Supporting Information

Substituent Effects on the Reactivity of Cyclic Tertiary Sulfamidates

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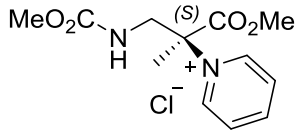
(*S*)-1-(1-Methoxy-3-((methoxycarbonyl)amino)-2-methyl-1-oxopropan-2-yl)pyridin-1-ium chloride 7



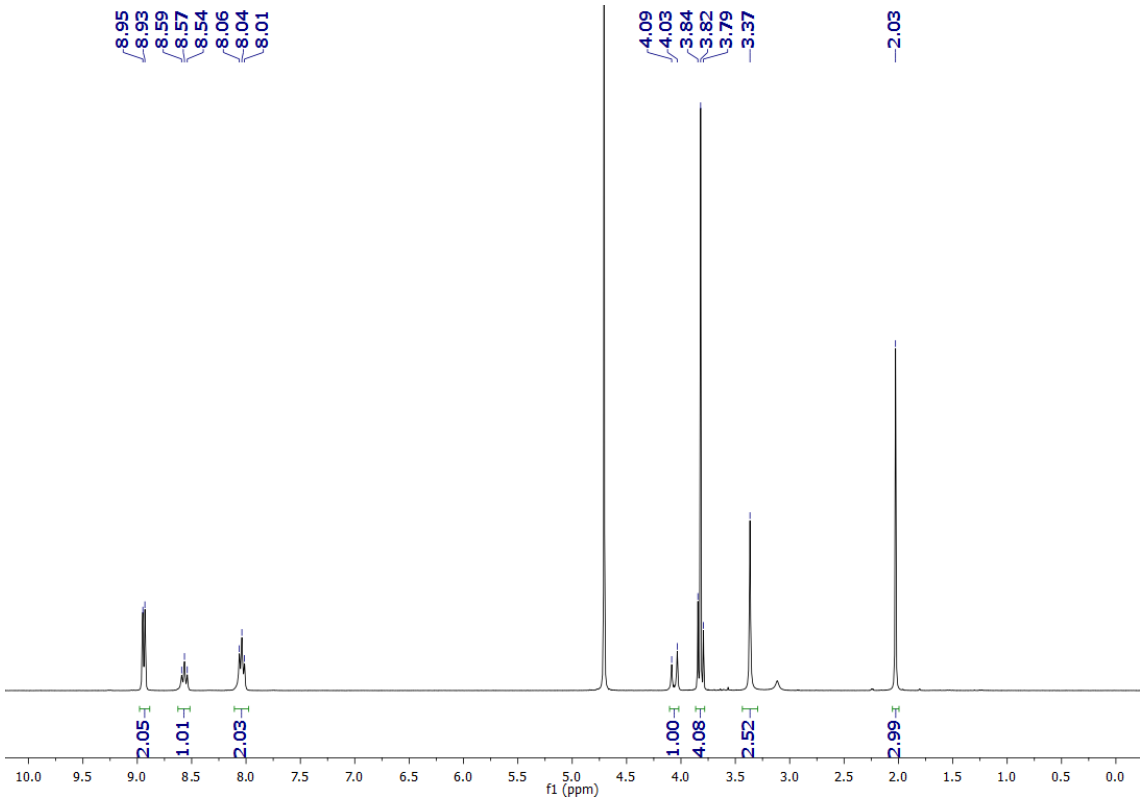
Compound **7'** (50 mg, 0.15 mmol, see ref. 21 for details) was dissolved in a 1:1 mixture of 2 M HCl/CH_2Cl_2. After stirring for 30 minutes at 25 ºC, the layers were separated, and the aqueous phase was lyophilized, affording compound **7** quantitatively (43 mg, 0.15 mmol).

HRMS (ESI) m/z = 253.1183, calculated for $C_{12}H_{17}N_2O_4$ (M^+) = 253.1183.

$[\alpha]_D^{20}$ = –8.5 (*c* 1.00 in H_2O).

^{1}H NMR (400 MHz, D_2O) δ (ppm): 2.03 (s, 3H, C*H*$_3$), 3.37 (s, 3H, NHCO$_2$C*H*$_3$), 3.75-3.90 (m, 4H, CO$_2$C*H*$_3$, C*H*$_2$), 4.06 (d, 1H, *J*= 15.3 Hz, C*H*$_2$), 8.04 (dd, 2H, *J*= 5.6, 7.2 Hz, Py$_{meta}$), 8.57 (t, 1H, *J*= 7.8 Hz Py$_{para}$), 8.94 (d, 2H, *J*= 5.6 Hz Py$_{orto}$).

^{13}C NMR (100 MHz, D_2O) δ (ppm): 20.2 (*C*H$_3$), 47.4 (*C*H$_2$), 52.7 (NHCO$_2$*C*H$_3$), 54.6 (CO$_2$*C*H$_3$), 76.7 (NHCH$_2$*C*), 127.8 (Py$_{meta}$), 143.5 (Py$_{orto}$), 147.3 (Py$_{para}$), 159.0 (NH*C*O$_2$CH$_3$), 170.1 (*C*O$_2$CH$_3$).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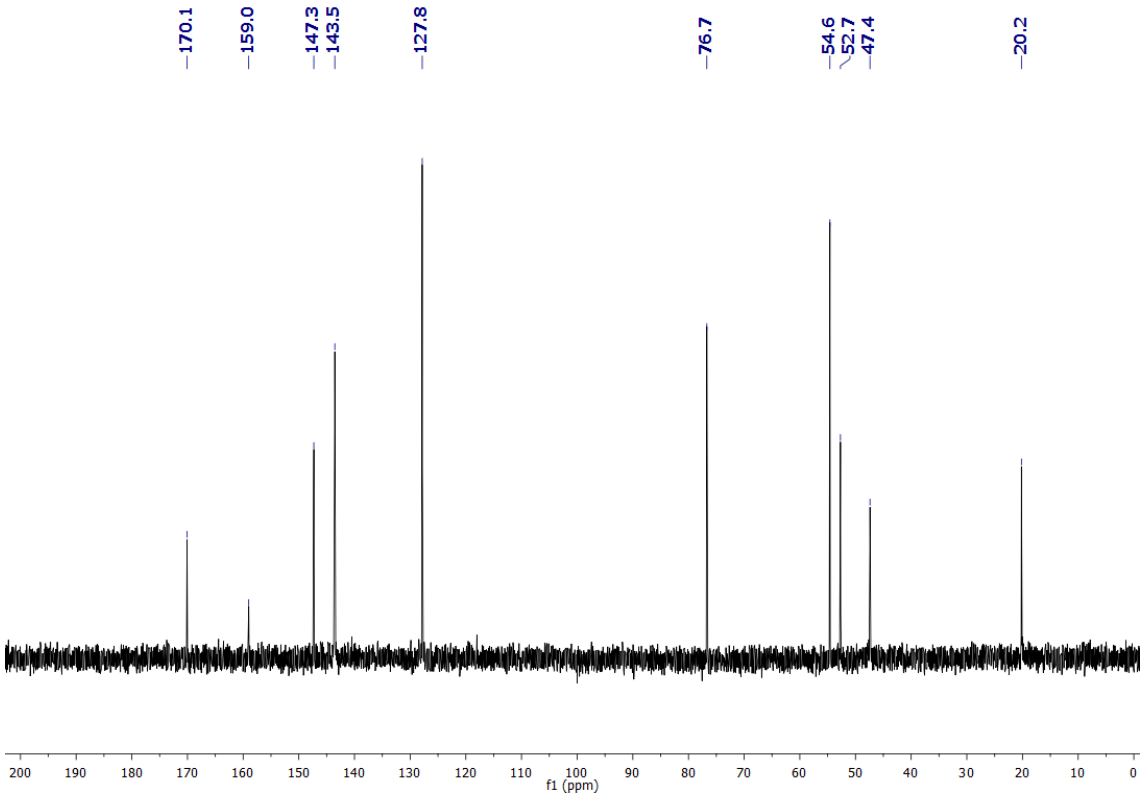
8.93
8.59
8.57
8.54
8.06
8.04
8.01
4.09
4.03
3.84
3.82
3.79
3.37
2.03
2.05
1.01
2.03
1.00
4.08
2.52
2.99
f1 (ppm)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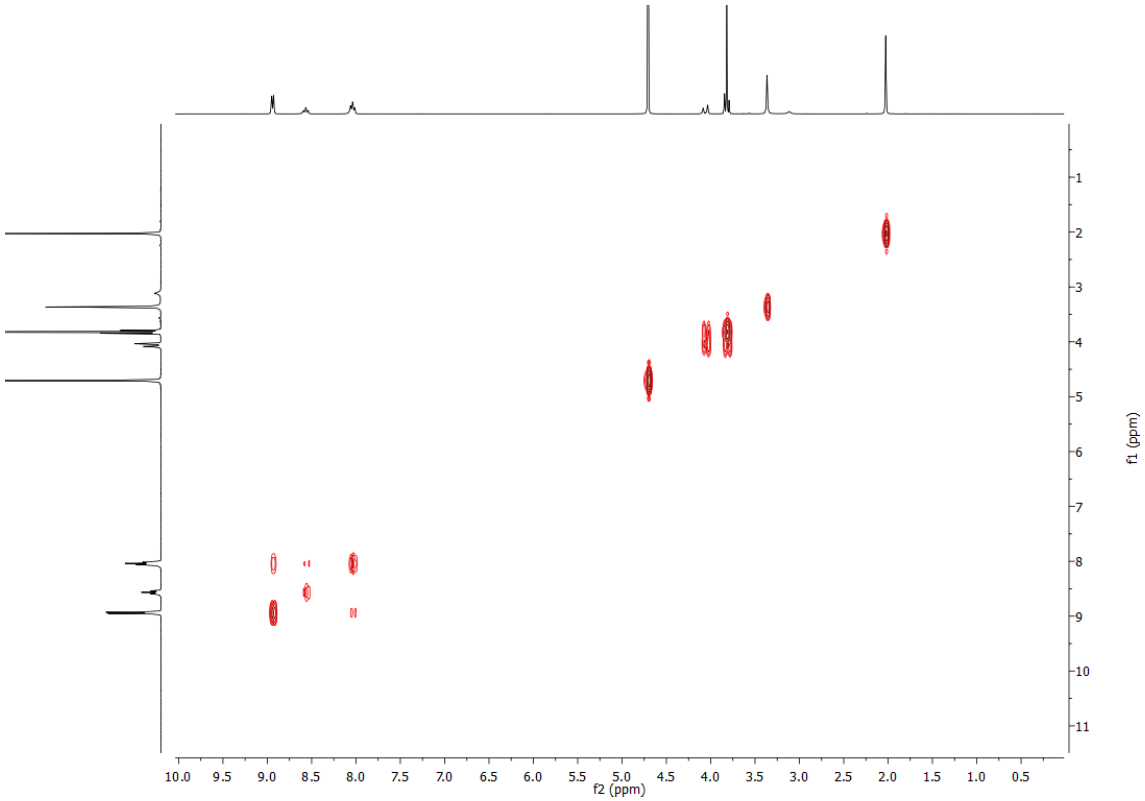
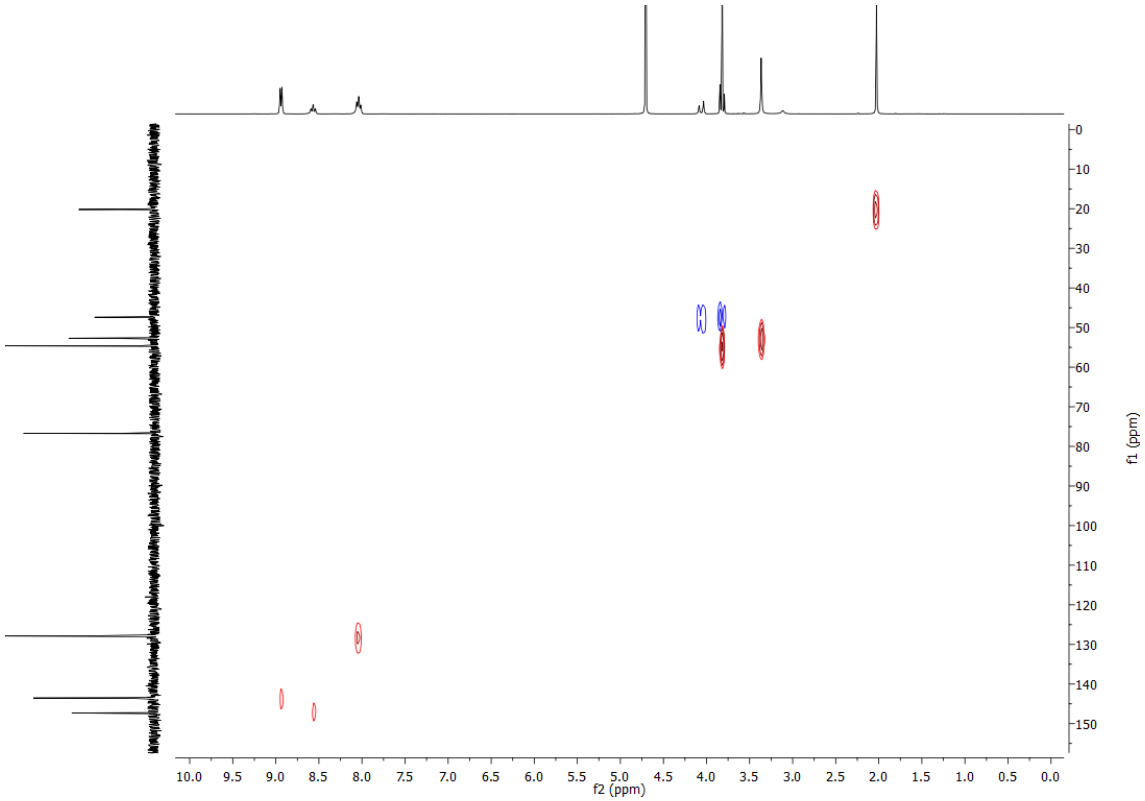
159.0
147.3
143.5
127.8
76.7
54.6
52.7
47.4
20.2
f1 (ppm)


f1 (ppm)
f2 (ppm)


f1 (ppm)
f2 (ppm)

Compounds **1**, **2**, **3** and **6** were fully characterized in ref. 21.

Compounds **4** and **5** were fully characterized in ref. 23.

Compounds **8** and **9** were fully characterized in ref. 24.

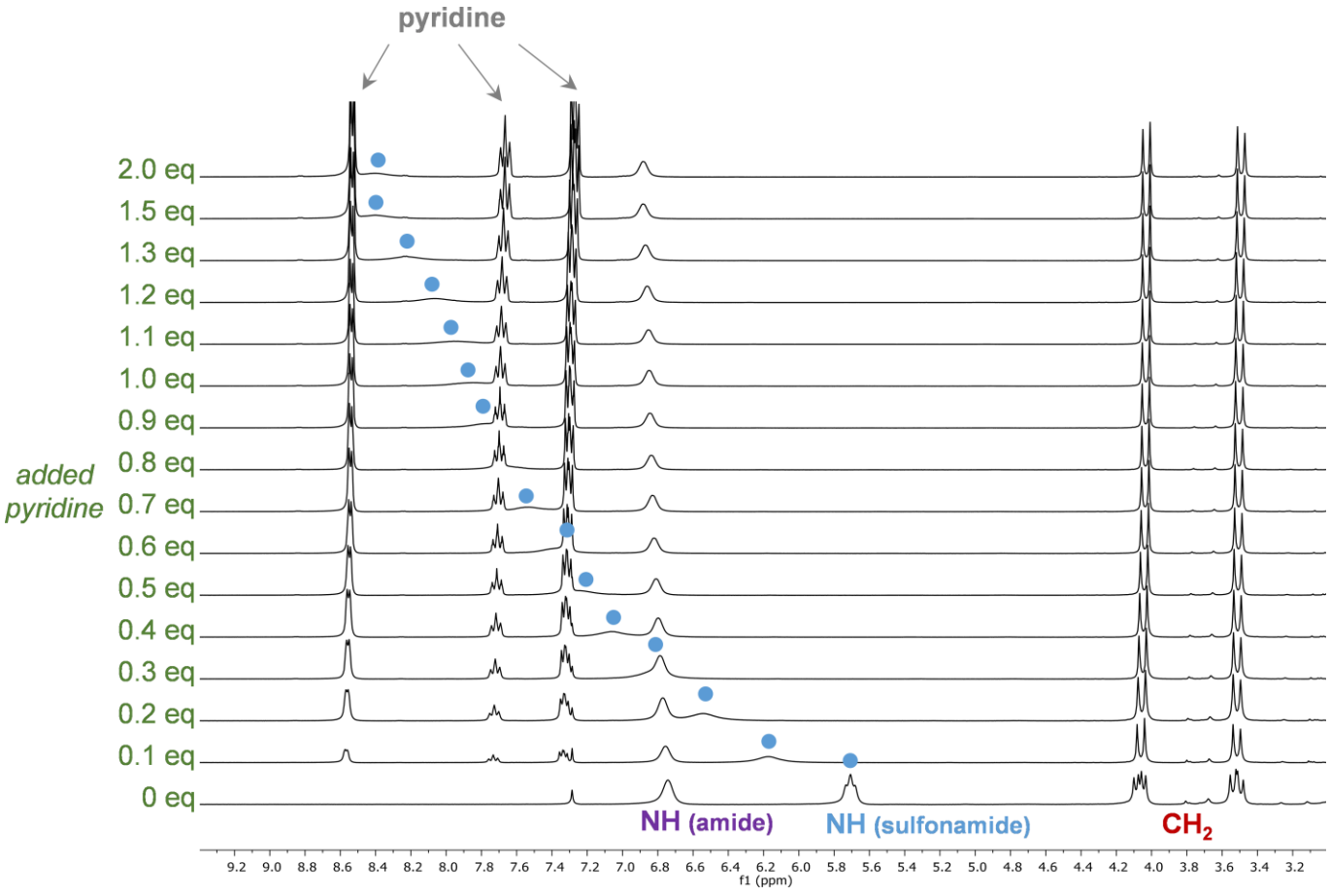


Figure S1. ^{1}H NMR titration experiments of sulfamidate **5** in $CDCl_3$. Incresaing amounts of pyridine cause the sulfonamide NH proton signal to and broaden and shift downfield due to competitive hydrogen bonding.

Table S1. **Energies, enthalpies, free energies, and entropies of the lowest energy structures calculated at the PCM(Pyridine)/M06-2X/6-31+G(d,p) level.**

All the computed conformations can be obtained from the authors upon request.

Compound	E0 (Hartree)[a]	E0+ZPE (Hartree)[a]	E0+DH (Hartree)[a]	E0+DG (Hartree)[a]	S (cal mol^{-1} K^{-1})[b]	E0+DG_corr (Hartree)[a]	Freq1 (cm^{-1})
Pyridine	–248.191435	–248.101816	–248.095535	–248.133104	70.8	–248.133104	386.4
1	–1177.302210	–1177.105495	–1177.085420	–1177.157524	135.8	–1177.153855	20.1
1-TS_{SN2}	–1425.465079	–1425.178056	–1425.151465	–1425.238394	163.7	–1425.233597	–540.1
1-TS_{E2}	–1425.451263	–1425.169603	–1425.142632	–1425.233195	170.6	–1425.225535	–1307.9
2	–1252.504173	–1252.301424	–1252.280341	–1252.354435	139.6	–1252.351259	25.8
2-TS_{SN2}	–1500.665332	–1500.372878	–1500.344976	–1500.435752	171.0	–1500.430120	–542.7
2-TS_{E2}	–1500.651927	–1500.364637	–1500.336454	–1500.430088	176.4	–1500.422145	–1293.5
3	–1024.703760	–1024.543845	–1024.528388	–1024.588651	113.5	–1024.586867	37.1
3-TS_{SN2}	–1272.860245	–1272.610532	–1272.588299	–1272.664505	143.5	–1272.661434	–542.6
3-TS_{E2}	–1272.848201	–1272.603554	–1272.581034	–1272.661029	150.7	–1272.654907	–1295.1
4	–1157.453084	–1157.243961	–1157.223517	–1157.296224	136.9	–1157.292471	25.1
4-TS_{SN2}	–1405.610215	–1405.310960	–1405.283892	–1405.371963	165.9	–1405.366860	–531.4
4-TS_{E2}	–1405.604506	–1405.310568	–1405.283241	–1405.373990	170.9	–1405.367074	–1276.5
5	–1004.855002	–1004.682857	–1004.666877	–1004.728625	116.3	–1004.726383	38.1
5-TS_{SN2}	–1253.007143	–1252.744682	–1252.722333	–1252.798272	143.0	–1252.795977	–532.4
5-TS_{E2}	–1252.999377	–1252.742776	–1252.719735	–1252.800294	151.7	–1252.794969	–1287.0

[a] 1 Hartree = 627.5 kcal mol^{-1}. [b] Thermal corrections at 333.15 K.

Cartesian coordinates of the structures calculated at the PCM(Pyridine)/M06-2X/6-31+G(d,p) level.

All the computed conformations can be obtained from the authors upon request.

Structure **Pyridine**

C	1.142544	0.721156	-0.000211
C	1.197132	-0.671811	-0.000121
C	0.000003	-1.382950	0.000092
C	-1.197128	-0.671816	0.000210
C	-1.142547	0.721150	0.000117
N	-0.000003	1.417379	-0.000094
H	0.000008	-2.468347	0.000163
H	2.059447	1.305126	-0.000372
H	2.155603	-1.178958	-0.000219
H	-2.155600	-1.178964	0.000373
H	-2.059452	1.305115	0.000195

Structure **1**

C	0.991461	0.601871	0.915170
C	-0.287969	1.421981	0.747450
N	-1.236049	0.469821	0.163290
S	-0.760219	-1.131389	0.381500
O	0.519191	-0.730489	1.264100
C	1.887901	1.075781	2.041480
C	1.780511	0.527011	-0.405610
O	1.676671	1.348681	-1.286240
C	3.393541	-0.667899	-1.608780
O	-0.353829	-1.698079	-0.886540
O	-1.669149	-1.872869	1.222280
H	-0.141999	2.256441	0.062170
H	-0.649749	1.778381	1.715310
H	2.762221	0.428681	2.125140
H	2.215781	2.097391	1.832260
H	1.330861	1.063701	2.979970
H	3.994081	-1.558049	-1.441210
H	4.026751	0.208441	-1.752320
H	2.736341	-0.799019	-2.469570
C	-2.358529	0.881381	-0.556440
O	-2.591169	2.070631	-0.641820
C	-3.195539	-0.198839	-1.183730
H	-2.623289	-0.704029	-1.966830
H	-3.496369	-0.943729	-0.442140
H	-4.079139	0.264921	-1.617600
O	2.602301	-0.508799	-0.417960

Structure **1-TS$_{SN2}$**

C	-0.204661	0.331151	0.540020
C	0.433679	-0.653549	-0.423220
N	1.850139	-0.779419	-0.103380
S	2.639439	0.723471	0.160920
O	1.392719	1.522261	0.467890
C	-0.133851	0.056841	2.011780
C	-0.937341	1.570111	0.054080
O	-1.439661	2.363341	0.813750
C	-1.643901	2.793771	-1.807940
O	3.511739	0.547831	1.315830
O	3.286459	1.136371	-1.080350
H	0.286809	-0.332379	-1.458020
H	-0.003511	-1.641559	-0.276980
H	0.902499	-0.136479	2.292610
H	-0.507251	0.911041	2.575970
H	-0.710301	-0.838299	2.251120
H	-1.545411	2.706741	-2.886850
H	-1.180141	3.712801	-1.448000
H	-2.693101	2.762701	-1.509240
C	-4.805881	-1.487240	-0.043240
C	-4.436681	-0.781450	1.099070
C	-3.132841	-0.310339	1.198090
C	-2.578701	-1.185649	-0.866390
C	-3.861961	-1.689880	-1.046420
H	-5.815461	-1.868720	-0.152430
H	-5.139561	-0.591720	1.901420
H	-2.805341	0.260491	2.062430
H	-1.819161	-1.315059	-1.631350
H	-4.105831	-2.226020	-1.955790
N	-2.223971	-0.522289	0.239860
C	2.503919	-1.973749	-0.377610
O	1.862109	-2.941049	-0.756990
O	-0.952501	1.655581	-1.266820
C	3.993119	-2.014089	-0.159710
H	4.492479	-1.206629	-0.700930
H	4.218669	-1.892739	0.901810
H	4.354099	-2.978019	-0.513350

Structure **1-TS$_{E2}$**

N	1.783519	-1.027190	-0.022930
S	2.859040	0.137959	0.629080
O	1.804970	0.947020	1.370940
C	0.087990	0.501390	0.779190
C	0.424459	-0.942850	0.492200
O	3.787229	-0.527531	1.536440
O	3.454820	0.856129	-0.491460
C	-0.875250	0.787411	1.759870
C	0.085510	1.395260	-0.450960
O	0.055290	0.950990	-1.576680
C	0.063311	3.590500	-1.255220
H	-0.249841	-1.325190	-0.279150
H	0.304429	-1.537390	1.403350
H	-1.094960	1.838671	1.931530
H	-0.846590	0.165471	2.653920

H	0.071781	4.585650	-0.818120
H	0.949181	3.429650	-1.871240
H	-0.837089	3.435581	-1.851690
H	-2.013170	0.327071	1.124790
N	-3.169601	-0.111399	0.610070
C	-3.596181	-1.344488	0.902630
C	-3.876660	0.683932	-0.199490
C	-4.782621	-1.840748	0.379160
H	-2.964171	-1.927759	1.565940
C	-5.073420	0.260332	-0.762090
H	-3.463570	1.670842	-0.387420
C	-5.530451	-1.022658	-0.465940
H	-5.107682	-2.843388	0.629130
H	-5.629150	0.922082	-1.415260
H	-6.461411	-1.382497	-0.890860
C	2.138949	-2.027250	-0.909020
O	1.302358	-2.844840	-1.264150
C	3.559739	-2.039041	-1.408420
H	4.273739	-1.944601	-0.587040
H	3.720848	-2.976431	-1.937630
H	3.714979	-1.196681	-2.086780
O	0.075130	2.682100	-0.141360

Structure **2**

C	-1.354942	-0.322371	1.002639
C	-0.055492	-1.090761	1.255409
N	0.952668	-0.293621	0.555989
S	0.424338	1.263449	0.174629
O	-0.949212	1.074019	0.991879
C	-2.391012	-0.487271	2.096209
C	-1.955812	-0.685381	-0.368691
O	-1.704742	-1.714801	-0.950851
C	-3.418122	0.000899	-2.061401
O	0.156338	1.361949	-1.242571
O	1.190608	2.291839	0.831439
H	-0.094462	-2.092991	0.829049
H	0.165548	-1.131871	2.324589
H	-3.274272	0.111989	1.870969
H	-2.678292	-1.539911	2.162489
H	-1.965932	-0.171061	3.050399
H	-4.064232	0.856749	-2.238031
H	-3.996412	-0.923121	-2.024061
H	-2.648772	-0.070801	-2.831541
C	2.139148	-0.833061	0.088419
O	2.463548	-1.979941	0.292379
O	-2.800592	0.242709	-0.784941
O	2.836188	0.080759	-0.577911
C	4.097288	-0.363081	-1.109621
H	3.934068	-1.179981	-1.812921
H	4.515208	0.504089	-1.613971
H	4.745998	-0.689021	-0.296161

Structure **2-TS$_{SN2}$**

C	0.470899	-0.457050	0.523910
C	-0.294812	0.477440	-0.398450
N	-1.703451	0.429979	-0.031660
S	-2.323071	-1.158201	0.218730
O	-0.970371	-1.825571	0.361110
C	0.373219	-0.256680	2.005810
C	1.353399	-1.570880	-0.013750
O	1.948680	-2.332910	0.709110
C	2.225060	-2.590339	-1.929220
O	-3.078241	-1.137282	1.463720
O	-3.036131	-1.583422	-0.978890
H	-0.145131	0.192470	-1.443120
H	0.037288	1.503970	-0.241330
H	-0.671971	-0.310161	2.313350
H	0.938369	-1.026110	2.531330
H	0.740218	0.737250	2.268660
H	2.120580	-2.460310	-3.003260
H	1.887620	-3.581020	-1.622850
H	3.259280	-2.434499	-1.617210
C	4.788198	1.957882	-0.015750
C	4.479348	1.290851	1.166680
C	3.251398	0.646841	1.267480
C	2.659028	1.280941	-0.873160
C	3.863428	1.950281	-1.056780
H	5.737518	2.470932	-0.126600
H	5.171458	1.261712	1.999720
H	2.976989	0.102981	2.166360
H	1.919208	1.238960	-1.666930
H	4.063268	2.448251	-1.998030
N	2.358788	0.656231	0.271770
C	-2.495242	1.531649	-0.290130
O	-2.050232	2.603149	-0.651490
O	-3.780592	1.266208	-0.078920
C	-4.684082	2.357568	-0.311100
H	-5.673422	1.959397	-0.099920
H	-4.449643	3.185118	0.359480
H	-4.613482	2.686328	-1.348600
O	1.384959	-1.584990	-1.337740

Structure **2-TS$_{E2}$**

N	1.608699	0.722089	-0.506979
S	2.574549	-0.681311	-0.732229
O	1.444909	-1.536630	-1.299649
C	-0.179731	-0.882130	-0.704409
C	0.213569	0.566580	-0.893169
O	3.607879	-0.405721	-1.718429
O	3.011629	-1.134601	0.581761
C	-1.248641	-1.394800	-1.458479
C	-0.110361	-1.353420	0.740951
O	-0.209691	-0.580970	1.670601
C	2.043330	1.873129	0.107561
O	3.342320	1.808589	0.394431

C	3.890100	2.963739	1.045861
O	0.003529	-2.663690	0.851191
C	0.067418	-3.172230	2.194671
O	1.320640	2.822800	0.338831
H	-0.392831	1.203260	-0.243519
H	0.055449	0.853900	-1.936439
H	-1.511191	-2.434960	-1.278829
H	-1.289341	-1.078190	-2.500279
H	3.389740	3.126399	2.001271
H	3.773840	3.842039	0.409711
H	4.942250	2.735329	1.197251
H	0.170958	-4.249290	2.092181
H	0.931779	-2.745530	2.705541
H	-0.846962	-2.918270	2.732691
H	-2.323491	-0.668660	-0.903609
N	-3.372581	-0.003699	-0.481559
C	-4.434631	0.135761	-1.282179
C	-3.353381	0.544871	0.739491
C	-5.552811	0.850891	-0.875479
H	-4.368581	-0.338829	-2.256399
C	-4.433931	1.275871	1.214961
H	-2.452371	0.384840	1.326371
C	-5.548811	1.429021	0.392951
H	-6.402711	0.950641	-1.539629
H	-4.396830	1.712631	2.205511
H	-6.407750	1.995031	0.737291

Structure **3**

C	-0.421730	0.799880	-0.094519
C	0.187120	0.808490	1.337971
N	1.146670	-0.300010	1.381661
S	1.889060	-0.297951	-0.109349
O	0.646830	0.346560	-0.951539
C	-0.882279	2.165560	-0.554969
C	-1.496620	-0.291799	-0.132039
O	-1.222831	-1.470679	-0.162129
C	-3.784030	-0.770318	0.033501
O	2.142039	-1.647231	-0.559619
O	2.957710	0.677059	-0.129029
H	-0.566600	0.680660	2.115381
H	0.716571	1.750580	1.500891
H	-1.312399	2.113001	-1.556559
H	-1.639749	2.549031	0.131551
H	-0.026449	2.843450	-0.563919
H	-4.700610	-0.191848	0.113701
H	-3.643831	-1.403028	0.910801
H	-3.787371	-1.382078	-0.869179
H	0.689069	-1.205680	1.503741
O	-2.723130	0.199581	-0.041199

Structure **3-TS$_{SN2}$**

C	0.210661	-0.385100	0.477141
C	0.629131	-0.988940	-0.858429
N	1.980411	-1.525289	-0.700879
S	3.010821	-0.291679	-0.183309
O	2.076030	0.287931	0.867461
C	0.161791	-1.276160	1.680001
C	-0.145820	1.081839	0.629251
O	-0.465230	1.565869	1.689401
C	-0.395711	3.134949	-0.460049
O	4.196501	-0.929548	0.385091
O	3.265640	0.653882	-1.276069
H	0.553971	-0.238070	-1.651279
H	-0.029598	-1.831261	-1.078129
H	1.108282	-1.812300	1.748821
H	0.006191	-0.689420	2.584801
H	-0.631988	-2.016391	1.565741
H	-0.271492	3.505239	-1.474449
H	0.287768	3.639860	0.223681
H	-1.425181	3.264979	-0.122019
C	-4.656199	-0.573603	-0.478379
C	-4.162379	-0.541983	0.823291
C	-2.785989	-0.503162	1.012581
C	-2.395579	-0.521242	-1.263779
C	-3.757479	-0.559423	-1.541669
H	-5.724949	-0.603504	-0.661539
H	-4.823339	-0.542733	1.681761
H	-2.356529	-0.458882	2.009431
H	-1.666089	-0.498902	-2.067409
H	-4.095239	-0.574943	-2.571019
N	-1.925339	-0.506232	-0.011449
O	-0.076991	1.735519	-0.520769
H	2.327392	-1.968439	-1.549789

Structure **3-TS$_{E2}$**

N	2.035431	-1.036659	-1.310541
S	3.197861	-0.800929	-0.108891
O	2.373610	-0.012789	0.925359
C	0.553020	-0.115090	0.444529
C	0.740001	-1.161670	-0.648651
O	3.560532	-2.114208	0.419179
O	4.267240	-0.003028	-0.704781
C	-0.285629	-0.419011	1.526529
C	0.559130	1.314460	-0.062831
O	0.646089	1.590120	-1.242141
O	0.439749	2.205630	0.907829
C	0.452038	3.583010	0.496999
H	-0.050009	-1.048221	-1.396511
H	0.654862	-2.155310	-0.201691
H	-0.410190	0.349499	2.285389
H	-0.225829	-1.440631	1.901029
H	0.363258	4.159980	1.413869
H	1.388748	3.807810	-0.014701

H	-0.390692	3.778209	-0.168211
H	-1.528449	-0.425932	0.894329
N	-2.758359	-0.456072	0.400129
C	-3.606229	-1.429293	0.748499
C	-3.133740	0.513757	-0.440081
C	-4.902289	-1.465764	0.251319
H	-3.224178	-2.178393	1.435099
C	-4.412160	0.545727	-0.980371
H	-2.386160	1.267368	-0.674531
C	-5.308139	-0.461484	-0.625831
H	-5.573188	-2.263224	0.546939
H	-4.693641	1.340896	-1.659911
H	-6.314669	-0.463735	-1.030251
H	2.051080	-0.217989	-1.919981

Structure **4**

C	1.039220	0.392250	1.000730
C	-0.175950	1.308340	0.854820
N	-1.096620	0.517199	0.037120
S	-0.928429	-1.127271	0.338350
O	0.481281	-0.956080	1.095260
C	1.840430	0.640500	2.263390
C	1.950790	0.501650	-0.235400
O	2.321770	1.615520	-0.598340
N	2.330551	-0.643080	-0.813070
C	3.231821	-0.636919	-1.954560
O	-0.752649	-1.852971	-0.900000
O	-1.897749	-1.613341	1.294360
H	0.084240	2.224680	0.326170
H	-0.617890	1.541459	1.828620
H	2.673740	-0.062180	2.328260
H	2.236320	1.658140	2.232990
H	1.198000	0.526060	3.138290
H	1.965001	-1.518670	-0.466460
H	3.426241	-1.666869	-2.247440
H	4.172690	-0.149089	-1.690160
H	2.782000	-0.098879	-2.792430
C	-2.187140	1.093129	-0.627050
O	-2.314480	2.299239	-0.594190
C	-3.103200	0.156869	-1.364500
H	-2.559629	-0.338431	-2.172800
H	-3.498739	-0.613182	-0.695690
H	-3.925830	0.740608	-1.772580

Structure **4-TS$_{SN2}$**

C	-0.185780	0.478870	0.314930
C	0.394720	-0.592871	-0.589230
N	1.779599	-0.824832	-0.196660
S	2.686980	0.617588	0.016370
O	1.501741	1.553279	0.076020
C	-0.116430	0.294720	1.802940
C	-0.872579	1.674780	-0.341520
O	-1.033879	1.700800	-1.556760
N	-1.262538	2.655620	0.483150
C	-1.868278	3.864801	-0.053350
O	3.391180	0.492417	1.288470
O	3.521581	0.831907	-1.161200
H	0.313500	-0.276611	-1.632720
H	-0.131301	-1.535150	-0.445880
H	0.756161	0.813009	2.203940
H	-1.005430	0.692700	2.293610
H	-0.015170	-0.766360	2.041690
H	-0.989218	2.638730	1.454570
H	-2.152967	4.506961	0.777990
H	-2.756328	3.607551	-0.633730
H	-1.165787	4.394510	-0.702330
C	-4.616201	-1.903097	-0.117700
C	-4.029741	-1.758258	1.135920
C	-2.841261	-1.042229	1.238980
C	-2.808260	-0.620939	-1.026770
C	-3.992271	-1.324838	-1.219520
H	-5.541382	-2.457657	-0.233710
H	-4.474271	-2.190478	2.024630
H	-2.358791	-0.922949	2.203370
H	-2.295070	-0.141209	-1.854510
H	-4.407861	-1.410528	-2.216630
N	-2.244590	-0.481919	0.181160
C	2.319379	-2.101142	-0.250160
O	1.607008	-3.053682	-0.528940
C	3.784289	-2.242613	0.069950
H	4.386809	-1.546343	-0.518310
H	3.955709	-2.022923	1.126050
H	4.075848	-3.267623	-0.151100

Structure **4-TS$_{E2}$**

N	1.685890	-0.969840	-0.159060
S	2.820820	-0.118940	0.815530
O	1.819180	0.777810	1.515790
C	0.039030	0.540960	0.729880
C	0.325090	-0.888660	0.352930
O	3.453090	-1.069240	1.725840
O	3.713190	0.598510	-0.087970
C	-0.931700	0.816910	1.703540
C	0.120590	1.520920	-0.435860
O	-0.648460	1.312010	-1.376610
C	1.025760	3.541460	-1.419310
H	-0.357150	-1.180100	-0.451180
H	0.171500	-1.549410	1.212710
H	-1.100990	1.865350	1.942910
H	-0.964370	0.135050	2.552720
H	1.684880	4.347000	-1.101520
H	1.422080	3.084480	-2.329990
H	0.033760	3.944620	-1.631920
H	-2.005580	0.457250	1.000340
N	-3.233870	0.032880	0.468130
C	-4.119490	-0.452540	1.344810

C	-3.535500	0.097530	-0.834940
C	-5.371660	-0.901980	0.945940
H	-3.804180	-0.474480	2.384350
C	-4.768010	-0.333920	-1.312430
H	-2.760810	0.500940	-1.479550
C	-5.698370	-0.840120	-0.407580
H	-6.068340	-1.289610	1.679520
H	-4.987050	-0.272000	-2.371780
H	-6.667940	-1.183550	-0.752730
N	0.944150	2.562930	-0.346880
H	1.599950	2.584360	0.422970
C	2.024860	-1.963980	-1.067920
O	1.151930	-2.681210	-1.530560
C	3.473990	-2.077010	-1.459730
H	4.107750	-2.205449	-0.578470
H	3.576130	-2.936690	-2.119250
H	3.795020	-1.167010	-1.970820

Structure **5**

C	-0.359361	0.993331	-0.229402
C	0.420529	1.353632	1.052228
N	1.197230	0.157483	1.406858
S	1.704091	-0.515076	-0.025792
O	0.527110	0.112902	-0.969892
C	-0.678153	2.195551	-1.097622
C	-1.649420	0.239669	0.133908
O	-2.464221	0.781228	0.879638
N	-1.816888	-0.973821	-0.404822
C	-3.025367	-1.742493	-0.153412
O	1.572893	-1.956206	0.014208
O	2.947440	0.079536	-0.460152
H	-0.251142	1.620291	1.866908
H	1.108037	2.179473	0.854178
H	-1.204272	1.885390	-2.003002
H	-1.316464	2.880230	-0.534702
H	0.247497	2.704472	-1.374192
H	-1.105058	-1.336650	-1.023342
H	-2.935466	-2.703392	-0.656472
H	-3.902378	-1.212514	-0.533202
H	-3.152997	-1.904143	0.919238
H	0.669241	-0.535398	1.938348

Structure **5-TS$_{SN2}$**

C	0.171529	-0.333000	0.600040
C	0.426100	-1.060540	-0.743740
N	1.759950	-1.638680	-0.868630
S	2.871789	-0.498660	-0.321520
O	2.168739	-0.020870	0.938250
C	0.008400	-1.124410	1.863190
C	0.002399	1.182100	0.738930
O	-0.548481	1.635479	1.734500
N	0.422729	1.937810	-0.292720
C	0.355729	3.387850	-0.177640
O	4.129720	-1.187860	-0.064500
O	2.878539	0.557370	-1.343880
H	0.250049	-0.374180	-1.575190
H	-0.287050	-1.878900	-0.829370
H	0.706119	-0.748700	2.610370
H	-0.996420	-0.989901	2.263610
H	0.205420	-2.184330	1.689850
H	1.128889	1.554940	-0.917310
H	-0.671151	3.694069	0.031430
H	0.676448	3.823510	-1.122520
H	0.996888	3.751350	0.631230
C	-4.663321	-0.526441	-0.642830
C	-4.009040	-1.606731	-0.055780
C	-2.663130	-1.473871	0.264350
C	-2.601691	0.687879	-0.533950
C	-3.946441	0.640539	-0.888390
H	-5.713731	-0.594402	-0.904990
H	-4.523140	-2.537201	0.153790
H	-2.118720	-2.296341	0.722130
H	-2.007401	1.579369	-0.712530
H	-4.411161	1.506099	-1.345540
N	-1.977731	-0.348971	0.034040
H	1.870360	-2.491130	-0.319550

Structure **5-TS$_{E2}$**

N	1.896970	-0.755820	-1.337340
S	3.101410	-0.982980	-0.170820
O	2.338170	-0.400320	1.012670
C	0.469940	-0.088430	0.457690
C	0.594500	-1.011490	-0.730570
O	3.367730	-2.414760	0.011070
O	4.252600	-0.176951	-0.575500
C	-0.391680	-0.421729	1.510630
C	0.552001	1.390810	0.098360
O	-0.360569	1.828631	-0.608030
C	1.623101	3.553260	0.315810
H	-0.187270	-0.740030	-1.448130
H	0.447770	-2.051000	-0.412470
H	-0.445719	0.278551	2.342620
H	-0.423960	-1.474879	1.787430
H	2.455722	3.968410	0.880700
H	1.786881	3.724260	-0.751500
H	0.697982	4.052200	0.612060
H	-1.564900	-0.251769	0.860160
N	-2.847510	-0.243109	0.358470
C	-3.682390	-1.146989	0.882390
C	-3.267269	0.601411	-0.592030
C	-5.003730	-1.245988	0.467040
H	-3.267620	-1.795739	1.648950
C	-4.575629	0.563242	-1.060660
H	-2.524439	1.301451	-0.961020
C	-5.454770	-0.373918	-0.522270
H	-5.657850	-1.987618	0.909500

H	-4.892409	1.256342	-1.830910	N	1.537111	2.131080	0.601850
H	-6.481280	-0.424798	-0.869660	H	2.280081	1.649900	1.091860
H	2.080540	-1.316520	-2.167300				