

# Supporting Information

## Theoretical and Experimental Investigation of Thermodynamics and Kinetics of Thiol-Michael Addition Reactions: A Case Study of Reversible Fluorescent Probes for Glutathione Imaging in Single Cells

Jianwei Chen,<sup>†,‡</sup> Xiqian Jiang,<sup>†,‡</sup> Shaina L. Carroll,<sup>†,¶</sup> Jia Huang,<sup>§</sup> and Jin Wang<sup>†,§,\*</sup>

<sup>†</sup>Department of Pharmacology, <sup>§</sup>Center for Drug Discovery, Dan L. Duncan Cancer Center, and Cardiovascular Research Institute, Baylor College of Medicine, Houston, Texas 77030, United States;

<sup>¶</sup>Department of Chemistry, Rice University, Houston, Texas 77251, United States;

<sup>§</sup>Sciclotron LLC., Sugar Land, Texas 77479, United States.

<sup>‡</sup> These authors contributed equally.

Email: [wangj@bcm.edu](mailto:wangj@bcm.edu)

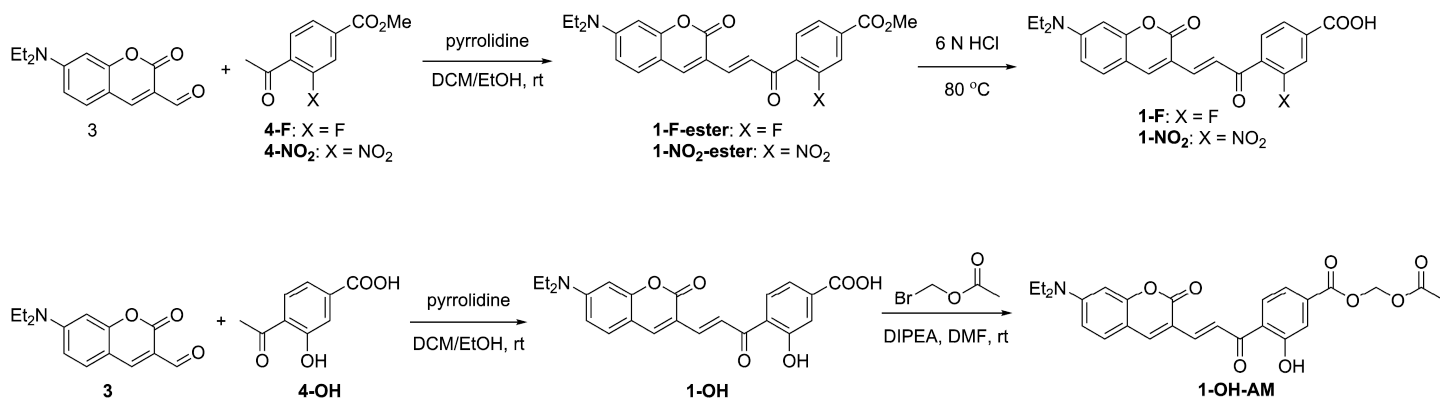
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## Materials and Methods

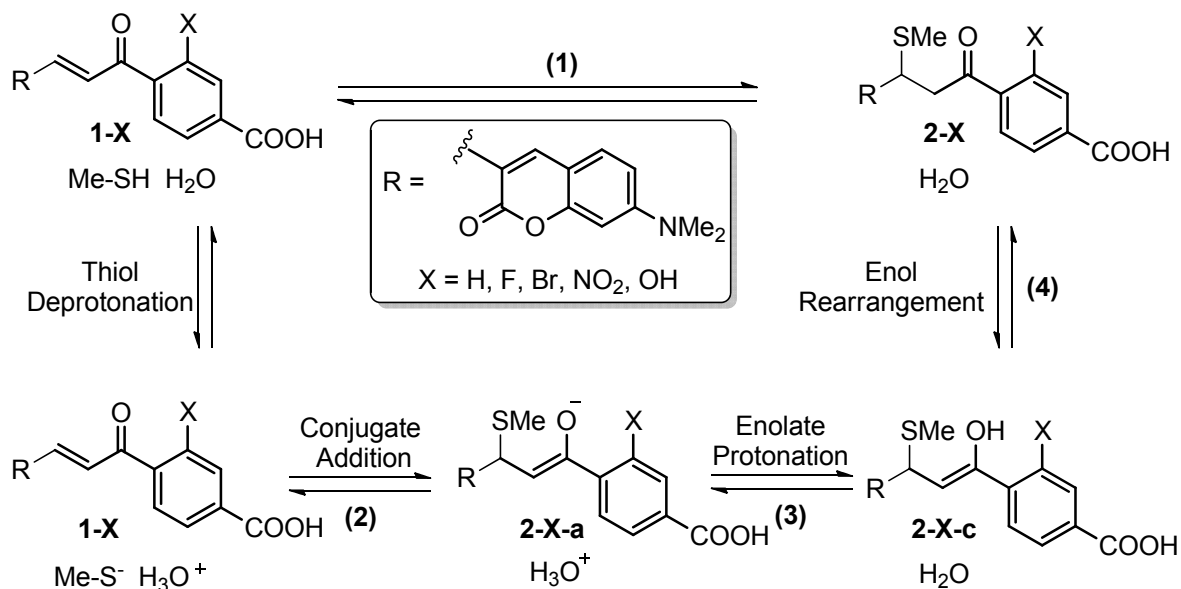
**Materials:** All the chemicals were purchased from Sigma-Aldrich or Alfa Aesar unless otherwise specified. All other solvents and reagents were used as obtained without further purification.

**Instrumentation:** NMR spectra were recorded on a Varian NMR ( $^1\text{H}$  at 400 MHz and  $^{13}\text{C}$  at 100 MHz) spectrometer. Chemical shifts ( $\delta$ ) were given in ppm with reference to solvent signals [ $^1\text{H}$  NMR:  $\text{CDCl}_3$  (7.26),  $\text{DMSO-}d_6$  (2.50);  $^{13}\text{C}$  NMR:  $\text{CDCl}_3$  (77.0),  $\text{DMSO-}d_6$  (40.0)]. UV-Vis measurements were performed in  $10 \times 10$  mm quartz cuvettes with a Cary 60 UV-Vis Spectrometer. Fluorescence measurements were performed in  $10 \times 10$  mm quartz cuvettes with a Cary Eclipse fluorescence spectrophotometer. Flash chromatography was performed on a Teledyne ISCO CombiFlash Rf 200. ESI mass spectrometry was measured on an Agilent Mass Spectrometer (6130 single quad). The Carl Zeiss LSM-780 confocal laser scanning microscope from the Optical Imaging and Vital Microscopy Core at Baylor College of Medicine was used for all cell imaging.

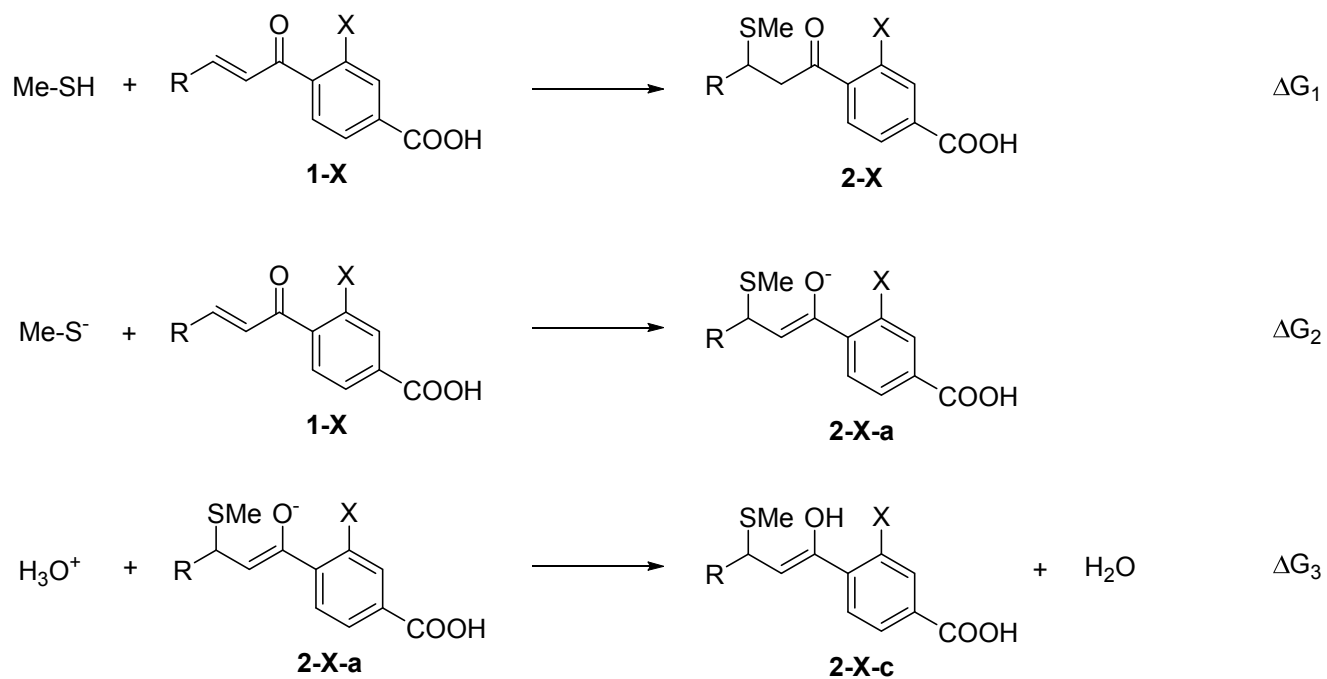


### Scheme S1. Synthetic route of compounds 1-F, 1-NO<sub>2</sub>, 1-OH and 1-OH-AM.

Compounds **1-H**<sup>S1</sup>, **1-Br**<sup>S1</sup>, **3**<sup>S1</sup>, **4-F**<sup>S2</sup>, **4-NO<sub>2</sub>**<sup>S3</sup> and **4-OH**<sup>S4</sup> were synthesized according to the literature.



**Scheme S2.** A general scheme for the mechanism of thiol-Michael addition reaction. To simplify calculations, methyl groups were used as substitutes for the ethyl groups in the coumarin moiety.



**Scheme S3.** Definition of  $\Delta G_1$ ,  $\Delta G_2$  and  $\Delta G_3$ .

**Table S1.** Gibbs free energies for Michael addition reactions computed by M06-2X/6-31G(d).

<b>X</b>	<b>1-X*</b>	<b>1-X-a*</b>	<b>1-X-b*</b>	<b>2-X*</b>
<b>Br**</b>	-3811.820694	-4249.897932	-4250.419190	-4250.440404
<b>H</b>	-1240.634867	-1678.782346	-1679.236039	-1679.251144
<b>F</b>	-1339.852664	-1778.00102	-1778.452895	-1778.468107
<b>Br</b>	-3811.852090	-4250.000578	-4250.452588	-4250.468143
<b>NO2</b>	-1445.063982	-1883.215301	-1883.666727	-1883.678798
<b>OH</b>	-1315.840037	-1753.993027	-1754.437886	-1754.455958

\*in Hartree

\*\*in the gas phase

**Table S2.** Summary of energies calculated with different DFT methods

Entry	M06-2X/6-31G(d)					6-311G(2d,p)			
	Electronic Energy	Zero-Point Energy	Thermal Correction to Energy	Thermal Correction to Enthalpy	Thermal Correction to Gibbs Free Energy	Electronic Energy (M06-2X)	Electronic Energy (B3LYP)	Electronic Energy (PBE1PBE)	Electronic Energy (wB97XD)
MeS <sup>-</sup>	-438.156891	0.046987	0.040170	0.041114	0.013534	-438.2010694	-438.2649071	-438.0488223	-438.2264258
H3O <sup>+</sup>	-76.809148	0.037134	0.037762	0.038706	0.015756	-76.84730862	-76.88399972	-76.80068734	-76.86222575
Water	-76.399062	0.021122	0.023957	0.024901	0.002800	-76.42628946	-76.46091933	-76.37612653	-76.43705682
MeSH	-438.631330	0.399029	0.050440	0.051384	0.022920	-438.6800671	-438.7479387	-438.5325888	-438.7114735
<b>1-H</b>	-1240.924250	0.348154	0.367022	0.367966	0.289383	-1241.250336	-1241.739484	-1240.317300	-1241.311241
<b>2-H-a</b>	-1679.105540	0.399732	0.409604	0.410548	0.323194	-1679.469350	-1680.001325	-1678.378198	-1679.552080
<b>2-H-b</b>	-1679.572320	0.386117	0.422978	0.423922	0.336281	-1679.948366	-1680.481677	-1678.858926	-1680.034870
<b>2-H</b>	-1679.588720	0.400840	0.423541	0.424485	0.337576	-1679.959726	-1680.493873	-1678.870356	-1680.051661
<b>1-Br</b>	-3812.127200	0.343724	0.358414	0.359358	0.275110	-3814.812808	-3815.269129	-3813.526991	-3814.872887
<b>2-Br-a</b>	-4250.312120	0.395833	0.401188	0.402132	0.311542	-4253.034184	-4253.531535	-4251.588924	-4253.115731
<b>2-Br-b</b>	-4250.775650	0.396622	0.414057	0.415001	0.323062	-4253.510250	-4254.011219	-4252.068338	-4253.596509
<b>2-Br</b>	-4250.794250	0.382761	0.415015	0.415959	0.326107	-4253.521703	-4254.017505	-4252.075671	-4253.612006
<b>1-F</b>	-1340.131510	0.333465	0.359254	0.360198	0.278846	-1340.486735	-1341.001976	-1339.490882	-1340.547370
<b>2-F-a</b>	-1778.314840	0.386819	0.402168	0.403112	0.313820	-1778.707848	-1779.265224	-1777.553221	-1778.789989
<b>2-F-b</b>	-1778.780020	0.372968	0.415437	0.416381	0.327125	-1779.185253	-1779.744924	-1778.033330	-1779.271449
<b>2-F</b>	-1778.796450	0.334953	0.416362	0.417307	0.328343	-1779.197230	-1779.756629	-1778.044316	-1779.288350
<b>1-NO<sub>2</sub></b>	-1445.350420	0.387487	0.371763	0.372708	0.286438	-1445.731652	-1446.290712	-1444.664857	-1445.798373
<b>2-NO<sub>2</sub>-a</b>	-1883.537480	0.388610	0.414834	0.415778	0.322179	-1883.956001	-1884.556957	-1882.730324	-1884.044237
<b>2-NO<sub>2</sub>-b</b>	-1884.000190	0.385408	0.427620	0.428564	0.333463	-1884.431421	-1885.033435	-1883.207108	-1884.523370
<b>2-NO<sub>2</sub></b>	-1884.014850	0.374460	0.428495	0.429439	0.336052	-1884.441482	-1885.041168	-1883.215366	-1884.539159
<b>1-OH</b>	-1316.133060	0.397648	0.372262	0.373206	0.293023	-1316.484932	-1316.997839	-1315.502690	-1316.546915
<b>2-OH-a</b>	-1754.319050	0.345551	0.413626	0.414570	0.326023	-1754.710625	-1755.265114	-1753.569670	-1754.793300
<b>2-OH-b</b>	-1754.777150	0.385332	0.427833	0.428777	0.339264	-1755.178268	-1755.734207	-1754.038110	-1755.265636
<b>2-OH</b>	-1754.796790	0.034898	0.428653	0.429597	0.340832	-1755.193801	-1755.751408	-1754.054746	-1755.286624

\*in Hartree

### Synthesis of compound 1-F

To the mixture of compound **3** (20 mg, 0.082 mmol) and compound **4-F** (32 mg, 0.16 mmol) in dry DCM/EtOH (1:1, 2 mL) was added pyrrolidine (0.018 mL, 0.25 mmol). The mixture was stirred at room temperature for 3 d. Then the solvent was removed and the residue was purified by flash chromatography (hexanes/EtOAc = 4:1 to 3:1) to afford compound **1-F-ester** (15 mg, 43%). Compound **1-F-ester**:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 – 7.86 (m, 2H), 7.86 – 7.75 (m, 3H), 7.60 (d,  $J = 15.6$  Hz, 1H), 7.32 (d,  $J = 8.8$  Hz, 1H), 6.61 (dd,  $J = 9.2, 2.4$  Hz, 1H), 6.48 (d,  $J = 2.4$  Hz, 1H), 3.95 (s, 3H), 3.45 (q,  $J = 7.2$  Hz, 4H), 1.23 (t,  $J = 7.2$  Hz, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  189.1, 165.3, 160.6 (d,  $J = 254.2$  Hz), 160.1, 156.8, 152.1, 145.9, 140.8, 134.7, 131.4, 130.8 (d,  $J = 2.9$  Hz), 130.2, 125.7 (d,  $J = 5.6$  Hz), 125.2 (d,  $J = 3.6$  Hz), 117.8 (d,  $J = 25.0$  Hz), 114.5, 109.6, 108.9, 96.9, 52.6, 45.1 (2C), 12.5 (2C); MS (ESI):  $m/z$  424.2  $[\text{M}+1]^+$ ; HRMS (ESI):  $m/z$  calcd for  $\text{C}_{24}\text{H}_{23}\text{FNO}_5$   $[\text{M}+\text{H}]^+$ : 424.1560, found: 424.1562.

The mixture of compound **1-F-ester** (10 mg, 0.047 mmol) and 6 N HCl (2 ml) was stirred at 80 °C for 8 h. Then the solvent was removed and the residue was purified by HPLC to obtain compound **1-F** (7 mg, 72%).

Compound **1-F**:  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.34 (s, 1H), 7.84 (dd,  $J = 8.0, 1.3$  Hz, 1H), 7.78 – 7.74 (m, 2H), 7.60 (dd,  $J = 15.6, 2.0$  Hz, 1H), 7.46 (d,  $J = 14.0$  Hz, 1H), 7.43 (d,  $J = 8.8$  Hz, 1H), 6.73 (dd,  $J = 8.8, 2.0$  Hz, 1H), 6.53 (d,  $J = 1.6$  Hz, 1H), 3.43 (q,  $J = 7.2$  Hz, 4H), 1.09 (t,  $J = 7.2$  Hz, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ )  $\delta$  189.1, 166.1 (d,  $J = 2.4$  Hz), 160.1, 160.0 (d,  $J = 251.3$  Hz), 157.1, 152.7, 147.6, 142.1, 136.1 (d,  $J = 7.7$  Hz), 131.4, 131.3 (d,  $J = 14.7$  Hz), 131.1 (d,  $J = 2.9$  Hz), 126.0 (d,  $J = 3.2$  Hz), 124.8 (d,  $J = 4.3$  Hz), 117.6 (d,  $J = 24.1$  Hz), 113.0, 110.5, 108.9, 96.7, 44.9 (2C), 12.9 (2C); MS (ESI):  $m/z$  410.1  $[\text{M}+1]^+$ ; HRMS (ESI):  $m/z$  calcd for  $\text{C}_{23}\text{H}_{21}\text{FNO}_5$   $[\text{M}+\text{H}]^+$ : 410.1404, found: 410.1408.

### Synthesis of compound 1-NO<sub>2</sub>

To the mixture of compound **3** (20 mg, 0.082 mmol) and compound **4-NO<sub>2</sub>** (33 mg, 0.15 mmol) in dry DCM/EtOH (1:1, 2 mL) was added pyrrolidine (0.0092 mL, 8.7 mmol). The mixture was stirred at room temperature for 3 d. Then the solvent was removed and the residue was purified by flash chromatography (hexanes/EtOAc = 4:1 to 3:1) to afford compound **1-NO<sub>2</sub>-ester** (23 mg, 63%). Compound **1-NO<sub>2</sub>-ester**:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.76 (d,  $J = 1.2$  Hz, 1H), 8.36 (dd,  $J = 7.6, 1.6$  Hz, 1H), 7.78 (s, 1H), 7.59 (d,  $J = 8.0$  Hz, 1H), 7.45 (d,  $J = 16.0$  Hz, 1H), 7.32 (d,  $J = 16.0$  Hz, 1H), 7.31 (d,  $J = 9.2$  Hz, 1H), 6.61 (dd,  $J = 8.8, 2.4$  Hz, 1H), 6.46 (d,  $J = 2.0$  Hz, 1H), 4.01 (s, 3H), 3.45 (q,  $J = 7.2$  Hz, 4H), 1.23 (t,  $J = 7.2$  Hz, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  191.9, 164.4, 160.1, 156.9, 152.3, 146.8, 145.5, 141.5, 140.5, 134.5, 132.4, 130.3, 129.0, 125.6, 125.1, 113.7, 109.7, 108.8, 96.9, 52.9, 45.1 (2C), 12.4 (2C); MS (ESI):  $m/z$  451.2  $[\text{M}+1]^+$ ; HRMS (ESI):  $m/z$  calcd for  $\text{C}_{24}\text{H}_{23}\text{N}_2\text{O}_7$   $[\text{M}+\text{H}]^+$ : 451.1505, found: 451.1505.

The mixture of compound **1-NO<sub>2</sub>-ester** (10 mg) and 6 N HCl (2 ml) was stirred at 80 °C for 3 h. And then the solvent was removed and the residue was purified by HPLC to obtain compound **1-NO<sub>2</sub>** (6 mg, 62%).

Compound **1-NO<sub>2</sub>**:  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.57 (s, 1H), 8.37 (d,  $J = 7.6$  Hz, 1H), 8.33 (s, 1H), 7.79 (d,  $J = 7.6$  Hz, 1H), 7.44 (d,  $J = 8.8$  Hz, 1H), 7.39 (d,  $J = 16.0$  Hz, 1H), 7.24 (d,  $J = 16.0$  Hz, 1H), 6.78 (d,  $J = 8.8$  Hz, 1H), 6.58 (s, 1H), 3.48 (d,  $J = 6.8$  Hz, 4H), 1.13 (t,  $J = 6.8$  Hz, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ )  $\delta$  192.2, 165.5, 159.9, 157.1, 152.8, 147.0, 143.3, 139.4, 135.1, 133.7, 131.4, 130.0, 125.6, 124.9, 112.5, 110.5, 110.0, 108.8, 96.6, 44.8 (2C), 12.8 (2C); MS (ESI):  $m/z$  437.1  $[\text{M}+1]^+$ ; HRMS (ESI):  $m/z$  calcd for  $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_7$   $[\text{M}+\text{H}]^+$ : 437.1349, found: 437.1346.

### Synthesis of compound 1-OH

To a solution of **3** (100 mg, 0.41 mmol) and compound **4-OH** (81 mg, 0.45 mmol) in  $\text{CH}_2\text{Cl}_2/\text{EtOH}$  (1:1, v/v, 2 mL) was added pyrrolidine (0.45 mmol, 0.038 mL). The resulting solution was stirred at r.t. for 24 h. Then the solvent was removed under vacuum. The crude product was then purified by reverse phase chromatography (C18 column, elute with ACN in water 5-40%) to obtain compound **1-OH** (40 mg, 24%). Compound **1-OH**:  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  13.32 (br s, 1H), 12.05 (s, 1H), 8.47 (s, 1H), 8.03 (d,  $J = 15.6$  Hz, 1H), 7.94 (d,  $J = 8.0$  Hz, 1H), 7.69 (d,  $J = 15.2$  Hz, 1H), 7.51 (s, 1H), 7.49 (m, 2H), 6.80 (dd,  $J = 8.8, 2.0$  Hz, 1H), 6.60 (d,  $J = 1.6$  Hz, 1H), 3.49 (q,  $J = 7.2$  Hz, 4H), 1.15 (t,  $J = 7.2$  Hz, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ )  $\delta$  192.7, 166.4, 159.8, 159.8, 156.6, 152.2, 146.4, 140.6, 136.2, 130.9, 130.2, 125.6, 121.5, 119.6, 118.1, 112.8, 110.1, 108.4, 96.2, 44.4 (2C), 12.4 (2C); MS (ESI):  $m/z$  408.1  $[\text{M}+1]^+$ ; HRMS (ESI):  $m/z$  calcd for  $\text{C}_{23}\text{H}_{22}\text{NO}_6$   $[\text{M}+\text{H}]^+$ : 408.1447, found: 408.1453.

## Synthesis of compound 1-OH-AM:

To a solution of compound **1-OH** (10 mg, 0.025 mmol) in anhydrous DMF (1 mL) were added bromomethyl acetate (0.014 mL, 0.15 mmol) and DIPEA (0.026 mL, 0.15 mmol). The reaction mixture was allowed to stir at room temperature overnight, and then concentrated under reduced pressure. The residue was purified by flash column chromatography (elute with ethyl acetate in hexane 10-50%) to afford **1-OH-AM** (6.0 mg, 52%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 12.92 (s, 1H), 8.37 (d, *J* = 14.8 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.83 (s, 1H), 7.74 (d, *J* = 15.2 Hz, 1H), 7.68 (d, *J* = 1.2 Hz, 1H), 7.59 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.36 (d, *J* = 8.8 Hz, 2H), 6.64 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.52 (d, *J* = 2.0 Hz, 1H), 6.00 (s, 2H), 3.47 (q, *J* = 7.2 Hz, 4H), 2.15 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 194.2, 169.5, 164.2, 163.0, 160.0, 156.8, 152.4, 147.6, 142.0, 135.0, 130.4, 130.2, 123.5, 120.8, 120.1, 119.6, 114.3, 109.8, 109.0, 96.9, 79.9, 45.1, 20.7 (2C), 12.5 (2C); MS (ESI): *m/z* 480.2 [M+1]<sup>+</sup>; HRMS (ESI): *m/z* calcd for C<sub>26</sub>H<sub>26</sub>NO<sub>8</sub> [M+H]<sup>+</sup>: 480.1658, found: 480.1673.

## Determination of *K<sub>d</sub>* of probes with GSH

The probe solution was mixed with a solution of GSH under anaerobic condition in a glovebox. The final probe concentrations were 16 μM (**1-H**), 16 μM (**1-F**), 15 μM (**1-Br**), 12 μM (**1-NO<sub>2</sub>**), and 15 μM (**1-OH**), respectively. The probe concentration was adjusted to ensure similar initial absorption. The GSH concentration varied from 0-80 mM (0, 0.2, 0.5, 1.0, 2.0, 4.0, 8.0, 10, 16, 20, and 80 mM), respectively. After 24 h, UV-Vis spectra of the mixture were taken.

## Determination of Reaction Kinetics of probes with GSH

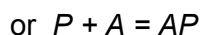
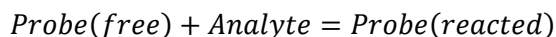
Forward reaction rate constants *k<sub>f</sub>* were determined by monitoring absorption changes of GSH probes **1-X** after mixing with GSH (2 mM in PBS at the final concentration); reverse reaction rate constants *k<sub>r</sub>* were measured by monitoring absorption changes of pre-equilibrated mixtures of GSH probes **1-X** and GSH upon addition of 5,6-dihydro-2H-pyran-2-one, a GSH scavenger.

## Cell Culture and Treatment for Imaging:

HeLa cells used in this study were purchased from American Type Culture Collection (ATCC) and grown in DMEM (Gibco, 11965) media supplemented with 10% FBS and 1% 1003 Pen Strep (Gibco). Cells were cultured under a controlled atmosphere (37°C, 5% CO<sub>2</sub>). Glass bottom dishes were used for cell culture due to confocal scanning requirements. Cells were treated with **1-OH-AM** (1 μM with 1% DMSO in culture media) for 30 min, followed by one washing step with trypan blue prior to imaging. Fluorescent images were acquired with 405 nm laser / 418 - 495 nm filter and 488 nm laser / 499 - 695 nm filter. All the microscope settings were kept consistent in each experiment.

## Deduction of Ratiometric Quantification

The reversible reaction equation is:



According to the reaction equation, the dissociation constant is:

$$K_d = \frac{[P][A]}{[AP]}$$

[*P*] and [*AP*] are the concentrations of free and reacted probes, respectively.

The absorptions at the two peak wavelengths are:

$$A_{\lambda 1} = \varepsilon_{P,\lambda 1}[P] + \varepsilon_{AP,\lambda 1}[AP]$$

$$A_{\lambda 2} = \varepsilon_{P,\lambda 2}[P] + \varepsilon_{AP,\lambda 2}[AP]$$

ε is the molar absorption coefficient, Subscripts *P*. and *AP*. stands for free and reacted probes, respectively.

The ratio can be described as:

$$R = \frac{A_{\lambda_1}}{A_{\lambda_2}} = \frac{\varepsilon_{P,\lambda_1}[P] + \varepsilon_{AP,\lambda_1}[AP]}{\varepsilon_{P,\lambda_2}[P] + \varepsilon_{AP,\lambda_2}[AP]}$$

From the dissociation constant, we can substitute all  $[P]$  with  $[AP]$ :

$$[AP] = [P][A]/K_d$$

$$R = \frac{\varepsilon_{P,\lambda_1} + \frac{\varepsilon_{AP,\lambda_1}}{K_d} [A]}{\varepsilon_{P,\lambda_2} + \frac{\varepsilon_{AP,\lambda_2}}{K_d} [A]}$$

So, the absorption ratio should fit in the following equation, which does not have a linear relationship to the analyte concentration:

$$R = \frac{\varepsilon_{P,\lambda_1}}{\varepsilon_{P,\lambda_2}} + \frac{\varepsilon_{AP,\lambda_1} - \frac{\varepsilon_{AP,\lambda_1}}{\varepsilon_{AP,\lambda_2}} \varepsilon_{P,\lambda_2}}{\varepsilon_{P,\lambda_2} + \frac{\varepsilon_{AP,\lambda_2}}{K_d} [A]} = P + \frac{Q}{S + T[A]}$$

The equation can be reduced to a linear fit when  $\varepsilon_{AP,\lambda_2} = 0$  or  $K_d$  is much larger than the analyte concentration.

Otherwise, the analyte concentration and  $R$  follows the relationship below:

$$[A] = K_d \left( \frac{R - \left( \frac{\varepsilon_{P,\lambda_1}}{\varepsilon_{P,\lambda_2}} \right)}{\left( \frac{\varepsilon_{AP,\lambda_1}}{\varepsilon_{AP,\lambda_2}} \right) - R} \right) \left( \frac{\varepsilon_{P,\lambda_2}}{\varepsilon_{AP,\lambda_2}} \right)$$

When there is no analyte present, only pure probe contributes to the absorbance:

$$A_{\lambda_1} = \varepsilon_{P,\lambda_1}[P]$$

$$A_{\lambda_2} = \varepsilon_{P,\lambda_2}[P]$$

$$R = \frac{\varepsilon_{P,\lambda_1}[P]}{\varepsilon_{P,\lambda_2}[P]} = \frac{\varepsilon_{P,\lambda_1}}{\varepsilon_{P,\lambda_2}} = R_{min}$$

When all the probe is saturated by analyte, only the bound probe contributes to the absorbance:

$$A_{\lambda_1} = \varepsilon_{AP,\lambda_1}[AP]$$

$$A_{\lambda_2} = \varepsilon_{AP,\lambda_2}[AP]$$

$$R = \frac{\varepsilon_{AP,\lambda_1}[AP]}{\varepsilon_{AP,\lambda_2}[AP]} = \frac{\varepsilon_{AP,\lambda_1}}{\varepsilon_{AP,\lambda_2}} = R_{max}$$

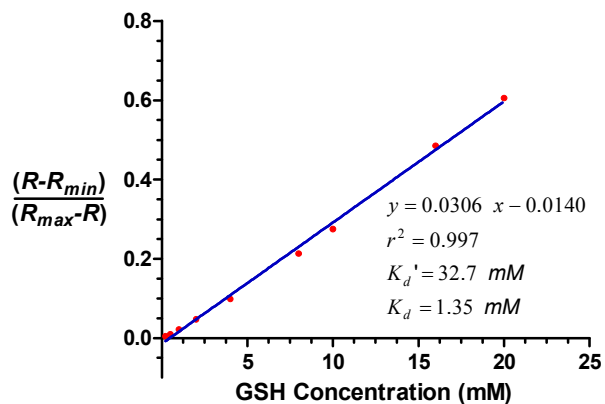
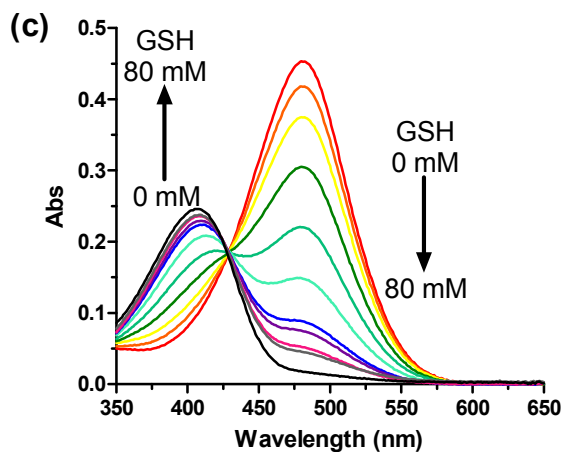
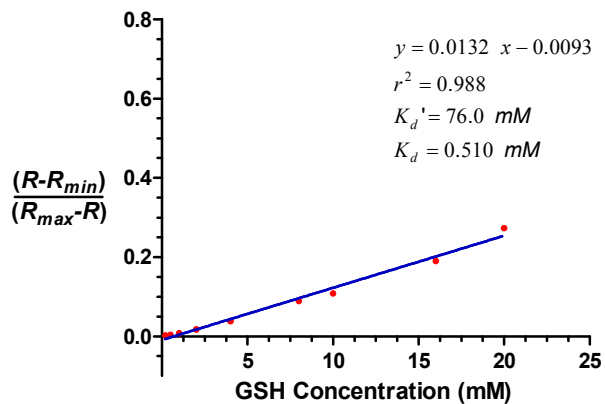
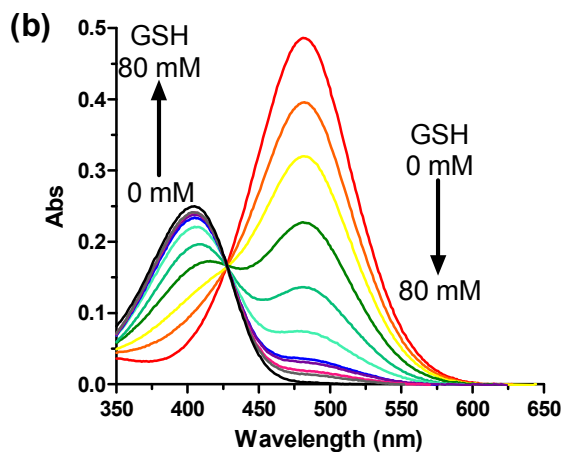
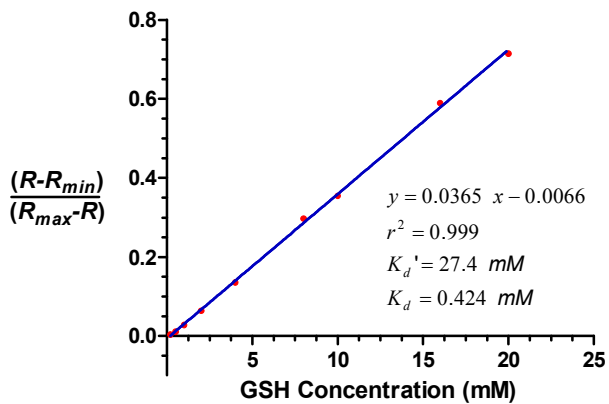
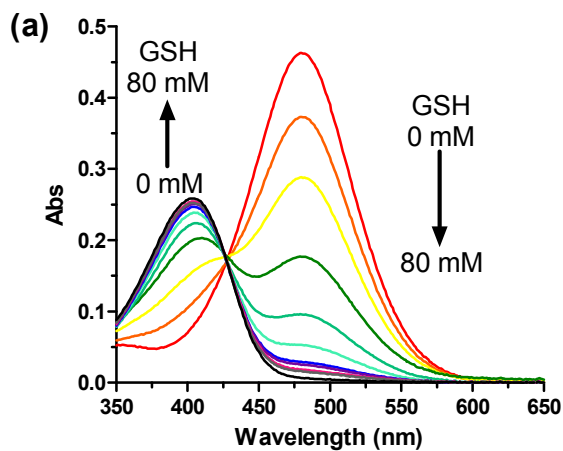
Combined all the above:

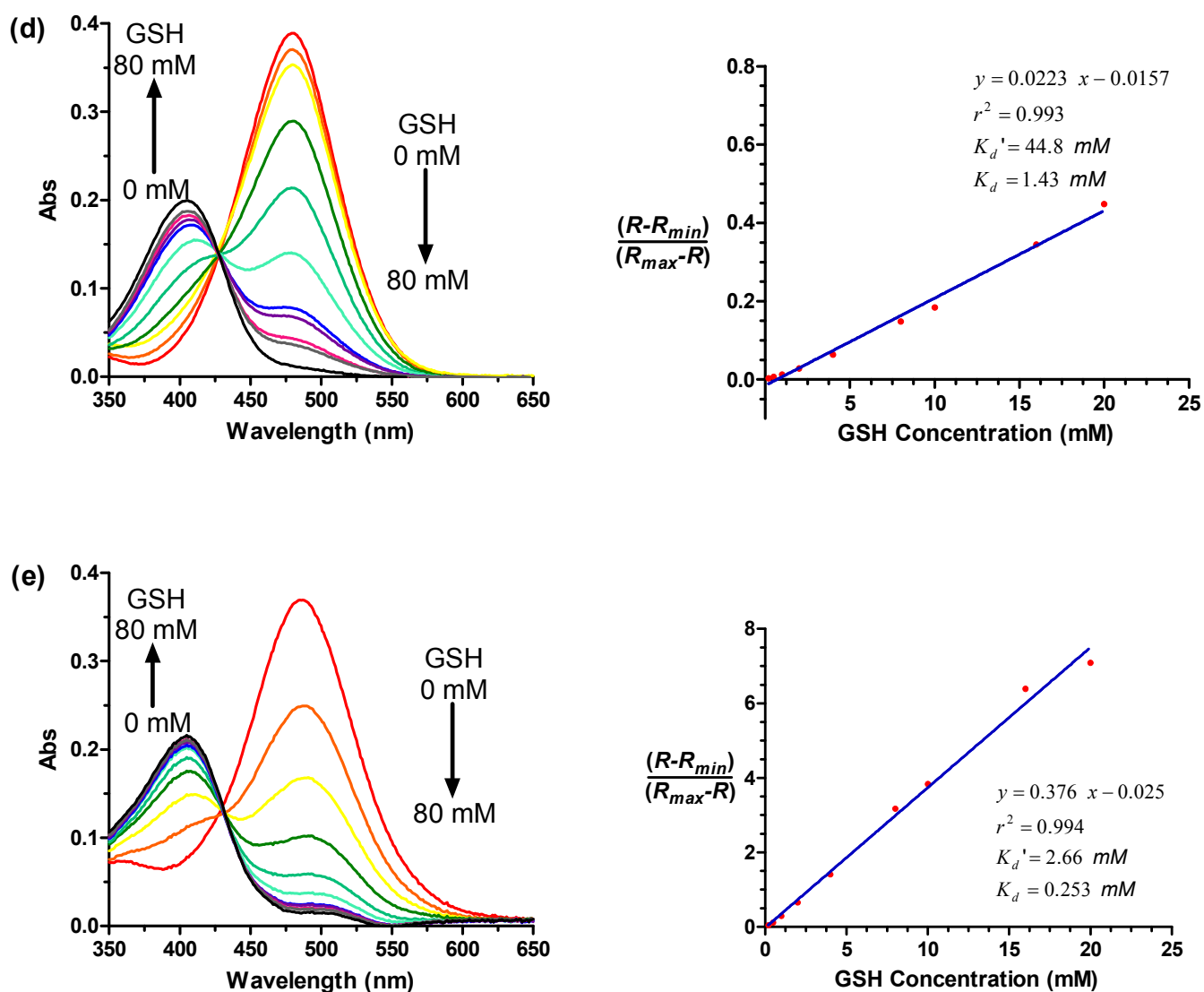
$$[A] = K_d \left( \frac{R - R_{min}}{R_{max} - R} \right) \left( \frac{\varepsilon_{P,\lambda_2}}{\varepsilon_{AP,\lambda_2}} \right)$$

$$[A] = K_d' \frac{R - R_{min}}{R_{max} - R}$$

Specific to **1-X**,  $\lambda_1 = 405$  nm, and  $\lambda_2 = 488$  nm.







**Figure S1.** Concentration dependent ratiometric spectra of **1-X** in PBS under anaerobic conditions for 24 h (left). Linear relationship between  $(R-R_{min})/(R_{max}-R)$  and GSH concentration (right). (a) **1-H**, (b) **1-F**, (c) **1-Br**, (d) **1-NO<sub>2</sub>**, (e) **1-OH**. Theoretically, all the lines should go through the origin. Deviation from the origin is due to random errors in experimental measurements. If the linear fitting is forced to go through the origin, less than 5% of difference in slope can be observed.

The ratio between the absorbance at two wavelengths, 405 nm and 488 nm, was calculated and recorded as  $R$ .  $R_{max}$  represents the ratio when GSH is 80 mM;  $R_{min}$  represents the ratio when GSH is 0 mM. Plotting  $(R-R_{min})/(R_{max}-R)$  as a function of GSH concentration afforded a linear relationship. The reciprocal of the slope yields  $K_d'$ . It is assumed that at a GSH concentration of 80 mM, all the probe molecules are fully converted to the probe GSH adduct probe-GSH. Comparing the absorption values of probe and probe-GSH at 488 nm, we can calculate the value of  $\frac{\epsilon_{probe,488\text{ nm}}}{\epsilon_{probe-GSH,488\text{ nm}}}$

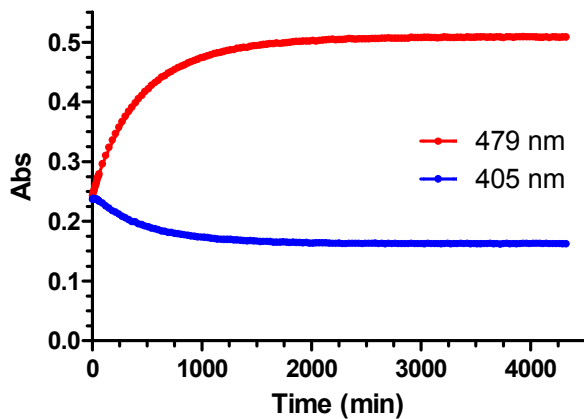
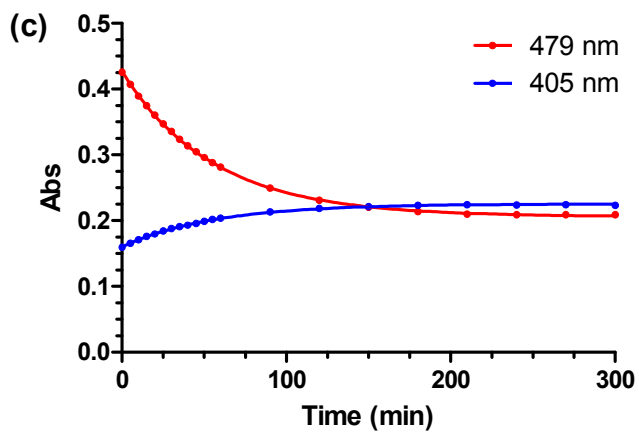
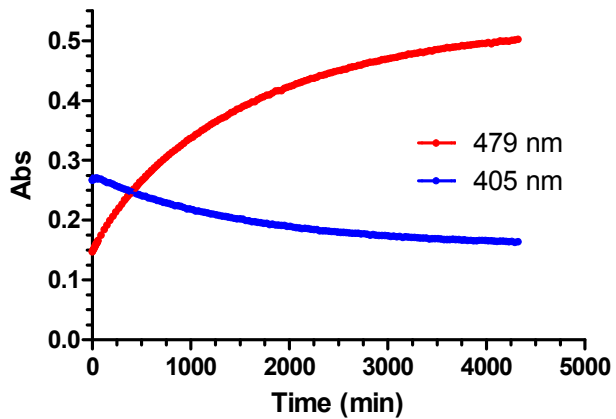
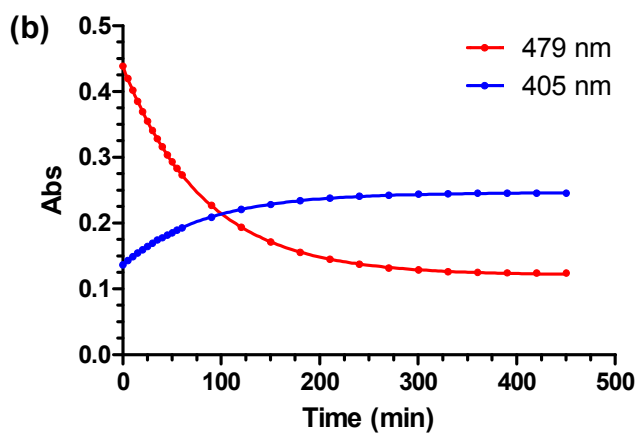
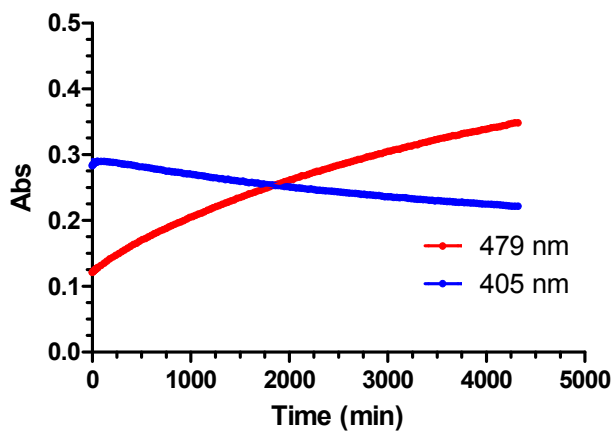
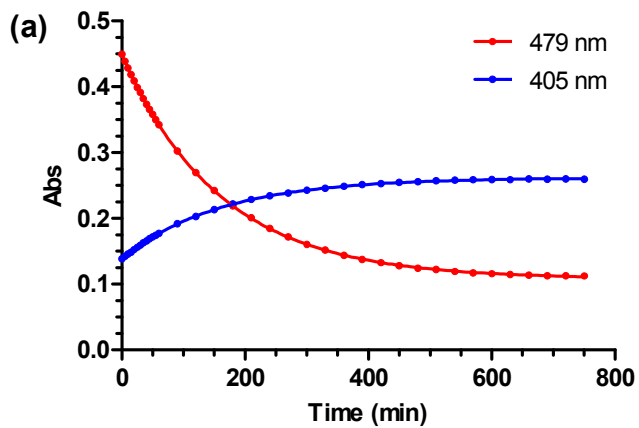
Based on the relationship

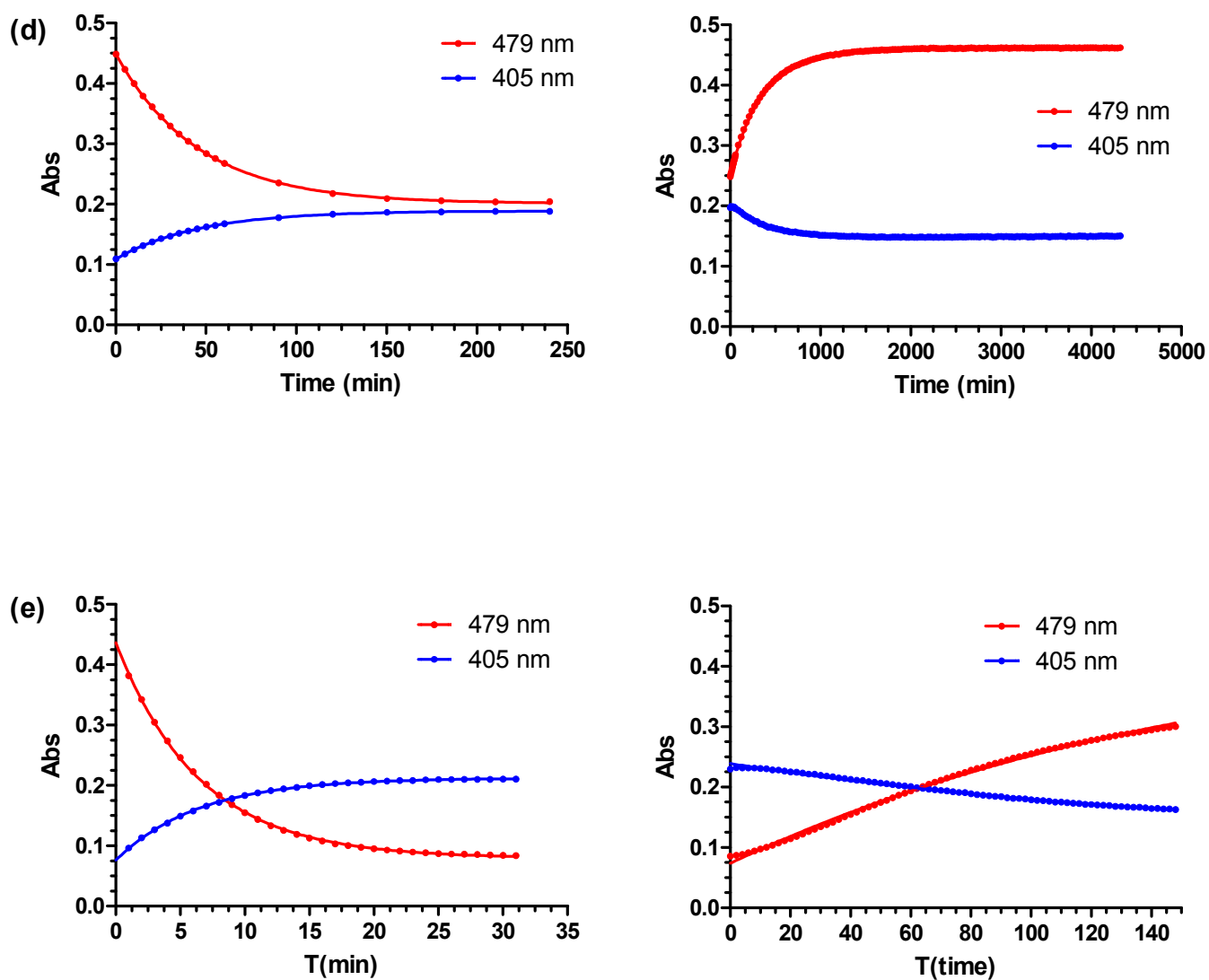
$$K_d' = K_d \frac{\epsilon_{probe,488\text{ nm}}}{\epsilon_{probe-GSH,488\text{ nm}}}$$

We can deduce  $K_d$  and the corresponding  $\Delta G$ .

The values used for the above calculations are listed below:

<b>X</b>	$K_d'$ (mM)	$\frac{\epsilon_{probe,488\text{ nm}}}{\epsilon_{probe-GSH,488\text{ nm}}}$	$K_d$ (mM)	$\Delta G_1$ (kcal·mol <sup>-1</sup> )
<b>H</b>	27.4	64.6	0.424	-4.67
<b>F</b>	76.0	149	0.510	-4.56
<b>Br</b>	32.7	24.2	1.35	-3.97
<b>NO2</b>	44.8	31.4	1.43	-3.94
<b>OH</b>	2.66	10.5	0.253	-4.98

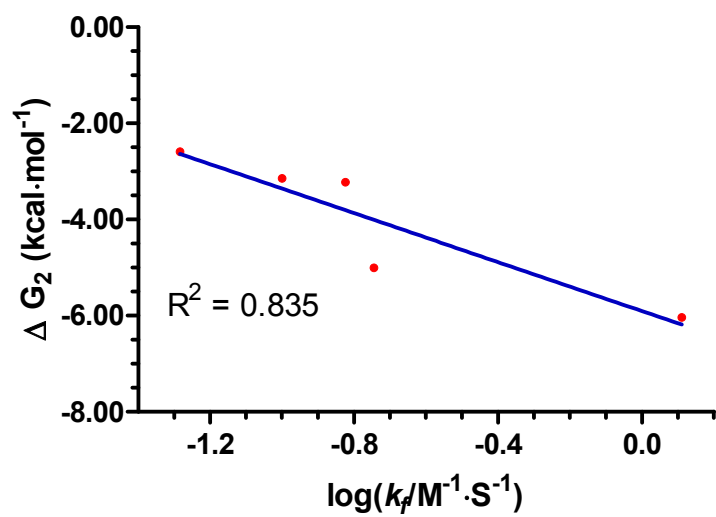
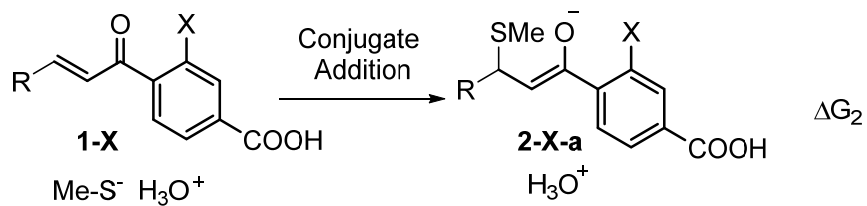




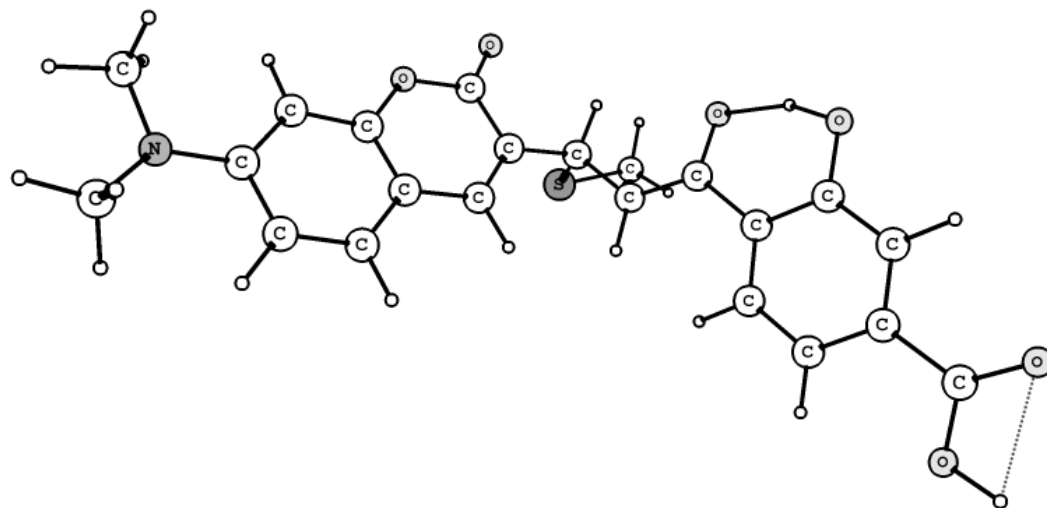
**Figure S2.** Kinetics of forward (left) and reverse (right) reactions between GSH probes and GSH (2 mM) in PBS (pH 7.4). (a) **1-H**, (b) **1-F**, (c) **1-Br**, (d) **1-NO<sub>2</sub>**, (e) **1-OH**.

The data obtained from the kinetic traces above are listed below:

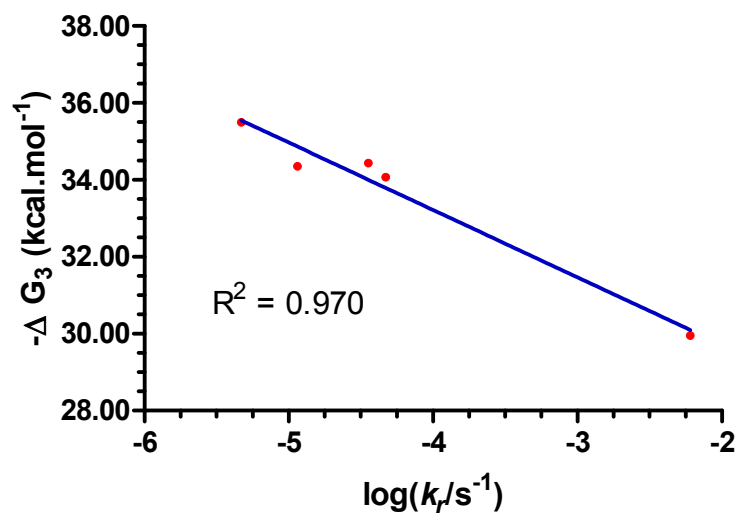
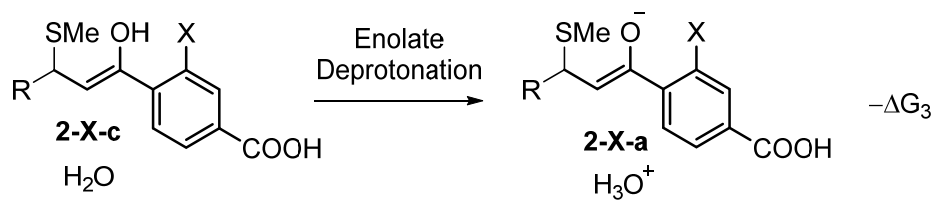
<b>X</b>	$k_f/(M^{-1}s^{-1})$	$\log [k_f/(M^{-1}\cdot s^{-1})]$	$k_r/(10^{-6}\cdot s^{-1})$	$\log [k_r/s^{-1}]$
<b>H</b>	0.052	-1.28	4.70	-5.33
<b>F</b>	0.10	-1.00	11.5	-4.94
<b>Br</b>	0.15	-0.82	35.7	-4.45
<b>NO<sub>2</sub></b>	0.18	-0.74	46.6	-4.33
<b>OH</b>	1.29	-0.11	6050	-2.22



**Figure S3.** Linear correlation between  $\Delta G_2$  and  $\log k_f$ .



**Figure S4.** Stable enolate intermediate of 1-OH-MeS<sup>-</sup> adduct (computational model)



**Figure S5.** Linear correlation between  $-\Delta G_3$  and  $\log k_r$ .

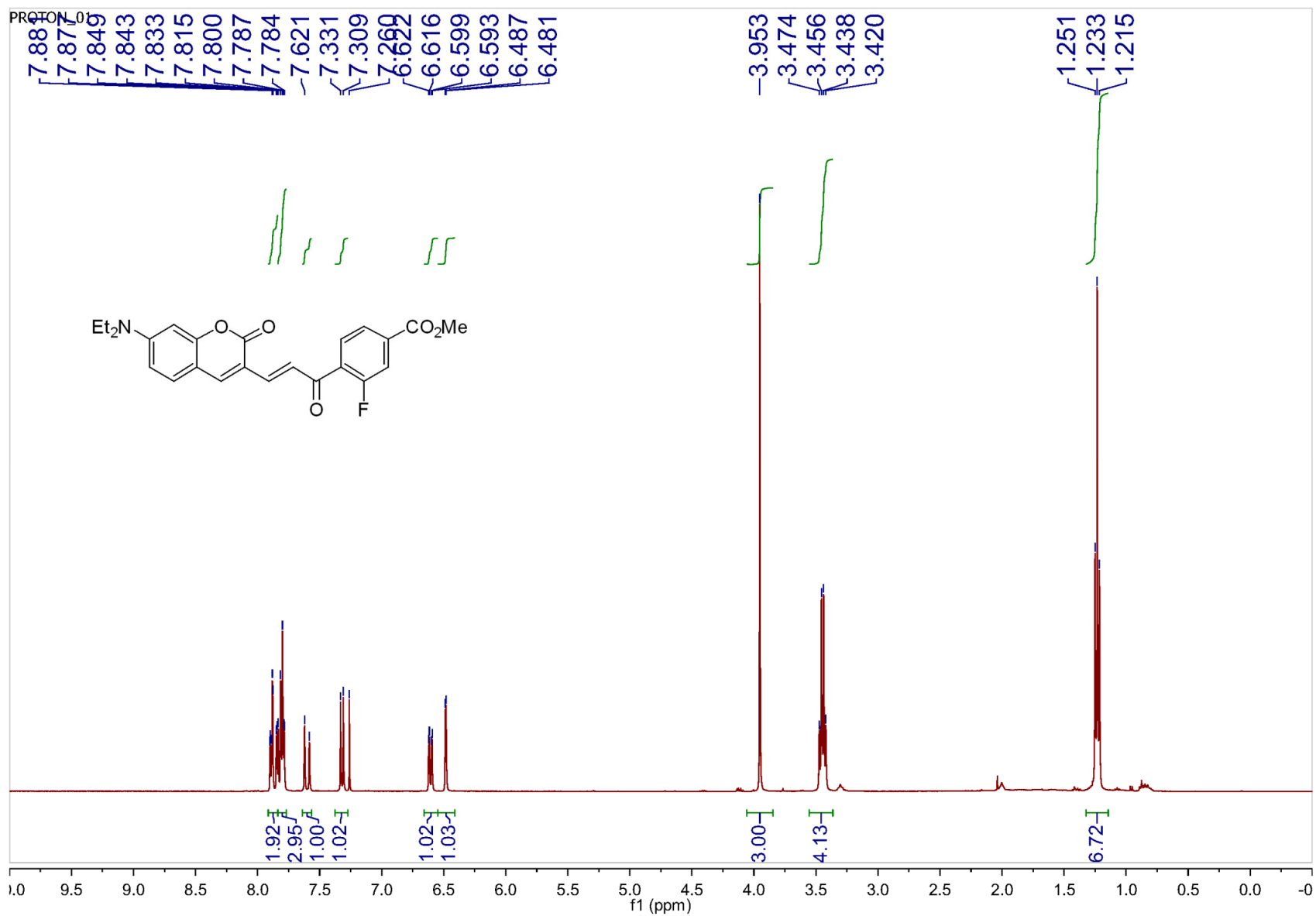


Figure S6. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of 1-F-ester



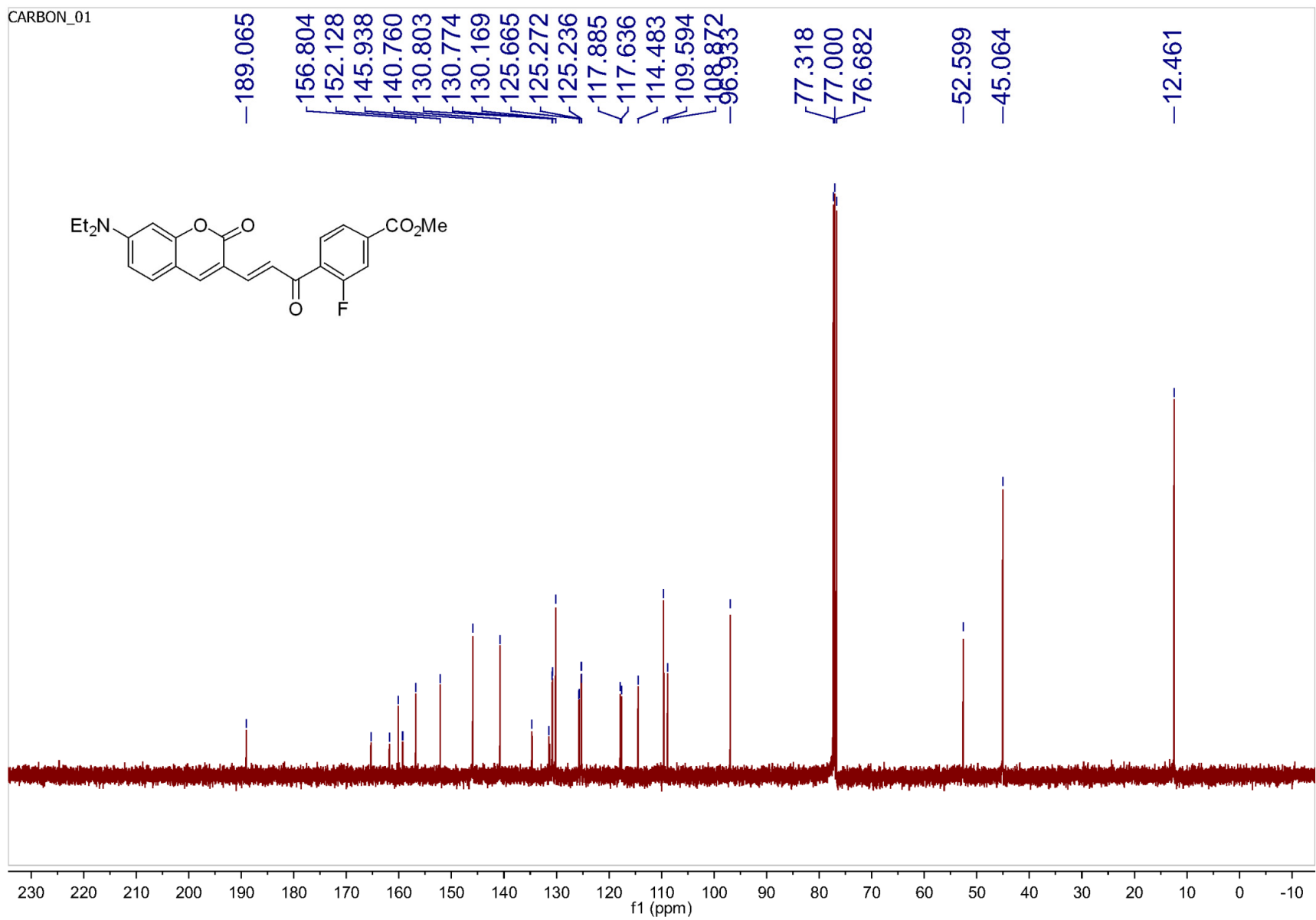


Figure S7.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of 1-F-ester

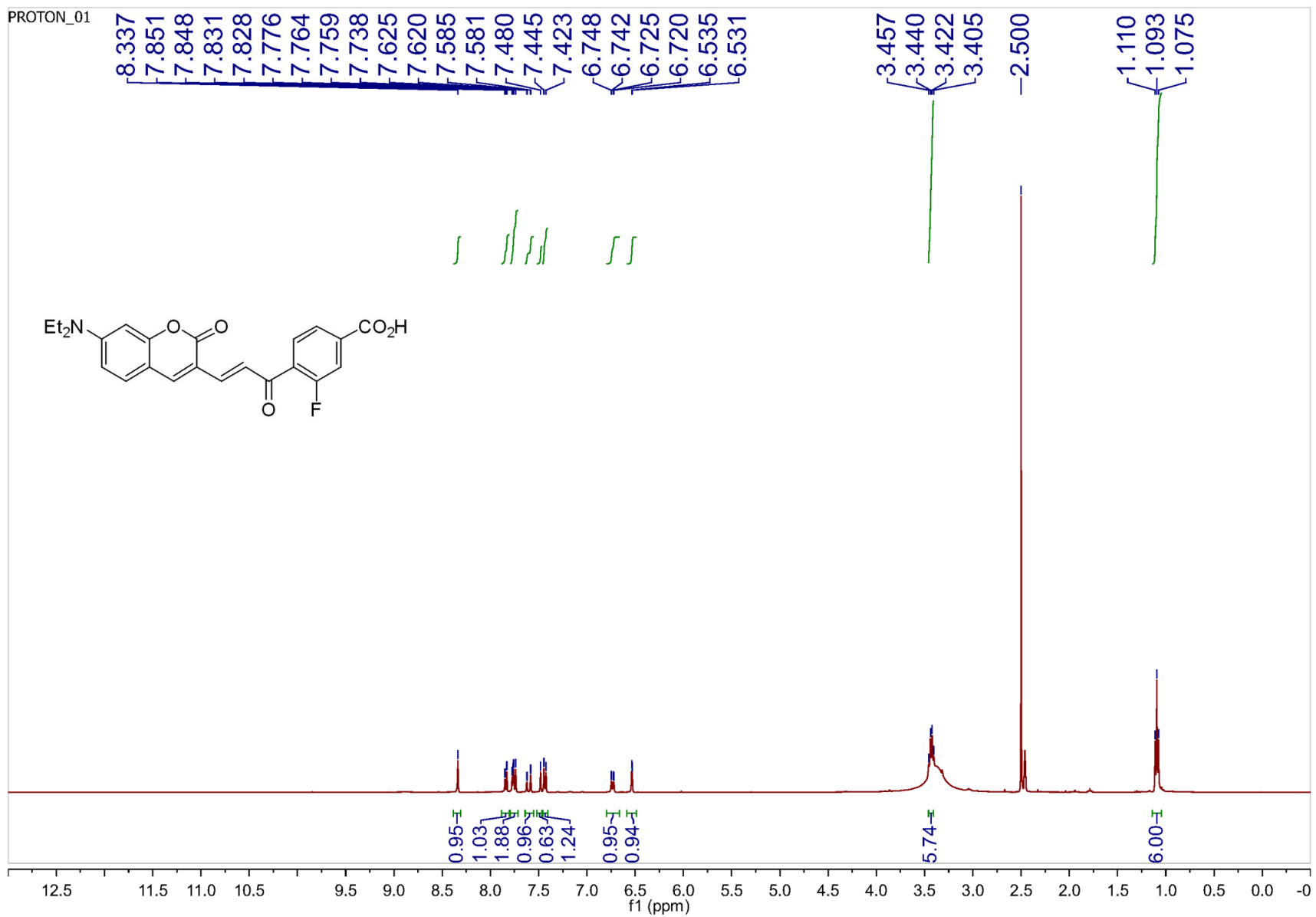


Figure S8.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) spectrum of 1-F

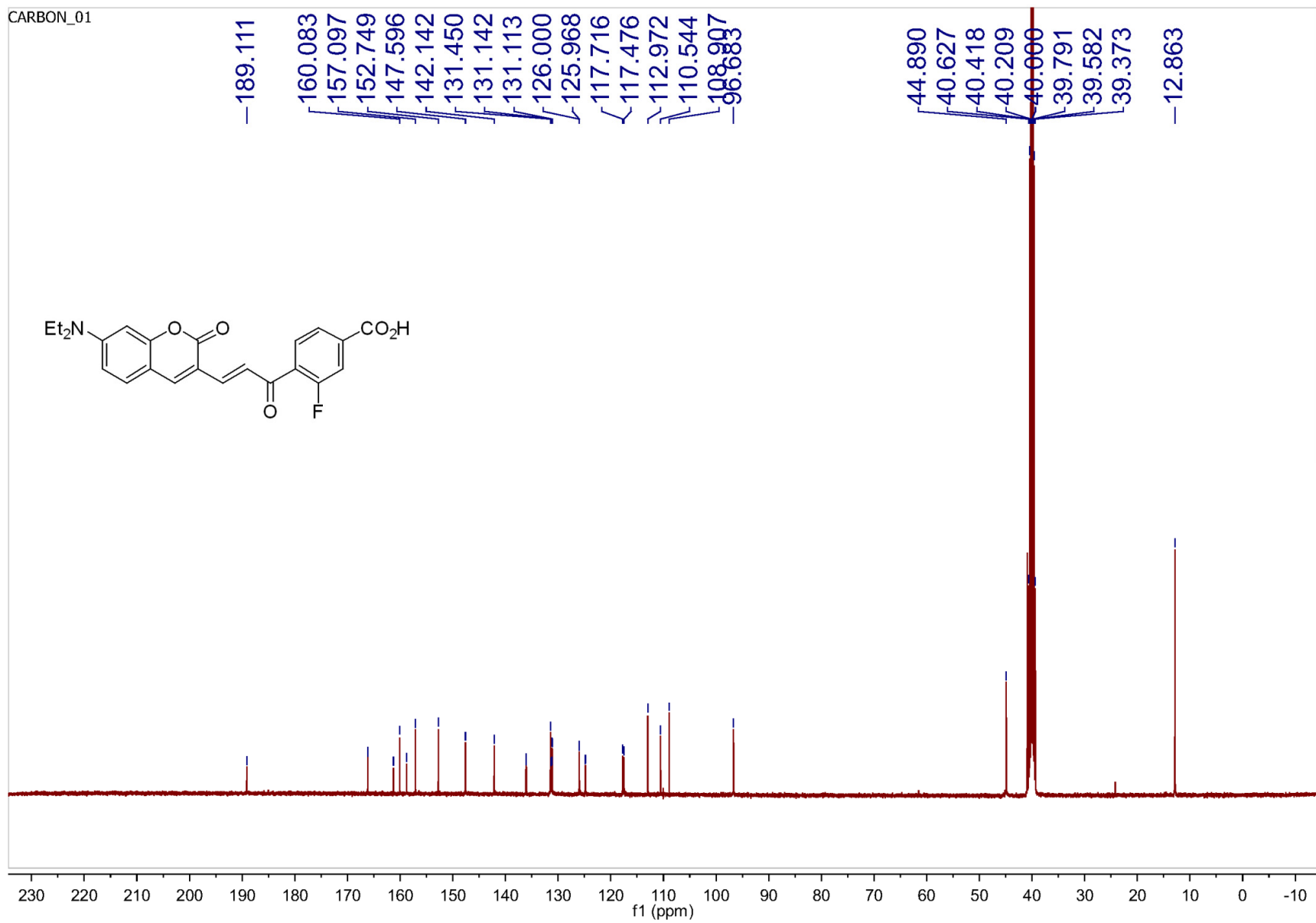


Figure S9.  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of 1-F

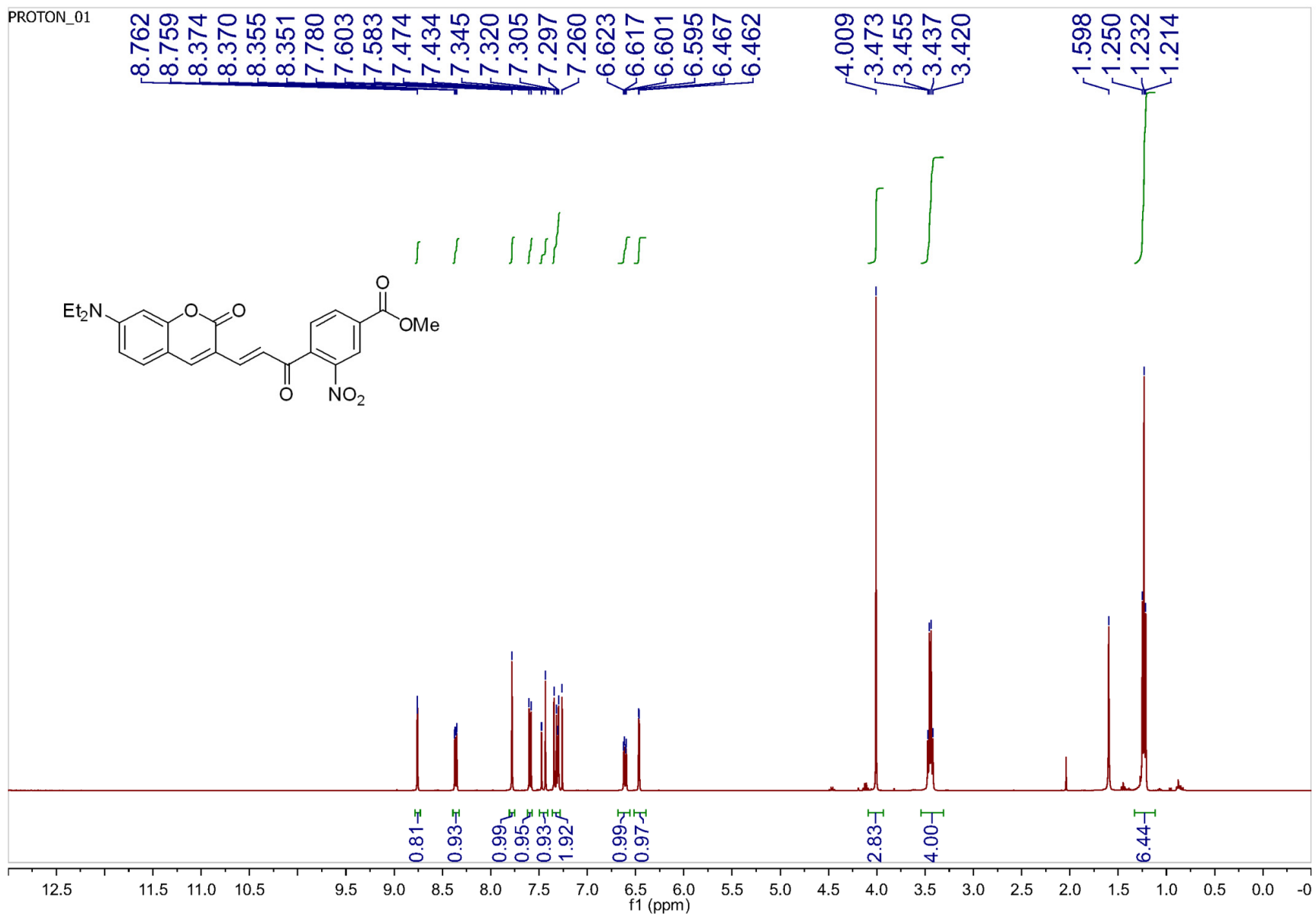
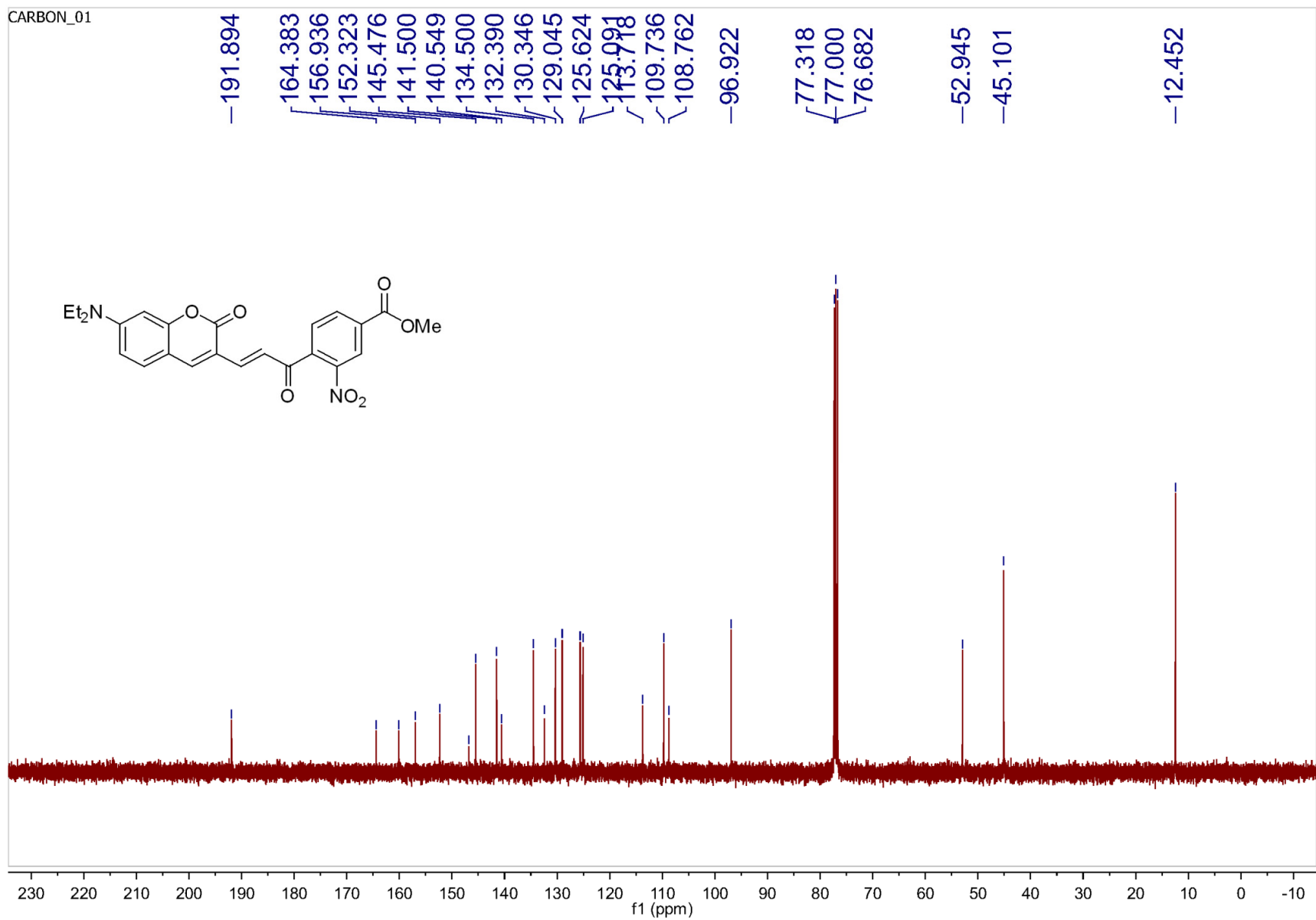
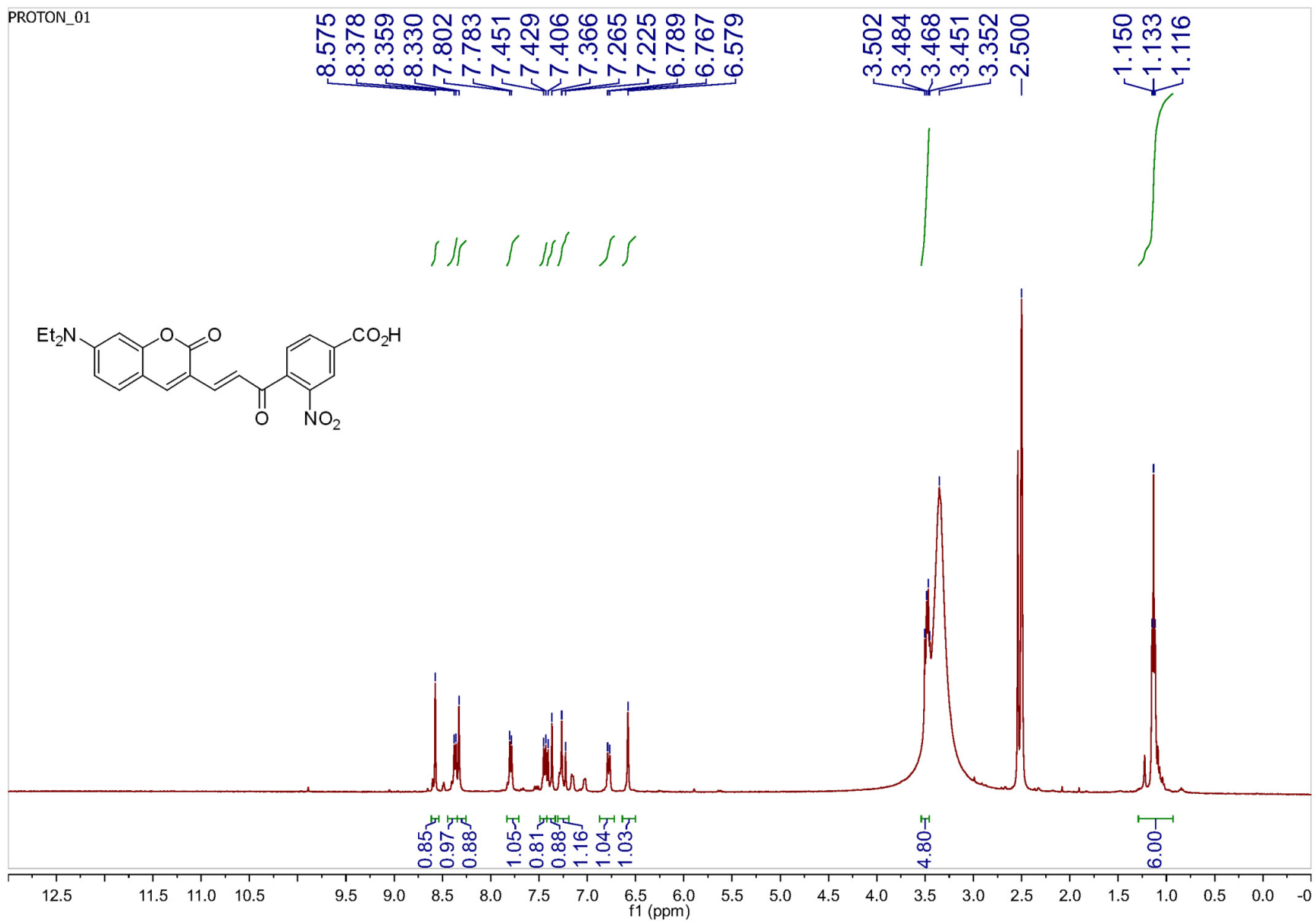


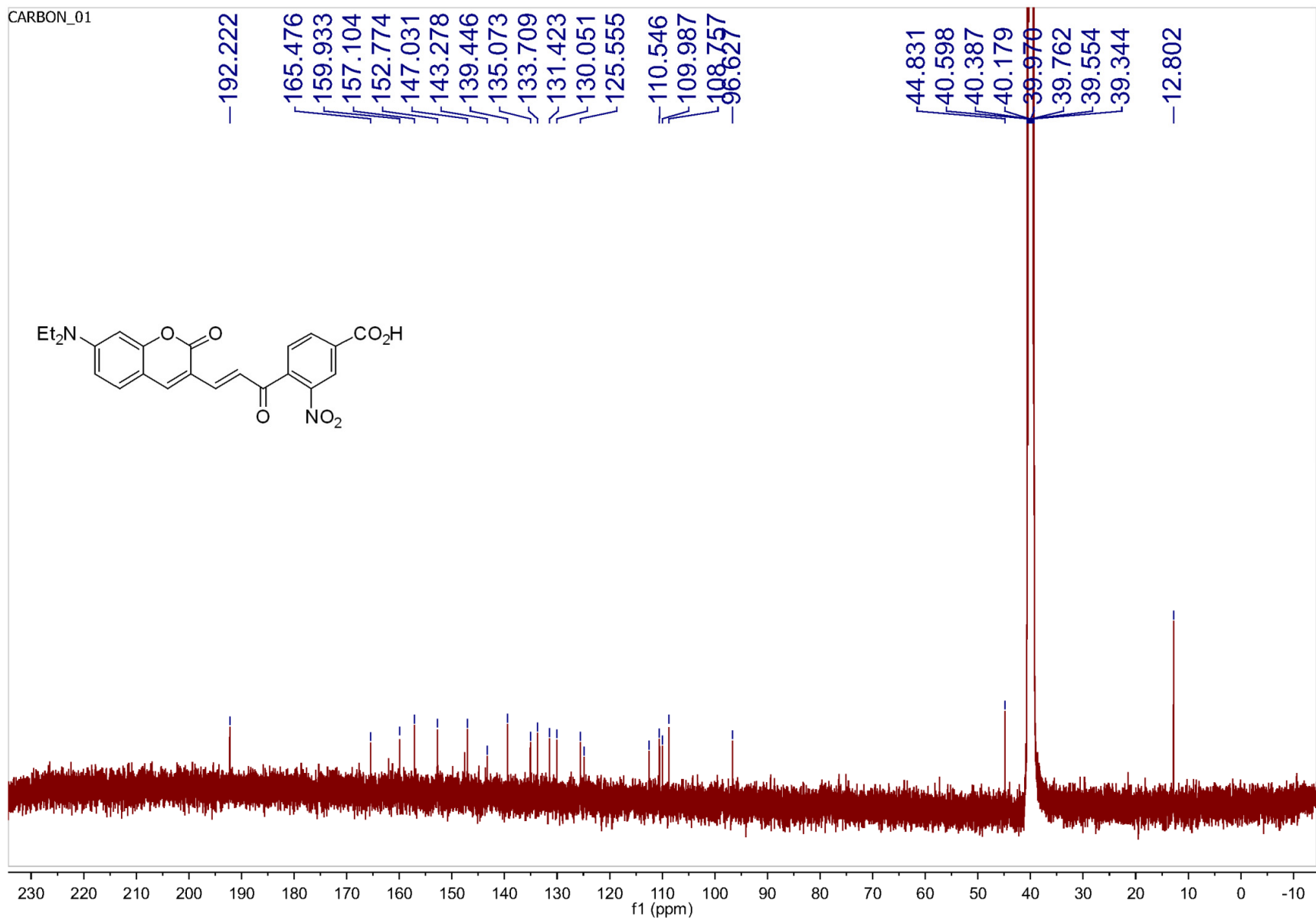
Figure S10. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of 1-NO<sub>2</sub>-ester



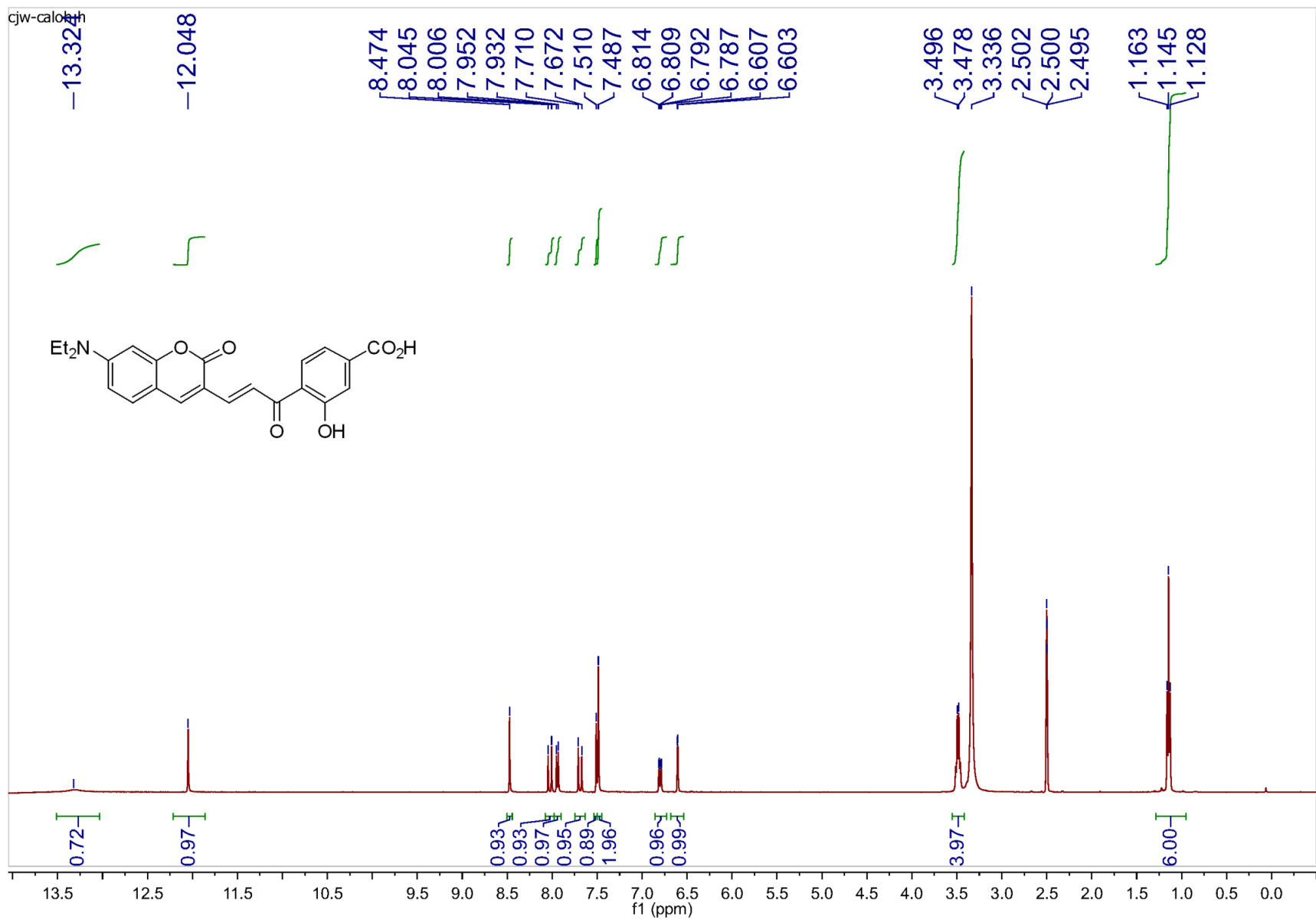
**Figure S11.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of 1- $\text{NO}_2$ -ester



**Figure S12.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of 1-NO<sub>2</sub>

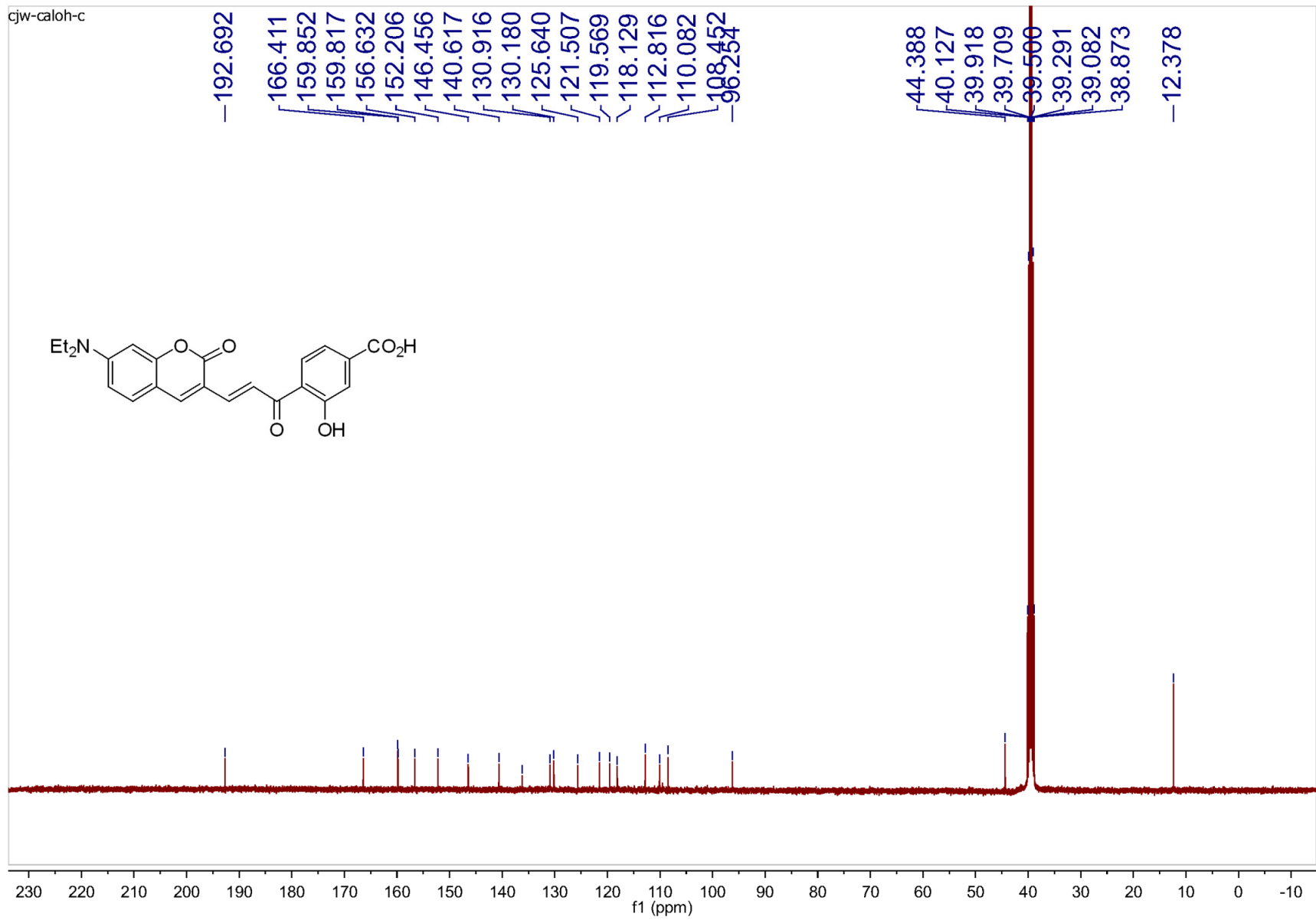


**Figure S13.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of 1- $\text{NO}_2$

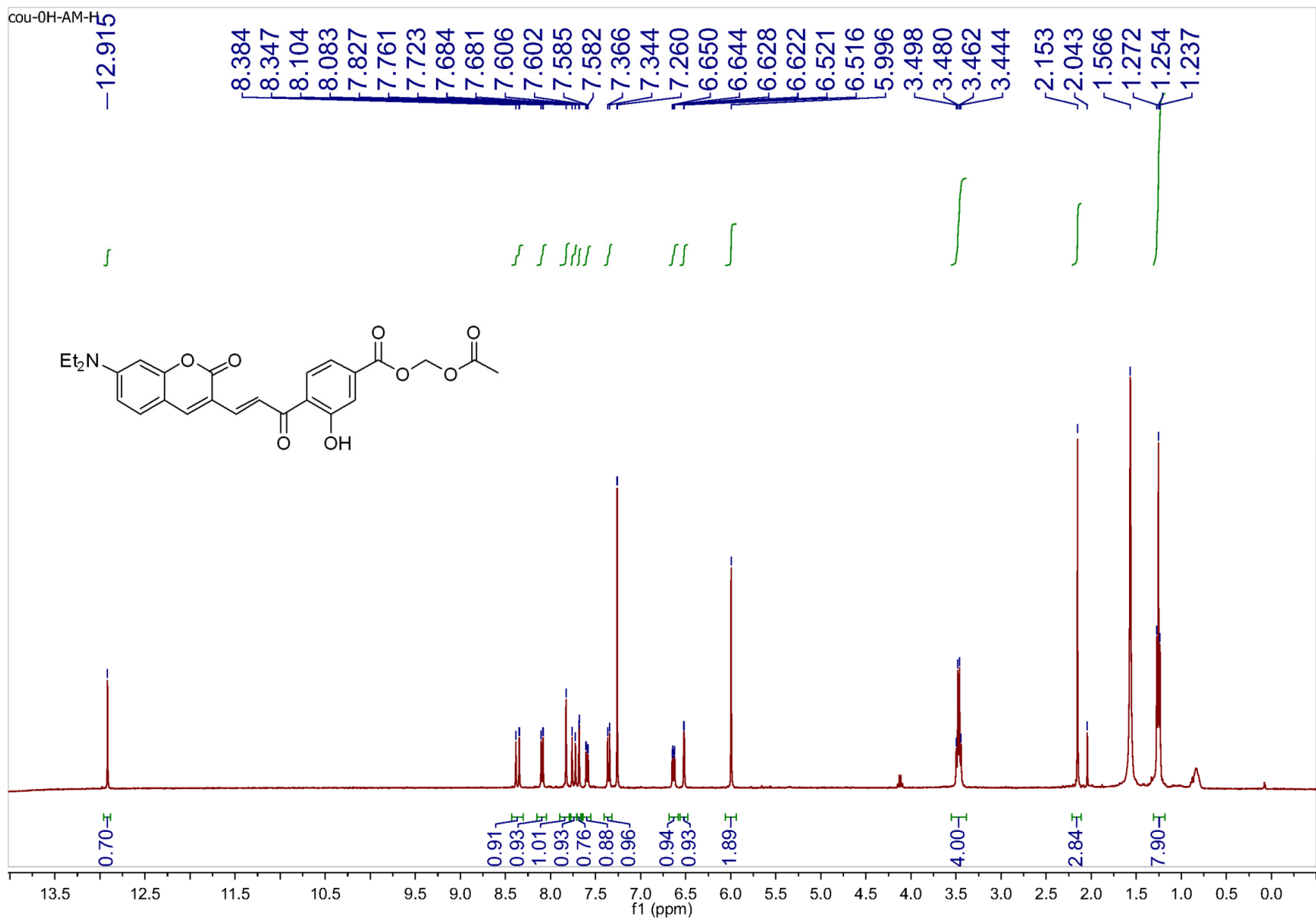


**Figure S14.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of 1-OH



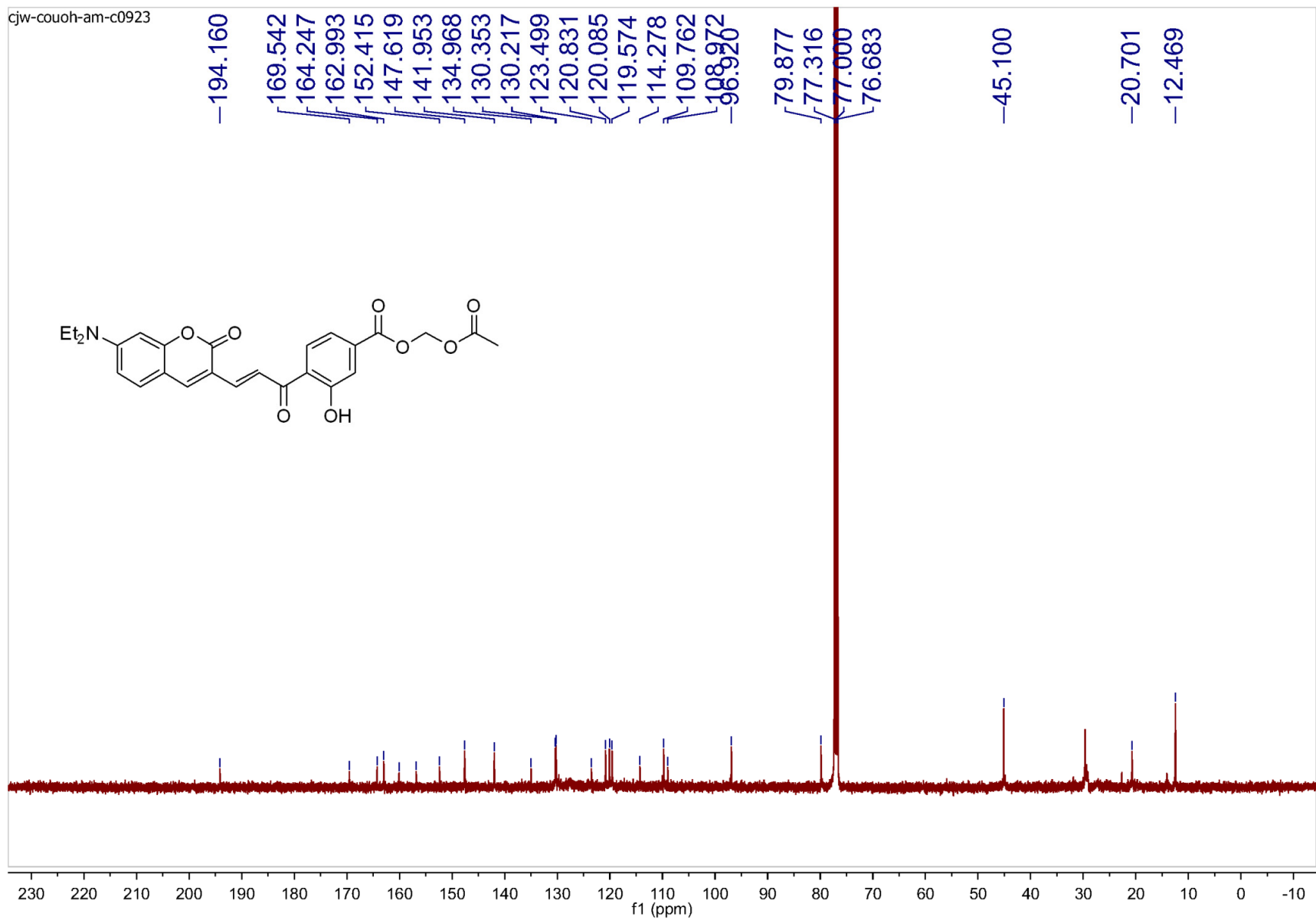


**Figure S15.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of 1-OH



**Figure S16.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of 1-OH-AM

cjw-couoh-am-c0923



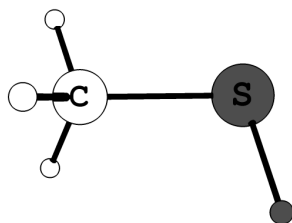
**Figure S17.** <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub> CDCl<sub>3</sub>) spectrum of 1-OH-AM

## Computational Methodology and Data

All DFT calculations were performed using the Gaussian 09 Version D.01 suite of programs<sup>S5</sup>. The geometries listed below were optimized at the M06-2X/6-31G(d) level of theory in the gas phase or with the SMD solvation method in water. Frequency analyses revealed no virtual frequencies in all the optimized structures. Thermochemical corrections were obtained from frequency calculations at the same level of theory without scaling. Single-point energies were computed using M06-2X, B3LYP, PBE1PBE and wB97XD DFT theories with a 6-311G(2d,p) basis set at the M06-2X/6-31G(d) geometries, and were used in conjunction with the M06-2X/6-31G(d) thermochemical corrections to obtain the free energies in water.

The geometries listed below were optimized at the M06-2X/6-31G(d) level of theory in the gas phase.

### MeSH

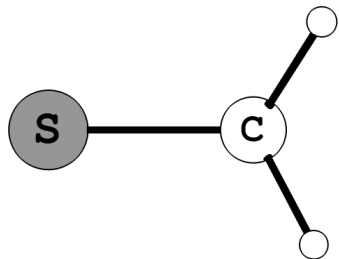


6	1.013174000	-0.096917000	-0.052025000
16	2.832526000	-0.062876000	0.040551000
1	0.644727000	-1.096548000	-0.287565000
1	0.636195000	0.623828000	-0.779203000
1	0.648707000	0.183712000	0.937703000
1	3.059402000	-0.452167000	-1.223776000

### Frequencies

325.9179	740.3729	818.4946	992.0486	1122.0626	1398.4898
1500.2169	1515.1432	2737.7458	3099.8752	3189.9767	3193.8322

E(RM062X)=	-438.629275
Zero-point correction=	0.047008 (Hartree/Particle)
Thermal correction to Energy=	0.050478
Thermal correction to Enthalpy=	0.051422
Thermal correction to Gibbs Free Energy=	0.022926
Sum of electronic and zero-point Energies=	-438.582267
Sum of electronic and thermal Energies=	-438.578797
Sum of electronic and thermal Enthalpies=	-438.577853
Sum of electronic and thermal Free Energies=	-438.606349

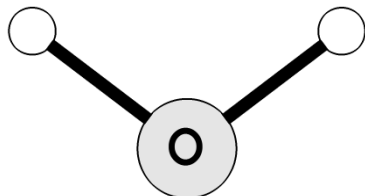
**MeS<sup>-</sup>**

6	1.099140000	0.064404000	-0.050063000
16	2.937606000	0.064293000	-0.050223000
1	0.688942000	0.869278000	-0.677021000
1	0.688834000	0.204766000	0.960280000
1	0.689141000	-0.880942000	-0.433612000

## Frequencies

726.6347    939.863    942.933    1358.6706    1507.2842    1510.9497

E(RM062X)=	-438.060636
Zero-point correction=	0.036655 (Hartree/Particle)
Thermal correction to Energy=	0.0397
Thermal correction to Enthalpy=	0.040644
Thermal correction to Gibbs Free Energy=	0.013051
Sum of electronic and zero-point Energies=	-438.023981
Sum of electronic and thermal Energies=	-438.020936
Sum of electronic and thermal Enthalpies=	-438.019992
Sum of electronic and thermal Free Energies=	-438.047585

**H<sub>2</sub>O**

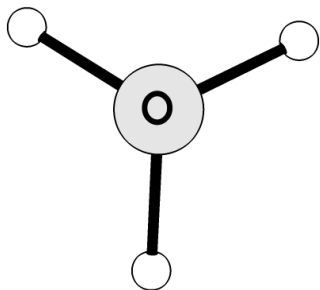
8	0.000029000	0.108787000	0.000000000
1	0.770470000	-0.473598000	0.000000000
1	-0.770499000	-0.473488000	0.000000000

## Frequencies

1665.13    3817.66    3941.03

E(RM062X)=	-76.3837478
Zero-point correction=	0.021469 (Hartree/Particle)
Thermal correction to Energy=	0.024304
Thermal correction to Enthalpy=	0.025248
Thermal correction to Gibbs Free Energy=	0.003164
Sum of electronic and zero-point Energies=	-76.3622788
Sum of electronic and thermal Energies=	-76.3594438
Sum of electronic and thermal Enthalpies=	-76.3584998
Sum of electronic and thermal Free Energies=	-76.3805838

H<sub>3</sub>O<sup>+</sup>



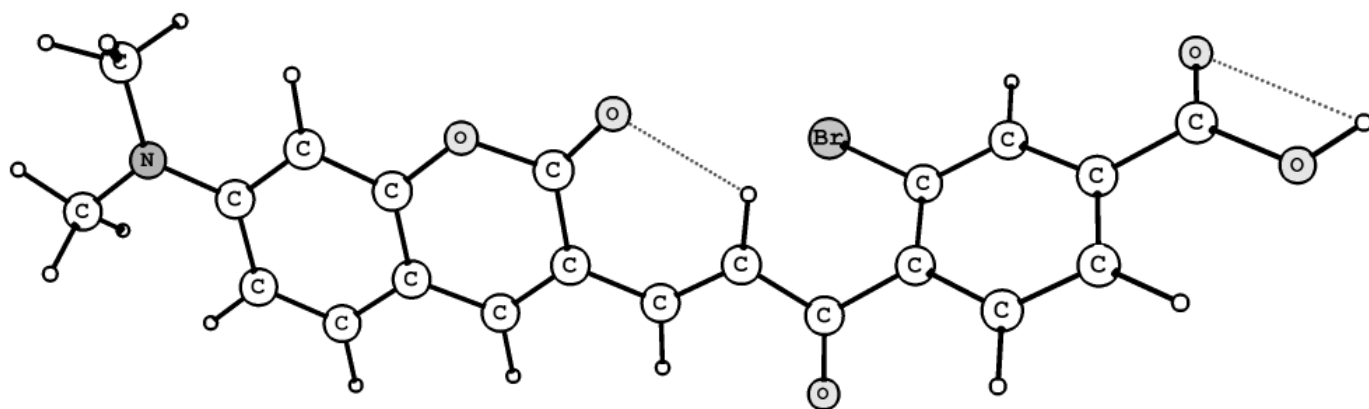
8	1.088100000	0.014662000	0.069461000
1	0.735877000	0.269670000	0.955671000
1	0.735930000	0.588161000	-0.652738000
1	2.073861000	-0.035329000	0.059504000

Frequencies

907.5629	1714.1075	1715.743	3542.0236	3638.283	3641.8869
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E(RM062X)=	-76.6542152
Zero-point correction=	0.034536 (Hartree/Particle)
Thermal correction to Energy=	0.037425
Thermal correction to Enthalpy=	0.038369
Thermal correction to Gibbs Free Energy=	0.015383
Sum of electronic and zero-point Energies=	-76.6196792
Sum of electronic and thermal Energies=	-76.6167902
Sum of electronic and thermal Enthalpies=	-76.6158462
Sum of electronic and thermal Free Energies=	-76.6388322

## 1-Br



6	-0.606978000	-4.971363000	-2.774539000
6	-0.461784000	-5.547311000	-1.478643000
6	-0.296167000	-4.747224000	-0.371038000
6	-0.261376000	-3.344213000	-0.474616000
6	-0.408510000	-2.790207000	-1.755799000
6	-0.577915000	-3.567394000	-2.890035000
6	-0.087192000	-2.448166000	0.619133000
6	-0.061979000	-1.093307000	0.454440000
6	-0.214589000	-0.538158000	-0.902784000
8	-0.386838000	-1.443157000	-1.930742000
7	-0.768918000	-5.762441000	-3.877437000
8	-0.202155000	0.628530000	-1.200800000
6	0.133101000	-0.220133000	1.600363000
6	0.203819000	1.122783000	1.619545000
6	0.420811000	1.814493000	2.910140000
6	0.678581000	3.301190000	2.863741000
6	-0.805716000	-7.205910000	-3.741829000
6	-0.921128000	-5.151895000	-5.183956000
6	-0.101245000	4.104600000	3.701892000
6	0.029047000	5.487035000	3.698545000
6	0.969928000	6.080089000	2.854751000
6	1.781023000	5.296571000	2.035086000
6	1.628387000	3.915969000	2.042823000
8	0.325318000	1.263153000	3.992764000
6	1.166295000	7.556318000	2.804049000
8	1.976171000	8.118013000	2.106495000
8	0.335209000	8.222675000	3.629687000
1	-0.481298000	-6.622389000	-1.352722000
1	-0.185476000	-5.203153000	0.609787000
1	-0.683230000	-3.060097000	-3.840315000
1	0.030665000	-2.863557000	1.619268000
1	0.244684000	-0.732335000	2.556919000
1	0.118632000	1.715002000	0.717048000
1	-1.639420000	-7.529629000	-3.105780000
1	-0.939232000	-7.650533000	-4.727728000
1	0.128745000	-7.593748000	-3.317386000
1	-1.806956000	-4.505134000	-5.222294000
1	-0.041174000	-4.552397000	-5.448996000
1	-1.038122000	-5.935178000	-5.932453000
1	-0.817280000	3.617416000	4.357239000
1	-0.588425000	6.104763000	4.341157000
1	2.523398000	5.773423000	1.403296000
1	0.534562000	9.169584000	3.530483000

35 2.790465000 2.889068000 0.961186000

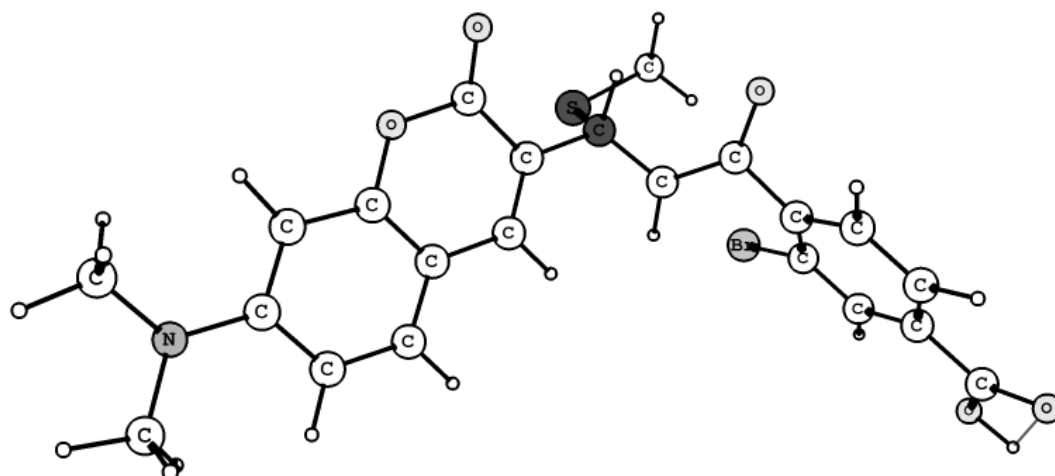
Frequencies

12.4404	21.8255	24.9127	32.3728	54.2308	61.9721
71.5211	79.54	91.8729	98.2898	117.8103	126.3756
143.0758	165.49	174.6183	189.6387	214.1416	230.1378
232.6635	271.2619	274.1276	283.156	291.3605	305.3237
330.3826	339.71	388.7007	405.6521	431.3525	433.5566
463.7948	473.9114	476.3256	488.9336	514.2039	535.7007
540.404	555.7961	577.3675	630.296	641.1007	657.2748
657.8462	691.4159	699.739	715.8124	726.9403	735.3408
765.7306	790.3049	807.0962	809.8627	822.1984	834.9821
859.6782	887.3498	888.8978	907.3854	917.2833	957.0188
966.5847	969.492	991.1652	1017.5898	1020.5567	1029.7128
1050.0564	1096.0696	1101.92	1124.0246	1150.1551	1152.8921
1157.6097	1170.9218	1186.0202	1199.2285	1224.5302	1229.2523
1251.0929	1267.4861	1286.6042	1307.0673	1318.7677	1331.7142
1345.6533	1353.849	1365.1513	1407.5396	1408.3213	1422.2289
1445.995	1448.5445	1466.8924	1505.013	1511.4359	1517.0196
1521.5635	1542.4149	1544.0129	1554.4208	1589.5864	1620.1419
1645.602	1683.1081	1689.79	1696.3961	1718.7249	1804.4901
1860.6924	1867.8493	3056.4594	3062.9416	3112.4807	3114.0119
3183.3248	3190.3197	3202.9135	3206.864	3224.6037	3229.9809
3245.8656	3260.6158	3269.5956	3271.3376	3273.2936	3759.6679

E(RM062X)=	-3812.09596
Zero-point correction=	0.334273 (Hartree/Particle)
Thermal correction to Energy=	0.359368
Thermal correction to Enthalpy=	0.360312
Thermal correction to Gibbs Free Energy=	0.275266
Sum of electronic and zero-point Energies=	-3811.761687
Sum of electronic and thermal Energies=	-3811.736592
Sum of electronic and thermal Enthalpies=	-3811.735648
Sum of electronic and thermal Free Energies=	-3811.820694



## 2-Br-a



6	0.350854000	-4.054305000	-2.481473000
6	1.602418000	-3.556098000	-2.044907000
6	1.698592000	-2.298134000	-1.475621000
6	0.575967000	-1.479970000	-1.299291000
6	-0.656312000	-1.990767000	-1.717617000
6	-0.783764000	-3.250601000	-2.294810000
6	0.599652000	-0.162099000	-0.716781000
6	-0.523237000	0.574225000	-0.570538000
6	-1.817876000	-0.002708000	-0.981620000
8	-1.794642000	-1.269360000	-1.558842000
7	0.249056000	-5.304640000	-3.089920000
8	-2.899917000	0.504310000	-0.847755000
6	-0.535946000	1.973321000	-0.014179000
6	0.595203000	2.338314000	0.864459000
6	0.378100000	3.037788000	2.036912000
6	1.617629000	3.332092000	2.871524000
8	-0.720408000	3.384986000	2.561454000
6	1.564754000	2.920925000	4.215254000
6	2.623842000	3.102049000	5.086227000
6	3.784580000	3.744944000	4.636097000
6	3.851576000	4.209793000	3.323000000
6	2.774499000	4.004382000	2.465232000
16	-0.640499000	3.077700000	-1.543400000
6	-0.956940000	4.634930000	-0.673522000
6	1.348934000	-6.233348000	-2.922220000
6	-1.072913000	-5.883004000	-3.224473000
6	4.907665000	3.928508000	5.576334000
8	5.971121000	4.572731000	5.032549000
8	4.931590000	3.557771000	6.731427000
1	2.501317000	-4.150543000	-2.150979000
1	2.667917000	-1.930271000	-1.147589000
1	-1.778044000	-3.568514000	-2.581238000
1	1.550245000	0.241956000	-0.378183000
1	-1.478300000	2.139454000	0.518781000
1	1.609833000	2.193305000	0.508127000
1	0.640736000	2.453203000	4.543297000
1	2.577094000	2.757317000	6.114959000
1	4.733714000	4.734536000	2.973302000
1	-0.925235000	5.441452000	-1.411411000
1	-1.935025000	4.616008000	-0.185984000
1	-0.183547000	4.793651000	0.082561000

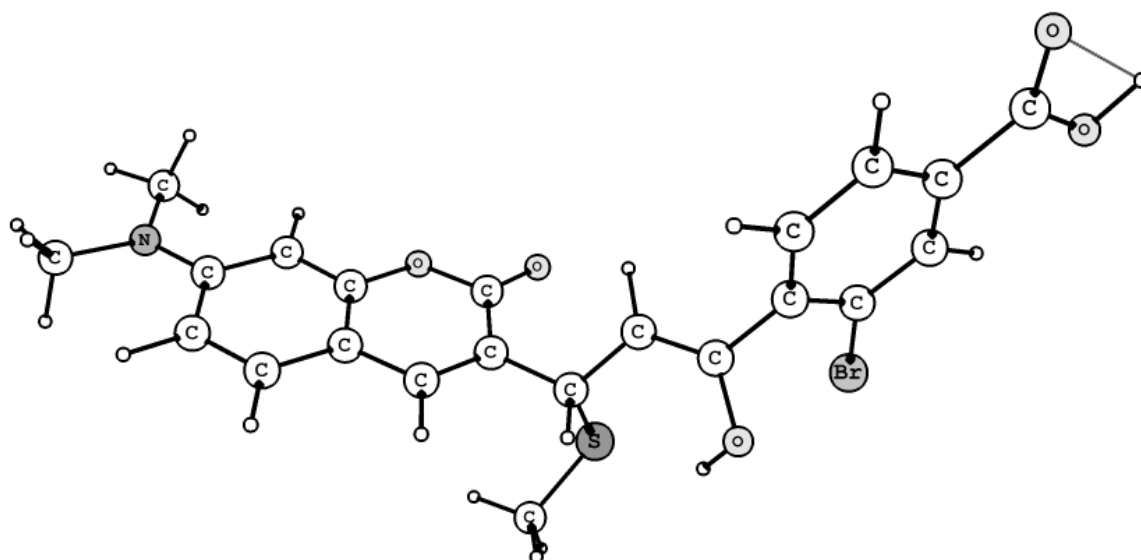
1	2.260818000	-5.841364000	-3.382554000
1	1.561889000	-6.453579000	-1.863416000
1	1.101870000	-7.167357000	-3.430417000
1	-1.703294000	-5.255548000	-3.861154000
1	-0.984682000	-6.858615000	-3.706341000
1	-1.579846000	-6.011437000	-2.254132000
1	6.637180000	4.629795000	5.737379000
35	2.952943000	4.716223000	0.710376000

Frequencies

15.999	17.7697	26.116	28.1936	40.4431	50.208
57.3042	64.0341	79.6353	88.4954	91.4368	103.4348
104.7666	122.4976	129.3316	141.5931	154.7822	165.9816
172.1095	192.3176	194.2826	243.4213	245.6384	249.4579
257.5441	284.5068	292.9865	310.5785	334.1541	348.8592
362.9504	394.7506	407.5541	434.0948	439.4749	469.4628
471.3837	480.0055	485.9634	511.8191	535.8995	539.6533
562.8772	587.8163	613.8159	636.3053	641.4805	650.5707
657.8757	671.5773	694.0674	697.5122	721.8282	732.3174
751.5057	758.6681	785.0821	790.2975	796.1102	805.3743
809.1616	828.9889	860.3271	887.5895	892.6827	922.2218
939.9729	942.4441	957.6332	972.3858	985.6557	993.8384
1013.7618	1016.8987	1052.549	1062.5936	1096.8828	1127.0939
1136.5748	1141.5666	1155.397	1169.7594	1173.8693	1181.1197
1189.2045	1197.9492	1219.4444	1223.8421	1249.0055	1256.456
1274.5341	1293.6544	1303.3253	1316.8939	1335.6689	1353.6036
1375.2029	1386.1521	1397.0446	1399.4334	1424.1074	1435.7289
1461.8088	1480.2598	1492.5395	1499.1642	1506.5244	1511.8464
1515.4232	1521.1058	1534.8925	1539.9203	1559.0775	1578.5828
1623.4692	1638.4804	1654.4661	1678.5945	1705.2299	1725.4637
1839.3046	1868.3334	3021.5415	3028.7687	3076.9255	3115.8269
3129.4472	3131.4788	3162.7446	3165.0688	3176.7409	3178.7861
3210.9074	3211.4564	3224.3633	3233.147	3237.9003	3244.7541

E(RM062X)=	-4250.20611
Zero-point correction=	0.3723 (Hartree/Particle)
Thermal correction to Energy=	0.401155
Thermal correction to Enthalpy=	0.402099
Thermal correction to Gibbs Free Energy=	0.308178
Sum of electronic and zero-point Energies=	-4249.83381
Sum of electronic and thermal Energies=	-4249.804955
Sum of electronic and thermal Enthalpies=	-4249.804011
Sum of electronic and thermal Free Energies=	-4249.897932

2-Br-b



8	1.591271000	0.022210000	2.010596000
6	2.539587000	-0.007404000	1.269476000
6	2.859175000	-1.100996000	0.336844000
6	1.981379000	-2.316786000	0.345799000
16	2.241002000	-3.312145000	1.893062000
6	3.911760000	-3.927341000	1.545081000
6	0.513207000	-2.044546000	0.169508000
6	-0.350251000	-3.033195000	-0.100613000
8	0.002128000	-4.346111000	-0.193185000
6	-1.793671000	-2.796043000	-0.348099000
6	-2.784129000	-3.384364000	0.447818000
6	-4.132710000	-3.176825000	0.191678000
6	-4.507773000	-2.356796000	-0.873738000
6	-5.940319000	-2.108739000	-1.192298000
8	-6.783063000	-2.756718000	-0.363516000
8	-6.331415000	-1.405529000	-2.093643000
6	-3.539815000	-1.743910000	-1.668448000
6	-2.195252000	-1.970319000	-1.403482000
6	3.951797000	-1.001597000	-0.457054000
6	4.813020000	0.144970000	-0.416793000
6	5.954283000	0.323452000	-1.214902000
6	6.733756000	1.456691000	-1.118480000
6	6.401223000	2.488306000	-0.196316000
7	7.175244000	3.613907000	-0.092106000
6	6.777778000	4.675755000	0.811124000
6	8.298980000	3.807000000	-0.986783000
6	5.255901000	2.321869000	0.605696000
6	4.493963000	1.169767000	0.483619000
8	3.397664000	1.071521000	1.284857000
1	2.312412000	-2.974068000	-0.471104000
1	4.190666000	-4.588325000	2.368637000
1	4.628492000	-3.102696000	1.498763000
1	3.939939000	-4.496609000	0.610957000
1	0.140830000	-1.036581000	0.308614000
1	0.716079000	-4.526449000	0.450116000
35	-2.309163000	-4.444445000	1.933255000
1	-4.885976000	-3.639135000	0.819549000

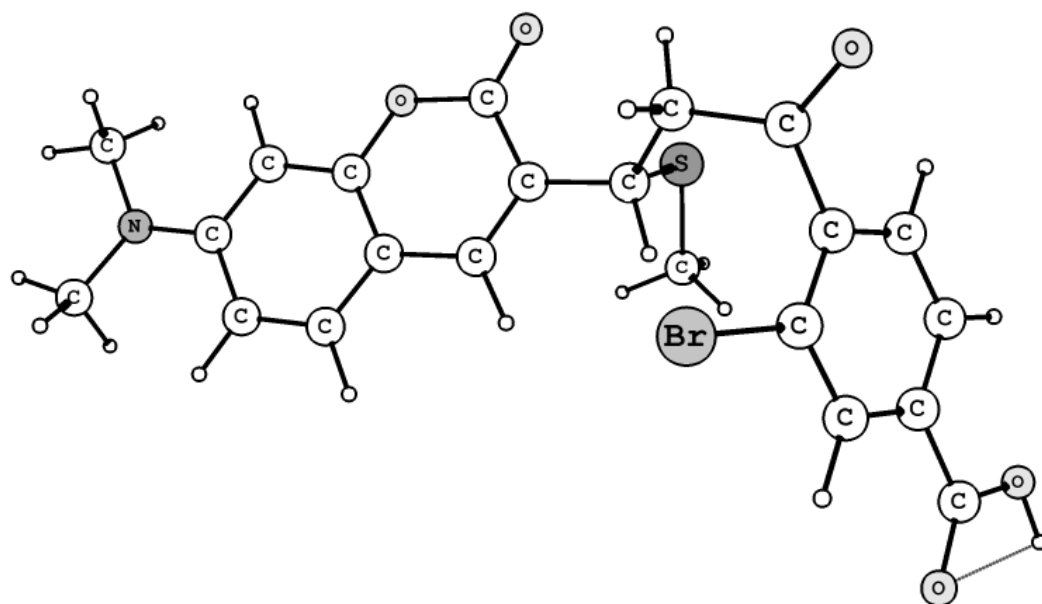
1	-7.687067000	-2.535718000	-0.646213000
1	-3.854336000	-1.108881000	-2.490367000
1	-1.428887000	-1.516817000	-2.025234000
1	4.191855000	-1.808796000	-1.149365000
1	6.224140000	-0.453821000	-1.926116000
1	7.604339000	1.552091000	-1.755169000
1	5.797206000	5.091888000	0.542174000
1	7.515588000	5.476835000	0.765837000
1	6.729192000	4.316083000	1.846082000
1	9.050456000	3.018345000	-0.859471000
1	8.772795000	4.761994000	-0.759611000
1	7.984279000	3.822225000	-2.038934000
1	4.933898000	3.065892000	1.322936000

#### Frequencies

16.0138	19.5096	21.5381	34.8957	38.9872	50.0124
56.0487	61.6138	74.3983	77.8308	90.0472	109.1717
118.8838	129.889	149.2588	152.0789	165.165	174.2553
182.3943	189.2866	210.5844	216.6502	247.1658	253.0982
265.8597	278.3687	291.1039	302.3143	325.3274	332.6023
372.504	407.515	414.5448	429.8656	454.1249	467.8222
471.7485	476.7672	501.7675	518.8294	527.1029	541.392
551.194	563.0477	580.5049	626.9326	630.5325	655.9134
657.8482	672.8234	699.049	700.0328	712.1457	729.6803
749.2965	756.4483	785.2419	791.5282	793.5666	806.0823
812.3791	826.6139	844.7034	857.8376	887.727	895.215
904.6417	947.642	957.0339	957.7261	975.5705	988.6221
992.8194	1013.1171	1013.8061	1049.1881	1094.804	1099.2447
1126.0921	1147.0838	1147.4446	1151.4953	1159.1906	1176.9764
1186.1667	1193.4105	1225.2147	1228.5428	1237.4314	1260.7233
1273.2694	1299.7721	1300.9857	1308.9002	1316.7349	1339.1986
1343.7892	1377.5046	1386.988	1402.7254	1405.4759	1419.1699
1424.1402	1450.0847	1456.1024	1462.3143	1490.5563	1502.8414
1506.2687	1509.7982	1512.7765	1520.5958	1544.8204	1553.833
1555.6637	1590.2012	1626.0701	1647.9086	1695.2723	1703.7824
1718.8304	1752.4654	1864.4887	1866.4659	3050.2529	3058.2145
3060.874	3074.9539	3109.05	3111.02	3159.9043	3177.5713
3178.8388	3181.4233	3190.6332	3200.728	3221.2337	3245.9649
3252.6834	3252.81	3258.5917	3261.5323	3636.1555	3765.1361

E(RM062X)=	-4250.74168
Zero-point correction=	0.386414 (Hartree/Particle)
Thermal correction to Energy=	0.415267
Thermal correction to Enthalpy=	0.416211
Thermal correction to Gibbs Free Energy=	0.32249
Sum of electronic and zero-point Energies=	-4250.355266
Sum of electronic and thermal Energies=	-4250.326413
Sum of electronic and thermal Enthalpies=	-4250.325469
Sum of electronic and thermal Free Energies=	-4250.41919

## 2-Br



8	0.91498000	0.580078000	1.225387000
6	2.073320000	0.437983000	0.924134000
6	2.702100000	-0.839561000	0.556124000
6	1.856714000	-2.077006000	0.605745000
16	1.349144000	-2.512252000	2.320989000
6	2.793917000	-3.518948000	2.750694000
6	0.612945000	-2.019825000	-0.286239000
6	-0.062367000	-3.369480000	-0.479406000
6	0.735278000	-4.652491000	-0.348657000
6	1.904781000	-4.954985000	-1.049850000
6	2.569188000	-6.160477000	-0.865995000
6	2.074461000	-7.075825000	0.061427000
6	0.911018000	-6.795790000	0.781521000
6	0.250827000	-5.592796000	0.567006000
8	-1.252758000	-3.450848000	-0.680387000
6	4.006975000	-0.865262000	0.195753000
6	4.804230000	0.328676000	0.179286000
6	6.155764000	0.392118000	-0.196423000
6	6.852577000	1.582404000	-0.193589000
6	6.216492000	2.793879000	0.195181000
7	6.907550000	3.978347000	0.209630000
6	6.205902000	5.209656000	0.513674000
6	8.260801000	4.030973000	-0.307220000
6	4.859196000	2.743625000	0.565446000
6	4.187808000	1.530509000	0.551227000
8	2.874485000	1.556521000	0.912028000
1	2.494741000	-2.901903000	0.277742000
1	2.691292000	-3.815809000	3.796798000
1	3.715290000	-2.938168000	2.642688000
1	2.844336000	-4.419671000	2.128831000
1	0.884724000	-1.624419000	-1.273300000
1	-0.138220000	-1.344196000	0.131816000
1	3.460801000	-6.403510000	-1.434628000
1	0.529525000	-7.515934000	1.497036000
1	-0.656375000	-5.354279000	1.113640000
1	4.468029000	-1.808119000	-0.099953000

1	6.659791000	-0.522732000	-0.499214000
1	7.892646000	1.583118000	-0.494854000
1	5.764929000	5.171905000	1.516578000
1	5.405008000	5.413976000	-0.210788000
1	6.913463000	6.038475000	0.488864000
1	8.308583000	3.729846000	-1.362997000
1	8.930595000	3.383027000	0.270181000
1	8.632049000	5.052603000	-0.225271000
1	4.302367000	3.623991000	0.859834000
6	2.826628000	-8.351081000	0.232644000
8	3.828289000	-8.641573000	-0.376355000
8	2.270344000	-9.164848000	1.149335000
1	2.818738000	-9.967360000	1.193420000
35	2.564723000	-3.780475000	-2.386723000

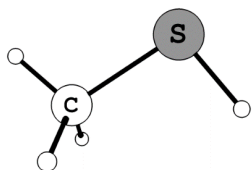
#### Frequencies

9.1214	17.5644	22.7697	35.8024	44.4386	49.6128
56.421	62.7632	71.0069	76.3392	83.8845	101.151
109.9919	116.1726	123.1901	140.7267	160.149	166.762
180.3891	191.9816	204.873	213.9621	242.612	256.0489
263.6519	278.8632	287.9297	294.8258	324.2481	331.8379
354.7145	390.7449	411.1645	428.665	444.5634	466.7147
471.0416	474.9301	492.0487	502.7252	517.7388	541.9016
552.6672	579.6302	607.2993	620.3514	637.288	644.5632
652.4616	685.8281	697.3946	702.2468	714.4327	726.0425
741.8189	754.2878	768.9246	788.0571	794.5626	817.0636
818.1171	861.7532	864.7297	888.9354	889.6991	945.5855
955.1978	965.0577	968.7522	974.9008	986.7315	1006.1824
1015.036	1019.7747	1041.3859	1092.9958	1097.9383	1119.7822
1129.928	1147.4366	1149.8513	1162.8964	1181.5538	1184.7313
1192.6375	1200.2426	1225.1025	1230.671	1259.6003	1275.4788
1287.5196	1295.7967	1299.8117	1313.5743	1322.124	1342.1121
1348.4844	1381.8967	1389.2921	1401.4977	1411.6217	1423.9016
1449.7376	1453.2228	1461.1974	1484.6815	1492.3168	1501.0602
1501.5062	1507.8112	1512.9436	1517.2384	1543.9331	1549.4299
1555.2243	1590.6336	1625.877	1646.5055	1698.6103	1706.5742
1717.0029	1845.072	1855.5899	1870.2926	3049.4122	3057.2091
3066.5055	3093.7345	3112.7762	3114.5938	3140.7593	3149.3604
3159.3806	3174.4896	3175.1306	3185.2122	3187.3564	3204.5088
3239.3987	3257.2095	3267.5604	3269.5388	3273.2596	3777.832

E(RM062X)=	-4250.76213
Zero-point correction=	0.386407 (Hartree/Particle)
Thermal correction to Energy=	0.41544
Thermal correction to Enthalpy=	0.416384
Thermal correction to Gibbs Free Energy=	0.321726
Sum of electronic and zero-point Energies=	-4250.375723
Sum of electronic and thermal Energies=	-4250.34669
Sum of electronic and thermal Enthalpies=	-4250.345746
Sum of electronic and thermal Free Energies=	-4250.440404

The geometries listed below were optimized with the SMD solvation model in water at the M06-2X/6-31G(d) level of theory .

### MeSH



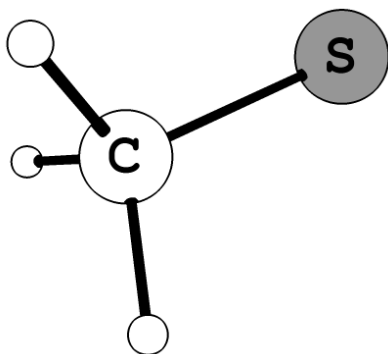
6	1.010871000	-0.095345000	-0.048499000
16	2.831520000	-0.062802000	0.037780000
1	0.649110000	-1.095966000	-0.289281000
1	0.638096000	0.623693000	-0.779317000
1	0.643700000	0.184063000	0.940885000
1	3.061435000	-0.454612000	-1.225882000

#### Frequencies

340.5178	737.1656	819.495	1005.6992	1115.3278	1393.9632
1474.4596	1494.791	2729.1588	3107.1758	3201.0039	3205.9331

E(RM062X)=	-438.63133
Zero-point correction=	0.046987 (Hartree/Particle)
Thermal correction to Energy=	0.05044
Thermal correction to Enthalpy=	0.051384
Thermal correction to Gibbs Free Energy=	0.02292
Sum of electronic and zero-point Energies=	-438.584343
Sum of electronic and thermal Energies=	-438.58089
Sum of electronic and thermal Enthalpies=	-438.579946
Sum of electronic and thermal Free Energies=	-438.60841

### MeS-



6	1.095680000	0.064485000	-0.050216000
16	2.935568000	0.064258000	-0.050164000
1	0.690724000	0.868018000	-0.675960000
1	0.690708000	0.204425000	0.958512000
1	0.690984000	-0.879387000	-0.432811000

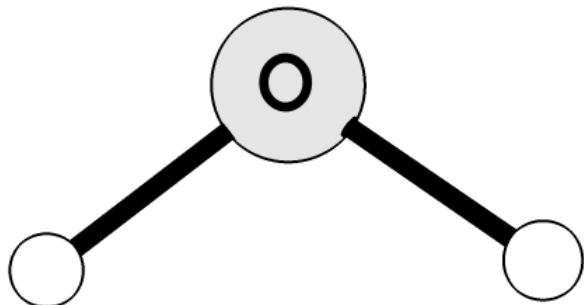
#### Frequencies

732.0494	961.6285	964.9579	1371.6824	1490.7574	1497.6598
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E(RM062X)=	-438.156891
Zero-point correction=	0.037134 (Hartree/Particle)
Thermal correction to Energy=	0.04017
Thermal correction to Enthalpy=	0.041114
Thermal correction to Gibbs Free Energy=	0.013534

Sum of electronic and zero-point Energies=	-438.119757
Sum of electronic and thermal Energies=	-438.116721
Sum of electronic and thermal Enthalpies=	-438.115777
Sum of electronic and thermal Free Energies=	-438.143357

## H<sub>2</sub>O

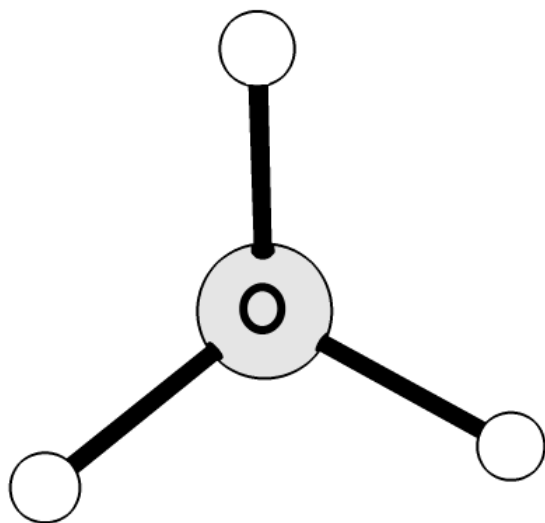


8	0.000028000	0.116390000	0.000000000
1	0.766442000	-0.477399000	0.000000000
1	-0.766470000	-0.477289000	0.000000000

### Frequencies

E(RM062X)=	-76.3990621
Zero-point correction=	0.021122 (Hartree/Particle)
Thermal correction to Energy=	0.023957
Thermal correction to Enthalpy=	0.024901
Thermal correction to Gibbs Free Energy=	0.0028
Sum of electronic and zero-point Energies=	-76.3779401
Sum of electronic and thermal Energies=	-76.3751051
Sum of electronic and thermal Enthalpies=	-76.3741611
Sum of electronic and thermal Free Energies=	-76.3962621

## H<sub>3</sub>O<sup>+</sup>



8	1.070116000	-0.036724000	0.059910000
1	0.754495000	0.287203000	0.933672000
1	0.755268000	0.595951000	-0.625733000
1	2.053889000	-0.009266000	0.064049000

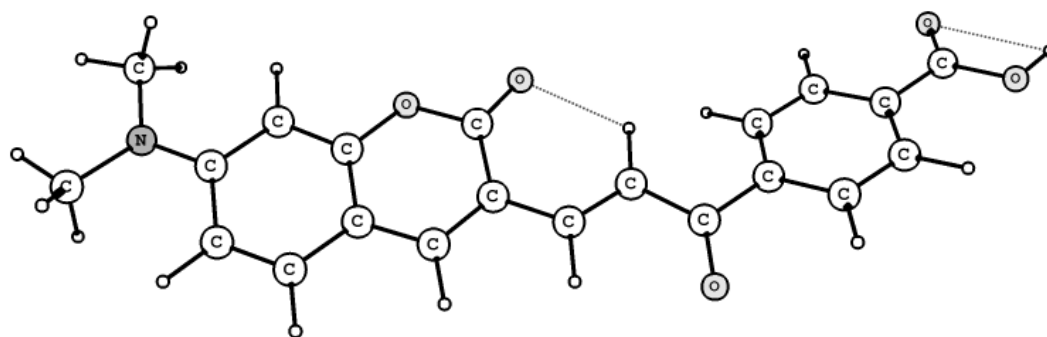
### Frequencies



1083.8111 1655.608 1689.1322 3581.8983 3652.4275 3655.5457

E(RM062X)=	-76.8091483
Zero-point correction=	0.034898 (Hartree/Particle)
Thermal correction to Energy=	0.037762
Thermal correction to Enthalpy=	0.038706
Thermal correction to Gibbs Free Energy=	0.015756
Sum of electronic and zero-point Energies=	-76.7742503
Sum of electronic and thermal Energies=	-76.7713863
Sum of electronic and thermal Enthalpies=	-76.7704423
Sum of electronic and thermal Free Energies=	-76.7933923

## 1-H



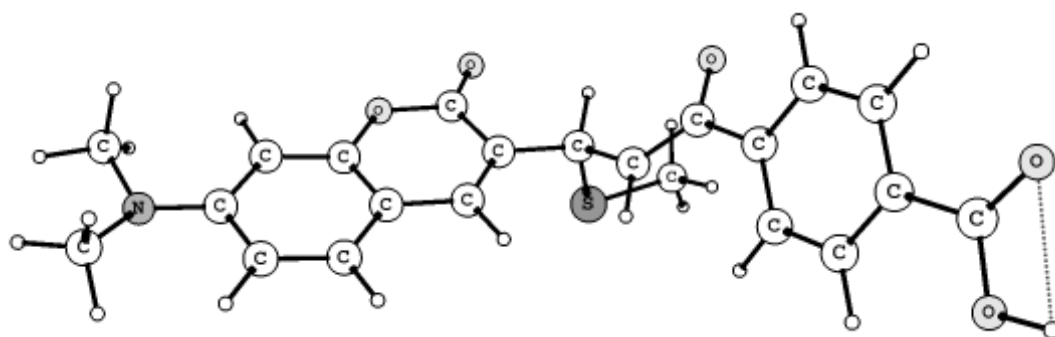
6	-0.589005000	-4.986850000	-2.768834000
6	-0.657596000	-5.530652000	-1.444551000
6	-0.501365000	-4.723964000	-0.346203000
6	-0.272465000	-3.333864000	-0.479232000
6	-0.207658000	-2.819050000	-1.787503000
6	-0.354820000	-3.597349000	-2.916062000
6	-0.122829000	-2.435538000	0.598207000
6	0.076300000	-1.085337000	0.408619000
6	0.152632000	-0.577717000	-0.954620000
8	0.008783000	-1.479353000	-1.980217000
7	-0.747505000	-5.780968000	-3.852620000
8	0.337973000	0.580518000	-1.290428000
6	0.193273000	-0.208615000	1.554474000
6	0.330878000	1.136601000	1.580336000
6	0.394494000	1.839753000	2.868905000
6	0.580273000	3.328776000	2.848101000
6	-1.035172000	-7.200965000	-3.693429000
6	-0.660307000	-5.210539000	-5.189366000
6	0.102393000	4.076925000	3.930351000
6	0.251564000	5.458154000	3.950358000
6	0.901036000	6.098525000	2.889354000
6	1.395488000	5.355990000	1.814962000
6	1.227623000	3.976172000	1.788903000
8	0.276993000	1.263553000	3.953575000
6	1.086510000	7.575368000	2.868157000
8	1.647496000	8.178173000	1.970282000
8	0.574406000	8.193051000	3.938756000
1	-0.831726000	-6.590069000	-1.302168000
1	-0.556335000	-5.148873000	0.652773000
1	-0.293687000	-3.122923000	-3.887616000
1	-0.176309000	-2.824582000	1.613847000
1	0.152150000	-0.726443000	2.513191000
1	0.364699000	1.719729000	0.670808000
1	-1.956267000	-7.356483000	-3.121191000
1	-1.165578000	-7.643786000	-4.679617000
1	-0.214199000	-7.720169000	-3.186777000
1	-1.448905000	-4.467416000	-5.356444000
1	0.312354000	-4.732169000	-5.349142000
1	-0.774222000	-6.008251000	-5.921511000
1	-0.399613000	3.571431000	4.749419000
1	-0.133752000	6.034233000	4.784985000
1	1.907007000	5.860178000	1.001471000
1	1.622782000	3.410620000	0.950974000
1	0.731988000	9.153749000	3.856614000

Frequencies

20.5476	27.1119	40.058	46.2422	65.0804	80.6172
102.6069	110.3406	112.259	129.6656	145.9741	156.8949
172.1643	180.113	209.2559	226.4596	231.093	255.4579
283.4234	293.3083	307.8988	314.0457	332.0831	382.6185
387.9541	412.4396	431.6224	444.8379	463.3916	472.2384
474.199	484.4277	509.5263	532.6203	535.8639	564.3926
580.8935	631.6851	639.8323	660.0592	661.5295	692.7112
700.9023	720.9825	733.7119	735.5473	775.6163	795.0865
806.5057	815.4281	828.1883	844.2638	869.4024	878.5648
881.5184	899.2691	911.8629	953.8968	978.535	1001.2224
1010.9799	1014.3919	1024.4627	1027.8779	1032.7563	1073.4705
1098.9908	1111.8254	1128.0266	1152.8791	1159.0411	1169.7794
1174.069	1194.459	1199.545	1221.8169	1227.7789	1243.4774
1261.7016	1296.4828	1317.6947	1326.7474	1337.7009	1349.8425
1361.5668	1374.4145	1395.8137	1406.4252	1424.4466	1446.7591
1456.1509	1467.8698	1498.4287	1503.2175	1509.609	1512.6082
1530.9211	1537.4153	1564.1194	1568.3943	1604.2136	1613.2849
1647.55	1658.8277	1684.8129	1702.0727	1727.9821	1757.7994
1771.5635	3077.1903	3084.3646	3139.8544	3144.3479	3197.0903
3209.4746	3217.8864	3221.0279	3226.2198	3235.1181	3245.5094
3263.5816	3265.4099	3266.3155	3267.6584	3301.4629	3696.6949

E(RM062X)=	-1240.92425
Zero-point correction=	0.343724 (Hartree/Particle)
Thermal correction to Energy=	0.367022
Thermal correction to Enthalpy=	0.367966
Thermal correction to Gibbs Free Energy=	0.289383
Sum of electronic and zero-point Energies=	-1240.580526
Sum of electronic and thermal Energies=	-1240.557228
Sum of electronic and thermal Enthalpies=	-1240.556284
Sum of electronic and thermal Free Energies=	-1240.634867

## 2-H-a



6	0.350379000	-4.026940000	-2.566087000
6	1.624428000	-3.495192000	-2.210094000
6	1.736133000	-2.244155000	-1.643740000
6	0.601726000	-1.451887000	-1.383977000
6	-0.640592000	-1.994536000	-1.726997000
6	-0.793203000	-3.246560000	-2.300430000
6	0.634037000	-0.152084000	-0.788403000
6	-0.501616000	0.553845000	-0.544377000
6	-1.784404000	-0.036087000	-0.907621000
8	-1.788415000	-1.280861000	-1.481022000
7	0.241425000	-5.261257000	-3.160073000
8	-2.881675000	0.477434000	-0.739748000
6	-0.531752000	1.942658000	0.042852000
6	0.577276000	2.278096000	0.976222000
6	0.362508000	2.929925000	2.164035000
6	1.566989000	3.248008000	3.015915000
8	-0.796422000	3.278690000	2.649273000
6	1.430772000	3.275531000	4.411718000
6	2.518307000	3.548903000	5.231789000
6	3.768887000	3.823600000	4.668833000
6	3.914810000	3.823302000	3.276816000
6	2.823793000	3.539986000	2.463760000
16	-0.585691000	3.101545000	-1.427653000
6	-0.970537000	4.642226000	-0.554109000
6	1.367036000	-6.184565000	-3.056165000
6	-1.081965000	-5.862834000	-3.257618000
6	4.906845000	4.116585000	5.570564000
8	6.056198000	4.364673000	4.924141000
8	4.835168000	4.135842000	6.788953000
1	2.524505000	-4.070255000	-2.388150000
1	2.716668000	-1.854088000	-1.382372000
1	-1.795230000	-3.593168000	-2.520897000
1	1.605197000	0.263777000	-0.528494000
1	-1.492869000	2.082447000	0.546013000
1	1.592392000	2.047627000	0.669636000
1	0.461256000	3.069985000	4.855046000
1	2.402288000	3.551576000	6.311530000
1	4.876173000	4.052459000	2.828270000
1	2.950071000	3.565318000	1.385452000
1	-0.995032000	5.446370000	-1.294061000
1	-1.945806000	4.578361000	-0.063917000
1	-0.196294000	4.862765000	0.186397000
1	2.250405000	-5.784312000	-3.559030000
1	1.622635000	-6.405105000	-2.010554000
1	1.098517000	-7.115446000	-3.555440000

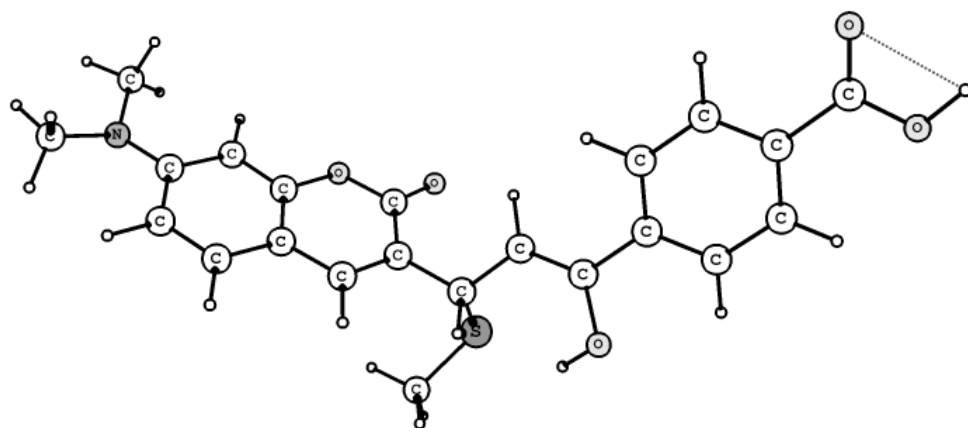
1	-1.745390000	-5.241868000	-3.864948000
1	-0.989911000	-6.831216000	-3.749207000
1	-1.541552000	-6.010511000	-2.269857000
1	6.753802000	4.547709000	5.582287000

Frequencies:

17.1283	27.4684	32.2058	38.2445	47.1036	64.8049
76.4057	79.5601	91.1456	102.694	103.7933	122.1509
131.4223	149.3526	170.9453	175.1841	193.1659	206.9243
214.4105	231.2756	245.7025	256.0814	258.0865	274.4813
297.4139	334.1915	345.7136	352.0746	384.8732	400.5593
419.3415	438.833	454.1438	464.6509	476.7326	481.1421
488.2688	506.9407	529.4565	545.2679	588.256	603.5786
641.8453	642.5605	645.1115	654.6172	670.4139	683.1719
703.9008	722.1175	726.4443	740.1582	748.3094	765.5977
792.6553	799.7295	808.5905	811.2241	819.0339	838.7032
868.7093	873.5553	892.4459	920.9746	952.8882	959.1007
984.2959	992.4281	1000.7403	1005.4106	1012.715	1018.3355
1031.5941	1054.5348	1098.3122	1111.8521	1122.8639	1143.5029
1150.7269	1153.1504	1175.979	1176.8566	1185.665	1197.0433
1207.4829	1225.1618	1229.8254	1240.1797	1268.1361	1282.2368
1291.4858	1310.7698	1328.3471	1339.5741	1354.5186	1377.7702
1387.4522	1389.5841	1404.9491	1421.6027	1441.7835	1461.3973
1467.9983	1469.5709	1488.3196	1490.1334	1496.9984	1504.1694
1508.14	1526.7622	1541.2577	1558.7528	1572.3945	1613.5456
1620.8428	1654.5641	1658.5277	1688.2674	1703.6314	1739.6935
1750.3986	3061.0586	3067.2751	3085.1976	3140.9392	3148.6173
3152.9726	3178.0041	3180.1615	3192.6727	3206.1683	3218.5494
3220.1085	3226.3453	3232.0757	3234.7336	3243.4787	3244.897

E(RM062X)=	-1679.10554
Zero-point correction=	0.382761 (Hartree/Particle)
Thermal correction to Energy=	0.409604
Thermal correction to Enthalpy=	0.410548
Thermal correction to Gibbs Free Energy=	0.323194
Sum of electronic and zero-point Energies=	-1678.722779
Sum of electronic and thermal Energies=	-1678.695936
Sum of electronic and thermal Enthalpies=	-1678.694992
Sum of electronic and thermal Free Energies=	-1678.782346

## 2-H-b



8	1.696805000	-0.016378000	2.252683000
6	2.618422000	-0.069304000	1.452941000
6	2.898452000	-1.171174000	0.543246000
6	2.007132000	-2.378202000	0.565545000
16	2.223214000	-3.354303000	2.132126000
6	3.914772000	-3.947571000	1.855074000
6	0.552215000	-2.071007000	0.346553000
6	-0.345574000	-3.016991000	0.022568000
8	-0.029541000	-4.351207000	-0.050592000
6	-1.766546000	-2.750216000	-0.293637000
6	-2.717178000	-3.769739000	-0.150640000
6	-4.058511000	-3.530377000	-0.430606000
6	-4.464260000	-2.266425000	-0.866334000
6	-5.883614000	-1.966551000	-1.179325000
8	-6.709394000	-3.002491000	-0.980874000
8	-6.281556000	-0.885207000	-1.578738000
6	-3.518861000	-1.247172000	-1.023979000
6	-2.181447000	-1.488131000	-0.745998000
6	3.983203000	-1.096198000	-0.273049000
6	4.837527000	0.047902000	-0.284019000
6	5.950426000	0.208026000	-1.130877000
6	6.709122000	1.356831000	-1.106562000
6	6.397650000	2.422573000	-0.211550000
7	7.170703000	3.557215000	-0.177211000
6	6.659203000	4.722776000	0.531444000
6	8.049958000	3.828293000	-1.309382000
6	5.281042000	2.274717000	0.637499000
6	4.539543000	1.106054000	0.582236000
8	3.455589000	1.016212000	1.422207000
1	2.353729000	-3.050572000	-0.230749000
1	4.162961000	-4.619192000	2.680494000
1	4.623644000	-3.115346000	1.851018000
1	3.981928000	-4.499723000	0.913727000
1	0.220572000	-1.044607000	0.449854000
1	0.789048000	-4.527700000	0.451906000
1	-2.406878000	-4.750963000	0.191809000
1	-4.785366000	-4.326393000	-0.307789000
1	-7.618316000	-2.727124000	-1.208818000
1	-3.835850000	-0.270720000	-1.376909000
1	-1.455355000	-0.696252000	-0.900356000
1	4.210067000	-1.922092000	-0.945952000
1	6.202090000	-0.593324000	-1.820957000

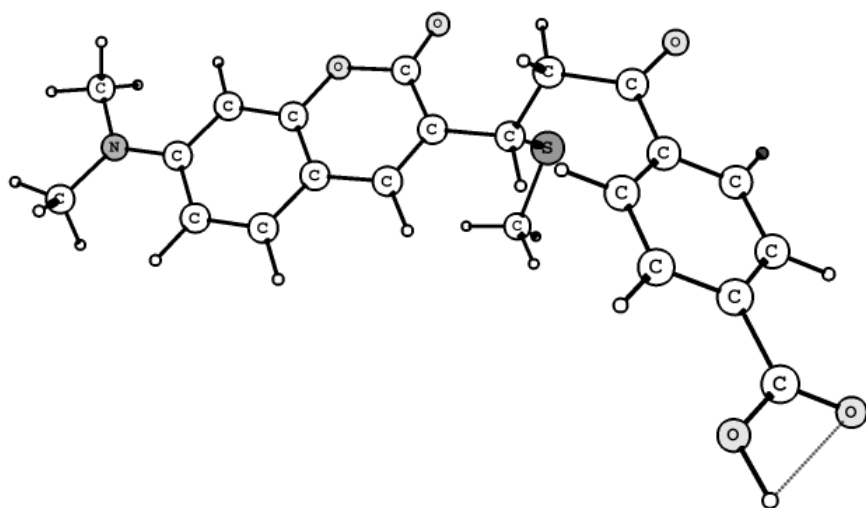
1	7.550887000	1.441043000	-1.782316000
1	5.715576000	5.085238000	0.098852000
1	7.401317000	5.518869000	0.473660000
1	6.495917000	4.495565000	1.587639000
1	8.826285000	3.064280000	-1.395226000
1	8.545277000	4.784598000	-1.142964000
1	7.494056000	3.879260000	-2.255810000
1	4.970302000	3.048460000	1.328655000

Frequencies:

14.1156	30.2742	36.9826	47.0967	52.3287	59.7213
72.0983	78.8161	90.6956	97.841	117.0799	125.0503
138.7118	151.9337	158.8121	171.4506	176.3384	201.4656
213.2454	225.36	235.7763	259.061	262.5132	268.2399
288.7624	309.9703	337.6364	376.9997	387.0323	401.4897
411.8239	417.9026	442.8413	464.8046	467.4709	478.7622
484.0593	505.3702	513.3583	534.5234	539.0964	571.9612
599.2028	629.4977	639.5418	654.4423	656.4726	659.574
698.9705	709.053	720.7959	728.943	746.7035	756.6576
784.9178	792.198	804.5763	815.1221	822.6314	836.4475
852.4809	860.1926	875.4371	896.77	901.2644	953.2216
963.0954	990.6778	1001.0224	1010.0975	1012.9532	1013.8332
1024.8906	1027.6413	1047.0902	1099.2498	1112.043	1126.9084
1140.0324	1148.5022	1151.7147	1158.7426	1186.7785	1190.8763
1197.3989	1226.6308	1235.3699	1237.4855	1243.3016	1247.2025
1283.166	1300.7533	1312.9021	1329.2725	1342.5717	1354.6622
1377.5947	1387.2019	1391.155	1394.1174	1397.7506	1419.8858
1449.0115	1462.2003	1463.1499	1469.7223	1488.5546	1493.6133
1496.5426	1502.489	1505.9681	1524.9804	1540.3052	1569.5124
1577.815	1615.447	1654.7186	1659.8111	1696.7209	1704.014
1736.0631	1744.1685	1760.6109	3058.4173	3065.1792	3084.3803
3091.7066	3150.2384	3152.1662	3177.3173	3186.7865	3197.9408
3206.2386	3207.9368	3217.5266	3238.9408	3243.8576	3248.2109
3255.2392	3256.6237	3259.7682	3265.3007	3667.974	3704.9697

E(RM062X)=	-1679.57232
Zero-point correction=	0.395833 (Hartree/Particle)
Thermal correction to Energy=	0.422978
Thermal correction to Enthalpy=	0.423922
Thermal correction to Gibbs Free Energy=	0.336281
Sum of electronic and zero-point Energies=	-1679.176487
Sum of electronic and thermal Energies=	-1679.149342
Sum of electronic and thermal Enthalpies=	-1679.148398
Sum of electronic and thermal Free Energies=	-1679.236039

## 2-H



8	0.807056000	0.715521000	1.071699000
6	1.981744000	0.467264000	0.843765000
6	2.575831000	-0.855817000	0.733283000
6	1.722534000	-2.077015000	0.930949000
16	1.173375000	-2.274414000	2.676790000
6	2.778438000	-2.684415000	3.412226000
6	0.494480000	-2.140601000	0.008649000
6	-0.255412000	-3.448681000	0.139756000
6	0.468060000	-4.739555000	-0.101105000
6	1.598095000	-4.805366000	-0.924026000
6	2.233295000	-6.024467000	-1.140055000
6	1.747355000	-7.178154000	-0.520108000
6	2.404148000	-8.499971000	-0.718863000
8	3.492375000	-8.441638000	-1.494429000
8	2.000113000	-9.540502000	-0.231922000
6	0.621706000	-7.116193000	0.307341000
6	-0.018337000	-5.901279000	0.510282000
8	-1.440205000	-3.463013000	0.445192000
6	3.912674000	-0.959333000	0.493689000
6	4.743226000	0.187940000	0.328014000
6	6.127116000	0.148448000	0.064356000
6	6.862179000	1.302008000	-0.087404000
6	6.240866000	2.584077000	0.021503000
7	6.966357000	3.725312000	-0.121562000
6	6.310937000	5.017839000	-0.010297000
6	8.389751000	3.658820000	-0.417689000
6	4.852181000	2.636061000	0.281866000
6	4.149566000	1.453134000	0.426195000
8	2.802830000	1.555354000	0.679383000
1	2.360575000	-2.942818000	0.725207000
1	2.611299000	-2.871272000	4.475689000
1	3.482169000	-1.854324000	3.306758000
1	3.193474000	-3.585806000	2.953043000
1	0.834372000	-2.025435000	-1.028763000
1	-0.207416000	-1.333804000	0.225984000
1	3.103066000	-6.073062000	-1.786134000
1	3.869079000	-9.338563000	-1.582871000
1	0.254843000	-8.017961000	0.787294000
1	-0.890947000	-5.843942000	1.153827000
1	4.369486000	-1.945687000	0.420525000



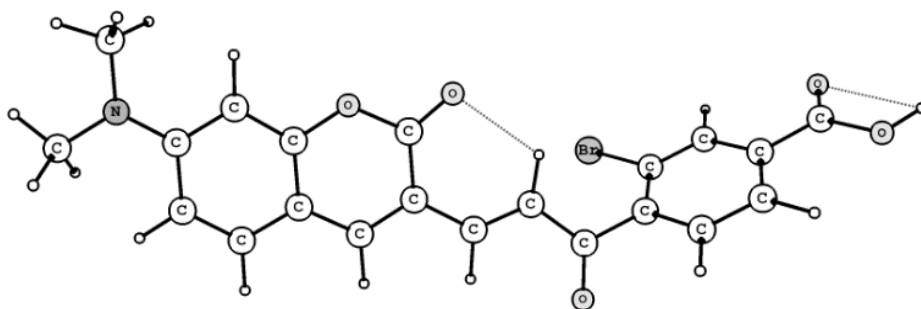
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1	7.923449000	1.228434000	-0.290540000
1	5.838516000	5.139955000	0.971482000
1	5.543617000	5.146111000	-0.783712000
1	7.055698000	5.803237000	-0.131365000
1	8.578696000	3.142119000	-1.366092000
1	8.939657000	3.142933000	0.377804000
1	8.778116000	4.673306000	-0.499003000
1	4.318030000	3.574114000	0.372411000
1	1.982650000	-3.914574000	-1.412753000

#### Frequencies

15.751	25.5635	38.2888	57.5697	59.2346	67.3648
73.5798	86.0381	91.6928	99.3246	113.9268	116.2406
127.9591	143.702	146.8728	176.3867	184.5411	197.8617
208.123	230.8941	234.3171	255.8652	266.1677	288.9014
298.1747	307.901	327.5452	353.2607	399.6143	410.4496
418.4496	439.1096	452.5858	458.5906	473.7112	478.3219
483.9455	495.0442	535.9446	546.6744	549.9285	572.1799
622.0759	630.2305	641.1969	660.8767	662.6049	694.588
701.8977	718.3765	729.2618	742.8395	751.9334	764.1887
793.9933	801.6561	815.1059	828.9858	831.2151	846.441
871.1402	888.4904	892.7273	952.0855	964.9227	976.6473
990.0976	999.2751	1006.2591	1011.0727	1017.0182	1020.2707
1031.2259	1066.2366	1097.0053	1103.3445	1114.3424	1130.1329
1148.5424	1159.9289	1168.5119	1170.1963	1177.6386	1192.9919
1203.1226	1228.586	1232.5371	1236.4348	1280.216	1280.9953
1294.6178	1318.389	1326.7853	1331.5456	1340.9982	1361.358
1378.1548	1378.8067	1399.3444	1404.6171	1423.1922	1452.7192
1458.5178	1470.8111	1474.0292	1477.1966	1487.5022	1496.467
1500.4001	1508.8568	1510.2275	1528.6804	1538.2638	1565.4135
1582.2686	1610.6369	1655.6164	1657.6766	1699.5951	1701.6568
1747.1594	1764.2593	1772.2646	3069.4845	3075.7839	3084.0116
3091.5328	3123.5514	3129.0446	3133.1764	3172.1088	3178.0832
3189.3248	3200.0957	3215.3049	3215.7838	3226.9651	3228.0757
3240.2556	3251.7262	3258.7422	3261.499	3262.9288	3714.539

E(RM062X)=	-1679.58872
Zero-point correction=	0.396622 (Hartree/Particle)
Thermal correction to Energy=	0.423541
Thermal correction to Enthalpy=	0.424485
Thermal correction to Gibbs Free Energy=	0.337576
Sum of electronic and zero-point Energies=	-1679.192098
Sum of electronic and thermal Energies=	-1679.165179
Sum of electronic and thermal Enthalpies=	-1679.164235
Sum of electronic and thermal Free Energies=	-1679.251144

## 1-Br



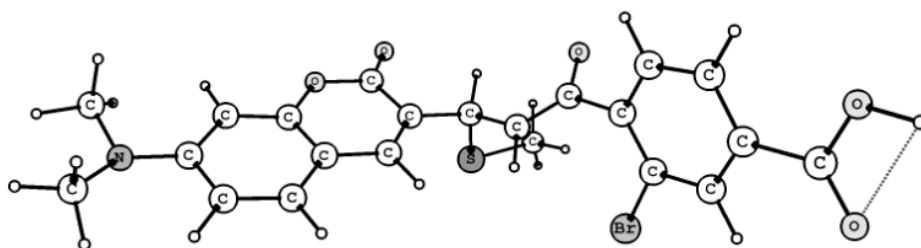
6	-0.661523000	-4.941287000	-2.770940000
6	-0.524863000	-5.527430000	-1.470042000
6	-0.320047000	-4.741175000	-0.365381000
6	-0.233711000	-3.332626000	-0.469347000
6	-0.374739000	-2.774912000	-1.754191000
6	-0.584149000	-3.531084000	-2.887866000
6	-0.015386000	-2.459782000	0.615959000
6	0.065945000	-1.093675000	0.455799000
6	-0.081690000	-0.537826000	-0.882568000
8	-0.298122000	-1.415479000	-1.916736000
7	-0.856569000	-5.717319000	-3.861495000
8	-0.034940000	0.642238000	-1.189287000
6	0.290764000	-0.249031000	1.607912000
6	0.418133000	1.096102000	1.656062000
6	0.607488000	1.770337000	2.942328000
6	0.770970000	3.266964000	2.901221000
6	-0.915013000	-7.168660000	-3.734391000
6	-1.001426000	-5.103424000	-5.173982000
6	-0.166941000	4.041675000	3.589076000
6	-0.113334000	5.429860000	3.551252000
6	0.902385000	6.055987000	2.826232000
6	1.864967000	5.300105000	2.156914000
6	1.787202000	3.915333000	2.195781000
8	0.570670000	1.207769000	4.035761000
6	1.014366000	7.539776000	2.752127000
8	1.901832000	8.123951000	2.158331000
8	0.036654000	8.175586000	3.403846000
1	-0.584712000	-6.602056000	-1.351144000
1	-0.216514000	-5.196793000	0.615955000
1	-0.680970000	-3.027104000	-3.841476000
1	0.093922000	-2.882621000	1.613376000
1	0.364844000	-0.792608000	2.550415000
1	0.371624000	1.714612000	0.769220000
1	-1.749023000	-7.478696000	-3.095163000
1	-1.061615000	-7.599767000	-4.723389000
1	0.016331000	-7.568373000	-3.318736000
1	-1.857502000	-4.419644000	-5.197000000
1	-0.099318000	-4.546401000	-5.452476000
1	-1.166418000	-5.885073000	-5.913775000
1	-0.954715000	3.541154000	4.144786000
1	-0.856912000	6.016695000	4.079030000
1	2.663460000	5.797704000	1.616274000
1	0.167929000	9.139774000	3.314533000
35	3.136405000	2.918871000	1.317136000

Frequencies

9.9976	21.2194	25.9354	40.5634	62.46	76.3273
83.1532	87.7973	98.6522	115.9552	123.5647	129.3352
142.9234	166.8537	175.2802	186.0111	210.7468	228.7337
231.8926	266.3717	280.754	284.6876	300.4701	305.7795
331.2794	343.8116	385.2589	398.2773	429.0569	436.5236
462.8194	475.4432	476.5547	490.4217	517.4868	533.5264
538.3842	554.7928	575.8847	620.053	632.6752	656.2797
661.4839	688.9575	701.062	722.5049	730.9135	736.0065
772.8084	782.5334	804.0189	809.2131	827.4644	834.5489
852.349	884.0534	888.6591	906.9312	909.1991	952.1177
970.6537	985.6003	1008.1845	1011.5932	1018.7218	1031.0703
1049.6979	1091.2841	1098.8213	1124.6588	1144.8302	1153.7371
1166.0719	1170.0574	1176.1246	1192.6973	1209.2759	1226.6865
1243.6448	1255.6803	1293.088	1297.3753	1319.1301	1330.6801
1343.1804	1344.858	1369.5287	1390.3745	1405.708	1424.3793
1442.6237	1447.5055	1466.9634	1497.8696	1500.7034	1502.8666
1506.9958	1528.3523	1532.5164	1547.6652	1567.6087	1604.3971
1613.126	1644.5646	1650.788	1686.2556	1695.8185	1735.4312
1761.0657	1777.8123	3073.3359	3082.9544	3133.5645	3144.0512
3195.6618	3210.3026	3220.5325	3229.3711	3240.1051	3244.9619
3258.5841	3266.3398	3269.7007	3273.0801	3290.1212	3704.5739

E(RM062X)=	-3812.1272
Zero-point correction=	0.333465 (Hartree/Particle)
Thermal correction to Energy=	0.358414
Thermal correction to Enthalpy=	0.359358
Thermal correction to Gibbs Free Energy=	0.27511
Sum of electronic and zero-point Energies=	-3811.793735
Sum of electronic and thermal Energies=	-3811.768786
Sum of electronic and thermal Enthalpies=	-3811.767842
Sum of electronic and thermal Free Energies=	-3811.85209

## 2-Br-a



6	0.484392000	-3.821364000	-2.843948000
6	1.703927000	-3.108458000	-2.660181000
6	1.726819000	-1.899397000	-1.999021000
6	0.552667000	-1.329933000	-1.472619000
6	-0.631872000	-2.052464000	-1.643078000
6	-0.692625000	-3.271331000	-2.299439000
6	0.492143000	-0.079760000	-0.779941000
6	-0.676092000	0.413210000	-0.292888000
6	-1.897817000	-0.358782000	-0.484809000
8	-1.810805000	-1.559630000	-1.138832000
7	0.455757000	-5.002611000	-3.558114000
8	-3.013843000	-0.037503000	-0.102050000
6	-0.809434000	1.742697000	0.404340000
6	0.385384000	2.186560000	1.171045000
6	0.288255000	2.775392000	2.398869000
6	1.575583000	3.172696000	3.082254000
8	-0.792973000	2.980024000	3.098959000
6	2.505020000	4.097195000	2.593032000
6	3.664559000	4.411513000	3.293589000
6	3.915023000	3.801524000	4.521285000
6	2.995163000	2.888974000	5.048887000
6	1.845039000	2.594584000	4.332274000
16	-1.276366000	2.966209000	-0.933216000
6	-1.662075000	4.386782000	0.120526000
6	1.709053000	-5.738099000	-3.708604000
6	-0.726846000	-5.846562000	-3.420056000
6	5.164259000	4.164258000	5.236385000
8	5.291182000	3.558429000	6.423499000
8	6.002455000	4.935708000	4.802665000
1	2.633835000	-3.506690000	-3.045309000
1	2.667923000	-1.369817000	-1.874071000
1	-1.654462000	-3.762292000	-2.377840000
1	1.418789000	0.475815000	-0.652903000
1	-1.679522000	1.700761000	1.066483000
1	1.358043000	2.139832000	0.690499000
1	4.371481000	5.132271000	2.896048000
1	3.178568000	2.412593000	6.006034000
1	1.124749000	1.888853000	4.737276000
1	-1.900228000	5.229982000	-0.533491000
1	-2.523816000	4.177045000	0.760144000
1	-0.794659000	4.643428000	0.734460000
1	2.445147000	-5.154086000	-4.264048000
1	2.138608000	-6.021219000	-2.737085000
1	1.510270000	-6.643959000	-4.281556000
1	-1.623460000	-5.319432000	-3.752447000
1	-0.603104000	-6.722318000	-4.057391000
1	-0.875686000	-6.181013000	-2.382909000
1	6.129008000	3.844032000	6.835927000

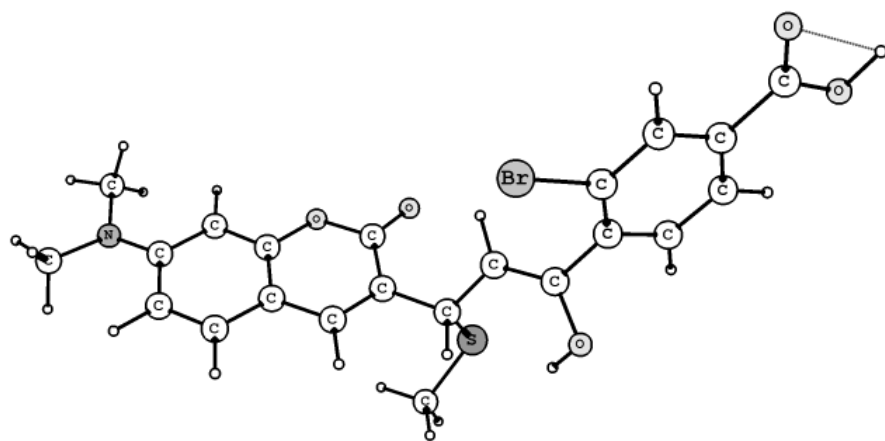
35 2.225667000 5.004961000 0.949910000

Frequencies

16.1867	19.5481	32.1791	35.218	52.354	65.5033
76.1248	88.9946	92.0691	95.8387	116.7312	118.8389
128.5449	136.1385	150.9486	170.4882	171.4867	182.1902
195.4719	200.6493	213.7277	243.1096	253.7418	257.5531
262.7458	286.7421	293.0123	311.7496	347.3993	356.2207
373.8254	392.2375	411.792	437.1217	445.7191	471.0426
478.3988	484.5754	496.1052	518.853	537.2594	542.0149
563.4704	587.4537	619.0485	640.5666	643.2388	657.7417
674.718	681.2076	692.181	724.5717	732.481	741.6557
747.6671	764.4425	783.8396	799.8338	801.6799	811.6884
826.1365	829.7803	850.6668	889.7605	893.1464	923.1919
951.8601	962.3767	972.7249	991.2809	999.3064	1000.3684
1012.8192	1022.5288	1046.2003	1066.0673	1095.564	1120.8089
1141.1857	1141.5464	1161.0701	1172.5851	1182.4435	1186.3764
1192.4308	1211.5835	1215.167	1226.2242	1240.5027	1267.2569
1282.1146	1294.6326	1301.8021	1312.3178	1337.6064	1349.7008
1378.7787	1384.7036	1387.7543	1407.3409	1420.2424	1439.4234
1454.2218	1467.3562	1474.2986	1484.4505	1491.2515	1501.44
1505.3095	1508.5211	1525.906	1542.9479	1545.8385	1574.7794
1616.9481	1630.2452	1644.5867	1661.5055	1692.0113	1703.0531
1736.9963	1764.2786	3055.2096	3062.4335	3086.6387	3138.3616
3157.3202	3157.3914	3177.7621	3183.7528	3195.8869	3202.9354
3210.3137	3218.9329	3224.3759	3241.027	3259.8303	3266.0605

E(RM062X)=	-4250.31231
Zero-point correction=	0.373493 (Hartree/Particle)
Thermal correction to Energy=	0.401599
Thermal correction to Enthalpy=	0.402543
Thermal correction to Gibbs Free Energy=	0.312042
Sum of electronic and zero-point Energies=	-4249.938817
Sum of electronic and thermal Energies=	-4249.910711
Sum of electronic and thermal Enthalpies=	-4249.909767
Sum of electronic and thermal Free Energies=	-4250.000268

2-Br-b



8	1.627329000	0.048321000	2.105808000
6	2.553460000	0.006928000	1.309520000
6	2.834841000	-1.076876000	0.381108000
6	1.969484000	-2.302018000	0.401150000
16	2.222411000	-3.291314000	1.953053000
6	3.931056000	-3.827809000	1.665608000
6	0.504395000	-2.032806000	0.202050000
6	-0.362434000	-2.996633000	-0.132285000
8	-0.031518000	-4.327153000	-0.230340000
6	-1.803933000	-2.770612000	-0.398849000
6	-2.729038000	-3.552215000	0.307365000
6	-4.096964000	-3.396699000	0.136554000
6	-4.567112000	-2.443087000	-0.769342000
6	-6.020648000	-2.226904000	-1.003792000
8	-6.799454000	-3.021951000	-0.263346000
8	-6.468954000	-1.410892000	-1.788606000
6	-3.669462000	-1.666936000	-1.499420000
6	-2.302490000	-1.838151000	-1.318535000
6	3.910725000	-0.976735000	-0.446115000
6	4.770032000	0.160722000	-0.428232000
6	5.895912000	0.326508000	-1.258200000
6	6.696632000	1.441223000	-1.164797000
6	6.417359000	2.465543000	-0.208731000
7	7.245251000	3.539996000	-0.079557000
6	6.881848000	4.624985000	0.818638000
6	8.318749000	3.749398000	-1.040108000
6	5.272958000	2.323984000	0.608483000
6	4.491910000	1.188536000	0.482356000
8	3.395103000	1.090399000	1.305103000
1	2.320562000	-2.956360000	-0.408277000
1	4.197759000	-4.509239000	2.477066000
1	4.615398000	-2.975479000	1.679371000
1	4.014971000	-4.357645000	0.712833000
1	0.137441000	-1.018609000	0.312012000
1	0.795157000	-4.500898000	0.261001000
1	-2.353265000	-4.286553000	1.013608000
1	-4.788800000	-4.007861000	0.705718000
1	-7.734862000	-2.827699000	-0.466809000
1	-4.044970000	-0.942225000	-2.214078000
35	-1.157728000	-0.789441000	-2.404651000
1	4.133458000	-1.786299000	-1.139981000
1	6.128600000	-0.449240000	-1.983438000

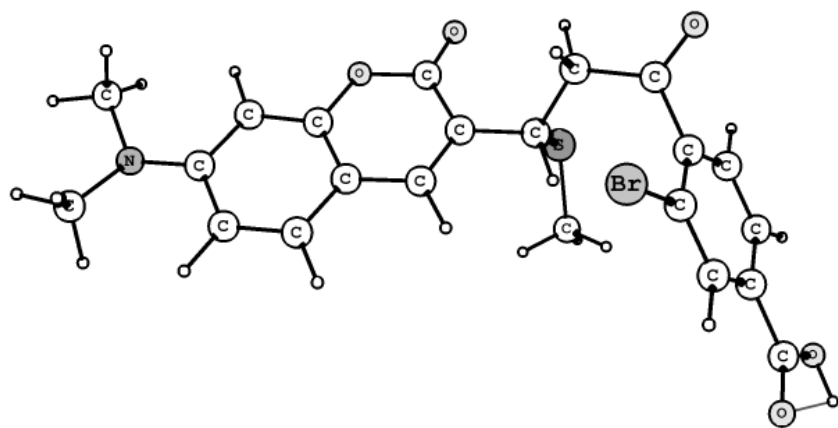
1	7.551853000	1.530747000	-1.822991000
1	5.943503000	5.108431000	0.515589000
1	7.676353000	5.370365000	0.808765000
1	6.769706000	4.260021000	1.844667000
1	9.022981000	2.911570000	-1.032787000
1	8.865351000	4.649624000	-0.761825000
1	7.932995000	3.876461000	-2.059835000
1	4.987548000	3.071674000	1.338540000

Frequencies

18.2944	22.3463	39.8506	45.5433	51.7599	57.8204
64.9055	78.094	93.4854	113.6035	122.1194	123.5442
134.1362	140.2508	153.4156	158.7578	165.5399	173.3539
185.1811	208.9804	213.7042	229.1255	252.8982	257.9879
267.8778	280.1677	288.2583	300.0271	326.9565	327.6011
375.8216	402.2745	421.3434	425.7366	451.2832	462.9259
471.9065	476.3908	482.5962	506.0812	526.3611	536.0045
540.1836	551.6007	573.7938	610.8499	629.533	653.3197
657.0497	673.1252	689.7572	701.2083	712.039	724.1374
747.3503	760.0941	781.9308	795.3503	800.1089	804.5704
815.2247	822.6341	833.2609	855.8486	885.1408	897.3359
902.7498	952.5804	963.0966	971.907	987.8958	998.6505
1008.1842	1012.171	1026.8915	1030.4124	1082.2496	1098.496
1113.7163	1145.0007	1150.7047	1158.907	1166.8049	1171.3924
1180.656	1191.6809	1209.9596	1234.1972	1236.485	1245.3273
1250.1859	1284.9567	1293.9562	1306.073	1319.8251	1329.8425
1338.3754	1371.0499	1383.6501	1389.105	1401.1739	1402.8622
1424.3826	1442.0543	1453.898	1466.119	1469.6505	1487.7978
1498.4614	1501.9524	1505.8646	1510.3233	1529.5767	1540.7771
1555.2029	1582.0619	1610.3487	1641.9542	1654.6302	1692.7052
1704.2635	1742.0905	1753.6373	1773.4402	3063.9365	3070.6388
3084.6544	3089.5981	3133.2011	3135.2197	3179.1613	3185.8814
3197.324	3207.1326	3208.0404	3220.8982	3248.7534	3248.9383
3249.4819	3260.5027	3260.9206	3263.8577	3659.291	3715.6336

E(RM062X)=	-4250.77449
Zero-point correction=	0.386116 (Hartree/Particle)
Thermal correction to Energy=	0.414546
Thermal correction to Enthalpy=	0.41549
Thermal correction to Gibbs Free Energy=	0.324986
Sum of electronic and zero-point Energies=	-4250.388374
Sum of electronic and thermal Energies=	-4250.359944
Sum of electronic and thermal Enthalpies=	-4250.359
Sum of electronic and thermal Free Energies=	-4250.449504

## 2-Br



8	0.962777000	0.554080000	1.291212000
6	2.122836000	0.420320000	0.932575000
6	2.738810000	-0.829052000	0.509913000
6	1.910884000	-2.081439000	0.541657000
16	1.449444000	-2.563721000	2.262444000
6	2.804481000	-3.730967000	2.564899000
6	0.652485000	-2.023004000	-0.329075000
6	-0.044104000	-3.359396000	-0.511960000
6	0.710499000	-4.654866000	-0.343730000
6	1.852860000	-5.003019000	-1.067293000
6	2.511934000	-6.204024000	-0.846351000
6	2.035575000	-7.067139000	0.139771000
6	0.894530000	-6.742626000	0.876572000
6	0.238983000	-5.543235000	0.627534000
8	-1.238978000	-3.406747000	-0.747498000
6	4.048869000	-0.832345000	0.147103000
6	4.836148000	0.360760000	0.170171000
6	6.194345000	0.437465000	-0.192996000
6	6.885768000	1.627823000	-0.137849000
6	6.248326000	2.826982000	0.296163000
7	6.951371000	4.004242000	0.393672000
6	6.198338000	5.243095000	0.544388000
6	8.220672000	4.109585000	-0.320049000
6	4.881944000	2.766263000	0.638431000
6	4.221867000	1.550850000	0.576319000
8	2.894957000	1.550077000	0.935516000
1	2.560704000	-2.888349000	0.191570000
1	2.704456000	-4.100641000	3.588239000
1	3.772298000	-3.232034000	2.460835000
1	2.744818000	-4.575947000	1.870256000
1	0.901987000	-1.630252000	-1.323819000
1	-0.091190000	-1.342666000	0.095377000
1	3.382867000	-6.478742000	-1.432395000
1	0.517598000	-7.419810000	1.634911000
1	-0.646178000	-5.277106000	1.197737000
1	4.525955000	-1.761021000	-0.164119000
1	6.699470000	-0.466499000	-0.524067000
1	7.928671000	1.639296000	-0.428656000
1	5.606997000	5.227386000	1.463185000
1	5.524803000	5.422576000	-0.305885000
1	6.902041000	6.072059000	0.618340000
1	8.101844000	3.940798000	-1.399198000



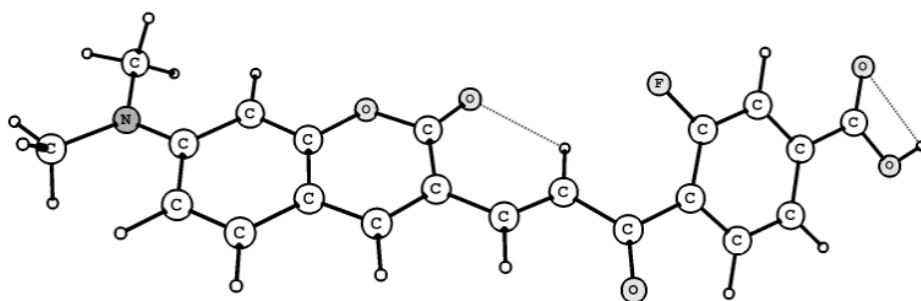
1	8.947755000	3.394825000	0.071940000
1	8.624077000	5.109915000	-0.164072000
1	4.322531000	3.638497000	0.952580000
6	2.772294000	-8.344579000	0.356198000
8	3.759094000	-8.671981000	-0.275940000
8	2.238032000	-9.102792000	1.316848000
1	2.756362000	-9.926921000	1.399070000
35	2.434721000	-3.913889000	-2.507661000

Frequencies

20.0944	23.6291	37.6949	44.5861	59.3957	60.1826
64.971	78.2306	91.8966	103.1792	109.934	118.2689
130.4389	142.8574	145.089	170.7941	171.8029	177.0518
205.0684	213.5274	225.5964	240.1425	253.8328	257.6957
274.3915	281.8617	294.3353	297.5018	335.0514	346.1663
361.194	399.9946	410.5077	435.2787	443.1772	466.9511
474.1782	481.3105	493.9861	504.9373	520.5605	536.994
552.7994	582.0795	608.418	620.8668	631.4985	640.5399
657.9498	685.9977	695.7917	704.7232	717.7364	726.0285
749.3666	756.7278	773.1559	791.3256	796.6867	816.1098
825.2639	854.6155	866.8156	891.1889	893.5895	951.3263
957.1361	968.8054	971.2642	989.1057	996.5342	1010.8027
1019.0369	1025.7203	1039.7045	1091.8942	1095.9197	1118.3771
1120.7346	1146.5251	1148.7357	1162.3499	1181.0953	1183.196
1190.2754	1198.4538	1219.1842	1227.6006	1236.283	1277.4373
1285.1389	1291.0324	1298.8152	1312.4207	1321.4476	1335.8367
1349.3875	1385.0281	1387.3454	1393.0127	1397.6546	1418.8752
1447.4483	1450.5272	1460.4415	1463.4589	1474.1871	1482.5058
1493.8595	1501.0829	1505.2339	1509.7751	1530.0822	1540.8857
1551.6934	1577.6881	1613.5064	1647.1284	1661.5832	1699.0422
1701.3768	1744.0588	1775.7202	1784.9233	3057.9042	3067.8308
3077.242	3093.2509	3143.1303	3149.7991	3157.0009	3162.1275
3164.0663	3183.5532	3197.2146	3206.1357	3207.9501	3221.8967
3251.2757	3264.7645	3266.0904	3275.0174	3282.0207	3702.4443

E(RM062X)=	-4250.79425
Zero-point correction=	0.386819 (Hartree/Particle)
Thermal correction to Energy=	0.415015
Thermal correction to Enthalpy=	0.415959
Thermal correction to Gibbs Free Energy=	0.326107
Sum of electronic and zero-point Energies=	-4250.407431
Sum of electronic and thermal Energies=	-4250.379235
Sum of electronic and thermal Enthalpies=	-4250.378291
Sum of electronic and thermal Free Energies=	-4250.468143

1-F



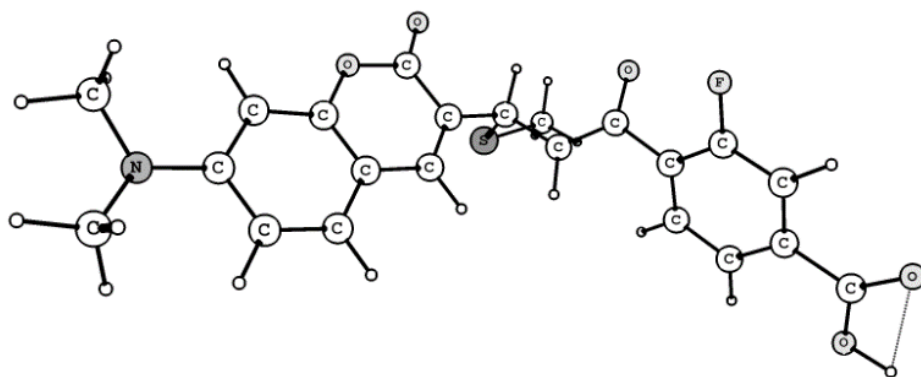
6	-0.484024000	-5.029083000	-2.756953000
6	-0.934061000	-5.483862000	-1.474471000
6	-0.972460000	-4.630555000	-0.401579000
6	-0.574769000	-3.277919000	-0.521432000
6	-0.145400000	-2.847383000	-1.790597000
6	-0.093496000	-3.674167000	-2.892818000
6	-0.577010000	-2.342522000	0.533677000
6	-0.172814000	-1.036689000	0.359608000
6	0.256695000	-0.610224000	-0.964826000
8	0.244375000	-1.545279000	-1.970918000
7	-0.428507000	-5.877120000	-3.810903000
8	0.629373000	0.506628000	-1.284288000
6	-0.191385000	-0.127853000	1.484527000
6	0.155912000	1.178675000	1.529612000
6	0.066442000	1.903558000	2.801633000
6	0.354938000	3.377934000	2.806755000
6	-0.922366000	-7.243072000	-3.683193000
6	-0.043857000	-5.377738000	-5.124002000
6	0.979820000	3.934571000	3.929086000
6	1.274805000	5.290311000	3.991568000
6	0.927285000	6.119770000	2.921139000
6	0.288757000	5.597171000	1.797126000
6	0.020634000	4.241459000	1.763426000
8	-0.188783000	1.356918000	3.876114000
6	1.214842000	7.582335000	2.936991000
8	0.941620000	8.335618000	2.020967000
8	1.806691000	7.993096000	4.062168000
1	-1.248108000	-6.512111000	-1.344096000
1	-1.314025000	-4.988850000	0.565994000
1	0.247082000	-3.264001000	-3.835323000
1	-0.906358000	-2.666899000	1.519602000
1	-0.543604000	-0.581924000	2.410955000
1	0.506142000	1.714075000	0.658201000
1	-1.984348000	-7.261641000	-3.412216000
1	-0.800653000	-7.748366000	-4.639953000
1	-0.356770000	-7.797604000	-2.927458000
1	-0.745546000	-4.614807000	-5.482753000
1	0.962067000	-4.946099000	-5.097419000
1	-0.040629000	-6.206983000	-5.829756000
1	1.245743000	3.280263000	4.753519000
1	1.771252000	5.698589000	4.864579000
1	-0.002796000	6.228082000	0.963810000
1	1.969665000	8.954831000	4.003735000
9	-0.625991000	3.760976000	0.680978000

Frequencies

17.1917	26.6554	33.239	41.1345	45.917	78.4142
93.5219	99.2807	111.2135	121.1145	142.9133	155.3004
161.8803	178.484	193.022	201.2631	215.7213	237.3398
258.9432	277.9362	283.8766	301.9666	311.4648	330.1759
366.6333	383.1252	390.2165	433.6971	438.9254	462.91
471.2487	473.0376	486.1052	506.0925	533.7351	538.0267
551.988	569.2381	593.986	616.0354	631.4701	655.2734
662.3457	695.0455	702.7611	723.5896	732.7697	748.0166
759.2432	779.6601	796.0451	810.2331	821.9063	850.1921
864.9831	873.8392	894.7179	899.7094	931.2734	952.9892
957.9858	978.4479	1001.9374	1007.1214	1013.4578	1026.4829
1071.1196	1100.5446	1107.4787	1127.1655	1153.5458	1160.3945
1166.2254	1176.2798	1194.1893	1196.6199	1223.611	1235.7616
1245.3575	1271.7159	1284.9788	1287.1759	1315.2671	1326.0785
1346.7684	1365.9034	1374.7989	1398.6377	1405.4453	1422.8724
1446.9182	1468.69	1479.5428	1495.5262	1502.7478	1505.1103
1510.3227	1526.6168	1540.5777	1553.5216	1565.8929	1602.678
1611.0216	1646.9889	1662.4716	1682.5608	1713.366	1727.3158
1758.7538	1771.1947	3074.8266	3084.8295	3140.0707	3146.5294
3200.3134	3205.8561	3216.004	3217.6803	3232.9445	3239.7015
3255.2727	3255.83	3257.5015	3275.2929	3288.1233	3702.2073

E(RM062X)=	-1340.13151
Zero-point correction=	0.334953 (Hartree/Particle)
Thermal correction to Energy=	0.359254
Thermal correction to Enthalpy=	0.360198
Thermal correction to Gibbs Free Energy=	0.278846
Sum of electronic and zero-point Energies=	-1339.796557
Sum of electronic and thermal Energies=	-1339.772256
Sum of electronic and thermal Enthalpies=	-1339.771312
Sum of electronic and thermal Free Energies=	-1339.852664

## 2-F-a



6	0.413541000	-3.967956000	-2.698245000
6	1.659865000	-3.455733000	-2.235414000
6	1.727065000	-2.253929000	-1.564273000
6	0.570621000	-1.497169000	-1.298871000
6	-0.647128000	-2.027975000	-1.734528000
6	-0.753410000	-3.230862000	-2.414718000
6	0.560250000	-0.236151000	-0.623254000
6	-0.592783000	0.446444000	-0.397103000
6	-1.853402000	-0.144447000	-0.832014000
8	-1.815551000	-1.351023000	-1.481784000
7	0.355229000	-5.139090000	-3.424313000
8	-2.964451000	0.334300000	-0.657745000
6	-0.664864000	1.800427000	0.263943000
6	0.488999000	2.150567000	1.135435000
6	0.333660000	2.703232000	2.378085000
6	1.579961000	3.140612000	3.110771000
8	-0.792551000	2.948064000	2.985786000
6	1.546382000	4.321933000	3.867674000
6	2.660342000	4.791113000	4.550999000
6	3.853656000	4.063923000	4.516046000
6	3.917493000	2.868333000	3.797801000
6	2.790828000	2.443089000	3.117112000
16	-0.863118000	3.035947000	-1.127714000
6	-1.260161000	4.500358000	-0.138010000
6	1.481999000	-6.063301000	-3.327476000
6	-0.949591000	-5.770555000	-3.583763000
6	5.032444000	4.580536000	5.254429000
8	6.102011000	3.776899000	5.182657000
8	5.046412000	5.631369000	5.872220000
1	2.575926000	-4.004668000	-2.412727000
1	2.688418000	-1.875643000	-1.226204000
1	-1.738584000	-3.567157000	-2.712642000
1	1.512777000	0.168818000	-0.288736000
1	-1.597145000	1.860234000	0.834205000
1	1.487664000	2.061280000	0.720253000
1	0.616514000	4.881460000	3.902474000
1	2.609786000	5.717551000	5.114091000
1	4.818588000	2.265403000	3.765098000
9	2.897436000	1.266735000	2.452215000
1	-1.336429000	5.351145000	-0.819974000
1	-2.214075000	4.374521000	0.381273000
1	-0.465371000	4.696121000	0.588128000
1	2.401430000	-5.602048000	-3.692816000
1	1.642560000	-6.410443000	-2.296893000

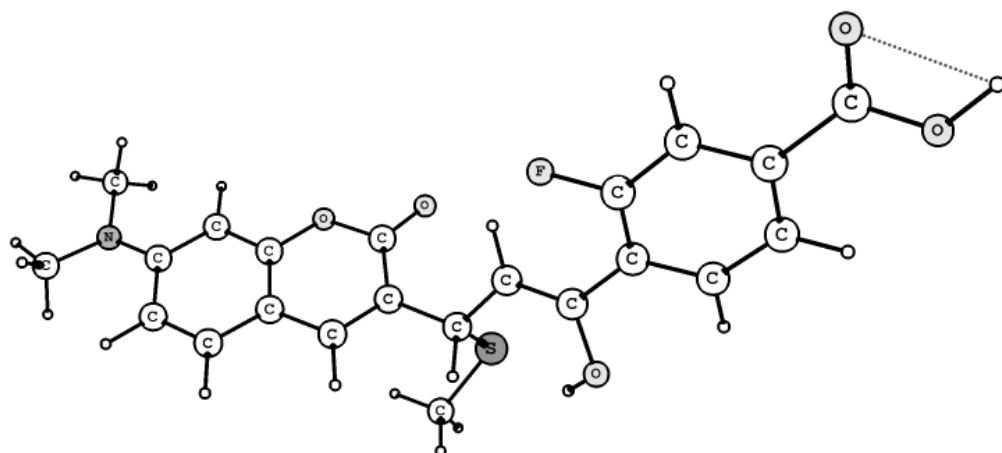
1	1.274891000	-6.926385000	-3.960379000
1	-1.631486000	-5.118615000	-4.134782000
1	-0.824551000	-6.685692000	-4.162802000
1	-1.405279000	-6.024576000	-2.615696000
1	6.835449000	4.179313000	5.686643000

Frequencies

20.2367	25.0232	29.2116	38.5947	45.1166	53.656
61.3057	80.6276	96.1484	104.5585	112.8819	117.6311
129.2494	147.3289	161.363	176.1869	188.1839	198.9025
203.9757	208.4966	228.9318	241.5509	249.0675	265.0254
275.8026	294.0048	337.8889	350.6288	360.9007	387.9353
393.1804	405.2307	434.5343	439.425	468.914	476.3093
483.4827	488.3202	498.2126	532.015	545.9273	564.9864
582.5703	602.2036	639.7139	642.168	651.059	657.8496
668.904	688.7811	704.9428	726.1761	739.6257	744.3394
754.2315	761.0083	787.3329	793.725	807.9103	812.3663
830.0755	856.6018	860.1619	879.1936	918.5746	930.0257
952.5486	962.5716	966.3965	992.1288	996.6521	1001.8417
1010.0807	1013.3396	1051.7681	1094.3999	1101.3472	1124.7408
1136.1588	1139.5269	1160.7966	1181.2617	1184.4369	1186.2853
1192.392	1208.8695	1212.7221	1235.4992	1249.325	1264.1943
1284.16	1288.6929	1294.3829	1309.9945	1341.0502	1360.9818
1375.712	1384.4886	1395.3	1406.8512	1421.4598	1443.1682
1461.9536	1468.2517	1470.2184	1489.6026	1489.9389	1499.8338
1505.2363	1510.8423	1522.5283	1535.7135	1555.3698	1573.601
1617.8897	1625.5406	1654.9667	1663.6908	1701.2386	1704.9682
1743.3972	1759.2983	3057.0964	3062.3515	3082.2258	3130.0067
3150.8261	3159.6934	3171.3771	3180.5373	3192.9616	3204.4003
3226.5497	3232.6482	3232.7663	3239.1819	3246.5749	3262.6458

E(RM062X)=	-1778.31505
Zero-point correction=	0.374812 (Hartree/Particle)
Thermal correction to Energy=	0.40246
Thermal correction to Enthalpy=	0.403404
Thermal correction to Gibbs Free Energy=	0.314276
Sum of electronic and zero-point Energies=	-1777.940238
Sum of electronic and thermal Energies=	-1777.91259
Sum of electronic and thermal Enthalpies=	-1777.911646
Sum of electronic and thermal Free Energies=	-1778.000774

## 2-F-b



8	1.631349000	0.190282000	2.100507000
6	2.557118000	0.109427000	1.306988000
6	2.816479000	-1.003398000	0.407519000
6	1.934022000	-2.214652000	0.469766000
16	2.189131000	-3.150408000	2.056685000
6	3.889680000	-3.715582000	1.777875000
6	0.469679000	-1.940380000	0.268270000
6	-0.404459000	-2.923908000	-0.004508000
8	-0.039193000	-4.248555000	-0.043958000
6	-1.845930000	-2.748808000	-0.282317000
6	-2.741938000	-3.791830000	-0.004848000
6	-4.101915000	-3.671161000	-0.261190000
6	-4.599555000	-2.492062000	-0.820615000
6	-6.045386000	-2.313841000	-1.117705000
8	-6.789278000	-3.374318000	-0.783975000
8	-6.520579000	-1.308804000	-1.615410000
6	-3.732852000	-1.440632000	-1.122514000
6	-2.387885000	-1.590103000	-0.848797000
6	3.894837000	-0.947935000	-0.420788000
6	4.776311000	0.172396000	-0.433492000
6	5.904448000	0.292943000	-1.268503000
6	6.729576000	1.391748000	-1.202904000
6	6.474745000	2.443208000	-0.270179000
7	7.328114000	3.500179000	-0.165198000
6	6.999362000	4.604891000	0.721490000
6	8.399290000	3.668472000	-1.136120000
6	5.328465000	2.347447000	0.551144000
6	4.520846000	1.227911000	0.451918000
8	3.422194000	1.173959000	1.276462000
1	2.275436000	-2.902653000	-0.314853000
1	4.151039000	-4.376575000	2.607820000
1	4.583601000	-2.871179000	1.765943000
1	3.963209000	-4.273691000	0.840599000
1	0.114724000	-0.920753000	0.343973000
1	0.767604000	-4.383393000	0.491312000
1	-2.355764000	-4.708835000	0.425984000
1	-4.769512000	-4.492697000	-0.026700000
1	-7.722057000	-3.188885000	-1.006175000
1	-4.092224000	-0.519608000	-1.570227000
9	-1.573793000	-0.563369000	-1.175206000
1	4.103030000	-1.781868000	-1.090046000

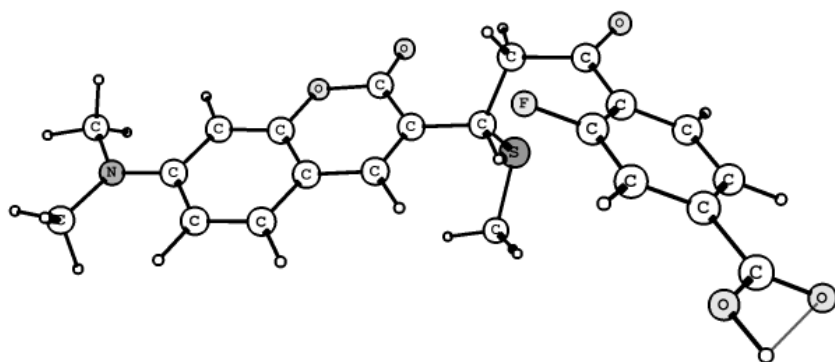
1	6.119604000	-0.505492000	-1.974268000
1	7.586673000	1.446158000	-1.862663000
1	6.074824000	5.112823000	0.415821000
1	7.815524000	5.326307000	0.702605000
1	6.879128000	4.253537000	1.751348000
1	9.090190000	2.819726000	-1.113427000
1	8.962095000	4.566058000	-0.882855000
1	8.009471000	3.777524000	-2.156309000
1	5.061985000	3.119472000	1.262756000

Frequencies

16.954	23.3987	28.9287	45.7229	50.2557	59.9541
66.9963	75.9448	93.7167	115.4528	122.6931	129.2129
144.9471	155.5231	163.6964	172.8874	183.5712	196.192
202.4067	211.2805	219.1802	237.5176	258.386	264.8681
276.9831	291.4333	319.3317	329.854	343.1828	374.935
386.0988	399.4907	406.2627	437.4212	457.2173	469.1287
473.1411	480.9495	499.6786	519.8179	537.8258	544.287
549.3751	576.2671	586.3029	616.1331	628.8968	649.9147
656.3724	660.2572	699.4377	709.8503	724.5288	737.135
742.7247	748.3458	759.0153	786.3804	802.0303	807.4683
816.8516	835.4556	837.8732	843.7955	879.8229	899.8174
923.724	953.484	956.4643	961.2153	987.7118	1001.2713
1010.6296	1011.8104	1015.5669	1037.4894	1103.2902	1108.6968
1122.8457	1143.5319	1157.3819	1162.8103	1165.561	1178.5465
1189.8805	1192.2642	1233.5869	1235.5924	1237.5926	1242.9954
1269.7657	1283.4847	1284.4704	1305.8284	1319.2411	1327.0151
1358.4384	1374.9076	1383.6081	1391.2657	1398.2001	1403.9547
1424.3177	1453.8464	1468.898	1470.5596	1481.3921	1489.0937
1496.6916	1502.3211	1505.1423	1509.4403	1530.3757	1542.6596
1563.7798	1583.1789	1611.192	1654.7401	1656.8328	1701.8481
1711.0535	1733.7209	1743.2554	1766.3834	3063.0847	3071.2628
3086.6515	3095.6437	3132.2623	3136.027	3180.1821	3187.4133
3200.8589	3210.1065	3211.6158	3221.0166	3249.8303	3251.5966
3255.5418	3265.9597	3266.3024	3270.2253	3629.5271	3726.3289

E(RM062X)=	-1778.78002
Zero-point correction=	0.387487 (Hartree/Particle)
Thermal correction to Energy=	0.415437
Thermal correction to Enthalpy=	0.416381
Thermal correction to Gibbs Free Energy=	0.327125
Sum of electronic and zero-point Energies=	-1778.392533
Sum of electronic and thermal Energies=	-1778.364583
Sum of electronic and thermal Enthalpies=	-1778.363639
Sum of electronic and thermal Free Energies=	-1778.452895

2-F



8	0.792658000	0.734545000	1.108301000
6	1.962586000	0.475244000	0.867730000
6	2.539182000	-0.853752000	0.743476000
6	1.667924000	-2.061909000	0.939487000
16	1.156366000	-2.284607000	2.693578000
6	2.766146000	-2.749811000	3.384113000
6	0.407404000	-2.079512000	0.062526000
6	-0.297726000	-3.416583000	0.084290000
6	0.468070000	-4.688945000	-0.146984000
6	1.596005000	-4.791008000	-0.960422000
6	2.278289000	-5.978653000	-1.156197000
6	1.816299000	-7.119771000	-0.501243000
6	2.514716000	-8.428142000	-0.658364000
8	3.585010000	-8.363720000	-1.454850000
8	2.151961000	-9.455485000	-0.117464000
6	0.687842000	-7.061290000	0.320993000
6	0.020997000	-5.855899000	0.486308000
8	-1.495049000	-3.488589000	0.314294000
6	3.871670000	-0.973765000	0.488304000
6	4.714706000	0.164746000	0.323231000
6	6.095803000	0.110880000	0.047555000
6	6.843123000	1.256709000	-0.103886000
6	6.237433000	2.545261000	0.015708000
7	6.973825000	3.679319000	-0.128941000
6	6.331041000	4.977942000	-0.014846000
6	8.394430000	3.599292000	-0.434827000
6	4.851827000	2.611795000	0.288460000
6	4.137069000	1.436517000	0.434066000
8	2.794294000	1.554027000	0.701652000
1	2.286928000	-2.933623000	0.703496000
1	2.617942000	-2.956912000	4.446608000
1	3.487297000	-1.934411000	3.281533000
1	3.147861000	-3.649766000	2.894208000
1	0.688050000	-1.848597000	-0.972130000
1	-0.314352000	-1.329181000	0.390713000
1	3.146410000	-5.996181000	-1.805939000
1	3.997182000	-9.247952000	-1.509109000
1	0.340906000	-7.955963000	0.827058000
1	-0.853633000	-5.797647000	1.126810000
1	4.314269000	-1.965612000	0.401715000
1	6.571090000	-0.862100000	-0.048328000
1	7.901918000	1.171821000	-0.315783000
1	5.865685000	5.105305000	0.969651000
1	5.560336000	5.112395000	-0.783828000

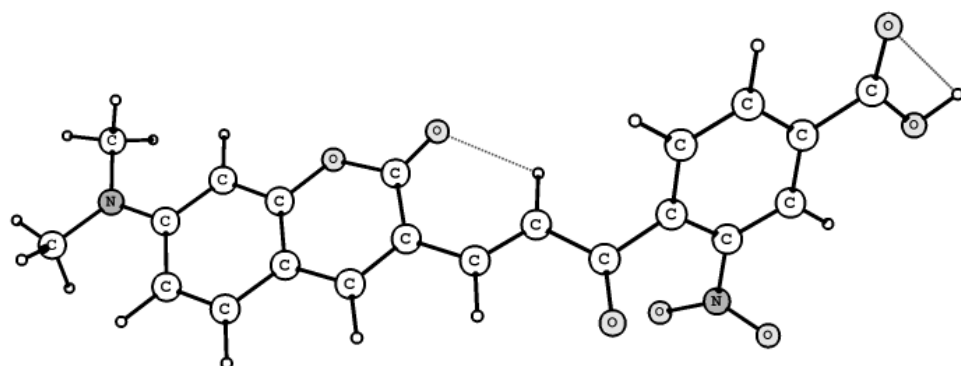


1	7.082136000	5.756483000	-0.140769000
1	8.572171000	3.084677000	-1.386542000
1	8.944008000	3.074615000	0.355080000
1	8.792580000	4.610108000	-0.514518000
1	4.329248000	3.555316000	0.388711000
9	2.052436000	-3.698074000	-1.607616000

Frequencies

17.8546	22.887	33.1747	46.5993	57.2627	58.2437
65.5072	82.6627	89.7142	100.6599	110.4143	118.1121
121.9646	135.6814	142.1909	181.6802	187.8037	192.2448
203.0952	214.6847	232.7143	242.9754	255.5673	273.0716
289.9715	303.0698	306.1383	328.129	351.3439	375.4619
401.8139	416.137	432.288	447.3443	453.3744	474.6761
479.229	483.4433	493.118	538.1781	539.445	547.4243
561.5229	608.7741	618.9636	625.9207	632.5548	656.8091
662.6682	695.9457	702.6092	723.4675	730.6719	747.8059
753.7189	764.6913	769.449	787.5709	799.6966	816.6884
833.2698	850.1733	875.9656	892.0407	928.9874	952.0238
961.158	966.1408	980.299	995.6451	1002.3653	1007.9708
1011.1983	1017.0534	1062.8768	1091.8615	1102.7787	1116.7336
1127.9767	1148.6032	1162.0308	1166.9862	1171.483	1185.5706
1193.8826	1194.7208	1234.9813	1237.2033	1259.4833	1273.9691
1288.7609	1292.3319	1299.0852	1319.1328	1328.5993	1336.0298
1364.5606	1376.4024	1388.4604	1406.6555	1409.1152	1427.6268
1457.6305	1469.0883	1470.3984	1476.5959	1477.395	1488.7388
1498.0724	1501.2236	1507.727	1509.5179	1529.7399	1538.5141
1555.7851	1582.7336	1611.0918	1656.5524	1658.7036	1700.2439
1714.34	1747.6147	1766.3889	1776.4619	3069.5552	3075.8654
3084.4602	3110.1711	3125.0462	3129.4061	3132.8451	3173.1159
3178.1147	3189.7468	3200.5229	3216.551	3217.0945	3231.6509
3246.8641	3257.0945	3261.0299	3261.4843	3269.1825	3706.6957

E(RM062X)=	-1778.79645
Zero-point correction=	0.38861 (Hartree/Particle)
Thermal correction to Energy=	0.416362
Thermal correction to Enthalpy=	0.417307
Thermal correction to Gibbs Free Energy=	0.328343
Sum of electronic and zero-point Energies=	-1778.40784
Sum of electronic and thermal Energies=	-1778.380088
Sum of electronic and thermal Enthalpies=	-1778.379143
Sum of electronic and thermal Free Energies=	-1778.468107

1-NO<sub>2</sub>

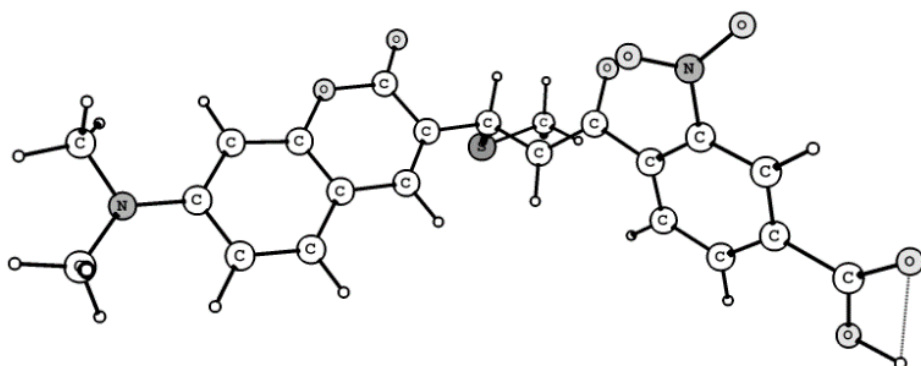
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6	-1.144380000	-5.382225000	-1.498388000
6	-1.281736000	-4.508645000	-0.451456000
6	-0.753871000	-3.196742000	-0.513241000
6	-0.079082000	-2.830838000	-1.694314000
6	0.076670000	-3.679396000	-2.769327000
6	-0.858546000	-2.244172000	0.518125000
6	-0.326275000	-0.976616000	0.403930000
6	0.371235000	-0.620050000	-0.823499000
8	0.460840000	-1.575528000	-1.806705000
7	-0.342260000	-5.847075000	-3.734150000
8	0.897396000	0.451450000	-1.073608000
6	-0.473822000	-0.042878000	1.494297000
6	-0.049567000	1.240280000	1.589067000
6	-0.310958000	1.989110000	2.816134000
6	0.145279000	3.427684000	2.839434000
6	-0.885626000	-7.196804000	-3.640982000
6	0.346414000	-5.430519000	-4.948219000
6	0.894136000	3.969407000	3.886537000
6	1.188772000	5.318289000	3.988251000
6	0.719219000	6.170044000	2.987935000
6	-0.022779000	5.661371000	1.922268000
6	-0.304529000	4.299650000	1.848976000
8	-0.903950000	1.549092000	3.799716000
6	1.004871000	7.632845000	3.025719000
8	0.607375000	8.417204000	2.185740000
8	1.741176000	7.997823000	4.077666000
1	-1.560812000	-6.378285000	-1.415051000
1	-1.806167000	-4.816211000	0.449567000
1	0.608296000	-3.323399000	-3.643234000
1	-1.380605000	-2.518588000	1.433562000
1	-1.007591000	-0.450593000	2.353415000
1	0.489112000	1.741159000	0.794789000
1	-1.969034000	-7.177960000	-3.481111000
1	-0.686271000	-7.719249000	-4.575236000
1	-0.417664000	-7.756259000	-2.823580000
1	-0.151388000	-4.568837000	-5.407124000
1	1.388884000	-5.164399000	-4.739321000
1	0.336159000	-6.254850000	-5.659563000
1	1.788392000	5.686197000	4.813684000
1	-0.382818000	6.333613000	1.150066000
1	-0.899755000	3.912700000	1.026856000
1	1.895253000	8.962200000	4.043022000
7	1.467239000	3.082165000	4.904689000

8	1.812594000	1.964539000	4.558144000
8	1.591863000	3.518704000	6.037310000

Frequencies

18.6166	26.8195	27.6482	37.7628	55.5243	61.4863
65.5969	72.8321	105.5281	109.9501	116.0273	116.9636
138.1518	152.6322	160.3088	164.9213	191.7014	201.6264
206.8712	225.8607	255.0834	280.3579	298.8004	303.0032
310.2252	328.5821	363.8465	368.9072	393.5194	417.6558
425.6523	437.7364	461.4909	472.7835	474.6911	485.481
510.7358	535.9348	551.9787	563.6596	601.0818	615.1148
633.0439	654.6278	667.2898	693.1344	701.3703	711.166
724.213	733.2065	752.3521	775.751	794.257	798.3592
808.6241	820.5069	835.5683	846.9972	871.4811	884.2353
897.4055	902.4304	946.2049	952.6352	954.9025	984.3121
1006.2207	1007.5237	1019.0235	1034.4876	1060.6406	1100.6924
1104.7714	1130.6598	1146.539	1150.7564	1166.534	1173.2581
1183.1993	1198.9712	1220.2903	1226.6868	1246.2556	1257.6951
1288.0922	1299.2327	1313.3305	1326.9008	1339.2209	1366.1781
1375.837	1405.2417	1408.332	1424.125	1448.0446	1452.7553
1467.6507	1478.6706	1491.0661	1497.3526	1504.5462	1509.9831
1527.9744	1544.1476	1557.3431	1563.5327	1598.9985	1609.6916
1635.5002	1647.2725	1656.1623	1684.1251	1714.8866	1732.6056
1760.5058	1779.9361	3075.9311	3081.5418	3141.227	3143.1717
3200.9848	3204.9643	3214.5167	3215.5836	3227.356	3234.6894
3253.5633	3261.3995	3262.5914	3273.8436	3289.5034	3697.9371

E(RM062X)=	-1445.35042
Zero-point correction=	0.345551 (Hartree/Particle)
Thermal correction to Energy=	0.371763
Thermal correction to Enthalpy=	0.372708
Thermal correction to Gibbs Free Energy=	0.286438
Sum of electronic and zero-point Energies=	-1445.004869
Sum of electronic and thermal Energies=	-1444.978657
Sum of electronic and thermal Enthalpies=	-1444.977712
Sum of electronic and thermal Free Energies=	-1445.063982

2-NO<sub>2</sub>-a

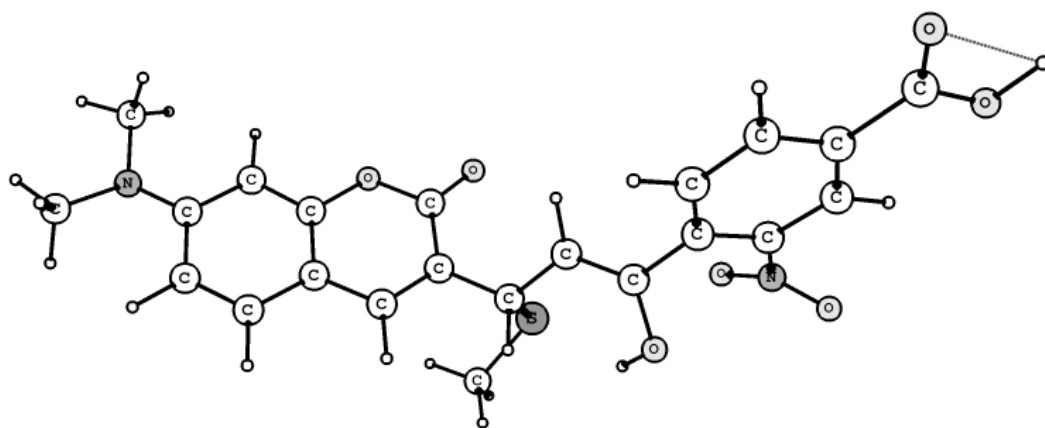
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6	1.527479000	-3.597669000	-2.083649000
6	1.682189000	-2.338033000	-1.547183000
6	0.581149000	-1.482876000	-1.352291000
6	-0.674812000	-1.973546000	-1.724667000
6	-0.871342000	-3.234414000	-2.263087000
6	0.659157000	-0.167232000	-0.798472000
6	-0.446565000	0.604392000	-0.624534000
6	-1.743235000	0.071767000	-1.023050000
8	-1.791269000	-1.191720000	-1.551752000
7	0.090861000	-5.317100000	-3.037198000
8	-2.816600000	0.649429000	-0.921438000
6	-0.424874000	2.011714000	-0.084162000
6	0.649001000	2.309235000	0.903053000
6	0.397943000	2.996362000	2.058777000
6	1.579668000	3.266140000	2.956171000
8	-0.742022000	3.454956000	2.483144000
6	1.511153000	3.093999000	4.343751000
6	2.523324000	3.449014000	5.218263000
6	3.695372000	3.987125000	4.688553000
6	3.813626000	4.170041000	3.307616000
6	2.764224000	3.823584000	2.462506000
16	-0.321166000	3.120899000	-1.586037000
6	-0.635712000	4.714522000	-0.782670000
6	1.189877000	-6.270561000	-2.935997000
6	-1.251332000	-5.873492000	-3.142273000
6	4.787496000	4.347569000	5.628849000
8	5.861161000	4.863511000	5.021346000
8	4.725125000	4.192930000	6.835496000
1	2.402224000	-4.223412000	-2.209435000
1	2.671128000	-1.990443000	-1.259107000
1	-1.881141000	-3.535739000	-2.512957000
1	1.640093000	0.206071000	-0.511811000
1	-1.400792000	2.224559000	0.362729000
1	1.670956000	2.027144000	0.666623000
1	2.413788000	3.286706000	6.286106000
1	4.720075000	4.597714000	2.892350000
1	2.848606000	4.009469000	1.395910000
1	-0.569819000	5.490006000	-1.550247000
1	-1.634817000	4.736928000	-0.339015000
1	0.117761000	4.910740000	-0.014414000
1	2.080017000	-5.895606000	-3.446890000
1	1.447353000	-6.493699000	-1.891406000
1	0.892052000	-7.196333000	-3.428162000

1	-1.884166000	-5.247206000	-3.776374000
1	-1.185361000	-6.857538000	-3.605799000
1	-1.731016000	-5.978112000	-2.158727000
1	6.535739000	5.073642000	5.696022000
7	0.335849000	2.450816000	4.941789000
8	-0.105621000	1.447753000	4.409540000
8	-0.116104000	2.932740000	5.970187000

Frequencies

14.7834	21.7768	32.3894	37.286	42.5801	60.8224
63.0486	71.5134	81.2497	93.706	106.1296	112.4947
125.8126	129.4072	138.257	149.9494	156.1911	162.9107
178.3621	187.8383	198.801	205.431	232.8221	242.6119
252.2527	254.5319	284.3264	296.4427	324.0475	334.4214
343.8655	367.5985	386.0642	403.9646	410.2747	437.8451
446.1002	471.2821	476.9644	481.825	491.3478	515.7273
530.3357	562.3431	588.1683	609.103	640.6176	643.6987
653.9989	658.3333	673.4132	683.4264	696.6853	705.0091
729.4247	731.6256	748.1651	758.0073	767.7018	792.7106
796.9231	802.7328	810.0073	815.3457	818.2468	854.6416
868.7085	890.56	918.5821	944.2776	953.8366	955.3397
960.6167	983.5917	988.7932	1000.0514	1010.5565	1022.1622
1050.5968	1093.931	1100.9597	1131.1794	1147.866	1153.2674
1155.9807	1177.5096	1181.1504	1182.7579	1189.2367	1208.7915
1222.1047	1230.1522	1237.4845	1260.9264	1278.4419	1289.8438
1296.2457	1311.0916	1340.4502	1356.4797	1372.7495	1389.748
1397.9355	1406.9938	1426.9518	1447.6866	1461.494	1464.8474
1471.1888	1481.6366	1490.5025	1491.4252	1500.9721	1506.4791
1507.5657	1527.1956	1541.8646	1546.8686	1574.5082	1614.8046
1625.9555	1631.4445	1654.0759	1657.0434	1702.6476	1706.7436
1735.5079	1764.2434	3061.1696	3067.6078	3083.1812	3139.0416
3148.227	3153.6876	3173.387	3182.4755	3194.9925	3207.0702
3216.2403	3217.9465	3226.7054	3233.1431	3255.8104	3255.9067

E(RM062X)=	-1883.53748
Zero-point correction=	0.385332 (Hartree/Particle)
Thermal correction to Energy=	0.414834
Thermal correction to Enthalpy=	0.415778
Thermal correction to Gibbs Free Energy=	0.322179
Sum of electronic and zero-point Energies=	-1883.152148
Sum of electronic and thermal Energies=	-1883.122646
Sum of electronic and thermal Enthalpies=	-1883.121702
Sum of electronic and thermal Free Energies=	-1883.215301

2-NO<sub>2</sub>-b

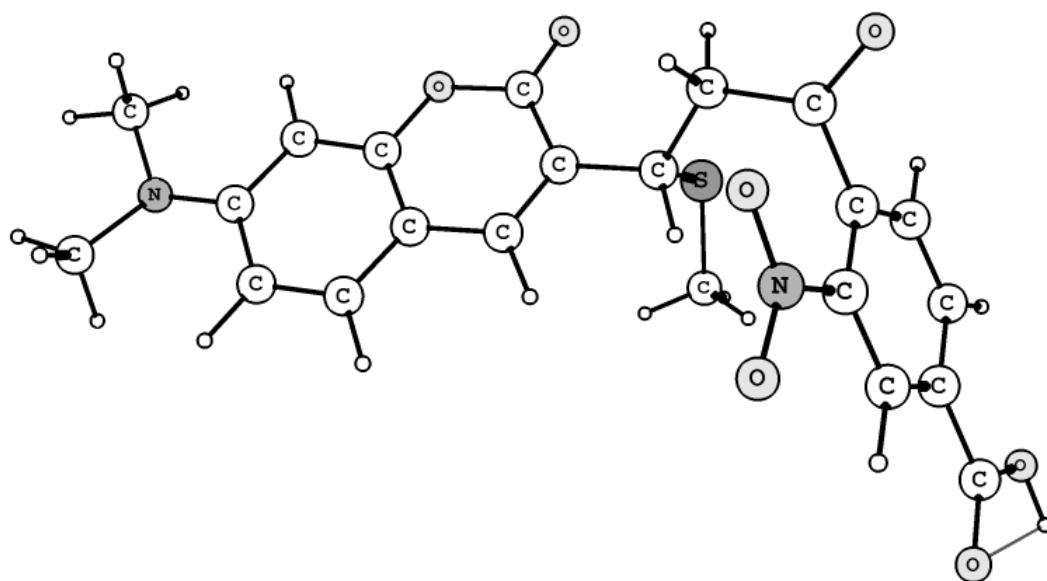
8	1.645073000	-0.057729000	2.101358000
6	2.577918000	-0.076804000	1.313097000
6	2.878981000	-1.144951000	0.370471000
6	2.008738000	-2.366682000	0.352070000
16	2.254439000	-3.400591000	1.876538000
6	3.952739000	-3.956663000	1.566201000
6	0.541181000	-2.092385000	0.179699000
6	-0.330313000	-3.060264000	-0.134381000
8	0.005809000	-4.377253000	-0.316994000
6	-1.770821000	-2.805864000	-0.362143000
6	-2.774747000	-3.642133000	0.143389000
6	-4.120133000	-3.474744000	-0.139793000
6	-4.497126000	-2.399300000	-0.943108000
6	-5.926299000	-2.148822000	-1.275744000
8	-6.759135000	-3.039011000	-0.729596000
8	-6.304423000	-1.228056000	-1.975312000
6	-3.527892000	-1.530255000	-1.447015000
6	-2.182001000	-1.743195000	-1.171434000
6	3.975816000	-1.034854000	-0.426366000
6	4.830351000	0.108180000	-0.375728000
6	5.973451000	0.294592000	-1.176273000
6	6.747457000	1.428657000	-1.067966000
6	6.420159000	2.453209000	-0.130993000
7	7.219317000	3.560372000	0.011979000
6	6.686699000	4.704939000	0.740128000
6	8.191085000	3.861842000	-1.034554000
6	5.263258000	2.287236000	0.658559000
6	4.512961000	1.131520000	0.524781000
8	3.404168000	1.016436000	1.327859000
1	2.350384000	-3.001343000	-0.476490000
1	4.217935000	-4.649414000	2.368508000
1	4.647865000	-3.113000000	1.582902000
1	4.020986000	-4.477763000	0.607525000
1	0.165925000	-1.086419000	0.332383000
1	0.802212000	-4.593632000	0.207870000
1	-4.853627000	-4.152794000	0.282715000
1	-7.675503000	-2.818824000	-0.987244000
1	-3.828156000	-0.696006000	-2.072851000
1	-1.429243000	-1.094335000	-1.607783000
1	4.217717000	-1.835375000	-1.124159000
1	6.239995000	-0.476777000	-1.894409000
1	7.614753000	1.532048000	-1.707964000

1	5.770758000	5.096376000	0.275046000
1	7.439675000	5.492644000	0.750984000
1	6.467737000	4.440128000	1.777539000
1	8.926599000	3.059492000	-1.126405000
1	8.727067000	4.769296000	-0.756905000
1	7.713604000	4.018585000	-2.011562000
1	4.936004000	3.030801000	1.374640000
7	-2.438634000	-4.715309000	1.085905000
8	-3.053487000	-5.766247000	0.994453000
8	-1.590224000	-4.491506000	1.932258000

#### Frequencies

9.5816	22.333	24.5369	41.758	49.7752	52.1085
58.5863	66.1253	79.0691	82.0321	92.5773	116.9202
122.1397	127.8063	139.7044	152.7181	157.2856	160.2999
168.5548	190.2297	204.4296	215.356	226.9123	241.9384
255.9451	257.2629	273.5293	287.9004	318.4825	331.5164
341.5671	365.837	381.4601	386.5058	405.4591	424.8425
433.1513	458.9234	465.6234	474.2648	479.255	509.6431
515.2575	534.5049	544.0841	555.332	599.1164	614.392
632.3838	652.9916	656.5835	659.4658	691.24	697.9748
708.1908	728.4898	739.964	746.7392	755.5575	785.888
795.8223	801.6597	808.292	817.3047	818.8989	845.3782
853.0486	854.0115	891.8277	901.6098	945.4622	951.6249
962.0277	966.8642	990.0096	999.837	1004.7003	1008.61
1024.4309	1032.9927	1088.2339	1107.5089	1124.3692	1138.1236
1139.0725	1147.8553	1156.6696	1181.5751	1184.1927	1188.6713
1220.0326	1229.7159	1233.8503	1239.3019	1249.2982	1278.3866
1292.1169	1307.0374	1308.0852	1325.2298	1356.3509	1371.6768
1385.9571	1389.836	1390.7885	1406.4438	1417.2479	1447.9389
1456.6375	1457.8666	1469.7102	1482.9671	1488.5133	1493.4306
1495.665	1501.9757	1509.2648	1520.9714	1534.5017	1563.3529
1572.4485	1612.9592	1630.2609	1650.6283	1658.7639	1704.5147
1711.2839	1743.2784	1746.0382	1774.8551	3056.279	3066.0098
3085.0559	3091.7869	3150.5535	3152.7539	3178.6133	3186.7719
3193.3756	3201.3628	3207.2258	3218.9134	3243.7512	3248.38
3259.4352	3259.8859	3261.3392	3274.3472	3663.7542	3715.5367

E(RM062X)=	-1884.00019
Zero-point correction=	0.397648 (Hartree/Particle)
Thermal correction to Energy=	0.42762
Thermal correction to Enthalpy=	0.428564
Thermal correction to Gibbs Free Energy=	0.333463
Sum of electronic and zero-point Energies=	-1883.602542
Sum of electronic and thermal Energies=	-1883.57257
Sum of electronic and thermal Enthalpies=	-1883.571626
Sum of electronic and thermal Free Energies=	-1883.666727

2-NO<sub>2</sub>

8	0.967943000	0.559072000	1.364044000
6	2.124664000	0.426769000	0.993664000
6	2.736673000	-0.820231000	0.559982000
6	1.906523000	-2.072113000	0.577227000
16	1.515039000	-2.614519000	2.295901000
6	2.920346000	-3.734941000	2.538903000
6	0.615021000	-1.982784000	-0.239285000
6	0.001473000	-3.317035000	-0.621743000
6	0.749288000	-4.622133000	-0.414336000
6	1.837262000	-5.077719000	-1.165853000
6	2.479782000	-6.278762000	-0.906381000
6	2.018229000	-7.066446000	0.143008000
6	0.922135000	-6.651427000	0.902689000
6	0.295272000	-5.441392000	0.620175000
8	-1.143698000	-3.378466000	-1.029470000
6	4.043382000	-0.822031000	0.185790000
6	4.831164000	0.371015000	0.205637000
6	6.186470000	0.448266000	-0.167625000
6	6.877395000	1.639342000	-0.118818000
6	6.242349000	2.838302000	0.318956000
7	6.945316000	4.016219000	0.410493000
6	6.192427000	5.255797000	0.555668000
6	8.215944000	4.117788000	-0.301084000
6	4.878711000	2.776611000	0.672334000
6	4.219382000	1.560285000	0.617911000
8	2.895940000	1.557622000	0.990271000
1	2.542007000	-2.861561000	0.162247000
1	2.849279000	-4.141712000	3.550544000
1	3.867134000	-3.196455000	2.438611000
1	2.880696000	-4.557353000	1.816555000
1	0.801327000	-1.443378000	-1.176012000
1	-0.161876000	-1.427360000	0.294469000
1	3.315860000	-6.599437000	-1.517740000
1	0.552891000	-7.269009000	1.714439000
1	-0.552549000	-5.118813000	1.216169000
1	4.511690000	-1.750374000	-0.139242000
1	6.689685000	-0.455570000	-0.501861000



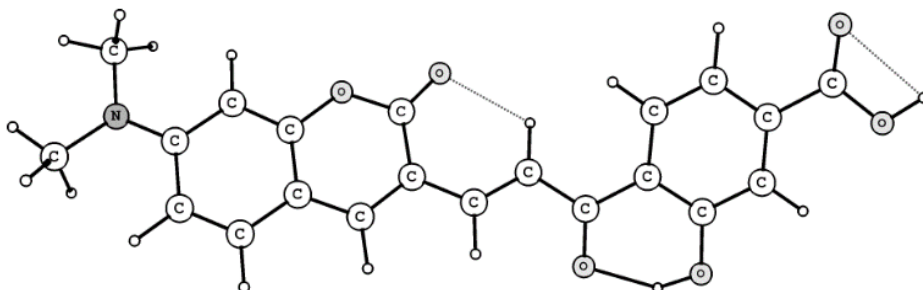
1	7.918075000	1.651285000	-0.417382000
1	5.604734000	5.246865000	1.476916000
1	5.515316000	5.428783000	-0.293129000
1	6.895963000	6.085654000	0.620321000
1	8.099524000	3.946221000	-1.380070000
1	8.940960000	3.402859000	0.094562000
1	8.620637000	5.117867000	-0.146820000
1	4.321286000	3.648675000	0.990543000
6	2.718351000	-8.356078000	0.406611000
8	3.687812000	-8.735489000	-0.221802000
8	2.172092000	-9.055453000	1.403041000
1	2.667406000	-9.890054000	1.517730000
7	2.317693000	-4.287764000	-2.302872000
8	3.325358000	-4.649553000	-2.883980000
8	1.674538000	-3.293810000	-2.608326000

#### Frequencies

14.6403	19.4779	31.0278	34.6845	40.5568	56.3735
61.3405	79.8821	84.945	92.0888	105.0642	111.6225
121.0595	127.5482	142.2758	154.6257	160.2661	173.6929
177.564	204.9022	209.7392	217.3115	239.5889	251.5448
253.2408	275.8852	278.0359	297.6758	301.4458	341.6621
352.1089	371.079	400.5661	408.7826	417.3757	440.8212
449.8627	464.7188	470.3587	478.8377	485.7203	513.603
531.2368	536.3144	566.1625	584.7455	614.5483	619.9098
628.0168	639.0745	660.7735	697.7646	699.2639	707.9511
717.8368	729.0901	742.3335	749.9013	759.6485	786.5267
799.5724	802.9384	815.8008	826.8615	828.3439	854.1862
883.6654	891.8891	941.3507	950.8626	958.6937	960.8307
976.6753	996.5048	1001.7539	1010.1643	1016.5625	1025.5542
1056.2477	1095.4964	1103.0367	1120.9462	1131.4164	1149.1394
1150.1128	1161.6717	1180.6936	1182.2491	1190.49	1203.3794
1217.4211	1228.1667	1236.0684	1276.8905	1284.0688	1291.3349
1298.3387	1308.7938	1312.947	1336.9711	1366.1449	1385.8432
1391.6484	1393.3409	1393.8311	1418.8881	1450.4557	1455.8506
1457.596	1463.7171	1464.0102	1470.509	1481.7538	1494.3155
1499.9294	1505.1798	1510.2365	1529.9092	1540.8531	1554.4662
1577.4165	1613.4585	1630.5189	1658.5079	1661.5053	1701.6609
1715.81	1743.6458	1777.5394	1787.0562	3057.0367	3067.4155
3078.6339	3098.8572	3121.2763	3148.6802	3156.3231	3161.7343
3165.9567	3186.0821	3196.7834	3206.1467	3214.6072	3222.0184
3251.0226	3260.7189	3273.4112	3277.8921	3281.6848	3688.6915

E(RM062X)=	-1884.01485
Zero-point correction=	0.399029 (Hartree/Particle)
Thermal correction to Energy=	0.428495
Thermal correction to Enthalpy=	0.429439
Thermal correction to Gibbs Free Energy=	0.336052
Sum of electronic and zero-point Energies=	-1883.615821
Sum of electronic and thermal Energies=	-1883.586355
Sum of electronic and thermal Enthalpies=	-1883.585411
Sum of electronic and thermal Free Energies=	-1883.678798

1-OH



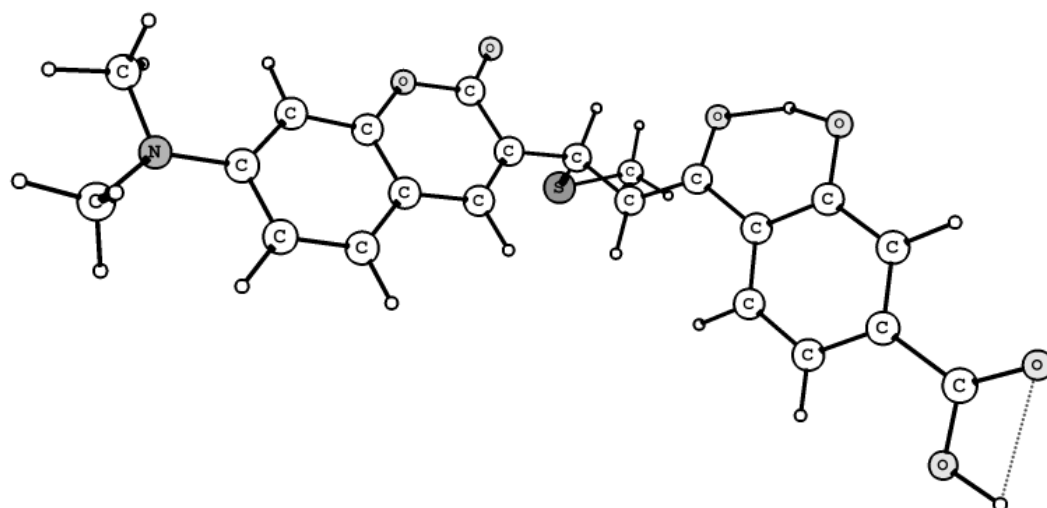
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6	11.236373000	2.847044000	0.396799000
6	10.060909000	2.476836000	0.997804000
6	8.964750000	3.367566000	1.081275000
6	9.134560000	4.648309000	0.522025000
6	10.302058000	5.059182000	-0.086197000
6	7.725785000	3.060107000	1.678802000
6	6.685878000	3.963087000	1.723054000
6	6.882343000	5.281145000	1.137564000
8	8.104040000	5.551990000	0.569992000
7	12.552207000	4.519369000	-0.757932000
8	6.066580000	6.187794000	1.097563000
6	5.437641000	3.579288000	2.344524000
6	4.281488000	4.276148000	2.435636000
6	3.139254000	3.665344000	3.122855000
6	1.793264000	4.292118000	3.030746000
6	13.666998000	3.583938000	-0.836659000
6	12.700313000	5.859278000	-1.308941000
6	0.712190000	3.748515000	3.763858000
6	-0.559847000	4.323321000	3.680962000
6	-0.766169000	5.429049000	2.867875000
6	0.286415000	5.979341000	2.125774000
6	1.544450000	5.410093000	2.213082000
8	3.279135000	2.618972000	3.786012000
6	-2.114281000	6.057266000	2.759262000
8	-2.345714000	7.054731000	2.101039000
8	-3.058514000	5.416917000	3.455972000
1	12.053937000	2.138525000	0.350853000
1	9.955378000	1.481654000	1.421818000
1	10.355819000	6.063003000	-0.489223000
1	7.586271000	2.073033000	2.116807000
1	5.454243000	2.580142000	2.779802000
1	4.185625000	5.262521000	2.007398000
1	13.389838000	2.684164000	-1.396620000
1	14.493024000	4.069019000	-1.353974000
1	14.009924000	3.287490000	0.160857000
1	11.968383000	6.044667000	-2.103210000
1	12.574866000	6.622320000	-0.532365000
1	13.698977000	5.958592000	-1.731112000
1	-1.365983000	3.882312000	4.257573000
1	0.111911000	6.838970000	1.487966000
1	2.345222000	5.841018000	1.623927000
1	-3.908789000	5.884618000	3.343129000
8	0.837842000	2.668689000	4.569115000
1	1.773200000	2.354923000	4.493132000

Frequencies

20.7605	33.2931	39.4836	47.8358	56.6905	81.9718
88.2654	99.9752	110.3845	123.9418	144.9413	151.191
162.8803	177.4736	200.1188	212.9754	224.4415	231.3333
280.4969	284.6961	308.3473	316.5718	324.8639	342.0137
364.424	392.9796	426.465	439.3171	446.4557	467.4347
472.6422	482.2255	483.7963	499.8233	537.0734	545.1028
555.8212	581.9014	585.875	604.7723	633.2262	665.1796
667.4599	687.423	702.4951	727.1989	735.7988	752.2485
753.4523	762.7329	775.5491	797.0743	810.6227	824.9542
857.0381	859.1794	863.8246	899.3769	902.5397	915.8589
953.4065	963.7983	990.019	997.0432	1010.0904	1012.8206
1033.0783	1057.0918	1102.6509	1106.0766	1124.786	1153.689
1169.5151	1171.41	1174.7862	1188.3276	1195.7721	1226.5658
1230.9671	1247.8033	1263.9196	1293.1184	1297.2203	1312.2065
1326.5884	1350.4361	1356.7189	1386.3575	1395.0603	1406.9524
1413.8054	1429.8495	1449.1176	1460.0269	1469.3001	1499.3263
1502.3451	1507.328	1511.3467	1530.2965	1538.5507	1554.9805
1569.8824	1599.3536	1609.797	1642.2919	1649.7312	1685.1774
1698.0213	1709.7595	1757.537	1774.9538	3075.0665	3080.8016
3137.4986	3138.9485	3205.7423	3210.0804	3223.5836	3235.4109
3238.0112	3246.9754	3253.3363	3259.9447	3261.0512	3265.7715

E(RM062X)=	-1316.13306
Zero-point correction=	0.348154 (Hartree/Particle)
Thermal correction to Energy=	0.372262
Thermal correction to Enthalpy=	0.373206
Thermal correction to Gibbs Free Energy=	0.293023
Sum of electronic and zero-point Energies=	-1315.784906
Sum of electronic and thermal Energies=	-1315.760798
Sum of electronic and thermal Enthalpies=	-1315.759854
Sum of electronic and thermal Free Energies=	-1315.840037

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6	0.352277000	-4.023412000	-2.563856000
6	1.626392000	-3.498883000	-2.197272000
6	1.740302000	-2.248909000	-1.629169000
6	0.608262000	-1.450239000	-1.379000000
6	-0.634268000	-1.985164000	-1.733708000
6	-0.789111000	-3.235952000	-2.308838000
6	0.643309000	-0.153106000	-0.778159000
6	-0.490544000	0.558969000	-0.543858000
6	-1.774284000	-0.024039000	-0.915366000
8	-1.780224000	-1.265381000	-1.496047000
7	0.240904000	-5.257609000	-3.156608000
8	-2.869748000	0.492165000	-0.746070000
6	-0.523318000	1.938583000	0.063661000
6	0.620621000	2.278887000	0.954392000
6	0.439592000	2.831819000	2.186466000
6	1.627252000	3.209093000	3.027073000
8	-0.744944000	3.054722000	2.741754000
6	1.461967000	3.353174000	4.424916000
6	2.550915000	3.656558000	5.241323000
6	3.813494000	3.844573000	4.680406000
6	3.992756000	3.742655000	3.296178000
6	2.902964000	3.432918000	2.492133000
16	-0.645661000	3.135784000	-1.364502000
6	-1.082643000	4.625754000	-0.429854000
6	1.363788000	-6.183960000	-3.051996000
6	-1.084269000	-5.854039000	-3.260779000
6	4.940714000	4.166315000	5.589716000
8	6.109402000	4.340811000	4.955371000
8	4.842140000	4.267308000	6.801727000
1	2.524512000	-4.079582000	-2.366637000
1	2.720585000	-1.865149000	-1.357814000
1	-1.791134000	-3.576617000	-2.538329000
1	1.614167000	0.253031000	-0.502828000
1	-1.462938000	2.050875000	0.611967000
1	1.624550000	2.141748000	0.567200000
1	2.399693000	3.747342000	6.312932000
1	4.967647000	3.907197000	2.850921000
1	3.049271000	3.372633000	1.418020000
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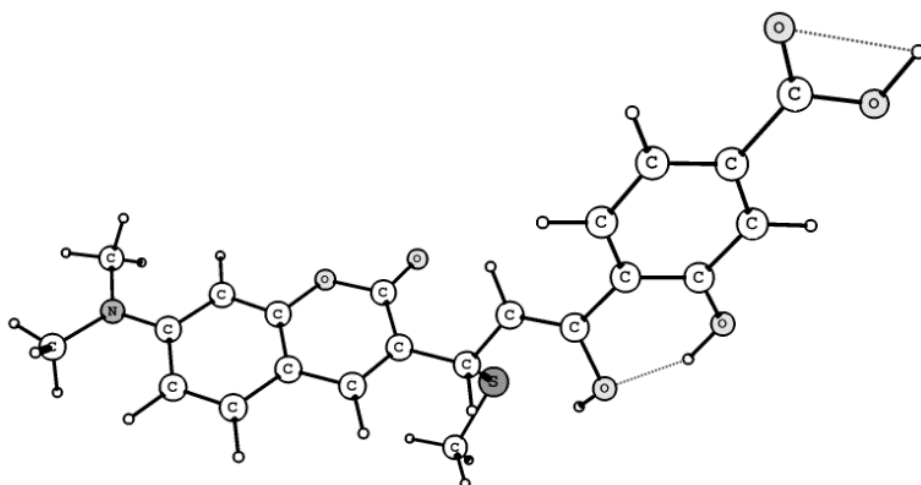
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1	-0.320165000	4.838261000	0.325334000
1	2.249077000	-5.784950000	-3.552542000
1	1.616897000	-6.406885000	-2.006292000
1	1.093830000	-7.113343000	-3.553246000
1	-1.741515000	-5.232407000	-3.874151000
1	-0.993034000	-6.824416000	-3.748500000
1	-1.550262000	-5.996555000	-2.275309000
1	6.797420000	4.549676000	5.616001000
8	0.240846000	3.186769000	4.997585000
1	-0.393559000	3.118359000	4.179050000

Frequencies

19.5939	21.6607	32.3034	38.3145	56.1809	58.2522
69.546	84.4478	92.3672	101.8494	108.5927	122.7633
130.1675	148.9631	172.9316	177.2109	193.2638	201.0564
208.8316	222.3517	240.5692	246.3896	255.3085	266.5323
292.9356	323.0146	325.8156	336.4337	364.371	385.7013
398.8166	411.423	438.175	452.7239	464.1538	475.269
479.6916	496.9993	509.7871	529.1034	558.0151	565.0945
585.8351	590.746	638.2086	643.1136	652.5626	654.1854
667.1926	680.2544	706.9668	728.4473	739.5828	747.1348
752.3874	761.0158	784.2757	796.3631	809.7992	814.1636
816.6263	839.2952	857.7659	864.2197	913.5133	918.4877
952.6025	953.573	957.4911	983.9438	992.2932	997.1936
1000.3469	1004.7547	1013.1041	1039.251	1090.2575	1099.4261
1121.4631	1150.8964	1152.1449	1156.163	1176.6373	1184.5425
1190.2333	1198.5202	1206.9527	1216.0941	1238.1325	1245.1237
1265.6551	1275.6834	1289.5865	1297.5463	1308.8708	1331.6457
1338.1685	1379.9674	1382.261	1385.6703	1391.943	1410.3957
1437.6921	1445.4246	1470.1886	1474.0995	1490.0337	1491.6684
1497.1041	1501.0578	1504.5389	1508.2054	1526.7847	1541.888
1572.4986	1574.3942	1614.1695	1649.9734	1657.5332	1665.7982
1696.8096	1705.0189	1740.8567	1753.8874	2473.4091	3061.3886
3067.4877	3087.8367	3138.9044	3148.1661	3153.7182	3179.8361
3182.4417	3192.8753	3207.072	3218.6081	3221.8907	3230.0099
3238.3561	3246.7653	3259.1842	3263.6874	3265.1683	3711.7416

E(RM062X)=	-1754.31905
Zero-point correction=	0.386117 (Hartree/Particle)
Thermal correction to Energy=	0.413626
Thermal correction to Enthalpy=	0.41457
Thermal correction to Gibbs Free Energy=	0.326023
Sum of electronic and zero-point Energies=	-1753.932933
Sum of electronic and thermal Energies=	-1753.905424
Sum of electronic and thermal Enthalpies=	-1753.90448
Sum of electronic and thermal Free Energies=	-1753.993027

2-OH-b



8	1.705217000	-0.008163000	2.249872000
6	2.614273000	-0.053693000	1.434129000
6	2.889664000	-1.152892000	0.523320000
6	2.016301000	-2.371773000	0.566306000
16	2.264156000	-3.343999000	2.130204000
6	3.948271000	-3.942132000	1.820953000
6	0.553390000	-2.086704000	0.368448000
6	-0.329683000	-3.049917000	0.063329000
8	0.025996000	-4.383733000	0.006336000
6	-1.751043000	-2.810248000	-0.266014000
6	-2.756420000	-3.748672000	0.041534000
6	-4.091562000	-3.473896000	-0.252671000
6	-4.439348000	-2.267531000	-0.854980000
6	-5.855826000	-1.950265000	-1.174656000
8	-6.705135000	-2.947659000	-0.898632000
8	-6.227239000	-0.888585000	-1.644178000
6	-3.455007000	-1.329287000	-1.180257000
6	-2.129176000	-1.613389000	-0.893821000
6	3.953645000	-1.062601000	-0.320862000
6	4.791026000	0.090390000	-0.353955000
6	5.886277000	0.259970000	-1.224042000
6	6.637805000	1.412113000	-1.214406000
6	6.331586000	2.477778000	-0.312914000
7	7.071585000	3.618248000	-0.307597000
6	6.742770000	4.692177000	0.615472000
6	8.151808000	3.795830000	-1.266033000
6	5.237608000	2.317103000	0.568450000
6	4.503476000	1.145323000	0.522837000
8	3.440108000	1.040794000	1.387940000
1	2.357143000	-3.043763000	-0.232383000
1	4.214751000	-4.603534000	2.648857000
1	4.655631000	-3.109159000	1.791922000
1	3.994036000	-4.504971000	0.884852000
1	0.202714000	-1.065124000	0.460569000
1	0.791755000	-4.546254000	0.595333000
1	-4.842039000	-4.215065000	0.002334000
1	-7.610559000	-2.664571000	-1.131175000
1	-3.727463000	-0.398364000	-1.666020000
1	-1.357470000	-0.901129000	-1.170428000
1	4.173910000	-1.885934000	-0.999201000

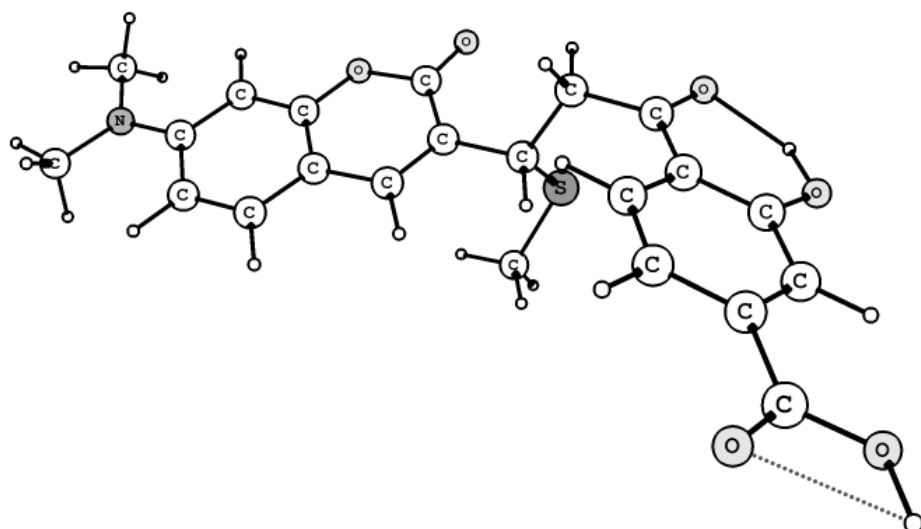
1	6.131717000	-0.541534000	-1.916336000
1	7.469633000	1.504444000	-1.901815000
1	5.735386000	5.086140000	0.431728000
1	7.459224000	5.501947000	0.484145000
1	6.795715000	4.349806000	1.655481000
1	8.937496000	3.044322000	-1.127480000
1	8.592589000	4.780753000	-1.118164000
1	7.785266000	3.733964000	-2.297436000
1	4.946149000	3.087352000	1.272221000
8	-2.506123000	-4.940776000	0.660695000
1	-1.541846000	-5.104072000	0.659491000

Frequencies

16.6736	26.4725	34.3083	47.8541	54.6441	59.4265
62.6071	81.209	83.591	91.2011	116.4486	124.3565
132.9134	144.3411	157.2469	168.5822	174.2342	196.8938
209.4734	211.3345	221.2565	235.3932	255.6643	288.7188
290.3451	301.3832	319.7078	324.8558	351.5386	373.8079
403.4781	423.9669	426.4612	452.2416	462.8482	471.8522
475.3219	481.2082	501.4571	516.5941	536.6628	546.4503
552.6792	567.2386	581.5338	596.0671	618.4276	630.7664
653.9199	658.1093	664.7974	699.2505	710.5161	729.3078
742.6076	749.0133	749.3281	761.234	782.6887	803.244
806.8367	819.2265	835.2347	842.6496	845.6837	865.3326
899.8876	911.9988	953.2774	960.0948	964.6077	990.3569
994.0292	999.6004	1009.1439	1010.5353	1035.1246	1104.5843
1109.4348	1122.5623	1139.3179	1151.1835	1152.4539	1161.6875
1176.7852	1188.0484	1191.5604	1219.661	1234.8045	1237.4712
1242.4676	1254.2271	1282.5354	1284.95	1296.8242	1321.8164
1327.2038	1330.5318	1370.9552	1376.3502	1384.2929	1389.3391
1399.2975	1406.3479	1425.0603	1454.6703	1466.8419	1469.7639
1486.6078	1488.6965	1493.6147	1498.0507	1501.2731	1505.3588
1527.5261	1541.1147	1561.6841	1585.6512	1610.7532	1650.8747
1652.6635	1702.3653	1704.9289	1739.5035	1741.6836	1761.8108
3066.4832	3074.859	3085.3211	3091.8922	3125.2148	3131.8461
3178.9963	3187.5627	3205.554	3207.4066	3216.4764	3216.9364
3227.858	3242.2442	3245.0298	3250.1944	3251.4181	3259.7651

E(RM062X)=	-1754.77715
Zero-point correction=	0.399732 (Hartree/Particle)
Thermal correction to Energy=	0.427833
Thermal correction to Enthalpy=	0.428777
Thermal correction to Gibbs Free Energy=	0.339264
Sum of electronic and zero-point Energies=	-1754.377418
Sum of electronic and thermal Energies=	-1754.349317
Sum of electronic and thermal Enthalpies=	-1754.348373
Sum of electronic and thermal Free Energies=	-1754.437886

2-OH



8	1.284383000	0.676442000	1.095152000
6	2.454963000	0.397926000	0.882062000
6	3.032676000	-0.936962000	0.864276000
6	2.177986000	-2.127030000	1.198570000
16	1.701939000	-2.163037000	2.977646000
6	3.347752000	-2.414206000	3.692525000
6	0.907014000	-2.249116000	0.336117000
6	0.167654000	-3.538707000	0.609943000
6	0.784260000	-4.840292000	0.254318000
6	1.912899000	-4.906309000	-0.582743000
6	2.504509000	-6.115445000	-0.900524000
6	1.972210000	-7.295766000	-0.364875000
6	0.855329000	-7.266971000	0.459500000
6	0.248348000	-6.044285000	0.762877000
8	-0.936929000	-3.500665000	1.158391000
6	4.362168000	-1.075091000	0.601853000
6	5.203822000	0.046730000	0.344835000
6	6.584233000	-0.029139000	0.071150000
6	7.336976000	1.102985000	-0.141794000
6	6.738845000	2.399469000	-0.085462000
7	7.484595000	3.520355000	-0.276240000
6	6.859381000	4.829115000	-0.180433000
6	8.909489000	3.417552000	-0.553703000
6	5.352445000	2.487273000	0.177512000
6	4.631231000	1.324817000	0.382509000
8	3.288048000	1.461262000	0.637318000
1	2.800235000	-3.014761000	1.041848000
1	3.218370000	-2.517017000	4.772622000
1	3.998156000	-1.557980000	3.494924000
1	3.803644000	-3.327337000	3.300034000
1	1.197912000	-2.195702000	-0.718976000
1	0.217711000	-1.428858000	0.542884000
1	0.429260000	-8.175554000	0.871314000
1	4.806416000	-2.069964000	0.592716000
1	7.055578000	-1.008020000	0.031507000
1	8.395670000	1.001587000	-0.347058000
1	6.399914000	4.978219000	0.803984000
1	6.087181000	4.960933000	-0.948087000



1	7.619495000	5.595862000	-0.323026000
1	9.098518000	2.854763000	-1.475089000
1	9.444597000	2.929400000	0.269321000
1	9.315323000	4.420731000	-0.678010000
1	4.833835000	3.437051000	0.227324000
6	2.629821000	-8.587854000	-0.718577000
8	3.591443000	-8.673996000	-1.459432000
8	2.062236000	-9.651593000	-0.142339000
1	2.539273000	-10.457700000	-0.420835000
1	3.370924000	-6.153712000	-1.551384000
1	2.323646000	-3.994465000	-1.004680000
8	-0.846527000	-6.087538000	1.555930000
1	-1.209214000	-5.175795000	1.628370000

#### Frequencies

15.9907	25.181	32.2191	51.7146	52.8933	66.1466
69.109	89.945	97.1863	105.632	117.456	121.433
128.3825	138.6896	141.179	173.4877	179.0595	193.7937
201.0128	207.3494	222.1817	254.5453	265.6034	277.2596
281.6133	302.0695	313.5445	327.0344	355.8472	396.8665
402.7952	421.3114	440.5367	448.8853	458.6026	472.1407
475.5391	481.1419	497.1568	536.8886	540.73	551.8112
554.418	584.8052	611.6365	620.4162	625.7192	653.1305
661.7253	672.0366	688.3524	701.3737	726.6633	735.9052
744.2524	751.8056	758.4308	778.6426	790.4744	798.8171
818.1673	826.0026	841.0575	868.862	890.7533	931.4087
951.135	957.9427	965.016	977.3704	990.3333	1000.9396
1006.8674	1011.6181	1016.9169	1048.6506	1082.7856	1098.4029
1110.4308	1125.1709	1158.7715	1163.0186	1167.5514	1169.1483
1177.7689	1191.376	1194.1651	1233.5129	1234.7029	1244.7368
1266.3242	1282.0988	1286.3255	1299.8126	1319.9719	1322.2445
1333.247	1364.6486	1378.5663	1385.439	1395.2869	1403.0478
1405.5063	1423.3916	1452.8621	1466.1877	1467.9732	1469.0383
1489.1748	1496.1447	1497.5515	1500.0501	1506.4145	1510.4858
1526.6651	1537.8431	1556.7529	1581.1734	1611.1007	1645.2812
1656.06	1698.9193	1709.6143	1720.8053	1746.2734	1775.149
3070.6025	3077.0082	3088.4206	3115.7	3123.4061	3129.2064
3132.2394	3178.4465	3186.8652	3192.0583	3203.9187	3207.9787
3217.8138	3219.2679	3246.9691	3256.7146	3257.4238	3260.4302

E(RM062X)=	-1754.79679
Zero-point correction=	0.40084 (Hartree/Particle)
Thermal correction to Energy=	0.428653
Thermal correction to Enthalpy=	0.429597
Thermal correction to Gibbs Free Energy=	0.340832
Sum of electronic and zero-point Energies=	-1754.39595
Sum of electronic and thermal Energies=	-1754.368137
Sum of electronic and thermal Enthalpies=	-1754.367193
Sum of electronic and thermal Free Energies=	-1754.455958

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