Supporting Information

Mechanistic Understanding Enables Chemoselective sp^3 over sp^2 C–H activation in Pd-Catalyzed Carbonylative Cyclization of Amines

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Experimental procedures and data

General Methods. The corresponding starting materials were synthetized using oven-dried glassware under an argon atmosphere containing a teflon-coated stirrer bar and dry septum. All reactions were performed at ambient argon pressure in oven-dried pressure tube, sealed with a Teflon-lined screw cap.

All general reagents were obtained from usual commercial sources and were used, except when noted, without further purification. Amino acid and iodoarene derivatives were purchased from Aldrich Chemical Co., TCI or Fluorochem and used without further purification. $Pd(OAc)_2$, silver acetate and molybdenum hexacarbonyl were purchased from Aldrich Chemical Co. Prior to use, benzoquinone was purified by sublimation.

Solvents were purified by standard procedures prior to use. All other compounds are commercially available and were used without further purification.

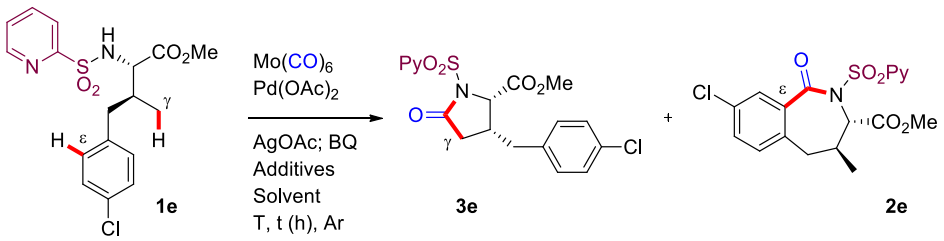
Flash column chromatography was performed using 230-400 mesh ultra-pure silica gel. NMR-spectra were obtained on 300 and 500 MHz spectrometers using acetone-d_6 and chloroform-d, as solvents, with proton and carbon resonances at 300/500 MHz and 75/125 MHz, respectively.

Infrared experiments were carried out in an *Agilent Cary 630 FTIR* spectrometer. Mass spectral data were acquired on a VG *AutoSpec mass* spectrometer. Melting points were determined in a *Büchi Melting Point* apparatus. Optical rotations were measured at 20 °C or 25 °C on an *Anton Paar Modular Compact Polarimeter* (MCP 150) using a 10 cm cell with the solvent and concentration stated, at 589 nm (sodium lamp).

The 2-pyridylsulfonyl chloride was synthesized from 2-mercaptopyridine following the procedure described in the literature.[1]

1. Additional information

1.1. Optimization studies for the derivatization of 1e (Table S1)



Entry	Additives, (equiv.)	Solvent	[1e] (M)	3e (%) [a]	2e (%) [a]
1	–	1,4-Dioxane	0.25	50	21
2	–	1,4-Dioxane	0.50	51	21
3	–	1,4-Dioxane	1.00	26	10
4[b]	–	1,4-Dioxane	0.25	32	16
5[c]	–	1,4-Dioxane	0.25	9	–
6	–	HFIP	0.25	20	49
7	–	HFIP	0.17	13	47
8	–	HFIP	0.12	10	50
9	–	HFIP	0.10	11	49
10	–	HFIP	0.07	8	35
11[d]	–	HFIP	0.12	8	13
12[d]	AcOH, (1.00)	HFIP	0.12	10	18
13[d]	AcOH, (3.00)	HFIP	0.12	7	40
14[d]	AcOH, (6.00)	HFIP	0.12	19	20
15	AcOH, (3.00)	HFIP	0.12	15	71
16	AcOH, (3.00)	1,4-Dioxane	0.25	25	30
17[e]	AcOH, (3.00)	HFIP	0.12	6	70
18[e,f]	2,5-diMe-BQ	HFIP	0.12	12	–
19[e,f]	Duroquinone	HFIP	0.12	7	–
20[e,f]	Naphthoquinone	HFIP	0.12	9	4
21[e,f]	Antraquinone	HFIP	0.12	–	–

Reaction conditions: Amino acid derivative (+)-**1** (0.10 mmol, 1.00 equiv), $Pd(OAc)_2$ (10 mol %, 0.01 mmol), $Mo(CO)_6$ (33 mol%, 0.033 mmol), AgOAc (0.15 mmol, 1.50 equiv) BQ (0.20 mmol, 2.00 equiv), Additive, Solvent (anh.), 110 °C, 16 h, Argon. [a] Determined by ^1H NMR of the crude mixture. [b] T = 100 °C. [c] T = 90 °C. [d] t = 4 h. [e] t = 8 h. [f] 3.00 equiv of AcOH were employed BQ = 1,4-benzoquinone. HFIP = 1,1,1,3,3,3-hexafluoro-2-propanol.

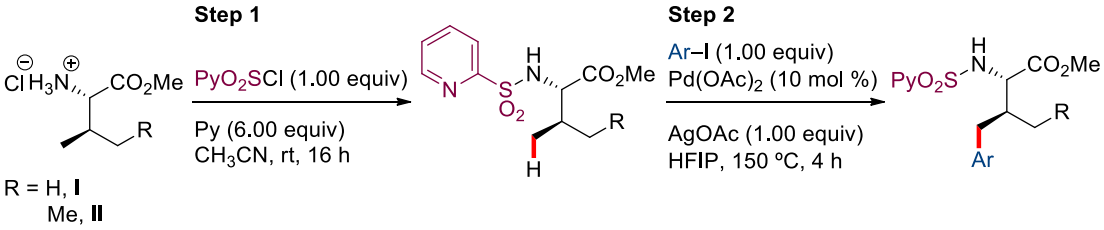
Table S1. Optimization studies for the derivatization of **1e**

We started our investigations by subjecting the γ-*p*-chlorobenzene-substituted L-valine derivative (+)-**1** to our previous carbonylation conditions,[2] employing $Mo(CO)_6$ (33 mol%) in the presence of a catalytic amount of $Pd(OAc)_2$ (10 mol%) and a combination of AgOAc (1.50 equiv) and 1,4-benzoquinone (BQ, 2.00 equiv) as oxidants in 1,4-dioxane (0.25 M) at 110 °C for 18 h. Under these reaction conditions (entry 1), we observed a high conversion of (+)-**1** leading to a mixture 2:1 of the benzazepinone product **2e** and the γ-lactam product **3e** (50 and 21% isolated yields, respectively). A change in the concentration (entries 2-3) had no influence in the outcome of the reaction. Further experiments proved that 110 °C was the optimal temperature for carrying out the reaction (entries 4 and 5). Nonetheless, the regioselectivity of the reaction switched towards the formation of the γ-lactam **3e** by using HFIP instead of 1,4-dioxane (entry 6,

20% of benzazepinone product **2e** and 49% of γ-lactam product **3e**. The more diluted was the solution, higher regiocontrol towards the γ-lactam product **3e** was obtained (entries 7-10). The optimal concentration was 0.12 M of (+)-**1**. Under these conditions γ-lactam product **3e** was obtained in 50% yield along with 10% of benzazepinone **2e** (entry 8). This little percentage of benzazepinone **2e** formed at the beginning of the reaction (entry 11) remained that low even when adding AcOH, a perfect additive to increase the conversion of (+)-**1** towards the formation of γ-lactam product **3e**. The optimal amount of AcOH was 3.00 equiv (entries 12-15), obtaining a 71% of the γ-lactam **3e** and an only 15% yield of the benzazepinone **2e**. The role of the acetic acid was also tested using 1,4-dioxane but the selectivity and the conversion were lower (entry 16). Higher levels of regioselectivity could even be obtained at shorter reaction times, isolating the corresponding γ-lactam **3e** in a 70% yield and the benzazepinone **2e** in a 6% yield (entry 17). Differently substituted quinones did not improved the yield or the selectivity of the system (entries 18-21).

2. Synthesis of starting materials

2.1. Typical procedure for the synthesis of *N*-SO_2Py protected γ-aryl aminoester derivatives



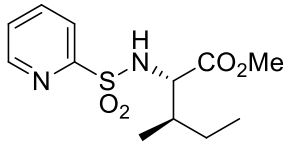
Step 1. Protection of the amino group.

Synthesis of (*S*)-methyl 3-methyl-2-(pyridine-2-sulfonamido)butanoate (I).[3] In a 100 mL round bottom flask, L-valine methyl ester hydrochloride (551 mg, 3.30 mmol, 1.00 equiv) was introduced and next flushed with Ar. Anhydrous CH_3CN (25.0 mL) and pyridine (1.46 mL, 18.0 mmol, 6.00 equiv) were then added. The mixture was placed in a 0 °C bath (ice-water) and 2-pyridylsulfonyl chloride (533 mg, 3.00 mmol, 1.00 equiv) was added dropwise. The mixture was stirred for 18 h at room temperature. The solvent was removed under reduced pressure and the resulted crude product was dissolved in CH_2Cl_2 and washed with 1 M HCl. The organic phase was then washed with water, brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The resulted residue was purified by flash column chromatography (cyclohexane:EtOAc 3:1) to obtain **I** as a white solid, yield: 881 mg (98%); mp = 108-109 °C. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.59 (ddd, *J* = 4.7, 1.5, 0.9 Hz, 1H), 7.93 (dt, *J* = 7.8, 1.1 Hz, 1H), 7.86 (td, *J* = 7.7, 1.7 Hz, 1H), 7.44 (ddd, *J* = 7.4, 4.7, 1.3 Hz, 1H), 5.56 (d, *J* = 9.6 Hz, 1H), 4.11 (dd, *J* = 9.7, 5.0 Hz, 1H), 3.53 (s, 3H), 2.15 – 1.99 (m, 1H), 0.96 (d, *J* = 6.8 Hz, 3H), 0.86 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.9, 157.9, 149.7, 138.1, 126.7, 121.8, 62.1, 52.2, 31.7, 19.0, 17.4. **HRMS-ESI (*m/z*):** calcd. for $C_{11}H_{17}N_2O_4S$ $(M+H)^+$: 273.0909; Found: 273.0911. **$[\alpha]_D^{25}$:** +17 (*c* = 1.0; CH_2Cl_2).

(2*S,3*R**)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)pentanoate (II).** The synthesis of compound **II** has two step, first the esterification of the acid group and second the protection of the amino group.

Step 1.1. Protection of the acid group. To a suspended mixture of DL-*allo*-isoleucine (2.00 g, 15.2 mmol, 1.00 equiv) in MeOH (30.5 mL) at 0 °C, thionyl chloride (1.22 mL, 16.7 mmol, 1.10 equiv) was added dropwise under Ar atmosphere. Once the thionyl chloride was added, the solution was refluxed for 3 h. After this time, the volatiles were removed *in vacuo* affording the pure aminoester hydrochloride, which was used without further purification.

Step 1.2. Protection of the amino group. The previously synthetized methyl ester hydrochloride (600 mg, 3.30 mmol, 1.10 equiv) was submitted to the conditions for the synthesis of *N*-SO_2Py protected amino acid derivatives, to give **II** as a white solid; total yield: 3.92 g (90%); mp = 111-112 °C. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.59 (d, *J* = 4.6 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.85 (td, *J* = 7.7, 1.6 Hz, 1H), 7.44 (ddd, *J* = 7.4, 4.7, 1.2 Hz, 1H), 5.47 (d, *J* = 9.9 Hz, 1H), 4.29 (dd, *J* = 9.9, 4.1 Hz, 1H), 3.52 (s, 3H), 1.88 – 1.75 (m, 1H), 1.56 – 1.42 (m, 1H), 1.30 – 1.15 (m, 1H), 0.90 (t, *J* = 7.4 Hz, 3H), 0.80 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.2, 157.9, 149.7, 138.1, 126.7, 121.8, 60.2, 52.3, 38.2, 26.0, 14.3, 11.5. **HRMS-ESI (*m/z*):** calcd. for $C_{12}H_{19}N_2O_4S$ $(M+H)^+$: 287.1066; Found: 287.1060.



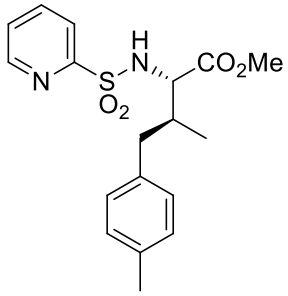
(*R*)-*N*-(3-Methylbutan-2-yl)pyridine-2-sulfonamide (III). Compound **III** was prepared following the typical procedure from (*R*)-3-methylbutan-2-amine (0.35 mL, 3.00 mmol, 1.00 equiv), to give **III** as a white solid; yield: 572 mg (83%); mp = 72-74 °C. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.70 (ddd, *J* = 4.7, 1.6, 0.8 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.89 (td, *J* = 7.7, 1.7 Hz, 1H), 7.47 (ddd, *J* = 7.6, 4.7, 1.2 Hz, 1H), 4.87 (d, *J* = 8.3 Hz, 1H), 3.35 – 3.24 (m, 1H), 1.74 – 1.59 (m, 1H), 0.94 (d, *J* = 6.7 Hz, 3H), 0.83 (d, *J* = 6.8 Hz, 6H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 158.5, 150.1, 138.0, 126.6, 122.0, 55.6, 33.6, 18.2, 18.1, 18.0. **HRMS-ESI (*m/z*):** calcd. for $C_{10}H_{17}N_2O_2S$ $(M+H)^+$: 229.1011; Found: 229.1006. **$[\alpha]_D^{25}$:** +10 (*c* = 1.0; CH_2Cl_2).

Step 2. Pd-catalyzed γ-monoarylation of *N*-SO_2Py aminoester derivatives[2]

Synthesis of (2*S*,3*S*)-methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-phenyl butanoate (1a). An oven-dried pressure tube was charged with $Pd(OAc)_2$ (5.61 mg, 0.025 mmol, 10 mol %), AgOAc (41.7 mg, 0.25 mmol), L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv), iodobenzene (28.0 µL, 0.25 mmol, 1.00 equiv) and HFIP (0.25 mL). The tube was sealed with a screw cap and then placed in an oil bath at 150 °C for 4 h. After the reaction time was completed, the reaction mixture was diluted with EtOAc, filtered through a short pad of Celite®, and concentrated *in vacuo*. The residue was purified by flash column chromatography (30:1 CH_2Cl_2:Et_2O) to obtain derivative (2*S*,3*S*)-methyl 3-methyl-2-(pyridine-2-sulfonamido)-4phenylbutanoate **1a** as a white oil in 62% yield (56.3 mg). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.61 (d, *J* = 4.2 Hz, 1H), 7.91 (d, *J* = 7.9 Hz, 1H), 7.84 (td, *J* = 7.7, 1.7 Hz, 1H), 7.43 (ddd, *J* = 7.4, 4.7, 1.3 Hz, 1H),

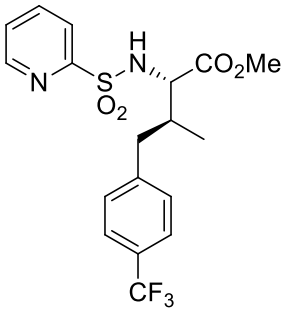
7.24 – 7.21 (m, 2H), 7.18 – 7.16 (m, 1H), 7.12 – 7.09 (m, 2H), 5.78 (d, *J* = 9.3 Hz, 1H), 4.23 (dd, *J* = 9.3, 4.7 Hz, 1H), 3.52 (s, 3H), 2.79 (dd, *J* = 12.9, 4.5 Hz, 1H), 2.40 – 2.23 (m, 2H), 0.91 (d, *J* = 6.5 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.5, 157.8, 149.8, 139.4, 138.1, 129.2, 128.4, 126.8, 126.2, 121.9, 61.2, 52.3, 38.9, 38.4, 15.9. **HRMS-ESI (*m/z*):** calcd. for $C_{17}H_{21}N_2O_4S$ $(M+H)^+$: 349.1222; Found: 349.1216. **IR** (ν_{max}/cm^{-1}): 1741, 1342, 1175. **$[\alpha]_D^{25}$:** +52 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*S*)-Methyl 3-methyl-4-(*p*-tolyl)-2-(pyridine-2-sulfonamido)butanoate (1b).



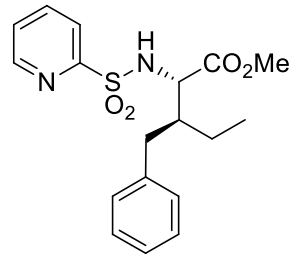
Compound **1b** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 4-iodotoluene (54.5 mg, 0.25 mmol, 1.00 equiv) to give **1b** as a yellow oil; yield: 51.6 mg (59%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.63 – 8.61 (m, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.86 (td, *J* = 7.7, 0.9 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.06 (d, *J* = 7.9 Hz, 2H), 7.00 (d, *J* = 7.9 Hz, 2H), 5.63 (d, *J* = 9.3 Hz, 1H), 4.24 (dd, *J* = 9.1, 4.3 Hz, 1H), 3.54 (s, 3H), 2.75 (dd, *J* = 12.7, 4.0 Hz, 1H), 2.37 – 2.21 (m, 5H), 0.92 (d, *J* = 6.1 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.6, 157.8, 149.8, 138.1, 136.3, 135.7, 129.1, 129.1, 126.8, 122.0, 61.2, 52.3, 39.0, 37.9, 21.1, 15.9. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{23}N_2O_4S$ $(M+H)^+$: 363.1379; Found: 363.1373. **IR** (ν_{max}/cm^{-1}): 1735, 1347, 1180. **$[\alpha]_D^{25}$:** +63 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(4-(trifluoromethyl)phenyl)-butanoate (1c).



Compound **1c** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 4-iodobenzotrifluoride (36.7 µL, 0.25 mmol, 1.00 equiv) to give **1c**, as a 87:13 diasteromeric mixture, as a yellow oil; yield: 46.9 mg (45%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.52 (ddd, *J* = 4.7, 1.7, 0.8 Hz, 1H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.77 (td, *J* = 7.7, 1.6 Hz, 1H), 7.42 – 7.35 (m, 3H), 7.16 (d, *J* = 8.0 Hz, 2H), 6.04 (d, *J* = 9.3 Hz, 1H), 4.12 (dd, *J* = 9.3, 5.2 Hz, 1H), 3.45 (s, 3H), 2.81 (dd, *J* = 13.5, 5.0 Hz, 1H), 2.38 (dd, *J* = 13.4, 9.5 Hz, 1H), 2.28 – 2.17 (m, 1H), 0.82 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.3, 157.6, 149.8, 143.7, 138.1, 129.6, 128.5 (q, *J* = 32.3 Hz), 126.8, 125.2 (q, *J* = 3.8 Hz), 124.3 (q, *J* = 271.8 Hz), 60.9, 52.3, 38.7, 38.2, 15.7. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{20}F_3N_2O_4S$ $(M+H)^+$: 417.1096; Found: 417.1090. **IR** (ν_{max}/cm^{-1}): 1742, 1325, 1120. **$[\alpha]_D^{25}$:** +53 (*c* = 1.0; CH_2Cl_2).

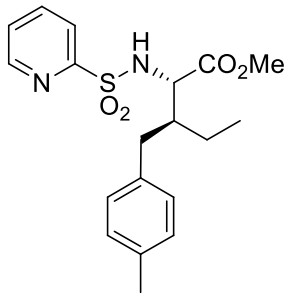
(2*S,3*S**)-Methyl 3-benzyl-2-(pyridine-2-sulfonamido)pentanoate (4a).** Compound



4a was prepared following the general protocol from DL-*allo*-isoleucine derivative **II** (71.6 mg, 0.25 mmol, 1.00 equiv) and iodobenzene (28.0 µL, 0.25 mmol, 1.00 equiv) to give **4a** as a yellow oil; yield: 63.6 mg (70%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.60 (d, *J* = 4.6 Hz, 1H), 7.90 (d, *J* = 7.8 Hz, 1H), 7.83 (td, *J* = 7.6, 1.6 Hz, 1H), 7.43 (ddd, *J* = 7.3, 4.7, 1.3 Hz, 1H), 7.25 – 7.21 (m, 2H), 7.18 – 7.14 (m, 1H), 7.13 – 7.07 (m, 2H), 5.60 (d, *J* = 9.5 Hz, 1H), 4.42 (dd, *J* = 9.5, 3.5 Hz, 1H), 3.46 (s, 3H), 2.61 – 2.46 (m, 2H), 2.16 – 2.06 (m, 1H), 1.61 – 1.46 (m, 1H), 1.39 – 1.25 (m, 1H), 0.94 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.0, 157.8, 149.8, 139.5, 138.0, 129.2, 128.4, 126.7,

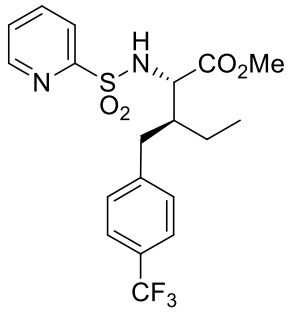
126.2, 121.9, 58.2, 52.4, 45.4, 35.9, 23.0, 11.5. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{23}N_2O_4S$ ($M+H^+$): 363.1379; Found: 363.1380. **IR** (ν_{max}/cm^{-1}): 1733, 1338, 1174.

(2*S,3*S**)-Methyl 3-(4-methylbenzyl)-2-(pyridine-2-sulfonamido)pentanoate (4b).**



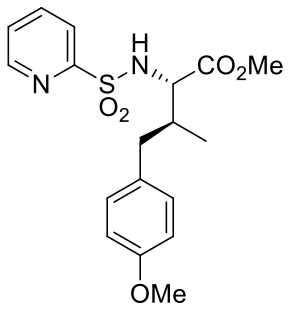
Compound **4b** was prepared following the general protocol from DL-*allo*-isoleucine derivative **II** (71.6 mg, 0.25 mmol, 1.00 equiv) and 4-iodotoluene (54.5 mg, 0.25 mmol, 1.00 equiv) to give **4b** as a white solid; yield: 67.9 mg (72%); mp = 96-97 °C. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.63 – 8.61 (m, 1H), 7.91 (d, *J* = 7.7 Hz, 1H), 7.85 (td, *J* = 7.6, 1.7 Hz, 1H), 7.44 (ddd, *J* = 7.4, 4.7, 1.4 Hz, 1H), 7.05 (d, *J* = 7.9 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 5.53 (d, *J* = 9.5 Hz, 1H), 4.43 (dd, *J* = 9.5, 3.5 Hz, 1H), 3.47 (s, 3H), 2.57 – 2.41 (m, 2H), 2.29 (s, 3H), 2.14 – 2.03 (m, 1H), 1.59 – 1.45 (m, 1H), 1.40 – 1.26 (m, 1H), 0.94 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.1, 157.8, 149.8, 138.0, 136.3, 135.7, 129.1, 129.1, 126.7, 121.9, 58.2, 52.4, 45.5, 35.4, 22.9, 21.1, 11.6. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{25}N_2O_4S$ ($M+H^+$): 377.1535; Found: 377.1530. **IR** (ν_{max}/cm^{-1}): 1735, 1174, 1339.

(2*S,3*S**)-Methyl 2-(pyridine-2-sulfonamido)-3-(4-(trifluoromethyl)benzyl)-pentanoate (4c).**



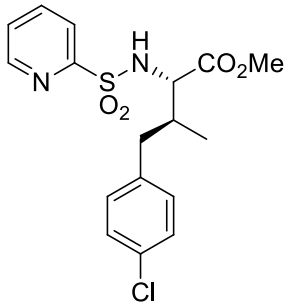
Compound **4c** was prepared following the general protocol from DL-*allo*-isoleucine derivative **II** (71.6 mg, 0.25 mmol, 1.00 equiv) and 4-iodobenzotrifluoride (36.7 µL, 0.25 mmol, 1.00 equiv) to give **4c** as a yellow solid; yield: 77.4 mg (72%); mp = 128-131 °C. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.61 – 8.58 (m, 1H), 7.89 (dt, *J* = 7.8, 1.3 Hz, 1H), 7.84 (td, *J* = 7.3, 1.7 Hz, 1H), 7.48 (d, *J* = 8.1 Hz, 2H), 7.45 – 7.41 (m, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 5.80 (d, *J* = 9.2 Hz, 1H), 4.36 (dd, *J* = 9.2, 3.7 Hz, 1H), 3.48 (s, 3H), 2.69 – 2.55 (m, 2H), 2.18 – 2.07 (m, 1H), 1.62 – 1.47 (m, 1H), 1.34 – 1.20 (m, 1H), 0.94 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.8, 157.7, 149.8, 143.9 (q, *J* = 1.2 Hz), 138.1, 129.6, 128.6 (q, *J* = 32.3 Hz), 126.8, 125.3 (q, *J* = 3.7 Hz), 124.3 (q, *J* = 271.8 Hz), 122.0, 58.1, 52.4, 45.3, 35.7, 22.9, 11.4. **^{19}F NMR (282 MHz, $CDCl_3$, δ):** -62.6. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{22}F_3N_2O_4S$ ($M+H^+$): 431.1247; Found: 431.1247. **IR** (ν_{max}/cm^{-1}): 1741, 1323, 1118.

(2*S*,3*S*)-Methyl 4-(4-methoxyphenyl)-3-methyl-2-(pyridine-2-sulfonamido)-butanoate (1d).

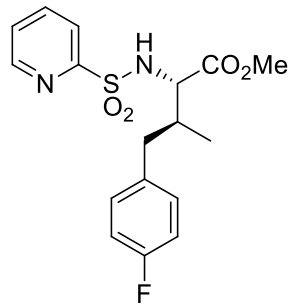


Compound **1d** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 4-iodoanisole (58.5 mg, 0.25 mmol, 1.00 equiv) to give **1d** as a white oil; yield: 60.6 mg (64%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.62 (d, *J* = 4.7 Hz, 1H), 7.92 (d, *J* = 7.2 Hz, 1H), 7.86 (t, *J* = 7.6 Hz, 1H), 7.47 – 7.42 (m, 1H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 8.3 Hz, 2H), 5.68 (d, *J* = 9.3 Hz, 1H), 4.22 (dd, *J* = 9.3, 4.5 Hz, 1H), 3.76 (s, 3H), 3.53 (s, 3H), 2.72 (dd, *J* = 13.1, 4.6 Hz, 1H), 2.35 – 2.20 (m, 2H), 0.90 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.6, 158.1, 157.8, 149.9, 138.1, 131.4, 130.2, 126.8, 122.0, 113.8, 61.1, 55.3, 52.3, 39.1, 37.5, 15.9. **HRMS-ESI (*m/z*):**

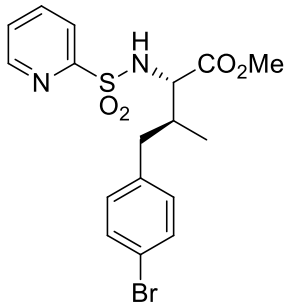
calcd. for $C_{18}H_{23}N_2O_5S$ $(M+H)^+$: 379.1328; Found: 379.1322. **IR** (ν_{max}/cm^{-1}): 1738, 1343, 1175. **$[\alpha]_D^{25}$:** +55 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*S*)-Methyl 4-(4-chlorophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1e). 

Compound **1e** was prepared following the general protocol L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 4-chloroiodobenzene (59.6 mg, 0.25 mmol, 1.00 equiv) to give **1d**, as a 89:11 diasteromeric mixture, yield: 50.1 mg (52%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.63 – 8.60 (m, 1H), 7.94 – 7.84 (m, 2H), 7.48 – 7.44 (m, 1H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.05 (d, *J* = 8.3 Hz, 2H), 5.75 (d, *J* = 9.2 Hz, 1H), 4.19 (dd, *J* = 9.2, 5.0 Hz, 1H), 3.55 (s, 3H), 2.78 (dd, *J* = 13.4, 5.1 Hz, 1H), 2.37 (dd, *J* = 13.4, 9.4 Hz, 1H), 2.30 – 2.18 (m, 1H), 0.90 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.4, 157.7, 149.9, 138.1, 138.0, 132.1, 130.6, 128.5, 126.8, 122.0, 61.0, 52.4, 39.0, 37.8, 15.8. **HRMS-ESI (*m/z*):** calcd. for $C_{17}H_{20}ClN_2O_4S$ $(M+H)^+$: 383.0832; Found: 383.0827. **IR** (ν_{max}/cm^{-1}): 1738, 1345, 1177. **$[\alpha]_D^{25}$:** +57 (*c* = 1.0; CH_2Cl_2).

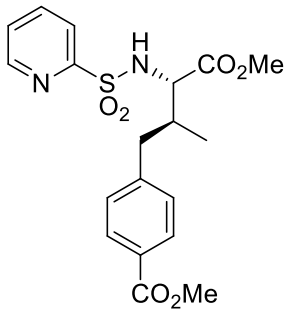
(2*S*,3*S*)-Methyl 4-(4-fluorophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1f). 

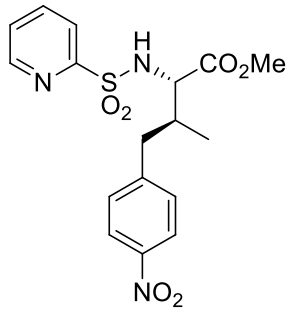
Compound **1f** was prepared following the general protocol L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 4-fluoroiodobenzene (28.8 µL, 0.25 mmol, 1.00 equiv) to give **1f**, as a 85:15 diasteromeric mixture, as a yellow oil; yield: 46.0 mg (50%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.62 (bd, *J* = 4.6 Hz, 1H), 7.93 (dt, *J* = 7.9, 1.2 Hz 1H), 7.88 (td, *J* = 7.6, 1.7 Hz, 1H), 7.46 (ddd, *J* = 7.2, 4.7, 1.4 Hz, 1H), 7.08 (dd, *J* = 8.6, 5.5 Hz, 2H), 6.94 (t, *J* = 8.7 Hz, 2H), 5.60 (d, *J* = 9.1 Hz, 1H), 4.21 (dd, *J* = 9.2, 4.9 Hz, 1H), 3.56 (s, 3H), 2.78 (dd, *J* = 13.5, 5.1 Hz, 1H), 2.37 (dd, *J* = 13.5, 9.4 Hz, 1H), 2.29 – 2.20 (m, 1H), 0.91 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.5, 161.5 (d, *J* = 243.9 Hz), 157.7, 149.8, 138.1, 135.1 (d, *J* = 3.3 Hz), 130.6 (d, *J* = 7.9 Hz), 126.8, 121.9, 115.1 (d, *J* = 21.1 Hz), 61.0, 52.3, 39.0, 37.6, 15.8. **HRMS-ESI (*m/z*):** calcd. for $C_{17}H_{20}FN_2O_4S$ $(M+H)^+$: 367.1128; Found: 367.1122. **IR** (ν_{max}/cm^{-1}): 1740, 1341, 1177. **$[\alpha]_D^{25}$:** +56 (*c* = 1.0; CH_2Cl_2).

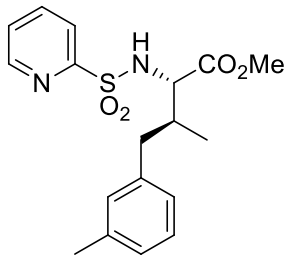
(2*S*,3*S*)-Methyl 4-(4-bromophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1g). 

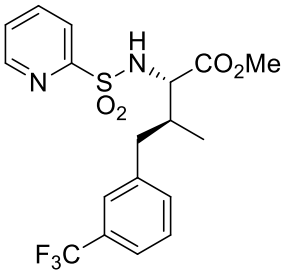
Compound **1g** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 4-bromoiodobenzene (70.7 mg, 0.25 mmol, 1.00 equiv) to give **1g** as a yellow oil; yield: 53.4 mg (50%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.60 – 8.58 (m, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.83 (td, *J* = 7.7, 1.5 Hz, 1H), 7.45 – 7.41 (m, 1H), 7.32 (d, *J* = 8.3 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 6.11 (d, *J* = 9.3 Hz, 1H), 4.16 (dd, *J* = 9.3, 5.1 Hz, 1H), 3.50 (s, 3H), 2.75 (dd, *J* = 13.2, 4.7 Hz, 1H), 2.33 (dd, *J* = 13.2, 9.5 Hz, 1H), 2.25 – 2.18 (m, 1H), 0.86 (d, *J* = 6.5 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.3, 157.5, 149.7, 138.4, 138.0, 131.3, 130.9, 126.8, 121.9, 119.9, 60.9, 52.2, 38.7, 37.7, 15.7. **HRMS-ESI (*m/z*):** calcd. for

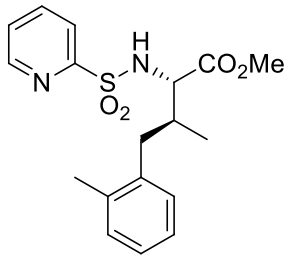
$C_{17}H_{20}BrN_2O_4S$ $(M+H)^+$: 427.0321; Found: 427.0310. **IR** (ν_{max}/cm^{-1}): 1742, 1339, 1181. **$[\alpha]_D^{25}$:** +50 (*c* = 1.0; CH_2Cl_2).

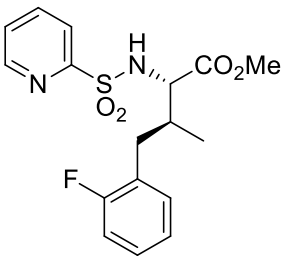
Methyl 4-((2*S*,3*S*)-4-methoxy-2-methyl-4-oxo-3-(pyridine-2-sulfonamido)butyl)-benzoate (1h).  Compound **1h** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and methyl 4-iodobenzoate (65.5 mg, 0.25 mmol, 1.00 equiv) to give **1h**, as a 86:14 diasteromeric mixture, yield: 51.8 mg (51%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.61 (ddd, *J* = 4.7, 1.6, 0.9 Hz, 1H), 7.97 – 7.91 (m, 3H), 7.89 (td, *J* = 7.6, 1.6 Hz, 1H), 7.46 (ddd, *J* = 7.3, 4.7, 1.5 Hz, 1H), 7.19 (d, *J* = 8.2 Hz, 2H), 5.66 (d, *J* = 9.2 Hz, 1H), 4.23 (dd, *J* = 9.2, 5.0 Hz, 1H), 3.89 (s, 3H), 3.56 (s, 3H), 2.87 (dd, *J* = 13.4, 5.0 Hz, 1H), 2.44 (dd, *J* = 13.4, 9.6 Hz, 1H), 2.36 – 2.25 (m, 1H), 0.91 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.4, 167.1, 157.8, 149.8, 145.1, 138.1, 129.7, 129.3, 128.3, 126.8, 122.0, 61.1, 52.4, 52.1, 38.8, 38.5, 15.9. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{23}N_2O_6S$ $(M+H^+)$: 407.1269; Found: 407.1271. **IR** (ν_{max}/cm^{-1}): 1742, 1714, 1336, 1175. **$[\alpha]_D^{20}$:** +60 (*c* = 1.0; CH_2Cl_2).

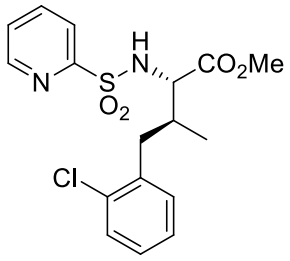
(2*S*,3*S*)-Methyl 3-methyl-4-(4-nitrophenyl)-2-(pyridine-2-sulfonamido)butanoate (1i).  Compound **1i** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 4-iodonitrobenzene (62.3 mg, 0.25 mmol, 1.00 equiv) to give **1i**, as a 85:15 diasteromeric mixture, yield: 33.4 mg (34%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.61 (bd, *J* = 4.7 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 2H), 7.95 (d, *J* = 7.2 Hz, 1H), 7.89 (td, *J* = 7.7, 1.4 Hz, 1H), 7.50 – 7.46 (m, 1H), 7.32 (d, *J* = 8.6 Hz, 2H), 5.59 (d, *J* = 9.0 Hz, 1H), 4.23 (dd, *J* = 9.0, 5.2 Hz, 1H), 3.60 (s, 3H), 2.97 (dd, *J* = 13.6, 5.2 Hz, 1H), 2.54 (dd, *J* = 13.6, 9.5 Hz, 1H), 2.38 – 2.27 (m, 1H), 0.93 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.3, 157.8, 149.9, 147.5, 146.8, 138.3, 130.1, 127.0, 123.8, 122.0, 61.1, 52.6, 39.0, 38.5, 15.8. **HRMS-ESI (*m/z*):** calcd. for $C_{17}H_{19}N_3O_6SNa$ $(M+H^+)$: 416.0887; Found: 416.0889. **$[\alpha]_D^{20}$:** +75 (*c* = 1.0; CH_2Cl_2).

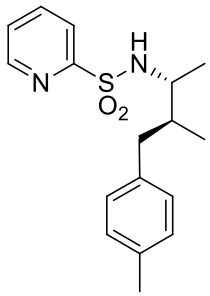
(2*S*,3*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(*m*-tolyl)butanoate (1j).  Compound **1j** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 3-iodotoluene (32.1 µL, 0.25 mmol, 1.00 equiv) to give **1j** as a yellow oil; yield: 44.5 mg (49%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.63 (d, *J* = 4.3 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.87 (td, *J* = 7.7, 1.7 Hz, 1H), 7.45 (ddd, *J* = 7.4, 4.7, 1.3 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 7.3 Hz, 1H), 6.93 – 6.90 (m, 2H), 5.67 (d, *J* = 9.3 Hz, 1H), 4.25 (dd, *J* = 9.3, 4.6 Hz, 1H), 3.55 (s, 3H), 2.77 (dd, *J* = 12.0, 3.3 Hz, 1H), 2.37 – 2.26 (m, 5H), 0.92 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.6, 157.8, 149.8, 139.4, 138.1, 137.9, 130.0, 128.3, 127.0, 126.8, 126.3, 122.0, 61.3, 52.3, 38.9, 38.3, 21.4, 16.0. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{23}N_2O_4S$ $(M+H)^+$: 363.1379; Found: 363.1373. **IR** (ν_{max}/cm^{-1}): 1738, 1343, 1175. **$[\alpha]_D^{25}$:** +55 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(3-(trifluoromethyl)phenyl)-butanoate (1k).  Compound **1k** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 3-iodobenzotrifluoride (36.0 µL, 0.25 mmol, 1.00 equiv) to give **1k**, as a 88:12 diasteromeric mixture, as a yellow oil; yield: 55.1 mg (53%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.61 (d, *J* = 4.6 Hz, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.87 (td, *J* = 7.6, 1.6 Hz, 1H), 7.48 – 7.44 (m, 2H), 7.41 – 7.32 (m, 3H), 5.75 (d, *J* = 9.2 Hz, 1H), 4.23 (dd, *J* = 9.2, 5.0 Hz, 1H), 3.56 (s, 3H), 2.89 (dd, *J* = 13.6, 5.1 Hz, 1H), 2.46 (dd, *J* = 13.6, 9.5 Hz, 1H), 2.35 – 2.24 (m, 1H), 0.92 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.4, 157.8, 149.9, 140.5, 138.2, 132.8, 130.8 (q, *J* = 32.0 Hz), 128.9, 126.9, 125.8 (q, *J* = 3.8 Hz), 124.3 (q, *J* = 272.3 Hz), 123.3 (q, *J* = 3.8 Hz), 122.0, 61.1, 52.4, 38.9, 38.3, 15.9. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{20}F_3N_2O_4S$ $(M+H)^+$: 417.1096; Found: 417.1090. **IR** (ν_{max}/cm^{-1}): 1738, 1323, 1116. **$[\alpha]_D^{25}$:** +50 (*c* = 1.0; CH_2Cl_2).

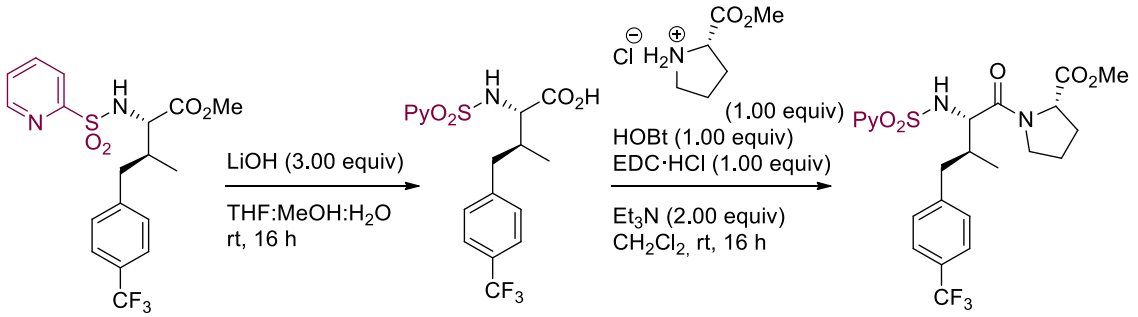
(2*S*,3*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(*o*-tolyl)butanoate (1l).  Compound **1l** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 2-iodotoluene (31.8 µL, 0.25 mmol, 1.00 equiv) to give **1l**, as a 73:27 diasteromeric mixture, as a brown oil; yield: 18.2 mg (20%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.63 (d, *J* = 4.6 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.87 (td, *J* = 7.7, 1.6 Hz, 1H), 7.46 (ddd, *J* = 7.4, 4.7, 1.2 Hz, 1H), 7.12 – 7.06 (m, 4H), 5.65 (d, *J* = 9.3 Hz, 1H), 4.30 (dd, *J* = 9.3, 4.3 Hz, 1H), 3.58 (s, 3H), 2.79 (dd, *J* = 12.9, 3.7 Hz, 1H), 2.39 – 2.31 (m, 1H), 2.27 – 2.24 (m, 4H), 0.95 (d, *J* = 6.5 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.6, 157.7, 149.8, 138.1, 137.6, 136.3, 130.4, 130.1, 126.7, 126.4, 125.7, 121.9, 61.4, 52.3, 37.3, 35.4, 19.3, 15.9. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{22}N_2O_4SNa$ $(M+Na)^+$: 385.1198; Found: 385.1192. **IR** (ν_{max}/cm^{-1}): 1753, 1342, 1185. **$[\alpha]_D^{25}$:** +58 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*S*)-Methyl 4-(2-fluorophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1m).  Compound **1m** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 2-fluoroiodobenzene (29.1 µL, 0.25 mmol, 1.00 equiv) to give **1m**, as a 85:15 diasteromeric mixture, as a yellow oil; yield: 49.7 mg (54%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.62 (d, *J* = 4.6 Hz, 1H), 7.96 (d, *J* = 7.4 Hz, 1H), 7.89 (td, *J* = 7.7, 1.5 Hz, 1H), 7.49 – 7.44 (m, 1H), 7.21 – 7.12 (m, 2H), 7.06 – 6.95 (m, 2H), 5.48 (d, *J* = 9.3 Hz, 1H), 4.29 (dd, *J* = 9.3, 4.3 Hz, 1H), 3.54 (s, 3H), 2.82 (dd, *J* = 12.8, 4.0 Hz, 1H), 2.44 – 2.28 (m, 2H), 0.97 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.6, 161.4 (d, *J* = 245.0 Hz), 158.0, 149.9, 138.1, 131.7 (d, *J* = 4.8 Hz), 128.2 (d, *J* = 8.2 Hz), 126.8, 126.5 (d, *J* = 15.5 Hz), 124.1 (d, *J* = 3.5 Hz), 122.0, 115.4 (d, *J* = 22.3 Hz), 61.3, 52.5, 37.8, 31.6, 16.3. **IR** (ν_{max}/cm^{-1}): 1744, 1338, 1175. **$[\alpha]_D^{20}$:** +13 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*S*)-Methyl 4-(2-chlorophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1n). 
Compound **1n** was prepared following the general protocol from L-valine derivative **I** (68.1 mg, 0.25 mmol, 1.00 equiv) and 2-chloroiodobenzene (30.5 µL, 0.25 mmol, 1.00 equiv) to give **1n** as a 78:22 mixture of diasteromers as a brown oil; yield: 26.0 mg (27%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.63 (d, *J* = 4.6 Hz, 1H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.89 (td, *J* = 7.6, 1.5 Hz, 1H), 7.49 – 7.45 (m, 1H), 7.33 – 7.30 (m, 1H), 7.20 – 7.13 (m, 3H), 5.47 (d, *J* = 9.3 Hz, 1H), 4.32 (dd, *J* = 9.3, 3.9 Hz, 1H), 3.58 (s, 3H), 2.95 – 2.89 (m, 1H), 2.48 – 2.37 (m, 2H), 0.98 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.61, 158.00, 149.89, 138.17, 137.13, 134.37, 131.83, 129.78, 127.99, 126.87, 126.78, 121.96, 77.16, 61.43, 52.49, 36.89, 35.86, 16.18. **HRMS-ESI (*m/z*):** calcd. for $C_{17}H_{20}ClN_2O_4S$ $(M+H)^+$: 383.0827; Found: 383.0832. **IR** (ν_{max}/cm^{-1}): 1742, 1343, 1178. **$[\alpha]_D^{25}$:** +31 (*c* = 1.0; CH_2Cl_2).

***N*-((2*R*,3*S*)-3-Methyl-4-(*p*-tolyl)butan-2-yl)pyridine-2-sulfonamide (6a).** 
Compound **6a** was prepared following the general protocol from (*R*)-*N*-(3-methylbutan-2-yl)pyridine-2-sulfonamide **III** (57.1 mg, 0.25 mmol, 1.00 equiv) and 4-iodotoluene (54.5 mg, 0.25 mmol, 1.00 equiv) to give **6a** as a brown oil; yield: 20.2 mg (25%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.69 (d, *J* = 4.6 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.86 (td, *J* = 7.7, 1.6 Hz, 1H), 7.46 (ddd, *J* = 7.5, 4.8, 1.1 Hz, 1H), 7.04 (d, *J* = 7.8 Hz, 2H), 6.93 (d, *J* = 7.9 Hz, 2H), 5.04 (d, *J* = 8.1 Hz, 1H), 3.44 – 3.33 (m, 1H), 2.65 (dd, *J* = 13.5, 5.7 Hz, 1H), 2.30 (s, 3H), 2.22 (dd, *J* = 13.5, 9.3 Hz, 1H), 1.93 – 1.79 (m, 1H), 1.02 (d, *J* = 6.8 Hz, 3H), 0.79 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 158.2, 150.1, 138.0, 137.2, 135.4, 129.1, 128.9, 126.6, 122.2, 53.9, 40.5, 39.1, 21.1, 17.0, 14.2. **HRMS-ESI (*m/z*):** calcd. for $C_{17}H_{23}N_2O_2S$ $(M+H^+)$: 319.1480; Found: 319.1488. **IR** (ν_{max}/cm^{-1}): 1332, 1173. **$[\alpha]_D^{20}$:** +45 (*c* = 1.0; CH_2Cl_2).

2.5. Typical procedure for the synthesis of peptide 8[4]



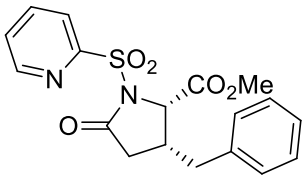
Step 1. Synthesis of (2*S*,3*S*)-3-methyl-2-(pyridine-2-sulfonamido)-4-(4-(trifluoro methyl)phenyl)butanoic acid (IV). An oven dried, nitrogen flushed 10.0 mL vessel was charged with (2*S*,3*S*)-methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(4-(trifluoromethyl)phenyl)-butanoate (**1c**) (125 mg, 0.30 mmol, 1.00 equiv) and LiOH·H_2O (37.8 mg, 0.90 mmol, 3.00 equiv). Then, a 3:1:1 mixture of THF:MeOH:H_2O (2.10 mL) was added via syringe. Next, the corresponding mixture was heated at 60 °C for 24 h. After that time, the reaction was allowed to reach room temperature and 1 M HCl was added until pH ≈ 2 and a solid could be observed. EtOAc (10.0 mL) was added to dissolve this solid and the organic phase was washed with water (10.0 mL), brine (10.0 mL), dried over Na_2SO_4, filtered and the solvent was eliminated *in vacuo* to obtain **III** as a white oil, which was used without further purification; yield: 120 mg (99%).

2.6. Typical procedure for the synthesis of peptides

Step 2. Synthesis of methyl *N*-(SO_2Py)-γ-(*p*-trifluoromethylphenyl)-L-valyl-prolinate (8). In a 10.0 mL round bottom flask, (2*S*,3*S*)-3-methyl-2-(pyridine-2-sulfonamido)-4-(4-(trifluoromethyl) phenyl) butanoic acid **IV** (402 mg, 1.00 mmol, 1.00 equiv), glycine methyl ester hydrochloride (125 mg, 1.00 mmol, 1.00 equiv), HOBt·H_2O (135 mg, 1.10 mmol, 1.10 equiv) and EDC·HCl (192 mg, 1.10 mmol, 1.10 equiv) were suspended in anhydrous CH_2Cl_2 (5.00 mL). Then, Et_3N (0.28 mL, 2.00 mmol, 2.00 equiv) was added via syringe, and the solution was left stirring at room temperature for 24 h. The reaction mixture was then diluted with CH_2Cl_2 and washed with an aqueous solution of citric acid 0.5 M (3 x 10.0 mL), $NaHCO_3$ (sat.) (3 x 10.0 mL) and brine (20.0 mL). The organic phase was dried over Na_2SO_4, filtered and the solvent was eliminated *in vacuo*. The residue was purified by flash column chromatography (cyclohexane-EtOAc 1:1) to obtain the dipeptide **8** as a 87:13 mixture of diasteromers as a white solid; yield: 477 mg (93%); mp = 138-139 °C. **^{1}H NMR (500 MHz, $CDCl_3$, δ):** 8.52 (ddd, *J* = 4.7, 1.6, 0.9 Hz, 1H), 7.99 (dt, *J* = 7.9, 0.9 Hz, 1H), 7.89 (td, *J* = 7.8, 1.7 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.46 (ddd, *J* = 7.6, 4.7, 1.1 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 2H), 5.70 (d, *J* = 9.3 Hz, 1H), 4.54 (dd, *J* = 9.3, 5.1 Hz, 1H), 4.27 (dd, *J* = 8.3, 5.2 Hz, 1H), 3.84 – 3.80 (m, 1H), 3.68 (s, 3H), 3.63 – 3.59 (m, 1H), 3.04 (dd, *J* = 13.2, 2.2 Hz, 1H), 2.32 (dd, *J* = 13.0, 11.3 Hz, 1H), 2.23 – 2.18 (m, 1H), 2.16 – 2.09 (m, 2H),

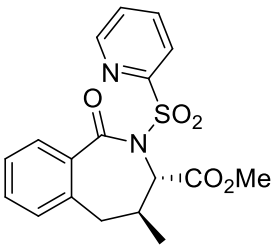
2.05 – 1.97 (m, 2H), 1.01 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR (126 MHz, $CDCl_3$, δ):** 172.1, 170.0, 158.6, 149.3, 144.6, 138.4, 129.8, 128.5 (q, *J* = 32.2 Hz), 126.9, 125.3 (q, *J* = 3.7 Hz), 124.5 (q, *J* = 271.7 Hz), 122.0, 60.5, 59.0, 52.5, 47.2, 38.6, 37.0, 29.2, 25.3, 15.9.**HRMS-ESI (*m/z*):** calcd. for $C_{23}H_{26}F_3N_3O_5SNa$ ($M+Na^+$): 536.1437; Found: 536.1441. **$[\alpha]_D^{20}$:** +34 (*c* = 1.0; CH_2Cl_2).

3. General protocol for the Pd-catalyzed γ-C(sp^3)–H carbonylative cyclization of γ-aryl-L-Valine type derivatives

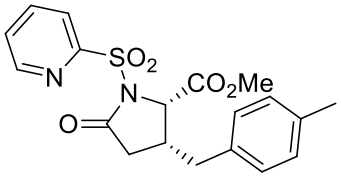


(2*S*,3*R*)-Methyl 3-benzyl-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3a). An oven-dried, argon flushed, pressure tube was charged with $Pd(OAc)_2$ (2.24 mg, 0.01 mmol, 0.10 equiv), AgOAc (25.0 mg, 0.15 mmol, 1.50 equiv), benzoquinone (21.6 mg, 0.20 mmol, 2.00 equiv), $Mo(CO)_6$ (8.67 mg, 0.33 mmol, 0.33 equiv) and (2*S*,3*S*)-methyl 4-phenyl-3-methyl-2-(pyridine-2-sulfonamido) butanoate (**1a**) (38.3 mg, 0.10 mmol, 1.00 equiv). The pressure tube was sealed with a rubber septum and flushed with argon. Under positive pressure of argon, HFIP (0.80 mL) and acetic acid (17 μL, 0.30 mmol, 3.00 equiv) were added *via* syringe. The septum was then replaced by a screw cap and finally placed in an oil bath at 110 °C for 8 h. The reaction mixture was then removed from the oil bath and allowed to cool to room temperature. The mixture was then diluted with EtOAc, filtered through a short pad of Celite® and concentrated *in vacuo*. The residue was purified by flash column chromatography (*n*-hexane:EtOAc 2:1) to afford **3a** as a yellow oil; yield: 25.0 mg (67%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.69 (bd, *J* = 4.6 Hz, 1H), 8.24 (d, *J* = 7.9 Hz, 1H), 7.95 (td, *J* = 7.8, 1.7 Hz, 1H), 7.55 (ddd, *J* = 7.7, 4.7, 1.0 Hz, 1H), 7.34 – 7.27 (m, 2H), 7.25 – 7.20 (m, 1H), 7.13 (d, *J* = 8.2 Hz, 2H), 5.10 (d, *J* = 8.0 Hz, 1H), 3.88 (s, 3H), 3.02 – 2.96 (m, 2H), 2.52 (dd, *J* = 17.0, 11.9 Hz, 1H), 2.37 (dd, *J* = 14.7, 11.7 Hz, 1H), 2.28 (dd, *J* = 17.0, 7.6 Hz, 1H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.3, 169.8, 155.7, 150.2, 138.2, 137.8, 129.0, 128.6, 128.0, 127.1, 124.5, 63.9, 52.8, 38.3, 36.6, 36.5. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{19}N_2O_5S$ ($M+H)^+$: 375.1009; Found: 375.0994. **IR** (ν_{max}/cm^{-1}): 1746, 1735, 1362, 1182. **$[\alpha]_D^{20}$:** -4 (*c* = 1.0; CH_2Cl_2).

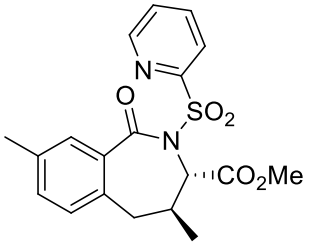
Along product **3a**, product **2a** was also isolated

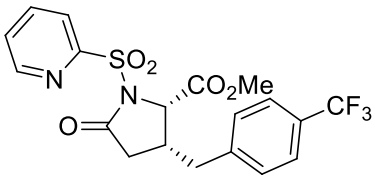


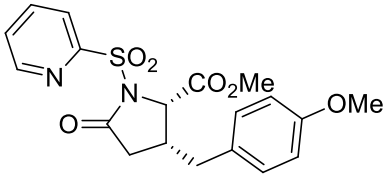
(3*S*,4*S*)-Methyl 4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2a). Yellow oil; yield: 9.8 mg (26%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.68 (bd, *J* = 4.0 Hz, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.01 (td, *J* = 7.8, 1.7 Hz, 1H), 7.54 (ddd, *J* = 7.6, 4.7, 0.9 Hz, 1H), 7.47 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.38 (td, *J* = 7.5, 1.3 Hz, 1H), 7.22 (t, *J* = 6.9 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 5.26 (s, 1H), 3.30 – 3.19 (m, 4H), 2.89 – 2.81 (m, 1H), 2.72 (dd, *J* = 13.6, 5.8 Hz, 1H), 1.49 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 170.0, 169.6, 156.6, 149.6, 138.7, 137.9, 133.0, 132.9, 129.8, 129.1, 127.5, 127.4, 125.6, 63.2, 52.6, 39.2, 37.8, 20.5. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{19}N_2O_5S$ ($M+H^+$): 375.1015; Found: 375.1007. **IR** (ν_{max}/cm^{-1}): 1742, 1690, 1353, 1181. **$[\alpha]_D^{20}$:** +8 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*R*)-Methyl 3-(4-methylbenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3b). 
Compound **3b** was prepared following the general protocol from (2*S*,3*S*)-methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(*p*-tolyl)butanoate (**1b**) (36.2 mg, 0.10 mmol, 1.00 equiv) to give **3b** as a yellow oil; yield: 16.7 mg (43%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.69 (bd, *J* = 4.7 Hz, 1H), 8.24 (d, *J* = 7.9 Hz, 1H), 7.95 (td, *J* = 7.8, 1.7 Hz, 1H), 7.54 (ddd, *J* = 7.7, 4.7, 1.0 Hz, 1H), 7.10 (d, *J* = 7.9 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 5.08 (d, *J* = 8.0 Hz, 1H), 3.87 (s, 3H), 2.97 – 2.91 (m, 2H), 2.51 (dd, *J* = 17.0, 12.0 Hz, 1H), 2.37 – 2.29 (m, 5H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.4, 169.8, 155.7, 150.2, 138.2, 136.7, 134.7, 129.6, 128.4, 128.0, 124.5, 63.9, 52.8, 38.3, 36.6, 36.0, 21.1. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{21}N_2O_6S$ $(M+H^+)$: 405.1114; **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{21}N_2O_5S$ $(M+H)^+$: 389.1166; Found: 389.1164. **$[\alpha]_D^{20}$:** -22 (*c* = 1.0; CH_2Cl_2).

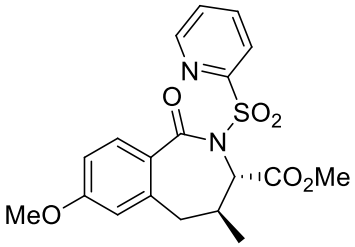
Along product **3b**, product **2b** was also isolated

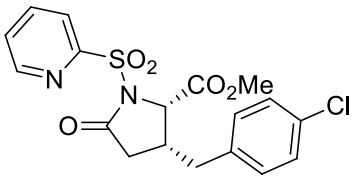

(3*S*,4*S*)-Methyl 4,8-dimethyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2b). White solid; yield: 13.6 mg (35%); mp = 185-186 °C. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.67 (dd, *J* = 4.7, 0.8 Hz, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.00 (td, *J* = 7.8, 1.7 Hz, 1H), 7.54 (ddd, *J* = 7.7, 4.7, 1.0 Hz, 1H), 7.27 (d, *J* = 1.3 Hz, 1H), 7.18 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.02 (d, *J* = 7.7 Hz, 1H), 5.24 (s, 1H), 3.29 – 3.16 (m, 4H), 2.84 – 2.75 (m, 1H), 2.68 (dd, *J* = 13.6, 5.9 Hz, 1H), 2.25 (s, 3H), 1.47 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 170.2, 169.7, 156.6, 149.6, 137.8, 137.2, 135.8, 133.8, 132.7, 130.0, 129.0, 127.4, 125.7, 63.3, 52.5, 39.3, 37.3, 20.9, 20.4. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{21}N_2O_5S$ $(M+H^+)$: 389.1165; Found: 389.1164. **IR** (ν_{max}/cm^{-1}): 1740, 1688, 1351, 1180. **$[\alpha]_D^{20}$:** +8 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*R*)-Methyl 5-oxo-1-(pyridin-2-ylsulfonyl)-3-(4-(trifluoromethyl)benzyl)pyrrolidine-2-carboxylate (3c). 
Compound **3c** was prepared following the general protocol from (2*S*,3*S*)-methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(4-(trifluoromethyl)phenyl)butanoate (**1c**) (41.6 mg, 0.10 mmol, 1.00 equiv) to give **3c** as a yellow oil; yield: 28.0 mg (63%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.69 (ddd, *J* = 4.7, 1.6, 0.8 Hz, 1H), 8.24 (dt, *J* = 7.9, 0.8 Hz, 1H), 7.96 (td, *J* = 7.8, 1.7 Hz, 1H), 7.58 – 7.53 (m, 3H), 7.26 (d, *J* = 8.0 Hz, 2H), 5.10 (d, *J* = 8.0 Hz, 1H), 3.88 (s, 3H), 3.08 – 2.93 (m, 2H), 2.57 – 2.43 (m, 2H), 2.28 (dd, *J* = 16.9, 7.6 Hz, 1H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.9, 169.6, 155.6, 150.2, 141.9, 138.3, 129.6 (q, *J* = 32.6 Hz), 129.0, 128.1, 125.9 (q, *J* = 3.7 Hz), 124.5, 124.2 (q, *J* = 274.4 Hz), 63.7, 52.9, 37.9, 36.4, 36.3. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{18}F_3N_2O_5S$ $(M+Na)^+$: 465.0702; Found: 465.0712. **IR** (ν_{max}/cm^{-1}): 1744, 1736, 1325, 1177. **$[\alpha]_D^{20}$:** -15 (*c* = 1.0; CH_2Cl_2).

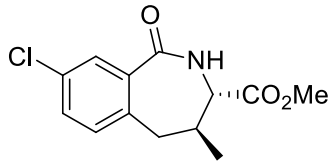
(2*S*,3*R*)-Methyl 3-(4-methoxybenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3d).  Compound **3d** was prepared following the general protocol from (2*S*,3*S*)-methyl 3-methyl-4-(4-methoxy)phenyl-2-(pyridine-2-sulfonamido) butanoate (**1d**) (34.8 mg, 0.10 mmol, 1.00 equiv) to give **3d** as a yellow oil; yield: 22.8 mg (56%). **^{1}H NMR (500 MHz, $CDCl_3$, δ):** 8.69 (ddd, *J* = 4.7, 1.6, 0.8 Hz, 1H), 8.23 (dt, *J* = 7.9, 0.9 Hz, 1H), 7.95 (td, *J* = 7.8, 1.7 Hz, 1H), 7.55 (ddd, *J* = 7.7, 4.7, 1.0 Hz, 1H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 5.08 (d, *J* = 8.1 Hz, 1H), 3.87 (s, 3H), 3.78 (s, 3H), 2.95 – 2.90 (m, 2H), 2.50 (dd, *J* = 17.0, 12.1 Hz, 1H), 2.32 – 2.25 (m, 2H). **^{13}C NMR (126 MHz, $CDCl_3$, δ):** 172.42, 169.79, 158.71, 155.69, 150.17, 138.23, 129.80, 129.56, 127.97, 124.53, 114.36, 63.86, 55.43, 52.80, 38.49, 36.58, 35.60. **$[\alpha]_D^{20}$:** -10 (*c* = 1.0; CH_2Cl_2).

Along product **3d**, product **2d** was also isolated

(3*S*,4*S*)-Methyl 8-methoxy-4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2d).  Yellow oil; yield: 6.9 mg (17%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.68 (dd, *J* = 4.6, 0.6 Hz, 1H), 8.42 (d, *J* = 7.9 Hz, 1H), 8.01 (td, *J* = 7.8, 1.7 Hz, 1H), 7.54 (ddd, *J* = 7.7, 4.7, 1.0 Hz, 1H), 7.04 (d, *J* = 8.3 Hz, 1H), 6.98 (d, *J* = 2.7 Hz, 1H), 6.92 (dd, *J* = 8.3, 2.8 Hz, 1H), 5.25 (s, 1H), 3.71 (s, 3H), 3.29 (s, 3H), 3.27 – 3.18 (m, 1H), 2.81 – 2.73 (m, 1H), 2.66 (dd, *J* = 13.7, 6.0 Hz, 1H), 1.46 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 170.0, 169.6, 158.7, 156.6, 149.6, 137.9, 133.7, 131.1, 130.4, 127.5, 125.6, 120.1, 113.3, 63.4, 55.6, 52.6, 39.7, 36.9, 20.4. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{21}N_2O_6S$ ($M+H^+$): 405.1114; Found: 405.1109. **IR** (ν_{max}/cm^{-1}): 1744, 1688, 1355, 1179. **$[\alpha]_D^{20}$:** +9 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*R*)-Methyl 3-(4-chlorobenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3e).  Compound **3e** was prepared following the general protocol from (2*S*,3*S*)-methyl 3-methyl-4-(4-chloro)phenyl-2-(pyridine-2-sulfonamido) butanoate (**1e**) (34.8 mg, 0.10 mmol, 1.00 equiv) to give **3e** as a yellow oil; yield: 28.8 mg (70%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.68 (ddd, *J* = 4.6, 1.6, 0.8 Hz, 1H), 8.23 (d, *J* = 7.9 Hz, 1H), 7.96 (td, *J* = 7.8, 1.7 Hz, 1H), 7.55 (ddd, *J* = 7.7, 4.7, 1.1 Hz, 1H), 7.27 (d, *J* = 8.3 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 5.08 (d, *J* = 8.0 Hz, 1H), 3.87 (s, 3H), 3.02 – 2.88 (m, 2H), 2.50 (dd, *J* = 17.0, 11.9 Hz, 1H), 2.37 (dd, *J* = 15.1, 11.8 Hz, 1H), 2.27 (dd, *J* = 17.0, 7.6 Hz, 1H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.0, 169.6, 155.6, 150.2, 138.3, 136.2, 133.0, 129.9, 129.1, 128.0, 124.5, 63.7, 52.9, 38.1, 36.4, 35.8. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{18}ClN_2O_5S$ $(M+H)^+$: 409.0619; Found: 409.0610. **IR** (ν_{max}/cm^{-1}): 1744, 1736, 1364, 1182. **$[\alpha]_D^{20}$:** -22 (*c* = 1.0; CH_2Cl_2).

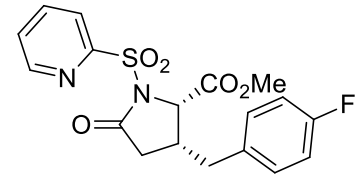
Along product **3e**, product **2e** was also isolated



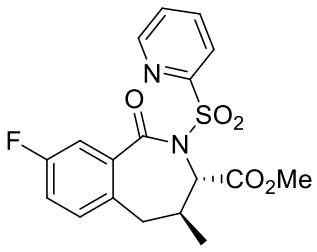
(3*S*,4*S*)-Methyl 8-chloro-4-methyl-1-oxo-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2e).

Further purification implied the *in situ* cleavage of the *N*–SO_2Py group[2] leading to the corresponding free benzazepinone derivative **2e**-deprotected as a white solid without further purification; yield: 1.60 mg (6%); mp = 110-113 °C. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 7.70 (d, *J* = 2.3 Hz, 1H), 7.39 (dd, *J* = 8.1, 2.3 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 1H), 6.71 (bs, 1H), 3.76 (s, 3H), 3.40 (dd, *J* = 10.3, 5.0 Hz, 1H), 3.21 (dd, *J* = 13.5, 6.6 Hz, 1H), 2.59 – 2.43 (m, 2H), 1.09 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.6, 170.1, 136.1, 134.4, 133.6, 131.7, 131.4, 129.0, 59.4, 53.0, 40.0, 37.9, 17.5. **HRMS-ESI (*m/z*):** calcd. for $C_{13}H_{15}ClNO_3$ ($M+Na^+$): 290.0554; Found: 290.0550. **IR** (ν_{max}/cm^{-1}): 1736, 1664. **$[\alpha]_D^{20}$:** -162 (*c* = 1.0; CH_2Cl_2).

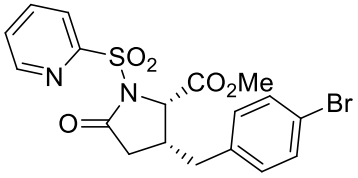
(2*S*,3*R*)-Methyl 5-oxo-1-(pyridin-2-ylsulfonyl)-3-(4-fluorobenzyl)pyrrolidine-2-carboxylate (3f). Compound **3f** was prepared following the general protocol from (2*S*,3*S*)-methyl 4-(4-fluorophenyl)-3-methyl-2-(pyridine-2-sulfonamido) butanoate (**1f**) (36.6 mg, 0.10 mmol, 1.00 equiv) to give **3f** as a yellow oil; yield: 33.2 mg (85%). **^{1}H NMR (500 MHz, $CDCl_3$, δ):** 8.69 (d, *J* = 4.6 Hz, 1H), 8.24 (d, *J* = 7.9 Hz, 1H), 7.96 (td, *J* = 7.8, 1.7 Hz, 1H), 7.56 – 7.54 (m, 1H), 7.09 (dd, *J* = 8.4, 5.5 Hz, 2H), 6.99 (t, *J* = 8.6 Hz, 2H), 5.09 (d, *J* = 8.0 Hz, 1H), 3.87 (s, 3H), 3.00 – 2.91 (m, 2H), 2.50 (dd, *J* = 17.0, 12.0 Hz, 1H), 2.37 (dd, *J* = 14.8, 11.7 Hz, 1H), 2.28 (dd, *J* = 17.0, 7.5 Hz, 1H). **^{13}C NMR (126 MHz, $CDCl_3$, δ):** 172.1, 169.7, 163.2 (d, *J* = 247.1 Hz), 155.6, 150.2, 138.3, 133.5 (d, *J* = 3.6 Hz), 130.1 (d, *J* = 7.8 Hz), 128.0, 124.5, 115.8 (d, *J* = 21.3 Hz), 63.8, 52.9, 38.3, 36.5, 35.7. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{18}FN_2O_5S$ ($M+H)^+$: 393.0914; Found: 393.0913. **IR** (ν_{max}/cm^{-1}): 1746, 1735, 1366, 1181. **$[\alpha]_D^{20}$:** -10 (*c* = 1.0; CH_2Cl_2).



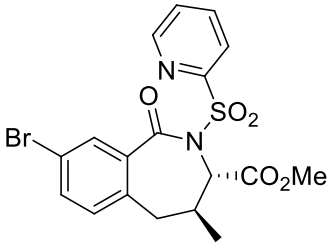
Along product **3f**, product **2f** was also isolated

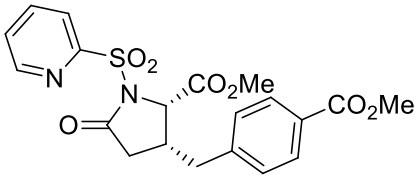


(3*S*,4*S*)-Methyl 8-fluoro-4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2f). Yellow oil; yield: 2.7 mg (7%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.67 (ddd, *J* = 4.6, 1.6, 0.8 Hz, 1H), 8.42 (dt, *J* = 7.9, 0.8 Hz, 1H), 8.02 (td, *J* = 7.8, 1.7 Hz, 1H), 7.55 (ddd, *J* = 7.6, 4.7, 1.1 Hz, 1H), 7.20 – 7.15 (m, 1H), 7.13 – 7.04 (m, 2H), 5.27 (s, 1H), 3.31 (s, 3H), 3.27 – 3.17 (m, 1H), 2.80 (t, *J* = 12.7 Hz, 1H), 2.70 (dd, *J* = 13.7, 6.1 Hz, 1H), 1.48 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 169.5, 168.8 (d, *J* = 2.5 Hz), 161.7 (d, *J* = 247.3 Hz), 156.4, 149.7, 137.9, 134.7 (d, *J* = 7.4 Hz), 134.5 (d, *J* = 3.3 Hz), 131.0 (d, *J* = 7.6 Hz), 127.6, 125.6, 120.0 (d, *J* = 21.4 Hz), 116.3 (d, *J* = 23.5 Hz), 63.3, 52.7, 39.4, 37.0, 20.4. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{18}FN_2O_5S$ ($M+H^+$): 393.0914; Found: 393.0907. **IR** (ν_{max}/cm^{-1}): 1741, 1688, 1353, 1180. **$[\alpha]_D^{20}$:** +5 (*c* = 1.0; CH_2Cl_2).

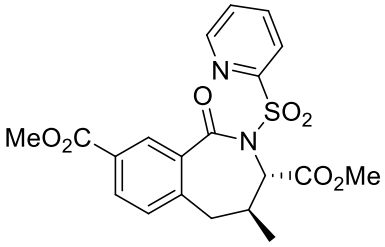
(2*S*,3*R*)-Methyl 5-oxo-1-(pyridin-2-ylsulfonyl)-3-(4-bromobenzyl)pyrrolidine-2-carboxylate (3g). 
Compound **3g** was prepared following the general protocol from (2*S*,3*S*)-methyl 4-(4-bromophenyl)-3-methyl-2-(pyridine-2-sulfonamido) butanoate (**1g**) (42.7 mg, 0.10 mmol, 1.00 equiv) to give **3g** as a yellow oil; yield: 31.5 mg (69%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.69 (ddd, *J* = 4.7, 1.6, 0.8 Hz, 1H), 8.24 (dt, *J* = 7.9, 0.9 Hz, 1H), 7.96 (td, *J* = 7.8, 1.7 Hz, 1H), 7.55 (ddd, *J* = 7.7, 4.7, 1.1 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.01 (d, *J* = 8.4 Hz, 2H), 5.08 (d, *J* = 8.0 Hz, 1H), 3.87 (s, 3H), 3.03 – 2.88 (m, 2H), 2.50 (dd, *J* = 16.9, 12.0 Hz, 1H), 2.40 – 2.23 (m, 2H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.0, 169.6, 155.6, 150.2, 138.3, 136.8, 132.1, 130.3, 128.0, 124.5, 121.1, 63.7, 52.9, 38.0, 36.5, 35.9. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{18}BrN_2O_5S$ $(M+H)^+$: 453.0114; Found: 453.0107. **IR** (ν_{max}/cm^{-1}): 1742, 1736, 1364, 1177. **$[\alpha]_D^{20}$:** -13 (*c* = 1.0; CH_2Cl_2).

Along product **3g**, product **2g** was also isolated

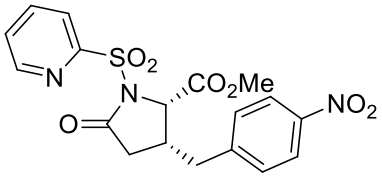

(3*S*,4*S*)-Methyl 8-bromo-4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2g). Yellow oil; yield: 4.6 mg (10%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.67 (dd, *J* = 4.7, 0.8 Hz, 1H), 8.42 (d, *J* = 7.9 Hz, 1H), 8.02 (td, *J* = 7.8, 1.7 Hz, 1H), 7.60 (d, *J* = 2.1 Hz, 1H), 7.56 (ddd, *J* = 7.7, 4.7, 1.0 Hz, 1H), 7.49 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 1H), 5.27 (s, 1H), 3.30 (s, 3H), 3.27 – 3.19 (m, 1H), 2.82 – 2.66 (m, 2H), 1.47 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 169.5, 168.5, 156.3, 149.6, 137.9, 137.5, 135.8, 134.7, 132.5, 130.8, 127.7, 125.7, 121.0, 63.3, 52.8, 39.1, 37.2, 20.4. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{18}BrN_2O_5S$ $(M+H^+)$: 453.0114; Found: 453.0105. **IR** (ν_{max}/cm^{-1}): 1740, 1686, 1353, 1179. **$[\alpha]_D^{20}$:** +16 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*R*)-Methyl 3-(4-(methoxycarbonyl)benzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3h). 
Compound **3h** was prepared following the general protocol from methyl 4-((2*S*,3*S*)-4-methoxy-2-methyl-4-oxo-3-(pyridine-2-sulfonamido)butyl) benzoate (**1h**) (40.6 mg, 0.10 mmol, 1.00 equiv) to give **3h** as a white oil; yield: 36.7 mg (85%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.69 (ddd, *J* = 4.7, 1.6, 0.8 Hz, 1H), 8.23 (dt, *J* = 7.9, 0.9 Hz, 1H), 7.98 – 7.93 (m, 3H), 7.55 (ddd, *J* = 7.7, 4.7, 1.1 Hz, 1H), 7.21 (d, *J* = 8.3 Hz, 2H), 5.10 (d, *J* = 8.0 Hz, 1H), 3.90 (s, 3H), 3.87 (s, 3H), 3.09 – 2.94 (m, 2H), 2.57 – 2.41 (m, 2H), 2.27 (dd, *J* = 17.0, 7.6 Hz, 1H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.0, 169.6, 166.8, 155.6, 150.2, 143.1, 138.3, 130.3, 129.3, 128.6, 128.0, 124.5, 63.7, 52.9, 52.3, 37.8, 36.4. **HRMS-ESI (*m/z*):** calcd. for $C_{20}H_{21}N_2O_7S$ $(M+H)^+$: 433.1063; Found: 433.1066. **IR** (ν_{max}/cm^{-1}): 1742, 1736, 1714, 1362, 1177. **$[\alpha]_D^{20}$:** -19 (*c* = 1.0; CH_2Cl_2).

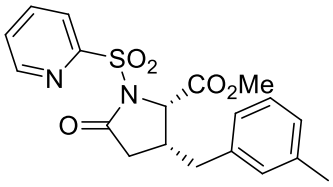
Along product **3h**, product **2h** was also isolated

(3*S*,4*S*)-Dimethyl 4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3,8-dicarboxylate (2h). 

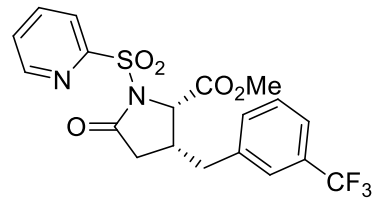
Yellow oil; yield: 3.4 mg (8%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.68 (dd, *J* = 4.7, 0.8 Hz, 1H), 8.44 (d, *J* = 7.9 Hz, 1H), 8.14 (d, *J* = 1.8 Hz, 1H), 8.06 – 8.00 (m, 2H), 7.56 (ddd, *J* = 7.6, 4.7, 1.0 Hz, 1H), 7.24 (d, *J* = 8.1 Hz, 1H), 5.28 (s, 1H), 3.86 (s, 3H), 3.31 – 3.19 (m, 4H), 2.92 – 2.84 (m, 1H), 2.79 (dd, *J* = 13.5, 6.1 Hz, 1H), 1.50 (d, *J* = 6.9 Hz, 4H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 169.4, 169.0, 165.9, 156.3, 149.6, 143.3, 137.9, 133.6, 133.4, 131.3, 129.7, 129.5, 127.7, 125.7, 63.2, 52.7, 52.4, 39.0, 37.8, 20.6. **HRMS-ESI (*m/z*):** calcd. for $C_{20}H_{21}N_2O_7S$ $(M+H^+)$: 433.1063; Found: 433.1059. **IR** (ν_{max}/cm^{-1}): 1741, 1720, 1688, 1353, 1177. **$[\alpha]_D^{20}$:** +32 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*R*)-Methyl 3-(4-nitrobenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3i). 

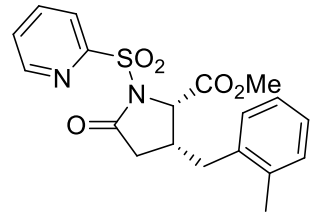
Compound **3i** was prepared following the general protocol from (2*S*,3*S*)-methyl 3-methyl-4-(4-nitrophenyl)-2-(pyridine-2-sulfonamido) butanoate (**1i**) (39.3 mg, 0.10 mmol, 1.00 equiv) to give **3i** as a white oil; yield: 21.0 mg (50%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.69 (ddd, *J* = 4.7, 1.5, 0.8 Hz, 1H), 8.23 (d, *J* = 7.9 Hz, 1H), 8.18 (d, *J* = 8.7 Hz, 2H), 7.97 (td, *J* = 7.8, 1.7 Hz, 1H), 7.56 (ddd, *J* = 7.7, 4.7, 1.0 Hz, 1H), 7.33 (d, *J* = 8.7 Hz, 2H), 5.11 (d, *J* = 8.0 Hz, 1H), 3.88 (s, 3H), 3.10 – 2.98 (m, 2H), 2.59 – 2.49 (m, 2H), 2.29 (dd, *J* = 16.8, 7.6 Hz, 1H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.6, 169.5, 155.5, 150.2, 147.3, 145.3, 138.3, 129.5, 128.1, 124.5, 124.2, 63.6, 53.0, 37.6, 36.4, 36.3. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{17}N_3O_7SNa$ $(M+Na)^+$: 422.0679; Found: 422.0684. **$[\alpha]_D^{20}$:** -7 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*R*)-Methyl 3-(3-methylbenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3j). 

Compound **3j** was prepared following the general protocol from (2*S*,3*S*)-methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(*m*-tolyl)butanoate (1**j**) (36.2 mg, 0.10 mmol, 1.00 equiv) to give **3j** as a 66:34 mixture of the γ-lactam and the benzazepinone as a yellow oil; yield: 38.4 mg (99%). **^{1}H NMR (500 MHz, $CDCl_3$, δ):** 8.69 (ddd, *J* = 4.7, 1.6, 0.8 Hz, 1H), 8.23 (d, *J* = 7.9 Hz, 1H), 7.95 (td, *J* = 7.8, 1.7 Hz, 1H), 7.54 – 7.52 (m, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 7.03 (d, *J* = 6.9 Hz, 1H), 6.93 (s, 1H), 6.91 (d, *J* = 7.7 Hz, 1H), 5.09 (d, *J* = 8.1 Hz, 1H), 3.87 (s, 3H), 2.96 – 2.93 (m, 1H), 2.51 (dd, *J* = 17.0, 12.2 Hz, 1H), 2.33 – 2.29 (m, 6H). **^{13}C NMR (126 MHz, $CDCl_3$, δ):** 172.4, 169.8, 155.6, 150.2, 138.6, 138.2, 137.7, 129.3, 128.8, 128.0, 127.8, 125.6, 124.5, 63.9, 52.8, 38.2, 36.6, 36.4, 21.5.

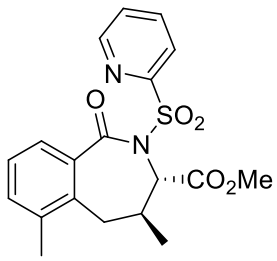


(2*S*,3*R*)-Methyl 5-oxo-1-(pyridin-2-ylsulfonyl)-3-(3-(trifluoromethyl)benzyl) pyrrolidine-2-carboxylate (3k). Compound **3k** was prepared following the general protocol from (2*S,*3*S*)-methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(3-(trifluoromethyl)phenyl) butanoate (**1k**) (41.6 mg, 0.10 mmol, 1.00 equiv) to give **3k** as a yellow oil; yield: 30.9 mg (70%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.71 – 8.67 (m, 1H), 8.23 (d, *J* = 7.7 Hz, 1H), 7.96 (td, *J* = 7.8, 1.7 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.46 – 7.39 (m, 2H), 7.35 – 7.32 (m, 1H), 5.09 (d, *J* = 7.9 Hz, 1H), 3.88 (s, 3H), 3.09 – 2.94 (m, 2H), 2.59 – 2.45 (m, 2H), 2.29 (dd, *J* = 17.0, 7.5 Hz, 1H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 171.9, 169.6, 155.6, 150.2, 138.8, 138.3, 132.0, 131.4 (q, *J* = 31.3 Hz), 129.5, 128.1, 125.4 (q, *J* = 3.7 Hz), 124.5, 124.1 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 272.4 Hz), 63.7, 52.9, 38.0, 36.4, 36.2. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{17}F_3N_2O_5SNa$ $(M+Na)^+$: 465.0709; Found: 465.0708. **IR** (ν_{max}/cm^{-1}): 1744, 1736, 1330, 1177. **$[\alpha]_D^{20}$:** -17 (*c* = 1.0; CH_2Cl_2).

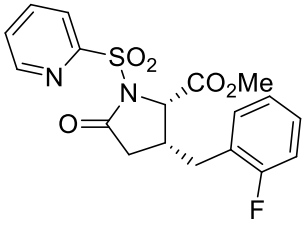


(2*S*,3*R*)-Methyl 3-(2-methylbenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3l). Compound **3l** was prepared following the general protocol from (2*S,*3*S*)-methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(*o*-tolyl)butanoate (**1l**) (36.2 mg, 0.10 mmol, 1.00 equiv) to give **3l** as a yellow oil; yield: 31.1 mg (80%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.70 – 8.68 (m, 1H), 8.24 (d, *J* = 7.9 Hz, 1H), 7.96 (td, *J* = 7.8, 1.7 Hz, 1H), 7.55 (ddd, *J* = 7.7, 4.7, 1.0 Hz, 1H), 7.17 – 7.12 (m, 3H), 7.04 – 7.01 (m, 1H), 5.12 (d, *J* = 8.1 Hz, 1H), 3.88 (s, 3H), 3.06 – 2.89 (m, 2H), 2.55 (dd, *J* = 16.9, 12.1 Hz, 1H), 2.39 – 2.30 (m, 4H), 2.24 – 2.20 (m, 1H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.4, 169.8, 155.6, 150.2, 138.2, 135.9, 135.9, 130.9, 129.1, 128.0, 127.2, 126.4, 124.6, 64.0, 52.8, 36.8, 36.6, 33.5, 19.5. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{21}N_2O_5S$ $(M+H)^+$: 389.1166; Found: 389.1160. **IR** (ν_{max}/cm^{-1}): 1748, 1736, 1364, 1182. **$[\alpha]_D^{20}$:** -25 (*c* = 1.0; CH_2Cl_2).

Along product **3l**, product **2l** was also isolated

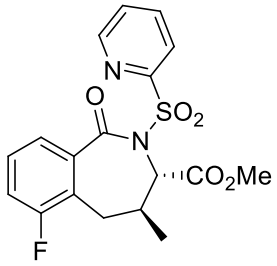


(3*S*,4*S*)-Methyl 4,6-dimethyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2l). White oil; yield: 6.6 mg (17%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.69 – 8.68 (m, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.00 (td, *J* = 7.8, 1.2 Hz, 1H), 7.54 (dd, *J* = 7.6, 4.8 Hz, 1H), 7.23 – 7.8 (m, 2H), 7.11 (d, *J* = 7.3 Hz, 1H), 5.23 (s, 1H), 3.26 – 3.18 (m, 4H), 2.93 (dd, *J* = 13.8, 5.2 Hz, 1H), 2.59 (t, *J* = 13.1 Hz, 1H), 2.35 (s, 3H), 1.50 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 170.4, 169.6, 156.6, 149.6, 137.9, 136.8, 135.7, 134.2, 133.6, 127.5, 127.5, 126.9, 125.7, 62.8, 52.5, 38.1, 32.7, 20.3, 19.6. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{20}N_2O_5SNa$ $(M+Na^+)$: 411.0985; Found: 411.0987. **$[\alpha]_D^{20}$:** +49 (*c* = 1.0; CH_2Cl_2).

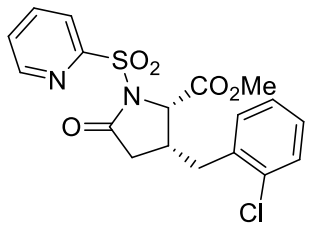
(2*S*,3*R*)-Methyl 5-oxo-1-(pyridin-2-ylsulfonyl)-3-(2-fluorobenzyl)pyrrolidine-2-carboxylate (3m). 

Compound **3m** was prepared following the general protocol from (2*S*,3*S*)-methyl 4-(2-fluorophenyl)-3-methyl-2-(pyridine-2-sulfonamido) butanoate (**1m**) (36.6 mg, 0.10 mmol, 1.00 equiv) to give **3m** as a yellow oil; yield: 33.1 mg (84%). **^{1}H NMR (500 MHz, $CDCl_3$, δ):** 8.69 (d, *J* = 4.7 Hz, 1H), 8.24 (d, *J* = 8.5 Hz, 1H), 7.95 (td, *J* = 7.7, 1.3 Hz, 1H), 7.55 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.25 – 7.20 (m, 1H), 7.15 – 7.01 (m, 3H), 5.09 (d, *J* = 8.0 Hz, 1H), 3.88 (s, 3H), 3.08 – 2.96 (m, 2H), 2.57 (dd, *J* = 16.9, 12.3 Hz, 1H), 2.48 – 2.43 (m, 1H), 2.28 (dd, *J* = 16.9, 7.5 Hz, 1H). **^{13}C NMR (126 MHz, $CDCl_3$, δ):** 172.2, 169.6, 161.0 (d, *J* = 245.4 Hz), 155.7, 150.2, 138.2, 130.8 (d, *J* = 4.5 Hz), 129.0 (d, *J* = 8.2 Hz), 128.0, 124.5 (d, *J* = 7.5 Hz), 124.5 (d, *J* = 3.9 Hz), 115.8 (d, *J* = 22.0 Hz), 63.8, 52.9, 37.0 (d, *J* = 1.2 Hz), 36.5, 29.8 (d, *J* = 1.9 Hz). **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{17}FN_2O_5SNa$ $(M+Na)^+$: 415.0734; Found: 415.0738. **$[\alpha]_D^{20}$:** -20 (*c* = 1.0; CH_2Cl_2).

Along product **3m**, product **2m** was also isolated

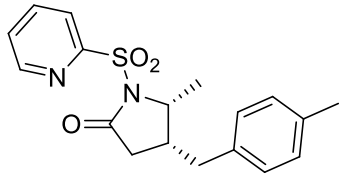


(3*S*,4*S*)-Methyl 6-fluoro-4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2m). Yellow oil; yield: 2.3 mg (6%). **^{1}H NMR (500 MHz, $CDCl_3$, δ):** 8.69 – 8.67 (m, 1H), 8.42 (d, *J* = 7.9 Hz, 1H), 8.01 (td, *J* = 7.8, 1.7 Hz, 1H), 7.55 (ddd, *J* = 7.7, 4.7, 1.0 Hz, 1H), 7.28 – 7.27 (m, 1H), 7.22 – 7.17 (m, 1H), 7.14 (td, *J* = 8.8, 1.2 Hz, 1H), 5.28 (s, 1H), 3.29 (s, 3H), 3.27 – 3.18 (m, 2H), 2.53 – 2.47 (m, 1H), 1.51 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR (126 MHz, $CDCl_3$, δ):** 169.5, 168.8 (d, *J* = 3.4 Hz), 159.2 (d, *J* = 247.1 Hz), 156.4, 149.7, 137.9, 135.3 (d, *J* = 3.2 Hz), 128.5 (d, *J* = 8.3 Hz), 127.6, 125.9 (d, *J* = 18.6 Hz), 125.6, 125.4 (d, *J* = 3.7 Hz), 119.4 (d, *J* = 23.3 Hz), 63.1, 52.7, 38.5, 28.0 (d, *J* = 3.8 Hz), 20.5. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{17}FN_2O_5SNa$ $(M+Na)^+$: 415.0734; Found: 415.0739. **$[\alpha]_D^{20}$:** +20 (*c* = 1.0; CH_2Cl_2).

(2*S*,3*R*)-Methyl 3-(2-chlorobenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3n). 

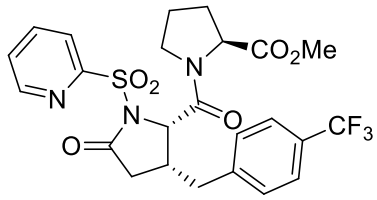
Compound **3n** was prepared following the general protocol from (2*S*,3*S*)-methyl 4-(2-chlorophenyl)-3-methyl-2-(pyridine-2-sulfonamido) butanoate (**1n**) (38.3 mg, 0.10 mmol, 1.00 equiv) to give **3n** as a 75:25 mixture of diasteromers, which came from both diasteromers presented in the starting material. Brown oil; yield: 34.7 mg (85%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.69 (bd, *J* = 4.5 Hz, 1H), 8.23 (d, *J* = 7.8 Hz, 1H), 7.95 (td, *J* = 7.8, 1.5 Hz, 1H), 7.55 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.37 – 7.34 (m, 1H), 7.21 – 7.13 (m, 3H), 5.11 (d, *J* = 8.0 Hz, 1H), 3.89 (s, 3H), 3.17 – 3.07 (m, 2H), 2.64 – 2.45 (m, 2H), 2.27 – 2.19 (m, 1H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.2, 169.7, 155.6, 150.2, 138.2, 135.5, 134.0, 130.7, 130.0, 128.7, 128.0, 127.3, 124.5, 63.8, 52.9, 36.4, 36.3, 33.9. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{17}ClN_2O_5SNa$ $(M+Na)^+$: 431.0439; Found: 431.0440. **$[\alpha]_D^{20}$:** -29 (*c* = 1.0; CH_2Cl_2).

(4*R*,5*R*)-5-Methyl-4-(4-methylbenzyl)-1-(pyridin-2-ylsulfonyl)pyrrolidin-2-one (7a).



Compound **7a** was prepared following the general protocol from *N*-((2*R*,3*S*)-3-methyl-4-(*p*-tolyl)butan-2-yl)pyridine-2-sulfonamide (**6a**) (31.8 mg, 0.10 mmol, 1.00 equiv) to give **7a** as a 81:19 mixture of diasteromers, which came from both diasteromers presented in the starting material. Yellow oil; yield: 34.7 mg (85%). **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.68 (ddd, *J* = 4.7, 1.6, 0.8 Hz, 1H), 8.22 (d, *J* = 7.9 Hz, 1H), 7.93 (td, *J* = 7.8, 1.7 Hz, 1H), 7.52 (ddd, *J* = 7.7, 4.7, 1.1 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.1 Hz, 2H), 4.65 (p, *J* = 6.7 Hz, 1H), 2.98 – 2.85 (m, 1H), 2.76 (dd, *J* = 13.6, 6.8 Hz, 1H), 2.63 (dd, *J* = 13.9, 9.1 Hz, 1H), 2.36 – 2.30 (m, 5H), 1.50 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 172.8, 156.0, 150.1, 138.0, 136.4, 135.4, 129.5, 128.4, 127.6, 124.6, 59.6, 39.1, 36.4, 35.5, 21.1, 15.8. **HRMS-ESI (*m/z*):** calcd. for $C_{18}H_{20}N_2O_3SNa$ $(M+Na)^+$: 367.1087; Found: 367.1099. **IR** (ν_{max}/cm^{-1}): 1737, 1736, 1340, 1174. **$[\alpha]_D^{20}$:** -42 (*c* = 1.0; CH_2Cl_2).

(*S*)-Methyl 1-((2S,3R)-5-oxo-1-(pyridin-2-ylsulfonyl)-3-(4-(trifluoromethyl) benzyl)pyrrolidine-2-carbonyl)pyrrolidine-2-carboxylateone (9).



Compound **9** was prepared following the general protocol from methyl *N*-(SO_2Py)-γ-(*p*-trifluoromethylphenyl)-L-valyl-prolinate (**8**) (31.8 mg, 0.10 mmol, 1.00 equiv) to give **9** as a 32:78 mixture of γ-lactam and the starting material as a yellow oil; yield: 52.1 mg (99%). **^{1}H NMR (500 MHz, $CDCl_3$, δ):** 8.64 (ddd, *J* = 4.6, 1.6, 0.8 Hz, 1H), 8.25 (d, *J* = 7.9 Hz, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.93 (td, *J* = 7.8, 1.7 Hz, 1H), 7.58 (d, *J* = 8.1 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.48 – 7.45 (m, 1H), 5.08 (d, *J* = 7.4 Hz, 1H), 4.54 – 4.52 (m, 1H), 3.90 – 3.85 (m, 1H), 3.76 (s, 3H), 3.19 – 3.15 (m, 1H), 2.94 – 2.84 (m, 3H), 2.34 – 2.28 (m, 2H), 2.21 – 2.08 (m, 2H), 2.05 – 1.96 (m, 2H).

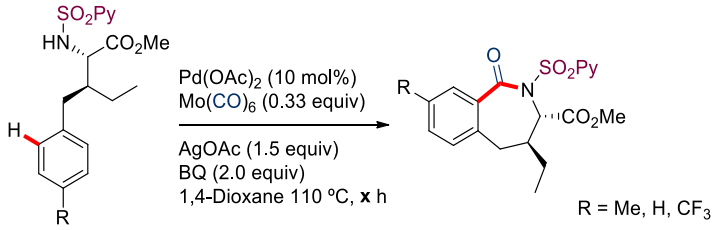
4. Mechanistic studies

4.1. Kinetic studies of the Pd-catalyzed carbonylative cyclization of amino acid derivatives.

These studies were performed in identical parallel reactions, stopped each of them at the corresponding time.

4.1.1. Evaluation of the substitution of the aryl ring

General procedure. An oven-dried, argon flushed, pressure tube was charged with $Pd(OAc)_2$ (2.24 mg, 0.010 mmol), AgOAc (25.0 mg, 0.15 mmol), benzoquinone (21.6 mg, 0.20 mmol), $Mo(CO)_6$ (8.67 mg, 0.33 mmol), the corresponding *N*-SO_2Py γ-arylated aminoester derivative (0.10 mmol, 1.00 equiv) and AcOH (34 μL, 0.60 mmol, 6.00 equiv) if corresponds. The pressure tube was sealed with a rubber septum and flushed with Ar. Under positive pressure of argon, 1,4-dioxane (0.40 mL) was added *via* syringe. The septum was then replaced by a teflon-lined screw cap and finally placed in a preheated oil bath at 110 °C for the given time. The final product percentage was determined by ^{1}H NMR spectroscopy.



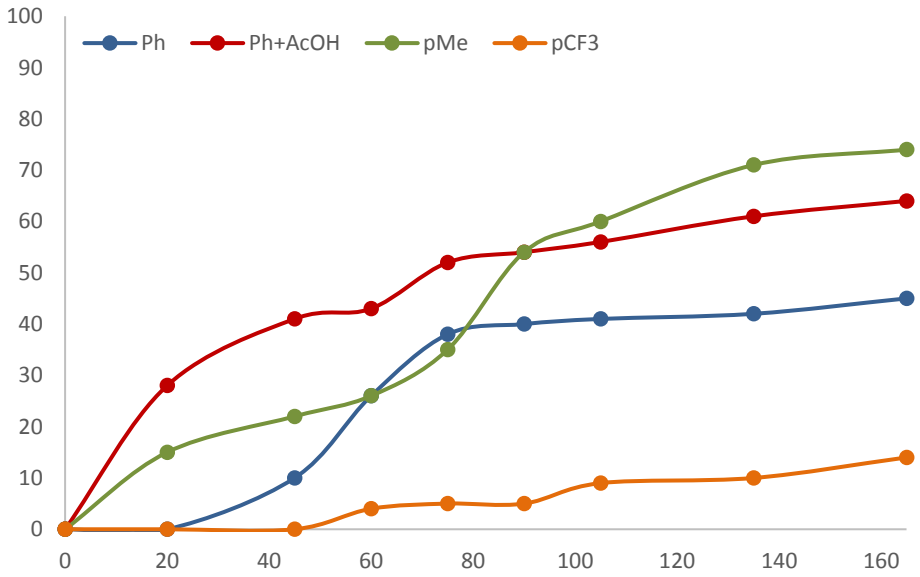
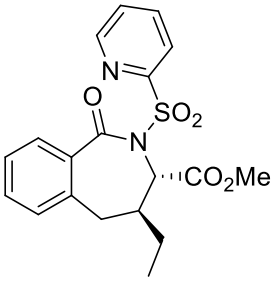
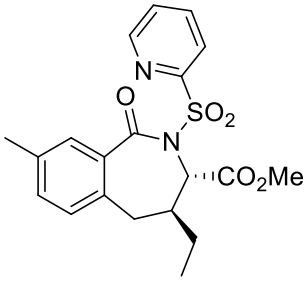


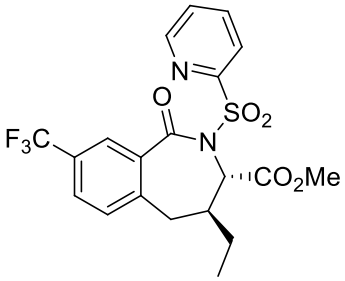
Figure S1. Conv. vs. time depending on the aryl ring nature and the addition of AcOH.

(3*S,4*S**)-Methyl 4-ethyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (5a).** 

Compound **5a** was prepared following the general procedure from (2*S*,3*S*)-methyl 3-benzyl-2-(pyridine-2-sulfonamido)pentanoate **(4a)** (36.2 mg, 0.10 mmol, 1.00 equiv) to give **5a** as a yellow oil. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.67 (ddd, *J* = 4.7, 1.7, 0.8 Hz, 1H), 8.43 (dt, *J* = 8.0, 0.9 Hz, 1H), 8.00 (td, *J* = 7.8, 1.7 Hz, 1H), 7.54 (ddd, *J* = 7.7, 4.7, 1.1 Hz, 1H), 7.46 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.38 (td, *J* = 7.5, 1.4 Hz, 1H), 7.22 (td, *J* = 7.6, 1.2 Hz, 1H), 7.15 (d, *J* = 7.5 Hz, 1H), 5.37 (s, 1H), 3.24 (s, 3H), 3.01 – 2.91 (m, 1H), 2.82 – 2.76 (m, 2H), 2.03 – 1.88 (m, 1H), 1.87 – 1.73 (m, 1H), 1.14 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 170.1, 169.9, 156.6, 149.6, 138.6, 137.8, 132.9, 129.8, 129.2, 127.5, 127.3, 125.7, 60.9, 52.6, 46.5, 36.1, 27.0, 12.1. **HRMS-ESI (*m/z*):** calcd. for $C_{19}H_{21}N_2O_5S$ $(M+H)^+$: 389.1165; Found: 389.1166. **IR** (ν_{max}/cm^{-1}): 1742, 1687, 1351, 1179.

(3*S,4*S**)-Methyl 4-ethyl-8-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (5b).** 

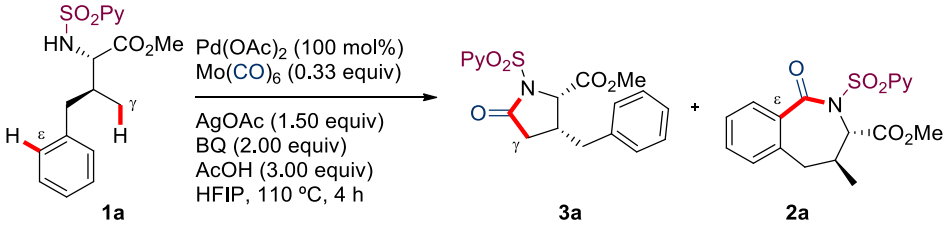
Compound **5b** was prepared following the general procedure from (2*S*,3*S*)-methyl 3-(4-methylbenzyl)-2-(pyridine-2-sulfonamido)pentanoate (**4b**) (37.6 mg, 0.10 mmol, 1.00 equiv) to give **5b** as a white solid; mp = 117-118 °C. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.67 (ddd, *J* = 4.7, 1.7, 0.8 Hz, 1H), 8.42 (dt, *J* = 7.9, 0.9 Hz, 1H), 8.00 (td, *J* = 7.8, 1.7 Hz, 1H), 7.53 (ddd, *J* = 7.6, 4.7, 1.1 Hz, 1H), 7.26 (s, 1H), 7.18 (d, *J* = 7.7 Hz, 1H), 7.02 (d, *J* = 7.7 Hz, 1H), 5.35 (s, 1H), 3.24 (s, 3H), 2.99 – 2.88 (m, 1H), 2.80 – 2.71 (m, 2H), 2.24 (s, 3H), 1.98 – 1.88 (m, 1H), 1.85 – 1.70 (m, 1H), 1.13 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 170.3, 169.9, 156.6, 149.5, 137.8, 137.1, 135.7, 133.8, 132.7, 130.0, 129.1, 127.4, 125.7, 61.1, 52.5, 46.5, 35.6, 27.0, 20.9, 12.1. **HRMS-ESI (*m/z*):** calcd. for $C_{20}H_{23}N_2O_5S$ $(M+H)^+$: 403.1328; Found: 403.1328. **IR** (ν_{max}/cm^{-1}): 1742, 1684, 1350, 1180

(3*S,4*S**)-Methyl 4-ethyl-1-oxo-2-(pyridin-2-ylsulfonyl)-8-(trifluoromethyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (5c).** 

Compound **5c** was prepared following the general procedure from (2*S*,3*S*)-methyl 2-(pyridine-2-sulfonamido)-3-(4-(trifluoromethyl)benzyl)pentanoate (**4c**) (43.0 mg, 0.10 mmol, 1.00 equiv) to give **5c** as a yellow solid; mp = 134-140 °C. **^{1}H NMR (300 MHz, $CDCl_3$, δ):** 8.68 (ddd, *J* = 4.7, 1.7, 0.8 Hz, 1H), 8.43 (dt, *J* = 7.9, 0.9 Hz, 1H), 8.03 (td, *J* = 7.8, 1.7 Hz, 1H), 7.74 (d, *J* = 1.2 Hz, 1H), 7.63 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.57 (ddd, *J* = 7.7, 4.7, 1.1 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 5.40 (s, 1H), 3.24 (s, 3H), 3.02 – 2.92 (m, 1H), 2.89 – 2.79 (m, 2H), 2.01 – 1.89 (m, 1H), 1.88 – 1.76 (m, 1H), 1.15 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$, δ):** 169.7, 168.8, 156.3, 149.7, 142.3, 138.0, 133.8, 130.1 (q, *J* = 33.4 Hz), 129.9, 129.2 (q, *J* = 3.5 Hz), 127.7, 127.0 (q, *J* = 3.8 Hz), 125.8 (s, *J* = 32.8 Hz), 123.5 (q, *J* = 272.4 Hz), 60.9, 52.7, 46.2, 36.0, 27.0, 12.0. **^{19}F NMR (282 MHz, $CDCl_3$, δ):** -63.0. **HRMS-ESI (*m/z*):**calcd. for

$C_{20}H_{20}F_3N_2O_5S$ $(M+H)^+$: 457.1039; Found: 457.1038. **IR** (ν_{max}/cm^{-1}): 1742, 1688, 1352, 1178.

4.2. Stoichiometric studies in γ-phenyl-valine derivative



General procedure. An oven-dried, Ar flushed, pressure tube was charged with $Pd(OAc)_2$ (22.4 mg, 0.010 mmol, 0.10 equiv), AgOAc (25.0 mg, 0.15 mmol, 1.50 equiv), benzoquinone (21.6 mg, 0.20 mmol, 2.00 equiv), $Mo(CO)_6$ (8.67 mg, 0.33 mmol, 0.33 equiv) and (2*S*,3*S*)-methyl 3-(4-benzyl)-2-(pyridine-2-sulfonamido)butanoate **1a** (34.8 mg, 0.10 mmol, 1.00 equiv). The pressure tube was sealed with a rubber septum and flushed with argon. Under positive pressure of argon, HFIP (0.80 mL) and acetic acid (17 μL, 0.30 mmol, 3.00 equiv) were added *via* syringe. The septum was then replaced by a screw cap and finally placed in an oil bath at 110 °C for 18 h. The reaction mixture was then removed from the oil bath and allowed to cool to room temperature. The mixture was then diluted with AcOEt, filtered through a short pad of Celite® and concentrated *in vacuo*. The residue was analyzed by ^{1}H NMR observing a conversion of 70% and 29% towards compounds **3a** and **2a** respectively.

Entry	Non-added additive	1a (%)[a]	3a (%)[a]	2a (%)[a]
1	none	–	70	29
2	AgOAc (1.50 equiv)	–	66	33
3	BQ (2.00 equiv)	41	51	8
4	AcOH	16	54	30

Reaction conditions: **1a** (0.10 mmol, 1.00 equiv), $Mo(CO)_6$ (0.033 mmol, 0.66 equiv), $Pd(OAc)_2$ (22.4 mg, 0.10 mmol, 1.00 equiv), AgOAc (0.15 mmol, 3.00 equiv), BQ (0.20 mmol, 4.00 equiv), AcOH (17 μL, 0.30 mmol, 3.00 equiv) HFIP (0.80 mL), 110 °C, 18 h, argon. [a] Conversion determined by ^{1}H NMR.

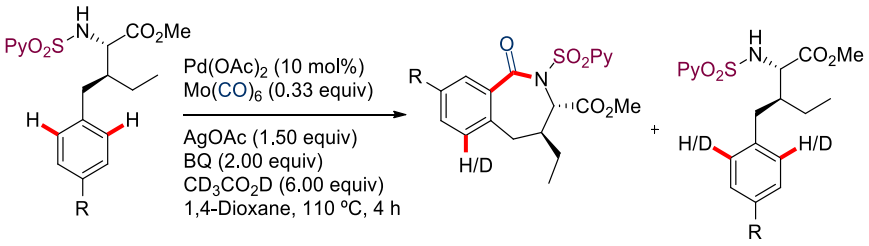
Table S2. Control experiments employing $Pd(OAc)_2$ in stoichiometric quantities

In control experiments employing stoichiometric quantities of $Pd(OAc)_2$, we could observe a complete conversion towards the benzazepinone and the γ-lactam in the presence of all the additives in 70% and 29% yields (entry 1). In the absence of the silver salt, the corresponding derivatives could be observed in a 66% of conversion and a 33% respectively, leading us to the conclusion that the presence of the silver is not required for a higher selectivity towards the γ-lactam product (entry 2). However, when no BQ was added to the reaction media, a higher selectivity was observed but with a higher decreased in yield (entry 3). When AcOH was not added to the reaction media, a higher formation of the g-lactam was observed but in lower selectivity compared to the standard stoichiometric reaction (entry 1) or in the absence of BQ (entry 3). This could indicate that the AcOH formed in the reaction media could be favoring the reversibility of the C-H activation step at the ε-position. The collection of this data is shown in Table S2.

4.3. H/D exchange experiments using deuterium donor species

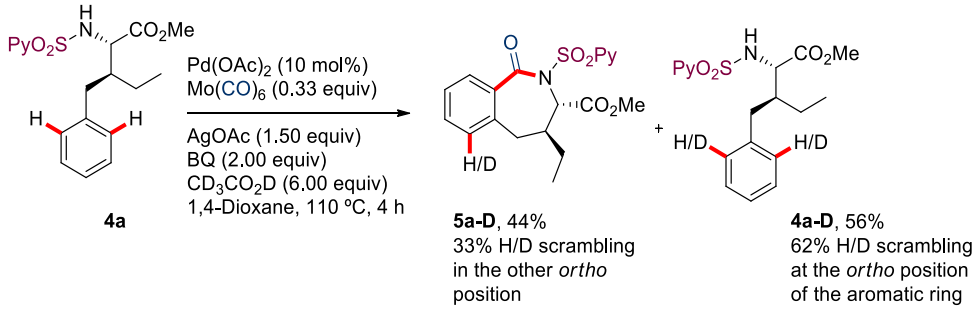
4.3.1. Experimental procedure for the aryl dependent H/D scrambling using CD_3CO_2D as deuterium donor

These studies were performed in identical parallel reactions, stopped each of them at 4 h.



General procedure. An oven-dried, Ar flushed, pressure tube was charged with $Pd(OAc)_2$ (2.24 mg, 0.010 mmol), AgOAc (25.0 mg, 0.15 mmol), benzoquinone (21.6 mg, 0.20 mmol), $Mo(CO)_6$ (8.67 mg, 0.33 mmol) and the corresponding γ-aryl-*allo*-Ile derivative (**4a-c**) (0.10 mmol, 1.00 equiv). The pressure tube was sealed with a rubber septum and flushed with Ar. Under positive pressure of argon, 1,4-dioxane (0.40 mL) and CD_3CO_2D (34.3 µL, 0.60 mmol, 6.00 equiv) were added *via* syringe. The septum was then replaced by a teflon-lined screw cap and finally placed in a preheated oil bath at 110 °C for 4 h. The reaction mixture was then removed from the oil bath and allowed to cool to room temperature. The mixture was then diluted with EtOAc, filtered through a short pad of Celite® and concentrated *in vacuo*. The residue was purified by flash column chromatography (cyclohexane:CH_2Cl_2:EtOAc 10:2:3) to afford the pure starting material **4a-c-D** and the pure benzazepinone **5a-c-D** (the corresponding yields and deuterium percentage are shown in the schemes).

4.3.2. H/D scrambling in electron neutral γ-aryl-*allo*-Ile derivative

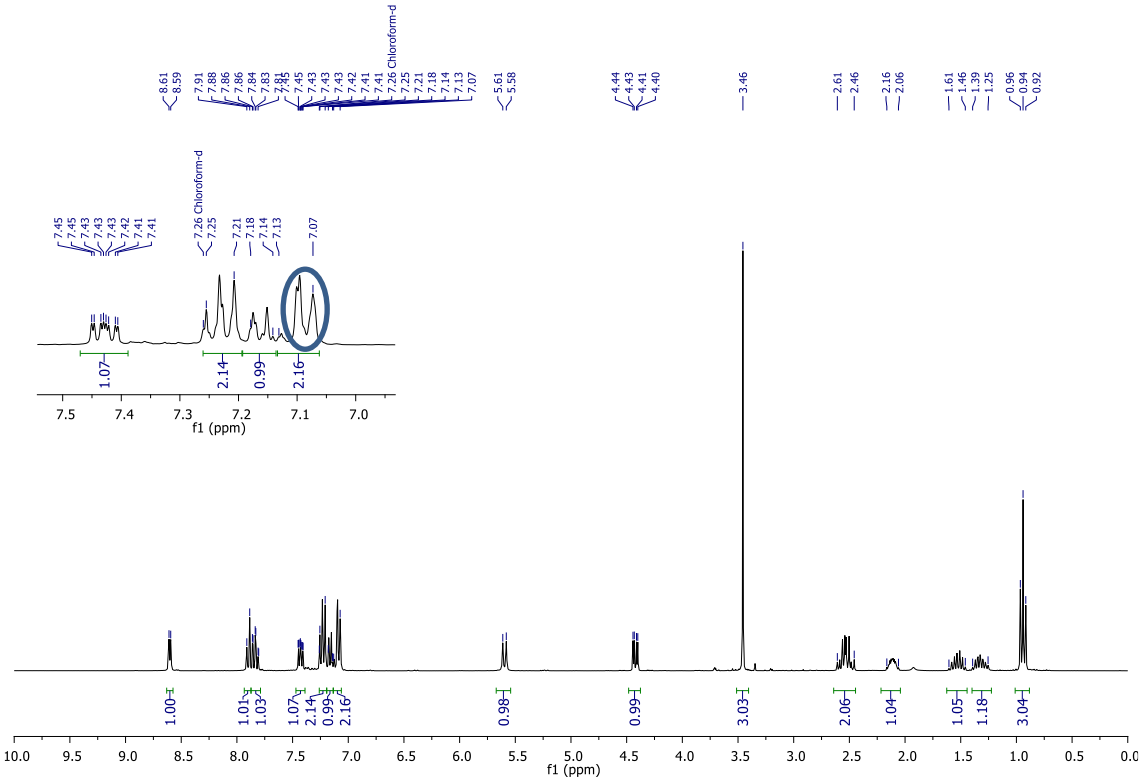


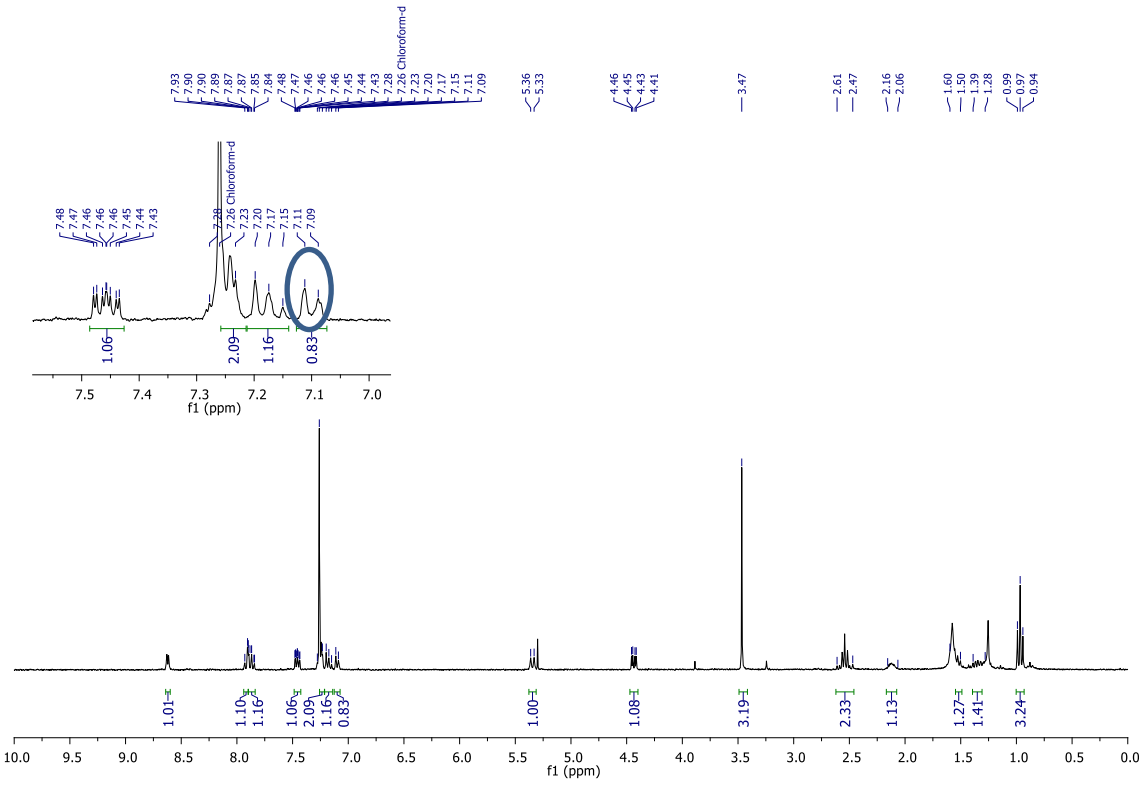
In the **4a-D** spectra, the integration of the doublet at 7.13-7.07 ppm (corresponding to the *o*-aryl positions) was 0.93 instead of 2.16 (62% H/D scrambling).

In the **5a-D** spectra, the integration of the doublet at 7.04-7.01 ppm (corresponding to the *o*-aryl positions) was 0.76 instead of 1.13 (33% H/D scrambling).

Spectra of 4a and 4a-D

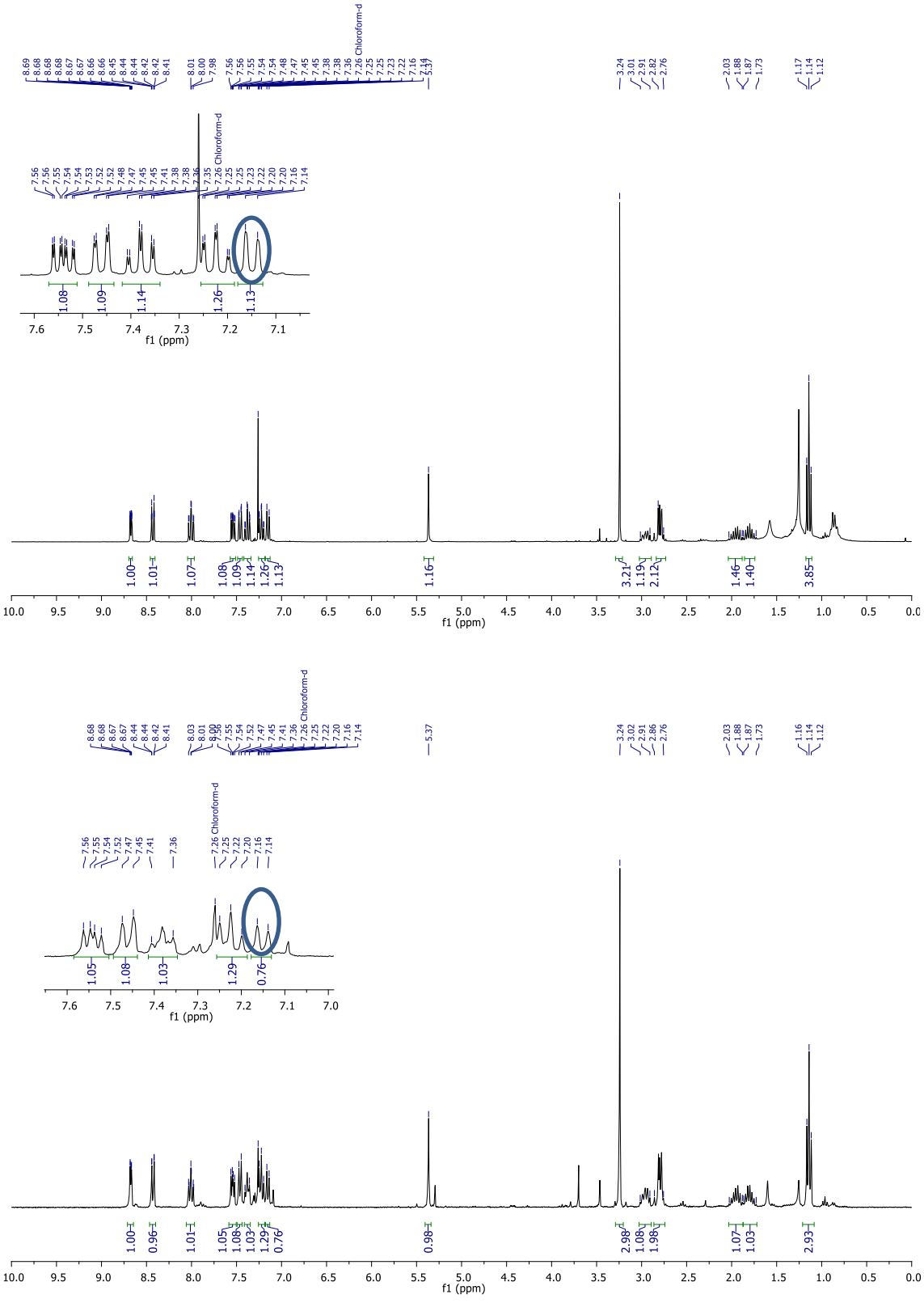
^{1}H NMR ($CDCl_3$, 300 MHz)



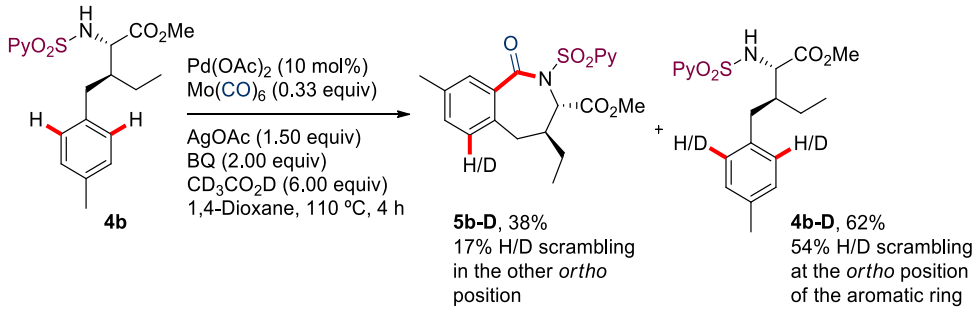


Spectra of 5a and 5a-D

^{1}H NMR ($CDCl_3$, 300 MHz)



4.3.3. H/D scrambling in electron rich γ-aryl-*allo*-Ile derivative

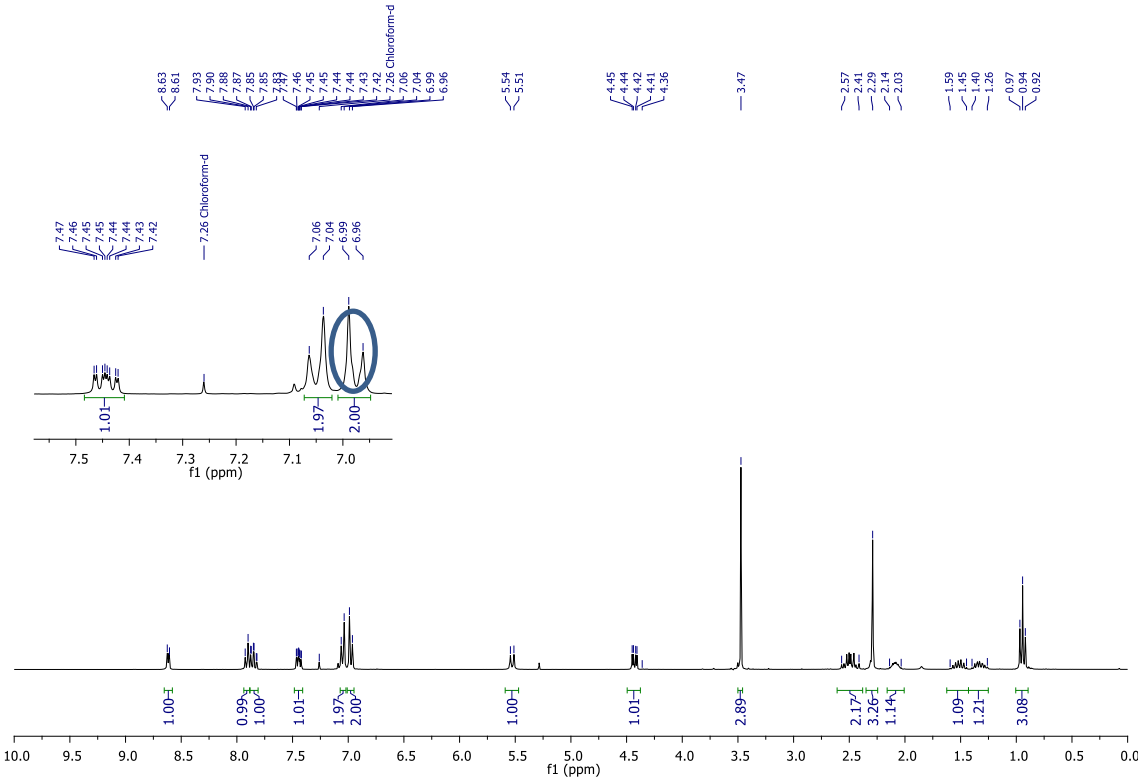


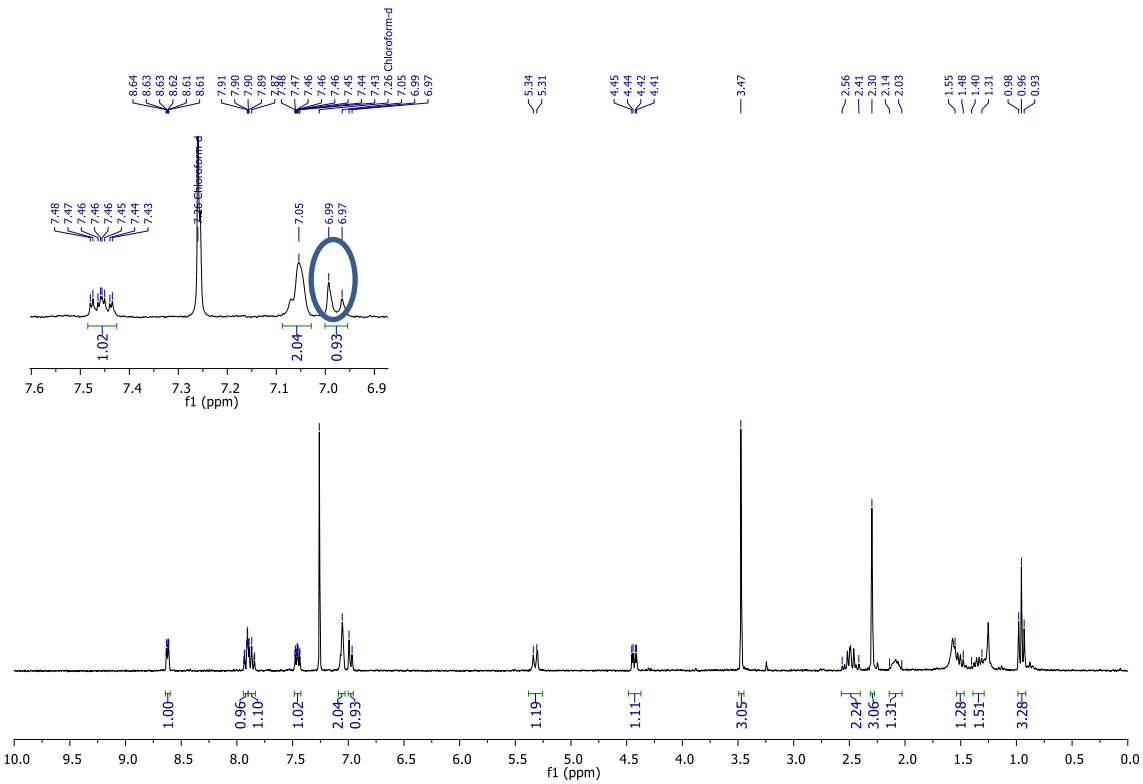
In the **4b-D** spectra, the integration of the doublet at 6.99-6.97 ppm (corresponding to the *o*-aryl positions) was 0.93 instead of 2.00 (54% H/D scrambling).

In the **5b-D** spectra, the integration of the doublet at 7.04-7.01 ppm (corresponding to the *o*-aryl positions) was 0.83 instead of 1.00 (17% H/D scrambling).

Spectra of 4b and 4b-D

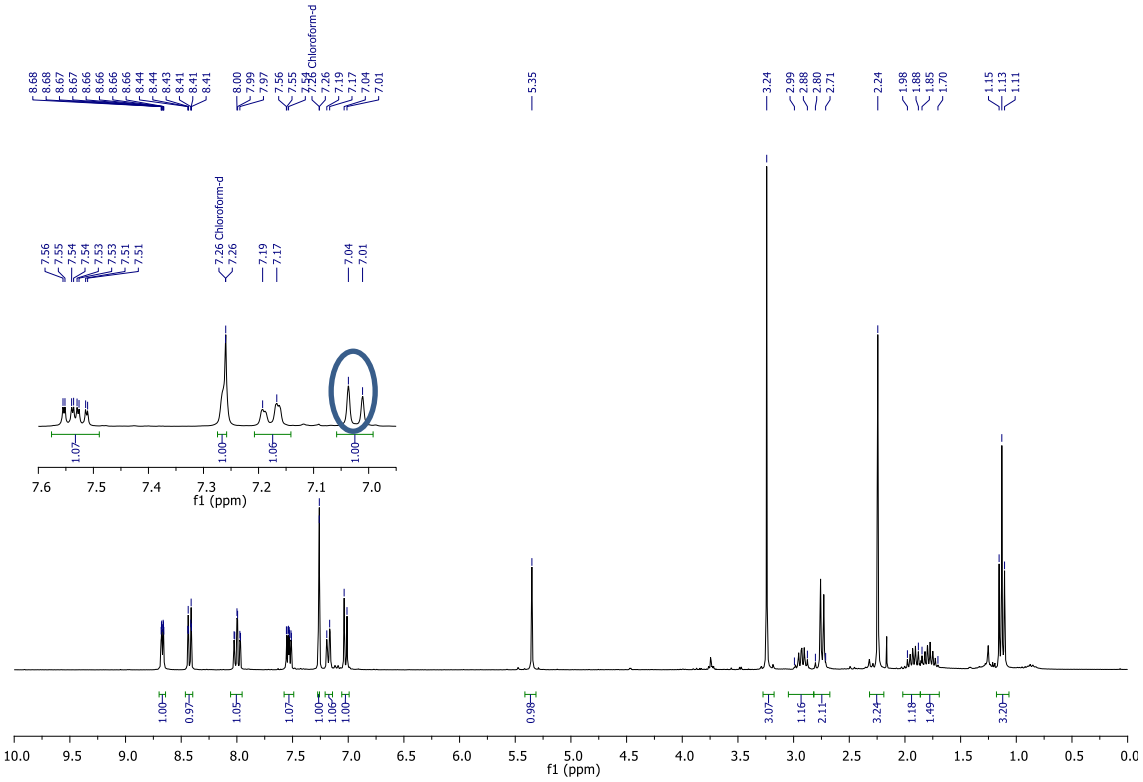
^{1}H NMR ($CDCl_3$, 300 MHz)

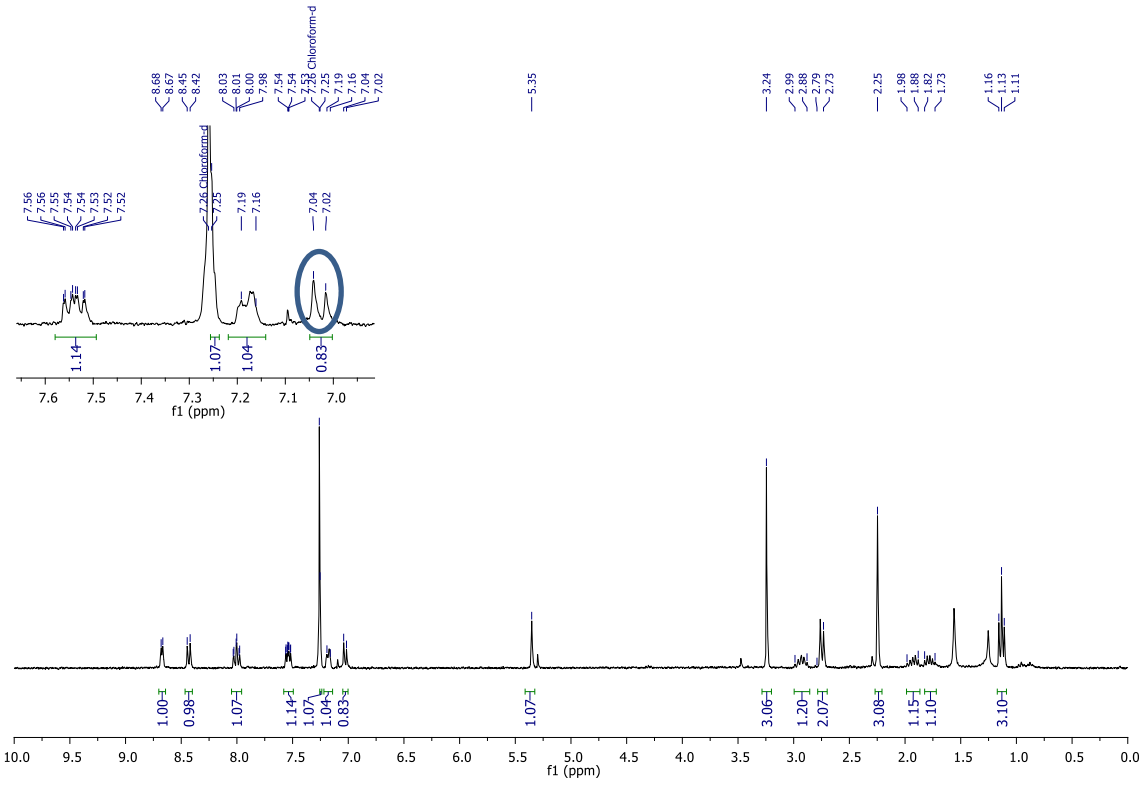




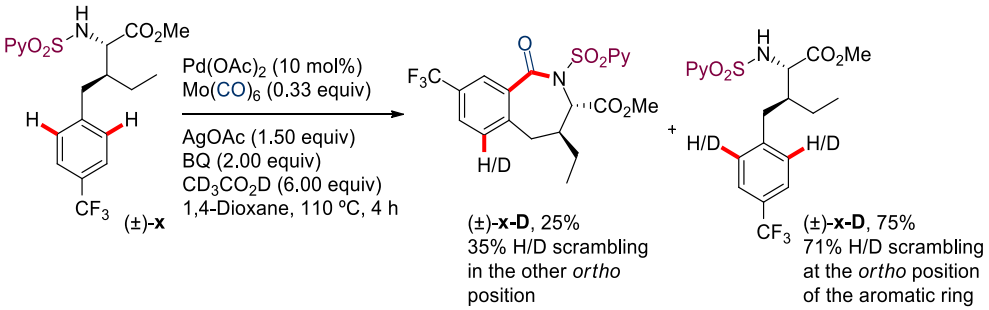
Spectra of 5b and 5b-D

^{1}H NMR ($CDCl_3$, 300 MHz)





4.3.4. H/D scrambling in electron poor γ-aryl-*allo*-Ile derivative

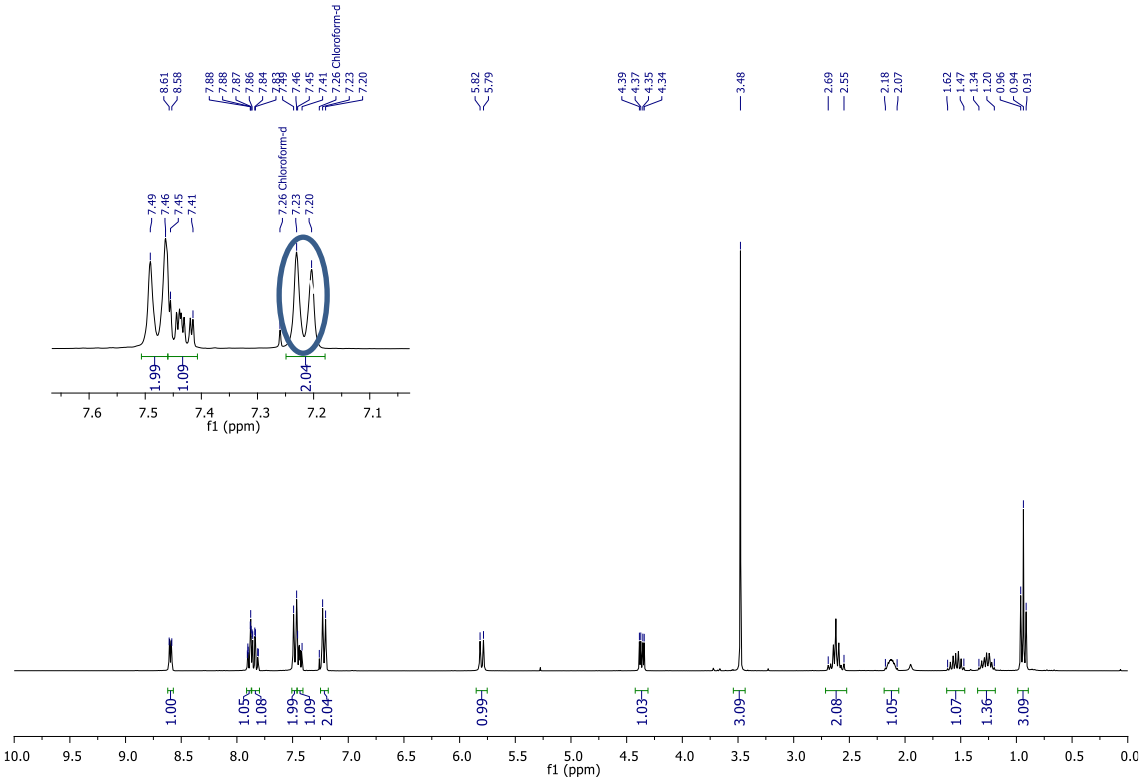


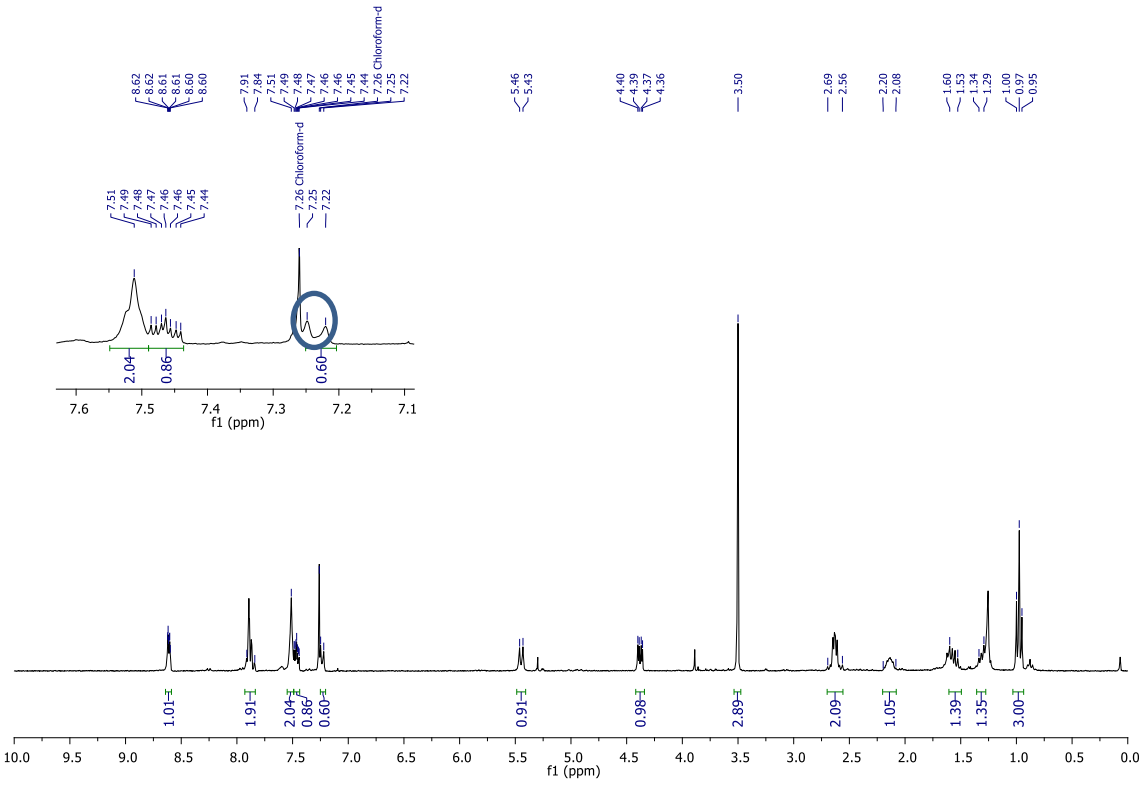
In the **4c-D** spectra, the integration of the doublet at 7.23-7.20 ppm (corresponding to the *o*-aryl positions) was 0.60 instead of 2.04 (71% H/D scrambling).

In the **5c-D** spectra, the integration of the doublet at 7.31-7.29 ppm (corresponding to the *o*-aryl positions) was 0.72 instead of 1.11 (35% H/D scrambling).

Spectra of 4c and 4c-D

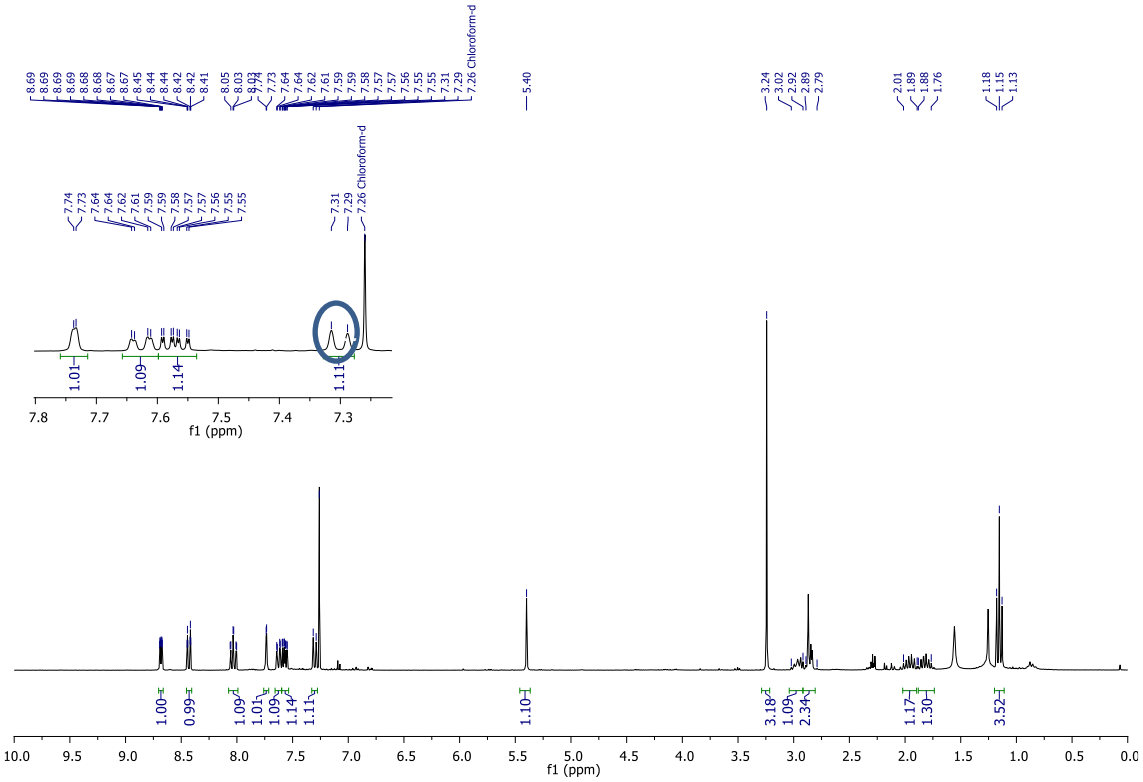
^{1}H NMR ($CDCl_3$, 300 MHz)

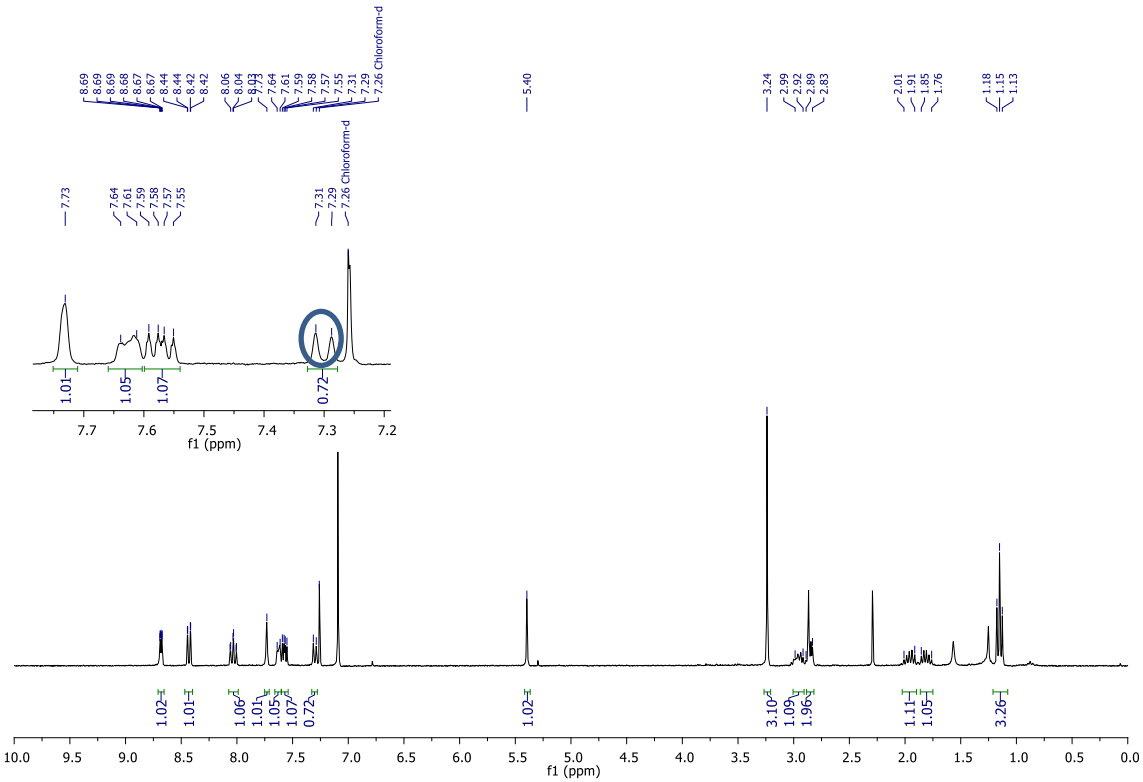




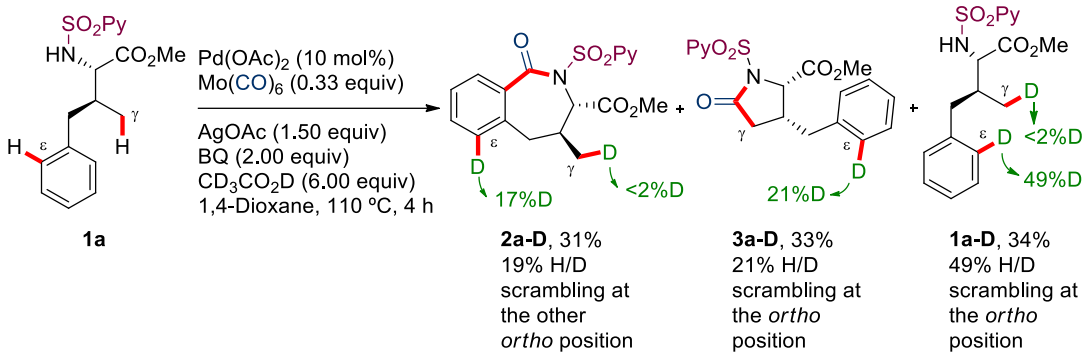
Spectra of 5c and 5c-D

^{1}H NMR ($CDCl_3$, 300 MHz)





4.3.5. H/D scrambling in intramolecular γ vs ε competition



1a

2a-D, 31%
19% H/D scrambling at the other *ortho* position

3a-D, 33%
21% H/D scrambling at the *ortho* position

1a-D, 34%
49% H/D scrambling at the *ortho* position

General procedure. An oven-dried, Ar flushed, pressure tube was charged with $Pd(OAc)_2$ (2.24 mg, 0.010 mmol), AgOAc (25.0 mg, 0.15 mmol), benzoquinone (21.6 mg, 0.20 mmol), $Mo(CO)_6$ (8.67 mg, 0.33 mmol) and (2*S*,3*S*)-methyl 3-(4-benzyl)-2-(pyridine-2-sulfonamido)butanoate **1a** (34.8 mg, 0.10 mmol, 1.00 equiv). The pressure tube was sealed with a rubber septum and flushed with Ar. Under positive pressure of argon, 1,4-dioxane (0.40 mL) and CD_3CO_2D (34.3 µL, 0.60 mmol, 6.00 equiv) were added *via* syringe. The septum was then replaced by a screw cap and finally placed in a preheated oil bath at 110 °C for 4 h. The reaction mixture was then removed from the oil bath and allowed to cool to room temperature. The mixture was then diluted with EtOAc, filtered through a short pad of Celite® and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexane:Et_2O:EtOAc 6:2:3) to afford the pure starting material **1a-D**, the pure benzazepinone **2a-D** and the pure γ-lactam **3a-D** (the corresponding yields and deuterium percentage are shown in the schemes).

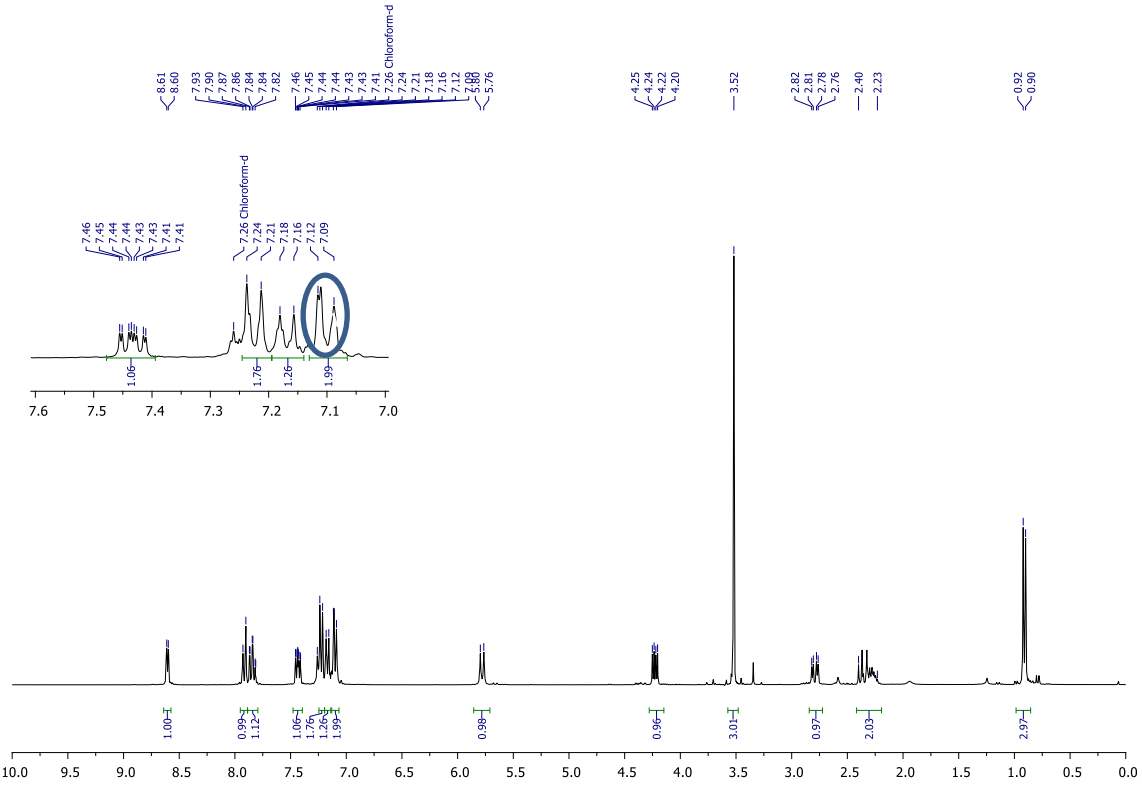
In the **1a-D** spectra, the integration of the doublet at 7.12-7.09 ppm (corresponding to the *o*-aryl positions) was 1.01 instead of 1.99 (49% H/D scrambling). The integration of the doublet at 0.92-0.90 was 3.12, so there is not D incorporation in the γ-methyl group.

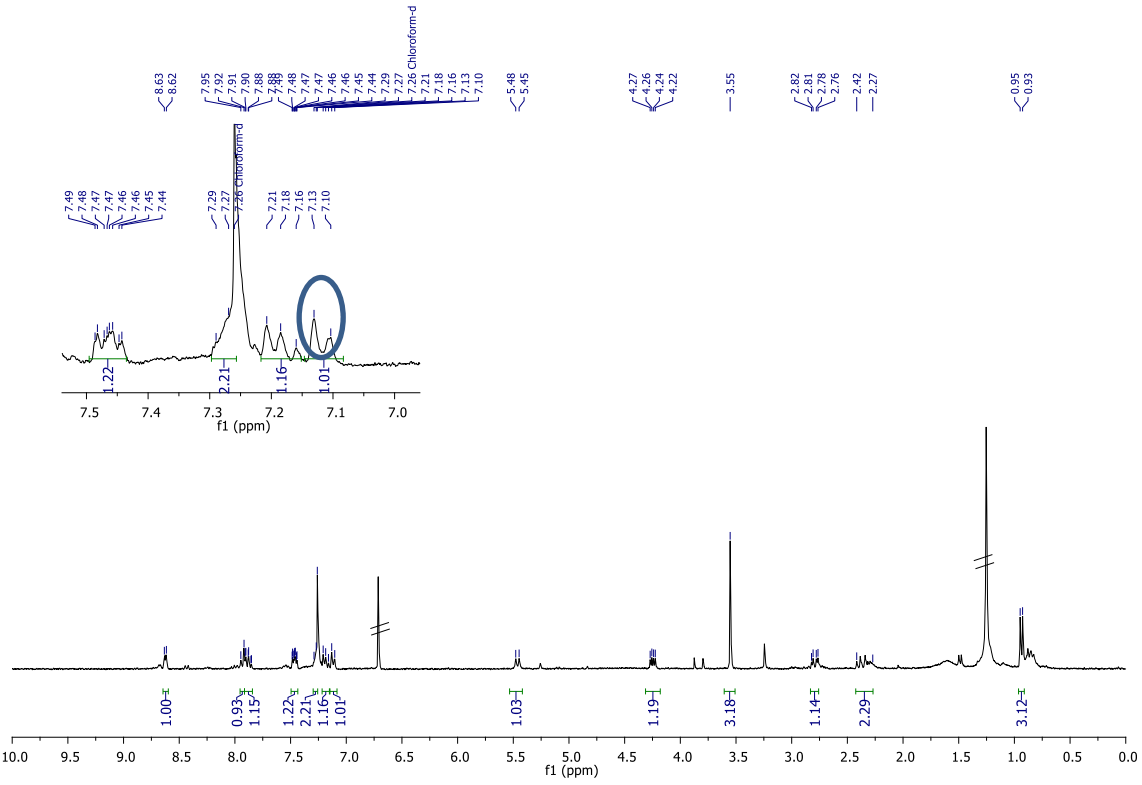
In the **2a-D** spectra, the integration of the doublet at 7.16-7.13 ppm (corresponding to the *o*-aryl positions) was 0.80 instead of 0.99 (19% H/D scrambling). The integration of the doublet at 1.50-1.48 was 3.64, so there is not D incorporation in the γ-methyl group.

In the **3a-D** spectra, the integration of the multiplet at 7.33-7.26 ppm (corresponding to the *o*-aryl positions) was 3.28 instead of 3.95 (17% H/D scrambling). The integration of the signals corresponding to the γ-methylene positions were 0.99, 1.38, 2.60 and 1.44 for the signals at 3.23-3.12, 3.03-2.96, 2.57-2.42 and 2.26-2.18 respectively, so there is not D incorporation in that positions.

Spectra of 1a and 1a-D

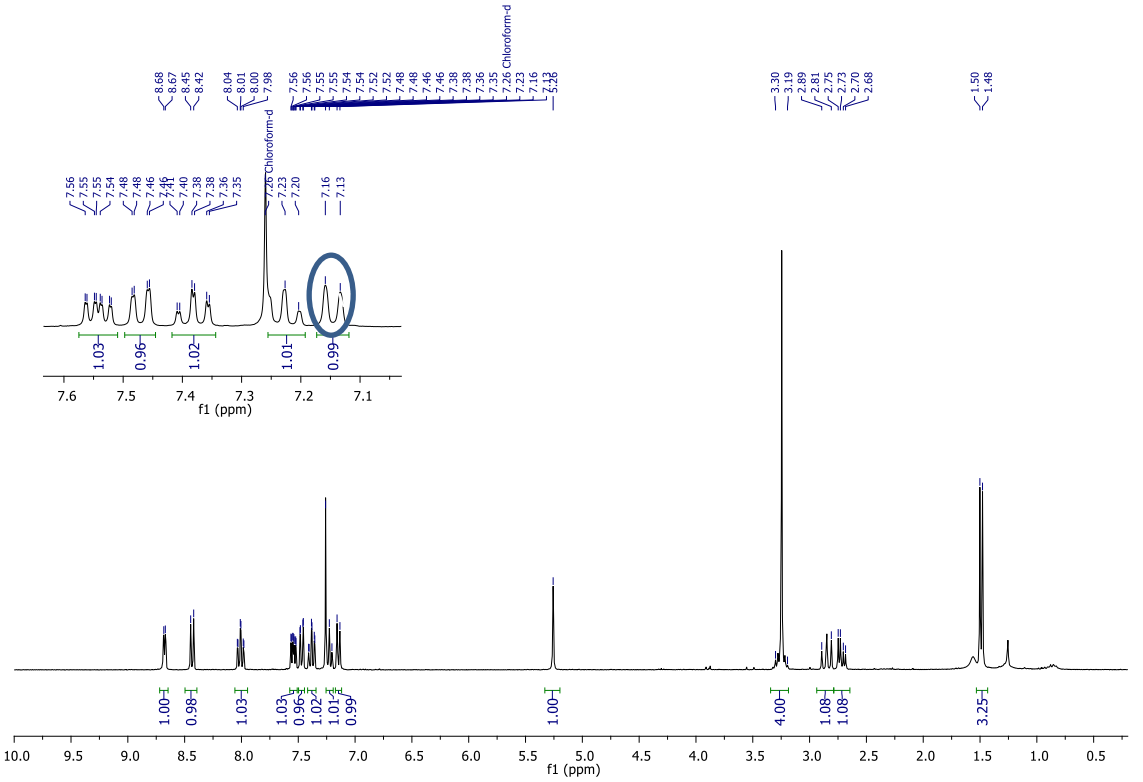
^{1}H NMR ($CDCl_3$, 300 MHz)

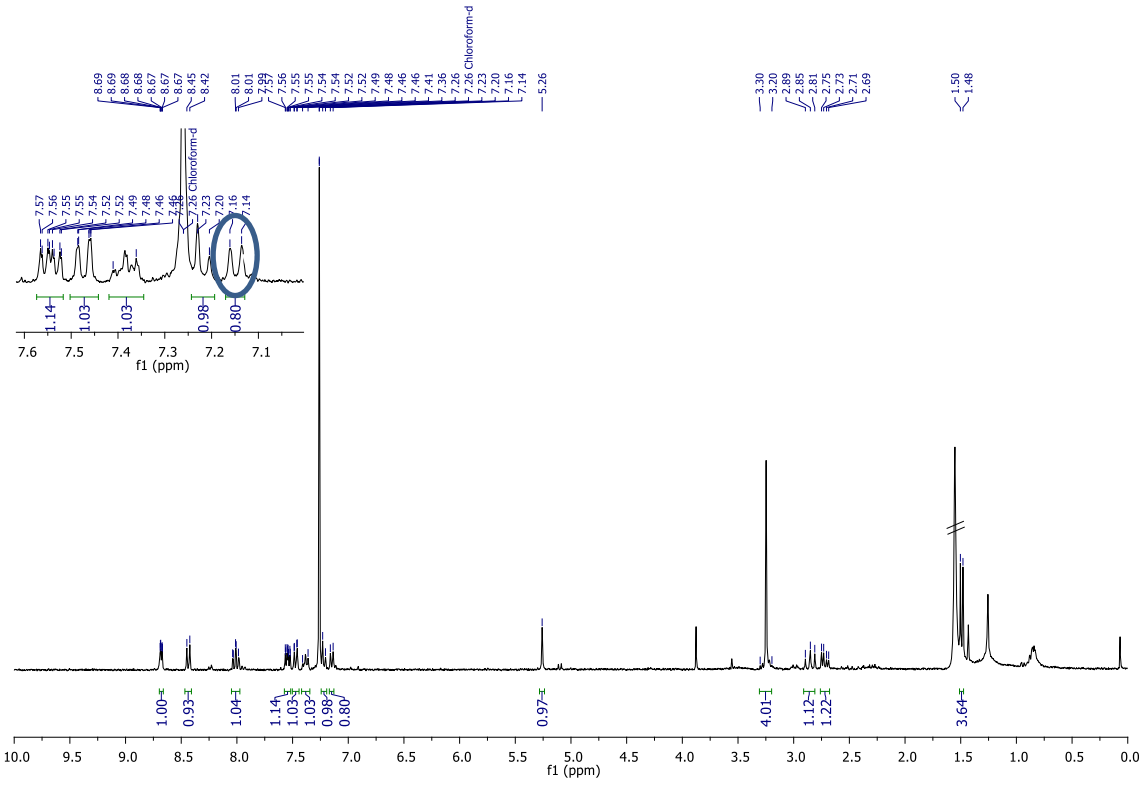




Spectra of 2a and 2a-D

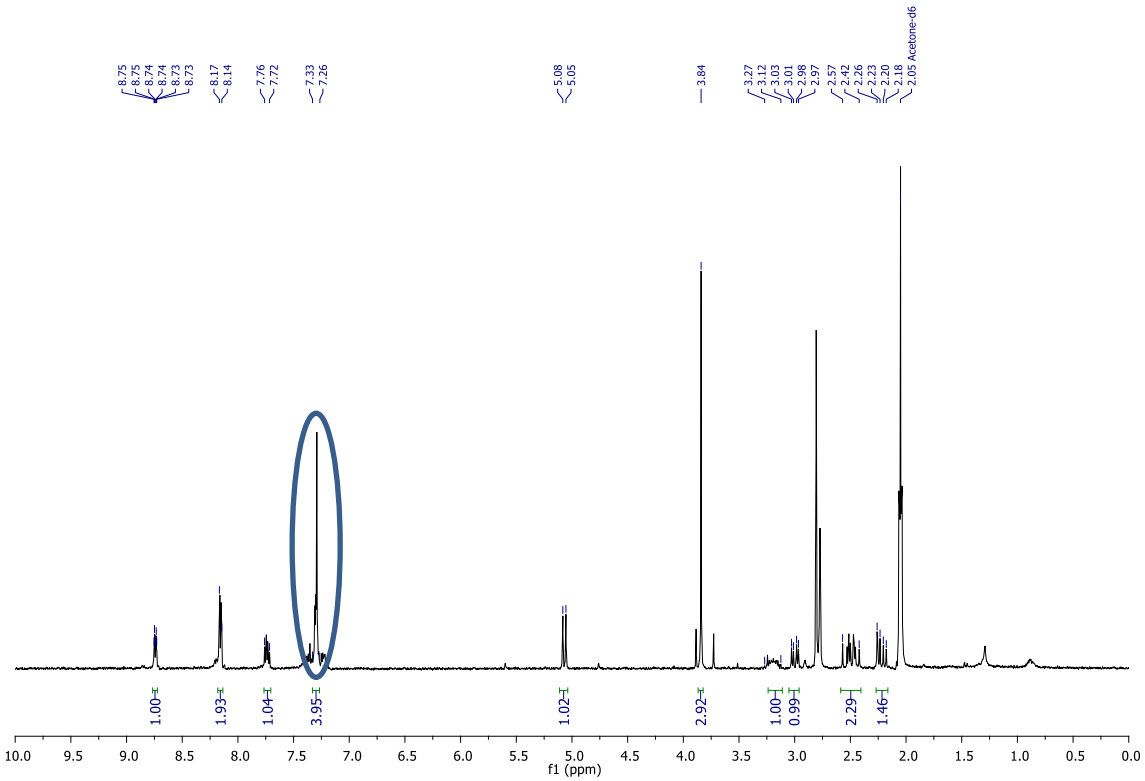
^{1}H NMR ($CDCl_3$, 300 MHz)

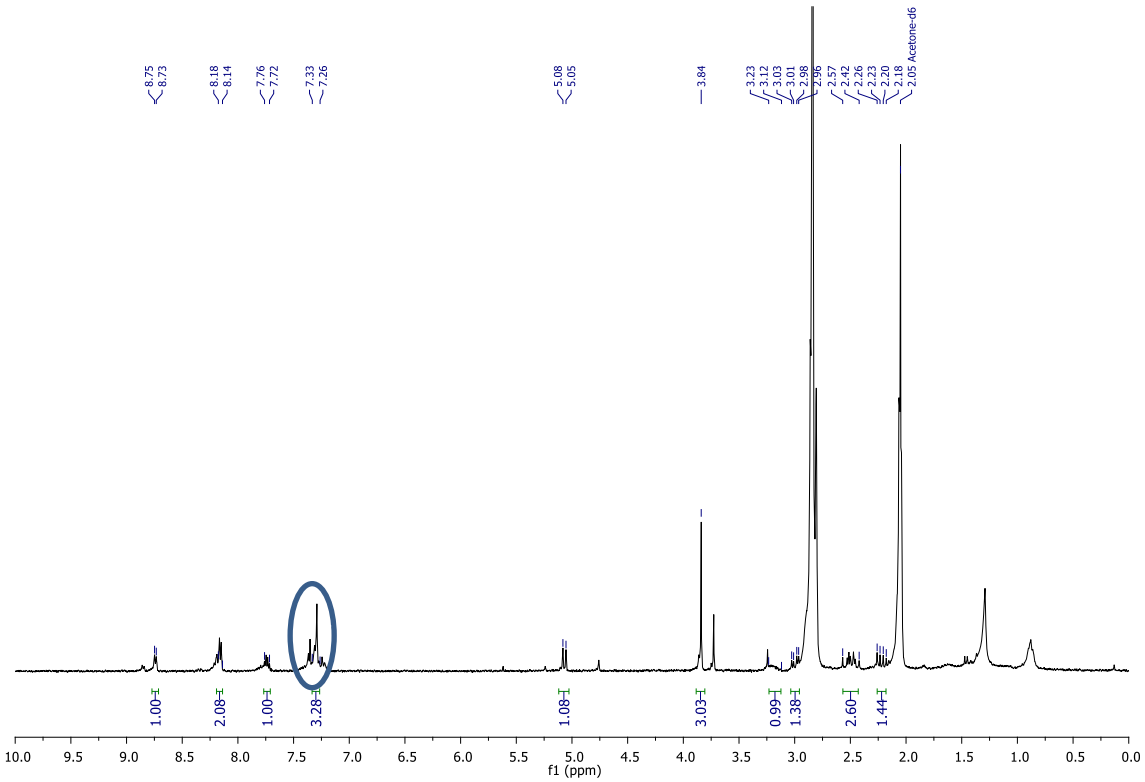




Spectra of 3a and 3a-D

^{1}H NMR ($CO(CD3)_2$, 300 MHz)





5. Theoretical calculations

5.1. Computational details

DFT calculations were performed with Gaussian 09.[5] Geometries were optimized with B3LYP-D3[6] in the gas phase. A mixed basis set of LANL2DZ(f) for Pd and Ag with 6-31G(d) for all other atoms was used in geometry optimizations. The LANL2DZ basis set was supplemented with an f-type polarization function (exponent 1.472 for Pd, 1.611 for Ag).[7] Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE). Single point energies were calculated with the M06 functional[8] and a mixed basis set of SDD for Pd and Ag with 6-311++G(d,p) for all other atoms. Solvation was introduced implicitly in all cases through the SMD[9] model, with 1,4-dioxane as the solvent. Although some experiments are conducted in HFIP, this solvent is not available in Gaussian 09. Instead, the solvation model for 2-propanol was used in M06 single-point energy calculations in these cases. The reported free energies include zero-point energies and thermal corrections calculated at 298 K with B3LYP-D3/LANL2DZ(f)-6-31G(d). Natural charges were calculated at the M06/SDD-6-311++G(d,p) level by means of the Natural Bond Orbital (NBO) analysis of Weinhold *et al.*[10]

5.2. Possible intermediates participating in alternative pathways for the Pd(II) catalysed transformation of substrate 1a into γ-lactam and benzazepinone complexes.

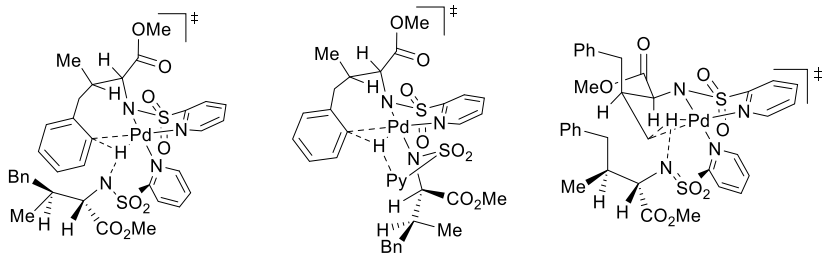


Figure S1. Structures and relative G values (kcal mol^{-1}, at 298 K in 1,4-dioxane) of alternative transition states for the C–H activation step from **IM1-1a**.

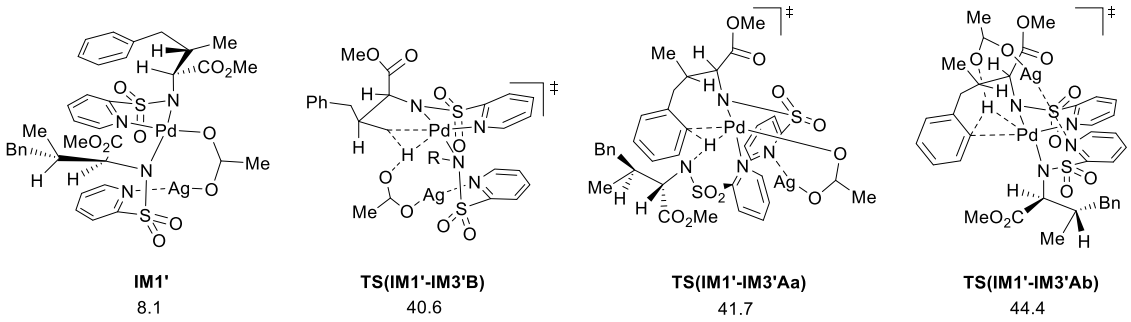


Figure S2. Structures and relative G values (kcal mol^{-1}, at 298 K in 1,4-dioxane) of alternative transition states for the C–H activation step from **IM1-1a** through the formation of bimetallic Pd-Ag complex **IM1'**. Energies are relative to **IM1-1a** + $Ag_2(OAc)_2$ and are mass balanced.

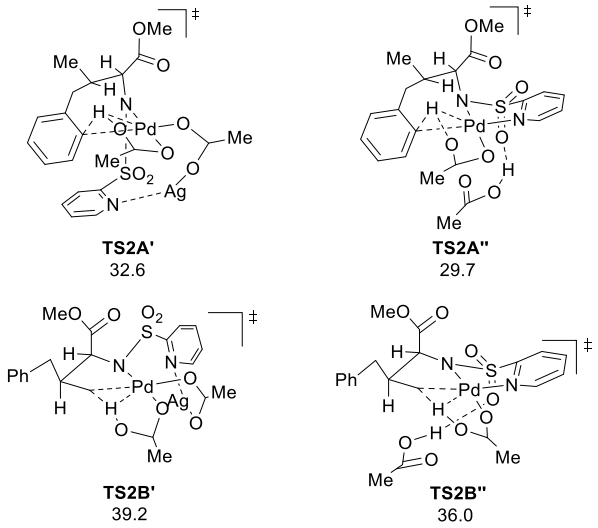


Figure S3. Structures and relative G values (kcal mol^{-1}, at 298 K in 1,4-dioxane) of alternative transition states for the C–H activation step from **IM2-1a** with the participation of AgOAc or HOAc (in the latter case, only the most stable structures are shown, which maintain the Py–Pd interaction). Energies are relative to **IM1-1a** + $Ag_2(OAc)_2$ and are mass balanced.

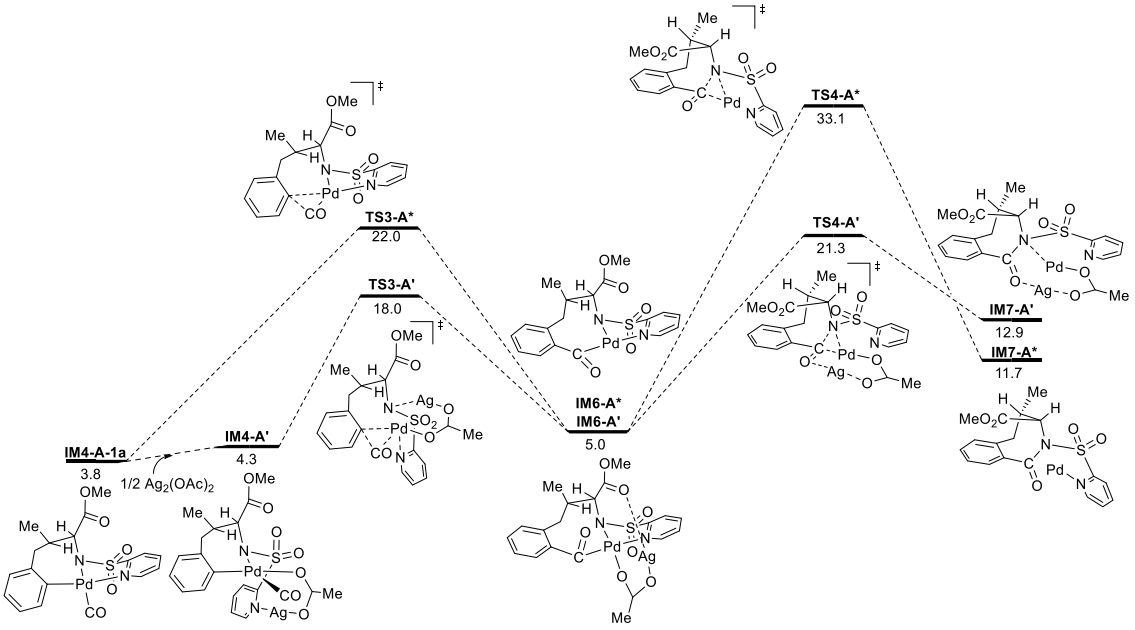


Figure S4. Energy profile for the CO migratory insertion and reductive elimination steps to transform intermediate **IM4-A-1a** into benzazepinone complexes considering the participation of intermediates carrying only one unit of CO or assisted by AgOAc. Energies are relative to **IM1-1a**.

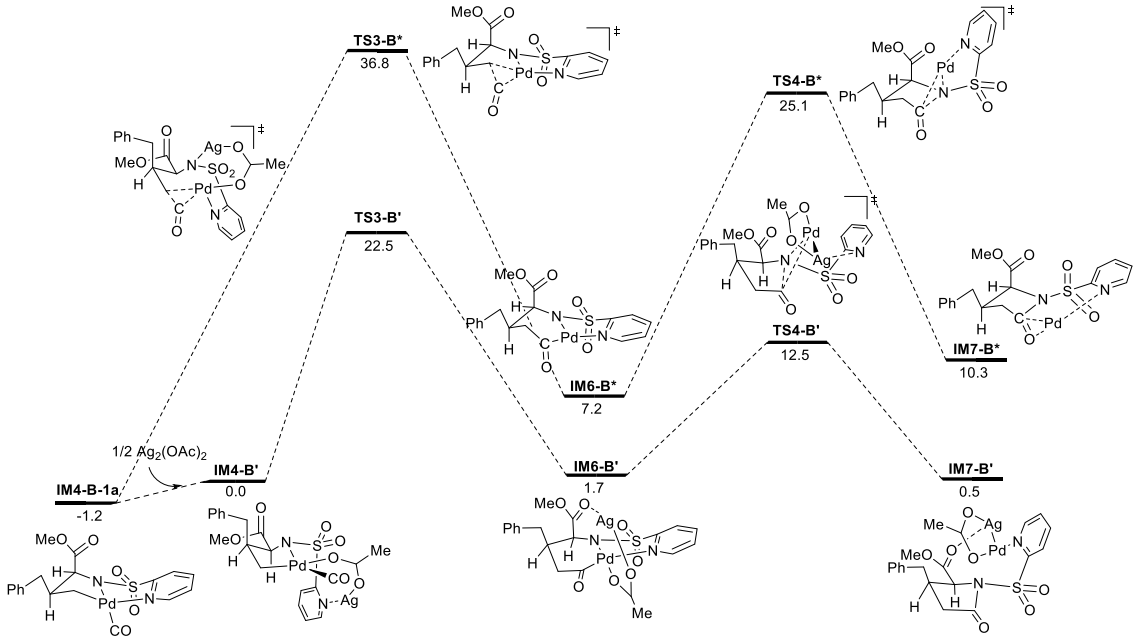


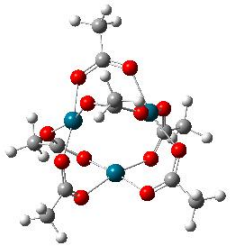
Figure S5. Energy profile for the CO migratory insertion and reductive elimination steps to transform intermediate **IM4-B-1a** into γ-lactam complexes considering the participation of intermediates carrying only one unit of CO or assisted by AgOAc. Energies are relative to **IM1-1a**.

5.3. Comparison of the key steps for the competitive synthesis of benzazepinone versus γ-lactam from 1a, 1b and 1c in 1,4-dioxane and 2-propanol, used as a model for HFIP (*).

		IM1 dissociation			C-H activation			CO coordination			CO insertion	
Ar	**Solvent**	**IM1**	**TS1**	**IM2**	**TS2-A**	**TS2-B**	**IM3-A**	**IM3-B**	**IM4-A**	**IM4-B**	**TS3-A**	**TS3-B**
C_6H_5 (**1a**)	1,4-dioxane	0	18.1 18.3**	13.0	27.1	33.8	17.7	18.8	3.8	-1.2	19.4 19.4**	22.6 23.6**
	HFIP*	0	15.8 16.9**	12.6	26.6	33.1	16.3	18.5	-0.3	-5.2	14.8 13.0**	15.3 14.9**
p-CH_3-C_6H_4 (**1c**)	1,4-dioxane	0	17.6	12.3	26.3	32.7	16.3	17.8	2.5	-2.1	18.1	21.6
	HFIP*	0	15.6	12.1	26.1	32.2	14.9	17.7	-1.4	-5.9	13.6	14.4
p-CF_3-C_6H_4 (**1c**)	1,4-dioxane	0	20.6	12.7	28.6	35.0	18.9	18.9	4.6	-0.1	21.9	25.3
	HFIP*	0	17.9	10.3	25.7	31.9	16.0	16.3	-2.1	-6.6	15.1	15.1

Table S1. Relative G values at 298 K (kcal·mol^{-1}). ($M06_{SMD}$ / 6-311++G(d,p) (C,H,N,O,S,F), SDD (Pd) // B3LYP-D3 / 6-31G(d) (C,H,N,O,S,F), LANL2DZ(f) (Pd)). The effect of including solvent during optimizations was tested by reoptimizing **TS1** and **TS3**, that seem to be more sensitive to solvent effects, for substrate **1a** (**).

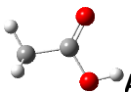
5.4. Cartesian coordinates (Å) and energies (hartrees) of all the optimized structure



$Pd_3(OAc)_6$

E(RB3LYP) = -1751.37803862
G(correction)= 0.245152
$E(RM06)_{dioxane}$ = -1754.44985719
$E(RM06)_{iPrOH}$ = -1754.46798176
Imaginary frequencies: 0

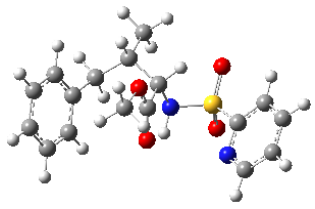
46	0	1.61119	0.92425	0.00545
8	0	2.31509	0.00299	-1.66137
8	0	2.64737	-0.34103	1.22557
8	0	1.15697	1.97807	1.68071
8	0	1.03049	2.44704	-1.22427
6	0	2.2771	-1.24775	-1.86621
6	0	2.22443	-1.35021	1.86424
6	0	0.05938	2.58056	1.87752
6	0	-0.04662	2.58172	-1.87624
8	0	1.59277	-2.11219	-1.2441
6	0	3.18057	-1.77662	-2.96087
8	0	1.15814	-2.00338	1.65838
6	0	3.0961	-1.81482	3.01234
8	0	-1.01818	2.45122	1.22524
6	0	0.02106	3.57263	3.02126
8	0	-1.14695	1.9842	-1.67966
6	0	-0.00376	3.574	-3.01966
46	0	-0.00466	-1.85413	-0.00027
1	0	3.456	-0.97526	-3.64866
1	0	4.09203	-2.16961	-2.49568
1	0	2.6881	-2.5949	-3.49076
1	0	4.12943	-1.90993	2.66649
1	0	3.07918	-1.05085	3.79684
1	0	2.73927	-2.76517	3.41136
46	0	-1.6064	0.93174	-0.00496
1	0	0.99538	3.64496	3.50612
1	0	-0.27888	4.55129	2.63363
1	0	-0.73939	3.25621	3.74202
1	0	-0.97872	3.65379	-3.50205
1	0	0.30475	4.55018	-2.63257
1	0	0.75233	3.25193	-3.74252
8	0	-1.60325	-2.10525	1.24349
8	0	-1.16791	-1.99636	-1.65935
8	0	-2.31509	0.01338	1.66134
8	0	-2.64937	-0.32741	-1.22556
6	0	-2.28351	-1.23767	1.86564
6	0	-2.23099	-1.33802	-1.86506
6	0	-3.19016	-1.76241	2.95964
6	0	-3.10438	-1.7973	-3.01398
1	0	-3.46062	-0.96023	3.64846
1	0	-4.10412	-2.14906	2.49399
1	0	-2.70279	-2.58442	3.48842
1	0	-3.08313	-1.0328	-3.79787
1	0	-2.75217	-2.74913	-3.41357
1	0	-4.13837	-1.88742	-2.6688



AcOH

E(RB3LYP) = -229.08478713
G(correction)= 0.034850
$E(RM06)_{dioxane}$ = -229.0364943
$E(RM06)_{iPrOH}$ = -229.04211179

8	0	0.64608	1.20331	0.00001
6	0	0.09322	0.12698	-0.00006
8	0	0.77586	-1.04831	-0.00001
6	0	-1.39645	-0.10917	0.00001
1	0	1.72236	-0.81171	0.00012
1	0	-1.68104	-0.69246	-0.88187
1	0	-1.68102	-0.69153	0.8825
1	0	-1.91648	0.84889	-0.00048

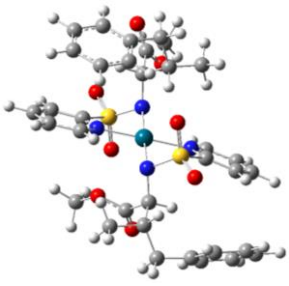


1a

E(RB3LYP) = -1468.43493783
G(correction)= 0.300746
$E(RM06)_{dioxane}$ = -1467.97004579
$E(RM06)_{iPrOH}$ = -1467.98518401
Imaginary frequencies: 0

1	0	-0.65327	0.67099	-1.40071
6	0	0.03913	0.69711	-0.55118
6	0	0.56976	-0.72381	-0.36537
7	0	-0.68419	1.09472	0.66414
6	0	1.15063	1.72358	-0.91455
8	0	0.47232	-1.3643	0.66051
8	0	1.16134	-1.16479	-1.48389
1	0	-0.52001	0.44203	1.43372
16	0	-2.3298	1.40108	0.53966

1	0	1.63916	1.33243	-1.81548
6	0	0.51345	3.07937	-1.24429
6	0	2.21479	1.88248	0.19743
6	0	1.8186	-2.44403	-1.36967
8	0	-2.77157	1.8421	1.85926
8	0	-2.53701	2.21287	-0.66464
6	0	-3.06698	-0.22465	0.19543
1	0	1.28118	3.78629	-1.5788
1	0	0.01524	3.49904	-0.36539
1	0	-0.24184	2.98814	-2.03086
1	0	2.79134	2.78853	-0.03098
1	0	1.70096	2.07972	1.14562
6	0	3.18086	0.72423	0.35106
1	0	2.24613	-2.63775	-2.35341
1	0	1.096	-3.21885	-1.10022
1	0	2.60264	-2.39028	-0.61153
6	0	-3.88216	-0.40051	-0.91989
7	0	-2.74239	-1.17042	1.07136
6	0	4.09151	0.42256	-0.67322
6	0	3.20049	-0.06407	1.50715
6	0	-4.40572	-1.67891	-1.12336
1	0	-4.08297	0.43007	-1.58645
6	0	-3.24605	-2.3895	0.85927
6	0	4.99474	-0.63174	-0.54603
1	0	4.09353	1.0261	-1.57845
6	0	4.10208	-1.12263	1.64139
1	0	2.49243	0.14295	2.30502
6	0	-4.08253	-2.69117	-0.22053
1	0	-5.05027	-1.87938	-1.97453
1	0	-2.96535	-3.15465	1.57929
6	0	5.00439	-1.40911	0.61622
1	0	5.69471	-0.84426	-1.35014
1	0	4.0961	-1.7225	2.54749
1	0	-4.46545	-3.69912	-0.3467
1	0	5.70999	-2.22918	0.7203

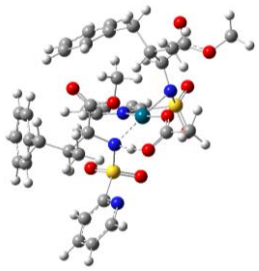


IM1-1a

E(RB3LYP) = -3062.45302679
G(correction)= 0.609762
$E(RM06)_{dioxane}$ = -3062.69751155
$E(RM06)_{iPrOH}$ = -3062.72493604
Imaginary frequencies: 0

6	0	-1.24625	-2.80398	0.13982
1	0	-0.46341	-2.84588	0.88723
6	0	-2.09803	-3.86816	-0.14698
7	0	-1.35256	-1.64491	-0.52469
1	0	-1.99972	-4.79293	0.41049
6	0	-3.07526	-3.7173	-1.13176
6	0	-2.28534	-1.49858	-1.48079
46	0	-0.18835	0.01179	-0.18268
1	0	-3.75707	-4.53176	-1.35798
6	0	-3.17728	-2.50387	-1.81667
16	0	-2.24681	0.14731	-2.27669
7	0	0.98026	1.68322	0.10224
1	0	-3.92681	-2.31707	-2.57761
7	0	-1.78887	1.07997	-0.99232
8	0	-1.1456	0.11016	-3.24937
8	0	-3.62013	0.40534	-2.73074
6	0	0.96766	2.76558	-0.69098
6	0	1.91578	1.56168	1.06042
6	0	-2.9018	1.28265	-0.03539
1	0	0.17782	2.79303	-1.43423
6	0	1.92981	3.76418	-0.54297
16	0	1.7791	-0.01543	1.96775
6	0	2.91954	2.49423	1.25461
1	0	-3.43069	0.34057	0.15209
6	0	-3.98183	2.23341	-0.54474
6	0	-2.37877	1.78676	1.34158
1	0	1.90693	4.62612	-1.20088
6	0	2.9222	3.62108	0.4278
7	0	1.43211	-1.02843	0.69939
8	0	0.58782	0.08148	2.82386
8	0	3.09015	-0.23265	2.59389
1	0	3.68776	2.30466	1.99477
8	0	-3.52592	3.14329	-1.41907
8	0	-5.12497	2.19872	-0.13364
1	0	-1.46351	1.2208	1.54864
6	0	-2.02345	3.27742	1.34639
6	0	-3.37477	1.43036	2.47048
1	0	3.70245	4.36864	0.53132
6	0	2.59742	-1.1653	-0.22071
6	0	-4.52562	4.0256	-1.95337
1	0	-1.38519	3.53503	0.49673
1	0	-2.92202	3.90338	1.29089
1	0	-1.49286	3.53384	2.27026
1	0	-2.96562	1.82715	3.40843
1	0	-4.32774	1.93818	2.28848
6	0	-3.58992	-0.06351	2.59735
6	0	3.67394	-2.17515	0.28048
6	0	2.16993	-1.52415	-1.63914
1	0	3.10058	-0.20104	-0.34814
1	0	-5.28925	3.44921	-2.48252
1	0	-3.99593	4.68396	-2.64252
1	0	-5.0008	4.6017	-1.15392
6	0	-4.76549	-0.66495	2.12674
6	0	-2.57988	-0.88096	3.12742
6	0	5.02306	-1.92214	-0.43937
1	0	3.81922	-1.94033	1.3371
6	0	3.22967	-3.63691	0.17329
8	0	2.73385	-1.09001	-2.6238
8	0	1.1664	-2.41552	-1.69101
1	0	-5.53654	-0.03958	1.68316
6	0	-4.93513	-2.05057	2.19449

6	0	-2.75083	-2.26395	3.20124
1	0	-1.64822	-0.43663	3.46422
1	0	4.91466	-2.13541	-1.50898
1	0	5.75128	-2.64173	-0.04276
6	0	5.53768	-0.50903	-0.24325
1	0	2.24127	-3.77059	0.6244
1	0	3.17217	-3.97203	-0.8687
1	0	3.93987	-4.28735	0.69636
6	0	0.6824	-2.73218	-3.01295
1	0	-5.85359	-2.49957	1.82453
6	0	-3.93042	-2.854	2.73752
1	0	-1.95968	-2.87947	3.62286
6	0	6.03774	-0.10248	1.00197
6	0	5.45697	0.44	-1.27293
1	0	-0.09422	-3.48244	-2.85799
1	0	0.26454	-1.83566	-3.47616
1	0	1.49127	-3.13282	-3.62886
1	0	-4.06462	-3.93137	2.79819
1	0	6.0842	-0.81907	1.81798
6	0	6.45601	1.21189	1.21292
6	0	5.8724	1.75771	-1.06523
1	0	5.03251	0.146	-2.22878
1	0	6.84529	1.5041	2.18501
6	0	6.37662	2.14799	0.17749
1	0	5.80122	2.47779	-1.87667
1	0	6.7098	3.17061	0.33802

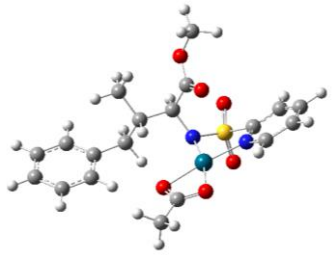


TS1-1a

E(RB3LYP) = -3291.54165576
G(correction)= 0.661349
$E(RM06)_{dioxane}$ = -3291.72189381
$E(RM06)_{iPrOH}$ = -3291.75857715
Imaginary frequencies: 1 (-984.1083 cm^{-1})

6	0	0.12606	1.8565	-1.30999
1	0	-0.60003	1.95759	-0.52047
6	0	0.37633	2.91147	-2.18208
7	0	0.77996	0.68804	-1.4063
1	0	-0.18753	3.82869	-2.05828
6	0	1.34159	2.76124	-3.1743
6	0	1.73142	0.55549	-2.35367
46	0	0.56116	-1.01223	-0.22025
1	0	1.55928	3.57232	-3.8629
6	0	2.04918	1.55998	-3.25206
16	0	2.66584	-1.00877	-2.24676
7	0	2.57166	-1.24432	-0.60497
1	0	2.85017	1.39447	-3.96388
8	0	1.90222	-2.04724	-2.93515
8	0	4.02922	-0.67359	-2.68567
6	0	3.46182	-0.33393	0.1398
1	0	3.37327	0.69661	-0.22247
6	0	4.94585	-0.66722	-0.02291
6	0	3.09498	-0.31822	1.64941
8	0	5.1827	-1.96427	-0.24915
8	0	5.81669	0.17183	0.11119
1	0	2.0022	-0.21124	1.67789
6	0	3.46102	-1.62492	2.36015
6	0	3.68009	0.93147	2.35343
6	0	6.5583	-2.30295	-0.48412
1	0	3.02692	-2.47595	1.82932
1	0	4.54701	-1.76214	2.41101
1	0	3.07916	-1.61739	3.38786
1	0	3.41898	0.86605	3.41817
1	0	4.77237	0.90907	2.28647
6	0	3.13813	2.22105	1.77213
1	0	6.92609	-1.7729	-1.36689
1	0	6.56785	-3.38016	-0.65144
1	0	7.17609	-2.03763	0.37886
6	0	3.85628	2.93828	0.80314
6	0	1.86106	2.67377	2.13123
1	0	4.8361	2.57756	0.50066
6	0	3.30619	4.07483	0.20541
6	0	1.31169	3.81152	1.53849
1	0	1.28161	2.13276	2.8733
1	0	3.87527	4.61437	-0.54751
6	0	2.03212	4.51603	0.57122
1	0	0.32231	4.14412	1.83742
1	0	1.60559	5.40251	0.10782
1	0	-1.82936	1.16333	0.56158
6	0	-2.00159	0.22062	1.07591
7	0	-1.60266	-0.88605	0.16493
6	0	-3.50015	0.22981	1.51117
6	0	-1.13489	0.27498	2.32692
16	0	-2.32452	-0.82908	-1.38123
6	0	-3.91737	1.62892	2.03396
1	0	-4.07735	0.07181	0.59794
6	0	-3.84742	-0.89002	2.49735
8	0	-0.9667	1.29542	2.96704
8	0	-0.64549	-0.91632	2.6892
6	0	-4.0146	-1.47711	-1.19467
8	0	-2.47163	0.57683	-1.79771
8	0	-1.59232	-1.78628	-2.21049
1	0	-3.40968	1.83729	2.98048
1	0	-4.9936	1.58837	2.24743
6	0	-3.62614	2.72658	1.03033
1	0	-3.51814	-1.86419	2.12548
1	0	-3.37676	-0.72012	3.47328
1	0	-4.93105	-0.93016	2.65537
6	0	0.15121	-0.94633	3.88592
7	0	-4.13095	-2.59592	-0.49377
6	0	-5.06097	-0.80201	-1.82421
6	0	-4.37457	2.82464	-0.1509
6	0	-2.5462	3.60192	1.21179
1	0	0.54236	-1.96113	3.94286

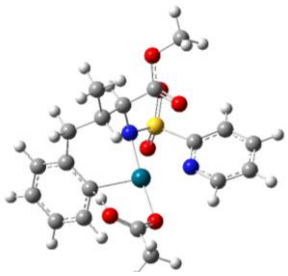
1	0	0.96892	-0.22605	3.81832
1	0	-0.46811	-0.71229	4.75607
6	0	-5.35847	-3.11401	-0.37687
6	0	-6.33405	-1.35917	-1.69873
1	0	-4.87195	0.11709	-2.36646
1	0	-5.20838	2.14417	-0.31156
6	0	-4.05183	3.76435	-1.12919
6	0	-2.221	4.54765	0.23565
1	0	-1.9434	3.50958	2.10987
1	0	-5.43637	-4.02671	0.20912
6	0	-6.48825	-2.5339	-0.96057
1	0	-7.19032	-0.88175	-2.16656
1	0	-4.63886	3.81898	-2.04203
6	0	-2.97184	4.63053	-0.93935
1	0	-1.38018	5.21823	0.39441
1	0	-7.4632	-2.99467	-0.83627
1	0	-2.72235	5.36679	-1.69914
1	0	-1.64741	-2.08997	0.64811
8	0	-1.51744	-3.19613	1.10455
6	0	-0.28632	-3.50543	1.20182
8	0	0.68754	-2.78773	0.83087
6	0	0.04816	-4.8571	1.78813
1	0	-0.72195	-5.16454	2.49908
1	0	0.07808	-5.58826	0.97197
1	0	1.03268	-4.83408	2.26



IM2-1a

E(RB3LYP) = -1823.090569
G(correction)= 0.333707
$E(RM06)_{dioxane}$ = -1823.73313904
$E(RM06)_{iPrOH}$ = -1823.75160052
Imaginary frequencies: 0

46	0	-0.6829	1.31698	-0.07098
7	0	-2.66848	0.84636	-0.01853
7	0	-0.42226	-0.53838	-0.8893
8	0	-0.54196	3.2488	0.76494
6	0	-3.06601	-0.2287	-0.71449
6	0	-3.53441	1.4773	0.79008
6	0	0.14127	-1.6133	-0.05842
16	0	-1.76138	-0.92009	-1.77162
6	0	0.72595	3.21152	0.60773
6	0	-4.3516	-0.74121	-0.63244
1	0	-3.14609	2.334	1.33064
6	0	-4.84839	1.03595	0.91742
6	0	1.59369	-1.25835	0.3665
1	0	0.18435	-2.52576	-0.66157
6	0	-0.73168	-1.92533	1.16041
8	0	-1.98896	-2.37073	-1.83592
8	0	-1.80075	-0.10655	-2.98799
8	0	1.23024	2.15713	0.08805
6	0	1.6019	4.36458	0.99423
6	0	-5.26126	-0.09026	0.20168
1	0	-4.60619	-1.62844	-1.20177
1	0	-5.52767	1.56506	1.5768
6	0	2.46332	-1.08029	-0.90328
6	0	2.17442	-2.32006	1.3113
1	0	1.56601	-0.29854	0.89764
8	0	-1.34157	-1.1044	1.81925
8	0	-0.74237	-3.24274	1.42964
1	0	1.04943	5.07112	1.61652
1	0	2.48519	3.99469	1.52292
1	0	1.94431	4.87237	0.08536
1	0	-6.27868	-0.4581	0.29618
1	0	2.45709	-2.02673	-1.46147
1	0	1.98461	-0.33245	-1.54258
6	0	3.88991	-0.6744	-0.60398
1	0	3.21754	-2.08536	1.53996
1	0	2.14139	-3.3163	0.85371
1	0	1.62696	-2.37053	2.25801
6	0	-1.50194	-3.633	2.58568
6	0	4.18801	0.63991	-0.21252
6	0	4.93886	-1.59992	-0.68608
1	0	-1.10402	-3.15475	3.48555
1	0	-1.40275	-4.71675	2.64926
1	0	-2.55092	-3.34755	2.46637
6	0	5.49828	1.01247	0.08991
1	0	3.38271	1.36579	-0.14952
6	0	6.25164	-1.22935	-0.38532
1	0	4.72368	-2.62192	-0.99089
6	0	6.53593	0.08011	0.00552
1	0	5.71219	2.03651	0.38745
1	0	7.05052	-1.9631	-0.45885
1	0	7.55654	0.37274	0.23853

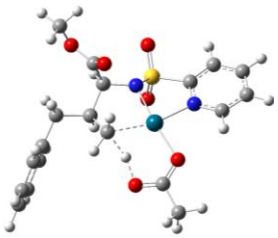


TS2-A-1a

E(RB3LYP) = -1823.06091585
G(correction)= 0.331537
$E(RM06)_{dioxane}$ = -1823.7084183
$E(RM06)_{iPrOH}$ = -1823.72712822
Imaginary frequencies: 1 (-1435.1322 cm^{-1})

46	0	-0.6358	0.72108	0.07814
7	0	0.37507	-0.95083	0.67358
8	0	-1.54978	2.42229	-0.75214

7	0	1.20092	1.74164	0.3703
16	0	1.49729	-0.50434	1.78116
6	0	0.79427	-1.90122	-0.36579
6	0	-2.40577	2.21699	-1.66462
6	0	2.10958	1.06792	1.08489
6	0	1.52953	2.92309	-0.1715
8	0	2.64148	-1.43142	1.79572
8	0	0.83689	-0.12066	3.03148
6	0	-0.32931	-2.06121	-1.42546
1	0	0.97802	-2.87761	0.09537
6	0	2.08203	-1.47936	-1.0816
8	0	-2.90999	1.07603	-1.93692
6	0	-2.88542	3.39321	-2.48212
6	0	3.40159	1.52899	1.29211
1	0	0.74624	3.41391	-0.73898
6	0	2.80124	3.46631	-0.00743
6	0	-1.63067	-2.61178	-0.81805
6	0	0.11931	-2.98288	-2.57363
1	0	-0.52092	-1.06611	-1.84703
8	0	2.32686	-0.3523	-1.4651
8	0	2.90507	-2.52498	-1.27123
1	0	-2.77158	3.16596	-3.54635
1	0	-3.95298	3.54707	-2.29284
1	0	-2.33023	4.29645	-2.2257
6	0	3.75108	2.75734	0.73154
1	0	4.09889	0.92496	1.86201
1	0	3.03979	4.42276	-0.4604
1	0	-1.41821	-3.6001	-0.38785
1	0	-2.31737	-2.80065	-1.65758
6	0	-2.4054	-1.79493	0.20039
1	0	-0.69664	-3.1133	-3.29266
1	0	0.40469	-3.97321	-2.19945
1	0	0.97544	-2.57197	-3.11652
6	0	4.14122	-2.21886	-1.93607
1	0	4.75278	3.1557	0.86505
6	0	-3.21349	-2.49688	1.10323
6	0	-2.43035	-0.37703	0.21724
1	0	3.95239	-1.8121	-2.93413
1	0	4.68211	-3.1633	-2.0002
1	0	4.70945	-1.48739	-1.35493
1	0	-3.19762	-3.58471	1.09664
6	0	-4.02793	-1.83263	2.0199
6	0	-3.27492	0.27306	1.15026
6	0	-4.06997	-0.4363	2.04353
1	0	-4.63193	-2.40814	2.71701
1	0	-3.3057	1.36058	1.15834
1	0	-4.7073	0.08503	2.75238
1	0	-2.5746	0.29534	-1.00771

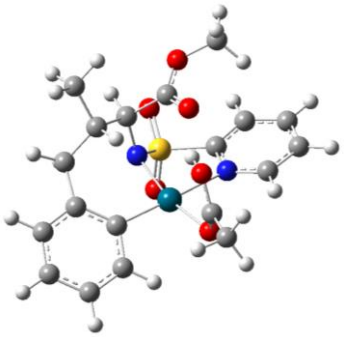


TS2-B-1a

E(RB3LYP) = -1823.0405888
G(correction)= 0.328847
$E(RM06)_{dioxane}$ = -1823.6950166
$E(RM06)_{iPrOH}$ = -1823.71410525
Imaginary frequencies: 1 (-1327.2642 cm^{-1})

46	0	0.88266	0.80198	-0.43012
7	0	0.8803	-1.16096	0.03943
7	0	2.92671	0.64682	-0.00789
8	0	1.08776	2.81808	-0.93136
6	0	-0.42741	-1.82748	0.09688
16	0	1.88067	-1.43571	1.31761
6	0	3.26838	-0.45043	0.68181
6	0	3.88372	1.48239	-0.44103
6	0	0.0602	3.52125	-0.66989
6	0	-1.53518	-0.74986	0.2237
1	0	-0.49524	-2.51829	0.94301
6	0	-0.6087	-2.64248	-1.18267
8	0	2.30526	-2.84203	1.38266
8	0	1.4599	-0.79238	2.57623
6	0	4.58408	-0.78954	0.96098
1	0	3.53572	2.35425	-0.98413
6	0	5.2304	1.22528	-0.19355
8	0	-1.03804	3.02993	-0.26936
6	0	0.1482	5.01824	-0.84859
6	0	-1.2711	0.39312	-0.77781
6	0	-2.95537	-1.35182	0.07149
1	0	-1.44237	-0.35955	1.24417
8	0	-0.34388	-2.26344	-2.30288
8	0	-1.16699	-3.84081	-0.9097
6	0	5.5852	0.07236	0.51036
1	0	4.79483	-1.70424	1.50414
1	0	5.98321	1.9169	-0.55628
1	0	-0.93267	1.70532	-0.37388
1	0	1.14058	5.31509	-1.19038
1	0	-0.60881	5.33816	-1.57148
1	0	-0.0826	5.50603	0.10366
1	0	-2.19912	0.97001	-0.90538
1	0	-1.0462	0.01571	-1.78108
1	0	-3.09783	-1.68309	-0.96477
1	0	-3.02711	-2.24836	0.70066
6	0	-4.03964	-0.36811	0.44966
6	0	-1.43959	-4.66572	-2.05531
1	0	6.62945	-0.15375	0.70443
6	0	-4.8159	0.26986	-0.52635
6	0	-4.25944	-0.0417	1.79602
1	0	-2.13452	-4.16208	-2.73389
1	0	-1.88169	-5.58064	-1.65995

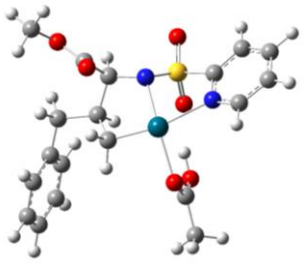
1	0	-0.5145	-4.88481	-2.59554
6	0	-5.78462	1.21177	-0.17024
1	0	-4.66017	0.02442	-1.57467
6	0	-5.22565	0.89669	2.15657
1	0	-3.66534	-0.5294	2.56611
6	0	-5.99198	1.52824	1.17273
1	0	-6.37624	1.69587	-0.94293
1	0	-5.38219	1.13488	3.20542
1	0	-6.74513	2.25989	1.45262



IM3-A-1a

E(RB3LYP) = -1823.0809401
G(correction)= 0.337756
$E(RM06)_{dioxane}$ = -1823.72961262
$E(RM06)_{iPrOH}$ = -1823.74981851
Imaginary frequencies: 0

46	0	0.52468	0.55716	-0.60414
7	0	-0.30959	-1.3202	-0.56859
6	0	2.39841	-0.14108	-0.58835
8	0	1.20564	2.59314	-0.02376
16	0	-1.6238	-1.36259	-1.55047
6	0	-0.46076	-1.87525	0.786
6	0	2.86091	-1.40375	-0.15954
6	0	3.3075	0.77833	-1.1364
6	0	1.41923	2.8006	1.17865
6	0	-2.48519	0.18839	-1.105
8	0	-2.54223	-2.45708	-1.20206
8	0	-1.18946	-1.16935	-2.93565
6	0	0.92686	-2.05537	1.44346
1	0	-0.96472	-2.8439	0.70698
6	0	-1.32501	-0.96589	1.66938
6	0	1.98568	-2.5071	0.41304
6	0	4.23468	-1.67715	-0.28237
6	0	4.6656	0.47563	-1.26276
1	0	2.95745	1.74906	-1.47739
8	0	0.9852	2.04896	2.1683
6	0	2.2583	3.96292	1.6307
7	0	-1.666	1.19951	-0.78744
6	0	-3.87154	0.29267	-1.08903
6	0	0.81168	-3.03414	2.62127
1	0	1.23208	-1.08	1.83951
8	0	-0.98214	0.12207	2.11851
8	0	-2.55107	-1.45756	1.86383
1	0	1.48415	-3.02967	-0.41093
1	0	2.64268	-3.24257	0.89213
1	0	4.60311	-2.64385	0.05645
6	0	5.13307	-0.76257	-0.82818
1	0	5.34525	1.20497	-1.69733
1	0	0.42246	1.27951	1.87336
1	0	1.92054	4.34154	2.59769
1	0	3.28984	3.60715	1.74267
1	0	2.24374	4.74704	0.87244
6	0	-2.2005	2.38277	-0.45551
6	0	-4.42678	1.52491	-0.74166
1	0	-4.47415	-0.57584	-1.33057
1	0	1.75432	-3.08155	3.17697
1	0	0.57433	-4.04566	2.26932
1	0	0.02556	-2.73186	3.32519
6	0	-3.46993	-0.6085	2.57772
1	0	6.18689	-1.0165	-0.90957
1	0	-1.49178	3.16655	-0.20642
6	0	-3.57875	2.58931	-0.4247
1	0	-5.50518	1.65389	-0.71609
1	0	-3.08202	-0.37374	3.57227
1	0	-4.39603	-1.17881	2.64562
1	0	-3.62814	0.32028	2.0225
1	0	-3.97419	3.56121	-0.14842



IM3-B-1a

E(RB3LYP) = -1823.06884904
G(correction)= 0.332939
$E(RM06)_{dioxane}$ = -1823.72310919
$E(RM06)_{iPrOH}$ = -1823.74142163
Imaginary frequencies: 0

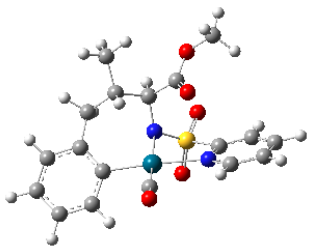
46	0	0.79001	0.44981	-0.9261
7	0	0.89356	-1.29165	0.17251
7	0	3.01367	0.48803	-0.4078
8	0	0.50864	2.52879	-1.43449
6	0	-0.434	-1.90575	0.38177
16	0	1.64809	-0.75877	1.52583
6	0	3.18434	-0.23654	0.7065
6	0	4.10365	0.94158	-1.04119
6	0	0.32199	3.29237	-0.47647
6	0	-1.50777	-0.78869	0.29116
1	0	-0.48584	-2.42351	1.34549
6	0	-0.6437	-2.94356	-0.71474
8	0	1.96298	-1.83099	2.48267
8	0	1.07428	0.49241	2.1195
6	0	4.42249	-0.55087	1.2486
1	0	3.92357	1.5159	-1.9449

6	0	5.39368	0.68843	-0.57343
8	0	0.3681	2.95684	0.79783
6	0	0.00023	4.74658	-0.68586
6	0	-1.19364	0.0722	-0.94368
6	0	-2.96753	-1.30473	0.31418
1	0	-1.35671	-0.17594	1.18861
8	0	-0.27586	-2.85131	-1.86428
8	0	-1.3751	-3.98086	-0.2445
6	0	5.55436	-0.06964	0.58737
1	0	4.47596	-1.15638	2.14642
1	0	6.25006	1.07509	-1.11603
1	0	0.58048	1.9955	0.96485
1	0	0.04652	4.98967	-1.74737
1	0	-1.005	4.94882	-0.30061
1	0	0.69937	5.3682	-0.11826
1	0	-1.77181	1.00146	-0.95742
1	0	-1.36214	-0.47856	-1.87716
1	0	-3.16663	-1.87861	-0.59906
1	0	-3.08503	-2.00172	1.15414
6	0	-3.95909	-0.16965	0.43824
6	0	-1.72064	-4.97632	-1.2215
1	0	6.54695	-0.28764	0.9705
6	0	-4.66563	0.3042	-0.67443
6	0	-4.14973	0.47082	1.67124
1	0	-2.31444	-4.5335	-2.02684
1	0	-2.30065	-5.72725	-0.684
1	0	-0.81843	-5.41965	-1.65208
6	0	-5.53969	1.38797	-0.56145
1	0	-4.52692	-0.18042	-1.63819
6	0	-5.02094	1.55388	1.7898
1	0	-3.60711	0.11506	2.54471
6	0	-5.71982	2.01718	0.67167
1	0	-6.08015	1.73875	-1.43706
1	0	-5.15699	2.03434	2.75538
1	0	-6.40113	2.85909	0.76257

CO

E(RB3LYP) = -113.30945509
G(correction)= -0.014107
$E(RM06)_{dioxane}$ = -113.28066693
$E(RM06)_{iPrOH}$ = -113.27784493

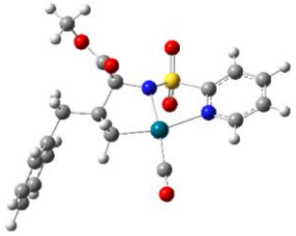
6	0	0.	0.	-0.65026
8	0	0.	0.	0.48769



IM4-A-1a

E(RB3LYP) = -1707.30685236
G(correction)= 0.283836
$E(RM06)_{dioxane}$ = -1707.99103113
$E(RM06)_{iPrOH}$ = -1708.0069701
Imaginary frequencies: 0

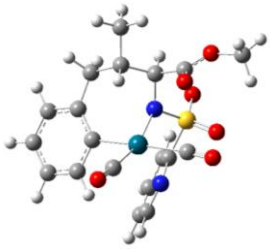
46	0	0.62973	-0.93294	-0.27119
7	0	-0.03641	0.66245	0.85712
6	0	2.56734	-0.34785	0.01232
6	0	1.18295	-2.21245	-1.58018
16	0	-1.15835	0.12393	1.91545
6	0	-0.33374	1.90561	0.13597
6	0	3.01719	0.97832	0.15449
6	0	3.47198	-1.40961	0.18862
8	0	1.43026	-2.9285	-2.43737
6	0	-2.20256	-0.93856	0.85746
8	0	-2.03401	1.20482	2.39321
8	0	-0.52314	-0.80144	2.85851
6	0	0.89328	2.29134	-0.72278
1	0	-0.52597	2.70154	0.86284
6	0	-1.55492	1.79417	-0.78217
6	0	2.17836	2.24888	0.12722
6	0	4.38502	1.17463	0.42933
6	0	4.81626	-1.18534	0.48654
1	0	3.13291	-2.43852	0.11495
7	0	-1.54007	-1.58653	-0.10795
6	0	-3.57382	-1.04561	1.05068
6	0	0.69814	3.68427	-1.34257
1	0	0.97044	1.55732	-1.53539
8	0	-1.73318	0.90444	-1.59237
8	0	-2.40781	2.8188	-0.60906
1	0	1.91492	2.49742	1.16491
1	0	2.83565	3.05812	-0.21319
1	0	4.74625	2.19638	0.53152
6	0	5.27975	0.1232	0.59701
1	0	5.48795	-2.02923	0.62081
6	0	-2.22917	-2.38942	-0.93043
6	0	-4.28923	-1.88371	0.19534
1	0	-4.04543	-0.47147	1.84049
1	0	1.53548	3.92406	-2.00658
1	0	0.65185	4.45538	-0.56373
1	0	-0.22362	3.75101	-1.93019
6	0	-3.58298	2.78732	-1.43661
1	0	6.32547	0.32588	0.81232
1	0	-1.65846	-2.88663	-1.70826
6	0	-3.60533	-2.56961	-0.80977
1	0	-5.36378	-1.99662	0.30715
1	0	-3.30951	2.81729	-2.49537
1	0	-4.15971	3.67027	-1.16075
1	0	-4.15601	1.87566	-1.24405
1	0	-4.12501	-3.22539	-1.50024



IM4-B-1a

E(RB3LYP) = -1707.30958426
G(correction)= 0.281392
$E(RM06)_{dioxane}$ = -1707.99652209
$E(RM06)_{iPrOH}$ = -1708.01233813
Imaginary frequencies: 0

46	0	-0.76484	-1.02629	-0.61001
7	0	-0.86748	0.88206	0.11837
6	0	1.24487	-0.56088	-0.77823
6	0	-0.46259	-2.76477	-1.31315
6	0	0.41621	1.59502	0.19083
16	0	-1.82588	0.96171	1.44125
6	0	1.52577	0.52062	0.27843
1	0	1.89886	-1.42609	-0.6542
1	0	1.32895	-0.17196	-1.79745
8	0	-0.25119	-3.81917	-1.70791
1	0	0.46554	2.26961	1.05129
6	0	0.57929	2.43919	-1.07128
6	0	-3.2444	0.07886	0.72008
8	0	-2.2569	2.33893	1.73355
8	0	-1.36244	0.14306	2.57946
6	0	2.96462	1.08508	0.16085
1	0	1.41468	0.0765	1.27522
8	0	0.25175	2.10973	-2.19013
8	0	1.21419	3.59738	-0.78738
7	0	-2.96276	-0.94379	-0.09929
6	0	-4.53683	0.44851	1.07109
1	0	3.1172	1.48346	-0.84989
1	0	3.06212	1.93382	0.84987
6	0	4.01464	0.04185	0.47063
6	0	1.49487	4.43639	-1.92066
6	0	-3.98174	-1.65681	-0.60398
6	0	-5.5922	-0.2993	0.54963
1	0	-4.6866	1.30392	1.72054
6	0	4.71451	-0.61136	-0.55187
6	0	4.27375	-0.32687	1.79848
1	0	2.13845	3.91389	-2.63478
1	0	1.99997	5.31487	-1.51812
1	0	0.56671	4.72044	-2.42414
1	0	-3.71224	-2.46925	-1.27123
6	0	-5.3109	-1.37128	-0.29926
1	0	-6.61892	-0.04625	0.79709
6	0	5.64865	-1.6076	-0.25841
1	0	4.52459	-0.33582	-1.58691
6	0	5.20584	-1.32079	2.097
1	0	3.73807	0.17184	2.60365
1	0	-6.1036	-1.97506	-0.72814
6	0	5.89712	-1.96567	1.06776
1	0	6.18274	-2.10149	-1.06614
1	0	5.39473	-1.59035	3.13287
1	0	6.62487	-2.73895	1.29873

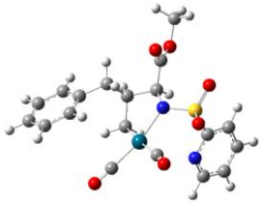


IM5-A-1a

E(RB3LYP) = -1820.6259794
G(correction)= 0.286344
$E(RM06)_{dioxane}$ = -1821.28290553
Imaginary frequencies: 0

46	0	-0.09997	0.60107	1.13611
7	0	0.59826	-0.2197	-0.65855
6	0	-1.55836	1.39546	-0.06564
6	0	-0.71451	1.82242	2.50187
6	0	1.33067	-0.42441	2.32105
16	0	0.74564	-1.85833	-0.72334
6	0	1.69636	0.54402	-1.26779
6	0	-1.35738	1.95891	-1.33424
6	0	-2.85976	1.19122	0.41921
8	0	-1.02971	2.60491	3.27111
8	0	2.0433	-0.92697	3.04664
6	0	-0.98106	-2.31222	-0.40479
8	0	1.55289	-2.40403	0.39329
8	0	1.07672	-2.29162	-2.09249
6	0	1.3121	2.0317	-1.34489
1	0	1.87535	0.15765	-2.27845
6	0	2.96779	0.35084	-0.43332
6	0	-0.03667	2.22621	-2.05292
6	0	-2.50572	2.30993	-2.07182
6	0	-3.97922	1.52915	-0.3408
1	0	-3.01266	0.74021	1.39563
7	0	-1.45982	-1.95865	0.78619
6	0	-1.70288	-2.98411	-1.38725
6	0	2.41294	2.8146	-2.07911
1	0	1.24973	2.41533	-0.31857
8	0	3.14732	0.84571	0.66653
8	0	3.81948	-0.50005	-1.01762
1	0	-0.02765	1.61383	-2.96682
1	0	-0.07756	3.26686	-2.40271
1	0	-2.36665	2.75	-3.05807
6	0	-3.79692	2.09998	-1.5996
1	0	-4.97695	1.35263	0.05277
6	0	-2.7352	-2.26487	1.04814
6	0	-3.02949	-3.3042	-1.09594
1	0	-1.23206	-3.22875	-2.33205
1	0	2.19058	3.88719	-2.07796
1	0	2.49764	2.48867	-3.12345
1	0	3.38891	2.67916	-1.60055

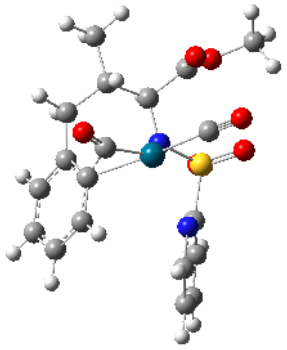
6	0	4.89876	-0.97206	-0.18921
1	0	-4.65179	2.38154	-2.2087
1	0	-3.1106	-1.9577	2.02159
6	0	-3.55754	-2.93806	0.14247
1	0	-3.64103	-3.82677	-1.82595
1	0	5.49154	-0.13486	0.18846
1	0	5.49801	-1.61626	-0.83239
1	0	4.48669	-1.54147	0.64814
1	0	-4.58581	-3.16532	0.4056



IM5-B-1a

E(RB3LYP) = -1820.63212245
G(correction)= 0.284389
$E(RM06)_{dioxane}$ = -1821.29377572
Imaginary frequencies: 0

46	0	-0.3343	-1.27379	0.31925
6	0	-1.62281	-2.60759	-0.17094
6	0	0.49141	-2.27362	1.99293
7	0	0.72905	0.48756	0.60762
6	0	-0.99753	-0.1577	-1.30748
8	0	-2.40323	-3.37753	-0.49311
8	0	0.81826	-2.91648	2.8698
6	0	0.40317	1.58762	-0.31744
16	0	2.32164	0.36535	0.98264
6	0	-1.01867	1.29505	-0.83791
1	0	-0.20869	-0.34231	-2.04472
1	0	-1.95918	-0.4835	-1.70447
1	0	1.07974	1.60969	-1.18418
6	0	0.48959	2.95089	0.37254
6	0	3.08185	-0.47218	-0.45283
8	0	2.46212	-0.56192	2.11706
8	0	2.94564	1.69866	1.02519
6	0	-2.11456	1.5921	0.22468
1	0	-1.21428	1.93297	-1.71456
8	0	0.13556	3.19272	1.50244
8	0	0.95006	3.88097	-0.49256
7	0	2.54283	-1.64592	-0.78125
6	0	4.1451	0.12593	-1.12539
1	0	-2.23095	2.67863	0.3035
1	0	-1.75796	1.25542	1.20209
6	0	-3.44087	0.94746	-0.1013
6	0	1.06723	5.20497	0.05363
6	0	3.06588	-2.29266	-1.82775
6	0	4.68261	-0.5603	-2.21656
1	0	4.5195	1.0876	-0.79509
6	0	-3.90931	-0.1425	0.64471
6	0	-4.21018	1.38832	-1.18792
1	0	0.09425	5.56939	0.39658
1	0	1.44749	5.82663	-0.75797
1	0	1.76207	5.20258	0.89796
1	0	2.60895	-3.24766	-2.07774
6	0	4.136	-1.79206	-2.57546
1	0	5.51228	-0.1379	-2.77647
6	0	-5.10507	-0.78321	0.31141
1	0	-3.32898	-0.48667	1.4977
6	0	-5.40485	0.75178	-1.52678
1	0	-3.86573	2.23785	-1.77429
1	0	4.52265	-2.35646	-3.41824
6	0	-5.85516	-0.34027	-0.77938
1	0	-5.45054	-1.62577	0.90507
1	0	-5.98656	1.10908	-2.3727
1	0	-6.78568	-0.83619	-1.04202

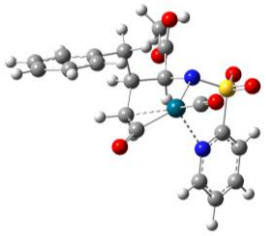


TS3-A-1a

E(RB3LYP) = -1820.60395373
G(correction)= 0.287198
$E(RM06)_{dioxane}$ = -1821.26429321
$E(RM06)_{iPrOH}$ = -1821.2782331
Imaginary frequencies: 1 (-275.8268 cm^{-1})

46	0	0.18967	-0.60758	1.17235
6	0	1.58429	-1.74112	0.02684
6	0	-1.07401	0.15613	2.50039
6	0	0.80284	-2.34714	1.59354
7	0	-0.5989	0.2808	-0.67528
6	0	1.17637	-2.0428	-1.29305
6	0	2.91706	-1.4104	0.32626
8	0	-1.77335	0.61508	3.27088
8	0	0.82026	-3.43012	2.02309
6	0	-1.74785	-0.46643	-1.20585
16	0	-0.68995	1.90535	-0.73574
6	0	-0.20639	-2.49006	-1.7466
6	0	2.17269	-1.9797	-2.27905
6	0	3.87895	-1.36099	-0.67704
1	0	3.19243	-1.18821	1.35304
6	0	-1.50779	-1.98763	-1.08869
1	0	-1.91656	-0.19192	-2.25549
6	0	-2.99278	-0.0923	-0.38674
6	0	1.03311	2.27345	-0.29293
8	0	-1.52189	2.49328	0.34308
8	0	-0.90111	2.41383	-2.10595
1	0	-0.27435	-2.28795	-2.82298
1	0	-0.2168	-3.58741	-1.65625
1	0	1.89602	-2.18454	-3.31017

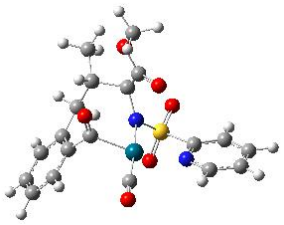
6	0	3.49499	-1.64534	-1.98782
1	0	4.90629	-1.10116	-0.44012
6	0	-2.69445	-2.74871	-1.70669
1	0	-1.49265	-2.22662	-0.01933
8	0	-3.21895	-0.50366	0.73678
8	0	-3.74755	0.81091	-1.02416
7	0	1.50758	1.67578	0.80148
6	0	1.75607	3.17644	-1.06845
1	0	4.22534	-1.60514	-2.7914
1	0	-2.56821	-3.83068	-1.58853
1	0	-2.78606	-2.53467	-2.77907
1	0	-3.63528	-2.47192	-1.22145
6	0	-4.72284	1.4911	-0.21104
6	0	2.76055	1.96355	1.17414
6	0	3.05794	3.47413	-0.66641
1	0	1.29866	3.6077	-1.95135
1	0	-5.38737	0.77393	0.2777
1	0	-5.27667	2.1323	-0.89689
1	0	-4.19746	2.08923	0.53784
1	0	3.12227	1.45345	2.0636
6	0	3.57166	2.85927	0.47673
1	0	3.66286	4.17284	-1.23747
1	0	4.57948	3.06465	0.82356



TS3-B-1a

E(RB3LYP) = -1820.58992256
G(correction)= 0.284589
$E(RM06)_{dioxane}$ = -1821.25654679
$E(RM06)_{iPrOH}$ = -1821.27487675
Imaginary frequencies: 1 (-246.5081 cm^{-1})

46	0	0.13798	-1.31504	-0.47325
6	0	1.38823	-1.83441	0.83043
6	0	0.17827	-2.60681	-1.90672
7	0	-0.85243	0.57038	-0.91843
6	0	1.09637	-0.16944	1.40789
8	0	2.05996	-2.62048	1.37244
8	0	0.18968	-3.37399	-2.7531
6	0	-0.45128	1.49408	0.15537
16	0	-2.45749	0.42494	-1.08513
6	0	0.99339	1.181	0.62934
1	0	0.28332	-0.28273	2.12915
1	0	2.05368	-0.17191	1.93211
1	0	-1.09553	1.40847	1.04406
6	0	-0.53736	2.956	-0.3057
6	0	-2.98369	-0.47851	0.43072
8	0	-2.73598	-0.48967	-2.20045
8	0	-3.15961	1.71888	-0.98899
6	0	2.0504	1.34459	-0.49522
1	0	1.22808	1.92059	1.41151
8	0	-0.14897	3.38321	-1.36757
8	0	-1.06353	3.72417	0.6724
7	0	-2.10804	-1.35392	0.93279
6	0	-4.24708	-0.25504	0.97628
1	0	2.08821	2.40473	-0.76183
1	0	1.70149	0.82264	-1.39126
6	0	3.41644	0.84381	-0.0906
6	0	-1.22765	5.11056	0.32919
6	0	-2.47147	-2.06972	2.00693
6	0	-4.61897	-1.00325	2.09205
1	0	-4.8946	0.49244	0.53213
6	0	3.92598	-0.3525	-0.61272
6	0	4.18104	1.53692	0.86031
1	0	-0.26437	5.56216	0.07395
1	0	-1.65474	5.58476	1.21362
1	0	-1.90292	5.20616	-0.52532
1	0	-1.73274	-2.77273	2.38473
6	0	-3.71697	-1.93177	2.61759
1	0	-5.59514	-0.86336	2.5479
6	0	5.16137	-0.85093	-0.19186
1	0	3.34886	-0.89361	-1.35917
6	0	5.415	1.04295	1.28426
1	0	3.80507	2.47401	1.26658
1	0	-3.96684	-2.53305	3.48588
6	0	5.90781	-0.1561	0.76077
1	0	5.53889	-1.7803	-0.60969
1	0	5.99493	1.59509	2.01919
1	0	6.86895	-0.54136	1.08978

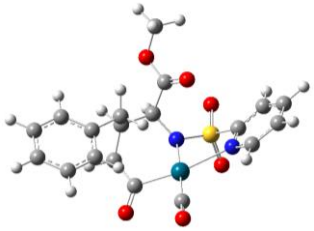


IM6-A-1a

E(RB3LYP) = -1820.64939175
G(correction)= 0.289492
$E(RM06)_{dioxane}$ = -1821.30775712
Imaginary frequencies: 0

46	0	-0.28614	-1.00481	-0.68365
7	0	-0.16393	0.63835	0.61311
6	0	1.58744	-0.44051	-1.18991
7	0	-2.4505	-1.07808	0.11383
6	0	-0.25603	-2.51587	-1.85857
6	0	0.23722	1.97836	0.2278
16	0	-1.12662	0.41812	1.89738
6	0	2.60203	-0.87532	-0.18206
8	0	1.77728	0.19823	-2.18654
6	0	-2.64482	-0.23546	1.13492
6	0	-3.52238	-1.62764	-0.47458
8	0	-0.29301	-3.43855	-2.5359

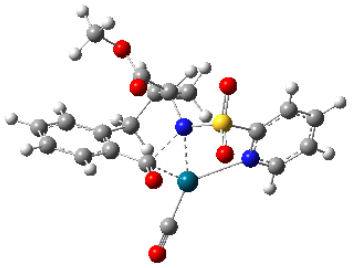
6	0	1.78842	2.21313	0.32592
1	0	-0.23475	2.69017	0.91985
6	0	-0.35007	2.30862	-1.15307
8	0	-1.4936	1.68929	2.54822
8	0	-0.63153	-0.69785	2.71554
6	0	2.98854	-0.10262	0.92949
6	0	3.14663	-2.14989	-0.41096
6	0	-3.90162	0.10844	1.61844
1	0	-3.32199	-2.29742	-1.30541
6	0	-4.82303	-1.3524	-0.05703
6	0	2.45944	1.26616	1.34634
6	0	2.05646	3.6708	0.74155
1	0	2.23613	2.06022	-0.65906
8	0	-1.28209	1.72415	-1.66605
8	0	0.27127	3.35201	-1.73374
6	0	3.95715	-0.67034	1.77601
6	0	4.10072	-2.68033	0.44863
1	0	2.81038	-2.72181	-1.27251
6	0	-5.01442	-0.46626	1.00463
1	0	-3.98172	0.81202	2.43938
1	0	-5.66247	-1.81707	-0.5634
1	0	1.77489	1.1082	2.18901
1	0	3.3199	1.80297	1.76473
1	0	3.12818	3.89685	0.70184
1	0	1.71109	3.84686	1.76869
1	0	1.53824	4.36931	0.08003
6	0	-0.20285	3.69847	-3.04652
1	0	4.2811	-0.09817	2.64238
6	0	4.50488	-1.93038	1.55496
1	0	4.52032	-3.66391	0.25882
1	0	-6.0165	-0.22392	1.34664
1	0	-0.07132	2.85337	-3.72765
1	0	0.40507	4.54708	-3.36152
1	0	-1.26142	3.9709	-3.01357
1	0	5.24517	-2.32579	2.24492



IM6-B-1a

E(RB3LYP) = -1820.65487987
G(correction)= 0.289867
$E(RM06)_{dioxane}$ = -1821.31733667
Imaginary frequencies: 0

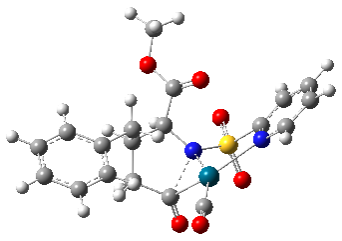
46	0	0.24072	-1.39919	-0.31723
6	0	-0.3776	-3.04326	0.48475
7	0	0.82518	0.38896	-1.1688
6	0	-1.45115	-1.21208	-1.44014
8	0	-0.75512	-4.00493	0.97303
6	0	0.10789	1.63677	-0.99641
16	0	2.43867	0.44016	-1.39668
8	0	-2.03987	-2.17782	-1.83365
6	0	-1.84975	0.21927	-1.81191
6	0	-1.42509	1.35209	-0.86404
1	0	0.24946	2.27275	-1.87793
6	0	0.58375	2.44201	0.21647
6	0	3.07533	-0.14579	0.20599
8	0	2.90926	1.82292	-1.58287
8	0	2.83632	-0.61285	-2.3398
1	0	-1.41197	0.38316	-2.80518
1	0	-2.93831	0.20011	-1.92098
6	0	-1.88526	1.126	0.60346
1	0	-1.9319	2.25638	-1.2186
8	0	1.20407	2.00233	1.16013
8	0	0.16613	3.72047	0.1211
7	0	2.37583	-1.14402	0.75406
6	0	4.22344	0.39449	0.77063
1	0	-1.74238	2.06487	1.15088
1	0	-1.2368	0.38531	1.08358
6	0	-3.33009	0.69579	0.71054
6	0	0.53359	4.57089	1.22147
6	0	2.80268	-1.65619	1.91643
6	0	4.66486	-0.14248	1.97936
1	0	4.7269	1.21634	0.2744
6	0	-3.66881	-0.63072	1.00529
6	0	-4.3639	1.61266	0.47103
1	0	0.09613	4.202	2.154
1	0	0.13997	5.5574	0.97512
1	0	1.6212	4.60379	1.32748
1	0	2.20354	-2.45961	2.33541
6	0	3.94523	-1.18728	2.5625
1	0	5.55414	0.25114	2.46323
6	0	-5.00429	-1.03602	1.05442
1	0	-2.87846	-1.35319	1.19401
6	0	-5.69956	1.21308	0.51904
1	0	-4.11659	2.64847	0.24663
1	0	4.25378	-1.62903	3.5042
6	0	-6.02401	-0.11502	0.8097
1	0	-5.24581	-2.07071	1.28234
1	0	-6.4877	1.93792	0.33247
1	0	-7.06395	-0.42762	0.84668



TS4-A-1a

E(RB3LYP) = -1820.63388269
G(correction)= 0.290895
$E(RM06)_{dioxane}$ = -1821.28931079
Imaginary frequencies: 1 (-209.9151 cm^{-1})

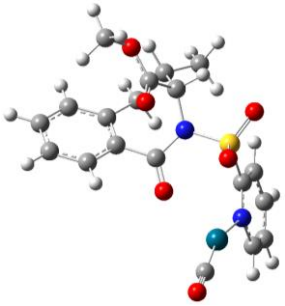
46	0	0.85574	1.56527	-0.06921
6	0	-0.95684	0.8298	-1.12986
7	0	0.16232	-0.5663	-0.32839
6	0	0.59702	3.43584	-0.00234
6	0	-2.27143	0.85055	-0.4144
8	0	-0.78569	1.02111	-2.29251
6	0	-0.5291	-1.46894	0.60604
16	0	1.3445	-1.30293	-1.25743
8	0	0.44985	4.57655	0.03814
6	0	-2.48594	0.72414	0.97572
6	0	-3.36934	0.98879	-1.28477
6	0	-0.75159	-0.85971	2.00971
1	0	0.0973	-2.35698	0.75782
6	0	-1.78931	-2.05254	-0.06524
6	0	2.84746	-0.93905	-0.27755
8	0	1.50416	-0.58068	-2.51646
8	0	1.2138	-2.7668	-1.23347
6	0	-1.36958	0.55582	1.97396
6	0	-3.80938	0.7275	1.43741
6	0	-4.6712	0.99248	-0.79963
1	0	-3.17662	1.0717	-2.34793
6	0	0.5528	-0.84616	2.81775
1	0	-1.46219	-1.52528	2.50903
8	0	-2.01625	-2.02915	-1.25121
8	0	-2.58674	-2.662	0.83828
7	0	2.9505	0.30468	0.19617
6	0	3.81693	-1.92149	-0.1032
1	0	-0.57454	1.2814	1.7569
1	0	-1.73806	0.79386	2.97825
1	0	-3.98416	0.62545	2.50542
6	0	-4.89357	0.85731	0.57234
1	0	-5.50495	1.09363	-1.48828
1	0	0.38455	-0.42047	3.81372
1	0	1.31795	-0.24101	2.31976
1	0	0.95026	-1.85978	2.94646
6	0	-3.79007	-3.23263	0.29372
6	0	4.05835	0.63244	0.87408
6	0	4.96758	-1.57452	0.60713
1	0	3.65618	-2.91375	-0.5087
1	0	-5.90559	0.85621	0.96814
1	0	-4.40596	-2.44698	-0.15311
1	0	-4.30412	-3.69295	1.13826
1	0	-3.55065	-3.97788	-0.46928
1	0	4.10473	1.65204	1.24524
6	0	5.09293	-0.27626	1.10258
1	0	5.7522	-2.30738	0.77193
1	0	5.97049	0.03177	1.6616



TS4-B-1a

E(RB3LYP) = -1820.64278683
G(correction)= 0.289592
$E(RM06)_{dioxane}$ = -1821.30312219
Imaginary frequencies: 1 (-154.8623 cm^{-1})

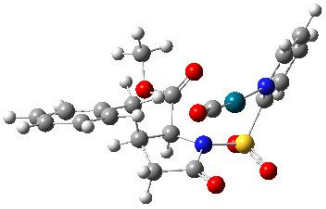
46	0	-0.27891	-1.50081	-0.09986
6	0	0.76861	-2.94314	-0.73338
7	0	-0.73849	0.23728	1.10024
8	0	1.42682	-3.79979	-1.12978
6	0	-0.01311	1.49282	1.00478
16	0	-2.35622	0.27801	1.44993
6	0	1.51124	1.15363	0.92431
1	0	-0.18351	2.08858	1.909
6	0	-0.44997	2.34966	-0.18004
6	0	-3.11717	-0.02209	-0.18014
8	0	-2.75327	1.63162	1.86615
8	0	-2.68597	-0.88936	2.26854
6	0	1.73677	-0.05467	1.84357
6	0	2.03018	0.95663	-0.52505
1	0	2.05347	2.00771	1.34084
8	0	-1.14566	1.98862	-1.10285
8	0	0.07893	3.58471	-0.07044
7	0	-2.51287	-0.92873	-0.94839
6	0	-4.28062	0.6518	-0.53071
6	0	0.5843	-1.04254	1.83827
1	0	1.83446	0.26209	2.88961
1	0	2.64471	-0.60474	1.57808
1	0	1.86538	1.89293	-1.0709
1	0	1.44024	0.18371	-1.02875
6	0	3.49989	0.60652	-0.57407
6	0	-0.24361	4.49013	-1.14179
6	0	-3.06016	-1.20732	-2.13832
6	0	-4.84655	0.35473	-1.77072
1	0	-4.70309	1.3877	0.14371
8	0	0.27659	-1.8329	2.66991
6	0	3.92462	-0.70515	-0.82451
6	0	4.47041	1.58933	-0.33129
1	0	0.1326	4.10464	-2.09388
1	0	0.24406	5.43132	-0.88716
1	0	-1.32643	4.62217	-1.21361
1	0	-2.53817	-1.94351	-2.74236
6	0	-4.22752	-0.59025	-2.5893
1	0	-5.75297	0.858	-2.09462
6	0	5.28361	-1.02878	-0.82868
1	0	3.18561	-1.47778	-1.01955
6	0	5.82843	1.2707	-0.33465
1	0	4.15593	2.61409	-0.14257
1	0	-4.63261	-0.84468	-3.56326
6	0	6.23949	-0.04192	-0.58232
1	0	5.59288	-2.05163	-1.02662
1	0	6.56637	2.04653	-0.14781
1	0	7.29701	-0.29151	-0.58626



IM7-A-1a

E(RB3LYP) = -1820.67366748
G(correction)= 0.289098
E(RM06)$_{dioxane}$ = -1821.33055604
Imaginary frequencies: 0

46	0	-3.14811	-1.1055	-0.16036
6	0	-4.05076	-2.70868	-0.31871
7	0	-2.69521	1.06108	0.36312
8	0	-4.60809	-3.7189	-0.41158
6	0	-1.63563	1.79636	0.02414
6	0	-3.53628	1.58696	1.27401
16	0	-0.53177	1.14132	-1.2669
6	0	-1.34689	3.05913	0.53249
1	0	-4.39839	0.97915	1.522
6	0	-3.32236	2.82886	1.87171
7	0	0.88682	0.68133	-0.36382
8	0	-1.15229	-0.00549	-1.91386
8	0	-0.08126	2.29944	-2.04914
6	0	-2.21046	3.58022	1.49539
1	0	-0.49019	3.61242	0.16815
1	0	-4.02655	3.19549	2.61112
6	0	2.18551	0.89851	-1.02769
6	0	0.70793	-0.3038	0.62766
1	0	-2.02325	4.5575	1.92987
6	0	3.13669	1.77191	-0.17226
1	0	1.97232	1.4573	-1.94459
6	0	2.73984	-0.45088	-1.52135
6	0	1.93841	-0.87663	1.25428
8	0	-0.41247	-0.65593	0.95856
6	0	3.0716	1.38655	1.32193
6	0	2.81879	3.26161	-0.34826
1	0	4.14885	1.57953	-0.53911
8	0	2.0603	-1.42743	-1.73203
8	0	4.06259	-0.38399	-1.75012
6	0	3.0712	-0.10247	1.57213
6	0	1.9112	-2.25028	1.52711
1	0	2.15928	1.82425	1.74867
1	0	3.91321	1.85629	1.84246
1	0	3.48089	3.87364	0.27463
1	0	1.78539	3.47366	-0.05296
1	0	2.93826	3.57873	-1.38956
6	0	4.65799	-1.60882	-2.22367
6	0	4.17739	-0.74657	2.13627
6	0	3.02568	-2.87486	2.07984
1	0	1.01581	-2.8112	1.28106
1	0	4.51915	-2.40002	-1.48204
1	0	5.71597	-1.38413	-2.35923
1	0	4.19994	-1.916	-3.16718
1	0	5.05602	-0.1598	2.39298
6	0	4.16327	-2.1205	2.3802
1	0	3.00761	-3.94286	2.27586
1	0	5.03674	-2.60008	2.8137

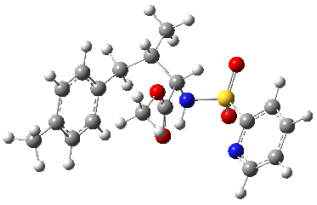


IM7-B-1a

E(RB3LYP) = -1820.67482008
G(correction)= 0.289416
E(RM06)$_{dioxane}$ = -1821.33546181
Imaginary frequencies: 0

46	0	-0.60097	-2.08759	-0.35646
6	0	0.89954	-3.17162	-0.38774
7	0	-2.50086	-0.99146	-0.63059
8	0	1.84537	-3.83622	-0.3937
6	0	-2.95331	0.11713	-0.03925
6	0	-3.16208	-1.41585	-1.7284
16	0	-2.2253	0.66779	1.54077
6	0	-4.04913	0.8523	-0.48324
1	0	-2.77822	-2.31652	-2.19244
6	0	-4.26906	-0.75231	-2.25051
7	0	-0.53264	0.65965	1.32834
8	0	-2.59188	2.08265	1.67392
8	0	-2.5887	-0.31253	2.55152
6	0	-4.72036	0.40399	-1.61828
1	0	-4.34705	1.74897	0.04542
1	0	-4.7584	-1.14257	-3.13647
6	0	0.13304	1.89902	0.89506
6	0	0.36018	-0.18224	2.07456
1	0	-5.57801	0.95032	-1.9991
6	0	1.63996	1.50104	0.85928
1	0	-0.03031	2.69258	1.63179
6	0	-0.35726	2.40715	-0.4486
6	0	1.72501	0.48704	2.0068
8	0	0.07244	-1.19874	2.64782
6	0	2.07169	0.8957	-0.49787
1	0	2.24184	2.39204	1.05613
8	0	-1.03989	1.79783	-1.2414
8	0	0.12838	3.64299	-0.6559
1	0	1.89072	0.98088	2.97288
1	0	2.5049	-0.26677	1.88114
1	0	1.88558	1.63614	-1.28546
1	0	1.44481	0.02436	-0.72477
6	0	3.53611	0.51717	-0.50945
6	0	-0.20651	4.2322	-1.92722
6	0	3.9401	-0.82081	-0.41856
6	0	4.52146	1.51281	-0.58223

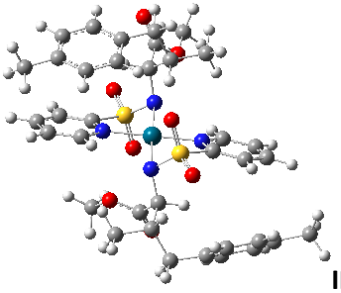
1	0	0.1831	3.61914	-2.74464
1	0	0.26142	5.21647	-1.92461
1	0	-1.29138	4.31858	-2.02973
6	0	5.29631	-1.15628	-0.39821
1	0	3.19205	-1.60616	-0.37162
6	0	5.87613	1.18168	-0.56197
1	0	4.22151	2.55629	-0.66199
6	0	6.26778	-0.15689	-0.46846
1	0	5.58916	-2.20056	-0.33056
1	0	6.62603	1.96615	-0.62334
1	0	7.32274	-0.41718	-0.45458



1b

E(RB3LYP) = -1507.75585048
G(correction)= 0.325041
$E(RM06)_{dioxane}$ = -1507.26450805
$E(RM06)_{iPrOH}$ = -1507.28002119
Imaginary frequencies: 0

1	0	-1.01018	0.7615	-1.39057
6	0	-0.30356	0.81705	-0.55425
6	0	0.36539	-0.55284	-0.44645
7	0	-1.03475	1.08642	0.6913
6	0	0.69307	1.96386	-0.88887
8	0	0.34393	-1.25138	0.54536
8	0	0.97943	-0.87925	-1.59199
1	0	-0.78822	0.42237	1.42837
16	0	-2.70476	1.23296	0.61345
1	0	1.1993	1.66266	-1.81435
6	0	-0.08146	3.26244	-1.1478
6	0	1.75869	2.17936	0.21189
6	0	1.75923	-2.092	-1.5468
8	0	-3.15536	1.5824	1.95728
8	0	-3.01957	2.06154	-0.55562
6	0	-3.28788	-0.44484	0.22583
1	0	0.60562	4.05421	-1.46753
1	0	-0.59595	3.59605	-0.2417
1	0	-0.84363	3.12887	-1.92171
1	0	2.24218	3.14472	0.01173
1	0	1.24612	2.28961	1.17489
6	0	2.83049	1.11182	0.30406
1	0	2.19981	-2.1892	-2.53904
1	0	1.11737	-2.94775	-1.32098
1	0	2.53706	-2.00231	-0.78574
6	0	-4.1019	-0.66353	-0.88276
7	0	-2.85569	-1.38254	1.06313
6	0	3.74774	0.93069	-0.74206
6	0	2.94468	0.27805	1.42072
6	0	-4.49837	-1.98043	-1.12451
1	0	-4.39751	0.16474	-1.51611
6	0	-3.23852	-2.63802	0.81475
6	0	4.73878	-0.04511	-0.6717
1	0	3.68135	1.56344	-1.62471
6	0	3.93709	-0.70136	1.4924
1	0	2.23592	0.38054	2.23818
6	0	-4.05928	-2.98534	-0.26339
1	0	-5.13501	-2.21546	-1.97279
1	0	-2.87047	-3.39516	1.50319
6	0	4.85473	-0.87828	0.4511
1	0	5.43676	-0.16228	-1.49826
1	0	3.99454	-1.33935	2.37142
1	0	-4.34147	-4.02183	-0.42019
6	0	5.95226	-1.91296	0.5402
1	0	6.17355	-2.35024	-0.44007
1	0	6.8851	-1.47026	0.91421
1	0	5.68261	-2.72723	1.22116

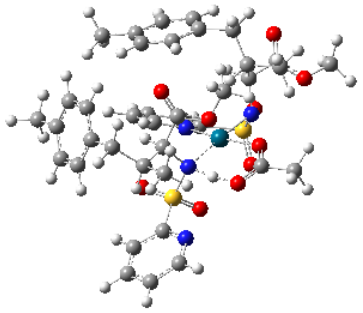


IM1-1b

E(RB3LYP) = -3141.095166
G(correction)= 0.661813
$E(RM06)_{dioxane}$ = -3141.28809986
$E(RM06)_{iPrOH}$ = -3141.31649267
Imaginary frequencies: 0

6	0	1.65718	-2.59097	0.20335
1	0	0.90904	-2.81675	-0.54645
6	0	2.6341	-3.49479	0.61407
7	0	1.5864	-1.36714	0.74592
1	0	2.67917	-4.47512	0.15353
6	0	3.55396	-3.1126	1.59142
6	0	2.46133	-0.9998	1.69684
46	0	0.21437	0.06559	0.21876
1	0	4.33225	-3.79943	1.9109
6	0	3.47112	-1.834	2.14845
16	0	2.16516	0.69123	2.32628
7	0	-1.1628	1.51742	-0.2708
7	0	1.62149	1.42309	0.94835
1	0	4.16566	-1.4705	2.89756
8	0	1.04866	0.58329	3.27582
8	0	3.47183	1.18788	2.77886
6	0	-1.31863	2.67794	0.38507
6	0	-2.03444	1.16672	-1.23266
6	0	2.72814	1.70132	0.00316
1	0	-0.57031	2.89557	1.13982
6	0	-2.38845	3.52215	0.08931
16	0	-1.66307	-0.47204	-1.94565
6	0	-3.13251	1.93806	-1.57108

1	0	3.39681	0.83647	-0.07899
6	0	3.63734	2.84517	0.44421
6	0	2.19104	1.99087	-1.42926
1	0	-2.50011	4.45064	0.63867
6	0	-3.31034	3.14434	-0.88794
7	0	-1.21966	-1.28037	-0.56586
8	0	-0.47046	-0.31233	-2.7905
8	0	-2.91417	-0.9342	-2.56238
1	0	-3.83533	1.56969	-2.30848
8	0	3.02311	3.75068	1.22103
8	0	4.78673	2.9451	0.06223
1	0	1.37128	1.28293	-1.59659
6	0	1.63793	3.41055	-1.59372
6	0	3.26808	1.66871	-2.49306
1	0	-4.16866	3.77175	-1.10682
6	0	-2.37294	-1.47729	0.35821
6	0	3.86445	4.81439	1.69406
1	0	0.9482	3.6647	-0.78433
1	0	2.44332	4.15481	-1.59145
1	0	1.10361	3.49808	-2.54641
1	0	2.84675	1.91654	-3.47573
1	0	4.13705	2.31664	-2.33605
6	0	3.68188	0.21292	-2.46173
6	0	-3.32337	-2.64262	-0.05666
6	0	-1.92394	-1.67262	1.80174
1	0	-2.98439	-0.57022	0.40572
1	0	4.689	4.40545	2.28415
1	0	3.22261	5.44066	2.31439
1	0	4.27262	5.38694	0.856
6	0	4.89681	-0.18255	-1.88379
6	0	2.81492	-0.7832	-2.93007
6	0	-4.70395	-2.48103	0.63082
1	0	-3.47864	-2.51969	-1.13024
6	0	-2.71962	-4.02956	0.18243
8	0	-2.56033	-1.25418	2.74814
8	0	-0.80732	-2.40951	1.92727
1	0	5.56354	0.57805	-1.48419
6	0	5.23451	-1.53236	-1.78164
6	0	3.15995	-2.13173	-2.83176
1	0	1.85073	-0.5089	-3.3472
1	0	-4.59159	-2.60569	1.7139
1	0	-5.34673	-3.29899	0.27969
6	0	-5.35465	-1.14536	0.32945
1	0	-1.71805	-4.09162	-0.25516
1	0	-2.6356	-4.26062	1.2507
1	0	-3.34747	-4.8003	-0.27899
6	0	-0.31016	-2.55944	3.273
1	0	6.17989	-1.81456	-1.32206
6	0	4.37434	-2.5304	-2.25876
1	0	2.46893	-2.88555	-3.20414
6	0	-5.86838	-0.87058	-0.94563
6	0	-5.37732	-0.11857	1.28292
1	0	0.57262	-3.19353	3.17982
1	0	-0.04121	-1.58119	3.67801
1	0	-1.06325	-3.03422	3.9068
6	0	4.75694	-3.98917	-2.16272
1	0	-5.83624	-1.64029	-1.71248
6	0	-6.38958	0.38485	-1.25498
6	0	-5.89678	1.13921	0.97008
1	0	-4.94149	-0.29722	2.26172
1	0	5.53401	-4.24898	-2.8934
1	0	5.15662	-4.2339	-1.17065
1	0	3.89921	-4.64396	-2.35327
1	0	-6.77861	0.57155	-2.25419
6	0	-6.41373	1.41299	-0.30166
1	0	-5.89191	1.92165	1.72624
6	0	-6.99355	2.76845	-0.63595
1	0	-6.77045	3.05892	-1.67
1	0	-8.08673	2.77411	-0.53256
1	0	-6.60296	3.54735	0.02897

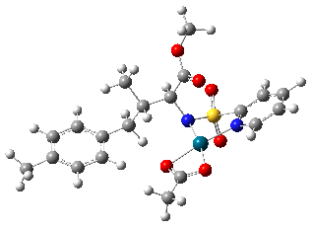


TS1-1b

E(RB3LYP) = -3370.18470737
G(correction)= 0.713322
$E(RM06)_{dioxane}$ = -3370.31326955
$E(RM06)_{iPrOH}$ = -3370.35046911
Imaginary frequencies: 1 (-988.3789 cm^{-1})

6	0	0.04842	1.75601	-1.16353
1	0	-0.6862	1.76658	-0.37549
6	0	0.25455	2.88013	-1.95741
7	0	0.75567	0.62806	-1.33673
1	0	-0.34735	3.76244	-1.775
6	0	1.23584	2.84697	-2.94454
6	0	1.71764	0.60638	-2.28236
46	0	0.60294	-1.16106	-0.27703
1	0	1.42219	3.71589	-3.56882
6	0	1.99739	1.68718	-3.10169
16	0	2.70244	-0.93057	-2.30092
7	0	2.61534	-1.3112	-0.68761
1	0	2.80947	1.60875	-3.81588
8	0	1.96864	-1.92571	-3.0802
8	0	4.0555	-0.51831	-2.70455
6	0	3.50423	-0.46776	0.13332
1	0	3.42029	0.5885	-0.14572
6	0	4.98772	-0.79221	-0.0491
6	0	3.13433	-0.57361	1.639
8	0	5.21995	-2.05944	-0.41042
8	0	5.86185	0.02168	0.18229
1	0	2.03952	-0.49306	1.671
6	0	3.52858	-1.92059	2.25249
6	0	3.68908	0.63347	2.43628
6	0	6.59708	-2.38245	-0.65686

1	0	3.11431	-2.74018	1.66013
1	0	4.6176	-2.03554	2.2967
1	0	3.14644	-1.99783	3.2773
1	0	3.3978	0.50051	3.48708
1	0	4.78301	0.6229	2.39902
6	0	3.15131	1.94772	1.91168
1	0	6.98595	-1.7625	-1.4693
1	0	6.60234	-3.43499	-0.94083
1	0	7.20065	-2.2187	0.2408
6	0	3.90457	2.7432	1.03649
6	0	1.8361	2.3381	2.19334
1	0	4.91294	2.43157	0.77639
6	0	3.35102	3.88479	0.45571
6	0	1.28494	3.47866	1.60954
1	0	1.22167	1.74058	2.86008
1	0	3.95088	4.47828	-0.23146
6	0	2.03277	4.27184	0.72966
1	0	0.25336	3.74009	1.83078
6	0	1.44506	5.516	0.10517
1	0	0.35255	5.4581	0.05293
1	0	1.6958	6.4141	0.68532
1	0	1.82449	5.67211	-0.91153
1	0	-1.87435	0.86956	0.67599
6	0	-1.99776	-0.11754	1.11724
7	0	-1.56279	-1.13607	0.12343
6	0	-3.48873	-0.20847	1.56716
6	0	-1.11681	-0.11995	2.35892
16	0	-2.29998	-1.00037	-1.40967
6	0	-3.95227	1.11816	2.22207
1	0	-4.06992	-0.30758	0.64785
6	0	-3.78051	-1.42405	2.45298
8	0	-0.96386	0.86293	3.05811
8	0	-0.59944	-1.32109	2.64347
6	0	-3.96361	-1.72375	-1.26002
8	0	-2.50542	0.42401	-1.72795
8	0	-1.53897	-1.86862	-2.30794
1	0	-3.46104	1.2422	3.19211
1	0	-5.02873	1.02284	2.41874
6	0	-3.68482	2.32686	1.34801
1	0	-3.41805	-2.34899	1.99666
1	0	-3.30556	-1.32084	3.43607
1	0	-4.86003	-1.51986	2.61568
6	0	0.21049	-1.4045	3.82883
7	0	-4.03441	-2.89069	-0.63601
6	0	-5.03804	-1.04844	-1.84031
6	0	-4.32009	2.46613	0.10551
6	0	-2.73133	3.28677	1.7082
1	0	0.62163	-2.41295	3.82357
1	0	1.01337	-0.66536	3.79546
1	0	-0.4039	-1.23331	4.71694
6	0	-5.24111	-3.46115	-0.55033
6	0	-6.28883	-1.65988	-1.74854
1	0	-4.88636	-0.09014	-2.32312
1	0	-5.05509	1.72718	-0.20573
6	0	-4.00027	3.5144	-0.75338
6	0	-2.42496	4.34831	0.85314
1	0	-2.2028	3.18134	2.65084
1	0	-5.2816	-4.41343	-0.02688
6	0	-6.39503	-2.88625	-1.09027
1	0	-7.16476	-1.18475	-2.18092
1	0	-4.49148	3.58377	-1.72137
6	0	-3.04503	4.47649	-0.39553
1	0	-1.69082	5.08774	1.16425
1	0	-7.35138	-3.39066	-0.99415
6	0	-2.71801	5.62501	-1.32257
1	0	-3.48002	6.41345	-1.26552
1	0	-1.75615	6.08544	-1.07111
1	0	-2.67431	5.29565	-2.36744
1	0	-1.56193	-2.37309	0.51741
8	0	-1.39184	-3.50531	0.8903
6	0	-0.15031	-3.77613	0.96514
8	0	0.79572	-2.99898	0.64554
6	0	0.23628	-5.15224	1.45432
1	0	-0.53372	-5.55141	2.11799
1	0	0.32476	-5.81427	0.58513
1	0	1.20697	-5.11829	1.95376

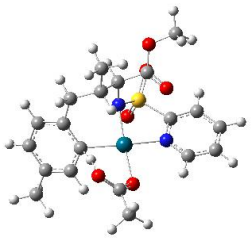


IM2-1b

E(RB3LYP) = -1862.41045004
G(correction)= 0.358595
$E(RM06)_{dioxane}$ = -1863.02752033
$E(RM06)_{iPrOH}$ = -1863.04632759
Imaginary frequencies: 0

46	0	0.9014	1.3175	0.0749
7	0	2.89582	0.88741	0.00554
7	0	0.68529	-0.54382	0.89259
6	0	3.32064	-0.1804	0.69646
6	0	3.74207	1.53667	-0.80936
6	0	0.13707	-1.62871	0.06431
16	0	2.03895	-0.89898	1.76349
6	0	4.6155	-0.66697	0.60285
1	0	3.33191	2.38586	-1.34559
6	0	5.0636	1.12211	-0.94815
6	0	-1.32661	-1.30354	-0.34548
1	0	0.11911	-2.54319	0.66569
6	0	1.00508	-1.91988	-1.16302
8	0	2.29684	-2.34468	1.82475
8	0	2.07193	-0.08565	2.98024
6	0	5.50494	0.00335	-0.23769
1	0	4.89253	-1.54979	1.16857
1	0	5.72663	1.66566	-1.6123
6	0	-2.18957	-1.15694	0.93282
6	0	-1.89133	-2.36944	-1.29515
1	0	-1.32555	-0.33854	-0.86774
8	0	1.59251	-1.08546	-1.82533

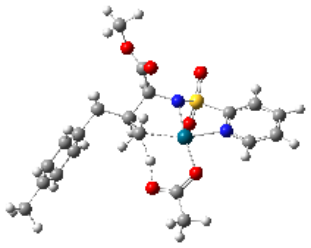
8	0	1.03977	-3.23624	-1.43586
1	0	6.52872	-0.34384	-0.34125
1	0	-2.16256	-2.11043	1.47841
1	0	-1.71856	-0.40923	1.5782
6	0	-3.62489	-0.77218	0.64975
1	0	-2.94262	-2.15828	-1.50886
1	0	-1.82791	-3.36941	-0.84906
1	0	-1.35404	-2.39577	-2.24874
6	0	1.79545	-3.60806	-2.60037
6	0	-3.95308	0.53815	0.27121
6	0	-4.66052	-1.71146	0.72702
1	0	1.37875	-3.13598	-3.495
1	0	1.71787	-4.69349	-2.66581
1	0	2.83955	-3.30147	-2.49097
6	0	-5.27084	0.88779	-0.01962
1	0	-3.16403	1.28136	0.20343
6	0	-5.97942	-1.35793	0.4367
1	0	-4.43149	-2.73517	1.016
6	0	-6.30895	-0.05094	0.05979
1	0	-5.50099	1.91127	-0.31088
1	0	-6.7637	-2.10925	0.50485
6	0	-7.7406	0.34441	-0.22028
1	0	-8.33109	-0.50764	-0.57508
1	0	-8.23266	0.72649	0.68457
1	0	-7.79849	1.13447	-0.97762
8	0	-1.03013	2.12031	-0.0678
6	0	-0.55042	3.18419	-0.59092
8	0	0.71534	3.24614	-0.75833
6	0	-1.45156	4.32027	-0.96991
1	0	-0.91687	5.03948	-1.59323
1	0	-2.32986	3.93371	-1.49502
1	0	-1.7997	4.81852	-0.05796



TS2-A-1b

E(RB3LYP) = -1862.38158337
G(correction)= 0.356953
$E(RM06)_{dioxane}$ = -1863.00344297
$E(RM06)_{iPrOH}$ = -1863.0223537
Imaginary frequencies: 1 (-1440.3607 cm^{-1})

46	0	0.49937	0.69193	0.09851
7	0	-0.48237	-0.93047	-0.66088
6	0	2.26275	-0.45895	0.14946
16	0	-1.44641	-0.42006	-1.88258
6	0	-1.04886	-1.90015	0.28579
6	0	2.19826	-1.87317	0.11967
6	0	3.23058	0.19312	-0.65335
6	0	-2.09086	1.15529	-1.22271
8	0	-2.60833	-1.3072	-2.06208
8	0	-0.62864	-0.02856	-3.03389
6	0	-0.06813	-2.12935	1.4677
1	0	-1.20147	-2.85537	-0.22817
6	0	-2.40284	-1.46035	0.85225
6	0	1.28257	-2.70051	1.00276
6	0	3.09935	-2.56396	-0.70048
6	0	4.11829	-0.4927	-1.47961
1	0	3.28628	1.27993	-0.61678
7	0	-1.25779	1.78009	-0.38254
6	0	-3.33214	1.66499	-1.57511
6	0	-0.67908	-3.07283	2.51876
1	0	0.09745	-1.15452	1.94408
8	0	-2.6629	-0.33757	1.23773
8	0	-3.27034	-2.48575	0.90674
1	0	1.09666	-3.66487	0.51025
1	0	1.85392	-2.94311	1.91212
1	0	3.06557	-3.65111	-0.73204
6	0	4.03001	-1.89252	-1.48903
6	0	5.1179	0.22976	-2.35126
6	0	-1.61484	2.95874	0.14716
6	0	-3.7112	2.89034	-1.02726
1	0	-3.97087	1.09946	-2.24452
1	0	0.04239	-3.25839	3.32174
1	0	-0.95121	-4.03826	2.07596
1	0	-1.57886	-2.65029	2.97572
6	0	-4.57269	-2.16065	1.41817
1	0	4.70278	-2.46566	-2.12426
1	0	6.11971	-0.2075	-2.26231
1	0	4.83126	0.17258	-3.40924
1	0	5.18718	1.28982	-2.08591
1	0	-0.89276	3.40988	0.81922
6	0	-2.8393	3.54847	-0.15673
1	0	-4.67585	3.32551	-1.27219
1	0	-4.50292	-1.78451	2.44333
1	0	-5.14138	-3.09031	1.38622
1	0	-5.04335	-1.39891	0.79049
1	0	-3.10281	4.50113	0.29037
1	0	2.27811	0.17603	1.40451
8	0	2.51777	0.92446	2.38615
6	0	2.08864	2.08801	2.08196
8	0	1.36172	2.34331	1.07512
6	0	2.49312	3.22721	2.98796
1	0	2.17153	3.00552	4.01049
1	0	3.58483	3.30703	2.99914
1	0	2.05296	4.1666	2.65089

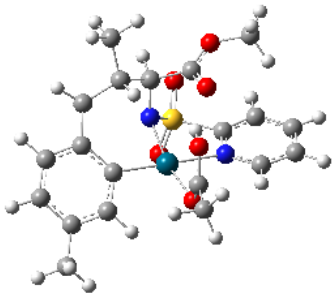


TS2-B-1b

E(RB3LYP) = -1862.36061705
G(correction)= 0.353211

E(RM06)$_{dioxane}$ = -1862.98955401
E(RM06)$_{iPrOH}$ = -1863.0088238
Imaginary frequencies: 1 (-1328.3151 cm^{-1})

46	0	-1.03475	-0.81505	-0.4618
7	0	-1.22194	1.12115	0.07654
7	0	-3.06594	-0.89218	0.03631
6	0	0.0093	1.92097	0.10876
16	0	-2.19474	1.24661	1.39851
6	0	-3.49418	0.13861	0.77815
6	0	-3.94519	-1.81231	-0.39029
6	0	1.22781	0.96337	0.16543
1	0	0.03589	2.59325	0.9719
6	0	0.05661	2.78255	-1.15193
8	0	-2.76371	2.59635	1.52858
8	0	-1.6597	0.61267	2.618
6	0	-4.82596	0.32388	1.11885
1	0	-3.52903	-2.62422	-0.97657
6	0	-5.30027	-1.71082	-0.0832
6	0	1.05059	-0.17161	-0.86418
6	0	2.57006	1.71748	-0.01193
1	0	1.21161	0.5356	1.17495
8	0	-0.21133	2.4071	-2.2726
8	0	0.50039	4.02473	-0.86446
6	0	-5.74697	-0.62634	0.675
1	0	-5.11061	1.19213	1.703
1	0	-5.98897	-2.46818	-0.44199
1	0	2.02984	-0.64189	-1.0387
1	0	0.75369	0.20823	-1.84761
1	0	2.63534	2.10098	-1.03804
1	0	2.57202	2.593	0.65037
6	0	3.76641	0.84194	0.28313
6	0	0.6478	4.89988	-1.99547
1	0	-6.80047	-0.52111	0.91652
6	0	4.5764	0.34135	-0.74228
6	0	4.07467	0.47598	1.60145
1	0	1.36946	4.48761	-2.70707
1	0	1.00452	5.84696	-1.58969
1	0	-0.31193	5.03268	-2.50236
6	0	5.65649	-0.49861	-0.46197
1	0	4.36383	0.61697	-1.77306
6	0	5.1523	-0.36098	1.88023
1	0	3.46412	0.85614	2.41802
6	0	5.9616	-0.86733	0.85246
1	0	6.27145	-0.87044	-1.27871
1	0	5.37292	-0.6248	2.91245
6	0	7.10931	-1.80135	1.15873
1	0	7.85489	-1.7988	0.35639
1	0	7.61459	-1.52431	2.09094
1	0	6.75763	-2.83521	1.27614
1	0	0.86713	-1.52503	-0.49504
8	0	1.11213	-2.83319	-0.4383
6	0	0.0579	-3.42454	-0.82192
8	0	-1.0454	-2.82585	-1.02807
6	0	0.12175	-4.91553	-1.05366
1	0	-0.85529	-5.31106	-1.33424
1	0	0.84926	-5.12313	-1.84498
1	0	0.48003	-5.40561	-0.14322

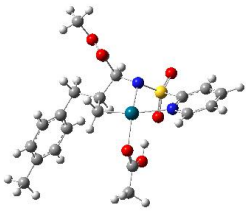


IM3-A-1b

E(RB3LYP) = -1862.40113401
G(correction)= 0.362228
E(RM06)$_{dioxane}$ = -1863.02465478
E(RM06)$_{iPrOH}$ = -1863.04546264
Imaginary frequencies: 0

46	0	-0.41316	-0.51542	-0.46967
7	0	0.55131	1.28242	-0.64969
6	0	-2.22347	0.33294	-0.39354
16	0	1.78672	1.12913	-1.71532
6	0	0.84322	1.92697	0.64048
6	0	-2.55647	1.65879	-0.04698
6	0	-3.23589	-0.54669	-0.80702
6	0	2.54267	-0.45238	-1.19594
8	0	2.81802	2.16046	-1.5261
8	0	1.23749	0.8643	-3.04696
6	0	-0.47456	2.27976	1.36816
1	0	1.41847	2.83859	0.44874
6	0	1.68939	1.01819	1.54167
6	0	-1.56611	2.73213	0.37358
6	0	-3.91139	2.02643	-0.11409
6	0	-4.58185	-0.16563	-0.88315
1	0	-2.98027	-1.56552	-1.08871
7	0	1.66507	-1.35249	-0.73259
6	0	3.91099	-0.68598	-1.27118
6	0	-0.19481	3.34166	2.44164
1	0	-0.82789	1.37119	1.86876
8	0	1.2891	0.00532	2.1049
8	0	2.96245	1.41347	1.61586
1	0	-1.08557	3.14996	-0.51981
1	0	-2.13288	3.55122	0.83215
1	0	-4.18765	3.04412	0.15667
6	0	-4.90716	1.14548	-0.52582
6	0	-5.64674	-1.15017	-1.30946
6	0	2.11781	-2.55184	-0.34108
6	0	4.38126	-1.93437	-0.86162
1	0	4.5663	0.10004	-1.62974
1	0	-1.08689	3.51759	3.05218
1	0	0.09604	4.2947	1.98283
1	0	0.61481	3.03505	3.11652
6	0	3.85704	0.54859	2.34137
1	0	-5.94189	1.47962	-0.56827
1	0	-6.41245	-0.66877	-1.92876

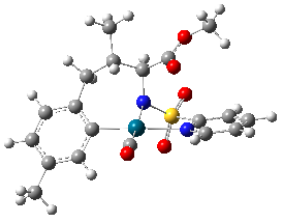
1	0	-5.21992	-1.97835	-1.88578
1	0	-6.16179	-1.58492	-0.44142
1	0	1.36493	-3.24295	0.02492
6	0	3.47007	-2.8854	-0.39451
1	0	5.44247	-2.16289	-0.90411
1	0	3.51022	0.41154	3.36871
1	0	4.82387	1.05091	2.31998
1	0	3.91777	-0.42491	1.84665
1	0	3.7983	-3.86625	-0.06665
1	0	-0.22601	-1.02105	2.04183
8	0	-0.83681	-1.71243	2.42423
6	0	-1.37729	-2.49956	1.51943
8	0	-1.20299	-2.40742	0.29575
6	0	-2.29024	-3.54464	2.09569
1	0	-1.96154	-3.85378	3.08994
1	0	-3.28919	-3.10025	2.18484
1	0	-2.3528	-4.39675	1.4172



IM3-B-1b

E(RB3LYP) = -1862.388875
G(correction)= 0.357737
$E(RM06)_{dioxane}$ = -1863.01787985
$E(RM06)_{iPrOH}$ = -1863.03647597
Imaginary frequencies: 0

46	0	-0.95787	-0.46493	-0.93241
7	0	-1.26164	1.22713	0.20142
6	0	0.95839	0.17066	-0.98223
6	0	-0.02457	2.01136	0.39281
16	0	-1.91063	0.57926	1.55859
6	0	1.18776	1.05153	0.25764
1	0	1.65179	-0.67533	-1.02205
1	0	1.0329	0.74932	-1.91128
1	0	-0.02026	2.51662	1.36454
6	0	0.0159	3.08573	-0.688
6	0	-3.3859	-0.11957	0.75946
8	0	-2.337	1.58645	2.54263
8	0	-1.17084	-0.5996	2.11463
6	0	2.56519	1.75926	0.25019
1	0	1.14716	0.41476	1.1504
8	0	-0.3776	2.9684	-1.82664
8	0	0.6291	4.19761	-0.21914
7	0	-3.1487	-0.7986	-0.37124
6	0	-4.64215	0.02748	1.33039
1	0	2.66122	2.36152	-0.66168
1	0	2.60925	2.45991	1.09405
6	0	3.70242	0.76692	0.33711
6	0	0.81607	5.24497	-1.18495
6	0	-4.18606	-1.3756	-0.99239
6	0	-5.71819	-0.58128	0.6813
1	0	-4.75246	0.60696	2.24011
6	0	4.41162	0.36621	-0.80117
6	0	4.0348	0.16974	1.56093
1	0	1.42332	4.89042	-2.02325
1	0	1.3265	6.04827	-0.6526
1	0	-0.14856	5.5879	-1.56955
1	0	-3.95408	-1.90818	-1.90974
6	0	-5.48769	-1.29426	-0.49624
1	0	-6.7222	-0.49597	1.08658
6	0	5.41851	-0.5971	-0.71977
1	0	4.16672	0.80859	-1.76421
6	0	5.04009	-0.79227	1.64201
1	0	3.49344	0.45876	2.45963
1	0	-6.29987	-1.77665	-1.03008
6	0	5.75282	-1.1917	0.50284
1	0	5.95266	-0.89106	-1.62106
1	0	5.27711	-1.24017	2.60492
6	0	6.86673	-2.20868	0.59932
1	0	7.8246	-1.72815	0.84058
1	0	7.00285	-2.7469	-0.34527
1	0	6.66929	-2.94739	1.38434
1	0	-0.51315	-2.00947	0.9095
8	0	-0.1933	-2.93595	0.71903
6	0	-0.13451	-3.23793	-0.56323
8	0	-0.43004	-2.48235	-1.49987
6	0	0.35348	-4.63879	-0.81153
1	0	0.29754	-4.86999	-1.87525
1	0	1.39016	-4.72143	-0.46727
1	0	-0.24192	-5.34985	-0.231

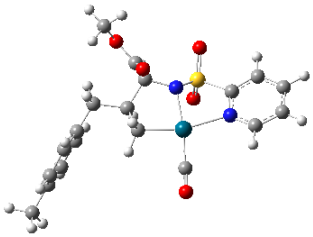


IM4-A-1b

E(RB3LYP) = -1746.62722759
G(correction)= 0.308352
$E(RM06)_{dioxane}$ = -1747.28588219
$E(RM06)_{iPrOH}$ = -1747.30229498
Imaginary frequencies: 0

46	0	0.53989	-0.78811	-0.3056
7	0	-0.27209	0.71555	0.85397
6	0	2.39815	0.0257	-0.07095
6	0	1.20388	-1.99604	-1.63148
16	0	-1.28568	0.03839	1.94242
6	0	-0.75053	1.9013	0.12983
6	0	2.68231	1.39599	0.06107
6	0	3.42778	-0.91869	0.08102
8	0	1.51164	-2.68143	-2.49423
6	0	-2.25503	-1.0975	0.88842
8	0	-2.24858	1.00573	2.48827

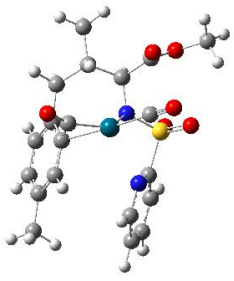
8	0	-0.51399	-0.83698	2.82972
6	0	0.39414	2.44448	-0.75528
1	0	-1.042	2.66664	0.85645
6	0	-1.95853	1.60611	-0.76762
6	0	1.70016	2.55989	0.0534
6	0	4.02449	1.74761	0.30585
6	0	4.75153	-0.55455	0.34774
1	0	3.20687	-1.98049	0.01407
7	0	-1.55604	-1.66405	-0.10291
6	0	-3.61038	-1.31989	1.09549
6	0	-0.00162	3.80482	-1.35134
1	0	0.53798	1.73379	-1.57916
8	0	-1.97696	0.76398	-1.64568
8	0	-3.00678	2.39632	-0.47893
1	0	1.44115	2.79046	1.09647
1	0	2.24807	3.43547	-0.31567
1	0	4.26849	2.80379	0.40657
6	0	5.03828	0.80945	0.45038
6	0	5.83538	-1.59795	0.48696
6	0	-2.18969	-2.49838	-0.93801
6	0	-4.26791	-2.19132	0.22632
1	0	-4.11527	-0.80464	1.90508
1	0	0.76748	4.15424	-2.04847
1	0	-0.11221	4.55984	-0.56313
1	0	-0.94916	3.75439	-1.89958
6	0	-4.18991	2.15959	-1.26043
1	0	6.05677	1.13807	0.64572
1	0	6.51538	-1.35742	1.31233
1	0	6.44403	-1.66461	-0.42486
1	0	5.41541	-2.59169	0.67586
1	0	-1.59225	-2.92472	-1.73749
6	0	-3.54513	-2.79327	-0.805
1	0	-5.32825	-2.3936	0.34779
1	0	-3.98791	2.31716	-2.32381
1	0	-4.9291	2.87341	-0.89658
1	0	-4.53918	1.13305	-1.11404
1	0	-4.02042	-3.46988	-1.50724



IM4-B-1b

E(RB3LYP) = -1746.62960171
G(correction)= 0.306032
$E(RM06)_{dioxane}$ = -1747.29098345
$E(RM06)_{iPrOH}$ = -1747.30702587
Imaginary frequencies: 0

46	0	-0.90642	-0.98859	-0.6679
7	0	-1.1904	0.85599	0.16873
6	0	1.03681	-0.30018	-0.85888
6	0	-0.43827	-2.64027	-1.47944
6	0	0.01114	1.69938	0.24763
16	0	-2.11781	0.77049	1.51255
6	0	1.23107	0.74828	0.24928
1	0	1.78285	-1.09456	-0.79732
1	0	1.04948	0.14774	-1.85709
8	0	-0.12343	-3.63973	-1.94251
1	0	0.01483	2.33105	1.14136
6	0	0.04432	2.61785	-0.97188
6	0	-3.45153	-0.22671	0.77853
8	0	-2.68712	2.07792	1.87961
8	0	-1.54077	-0.04332	2.60113
6	0	2.59739	1.46994	0.12911
1	0	1.19756	0.24214	1.22197
8	0	-0.27915	2.30981	-2.09806
8	0	0.55933	3.82303	-0.6439
7	0	-3.08449	-1.17062	-0.09943
6	0	-4.76616	-0.01827	1.17701
1	0	2.6696	1.95009	-0.85482
1	0	2.63069	2.27592	0.87359
6	0	3.76316	0.52794	0.32897
6	0	0.71674	4.74086	-1.73913
6	0	-4.03448	-1.96408	-0.61848
6	0	-5.74897	-0.84963	0.64042
1	0	-4.98939	0.78236	1.8735
6	0	4.49868	0.03601	-0.75527
6	0	4.10479	0.07938	1.61234
1	0	1.38839	4.32367	-2.49541
1	0	1.14065	5.64679	-1.30496
1	0	-0.25088	4.95041	-2.20337
1	0	-3.69757	-2.70797	-1.33337
6	0	-5.37766	-1.84066	-0.26998
1	0	-6.78968	-0.7225	0.92357
6	0	5.54055	-0.87342	-0.56448
1	0	4.25018	0.3653	-1.76192
6	0	5.14504	-0.82813	1.80229
1	0	3.54485	0.44333	2.47152
1	0	-6.11235	-2.50488	-0.71262
6	0	5.88413	-1.31978	0.71692
1	0	6.0949	-1.24117	-1.42542
1	0	5.38894	-1.1609	2.80903
6	0	7.0331	-2.278	0.9305
1	0	7.9621	-1.73907	1.16082
1	0	7.22145	-2.88494	0.03823
1	0	6.83774	-2.95792	1.76735

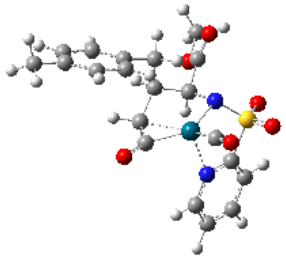


TS3-A-1b

E(RB3LYP) = -1859.9259345

G(correction)= 0.312811
$E(RM06)_{dioxane}$ = -1860.56026923
$E(RM06)_{iPrOH}$ = -1860.57469735
Imaginary frequencies: 1 (-273.1962 cm^{-1})

46	0	-0.00988	-0.64113	1.18382
6	0	1.46033	-1.65567	0.02645
6	0	-1.32941	0.04294	2.49924
6	0	0.70739	-2.35198	1.57899
6	0	1.08118	-1.93555	-1.30506
6	0	2.75981	-1.23553	0.35053
8	0	-2.06305	0.46128	3.26095
8	0	0.79486	-3.44136	1.98161
6	0	-0.26813	-2.4494	-1.78474
6	0	2.08192	-1.76271	-2.27136
6	0	3.73607	-1.05391	-0.62983
1	0	3.00656	-1.03202	1.38929
6	0	-1.60189	-1.99025	-1.15726
1	0	-0.32109	-2.25872	-2.86398
1	0	-0.2405	-3.54545	-1.68387
1	0	1.83725	-1.95174	-3.31364
6	0	3.36839	-1.33199	-1.95084
6	0	5.10616	-0.52623	-0.27985
6	0	-1.87644	-0.47221	-1.24011
6	0	-2.75075	-2.76253	-1.82981
1	0	-1.61265	-2.25711	-0.09427
1	0	4.09801	-1.20343	-2.74716
1	0	5.86509	-0.8747	-0.98806
1	0	5.11156	0.57157	-0.3015
1	0	5.41191	-0.83541	0.72552
7	0	-0.76985	0.28759	-0.64245
1	0	-2.01254	-0.16872	-2.28633
6	0	-3.15603	-0.14842	-0.45382
1	0	-2.59605	-3.84393	-1.74476
1	0	-2.82182	-2.51502	-2.89655
1	0	-3.71056	-2.5287	-1.35944
16	0	-0.8805	1.91204	-0.68038
8	0	-3.41399	-0.60183	0.64655
8	0	-3.89967	0.76981	-1.08305
6	0	0.83521	2.29277	-0.2167
8	0	-1.73174	2.47268	0.39651
8	0	-1.08198	2.43148	-2.048
6	0	-4.91001	1.40939	-0.27984
7	0	1.28401	1.73014	0.90622
6	0	1.58128	3.15753	-1.01435
1	0	-5.5855	0.66814	0.15497
1	0	-5.444	2.07341	-0.95966
1	0	-4.41859	1.98145	0.51129
6	0	2.53403	2.01787	1.28814
6	0	2.88065	3.45387	-0.60339
1	0	1.14275	3.56154	-1.91939
1	0	2.87611	1.53764	2.20177
6	0	3.36817	2.87699	0.57105
1	0	3.50316	4.12355	-1.19018
1	0	4.37151	3.08626	0.92883

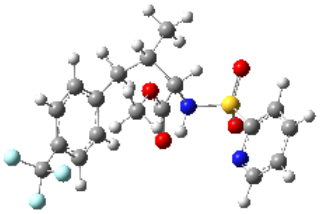


TS3-B-1b

E(RB3LYP) = -1859.9101771
G(correction)= 0.309358
$E(RM06)_{dioxane}$ = -1860.55134184
$E(RM06)_{iPrOH}$ = -1860.56995943
Imaginary frequencies: 1 (-251.254 cm^{-1})

46	0	-0.03247	-1.27367	-0.51941
6	0	1.29726	-1.72997	0.72817
6	0	0.02573	-2.5524	-1.96285
7	0	-1.14017	0.56237	-0.89889
8	0	2.04048	-2.47895	1.22734
8	0	0.04931	-3.31297	-2.81504
6	0	-0.75421	1.49954	0.16781
16	0	-2.73902	0.33285	-1.01725
6	0	0.71832	1.25723	0.59585
1	0	-1.36716	1.37921	1.07445
6	0	-0.92222	2.95747	-0.28287
6	0	-3.16914	-0.61412	0.50243
8	0	-3.00354	-0.58317	-2.13495
8	0	-3.50607	1.58603	-0.88256
6	0	0.91492	-0.0979	1.34638
6	0	1.72912	1.49747	-0.55826
1	0	0.93593	1.99536	1.38408
8	0	-0.60709	3.4018	-1.36157
8	0	-1.42336	3.70341	0.72587
7	0	-2.23772	-1.4552	0.9611
6	0	-4.42132	-0.45502	1.09441
1	0	0.12503	-0.2712	2.08138
1	0	1.88139	-0.05455	1.85143
1	0	1.72672	2.56836	-0.78217
1	0	1.36034	1.00276	-1.46178
6	0	3.1233	1.02173	-0.2279
6	0	-1.65048	5.08493	0.39947
6	0	-2.53118	-2.20036	2.03652
6	0	-4.71999	-1.23344	2.21149
1	0	-5.11672	0.26805	0.68352
6	0	3.65699	-0.12301	-0.83198
6	0	3.89959	1.67604	0.74034
1	0	-0.71656	5.56962	0.09955
1	0	-2.0486	5.54095	1.3067
1	0	-2.36983	5.16205	-0.42025
1	0	-1.74891	-2.87392	2.37873
6	0	-3.7595	-2.12703	2.6919
1	0	-5.68476	-1.14345	2.70286
6	0	4.91765	-0.60491	-0.47462
1	0	3.07668	-0.64262	-1.59122

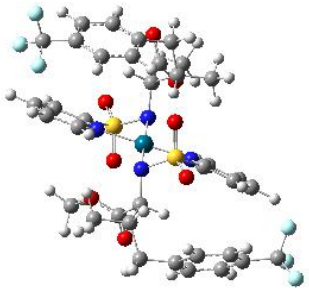
6	0	5.1574	1.19354	1.09731
1	0	3.51181	2.57286	1.22012
1	0	-3.95148	-2.75017	3.55951
6	0	5.68945	0.04276	0.49664
1	0	5.30551	-1.4986	-0.95816
1	0	5.73894	1.71836	1.8523
6	0	7.06637	-0.45884	0.86421
1	0	7.84106	0.03965	0.26637
1	0	7.29601	-0.26562	1.91795
1	0	7.16157	-1.53566	0.68855



1c

E(RB3LYP) = -1805.47933299
G(correction)= 0.299745
$E(RM06)_{dioxane}$ = --1805.00502184
$E(RM06)_{iPrOH}$ = -1805.02206986
Imaginary frequencies: 0

1	0	-1.83643	-0.959	1.37664
6	0	-1.05279	-1.06707	0.61669
6	0	-0.14208	0.15392	0.78438
7	0	-1.6609	-1.02855	-0.71983
6	0	-0.3682	-2.43765	0.88899
8	0	0.01475	1.01238	-0.05782
8	0	0.42904	0.1728	1.99751
1	0	-1.20408	-0.34316	-1.32539
16	0	-3.32734	-0.82576	-0.83066
1	0	0.16744	-2.32662	1.83981
6	0	-1.43434	-3.52977	1.04181
6	0	0.6488	-2.83985	-0.20681
6	0	1.3167	1.28468	2.24411
8	0	-3.6661	-0.95074	-2.24456
8	0	-3.93914	-1.67472	0.19778
6	0	-3.60146	0.89486	-0.31519
1	0	-0.96341	-4.49475	1.26076
1	0	-2.02352	-3.62963	0.12564
1	0	-2.13243	-3.29505	1.85172
1	0	1.01175	-3.84695	0.03579
1	0	0.11853	-2.9153	-1.16226
6	0	1.82306	-1.89691	-0.32949
1	0	1.68607	1.13773	3.25907
1	0	0.76999	2.22791	2.16393
1	0	2.14182	1.28264	1.52902
6	0	-4.43549	1.17781	0.76329
7	0	-2.92986	1.79217	-1.02963
6	0	2.77185	-1.81663	0.70214
6	0	1.96037	-1.04271	-1.42887
6	0	-4.57927	2.52246	1.11256
1	0	-4.93703	0.37614	1.29271
6	0	-3.07284	3.07294	-0.679
6	0	3.79757	-0.88016	0.6602
1	0	2.68934	-2.48545	1.55524
6	0	2.97912	-0.09227	-1.47761
1	0	1.24	-1.09728	-2.24053
6	0	-3.88652	3.48634	0.38134
1	0	-5.21807	2.80884	1.94321
1	0	-2.51137	3.79547	-1.26652
6	0	3.88959	-0.00276	-0.42575
1	0	4.52171	-0.81708	1.4664
1	0	3.05638	0.5879	-2.31886
1	0	-3.96794	4.54114	0.62466
6	0	4.89436	1.10955	-0.37826
9	0	4.43238	2.14275	0.37942
9	0	6.06219	0.71808	0.18116
9	0	5.17265	1.61261	-1.59889

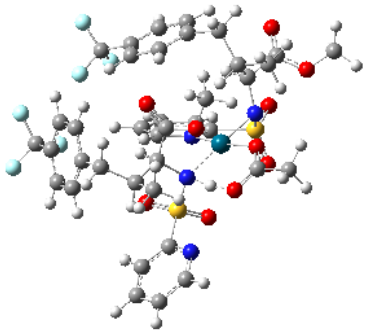


IM1-1c

E(RB3LYP) = -3736.54680603
G(correction)= 0.611453
$E(RM06)_{dioxane}$ = -3736.77268895
$E(RM06)_{iPrOH}$ = -3736.79966982
Imaginary frequencies: 0

6	0	2.23752	-2.0105	0.61705
1	0	1.5235	-2.47335	-0.05343
6	0	3.41801	-2.62309	1.02817
7	0	1.91918	-0.77864	1.04118
1	0	3.67514	-3.59933	0.63698
6	0	4.28147	-1.9385	1.88477
6	0	2.73533	-0.12684	1.88654
46	0	0.26489	0.27257	0.43045
1	0	5.22374	-2.38772	2.18133
6	0	3.93244	-0.66235	2.3339
16	0	2.10863	1.52506	2.35602
7	0	-1.39569	1.34579	-0.14167
7	0	1.37156	1.96661	0.94285
1	0	4.56587	-0.0734	2.98791
8	0	1.07561	1.30283	3.37707
8	0	3.29505	2.33208	2.67174
6	0	-1.78908	2.50091	0.41736
6	0	-2.17838	0.7383	-1.05143
6	0	2.36273	2.35446	-0.08793
1	0	-1.10011	2.93432	1.13438
6	0	-3.01302	3.075	0.07487
16	0	-1.47237	-0.84569	-1.62613
6	0	-3.41265	1.23516	-1.43281

1	0	3.19539	1.64221	-0.11119
6	0	3.02856	3.70323	0.17348
6	0	1.73378	2.36012	-1.51241
1	0	-3.31526	4.00319	0.54766
6	0	-3.83764	2.43359	-0.85027
7	0	-0.85068	-1.41452	-0.19594
8	0	-0.35071	-0.51556	-2.51835
8	0	-2.60185	-1.62316	-2.15387
1	0	-4.02991	0.67866	-2.12684
8	0	2.26695	4.55125	0.87807
8	0	4.1195	3.98494	-0.28367
1	0	1.09394	1.47235	-1.56876
6	0	0.86684	3.59373	-1.7861
6	0	2.82179	2.18037	-2.60036
1	0	-4.81186	2.83806	-1.10149
6	0	-1.93357	-1.8028	0.75015
6	0	2.88306	5.81343	1.18291
1	0	0.16667	3.77456	-0.96657
1	0	1.481	4.49433	-1.90426
1	0	0.29374	3.4543	-2.70945
1	0	2.3199	2.19799	-3.57575
1	0	3.51405	3.02779	-2.56861
6	0	3.57409	0.87866	-2.43279
6	0	-2.51062	-3.22675	0.47784
6	0	-1.49841	-1.68899	2.20643
1	0	-2.76717	-1.09707	0.68247
1	0	3.78946	5.65371	1.77286
1	0	2.14233	6.36775	1.75971
1	0	3.1412	6.34929	0.26491
6	0	4.85566	0.85797	-1.8617
6	0	2.956	-0.34008	-2.74952
6	0	-3.90453	-3.38727	1.1441
1	0	-2.66008	-3.27169	-0.60352
6	0	-1.55463	-4.35471	0.87651
8	0	-2.24903	-1.31529	3.08649
8	0	-0.24272	-2.10677	2.42602
1	0	5.32314	1.79763	-1.57974
6	0	5.49976	-0.34957	-1.59988
6	0	3.59867	-1.55051	-2.49824
1	0	1.9502	-0.34586	-3.15763
1	0	-3.80255	-3.33117	2.23369
1	0	-4.27658	-4.39144	0.90436
6	0	-4.87971	-2.33781	0.65507
1	0	-0.56042	-4.1791	0.45402
1	0	-1.44813	-4.43611	1.96413
1	0	-1.92543	-5.31528	0.5015
6	0	0.24645	-1.94586	3.77484
1	0	6.48032	-0.35742	-1.13392
6	0	4.86803	-1.55627	-1.91398
1	0	3.10561	-2.48762	-2.73482
6	0	-5.39898	-2.41076	-0.64642
6	0	-5.17482	-1.20934	1.43239
1	0	1.23825	-2.39971	3.77245
1	0	0.31178	-0.88241	4.0147
1	0	-0.41218	-2.45514	4.48225
6	0	5.57425	-2.84798	-1.62798
1	0	-5.17002	-3.27281	-1.26654
6	0	-6.15378	-1.36964	-1.17447
6	0	-5.92741	-0.15725	0.90963
1	0	-4.75215	-1.12798	2.42922
9	0	6.50789	-3.1482	-2.55588
9	0	4.71807	-3.90207	-1.57509
9	0	6.22044	-2.81098	-0.43056
1	0	-6.52398	-1.42388	-2.19397
6	0	-6.40232	-0.23059	-0.40027
1	0	-6.11958	0.72707	1.50734
6	0	-7.12917	0.91827	-1.03042
9	0	-6.49658	1.32689	-2.1737
9	0	-7.19221	2.0033	-0.2234
9	0	-8.39006	0.60609	-1.39266

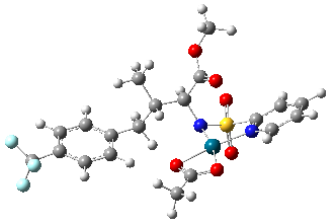


TS1-1c

E(RB3LYP) = -3965.63464401
G(correction)= 0.665087
$E(RM06)_{dioxane}$ = -3965.79508451
$E(RM06)_{iPrOH}$ = -3965.83209835
Imaginary frequencies: 1 (-1020.0882 cm^{-1})

6	0	-0.34975	1.20125	-1.08551
1	0	-1.05457	0.87673	-0.33764
6	0	-0.53684	2.39907	-1.76768
7	0	0.70925	0.40728	-1.31855
1	0	-1.40113	3.0079	-1.53704
6	0	0.40811	2.79857	-2.70972
6	0	1.61819	0.79804	-2.23545
46	0	1.21777	-1.36459	-0.34626
1	0	0.29647	3.74457	-3.22926
6	0	1.51469	1.98133	-2.94772
16	0	3.06796	-0.30104	-2.34851
7	0	3.14906	-0.77288	-0.75569
1	0	2.30703	2.24945	-3.63767
8	0	2.70687	-1.44924	-3.17731
8	0	4.19025	0.57053	-2.72785
6	0	3.69452	0.29163	0.10599
1	0	3.23626	1.26078	-0.12133
6	0	5.19349	0.52756	-0.09303
6	0	3.41547	-0.00644	1.60529
8	0	5.85516	-0.55125	-0.5222
8	0	5.72211	1.58817	0.18451
1	0	2.36006	-0.30856	1.64457
6	0	4.26364	-1.16174	2.14566
6	0	3.54336	1.2766	2.46653

6	0	7.25024	-0.34611	-0.79711
1	0	4.135	-2.04617	1.51731
1	0	5.32713	-0.89891	2.16846
1	0	3.96286	-1.40948	3.17022
1	0	3.32016	1.00392	3.5065
1	0	4.57667	1.63518	2.43666
6	0	2.59223	2.3574	2.0004
1	0	7.36703	0.40358	-1.58437
1	0	7.6258	-1.31378	-1.12995
1	0	7.77731	-0.01143	0.10107
6	0	3.03546	3.40221	1.17435
6	0	1.2237	2.25976	2.28521
1	0	4.08883	3.45904	0.91573
6	0	2.13029	4.31109	0.63136
6	0	0.31232	3.16404	1.74306
1	0	0.85534	1.45582	2.91436
1	0	2.47829	5.10089	-0.02742
6	0	0.76505	4.18748	0.90784
1	0	-0.74632	3.05159	1.94741
6	0	-0.18896	5.17648	0.3058
9	0	-0.14099	6.3783	0.92022
9	0	0.08637	5.40358	-1.00542
9	0	-1.47843	4.75322	0.36653
1	0	-3.11949	3.55808	1.70478
6	0	-3.56263	2.62616	1.37475
6	0	-3.38673	1.45639	2.11369
6	0	-4.31187	2.59719	0.19672
6	0	-3.96261	0.24822	1.69707
1	0	-2.77311	1.47002	3.00855
6	0	-4.896	1.40141	-0.23072
6	0	-4.45349	3.83339	-0.64516
6	0	-3.70961	-1.0396	2.45347
6	0	-4.72406	0.24202	0.51919
1	0	-5.48176	1.38356	-1.14392
9	0	-4.28221	4.96352	0.06836
9	0	-3.53548	3.86146	-1.65267
9	0	-5.66537	3.89995	-1.24109
6	0	-2.85522	-2.05174	1.64848
1	0	-3.2214	-0.82259	3.40869
1	0	-4.66362	-1.53072	2.68633
1	0	-5.17492	-0.68589	0.17683
6	0	-1.52182	-1.39713	1.17017
1	0	-3.41967	-2.27081	0.73902
6	0	-2.65062	-3.36266	2.41528
1	0	-1.7778	-0.4023	0.81037
7	0	-0.80926	-2.12103	0.08244
6	0	-0.63145	-1.16381	2.38233
1	0	-2.01054	-4.05499	1.86278
1	0	-2.18846	-3.18192	3.39285
1	0	-3.61668	-3.84983	2.58903
16	0	-1.64492	-2.14044	-1.40862
8	0	-0.75887	-0.20166	3.11621
8	0	0.23612	-2.15629	2.60504
6	0	-2.88751	-3.4663	-1.29296
8	0	-2.40885	-0.88746	-1.55151
8	0	-0.67041	-2.54786	-2.41998
6	0	1.07624	-2.0242	3.76494
7	0	-2.46118	-4.61915	-0.79884
6	0	-4.1752	-3.21466	-1.768
1	0	1.79319	-2.84077	3.69403
1	0	1.59096	-1.06164	3.75609
1	0	0.47499	-2.10545	4.67461
6	0	-3.34439	-5.62229	-0.74731
6	0	-5.08297	-4.2731	-1.71437
1	0	-4.43839	-2.23462	-2.14851
1	0	-2.97873	-6.55778	-0.33077
6	0	-4.66304	-5.49833	-1.19368
1	0	-6.10037	-4.14151	-2.07133
1	0	-5.34096	-6.34383	-1.13213
1	0	-0.35821	-3.30091	0.37131
8	0	0.2158	-4.32396	0.66173
6	0	1.47113	-4.13389	0.74608
8	0	2.0704	-3.04761	0.49528
6	0	2.32854	-5.30794	1.15653
1	0	1.77495	-5.96479	1.83136
1	0	2.58606	-5.8773	0.2559
1	0	3.25567	-4.96131	1.61755

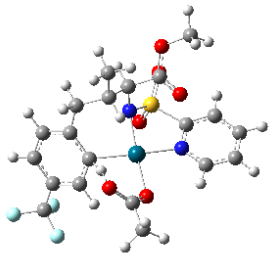


IM2-1c

E(RB3LYP) = -2160.13169566
G(correction)= 0.331679
$E(RM06)_{dioxane}$ = -2160.76904386
$E(RM06)_{iPrOH}$ = -2160.78847565
Imaginary frequencies: 0

46	0	1.53249	1.31152	0.07806
7	0	3.53881	0.94456	0.00853
7	0	1.37443	-0.5606	0.88485
6	0	3.99713	-0.11505	0.69073
6	0	4.36477	1.62827	-0.79918
6	0	0.85432	-1.65578	0.0537
16	0	2.73978	-0.88233	1.75214
6	0	5.30712	-0.55864	0.5952
1	0	3.92811	2.46842	-1.32868
6	0	5.69933	1.25805	-0.93892
6	0	-0.62451	-1.37484	-0.33276
1	0	0.8754	-2.57642	0.64563
6	0	1.71544	-1.90686	-1.18795
8	0	3.03993	-2.32023	1.79953
8	0	2.74702	-0.07974	2.97614
6	0	6.17563	0.14783	-0.23773
1	0	5.61217	-1.43675	1.15379
1	0	6.34548	1.82897	-1.59669
6	0	-1.46893	-1.26664	0.9619
6	0	-1.17187	-2.44993	-1.28216
1	0	-0.662	-0.40547	-0.84521

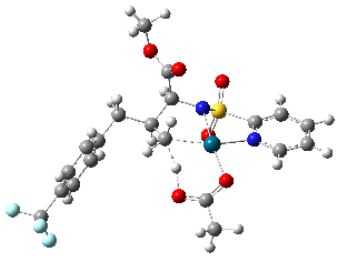
8	0	2.27182	-1.04761	-1.84478
8	0	1.78273	-3.21791	-1.47749
1	0	7.2103	-0.16493	-0.34231
1	0	-1.414	-2.22616	1.49361
1	0	-1.00617	-0.51601	1.60976
6	0	-2.91449	-0.90751	0.70367
1	0	-2.23224	-2.2707	-1.48073
1	0	-1.07039	-3.45109	-0.84621
1	0	-0.64879	-2.45148	-2.24365
6	0	2.5373	-3.55584	-2.65377
6	0	-3.26464	0.40009	0.33037
6	0	-3.92974	-1.86838	0.80049
1	0	2.09955	-3.08448	-3.53857
1	0	2.48791	-4.64204	-2.73124
1	0	3.57369	-3.2227	-2.54969
6	0	-4.58926	0.73248	0.0605
1	0	-2.48684	1.15318	0.24996
6	0	-5.25913	-1.54254	0.53373
1	0	-3.67575	-2.88618	1.08627
6	0	-5.58995	-0.23924	0.15983
1	0	-4.85185	1.7444	-0.2326
1	0	-6.03598	-2.29652	0.60712
6	0	-7.02337	0.14079	-0.0761
9	0	-7.77599	-0.91875	-0.45316
9	0	-7.59957	0.65256	1.03908
9	0	-7.14195	1.08575	-1.0392
8	0	-0.42436	2.05791	-0.06822
6	0	0.02742	3.13937	-0.58195
8	0	1.29136	3.23704	-0.74306
6	0	-0.90272	4.25288	-0.95662
1	0	-0.38338	4.99443	-1.5665
1	0	-1.76445	3.84799	-1.49531
1	0	-1.2739	4.73029	-0.0426



TS2-A-1c

E(RB3LYP) = -2160.10116604
G(correction)= 0.330606
$E(RM06)_{dioxane}$ = -2160.74256878
$E(RM06)_{iPrOH}$ = -2160.76277577
Imaginary frequencies: 1 (-1429.4095 cm^{-1})

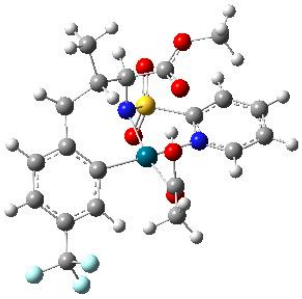
46	0	0.00778	0.61803	0.35361
7	0	-0.86376	-0.9037	-0.68961
6	0	1.6902	-0.62444	0.66522
16	0	-1.56185	-0.27439	-2.03505
6	0	-1.64392	-1.88799	0.07265
6	0	1.59128	-2.02531	0.47696
6	0	2.81723	0.04981	0.14242
6	0	-2.25088	1.29176	-1.40213
8	0	-2.70481	-1.08883	-2.47903
8	0	-0.52472	0.13457	-2.98466
6	0	-0.88849	-2.27589	1.37226
1	0	-1.77098	-2.78931	-0.53649
6	0	-3.04119	-1.38505	0.4507
6	0	0.4936	-2.88266	1.07761
6	0	2.61069	-2.68936	-0.22068
6	0	3.81589	-0.62312	-0.5504
1	0	2.91256	1.12067	0.29584
7	0	-1.56515	1.82119	-0.38207
6	0	-3.37775	1.88968	-1.94674
6	0	-1.70893	-3.27243	2.21018
1	0	-0.76466	-1.36008	1.96416
8	0	-3.28442	-0.27641	0.88522
8	0	-3.97177	-2.33805	0.27576
1	0	0.35407	-3.76929	0.44446
1	0	0.88701	-3.26466	2.03213
1	0	2.54277	-3.76458	-0.36834
6	0	3.70481	-2.00456	-0.73821
6	0	4.97474	0.12257	-1.14836
6	0	-1.96058	2.98881	0.1456
6	0	-3.79643	3.10397	-1.40272
1	0	-3.90272	1.39885	-2.75881
1	0	-1.14929	-3.56203	3.10602
1	0	-1.93267	-4.18158	1.63955
1	0	-2.65977	-2.84385	2.53961
6	0	-5.31666	-1.95253	0.6045
1	0	4.47983	-2.53923	-1.2788
9	0	5.20449	1.29498	-0.51368
9	0	4.76581	0.41301	-2.45251
9	0	6.11742	-0.60276	-1.08928
1	0	-1.36021	3.36144	0.96842
6	0	-3.07559	3.66341	-0.34534
1	0	-4.67539	3.60672	-1.79564
1	0	-5.38867	-1.66253	1.65699
1	0	-5.93101	-2.83021	0.40278
1	0	-5.62968	-1.11098	-0.01957
1	0	-3.37356	4.60512	0.10314
1	0	1.43878	-0.08855	1.9299
8	0	1.50063	0.57973	3.00719
6	0	1.2131	1.78686	2.70897
8	0	0.7273	2.15191	1.59435
6	0	1.49698	2.84258	3.75068
1	0	1.06209	2.53753	4.7069
1	0	2.58053	2.9176	3.89187
1	0	1.09903	3.81002	3.44176



TS2-B-1c

E(RB3LYP) = -2160.08064161
G(correction)= 0.328021
$E(RM06)_{dioxane}$ = -2160.7299108
$E(RM06)_{iPrOH}$ = -2160.75039736
Imaginary frequencies: 1 (-1321.6248 cm^{-1})

46	0	-1.59431	-0.82715	-0.51019
7	0	-1.98178	1.05083	0.12208
7	0	-3.56059	-1.17677	0.10665
6	0	-0.85633	1.99372	0.12112
16	0	-2.86946	1.00101	1.50902
6	0	-4.06161	-0.23746	0.92103
6	0	-4.34645	-2.1826	-0.30832
6	0	0.4699	1.19153	0.06531
1	0	-0.85794	2.63023	1.01141
6	0	-0.9895	2.9036	-1.09937
8	0	-3.58973	2.26192	1.73852
8	0	-2.17208	0.39465	2.65833
6	0	-5.38015	-0.2341	1.35116
1	0	-3.87343	-2.9117	-0.9569
6	0	-5.68015	-2.26391	0.08606
6	0	0.36829	0.08759	-1.0073
6	0	1.69813	2.11395	-0.14643
1	0	0.56497	0.72362	1.05241
8	0	-1.27655	2.54146	-2.21958
8	0	-0.68227	4.17812	-0.779
6	0	-6.205	-1.27471	0.92052
1	0	-5.7301	0.56829	1.99134
1	0	-6.29302	-3.08712	-0.26505
1	0	1.38176	-0.24959	-1.26958
1	0	-0.0424	0.46646	-1.94921
1	0	1.65835	2.54529	-1.15409
1	0	1.63514	2.95292	0.55824
6	0	3.0049	1.38004	0.0449
6	0	-0.71681	5.11149	-1.8728
1	0	-7.24489	-1.31215	1.23102
6	0	3.8063	1.02494	-1.04739
6	0	3.41939	0.99648	1.32991
1	0	0.00137	4.82239	-2.64587
1	0	-0.45254	6.07784	-1.44268
1	0	-1.71679	5.14422	-2.31371
6	0	4.98911	0.307	-0.86886
1	0	3.50027	1.31269	-2.05009
6	0	4.59647	0.27954	1.51824
1	0	2.80792	1.25999	2.18956
6	0	5.38375	-0.06772	0.41541
1	0	5.59885	0.03198	-1.72292
1	0	4.90456	-0.01931	2.51511
6	0	6.68288	-0.79095	0.63303
9	0	6.59206	-1.69428	1.63628
9	0	7.09004	-1.45128	-0.47441
9	0	7.67924	0.06367	0.97021
1	0	0.37201	-1.28574	-0.68486
8	0	0.78286	-2.55593	-0.69341
6	0	-0.21173	-3.26301	-1.03808
8	0	-1.3915	-2.80039	-1.15694
6	0	0.01759	-4.72876	-1.31882
1	0	-0.90134	-5.21323	-1.65134
1	0	0.79674	-4.83285	-2.07991
1	0	0.38467	-5.21158	-0.40728

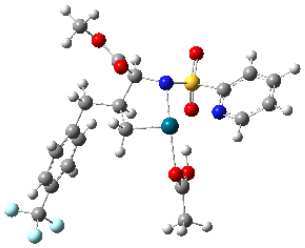


IM3-A-1c

E(RB3LYP) = -2160.12593627
G(correction)= 0.338781
$E(RM06)_{dioxane}$ = -2160.76631381
$E(RM06)_{iPrOH}$ = -2160.78645403
Imaginary frequencies: 0

46	0	0.06375	-0.4259	-0.40362
7	0	1.24098	1.20076	-0.77192
6	0	-1.62818	0.65019	-0.36376
16	0	2.43473	0.78028	-1.8181
6	0	1.63102	1.92025	0.45171
6	0	-1.79528	2.03823	-0.14462
6	0	-2.7658	-0.14014	-0.56713
6	0	2.97623	-0.82766	-1.14143
8	0	3.59267	1.68151	-1.73053
8	0	1.83471	0.46321	-3.11532
6	0	0.39102	2.56901	1.11315
1	0	2.35568	2.69298	0.17612
6	0	2.30773	0.98043	1.46111
6	0	-0.65169	3.01522	0.0621
6	0	-3.10151	2.55499	-0.10028
6	0	-4.05523	0.39491	-0.49602
1	0	-2.66633	-1.20196	-0.76711
7	0	1.99	-1.53974	-0.57912
6	0	4.29481	-1.26249	-1.20289
6	0	0.84257	3.7294	2.01174
1	0	-0.07824	1.81039	1.74946
8	0	1.73573	0.13737	2.14341
8	0	3.63416	1.12885	1.48251
1	0	-0.14891	3.18947	-0.89614
1	0	-1.07579	3.97582	0.37584
1	0	-3.2351	3.62003	0.07583
6	0	-4.2303	1.75486	-0.25897
6	0	-5.21857	-0.5454	-0.5687

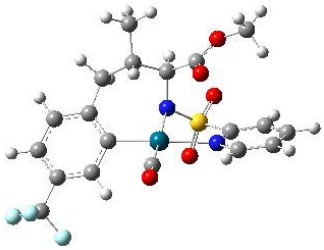
6	0	2.27438	-2.74587	-0.06596
6	0	4.5907	-2.51666	-0.66762
1	0	5.04768	-0.62051	-1.64663
1	0	-0.00024	4.12181	2.59074
1	0	1.25632	4.55033	1.41338
1	0	1.61567	3.41188	2.7233
6	0	4.36637	0.20232	2.3085
1	0	-5.22677	2.17894	-0.19635
9	0	-6.39558	0.08727	-0.75563
9	0	-5.08204	-1.45991	-1.5552
9	0	-5.34169	-1.26213	0.59149
1	0	1.43865	-3.2787	0.37638
6	0	3.56419	-3.27298	-0.09544
1	0	5.60711	-2.8991	-0.69401
1	0	4.03005	0.26594	3.34635
1	0	5.41079	0.49951	2.2181
1	0	4.22263	-0.81821	1.943
1	0	3.75699	-4.25217	0.33017
1	0	0.05704	-0.62836	2.18917
8	0	-0.71821	-1.11367	2.58734
6	0	-1.30408	-1.93462	1.74274
8	0	-0.95507	-2.10133	0.56215
6	0	-2.49959	-2.6528	2.29454
1	0	-2.53038	-2.61307	3.38406
1	0	-3.39083	-2.16102	1.88352
1	0	-2.50201	-3.68594	1.93896



IM3-B-1c

E(RB3LYP) = -2160.10950624
G(correction)= 0.331114
$E(RM06)_{dioxane}$ = -2160.75866397
$E(RM06)_{iPrOH}$ = -2160.77832548
Imaginary frequencies: 0

46	0	-1.52211	-0.47915	-0.94186
7	0	-2.044	1.12368	0.23767
6	0	0.27484	0.43767	-1.02838
6	0	-0.93614	2.08379	0.41312
16	0	-2.54478	0.35677	1.5977
6	0	0.40316	1.32206	0.22406
1	0	1.08553	-0.29422	-1.10313
1	0	0.23673	1.03756	-1.94597
1	0	-0.97979	2.56694	1.39508
6	0	-1.09017	3.16938	-0.64647
6	0	-3.9193	-0.5437	0.82178
8	0	-3.08746	1.26854	2.61635
8	0	-1.61571	-0.70521	2.10183
6	0	1.65211	2.23861	0.19455
1	0	0.48766	0.67098	1.103
8	0	-1.48121	3.00826	-1.78049
8	0	-0.65554	4.35747	-0.16581
7	0	-3.61395	-1.15384	-0.33179
6	0	-5.16523	-0.60525	1.42916
1	0	1.62408	2.86627	-0.70411
1	0	1.61709	2.91858	1.05518
6	0	2.93037	1.43422	0.22253
6	0	-0.66657	5.4399	-1.11164
6	0	-4.56743	-1.87201	-0.94009
6	0	-6.15288	-1.36056	0.79337
1	0	-5.33674	-0.0691	2.35584
6	0	3.66003	1.18759	-0.94764
6	0	3.38113	0.8639	1.42235
1	0	-0.01788	5.21229	-1.9629
1	0	-0.29664	6.30956	-0.56764
1	0	-1.68122	5.61622	-1.47917
1	0	-4.2832	-2.34252	-1.87641
6	0	-5.85034	-2.00449	-0.40737
1	0	-7.14531	-1.44088	1.22712
6	0	4.80895	0.3982	-0.9253
1	0	3.32009	1.61443	-1.88761
6	0	4.5263	0.07317	1.45552
1	0	2.82277	1.03938	2.3388
1	0	-6.5937	-2.59623	-0.93127
6	0	5.2426	-0.16165	0.27802
1	0	5.36394	0.20984	-1.83856
1	0	4.86312	-0.36793	2.38813
6	0	6.51187	-0.9635	0.32416
9	0	6.46504	-1.92764	1.27305
9	0	6.77253	-1.56971	-0.85747
9	0	7.5856	-0.18823	0.61062
1	0	-0.81531	-1.99895	0.84258
8	0	-0.37429	-2.86471	0.61492
6	0	-0.30626	-3.11708	-0.67793
8	0	-0.72707	-2.38115	-1.58205
6	0	0.36158	-4.42939	-0.98284
1	0	0.33594	-4.62055	-2.05557
1	0	1.3995	-4.39268	-0.63487
1	0	-0.13751	-5.23598	-0.43707



IM4-A-1c

E(RB3LYP) = -2044.3480141
G(correction)= 0.282935
$E(RM06)_{dioxane}$ = -2045.02638699
$E(RM06)_{iPrOH}$ = -2045.04406453
Imaginary frequencies: 0

46	0	0.06472	-0.60799	-0.33252
7	0	-0.90041	0.77774	0.84885
6	0	1.80467	0.44138	-0.13603
6	0	0.83958	-1.73793	-1.67402
16	0	-1.7878	-0.0294	1.96205
6	0	-1.54918	1.88244	0.12662
6	0	1.91958	1.8388	0.01571
6	0	2.95334	-0.35693	-0.03485
8	0	1.20243	-2.38612	-2.54269
6	0	-2.63936	-1.26227	0.91596
8	0	-2.84074	0.80675	2.55319
8	0	-0.88071	-0.80975	2.80801
6	0	-0.49447	2.59194	-0.74942
1	0	-1.95629	2.58786	0.85848
6	0	-2.69387	1.40249	-0.77523
6	0	0.79152	2.86072	0.05447
6	0	3.20786	2.36928	0.22436
6	0	4.21319	0.19805	0.19337
1	0	2.88772	-1.43689	-0.10507
7	0	-1.90006	-1.72473	-0.10105
6	0	-3.95276	-1.65017	1.14671
6	0	-1.07571	3.89833	-1.31236
1	0	-0.26441	1.92565	-1.59034
8	0	-2.55846	0.62909	-1.70496
8	0	-3.87774	1.923	-0.41199
1	0	0.51944	3.01597	1.10776
1	0	1.21215	3.8137	-0.28773
1	0	3.30962	3.44647	0.33681
6	0	4.34598	1.57862	0.31488
6	0	5.41988	-0.69516	0.22312
6	0	-2.44756	-2.61566	-0.939
6	0	-4.51968	-2.58213	0.27591
1	0	-4.49788	-1.21215	1.97547
1	0	-0.36944	4.3643	-2.00768
1	0	-1.28208	4.61467	-0.5075
1	0	-2.01213	3.72801	-1.85612
6	0	-5.0105	1.47202	-1.17477
1	0	5.3204	2.02426	0.48438
9	0	6.43686	-0.1497	0.92726
9	0	5.89284	-0.93761	-1.0254
9	0	5.14391	-1.90162	0.77096
1	0	-1.82263	-2.9526	-1.75957
6	0	-3.7538	-3.07484	-0.78193
1	0	-5.54419	-2.91439	0.41672
1	0	-4.88658	1.71931	-2.2328
1	0	-5.87189	1.99039	-0.75352
1	0	-5.12405	0.3884	-1.07359
1	0	-4.15968	-3.79316	-1.4862

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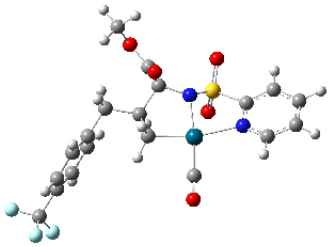
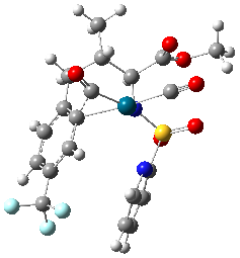


IM4-B-1c

E(RB3LYP) = -2044.34961646
G(correction)= 0.280446
$E(RM06)_{dioxane}$ = -2045.03132412
$E(RM06)_{iPrOH}$ = -2045.04883662
Imaginary frequencies: 0

46	0	-1.49036	-0.91214	-0.78066
7	0	-1.97207	0.80918	0.2164
6	0	0.32879	0.04866	-1.00875
6	0	-0.85993	-2.42213	-1.74756
6	0	-0.88902	1.79949	0.30479
16	0	-2.75741	0.47223	1.61325
6	0	0.44315	1.02464	0.17492
1	0	1.17544	-0.63976	-1.04901
1	0	0.22713	0.57098	-1.96475
8	0	-0.4472	-3.33243	-2.30656
1	0	-0.9181	2.3597	1.24467
6	0	-1.04744	2.80048	-0.83747
6	0	-3.99405	-0.64777	0.88646
8	0	-3.47224	1.64386	2.14546
8	0	-1.97248	-0.33298	2.57066
6	0	1.69138	1.93695	0.06081
1	0	0.52615	0.4453	1.10263
8	0	-1.39179	2.53418	-1.9679
8	0	-0.67879	4.03675	-0.43709
7	0	-3.57121	-1.44959	-0.1009
6	0	-5.28642	-0.67162	1.39535
1	0	1.65558	2.4866	-0.88751
1	0	1.64822	2.68691	0.86073
6	0	2.98073	1.15513	0.15639
6	0	-0.7152	5.04941	-1.45758
6	0	-4.43873	-2.32978	-0.62464
6	0	-6.18252	-1.59265	0.8531
1	0	-5.56185	0.02535	2.17911
6	0	3.73353	0.85211	-0.98508
6	0	3.42534	0.67402	1.39713
1	0	-0.03512	4.79397	-2.27572
1	0	-0.39997	5.97123	-0.96804
1	0	-1.72752	5.15049	-1.85815
1	0	-4.06068	-2.953	-1.42868
6	0	-5.75179	-2.43726	-0.17154
1	0	-7.20315	-1.64664	1.22012
6	0	4.9012	0.09476	-0.89594
1	0	3.40054	1.21222	-1.95521
6	0	4.58828	-0.08402	1.49653
1	0	2.84997	0.89487	2.293
1	0	-6.41915	-3.16408	-0.62231
6	0	5.32896	-0.37498	0.34672

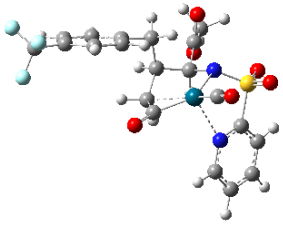
1	0	5.47523	-0.13675	-1.78705
1	0	4.92106	-0.45643	2.46006
6	0	6.61709	-1.13926	0.46757
9	0	6.55529	-2.07667	1.44128
9	0	7.654	-0.32418	0.77831
9	0	6.94448	-1.76885	-0.68378



TS3-A-1c

E(RB3LYP) = -2157.64563893
G(correction)= 0.287937
$E(RM06)_{dioxane}$ = -2158.29857936
$E(RM06)_{iPrOH}$ = -2158.31365476
Imaginary frequencies: 1 (-269.2622 cm^{-1})

46	0	-0.50084	-0.68552	1.16614
6	0	1.01859	-1.62548	0.00416
6	0	-1.85354	-0.09382	2.48665
6	0	0.22888	-2.41216	1.47055
6	0	0.68303	-1.78852	-1.36035
6	0	2.2866	-1.17659	0.39879
8	0	-2.61004	0.27594	3.25051
8	0	0.29676	-3.52898	1.7959
6	0	-0.63121	-2.32042	-1.90926
6	0	1.68519	-1.46763	-2.29028
6	0	3.24413	-0.84673	-0.55231
1	0	2.51266	-1.05371	1.45178
6	0	-1.99581	-1.93981	-1.29376
1	0	-0.66075	-2.07408	-2.9776
1	0	-0.56387	-3.41842	-1.86316
1	0	1.4616	-1.55761	-3.34958
6	0	2.93606	-0.99386	-1.90639
6	0	4.59309	-0.3244	-0.14553
6	0	-2.30614	-0.42658	-1.28917
6	0	-3.10313	-2.69892	-2.04496
1	0	-2.0267	-2.27349	-0.25037
1	0	3.66931	-0.72271	-2.65985
9	0	5.56707	-1.24117	-0.33297
9	0	4.93537	0.76481	-0.87357
9	0	4.62674	0.03648	1.15948
7	0	-1.22175	0.31481	-0.63238
1	0	-2.43565	-0.06129	-2.31633
6	0	-3.60166	-0.17855	-0.50135
1	0	-2.92186	-3.77925	-2.0216
1	0	-3.15326	-2.38712	-3.09576
1	0	-4.08049	-2.51852	-1.58742
16	0	-1.3514	1.94261	-0.58395
8	0	-3.86699	-0.71385	0.56018
8	0	-4.34721	0.77372	-1.07271
6	0	0.36855	2.30259	-0.12362
8	0	-2.20313	2.42464	0.52844
8	0	-1.57347	2.52251	-1.92318
6	0	-5.37772	1.34306	-0.24185
7	0	0.81012	1.72341	0.99431
6	0	1.13392	3.13801	-0.9331
1	0	-6.04923	0.56475	0.12941
1	0	-5.91017	2.04657	-0.88177
1	0	-4.90541	1.86453	0.59458
6	0	2.07852	1.95964	1.35272
6	0	2.45519	3.37085	-0.55014
1	0	0.69725	3.56112	-1.83025
1	0	2.42093	1.46477	2.25742
6	0	2.93956	2.77042	0.61231
1	0	3.09905	4.00355	-1.15441
1	0	3.96633	2.90599	0.93385

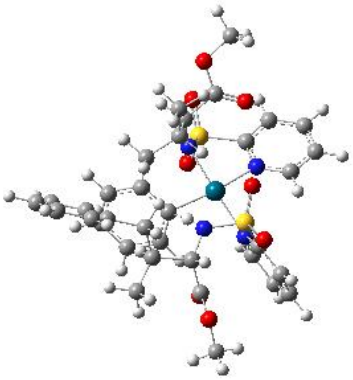


TS3-B-1c

E(RB3LYP) = -2157.6289989
G(correction)= 0.284134
$E(RM06)_{dioxane}$ = -2158.28930239
$E(RM06)_{iPrOH}$ = -2158.30992684
Imaginary frequencies: 1 (-259.1647 cm^{-1})

46	0	-0.62833	-1.30913	-0.54769
6	0	0.81784	-1.68698	0.59323
6	0	-0.69033	-2.66598	-1.91942
7	0	-1.78671	0.52737	-0.88264
8	0	1.64432	-2.38885	1.02259
8	0	-0.74247	-3.47155	-2.72703
6	0	-1.37652	1.47138	0.171
16	0	-3.38607	0.26937	-0.9577
6	0	0.13061	1.2892	0.48906
1	0	-1.91723	1.30437	1.11567
6	0	-1.66239	2.92232	-0.24593
6	0	-3.77018	-0.63208	0.59966
8	0	-3.65174	-0.68619	-2.04214
8	0	-4.17117	1.51425	-0.85544
6	0	0.42233	-0.04892	1.23527
6	0	1.04597	1.54596	-0.7385
1	0	0.38351	2.04297	1.25225
8	0	-1.3061	3.43661	-1.28167
8	0	-2.34502	3.56443	0.72213
7	0	-2.82753	-1.46468	1.05074
6	0	-5.00233	-0.44931	1.22527
1	0	-0.31306	-0.24506	2.01909
1	0	1.41795	0.01817	1.67586
1	0	0.968	2.60601	-0.99333
1	0	0.64766	1.00031	-1.59891

6	0	2.48213	1.15795	-0.48446
6	0	-2.76245	4.89874	0.38538
6	0	-3.09096	-2.17791	2.15478
6	0	-5.26925	-1.19566	2.37221
1	0	-5.70687	0.26584	0.8163
6	0	3.03172	0.01256	-1.07429
6	0	3.28325	1.90711	0.39264
1	0	-1.89861	5.52852	0.15365
1	0	-3.28944	5.27254	1.26389
1	0	-3.42798	4.86898	-0.48145
1	0	-2.30189	-2.8463	2.49148
6	0	-4.29804	-2.08054	2.84626
1	0	-6.21777	-1.0874	2.8907
6	0	4.33648	-0.39015	-0.7877
1	0	2.42948	-0.56957	-1.76727
6	0	4.58637	1.51479	0.68343
1	0	2.88017	2.81005	0.84569
1	0	-4.46534	-2.6791	3.736
6	0	5.11292	0.35944	0.09562
1	0	4.75121	-1.2788	-1.2511
1	0	5.20183	2.10467	1.35543
6	0	6.49865	-0.08848	0.47003
9	0	7.34723	0.95899	0.5841
9	0	6.50496	-0.72471	1.6662
9	0	7.02123	-0.94261	-0.43612



TS(IM1-IM3-Aa)

E(RB3LYP) = -3062.39356893

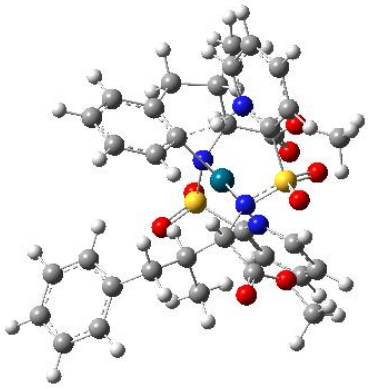
G(correction)= 0.602766

$E(RM06)_{dioxane}$ = -3062.64470287

Imaginary frequencies: 1 (-1425.5891 cm^{-1})

6	0	3.84767	1.8141	-0.7151
1	0	3.10902	2.4924	-1.12697
6	0	5.20199	1.92107	-1.02036
7	0	3.38293	0.84609	0.08732
1	0	5.54218	2.71156	-1.68077
6	0	6.09311	0.98957	-0.48367
6	0	4.23872	-0.05719	0.58165
1	0	7.1531	1.04666	-0.71389
6	0	5.60262	-0.02933	0.33185
16	0	3.43177	-1.37097	1.55411
1	0	6.23569	-0.80572	0.74664
7	0	2.00369	-1.50065	0.77582
8	0	4.25263	-2.58193	1.39691
8	0	3.22397	-0.78042	2.88157
46	0	1.32046	0.40455	0.49379
6	0	1.85591	-2.51941	-0.26812
6	0	-0.582	-0.24127	1.18767
1	0	1.85784	-3.51213	0.19591
6	0	2.98458	-2.50357	-1.30326
6	0	0.4935	-2.30908	-0.98252
6	0	-0.79469	-1.65225	1.22417
6	0	-0.87448	0.50711	2.3569
1	0	-1.05465	0.32561	0.06383
8	0	3.29268	-3.7545	-1.6952
8	0	3.52417	-1.51113	-1.74742
1	0	0.47253	-1.28006	-1.35601
6	0	0.3218	-3.24345	-2.19049
6	0	-0.67559	-2.52552	-0.00663
6	0	-1.26099	-2.24203	2.40295
6	0	-1.34479	-0.09323	3.52016
1	0	-0.76654	1.58435	2.32483
7	0	-1.68724	0.87517	-1.04933
6	0	4.31905	-3.84629	-2.69557
1	0	1.05196	-3.02767	-2.97594
1	0	0.43259	-4.2964	-1.90541
1	0	-0.67502	-3.10817	-2.62386
1	0	-1.60127	-2.38725	-0.58292
1	0	-0.6804	-3.57878	0.30483
1	0	-1.41995	-3.31769	2.43378
6	0	-1.52369	-1.4779	3.54238
1	0	-1.56411	0.50482	4.40036
16	0	-0.66329	1.73954	-1.94633
6	0	-3.03342	1.42245	-0.85893
1	0	4.01704	-3.32077	-3.60653
1	0	4.44606	-4.91176	-2.88946
1	0	5.24947	-3.40782	-2.3242
1	0	-1.87522	-1.96817	4.44691
6	0	0.08942	2.93423	-0.77493
8	0	0.45818	0.88065	-2.35974
8	0	-1.3511	2.59175	-2.93274
6	0	-3.93439	0.32776	-0.22308
6	0	-3.03965	2.67947	0.01487
1	0	-3.46194	1.70478	-1.82692
7	0	0.77695	2.43714	0.26628
6	0	-0.1252	4.29991	-0.94627
6	0	-4.07897	-0.84327	-1.22056
6	0	-5.30817	0.87268	0.191
1	0	-3.41704	-0.02742	0.67629
8	0	-2.32781	2.87695	0.97959
8	0	-3.95517	3.5696	-0.41608
6	0	1.25141	3.29008	1.1958
6	0	0.37633	5.1807	0.00887
1	0	-0.68472	4.63311	-1.81206
1	0	-3.07737	-1.12283	-1.567
1	0	-4.61761	-0.47897	-2.10583
6	0	-4.79362	-2.05476	-0.65912

1	0	-5.23137	1.61223	0.99517
1	0	-5.81422	1.34953	-0.65683
1	0	-5.93945	0.05424	0.54985
6	0	-4.0709	4.76362	0.37424
1	0	1.79156	2.84035	2.022
6	0	1.06891	4.6654	1.105
1	0	0.22423	6.25112	-0.09624
6	0	-4.33181	-2.68718	0.50527
6	0	-5.92906	-2.57879	-1.29044
1	0	-4.83539	5.36748	-0.1152
1	0	-4.36838	4.51923	1.39833
1	0	-3.1158	5.29623	0.40234
1	0	1.46583	5.31034	1.88154
1	0	-3.46283	-2.29467	1.02307
6	0	-4.97887	-3.8122	1.01576
6	0	-6.57944	-3.70692	-0.78424
1	0	-6.30588	-2.09851	-2.1909
1	0	-4.60092	-4.28511	1.919
6	0	-6.10574	-4.32943	0.37174
1	0	-7.45762	-4.09649	-1.29301
1	0	-6.61031	-5.20654	0.76826



TS(IM1-IM3-Ab)

E(RB3LYP) = -3062.38332803

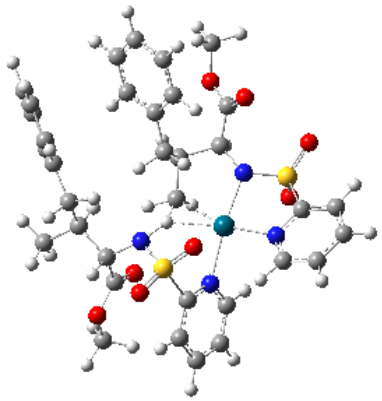
G(correction)= 0.603637

$E(RM06)_{dioxane}$ = -3062.63338878

Imaginary frequencies: 1 (-1432.4147cm^{-1})

6	0	-2.66664	2.52715	2.57235
1	0	-2.78048	1.72432	3.2954
6	0	-3.17236	3.80504	2.76715
7	0	-1.97079	2.21241	1.46993
1	0	-3.74561	4.03399	3.65881
6	0	-2.89999	4.78106	1.80264
6	0	-1.70987	3.13183	0.53441
1	0	-3.26166	5.79665	1.93443
6	0	-2.15194	4.44713	0.67521
16	0	-0.83859	2.63507	-1.00789
1	0	-1.89842	5.17085	-0.09033
7	0	0.26619	1.5324	-0.63968
8	0	-1.93581	2.02986	-1.78658
8	0	-0.23631	3.90142	-1.46547
6	0	1.68155	1.94741	-0.64734
46	0	-0.45912	-0.32799	0.04965
1	0	1.85821	2.7474	0.08303
6	0	2.16548	2.53902	-1.97188
6	0	2.60948	0.74078	-0.28634
7	0	-0.3901	-1.19461	-1.92069
7	0	-1.16441	-2.16694	0.56428
8	0	1.49349	2.07449	-3.04423
8	0	3.11956	3.28309	-2.04668
1	0	2.04035	0.1161	0.4082
6	0	2.97471	-0.14173	-1.48796
6	0	3.86691	1.24304	0.45784
6	0	-0.4637	-0.52221	-3.08151
6	0	-0.3543	-2.53629	-1.94058
16	0	-0.28351	-3.26664	-0.27792
6	0	-2.6263	-2.29209	0.61416
6	0	1.92143	2.60785	-4.30576
1	0	2.08725	-0.41767	-2.05901
1	0	3.67382	0.37152	-2.15949
1	0	3.45267	-1.05966	-1.13669
1	0	4.42811	1.91496	-0.20189
1	0	3.54362	1.84838	1.31715
6	0	4.7478	0.11259	0.94388
1	0	-0.49911	0.55506	-3.00496
6	0	-0.49568	-1.19597	-4.30093
6	0	-0.39514	-3.28363	-3.10692
8	0	1.11831	-3.13666	0.13769
8	0	-0.92324	-4.5854	-0.32849
6	0	-3.14	-1.4103	1.7703
6	0	-3.26884	-1.95347	-0.74201
1	0	-2.87173	-3.34212	0.81174
1	0	1.7748	3.69109	-4.32529
1	0	1.29547	2.12279	-5.05603
1	0	2.97751	2.38389	-4.48018
6	0	4.26899	-0.79672	1.8997
6	0	6.03868	-0.07072	0.43517
1	0	-0.55837	-0.62499	-5.22131
6	0	-0.46322	-2.59177	-4.31604
1	0	-0.39988	-4.36595	-3.04577
6	0	-2.24402	-1.57011	3.00649
1	0	-3.11318	-0.36899	1.43511
6	0	-4.59919	-1.76324	2.09195
8	0	-3.41571	-2.75413	-1.64163
8	0	-3.57195	-0.645	-0.85596
1	0	3.26614	-0.67582	2.30195
6	0	5.06028	-1.86049	2.33136
6	0	6.83668	-1.13265	0.86856
1	0	6.4201	0.62422	-0.30972
1	0	-0.5016	-3.13402	-5.25636
1	0	-1.96374	-2.62802	3.10378
1	0	-2.85094	-1.34648	3.89618
6	0	-0.97222	-0.73521	3.13106
1	0	-5.23053	-1.69039	1.19938
1	0	-4.6803	-2.78514	2.48274
1	0	-5.01021	-1.08149	2.84563
6	0	-4.02616	-0.21813	-2.15322

1	0	4.6681	-2.55917	3.06576
6	0	6.34879	-2.03213	1.81744
1	0	7.83688	-1.25779	0.46126
6	0	-0.42433	0.14019	2.1518
6	0	-0.33379	-0.83349	4.38079
1	0	-4.10307	0.86459	-2.09022
1	0	-3.2957	-0.49825	-2.91568
1	0	-4.98821	-0.68374	-2.38599
1	0	6.965	-2.86239	2.15254
6	0	0.70132	0.91712	2.52664
1	0	-1.32085	1.07257	1.5328
6	0	0.80837	-0.10397	4.69315
1	0	-0.7502	-1.50974	5.12523
1	0	1.07566	1.65234	1.82543
6	0	1.32453	0.80201	3.76219
1	0	1.27919	-0.22316	5.66558
1	0	2.19729	1.40516	3.99724

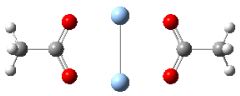


TS(IM1-IM3-B)

E(RB3LYP) = -3062.36261102
G(correction)= 0.602422
$E(RM06)_{dioxane}$ = -3062.62036625
Imaginary frequencies: 1 (-1335.8335 cm^{-1})

46	0	-1.74154	-0.49248	-0.32778
7	0	-0.85203	-2.30911	-0.51492
7	0	-3.2225	-1.64245	0.6359
6	0	0.39429	-2.34288	-1.29121
16	0	-2.05976	-3.3125	-1.06749
6	0	-3.19249	-2.93841	0.29692
6	0	-3.98675	-1.2489	1.66545
6	0	1.1153	-0.98719	-1.07478
1	0	0.20767	-2.43087	-2.37172
6	0	1.26816	-3.5307	-0.87864
8	0	-1.70744	-4.73377	-1.00261
8	0	-2.70913	-2.81764	-2.3003
6	0	-3.9417	-3.9125	0.93635
1	0	-3.91542	-0.20407	1.94317
6	0	-4.78473	-2.15772	2.358
6	0	0.09683	0.12525	-1.40222
6	0	1.7072	-0.80319	0.34606
1	0	1.93858	-0.94482	-1.79909
8	0	1.11867	-4.22875	0.09393
8	0	2.27525	-3.65926	-1.7682
6	0	-4.76702	-3.50339	1.98602
1	0	-3.84831	-4.94672	0.6241
1	0	-5.3912	-1.81151	3.18793
1	0	-0.50142	-0.10802	-2.29473
1	0	0.57852	1.06372	-1.69504
1	0	-0.21632	0.90986	-0.30844
1	0	1.90872	0.26479	0.46787
1	0	0.93784	-1.04368	1.08752
6	0	2.98642	-1.55772	0.64792
6	0	3.26281	-4.65022	-1.43099
1	0	-5.3724	-4.2291	2.52087
7	0	-0.01758	2.00175	0.69731
6	0	4.15726	-1.29329	-0.07627
6	0	3.04705	-2.4904	1.69073
1	0	3.74652	-4.38997	-0.48697
1	0	3.98374	-4.63313	-2.24922
1	0	2.79752	-5.63614	-1.34516
16	0	-1.21947	2.04018	1.76998
6	0	0.39623	3.31744	0.18494
6	0	5.35331	-1.94179	0.22898
1	0	4.1425	-0.54993	-0.86773
6	0	4.24338	-3.13917	2.00512
1	0	2.14276	-2.72464	2.24423
6	0	-2.69689	2.24786	0.70934
8	0	-1.37577	0.7058	2.37438
8	0	-1.22139	3.23774	2.62843
6	0	1.86228	3.27409	-0.31947
6	0	-0.5219	3.76664	-0.95492
1	0	0.33527	4.06757	0.98067
6	0	5.40237	-2.86754	1.27474
1	0	6.24936	-1.7066	-0.33856
1	0	4.26595	-3.86102	2.81752
7	0	-2.8999	1.29082	-0.21077
6	0	-3.48593	3.39191	0.78795
6	0	2.80107	2.89513	0.83607
6	0	2.2512	4.62165	-0.95171
1	0	1.91338	2.49361	-1.08762
8	0	-0.84178	3.08101	-1.906
8	0	-0.9528	5.03356	-0.78105
1	0	6.33488	-3.37041	1.51869
6	0	-3.90208	1.4369	-1.09549
6	0	-4.53043	3.5407	-0.12425
1	0	-3.25783	4.13022	1.54713
1	0	2.30024	2.14529	1.45902
1	0	2.92889	3.77662	1.48215
6	0	4.17404	2.36253	0.45273
1	0	1.70718	4.81128	-1.88399
1	0	2.03305	5.44546	-0.26155
1	0	3.32067	4.65124	-1.17727
6	0	-1.80024	5.54174	-1.82534
1	0	-4.01942	0.63915	-1.8214
6	0	-4.74006	2.54883	-1.08357
1	0	-5.16773	4.41981	-0.09056
6	0	4.62332	2.22813	-0.86738

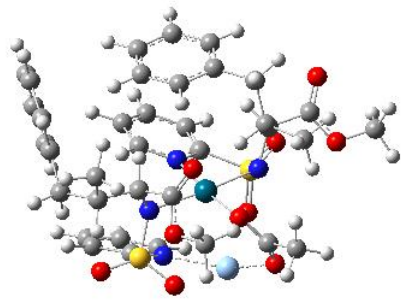
6	0	5.04033	1.96315	1.48346
1	0	-2.03573	6.56727	-1.53933
1	0	-1.28094	5.51784	-2.78747
1	0	-2.71122	4.94092	-1.89945
1	0	-5.5333	2.6292	-1.81892
1	0	3.984	2.51149	-1.69715
6	0	5.89836	1.72494	-1.14804
6	0	6.30814	1.45693	1.20994
1	0	4.70378	2.04243	2.51497
1	0	6.222	1.63404	-2.18193
6	0	6.74704	1.33986	-0.11213
1	0	6.95191	1.14461	2.02777
1	0	7.73666	0.94685	-0.3292



$Ag_2(OAc)_2$

E(RB3LYP) = -748.61917282
G(correction)= 0.056713
$E(RM06)_{dioxane}$ = -750.95643742
$E(RM06)_{iPrOH}$ = -750.96959237

6	0	-2.69555	-0.00003	-0.00692
8	0	-2.13328	1.13858	-0.0062
8	0	-2.13328	-1.13863	-0.00622
8	0	2.13328	1.13863	-0.0062
8	0	2.13328	-1.13858	-0.0062
6	0	2.69555	0.00003	-0.00691
6	0	4.21522	-0.00001	0.03104
1	0	4.53481	-0.00081	1.07996
1	0	4.61002	-0.89882	-0.44681
1	0	4.61009	0.89946	-0.44553
6	0	-4.21522	0.	0.03101
1	0	-4.61002	0.89883	-0.44681
1	0	-4.61008	-0.89945	-0.44557
1	0	-4.53481	0.00079	1.07994
47	0	0.00001	-1.40052	-0.00496
47	0	-0.00001	1.40052	-0.00495



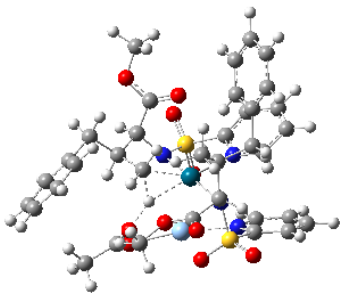
IM1'

E(RB3LYP) = -3436.78210106
G(correction)= 0.656270
$E(RM06)_{dioxane}$ = -3438.18098115

Imaginary frequencies: 0

6	0	-1.36273	0.93584	-1.75988
1	0	-2.09275	0.59608	-1.03936
6	0	-1.71079	1.64443	-2.90754
7	0	-0.08474	0.63459	-1.49047
1	0	-2.75234	1.88547	-3.07543
6	0	-0.71389	2.05906	-3.78796
6	0	0.87728	1.03443	-2.3423
46	0	0.57769	-0.31289	0.23143
1	0	-0.96477	2.62773	-4.67866
6	0	0.61693	1.75179	-3.49761
16	0	2.55737	0.5734	-1.81607
7	0	2.40009	0.63832	-0.18514
7	0	-1.34977	-1.16709	0.5387
8	0	1.397	-1.07898	1.95611
1	0	1.44582	2.06866	-4.12097
8	0	2.73172	-0.82895	-2.2579
8	0	3.45024	1.59466	-2.37849
6	0	2.45298	2.03286	0.31778
16	0	-1.39798	-2.77655	0.20906
6	0	-2.0743	-0.55243	1.67752
6	0	2.45564	-1.80358	2.03054
1	0	1.79651	2.68128	-0.27372
6	0	3.82849	2.68548	0.20681
6	0	1.97048	2.11219	1.79734
6	0	-1.23599	-2.64166	-1.61583
8	0	-0.22684	-3.54631	0.67521
8	0	-2.73	-3.36797	0.43286
6	0	-3.52328	-1.02011	2.01079
6	0	-1.24457	-0.62642	2.96301
1	0	-2.11946	0.51041	1.42229
8	0	3.00588	-2.45507	1.11603
6	0	3.08016	-1.89227	3.4158
8	0	4.84308	1.81191	0.25454
8	0	3.96675	3.89201	0.15237
1	0	1.15982	1.38623	1.90698
6	0	3.05867	1.73394	2.80592
6	0	1.36197	3.50439	2.09165
7	0	-0.00947	-2.58132	-2.14065
6	0	-2.39891	-2.52985	-2.37848
6	0	-4.53132	-0.91786	0.83939
1	0	-3.47211	-2.08441	2.24736
6	0	-3.99861	-0.29083	3.28297
8	0	-0.79359	0.33675	3.55043
8	0	-1.12535	-1.89474	3.37617
47	0	1.88531	-2.76212	-0.76367
1	0	4.16745	-1.9362	3.3174
1	0	2.79152	-1.04579	4.04062
1	0	2.74844	-2.8222	3.8913
6	0	6.15114	2.38724	0.11747
1	0	3.55351	0.80543	2.51241
1	0	3.82275	2.51706	2.88409
1	0	2.61317	1.5948	3.79678
1	0	1.0969	3.53101	3.15592
1	0	2.11995	4.27635	1.92003
6	0	0.13281	3.76844	1.24873

6	0	0.11476	-2.33411	-3.45697
6	0	-2.26698	-2.29273	-3.74467
1	0	-3.36535	-2.63054	-1.8998
1	0	-5.4607	-1.37958	1.20254
1	0	-4.17296	-1.57038	0.04247
6	0	-4.88392	0.43257	0.24532
1	0	-3.44578	-0.63183	4.16347
1	0	-3.86568	0.79417	3.21489
1	0	-5.05891	-0.49833	3.46558
6	0	-0.34013	-2.1061	4.55783
1	0	6.23727	2.89562	-0.84688
1	0	6.84544	1.54859	0.17347
1	0	6.34365	3.1052	0.92011
6	0	0.19202	4.59326	0.11677
6	0	-1.07467	3.11469	1.54131
1	0	1.131	-2.24139	-3.82491
6	0	-0.98737	-2.17408	-4.29233
1	0	-3.14862	-2.19674	-4.37209
6	0	-4.70884	0.65214	-1.12992
6	0	-5.49545	1.45548	0.9909
1	0	-0.17875	-3.18278	4.61287
1	0	0.60515	-1.57188	4.47504
1	0	-0.88453	-1.7531	5.43982
1	0	1.12927	5.08913	-0.12614
6	0	-0.92574	4.76054	-0.70661
6	0	-2.19332	3.2853	0.72408
1	0	-1.12467	2.45524	2.40454
1	0	-0.84058	-1.97089	-5.34795
1	0	-4.27297	-0.13741	-1.73857
6	0	-5.10874	1.84592	-1.73585
6	0	-5.87331	2.66027	0.39604
1	0	-5.69815	1.30664	2.04507
1	0	-0.85844	5.40263	-1.58167
6	0	-2.12215	4.10787	-0.40423
1	0	-3.12424	2.77982	0.96157
1	0	-4.99557	1.9734	-2.81004
6	0	-5.67955	2.86436	-0.97195
1	0	-6.33379	3.43631	1.00143
1	0	-2.99779	4.23284	-1.03532
1	0	-5.98898	3.79559	-1.43822



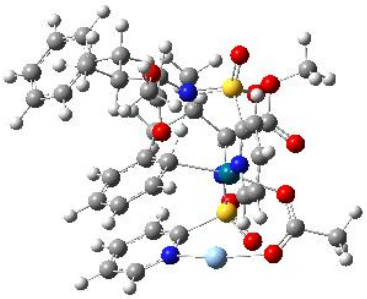
TS(IM1'-IM3'B)

E(RB3LYP) = -3436.71517365
G(correction)= 0.602422
$E(RM06)_{dioxane}$ = -3438.11843897

Imaginary frequencies: 1 (-1304.4346 cm^{-1})

46	0	0.18584	-0.20603	-0.12111
7	0	-0.2327	-0.185	-2.12908
7	0	2.26228	-0.38594	-0.73437
7	0	0.68711	-0.43876	1.91436
6	0	-1.00059	0.97078	-2.58229
16	0	0.99345	-0.74622	-3.04823
6	0	2.45117	-0.32015	-2.06138
6	0	3.31158	-0.18331	0.07367
16	0	0.58882	-2.01294	2.41029
6	0	0.40396	0.53288	2.99976
6	0	-2.19395	1.04334	-1.59278
1	0	-1.38105	0.81217	-3.59647
6	0	-0.15541	2.24782	-2.61741
8	0	1.08422	-0.05779	-4.34393
8	0	0.99894	-2.22504	-3.01917
6	0	3.67215	-0.0247	-2.6472
1	0	3.092	-0.24858	1.13075
6	0	4.58068	0.10235	-0.42334
6	0	1.88349	-2.81549	1.39166
8	0	1.06001	-2.12809	3.80265
8	0	-0.66769	-2.68993	2.03708
6	0	0.78672	1.96306	2.5271
6	0	-1.00999	0.48691	3.59393
1	0	1.03831	0.28666	3.85812
6	0	-1.67444	0.94848	-0.1527
6	0	-3.13217	2.25907	-1.78428
1	0	-2.77718	0.13975	-1.79936
8	0	0.91564	2.39309	-2.06148
8	0	-0.74612	3.20823	-3.34698
6	0	4.76148	0.19797	-1.80295
1	0	3.7427	0.03914	-3.72749
1	0	5.39965	0.27073	0.26742
7	0	1.57189	-3.19323	0.14585
6	0	3.14947	-2.98594	1.94854
6	0	2.31503	2.16224	2.65399
1	0	0.52491	2.02878	1.46729
6	0	0.0383	3.08367	3.26073
8	0	-1.23689	0.7447	4.75774
8	0	-1.94932	0.16126	2.69797
1	0	-2.46807	1.04013	0.58808
1	0	-0.98788	1.77481	0.07262
1	0	-1.80549	-0.41479	0.1544
1	0	-2.60251	3.18199	-1.52227
1	0	-3.39772	2.34264	-2.84515
6	0	-4.37894	2.11557	-0.93823
6	0	-0.03109	4.45614	-3.42377
1	0	5.73457	0.44569	-2.21658
6	0	2.54357	-3.70934	-0.62788
6	0	4.14717	-3.54549	1.15173
1	0	3.32242	-2.68319	2.97463
1	0	2.81116	1.21895	2.40313
1	0	2.55698	2.36312	3.70579
6	0	2.85868	3.26586	1.77181
1	0	-1.03554	3.05903	3.04637

1	0	0.16063	2.99988	4.34523
1	0	0.4275	4.05473	2.93596
6	0	-3.29217	0.03061	3.19888
8	0	-2.91752	-1.24771	0.35733
6	0	-4.48966	2.75665	0.30262
6	0	-5.41973	1.27117	-1.34733
1	0	0.15	4.85653	-2.4224
1	0	-0.67115	5.1244	-3.99982
1	0	0.92767	4.30971	-3.92885
1	0	2.26056	-3.94518	-1.64758
6	0	3.84363	-3.89778	-0.16428
1	0	5.14648	-3.69733	1.54952
6	0	3.53858	4.36682	2.30648
6	0	2.68002	3.20387	0.38135
1	0	-3.88226	-0.26764	2.33526
1	0	-3.32204	-0.73436	3.97894
1	0	-3.63632	0.98272	3.61331
6	0	-3.36841	-2.19876	-0.35878
6	0	-5.60296	2.5514	1.12076
1	0	-3.69061	3.41645	0.63391
6	0	-6.53768	1.06732	-0.53736
1	0	-5.34814	0.76366	-2.30711
1	0	4.59406	-4.31954	-0.82462
1	0	3.68043	4.43547	3.3829
6	0	4.0336	5.3763	1.47581
6	0	3.16463	4.21152	-0.45133
1	0	2.14417	2.37354	-0.06319
8	0	-2.69815	-2.95792	-1.11342
6	0	-4.8648	-2.44597	-0.25006
6	0	-6.63036	1.70323	0.70378
1	0	-5.6665	3.05487	2.08187
1	0	-7.33619	0.41145	-0.87456
1	0	4.55857	6.22299	1.91103
6	0	3.84832	5.30216	0.09378
1	0	2.99296	4.13569	-1.52132
47	0	-0.55997	-3.01717	-0.70687
1	0	-5.21321	-3.08964	-1.06016
1	0	-5.06464	-2.94154	0.70742
1	0	-5.4	-1.4928	-0.25007
1	0	-7.49826	1.54201	1.33726
1	0	4.22863	6.09025	-0.55125



TS(IM1'-IM3'Aa)

E(RB3LYP) = -3436.71796822

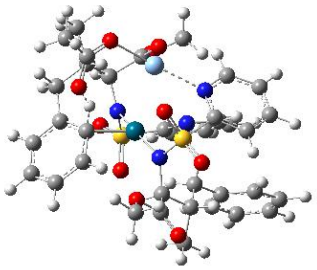
G(correction)= 0.647297

$E(RM06)_{dioxane}$ = -3438.11846514

Imaginary frequencies: 1 (-860.7539 cm^{-1})

6	0	-2.22454	-3.02136	-2.86892
1	0	-2.28621	-2.48986	-3.8124
6	0	-1.86381	-4.3644	-2.81983
7	0	-2.51396	-2.30699	-1.76821
1	0	-1.64998	-4.9001	-3.73866
6	0	-1.78465	-4.98877	-1.57509
6	0	-2.43745	-2.9129	-0.57176
1	0	-1.50879	-6.03655	-1.49759
6	0	-2.07224	-4.25124	-0.42882
16	0	-2.847	-1.94394	0.93808
1	0	-2.04561	-4.68621	0.56275
7	0	-1.5228	-1.05915	1.20235
8	0	-4.00585	-1.13108	0.52057
8	0	-3.0232	-2.96986	1.97841
46	0	-1.08182	0.73212	0.28113
6	0	-0.76232	-1.30067	2.43619
6	0	0.51175	-0.29115	-0.76214
8	0	-2.81446	1.68578	0.98065
1	0	-1.10001	-2.25688	2.85745
6	0	-1.1745	-0.23908	3.4777
6	0	0.75434	-1.43546	2.14821
6	0	0.76878	-1.66578	-0.49819
6	0	0.45151	0.12946	-2.1206
1	0	1.21891	0.50689	-0.04636
6	0	-3.81022	1.9696	0.25161
8	0	-0.1888	0.05927	4.34191
8	0	-2.28324	0.24029	3.52895
1	0	1.18551	-0.43901	2.03093
6	0	1.48191	-2.1473	3.30385
6	0	0.97697	-2.26777	0.87563
6	0	0.94954	-2.54067	-1.57976
6	0	0.61524	-0.75546	-3.17847
1	0	0.33585	1.18418	-2.33224
7	0	2.24059	1.34063	0.60146
8	0	-3.93009	1.75472	-0.9996
6	0	-4.97974	2.61829	0.96395
6	0	-0.47226	1.14547	5.23977
1	0	1.33531	-1.62765	4.25028
1	0	1.11844	-3.17863	3.41256
1	0	2.55801	-2.19848	3.09962
1	0	2.01243	-2.63294	0.88746
1	0	0.36017	-3.17705	0.94169
1	0	1.17246	-3.5849	-1.37611
6	0	0.86665	-2.10366	-2.8992
1	0	0.57782	-0.40035	-4.20497
16	0	1.55056	2.55771	1.38678
6	0	3.4932	1.59714	-0.10478
47	0	-3.10207	-0.1297	-1.73763
1	0	-4.63842	3.18621	1.83156
1	0	-5.5482	3.2489	0.27658
1	0	-5.63037	1.81032	1.31881
1	0	-0.618	2.06077	4.6623

1	0	0.40842	1.23231	5.87713
1	0	-1.36511	0.93242	5.83405
1	0	1.01188	-2.81314	-3.71056
6	0	0.47953	3.37841	0.14602
8	0	0.60235	2.00577	2.36965
8	0	2.5111	3.60111	1.79096
6	0	4.06624	0.23717	-0.5953
6	0	3.31651	2.54294	-1.29596
1	0	4.2214	2.06184	0.57038
7	0	-0.51091	2.66772	-0.4233
6	0	0.76169	4.69435	-0.21165
6	0	4.32389	-0.65957	0.62708
6	0	5.33576	0.41907	-1.4394
1	0	3.28674	-0.21494	-1.21947
8	0	2.36411	2.55854	-2.05114
8	0	4.36697	3.37689	-1.42266
6	0	-1.2476	3.25801	-1.38589
6	0	0.00194	5.29795	-1.20926
1	0	1.56987	5.2065	0.29606
1	0	3.46253	-0.57167	1.29905
1	0	5.17669	-0.24777	1.18608
6	0	4.57131	-2.1347	0.36706
1	0	5.13082	0.93067	-2.38573
1	0	6.08284	1.00907	-0.89543
1	0	5.77792	-0.55423	-1.67309
6	0	4.30001	4.2852	-2.53376
1	0	-2.06415	2.67334	-1.78648
6	0	-1.01697	4.56217	-1.80998
1	0	0.20067	6.32283	-1.5096
6	0	4.25734	-2.77163	-0.84081
6	0	5.07261	-2.92419	1.41527
1	0	5.2025	4.89365	-2.47105
1	0	4.26974	3.73524	-3.4792
1	0	3.40536	4.91029	-2.461
1	0	-1.64097	4.98328	-2.591
1	0	3.85901	-2.19885	-1.671
6	0	4.42971	-4.15087	-0.99271
6	0	5.24405	-4.29986	1.26943
1	0	5.32258	-2.44794	2.36115
1	0	4.17753	-4.61961	-1.94098
6	0	4.9211	-4.92208	0.06008
1	0	5.6298	-4.88635	2.0993
1	0	5.05486	-5.994	-0.05846

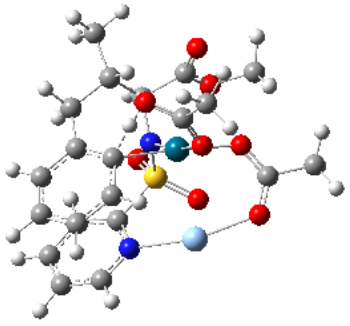


TS(IM1'-IM3'Ab)

E(RB3LYP) = -3436.70997552
G(correction)= 0.642417
$E(RM06)_{dioxane}$ = -3438.1092789
Imaginary frequencies: 1 (-1471.789 cm^{-1})

46	0	-0.56133	0.0347	0.59925
7	0	-0.39558	-1.91406	1.18327
6	0	-2.3713	0.19665	1.6379
7	0	-0.28215	2.04928	0.07461
16	0	0.8781	-2.21185	2.15164
6	0	-1.10286	-3.03952	0.58242
6	0	-2.76973	-0.9469	2.41446
6	0	-2.34523	1.46946	2.28261
1	0	-3.24499	0.27199	0.5833
16	0	-0.55487	2.58009	-1.42634
6	0	0.49939	2.89321	1.00892
6	0	2.30249	-2.42626	1.03402
8	0	0.73479	-3.48779	2.8716
8	0	1.1661	-0.97458	2.90295
6	0	-2.59337	-2.70893	0.45339
1	0	-0.98353	-3.92403	1.21753
6	0	-0.45421	-3.33991	-0.77229
6	0	-3.1645	-2.28012	1.80824
6	0	-3.03968	-0.77428	3.77504
6	0	-2.64602	1.61623	3.62836
1	0	-2.11608	2.34279	1.68532
6	0	0.54357	1.57614	-2.49454
8	0	-1.91837	2.21395	-1.86014
8	0	-0.08396	3.9651	-1.60707
6	0	2.04394	2.81284	0.88011
6	0	0.00701	4.3544	1.02644
1	0	0.24045	2.49002	1.99721
7	0	2.2853	-1.6849	-0.0691
6	0	3.34085	-3.28309	1.39742
6	0	-3.3768	-3.89636	-0.1195
1	0	-2.69962	-1.88002	-0.24819
8	0	-0.68037	-2.76416	-1.82541
8	0	0.47592	-4.29876	-0.65602
1	0	-2.98597	-3.07462	2.54546
1	0	-4.2578	-2.22389	1.6884
1	0	-3.33877	-1.63507	4.36893
6	0	-2.95358	0.47842	4.3828
1	0	-2.63047	2.59967	4.08986
7	0	0.19641	0.2971	-2.68454
6	0	1.7174	2.13189	-2.99873
6	0	2.4607	1.35131	0.62634

1	0	2.34578	3.43729	0.02968
6	0	2.71926	3.34351	2.15503
8	0	0.71049	5.33832	1.03806
8	0	-1.34117	4.40413	1.09164
6	0	3.36227	-1.7401	-0.86355
6	0	4.4502	-3.34023	0.55471
1	0	3.26352	-3.87391	2.30286
1	0	-4.42523	-3.62115	-0.27383
1	0	-3.34432	-4.76044	0.55656
1	0	-2.9758	-4.20235	-1.09151
6	0	1.25982	-4.57229	-1.82978
1	0	-3.15542	0.56977	5.4473
6	0	1.0307	-0.50247	-3.3681
47	0	-1.94798	-0.4076	-2.13341
6	0	2.56921	1.30591	-3.73142
1	0	1.9325	3.17759	-2.81323
1	0	2.00013	1.00433	-0.30318
1	0	2.05346	0.72939	1.43163
6	0	3.94602	1.10062	0.52913
1	0	2.43803	4.37831	2.35417
1	0	2.43811	2.72492	3.01855
1	0	3.80824	3.29406	2.05754
6	0	-1.91218	5.71543	0.95936
1	0	3.33904	-1.10111	-1.74056
6	0	4.46755	-2.5477	-0.59385
1	0	5.29047	-3.98538	0.79556
1	0	0.61722	-4.90179	-2.65084
1	0	1.95255	-5.36152	-1.53831
1	0	1.80858	-3.67641	-2.13033
1	0	0.7204	-1.53845	-3.45289
6	0	2.22548	-0.03501	-3.91405
8	0	-4.10927	-0.76689	-1.88753
1	0	3.49132	1.70128	-4.14755
6	0	4.61578	0.37407	1.52194
6	0	4.67674	1.54261	-0.58336
1	0	-2.99128	5.57032	1.01698
1	0	-1.56319	6.37267	1.76083
1	0	-1.63114	6.14041	-0.00788
1	0	5.32205	-2.54005	-1.26235
1	0	2.86774	-0.71156	-4.46857
6	0	-4.81242	-0.16291	-1.03744
1	0	4.05394	0.01354	2.38001
6	0	5.97627	0.0846	1.40099
6	0	6.03687	1.25803	-0.70794
1	0	4.1661	2.10687	-1.36012
8	0	-4.40774	0.39403	0.04114
6	0	-6.30466	-0.04678	-1.29913
1	0	6.47599	-0.48856	2.17786
6	0	6.69179	0.52264	0.28445
1	0	6.58682	1.60801	-1.57843
1	0	-6.86509	-0.08476	-0.36189
1	0	-6.49646	0.92596	-1.76738
1	0	-6.63359	-0.83218	-1.98281
1	0	7.75084	0.29739	0.18886

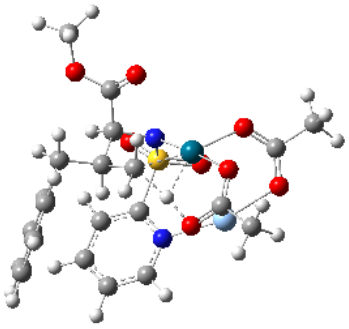


TS2A'

E(RB3LYP) = -2197.38906978
G(correction)= 0.374972
$E(RM06)_{dioxane}$ = -2199.19298298
Imaginary frequencies: 1 (-1293.0767 cm^{-1})

46	0	-0.88041	0.15443	-0.61918
7	0	-0.06621	0.54017	1.21902
6	0	0.56588	1.49246	-1.42869
8	0	-1.89157	0.03223	-2.43482
8	0	-2.2321	-1.26504	0.12174
16	0	0.78176	-0.50679	2.11655
6	0	-0.76669	1.65052	1.87797
6	0	1.32661	2.35037	-0.59445
6	0	1.21323	0.8537	-2.51788
6	0	-2.18676	1.15182	-2.95996
6	0	-2.20527	-2.48278	-0.24735
6	0	2.41459	-0.5077	1.28261
8	0	0.31472	-1.90195	1.99072
8	0	1.0449	0.04492	3.45588
6	0	-0.67197	2.93885	1.03721
1	0	-0.3134	1.82027	2.86157
6	0	-2.22884	1.22155	2.08431
6	0	0.76429	3.17898	0.55066
6	0	2.69233	2.51623	-0.87229
6	0	2.56598	1.03022	-2.77951
1	0	0.61879	0.21877	-3.17045
8	0	-1.65372	2.26274	-2.63412
6	0	-3.25709	1.1644	-4.02564
8	0	-1.28355	-3.06554	-0.88774
6	0	-3.40659	-3.31475	0.16771
7	0	2.554	-1.19826	0.13895
6	0	3.46407	0.19132	1.87688
6	0	-1.16235	4.13537	1.86761
1	0	-1.34219	2.84046	0.17692
8	0	-3.1763	1.64779	1.45608
8	0	-2.30679	0.25359	3.00809
1	0	1.44735	3.08541	1.40817
1	0	0.83883	4.23088	0.23714
1	0	3.28348	3.17211	-0.23605
6	0	3.30926	1.86484	-1.9382
1	0	3.03789	0.53322	-3.62315
1	0	-0.63312	1.9527	-1.87659
1	0	-4.2152	1.38778	-3.54175
1	0	-3.05413	1.94675	-4.76001
1	0	-3.33048	0.18597	-4.50381
47	0	0.72895	-2.26679	-0.66685

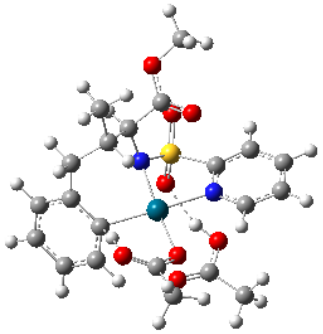
1	0	-4.32244	-2.72193	0.10429
1	0	-3.48368	-4.21106	-0.45044
1	0	-3.26784	-3.6181	1.21218
6	0	3.75591	-1.1968	-0.4632
6	0	4.71107	0.16976	1.25705
1	0	3.28741	0.71343	2.80928
1	0	-1.17559	5.04849	1.26199
1	0	-0.5073	4.31175	2.73108
1	0	-2.17873	3.96259	2.23255
6	0	-3.56913	-0.43131	3.08264
1	0	4.37108	2.01515	-2.11736
1	0	3.82322	-1.74871	-1.39458
6	0	4.86093	-0.53492	0.06303
1	0	5.55284	0.69397	1.7003
1	0	-4.3716	0.2658	3.33996
1	0	-3.44466	-1.18336	3.86221
1	0	-3.77811	-0.89888	2.11781
1	0	5.81193	-0.57549	-0.45731



TS2B'

E(RB3LYP) = -2197.36943228
G(correction)= 0.371585
$E(RM06)_{dioxane}$ = -2199.17905481
Imaginary frequencies: 1 (-1386.7515 cm^{-1})

46	0	-1.05215	0.74341	-0.86404
7	0	-0.30373	1.45583	0.90682
8	0	-1.74996	-0.07778	-2.65308
8	0	-3.01581	1.29192	-0.49693
6	0	1.09534	1.88236	0.74086
16	0	-0.65371	0.7688	2.34038
6	0	-1.27182	-1.2358	-2.83914
6	0	-3.97473	0.45564	-0.53034
6	0	1.85278	0.8132	-0.0828
1	0	1.57778	2.02071	1.71205
6	0	1.12259	3.23084	0.02592
6	0	0.25941	-0.83697	2.40323
8	0	-2.07915	0.41182	2.37612
8	0	-0.05249	1.53841	3.44015
8	0	-0.29721	-1.70723	-2.15693
6	0	-1.92003	-2.10713	-3.88493
8	0	-3.89413	-0.80603	-0.45021
6	0	-5.35391	1.06182	-0.7173
6	0	1.09639	0.4937	-1.37629
6	0	3.33664	1.18135	-0.33754
1	0	1.85292	-0.08816	0.53956
8	0	0.41659	3.55043	-0.9058
8	0	2.10169	4.01274	0.52676
7	0	-0.17664	-1.85078	1.63701
6	0	1.42864	-0.91597	3.15992
1	0	0.20125	-0.63415	-1.52589
1	0	-2.18643	-1.50809	-4.75888
1	0	-1.26514	-2.93367	-4.16461
1	0	-2.84817	-2.50692	-3.45966
47	0	-2.11792	-1.58861	0.51487
1	0	-5.5147	1.23194	-1.78846
1	0	-6.12399	0.38178	-0.348
1	0	-5.4134	2.0272	-0.20986
1	0	1.68125	-0.23897	-1.95067
1	0	1.01938	1.36547	-2.03576
1	0	3.39516	1.97309	-1.09432
1	0	3.76151	1.59834	0.58451
6	0	4.13576	-0.0265	-0.77142
6	0	2.26558	5.28439	-0.12722
6	0	0.56833	-2.96787	1.56388
6	0	2.19206	-2.08028	3.0868
1	0	1.71329	-0.07346	3.77839
6	0	4.47658	-0.2405	-2.11257
6	0	4.49879	-0.99945	0.17213
1	0	2.51075	5.14201	-1.18381
1	0	3.08421	5.77922	0.39589
1	0	1.34658	5.87162	-0.05242
1	0	0.18975	-3.75337	0.91826
6	0	1.76367	-3.12017	2.26179
1	0	3.11034	-2.17092	3.66005
6	0	5.15907	-1.39577	-2.50338
1	0	4.20388	0.50457	-2.85646
6	0	5.17999	-2.15356	-0.21206
1	0	4.23892	-0.84594	1.21752
1	0	2.33581	-4.03574	2.15803
6	0	5.51207	-2.35645	-1.55471
1	0	5.41482	-1.54303	-3.54934
1	0	5.45713	-2.89324	0.53518
1	0	6.04449	-3.25416	-1.85695

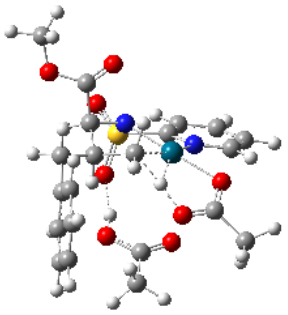


TS2A''

E(RB3LYP) = -2052.16908048
G(correction)= 0.386386

$E(RM06)_{dioxane}$ = -2052.76084145
Imaginary frequencies: 1 (-1404.428 cm^{-1})

46	0	0.63381	-0.17733	0.35895
7	0	-1.01652	-0.57191	-0.79549
6	0	1.39519	-2.04759	-0.22181
8	0	2.15477	0.25386	1.73486
16	0	-1.36174	0.77914	-1.62723
6	0	-2.13678	-1.32959	-0.21562
6	0	0.50988	-3.08286	-0.62331
6	0	2.57816	-1.83446	-0.96985
1	0	1.73956	-2.01077	1.12504
6	0	2.59996	-0.70076	2.43859
6	0	-1.09559	2.09074	-0.38616
8	0	-2.76721	0.84651	-2.0533
8	0	-0.29799	1.02832	-2.62478
6	0	-1.60202	-2.36731	0.80922
1	0	-2.66422	-1.8633	-1.01378
6	0	-3.15465	-0.43251	0.49636
6	0	-0.73515	-3.46064	0.15632
6	0	0.84242	-3.86283	-1.73548
6	0	2.8927	-2.61759	-2.07595
1	0	3.24532	-1.02942	-0.67918
8	0	2.32166	-1.93119	2.24705
6	0	3.54858	-0.37697	3.56943
7	0	-0.1632	1.78813	0.52285
6	0	-1.76273	3.30535	-0.41656
6	0	-2.75235	-3.04085	1.57848
1	0	-0.99317	-1.80835	1.5312
8	0	-2.87074	0.48261	1.24376
8	0	-4.41458	-0.8113	0.2252
1	0	-1.38296	-4.06791	-0.49036
1	0	-0.41685	-4.1327	0.96814
1	0	0.1704	-4.65878	-2.04936
6	0	2.01321	-3.63157	-2.46012
1	0	3.80263	-2.43236	-2.63976
1	0	3.24794	-0.91957	4.46996
1	0	4.55145	-0.72216	3.29511
1	0	3.57365	0.69707	3.75931
6	0	0.17068	2.69534	1.45096
6	0	-1.42221	4.25384	0.54754
1	0	-2.52145	3.48198	-1.17072
1	0	-2.3553	-3.81635	2.24224
1	0	-3.46699	-3.5126	0.89389
1	0	-3.30273	-2.32688	2.19883
6	0	-5.43968	-0.02375	0.85274
1	0	2.23532	-4.24622	-3.32915
1	0	0.93879	2.38736	2.15242
6	0	-0.43912	3.94705	1.49107
1	0	-1.91741	5.22033	0.56433
1	0	-5.35412	-0.07645	1.94227
1	0	-6.38489	-0.45235	0.51887
1	0	-5.35613	1.02	0.53799
1	0	-0.15098	4.66137	2.2551
1	0	1.07231	2.13706	-2.22182
8	0	1.55886	2.90616	-1.83
6	0	2.66406	2.47065	-1.2064
8	0	3.03833	1.31448	-1.21033
6	0	3.36413	3.59652	-0.47903
1	0	3.53369	4.44112	-1.15402
1	0	2.72011	3.95101	0.33387
1	0	4.30984	3.23941	-0.07005

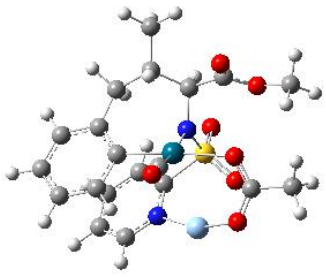


TS2B''

E(RB3LYP) = -2052.15863746
G(correction)= 0.387607
$E(RM06)_{dioxane}$ = -2052.75195807
Imaginary frequencies: 1 (-1297.0344 cm^{-1})

46	0	-0.88702	-0.36301	-0.89926
7	0	-1.005	1.44055	0.03119
7	0	-2.90258	-0.50751	-0.39009
8	0	-0.94543	-2.22909	-1.80941
6	0	0.27075	2.1354	0.27331
16	0	-2.02265	1.37207	1.30658
6	0	-3.32032	0.37962	0.52144
6	0	-3.78156	-1.36604	-0.92866
6	0	0.1099	-2.91195	-1.61473
6	0	1.41786	1.10332	0.11957
1	0	0.31736	2.57232	1.27593
6	0	0.41604	3.27012	-0.73722
8	0	-2.58218	2.67887	1.67276
8	0	-1.52438	0.55049	2.44537
6	0	-4.64229	0.49042	0.92497
1	0	-3.37044	-2.07323	-1.64023
6	0	-5.12787	-1.33564	-0.5707
8	0	1.2015	-2.40829	-1.20695
6	0	0.03542	-4.40095	-1.82875
6	0	1.21469	0.29054	-1.17524
6	0	2.82759	1.72838	0.22324
1	0	1.2995	0.43131	0.97379
8	0	0.11295	3.21645	-1.90866
8	0	0.99924	4.34302	-0.1607
6	0	-5.56554	-0.39096	0.35941
1	0	-4.91884	1.24634	1.65174
1	0	-5.8169	-2.04166	-1.02161
1	0	-0.69185	-4.64673	-2.60516
1	0	1.01895	-4.80737	-2.07091
1	0	-0.30504	-4.83399	-0.88067
1	0	2.17645	-0.14413	-1.4854

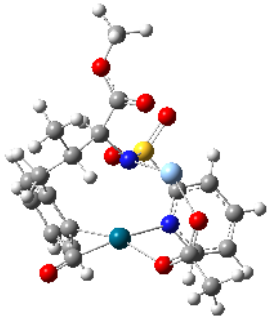
1	0	0.91392	0.91325	-2.02412
1	0	0.99934	-1.09419	-1.10079
1	0	3.0171	2.37265	-0.64417
1	0	2.86296	2.37654	1.10892
6	0	3.89767	0.65992	0.31545
6	0	1.25239	5.45082	-1.04186
1	0	-6.61228	-0.34232	0.64393
6	0	4.85233	0.50113	-0.69623
6	0	3.92189	-0.22881	1.40238
1	0	1.92024	5.14958	-1.85434
1	0	1.7193	6.21748	-0.42296
1	0	0.31601	5.81724	-1.47142
6	0	5.81089	-0.51393	-0.62834
1	0	4.84361	1.17898	-1.54704
6	0	4.87631	-1.24331	1.47289
1	0	3.17841	-0.13794	2.19053
6	0	5.82559	-1.39007	0.45696
1	0	6.54202	-0.61945	-1.42567
1	0	4.87838	-1.92129	2.32256
1	0	6.56819	-2.18151	0.51208
1	0	-0.30644	-0.73315	2.39334
8	0	0.52324	-1.27562	2.43982
6	0	0.34773	-2.44519	1.80287
8	0	-0.69846	-2.77257	1.27099
6	0	1.61077	-3.27073	1.80726
1	0	2.33891	-2.80222	1.13783
1	0	2.04296	-3.30308	2.81184
1	0	1.39336	-4.27837	1.45124



IM4-A'

E(RB3LYP) = -2081.64132943
G(correction)= 0.327016
$E(RM06)_{dioxane}$ = -2083.48326321
Imaginary frequencies: 0

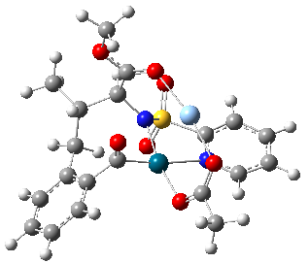
46	0	-0.52455	0.01796	-1.11886
7	0	-0.336	1.03706	0.66657
6	0	1.40405	0.54148	-1.51365
6	0	-0.7672	-0.68542	-2.88791
16	0	-0.05356	0.37028	2.11034
6	0	-0.85274	2.40679	0.57984
6	0	2.023	1.75047	-1.14102
6	0	2.18121	-0.48197	-2.08879
8	0	-0.97804	-1.08942	-3.93383
6	0	1.66105	-0.22746	1.88926
8	0	-0.847	-0.85416	2.35475
8	0	0.01579	1.39491	3.16411
6	0	-0.14022	3.17182	-0.54917
1	0	-0.68014	2.91531	1.53608
6	0	-2.36667	2.31381	0.3411
6	0	1.38067	2.9582	-0.46293
6	0	3.40909	1.87068	-1.36926
6	0	3.5539	-0.34083	-2.29191
1	0	1.71844	-1.42391	-2.37112
7	0	1.85564	-1.38098	1.23067
6	0	2.70605	0.5664	2.35636
6	0	-0.49109	4.66525	-0.47188
1	0	-0.50923	2.78995	-1.50866
8	0	-2.92076	2.54615	-0.7139
8	0	-2.98997	1.86726	1.44101
1	0	1.6667	2.93977	0.60045
1	0	1.87017	3.848	-0.87838
1	0	3.89575	2.80276	-1.08645
6	0	4.17485	0.85243	-1.92729
1	0	4.12264	-1.15283	-2.73849
6	0	3.12051	-1.76679	0.98443
6	0	4.01199	0.15608	2.10235
1	0	2.47621	1.4759	2.89811
1	0	-0.05472	5.20966	-1.31677
1	0	-0.105	5.11294	0.45345
1	0	-1.57451	4.81259	-0.5027
6	0	-4.36102	1.47521	1.25586
1	0	5.24097	0.99451	-2.08422
1	0	3.23908	-2.69304	0.43266
6	0	4.2243	-1.02925	1.39811
1	0	4.8514	0.75395	2.44488
1	0	-4.96559	2.32745	0.93256
1	0	-4.69287	1.11263	2.22913
1	0	-4.40821	0.68321	0.50491
1	0	5.22396	-1.37952	1.16567
47	0	0.02819	-2.43255	0.41458
8	0	-1.94175	-2.88404	-0.36863
6	0	-2.78486	-1.93346	-0.40531
8	0	-2.53445	-0.70467	-0.59228
6	0	-4.24278	-2.29801	-0.17861
1	0	-4.46389	-2.16362	0.88707
1	0	-4.89888	-1.63711	-0.74999
1	0	-4.42339	-3.34271	-0.43919



TS3-A'

E(RB3LYP) = -2081.61722238
G(correction)= 0.323916
$E(RM06)_{dioxane}$ = -2083.45835808
Imaginary frequencies: 1 (-312.8406 cm^{-1})

46	0	1.19067	0.92216	-0.83202
6	0	0.02148	2.65705	-0.51429
6	0	0.87181	2.15699	-2.17176
7	0	-0.93469	-0.336	0.45717
8	0	2.74718	-0.44772	-1.52075
6	0	-1.3866	2.64648	-0.59466
6	0	0.70487	3.55646	0.31608
8	0	0.83293	2.72203	-3.18596
16	0	-0.8301	-0.05098	2.05172
6	0	-2.292	-0.22337	-0.07462
6	0	2.87027	-1.70137	-1.69788
6	0	-2.18584	1.84519	-1.60522
6	0	-2.07145	3.52127	0.25655
6	0	-0.00918	4.40943	1.15511
1	0	1.79043	3.5743	0.3186
6	0	0.97317	-0.21123	2.2791
8	0	-1.41717	-1.11443	2.89955
8	0	-1.19852	1.33641	2.40237
6	0	-2.20946	0.29703	-1.53949
1	0	-2.91049	0.46998	0.50886
6	0	-2.97285	-1.59521	-0.03229
8	0	2.02406	-2.60501	-1.44771
6	0	4.19418	-2.14456	-2.30745
1	0	-3.22545	2.1885	-1.53678
1	0	-1.84844	2.12253	-2.614
1	0	-3.1581	3.5297	0.23282
6	0	-1.40211	4.3771	1.13128
1	0	0.51867	5.08711	1.81975
7	0	1.80451	0.18552	1.30801
6	0	1.41241	-0.7196	3.50087
6	0	-3.34551	-0.20994	-2.44217
1	0	-1.26388	-0.08968	-1.94036
8	0	-2.42318	-2.65058	-0.30535
8	0	-4.26509	-1.50742	0.30018
47	0	0.17145	-2.07737	-0.4355
1	0	4.34474	-3.21696	-2.17129
1	0	4.17881	-1.92031	-3.38031
1	0	5.02035	-1.58063	-1.86566
1	0	-1.97389	5.02857	1.78591
6	0	3.12833	0.07083	1.51811
6	0	2.78459	-0.80879	3.72296
1	0	0.68082	-1.04906	4.22923
1	0	-3.27309	0.24533	-3.43618
1	0	-4.32728	0.0418	-2.02455
1	0	-3.29717	-1.29622	-2.57033
6	0	-4.98644	-2.7542	0.35113
1	0	3.76219	0.35119	0.68379
6	0	3.6597	-0.40956	2.71187
1	0	3.1641	-1.19819	4.66323
1	0	-4.98115	-3.23729	-0.62995
1	0	-6.00175	-2.4908	0.64756
1	0	-4.52878	-3.42276	1.08452
1	0	4.73563	-0.47715	2.8348

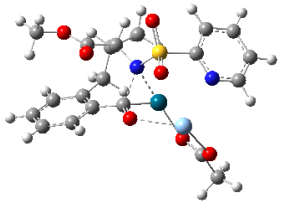


IM6-A'

E(RB3LYP) = -2081.64690748
G(correction)= 0.328955
$E(RM06)_{dioxane}$ = -2083.48411775
Imaginary frequencies: 0

46	0	-0.18783	0.69242	-0.54827
7	0	0.10794	-1.36397	-0.40697
6	0	1.45527	1.10878	0.43213
8	0	-0.80984	2.72318	-0.38122
6	0	1.09673	-2.0775	0.36859
16	0	-0.65126	-2.199	-1.58722
6	0	2.63781	1.40992	-0.43221
8	0	1.46913	1.2013	1.64553
6	0	-1.59094	3.10994	0.54643
6	0	2.61239	-1.7174	0.07058
1	0	0.9804	-3.15416	0.17291
6	0	0.77591	-1.96183	1.86619
6	0	-2.23481	-1.31335	-1.60654
8	0	-0.91929	-3.59144	-1.17554
8	0	-0.07907	-1.98129	-2.92983
6	0	3.26302	0.43787	-1.24195
6	0	3.0943	2.7364	-0.40984
8	0	-2.09994	2.40723	1.46857
6	0	-1.9445	4.58955	0.54789
6	0	2.82298	-1.01315	-1.30175
6	0	3.47084	-2.99158	0.14447
1	0	2.95351	-1.04259	0.86181
8	0	-0.25272	-1.52519	2.37631
8	0	1.74765	-2.46799	2.6233
7	0	-2.15802	0.01187	-1.4544
6	0	-3.42407	-1.99759	-1.82621
6	0	4.35451	0.85524	-2.01554
6	0	4.1667	3.12633	-1.20755
1	0	2.59122	3.45394	0.23171
47	0	-1.38517	0.37366	1.92847
1	0	-2.99449	4.72529	0.82016
1	0	-1.3372	5.08925	1.31172
1	0	-1.73406	5.04467	-0.4217
1	0	1.91448	-1.0874	-1.90657
1	0	3.58657	-1.56576	-1.85959
1	0	4.5325	-2.74472	0.03088
1	0	3.19778	-3.68323	-0.66286

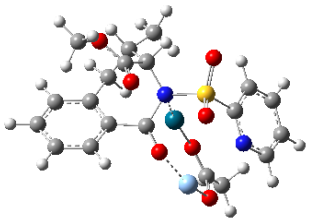
1	0	3.342	-3.50949	1.09849
6	0	1.55355	-2.40443	4.05129
6	0	-3.2844	0.73475	-1.5242
6	0	-4.59622	-1.24304	-1.89987
1	0	-3.41284	-3.07746	-1.92195
1	0	4.8662	0.12147	-2.63381
6	0	4.79792	2.17815	-2.01442
1	0	4.51113	4.15655	-1.19225
1	0	1.43761	-1.36448	4.36658
1	0	2.45352	-2.84239	4.48193
1	0	0.66698	-2.975	4.339
1	0	-3.16492	1.80355	-1.3831
6	0	-4.52641	0.14412	-1.75306
1	0	-5.55171	-1.73161	-2.06749
1	0	5.6415	2.46416	-2.63699
1	0	-5.41707	0.76147	-1.80485



TS4-A'

E(RB3LYP) = -2081.61276631
G(correction)= 0.327654
$E(RM06)_{dioxane}$ = -2083.45684987
Imaginary frequencies: 1 (-252.9011 cm^{-1})

46	0	-0.56008	-0.57975	0.8723
6	0	0.86217	-0.86881	-0.57485
7	0	0.73727	0.86883	-0.10392
6	0	2.20243	-1.42227	-0.1492
8	0	0.36183	-1.21362	-1.64509
6	0	1.95119	1.48462	0.48628
16	0	-0.14059	1.94585	-1.13048
6	0	2.81606	-1.24859	1.11154
6	0	2.8592	-2.17163	-1.14127
6	0	2.21149	1.09059	1.95772
1	0	1.80071	2.56944	0.4891
6	0	3.13382	1.30632	-0.48444
6	0	-1.699	2.20184	-0.205
8	0	-0.50205	1.29098	-2.38881
8	0	0.53251	3.25125	-1.13313
6	0	2.18663	-0.43409	2.21296
6	0	4.0748	-1.82529	1.32414
6	0	4.10879	-2.73487	-0.9085
1	0	2.37285	-2.28359	-2.10272
6	0	1.24135	1.81457	2.90081
1	0	3.22485	1.44595	2.16739
8	0	3.01136	1.12196	-1.67262
8	0	4.32092	1.45864	0.13496
7	0	-2.68762	1.35202	-0.47248
6	0	-1.77599	3.23351	0.7264
1	0	1.14364	-0.75854	2.35746
1	0	2.69834	-0.6315	3.16175
1	0	4.55179	-1.68921	2.29156
6	0	4.72259	-2.56053	0.33367
1	0	4.60054	-3.30369	-1.69253
1	0	1.42693	1.5247	3.94134
1	0	0.20095	1.56132	2.66374
1	0	1.35417	2.90296	2.82695
6	0	5.47262	1.28822	-0.71198
6	0	-3.82293	1.46919	0.22718
6	0	-2.9663	3.35523	1.44596
1	0	-0.93864	3.90581	0.8697
1	0	5.6984	-2.99582	0.53216
1	0	5.49116	0.27024	-1.11026
1	0	6.3356	1.46699	-0.06981
1	0	5.44902	2.00069	-1.54053
1	0	-4.58972	0.73174	0.00877
6	0	-4.00371	2.45512	1.20016
1	0	-3.07848	4.13986	2.18853
1	0	-4.93851	2.5113	1.74834
8	0	-1.98351	-1.99062	1.54346
6	0	-3.05764	-2.35116	0.95714
8	0	-3.44038	-2.0408	-0.20415
6	0	-3.95592	-3.27538	1.76997
47	0	-2.05188	-0.90866	-1.58749
1	0	-4.92887	-3.39707	1.29031
1	0	-3.47049	-4.25436	1.85411
1	0	-4.07563	-2.88335	2.78439

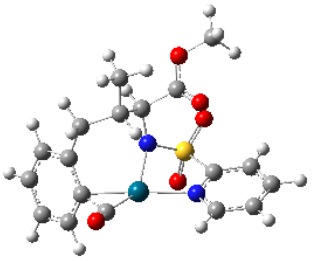


IM7-A'

E(RB3LYP) = -2081.61948785
G(correction)= 0.325255
$E(RM06)_{dioxane}$ = -2083.46779162
Imaginary frequencies: 0

46	0	-0.66762	-0.26934	0.98714
47	0	-1.77363	-1.37448	-1.36379
7	0	-2.46983	1.33214	-1.32844
8	0	-3.53604	-1.89451	-0.15579
6	0	-1.66641	1.99666	-0.50729
6	0	-3.76524	1.26625	-0.98481
6	0	-3.45125	-1.67184	1.09126
16	0	0.07843	2.19331	-1.03748
6	0	-2.0703	2.68249	0.64262
1	0	-4.40419	0.69374	-1.65013
6	0	-4.27962	1.868	0.1638
8	0	-2.46704	-1.18627	1.72408

6	0	-4.67769	-2.0054	1.93141
7	0	0.93543	0.88663	-0.05641
8	0	0.20761	1.98886	-2.46739
8	0	0.54332	3.43157	-0.39742
6	0	-3.41683	2.59542	0.98602
1	0	-1.3551	3.24039	1.23333
1	0	-5.33455	1.77291	0.39913
1	0	-5.42471	-2.54396	1.34574
1	0	-4.37874	-2.59794	2.80101
1	0	-5.11241	-1.07201	2.30754
6	0	2.16322	1.40473	0.6185
6	0	0.96905	-0.43618	-0.64362
1	0	-3.7846	3.08738	1.88142
6	0	2.37245	0.88476	2.05893
1	0	2.01396	2.48524	0.69675
6	0	3.35436	1.25964	-0.34322
6	0	2.10155	-1.3527	-0.2594
8	0	0.32343	-0.67436	-1.69923
6	0	2.18395	-0.64193	2.18825
6	0	1.47932	1.63185	3.05795
1	0	3.41631	1.11806	2.28831
8	0	3.23918	1.21237	-1.54644
8	0	4.53261	1.26411	0.30277
6	0	2.7014	-1.4366	1.01815
6	0	2.59406	-2.14453	-1.31033
1	0	1.10586	-0.85352	2.30493
1	0	2.66578	-0.97538	3.1139
1	0	1.64267	1.25261	4.07305
1	0	0.41858	1.48695	2.8163
1	0	1.69235	2.70715	3.05659
6	0	5.68916	1.12287	-0.54546
6	0	3.78957	-2.30028	1.18797
6	0	3.67695	-2.99645	-1.11911
1	0	2.12304	-2.05568	-2.28197
1	0	5.64635	0.16608	-1.0727
1	0	6.54743	1.15792	0.12567
1	0	5.72999	1.93553	-1.27508
1	0	4.25205	-2.36838	2.16948
6	0	4.2814	-3.07337	0.13713
1	0	4.04923	-3.59214	-1.94767
1	0	5.12854	-3.7341	0.30063

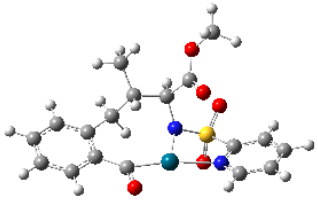


TS3-A*

E(RB3LYP) = -1707.2723742
G(correction)= 0.285463
$E(RM06)_{dioxane}$ = -1707.96357759

Imaginary frequencies: 1 (-146.7911 cm^{-1})

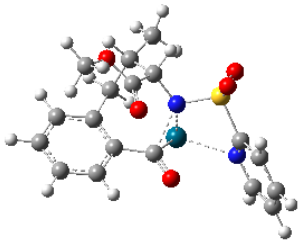
46	0	0.83827	-1.01712	-0.20121
6	0	2.82041	-0.32469	-0.21398
6	0	2.23321	-1.38962	-1.41732
6	0	2.76709	1.09566	-0.22445
6	0	3.63714	-1.0127	0.70745
8	0	2.70221	-1.66969	-2.4598
6	0	1.94586	1.92493	-1.19495
6	0	3.56536	1.76533	0.70969
6	0	4.43504	-0.31372	1.60577
1	0	3.64284	-2.09882	0.70124
6	0	0.39664	1.81375	-1.30237
1	0	2.18461	2.97672	-0.99706
1	0	2.3283	1.7178	-2.2052
1	0	3.53027	2.85086	0.74616
6	0	4.3886	1.08111	1.60576
1	0	5.07222	-0.84766	2.30394
6	0	-0.40817	1.82723	0.03611
6	0	-0.06434	2.95859	-2.22782
1	0	0.13988	0.86748	-1.7945
1	0	4.99075	1.64431	2.31348
7	0	-0.15022	0.61798	0.83385
1	0	-0.12867	2.71753	0.61271
6	0	-1.88567	1.96199	-0.35663
1	0	0.56554	3.00644	-3.12296
1	0	0.00086	3.92729	-1.71742
1	0	-1.09636	2.81532	-2.55843
16	0	-1.30478	-0.07487	1.71349
8	0	-2.49851	1.12552	-0.99186
8	0	-2.40423	3.13231	0.0407
6	0	-2.01497	-1.30798	0.55177
8	0	-2.4207	0.81686	2.08424
8	0	-0.6729	-0.91889	2.73959
6	0	-3.81437	3.28293	-0.19488
7	0	-1.13884	-1.88664	-0.28723
6	0	-3.36538	-1.63392	0.57087
1	0	-4.03913	3.21284	-1.26324
1	0	-4.07279	4.26944	0.19087
1	0	-4.35872	2.50192	0.34251
6	0	-1.58081	-2.81942	-1.14847
6	0	-3.8233	-2.60125	-0.32023
1	0	-4.02044	-1.11238	1.25914
1	0	-0.83505	-3.24819	-1.80898
6	0	-2.91629	-3.20608	-1.19381
1	0	-4.87388	-2.87684	-0.34052
1	0	-3.23385	-3.95982	-1.90641



IM6-A*

E(RB3LYP) = -1707.31268882
G(correction)= 0.288482
$E(RM06)_{dioxane}$ = -1707.99372794
Imaginary frequencies: 0

46	0	0.063	-1.31505	-0.13483
7	0	-0.40688	0.41709	0.93167
6	0	-0.10222	1.73828	0.39063
16	0	-1.84272	0.23548	1.68693
6	0	1.37603	1.74849	-0.08239
1	0	-0.22908	2.49617	1.17145
6	0	-1.02457	2.11395	-0.77272
6	0	-2.83475	-0.66789	0.45749
8	0	-2.5145	1.5314	1.89642
8	0	-1.7068	-0.70972	2.80151
6	0	2.28908	1.17403	1.03676
6	0	1.85916	3.13164	-0.53334
1	0	1.42133	1.07392	-0.94661
8	0	-1.50168	1.32628	-1.56428
8	0	-1.23568	3.44313	-0.82668
7	0	-2.14799	-1.54562	-0.28335
6	0	-4.20406	-0.46723	0.34102
6	0	3.45068	0.37671	0.50169
1	0	1.68389	0.53988	1.68992
1	0	2.66767	2.00018	1.64984
1	0	2.91455	3.07741	-0.82472
1	0	1.76722	3.86357	0.278
1	0	1.28955	3.50844	-1.38729
6	0	-2.09743	3.88663	-1.88822
6	0	-2.81623	-2.27903	-1.18637
6	0	-4.89587	-1.23264	-0.59707
1	0	-4.68828	0.27709	0.96315
6	0	3.28231	-0.87982	-0.13266
6	0	4.75493	0.87326	0.61551
1	0	-1.67453	3.62553	-2.86283
1	0	-2.16839	4.96888	-1.77603
1	0	-3.08345	3.42342	-1.79361
1	0	-2.22168	-2.97188	-1.77383
6	0	-4.19165	-2.15636	-1.37148
1	0	-5.96721	-1.10784	-0.72616
6	0	4.39827	-1.59279	-0.6172
6	0	1.96728	-1.49785	-0.34554
1	0	4.9065	1.83471	1.09868
6	0	5.85538	0.16472	0.13212
1	0	-4.69218	-2.76738	-2.11519
6	0	5.68052	-1.07667	-0.48661
1	0	4.23131	-2.55251	-1.09559
8	0	1.76417	-2.56127	-0.93482
1	0	6.8527	0.58304	0.23953
1	0	6.5348	-1.63149	-0.86292

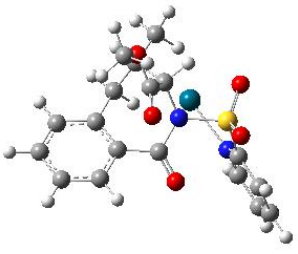


TS4-A*

E(RB3LYP) = -1707.25808767
G(correction)= 0.285008
$E(RM06)_{dioxane}$ = -1707.94546321
Imaginary frequencies: 1 (-182.6033 cm^{-1})

46	0	-0.9186	-1.0397	1.39178
7	0	-3.03049	-0.45758	0.29515
6	0	-2.72854	0.50626	-0.58251
6	0	-3.99093	-1.32598	-0.04986
16	0	-1.47314	1.71671	-0.07289
6	0	-3.34301	0.66829	-1.8175
1	0	-4.21445	-2.10252	0.67592
6	0	-4.67468	-1.25452	-1.26467
7	0	-0.13117	0.76159	0.13139
8	0	-1.29945	2.66386	-1.18813
8	0	-1.91204	2.26472	1.22566
6	0	-4.34377	-0.24156	-2.16285
1	0	-3.03041	1.47397	-2.47077
1	0	-5.44603	-1.98253	-1.49465
6	0	1.09809	1.53419	0.29547
1	0	-4.85175	-0.16108	-3.11941
6	0	1.83328	1.20783	1.62502
1	0	0.85828	2.60638	0.34259
6	0	1.96974	1.42921	-0.97165
6	0	1.97787	-0.31095	1.87315
6	0	1.12007	1.87094	2.80939
1	0	2.84144	1.62348	1.53153
8	0	1.61432	0.99246	-2.03974
8	0	3.19755	1.95613	-0.75219
6	0	2.39608	-1.09868	0.65509
1	0	1.01982	-0.70474	2.26933
1	0	2.70157	-0.4622	2.68184
1	0	1.5827	1.5757	3.75872
1	0	0.06147	1.58921	2.82959
1	0	1.16533	2.96291	2.73383
6	0	4.08804	1.90261	-1.87863
6	0	1.49447	-1.47376	-0.36378
6	0	3.7486	-1.4227	0.49092
1	0	4.27318	0.86191	-2.16088
1	0	5.01024	2.38195	-1.54752
1	0	3.66084	2.43356	-2.73358
6	0	1.95864	-2.17398	-1.49037
6	0	0.02435	-1.16246	-0.39103

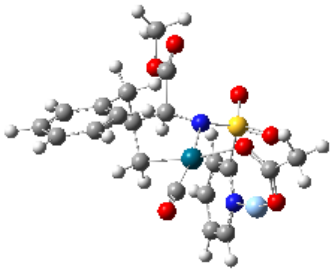
1	0	4.45249	-1.12736	1.26491
6	0	4.20689	-2.11018	-0.63237
6	0	3.30486	-2.4926	-1.62719
1	0	1.24511	-2.43616	-2.26276
8	0	-0.74086	-1.53169	-1.24632
1	0	5.26275	-2.34928	-0.72657
1	0	3.64839	-3.02775	-2.5077



IM7-A*

E(RB3LYP) = -1707.29783204
G(correction)= 0.287547
$E(RM06)_{dioxane}$ = -1707.98212852
Imaginary frequencies: 0

46	0	-1.79836	2.06909	0.0611
7	0	-2.87805	0.02743	0.34073
6	0	-2.46324	-1.12952	-0.17467
6	0	-3.95621	-0.01912	1.15019
16	0	-1.07704	-1.10364	-1.35626
6	0	-3.06116	-2.36599	0.05342
1	0	-4.27292	0.92987	1.5673
6	0	-4.63374	-1.20008	1.43956
7	0	0.26008	-0.43144	-0.46091
8	0	-0.79739	-2.49026	-1.72654
8	0	-1.35046	-0.11527	-2.40462
6	0	-4.18055	-2.39585	0.88033
1	0	-2.63994	-3.2589	-0.39027
1	0	-5.49855	-1.17558	2.09461
6	0	1.30567	0.18537	-1.29251
6	0	0.51918	-0.99754	0.7989
1	0	-4.68188	-3.33559	1.0906
6	0	1.6784	1.64173	-0.87352
1	0	0.8896	0.25358	-2.30197
6	0	2.50002	-0.77238	-1.4269
6	0	1.7069	-0.49568	1.55603
8	0	-0.22621	-1.84868	1.26195
6	0	1.49019	1.86645	0.63709
6	0	0.87389	2.66529	-1.68263
1	0	2.73963	1.77251	-1.10858
8	0	2.56892	-1.88653	-0.96408
8	0	3.45627	-0.21144	-2.19206
6	0	2.17156	0.83314	1.49669
6	0	2.33568	-1.43046	2.39
1	0	0.40132	1.8735	0.84974
1	0	1.86497	2.86468	0.88805
1	0	1.10799	3.68679	-1.36386
1	0	-0.2115	2.49523	-1.54859
1	0	1.08543	2.58246	-2.75449
6	0	4.61364	-1.03658	-2.42413
6	0	3.28287	1.18027	2.27613
6	0	3.4443	-1.06877	3.14794
1	0	1.94054	-2.43997	2.42065
1	0	5.09366	-1.29115	-1.47531
1	0	5.27863	-0.4379	-3.04689
1	0	4.32624	-1.95846	-2.93675
1	0	3.64473	2.2053	2.24776
6	0	3.9207	0.24356	3.08831
1	0	3.9334	-1.80307	3.7815
1	0	4.78405	0.53934	3.6785

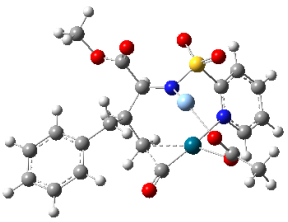


IM4-B'

E(RB3LYP) = -2081.63952028
G(correction)= 0.323622
$E(RM06)_{dioxane}$ = -2083.48670593
Imaginary frequencies: 0

46	0	-0.56916	-0.87987	0.00025
6	0	-1.40491	-2.37233	-0.82487
7	0	0.18572	0.95145	0.69148
6	0	-1.37433	0.41984	-1.37855
8	0	0.02099	-2.20525	1.68147
8	0	-1.88543	-3.28151	-1.32398
6	0	-0.45677	2.14419	0.09513
16	0	1.75012	1.17466	1.06455
6	0	-1.76413	1.65201	-0.56087
1	0	-0.56388	0.63452	-2.08405
1	0	-2.22272	-0.01023	-1.91261
6	0	0.78562	-3.20945	1.65192
1	0	0.16026	2.57248	-0.70788
6	0	-0.68089	3.24779	1.13072
6	0	2.60735	1.31737	-0.5657
8	0	2.29351	-0.03738	1.69608
8	0	1.9731	2.49425	1.6744
6	0	-2.89859	1.38562	0.46961
1	0	-2.11752	2.43027	-1.2563
8	0	1.62894	-3.49132	0.73745
6	0	0.72455	-4.16821	2.82936
8	0	-1.17382	3.10162	2.22402
8	0	-0.2892	4.4431	0.63149
7	0	2.85991	0.19473	-1.26093
6	0	2.89865	2.58899	-1.05913

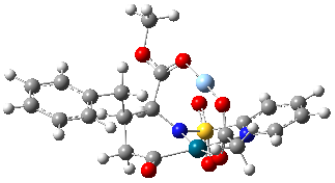
1	0	-3.27501	2.35165	0.82283
1	0	-2.47606	0.89022	1.34859
6	0	-4.02932	0.56192	-0.10119
47	0	2.3139	-1.77728	-0.35265
1	0	1.54877	-3.92774	3.51094
1	0	-0.21817	-4.06182	3.369
1	0	0.86259	-5.19686	2.48664
6	0	-0.41787	5.54478	1.54574
6	0	3.42494	0.30612	-2.47682
6	0	3.47433	2.6975	-2.32484
1	0	2.67377	3.45432	-0.44734
6	0	-4.22792	-0.76334	0.30949
6	0	-4.8764	1.08673	-1.08775
1	0	-1.45824	5.66654	1.86081
1	0	-0.0753	6.42439	0.99903
1	0	0.20316	5.37052	2.42875
1	0	3.62017	-0.62332	-3.00188
6	0	3.74495	1.53574	-3.04671
1	0	3.70919	3.67393	-2.7385
6	0	-5.23521	-1.54819	-0.25696
1	0	-3.58584	-1.17991	1.08216
6	0	-5.88386	0.30735	-1.6577
1	0	-4.74198	2.1168	-1.41238
1	0	4.19433	1.57153	-4.03342
6	0	-6.06429	-1.01639	-1.24629
1	0	-5.37182	-2.57366	0.07675
1	0	-6.53043	0.73308	-2.4209
1	0	-6.84886	-1.62439	-1.68864
8	0	2.49339	1.68722	1.63909
8	0	1.4126	3.49134	0.18034
8	0	1.43378	-2.47692	2.11843
6	0	3.1072	-4.07632	1.60418
6	0	-1.10708	-0.30864	-1.7686
6	0	-2.63912	-0.07134	0.30136
1	0	-2.48313	1.22824	-1.38577
8	0	-1.44138	2.65276	1.95835
8	0	-2.48216	3.3688	0.08241
7	0	2.6284	0.26261	-1.37191
6	0	3.68397	2.42046	-1.43054
1	0	2.51496	-4.86533	2.07744
1	0	3.64182	-4.4731	0.7398
1	0	3.82477	-3.71476	2.34853
1	0	-0.41696	0.20426	-2.44728
1	0	-1.84457	-0.81999	-2.38907
1	0	-2.82541	0.62489	1.1261
1	0	-2.08546	-0.90689	0.74191
6	0	-3.97468	-0.54813	-0.23744
6	0	-3.28871	4.2394	0.89708
6	0	3.50936	-0.17214	-2.29344
6	0	4.57927	1.97123	-2.39732
1	0	3.69993	3.43597	-1.05199
6	0	-4.31648	-1.90408	-0.28789
6	0	-4.91169	0.39656	-0.68675
1	0	-3.87971	3.65674	1.60984
1	0	-3.9389	4.77233	0.20258
1	0	-2.65433	4.93827	1.44838
1	0	3.40417	-1.20883	-2.59785
6	0	4.4991	0.64544	-2.82901
1	0	5.33219	2.64097	-2.8028
6	0	-5.55686	-2.30915	-0.78934
1	0	-3.61045	-2.64885	0.06461
6	0	-6.14918	-0.00414	-1.18769
1	0	-4.66556	1.45566	-0.63399
1	0	5.18461	0.24828	-3.57021
6	0	-6.47513	-1.36251	-1.24388
1	0	-5.80254	-3.36734	-0.82231
1	0	-6.86198	0.74236	-1.52859
1	0	-7.4392	-1.67767	-1.63391
47	0	0.57108	-0.45129	1.94793



TS3-B'

E(RB3LYP) = -2081.60088839
G(correction)= 0.322009
$E(RM06)_{dioxane}$ = -2083.44929944
Imaginary frequencies: 1 (-315.6126 cm^{-1})

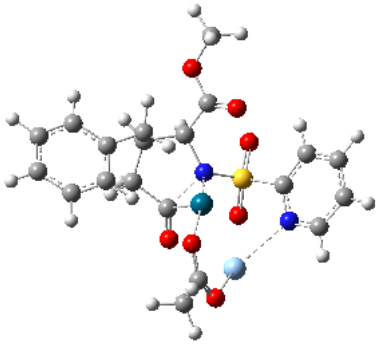
46	0	0.91368	-1.15389	-0.88185
6	0	-0.6657	-2.05455	-1.04479
7	0	0.36365	1.1456	0.42471
8	0	2.27971	-2.52876	0.00345
8	0	-1.41188	-2.94745	-0.99334
6	0	-0.80328	1.72069	-0.21294
16	0	1.68546	2.06959	0.46297
6	0	2.18834	-2.9286	1.21226
6	0	-1.77999	0.64671	-0.77493
1	0	-0.51522	2.35436	-1.06281
6	0	-1.57291	2.62828	0.75682
6	0	2.73466	1.52471	-0.93831



IM6-B'

E(RB3LYP) = -2081.64590708
G(correction)= 0.327801
$E(RM06)_{dioxane}$ = -2083.48818413
Imaginary frequencies: 0

46	0	0.68689	0.90241	1.07842
7	0	0.53761	-1.15142	1.19135
6	0	-1.18257	1.10116	1.65872
8	0	0.92903	2.9476	0.55808
6	0	-0.56044	-1.94871	0.6831
16	0	1.95603	-1.92681	1.40437
8	0	-1.69492	2.18731	1.75274
6	0	-1.91895	-0.19887	2.01551
6	0	0.76777	3.38547	-0.62022
6	0	-1.95595	-1.22912	0.86846
1	0	-0.62323	-2.89045	1.23674
6	0	-0.36449	-2.36582	-0.77903
6	0	3.12351	-0.89346	0.46137
8	0	1.92387	-3.24841	0.73997
8	0	2.43691	-1.83932	2.78922
1	0	-1.41979	-0.63247	2.8891
1	0	-2.94209	0.07639	2.2884
8	0	0.57937	2.70743	-1.67959
6	0	0.77959	4.89691	-0.77975
6	0	-2.57232	-0.61409	-0.4178
1	0	-2.64546	-2.02148	1.17974
8	0	0.17649	-1.70825	-1.67157
8	0	-0.90142	-3.55241	-1.02553
7	0	2.85387	0.41446	0.43093
6	0	4.24713	-1.4605	-0.13043
47	0	0.4652	0.53015	-1.67815
1	0	-0.25211	5.25597	-0.68593
1	0	1.37365	5.36231	0.00952
1	0	1.15158	5.17878	-1.76733
1	0	-2.50545	-1.3407	-1.23563
1	0	-1.99436	0.26564	-0.7272
6	0	-4.02671	-0.2315	-0.23737
6	0	-0.78705	-4.05162	-2.37555
6	0	3.71314	1.23884	-0.18707
6	0	5.13913	-0.60294	-0.77535
1	0	4.39474	-2.53383	-0.08715
6	0	-4.4045	1.08029	0.07849
6	0	-5.02379	-1.20949	-0.35856
1	0	-1.26692	-3.36384	-3.07685
1	0	-1.29331	-5.01617	-2.36874
1	0	0.26688	-4.16723	-2.63849
1	0	3.43499	2.28776	-0.18514
6	0	4.87398	0.76893	-0.79885
1	0	6.02954	-0.99943	-1.25479
6	0	-5.7495	1.40424	0.26918
1	0	-3.64227	1.84456	0.19762
6	0	-6.3681	-0.88817	-0.16827
1	0	-4.74186	-2.23112	-0.60758
1	0	5.54713	1.46428	-1.28928
6	0	-6.73484	0.4227	0.14617
1	0	-6.02496	2.42604	0.51606
1	0	-7.1282	-1.65848	-0.26955
1	0	-7.78117	0.67648	0.29336

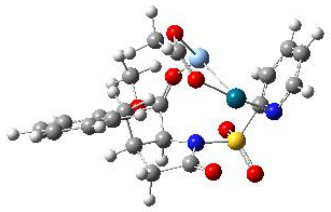


TS4-B'

E(RB3LYP) = -2081.62599584
G(correction)= 0.327458
$E(RM06)_{dioxane}$ = -2083.47064298
Imaginary frequencies: 1 (-189.1804 cm^{-1})

46	0	0.09683	-0.56301	-0.4155
6	0	0.54926	-0.32907	1.58262
8	0	0.42963	-2.44682	-1.283
6	0	1.94756	0.21972	1.83362
8	0	-0.05577	-1.06968	2.338
6	0	-0.23153	-3.50408	-1.00281
6	0	2.216	1.44559	0.95033
1	0	1.97541	0.49121	2.89686
1	0	2.67604	-0.57906	1.67573
8	0	-1.25627	-3.59694	-0.27688
6	0	0.31644	-4.78398	-1.62032
6	0	0.83437	2.17687	0.87337
6	0	2.81704	1.12994	-0.44842
1	0	2.91541	2.11325	1.46179
47	0	-2.11306	-1.82319	0.83942
1	0	-0.38726	-5.60924	-1.49923
1	0	0.53836	-4.62294	-2.67936
1	0	1.25964	-5.03804	-1.12296
7	0	-0.18952	1.12689	0.8758
1	0	0.72692	2.80698	1.76215
6	0	0.72027	3.08658	-0.34179
1	0	3.12131	2.08205	-0.90031
1	0	2.03919	0.70321	-1.09536
6	0	3.99641	0.1871	-0.39576
16	0	-1.76777	1.60547	1.26445
8	0	0.01099	2.89858	-1.30632
8	0	1.54833	4.13857	-0.20477
6	0	3.83959	-1.17536	-0.69221
6	0	5.25978	0.65091	-0.00404
6	0	-2.73248	1.29717	-0.25202
8	0	-1.76748	3.05773	1.48409
8	0	-2.31216	0.69582	2.27806
6	0	1.55818	5.06619	-1.30543
6	0	4.92426	-2.05012	-0.5945
1	0	2.86562	-1.55603	-0.99367
6	0	6.3439	-0.22228	0.09375
1	0	5.39385	1.70694	0.22336
7	0	-3.18304	0.05188	-0.41889
6	0	-2.96722	2.3464	-1.13279
1	0	1.87815	4.5646	-2.22314

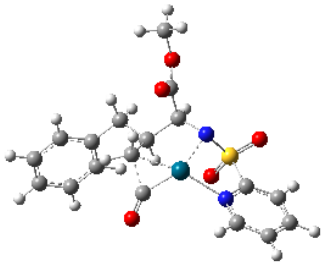
1	0	2.26618	5.84599	-1.02466
1	0	0.56031	5.48658	-1.45663
6	0	6.17792	-1.57804	-0.20039
1	0	4.78656	-3.10262	-0.82826
1	0	7.31728	0.15515	0.39656
6	0	-3.90302	-0.20553	-1.52025
6	0	-3.71838	2.06726	-2.27506
1	0	-2.55735	3.32652	-0.93015
1	0	7.02083	-2.25993	-0.12552
1	0	-4.24643	-1.22895	-1.63761
6	0	-4.19401	0.77175	-2.47333
1	0	-3.92367	2.84997	-2.99912
1	0	-4.77835	0.51349	-3.35041



IM7-B'

E(RB3LYP) = -2081.64123456
G(correction)= 0.327399
$E(RM06)_{dioxane}$ = -2083.48964972
Imaginary frequencies: 0

46	0	1.01711	1.87644	0.74209
7	0	2.82936	0.90479	1.15431
8	0	-0.7878	2.77003	0.07395
6	0	2.85332	-0.24692	0.44732
6	0	3.43809	1.97781	0.56223
6	0	-1.23208	2.77672	-1.11896
16	0	2.15425	-1.70436	1.27939
6	0	3.54652	-0.45192	-0.7443
1	0	3.53179	2.86817	1.17637
6	0	4.10562	1.8859	-0.67347
8	0	-0.83636	2.0585	-2.08137
6	0	-2.40819	3.70523	-1.38734
7	0	0.43206	-1.51964	1.19935
8	0	2.40085	-2.86729	0.41523
8	0	2.5597	-1.70018	2.67678
6	0	4.18731	0.65735	-1.31768
1	0	3.57462	-1.43669	-1.19397
1	0	4.57558	2.77157	-1.08851
47	0	0.59923	0.41592	-1.50379
1	0	-2.4111	4.02895	-2.43038
1	0	-3.33377	3.14779	-1.19918
1	0	-2.38183	4.56561	-0.71502
6	0	-0.37469	-2.56621	0.56042
6	0	-0.29841	-0.83775	2.208
1	0	4.73165	0.55051	-2.2507
6	0	-1.83662	-2.05882	0.80148
1	0	-0.23332	-3.53041	1.06007
6	0	-0.05505	-2.77896	-0.90963
6	0	-1.70256	-1.41781	2.19024
8	0	0.14145	0.03014	2.92219
6	0	-2.30351	-1.03678	-0.2629
1	0	-2.51671	-2.9151	0.80498
8	0	0.42681	-1.96807	-1.68588
8	0	-0.44312	-3.99581	-1.284
1	0	-1.7541	-2.17336	2.98533
1	0	-2.44467	-0.64789	2.40502
1	0	-2.3454	-1.53134	-1.24122
1	0	-1.55709	-0.23852	-0.3445
6	0	-3.64507	-0.41825	0.05715
6	0	-0.24917	-4.32538	-2.67685
6	0	-3.71903	0.87599	0.59223
6	0	-4.83143	-1.135	-0.14743
1	0	-0.79833	-3.62499	-3.31135
1	0	-0.63526	-5.3378	-2.78896
1	0	0.81441	-4.28448	-2.92331
6	0	-4.95642	1.43864	0.91532
1	0	-2.80683	1.44846	0.74536
6	0	-6.06776	-0.57416	0.17572
1	0	-4.78619	-2.13755	-0.56907
6	0	-6.13307	0.71551	0.70958
1	0	-4.99662	2.44371	1.32658
1	0	-6.97956	-1.14114	0.00695
1	0	-7.09533	1.15407	0.95948

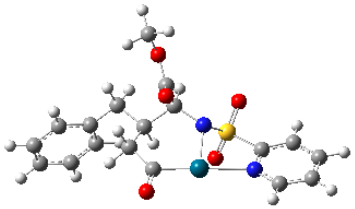


TS3-B*

E(RB3LYP) = -1707.2463649
G(correction)= 0.282912
$E(RM06)_{dioxane}$ = --1707.93752045
Imaginary frequencies: 1 (-201.8188 cm^{-1})

46	0	-0.96011	-0.34794	-1.2941
6	0	0.37699	-1.64502	-1.28142
6	0	1.33199	-0.27598	-1.1442
8	0	0.63616	-2.77694	-1.09673
6	0	1.3863	0.36078	0.28046
1	0	2.27474	-0.7718	-1.39318
1	0	1.17367	0.48116	-1.92484
6	0	0.3799	1.5552	0.50554
6	0	2.83724	0.80745	0.59693
1	0	1.09308	-0.39505	1.01457
7	0	-1.04883	1.2598	0.29195
1	0	0.56971	1.91741	1.52173
6	0	0.69471	2.69404	-0.45786

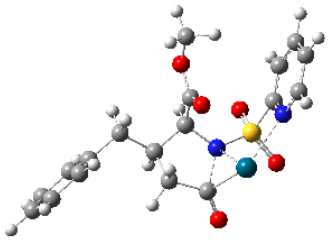
1	0	3.16532	1.55133	-0.14073
1	0	2.83098	1.31441	1.56978
6	0	3.81021	-0.35068	0.62887
16	0	-1.80373	0.5757	1.54976
8	0	0.5656	2.62966	-1.66707
8	0	1.16386	3.77967	0.17878
6	0	4.79131	-0.50371	-0.35925
6	0	3.71614	-1.32311	1.63606
6	0	-3.14015	-0.35731	0.6777
8	0	-2.53594	1.51329	2.422
8	0	-0.98126	-0.45181	2.23887
6	0	1.47579	4.90491	-0.66352
6	0	5.65899	-1.59958	-0.34509
1	0	4.88028	0.24552	-1.14347
6	0	4.58007	-2.41701	1.65384
1	0	2.95861	-1.22023	2.40995
7	0	-2.87023	-0.98216	-0.48315
6	0	-4.37144	-0.47462	1.31596
1	0	2.24707	4.63608	-1.39101
1	0	1.83439	5.68309	0.01038
1	0	0.58246	5.23719	-1.19897
6	0	5.5548	-2.55963	0.66163
1	0	6.41468	-1.69967	-1.11979
1	0	4.49301	-3.15976	2.44228
6	0	-3.81307	-1.76116	-1.04234
6	0	-5.35046	-1.27846	0.73393
1	0	-4.53418	0.06907	2.23931
1	0	6.22718	-3.41304	0.67526
1	0	-3.53991	-2.24486	-1.97365
6	0	-5.06608	-1.93743	-0.46281
1	0	-6.32191	-1.38799	1.2071
1	0	-5.79788	-2.57522	-0.94718



IM6-B*

E(RB3LYP) = -1707.30178176
G(correction)= 0.284501
$E(RM06)_{dioxane}$ = -1707.9863206
Imaginary frequencies: 0

46	0	-1.24229	-0.31622	-1.4233
6	0	0.54436	-0.21991	-2.05871
7	0	-0.90576	0.54904	0.42773
8	0	0.49538	-0.56381	-3.21914
6	0	0.4132	1.08584	0.74811
16	0	-1.54818	-0.44472	1.56603
6	0	1.59532	0.18155	0.26832
1	0	0.50256	1.20495	1.83372
6	0	0.51834	2.47176	0.11894
6	0	-3.21928	-0.57005	0.84733
8	0	-1.68055	0.2383	2.86612
8	0	-0.98729	-1.81244	1.57683
6	0	1.77421	0.15033	-1.25986
6	0	2.91803	0.58872	0.95783
1	0	1.32805	-0.82816	0.60247
8	0	0.19266	2.74915	-1.0165
8	0	1.0901	3.35015	0.96674
7	0	-3.30767	-0.66917	-0.48668
6	0	-4.31655	-0.60641	1.69982
1	0	2.55423	-0.56876	-1.53262
1	0	2.09445	1.12955	-1.63893
1	0	3.20718	1.5963	0.63334
1	0	2.73094	0.65446	2.03737
6	0	4.04388	-0.38805	0.69556
6	0	1.28838	4.6749	0.43902
6	0	-4.52635	-0.81846	-1.02861
6	0	-5.5788	-0.76847	1.12858
1	0	-4.1664	-0.49725	2.76795
6	0	5.11049	-0.06244	-0.15131
6	0	4.01539	-1.6647	1.27632
1	0	1.92966	4.64262	-0.44651
1	0	1.76364	5.24074	1.24048
1	0	0.3291	5.122	0.16491
1	0	-4.56098	-0.88661	-2.1116
6	0	-5.68656	-0.87872	-0.25825
1	0	-6.46454	-0.80278	1.75617
6	0	6.12515	-0.98623	-0.41403
1	0	5.1475	0.92439	-0.60802
6	0	5.02596	-2.59012	1.01679
1	0	3.19364	-1.93205	1.93739
1	0	-6.64995	-1.00219	-0.74169
6	0	6.08516	-2.25354	0.16912
1	0	6.94544	-0.71419	-1.07317
1	0	4.98812	-3.57364	1.47765
1	0	6.87322	-2.97381	-0.03326

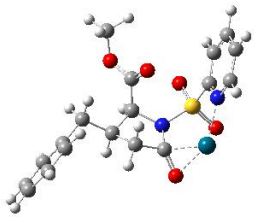


TS4-B*

E(RB3LYP) = -1707.26576673
G(correction)= 0.283082
$E(RM06)_{dioxane}$ = -1707.95634127
Imaginary frequencies: 1 (-232.1362 cm^{-1})

46	0	-1.06448	-1.64153	-1.09038
7	0	-0.40142	-0.54735	1.01803

6	0	0.34891	0.68584	0.87128
16	0	-1.84422	-0.52735	1.78841
6	0	1.80155	0.20811	0.61412
1	0	0.31123	1.28683	1.7847
6	0	-0.16401	1.54409	-0.29113
6	0	-3.00461	0.24083	0.58406
8	0	-1.8128	0.41982	2.91591
8	0	-2.28261	-1.91022	1.97658
6	0	1.74282	-0.99032	-0.34887
6	0	2.74236	1.32712	0.12949
1	0	2.16051	-0.16117	1.58234
8	0	-0.39475	1.13282	-1.41476
8	0	-0.33025	2.825	0.07203
7	0	-3.09287	-0.33243	-0.623
6	0	-3.71305	1.38112	0.95303
6	0	0.56056	-1.89267	0.01445
1	0	2.65251	-1.59361	-0.29513
1	0	1.61984	-0.63371	-1.3771
1	0	2.4022	1.68511	-0.8508
1	0	2.65726	2.17379	0.82351
6	0	4.18187	0.87026	0.03661
6	0	-0.85121	3.69788	-0.94864
6	0	-3.91636	0.2241	-1.52123
6	0	-4.56512	1.95654	0.00763
1	0	-3.58281	1.7904	1.94758
8	0	0.56723	-3.02884	0.41066
6	0	4.75162	0.52352	-1.19475
6	0	4.95918	0.73815	1.19573
1	0	-0.19108	3.70746	-1.82001
1	0	-0.90209	4.68532	-0.48994
1	0	-1.84554	3.36063	-1.25532
1	0	-3.96544	-0.26397	-2.49021
6	0	-4.67059	1.36819	-1.25167
1	0	-5.13519	2.84814	0.25319
6	0	6.06464	0.05334	-1.26893
1	0	4.16138	0.62407	-2.10304
6	0	6.27103	0.26909	1.12682
1	0	4.5304	1.00659	2.15909
1	0	-5.31934	1.78179	-2.01711
6	0	6.82802	-0.07602	-0.10744
1	0	6.49012	-0.20977	-2.23375
1	0	6.85951	0.17512	2.03562
1	0	7.85014	-0.44045	-0.16263

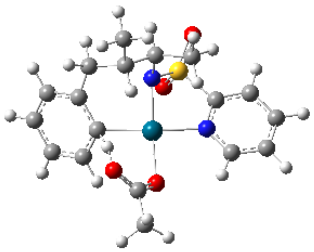


IM7-B*

E(RB3LYP) = -1707.29325834
G(correction)= 0.287119
$E(RM06)_{dioxane}$ = -1707.98397552

Imaginary frequencies: 0

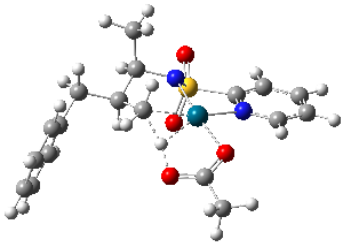
46	0	-1.45762	-2.21519	-0.24584
7	0	-2.69689	-0.61142	-0.92905
6	0	-2.80789	0.41686	-0.07448
6	0	-3.33171	-0.51501	-2.11297
16	0	-1.98308	0.31698	1.57396
6	0	-3.55032	1.56241	-0.34089
1	0	-3.21191	-1.35789	-2.78444
6	0	-4.0975	0.59228	-2.46729
7	0	-0.36454	-0.02722	1.31545
8	0	-2.01172	1.69114	2.09374
8	0	-2.61311	-0.78436	2.29456
6	0	-4.2125	1.64794	-1.5642
1	0	-3.58807	2.35637	0.3944
1	0	-4.58794	0.61826	-3.43477
6	0	0.57955	1.08517	1.13264
6	0	0.1391	-1.29514	0.69675
1	0	-4.80183	2.52671	-1.80852
6	0	1.88079	0.34663	0.69683
1	0	0.71524	1.62723	2.06956
6	0	0.15131	2.07809	0.0558
6	0	1.33986	-0.83112	-0.12926
8	0	0.10251	-2.41347	1.28616
6	0	2.91827	1.22746	-0.02113
1	0	2.33532	-0.0526	1.61215
8	0	-0.45306	1.79512	-0.95884
8	0	0.59653	3.31085	0.34642
1	0	2.05412	-1.64628	-0.24593
1	0	1.02037	-0.47616	-1.11452
1	0	2.49925	1.57597	-0.97383
1	0	3.11198	2.12009	0.5863
6	0	4.20681	0.47493	-0.27259
6	0	0.31345	4.31719	-0.64205
6	0	4.43371	-0.18006	-1.4898
6	0	5.17887	0.37731	0.73207
1	0	0.78372	4.05946	-1.59544
1	0	0.72834	5.24326	-0.24441
1	0	-0.76597	4.40778	-0.79002
6	0	5.60142	-0.9165	-1.69876
1	0	3.68792	-0.11294	-2.27879
6	0	6.34787	-0.35665	0.52783
1	0	5.0165	0.88256	1.68205
6	0	6.56223	-1.00718	-0.6897
1	0	5.76047	-1.41788	-2.64981
1	0	7.09151	-0.41922	1.31791
1	0	7.472	-1.579	-0.85095



TS2-A-6b

E(RB3LYP) = -1634.4972078
G(correction)= 0.321864
E(RM06)$_{dioxane}$ = -1635.17692186
Imaginary frequencies: 1 (-1434.7286 cm^{-1})

46	0	0.10774	0.60902	-0.14996
7	0	-0.33935	-1.37508	0.01149
6	0	2.13029	0.10036	-0.41952
8	0	0.50058	2.6778	0.00859
16	0	-1.65088	-1.66601	-0.91545
6	0	-0.3231	-1.89897	1.39972
6	0	2.5886	-1.2123	-0.14136
6	0	2.61073	0.75316	-1.58478
1	0	2.16587	1.07227	0.58998
6	0	1.46278	2.99052	0.77469
6	0	-2.69628	-0.2079	-0.55407
8	0	-2.40616	-2.84659	-0.46817
8	0	-1.30256	-1.50685	-2.33054
6	0	1.07006	-1.59598	2.00859
1	0	-0.4222	-2.99011	1.32123
6	0	-1.46679	-1.37157	2.2847
6	0	2.22045	-2.03267	1.08429
6	0	3.5109	-1.8009	-1.01965
6	0	3.51525	0.15152	-2.44914
1	0	2.26493	1.76266	-1.79516
8	0	2.32024	2.16267	1.23099
6	0	1.63315	4.44117	1.16193
7	0	-1.99885	0.89381	-0.23956
6	0	-4.0834	-0.22647	-0.62178
6	0	1.24	-2.29178	3.37129
1	0	1.13822	-0.51167	2.17575
1	0	-1.45649	-1.8462	3.26991
1	0	-1.38142	-0.28688	2.42261
1	0	-2.43707	-1.5939	1.83319
1	0	2.0244	-3.06309	0.75616
1	0	3.13335	-2.09303	1.69558
1	0	3.87071	-2.80622	-0.8093
6	0	3.96243	-1.1415	-2.15976
1	0	3.86675	0.67317	-3.33501
1	0	1.76488	4.51822	2.24506
1	0	2.54459	4.82749	0.69297
1	0	0.77586	5.03307	0.83819
6	0	-2.64913	2.0436	0.00089
6	0	-4.76561	0.96341	-0.36786
1	0	-4.59166	-1.15505	-0.8578
1	0	2.22827	-2.07314	3.79088
1	0	1.1543	-3.38133	3.26855
1	0	0.49638	-1.96318	4.10242
1	0	4.66604	-1.63705	-2.82416
1	0	-2.02162	2.89649	0.23779
6	0	-4.03836	2.11616	-0.05768
1	0	-5.85057	0.99355	-0.41075
1	0	-4.53656	3.05862	0.1435



TS2-B-6b

E(RB3LYP) = -1634.48220545
G(correction)= 0.318932
E(RM06)$_{dioxane}$ = -1635.16767363
Imaginary frequencies: 1 (-1321.4004 cm^{-1})

46	0	0.75021	0.65112	-0.4405
7	0	0.89841	-1.36227	-0.54404
7	0	2.78518	0.53713	0.03507
8	0	0.81224	2.74256	-0.35807
6	0	-0.36328	-2.12276	-0.73759
16	0	1.87766	-1.90434	0.66127
6	0	3.19771	-0.68162	0.41
6	0	3.67848	1.53157	-0.08846
6	0	-0.281	3.27591	0.01502
6	0	-1.53383	-1.18839	-0.3552
1	0	-0.38915	-2.98841	-0.06269
6	0	-0.38388	-2.64827	-2.17627
8	0	2.42552	-3.2356	0.35698
8	0	1.36534	-1.67695	2.02633
6	0	4.5278	-0.9849	0.66209
1	0	3.27353	2.49295	-0.38481
6	0	5.03275	1.3175	0.15795
8	0	-1.35308	2.62152	0.18673
6	0	-0.30288	4.76319	0.27748
6	0	-1.35216	0.20078	-1.00055
6	0	-2.91632	-1.80923	-0.67829
1	0	-1.47718	-1.06742	0.73367
1	0	0.50493	-3.26334	-2.34218
1	0	-1.27164	-3.26102	-2.36825
1	0	-0.36304	-1.82583	-2.89959
6	0	5.46345	0.04235	0.53163
1	0	4.79905	-1.99743	0.94022
1	0	5.73323	2.13863	0.04963
1	0	0.64029	5.2269	-0.01472
1	0	-1.13558	5.21697	-0.26749
1	0	-0.48031	4.93003	1.34533
1	0	-2.32274	0.7196	-0.99825
1	0	-1.09153	0.14643	-2.06431
1	0	-1.13122	1.38227	-0.26093

1	0	-3.05138	-1.85682	-1.76529
1	0	-2.92684	-2.84514	-0.31191
6	0	-4.05863	-1.03818	-0.05489
1	0	6.51599	-0.1496	0.71782
6	0	-4.89188	-0.21993	-0.82843
6	0	-4.27974	-1.0956	1.32932
6	0	-5.91736	0.52403	-0.23862
1	0	-4.73713	-0.16821	-1.90409
6	0	-5.30241	-0.35666	1.92257
1	0	-3.64147	-1.72636	1.94459
6	0	-6.12542	0.45792	1.13931
1	0	-6.55251	1.15285	-0.85725
1	0	-5.45874	-0.4166	2.99654
1	0	-6.92245	1.03456	1.60099

IM1-1a(dioxane)

E(RB3LYP) = -3062.48302449
G(correction)= 0.609080
E(RM06) = -3062.69818394
Imaginary frequencies: 0

6	0	-1.25488	-2.8155	0.1508
1	0	-0.48498	-2.85924	0.91098
6	0	-2.10251	-3.88077	-0.14422
7	0	-1.34886	-1.65823	-0.51948
1	0	-2.01044	-4.80418	0.41667
6	0	-3.0641	-3.73417	-1.14404
6	0	-2.27057	-1.51637	-1.4877
46	0	-0.18257	-0.00401	-0.16302
1	0	-3.74088	-4.54972	-1.38017
6	0	-3.15627	-2.52273	-1.8341
16	0	-2.22087	0.12586	-2.28376
7	0	0.9888	1.66369	0.15117
1	0	-3.8941	-2.34654	-2.60879
7	0	-1.76998	1.0646	-1.00376
8	0	-1.11687	0.08493	-3.256
8	0	-3.58848	0.39738	-2.75391
6	0	0.98894	2.75404	-0.63104
6	0	1.9017	1.54319	1.13166
6	0	-2.89863	1.30639	-0.07422
1	0	0.22475	2.78437	-1.3997
6	0	1.93116	3.76434	-0.44361
16	0	1.76799	-0.04838	2.00851
6	0	2.88117	2.49035	1.37056
1	0	-3.46415	0.38356	0.10077
6	0	-3.9297	2.29522	-0.61349
6	0	-2.3938	1.79694	1.31523
1	0	1.91577	4.63213	-1.09394
6	0	2.89108	3.62845	0.55894
7	0	1.43296	-1.04703	0.72757
8	0	0.5732	0.02072	2.86587
8	0	3.07306	-0.27519	2.64782
1	0	3.62463	2.31357	2.13873
8	0	-3.41846	3.19149	-1.46937
8	0	-5.08665	2.29831	-0.238
1	0	-1.49268	1.21331	1.53455
6	0	-2.01256	3.28037	1.33762
6	0	-3.41724	1.45571	2.42375
1	0	3.65036	4.39107	0.70101
6	0	2.59252	-1.16871	-0.20407
6	0	-4.36357	4.13117	-2.00856
1	0	-1.36222	3.53991	0.49792
1	0	-2.8988	3.92485	1.28526
1	0	-1.48378	3.5181	2.26795
1	0	-3.02541	1.85485	3.3681
1	0	-4.36071	1.97288	2.21927
6	0	-3.65252	-0.03432	2.5572
6	0	3.69691	-2.15492	0.28426
6	0	2.13561	-1.54454	-1.60998
1	0	3.07218	-0.19464	-0.34624
1	0	-5.15241	3.6062	-2.5547
1	0	-3.79127	4.76556	-2.687
1	0	-4.81334	4.73184	-1.2121
6	0	-4.83289	-0.62571	2.08626
6	0	-2.65597	-0.86187	3.09745
6	0	5.01986	-1.90449	-0.48402
1	0	3.87538	-1.89349	1.32933
6	0	3.27418	-3.625	0.22721
8	0	2.62837	-1.06753	-2.61401
8	0	1.1891	-2.49547	-1.6291
1	0	-5.59819	0.00434	1.6395
6	0	-5.02006	-2.00869	2.16161
6	0	-2.84347	-2.2421	3.1797
1	0	-1.72092	-0.42633	3.43687
1	0	4.87516	-2.12178	-1.54876
1	0	5.75989	-2.62429	-0.11106
6	0	5.54353	-0.49284	-0.30773
1	0	2.30229	-3.76705	0.71099
1	0	3.19468	-3.99152	-0.80271
1	0	4.01025	-4.24855	0.74824
6	0	0.67092	-2.83681	-2.93103
1	0	-5.94209	-2.44865	1.78955
6	0	-4.02758	-2.82111	2.71343
1	0	-2.06147	-2.8648	3.60773
6	0	6.12169	-0.09866	0.90751
6	0	5.39367	0.46882	-1.31784
1	0	-0.08219	-3.6047	-2.74821
1	0	0.22031	-1.95729	-3.39669
1	0	1.46687	-3.23072	-3.56898
1	0	-4.17405	-3.89654	2.77778
1	0	6.23369	-0.82797	1.70624
6	0	6.54183	1.21673	1.1095
6	0	5.81056	1.78737	-1.11918
1	0	4.91697	0.18409	-2.25165
1	0	6.99075	1.49974	2.05846
6	0	6.38724	2.16627	0.09513
1	0	5.68274	2.5173	-1.91483
1	0	6.71759	3.19065	0.24954

IM1-1a(iPrOH)

E(RB3LYP) = -3062.51062052

G(correction)= 0.608299
E(RM06) = -3062.7284721
Imaginary frequencies: 0

6	0	-1.30516	-2.8057	0.24726
1	0	-0.56492	-2.84352	1.03618
6	0	-2.1591	-3.86897	-0.04031
7	0	-1.36032	-1.66741	-0.45954
1	0	-2.09648	-4.7743	0.55303
6	0	-3.08456	-3.7446	-1.07563
6	0	-2.25324	-1.54979	-1.45896
46	0	-0.17434	-0.01814	-0.12833
1	0	-3.76202	-4.5595	-1.31042
6	0	-3.13919	-2.5535	-1.80656
16	0	-2.16821	0.06841	-2.28107
7	0	1.00733	1.64602	0.18426
1	0	-3.8488	-2.40067	-2.61209
7	0	-1.74684	1.0447	-1.02439
8	0	-1.04213	0.01423	-3.23467
8	0	-3.51712	0.34906	-2.81139
6	0	0.99338	2.75392	-0.57311
6	0	1.91817	1.52809	1.16838
6	0	-2.8981	1.31546	-0.12821
1	0	0.24184	2.79066	-1.35282
6	0	1.90852	3.78281	-0.35322
16	0	1.81692	-0.07589	2.01091
6	0	2.86725	2.49444	1.44522
1	0	-3.45902	0.39564	0.07287
6	0	-3.91995	2.27162	-0.73612
6	0	-2.42668	1.87365	1.24876
1	0	1.87723	4.66378	-0.98487
6	0	2.85606	3.65272	0.66065
7	0	1.45045	-1.07208	0.74459
8	0	0.64787	-0.04367	2.91255
8	0	3.13568	-0.30646	2.63015
1	0	3.5995	2.33173	2.22731
8	0	-3.38965	3.16295	-1.57917
8	0	-5.09875	2.2533	-0.42166
1	0	-1.52272	1.3098	1.50412
6	0	-2.06791	3.36265	1.21997
6	0	-3.46636	1.56116	2.35183
1	0	3.58767	4.43501	0.83529
6	0	2.56969	-1.2012	-0.23775
6	0	-4.31423	4.10701	-2.15978
1	0	-1.39662	3.60055	0.39025
1	0	-2.96244	3.99018	1.12033
1	0	-1.56712	3.64242	2.15394
1	0	-3.1109	2.02764	3.2791
1	0	-4.42154	2.03396	2.0977
6	0	-3.65126	0.07374	2.56554
6	0	3.7292	-2.14058	0.22049
6	0	2.03373	-1.65115	-1.59271
1	0	3.00686	-0.21938	-0.44421
1	0	-5.07721	3.57971	-2.73933
1	0	-3.71124	4.73989	-2.81158
1	0	-4.79114	4.70626	-1.37907
6	0	-4.77706	-0.59978	2.07026
6	0	-2.65153	-0.67555	3.20577
6	0	5.01367	-1.83799	-0.59375
1	0	3.93503	-1.86784	1.25691
6	0	3.37873	-3.63108	0.18964
8	0	2.41721	-1.17499	-2.64859
8	0	1.1554	-2.65341	-1.50939
1	0	-5.54982	-0.03315	1.5557
6	0	-4.90391	-1.9853	2.2112
6	0	-2.77542	-2.0583	3.35117
1	0	-1.76571	-0.17171	3.58229
1	0	4.83414	-2.04434	-1.65574
1	0	5.78757	-2.54013	-0.25877
6	0	5.50045	-0.41399	-0.41164
1	0	2.43224	-3.82383	0.70614
1	0	3.28946	-4.0122	-0.83427
1	0	4.16476	-4.20589	0.69338
6	0	0.58754	-3.11839	-2.75336
1	0	-5.78268	-2.48941	1.8165
6	0	-3.90379	-2.71899	2.85385
1	0	-1.98896	-2.6201	3.84937
6	0	6.0904	-0.01719	0.79874
6	0	5.30828	0.55584	-1.40696
1	0	-0.12804	-3.89039	-2.47043
1	0	0.08462	-2.29577	-3.26675
1	0	1.36999	-3.53728	-3.39207
1	0	-3.99955	-3.79624	2.96311
1	0	6.24262	-0.75437	1.58404
6	0	6.47311	1.30873	1.01091
6	0	5.68639	1.88543	-1.19828
1	0	4.83648	0.26912	-2.34345
1	0	6.92828	1.59454	1.95613
6	0	6.26983	2.26711	0.01244
1	0	5.52148	2.62184	-1.98098
1	0	6.56341	3.30068	0.17768

AcOH(dioxane)

E(RB3LYP) = -229.090190093
G(correction)= 0.034993
E(RM06) = -229.03655315

8	0	0.64571	1.20304	-0.00007
6	0	0.09218	0.12469	-0.00004
8	0	0.77581	-1.04621	0.00006
6	0	-1.39481	-0.10925	0.00001
1	0	1.7244	-0.81312	0.00009
1	0	-1.68144	-0.69132	-0.88261
1	0	-1.68146	-0.69047	0.88318
1	0	-1.91783	0.84771	-0.00044

AcOH(iPrOH)

E(RB3LYP) = -229.094717955
G(correction)= 0.034559
E(RM06) = -229.04237754

8	0	0.64608	1.20331	0.00001
6	0	0.09322	0.12698	-0.00006
8	0	0.77586	-1.04831	-0.00001
6	0	-1.39645	-0.10917	0.00001
1	0	1.72236	-0.81171	0.00012
1	0	-1.68104	-0.69246	-0.88187
1	0	-1.68102	-0.69153	0.8825
1	0	-1.91648	0.84889	-0.00048

TS1-1a(dioxane)

E(RB3LYP) = -3291.57291874
G(correction)= 0.660621
E(RM06) = -3291.72212532
Imaginary frequencies: 1 (-1006.6164cm^{-1})

6	0	0.13524	1.8723	-1.29939
1	0	-0.59537	1.9592	-0.51208
6	0	0.38654	2.9408	-2.15528
7	0	0.79229	0.70698	-1.41049
1	0	-0.17725	3.85686	-2.02189
6	0	1.35165	2.80716	-3.14904
6	0	1.74819	0.59343	-2.35673
46	0	0.56838	-1.01362	-0.25379
1	0	1.5676	3.62726	-3.82696
6	0	2.06289	1.609	-3.24228
16	0	2.69747	-0.95986	-2.25487
7	0	2.59019	-1.21825	-0.62048
1	0	2.86188	1.4605	-3.95996
8	0	1.9606	-2.00693	-2.96602
8	0	4.0648	-0.61595	-2.67984
6	0	3.47375	-0.31259	0.14107
1	0	3.40217	0.71706	-0.22716
6	0	4.9562	-0.66639	0.00844
6	0	3.07817	-0.28514	1.64419
8	0	5.1811	-1.96576	-0.21111
8	0	5.83706	0.16079	0.15801
1	0	1.9853	-0.17449	1.6525
6	0	3.4311	-1.58493	2.37242
6	0	3.65581	0.96449	2.35373
6	0	6.56109	-2.33357	-0.37431
1	0	3.00118	-2.44308	1.8493
1	0	4.51629	-1.72601	2.43923
1	0	3.03978	-1.56752	3.39601
1	0	3.37527	0.9017	3.41321
1	0	4.74911	0.9351	2.30857
6	0	3.13711	2.26074	1.7663
1	0	6.99694	-1.80321	-1.22573
1	0	6.55639	-3.40856	-0.55917
1	0	7.1348	-2.10317	0.52865
6	0	3.88226	2.97729	0.81761
6	0	1.86048	2.72969	2.10795
1	0	4.86313	2.60784	0.5297
6	0	3.36278	4.13044	0.22442
6	0	1.34204	3.88564	1.52145
1	0	1.26114	2.18527	2.83146
1	0	3.95385	4.66899	-0.51218
6	0	2.09134	4.59018	0.57576
1	0	0.3544	4.23616	1.80868
1	0	1.6893	5.49065	0.11769
1	0	-1.80556	1.12004	0.59228
6	0	-1.98306	0.16223	1.07584
7	0	-1.59492	-0.91706	0.12459
6	0	-3.47693	0.16676	1.52823
6	0	-1.10288	0.1613	2.3184
16	0	-2.33341	-0.81631	-1.41104
6	0	-3.87607	1.5488	2.10687
1	0	-4.06745	0.04678	0.61809
6	0	-3.82477	-0.98095	2.48057
8	0	-0.87276	1.1671	2.96372
8	0	-0.68238	-1.05788	2.66833
6	0	-4.03393	-1.43115	-1.21623
8	0	-2.44715	0.59729	-1.81175
8	0	-1.62679	-1.77507	-2.26544
1	0	-3.32689	1.73679	3.03457
1	0	-4.9402	1.49358	2.37014
6	0	-3.6462	2.67561	1.12083
1	0	-3.48777	-1.94398	2.08751
1	0	-3.36657	-0.83668	3.46669
1	0	-4.90986	-1.03281	2.62598
6	0	0.12282	-1.14576	3.85784
7	0	-4.16072	-2.55408	-0.52359
6	0	-5.07458	-0.72974	-1.82391
6	0	-4.49501	2.83139	0.01586
6	0	-2.53623	3.52499	1.23557
1	0	0.47309	-2.17678	3.8946
1	0	0.96658	-0.45538	3.80364
1	0	-0.48202	-0.91251	4.73896
6	0	-5.39613	-3.05039	-0.39298
6	0	-6.35633	-1.26365	-1.68313
1	0	-4.88186	0.19028	-2.36289
1	0	-5.35665	2.17514	-0.09026
6	0	-4.24353	3.80457	-0.95104
6	0	-2.28093	4.50226	0.26952
1	0	-1.8582	3.39282	2.0736
1	0	-5.48408	-3.96741	0.18445
6	0	-6.52223	-2.44118	-0.95324
1	0	-7.20948	-0.76491	-2.13375
1	0	-4.9116	3.90742	-1.80228
6	0	-3.133	4.64379	-0.82832
1	0	-1.4166	5.15306	0.37649
1	0	-7.50412	-2.88359	-0.8179
1	0	-2.93729	5.40409	-1.58011
1	0	-1.63703	-2.14454	0.56397
8	0	-1.49915	-3.26303	0.97608
6	0	-0.26493	-3.55007	1.10521
8	0	0.70264	-2.81261	0.75414
6	0	0.07825	-4.89423	1.69637
1	0	0.08746	-5.63464	0.88715
1	0	1.07064	-4.87317	2.15178
1	0	-0.67822	-5.19442	2.42568

TS1-1a(iPrOH)

E(RB3LYP) = -3291.60961812
G(correction)= 0.660622
E(RM06) = -3291.76172171
Imaginary frequencies: 1 (-977.5816 cm^{-1})

6	0	0.12477	1.9235	-1.21915
1	0	-0.58154	1.99253	-0.40738
6	0	0.35797	3.0084	-2.06181
7	0	0.7801	0.76166	-1.36712
1	0	-0.20162	3.92279	-1.90133
6	0	1.3031	2.89643	-3.07689
6	0	1.71879	0.67283	-2.33421
46	0	0.57166	-0.97729	-0.23583
1	0	1.5034	3.72922	-3.74347
6	0	2.01756	1.70142	-3.20764
16	0	2.64456	-0.88521	-2.27827
7	0	2.58862	-1.19356	-0.65719
1	0	2.7986	1.57285	-3.94894
8	0	1.86926	-1.91474	-2.99211
8	0	4.01008	-0.58612	-2.75068
6	0	3.50881	-0.3186	0.10483
1	0	3.45564	0.71578	-0.25204
6	0	4.97383	-0.71714	-0.05868
6	0	3.13966	-0.29743	1.61716
8	0	5.15762	-2.02431	-0.26069
8	0	5.8851	0.0869	0.05136
1	0	2.0473	-0.19738	1.64854
6	0	3.52155	-1.58555	2.35199
6	0	3.7202	0.95956	2.31142
6	0	6.53008	-2.45664	-0.38001
1	0	3.12202	-2.46388	1.83729
1	0	4.60984	-1.69654	2.43138
1	0	3.11491	-1.5702	3.36903
1	0	3.47959	0.8829	3.37902
1	0	4.81217	0.95289	2.22669
6	0	3.14967	2.24678	1.75315
1	0	7.0097	-1.96165	-1.22903
1	0	6.48073	-3.53325	-0.54482
1	0	7.08143	-2.23444	0.53804
6	0	3.85193	3.01428	0.81187
6	0	1.85873	2.65727	2.11905
1	0	4.84696	2.69974	0.50648
6	0	3.27831	4.1586	0.2491
6	0	1.28257	3.80033	1.56117
1	0	1.29701	2.07295	2.84133
1	0	3.83696	4.73659	-0.48299
6	0	1.99206	4.55638	0.62289
1	0	0.27923	4.09671	1.85546
1	0	1.54483	5.44466	0.18411
1	0	-1.84245	1.12908	0.58008
6	0	-2.00342	0.17254	1.07199
7	0	-1.58456	-0.90812	0.13143
6	0	-3.49793	0.14538	1.52116
6	0	-1.12021	0.19479	2.31185
16	0	-2.30718	-0.85699	-1.40649
6	0	-3.92937	1.52485	2.08219
1	0	-4.08585	0.00011	0.61362
6	0	-3.8243	-0.99448	2.48959
8	0	-0.91898	1.2113	2.9533
8	0	-0.66222	-1.00708	2.66015
6	0	-3.99987	-1.48621	-1.23267
8	0	-2.40616	0.53914	-1.87245
8	0	-1.57112	-1.83891	-2.22276
1	0	-3.40942	1.72402	3.02461
1	0	-4.9998	1.45429	2.31348
6	0	-3.68426	2.65014	1.09785
1	0	-3.48643	-1.96035	2.10321
1	0	-3.35454	-0.8357	3.46808
1	0	-4.90744	-1.05196	2.64537
6	0	0.1598	-1.07783	3.84567
7	0	-4.09675	-2.65463	-0.61035
6	0	-5.05616	-0.75673	-1.77207
6	0	-4.42739	2.72252	-0.09073
6	0	-2.65816	3.58448	1.30076
1	0	0.50022	-2.11143	3.89632
1	0	1.00883	-0.39717	3.76108
1	0	-0.43596	-0.82377	4.72656
6	0	-5.32813	-3.16289	-0.47233
6	0	-6.33202	-1.30658	-1.62648
1	0	-4.89016	0.19394	-2.26441
1	0	-5.22456	2.00303	-0.26608
6	0	-4.14397	3.68983	-1.05648
6	0	-2.37342	4.55839	0.33862
1	0	-2.06436	3.53026	2.20854
1	0	-5.39994	-4.11447	0.04814
6	0	-6.47159	-2.52415	-0.96115
1	0	-7.19876	-0.78666	-2.02325
1	0	-4.7266	3.72413	-1.97378
6	0	-3.11253	4.61115	-0.84642
1	0	-1.57242	5.27206	0.51452
1	0	-7.44724	-2.97831	-0.82105
1	0	-2.89032	5.36437	-1.59798
1	0	-1.60774	-2.14471	0.59346
8	0	-1.46523	-3.24273	1.01273
6	0	-0.22575	-3.5263	1.14957
8	0	0.72852	-2.79627	0.75143
6	0	0.10912	-4.82642	1.827
1	0	-0.39686	-4.86704	2.79738
1	0	-0.27351	-5.65303	1.21741
1	0	1.18679	-4.93488	1.95874

1a(dioxane)

E(RB3LYP) = -1468.45092328
G(correction)= 0.301081
E(RM06) = -1467.97042798

1	0	-0.64537	0.73817	-1.42824
6	0	0.05483	0.73896	-0.58508
6	0	0.55179	-0.69922	-0.43237

7	0	-0.65614	1.13444	0.63922
6	0	1.17728	1.75479	-0.94162
8	0	0.41469	-1.37138	0.56903
8	0	1.14604	-1.12106	-1.555
1	0	-0.46357	0.49873	1.41618
16	0	-2.30902	1.40607	0.54344
1	0	1.66734	1.36079	-1.83982
6	0	0.55412	3.11478	-1.2761
6	0	2.23647	1.90909	0.1747
6	0	1.75436	-2.4281	-1.48235
8	0	-2.73223	1.84133	1.87427
8	0	-2.55081	2.22919	-0.64791
6	0	-3.0279	-0.22787	0.20973
1	0	1.32972	3.81798	-1.60108
1	0	0.0491	3.54059	-0.40349
1	0	-0.18872	3.03129	-2.07622
1	0	2.84556	2.7876	-0.07565
1	0	1.72307	2.15052	1.11301
6	0	3.15715	0.72152	0.37119
1	0	2.26165	-2.56569	-2.43783
1	0	0.9884	-3.19648	-1.34265
1	0	2.47099	-2.46625	-0.65939
6	0	-3.76962	-0.44839	-0.94692
7	0	-2.75163	-1.1397	1.13683
6	0	4.05226	0.343	-0.64156
6	0	3.14459	-0.02354	1.55606
6	0	-4.26917	-1.73878	-1.13808
1	0	-3.94208	0.35425	-1.65415
6	0	-3.23374	-2.36955	0.93791
6	0	4.90706	-0.74577	-0.47599
1	0	4.07985	0.91207	-1.56841
6	0	3.99887	-1.11526	1.72893
1	0	2.45273	0.24799	2.3495
6	0	-3.99702	-2.71535	-0.18206
1	0	-4.85756	-1.97375	-2.02036
1	0	-2.99698	-3.10699	1.70109
6	0	4.88395	-1.48018	0.7138
1	0	5.59491	-1.01911	-1.27233
1	0	3.96945	-1.68002	2.65712
1	0	-4.36484	-3.73024	-0.29595
1	0	5.55176	-2.32736	0.84714

1a(iPrOH)

E(RB3LYP) = -1468.46714763
G(correction)= 0.301207
E(RM06) = -1467.98903399

1	0	-0.55867	1.26775	-1.54309
6	0	0.15725	1.05483	-0.74325
6	0	0.43116	-0.45067	-0.81962
7	0	-0.47166	1.40756	0.53599
6	0	1.39753	1.95046	-1.0171
8	0	0.22003	-1.24238	0.07858
8	0	0.88858	-0.79063	-2.03037
1	0	-0.09524	0.8805	1.32584
16	0	-2.14407	1.44071	0.61626
1	0	1.87985	1.53231	-1.90779
6	0	0.93957	3.37902	-1.3321
6	0	2.42182	1.95778	0.14086
6	0	1.15801	-2.198	-2.22586
8	0	-2.47515	1.80945	1.99762
8	0	-2.60354	2.26858	-0.50996
6	0	-2.70546	-0.25377	0.30534
1	0	1.80221	4.01996	-1.54716
1	0	0.39726	3.81236	-0.48398
1	0	0.27471	3.39861	-2.20378
1	0	3.25165	2.60625	-0.16934
1	0	1.96476	2.43453	1.01602
6	0	2.95872	0.59563	0.52505
1	0	1.53538	-2.2817	-3.24531
1	0	0.23653	-2.77514	-2.10831
1	0	1.90749	-2.54172	-1.50873
6	0	-3.09114	-0.62431	-0.97935
7	0	-2.60398	-1.06687	1.35221
6	0	3.69664	-0.16754	-0.39328
6	0	2.70504	0.05126	1.79112
6	0	-3.38515	-1.9751	-1.18209
1	0	-3.15674	0.1038	-1.77921
6	0	-2.8957	-2.35542	1.14082
6	0	4.15394	-1.44354	-0.0601
1	0	3.90737	0.23939	-1.37962
6	0	3.1588	-1.22593	2.12924
1	0	2.13359	0.62984	2.51427
6	0	-3.2814	-2.85516	-0.1071
1	0	-3.68785	-2.32746	-2.1636
1	0	-2.81399	-3.01537	2.00103
6	0	3.88214	-1.97983	1.20277
1	0	4.72375	-2.01908	-0.78555
1	0	2.94371	-1.6319	3.11458
1	0	-3.49556	-3.91269	-0.22433
1	0	4.23458	-2.97497	1.46161

CO(dioxane)

E(RB3LYP) = -113.304460442
G(correction)= -0.014105
E(RM06) = -113.28067631

6	0	0.	0.	-0.65015
8	0	0.	0.	0.48762

CO(iPrOH)

E(RB3LYP) = -113.301484109
G(correction)= -0.014118
E(RM06) = -113.27785817

6	0	0.	0.	-0.65011
8	0	0.	0.	0.48758

TS3A-1a(dioxane)

E(RB3LYP) = -1820.62171125
G(correction)= 0.286296
E(RM06) = -1821.2646599
Imaginary frequencies: 1 (-275.7981 cm^{-1})

46	0	0.23452	-0.55195	1.17366
6	0	1.58916	-1.72054	0.0319
6	0	-0.97512	0.28619	2.50619
6	0	0.81791	-2.27958	1.6558
7	0	-0.61315	0.28009	-0.68324
6	0	1.16644	-2.08184	-1.26704
6	0	2.93389	-1.42469	0.31579
8	0	-1.61946	0.7871	3.2994
8	0	0.84856	-3.34376	2.12669
6	0	-1.77387	-0.48417	-1.15584
16	0	-0.70062	1.89646	-0.80522
6	0	-0.23062	-2.49919	-1.70847
6	0	2.16514	-2.1144	-2.25366
6	0	3.8953	-1.47007	-0.68796
1	0	3.22001	-1.15996	1.32959
6	0	-1.51784	-2.00297	-1.02084
1	0	-1.98018	-0.23947	-2.20578
6	0	-3.0062	-0.11628	-0.31419
6	0	1.01813	2.28656	-0.36627
8	0	-1.54476	2.5355	0.23731
8	0	-0.91182	2.35472	-2.1967
1	0	-0.31207	-2.27021	-2.77856
1	0	-0.24984	-3.59802	-1.64569
1	0	1.88011	-2.36984	-3.27124
6	0	3.49923	-1.81553	-1.98058
1	0	4.93245	-1.23803	-0.46494
6	0	-2.71208	-2.77976	-1.60184
1	0	-1.47239	-2.22827	0.0508
8	0	-3.17201	-0.45519	0.84399
8	0	-3.85381	0.66866	-0.991
7	0	1.49157	1.70513	0.73747
6	0	1.73627	3.1902	-1.14337
1	0	4.23003	-1.8517	-2.78402
1	0	-2.58412	-3.85822	-1.45553
1	0	-2.81909	-2.59584	-2.67845
1	0	-3.65105	-2.49408	-1.11587
6	0	-4.90971	1.26115	-0.21069
6	0	2.73781	2.01055	1.11962
6	0	3.0317	3.50653	-0.73318
1	0	1.28679	3.61279	-2.03432
1	0	-5.54346	0.48916	0.23526
1	0	-5.48363	1.87013	-0.91034
1	0	-4.47957	1.88633	0.57607
1	0	3.09761	1.51362	2.01678
6	0	3.54284	2.90932	0.4194
1	0	3.63246	4.20675	-1.30646
1	0	4.54537	3.12968	0.77193

TS3A-1a(iPrOH)

E(RB3LYP) = -1820.63433397
G(correction)= 0.284931
E(RM06) = -1821.28054299
Imaginary frequencies: 1 (-289.4109 cm^{-1})

46	0	0.22515	-0.65222	1.18809
6	0	1.57114	-1.68834	-0.07115
6	0	-0.97118	0.10199	2.58401
6	0	0.91532	-2.36283	1.60193
7	0	-0.62701	0.32905	-0.59364
6	0	1.0868	-2.01611	-1.35746
6	0	2.91471	-1.34958	0.15779
8	0	-1.63637	0.55971	3.38708
8	0	1.05662	-3.42921	2.03986
6	0	-1.78744	-0.38932	-1.14119
16	0	-0.64703	1.93892	-0.67664
6	0	-0.3207	-2.46481	-1.72678
6	0	2.02833	-1.96642	-2.39833
6	0	3.81903	-1.31558	-0.90073
1	0	3.24568	-1.10734	1.16323
6	0	-1.5882	-1.91908	-1.0341
1	0	-1.93987	-0.11414	-2.19209
6	0	-3.03914	0.0009	-0.34403
6	0	1.08406	2.27153	-0.26373
8	0	-1.4747	2.59953	0.37509
8	0	-0.8893	2.43454	-2.05815
1	0	-0.43439	-2.31034	-2.80659
1	0	-0.34371	-3.55532	-1.58262
1	0	1.69739	-2.19096	-3.40927
6	0	3.36473	-1.62431	-2.18361
1	0	4.85658	-1.0476	-0.72447
6	0	-2.81058	-2.63957	-1.62958
1	0	-1.54938	-2.16371	0.03411
8	0	-3.25157	-0.333	0.81021
8	0	-3.85144	0.80173	-1.04537
7	0	1.51254	1.72368	0.87504
6	0	1.86029	3.0612	-1.10415
1	0	4.0503	-1.59669	-3.02644
1	0	-2.7017	-3.72547	-1.53157
1	0	-2.92547	-2.40592	-2.6955
1	0	-3.73705	-2.3553	-1.11812
6	0	-4.98226	1.3429	-0.32621
6	0	2.78679	1.94272	1.22585
6	0	3.18536	3.28783	-0.72344
1	0	1.4451	3.46946	-2.01815
1	0	-5.62535	0.53686	0.03761
1	0	-5.51627	1.96196	-1.04766
1	0	-4.63318	1.949	0.51435
1	0	3.11699	1.47544	2.14956
6	0	3.65756	2.72006	0.45936
1	0	3.83619	3.89502	-1.34562
1	0	4.68126	2.86992	0.78681

TS3B-1a(dioxane)

E(RB3LYP) = -1820.61074871

G(correction)= 0.285532
E(RM06) = -1821.25717398
Imaginary frequencies: 1 (-242.4261 cm^{-1})

46	0	0.09724	-1.27615	-0.49361
6	0	1.28869	-1.89431	0.81438
6	0	0.15763	-2.47615	-2.00418
7	0	-0.87821	0.62434	-0.90556
6	0	1.03241	-0.20097	1.40892
8	0	1.89002	-2.71579	1.38396
8	0	0.2003	-3.19419	-2.89235
6	0	-0.44879	1.53418	0.16848
16	0	-2.48568	0.49637	-1.04761
6	0	0.97851	1.16884	0.66488
1	0	0.21582	-0.30655	2.12666
1	0	1.9873	-0.24872	1.93506
1	0	-1.10541	1.48157	1.04975
6	0	-0.45737	2.99544	-0.29998
6	0	-3.00118	-0.45796	0.43815
8	0	-2.78992	-0.36788	-2.2001
8	0	-3.17792	1.79379	-0.90439
6	0	2.05457	1.34389	-0.44139
1	0	1.2166	1.88155	1.46887
8	0	-0.23097	3.38177	-1.42266
8	0	-0.69357	3.814	0.748
7	0	-2.11908	-1.35213	0.89213
6	0	-4.25457	-0.25437	1.01089
1	0	2.15191	2.41611	-0.64042
1	0	1.69165	0.89325	-1.36984
6	0	3.39373	0.75647	-0.06582
6	0	-0.70414	5.21938	0.43664
6	0	-2.46223	-2.10659	1.94568
6	0	-4.60649	-1.04229	2.10647
1	0	-4.91626	0.50362	0.6075
6	0	3.83045	-0.45033	-0.62976
6	0	4.20289	1.37596	0.89865
1	0	0.2607	5.53357	0.02691
1	0	-0.90123	5.72992	1.3807
1	0	-1.49127	5.4427	-0.28911
1	0	-1.71705	-2.82239	2.28424
6	0	-3.69651	-1.988	2.58294
1	0	-5.57464	-0.91828	2.58318
6	0	5.04004	-1.02885	-0.23713
1	0	3.21782	-0.93641	-1.38626
6	0	5.41116	0.80101	1.29414
1	0	3.88257	2.31849	1.33851
1	0	-3.93187	-2.61885	3.43405
6	0	5.83221	-0.40631	0.72874
1	0	5.36204	-1.96402	-0.68771
1	0	6.02692	1.29648	2.04043
1	0	6.77345	-0.85419	1.03578

G(correction)= 0.285233
E(RM06) = -1821.27776206
Imaginary frequencies: 1 (-252.5046 cm^{-1})

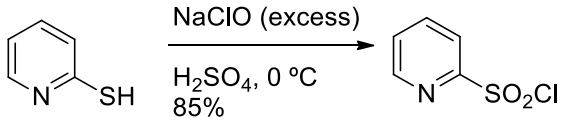
46	0	0.05842	-1.41789	-0.41721
6	0	1.431	-1.93686	0.74456
6	0	-0.18443	-2.83756	-1.71468
7	0	-0.85838	0.55517	-0.8931
6	0	1.06184	-0.23854	1.36627
8	0	2.19946	-2.68863	1.19072
8	0	-0.30997	-3.69282	-2.46154
6	0	-0.36796	1.50393	0.12042
16	0	-2.46128	0.54696	-1.06496
6	0	1.05695	1.10955	0.6036
1	0	0.20675	-0.35486	2.03655
1	0	1.98207	-0.30606	1.94723
1	0	-1.00248	1.52234	1.01847
6	0	-0.32296	2.93569	-0.424
6	0	-3.13453	-0.24078	0.44096
8	0	-2.80046	-0.35313	-2.1916
8	0	-3.046	1.91234	-1.07444
6	0	2.12386	1.21304	-0.5154
1	0	1.32791	1.83549	1.38363
8	0	-0.15312	3.24711	-1.58597
8	0	-0.43898	3.82193	0.57911
7	0	-2.47523	-1.32684	0.84783
6	0	-4.25849	0.27856	1.0759
1	0	2.20413	2.26697	-0.80279
1	0	1.77601	0.6682	-1.3989
6	0	3.47746	0.69224	-0.09096
6	0	-0.34222	5.21408	0.20592
6	0	-2.926	-1.95943	1.9386
6	0	-4.72297	-0.38974	2.21177
1	0	-4.74251	1.17144	0.69786
6	0	3.97986	-0.5088	-0.60963
6	0	4.23872	1.38055	0.86701
1	0	0.63062	5.41981	-0.24976
1	0	-0.45416	5.77378	1.13517
1	0	-1.13987	5.47426	-0.4954
1	0	-2.36654	-2.83787	2.25019
6	0	-4.04723	-1.52762	2.65128
1	0	-5.59571	-0.0227	2.74403
6	0	5.20954	-1.01632	-0.17958
1	0	3.40054	-1.05176	-1.35348
6	0	5.46661	0.87717	1.29935
1	0	3.86362	2.31697	1.27478
1	0	-4.37339	-2.07227	3.53155
6	0	5.95539	-0.32583	0.77798
1	0	5.58216	-1.95011	-0.59318
1	0	6.04379	1.42353	2.04124
1	0	6.91165	-0.71825	1.11427

TS3B-1a(iPrOH)

E(RB3LYP) = -1820.62873213

6. References

[1] The *N*-(2-pyridyl)sulfonyl group is prepared *in situ* by oxidation of the commercial 2-mercaptopyridine with sodium hypochlorite (commercial bleach, see scheme below), following the protocol described by Walsh. See, for instance: S. Diltz, G. Aguirre, F. Ortega, P. J. Walsh, *Tetrahedron: Asymmetry* **1997**, *8*, 3559.



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[6] a) A.D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648. b) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.

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7. NMR Spectra

The chemical shifts of the solvents signals (used in this SI) observed for ^{1}H NMR and ^{13}C NMR spectra are listed in the following chart. The multiplicity is shown as 1 for singlet, 2 for doublet, etc.

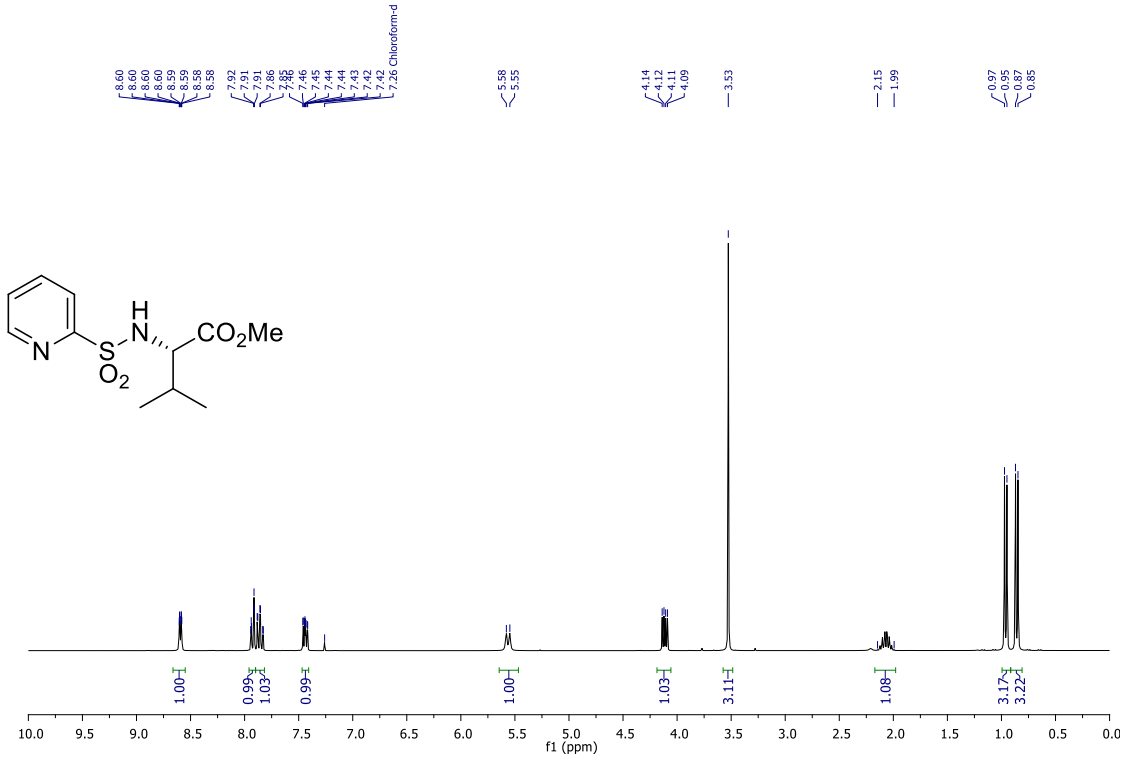
Solvent	^{1}H NMR Chemical Shift (ppm)	^{13}C NMR Chemical Shift (ppm)	^{19}F NMR Chemical Shift (ppm)
$CDCl_3$	7.26 (1)	77.2 (3)	–
HFIP	–	–	-75.7 (1)

In the following table are the chemical shifts of the water signal in the solvents listed before (H_2O in aprotic solvents or HOD in protic solvents).

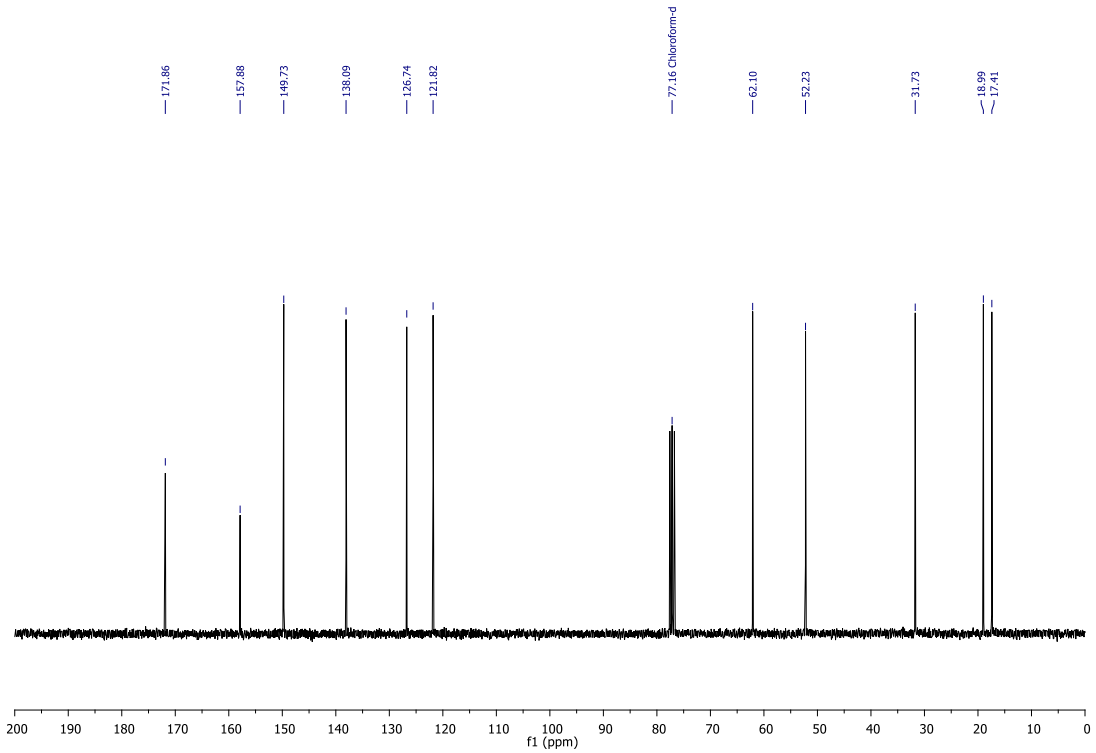
Solvent	^{1}H NMR Chemical Shift (ppm)
Acetone	2.84
Chloroform	1.56

(*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)butanoate (I)

^{1}H NMR ($CDCl_3$, 300 MHz)

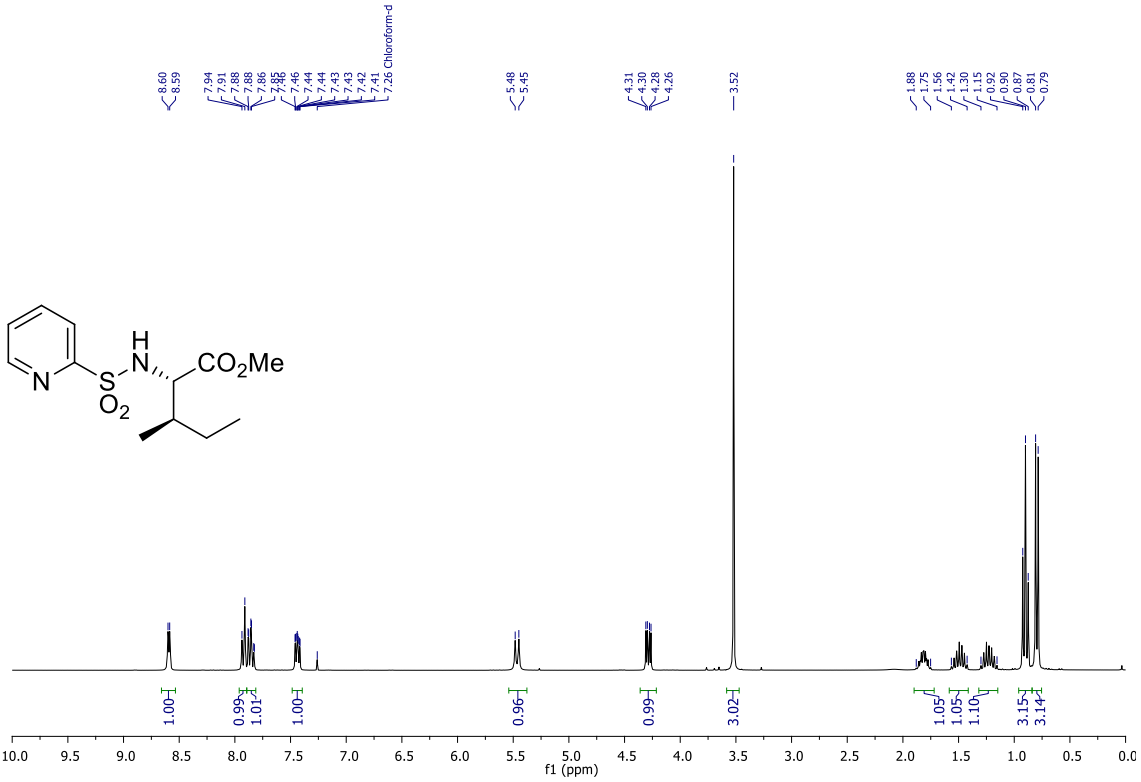


^{13}C NMR ($CDCl_3$, 75 MHz)

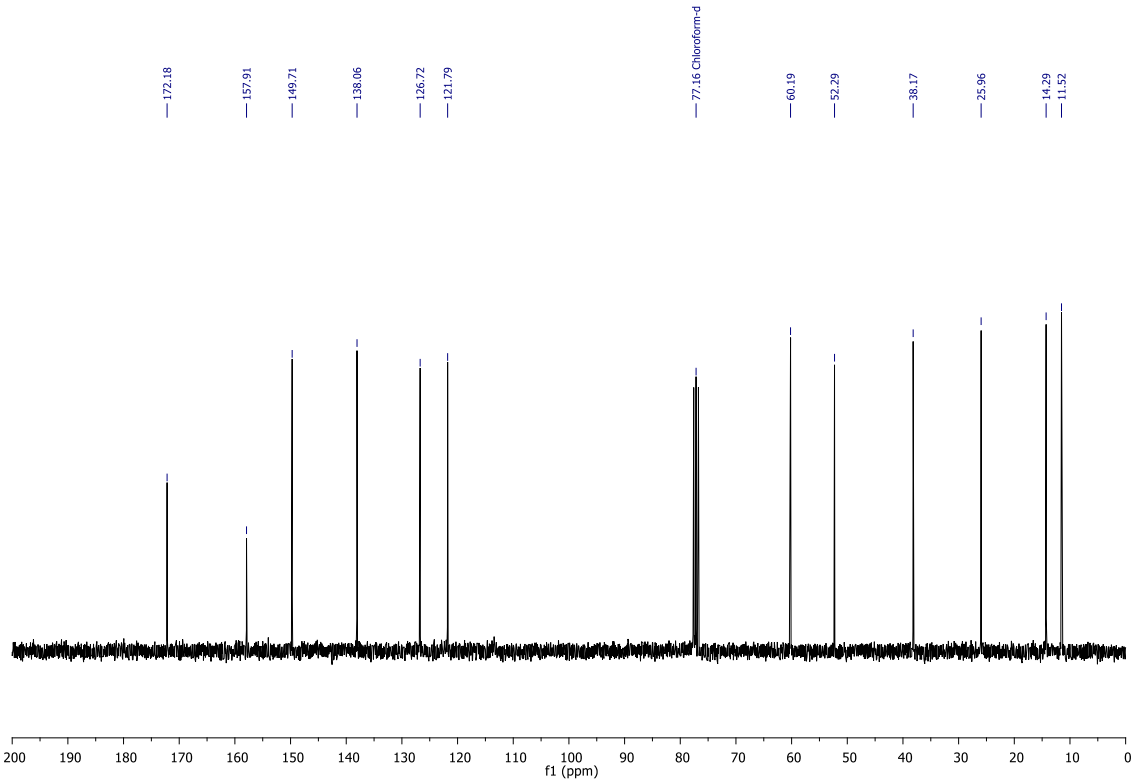


(2*S,3*R**)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)pentanoate (II)**

^{1}H NMR ($CDCl_3$, 300 MHz)

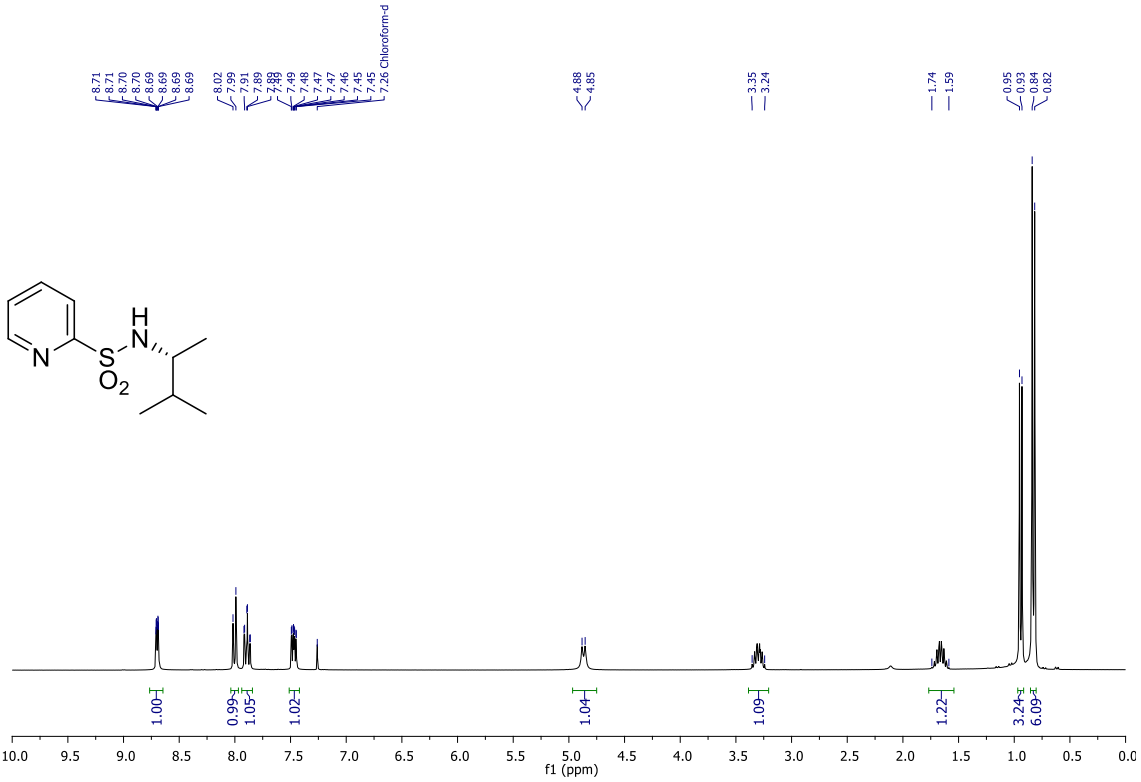


^{13}C NMR ($CDCl_3$, 75 MHz)

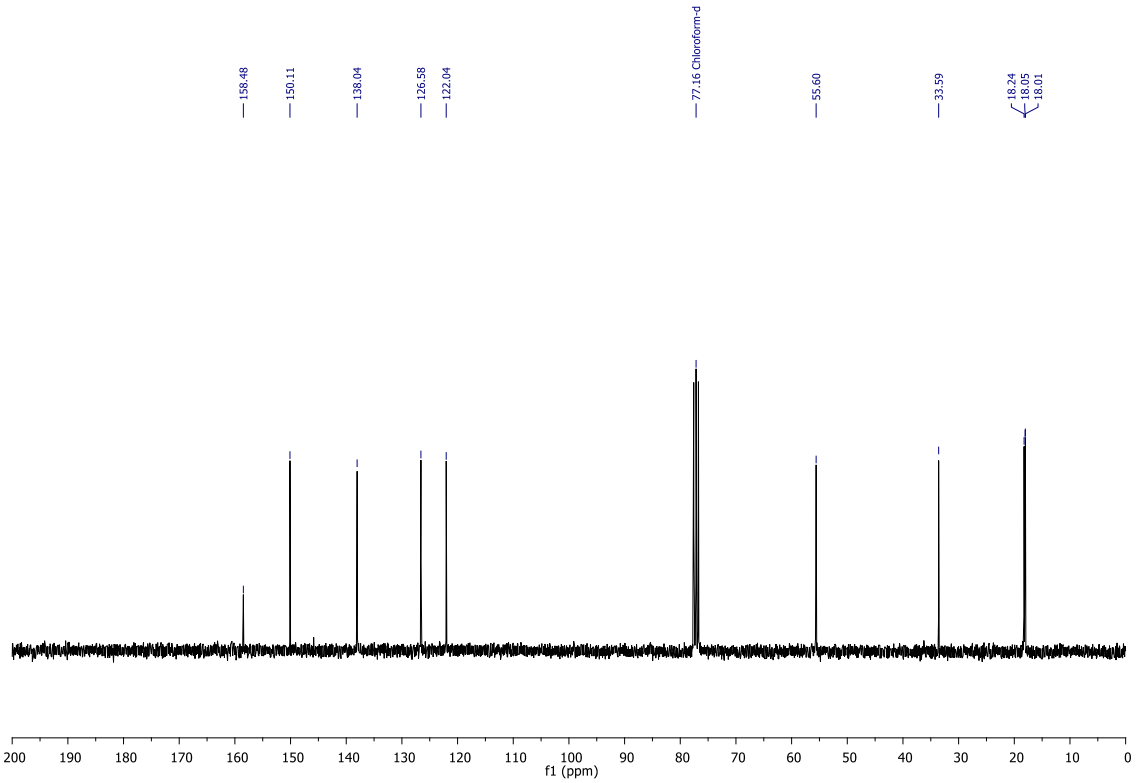


(*R*)-*N*-(3-Methylbutan-2-yl)pyridine-2-sulfonamide (III)

^{1}H NMR ($CDCl_3$, 300 MHz)

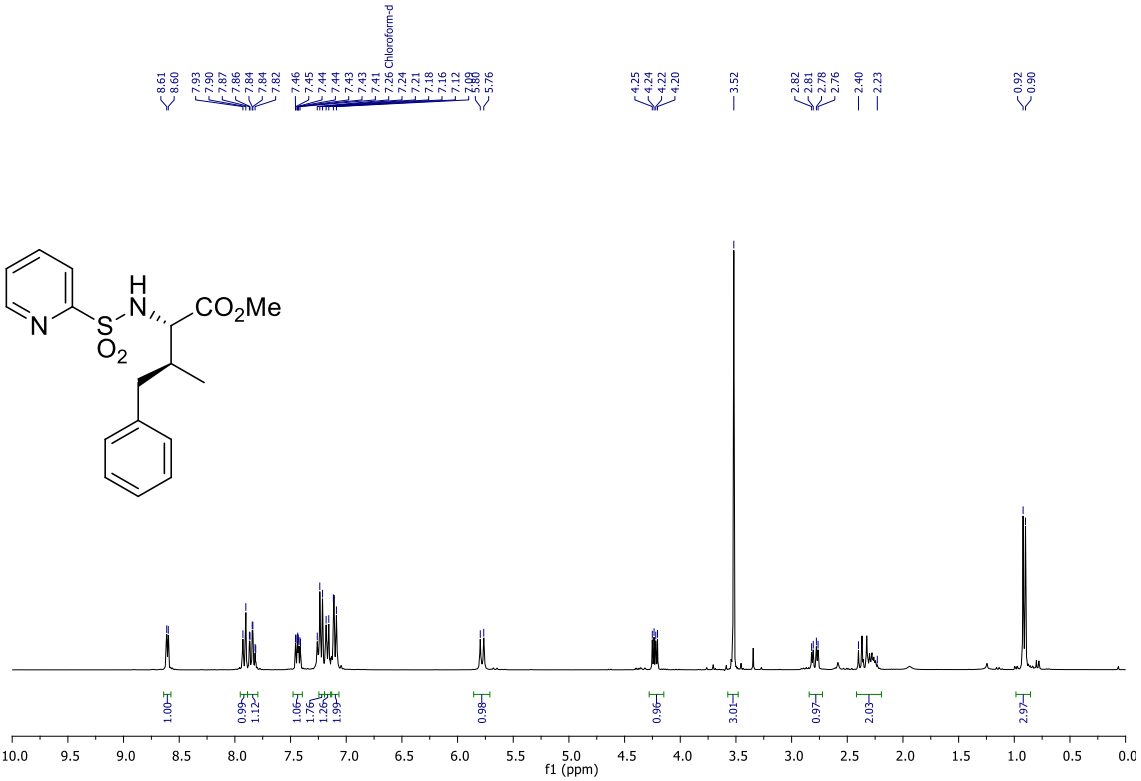


^{13}C NMR ($CDCl_3$, 75 MHz)

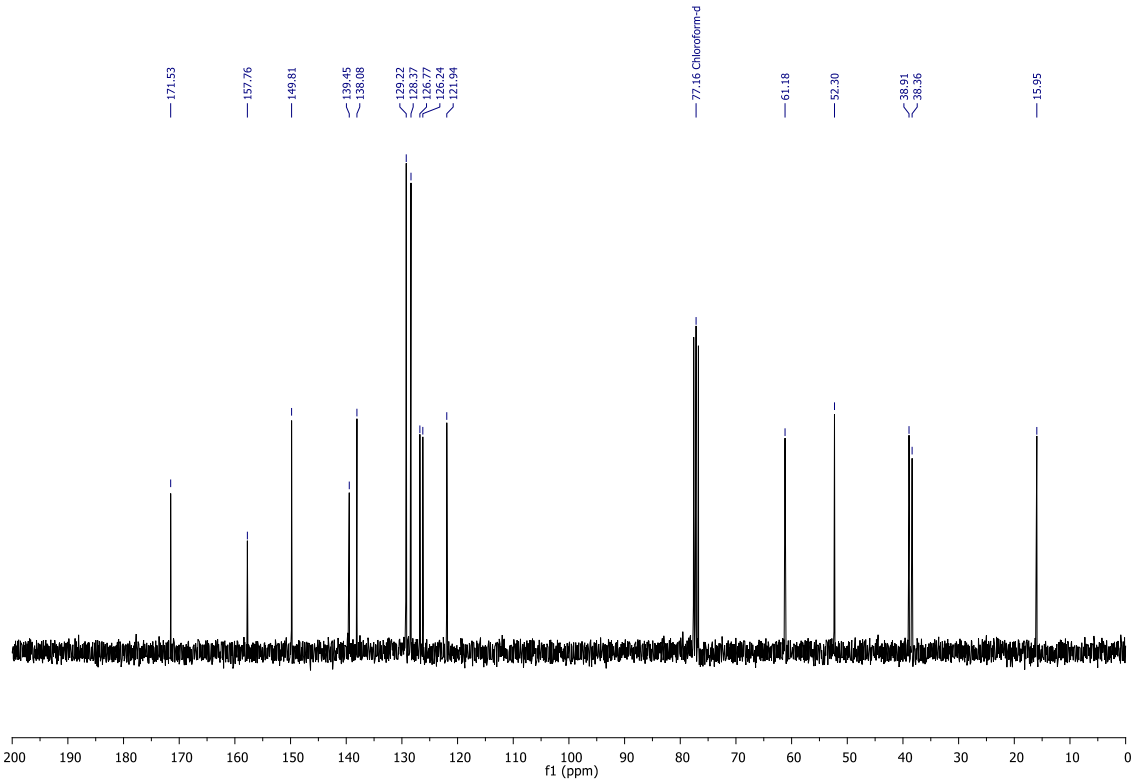


(2*S*,3*S*)-Methyl 3-methyl-4-phenyl-2-(pyridine-2-sulfonamido)butanoate (1a)

^{1}H NMR ($CDCl_3$, 300 MHz)

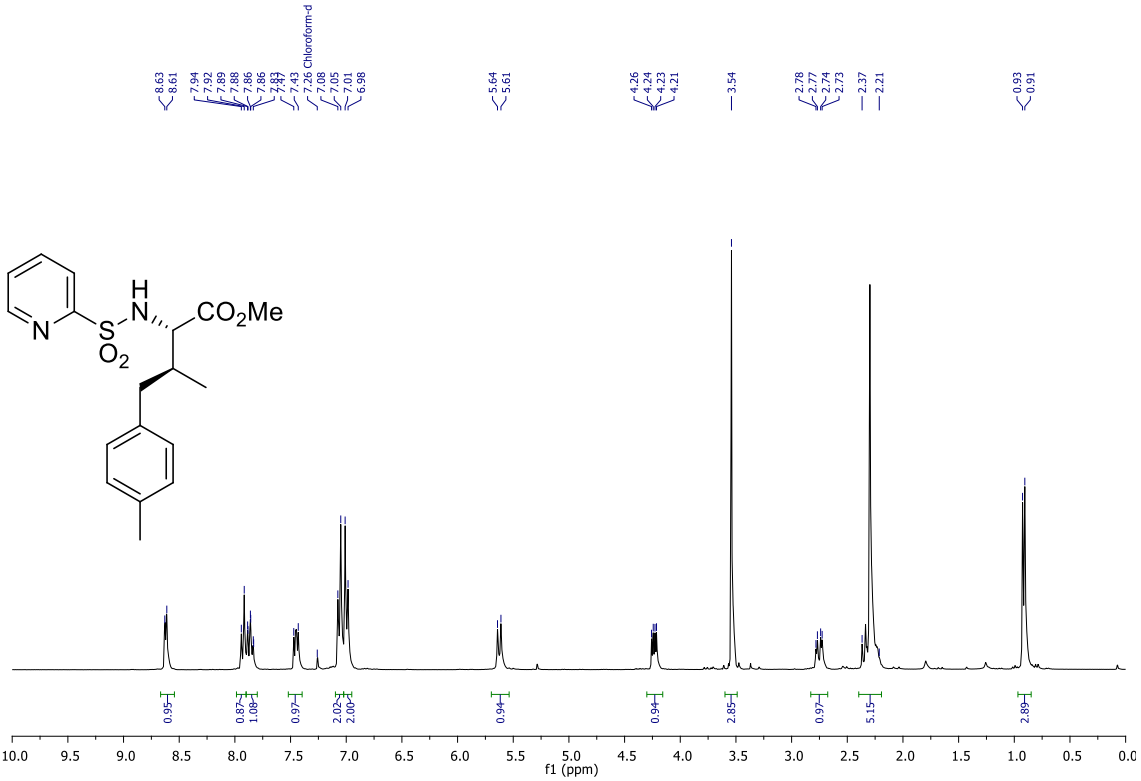


^{13}C NMR ($CDCl_3$, 75 MHz)

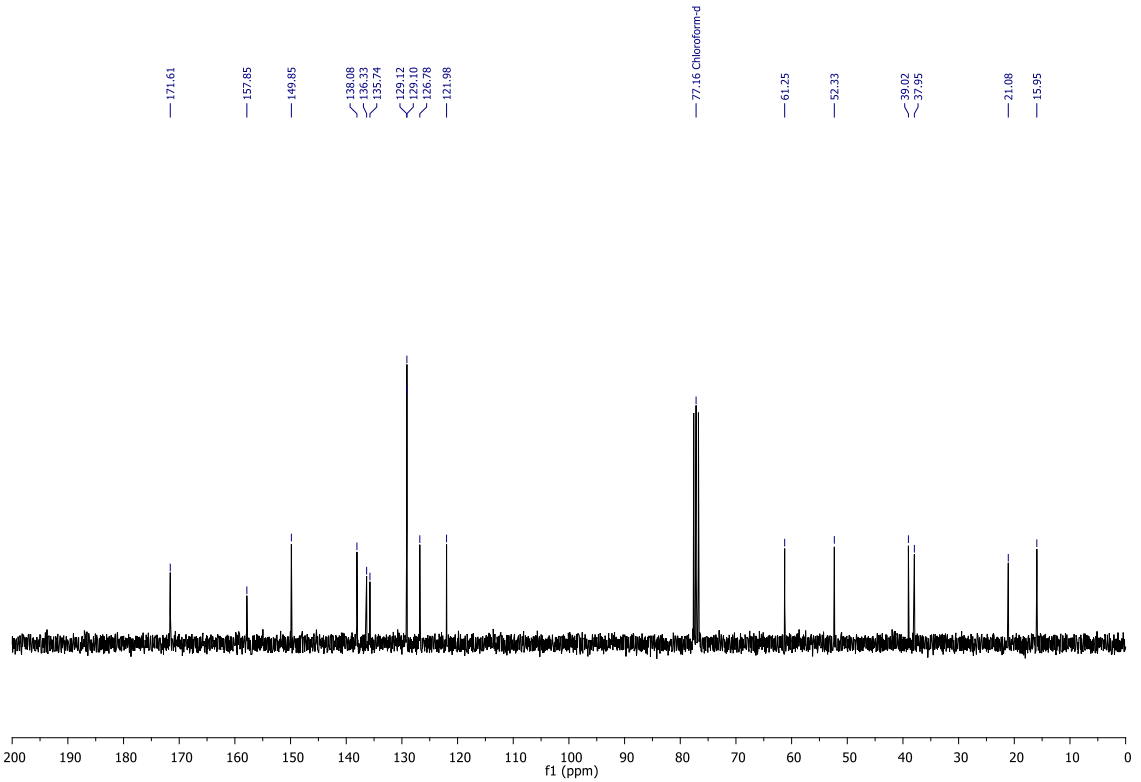


(2*S*,3*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(*p*-tolyl)butanoate (1b)

^{1}H NMR ($CDCl_3$, 300 MHz)

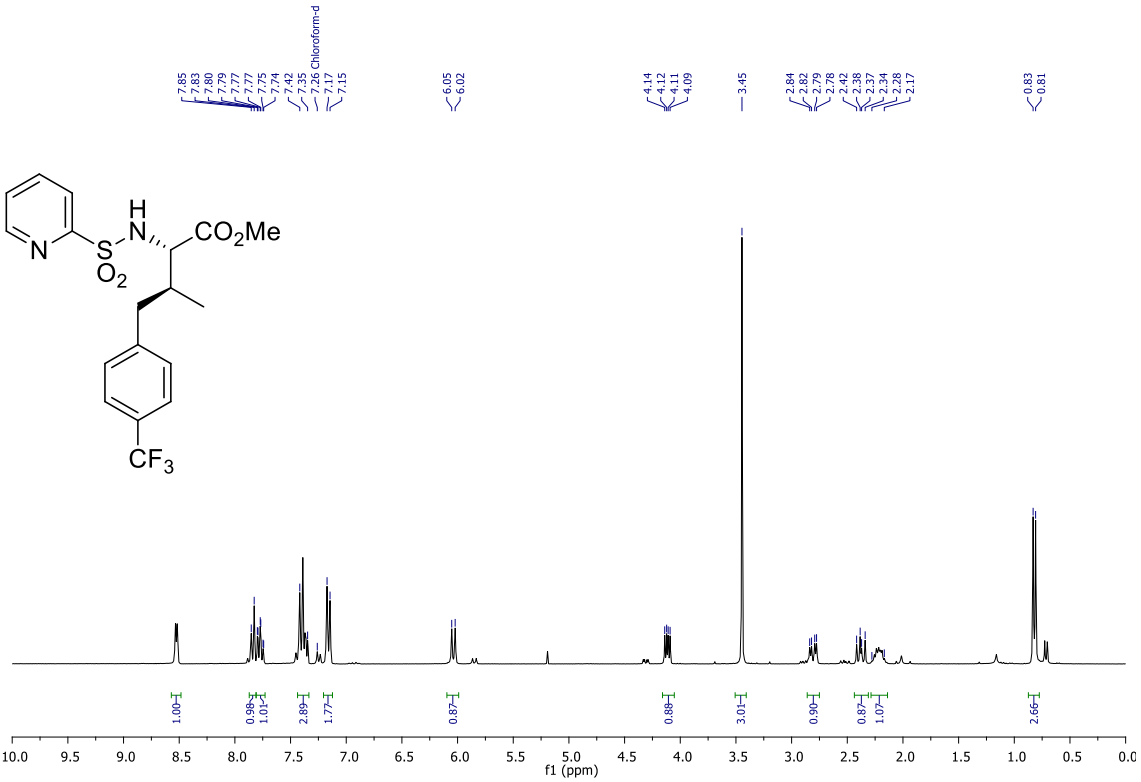


^{13}C NMR ($CDCl_3$, 75 MHz)

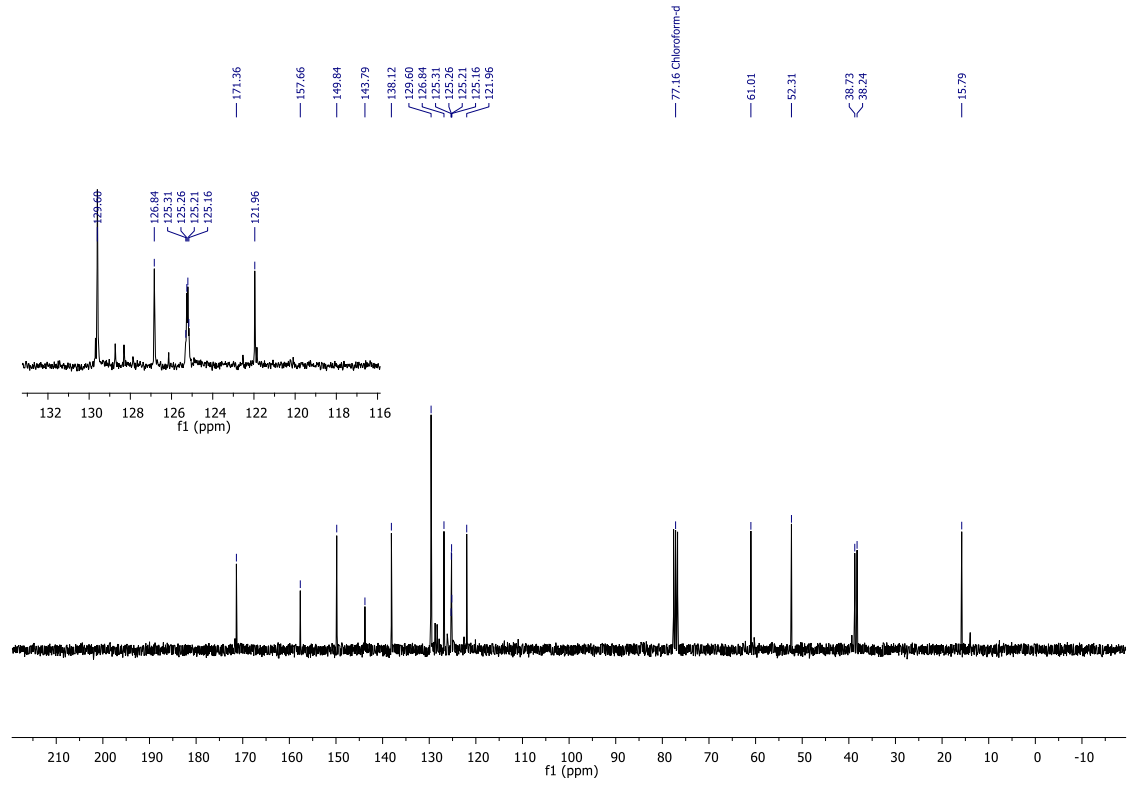


(2*S*,3*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(4-(trifluoromethyl)phenyl) butanoate (1c)

^{1}H NMR ($CDCl_3$, 300 MHz)

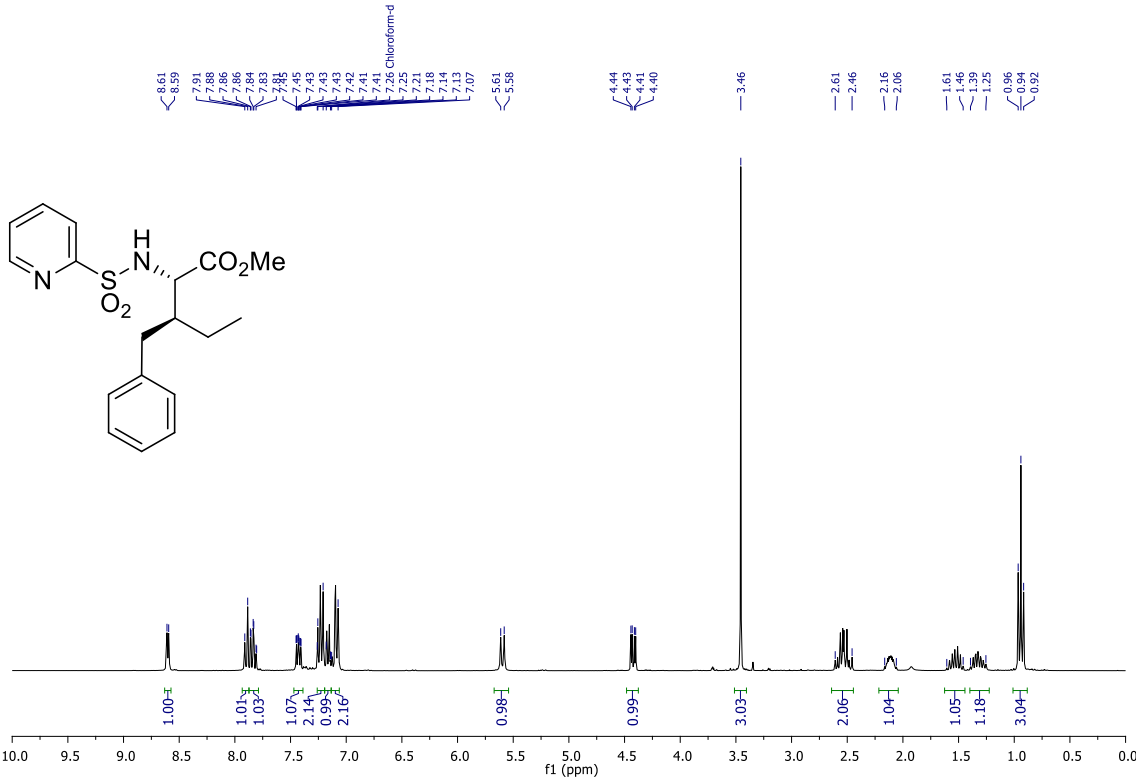


^{13}C NMR ($CDCl_3$, 75 MHz)

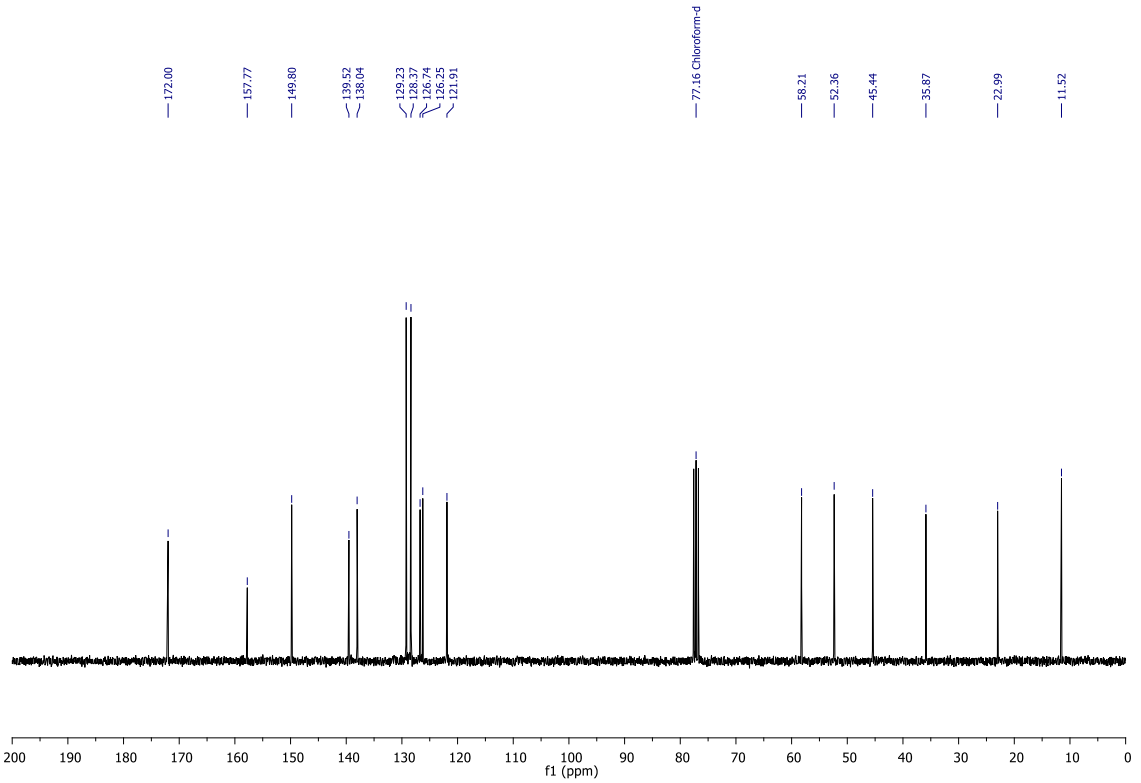


(2*S**,3*S**)-Methyl 3-benzyl-2-(pyridine-2-sulfonamido)pentanoate (4a)

^{1}H NMR ($CDCl_3$, 300 MHz)

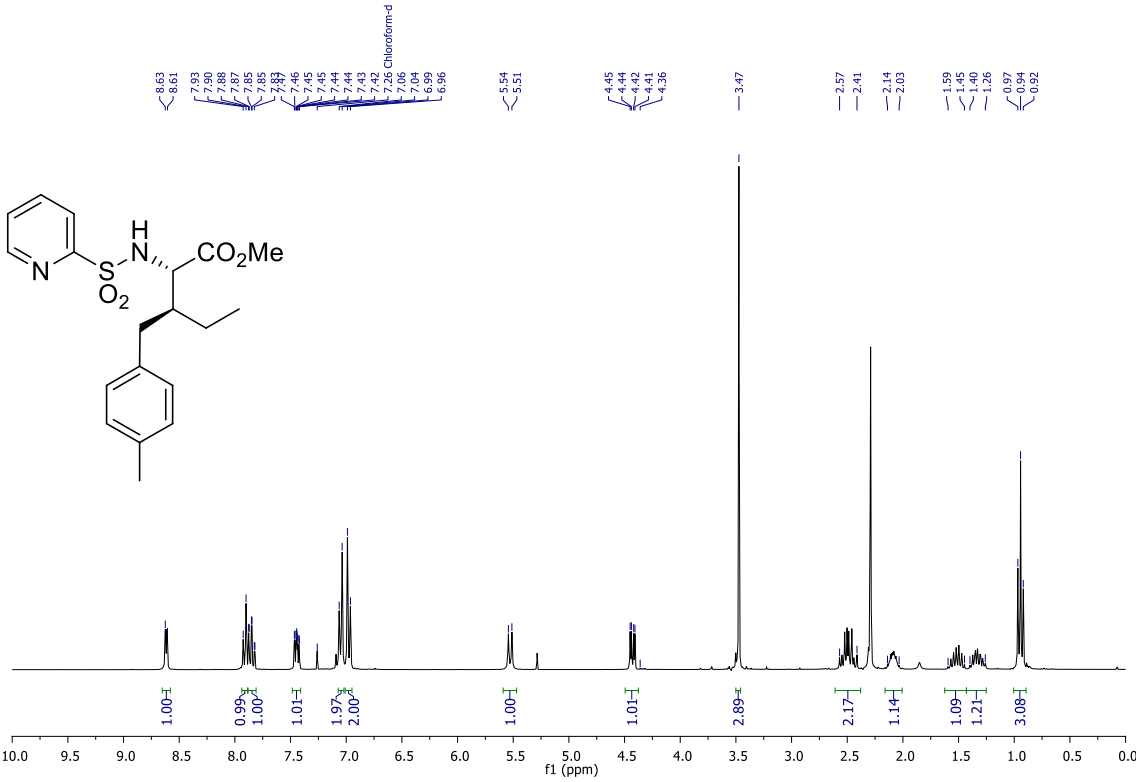


^{13}C NMR ($CDCl_3$, 75 MHz)

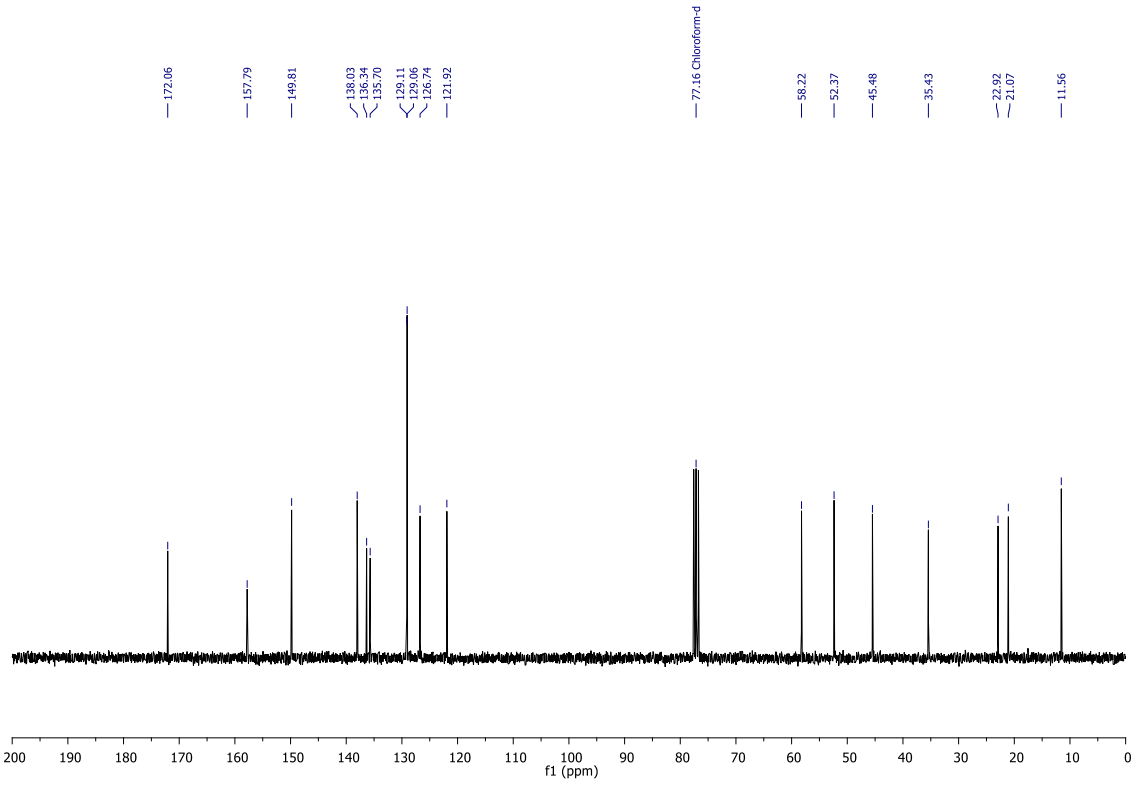


(2*S,3*S**)-Methyl 3-(4-methylbenzyl)-2-(pyridine-2-sulfonamido)pentanoate (4b)**

^{1}H NMR ($CDCl_3$, 300 MHz)

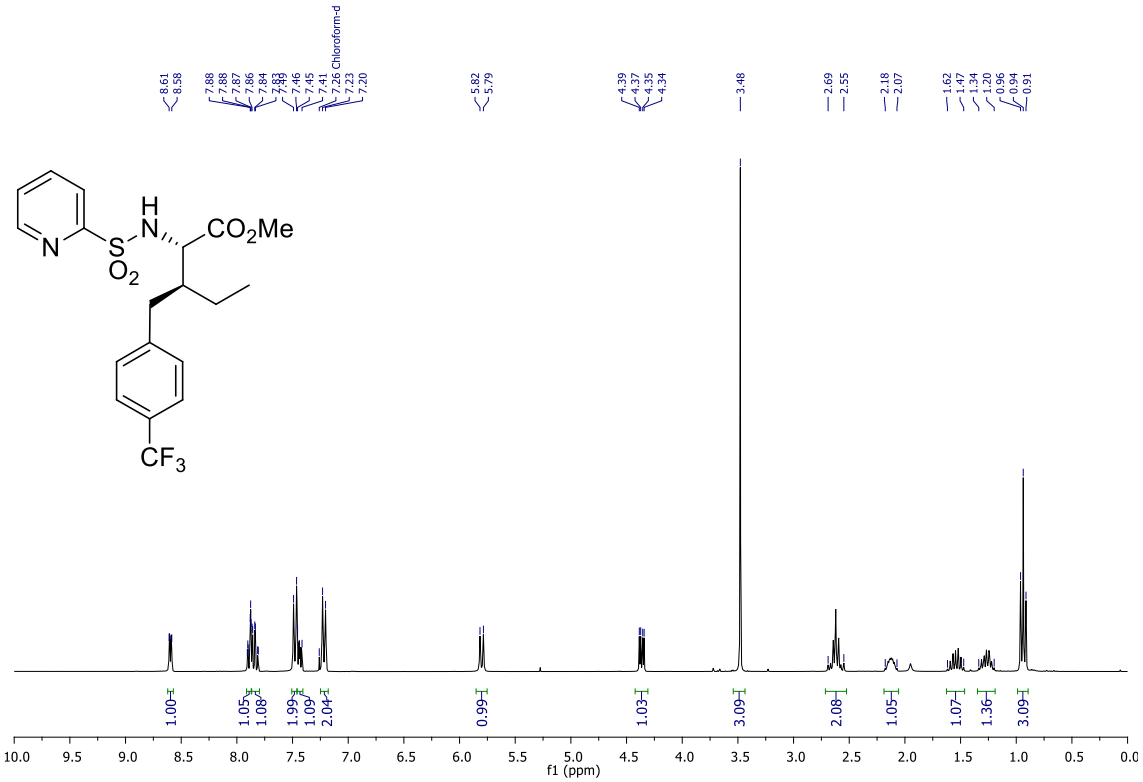


^{13}C NMR ($CDCl_3$, 75 MHz)

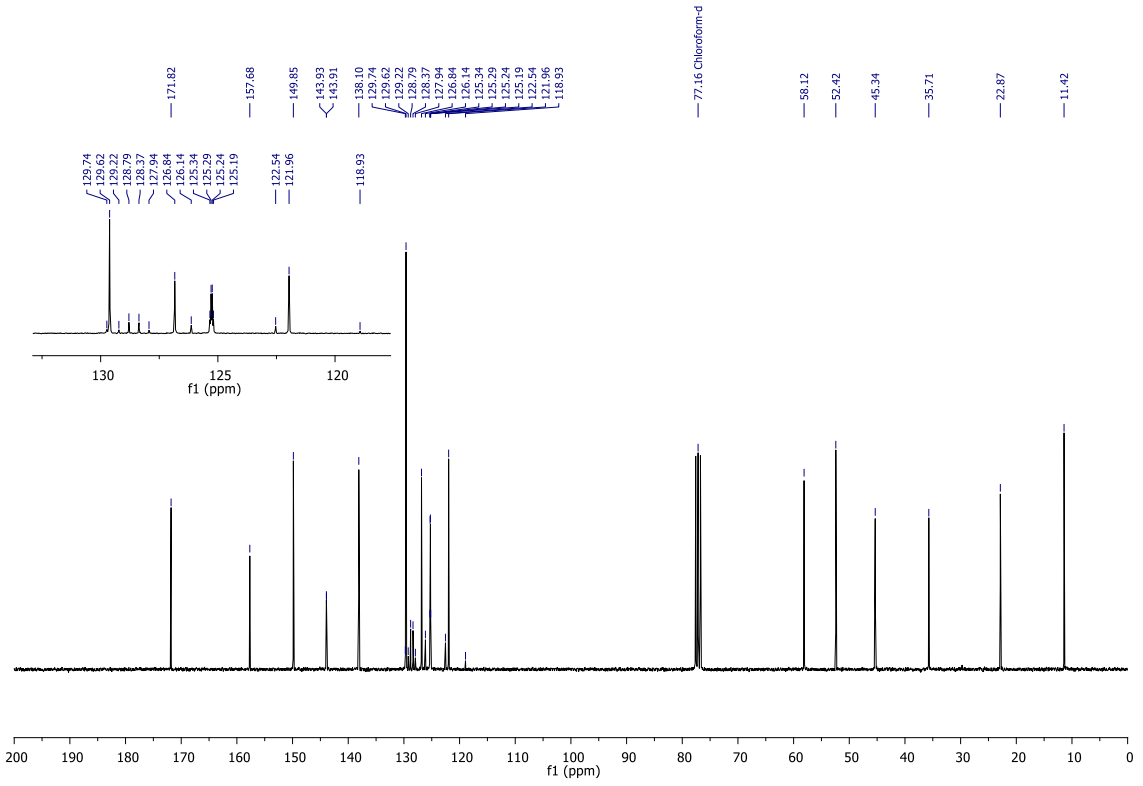


(2*S,3*S**)-Methyl 2-(pyridine-2-sulfonamido)-3-(4-(trifluoromethyl)benzyl) pentanoate (4c)**

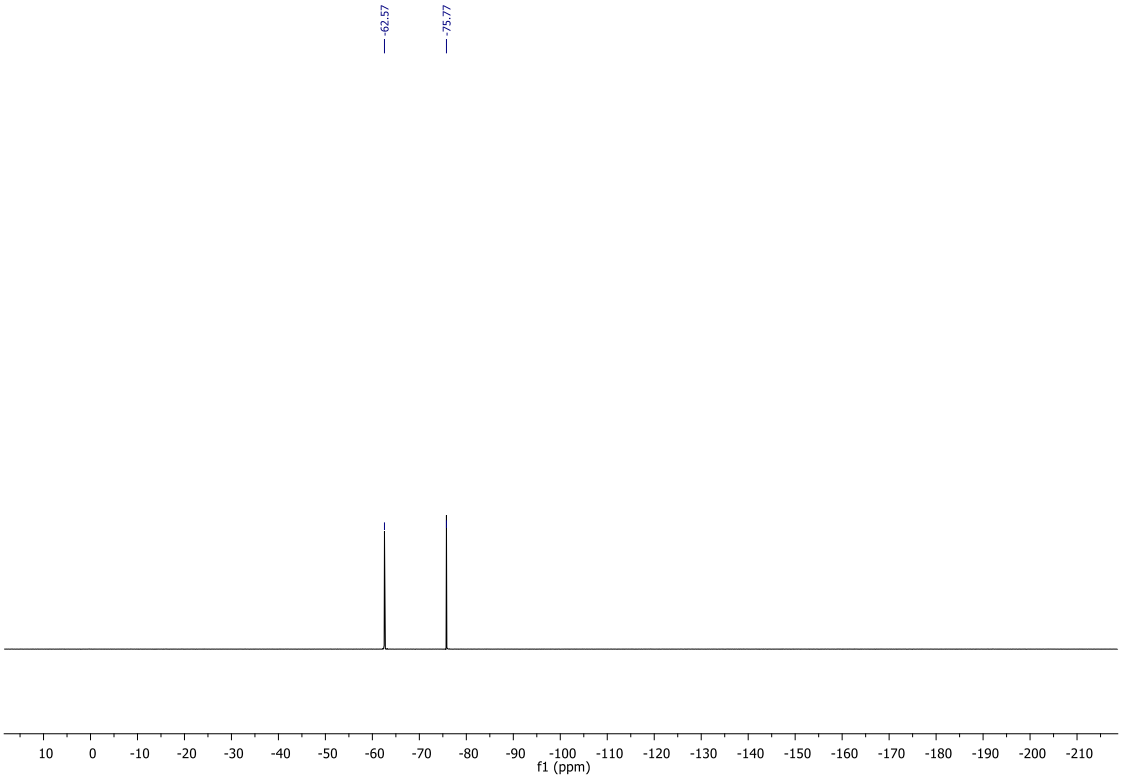
^{1}H NMR ($CDCl_3$, 300 MHz)



^{13}C NMR ($CDCl_3$, 75 MHz)

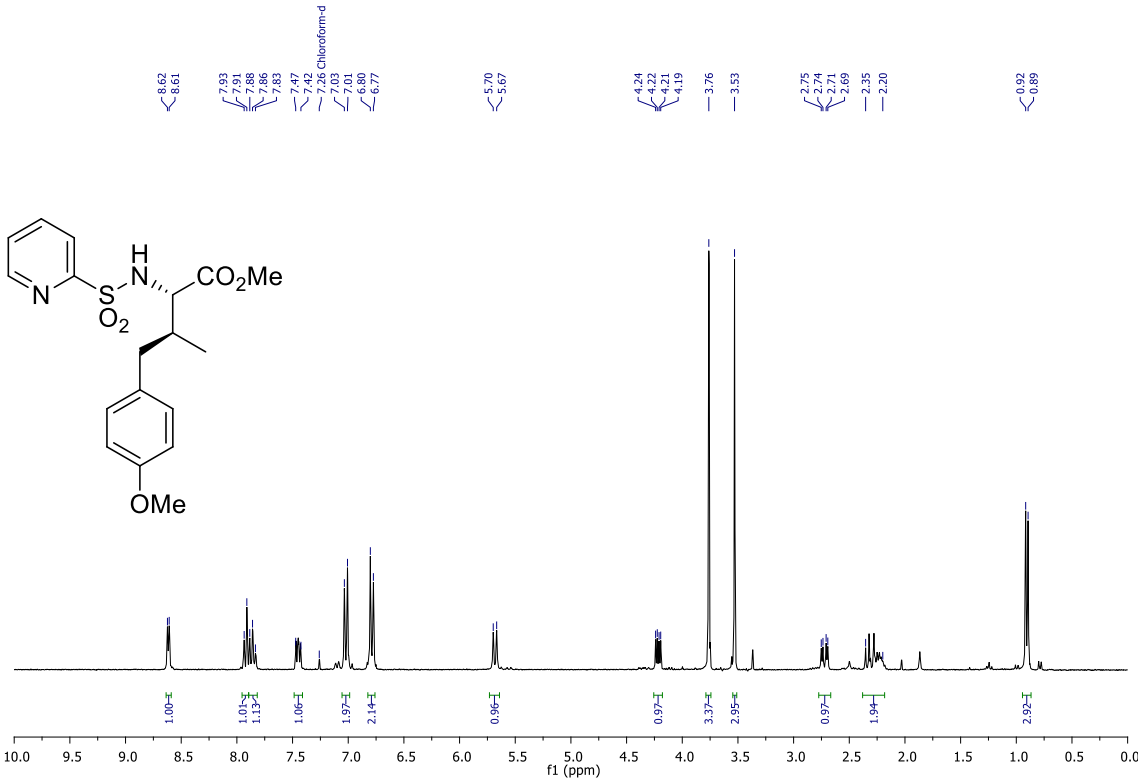


^{19}F NMR ($CDCl_3$, 282 MHz)

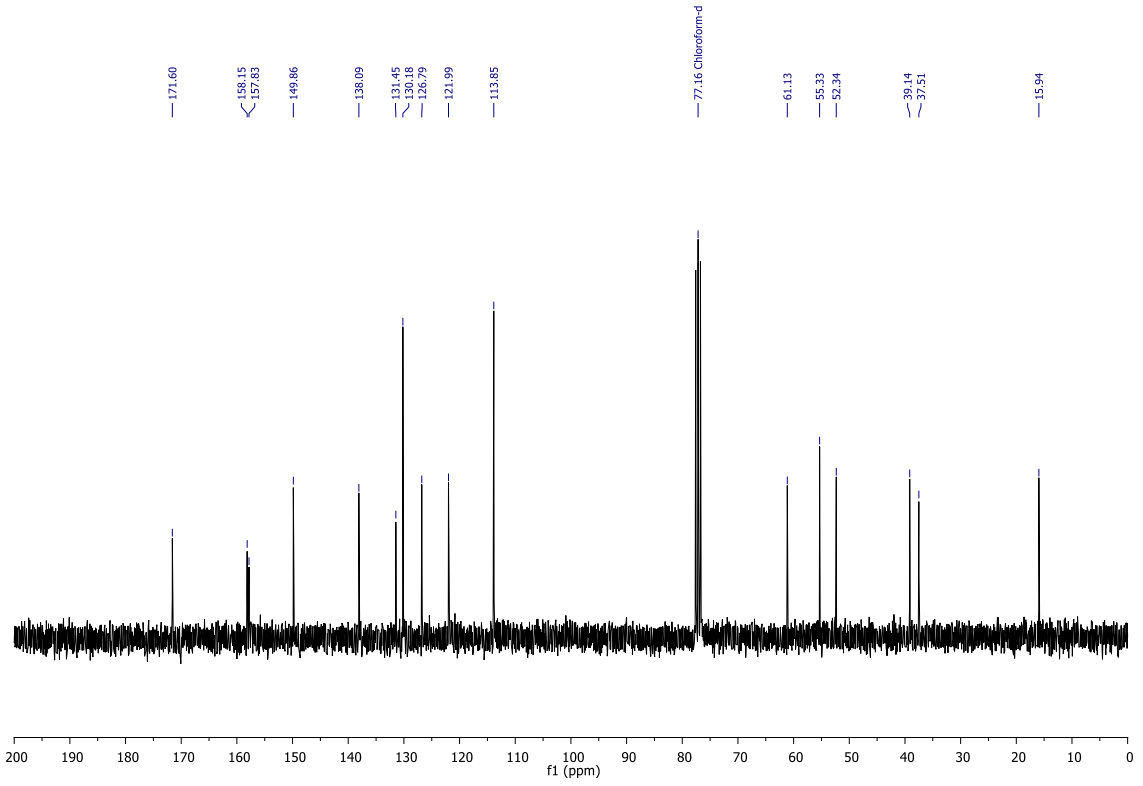


(2*S*,3*S*)-Methyl 4-(4-methoxyphenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1d)

^{1}H NMR ($CDCl_3$, 300 MHz)

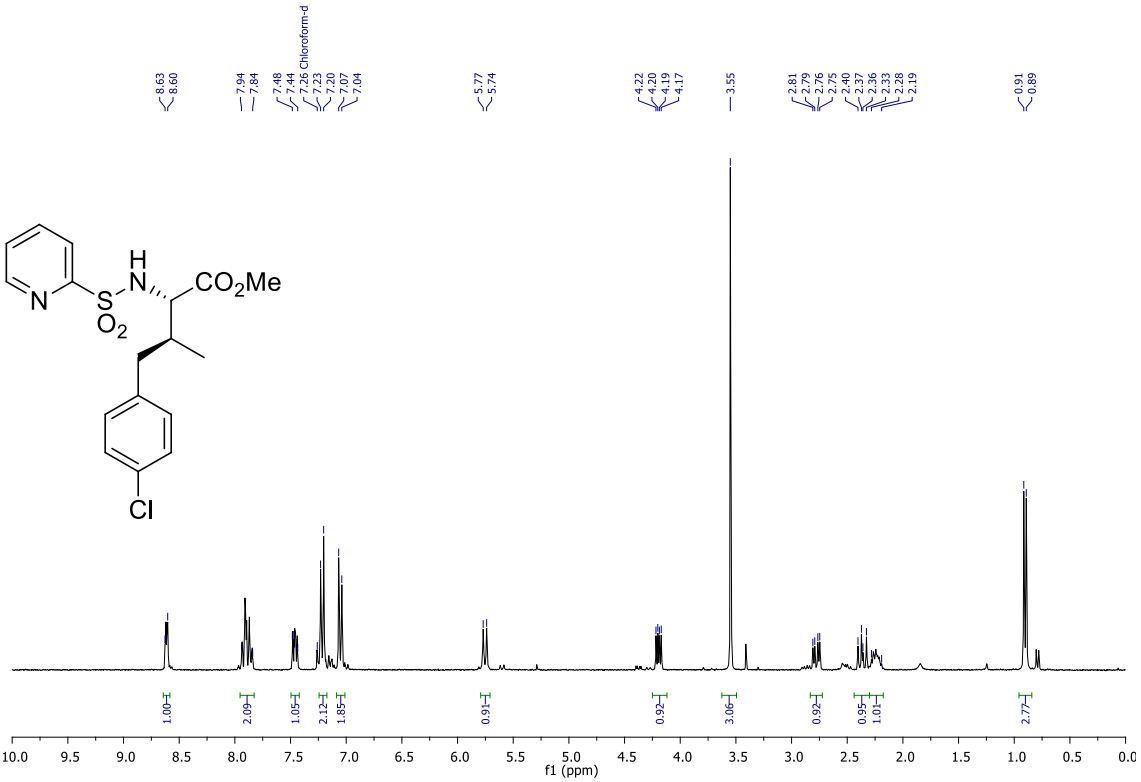


^{13}C NMR ($CDCl_3$, 75 MHz)

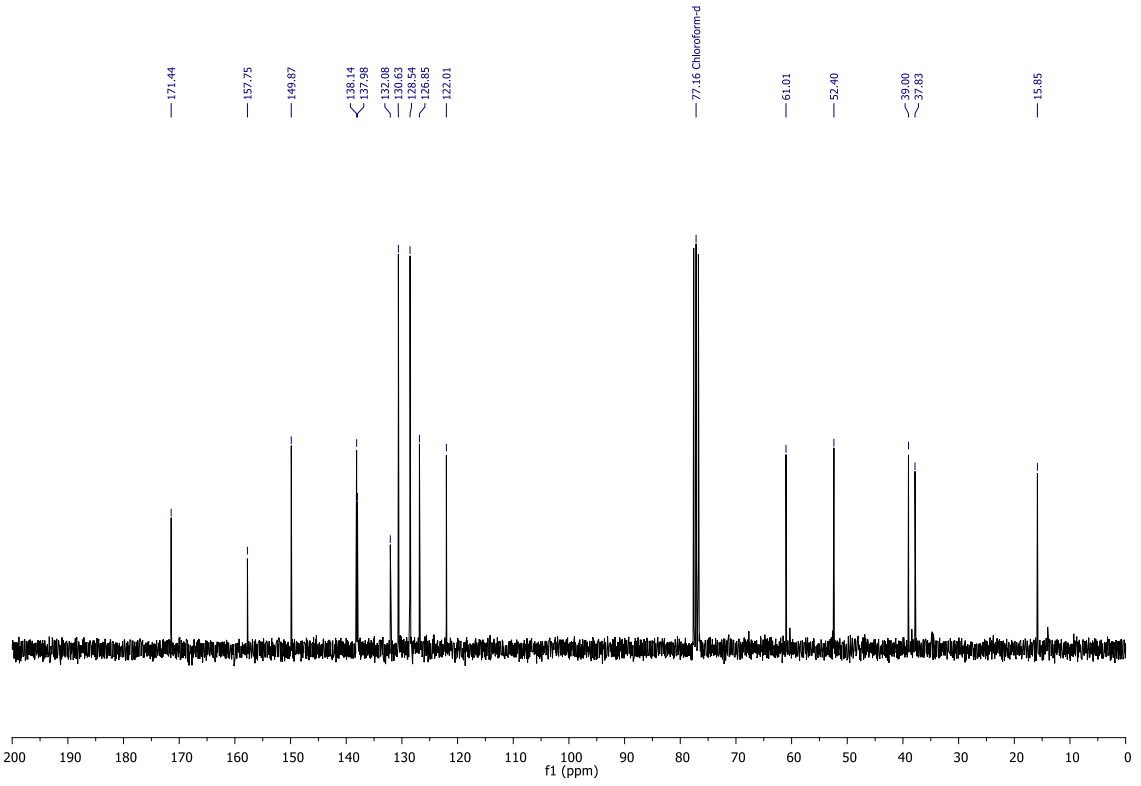


(2*S*,3*S*)-Methyl 4-(4-chlorophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1e)

^{1}H NMR ($CDCl_3$, 300 MHz)

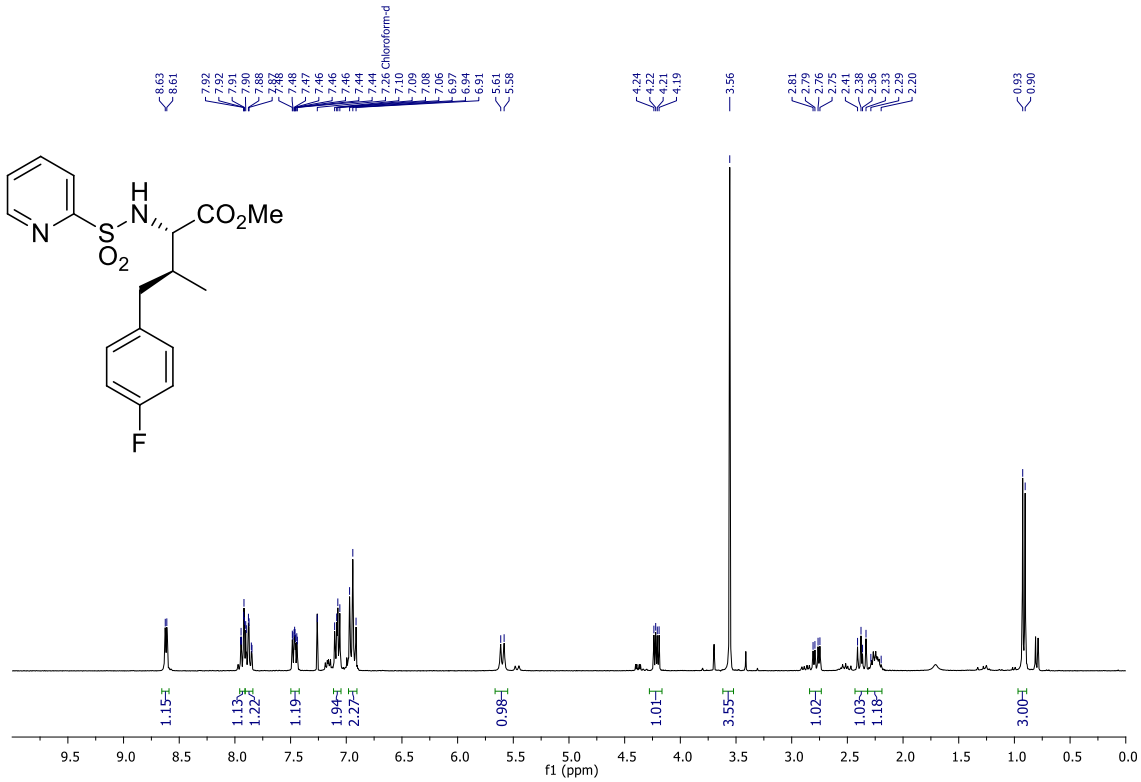


^{13}C NMR ($CDCl_3$, 75 MHz)

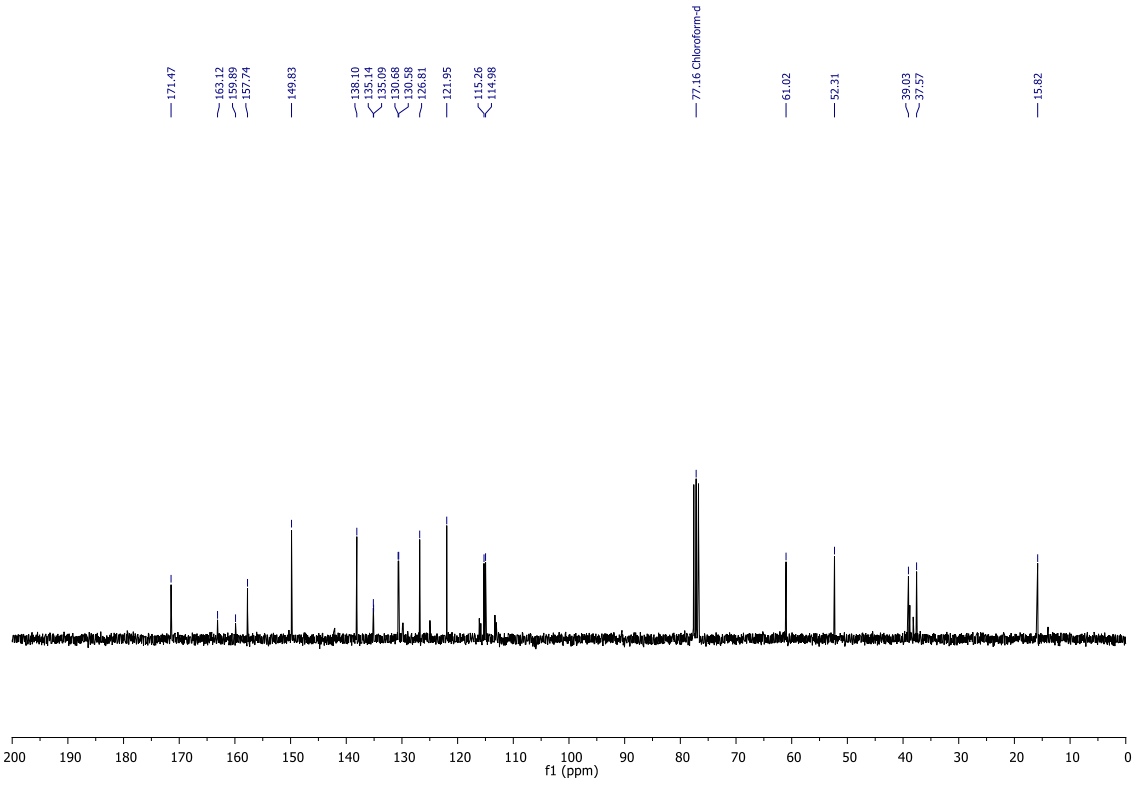


(2*S*,3*S*)-Methyl 4-(4-fluorophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1f)

^{1}H NMR ($CDCl_3$, 300 MHz)

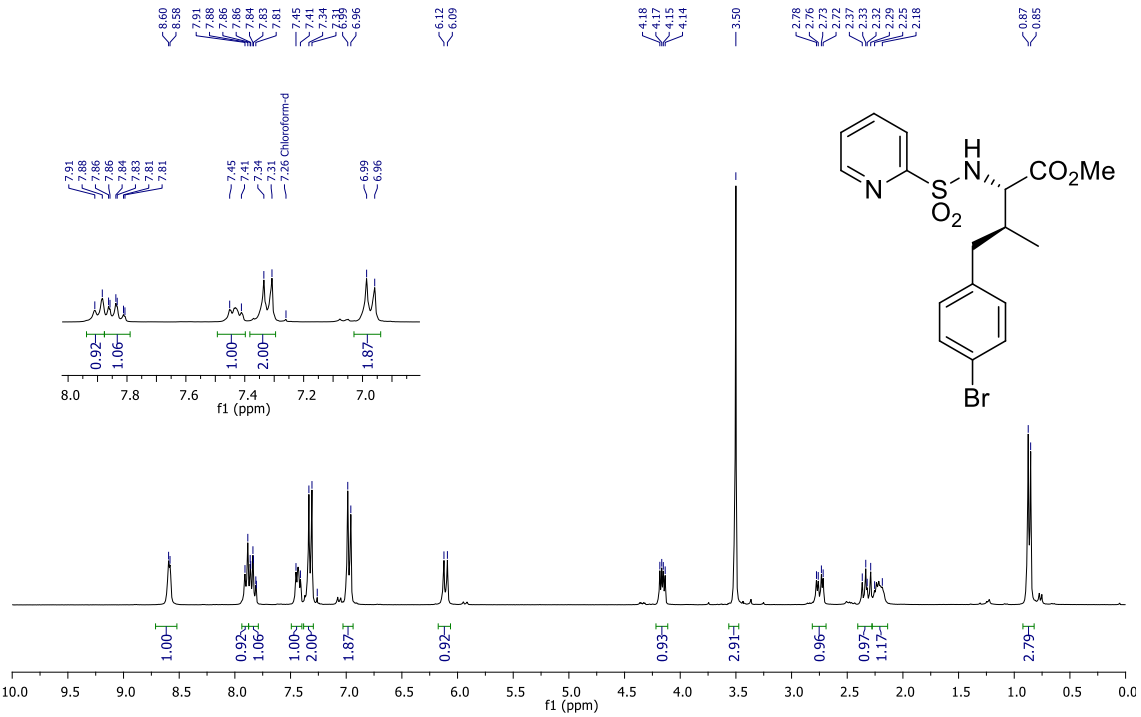


^{13}C NMR ($CDCl_3$, 75 MHz)

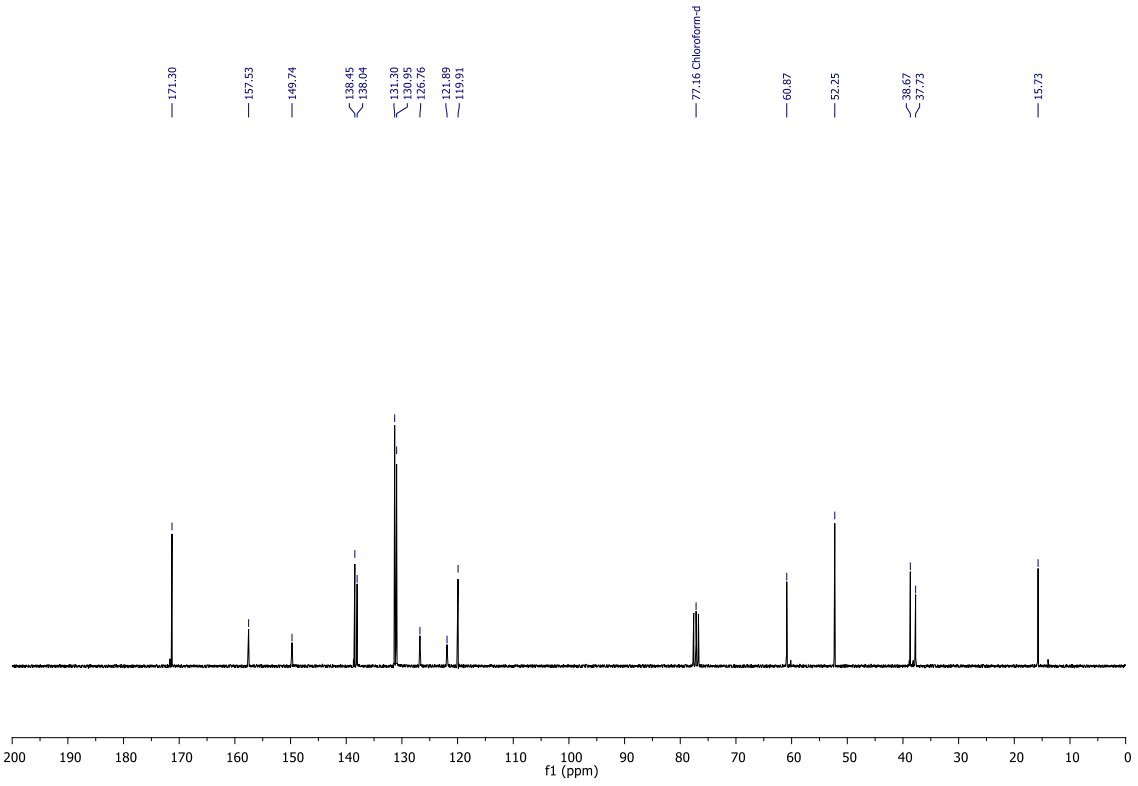


(2*S*,3*S*)-Methyl 4-(4-bromophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1g)

^{1}H NMR ($CDCl_3$, 300 MHz)

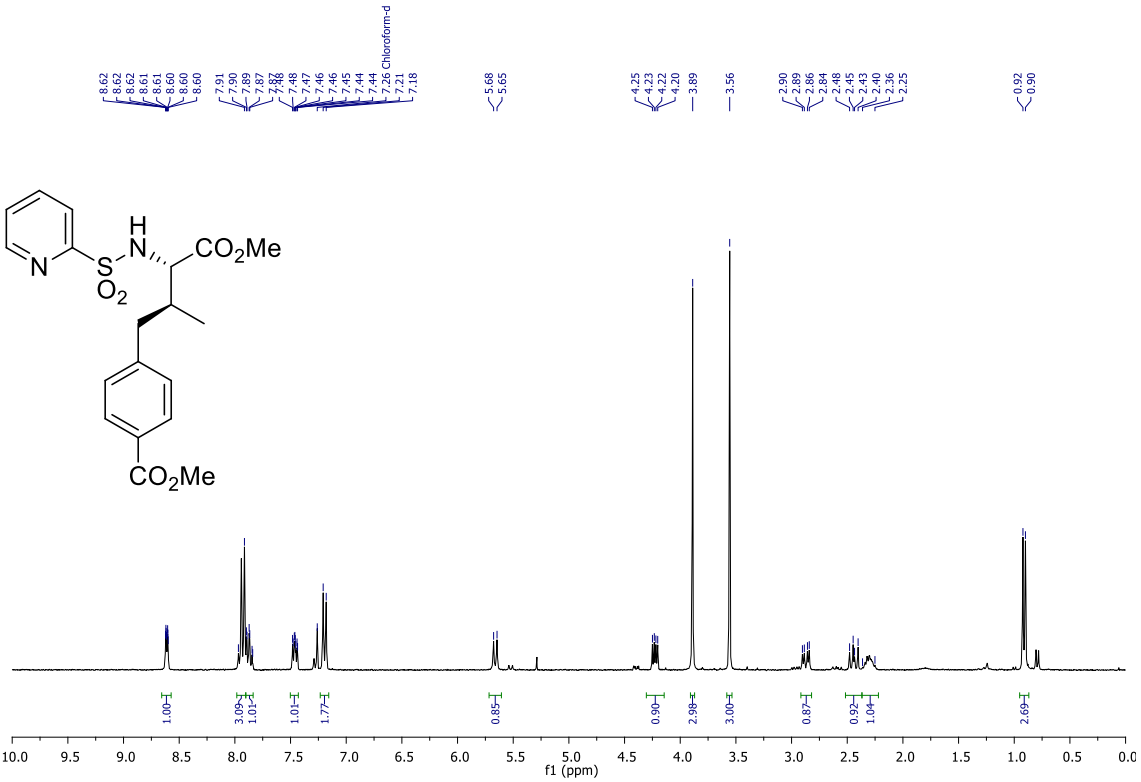


^{13}C NMR ($CDCl_3$, 75 MHz)

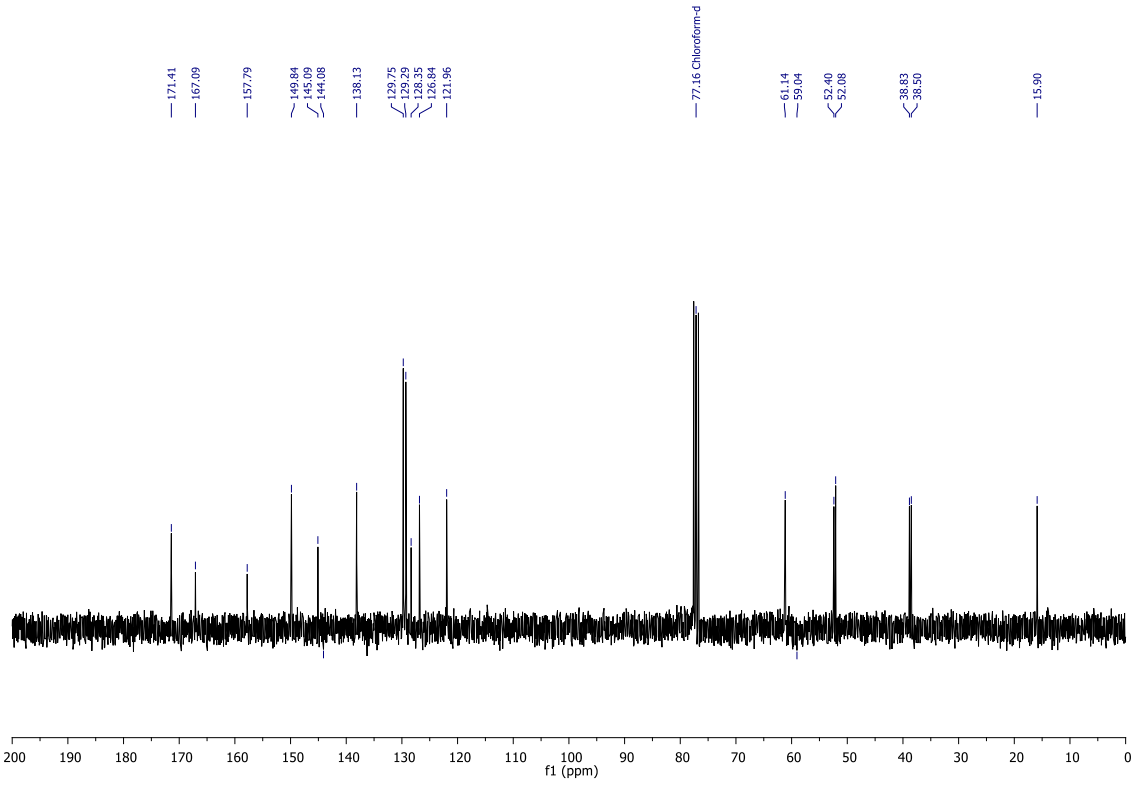


Methyl 4-((2*S*,3*S*)-4-methoxy-2-methyl-4-oxo-3-(pyridine-2-sulfonamido)butyl) benzoate (1h)

^{1}H NMR ($CDCl_3$, 300 MHz)

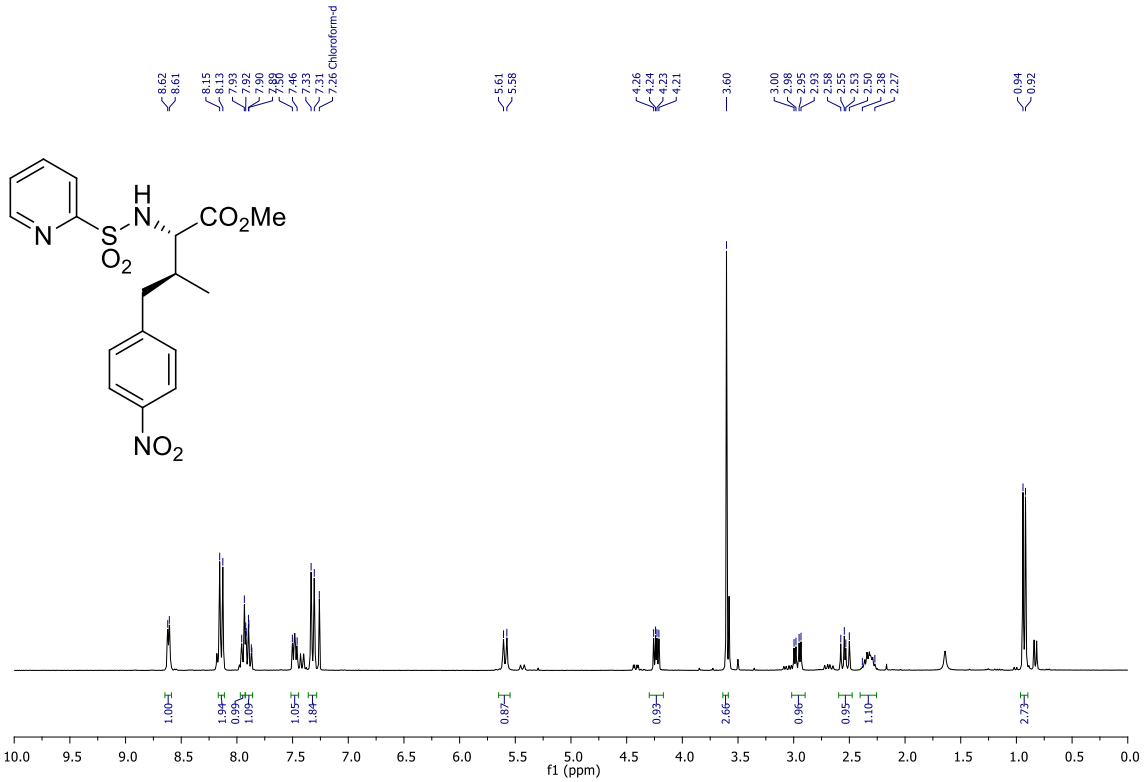


^{13}C NMR ($CDCl_3$, 75 MHz)

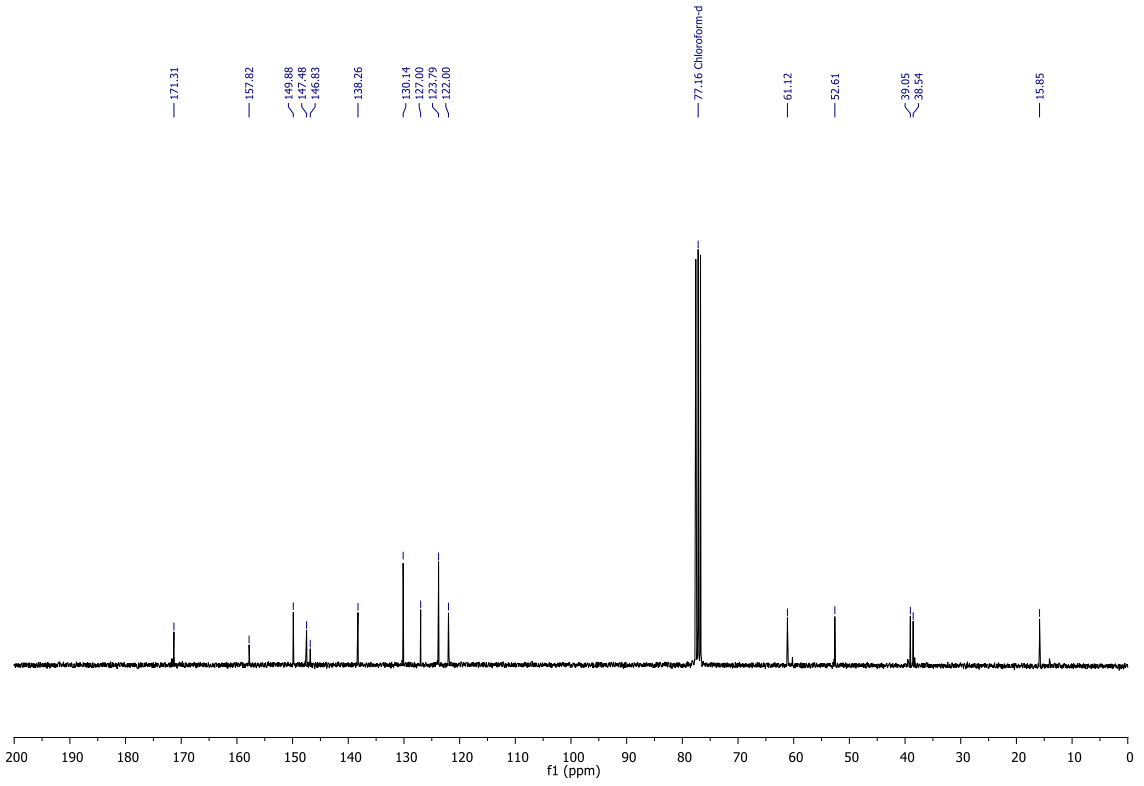


(2*S*,3*S*)-Methyl 3-methyl-4-(4-nitrophenyl)-2-(pyridine-2-sulfonamido)butanoate (1i)

^{1}H NMR ($CDCl_3$, 300 MHz)

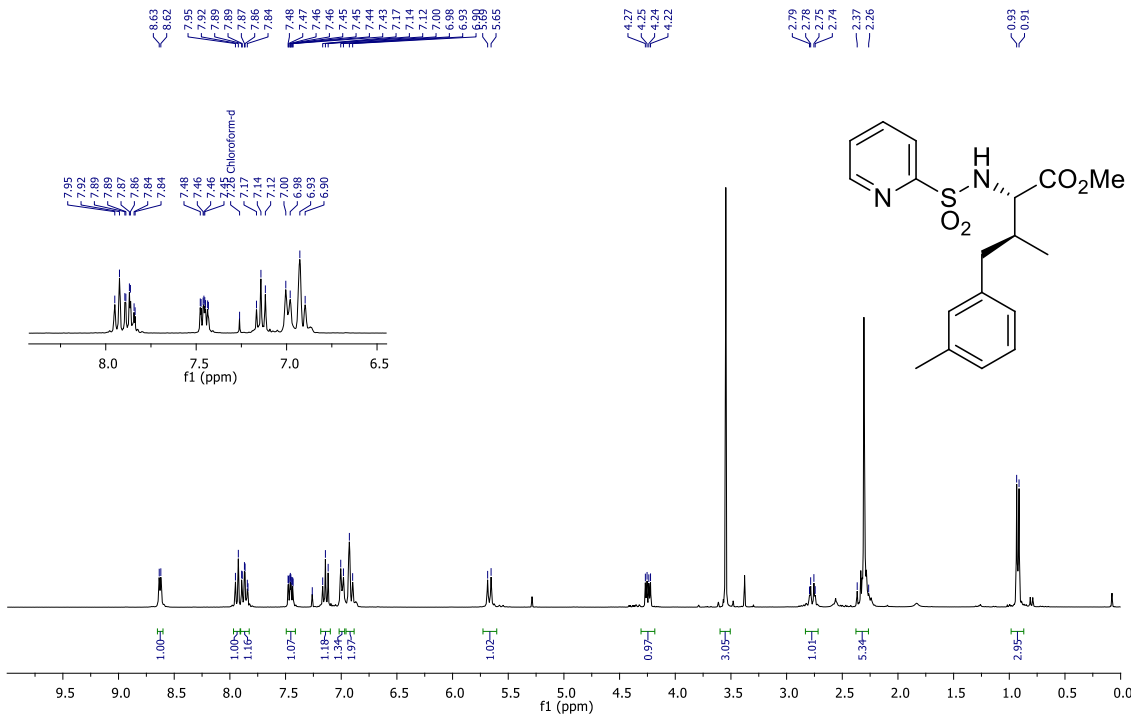


^{13}C NMR ($CDCl_3$, 75 MHz)

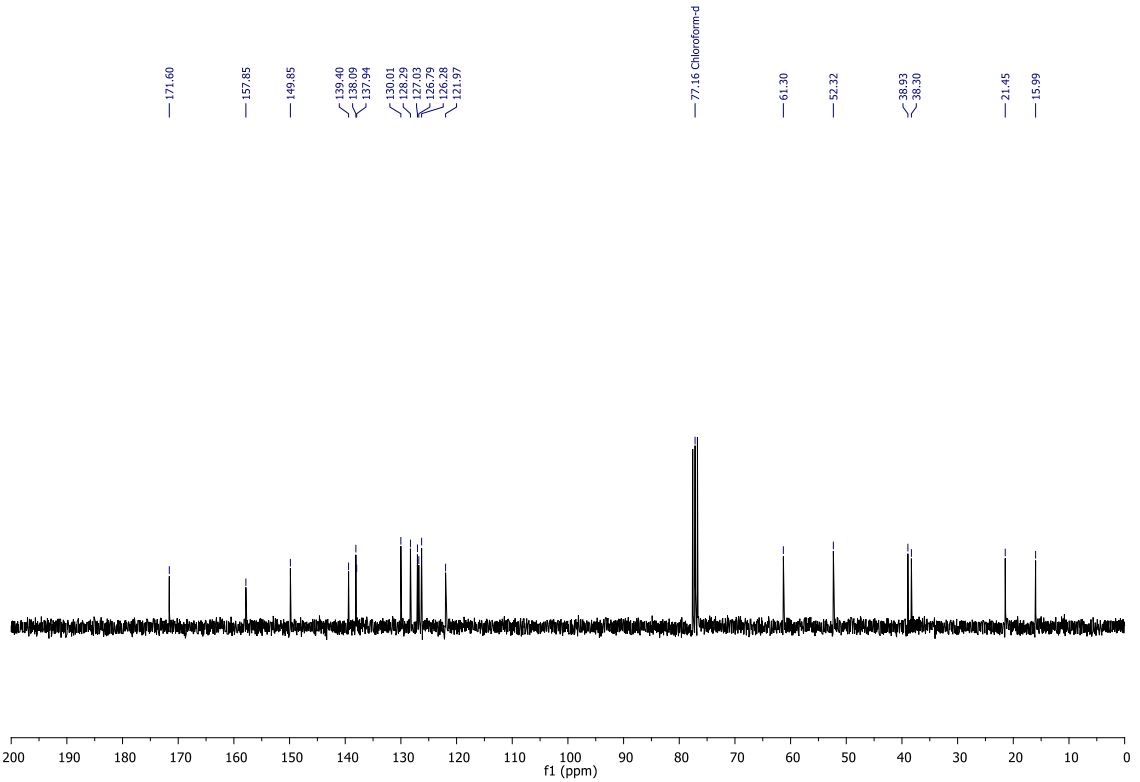


(2*S*,3*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(*m*-tolyl)butanoate (1j)

^{1}H NMR ($CDCl_3$, 300 MHz)

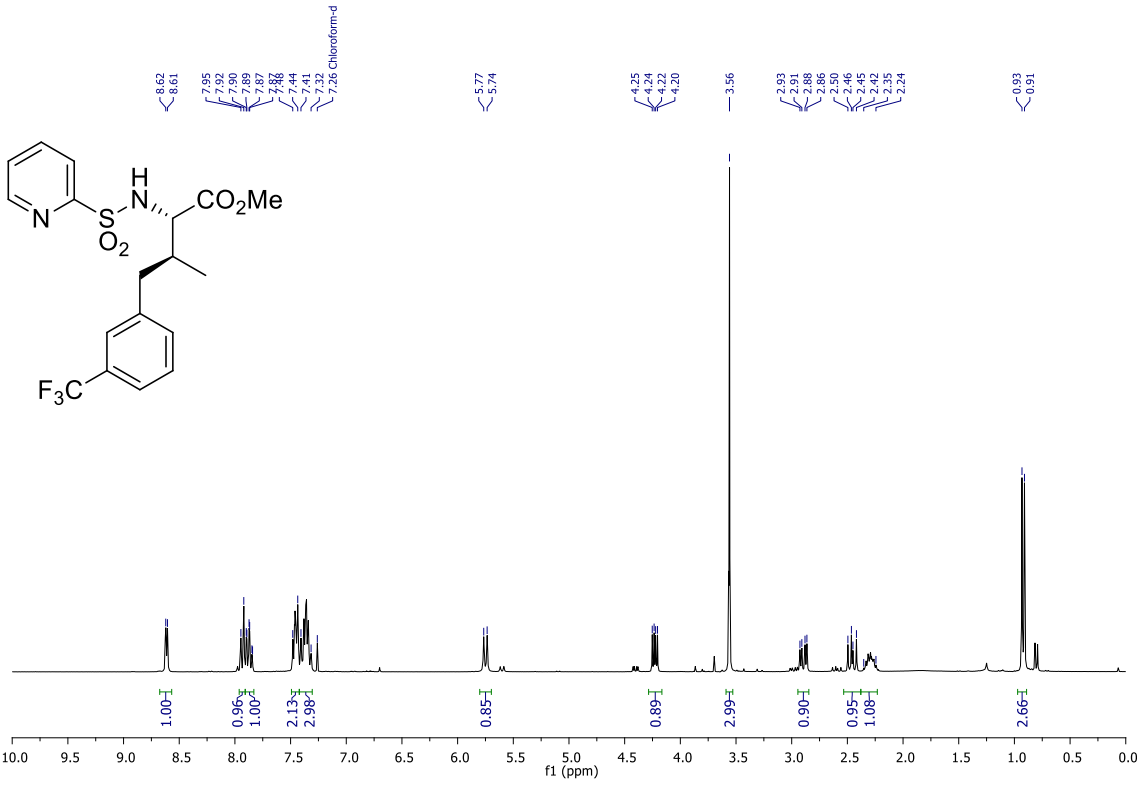


^{13}C NMR ($CDCl_3$, 75 MHz)

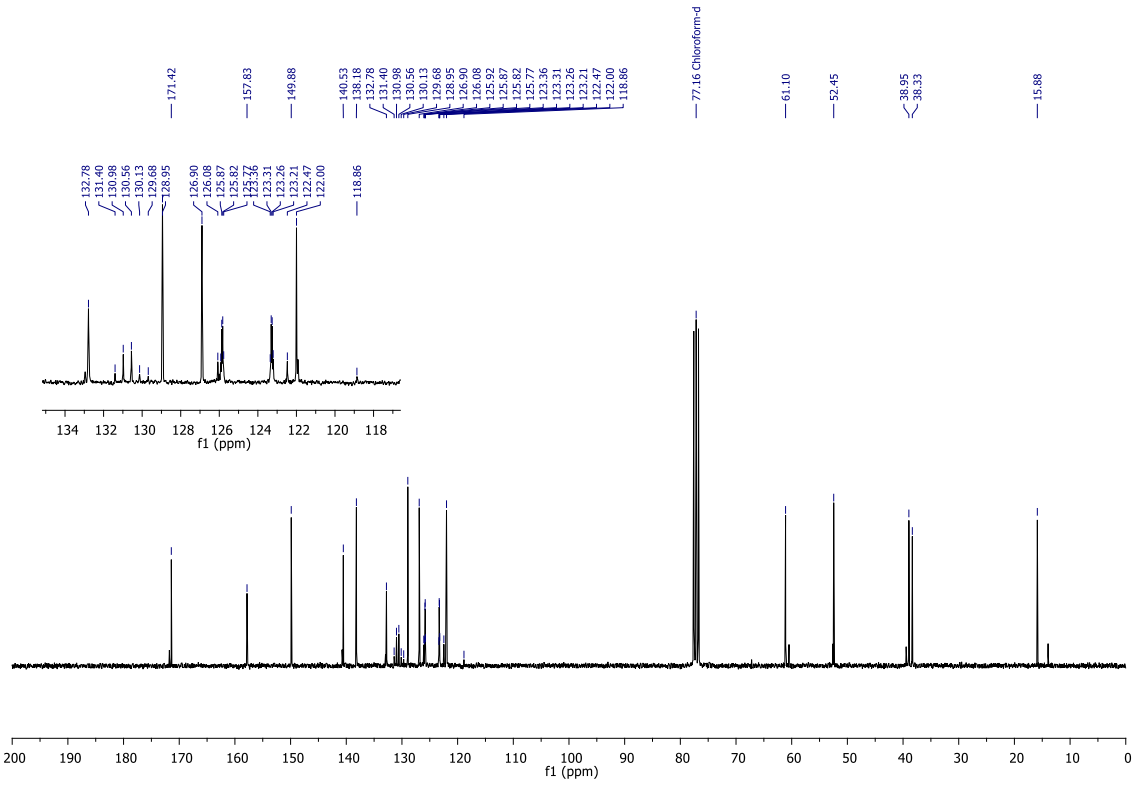


(2*S*,3*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(3-(trifluoromethyl)phenyl)-butanoate (1k).

^{1}H NMR ($CDCl_3$, 300 MHz)

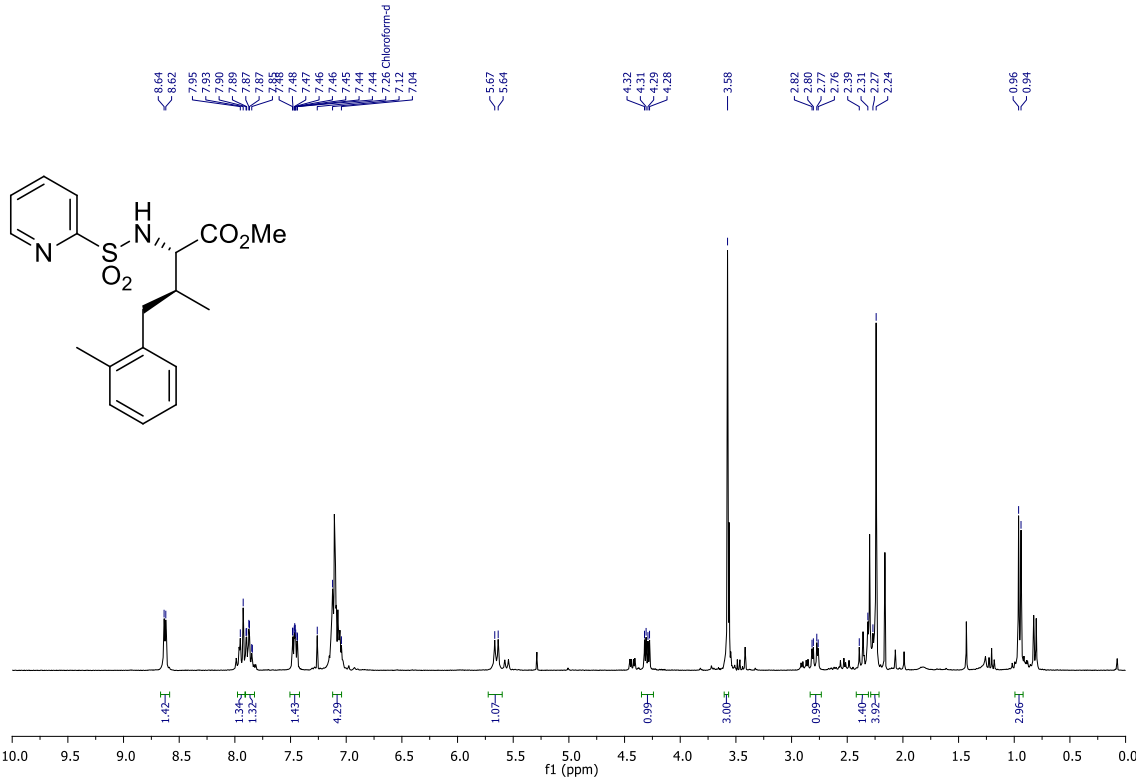


^{13}C NMR ($CDCl_3$, 75 MHz)

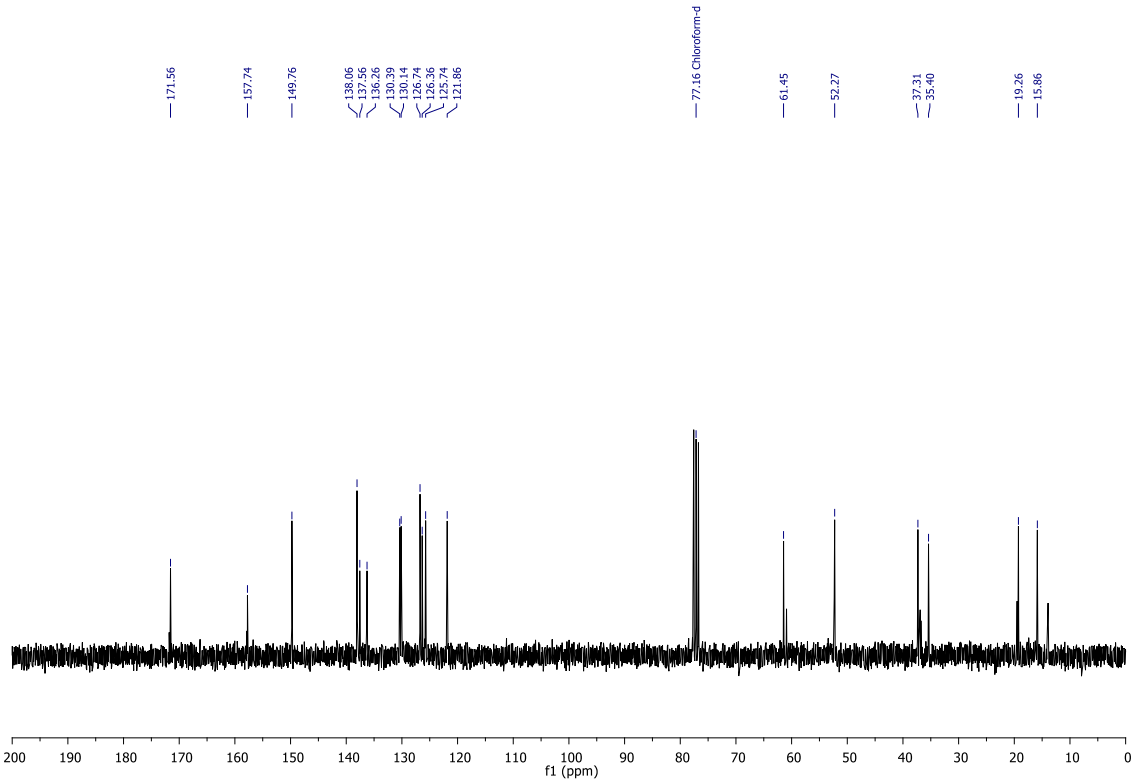


(2*S*,3*S*)-Methyl 3-methyl-2-(pyridine-2-sulfonamido)-4-(*o*-tolyl)butanoate (1l)

^{1}H NMR ($CDCl_3$, 300 MHz)

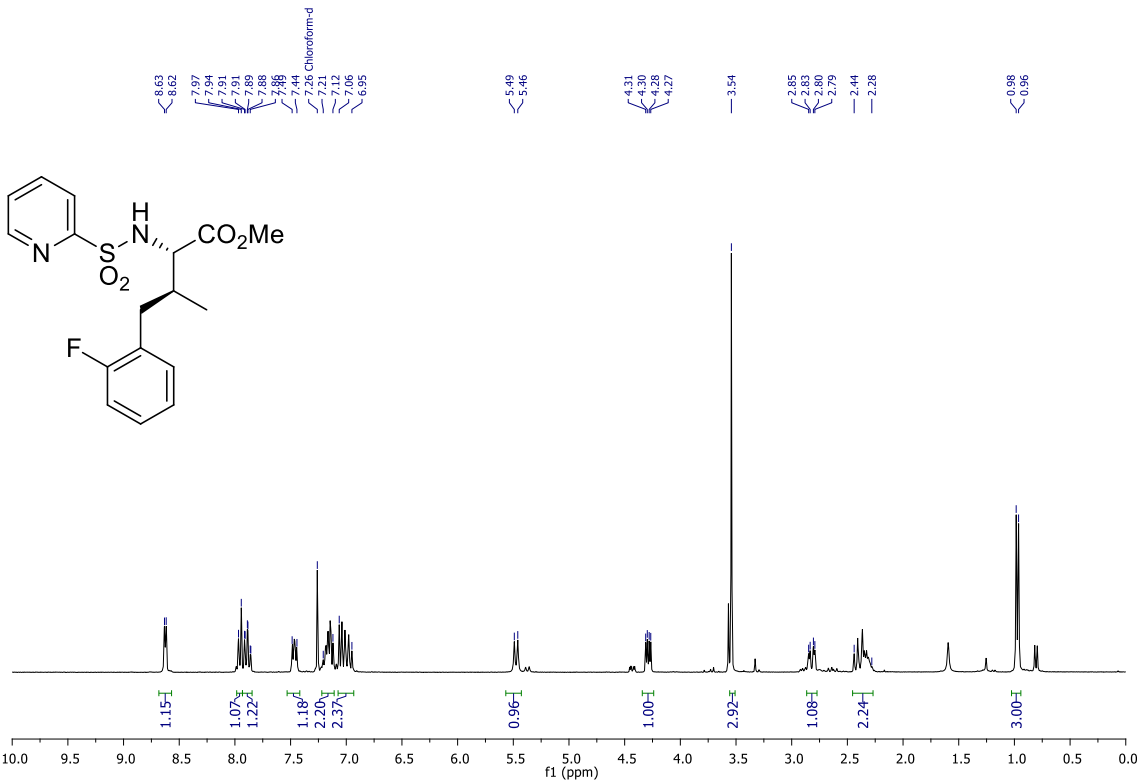


^{13}C NMR ($CDCl_3$, 75 MHz)

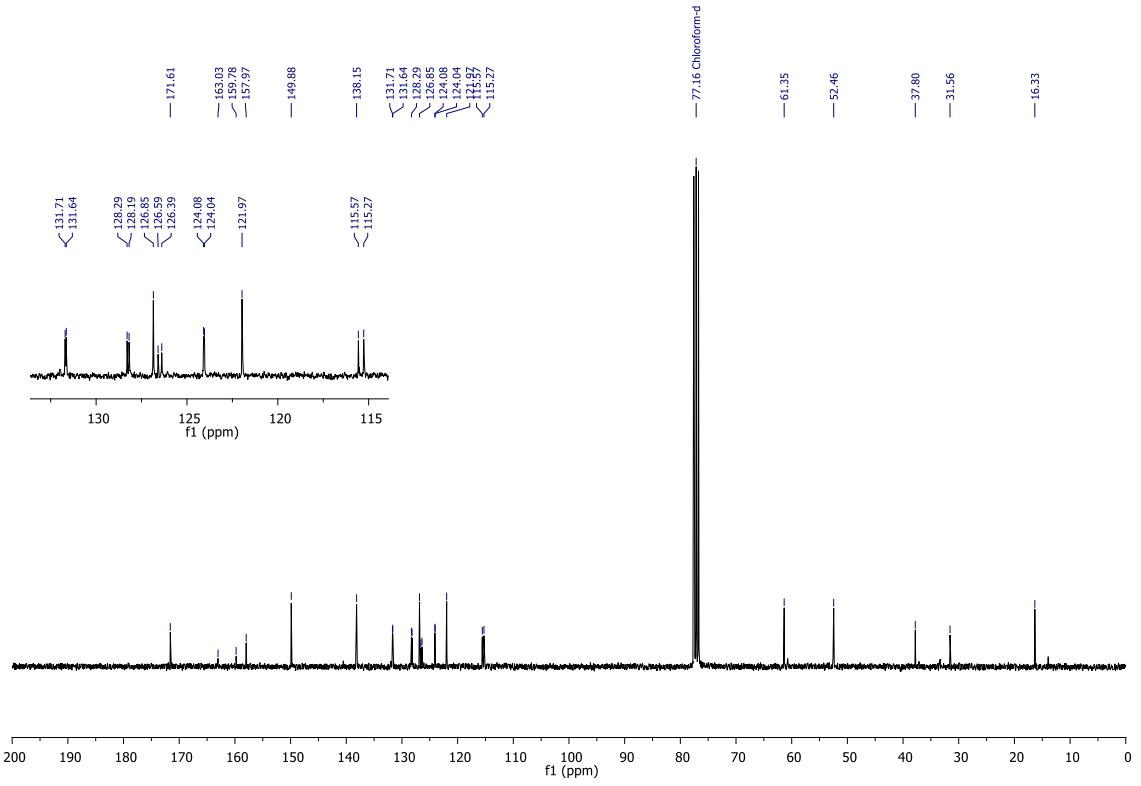


(2*S*,3*S*)-Methyl 4-(2-fluorophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1m).

^{1}H NMR ($CDCl_3$, 300 MHz)

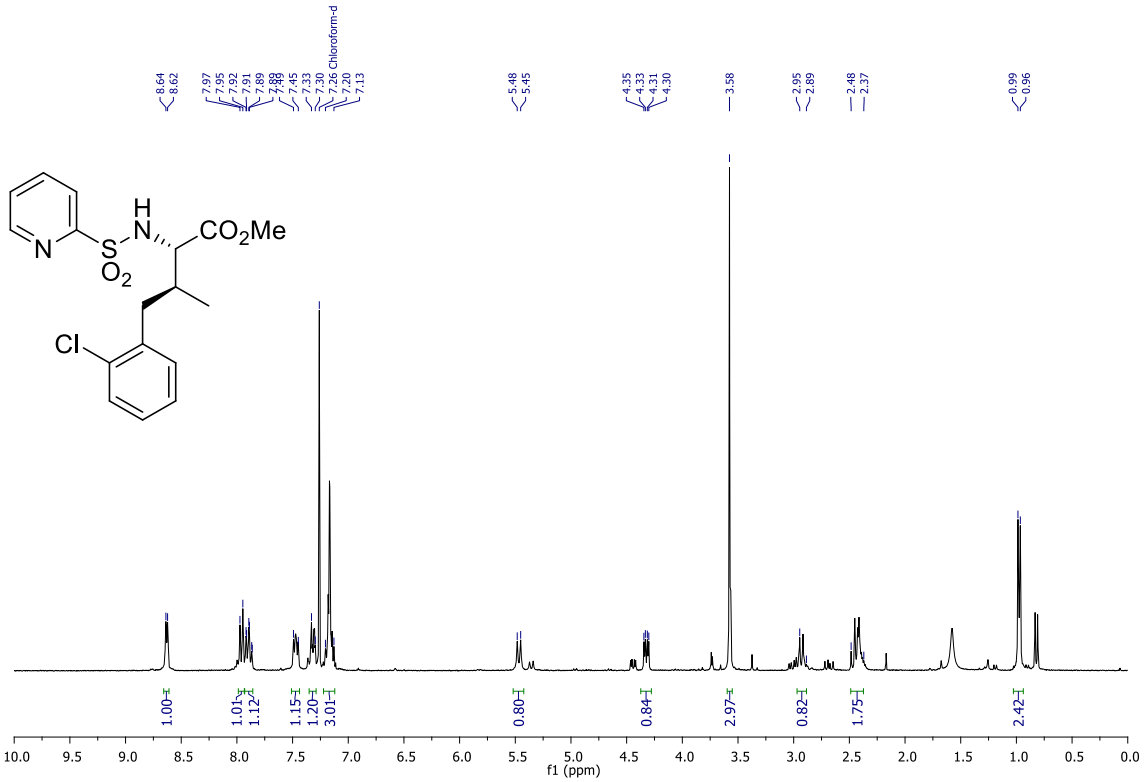


^{13}C NMR ($CDCl_3$, 75 MHz)

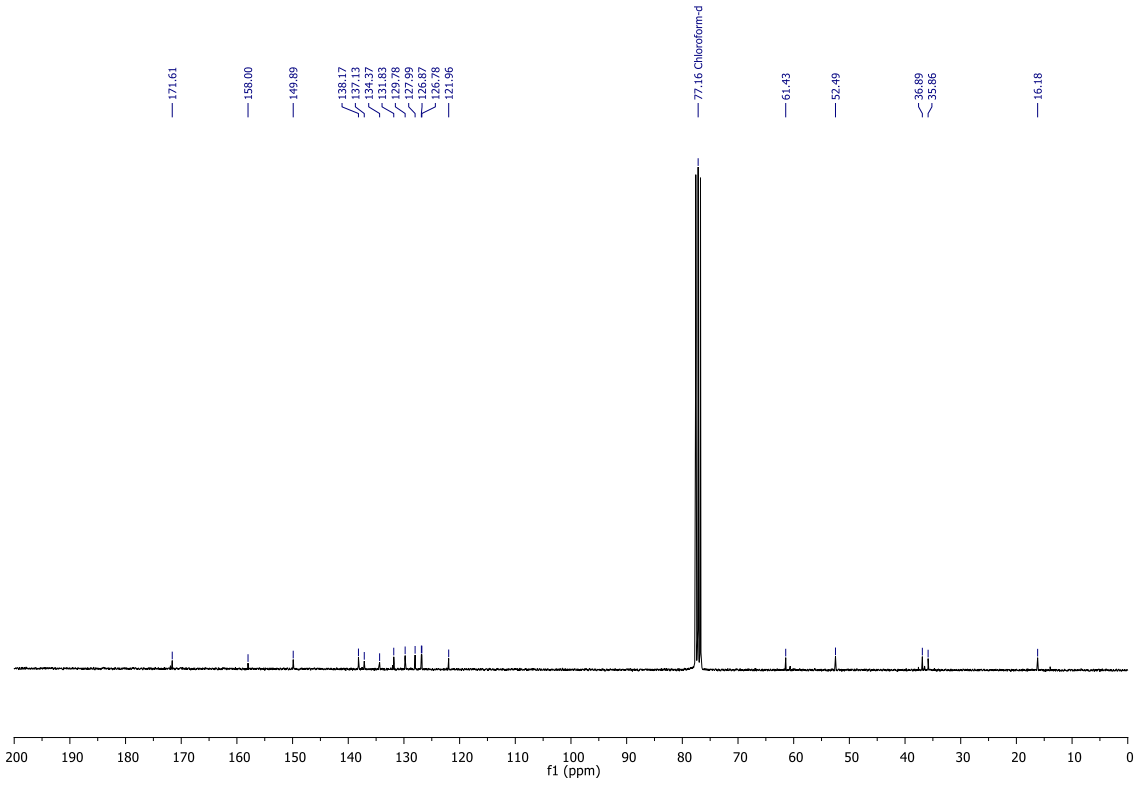


(2*S*,3*S*)-Methyl 4-(2-chlorophenyl)-3-methyl-2-(pyridine-2-sulfonamido)butanoate (1n).

^{1}H NMR ($CDCl_3$, 300 MHz)

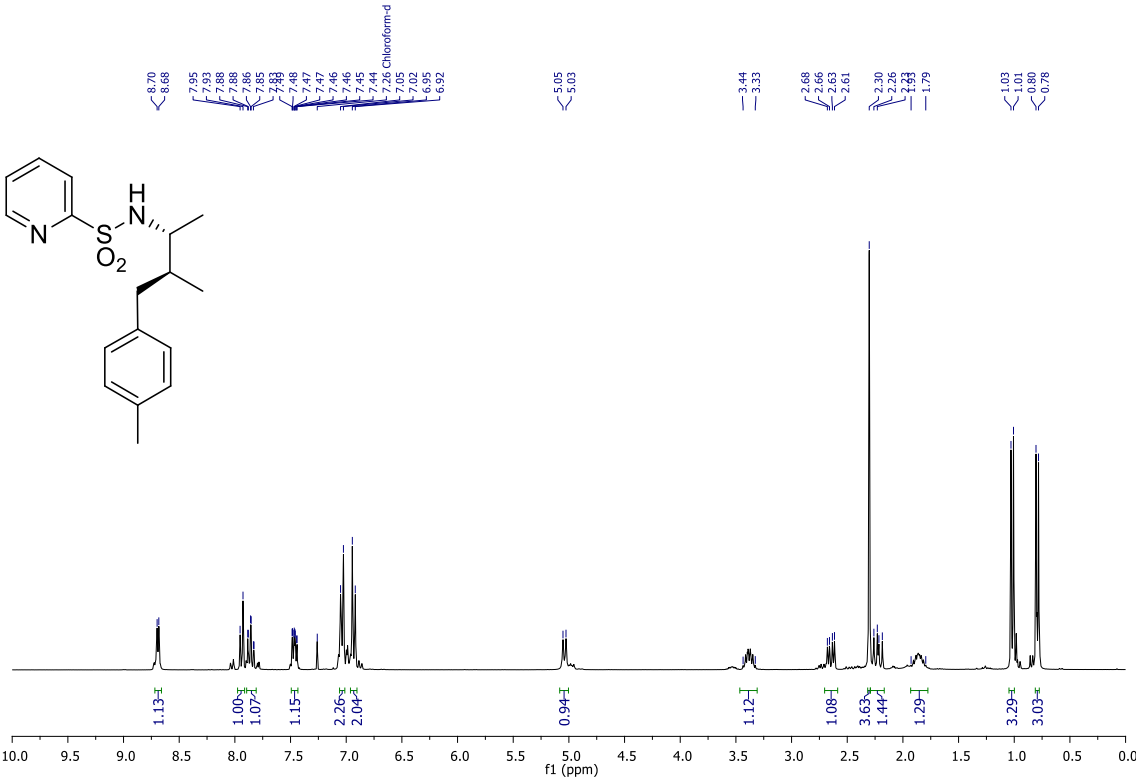


^{13}C NMR ($CDCl_3$, 75 MHz)

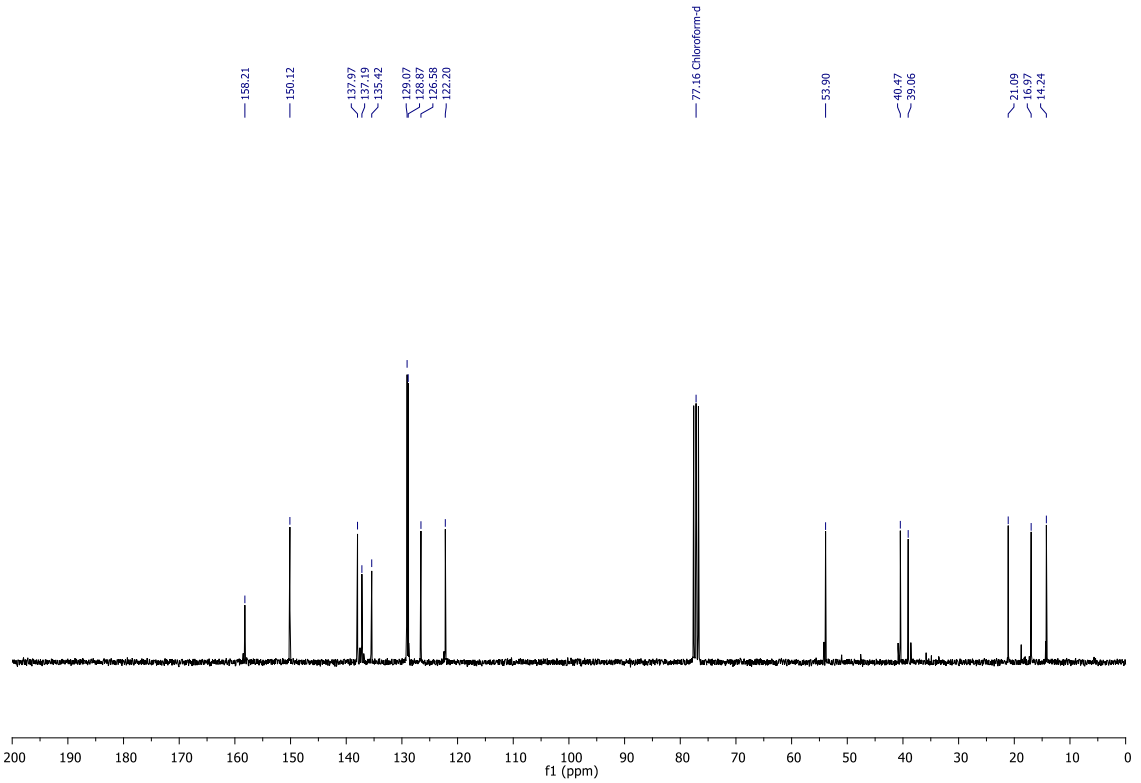


N-((2*R*,3*S*)-3-Methyl-4-(*p*-tolyl)butan-2-yl)pyridine-2-sulfonamide (6a)

^{1}H NMR ($CDCl_3$, 300 MHz)

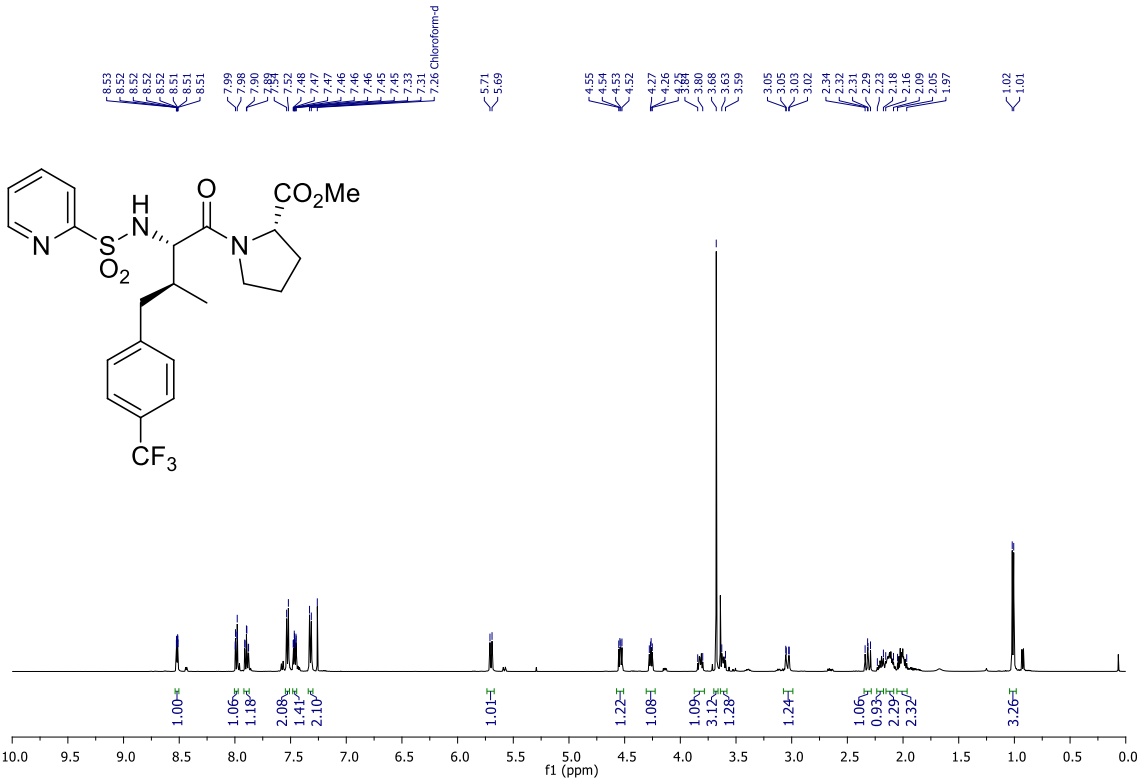


^{13}C NMR ($CDCl_3$, 75 MHz)

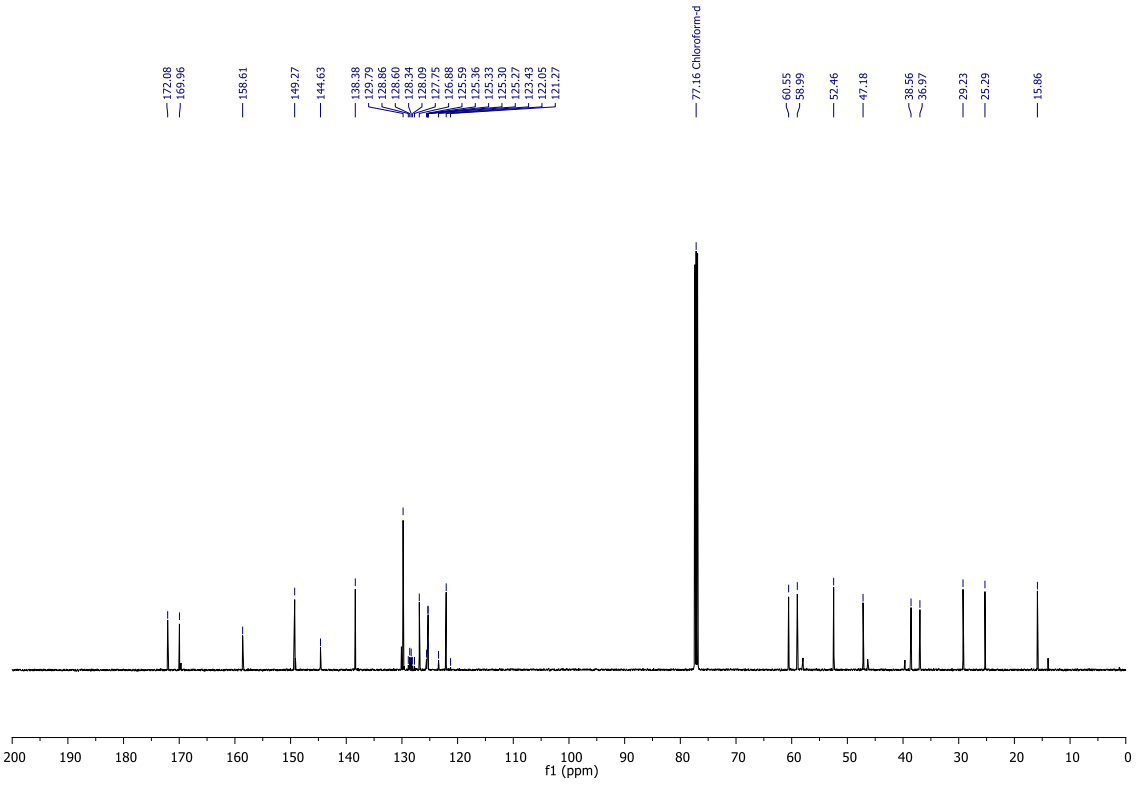


Methyl *N*-(SO_2Py)-γ-(*p*-trifluoromethylphenyl)-L-valyl-glycinate (8)

^{1}H NMR ($CDCl_3$, 300 MHz)

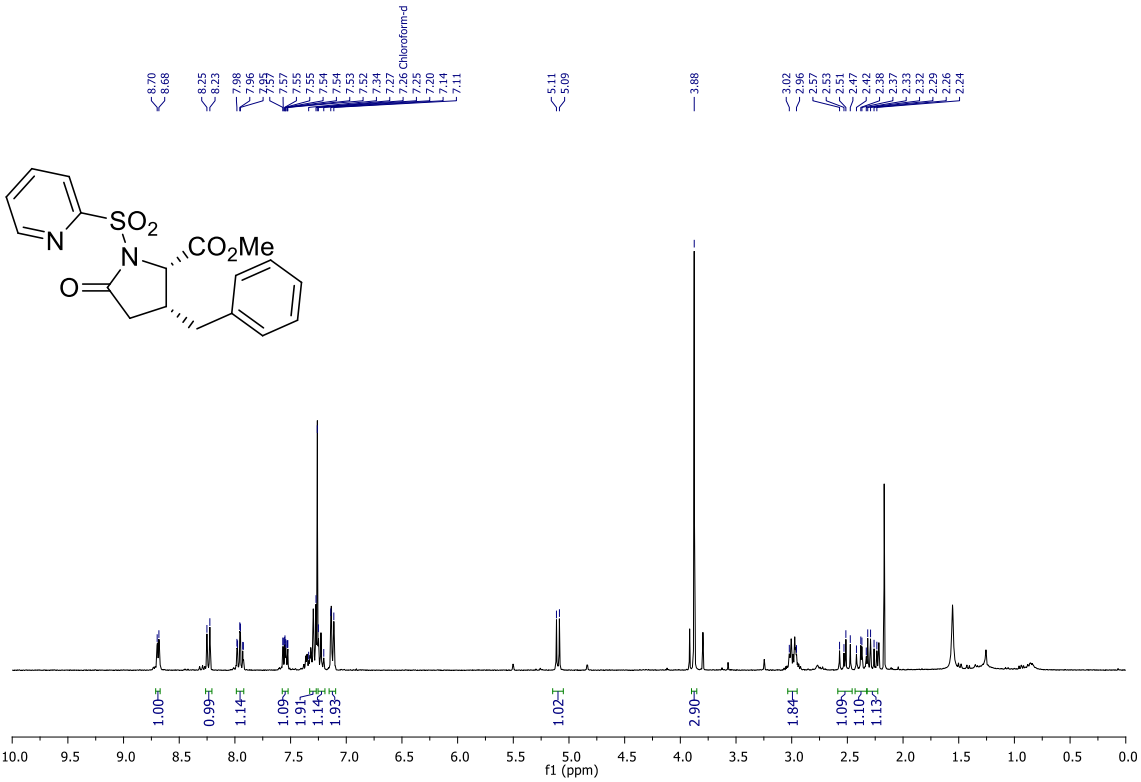


^{13}C NMR ($CDCl_3$, 75 MHz)

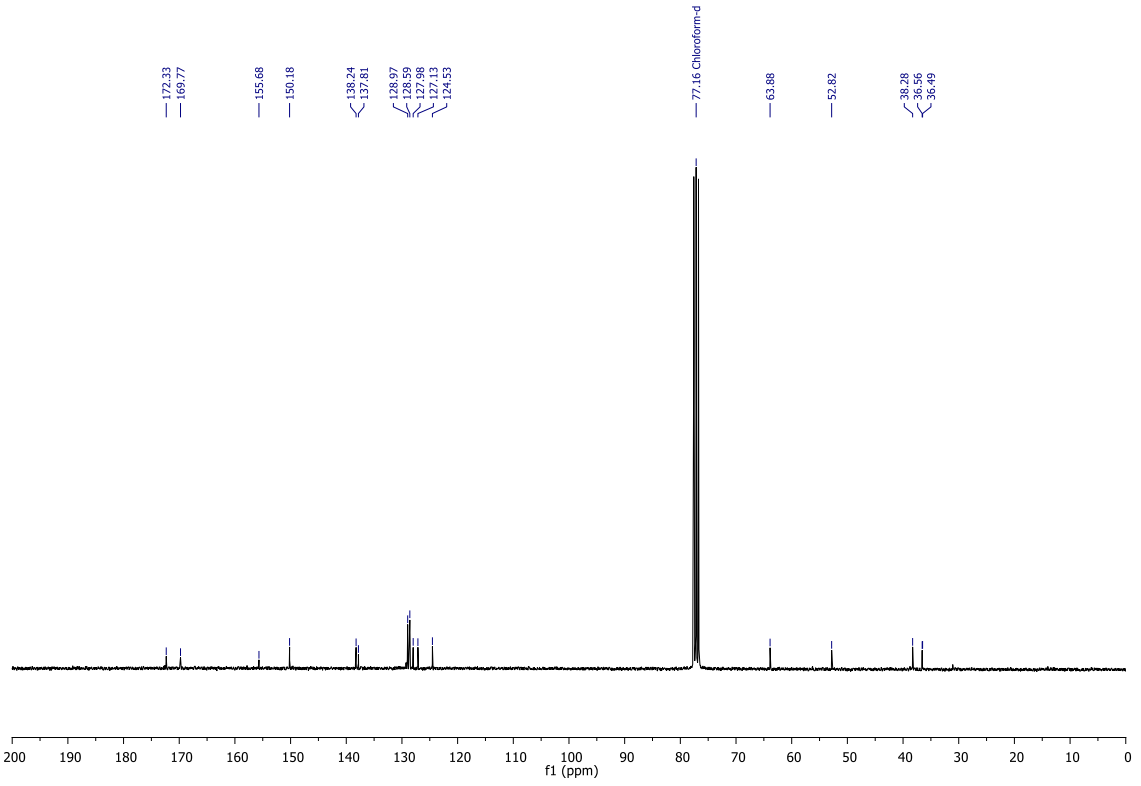


(2*S*,3*R*)-Methyl 3-benzyl-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3a)

^{1}H NMR ($CDCl_3$, 300 MHz)

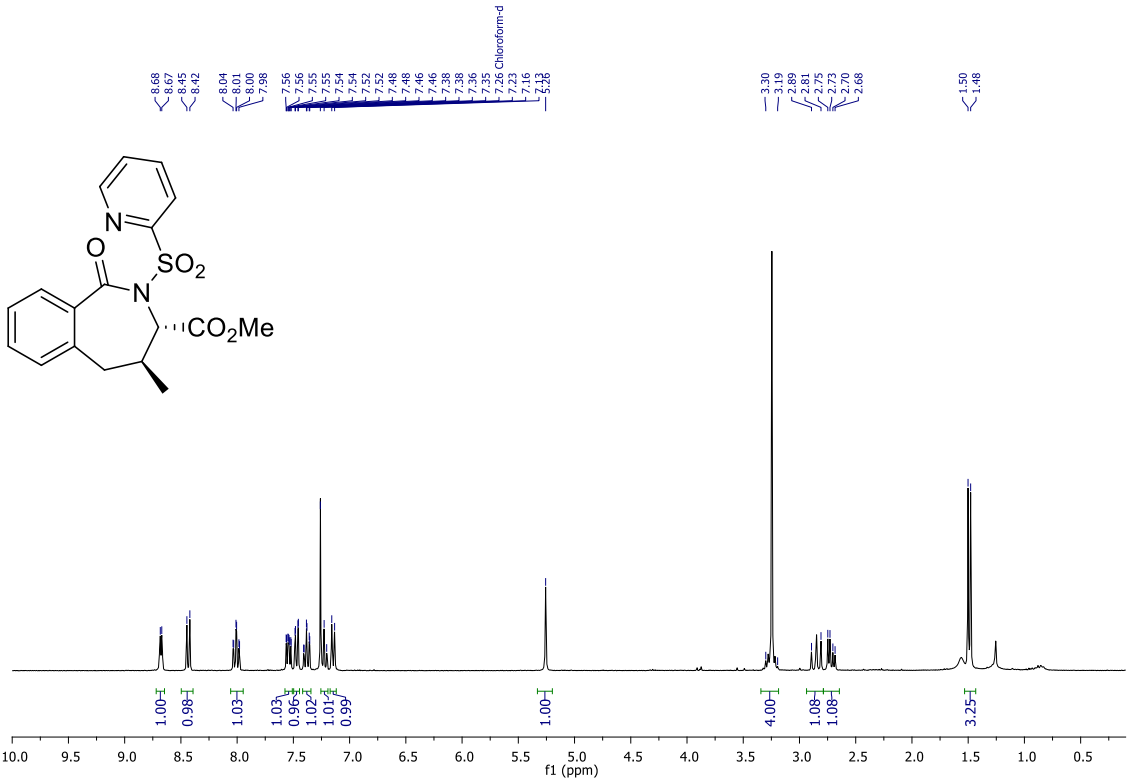


^{13}C NMR ($CDCl_3$, 75 MHz)

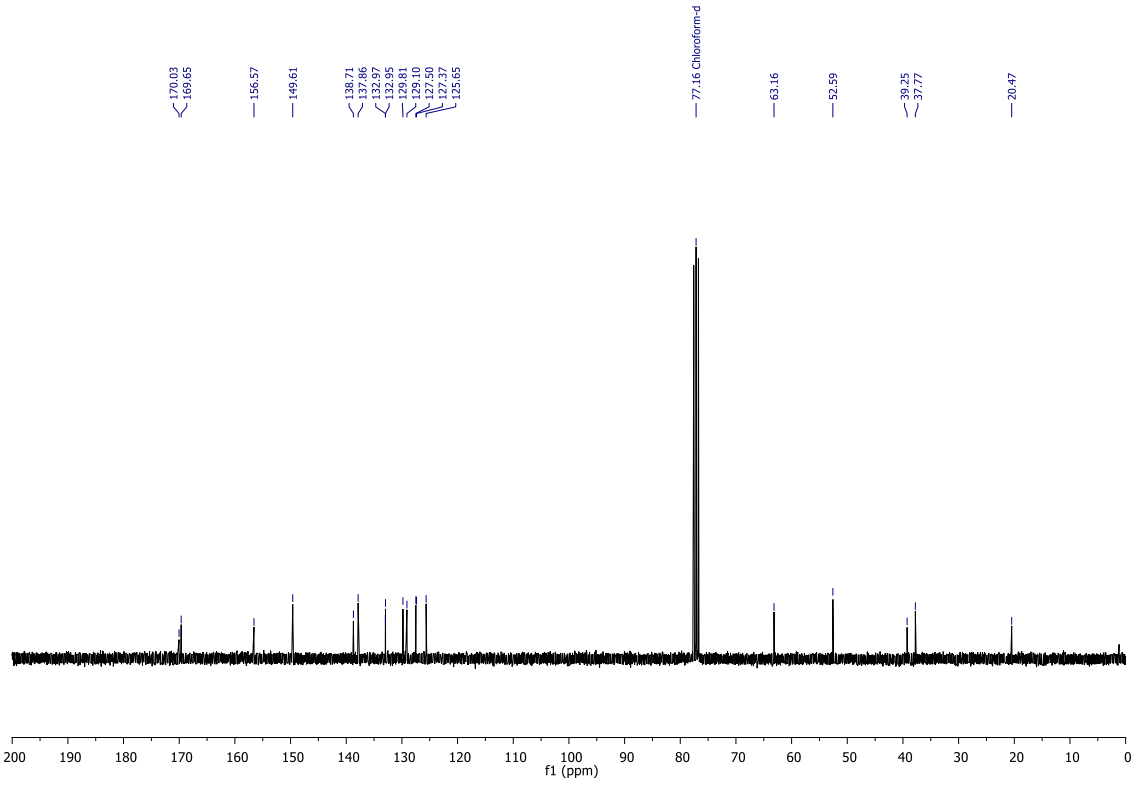


(3*S*,4*S*)-Methyl 4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2a)

^{1}H NMR ($CDCl_3$, 300 MHz)

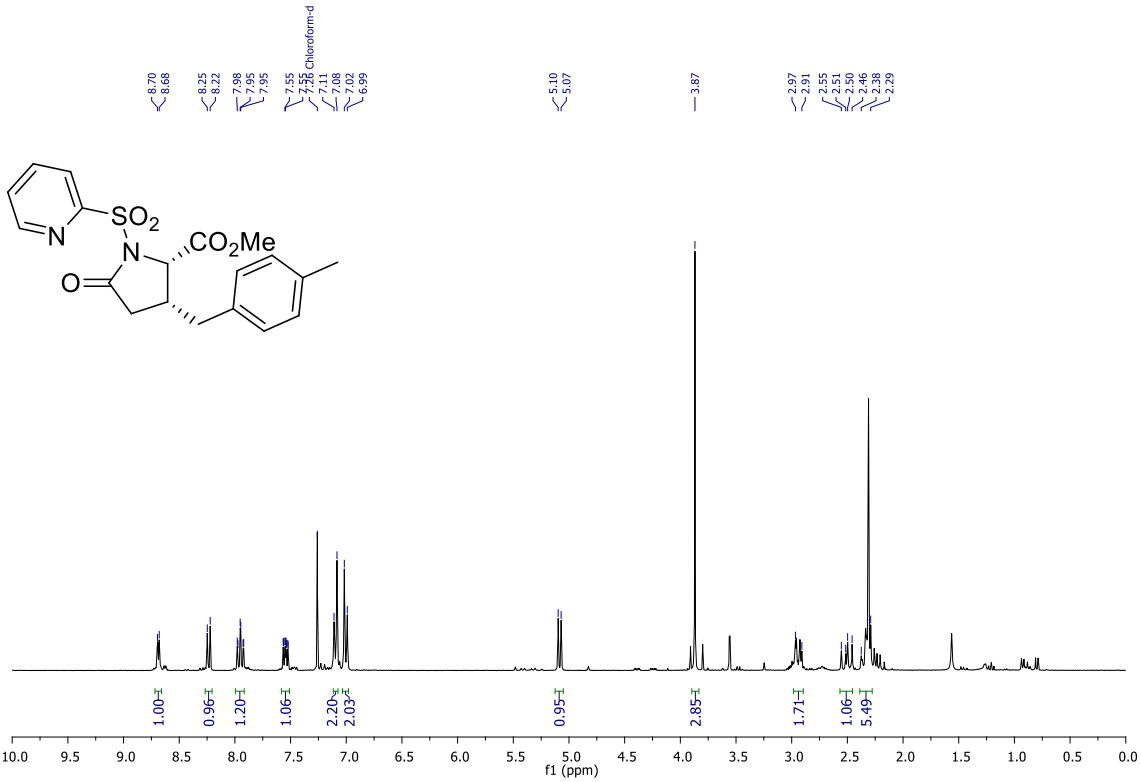


^{13}C NMR ($CDCl_3$, 75 MHz)

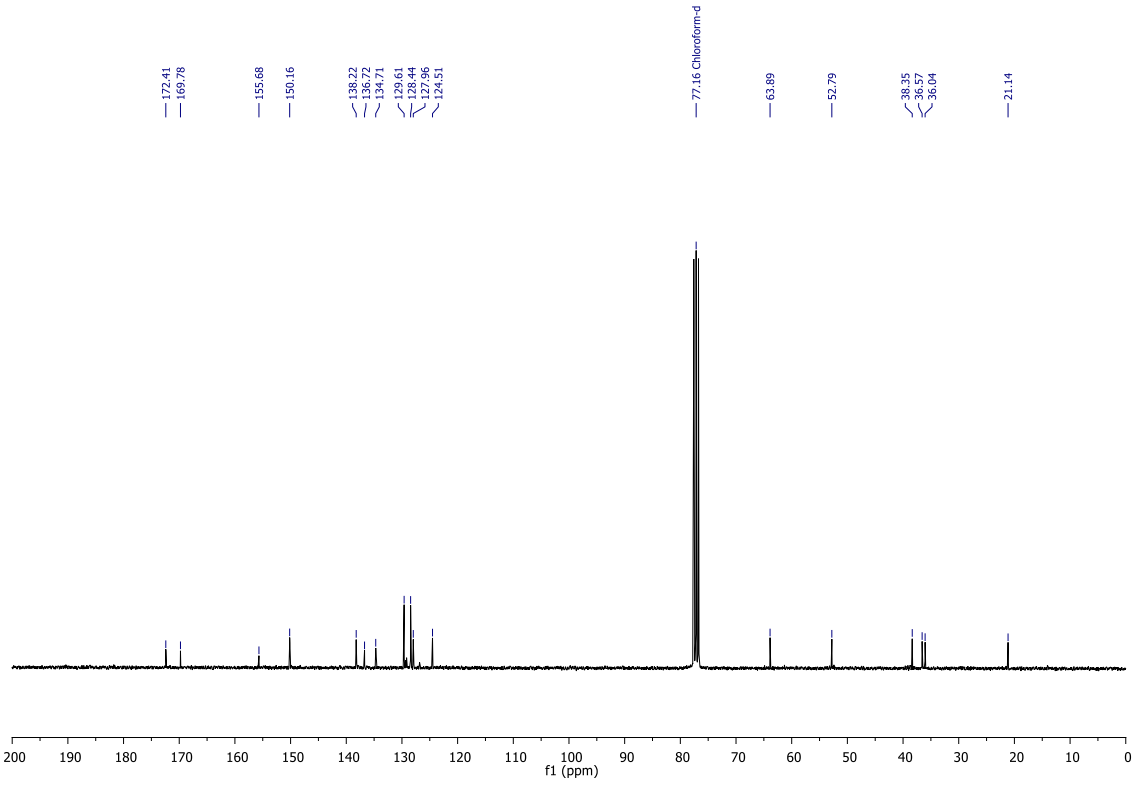


(2*S*,3*R*)-Methyl 3-(4-methylbenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3b)

^{1}H NMR ($CDCl_3$, 300 MHz)

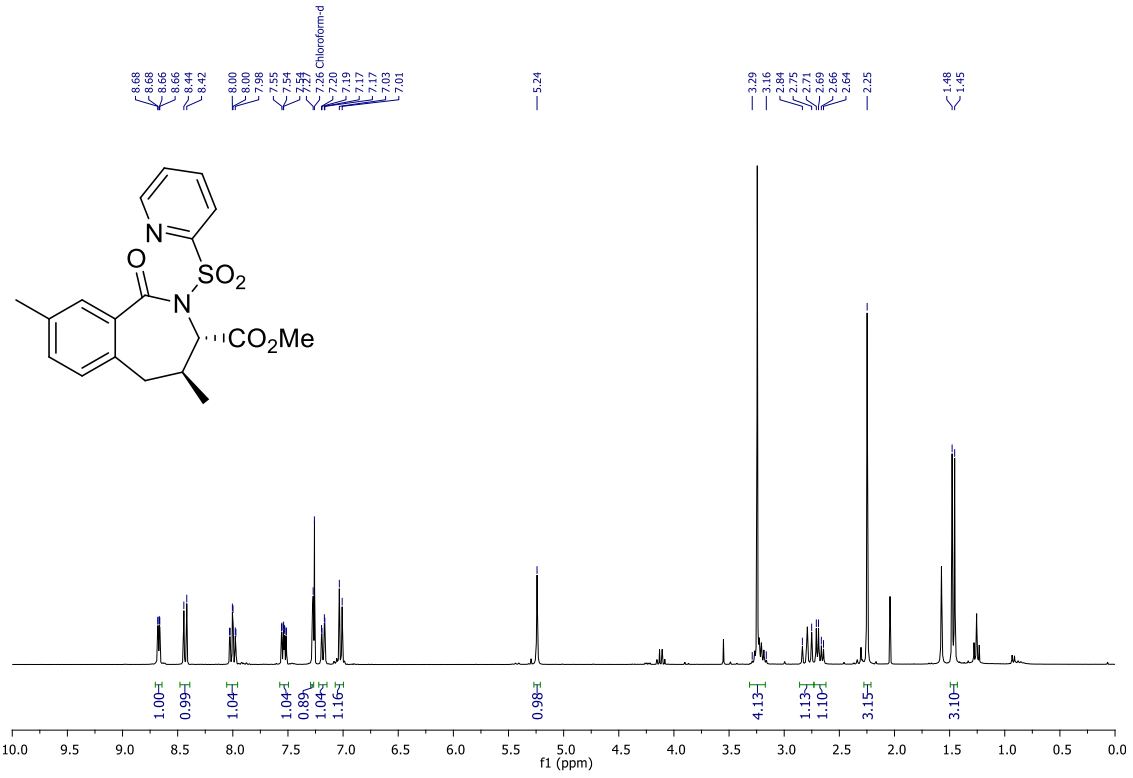


^{13}C NMR ($CDCl_3$, 75 MHz)

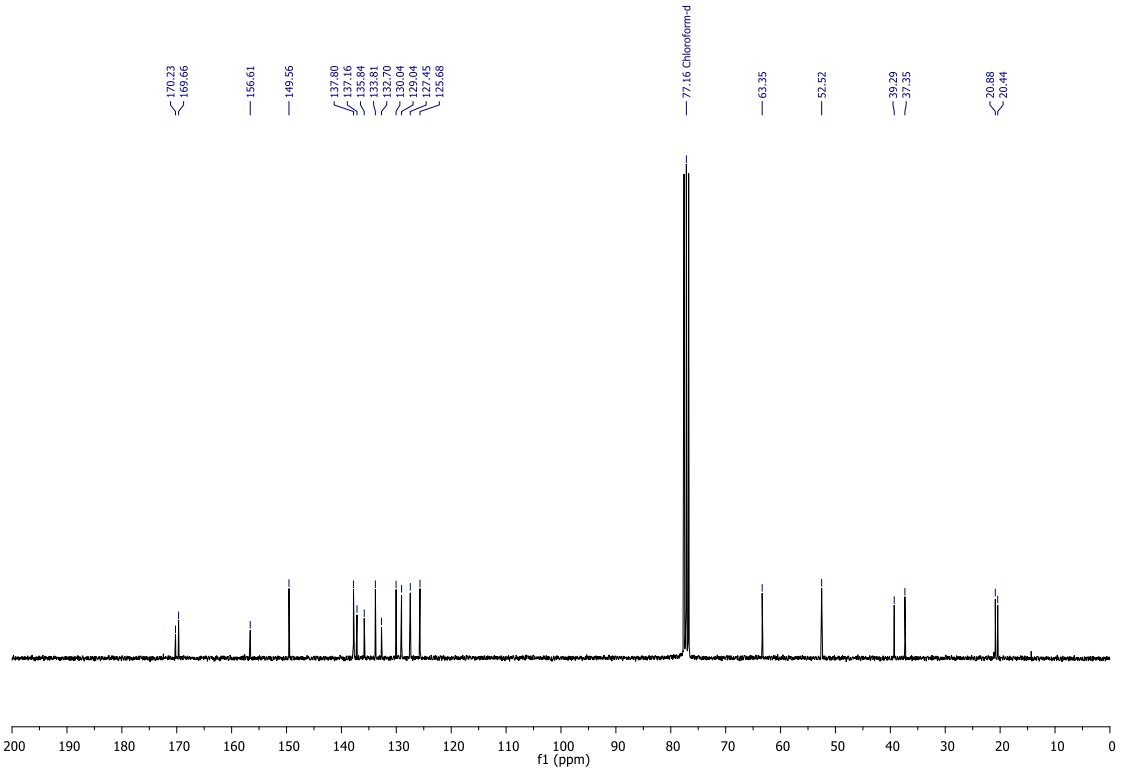


(3*S*,4*S*)-Methyl 4,8-dimethyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2b)

^{1}H NMR ($CDCl_3$, 300 MHz)

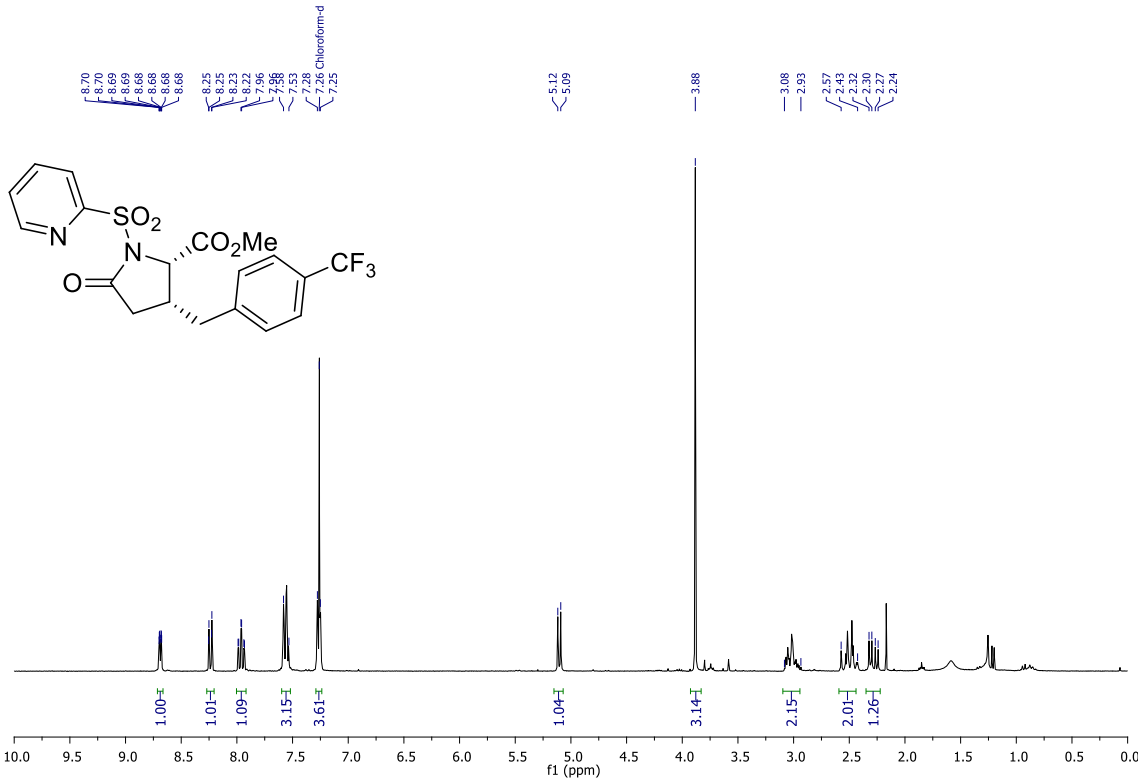


^{13}C NMR ($CDCl_3$, 75 MHz)

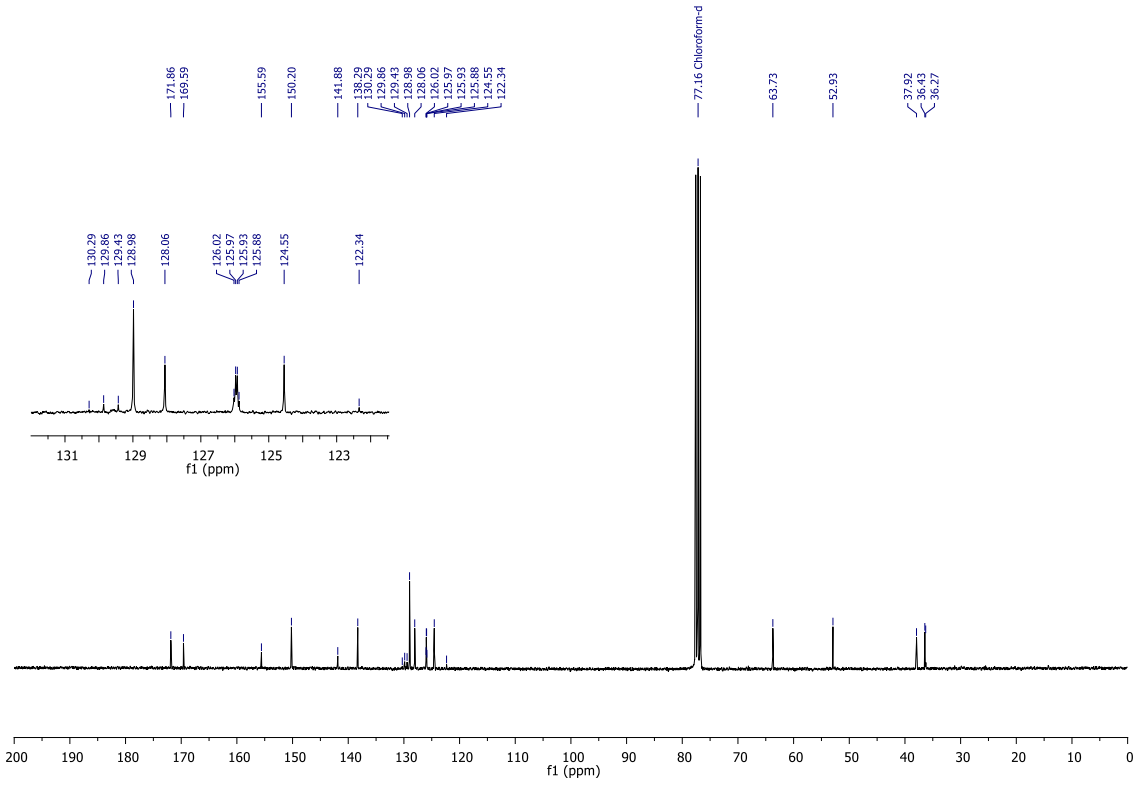


(2*S*,3*R*)-Methyl 5-oxo-1-(pyridin-2-ylsulfonyl)-3-(4-(trifluoromethyl)benzyl)pyrrolidine-2-carboxylate (3c)

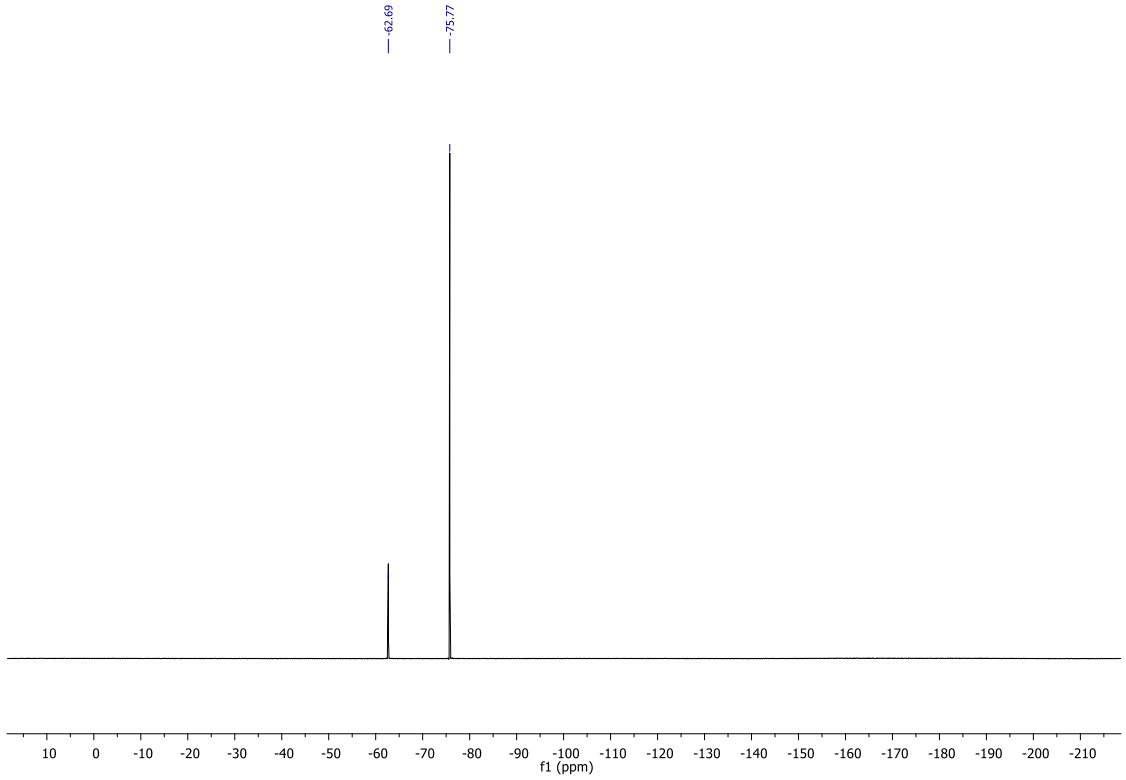
^{1}H NMR ($CDCl_3$, 300 MHz)



^{13}C NMR ($CDCl_3$, 75 MHz)

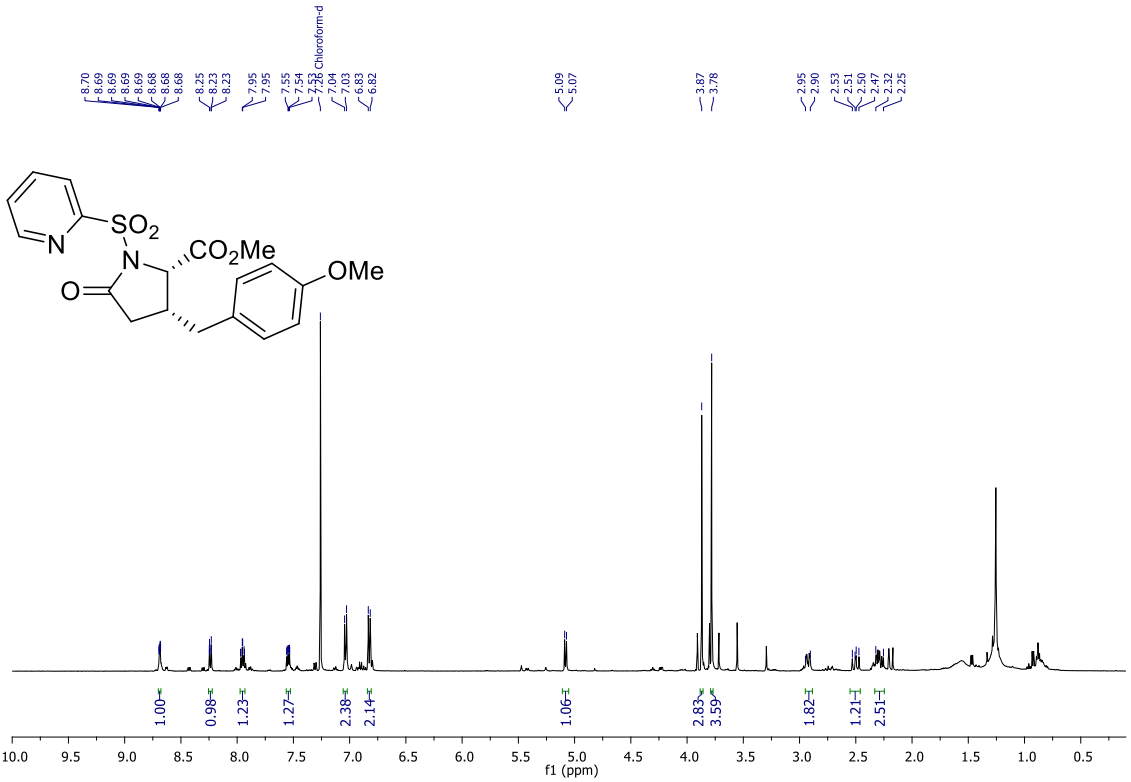


^{19}F NMR ($CDCl_3$, 282 MHz)

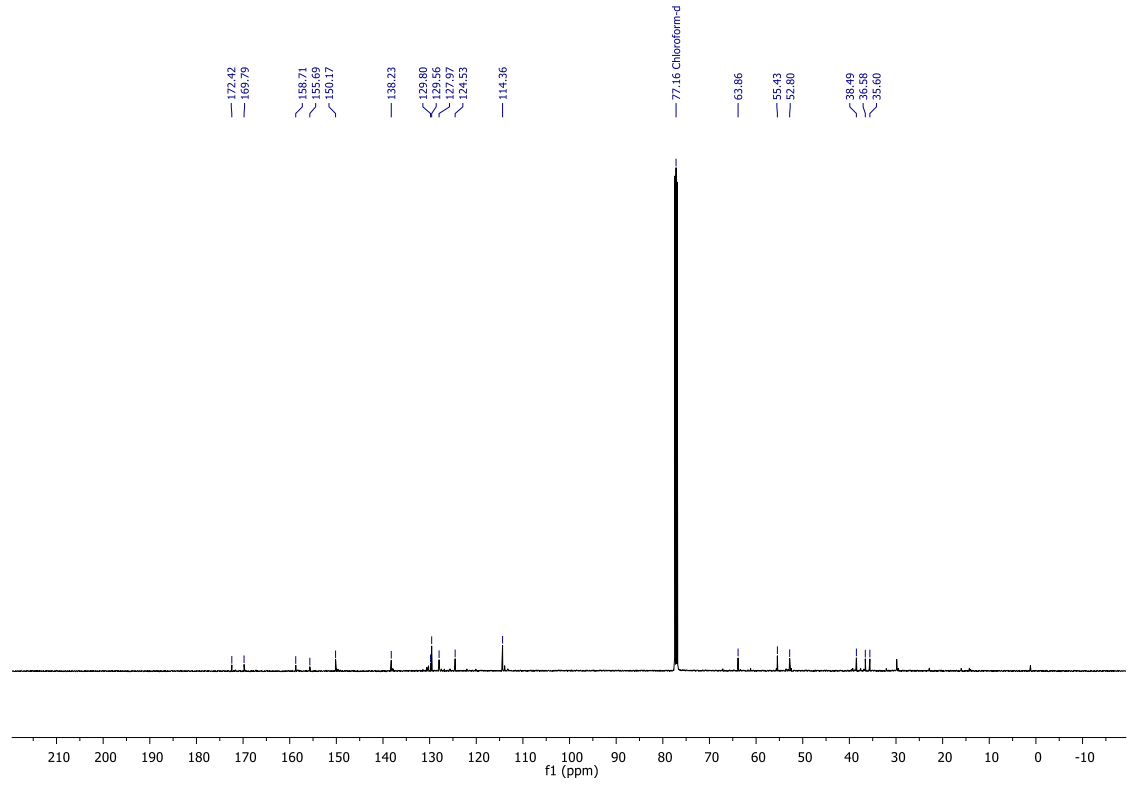


(2*S*,3*R*)-Methyl 3-(4-methoxybenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3d)

^{1}H NMR ($CDCl_3$, 500 MHz)

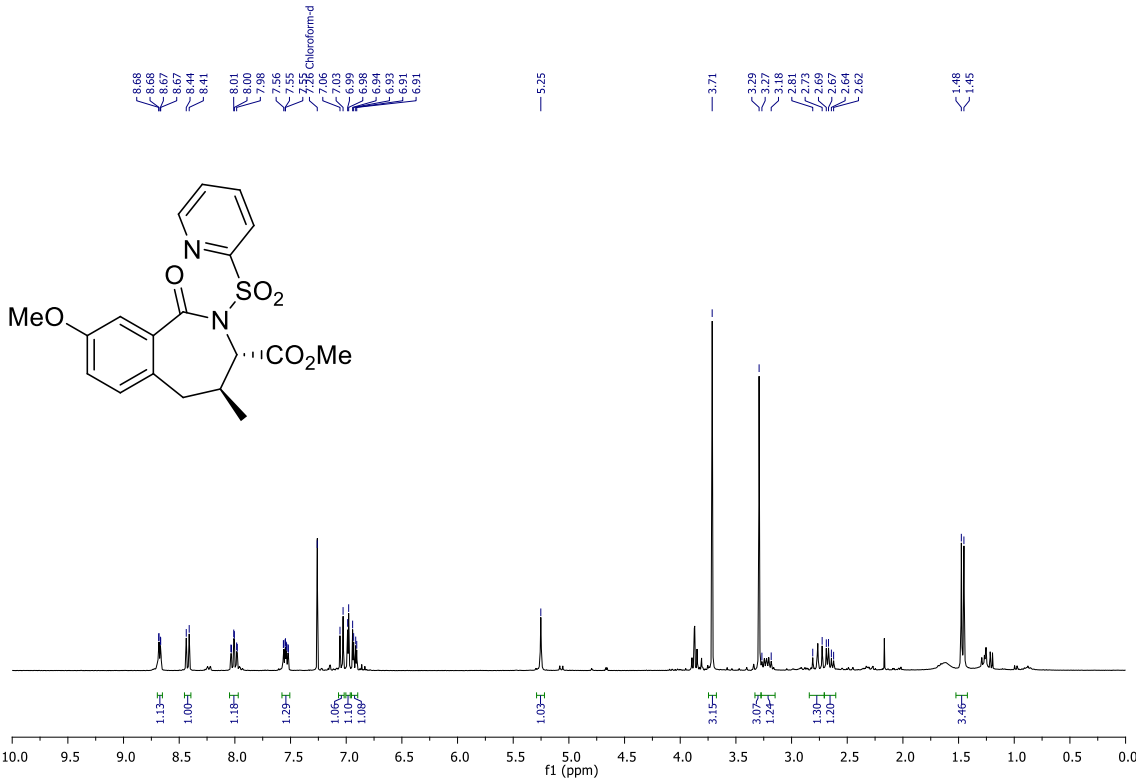


^{13}C NMR ($CDCl_3$, 126 MHz)

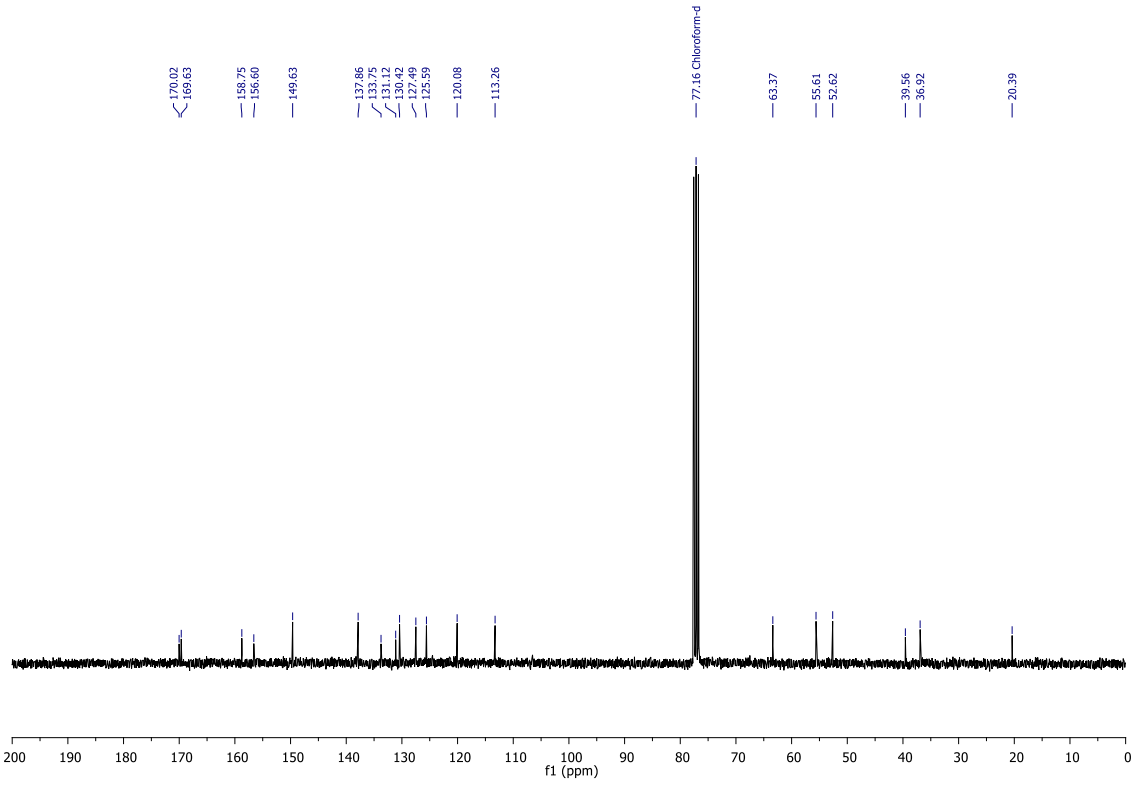


(3*S*,4*S*)-Methyl 8-methoxy-4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2d)

^{1}H NMR ($CDCl_3$, 300 MHz)

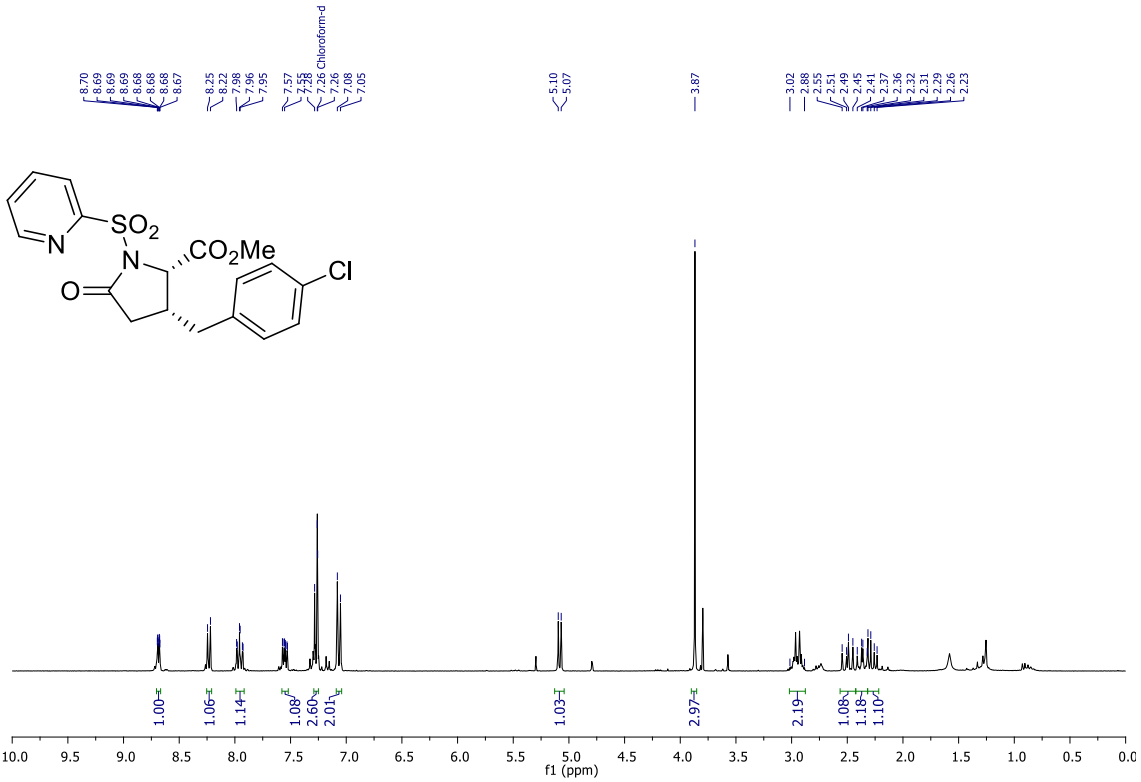


^{13}C NMR ($CDCl_3$, 75 MHz)

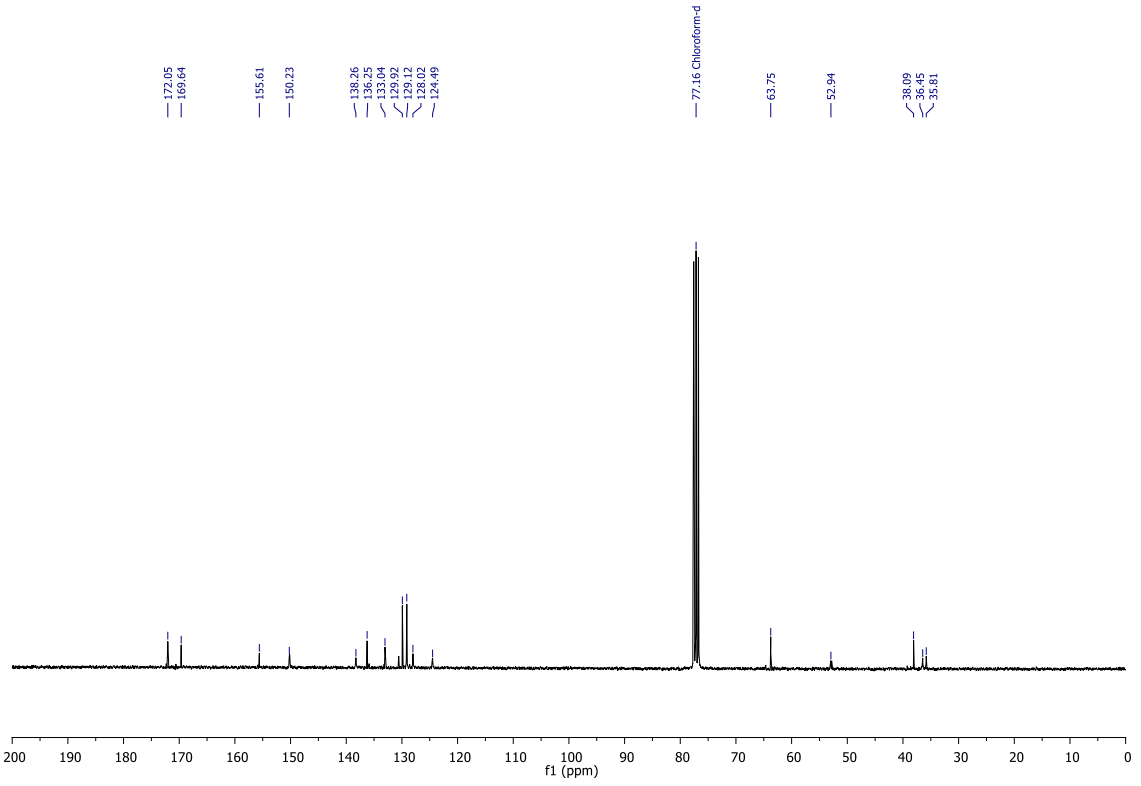


(2*S*,3*R*)-Methyl 5-oxo-1-(pyridin-2-ylsulfonyl)-3-(4-chlorobenzyl)pyrrolidine-2-carboxylate (3e)

^{1}H NMR ($CDCl_3$, 300 MHz)

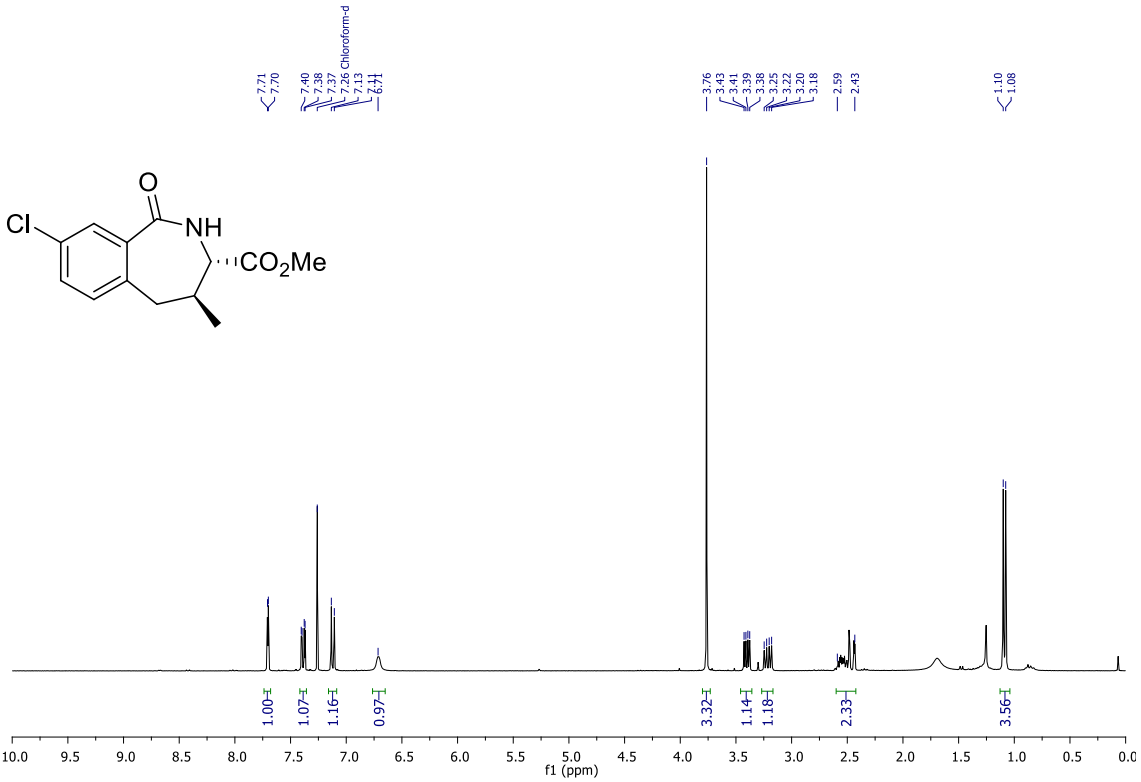


^{13}C NMR ($CDCl_3$, 75 MHz)

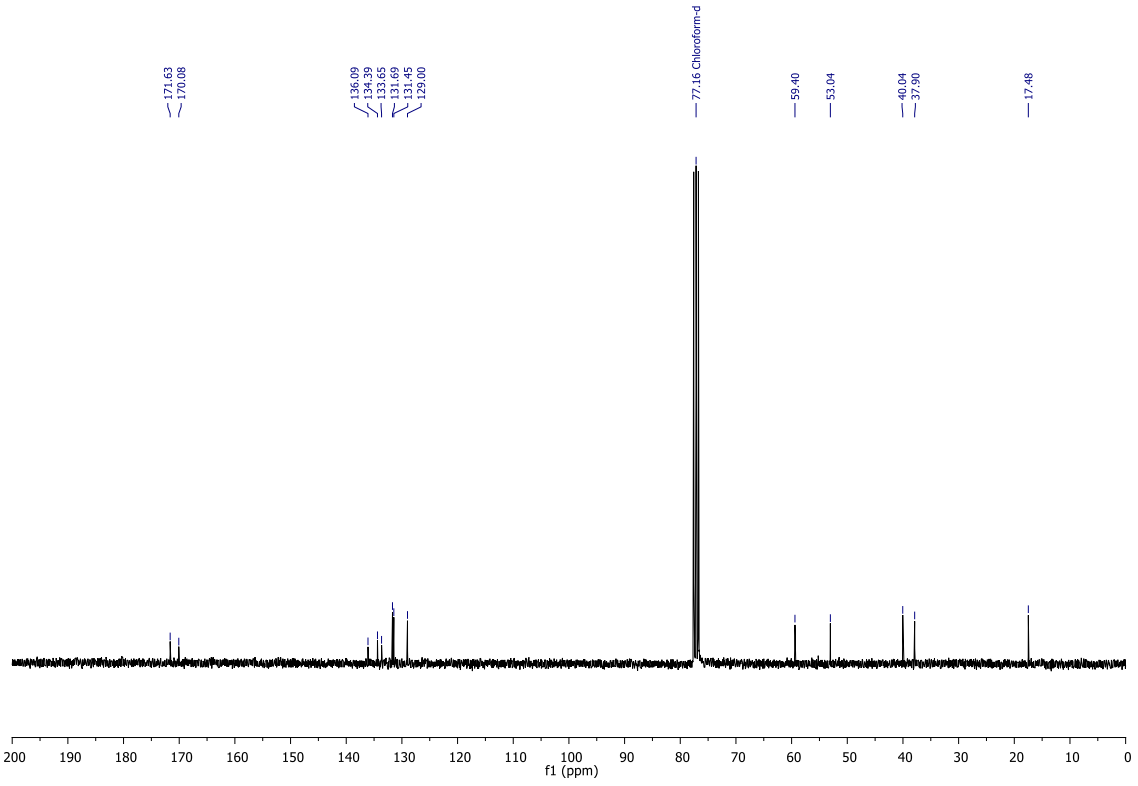


(3*S*,4*S*)-Methyl 8-chloro-4-methyl-1-oxo-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2e)

^{1}H NMR ($CDCl_3$, 300 MHz)

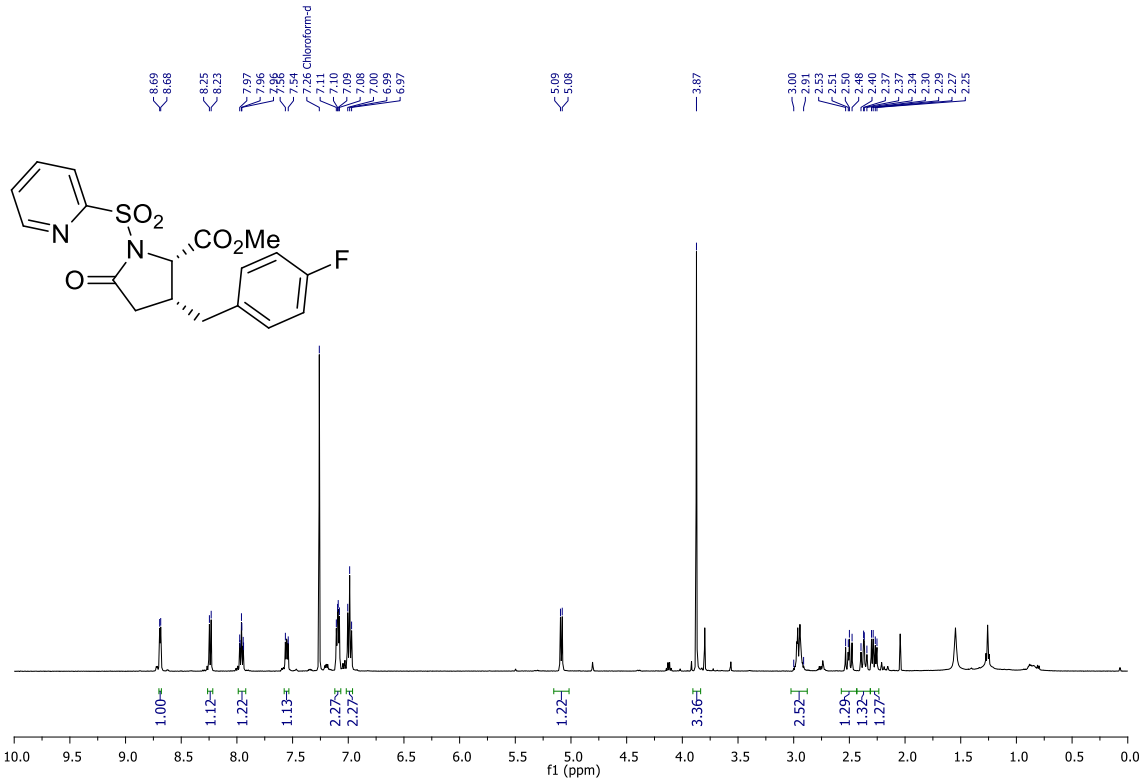


^{13}C NMR ($CDCl_3$, 75 MHz)

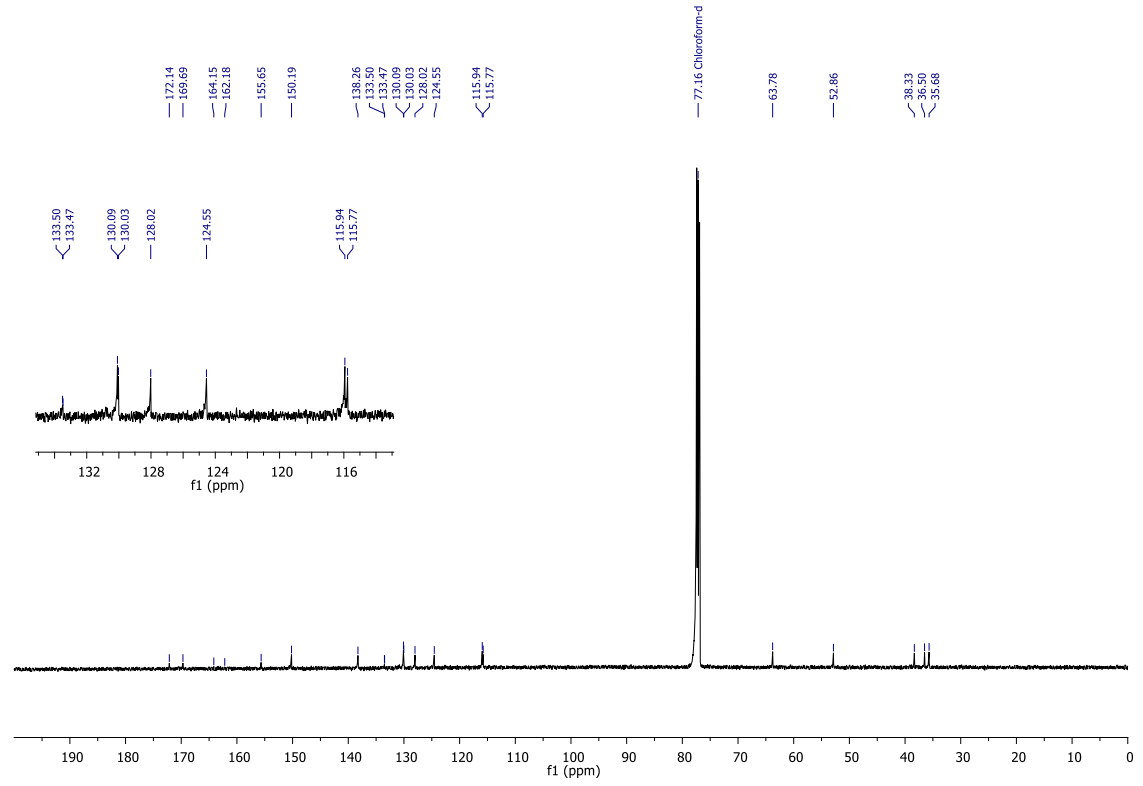


(2*S*,3*R*)-Methyl 3-(4-fluorobenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3f)

^{1}H NMR ($CDCl_3$, 500 MHz)

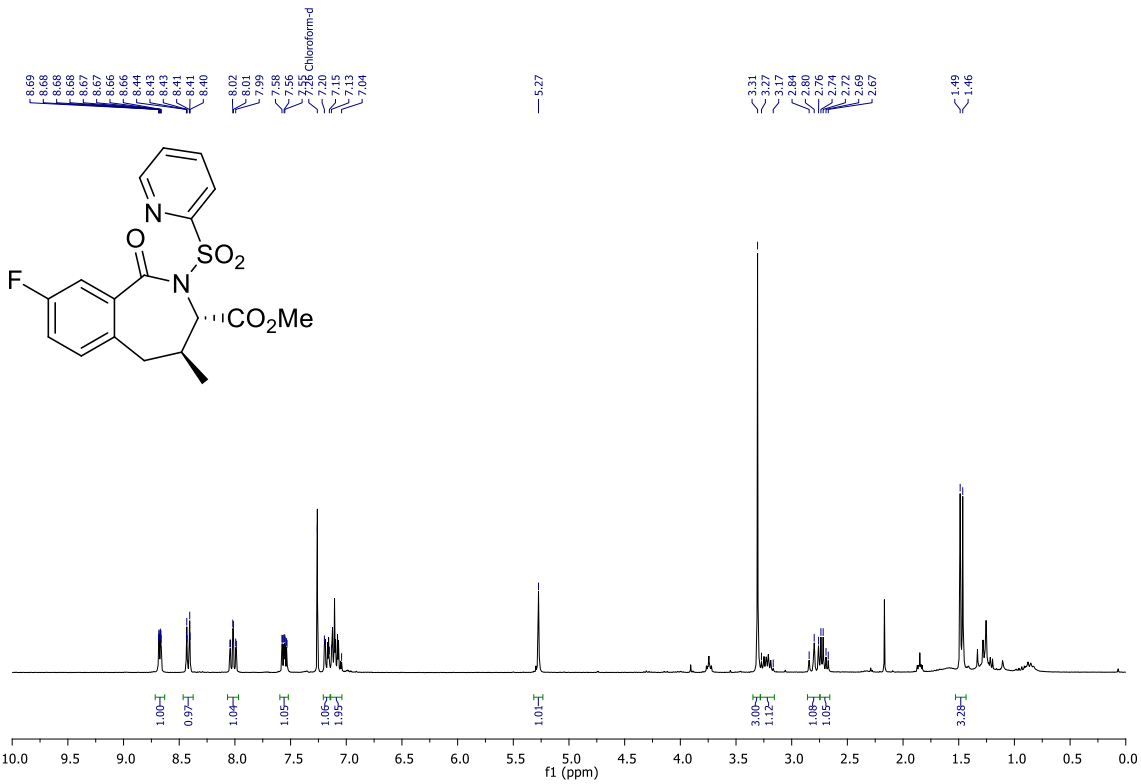


^{13}C NMR ($CDCl_3$, 126 MHz)

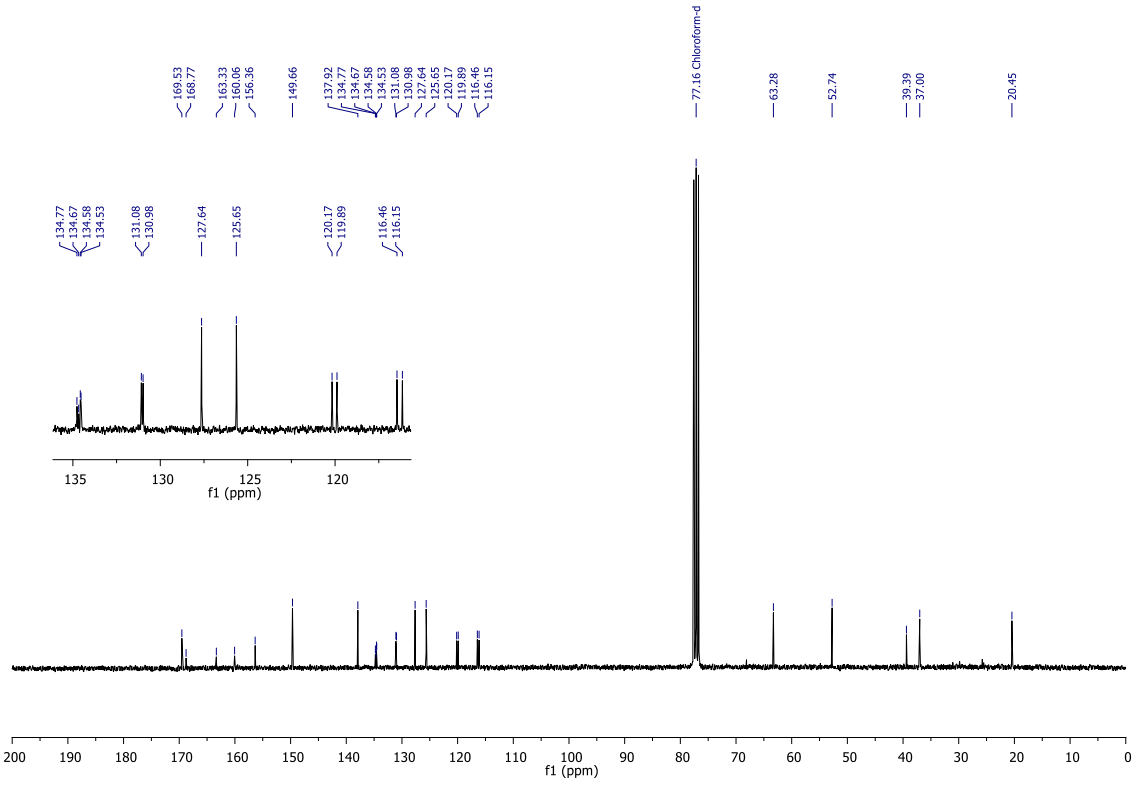


(3*S*,4*S*)-Methyl 8-fluoro-4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2f)

^{1}H NMR ($CDCl_3$, 300 MHz)

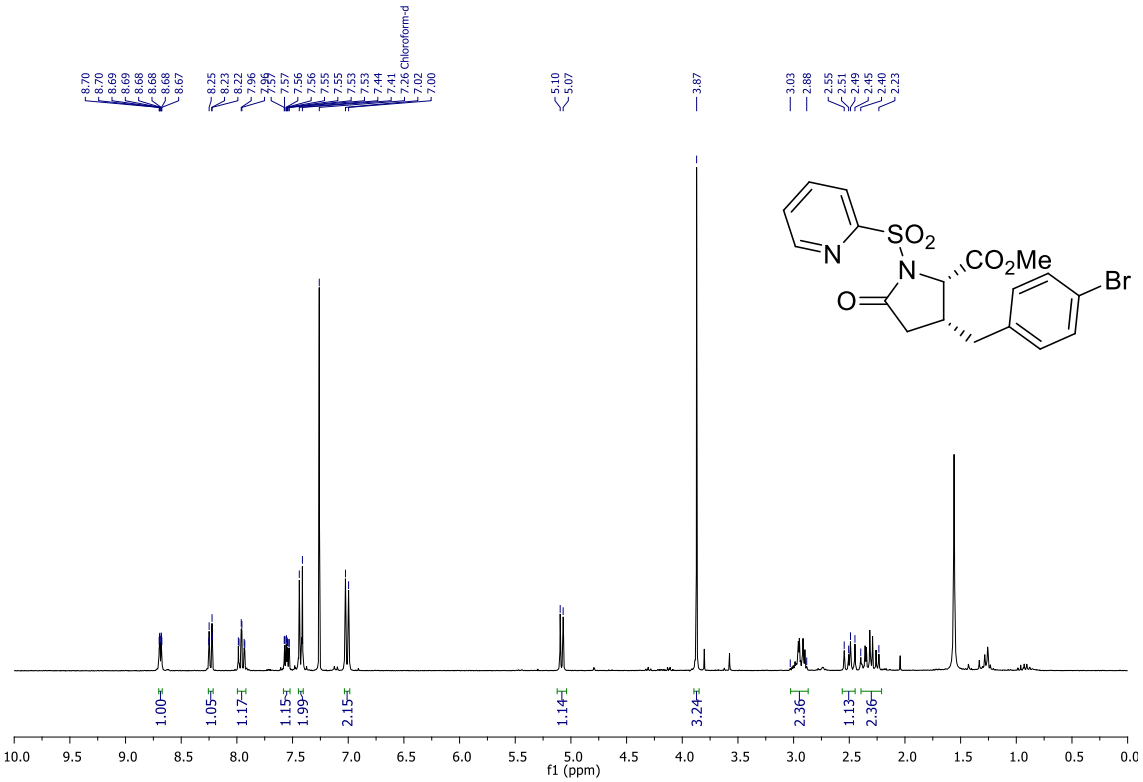


^{13}C NMR ($CDCl_3$, 75 MHz)

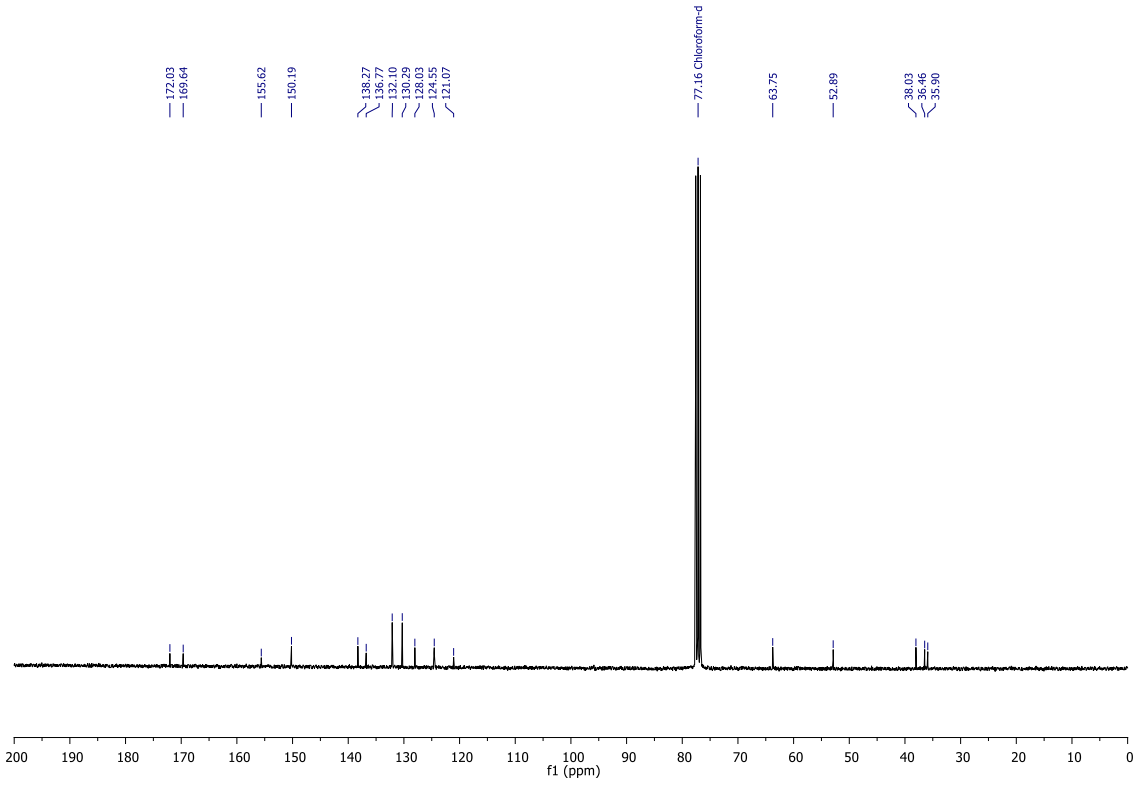


(2*S*,3*R*)-Methyl 5-oxo-1-(pyridin-2-ylsulfonyl)-3-(4-bromobenzyl)pyrrolidine-2-carboxylate (3g)

^{1}H NMR ($CDCl_3$, 300 MHz)

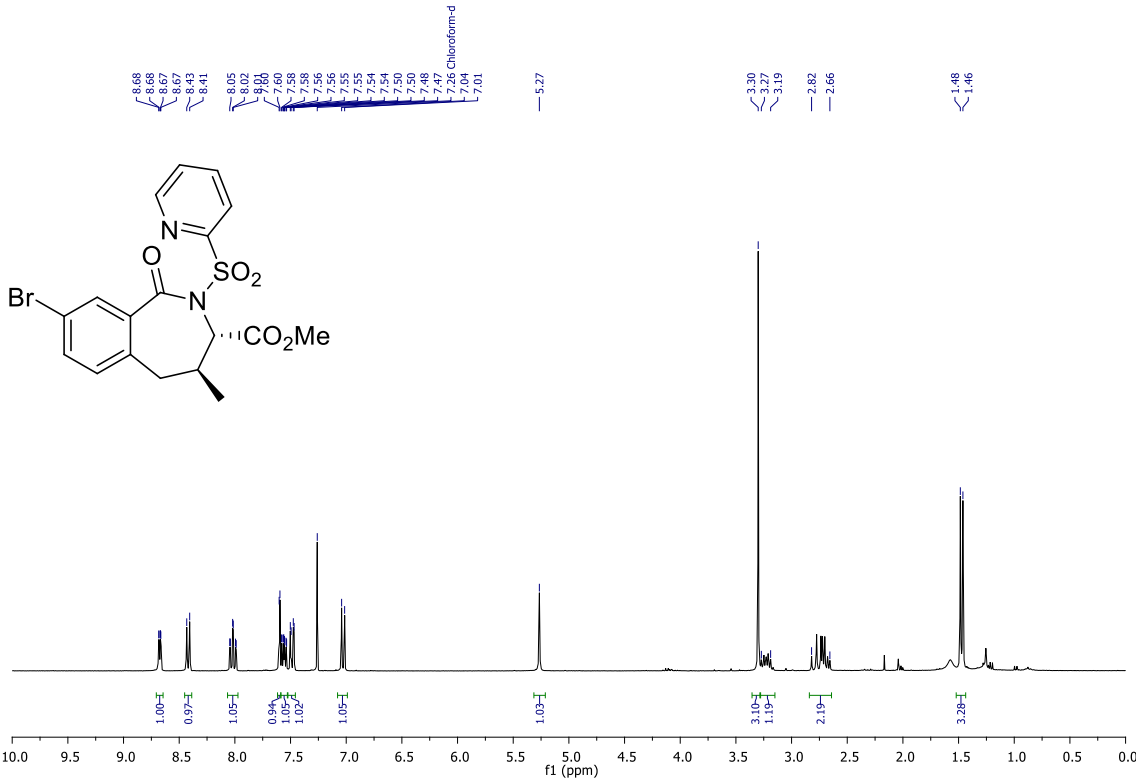


^{13}C NMR ($CDCl_3$, 75 MHz)

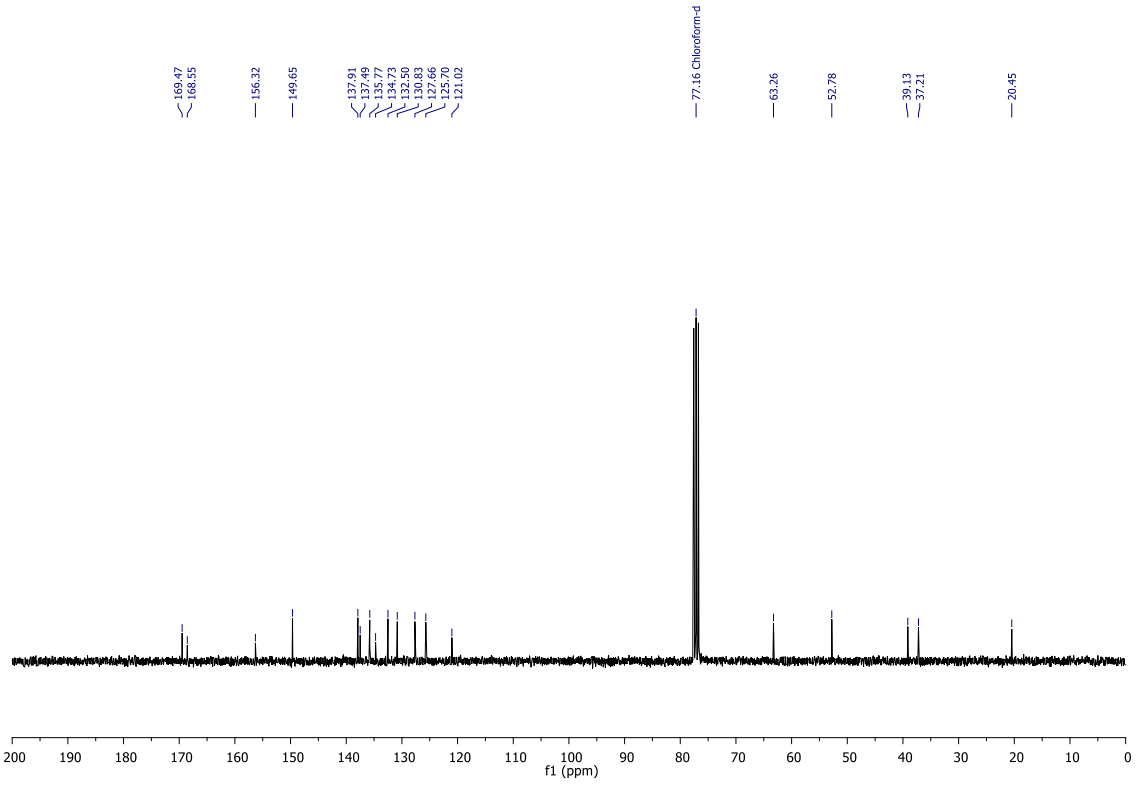


(3*S*,4*S*)-Methyl 8-bromo-4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2g)

^{1}H NMR ($CDCl_3$, 300 MHz)

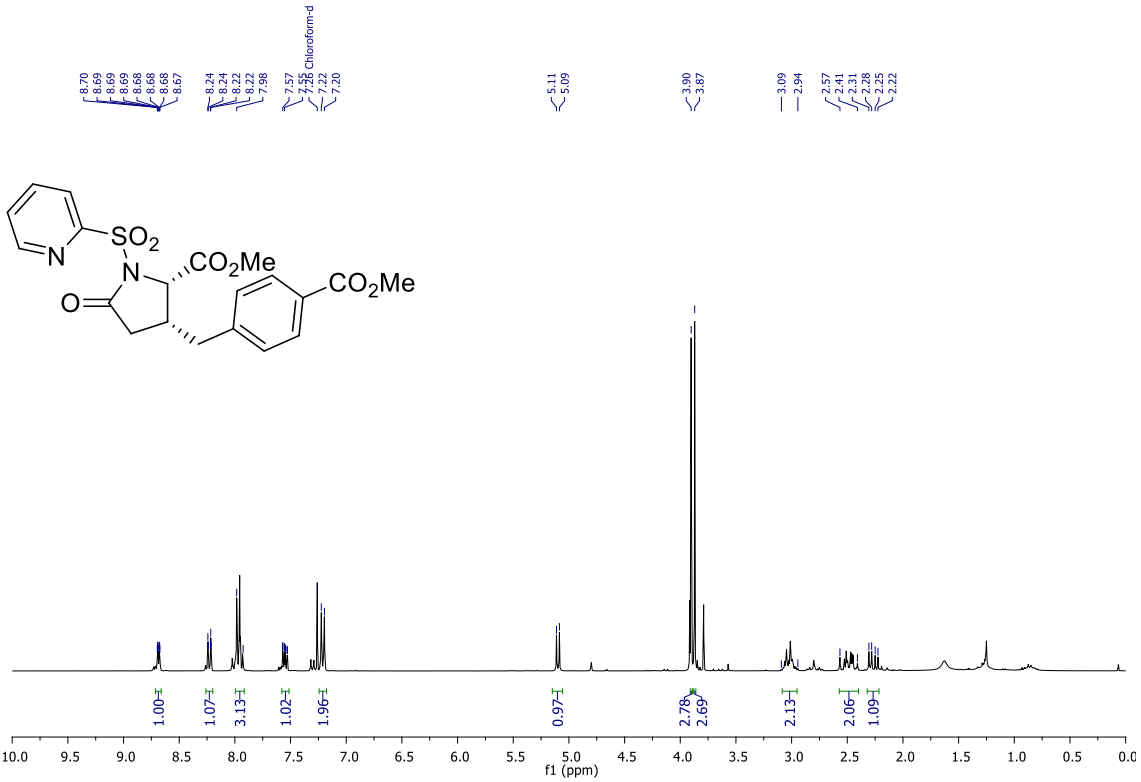


^{13}C NMR ($CDCl_3$, 75 MHz)

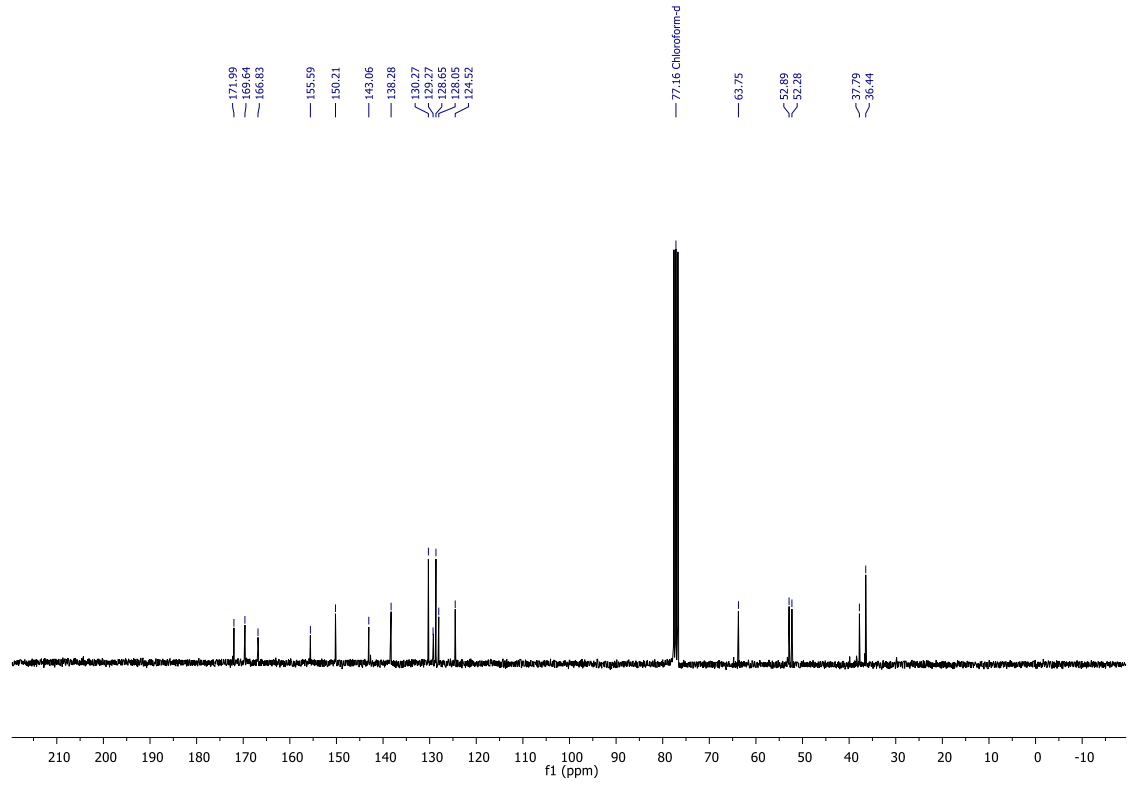


(2*S*,3*R*)-Methyl 3-(4-(methoxycarbonyl)benzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3h)

^{1}H NMR ($CDCl_3$, 300 MHz)

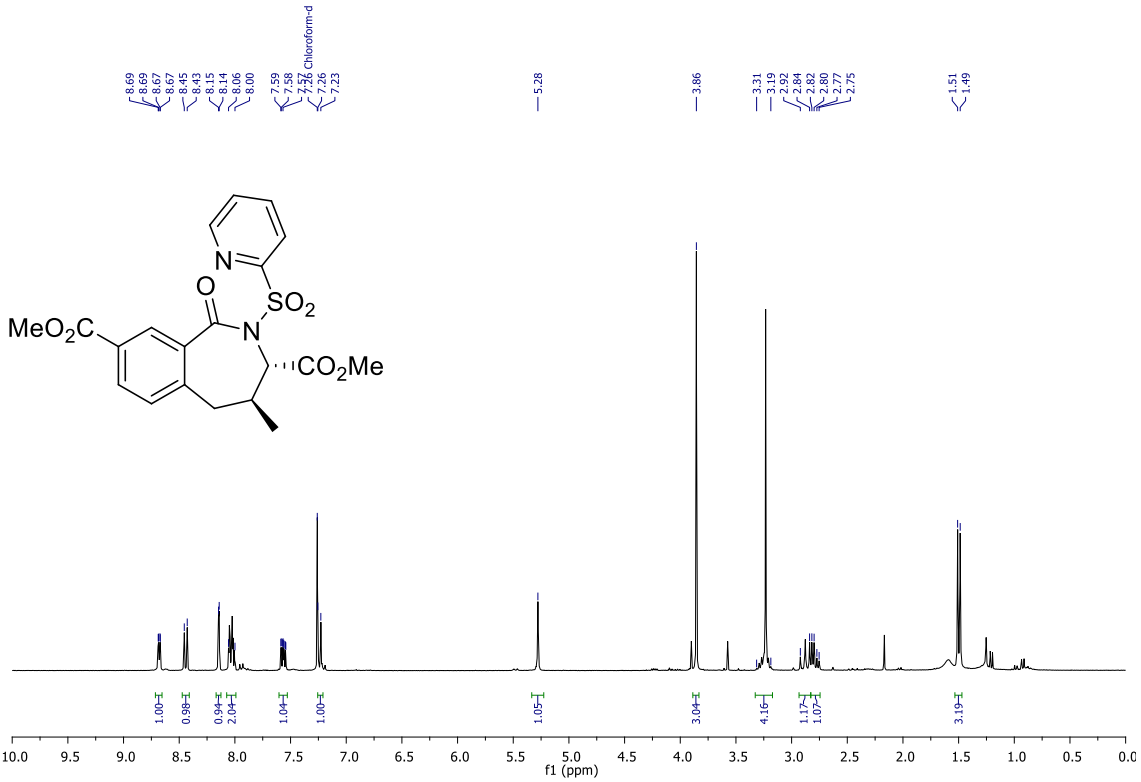


^{13}C NMR ($CDCl_3$, 75 MHz)

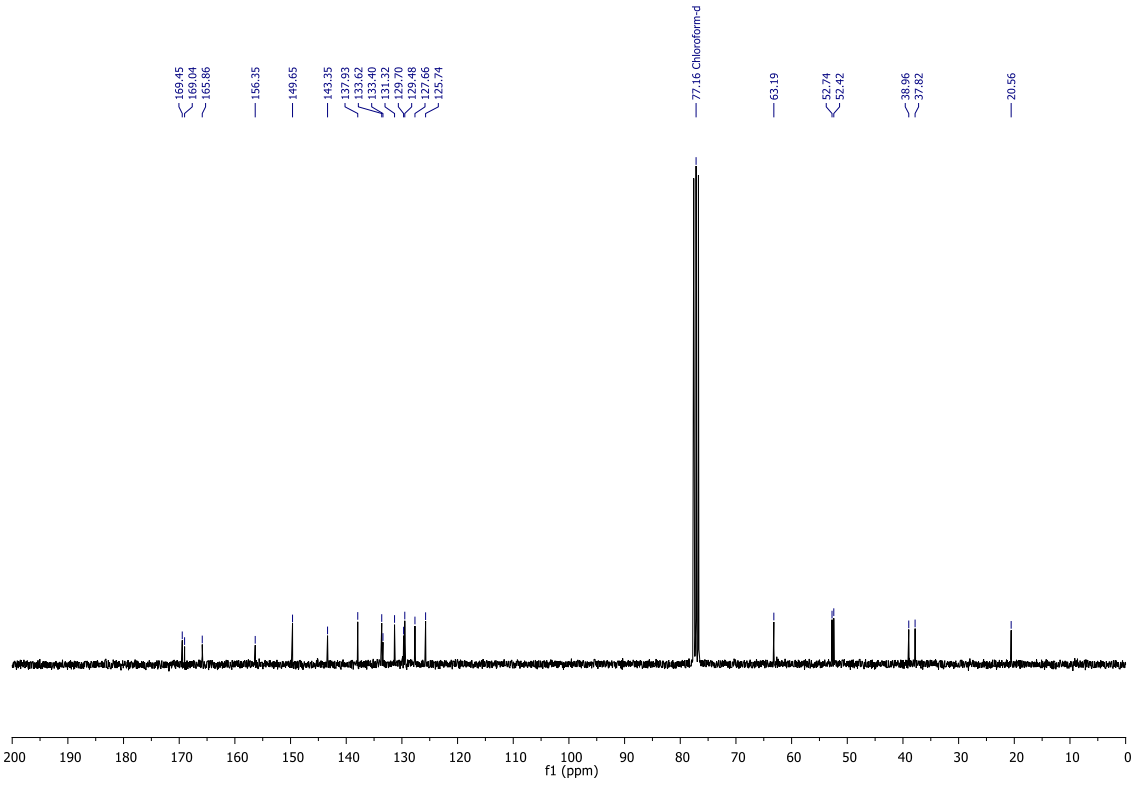


(3*S*,4*S*)-Dimethyl 4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3,8-dicarboxylate (2h)

^{1}H NMR ($CDCl_3$, 300 MHz)

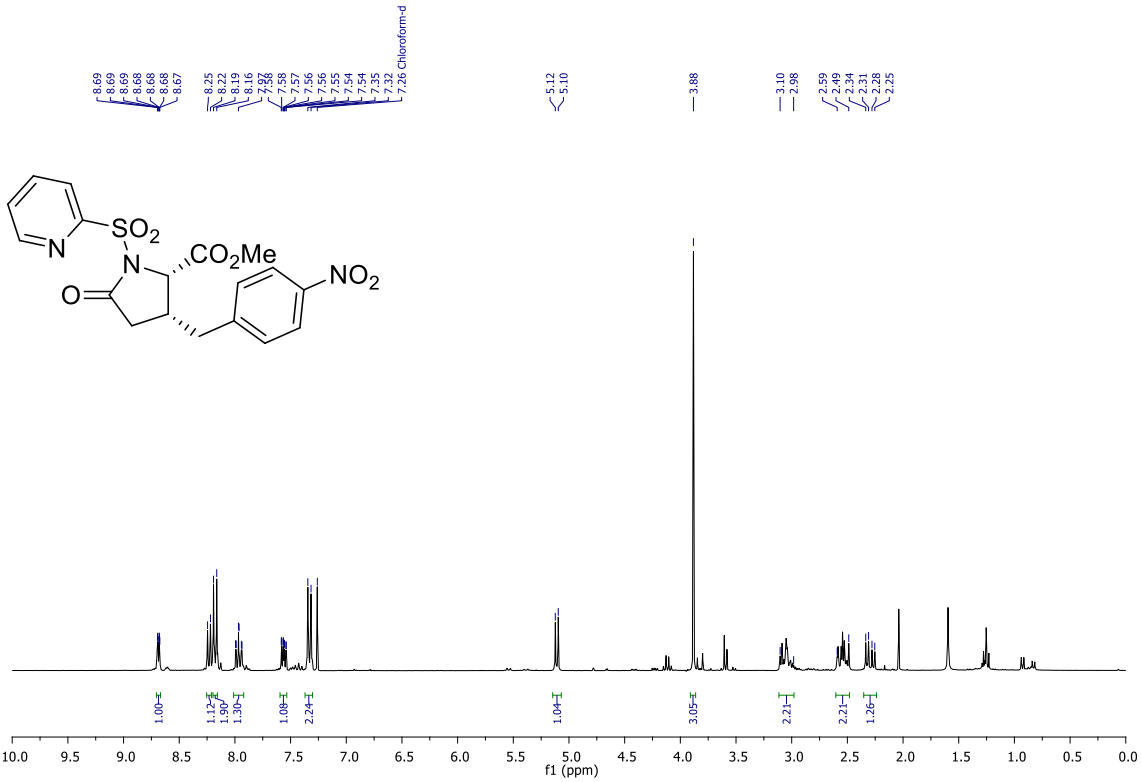


^{13}C NMR ($CDCl_3$, 75 MHz)

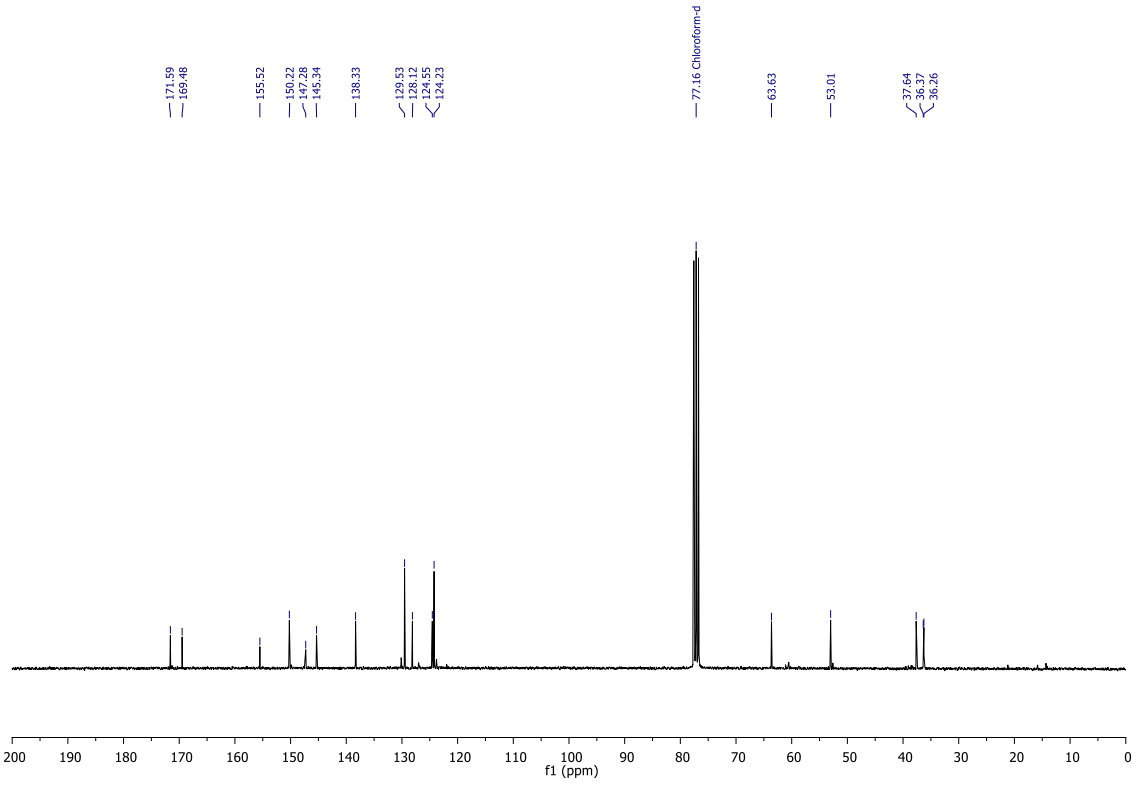


(2*S*,3*R*)-Methyl 3-(4-nitrobenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3i)

^{1}H NMR ($CDCl_3$, 300 MHz)

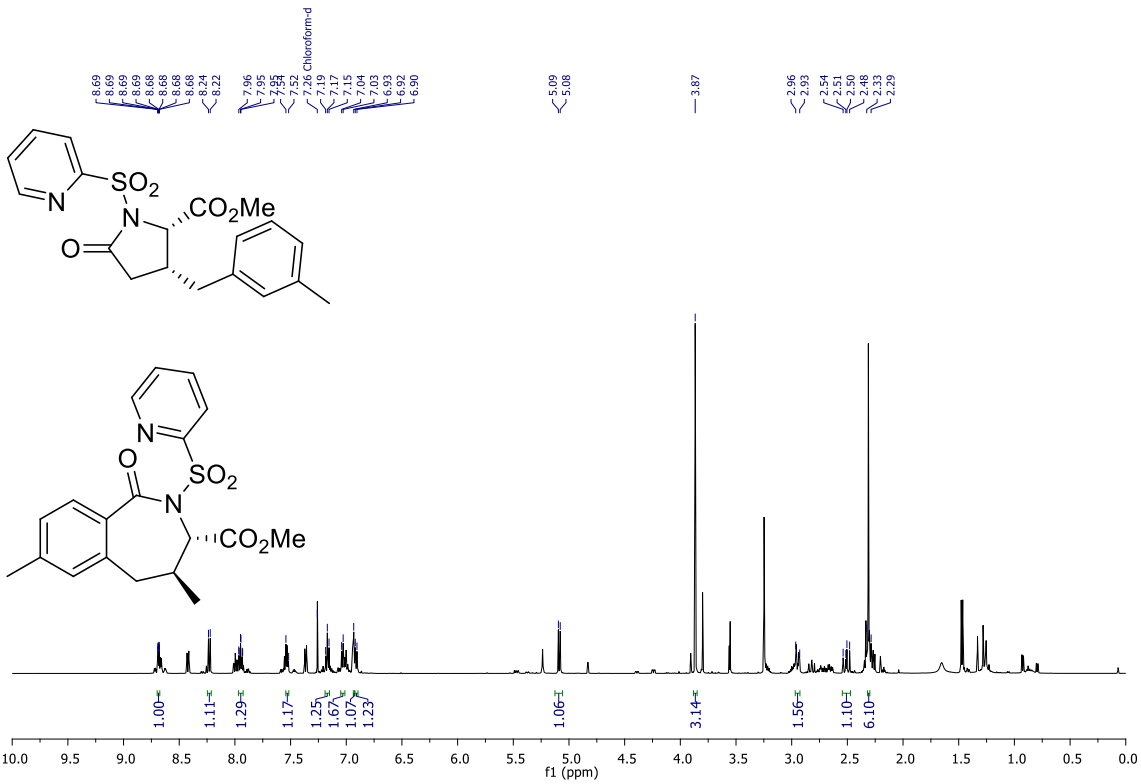


^{13}C NMR ($CDCl_3$, 75 MHz)

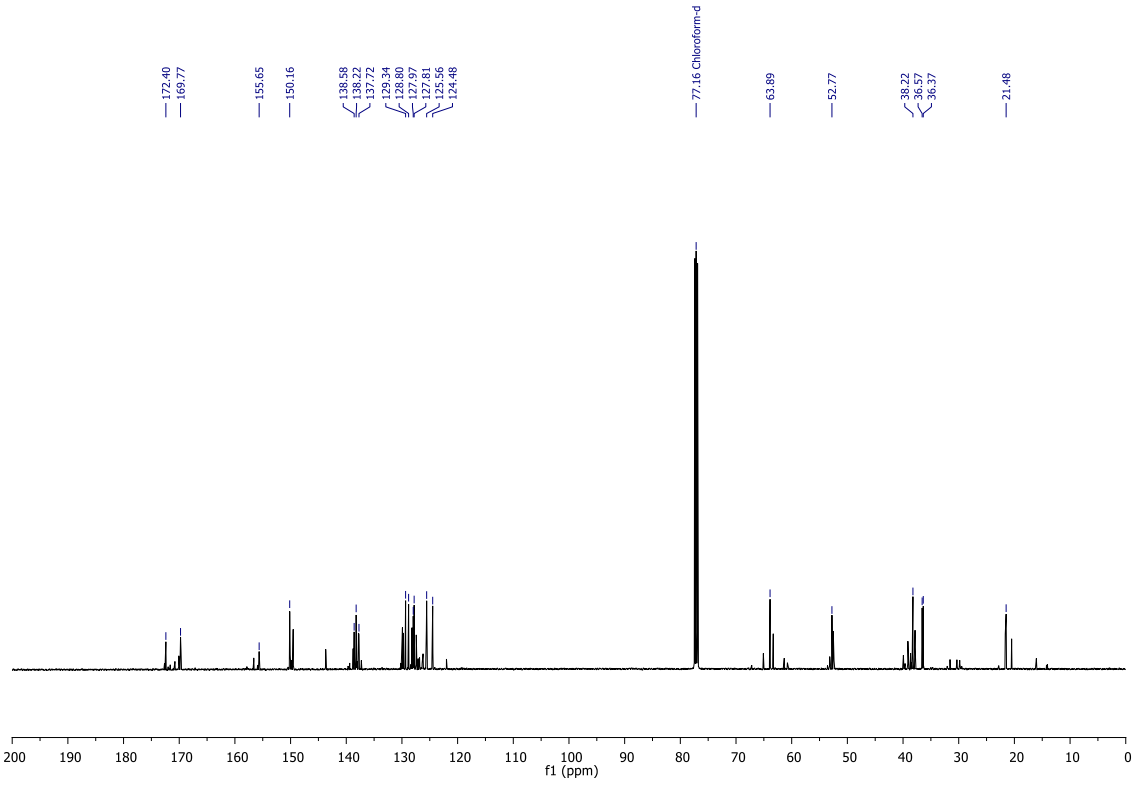


(2*S*,3*R*)-Methyl 3-(3-methylbenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3j+2j)

^{1}H NMR ($CDCl_3$, 500 MHz)

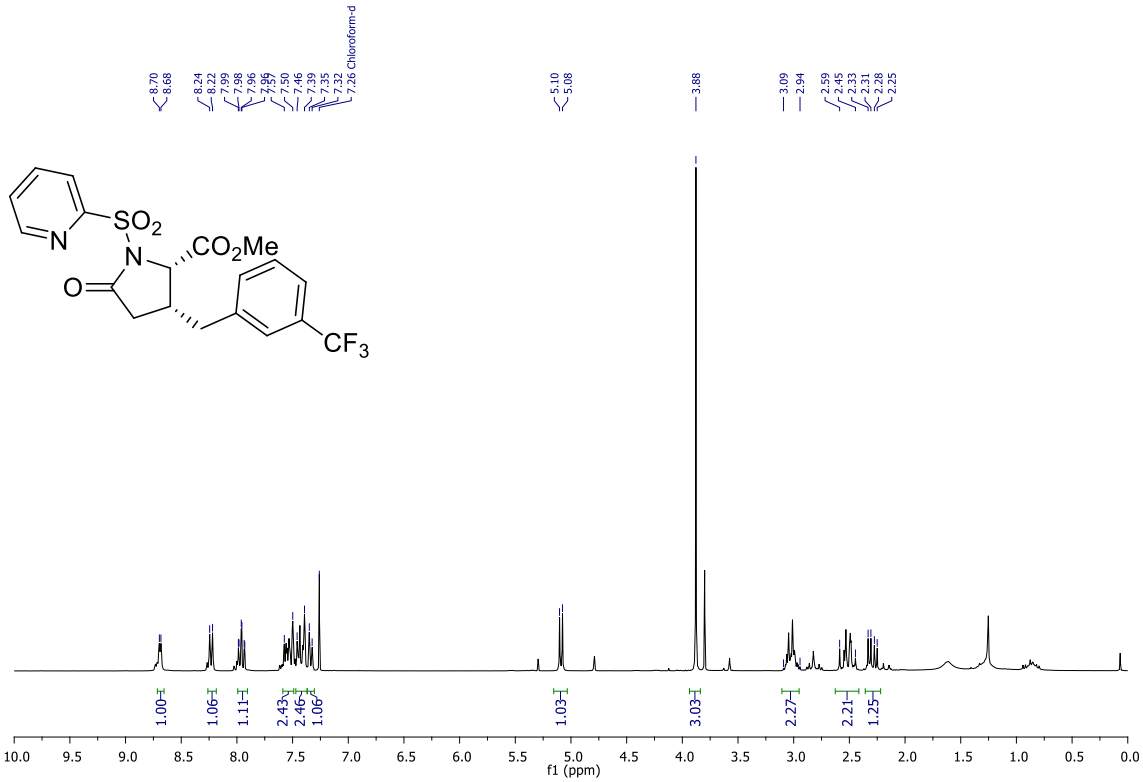


^{13}C NMR ($CDCl_3$, 126 MHz)

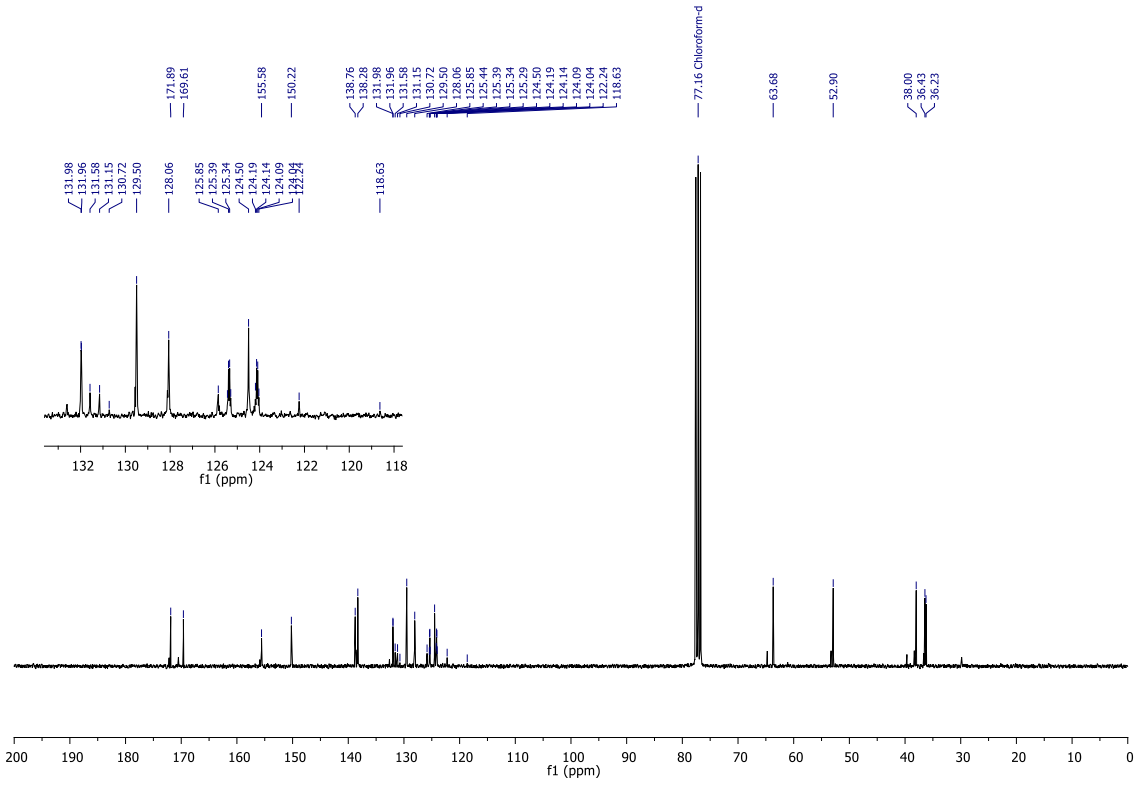


(2*S*,3*R*)-Methyl 5-oxo-1-(pyridin-2-ylsulfonyl)-3-(3-(trifluoromethyl)benzyl) pyrrolidine-2-carboxylate (3k)

^{1}H NMR ($CDCl_3$, 300 MHz)

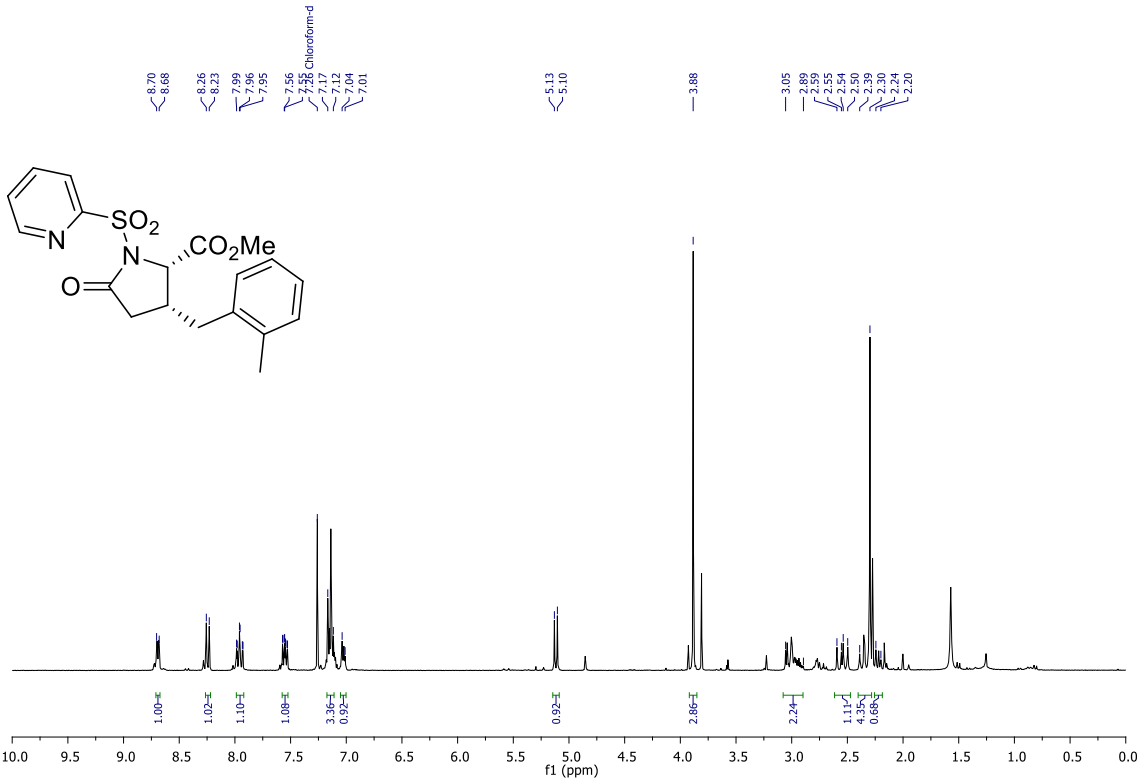


^{13}C NMR ($CDCl_3$, 75 MHz)

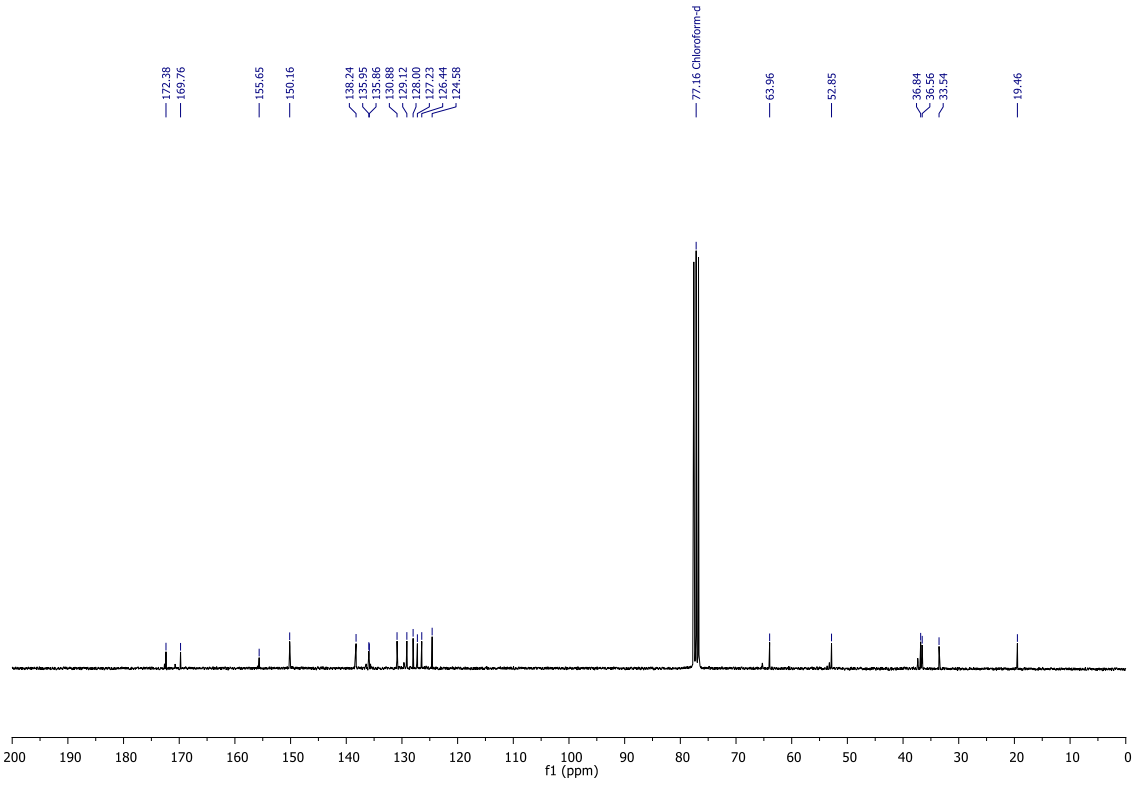


(2*S*,3*R*)-Methyl 3-(2-methylbenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3l)

^{1}H NMR ($CDCl_3$, 300 MHz)

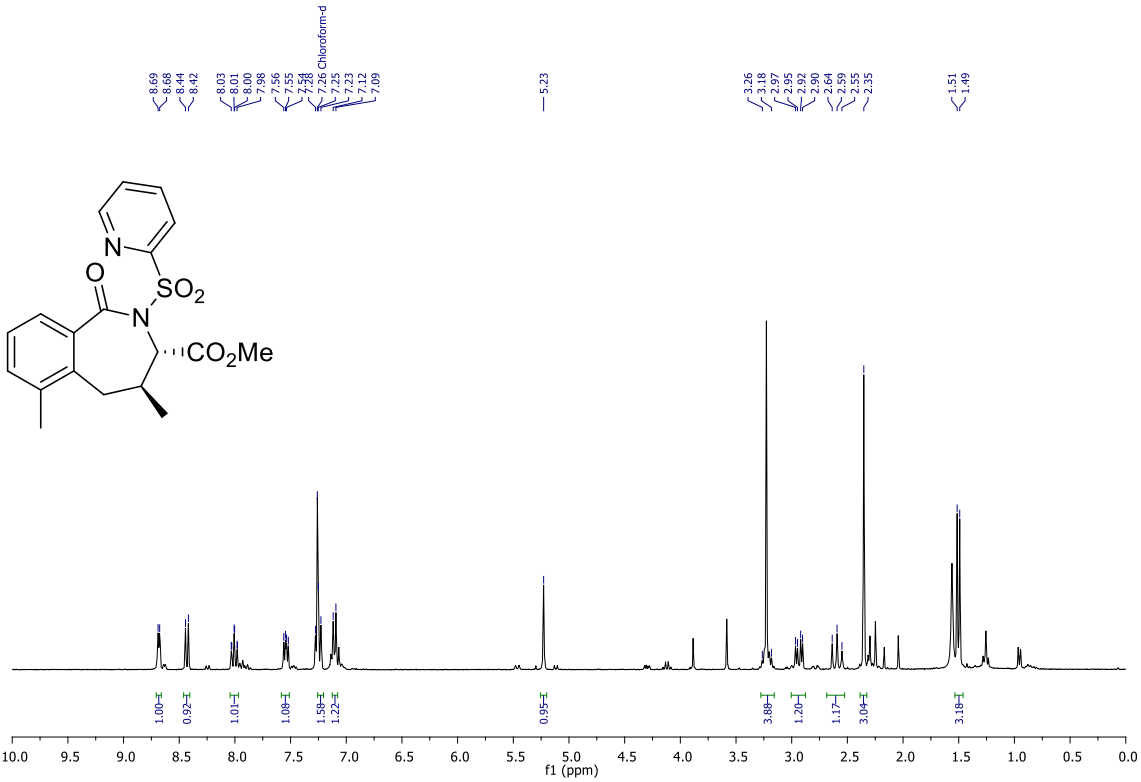


^{13}C NMR ($CDCl_3$, 75 MHz)

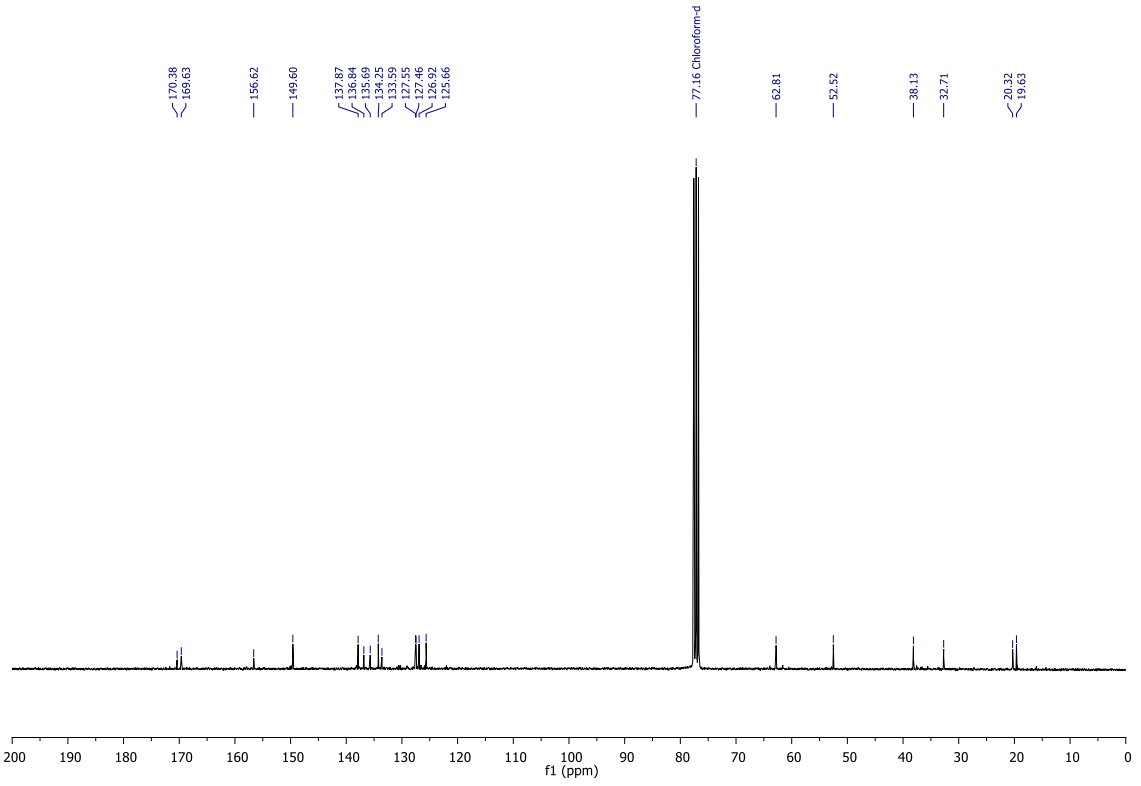


(3*S*,4*S*)-Methyl 4,6-dimethyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2l)

^{1}H NMR ($CDCl_3$, 300 MHz)

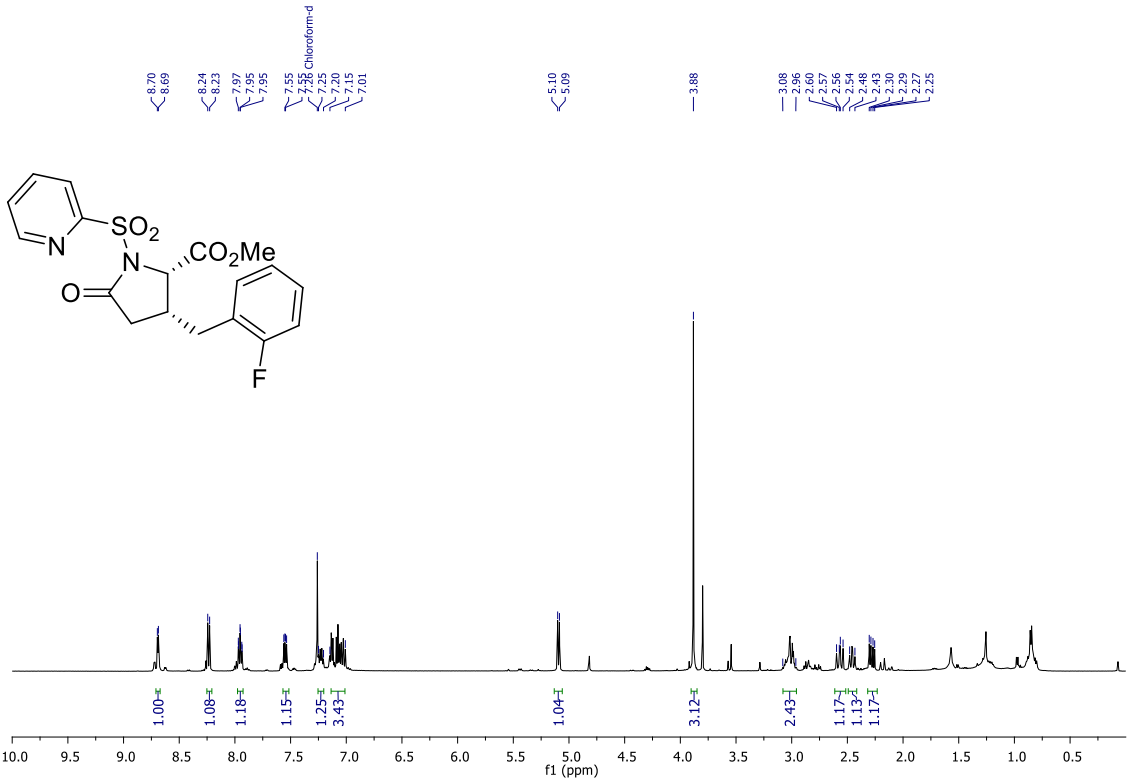


^{13}C NMR ($CDCl_3$, 75 MHz)

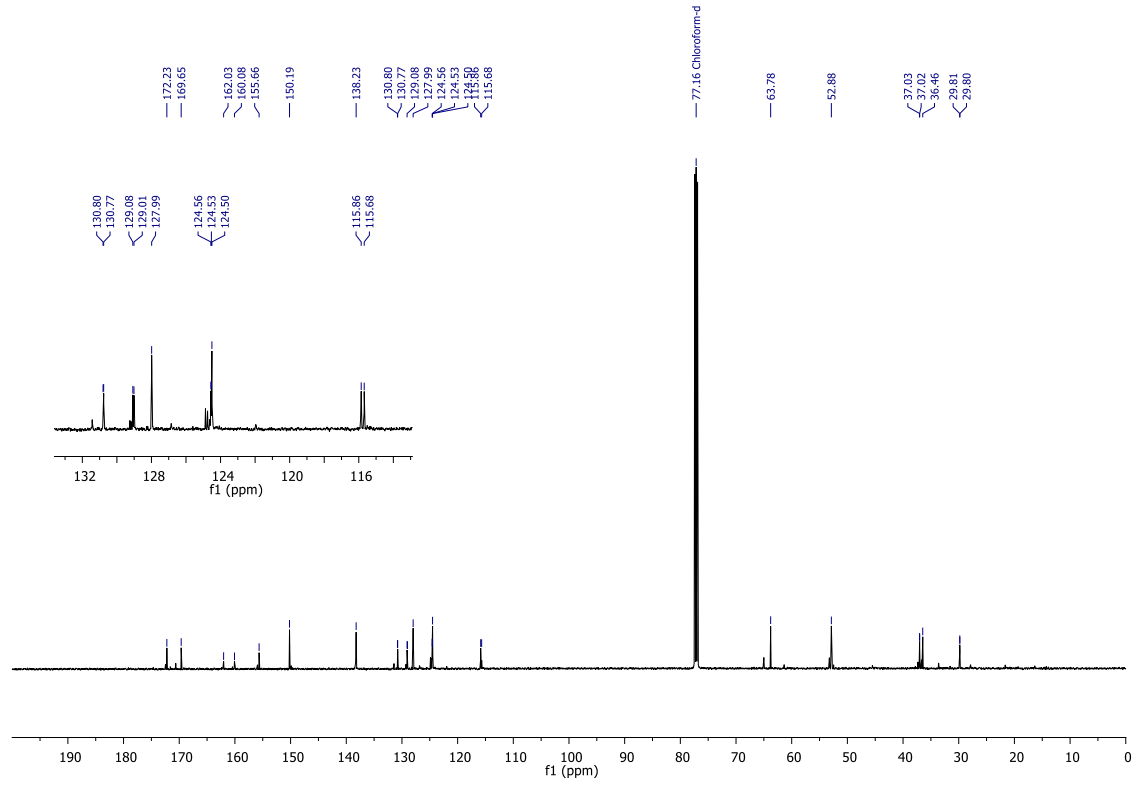


(2*S*,3*R*)-Methyl 3-(2-fluorobenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3m)

^{1}H NMR ($CDCl_3$, 500 MHz)

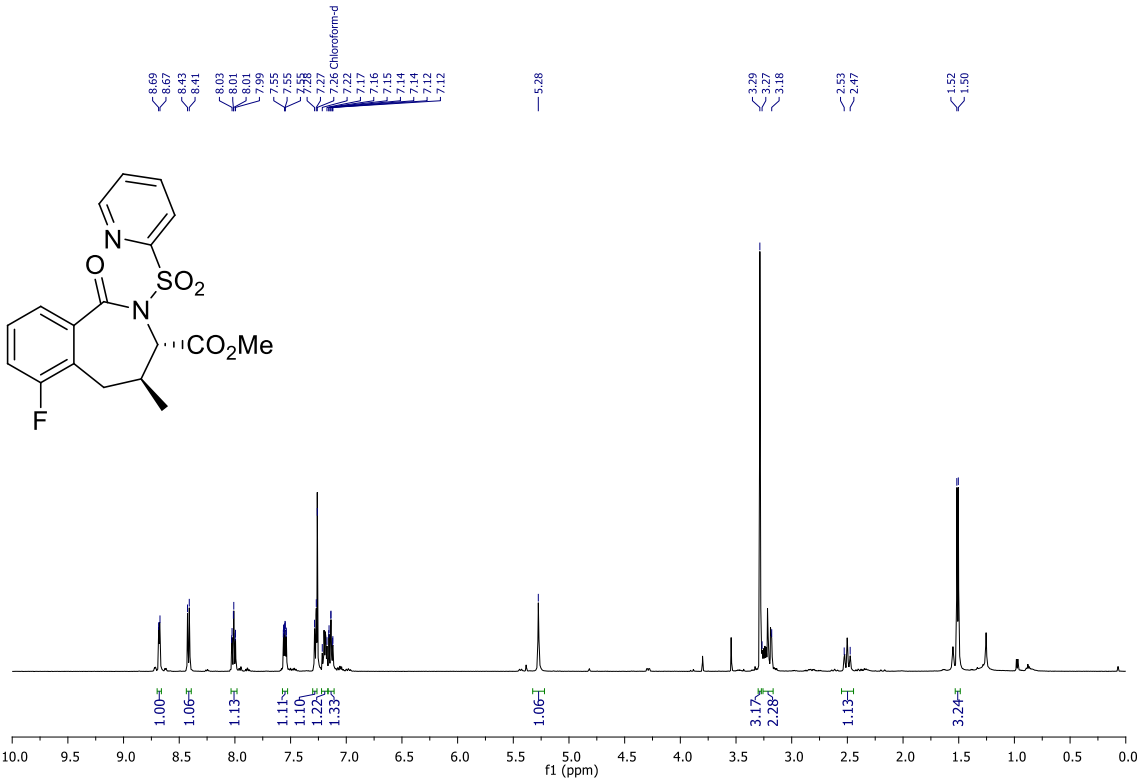


^{13}C NMR ($CDCl_3$, 126 MHz)

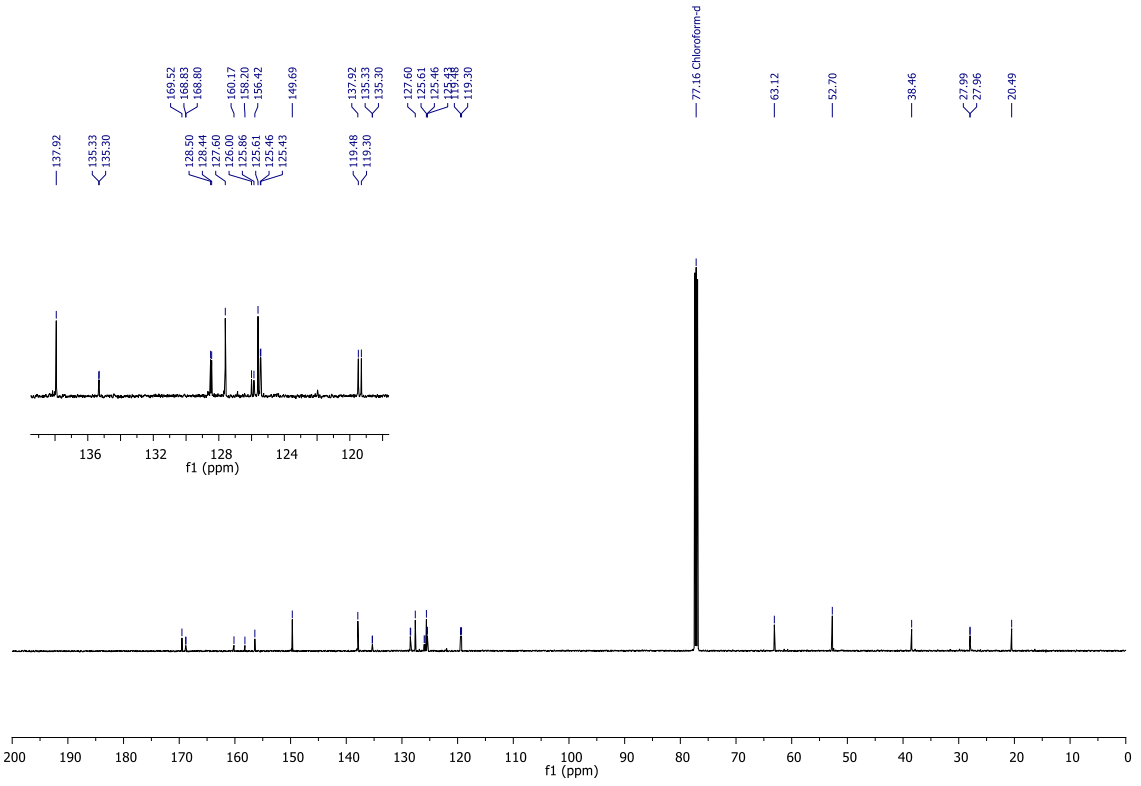


(3*S*,4*S*)-Methyl 6-fluoro-4-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (2m)

^{1}H NMR ($CDCl_3$, 500 MHz)

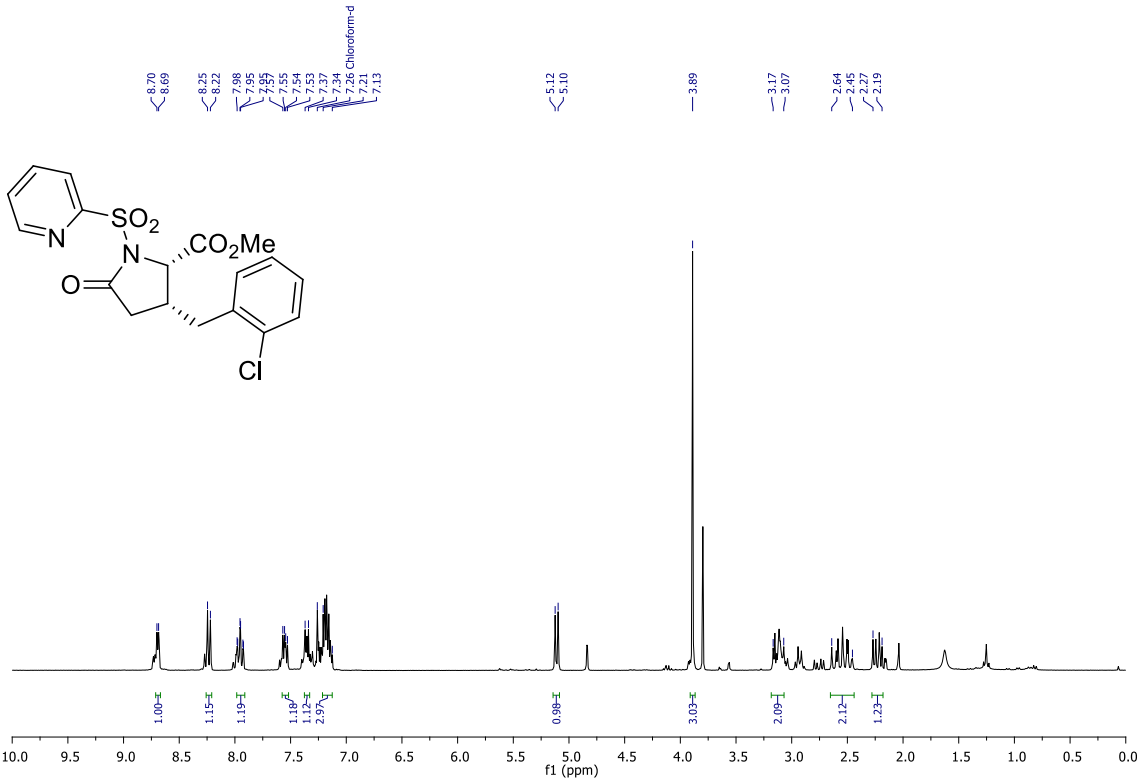


^{13}C NMR ($CDCl_3$, 126 MHz)

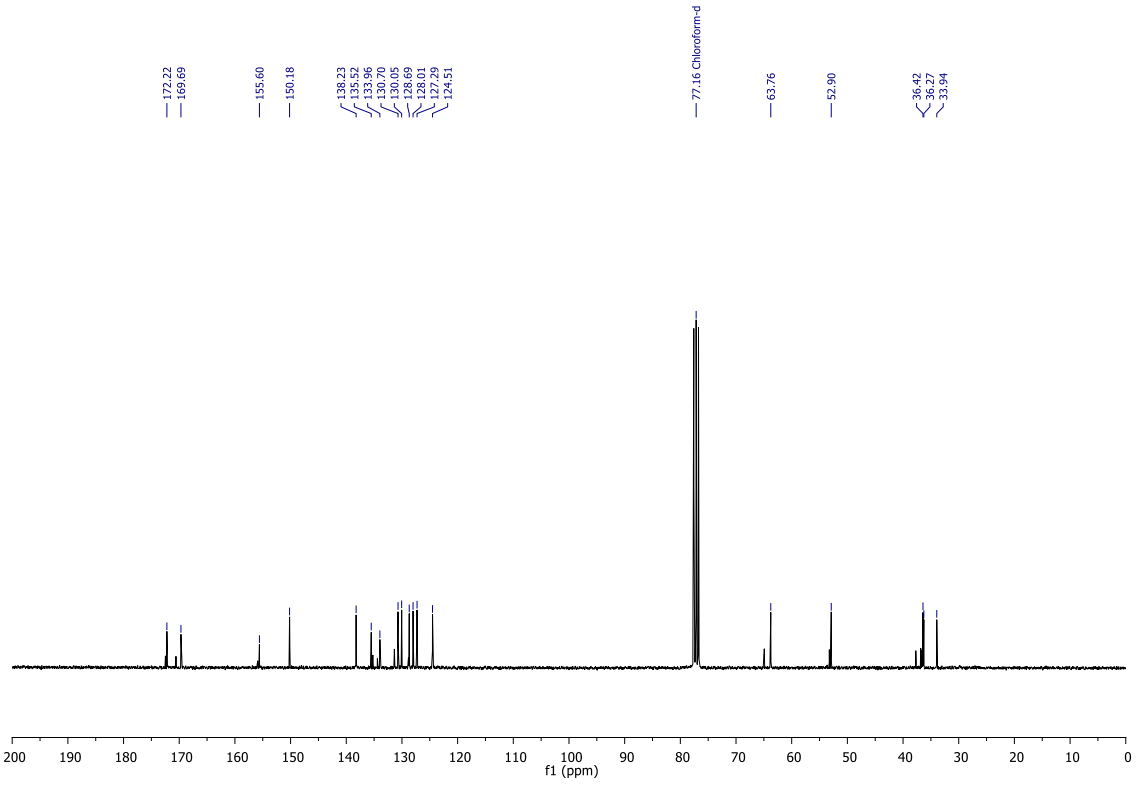


(2*S*,3*R*)-Methyl 3-(2-chlorobenzyl)-5-oxo-1-(pyridin-2-ylsulfonyl)pyrrolidine-2-carboxylate (3n)

^{1}H NMR ($CDCl_3$, 300 MHz)

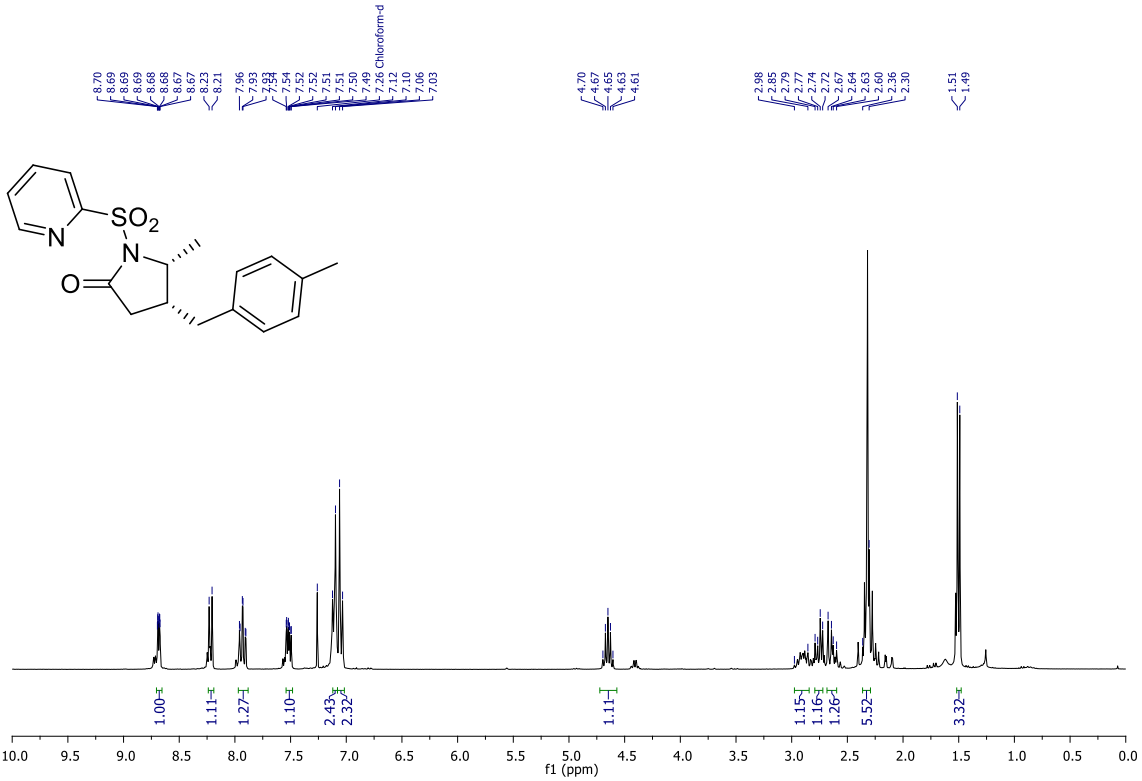


^{13}C NMR ($CDCl_3$, 75 MHz)

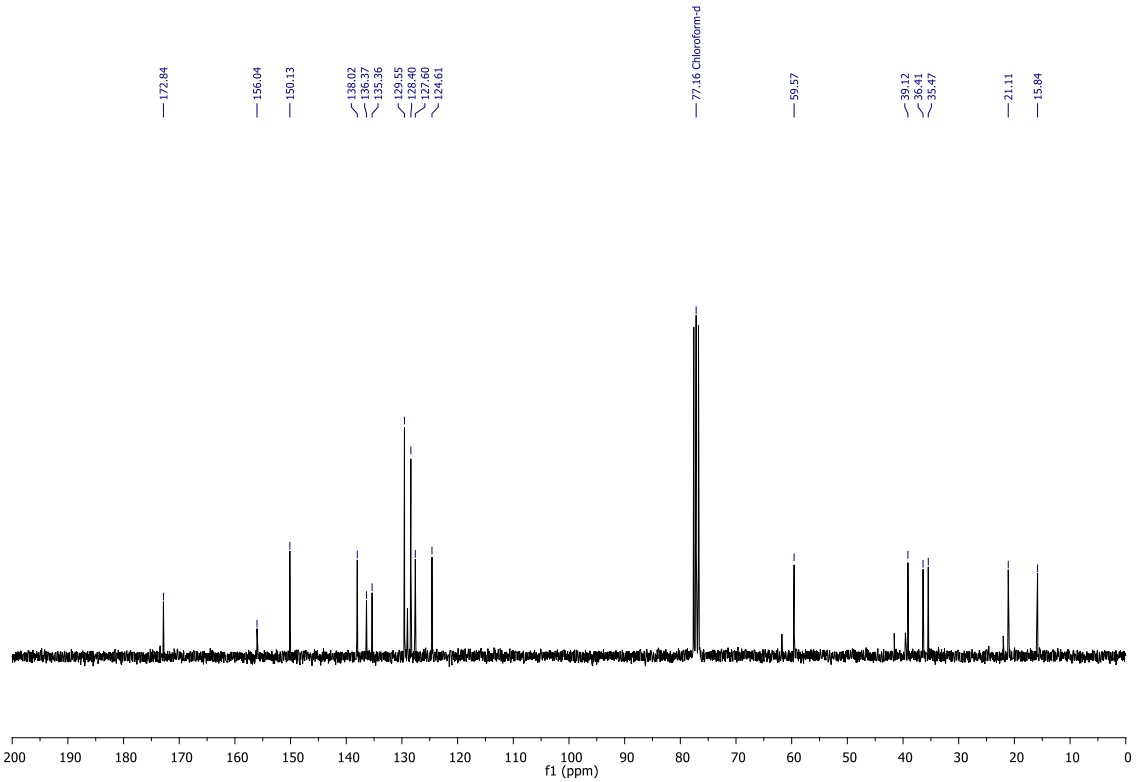


(4*R*,5*R*)-5-Methyl-4-(4-methylbenzyl)-1-(pyridin-2-ylsulfonyl)pyrrolidin-2-one (7a)

^{1}H NMR ($CDCl_3$, 300 MHz)

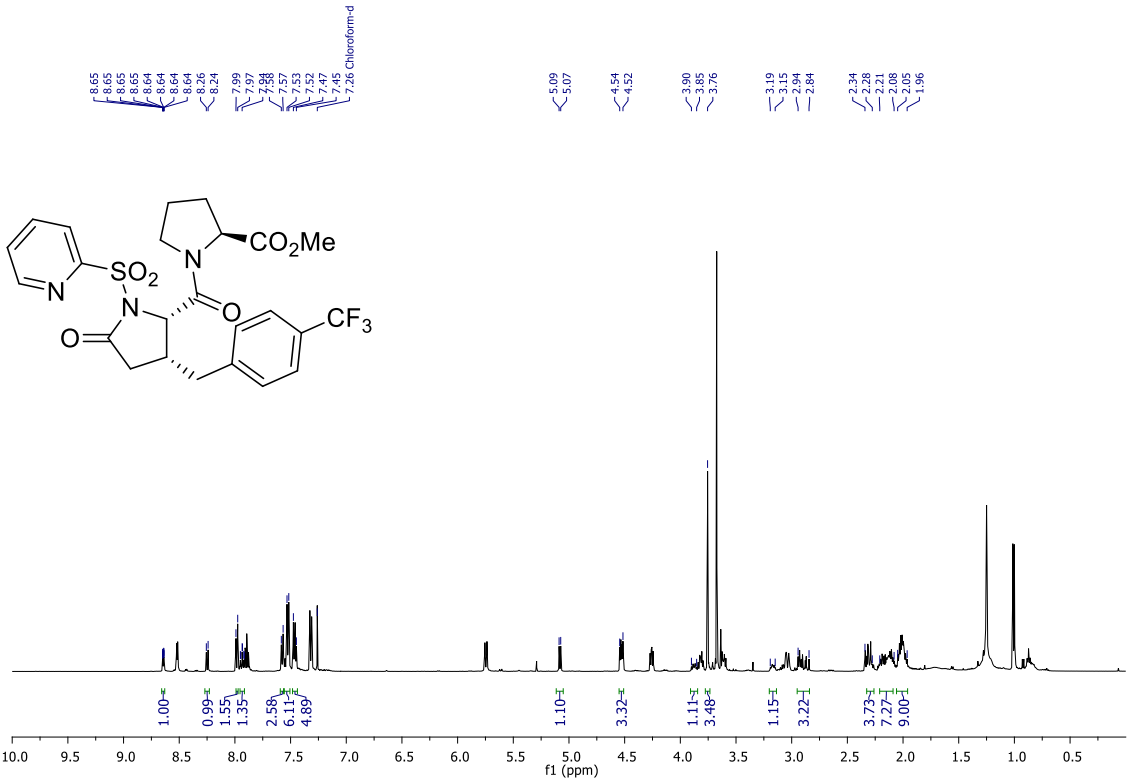


^{13}C NMR ($CDCl_3$, 75 MHz)

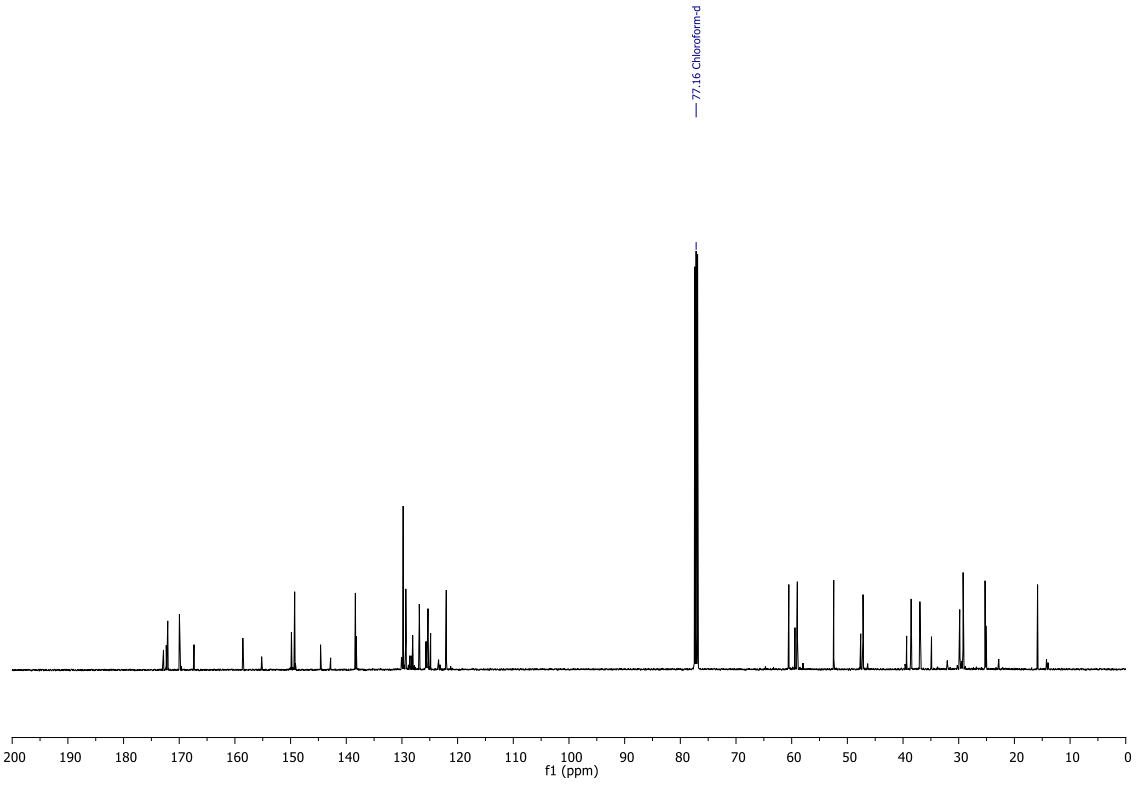


(*S*)-Methyl 1-((2S,3R)-5-oxo-1-(pyridin-2-ylsulfonyl)-3-(4-(trifluoromethyl) benzyl)pyrrolidine-2-carbonyl)pyrrolidine-2-carboxylateone (9)

^{1}H NMR ($CDCl_3$, 500 MHz)

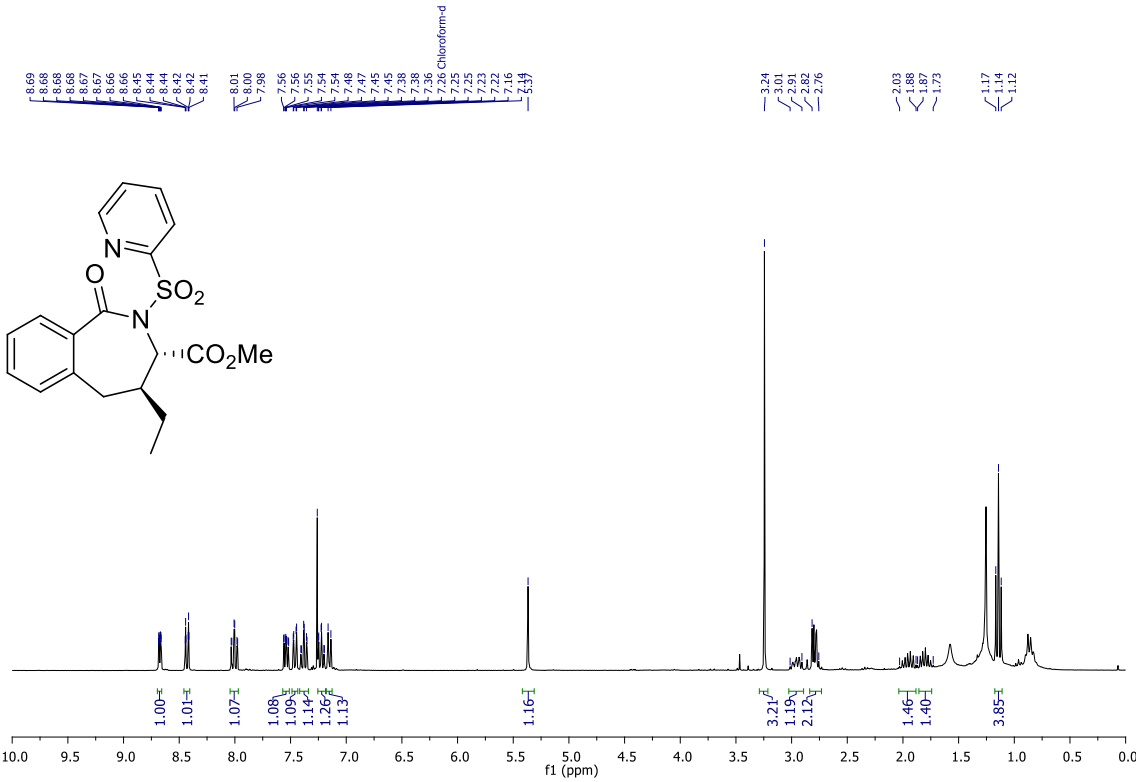


^{13}C NMR ($CDCl_3$, 126 MHz)

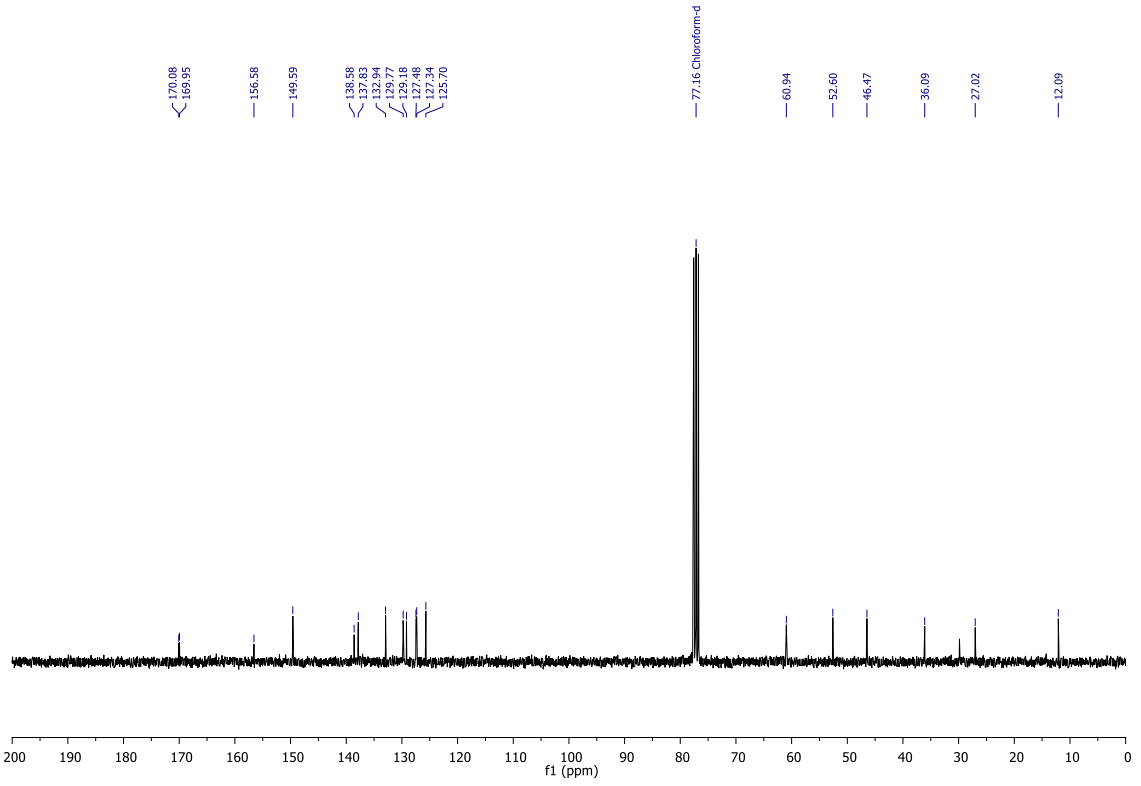


(3*S,4*S**)-Methyl 4-ethyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (5a)**

^{1}H NMR ($CDCl_3$, 300 MHz)

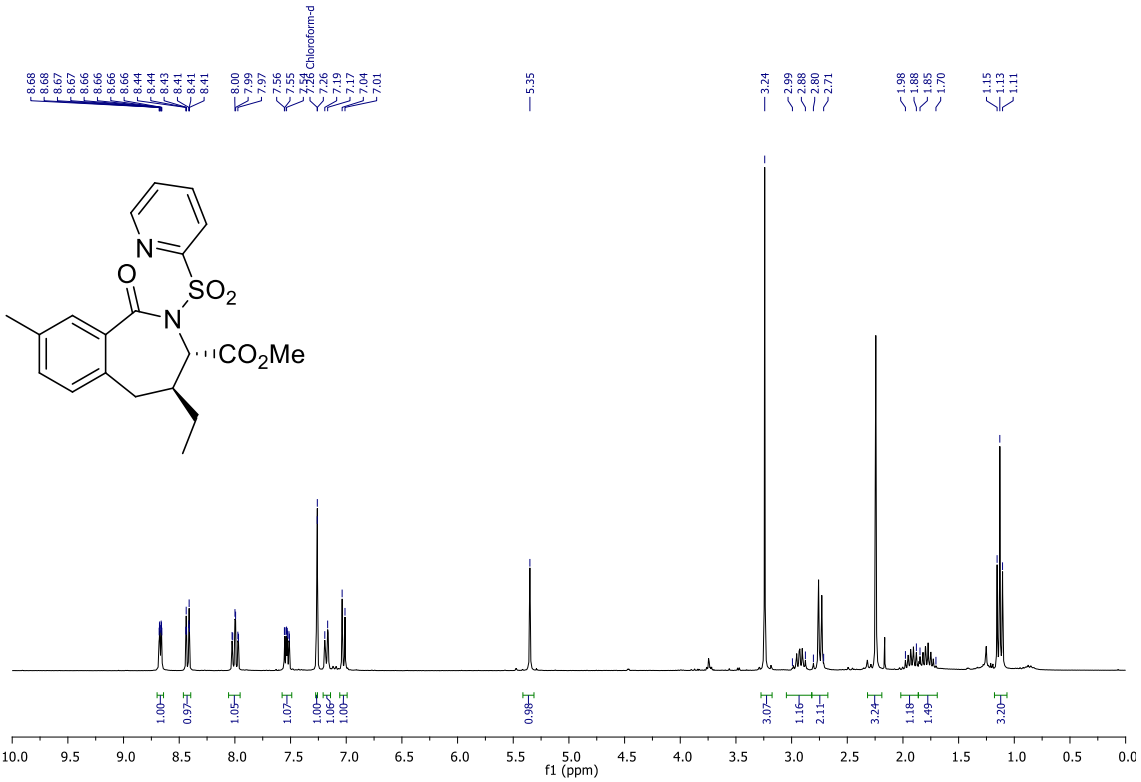


^{13}C NMR ($CDCl_3$, 75 MHz)

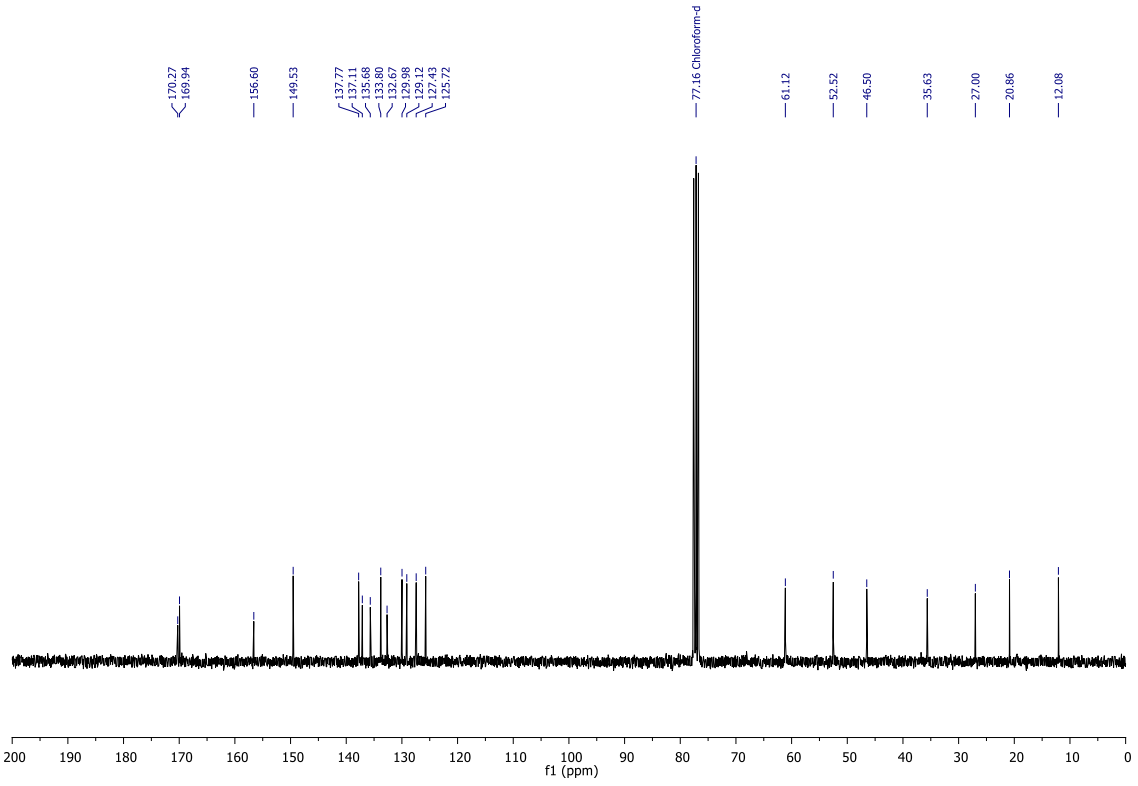


(3*S,4*S**)-Methyl 4-ethyl-8-methyl-1-oxo-2-(pyridin-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (5b)**

^{1}H NMR ($CDCl_3$, 300 MHz)

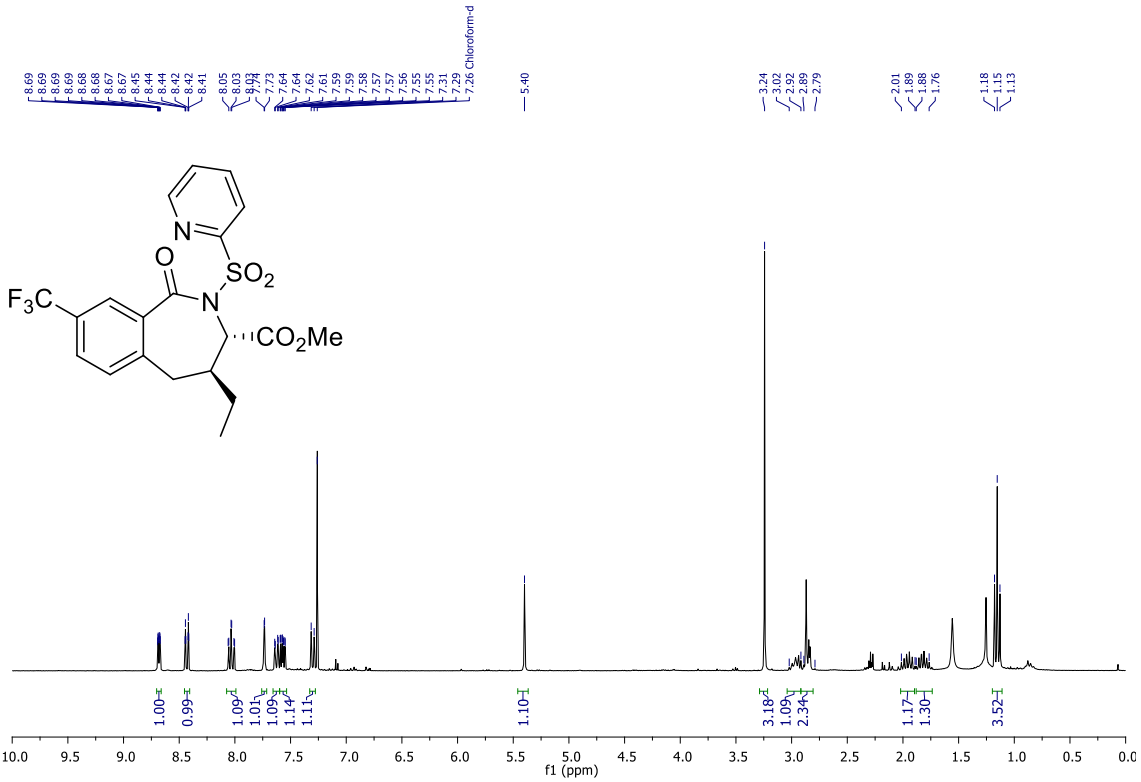


^{13}C NMR ($CDCl_3$, 75 MHz)

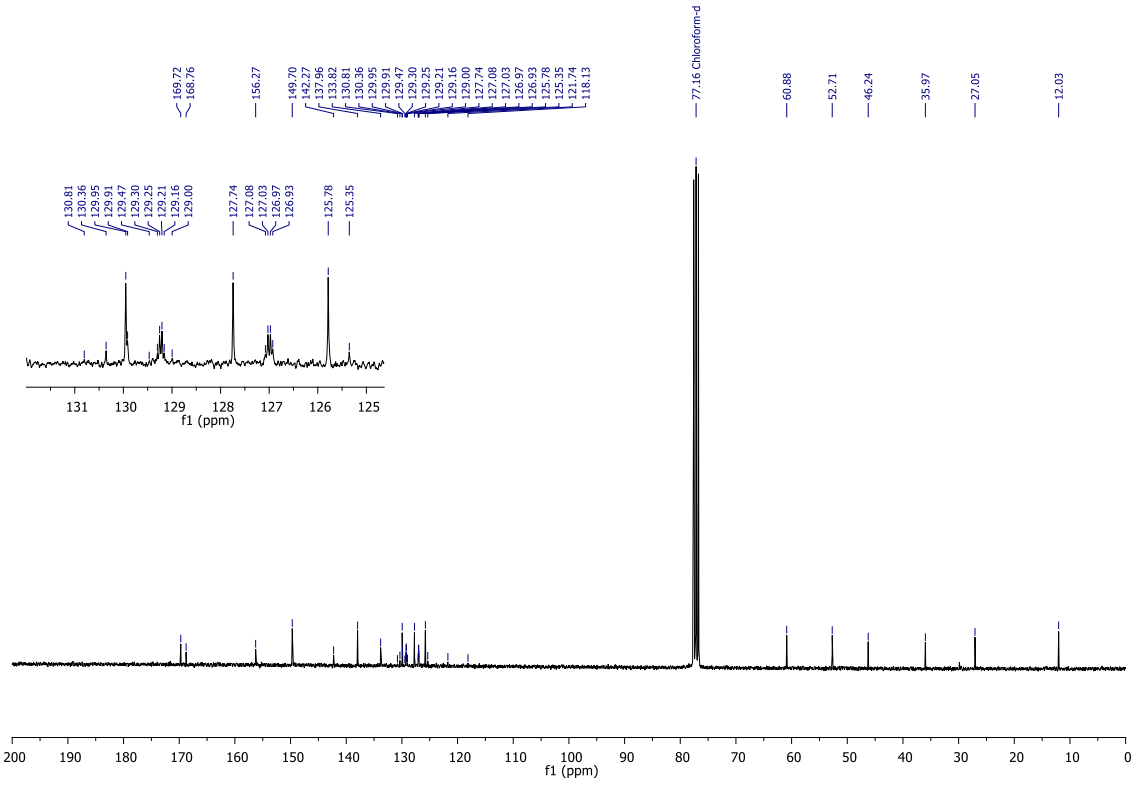


(3*S,4*S**)-Methyl 4-ethyl-1-oxo-2-(pyridin-2-ylsulfonyl)-8-(trifluoromethyl)-2,3,4,5-tetrahydro-1*H*-benzo[*c*]azepine-3-carboxylate (5c)**

^{1}H NMR ($CDCl_3$, 300 MHz)



^{13}C NMR ($CDCl_3$, 75 MHz)



^{19}F NMR ($CDCl_3$, 282 MHz)