Supplementary Information

Experimental and theoretical studies of the rhodium(I)-catalyzed C−H oxidative alkenylation/cyclization of *N*-(2-(methylthio)phenyl)benzamides with maleimides

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Contents

I. General Information:

^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer in $CDCl_3$ with tetramethylsilane as the internal standard. All the data are reported as follow: chemical shift (δ) peaking in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q= quartet, quin = quintet, sx = sextuplet and m = multiple), coupling constant (*J*) in Hz, and integration. Infrared spectra (IR) were obtained using a JASCO FT/IR-4200 spectrometer; absorptions are reported in reciprocal centimeters with the following relative intensities: s (strong), m (medium), or w (weak). Mass spectra and high-resolution mass spectra (HRMS) were obtained on a JEOL JMS-700 spectrometer. Melting points were determined using a OptiMelt MPA 100 Automated melting point system (temperature measurement accuracy is 0.1 ºC). Column chromatography was performed with SiO_2 (Silicycle Silica Flash F60 (230-400 mesh)) or NH Silica (Silica Gel 60 (special) NH_2 (40-50 μm)) for some starting materials. Also, we proceed the isolation for some product using there is compound was purified by LC-908 HPLC (GPC).

II. Materials:

2-(methylthio)aniline (CAS 2987-53-3) from Tokyo Chemical Industry Co., Ltd. (TCI), oxalyl chloride (CAS 79-37-8) from TCI, pivalic acid (CAS 75-98-9) from (TCI), $[Rh(COD)Cl]_2$ (CAS 12092-47-6) from Wako Pure Chemical Co., Ltd. (Wako), 2,3-difluorobenzoic acid (CAS 4519-39-5) from (TCI), 1,4-benzoquinone (CAS 106-51-4) from (TCI), silver hexafluoroantimoinate (CAS 26042-64-8) from (TCI), biphenyl-2-carboxylic acid (CAS 947-84-2) from (TCI), *o*-toluic Acid (CAS 118-90-1) from (TCI), $[Rh(CF_3CO_2)_2]_2$ dimer (CAS 31326-95-1) from Aldrich, $[Rh(OAc)_2)]_2$ (CAS 15956-28-2) from (TCI), $[Rh(CO)Cl(PPh_3)_2]$ (CAS 13938-94-8) from Strem Chemicals, $[Rh(acac)(CO)_2]$ (CAS 14874-82-9) from Aldrich, $RhCl_3 \cdot 3H_2O$ (CAS 20765-98-4) from Aldrich, $[RhCp^*Cl_2]_2$ (CAS 12354-85-7) from Aldrich, acetic acid (CAS 64-19-7) from Chameleon reagent, cyclohexyl carboxylic acid (CAS 98-89-5) from TCI, copper (II) chloride (CAS 7447-39-4) from Wako, copper (II) acetate$\cdot 2H_2O$ (CAS 6046-93-1) from Wako, manganese dioxide (CAS 1313-13-9) from Wako, silver acetate (CAS 563-63-3) from Wako, triethylamine (CAS 121-44-8) from Nacalei Tesque, 4-dimethylaminopyridine (CAS 1122-58-3) from Wako, *p*-toluoyl chloride (CAS 874-60-2) from TCI, *o*-toluoyl chloride (CAS 874-60-2) from TCI, 2-chlorobenzoyl chloride (CAS 609-65-4) from TCI, 2-bromobenzoyl chloride (CAS 7154-66-7) from TCI, 4-chlorobenzoyl chloride (CAS 122-01-0) from TCI, 4-butylbenzoyl chloride (CAS 28788-62-7) from TCI, *m*-toluoyl chloride (CAS 1711-06-4) from TCI, benzo[*b*]thiophene-2-carbonyl chloride (CAS 39827-11-7), from TCI, 1-naphthoyl chloride (CAS 879-18-5), from TCI, 3-bromo-2-methylbenzoic acid (CAS 76006-33-2) benzoic acid-d_5 (CAS 1079-02-3) from Cambridge Isotope Laboratories Inc., *N*-methylmaleimide (CAS 930-88-1) from TCI, *N*-ethylmaleimide (CAS 128-53-0) from TCI, *N*-phenylmaleimide (CAS 941-69-5) from TCI, *N*-cyclohexylmaleimide (CAS 1631-25-0) from TCI, *N*-benzylmaleimide (CAS 1631-26-1) from TCI.

III. Synthesis of Starting Materials:

1. General Procedure for the Preparation of Starting Amides:[1,2]

All amides bearing a 2-methylthiophenyl moiety were prepared by reacting the corresponding acids or the corresponding acid chlorides with 2-(methylthio)aniline (CAS 2987-53-3).

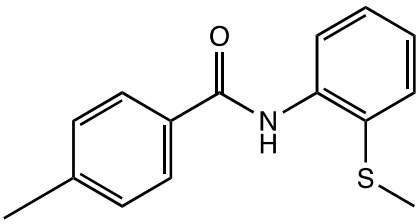
a. Synthesis of Amides from Acid Chlorides:

The acid chloride (5 mmol) was dissolved in CH_2Cl_2 (20 mL). After cooling the reaction mixture to 0 °C, a solution of 2-(methylthio)aniline (5 mmol) and triethylamine (12 mmol) in 10 mL of CH_2Cl_2 was added dropwise. The resulting mixture was allowed to slowly warm to room temperature and was then stirred overnight. The crude mixture was then washed with saturated aqueous $NaHCO_3$ (10 mL), and then extracted with CH_2Cl_2 (3x10 mL). The combined organic layers were washed with a 1 M solution of HCl aq. (10 mL). The organic phase was dried over anhydrous Na_2SO_4 and the resulting solution evaporated to dryness. The resulting crude amide was purified by flash chromatography on silica gel (hexanes/EtOAc = 5/1 as the eluent).

b. Synthesis of Amides from Carboxylic Acids:

To a stirred solution of a carboxylic acid (5 mmol) and in CH_2Cl_2 (10 mL) that contained 5 drops of DMF, $COCl_2$ (0.5 mL, 6 mmol) was added dropwise at 0 ºC. The solution was then magnetically stirred at room temperature for approximately for 2 h. The solvent was then removed under reduced pressure, and the resulting residue was dissolved in CH_2Cl_2 (10 mL). After cooling the reaction mixture to 0 °C, 2-(methylthio)aniline (5 mmol) and triethylamine (12 mmol) in 10 mL of CH_2Cl_2 were added dropwise. The resulting mixture was allowed to warm to room temperature and then stirred overnight. The crude product was washed with saturated aqueous $NaHCO_3$ (20 mL), and CH_2Cl_2 (3x10 mL). After washing with a 1 M solution of HCl aq. (20 mL), the organic phase was dried over anhydrous Na_2SO_4 and the solvent was removed by evaporation. The resulting crude amide was purified by flash chromatography on silica gel (hexanes/EtOAc = 5/1 as the eluent).

2. Spectroscopic Data of Staring Amides:

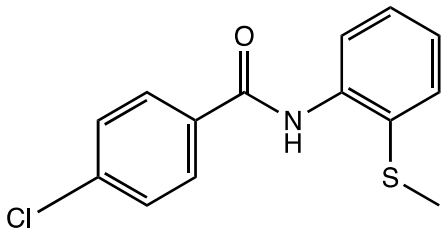


4-methyl-*N*-(2-(methylthio)phenyl)benzamide [CAS 701289-62-5] (1a)[3]

Quantitative yield. R_f = 0.26 (hexane/ Et_2O = 8/2). A white solid. Mp = 76.6 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.23 (brs, 1H), 8.54 (dd, *J* = 8.2 Hz and 1.2 Hz, 1H), 7.84-7.87 (m, 2H), 7.54 (dd, *J* = 7.6 Hz and 1.5 Hz, 1H), 7.30-7.38 (m, 3H), 7.08 (td, *J* = 7.6 Hz and 1.2 Hz, 1H), 2.44 (s, 3H), 2.40 (s, 3H).

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{15}H_{15}NOS$: 257.0874; Found: 257.0875.



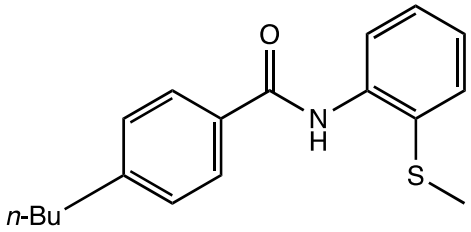
4-chloro-*N*-(2-(methylthio)phenyl)benzamide [CAS 450364-76-8] (1b)

95% yield. R_f = 0.43 (hexane/ Et_2O = 8/2). A white solid. Mp = 113.9 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.19 (brs, 1H), 8.48 (dd, *J* = 7.7 Hz and 0.7 Hz, 1H), 7.88-7.91 (m, 2H), 7.47-7.55 (m, 3H), 7.36 (td, *J* = 8.4 Hz and 1.2 Hz, 1H), 7.11 (td, *J* = 7.6 Hz and 1.1 Hz, 1H), 2.41 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.2, 138.5, 138.4, 133.4, 133.3, 129.4, 129.3, 128.65, 125.7, 124.8, 120.6, 19.4.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{18}H_{21}NOS$: 277.0328; Found: 277.0327.



4-butyl-*N*-(2-(methylthio)phenyl)benzamide (1c)

89% yield. R_f = 0.47 (hexane/ Et_2O = 8/2). A colorless oil.

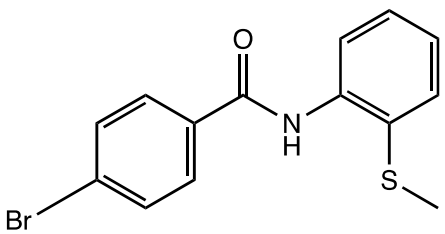
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.20 (brs, 1H), 8.51 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.07-7.33 (m, 3H), 7.05 (t, *J* = 7.6 Hz, 1H), 2.65 (t, *J* = 7.5 Hz, 2H), 2.36 (s, 3H), 1.60 (quin, *J* = 7.5 Hz, 2H), 1.34 (sext, *J* = 7.5 Hz, 2H), 0.92 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.0, 147.3, 138.6, 133.1, 132.1, 129.0, 128.8, 127.1, 125.5, 124.2, 120.4, 35.5, 33.2, 22.2, 19.0, 13.99.

IR (ATR) (neat, ν/cm^{-1}): 3348 w, 2955 w, 2926 w, 2858 w, 2360 w, 2340 w, 1523 m, 1502 s, 1432 s, 1304 m, 754 m.

MS m/z (relative intensity, %): 299 (M^+, 20), 253 (12), 252 (64), 162 (15), 161 (100), 91 (17).

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{18}H_{21}NOS$: 299.1344; Found: 299.1347.



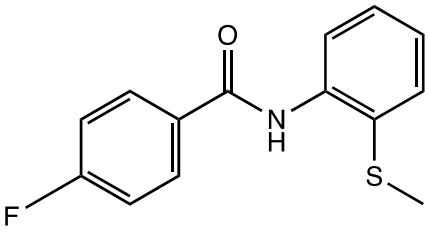
4-bromo-*N*-(2-(methylthio)phenyl)benzamide [CAS 862657-83-8] (1d)

Quantitative yield. R_f = 0.28 (hexane/ Et_2O = 8/2). A white solid. Mp = 117.9 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.20 (brs, 1H), 8.50 (dd, *J* = 8.2 Hz and 1.1 Hz, 1H), 7.74-7.84 (m, 2H), 7.68-7.65 (m, 2H), 7.55 (dd, *J* = 7.7. Hz and 1.1 Hz, 1H), 7.35-7.39 (m, 1H) 7.12-7.15 (m, 2H), 2.41 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.3, 138.40, 133.8, 133.4, 132.24, 129.3, 128.8, 126.9, 125.7, 124.8, 120.6, 19.4.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{14}H_{21}BrNOS$: 320.9823; Found: 320.9821.



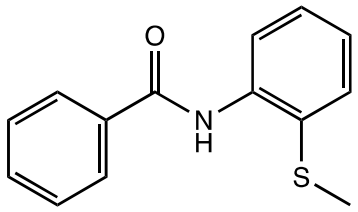
4-fluoro-*N*-(2-(methylthio)phenyl)benzamide [CAS 708243-62-3] (1e)

Quantitative yield. R_f = 0.25 (hexane/ Et_2O = 8/2). A white solide. Mp = 77.6 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.18 (brs, 1H), 8.50 (dd, *J* = 8.2 Hz and 1.1 Hz, 1H), 7.95-7.98 (m, 2H), 7.55 (dd, *J* = 7.8 Hz and 1.6 Hz, 1H), 7.36 (td, *J* = 8.4 Hz and 1.3 Hz, 1H), 7.19-7.22 (tm, 2H) 7.12 (td, *J* = 7.6 Hz and 1.3 Hz, 1H), 2.41 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.1 (d, *J* = 251 Hz), 164.2, 138.5, 133.4, 131.1 (d, *J* = 3.8 Hz), 129.60 (d, *J* = 9.6 Hz), 129.3, 125.7, 124.7, 120.6, 116.08 (*J* = 22.1 Hz), 19.3.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{14}H_{12}FNOS$: 261.0624; Found: 261.0627.



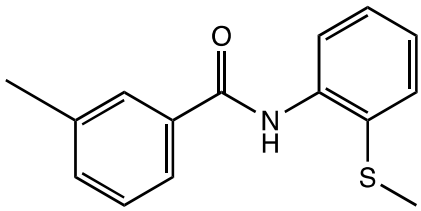
***N*-(2-(methylthio)phenyl)benzamide [CAS 51942-32-6] (1f)[3]**

Quantitative yield. R_f = 0.38 (hexane/ Et_2O = 8/2). A pale yellow solid. Mp = 96.1 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.25 (brs, 1H), 8.53 (dd, *J* = 8.2 Hz and 1.1 Hz, 1H), 7.94-7.97 (m, 2H), 7.50-7.59 (m, 4H), 7.36 (td, *J* = 8.4 Hz and 1.3 Hz, 1H), 7.10 (td, *J* = 7.5 Hz and 1.0 Hz, 1H), 2.38 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.3, 138.8, 135.0, 133.5, 132.1, 129.4, 129.0, 127.2, 125.5, 124.6, 120.5, 19.4.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{14}H_{13}NOS$: 243.0718; Found: 243.0718.



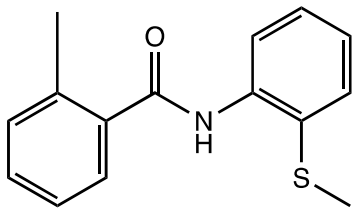
3-methyl-*N*-(2-(methylthio)phenyl)benzamide [CAS 903797-73-9] (1g)[3]

73% yield. R_f = 0.27 (hexane/ Et_2O = 8/2). A pale yellow solid. Mp= 99.4 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.21 (s, 1H), 8.53 (dd, *J* = 8.2 Hz and 1.5 Hz, 1H), 7.78 (s, 1H), 7.72-7.73 (m, 1H), 7.53-7.56 (dd, *J* = 7.7 Hz, and 1.3 Hz, 1H), 7.34-7.42 (m, 3H), 7.11 (td, *J* = 7.5 Hz and 1.4 Hz, 1H), 2.46 (s, 3H), 2.41 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.6, 139.0, 138.8, 135.0, 133.5,132.9, 129.4, 128.9, 128.1, 125.6, 124.6, 124.1, 120.6, 21.6, 19.4.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{15}H_{15}NOS$: 257.0874; Found:257.0876.



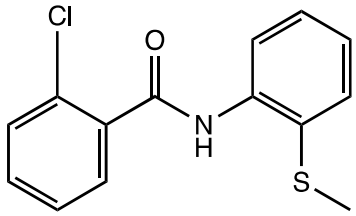
2-methyl-*N*-(2-(methylthio)phenyl)benzamide [CAS 708220-13-7] (1h)[4]

92% yield. R_f = 0.22 (hexane/ Et_2O = 8/2). A white solid. Mp = 65.4 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.65 (brs, 1H), 8.50 (d, *J* = 7.8 Hz, 1H), 7.59-7.57 (m, 1H), 7.52 (dd, *J* = 7.7 Hz and 1.3 Hz, 1H), 7.33-7.41 (m, 2H), 7.27-7.31 (m, 2H), 7.12 (td, J= 7.5 Hz and 1.3 Hz, 1H), 2.57 (s, 3H), 2.39 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.1, 138.6, 136.9, 136.4, 133.1, 131.6, 130.6, 129.1, 127.0, 126.2, 125.8, 124.8, 120.8, 20.3, 19.2.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{15}H_{15}NOS$: 257.0874; Found: 257.0876.



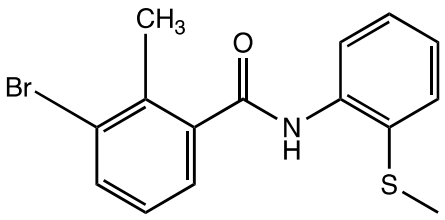
2-chloro-*N*-(2-(methylthio)phenyl)benzamide [CAS 450364-76-8] (1i)

Quantitative yield. R_f = 0.26 (hexane/ Et_2O = 8/2). A white solid. Mp = 45.0 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.99 (brs, 1H), 8.51 (d, *J* = 8.2 Hz, 1H), 7.75 (dd, *J* = 7.5 Hz and 2.0 Hz, 1H), 7.51 (dd, *J* = 7.8 Hz and 1.4 Hz, 1H), 7.32-7.46 (m, 4H), 7.11 (td, *J* = 7.4 Hz and 1.4 Hz 1H), 2.36 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.7, 138.2, 135.4, 133.2, 131.7, 130.7, 130.5, 130.2, 129.0, 127.3, 126.0, 124.9, 120.9, 19.3.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{14}H_{12}ClNOS$: 277.0328; Found: 277.0328.



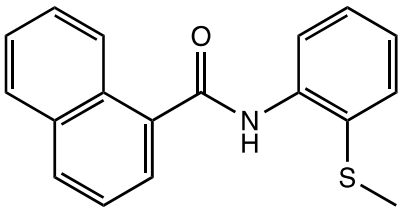
3-bromo-2-methyl-*N*-(2-(methylthio)phenyl)benzamide [CAS 1498493-84-7] (1j)

76% yield. R_f = 0.25 (hexane/ Et_2O = 8/2). A white solid. Mp = 97.6 ºC

^{11}H NMR ($CDCl_3$, 400 MHz): δ 8.65 (brs, 1H), 8.52 (d, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 7.1 Hz, 1H), 7.28-7.39 (m, 4H), 7.12 (td, *J* = 7.7 Hz and 0.8 Hz, 1H), 2.48 (s, 3H), 2.38 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.7, 139.7, 139.3, 138.4, 133.4, 132.4, 129.2, 127.6, 126.4, 125.8, 125.0, 121.7, 120.90, 23.7, 19.5.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{15}H_{14}BrNOS$: 334.9979; Found: 334.9982.



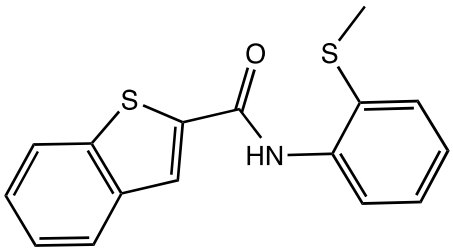
***N*-(2-(methylthio)phenyl)-1-naphthamide [CAS 920228-77-9] (1k)**

86% yield. R_f = 0.13 (hexane/ Et_2O = 8/2). A white yellow solid. Mp = 100.4 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.87 (brs, 1H), 8.60 (d, J= 7.5 Hz, 1H), 8.47 (d, *J* = 8.2 Hz, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 7.5 Hz, 1H), 7.81 (d, *J* = 6.6 Hz, 1H), 7.51-7.61 (m, 4H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.13 (td, *J* = 7.5 Hz and 1.1 Hz, 1H) 2.36 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.6, 138.6, 134.5, 134.0, 133.1, 131.4, 130.3, 129.1, 128.6, 127.5, 126.7, 125.5, 125.4, 125.0, 124.9, 120.9, 19.2.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{18}H_{15}NOS$: 293.0874; Found: 293.0878.



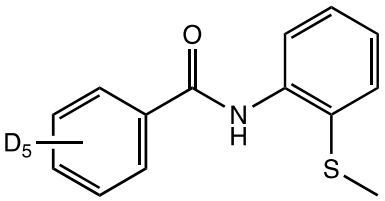
***N*-(2-(methylthio)phenyl)benzo[*b*]thiophene-2-carboxamide [CAS 1801979-19-0] (1l)[5]**

Quantitative yield. R_f = 0.40 (hexane/ Et_2O = 8/2). A white solid. Mp = 100.8 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.28 (brs, 1H), 8.50 (d, *J* = 8.0 Hz, 1H), 7.90-7.94 (m, 3H), 7.36-7.58 (c, 4H), 7.12 (t, *J* = 7.3 Hz, 1H), 2.45 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.3, 141.4, 139.3, 139.2, 138.5, 133.8, 129.6, 126.8, 125.7, 125.4, 125.3, 124.8, 122.9, 120.5, 19.6.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{16}H_{13}NOS_2$: 299.0439; Found: 299.0443.



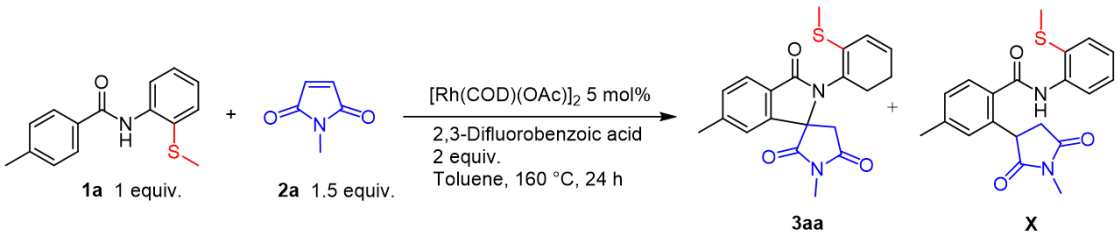
***N*-(2-(methylthio)phenyl)benzamide-*d*$_5$ (1f-*d*$_5$)**

Quantitative yield. R_f = 0.38 (hexane/ Et_2O = 8/2). A pale yellow solid. Mp = 96.1 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.24 (brs, 1H), 8.53 (dd, *J* = 8.2 Hz and 1.0 Hz, 1H), 7.54 (dd, *J* = 7.8 Hz and 1.4 Hz), 7.36 (td, *J* = 7.8 Hz and 1.4 Hz, 1H), 7.10 (td, *J* = 8.4 Hz and 1.4 Hz, 1H), 2.40 (s, 3H).

IV. Optimization of Reaction Conditions Using 4-Methyl-*N*-(2-(methylthio)phenyl)benzamide:

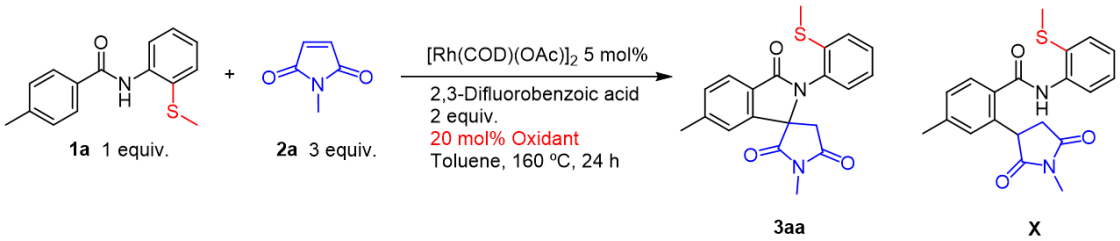
1. Table S1: Screening of Rhodium Catalysts.



1a 1 equiv. **2a** 1.5 equiv. **3aa** **X**

Reaction Number	Entry	Catalyst	Catalyst Loading	NMR Yields%		
				3aa	X	SM
ac 507	1	$[Rh(II)(OAc)_2]_2$	5 mol%	48	n.d	50
ac 508	2	$[Rh(I)(COD)Cl]_2$	5 mol%	84	n.d	12
ac 509	3	$[Rh(CF_3COO)_2]_2$	5 mol%	56	n.d	41
ac 510	4	$[Rh(COD)(OAc)]_2$	5 mol%	52	n.d	49
ac 511	5	$[Rh(CO)Cl(Pph_3)_2$	10 mol%	n.d	n.d	97
ac 512	6	$[Rh(acac)(CO)_2]$	10 mol%	39	n.d	61
ac 513	7	$RhCl_3.3H_2O$	10 mol%	Tr	n.d	96
ac 520	8	$RhCp^*Cl_2$	10 mol%	43	n.d	51

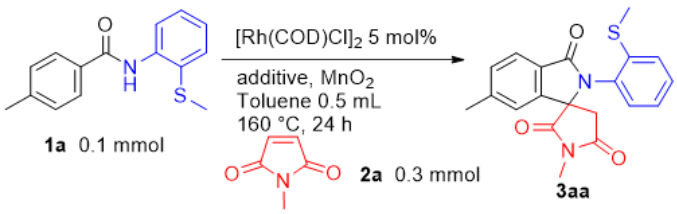
2. Table S2: Screening of Oxidants.



1a 1 equiv. **2a** 3 equiv. **3aa** **X**

Reaction Number	Entry	Oxidant	Oxidant Loading	NMR Yields%		
				3aa	X	SM
ac 531	1	$CuCl_2$	20 mol%	17	n.d	81
ac 532	2	$Cu(OAc).H_2O$	20 mol%	32	n.d	67
ac 533	3	MnO_2	20 mol%	48	n.d	51
ac 534	4	AgOAc	20 mol%	22	n.d	75
ac 535	5	$AgSbF_6$	20 mol%	n.d	n.d	98
ac 542	6	p-benzoquinone	20 mol%	24	n.d	74

3. Table S3: Optimization of Reaction Conditions[a]



Entry	Additive	Maleimide	MnO_2	Yields (%)
1	2,3-Difluorobenzoic acid 2 equiv.	3 equiv.	0.5 equiv.	62
2	2,3-Difluorobenzoic acid 2 equiv.	3 equiv.	1 equiv.	50
3	2,3-Difluorobenzoic acid 2 equiv.	3 equiv.	2 equiv.	trace
4	2,3-Difluorobenzoic acid 0.5 equiv.	3 equiv.	0.5 equiv.	49
5	2,3-Difluorobenzoic acid 1 equiv.	3 equiv.	0.5 equiv.	53
6	2,3-Difluorobenzoic acid 3 equiv.	3 equiv.	0.5 equiv.	77
7	AcOH 3 equiv.	3 equiv.	0.5 equiv.	0
8	PivOH 3 equiv.	3 equiv.	0.5 equiv.	97 (85)
9	2-toluic acid 3 equiv.	3 equiv.	0.5 equiv.	61
10	2-biphenylbenzoic acid 3 equiv.	3 equiv.	0.5 equiv.	65
11	$C_6H_{11}CO_2H$ 3 equiv.	3 equiv.	0.5 equiv.	39
12	PivOH 3 equiv.	1.2 equiv.	0.5 equiv.	45
13	PivOH 3 equiv.	2.5 equiv.	0.5 equiv.	83
14[b]	PivOH 3 equiv.	3 equiv.	0.5 equiv.	41
15[c,d]	PivOH 3 equiv.	3 equiv.	-	64
16[c,e]	PivOH 3 equiv.	3 equiv.	-	78
17[c,f]	PivOH 3 equiv.	3 equiv.	-	86
18[f]	PivOH 3 equiv.	3 equiv.	-	96 (91)
19[f,g]	PivOH 3 equiv.	3 equiv.	-	58

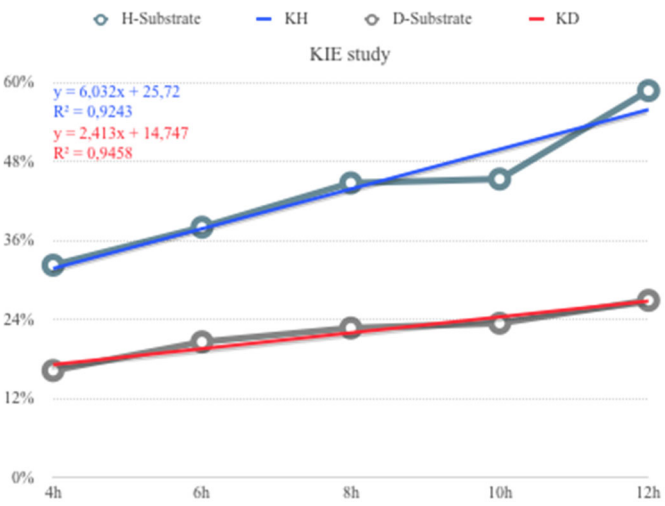
[a] Reaction conditions: **1a** (0.1 mmol), **2a**, $[Rh(COD)Cl]_2$ (0.005mmol), additive, MnO_2, at 160 °C for 24 h. The number in the parenthesis refers to the isolated yield. [b] 2.5 mol% of $[Rh(COD)Cl]_2$ was used as the catalyst. [c] The reaction was carried out at 140 °C. [d] Toluene (1 mL) was used. [e] Toluene (0.4 mL) was used. [f] No solvent. [g] The reaction was carried out under an atmosphere of N_2.

V. Kinetic Isotope Experiments:

In a 20 mL sealed tube containing **1** (48.7 mg, 0.2 mmol) or the deuterated starting material **1-*d*$_7$** (49.7 mg, 0.2 mmol), *N*-benzylmaleimide (**2**) (112.3 mg, 0.6 mmol), $[Rh(COD)Cl]_2$ (4.9 mg, 0.01 mmol), pivalic acid (61.3 mg, 0.6 mmol) the reaction was stirred in an aerobic atmosphere at 140 ºC. After stirring for 10 h, the mixture was diluted with ethyl acetate (5 mL) and filtered through a short pad of celite pad, which was then washed three times with ethyl acetate (3 × 3 mL). The combined filtrates were concentrated under reduced pressure and the crude mixture was analyzed by ^{1}H NMR to calculate the yield of the product and the remaining starting material. The experiment was conducted using parallel reaction conditions. Product yields were determined at 2 h intervals from 4 h to 12 h. In addition, the ratio of the two products was determined by ^{1}H NMR spectra of a mixture of **3c** and **1** or **3c-*d*$_4$** and **1-*d*$_5$** and the results are listed in the table below. Using these findings, the slope of the yield curve for both substrates was taken as k_H and k_D to determinate value KIE. KIE = k_H/k_D = 2.50.

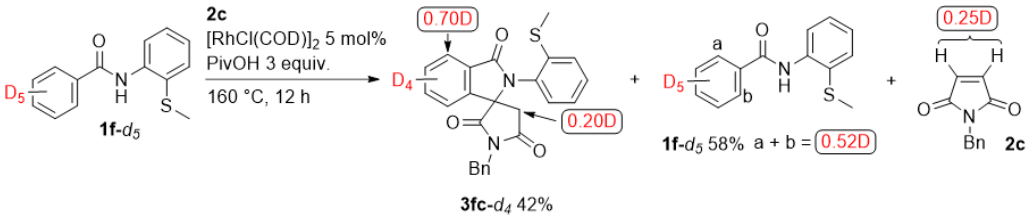
1. Table S4: Reaction Values of Kinetic Isotopic Effect.

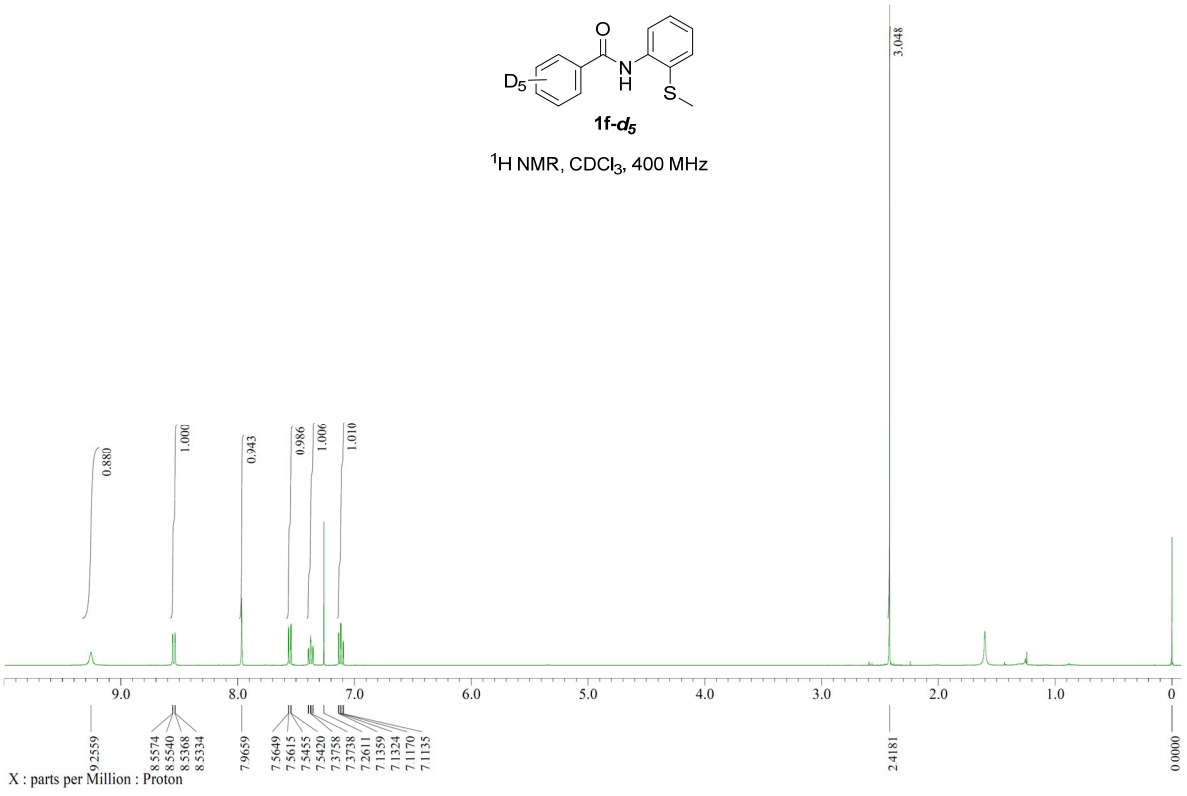
Time	k_H	k_D	k_H/k_D
4 h	32.25	16.26	1.983
6 h	38.01	20.61	1.844
8 h	44.74	22.71	1.970
10 h	45.33	23.44	1.933
12 h	58.75	26.91	2.183
Average	43.816	21.986	1.9826

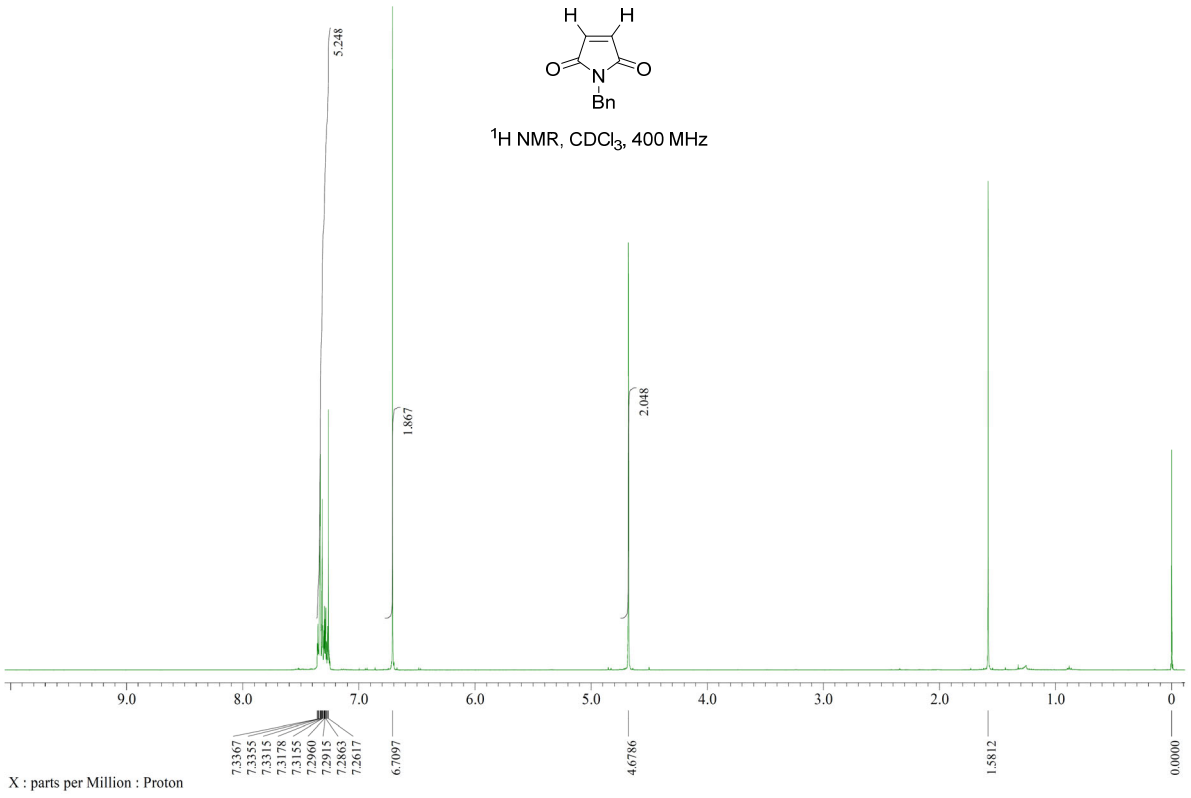


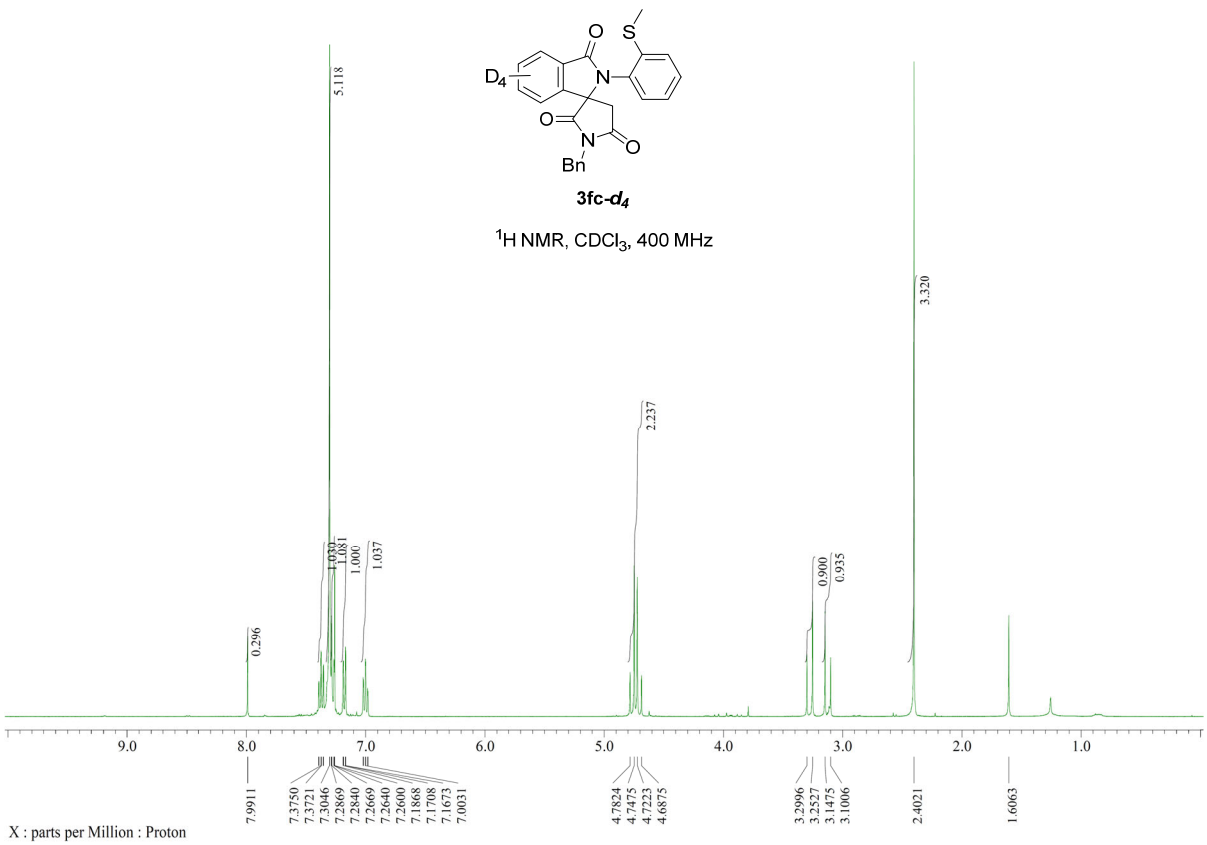
2. Deuterium Labelling Experiments:

Scheme S1: Deuterium labeling experiment using deuterated N-(2-(methylthio)phenyl) benzamide.

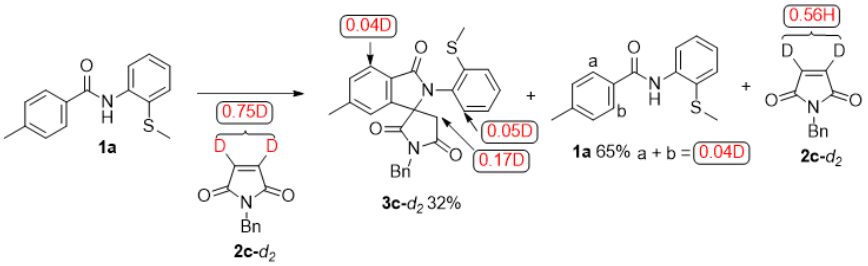


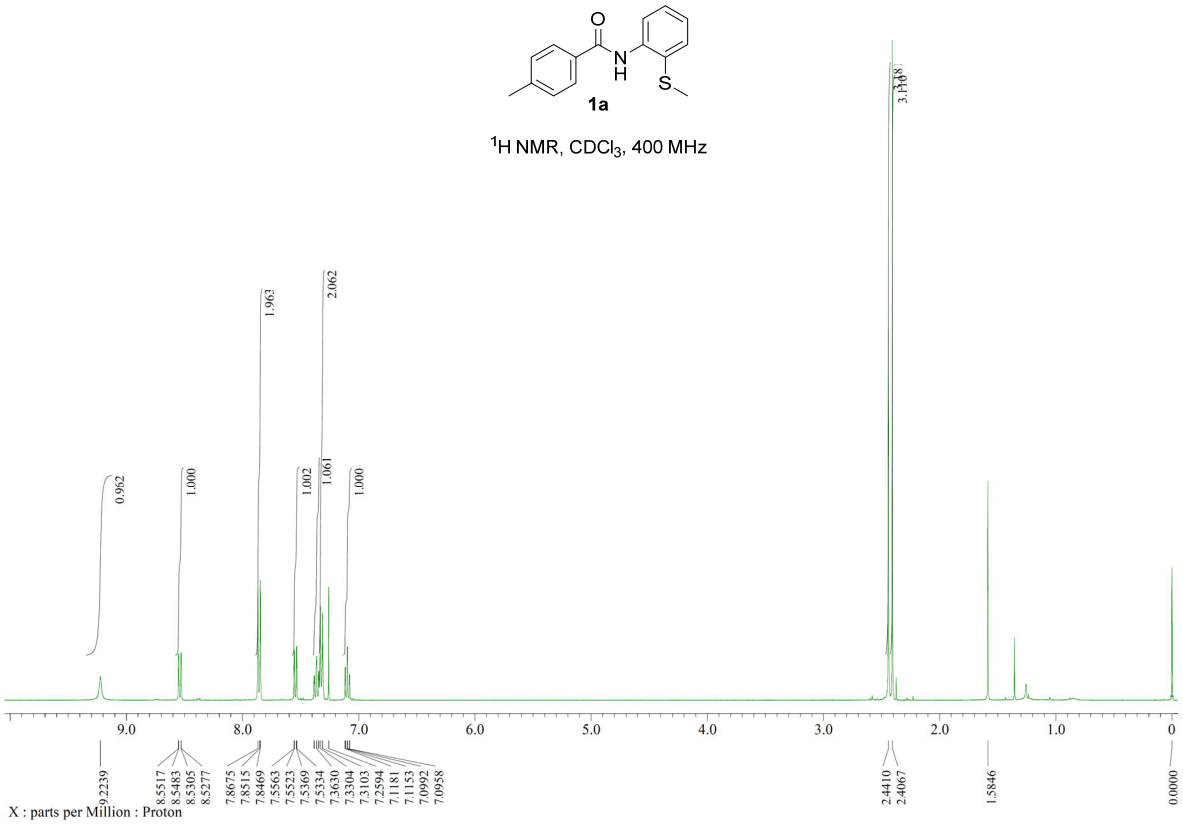


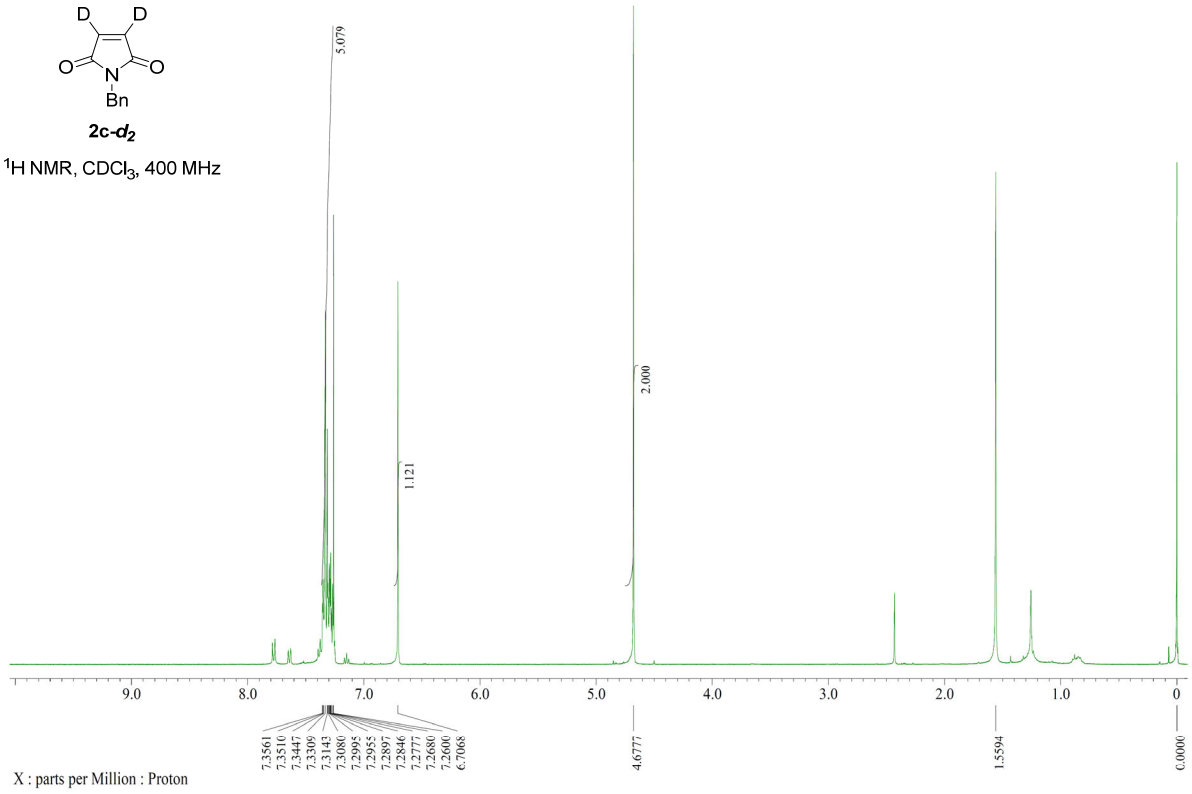

H
H
O
O
N
Bn
^{1}H NMR, CDCl$_3$, 400 MHz
5.248
1.867
2.048
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.3367
7.3355
7.3315
7.3178
7.3155
7.2960
7.2915
7.2863
7.2617
6.7097
4.6786
1.5812
0.0000
X : parts per Million : Proton


O
S
D$_4$
N
O
N
O
Bn
3fc-*d*$_4$
^{1}H NMR, CDCl$_3$, 400 MHz
5.118
3.320
2.237
0.900
0.935
1.030
1.081
1.000
1.037
0.296
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.9911
7.3750
7.3721
7.3046
7.2869
7.2840
7.2669
7.2640
7.2600
7.1868
7.1708
7.1673
7.0031
4.7824
4.7475
4.7223
4.6875
3.2996
3.2527
3.1475
3.1006
2.4021
1.6063
X : parts per Million : Proton

Scheme S2: Deuterium labeling experiment using deuterated *N*-benzylmaleimide.

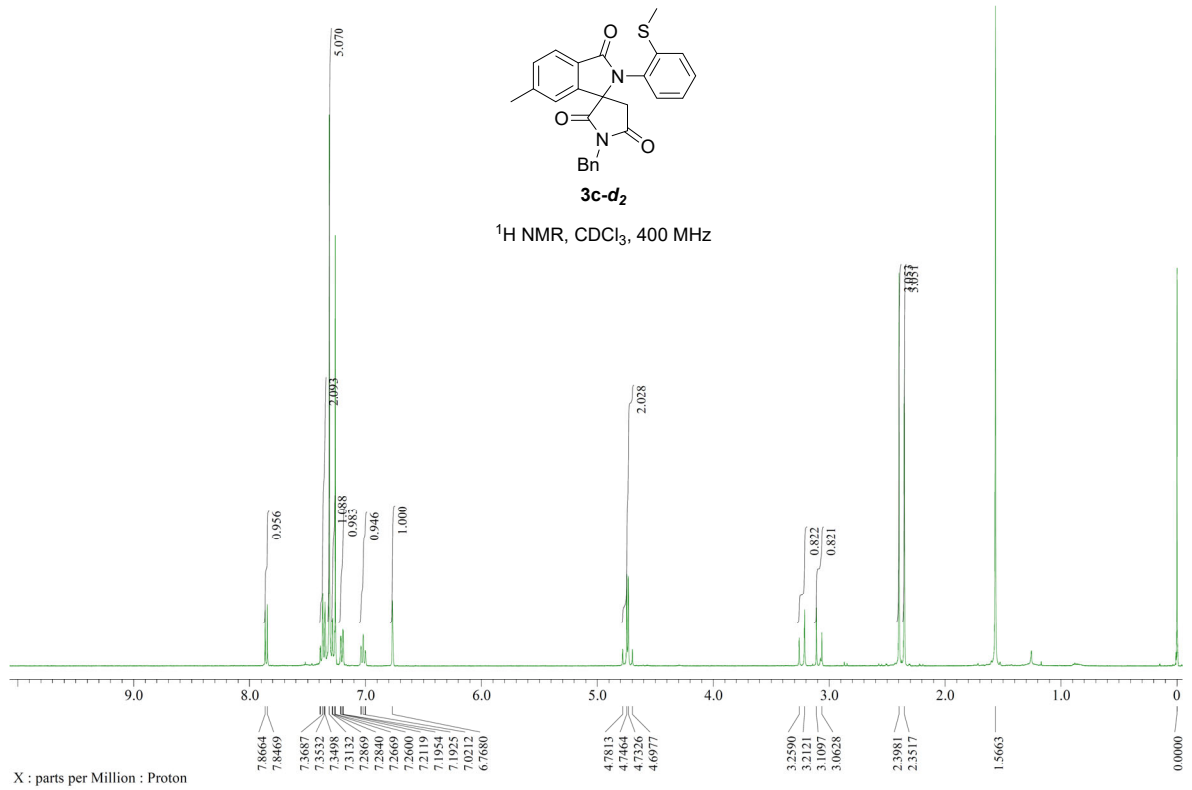






2c-d_2

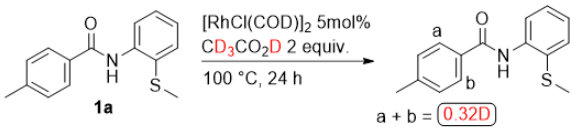
^{1}H NMR, $CDCl_3$, 400 MHz

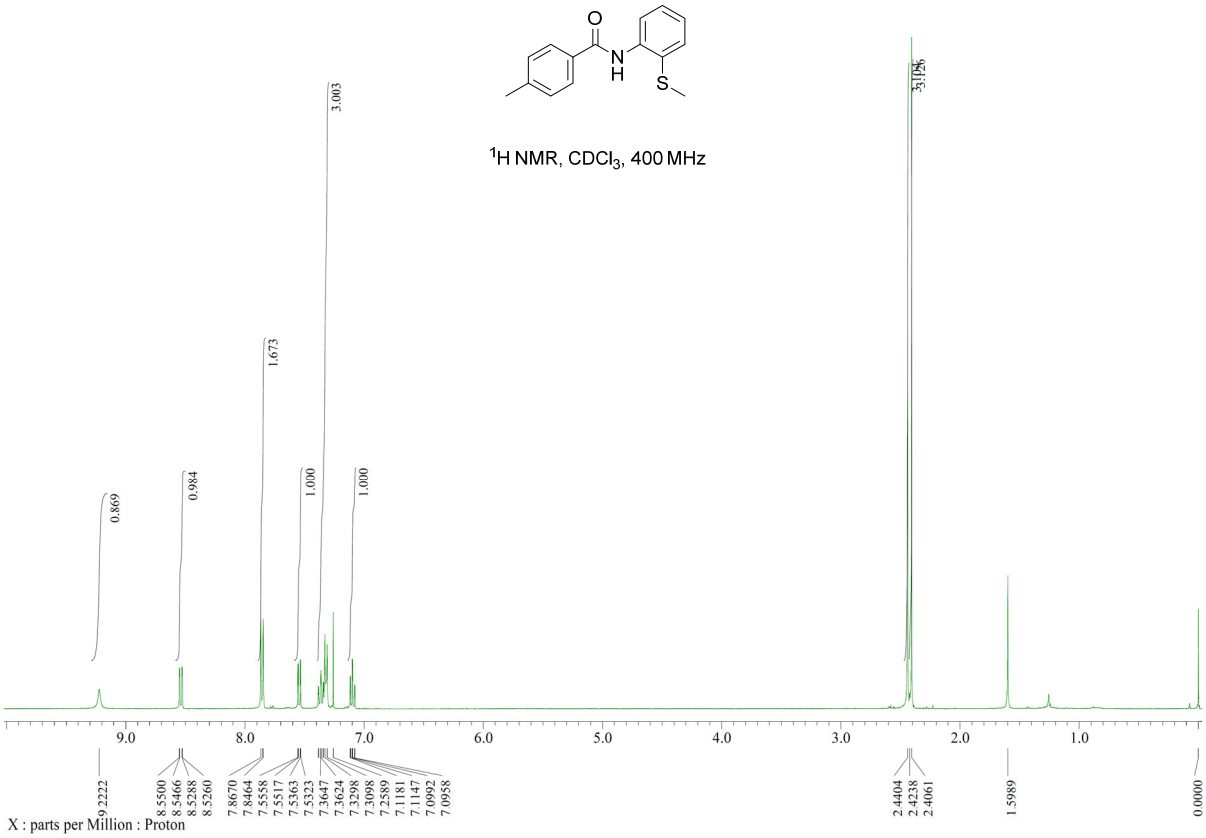


3c-d_2

^{1}H NMR, $CDCl_3$, 400 MHz

Scheme S3: Deuterium labeling experiment using CD_3CO_2D.





VI. General Procedure for the Rh(I)-Catalyzed Reaction of Aromatic Amides with Maleimides:

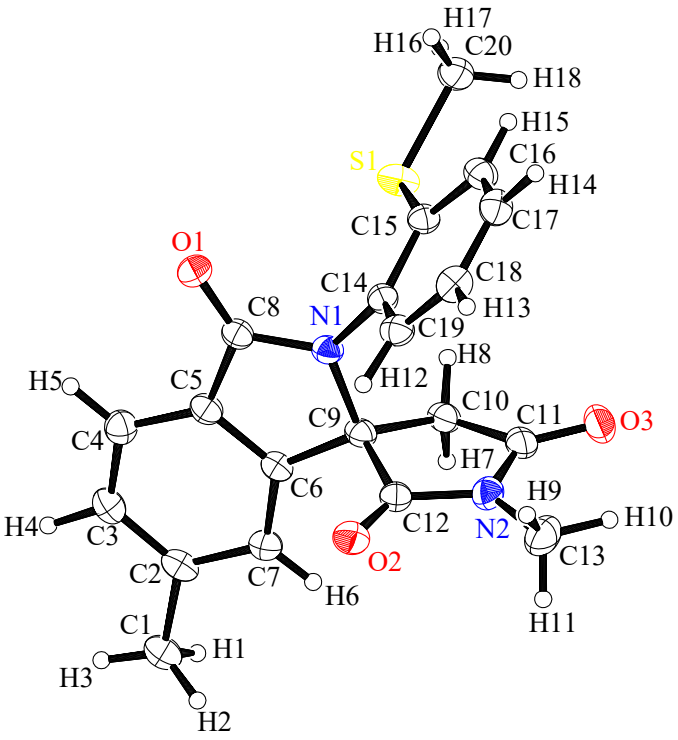
After oven-drying a 20 mL screw-capped vial, 4-methyl-*N*-(2-(methylthio)phenyl)benzamide (**1a**) (25.7 mg, 0.1 mmol), *N*-methylmaleimide (**2a**; 33.3 mg, 0.3 mmol), $[RhCl(COD)]_2$ (2.5 mg, 0.005 mmol), and pivalic acid (30.6 mg, 0.3 mmol) were added. The mixture was stirred at 160 °C for 24 h and then allowed to cool to room temperature. The resulting mixture was filtered through a celite pad, and the organic phase was concentrated in vacuo. The residue was purified by column chromatography (hexane/Et_2O = 2/8 as the eluent) to afford the desired product **3aa** (33.3 mg, 91%) as a pale-orange solid.

In the case of a 2 g scale synthesis of **3ac**: In an oven dried 40 mL seal tube, 4-methyl-*N*-(2-(methylthio)phenyl)benzamide (**1a**) (2 g, 7.77 mmol), *N*-benzylmaleimide (4.363 g, 23.31 mmol) (**2c**), $[Rh(COD)Cl]_2$ (191.6 mg, 0.388 mmol), and pivalic acid (2.380 g, 23.31 mmol) were added. The mixture was stirred at 160 °C for 24 h in an oil bath and then allowed to cool to room temperature. After completion of the reaction, the mixture was filtered through a celite pad, and the filtrate was then concentrated in vacuo. The residue was purified by column chromatography on (eluent: hexane/Et_2O = 2/8) to afford the desired products **3c** (2.758 g, 81%) as a light yellow solid.

VII. X-Ray Crystallographic Structure Analysis:

CCDC 1966217 contains the supplementary crystallographic data. X-Ray crystallographic structure analysis of 1',6-dimethyl-2-(2-(methylthio)phenyl)spiro[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (**3a**) was performed on Rigaku XtaLAB P200 imaging plate diffractometer with graphite monochromated Cu Kα radiation. The data was collected at 150 K±1 K using ω scan in the 2θ range of 68.16º. A total of 21993 reflection were measured, of which 5543 were independent reflections (Rint = 0.0484). The structure was solved by direct methods (SIR92) and refined by the full matrix least-squares on F2 (Crystals). All nonhydrogen atoms were refined anisotropically and all hydrogen atoms were placed using riding model. The crystal data are as follows: (**3aa_CCDC 1966217**):

A. Crystal Data	
Empirical Formula	$C_{20}\ H_{18}\ N_2\ O_3\ S$
Formula Weight	366.43
Crystal Color, Habit	Colorless crystal
Crystal Description	Plate
Crystal Dimensions	0.05 x 0.5 x 0.6
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 7.3302(6) Å
	b = 7.6156(5) Å
	c = 15.7854(10) Å
	a = 85.339(5) º
	b = 82.972(6) º
	g = 83.511(6) º
	V = 866.94(11) $Å^3$
Space Group P-1 (#2)	
Z value 2	
D_{calc}	1.404 g/cm^3
Radiation Type	Cu K\a
Radiation Wavelength	1.54184
Measurement Temperature	148ºC
F000	384.00
m(CuKa)	71.294 cm^{-1}


H17
H16
C20
H18
H15
S1
C16
H14
C15
C17
O1
C18
C14
C8
N1
H13
C19
H8
H5
C5
H12
C10
C9
C11
O3
C4
H7
C6
H9
H4
C3
C12
N2
H10
O2
C13
C2
C7
H6
C1
H1
H3
H11
H2

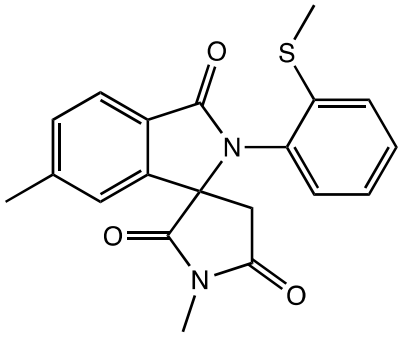
1. **Table S5: Bond lengths (Å)**

atom	atom	distance	atom	atom	distance
S1	C15	1.760(2)	C6	C9	1.509(3)
S1	C20	1.802(3)	C7	H6	0.91(2)
O1	C8	1.222(3)	C9	C10	1.536(3)
O2	C12	1.202(3)	C9	C12	1.547(3)
O3	C11	1.207(3)	C10	C11	1.506(4)
N1	C8	1.378(3)	C10	H7	0.94(3)
N1	C14	1.441(3)	C10	H8	0.95(3)
N1	C9	1.480(3)	C13	H9	0.93(5)
N2	C12	1.375(3)	C13	H10	1.04(6)
N2	C11	1.387(4)	C13	H11	0.94(5)
N2	C13	1.457(4)	C14	C19	1.390(3)
C1	C2	1.506(3)	C14	C15	1.405(3)
C1	H1	0.90(6)	C15	C16	1.395(3)
C1	H2	0.98(5)	C16	C17	1.383(4)
C1	H3	0.94(6)	C16	C15	0.92(3)
C2	C7	1.394(3)	C17	C18	1.373(4)
C2	C3	1.401(3)	C17	H14	0.99(3)
C3	C4	1.384(3)	C18	C19	1.391(3)
C3	H4	1.03(3)	C18	H13	0.87(3)
C4	C5	1.391(3)	C19	H12	1.00(3)
C4	H5	0.98(2)	C20	H16	1.01(4)
C5	C6	1.381(3)	C20	H17	0.99(3)
C5	C8	1.488(3)	C20	H18	0.94(3)

2. Table S6: Bond angles (º)

atom	atom	atom	angle	atom	atom	atom	angle
C15	S1	C20	102.51(12)	C11	C10	H7	103.3(18)
C8	N1	C14	124.34(17)	C9	C10	H7	110.1(18)
C8	N1	C9	113.48(17)	C11	C10	H8	113.2(15)
C14	N1	C9	121.67(17)	C9	C10	H8	112.0(15)
C12	N2	C11	113.2(2)	H7	C10	H8	113(2)
C12	N2	C13	122.3(2)	O3	C11	N2	124.6(3)
C11	N2	C13	124.4(2)	O3	C11	C10	127.3(3)
C2	C1	H1	108(4)	N2	NC11	C10	108.09(19)
C2	C1	H2	109(3)	O2	C12	N2	125.5(2)
H1	C1	H2	93(4)	O2	C12	C9	126.7(2)
C2	C1	H3	111(4)	N2	C12	C9	107.6(2)
H1	C1	H3	113(5)	N2	C13	H9	111(3)
H2	C1	H3	120(5)	N2	C13	H10	107(3)
C7	C2	C3	119.4(2)	H9	C13	H10	110(4)
C7	C2	C1	120.2(2)	N2	C13	H11	114(2)
C3	C2	C1	120.3(2)	H9	C13	H11	111(4)
C4	C3	C2	122.2(2)	H10	C13	H11	103(4)
C4	C3	H4	123.0(16)	C19	C14	C15	120.42(19)
C2	C3	H4	114.8(16)	C19	C14	N1	119.4(2)
C3	C4	C5	117.6(2)	C15	C14	N1	120.12(19)
C3	C4	H5	121.4(14)	C16	C15	C14	118.5(2)
C5	C4	H5	121.0(14)	C16	C15	S1	123.49(19)
C6	C5	C4	120.9(2)	C14	C15	S1	118.04(15)
C6	C5	C8	109.38(19)	C17	C16	C15	120.4(2)
C4	C5	C8	129.6(2)	C17	C16	H15	121.0(16)
C5	C6	C7	121.5(2)	C15	C16	H15	118.6(16)
C5	C6	C9	110.00(18)	C18	C17	C16	121.1(2)
C7	C6	C9	128.4(2)	C18	C17	H14	120.3(19)
C6	C7	C2	118.3(2)	C16	C17	H14	118.6(19)
C6	C7	H6	119.3(14)	C17	C18	C19	119.6(2)
C2	C7	H6	122.4(14)	C17	C18	H13	121(2)
O1	C8	N1	125.77(19)	C19	C18	H13	120(2)
O1	C8	C5	128.7(2)	C14	C19	C18	120.0(2)
N1	C8	C5	105.57(18)	C14	C19	H12	118.6(14)
N1	C9	C6	101.56(16)	C18	C19	H12	121.4(14)
N1	C9	C10	113.17(18)	S1	C20	H16	106(2)
C6	C9	C10	117.53(18)	S1	C20	H17	104.9(18)
N1	C9	C12	108.57(17)	H16	C20	H17	112(3)
C6	C9	C12	113.33(18)	S1	C20	H18	112.8(18)
C10	C9	C12	102.76(18)	H16	C20	H18	112(2)
C11	C10	C9	104.2(2)	H17	C20	H18	108(3)

VIII. Spectroscopic Data of Products:



1',6-dimethyl-2-(2-(methylthio)phenyl)spiro[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3aa)

91% yield. R_f = 0.13 (hexane/EtOAc = 6/4). An orange solid. Mp = 193.5 ºC

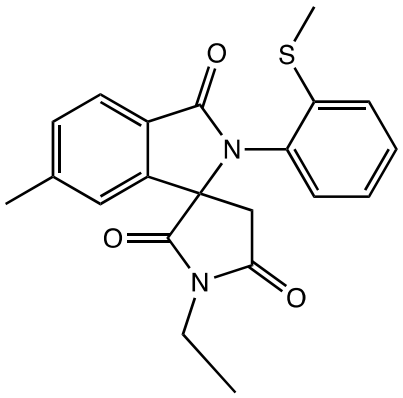
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.88 (d, *J* = 7.8 Hz, 1H), 7.39-7.44 (m, 2H), 7.29-7.32 (m, 2H), 7.17-7.21 (m, 1H), 7.07 (s, 1H), 3.29 (d, *J* = 18.9 Hz, 1H), 3.14 (d, *J* = 18.9 Hz, 1H), 3.10 (s, 3 H), 2.48 (s, 3H), 2.41 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 175.1, 173.8, 167.5, 144.7, 144.4, 140.7, 131.8, 131.1, 130.4, 130.1, 128,2, 126.2, 126.0, 125.1, 120.5, 70.6, 36.9, 25.9, 22.2, 15.0.

IR (ATR) (neat, ν/cm^{-1}): 2971 w, 2926 w, 2360 w, 1712 s, 1616 w, 1435 w, 1356 m, 1219 w, 1204 w.

MS m/z (relative intensity, %): 366 (M^+, 21), 320 (23), 266 (28), 234 (10).

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{21}H_{20}N_2O_3S$: 366.1038; Found: 366.1189.



1'-ethyl-6-methyl-2-(2-(methylthio)phenyl)spiro[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3ab)

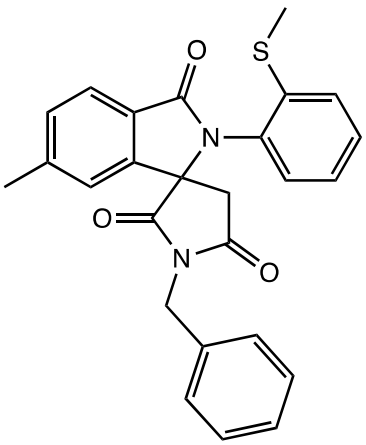
96% yield. R_f = 0.26 (hexane/EtOAc = 6/4). A pale yellow solid. Mp = 194.4 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.88 (d, *J* = 7.8 Hz, 1H), 7.38-7.43 (m, 2H), 7.29-7.32 (m, 2H), 7.17 (td, *J* = 7.6 Hz and 1.4 Hz, 1H) 7.06 (d, *J* = 0.5 Hz, 1H), 3.65 (q, *J* = 7.2 Hz, 2H), 3.26 (d, *J* = 18.7 Hz, 1H), 3.10 (d, *J* = 18.7 Hz, 1H), 2.47 (s, 3H), 2.41 (s, 3H), 1.17 (t, *J* = 7.2 Hz, 3H)

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.8, 173.5, 167.5, 144.8, 144.3, 140.6, 131.8, 131.1, 130.3, 130.0, 128.3, 126.0, 126.0, 125.1, 120.5, 70.3, 36.9, 34.8, 22.2, 14.9, 13.1.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{20}H_{18}N_2O_3S$: 380.1195; Found: 380.1189.

1'-benzyl-6-methyl-2-(2-(methylthio)phenyl)spiro[iso-indoline-1,3'-pyrrolidine]-2',3,5'-trione (3ac)



99% yield. R_f = 0.18 (hexane/EtOAc = 6/4). A white solid. Mp = 212.3 ºC

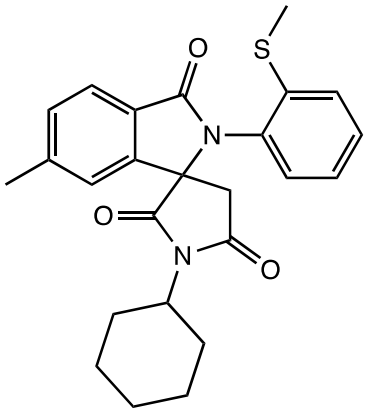
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.85 (d, *J* = 7.8 Hz, 1H), 7.34-7.39 (m, 2H), 7.19-7.39 (c, 7H), 7.01 (dd, *J* = 7.6. Hz and 1.4 Hz, 1H), 6.77 (t, *J* = 1.4 Hz, 1H), 4.76 (d, *J* = 12.2 Hz, 1H), 4.71 (d, *J* = 12.2 Hz, 1H), 3.23 (d, *J* = 18.7 Hz, 1H), 3.09 (d, *J* = 18.7 Hz, 1H), 2.39 (s, 3H), 2.34 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.6, 173.2, 167.5, 144.7, 144.3, 140.5, 135.2, 131.7, 131.0, 130.2, 130.1, 128.9, 128.9, 128.5, 128.1, 126.0, 125.9, 125.1,120.5, 70.3, 43.3, 36.9, 22.0, 15.0.

IR (ATR) (neat, ν/cm^{-1}): 3340 w, 3033 w, 2921 w, 2360 w, 2338 w, 1713 s, 1390 m, 1352 m, 1173 m, 756 w, 702 m.

MS m/z (relative intensity, %): 442 (M^+, 29), 396 (27), 395 (100), 266 (32), 91(11).

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{26}H_{22}N_2O_3S$: 442.1351; Found: 442.1351.



1'-cyclohexyl-6-methyl-2-(2-(methylthio)phenyl)spiro[indene-1,3'-pyrrolidine]-2',3,5'(2H)-trione (3ad)

80% yield. R_f = 0.23 (hexane/Et_2O = 3/7). A white solid. Mp = 169.9 ºC

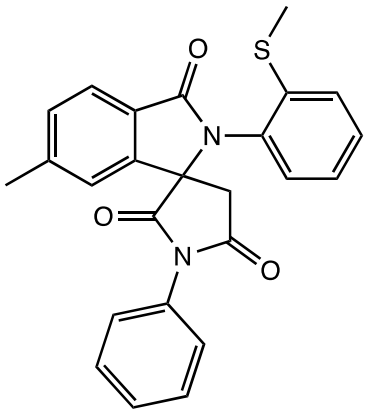
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.37-7.43 (m, 2H), 7.15-7.20 (m, 1H), 7.15-7.20 (m, 1H), 7.03 (d, *J* = 1.1 Hz, 1H), 3.95-4.95 (m, 1H), 3.20 (d, *J* = 18.5 Hz, 1H), 3.06 (d, *J* = 18.5 Hz, 1H), 2.47 (s, 3H), 2.41 (s, 3H), 2.01-2.24 (m, 2H), 1.82-1.84 (m, 2H), 1.54-1.67 (m, 3H), 1.17-1.37 (m, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.9, 173.8, 167.6, 145.1, 144.3, 140.7, 132.0, 131.0, 130.3, 130.0, 128.4, 126.1, 126.0, 125.1, 120.3, 70.0, 52.8, 36.7, 29.1, 28.9, 25.9, 25.8, 25.0, 22.2, 15.0.

IR (ATR) (neat, ν/cm^{-1}): 2930 w, 2853 w, 2360 w, 1710 s, 1351 m, 1199 w, 1054 w, 757 w.

MS m/z (relative intensity, %): 434 (M^+, 22), 388 (26), 387 (100), 266 (45), 234 (11).

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{25}H_{26}N_2O_3S$: 434.1664; Found: 434.1665.



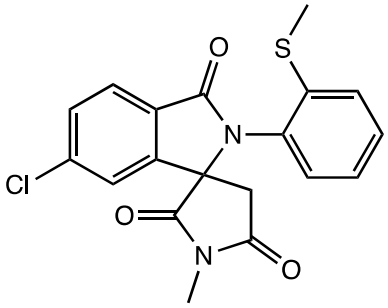
6-methyl-2-(2-(methylthio)phenyl)-1'-phenylspiro[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3ae)

65% yield. R_f = 0.23 (hexane/EtOAc = 6/4). A golden solid. Mp = 103.1 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91 (d, *J* = 8.0 Hz, 1H), 7.40-7.51 (c, 7H), 7.32-7.35 (m, 1H), 7.20-7.26 (c, 2H), 3.48 (d, *J* = 18.8 Hz), 3.30 (d, *J* = 18.8 Hz), 2.51 (s, 3H), 2.44 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.0, 172.7, 167.6, 144.7, 144.5, 140.78, 131.83, 131.43, 131.28, 130.48, 130.23, 129.49, 129.31, 128.31, 126.3, 126.2, 126.1, 125.3, 120.5, 70.5, 37.1, 22.2, 15.0.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{25}H_{20}N_2O_3S$: 428.1195; Found: 428.1190.



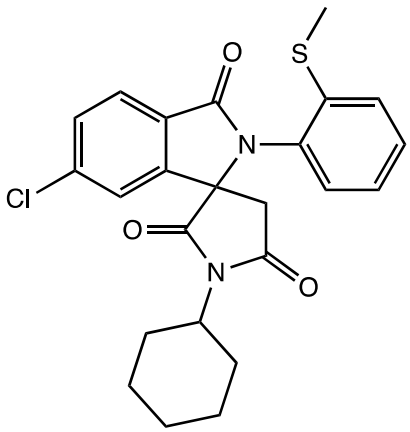
6-chloro-1'-methyl-2-(2-(methylthio)phenyl)spiro[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3ba)

72% yield. R_f = 0.33 (hexane/Et_2O = 3/7). A yellow solid. Mp = 213.7 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (dd, *J* = 8.2 Hz and 0.8 Hz, 1H), 7.58 (dd, *J* = 8.0 Hz and 1.6 Hz, 1H), 7.43 (td, *J* = 8.0 Hz and 1.6 Hz, 1H), 7.27-7.30 (c, 3H), 7.19 (td, *J* = 7.6. Hz and 1.4 Hz, 1H), 3.31 (d, *J* = 18.8 Hz, 1H), 3.14 (d, *J* = 18.8 Hz, 1H), 3.10 (s, 3H), 2.42 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.33, 173.1, 166.3, 145.7, 140.6, 139.6, 131.5, 130.8, 130.6, 129.9, 129.4, 126.5, 126.3, 120.869, 70.4, 36.7, 26.0, 15.0.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{19}H_{15}ClN_2O_3S$: 386.0492; Found: 386.0492.



6-chloro-1'-cyclohexyl-2-(2-(methylthio)phenyl)spiro-[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3bd)

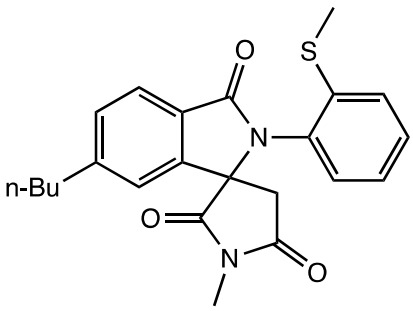
86% yield. R_f = 0.43 (hexane/Et_2O = 3/7). A light yellow solid. Mp = 211.1 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (dd, *J* = 8.0 Hz and 0.5 Hz, 1H), 7.57 (dd, *J* = 7.7 Hz and 1.6 Hz, 1H), 7.42 (td, *J* = 7.7 Hz and 1.6 Hz, 1H), 7.25-7.32 (c, 3H), 7.18 (td, *J* = 7.7 Hz and 1.4 Hz, 1H), 4.03-

4.95 (m, 1H), 3.22 (d, J = 18.8 Hz, 1H), 3.07 (d, J = 18.8 Hz, 1H), 2.42 (s, 3H), 2.00-2.19 (m, 2H), 1.80-1.90 (c, 2H), 1.51-1.70 (c, 3H), 1.17-1.37 (m, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.2, 173.1, 166.4, 146.0, 140.5, 139.5, 131.4, 130.6, 130.5, 129.8, 129.5, 126.5, 126.2, 126.1, 120.6, 69.7, 53.0, 36.4, 29.0, 28.8, 25.8, 25.8, 25.0,15.0.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{24}H_{23}N_2O_3S$: 454.1118; Found: 454.1119.



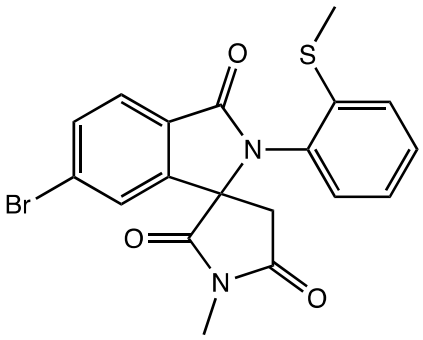
6-butyl-1'-methyl-2-(2-(methylthio)phenyl)spiro[iso-indoline-1,3'-pyrrolidine]-2',3,5'-trione (3ca)

92% yield. R_f = 0.32 (hexane/Et_2O = 3/7). An orange solid. Mp = 100.5 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.89 (d, J = 8.0 Hz, 1H), 7.39-7.44 (m, 2H), 7.29-7.32 (m, 2H), 7.16-7.21 (m, 1H), 7.05 (d, J = 0.5 Hz, 1H), 3.29 (d, J = 18.3 Hz, 1H), 3.13 (d, J = 18.3 Hz, 1H), 3.09 (s, 3H), 2.69-2.73 (m, 2H), 2.41 (s, 3H), 1.59-1.66 (m, 2H), 1.36-1.41 (m, 2H), 0.92 (t, J = 7.3 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100.53 MHz): δ 175.11, 173.8, 167.6, 149.4, 144.6, 140.7, 131.9, 130.5, 130.3, 130.1, 128.4, 126.1, 126.1, 125.1, 119.8, 70.6, 37.0, 36.3, 33.7, 25.9, 22.6, 15.0, 14.0.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{23}H_{24}N_2O_3S$: 408.1508; Found: 406.1509.



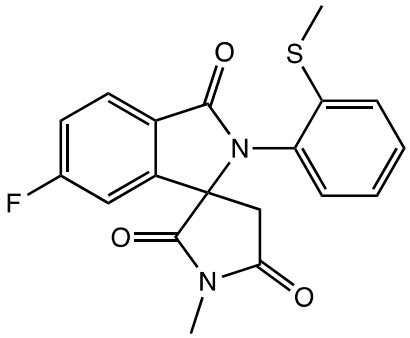
6-bromo-1'-methyl-2-(2-(methylthio)phenyl)spiro[iso-indoline-1,3'-pyrrolidine]-2',3,5'-trione (3da)

84% yield. R_f = 0.27 (hexane/Et_2O = 3/7). A light orange solid. Mp = 225.1 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86 (d, J = 8.2 Hz, 1H), 7.74 (dd, J = 8.2 Hz and 1.5 Hz, 1H), 7.41-7.45 (m, 2H), 7.26-7.31(m, 2H), 7.18 (td, J = 7.6 Hz and 1.4 Hz, 1H), 3.30 (d, J = 18.8 Hz, 1H), 3.15 (d, J = 18.8 Hz, 1H), 3.10 (s, 3H), 2.42 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.3, 173.2, 166.4, 145.8, 140.5, 133.6, 131.2, 130.6, 129.8, 129.8, 127.9, 126.7, 126.2, 126.1, 123.8, 70.3, 36.6, 26.0, 14.9.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{19}H_{15}BrN_2O_3S$: 429.9987; Found: 429.9980



6-fluoro-1'-methyl-2-(2-(methylthio)phenyl)spiro[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3ea)

91% yield. R_f = 0.23 (hexane/Et_2O = 3/7). A white solid. Mp = 210.1 ºC

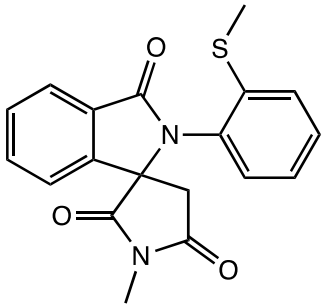
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.99 (dd, *J* = 8.2 Hz and 4.8 Hz, 1H), 7.43 (td, *J* = 7.7 Hz and 1.3 Hz, 1H), 7.24-7.32 (m, 3H), 7.19 (td, *J* = 7.5 Hz and 1.1 Hz, 1H), 6.99 (dd, *J* = 7.5 Hz and 2.0 Hz, 1H), 3.31 (d, *J* = 18.8 Hz, 1H), 3.14 (d, *J* = 18.8 Hz, 1H), 3.09 (s, 3H), 2.42 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.3, 173.2, 166.3, 165.9 (*J* = 253 Hz), 146.4 (d, *J* = 9.6 Hz), 140.5, 131.4, 130.6, 129.9, 127.5 (d, *J* = 9.6 Hz), 126.9, 126.1 (d, *J* = 15.3 Hz), 117.97 (d, *J* = 23.0 Hz), 108.04 (d, *J* = 24.9 Hz), 70.3, 36.7, 26.0, 14.9.

IR (ATR) (neat, ν/cm^{-1}): 3064 w, 2925 w, 2855 w, 1711 s, 1606 m, 1469 m, 1435 m, 1355 m, 1240 m, 1140 w, 1049 w, 757 w.

MS m/z (relative intensity, %): 370 (M+, 29), 324 (20), 323 (100), 270 (40), 238 (13).

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{19}H_{15}FN_2O_3S$: 370.0787; Found: 370.0783.



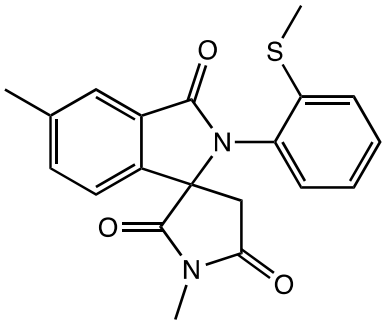
1'-methyl-2-(2-(methylthio)phenyl)spiro[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3fa)

64% yield. R_f = 0.20 (hexane/Et_2O = 3/7). A ivory solid. Mp = 229.3 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.99-8.02 (m, 1H), 7.58-7.66 (m, 2H), 7.41-7.45 (m, 1H), 7.28-7.32 (m, 3H), 7.19 (td, *J* = 7.6 Hz and 1.4 Hz, 1H), 3.31 (d, *J* = 18.7 Hz, 1H), 3.15 (d, *J* = 18.7 Hz, 1H), 3.09 (s, 3H), 2.41 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.9, 173.7, 167.5, 144.3, 140.6, 133.3, 131.7, 130.8, 130.4, 130.2, 130.0, 126.2, 126.1, 125.3, 120.2, 70.8, 36.9, 25.9, 15.0.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{19}H_{16}N_2O_3S$: 352.0882; Found: 352.0878.



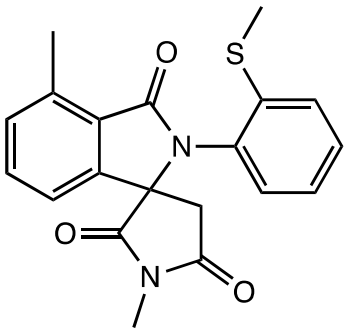
1',5-dimethyl-2-(2-(methylthio)phenyl)spiro[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3ga)

94% yield. R_f = 0.22 (hexane/EtOAc = 7/3). A golden solid. Mp = 180.3 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.81 (q, *J* = 0.7 Hz, 1H), 7.40-7.46 (m, 2H), 7.29-7.32 (m, 2H), 7.17-7.21 (m, 2H), 3.27 (d, *J* = 18.9 Hz, 1H), 3.12 (d, *J* = 18.9 Hz, 1H), 3.08 (s, 3H), 2.48 (s, 3H), 2.42 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 175.1, 173.7, 167.7, 141.6, 140.6, 134.2, 131.9, 130.9, 130.384, 130.0, 126.2, 126,1, 125.5, 119.9, 70.6, 36.9, 25.8, 21.6, 15.0.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{20}H_{18}N_2O_3S$: 366.1038; Found: 366.1337.



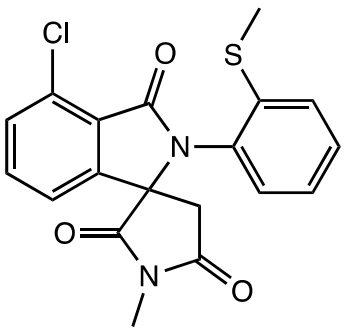
1',4-dimethyl-2-(2-(methylthio)phenyl)spiro[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3ha)

60% yield. R_f = 0.32 (hexane/Et_2O = 3/7). A light orange solid. Mp = 158.7 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49 (t, J= 7.5 Hz, 1H), 7.42 (td, *J* = 7.8 Hz, and1.4 Hz, 1H), 7.27-7.34 (m, 3), 7.18 (td, *J* = 7.8 Hz and 1.3 Hz, 1), 7.08 (d, *J* = 7.8 Hz, 1H), 3.32 (d, *J* = 18.8 Hz, 1H), 3.13 (d, *J* = 18.8 Hz, 1H), 3.08 (s, 3H), 2.78 (s, 3H), 2.40 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 175.2, 173.8, 168.2, 144.9, 140.7, 139.7, 132.7, 132.2, 132.0, 130.3, 130.2, 127.8, 126.1, 125.8, 117.4, 70.1, 37.2, 25.8, 17.4, 14.9.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{20}H_{18}N_2O_3S$: 366.1038; Found: 406.1323.



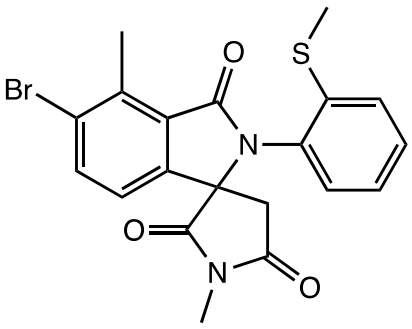
4-chloro-1'-methyl-2-(2-(methylthio)phenyl)spiro[iso-indoline-1,3'-pyrrolidine]-2',3,5'-trione (3ia)

81% yield. R_f = 0.19 (hexane/Et_2O = 2/8). A beige solid. Mp = 146.3 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.54 (t, *J* = 2.7 Hz, 2H), 7.41-7.45 (m, 1H), 7.28-7.31 (m, 2H), 7.17-7.21 (m, 2H), 3.33 (d, *J* = 18.3 Hz, 1H), 3.12 (d, *J* = 18.7 Hz, 1H), 3.08 (s, 3H), 2.42 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.5, 173.4, 164.9, 146.5, 140.6, 133.88, 133.3, 131.9, 131.5, 130.6, 130.1, 127.0, 126.2, 126.1, 118.7, 69.7, 37.0, 26.0,15.0.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{19}H_{15}ClN_2O_3S$: 386.0492; Found: 386.0487.



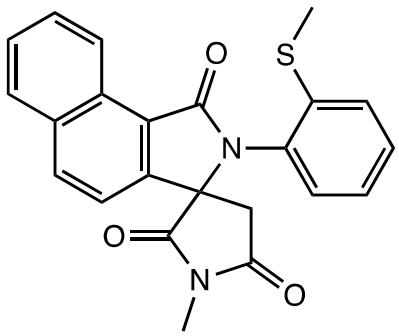
5-bromo-1',4-dimethyl-2-(2-(methylthio)phenyl)spiro-[isoindoline-1,3'-pyrrolidine]-2',3,5'-trione (3ja)

74% yield. R_f = 0.35 (hexane/ Et_2O = 3/7). A light orange solid. Mp = 238.4 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49 (d, *J* = 7.8 Hz, 1H), 7.42 (td, *J* = 7.5 Hz and 1.4 Hz, 1H), 7.28-7.30 (m, 2H), 7.18 (td, *J* = 7.8 Hz and 1.4 Hz, 1H), 7.11 (d, *J* = 7.8 Hz, 1H), 3.33 (d, *J* = 18.6Hz, 1H), 3.11 (d, *J* = 18.6 Hz, 1H), 3.07 (s, 3H), 2.53 (s, 3H), 2.41 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.7, 173.5, 165.6, 144.2, 141.7, 140.6, 135.0, 131.6, 130.5, 130.1, 128.6, 126.1, 125.9,122.9, 118.6, 68.8, 37.0, 25.9, 22.8, 14.9.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{20}H_{17}BrN_2O_3S$: 444.0143; Found: 444.0129.



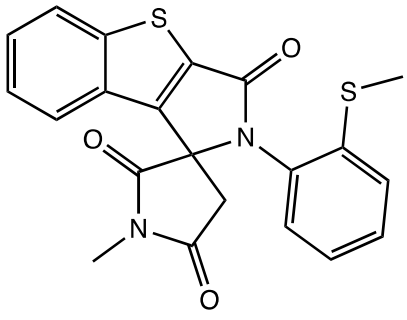
1'-methyl-2-(2-(methylthio)phenyl)spiro[benzo[*e*]iso-indole-3,3'-pyrrolidine]-1,2',5'(2*H*)-trione (3ka)

90% yield. R_f = 0.25 (hexane/EtOAc = 7/3). A white solid. Mp = 273.2 ºC

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.25 (dt, *J* = 8.5 Hz and 0.5 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.71-7.75 (m, 1H), 7.63-7.66 (m, 1H), 7.42-7.47 (m, 1H), 7.30-7.38 (m, 3H), 7.19-7.23 (m, 1H), 3.40 (d, *J* = 18.8 Hz, 1H), 3.23 (d, *J* = 18.8 Hz, 1H), 3.12 (s, 3H), 2.42 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.8, 173.7, 168.4, 144.1, 140.8, 134.6, 134.0, 131.9, 130.4, 130.2, 129.6, 129.1, 128.4, 127.7, 126.1, 125.9, 125.2, 124.6, 116.6, 70.5, 36.5, 26.0, 14.9.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{23}H_{18}N_2O_3S$: 402.1038; Found: 406.1040.



1'-methyl-2-(2-(methylthio)phenyl)spiro[benzo[4,5]thie-no[2,3-*c*]pyrrole-1,3'-pyrrolidine]-2',3,5'(2*H*)-trione (3la)

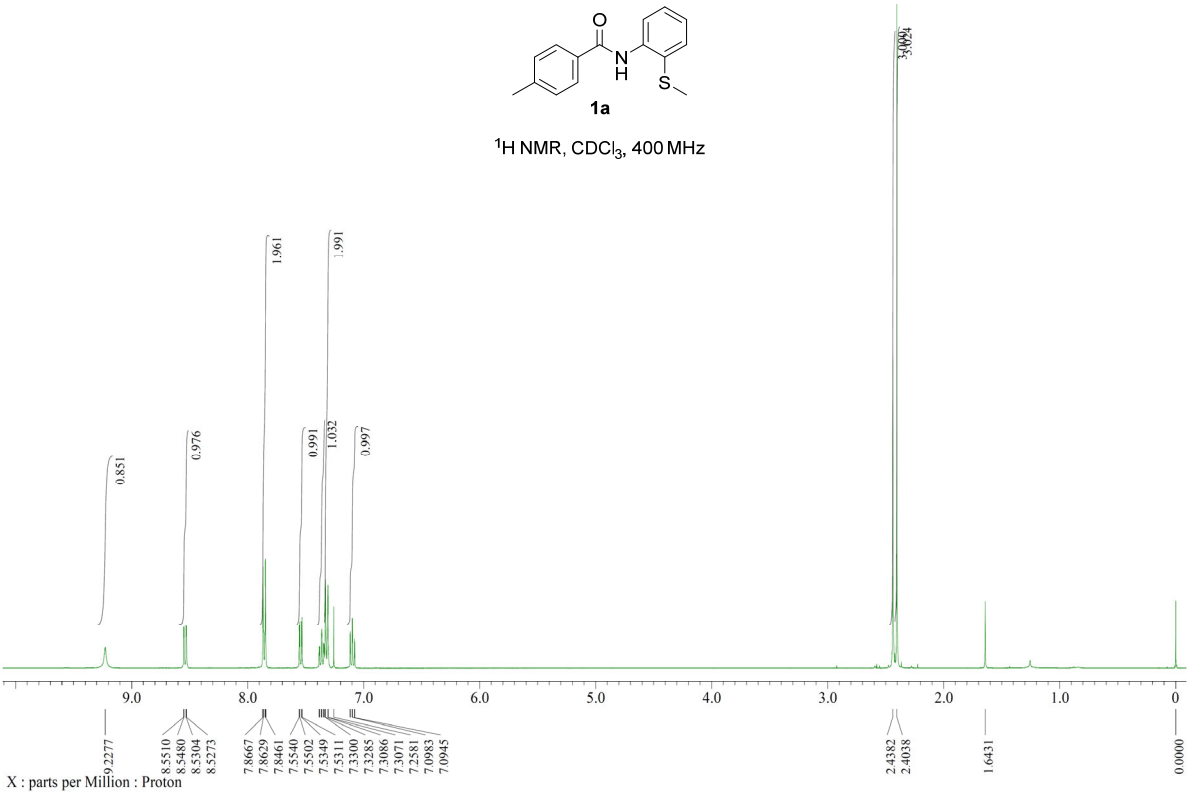
27% yield. R_f = 0.38 (hexane/Et_2O = 3/7). A white solid. Mp = 231.3 ºC

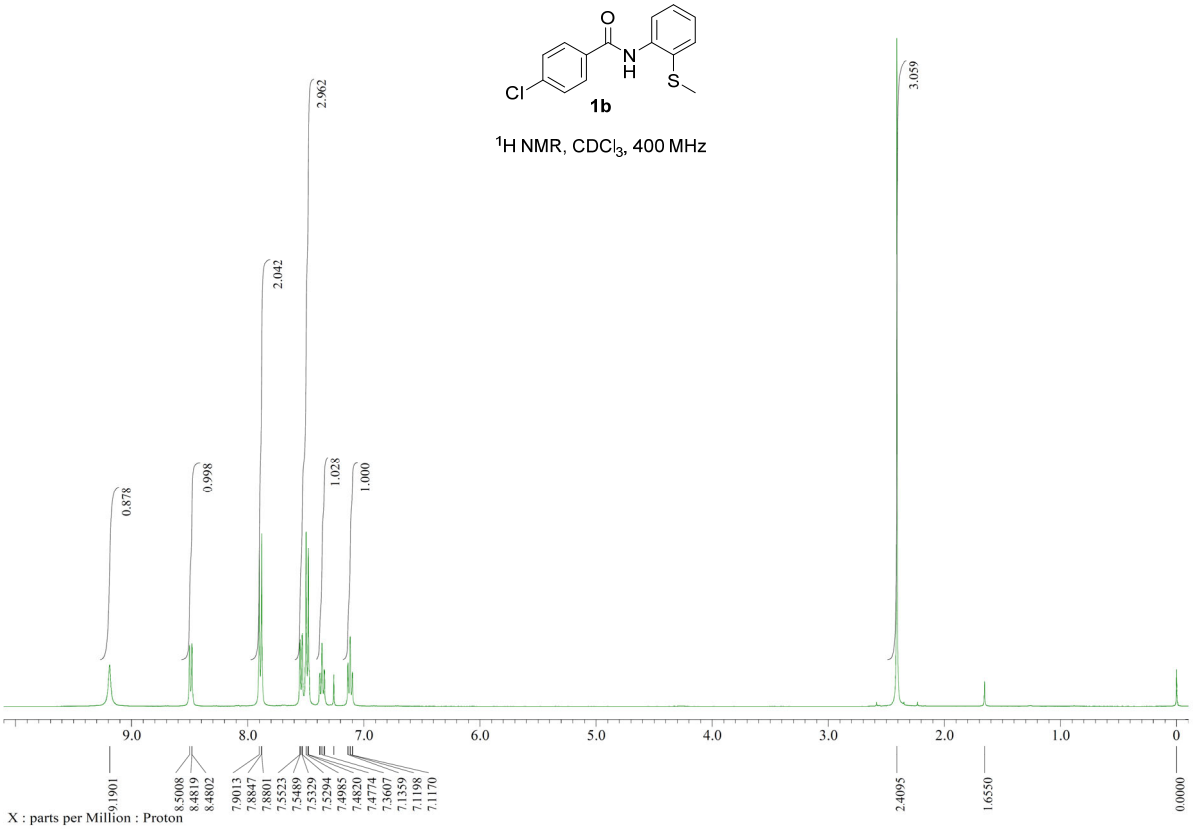
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.56-8.58 (m, 1H), 7.94 (dd, *J* = 8.0 Hz and 1.5 Hz, 1H),7.88-7.91 (m, 1H), 7.49-7.54 (m, 2H), 7.41(td, *J* = 7.8 Hz and 1.6 Hz, 1H), 7.33 (td, *J* = 7.8 Hz and 1.6 Hz, 1H), 7.26 (dd, *J* = 7.8 Hz and 1.4 Hz, 1H), 5.11 (d, *J* = 8.5 Hz, 1H), 5.01 (d, *J* = 8.5 Hz, 1H), 2.99 (s, 3H), 2.41 (s, 3H).

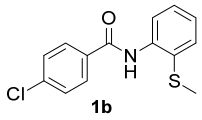
^{13}C NMR ($CDCl_3$, 100 MHz): δ 174.6, 172.2, 158.8, 142.7, 137.2, 136.1, 133.9, 132.3, 131.4, 129.5, 127.6, 126.0, 125.7, 125.6, 125.5, 123.2, 60.9, 43.9, 25.6 14.8.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{21}H_{16}N_2O_3S_2$: 408.0602; Found: 408.0606.

VIII. Copies of ^{1}H & ^{13}C NMR Spectra:

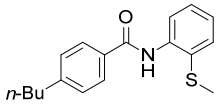






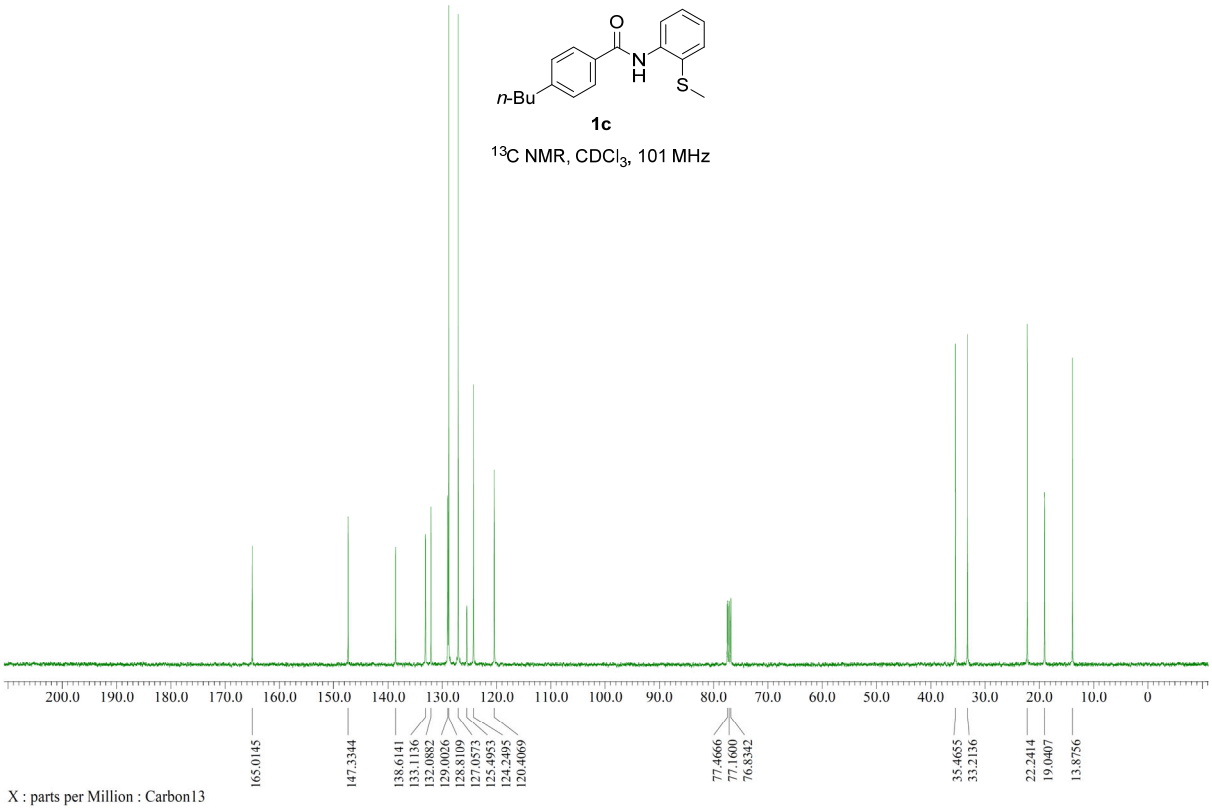
1b

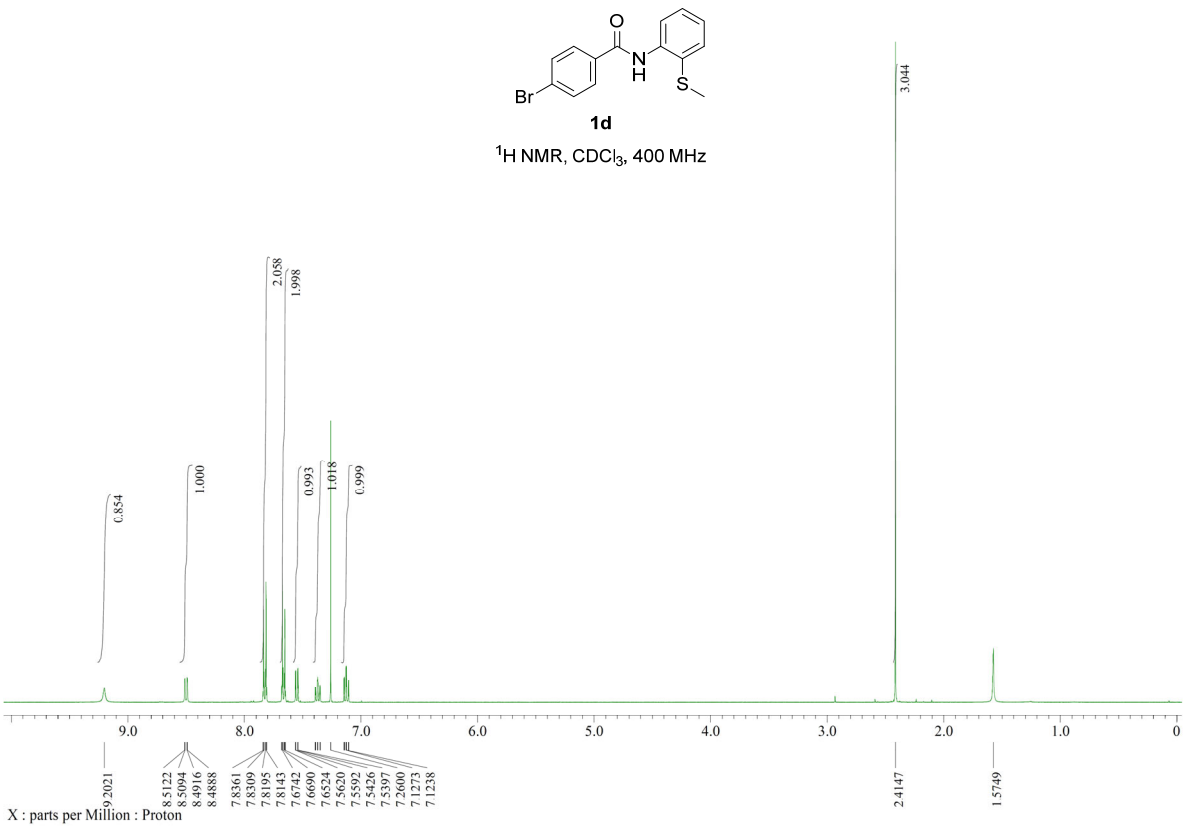
^{13}C NMR, $CDCl_3$, 101 MHz

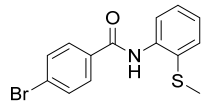


1c

^{1}H NMR, $CDCl_3$, 400 MHz

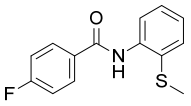

n-Bu
1c
13C NMR, CDCl3, 101 MHz
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
165.0145
147.3344
138.6141
133.1136
132.0882
129.0026
128.8109
127.0573
125.4953
124.2495
120.4069
77.4666
77.1600
76.8342
35.4655
33.2136
22.2414
19.0407
13.8756
X : parts per Million : Carbon13


Br
1d
1H NMR, CDCl3, 400 MHz
3.044
2.058
1.998
1.000
0.993
1.018
0.999
0.854
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
9.2021
8.5122
8.5094
8.4916
8.4888
7.8361
7.8309
7.8195
7.8143
7.6742
7.6690
7.6624
7.5620
7.5592
7.5426
7.5397
7.2600
7.1273
7.1238
2.4147
1.5749
X : parts per Million : Proton



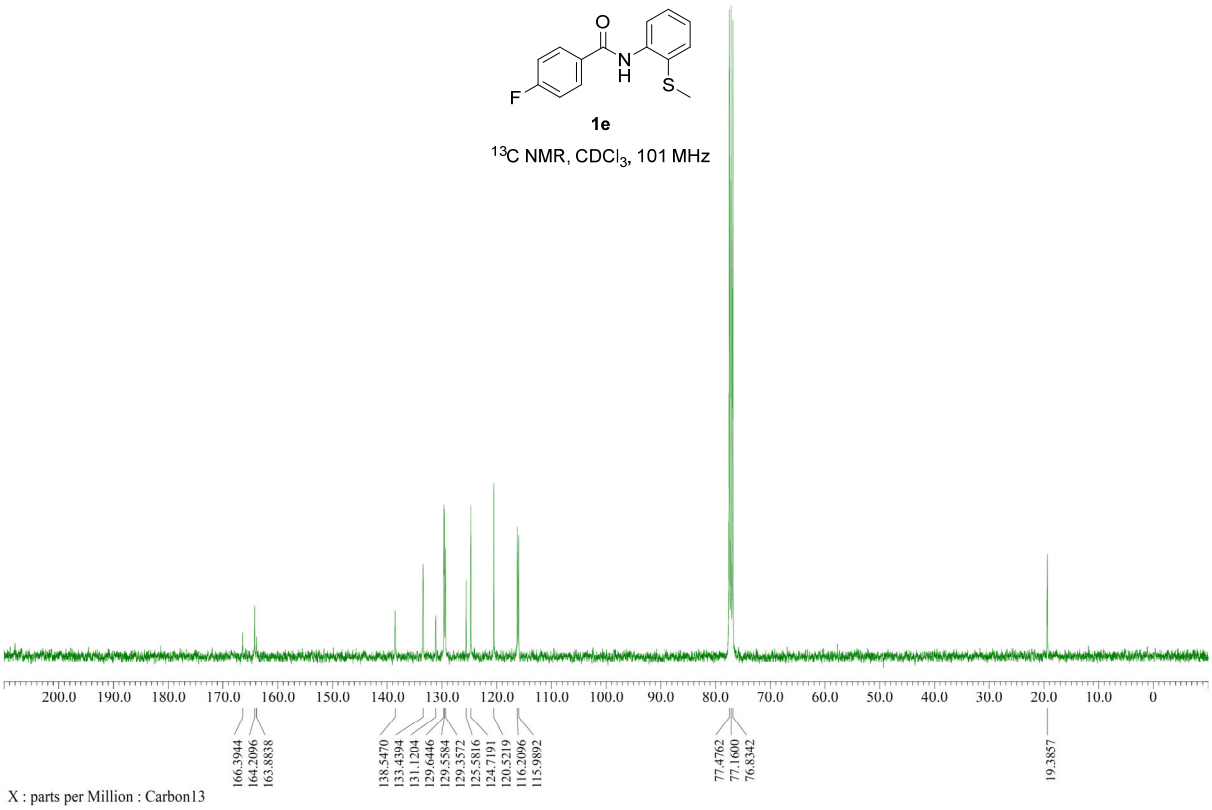
1d

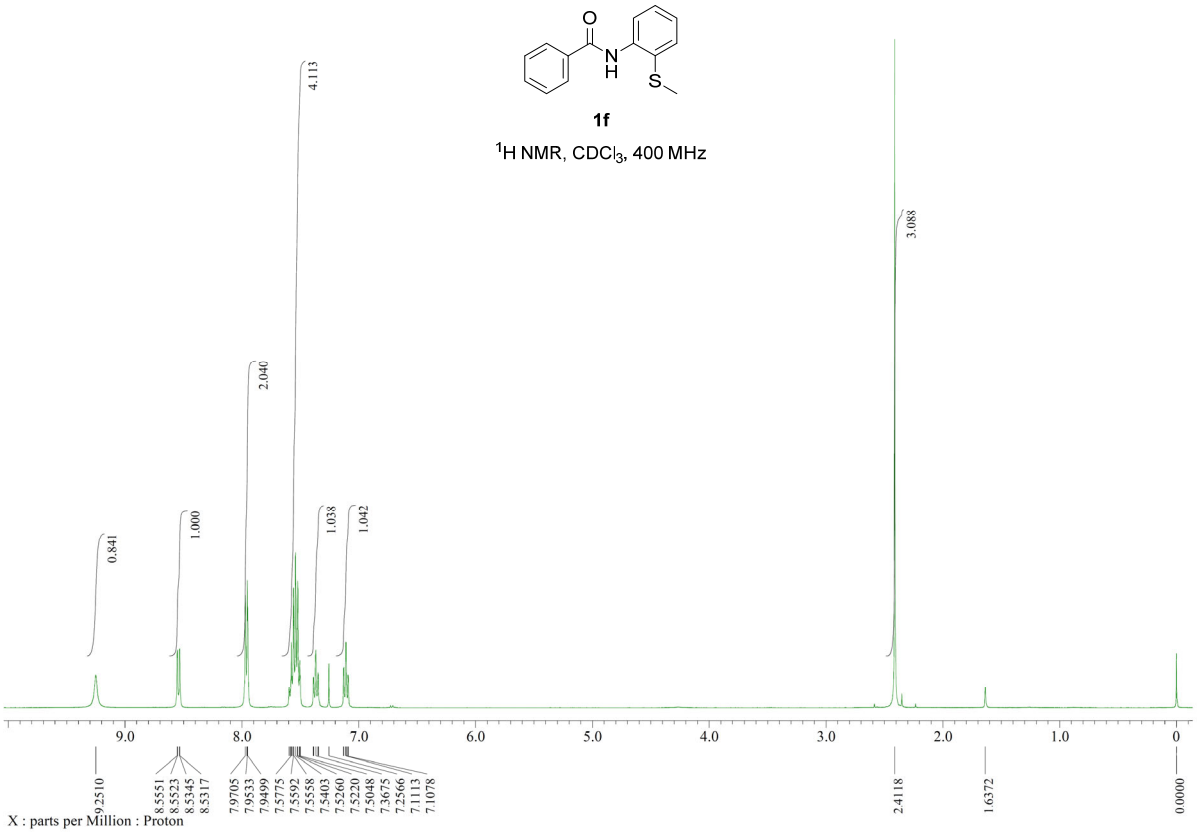
^{13}C NMR, $CDCl_3$, 101 MHz

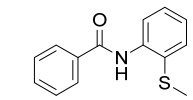


1e

^{1}H NMR, $CDCl_3$, 400 MHz

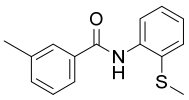

1e
^{13}C NMR, $CDCl_3$, 101 MHz
166.3944
164.2096
163.8838
138.5470
133.4394
131.1204
129.6446
129.5584
129.3572
125.5816
124.7191
120.5219
116.2096
115.9892
77.4762
77.1600
76.8342
19.3857
X : parts per Million : Carbon13


1f
^{1}H NMR, $CDCl_3$, 400 MHz
0.841
1.000
2.040
4.113
1.038
1.042
3.088
9.2510
8.5551
8.5523
8.5345
8.5317
7.9705
7.9533
7.9499
7.5775
7.5592
7.5558
7.5403
7.5260
7.5220
7.5048
7.3675
7.2566
7.1113
7.1078
2.4118
1.6372
0.0000
X : parts per Million : Proton



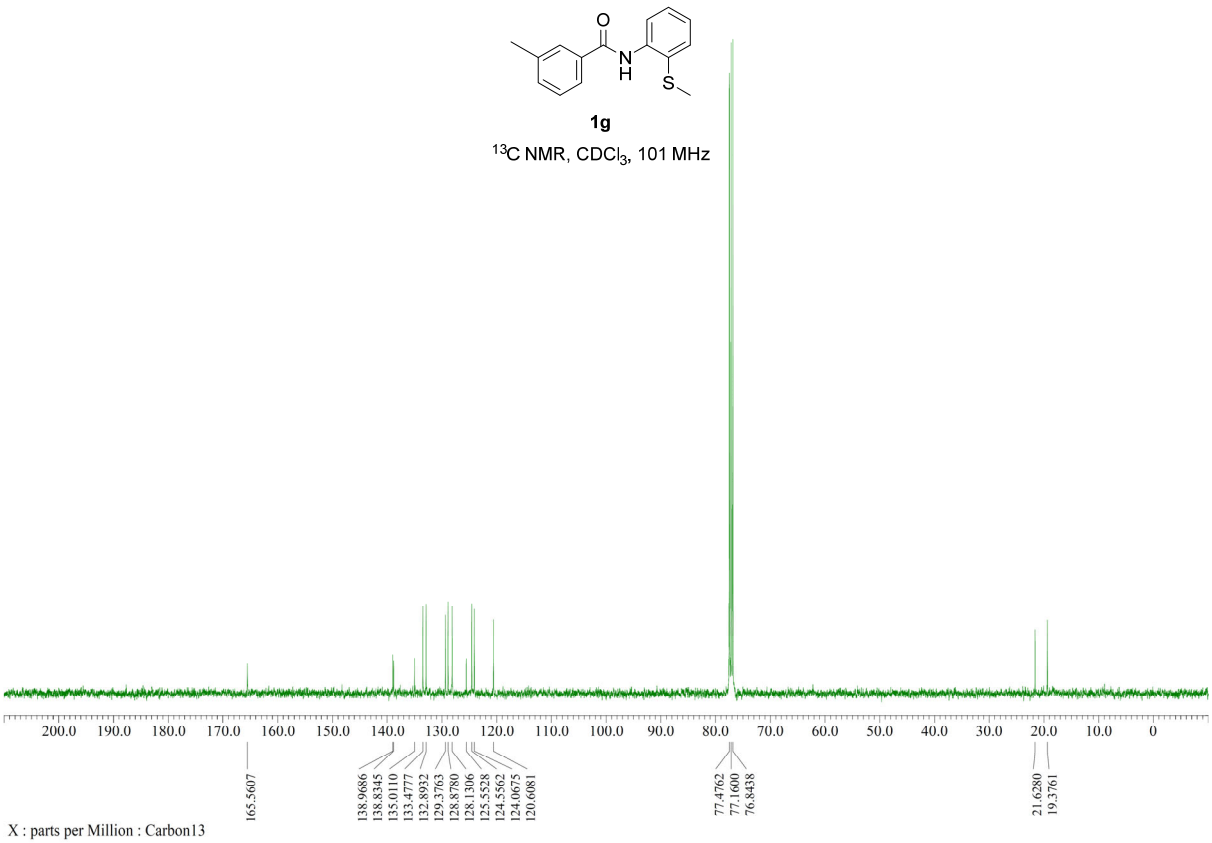
1f

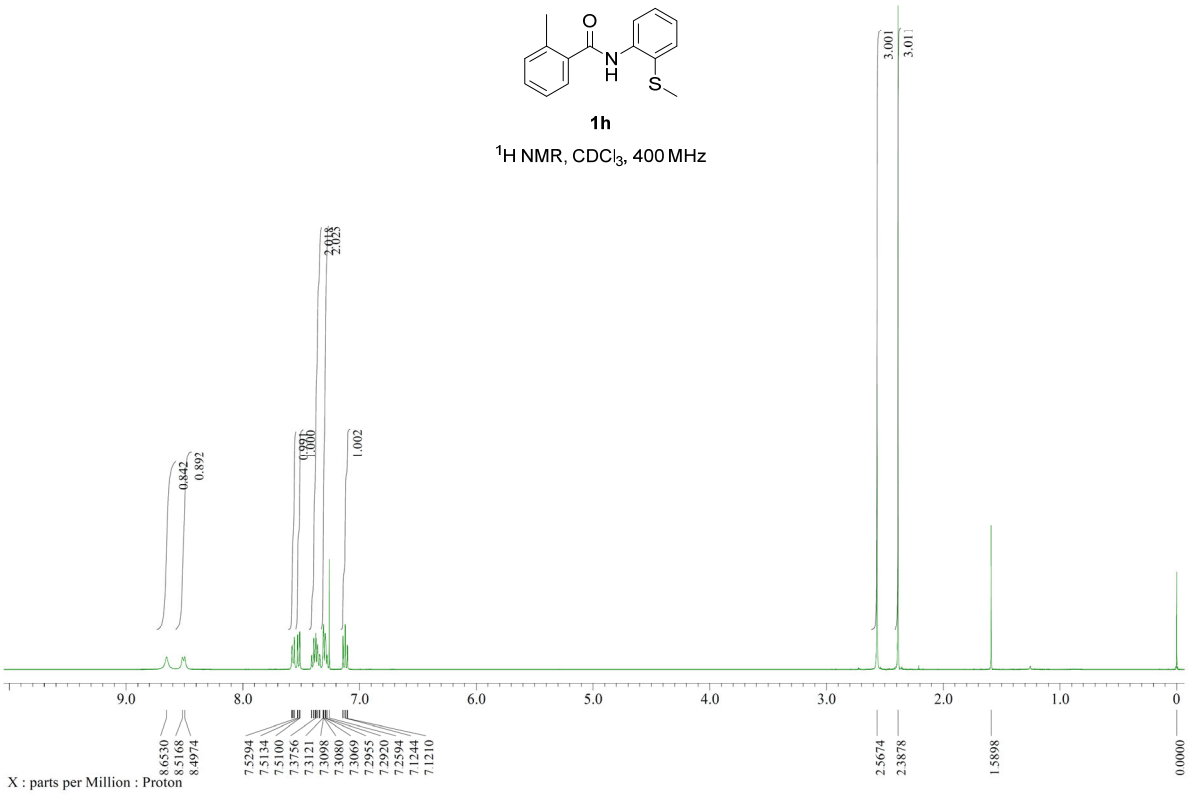
^{13}C NMR, $CDCl_3$, 101 MHz

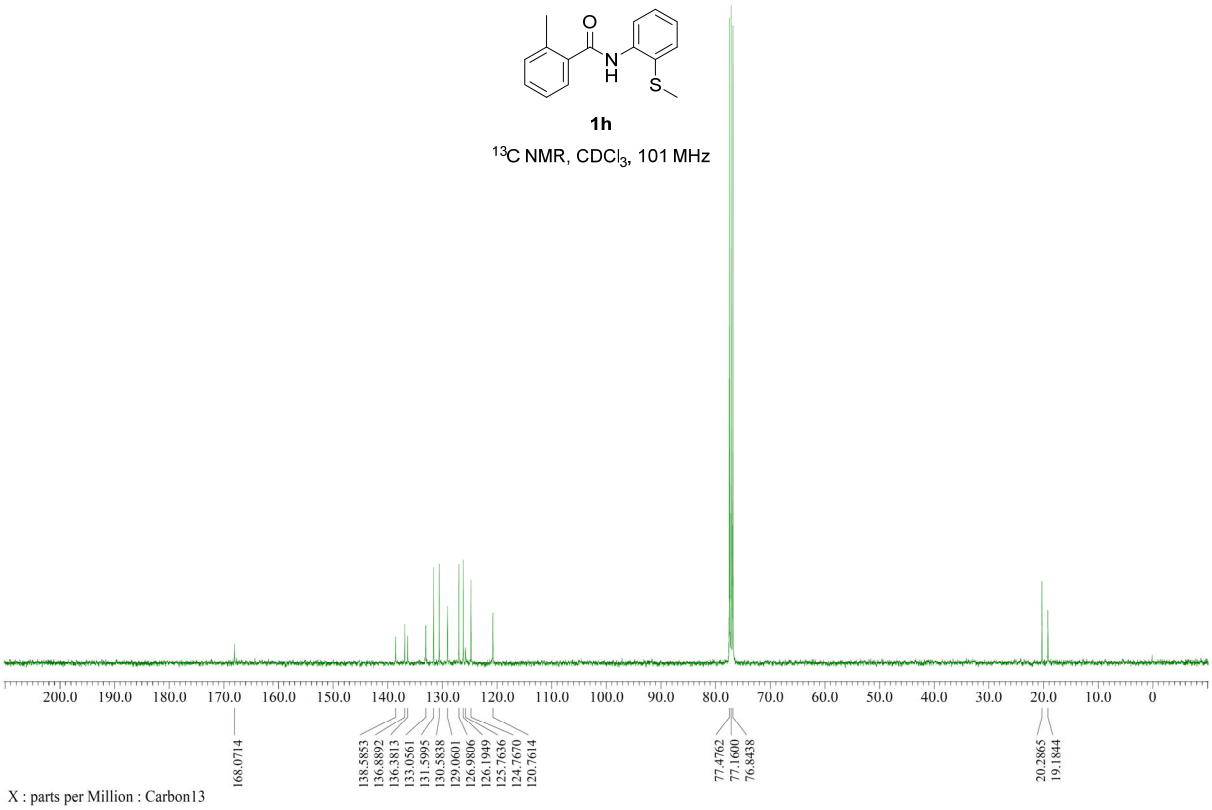


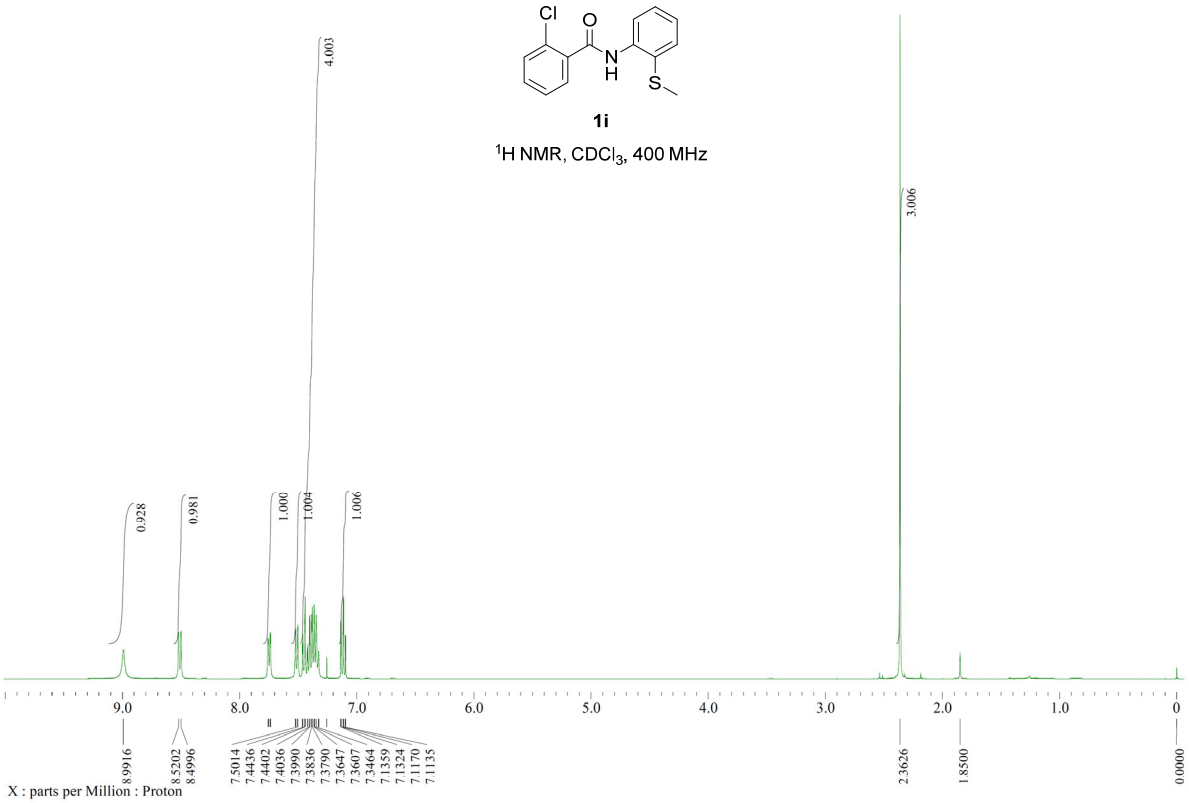
1g

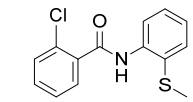
^{1}H NMR, $CDCl_3$, 400 MHz


1g
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13


1h
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton


1h
13C NMR, CDCl3, 101 MHz
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
168.0714
138.5853
136.8892
136.3813
133.0561
131.5995
130.5838
129.0601
126.9806
126.1949
125.7636
124.7670
120.7614
77.4762
77.1600
76.8438
20.2865
19.1844
X : parts per Million : Carbon13

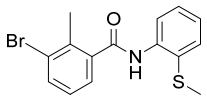

1i
1H NMR, CDCl3, 400 MHz
4.003
3.006
0.928
0.981
1.000
1.004
1.006
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.9916
8.5202
8.4996
7.5014
7.4436
7.4402
7.4036
7.3990
7.3836
7.3790
7.3647
7.3607
7.3464
7.1359
7.1324
7.1170
7.1135
2.3626
1.8500
0.0000
X : parts per Million : Proton



1i

^{13}C NMR, $CDCl_3$, 101 MHz

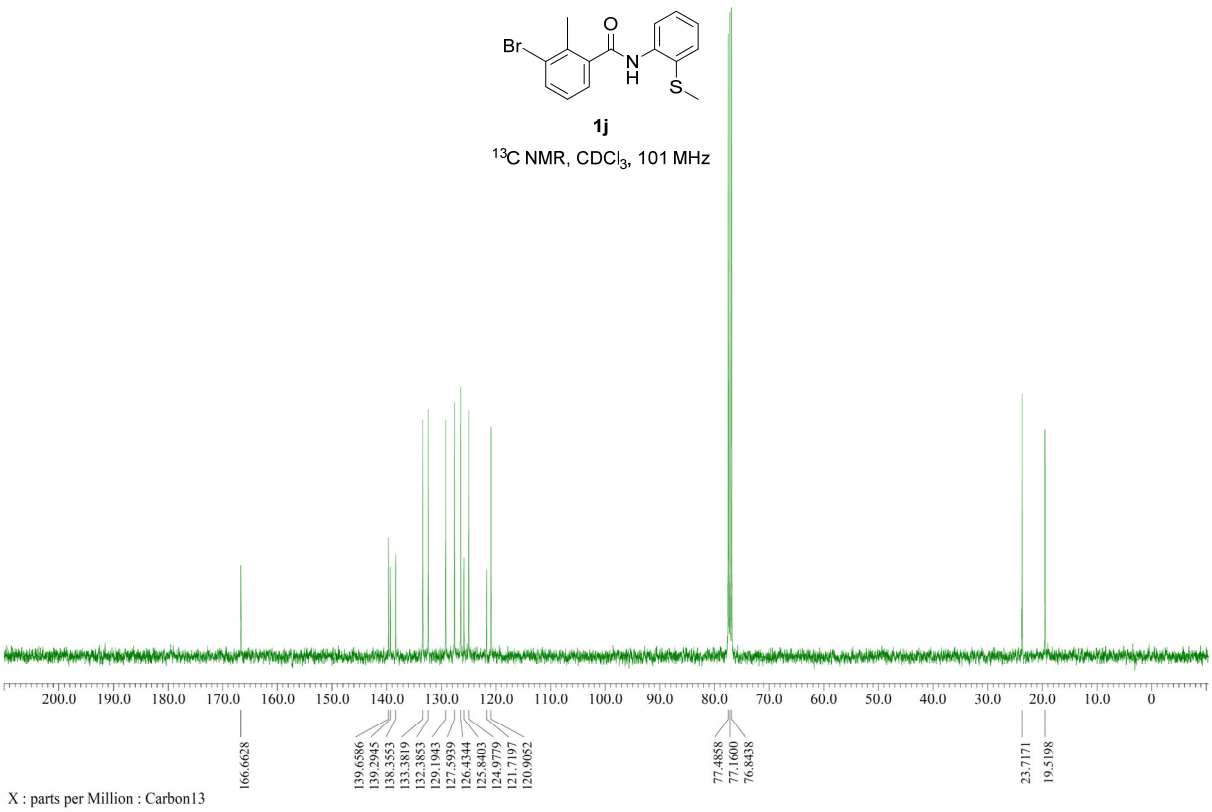
X : parts per Million : Carbon13

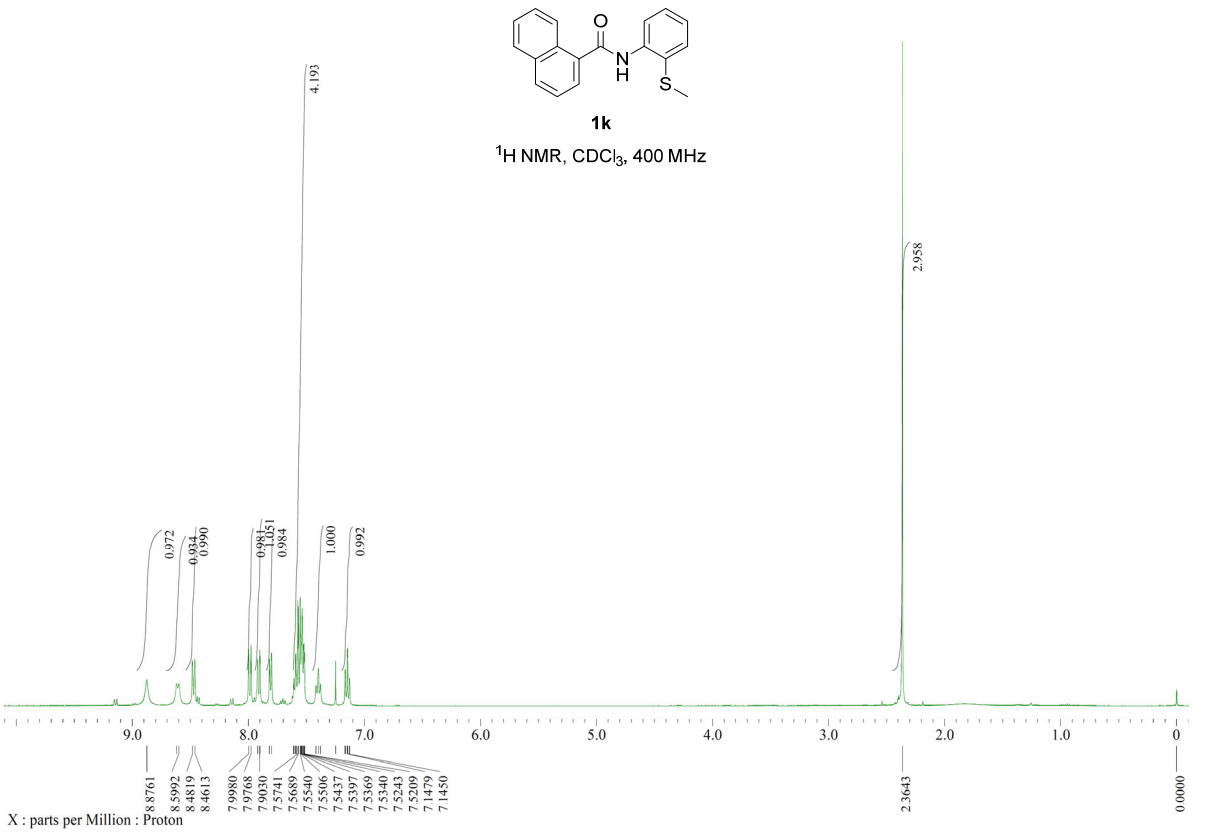


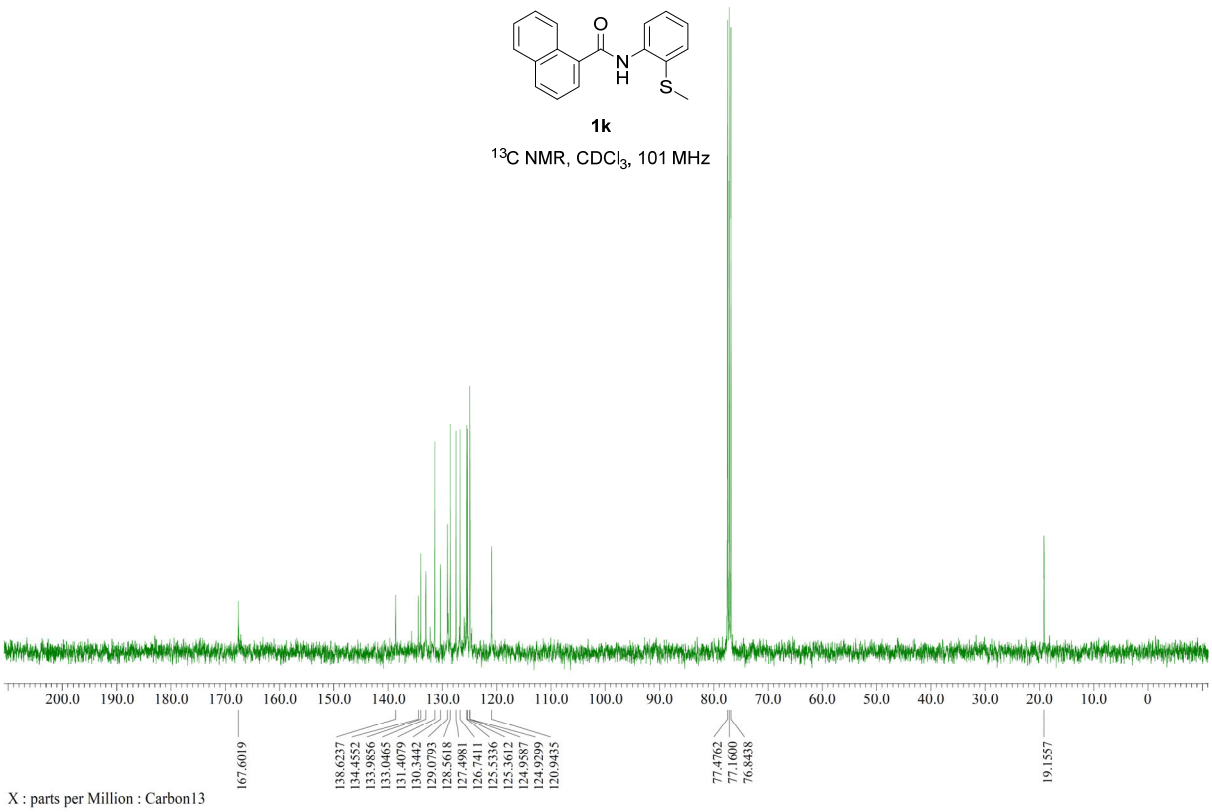
1j

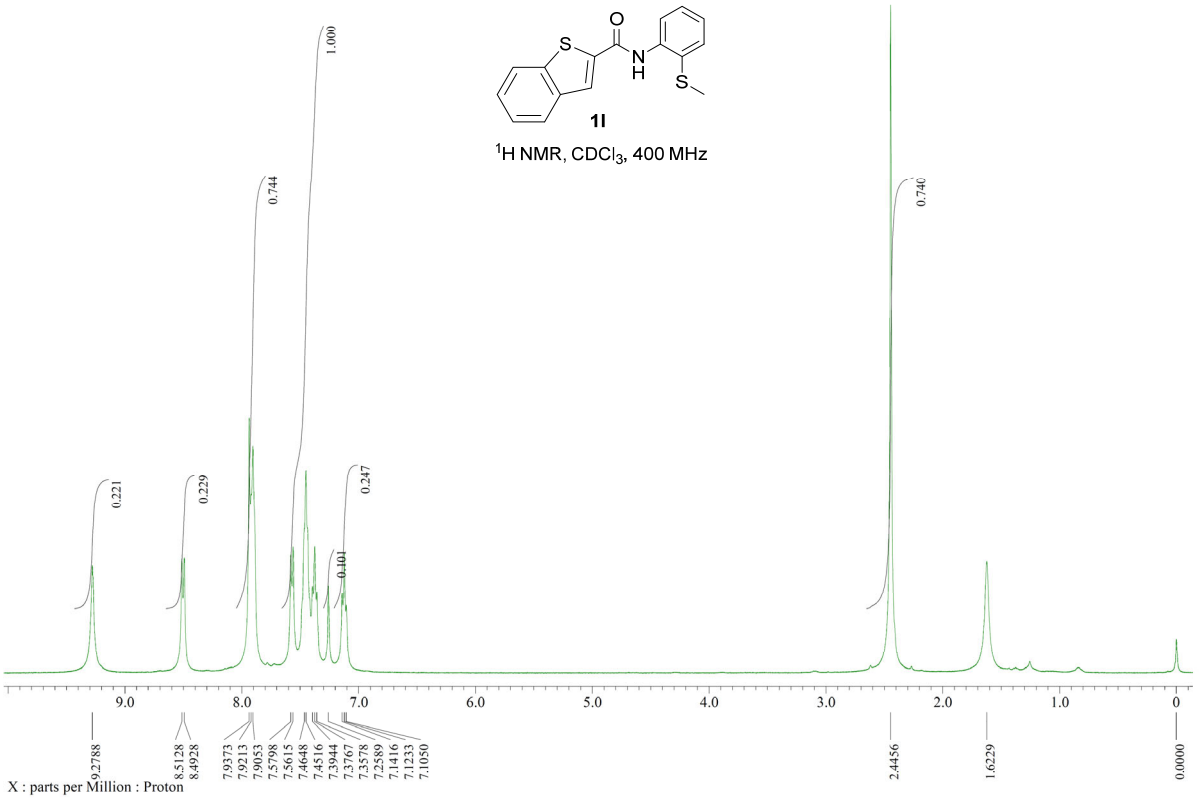
^{1}H NMR, $CDCl_3$, 400 MHz

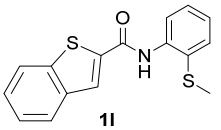
X : parts per Million : Proton


Br
O
N
H
S
1j
13C NMR, CDCl3, 101 MHz
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
166.6628
139.6586
139.2945
138.3553
133.3819
132.3853
129.1943
127.5939
126.4344
125.8403
124.9779
121.7197
120.9052
77.4858
77.1600
76.8438
23.7171
19.5198
X : parts per Million : Carbon13


O
N
H
S
1k
1H NMR, CDCl3, 400 MHz
4.193
2.958
0.972
0.934
0.990
0.984
1.000
0.992
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.8761
8.5992
8.4819
8.4613
7.9980
7.9768
7.9030
7.5741
7.5689
7.5540
7.5506
7.5437
7.5397
7.5369
7.5340
7.5243
7.5209
7.1479
7.1450
2.3643
0.0000
X : parts per Million : Proton

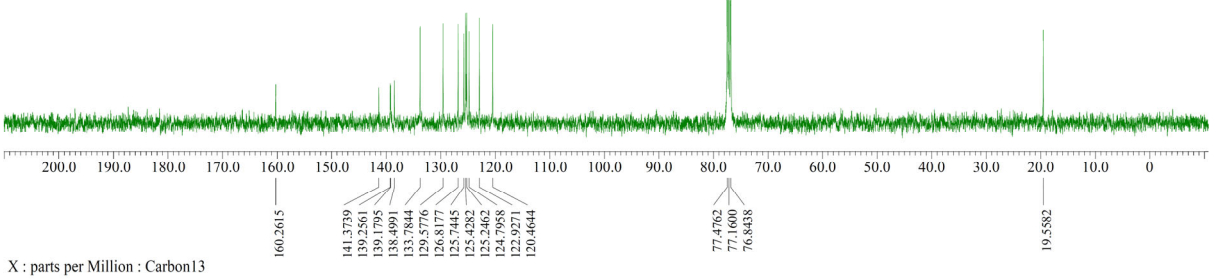

1k
13C NMR, CDCl3, 101 MHz
167.6019
138.6237
134.4552
133.9856
133.0465
131.4079
130.3442
129.0793
128.5618
127.4981
126.7411
125.5336
125.3612
124.9587
124.9299
120.9435
77.4762
77.1600
76.8438
19.1557
X : parts per Million : Carbon13

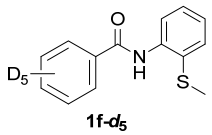

1l
1H NMR, CDCl3, 400 MHz
0.221
0.229
0.744
1.000
0.101
0.247
0.740
9.2788
8.5128
8.4928
7.9373
7.9213
7.9053
7.5798
7.5615
7.4648
7.4516
7.3944
7.3767
7.3578
7.2589
7.1416
7.1233
7.1050
2.4456
1.6229
0.0000
X : parts per Million : Proton



1l

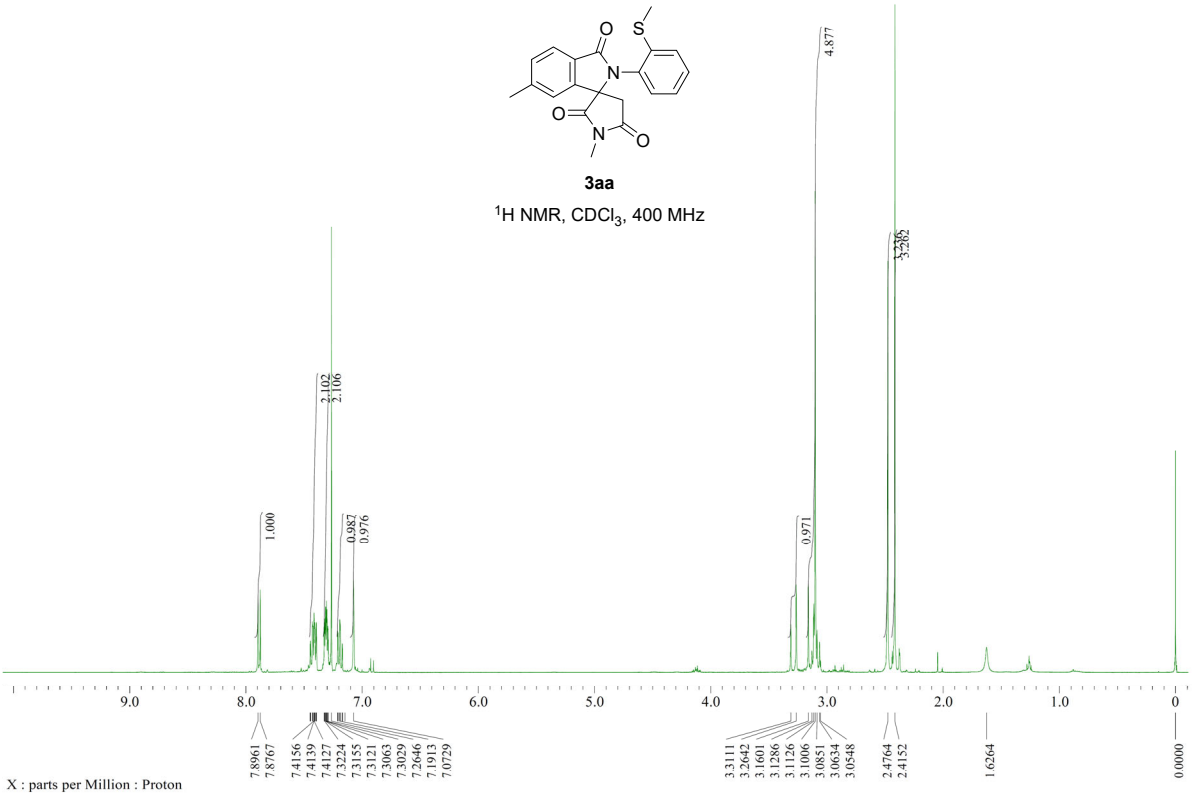
^{13}C NMR, $CDCl_3$, 101 MHz

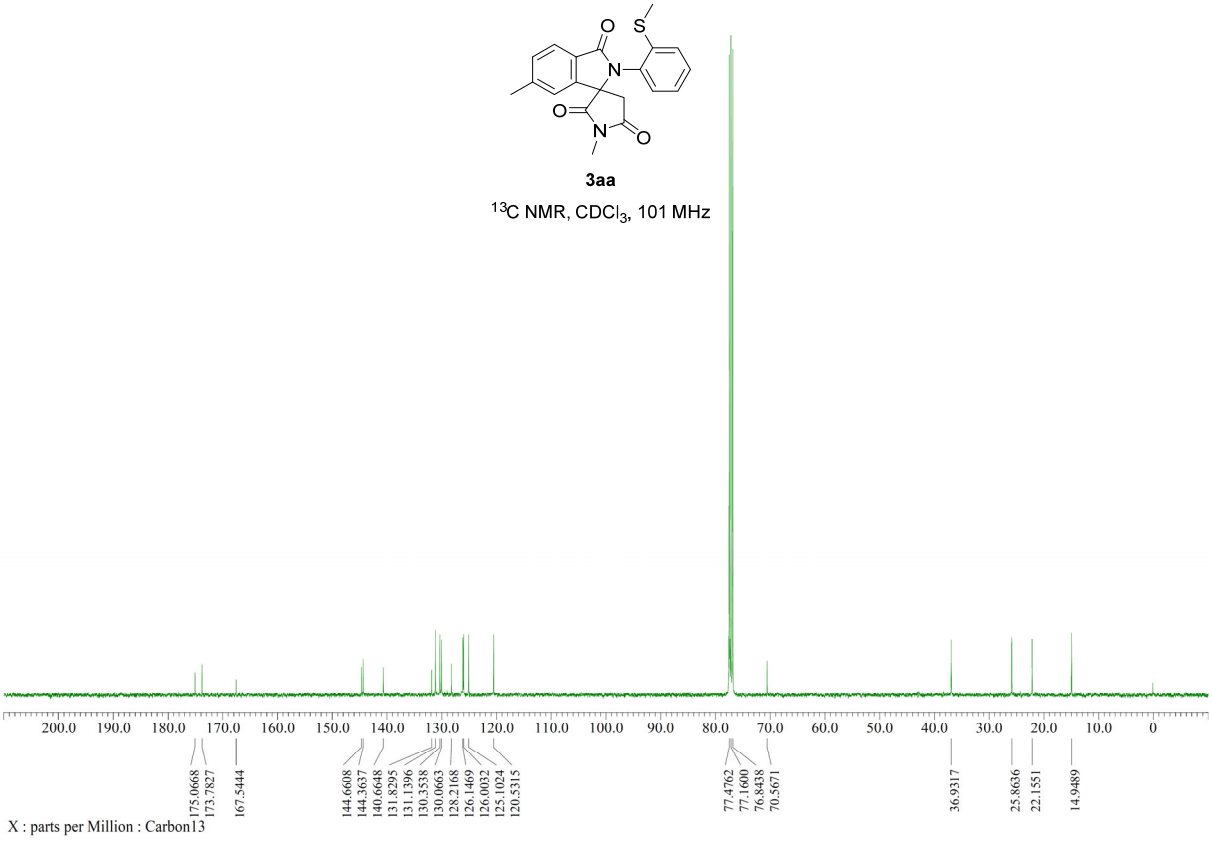


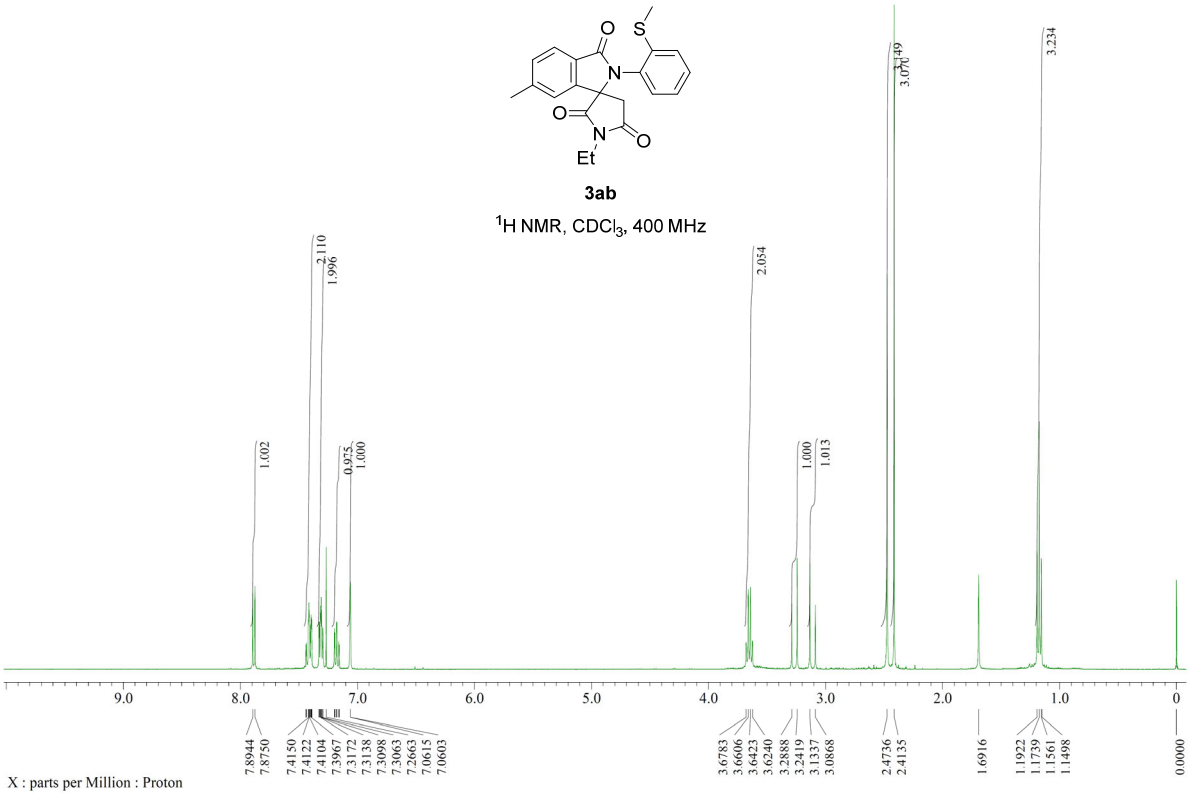


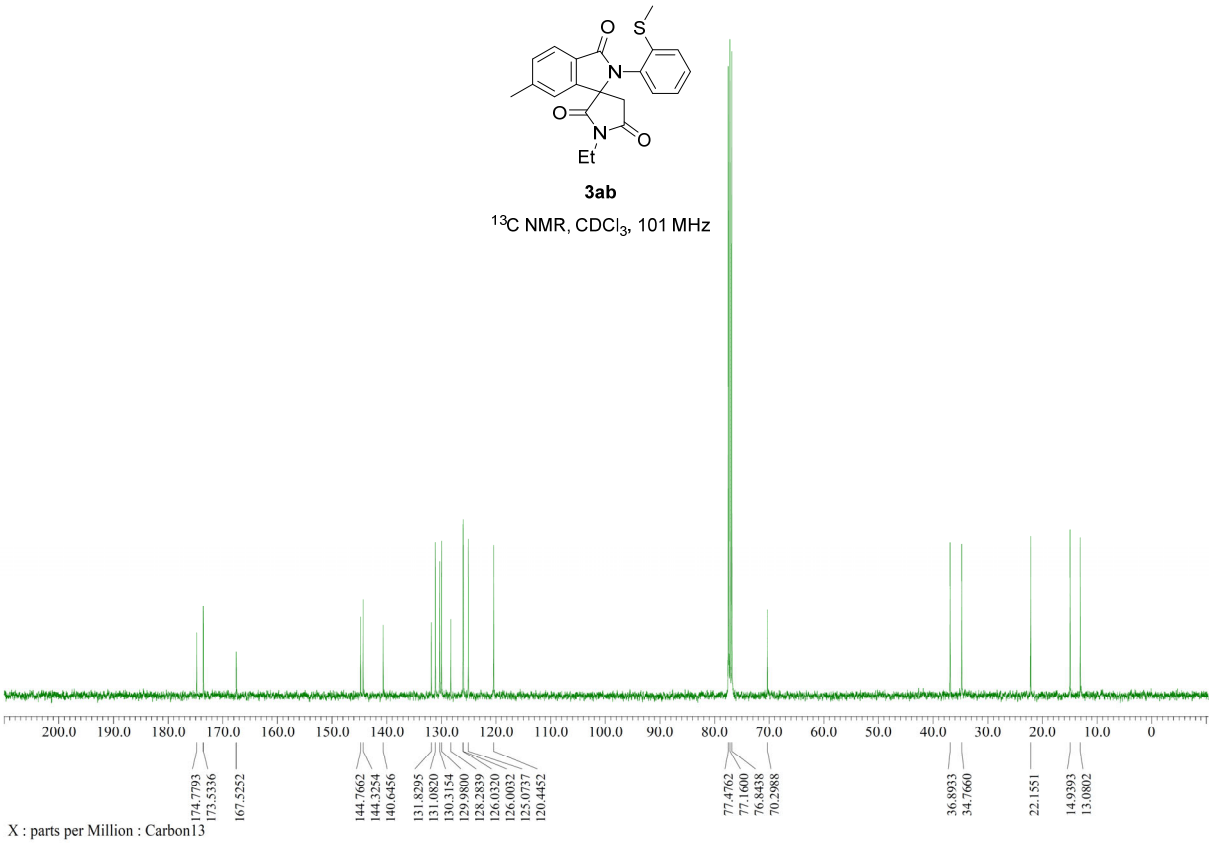
1f-d_5

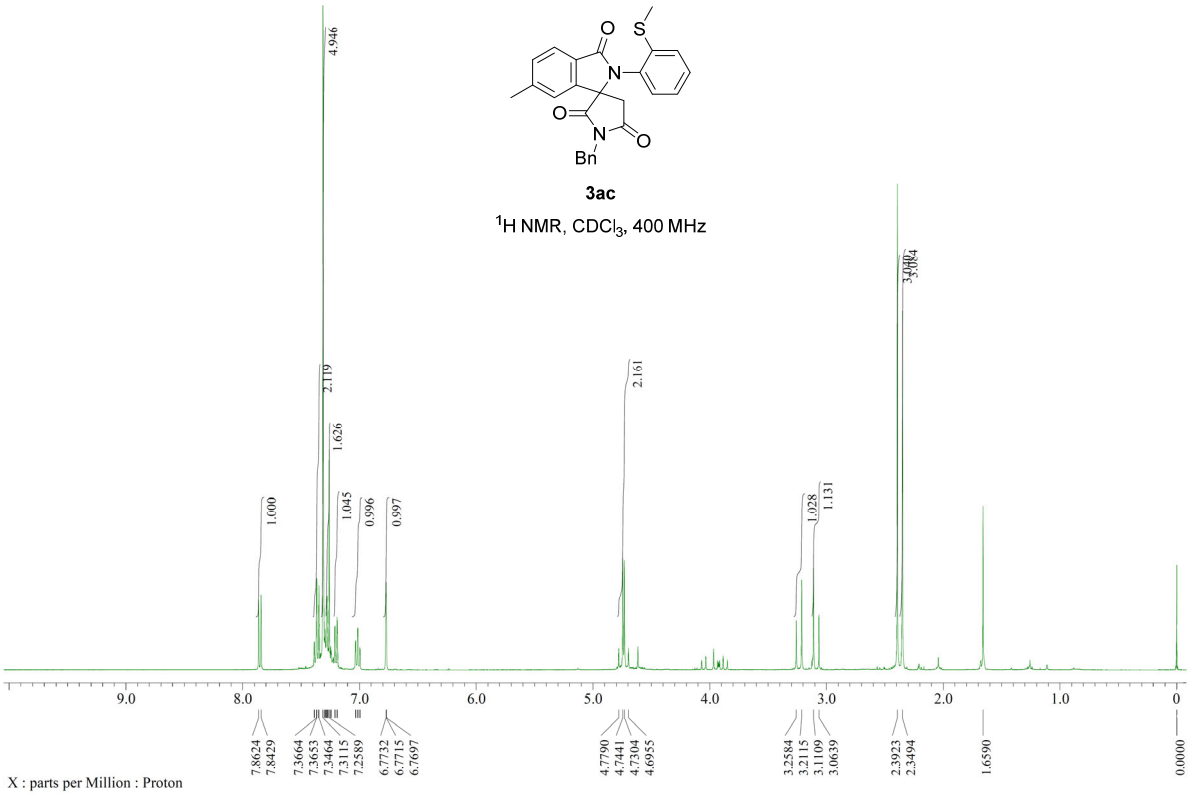
^{1}H NMR, $CDCl_3$, 400 MHz

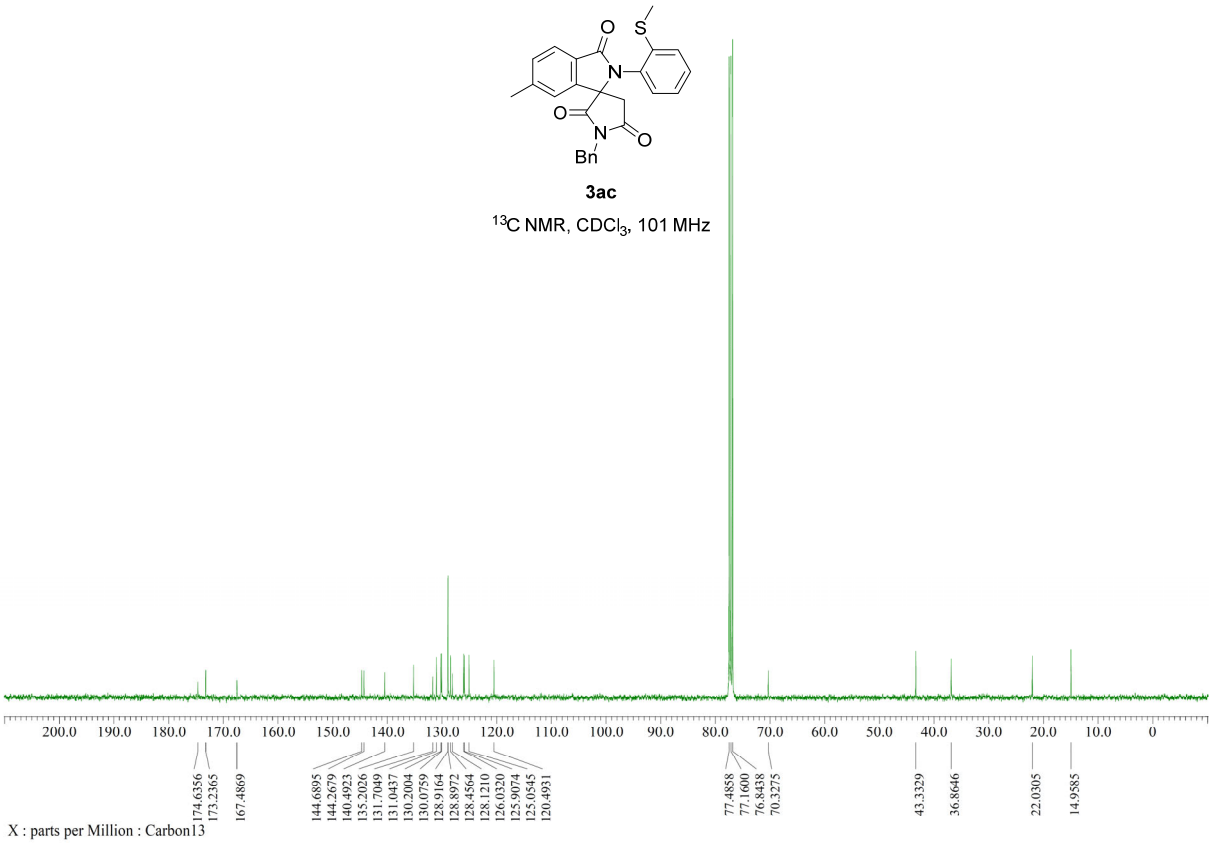

3aa
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton

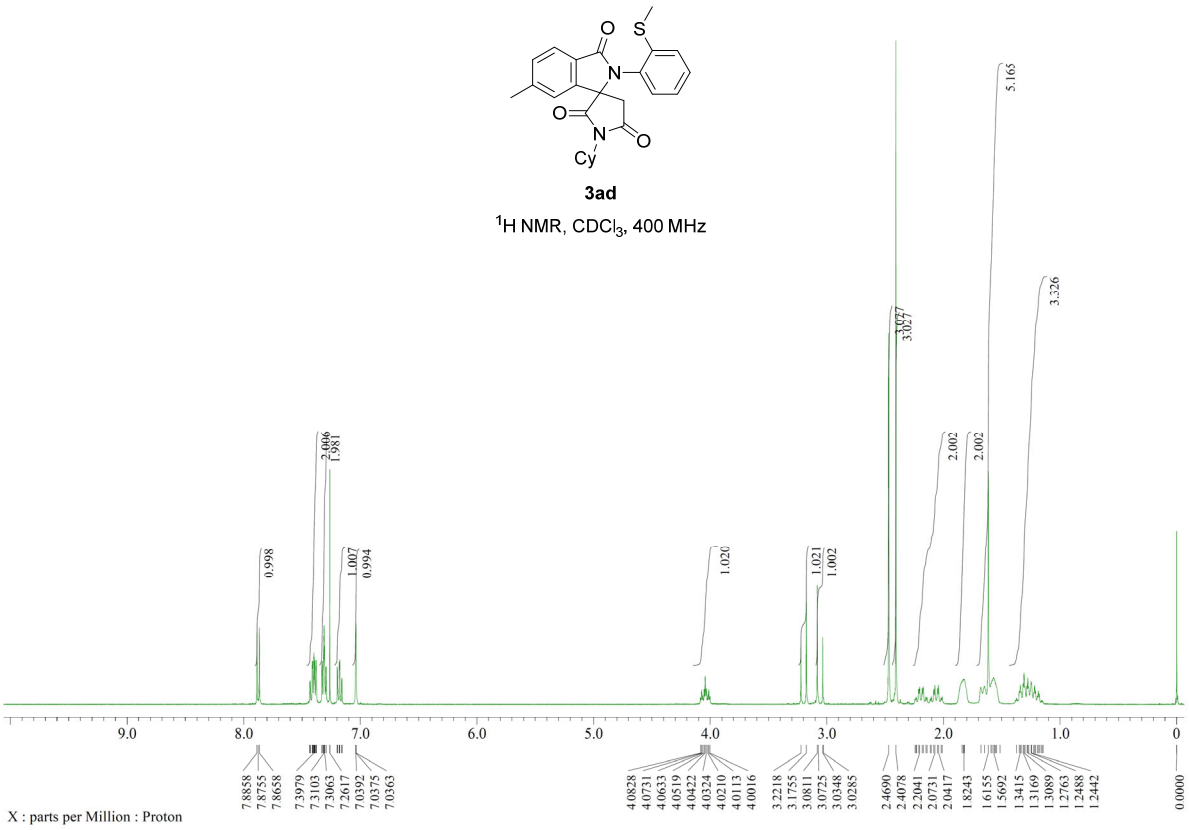

3aa
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13

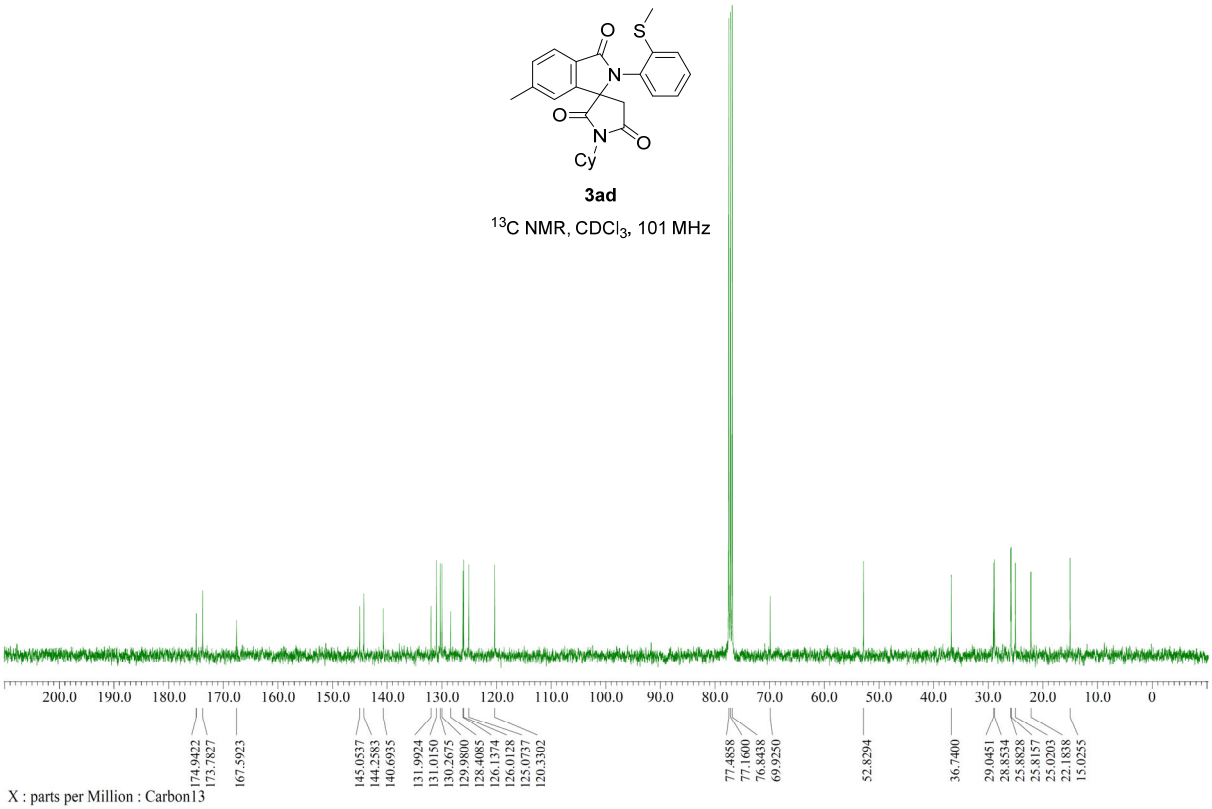

3ab
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton

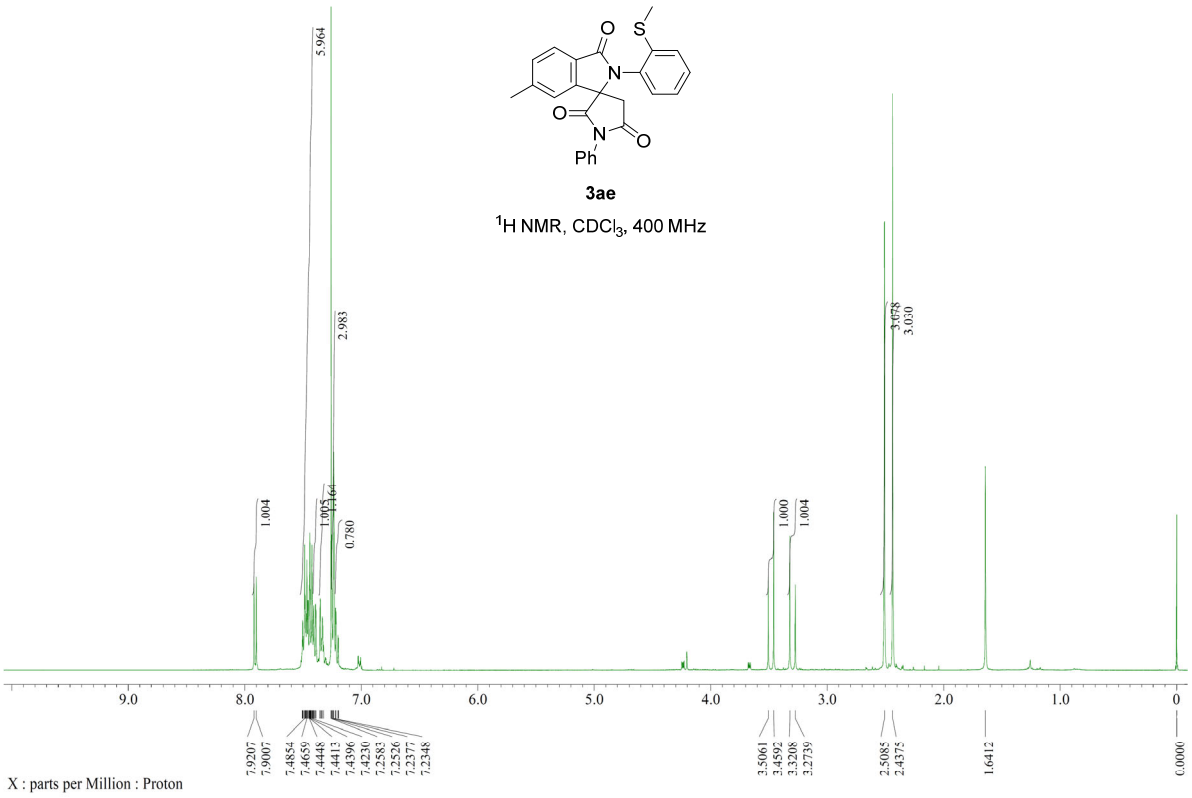

3ab
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13

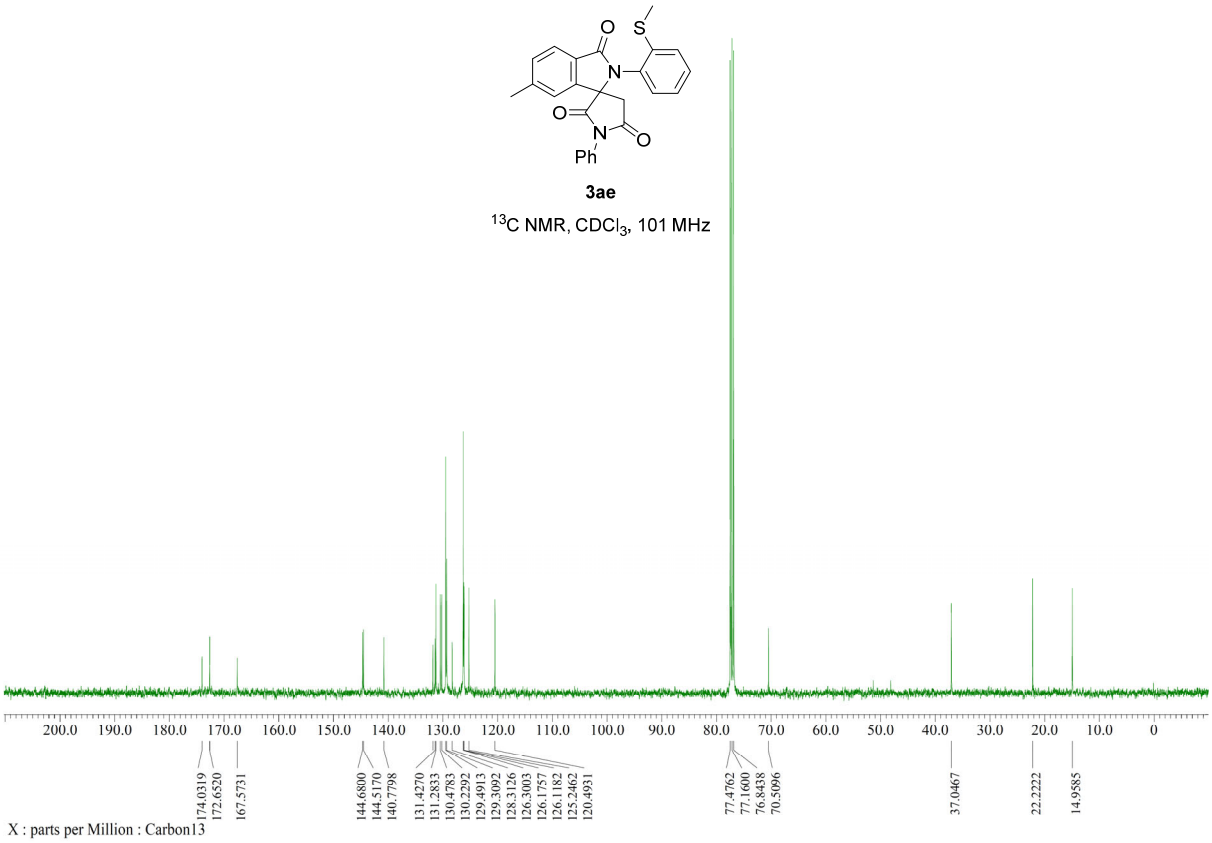

Bn
3ac
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton

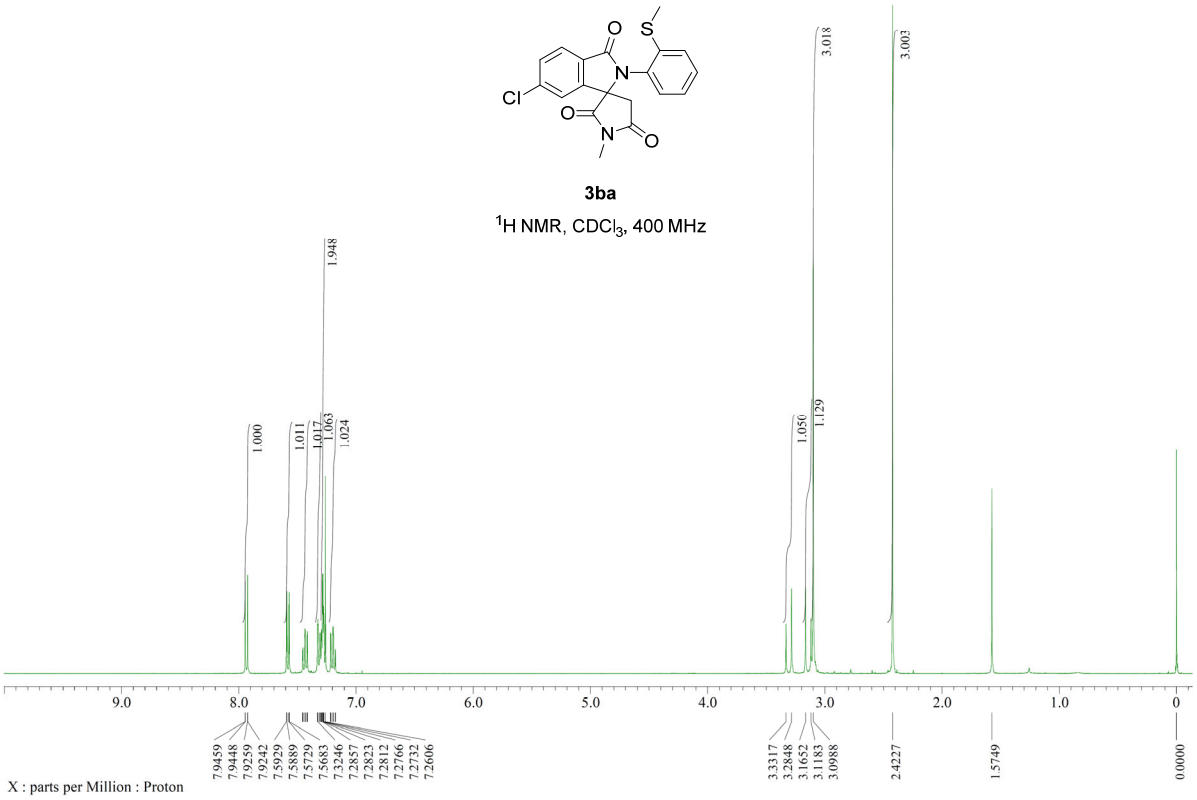

Bn
3ac
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13

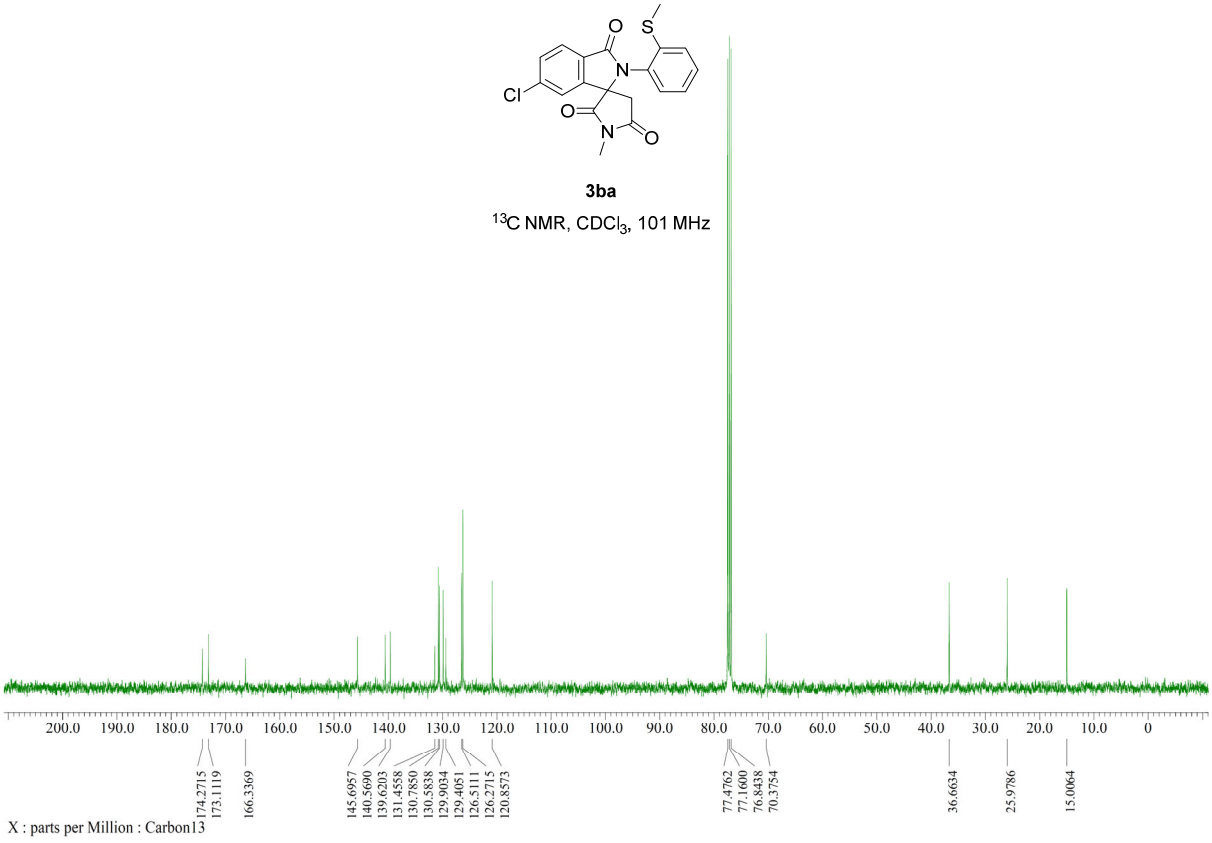

3ad
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton

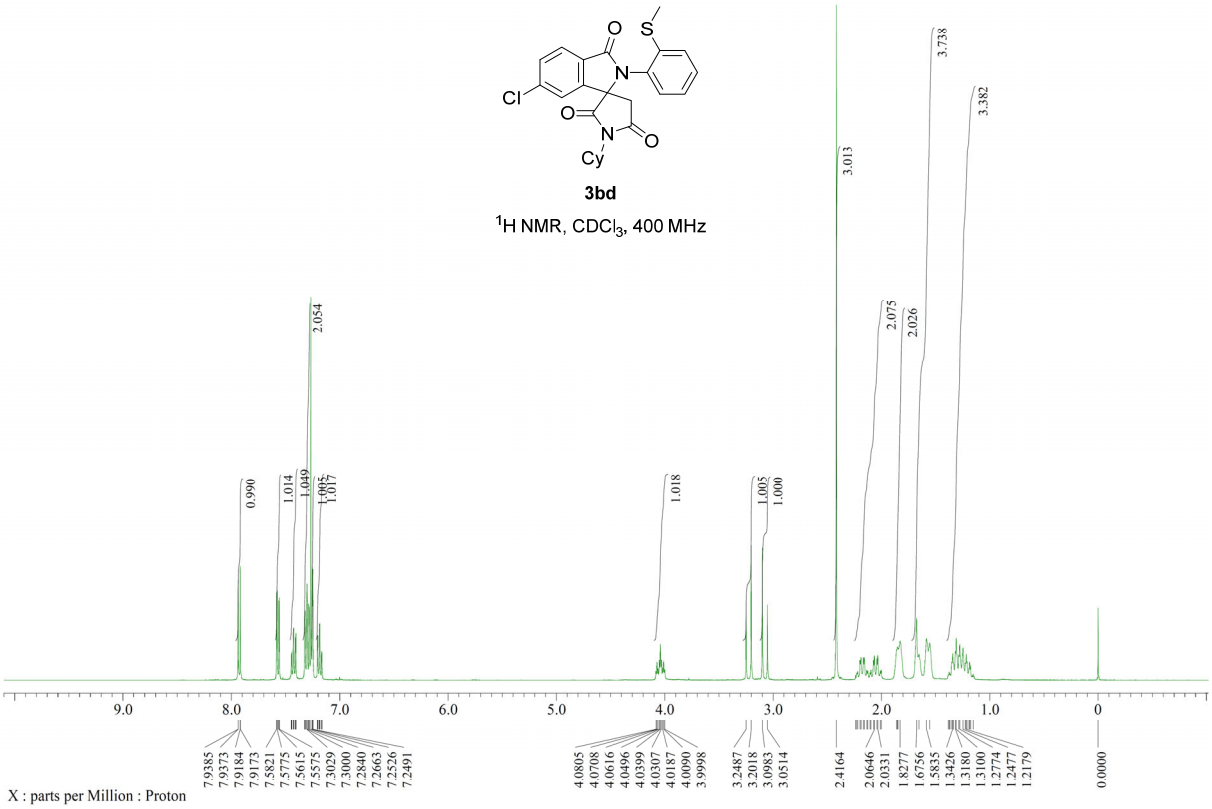

3ad
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13

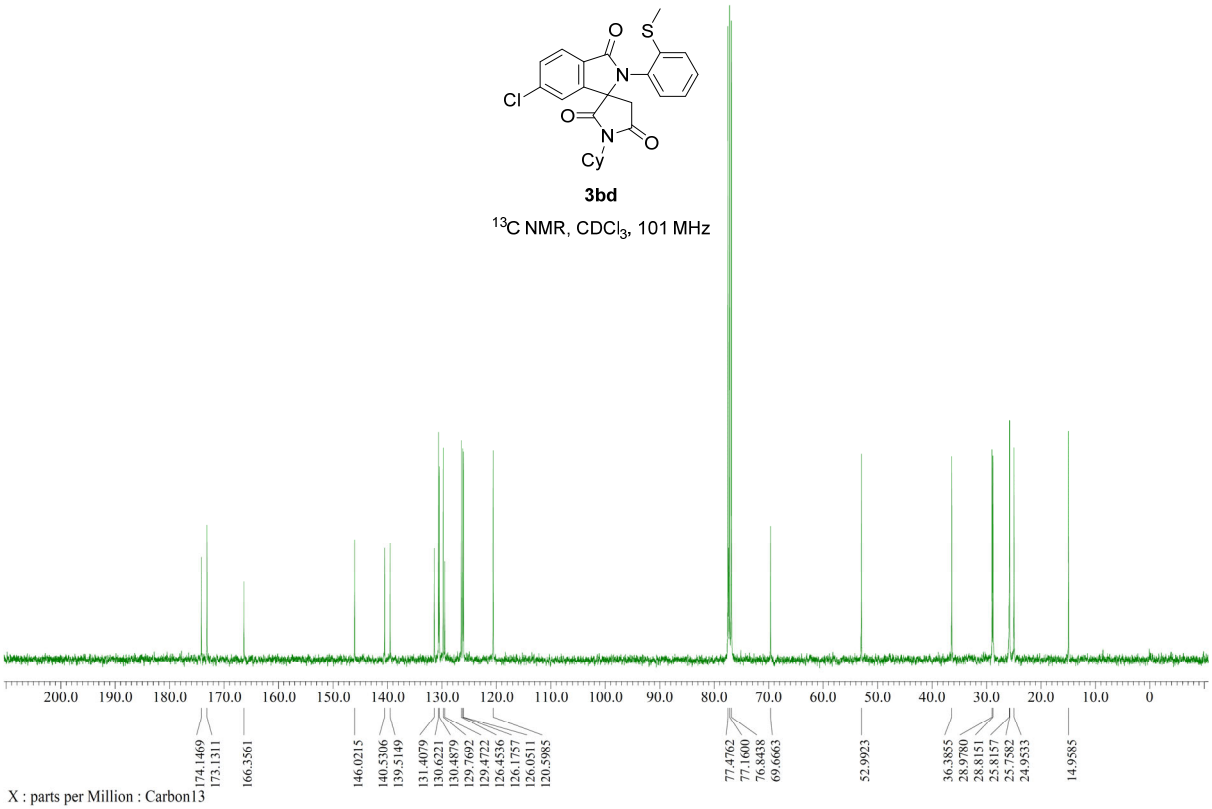

3ae
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton

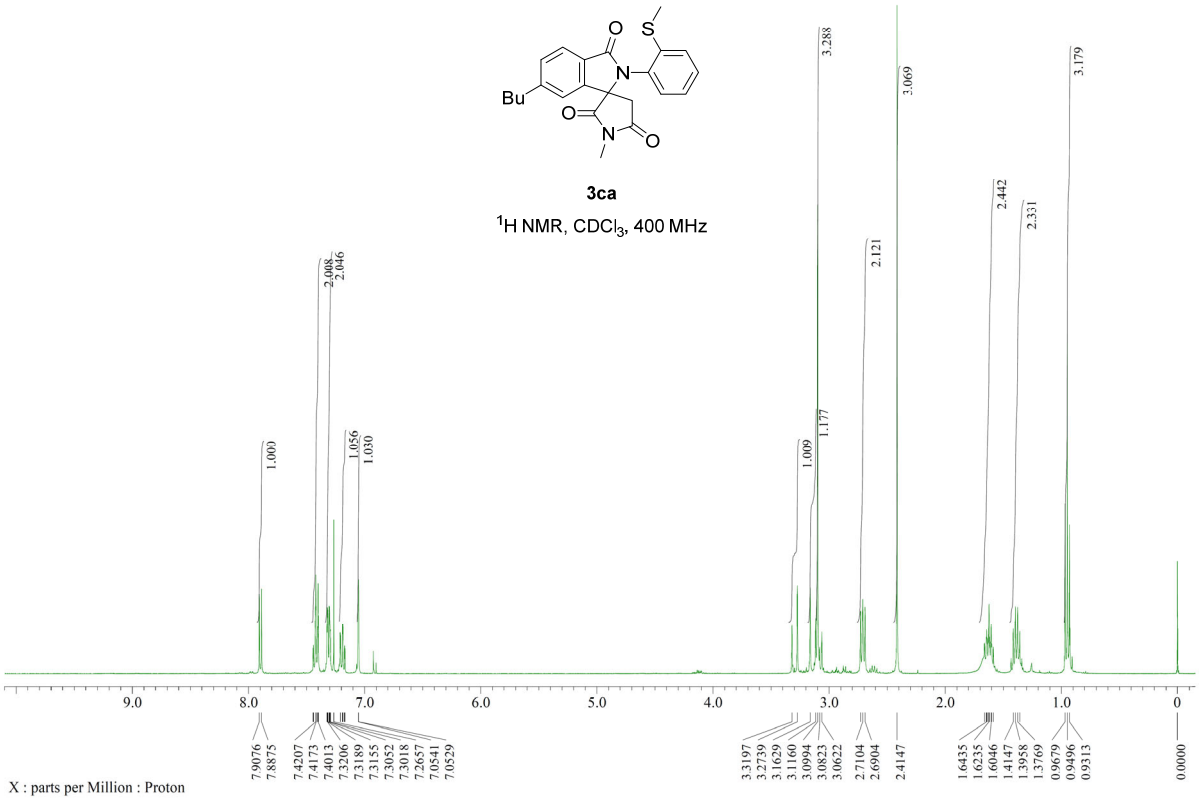

3ae
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13

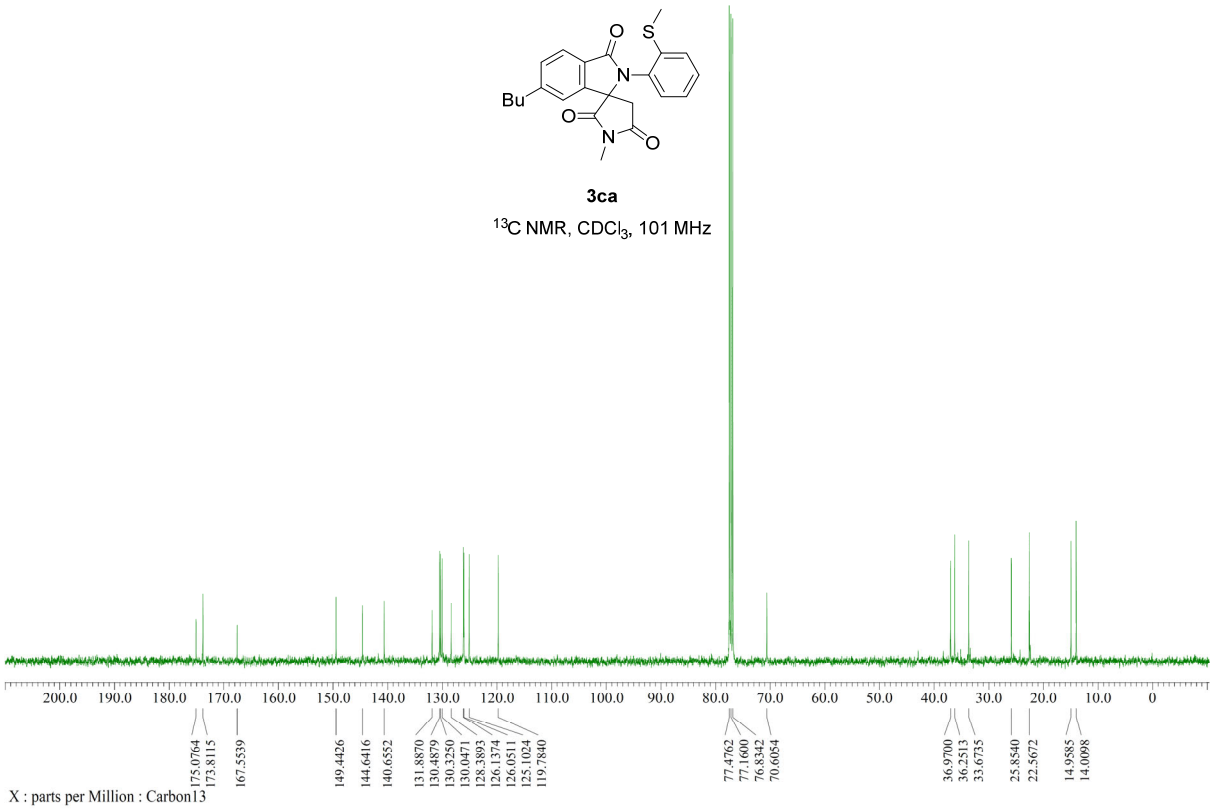

3ba
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton

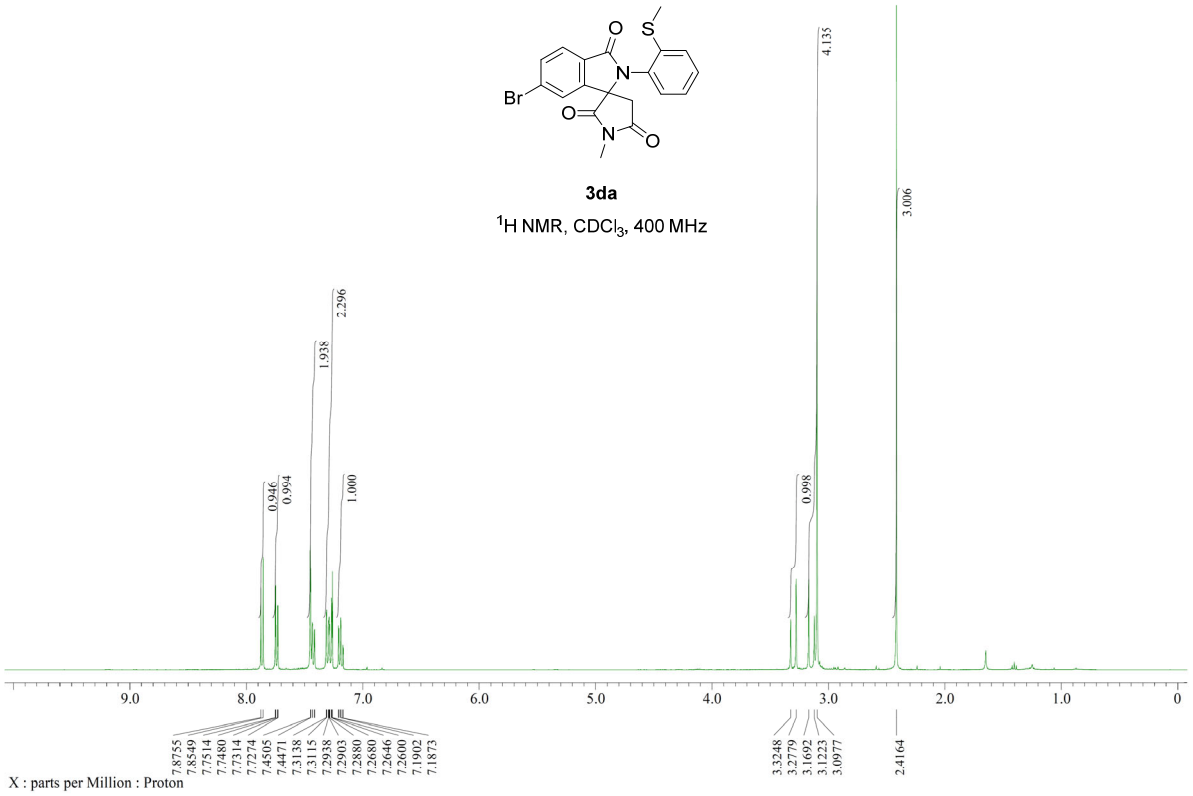

3ba
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13

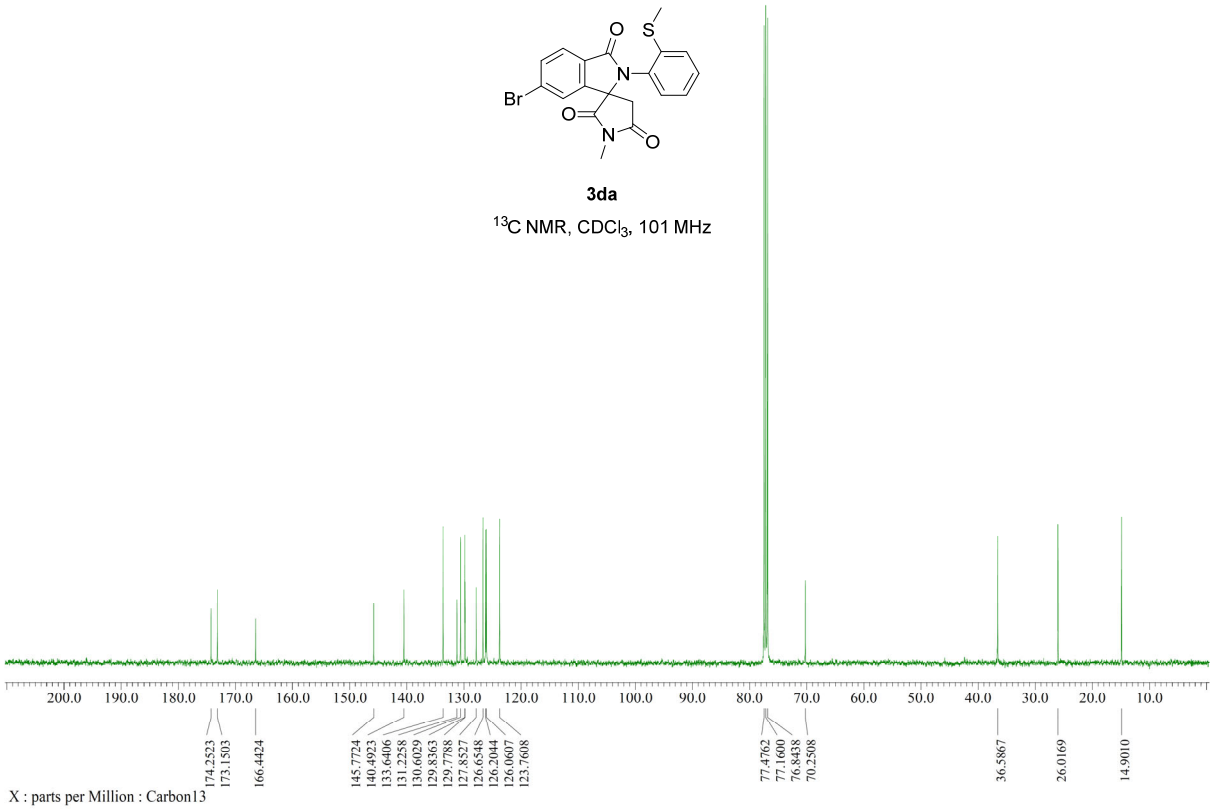

3bd
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton

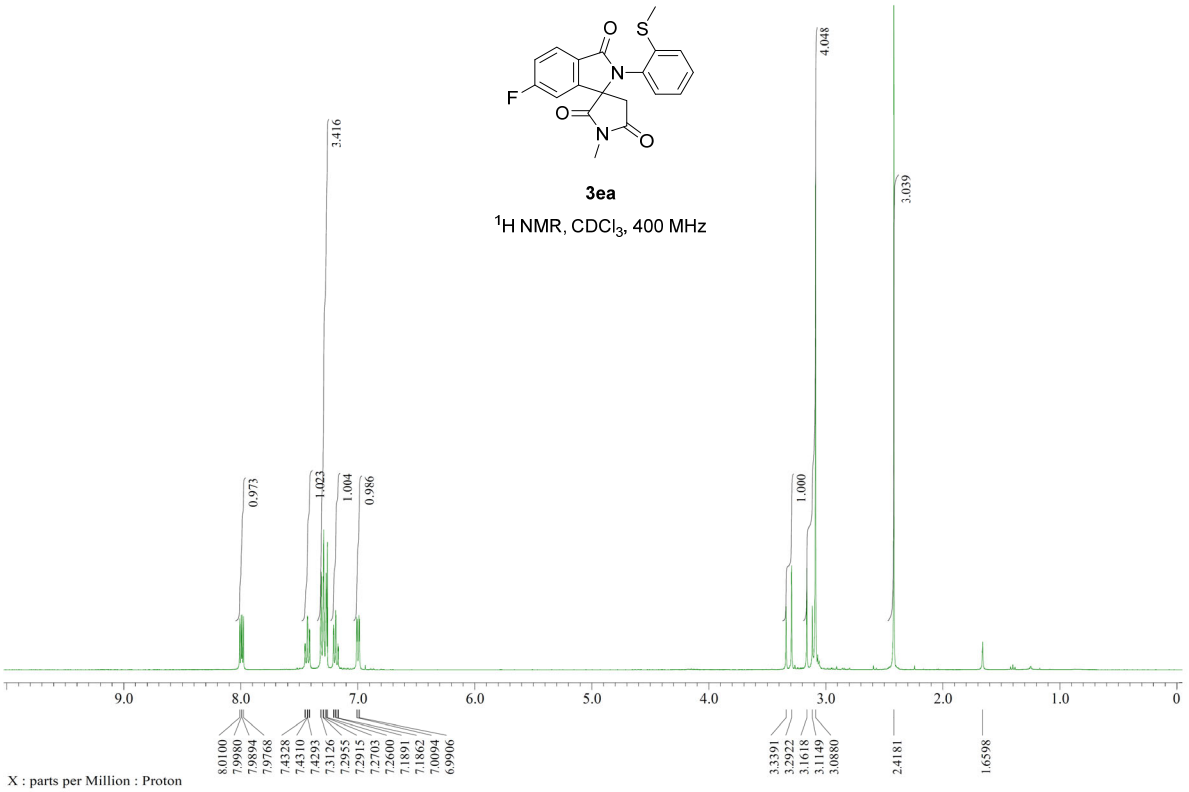

3bd
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13

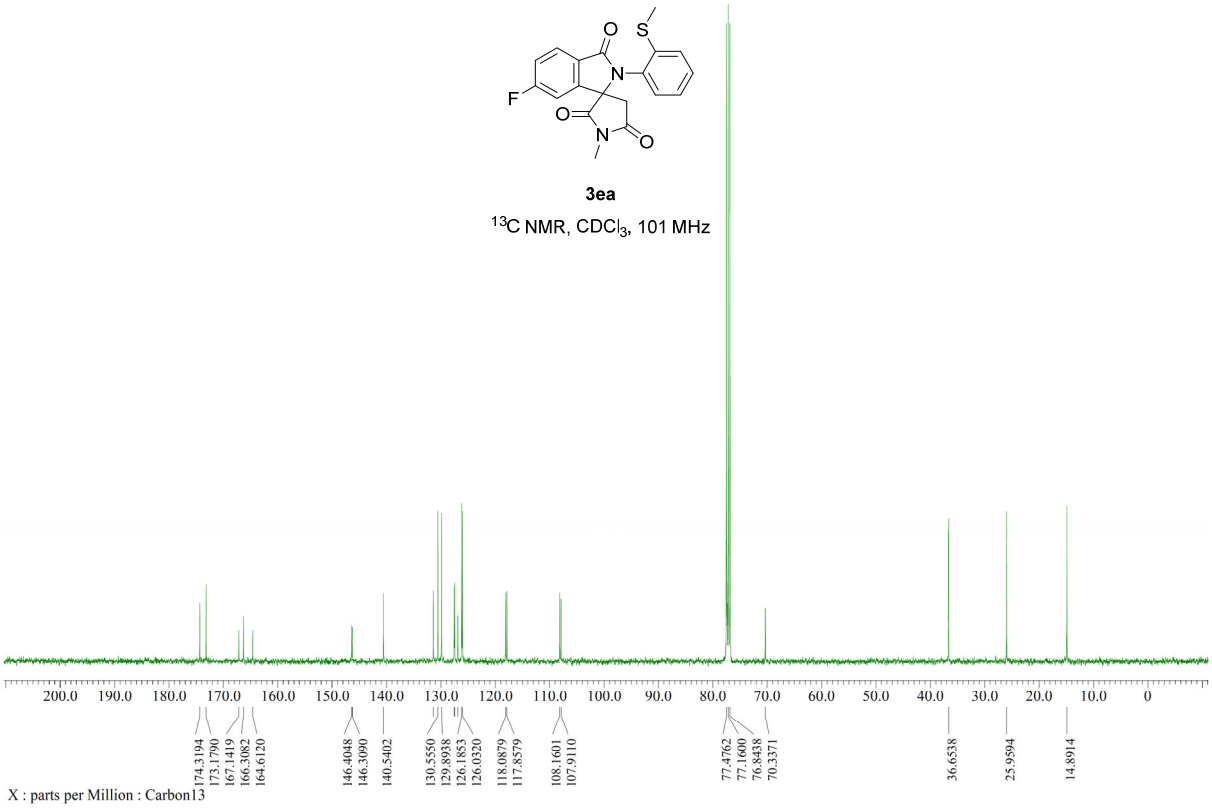

Bu
O
S
N
O
N
O
3ca
1H NMR, CDCl3, 400 MHz
1.000
2.068
2.046
1.056
1.030
1.009
1.177
3.288
2.121
3.069
2.442
2.331
3.179
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.9076
7.8875
7.4207
7.4173
7.4013
7.3206
7.3189
7.3155
7.3052
7.3018
7.2657
7.0541
7.0529
3.3197
3.2739
3.1629
3.1160
3.0994
3.0823
3.0622
2.7104
2.6904
2.4147
1.6435
1.6235
1.6046
1.4147
1.3958
1.3769
0.9679
0.9496
0.9313
0.0000
X : parts per Million : Proton

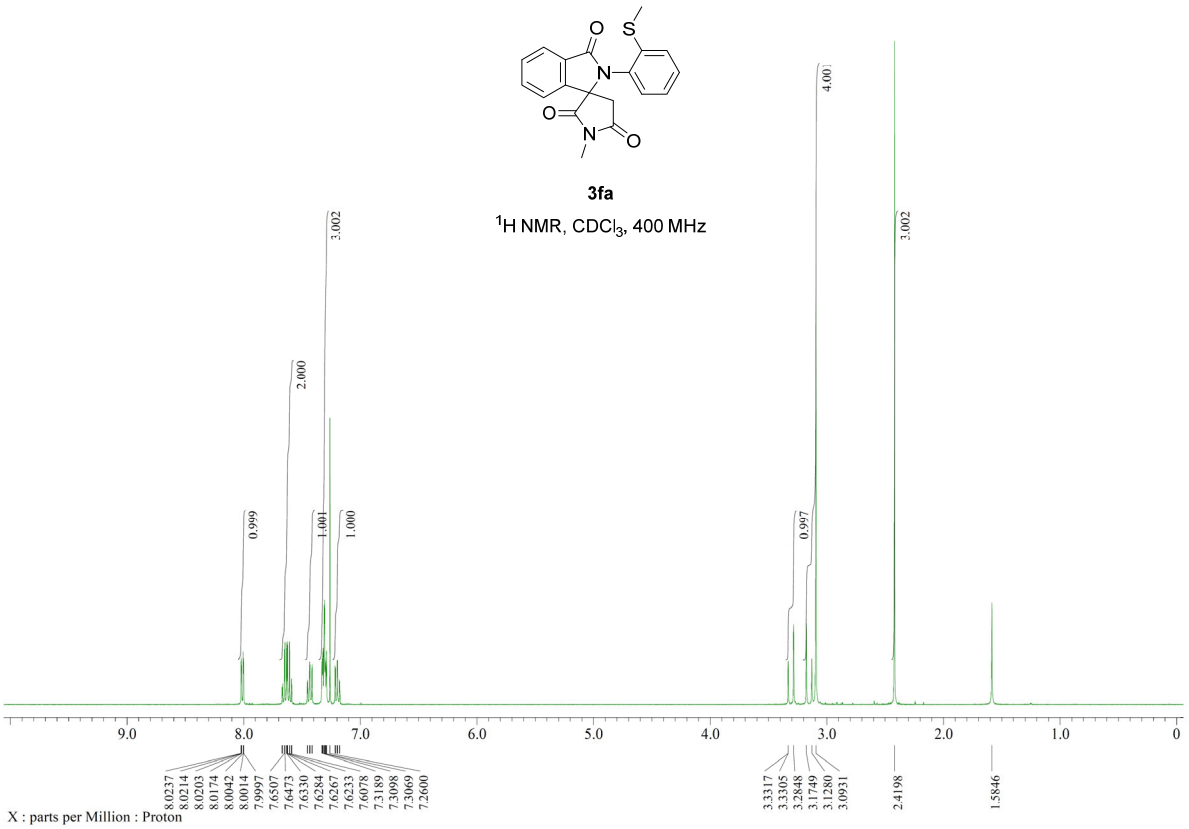

Bu
O
S
N
O
N
O
3ca
13C NMR, CDCl3, 101 MHz
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
175.0764
173.8115
167.5539
149.4426
144.6416
140.6552
131.8870
130.4879
130.3250
130.0471
128.3893
126.1374
126.0511
125.1024
119.7840
77.4762
77.1600
76.8342
70.6054
36.9700
36.2513
33.6735
25.8540
22.5672
14.9585
14.0098
X : parts per Million : Carbon13

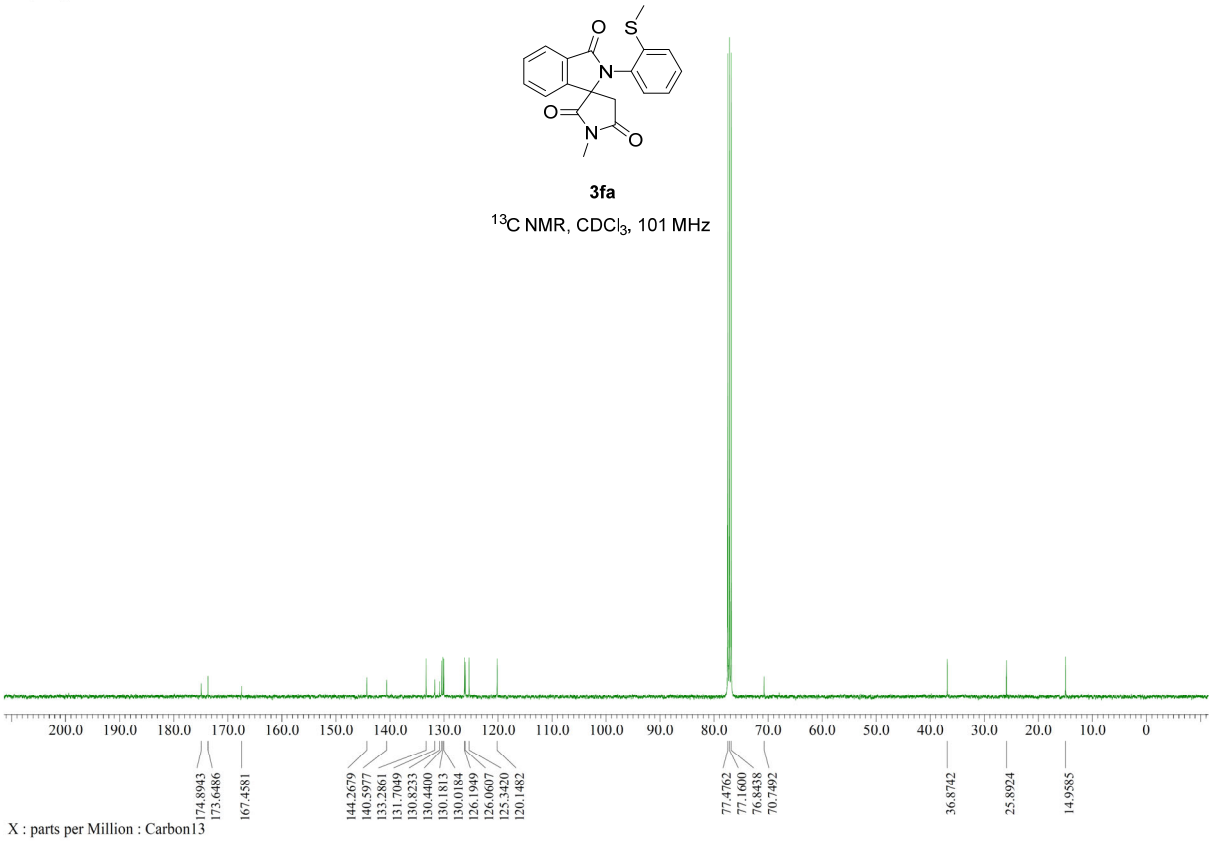

3da
1H NMR, CDCl3, 400 MHz
4.135
3.006
2.296
1.938
1.000
0.998
0.994
0.946
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8755
7.8549
7.7514
7.7480
7.7314
7.7274
7.4505
7.4471
7.3138
7.3115
7.2938
7.2903
7.2880
7.2646
7.2680
7.2600
7.1902
7.1873
3.3248
3.2779
3.1692
3.1223
3.0977
2.4164
X : parts per Million : Proton

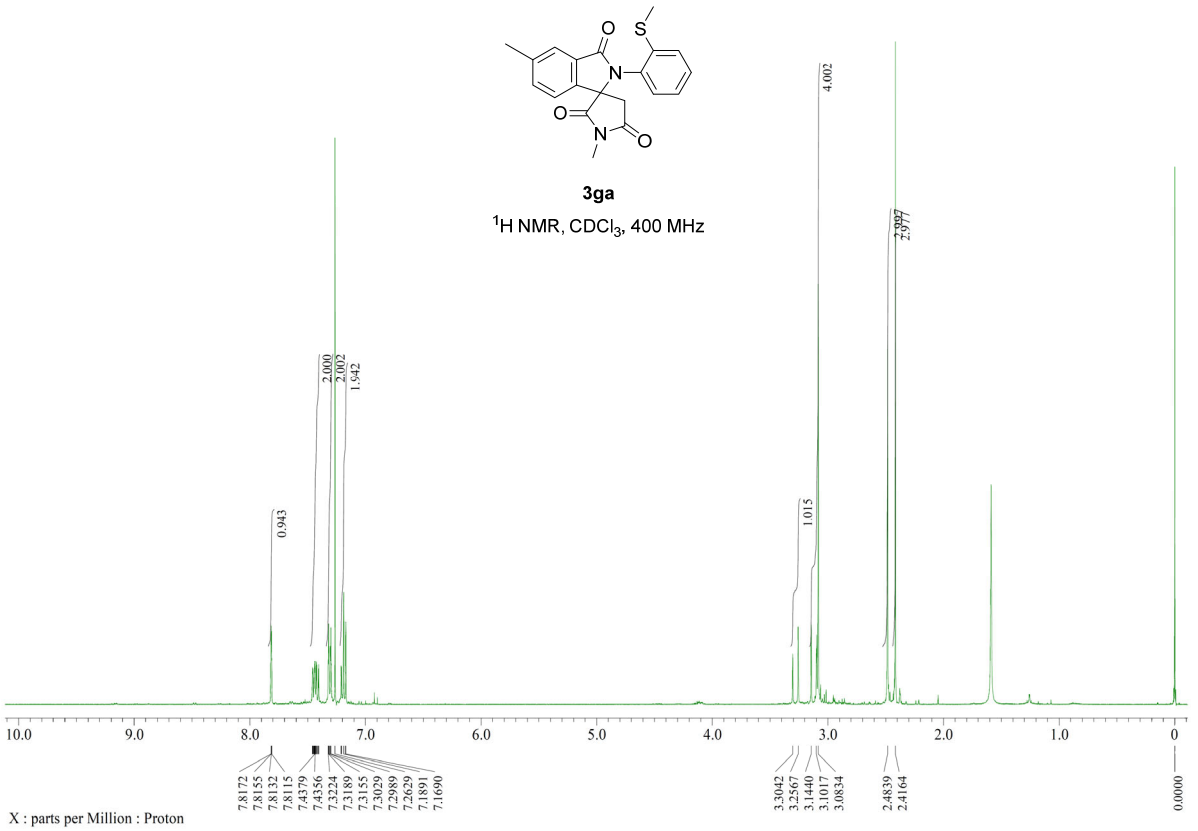

3da
13C NMR, CDCl3, 101 MHz
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
174.2523
173.1503
166.4424
145.7724
140.4923
133.6406
131.2258
130.6029
129.8363
129.7788
127.8527
126.6548
126.2044
126.0607
123.7608
77.4762
77.1600
76.8438
70.2508
36.5867
26.0169
14.9010
X : parts per Million : Carbon13

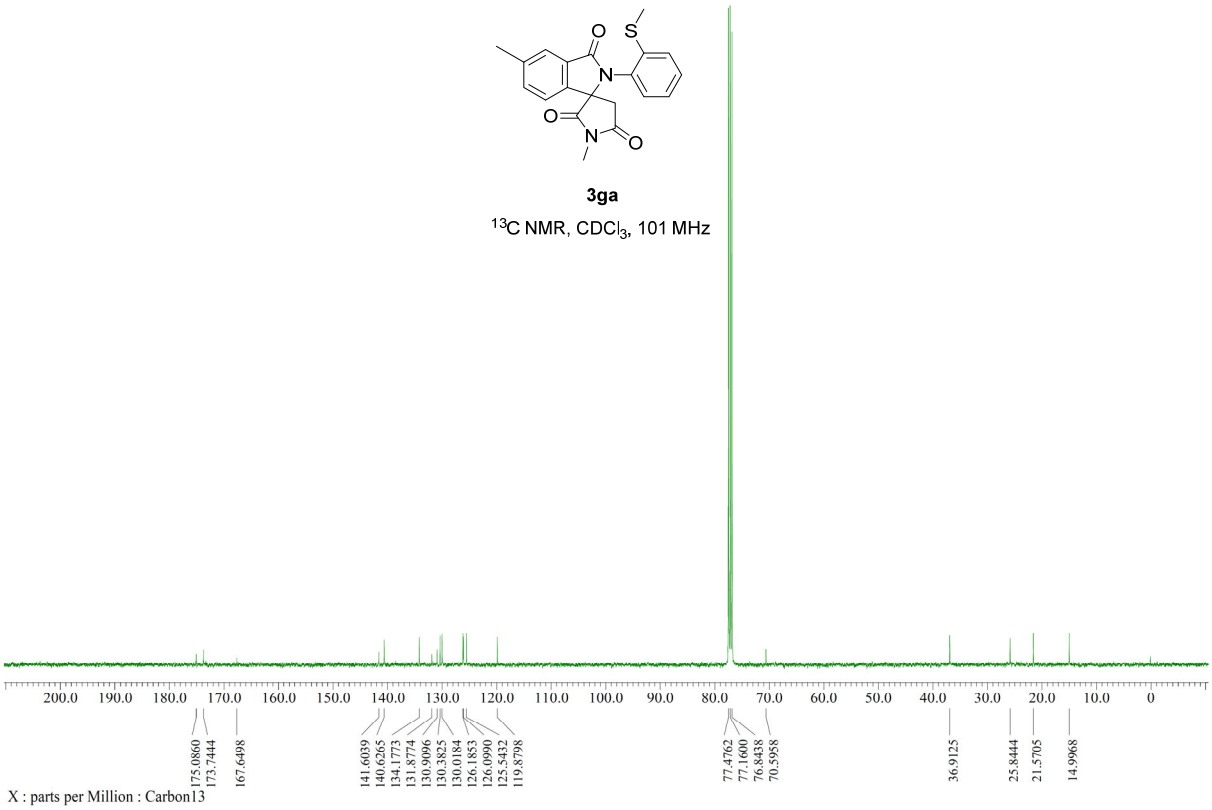

3ea
1H NMR, CDCl3, 400 MHz
3.416
4.048
3.039
0.973
1.023
1.004
0.986
1.000
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.0100
7.9980
7.9894
7.9768
7.4328
7.4310
7.4293
7.3126
7.2955
7.2915
7.2703
7.2600
7.1891
7.1862
7.0094
6.9906
3.3391
3.2922
3.1618
3.1149
3.0880
2.4181
1.6598
X : parts per Million : Proton

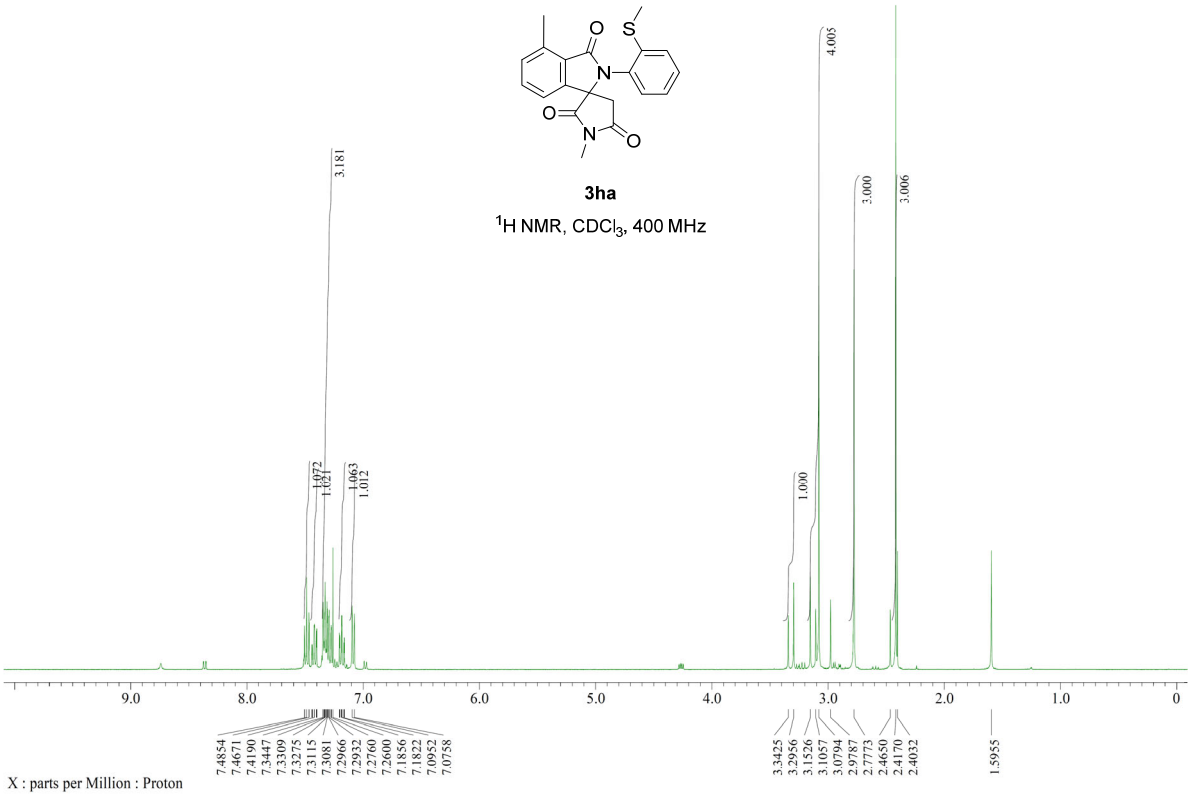

3ea
13C NMR, CDCl3, 101 MHz
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
174.3194
173.1790
167.1419
166.3082
164.6120
146.4048
146.3090
140.5402
130.5550
129.8938
126.1853
126.0320
118.0879
117.8579
108.1601
107.9110
77.4762
77.1600
76.8438
70.3371
36.6538
25.9594
14.8914
X : parts per Million : Carbon13

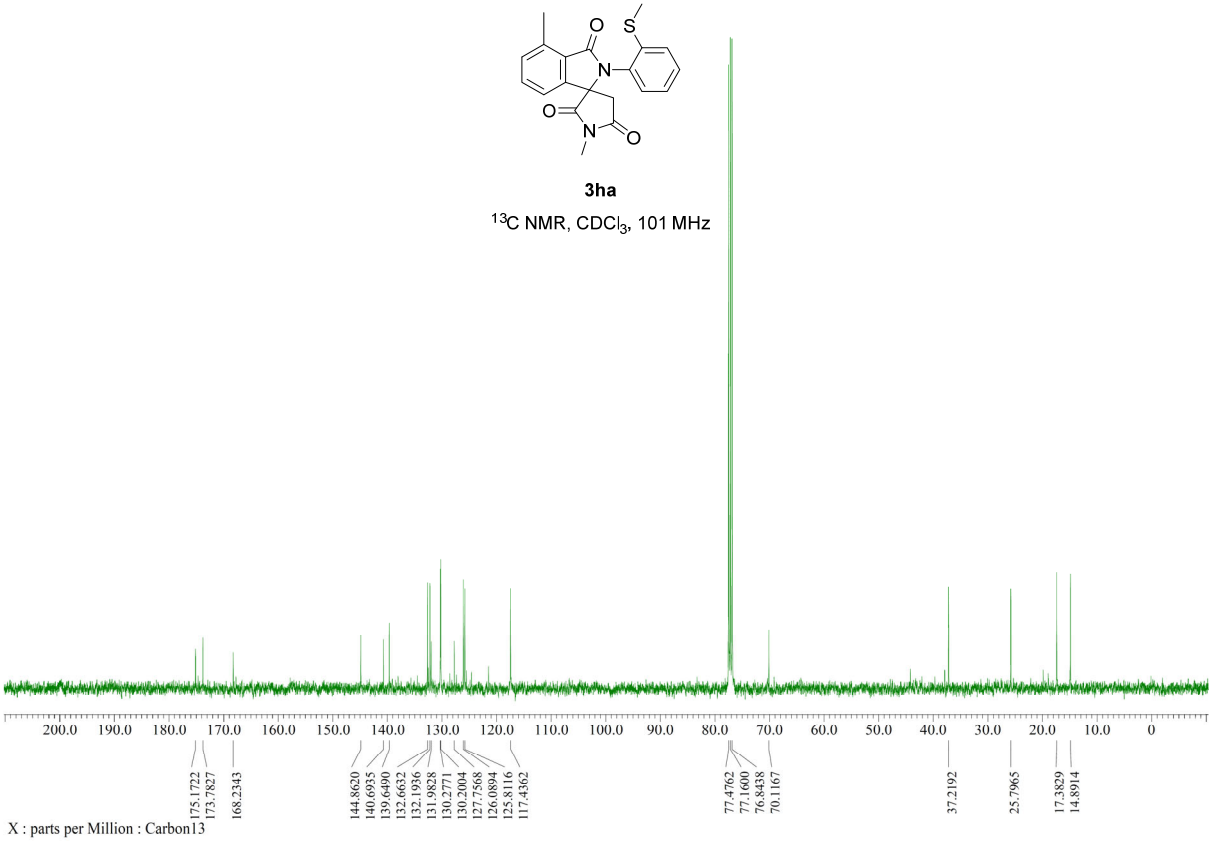

3fa
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton

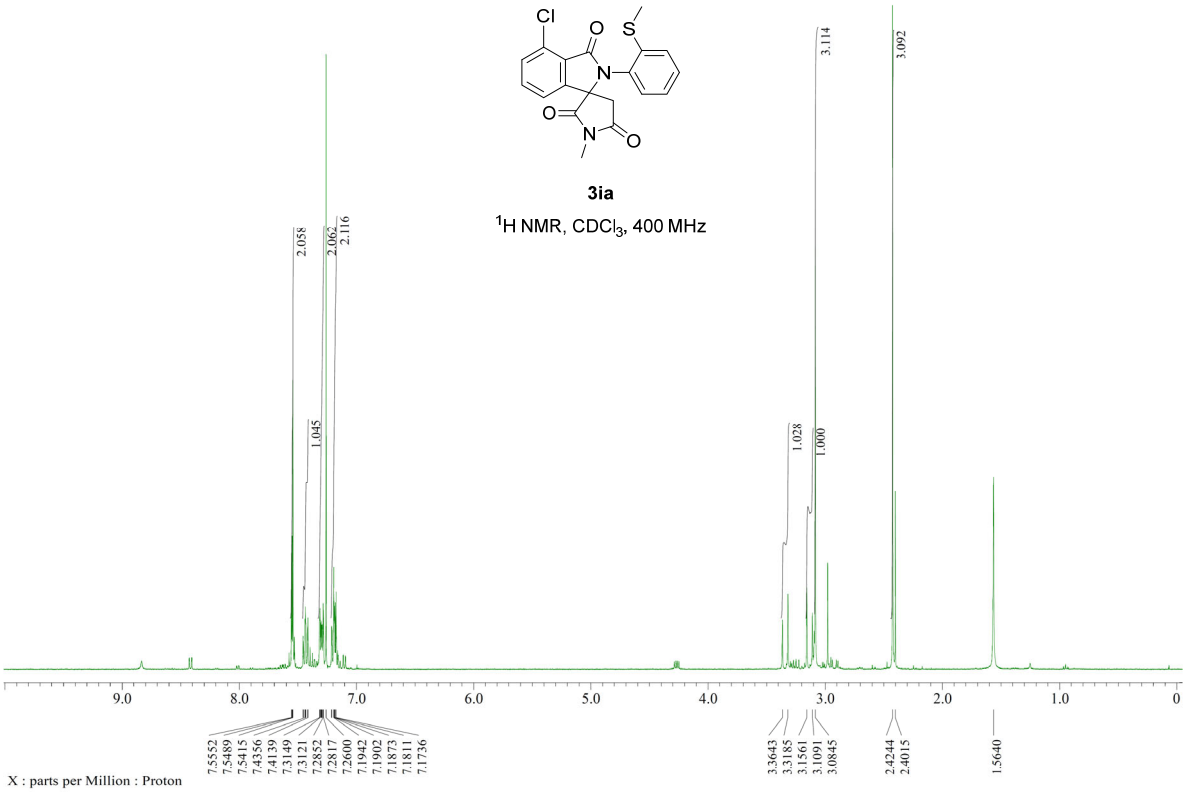

3fa
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13

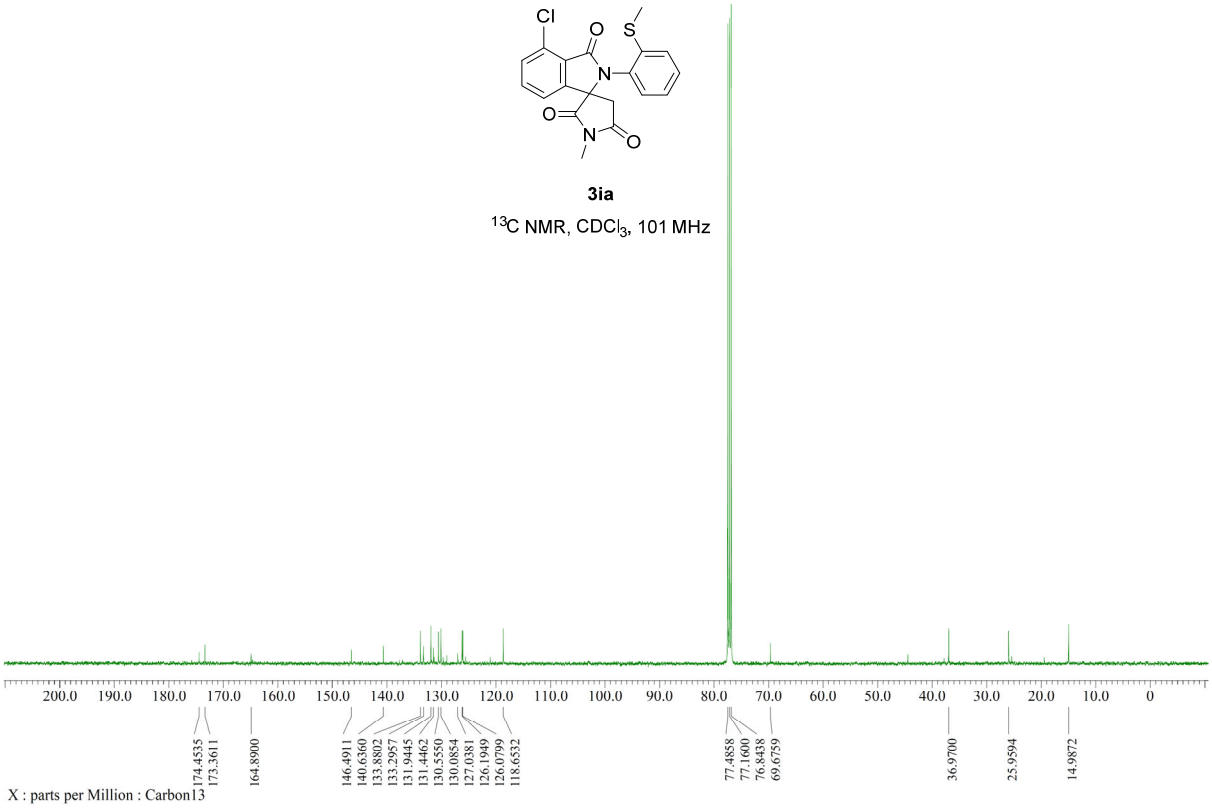

3ga
1H NMR, CDCl3, 400 MHz
4.002
2.997
2.977
2.000
2.002
1.942
1.015
0.943
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8172
7.8155
7.8132
7.8115
7.4379
7.4356
7.3224
7.3189
7.3155
7.3029
7.2989
7.2629
7.1891
7.1690
3.3042
3.2567
3.1440
3.1017
3.0834
2.4839
2.4164
0.0000
X : parts per Million : Proton

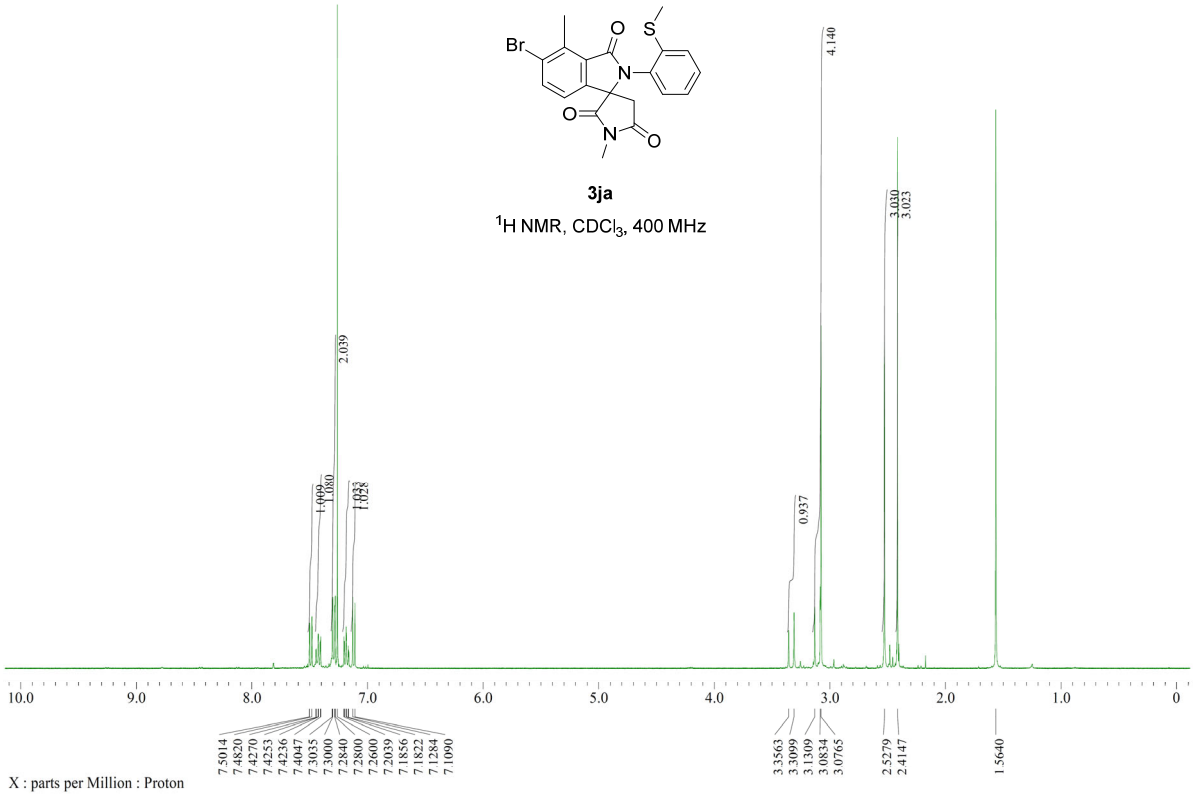

3ga
13C NMR, CDCl3, 101 MHz
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
175.0860
173.7444
167.6498
141.6039
140.6265
134.1773
131.8774
130.9096
130.3825
130.0184
126.1853
126.0990
125.5432
119.8798
77.4762
77.1600
76.8438
70.5958
36.9125
25.8444
21.5705
14.9968
X : parts per Million : Carbon13

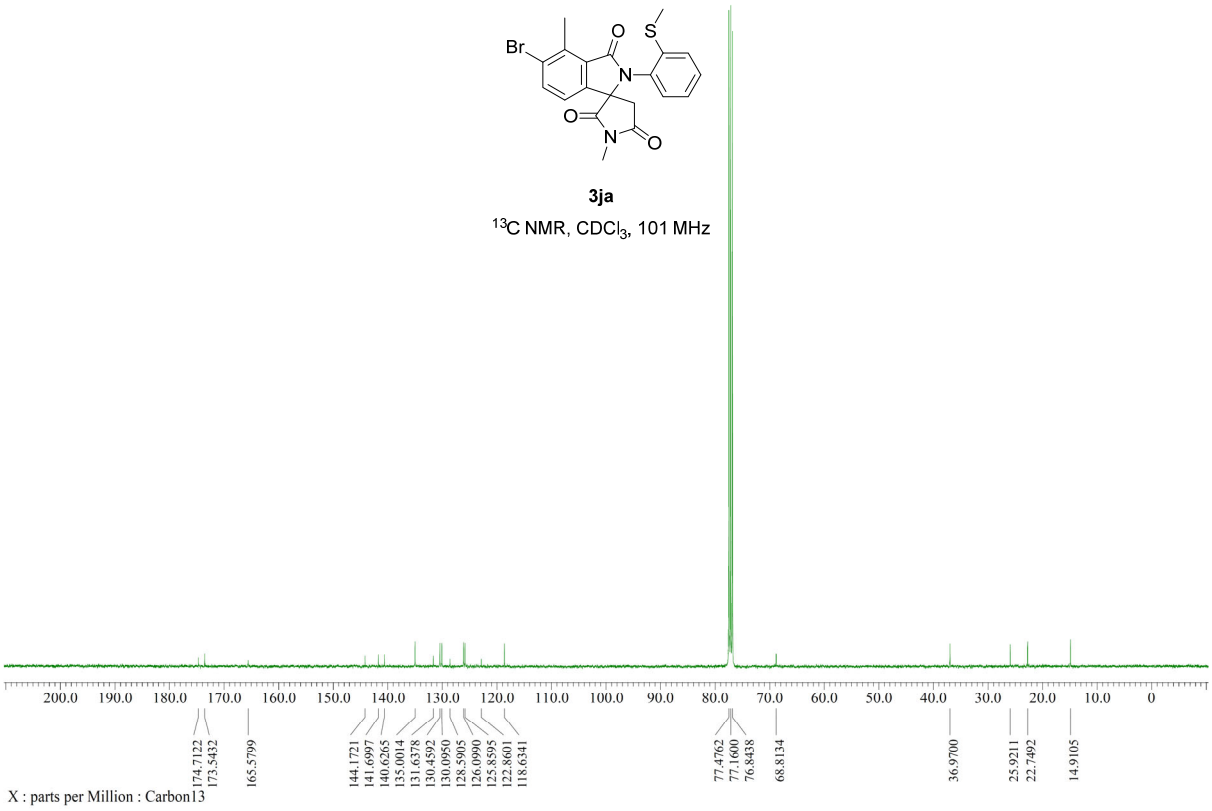

3ha
1H NMR, CDCl3, 400 MHz
3.181
1.072
1.021
1.063
1.012
1.000
4.005
3.000
3.006
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4854
7.4671
7.4190
7.3447
7.3309
7.3275
7.3115
7.3081
7.2966
7.2932
7.2760
7.2600
7.1856
7.1822
7.0952
7.0758
3.3425
3.2956
3.1526
3.1057
3.0794
2.9787
2.7773
2.4650
2.4170
2.4032
1.5955
X : parts per Million : Proton

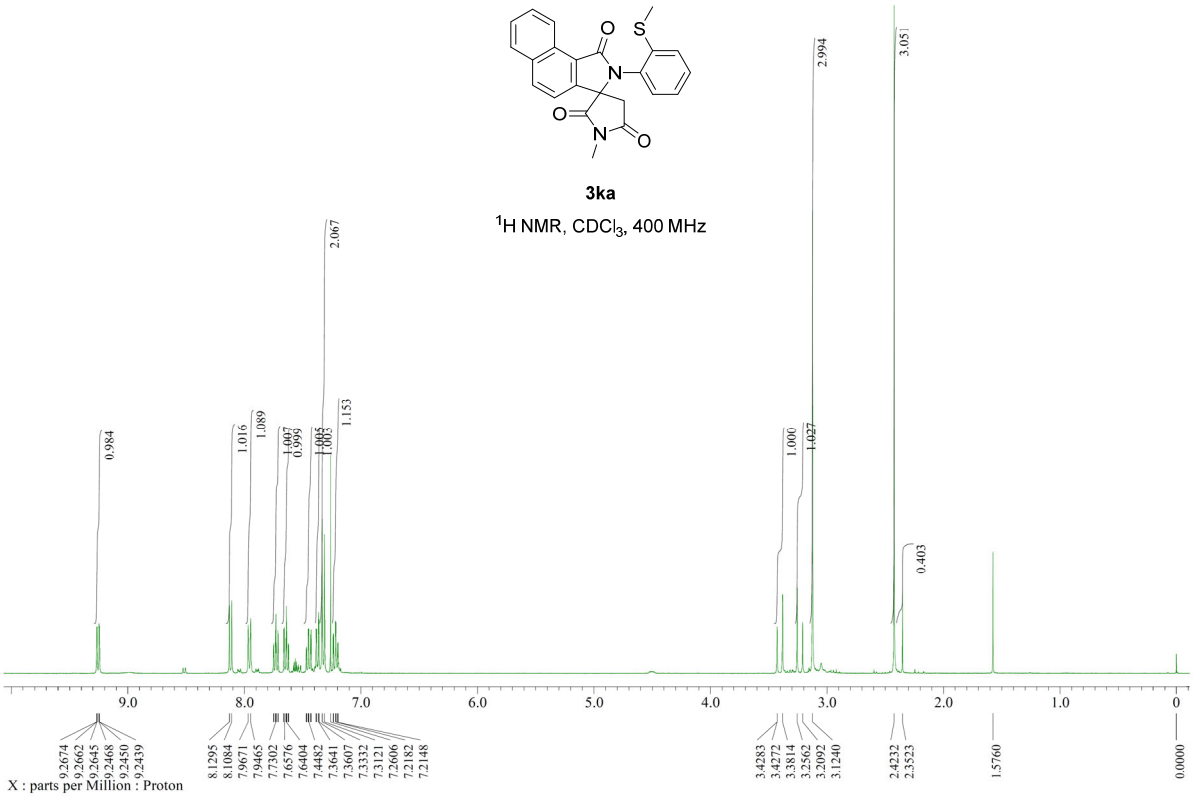

3ha
13C NMR, CDCl3, 101 MHz
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
175.1722
173.7827
168.2343
144.8620
140.6935
139.6490
132.6632
132.1936
131.9828
130.2771
130.2004
127.7568
126.0894
125.8116
117.4362
77.4762
77.1600
76.8438
70.1167
37.2192
25.7965
17.3829
14.8914
X : parts per Million : Carbon13

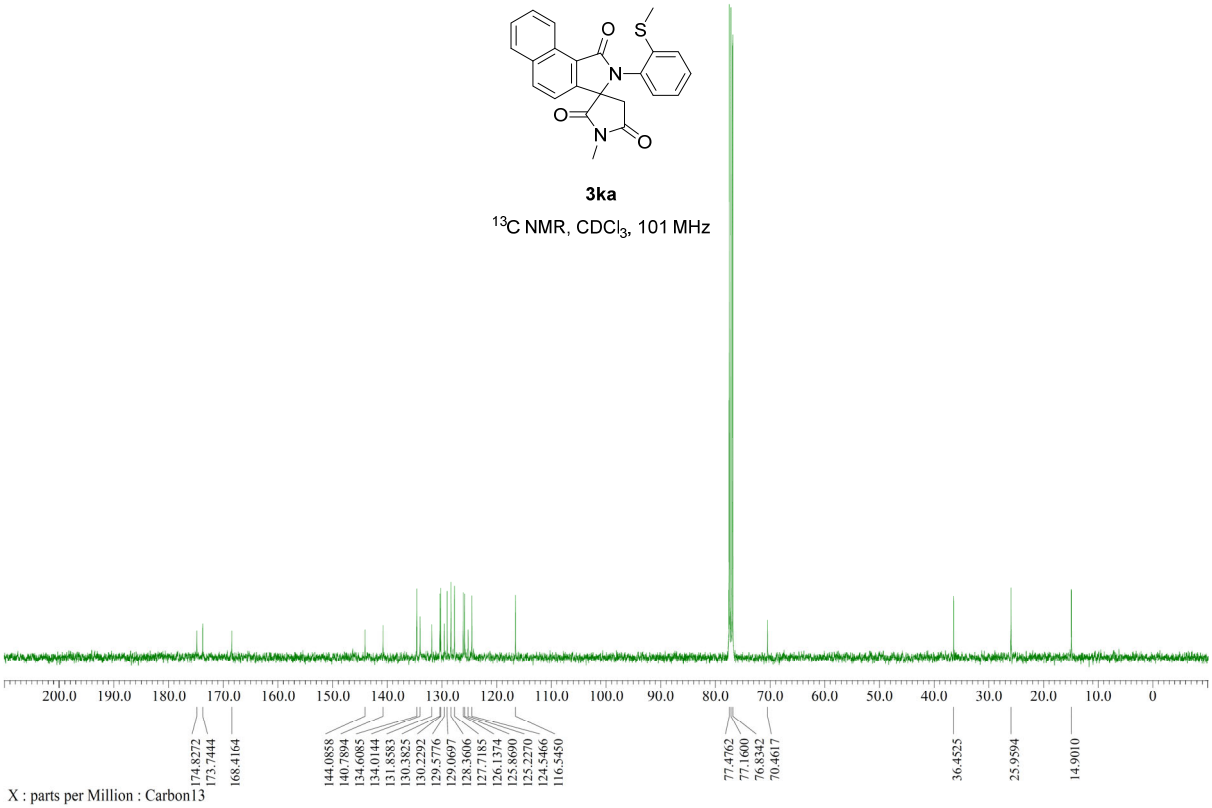

Cl
O
S
N
O
N
O
3ia
1H NMR, CDCl3, 400 MHz
2.058
2.062
2.116
1.045
1.028
1.000
3.114
3.092
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.5552
7.5489
7.5415
7.4356
7.4139
7.3149
7.3121
7.2852
7.2817
7.2600
7.1942
7.1902
7.1873
7.1811
7.1736
3.3643
3.3185
3.1561
3.1091
3.0845
2.4244
2.4015
1.5640
X : parts per Million : Proton

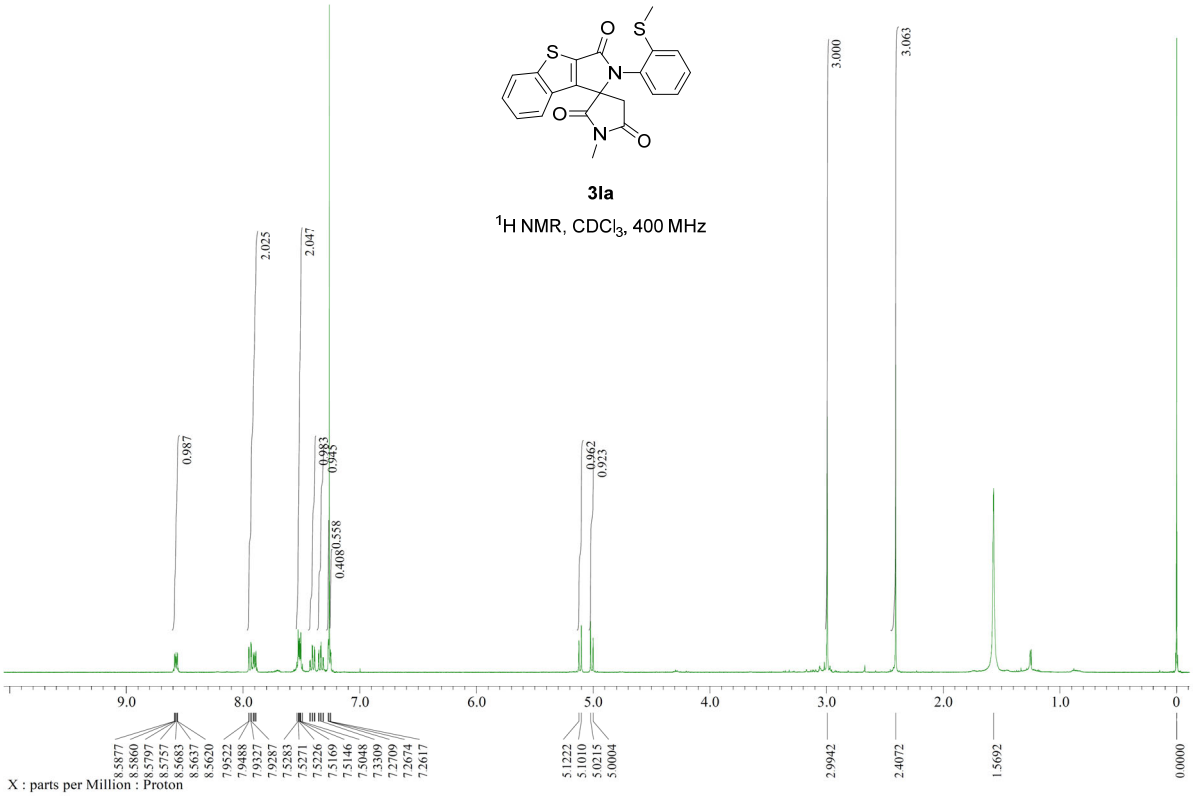

Cl
O
S
N
O
N
O
3ia
13C NMR, CDCl3, 101 MHz
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
174.4535
173.3611
164.8900
146.4911
140.6360
133.8802
133.2957
131.9445
131.4462
130.5550
130.0854
127.0381
126.1949
126.0799
118.6532
77.4858
77.1600
76.8438
69.6759
36.9700
25.9594
14.9872
X : parts per Million : Carbon13

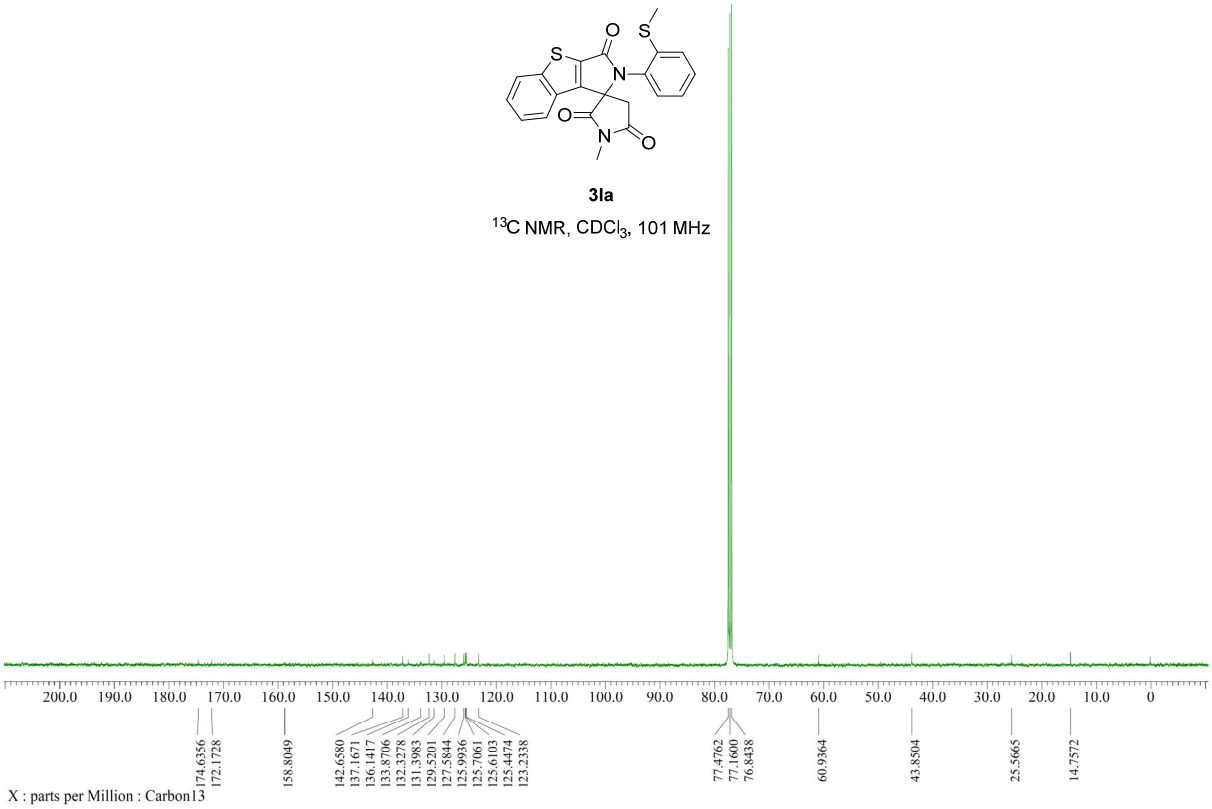

Br
O
S
N
O
O
N
O
3ja
^{1}H NMR, CDCl$_3$, 400 MHz
4.140
3.030
3.023
2.039
1.099
1.080
1.033
1.028
0.937
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.5014
7.4820
7.4270
7.4253
7.4236
7.4047
7.3035
7.3000
7.2840
7.2800
7.2600
7.2039
7.1856
7.1822
7.1284
7.1090
3.3563
3.3099
3.1309
3.0834
3.0765
2.5279
2.4147
1.5640
X : parts per Million : Proton


Br
O
S
N
O
O
N
O
3ja
^{13}C NMR, CDCl$_3$, 101 MHz
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
174.7122
173.5432
165.5799
144.1721
141.6997
140.6265
135.0014
131.6378
130.4592
130.0950
128.5905
126.0990
125.8595
122.8601
118.6341
77.4762
77.1600
76.8438
68.8134
36.9700
25.9211
22.7492
14.9105
X : parts per Million : Carbon13


3ka
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton


3ka
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13


3Ia
1H NMR, CDCl3, 400 MHz
X : parts per Million : Proton


3Ia
13C NMR, CDCl3, 101 MHz
X : parts per Million : Carbon13

IX. Computational details:

The reaction path of Rhodium(I)-catalyzed C−H alkylation of the 2-(methylthio)aniline aromatic amide with maleimide was investigated by Density Functional Theory (DFT) calculations, using the Gaussian 16[6] (Rev. A. 03) and Orca[7] (version 4.2.1) software packages. The B3LYP+D3BJ[8-10] and M06[11] functionals at the def2-SVP[12] level basis sets were employed to carry out lower level pre-geometry optimizations and conformational analyses. The final geometry optimization was performed at the M06/def2-TZVP/SMD[13] level using dielectric constant 2.3741 (toluene) and additional parameters to account for the solvent effect and at the DLPNO-CCSD(T)/def2-TZVP[12,14] level also. On all functionals and basis sets, the thermal corrections to the electronic energies had been estimated at 433.15 K (160°C) and 1 atm (to mimic the experimental conditions) using the normal coordinate analysis achieving the Gibbs free energies. The 1-methyl-2,5-pyrroledione was used as the representative of maleimide, 2-(methylthio)aniline as a directing group of aromatic amide, and Rh(COD)(OPiv) as the catalyst as in the experimental conditions. Transitional entropies have also been corrected using the method developed by Whitesides (W)[15,16], and the concentration correction (cc) was also considered on the Gibbs free energy based on the experimental condition. The analysis of electron density was carried out with the quantum theory of atoms in molecules (QTAIM[17]), while further Mayer bond order (MBO[18]) analyses to clarify the nature of bonding and structure. Furthermore, the natural population analysis (NPA[19]) was applied to determine the atomic charges, and localized orbital bonding analysis (LOBA[20]) to determine the oxidation state of rhodium. The energy decomposition analysis (EDA[21]) was also performed to gain insight into the difference in the reaction paths' intermediate and transition state structures. These analyses were conducted with MultiWFN 3.7[22] and NBO 6.0[23] software. The energetic span model[24] and AUTOF[25] software were used to determine the rate-determining step, utilizing the TDTS (TOF-determining transition state), TDI (TOF-determining intermediate), and energetic span for the preferable reaction paths for the formation of isoindolone spirosuccinimides. The conformation analyses were carried out with the GFN2-xTB[26] (Density Functional Tight Binding) method applied in the xTB[27] software. The noncovalent interactions in the final products were evaluated by the NCI[28] method and visualized by the Chemcraft[29] software to explain the deuterium labeling experimental results. Furthermore, the Kinetic Isotopic Effect (KIE) was calculated by the python version of kinisot[30].

X. Whitesides correction and concentration correction:

The Sackur-Tetrode equation (S_{trans}) fails in the assumption that molecules have no volume, which is reasonable in the gas phase, where the volume occupied by molecules is very small compared to the total volume. Thus, the translation entropy correction in the solution can be applied with the following equation:

$$S_{trans}^{corr} = S_{trans} + R \ln V_{free}$$

$$V_{free} = C_{free}\left(\sqrt[3]{\left(\frac{10^{27}}{[X]N_A}\right)} - \sqrt[3]{V_{molec}}\right)^3$$

whereas V_{free} is the "free volume", C_{free} is 8, N_A is the Avogadro's number ($6.022*10^{23}$ mol^{-1}), while the density of toluene at 25°C is 0.8623 g/cm^3 and M is 92.14 g/mol, therefore the [X] = 9.3585 mol/L. The volume of the molecule (Table S2, V_{mol}) on the different levels of theory was obtained from Gaussian 16 simulations, and V_{molec} was calculated with $V_{molec} = V_{mol}/N_A$ equation.

1. Table S7: The values of the Whitesides correction of translational entropy

	B3LYP+D3BJ/ def-2SVP	**M06/ def2-SVP**	**M06/ def2-TZVP**
V_{mol} [cm^3]	83.96	82.95	83.78
V_{molec} [$Å^3$]	139	138	139
V_{free} [$Å^3$]	3.72	3.54	3.89
$R\ln V_{free}$ [kJ/mol*K]	0.0109	0.0113	0.0109

Experimental conditions

$C_{2\text{-met}}$ = 0.1 mmol, C_{mal} = 0.3 mmol, $C_{Rh(I)}$ = 0.01 mmol (5 mol%), toluene (1 equiv)

Gibbs free energy concentration correction

$C_{2\text{-met}}$ = 0.1 M, C_{mal} = 0.3 M, C_{prod} = 0.9 M (90% yield)

$G_{corr} = 2.303\ RT \log_{10}K$, $K = [C_{prod}/(C_{2\text{-met}}\ C_{mal})]$

R = 8.314E-03 [kJ/mol K], T = 433.15 [K]

G_{corr} = -4.0 [kJ/mol]

XI. Energy decomposition analysis (EDA)

A simple energy decomposition analysis (EDA), based on the work of Kitaura and Morokuma, was performed with the combination of the two A and B fragments' wavefunction from the optimized AB structure and the total energy variation of forming complex was determined with the following equation:

$$\Delta E_{int} = E_{AB} - (E_A + E_B) = \Delta E_{steric} + \Delta E_{orb}$$

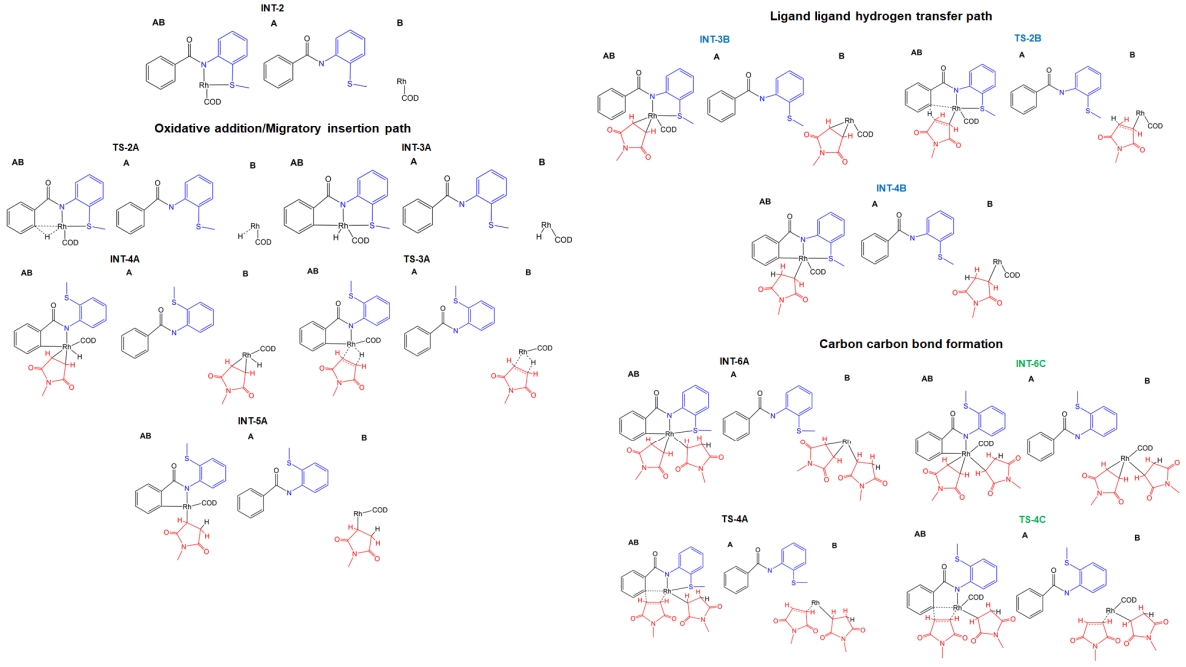
where ΔE_{steric} consists of the electrostatic interaction and exchange repulsion term and E_{orb} is the orbital interaction term, which is sometimes known as the induction or polarization term. The ΔE_{orb} and ΔE_{steric} can be determined with the following equations:

$$\Delta E_{orb} = E_{SCF,last} - E_{SCF,1st}$$

$$\Delta E_{steric} = \Delta E_{int} - \Delta E_{orb}$$

Furthermore, the dispersion interaction (ΔE_{disp}) was also determined with the difference of B3LYP/def2-SVP and B3LYP+D3/def2-SVP single point energy calculations on the optimized AB structure.

2. Figure S1: The fragmentation for the energy decomposition analysis of the structures involved in the OA/MI, LLHT and CCBF paths.



3. **Table S8: The energy decomposition analysis of the structures involved in the OA/MI, LLHT and CCBF paths.**

	E_A (a.u.)	E_B (a.u.)	E_{AB} (a.u.)	ΔE_{int} (kJ/mol)	ΔE_{orb} (kJ/mol)	ΔE_{steric} (kJ/mol)	ΔE_{disp} (kJ/mol)
INT-2	-1068.2649	-422.4677	-1491.2005	-1228	-1473	245	-375
TS-2A	-1067.8358	-423.0182	-1491.1278	-719	-1225	506	-392
INT-3B	-1068.2782	-821.2125	-1889.8589	-967	-1104	138	-506
INT-3A	-1067.8439	-423.0174	-1491.1576	-778	-1160	382	-398
TS-2B	-1067.8545	-821.6843	-1889.7798	-633	-1519	886	-522
INT-4A	-1067.8596	-821.7358	-1889.8227	-597	-916	319	-526
INT-4B	-1067.8472	-821.7729	-1889.8682	-651	-1021	370	-536
TS-3A	-1067.8556	-821.7200	-1889.8061	-605	-919	314	-528
INT-5A	-1067.8651	-821.7654	-1889.8328	-531	-873	342	-500
INT-6A	-1067.8534	-908.5019	-1976.6135	-678	-1049	371	-465
INT-6C	-1067.8493	-1220.3913	-2288.4553	-564	-872	309	-650
TS-4A	-1067.8505	-908.4840	-1976.5887	-667	-1369	702	-452
TS-4C	-1067.8501	-1220.3900	-2288.4530	-559	-900	341	-652

XII. Kinetic isotopic effect of the calculated reaction paths:

The kinetic isotopic effect (KIE) of the calculated reaction paths was determined using the kinisot python code. The determination of KIE was compared between INT-0 and TS-2A, TS-2B, TS-3A, TS-7C and TS-7D transition states. The temperature was set 433.15 K to reproduce the experimental conditions, while the scaling factor for vibrational frequencies was set to default (0.982) to apply automatically for the combination of functional/basis set (M06/def2-TZVP). Furthermore, the quantum mechanical tunnelling correction (1D-Tunn) is computed also.

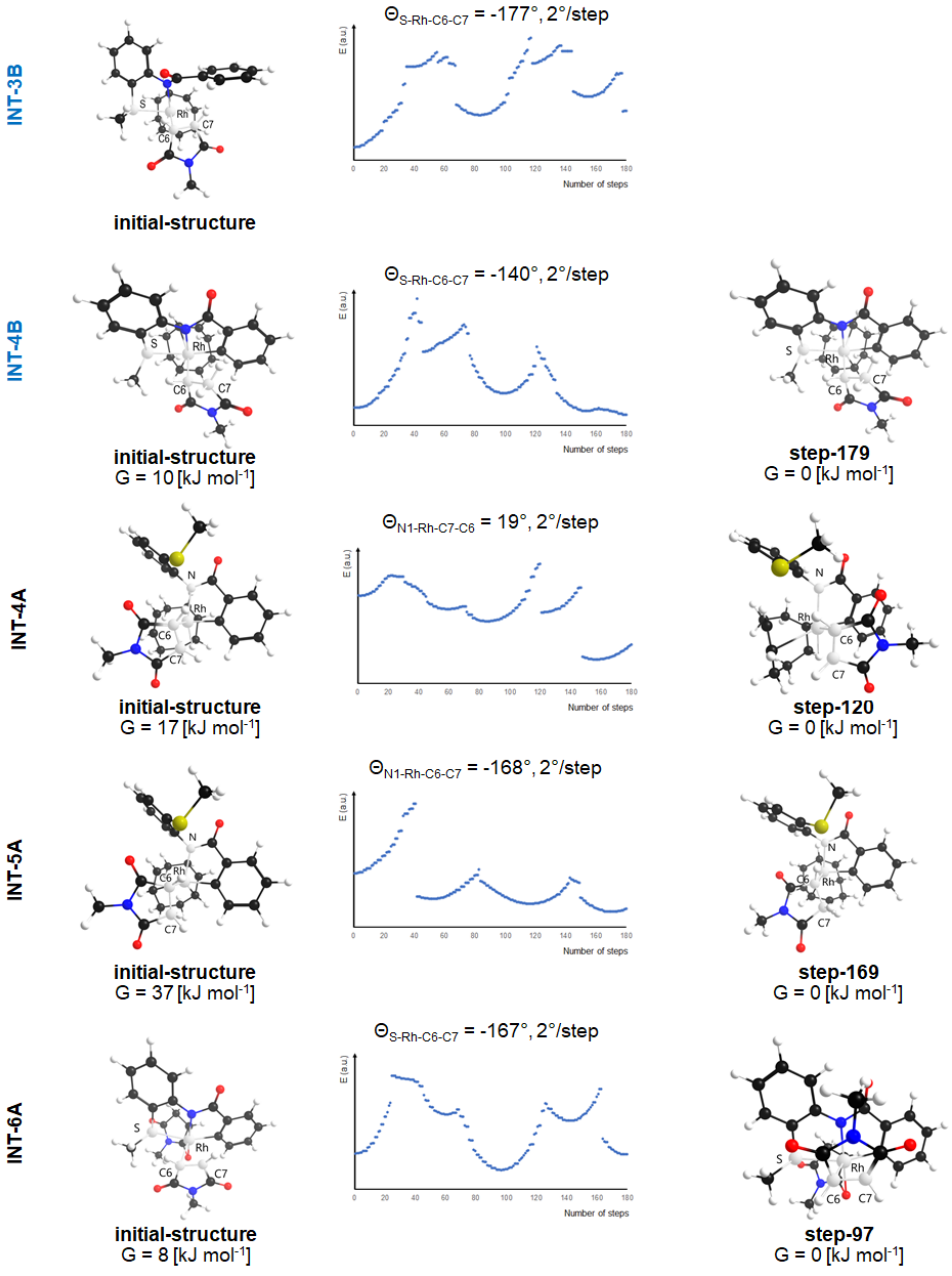
1. Table S9: The theoretical kinetic isotopic effect determined for the most important transition states of the reaction paths.

	INT-0 TS-2A	INT-0 TS-2B	INT-0 TS-3A	INT-0 TS-7C	INT-0 TS-7D	Exp.
KIE	2.89	3.39	2.95	1.02	0.97	2.5
KIE (corr.)	3.36	9.31	3.12	1.02	0.97	N/A

XIII. Conformational analysis of maleimide coordinated structures:

Conformational analyses were carried out both reaction paths' (LLHT, OA/MI, CCBF) maleimide coordinated structures (INT-3B, INT-4B, INT-4A, INT-5A, INT-6A) to determine the energetically most preferable conformation structures. The GFN2-xTB method was used to perform the relaxed scan geometry optimizations to save computational time. The lowest energy structure of the relaxed scan was further optimized on the B3LYP+D3BJ/def2-SVP level. The more stable conformation structure had been used in the further reaction path determination. The N1-Rh-C6-C7 dihedral angle was scanned for INT-4A and INT-5A, while S-Rh-C6-C7 dihedral angle for INT-3B, INT-4B and INT-6A structures with 2° stepwise condition for the relaxed scan simulations (Figure S2). The relaxed scan of INT-3B did not conclude into a lower energy structure then the initial structure. However, in the other relaxed scan analyses for INT-4B, INT-4A, INT-5A and INT-6A, a lower energy structure had been found. The further geometry optimization with B3LYP+D3BJ/def2-SVP and energy comparison with the initial structure showed that all lower energy structures are global minima, therefore these structures were used for further computational simulations.

1. **Figure S2: The fragmentation for the energy decomposition analysis of the structures involved in the OA/MI, LLHT and CCBF paths.**



XIV. The usability of SMD single point calculations results

The single point energy calculations with M06/def2-TZVP/SMD on the geometry optimized M06/def2-TZVP gave some significant an some neglectable differences throughout the whole reaction path (Table S9), showing that the usage of SMD is crucial.

1. **Table S10: The relative Gibbs free energies of LLHT, OA/MI and CCBF pathways with a different selection of DFT (B3LYP+D3BJ, M06) and post-HF (DLPNO-CCSD(T)) methods with different basis sets (def-2SVP, def2-TZVP, def2-TZVPP) and applied Whitesides (W) and concentration correction(cc).**

	B3LYP +D3BJ/ def2-SVP -W	M06/ def2-SVP -W	M06/ def2-TZVP -W	M06/ def2-TZVP -W-cc	**M06/ def2-TZVP /SMD -W-cc**	DLPNO-CCSD(T)/ def2-TZVPP -W-cc
INT-0	0	0	0	0	**0**	0
INT-1	-11	19	20	16	**32(27)**	25
TS-1	88	135	141	137	**152(140)**	149
INT-2	15	24	17	13	**12(8)**	11
TS-2A	188	208	205	201	**203(197)**	163
INT-3B	72	97	108	104	**120(105)**	80
INT-3A	97	135	131	127	**129(125)**	76
TS-2B	243	289	306	302	**292(304)**	292
INT-4A	166	186	206	202	**161(155)**	161
INT-4B	33	82	102	98	**111(112)**	40
TS-3A	180	222	243	239	**250(255)**	177
INT-5A	113	154	171	167	**174(168)**	129
INT-6A	-221	-172	-129	-133	**-75**	-218
INT-6C	273	328	364	361	**390**	299
TS-4A	-149	-108	-56	-60	**-3**	-139
TS-4C	187	335	376	372	**403**	309
INT-7A	-220	-179	-135	-139	**-85**	-218
INT-7C	94	145	189	185	**213**	123
TS-5A	-91	-67	-38	-42	**2**	-79
TS-5C	177	214	251	247	**264**	213
INT-8	-66	-52	-13	-17	**-1**	-43
TS-6A	19	31	66	62	**77**	42
INT-9C	-20	8	55	51	**78**	36
INT-9A	-66	-76	-38	-42	**-32**	-49
TS-6C	-14	28	67	63	**95**	40
INT-10A	-37	-33	13	9	**32**	0
INT-10C	-58	-54	-34	-38	**-33**	-44
INT-10D	-15	28	65	61	**92**	41
TS-7A	37	49	109	105	**130**	95
TS-7C	164	157	195	191	**196**	181
TS-7D	152	204	249	245	**236**	258
FP	-87	-105	-85	-89	**-87**	-83

Furthermore, it needs to be ensured that the single-point energy calculations are trustable, therefore the key steps of LLHT and OA/MI (from INT-1 to INT-4B/INT-5A) structures were also geometry optimized with M06/def2-TZVP/SMD level. Thus, the difference between the single-point energy and optimized energy (values are shown in brackets of Table S8 at M06/def2-TZVP/SMD level) is reasonably small (<10 kJ/mol), which support the usage of the single point energy results.

XV. The bonding system of Rh-L during the reaction path

The proposed mechanism pathway (Figure 1 black line) intermediate and transition state structures of the Rh transition metal bonding system was evaluated with Rh-L bond distances (Table S11), NPA (Natural Population Analysis) charges (Table S12), MBO (Mayor Bond Order) for Rh-L bond order (Table S13) and QTAIM (Quantum Theory of Atoms in Molecule) for the Rh-L bond critical points (CP(3,-1)) and the values (a.u.) of electron density (ρ) distribution (Table S14).

The Rh catalyst coordinates to N-(2-methylthio)phenyl)benzamides as the first step (INT-1) of the reaction path, where the Rh ion forms bond with S of 2-(methylthio)aniline, while keeping bond with one of the O of PivOH. During the protonation of amide group (TS-1) the Rh−O(PivOH) bond breaks and Rh form a bond with the N of amide group (INT-2). This can be followed up by the decreasing bond order (Table S13) and electron density distribution (Table S14) of Rh−O(PivOH) bond and the opposite of Rh−N(2met) bond. The oxidative addition TS-2A and INT-3A steps, the Rh−S bond distance increase and parallel to that the bond order and electron density distribution decrease, while the formation of Rh−C5(Ph) bond formation occurs. The migratory insertion TS-3A and INT-5A steps, the Rh−S(2met) bond breaks, while the Rh−C5(Ph) stays a stable bond. Furthermore, first the Rh forms bonds each of the C6/C7 of maleimide, but as one of the C7 gets protonated during the migratory insertion (TS-3A) the bond breaks between Rh-C7. Interestingly the Rh−COD bonds (C1, C2, C3, C4) also weakens during the migratory insertion steps, which is a proof that the COD and second maleimide ligand substitution is possible. The bonding of second maleimide C8/C9 atoms to Rh is quite similar as the first maleimide C6/C7 atoms bonded to Rh before the migratory insertion. During the C−C bond formation the bonding of C8 breaks with Rh and forms a C−C bond with C5(Ph) and parallel to this the Rh−C5(Ph) bond also breaks (TS-4A). During the ligand-ligand hydrogen transfer the first maleimide C7 bond breaks with Rh and dissociates from the complex, while the COD re-coordinates to complex (INT-8). The C−N bond formation step between the second maleimide and amide group (TS-6) showed the N amide group bond breaking with Rh and formation of Rh−O when PivOH re-coordinates (INT-10A). The last transition state step (TS-7A) as maleimide gets protonated by the PivOH, the bonds between Rh−S(2met) and Rh−C9(maleimide) weakens greatly, thus getting ready for the dissociation of Rh catalyst and final product formation.

1. **Table S111: The bond distances around the Rh(I) ion for the proposed mechanism intermediate and transition states, computed at the M06/def2-TZVP level.**

	Rh-S (2MA)	Rh-N (2MA)	Rh-O (PivOH)	Rh-C1 (COD)	Rh-C2 (COD)	Rh-C3 (COD)	Rh-C4 (COD)	Rh-C5 (Ph)	Rh-C6 (Mal)	Rh-C7 (Mal)	Rh-C8 (Mal)	Rh-C9 (Mal)
INT-1	2.40	3.65	2.08	2.15	2.15	2.15	2.14	-	-	-	-	-
TS-1	2.28	2.17	2.13	2.16	2.20	-	-	-	-	-	-	-
INT-2	2.37	2.13	-	2.22	2.18	2.16	2.14	-	-	-	-	-
TS-2A	2.41	2.20	-	2.16	2.18	2.19	2.17	2.16	-	-	-	-
INT-3A	2.42	2.15	-	2.16	2.40	2.43	2.02	2.02	-	-	-	-
INT-4A	-	2.12	-	-	2.62	2.63	2.01	2.01	2.39	2.34	-	-
TS-3A	-	2.20	-	2.24	2.56	2.54	2.02	2.02	2.24	2.26	-	-
INT-5A	-	2.05	-	2.33	2.53	2.48	2.01	2.03		2.09	-	-
INT-6A	2.50	2.03	-	-	-	-	-	2.03		2.13	2.32	2.33
TS-4A	2.36	2.03	-	-	-	-	-	2.14		2.25	-	2.13
INT-7A	2.29	2.01	-	-	-	-	-	2.41		2.32	-	2.09
TS-5A	2.43	2.03	-	-	-	-	-	-	-	-	-	2.05
INT-8	2.53	2.11	-	2.20	2.21	2.26	2.27	-	-	-	-	2.19
TS-6A	2.62	2.28	-	2.11	2.12	2.19	2.22	-	-	-	-	2.24
INT-9A	2.39	-	-	2.16	2.16	2.21	2.23	-	-	-	-	2.13
INT-10A	-	-	2.20	2.12	2.13	2.19	2.20	-	-	-	-	2.16
TS-7A	-	-	2.11	2.12	2.13	2.14	2.16	-	-	-	-	2.60

2. **Table S12: The NPA charges of Rh(I) and connecting ligands for the proposed mechanism intermediate and transition states, computed at the M06/def2-TZVP level.**

	Rh	S (2MA)	N (2MA)	O (PivOH)	C1 (COD)	C2 (COD)	C3 (COD)	C4 (COD)	C5 (Ph)	C6 (Mal)	C7 (Mal)	C8 (Mal)	C9 (Mal)
INT-1	0.35	0.39	-0.65	-0.72	-0.19	-0.19	-0.22	-0.19	-	-	-	-	-
TS-1	0.26	0.48	-0.73	-0.66	-0.19	-0.22	-0.16	-0.20	-	-	-	-	-
INT-2	0.28	0.42	-0.66	-	-0.21	-0.17	-0.20	-0.20	-	-	-	-	-
TS-2A	0.32	0.49	-0.70	-	-0.17	-0.16	-0.28	-0.20	-0.12	-	-	-	-
INT-3A	0.27	0.47	-0.68	-	-0.18	-0.18	-0.20	-0.18	0.03	-	-	-	-
INT-4A	0.47	0.21	-0.59	-	-0.40	-0.16	-0.18	-0.19	0.06	-0.32	-0.31	-	-
TS-3A	0.33	0.20	-0.66	-	-0.14	-0.19	-0.18	-0.19	0.07	-0.25	-0.34	-	-
INT-5A	0.50	0.22	-0.55	-	-0.23	-0.16	-0.17	-0.21	0.05	-0.51	-0.36	-	-
INT-6A	0.53	0.35	-0.54	-	-	-	-	-	0.03	-	-0.35	-0.32	-0.25
TS-4A	0.53	0.48	-0.52	-	-	-	-	-	-0.02	-	-0.41		-0.42
INT-7A	0.57	0.58	-0.52	-	-	-	-	-	-0.04	-	-0.46		-0.42
TS-5A	0.10	0.37	-0.60	-	-	-	-	-	-	-	-	-	-0.35
INT-8	0.44	0.37	-0.60	-	-0.20	-0.21	-0.17	-0.17	-	-	-	-	-0.37
TS-6A	0.38	0.30	-0.57	-	-0.18	-0.19	-0.25	-0.19	-	-	-	-	-0.52
INT-9A	0.18	0.42	-	-	-0.21	-0.21	-0.20	-0.18	-	-	-	-	-0.53
INT-10A	0.33	-	-	-0.61	-0.19	-0.20	-0.22	-0.21	-	-	-	-	-0.55
TS-7A	0.46	-	-	-0.68	-0.20	-0.20	-0.19	-0.16	-	-	-	-	-0.68

3. **Table S13: The bond orders (MBO) around Rh(I) ion for the proposed mechanism intermediate and transition states, computed at the M06/def2-TZVP level.**

	Rh-S (2MA)	Rh-N (2MA)	Rh-O (PivOH)	Rh-C1 (COD)	Rh-C2 (COD)	Rh-C3 (COD)	Rh-C4 (COD)	Rh-C5 (Ph)	Rh-C6 (Mal)	Rh-C7 (Mal)	Rh-C8 (Mal)	Rh-C9 (Mal)
INT-1	0.60	-	0.41	0.55	0.52	0.56	0.57	-	-	-	-	-
TS-1	0.75	0.42	0.31	0.52	0.48	-	-	-	-	-	-	-
INT-2	0.66	0.48	-	0.44	0.52	0.55	0.55	-	-	-	-	-
TS-2A	0.69	0.48	-	0.55	0.53	0.52	0.54	0.51	-	-	-	-
INT-3A	0.68	0.53	-	0.50	0.56	0.30	0.32	0.67	-	-	-	-
INT-4A	-	0.70	-	0.26	0.77	0.22	0.23	0.67	0.46	0.43	-	-
TS-3A	-	0.60	-	0.42	0.50	0.24	0.24	0.64	0.44	0.52	-	-
INT-5A	-	0.69	-	0.42	0.40	0.23	0.29	0.64	-	0.69	-	-
INT-6A	0.57	0.67	-	-	-	-	-	0.69	-	0.63	0.38	0.38
TS-4A	0.68	0.63	-	-	-	-	-	0.38	-	0.46		0.57
INT-7A	0.80	0.58	-	-	-	-	-	0.26	-	0.36		0.63
TS-5A	0.63	0.64	-	-	-	-	-	-	-	-	-	0.74
INT-8	0.57	0.50	-	0.51	0.50	0.45	0.41	-	-	-	-	0.57
TS-6A	0.43	0.33	-	0.54	0.47	0.61	0.58	-	-	-	-	0.35
INT-9A	0.58	-	-	0.50	0.47	0.53	0.46	-	-	-	-	0.57
INT-10A	-	-	0.29	0.59	0.55	0.49	0.47	-	-	-	-	0.54
TS-7A	-	-	0.39	0.56	0.53	0.58	0.60	-	-	-	-	-

4. **Table S14: The critical points (3, -1) and the values (a.u.) of electron density (ρ) distribution around the Rh(I) ion for the proposed mechanism intermediate and transition states, computed at the M06/def2-TZVP level.**

	Rh-S (2MA)	Rh-N (2MA)	Rh-O (PivOH)	Rh-C1 (COD)	Rh-C2 (COD)	Rh-C3 (COD)	Rh-C4 (COD)	Rh-C5 (Ph)	Rh-C6 (Mal)	Rh-C7 (Mal)	Rh-C8 (Mal)	Rh-C9 (Mal)
INT-1	0.075	-	0.088	0.095	0.096	0.097	0.099	-	-	-	-	-
TS-1	0.097	0.081	0.073	0.092	0.086	-	-	-	-	-	-	-
INT-2	0.082	0.090	-	0.089	-	0.095	0.098	-	-	-	-	-
TS-2A	0.077	0.081	-	0.086	0.094	0.092	0.090	0.096	-	-	-	-
INT-3A	0.075	0.089	-	0.090	0.095	-	0.056	0.134	-	-	-	-
INT-4A	-	0.096	-	0.119	0.038	-	-	0.119	0.070	0.064	-	-
TS-3A	-	0.079	-	0.079	0.044	-	-	0.135	0.080	0.083	-	-
INT-5A	-	0.099	-	0.069	0.049	-	-	0.139	-	0.114	-	-
INT-6A	0.064	0.117	-	-	-	-	-	0.133	-	0.102	0.064	0.065
TS-4A	0.083	0.117	-	-	-	-	-	0.095	-	0.078	0.095	0.068
INT-7A	0.099	0.120	-	-	-	-	-	0.050	-	0.068	-	0.111
TS-5A	0.074	0.115	-	-	-	-	-	-	-	-	-	0.117
INT-8	0.063	0.096	-	0.085	0.087	0.076	0.074	-	-	-	-	0.103
TS-6A	0.048	0.062	-	0.084	0.087	0.105	0.105	-	-	-	-	0.074
INT-9A	0.075	-	-	0.081	0.084	0.094	0.094	-	-	-	-	0.103
INT-10A	-	-	0.062	0.100	0.104	0.085	0.087	-	-	-	-	0.097
TS-7A	-	-	0.082	0.095	0.098	0.102	0.103	-	-	-	-	0.042

XVI. Cartesian coordinates, absolute energies, and imaginary frequency of transition states

All cartesian coordinates are given here in angstrom, and energies are the total energies in Hartree (a.u.) as reported by the Gaussian 16 on the M06/def2-TZVP/SMD level of theory.

RhCODPivO
E(RM06) = -768.905626074

Rh	0.436951000	0.018270000	0.013771000
C	1.789132000	-1.480277000	0.609063000
C	1.948789000	-0.376049000	1.450679000
C	3.103668000	0.594936000	1.376023000
C	2.762247000	1.808225000	0.509383000
C	1.822842000	1.472149000	-0.614564000
C	1.925985000	0.363607000	-1.459247000
C	3.050327000	-0.644447000	-1.411459000
C	2.689681000	-1.846556000	-0.537164000
H	1.160415000	-2.291000000	0.975513000
H	1.416882000	-0.405259000	2.399658000
H	1.212292000	2.303172000	-0.965874000
H	1.373248000	0.410627000	-2.395542000
H	3.273443000	-0.986346000	-2.424409000
H	3.964507000	-0.164159000	-1.053046000
H	2.158787000	-2.583111000	-1.146606000
H	3.595986000	-2.350149000	-0.175221000
H	3.993343000	0.085050000	0.997472000
H	3.675913000	2.281204000	0.125347000
H	3.360934000	0.929522000	2.383302000
H	2.271043000	2.562155000	1.130716000
C	-2.027225000	0.050516000	0.038206000
O	-1.388594000	-0.661185000	0.868459000
O	-1.387666000	0.755088000	-0.796816000
C	-3.538875000	0.005640000	0.002805000
C	-4.093801000	-0.243625000	1.396877000
H	-3.708042000	-1.172690000	1.817436000
H	-3.832234000	0.569216000	2.078650000
H	-5.184223000	-0.308755000	1.349747000
C	-3.905638000	-1.163661000	-0.913412000
H	-3.510733000	-1.010371000	-1.920630000
H	-3.511018000	-2.104833000	-0.523730000
H	-4.993605000	-1.248847000	-0.981162000
C	-4.098381000	1.298571000	-0.568983000
H	-3.831926000	2.155781000	0.053794000
H	-3.721093000	1.484779000	-1.574939000
H	-5.189136000	1.236474000	-0.612553000

Mal
E(RM06) = -398.666378615

N	-0.010856000	0.588248000	0.000028000
C	1.148735000	-0.177879000	0.000086000
C	-0.629292000	-1.628674000	-0.000050000
C	0.694836000	-1.602025000	-0.000075000
C	-1.136850000	-0.223049000	0.000125000
O	2.270899000	0.242383000	-0.000047000
O	-2.272452000	0.160649000	0.000037000
C	-0.051657000	2.026699000	-0.000028000
H	-1.298856000	-2.476155000	-0.000140000
H	0.974963000	2.389541000	-0.000145000
H	-0.570509000	2.397771000	-0.885011000
H	-0.570328000	2.397845000	0.885031000
H	1.398518000	-2.421433000	-0.000190000

Mal
E(RM06) = -399.904066920

H	1.137510000	-2.108588000	0.874276000
N	0.016814000	0.620438000	-0.000039000
C	-1.168197000	-0.102254000	-0.000116000
C	0.710959000	-1.614859000	0.000031000
C	-0.807418000	-1.568810000	0.000017000
C	1.154161000	-0.171453000	-0.000046000
O	-2.266011000	0.378140000	0.000041000
O	2.274865000	0.253971000	0.000008000
C	0.076259000	2.060024000	0.000032000
H	1.137537000	-2.108702000	-0.874134000
H	-0.944358000	2.438045000	0.000154000
H	0.606423000	2.417750000	0.883346000
H	0.606235000	2.417851000	-0.883355000
H	-1.263225000	-2.036155000	-0.874014000
H	-1.263239000	-2.036042000	0.874102000

PivOH
E(RM06) = -346.951160434

H	2.545366000	-0.762733000	0.000041000
C	0.938926000	0.186834000	-0.000027000
O	1.510610000	1.239943000	-0.000155000
O	1.603816000	-0.983917000	0.000076000
C	-0.563931000	-0.011968000	0.000008000
C	-1.244320000	1.345373000	-0.000176000
H	-0.968294000	1.927624000	0.880605000
H	-0.968307000	1.927378000	-0.881124000
H	-2.328703000	1.210120000	-0.000149000
C	-0.961616000	-0.794778000	1.249064000
H	-0.507643000	-1.786464000	1.263098000
H	-0.664269000	-0.265646000	2.158136000
H	-2.048004000	-0.913498000	1.270454000
C	-0.961646000	-0.795134000	-1.248813000
H	-2.048034000	-0.913866000	-1.270139000
H	-0.664328000	-0.266260000	-2.158044000
H	-0.507668000	-1.786822000	-1.262580000

RhPivO
E(RM06) = -456.882764239

Rh	1.846138000	0.000000000	0.002588000
C	-0.541794000	0.000001000	-0.059667000
O	0.127783000	-1.075816000	-0.051506000
O	0.127784000	1.075818000	-0.051507000
C	-2.044700000	0.000000000	-0.009105000
C	-2.590075000	-1.251527000	-0.679904000
H	-2.320194000	-1.285030000	-1.737795000
H	-2.209372000	-2.156593000	-0.205119000
H	-3.680532000	-1.255216000	-0.606551000
C	-2.590076000	1.251554000	-0.679852000
H	-2.209375000	2.156602000	-0.205030000
H	-2.320195000	1.285103000	-1.737741000
H	-3.680534000	1.255239000	-0.606499000
C	-2.421475000	-0.000031000	1.474661000

H	-2.030845000	-0.887010000	1.978400000
H	-2.030844000	0.886928000	1.978437000
H	-3.510154000	-0.000032000	1.572736000

INT-0
E(RM06) = -1069.27126107

C	-2.292479000	-0.452475000	-0.039235000
C	-2.495308000	0.791496000	-0.629173000
C	-3.765255000	1.336458000	-0.694924000
C	-4.844853000	0.647573000	-0.169415000
C	-4.652437000	-0.594252000	0.413935000
C	-3.385816000	-1.142114000	0.472267000
C	-0.959858000	-1.125906000	0.065674000
O	-0.866941000	-2.310072000	0.300487000
N	0.114495000	-0.293334000	-0.104823000
C	1.473125000	-0.592216000	-0.120153000
C	1.970974000	-1.891224000	-0.050245000
C	3.334912000	-2.112196000	-0.092261000
C	4.228657000	-1.061553000	-0.204283000
C	3.741127000	0.230566000	-0.269998000
C	2.378164000	0.479599000	-0.223760000
S	1.801507000	2.161205000	-0.315230000
C	1.617220000	2.497657000	1.458586000
H	-1.672922000	1.343822000	-1.073413000
H	-5.838599000	1.077055000	-0.220285000
H	-5.495485000	-1.138834000	0.822585000
H	-3.214101000	-2.116544000	0.913339000
H	-3.912024000	2.301552000	-1.165125000
H	-0.070050000	0.692832000	-0.237866000
H	1.275650000	-2.712162000	0.039068000
H	3.701390000	-3.130897000	-0.038328000
H	5.295579000	-1.244339000	-0.239872000
H	4.417193000	1.073621000	-0.358532000
H	0.903241000	1.811469000	1.915162000
H	2.582134000	2.410221000	1.957224000
H	1.248904000	3.518349000	1.557485000

INT-1
E(RM06) = -1838.20300249

C	1.792506000	2.499644000	-1.138468000
C	1.802690000	1.232528000	-1.705410000
C	2.952901000	0.737765000	-2.290289000
C	4.109374000	1.500191000	-2.296633000
C	4.106335000	2.765426000	-1.730849000
C	2.948595000	3.268267000	-1.167013000
C	0.559830000	3.103983000	-0.559800000
O	0.364985000	4.297613000	-0.608104000
N	-0.322219000	2.197593000	0.002251000
C	-1.645851000	2.434646000	0.344668000
C	-2.329025000	3.572100000	-0.098670000
C	-3.668404000	3.753803000	0.176955000
C	-4.384623000	2.820227000	0.906156000
C	-3.725908000	1.699054000	1.365541000
C	-2.374794000	1.498069000	1.103188000
S	-1.694063000	-0.008016000	1.756563000
C	-0.579594000	0.598007000	3.044943000
H	0.901036000	0.629154000	-1.690243000
H	5.014777000	1.108783000	-2.746159000
H	5.009459000	3.364319000	-1.736294000
H	2.920580000	4.263989000	-0.740394000
H	2.949543000	-0.250639000	-2.738130000
H	0.094433000	1.299757000	0.266054000
H	-1.784091000	4.314312000	-0.661100000
H	-4.159406000	4.647214000	-0.191503000
H	-5.435931000	2.965027000	1.120688000
H	-4.251492000	0.951451000	1.949322000
H	0.205820000	1.228479000	2.635539000
H	-1.182667000	1.127202000	3.781575000
H	-0.130089000	-0.285953000	3.497909000
Rh	-0.750500000	-1.427059000	0.066720000
C	-0.446851000	-3.319473000	-0.910723000
C	0.280417000	-2.342510000	-1.581184000
C	-0.132617000	-1.720064000	-2.884236000
C	-1.580065000	-1.219893000	-2.883585000
C	-2.088526000	-0.841738000	-1.508575000
C	-2.743234000	-1.721977000	-0.646334000
C	-2.957368000	-3.193181000	-0.865865000
C	-1.732619000	-3.908380000	-1.434028000
H	0.075335000	-3.885726000	-0.142987000
H	1.330970000	-2.230191000	-1.315057000
H	-2.299731000	0.217273000	-1.368744000
H	-3.432744000	-1.281435000	0.073137000
H	-3.205986000	-3.632417000	0.104662000
H	-3.834142000	-3.361476000	-1.505989000
H	-1.779236000	-4.967623000	-1.172050000
H	-1.737654000	-3.870788000	-2.526625000
H	0.023625000	-2.430943000	-3.706433000
H	-2.244974000	-1.973691000	-3.315615000
H	0.538725000	-0.883416000	-3.090860000
H	-1.657697000	-0.349758000	-3.538798000
C	1.794832000	-0.865257000	1.342474000
O	0.965165000	-1.822178000	1.174503000
O	1.591286000	0.305740000	1.020866000
C	3.147344000	-1.233686000	1.958037000
C	3.190560000	-2.671109000	2.444783000
H	2.437306000	-2.854570000	3.214380000
H	3.008706000	-3.374137000	1.629845000
H	4.174588000	-2.886726000	2.871900000
C	3.433244000	-0.284873000	3.114765000
H	3.403075000	0.754060000	2.783853000
H	2.701336000	-0.411266000	3.918746000
H	4.423255000	-0.490842000	3.531807000
C	4.186420000	-1.027829000	0.858792000
H	5.186020000	-1.260372000	1.237625000
H	3.988198000	-1.686826000	0.006410000
H	4.175846000	0.004435000	0.500621000

TS-1
E(RM06) = -1838.15570781

C	1.697977000	0.922512000	1.895734000
C	1.471779000	-0.094635000	2.814675000
C	2.524003000	-0.855274000	3.287299000
C	3.818663000	-0.580779000	2.873122000
C	4.052653000	0.458224000	1.989133000
C	2.994776000	1.204905000	1.494635000
C	0.526976000	1.723618000	1.420207000
O	-0.144309000	2.346008000	2.217373000
N	0.266590000	1.680148000	0.051072000
C	-0.738385000	2.601610000	-0.354239000
C	-0.413402000	3.903361000	-0.700738000
C	-1.402967000	4.791557000	-1.083579000
C	-2.729762000	4.393697000	-1.115760000
C	-3.063710000	3.096347000	-0.768799000
C	-2.068529000	2.211512000	-0.391756000

S	-2.467122000	0.516931000	0.020347000
C	-2.934734000	0.755150000	1.760580000
H	0.454465000	-0.290315000	3.139845000
H	4.646430000	-1.170419000	3.249736000
H	5.066600000	0.691954000	1.683201000
H	3.180953000	2.009483000	0.791612000
H	2.337211000	-1.660958000	3.987862000
H	0.626471000	4.209705000	-0.660939000
H	-1.135744000	5.804794000	-1.359933000
H	-3.502103000	5.089103000	-1.421321000
H	-4.095128000	2.760067000	-0.799564000
H	-2.096446000	1.166539000	2.323803000
H	-3.784308000	1.438108000	1.793464000
H	-3.235733000	-0.221498000	2.139583000
Rh	-0.378896000	-0.375371000	-0.186584000
C	2.395191000	-0.191379000	-1.263988000
O	1.615687000	-0.949215000	-0.664823000
O	2.176873000	1.053220000	-1.458498000
C	3.663529000	-0.767743000	-1.866506000
C	4.783933000	0.261461000	-1.859316000
H	4.513622000	1.152043000	-2.426987000
H	5.028735000	0.570002000	-0.839320000
H	5.681882000	-0.174415000	-2.304955000
C	3.310069000	-1.136847000	-3.308657000
H	2.499695000	-1.870387000	-3.336863000
H	3.002408000	-0.256414000	-3.877304000
H	4.183603000	-1.574724000	-3.798809000
C	4.089802000	-2.014789000	-1.107655000
H	5.001069000	-2.419617000	-1.555597000
H	4.292887000	-1.787528000	-0.057594000
H	3.317355000	-2.784346000	-1.139680000
H	1.304027000	1.398560000	-0.824785000
C	-4.117767000	-2.086735000	-0.549797000
C	-3.965654000	-2.668650000	0.633350000
C	-2.863779000	-3.559073000	1.115497000
C	-1.594601000	-2.825901000	1.545474000
C	-0.631490000	-2.422649000	0.462059000
C	-0.785295000	-2.411253000	-0.922392000
C	-1.943560000	-2.852166000	-1.788546000
C	-3.277979000	-2.125529000	-1.778716000
H	-4.999990000	-1.458863000	-0.663695000
H	-4.734380000	-2.454517000	1.373658000
H	0.403541000	-2.515397000	0.793924000
H	0.155432000	-2.527083000	-1.458830000
H	-1.587557000	-2.795307000	-2.821233000
H	-2.111560000	-3.921910000	-1.612983000
H	-3.113275000	-1.088928000	-2.098097000
H	-3.889366000	-2.561473000	-2.579825000
H	-2.603773000	-4.314816000	0.371035000
H	-1.033633000	-3.488527000	2.214808000
H	-3.235063000	-4.116169000	1.979663000
H	-1.852643000	-1.960380000	2.169002000

INT-2

E(RM06) = -1491.22536898

C	1.270716000	2.335986000	-0.020770000
C	1.713127000	1.750165000	1.159724000
C	3.033583000	1.876872000	1.556720000
C	3.929966000	2.582433000	0.770576000
C	3.491739000	3.189327000	-0.396176000
C	2.165998000	3.082550000	-0.776668000
C	-0.150313000	2.246071000	-0.497533000
O	-0.643950000	3.239090000	-1.010766000
N	-0.773321000	1.056237000	-0.265093000
C	-2.163041000	0.966359000	-0.366685000
C	-2.983902000	1.741673000	-1.193864000
C	-4.355916000	1.559794000	-1.200114000
C	-4.971851000	0.618190000	-0.393098000
C	-4.183881000	-0.163219000	0.432904000
C	-2.812893000	0.011653000	0.436362000
S	-1.806331000	-1.006306000	1.494446000
C	-1.564394000	0.125202000	2.893207000
H	1.018622000	1.183969000	1.771953000
H	4.966444000	2.672569000	1.074947000
H	4.186347000	3.753549000	-1.007830000
H	1.800606000	3.569227000	-1.673546000
H	3.364759000	1.423904000	2.484676000
H	-2.527922000	2.487874000	-1.825021000
H	-4.957422000	2.171702000	-1.863439000
H	-6.046449000	0.485633000	-0.412896000
H	-4.624161000	-0.919675000	1.073872000
H	-1.234995000	1.096327000	2.526599000
H	-2.504887000	0.222753000	3.434690000
H	-0.804222000	-0.310270000	3.542388000
Rh	0.099692000	-0.848098000	0.097652000
C	1.992173000	-0.687165000	-1.060167000
C	0.944562000	-1.011144000	-1.902275000
C	0.609116000	-2.379515000	-2.417961000
C	0.751632000	-3.473426000	-1.361877000
C	0.324247000	-2.992172000	0.003876000
C	1.171904000	-2.471942000	0.979953000
C	2.645264000	-2.224589000	0.831128000
C	3.030024000	-1.643504000	-0.529684000
H	2.267533000	0.359990000	-1.013618000
H	0.483875000	-0.188143000	-2.445779000
H	-0.622978000	-3.396702000	0.353922000
H	0.832317000	-2.545624000	2.013903000
H	2.938054000	-1.513013000	1.609905000
H	3.214173000	-3.142673000	1.031952000
H	3.976655000	-1.107128000	-0.429868000
H	3.213170000	-2.440803000	-1.254107000
H	1.224022000	-2.609710000	-3.298631000
H	1.777641000	-3.846303000	-1.323673000
H	-0.425484000	-2.356263000	-2.771232000
H	0.137129000	-4.329873000	-1.648313000

TS-2A

E(RM06) = -1491.15155220

C	1.091891000	2.220914000	-0.417934000
C	1.737844000	1.227259000	0.334088000
C	3.052636000	1.474365000	0.734050000
C	3.697796000	2.659539000	0.419376000
C	3.042644000	3.635785000	-0.310068000
C	1.744103000	3.409304000	-0.720527000
C	-0.327874000	2.069844000	-0.872259000
O	-0.996344000	3.043221000	-1.187696000
N	-0.771802000	0.789038000	-0.792927000
C	-2.132797000	0.600982000	-0.588029000
C	-3.133802000	0.858253000	-1.518200000
C	-4.459464000	0.615052000	-1.200026000
C	-4.822907000	0.123117000	0.044284000
C	-3.843829000	-0.119042000	0.994505000
C	-2.523055000	0.126575000	0.669879000
S	-1.213759000	-0.103088000	1.866967000

C	-1.036587000	1.599079000	2.452426000
H	1.598454000	-0.000174000	1.345529000
H	4.715561000	2.818807000	0.758465000
H	3.542186000	4.565246000	-0.557086000
H	1.188887000	4.146373000	-1.291255000
H	3.588762000	0.734169000	1.321330000
H	-2.852854000	1.256990000	-2.485036000
H	-5.226595000	0.812698000	-1.940363000
H	-5.863010000	-0.071720000	0.274946000
H	-4.100582000	-0.495579000	1.978851000
H	-0.915824000	2.280452000	1.611291000
H	-1.930193000	1.857210000	3.019454000
H	-0.156679000	1.635716000	3.093646000
Rh	0.549544000	-0.587530000	0.298609000
C	2.334315000	-1.512032000	-0.635866000
C	1.448125000	-1.061899000	-1.611153000
C	0.465608000	-1.912198000	-2.363592000
C	-0.245301000	-2.950349000	-1.496927000
C	-0.485375000	-2.463080000	-0.083084000
C	0.404243000	-2.657619000	0.989647000
C	1.722372000	-3.375365000	0.926077000
C	2.548651000	-2.963661000	-0.280411000
H	3.159768000	-0.847560000	-0.404766000
H	1.660545000	-0.097200000	-2.066319000
H	-1.533818000	-2.341094000	0.181144000
H	-0.039628000	-2.650796000	1.982887000
H	2.276137000	-3.130876000	1.836639000
H	1.566955000	-4.463537000	0.947028000
H	3.609736000	-3.126006000	-0.076929000
H	2.314523000	-3.587170000	-1.146875000
H	0.966442000	-2.387774000	-3.218352000
H	0.309578000	-3.893138000	-1.476470000
H	-0.282376000	-1.236049000	-2.786753000
H	-1.207378000	-3.188714000	-1.955349000

INT-3B

E(RM06) = -1889.88840342

C	2.176663000	2.149525000	-0.668477000
C	2.844535000	2.191793000	0.549607000
C	3.278380000	3.400316000	1.067209000
C	3.028456000	4.575730000	0.379243000
C	2.368089000	4.540093000	-0.839820000
C	1.962931000	3.330682000	-1.370334000
C	1.817301000	0.841496000	-1.289579000
O	1.880241000	0.709128000	-2.492300000
N	1.456067000	-0.187937000	-0.417037000
C	2.159481000	-1.362814000	-0.528751000
C	3.489365000	-1.386640000	-1.004030000
C	4.235845000	-2.539488000	-1.000866000
C	3.718053000	-3.739173000	-0.520340000
C	2.424974000	-3.747587000	-0.050237000
C	1.656357000	-2.588248000	-0.068324000
S	-0.024980000	-2.678406000	0.469308000
C	-0.779912000	-3.508905000	-0.952317000
H	3.035512000	1.262914000	1.077182000
H	3.356889000	5.523760000	0.789432000
H	2.178938000	5.459495000	-1.381240000
H	1.479569000	3.281754000	-2.339975000
H	3.812937000	3.424774000	2.009646000
H	3.931051000	-0.469782000	-1.376337000
H	5.253670000	-2.503338000	-1.373190000
H	4.316274000	-4.641170000	-0.511658000
H	1.982222000	-4.660736000	0.335461000
H	-0.447813000	-3.043106000	-1.877940000
H	-0.489376000	-4.559126000	-0.932088000
H	-1.862591000	-3.412414000	-0.876247000
Rh	-0.525754000	-0.228727000	0.387071000
C	0.015592000	1.144310000	2.088243000
C	0.457897000	-0.139687000	2.368490000
C	-0.206480000	-1.074661000	3.338399000
C	-1.713371000	-1.232706000	3.115597000
C	-2.188970000	-0.941373000	1.709722000
C	-2.543898000	0.307816000	1.241985000
C	-2.453084000	1.609275000	1.980730000
C	-1.169792000	1.766986000	2.779756000
H	0.716889000	1.830432000	1.627977000
H	1.494626000	-0.371451000	2.135868000
H	-2.622963000	-1.782876000	1.174172000
H	-3.257825000	0.307867000	0.427836000
H	-2.521920000	2.412328000	1.242822000
H	-3.336505000	1.718270000	2.625137000
H	-0.973745000	2.829480000	2.937753000
H	-1.276170000	1.331814000	3.777929000
H	-0.012500000	-0.747131000	4.367856000
H	-2.269806000	-0.583571000	3.798785000
H	0.271664000	-2.052213000	3.245087000
H	-2.005095000	-2.253413000	3.371580000
N	-3.304098000	0.532647000	-1.848377000
C	-2.550922000	-0.630688000	-1.991506000
C	-1.131780000	1.094037000	-1.309118000
C	-1.140934000	-0.256689000	-1.700132000
C	-2.524540000	1.596634000	-1.398794000
O	-3.009122000	-1.702667000	-2.296578000
O	-2.960594000	2.691728000	-1.153481000
C	-4.737136000	0.594013000	-1.951370000
H	-0.343687000	1.813452000	-1.475159000
H	-5.089581000	-0.372782000	-2.307334000
H	-5.192530000	0.816080000	-0.982141000
H	-5.034246000	1.375881000	-2.650742000
H	-0.341873000	-0.750751000	-2.240728000

INT-3A

E(RM06) = -1491.18134917

C	1.155349000	-2.096505000	0.667638000
C	1.649183000	-1.175033000	-0.259657000
C	2.837472000	-1.459073000	-0.918911000
C	3.515806000	-2.643003000	-0.656422000
C	3.024423000	-3.549428000	0.269809000
C	1.838403000	-3.276290000	0.926302000
C	-0.201255000	-1.865187000	1.243200000
O	-0.805800000	-2.717026000	1.868870000
N	-0.704484000	-0.651772000	0.846681000
C	-2.059314000	-0.575265000	0.564444000
C	-3.087860000	-0.775975000	1.481532000
C	-4.409312000	-0.655145000	1.085529000
C	-4.744384000	-0.339469000	-0.222242000
C	-3.738150000	-0.160839000	-1.157555000
C	-2.419305000	-0.288410000	-0.762061000
S	-1.087264000	-0.164665000	-1.949560000
C	-0.852218000	-1.919569000	-2.322230000
H	1.508444000	1.026567000	-1.573904000
H	4.439495000	-2.856091000	-1.184382000
H	3.562061000	-4.468878000	0.470084000
H	1.403898000	-3.971650000	1.637262000

H	3.241779000	-0.765266000	-1.648711000
H	-2.829140000	-1.029511000	2.501384000
H	-5.195652000	-0.804480000	1.817061000
H	-5.782207000	-0.235855000	-0.513953000
H	-3.971788000	0.070264000	-2.191387000
H	-0.718637000	-2.485048000	-1.401139000
H	-1.725743000	-2.275496000	-2.867130000
H	0.042698000	-2.003823000	-2.937915000
Rh	0.595782000	0.548985000	-0.370775000
C	2.305903000	1.696489000	0.368891000
C	1.615422000	1.126318000	1.441287000
C	0.657362000	1.813220000	2.368908000
C	-0.243721000	2.858470000	1.714817000
C	-0.721855000	2.466087000	0.345132000
C	-0.105171000	2.806146000	-0.815329000
C	1.169723000	3.588799000	-0.941041000
C	2.280151000	3.170135000	0.023636000
H	3.195410000	1.161663000	0.051710000
H	2.034681000	0.210152000	1.850017000
H	-1.722359000	2.049851000	0.281531000
H	-0.662005000	2.672437000	-1.738945000
H	1.531215000	3.468369000	-1.964713000
H	0.955430000	4.658982000	-0.820728000
H	3.241633000	3.439851000	-0.418882000
H	2.214907000	3.743320000	0.952969000
H	1.218157000	2.264990000	3.198414000
H	0.264704000	3.824156000	1.656656000
H	0.030620000	1.036514000	2.815067000
H	-1.113689000	3.019079000	2.355668000

INT-4A

E(RM06) = -1889.85449783

C	1.165686000	-1.368238000	1.625788000
C	1.586580000	-0.132976000	1.159462000
C	2.820253000	0.367352000	1.550565000
C	3.632200000	-0.392966000	2.383679000
C	3.221422000	-1.640899000	2.827640000
C	1.983942000	-2.127939000	2.448123000
C	-0.212079000	-1.801764000	1.295582000
O	-0.703600000	-2.828815000	1.726917000
N	-0.863990000	-0.903217000	0.493054000
C	-2.270641000	-0.987498000	0.497748000
C	-2.939509000	-0.841907000	1.717445000
C	-4.314986000	-0.813905000	1.804943000
C	-5.080394000	-0.942932000	0.656545000
C	-4.446628000	-1.153808000	-0.551601000
C	-3.056992000	-1.202428000	-0.644454000
S	-2.383976000	-1.539098000	-2.252036000
H	1.325874000	2.343908000	0.113063000
H	4.599121000	-0.001696000	2.681643000
H	3.864271000	-2.224801000	3.475815000
H	1.611541000	-3.088863000	2.787748000
H	3.185941000	1.326427000	1.197588000
H	-2.335561000	-0.752991000	2.614439000
H	-4.790906000	-0.692101000	2.771227000
H	-6.162369000	-0.915279000	0.706049000
Rh	0.280295000	0.809227000	-0.036777000
C	0.663519000	2.894827000	0.910221000
C	-0.291001000	1.950951000	1.567366000
C	-1.749583000	2.275839000	1.709712000
C	-2.523197000	2.522883000	0.408508000
C	-1.898210000	1.922282000	-0.815321000
C	-0.919282000	2.485329000	-1.546509000
C	-0.238836000	3.799124000	-1.284200000
C	0.109552000	4.106737000	0.170449000
H	1.474255000	3.146475000	1.600240000
H	0.108381000	1.527686000	2.489713000
H	-2.371524000	1.039113000	-1.226387000
H	-0.709853000	2.027520000	-2.510347000
H	0.687834000	3.824374000	-1.867739000
H	-0.858413000	4.606481000	-1.693751000
H	0.856783000	4.903181000	0.180257000
H	-0.751484000	4.499937000	0.714530000
H	-1.864096000	3.136572000	2.383751000
H	-2.655513000	3.596236000	0.241283000
H	-2.212030000	1.438898000	2.233896000
H	-3.527367000	2.106632000	0.519034000
N	3.163795000	-0.933091000	-1.398678000
C	3.069939000	0.432100000	-1.576553000
C	0.960945000	-0.476508000	-1.934504000
C	1.644372000	0.703716000	-1.940929000
C	1.925184000	-1.552314000	-1.562867000
O	3.960503000	1.232877000	-1.468667000
O	1.733000000	-2.730022000	-1.448236000
C	4.325568000	-1.622014000	-0.898539000
H	-0.011692000	-0.701657000	-2.354766000
H	4.633845000	-2.403562000	-1.593622000
H	5.125691000	-0.891808000	-0.787005000
H	4.107332000	-2.076362000	0.070321000
H	1.399743000	1.619842000	-2.458261000
C	-1.524344000	-3.098752000	-1.921155000
H	-2.240574000	-3.849512000	-1.590807000
H	-1.071412000	-3.411290000	-2.862237000
H	-0.739783000	-2.971798000	-1.178271000
H	-5.026415000	-1.315117000	-1.453457000

TS-2B

E(RM06) = -1889.81082912

C	-0.690401000	2.514397000	-0.730755000
C	-1.427528000	1.317583000	-0.683766000
C	-2.823720000	1.409079000	-0.740782000
C	-3.458260000	2.634394000	-0.765696000
C	-2.706944000	3.804437000	-0.748235000
C	-1.324589000	3.743886000	-0.754215000
C	0.795032000	2.458478000	-0.794327000
O	1.457155000	3.443473000	-1.064956000
N	1.279281000	1.202984000	-0.530017000
C	2.622547000	0.889328000	-0.658300000
C	3.534405000	1.582676000	-1.469939000
C	4.837611000	1.150592000	-1.589474000
C	5.298079000	0.033685000	-0.905219000
C	4.426824000	-0.654779000	-0.087650000
C	3.110376000	-0.233156000	0.021824000
S	1.991519000	-1.030423000	1.149125000
C	2.261621000	-2.778347000	0.775337000
H	-1.049072000	0.417448000	-1.461587000
H	-4.539649000	2.685702000	-0.822969000
H	-3.207185000	4.766014000	-0.760665000
H	-0.713110000	4.638926000	-0.783003000
H	-3.412712000	0.500489000	-0.826551000
H	3.194892000	2.459593000	-1.999387000
H	5.512508000	1.699497000	-2.236225000
H	6.325861000	-0.292411000	-1.003633000
H	4.770676000	-1.516858000	0.472589000

H	2.220871000	-2.964663000	-0.295603000
H	3.228749000	-3.066174000	1.184725000
H	1.471467000	-3.344215000	1.265040000
Rh	-0.020241000	-0.135982000	0.375482000
C	-1.146449000	1.580490000	2.552354000
C	0.060869000	1.118262000	2.882475000
C	0.308014000	-0.084099000	3.745686000
C	-0.437394000	-1.383210000	3.371574000
C	-0.846766000	-1.619400000	1.932721000
C	-1.949092000	-1.058196000	1.340538000
C	-2.936660000	-0.150439000	2.016339000
C	-2.413726000	0.921941000	2.982520000
H	-1.220600000	2.484825000	1.955405000
H	0.934490000	1.689399000	2.576410000
H	-0.495316000	-2.540359000	1.480428000
H	-2.354147000	-1.574189000	0.472480000
H	-3.548947000	0.332775000	1.256833000
H	-3.627948000	-0.802520000	2.568319000
H	-3.197059000	1.675649000	3.095931000
H	-2.269841000	0.487698000	3.975485000
H	0.059222000	0.163647000	4.784618000
H	-1.344389000	-1.468518000	3.979463000
H	1.379767000	-0.285540000	3.747675000
H	0.192309000	-2.222455000	3.680394000
N	-1.832491000	-2.416985000	-2.015683000
C	-0.724874000	-2.564103000	-1.230994000
C	-0.515875000	-0.609618000	-2.510626000
C	0.127786000	-1.345674000	-1.452474000
C	-1.726132000	-1.285295000	-2.889163000
O	-0.513565000	-3.513765000	-0.503422000
O	-2.568983000	-1.031407000	-3.716707000
C	-2.917798000	-3.355476000	-2.048766000
H	-0.009215000	0.069336000	-3.182549000
H	-2.563536000	-4.353734000	-2.313049000
H	-3.409755000	-3.419790000	-1.074272000
H	-3.628756000	-3.008449000	-2.797792000
H	1.200843000	-1.518210000	-1.486537000

TS-3A

E(RM06) = -1889.83748762

C	1.097365000	-1.380526000	1.610178000
C	1.611496000	-0.177365000	1.147865000
C	2.872932000	0.236440000	1.551094000
C	3.625918000	-0.575081000	2.390684000
C	3.126349000	-1.791419000	2.829217000
C	1.861740000	-2.190249000	2.438668000
C	-0.303070000	-1.763824000	1.280894000
O	-0.796384000	-2.797510000	1.701490000
N	-0.944722000	-0.837758000	0.512845000
C	-2.347264000	-0.951942000	0.466950000
C	-3.059191000	-0.916703000	1.672554000
C	-4.436090000	-0.908840000	1.718794000
C	-5.167808000	-0.949862000	0.541544000
C	-4.494281000	-1.057546000	-0.657298000
C	-3.100960000	-1.085812000	-0.710007000
S	-2.379631000	-1.336304000	-2.314131000
H	1.538643000	1.882243000	-0.331171000
H	4.614009000	-0.248752000	2.697013000
H	3.720955000	-2.419913000	3.481808000
H	1.420269000	-3.123894000	2.771413000
H	3.304031000	1.169280000	1.201607000
H	-2.487206000	-0.894394000	2.594083000
H	-4.940888000	-0.871093000	2.677449000
H	-6.250975000	-0.936188000	0.560127000
Rh	0.354284000	0.839407000	-0.056328000
C	0.591802000	2.729857000	1.139762000
C	-0.365273000	1.899347000	1.726199000
C	-1.837910000	2.175501000	1.727064000
C	-2.467622000	2.555274000	0.381368000
C	-1.783844000	1.996310000	-0.831128000
C	-0.755678000	2.576191000	-1.480193000
C	-0.049548000	3.841543000	-1.089978000
C	0.231984000	4.002956000	0.405733000
H	1.583484000	2.699608000	1.579992000
H	-0.022731000	1.277252000	2.550278000
H	-2.250247000	1.143086000	-1.308959000
H	-0.513936000	2.176964000	-2.462206000
H	0.901706000	3.882740000	-1.629041000
H	-0.623531000	4.705506000	-1.447560000
H	1.048428000	4.717983000	0.525490000
H	-0.631307000	4.450048000	0.906859000
H	-2.038145000	2.969173000	2.459643000
H	-2.517533000	3.643513000	0.280070000
H	-2.343394000	1.291206000	2.109879000
H	-3.501989000	2.202148000	0.379945000
N	3.145997000	-0.978389000	-1.402154000
C	3.155881000	0.388430000	-1.545938000
C	0.953562000	-0.365744000	-1.842179000
C	1.733761000	0.783319000	-1.850856000
C	1.859664000	-1.510799000	-1.541221000
O	4.106188000	1.118029000	-1.462445000
O	1.606657000	-2.678623000	-1.464540000
C	4.267387000	-1.763795000	-0.952366000
H	0.012803000	-0.526135000	-2.356423000
H	4.504154000	-2.540967000	-1.679396000
H	5.119319000	-1.096275000	-0.833704000
H	4.033176000	-2.234976000	0.004548000
H	1.581609000	1.663038000	-2.461549000
C	-1.582651000	-2.939876000	-2.040238000
H	-2.338990000	-3.690137000	-1.814328000
H	-1.068626000	-3.201733000	-2.965263000
H	-0.851369000	-2.883890000	-1.236172000
H	-5.042921000	-1.154759000	-1.587465000

INT-4B

E(RM06) = -1889.89870197

C	0.797824000	2.140665000	-1.234425000
C	1.382616000	0.923002000	-0.885959000
C	2.766887000	0.855207000	-0.858732000
C	3.539874000	1.955034000	-1.211399000
C	2.946632000	3.137573000	-1.615619000
C	1.567942000	3.228834000	-1.618863000
C	-0.660518000	2.324165000	-1.039088000
O	-1.245046000	3.323911000	-1.413721000
N	-1.211586000	1.265165000	-0.353724000
C	-2.501300000	1.279010000	0.155936000
C	-3.299383000	2.437536000	0.240348000
C	-4.564353000	2.398895000	0.783544000
C	-5.117859000	1.218258000	1.258699000
C	-4.363505000	0.068766000	1.185127000
C	-3.077031000	0.100894000	0.662020000
S	-2.162310000	-1.420214000	0.619576000
C	-2.061930000	-1.858566000	2.378199000
H	1.151262000	2.196702000	1.229180000

H	4.620174000	1.881981000	-1.150644000
H	3.555853000	3.988729000	-1.894653000
H	1.053187000	4.146713000	-1.882405000
H	3.285272000	-0.035634000	-0.522124000
H	-2.899554000	3.364272000	-0.138102000
H	-5.135441000	3.319338000	0.831594000
H	-6.118533000	1.195201000	1.671549000
H	-4.764806000	-0.876305000	1.536573000
H	-2.052872000	-0.959803000	2.992361000
H	-2.928801000	-2.466432000	2.631794000
H	-1.137965000	-2.417379000	2.534876000
Rh	-0.062812000	-0.448054000	-0.320427000
C	-0.066613000	-0.678586000	-2.717862000
C	-1.225414000	-1.232060000	-2.273843000
C	-1.459462000	-2.708361000	-2.160830000
C	-0.380206000	-3.477738000	-1.382304000
C	0.438890000	-2.692152000	-0.383735000
C	1.574309000	-2.005329000	-0.731578000
C	2.102989000	-1.940948000	-2.135926000
C	1.100640000	-1.491488000	-3.207793000
H	-0.075902000	0.372692000	-2.978599000
H	-2.101091000	-0.590978000	-2.212240000
H	0.336507000	-2.956133000	0.663331000
H	2.300694000	-1.820589000	0.054668000
H	2.963842000	-1.275908000	-2.158156000
H	2.492816000	-2.934031000	-2.395416000
H	1.636016000	-0.905529000	-3.957042000
H	0.706415000	-2.364657000	-3.737873000
H	-1.546292000	-3.128043000	-3.170818000
H	0.317321000	-3.944026000	-2.086024000
H	-2.429026000	-2.871478000	-1.690712000
H	-0.860532000	-4.303563000	-0.853186000
N	2.651487000	-0.331193000	2.424935000
C	1.407943000	-0.922953000	2.243500000
C	1.191396000	1.425485000	1.995364000
C	0.486920000	0.109495000	1.703250000
C	2.621089000	1.049846000	2.276860000
O	1.190176000	-2.090492000	2.492770000
O	3.581614000	1.757779000	2.402844000
C	3.849121000	-1.049383000	2.769234000
H	0.793252000	1.876787000	2.911798000
H	3.591648000	-2.100804000	2.887835000
H	4.598233000	-0.933598000	1.982059000
H	4.275189000	-0.665538000	3.697054000
H	-0.481599000	0.055851000	2.190934000

INT-5A

E(RM06) = -1889.86532146

C	-0.612579000	2.570784000	0.213320000
C	0.572410000	1.914946000	0.531153000
C	1.459735000	2.513921000	1.406742000
C	1.194382000	3.787455000	1.898144000
C	0.043278000	4.463539000	1.532222000
C	-0.867331000	3.843594000	0.697555000
C	-1.653637000	1.814584000	-0.521672000
O	-2.728153000	2.286897000	-0.847305000
N	-1.252215000	0.533554000	-0.737010000
C	-2.193262000	-0.481054000	-0.954759000
C	-2.120075000	-1.269559000	-2.102695000
C	-2.997360000	-2.308627000	-2.333650000
C	-3.988695000	-2.592049000	-1.411439000
C	-4.078011000	-1.829215000	-0.262716000
C	-3.200900000	-0.780759000	-0.016348000
S	-3.373495000	0.099308000	1.522297000
C	-4.828270000	1.106823000	1.133119000
H	1.679799000	0.184391000	2.759208000
H	1.902607000	4.246931000	2.579241000
H	-0.152069000	5.456424000	1.919340000
H	-1.809203000	4.306998000	0.421958000
H	2.366852000	2.018857000	1.732925000
H	-1.354685000	-1.052006000	-2.836411000
H	-2.907016000	-2.897250000	-3.239172000
H	-4.682074000	-3.407732000	-1.578403000
H	-4.835738000	-2.050726000	0.481400000
H	-4.603537000	1.746365000	0.279573000
H	-5.690814000	0.470577000	0.933040000
H	-5.029050000	1.717110000	2.013477000
Rh	0.732197000	0.117622000	-0.405150000
C	1.562773000	1.448440000	-2.318649000
C	1.034957000	0.277066000	-2.746193000
C	1.750509000	-1.010519000	-3.022479000
C	2.966927000	-1.293816000	-2.136112000
C	2.781433000	-0.956681000	-0.678920000
C	3.068062000	0.239476000	-0.091282000
C	3.609621000	1.452585000	-0.783885000
C	3.027661000	1.743745000	-2.168640000
H	0.885544000	2.294526000	-2.251794000
H	-0.009701000	0.303858000	-3.036248000
H	2.653723000	-1.808336000	-0.018918000
H	3.166440000	0.237447000	0.990837000
H	3.444883000	2.319008000	-0.142593000
H	4.699325000	1.346224000	-0.863487000
H	3.189420000	2.800780000	-2.389824000
H	3.578980000	1.195376000	-2.935424000
H	2.051445000	-1.051620000	-4.076969000
H	3.847347000	-0.770449000	-2.515766000
H	1.026835000	-1.822183000	-2.890947000
H	3.196440000	-2.358956000	-2.210890000
N	1.282920000	-2.779606000	1.812299000
C	0.410432000	-2.138540000	0.939598000
C	0.971889000	-0.644823000	2.706686000
C	0.186601000	-0.760373000	1.420786000
C	1.717850000	-1.949192000	2.837283000
O	0.030271000	-2.622445000	-0.109303000
O	2.557093000	-2.255018000	3.639048000
C	1.837335000	-4.088883000	1.583084000
H	0.319835000	-0.530007000	3.577411000
H	2.927819000	-4.037301000	1.557868000
H	1.549843000	-4.775551000	2.380060000
H	1.455437000	-4.453418000	0.630372000
H	-0.864650000	-0.501559000	1.517075000

INT-6A

E(RM06) = -1976.64368414

C	2.038417000	-1.224421000	-1.315513000
C	1.232403000	-1.861263000	-0.387173000
C	1.419144000	-3.199504000	-0.094902000
C	2.441303000	-3.890306000	-0.732737000
C	3.260312000	-3.254793000	-1.655226000
C	3.058950000	-1.920096000	-1.948921000
C	1.792815000	0.206570000	-1.595537000
O	2.483931000	0.844512000	-2.367899000
N	0.713564000	0.697232000	-0.880392000
C	0.157629000	1.957036000	-1.087009000

C	0.775379000	2.967983000	-1.847444000
C	0.176436000	4.195891000	-2.030478000
C	-1.064371000	4.487276000	-1.487316000
C	-1.691964000	3.517309000	-0.737800000
C	-1.087500000	2.286881000	-0.521520000
S	-1.962367000	1.123172000	0.500068000
C	-2.138049000	2.040975000	2.052389000
H	-2.445737000	-0.033206000	-2.149044000
H	2.602173000	-4.937535000	-0.500097000
H	4.057134000	-3.805560000	-2.140435000
H	3.679495000	-1.389291000	-2.662850000
H	0.786165000	-3.704641000	0.627949000
H	1.735725000	2.761950000	-2.290144000
H	0.697419000	4.942555000	-2.619095000
H	-1.534344000	5.449543000	-1.646039000
H	-2.668904000	3.707867000	-0.306641000
H	-1.192160000	2.511250000	2.323681000
H	-2.919774000	2.789570000	1.933764000
H	-2.451550000	1.323029000	2.812034000
Rh	-0.178238000	-0.619464000	0.377891000
N	-3.416797000	-1.857059000	0.166408000
C	-2.067375000	-2.044551000	0.220034000
C	-2.545104000	-1.089333000	-1.881031000
C	-1.433161000	-1.636136000	-1.022309000
C	-3.798131000	-1.254812000	-1.048914000
O	-1.428614000	-2.290816000	1.260627000
O	-4.916132000	-0.922371000	-1.304607000
C	-4.285188000	-1.936211000	1.314123000
H	-2.660379000	-1.633403000	-2.821042000
H	-3.981184000	-1.207817000	2.070633000
H	-5.297672000	-1.715426000	0.981048000
H	-4.246821000	-2.931540000	1.755355000
H	-0.773899000	-2.362451000	-1.484173000
N	2.634037000	1.172184000	1.551103000
C	2.755089000	-0.212494000	1.604410000
C	0.626943000	0.353291000	2.328098000
C	1.421803000	-0.723799000	2.061541000
C	1.396243000	1.593656000	1.998362000
O	3.749682000	-0.833090000	1.367231000
O	1.039861000	2.736005000	2.117859000
C	3.625647000	2.035796000	0.957461000
H	-0.241906000	0.380537000	2.968627000
H	3.372198000	3.064439000	1.207587000
H	4.611441000	1.788127000	1.349428000
H	3.634979000	1.916922000	-0.129855000
H	1.304718000	-1.739879000	2.412051000

INT-6C

E(RM06) = -2288.49039981

C	-0.900861000	-2.888439000	-0.246910000
C	-1.706186000	-1.771953000	-0.077807000
C	-3.013765000	-1.973405000	0.332355000
C	-3.519092000	-3.255647000	0.494089000
C	-2.723403000	-4.363475000	0.261261000
C	-1.404003000	-4.173366000	-0.094762000
C	0.536116000	-2.711446000	-0.536238000
O	1.289710000	-3.661522000	-0.686395000
N	0.932031000	-1.407400000	-0.587299000
C	2.333852000	-1.264206000	-0.702016000
C	2.920879000	-0.974263000	-1.929534000
C	4.289368000	-0.848129000	-2.073582000
C	5.116847000	-1.030970000	-0.979400000
C	4.557898000	-1.355246000	0.242415000
C	3.183735000	-1.486445000	0.393298000
S	2.555794000	-1.897721000	2.007682000
C	3.009193000	-3.653166000	2.055708000
H	2.471897000	0.772921000	0.796159000
H	-4.545323000	-3.378806000	0.822477000
H	-3.123610000	-5.362681000	0.384436000
H	-0.720296000	-5.000813000	-0.250875000
H	-3.672655000	-1.150177000	0.577795000
H	2.285134000	-0.881139000	-2.801539000
H	4.709488000	-0.619775000	-3.046205000
H	6.190984000	-0.927993000	-1.076126000
H	5.190514000	-1.502143000	1.111083000
H	2.562871000	-4.163318000	1.201922000
H	4.093199000	-3.767664000	2.052858000
H	2.608325000	-4.054275000	2.986173000
Rh	-0.591157000	0.070396000	-0.539705000
C	-1.302393000	-0.751111000	-2.504787000
C	-0.402089000	0.267598000	-2.767239000
C	-0.734417000	1.623046000	-3.302879000
C	-1.879193000	2.317567000	-2.582475000
C	-1.987865000	1.940782000	-1.132041000
C	-2.791687000	0.906525000	-0.743467000
C	-3.607138000	0.137952000	-1.747587000
C	-2.788606000	-0.691955000	-2.744618000
H	-0.881239000	-1.749170000	-2.512959000
H	0.617848000	-0.053573000	-2.938926000
H	-1.665366000	2.674590000	-0.405543000
H	-3.121074000	0.867082000	0.289059000
H	-4.303344000	-0.517019000	-1.231141000
H	-4.231425000	0.859917000	-2.285454000
H	-3.163171000	-1.717031000	-2.736579000
H	-2.941969000	-0.319279000	-3.764771000
H	-0.960746000	1.512914000	-4.372333000
H	-2.827548000	2.084570000	-3.075088000
H	0.149371000	2.258709000	-3.245817000
H	-1.733594000	3.393448000	-2.648831000
N	1.526691000	3.738388000	0.440465000
C	0.831722000	3.195082000	-0.635073000
C	2.421717000	1.628225000	0.123719000
C	1.196552000	1.755783000	-0.770984000
C	2.485966000	2.889488000	0.945268000
O	0.106356000	3.880472000	-1.320569000
O	3.224960000	3.133593000	1.861249000
C	1.312980000	5.085724000	0.899825000
H	3.343160000	1.563401000	-0.464927000
H	1.475278000	5.793796000	0.086191000
H	0.290806000	5.196014000	1.263024000
H	2.017256000	5.277243000	1.707583000
H	1.434774000	1.540216000	-1.806833000
N	-2.267944000	1.165004000	2.569284000
C	-1.222913000	1.902965000	2.033914000
C	-0.673200000	-0.350958000	1.862649000
C	-0.190260000	0.904038000	1.616480000
C	-1.990091000	-0.199499000	2.563109000
O	-1.184380000	3.100036000	1.953995000
O	-2.662281000	-1.031954000	3.097768000
C	-3.484985000	1.722925000	3.098613000
H	-0.082117000	-1.252912000	1.948714000
H	-3.429757000	2.805735000	2.999806000
H	-4.350550000	1.346815000	2.547723000
H	-3.604086000	1.452967000	4.148331000

H	0.847866000	1.172071000	1.591064000

TS-4A

E(RM06) = -1976.61884323

C	-1.161031000	2.460563000	0.910775000
C	-1.766857000	1.256176000	0.529621000
C	-2.974153000	0.884459000	1.107204000
C	-3.584143000	1.722224000	2.025548000
C	-3.005008000	2.934563000	2.367397000
C	-1.787942000	3.297864000	1.815137000
C	0.214261000	2.781632000	0.446396000
O	0.673900000	3.904855000	0.531710000
N	0.866297000	1.667820000	-0.022552000
C	2.190884000	1.662320000	-0.443692000
C	2.945968000	2.817727000	-0.706857000
C	4.248477000	2.723185000	-1.149357000
C	4.865863000	1.495421000	-1.336657000
C	4.149660000	0.347706000	-1.072848000
C	2.832027000	0.431851000	-0.648988000
S	1.958404000	-1.067338000	-0.259733000
C	2.097513000	-2.008055000	-1.794907000
H	1.883447000	-0.456507000	2.945836000
H	-4.526651000	1.425484000	2.470948000
H	-3.495865000	3.588821000	3.078037000
H	-1.285821000	4.218581000	2.091005000
H	-3.444489000	-0.054443000	0.845849000
H	2.484597000	3.780663000	-0.557326000
H	4.795700000	3.636883000	-1.351461000
H	5.892552000	1.434115000	-1.674839000
H	4.614115000	-0.625743000	-1.186657000
H	1.801996000	-1.406648000	-2.651100000
H	3.119273000	-2.372663000	-1.891814000
H	1.414112000	-2.852604000	-1.706214000
Rh	-0.168074000	-0.072910000	0.022871000
N	0.272642000	-2.886782000	1.874060000
C	-0.542327000	-1.838317000	1.506253000
C	0.960248000	-1.020939000	3.109541000
C	-0.177507000	-0.646036000	2.202483000
C	1.228928000	-2.478104000	2.808437000
O	-1.306151000	-1.884017000	0.505464000
O	2.105632000	-3.183587000	3.218103000
C	0.358779000	-4.143717000	1.174486000
H	0.717137000	-0.910814000	4.169901000
H	-0.183074000	-4.052173000	0.232983000
H	1.407830000	-4.381097000	0.988988000
H	-0.076614000	-4.954300000	1.760637000
H	-0.950757000	0.023268000	2.557160000
N	-2.467211000	-1.034566000	-2.372139000
C	-1.101784000	-0.956826000	-2.656450000
C	-1.718632000	0.946938000	-1.416084000
C	-0.606796000	0.287012000	-2.033782000
C	-2.933263000	0.082246000	-1.719952000
O	-0.506696000	-1.763714000	-3.323446000
O	-4.086439000	0.319066000	-1.492533000
C	-3.310423000	-2.141584000	-2.738775000
H	-1.863902000	2.011353000	-1.559167000
H	-2.740444000	-2.792259000	-3.399504000
H	-3.618954000	-2.699451000	-1.852334000
H	-4.201747000	-1.778277000	-3.250366000
H	0.205905000	0.820195000	-2.513560000

TS-4C

E(RM06) = -2288.48768209

C	-0.556070000	-2.877651000	-0.322198000
C	-1.461201000	-1.866116000	-0.025077000
C	-2.768961000	-2.219462000	0.272281000
C	-3.179001000	-3.540513000	0.204114000
C	-2.281154000	-4.536070000	-0.144673000
C	-0.964686000	-4.201006000	-0.394661000
C	0.865299000	-2.546290000	-0.573322000
O	1.705666000	-3.421201000	-0.721605000
N	1.130403000	-1.210267000	-0.604338000
C	2.512219000	-0.925355000	-0.706505000
C	3.072250000	-0.541345000	-1.920358000
C	4.419604000	-0.262071000	-2.047725000
C	5.254234000	-0.380703000	-0.950467000
C	4.725422000	-0.795227000	0.257315000
C	3.373282000	-1.081544000	0.391323000
S	2.781361000	-1.594468000	1.990356000
C	3.473992000	-3.268243000	2.036715000
H	2.280447000	0.989281000	0.924325000
H	-4.206321000	-3.790356000	0.444445000
H	-2.604144000	-5.568895000	-0.197208000
H	-0.215904000	-4.944649000	-0.644506000
H	-3.494627000	-1.483204000	0.598836000
H	2.435910000	-0.493051000	-2.795157000
H	4.818325000	0.036926000	-3.010097000
H	6.311079000	-0.157347000	-1.033783000
H	5.364339000	-0.891681000	1.128455000
H	3.111955000	-3.830836000	1.177233000
H	4.563327000	-3.233392000	2.046455000
H	3.121988000	-3.726638000	2.960434000
Rh	-0.537029000	0.110146000	-0.585409000
C	-1.150201000	-0.779333000	-2.567179000
C	-0.356628000	0.322028000	-2.819138000
C	-0.810472000	1.652503000	-3.328598000
C	-2.019036000	2.222239000	-2.602502000
C	-2.092532000	1.821476000	-1.155504000
C	-2.791908000	0.707896000	-0.779212000
C	-3.528204000	-0.131802000	-1.787375000
C	-2.636891000	-0.872578000	-2.792549000
H	-0.631763000	-1.730933000	-2.567113000
H	0.690882000	0.105654000	-2.990204000
H	-1.864589000	2.572812000	-0.410811000
H	-3.129699000	0.635518000	0.249568000
H	-4.156817000	-0.853430000	-1.271687000
H	-4.221610000	0.529562000	-2.318974000
H	-2.903797000	-1.931390000	-2.780561000
H	-2.842121000	-0.520114000	-3.810630000
H	-1.017937000	1.552369000	-4.402576000
H	-2.939931000	1.899185000	-3.097590000
H	0.010271000	2.365219000	-3.242700000
H	-1.982961000	3.308159000	-2.661235000
N	0.938846000	3.828752000	0.623563000
C	0.499879000	3.290259000	-0.580812000
C	2.151089000	1.883965000	0.319813000
C	1.024155000	1.898441000	-0.704742000
C	1.908839000	3.060841000	1.228420000
O	-0.162616000	3.941693000	-1.356170000
O	2.448379000	3.309375000	2.273321000
C	0.478170000	5.097140000	1.123343000
H	3.123769000	2.031570000	-0.164312000
H	0.676404000	5.887093000	0.397890000
H	-0.595106000	5.053822000	1.313520000

H	1.007997000	5.300570000	2.052339000
H	1.385806000	1.731823000	-1.715197000
N	-2.449099000	0.549947000	2.626260000
C	-1.561478000	1.469802000	2.068721000
C	-0.691699000	-0.671546000	1.760978000
C	-0.409419000	0.675769000	1.557949000
C	-1.957769000	-0.746344000	2.571007000
O	-1.734232000	2.657899000	2.042557000
O	-2.432629000	-1.686185000	3.139185000
C	-3.701146000	0.894037000	3.248108000
H	0.069962000	-1.431834000	1.873302000
H	-3.711754000	0.570529000	4.289345000
H	-3.816245000	1.975402000	3.195584000
H	-4.531852000	0.409014000	2.729554000
H	0.581790000	1.077285000	1.669167000

INT-7A

E(RM06) = -1976.64957035

C	1.163757000	-1.408663000	1.876123000
C	2.082485000	-0.856188000	0.952899000
C	2.977337000	0.116775000	1.435481000
C	2.994113000	0.483088000	2.758828000
C	2.141893000	-0.138893000	3.668152000
C	1.233371000	-1.071799000	3.227223000
C	0.035208000	-2.313849000	1.461172000
O	-0.141598000	-3.411631000	1.947411000
N	-0.729340000	-1.643377000	0.569322000
C	-1.932980000	-2.048608000	0.030209000
C	-2.527897000	-3.298608000	0.249915000
C	-3.733781000	-3.601234000	-0.346960000
C	-4.392053000	-2.689879000	-1.162444000
C	-3.826282000	-1.450176000	-1.378816000
C	-2.607636000	-1.143548000	-0.794777000
S	-1.895615000	0.474656000	-1.013976000
C	-1.696198000	0.530907000	-2.807091000
H	-2.680972000	1.482001000	2.222033000
H	3.695310000	1.235852000	3.097344000
H	2.186500000	0.121025000	4.719349000
H	0.545034000	-1.554383000	3.911442000
H	3.689373000	0.569653000	0.756974000
H	-2.020734000	-4.009510000	0.885920000
H	-4.173987000	-4.575805000	-0.169673000
H	-5.342173000	-2.940942000	-1.616742000
H	-4.333598000	-0.712830000	-1.991670000
H	-1.209775000	-0.371234000	-3.168730000
H	-2.686367000	0.653136000	-3.246121000
H	-1.067028000	1.389603000	-3.033305000
Rh	0.057574000	0.157285000	0.124408000
N	-1.056939000	3.348912000	0.337993000
C	-0.095815000	2.416265000	0.693434000
C	-1.861584000	2.207415000	2.212410000
C	-0.526676000	1.654518000	1.804134000
C	-2.169815000	3.260444000	1.169190000
O	0.896525000	2.153204000	-0.045201000
O	-3.179552000	3.889402000	1.013516000
C	-1.057870000	4.089395000	-0.897531000
H	-1.855578000	2.677977000	3.200308000
H	-0.820598000	5.141628000	-0.731784000
H	-0.306567000	3.656579000	-1.559066000
H	-2.048190000	4.030787000	-1.352774000
H	0.192406000	1.312660000	2.537916000
N	3.132655000	-0.088275000	-2.125890000
C	1.753095000	-0.065262000	-2.353781000
C	2.227904000	-1.444575000	-0.457971000
C	1.107471000	-0.926243000	-1.336099000
C	3.504500000	-0.946809000	-1.115970000
O	1.262029000	0.549015000	-3.268296000
O	4.633815000	-1.210520000	-0.802676000
C	4.064961000	0.631209000	-2.955339000
H	2.276739000	-2.534474000	-0.381606000
H	3.990024000	0.299985000	-3.992051000
H	3.847541000	1.699127000	-2.921412000
H	5.068548000	0.440425000	-2.579394000
H	0.453643000	-1.674250000	-1.784048000

INT-7C

E(RM06) = -2288.55949859

C	-0.287467000	-2.668412000	-0.354780000
C	-1.103923000	-2.338088000	0.737160000
C	-2.327518000	-2.995982000	0.868122000
C	-2.739114000	-3.944653000	-0.046263000
C	-1.928489000	-4.270230000	-1.124855000
C	-0.712024000	-3.641070000	-1.263401000
C	1.132360000	-2.198617000	-0.529977000
O	1.999660000	-3.052850000	-0.650171000
N	1.322181000	-0.869077000	-0.604744000
C	2.661058000	-0.449684000	-0.749531000
C	3.090231000	0.058758000	-1.971120000
C	4.378374000	0.522986000	-2.156706000
C	5.283131000	0.474628000	-1.110663000
C	4.884044000	-0.053891000	0.102783000
C	3.592300000	-0.527063000	0.298127000
S	3.169199000	-1.157904000	1.909610000
C	3.981923000	-2.776063000	1.811416000
H	1.962891000	1.189570000	0.998511000
H	-3.690288000	-4.445037000	0.093111000
H	-2.237242000	-5.027455000	-1.835763000
H	-0.033003000	-3.918693000	-2.062316000
H	-2.958538000	-2.793116000	1.725302000
H	2.392682000	0.054355000	-2.800245000
H	4.677370000	0.912475000	-3.122936000
H	6.294549000	0.841485000	-1.237976000
H	5.578982000	-0.097655000	0.934539000
H	3.585098000	-3.330303000	0.960903000
H	5.062058000	-2.653687000	1.728928000
H	3.750322000	-3.296832000	2.740222000
Rh	-0.480931000	0.188718000	-0.751739000
C	-0.818936000	-0.562602000	-3.083669000
C	-0.356490000	0.699110000	-3.204310000
C	-1.167005000	1.935414000	-3.425851000
C	-2.478727000	2.013944000	-2.645375000
C	-2.444357000	1.453689000	-1.248835000
C	-2.753775000	0.159892000	-0.948974000
C	-3.079376000	-0.923468000	-1.933490000
C	-2.261460000	-0.955796000	-3.230396000
H	-0.084439000	-1.363311000	-3.051900000
H	0.717552000	0.827584000	-3.284429000
H	-2.464966000	2.160640000	-0.430112000
H	-3.054321000	-0.060474000	0.072764000
H	-2.984291000	-1.885458000	-1.427995000
H	-4.145505000	-0.837062000	-2.183886000
H	-2.305082000	-1.973242000	-3.626599000
H	-2.723332000	-0.318056000	-3.987541000
H	-1.372019000	2.037149000	-4.499523000

H	-3.278551000	1.512651000	-3.197970000
H	-0.561733000	2.801993000	-3.153943000
H	-2.759837000	3.064792000	-2.574984000
N	0.080463000	3.751564000	1.000475000
C	-0.220667000	3.300869000	-0.269430000
C	1.660090000	2.123522000	0.538615000
C	0.595397000	2.063285000	-0.541733000
C	1.127962000	3.065646000	1.584900000
O	-0.976259000	3.886078000	-1.006019000
O	1.529201000	3.230720000	2.703382000
C	-0.656806000	4.807886000	1.642224000
H	2.583432000	2.556509000	0.133304000
H	-0.592027000	5.726434000	1.057926000
H	-1.704655000	4.519075000	1.735124000
H	-0.226535000	4.961620000	2.630182000
H	1.009840000	2.106532000	-1.547639000
N	-2.203179000	-0.096353000	2.974782000
C	-1.707931000	0.780864000	2.013730000
C	-0.622198000	-1.355950000	1.789000000
C	-0.574947000	0.095690000	1.314238000
C	-1.552910000	-1.317135000	2.986182000
O	-2.128046000	1.901003000	1.861602000
O	-1.746570000	-2.175731000	3.801589000
C	-3.202279000	0.258541000	3.951430000
H	0.367154000	-1.681425000	2.128879000
H	-3.575434000	1.250688000	3.705194000
H	-4.018455000	-0.464700000	3.934389000
H	-2.771665000	0.263380000	4.953697000
H	0.331735000	0.560937000	1.699234000

TS-5A

E(RM06) = -1976.60609068

C	-2.069638000	-1.902826000	-0.214840000
C	-2.908942000	-0.820958000	-0.514994000
C	-3.917307000	-1.001861000	-1.465919000
C	-4.093939000	-2.205119000	-2.115439000
C	-3.266124000	-3.272269000	-1.810215000
C	-2.277388000	-3.116585000	-0.859656000
C	-0.951230000	-1.908707000	0.788884000
O	-0.965097000	-2.752778000	1.664478000
N	0.070863000	-1.021085000	0.602686000
C	1.077782000	-1.014291000	1.587916000
C	0.823674000	-0.705141000	2.919380000
C	1.860083000	-0.686364000	3.835073000
C	3.161852000	-0.979229000	3.456496000
C	3.429198000	-1.301216000	2.137863000
C	2.390021000	-1.315307000	1.224136000
S	2.671445000	-1.711929000	-0.487104000
C	2.113905000	-3.440468000	-0.513850000
H	1.622499000	0.112100000	-2.814960000
H	-4.888053000	-2.315200000	-2.844204000
H	-3.399912000	-4.228375000	-2.302300000
H	-1.640774000	-3.951555000	-0.588612000
H	-4.592441000	-0.177642000	-1.668335000
H	-0.194046000	-0.485259000	3.218407000
H	1.646502000	-0.434214000	4.867486000
H	3.964578000	-0.953446000	4.183105000
H	4.436911000	-1.532782000	1.811105000
H	2.042439000	-3.746207000	-1.556782000
H	2.850721000	-4.050602000	0.006784000
H	1.143316000	-3.522462000	-0.025265000
Rh	0.772821000	-0.375798000	-1.190041000
N	2.103552000	2.574262000	-0.993903000
C	0.759669000	2.332275000	-0.702846000
C	1.338658000	1.236346000	-2.748307000
C	0.206306000	1.496790000	-1.815924000
C	2.531719000	1.973440000	-2.161115000
O	0.196898000	2.745985000	0.272774000
O	3.640302000	2.014015000	-2.611779000
C	2.975199000	3.261908000	-0.074189000
H	1.179162000	1.460132000	-3.804387000
H	2.575231000	4.249657000	0.154088000
H	3.058704000	2.699023000	0.858318000
H	3.954158000	3.352996000	-0.540606000
H	-0.735630000	1.867076000	-2.213731000
N	-2.504418000	2.152096000	1.685705000
C	-2.784415000	2.779022000	0.476209000
C	-2.789859000	0.503973000	0.085586000
C	-2.982381000	1.685674000	-0.504797000
C	-2.490870000	0.781905000	1.538609000
O	-2.859244000	3.962262000	0.296709000
O	-2.318686000	-0.013021000	2.421196000
C	-2.111186000	2.832343000	2.889473000
H	-0.679402000	0.164397000	-1.461328000
H	-1.073489000	2.597111000	3.136276000
H	-2.204359000	3.902351000	2.711078000
H	-2.749044000	2.539906000	3.724353000
H	-3.229251000	1.886146000	-1.538632000

TS-5C

E(RM06) = -2288.53415209

C	2.132855000	1.921780000	0.773043000
C	2.360676000	1.901609000	-0.606409000
C	2.633951000	3.099267000	-1.268238000
C	2.725857000	4.293353000	-0.578607000
C	2.578073000	4.298125000	0.798588000
C	2.287881000	3.119750000	1.460891000
C	1.691582000	0.751440000	1.607420000
O	2.366627000	0.453949000	2.582115000
N	0.520836000	0.154480000	1.282182000
C	0.111817000	-0.875485000	2.165356000
C	-0.829088000	-0.578115000	3.149781000
C	-1.305191000	-1.540640000	4.018378000
C	-0.838827000	-2.837917000	3.927341000
C	0.108832000	-3.149785000	2.969940000
C	0.598138000	-2.189477000	2.095287000
S	1.839461000	-2.683294000	0.922063000
C	3.303855000	-2.610408000	1.989302000
H	-0.886780000	-0.588325000	-3.056723000
H	2.948234000	5.210205000	-1.111353000
H	2.684571000	5.220961000	1.356577000
H	2.157502000	3.108129000	2.537447000
H	2.819974000	3.072497000	-2.336715000
H	-1.163177000	0.447623000	3.251305000
H	-2.036795000	-1.272409000	4.771663000
H	-1.206328000	-3.605228000	4.598126000
H	0.490180000	-4.161846000	2.886914000
H	3.388115000	-1.612256000	2.418302000
H	3.237516000	-3.370058000	2.768528000
H	4.166878000	-2.804813000	1.352530000
Rh	-1.147971000	0.683992000	0.134045000
C	-0.974136000	3.010104000	0.356556000
C	-1.538271000	2.485825000	1.486443000
C	-3.001887000	2.387051000	1.800799000

C	-3.884583000	2.097979000	0.587112000
C	-3.279560000	1.104433000	-0.374855000
C	-2.505124000	1.401788000	-1.477526000
C	-2.030260000	2.754232000	-1.915835000
C	-1.691649000	3.699288000	-0.769509000
H	0.099771000	3.142143000	0.367936000
H	-0.861529000	2.297216000	2.317305000
H	-3.742850000	0.121907000	-0.361330000
H	-2.480072000	0.658528000	-2.268092000
H	-1.133734000	2.603915000	-2.527937000
H	-2.773171000	3.209346000	-2.583654000
H	-1.045275000	4.495449000	-1.146879000
H	-2.590258000	4.192571000	-0.394823000
H	-3.343446000	3.299138000	2.306694000
H	-4.127744000	3.020763000	0.057064000
H	-3.133845000	1.580042000	2.529066000
H	-4.838173000	1.698901000	0.938372000
N	-3.036713000	-2.195694000	-1.407286000
C	-2.193658000	-1.874292000	-0.343748000
C	-1.081097000	-1.449070000	-2.414287000
C	-0.961698000	-1.228954000	-0.908941000
C	-2.486661000	-1.937682000	-2.650531000
O	-2.491498000	-2.088362000	0.803812000
O	-3.049935000	-2.086134000	-3.699850000
C	-4.343236000	-2.767962000	-1.210154000
H	-0.395261000	-2.229412000	-2.759599000
H	-4.267015000	-3.722437000	-0.688030000
H	-4.966091000	-2.103463000	-0.607895000
H	-4.796326000	-2.912949000	-2.189391000
H	-0.060615000	-1.666652000	-0.484583000
N	3.213039000	-1.410170000	-2.027502000
C	2.290609000	-0.992920000	-2.974390000
C	2.417300000	0.667434000	-1.382394000
C	1.836103000	0.352662000	-2.539083000
C	3.374938000	-0.450223000	-1.039833000
O	1.945465000	-1.617068000	-3.941827000
O	4.182898000	-0.475421000	-0.158122000
C	3.907441000	-2.669563000	-2.052628000
H	-0.304008000	0.359563000	-1.115686000
H	3.426506000	-3.396060000	-1.391793000
H	3.892530000	-3.053103000	-3.071637000
H	4.936523000	-2.522198000	-1.725175000
H	1.133024000	0.937563000	-3.117948000

INT-8

E(RM06) = -1888.70535907

C	-0.650201000	2.716001000	-0.322345000
C	-1.781627000	1.892252000	-0.210192000
C	-2.946932000	2.448536000	0.329810000
C	-3.001537000	3.771821000	0.721693000
C	-1.898669000	4.589309000	0.562796000
C	-0.740054000	4.055909000	0.033199000
C	0.720017000	2.299708000	-0.763826000
O	1.370222000	3.066254000	-1.455662000
N	1.201058000	1.117658000	-0.269434000
C	2.583429000	0.904210000	-0.321670000
C	3.517415000	1.926486000	-0.103883000
C	4.868679000	1.658147000	-0.051789000
C	5.357788000	0.369234000	-0.215814000
C	4.459555000	-0.654704000	-0.431954000
C	3.099468000	-0.384413000	-0.486926000
S	1.966367000	-1.709328000	-0.801494000
C	1.884921000	-1.576612000	-2.607000000
H	-3.922142000	4.165378000	1.136988000
H	-1.936109000	5.633392000	0.850037000
H	0.138534000	4.673009000	-0.109065000
H	-3.826683000	1.830474000	0.429949000
H	3.166000000	2.939745000	0.026733000
H	5.557096000	2.475659000	0.130548000
H	6.420749000	0.168233000	-0.168902000
H	4.797303000	-1.677701000	-0.561068000
H	1.734223000	-0.534598000	-2.888419000
H	2.828525000	-1.937400000	-3.016004000
H	1.047280000	-2.175909000	-2.961933000
Rh	0.015020000	-0.534406000	0.289622000
C	-0.091380000	0.157733000	2.390298000
C	1.141474000	-0.450959000	2.173065000
C	1.536456000	-1.826008000	2.626313000
C	0.493382000	-2.898452000	2.319214000
C	-0.366073000	-2.606990000	1.112009000
C	-1.559985000	-1.924522000	1.157151000
C	-2.176060000	-1.268091000	2.357189000
C	-1.188654000	-0.479394000	3.206143000
H	-0.128031000	1.239716000	2.289122000
H	1.978552000	0.209528000	1.969567000
H	-0.217651000	-3.254864000	0.252244000
H	-2.258454000	-2.162016000	0.364293000
H	-2.960578000	-0.597366000	1.998910000
H	-2.689770000	-2.029422000	2.960037000
H	-1.728769000	0.300067000	3.747530000
H	-0.738295000	-1.117050000	3.973485000
H	1.770994000	-1.822181000	3.698941000
H	-0.168336000	-3.043503000	3.178465000
H	2.473444000	-2.081792000	2.122405000
H	0.995773000	-3.855649000	2.164592000
N	-2.913211000	-1.267527000	-1.707591000
C	-1.642066000	-1.242020000	-2.264742000
C	-1.783204000	0.502455000	-0.685894000
C	-0.934494000	-0.106715000	-1.636064000
C	-3.060102000	-0.305623000	-0.720617000
O	-1.248733000	-2.019503000	-3.097870000
O	-4.060971000	-0.216117000	-0.055143000
C	-3.897686000	-2.285738000	-1.961097000
H	-3.528576000	-2.909851000	-2.773062000
H	-4.067431000	-2.900733000	-1.073389000
H	-4.847258000	-1.831906000	-2.245011000
H	-0.190410000	0.408915000	-2.227910000

TS-6A

E(RM06) = -1888.67342913

C	1.635000000	2.272529000	-0.387769000
C	2.281828000	1.192528000	0.196033000
C	3.665214000	1.152832000	0.241762000
C	4.389240000	2.210015000	-0.288766000
C	3.740602000	3.293751000	-0.861841000
C	2.357244000	3.327661000	-0.912675000
C	0.154061000	2.221495000	-0.404736000
O	-0.529936000	3.171564000	-0.720925000
N	-0.325921000	0.976226000	-0.032556000
C	-1.556787000	0.895041000	0.628671000
C	-1.946549000	1.910261000	1.513658000
C	-3.121952000	1.835622000	2.226344000
C	-3.957195000	0.737933000	2.086603000
C	-3.593500000	-0.277669000	1.226462000

C	-2.401245000	-0.220721000	0.514041000
S	-1.986774000	-1.565790000	-0.571477000
C	-2.183096000	-2.996078000	0.520510000
H	5.472014000	2.187771000	-0.251409000
H	4.319559000	4.112771000	-1.271648000
H	1.818907000	4.157522000	-1.356468000
H	4.171781000	0.307275000	0.694252000
H	-1.298672000	2.766818000	1.637661000
H	-3.385712000	2.640827000	2.901541000
H	-4.886694000	0.674983000	2.639366000
H	-4.245144000	-1.134361000	1.096541000
H	-1.737313000	-2.817680000	1.495787000
H	-3.238994000	-3.243654000	0.621508000
H	-1.657795000	-3.823539000	0.045138000
Rh	0.314681000	-0.666251000	-1.479314000
C	-0.050945000	0.675117000	-3.204060000
C	-0.995259000	-0.339032000	-3.201894000
C	-0.960621000	-1.582995000	-4.041361000
C	0.416473000	-2.244050000	-4.089802000
C	1.198798000	-2.046871000	-2.807244000
C	2.086024000	-0.964798000	-2.595932000
C	2.377352000	0.162046000	-3.545381000
C	1.115098000	0.747826000	-4.157698000
H	-0.358040000	1.618977000	-2.760523000
H	-1.973572000	-0.087900000	-2.796047000
H	1.421206000	-2.960028000	-2.256946000
H	2.919416000	-1.151159000	-1.919862000
H	2.893525000	0.941239000	-2.973803000
H	3.083788000	-0.159293000	-4.323842000
H	1.285137000	1.792448000	-4.429071000
H	0.857592000	0.233542000	-5.087767000
H	-1.328403000	-1.370235000	-5.054214000
H	0.997516000	-1.863653000	-4.935765000
H	-1.677895000	-2.285443000	-3.605126000
H	0.292515000	-3.312616000	-4.278349000
N	0.400493000	-1.085799000	2.373435000
C	0.848137000	-2.013580000	1.412377000
C	1.426438000	0.121152000	0.714679000
C	1.491829000	-1.236007000	0.341138000
C	0.813347000	0.195248000	2.089975000
O	0.719579000	-3.204197000	1.522876000
O	0.710103000	1.152691000	2.806312000
C	-0.337202000	-1.421401000	3.562756000
H	-0.396612000	-2.507161000	3.628407000
H	0.167016000	-1.026809000	4.445379000
H	-1.343455000	-0.994399000	3.518379000
H	2.353902000	-1.668292000	-0.148596000

INT-9C

E(RM06) = -2235.65769756

C	0.340678000	1.682231000	1.793454000
C	1.647899000	1.919113000	1.348453000
C	2.030960000	3.235484000	1.069642000
C	1.179646000	4.296018000	1.302423000
C	-0.084477000	4.062250000	1.818556000
C	-0.494706000	2.764078000	2.046525000
C	-0.243482000	0.335170000	2.143408000
O	0.058886000	-0.179448000	3.207295000
N	-1.135190000	-0.162240000	1.235332000
C	-2.185328000	-0.972830000	1.703782000
C	-2.769878000	-0.713866000	2.951258000
C	-3.858463000	-1.421247000	3.407691000
C	-4.427797000	-2.413402000	2.623360000
C	-3.886625000	-2.668726000	1.382743000
C	-2.766893000	-1.981680000	0.919334000
S	-2.174116000	-2.377003000	-0.717222000
C	-1.756609000	-4.124952000	-0.476549000
H	1.511457000	5.307213000	1.099265000
H	-0.751919000	4.888502000	2.035191000
H	-1.488629000	2.569547000	2.437916000
H	3.025522000	3.419464000	0.685760000
H	-2.338862000	0.059546000	3.574445000
H	-4.275565000	-1.186344000	4.380193000
H	-5.294516000	-2.965147000	2.966303000
H	-4.342506000	-3.412328000	0.737758000
H	-0.919658000	-4.229195000	0.215453000
H	-2.613959000	-4.689503000	-0.112415000
H	-1.473287000	-4.515477000	-1.454258000
Rh	-1.039014000	0.634261000	-0.755425000
C	-2.551274000	2.090673000	-0.442954000
C	-3.117724000	0.921402000	-0.963654000
C	-3.527140000	0.691629000	-2.390915000
C	-2.494756000	1.191774000	-3.398557000
C	-1.088315000	1.031452000	-2.876448000
C	-0.386101000	2.032875000	-2.212608000
C	-0.909711000	3.393320000	-1.851112000
C	-2.307592000	3.356153000	-1.233956000
H	-2.651604000	2.221944000	0.630862000
H	-3.612463000	0.266274000	-0.247720000
H	-0.499465000	0.228648000	-3.317196000
H	0.700035000	1.939980000	-2.184301000
H	-0.215078000	3.821039000	-1.121720000
H	-0.886591000	4.060697000	-2.723028000
H	-2.428530000	4.218279000	-0.573337000
H	-3.078414000	3.460502000	-2.003210000
H	-4.509136000	1.146664000	-2.578908000
H	-2.676398000	2.239335000	-3.653414000
H	-3.663580000	-0.386098000	-2.520576000
H	-2.601831000	0.636731000	-4.333117000
N	4.559991000	-0.193649000	0.464337000
C	4.078245000	-0.907162000	1.563625000
C	2.651681000	0.868909000	1.238035000
C	2.852280000	-0.207941000	2.006163000
C	3.758161000	0.905963000	0.208594000
O	4.604917000	-1.883445000	2.022083000
O	3.932447000	1.699036000	-0.676453000
C	5.789273000	-0.497437000	-0.218407000
H	5.744792000	-1.484914000	-0.682742000
H	5.940581000	0.257149000	-0.989307000
H	6.629390000	-0.484247000	0.477855000
H	2.261975000	-0.535722000	2.849897000
H	0.193236000	-1.546514000	0.723010000
C	1.265346000	-1.501101000	-0.810163000
O	0.882590000	-0.384184000	-1.130028000
O	0.886913000	-2.102265000	0.287925000
C	2.155750000	-2.318169000	-1.717975000
C	1.189655000	-3.116438000	-2.601222000
H	0.602937000	-3.819183000	-2.006431000
H	0.504987000	-2.455629000	-3.139710000
H	1.765932000	-3.686435000	-3.333964000
C	3.040389000	-3.281714000	-0.941802000
H	2.450235000	-3.984526000	-0.352620000
H	3.648006000	-3.854564000	-1.646782000
H	3.716033000	-2.764634000	-0.257733000

C	2.987326000	-1.395181000	-2.595235000
H	3.602600000	-1.996598000	-3.268578000
H	2.354679000	-0.740401000	-3.196894000
H	3.648917000	-0.759954000	-2.003464000

INT-9A
E(RM06) = -1888.71519443

C	1.665028000	2.420558000	-0.435488000
C	2.131920000	1.259394000	0.148923000
C	3.487934000	1.004793000	0.214855000
C	4.355561000	1.934766000	-0.336807000
C	3.879267000	3.094433000	-0.941308000
C	2.520822000	3.352724000	-0.990841000
C	0.194812000	2.473602000	-0.315717000
O	-0.558272000	3.356260000	-0.640467000
N	-0.171432000	1.273709000	0.275374000
C	-1.435687000	1.097556000	0.887566000
C	-1.728424000	1.850724000	2.020419000
C	-2.914173000	1.678511000	2.704447000
C	-3.830685000	0.740657000	2.259318000
C	-3.567124000	0.006777000	1.120310000
C	-2.376305000	0.178322000	0.422758000
S	-2.169368000	-0.644208000	-1.142612000
C	-2.720447000	-2.325204000	-0.741565000
H	5.424163000	1.758766000	-0.293381000
H	4.582090000	3.802204000	-1.364566000
H	2.122566000	4.255393000	-1.440131000
H	3.867688000	0.103886000	0.686371000
H	-0.987355000	2.563466000	2.362525000
H	-3.120143000	2.272555000	3.586356000
H	-4.764501000	0.591719000	2.788253000
H	-4.309797000	-0.691544000	0.754262000
H	-2.136279000	-2.722748000	0.087988000
H	-3.787939000	-2.336525000	-0.527646000
H	-2.527711000	-2.922009000	-1.632347000
Rh	0.055164000	-1.040540000	-1.935665000
C	-0.468989000	-0.408534000	-4.006054000
C	-0.899964000	-1.706034000	-3.811173000
C	-0.192303000	-2.963005000	-4.225423000
C	1.319513000	-2.918477000	-4.005705000
C	1.710656000	-2.151675000	-2.764536000
C	2.043215000	-0.802067000	-2.740449000
C	1.987391000	0.163557000	-3.885635000
C	0.762712000	-0.014976000	-4.780841000
H	-1.206060000	0.378415000	-3.861999000
H	-1.960587000	-1.839068000	-3.599550000
H	2.068892000	-2.760823000	-1.936867000
H	2.668015000	-0.459542000	-1.918958000
H	1.972036000	1.169711000	-3.452393000
H	2.908966000	0.107703000	-4.481378000
H	0.567424000	0.921549000	-5.308082000
H	0.960203000	-0.756591000	-5.559012000
H	-0.416726000	-3.211439000	-5.271821000
H	1.821093000	-2.486842000	-4.875682000
H	-0.608742000	-3.780843000	-3.627577000
H	1.695352000	-3.941000000	-3.925328000
N	0.407570000	-1.084216000	2.297262000
C	0.342443000	-1.820786000	1.098121000
C	0.991047000	0.415022000	0.612584000
C	0.917156000	-0.984756000	0.008077000
C	0.922627000	0.175933000	2.127910000
O	-0.076834000	-2.949907000	1.058137000
O	1.176778000	0.956220000	3.004848000
C	-0.036533000	-1.572613000	3.576690000
H	-0.415462000	-2.583382000	3.435851000
H	0.785968000	-1.581358000	4.293083000
H	-0.827145000	-0.927273000	3.967394000
H	1.939964000	-1.364388000	-0.116918000

TS-6C
E(RM06) = -2235.64535329

C	-0.444964000	1.702914000	1.904313000
C	0.541638000	2.467946000	1.271207000
C	0.304772000	3.831282000	1.083803000
C	-0.852162000	4.429617000	1.542424000
C	-1.805143000	3.671592000	2.198853000
C	-1.597955000	2.315754000	2.374047000
C	-0.307710000	0.232199000	2.161472000
O	0.308176000	-0.178484000	3.103204000
N	-0.941411000	-0.657222000	1.229282000
C	-1.975505000	-1.466603000	1.770600000
C	-2.576414000	-1.161020000	2.992600000
C	-3.614631000	-1.917275000	3.499263000
C	-4.094143000	-3.007898000	2.797420000
C	-3.513580000	-3.321354000	1.584637000
C	-2.459491000	-2.579273000	1.065131000
S	-1.805167000	-3.070409000	-0.516992000
C	-0.833549000	-4.503528000	0.024227000
H	-1.003618000	5.492037000	1.394426000
H	-2.711591000	4.131736000	2.574097000
H	-2.353849000	1.718832000	2.873240000
H	1.050747000	4.425780000	0.573166000
H	-2.204546000	-0.332487000	3.582743000
H	-4.049042000	-1.646012000	4.454377000
H	-4.912570000	-3.602441000	3.183943000
H	-3.878732000	-4.161685000	1.003683000
H	0.020715000	-4.176563000	0.618603000
H	-1.459429000	-5.191161000	0.592641000
H	-0.481824000	-5.007912000	-0.875945000
Rh	-1.135041000	0.147263000	-0.855010000
C	-2.902258000	1.306602000	-0.532669000
C	-3.245630000	0.042688000	-1.016489000
C	-3.621725000	-0.304247000	-2.429098000
C	-2.722797000	0.366148000	-3.463206000
C	-1.304724000	0.484620000	-2.962116000
C	-0.792344000	1.621864000	-2.337914000
C	-1.562045000	2.866159000	-2.004103000
C	-2.912016000	2.581341000	-1.345621000
H	-3.005283000	1.443673000	0.540248000
H	-3.595694000	-0.675659000	-0.275828000
H	-0.580300000	-0.202567000	-3.395379000
H	0.289203000	1.746402000	-2.343862000
H	-0.943664000	3.451150000	-1.316760000
H	-1.689453000	3.488602000	-2.899894000
H	-3.169904000	3.416080000	-0.688021000
H	-3.709117000	2.531055000	-2.093611000
H	-4.677683000	-0.062856000	-2.611516000
H	-3.105842000	1.355918000	-3.726036000
H	-3.538086000	-1.390733000	-2.531062000
H	-2.735547000	-0.213815000	-4.388590000
N	3.713581000	1.764700000	-0.491991000
C	3.844366000	0.862499000	0.563018000
C	1.813522000	1.913088000	0.823521000
C	2.612005000	0.996308000	1.376226000

C	2.498537000	2.410168000	-0.428389000
O	4.787721000	0.143304000	0.745757000
O	2.095382000	3.205038000	-1.235575000
C	4.682371000	1.980992000	-1.532832000
H	5.539625000	1.340458000	-1.330542000
H	4.262995000	1.732347000	-2.509167000
H	5.002176000	3.024045000	-1.547725000
H	2.464730000	0.429652000	2.283389000
H	-0.009368000	-1.326757000	0.886346000
C	1.419824000	-1.446633000	-0.671724000
O	0.874929000	-0.446114000	-1.209120000
O	1.096108000	-1.913975000	0.448156000
C	2.477878000	-2.185614000	-1.486058000
C	1.685172000	-3.075647000	-2.446519000
H	1.046839000	-3.773306000	-1.899812000
H	1.054920000	-2.476940000	-3.109290000
H	2.377117000	-3.658435000	-3.060390000
C	3.360559000	-3.043839000	-0.595680000
H	2.776706000	-3.786227000	-0.049637000
H	4.097780000	-3.568072000	-1.210230000
H	3.898710000	-2.433284000	0.133222000
C	3.333161000	-1.224229000	-2.296144000
H	3.952569000	-1.790287000	-2.997173000
H	2.717621000	-0.523352000	-2.864049000
H	4.007069000	-0.660497000	-1.648690000

INT-10A

E(RM06) = -2235.67273226

C	-0.926927000	0.757574000	2.481983000
C	-0.371307000	-0.364499000	1.908630000
C	0.678965000	-1.018309000	2.523941000
C	1.193700000	-0.474054000	3.690383000
C	0.654006000	0.683829000	4.244424000
C	-0.428739000	1.305756000	3.649133000
C	-2.028319000	1.237565000	1.632824000
O	-2.702812000	2.230577000	1.771886000
N	-2.132753000	0.330527000	0.589436000
C	-2.818246000	0.685811000	-0.600747000
C	-2.346203000	1.781204000	-1.316033000
C	-2.888908000	2.140439000	-2.530927000
C	-3.935661000	1.394587000	-3.049562000
C	-4.449417000	0.338092000	-2.326408000
C	-3.917186000	-0.022863000	-1.088558000
S	-4.683062000	-1.378230000	-0.254293000
C	-4.881113000	-0.747177000	1.433100000
H	2.025395000	-0.963681000	4.185360000
H	1.076160000	1.084955000	5.158257000
H	-0.883265000	2.196826000	4.068054000
H	1.082567000	-1.937708000	2.112861000
H	-1.519882000	2.344243000	-0.893718000
H	-2.491968000	2.990308000	-3.073891000
H	-4.371773000	1.653488000	-4.007080000
H	-5.302001000	-0.217091000	-2.700837000
H	-4.020869000	-0.995317000	2.052917000
H	-5.042217000	0.329872000	1.406908000
H	-5.770187000	-1.233262000	1.833420000
Rh	1.849273000	-0.484854000	-0.294517000
C	2.593247000	-1.927694000	-1.676537000
C	2.363474000	-2.531617000	-0.434667000
C	3.419270000	-2.875585000	0.580055000
C	4.434370000	-1.755221000	0.820185000
C	3.843443000	-0.380377000	0.636003000
C	3.868863000	0.325736000	-0.552784000
C	4.405758000	-0.167843000	-1.866325000
C	3.973409000	-1.595406000	-2.198557000
H	1.813065000	-2.054748000	-2.423074000
H	1.454871000	-3.124408000	-0.338398000
H	3.660257000	0.193061000	1.543238000
H	3.762884000	1.407734000	-0.481309000
H	4.037909000	0.505914000	-2.647180000
H	5.500497000	-0.082498000	-1.894859000
H	3.986184000	-1.730585000	-3.282238000
H	4.695850000	-2.314940000	-1.802956000
H	3.934510000	-3.801855000	0.291674000
H	5.295603000	-1.872089000	0.156753000
H	2.913966000	-3.105951000	1.523031000
H	4.830594000	-1.841889000	1.834652000
N	-1.397003000	-2.832523000	-0.345090000
C	-0.644086000	-2.090231000	-1.275198000
C	-1.083598000	-0.716029000	0.631449000
C	-0.250486000	-0.820968000	-0.645955000
C	-1.688176000	-2.129675000	0.788876000
O	-0.385333000	-2.509095000	-2.377540000
O	-2.264284000	-2.553132000	1.755391000
C	-1.893553000	-4.161721000	-0.583892000
H	-1.530215000	-4.483647000	-1.558413000
H	-1.545645000	-4.844820000	0.192587000
H	-2.985595000	-4.158882000	-0.576581000
H	-0.454167000	-0.008221000	-1.347127000
H	1.513511000	1.222144000	-1.958211000
C	1.196141000	2.443033000	-0.580810000
O	1.270325000	1.565398000	0.265094000
O	1.340102000	2.190089000	-1.866261000
C	1.041853000	3.902750000	-0.230658000
C	0.312531000	4.047870000	1.096281000
H	-0.721119000	3.695107000	1.039424000
H	0.814256000	3.490488000	1.888928000
H	0.289640000	5.103482000	1.376228000
C	0.324833000	4.681094000	-1.324617000
H	-0.693256000	4.315217000	-1.478508000
H	0.256630000	5.729401000	-1.025410000
H	0.855354000	4.630658000	-2.275857000
C	2.479401000	4.419668000	-0.089453000
H	2.452946000	5.479014000	0.175672000
H	3.012182000	3.883220000	0.699798000
H	3.035332000	4.315399000	-1.024602000

INT-10C

E(RM06) = -1466.74919253

C	-1.557326000	-1.945691000	0.195662000
C	-2.241100000	-0.731380000	0.044513000
C	-3.529941000	-0.751380000	-0.489965000
C	-4.136684000	-1.944473000	-0.829133000
C	-3.470213000	-3.142313000	-0.635234000
C	-2.186077000	-3.138361000	-0.122663000
C	-0.138465000	-2.026295000	0.673899000
O	0.165364000	-2.647814000	1.666649000
N	0.734038000	-1.365459000	-0.143671000
C	2.092733000	-1.108967000	0.029821000
C	2.834123000	-1.637190000	1.084101000
C	4.177718000	-1.334616000	1.202399000
C	4.810718000	-0.517387000	0.282261000
C	4.080734000	0.002904000	-0.770030000
C	2.729460000	-0.275412000	-0.905923000

S	1.823746000	0.430945000	-2.266628000
C	1.453919000	2.053031000	-1.544877000
H	-5.139824000	-1.938685000	-1.238109000
H	-3.947434000	-4.080677000	-0.891294000
H	-1.646562000	-4.066644000	0.027367000
H	-4.058377000	0.183934000	-0.623116000
H	2.342668000	-2.281219000	1.798255000
H	4.737995000	-1.753452000	2.030230000
H	5.865308000	-0.290468000	0.378676000
H	4.553815000	0.639540000	-1.509843000
H	0.943370000	1.938041000	-0.587358000
H	2.370661000	2.624715000	-1.401106000
H	0.801075000	2.575220000	-2.244982000
N	-1.304029000	2.813724000	0.575257000
C	-0.665715000	2.241040000	1.677742000
C	-1.687793000	0.531620000	0.518089000
C	-0.945163000	0.787599000	1.598918000
C	-1.922831000	1.845814000	-0.189123000
O	-0.026815000	2.840737000	2.495099000
O	-2.498889000	2.040888000	-1.224488000
C	-1.237428000	4.205321000	0.217970000
H	-0.749486000	4.735867000	1.034047000
H	-0.662235000	4.345571000	-0.700168000
H	-2.238628000	4.608036000	0.062692000
H	-0.588643000	0.097884000	2.352055000
H	0.345014000	-0.924327000	-0.971042000

INT-10D

E(RM06) = -2235.64934858

C	-0.430645000	1.618822000	2.063310000
C	0.320718000	2.447377000	1.218246000
C	0.010876000	3.807916000	1.181125000
C	-0.979408000	4.342095000	1.982997000
C	-1.663596000	3.529389000	2.866713000
C	-1.381430000	2.175132000	2.905927000
C	-0.269332000	0.131657000	2.119565000
O	0.316564000	-0.421264000	2.997593000
N	-0.917444000	-0.644377000	1.056914000
C	-1.994865000	-1.470317000	1.516680000
C	-2.675413000	-1.174508000	2.692285000
C	-3.777291000	-1.908458000	3.091514000
C	-4.224554000	-2.968144000	2.327048000
C	-3.547194000	-3.280269000	1.163483000
C	-2.439162000	-2.554238000	0.746884000
S	-1.676608000	-3.014870000	-0.790872000
C	-0.570183000	-4.307638000	-0.156570000
H	-1.195198000	5.402681000	1.934934000
H	-2.418327000	3.941785000	3.525274000
H	-1.923455000	1.540701000	3.596659000
H	0.575208000	4.450897000	0.518974000
H	-2.337064000	-0.367726000	3.327460000
H	-4.282662000	-1.644477000	4.012913000
H	-5.088410000	-3.546340000	2.630580000
H	-3.875449000	-4.104672000	0.539920000
H	0.210573000	-3.866402000	0.463466000
H	-1.142733000	-5.051235000	0.397890000
H	-0.108645000	-4.783263000	-1.022214000
Rh	-1.322867000	0.360247000	-0.946953000
C	-2.935942000	1.632988000	-0.328168000
C	-3.432326000	0.380817000	-0.694479000
C	-4.078785000	0.016161000	-2.001182000
C	-3.361804000	0.612254000	-3.208833000
C	-1.871199000	0.676682000	-2.986724000
C	-1.198500000	1.799102000	-2.504926000
C	-1.830045000	3.088372000	-2.069470000
C	-3.049298000	2.882209000	-1.173142000
H	-2.814892000	1.806131000	0.739542000
H	-3.683064000	-0.297779000	0.118784000
H	-1.271536000	-0.058996000	-3.519246000
H	-0.133207000	1.861396000	-2.720225000
H	-1.066010000	3.648876000	-1.523556000
H	-2.087974000	3.701025000	-2.943686000
H	-3.161561000	3.747085000	-0.514284000
H	-3.967792000	2.838347000	-1.765705000
H	-5.140524000	0.297812000	-1.997442000
H	-3.745649000	1.611037000	-3.433041000
H	-4.057159000	-1.076469000	-2.077084000
H	-3.570832000	0.005795000	-4.092733000
N	3.125031000	1.970624000	-1.150494000
C	3.429127000	0.965870000	-0.233184000
C	1.478173000	1.964623000	0.474871000
C	2.354233000	1.006428000	0.788498000
C	1.956865000	2.608705000	-0.804093000
O	4.388285000	0.247870000	-0.283837000
O	1.457232000	3.510924000	-1.424364000
C	3.907162000	2.314919000	-2.307452000
H	4.820535000	1.722437000	-2.283861000
H	3.358397000	2.097947000	-3.225917000
H	4.157905000	3.376442000	-2.292759000
H	2.370929000	0.345899000	1.642363000
H	-0.132017000	-1.227164000	0.657763000
C	1.259840000	-1.251777000	-1.292367000
O	0.540741000	-0.277453000	-1.689990000
O	1.283543000	-1.696401000	-0.138026000
C	2.101086000	-1.923569000	-2.387286000
C	1.125446000	-2.727196000	-3.246783000
H	0.613994000	-3.492730000	-2.657638000
H	0.367828000	-2.080522000	-3.695759000
H	1.670373000	-3.231828000	-4.049739000
C	3.136797000	-2.853928000	-1.780213000
H	2.666693000	-3.630660000	-1.174433000
H	3.710314000	-3.336501000	-2.577295000
H	3.831408000	-2.305549000	-1.140075000
C	2.790994000	-0.889340000	-3.265037000
H	3.283490000	-1.389394000	-4.104173000
H	2.075607000	-0.166842000	-3.665011000
H	3.561144000	-0.354697000	-2.704600000

TS-7A

E(RM06) = -2235.63611024

C	-0.774051000	1.412850000	2.102152000
C	-0.401926000	0.135261000	1.747391000
C	0.416205000	-0.611581000	2.572438000
C	0.904068000	-0.014268000	3.723557000
C	0.558696000	1.291579000	4.057706000
C	-0.300026000	2.017988000	3.251908000
C	-1.722257000	1.937192000	1.103069000
O	-2.231570000	3.028663000	1.057804000
N	-1.929850000	0.905729000	0.195860000
C	-2.513126000	1.176357000	-1.072864000
C	-1.849313000	2.060948000	-1.917495000
C	-2.320428000	2.322723000	-3.188070000
C	-3.474013000	1.697070000	-3.630345000
C	-4.162994000	0.850118000	-2.786284000

C	-3.707773000	0.588140000	-1.495383000
S	-4.690002000	-0.506122000	-0.515702000
C	-4.837544000	0.386941000	1.054559000
H	1.556846000	-0.577017000	4.381356000
H	0.951824000	1.731495000	4.966640000
H	-0.611036000	3.026236000	3.502885000
H	0.666414000	-1.641789000	2.335371000
H	-0.931633000	2.516837000	-1.561559000
H	-1.782818000	3.006987000	-3.833000000
H	-3.853372000	1.887582000	-4.627436000
H	-5.092397000	0.393528000	-3.107087000
H	-4.045693000	0.105804000	1.747309000
H	-4.825858000	1.460216000	0.868617000
H	-5.803283000	0.105849000	1.473222000
Rh	2.227558000	-1.194234000	0.098680000
C	2.480114000	-3.027086000	-1.013515000
C	1.861693000	-3.301742000	0.203605000
C	2.537206000	-3.861194000	1.426219000
C	3.870346000	-3.184155000	1.742873000
C	3.880479000	-1.735270000	1.321274000
C	4.342902000	-1.280730000	0.081141000
C	4.829345000	-2.134064000	-1.051014000
C	3.928425000	-3.337514000	-1.307057000
H	1.827063000	-2.919374000	-1.874756000
H	0.784535000	-3.458090000	0.189025000
H	3.849489000	-0.999776000	2.123101000
H	4.649554000	-0.237672000	0.033489000
H	4.852670000	-1.506632000	-1.945912000
H	5.866735000	-2.448691000	-0.874847000
H	4.021609000	-3.646005000	-2.350257000
H	4.249998000	-4.197127000	-0.713117000
H	2.668149000	-4.946582000	1.324460000
H	4.696761000	-3.712458000	1.260228000
H	1.858036000	-3.726137000	2.273559000
H	4.063548000	-3.248075000	2.815771000
N	-1.566536000	-2.459761000	-0.238607000
C	-0.612170000	-2.001125000	-1.153115000
C	-1.071900000	-0.265239000	0.460851000
C	-0.174549000	-0.644243000	-0.727228000
C	-1.875029000	-1.553148000	0.741998000
O	-0.292603000	-2.623353000	-2.131815000
O	-2.583024000	-1.762969000	1.687618000
C	-2.201255000	-3.750479000	-0.322582000
H	-1.780452000	-4.276565000	-1.177741000
H	-2.025937000	-4.317708000	0.593106000
H	-3.278041000	-3.628584000	-0.452067000
H	-0.472124000	-0.039257000	-1.596723000
H	0.855829000	0.209896000	-0.804257000
C	2.069752000	1.709582000	0.066288000
O	2.586261000	0.782781000	0.738518000
O	1.261392000	1.493397000	-0.871608000
C	2.487836000	3.142075000	0.353601000
C	3.126455000	3.262705000	1.727122000
H	2.431665000	2.960249000	2.513991000
H	4.018368000	2.640019000	1.810445000
H	3.414117000	4.302433000	1.903710000
C	1.288421000	4.073726000	0.248517000
H	0.517417000	3.826212000	0.983662000
H	1.609394000	5.102210000	0.433074000
H	0.835022000	4.031645000	-0.742648000
C	3.515061000	3.498780000	-0.722393000
H	3.869437000	4.520749000	-0.564507000
H	4.379606000	2.829844000	-0.677027000
H	3.077957000	3.434963000	-1.720838000

TS-7C

E(RM06) = -1466.66286966

C	2.328151000	-0.504968000	-0.735272000
C	2.006992000	0.601237000	0.033520000
C	2.970202000	1.207208000	0.816018000
C	4.246066000	0.668367000	0.819287000
C	4.566096000	-0.443494000	0.043997000
C	3.605352000	-1.041596000	-0.746776000
C	1.167881000	-0.998271000	-1.469508000
O	1.045744000	-1.888386000	-2.247773000
N	0.047278000	-0.092090000	-1.121874000
C	-1.257665000	-0.659421000	-0.884302000
C	-2.338141000	-0.034312000	-1.490875000
C	-3.626402000	-0.454102000	-1.225218000
C	-3.831638000	-1.520242000	-0.366574000
C	-2.753729000	-2.166140000	0.206564000
C	-1.448985000	-1.747719000	-0.030390000
S	-0.082483000	-2.612525000	0.688256000
C	-0.562170000	-2.617162000	2.431061000
H	5.012763000	1.121346000	1.437075000
H	5.574216000	-0.838694000	0.066100000
H	3.822445000	-1.911026000	-1.356321000
H	2.727833000	2.078601000	1.414286000
H	-2.159478000	0.798876000	-2.161840000
H	-4.463812000	0.046058000	-1.695148000
H	-4.836750000	-1.867221000	-0.158290000
H	-2.919293000	-3.025405000	0.845710000
H	-0.735992000	-1.594680000	2.762055000
H	-1.432692000	-3.247993000	2.606408000
H	0.287548000	-3.037547000	2.968197000
N	-1.064663000	2.327244000	0.771246000
C	-0.649969000	3.037888000	-0.427713000
C	0.608346000	1.050042000	-0.174525000
C	0.365860000	2.243039000	-1.049800000
C	-0.315809000	1.235027000	1.029425000
O	-1.158664000	4.088962000	-0.722116000
O	-0.376429000	0.518044000	1.999875000
C	-2.145972000	2.755874000	1.613410000
H	-2.936910000	2.001146000	1.634703000
H	-1.800857000	2.920665000	2.635459000
H	-2.532454000	3.686410000	1.199465000
H	1.194296000	2.739040000	-1.540959000
H	-0.051458000	0.868259000	-1.808456000

TS-7D

E(RM06) = -2235.58091287

C	2.700992000	-1.043408000	-1.460708000
C	2.784421000	0.357951000	-1.279450000
C	4.032996000	0.938720000	-1.035447000
C	5.186027000	0.175481000	-1.032515000
C	5.112314000	-1.181795000	-1.278448000
C	3.874565000	-1.776996000	-1.475987000
C	1.435485000	-1.887659000	-1.492727000
O	1.528552000	-3.017052000	-1.914415000
N	0.236538000	-1.352128000	-1.001895000
C	-0.903424000	-2.119536000	-1.374854000
C	-1.166512000	-2.327570000	-2.727791000
C	-2.317830000	-2.954634000	-3.146458000
C	-3.237152000	-3.415133000	-2.215191000

C	-2.989327000	-3.231501000	-0.873460000
C	-1.837150000	-2.578395000	-0.453229000
S	-1.544036000	-2.309070000	1.263392000
C	-3.164193000	-1.770456000	1.848805000
H	6.143194000	0.650320000	-0.852478000
H	6.010542000	-1.787032000	-1.297733000
H	3.792734000	-2.848000000	-1.613256000
H	4.082433000	2.007826000	-0.873453000
H	-0.453752000	-1.967056000	-3.460960000
H	-2.503335000	-3.082526000	-4.206124000
H	-4.142254000	-3.916222000	-2.536044000
H	-3.700173000	-3.589395000	-0.137891000
H	-3.614821000	-1.122975000	1.098356000
H	-3.803062000	-2.626074000	2.065079000
H	-2.991335000	-1.214956000	2.772434000
Rh	0.241381000	-0.273808000	0.965318000
C	2.259713000	-0.865427000	1.678003000
C	1.318900000	-1.779596000	2.119996000
C	0.769606000	-1.806728000	3.519438000
C	0.312235000	-0.434537000	4.027079000
C	-0.120200000	0.501885000	2.921451000
C	0.735727000	1.386652000	2.261600000
C	2.210152000	1.511523000	2.498291000
C	2.911956000	0.164051000	2.569682000
H	2.829276000	-1.139755000	0.800446000
H	1.226110000	-2.710843000	1.562975000
H	-1.179970000	0.751283000	2.893825000
H	0.268318000	2.239600000	1.775058000
H	2.626243000	2.097365000	1.675804000
H	2.389886000	2.098415000	3.409598000
H	3.954375000	0.278765000	2.263041000
H	2.943029000	-0.214364000	3.595487000
H	1.520642000	-2.234067000	4.196335000
H	1.104766000	0.041695000	4.611508000
H	-0.073827000	-2.500961000	3.539087000
H	-0.521102000	-0.571407000	4.720065000
N	0.356531000	3.092886000	-1.534004000
C	-0.253859000	2.163273000	-2.385034000
C	1.635654000	1.200826000	-1.423923000
C	0.562372000	0.920557000	-2.305370000
C	1.491792000	2.596878000	-0.934926000
O	-1.206783000	2.396026000	-3.071617000
O	2.220788000	3.232839000	-0.208939000
C	-0.087729000	4.448524000	-1.353204000
H	-1.101894000	4.532062000	-1.740521000
H	-0.067614000	4.707888000	-0.294352000
H	0.561495000	5.144592000	-1.889285000
H	0.780768000	0.450654000	-3.266349000
H	0.100047000	-0.073120000	-1.720091000
C	-2.388867000	1.010096000	-0.119195000
O	-1.189946000	1.129627000	0.345358000
O	-2.826241000	0.069563000	-0.756899000
C	-3.331419000	2.189088000	0.213403000
C	-4.495748000	1.614329000	1.015379000
H	-5.012599000	0.837330000	0.449388000
H	-4.149988000	1.185464000	1.962576000
H	-5.212583000	2.406058000	1.252745000
C	-3.863802000	2.769458000	-1.090980000
H	-4.342257000	1.992252000	-1.688701000
H	-4.599350000	3.551377000	-0.877650000
H	-3.064336000	3.202559000	-1.697981000
C	-2.664704000	3.275566000	1.037279000
H	-3.377460000	4.083609000	1.230056000
H	-2.318793000	2.894391000	2.001482000
H	-1.802347000	3.700673000	0.522956000

FP

E(RM06) = -1466.77460042

C	-1.486446000	-1.886412000	-0.596262000
C	-1.914628000	-0.768592000	0.091145000
C	-3.183497000	-0.708508000	0.631059000
C	-4.011149000	-1.808793000	0.462407000
C	-3.579874000	-2.933166000	-0.232967000
C	-2.305353000	-2.983888000	-0.771107000
C	-0.087670000	-1.690281000	-1.032222000
O	0.621572000	-2.432854000	-1.654388000
N	0.271342000	-0.438688000	-0.540893000
C	1.563890000	0.117273000	-0.719192000
C	1.802060000	1.014507000	-1.745682000
C	3.063553000	1.555517000	-1.924933000
C	4.087964000	1.179449000	-1.076231000
C	3.864917000	0.271056000	-0.055642000
C	2.600906000	-0.273367000	0.138875000
S	2.196640000	-1.434666000	1.398507000
C	3.752165000	-1.604905000	2.282186000
H	-5.011195000	-1.792397000	0.879619000
H	-4.250415000	-3.776203000	-0.349276000
H	-1.943024000	-3.850316000	-1.312378000
H	-3.529148000	0.164933000	1.175304000
H	0.981734000	1.268301000	-2.407249000
H	3.245275000	2.255800000	-2.730611000
H	5.082131000	1.590513000	-1.208897000
H	4.688889000	-0.012373000	0.586003000
H	4.530416000	-2.025392000	1.644598000
H	4.084227000	-0.657123000	2.707275000
H	3.550913000	-2.302990000	3.093566000
N	-1.605023000	2.486351000	0.150980000
C	-1.237510000	2.208596000	1.466178000
C	-0.820473000	0.266110000	0.099606000
C	-0.533175000	0.877878000	1.466320000
C	-1.310002000	1.469643000	-0.730232000
O	-1.441308000	2.933339000	2.396528000
O	-1.456150000	1.513786000	-1.917660000
C	-2.206258000	3.728956000	-0.269349000
H	-3.148037000	3.535115000	-0.783173000
H	-2.381658000	4.333504000	0.618347000
H	-1.543413000	4.258390000	-0.954653000
H	-0.853764000	0.262331000	2.306515000
H	0.537157000	1.068333000	1.588716000

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