Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

A one-pot route to thioamides discovered by gas-phase studies: palladium-mediated CO_2 extrusion followed by insertion of isothiocyanates

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Contents:

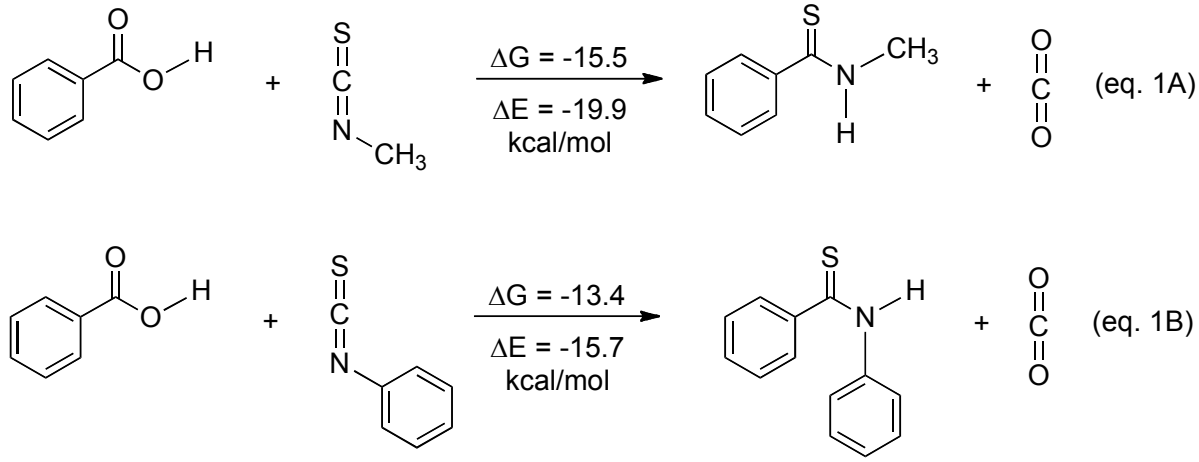
1 DFT Calculations

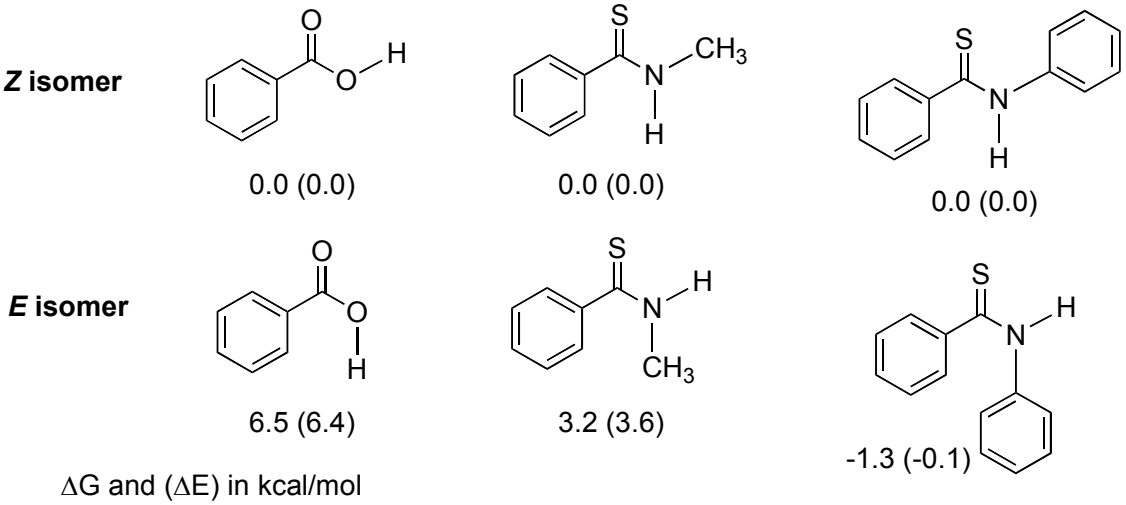
Gaussian 09[1] was used to fully optimize all the structures reported in this paper at the M06[2] level of density functional theory (DFT). For the DMSO system (in solution), the effective-core potential of Hay and Wadt with a double-ξ valence basis set (LANL2DZ)[3] was chosen to describe Pd. The 6-31G(d) basis set was used for other atoms.[4] A polarization function of $\xi_f = 1.472$ was also added for Pd.[5] This basis set combination will be referred to as BS1. Solvation effects of DMSO on the optimized structures were accounted for using the CPCM model.[6] For the phenanthroline system (gas phase), we employed the Stuttgart ECP basis set (SDD)[7] for Pd and the 6-31+G(d) basis set for other atoms. This basis set combination will be referred to as BS2. Frequency calculations were carried out at the same level of theory as those for the structural optimization. Transition structures were located using the Berny algorithm. Intrinsic reaction coordinate (IRC)[8] calculations were used to confirm the connectivity between transition structures and minima. To further refine the energies obtained from the M06/(BS1 or BS2) calculations, we carried out single-point energy calculations for all of the structures with a larger basis set (BS3) at the B3LYP-D3BJ level of theory.[9,10] BS3 utilizes def2-TZVP[11] for all atoms along with the effective core potential including scalar relativistic effects for Pd.[12] The solvent effect using the CPCM approach was considered for the DMSO system in the single point calculations. The B3LYP-D3BJ calculations were used to overcome the deficiency of the M06 level in incorporating long-range correlation for dispersion forces.[13] To estimate the corresponding enthalpy, ΔH, and Gibbs energies, ΔG, the corrections were calculated at the M06/(BS1 or BS2) levels and finally added to the corresponding single-point energies. Entropy calculations for the DMSO system were adjusted by the method proposed by Okuno.[14a] An additional correction was made to account for the fact that DMSO participates in the equilibrium between **14** and **14a**. Thus when calculating the energy profiles for Figure 3 and Figure S43 the concentration of DMSO was set using the method of Keith and Carter (we utilized eq. 6 of their paper).[14b] We have used the corrected enthalpy and Gibbs free energies obtained from the B3LYP-D3BJ/BS3//M06/(BS1 or BS2) calculations throughout the paper unless otherwise stated.

Scheme S1: DFT calculated thermochemistry for transformation of aromatic carboxylic acids into thioamides. The relative Gibbs and enthalpy energies are given in kcal/mol and were calculated at the B3LYP-D3BJ/BS3//M06/BS1 level of theory in DMSO using the CPCM approach.

$$PhCO_2H + MeNCS \rightarrow PhC(S)NHMe + CO_2 \qquad (1A)$$

$$PhCO_2H + PhNCS \rightarrow PhC(S)NHPh + CO_2 \qquad (1B)$$





ΔG and (ΔE) in kcal/mol

DFT calculated relative energies ΔG and (ΔH) of *Z*-6a versus *E*-6a and *Z*-6e versus *E*-6e in the gas-phase and in DMSO solvent (PCM model):

Table S1: M06/6-31G(d) calculated relative energies in kcal mol^{-1}.

Species	**phase**	**Relative energy of *Z* isomer ΔG (ΔH)**	**Relative energy of *E* isomer ΔG (ΔH)**
6a	Gas phase	-1.0 (-0.9)[(a)]	0 (0)
6a	DMSO	-1.8 (-1.7)	0 (0)
6e	Gas phase	0.9 (0.9)	0 (0)[(a)] -0.8 (-0.2)[(b)]
6e	DMSO	0.3(0.9)	0 (0)[(a)] -0.002(-0.001)[(b)]

(a) Structure reoptimized from X-ray structure.

(b) More stable isomer found.

2 Gas-phase Experiments

The gas-phase CID of $[(phen)Pd(O_2CC_6H_5)]^+$ to form $[(phen)Pd(C_6H_5)]^+$ for subsequent ion-molecule reaction studies were conducted in a similar manner to those reported for the reactivity studies of $[(phen)M(CH_3)]^+$.[15] Briefly, 30 μL of methanolic solutions of palladium acetate (5mM), benzoic acid (10mM) and phen (10mM) were mixed and then diluted to a final concentration of 0.1 mM in Pd. The solution was transferred via syringe pump operating at 5 μL min^{-1} to the electrospray source of a Finnigan LTQ FT hybrid linear ion trap (Finnigan, Bremen, Germany) previously modified to allow the introduction of neutral reagents into the ion trap.[16]

Typical electrospray source conditions were:

CID: Sheath Gas = 5 arbitrary units, Auxiliary Gas = 0 arbitrary units, Sweep Gas = 0 arbitrary units, Spray Voltage = 4.8 kV, Capillary Temp. = 250 °C, Capillary Voltage = 50 V, Tube Lens Voltage = 130 V. The precursor ion was mass selected with a window of 1 *m/z* and and collision induced dissociation was carried out using the helium bath gas by activating the ion with an activation time of 30ms. A normalized collision energy (NCE) was chosen to deplete the precursor ion to 10%.

IMR: Sheath Gas = 5 arbitrary units, Auxiliary Gas = 0 arbitrary units, Sweep Gas = 0 arbitrary units, Spray Voltage = 4 kV, Capillary Temp. = 250 °C, Capillary Voltage = 38 V, Tube Lens Voltage = 105 V.

Comparision of the CID spectra of the IMR product $[(phen)Pd(SC(NMe)C_6H_5)]^+$ with an "authentic sample".

We confirmed that the C-C bond coupled product $[(phen)Pd(SC(NMe)C_6H_5)]^+$ was formed rather than the complex $[(phen)Pd(C_6H_5)(MeNCS)]^+$ by comparing the CID spectra of the IMR product versus that of an "authentic standard" of the deprotonated, coordinated N-methylbenzothioamide (Figure S1). The N-methylbenzothioamide neutral was prepared, purified and characterized as discussed below (see page S7).

The product of the IMR was formed and subjected to CID via the following sequence of gas-phase reactions: (i) CID of $[(phen)Pd(O_2CC_6H_5)]^+$ (*m/z* 407, NCE of 14% and reaction time of 10ms) to form $[(phen)Pd(C_6H_5)]^+$; (ii) ion-molecule reaction of $[(phen)Pd(C_6H_5)]^+$ (*m/z* 363) with MeNCS (concentration was 1.65 x 10^9 molecule/cm^3 and reaction time was 30 ms) to give the ion formulated as $[(phen)Pd(SC(NMe)C_6H_5)]^+$ (*m/z* 436); (iii) CID of *m/z* 436 (NCE of 15%, Figure S1(a)).

An authentic sample of $[(phen)Pd(SC(NMe)C_6H_5)]^+$ (*m/z* 436) was formed by carrying out ESI on a methanolic solution formed by mixing 30 μL of methanolic solutions of palladium acetate (5 mM), N-methylbenzothioamide (10 mM) and phen (10 mM) and then diluted to a final concentration of 0.1 mM in Pd. This solution was transferred via syringe pump operating at 5 μL min^{-1} to the electrospray source of a Finnigan LTQ FT hybrid linear ion trap (Finnigan, Bremen, Germany). The $[(phen)Pd(SC(NMe)C_6H_5)]^+$ (*m/z* 436) was mass selected and subjected to CID (NCE of 15%, Figure S1(b)).

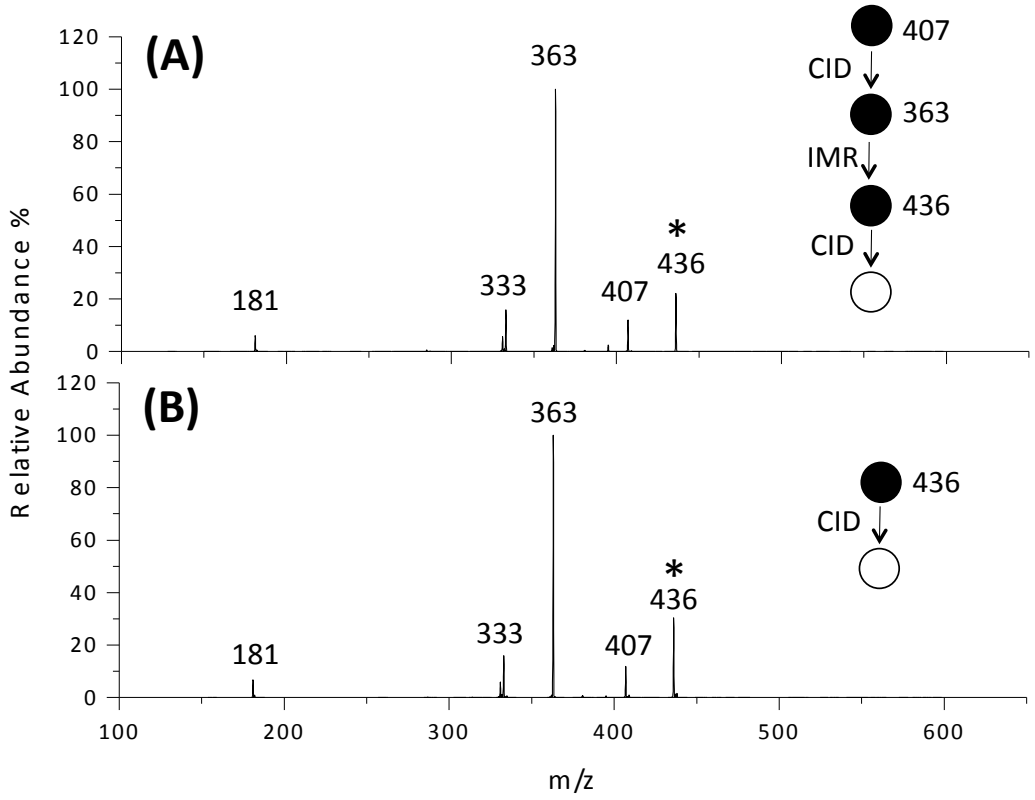


Figure S1. Gas-phase experiments (LTQ ion trap) comparing the CID spectra of $[(phen)Pd(SC(NMe)C_6H_5)]^+$ formed via: (a) ion-molecule reaction of $[(phen)Pd(C_6H_5)]^+$ with MeNCS; (b) ESI-MS of a solution containing the "authentic sample" prepared as described above. In both cases the ion at *m/z* 436 was mass selected with a window of 1.0 and CID was carried out (NCE of 15%, activation time of 30ms).

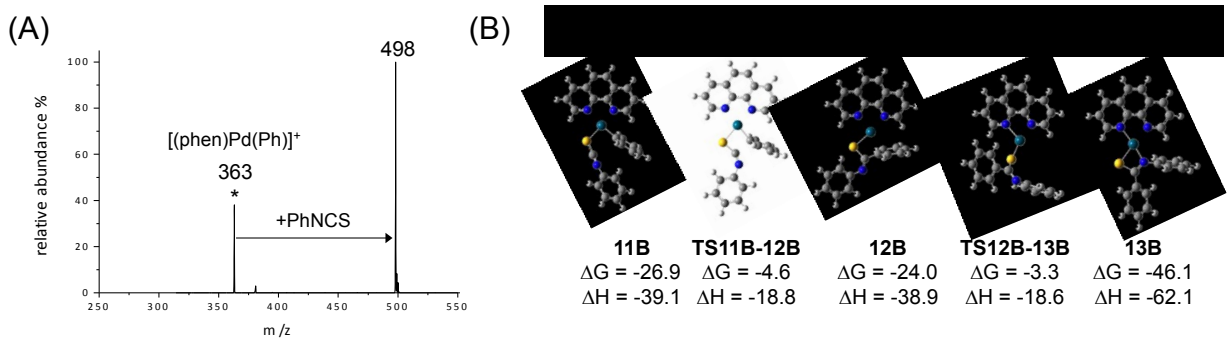


Figure S2. Gas-phase experiments (LTQ ion trap) and DFT calculations (B3LYP-gd3bj/SDD6-31+G(d)//M06/SDD6-31+G(d)) on: (**A**,**B**) insertion of PhNCS into the Pd-C bond (eq. 4, MS^3 IMR, concentration of PhNCS is 1.9 x 10^9 molecule/cm^3 and reaction time is 260 ms). DFT calculated species are orientated to highlight the direct relationship between carbon dioxide extrusion and isothiocyanate insertion for isoelectronic CO_2 and SCNR via the three coordinate complex, **10**.

3 General Experimental and Materials.

Unless otherwise stated, all reagents were purchased from commercial sources and used without further purification. Flash column chromatography was carried out using silica gel (40-63 microns) as the stationary phase. Analytical TLC was performed on pre-coated silica gel plates (0.25 mm thick, 60F254, Merck, Germany) and visualized under UV light. ^{1}H, ^{13}C NMR spectra were recorded either on a 600 MHz Varian/Agilent 600-MR or 500 MHz AR spectrometer at 298 K. Chemical shifts are reported in parts per million (ppm) and referenced to residual solvent peak. Coupling constants (*J*) are reported in Hertz (Hz). Standard abbreviations indicating multiplicity were used as follows: m = multiplet, quint. = quintet, q = quartet, t = triplet, d = doublet, s = singlet, br = broad. ESI-MS spectra were recorded on an Agilent 6510 ESI-TOF LC/MS mass spectrometer. High resolution electrospray ionization mass spectra (HR-ESI-MS) were collected on a Finnigan hybrid linear quadrupole Fourier transform ion-cyclotron resonance (LTQ FTICR) mass spectrometer.

Procedure for preparation of N-methylbenzothioamide for "authentic standard" studies (Figure S1).

To a mixture of magnesium (1.1 equiv), and an iodine crystal in THF was added dropwise the phenyl bromide (1 equiv). The reaction mixture was heated at reflux for 2 h. The mixture was allowed to cool at 0 °C and a solution of methylisothiocyanate (1.2 equiv) in THF was added. The reaction mixture was stirred for 16 h at room temperature. Water was added and the mixture was extracted twice with dichloromethane. The combined organic phases were washed with brine and dried over magnesium sulfate. After filtration the solvent was removed under reduced pressure and the residue (a yellow solid) was purified by chromatography on silica gel and elution with petroleum ether/ethyl acetate (8:2). ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.26 (s, 1H), 7.79 – 7.74 (m, 2H), 7.50 – 7.45 (m, 1H), 7.44 – 7.36 (m, 2H), 3.14 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 197.93, 141.36, 131.01, 128.45, 127.52, 3.88. ; HR-ESMS (ESI): m/z = 152.05291 $[M + H]^+$ (calc. for $C_8H_{10}NS$, *m/z* 152.05285).

^{1}H NMR monitoring experiments.

A small sample tube was charged with 2,6-dimethoxybenzoic acid (6 mg, 0.03 mmol) and palladium(II) acetate (8 mg, 0.036 mmol) and purged with N_2. DMSO-d_6 (0.75 ml) was added under N_2 and the mixture was stirred for 5 min at RT. For all sequential NMR experiments used to monitor reaction outcomes, a 100µl aliquot of the reaction mixture were withdrawn from the sample tube and transferred to a NMR tube, diluted via the addition of 700 µL DMSO-d_6 and then a ^{1}H NMR spectrum was taken. The mixture was then warmed to 65°C and stirred for 4 hours. ^{1}H NMR spectrum was

recorded and the formation of aryl palladium species was confirmed by the upfield shifts and peak broadening of the aromatic protons H_{para} and H_{meta} (Supplementary Information, Figure S1). The mixture was cooled to RT, RNCS (2 eq.) was added and stirred for 1 h and then a ^{1}H NMR spectrum was recorded. $NaBH_4$ (5 eq.) was added to the NMR sample and the mixture was stirred for another 1 h at RT. A final ^{1}H NMR spectrum was recorded. The recorded stacked spectra were stacked and are shown in supplementry information (Figure S1-S5). HRMS analyses was conducted for the NMR samples by diluting in acetonitrile.

General Procedure for the Insertion of Aliphatic Isothiocyanates.

To a solution of 2,6-dimethoxybenzoic acid (1 eq.) in DMSO (10 ml) was added palladium(II) acetate (1.1 eq). The mixture was heated to 65 °C for 4 hours under N_2, then cooled to RT. R-NCS was added and the mixture was then stirred for 1 hour at RT. $NaBH_4$ (5 eq.) was added and the reaction mixture was further stirred for an additional 1 hour at RT. Methanol (5 mL) was added to the mixture followed by water (100 mL) and the aqueous layer was extracted with diethyl ether (3 × 100 mL). The combined organic layer was washed with water (100 mL) and brine (100 mL) and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by column chromatography (silica gel, ethyl acetate/hexane, 1:4) to give the thioamides **6a-d**.

2,6-dimethoxy-N-methylbenzothioamide, 6a. Using the general procedure above using the following reagents: 2,6-dimethoxybenzoic acid (100 mg, 0.549 mmol), palladium(II) acetate (136 mg, 0.604 mmol), methylisothiocyanate (60 mg, 0.823 mmol) and $NaBH_4$ (104 mg, 2.74 mmol). Column chromatography (silica gel, ethyl acetate/hexane, 1:4), white solid (54 mg, 47%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.21 – 10.00 (m, *J* = 3.4 Hz, 1H), 7.24 (t, *J* = 8.4 Hz, 1H), 6.66 (d, *J* = 8.4 Hz, 2H), 3.71 (s, 6H), 3.02 (d, *J* = 4.7 Hz, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 194.18, 155.82, 129.52, 122.44, 104.79, 56.29, 32.50; HR-ESMS (ESI): m/z = 212.07395 [**6a** + H]$^+$ (calc. for $C_{10}H_{14}NO_2S$, *m/z* = 212.07398).

2,6-dimethoxy-N-ethylbenzothioamide, 6b. Using the general procedure above using the following reagents: 2,6-dimethoxybenzoic acid (100 mg, 0.549 mmol), palladium(II) acetate (136 mg, 0.604 mmol), ethylisothiocyanate (72 µL, 0.823 mmol) and $NaBH_4$ (104 mg, 2.74 mmol). Column chromatography (silica gel, ethyl acetate/hexane, 1:4), white solid (62 mg, 50%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.08 (s, 1H), 7.24 (t, *J* = 8.4 Hz, 1H), 6.66 (d, *J* = 8.4 Hz, 2H), 3.71 (s, 6H), 3.62 – 3.54 (m, *J* = 7.3, 5.3 Hz, 2H), 1.15 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 193.00, 155.78, 129.40, 122.68, 104.88, 56.36, 13.05. HR-ESMS (ESI): *m/z* = 226.08957 [**6b** + H]$^+$ (calc. for $C_{11}H_{16}NO_2S$, *m/z* = 226.08963).

2,6-dimethoxy-N-(isopropyl)benzothioamide, 6c. Using the general procedure above using the following reagents: 2,6-dimethoxybenzoic acid (100 mg, 0.549 mmol), palladium(II) acetate (136 mg, 0.604 mmol), isopropylisothiocyanate (89 µL, 0.823 mmol) and $NaBH_4$ (104 mg, 2.74 mmol). Column chromatography (silica gel, ethyl acetate/hexane, 1:4), yellow oil (75 mg, 57%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.96 (d, *J* = 7.3 Hz, 1H), 7.23 (t, *J* = 8.4 Hz, 1H), 6.65 (d, *J* = 8.4 Hz, 2H), 4.69 – 4.54 (m, 1H), 3.71 (s, 6H), 1.17 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 191.66, 155.77, 129.31, 122.85, 104.97, 56.44, 46.61, 21.07.; HR-ESMS (ESI): *m/z* = 240.10520 [**6c** + H]$^+$ (calc. for $C_{12}H_{18}NO_2S$, *m/z* = 240.10528).

2,6-dimethoxy-N-(tert-butyl)benzothioamide, 6d. Using the general procedure above using the following reagents: 2,6-dimethoxybenzoic acid (100 mg, 0.549 mmol), palladium(II) acetate (136 mg, 0.604 mmol), tert-butylisothiocyanate (348 µL, 2.74 mmol) and $NaBH_4$ (104 mg, 2.74 mmol). Column chromatography (silica gel, ethyl acetate/hexane, 1:4), white solid (17 mg, 12%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.51 (s, 1H), 7.18 (t, *J* = 8.4 Hz, 1H), 6.62 (d, *J* = 8.4 Hz, 2H), 3.70 (s, 6H), 1.51 (s, 9H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 192.63, 155.14, 128.30, 124.20, 104.58, 55.07, 40.02, 39.85, 39.69, 39.52, 39.35, 39.19, 39.02, 27.36; HR-ESMS (ESI): *m/z* = 254.12093 [**6d** + H]$^+$ (calc. for $C_{13}H_{20}NO_2S$, *m/z* = 254.12083).

General Procedure for the Insertion of Aromatic Isothiocyanates.

To a solution of 2,6-dimethoxybenzoic acid (1 eq.) in DMSO (10 ml) was added palladium(II) acetate (1.1 eq). The mixture was heated to 65 °C for 4 hours under N_2, then cooled to RT. K_2CO_3 (2 eq) was added to the mixture followed by the Ar-NCS and the mixture was then stirred for 2 hour at RT. $NaBH_4$ was added and the reaction mixture was further stirred for an additional 1 hour at RT. Methanol (5 mL) was added to the mixture followed by water (100 mL) and the aqueous layer was extracted with ethyl acetate (3 × 100 mL). The combined organic layer was washed with water (100 mL) and brine (100 mL) and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by column chromatography (silica gel, ethyl acetate/hexane, 1:4) to give the thioamides.

2,6-dimethoxy-N-phenylbenzothioamide, 6e and 2,6-dimethoxy-N-phenylbenzamide byproduct. Using the general procedure above using the following reagents: 2,6-dimethoxybenzoic acid (50 mg, 0.274 mmol), palladium(II) acetate (67.8 mg, 0.302 mmol). K_2CO_3 (76 mg, 0.549 mmol) and isothiocyanatobenzene (82 µl, 0.686 mmol). colorless solid (45mg, 60%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.75 (s, 1H), 8.06 (dd, *J* = 8.6, 1.0 Hz, 2H), 7.40 (3, *J* = 8.4, 7.5 Hz, 2H), 7.29 (t, *J* = 8.4 Hz, 1H), 7.25 – 7.19 (m, 1H), 6.72 (d, *J* = 8.4 Hz, 2H), 3.76 (s, 6H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 192.83, 155.66, 140.38, 129.64, 128.82, 126.19, 123.78, 122.65, 104.97, 56.46, 56.45; HR-ESMS (ESI): *m/z* = 274.08974 [**6e** + H]$^+$ (calc. for $C_{15}H_{16}NO_2S$, *m/z* = 274.08963).

From experiment entry **6** in **Table 1** (main paper) a second fraction from column chromatography gave the hydrolyzed amide as byproduct (10 mg, 7% yield). ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.17 (s, 1H), 7.70 (d, *J* = 7.7 Hz, 2H), 7.35 (t, *J* = 8.4 Hz, 1H), 7.29 (t, *J* = 7.9 Hz, 2H), 7.04 (t, *J* = 7.3 Hz, 1H), 6.73 (d, *J* = 8.4 Hz, 2H), 3.75 (s, 6H).; ^{13}C NMR (126 MHz, DMSO-d_6) δ 163.75, 157.14, 140.11, 130.76, 129.04, 123.49, 119.34, 117.34, 104.68, 56.21.; HR-ESMS (ESI): *m/z* = 258.11225 $[M + H]^+$ (calc. for $C_{15}H_{16}NO_3$, *m/z* = 258.11247).

2,6-dimethoxy-N-(4-chlorophenyl)benzothioamide, 6f. Using the general procedure above using the following reagents: 2,6-dimethoxybenzoic acid (50 mg, 0.274 mmol), palladium(II) acetate (67.8 mg, 0.302 mmol), K_2CO_3 (76 mg, 0.549 mmol) and 1-chloro-4-isothiocyanatobenzene (116 mg, 0.686 mmol), colorless solid (45 mg, 53%); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.84 (s, 1H), 8.10 (d, *J* = 8.9 Hz, 2H), 7.44 (d, *J* = 8.9 Hz, 2H), 7.28 (t, *J* = 8.4 Hz, 1H), 6.70 (d, *J* = 8.4 Hz, 2H), 3.73 (s, 6H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 193.29, 155.65, 139.22, 129.81, 129.69, 128.80, 124.15, 123.56, 104.96, 56.46; HR-ESMS (ESI): *m/z* = 308.05066 [**6f** + H]$^+$ (calc. for $C_{15}H_{15}NClO_2S$, *m/z* = 308.05065).

2,6-dimethoxy-N-(4-trifluoromethylphenyl)benzothioamide, 6g. Using the general procedure above using the following reagents: 2,6-dimethoxybenzoic acid (50 mg, 0.274 mmol), palladium(II) acetate (67.8 mg, 0.302 mmol), K_2CO_3 (76 mg, 0.549 mmol) and 1-trifluoromethyl-4-isothiocyanatobenzene (116 mg, 0.686 mmol). Colorless solid (48 mg, 41%); ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.05 (s, 2H), 8.32 (d, *J* = 8.5 Hz, 2H), 7.78 (d, *J* = 8.6 Hz, 2H), 7.31 (t, *J* = 8.4 Hz, 1H), 6.74 (d, *J* = 8.4 Hz, 2H), 3.76 (s, 6H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 194.03, 155.20, 143.22, 129.49, 125.75, 125.72, 123.11, 122.74, 122.14, 104.52, 56.03; HR-ESMS (ESI): *m/z* = 342.07717 [**6g** + H]$^+$ (calc. for $C_{16}H_{15}F_3NO_2S$, *m/z* = 342.07701).

2,6-dimethoxy-N-(4-nitrophenyl)benzothioamide, 6h. Using the general procedure above using the following reagents without adding $NaBH_4$: 2,6-dimethoxybenzoic acid (100 mg, 0.549 mmol), palladium(II) acetate (136 mg, 0.604 mmol), K_2CO_3 (150 mg, 1.1 mmol) and 1-nitro-4-isothiocyanatobenzene (148 mg, 1.5 mmol). Off-white solid (38 mg, 22%); ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.24 (s, 1H), 8.43 (d, *J* = 8.7 Hz, 2H), 8.29 (d, *J* = 8.8 Hz, 2H), 7.32 (t, *J* = 8.4 Hz, 1H), 6.74 (d, *J* = 8.3 Hz, 2H), 3.75 (s, 6H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 195.29, 155.66, 145.96, 144.18, 130.13, 124.94, 123.56, 122.11, 104.98, 56.50; HR-ESMS (ESI): *m/z* = 319.07450 [**6h** + H]$^+$ (calc. for $C_{15}H_{15}N_2O_4S$, *m/z* = 319.07470).

4 Selected ^{1}H NMR Spectrum.

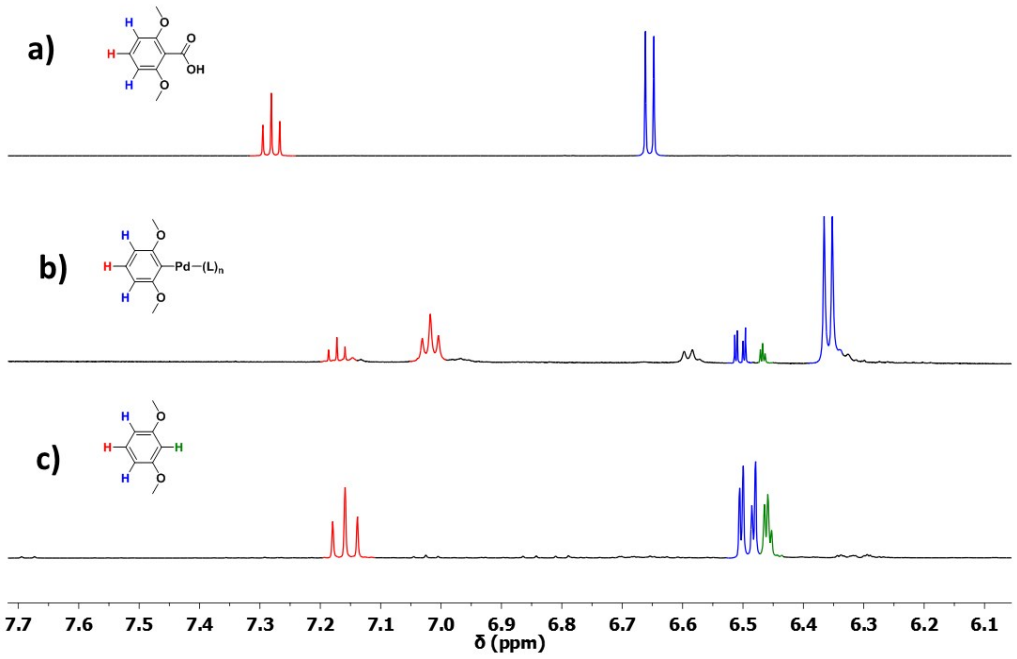


Figure S3 Partial Stacked ^{1}H NMR spectra (600 MHz, DMSO-d_6) of **a)** 2,3-dimethoxybenzoic acid, **b)** After adding Pd(II) acetate and heating for 4h at 65 °C, **c)** After heating at 70 °C for 24 h.

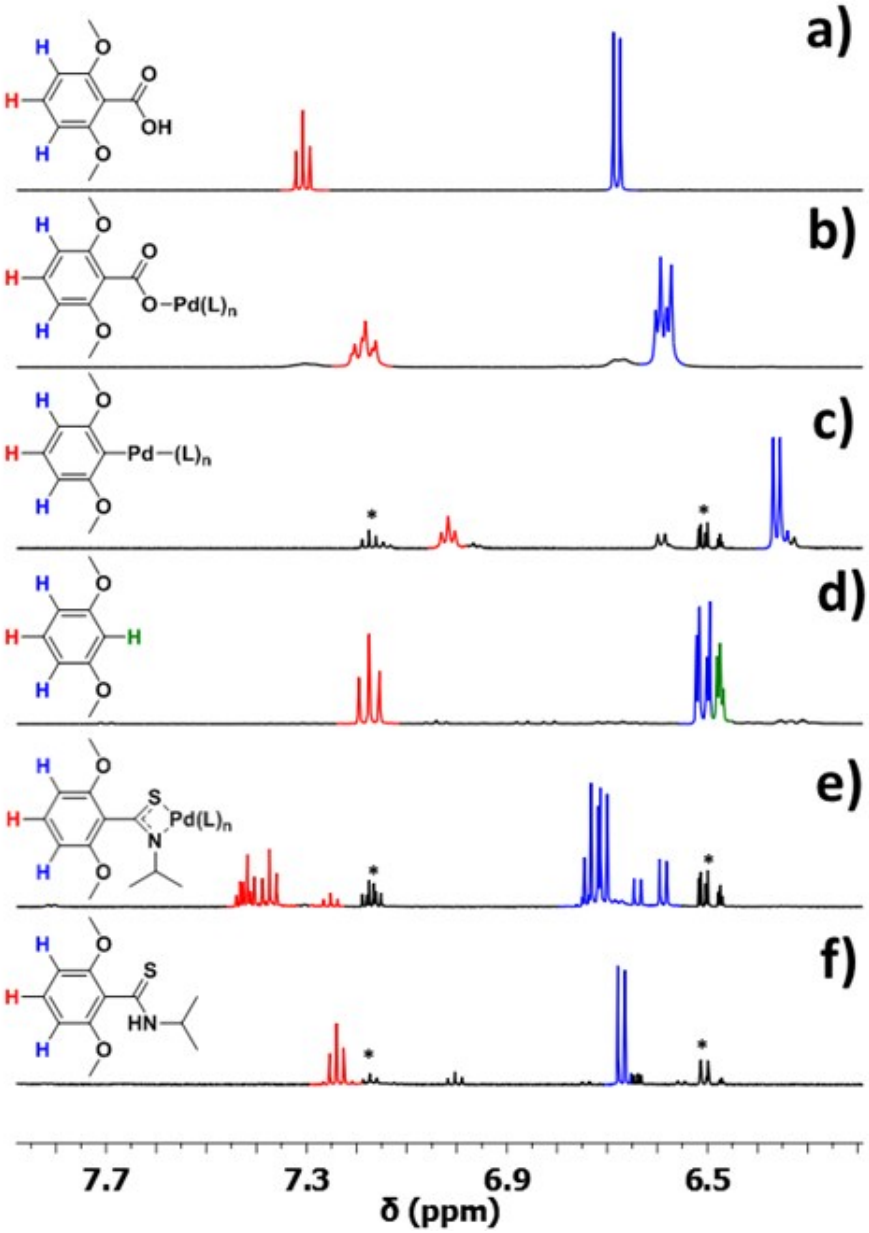


Figure S4 Transformation of 2,6-dimethoxybenzoic acid to N-isopropyl-2,6-dimethoxybenzamide monitored using 1H NMR spectroscopy (only the resonances due to the aromatic protons are shown): (a) free 2,6-dimethoxybenzoic acid; (b) binding to the metal center (eq. 2); (c) decarboxylation (eq. 3); (d) no addition of iPrNCS, showing protonation (eq. 6) occuring at longer reaction times to yield protodecarboxylation product (eq. 7); (e) insertion of iPrNCS into the Pd-C bond (eq. 4) and (f) reaction of the palladium thioamidate with NaBH4 to release the free thioamide (eq. 5). * highlights peaks due to proto decarboxylated product, 1,3-dimethoxybenzene. Ligand 'L' is either DMSO or acetate.

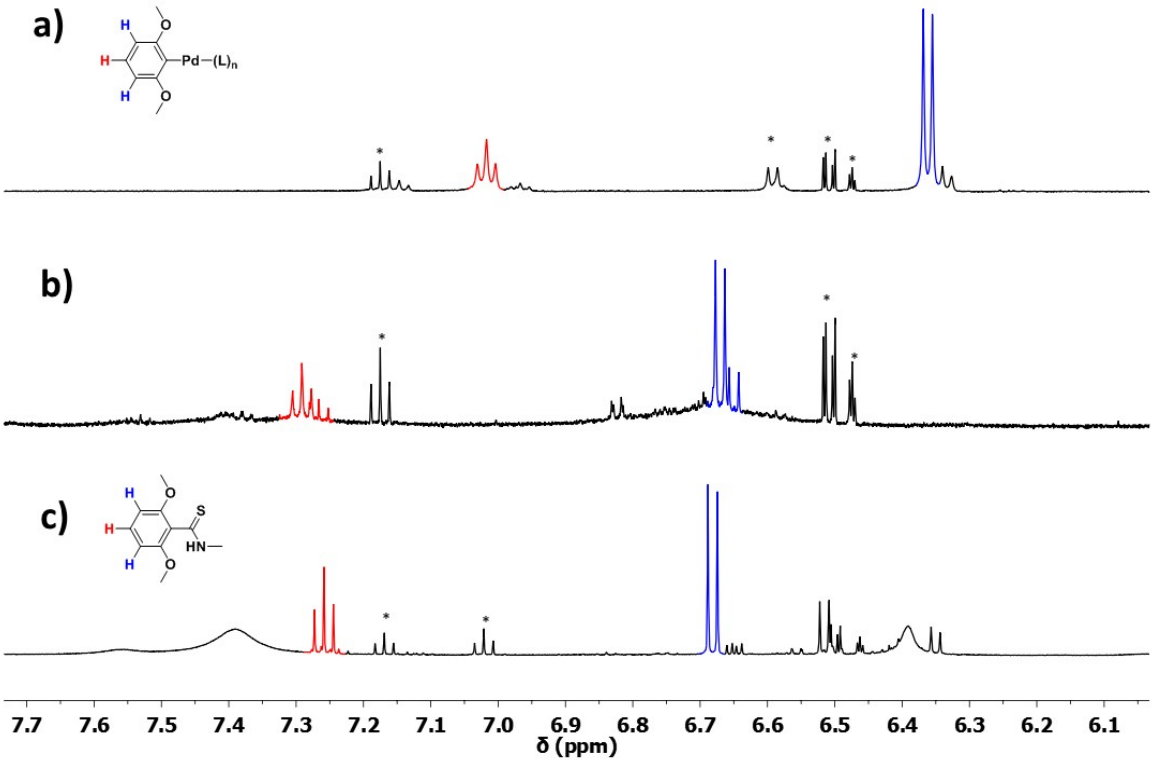


Figure S5 Partial Stacked ^{1}H NMR spectra (600 MHz, DMSO-d_6) of **a)** preformed aryl palladium complex, **b)** after stirring with methylisothiocyanate for 1h at RT,**c)** After addition of $NaBH_4$ at RT. * highlights peaks due to proto decarboxylated product, 1,3-dimethoxybenzene. Ligand 'L' is either DMSO or acetate.

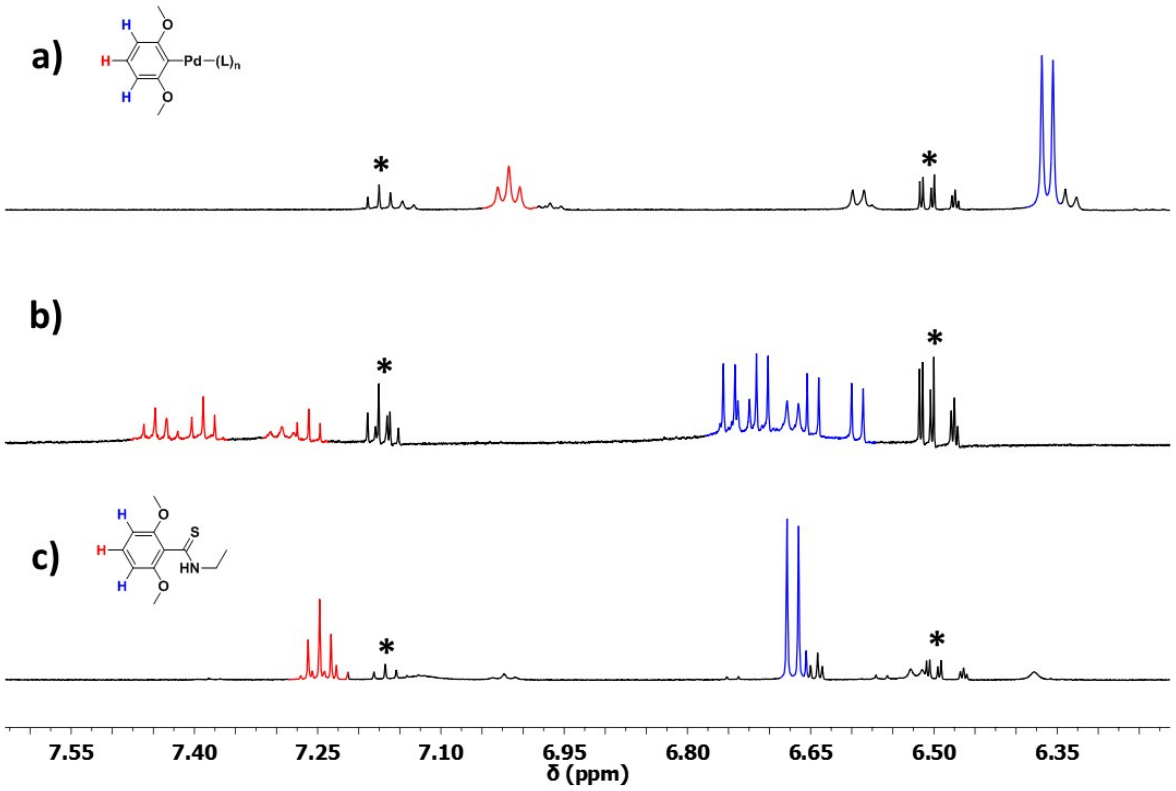


Figure S6 Partial Stacked ^{1}H NMR spectra (600 MHz, DMSO-d_6) of **a)** preformed aryl palladium complex, **b)** after stirring with ethylisothiocyanate for 1h at RT, **c)** After 1 h addition of $NaBH_4$ at RT. * highlights peaks due to proto decarboxylated product, 1,3-dimethoxybenzene. Ligand 'L' is either DMSO or acetate.

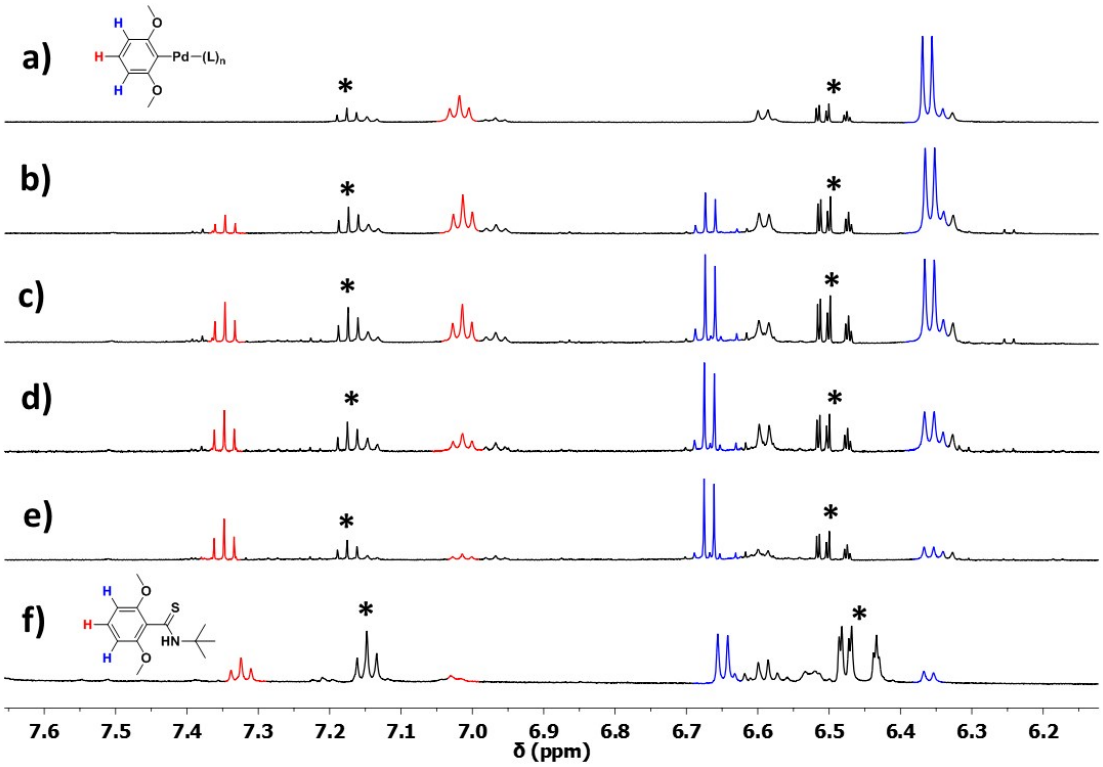


Figure S7 Partial Stacked ^{1}H NMR spectra (600 MHz, DMSO-d_6) of **a)** preformed aryl palladium complex, **b)** after stirring with *t*-butylisothiocyanate for 1h at RT, **c)** after 2h at RT, **d)** after 3h at RT, **e)** after 4h at RT, **f)**after 1 h addition of $NaBH_4$ at RT. * highlights peaks due to proto decarboxylated product, 1,3-dimethoxybenzene. Ligand 'L' is either DMSO or acetate.

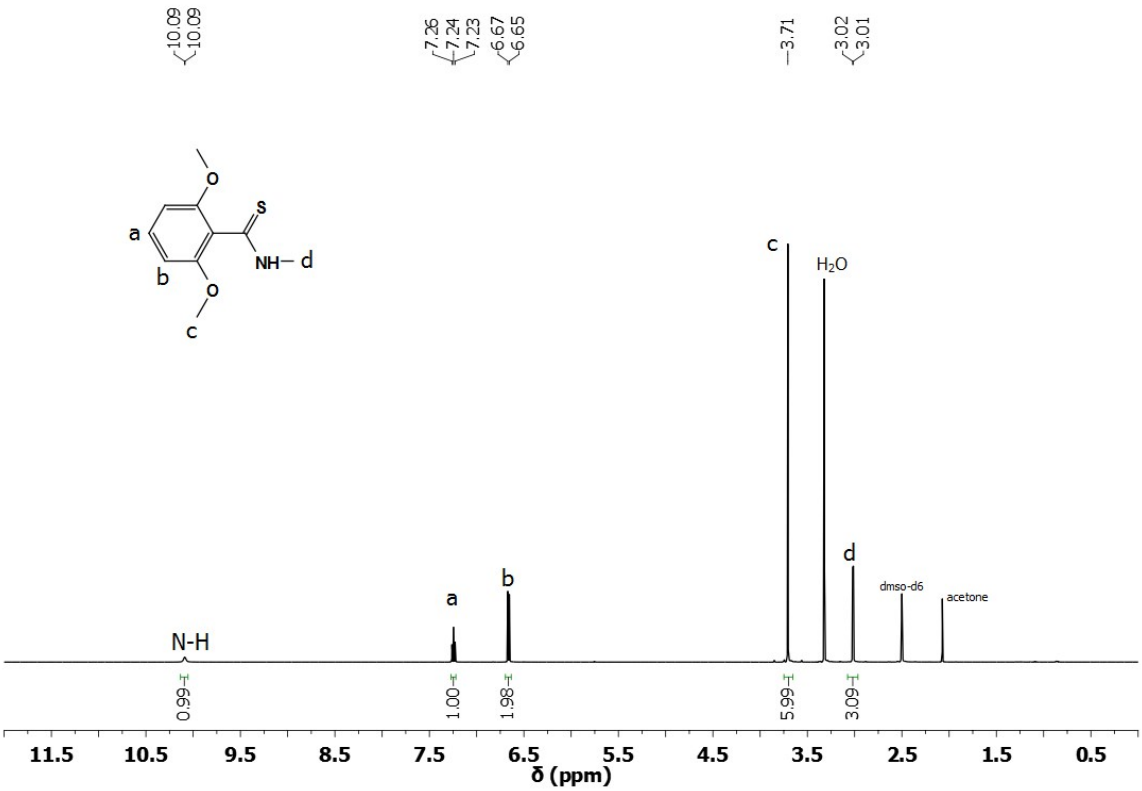


Figure S8 [1]H NMR spectra (500 MHz, DMSO-d6) of **6a**

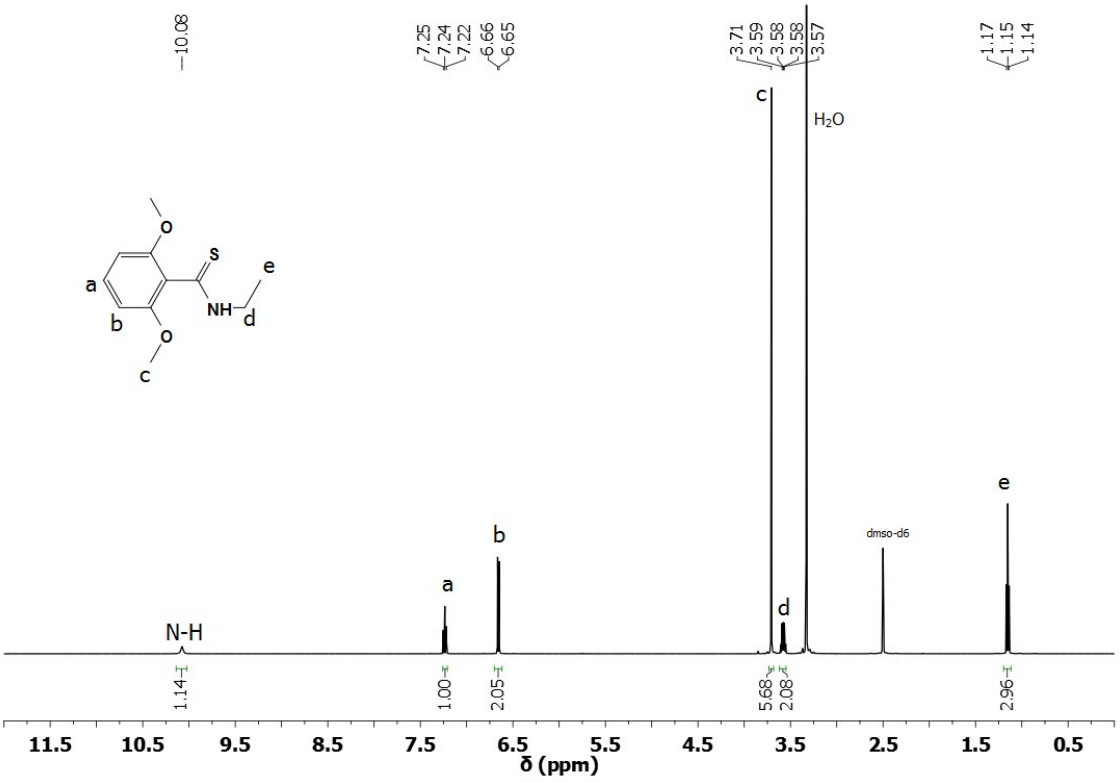


Figure S9 [1]H NMR spectra (500 MHz, DMSO-d6) of **6b**

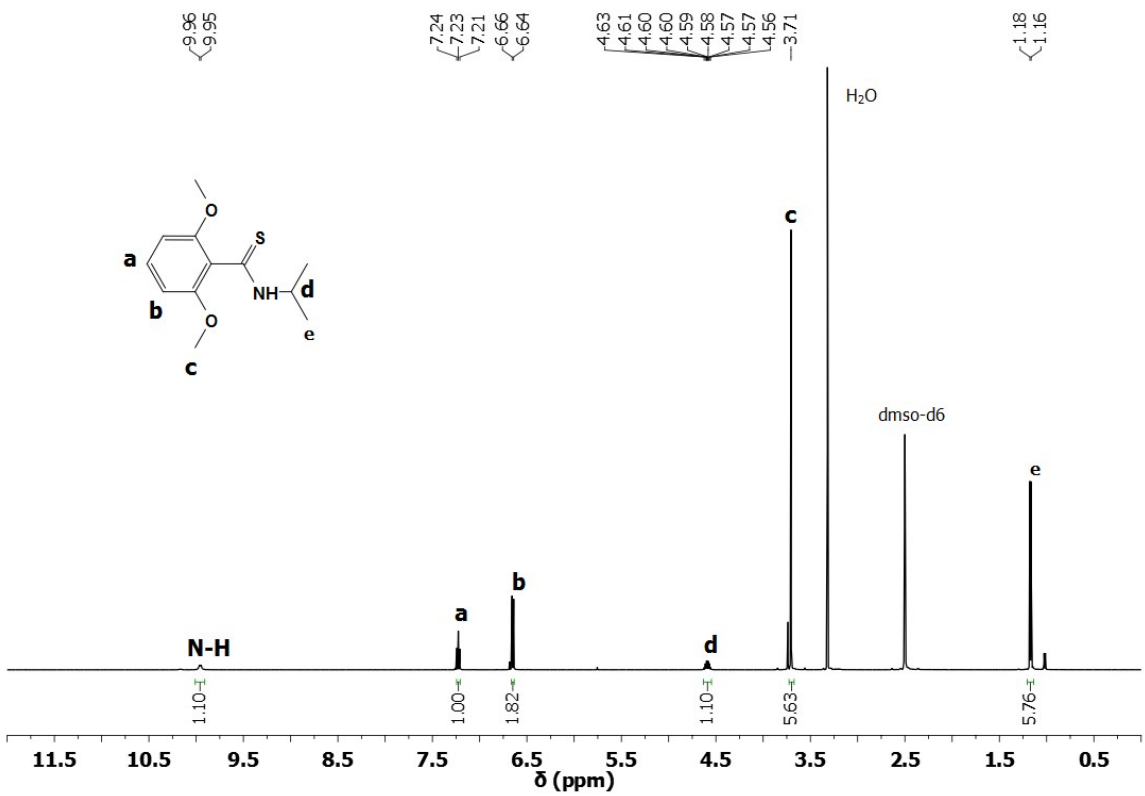


Figure S10 ^{1}H NMR spectra (500 MHz, DMSO-d6) of **6c**

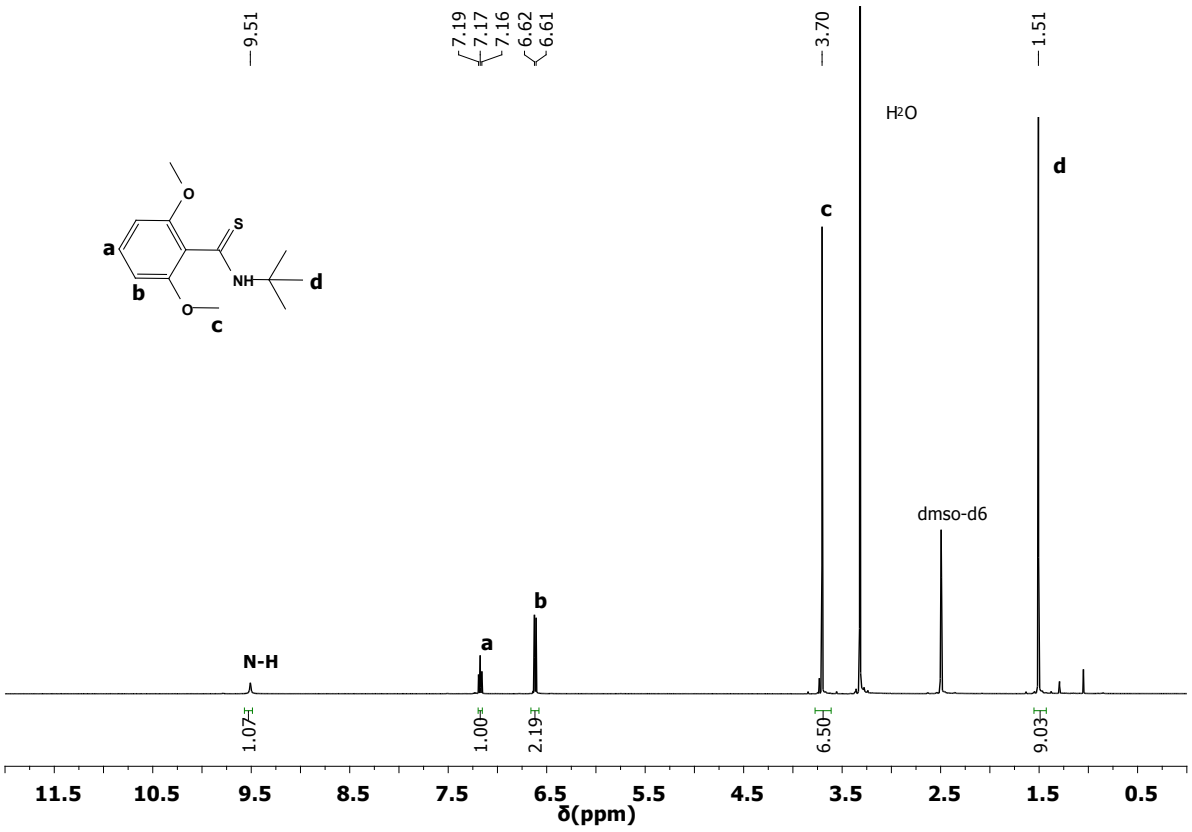


Figure S11 [1]H NMR spectra (500 MHz, DMSO-d6) of **6d**

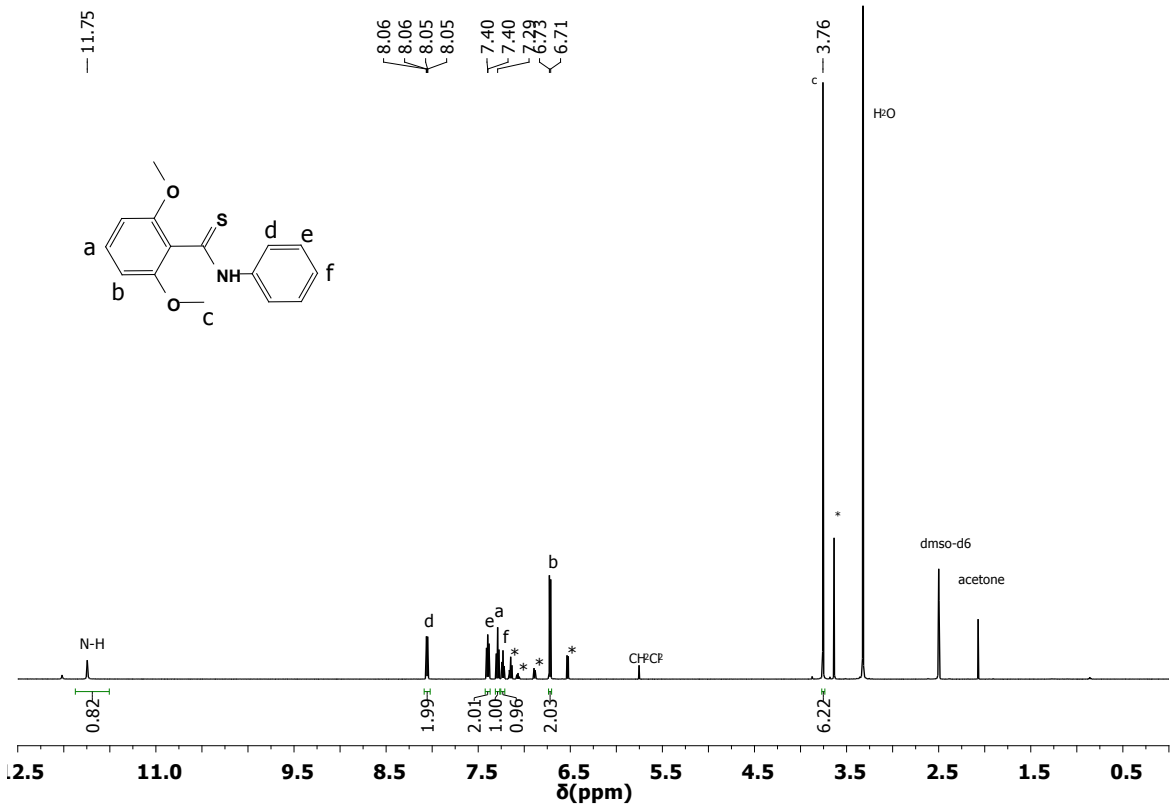


Figure S12 [1]H NMR spectra (500 MHz, DMSO-d6) of **6e**

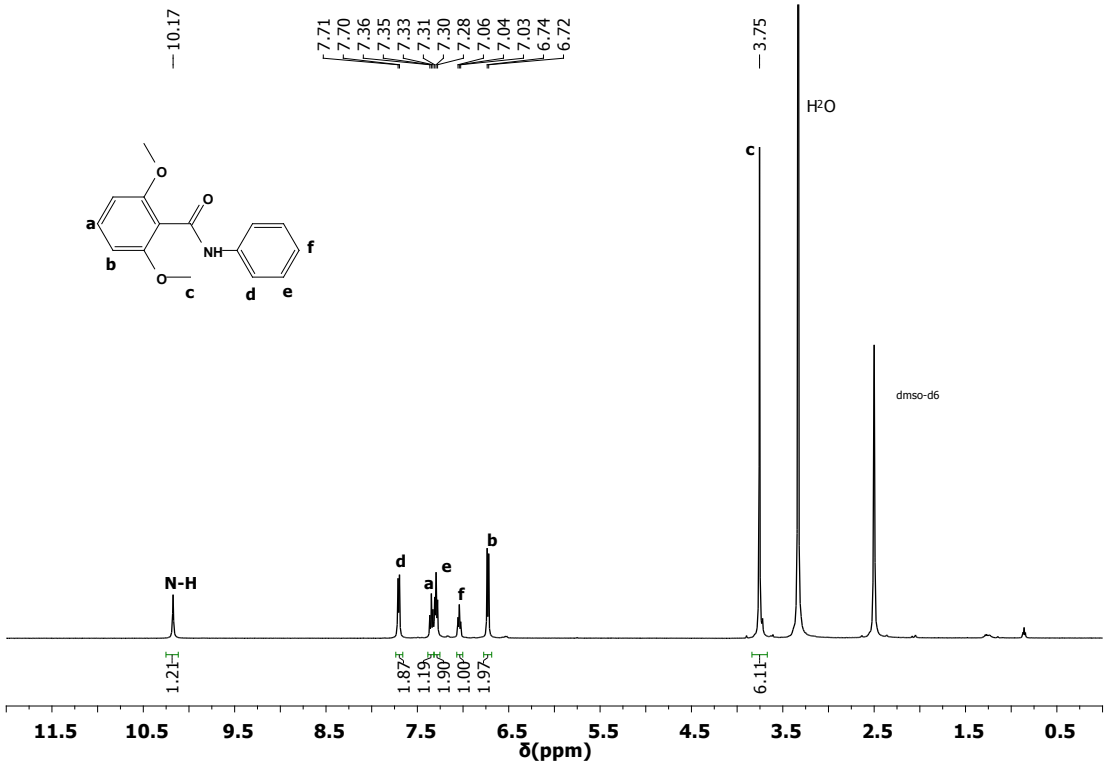


Figure S13 [1]H NMR spectra (500 MHz, DMSO-d6) of amide byproduct of **6e**

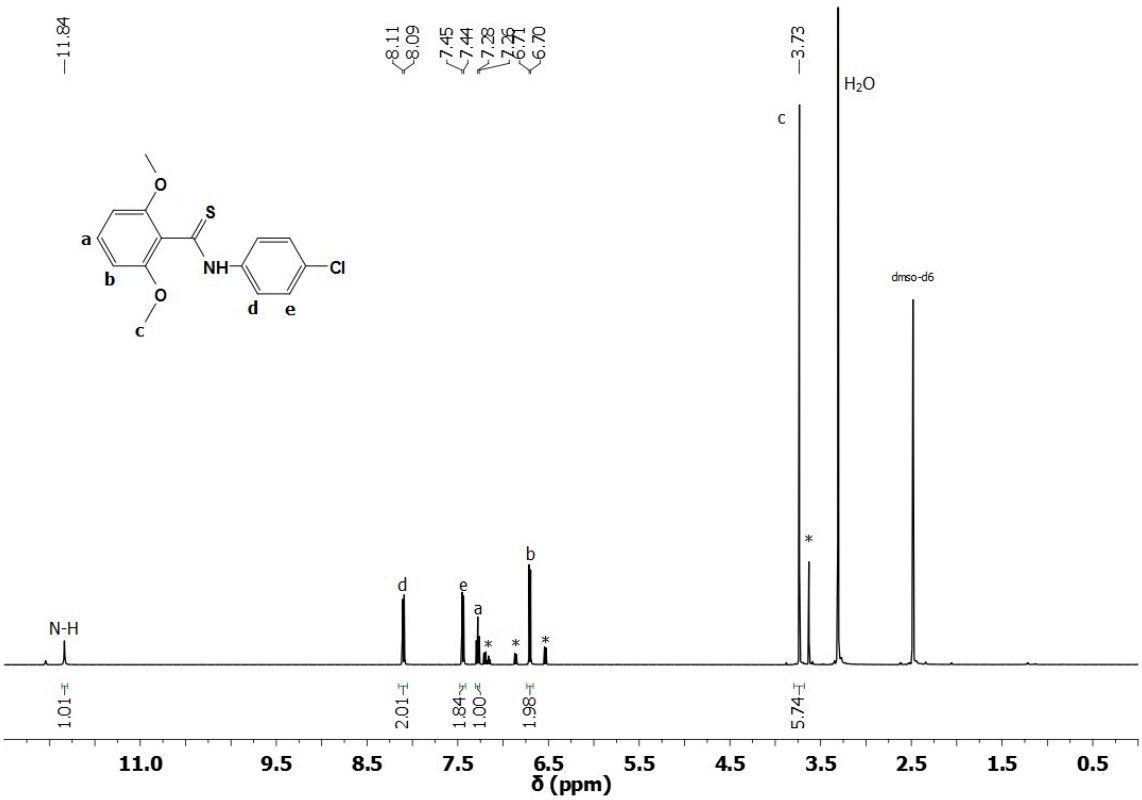


Figure S14 [1]H NMR spectra (500 MHz, DMSO-d6) of **6f**

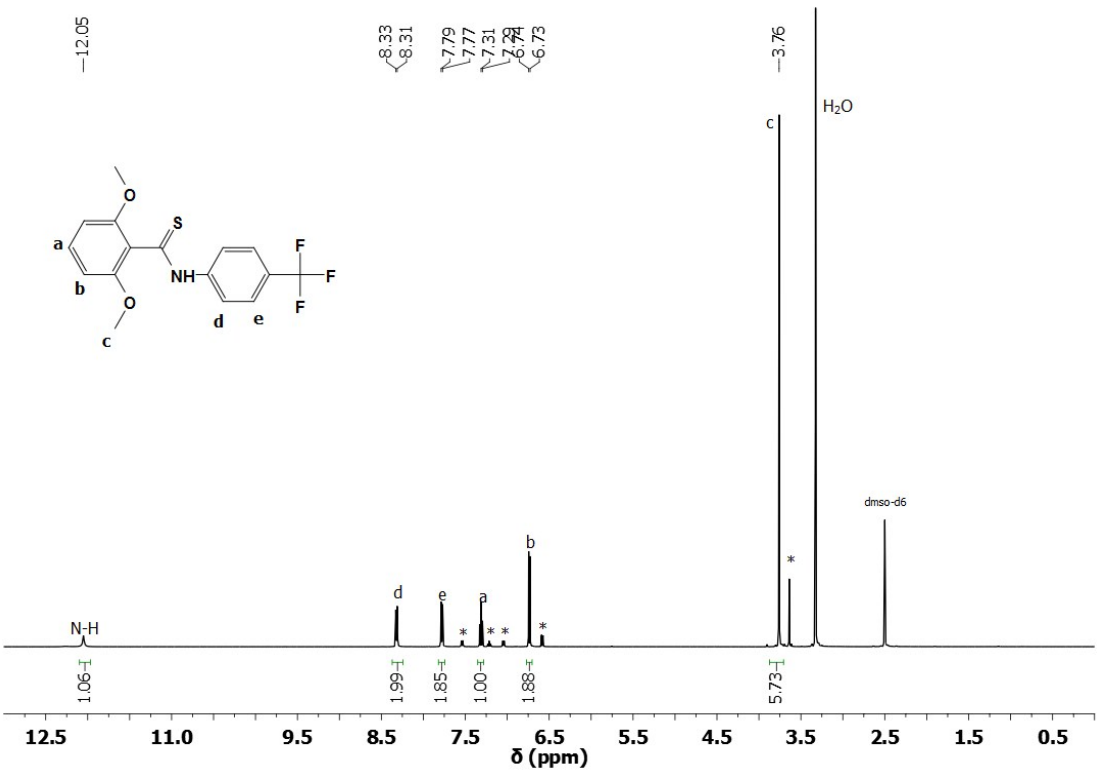


Figure S15 [1]H NMr spectra (500 MHz, DMSO-d6) of **6g**

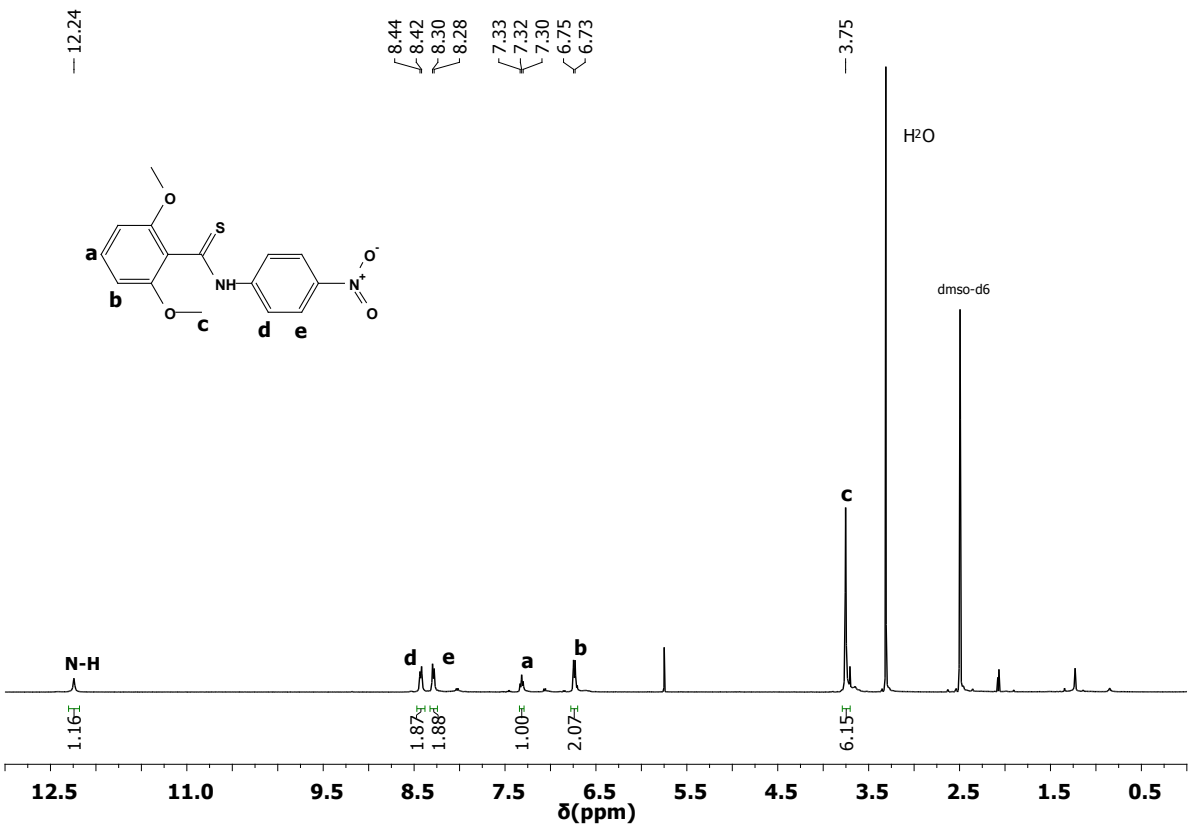


Figure S16 [1]H NMr spectra (500 MHz, DMSO-d6) of **6h**

5 Selected HR-ESMS Spectrum

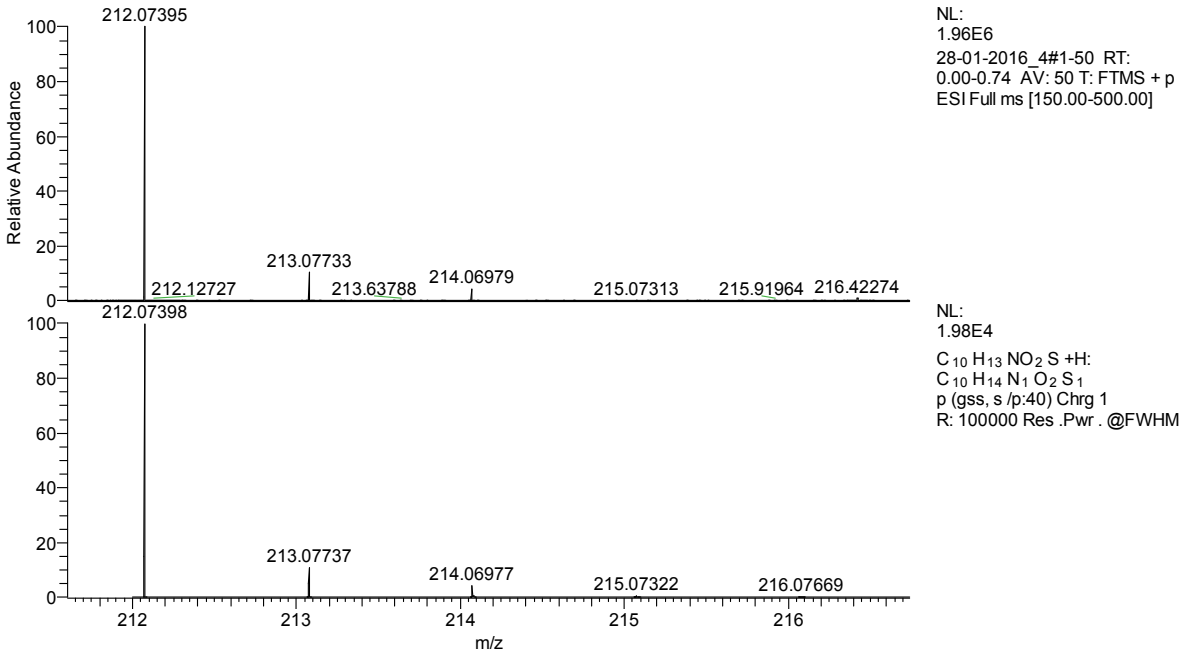


Figure S17 Observed (top) and calculated (bottom) isotopic distribution patterns of **6a**

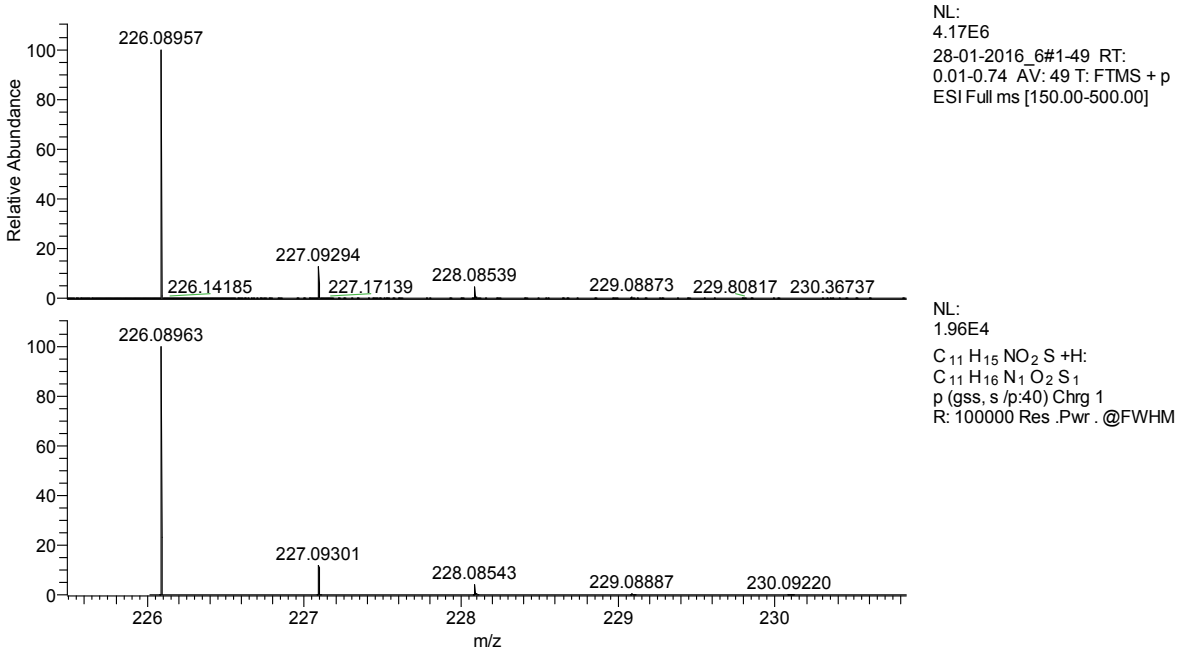


Figure S18 Observed (top) and calculated (bottom) isotopic distribution patterns of **6b**

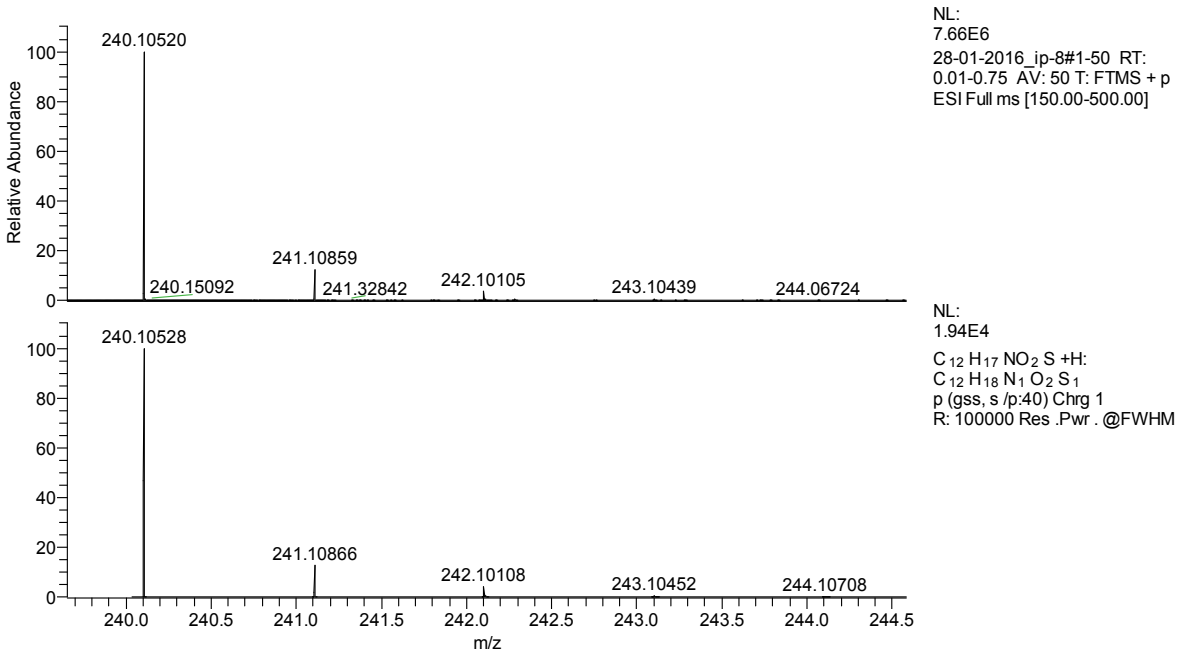


Figure S19 Observed (top) and calculated (bottom) isotopic distribution patterns of **6c**

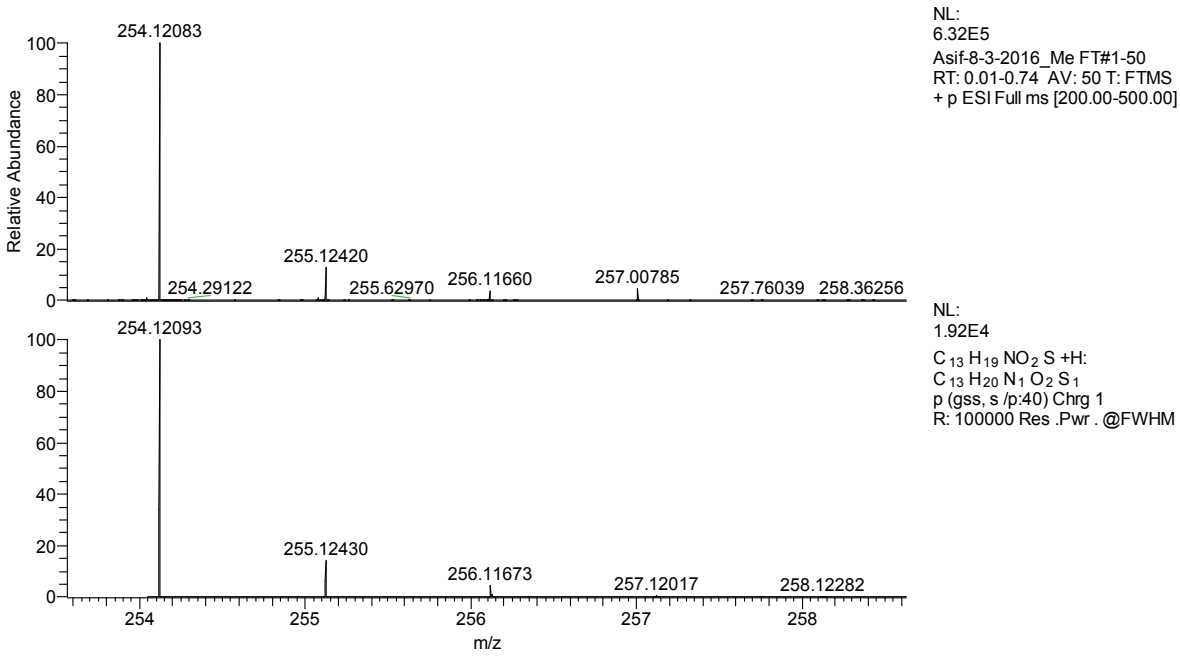


Figure S20 Observed (top) and calculated (bottom) isotopic distribution patterns of **6d**

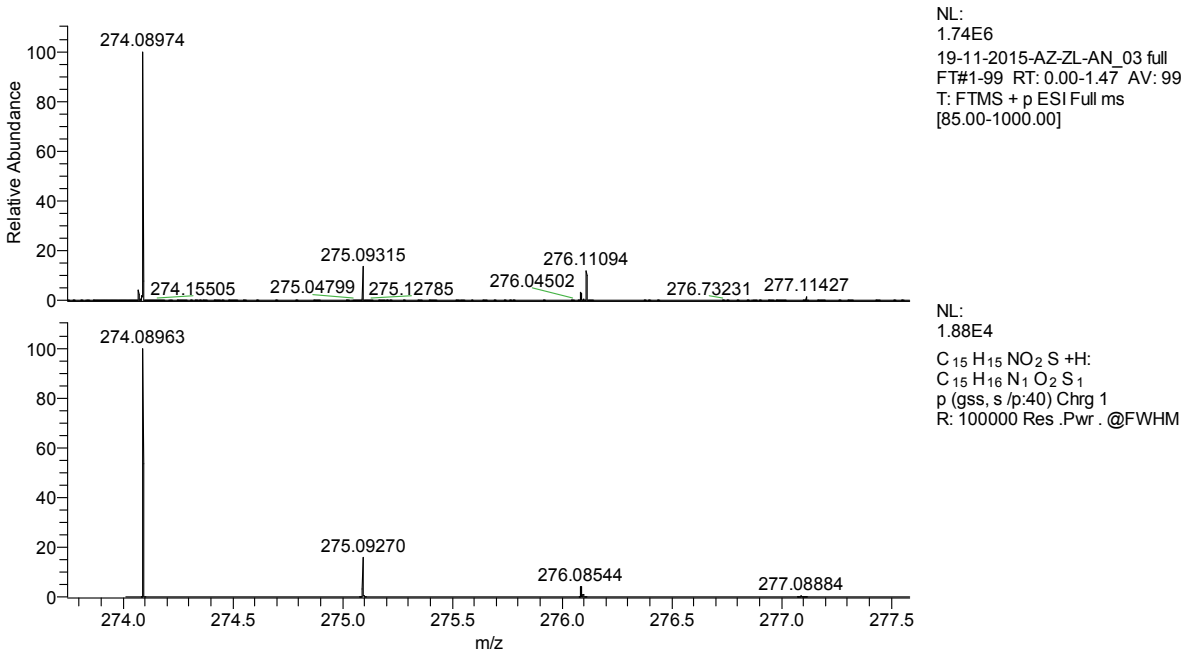


Figure S21 Observed (top) and calculated (bottom) isotopic distribution patterns of **6e**

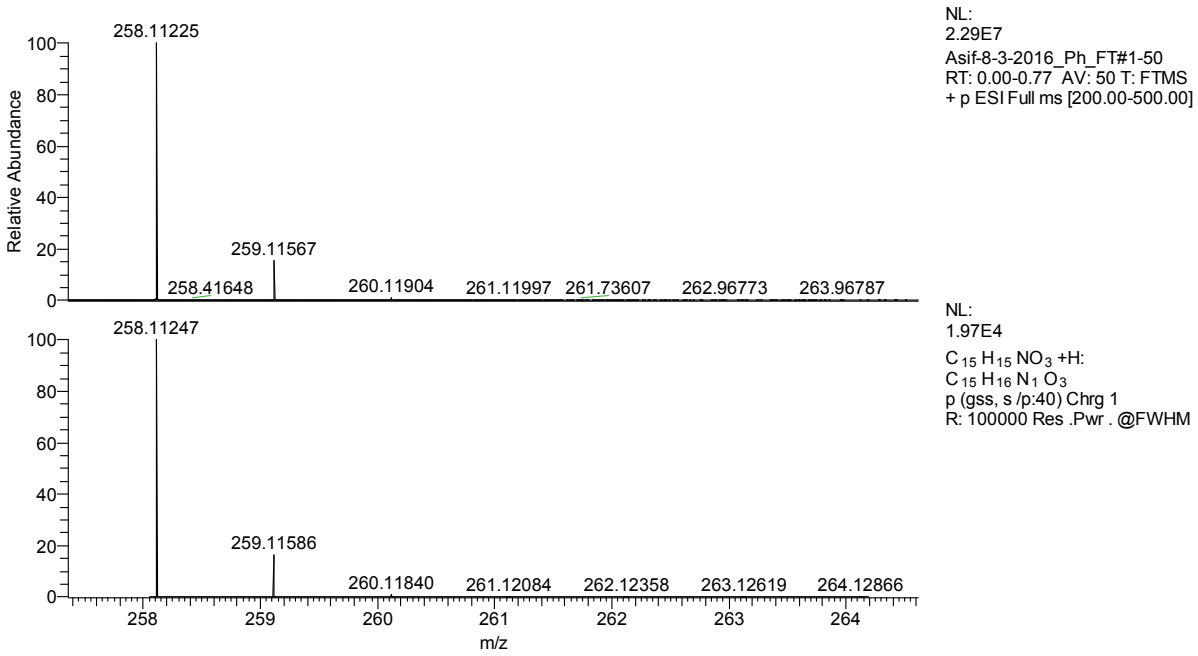


Figure S22 Observed (top) and calculated (bottom) isotopic distribution patterns for the amide byproduct of **6e**

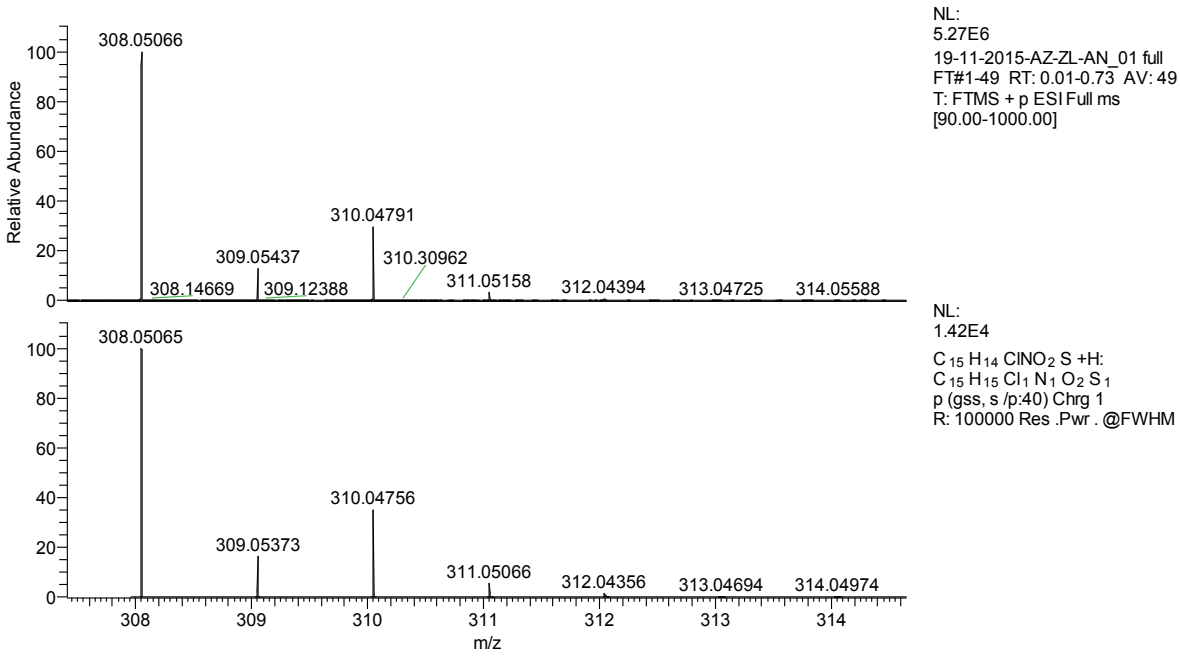


Figure S23 Observed (top) and calculated (bottom) isotopic distribution patterns of **6f**

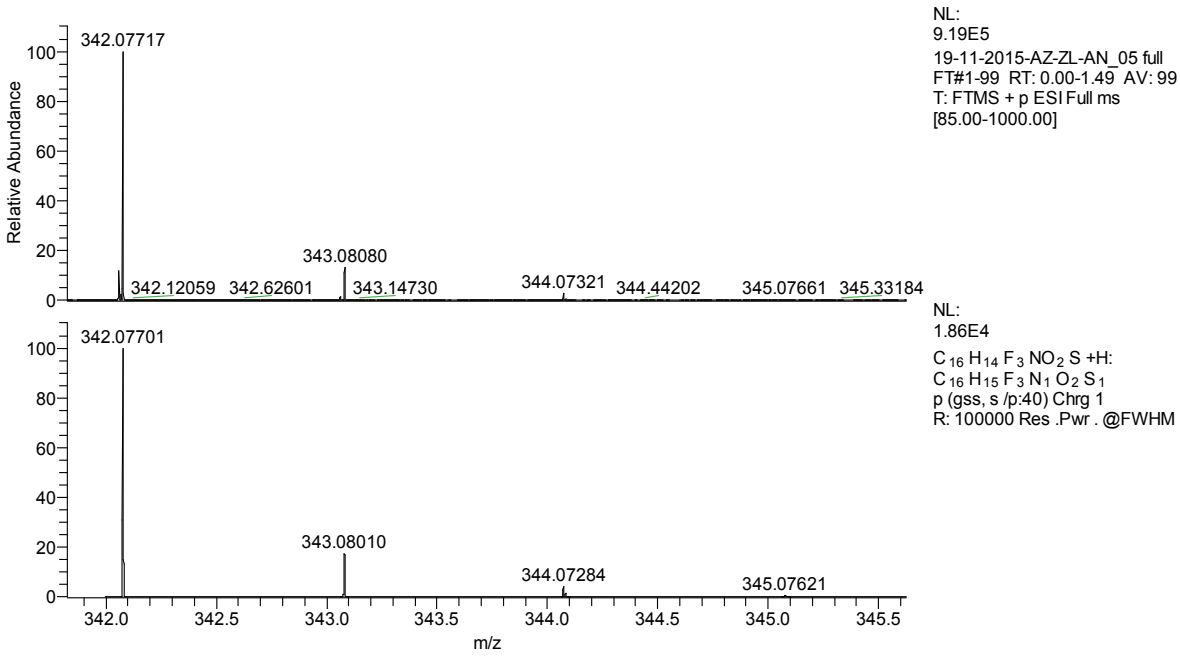


Figure S24 Observed (top) and calculated (bottom) isotopic distribution patterns of **6g**

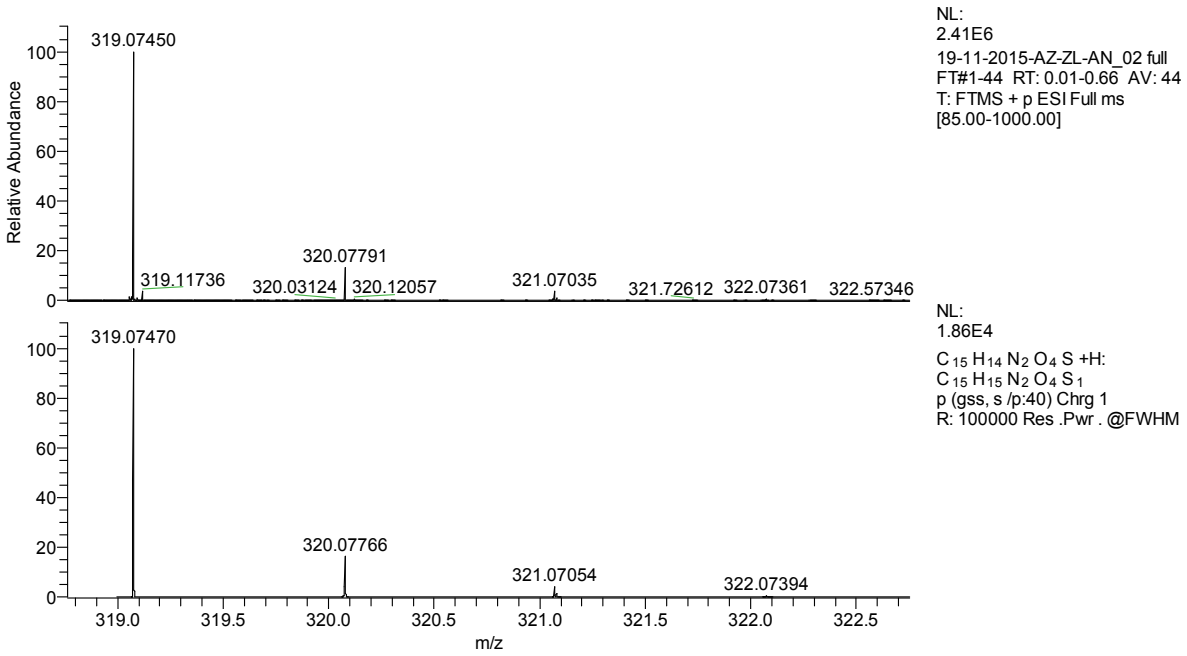


Figure S25 Observed (top) and calculated (bottom) isotopic distribution patterns of **6h**

6 X-ray Crystallography

The molecular structures of the thioamides **6a**, **6b**, **6d**, **6e**, **6f** and **6g** were confirmed by X-ray crystallography. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of compounds dissolved in mixtures of pentane and dichloromethane (1:1). The molecular structures reveal different *E* versus *Z* arrangements about the central C-N bond of the thioamide that depend on the nature of the R group used in the isothiocyanate. In the case of aliphatic groups, a *Z* arrangement is found (Figure S24 (**6a**) and Figure S27 (**6b**) and S30 (**6d**)), while the aromatic groups give rise to a *E* arrangement (Figures S33 (**6e**), S35 (**6f**) and S37 (**6g**)). The *E* versus *Z* arrangements influence the intermolecular hydrogen bonded arrangements. The *E* arrangements found in **6e**, **6f** and **6g** give rise to strong hydrogen bonding through the sulfur and the N-H group of the neighboring molecule resulting in the formation of hydrogen bonded dimers.[17, 18] The H-bond lengths are similar in all cases (S1···H10-N, 2.35 (2) Å in **6e** and 2.39 (2) Å in **6f** while slightly longer 2.57 Å in **6g**). The sulfur atom S1 in **6f** and **6g** was also found to be weakly bonded to the aromatic hydrogen (S1···H14, 2.87(2) Å in **6f** and in **6g** S1···H13 3.01(2) Å) of the neighboring molecule further stabilizing the dimeric arrangement of the two molecules. In contrast, formation of the dimeric "synthon" [17] is not possible for the *Z* arrangements found in **6a, 6b** and **6d**, which instead form hydrogen bonded linear chain structures Figures S26, S29 and S32). DFT calculations reveal that the *Z* form is more stable for both $PhC(S)NHCH_3$ and **6a**, while the *E* form in more stable for both PhC(S)NHPh and **6e** (Table S1). These stability orders remain the same in both the gas-phase and in DMSO (Table S1). Thus the differences between the X-ray structures likely arises from intrinsic differences in stabilities rather than the crystal packing forces

Data Collection

X-ray data benzothioamides were collected at 130 K on an Agilent Technologies Dual source Supernova system using Cu Kαradiation, and data were treated using CrysAlisPro[19] software. The structures were solved using SHELXT running within the WinGX[20] package program.

Data Refinement

X-Ray data refinement for 2,6-dimethoxy-N-methylbenzothioamide,6a

The structure was solved by direct methods using SHELXT running within the WinGX[20] package. All non-hydrogen atoms were refined anisotropically. The structure was solved in the orthorhombic space group $Pna2_1$ and refined to an R_1 value of 2.5%.

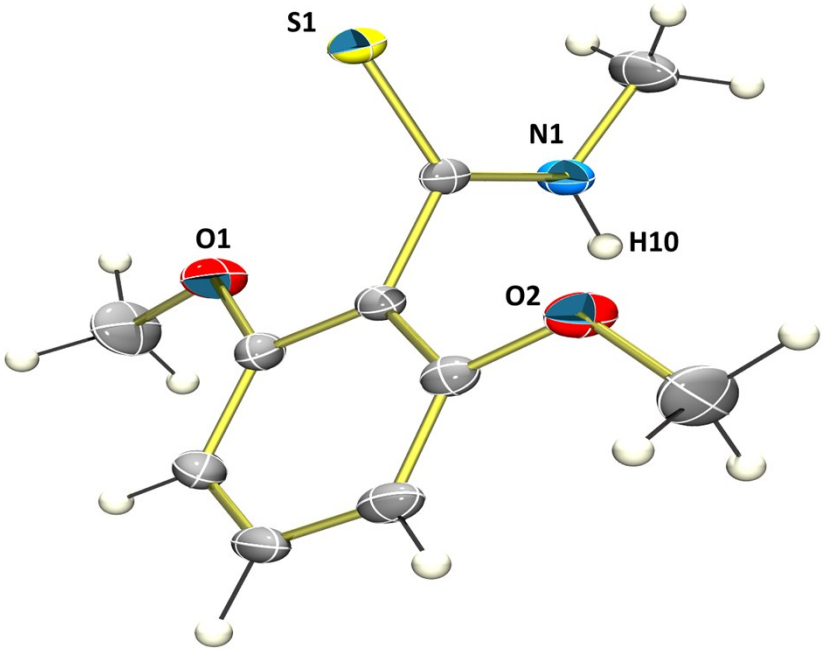


Figure S26 ORTEP-3 representations of the molecular structures of **6a**. The thermal ellipsoids are shown at the 50% probability level.

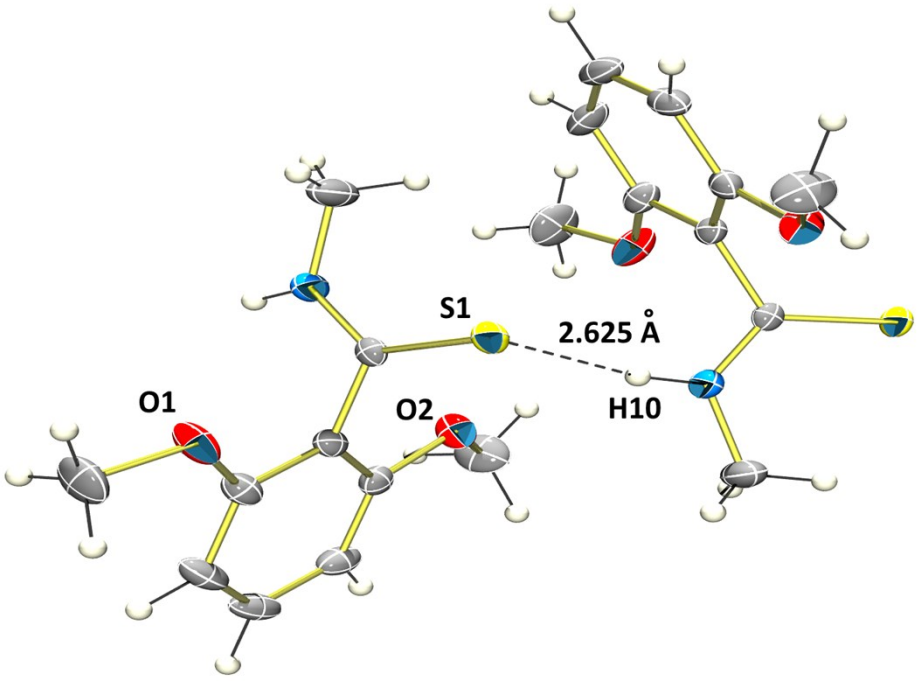


Figure S27 ORTEP-3 representations of the intermolecular hydrogen bonded arrangement for **6a**. The thermal ellipsoids are shown at the 50% probability level.

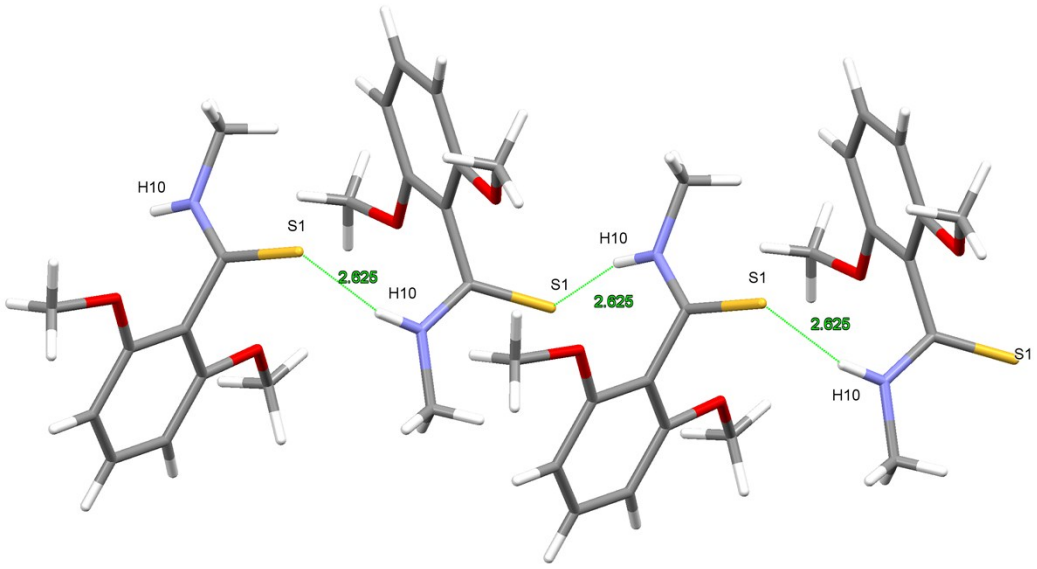


Figure S28 Mercury diagrams (capped stick) for the intermolecular hydrogen bonded linear chain of **6a.**

X-Ray data refinement for2,6-dimethoxy-N-ethylbenzothioamide,6b

The structure was solved by direct methods using SHELXT running within the WinGX[20] package. All non-hydrogen atoms were refined anisotropically. The structure was solved in the monoclinic space group $P2_1/c$ and refined to an R_1 value of 3.5%.

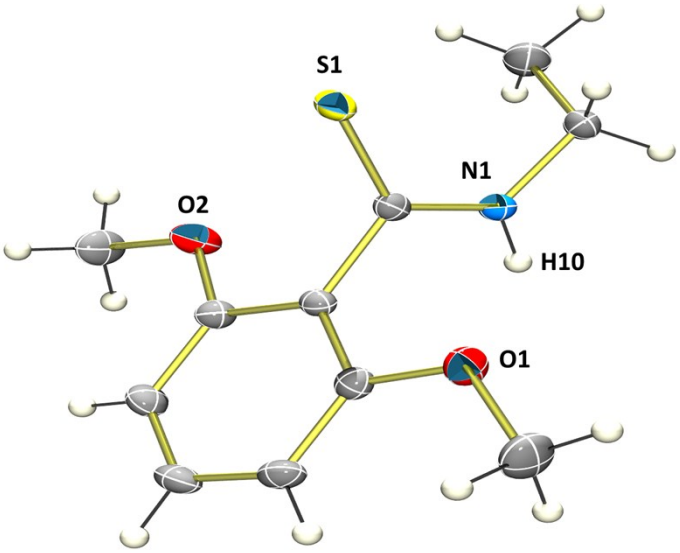


Figure S29 ORTEP-3 representations of the molecular structures of **6b**. The thermal ellipsoids are shown at the 50% probability level**.**

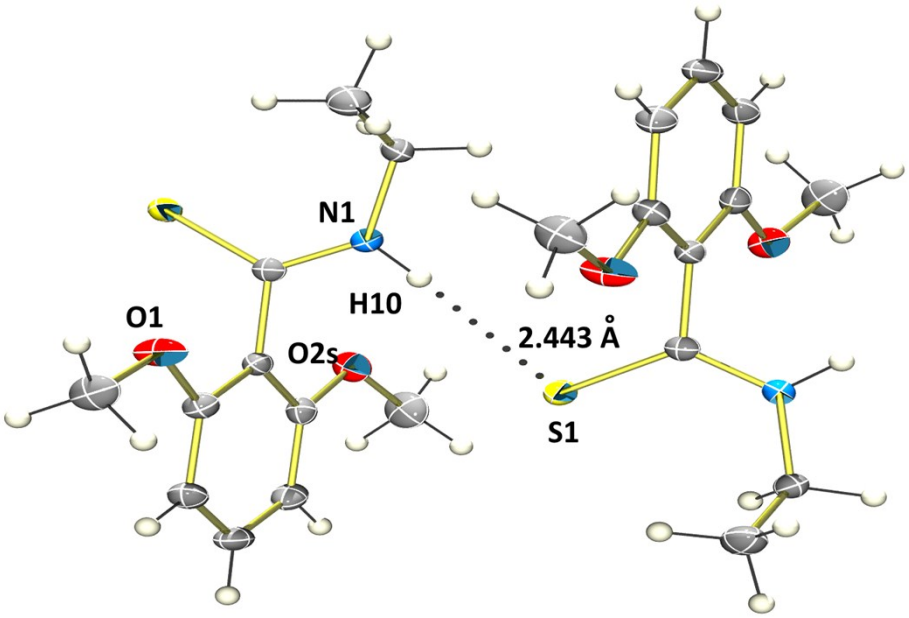


Figure S30 ORTEP-3 representations of the intermolecular hydrogen bonded arrangement for **6b**. The thermal ellipsoids are shown at the 50% probability level.

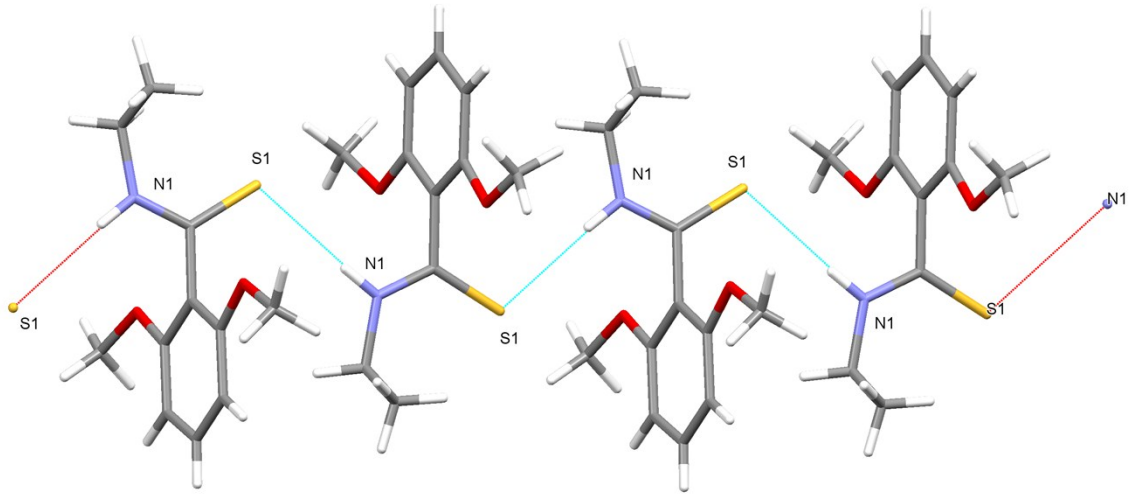


Figure S31 Mercury diagrams (capped stick) for the intermolecular hydrogen bonded linear chain of **6b.**

X-Ray data refinement for 2,6-dimethoxy-N-t-butylbenzothioamide,6d

The structure was solved by direct methods using SHELXT running within the WinGX[20] package. All non-hydrogen atoms were refined anisotropically. The structure was solved in the monoclinic space group P-1 and refined to an R_1 value of 3.6%.

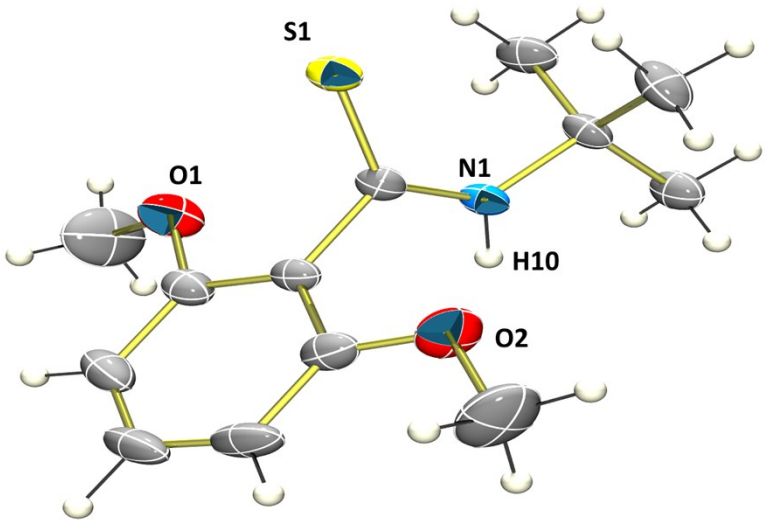


Figure S32 ORTEP-3 representations of the molecular structures of **6d**. The thermal ellipsoids are shown at the 50% probability level**.**

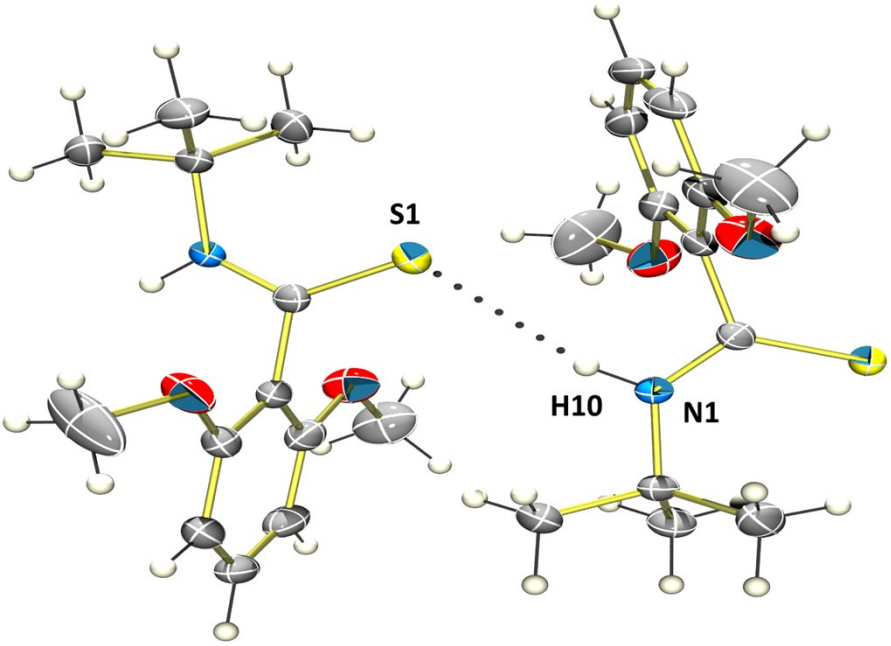


Figure S33 ORTEP-3 representations of the intermolecular hydrogen bonded arrangement for **6d**. The thermal ellipsoids are shown at the 50% probability level.

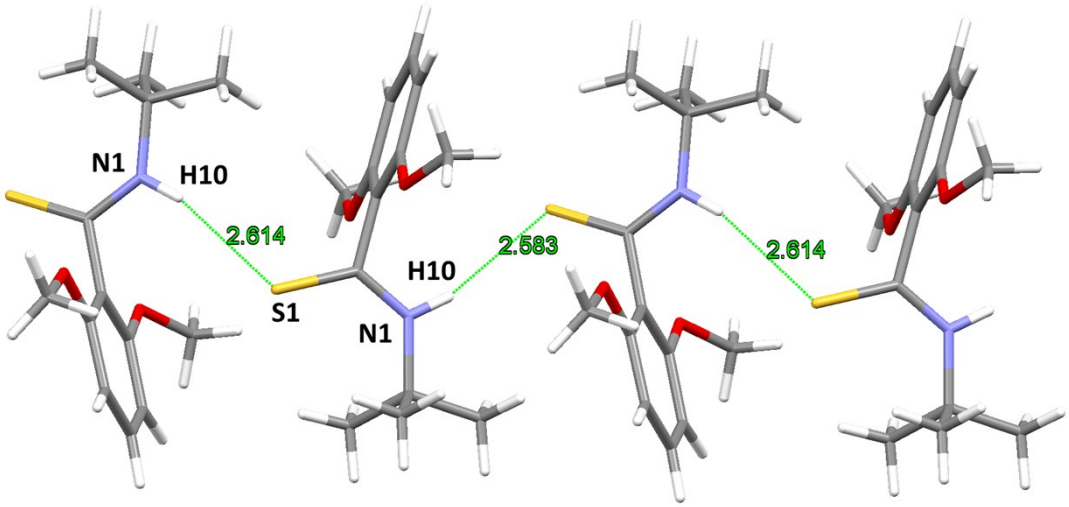


Figure S34 Mercury diagrams (capped stick) for the intermolecular hydrogen bonded linear chain of **6d**

X-Ray data refinement for 2,6-dimethoxy-N-phenylbenzothioamide,6e

The structure was solved by direct methods using SHELXT running within the WinGX[20] package. All non-hydrogen atoms were refined anisotropically. The structure was solved in the orthorhombic space group Pbca and refined to an R_1 value of 2.9%.

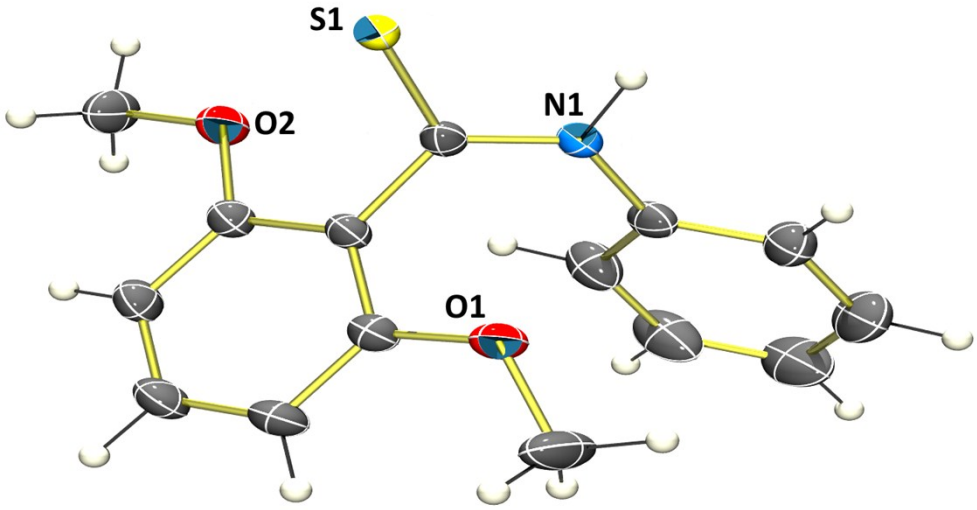


Figure S35 ORTEP-3 representations of the molecular structures of **6e**. The thermal ellipsoids are shown at the 50% probability level.

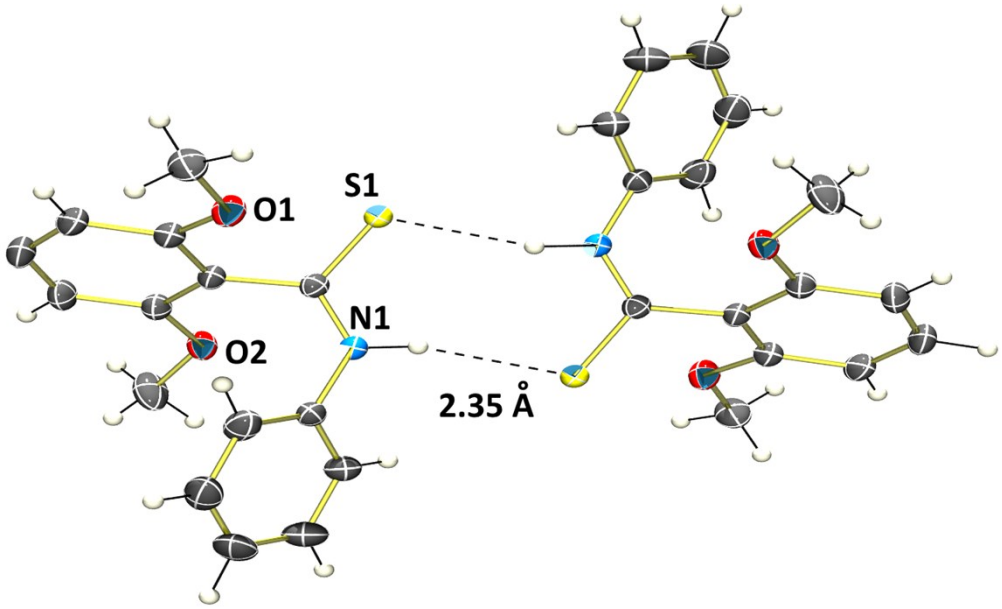


Figure S36 ORTEP-3 representations of the intermolecular hydrogen bonded arrangement for **6e**. The thermal ellipsoids are shown at the 50% probability level.

X-Ray data refinement for 2,6-dimethoxy-N-(4-chlorophenyl)benzothioamide, 6f

The structure was solved by direct methods using SHELXT running within the WinGX[20] package. All non-hydrogen atoms were refined anisotropically. The structure was solved in the triclinic space group *P-1* and refined to an R_1 value of 3.2%.

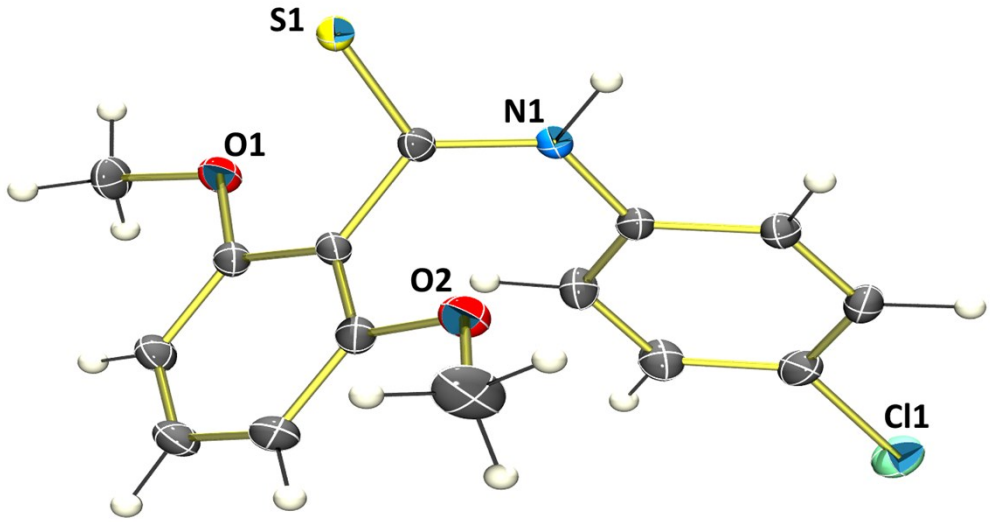


Figure S37 ORTEP-3 representations of the molecular structures of **6f**. The thermal ellipsoids are shown at the 50% probability level.

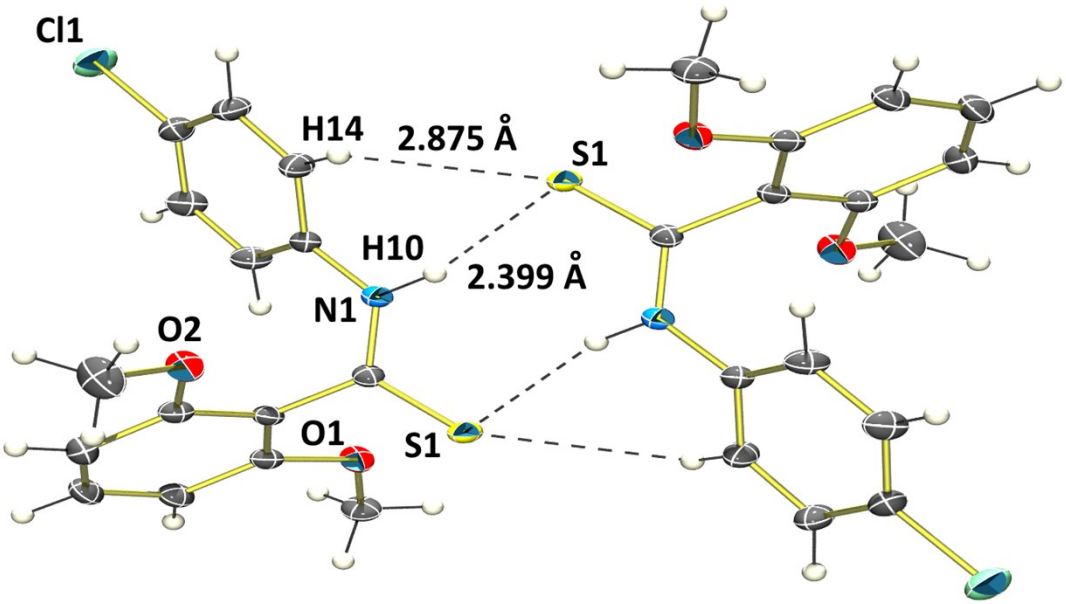


Figure S38 ORTEP-3 representations of the intermolecular hydrogen bonded arrangement for **6f**. The thermal ellipsoids are shown at the 50% probability level**.**

X-Ray data refinement for 2,6-dimethoxy-N-(4-trifluorophenyl)benzothioamide,6g

The structure was solved by direct methods using SHELXT running within the WinGX[20] package. All non-hydrogen atoms were refined anisotropically. The structure was solved in the monoclinic space group $P2_1/n$and refined to an R_1 value of 3.2%.

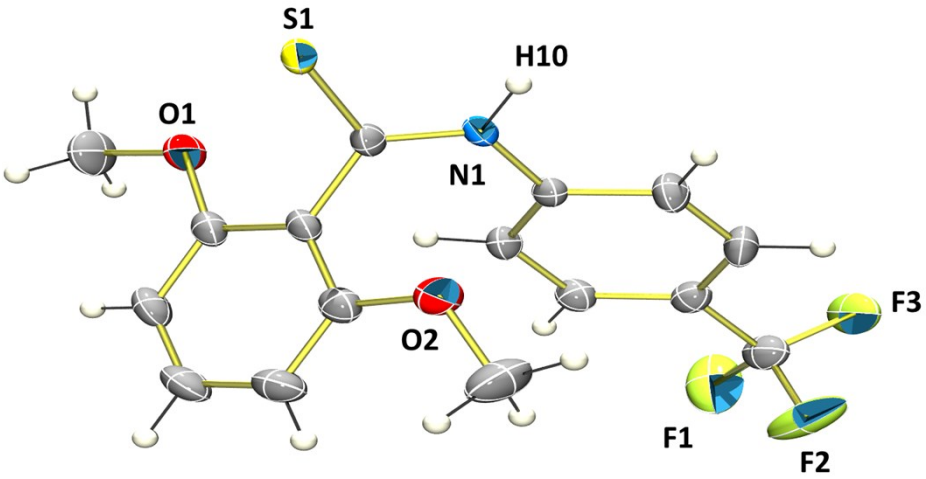


Figure S39 ORTEP-3 representations of the molecular structures of **6g**. The thermal ellipsoids are shown at the 50% probability level.

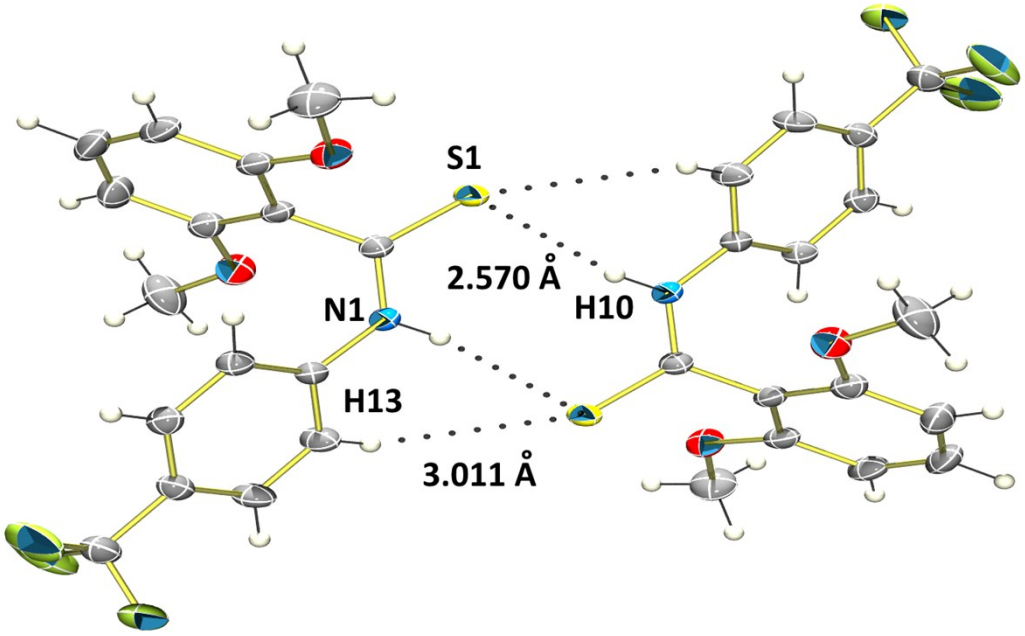


Figure S40 ORTEP-3 representations of the intermolecular hydrogen bonded arrangement for **6g**. The thermal ellipsoids are shown at the 50% probability level.

Crystallographic Data

Table S2. Crystal data and structure refinement for 6a

CCDC	1468845
Empirical formula	$C_{10}H_{13}NO_2S$
Formula weight	211.27
Temperature	130.00(10) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	a = 15.1567(2) Å, α = 90°.
	b = 8.34180(10) Å, β = 90°.
	c = 8.61660(10) Å, γ = 90°.
Volume	1089.43(2) $Å^3$
Z	4
Density (calculated)	1.288 Mg/m^3
Absorption coefficient	2.445 mm^{-1}
F(000)	448
Crystal size	0.723 x 0.431 x 0.358 mm^3
Theta range for data collection	6.055 to 77.001°.
Index ranges	-19<=h<=12, -9<=k<=10, -10<=l<=10
Reflections collected	8872
Independent reflections	2220 [R(int) = 0.0248]
Completeness to theta = 67.684°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.57275
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2220 / 1 / 179
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0251, wR2 = 0.0658
R indices (all data)	R1 = 0.0252, wR2 = 0.0659
Absolute structure parameter	0.003(7)
Extinction coefficient	n/a
Largest diff. peak and hole	0.179 and -0.261 $e.Å^{-3}$

Table S3. Crystal data and structure refinement for 6b

CCDC	1468846
Empirical formula	$C_{11}H_{15}NO_2S$
Formula weight	225.30
Temperature	130.00(10) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 7.0891(2) Å, α = 90°.
	b = 17.2751(3) Å, β = 106.161(2)°.
	c = 10.1191(2) Å, γ = 90°.
Volume	1190.26(5) $Å^3$
Z	4
Density (calculated)	1.257 Mg/m^3
Absorption coefficient	2.268 mm^{-1}
F(000)	480
Crystal size	0.982 x 0.314 x 0.118 mm^3
Theta range for data collection	5.121 to 77.096°.
Index ranges	-8<=h<=8, -19<=k<=21, -12<=l<=10
Reflections collected	10054
Independent reflections	2503 [R(int) = 0.0379]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.48261
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2503 / 0 / 196
Goodness-of-fit on F^2	1.073
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0951
R indices (all data)	R1 = 0.0359, wR2 = 0.0964
Extinction coefficient	n/a
Largest diff. peak and hole	0.332 and -0.365 $e.Å^{-3}$

Table S4. Crystal data and structure refinement for 6d

CCDC	1468847
Empirical formula	$C_{13}H_{19}NO_2S$
Formula weight	253.35
Temperature	130 K
Wavelength	1.54184 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 10.1980(4) Å, □= 73.111(5)°.
	b = 10.3995(6) Å, □= 81.002(4)°.
	c = 14.5146(7) Å, □ = 73.607(4)°.
Volume	1408.41(13) $Å^3$
Z	4
Density (calculated)	1.195 Mg/m^3
Absorption coefficient	1.969 mm^{-1}
F(000)	544
Crystal size	0.414 x 0.253 x 0.142 mm^3
Theta range for data collection	3.192 to 76.988°.
Index ranges	-11<=h<=12, -12<=k<=13, -18<=l<=17
Reflections collected	12929
Independent reflections	5879 [R(int) = 0.0266]
Completeness to theta = 67.684°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.90488
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5879 / 0 / 435
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0363, wR2 = 0.0954
R indices (all data)	R1 = 0.0435, wR2 = 0.1010
Extinction coefficient	n/a
Largest diff. peak and hole	0.282 and -0.334 $e.Å^{-3}$

Table S5. Crystal data and structure refinement for 6e

CCDC	1468848
Empirical formula	$C_{15}H_{15}NO_2S$
Formula weight	273.34
Temperature	129.95(11) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	P b c a
Unit cell dimensions	a = 13.0843(2) Å, α = 90°.
	b = 12.4311(2) Å, β = 90°.
	c = 17.6208(2) Å, γ = 90°.
Volume	2866.06(7) $Å^3$
Z	8
Density (calculated)	1.267 Mg/m^3
Absorption coefficient	1.984 mm^{-1}
F(000)	1152
Crystal size	0.280 x 0.123 x 0.096 mm^3
Theta range for data collection	5.020 to 76.924°.
Index ranges	-16<=h<=16, -15<=k<=14, -22<=l<=22
Reflections collected	29121
Independent reflections	3026 [R(int) = 0.0332]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.86861
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3026 / 0 / 232
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0298, wR2 = 0.0795
R indices (all data)	R1 = 0.0343, wR2 = 0.0842
Extinction coefficient	n/a
Largest diff. peak and hole	0.272 and -0.194 $e.Å^{-3}$

Table S6. Crystal data and structure refinement for 6f

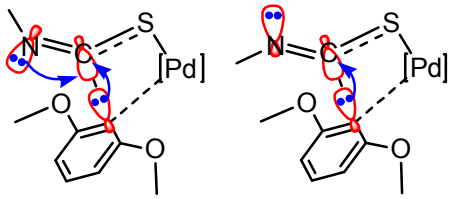
CCDC	1468849
Empirical formula	$C_{15}H_{14}ClNO_2S$
Formula weight	307.78
Temperature	130 K
Wavelength	1.54184 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 7.7838(2) Å, α = 76.510(3)°.
	b = 13.8454(5) Å, β = 76.082(3)°.
	c = 14.3496(5) Å, γ = 83.060(2)°.
Volume	1456.20(9) $Å^3$
Z	4
Density (calculated)	1.404 Mg/m^3
Absorption coefficient	3.667 mm^{-1}
F(000)	640
Crystal size	0.441 x 0.371 x 0.24 mm^3
Theta range for data collection	3.247 to 76.953°.
Index ranges	-8<=h<=9, -17<=k<=17, -18<=l<=17
Reflections collected	13965
Independent reflections	6079 [R(int) = 0.0199]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.88076
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6079 / 0 / 473
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0322, wR2 = 0.0829
R indices (all data)	R1 = 0.0337, wR2 = 0.0841
Extinction coefficient	n/a
Largest diff. peak and hole	0.285 and -0.353 $e.Å^{-3}$

Table S7. Crystal data and structure refinement for 6g

CCDC	1468850
Empirical formula	$C_{16}H_{14}F_3NO_2S$
Formula weight	341.34
Temperature	130.00(10) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 11.2091(2) Å, α = 90°.
	b = 7.59230(10) Å, β = 90.543(2)°.
	c = 18.4855(3) Å, γ = 90°.
Volume	1573.10(4) $Å^3$
Z	4
Density (calculated)	1.441 Mg/m^3
Absorption coefficient	2.210 mm^{-1}
F(000)	704
Crystal size	0.492 x 0.360 x 0.226 mm^3
Theta range for data collection	4.594 to 76.906°.
Index ranges	-14<=h<=12, -9<=k<=7, -22<=l<=23
Reflections collected	14080
Independent reflections	3294 [R(int) = 0.0221]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.80174
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3294 / 0 / 264
Goodness-of-fit on F^2	0.925
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0854
R indices (all data)	R1 = 0.0345, wR2 = 0.0874
Extinction coefficient	n/a
Largest diff. peak and hole	0.285 and -0.358 $e.Å^{-3}$

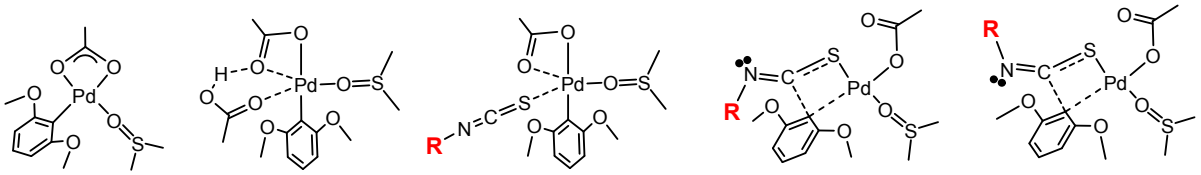
7 DFT calculated mechanisms for solution phase reactions: decarboxylation; insertion and protonation

Scheme S2: Orbital interaction scheme showing the presence of the interference from the interaction of the lone pair on N with the carbon of RNCS in $TS_{15\text{-}16'}$ and the absence of the corresponding interference in $TS_{15\text{-}16}$.



$TS_{15\text{-}16'}$ $TS_{15\text{-}16}$

Scheme S3. Calculated relative energies of vital transition structures for competition between protonation and insertion starting from **14** + $(AcOH)_2$ + RNCS where the R substituents are Ph, Me, Et, *i*Pr, and *t*Bu. The relative Gibbs and enthalpy energies (in parentheses) are given in kcal/mol and were calculated at the B3LYP-D3BJ/BS3//M06/BS1 level of theory in DMSO using the CPCM approach.



14 $TS_{14\text{-}17}$ $TS_{14\text{-}15}$ $TS_{15\text{-}16}$ $TS_{15\text{-}16'}$

R					
Ph	0.0 (0.0)	14.6 (8.7)	13.1 (2.0)	10.6 (-1.2)	12.2 (2.5)
Me	0.0 (0.0)	14.6 (8.7)	13.5 (2.8)	11.5 (0.4)	14.3 (5.1)
Et	0.0 (0.0)	14.6 (8.7)	12.6 (3.2)	11.4 (0.9)	13.8 (4.4)
iPr	0.0 (0.0)	14.6 (8.7)	13.7 (3.0)	11.2 (0.1)	16.1 (4.8)
tBu	0.0 (0.0)	14.6 (8.7)	13.7 (3.1)	14.4 (3.4)	16.3 (4.8)

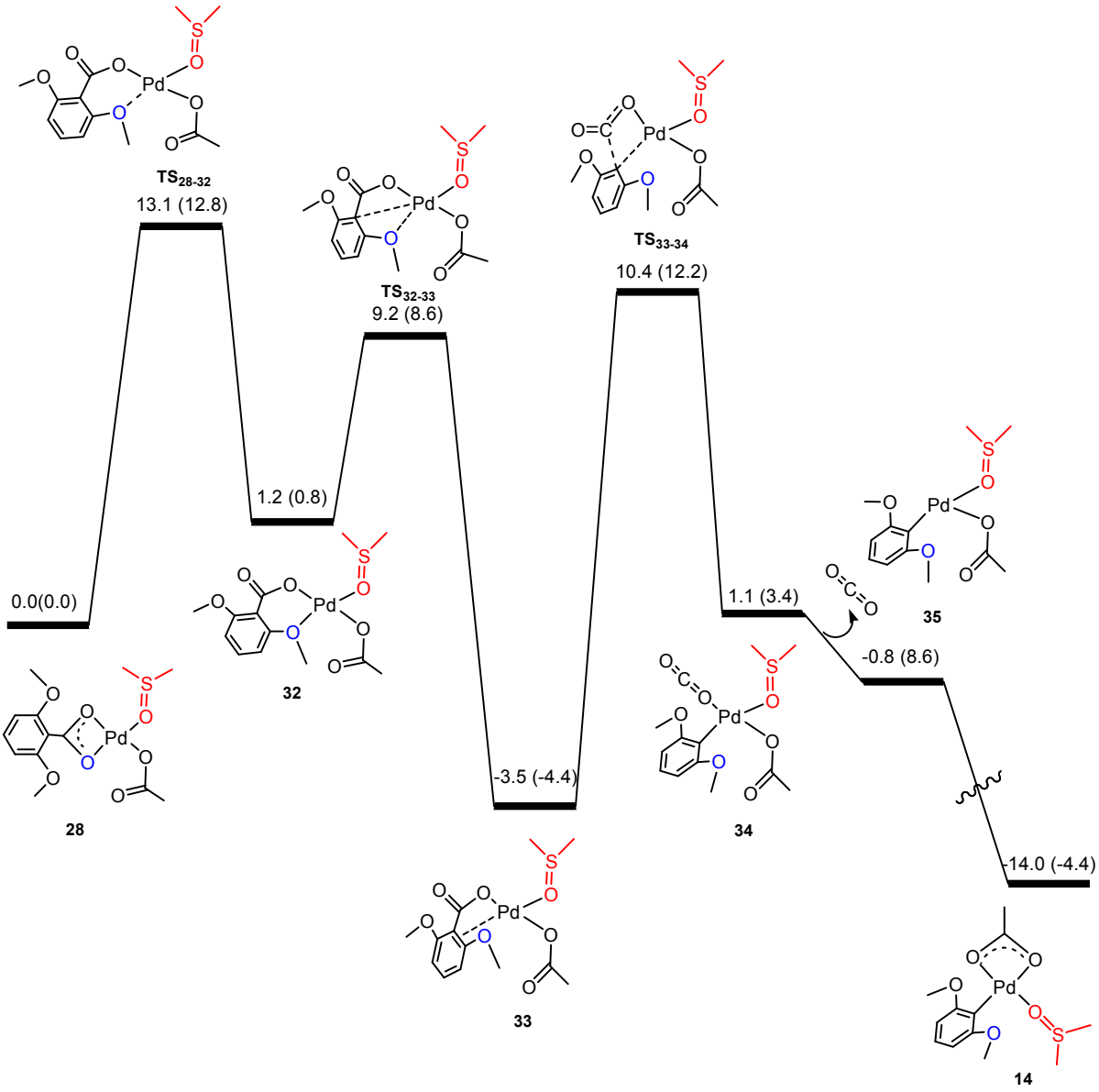


Figure S41: DFT calculated potential energy diagram for decarboxylation via trans intermediate, **2**. The relative Gibbs and enthalpy energies (in parentheses) are given in kcal/mol and were calculated at the B3LYP-D3BJ/BS3//M06/BS1 level of theory in DMSO using the CPCM approach.

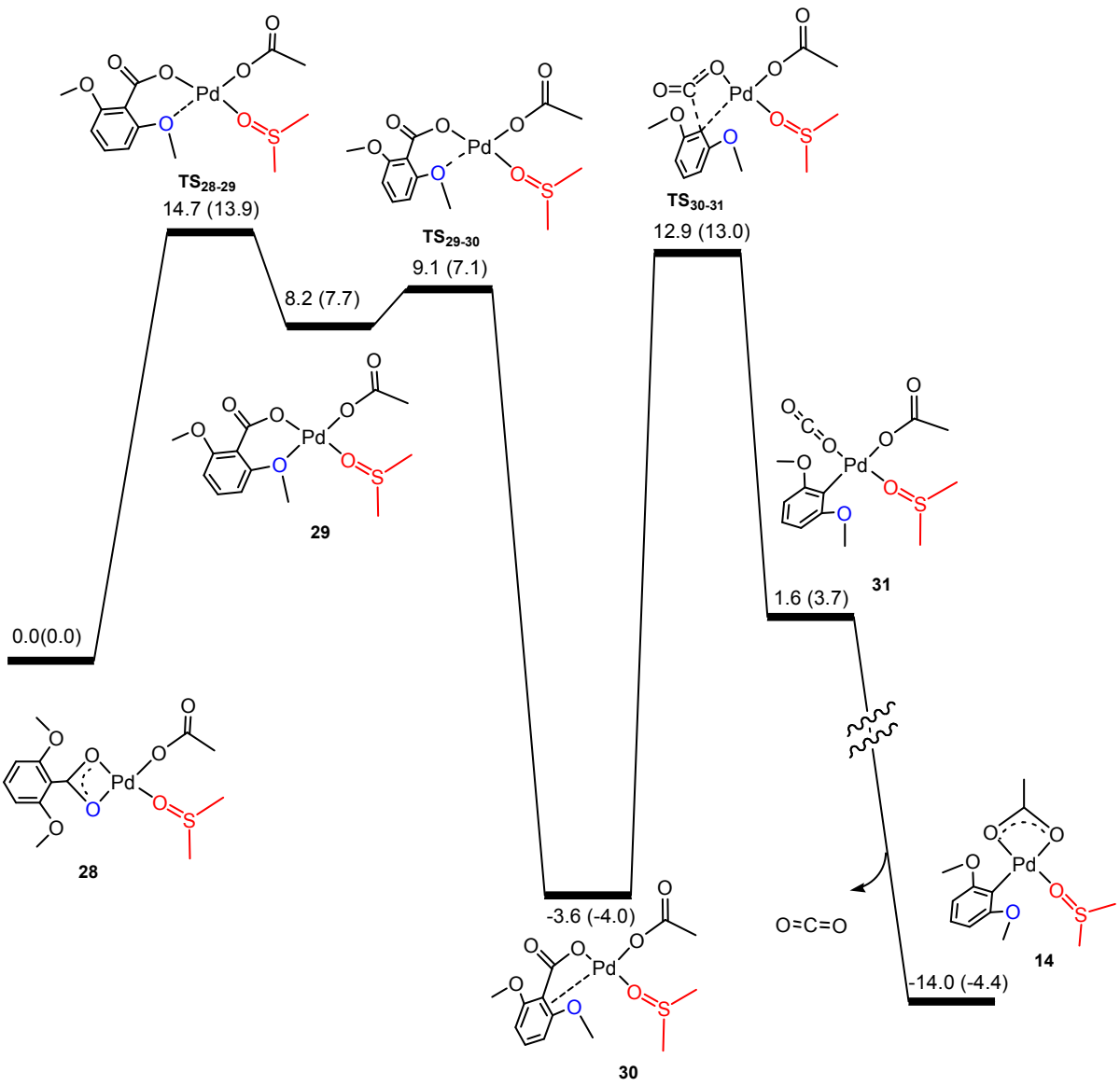


Figure S42: DFT calculated potential energy diagram for decarboxylation via trans intermediate, **2a**. The relative Gibbs and enthalpy energies (in parentheses) are given in kcal/mol and were calculated at the B3LYP-D3BJ/BS3//M06/BS1 level of theory in DMSO using the CPCM approach.

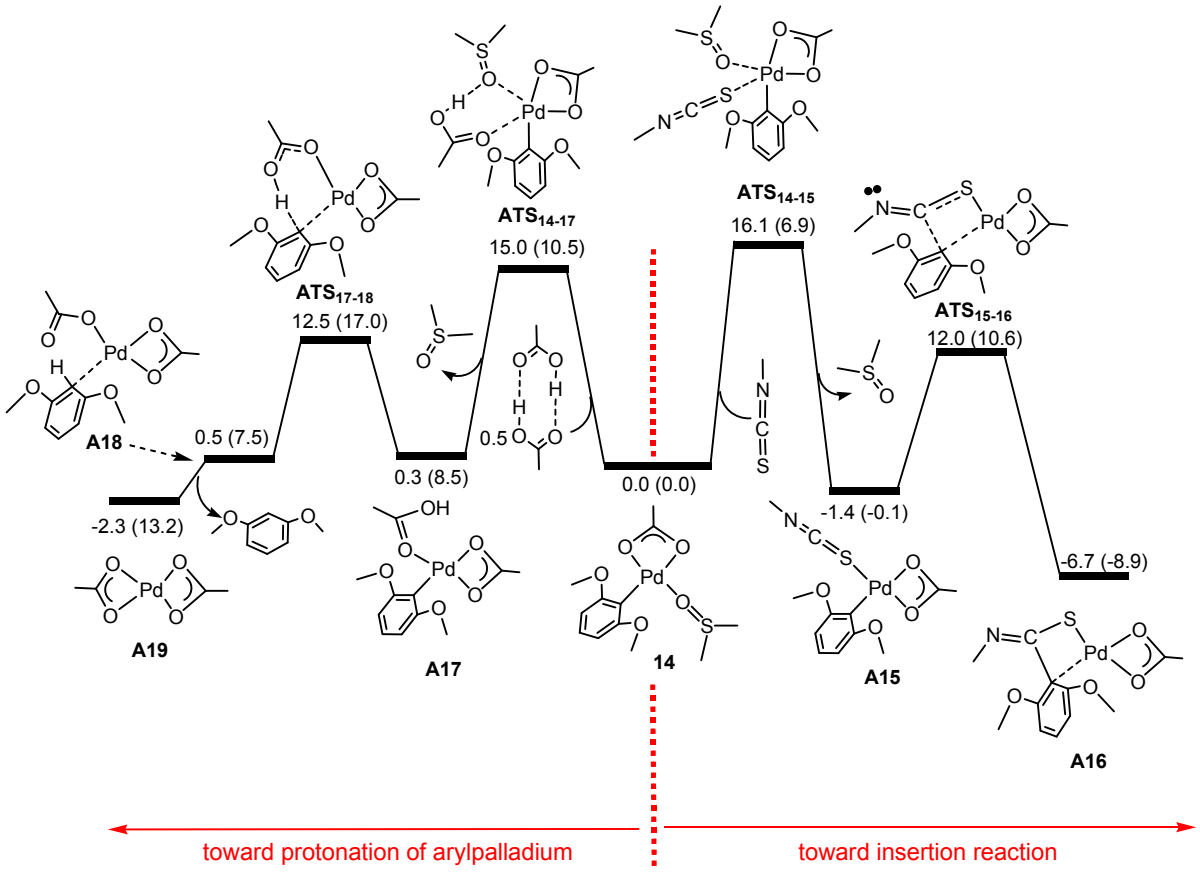


Figure S43: DFT calculated potential energy diagram for competition between protonation and insertion via intermediate, **14** involving ligand substitution in which the coordinated DMSO ligand is exchanged. The relative Gibbs and enthalpy energies (in parentheses) are given in kcal/mol and were calculated at the B3LYP-D3BJ/BS3//M06/BS1 level of theory in DMSO using the CPCM approach.

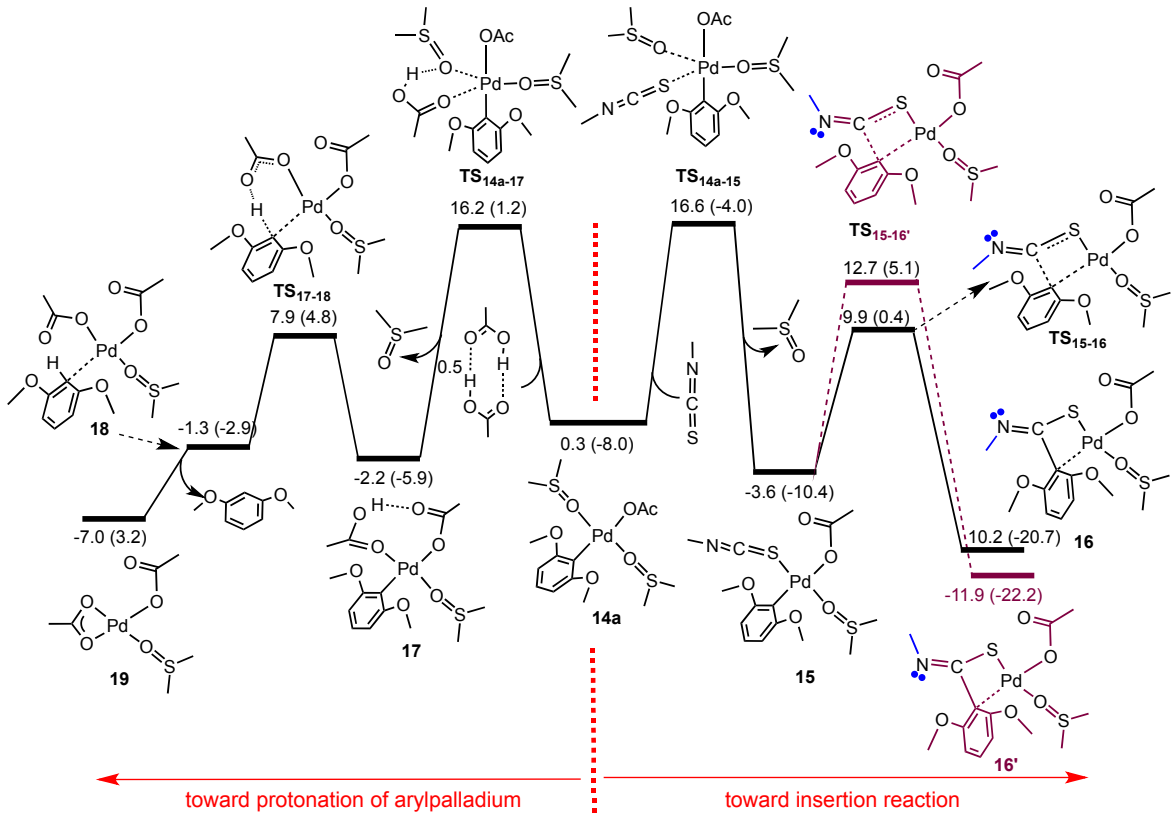
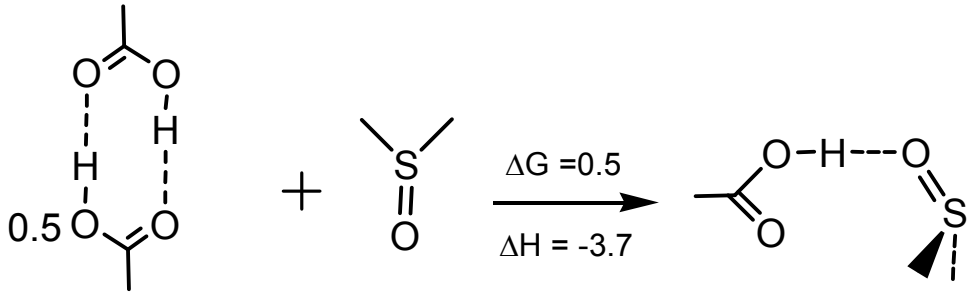


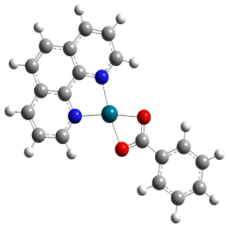
Figure S44: DFT calculated potential energy diagram for competition between protonation and insertion [$(DMSO)_2Pd(O_2CCH_3)(Ar)$], **14a** involving ligand substitution in which one of the coordinated DMSO ligand is exchanged. The relative Gibbs and enthalpy energies (in parentheses) are given in kcal/mol and were calculated at the B3LYP-D3BJ/BS3//M06/BS1 level of theory in DMSO using the CPCM approach.

Scheme S4: DFT calculated eneregtics associated with the equilibrium between the acetic acid homodimer and the 1:1 complex between DMSO and acetic acid. The relative Gibbs and enthalpy energies (in parentheses) are given in kcal/mol and were calculated at the B3LYP-D3BJ/BS3//M06/BS1 level of theory in DMSO using the CPCM approach.



8 Cartesian coordinates associated with M06/BS2 DFT calculated species (all energies are in Hartrees).

[(phen)Pd(O_2CPh)]$^+$ Decarboxylation (Figure 1B)



7

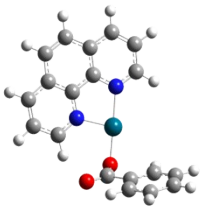
E = -1118.9063565

H = -1118.607748

G = -1118.674919

N	1.41585400	-1.32303300	-0.00097900
C	2.63005000	-0.71028400	-0.00065200
C	3.83972600	-1.42214200	0.00005700
C	3.74932300	-2.83026800	0.00072400
C	2.51047100	-3.43677900	0.00075700
C	1.34908800	-2.64671300	-0.00014800
Pd	-0.14613300	-0.00006400	-0.00104400
H	4.65925600	-3.42941200	0.00130300
H	2.41383500	-4.51915300	0.00145600
H	0.35101400	-3.08360200	-0.00026000
N	1.41576600	1.32303800	-0.00095600
C	1.34893600	2.64671400	-0.00006500
C	2.51028300	3.43683800	0.00089300
C	3.74916800	2.83039600	0.00084100
C	3.83964600	1.42227500	0.00011400
C	2.63000600	0.71035700	-0.00063100
H	0.35084300	3.08356000	-0.00018100
H	2.41359400	4.51920800	0.00164700
H	4.65907100	3.42958600	0.00145300
C	5.06677800	0.68152600	0.00027400
C	5.06681700	-0.68133000	0.00024500

H	6.00589900	1.23290600	0.00051500
H	6.00596800	-1.23265900	0.00046100
O	-1.87806300	-1.08709400	0.00152900
O	-1.87803600	1.08682200	0.00146000
C	-2.56692400	-0.00014400	0.00174500
C	-4.02175100	-0.00001500	0.00125300
C	-4.71600100	1.21604600	0.00053600
C	-4.71611700	-1.21601100	0.00089600
C	-6.10379600	1.21172400	-0.00049100
H	-4.16083200	2.15205200	0.00070100
C	-6.10390800	-1.21157900	-0.00012400
H	-4.16101800	-2.15206100	0.00135000
C	-6.79543300	0.00010500	-0.00082500
H	-6.65100900	2.15216100	-0.00107800
H	-6.65119800	-2.15196800	-0.00041800
H	-7.88401700	0.00015800	-0.00168000



TS7-8

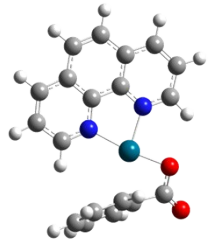
E = -1118.8467541

H = -1118.55017

G =-1118.617651

C	2.18007000	1.57286400	-1.56286100
H	-4.41194800	4.52766400	1.73350300
C	-3.83127100	3.61665000	1.59658400
C	-2.77858900	3.61983400	0.62502600
C	-4.10398300	2.50610800	2.33779700
C	-2.03178600	2.44513100	0.44701200
C	-2.42519800	4.73096100	-0.17211900
C	-3.34619600	1.30237400	2.16943600
H	-4.90629100	2.51709100	3.07381100
N	-1.00910000	2.37183600	-0.45051900

C	-2.31247300	1.28629000	1.21720600
C	-1.38216900	4.63031300	-1.06549900
H	-2.97812700	5.66403200	-0.06902600
C	-3.56186800	0.11379400	2.89829300
C	-0.67375100	3.42075000	-1.18979100
N	-1.53732000	0.18950900	0.98821100
H	-1.08291700	5.47269500	-1.68352000
C	-2.77072400	-0.98943500	2.65703000
H	-4.35256600	0.07596800	3.64668800
H	0.18670700	3.30450300	-1.85427800
C	-1.75864700	-0.91588300	1.68712500
H	-2.91495800	-1.91805700	3.20269600
H	-1.11687600	-1.76995200	1.47427500
Pd	-0.13330100	0.54115200	-0.48965900
C	3.24751300	0.80916500	-0.86904200
C	3.15622700	-0.58050600	-0.69262700
C	4.35474800	1.50099000	-0.36555900
C	4.14953700	-1.26267100	0.00396500
H	2.33566500	-1.12969200	-1.15437900
C	5.34546000	0.81635000	0.32446000
H	4.41598700	2.57615800	-0.52265700
C	5.24154800	-0.56448200	0.51309300
H	4.08405800	-2.34187000	0.12953900
H	6.20544100	1.35498700	0.71787500
H	6.02533400	-1.09791800	1.04826500
O	1.11929100	0.84925900	-1.95484900
O	2.23448200	2.77745300	-1.75048200



8

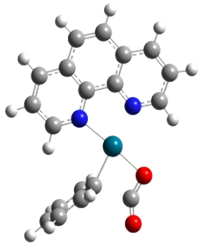
E = -1118.8839801

H = -1118.585943

G = -1118.652919

C	-2.82700800	-1.87125500	0.16732700
H	5.60897700	-0.23328800	0.27795500
C	4.57237800	0.09288000	0.20797800
C	3.54565900	-0.90127200	0.11575600
C	4.26330400	1.41930600	0.21473700
C	2.20949000	-0.47927600	0.01773000
C	3.77821500	-2.29365800	0.12328900
C	2.90440500	1.86521100	0.12603700
H	5.04922100	2.16904200	0.29387100
N	1.18051600	-1.36016300	-0.06356500
C	1.88075300	0.90658700	0.01668300
C	2.71627400	-3.16909800	0.04208200
H	4.79906100	-2.66683800	0.19777900
C	2.51622200	3.22063200	0.15105700
C	1.40806800	-2.66522500	-0.05102100
N	0.56051700	1.24179300	-0.07548200
H	2.86983800	-4.24490900	0.05017400
C	1.17939500	3.54559500	0.07764500
H	3.27519300	3.99757900	0.23661900
H	0.53048300	-3.30973100	-0.11134800
C	0.22448900	2.52349900	-0.03748900
H	0.84840200	4.58045400	0.10330600
H	-0.83997400	2.74963800	-0.10025500
Pd	-0.65710500	-0.45187600	-0.22373000
C	-2.97637400	-0.36899700	0.11914600
C	-2.70861600	0.31740100	-1.09513000
C	-3.44518700	0.34720800	1.24276100
C	-2.96873400	1.70153500	-1.18057400
H	-2.51646600	-0.25131900	-2.00748300
C	-3.66466300	1.70496300	1.14284900
H	-3.66680000	-0.19943600	2.15812100
C	-3.43720400	2.38185100	-0.07388200
H	-2.83285300	2.21365700	-2.13188700
H	-4.04593200	2.25669700	2.00017200
H	-3.66216400	3.44526200	-0.14388400

O	-1.61738600	-2.19744600	-0.24933200
O	-3.68293700	-2.62246400	0.55931500



TS8-9

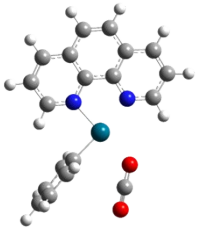
E = -1118.8636726

H = -1118.567704

G = -1118.636125

C	2.71791200	-2.01070200	-0.01535700
H	-5.70861000	0.53102100	0.01956100
C	-4.62911900	0.67493900	0.01251500
C	-3.78384900	-0.48094300	0.01013400
C	-4.09938200	1.92858200	0.00582200
C	-2.38846600	-0.30365500	0.00121400
C	-4.26262900	-1.80810900	0.01612000
C	-2.68140600	2.13325300	-0.00303700
H	-4.74793600	2.80353700	0.00729300
N	-1.52254000	-1.34886500	-0.00199600
C	-1.83018400	1.01206600	-0.00463800
C	-3.37030500	-2.85803900	0.01276600
H	-5.33674400	-1.99069400	0.02327000
C	-2.07410800	3.40603100	-0.01016400
C	-1.99204900	-2.58667300	0.00356500
N	-0.47074200	1.12675600	-0.01146000
H	-3.71175600	-3.88975600	0.01707800
C	-0.70019000	3.50510400	-0.01764900
H	-2.69730100	4.29975000	-0.00968600
H	-1.25322500	-3.38783500	0.00065300
C	0.07555200	2.33678800	-0.01754900
H	-0.20330600	4.47168800	-0.02348000
H	1.16339100	2.38320800	-0.02276700

Pd	0.49350700	-0.70232100	-0.00850600
C	2.47021400	-0.10606700	-0.00088400
C	2.96625600	0.38274800	1.22949800
C	2.98409600	0.41179600	-1.21195400
C	3.97884900	1.33033200	1.24560600
H	2.57328200	-0.01402300	2.16687600
C	3.99698000	1.35855600	-1.18992400
H	2.60510300	0.03714500	-2.16401600
C	4.49334200	1.80981600	0.03730700
H	4.37893000	1.69230400	2.19087300
H	4.41157400	1.74191700	-2.12043100
H	5.29869100	2.54261800	0.05199900
O	1.55236500	-2.44564700	-0.00510800
O	3.85394300	-2.32613900	-0.02890700



9

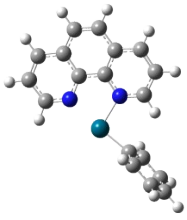
E = -1118.8906052

H = -1118.593255

G = -1118.66482

C	2.94646700	-2.42672100	-0.00061200
H	-5.79035900	0.12632400	0.00083600
C	-4.72779600	0.36540100	0.00060200
C	-3.78434500	-0.71040400	0.00063700
C	-4.30746800	1.65829200	0.00026300
C	-2.40382800	-0.42475400	0.00023500
C	-4.16329900	-2.06907100	0.00101300
C	-2.91229400	1.97975200	-0.00005200
H	-5.02629200	2.47643900	0.00022600
N	-1.46147400	-1.40219800	0.00011000
C	-1.96009300	0.93983000	-0.00008800
C	-3.19647400	-3.04910300	0.00099600

H	-5.22130000	-2.32957800	0.00129700
C	-2.43591600	3.30596600	-0.00036200
C	-1.84478200	-2.66892100	0.00048800
N	-0.61863000	1.19803100	-0.00042100
H	-3.45947400	-4.10368700	0.00128400
C	-1.08071200	3.54417000	-0.00065700
H	-3.14828900	4.13029600	-0.00035400
H	-1.05069400	-3.41534800	0.00031100
C	-0.19459000	2.45815500	-0.00068200
H	-0.68100400	4.55474400	-0.00088700
H	0.88263500	2.60979100	-0.00092700
Pd	0.53511500	-0.51413900	-0.00089900
C	2.26186900	0.45951600	0.00020300
C	2.88411800	0.74061500	1.21582700
C	2.88531800	0.74128700	-1.21466400
C	4.16540500	1.29921000	1.20900500
H	2.38833200	0.52862900	2.16499500
C	4.16656500	1.29990500	-1.20632100
H	2.39040400	0.52985400	-2.16441400
C	4.80479400	1.57256000	0.00173900
H	4.66232300	1.51556400	2.15378000
H	4.66439300	1.51682700	-2.15048600
H	5.80459600	2.00250400	0.00235200
O	1.76759400	-2.38496000	-0.00130300
O	4.09647400	-2.50965200	0.00006500



10

E = -930.3625207

H = -930.082701

G = -930.146300

N	-1.38609500	-1.46361200	0.00889800

C	-2.14142900	-0.33374200	0.00223500
C	-3.55142000	-0.37127500	0.00895200
C	-4.16738100	-1.64024100	0.02285200
C	-3.39053200	-2.77611500	0.02915800
C	-1.99312000	-2.64084200	0.02183800
Pd	0.75234300	-0.92831500	0.00445600
H	-5.25476700	-1.70755400	0.02838000
H	-3.83495700	-3.76791200	0.04011900
H	-1.35038200	-3.52072300	0.02673700
N	-0.10630500	0.96839100	-0.01916700
C	0.52785700	2.13744900	-0.03749400
C	-0.16001600	3.35814900	-0.04761900
C	-1.53571900	3.35195400	-0.03874600
C	-2.23029200	2.12580400	-0.02159500
C	-1.47030600	0.93725300	-0.01272700
H	1.61468500	2.10439800	-0.04449300
H	0.40581400	4.28592500	-0.06195700
H	-2.09959100	4.28422100	-0.04551400
C	-3.65944600	2.05147600	-0.01354300
C	-4.29538400	0.85060900	0.00120400
H	-4.22653200	2.98121400	-0.01980900
H	-5.38305600	0.79671200	0.00696600
H	2.76398700	-0.41857700	-2.15830500
C	3.28142900	-0.26725000	-1.20950800
C	4.66205900	-0.05193200	-1.18909100
C	2.60141000	-0.29691900	0.00469100
C	5.31873300	0.17018200	0.01959400
C	3.22847300	-0.03627600	1.22015300
C	4.60872200	0.17840800	1.21906400
H	2.66812300	-0.01374900	2.15624800
H	5.21842700	-0.04743200	-2.12516600
H	5.12386200	0.35918000	2.16137200
H	6.39158100	0.35319100	0.02580000

CO_2

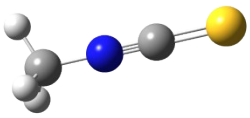
E = -188.5096102

H = -188.494117

G = -188.518367

C	0.00000000	0.000000000.00000000	
O	0.00000000	0.00000000	1.16416200
O	0.00000000	0.00000000	-1.16416200

[(phen)Pd(Ph)]$^{+}$ + MeNCS (Figure 1D)



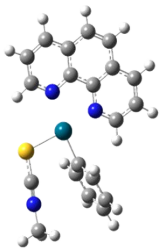
MeNCS

E = -530.8268768

H = -530.772767

G = -530.808123

C	0.00000000	0.00000000	0.19030500
N	0.00000000	0.00000000	-0.99146600
C	0.00000000	0.00000000	-2.39776100
H	0.00000000	1.02862500	-2.77923300
H	0.89081500	-0.51431200	-2.77923300
H	-0.89081500	-0.51431200	-2.77923300
S	0.00000000	0.00000000	1.78266900



11A

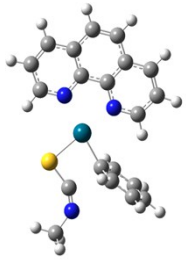
E = -1461.2443366

H = -1460.907278

G = -1460.982938

C	-3.14181600	-1.96822900	-0.04883400
H	6.07411300	-0.11365700	-0.06476800
C	5.02615300	0.18289100	-0.05215600
C	4.02642000	-0.84065800	-0.02978600
C	4.67715300	1.49647300	-0.05742100
C	2.66178800	-0.48219500	-0.01205700
C	4.33761300	-2.21561200	-0.02439900
C	3.30183500	1.89250900	-0.04066500
H	5.43950500	2.27416800	-0.07507600
N	1.66970300	-1.41000500	0.01050300
C	2.29341100	0.90623200	-0.01842200
C	3.32223200	-3.14462400	-0.00364400
H	5.38136900	-2.52816700	-0.03711000
C	2.89745500	3.24253100	-0.04524600
C	1.99367500	-2.69401600	0.01327100
N	0.96968200	1.23040100	-0.00269000
H	3.52913500	-4.21162000	0.00006400
C	1.55667500	3.55051700	-0.02705700
H	3.65273600	4.02763100	-0.06340900
H	1.16899500	-3.40691600	0.02835800
C	0.61670400	2.50987400	-0.00524400
H	1.21065700	4.58079500	-0.02900100
H	-0.45203600	2.72051100	0.00946900
S	-1.58711200	-2.44627300	0.11226000
N	-4.27116200	-1.69793700	-0.15935000
C	-5.61346700	-1.26268000	-0.27101400
H	-5.89155700	-0.70409500	0.62891500
H	-5.71279000	-0.61764200	-1.15047000
H	-6.26966300	-2.13234700	-0.37979300
Pd	-0.30283800	-0.45600300	0.03583100
C	-1.94336800	0.67669500	0.05002200
C	-2.45674300	1.15797400	-1.15538900
C	-2.49988500	1.07885500	1.26476800
C	-3.51505000	2.07068500	-1.14053200
H	-2.02949900	0.83890600	-2.10786300
C	-3.55780900	1.99243000	1.27102200

H	-2.10846300	0.69629900	2.20898800
C	-4.06273900	2.49150100	0.07097600
H	-3.90480100	2.45913700	-2.08142200
H	-3.98123500	2.31958000	2.22040500
H	-4.88108600	3.20980200	0.07993400



TS11A-12A

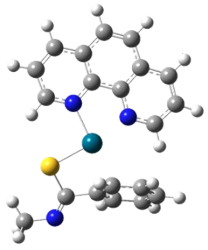
E = -1461.2123834

H = -1460.877534

G = -1460.952006

C	3.08955000	-1.27601300	-0.30064900
H	-6.07513400	-0.19078000	0.09647200
C	-5.02983800	0.11446000	0.07354100
C	-4.02375000	-0.90060000	-0.00888400
C	-4.69164100	1.43044500	0.12264900
C	-2.66418600	-0.52810300	-0.04108600
C	-4.32108700	-2.27762300	-0.05936700
C	-3.31988100	1.83881800	0.09429200
H	-5.46050200	2.19924900	0.18742600
N	-1.66283000	-1.44337100	-0.11995800
C	-2.30727100	0.86085700	0.01317700
C	-3.29620500	-3.19369300	-0.13667900
H	-5.36081700	-2.60267000	-0.03619300
C	-2.91772100	3.18872600	0.14555700
C	-1.97204500	-2.73071600	-0.16526600
N	-0.98648500	1.18560300	-0.01432500
H	-3.49217900	-4.26200700	-0.17589500
C	-1.57711200	3.50097700	0.11662800
H	-3.67331200	3.97113600	0.21012900

H	-1.14028900	-3.43196000	-0.22704900
C	-0.63671700	2.46306300	0.03637300
H	-1.23481200	4.53183800	0.15500200
H	0.43183400	2.67631400	0.01334400
S	1.73563400	-2.29431300	-0.30131800
N	4.28666200	-1.14031200	-0.34512400
C	5.42531700	-2.01854900	-0.44783400
H	5.98267000	-1.77180700	-1.35742100
H	6.08584400	-1.84414800	0.40754900
H	5.12205800	-3.07311300	-0.47362100
Pd	0.28787500	-0.52220200	-0.14820800
C	2.06849200	0.46784100	-0.14115500
C	2.51414800	0.94914000	1.10998900
C	2.44002000	1.14945400	-1.32171100
C	3.34245800	2.05968000	1.17434600
H	2.23663400	0.41383700	2.01929300
C	3.27052600	2.25775700	-1.25236900
H	2.10207800	0.77153200	-2.28786300
C	3.72877500	2.70071700	-0.00693300
H	3.70458300	2.42217900	2.13495000
H	3.57629200	2.77417500	-2.16073700
H	4.39823600	3.55833000	0.04259900



12A

E = -1461.2528148

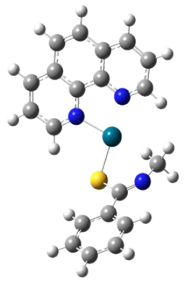
H = -1460.915305

G = -1460.988478

C	3.22422100	-0.83636400	-0.21942700
H	-5.73557300	-1.20104400	-0.33061800
C	-4.78426100	-0.67424000	-0.27114700

C	-3.58771200	-1.44255200	-0.11186500
C	-4.73556200	0.68181500	-0.35520900
C	-2.34744600	-0.77805100	-0.02520500
C	-3.58031200	-2.85008000	-0.04358300
C	-3.48741900	1.37813100	-0.28140900
H	-5.64733800	1.26329200	-0.48409500
N	-1.17586400	-1.45647600	0.11538900
C	-2.29471400	0.64767400	-0.10276500
C	-2.38491000	-3.51840900	0.09162500
H	-4.52193000	-3.39478000	-0.10459000
C	-3.38270300	2.77956800	-0.38747500
C	-1.19364500	-2.78269200	0.16476100
N	-1.07492800	1.24890300	-0.01550900
H	-2.34199500	-4.60313400	0.14041200
C	-2.14304500	3.37214200	-0.31906700
H	-4.28316200	3.37660700	-0.52749900
H	-0.23063800	-3.28300800	0.25750700
C	-1.00991400	2.56621000	-0.12782600
H	-2.02372000	4.44906400	-0.40477200
H	-0.01761100	3.00897900	-0.05715400
S	1.98760700	-1.95354700	0.44119400
N	4.31427500	-1.07411900	-0.80653200
C	4.77820300	-2.42661100	-0.99314800
H	5.21356600	-2.52414600	-1.99385600
H	5.58035900	-2.63111200	-0.27175800
H	3.98881000	-3.18574700	-0.86749700
Pd	0.49894100	-0.20452200	0.27301700
C	2.73231000	0.55955300	-0.04309300
C	2.28904800	1.01508100	1.22656600
C	2.89074000	1.49273400	-1.09770200
C	2.08619500	2.39467000	1.44147300
H	2.32947700	0.34285300	2.08434800
C	2.69132600	2.83553500	-0.86320200
H	3.24080500	1.12713400	-2.06128300
C	2.30486700	3.29119400	0.41510000
H	1.80451300	2.74336400	2.43341600

H	2.86105700	3.55607700	-1.66155800
H	2.19437500	4.36033300	0.59323200



TS12A-13A

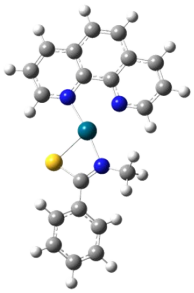
E = -1461.2147846

H = -1460.879337

G = -1460.952299

C	3.14936300	-0.18472000	-0.25211600
H	-5.44218000	-1.47943600	0.75240300
C	-4.57231600	-0.94110800	0.37886100
C	-3.31270400	-1.62200800	0.34858200
C	-4.68465200	0.34744000	-0.04317600
C	-2.17955000	-0.94096600	-0.13596000
C	-3.13547100	-2.95039900	0.78685400
C	-3.54537800	1.06107700	-0.53526800
H	-5.64558400	0.85889600	-0.01193600
N	-0.94929800	-1.53020400	-0.18382400
C	-2.29853400	0.40897200	-0.58502500
C	-1.88498800	-3.52396300	0.73435800
H	-3.99020300	-3.50974900	1.16546600
C	-3.59116700	2.39994500	-0.97681300
C	-0.80274800	-2.77952400	0.24277900
N	-1.17412900	1.02131100	-1.04088800
H	-1.71424400	-4.54400800	1.06828200
C	-2.44196500	3.00935600	-1.42992300
H	-4.53620800	2.94147600	-0.95309800
H	0.20026500	-3.19877900	0.19826700
C	-1.24313100	2.27974600	-1.44765500
H	-2.44528500	4.04066900	-1.77256100
H	-0.31656200	2.73157700	-1.80115400

S	2.28434600	-1.70704300	-0.72780100
N	3.00131800	0.91191300	-0.90427600
C	2.38933200	1.04648700	-2.20459600
H	1.82927000	1.98778200	-2.25626100
H	3.17794200	1.11518100	-2.96986100
H	1.74402900	0.19963100	-2.56592400
Pd	0.49587000	-0.28803200	-0.95764500
C	3.99558600	-0.21063800	0.95912500
C	4.06815100	-1.33121600	1.79462200
C	4.77154900	0.91834000	1.26349800
C	4.89401600	-1.32281700	2.91361000
H	3.47144300	-2.21431500	1.57294000
C	5.59049200	0.92511100	2.38317900
H	4.72227100	1.78386100	0.60689400
C	5.65399900	-0.19544600	3.21197300
H	4.94233700	-2.20110200	3.55465600
H	6.18807600	1.80601400	2.61072600
H	6.30018200	-0.18999800	4.08816800



13A

E = -1461.2787872

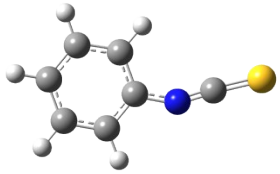
H = -1460.940208

G = -1461.012342

C	3.22422100	-0.83636400	-0.21942700
H	-5.73557300	-1.20104400	-0.33061800
C	-4.78426100	-0.67424000	-0.27114700
C	-3.58771200	-1.44255200	-0.11186500
C	-4.73556200	0.68181500	-0.35520900
C	-2.34744600	-0.77805100	-0.02520500
C	-3.58031200	-2.85008000	-0.04358300

C	-3.48741900	1.37813100	-0.28140900
H	-5.64733800	1.26329200	-0.48409500
N	-1.17586400	-1.45647600	0.11538900
C	-2.29471400	0.64767400	-0.10276500
C	-2.38491000	-3.51840900	0.09162500
H	-4.52193000	-3.39478000	-0.10459000
C	-3.38270300	2.77956800	-0.38747500
C	-1.19364500	-2.78269200	0.16476100
N	-1.07492800	1.24890300	-0.01550900
H	-2.34199500	-4.60313400	0.14041200
C	-2.14304500	3.37214200	-0.31906700
H	-4.28316200	3.37660700	-0.52749900
H	-0.23063800	-3.28300800	0.25750700
C	-1.00991400	2.56621000	-0.12782600
H	-2.02372000	4.44906400	-0.40477200
H	-0.01761100	3.00897900	-0.05715400
S	1.98760700	-1.95354700	0.44119400
N	4.31427500	-1.07411900	-0.80653200
C	4.77820300	-2.42661100	-0.99314800
H	5.21356600	-2.52414600	-1.99385600
H	5.58035900	-2.63111200	-0.27175800
H	3.98881000	-3.18574700	-0.86749700
Pd	0.49894100	-0.20452200	0.27301700
C	2.73231000	0.55955300	-0.04309300
C	2.28904800	1.01508100	1.22656600
C	2.89074000	1.49273400	-1.09770200
C	2.08619500	2.39467000	1.44147300
H	2.32947700	0.34285300	2.08434800
C	2.69132600	2.83553500	-0.86320200
H	3.24080500	1.12713400	-2.06128300
C	2.30486700	3.29119400	0.41510000
H	1.80451300	2.74336400	2.43341600
H	2.86105700	3.55607700	-1.66155800
H	2.19437500	4.36033300	0.59323200

[(phen)Pd(Ph)]$^{+}$ + PhNCS (Figure 1F)



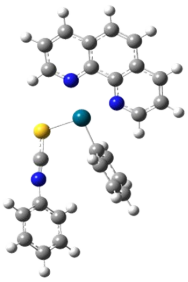
PhNCS

E = -722.4286484

H =-722.319106

G = -722.361024

C	2.06125700	-0.17446200	0.00010400
N	0.91020900	-0.49901300	0.00010700
S	3.60930700	0.14371800	-0.00007100
C	-0.44284400	-0.22241100	0.00004600
C	-1.35527000	-1.28000100	0.00003400
C	-0.89370600	1.10253800	0.00001000
C	-2.71808400	-1.00816400	-0.00002300
H	-0.98072900	-2.30155700	0.00006900
C	-2.25867500	1.35914200	-0.00004200
H	-0.16721700	1.91352000	0.00002400
C	-3.17460800	0.30810100	-0.00005100
H	-3.42878000	-1.83268400	-0.00003500
H	-2.60914100	2.38988400	-0.00006900
H	-4.24293200	0.51597600	-0.00007100



11B

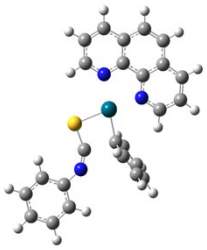
E = -1652.8402318

H = -1652.44851

G = -1652.534613

C	-2.27351100	-1.73919200	0.40882800
H	6.84040700	-0.60595100	-0.84197200
C	5.83680600	-0.21136300	-0.68856800
C	4.78156400	-1.12828800	-0.38532100
C	5.59312800	1.12259900	-0.78135800
C	3.47288000	-0.64336000	-0.17950200
C	4.98473600	-2.51901400	-0.27759100
C	4.27591000	1.64504500	-0.58241000
H	6.39740100	1.82062600	-1.01016400
N	2.43468700	-1.46750800	0.11762400
C	3.21408300	0.76534300	-0.28581000
C	3.92177500	-3.34271200	0.01627900
H	5.98359000	-2.92700100	-0.43006800
C	3.98247000	3.02048700	-0.66990800
C	2.65484000	-2.77011500	0.20724300
N	1.94124500	1.21357900	-0.09533700
H	4.04495300	-4.41911100	0.10365800
C	2.69304800	3.45523900	-0.46654800
H	4.78247100	3.72473000	-0.89662500
H	1.79201200	-3.39590700	0.43710500
C	1.69301000	2.51479700	-0.17938200
H	2.43289400	4.50898600	-0.52359200
H	0.66160500	2.82479800	-0.01422200
S	-0.81485300	-2.14513900	1.01000300
N	-3.34142000	-1.51554400	-0.01870300
Pd	0.56861800	-0.33326900	0.35757000
C	-0.96076700	0.94136700	0.48580100
C	-1.57323800	1.38451400	-0.68828400
C	-1.32337600	1.48452000	1.71810300
C	-2.52788800	2.40281300	-0.62916100
H	-1.30379000	0.95172800	-1.65401900
C	-2.27640300	2.50663800	1.76834000
H	-0.85973200	1.12996900	2.63985400
C	-2.87302900	2.97006700	0.59686800
H	-3.00106400	2.75200900	-1.54666400
H	-2.54805500	2.94143200	2.72996100

H	-3.61057900	3.77041300	0.63933900
C	-4.59696900	-1.04417800	-0.35265300
C	-5.33988500	-1.70068000	-1.33604400
C	-5.08465700	0.08885200	0.30564400
C	-6.59772100	-1.20862000	-1.66078100
H	-4.92941100	-2.58057300	-1.82697500
C	-6.34084700	0.56925600	-0.03823100
H	-4.47135900	0.57872400	1.06114400
C	-7.09667100	-0.07731600	-1.01620400
H	-7.19132100	-1.71067400	-2.42175400
H	-6.73362900	1.45194100	0.46273600
H	-8.08249100	0.30256400	-1.27717800



TS11B-12B

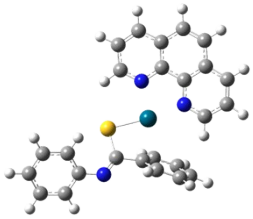
E = -1652.8096429

H = -1652.419642

G = -1652.502431

C	3.02164400	-1.39975700	-0.29620400
H	-6.08786900	-0.08684200	0.37429000
C	-5.03743200	0.18947700	0.29309800
C	-4.05854600	-0.85438400	0.25004100
C	-4.66771500	1.49663300	0.23555900
C	-2.69280400	-0.51949700	0.14386500
C	-4.38780100	-2.22387000	0.30993200
C	-3.28899800	1.86710700	0.12652300
H	-5.41625400	2.28706000	0.27139700
N	-1.71527000	-1.46248000	0.09929500
C	-2.30302000	0.86020200	0.07785000
C	-3.38673200	-3.16806300	0.26465600

H	-5.43290300	-2.52106000	0.39128200
C	-2.85455800	3.20633200	0.06252800
C	-2.05415200	-2.74156700	0.15798800
N	-0.97806000	1.14824400	-0.03082800
H	-3.60782500	-4.23128500	0.30896100
C	-1.50990500	3.48150000	-0.04507500
H	-3.58905000	4.01028400	0.09970600
H	-1.24072900	-3.46555800	0.11799500
C	-0.59788900	2.41663500	-0.09051300
H	-1.14313200	4.50333500	-0.09669100
H	0.47277000	2.59968700	-0.17796800
S	1.65982500	-2.40192400	-0.16229100
N	4.22265600	-1.28971800	-0.38550900
Pd	0.25088400	-0.59669300	-0.09073000
C	2.05706900	0.33375600	-0.29280300
C	2.57343700	0.97873200	0.85496300
C	2.35511900	0.85171600	-1.57417600
C	3.41063500	2.07517000	0.71985700
H	2.34971600	0.57305000	1.84271600
C	3.19223300	1.94962800	-1.70487900
H	1.96202000	0.34900400	-2.45902600
C	3.72900700	2.54616500	-0.55910200
H	3.83237500	2.55855900	1.59948900
H	3.44482200	2.33574900	-2.69091400
H	4.40757600	3.39174400	-0.66405500
C	5.39464100	-2.04398600	-0.41921800
C	5.36384400	-3.44015300	-0.32736100
C	6.60800500	-1.36333600	-0.54286700
C	6.55860800	-4.14830400	-0.35940800
H	4.41177300	-3.96072400	-0.22931200
C	7.79597000	-2.08267200	-0.57440800
H	6.59593200	-0.27668400	-0.61185300
C	7.77313400	-3.47339600	-0.48219800
H	6.54232200	-5.23414000	-0.28742200
H	8.74445800	-1.55790400	-0.67125300
H	8.70504000	-4.03506800	-0.50595800



12B

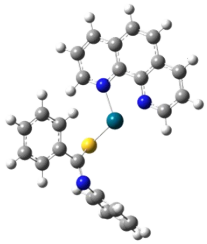
E = -1652.8471074

H = -1652.453854

G = -1652.535652

C	-2.44355400	0.62338600	0.07239500
H	5.74433300	-3.09000400	-0.39025400
C	5.05940000	-2.24465300	-0.34288200
C	3.68084800	-2.49941300	-0.05671400
C	5.50337600	-0.97788500	-0.55815300
C	2.77922900	-1.41827300	0.01619800
C	3.16527100	-3.79409100	0.15245900
C	4.60605300	0.13545600	-0.49686100
H	6.55157300	-0.78676400	-0.78404000
N	1.45448500	-1.60109300	0.26831900
C	3.24667300	-0.08405900	-0.19464100
C	1.82260200	-3.95912300	0.40549600
H	3.83491400	-4.65231700	0.10787800
C	5.01437100	1.46323300	-0.73426200
C	0.99120300	-2.83086700	0.45121000
N	2.34394200	0.93272700	-0.10889800
H	1.39042000	-4.94331300	0.56619100
C	4.08798400	2.47796200	-0.66760400
H	6.05719600	1.67056100	-0.97252600
H	-0.07798700	-2.93240300	0.63261500
C	2.75774900	2.16778800	-0.34571200
H	4.36479600	3.51235700	-0.85422000
H	2.00574500	2.95200600	-0.27095400
S	-1.65686200	-0.86442000	0.66498300
N	-3.62427300	0.85008900	-0.32105000

Pd	0.36629200	0.19536500	0.36156700
C	-1.43604000	1.72037500	0.09028500
C	-1.31512200	2.58870600	-1.02337400
C	-0.75885000	2.03890600	1.29737800
C	-0.61223000	3.76697500	-0.90250300
H	-1.85042700	2.33626500	-1.93696700
C	-0.04183100	3.25014300	1.39629800
H	-0.98759300	1.47806700	2.20463800
C	0.01086100	4.10874500	0.31709900
H	-0.56288700	4.45604400	-1.74393400
H	0.42216600	3.51919400	2.34347400
H	0.52157500	5.06679200	0.40868400
C	-4.63204500	-0.12980900	-0.38007300
C	-4.43876300	-1.38424700	-0.97110100
C	-5.89298800	0.21632100	0.11622900
C	-5.49578800	-2.28789800	-1.03574400
H	-3.47644000	-1.63514900	-1.41519800
C	-6.93451200	-0.70209800	0.07029600
H	-6.03353000	1.20928600	0.54043700
C	-6.74054700	-1.95695800	-0.50600400
H	-5.34539600	-3.25703000	-1.50929100
H	-7.90908200	-0.43110400	0.47273500
H	-7.56225200	-2.66894900	-0.55557900



TS12B-13B

E = -1652.8084724

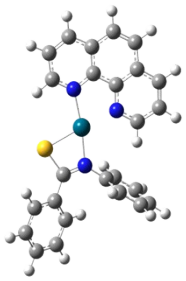
H = -1652.416805

G = -1652.497898

C	-2.36595900	0.74524100	0.15546400
H	5.75727500	-2.71817600	-1.55011600

C	5.13116800	-1.96152400	-1.07945900
C	3.73865700	-2.24441300	-0.90116100
C	5.66414500	-0.77819200	-0.67101500
C	2.91479800	-1.27355600	-0.29853400
C	3.13379700	-3.45446200	-1.29604600
C	4.84883600	0.21850800	-0.04429000
H	6.72422100	-0.57090700	-0.81067000
N	1.58135100	-1.47358100	-0.11179300
C	3.47676400	-0.03527500	0.14124300
C	1.78676900	-3.64684100	-1.08092500
H	3.73921300	-4.22923400	-1.76527700
C	5.34168700	1.45860600	0.41221800
C	1.03336900	-2.62642300	-0.48184600
N	2.64303100	0.85522300	0.73902900
H	1.29218800	-4.57148200	-1.36689000
C	4.48451200	2.35466800	1.01199000
H	6.39781000	1.69550800	0.28746000
H	-0.03383200	-2.74457500	-0.30437100
C	3.13054800	2.01245800	1.16078500
H	4.83606500	3.31690500	1.37508300
H	2.42564500	2.69441800	1.63509400
S	-1.49077400	-0.37593800	1.30698400
N	-2.96903100	1.78863700	0.57864400
Pd	0.63394000	0.13592300	0.84195300
C	-2.46047400	0.36634700	-1.26996400
C	-3.61896000	0.73153300	-1.97024400
C	-1.45254100	-0.32778400	-1.94686200
C	-3.76560900	0.39463500	-3.30958500
H	-4.40041900	1.27718500	-1.44538900
C	-1.59525500	-0.65504600	-3.29040400
H	-0.52651900	-0.57467300	-1.42878400
C	-2.75619300	-0.30075800	-3.97340400
H	-4.67320100	0.67634800	-3.84023200
H	-0.79401500	-1.17952400	-3.80938600
H	-2.87233500	-0.56105000	-5.02399100
C	-3.07860100	2.09752100	1.93019700

C	-3.51646300	1.15241400	2.87657600
C	-2.80807600	3.41060900	2.33841900
C	-3.61845700	1.50795500	4.22038700
H	-3.86373400	0.17513100	2.54191200
C	-2.88960800	3.74564500	3.68172300
H	-2.51958300	4.14313000	1.58647400
C	-3.29254000	2.79573400	4.62831300
H	-3.97370800	0.77679000	4.94432300
H	-2.65429400	4.76038500	3.99843200
H	-3.37707900	3.07496000	5.67671000



13B

E = -1652.8794095

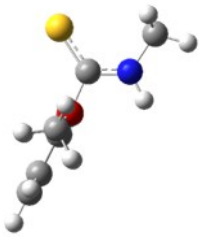
H = -1652.485281

G = -1652.565292

C	2.42771300	-0.37844800	-0.01887800
H	-6.48853600	-0.73583800	-0.87874800
C	-5.52098800	-0.38303300	-0.52426200
C	-4.33854200	-1.01388300	-1.02788400
C	-5.44103900	0.63075500	0.37959900
C	-3.08063700	-0.56921000	-0.57829300
C	-4.35577000	-2.07177500	-1.95980300
C	-4.17267200	1.10183600	0.84849900
H	-6.34434200	1.10278500	0.76375000
N	-1.91698400	-1.13080900	-1.00356500
C	-2.99449000	0.50490900	0.36055000
C	-3.16846700	-2.62405800	-2.38665700
H	-5.30954400	-2.44291800	-2.33371600
C	-4.02804900	2.14334100	1.78803800
C	-1.95895600	-2.12499300	-1.88021700

N	-1.75407300	0.90615900	0.75160400
H	-3.14878800	-3.44005200	-3.10413700
C	-2.76817900	2.52899700	2.18616600
H	-4.91564600	2.62916300	2.19223000
H	-1.00246200	-2.54022700	-2.19308800
C	-1.64691400	1.88269000	1.64085100
H	-2.62236400	3.32329900	2.91352400
H	-0.63614300	2.16930500	1.93279200
S	1.54740900	-1.52335800	-1.01803100
N	1.56883900	0.45835900	0.49400900
Pd	-0.22160200	-0.25198500	-0.17526000
C	3.88037500	-0.41880700	0.13917100
C	4.54444900	-1.63420400	-0.08503600
C	4.62851100	0.72196700	0.47319200
C	5.92460600	-1.71286600	0.03835800
H	3.96904700	-2.52288700	-0.34289800
C	6.01016100	0.63933300	0.58097800
H	4.13826400	1.68085000	0.62694000
C	6.65920800	-0.57624800	0.37052500
H	6.42869000	-2.66303400	-0.12615900
H	6.58490900	1.52963900	0.82833000
H	7.74219600	-0.63684300	0.46154000
C	1.78242500	1.51375600	1.41064700
C	1.68104500	2.83135800	0.95694600
C	2.03091200	1.24088600	2.75689700
C	1.86370500	3.88081700	1.85271200
H	1.47233000	3.01632100	-0.09717800
C	2.20798300	2.29791200	3.64556800
H	2.09063700	0.20522900	3.09054200
C	2.12775600	3.61594000	3.19656000
H	1.80209000	4.90879900	1.49963100
H	2.41425700	2.09024300	4.69411300
H	2.27200900	4.43724400	3.89594600

***Z*-6a gas phase**



E = -991.588123

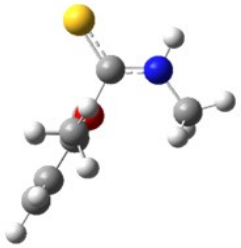
H = -991.572743

G = -991.630041

S	-2.04158100	-0.00669600	1.52786400
O	0.16637700	-2.32583800	-0.06906400
O	0.15457600	2.32657700	-0.06786100
N	-1.90115700	-0.00342600	-1.12264900
C	0.21774400	0.00052600	-0.05171000
C	0.92108700	1.21097800	-0.07359100
C	2.31743100	1.21919200	-0.10843700
C	0.92717300	-1.20632400	-0.07413200
C	-1.26796200	-0.00326800	0.06140800
C	2.32354000	-1.20755100	-0.10891300
C	2.99714900	0.00753000	-0.12147000
C	0.79770700	3.57012800	0.05516600
C	0.81608500	-3.56597100	0.05400100
C	-3.33873300	-0.00693000	-1.26243200
H	2.88254400	-2.13886100	-0.12710800
H	0.02780100	-4.31839000	0.13715500
H	2.87171400	2.15330400	-0.12625000
H	4.08552300	0.01029900	-0.14862100
H	0.00539900	4.31833400	0.13815800
H	-1.32760200	-0.00073400	-1.95728400
H	1.43708900	-3.79031900	-0.82686300
H	1.44566700	-3.60128700	0.95519300
H	1.42689300	3.60893500	0.95648800
H	-3.77447000	0.87722300	-0.77957700
H	1.41761800	3.79773500	-0.82560700
H	-3.76994200	-0.89345400	-0.77985100

H	-3.58978400	-0.00744800	-2.32705100

_E_-6a gas phase



E = -991.586766

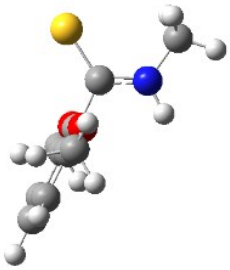
H = -991.571256

G = -991.628426

C	-0.00905800	-0.06031000	-0.03719500
C	-1.22592200	-0.75136000	-0.02438000
C	-1.24941900	-2.14705700	-0.06264000
C	-0.04520100	-2.83945500	-0.09796100
C	1.17695400	-2.17841000	-0.08509900
C	1.18895600	-0.78242100	-0.05082900
H	-2.18978700	-2.69116100	-0.06240400
H	-0.05986000	-3.92758500	-0.12878500
H	2.10271600	-2.74667900	-0.10070300
C	0.01199400	1.42692000	-0.11664300
S	-0.02681400	2.21153200	-1.57908100
N	0.06456100	2.07598900	1.05739200
H	0.10441500	3.08700100	0.98548400
O	2.31528400	-0.03008700	-0.01859700
O	-2.32996300	0.02950400	0.04695400
C	-3.58743300	-0.58528200	-0.08195600
H	-3.67515400	-1.12466300	-1.03643400
H	-3.78708800	-1.28290900	0.74564900
H	-4.32543700	0.22029100	-0.05595800
C	3.55084800	-0.68232500	-0.17432000
H	3.76772800	-1.35181600	0.67209100
H	3.58368300	-1.26233000	-1.10812900
H	4.30955200	0.10328400	-0.21301000
C	0.14912200	1.45797400	2.36442600

H	-0.63638800	0.70331000	2.48852900
H	1.12598000	0.98083800	2.52436400
H	0.00911900	2.23100900	3.12556400

_Z_-6aDMSO



E = -991.606164

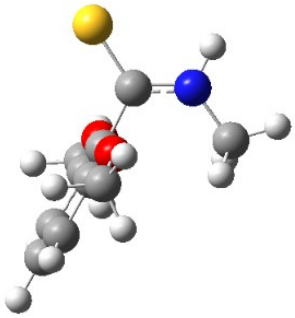
H = -991.591230

G = -991.647572

S	2.07677400	-0.00424300	1.53152600
O	-0.15423800	2.32763200	-0.01172700
O	-0.16364300	-2.32713700	-0.01189200
N	1.87608500	-0.00350700	-1.11805300
C	-0.22117300	0.00039900	-0.01112500
C	-0.92673500	-1.21024100	-0.03552500
C	-2.32269200	-1.21078800	-0.08476900
C	-0.92188300	1.21386100	-0.03547500
C	1.26492100	-0.00252300	0.06401200
C	-2.31781700	1.22001000	-0.08475500
C	-2.99477000	0.00596400	-0.10690500
C	-0.81964100	-3.57918700	-0.02888200
C	-0.80504100	3.58238700	-0.02876200
C	3.31191700	-0.00638800	-1.30375000
H	-2.87413400	2.15244800	-0.10836700
H	-0.01668900	4.33586300	0.03115100
H	-2.88276200	-2.14097800	-0.10837200
H	-4.08245700	0.00815800	-0.14673100
H	-0.03441400	-4.33592900	0.03089900
H	1.28703700	-0.00221000	-1.94472500
H	-1.37431500	3.72473200	-0.95767500
H	-1.47970200	3.69417900	0.83091400

H	-1.49464200	-3.68819000	0.83088400
H	3.75649400	-0.89555900	-0.84017300
H	-1.38963500	-3.71911700	-0.95771800
H	3.76024300	0.88011500	-0.83870100
H	3.52451700	-0.00598800	-2.37486600

***E*-6aDMSO**



E = -991.603685

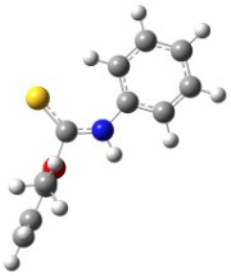
H = -991.588446

G = -991.644707

C	0.00896700	0.05961000	-0.07080700
C	1.22944600	0.74725500	-0.06422100
C	1.25157700	2.14286800	-0.10686900
C	0.04532800	2.83326600	-0.14514000
C	-1.17888500	2.17437400	-0.13328500
C	-1.19261700	0.77849700	-0.09052900
H	2.19047700	2.68875200	-0.10805300
H	0.06016300	3.92097400	-0.17990800
H	-2.10311000	2.74426800	-0.15598800
C	-0.01381500	-1.42689300	-0.10346100
S	0.02715100	-2.25879500	-1.56423100
N	-0.07047300	-2.04693400	1.07075600
H	-0.10503900	-3.06171500	1.03834000
O	-2.31645000	0.02446600	-0.05922500
O	2.33208100	-0.03483800	0.00032600
C	3.59564100	0.59952700	0.00863200
H	3.76488900	1.16404700	-0.91851100
H	3.69724800	1.27522800	0.86883200
H	4.33736900	-0.19829900	0.08655300

C	-3.56265800	0.69239900	-0.08255100
H	-3.66667100	1.37335000	0.77316600
H	-3.69425400	1.25817400	-1.01495800
H	-4.32693900	-0.08517400	-0.02011000
C	-0.14137800	-1.40035100	2.37168600
H	0.65105400	-0.65158300	2.47353400
H	-1.11444100	-0.91567000	2.51882300
H	-0.00651800	-2.16343600	3.14113900

_Z_-6e gas phase



E = -1183.118877

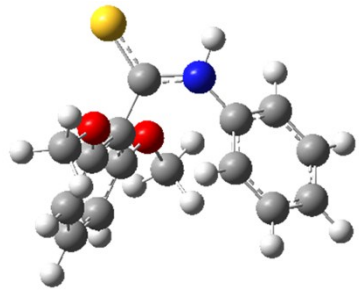
H = -1183.101068

G = -1183.164377

C	2.51764322	0.01139863	-3.09421071
C	3.16198427	-1.21334206	-2.88040564
C	4.48950245	-1.24860453	-2.44760713
C	5.15724848	-0.05004068	-2.22836777
C	4.53626611	1.17834429	-2.41798477
C	3.20858643	1.20481895	-2.85089591
H	4.99998786	-2.19366847	-2.28530193
H	6.19328399	-0.07408387	-1.89457263
H	5.08268050	2.09881775	-2.23292946
C	1.13216997	0.04490039	-3.65105410
S	0.91548065	0.06886469	-5.29123634
N	0.19660443	0.05113042	-2.66936200
O	2.49633843	2.33709597	-3.05480891
O	2.40672258	-2.31201159	-3.11152742
C	3.01856944	-3.57271432	-3.00018420
H	3.85446284	-3.67788214	-3.70723472
H	3.38506502	-3.75759267	-1.97905024

H	2.24815586	-4.30870093	-3.24282127
C	3.15629882	3.57018873	-2.91321114
H	3.52914679	3.71601600	-1.88806062
H	3.99598492	3.66013639	-3.61786860
H	2.41495884	4.34100519	-3.13759627
H	0.59571397	0.03219599	-1.73532257
C	-1.21089445	0.07842147	-2.66954741
C	-1.82655334	0.07545010	-1.41026045
C	-2.00317313	0.10735902	-3.81977804
C	-3.20775089	0.10093258	-1.30055599
H	-1.20956352	0.05283520	-0.51030005
C	-3.38815573	0.13272042	-3.69270890
H	-1.53201000	0.10973549	-4.79621461
C	-4.00024846	0.12985363	-2.44505910
H	-3.66638128	0.09816133	-0.31313721
H	-3.99574907	0.15519047	-4.59602263
H	-5.08513807	0.14992662	-2.36177244

_E_-6e gas phase E1



E = -1183.120586

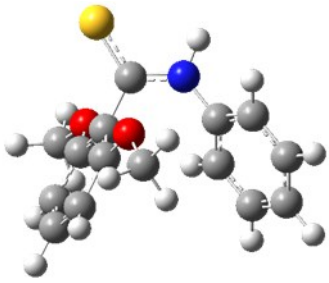
H = -1183.102525

G = -1183.165821

C	0.98935600	0.01234300	-0.40228200
C	2.05682900	0.51010600	0.36048000
C	2.36966600	1.87092200	0.33427400
C	1.60401600	2.72792200	-0.44678500
C	0.53605600	2.26383300	-1.20252900
C	0.23925300	0.90050400	-1.18536100
H	3.19078800	2.26290400	0.92783200
H	1.84590100	3.78938700	-0.46256700

H	-0.04649000	2.95294500	-1.80767600
C	0.64541500	-1.43123500	-0.39868900
S	1.64981500	-2.58008300	-1.04547400
N	-0.56893200	-1.77309300	0.10782800
O	-0.76750500	0.34080500	-1.89704600
O	2.68479900	-0.38821700	1.14864500
C	3.81454700	0.03287000	1.87091200
H	4.59093400	0.43470400	1.20367200
H	3.55663100	0.79363500	2.62341500
H	4.20052000	-0.85563900	2.37644600
C	-1.81350800	1.17958700	-2.32456700
H	-2.22294500	1.75521800	-1.47990600
H	-1.49113500	1.86756100	-3.11987000
H	-2.59073900	0.52072200	-2.72131800
H	-0.81329900	-2.74507100	-0.06334200
C	-1.59926200	-0.94100200	0.60015400
C	-2.90609900	-1.18783900	0.17448300
C	-1.35060000	0.08298800	1.51570700
C	-3.95406600	-0.40764200	0.64672000
H	-3.08767500	-1.98504400	-0.54663900
C	-2.40213300	0.87315500	1.96505800
H	-0.33824600	0.24618700	1.87922900
C	-3.70495200	0.63386000	1.53621700
H	-4.96935600	-0.60979100	0.30938800
H	-2.20078200	1.67220500	2.67655500
H	-4.52408000	1.25011600	1.90203800

***E*-6e gas phase E2**



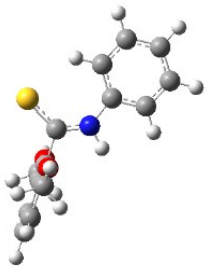
E = -1183.121203

H = -1183.102817

G = -1183.167171

S	-1.67083000	-2.57101200	-1.05045100
O	0.77950900	0.28490000	-1.93079200
O	-2.62655900	-0.33751200	1.18468800
N	0.55716100	-1.79989000	0.11531700
C	-0.96300200	0.00968100	-0.40952900
C	-0.64839700	-1.44191300	-0.39777800
C	1.57323400	-0.96226500	0.63136400
C	-0.21279400	0.87178000	-1.22095500
C	-2.00959300	0.53727100	0.36053300
C	-0.49739000	2.23712800	-1.26778500
C	-2.31164600	1.89956900	0.30510500
C	-1.55096200	2.72926900	-0.50971100
C	1.29839500	-0.00729800	1.61028400
C	2.87710300	-1.12136900	0.16045900
C	-3.73898200	0.10729500	1.91983000
C	2.32022200	0.80923700	2.08066100
C	3.89674800	-0.31416300	0.65022900
C	1.79810700	1.10912500	-2.44161900
C	3.61984100	0.66189500	1.60363700
H	0.79784200	-2.77319900	-0.05267100
H	0.28742800	0.07966800	2.00389200
H	-3.11878000	2.31616900	0.90095700
H	0.08468600	2.90532600	-1.89643700
H	-4.10993800	-0.76339200	2.46599700
H	-4.53306800	0.48442900	1.25915400
H	-3.46371700	0.89389800	2.63885000
H	-1.78399300	3.79210900	-0.54898900
H	3.07641100	-1.86681600	-0.60969300
H	2.10024600	1.55639100	2.84121300
H	4.41691400	1.29934200	1.98181900
H	4.91105000	-0.44256500	0.27568400
H	2.56748300	0.43744400	-2.83259200
H	2.23461400	1.73528700	-1.64783000
H	1.43706800	1.75077900	-3.25888000

***Z*-6eDMSO**



E = -1183.135425

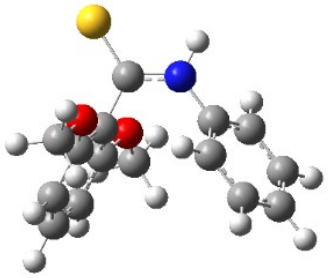
H = -1183.117260

G = -1183.182823

C	-1.38371100	0.00001500	0.08848800
C	-2.04170900	-1.21206500	-0.16114100
C	-3.34954600	-1.21437300	-0.65146900
C	-3.98146300	0.00157100	-0.88605000
C	-3.34835700	1.21676400	-0.65080300
C	-2.04053100	1.21288000	-0.16045900
H	-3.87045100	-2.14635000	-0.85081600
H	-5.00070800	0.00217500	-1.26797500
H	-3.86834600	2.14936300	-0.84962600
C	-0.00024700	-0.00076200	0.64549300
S	0.22652400	-0.00116400	2.30043400
N	0.93443700	-0.00054100	-0.32348500
O	-1.32038700	2.32748300	0.10189800
O	-1.32265100	-2.32754200	0.10047900
C	-1.93978700	-3.58073500	-0.11726900
H	-2.83840400	-3.69643000	0.50388200
H	-2.20854300	-3.71557100	-1.17392900
H	-1.20434100	-4.33618100	0.16753700
C	-1.93621600	3.58142600	-0.11522200
H	-2.20444100	3.71724800	-1.17189100
H	-2.83495100	3.69757800	0.50567200
H	-1.20014000	4.33595400	0.17039000
H	0.53877000	-0.00005300	-1.26144000
C	2.34696900	-0.00051900	-0.32794600
C	2.94710000	0.00056500	-1.59485900
C	3.15001100	-0.00145400	0.81504100

C	4.32787100	0.00077200	-1.71766700
H	2.32164700	0.00127100	-2.48776900
C	4.53531000	-0.00124000	0.67524400
H	2.69412000	-0.00234000	1.79797100
C	5.13250200	-0.00011000	-0.58004000
H	4.77626300	0.00167000	-2.70919300
H	5.15277100	-0.00193500	1.57178700
H	6.21643600	0.00007200	-0.67421600

***E1*-6eDMSO**



E = -1183.136888

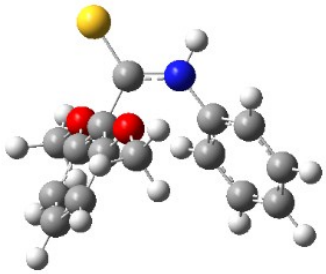
H = -1183.118664

G = -1183.183222

C	0.93031500	0.41515700	0.02322400
C	1.81221300	-0.55487100	0.51513700
C	2.10418900	-0.61336200	1.87926500
C	1.50332300	0.30130400	2.73694700
C	0.61724600	1.26730500	2.27490000
C	0.33255400	1.32214000	0.90940700
H	2.78233900	-1.36394900	2.27437900
H	1.73017000	0.25662800	3.80052000
H	0.16181000	1.96667200	2.96989200
C	0.61473600	0.51860200	-1.42394900
S	1.67163900	1.24445200	-2.50296200
N	-0.58544500	0.06159300	-1.80864000
O	-0.50563800	2.21787800	0.33915200
O	2.29384300	-1.42381500	-0.40407700
C	3.16783100	-2.44269300	0.04162400
H	4.07982900	-2.02004600	0.48447700
H	2.67644100	-3.09682900	0.77486000

H	3.43264000	-3.02580900	-0.84303200
C	-1.26847100	3.04950900	1.19005900
H	-1.89724800	2.45287000	1.86588600
H	-0.62770900	3.71685900	1.78229000
H	-1.90658300	3.65006600	0.53771600
H	-0.84287800	0.25764300	-2.77396400
C	-1.56290400	-0.56395800	-0.97938100
C	-2.82725300	0.01123500	-0.87436500
C	-1.26266400	-1.74783800	-0.30774200
C	-3.79533100	-0.60105100	-0.08522600
H	-3.03855400	0.94142100	-1.40034700
C	-2.23223900	-2.34587800	0.48930800
H	-0.27692800	-2.19594300	-0.42555500
C	-3.49833200	-1.77612200	0.60105200
H	-4.78313700	-0.15229800	-0.00003200
H	-1.99907500	-3.26865400	1.01703300
H	-4.25613700	-2.25039100	1.22159000

***E2*-6eDMSO**



E = -1183.136890

H = -1183.118666

G = -1183.183219

S	-1.67174400	1.24108000	-2.50428100
O	0.50513300	2.21874400	0.33649100
O	-2.29257600	-1.42528100	-0.40215000
N	0.58568900	0.05949600	-1.80881100
C	-0.93002100	0.41495300	0.02280900
C	-0.61451300	0.51674300	-1.42452300
C	1.56322100	-0.56506100	-0.97881000
C	-0.33270400	1.32334900	0.90784600

C	-1.81166100	-0.55469800	0.51591200
C	-0.61764200	1.27026400	2.27336400
C	-2.10392000	-0.61140700	1.88004800
C	-1.50349500	0.30461800	2.73657900
C	1.26311000	-1.74857800	-0.30645700
C	2.82731300	0.01064500	-0.87374700
C	-3.16920200	-2.44162200	0.04418400
C	2.23257500	-2.34572900	0.49139000
C	3.79529200	-0.60075800	-0.08378600
C	1.26812300	3.05126200	1.18640900
C	3.49841400	-1.77543300	0.60322200
H	0.84297800	0.25423100	-2.77443700
H	0.27752200	-2.19700200	-0.42429500
H	-2.78181200	-1.36176400	2.27604900
H	-0.16249200	1.97063900	2.96752500
H	-3.43478500	-3.02514000	-0.83997800
H	-4.08045600	-2.01632600	0.48601300
H	-2.67988200	-3.09617100	0.77844500
H	-1.73049600	0.26134700	3.80017900
H	3.03854500	0.94045200	-1.40043100
H	1.99952800	-3.26817700	1.01974200
H	4.25616800	-2.24895900	1.22439300
H	4.78290400	-0.15160300	0.00152100
H	1.90626500	3.65100000	0.53333900
H	1.89684900	2.45531200	1.86289900
H	0.62745000	3.71941100	1.77784300

9 Cartesian coordinates associated with the B3LYP-D3BJ/BS3//M06/BS1 calculations in DMSO using the CPCM approach (solution phase) (all energies are in Hartrees).

14

E (M06/BS1) = -1368.580509 au

H(M06/BS1) = -1368.269103 au

G(M06/BS1) = -1368.345382 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1370.846983 au

C	-0.48059300	-0.89011600	-0.05698200
C	-1.18145400	-1.39100500	1.04478500
C	-0.90235900	-1.21763600	-1.34996800
C	-2.29201500	-2.22533100	0.86030900
C	-2.01665100	-2.04457900	-1.54444600
C	-2.69282900	-2.53779300	-0.43468800
H	-2.35625400	-2.30455100	-2.54360400
H	-3.55752700	-3.18249700	-0.58236300
C	3.54431700	-0.17460900	0.14731600
O	3.25788700	1.03014200	0.36096000
C	4.96735600	-0.63056700	0.04062900
O	2.61626300	-1.04601300	-0.01350200
Pd	1.05791600	0.31941300	0.20423900
C	-2.91667000	1.57300000	0.61899300
H	-2.78090000	2.00873000	1.61577900
H	-3.83569200	1.94278100	0.15180300
H	-2.93867100	0.47932900	0.67684900
C	-1.76195300	3.82491300	-0.36839600
H	-0.91428100	4.28762700	-0.88091800
H	-2.69198400	4.06601400	-0.89292200
H	-1.80322200	4.15502000	0.67525900
S	-1.50881300	2.04402000	-0.40560300
O	-0.27162900	1.89912300	0.53298900
H	-2.84327300	-2.62265900	1.70864400
O	-0.74068900	-0.99587200	2.27086600
O	-0.18823200	-0.67203200	-2.37277300
C	-0.60063100	-0.95700200	-3.69234800
H	-1.62743800	-0.61000800	-3.87700700
H	0.08415800	-0.41763500	-4.35093300
H	-0.53968800	-2.03252800	-3.91122600
C	-1.50205600	-1.37542200	3.39699000
H	-1.01792100	-0.91852600	4.26337600
H	-2.53618600	-1.00692700	3.32288200
H	-1.51876300	-2.46675400	3.52787800
H	5.29598400	-0.54179500	-1.00259400
H	5.06586100	-1.67904700	0.33755500

H	5.61709600	0.00020200	0.65471900

14a

E (M06/BS1) = -1921.659037 au

H(M06/BS1) = -1921.258399 au

G(M06/BS1) = -1921.349693 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1924.195395 au

O	-1.13917000	-0.26231700	0.00000000
C	0.37079800	1.56030200	0.06716400
C	1.48937400	2.11150000	-0.56720600
C	-0.48106200	2.41878900	0.76654600
C	1.74125600	3.48856300	-0.52666500
C	-0.24792100	3.79798500	0.82112000
C	0.86495200	4.31523000	0.16766600
H	-0.91390900	4.46118700	1.36776100
H	1.05607100	5.38660700	0.20275200
C	-1.12078900	-3.13660600	0.21919800
O	-0.09259300	-2.55864000	-0.27459200
C	-1.20597600	-4.63123100	-0.03548500
O	-2.04130300	-2.57790200	0.84163700
Pd	0.03686600	-0.40070300	-0.03623300
C	-3.82063600	1.43996300	-1.00221500
H	-3.86036400	1.36612000	-2.09443200
H	-4.82561300	1.55054300	-0.58088500
H	-3.19432900	2.28775200	-0.70636900
C	-4.05500800	-1.26116300	-1.18475100
H	-3.67355200	-2.23835200	-0.87578900
H	-5.09810300	-1.14468500	-0.87124300
H	-3.95376700	-1.11480300	-2.26579000
S	-3.04476500	-0.04171900	-0.33013700
O	-1.71167100	-0.07480300	-1.13636800
H	2.60573800	3.91944300	-1.02542200
O	2.30638800	1.23021700	-1.22576600
O	-1.54485200	1.82297400	1.39024300
C	-2.43735500	2.63726900	2.11684000
H	-2.90755500	3.40037000	1.47789400

H	-3.21286700	1.96948600	2.50393600
H	-1.93610400	3.13796900	2.95741100
C	3.40006300	1.75073600	-1.94771700
H	3.89800900	0.89315900	-2.41038300
H	3.07242100	2.44588300	-2.73394800
H	4.11411400	2.26918200	-1.29015100
H	-0.21339000	-5.08643800	-0.12486600
H	-1.73475000	-4.79935600	-0.98377300
H	-1.77634700	-5.12869800	0.75579500
C	4.40256700	-0.76665100	0.65610800
H	4.45462600	-0.85697500	1.74653700
H	5.22997800	-1.29988500	0.17695600
H	4.40789200	0.28667800	0.36099300
C	2.96614700	-3.08656400	0.83287900
H	2.00135400	-3.56801800	0.64308300
H	3.77765900	-3.64384500	0.35351400
H	3.14272700	-2.97920000	1.90880900
S	2.84196800	-1.45319800	0.08590300
O	1.82034600	-0.71582400	1.00249100

15

E (M06/BS1) = -1899.418350 au

H(M06/BS1) = -1899.049730 au

G(M06/BS1) = -1899.142410 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1901.913516 au

C	-1.10872000	0.49651500	0.20749000
C	-2.13041600	0.32833500	1.14673800
C	-1.18768000	1.57436900	-0.67771000
C	-3.20939500	1.22160600	1.20880200
C	-2.26162000	2.47256200	-0.63854600
C	-3.25881000	2.28367400	0.31160200
H	-2.32603600	3.30752800	-1.33140000
H	-4.09468800	2.98008600	0.35447400
C	3.19573500	-1.75926800	-0.34154700
O	2.11497200	-2.12750500	0.23854100
C	4.39207900	-2.66287500	-0.10292000

O	3.34248300	-0.73612700	-1.03102500
Pd	0.46659900	-0.74001600	0.16392200
C	1.71170500	3.33461900	0.74846800
H	1.86883900	3.41825600	1.82946700
H	2.22503400	4.14112200	0.21356500
H	0.63887200	3.35745200	0.52365800
C	3.98421200	1.82391400	0.84835000
H	4.45790000	0.86953800	0.60055300
H	4.52482800	2.64885300	0.37226200
H	3.92591200	1.96723300	1.93281400
S	2.32174200	1.74027100	0.16916100
O	1.61001900	0.75634300	1.14490000
H	-4.00147100	1.09997400	1.94360300
C	-2.21899000	-1.92128700	-1.09956000
O	-2.01357000	-0.75220900	1.97149700
O	-0.15136400	1.69313600	-1.56169200
C	-0.14271900	2.79532700	-2.44288300
H	-0.15807500	3.75090600	-1.89764900
H	0.78777900	2.72363600	-3.01256100
H	-0.99534300	2.76627700	-3.13592700
C	-3.08698700	-1.03738600	2.84003600
H	-2.82566600	-1.96181600	3.36091400
H	-3.23567400	-0.23930000	3.58153100
H	-4.02558800	-1.18835800	2.28488900
N	-3.31260200	-1.54383000	-1.24410700
S	-0.69524300	-2.49364700	-0.92294700
C	-4.60911800	-0.99164300	-1.37406200
H	4.09093500	-3.68818500	0.13417300
H	4.96315200	-2.27291600	0.75081200
H	5.05686600	-2.65862000	-0.97321200
H	-4.64353500	-0.05743900	-0.80072300
H	-4.82059700	-0.78874300	-2.42822100
H	-5.34875200	-1.69379300	-0.97741900

16

E (M06/BS1) = -1899.443781 au

H(M06/BS1) = -1899.074018 au

G(M06/BS1) = -1899.160908 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1901.931014 au

C	1.65918500	0.06463900	0.20461800
C	2.05263700	0.63869900	-1.05225000
C	1.19112200	0.94865600	1.23424000
C	1.86331000	1.99471400	-1.30286600
C	1.00091100	2.30434400	0.96845300
C	1.35278000	2.79539600	-0.28622000
H	0.62949100	2.98292700	1.73082200
H	1.24013100	3.86215100	-0.47584200
C	-2.86661500	-1.92518000	0.03769200
O	1.00232900	0.37734100	2.42447700
C	0.36671800	1.13527200	3.44720800
H	-0.61317400	1.49454300	3.10650800
H	0.23763500	0.45216800	4.28777100
H	0.99159600	1.98262600	3.75450600
O	-1.92640700	-1.96390400	-0.84191500
C	-4.10706500	-2.70055500	-0.35171800
O	-2.83462400	-1.28753700	1.09860800
Pd	-0.31839100	-0.73021800	-0.35992700
C	-2.23451000	3.44565600	-0.56351600
H	-2.62750700	3.40153200	-1.58532400
H	-2.86393500	4.07754300	0.07141500
H	-1.20875300	3.82385000	-0.56869600
C	-3.94916800	1.40386700	-0.10949300
H	-4.11250400	0.40395700	0.30320700
H	-4.53917600	2.14251300	0.44356900
H	-4.18115000	1.44076500	-1.18002200
S	-2.19763700	1.77598400	0.11185300
O	-1.47179700	0.98078300	-1.00529400
H	2.13895000	2.43632600	-2.25516400
O	2.63527400	-0.21191300	-1.89738600
C	3.00302500	0.25739700	-3.18847100
H	3.73867800	1.06736600	-3.11376100
H	3.44949100	-0.59614700	-3.70047600

H	2.12114100	0.60099200	-3.74318600
C	2.24963000	-1.27471400	0.59527800
N	3.41490500	-1.51342800	1.02873700
S	1.00161200	-2.49109200	0.30802500
H	-4.67105300	-2.99200600	0.53950500
H	-4.74824400	-2.04984000	-0.96225000
H	-3.86293300	-3.58305400	-0.95099300
C	4.35435400	-0.42710800	1.19545500
H	5.18706000	-0.56007100	0.49108200
H	3.93503000	0.58194000	1.04083100
H	4.78119700	-0.46896900	2.20555800

16'

E (M06/BS1) = -1899.446297 au

H(M06/BS1) = -1899.076488 au

G(M06/BS1) = -1899.163551 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1901.933515 au

C	1.63770600	0.49391100	0.24074600
C	1.87132800	1.24727800	-0.96044600
C	0.99114700	1.15206000	1.34116700
C	1.37119000	2.54075000	-1.08933600
C	0.49589000	2.44690900	1.19542400
C	0.70536700	3.11090700	-0.01041000
H	-0.01251500	2.95227600	2.01154900
H	0.34488500	4.13407500	-0.10927600
C	-2.35782900	-2.39077400	-0.17537400
O	0.92880600	0.44183800	2.46840700
C	0.14415200	0.94245000	3.54345700
H	-0.89561500	1.09346900	3.22487500
H	0.18406700	0.17936000	4.32209500
H	0.55761400	1.88189400	3.93058900
O	-1.48107300	-2.09669400	-1.07245300
C	-3.39141300	-3.39847700	-0.63216400
O	-2.42774200	-1.88783700	0.95325200
Pd	-0.15675000	-0.61805500	-0.44683800
C	-2.94870500	3.03938200	-0.16749800

H	-3.30462100	3.04716400	-1.20371300
H	-3.71918500	3.41450300	0.51365800
H	-2.04181200	3.64312300	-0.07380900
C	-4.15173600	0.62021400	-0.04217100
H	-4.09014100	-0.43457400	0.23838800
H	-4.89811300	1.12948600	0.57670600
H	-4.37902800	0.74136900	-1.10735000
S	-2.53255500	1.34531000	0.28625700
O	-1.63669500	0.89392500	-0.89749100
H	1.51897000	3.11411400	-1.99887800
O	2.60772900	0.62855000	-1.88398400
C	2.78995600	1.26407200	-3.14219500
H	3.31871400	2.21801600	-3.02653100
H	3.39551600	0.58043300	-3.73886800
H	1.82382400	1.42977000	-3.63551900
C	2.46886100	-0.73304100	0.50188000
N	3.64258200	-0.66353200	0.97354000
S	1.50158500	-2.14446600	0.03265400
H	-3.81740700	-3.92432800	0.22767500
H	-4.20488000	-2.86118900	-1.13883700
H	-2.97243800	-4.11555500	-1.34476200
C	4.34900100	-1.91066000	1.18235100
H	4.48153800	-2.45943600	0.23613700
H	5.33912700	-1.71607500	1.60752600
H	3.80173300	-2.57428800	1.87110900

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E (M06/BS1) = -1597.565397 au

H(M06/BS1) = -1597.184294 au

G(M06/BS1) = -1597.271954 au

E(B3LYP- D3BJ/BS2 /BS2//M06/BS1) = -1600.072962 au

C	-1.21681500	-0.63048100	0.21416600
C	-2.37345000	-0.32354500	0.93726500
C	-1.30725300	-1.51171400	-0.86757000
C	-3.61076600	-0.87396600	0.57493600
C	-2.53688400	-2.06328700	-1.24727100

C	-3.67337100	-1.73359900	-0.51686100
H	-2.61321500	-2.73555500	-2.09829700
H	-4.63355400	-2.15817600	-0.80545100
C	3.23428200	1.21404800	0.23455600
O	2.42015600	1.14679000	1.20298100
C	4.32448700	2.25531700	0.33608100
O	3.18039100	0.50639500	-0.80517400
Pd	0.53612000	0.18493000	0.67935100
C	-2.49897200	2.33012100	-1.18160100
H	-2.66257800	3.04767400	-0.36884200
H	-2.91562300	2.70242300	-2.12360500
H	-2.93887400	1.35803900	-0.93202100
C	-0.30583300	3.77861200	-1.87821300
H	0.78337400	3.83784500	-1.95392900
H	-0.76027000	3.98761200	-2.85188500
H	-0.67469800	4.47353600	-1.11601400
S	-0.72031200	2.09879000	-1.38378800
O	-0.15411700	2.06233300	0.06834000
H	-4.51472900	-0.63687900	1.13031300
O	-2.22188100	0.54052100	1.97903300
O	-0.13744300	-1.77425100	-1.51723900
C	-0.14111300	-2.74301400	-2.54207600
H	-0.73980300	-2.42183900	-3.40646900
H	0.90232800	-2.86130400	-2.84752500
H	-0.52500400	-3.70876900	-2.18097100
C	-3.38460600	0.98136200	2.64440800
H	-3.05411600	1.70586100	3.39275800
H	-4.08205000	1.47132600	1.94861400
H	-3.90398800	0.15459800	3.15019300
H	4.60265500	2.43432800	1.37940200
H	3.94710200	3.20167700	-0.07365200
H	5.20356300	1.96265600	-0.24616900
O	1.17787800	-1.74915900	1.20464500
O	2.63986400	-1.98332400	-0.50215500
C	1.89077400	-2.43595400	0.45312800
H	2.67127300	-0.95695500	-0.57830600

C	1.90804800	-3.92070300	0.60107900
H	1.19890900	-4.34093200	-0.12526600
H	2.89792000	-4.32824500	0.37839200
H	1.58488900	-4.20997600	1.60357400

18

E (M06/BS1) = -1597.563914 au

H(M06/BS1) = -1597.182076 au

G(M06/BS1) = -1597.273109 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1600.068972 au

Ag	1.83868900	1.14866000	0.00035900
C	0.34245300	-1.92939500	0.03597900
C	1.50003500	-1.83413200	-0.79439500
C	0.51319300	-1.89044800	1.45514500
C	2.74754600	-1.56872600	-0.23875000
C	1.75674100	-1.56995700	2.00429100
C	2.84300900	-1.43239300	1.14599100
H	1.89896200	-1.48165600	3.07649900
H	3.82013700	-1.21977500	1.57872600
C	-1.77230300	2.60559300	0.27739600
O	-1.60975900	1.81322000	-0.72527200
C	-2.50863000	3.88352000	-0.06430500
O	-1.33655600	2.41952000	1.42043200
Pd	-0.55667200	0.09190400	-0.26274800
C	3.63187000	1.95740100	-0.39298600
H	3.48786700	2.46122900	-1.35514300
H	4.27007900	2.55084800	0.26953000
H	4.06513200	0.96457500	-0.54215900
C	1.53151800	3.47587000	0.42656500
H	0.55480100	3.51560700	0.91890600
H	2.27189500	4.03855000	1.00493900
H	1.47327000	3.84531000	-0.60375500
S	2.02291000	1.74168400	0.38493000
O	1.19365100	1.12444500	-0.78092500
H	3.63684900	-1.48973900	-0.85730200
O	1.27331900	-2.00822200	-2.09760700

O	-0.56550400	-2.20511500	2.16991900
C	-0.50610800	-2.06841300	3.58292200
H	-0.28957600	-1.02978900	3.86376500
H	-1.49302500	-2.35015200	3.95322200
H	0.25063200	-2.73705400	4.01181800
C	2.34640100	-1.78901500	-3.00281200
H	1.92565600	-1.90926200	-4.00241300
H	2.74909900	-0.77351900	-2.89109900
H	3.14551700	-2.52550000	-2.85122400
H	-1.78196500	4.61164900	-0.45029000
H	-2.97076800	4.30742100	0.83240300
H	-3.26379500	3.72401700	-0.84009200
C	-4.33924400	-1.74488200	-0.58125600
O	-2.33180100	-0.77727400	0.15177600
O	-2.47150000	-1.31622500	-2.02533800
C	-2.93982600	-1.25869100	-0.88903500
H	-0.51718500	-2.46884100	-0.36271600
H	-4.38995900	-2.22170900	0.40289800
H	-5.02175400	-0.88575900	-0.56697400
H	-4.67620600	-2.44174200	-1.35441100

19

E (M06/BS1) = -1136.569155 au

H(M06/BS1) = -1136.366067 au

G(M06/BS1) = -1136.431846 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1138.540607 au

C	1.29096800	2.12161500	0.24897100
O	0.31098000	1.88996400	-0.56697600
C	2.04980600	3.39070400	-0.06096300
O	1.63163200	1.39150400	1.18260100
Pd	-0.69885100	0.17282000	-0.26637100
C	2.04402200	-3.16746200	-0.09306900
H	2.40461300	-3.19620800	-1.12677200
H	2.75822800	-3.64679600	0.58448100
H	1.07029300	-3.65891900	-0.01378100
C	3.48561900	-0.85969700	0.05507700

H	3.48975300	0.20740800	0.29287900
H	4.19337200	-1.39573400	0.69587600
H	3.70424800	-1.03622400	-1.00366500
S	1.82491900	-1.45189000	0.40661800
O	0.98762100	-0.88787700	-0.79089600
H	2.94286500	3.12917600	-0.64369400
H	2.38566800	3.85898900	0.86968600
H	1.45306300	4.09658800	-0.64537300
C	-4.47862300	-0.62239400	0.46459300
O	-2.61021600	0.86216700	0.16480400
O	-2.19864000	-1.27470600	0.03451500
C	-3.04062500	-0.33947900	0.22124000
H	-4.90078500	0.11772800	1.15113200
H	-5.02314000	-0.55147200	-0.48522800
H	-4.60776500	-1.63215300	0.86416000

20

E (M06/BS1) = -1899.428004 au

H(M06/BS1) = -1899.057949 au

G(M06/BS1) = -1899.144312 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1901.923267 au

C	2.29004100	0.30034700	-0.04856500
C	1.35554300	1.27471200	-0.39619200
C	3.14925600	0.56920900	1.03011300
C	1.27459500	2.50385500	0.24257700
C	3.09206800	1.80255900	1.68716400
C	2.16327300	2.75388700	1.28346400
H	3.76129300	2.02112400	2.51431200
H	2.12116200	3.70920300	1.80225600
C	-2.52228300	-2.05010600	1.07554300
O	3.99456600	-0.42720400	1.36590100
C	4.92122000	-0.19600600	2.41006800
H	4.41028200	-0.01084400	3.36455200
H	5.51901300	-1.10609000	2.49096400
H	5.57926000	0.65186200	2.17672400
O	-2.03342300	-2.16543000	-0.11923100

C	-3.50586700	-3.14203400	1.42776300
O	-2.27731000	-1.13418500	1.86371500
Pd	-0.86065300	-0.62140600	-0.68623100
C	-3.42177800	3.10064200	-0.22495500
H	-4.19299700	2.89456200	-0.97528400
H	-3.81982800	3.72220200	0.58376100
H	-2.56832200	3.60572400	-0.68675100
C	-4.44189300	0.94889100	1.06353000
H	-4.26399600	-0.02025100	1.53856000
H	-4.82682300	1.66312400	1.79907900
H	-5.12383500	0.86165400	0.21031100
S	-2.84647200	1.53621200	0.46385300
O	-2.57179500	0.69252500	-0.81353500
H	0.52929800	3.24122400	-0.04467500
O	0.47808900	0.91013000	-1.40929000
C	-0.04052100	1.93996000	-2.25864700
H	0.79046400	2.56360000	-2.60413300
H	-0.51402500	1.42700100	-3.09797500
H	-0.78728800	2.54768700	-1.73818700
C	2.33175900	-1.00778800	-0.76766500
N	3.29246200	-1.46142500	-1.46663600
S	0.91297400	-2.08768900	-0.54849300
H	-3.50698400	-3.30987200	2.50893900
H	-4.51193100	-2.81214100	1.13542200
H	-3.29033200	-4.07488600	0.89892800
C	4.50577400	-0.69750800	-1.63991900
H	4.79761300	-0.73682800	-2.69710400
H	4.43223100	0.35719500	-1.33196400
H	5.31636500	-1.16738100	-1.06656500

21

E (M06/BS1) = -1899.456143 au

H(M06/BS1) = -1899.085327 au

G(M06/BS1) = -1899.173084 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1901.949286 au

C	2.90443200	0.08291900	0.08482400

C	3.30550600	1.16592000	0.88518700
C	3.87144800	-0.68771500	-0.58136600
C	4.65955000	1.47696000	1.01982100
C	5.22661500	-0.37828500	-0.44988200
C	5.59543300	0.69731400	0.34983900
H	5.98738800	-0.95792600	-0.96376400
H	6.65186400	0.93850800	0.45253700
C	-3.47453600	-1.46336600	1.25190800
O	3.39144700	-1.69285600	-1.34310300
C	4.32074900	-2.51293000	-2.02693200
H	5.00181000	-3.01265200	-1.32519300
H	3.73148700	-3.26371400	-2.55700000
H	4.90614100	-1.93101600	-2.75140800
O	-2.59265600	-1.97607000	0.46541000
C	-4.62098300	-2.38883400	1.59490400
O	-3.46049900	-0.30255000	1.68447400
Pd	-1.13240500	-0.65685700	-0.13197200
C	-3.32283700	2.86544100	-1.93934200
H	-3.77615900	2.38107300	-2.81109900
H	-3.91958100	3.72501400	-1.61696200
H	-2.30509400	3.18957100	-2.17316800
C	-4.97717700	1.24783300	-0.52969600
H	-5.08521400	0.49612400	0.25741600
H	-5.55101000	2.14564100	-0.27621500
H	-5.27868000	0.85481800	-1.50716700
S	-3.22686000	1.67161100	-0.59197500
O	-2.55823100	0.45337200	-1.28802000
H	4.98497000	2.31012200	1.63535900
O	2.30453400	1.83774800	1.49373300
C	2.64671900	2.92372800	2.33508400
H	3.16580300	3.71340100	1.77561500
H	1.70434100	3.31527400	2.72349000
H	3.27703700	2.59424900	3.17184900
C	1.47949400	-0.26954700	0.00284700
N	0.55186900	0.37718300	-0.61452700
S	0.76699400	-1.64860600	0.84243600

H	-5.03296000	-2.13673200	2.57696100
H	-5.41734000	-2.24956400	0.85077100
H	-4.32024700	-3.44064900	1.56996000
C	0.71136400	1.60636700	-1.35363300
H	0.34409800	2.44844100	-0.75175100
H	1.76538800	1.78253500	-1.60300700
H	0.11995500	1.55253900	-2.27356400

22

E (M06/BS1) = -1535.972029 au

H(M06/BS1) = -1535.645622 au

G(M06/BS1) = -1535.728977 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1538.277848 au

C	-2.31849600	-0.00126200	-0.09396300
C	-2.72915900	1.33269000	0.06113800
C	-3.25827900	-0.98707300	-0.43283000
C	-4.06819800	1.68126600	-0.11805700
C	-4.59977600	-0.64306500	-0.61159600
C	-4.97897700	0.68476000	-0.45248700
H	-5.34166700	-1.39363500	-0.86721000
H	-6.02437600	0.95344600	-0.59262300
C	3.99406200	0.28352300	-1.00717400
O	-2.77097300	-2.24070700	-0.54542600
C	-3.66979200	-3.27713700	-0.89376400
H	-4.12832100	-3.09425500	-1.87487300
H	-3.07551800	-4.19213100	-0.93642600
H	-4.45780900	-3.39128700	-0.13718200
O	3.53591700	-0.76590800	-0.42923200
C	5.33696300	0.10864200	-1.67878600
O	3.43801100	1.39372100	-1.04068200
Pd	1.70522900	-0.56924200	0.49988300
H	-4.40300700	2.70798800	-0.00383800
O	-1.74663400	2.20776400	0.37665200
C	-2.09318700	3.57419400	0.51653200
H	-2.82059100	3.71795600	1.32632200
H	-1.16703100	4.09838500	0.76191800

H	-2.50375200	3.97632700	-0.41938200
C	-0.88901200	-0.32568800	0.03201400
N	-0.21305200	-0.38160400	1.12914400
S	0.15744500	-0.56715100	-1.36394500
H	5.28215300	0.47718300	-2.70936100
H	6.08165000	0.72084400	-1.15562200
H	5.66772400	-0.93339100	-1.67733300
C	-0.72663600	-0.14190000	2.45758800
H	-0.40033500	0.84851200	2.80180800
H	-1.82267900	-0.18622000	2.46865500
H	-0.31564000	-0.89100800	3.14256400
H	2.52261800	-0.14080100	2.00877000
B	2.71185300	-1.26892400	2.65557100
H	2.33255200	-2.29043100	2.09931300
H	3.92438200	-1.24974300	2.77293400
H	2.08265600	-1.05556900	3.67653900
Na	1.44470800	2.46368900	-0.60004500

22'

E (M06/BS1) = -1373.723714 au

H(M06/BS1) = -1373.40096 au

G(M06/BS1) = -1373.482331 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1376.003057 au

C	-2.26366200	0.04738400	-0.12068800
C	-2.75714400	1.36228300	-0.12959700
C	-3.14773600	-1.02870000	-0.29295700
C	-4.11976100	1.60222900	-0.31547200
C	-4.51278200	-0.79391800	-0.47301100
C	-4.97316400	0.51777500	-0.48482700
H	-5.21252500	-1.61440500	-0.59979600
H	-6.03643700	0.70129700	-0.62856600
C	4.13863000	0.42974700	-1.02596900
O	-2.58560600	-2.25597100	-0.25293900
C	-3.42485100	-3.37880100	-0.44501700
H	-3.92566000	-3.33859200	-1.42174700
H	-2.77471400	-4.25525400	-0.40756100

H	-4.18044900	-3.45235500	0.34891300
O	3.60571000	-0.61941200	-0.49262100
C	5.49070100	0.16664200	-1.66020300
O	3.65660800	1.56506200	-1.02392000
Pd	1.80123100	-0.29400300	0.43556900
H	-4.51509900	2.61337000	-0.33026000
O	-1.82915400	2.32952900	0.04285600
C	-2.26142400	3.67701200	0.01793500
H	-2.99251600	3.87516900	0.81326700
H	-1.37044500	4.28540900	0.18524900
H	-2.70209000	3.93461400	-0.95461300
C	-0.81223000	-0.17695400	0.00186600
N	-0.11173800	-0.05889800	1.07830600
S	0.21375000	-0.55073500	-1.37743100
H	5.69714100	0.91137200	-2.43522400
H	6.26958500	0.25169900	-0.89135000
H	5.55135100	-0.84148500	-2.08263700
C	-0.61198500	0.30984100	2.38093500
H	-0.28505200	1.32933800	2.62422300
H	-1.70810200	0.26617300	2.40824400
H	-0.19041100	-0.36661600	3.13273300
H	2.64399600	0.31528300	1.86953200
B	2.84670200	-0.71415400	2.65403900
H	2.45241800	-1.79881500	2.24855700
H	4.06212800	-0.69063600	2.74695000
H	2.24086900	-0.36750500	3.65351300

23

E (M06/BS1) = -1535.951836 au

H(M06/BS1) = -1535.626892 au

G(M06/BS1) = -1535.71173 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1538.255491 au

C	2.36444600	0.14352900	-0.03484200
C	3.03224700	1.37404600	0.10187200
C	3.11236200	-1.04830300	-0.06368100
C	4.42198700	1.41321600	0.22338000

C	4.50253000	-1.01180900	0.06228200
C	5.13227400	0.21851200	0.20601200
H	5.09007400	-1.92479200	0.05158200
H	6.21599100	0.24822000	0.30244400
C	-4.49289100	0.06197300	0.48113700
O	2.39835900	-2.18498300	-0.20399700
C	3.09599700	-3.41688200	-0.20677700
H	3.62562300	-3.57496800	0.74208100
H	2.33852600	-4.19310000	-0.33292600
H	3.81088200	-3.46809500	-1.03878800
O	-3.52512900	-0.74909100	0.69970200
C	-5.70599500	-0.18629800	1.35189100
O	-4.49534400	0.99468300	-0.33853300
Pd	-1.72685600	-0.53061300	-0.29475100
H	4.94889400	2.35725400	0.32364700
O	2.24521600	2.46937400	0.07062600
C	2.85534700	3.73705900	0.22445000
H	3.58171500	3.92846700	-0.57669300
H	2.04928100	4.47108600	0.16436500
H	3.35530700	3.82348500	1.19856300
C	0.89637300	0.08645200	-0.07075100
N	0.17197000	-0.36715500	-1.03184800
S	-0.09989100	0.59227400	1.33220300
H	-6.55253000	0.42652100	1.02989200
H	-5.98441900	-1.24572700	1.32861500
H	-5.46451100	0.05993300	2.39341200
C	0.70039900	-0.81997200	-2.30294700
H	1.72268700	-0.45696100	-2.46584500
H	0.70118300	-1.91619100	-2.32068200
H	0.04470300	-0.46043300	-3.10236000
B	0.40343300	-0.81011000	2.70299300
H	1.60092700	-0.70280100	2.87212100
H	-0.25461600	-0.45993100	3.66193800
H	0.05892100	-1.88240100	2.24272000
H	-2.35333900	-1.24502300	-1.55568100
Na	-3.01799100	1.83808300	-1.87469700

24

E (M06/BS1) = -1535.965932 au

H(M06/BS1) = -1535.640063 au

G(M06/BS1) = -1535.725243 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1538.271676 au

C	2.36444600	0.14352900	-0.03484200
C	3.03224700	1.37404600	0.10187200
C	3.11236200	-1.04830300	-0.06368100
C	4.42198700	1.41321600	0.22338000
C	4.50253000	-1.01180900	0.06228200
C	5.13227400	0.21851200	0.20601200
H	5.09007400	-1.92479200	0.05158200
H	6.21599100	0.24822000	0.30244400
C	-4.49289100	0.06197300	0.48113700
O	2.39835900	-2.18498300	-0.20399700
C	3.09599700	-3.41688200	-0.20677700
H	3.62562300	-3.57496800	0.74208100
H	2.33852600	-4.19310000	-0.33292600
H	3.81088200	-3.46809500	-1.03878800
O	-3.52512900	-0.74909100	0.69970200
C	-5.70599500	-0.18629800	1.35189100
O	-4.49534400	0.99468300	-0.33853300
Pd	-1.72685600	-0.53061300	-0.29475100
H	4.94889400	2.35725400	0.32364700
O	2.24521600	2.46937400	0.07062600
C	2.85534700	3.73705900	0.22445000
H	3.58171500	3.92846700	-0.57669300
H	2.04928100	4.47108600	0.16436500
H	3.35530700	3.82348500	1.19856300
C	0.89637300	0.08645200	-0.07075100
N	0.17197000	-0.36715500	-1.03184800
S	-0.09989100	0.59227400	1.33220300
H	-6.55253000	0.42652100	1.02989200
H	-5.98441900	-1.24572700	1.32861500
H	-5.46451100	0.05993300	2.39341200

C	0.70039900	-0.81997200	-2.30294700
H	1.72268700	-0.45696100	-2.46584500
H	0.70118300	-1.91619100	-2.32068200
H	0.04470300	-0.46043300	-3.10236000
B	0.40343300	-0.81011000	2.70299300
H	1.60092700	-0.70280100	2.87212100
H	-0.25461600	-0.45993100	3.66193800
H	0.05892100	-1.88240100	2.24272000
H	-2.35333900	-1.24502300	-1.55568100
Na	-3.01799100	1.83808300	-1.87469700

25

E (M06/BS1) = -1535.959853 au

H(M06/BS1) = -1535.635213 au

G(M06/BS1) = -1535.718497 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1538.266764 au

C	2.33326500	-0.04198700	-0.13931700
C	2.99676800	1.13189100	-0.51276800
C	3.07407100	-1.18521500	0.18248900
C	4.39181500	1.17068300	-0.55664700
C	4.46941600	-1.15698200	0.14116100
C	5.10490600	0.02421000	-0.22471000
H	5.05722200	-2.03537700	0.39032500
H	6.19259800	0.05091400	-0.25739800
C	-4.72769600	0.05884300	0.17213600
O	2.34243600	-2.27013700	0.53090800
C	3.03446500	-3.41132100	0.99755600
H	3.63479000	-3.17305500	1.88688300
H	2.27048800	-4.14578800	1.26133400
H	3.68691500	-3.83192900	0.22028200
O	-3.99004800	-0.82228300	-0.40103300
C	-6.18506900	-0.33679500	0.26642900
O	-4.34705800	1.15123400	0.61926200
Pd	-1.96465800	-0.56631400	-0.61588700
H	4.92051300	2.07483700	-0.84376900
O	2.19498900	2.18028100	-0.81631200

C	2.80847800	3.43593600	-1.02993700
H	3.44913700	3.42379800	-1.92241000
H	1.99859900	4.15331600	-1.17914100
H	3.40627500	3.73553300	-0.15735400
C	0.86056700	-0.04703700	0.03111900
N	0.05795200	-0.39714000	-0.92437700
S	0.22106400	0.40108600	1.59315700
H	-6.75742700	0.40465300	0.83048100
H	-6.60871000	-0.43053100	-0.74084200
H	-6.28039400	-1.31781000	0.74603100
C	0.60641900	-0.79439200	-2.22019600
H	1.32964900	-0.05790200	-2.59298000
H	1.10721700	-1.76911900	-2.14447900
H	-0.21175200	-0.87935800	-2.93956600
B	1.76919200	0.92660900	2.75459200
H	2.33260200	1.87223800	2.23667800
H	1.17666500	1.22944000	3.77616700
H	2.48200900	-0.04894100	2.89717800
H	-2.14002900	0.67236000	-1.49600100
Na	-2.33343100	2.07754000	1.22364100

26

E (M06/BS1) = -1535.986371 au

H(M06/BS1) = -1535.656904 au

G(M06/BS1) = -1535.743662 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1538.273582 au

C	1.80765500	0.36812800	0.24705900
C	3.15441200	-0.00377000	0.08771300
C	1.45434100	1.70909300	0.05552400
C	4.10352300	0.92900400	-0.33523600
C	2.39416000	2.64866100	-0.37119100
C	3.70626200	2.24058100	-0.57122600
H	2.10837600	3.68500500	-0.53018400
H	4.44494300	2.96678700	-0.90572000
C	-4.09823700	0.54162600	0.05003300
O	0.16190800	2.03085100	0.32331300

C	-0.39887400	3.16213000	-0.32388500
H	-0.15849200	3.14963900	-1.39661500
H	-1.47980900	3.06874400	-0.19048400
H	-0.04160200	4.09919000	0.12290000
O	-2.93346700	1.00865900	-0.16226000
C	-5.18728300	1.58512200	0.21753000
O	-4.40068900	-0.66603000	0.14438800
Pd	-1.13782200	-0.22558400	-0.17644000
H	5.14083700	0.64213100	-0.48090100
O	3.43985600	-1.29678100	0.35655400
C	4.73459600	-1.76884200	0.04404200
H	5.50260300	-1.27371700	0.65402100
H	4.73310500	-2.83771600	0.26861000
H	4.96336700	-1.61936900	-1.02057500
C	0.79247200	-0.68970600	0.52401800
N	0.66401200	-1.07235700	1.82815300
S	0.43927800	-1.89772900	-0.73765600
H	-6.18398600	1.13787300	0.15723000
H	-5.07837200	2.06474100	1.19905100
H	-5.08631400	2.37255100	-0.53759000
C	1.20951200	-0.33844800	2.95224300
H	2.30579400	-0.40022400	2.97946800
H	0.91692400	0.71917900	2.92371200
H	0.81603700	-0.77861900	3.87192100
B	1.24882700	-1.23411700	-2.47317000
H	2.41730700	-1.56312800	-2.42449000
H	0.60372800	-1.86862000	-3.28521200
H	1.06861200	-0.03586100	-2.54569200
H	0.07465600	-1.87339200	2.02208100
Na	-3.16587700	-2.55933200	-0.19542800

27

E (M06/BS1) = -2089.005350 au

H(M06/BS1) = -2088.594278 au

G(M06/BS1) = -2088.690646 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -2091.575710 au

C	-2.19976700	0.06481500	-0.11912800
C	-2.53981200	1.41677000	0.02288900
C	-3.20038100	-0.88063000	-0.37940200
C	-3.86676600	1.82800200	-0.11257400
C	-4.53113800	-0.47791100	-0.51356000
C	-4.83973700	0.87105200	-0.38060800
H	-5.31786200	-1.19965300	-0.71286700
H	-5.87584800	1.18804800	-0.48378900
C	4.22848400	0.24126000	-0.51617700
O	-2.77495200	-2.16111700	-0.47075400
C	-3.73557500	-3.16178500	-0.74786200
H	-4.23232200	-2.98216500	-1.71104000
H	-3.18727200	-4.10504300	-0.79484500
H	-4.49157300	-3.22143600	0.04691600
O	3.75164200	-0.86249500	-0.07709000
C	5.62454500	0.15894000	-1.09371900
O	3.64678500	1.34202700	-0.51075700
Pd	1.78779400	-0.79426700	0.60316900
H	-4.14554000	2.87230900	-0.00851700
O	-1.50804000	2.25291600	0.30131800
C	-1.80273900	3.62856400	0.46966400
H	-2.50707700	3.78382600	1.29758400
H	-0.85538200	4.11972100	0.70336600
H	-2.21991000	4.05990900	-0.45019700
C	-0.78150900	-0.34200600	-0.01855800
N	-0.18613400	-0.64802300	1.08827500
S	0.25050300	-0.36793100	-1.43657100
H	5.58859000	0.41267500	-2.16032900
H	6.26708400	0.90315100	-0.60904100
H	6.06434000	-0.83535100	-0.97697600
C	-0.82565800	-0.64425200	2.38585000
H	-0.40008100	0.16004400	2.99998700
H	-1.91082100	-0.50123500	2.30398500
H	-0.62112800	-1.59461000	2.89255900
H	2.30996700	-1.02873300	2.07506700
Na	1.49891200	2.19457400	-0.42845800

28

E (M06/BS1) = --1557.074748 au

H(M06/BS1) = -1556.745361 au

G(M06/BS1) = -1556.828916 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.516145 au

C	2.83522900	0.06147300	0.04437300
C	3.64461200	-0.97036700	-0.45665200
C	3.41631000	1.13472700	0.73734800
C	5.02765000	-0.92665700	-0.27113100
C	4.79822100	1.17790800	0.92981900
C	5.57851900	0.14639500	0.41988400
H	5.26367400	1.99788200	1.46830100
H	6.65652400	0.18032700	0.56628600
C	-3.25520000	1.65256600	-1.07270100
O	2.55454500	2.06353500	1.20241100
C	3.08214000	3.16076500	1.92444000
H	3.76935300	3.75133500	1.30390200
H	2.22653300	3.77836300	2.20500100
H	3.60351400	2.82680800	2.83152700
O	-2.30243800	1.02659600	-1.68995400
C	-4.19917100	2.37138800	-2.00898500
O	-3.43145500	1.66486000	0.14739300
Pd	-1.04063700	-0.03884400	-0.53520500
C	-4.93310100	-0.89497600	1.17941600
H	-5.23488100	-1.75539900	0.57237800
H	-5.43997200	-0.90244900	2.15005400
H	-5.12131100	0.04718200	0.65836600
C	-3.07710800	-2.60202100	2.21734800
H	-2.02096400	-2.83373700	2.38163000
H	-3.60470000	-2.57238900	3.17620600
H	-3.52916300	-3.33718900	1.54319200
S	-3.15858100	-0.97476500	1.45238000
O	-2.59773700	-1.27464000	0.02098400
H	5.67075800	-1.71040200	-0.65944100
O	2.99848500	-1.94880600	-1.12511800

C	3.76701500	-3.01080000	-1.65952700
H	4.31203600	-3.54305700	-0.86845800
H	3.05637500	-3.69255800	-2.13089100
H	4.47863900	-2.64686500	-2.41275200
H	-4.66137900	3.22095600	-1.49737200
H	-4.99670900	1.67795700	-2.30568900
H	-3.69139100	2.70727300	-2.91797400
O	0.65098900	-0.86308500	0.40551400
O	0.79247400	0.86620800	-0.91518200
C	1.37333900	0.01821300	-0.15884900

29

E (M06/BS1) = -1557.058918 au

H(M06/BS1) = -1556.728428 au

G(M06/BS1) = -1556.811162 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.505029 au

C	-2.51260000	-0.03552000	0.14663400
C	-3.90721900	-0.19749700	0.30011800
C	-2.03366100	1.23666600	-0.19062300
C	-4.77613400	0.88214000	0.13394900
C	-2.89329900	2.32359200	-0.34778000
C	-4.25717700	2.12871400	-0.18060700
H	-2.52456400	3.31492100	-0.58447900
H	-4.93116200	2.97420500	-0.30065400
C	2.69770000	-2.18460900	-0.05185700
O	-0.66148000	1.40981700	-0.32067800
C	-0.20727000	2.66541700	-0.85401400
H	-0.40638300	3.46656700	-0.13428700
H	0.86716100	2.55632600	-1.00688700
H	-0.70257400	2.87001800	-1.80905600
O	1.94356500	-1.77262500	-1.02448300
C	3.61652300	-3.31353500	-0.45543000
O	2.72411000	-1.70787700	1.08331200
Pd	0.74388600	-0.22975600	-0.60353400
C	4.66971300	0.72493700	0.82425700
H	5.10149500	1.13483600	-0.09511400

H	5.21156200	1.08313000	1.70607500
H	4.65700200	-0.36798500	0.81026200
C	3.24254400	3.03815600	0.92414300
H	2.27097400	3.53742300	0.97628300
H	3.84011200	3.30977200	1.80031700
H	3.76394600	3.30232700	-0.00221500
S	2.95653600	1.26042900	0.94536300
O	2.39750400	1.02283200	-0.50326400
H	-5.84874300	0.75684300	0.24408300
O	-4.33694900	-1.44829900	0.56699100
C	-5.72757200	-1.67125500	0.68001600
H	-6.25295000	-1.42435000	-0.25294100
H	-5.84643300	-2.73686800	0.88841000
H	-6.16223200	-1.09159600	1.50586800
H	3.85116800	-3.93146800	0.41638400
H	4.55491400	-2.88369200	-0.83007600
H	3.18481600	-3.92740500	-1.25094000
O	-1.73229200	-1.96710000	1.28708600
O	-0.81659400	-1.49312500	-0.69668700
C	-1.62727400	-1.24555600	0.30744400

30

E (M06/BS1) = -1557.083882 au

H(M06/BS1) = -1556.753854 au

G(M06/BS1) = -1556.836812 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.523179 au

C	-1.78617700	-0.22861500	0.43086400
C	-1.42364100	0.77487900	1.38512700
C	-2.41298300	0.17942900	-0.78983600
C	-1.55100900	2.12459800	1.06559200
C	-2.53892900	1.53178400	-1.09893500
C	-2.11408800	2.46931200	-0.16255300
H	-2.98337600	1.86046600	-2.03310000
H	-2.23492200	3.52608800	-0.39747900
C	2.88555500	-1.62992400	0.04347800
O	1.87431400	-1.94278400	-0.69230400
C	4.15803900	-2.36889200	-0.30707200

O	2.88258000	-0.77599500	0.93972500
Pd	0.19559800	-0.81231500	-0.25960600
C	3.52935600	1.80700600	-0.64927600
H	3.59517100	1.83325100	-1.74250500
H	4.02732800	2.67612300	-0.20656500
H	3.94608800	0.88225400	-0.24116800
C	1.36467700	3.41575600	-0.94252600
H	0.28583500	3.55463300	-0.82318500
H	1.90536900	4.21988300	-0.43292600
H	1.62876100	3.37764200	-2.00492600
S	1.79125700	1.84238400	-0.17753700
O	1.10783500	0.83164300	-1.15424100
H	-1.25377700	2.90122700	1.76408700
C	-1.93176300	-1.68443400	0.88666800
O	-0.97561800	0.30412000	2.55071400
O	-2.85145300	-0.82351300	-1.55130300
C	-3.41930500	-0.51997300	-2.82003800
H	-2.68406700	-0.02494000	-3.46613200
H	-3.70555400	-1.47815800	-3.25559800
H	-4.30731700	0.11355900	-2.70826600
C	-0.48754000	1.22963400	3.51469100
H	-0.16156900	0.63051400	4.36592800
H	0.36230900	1.79575000	3.11308200
H	-1.28068100	1.91770200	3.83106400
H	4.68885500	-1.80088000	-1.08318000
H	4.81093500	-2.43498400	0.56854100
H	3.95409200	-3.36766000	-0.70460100
O	-0.85407900	-2.33833600	0.57384500
O	-2.91911000	-2.11732000	1.44635100

31

E (M06/BS1) = -1557.070355 au

H(M06/BS1) = -1556.741254 au

G(M06/BS1) = -1556.828160 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.509988 au

C	-1.08767100	0.67824300	-0.33999400

C	-2.24964800	0.39149600	-1.06421600
C	-1.08820500	1.75701300	0.54868600
C	-3.40232000	1.16707900	-0.89003300
C	-2.23299100	2.53764200	0.73732800
C	-3.37697900	2.22688600	0.01017100
H	-2.23830700	3.37363200	1.43187300
H	-4.27405800	2.82812500	0.14761600
C	3.40715300	-0.89601400	-0.25436200
O	2.41958300	-1.44149600	-0.86080600
C	4.72445900	-1.63165000	-0.39584500
O	3.34671100	0.15277700	0.41299400
Pd	0.59529100	-0.35738300	-0.56395800
C	-1.65800600	-3.58628700	1.82009700
H	-0.69339700	-3.94143300	2.19830500
H	-2.41914800	-3.60196200	2.60695000
H	-1.98499200	-4.19723500	0.97440700
C	-0.79816800	-1.17229500	2.73505500
H	-0.50718800	-0.14197500	2.50151700
H	-1.57185900	-1.17867400	3.51003200
H	0.07757800	-1.75218500	3.04738700
S	-1.46843700	-1.89837700	1.22754600
O	-0.22563800	-2.06830600	0.29363300
H	-4.31159600	0.95075500	-1.44501100
C	2.16830900	2.19034900	-0.58863200
O	-2.18348000	-0.67411400	-1.90755100
O	0.09081200	1.97629500	1.20890200
C	0.14077200	3.03186100	2.14911100
H	-0.58066600	2.87427600	2.96275800
H	1.15494800	3.02810400	2.55512400
H	-0.05375100	4.00237100	1.67151000
C	-3.34430700	-1.01556000	-2.63461300
H	-3.08153500	-1.88573900	-3.24079000
H	-4.17614200	-1.27938100	-1.96594200
H	-3.66100800	-0.19715500	-3.29663500
H	4.97756300	-1.74762600	-1.45665400
H	5.53217200	-1.09882400	0.11459600

H	4.63496800	-2.64140600	0.02303200
O	1.56971100	1.53426000	-1.36107100
O	2.74150300	2.93901200	0.08448900

32

E (M06/BS1) = -1557.069502 au

H(M06/BS1) = -1556.738946 au

G(M06/BS1) = -1556.821800 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.516082 au

C	2.47312600	0.08440100	0.32230400
C	3.71354300	0.36859500	-0.29681100
C	2.04349300	-1.25047700	0.32408800
C	4.48760600	-0.66545200	-0.84600400
C	2.80109700	-2.29186000	-0.20744100
C	4.03108000	-1.97923700	-0.78568600
H	2.44885600	-3.31513300	-0.18923400
H	4.63647200	-2.77441900	-1.21011600
C	-2.99019200	-1.91373700	-0.21707200
O	0.78788900	-1.48327700	0.90235200
C	0.43235700	-2.83374100	1.28588600
H	1.24895400	-3.25555400	1.87500800
H	-0.46532300	-2.73433200	1.89316400
H	0.22340800	-3.44162500	0.40402600
O	-1.77529500	-1.78257600	-0.67429700
C	-3.74696500	-3.08038900	-0.83802000
O	-3.52261100	-1.17238300	0.61923600
Pd	-0.68698700	-0.22687700	0.01590100
C	-2.56246500	3.63391200	-0.31306100
H	-2.69814600	3.74895200	-1.39081300
H	-3.25397400	4.27382200	0.24125600
H	-1.53296500	3.85747100	-0.02671800
C	-4.53875500	1.68284000	-0.51093600
H	-4.78052500	0.63223600	-0.34319800
H	-5.22217000	2.33082200	0.04416000
H	-4.54002400	1.92884800	-1.57554200
S	-2.86981900	1.91006600	0.15713300

O	-1.96250900	1.11054300	-0.86368500
H	5.43631300	-0.45217600	-1.32173300
O	4.07575500	1.67509600	-0.34897300
C	5.30644100	2.02229200	-0.98166000
H	5.30941400	1.73021300	-2.03826600
H	5.37884200	3.10783800	-0.90469800
H	6.16148000	1.56315500	-0.47206000
H	-4.59701300	-3.35480300	-0.20947800
H	-3.09198100	-3.94375800	-0.98264800
H	-4.12401400	-2.77992600	-1.82307500
O	2.26102900	1.96661200	1.76661500
O	0.40707000	1.30293000	0.74222200
C	1.68468100	1.19253400	1.00385400

33

E (M06/BS1) = -1557.085549 au

H(M06/BS1) = -1556.755106 au

G(M06/BS1) = -1556.837186 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.524210 au

C	1.72588000	-0.44513200	0.58756900
C	2.59520400	-0.45029300	-0.55580900
C	1.56594200	0.78035900	1.31904500
C	3.14234700	0.73650800	-1.02600300
C	2.11294700	1.96441400	0.82953800
C	2.88223500	1.91566500	-0.32773700
H	1.95228700	2.90992800	1.33840000
H	3.31076200	2.84362600	-0.70278200
C	-0.89814400	2.22039500	-0.80906800
O	-0.27448200	1.25972400	-1.40927300
C	-0.79906800	3.54453200	-1.52928600
O	-1.49883200	2.11397400	0.26696100
Pd	-0.20712200	-0.45641000	-0.32199300
C	-4.28321200	0.59080700	-0.36754100
H	-4.58116200	0.37724900	-1.40011500
H	-5.15841300	0.66143800	0.28675800
H	-3.68562600	1.50569600	-0.30879400

C	-4.35101200	-2.11496000	-0.05094400
H	-3.81292900	-3.03447700	0.19502100
H	-5.21587700	-1.99964600	0.61035200
H	-4.65930700	-2.12156800	-1.10216200
S	-3.22105400	-0.73939600	0.21409300
O	-2.19238200	-0.92815700	-0.93873900
H	3.76969000	0.75659400	-1.91159600
C	1.34070800	-1.77887200	1.24278600
O	2.80525000	-1.65647800	-1.08686400
O	0.87822900	0.67071300	2.45616700
C	0.38786900	1.86479400	3.06138300
H	-0.23909600	2.41007300	2.34376500
H	-0.21092900	1.54181900	3.91455700
H	1.21399500	2.49350000	3.41458100
C	3.56287200	-1.74238700	-2.28734400
H	3.59154200	-2.80103600	-2.54865500
H	3.07810800	-1.17511300	-3.09169500
H	4.58389600	-1.37336900	-2.13168800
H	-0.91283500	3.41754600	-2.61091100
H	-1.54828700	4.24610900	-1.15142500
H	0.19939500	3.96615300	-1.35225400
O	0.15238400	-2.11047800	0.84126800
O	2.06506300	-2.38858700	2.00488800

34

E (M06/BS1) = -1557.073230 au

H(M06/BS1) = -1556.743977 au

G(M06/BS1) = -1556.831253 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.510587 au

C	-1.70465700	-0.01740400	-0.05286400
C	-2.68447500	-0.83597400	-0.62236300
C	-2.08153000	0.98142800	0.84730300
C	-4.03188200	-0.66465500	-0.27985500
C	-3.42395300	1.16114200	1.19908600
C	-4.38033000	0.32686600	0.63076800
H	-3.72620700	1.93482200	1.90003400

H	-5.42739300	0.45900600	0.89829900
C	0.95766100	-2.00903500	1.52164300
O	0.21624200	-2.02029000	0.46429400
C	1.13476700	-3.37262500	2.15556700
O	1.52777400	-1.02156300	1.99847800
Pd	0.20580500	-0.21069900	-0.50489700
C	4.37994400	-0.87350200	0.55688000
H	4.73897300	-1.50553600	-0.26328700
H	5.21521800	-0.38762500	1.07205400
H	3.78094500	-1.44925000	1.26817400
C	4.46041200	1.14133100	-1.26175500
H	3.91795600	1.90185900	-1.83120300
H	5.27106600	1.61041900	-0.69440900
H	4.85011500	0.36954300	-1.93486300
S	3.28562800	0.38651500	-0.12092300
O	2.33847600	-0.38827700	-1.06362300
H	-4.80382100	-1.29298000	-0.71704700
C	0.03710400	2.90541200	-0.93860100
O	-2.25339900	-1.76392800	-1.51880000
O	-1.06477500	1.76423700	1.32594600
C	-1.38890800	2.76378900	2.27136600
H	-1.82503300	2.32604300	3.17984100
H	-0.45017600	3.26261100	2.52435200
H	-2.08907500	3.50158100	1.85430600
C	-3.21366700	-2.62298600	-2.09233500
H	-2.66643300	-3.29259700	-2.76025100
H	-3.73056000	-3.21994400	-1.32715800
H	-3.96038300	-2.06433400	-2.67499700
H	2.06692400	-3.81451600	1.77889000
H	1.23012800	-3.27134000	3.24127000
H	0.31299400	-4.05168500	1.91088900
O	0.21590000	1.87212400	-1.46360700
O	-0.11837200	3.95634000	-0.47692300

35

E (M06/BS1) = -1368.559413 au

H(M06/BS1) = -1368.248145 au

G(M06/BS1) = -1368.325888 au

E(B3LYP- D3BJ/BS2//M06/BS1) =-1370.825824 au

C	-1.70100500	0.16854600	-0.29873400
C	-2.65823200	-0.84465900	-0.40917300
C	-2.10647700	1.47353200	-0.00184700
C	-4.01879400	-0.55212300	-0.25215800
C	-3.46464500	1.77580800	0.15527900
C	-4.40070800	0.75510200	0.02943300
H	-3.79252500	2.78857700	0.37546900
H	-5.45784100	0.98515000	0.15257200
C	0.99609800	-0.53960400	2.12401400
O	0.20070100	-1.11284700	1.28439100
C	1.13181900	-1.28360000	3.43670100
O	1.64166500	0.49480300	1.92721900
Pd	0.20228600	-0.22127300	-0.57718100
C	4.41663100	-0.26956000	0.58494100
H	4.75203900	-1.24562400	0.21642000
H	5.26744400	0.40133300	0.74480900
H	3.83904800	-0.37101500	1.50740300
C	4.44934500	0.47048200	-2.02364400
H	3.89010700	0.80040300	-2.90368400
H	5.26577700	1.17092200	-1.81888700
H	4.83486300	-0.54337400	-2.17881500
S	3.30415100	0.46028100	-0.62980000
O	2.32620600	-0.67767600	-0.99734500
H	-4.77502800	-1.32704400	-0.34825600
O	-2.18760800	-2.09140400	-0.68896000
O	-1.11232200	2.40022400	0.10849200
C	-1.48098900	3.73367200	0.38509200
H	-1.98859800	3.82000600	1.35662500
H	-0.55351000	4.31059600	0.41301600
H	-2.13610400	4.14130000	-0.39829500
C	-3.12414300	-3.14069200	-0.79255800
H	-2.55097600	-4.04430900	-1.01408800
H	-3.67510900	-3.28410800	0.14817200

H	-3.84361600	-2.96364000	-1.60508300
H	2.02988800	-1.91379500	3.39156500
H	1.26851500	-0.56957000	4.25503300
H	0.27148800	-1.92794000	3.63867400

A15

E (M06/BS1) = -1346.339555 au

H(M06/BS1) = -1346.059342 au

G(M06/BS1) = -1346.136832 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1348.562207 au

C	-0.52697200	0.25203200	0.57711900
C	-1.04032300	1.54673200	0.68202800
C	-1.18423100	-0.81312400	1.19739300
C	-2.20544300	1.78233700	1.42408200
C	-2.34232200	-0.58378600	1.95222600
C	-2.83494400	0.71392900	2.05201800
H	-2.85716400	-1.39876700	2.45508200
H	-3.73673000	0.89685100	2.63387300
C	3.53483000	-0.19068300	0.45016000
O	3.38467900	-0.36425700	-0.78887300
C	4.89532500	-0.19564600	1.07745200
O	2.52168200	0.01513200	1.20366200
Pd	1.15265600	-0.08534800	-0.41732900
H	-2.61748900	2.78366700	1.51847600
O	-0.35551800	2.52179900	0.02608600
O	-0.64501400	-2.04725200	1.00168300
C	-1.35430400	-3.16089400	1.50246600
H	-2.36444600	-3.21855100	1.06979600
H	-0.78490600	-4.04560600	1.20841800
H	-1.43346500	-3.13220500	2.59825400
C	-0.85558900	3.84069700	0.09165100
H	-0.17938700	4.45493600	-0.50759700
H	-1.86978400	3.90897000	-0.32677900
H	-0.86585200	4.21750100	1.12412100
H	5.17023100	0.82960000	1.35446600
H	5.64284000	-0.58669900	0.38175000

H	4.88873500	-0.79175300	1.99622900
C	-1.62348000	-0.50682000	-1.97484900
S	-0.07584800	-0.25139700	-2.44849000
N	-2.73945200	-0.69861700	-1.69801000
C	-4.07088600	-0.89379100	-1.25923700
H	-4.47425600	-1.80904300	-1.70247800
H	-4.06319800	-0.98268200	-0.16615900
H	-4.68413700	-0.03682800	-1.55391900

A16

E (M06/BS1) = -1346.362770 au

H(M06/BS1) = -1346.081379 au

G(M06/BS1) = -1346.153266 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1348.577433 au

C	-1.11958500	0.00504800	0.10876300
C	-1.08317900	-1.23560700	0.84554200
C	-1.06910400	1.23705900	0.85867600
C	-0.82164800	-1.23457600	2.21190800
C	-0.80720400	1.21804100	2.22524200
C	-0.68628000	-0.01238400	2.86632800
H	-0.73070400	2.13735100	2.79672600
H	-0.49532600	-0.01937400	3.93775200
C	3.37771400	-0.00487500	0.10529500
O	-1.31701000	2.33303500	0.14717800
C	-1.17242800	3.60020800	0.77967300
H	-0.15683000	3.71955600	1.17660400
H	-1.35481600	4.34415400	0.00322800
H	-1.90739700	3.71813700	1.58486500
O	3.01764300	0.00745300	-1.11651200
C	4.82821500	-0.04796900	0.45600700
O	2.49022500	-0.00611000	1.01215900
Pd	0.94836100	0.00472100	-0.52673400
H	-0.75568200	-2.16056700	2.77385900
O	-1.34079400	-2.32090400	0.12111800
C	-1.21444900	-3.59650400	0.74034400
H	-1.95334800	-3.71334900	1.54209700

H	-1.40404300	-4.32973000	-0.04451100
H	-0.20178300	-3.73313100	1.13909700
C	-1.75459600	0.01404000	-1.26374900
N	-2.98104500	0.00693300	-1.56958900
S	-0.39988600	0.02567300	-2.39790800
H	4.99551300	0.37097200	1.45253500
H	5.16576400	-1.09194800	0.46056900
H	5.41956300	0.49364100	-0.28859200
C	-3.97393800	-0.01602900	-0.51899400
H	-4.54781700	-0.95025300	-0.58487300
H	-3.56980300	0.06510500	0.50482000
H	-4.68401700	0.80643900	-0.67252900

A17

E (M06/BS1) = -1044.481053 au

H(M06/BS1) = -1044.187441 au

G(M06/BS1) = -1044.265991 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1046.71613 au

C	-0.81283300	-0.62996100	0.17993600
C	-1.61480600	-0.16760700	1.22066600
C	-1.20933400	-1.75738900	-0.54576600
C	-2.80772200	-0.81491000	1.55445000
C	-2.39850800	-2.41968800	-0.21930900
C	-3.17929800	-1.93940000	0.82660600
H	-2.71673400	-3.30050400	-0.77155400
H	-4.10428000	-2.45451600	1.07924600
C	3.19293700	-0.40746000	0.71314200
O	3.21286700	0.55302700	-0.09499900
C	4.44406200	-0.94715100	1.33208500
O	2.08005500	-0.97546100	1.01648000
Pd	0.92723000	0.22337500	-0.21182100
H	-3.43963700	-0.45892900	2.36335500
O	-1.15809000	0.95521600	1.87411700
O	-0.38125500	-2.14683700	-1.55184900
C	-0.74797300	-3.28394300	-2.30445300
H	-1.71575400	-3.13998000	-2.80529900

H	0.03064100	-3.41693900	-3.05913200
H	-0.79838200	-4.18385300	-1.67513200
C	-1.95878400	1.49349100	2.91628900
H	-1.42095100	2.36669000	3.29158500
H	-2.94425800	1.80081600	2.54100500
H	-2.08346200	0.76489700	3.72673500
H	5.26084500	-0.22640600	1.23750300
H	4.73100900	-1.87325200	0.81879400
H	4.27550300	-1.19244500	2.38572500
C	-1.17660200	3.42318800	-2.39046400
O	-0.00596500	1.51293200	-1.58732000
O	-1.12799900	2.81030000	-0.12617100
C	-0.71786600	2.48956100	-1.32618800
H	-0.87509500	2.13360300	0.55781900
H	-0.82425600	3.08857900	-3.36747900
H	-2.27027000	3.48258700	-2.38253100
H	-0.79401200	4.42859100	-2.18089000

A18

E (M06/BS1) = -1044.484265 au

H(M06/BS1) = -1044.191213 au

G(M06/BS1) = -1044.267704 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1046.717175 au

C	0.80889400	1.27941900	0.32836900
C	1.44416900	0.70193800	1.47905700
C	1.52131300	1.28710900	-0.91747800
C	2.64044100	0.01069300	1.34464200
C	2.70720900	0.56233800	-1.04993000
C	3.23601400	-0.04878800	0.08200500
H	3.23661800	0.50924600	-1.99577700
H	4.17570900	-0.58950800	-0.01710900
C	-0.42644800	-2.81079600	-0.54858600
O	-1.51778600	-2.19692900	-0.74843600
C	-0.31032900	-4.28098100	-0.75151000
O	0.59318000	-2.12758100	-0.19150800
Pd	-0.49998300	-0.34975600	-0.25675100

H	3.12184000	-0.46611000	2.19257700
O	0.79199000	0.89492000	2.62535200
O	0.97561900	2.03959800	-1.87027100
C	1.51901900	1.96576100	-3.18281800
H	1.47367800	0.93634300	-3.56038800
H	0.89653800	2.61299000	-3.80225900
H	2.55481700	2.32566000	-3.19980300
C	1.28686600	0.25680600	3.79562500
H	0.59453700	0.51799900	4.59713500
H	1.30568000	-0.83214500	3.66231900
H	2.29175900	0.61962000	4.04409800
H	-1.28528000	-4.76249800	-0.63333700
H	0.41383300	-4.70733900	-0.05066400
H	0.04986200	-4.47480600	-1.76958200
C	-3.85474100	2.17131100	0.09625400
O	-1.87166800	1.10004100	-0.55077800
O	-2.76610300	0.47976300	1.41281500
C	-2.77047000	1.16048400	0.38987300
H	0.08319800	2.07510900	0.49804000
H	-4.38801700	1.89308200	-0.82040500
H	-4.56324000	2.21962600	0.92777000
H	-3.41580400	3.16123400	-0.07246700

A19

E (M06/BS1) = -583.487108 au

H(M06/BS1) = -583.374281 au

G(M06/BS1) = -583.420300 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -585.188003 au

C	-2.43658900	0.00017000	0.01946700
O	-1.76400800	1.08391400	0.02235100
C	-3.91783100	-0.00000100	-0.01758600
O	-1.76416500	-1.08372300	0.02242200
Pd	0.00000000	-0.00000700	0.00002200
H	-4.31021200	0.90694400	0.45120800
H	-4.31033100	-0.89160300	0.47984300
H	-4.24880600	-0.01739100	-1.06337900

C	3.91784000	-0.00002200	0.01748700
O	1.76402200	1.08386300	-0.02234100
O	1.76412900	-1.08375800	-0.02241900
C	2.43660400	0.00009800	-0.01951700
H	4.24880200	-0.01117700	1.06337400
H	4.31029600	-0.89448100	-0.47478500
H	4.31026600	0.90421300	-0.45649700

$ATS_{14\text{-}15}$

E (M06/BS1) = -1899.393036 au

H(M06/BS1) = -1899.025455 au

G(M06/BS1) = -1899.116953 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1901.884874 au

C	-0.48964100	1.40564100	0.34188700
C	0.44102500	2.45071700	0.30249000
C	-1.85646500	1.69818100	0.39557700
C	0.00272700	3.77853500	0.21797400
C	-2.29891700	3.02434300	0.31437500
C	-1.36128700	4.04569400	0.21534400
H	-3.35933700	3.26241900	0.33210100
H	-1.70213600	5.07746500	0.14795300
C	0.67485000	-1.98414100	2.37948500
O	0.85577700	-2.45823900	1.22195500
C	1.00373900	-2.80820200	3.58876000
O	0.22824900	-0.80097600	2.54093300
Pd	0.12990500	-0.45365300	0.39805600
C	3.39399400	-2.13989900	-0.92845300
H	3.13822800	-2.54349100	-1.91537300
H	4.44138000	-2.34553100	-0.68178400
H	2.73169300	-2.55871200	-0.16146600
C	4.18147200	0.05083400	-2.32567000
H	4.08601400	1.12455100	-2.51440000
H	5.21902700	-0.19145900	-2.07171500
H	3.85191800	-0.51712000	-3.20322700
S	3.10841400	-0.35605200	-0.92942000
O	1.68903400	-0.18172100	-1.47652900

H	0.71494000	4.59796800	0.16410100
O	1.75342800	2.10149100	0.37536900
O	-2.69813600	0.63758800	0.54273200
C	-4.08510000	0.88798200	0.57029000
H	-4.43687300	1.32290200	-0.37736200
H	-4.56696700	-0.08199700	0.72255200
H	-4.36245000	1.55483300	1.39899200
C	2.72137900	3.11814200	0.24767000
H	3.69401800	2.62276500	0.32022900
H	2.64569300	3.62579700	-0.72523600
H	2.63839400	3.86526800	1.05017300
H	2.09231700	-2.91784100	3.66738300
H	0.58142000	-3.81338700	3.48231700
H	0.62718500	-2.34106200	4.50305300
C	-2.52686100	-1.47646100	-1.70664800
S	-0.97884900	-1.07674600	-1.95750200
N	-3.65145800	-1.77217100	-1.55119300
C	-4.98924000	-2.20996600	-1.42380300
H	-5.13881600	-2.66368300	-0.43807600
H	-5.67259400	-1.36135400	-1.53610400
H	-5.20837300	-2.95388600	-2.19694500

$ATS_{14\text{-}17}$

E (M06/BS1) = -1597.543907 au

H(M06/BS1) = -1597.163181 au

G(M06/BS1) = -1597.252200 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1600.046479 au

C	-1.45890700	-0.34654800	0.28055100
C	-1.74313500	-1.10626600	1.42261800
C	-2.45057600	0.47081000	-0.27211600
C	-2.99688300	-1.01130600	2.03855400
C	-3.70394100	0.57237000	0.34629800
C	-3.95757800	-0.16712800	1.49438500
H	-4.47763300	1.21654500	-0.06290800
H	-4.93207100	-0.08855000	1.97348300
C	1.22780500	-2.56385300	-1.84035700

O	2.01740900	-1.59449200	-1.68149800
C	1.63827700	-3.77680300	-2.61945200
O	0.04173200	-2.52629100	-1.36436700
Pd	0.30772700	-0.56879400	-0.54455400
C	3.53595100	0.85504700	0.10479000
H	3.10924500	1.73561600	-0.38878400
H	4.61290800	0.96976000	0.26874200
H	3.33384200	-0.03921900	-0.49623600
C	3.11669700	2.23603500	2.40632800
H	2.63007800	2.29743200	3.38380900
H	4.20062600	2.33666900	2.52414300
H	2.72612300	3.01227600	1.73797000
S	2.74239500	0.61393100	1.70939000
O	1.21820200	0.64580000	1.46640600
H	-3.22867100	-1.58877700	2.92940700
O	-0.75304900	-1.92490300	1.86903500
O	-2.13401600	1.13614400	-1.41923000
C	-3.16660300	1.84206600	-2.07347800
H	-3.51561600	2.69659500	-1.47515800
H	-2.74240800	2.21070500	-3.01101200
H	-4.02125100	1.18870800	-2.29844300
C	-1.01826700	-2.72687000	2.99878300
H	-0.10651900	-3.29766000	3.19091200
H	-1.25342400	-2.11685400	3.88284300
H	-1.84814900	-3.42426200	2.81418000
H	2.72816600	-3.85061300	-2.67420900
H	1.24390400	-3.69854800	-3.64045400
H	1.21987800	-4.68409000	-2.17192400
C	-0.25122400	3.86945100	-1.59484800
O	0.73952400	1.70057500	-1.31584100
O	0.00669800	2.80724800	0.48755600
C	0.20553300	2.68290700	-0.81205800
H	0.41742800	2.00612800	0.93253100
H	-0.23716700	3.64627100	-2.66394500
H	-1.25933100	4.16189600	-1.28029200
H	0.41139500	4.71949600	-1.39187200

$ATS_{15\text{-}16}$

E (M06/BS1) = -1346.324155 au

H(M06/BS1) = -1346.045066 au

G(M06/BS1) = -1346.118227 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1348.544094 au

C	0.69757600	-0.00565600	-0.28956500
C	1.16335800	-1.27575200	-0.71964700
C	1.21009300	1.15954600	-0.91632100
C	2.11816900	-1.37451800	-1.73523900
C	2.17302400	1.05690500	-1.92260500
C	2.59562300	-0.20667500	-2.32243100
H	2.57543900	1.93981000	-2.41061300
H	3.33433200	-0.28574200	-3.11796300
C	-3.48795800	-0.10531600	-0.55900100
O	-3.39159800	0.11565800	0.68412000
C	-4.83648600	-0.27239000	-1.18935100
O	-2.44070600	-0.21145600	-1.27401200
Pd	-1.17484800	0.09138400	0.45706200
H	2.47964200	-2.33940900	-2.07938800
C	1.51800200	0.14221300	1.65440100
O	0.63686200	-2.33629200	-0.08229600
O	0.71570200	2.32985500	-0.47408300
C	1.26258800	3.53060200	-0.99340600
H	1.07687700	3.61672400	-2.07193500
H	0.75415000	4.34395900	-0.47228500
H	2.34198900	3.58961600	-0.80096600
C	1.16212800	-3.62230700	-0.36832000
H	0.64016200	-4.31531600	0.29391600
H	0.97354300	-3.90443600	-1.41215200
H	2.24069800	-3.66144200	-0.16417100
N	2.70342700	0.02813400	1.81601100
S	0.01863800	0.38631800	2.39460200
H	-4.77983600	-0.15480300	-2.27515800
H	-5.54504300	0.44816200	-0.76813400
H	-5.21613700	-1.27748100	-0.96677800

C	3.92973000	-0.19508900	1.11997100
H	4.71016300	-0.48468700	1.82888200
H	3.79853400	-0.99247600	0.37663400
H	4.23914200	0.72436000	0.60879900

ATS_{17-18}

E (M06/BS1) = -1044.460948 au

H(M06/BS1) = -1044.174037 au

G(M06/BS1) = -1044.246271 au

E(B3LYP- D3BJ/BS2/M06/BS1) = -1046.696251 au

C	0.90281000	-0.54506300	0.10348600
C	0.78562000	-1.76129100	0.83640500
C	1.71255100	-0.55151700	-1.06872400
C	1.47993400	-2.90564400	0.45031000
C	2.40849300	-1.69381800	-1.46037900
C	2.26898100	-2.84832400	-0.69584600
H	3.04162900	-1.70151600	-2.34259400
H	2.80533600	-3.74460900	-1.00354800
C	-3.10855100	-0.19196800	-0.73405700
O	-2.96300800	1.02969600	-0.44217600
C	-4.41659500	-0.72508900	-1.21327200
O	-2.10173500	-0.97795400	-0.63979700
Pd	-0.84681100	0.56144900	-0.02973100
H	1.41189500	-3.83153800	1.01366800
O	0.00043500	-1.69602500	1.92162600
O	1.78366000	0.62228300	-1.71394700
C	2.64857100	0.72781900	-2.83410700
H	2.33157300	0.05477800	-3.64093600
H	2.57660300	1.76211200	-3.17496800
H	3.68619800	0.50466200	-2.55443600
C	-0.09264500	-2.83678800	2.76066100
H	-0.73293300	-2.54622800	3.59546100
H	-0.54787700	-3.68155700	2.22812900
H	0.89465400	-3.12872100	3.14080500
H	-5.24262200	-0.19330900	-0.73124700
H	-4.49216900	-1.79936000	-1.02188100

H	-4.49593300	-0.56194400	-2.29534300
C	1.51501600	3.82969100	1.56616900
O	0.00037400	2.35031600	0.51620600
O	1.82338300	1.47816500	1.48931500
C	1.08088000	2.44728800	1.17008200
H	1.34212800	0.40321900	0.86246500
H	0.66864100	4.52069200	1.56928800
H	1.99513200	3.80676100	2.54866400
H	2.25578200	4.18625800	0.83995000

$TS_{14\text{-}15}$(R=Et)

E (M06/BS1) = -1938.681449 au

H(M06/BS1) = -1938.284153 au

G(M06/BS1) = -1938.378756 au

E(B3LYP- D3BJ/BS2/BS2//M06/BS1) = -1941.226375 au

C	0.97185700	0.89564900	0.30244500
C	1.17543000	1.08535100	1.67377000
C	1.53689400	1.80371700	-0.60095400
C	1.92391300	2.17116300	2.14316600
C	2.27391900	2.90092900	-0.14250100
C	2.45922300	3.06759100	1.22515400
H	2.70984900	3.61173400	-0.83992100
H	3.03835900	3.91645400	1.58458800
C	-2.27329700	-2.09187300	-0.03744200
O	-1.33412000	-2.37358600	-0.84784400
C	-3.51305100	-2.94599500	-0.06124000
O	-2.20927400	-1.10480000	0.74274700
Pd	-0.04641100	-0.67308700	-0.33883100
C	3.15903600	-1.83680300	1.39899600
H	2.98625100	-2.91819600	1.36046200
H	4.12599200	-1.60956800	1.86009700
H	2.34915700	-1.34474300	1.94957700
C	4.29470700	-2.33492200	-1.01960100
H	4.36414000	-2.10083000	-2.08531100
H	5.27384000	-2.20944100	-0.54570500
H	3.91581700	-3.35258900	-0.87582500

S	3.13482100	-1.17437100	-0.27760400
O	1.78568000	-1.66794700	-0.87430500
H	2.08712700	2.32258000	3.20702100
O	0.62567500	0.14438200	2.49722000
O	1.34603400	1.53626800	-1.92228500
C	1.68436200	2.53998000	-2.85595600
H	2.76847200	2.71714400	-2.89146200
H	1.34962900	2.17591000	-3.83064600
H	1.17067700	3.48488600	-2.62538000
C	0.85878400	0.26569500	3.88516700
H	0.35400500	-0.58073600	4.35667000
H	1.93384800	0.22131000	4.11571200
H	0.44380800	1.20190200	4.28394600
H	-3.99030600	-2.97378300	0.92382700
H	-3.28318400	-3.96240600	-0.39593600
H	-4.23026300	-2.51298900	-0.77245200
C	-3.07416900	0.99141500	-1.02815900
S	-1.65271300	1.21389600	-1.74872800
N	-4.14135300	0.86336700	-0.53652700
C	-5.03103200	0.40768700	0.49190100
H	-5.87452100	-0.10266300	0.01036600
H	-4.46071200	-0.33483300	1.07099700
C	-5.51491500	1.55443600	1.35780500
H	-6.05661000	2.29728100	0.76165800
H	-6.19296400	1.16938400	2.12741300
H	-4.67368200	2.05160200	1.85397600

$TS_{14\text{-}15}$(R=iPr)

E (M06/BS1) = -1977.965471 au

H(M06/BS1) = -1977.538787 au

G(M06/BS1) = -1977.634801 au

E(B3LYP- D3BJ/BS2/BS2//M06/BS1) = -1980.563453 au

C	1.19228900	0.89486600	0.29269500
C	1.41145800	1.08536900	1.66158900
C	1.76616500	1.78924700	-0.61872500
C	2.18469800	2.15812800	2.12059700

C	2.52879100	2.87319800	-0.17076700
C	2.72920000	3.04070700	1.19468400
H	2.97187600	3.57368200	-0.87404900
H	3.32763800	3.87952900	1.54600600
C	-2.10342500	-2.04437400	0.01136000
O	-1.17287100	-2.34953100	-0.80109600
C	-3.35899100	-2.87570000	-0.01038700
O	-2.01889300	-1.05360700	0.78384400
Pd	0.14162500	-0.66095600	-0.32839800
C	3.34826900	-1.86335900	1.38420400
H	3.15978100	-2.94256300	1.36168100
H	4.32305200	-1.64395700	1.83243300
H	2.55105200	-1.35269100	1.93646300
C	4.44515300	-2.41349100	-1.04077500
H	4.51107400	-2.19147900	-2.10926300
H	5.43026000	-2.30396900	-0.57538300
H	4.04610700	-3.42150100	-0.88378700
S	3.31539400	-1.22236600	-0.30057000
O	1.94995800	-1.69795300	-0.87377000
H	2.36026600	2.31003400	3.18241100
O	0.85203700	0.15722900	2.49300600
O	1.55582300	1.52139800	-1.93687600
C	1.93476200	2.50065200	-2.88075800
H	3.02486100	2.63705700	-2.91253300
H	1.59112800	2.13698600	-3.85241700
H	1.45534300	3.46671000	-2.66502500
C	1.09827400	0.27933900	3.87866100
H	0.58357500	-0.55718800	4.35707900
H	2.17425100	0.21798700	4.10073500
H	0.70168000	1.22353600	4.27730500
H	-3.90166500	-2.80158500	0.93781500
H	-3.13090400	-3.92340800	-0.23200300
H	-4.01335100	-2.50493600	-0.81173900
C	-2.88019300	0.99755100	-1.04130600
S	-1.44143200	1.22169000	-1.72475000
N	-3.96675800	0.85929600	-0.59064700

C	-4.83271600	0.47177800	0.50435700
H	-4.27609100	-0.32904100	1.01940300
C	-5.02059300	1.65447300	1.43981500
H	-5.52889600	2.47843900	0.92269000
H	-5.63821600	1.35006400	2.29343000
H	-4.05846800	2.01789300	1.81873900
C	-6.15179900	-0.04924100	-0.03429000
H	-6.77558300	-0.39518600	0.79833800
H	-6.69302400	0.74648300	-0.56252800
H	-6.00308500	-0.88629300	-0.72645800

$TS_{14\text{-}15}$(R=Ph)

E (M06/BS1) = -2090.989194 au

H(M06/BS1) = -2090.566225 au

G(M06/BS1) = -2090.663097 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -2093.721911 au

C	1.76082800	0.65996000	0.65444800
C	1.99446800	0.20066800	1.95537100
C	2.48515400	1.76085000	0.18259100
C	2.94218600	0.82360700	2.77562700
C	3.42225400	2.40334700	0.99939600
C	3.64014900	1.92122700	2.28542800
H	3.98397300	3.26128300	0.63886900
H	4.37421900	2.41278900	2.92152800
C	-1.86369600	-1.50991200	-0.66642900
O	-1.00463100	-1.47833300	-1.60804400
C	-3.16426200	-2.22502500	-0.92754300
O	-1.66119600	-0.94241400	0.43712100
Pd	0.50922300	-0.31981500	-0.52599000
C	3.42311700	-2.61877900	0.35392400
H	3.06678400	-3.52166700	-0.15474200
H	4.39789800	-2.79003200	0.82293300
H	2.69256800	-2.29383300	1.10373000
C	4.54827200	-2.15890000	-2.08090900
H	4.69846800	-1.48312100	-2.92721200
H	5.51529400	-2.42807900	-1.64289900

H	3.99782600	-3.05147600	-2.39757400
S	3.57254900	-1.28210100	-0.84769100
O	2.18299700	-1.22335300	-1.54238400
H	3.13294300	0.46361700	3.78333600
O	1.26957300	-0.88840300	2.34489300
O	2.23375000	2.13619800	-1.10255500
C	2.94619800	3.23943700	-1.62193600
H	4.02943200	3.05368300	-1.62354000
H	2.60169600	3.36840300	-2.65069800
H	2.73782700	4.15727400	-1.05410200
C	1.50473900	-1.41142000	3.63584700
H	0.82162300	-2.25567500	3.75342100
H	2.54126400	-1.76546100	3.74210000
H	1.29721200	-0.66607800	4.41614800
H	-3.69945500	-2.42921500	0.00534700
H	-2.98576900	-3.15822600	-1.47286800
H	-3.80367600	-1.59181900	-1.55812100
C	-2.32159100	1.69942400	-0.64332900
S	-0.78870300	2.12933200	-0.79434300
N	-3.47124300	1.39968400	-0.61708900
C	-4.58623500	0.78722500	-0.07429100
C	-4.53539000	0.29773400	1.23523900
C	-5.73368600	0.64059900	-0.85602500
C	-5.64617000	-0.35436900	1.75277500
H	-3.61922800	0.41116900	1.80893500
C	-6.83446000	-0.01855200	-0.32347100
H	-5.74278600	1.03263300	-1.87064200
C	-6.79297800	-0.51701100	0.97698800
H	-5.61435700	-0.74239800	2.76887100
H	-7.73002500	-0.14335200	-0.92833600
H	-7.65814600	-1.03265100	1.38876300

$TS_{14\text{-}15}$(R=tBu)

E (M06/BS1) = -2017.249486 au

H(M06/BS1) = -2016.794061 au

G(M06/BS1) = -2016.893054 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -2019.899350 au

C	1.30785400	0.90153200	0.35504900
C	1.53622700	1.01371300	1.73072100
C	1.78511400	1.90334600	-0.49831700
C	2.22237800	2.11641200	2.25398100
C	2.45953000	3.01648300	0.01475200
C	2.67058100	3.10555600	1.38620800
H	2.82821900	3.79921200	-0.64334700
H	3.20023600	3.96714100	1.78911400
C	-1.70883900	-2.28450100	-0.08490200
O	-0.81500900	-2.42046900	-0.98272300
C	-2.91448700	-3.18440600	-0.14818700
O	-1.63148300	-1.40280400	0.80809900
Pd	0.38207200	-0.68187900	-0.37833300
C	3.62573200	-1.83955100	1.20216700
H	3.49625400	-2.91487800	1.03524600
H	4.57770700	-1.63106700	1.70224500
H	2.79189100	-1.44500100	1.79491000
C	4.81960500	-1.98778000	-1.24048700
H	4.87195800	-1.63457100	-2.27397400
H	5.79092600	-1.85462400	-0.75268800
H	4.50537300	-3.03663400	-1.21140000
S	3.59109000	-0.98644200	-0.38651500
O	2.27823700	-1.46902400	-1.06382200
H	2.40289100	2.21120900	3.32148000
O	1.07061200	-0.01264500	2.50130800
O	1.57282200	1.70847300	-1.82936100
C	1.84981700	2.77762700	-2.70863600
H	2.92246800	3.01546000	-2.73665800
H	1.53097700	2.44750400	-3.70053500
H	1.28626100	3.67961300	-2.42808000
C	1.34774800	0.02365700	3.88578500
H	0.92522400	-0.89169100	4.30694500
H	2.43125000	0.04393400	4.07622800
H	0.88028200	0.89314700	4.36872400
H	-3.42023000	-3.23954000	0.82145800

H	-2.63699700	-4.18933500	-0.48352000
H	-3.61983000	-2.77511800	-0.88464800
C	-2.84032600	0.82336600	-1.00225300
S	-1.37188400	1.14141500	-1.58480700
N	-3.93239200	0.56586000	-0.63053300
C	-5.04929300	0.56976000	0.30604800
C	-5.64645300	1.97260400	0.30466200
H	-6.01754400	2.24055400	-0.69219600
H	-6.48724700	2.00762600	1.00918900
H	-4.90055400	2.71445800	0.61567000
C	-6.07470900	-0.45248700	-0.16409000
H	-6.94374000	-0.42743900	0.50492400
H	-6.41416200	-0.22798800	-1.18257900
H	-5.65765800	-1.46665200	-0.14586800
C	-4.49506000	0.20257500	1.67751800
H	-5.32154600	0.12641800	2.39570600
H	-3.95774800	-0.75293300	1.63476300
H	-3.79445800	0.97133700	2.02897500

TS_{14-15}

E (M06/BS1) = -1899.399371 au

H(M06/BS1) = -1899.032895 au

G(M06/BS1) = -1899.121631 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1901.890582 au

C	0.91960400	0.77720700	0.47261400
C	1.25383100	0.59906900	1.82017500
C	1.51865900	1.81919700	-0.24421500
C	2.16489100	1.45302200	2.45199700
C	2.41604000	2.69131900	0.38250500
C	2.72925700	2.49321800	1.72247000
H	2.87790900	3.50739500	-0.16752400
H	3.43385800	3.16494200	2.20976800
C	-2.66988100	-1.73058600	-0.11498700
O	-1.85601600	-1.90484800	-1.07793800
C	-3.97979000	-2.47224900	-0.15815600
O	-2.42518700	-0.93621200	0.83123300

Pd	-0.33745800	-0.48525800	-0.38499700
C	2.78183100	-2.40458100	0.66991700
H	2.48372100	-3.41748100	0.37674100
H	3.79146400	-2.39879300	1.09436000
H	2.06476200	-1.99248500	1.38953800
C	3.69145300	-2.37878400	-1.89425900
H	3.73294500	-1.87980800	-2.86620100
H	4.70327500	-2.49780600	-1.49313000
H	3.18870600	-3.34793500	-1.98262200
S	2.74272500	-1.33138700	-0.77871600
O	1.30479400	-1.49661500	-1.34786000
H	2.42891500	1.31645600	3.49746100
O	0.65511600	-0.45573300	2.44789300
O	1.19641800	1.90913700	-1.56417600
C	1.59835100	3.06436400	-2.26831400
H	2.69211300	3.13323300	-2.35134500
H	1.16959400	2.97612400	-3.26982500
H	1.21318300	3.97578000	-1.78799000
C	1.00255800	-0.70855800	3.79363900
H	0.43258800	-1.59018500	4.09616300
H	2.07775900	-0.91845800	3.89727300
H	0.73523700	0.13553600	4.44448000
H	-4.39969500	-2.59582200	0.84527200
H	-3.85708300	-3.44932300	-0.63658800
H	-4.69537900	-1.89629700	-0.76080600
C	-3.18487500	1.55426900	-0.42685700
S	-1.78747400	1.82154800	-1.17925500
N	-4.22876800	1.39659600	0.10099600
C	-5.11330400	0.82822000	1.05639900
H	-5.40003700	1.58326600	1.79566800
H	-6.01732800	0.46048100	0.56053200
H	-4.58885300	-0.00228200	1.54841300

$TS_{14\text{-}17}$

E (M06/BS1) = -1597.547469 au

H(M06/BS1) = -1597.166236 au

G(M06/BS1) = -1597.252979 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1600.049813 au

C	0.65596800	0.60841700	0.50441500
C	1.04763600	0.41986800	1.83653300
C	1.26353400	1.61816400	-0.25188100
C	2.00678600	1.25282300	2.42463500
C	2.22736900	2.45449300	0.32908300
C	2.58228900	2.26117000	1.65854500
H	2.70105100	3.24457900	-0.24750900
H	3.33056000	2.91103500	2.10890200
C	-3.18601700	-1.48591400	0.09047400
O	-2.37870500	-1.95447600	-0.76184500
C	-4.61229700	-1.96198900	0.09671500
O	-2.83461700	-0.61800100	0.94741700
Pd	-0.66628700	-0.64436800	-0.24249500
C	3.41792400	-1.63776100	0.20269000
H	3.26707400	-2.63486800	0.63226800
H	4.44544700	-1.51798500	-0.15715300
H	3.18711000	-0.86156500	0.94109700
C	2.88526000	-2.79022000	-2.19919000
H	2.23721800	-2.85439100	-3.07745700
H	3.91406600	-2.57939900	-2.50876100
H	2.83347700	-3.71666100	-1.61692000
S	2.28565500	-1.42940000	-1.18439600
O	0.93056200	-2.00052100	-0.67407700
H	2.30938800	1.11615800	3.45955000
O	0.46043500	-0.62072800	2.48765400
O	0.87541000	1.72062500	-1.54948300
C	1.55077500	2.64736500	-2.37053400
H	2.62843600	2.43220400	-2.41721400
H	1.11830300	2.54347000	-3.36890900
H	1.40540200	3.68094500	-2.02310900
C	0.92088300	-0.93612600	3.78444600
H	0.36531200	-1.82270400	4.09883600
H	1.99708200	-1.16425300	3.78232300
H	0.72688200	-0.12026900	4.49490900

H	-4.77173000	-2.76302300	-0.63045500
H	-5.27467000	-1.12078800	-0.14207000
H	-4.88584900	-2.31179400	1.09877800
C	-1.79559600	3.56681500	-0.87056600
O	-1.96485800	1.20165500	-1.24925700
O	-2.64544800	2.04110300	0.71067100
C	-2.13948000	2.15936400	-0.50733000
H	-2.83081000	1.07028400	0.85907400
H	-1.40302300	3.60467100	-1.88904100
H	-2.67526000	4.21343200	-0.77749100
H	-1.03918100	3.94615700	-0.17139600

TS_{14a-15}

E (M06/BS1) = -2452.473993 au

H(M06/BS1) = -2452.017709 au

G(M06/BS1) = -2452.119239 au

E(B3LYP- D3BJ/BS2/M06/BS1) = -2455.237299 au

C	0.04597000	1.69743900	-0.33688800
C	0.99847900	2.56022600	0.22028000
C	-1.12476900	2.25101000	-0.86738900
C	0.81906100	3.94907200	0.18996300
C	-1.31911100	3.63885000	-0.90231000
C	-0.33822700	4.47087200	-0.37576100
H	-2.22515700	4.06982100	-1.32066000
H	-0.48321600	5.54973000	-0.39900900
C	-0.36130800	-3.09549300	0.72456500
O	0.59919600	-2.35337300	0.32458100
C	0.04495500	-4.52262900	1.05465200
O	-1.54513300	-2.74720100	0.88399900
Pd	0.26882800	-0.25448700	-0.09125100
C	3.79553600	-2.44409200	-0.08632100
H	4.16638000	-2.64127100	-1.09932400
H	4.51776900	-2.77990500	0.66608800
H	2.81967000	-2.92159700	0.06824000
C	5.13265800	-0.09896100	-0.39852600
H	5.11012300	0.99539100	-0.41256000

H	5.88262700	-0.44774100	0.31971500
H	5.34902400	-0.47998500	-1.40348200
S	3.49116600	-0.67185500	0.10280000
O	2.57795500	-0.29974500	-1.06279200
H	1.56332000	4.62012400	0.61138600
O	2.07894500	1.97084600	0.80927900
O	-2.06841700	1.36371000	-1.30153900
C	-3.31734600	1.86775700	-1.71150400
H	-3.22841200	2.52227400	-2.59062400
H	-3.92683200	1.00005200	-1.98031200
H	-3.81752100	2.42255900	-0.90267300
C	3.00588500	2.79724900	1.47440000
H	3.75254700	2.12675000	1.91049700
H	3.50681200	3.48916600	0.78141200
H	2.53017400	3.37777300	2.27833700
H	0.52973500	-4.54098000	2.03989100
H	0.77238800	-4.90379000	0.32857600
H	-0.82763900	-5.18280000	1.08956300
C	-1.54169600	-1.33094900	-2.25830500
S	-0.05388400	-0.83346500	-2.64951500
N	-2.63269200	-1.70075400	-2.02291800
C	-3.76318200	-2.20544400	-1.33209700
H	-3.41165000	-2.68306600	-0.40970300
H	-4.44496300	-1.38275900	-1.08742200
H	-4.29364700	-2.92858900	-1.95954600
C	-2.67050300	-0.93022100	3.17845200
H	-2.13307000	-0.54723800	4.05335700
H	-3.75360900	-0.84412100	3.31618000
H	-2.39150900	-1.96552000	2.96014500
C	-2.66074200	1.65862000	2.30522600
H	-2.28078200	2.37753300	1.56755000
H	-3.75313300	1.72075700	2.36061700
H	-2.20732800	1.84968600	3.28444300
S	-2.17737900	0.01636200	1.73046300
O	-0.62901400	0.06362400	1.85605900

$TS_{14a\text{-}17}$

E (M06/BS1) = -2150.620973 au

H(M06/BS1) = -2150.151325 au

G(M06/BS1) = -2150.251831 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -2153.396616 au

C	1.22623900	-0.82178400	0.16190100
C	1.72762800	-1.09651900	1.44063300
C	1.85726100	-1.40776600	-0.94401700
C	2.81990200	-1.95714000	1.61713200
C	2.93557700	-2.28720700	-0.78064200
C	3.40292800	-2.54825800	0.50323900
H	3.41904000	-2.75019800	-1.63716100
H	4.24600200	-3.22406800	0.63689900
C	-1.96434400	2.39184800	-1.50479900
O	-1.85181000	1.87714700	-0.33143400
C	-3.14752200	3.33391400	-1.65110100
O	-1.21374200	2.17630500	-2.46425700
Pd	-0.24111000	0.48175700	-0.11097300
C	-4.14436100	-0.34345400	0.01675800
H	-4.15354500	-1.42641400	-0.15185500
H	-5.16497000	0.04101000	0.11992100
H	-3.62040000	0.16830900	-0.79435900
C	-4.17428800	-1.07576000	2.61883800
H	-3.73244600	-1.01249700	3.61718300
H	-5.22200900	-0.75886500	2.65519700
H	-4.09114800	-2.09865200	2.23299500
S	-3.24726700	0.03435400	1.53696500
O	-1.86978700	-0.65296600	1.43134100
H	3.21322500	-2.16861600	2.60824500
O	1.11631100	-0.45932900	2.47876400
O	1.37895900	-1.04444600	-2.16804900
C	2.07917900	-1.48564700	-3.30908100
H	2.04325600	-2.58047500	-3.41350000
H	1.58157600	-1.03086900	-4.16949500
H	3.13133800	-1.16388900	-3.28615400
C	1.75866100	-0.48054400	3.73327700

H	1.17130900	0.16570500	4.39064500
H	1.78823200	-1.49164600	4.16411800
H	2.78463800	-0.08928600	3.65995200
H	-3.06026900	4.16208500	-0.93694300
H	-4.08099800	2.80775700	-1.41217500
H	-3.20998300	3.73780100	-2.66634800
C	-1.05386400	-3.38606600	-2.24894900
O	-1.44479100	-1.15261000	-1.45930200
O	-1.47618800	-2.85054600	0.00207300
C	-1.34492400	-2.34829800	-1.21428300
H	-1.64617200	-2.08060600	0.62613500
H	-0.98734100	-2.92878500	-3.23868300
H	-0.10096500	-3.87426800	-2.00638200
H	-1.82611500	-4.16332300	-2.24065000
C	3.80673600	1.50263800	-0.47173000
H	3.69207500	2.05606400	-1.41104200
H	4.78062200	1.70699200	-0.01378600
H	3.69309800	0.42638100	-0.64291600
C	2.95011600	3.76082700	0.76373500
H	2.19222500	4.26001600	1.37363800
H	3.93269800	3.85601400	1.23729200
H	2.96084500	4.18039100	-0.24816500
S	2.50566200	2.01819800	0.66756000
O	1.21272000	2.07739200	-0.18984800

$TS_{15\text{-}16}$(R=Et)

E (M06/BS1) = -1938.681919 au

H(M06/BS1) = -1938.285003 au

G(M06/BS1) = -1938.377926 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1941.229629 au

C	1.15924400	0.33485500	0.23986200
C	1.75224300	1.25504300	-0.65650900
C	1.41243800	0.48788200	1.62347900
C	2.53381700	2.31661500	-0.18638900
C	2.20858000	1.53436300	2.09650600
C	2.73576900	2.44287800	1.18402800

H	2.39842000	1.66535800	3.15804700
H	3.33930300	3.27044000	1.55272300
C	-3.17316700	-1.90197700	0.00524900
O	-2.53808000	-1.23447300	-0.89819400
C	-4.59387500	-2.25859300	-0.38896600
O	-2.73168300	-2.20888800	1.11674600
Pd	-0.63531900	-0.47281500	-0.28622600
C	-3.37641200	3.12421100	0.77352900
H	-2.93719500	3.83063500	0.06074300
H	-4.45574900	3.28321700	0.86605400
H	-2.90078400	3.22693900	1.75266300
C	-3.82720000	1.60792300	-1.43688600
H	-3.66139100	0.65008200	-1.93827600
H	-4.90020000	1.79691700	-1.32185500
H	-3.33912100	2.42789100	-1.97568000
S	-3.07746800	1.44682900	0.19356700
O	-1.54574300	1.46940400	-0.06120400
H	2.97628900	3.03779700	-0.86782300
C	2.06695400	-1.56260300	-0.28050200
O	1.51416900	1.03353300	-1.96624000
O	0.83265800	-0.42534400	2.43230400
C	1.10887400	-0.36267400	3.81929300
H	0.73862300	0.57420200	4.25693900
H	0.58295700	-1.20534400	4.27275600
H	2.18545200	-0.45672400	4.01540100
C	2.21281300	1.81825300	-2.91557300
H	1.92599300	1.43464300	-3.89670400
H	1.93245100	2.87746900	-2.84468600
H	3.29994200	1.71854300	-2.78599200
N	3.26904000	-1.60592300	-0.29372400
S	0.61924300	-2.38155300	-0.52485500
H	-5.02967700	-2.97849500	0.31042400
H	-4.63295200	-2.65811600	-1.40851700
H	-5.20383900	-1.34415700	-0.37846200
C	4.43207100	-0.78847200	-0.07952600
H	4.11898800	0.26640000	-0.10759700

H	4.80866300	-1.00074600	0.93011100
C	5.49432300	-1.06998200	-1.12343800
H	6.37567300	-0.44848300	-0.93126600
H	5.80034300	-2.12205200	-1.09967200
H	5.12138500	-0.84005400	-2.12849900

$TS_{15\text{-}16}$(R=iPr)

E (M06/BS1) = -1977.967128 au

H(M06/BS1) = -1977.541279 au

G(M06/BS1) = -1977.637005 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1980.567252 au

C	0.98670500	0.32483800	0.27966100
C	1.48761100	1.48038100	-0.36405100
C	1.30743100	0.12377900	1.64328200
C	2.23825600	2.42874200	0.34005200
C	2.08506600	1.05106000	2.34191100
C	2.51782500	2.19758400	1.68282800
H	2.33040800	0.90529200	3.39025800
H	3.10387700	2.93189700	2.23262100
C	-3.28559000	-1.91955000	-0.17622000
O	-2.69319300	-1.15432300	-1.03027800
C	-4.70460300	-2.28261800	-0.56880900
O	-2.80288700	-2.31330100	0.89006900
Pd	-0.79641900	-0.42109100	-0.35932700
C	-3.66818000	2.91740900	1.21017100
H	-3.16026100	3.71304900	0.65442700
H	-4.75185700	3.07326400	1.21380100
H	-3.29547500	2.87410700	2.23729500
C	-3.89449600	1.71841600	-1.22719100
H	-3.66476000	0.83439800	-1.83169000
H	-4.97636700	1.88816900	-1.19327700
H	-3.36958700	2.60545900	-1.59984000
S	-3.30419000	1.33656500	0.43138100
O	-1.75496100	1.38758000	0.33225600
H	2.60678500	3.32900300	-0.14368400
C	1.93848900	-1.32326700	-0.76233400

O	1.20387600	1.58897600	-1.67880700
O	0.81029600	-0.99929800	2.20505500
C	1.16129900	-1.29338100	3.54452800
H	0.79047200	-0.52232900	4.23303800
H	0.68420500	-2.24699700	3.77963500
H	2.24950700	-1.39272900	3.66024200
C	1.81816800	2.63579700	-2.40865100
H	1.52905000	2.49015700	-3.45128000
H	1.46879300	3.61953600	-2.06808800
H	2.91314300	2.58731200	-2.32113200
N	3.13322800	-1.26673400	-0.89862400
S	0.51610700	-2.16281900	-1.07863200
H	-5.13284800	-3.01364800	0.12347100
H	-4.73814200	-2.67656000	-1.59107700
H	-5.32225800	-1.37357200	-0.55628500
C	4.26660700	-0.43095600	-0.55678300
H	3.86828000	0.58516700	-0.39502900
C	5.24478900	-0.41695100	-1.71747200
H	6.09003400	0.23997400	-1.48033500
H	5.63330700	-1.42644600	-1.90456800
H	4.76700600	-0.05093200	-2.63383900
C	4.89901000	-0.94296200	0.72705800
H	5.72729700	-0.28465900	1.01653700
H	4.16940900	-0.96247000	1.54660600
H	5.29661700	-1.95606500	0.58336800

$TS_{15\text{-}16}$(R=Ph)

E (M06/BS1) = -2090.991270 au

H(M06/BS1) = -2090.567990 au

G(M06/BS1) = -2090.663688 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -2093.727319 au

C	0.63813400	0.15233600	0.28477200
C	1.28383600	1.25471600	-0.32249300
C	0.98956500	-0.18315900	1.61284000
C	2.21310300	2.01996300	0.38444400
C	1.92552700	0.57692000	2.32142100

C	2.51044800	1.67265500	1.69800700
H	2.19478200	0.33107200	3.34490100
H	3.23759200	2.26716300	2.24881100
C	-3.83311300	-1.66786300	-0.39182900
O	-3.17262000	-0.81900400	-1.10521300
C	-5.28300400	-1.81742300	-0.81002600
O	-3.38814900	-2.29286300	0.57567100
Pd	-1.21455900	-0.36716000	-0.37409700
C	-3.68535600	3.00745800	1.65202100
H	-3.19505800	3.83479600	1.12760700
H	-4.75061300	3.21359000	1.79925800
H	-3.20419800	2.83187300	2.61801400
C	-4.26541200	2.10761500	-0.85031200
H	-4.15694900	1.29407200	-1.57462400
H	-5.32475700	2.31652300	-0.66488000
H	-3.73981400	3.01011400	-1.18236700
S	-3.50674300	1.50989600	0.67009900
O	-1.97979700	1.50400300	0.38235200
H	2.70944000	2.87209300	-0.07156400
C	1.36847500	-1.55194400	-0.89904800
O	0.94148200	1.49939200	-1.60839000
O	0.35648200	-1.25526000	2.14070400
C	0.77033300	-1.71192000	3.41415900
H	0.57149300	-0.96305700	4.19258600
H	0.18556700	-2.61059200	3.62137800
H	1.84028400	-1.96331000	3.41759600
C	1.60099400	2.55348900	-2.28374600
H	1.20161100	2.56201200	-3.30001500
H	1.40017100	3.52174300	-1.80539500
H	2.68716000	2.38500600	-2.31889800
N	2.55933900	-1.54303900	-1.09371100
S	-0.12413700	-2.24306000	-1.16290500
H	-5.74937400	-2.67713000	-0.31930900
H	-5.37287400	-1.91386900	-1.89772100
H	-5.82998800	-0.90873400	-0.52126100
C	3.72721500	-0.88788100	-0.72463800

C	4.32095300	0.00169400	-1.62348500
C	4.29108100	-1.13169400	0.52880200
C	5.46225800	0.69235400	-1.23656000
H	3.86819000	0.15025000	-2.60258100
C	5.43389600	-0.43572500	0.89954300
H	3.81327900	-1.84172500	1.20194000
C	6.01510700	0.48137100	0.02510800
H	5.91998900	1.40028100	-1.92472000
H	5.87068900	-0.60505900	1.88180200
H	6.90836900	1.02621800	0.32392100

$TS_{15\text{-}16}$(R=tBu)

E (M06/BS1) = -2017.248466 au

H(M06/BS1) = -2016.793638 au

G(M06/BS1) = -2016.892111 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -2019.898305 au

C	0.84508600	0.49040400	0.03983100
C	1.26237100	1.43939400	-0.92737800
C	1.08106000	0.77879900	1.40790100
C	1.87771800	2.63325000	-0.54499000
C	1.69520700	1.97068900	1.79645700
C	2.07633200	2.87744000	0.81087700
H	1.87416800	2.20466300	2.84221200
H	2.55023700	3.81020500	1.11202900
C	-3.27671800	-2.14802500	0.09797300
O	-2.77141000	-1.40602900	-0.82892200
C	-4.68647100	-2.62202200	-0.20257800
O	-2.73423900	-2.43664900	1.16895600
Pd	-0.91197400	-0.46805700	-0.35298900
C	-3.93393400	2.79387200	1.06921200
H	-3.61551600	3.55380400	0.34727800
H	-5.01560200	2.83932300	1.23275500
H	-3.40887500	2.92821100	2.01879400
C	-4.40372200	1.26832600	-1.12950800
H	-4.16271900	0.34855900	-1.67082300
H	-5.47778900	1.31770700	-0.91961400

H	-4.07105700	2.15423300	-1.68216900
S	-3.50185500	1.16836700	0.42725900
O	-2.01086800	1.36189700	0.04605900
H	2.19646500	3.36961400	-1.27750400
C	1.91355800	-1.27485600	-0.38530000
O	1.03619800	1.10343600	-2.21307400
O	0.68535900	-0.16959000	2.28047900
C	0.93840000	0.03537500	3.65942700
H	0.40971200	0.92236900	4.03262700
H	0.56235200	-0.85273900	4.17096300
H	2.01383400	0.14161400	3.85716900
C	1.51620300	1.96749700	-3.22799700
H	1.27522800	1.48362500	-4.17657300
H	1.02194300	2.94693700	-3.18355900
H	2.60398000	2.10241700	-3.15272600
N	3.10668600	-1.34971000	-0.29878000
S	0.52619700	-2.18424000	-0.77268000
H	-4.96784700	-3.45757400	0.44567800
H	-4.79670500	-2.90862200	-1.25401800
H	-5.38309000	-1.79159500	-0.01804200
C	4.42970700	-0.82924400	-0.00203100
C	5.42331600	-1.95915000	-0.25732100
H	6.44035500	-1.61219700	-0.03457100
H	5.20235500	-2.82340600	0.38133000
H	5.38704400	-2.28067900	-1.30569600
C	4.47009400	-0.40693000	1.46239100
H	3.78281400	0.42804500	1.64909900
H	4.19814000	-1.24511700	2.11708600
H	5.48707800	-0.08203500	1.71758000
C	4.71702400	0.34839900	-0.92641500
H	4.61341100	0.05325300	-1.97870800
H	4.03663300	1.18460100	-0.72301400
H	5.74626600	0.69354700	-0.76316300

$TS_{15\text{-}16}$

E (M06/BS1) = -1899.399608 au

H(M06/BS1) = -1899.033740 au

G(M06/BS1) = -1899.122229 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1901.893480 au

C	1.37808400	0.19314400	0.12593000
C	1.96093600	1.22180900	-0.65079600
C	1.74722200	0.08638700	1.48769400
C	2.85831500	2.13196500	-0.08069500
C	2.65512100	0.98233000	2.05752200
C	3.17842500	2.00074200	1.26690600
H	2.93634500	0.91311700	3.10462800
H	3.87281800	2.71057000	1.71314200
C	-3.07720100	-1.75180000	-0.03773800
O	-2.47689200	-1.02398200	-0.91820500
C	-4.54511500	-1.98519200	-0.34008700
O	-2.56867900	-2.19908500	0.99485400
Pd	-0.49197500	-0.43207700	-0.37812300
C	-2.94578500	3.14395500	1.33895500
H	-2.50278100	3.89890100	0.68032300
H	-4.00760400	3.34944800	1.51022400
H	-2.41399000	3.11228600	2.29376500
C	-3.61530100	1.89836500	-0.98486300
H	-3.54344400	0.98736000	-1.58729600
H	-4.66375800	2.13621400	-0.77409000
H	-3.11248200	2.74055400	-1.47366600
S	-2.77811800	1.52638800	0.56588100
O	-1.26454200	1.49674200	0.22035700
H	3.29906500	2.93511300	-0.66471800
C	2.14076500	-1.63413700	-0.74713500
O	1.59162700	1.25561500	-1.94795700
O	1.16168900	-0.91665400	2.17666400
C	1.54740700	-1.12151300	3.52343600
H	1.28680900	-0.25682700	4.14842400
H	0.99154200	-1.99614800	3.86734000
H	2.62487200	-1.31921300	3.60409500
C	2.22955900	2.18691000	-2.80309400

H	1.81639700	2.01665500	-3.79932100
H	2.02039400	3.22036300	-2.49646600
H	3.31617200	2.02438700	-2.82447900
N	3.33710900	-1.74312500	-0.81113400
S	0.63671200	-2.31334600	-1.06289300
H	-4.95390800	-2.78877200	0.27995500
H	-4.70272000	-2.21211700	-1.40020800
H	-5.09868100	-1.06066000	-0.12165200
C	4.53495800	-1.03428200	-0.49275700
H	5.34123500	-1.35102900	-1.16011900
H	4.36901600	0.04658900	-0.60261700
H	4.82834200	-1.25125500	0.54115800

$TS_{15\text{-}16'}$(R=Et)

E (M06/BS1) = -1938.681449 au

H(M06/BS1) = -1938.284153 au

G(M06/BS1) = -1938.378756 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1941.226375 au

C	1.05907200	0.70095900	0.23023700
C	1.54421700	1.64020300	-0.71594400
C	1.48332000	0.81594500	1.57909700
C	2.50605400	2.58012200	-0.35652200
C	2.44739600	1.75381000	1.94394300
C	2.95064600	2.60460800	0.96392100
H	2.80795800	1.83428100	2.96529700
H	3.70969400	3.33294300	1.24523500
C	-2.85363100	-2.22426800	0.13526200
O	-2.32911200	-1.48701900	-0.78317100
C	-4.17627000	-2.84817800	-0.26971800
O	-2.38952000	-2.41012400	1.26482300
Pd	-0.58726700	-0.36928200	-0.20826900
C	-4.01768300	2.67512100	0.73702600
H	-3.62728700	3.43682600	0.05333300
H	-5.11167400	2.64515400	0.70504400
H	-3.68010100	2.87223000	1.75816700
C	-3.96661500	1.06161400	-1.45458200

H	-3.57939300	0.13770300	-1.89717200
H	-5.06215700	1.05635400	-1.45167200
H	-3.57994300	1.94668800	-1.97260000
S	-3.37169800	1.06794800	0.24625500
O	-1.85083700	1.36018800	0.14254700
H	2.91093500	3.28575400	-1.07634100
C	2.33709100	-0.91854500	-0.28759300
O	1.05668100	1.50931600	-1.96509800
O	0.93505300	-0.06550500	2.43715400
C	1.41503800	-0.08956200	3.77077000
H	1.21262900	0.86105200	4.28141100
H	0.87381700	-0.89319500	4.27385300
H	2.49239900	-0.29929300	3.80037200
C	1.58716600	2.34424500	-2.98004300
H	1.07919700	2.05922500	-3.90341800
H	1.38713000	3.40257900	-2.76628200
H	2.66862300	2.19188800	-3.09412000
N	3.51105300	-0.68148000	-0.22898400
S	1.03085000	-1.95531300	-0.59327200
H	-4.51785300	-3.57408400	0.47430100
H	-4.09570700	-3.33097000	-1.25040900
H	-4.93157900	-2.05537400	-0.36492000
C	4.80024200	-1.27925900	-0.49505300
H	5.32880900	-0.61216400	-1.18778100
H	5.36661400	-1.25918000	0.44471400
C	4.69215500	-2.68472700	-1.05009900
H	4.18706500	-3.35036500	-0.33943100
H	4.13116800	-2.69219500	-1.99269000
H	5.69281600	-3.08805900	-1.24364100

$TS_{15\text{-}16'}$(R=iPr)

E (M06/BS1) = -1977.965471 au

H(M06/BS1) = -1977.538787 au

G(M06/BS1) = -1977.634801 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1980.563453 au

C	0.85848100	0.77694700	0.08327000

C	1.26847200	1.79749400	-0.81564800
C	1.32019700	0.83336000	1.42591200
C	2.21258900	2.74779800	-0.43101400
C	2.25960400	1.78178300	1.81608400
C	2.70236600	2.70685600	0.87109100
H	2.65104000	1.81487000	2.82888200
H	3.44556700	3.44348000	1.17253800
C	-2.89870200	-2.31566100	0.00533600
O	-2.50900200	-1.47020700	-0.88631500
C	-4.23371100	-2.96332900	-0.31103600
O	-2.30714100	-2.57714400	1.05835500
Pd	-0.77107200	-0.32486200	-0.34613200
C	-4.19776400	2.34113300	1.40245700
H	-3.92803000	3.21724000	0.80269000
H	-5.28502300	2.24963600	1.49368800
H	-3.74572700	2.40800900	2.39584900
C	-4.35232600	1.07015300	-0.99629200
H	-3.98500000	0.25012900	-1.62088200
H	-5.43706300	0.99199300	-0.86410000
H	-4.07707900	2.04455500	-1.41563300
S	-3.54775900	0.86565200	0.60264900
O	-2.06591600	1.26164500	0.36689000
H	2.56771700	3.50956300	-1.11900400
C	2.15437100	-0.71732900	-0.56873000
O	0.73291900	1.73417000	-2.04792300
O	0.84901100	-0.13108100	2.23878200
C	1.41291100	-0.24433900	3.53433600
H	1.19965500	0.64727300	4.13848000
H	0.94325800	-1.11507700	3.99584900
H	2.49907100	-0.39808700	3.47783600
C	1.21246000	2.63236600	-3.03513400
H	0.68089500	2.38193000	-3.95517800
H	0.99636700	3.67349800	-2.76180100
H	2.29247500	2.51008600	-3.18984400
N	3.32160900	-0.48481000	-0.41938600
S	0.89151200	-1.73670000	-1.07709600

H	-4.43943100	-3.79986800	0.36359600
H	-4.26983500	-3.30507300	-1.35155800
H	-5.02703800	-2.21138100	-0.19217100
C	4.64211600	-1.08856400	-0.40315400
H	5.25167400	-0.50256600	-1.10625000
C	4.58668100	-2.53869100	-0.84988900
H	3.97672900	-3.13001600	-0.15309100
H	4.15763200	-2.63199300	-1.85499700
H	5.59775400	-2.96412300	-0.86542300
C	5.21528300	-0.93018700	0.99640500
H	6.24365100	-1.30943500	1.02625400
H	5.21769300	0.12246300	1.30358600
H	4.61388900	-1.50080300	1.71734900

$TS_{15\text{-}16'}$(R=Ph)

E (M06/BS1) = -2090.989194 au

H(M06/BS1) = -2090.566225 au

G(M06/BS1) = -2090.663097 au

E(B3LYP- D3BJ /BS2//M06/BS1) = -2093.721911 au

C	0.28944700	0.90274900	0.08062200
C	0.76530800	1.71121800	-0.98275500
C	0.59955200	1.27823600	1.41204400
C	1.62004700	2.78249100	-0.73292200
C	1.45150900	2.35021200	1.66847000
C	1.95770700	3.06934200	0.58795100
H	1.72241200	2.63389400	2.68151400
H	2.62951800	3.90333700	0.78550600
C	-3.19861200	-2.48079800	0.29389200
O	-2.81102400	-1.75261500	-0.69735100
C	-4.46460800	-3.26873200	0.01376800
O	-2.65601100	-2.53596800	1.40227800
Pd	-1.20397400	-0.40037700	-0.25162400
C	-4.88709100	2.30072100	0.64511600
H	-4.68851200	3.03177200	-0.14599200
H	-5.96316500	2.13775000	0.76475300
H	-4.45489600	2.63780500	1.59134800

C	-4.88116400	0.50648200	-1.39836300
H	-4.43989300	-0.40659900	-1.80908500
H	-5.96087700	0.38225500	-1.26103200
H	-4.66269400	1.37442700	-2.03096700
S	-4.10215300	0.74128200	0.20914600
O	-2.65178700	1.19539800	-0.11008800
H	2.02127300	3.39221000	-1.53747600
C	1.76280800	-0.63707900	-0.11395900
O	0.38151700	1.33209200	-2.21683100
O	0.06098800	0.50187100	2.37209300
C	0.43217900	0.74655200	3.71805600
H	0.10914500	1.74424500	4.04342000
H	-0.07822800	-0.01149200	4.31519800
H	1.51752900	0.65014100	3.85324100
C	0.92708900	2.02126100	-3.32889000
H	0.51286300	1.53977300	-4.21682600
H	0.63630500	3.07998600	-3.32052000
H	2.02207100	1.94217200	-3.34611800
N	2.89631100	-0.26830100	0.03596200
S	0.60317300	-1.82302500	-0.40547900
H	-4.64406800	-4.01959000	0.78938500
H	-4.41997400	-3.75050500	-0.96939300
H	-5.31692700	-2.57444600	-0.00639800
C	4.24318500	-0.59797600	-0.01717300
C	4.64834900	-1.85691700	-0.47469300
C	5.18421200	0.35116500	0.38682100
C	6.00317700	-2.15616800	-0.52448700
H	3.89868200	-2.58190700	-0.78831100
C	6.53604900	0.03615900	0.33778700
H	4.83729700	1.32203200	0.73594000
C	6.94760800	-1.21427700	-0.11818000
H	6.32476000	-3.13246100	-0.88184200
H	7.27214800	0.77156000	0.65583600
H	8.00754300	-1.45709700	-0.15732200

$TS_{15\text{-}16'}$(R=tBu)

E (M06/BS1) = -2017.249486 au

H(M06/BS1) = -2016.794061 au

G(M06/BS1) = -2016.893054 au

E(B3LYP- D3BJ /BS2//M06/BS1) = -2019.899350 au

C	0.68569600	0.75024800	0.13130800
C	1.18734800	1.67758200	-0.82339700
C	1.05122600	0.92212700	1.49525600
C	2.13660600	2.62917200	-0.46046700
C	1.99875100	1.87186600	1.86334600
C	2.53931100	2.68945600	0.87196400
H	2.32426700	1.98709700	2.89316400
H	3.28939800	3.42590100	1.15670000
C	-3.13688300	-2.28964900	0.00036800
O	-2.67981700	-1.47683200	-0.88947300
C	-4.47211600	-2.91015300	-0.36758400
O	-2.60901600	-2.54233200	1.08853200
Pd	-0.94395300	-0.34740900	-0.31620700
C	-4.34842900	2.47884700	1.13955100
H	-4.08709500	3.31843100	0.48631200
H	-5.43405900	2.39901800	1.25785300
H	-3.87582800	2.59767500	2.11843400
C	-4.56369800	1.07555200	-1.17703400
H	-4.20989000	0.22558000	-1.76748400
H	-5.64495400	1.00417500	-1.01696200
H	-4.29886700	2.02615700	-1.65352100
S	-3.72235000	0.95656700	0.41067800
O	-2.24629200	1.33018700	0.11147900
H	2.56354000	3.31615500	-1.18552300
C	1.97087400	-0.78543700	-0.29211800
O	0.74488100	1.50788300	-2.08214900
O	0.48771100	0.05490000	2.35560400
C	0.96055600	0.03716800	3.69243900
H	0.74690600	0.98611400	4.20129600
H	0.42502900	-0.77123200	4.19380200
H	2.04036900	-0.16152600	3.72426300
C	1.35898700	2.26193000	-3.11449000

H	0.90379900	1.92502500	-4.04777000
H	1.17254700	3.33597400	-2.98534600
H	2.44122800	2.07746100	-3.14582900
N	3.13019200	-0.53596100	-0.12122400
S	0.73247300	-1.86925900	-0.74142800
H	-4.70472600	-3.76155400	0.27936200
H	-4.49008200	-3.22145500	-1.41789400
H	-5.25840000	-2.15198400	-0.24207100
C	4.50352100	-1.01957500	-0.14107800
C	4.53321000	-2.45687700	-0.64392500
H	3.93695100	-3.10918600	0.00807100
H	4.13174000	-2.52127700	-1.66401500
H	5.56606400	-2.82915500	-0.65450200
C	5.02446500	-0.92120200	1.28856400
H	6.07739300	-1.22945200	1.32165800
H	4.94680600	0.11061600	1.65690000
H	4.44883200	-1.57371000	1.95780900
C	5.28729900	-0.09114300	-1.06109300
H	4.89856200	-0.13910100	-2.08656100
H	5.21460000	0.94624000	-0.70889300
H	6.34430900	-0.38629800	-1.07477500

$TS_{15\text{-}16'}$

E (M06/BS1) = -1899.392930 au

H(M06/BS1) = -1899.026122 au

G(M06/BS1) = -1899.117560 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1901.887004 au

C	1.28698200	0.39752800	0.22915800
C	1.86783000	1.46851000	-0.49728900
C	1.74981500	0.13994100	1.54503600
C	2.94700300	2.17779200	0.02348100
C	2.83048000	0.84452400	2.07040900
C	3.41686100	1.83782400	1.29044100
H	3.21627900	0.63786100	3.06473200
H	4.26651700	2.38523900	1.69560500
C	-2.93565800	-1.94810300	-0.17393300

O	-2.38268600	-1.13040000	-1.00350900
C	-4.34490600	-2.35054100	-0.56584800
O	-2.42636600	-2.36670200	0.87119000
Pd	-0.49211100	-0.34885100	-0.34179600
C	-3.47631200	2.79862500	1.43203600
H	-2.99159300	3.63055800	0.90958300
H	-4.56409400	2.92225300	1.44058200
H	-3.10219800	2.72470700	2.45688400
C	-3.65682700	1.70124800	-1.05416800
H	-3.41688800	0.84362600	-1.69193500
H	-4.74040500	1.85816600	-1.01422100
H	-3.14150800	2.60821000	-1.39075500
S	-3.06366700	1.26254300	0.58973300
O	-1.51665200	1.36086600	0.50682500
H	3.42422400	2.98046500	-0.53134700
C	2.33987500	-1.19163900	-0.71742700
O	1.34194800	1.69331000	-1.71699000
O	1.11156300	-0.84965500	2.19857900
C	1.61076800	-1.24860000	3.46375700
H	1.53136300	-0.43406000	4.19559700
H	0.98796800	-2.08582700	3.78473000
H	2.65611400	-1.57687700	3.39237000
C	1.94045900	2.68629600	-2.53215700
H	1.37649700	2.69104300	-3.46693200
H	1.87365800	3.67628400	-2.06172900
H	2.99232400	2.44977100	-2.74046200
N	3.53353700	-1.13005400	-0.64647700
S	0.90896000	-1.94805400	-1.21770000
H	-4.74875700	-3.10401900	0.11706000
H	-4.36728500	-2.73319000	-1.59294300
H	-4.99165400	-1.46223600	-0.54279500
C	4.74096500	-1.79327500	-1.04106400
H	5.34283600	-1.11371300	-1.65311300
H	5.32189400	-2.04713600	-0.14860100
H	4.52589800	-2.70552900	-1.61026800

$TS_{17\text{-}18}$

E (M06/BS1) = -1597.543973 au

H(M06/BS1) = -1597.168089 au

G(M06/BS1) = -1597.256653 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1600.050777 au

C	-1.46382200	0.21624200	0.09224800
C	-2.27498300	-0.32682100	-0.93671400
C	-1.63206200	-0.29715000	1.40431200
C	-3.22507400	-1.31419300	-0.67018500
C	-2.56621900	-1.29528000	1.68383400
C	-3.34534300	-1.78148000	0.63604400
H	-2.70020400	-1.69006400	2.68674500
H	-4.07915100	-2.55814700	0.84662700
C	3.35709600	0.29425100	-0.12408300
O	2.55095300	0.87169000	-0.94001400
C	4.81204400	0.32243200	-0.54328700
O	3.02920100	-0.29641800	0.91768400
Pd	0.53935100	0.62755000	-0.41489200
C	-0.23839000	-3.69733100	-0.12819700
H	-0.00441700	-4.04537100	-1.14021700
H	-0.11850600	-4.50447100	0.60209300
H	-1.25921400	-3.30249100	-0.08659400
C	2.42900300	-3.17745800	-0.04446000
H	3.22054500	-2.45514600	0.17515000
H	2.51379300	-4.05075800	0.61093500
H	2.43737100	-3.47783100	-1.09809500
S	0.87055600	-2.34512700	0.30088600
O	0.68451700	-1.38947900	-0.92029500
H	-3.85929500	-1.72395200	-1.45076000
O	-2.07437100	0.20073300	-2.15718800
O	-0.84553700	0.26914400	2.33906000
C	-0.94702100	-0.19636400	3.67403300
H	-0.69916500	-1.26468100	3.73734100
H	-0.22238900	0.37950500	4.25260000
H	-1.95374600	-0.02992000	4.07929200
C	-2.90889700	-0.22323400	-3.22188600

H	-2.60263000	0.35398400	-4.09640100
H	-2.77570000	-1.29359500	-3.42605300
H	-3.96502300	-0.01975300	-3.00115300
H	5.02946500	-0.59284600	-1.11107400
H	5.46239700	0.32918000	0.33727100
H	5.03893700	1.17873500	-1.18569100
C	-0.36533400	4.77118100	0.51567600
O	0.54426900	2.64353000	0.01223600
O	-1.67769300	2.81613200	0.26894000
C	-0.51137200	3.30054600	0.24682500
H	-1.56110200	1.51133100	0.12238700
H	0.68356800	5.07545100	0.50673600
H	-0.91868700	5.33304400	-0.24515500
H	-0.81436700	5.00781000	1.48652300

$TS_{22\text{-}23}$

E (M06/BS1) = -1535.951720 au

H(M06/BS1) = -1535.627766 au

G(M06/BS1) = -1535.711225 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1538.254744 au

C	-2.29018700	0.10368700	-0.15198100
C	-2.77429800	1.40370500	0.04448700
C	-3.18214300	-0.93790300	-0.43862400
C	-4.14006700	1.67067400	-0.07194500
C	-4.54958900	-0.67909400	-0.55724000
C	-5.00289700	0.62272700	-0.37491600
H	-5.25495900	-1.47354200	-0.78259700
H	-6.06813700	0.82720500	-0.46593100
C	4.15806600	0.45475600	-0.61821800
O	-2.61870300	-2.16082700	-0.56903300
C	-3.46564100	-3.25051500	-0.87997300
H	-3.96008900	-3.10536300	-1.85022400
H	-2.82314300	-4.13215600	-0.92842200
H	-4.22713200	-3.39816200	-0.10207400
O	3.68574000	-0.68456800	-0.27173900
C	5.54968500	0.42789700	-1.20659600

O	3.57357100	1.54557700	-0.49093200
Pd	1.74805800	-0.59613500	0.47126800
H	-4.53302800	2.67282800	0.07204200
O	-1.83609000	2.33126100	0.35196400
C	-2.26508200	3.66350800	0.56158900
H	-2.97544300	3.72589900	1.39693500
H	-1.36888600	4.23786600	0.80617100
H	-2.72870000	4.07976400	-0.34307100
C	-0.83751500	-0.16163100	-0.08202300
N	-0.20288400	-0.43338100	1.01235400
S	0.16086100	-0.10090200	-1.51792400
H	5.58164000	1.04825000	-2.10898400
H	6.25169400	0.86635700	-0.48631300
H	5.87745400	-0.58815200	-1.44285100
C	-0.80506400	-0.52194400	2.32291400
H	-0.37273400	0.24718200	2.97559100
H	-1.89293800	-0.38635600	2.27623400
H	-0.57900300	-1.50225800	2.76011900
B	1.63646700	-2.92631700	1.13719200
H	0.77997400	-3.09095900	0.30670000
H	2.77164800	-3.19850900	0.85876400
H	1.30631400	-2.96941800	2.29139900
H	2.31652300	-0.85158000	1.91162800
Na	1.57678100	2.60602400	-0.06872900

$TS_{23\text{-}24}$

E (M06/BS1) = -1535.944500 au

H(M06/BS1) = -1535.620778 au

G(M06/BS1) = -1535.703512 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1538.245401 au

C	-2.24821800	0.08178200	-0.08564700
C	-2.55860600	1.44952800	-0.03112400
C	-3.26241700	-0.84779500	-0.36168800
C	-3.86558600	1.88682400	-0.25072800
C	-4.57295500	-0.41636100	-0.57910600
C	-4.85099800	0.94397600	-0.52148700

H	-5.36905900	-1.12526200	-0.78604300
H	-5.87139500	1.28218700	-0.69185200
C	4.12691200	0.43529900	-0.64371800
O	-2.87619100	-2.14189800	-0.37371900
C	-3.85463800	-3.12802000	-0.64088900
H	-4.29339300	-2.99556500	-1.63926700
H	-3.33714500	-4.08875700	-0.59820600
H	-4.65315500	-3.11101300	0.11309300
O	3.69961900	-0.61046500	-0.04380500
C	5.53714400	0.34410100	-1.18367400
O	3.49119400	1.49309500	-0.80595400
Pd	1.74971500	-0.51144200	0.68754300
H	-4.11889400	2.94199700	-0.21593300
O	-1.51844500	2.28061900	0.23489200
C	-1.80510800	3.66106700	0.38862100
H	-2.53958500	3.82316900	1.18823700
H	-0.86326200	4.14280800	0.66013800
H	-2.18115400	4.09502200	-0.54730800
C	-0.84736400	-0.34874900	0.09676000
N	-0.21730500	-0.35284700	1.22734800
S	0.15633000	-0.78208800	-1.27733500
H	5.97490300	-0.64727000	-1.03858400
H	5.53701500	0.59209700	-2.25145900
H	6.16374800	1.09088800	-0.68095600
C	-0.79995200	0.04244600	2.49111000
H	-0.47566600	1.06083300	2.74444700
H	-1.89656700	0.01415600	2.45567600
H	-0.44312300	-0.63246300	3.27653600
B	1.43257300	-3.18102100	0.09139600
H	1.87882600	-3.32653700	-1.00773900
H	2.18568800	-3.08359900	1.01839300
H	0.28239600	-3.43144900	0.30101200
H	2.34947700	-0.21685700	2.12466800
Na	1.33470300	2.29409200	-0.80225100

$TS_{25\text{-}26}$

E (M06/BS1) = -1535.935101 au

H(M06/BS1) = -1535.611104 au

G(M06/BS1) = -1535.697726 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1538.233616 au

C	2.37192200	-0.06121800	-0.13436400
C	3.08431000	1.06366100	-0.56523600
C	3.05490800	-1.23623100	0.20059300
C	4.47706200	1.02258100	-0.64991300
C	4.44668100	-1.28940300	0.10781200
C	5.13388000	-0.15470700	-0.30994800
H	4.99333900	-2.19322500	0.35996100
H	6.21960200	-0.19164100	-0.37767600
C	-4.85729100	0.04176100	0.06903200
O	2.27292100	-2.26016100	0.61292000
C	2.90927500	-3.45098500	1.03596800
H	3.59047800	-3.25978400	1.87630500
H	2.11263600	-4.12372300	1.36037200
H	3.46700000	-3.91939100	0.21374100
O	-4.04466300	-0.81167600	-0.42443300
C	-6.31092600	-0.38206000	0.02204700
O	-4.55563300	1.14957200	0.54899600
Pd	-1.96985900	-0.56830000	-0.53582600
H	5.04549700	1.88860600	-0.97603600
O	2.32810400	2.14082700	-0.87852000
C	2.99407800	3.36899300	-1.09916100
H	3.62803400	3.32870200	-1.99528500
H	2.21400200	4.11926500	-1.24559600
H	3.60678300	3.64285300	-0.22862300
C	0.91319300	0.04015900	0.09044600
N	0.07018200	-0.27010500	-0.87187800
S	0.34560600	0.55531000	1.63035900
H	-6.95274900	0.33772500	0.53777900
H	-6.63498600	-0.46729400	-1.02262900
H	-6.43122200	-1.37302200	0.47514700
C	0.57219200	-0.72685000	-2.17260200
H	1.32137500	-0.03498200	-2.57598400

H	1.01602200	-1.72420800	-2.07094500
H	-0.27149100	-0.78464800	-2.86431900
B	1.94946800	1.17437700	2.67259200
H	2.45681500	2.09238300	2.05946400
H	1.40621900	1.52763700	3.70325200
H	2.68087600	0.21620700	2.82449600
H	-1.04332400	0.63965100	-1.02910300
Na	-2.57466100	2.03562300	1.25803200

$TS_{28\text{-}29}$

E (M06/BS1) = -1557.048395 au

H(M06/BS1) = -1556.719783 au

G(M06/BS1) = -1556.801948 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.493271 au

C	2.72342900	-0.03301100	0.13694600
C	4.04283200	0.41244800	0.27817900
C	2.46761400	-1.40327000	-0.01703300
C	5.09966700	-0.50158000	0.25144300
C	3.51514100	-2.32451800	-0.04118500
C	4.81735700	-1.85351200	0.09224900
H	3.33105100	-3.38915000	-0.15093900
H	5.63999700	-2.56610700	0.07576000
C	-2.50134700	2.28290900	0.09010400
O	1.15279200	-1.75504500	-0.09486300
C	0.83278100	-3.12128800	-0.29051700
H	1.16837400	-3.73200600	0.55782600
H	-0.25652900	-3.17003500	-0.36421800
H	1.27548100	-3.50506000	-1.21911200
O	-1.83756300	1.86857500	-0.94613100
C	-3.23937000	3.57693200	-0.16838100
O	-2.58051700	1.70433900	1.17293200
Pd	-0.93402000	0.08555900	-0.71436300
C	-4.90488400	-0.37868900	0.87062900
H	-5.45382800	-0.61461200	-0.04740500
H	-5.44190300	-0.74234400	1.75288200
H	-4.71666900	0.69405300	0.95985600

C	-3.86146300	-2.87489000	0.59343200
H	-2.97997200	-3.51356900	0.49542600
H	-4.43521400	-3.16858600	1.47840700
H	-4.47914200	-2.93145100	-0.30917700
S	-3.29550700	-1.17911800	0.80617800
O	-2.77785700	-0.83623000	-0.63101400
H	6.13027700	-0.17373100	0.34975300
O	4.19793200	1.75031100	0.40435600
C	5.51112400	2.25737700	0.52898000
H	6.11914100	2.01714600	-0.35424000
H	5.41262700	3.34170200	0.61513100
H	6.00737700	1.86621800	1.42787100
H	-3.26070500	4.17684900	0.74659400
H	-4.27599400	3.33704900	-0.43872500
H	-2.79454100	4.14948700	-0.98660200
O	1.25172400	1.56231800	1.13609500
O	0.89016100	0.85882000	-0.97874800
C	1.55208800	0.89935800	0.15377400

$TS_{28\text{-}32}$

E (M06/BS1) = -1557.051159 au

H(M06/BS1) = -1556.722772 au

G(M06/BS1) = -1556.805772 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.494768 au

C	2.50016900	-0.07567600	0.07325500
C	3.79457000	0.45529100	0.11574200
C	2.30575700	-1.44116200	0.33059700
C	4.88556700	-0.36996100	0.40210700
C	3.38688400	-2.27228100	0.62492700
C	4.66279400	-1.71944300	0.65267500
H	3.24653400	-3.32865000	0.83427400
H	5.51177300	-2.36104600	0.88166100
C	-3.35270400	-1.44332400	0.43962000
O	1.01303500	-1.86546800	0.31048000
C	0.73705000	-3.21803700	0.62618600
H	1.08769200	-3.46688200	1.63647900

H	-0.35071100	-3.31949300	0.58197400
H	1.19697100	-3.90065600	-0.10065000
O	-2.80075300	-1.51277500	-0.73300100
C	-4.67322000	-2.16787400	0.52751700
O	-2.88875700	-0.82481800	1.39996100
Pd	-1.10078500	-0.46880100	-0.94994400
C	-1.56127300	3.62274300	0.28538200
H	-2.20929200	3.99514700	-0.51497500
H	-1.65207300	4.24301200	1.18322600
H	-0.51777100	3.57004300	-0.03564600
C	-3.76906000	2.22856300	1.08159900
H	-4.20920200	1.25021100	1.29343700
H	-3.82485400	2.86750200	1.96932400
H	-4.25612200	2.70657100	0.22519000
S	-2.03670000	1.93851400	0.69284600
O	-2.14027300	1.29423100	-0.73894000
H	5.89632800	0.02706900	0.42943800
O	3.89433400	1.77618100	-0.16039700
C	5.17932200	2.36321200	-0.13371700
H	5.84133200	1.91610100	-0.88825900
H	5.03580200	3.42173300	-0.36183900
H	5.64336000	2.26612300	0.85767500
H	-4.89170100	-2.42880500	1.56720500
H	-4.68359600	-3.06520500	-0.09900800
H	-5.46572700	-1.49929800	0.16647000
O	0.92216900	1.66214100	0.51745900
O	0.68598600	0.38537400	-1.32005600
C	1.29391900	0.76065200	-0.22891800

$TS_{29\text{-}30}$

E (M06/BS1) = -1557.059939 au

H(M06/BS1) = -1556.730925 au

G(M06/BS1) = -1556.811194 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.504515 au

C	-2.04857600	-0.14706900	-0.21361100
C	-2.50616800	-0.11072100	1.11676700

C	-1.67403800	1.06276900	-0.82532200
C	-2.59884800	1.10564100	1.79917200
C	-1.79294900	2.28493200	-0.16662600
C	-2.25319900	2.28260000	1.14654500
H	-1.53413900	3.21801000	-0.65937600
H	-2.33856700	3.22852700	1.67773700
C	2.41121400	-2.00983400	0.53285800
O	-1.16542600	0.93151000	-2.09538400
C	-0.69905000	2.09892800	-2.76070300
H	0.12506700	2.56356700	-2.20241500
H	-0.33560300	1.76025500	-3.73254600
H	-1.51551000	2.81752000	-2.90106300
O	1.96554400	-1.88478400	-0.67788900
C	3.53239000	-3.01755300	0.65115000
O	2.02122700	-1.37076500	1.51131200
Pd	0.52602200	-0.47067300	-0.91251800
C	3.49957400	1.37124400	1.50723900
H	4.15714000	1.78508900	0.73537300
H	3.63176500	1.89633500	2.45874600
H	3.66382200	0.29914200	1.64260500
C	1.77337600	3.34796400	0.77161600
H	0.78008700	3.62710400	0.40807300
H	1.95225200	3.81196000	1.74736700
H	2.54561900	3.63795900	0.05106600
S	1.79379100	1.56017400	0.97190400
O	1.83276100	1.07657600	-0.52266500
H	-2.94383100	1.14236800	2.82797900
O	-2.81235300	-1.30371500	1.66061400
C	-3.29186100	-1.33261200	2.99228500
H	-4.22470100	-0.76171700	3.09099100
H	-3.48546000	-2.38260500	3.22079900
H	-2.54508900	-0.93957800	3.69505100
H	3.53786900	-3.44953400	1.65631000
H	4.48707600	-2.49753500	0.49861300
H	3.45314800	-3.80733100	-0.10114200
O	-3.04424800	-2.08504600	-1.19077700

O	-0.83595600	-1.87518100	-1.33541200
C	-2.01870100	-1.46464200	-0.96590900

TS_{30-31}

E (M06/BS1) = -1557.054805 au

H(M06/BS1) = -1556.726902 au

G(M06/BS1) = -1556.810611 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1556.810611 au

C	1.34749700	-0.14816900	0.14236600
C	2.31411500	-0.29299000	-0.88397100
C	1.65310100	0.68302300	1.24794200
C	3.56330900	0.31463700	-0.77565200
C	2.90693900	1.28132500	1.36973400
C	3.83575600	1.08410300	0.35263000
H	3.16387500	1.89795800	2.22601900
H	4.81477400	1.55199900	0.44198300
C	-3.32339700	-1.01761200	0.48090200
O	-2.57545800	-1.29354800	-0.52507500
C	-4.76762400	-1.45308600	0.33997100
O	-2.95884900	-0.39779000	1.49326600
Pd	-0.57770500	-0.63809500	-0.22220200
C	-2.82706600	2.13569900	-0.62295900
H	-2.69212700	1.53735500	0.28926800
H	-3.13900500	3.15922500	-0.38648900
H	-3.56767000	1.66578600	-1.27747200
C	-0.26154300	2.96200200	-0.24972700
H	0.77622100	2.94049500	-0.59970100
H	-0.58532400	3.99877100	-0.10800500
H	-0.36769300	2.38816200	0.67937800
S	-1.28216000	2.23018600	-1.54119900
O	-0.77920900	0.77996600	-1.74293300
H	4.32107100	0.20140800	-1.54536600
C	1.29249700	-1.98789000	1.11237400
O	1.95057700	-1.08017700	-1.91211900
O	0.66666100	0.82362700	2.15914600
C	0.92517700	1.61414800	3.30871900

H	1.15152400	2.65182300	3.02696800
H	0.01125200	1.58964300	3.90491600
H	1.75675800	1.20145900	3.89404300
C	2.89541000	-1.31617500	-2.94272400
H	2.41215400	-1.99445500	-3.64828300
H	3.15975200	-0.38248800	-3.45637200
H	3.80475300	-1.78645900	-2.54606900
H	-5.31871300	-0.67440600	-0.20517400
H	-4.85442100	-2.38179900	-0.23338200
H	-5.23485400	-1.57179100	1.32273000
O	0.08686200	-2.16229200	1.11824700
O	2.37837200	-2.35446100	1.38744800

TS_{32-33}

E (M06/BS1) = -1557.056899 au

H(M06/BS1) = -1556.728267 au

G(M06/BS1) = -1556.810873 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.501691 au

C	-1.93339900	-0.60017000	-0.26185400
C	-2.19141200	-1.21300200	0.97919300
C	-2.18983100	0.77835700	-0.39680300
C	-2.72431100	-0.47323600	2.03606500
C	-2.73472900	1.52254500	0.64824000
C	-2.99234100	0.87894100	1.85230400
H	-2.93945500	2.58287500	0.53895400
H	-3.40778100	1.45213200	2.67860800
C	1.39653600	2.09001000	1.28298100
O	-1.84691800	1.31590000	-1.61581000
C	-1.99953100	2.71959400	-1.79176800
H	-1.39835300	3.27110700	-1.05661200
H	-1.63772900	2.93286200	-2.79919800
H	-3.05514300	3.00670900	-1.70995900
O	0.89742100	2.23019100	0.09092700
C	1.78819600	3.39949400	1.92213200
O	1.56581900	1.00994800	1.85233800
Pd	0.40169400	0.51133200	-0.82028600

C	3.34500500	-2.56499800	-0.83753700
H	4.18265400	-2.13004300	-1.39332600
H	3.68255000	-3.38776000	-0.19871400
H	2.57259100	-2.92107900	-1.52521200
C	4.05272100	-0.77149300	1.10256200
H	3.73493100	0.06953800	1.72478900
H	4.39465300	-1.60386800	1.72634500
H	4.82802900	-0.46987600	0.39020800
S	2.59490900	-1.29330300	0.19038400
O	2.39033600	-0.12758900	-0.83670100
H	-2.92726300	-0.93968600	2.99567900
O	-1.87527600	-2.52072800	1.05749600
C	-2.09031600	-3.18589100	2.28809200
H	-3.15475800	-3.18862600	2.55859200
H	-1.75246300	-4.21348300	2.14025700
H	-1.50887400	-2.72365400	3.09714000
H	1.94064200	3.26605900	2.99690700
H	1.02810200	4.16688500	1.74232000
H	2.72529800	3.75418600	1.47493600
O	-2.08657600	-2.32476400	-1.91291400
O	-0.19499200	-1.15461100	-1.78205400
C	-1.41035800	-1.44339700	-1.41043000

TS_{33-34}

E (M06/BS1) = -1557.056972 au

H(M06/BS1) = -1556.729515 au

G(M06/BS1) = -1556.815794 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1559.494846 au

C	1.61234100	-0.01269100	0.08146000
C	2.52656300	-0.23359800	-0.98142300
C	2.01211400	0.81278700	1.16471300
C	3.82584000	0.26510600	-0.91499500
C	3.31167200	1.31312200	1.23345900
C	4.19004100	1.02612400	0.19303900
H	3.64187800	1.92120500	2.07064900
H	5.20512700	1.41623200	0.24602700

C	-1.43278200	2.11444600	-0.92731300
O	-0.59868200	1.24581500	-1.39135200
C	-1.74970400	3.23624400	-1.89231300
O	-1.98690700	2.06795600	0.17693700
Pd	-0.33457400	-0.40283900	-0.21181100
C	-4.59967700	0.46380800	-0.25526700
H	-4.90668400	-0.03753900	-1.18021000
H	-5.45954300	0.62785400	0.40325500
H	-4.09353700	1.41262100	-0.46039000
C	-4.44637200	-2.03441200	0.78944100
H	-3.83756500	-2.82019200	1.24539300
H	-5.28897300	-1.78955700	1.44437900
H	-4.79969700	-2.35301000	-0.19762200
S	-3.40010100	-0.57873800	0.59575800
O	-2.41097500	-1.02106100	-0.50953300
H	4.54974500	0.08162800	-1.70338000
C	1.55679700	-1.85836800	1.01460200
O	2.05998400	-0.98602700	-1.99336800
O	1.08228900	1.01307200	2.11541000
C	1.45225100	1.73836300	3.27735400
H	1.73541800	2.76868200	3.02608200
H	0.56931800	1.75085100	3.91890300
H	2.28111400	1.24584300	3.80214100
C	2.94695100	-1.32727600	-3.04672200
H	2.37142700	-1.94902100	-3.73485200
H	3.29881300	-0.43002300	-3.57200600
H	3.80725800	-1.89613600	-2.67095600
H	-2.67686700	2.98520100	-2.42541700
H	-1.92524400	4.16723400	-1.34399700
H	-0.95942100	3.37915300	-2.63505400
O	0.36171100	-2.08072300	0.91444100
O	2.62299000	-2.20310500	1.38272000

TS_{27}

E (M06/BS1) = -1509.308821 au

H(M06/BS1) = -1509.018584 au

G(M06/BS1) = -1509.099597 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1511.561600 au

C	-2.42397700	0.00426300	0.13765700
C	-3.27123600	-1.06804100	-0.16928900
C	-2.96848800	1.28019200	0.33237500
C	-4.65176100	-0.87628600	-0.25821700
C	-4.34863600	1.48058900	0.24807700
C	-5.16869600	0.39628800	-0.04244100
H	-4.78317800	2.46413600	0.40133000
H	-6.24428800	0.54896200	-0.11001500
C	4.75520600	0.02710300	0.06242100
O	-2.07124500	2.26149200	0.59463600
C	-2.56499400	3.56539100	0.82857800
H	-3.24675700	3.58559000	1.68983100
H	-1.69373700	4.18755800	1.04448100
H	-3.08386400	3.96202000	-0.05485900
O	3.94122700	0.60626800	-0.73240500
C	6.21295900	0.40432300	-0.10788600
O	4.46117700	-0.82175100	0.92557500
Pd	1.86336400	0.32275900	-0.64334200
H	-5.31719800	-1.70148900	-0.49522600
O	-2.65049200	-2.25395100	-0.37919400
C	-3.45211000	-3.37814400	-0.68280300
H	-4.00472100	-3.23364500	-1.62133700
H	-2.76575100	-4.22023900	-0.79477400
H	-4.16202100	-3.59404100	0.12727600
C	-0.95664800	-0.21010300	0.29259700
N	-0.18704800	-0.01304500	-0.76646700
S	-0.38760300	-0.66888300	1.82829500
H	6.73439500	-0.41019200	-0.62717000
H	6.33358000	1.32078800	-0.69278300
H	6.69013000	0.52129800	0.87125800
C	-0.76740400	0.31598700	-2.07009500
H	-1.62539100	-0.32506600	-2.30765400
H	-1.08732300	1.36571300	-2.09069500
H	0.00235900	0.17400600	-2.83365900

H	0.96247100	-0.96754500	-0.85581100
Na	2.47972100	-1.61065100	1.76012100

TS'$_{25\text{-}26}$

E (M06/BS1) = -1373.685243 au

H(M06/BS1) = -1373.364292 au

G(M06/BS1) = -1373.445256 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1375.957103 au

C	-2.21521800	-0.01002000	-0.07984900
C	-2.90469100	-1.21930100	0.08631900
C	-2.92612900	1.16705500	-0.34078100
C	-4.29729600	-1.25290600	0.00490800
C	-4.32041000	1.14256700	-0.41746600
C	-4.98153000	-0.06738800	-0.24096900
H	-4.88765400	2.04639400	-0.61863600
H	-6.06803300	-0.08910700	-0.30288600
C	4.82506100	0.08193200	0.51760200
O	-2.17146300	2.27302500	-0.51930200
C	-2.83569300	3.51699200	-0.61754100
H	-3.43682400	3.71423400	0.28129000
H	-2.05444400	4.27503900	-0.70599600
H	-3.48080600	3.55892900	-1.50575000
O	4.25628800	-0.02248200	-0.63288500
C	6.33512100	0.23329000	0.43619100
O	4.26082600	0.06258400	1.61663500
Pd	2.16153200	-0.09907800	-0.67716900
H	-4.84581400	-2.18103100	0.13481000
O	-2.12432200	-2.29596500	0.33604900
C	-2.76067300	-3.54362300	0.53463500
H	-3.33943500	-3.84122200	-0.35044200
H	-1.96339500	-4.26991800	0.70587800
H	-3.42357600	-3.51674300	1.41019900
C	-0.75328500	0.02046300	0.13806900
N	0.08517300	-0.39701100	-0.79127100
S	-0.14606500	0.54877800	1.65876900
H	6.77703700	0.33658200	1.43190300

H	6.77431400	-0.63808100	-0.06514300
H	6.59491200	1.11129600	-0.16791800
C	-0.37173400	-0.89609500	-2.08883500
H	-0.16752800	-1.97134800	-2.15829500
H	-1.44464600	-0.72439700	-2.22207800
H	0.17956600	-0.38572200	-2.88502900
B	-1.73031800	0.87478300	2.84741400
H	-2.38445500	-0.14866500	2.89421800
H	-1.16109700	1.12308200	3.89479900
H	-2.33925500	1.83015200	2.40513100
H	1.10133300	-1.22226600	-0.26243700

TS_m

E (M06/BS1) = -1373.681533 au

H(M06/BS1) = -1373.362662 au

G(M06/BS1) = -1373.443303 au

E(B3LYP- D3BJ/BS2//M06/BS1) = -1375.951565 au

C	2.26084100	0.21138300	0.16916400
C	2.61363800	1.55570000	-0.00091100
C	3.23899000	-0.78261200	0.04104900
C	3.93985900	1.91058900	-0.25935100
C	4.56716400	-0.43726100	-0.21813100
C	4.89632100	0.90648700	-0.35932600
H	5.33464300	-1.19964100	-0.31743800
H	5.93050700	1.17879400	-0.56239400
C	-4.33222700	0.69536800	0.07370000
O	2.79010400	-2.05507900	0.16482000
C	3.73559600	-3.10045700	0.05907800
H	4.51229600	-3.01496300	0.83151200
H	3.18158900	-4.03047700	0.20461800
H	4.21032700	-3.11162400	-0.93178000
O	-4.18276800	-0.56872900	0.02628900
C	-5.72227900	1.25274500	0.20549200
O	-3.34648000	1.47387300	-0.01550000
Pd	-2.04144800	-0.45790600	-0.21976100
H	4.22688900	2.95056300	-0.38576600

O	1.59082300	2.43864500	0.09896900
C	1.88039000	3.81077100	-0.07698000
H	2.28866100	4.00774500	-1.07790600
H	0.93115600	4.33924300	0.03607500
H	2.58881200	4.17183200	0.68129100
C	0.85571600	-0.16164400	0.49251400
N	0.02083700	-0.35647800	-0.52438100
S	0.40397400	-0.32778800	2.11329700
H	-6.09218000	1.53406400	-0.78880600
H	-6.40841500	0.51321500	0.62894700
H	-5.71577300	2.15690800	0.82275600
C	0.44572800	-0.24150000	-1.91814000
H	1.44772000	-0.65896600	-2.07461600
H	-0.26800200	-0.79336800	-2.53873400
H	0.44039600	0.81009000	-2.23164300
H	-0.72562300	-1.56281100	-0.34988600
B	-1.71233300	-2.71080100	-0.41711300
H	-0.54645700	-3.09769100	-0.47904300
H	-2.26582300	-3.03659600	0.60505300
H	-2.30376700	-2.82577000	-1.46530100

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