Supporting Information

New Insights into the Torquoselectivity of the Staudinger Reaction

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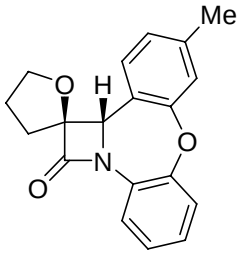
Content

1. Experimental Details and Spectroscopic Data

General. 2-Tetrahydrofuroyl chloride (precursor of ketene **1**)[1] and cyclic imines **2a**−**d**,[2] **2e**,[3] and **2g**[4] were prepared according to the published procedures. Toluene was refluxed with sodium and freshly distilled prior to use. Reactions of **1** with imines **2a**−**e** and **2g** were performed according to the published procedure.[1]

General procedure for the kinetic competition experiments. To a solution of imine **2c** (0.5 mmol), imine **2x** (**x** = **a**, **b**, **d**, or **e**, 0.5 mmol), and Et_3N (73 mg, 0.72 mmol) in refluxing toluene (10 mL) was added dropwise a solution of 2-tetrahydrofuroyl chloride (precursor of ketene **1**, 67 mg, 0.5 mmol) in toluene (5 mL). The reaction mixture was refluxed for 13 h, cooled to room temperature, and washed successively with saturated sodium bicarbonate and brine. The organic layer was dried (Na_2SO_4), concentrated *in vacuo*, and submitted to ^{1}H NMR analysis to determine the product ratio. In each case, the total conversion of two imines was less than 20% as shown in ^{1}H NMR spectrum of the reaction mixture.

***Rel*-(1*S*,12b*S*)-Spiro[10-methylazeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclopentane)]-2(12b*H*)-one (3a)**



Pale yellow oil. R_f = 0.36 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.02 (m, 4H), 2.34 (s, 3H), 4.09 (m, 2H), 5.11 (s, 1H), 6.98−7.61 (m, 7H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 20.8, 25.4, 28.5, 66.8, 70.5, 95.9, 122.7, 124.9, 125.2, 125.4, 127.6, 127.9, 128.5, 139.8, 151.6, 153.8, 168.4. IR ν (cm^{-1}): 1766. MS (ESI) m/z: 308 $[M+H]^+$. Calcd for $C_{19}H_{18}NO_3^+$ $[M+H]^+$: 308.1287. Found: 308.1285.

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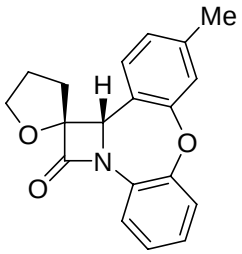
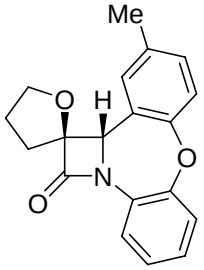
[1] Alonso, E.; del Pozo, C.; González, J. *J. Chem. Soc., Perkin Trans. 1* **2002**, 571.
[2] Wardrop, A. W. H.; Sainsbury, G. L.; Harrison, J. M.; Inch, T. D. *J. Chem. Soc., Perkin Trans. 1* **1976**, 1279.
[3] Nagarajan, K.; Venkateswarlu, A.; Kulkarni, C. L.; Shah, R. K. *Indian J. Chem.* **1974**, *12*, 227.
[4] Gauss, W.; Heitzer, H. *Liebigs Ann. Chem.* **1970**, *733*, 59.

***Rel*-(1*R*,12b*S*)-Spiro[10-methylazeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclope ntane)]-2(12b*H*)-one (4a)**



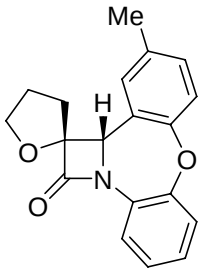
Pale yellow oil. R_f = 0.41 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.06 (m, 1H), 2.20 (m, 1H), 2.31 (s, 3H), 2.37 (m, 1H), 2.57 (m, 1H), 4.18 (dd, J = 6.0, 6.6 Hz, 2H), 5.48 (s, 1H), 6.95−8.01 (m, 7H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 21.0, 25.5, 33.0, 62.6, 70.5, 94.0, 120.6, 121.3, 121.6, 124.8, 125.4, 125.8, 128.5, 129.0, 129.9, 144.9, 157.6, 160.5, 166.9. IR ν (cm^{-1}): 1754. MS (ESI) m/z: 308 $[M+H]^+$. Calcd for $C_{19}H_{18}NO_3^+$ $[M+H]^+$: 308.1287. Found: 308.1279.

***Rel*-(1*S*,12b*S*)-Spiro[11-methylazeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclope ntane)]-2(12b*H*)-one (3b)**



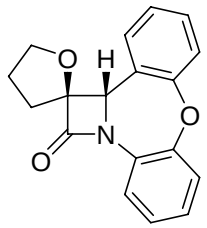
Pale yellow oil. R_f = 0.36 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.02 (m, 4H), 2.30 (s, 3H), 4.10 (m, 2H), 5.08 (s, 1H), 6.87−7.59 (m, 7H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 20.4, 25.2, 28.5, 66.8, 70.4, 95.8, 121.1, 121.9, 124.3, 124.8, 125.4, 127.8, 128.0, 128.4, 129.9, 133.9, 151.8, 168.3. IR ν (cm^{-1}): 1763. MS (ESI) m/z: 308 $[M+H]^+$. Calcd for $C_{19}H_{18}NO_3^+$ $[M+H]^+$: 308.1287. Found: 308.1283.

***Rel*-(1*R*,12b*S*)-Spiro[11-methylazeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclopentane)]-2(12b*H*)-one (4b)**



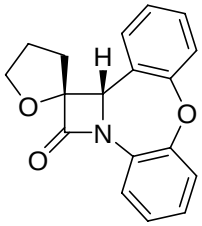
Pale yellow oil. R_f = 0.44 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.10 (m, 1H), 2.24 (m, 1H), 2.33 (s, 3H), 2.39 (m, 1H), 2.59 (m, 1H), 4.22 (t, J = 6.6 Hz, 2H), 5.53 (s, 1H), 6.98−8.03 (m, 7H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 21.2, 25.5, 33.2, 62.8, 70.6, 94.1, 120.6, 120.8, 121.3, 124.9, 125.0, 126.6, 128.7, 129.7, 134.4, 145.1, 155.7, 160.7, 166.9. IR ν (cm^{-1}): 1754. MS (ESI) m/z: 308 $[M+H]^+$. Calcd for $C_{19}H_{18}NO_3^+$ $[M+H]^+$: 308.1287. Found: 308.1283.

***Rel*-(1*S*,12b*S*)-Spiro[azeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclopentane)]-2(12b*H*)-one (3c)**



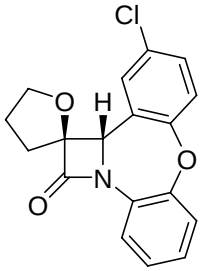
Colorless crystals, m.p. 135-136 °C. R_f = 0.35 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.94 (m, 2H), 2.09 (m, 1H), 2.20 (m, 1H), 4.13 (m, 2H), 5.17 (s, 1H), 7.10−7.64 (m, 8H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 25.5, 28.7, 67.0, 70.7, 96.1, 121.4, 122.6, 124.5, 125.1, 125.2, 125.6, 128.0, 128.1, 128.6, 129.5, 151.7, 154.2, 168.4. IR ν (cm^{-1}): 1764. MS (ESI) m/z: 294 $[M+H]^+$. Calcd for $C_{18}H_{16}NO_3^+$ $[M+H]^+$: 294.1130. Found: 294.1133.

***Rel*-(1*R*,12b*S*)-Spiro[azeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclopentane)]-2(12b*H*)-one (4c)**



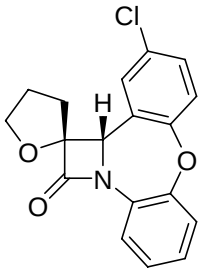
Pale yellow oil. R_f = 0.41 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.06 (m, 1H), 2.20 (m, 1H), 2.36 (m, 1H), 2.56 (m, 1H), 4.18 (m, 2H), 5.52 (s, 1H), 6.98−8.01 (m, 8H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 25.5, 33.1, 62.7, 70.5, 94.1, 120.5, 121.1, 121.3, 124.80, 124.84, 124.97, 124.99, 126.2, 129.37, 129.40, 144.8, 157.8, 166.8. IR ν (cm^{-1}): 1754. MS (ESI) m/z: 294 $[M+H]^+$. Calcd for $C_{18}H_{16}NO_3^+$ $[M+H]^+$: 294.1130. Found: 294.1126.

***Rel*-(1*S*,12b*S*)-Spiro[11-chloroazeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclopentane)]-2(12b*H*)-one (3d)**



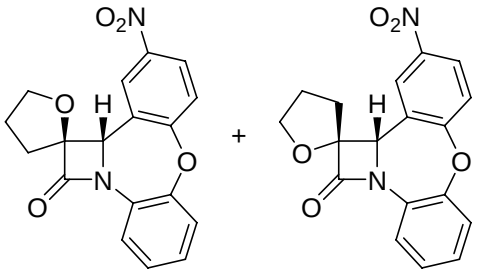
Colorless crystals, m.p. 107-108 °C. R_f = 0.40 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.95 (m, 2H), 2.17 (m, 2H), 4.14 (m, 2H), 5.10 (s, 1H), 7.09−7.64 (m, 7H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 25.5, 28.8, 66.5, 70.8, 96.3, 121.3, 124.0, 125.5, 125.7, 126.7, 127.6, 128.3, 128.4, 129.4, 129.6, 151.4, 152.6, 168.1. IR ν (cm^{-1}): 1767. MS (ESI) m/z: 328 $[M+H]^+$. Calcd for $C_{18}H_{15}ClNO_3^+$ $[M+H]^+$: 328.0740. Found: 328.0753.

***Rel*-(1*R*,12b*S*)-Spiro[11-chloroazeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclopentane)]-2(12b*H*)-one (4d)**



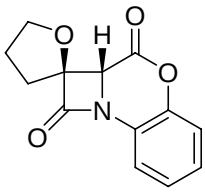
Colorless crystals, m.p. 124-125 °C. R_f = 0.48 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.09 (m, 1H), 2.24 (m, 1H), 2.39 (m, 1H), 2.59 (m, 1H), 4.22 (dd, J = 6.0, 6.6 Hz, 2H), 5.48 (s, 1H), 6.99−8.00 (m, 7H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 25.4, 33.1, 62.0, 70.7, 94.1, 120.6, 121.3, 122.5, 125.0, 125.3, 126.5, 129.2, 130.0, 130.7, 144.4, 156.3, 166.6. IR ν (cm^{-1}): 1754. MS (ESI) m/z: 328 $[M+H]^+$. Calcd for $C_{18}H_{15}ClNO_3^+$ $[M+H]^+$: 328.0740. Found: 328.0750.

***Rel*-(1*S*,12b*S*)-Spiro[11-nitroazeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclopentane)]-2(12b*H*)-one (3e) and**
***Rel*-(1*R*,12b*S*)-Spiro[11-nitroazeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepine-1,2'-(2-oxacyclopentane)]-2(12b*H*)-one (4e)**



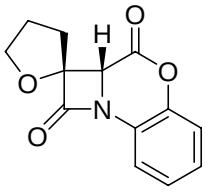
Inseparable mixture, white solid. R_f = 0.30 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): **3e:** δ 1.93 (m, 2H), 2.17 (m, 2H), 4.13 (m, 2H), 5.21 (s, 1H), 7.07−8.05 (m, 7H). **4e:** δ 2.18 (m, 1H), 2.31 (m, 1H), 2.47 (m, 1H), 2.65 (m, 1H), 4.28 (m, 2H), 5.48 (s, 1H), 7.09−8.64 (m, 7H). ^{13}C NMR (75.5 MHz, $CDCl_3$): **3e:** δ 25.5, 28.7, 66.3, 70.9, 96.7, 124.8, 125.3, 125.9, 128.2, 128.6, 129.7, 144.1, 149.8, 158.2, 167.3. **4e:** δ 25.6, 32.9, 62.0, 71.0, 94.4, 121.2, 121.4, 122.4, 123.0, 123.8, 125.1, 125.6, 125.7, 144.0, 162.0, 166.4. IR ν (cm^{-1}): 1759. MS (ESI) m/z: 339 $[M+H]^+$. Calcd for $C_{18}H_{15}N_2O_5^+$ $[M+H]^+$: 339.0981. Found: 339.0990.

***Rel*-(2*S*,2a*R*)-Spiro[azeto[1,2-*d*]benzo[*b*][1,4]oxazine-2,2'-(2-oxacyclopentane)]-1(2a*H*),3-dione (3g)**



Colorless crystals, m.p. 134-135 °C. R_f = 0.43 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.10−2.30 (m, 3H), 2.42 (m, 1H), 4.13 (m, 2H), 4.44 (s, 1H), 7.12−7.49 (m, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 25.5, 29.7, 59.7, 71.4, 98.2, 117.2, 120.6, 121.6, 125.4, 126.5, 144.5, 161.9, 168.9. IR ν (cm^{-1}): 1771. MS (ESI) m/z: 246 $[M+H]^+$. Calcd for $C_{13}H_{11}NO_4$: C, 63.67; H, 4.52; N, 5.71. Found: C, 63.57; H, 4.77; N, 5.61.

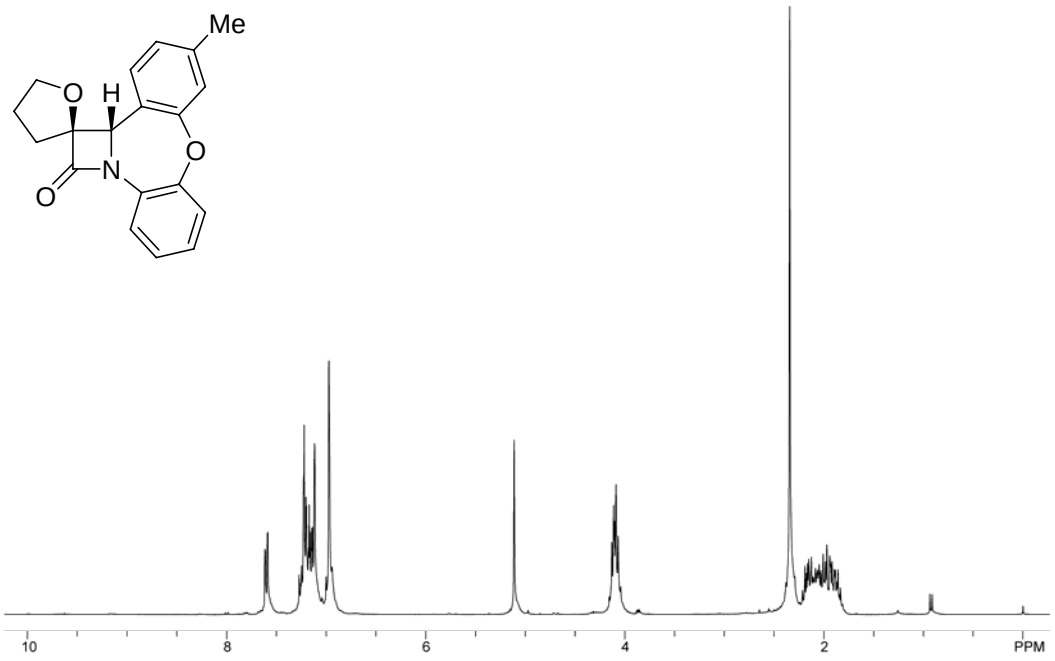
***Rel*-(2*R*,2a*R*)-Spiro[azeto[1,2-*d*]benzo[*b*][1,4]oxazine-2,2'-(2-oxacyclopentane)]-1(2a*H*),3-dione (4g)**



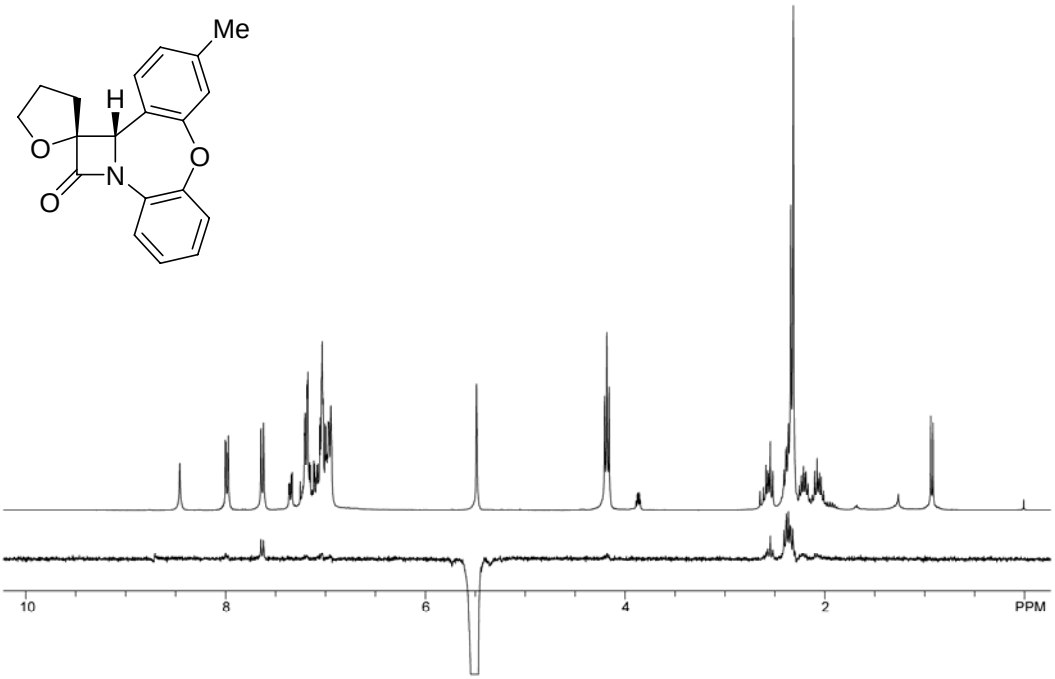
Colorless crystals, m.p. 150-151 °C. R_f = 0.33 [silica gel plate, petroleum ether (60-90 °C):AcOEt = 5:1, v/v]. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.19 (m, 2H), 2.46 (m, 2H), 4.11 (m, 1H), 4.23 (m, 1H), 4.30 (s, 1H), 7.12−7.40 (m, 4H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 25.2, 31.9, 59.2, 70.9, 99.0, 117.4, 121.1, 121.6, 125.2, 127.2, 145.5, 160.7, 169.5. IR ν (cm^{-1}): 1778. MS (ESI) m/z: 246 $[M+H]^+$. Calcd for $C_{13}H_{11}NO_4$: C, 63.67; H, 4.52; N, 5.71. Found: C, 63.64; H, 4.73; N, 5.64.

2. Copies of ^{1}H NMR Spectra

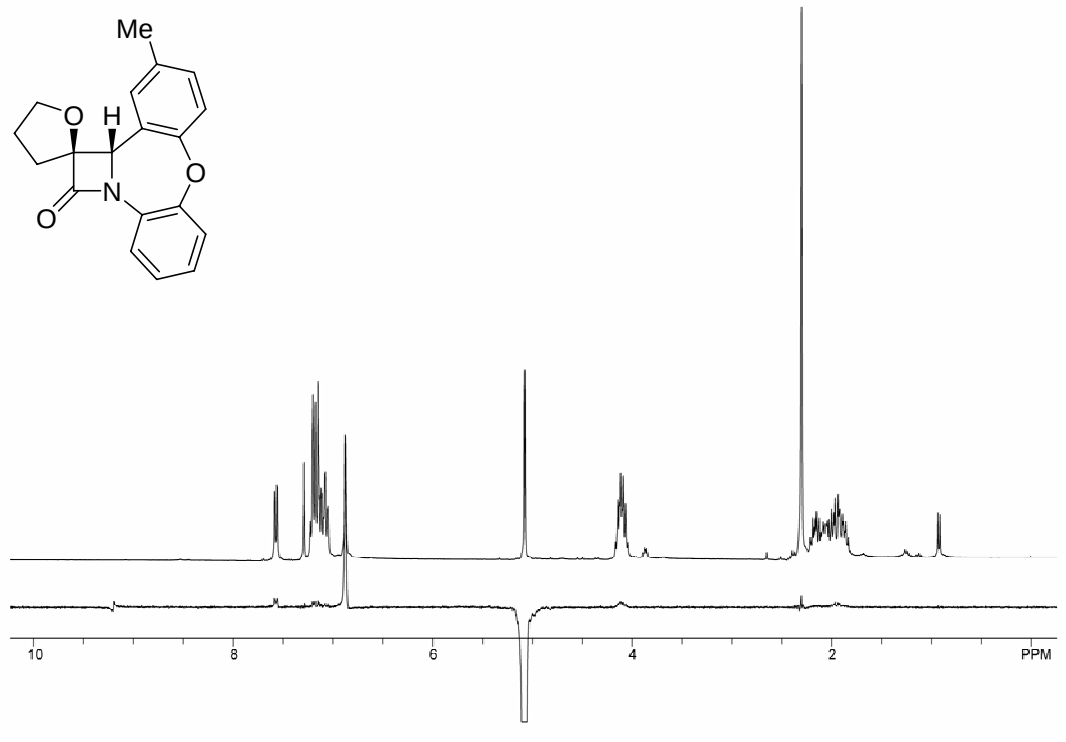
3a



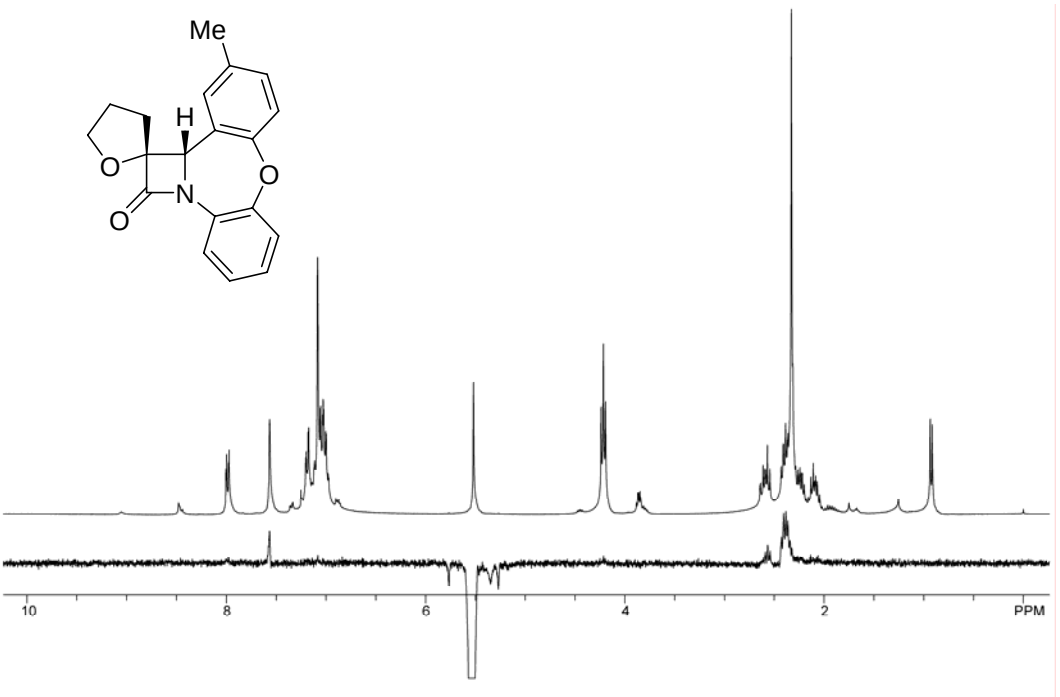
4a



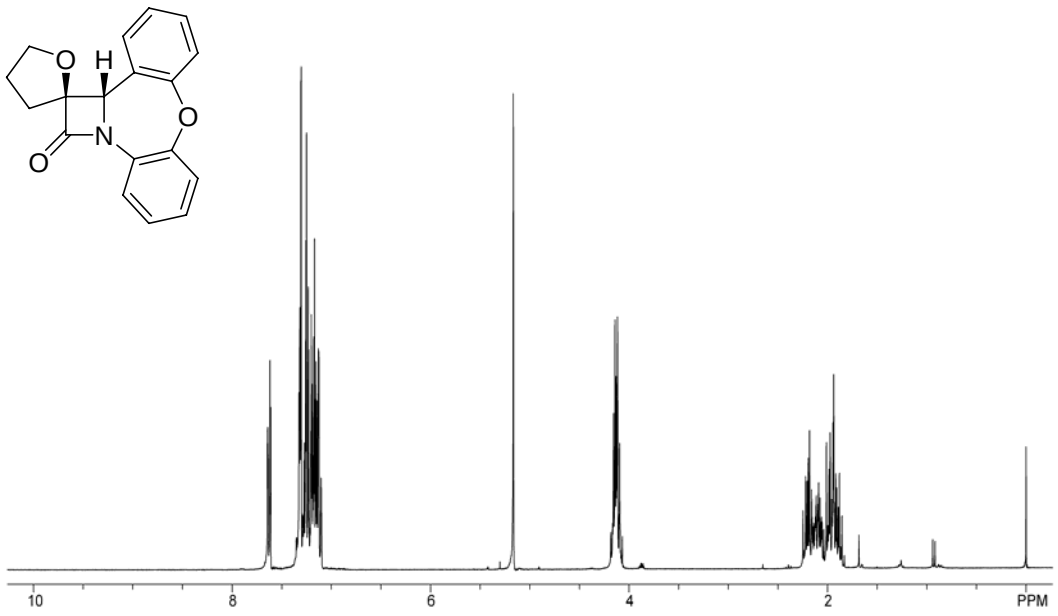
3b



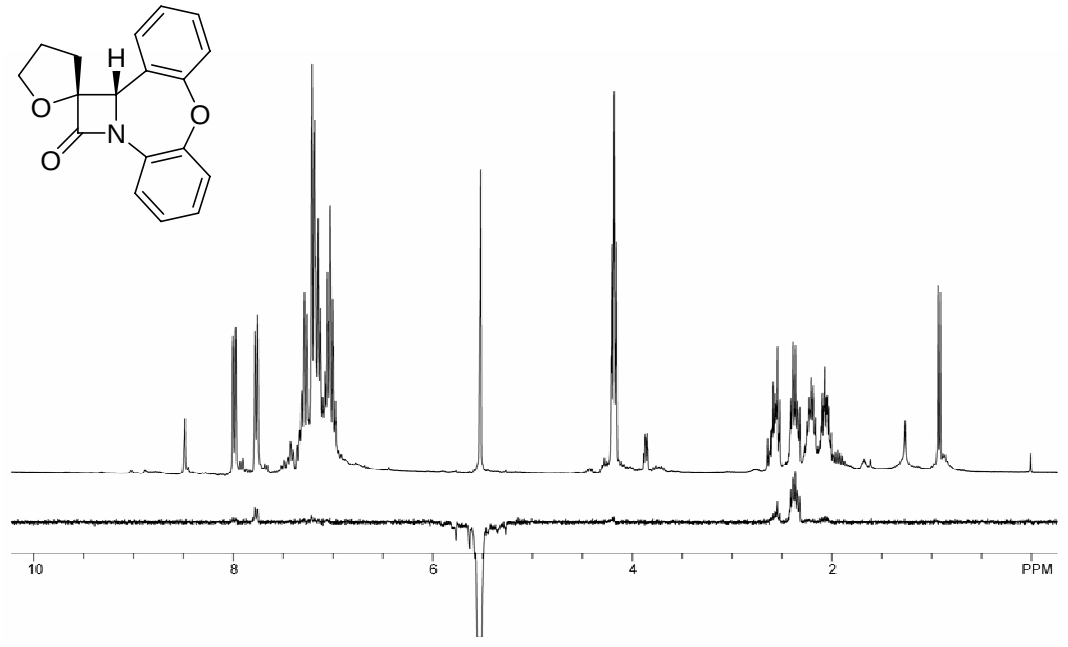
4b



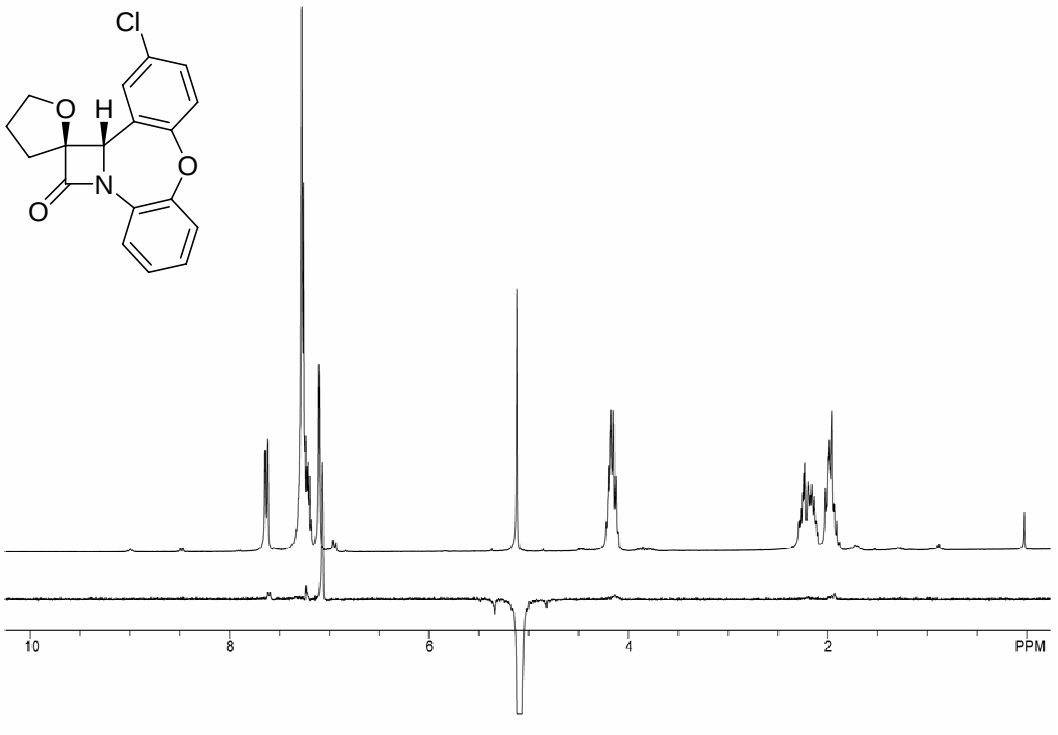
3c



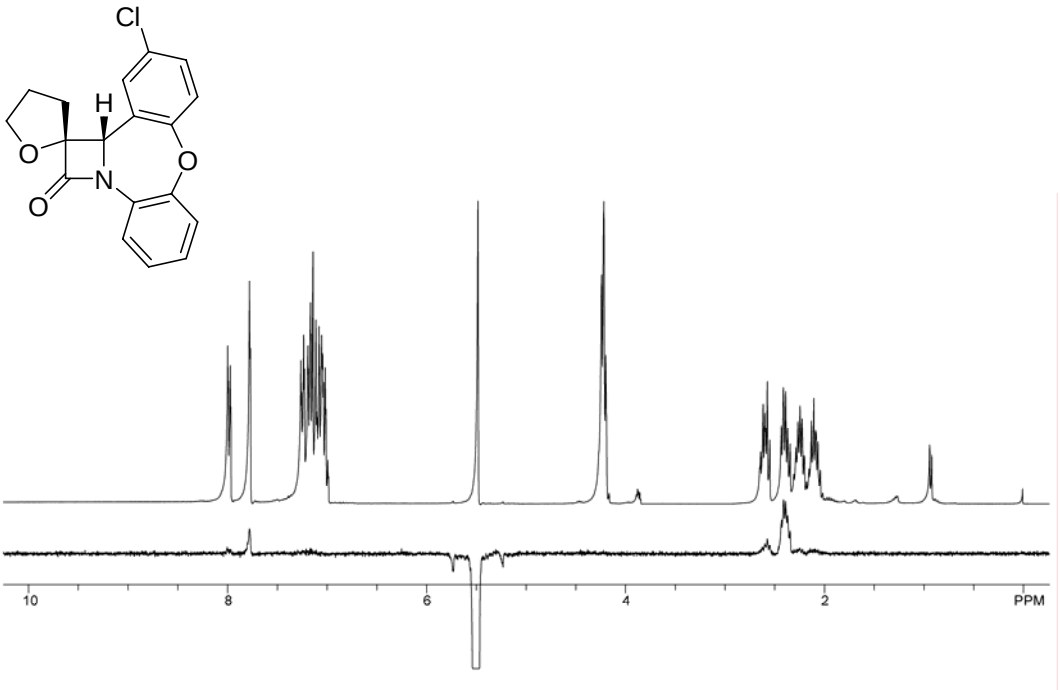
4c



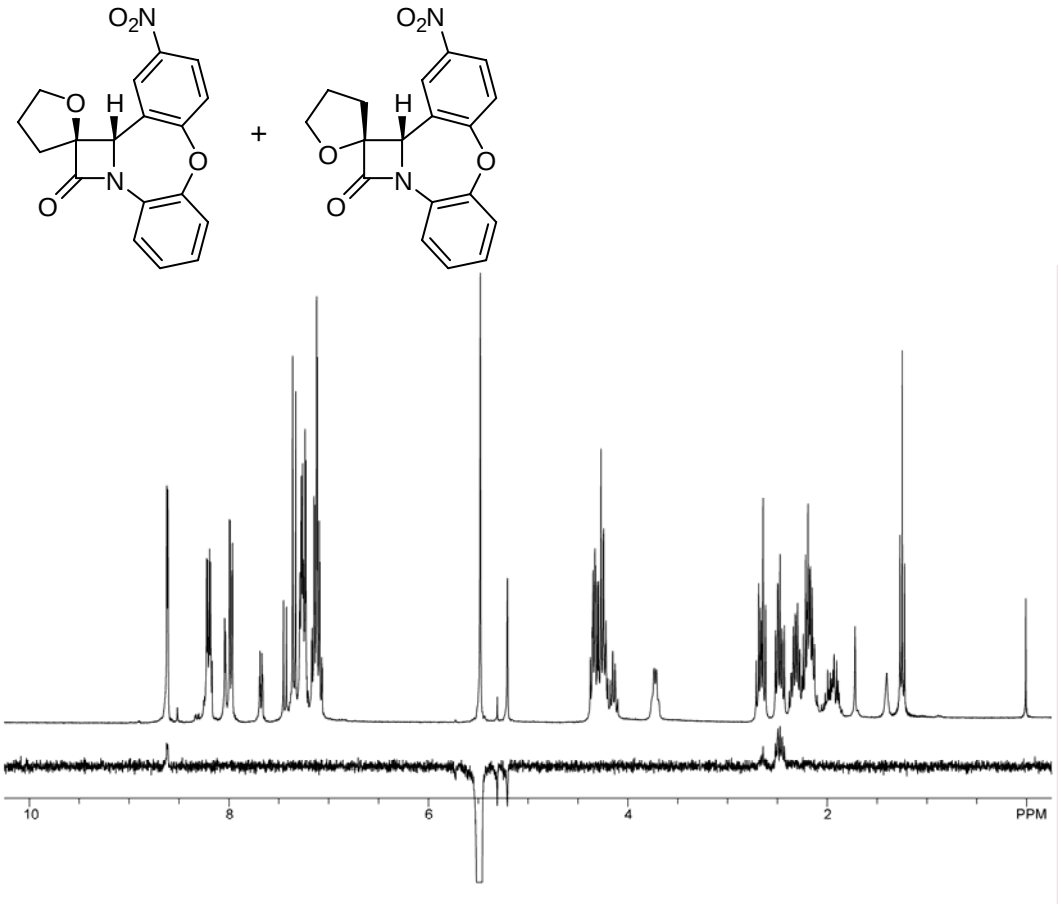
3d



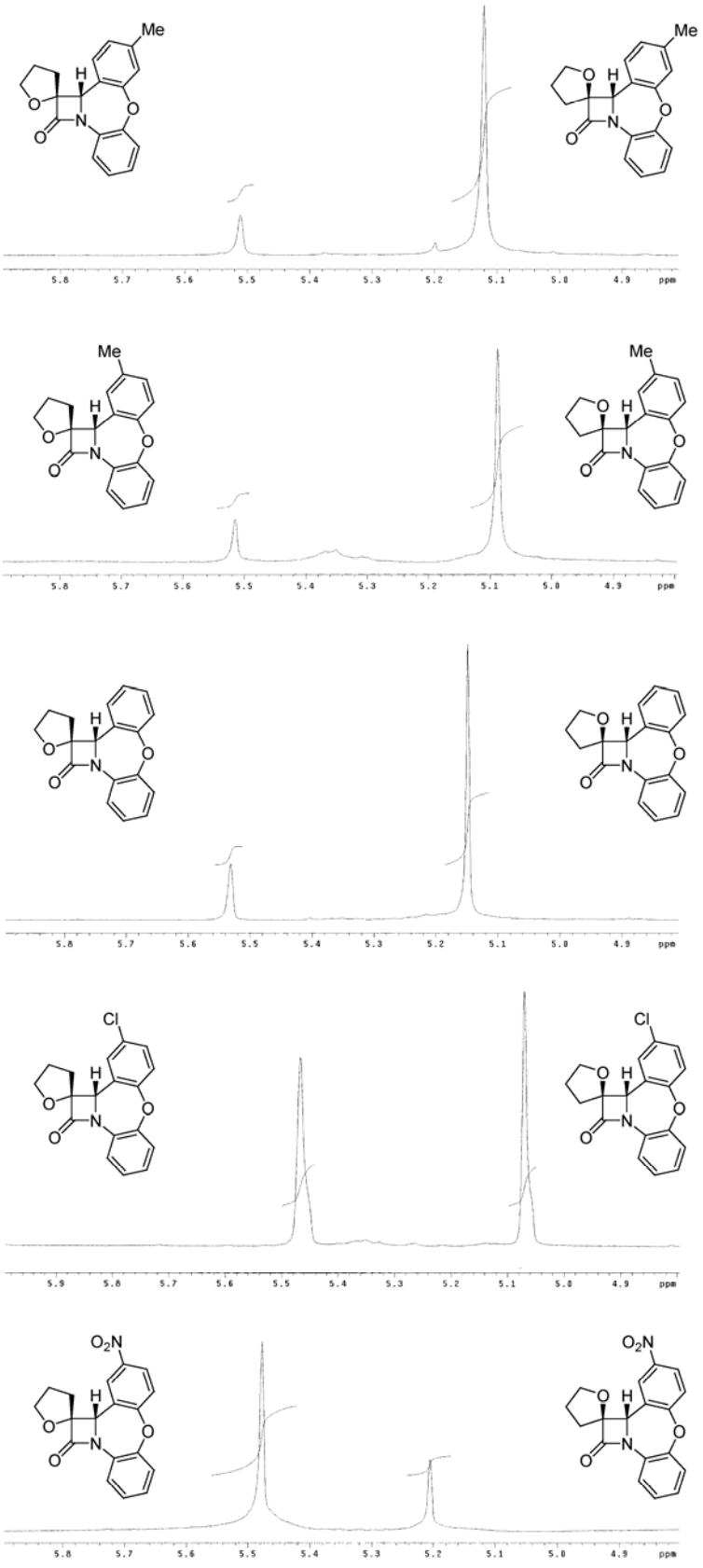
4d



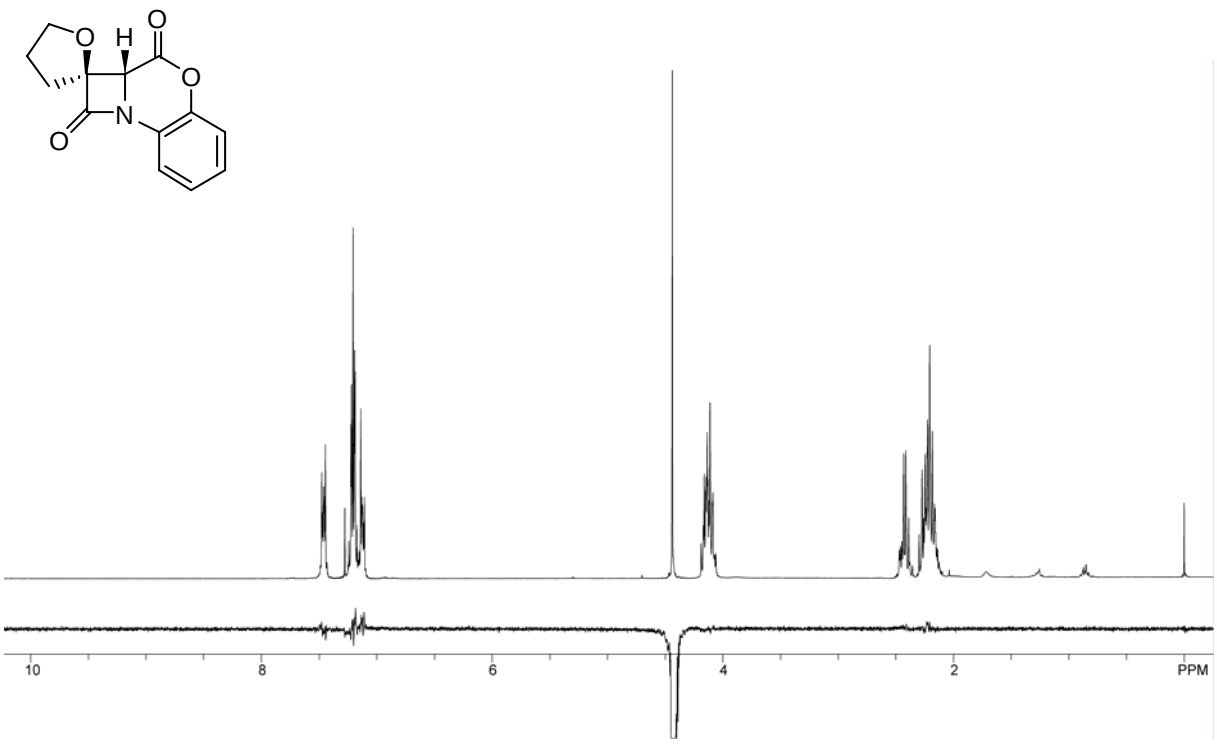
3e + **4e**



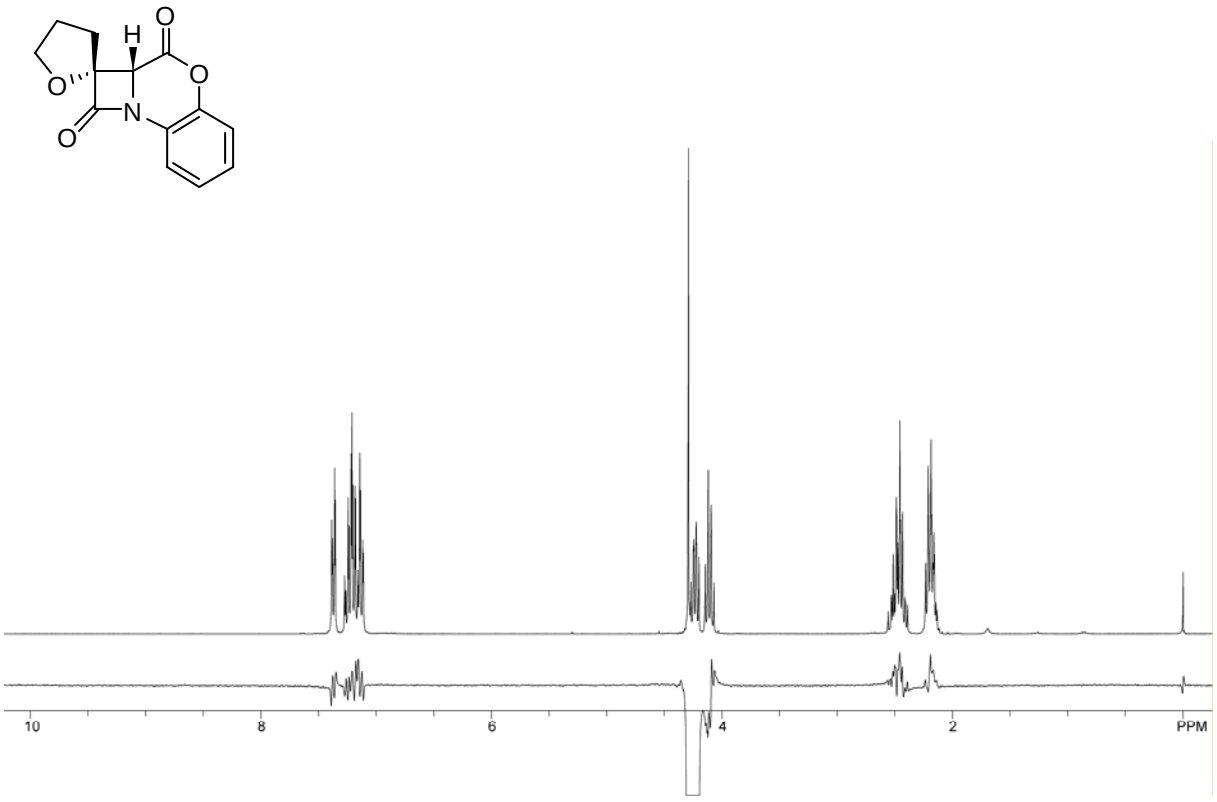
Determination of product ratios (**3**/**4** ratio) of the reactions of **1** with **2a-e**



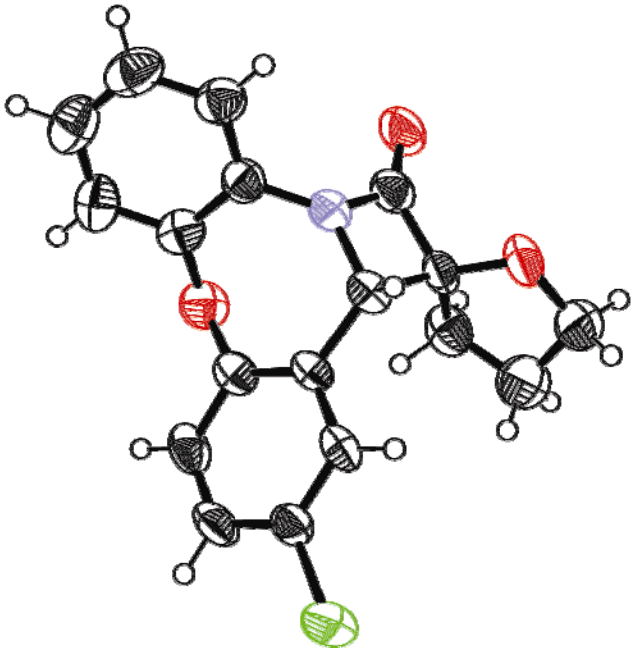
3g



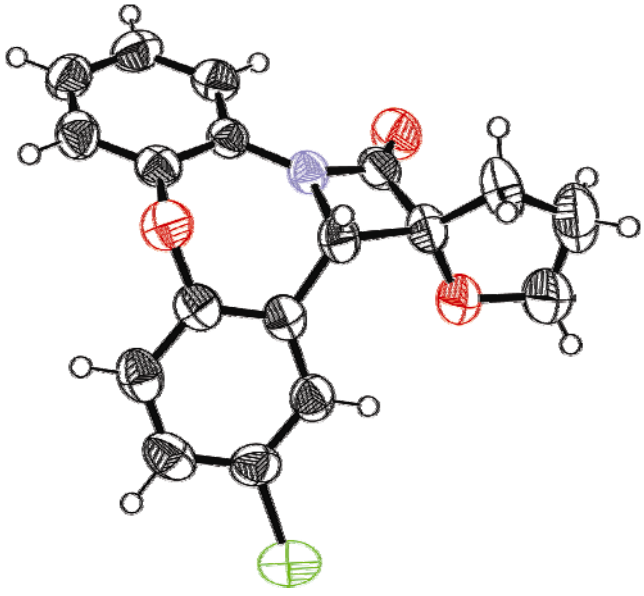
4g



3. Crystal Structures of 3d and 4d



3d



4d

Ellipsoids are drawn at 50% probability.

4. Details of Calculations

All of the DFT calculations were performed with the Gaussian 03 program package.[5] The geometry optimization of all the minima and transition states involved were performed at the B3LYP levels of theory[6] with the 6-31G(d) basis set.[7] The vibrational frequencies were computed at the same level of theory to check whether every optimized geometrical structure is an energy minimum or a transition state, and to evaluate its zero-point vibration energy (ZPVE). IRC calculations[8] were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. Solvent effects were computed by the CPCM model[9] at the B3LYP/6-31G(d) level using the gas phase optimized structures.

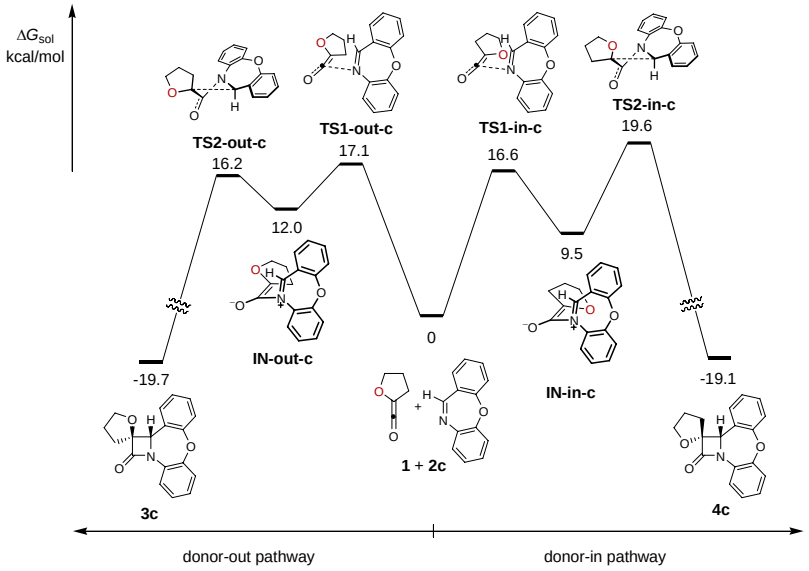


Figure S1. The calculated energy surfaces for the reaction of ketene **1** with imine **2c** at the B3LYP/6-31+G(d)//B3LYP/6-31G(d) + ΔZPVE level of theory (toluene was used as solvent within the CPCM method). **TS2-out-c** is calculated on the B3LYP/6-31+G(d)//B3LYP/6-31G level.

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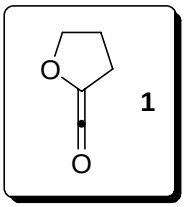
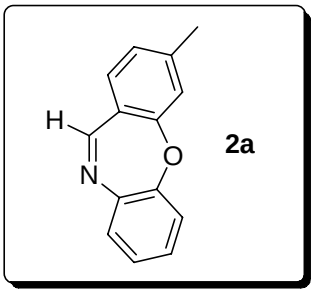
5. Coordinates of All Stationary Points



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.341056	-1.150574	-0.227141
2	6	0	1.654186	-0.831556	0.252139
3	6	0	1.868674	0.629059	-0.155097
4	6	0	0.469004	1.249092	0.076098
5	6	0	-0.414532	0.018905	-0.070155
6	6	0	-1.729577	-0.025897	0.017810
7	8	0	-2.910082	-0.009746	0.040109
8	1	0	2.346368	-1.536964	-0.213981
9	1	0	1.698961	-0.951516	1.345435
10	1	0	2.135443	0.682920	-1.215418
11	1	0	2.650451	1.126519	0.426281
12	1	0	0.240920	2.036614	-0.649452
13	1	0	0.393528	1.687366	1.078617



Standard orientation:

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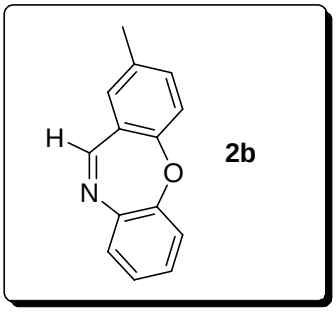
1	6	0	-2.169713	-1.714018	0.183407
2	6	0	-1.449550	-0.547590	0.424625
3	6	0	-1.976884	0.716855	0.091513

4	6	0	-3.258041	0.753425	-0.486221
5	6	0	-3.976146	-0.410181	-0.746192
6	6	0	-3.432969	-1.650465	-0.405430
7	8	0	-0.240647	-0.685493	1.100867
8	6	0	0.891616	-0.191530	0.478397
9	6	0	1.956819	-1.065540	0.299317
10	6	0	3.180571	-0.612059	-0.213583
11	6	0	3.304462	0.745095	-0.536941
12	6	0	2.236576	1.618324	-0.349723
13	6	0	1.002867	1.170792	0.145988
14	6	0	4.329337	-1.573046	-0.404574
15	6	0	-0.092598	2.133240	0.331463
16	7	0	-1.363940	1.960200	0.313451
17	1	0	0.234490	3.170389	0.455928
18	1	0	-3.666377	1.731439	-0.721152
19	1	0	-4.961805	-0.348504	-1.198433
20	1	0	-3.990583	-2.565185	-0.585547
21	1	0	-1.726793	-2.661236	0.475087
22	1	0	1.823359	-2.104299	0.587702
23	1	0	2.350148	2.672095	-0.593656
24	1	0	4.246478	1.120733	-0.927439
25	1	0	5.238171	-1.052199	-0.720504
26	1	0	4.554490	-2.114644	0.521899
27	1	0	4.093102	-2.325861	-1.167245

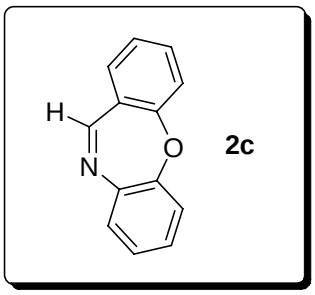


2b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.358876	-0.031883	0.360589
2	6	0	-2.942891	-1.355372	0.150317
3	6	0	-1.652425	-1.646658	-0.287139
4	6	0	-0.749643	-0.613131	-0.523440
5	6	0	-1.125365	0.723433	-0.319434
6	6	0	-2.437676	0.985959	0.108979

7	8	0	0.478572	-0.940594	-1.070440
8	6	0	1.609149	-0.527944	-0.371348
9	6	0	1.881552	0.835847	-0.139906
10	6	0	3.105646	1.159035	0.471023
11	6	0	4.009665	0.174880	0.860405
12	6	0	3.717570	-1.169030	0.619368
13	6	0	2.516549	-1.515927	-0.000353
14	7	0	1.063675	1.919553	-0.497702
15	6	0	-0.215493	1.852882	-0.568951
16	1	0	-0.719234	2.795748	-0.804023
17	1	0	3.318248	2.212174	0.626441
18	1	0	4.945055	0.456270	1.335463
19	1	0	4.422860	-1.945762	0.901037
20	1	0	2.267626	-2.550243	-0.216455
21	1	0	-1.335573	-2.668152	-0.471666
22	1	0	-3.641831	-2.170896	0.321851
23	1	0	-2.735701	2.023202	0.249667
24	6	0	-4.758943	0.274340	0.839817
25	1	0	-4.956912	1.350624	0.831602
26	1	0	-5.513731	-0.210087	0.208982
27	1	0	-4.918031	-0.083594	1.864977



Standard orientation:

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3	7	0	-0.706604	1.935816	0.424168
4	6	0	-1.511816	0.818878	0.150342
5	6	0	-2.785090	1.088591	-0.380702
6	1	0	-3.041998	2.130391	-0.545208
7	6	0	-3.681118	0.067403	-0.683412
8	1	0	-4.655737	0.307588	-1.098375
9	6	0	-3.329310	-1.260299	-0.432593

10	1	0	-4.026535	-2.065429	-0.646281
11	6	0	-2.077591	-1.554163	0.109390
12	1	0	-1.780749	-2.574512	0.331245
13	6	0	-1.179600	-0.529416	0.393033
14	8	0	0.009980	-0.890050	1.020340
15	6	0	1.187833	-0.541959	0.384642
16	6	0	1.503460	0.802953	0.123931
17	6	0	2.099669	-1.559051	0.114717
18	1	0	1.820787	-2.582062	0.345599
19	6	0	3.351485	-1.245338	-0.416610
20	1	0	4.063501	-2.040858	-0.617875
21	6	0	2.774993	1.094454	-0.397118
22	1	0	3.035383	2.133597	-0.584380
23	6	0	3.691472	0.084306	-0.676762
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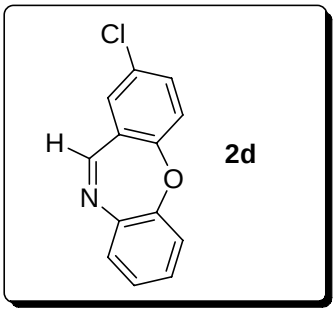

2d

Standard orientation:

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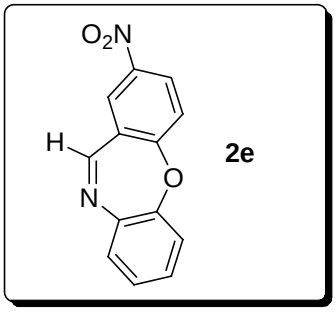
2	6	0	-2.583893	-1.433741	0.015752
3	6	0	-1.270686	-1.697491	-0.371526
4	6	0	-0.379226	-0.649992	-0.589760
5	6	0	-0.781888	0.685652	-0.418509
6	6	0	-2.109265	0.941525	-0.041071
7	8	0	0.870381	-0.963554	-1.085452
8	6	0	1.971274	-0.524361	-0.352423
9	6	0	2.214979	0.846070	-0.131708
10	6	0	3.411700	1.197162	0.516660
11	6	0	4.315183	0.231884	0.951670
12	6	0	4.051595	-1.119426	0.719390
13	6	0	2.878685	-1.493778	0.062581
14	7	0	1.393753	1.910750	-0.534578
15	6	0	0.120239	1.827499	-0.652998

16	1	0	-0.388260	2.757757	-0.923429
17	1	0	3.603291	2.255358	0.664245
18	1	0	5.228836	0.533658	1.455347
19	1	0	4.757953	-1.881237	1.036468
20	1	0	2.653891	-2.534616	-0.148178
21	1	0	-0.929114	-2.715322	-0.528040
22	1	0	-3.284484	-2.245368	0.179393
23	1	0	-2.444113	1.967225	0.079010
24	17	0	-4.646934	0.234665	0.663066



2e

Standard orientation:

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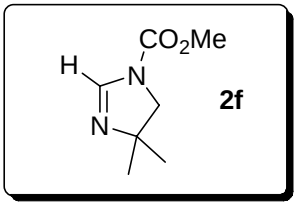
2	6	0	0.367408	1.808749	-0.676128
3	1	0	-0.144805	2.733081	-0.958094
4	6	0	-0.534453	0.664162	-0.445126
5	6	0	-0.129220	-0.677101	-0.600194
6	8	0	1.126502	-1.000928	-1.047599
7	6	0	2.226278	-0.531509	-0.324289
8	6	0	2.463076	0.843046	-0.129992
9	6	0	3.135653	-1.490581	0.107840
10	1	0	2.915184	-2.535788	-0.084517
11	6	0	4.306659	-1.099956	0.758866
12	1	0	5.015159	-1.853477	1.090131
13	6	0	4.564853	0.256121	0.966341
14	1	0	5.476811	0.570733	1.464922
15	6	0	3.657981	1.209755	0.512991
16	1	0	3.844881	2.271162	0.641492
17	6	0	-1.028141	-1.729229	-0.411594
18	1	0	-0.676189	-2.744803	-0.556352
19	6	0	-2.348464	-1.467398	-0.063952
20	1	0	-3.065840	-2.264701	0.085704
21	6	0	-2.750261	-0.140447	0.087496

22	7	0	-4.144382	0.149314	0.446540
23	8	0	-4.469652	1.330249	0.568515
24	8	0	-4.902866	-0.807252	0.604243
25	6	0	-1.869250	0.917226	-0.110030
26	1	0	-2.228768	1.934520	-0.003996



Standard orientation:

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3	7	0	-1.756922	1.266155	-0.000392
4	6	0	-1.984681	-0.203427	-0.000024
5	6	0	-0.554129	-0.854411	-0.000258
6	1	0	-0.365687	-1.468261	0.886195
7	1	0	-0.365778	-1.467660	-0.887164
8	7	0	0.313230	0.330641	0.000069
9	6	0	1.687553	0.373562	0.000013
10	8	0	2.350268	1.393618	-0.000001
11	8	0	2.195436	-0.882605	0.000010
12	6	0	3.630277	-0.945673	0.000023
13	1	0	4.037322	-0.458952	0.890042
14	1	0	4.037337	-0.458984	-0.890006
15	1	0	3.872143	-2.008953	0.000043
16	6	0	-2.774609	-0.573985	-1.262665
17	1	0	-2.974721	-1.651931	-1.294276
18	1	0	-3.730608	-0.041526	-1.280134
19	1	0	-2.216938	-0.299574	-2.164873
20	6	0	-2.773810	-0.573297	1.263350
21	1	0	-3.729999	-0.041188	1.280884
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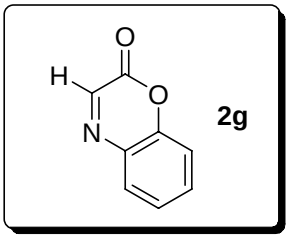
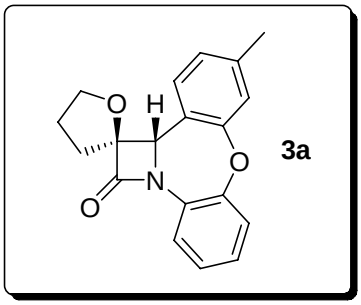
23	1	0	-2.215770	-0.297952	2.165047



2g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.633969	1.685234	-0.000002
2	6	0	1.820378	1.182928	-0.000029
3	1	0	2.682973	1.846679	0.000093
4	6	0	2.136921	-0.262525	-0.000083
5	8	0	3.248468	-0.729413	0.000077
6	8	0	1.040251	-1.106026	-0.000029
7	6	0	-0.231085	-0.594776	-0.000010
8	6	0	-0.438189	0.797552	0.000003
9	6	0	-1.300971	-1.487154	-0.000001
10	6	0	-1.754379	1.287346	0.000015
11	6	0	-2.827518	0.406406	0.000011
12	6	0	-2.597045	-0.978171	0.000010
13	1	0	-1.102411	-2.553877	0.000000
14	1	0	-1.894714	2.363739	0.000019
15	1	0	-3.437766	-1.665858	0.000037
16	1	0	-3.844289	0.786562	-0.000011

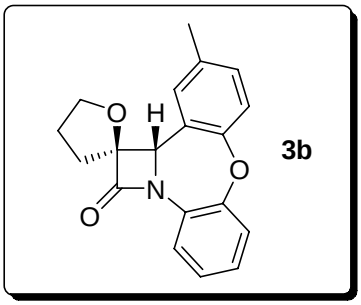


3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.685617	0.820836	0.294705
2	6	0	2.345455	0.435173	0.270850
3	6	0	1.993388	-0.855913	-0.152281

4	6	0	2.995105	-1.759696	-0.524055
5	6	0	4.334495	-1.377788	-0.478738
6	6	0	4.678423	-0.083973	-0.079932
7	8	0	1.435462	1.319577	0.814645
8	6	0	0.256909	1.754002	0.229395
9	6	0	-0.661386	0.962847	-0.474283
10	6	0	-1.815206	1.599449	-0.964802
11	6	0	-2.075622	2.943497	-0.735363
12	6	0	-1.167583	3.724726	-0.003774
13	6	0	-0.006027	3.111130	0.459582
14	6	0	-0.497040	-0.500648	-0.777982
15	7	0	0.636672	-1.208364	-0.169486
16	6	0	-0.096291	-2.291039	0.287360
17	8	0	0.220319	-3.339752	0.799423
18	6	0	-1.441608	5.184594	0.270641
19	6	0	-1.428215	-1.586731	-0.113761
20	6	0	-2.330585	-1.221689	1.067626
21	6	0	-3.283187	-2.426665	1.088151
22	6	0	-3.459622	-2.710601	-0.407726
23	8	0	-2.237971	-2.281367	-1.039375
24	1	0	-0.509620	-0.654113	-1.865535
25	1	0	2.705418	-2.759029	-0.831804
26	1	0	5.106314	-2.086842	-0.763084
27	1	0	5.720442	0.221504	-0.052675
28	1	0	3.929067	1.822832	0.633336
29	1	0	0.736831	3.676823	1.014172
30	1	0	-2.521326	1.005803	-1.541920
31	1	0	-2.984689	3.392158	-1.128178
32	1	0	-4.295498	-2.139451	-0.835379
33	1	0	-3.612228	-3.770452	-0.634448
34	1	0	-2.799266	-3.276049	1.581667
35	1	0	-4.230624	-2.221888	1.595663
36	1	0	-1.776602	-1.083962	1.999855
37	1	0	-2.870688	-0.292557	0.851413
38	1	0	-1.746834	5.711948	-0.640713
39	1	0	-2.253591	5.305333	0.999425
40	1	0	-0.558405	5.689752	0.673378

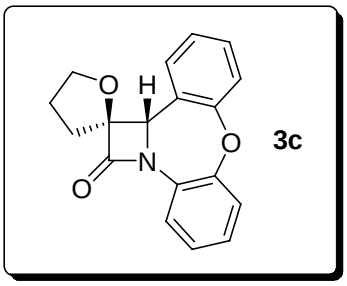


3b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.945444	-3.187926	0.626701
2	6	0	0.419665	-2.180390	0.213121
3	6	0	-1.035668	-1.707315	-0.087420
4	8	0	-1.744985	-2.469933	-1.041648
5	6	0	-2.825414	-3.181054	-0.406830
6	1	0	-2.773954	-4.231767	-0.709313
7	1	0	-3.776970	-2.762882	-0.763494
8	6	0	-2.640502	-2.972285	1.100714
9	1	0	-1.982006	-3.743889	1.513194
10	1	0	-3.586331	-2.991144	1.650452
11	6	0	-1.937327	-1.607073	1.145313
12	1	0	-1.379335	-1.431949	2.068878
13	1	0	-2.653514	-0.786736	1.018155
14	7	0	0.921323	-0.950909	-0.178820
15	6	0	-0.348661	-0.424532	-0.694629
16	1	0	-0.383021	-0.502359	-1.789749
17	6	0	-0.759692	0.960641	-0.277227
18	6	0	-2.040643	1.391624	-0.667176
19	1	0	-2.651575	0.701329	-1.246693
20	6	0	-2.554049	2.646180	-0.344717
21	6	0	-3.941003	3.065515	-0.772667
22	1	0	-4.432667	2.282627	-1.358612
23	1	0	-4.579109	3.284227	0.092783
24	1	0	-3.912956	3.973539	-1.387704
25	6	0	-1.731186	3.512040	0.392653
26	1	0	-2.091112	4.502122	0.662872
27	6	0	-0.452134	3.126948	0.766811
28	1	0	0.196626	3.796368	1.322718
29	6	0	0.046272	1.860436	0.432541
30	8	0	1.318810	1.620420	0.926492
31	6	0	2.337200	0.943889	0.286166
32	6	0	3.588245	1.560568	0.271480

33	1	0	3.671416	2.570549	0.659998
34	6	0	4.701463	0.868404	-0.204251
35	1	0	5.673499	1.353193	-0.206456
36	6	0	4.568283	-0.443362	-0.665812
37	1	0	5.435327	-0.987309	-1.028646
38	6	0	3.316296	-1.055009	-0.672951
39	1	0	3.189274	-2.072484	-1.027655
40	6	0	2.194354	-0.364821	-0.200343

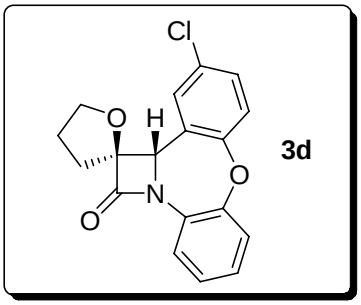


3c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.607379	-0.052388	-0.759338
2	6	0	-1.777768	-0.893745	-0.118387
3	6	0	1.719049	-1.021274	-0.158760
4	6	0	2.468706	-2.131373	-0.563307
5	6	0	3.860989	-2.086843	-0.523578
6	6	0	4.510790	-0.925938	-0.097608
7	6	0	3.769669	0.182910	0.310173
8	6	0	2.376145	0.134013	0.291573
9	8	0	1.707361	1.196729	0.866666
10	6	0	0.673496	1.923472	0.299295
11	6	0	-0.411455	1.400469	-0.421814
12	6	0	0.747016	3.296860	0.567005
13	6	0	-0.239020	4.164976	0.114005
14	6	0	-1.379423	2.303537	-0.894652
15	6	0	-1.310896	3.667074	-0.631497
16	1	0	-0.654264	-0.171426	-1.850195
17	1	0	1.943583	-3.022067	-0.892223
18	1	0	4.436274	-2.954096	-0.833770
19	1	0	5.595919	-0.883444	-0.074839
20	1	0	4.251266	1.086385	0.670311
21	1	0	1.599647	3.656362	1.134095
22	1	0	-0.163061	5.226868	0.330253
23	1	0	-2.205542	1.906200	-1.480800

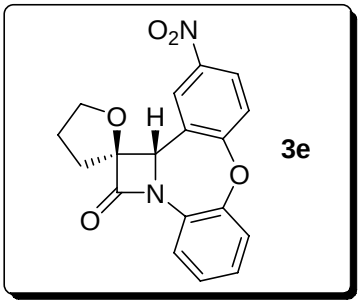
24	1	0	-2.082156	4.334070	-1.005207
25	6	0	-0.658555	-1.910879	0.262216
26	8	0	-0.608677	-3.017385	0.747114
27	7	0	0.317383	-1.029040	-0.171064
28	8	0	-2.727099	-1.347432	-1.060206
29	6	0	-4.015220	-1.502125	-0.432878
30	6	0	-3.781775	-1.295908	1.068446
31	6	0	-2.571564	-0.349352	1.071222
32	1	0	-4.698958	-0.748475	-0.847524
33	1	0	-4.403443	-2.495323	-0.679607
34	1	0	-3.513462	-2.244605	1.545023
35	1	0	-4.656039	-0.883421	1.580846
36	1	0	-2.004520	-0.365110	2.005661
37	1	0	-2.876434	0.685141	0.874139



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	4.533607	-1.839715	-0.636871
2	8	0	-1.176808	-1.792940	0.917950
3	8	0	-2.007645	2.980755	0.656058
4	8	0	0.826554	2.956943	-0.942773
5	7	0	-1.397925	0.823240	-0.132961
6	6	0	-1.233987	2.141184	0.261214
7	6	0	0.300754	2.055043	0.006585
8	6	0	-0.027420	0.638103	-0.620180
9	6	0	0.704560	-0.607263	-0.200025
10	6	0	0.127087	-1.696340	0.472693
11	6	0	0.914426	-2.803724	0.818043
12	6	0	2.263863	-2.859825	0.496705
13	6	0	2.831586	-1.790742	-0.197715
14	6	0	2.063696	-0.688558	-0.546923
15	6	0	-2.486895	-0.055730	-0.201123
16	6	0	-2.315745	-1.370255	0.257724

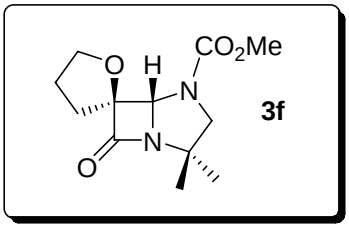
17	6	0	-3.373785	-2.276408	0.197321
18	6	0	-4.611493	-1.868511	-0.298823
19	6	0	-4.794565	-0.553598	-0.733527
20	6	0	-3.733061	0.348075	-0.694078
21	6	0	1.165369	2.166925	1.279805
22	6	0	2.406417	2.935663	0.794763
23	6	0	1.814546	3.793897	-0.322804
24	1	0	0.013771	0.732803	-1.713640
25	1	0	0.434907	-3.622965	1.343557
26	1	0	2.863103	-3.722451	0.766670
27	1	0	2.516105	0.132331	-1.095248
28	1	0	-3.214386	-3.284447	0.566441
29	1	0	-5.433549	-2.577268	-0.337455
30	1	0	-5.760046	-0.231426	-1.111945
31	1	0	-3.853156	1.373601	-1.027011
32	1	0	0.620580	2.753890	2.027657
33	1	0	1.396423	1.192429	1.716492
34	1	0	2.876191	3.528010	1.585403
35	1	0	3.156830	2.247561	0.389780
36	1	0	1.338974	4.700863	0.076747
37	1	0	2.529488	4.083840	-1.097726



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.447423	2.733108	0.623704
2	6	0	-1.585645	1.972924	0.249775
3	6	0	-0.057418	2.053393	-0.049613
4	8	0	0.325790	2.992583	-1.027744
5	6	0	1.086692	4.060070	-0.423921
6	1	0	2.124869	3.989452	-0.774450
7	1	0	0.668425	5.013130	-0.761127
8	6	0	0.977749	3.847489	1.089731
9	1	0	0.083866	4.344562	1.480778

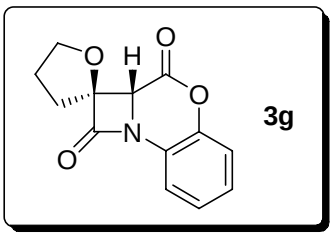
10	1	0	1.850412	4.219802	1.634023
11	6	0	0.812043	2.322378	1.182739
12	1	0	0.346480	1.988475	2.113841
13	1	0	1.779242	1.816531	1.084315
14	7	0	-1.603129	0.627592	-0.087827
15	6	0	-0.239535	0.595376	-0.627541
16	1	0	-0.253241	0.661613	-1.723836
17	6	0	0.649910	-0.538833	-0.200650
18	6	0	2.019403	-0.407290	-0.458290
19	1	0	2.394846	0.483225	-0.949954
20	6	0	2.916089	-1.402507	-0.092535
21	7	0	4.342174	-1.215101	-0.366536
22	8	0	4.691364	-0.161572	-0.902313
23	8	0	5.109743	-2.122362	-0.042714
24	6	0	2.483148	-2.573276	0.532601
25	1	0	3.199751	-3.336459	0.808776
26	6	0	1.128697	-2.728556	0.765665
27	1	0	0.741769	-3.628559	1.231053
28	6	0	0.202888	-1.734373	0.396298
29	8	0	-1.081501	-2.075125	0.724338
30	6	0	-2.284819	-1.674507	0.168024
31	6	0	-3.257847	-2.670905	0.081749
32	1	0	-2.982919	-3.685398	0.351512
33	6	0	-4.554055	-2.347678	-0.313189
34	1	0	-5.306913	-3.127959	-0.372260
35	6	0	-4.882506	-1.024533	-0.619721
36	1	0	-5.893823	-0.766074	-0.918671
37	6	0	-3.908621	-0.031839	-0.555496
38	1	0	-4.142009	1.001363	-0.788559
39	6	0	-2.600817	-0.349699	-0.165137



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.556288	-0.441615	0.064800
2	6	0	1.807922	1.063776	-0.238492

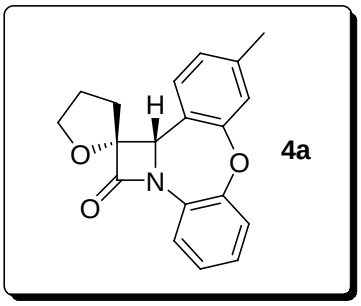
3	7	0	0.679121	1.453893	0.500581
4	6	0	0.234176	0.078446	0.749045
5	8	0	2.611169	1.692048	-0.884402
6	6	0	-0.446994	2.331964	0.114994
7	6	0	-1.391449	1.301471	-0.582981
8	7	0	-1.041829	0.017212	0.041730
9	6	0	-1.843432	-1.078424	0.158335
10	8	0	-3.034848	-0.892013	-0.467989
11	6	0	-3.927842	-2.012982	-0.396209
12	8	0	-1.526062	-2.102232	0.744382
13	6	0	-0.008252	3.457244	-0.822293
14	6	0	-1.096830	2.892121	1.389519
15	8	0	2.464021	-1.028492	0.972397
16	6	0	2.813525	-2.358720	0.543169
17	6	0	1.769976	-2.742943	-0.506979
18	6	0	1.456594	-1.378122	-1.140594
19	1	0	0.130274	-0.225543	1.793819
20	1	0	-1.200517	1.274238	-1.663946
21	1	0	-2.448899	1.526598	-0.427397
22	1	0	-4.815888	-1.710720	-0.952686
23	1	0	-4.184794	-2.238105	0.642215
24	1	0	-3.474344	-2.898269	-0.849592
25	1	0	-0.883673	4.040373	-1.129538
26	1	0	0.487567	3.070251	-1.715727
27	1	0	0.690880	4.129319	-0.316197
28	1	0	-1.964718	3.511862	1.136571
29	1	0	-0.378627	3.506002	1.941425
30	1	0	-1.435387	2.086412	2.050243
31	1	0	2.812700	-3.008024	1.424165
32	1	0	3.828397	-2.342272	0.121647
33	1	0	0.870290	-3.142890	-0.029057
34	1	0	2.144239	-3.475709	-1.228406
35	1	0	2.223704	-1.094606	-1.871215
36	1	0	0.481430	-1.334426	-1.631475



Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

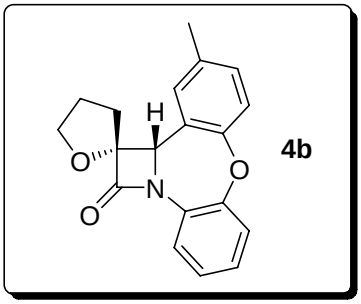
Number	Number	Type	X	Y	Z
1	6	0	-1.773110	-0.181085	-0.179120
2	6	0	-0.769284	-1.353473	0.087329
3	7	0	0.286310	-0.606094	-0.441767
4	6	0	-0.522291	0.565980	-0.784127
5	6	0	-2.465048	0.380512	1.071662
6	6	0	-3.849074	-0.278847	0.976913
7	6	0	-4.082377	-0.277699	-0.533986
8	8	0	-2.778460	-0.461897	-1.120871
9	6	0	1.663460	-0.529195	-0.215909
10	6	0	2.169055	0.754528	0.034690
11	8	0	1.331388	1.861995	0.157561
12	6	0	-0.004172	1.842769	-0.159296
13	6	0	2.526572	-1.627313	-0.220185
14	6	0	3.887974	-1.428394	0.007971
15	6	0	4.389630	-0.141160	0.220288
16	6	0	3.529210	0.958024	0.235099
17	8	0	-0.669893	2.826714	0.036745
18	8	0	-0.817137	-2.454101	0.575337
19	1	0	-0.635076	0.719800	-1.864659
20	1	0	-2.536950	1.469593	0.988484
21	1	0	-1.929734	0.140067	1.994528
22	1	0	-4.620971	0.266237	1.527960
23	1	0	-3.807587	-1.306012	1.354688
24	1	0	-4.500874	0.677604	-0.879945
25	1	0	-4.723394	-1.090673	-0.886068
26	1	0	2.118573	-2.616841	-0.396446
27	1	0	4.560003	-2.281214	0.008533
28	1	0	5.452123	0.010163	0.384752
29	1	0	3.889259	1.964366	0.422391



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.335160	0.038416	1.289216
2	6	0	-2.216803	0.113862	0.244139
3	8	0	-2.620916	1.096121	-0.692978
4	6	0	-4.027967	1.376777	-0.547241
5	6	0	-4.571368	0.327171	0.427482
6	6	0	-0.729690	0.174852	0.755270
7	7	0	-0.530834	-1.139519	0.089216
8	6	0	-1.817176	-1.242013	-0.400547
9	8	0	-2.384719	-2.091017	-1.055338
10	6	0	0.269073	1.220711	0.327212
11	6	0	1.621776	0.912690	0.548721
12	6	0	2.636389	1.812341	0.248952
13	6	0	2.331590	3.068774	-0.293416
14	6	0	0.987436	3.379594	-0.518542
15	6	0	-0.030606	2.472616	-0.213147
16	8	0	1.974530	-0.279885	1.179096
17	6	0	1.842333	-1.487379	0.500825
18	6	0	2.972931	-2.295192	0.417884
19	6	0	2.902380	-3.549970	-0.187207
20	6	0	1.689388	-3.992855	-0.717206
21	6	0	0.549352	-3.197131	-0.632497
22	6	0	0.611181	-1.939369	-0.011690
23	6	0	3.434042	4.048329	-0.621470
24	1	0	0.726502	4.347166	-0.940155
25	1	0	3.663958	1.523114	0.451216
26	1	0	-1.063970	2.728914	-0.407303
27	1	0	-0.683428	0.059343	1.847117
28	1	0	-0.400369	-3.528419	-1.036020
29	1	0	1.624212	-4.964930	-1.197493
30	1	0	3.791091	-4.171165	-0.248403
31	1	0	3.900442	-1.917926	0.837040
32	1	0	-3.372930	-0.928029	1.799905
33	1	0	-3.189677	0.821297	2.044623
34	1	0	-4.868099	-0.577630	-0.112828
35	1	0	-5.428779	0.688092	1.003170
36	1	0	-4.489405	1.332297	-1.538380
37	1	0	-4.143648	2.396149	-0.153327
38	1	0	3.031211	4.975339	-1.040813
39	1	0	4.015525	4.309323	0.271566
40	1	0	4.137441	3.628599	-1.351105

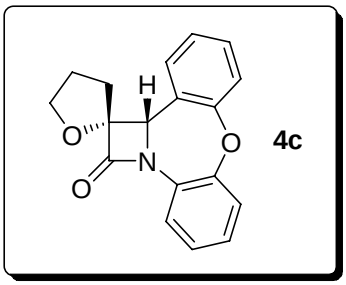


4b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.158707	-3.072861	-1.052765
2	6	0	-0.318885	-2.071861	-0.386285
3	6	0	-1.529289	-1.380717	0.298773
4	6	0	-2.247962	-2.224758	1.357113
5	1	0	-1.585636	-2.944997	1.845760
6	1	0	-2.673517	-1.569647	2.128094
7	1	0	-4.047827	-2.085703	-1.425205
8	1	0	-2.942267	-3.724386	-0.042853
9	1	0	-4.202503	-3.228543	1.110088
10	6	0	-3.726253	-1.739359	-0.438335
11	6	0	-3.353120	-2.877763	0.516549
12	1	0	-4.514050	-1.098115	-0.019236
13	6	0	-0.488169	-0.307982	0.789838
14	1	0	-0.343068	-0.370887	1.877249
15	6	0	-0.507600	1.144651	0.381609
16	6	0	-1.616745	1.836339	-0.115148
17	1	0	-2.536961	1.290404	-0.282665
18	6	0	-1.555485	3.203191	-0.414901
19	6	0	-2.764303	3.931945	-0.954806
20	1	0	-2.562247	4.368513	-1.940969
21	1	0	-3.621080	3.259253	-1.059940
22	1	0	-3.065749	4.755791	-0.295475
23	6	0	-0.347499	3.880199	-0.204103
24	1	0	-0.278201	4.942197	-0.429260
25	6	0	0.771206	3.212545	0.290103
26	1	0	1.709283	3.729895	0.465033
27	6	0	0.685806	1.853765	0.577351
28	8	0	1.787051	1.235268	1.167708
29	6	0	2.510505	0.283916	0.456169
30	6	0	3.882112	0.488139	0.335481
31	1	0	4.300694	1.397929	0.754256
32	6	0	4.683663	-0.456272	-0.305808

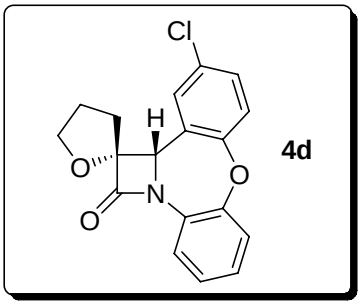
33	1	0	5.752380	-0.285772	-0.396389
34	6	0	4.102058	-1.610036	-0.833924
35	1	0	4.715017	-2.348727	-1.342302
36	6	0	2.732049	-1.829676	-0.711439
37	1	0	2.266514	-2.722146	-1.113098
38	6	0	1.922742	-0.889290	-0.054414
39	7	0	0.548498	-1.106954	0.084025
40	8	0	-2.530750	-0.949685	-0.605467



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.160492	-0.236233	-0.528679
2	8	0	-2.772669	0.116929	-0.701866
3	6	0	-1.974597	-0.548863	0.260309
4	6	0	-2.940104	-1.044300	1.342644
5	6	0	-4.184756	-1.366854	0.504685
6	6	0	-0.649881	0.166619	0.718907
7	6	0	-0.196765	1.514629	0.213643
8	6	0	1.161147	1.818644	0.404738
9	6	0	1.694118	3.048247	0.031112
10	6	0	0.862345	4.005268	-0.552130
11	6	0	-0.488392	3.722522	-0.752471
12	6	0	-1.015020	2.486021	-0.371147
13	8	0	1.992698	0.924541	1.076601
14	6	0	2.382415	-0.259350	0.458176
15	6	0	1.455944	-1.216753	0.003629
16	6	0	1.928601	-2.413670	-0.557423
17	6	0	3.297978	-2.654717	-0.639929
18	6	0	4.212226	-1.711955	-0.166849
19	6	0	3.748342	-0.514767	0.378281
20	1	0	-1.138817	4.464075	-1.207710
21	7	0	0.083300	-0.970842	0.103446
22	6	0	-1.041647	-1.636436	-0.339448
23	8	0	-1.199900	-2.679322	-0.938543

24	1	0	2.747507	3.240028	0.208845
25	1	0	1.272057	4.967052	-0.848170
26	1	0	-2.060412	2.260774	-0.537139
27	1	0	-0.546459	0.141117	1.812516
28	1	0	1.206304	-3.137160	-0.917046
29	1	0	3.648010	-3.587040	-1.073569
30	1	0	5.280072	-1.900529	-0.226262
31	1	0	4.431354	0.241703	0.751808
32	1	0	-2.550653	-1.902641	1.897373
33	1	0	-3.144116	-0.235757	2.056232
34	1	0	-4.058860	-2.336172	0.011692
35	1	0	-5.109683	-1.387506	1.088461
36	1	0	-4.563226	-0.527380	-1.503476
37	1	0	-4.705984	0.649817	-0.175502

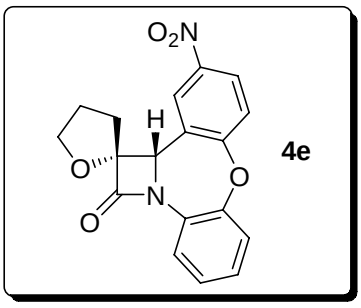


4d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	4.247211	-2.195816	-0.776700
2	8	0	-1.297410	-1.766589	1.213978
3	8	0	1.647970	2.072778	-0.541503
4	8	0	-1.406491	2.894076	-1.142625
5	7	0	-1.203606	0.856055	0.065255
6	6	0	-0.019527	-1.839799	0.672092
7	6	0	0.522284	-3.099971	0.439138
8	6	0	1.838333	-3.218076	-0.007208
9	6	0	2.585292	-2.060739	-0.212305
10	6	0	2.050792	-0.793549	0.020575
11	6	0	0.734255	-0.671817	0.471580
12	6	0	0.050385	0.626693	0.825458
13	6	0	-2.328867	0.040793	-0.091556
14	6	0	-3.449915	0.499673	-0.801189
15	6	0	-4.570791	-0.315099	-0.941423
16	6	0	-4.592362	-1.592832	-0.379713

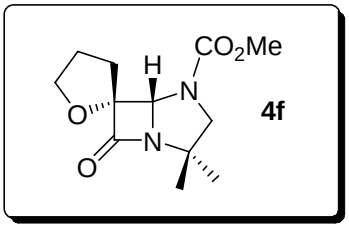
17	6	0	-3.475778	-2.059854	0.313509
18	6	0	-2.347257	-1.257474	0.451797
19	6	0	-0.840193	2.094205	-0.429241
20	6	0	0.522424	2.039032	0.315732
21	6	0	0.744963	3.142400	1.356544
22	6	0	1.497092	4.190294	0.524525
23	6	0	2.378679	3.304506	-0.360237
24	1	0	-0.088908	-3.978610	0.617584
25	1	0	2.274944	-4.193228	-0.193609
26	1	0	2.641674	0.093414	-0.160754
27	1	0	-0.145612	0.639176	1.906441
28	1	0	-3.419621	1.494874	-1.229154
29	1	0	-5.431357	0.055831	-1.490495
30	1	0	-5.467580	-2.227056	-0.484248
31	1	0	-3.456846	-3.049251	0.759557
32	1	0	-0.189098	3.512926	1.788274
33	1	0	1.373959	2.761129	2.171071
34	1	0	0.788705	4.756790	-0.088513
35	1	0	2.075815	4.892879	1.131187
36	1	0	2.575971	3.730333	-1.348303
37	1	0	3.339216	3.074831	0.120816



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.090493	2.328928	-0.551058
2	6	0	1.641439	3.654081	-0.383416
3	1	0	2.633564	3.564191	0.078360
4	1	0	1.757993	4.099098	-1.375587
5	6	0	0.654895	4.407615	0.514029
6	1	0	-0.132106	4.870908	-0.089843
7	1	0	1.137176	5.183909	1.114953
8	6	0	0.064635	3.267236	1.354955
9	1	0	0.746023	2.984686	2.167456

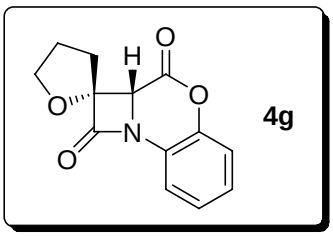
10	1	0	-0.910090	3.503517	1.791132
11	6	0	-0.004685	2.137072	0.322449
12	6	0	-1.363066	1.974223	-0.414717
13	8	0	-2.057235	2.673163	-1.119628
14	7	0	-1.514051	0.686373	0.067470
15	6	0	-0.248523	0.668767	0.838718
16	1	0	-0.452878	0.655104	1.918489
17	6	0	0.652760	-0.492637	0.499613
18	6	0	1.986262	-0.378207	0.111238
19	1	0	2.435540	0.592264	-0.038376
20	6	0	2.737566	-1.532757	-0.103561
21	7	0	4.144252	-1.394827	-0.506549
22	8	0	4.602032	-0.257235	-0.614560
23	8	0	4.784159	-2.427415	-0.708726
24	6	0	2.205381	-2.809868	0.058055
25	1	0	2.826746	-3.678401	-0.120940
26	6	0	0.876458	-2.928842	0.449457
27	1	0	0.418231	-3.900361	0.599889
28	6	0	0.111444	-1.781467	0.664967
29	8	0	-1.166409	-1.952334	1.160878
30	6	0	-2.292216	-1.593982	0.416040
31	6	0	-3.274716	-2.568573	0.269897
32	1	0	-3.089008	-3.550083	0.694320
33	6	0	-4.459133	-2.277620	-0.405874
34	1	0	-5.219198	-3.044824	-0.518074
35	6	0	-4.652292	-1.002636	-0.940643
36	1	0	-5.566953	-0.766984	-1.476656
37	6	0	-3.679391	-0.018068	-0.789568
38	1	0	-3.817000	0.976768	-1.196617
39	6	0	-2.490779	-0.299583	-0.096676



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.133649	-1.564267	0.083523
2	6	0	1.363430	-1.544996	-0.338411

3	7	0	1.652180	-0.456872	0.513269
4	6	0	0.238986	-0.249180	0.869778
5	8	0	2.048885	-2.172274	-1.105911
6	6	0	2.279582	0.832298	0.120588
7	6	0	1.052984	1.576157	-0.494486
8	7	0	-0.084763	1.021845	0.247139
9	6	0	-1.369989	1.467025	0.231040
10	8	0	-1.486548	2.609434	-0.494366
11	6	0	-2.812932	3.151182	-0.546045
12	8	0	-2.296928	0.924099	0.814945
13	6	0	3.416901	0.640208	-0.882452
14	6	0	2.775888	1.544709	1.387545
15	6	0	-0.701004	-2.737549	0.877224
16	6	0	-2.210861	-2.550047	0.652367
17	6	0	-2.257069	-2.022020	-0.785967
18	8	0	-0.988241	-1.370161	-1.017600
19	1	0	0.008656	-0.241196	1.939716
20	1	0	0.966323	1.359611	-1.567526
21	1	0	1.106255	2.659777	-0.362003
22	1	0	-2.733941	4.052477	-1.155405
23	1	0	-3.171587	3.397423	0.456964
24	1	0	-3.503768	2.439179	-1.005437
25	1	0	3.803061	1.619348	-1.187158
26	1	0	3.087151	0.099599	-1.772215
27	1	0	4.237591	0.075143	-0.430224
28	1	0	3.215015	2.515572	1.131013
29	1	0	3.538365	0.939727	1.887714
30	1	0	1.957499	1.719344	2.094424
31	1	0	-0.406636	-2.721431	1.930993
32	1	0	-0.346997	-3.676611	0.435502
33	1	0	-2.602684	-1.792552	1.337581
34	1	0	-2.782996	-3.473625	0.782221
35	1	0	-3.051663	-1.287178	-0.941699
36	1	0	-2.362511	-2.829308	-1.522073

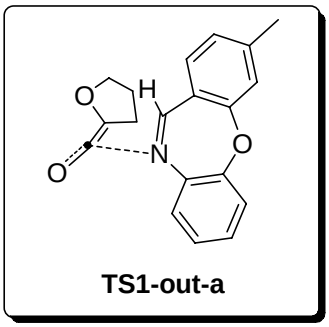


4g

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	1.750031	-0.419007	0.161284
2	6	0	0.654361	-1.489558	-0.153957
3	7	0	-0.330680	-0.719058	0.474168
4	6	0	0.564630	0.379236	0.846321
5	8	0	2.212765	0.149250	-1.038105
6	6	0	3.550627	0.630939	-0.826559
7	6	0	4.174715	-0.410347	0.102558
8	6	0	2.985568	-0.783998	1.013634
9	6	0	-1.695655	-0.510164	0.235194
10	6	0	-2.075792	0.815183	-0.022821
11	8	0	-1.143499	1.845607	-0.119520
12	6	0	0.171053	1.713005	0.254790
13	6	0	-2.656096	-1.523296	0.224117
14	6	0	-3.989517	-1.202193	-0.029299
15	6	0	-4.366053	0.125170	-0.251408
16	6	0	-3.408408	1.140735	-0.248267
17	8	0	0.916266	2.650208	0.146902
18	8	0	0.614018	-2.552314	-0.715275
19	1	0	0.668168	0.499975	1.933076
20	1	0	3.515946	1.627603	-0.366956
21	1	0	4.023112	0.702844	-1.808865
22	1	0	5.032325	-0.025359	0.662099
23	1	0	4.501561	-1.280219	-0.475936
24	1	0	2.984530	-1.842584	1.288583
25	1	0	2.994680	-0.197804	1.938338
26	1	0	-2.344308	-2.546317	0.406072
27	1	0	-4.736524	-1.990016	-0.043459
28	1	0	-5.406742	0.373298	-0.436743
29	1	0	-3.671174	2.175753	-0.440909

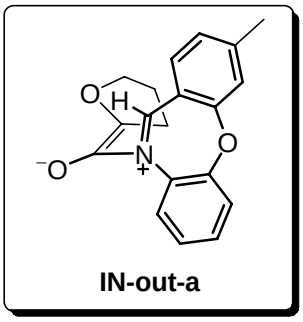


TS1-out-a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.674103	0.035647	0.628897
2	6	0	-2.360164	-0.280266	1.207455
3	8	0	-2.511787	0.114595	2.350299
4	6	0	-2.982695	-0.824974	0.141121
5	6	0	-2.512423	-1.198951	-1.251780
6	1	0	-1.971029	-0.398199	-1.768047
7	1	0	-1.855660	-2.081967	-1.257475
8	6	0	-3.845430	-1.537285	-1.953192
9	1	0	-4.282653	-0.634604	-2.394211
10	1	0	-3.740343	-2.291114	-2.740026
11	6	0	-4.705271	-2.003267	-0.774094
12	1	0	-4.478190	-3.052170	-0.516288
13	1	0	-5.782962	-1.909969	-0.938399
14	8	0	-4.351288	-1.135974	0.295950
15	6	0	0.138893	-0.960719	0.736335
16	1	0	-0.320200	-1.876457	1.108254
17	6	0	1.567233	-1.004710	0.463791
18	6	0	2.366473	-1.955424	1.125602
19	1	0	1.900820	-2.619700	1.849145
20	6	0	3.729666	-2.040799	0.879806
21	1	0	4.328538	-2.773735	1.413467
22	6	0	4.341356	-1.197759	-0.062992
23	6	0	5.814903	-1.320255	-0.363955
24	1	0	6.396769	-1.468109	0.552221
25	1	0	6.197160	-0.430331	-0.872599
26	1	0	6.010568	-2.182970	-1.014184
27	6	0	3.548359	-0.263203	-0.740169
28	1	0	3.978023	0.392172	-1.491559
29	6	0	2.184959	-0.169532	-0.483880
30	8	0	1.435849	0.686397	-1.268061
31	6	0	0.717058	1.677790	-0.602717
32	6	0	1.002545	3.000271	-0.928229
33	1	0	1.799029	3.195551	-1.639003
34	6	0	0.258050	4.032850	-0.360032
35	1	0	0.479748	5.063489	-0.621408
36	6	0	-0.769271	3.735451	0.538442
37	1	0	-1.350010	4.534314	0.989423
38	6	0	-1.061266	2.413899	0.861192
39	1	0	-1.844665	2.163339	1.567892
40	6	0	-0.321045	1.363680	0.291464

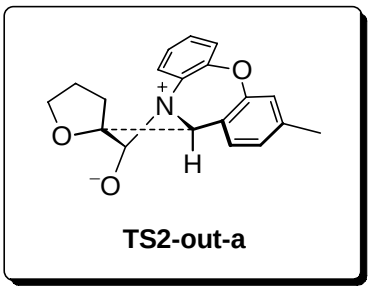


IN-out-a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.532811	-0.694057	0.355514
2	6	0	-1.803957	-1.447695	0.475602
3	6	0	-2.925835	-0.848802	-0.104416
4	8	0	-1.728356	-2.596079	0.952703
5	6	0	-3.146239	0.315255	-1.047060
6	1	0	-2.669649	1.247522	-0.746934
7	1	0	-2.769878	0.071513	-2.053539
8	6	0	-4.682572	0.419565	-1.071140
9	1	0	-5.073635	0.844584	-2.000130
10	1	0	-5.033487	1.034106	-0.234358
11	6	0	-5.089254	-1.039339	-0.863202
12	1	0	-6.052321	-1.177212	-0.364288
13	1	0	-5.102204	-1.594331	-1.812422
14	6	0	0.569595	-1.447473	0.460062
15	1	0	0.340722	-2.478201	0.709781
16	6	0	1.920583	-1.039089	0.231875
17	6	0	2.978474	-1.854655	0.703009
18	1	0	2.729772	-2.733348	1.291993
19	6	0	4.303247	-1.556401	0.427905
20	1	0	5.087892	-2.204907	0.809354
21	6	0	4.648309	-0.434839	-0.346453
22	6	0	6.091522	-0.098505	-0.628862
23	1	0	6.538479	0.460913	0.204467
24	1	0	6.693348	-1.003157	-0.768346
25	1	0	6.191971	0.518997	-1.527186
26	6	0	3.612795	0.372231	-0.836079
27	1	0	3.826938	1.232676	-1.463418
28	6	0	2.286138	0.077425	-0.557344
29	8	0	1.310541	0.861135	-1.164588
30	6	0	0.446908	1.481384	-0.275377
31	6	0	0.491534	2.869189	-0.162139
32	1	0	1.203938	3.412638	-0.774420

33	6	0	-0.367015	3.523611	0.719675
34	1	0	-0.335227	4.606180	0.801545
35	6	0	-1.246750	2.780430	1.509920
36	1	0	-1.897317	3.278461	2.222618
37	6	0	-1.289249	1.392310	1.397294
38	1	0	-1.965258	0.805172	2.007649
39	6	0	-0.469946	0.731451	0.470093
40	8	0	-4.076451	-1.594996	-0.014507

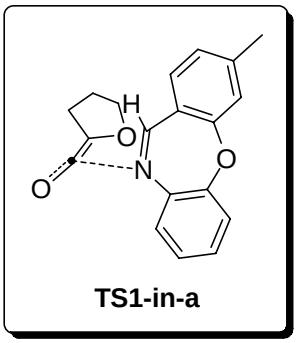


TS2-out-a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.409547	-1.230217	-0.212310
2	6	0	0.096732	-0.504161	-1.178746
3	1	0	0.479524	-1.080659	-2.009201
4	7	0	0.920277	0.490540	-0.719916
5	6	0	2.312416	0.104634	-0.723781
6	8	0	3.237293	0.841840	-1.157553
7	8	0	3.638943	-1.848385	-0.365941
8	6	0	3.871643	-2.816025	0.743137
9	1	0	4.906485	-2.682435	1.060107
10	1	0	3.735944	-3.824064	0.337835
11	6	0	2.819338	-2.447645	1.797121
12	1	0	3.200579	-1.663586	2.460151
13	1	0	2.520773	-3.303264	2.408932
14	6	0	1.655665	-1.899155	0.924174
15	1	0	0.995389	-1.209757	1.453785
16	1	0	1.046105	-2.742466	0.573256
17	6	0	-1.257895	-0.740086	-0.780442
18	6	0	-2.026439	-1.696249	-1.496245
19	1	0	-1.568223	-2.193965	-2.345847
20	6	0	-3.328656	-2.011889	-1.129429
21	1	0	-3.881519	-2.753274	-1.697976
22	6	0	-3.941718	-1.385422	-0.025747

23	6	0	-5.367413	-1.701312	0.359488
24	1	0	-6.074263	-1.033681	-0.152861
25	1	0	-5.528602	-1.579621	1.435713
26	1	0	-5.636596	-2.727574	0.088718
27	6	0	-3.196832	-0.434862	0.692526
28	1	0	-3.619078	0.067174	1.555984
29	6	0	-1.894569	-0.119426	0.323666
30	8	0	-1.204574	0.780687	1.161686
31	6	0	-0.567627	1.920356	0.609533
32	6	0	-0.976044	3.172669	1.061201
33	1	0	-1.801978	3.229391	1.760263
34	6	0	-0.297017	4.316877	0.627828
35	1	0	-0.606507	5.293649	0.983929
36	6	0	0.781665	4.194813	-0.255327
37	1	0	1.315097	5.078273	-0.589017
38	6	0	1.182497	2.937164	-0.718287
39	1	0	2.027024	2.815683	-1.383091
40	6	0	0.503810	1.787146	-0.286158

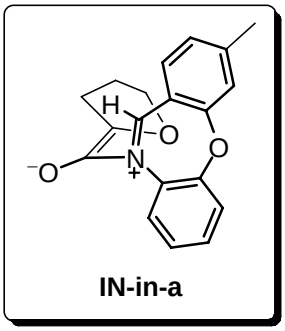


TS1-in-a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.686926	0.084983	0.637517
2	6	0	-2.466615	-0.221667	1.229678
3	8	0	-2.622833	0.197903	2.359210
4	6	0	-3.049203	-0.848573	0.198083
5	8	0	-2.394561	-1.178864	-1.005219
6	6	0	-3.414030	-1.517003	-1.945119
7	1	0	-3.783854	-0.609278	-2.449763
8	1	0	-2.967931	-2.177539	-2.694527
9	6	0	-4.525281	-2.165006	-1.111691
10	1	0	-4.259447	-3.203386	-0.883423
11	1	0	-5.497350	-2.160499	-1.614870

12	6	0	-4.493716	-1.307050	0.171664
13	1	0	-4.781390	-1.873383	1.064447
14	1	0	-5.191486	-0.461141	0.089947
15	6	0	0.104099	-0.924051	0.734391
16	1	0	-0.367370	-1.838685	1.093469
17	6	0	1.537102	-0.992896	0.472065
18	6	0	2.312092	-1.954760	1.141874
19	1	0	1.826981	-2.612885	1.858330
20	6	0	3.678511	-2.063846	0.912820
21	1	0	4.257925	-2.807616	1.452753
22	6	0	4.314895	-1.231887	-0.020158
23	6	0	5.788430	-1.375283	-0.312955
24	1	0	6.319290	-1.838195	0.524604
25	1	0	5.952209	-2.007180	-1.195909
26	1	0	6.252235	-0.404893	-0.518652
27	6	0	3.544738	-0.282154	-0.705165
28	1	0	3.994014	0.368113	-1.449855
29	6	0	2.180658	-0.166470	-0.466474
30	8	0	1.459738	0.704382	-1.259712
31	6	0	0.731518	1.697927	-0.612034
32	6	0	1.022412	3.015595	-0.951942
33	1	0	1.827751	3.198556	-1.656071
34	6	0	0.274926	4.059378	-0.407850
35	1	0	0.502904	5.085289	-0.682481
36	6	0	-0.762707	3.778095	0.482628
37	1	0	-1.346879	4.584612	0.915512
38	6	0	-1.060841	2.460506	0.817846
39	1	0	-1.854994	2.224184	1.517144
40	6	0	-0.319135	1.397759	0.274420

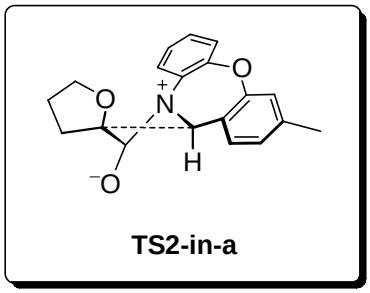


IN-in-a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.533268	-0.705285	0.359022
2	6	0	-1.788317	-1.486544	0.439788
3	8	0	-1.686103	-2.673633	0.835870
4	6	0	-2.947897	-0.921074	-0.067077
5	8	0	-3.057940	0.311681	-0.668857
6	6	0	-4.446702	0.552649	-0.959406
7	1	0	-4.486920	1.192107	-1.844580
8	1	0	-4.902041	1.088151	-0.113250
9	6	0	-5.062268	-0.838236	-1.141851
10	1	0	-4.893604	-1.190660	-2.165252
11	1	0	-6.138835	-0.849236	-0.948523
12	6	0	-4.244715	-1.679171	-0.141672
13	1	0	-4.735781	-1.724567	0.842057
14	1	0	-4.083017	-2.714990	-0.455135
15	6	0	0.575160	-1.442243	0.465288
16	1	0	0.354433	-2.477526	0.706377
17	6	0	1.925680	-1.022092	0.244750
18	6	0	2.985653	-1.823487	0.734751
19	1	0	2.739409	-2.693641	1.337361
20	6	0	4.309143	-1.519286	0.463897
21	1	0	5.097012	-2.153627	0.862504
22	6	0	4.648693	-0.408634	-0.330253
23	6	0	6.091754	-0.090130	-0.634327
24	1	0	6.662668	0.084886	0.286269
25	1	0	6.183141	0.802355	-1.260415
26	1	0	6.579979	-0.920502	-1.159853
27	6	0	3.611603	0.384216	-0.835611
28	1	0	3.822992	1.238138	-1.472429
29	6	0	2.283804	0.085244	-0.558087
30	8	0	1.306706	0.851588	-1.174993
31	6	0	0.428753	1.472522	-0.295766
32	6	0	0.478392	2.860643	-0.183700
33	1	0	1.202031	3.399417	-0.786847
34	6	0	-0.386464	3.518892	0.686925
35	1	0	-0.350245	4.601265	0.770298
36	6	0	-1.282657	2.778875	1.462190
37	1	0	-1.944502	3.279628	2.162577
38	6	0	-1.329607	1.393341	1.347240
39	1	0	-2.018606	0.808841	1.946188
40	6	0	-0.492766	0.726159	0.443478

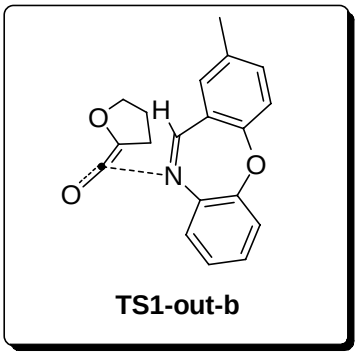


TS2-in-a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.392220	-1.178981	0.104065
2	6	0	-0.204283	-0.397711	1.172951
3	1	0	-0.585106	-0.844721	2.082926
4	7	0	-0.970100	0.598995	0.619098
5	6	0	-2.326083	0.187861	0.575326
6	8	0	-3.288097	0.842150	0.996667
7	6	0	-3.625516	-2.027680	0.293735
8	1	0	-4.506911	-1.398516	0.443596
9	1	0	-3.520788	-2.654762	1.191144
10	6	0	-3.664014	-2.883802	-0.987491
11	1	0	-4.265053	-2.390241	-1.758548
12	1	0	-4.064414	-3.889366	-0.831579
13	6	0	-2.187913	-2.893017	-1.395723
14	1	0	-1.625035	-3.680504	-0.874104
15	1	0	-2.007040	-2.979388	-2.469467
16	8	0	-1.683792	-1.609080	-0.985711
17	6	0	1.137643	-0.701668	0.791007
18	6	0	1.848246	-1.692539	1.513296
19	1	0	1.348919	-2.169902	2.353217
20	6	0	3.130034	-2.080570	1.164039
21	1	0	3.632870	-2.855444	1.737396
22	6	0	3.786724	-1.486930	0.071694
23	6	0	5.194644	-1.882953	-0.299171
24	1	0	5.932631	-1.351834	0.317618
25	1	0	5.415287	-1.648911	-1.345522
26	1	0	5.361193	-2.955181	-0.147434
27	6	0	3.108932	-0.491269	-0.639910
28	1	0	3.577115	0.001769	-1.486988
29	6	0	1.820132	-0.097075	-0.294495
30	8	0	1.247494	0.857768	-1.111767
31	6	0	0.630455	1.981993	-0.580728
32	6	0	1.101458	3.228612	-0.983516

33	1	0	1.975572	3.269176	-1.625666
34	6	0	0.430125	4.386199	-0.586625
35	1	0	0.795345	5.356893	-0.909729
36	6	0	-0.708693	4.291697	0.214469
37	1	0	-1.237219	5.189610	0.521459
38	6	0	-1.173500	3.044797	0.634010
39	1	0	-2.060035	2.942543	1.248405
40	6	0	-0.503083	1.882885	0.237414

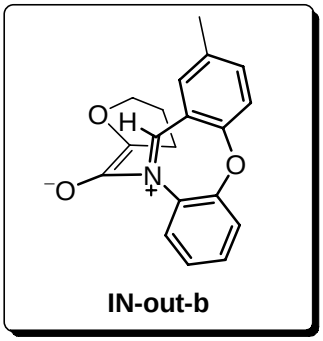


TS1-out-b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.558722	-0.013633	0.575991
2	6	0	-2.145363	-0.561627	1.246763
3	8	0	-2.217084	-0.329011	2.441072
4	6	0	-2.820295	-1.028395	0.175553
5	8	0	-4.138954	-1.478648	0.404282
6	6	0	-4.538135	-2.212492	-0.746812
7	1	0	-5.630386	-2.179476	-0.802827
8	1	0	-4.222630	-3.266988	-0.664934
9	6	0	-3.826843	-1.523298	-1.915444
10	1	0	-4.361065	-0.604614	-2.182079
11	1	0	-3.749148	-2.151186	-2.808754
12	6	0	-2.457917	-1.182837	-1.288631
13	1	0	-2.015872	-0.285202	-1.735118
14	1	0	-1.752678	-2.008473	-1.468681
15	6	0	0.354172	-0.922194	0.505708
16	1	0	0.024118	-1.916892	0.804185
17	6	0	1.753150	-0.777567	0.124997
18	6	0	2.695224	-1.694126	0.627105
19	1	0	2.351357	-2.472443	1.304799
20	6	0	4.046374	-1.622368	0.289581
21	6	0	5.053226	-2.589770	0.865931

22	1	0	5.670725	-2.108026	1.634738
23	1	0	4.560728	-3.449260	1.330669
24	1	0	5.733031	-2.966818	0.093733
25	6	0	4.443715	-0.615330	-0.605069
26	1	0	5.487489	-0.547912	-0.902548
27	6	0	3.528670	0.292955	-1.134396
28	1	0	3.834002	1.053824	-1.845161
29	6	0	2.188071	0.212569	-0.771702
30	8	0	1.283831	1.046122	-1.403137
31	6	0	0.537561	1.885535	-0.578979
32	6	0	0.655921	3.257004	-0.782300
33	1	0	1.355623	3.608327	-1.533762
34	6	0	-0.128885	4.139519	-0.041659
35	1	0	-0.038359	5.209153	-0.207078
36	6	0	-1.027494	3.643656	0.906222
37	1	0	-1.637066	4.325620	1.491153
38	6	0	-1.153718	2.272643	1.106634
39	1	0	-1.834578	1.868022	1.847412
40	6	0	-0.371866	1.372801	0.362261

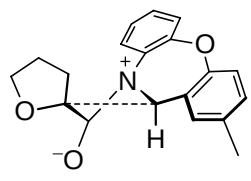


IN-out-b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.852729	-1.901794	0.081485
2	6	0	-4.969045	-1.446198	-0.694133
3	1	0	-5.879730	-1.702827	-0.146371
4	1	0	-4.974530	-1.978168	-1.656459
5	6	0	-4.740432	0.053639	-0.881836
6	1	0	-5.230488	0.452375	-1.774788
7	1	0	-5.108154	0.605520	-0.009368
8	6	0	-3.203164	0.123269	-0.946851
9	1	0	-2.815968	1.095684	-0.645154
10	1	0	-2.861940	-0.052011	-1.979684

11	6	0	-2.798576	-1.031466	-0.055109
12	6	0	-1.582298	-1.520463	0.431532
13	8	0	-1.352817	-2.668185	0.857660
14	7	0	-0.411946	-0.625958	0.267100
15	6	0	-0.501577	0.793082	0.434915
16	6	0	-1.333422	1.323848	1.432094
17	1	0	-1.901370	0.643031	2.055026
18	6	0	-1.440540	2.703063	1.598239
19	1	0	-2.099247	3.099121	2.365329
20	6	0	-0.698076	3.567956	0.791329
21	1	0	-0.783028	4.643694	0.914969
22	6	0	0.175249	3.046508	-0.162022
23	1	0	0.784619	3.688796	-0.789602
24	6	0	0.280736	1.667378	-0.328622
25	8	0	1.154728	1.179428	-1.287033
26	6	0	2.243565	0.488348	-0.764717
27	6	0	3.516793	0.932637	-1.094669
28	1	0	3.615443	1.832114	-1.694234
29	6	0	4.636155	0.210732	-0.681603
30	1	0	5.628192	0.564107	-0.951796
31	6	0	4.498461	-0.971350	0.067901
32	6	0	5.716985	-1.745552	0.514208
33	1	0	5.437942	-2.693245	0.984586
34	1	0	6.307887	-1.174777	1.241772
35	1	0	6.377999	-1.971954	-0.330883
36	6	0	3.214655	-1.403334	0.383100
37	1	0	3.081185	-2.321447	0.950298
38	6	0	2.053991	-0.689578	-0.006332
39	6	0	0.770416	-1.254414	0.276741
40	1	0	0.672096	-2.312532	0.494770

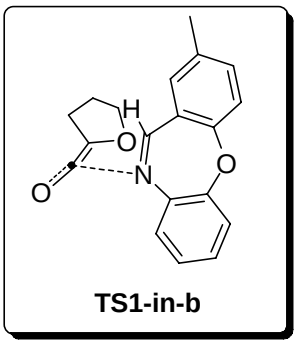


TS2-out-b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.076296	-1.568704	-0.234805
2	6	0	-0.169490	-0.497282	-1.011006
3	1	0	0.005163	-1.187026	-1.824710
4	7	0	0.861584	0.359813	-0.725154
5	6	0	2.154499	-0.270249	-0.838426
6	8	0	3.139270	0.258320	-1.418905
7	8	0	3.151622	-2.407353	-0.469325
8	6	0	3.344285	-3.334301	0.681985
9	1	0	4.417006	-3.371360	0.874269
10	1	0	2.988636	-4.322969	0.374227
11	6	0	2.505055	-2.719500	1.809609
12	1	0	3.092906	-1.980132	2.364065
13	1	0	2.137703	-3.469358	2.515431
14	6	0	1.358644	-2.021675	1.025125
15	1	0	0.575352	-2.759892	0.808205
16	1	0	0.894565	-1.194447	1.565601
17	6	0	-1.488420	-0.457195	-0.452481
18	6	0	-2.488663	-1.297114	-1.012750
19	1	0	-2.218442	-1.912234	-1.866924
20	6	0	-3.786395	-1.362287	-0.505913
21	6	0	-4.826047	-2.268225	-1.128436
22	1	0	-5.672664	-1.692142	-1.522686
23	1	0	-5.230850	-2.976150	-0.394649
24	1	0	-4.405593	-2.848451	-1.955342
25	6	0	-4.109065	-0.557767	0.606742
26	1	0	-5.111537	-0.590985	1.022482
27	6	0	-3.153582	0.285458	1.179471
28	1	0	-3.388172	0.904219	2.037637
29	6	0	-1.864915	0.337378	0.657275
30	8	0	-0.932467	1.145174	1.342086
31	6	0	-0.184545	2.116721	0.631616
32	6	0	-0.313936	3.448264	1.017758
33	1	0	-1.024555	3.697498	1.796819
34	6	0	0.491065	4.421625	0.415348
35	1	0	0.399420	5.458952	0.719052
36	6	0	1.414674	4.051714	-0.568775
37	1	0	2.045081	4.801937	-1.033675
38	6	0	1.534845	2.715285	-0.964350
39	1	0	2.257750	2.402186	-1.705503
40	6	0	0.728984	1.736609	-0.362832

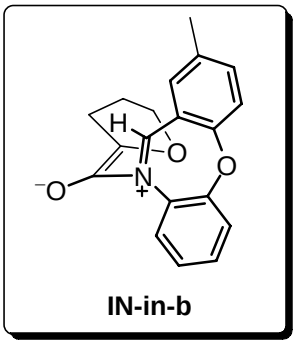


TS1-in-b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.569844	0.010785	0.600031
2	6	0	-2.223266	-0.551843	1.290300
3	8	0	-2.300420	-0.316659	2.481486
4	6	0	-2.857293	-1.087866	0.237068
5	6	0	-4.255326	-1.672310	0.271953
6	1	0	-5.020584	-0.895947	0.414648
7	1	0	-4.394611	-2.407679	1.072522
8	6	0	-4.368178	-2.301308	-1.134296
9	1	0	-5.386553	-2.290422	-1.535474
10	1	0	-4.015283	-3.338648	-1.117966
11	6	0	-3.394448	-1.436257	-1.943030
12	1	0	-3.872348	-0.490182	-2.246485
13	1	0	-2.988108	-1.925704	-2.833021
14	8	0	-2.306223	-1.177967	-1.056588
15	6	0	0.333407	-0.899936	0.516226
16	1	0	0.002745	-1.897657	0.803914
17	6	0	1.736263	-0.760853	0.135883
18	6	0	2.672065	-1.680688	0.641274
19	1	0	2.321405	-2.458611	1.316066
20	6	0	4.025468	-1.616798	0.309250
21	6	0	5.023927	-2.590663	0.889637
22	1	0	5.633780	-2.116860	1.669572
23	1	0	4.524344	-3.452903	1.341798
24	1	0	5.711888	-2.963313	0.122497
25	6	0	4.431780	-0.612023	-0.582903
26	1	0	5.476888	-0.549961	-0.877082
27	6	0	3.522865	0.301291	-1.113971
28	1	0	3.834259	1.061616	-1.822733
29	6	0	2.179839	0.227770	-0.757181
30	8	0	1.287530	1.069381	-1.393397
31	6	0	0.524057	1.901468	-0.580778

32	6	0	0.628694	3.271862	-0.797976
33	1	0	1.330274	3.621257	-1.548645
34	6	0	-0.169400	4.156516	-0.073546
35	1	0	-0.087821	5.224845	-0.252125
36	6	0	-1.068788	3.663780	0.873931
37	1	0	-1.689061	4.346288	1.447081
38	6	0	-1.182205	2.292920	1.086339
39	1	0	-1.865564	1.891961	1.826626
40	6	0	-0.388433	1.389667	0.359584

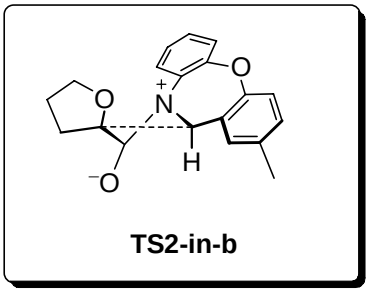


IN-in-b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.096990	0.124847	-0.558888
2	6	0	-4.519079	0.213666	-0.765512
3	1	0	-4.681271	0.867522	-1.625856
4	1	0	-4.980745	0.672231	0.121231
5	6	0	-4.985880	-1.232229	-0.960395
6	1	0	-6.039918	-1.370545	-0.702872
7	1	0	-4.845470	-1.533754	-2.004091
8	6	0	-4.018011	-2.004331	-0.042492
9	1	0	-4.437637	-2.136368	0.966152
10	1	0	-3.760133	-3.004337	-0.403961
11	6	0	-2.812297	-1.105967	-0.015544
12	6	0	-1.566586	-1.556169	0.395065
13	8	0	-1.312119	-2.739174	0.729605
14	7	0	-0.411537	-0.639705	0.269984
15	6	0	0.774243	-1.253320	0.278289
16	1	0	0.682938	-2.314546	0.487161
17	6	0	2.056685	-0.678384	0.000458
18	6	0	3.218868	-1.378767	0.405960
19	1	0	3.089231	-2.290362	0.984457
20	6	0	4.501281	-0.941405	0.091371

21	6	0	5.723783	-1.700618	0.552353
22	1	0	6.328420	-1.101395	1.244726
23	1	0	5.448660	-2.625815	1.067670
24	1	0	6.370698	-1.967184	-0.292136
25	6	0	4.632416	0.229727	-0.676050
26	1	0	5.623159	0.586531	-0.946838
27	6	0	3.510403	0.937109	-1.105850
28	1	0	3.605410	1.828374	-1.718036
29	6	0	2.238025	0.489758	-0.773617
30	8	0	1.147140	1.161551	-1.305773
31	6	0	0.262446	1.652502	-0.354687
32	6	0	-0.522144	0.784031	0.409280
33	6	0	-1.367639	1.322782	1.387644
34	1	0	-1.947115	0.645395	2.004459
35	6	0	-1.467937	2.700375	1.552785
36	1	0	-2.134560	3.100813	2.310785
37	6	0	-0.711715	3.560925	0.753252
38	1	0	-0.790885	4.637309	0.875655
39	6	0	0.163648	3.033093	-0.192549
40	1	0	0.782682	3.669623	-0.816509

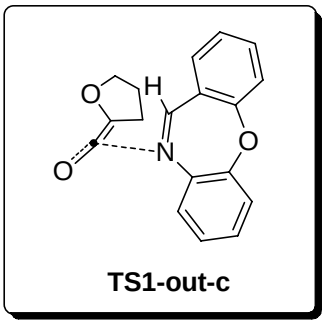


TS2-in-b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.830349	-1.804447	-0.135442
2	6	0	-0.115102	-0.399726	-1.022619
3	1	0	-0.016345	-0.992873	-1.923179
4	7	0	0.992080	0.316185	-0.637927
5	6	0	2.141136	-0.510217	-0.706074
6	8	0	3.200122	-0.222625	-1.277585
7	6	0	2.694204	-3.015368	-0.389249
8	1	0	2.279801	-3.610117	-1.216293
9	1	0	3.702472	-2.713806	-0.685176
10	6	0	2.624124	-3.783720	0.944958

11	1	0	3.445964	-3.482012	1.602892
12	1	0	2.659371	-4.870344	0.827905
13	6	0	1.288196	-3.294311	1.512411
14	1	0	1.231002	-3.270706	2.602903
15	1	0	0.440872	-3.876546	1.122667
16	8	0	1.169317	-1.934709	1.055094
17	6	0	1.009800	1.698406	-0.316805
18	6	0	1.956666	2.560879	-0.878748
19	1	0	2.678626	2.149556	-1.574071
20	6	0	1.968549	3.908474	-0.516928
21	1	0	2.710033	4.571813	-0.952825
22	6	0	1.031465	4.402617	0.391512
23	1	0	1.037205	5.452612	0.669899
24	6	0	0.085269	3.544178	0.953717
25	1	0	-0.640585	3.894406	1.680735
26	6	0	0.081332	2.195647	0.608081
27	8	0	-0.784744	1.355633	1.293368
28	6	0	-1.731144	0.606481	0.620748
29	6	0	-3.028364	0.666786	1.122775
30	1	0	-3.219275	1.316942	1.970750
31	6	0	-4.047898	-0.087945	0.548653
32	1	0	-5.053624	-0.025283	0.957226
33	6	0	-3.794704	-0.916382	-0.559540
34	6	0	-4.905915	-1.724096	-1.189273
35	1	0	-5.720857	-1.078474	-1.539387
36	1	0	-5.342218	-2.432155	-0.473597
37	1	0	-4.544859	-2.298692	-2.047899
38	6	0	-2.495857	-0.967591	-1.048813
39	1	0	-2.271373	-1.608711	-1.899016
40	6	0	-1.425160	-0.233879	-0.476875

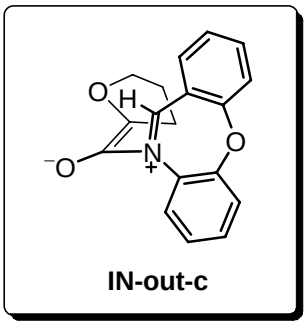


TS1-out-c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.341178	-0.022702	0.629401
2	6	0	-2.044721	-0.165849	1.239249
3	8	0	-2.125923	0.207914	2.395654
4	6	0	-2.745112	-0.604118	0.172436
5	8	0	-4.137766	-0.753099	0.350837
6	6	0	-4.626549	-1.502237	-0.755298
7	1	0	-5.683010	-1.250926	-0.889030
8	1	0	-4.545549	-2.584994	-0.557660
9	6	0	-3.729509	-1.097250	-1.928966
10	1	0	-4.043358	-0.120598	-2.313877
11	1	0	-3.743054	-1.815958	-2.754506
12	6	0	-2.352096	-0.984331	-1.241707
13	1	0	-1.706323	-0.250563	-1.736428
14	1	0	-1.833013	-1.953413	-1.294452
15	6	0	0.360024	-1.103476	0.688454
16	1	0	-0.184069	-1.974946	1.051755
17	6	0	1.770899	-1.291925	0.374101
18	6	0	2.478633	-2.332115	1.003375
19	1	0	1.960809	-2.955746	1.727526
20	6	0	3.820853	-2.557091	0.717472
21	1	0	4.357099	-3.357174	1.218041
22	6	0	4.468919	-1.757135	-0.228443
23	1	0	5.512980	-1.936635	-0.468601
24	6	0	3.780306	-0.733277	-0.880795
25	1	0	4.258592	-0.117968	-1.635605
26	6	0	2.440980	-0.504982	-0.580946
27	8	0	1.756066	0.435154	-1.326585
28	6	0	1.175984	1.486719	-0.619497
29	6	0	1.591618	2.777118	-0.932504
30	1	0	2.378278	2.901116	-1.669724
31	6	0	0.985015	3.870803	-0.316518
32	1	0	1.307742	4.877092	-0.567207
33	6	0	-0.034777	3.666319	0.616148
34	1	0	-0.507758	4.513227	1.103800
35	6	0	-0.457376	2.377431	0.925882
36	1	0	-1.238069	2.196828	1.656592
37	6	0	0.143232	1.267034	0.308274

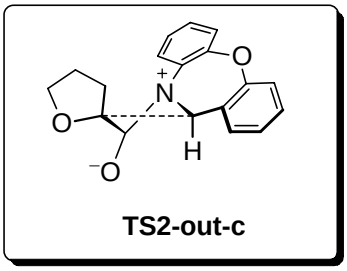


IN-out-c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.464482	-1.445226	0.483833
2	8	0	-1.380523	-2.596887	0.950685
3	6	0	-2.603444	-0.840025	-0.058461
4	8	0	-3.749770	-1.585251	0.061645
5	6	0	-4.788502	-1.025250	-0.753391
6	6	0	-4.387440	0.434255	-0.966667
7	6	0	-2.850976	0.330364	-0.986648
8	1	0	-4.829860	-1.576821	-1.703571
9	1	0	-5.735445	-1.165576	-0.225403
10	1	0	-4.714484	1.045436	-0.117891
11	1	0	-4.804554	0.862992	-1.882442
12	1	0	-2.366415	1.260694	-0.693731
13	1	0	-2.502158	0.092859	-2.004363
14	6	0	0.906111	-1.454383	0.394560
15	7	0	-0.197005	-0.697004	0.326903
16	6	0	-0.126298	0.728234	0.442399
17	6	0	-0.909964	1.389900	1.399074
18	6	0	-0.858874	2.777800	1.511553
19	6	0	-0.005362	3.518992	0.691195
20	6	0	0.819214	2.863154	-0.221578
21	6	0	0.765971	1.475730	-0.334426
22	8	0	1.594907	0.851212	-1.252803
23	6	0	2.590746	0.067561	-0.679027
24	6	0	2.251463	-1.050283	0.122300
25	6	0	3.909221	0.362235	-0.997763
26	6	0	4.938743	-0.457679	-0.530055
27	6	0	3.317324	-1.870265	0.568133
28	6	0	4.636927	-1.576086	0.255977
29	1	0	0.682962	-2.484851	0.649719
30	1	0	-1.565036	0.804242	2.033305
31	1	0	-1.481742	3.277153	2.247658
32	1	0	0.032998	4.601304	0.773355

33	1	0	1.511149	3.405318	-0.857976
34	1	0	4.111109	1.221913	-1.628802
35	1	0	5.969030	-0.228046	-0.785356
36	1	0	3.078834	-2.744254	1.168114
37	1	0	5.433472	-2.220098	0.616818

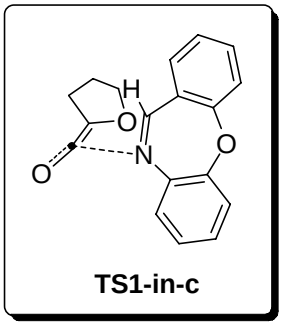


TS2-out-c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.042500	-0.668939	-1.142728
2	6	0	2.485374	-0.298145	-0.235658
3	6	0	1.808802	0.834300	-0.790631
4	8	0	2.315721	1.875084	-1.288260
5	7	0	0.384013	0.592079	-0.735606
6	1	0	0.623930	-1.068227	-1.961829
7	8	0	3.858819	-0.320104	-0.402554
8	6	0	4.502797	-1.058953	0.719938
9	1	0	5.379029	-0.479031	1.011439
10	1	0	4.815647	-2.035719	0.336851
11	6	0	3.406605	-1.157610	1.788733
12	1	0	3.414392	-0.267902	2.427476
13	1	0	3.518059	-2.040610	2.423750
14	6	0	2.110878	-1.196063	0.930603
15	1	0	1.926136	-2.230374	0.611238
16	1	0	1.221848	-0.848510	1.460424
17	6	0	-0.525254	1.606717	-0.301497
18	6	0	-0.408746	2.921961	-0.777194
19	1	0	0.384100	3.146697	-1.477724
20	6	0	-1.284875	3.907886	-0.311185
21	1	0	-1.184989	4.923438	-0.678611
22	6	0	-2.282457	3.591738	0.617973
23	1	0	-2.961135	4.358411	0.976060
24	6	0	-2.401629	2.281408	1.094553
25	1	0	-3.149523	2.006846	1.828901
26	6	0	-1.521146	1.303852	0.638924

27	8	0	-1.598610	0.016435	1.227755
28	6	0	-1.885670	-1.106465	0.424134
29	6	0	-2.934182	-1.921150	0.839236
30	1	0	-3.505500	-1.622756	1.710229
31	6	0	-3.222010	-3.100297	0.142262
32	1	0	-4.039988	-3.733751	0.467635
33	6	0	-2.451043	-3.455450	-0.975520
34	1	0	-2.669492	-4.367520	-1.520372
35	6	0	-1.402361	-2.638311	-1.384533
36	1	0	-0.801784	-2.914136	-2.246211
37	6	0	-1.081960	-1.436933	-0.696666

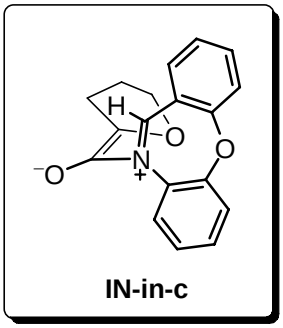


TS1-in-c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.358672	0.032372	0.643523
2	6	0	-2.119184	-0.062898	1.252699
3	8	0	-2.213617	0.351136	2.393981
4	6	0	-2.803723	-0.594485	0.228373
5	8	0	-2.223977	-0.983660	-0.995858
6	6	0	-3.297375	-1.118012	-1.926953
7	1	0	-3.532477	-0.141486	-2.381467
8	1	0	-2.969041	-1.802238	-2.714873
9	6	0	-4.480328	-1.629261	-1.096716
10	1	0	-4.373195	-2.706206	-0.924504
11	1	0	-5.448665	-1.452116	-1.575340
12	6	0	-4.297230	-0.851987	0.225642
13	1	0	-4.873660	0.084095	0.211702
14	1	0	-4.637290	-1.422151	1.097612
15	6	0	0.307183	-1.065860	0.700413
16	1	0	-0.261755	-1.925109	1.054181
17	6	0	1.717334	-1.295525	0.398432
18	6	0	2.389227	-2.348936	1.043059
19	1	0	1.845734	-2.953201	1.764892

20	6	0	3.727965	-2.614802	0.774233
21	1	0	4.235282	-3.426291	1.286621
22	6	0	4.408376	-1.841380	-0.170391
23	1	0	5.449335	-2.052166	-0.398567
24	6	0	3.755462	-0.803484	-0.836779
25	1	0	4.258491	-0.206916	-1.590581
26	6	0	2.419508	-0.534826	-0.553765
27	8	0	1.775028	0.419943	-1.314827
28	6	0	1.198635	1.486078	-0.630498
29	6	0	1.635043	2.764220	-0.964610
30	1	0	2.430060	2.860981	-1.696970
31	6	0	1.040489	3.880405	-0.377236
32	1	0	1.381094	4.876030	-0.646545
33	6	0	0.010484	3.710903	0.549884
34	1	0	-0.454180	4.574462	1.016115
35	6	0	-0.433755	2.433709	0.879461
36	1	0	-1.225007	2.281144	1.605067
37	6	0	0.152974	1.300343	0.291690

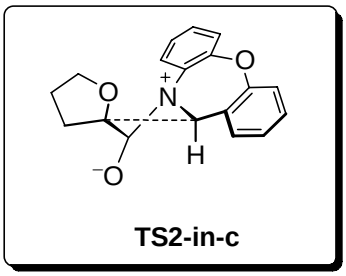


IN-in-c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.449820	-1.485255	0.441961
2	8	0	-1.340971	-2.678068	0.817903
3	6	0	-2.625749	-0.911407	-0.019247
4	8	0	-2.754772	0.326534	-0.601979
5	6	0	-4.152118	0.570495	-0.850321
6	6	0	-4.774200	-0.818621	-1.023051
7	6	0	-3.924684	-1.668157	-0.057486
8	1	0	-4.580270	1.101475	0.012408
9	1	0	-4.217163	1.215425	-1.729915
10	1	0	-4.640440	-1.163268	-2.054182
11	1	0	-5.843625	-0.830376	-0.793793
12	1	0	-3.773509	-2.701356	-0.384233

13	1	0	-4.381952	-1.721289	0.941964
14	6	0	0.912100	-1.451203	0.393045
15	7	0	-0.196932	-0.709748	0.325370
16	6	0	-0.148555	0.721519	0.413464
17	6	0	-0.949214	1.389780	1.348360
18	6	0	-0.893505	2.775123	1.462379
19	6	0	-0.024481	3.512984	0.654728
20	6	0	0.805859	2.853091	-0.247738
21	6	0	0.747694	1.465289	-0.358528
22	8	0	1.591378	0.839356	-1.266822
23	6	0	2.590087	0.076347	-0.680437
24	6	0	2.258026	-1.033731	0.133371
25	6	0	3.909049	0.376696	-0.995101
26	6	0	4.941428	-0.427345	-0.507403
27	6	0	3.325555	-1.838849	0.598557
28	6	0	4.645258	-1.536681	0.293290
29	1	0	0.696490	-2.486868	0.636125
30	1	0	-1.617081	0.807137	1.972593
31	1	0	-1.527001	3.277441	2.187395
32	1	0	0.018142	4.595134	0.737694
33	1	0	1.508625	3.390298	-0.876404
34	1	0	4.108325	1.228927	-1.636874
35	1	0	5.971598	-0.192194	-0.758539
36	1	0	3.089699	-2.707565	1.207228
37	1	0	5.445231	-2.167701	0.669064

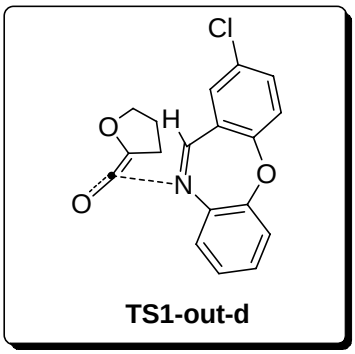


TS2-in-c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.256186	0.461154	-1.145410
2	6	0	-2.431082	-0.424630	-0.129449
3	6	0	-1.471448	-1.395363	-0.615262
4	8	0	-1.757691	-2.511646	-1.065023
5	7	0	-0.182490	-0.808788	-0.626974
6	6	0	1.011033	-1.477372	-0.250054

7	1	0	0.556728	-3.270062	-1.322304
8	6	0	1.280770	-2.779708	-0.682648
9	1	0	2.649208	-4.434265	-0.600724
10	6	0	2.447660	-3.421021	-0.265328
11	6	0	3.352322	-2.764845	0.570556
12	1	0	4.263046	-3.262085	0.891961
13	1	0	3.758368	-0.938576	1.673215
14	6	0	3.085167	-1.465276	1.004338
15	6	0	1.914088	-0.828701	0.602977
16	8	0	1.622457	0.405670	1.166592
17	6	0	1.443142	1.525259	0.377623
18	6	0	2.153278	2.659082	0.762240
19	1	0	2.819605	2.578711	1.615216
20	6	0	2.006112	3.858543	0.065952
21	1	0	2.566283	4.735373	0.377523
22	1	0	1.032936	4.847988	-1.592215
23	6	0	1.147791	3.920693	-1.038483
24	6	0	0.439587	2.792587	-1.421776
25	1	0	-0.236462	2.837962	-2.272329
26	6	0	0.547388	1.564453	-0.721889
27	1	0	-0.829343	0.576135	-2.056979
28	8	0	-2.197199	0.336569	0.982079
29	6	0	-3.432635	0.939575	1.410599
30	1	0	-3.360774	1.080565	2.491330
31	1	0	-3.534615	1.922221	0.928281
32	6	0	-3.914757	-0.598729	-0.341692
33	1	0	-4.155320	-1.646982	-0.536871
34	1	0	-4.241877	-0.022990	-1.219840
35	6	0	-4.523929	-0.034184	0.956870
36	1	0	-4.649786	-0.831384	1.697112
37	1	0	-5.490921	0.455069	0.811270

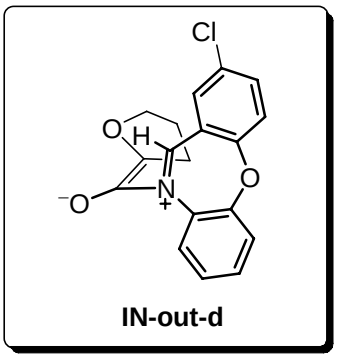


TS1-out-d

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-0.811974	0.048414	0.587225
2	6	0	-2.347943	-0.708807	1.255008
3	8	0	-2.492840	-0.433479	2.429857
4	6	0	-2.905394	-1.310670	0.183344
5	8	0	-4.154919	-1.929300	0.398791
6	6	0	-4.432888	-2.734986	-0.741445
7	1	0	-5.519226	-2.835977	-0.821906
8	1	0	-3.994371	-3.740171	-0.621067
9	6	0	-3.780481	-1.994438	-1.912188
10	1	0	-4.414711	-1.155408	-2.219150
11	1	0	-3.602060	-2.631732	-2.783982
12	6	0	-2.480772	-1.473565	-1.263245
13	1	0	-2.130599	-0.547309	-1.730928
14	1	0	-1.681888	-2.219491	-1.390914
15	6	0	0.197492	-0.746668	0.482013
16	1	0	-0.001963	-1.775661	0.779462
17	6	0	1.558504	-0.436292	0.054170
18	6	0	2.612946	-1.241780	0.518042
19	1	0	2.406190	-2.060360	1.200085
20	6	0	3.916490	-0.983733	0.111355
21	17	0	5.225145	-1.987025	0.708008
22	6	0	4.194715	0.056566	-0.778658
23	1	0	5.214981	0.237993	-1.098873
24	6	0	3.152082	0.848085	-1.258177
25	1	0	3.338783	1.646920	-1.967925
26	6	0	1.844463	0.604143	-0.848479
27	8	0	0.829166	1.328626	-1.437496
28	6	0	0.015938	2.070889	-0.581066
29	6	0	-0.032552	3.447123	-0.775887
30	1	0	0.598367	3.882683	-1.543924
31	6	0	-0.893376	4.227091	-0.004608
32	1	0	-0.933137	5.300936	-0.161972
33	6	0	-1.700714	3.622701	0.961746
34	1	0	-2.370451	4.224228	1.568650
35	6	0	-1.659364	2.245182	1.153168
36	1	0	-2.273019	1.758863	1.903344
37	6	0	-0.797779	1.447196	0.380435

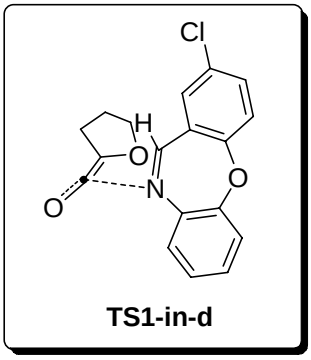


IN-out-d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.241627	-0.572586	-0.051735
2	6	0	4.319608	0.618484	-0.779999
3	6	0	3.135972	1.255968	-1.155593
4	6	0	1.905789	0.714746	-0.809657
5	6	0	1.809214	-0.487339	-0.065620
6	6	0	3.020360	-1.126859	0.296895
7	8	0	0.763685	1.334973	-1.300842
8	6	0	-0.124525	1.750115	-0.320489
9	6	0	-0.831437	0.813013	0.441303
10	6	0	-1.678136	1.270543	1.461877
11	6	0	-1.875427	2.636804	1.651783
12	6	0	-1.208912	3.562287	0.845863
13	6	0	-0.319529	3.116053	-0.130751
14	7	0	-0.650278	-0.593430	0.243271
15	6	0	0.573706	-1.143443	0.231026
16	6	0	-1.752612	-1.560323	0.401418
17	6	0	-3.008858	-1.142177	-0.060601
18	8	0	-3.994264	-2.082861	0.065637
19	6	0	-5.162460	-1.678707	-0.665416
20	6	0	-5.031376	-0.164042	-0.823970
21	6	0	-3.503173	0.004631	-0.915783
22	8	0	-1.450587	-2.702628	0.792477
23	1	0	-5.162855	-2.191402	-1.637471
24	1	0	-6.036579	-2.004723	-0.096015
25	1	0	-5.416460	0.346331	0.065926
26	1	0	-5.562185	0.220423	-1.699484
27	1	0	-3.169914	0.991770	-0.598979
28	1	0	-3.170877	-0.128252	-1.957669
29	1	0	0.551878	-2.208189	0.435228
30	1	0	-2.184912	0.544351	2.086524
31	1	0	-2.544394	2.975648	2.437099

32	1	0	-1.364309	4.627661	0.988428
33	1	0	0.233223	3.807838	-0.758091
34	1	0	3.157269	2.169592	-1.740752
35	1	0	5.283805	1.032610	-1.052141
36	1	0	2.981997	-2.057531	0.853078
37	17	0	5.726271	-1.386529	0.424115

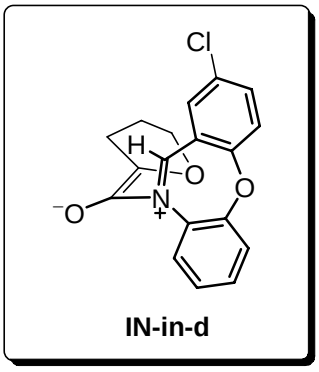


TS1-in-d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.855569	0.107801	0.588301
2	6	0	-2.406520	-0.636091	1.241014
3	8	0	-2.613321	-0.308568	2.397799
4	6	0	-2.902043	-1.368908	0.229789
5	6	0	-4.194739	-2.155888	0.290097
6	1	0	-5.074782	-1.496658	0.292793
7	1	0	-4.268994	-2.789976	1.180506
8	6	0	-4.127302	-2.973148	-1.018227
9	1	0	-3.613804	-3.926077	-0.847397
10	1	0	-5.110103	-3.184326	-1.451184
11	6	0	-3.262899	-2.070041	-1.904993
12	1	0	-2.733577	-2.595233	-2.705474
13	1	0	-3.869341	-1.264920	-2.351061
14	8	0	-2.281087	-1.518227	-1.026933
15	6	0	0.141091	-0.697595	0.481145
16	1	0	-0.070927	-1.726580	0.767380
17	6	0	1.510546	-0.401456	0.065182
18	6	0	2.549116	-1.216556	0.545871
19	1	0	2.323571	-2.030844	1.227028
20	6	0	3.861084	-0.976048	0.155185
21	17	0	5.150180	-1.992503	0.773727
22	6	0	4.162680	0.055903	-0.736166
23	1	0	5.188792	0.223576	-1.045091

24	6	0	3.135403	0.857394	-1.231632
25	1	0	3.340023	1.650948	-1.942338
26	6	0	1.819424	0.631518	-0.837126
27	8	0	0.824305	1.368246	-1.441592
28	6	0	-0.005825	2.111567	-0.605164
29	6	0	-0.053556	3.484869	-0.820037
30	1	0	0.589455	3.908848	-1.584515
31	6	0	-0.927366	4.276810	-0.075814
32	1	0	-0.964879	5.348012	-0.251313
33	6	0	-1.749660	3.687010	0.885675
34	1	0	-2.430506	4.296589	1.471983
35	6	0	-1.709245	2.312013	1.097546
36	1	0	-2.336280	1.835633	1.842980
37	6	0	-0.835507	1.501538	0.352663

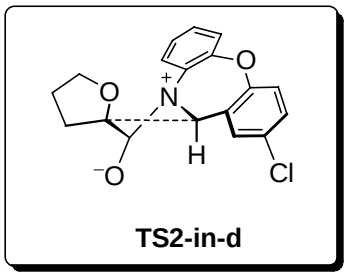


IN-in-d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.239772	-0.553572	-0.036303
2	6	0	4.312344	0.624050	-0.786379
3	6	0	3.127325	1.247743	-1.179270
4	6	0	1.897869	0.706624	-0.827479
5	6	0	1.808571	-0.482786	-0.063828
6	6	0	3.019865	-1.109753	0.315334
7	8	0	0.754598	1.308067	-1.327958
8	6	0	-0.139132	1.730866	-0.351729
9	6	0	-0.848053	0.802940	0.415279
10	6	0	-1.700921	1.271659	1.422596
11	6	0	-1.884718	2.637691	1.611359
12	6	0	-1.205871	3.556383	0.807167
13	6	0	-0.321421	3.099673	-0.167034
14	7	0	-0.651000	-0.608436	0.244985
15	6	0	0.573840	-1.146654	0.229607

16	6	0	-1.739655	-1.592481	0.362924
17	6	0	-3.022175	-1.211497	-0.015505
18	8	0	-3.394139	0.009705	-0.512470
19	6	0	-4.823300	0.012721	-0.706175
20	6	0	-5.198128	-1.455341	-0.930126
21	6	0	-4.166836	-2.185242	-0.047411
22	8	0	-1.413463	-2.767492	0.657833
23	1	0	-5.300645	0.422067	0.195511
24	1	0	-5.033155	0.674765	-1.549423
25	1	0	-5.057089	-1.722601	-1.982943
26	1	0	-6.236063	-1.667942	-0.659068
27	1	0	-3.850058	-3.157412	-0.436213
28	1	0	-4.557294	-2.366983	0.965119
29	1	0	0.557029	-2.213843	0.424455
30	1	0	-2.219581	0.550733	2.044353
31	1	0	-2.555555	2.983772	2.391978
32	1	0	-1.350819	4.623461	0.948411
33	1	0	0.240318	3.783724	-0.794858
34	1	0	3.146126	2.150953	-1.780338
35	1	0	5.275304	1.039296	-1.061534
36	1	0	2.984251	-2.031990	0.885580
37	17	0	5.727177	-1.348785	0.460981

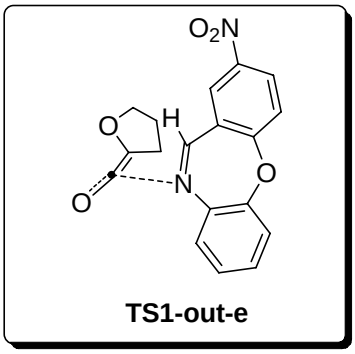


TS2-in-d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.636915	2.153693	-0.147442
2	6	0	0.009864	0.337041	-0.961459
3	6	0	-2.182494	0.952455	-0.749536
4	8	0	-3.254447	0.903895	-1.365215
5	7	0	-1.249827	-0.105437	-0.638342
6	1	0	0.093674	0.949897	-1.849980
7	6	0	1.216293	-0.126503	-0.353541
8	6	0	2.451214	0.351601	-0.858834
9	1	0	2.445775	1.033789	-1.703045

10	6	0	3.651219	-0.020285	-0.278188
11	17	0	5.160243	0.612328	-0.927436
12	6	0	3.686051	-0.886446	0.818423
13	1	0	4.632135	-1.170540	1.265226
14	6	0	2.482626	-1.386288	1.313898
15	1	0	2.470754	-2.068532	2.157654
16	6	0	1.265573	-1.024526	0.744221
17	8	0	0.137454	-1.535577	1.352419
18	6	0	-0.856152	-2.155957	0.605961
19	6	0	-1.178043	-3.472905	0.920321
20	1	0	-0.590718	-3.984669	1.676020
21	6	0	-2.257326	-4.092161	0.287815
22	1	0	-2.511760	-5.117553	0.540118
23	6	0	-3.007527	-3.391506	-0.657549
24	1	0	-3.850838	-3.868463	-1.148454
25	6	0	-2.677791	-2.075896	-0.985650
26	1	0	-3.250296	-1.506970	-1.708185
27	6	0	-1.597209	-1.453079	-0.353173
28	8	0	-1.000376	2.144151	1.057206
29	6	0	-0.887214	3.495862	1.548843
30	1	0	-0.895405	3.439069	2.639386
31	1	0	0.075669	3.910102	1.219229
32	6	0	-2.073810	4.239497	0.929715
33	1	0	-2.970914	4.094594	1.540693
34	1	0	-1.893018	5.313448	0.833813
35	6	0	-2.223346	3.515031	-0.422316
36	1	0	-1.648978	4.019945	-1.212848
37	1	0	-3.252539	3.426834	-0.779143

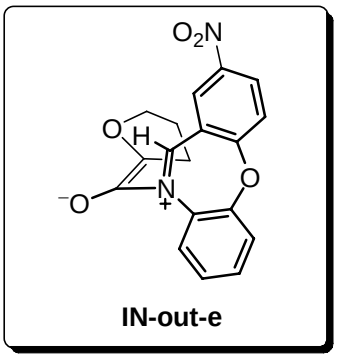


TS1-out-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.003598	0.058295	0.606868

2	6	0	-2.500706	-0.840112	1.245268
3	8	0	-2.689501	-0.586160	2.415871
4	6	0	-2.980943	-1.470494	0.152385
5	8	0	-4.185314	-2.179343	0.334139
6	6	0	-4.391958	-2.979114	-0.826763
7	1	0	-3.896515	-3.957778	-0.712790
8	1	0	-5.468419	-3.142989	-0.930658
9	6	0	-3.762954	-2.179046	-1.970287
10	1	0	-4.441166	-1.375333	-2.277562
11	1	0	-3.526695	-2.788756	-2.847863
12	6	0	-2.512008	-1.590748	-1.284539
13	1	0	-2.205292	-0.640563	-1.733599
14	1	0	-1.669563	-2.289020	-1.398854
15	6	0	0.062091	-0.656219	0.485196
16	1	0	-0.050828	-1.699867	0.776611
17	6	0	1.391679	-0.245442	0.038956
18	6	0	2.503164	-0.989489	0.458355
19	1	0	2.386513	-1.835977	1.125593
20	6	0	3.771914	-0.638488	0.016228
21	7	0	4.928459	-1.424635	0.471774
22	8	0	4.712425	-2.363599	1.236110
23	8	0	6.037967	-1.092203	0.057936
24	6	0	3.976721	0.425401	-0.863409
25	1	0	4.981295	0.658710	-1.194008
26	6	0	2.877083	1.155621	-1.301364
27	1	0	2.989943	1.976044	-2.001485
28	6	0	1.596437	0.825289	-0.856985
29	8	0	0.536867	1.499901	-1.408084
30	6	0	-0.337395	2.155692	-0.535697
31	6	0	-0.491355	3.526149	-0.711488
32	1	0	0.103586	4.020296	-1.472670
33	6	0	-1.409528	4.226280	0.070394
34	1	0	-1.531697	5.295948	-0.071246
35	6	0	-2.167829	3.546502	1.026023
36	1	0	-2.882603	4.084692	1.640852
37	6	0	-2.019667	2.173614	1.196895
38	1	0	-2.595666	1.630652	1.937995
39	6	0	-1.099156	1.454528	0.414401

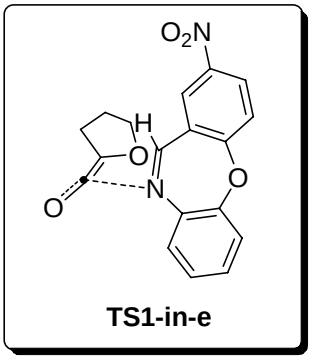


IN-out-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.126734	-2.163612	0.024671
2	6	0	-5.307491	-1.794154	-0.707961
3	1	0	-6.170286	-2.157406	-0.144433
4	1	0	-5.283682	-2.297531	-1.684084
5	6	0	-5.228622	-0.273866	-0.847657
6	1	0	-5.636626	0.211511	0.045875
7	1	0	-5.767436	0.102377	-1.721666
8	6	0	-3.706888	-0.049968	-0.927905
9	1	0	-3.408891	0.943309	-0.595532
10	1	0	-3.363038	-0.158317	-1.968720
11	6	0	-3.177088	-1.190918	-0.086528
12	6	0	-1.905026	-1.573886	0.371445
13	8	0	-1.568945	-2.713069	0.739493
14	7	0	-0.839339	-0.569806	0.231642
15	6	0	0.405008	-1.076990	0.212520
16	1	0	0.423845	-2.144122	0.402724
17	6	0	1.614919	-0.375816	-0.082775
18	6	0	2.848215	-0.984265	0.244197
19	1	0	2.868324	-1.927790	0.776362
20	6	0	4.041736	-0.380015	-0.116375
21	7	0	5.307030	-1.037668	0.247654
22	8	0	5.245126	-2.097985	0.868376
23	8	0	6.353076	-0.484684	-0.091859
24	6	0	4.086983	0.825730	-0.821540
25	1	0	5.041822	1.258814	-1.089578
26	6	0	2.881000	1.432096	-1.164382
27	1	0	2.860623	2.357288	-1.730462
28	6	0	1.672003	0.845932	-0.806662
29	8	0	0.512979	1.445746	-1.266748
30	6	0	-0.392424	1.802615	-0.276036
31	6	0	-0.629940	3.156548	-0.054551

32	1	0	-0.097911	3.880367	-0.663293
33	6	0	-1.535721	3.550856	0.929341
34	1	0	-1.724498	4.606959	1.097408
35	6	0	-2.175074	2.585231	1.709489
36	1	0	-2.856383	2.883176	2.500666
37	6	0	-1.933257	1.230964	1.487807
38	1	0	-2.415569	0.474692	2.095870
39	6	0	-1.069692	0.824543	0.459627

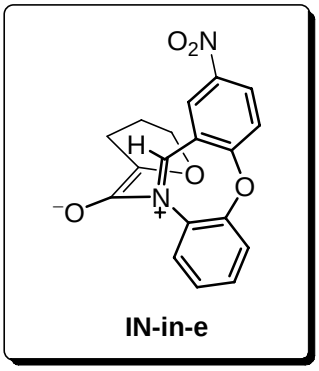


TS1-in-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.067500	0.130618	0.614830
2	6	0	-2.581324	-0.758786	1.205711
3	8	0	-2.900966	-0.416952	2.330256
4	6	0	-2.931201	-1.572133	0.193870
5	6	0	-4.158290	-2.461934	0.204553
6	1	0	-4.230751	-3.079144	1.106815
7	1	0	-5.086157	-1.875861	0.142580
8	6	0	-3.951113	-3.301953	-1.074552
9	1	0	-3.383835	-4.211365	-0.846882
10	1	0	-4.887760	-3.592986	-1.559952
11	6	0	-3.099166	-2.360919	-1.932730
12	1	0	-2.482946	-2.865211	-2.682557
13	1	0	-3.730128	-1.611496	-2.437233
14	8	0	-2.216414	-1.718469	-1.010051
15	6	0	-0.007336	-0.587743	0.502268
16	1	0	-0.125213	-1.630046	0.793201
17	6	0	1.328508	-0.186710	0.061561
18	6	0	2.430322	-0.929703	0.505218
19	1	0	2.300641	-1.764061	1.185073
20	6	0	3.706422	-0.596795	0.069125
21	7	0	4.852319	-1.381058	0.551398

22	8	0	4.623380	-2.299915	1.336495
23	8	0	5.968120	-1.067944	0.138697
24	6	0	3.926219	0.447205	-0.830193
25	1	0	4.935146	0.666498	-1.157174
26	6	0	2.836109	1.176598	-1.291362
27	1	0	2.960803	1.982668	-2.005956
28	6	0	1.548365	0.865606	-0.851305
29	8	0	0.503911	1.542392	-1.422583
30	6	0	-0.390295	2.202726	-0.576414
31	6	0	-0.548481	3.567784	-0.786606
32	1	0	0.057328	4.045416	-1.549746
33	6	0	-1.482742	4.283754	-0.038553
34	1	0	-1.606445	5.349070	-0.209322
35	6	0	-2.253995	3.624119	0.919232
36	1	0	-2.983022	4.172736	1.507707
37	6	0	-2.101093	2.256041	1.125678
38	1	0	-2.692018	1.726100	1.864255
39	6	0	-1.164846	1.520817	0.378346

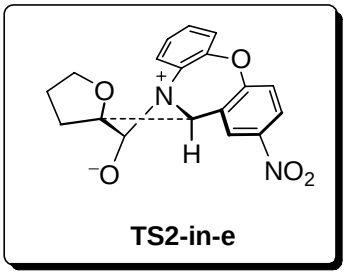


IN-in-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.601929	-0.043531	-0.507992
2	6	0	-5.027637	-0.088907	-0.734497
3	1	0	-5.239732	0.568410	-1.580690
4	1	0	-5.536599	0.300160	0.158133
5	6	0	-5.346658	-1.567301	-0.976164
6	1	0	-5.183079	-1.819664	-2.029286
7	1	0	-6.379650	-1.818962	-0.720614
8	6	0	-4.301171	-2.269806	-0.088403
9	1	0	-4.694567	-2.471627	0.919146
10	1	0	-3.946681	-3.227286	-0.480464
11	6	0	-3.191333	-1.258432	-0.036166

12	6	0	-1.893686	-1.604149	0.334148
13	8	0	-1.532296	-2.773794	0.603418
14	7	0	-0.840746	-0.585094	0.235302
15	6	0	0.403043	-1.082322	0.211415
16	1	0	0.425720	-2.151507	0.392767
17	6	0	1.612555	-0.375324	-0.084045
18	6	0	2.845709	-0.971740	0.259221
19	1	0	2.868015	-1.905798	0.807701
20	6	0	4.037919	-0.367626	-0.107706
21	7	0	5.305018	-1.009059	0.275227
22	8	0	5.246604	-2.060946	0.910803
23	8	0	6.349366	-0.452879	-0.064390
24	6	0	4.077429	0.823601	-0.837201
25	1	0	5.030778	1.257029	-1.110368
26	6	0	2.870334	1.416893	-1.197040
27	1	0	2.847685	2.330623	-1.781224
28	6	0	1.662185	0.832840	-0.829772
29	8	0	0.502223	1.414783	-1.297997
30	6	0	-0.405097	1.782138	-0.308526
31	6	0	-0.626769	3.140154	-0.092699
32	1	0	-0.086098	3.855089	-0.704296
33	6	0	-1.523372	3.547462	0.892210
34	1	0	-1.699568	4.606046	1.058635
35	6	0	-2.173463	2.590136	1.674669
36	1	0	-2.853090	2.897393	2.463781
37	6	0	-1.948488	1.235012	1.454599
38	1	0	-2.442524	0.485128	2.061892
39	6	0	-1.083546	0.814867	0.436033

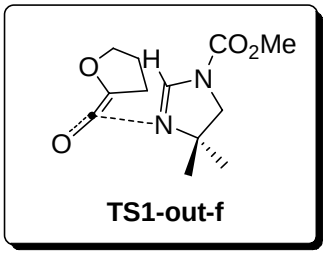


TS2-in-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.682279	2.235827	-0.110332
2	6	0	-0.139396	0.312806	-0.939858
3	1	0	-0.002388	0.937843	-1.812894

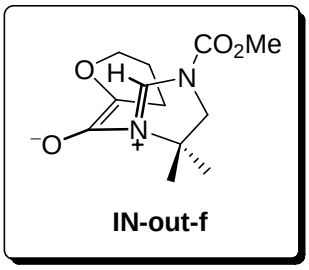
4	7	0	-1.430503	-0.041306	-0.633810
5	6	0	-2.288057	1.078792	-0.741371
6	8	0	-3.354196	1.110560	-1.367807
7	6	0	-2.186965	3.632272	-0.363999
8	1	0	-3.217544	3.610369	-0.726523
9	1	0	-1.579770	4.113841	-1.144520
10	6	0	-1.999748	4.323921	1.000521
11	1	0	-2.905483	4.220973	1.607105
12	1	0	-1.757096	5.386874	0.922481
13	6	0	-0.859100	3.504400	1.609407
14	1	0	-0.877809	3.422616	2.698070
15	1	0	0.127317	3.870357	1.294126
16	8	0	-1.040808	2.169602	1.085648
17	6	0	1.025555	-0.230220	-0.318528
18	6	0	2.292367	0.196976	-0.775872
19	1	0	2.363847	0.895691	-1.601206
20	6	0	3.452794	-0.244973	-0.162819
21	7	0	4.746748	0.238747	-0.659548
22	8	0	4.742331	1.021725	-1.610377
23	8	0	5.762845	-0.166631	-0.094203
24	6	0	3.427220	-1.129353	0.919404
25	1	0	4.353752	-1.454354	1.374631
26	6	0	2.191099	-1.579444	1.368391
27	1	0	2.118015	-2.275666	2.197038
28	6	0	1.007345	-1.153630	0.764445
29	8	0	-0.147489	-1.633701	1.328254
30	6	0	-1.190127	-2.146111	0.561886
31	6	0	-1.609009	-3.442302	0.846243
32	1	0	-1.060250	-4.014309	1.587467
33	6	0	-2.732002	-3.963975	0.202697
34	1	0	-3.061481	-4.973342	0.431009
35	6	0	-3.428559	-3.185990	-0.722889
36	1	0	-4.305338	-3.586106	-1.223473
37	6	0	-3.001463	-1.891445	-1.019996
38	1	0	-3.529125	-1.264834	-1.728607
39	6	0	-1.876646	-1.364964	-0.376217



TS1-out-f

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.056379	0.834279	-0.555761
2	7	0	-0.224481	0.633278	-0.204303
3	6	0	0.588738	-0.322000	-0.468310
4	1	0	0.324614	-1.257461	-0.943807
5	7	0	1.891090	-0.088238	-0.088901
6	6	0	1.934809	1.178593	0.663737
7	1	0	2.055894	0.969454	1.733020
8	1	0	2.767681	1.799508	0.329283
9	6	0	0.544043	1.805851	0.327730
10	6	0	0.676437	2.851518	-0.793653
11	1	0	1.230020	3.722102	-0.422220
12	1	0	-0.312358	3.163931	-1.131580
13	1	0	1.222691	2.435540	-1.648078
14	6	0	-0.153246	2.386285	1.559258
15	1	0	-0.281435	1.623792	2.335189
16	1	0	0.442914	3.206454	1.975299
17	1	0	-1.136096	2.772770	1.279715
18	6	0	2.905273	-1.019954	-0.256670
19	8	0	2.765573	-2.081997	-0.826036
20	8	0	4.044485	-0.563797	0.297116
21	6	0	5.172699	-1.449970	0.169345
22	1	0	4.963808	-2.405212	0.656635
23	1	0	5.401763	-1.624604	-0.884530
24	1	0	5.997252	-0.936660	0.663552
25	8	0	-2.270196	1.973998	-0.901727
26	6	0	-2.601072	-0.388887	-0.380567
27	8	0	-3.988350	-0.473892	-0.613312
28	6	0	-4.501871	-1.232609	0.478394
29	1	0	-4.592675	-0.598371	1.374934
30	1	0	-5.494295	-1.597262	0.197796
31	6	0	-3.464062	-2.344844	0.699098
32	1	0	-3.451331	-2.712892	1.729989
33	1	0	-3.677221	-3.193102	0.040870
34	6	0	-2.126262	-1.665586	0.283211
35	1	0	-1.481365	-1.472692	1.148514
36	1	0	-1.572859	-2.341124	-0.385348

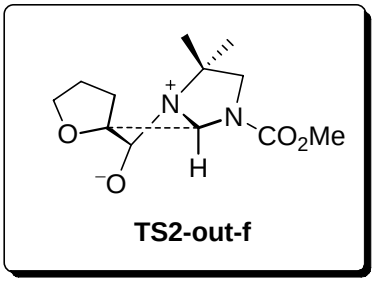


IN-out-f

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.300306	0.677200	-0.256165
2	6	0	1.753099	0.800855	-0.523725
3	6	0	-0.483783	1.835107	0.315041
4	6	0	-1.799896	1.120155	0.736716
5	7	0	-1.775200	-0.116137	-0.065532
6	6	0	-2.802161	-1.022744	-0.264734
7	8	0	-2.686279	-2.048977	-0.904301
8	8	0	-3.923199	-0.594198	0.350293
9	6	0	-5.059709	-1.464135	0.199175
10	6	0	-0.730164	2.853931	-0.808226
11	6	0	0.251301	2.458355	1.500509
12	1	0	-0.257274	-1.170147	-1.153108
13	1	0	-1.812736	0.866418	1.803247
14	1	0	-2.685998	1.711760	0.502903
15	1	0	-4.841848	-2.451959	0.612170
16	1	0	-5.325111	-1.565234	-0.855969
17	1	0	-5.864825	-0.983068	0.754363
18	1	0	-1.290109	3.710255	-0.414185
19	1	0	0.233150	3.182554	-1.202097
20	1	0	-1.312736	2.405146	-1.621268
21	1	0	1.198187	2.878849	1.156362
22	1	0	-0.363580	3.253258	1.937023
23	1	0	0.454165	1.710860	2.274989
24	6	0	-0.508466	-0.305759	-0.558882
25	8	0	2.167521	1.933355	-0.859358
26	6	0	2.441343	-0.377304	-0.284468
27	8	0	3.816644	-0.326271	-0.460907
28	6	0	4.408653	-1.520050	0.061331
29	6	0	3.363005	-2.127097	1.001039
30	6	0	2.052474	-1.709916	0.299437
31	1	0	4.644567	-2.201367	-0.770434
32	1	0	5.344438	-1.245614	0.557976
33	1	0	3.425416	-1.660767	1.990601

34	1	0	3.471322	-3.209649	1.119281
35	1	0	1.194252	-1.654576	0.980666
36	1	0	1.801304	-2.463817	-0.465726

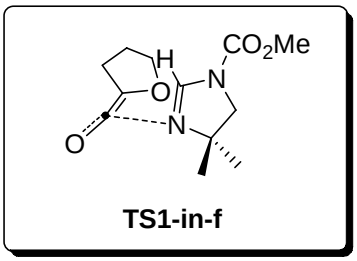


TS2-out-f

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.034166	-0.567852	-0.396639
2	6	0	-0.344733	-0.066401	-0.846939
3	1	0	-0.290841	-0.590174	-1.786869
4	7	0	0.373471	1.010748	-0.491614
5	6	0	1.791754	0.848202	-0.591382
6	8	0	2.559971	1.756280	-0.907871
7	8	0	3.243861	-1.018983	-0.860136
8	6	0	3.818909	-1.978008	0.052300
9	1	0	3.701749	-2.984124	-0.372735
10	1	0	4.886509	-1.755460	0.136650
11	6	0	3.036993	-1.810210	1.356531
12	1	0	3.468529	-1.000932	1.956232
13	1	0	3.019128	-2.722006	1.961489
14	6	0	1.648737	-1.403882	0.816194
15	1	0	1.100863	-2.312675	0.533571
16	1	0	1.038964	-0.859627	1.541903
17	7	0	-1.517821	-0.099477	-0.102957
18	6	0	-1.538559	1.029913	0.847428
19	1	0	-1.323680	0.673264	1.861824
20	1	0	-2.520895	1.504224	0.844694
21	6	0	-0.417541	1.977369	0.313396
22	6	0	0.424412	2.588782	1.433263
23	1	0	-0.181346	3.286898	2.020956
24	1	0	0.810256	1.815054	2.105513
25	1	0	1.276365	3.126754	1.009902
26	6	0	-0.981988	3.061127	-0.617835
27	1	0	-1.596994	2.617193	-1.408411
28	1	0	-0.159266	3.605803	-1.090343

29	1	0	-1.600086	3.770560	-0.055044
30	6	0	-2.536578	-0.995953	-0.348096
31	8	0	-2.487875	-1.873339	-1.188063
32	8	0	-3.581926	-0.759991	0.479538
33	6	0	-4.696090	-1.650001	0.300604
34	1	0	-5.088595	-1.575032	-0.716588
35	1	0	-4.396336	-2.683267	0.493009
36	1	0	-5.443017	-1.325607	1.025551

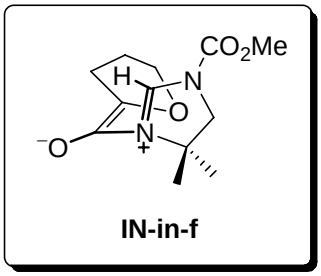


TS1-in-f

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.210706	1.014895	-0.105912
2	7	0	0.213971	0.717876	-0.045316
3	6	0	-0.669737	1.918677	0.073931
4	6	0	-0.308366	2.710046	1.337896
5	1	0	0.719206	3.073135	1.275394
6	1	0	-0.984076	3.566777	1.447604
7	1	0	-0.404627	2.080508	2.229595
8	6	0	-0.517045	2.777475	-1.191322
9	1	0	-0.802585	2.206807	-2.082450
10	1	0	-1.165588	3.659377	-1.125491
11	1	0	0.518899	3.102625	-1.302699
12	6	0	-2.112866	1.311265	0.173221
13	1	0	-2.786943	1.700698	-0.594260
14	1	0	-2.571374	1.476698	1.153481
15	7	0	-1.867218	-0.123592	-0.035525
16	6	0	-0.506120	-0.339647	-0.116804
17	1	0	-0.112583	-1.339509	-0.228263
18	6	0	-2.800235	-1.143586	-0.079397
19	8	0	-2.531329	-2.317997	-0.227218
20	8	0	-4.043399	-0.635763	0.063659
21	6	0	-5.097619	-1.613175	0.027402
22	1	0	-5.097355	-2.141206	-0.929337
23	1	0	-4.976668	-2.337185	0.836966

24	1	0	-6.019884	-1.045850	0.153431
25	8	0	2.401106	2.203570	-0.190287
26	6	0	2.762036	-0.200958	-0.052933
27	8	0	2.063796	-1.418478	-0.002812
28	6	0	2.999070	-2.412237	0.426078
29	1	0	2.638749	-3.379865	0.066198
30	1	0	3.046767	-2.435631	1.526464
31	6	0	4.338875	-1.971586	-0.170498
32	1	0	4.383580	-2.253073	-1.228219
33	1	0	5.199646	-2.412312	0.341700
34	6	0	4.261727	-0.435940	-0.024662
35	1	0	4.710828	-0.111296	0.924489
36	1	0	4.792780	0.087287	-0.827446

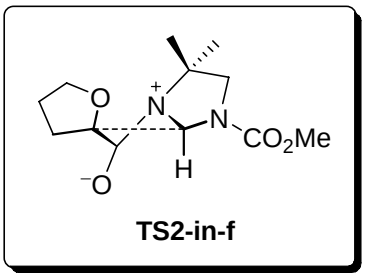


IN-in-f

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.313699	0.715048	-0.139482
2	6	0	-1.799067	0.878884	-0.285902
3	6	0	0.549896	1.924242	0.144019
4	6	0	1.938170	1.270159	0.420385
5	7	0	1.754859	-0.116449	-0.034782
6	6	0	2.720936	-1.107175	-0.124588
7	8	0	2.497760	-2.249990	-0.466236
8	8	0	3.924530	-0.603433	0.218005
9	6	0	5.009160	-1.546673	0.152207
10	6	0	0.038750	2.687032	1.369471
11	6	0	0.585633	2.806755	-1.112301
12	1	0	0.060402	-1.324893	-0.558007
13	1	0	2.741906	1.753739	-0.138088
14	1	0	2.196355	1.278496	1.484723
15	1	0	5.124565	-1.924959	-0.866415
16	1	0	4.827601	-2.384895	0.829201
17	1	0	5.893846	-0.988521	0.458379
18	1	0	0.724310	3.512835	1.593153

19	1	0	-0.959174	3.075838	1.163636
20	1	0	-0.005495	2.029867	2.245233
21	1	0	-0.431215	3.120190	-1.353695
22	1	0	1.215743	3.684491	-0.926207
23	1	0	1.005052	2.255900	-1.962502
24	6	0	0.429948	-0.351820	-0.278625
25	8	0	-2.222548	2.056400	-0.429828
26	6	0	-2.530003	-0.279698	-0.202996
27	8	0	-1.963342	-1.554143	-0.046087
28	6	0	-3.028943	-2.505131	0.133037
29	6	0	-4.244978	-1.689183	0.583683
30	6	0	-4.024503	-0.355741	-0.160295
31	1	0	-3.217615	-3.008008	-0.826497
32	1	0	-2.692495	-3.252402	0.858122
33	1	0	-4.211361	-1.529724	1.667353
34	1	0	-5.190802	-2.181632	0.337890
35	1	0	-4.459134	0.511773	0.344931
36	1	0	-4.471786	-0.398877	-1.166757

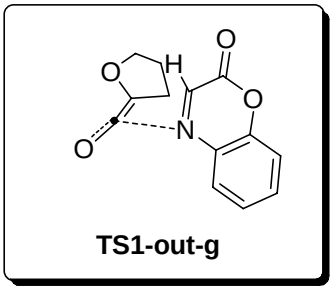


TS2-in-f

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.250140	0.359276	-1.133716
2	6	0	1.769594	-0.697210	-0.391433
3	6	0	1.927845	0.692554	-0.747459
4	8	0	2.907459	1.232606	-1.251872
5	7	0	0.600481	1.321456	-0.691180
6	1	0	-0.297088	-0.011091	-2.146438
7	8	0	1.064455	-1.047418	0.778628
8	6	0	1.417390	-2.391389	1.128024
9	1	0	0.766920	-3.097468	0.589111
10	1	0	1.248057	-2.503358	2.202205
11	6	0	2.875890	-2.539500	0.689277
12	1	0	3.540282	-2.098899	1.442020
13	1	0	3.170091	-3.582409	0.538311

14	6	0	2.888975	-1.697251	-0.602715
15	1	0	2.686348	-2.324249	-1.481690
16	1	0	3.836181	-1.180634	-0.787025
17	7	0	-1.330492	0.240402	-0.294653
18	6	0	-1.146346	1.092514	0.895409
19	1	0	-0.874505	0.469540	1.751854
20	1	0	-2.069204	1.631364	1.115092
21	6	0	0.011212	2.051958	0.468384
22	6	0	-0.541179	3.396158	-0.028619
23	1	0	0.271554	4.009804	-0.429924
24	1	0	-1.023970	3.944584	0.788443
25	1	0	-1.277531	3.246648	-0.826373
26	6	0	1.045476	2.249746	1.577265
27	1	0	0.602921	2.804954	2.410586
28	1	0	1.899862	2.820125	1.199450
29	1	0	1.406371	1.285770	1.947744
30	6	0	-2.373960	-0.633574	-0.534835
31	8	0	-2.462900	-1.339308	-1.519383
32	8	0	-3.271508	-0.580575	0.475303
33	6	0	-4.398237	-1.459716	0.320694
34	1	0	-5.011965	-1.299429	1.206607
35	1	0	-4.956455	-1.212465	-0.585836
36	1	0	-4.066962	-2.499619	0.263641

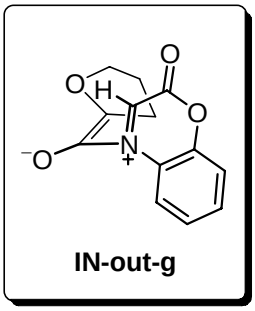


TS1-out-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.200199	0.231834	0.574912
2	6	0	-1.356166	-0.661422	1.080138
3	8	0	-1.112444	-1.474728	1.938048
4	6	0	-2.335853	-0.101987	0.327802
5	8	0	-3.606882	-0.659708	0.518959
6	6	0	-4.219482	-0.697381	-0.770911
7	1	0	-3.859591	-1.572697	-1.334021

8	1	0	-5.298668	-0.788510	-0.623043
9	6	0	-3.781997	0.609858	-1.442629
10	1	0	-4.449798	1.423864	-1.143804
11	1	0	-3.788859	0.549201	-2.535021
12	6	0	-2.360693	0.844900	-0.862288
13	1	0	-2.243437	1.901891	-0.598019
14	1	0	-1.582192	0.608889	-1.597803
15	6	0	0.289200	1.521616	0.671202
16	1	0	-0.555756	2.078552	1.059840
17	6	0	1.475449	2.294615	0.274322
18	8	0	1.559703	3.496016	0.329624
19	8	0	2.540722	1.546490	-0.186331
20	6	0	2.469553	0.178281	-0.244727
21	6	0	3.589671	-0.507295	-0.709396
22	1	0	4.468192	0.057919	-1.001560
23	6	0	3.543252	-1.895335	-0.783604
24	1	0	4.412386	-2.438902	-1.141848
25	6	0	2.390956	-2.595214	-0.393880
26	1	0	2.372574	-3.679144	-0.445116
27	6	0	1.274334	-1.913470	0.067489
28	1	0	0.391041	-2.437702	0.410270
29	6	0	1.302432	-0.508959	0.140373

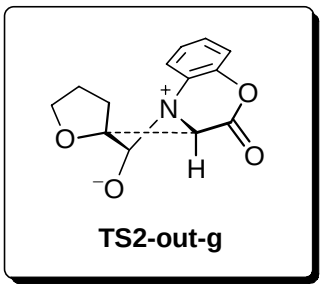


IN-out-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.275705	-1.083721	-0.318083
2	6	0	-4.313568	-0.588476	0.565055
3	1	0	-4.761701	-1.457498	1.050990
4	1	0	-5.072285	-0.093986	-0.053910
5	6	0	-3.600856	0.378579	1.509249
6	1	0	-4.259925	1.164062	1.887859
7	1	0	-3.178281	-0.161658	2.362892
8	6	0	-2.474647	0.916764	0.599876

9	1	0	-2.848873	1.768499	0.015140
10	1	0	-1.586027	1.273040	1.131665
11	6	0	-2.198057	-0.277084	-0.275523
12	6	0	-1.018132	-0.847420	-0.839183
13	8	0	-0.935948	-1.975522	-1.340974
14	7	0	0.134516	-0.000953	-0.646958
15	6	0	0.024540	1.328898	-0.879031
16	1	0	-0.791095	1.679161	-1.491370
17	6	0	0.966685	2.292112	-0.385414
18	8	0	0.861976	3.496347	-0.481107
19	8	0	2.102510	1.767373	0.235398
20	6	0	2.331391	0.416129	0.244623
21	6	0	1.374783	-0.518996	-0.196341
22	6	0	1.671225	-1.890329	-0.138399
23	6	0	3.561382	-0.011213	0.741556
24	6	0	2.898526	-2.306209	0.366440
25	6	0	3.843052	-1.372138	0.805237
26	1	0	0.938645	-2.593147	-0.510977
27	1	0	3.123095	-3.367683	0.403606
28	1	0	4.802965	-1.703410	1.190268
29	1	0	4.271242	0.739773	1.071793

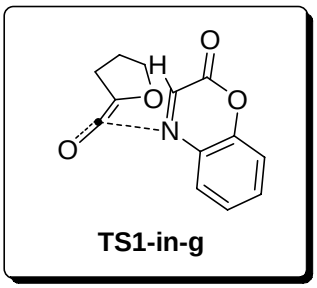


TS2-out-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.111715	-0.283734	-0.262109
2	6	0	-0.126004	1.117183	-1.027956
3	1	0	-0.781154	1.312920	-1.861590
4	7	0	0.173573	-0.178415	-0.689522
5	6	0	-0.940057	-1.044736	-0.694484
6	8	0	-0.928842	-2.233061	-1.011160
7	8	0	-3.283745	-0.869218	-0.526455
8	6	0	-4.299622	-0.461155	0.435316
9	1	0	-4.893170	-1.349679	0.658183
10	1	0	-4.937008	0.287792	-0.048431

11	6	0	-3.504914	0.101529	1.611773
12	1	0	-4.065201	0.846625	2.182418
13	1	0	-3.205179	-0.705008	2.289287
14	6	0	-2.278234	0.696017	0.885575
15	1	0	-1.378926	0.780945	1.500328
16	1	0	-2.524663	1.699722	0.522042
17	6	0	0.635634	2.209653	-0.481038
18	8	0	0.369039	3.386817	-0.587964
19	8	0	1.789643	1.850758	0.227582
20	6	0	2.253923	0.555230	0.220908
21	6	0	1.461471	-0.515716	-0.225785
22	6	0	1.948765	-1.826750	-0.166982
23	1	0	1.319080	-2.632671	-0.522387
24	6	0	3.227869	-2.052375	0.336507
25	1	0	3.610950	-3.067355	0.380185
26	6	0	4.019139	-0.984461	0.771903
27	1	0	5.017801	-1.167316	1.157445
28	6	0	3.535206	0.321437	0.713593
29	1	0	4.124930	1.167826	1.049818

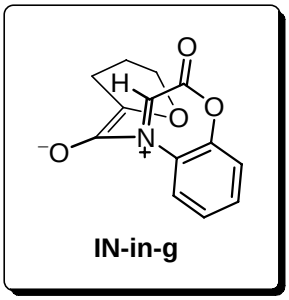


TS1-in-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.182156	0.125177	0.450084
2	6	0	-1.303040	-0.968768	0.873258
3	8	0	-0.957443	-1.912844	1.552108
4	6	0	-2.368391	-0.431804	0.250626
5	8	0	-2.375831	0.758500	-0.487565
6	6	0	-3.717408	0.983522	-0.948468
7	1	0	-3.652581	1.474208	-1.923647
8	1	0	-4.236097	1.656468	-0.249271
9	6	0	-4.379754	-0.396627	-0.979463
10	1	0	-4.105888	-0.925231	-1.899128
11	1	0	-5.470978	-0.342599	-0.922511
12	6	0	-3.733408	-1.078330	0.242926

13	1	0	-3.681378	-2.167848	0.156476
14	1	0	-4.302381	-0.849811	1.156550
15	6	0	0.127124	1.414182	0.563575
16	1	0	-0.812652	1.877441	0.834768
17	6	0	1.264408	2.313785	0.315528
18	8	0	1.221768	3.513861	0.427792
19	8	0	2.437454	1.697309	-0.064450
20	6	0	2.507725	0.333174	-0.180083
21	6	0	1.391170	-0.483066	0.085950
22	6	0	1.517090	-1.877287	-0.055950
23	1	0	0.668987	-2.504509	0.185899
24	6	0	2.730023	-2.419381	-0.457188
25	1	0	2.824749	-3.495620	-0.561629
26	6	0	3.830984	-1.591297	-0.719523
27	1	0	4.776644	-2.025830	-1.029866
28	6	0	3.725307	-0.211827	-0.581552
29	1	0	4.557920	0.454829	-0.779127

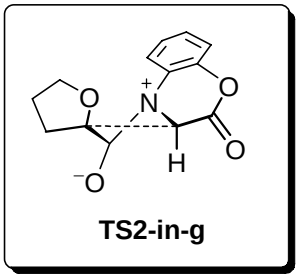


IN-in-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.375189	-1.334143	-0.021582
2	1	0	3.030339	-2.349389	0.187929
3	1	0	4.046917	-1.395860	-0.891431
4	6	0	4.062686	-0.623981	1.163067
5	1	0	3.615214	-0.945872	2.109178
6	1	0	5.139269	-0.806046	1.214729
7	6	0	3.737214	0.847930	0.892311
8	1	0	4.486928	1.336067	0.259242
9	1	0	3.576186	1.454579	1.786005
10	8	0	2.485440	0.842789	0.145123
11	6	0	2.230425	-0.411937	-0.302834
12	6	0	1.010002	-0.869809	-0.833812
13	8	0	0.859092	-2.010451	-1.315599

14	7	0	-0.121398	0.022188	-0.621753
15	6	0	0.010814	1.354169	-0.769580
16	1	0	0.898660	1.733166	-1.246898
17	6	0	-0.954123	2.312518	-0.308476
18	8	0	-0.835386	3.516514	-0.384980
19	8	0	-2.113326	1.789163	0.259053
20	6	0	-2.337396	0.439505	0.252266
21	6	0	-1.379272	-0.492439	-0.194133
22	6	0	-1.693933	-1.861960	-0.161234
23	6	0	-3.575382	0.013977	0.732381
24	6	0	-2.927980	-2.276478	0.326728
25	6	0	-3.869766	-1.343835	0.773257
26	1	0	-0.964597	-2.564615	-0.538522
27	1	0	-4.280821	0.767578	1.065993
28	1	0	-3.159654	-3.336986	0.343287
29	1	0	-4.836084	-1.673155	1.143829



TS2-in-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.116726	-0.376219	-0.169399
2	6	0	-0.153528	1.055852	-0.992260
3	7	0	0.190203	-0.221936	-0.591797
4	6	0	-0.896576	-1.093845	-0.574479
5	8	0	-0.902194	-2.282204	-0.910648
6	1	0	-0.775774	1.190507	-1.862800
7	6	0	0.593500	2.182674	-0.503324
8	8	0	0.328744	3.352527	-0.673137
9	8	0	1.760079	1.866320	0.215706
10	6	0	2.274393	0.591269	0.211632
11	6	0	1.507371	-0.515890	-0.187296
12	6	0	2.039967	-1.807471	-0.125622
13	1	0	1.426780	-2.642793	-0.440949
14	6	0	3.345385	-1.980244	0.330626
15	1	0	3.765675	-2.980358	0.376986

16	6	0	4.113478	-0.877511	0.717457
17	1	0	5.131732	-1.018742	1.067789
18	6	0	3.581436	0.409926	0.657231
19	1	0	4.153440	1.281559	0.957801
20	8	0	-2.171660	0.317187	0.979775
21	6	0	-3.552340	0.618270	1.308022
22	1	0	-3.789064	1.606338	0.894370
23	1	0	-3.612455	0.658992	2.396737
24	6	0	-4.358062	-0.505147	0.650591
25	1	0	-4.421699	-1.369083	1.319775
26	1	0	-5.373486	-0.194228	0.393114
27	6	0	-3.490100	-0.840361	-0.578804
28	1	0	-3.811931	-0.279031	-1.467886
29	1	0	-3.473568	-1.898062	-0.852180

6. Computed Energies

Table S1. Reaction of **1** with **2a**. Sum of electronic and zero-point energies (*E*, in a.u.), sum of electronic and thermal enthalpies (*H*, in a.u.), sum of electronic and thermal free energies (*G*, in a.u.), thermal correction to Gibbs free energy (*TCGFE*, in a.u.), total free energy in solution (G_S, in a.u., solvent = toluene)

Structure	*E*	*H*	*G*	*TCGFE*	G_s
1	-344.419239	-344.411865	-344.450328	0.072048	-344.52161
2a	-669.860801	-669.847585	-669.900534	0.174155	-670.073757
TS1-out-a	-1014.271171	-1014.251033	-1014.321	0.268805	-1014.59094
IN-out-a	-1014.280105	-1014.260146	-1014.328152	0.272174	-1014.601453
TS2-out-a	-1014.2767*	-1014.257628*	-1014.323854*	0.274634**	-1014.598174*
3a	-1014.336764	-1014.317039	-1014.385324	0.27365	-1014.655869
TS1-in-a	-1014.276117	-1014.25589	-1014.326466	0.268428	-1014.591891
IN-in-a	-1014.287069	-1014.266968	-1014.336449	0.270573	-1014.606045
TS2-in-a	-1014.273635	-1014.254047	-1014.321898	0.270912	-1014.589595
4a	-1014.338913	-1014.319316	-1014.387655	0.273804	-1014.658257

* Calculated at the B3LYP/6-31G(d)//B3LYP/6-31G level of theory.

** Calculated at the B3LYP/6-31G level of theory.

Table S2. Reaction of **1** with **2a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_{sol}, in kcal/mol)

Structure	3a	TS2-out-a*	IN-out-a	TS1-out-a	TS1-in-a	IN-in-a	TS2-in-a	4a
ΔE	-35.59	2.10	-0.04	5.57	2.46	-4.41	4.02	-36.94
ΔH	-36.14	1.14	-0.44	5.28	2.23	-4.72	3.39	-37.57
ΔG	-21.63	16.95	14.25	18.74	15.31	9.04	18.18	-23.09
ΔG_{sol}	-20.74	16.08	12.48	16.96	16.13	8.59	19.13	-22.14

* Calculated at the B3LYP/6-31G(d)//B3LYP/6-31G level of theory.

Table S3. Reaction of **1** with **2b**. Sum of electronic and zero-point energies (*E*, in a.u.), sum of electronic and thermal enthalpies (*H*, in a.u.), sum of electronic and thermal free energies (*G*, in a.u.), thermal correction to Gibbs free energy (*TCGFE*, in a.u.), total free energy in solution (G_S, in a.u., solvent = toluene)

Structure	*E*	*H*	*G*	*TCGFE*	G_s
1	-344.419239	-344.411865	-344.450328	0.072048	-344.52161
2b	-669.859908	-669.846716	-669.899278	0.174561	-670.072886
TS1-out-b	-1014.270103	-1014.249992	-1014.319598	0.269185	-1014.589854
IN-out-b	-1014.279348	-1014.25934	-1014.327759	0.271795	-1014.600456
TS2-out-b	-1014.275959*	-1014.256969*	-1014.322427*	0.275426**	-1014.597299*
3b	-1014.336301	-1014.31659	-1014.384681	0.27384	-1014.65489
TS1-in-b	-1014.275076	-1014.254885	-1014.325163	0.268741	-1014.590972
IN-in-b	-1014.286136	-1014.266097	-1014.33451	0.271692	-1014.605081
TS2-in-b	-1014.272744	-1014.253226	-1014.320445	0.2716	-1014.588665
4b	-1014.338231	-1014.318701	-1014.386177	0.274707	-1014.657174

* Calculated at the B3LYP/6-31G(d)//B3LYP/6-31G level of theory.

** Calculated at the B3LYP/6-31G level of theory.

Table S4. Reaction of **1** with **2b**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_{sol}, in kcal/mol)

Structure	3b	TS2-out-b*	IN-out-b	TS1-out-b	TS1-in-b	IN-in-b	TS2-in-b	4b
ΔE	-35.86	2.00	-0.13	5.68	2.55	-4.39	4.02	-37.08
ΔH	-36.40	1.01	-0.48	5.39	2.32	-4.72	3.36	-37.73
ΔG	-22.01	17.06	13.71	18.83	15.34	9.47	18.30	-22.95
ΔG_{sol}	-20.81	16.32	12.06	17.08	16.10	9.10	19.34	-21.70

* Calculated at the B3LYP/6-31G(d)//B3LYP/6-31G level of theory.

Table S5. Reaction of **1** with **2c**. Sum of electronic and zero-point energies (*E*, in a.u.), sum of electronic and thermal enthalpies (*H*, in a.u.), sum of electronic and thermal free energies (*G*, in a.u.), thermal correction to Gibbs free energy (*TCGFE*, in a.u.), total free energy in solution (G_S, in a.u., solvent = toluene)

Structure	*E*	*H*	*G*	*TCGFE*	G_s
1	-344.419239	-344.411865	-344.450328	0.072048	-344.52161
2c	-630.569519	-630.558241	-630.605847	0.150057	-630.757882
TS1-out-c	-974.979348	-974.961115	-975.026211	0.244253	-975.274489
IN-out-c	-974.988842	-974.970799	-975.034048	0.247505	-975.285492
TS2-out-c	-974.985694*	-974.968544*	-975.029744*	0.250099**	-975.282411*
3c	-975.045867	-975.028051	-975.091668	0.248909	-975.340525
TS1-in-c	-974.984425	-974.966119	-975.032049	0.243652	-975.276001
IN-in-c	-974.995687	-974.977586	-975.041123	0.247115	-975.290083
TS2-in-c	-974.982441	-974.964777	-975.027737	0.246364	-975.273804
4c	-975.047972	-975.030404	-975.092707	0.250461	-975.342867

* Calculated at the B3LYP/6-31G(d)//B3LYP/6-31G level of theory.

** Calculated at the B3LYP/6-31G level of theory.

Table S6. Reaction of **1** with **2c**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_{sol}, in kcal/mol)

Structure	3c	TS2-out-c*	IN-out-c	TS1-out-c	TS1-in-c	IN-in-c	TS2-in-c	4c
ΔE	-35.84	1.92	-0.05	5.90	2.72	-4.35	3.96	-37.16
ΔH	-36.36	0.98	-0.43	5.64	2.50	-4.69	3.34	-37.84
ΔG	-22.27	16.59	13.88	18.80	15.14	9.45	17.85	-22.92
ΔG_{sol}	-21.48	15.73	12.17	17.04	15.71	9.05	18.79	-21.97

* Calculated at the B3LYP/6-31G(d)//B3LYP/6-31G level of theory.

Table S7. Reaction of **1** with **2d**. Sum of electronic and zero-point energies (*E*, in a.u.), sum of electronic and thermal enthalpies (*H*, in a.u.), sum of electronic and thermal free energies (*G*, in a.u.), thermal correction to Gibbs free energy (*TCGFE*, in a.u.), total free energy in solution (G_S, in a.u., solvent = toluene)*

Structure	*E*	*H*	*G*	*TCGFE*	G_s
1	-344.419239	-344.411865	-344.450328	0.072048	-344.52161
2d	-1090.173531	-1090.160984	-1090.212004	0.138178	-1090.351968
TS1-out-d	-1434.581977	-1434.562428	-1434.631079	0.232123	-1434.866599
IN-out-d	-1434.592824	-1434.573476	-1434.640214	0.235549	-1434.879297
3d	-1434.650590	-1434.631559	-1434.698324	0.23733	-1434.934983
TS1-in-d	-1434.587291	-1434.567711	-1434.636986	0.23175	-1434.869098
IN-in-d	-1434.599673	-1434.580267	-1434.647247	0.235166	-1434.883934
TS2-in-d	-1434.587166	-1434.568242	-1434.634321	0.234825	-1434.868632
4d	-1434.653062	-1434.634164	-1434.700061	0.238357	-1434.937539

* Transition state **TS2-out-d** was not located.

Table S8. Reaction of **1** with **2d**. Electronic energies (Δ*E*, in kcal/mol), enthalpies (Δ*H*, in kcal/mol), Gibbs free energies at 298 K (Δ*G*, in kcal/mol), Gibbs free energies in solution (ΔG_{sol}, in kcal/mol)

Structure	3d	TS2-out-d*	IN-out-d	TS1-out-d	TS1-in-d	IN-in-d	TS2-in-d	4d
Δ*E*	-36.28	–	-0.03	6.77	3.44	-4.33	3.52	-37.83
Δ*H*	-36.84	–	-0.39	6.54	3.22	-4.65	2.89	-38.48
Δ*G*	-22.59	–	13.88	19.61	15.90	9.47	17.58	-23.68
ΔG_{sol}	-21.52	–	12.30	18.12	16.32	9.15	18.54	-22.48

* Transition state **TS2-out-d** was not located.

Table S9. Reaction of **1** with **2e**. Sum of electronic and zero-point energies (*E*, in a.u.), sum of electronic and thermal enthalpies (*H*, in a.u.), sum of electronic and thermal free energies (*G*, in a.u.), thermal correction to Gibbs free energy (*TCGFE*, in a.u.), total free energy in solution (G_S, in a.u., solvent = toluene)*

Structure	*E*	*H*	*G*	*TCGFE*	G_s
1	-344.419239	-344.411865	-344.450328	0.072048	-344.52161
2e	-835.067145	-835.053266	-835.10765	0.148368	-835.258607
TS1-out-e	-1179.474185	-1179.45326	-1179.525348	0.242112	-1179.771391
IN-out-e	-1179.486109	-1179.465432	-1179.53552	0.245728	-1179.78543
3e	-1179.545041	-1179.524655	-1179.594389	0.248013	-1179.842313
TS1-in-e	-1179.479850	-1179.458929	-1179.531245	0.242155	-1179.774289
IN-in-e	-1179.493119	-1179.472379	-1179.542712	0.245347	-1179.790267
TS2-in-e	-1179.481771	-1179.461507	-1179.53099	0.244988	-1179.776118
4e	-1179.547258	-1179.527004	-1179.596306	0.248465	-1179.844701

* Transition state **TS2-out-e** was not located.

Table S10. Reaction of **1** with **2e**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_{sol}, in kcal/mol)

Structure	3e	TS2-out-e*	IN-out-e	TS1-out-e	TS1-in-e	IN-in-e	TS2-in-e	4e
ΔE	-36.81	–	0.17	7.65	4.10	-4.23	2.89	-38.20
ΔH	-37.35	–	-0.19	7.45	3.89	-4.55	2.27	-38.83
ΔG	-22.85	–	14.09	20.48	16.78	9.58	16.94	-24.05
ΔG_{sol}	-21.65	–	12.61	19.15	17.36	9.34	17.99	-22.86

* Transition state **TS2-out-e** was not located.

Table S11. Reaction of **1** with **2f**. Sum of electronic and zero-point energies (*E*, in a.u.), sum of electronic and thermal enthalpies (*H*, in a.u.), sum of electronic and thermal free energies (*G*, in a.u.), thermal correction to Gibbs free energy (*TCGFE*, in a.u.), total free energy in solution (G_S, in a.u., solvent = acetonitrile)

Structure	*E*	*H*	*G*	*TCGFE*	G_s
1	-344.419239	-344.411865	-344.450328	0.072048	-344.519107
2f	-533.742367	-533.729856	-533.78039	0.155804	-533.928347
TS1-out-f	-878.151607	-878.13231	-878.199603	0.250884	-878.445876
IN-out-f	-878.157830	-878.13854	-878.204767	0.252886	-878.459635
TS2-out-f	-878.148574	-878.130091	-878.19424	0.253873	-878.445202
3f	-878.207882	-878.189388	-878.253349	0.257048	-878.499862
TS1-in-f	-878.161808	-878.142326	-878.21071	0.249859	-878.447923
IN-in-f	-878.167937	-878.148656	-878.215241	0.252798	-878.461941
TS2-in-f	-878.144095	-878.12555	-878.190166	0.253183	-878.434621
4f	-878.207620	-878.189183	-878.25285	0.257326	-878.498975

Table S12. Reaction of **1** with **2f**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_{sol}, in kcal/mol)

Structure	3f	TS2-out-f	IN-out-f	TS1-out-f	TS1-in-f	IN-in-f	TS2-in-f	4f
ΔE	-29.04	8.18	2.37	6.27	-0.13	-3.97	10.99	-28.87
ΔH	-29.91	7.30	2.00	5.91	-0.38	-4.35	10.15	-29.78
ΔG	-14.20	22.89	16.28	19.52	12.56	9.71	25.45	-13.89
ΔG_{sol}	-14.57	17.74	8.07	15.44	13.52	6.56	23.95	-13.83

Table S13. Reaction of **1** with **2g**. Sum of electronic and zero-point energies (*E*, in a.u.), sum of electronic and thermal enthalpies (*H*, in a.u.), sum of electronic and thermal free energies (*G*, in a.u.), thermal correction to Gibbs free energy (*TCGFE*, in a.u.), total free energy in solution (G_S, in a.u., solvent = toluene)

Structure	*E*	*H*	*G*	*TCGFE*	G_s
1	-344.419239	-344.411865	-344.450328	0.072048	-344.52161
2g	-512.938480	-512.929983	-512.971087	0.082989	-513.057331
TS1-out-g	-857.340845	-857.325252	-857.384635	0.176005	-857.564587
IN-out-g	-857.357426	-857.342231	-857.399431	0.180027	-857.584995
TS2-out-g	-857.355803	-857.341371	-857.396533	0.181185	-857.582134
3g	-857.410591	-857.395724	-857.452186	0.182242	-857.636383
TS1-in-g	-857.348851	-857.33328	-857.392483	0.17625	-857.570158
IN-in-g	-857.360505	-857.345214	-857.402771	0.179667	-857.586183
TS2-in-g	-857.346160	-857.331352	-857.387698	0.179404	-857.570592
4g	-857.407272	-857.392404	-857.449074	0.181998	-857.633646

Table S14. Reaction of **1** with **2g**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_{sol}, in kcal/mol)

Structure	3g	TS2-out-g	IN-out-g	TS1-out-g	TS1-in-g	IN-in-g	TS2-in-g	4g
ΔE	-33.18	1.20	0.18	10.59	5.56	-1.75	7.25	-31.10
ΔH	-33.81	0.30	-0.24	10.41	5.38	-2.11	6.59	-31.72
ΔG	-19.31	15.61	13.80	23.08	18.16	11.70	21.16	-17.36
ΔG_{sol}	-18.97	14.40	11.88	22.16	18.82	10.91	20.53	-17.41