O-phenylenediamine: A Privileged Pharmacophore of Ferrostatins for Radical-Trapping Activity in Blocking Ferroptosis

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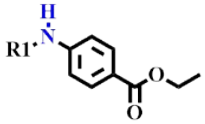
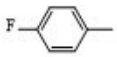
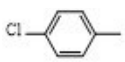
Tab. S1 The experimental and computational data of compound **1-13.**



NO.	R1-Compounds	cLogP[a]	MNTD[b]	EC_{50} (nM)	BDE kcal mol^{-1}	ΔE kcal mol^{-1}
Fer	/	2.9	125000	50	80	10.45
1		4.91	12500	>12500	88	18.80
2		3.67	12500	>12500	87	18.11
3	CH_3-	2.72	12500	>12500	88	19.85
4		3.68	12500	>12500	88	21.32
5		3.78	12500	>12500	88	17.58
6		4.29	6250	>6250	88	18.29
7		3.77	12500	>12500	88	17.74
8		2.99	12500	>12500	89	18.39
9		2.50	12500	>12500	88	19.85
10		3.74	12500	>12500	89	17.51
11		4.19	12500	>12500	89	17.23
12		3.90	12500	>12500	89	17.25
13		4.42	12500	>12500	89	17.41

a: The calculated octanol-water partition coefficient (clog P) is predicted by using the Molinspiration Cheminformatics server (http://www.molinspiration.com). b: MNTD means the maximum non-toxic dose.

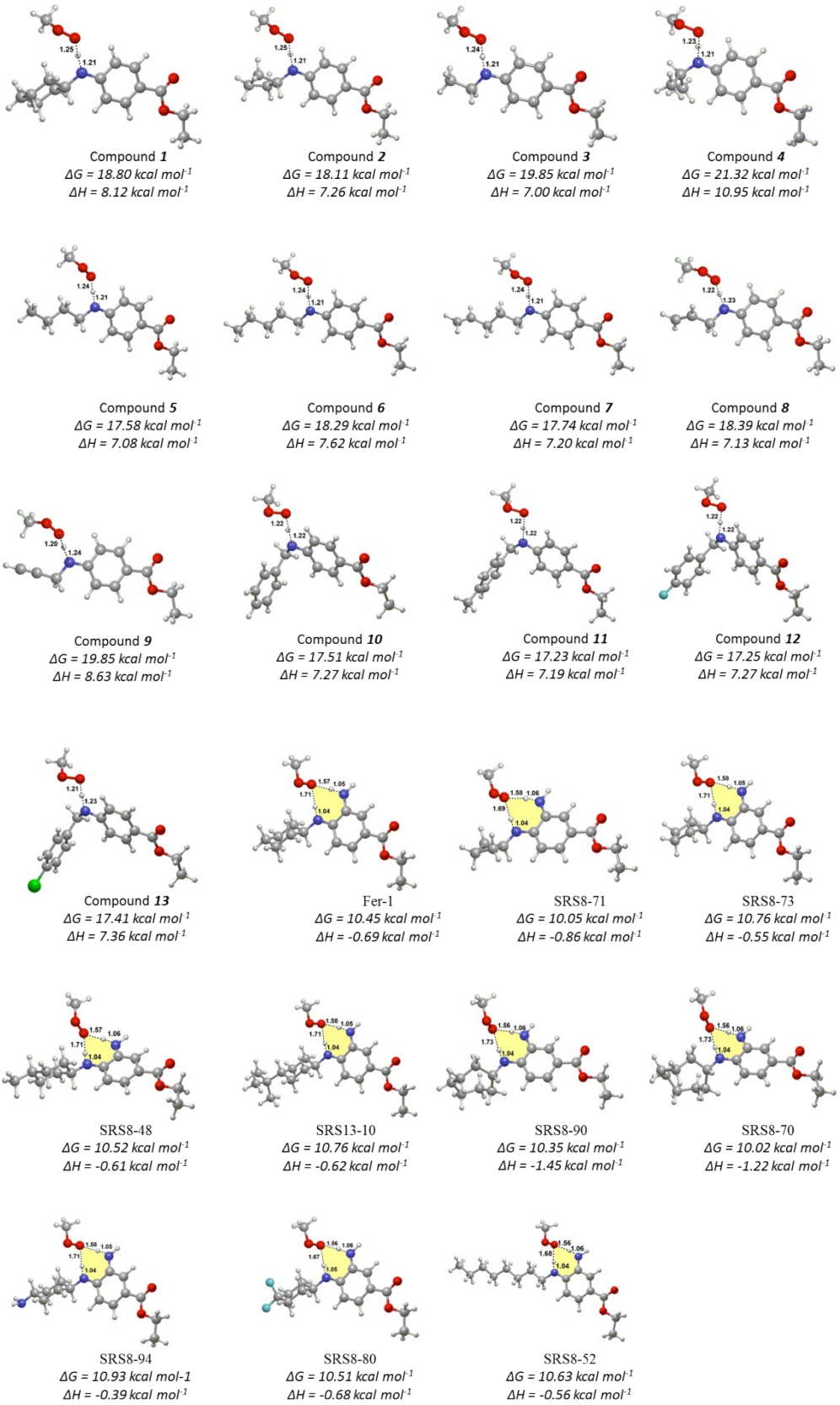


Fig S1 Transition States Structures of serial *R1* and serial *R2*

Site Selectivity of H-atom Abstraction

Fer-1 possesses three candidate hydrogen from two –$NH_{(2)}$ groups that may represent attack sites by lipid peroxide radical. Therefore, we first check the H-atom transfer reaction between each -NH group and $CH_3OO\cdot$ to determine the most reactive site. However, we have just found two possible H-abstraction paths occur at position $H_{3'}$ and $H_{3''}$ by quantum calculation. The possible mechanisms are listed in Figure S1. The required energy barrier for transferring the hydrogen atom from -NH groups to methylperoxyl radical is calculated: 10.45 ($H_{3'}$) and 17.57 ($H_{3''}$). It is clear that the reactivity order is $H_{3'} > H_{3''}$. Corresponding, the BDE (N-H) value at position 3′ is 79.81 kcal mol^{-1}, which is also significantly smaller than that of position 3″ with the value of 87.23 kcal mol^{-1}.

The most obvious difference between two reaction paths is geometric feature of transition state. For position 3′, the two hydrogen atoms of *ortho*-diamines interact with methylperoxyl radical together and form a stable seven-membered ring in help of the reaction energetically favorable. For position 3′, one hydrogen atom of –NH group interacts with radical and forms a linear transition structure with less compact, leading the H-atom abstract reaction is endothermic. The above results reveal that $H_{3'}$ is the most favorable site in trapping lipid radical.

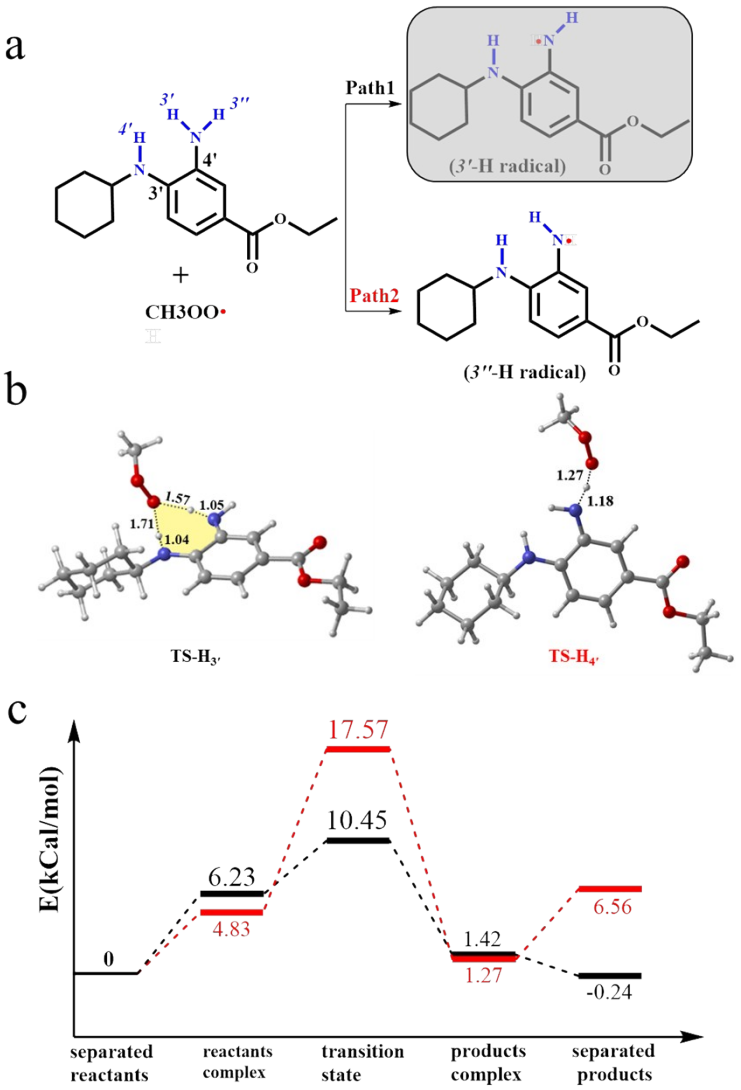


Fig S2 (a) Possible Reactions between Fer-1 and $CH_3OO\cdot$. (b) Optimized structures of transition state for the two reactions. (c) Potential energy profiles for $CH_3OO\cdot$ with the $H_{3'}$ (black line) and $H_{3''}$ (blue line) site of Fer-1 (values are given in kcal/mol).

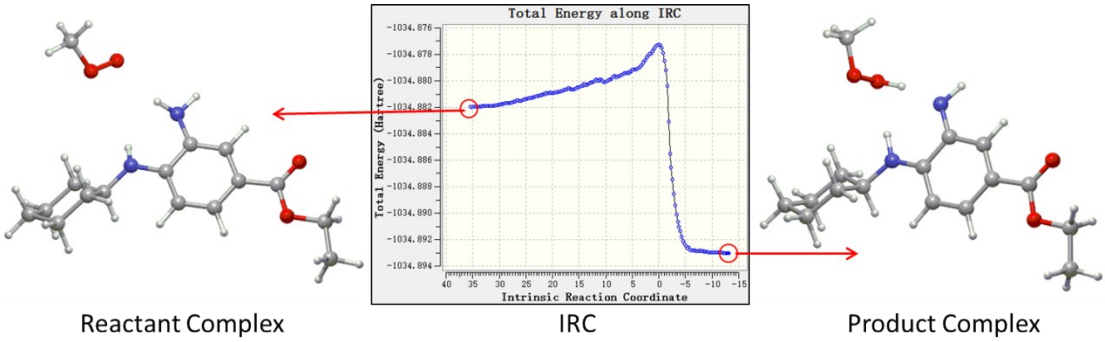
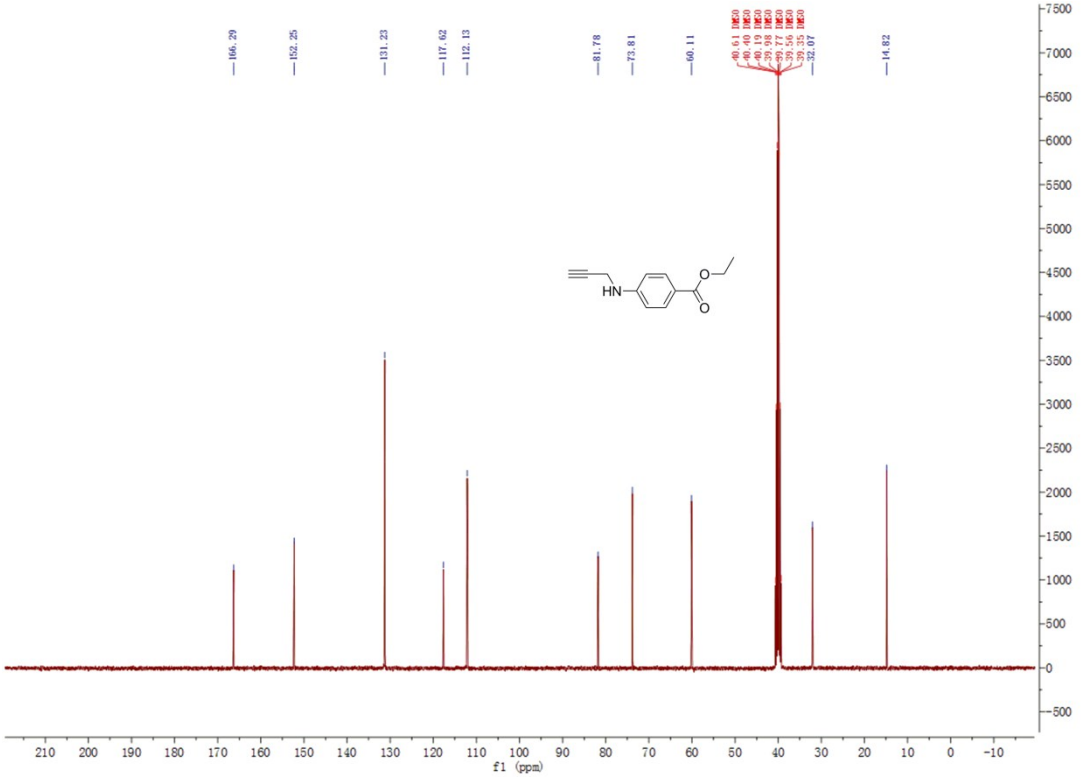
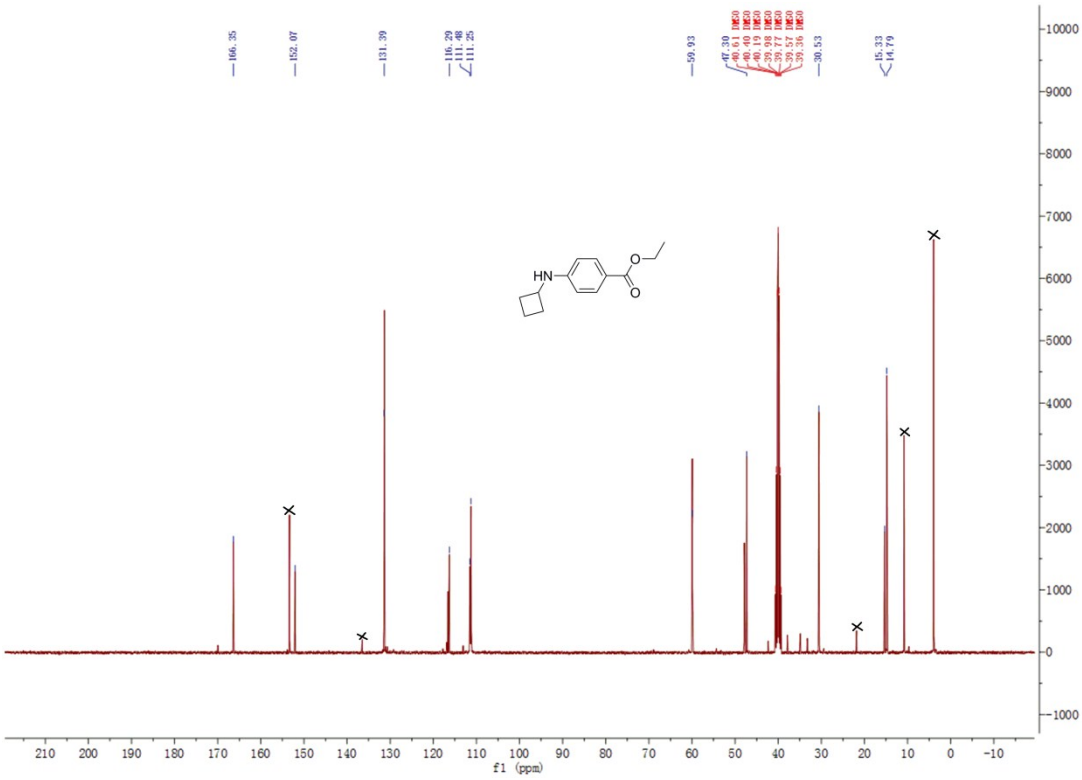
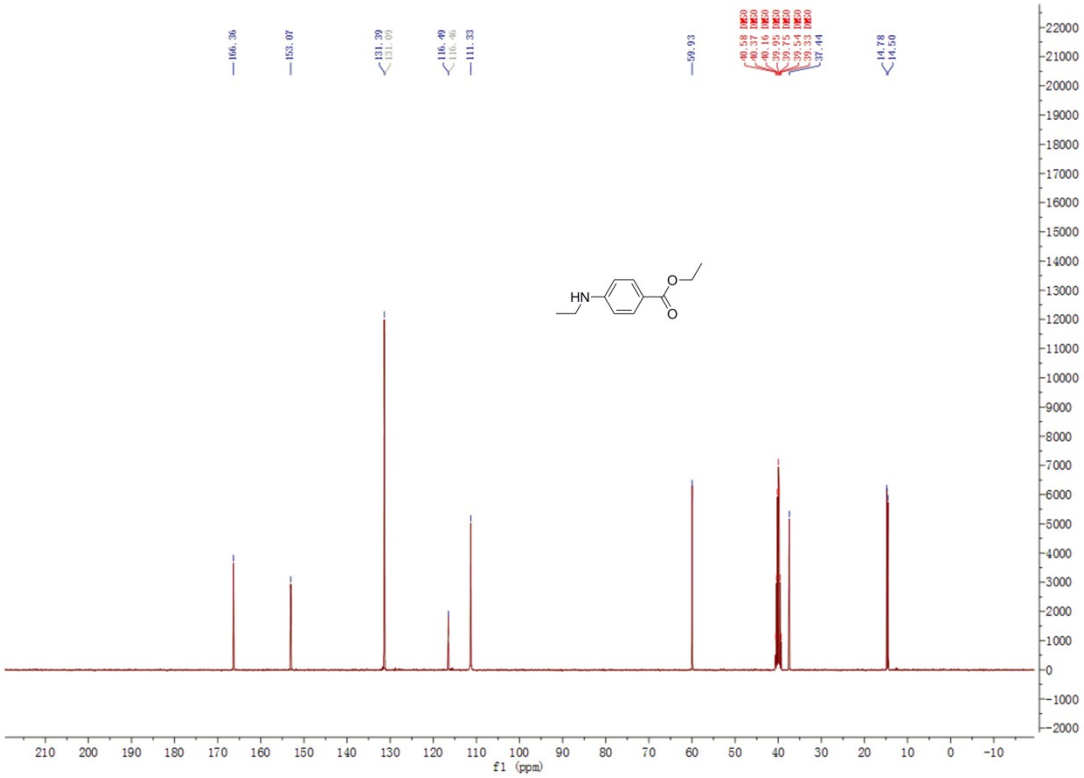


Fig S3 Intrinsic Reaction Coordinate (IRC) of the reaction between Fer-1 and methylperoxyl radical

The 13C NMR spectra of the synthetic compounds



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131.09
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116.46
111.33
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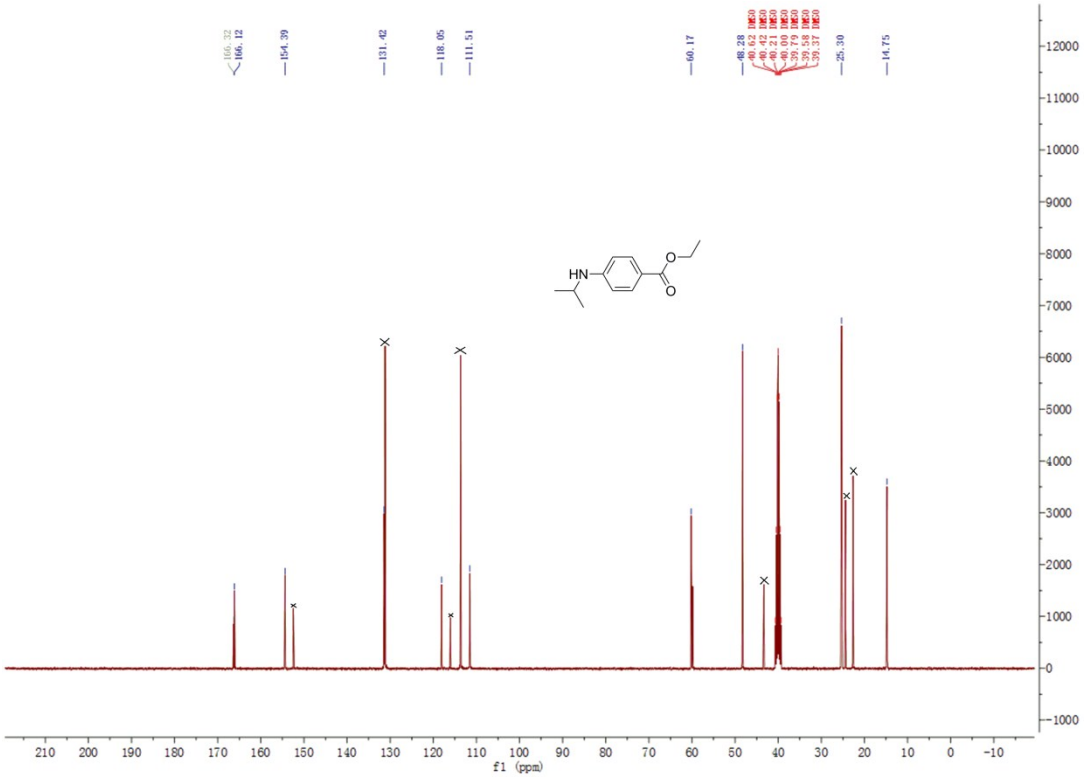
39.75
39.54
39.33
37.44
14.78
14.50
HN
O
O
f1 (ppm)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25.30
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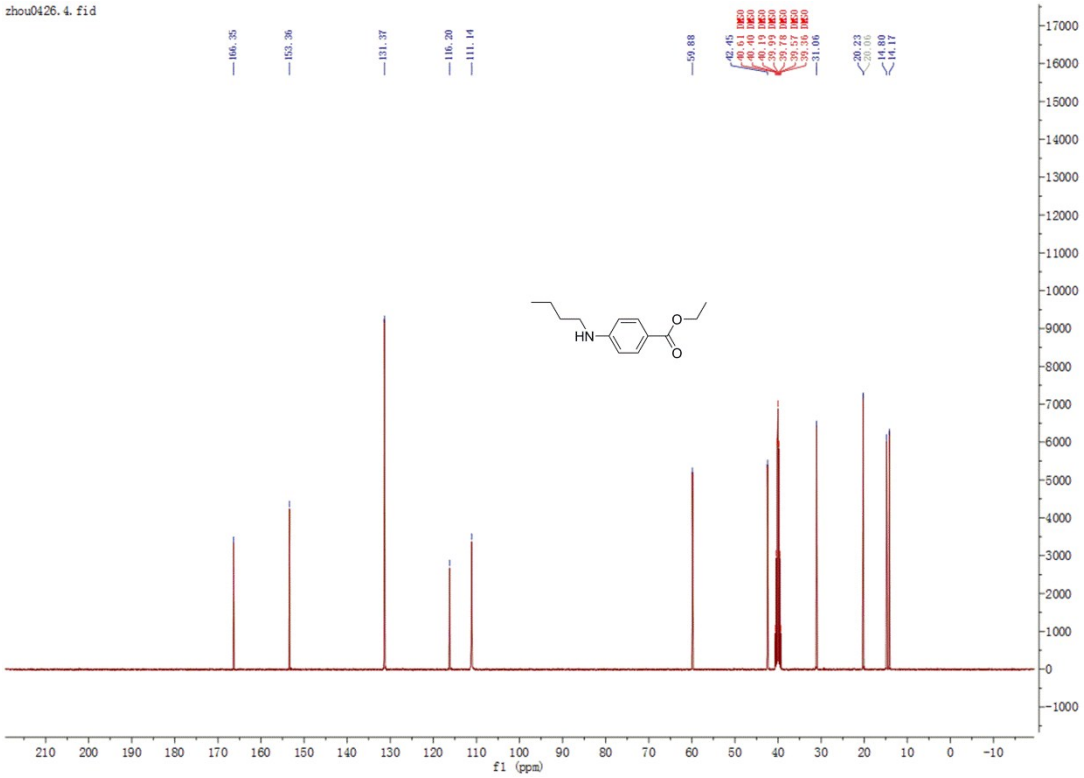
O
O
f1 (ppm)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39.57
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31.06
20.23
14.80
14.17
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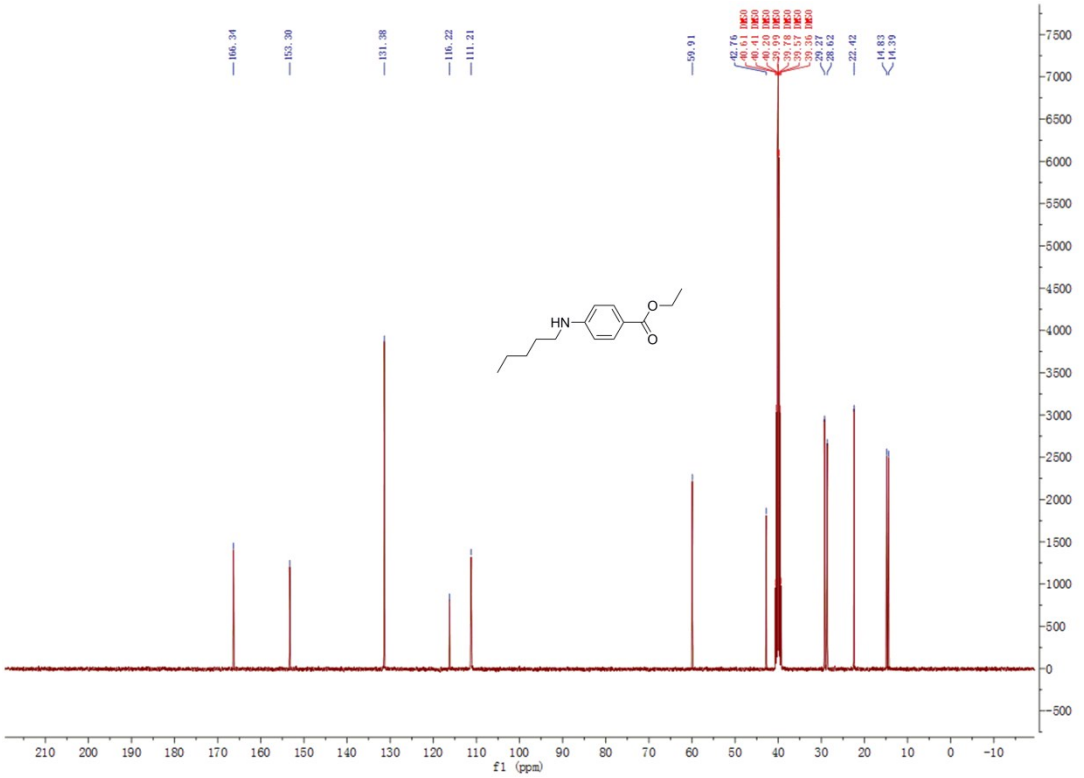
O
O
f1 (ppm)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HN
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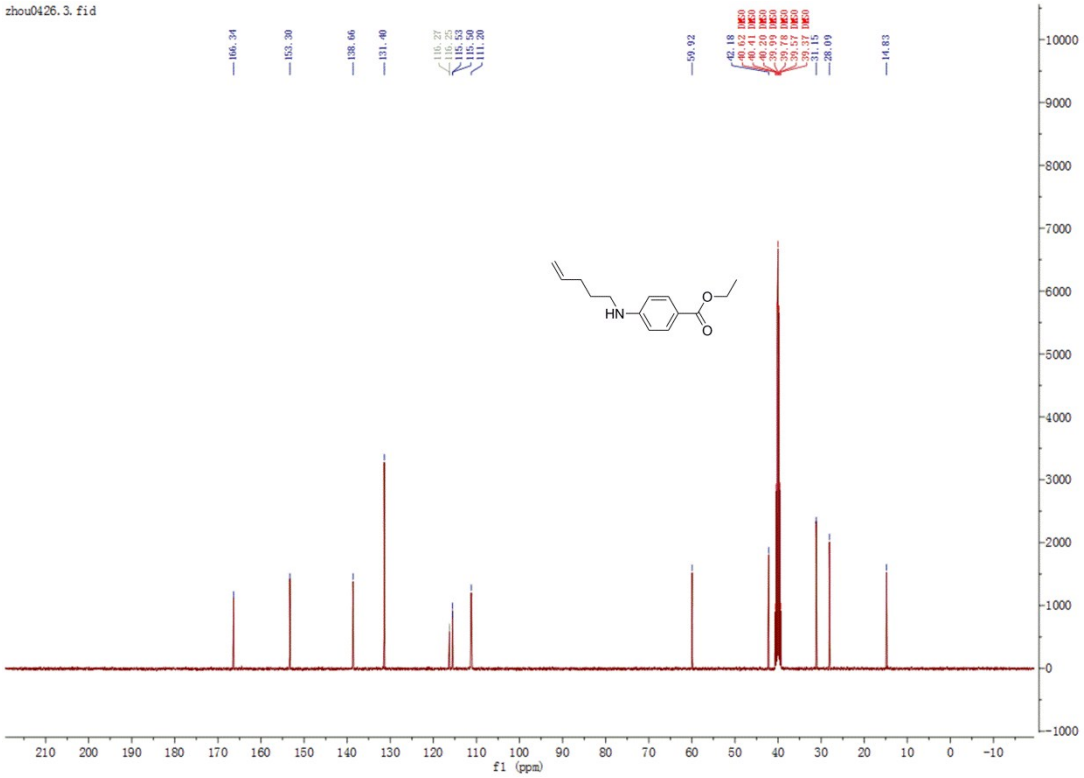
O
f1 (ppm)

zhou0426.3.fid



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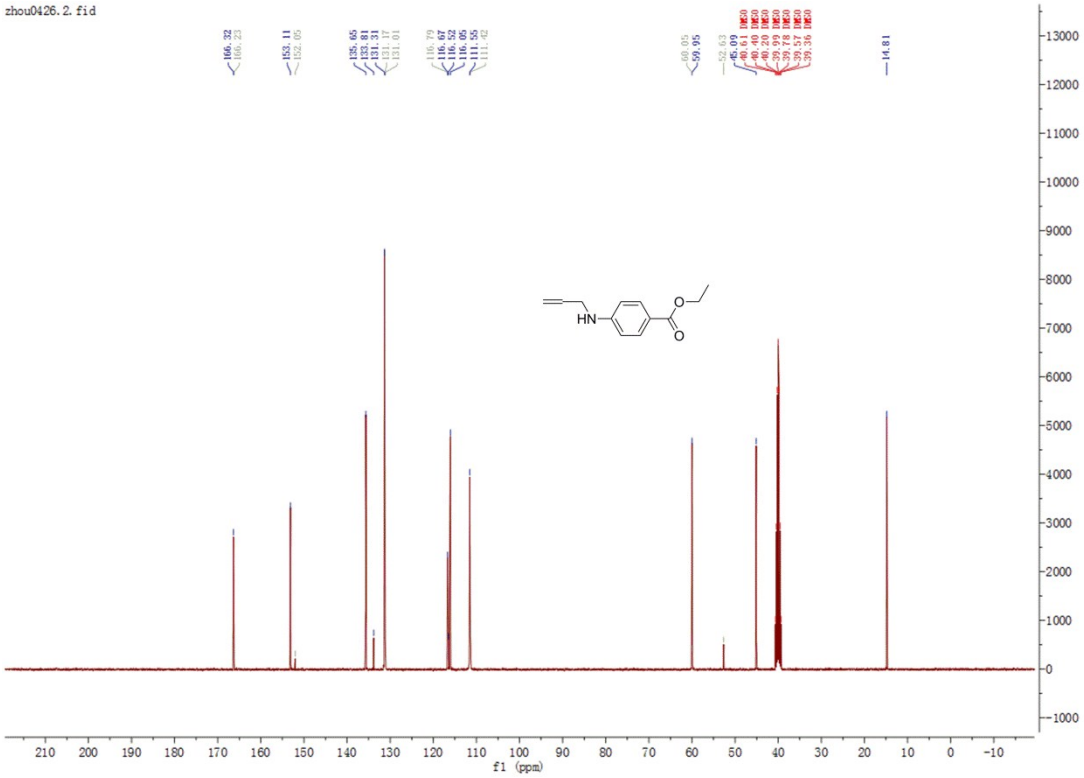

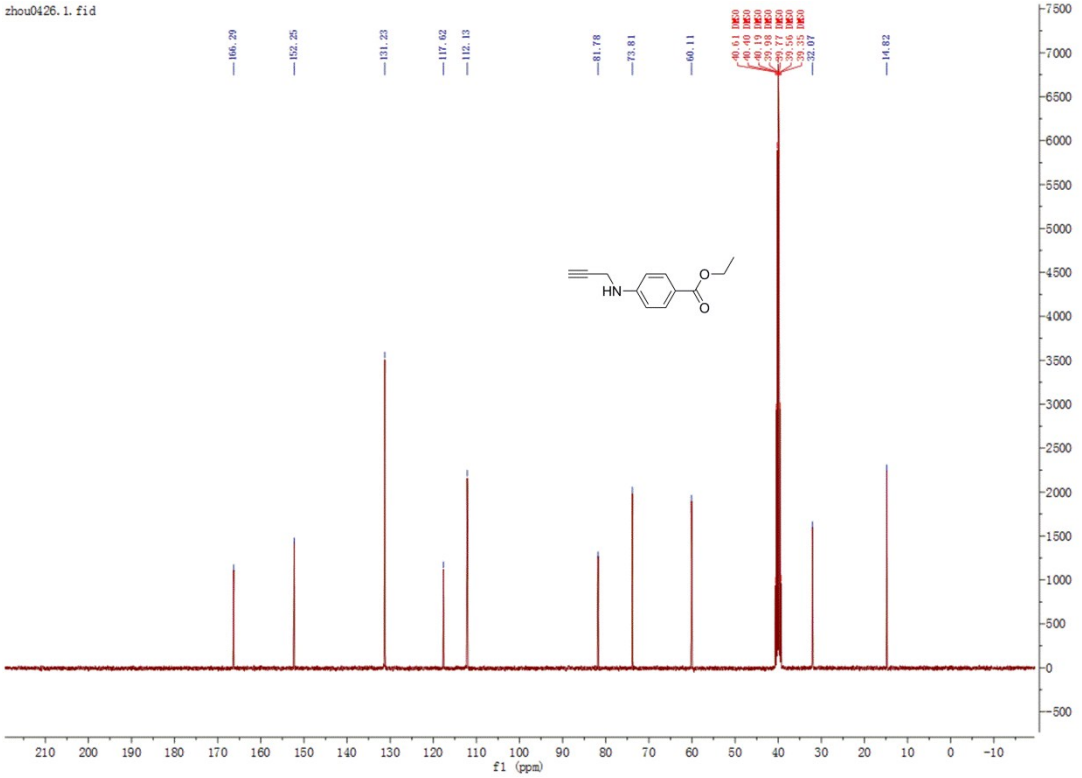
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73.81
60.11
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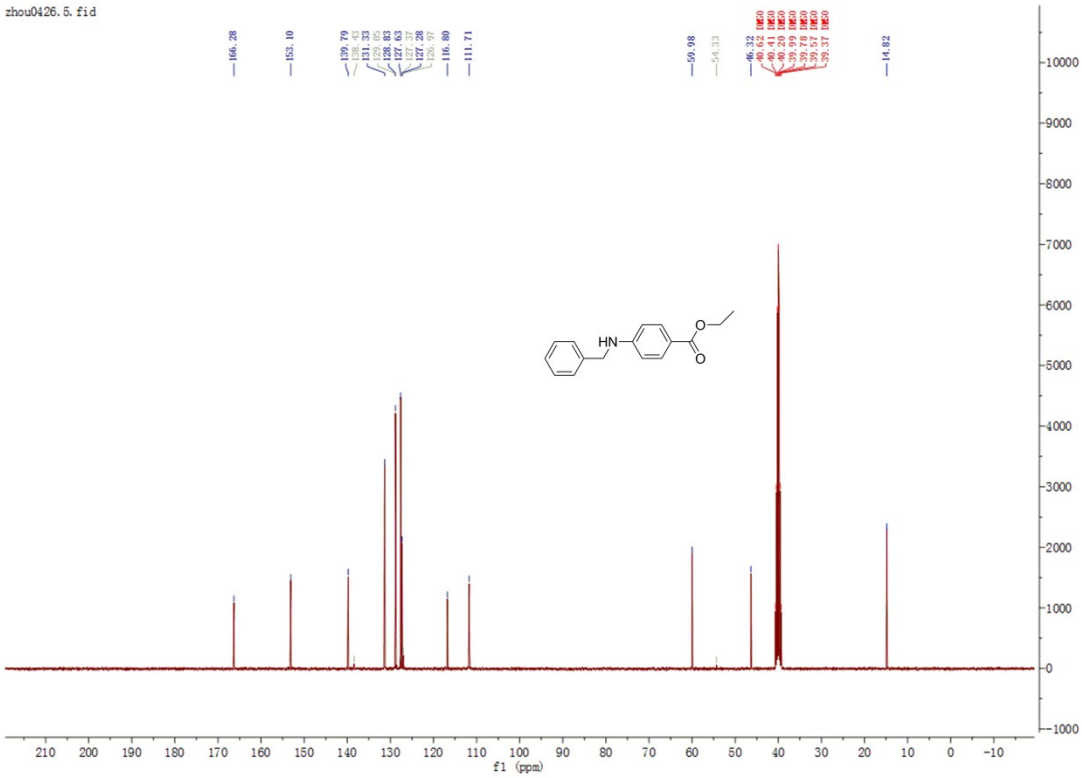
39.98 DMSO
39.77 DMSO
39.56 DMSO
39.35 DMSO
32.07
14.82
HN
O
O
f1 (ppm)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59.98
54.33
46.32
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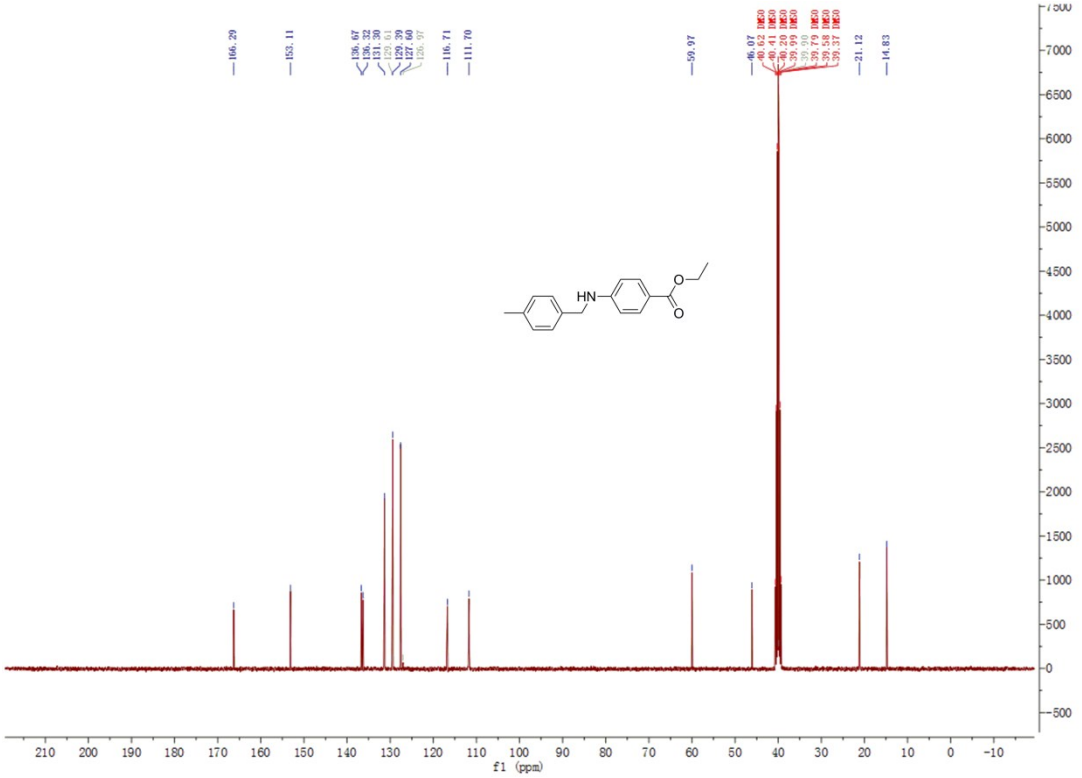
39.37 DMSO
14.82
HN
O
O
f1 (ppm)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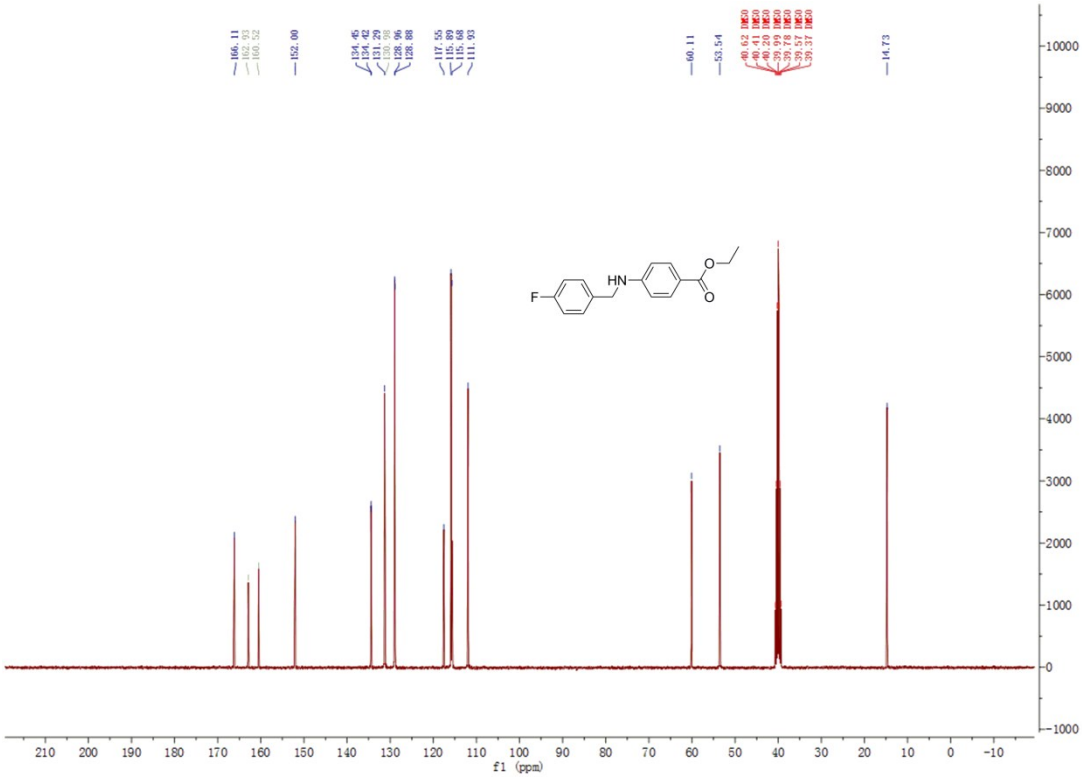
O
f1 (ppm)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111.93
60.11
53.54
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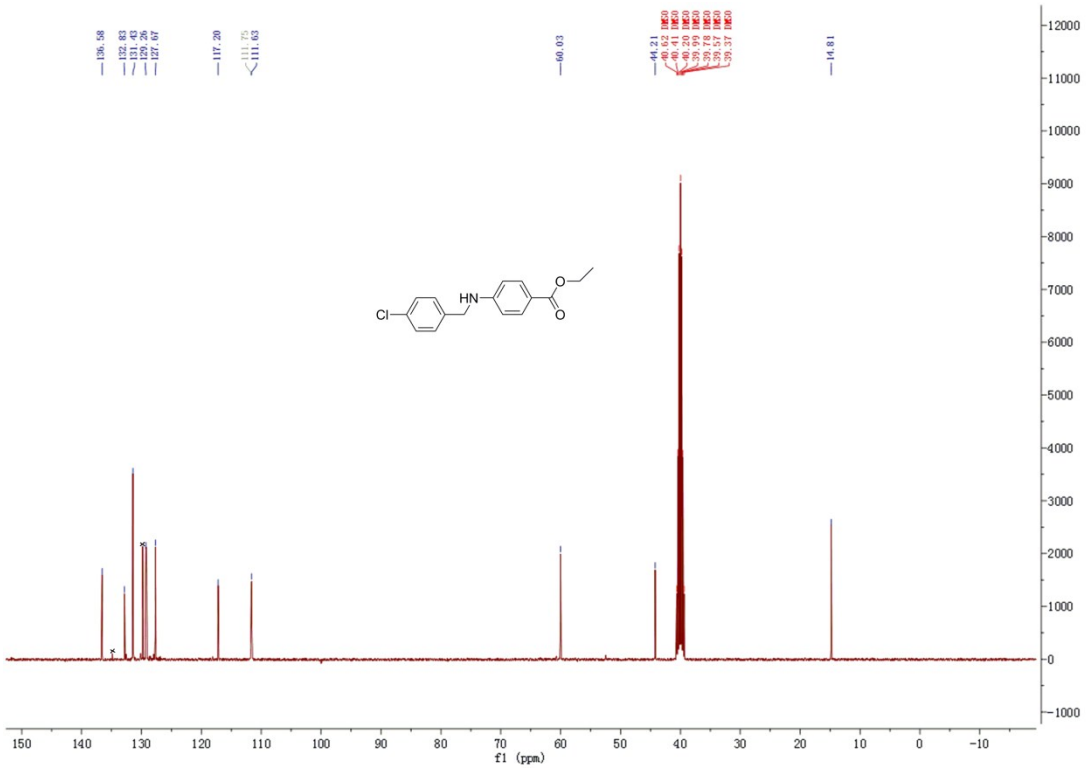
40.20
39.99
39.78
39.57
39.37
14.73
F
HN
O
O
f1 (ppm)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44.21
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40.41
40.20
39.99
39.78
39.57
39.37
14.81
Cl
HN
O
O
f1 (ppm)

COORDINATES OF THE STATIONARY POINTS

Optimized molecular geometries in Cartesian coordinates

[Fer-1]

C	0.20167	-1.21896	-0.02942
C	-0.0682	0.15094	-0.00106
C	0.99424	1.06237	-0.00113
C	2.31093	0.62868	-0.01387
C	2.58174	-0.75868	0.00276
C	1.51747	-1.6632	-0.02744
H	-0.61458	-1.93023	-0.04125
H	0.7635	2.12314	-0.00166
H	1.72924	-2.72848	-0.02965
N	3.40721	1.50714	0.02671
H	3.13654	2.47935	-0.01742
H	4.09798	1.30869	-0.68812
N	3.90972	-1.16641	-0.00597
H	4.52273	-0.56815	0.53324
C	-1.44127	0.69706	0.01323
O	-1.71115	1.88245	0.03732
O	-2.38525	-0.2628	-0.00372
C	-3.7442	0.19697	0.00925
H	-3.90199	0.80552	0.90385
H	-3.90716	0.84037	-0.85968
C	-4.63835	-1.02039	-0.01219
H	-4.46094	-1.65238	0.86116
H	-5.68613	-0.70884	-0.00255
H	-4.46675	-1.61698	-0.91122
C	4.12323	-2.58996	0.29205
C	4.80332	-3.25898	-0.88508
C	4.95075	-2.72617	1.55427
H	3.11572	-3.0554	0.45468
C	5.11808	-4.71103	-0.58836
H	5.75353	-2.71342	-1.12557
H	4.14087	-3.19533	-1.78716
C	5.26481	-4.1783	1.85143
H	5.90836	-2.15409	1.4358
H	4.39491	-2.27776	2.41822
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H	4.16053	-5.28365	-0.47178
H	5.92762	-4.24197	2.75319
H	4.31428	-4.72304	2.09275
H	6.10411	-5.93436	0.90181
H	6.95251	-4.38532	0.51249

[Fer-1] _TS (H3')

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C	2.50643	0.0923	-0.37388
C	1.81121	1.1542	-0.96971
C	0.42909	1.16016	-1.04359
C	-0.30279	0.05776	-0.5217
C	0.39803	-0.98573	0.09834
H	2.31221	-1.79226	0.64136
H	2.38451	1.98236	-1.37506
H	-0.14342	-1.82829	0.51132
N	-0.29958	2.17611	-1.69026
H	0.29896	2.86117	-2.13009
H	-0.96657	2.65038	-1.08571
N	-1.67658	0.09447	-0.64613
H	-1.97024	0.70123	-1.40295
C	3.97973	0.16574	-0.33777
O	4.63736	1.07956	-0.79839
O	4.54208	-0.89821	0.26895
C	5.97457	-0.8932	0.33585
H	6.37552	-0.84379	-0.68028
H	6.30086	0.00826	0.86179
C	6.40312	-2.15216	1.05225
H	6.07034	-3.04279	0.51398

H	7.49349	-2.18306	1.12424
H	5.99211	-2.18653	2.06402
C	-2.52589	-1.06622	-0.4239
C	-2.95102	-1.18942	1.04387
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H	-3.47184	-0.26435	1.32304
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H	-4.29124	-0.04184	-1.09703
H	-3.44504	-0.92205	-2.37195
C	-5.102	-2.31008	0.35446
H	-4.17702	-2.44118	2.31137
H	-3.3254	-3.31613	1.04955
H	-5.5835	-2.05115	-1.74424
H	-4.19463	-3.08268	-1.44213
H	-5.73067	-3.19694	0.48632
H	-5.7127	-1.44637	0.64902
C	-1.34284	2.68698	1.97276
H	-1.46953	2.60491	3.05147
H	-0.40453	3.18516	1.72655
H	-1.40733	1.71209	1.48776
O	-2.44302	3.5046	1.52445
O	-2.4194	3.68343	0.23111

[Fer-1] _TS (H3′)

C	1.99112	-0.96769	-0.10194
C	2.63456	0.28186	-0.20451
C	1.88201	1.41452	-0.46196
C	0.49415	1.35285	-0.6574
C	-0.17019	0.07425	-0.53098
C	0.62758	-1.06208	-0.25174
H	2.57864	-1.85257	0.10686
H	2.39365	2.36857	-0.53751
H	0.14953	-2.02756	-0.15007
N	-0.20737	2.45625	-1.02441
H	0.31245	3.31984	-0.96155
H	-1.22882	2.54674	-0.764
N	-1.50555	0.01238	-0.69134
H	-2.0423	0.90248	-0.68495
C	4.0953	0.44684	-0.04415
O	4.67905	1.50797	-0.11834
O	4.72067	-0.71989	0.19494
C	6.14287	-0.63304	0.35439
H	6.57322	-0.18433	-0.54505
H	6.36588	0.03705	1.18918
C	6.66032	-2.03104	0.59446
H	6.42603	-2.68395	-0.24903
H	7.74534	-2.00897	0.72004
H	6.21963	-2.46158	1.49621
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C	-2.59856	-1.39288	1.02815
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H	-3.4415	3.50372	2.55555
H	-4.04157	4.11077	0.97914
H	-2.30546	4.23273	1.37862
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[Fer-1] _PC(H3′)

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C	2.7083	0.38208	-0.12681
C	1.90406	1.49254	-0.26689
C	0.48451	1.39941	-0.35924
C	-0.11059	0.06293	-0.32332
C	0.74489	-1.05041	-0.16432
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H	2.36723	2.47387	-0.30293
H	0.32103	-2.045	-0.11182
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H	0.24948	3.31241	-0.49027
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O	4.84424	-0.56984	0.11019
C	6.2729	-0.45525	0.20729
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C	6.83241	-1.84692	0.38256
H	6.57758	-2.48289	-0.46843
H	7.92166	-1.79836	0.45933
H	6.44604	-2.31361	1.29167
C	-2.20261	-1.28977	-0.38465
C	-2.46608	-1.71725	1.06556
C	-3.51736	-1.11635	-1.14622
H	-1.62419	-2.07625	-0.88737
C	-3.30557	-2.99343	1.1212
H	-2.994	-0.8991	1.57056
H	-1.51627	-1.85308	1.59313
C	-4.36228	-2.38844	-1.08559
H	-4.07213	-0.27872	-0.70537
H	-3.30405	-0.84331	-2.18473
C	-4.61763	-2.82933	0.35526
H	-3.50134	-3.26279	2.16422
H	-2.73484	-3.82627	0.68783
H	-5.3097	-2.22482	-1.60904
H	-3.84576	-3.19417	-1.62453
H	-5.18645	-3.76502	0.37024
H	-5.23717	-2.07615	0.85922
C	-4.1067	3.76133	1.0128
H	-4.44743	3.71631	2.05041
H	-4.96901	3.83246	0.34202
H	-3.4582	4.63373	0.87431
O	-3.40353	2.5583	0.80804
O	-2.99044	2.54897	-0.56531

[Fer-1] _RC (H3″)

C	-1.62343	-1.36449	0.1094
C	-2.30469	-0.17193	-0.13192
C	-1.58775	0.97433	-0.47519
C	-0.20116	0.94766	-0.56714
C	0.50034	-0.23672	-0.21306
C	-0.23374	-1.38749	0.0776
H	-2.17723	-2.2643	0.34342
H	-2.13315	1.88151	-0.71024
H	0.28317	-2.31137	0.30737
N	0.49773	2.044	-0.99971
H	0.09764	2.96204	-0.9172
H	1.46126	1.9548	-1.26123
N	1.89566	-0.16507	-0.19547
H	2.20153	0.70152	0.23196
C	-3.77785	-0.07058	-0.08199
O	-4.41382	0.94332	-0.28336
O	-4.36048	-1.2486	0.21669
C	-5.78853	-1.23075	0.28482
H	-6.10203	-0.5076	1.0432
H	-6.18897	-0.88734	-0.67326
C	-6.24021	-2.63303	0.61828
H	-5.82678	-2.95743	1.57577
H	-7.33019	-2.67006	0.68442
H	-5.91866	-3.33858	-0.15095

C	2.71702	-1.29785	0.2066
C	2.92941	-2.26661	-0.96091
C	4.06504	-0.78859	0.71744
H	2.23743	-1.84642	1.03538
C	3.84354	-3.4268	-0.56888
H	3.37515	-1.70028	-1.78758
H	1.96549	-2.63655	-1.32266
C	4.99266	-1.93833	1.10863
H	4.53334	-0.18935	-0.07504
H	3.90679	-0.12289	1.57474
C	5.18678	-2.92101	-0.04515
H	3.99293	-4.0903	-1.42627
H	3.35613	-4.03036	0.20807
H	5.95695	-1.54056	1.4404
H	4.56368	-2.46924	1.96793
H	5.81405	-3.75935	0.27443
H	5.72527	-2.41973	-0.85978
C	2.41052	5.22178	0.58763
H	2.96855	5.96009	0.01237
H	2.98162	4.29614	0.68488
H	2.15151	5.60976	1.57318
O	1.21402	4.96947	-0.15449
O	0.4182	4.1685	0.52996

[Fer-1] _TS (H3'')

C	-1.67462	-1.30005	0.08293
C	-2.36874	-0.10232	-0.15027
C	-1.65779	1.04456	-0.46704
C	-0.25399	1.03718	-0.55365
C	0.45006	-0.1725	-0.22056
C	-0.29085	-1.33281	0.04613
H	-2.23054	-2.20056	0.31165
H	-2.1921	1.96139	-0.68743
H	0.22129	-2.26163	0.2633
N	0.38432	2.16214	-0.96795
H	0.2171	3.18665	-0.38332
H	1.36533	2.01971	-1.17984
N	1.82025	-0.13122	-0.17905
H	2.19714	0.77178	0.07025
C	-3.84617	-0.01513	-0.0983
O	-4.48312	0.99603	-0.29859
O	-4.41811	-1.19644	0.20162
C	-5.84988	-1.18376	0.27268
H	-6.16069	-0.4608	1.03183
H	-6.24961	-0.8396	-0.68504
C	-6.30129	-2.58573	0.60573
H	-5.88989	-2.91126	1.56365
H	-7.39127	-2.61961	0.67158
H	-5.98246	-3.29196	-0.16396
C	2.65787	-1.25846	0.19732
C	2.86804	-2.22043	-0.97664
C	4.00221	-0.74094	0.70736
H	2.17976	-1.80959	1.02303
C	3.78141	-3.38034	-0.58335
H	3.31511	-1.65345	-1.80207
H	1.90416	-2.58961	-1.33939
C	4.93004	-1.89099	1.09627
H	4.47073	-0.14234	-0.08562
H	3.84147	-0.07593	1.56376
C	5.12349	-2.87327	-0.05802
H	3.93156	-4.04333	-1.44068
H	3.29215	-3.98352	0.19267
H	5.89396	-1.49218	1.42655
H	4.50235	-2.42118	1.95653
H	5.75011	-3.71161	0.2619
H	5.66276	-2.37251	-0.87225
C	2.30119	5.23993	0.56948
H	2.87719	6.0009	0.03856
H	2.89639	4.32388	0.66881
H	2.03258	5.60151	1.5666
O	1.1492	5.01234	-0.20928
O	0.36299	4.08915	0.46093

[Fer-1] _PC (H3″)

C	-1.61247	-1.3585	0.10126
C	-2.30626	-0.15438	-0.13917
C	-1.59728	0.9832	-0.45929
C	-0.18065	0.96368	-0.58413
C	0.51907	-0.25383	-0.21166
C	-0.22893	-1.40494	0.07082
H	-2.17546	-2.25279	0.33687
H	-2.11923	1.90691	-0.67952
H	0.27366	-2.33596	0.30067
N	0.41881	2.05384	-1.04541
H	0.22442	3.46633	-0.15572
H	1.40344	1.89478	-1.25314
N	1.87599	-0.2057	-0.14828
H	2.27585	0.71197	-0.02734
C	-3.78475	-0.06358	-0.08442
O	-4.41851	0.94855	-0.28542
O	-4.35479	-1.24414	0.2153
C	-5.78725	-1.23296	0.28599
H	-6.09799	-0.51007	1.04507
H	-6.18598	-0.88896	-0.67211
C	-6.23657	-2.63529	0.61878
H	-5.8251	-2.96031	1.57681
H	-7.32646	-2.67025	0.68454
H	-5.91716	-3.34104	-0.15108
C	2.73136	-1.32018	0.21435
C	2.94016	-2.2761	-0.96414
C	4.07164	-0.7926	0.72271
H	2.25805	-1.87529	1.03879
C	3.85427	-3.43431	-0.57143
H	3.3864	-1.70742	-1.78895
H	1.97534	-2.64457	-1.32523
C	5.0014	-1.94158	1.10984
H	4.53863	-0.1933	-0.07084
H	3.90803	-0.12795	1.57822
C	5.19459	-2.92396	-0.04468
H	4.0067	-4.09694	-1.4285
H	3.36461	-4.03798	0.20394
H	5.96532	-1.54195	1.43858
H	4.57536	-2.47159	1.97101
H	5.82232	-3.76127	0.27542
H	5.73345	-2.42285	-0.8589
C	2.39037	5.2021	0.58643
H	3.00488	5.92981	0.04961
H	2.9528	4.26578	0.70747
H	2.14464	5.59662	1.57897
O	1.24373	5.0296	-0.1964
O	0.39614	4.14589	0.54732

[SRS9-01] _TS(H4′)

N	1.09022	0.00287	-0.02838
C	-0.18769	-0.39475	0.00404
C	-1.17829	0.4956	0.58
C	-0.6658	-1.62052	-0.55145
C	-2.54016	0.23637	0.36589
C	-2.00697	-1.87288	-0.68728
H	0.04461	-2.34812	-0.92006
C	-2.9633	-0.92895	-0.25836
H	-3.28489	0.91948	0.75264
H	-2.35658	-2.79295	-1.14127
N	-0.78005	1.60884	1.27864
C	-4.39388	-1.2476	-0.44839
O	-5.13154	-0.37194	-0.04161
H	1.31327	1.1024	-0.08246
C	2.13883	-0.85405	-0.57389
C	2.53566	-1.92604	0.46702
H	1.75115	-1.39021	-1.45287
C	3.29967	0.01922	-1.05412
C	3.40527	-1.47672	1.65012
H	3.03197	-2.75659	-0.04811
H	1.60366	-2.34676	0.85893
H	3.56902	0.7114	-0.25186
H	2.93543	0.65654	-1.86268
C	4.52438	-0.79454	-1.50142
C	4.9351	-1.58472	1.49985
H	3.14058	-0.45188	1.94009

H	3.12744	-2.10431	2.5043
C	5.80398	-0.48844	-0.71703
H	4.31225	-1.866	-1.42392
H	4.72239	-0.62055	-2.56406
C	5.66611	-0.42483	0.80822
H	5.34266	-1.66211	2.51428
H	5.18732	-2.53589	1.01113
H	6.21246	0.47195	-1.05517
H	6.557	-1.24334	-0.97597
H	5.18252	0.5144	1.10225
H	6.68111	-0.36279	1.21784
C	0.24497	1.55937	2.3067
H	-0.22477	1.72943	3.28442
H	0.73465	0.58928	2.31139
H	0.99722	2.33333	2.12719
C	-1.6457	2.76121	1.3751
H	-2.19429	2.90225	0.44422
H	-2.35905	2.67676	2.20784
H	-1.02037	3.64046	1.54307
C	1.26003	3.9755	-1.71929
H	1.55467	4.20892	-2.74587
H	1.6714	4.72734	-1.03568
H	0.16634	3.96898	-1.63938
O	1.79239	2.70503	-1.44714
O	1.45506	2.3841	-0.11913
O	-4.84792	-2.38035	-1.01264
C	-6.27608	-2.3434	-1.07501
H	-6.67438	-2.2639	-0.08509
H	-6.58609	-1.4981	-1.65315
C	-6.79467	-3.63465	-1.73481
H	-6.47913	-4.48035	-1.16025
H	-7.8636	-3.60991	-1.77557
H	-6.40158	-3.71087	-2.72707

[SRS12-12] _TS(H3′)

C	-4.19065	1.23743	-0.63475
C	-4.76383	0.02655	-0.21301
C	-3.92864	-1.01053	0.16392
C	-2.52407	-0.8963	0.12626
C	-1.93723	0.3195	-0.38226
C	-2.81597	1.37278	-0.7104
H	-4.83114	2.05894	-0.93103
H	-4.37484	-1.92826	0.53488
H	-2.41483	2.30321	-1.08877
N	-1.7302	-1.89991	0.58875
H	-2.28626	-2.68734	0.90628
H	-0.95426	-1.64348	1.43325
N	-0.56704	0.44833	-0.51298
C	-6.22727	-0.18438	-0.1253
O	-6.75007	-1.21706	0.24241
O	-6.92717	0.90021	-0.49896
C	-8.3572	0.77629	-0.43557
H	-8.66451	-0.06213	-1.06623
H	-8.64239	0.5386	0.59276
C	-8.95048	2.08473	-0.90073
H	-8.6593	2.30422	-1.93056
H	-10.04128	2.02959	-0.85799
H	-8.62478	2.91135	-0.265
C	-0.04874	1.80265	-0.67784
C	1.42333	1.97888	-0.32287
H	-0.6289	2.45363	-0.01884
H	-0.21063	2.15527	-1.71169
C	1.81331	3.45599	-0.31104
H	1.61352	1.53512	0.66007
H	2.05718	1.45146	-1.04321
H	1.57177	3.9091	-1.28211
H	1.20487	3.98665	0.43317
C	3.29159	3.68343	-0.00578
C	3.68147	5.15855	0.03925
H	3.90134	3.16969	-0.76082
H	3.53854	3.21336	0.95505
C	5.16474	5.38759	0.31689
H	3.4137	5.63463	-0.91366
H	3.08622	5.66663	0.80971
H	5.43548	4.90379	1.26499

H	5.76081	4.88776	-0.45852
C	5.55443	6.86243	0.37663
C	7.03669	7.07994	0.66133
H	4.95592	7.36243	1.14847
H	5.28881	7.34478	-0.57247
H	7.32231	6.64223	1.62318
H	7.65961	6.61497	-0.10955
H	7.2877	8.14382	0.69329
C	0.17163	-0.6136	-1.22259
C	1.32861	-1.26809	-0.47193
H	0.53677	-0.17661	-2.16492
H	-0.54511	-1.38929	-1.49509
C	1.88234	-2.46735	-1.2385
H	2.13583	-0.55053	-0.30392
H	0.98691	-1.5829	0.51521
H	1.08815	-3.21456	-1.36702
H	2.18197	-2.16086	-2.25088
C	3.07253	-3.11325	-0.53441
C	3.65737	-4.30817	-1.28293
H	2.76433	-3.4269	0.47093
H	3.85793	-2.35925	-0.38921
C	4.8504	-4.94031	-0.57144
H	2.8761	-5.0671	-1.42427
H	3.96094	-3.9944	-2.29104
H	5.62656	-4.17798	-0.41924
H	4.54352	-5.26265	0.43262
C	5.4536	-6.12752	-1.31811
C	6.63696	-6.75585	-0.58996
H	5.76915	-5.80267	-2.31769
H	4.67708	-6.88632	-1.47775
H	7.4405	-6.02752	-0.44029
H	6.34177	-7.12689	0.39673
H	7.05263	-7.59798	-1.15046
C	-0.5131	-3.18774	4.04448
H	-0.05978	-4.1574	4.2626
H	-1.59285	-3.30184	3.89572
H	-0.33043	-2.49097	4.86767
O	0.11193	-2.73044	2.86296
O	-0.38053	-1.46596	2.5685

[SRS11-89] _TS(H3′)

C	2.74761	-3.39341	1.13596
C	3.57351	-4.67309	1.01077
C	2.71882	-5.8345	0.50463
C	2.02156	-5.4759	-0.80745
C	1.21283	-4.18483	-0.68433
C	2.08164	-3.02575	-0.19491
H	3.33221	-6.73238	0.37374
H	4.4063	-4.50529	0.31425
H	4.0247	-4.9223	1.97678
H	1.95356	-3.53097	1.88067
H	3.36817	-2.56602	1.49375
H	2.77506	-5.35623	-1.59713
H	1.36636	-6.2927	-1.12763
H	0.75805	-3.92496	-1.64655
H	0.39144	-4.33126	0.03022
H	2.86869	-2.86503	-0.95032
H	1.96164	-6.07978	1.26127
N	1.25988	-1.83236	-0.07483
H	0.33893	-1.90369	-0.49515
C	1.7679	-0.56108	-0.08653
C	0.9042	0.56283	0.0283
C	3.15173	-0.29793	-0.17228
C	1.42183	1.84941	0.04206
C	3.65406	0.98979	-0.14259
H	3.84228	-1.12689	-0.25599
C	2.79661	2.08698	-0.03482
H	0.741	2.68956	0.12531
H	4.72182	1.16611	-0.20684
N	-0.4924	0.43135	0.25735
H	-1.00913	1.26379	1.08102
C	3.3743	3.44318	-0.00724
O	4.68464	3.71339	-0.08199
O	2.52715	4.31527	0.09369
C	-1.39301	-0.26104	-0.48528

O	-1.133	-1.06019	-1.37178
O	-2.64423	0.04104	-0.08759
C	-3.69621	-0.67412	-0.76705
H	-3.57489	-1.74252	-0.57253
H	-3.59282	-0.51077	-1.8419
C	-5.00729	-0.16311	-0.24983
C	-5.62971	0.93028	-0.85688
C	-5.61791	-0.76394	0.8533
C	-6.83845	1.41826	-0.36808
H	-5.16415	1.40093	-1.71781
C	-6.827	-0.27912	1.34494
H	-5.1429	-1.61671	1.32939
C	-7.43871	0.81398	0.7348
H	-7.31347	2.26651	-0.84954
H	-7.29279	-0.75579	2.20098
H	-8.38249	1.19089	1.11464
C	5.12471	5.02474	-0.44476
H	4.86179	5.71586	0.32863
H	4.65477	5.31815	-1.36017
C	6.6534	5.01999	-0.63103
H	6.99493	6.01943	-0.80239
H	7.11885	4.63015	0.25004
H	6.90855	4.40708	-1.47016
C	-3.34772	3.40732	2.24083
H	-4.41244	3.25164	2.4117
H	-3.17715	3.99282	1.33675
H	-2.87754	3.88177	3.10288
O	-2.79177	2.09271	2.06386
O	-1.50349	2.14761	1.84742

[SRS11-89] _TS (H4′)

C	-1.57059	-2.91776	-1.92831
C	-2.11471	-4.21404	-2.52838
C	-1.25928	-5.41772	-2.13728
C	-1.11323	-5.51365	-0.61984
C	-0.57181	-4.21555	-0.0217
C	-1.44437	-3.01784	-0.40011
H	-1.69367	-6.33945	-2.53925
H	-3.14375	-4.37224	-2.17844
H	-2.16943	-4.11967	-3.61822
H	-0.57503	-2.70436	-2.33745
H	-2.2127	-2.07364	-2.1992
H	-2.09235	-5.73847	-0.17541
H	-0.45497	-6.34611	-0.3504
H	-0.50816	-4.29668	1.06683
H	0.44483	-4.02877	-0.38962
H	-2.45136	-3.19479	0.01287
H	-0.26433	-5.31584	-2.59078
N	-0.85008	-1.79515	0.13286
H	-0.50826	-1.97616	1.32447
C	-1.55751	-0.61838	0.02555
C	-0.8488	0.61334	-0.10288
C	-2.97108	-0.55738	0.01357
C	-1.55199	1.80699	-0.23809
C	-3.65589	0.63394	-0.11606
H	-3.5298	-1.47927	0.12201
C	-2.94663	1.83293	-0.24774
H	-1.00096	2.7344	-0.34359
H	-4.73942	0.66307	-0.11427
N	0.54492	0.66859	-0.27393
H	0.88886	1.29261	-0.98735
C	-3.71508	3.09438	-0.38897
O	-5.04333	3.16163	-0.37793
O	-3.00254	4.06372	-0.51846
C	1.50486	0.16439	0.56308
O	1.32233	-0.42071	1.60305
O	2.72143	0.45421	0.04347
C	3.8365	0.00068	0.83326
H	3.84874	-1.09246	0.81986
H	3.69336	0.32282	1.86672
C	5.08824	0.57553	0.23992
C	5.64483	1.74677	0.75819
C	5.71077	-0.04646	-0.84552
C	6.80058	2.2898	0.2021
H	5.17078	2.23448	1.60491

C	6.86427	0.49442	-1.40618
H	5.28736	-0.96014	-1.25215
C	7.41137	1.66465	-0.88254
H	7.2253	3.19791	0.61701
H	7.33933	0.00104	-2.24768
H	8.31331	2.08454	-1.31546
C	-2.39211	-1.56096	3.73658
H	-2.70224	-0.65919	4.26795
H	-2.25545	-2.38527	4.44253
H	-3.14203	-1.83178	2.98754
O	-1.16107	-1.22638	3.12235
O	-0.69661	-2.33753	2.45152
C	-5.45028	4.51439	-0.1558
H	-5.16107	5.11577	-0.99222
H	-4.981	4.88704	0.73066
C	-6.98019	4.56934	0.0114
H	-7.29219	5.58839	0.10674
H	-7.44855	4.13159	-0.84528
H	-7.26281	4.02621	0.88892

[SRS11-97] _TS (H3′)

C	2.7678	-3.42839	1.10256
C	3.59371	-4.70807	0.97738
C	2.73901	-5.86948	0.47123
C	2.04176	-5.51088	-0.84085
C	1.23303	-4.21981	-0.71773
C	2.10183	-3.06073	-0.2283
H	3.3524	-6.76736	0.34035
H	4.4265	-4.54027	0.28085
H	4.04489	-4.95728	1.94339
H	1.97375	-3.56595	1.84727
H	3.38836	-2.60099	1.46035
H	2.79526	-5.3912	-1.63052
H	1.38655	-6.32767	-1.16103
H	0.77824	-3.95994	-1.67994
H	0.41163	-4.36623	-0.00317
H	2.88888	-2.90001	-0.98372
H	1.98183	-6.11476	1.22787
N	1.28008	-1.86734	-0.10822
H	0.35912	-1.93867	-0.52854
C	1.78809	-0.59606	-0.11992
C	0.92439	0.52785	-0.00509
C	3.17193	-0.33291	-0.20567
C	1.44202	1.81443	0.00867
C	3.67426	0.95481	-0.17599
H	3.86247	-1.16187	-0.28939
C	2.8168	2.052	-0.06822
H	0.76119	2.65458	0.09192
H	4.74202	1.13113	-0.24023
N	-0.47221	0.39637	0.22396
H	-0.9263	1.2653	1.01538
C	3.39449	3.4082	-0.04063
O	4.70484	3.67841	-0.11538
O	2.54734	4.28029	0.06029
C	-1.37281	-0.29602	-0.51867
O	-1.11281	-1.09517	-1.40518
O	-2.62404	0.00606	-0.12098
C	-3.67602	-0.7091	-0.80044
H	-3.58261	-1.75603	-0.60014
H	-3.59979	-0.53936	-1.85414
C	5.14491	4.98976	-0.47815
H	4.88199	5.68088	0.29524
H	4.67497	5.28317	-1.39356
C	6.67359	4.98501	-0.66442
H	7.01513	5.98445	-0.83578
H	7.13904	4.59517	0.21664
H	6.92874	4.3721	-1.50356
H	-4.62617	-0.36252	-0.45116
C	-2.97853	3.52368	1.04266
H	-4.03778	3.63607	0.94135
H	-2.52442	3.53467	0.07387
H	-2.58874	4.3298	1.62844
O	-2.69073	2.28146	1.68993
O	-1.384	2.14114	1.81308

[SRS11-97] _TS (H4′)

C	-1.57059	-2.91776	-1.92831
C	-2.11471	-4.21404	-2.52838
C	-1.25928	-5.41772	-2.13728
C	-1.11323	-5.51365	-0.61984
C	-0.57181	-4.21555	-0.0217
C	-1.44437	-3.01784	-0.40011
H	-1.69367	-6.33945	-2.53925
H	-3.14375	-4.37224	-2.17844
H	-2.16943	-4.11967	-3.61822
H	-0.57503	-2.70436	-2.33745
H	-2.2127	-2.07364	-2.1992
H	-2.09235	-5.73847	-0.17541
H	-0.45497	-6.34611	-0.3504
H	-0.50816	-4.29668	1.06683
H	0.44483	-4.02877	-0.38962
H	-2.45136	-3.19479	0.01287
H	-0.26433	-5.31584	-2.59078
N	-0.85008	-1.79515	0.13286
H	-0.50826	-1.97616	1.32447
C	-1.55751	-0.61838	0.02555
C	-0.8488	0.61334	-0.10288
C	-2.97108	-0.55738	0.01357
C	-1.55199	1.80699	-0.23809
C	-3.65589	0.63394	-0.11606
H	-3.5298	-1.47927	0.12201
C	-2.94663	1.83293	-0.24774
H	-1.00096	2.7344	-0.34359
H	-4.73942	0.66307	-0.11427
N	0.54492	0.66859	-0.27393
H	0.88886	1.29261	-0.98735
C	-3.71508	3.09438	-0.38897
O	-5.04333	3.16163	-0.37793
O	-3.00254	4.06372	-0.51846
C	1.50486	0.16439	0.56308
O	1.32233	-0.42071	1.60305
O	2.72143	0.45421	0.04347
C	3.8365	0.00068	0.83326
H	3.87805	-1.06828	0.81092
H	3.71614	0.3319	1.84356
C	-2.39211	-1.56096	3.73658
H	-2.70224	-0.65919	4.26795
H	-2.25545	-2.38527	4.44253
H	-3.14203	-1.83178	2.98754
O	-1.16107	-1.22638	3.12235
O	-0.69661	-2.33753	2.45152
C	-5.45028	4.51439	-0.1558
H	-5.16107	5.11577	-0.99222
H	-4.981	4.88704	0.73066
C	-6.98019	4.56934	0.0114
H	-7.29219	5.58839	0.10674
H	-7.44855	4.13159	-0.84528
H	-7.26281	4.02621	0.88892
H	4.744	0.40135	0.43227

[SRS11-98]_TS (H3′)

C	2.74761	-3.39341	1.13596
C	3.57351	-4.67309	1.01077
C	2.71882	-5.8345	0.50463
C	2.02156	-5.4759	-0.80745
C	1.21283	-4.18483	-0.68433
C	2.08164	-3.02575	-0.19491
H	3.33221	-6.73238	0.37374
H	4.4063	-4.50529	0.31425
H	4.0247	-4.9223	1.97678
H	1.95356	-3.53097	1.88067
H	3.36817	-2.56602	1.49375
H	2.77506	-5.35623	-1.59713
H	1.36636	-6.2927	-1.12763
H	0.75805	-3.92496	-1.64655
H	0.39144	-4.33126	0.03022
H	2.86869	-2.86503	-0.95032
H	1.96164	-6.07978	1.26127
N	1.25988	-1.83236	-0.07483

H	0.33893	-1.90369	-0.49515
C	1.7679	-0.56108	-0.08653
C	0.9042	0.56283	0.0283
C	3.15173	-0.29793	-0.17228
C	1.42183	1.84941	0.04206
C	3.65406	0.98979	-0.14259
H	3.84228	-1.12689	-0.25599
C	2.79661	2.08698	-0.03482
H	0.741	2.68956	0.12531
H	4.72182	1.16611	-0.20684
N	-0.4924	0.43135	0.25735
H	-1.00509	1.25728	1.07459
C	3.3743	3.44318	-0.00724
O	4.68464	3.71339	-0.08199
O	2.52715	4.31527	0.09369
C	-1.39301	-0.26104	-0.48528
O	-1.133	-1.06019	-1.37178
C	5.12471	5.02474	-0.44476
H	4.86179	5.71586	0.32863
H	4.65477	5.31815	-1.36017
C	6.6534	5.01999	-0.63103
H	6.99493	6.01943	-0.80239
H	7.11885	4.63015	0.25004
H	6.90855	4.40708	-1.47016
C	-2.82329	0.08427	-0.03068
H	-3.05035	1.09366	-0.30356
H	-3.51767	-0.578	-0.50409
H	-2.8956	-0.02293	1.03148
C	-2.31517	4.18237	0.73744
H	-3.29779	4.4803	0.37307
H	-1.57266	4.22159	-0.06032
H	-2.00703	4.79864	1.58274
O	-2.46567	2.82084	1.17583
O	-1.33972	2.34447	1.63934

[SRS11-98]_TS (H4′)

C	-1.57059	-2.91776	-1.92831
C	-2.11471	-4.21404	-2.52838
C	-1.25928	-5.41772	-2.13728
C	-1.11323	-5.51365	-0.61984
C	-0.57181	-4.21555	-0.0217
C	-1.44437	-3.01784	-0.40011
H	-1.69367	-6.33945	-2.53925
H	-3.14375	-4.37224	-2.17844
H	-2.16943	-4.11967	-3.61822
H	-0.57503	-2.70436	-2.33745
H	-2.2127	-2.07364	-2.1992
H	-2.09235	-5.73847	-0.17541
H	-0.45497	-6.34611	-0.3504
H	-0.50816	-4.29668	1.06683
H	0.44483	-4.02877	-0.38962
H	-2.45136	-3.19479	0.01287
H	-0.26433	-5.31584	-2.59078
N	-0.85008	-1.79515	0.13286
H	-0.50826	-1.97616	1.32447
C	-1.55751	-0.61838	0.02555
C	-0.8488	0.61334	-0.10288
C	-2.97108	-0.55738	0.01357
C	-1.55199	1.80699	-0.23809
C	-3.65589	0.63394	-0.11606
H	-3.5298	-1.47927	0.12201
C	-2.94663	1.83293	-0.24774
H	-1.00096	2.7344	-0.34359
H	-4.73942	0.66307	-0.11427
N	0.54492	0.66859	-0.27393
H	0.88886	1.29261	-0.98735
C	-3.71508	3.09438	-0.38897
O	-5.04333	3.16163	-0.37793
O	-3.00254	4.06372	-0.51846
C	1.50486	0.16439	0.56308
O	1.32233	-0.42071	1.60305
C	-2.39211	-1.56096	3.73658
H	-2.70224	-0.65919	4.26795
H	-2.25545	-2.38527	4.44253
H	-3.14203	-1.83178	2.98754

O	-1.16107	-1.22638	3.12235
O	-0.69661	-2.33753	2.45152
C	-5.45028	4.51439	-0.1558
H	-5.16107	5.11577	-0.99222
H	-4.981	4.88704	0.73066
C	-6.98019	4.56934	0.0114
H	-7.29219	5.58839	0.10674
H	-7.44855	4.13159	-0.84528
H	-7.26281	4.02621	0.88892
C	2.88828	0.49396	-0.02779
H	3.09707	1.53409	0.11161
H	3.63594	-0.08944	0.46774
H	2.89304	0.2662	-1.07326

[SRS8-91]_TS (H3′)

N	-0.83890	-1.23113	-0.59564
H	-1.39652	-0.42792	-0.89810
C	0.48057	-0.98525	-0.48327
C	0.96842	0.37097	-0.35451
C	1.43577	-2.03615	-0.47741
C	2.35944	0.57146	-0.27224
C	2.78435	-1.79178	-0.38447
H	1.09241	-3.05935	-0.55352
C	3.26775	-0.47045	-0.28771
H	2.72471	1.58723	-0.17972
H	3.48546	-2.61733	-0.39217
N	0.21651	1.50972	-0.16866
H	0.51169	2.10290	0.89732
C	4.70857	-0.14820	-0.20035
O	5.48155	-1.24998	-0.19880
O	5.16076	0.97700	-0.13796
C	-0.99984	1.82290	-0.68779
O	-1.62635	1.17684	-1.53076
O	-1.40397	2.99641	-0.19030
C	6.89666	-1.02004	-0.11472
H	7.10704	-0.46394	0.80277
H	7.20088	-0.39358	-0.95754
C	7.58120	-2.36598	-0.13181
H	8.66377	-2.22886	-0.06827
H	7.26408	-2.97880	0.71525
H	7.35903	-2.90829	-1.05392
C	1.37662	4.54354	1.59083
H	1.11499	5.56343	1.87931
H	1.29240	4.42968	0.50513
H	2.39331	4.30459	1.91535
O	0.44157	3.71156	2.25396
O	0.76159	2.39180	2.03233
C	-1.45244	-2.55033	-0.68993
C	-2.79878	-2.42165	-1.42048
H	-0.81733	-3.18051	-1.32826
C	-1.54207	-3.19167	0.70139
C	-3.99631	-1.86141	-0.63800
H	-3.06914	-3.40255	-1.82396
H	-2.61689	-1.79163	-2.29803
H	-2.02453	-2.46871	1.36474
H	-0.52971	-3.31488	1.09672
C	-2.30246	-4.52702	0.71131
C	-4.89893	-2.86570	0.10474
H	-3.66927	-1.08212	0.06228
H	-4.63008	-1.34444	-1.36613
C	-3.54320	-4.53334	1.61063
H	-2.60378	-4.78812	-0.30866
H	-1.63985	-5.33842	1.02921
C	-4.46712	-3.31350	1.50922
H	-5.87761	-2.38422	0.20851
H	-5.07140	-3.74257	-0.53426
H	-3.22864	-4.62660	2.65742
H	-4.12237	-5.43832	1.39016
H	-4.01771	-2.45617	2.02520
H	-5.36714	-3.55050	2.08788
C	-2.70034	3.57770	-0.53492
C	-2.74998	3.90650	-2.02330
C	-3.82835	2.64367	-0.10949
C	-2.72217	4.85250	0.29937
H	-1.90636	4.54471	-2.29927

H	-2.72298	3.00185	-2.63008
H	-3.67259	4.45121	-2.24231
H	-3.71969	2.37477	0.94457
H	-4.78629	3.15645	-0.23163
H	-3.84304	1.73587	-0.71220
H	-3.66445	5.38310	0.14196
H	-2.62044	4.61873	1.36116
H	-1.90070	5.51330	0.01282

[SRS8-91]_TS (H4′)

C	1.78419	-2.49964	-1.73381
C	2.62108	-3.70605	-2.15840
C	4.10938	-3.47847	-1.89993
C	4.35911	-3.10399	-0.44042
C	3.52137	-1.89834	-0.01723
C	2.03025	-2.13585	-0.26100
H	4.68284	-4.37186	-2.16997
H	2.28863	-4.59319	-1.60247
H	2.44403	-3.92083	-3.21774
H	2.04549	-1.62759	-2.34644
H	0.72033	-2.69672	-1.89982
H	4.11377	-3.96152	0.20088
H	5.42052	-2.89112	-0.27607
H	3.68972	-1.67116	1.03896
H	3.82497	-1.01216	-0.58876
H	1.72300	-2.99598	0.35690
H	4.46805	-2.66741	-2.54765
N	1.28478	-0.92901	0.08598
H	1.68383	-0.48604	1.18527
C	-0.09239	-0.97890	0.07103
C	-0.82962	0.19227	-0.27727
C	-0.83096	-2.14943	0.36218
C	-2.21992	0.14520	-0.32674
C	-2.21017	-2.18050	0.31384
H	-0.29123	-3.04606	0.64296
C	-2.91953	-1.02663	-0.03721
H	-2.76737	1.03987	-0.59996
H	-2.76117	-3.08402	0.54829
N	-0.20603	1.36263	-0.74026
H	-0.59652	1.79470	-1.56284
C	-4.40103	-1.09684	-0.07979
O	-5.04133	-2.09583	0.17611
O	-4.96587	0.06846	-0.43430
C	-6.40235	0.07776	-0.49101
H	-6.72852	-0.68009	-1.20822
H	-6.79226	-0.20524	0.49022
C	-6.83487	1.46674	-0.89547
H	-7.92563	1.51049	-0.94984
H	-6.49888	2.21011	-0.16888
H	-6.43306	1.73349	-1.87572
C	0.72983	2.11258	-0.07045
O	1.14422	1.88047	1.04062
O	1.07819	3.14979	-0.85935
C	2.03567	4.15139	-0.38993
C	0.61434	-1.41873	3.92911
H	-0.28640	-1.15473	4.48656
H	1.45687	-1.54738	4.61488
H	0.44926	-2.34169	3.36515
O	0.84659	-0.32692	3.05852
O	1.99507	-0.58442	2.33987
C	2.11408	5.11374	-1.56833
H	1.13464	5.55211	-1.77517
H	2.81460	5.92192	-1.34417
H	2.45890	4.59561	-2.46647
C	1.49359	4.85785	0.84806
H	0.50311	5.27482	0.64585
H	1.42609	4.17498	1.69452
H	2.15994	5.68276	1.11515
C	3.38994	3.49894	-0.13509
H	3.33787	2.79450	0.69468
H	3.73138	2.97105	-1.02961
H	4.12511	4.27216	0.10489

[SRS8-24]_TS (H4′)

C	-3.02950	-1.69093	1.00011	N	0.40944	1.86360	1.14168
C	-4.20990	-2.63374	0.76953	O	1.31194	2.68928	1.09189
C	-5.49726	-1.86099	0.48987	O	-0.62303	2.01167	1.77661
C	-5.30978	-0.88922	-0.67310	C	-1.04629	4.03234	-0.69311
C	-4.12690	0.05110	-0.44348	H	-0.08141	4.53859	-0.74260
C	-2.83814	-0.73615	-0.19326	H	-1.33483	3.86797	0.34914
H	-6.31797	-2.55453	0.27895	H	-1.81302	4.61476	-1.21059
H	-3.98958	-3.29379	-0.08025	O	-0.85216	2.79423	-1.36366
H	-4.33260	-3.28253	1.64302	O	-2.03995	2.08333	-1.34164
H	-3.20327	-1.07985	1.89353				
H	-2.11301	-2.26067	1.18266	**[SRS9-14] _TS**			
H	-5.14849	-1.45712	-1.59933				
H	-6.21874	-0.29966	-0.82910	C	2.49258	-1.09954	0.39787
H	-3.99809	0.71259	-1.30427	C	3.14772	0.05795	-0.05119
H	-4.31873	0.68978	0.42744	C	2.39461	1.15928	-0.44222
H	-2.63163	-1.33267	-1.09566	C	0.99358	1.14300	-0.42198
H	-5.78350	-1.29979	1.38892	C	0.31828	-0.03426	0.07726
N	-1.74386	0.17907	0.10026	C	1.11417	-1.13802	0.45847
H	-1.92074	1.28455	-0.45115	H	3.07266	-1.96180	0.70185
C	-0.45853	-0.24470	0.02261	H	2.92660	2.03587	-0.78910
C	0.62284	0.59483	0.44139	H	0.63207	-2.03932	0.81319
C	-0.08112	-1.51451	-0.49694	N	0.26574	2.18472	-0.91870
C	1.94697	0.21977	0.29284	H	-0.70969	2.30761	-0.60272
C	1.23678	-1.89719	-0.61535	N	-1.03170	-0.05360	0.16760
H	-0.85362	-2.19156	-0.83482	H	-1.55570	0.81223	0.00855
C	2.26934	-1.02984	-0.23342	C	4.61905	0.16493	-0.13125
H	2.72243	0.90228	0.61296	O	5.21897	1.14836	-0.52043
H	1.49861	-2.86732	-1.02243	O	5.24406	-0.95496	0.27852
C	3.67277	-1.48894	-0.39436	C	6.67790	-0.92412	0.22926
O	3.97485	-2.57617	-0.84062	H	6.99043	-0.73603	-0.80158
O	4.56207	-0.57346	0.00562	H	7.03322	-0.08888	0.83881
C	5.94866	-0.94137	-0.12250	C	7.18171	-2.25319	0.74026
H	6.11806	-1.85786	0.44847	H	6.81537	-3.07603	0.12188
H	6.15196	-1.16130	-1.17369	H	8.27447	-2.26709	0.71611
C	6.77633	0.21203	0.38983	H	6.85991	-2.42488	1.77010
H	7.83780	-0.03357	0.30391	C	-3.13819	4.15267	1.15810
H	6.58715	1.11929	-0.18815	H	-3.48393	4.33284	2.17767
H	6.55687	0.41782	1.43987	H	-3.95284	4.30725	0.44506

H	-2.30303	4.81784	0.91715
O	-2.71254	2.80249	1.12940
O	-2.29137	2.49314	-0.13235
C	-1.82713	-1.19599	0.59848
C	-1.97110	-2.22300	-0.54289
H	-1.29224	-1.69632	1.41682
C	-3.14306	-0.66302	1.17275
C	-2.89637	-1.85672	-1.71051
H	-2.28067	-3.18643	-0.12176
H	-0.96286	-2.38930	-0.93651
H	-3.56379	0.05754	0.46505
H	-2.90556	-0.08077	2.06738
C	-4.17266	-1.75996	1.48527
C	-4.37245	-2.28404	-1.61568
H	-2.83753	-0.77881	-1.90941
H	-2.48423	-2.33725	-2.60444
C	-5.47142	-1.65129	0.67828
H	-3.72939	-2.74640	1.31556
H	-4.42714	-1.74154	2.54980
C	-5.32522	-1.37792	-0.82273
H	-4.75016	-2.32816	-2.64339
H	-4.43119	-3.31442	-1.23843
H	-6.09017	-0.85083	1.10292
H	-6.04223	-2.57768	0.81815
H	-5.03196	-0.33414	-0.98806
H	-6.32753	-1.46373	-1.25822
C	0.89408	3.40444	-1.36575
H	1.48892	3.89111	-0.58135
H	1.55006	3.20926	-2.21959
H	0.11046	4.09101	-1.68573

[Compound 1] _TS

C	3.51294	-0.78672	-1.23254
C	4.37219	-2.04629	-1.13187
C	4.68475	-2.40011	0.32162
C	3.40363	-2.53321	1.14364
C	2.54189	-1.27491	1.04682
C	2.22321	-0.93196	-0.42021
H	5.26499	-3.32754	0.37164
H	3.84542	-2.88745	-1.60307
H	5.29835	-1.90660	-1.69874
H	4.06667	0.08235	-0.85948
H	3.25886	-0.57336	-2.27576
H	2.82959	-3.39766	0.78294
H	3.64081	-2.73607	2.19338
H	1.61029	-1.39589	1.60933
H	3.06909	-0.42104	1.48795
H	1.64703	-1.76336	-0.84826
H	5.31292	-1.61250	0.75807
N	1.44184	0.28342	-0.52541
H	1.98496	1.32440	-0.23948
C	0.09547	0.29797	-0.38818
C	-0.71046	-0.85684	-0.19276
C	-0.55560	1.56284	-0.46706
C	-2.08316	-0.74522	-0.09360
C	-1.92516	1.65883	-0.35050
H	0.05434	2.44624	-0.62016
C	-2.70899	0.50896	-0.16842
H	-2.68901	-1.63168	0.05024
H	-2.42171	2.62067	-0.40822
C	-4.17796	0.67125	-0.06584
O	-4.75203	1.73902	-0.13321
O	-4.81677	-0.49742	0.11235
C	-6.24761	-0.41850	0.22325
H	-6.49757	0.23659	1.06197
H	-6.64370	0.04220	-0.68562
C	-6.76910	-1.82141	0.42258
H	-7.85828	-1.79914	0.51100
H	-6.50792	-2.46166	-0.42323
H	-6.36147	-2.26650	1.33322
H	-0.25380	-1.83544	-0.11688
C	4.47557	2.97378	0.99646
H	5.49296	3.10281	0.62026
H	4.46345	2.24569	1.81487
H	4.08244	3.93067	1.35364

O	3.72029	2.50826	-0.10001
O	2.40212	2.35634	0.32685

[Compound 2] _TS

N	1.89328	-0.17519	-0.58823
H	2.55223	0.78320	-0.25510
C	0.55669	-0.00963	-0.43257
C	-0.36028	-1.07453	-0.22761
C	0.04520	1.31643	-0.49814
C	-1.71287	-0.82066	-0.11167
C	-1.30605	1.55511	-0.36531
H	0.74381	2.13074	-0.65446
C	-2.20316	0.49288	-0.17716
H	-2.40714	-1.63816	0.04043
H	-1.70022	2.56369	-0.41376
C	-3.64605	0.80896	-0.05428
O	-4.10513	1.93119	-0.11557
O	-4.40136	-0.28577	0.13524
C	-5.81442	-0.05742	0.26681
H	-5.98143	0.62994	1.10025
H	-6.17541	0.43089	-0.64226
C	-6.47439	-1.39654	0.49313
H	-7.55394	-1.26123	0.59729
H	-6.29390	-2.07077	-0.34730
H	-6.09979	-1.86961	1.40381
H	-0.00141	-2.09343	-0.15289
C	5.25672	2.06910	0.91795
H	6.24909	2.16028	0.47085
H	5.24037	1.24601	1.64066
H	4.98239	3.00177	1.42003
O	4.37833	1.81074	-0.15593
O	3.08783	1.72362	0.36062
C	2.50026	-1.47136	-0.51123
C	4.00464	-1.56435	-0.82747
C	2.80198	-2.10216	0.88246
H	1.93382	-2.17924	-1.12753
C	4.13309	-2.61644	0.29655
H	4.50805	-0.62915	-0.57279
H	4.28311	-1.85261	-1.84352
H	2.95875	-1.31220	1.62110
H	2.08740	-2.82821	1.27792
H	5.01550	-2.56388	0.93684
H	4.04030	-3.63647	-0.08571

[Compound 3] _TS

N	-2.23175	0.71979	-0.27801
H	-2.96882	-0.20349	-0.00014
C	-0.91597	0.41410	-0.20379
C	0.11256	1.37494	-0.00849
C	-0.54331	-0.95193	-0.35500
C	1.43698	0.98505	0.02273
C	0.78219	-1.32634	-0.30301
H	-1.32709	-1.68563	-0.50500
C	1.78920	-0.36645	-0.11966
H	2.21676	1.72374	0.16354
H	1.07104	-2.36528	-0.41311
C	3.19735	-0.82747	-0.08861
O	3.53772	-1.98576	-0.21705
O	4.06768	0.17863	0.09905
C	5.45537	-0.19401	0.14143
H	5.59546	-0.92940	0.93805
H	5.71605	-0.67694	-0.80413
C	6.25964	1.06155	0.37900
H	7.32358	0.81409	0.41696
H	6.10587	1.78546	-0.42465
H	5.98417	1.53110	1.32615
H	-0.13632	2.42200	0.11137
C	-5.86702	-1.38550	0.53280
H	-6.72685	-1.45717	-0.13674
H	-5.98961	-0.53867	1.21667
H	-5.76003	-2.30855	1.11062
O	-4.74774	-1.19653	-0.30482
O	-3.61321	-1.13758	0.49858
C	-2.68875	2.07624	-0.07168

H	-2.24285	2.71362	-0.84766
H	-2.32848	2.46247	0.89335
C	-4.20296	2.17340	-0.13526
H	-4.66429	1.60015	0.67151
H	-4.57982	1.78650	-1.08431
H	-4.51380	3.21600	-0.03538

[Compound 4] _TS

N	-2.17662	0.33004	-0.37083
H	-2.86863	-0.64991	-0.18483
C	-0.84443	0.12825	-0.26480
C	0.13736	1.13186	-0.03625
C	-0.39174	-1.21384	-0.43450
C	1.47869	0.80614	0.01187
C	0.94772	-1.52620	-0.36311
H	-1.13195	-1.98514	-0.61717
C	1.90324	-0.52202	-0.14324
H	2.21648	1.58219	0.17639
H	1.28787	-2.54816	-0.48525
C	3.33159	-0.91196	-0.08921
O	3.73268	-2.04963	-0.22667
O	4.14539	0.13404	0.13141
C	5.54917	-0.16729	0.20057
H	5.70981	-0.90401	0.99208
H	5.85539	-0.62440	-0.74411
C	6.28134	1.12547	0.47020
H	7.35560	0.93345	0.53090
H	6.10836	1.84964	-0.32930
H	5.95950	1.56891	1.41531
H	-0.15600	2.16401	0.08933
C	-5.77741	-1.49311	0.72872
H	-6.74370	-1.30511	0.25541
H	-5.61935	-0.79412	1.55739
H	-5.73592	-2.52013	1.10400
O	-4.81384	-1.29871	-0.28332
O	-3.55844	-1.56408	0.26679
C	-2.87975	1.58684	-0.13905
C	-2.68984	2.16999	1.26549
C	-2.61923	2.60242	-1.25697
H	-2.86653	1.40215	2.02223
H	-1.69435	2.58599	1.42914
H	-3.41461	2.97398	1.42099
H	-2.79714	2.14810	-2.23401
H	-3.30288	3.44778	-1.14254
H	-1.59920	2.99157	-1.24339
H	-3.93309	1.30064	-0.22084

[Compound 5] _TS

N	1.64840	-0.04676	-0.28727
H	2.22691	0.98843	-0.03059
C	0.30051	0.04962	-0.21228
C	-0.56210	-1.05434	0.02467
C	-0.28462	1.33306	-0.40655
C	-1.93153	-0.87845	0.05293
C	-1.65264	1.49439	-0.35689
H	0.37233	2.17610	-0.58778
C	-2.49428	0.39405	-0.13344
H	-2.58366	-1.72595	0.22615
H	-2.10273	2.47014	-0.49935
C	-3.95752	0.62734	-0.10492
O	-4.47730	1.71358	-0.25953
O	-4.65727	-0.49868	0.11306
C	-6.08613	-0.34928	0.15891
H	-6.33796	0.35837	0.95323
H	-6.42312	0.08203	-0.78736
C	-6.68100	-1.71511	0.40491
H	-7.77051	-1.63899	0.44697
H	-6.41746	-2.40860	-0.39704
H	-6.33068	-2.13143	1.35226
H	-0.14969	-2.04343	0.18038
C	4.87034	2.63317	0.61843
H	5.75046	2.81898	-0.00092
H	5.07727	1.83621	1.34087
H	4.58502	3.54453	1.15274

O	3.85051	2.24685	-0.27654
O	2.69150	2.02756	0.46107
C	2.31141	-1.30843	-0.04511
H	1.94967	-2.03989	-0.78202
H	2.03955	-1.70532	0.94531
C	3.82455	-1.18832	-0.15302
C	4.52375	-2.53371	0.02051
H	4.18324	-0.48329	0.60456
H	4.08056	-0.75413	-1.12555
C	6.04191	-2.42697	-0.07424
H	4.24818	-2.96730	0.99012
H	4.15983	-3.23465	-0.74143
H	6.34902	-2.02245	-1.04358
H	6.44075	-1.76525	0.70083
H	6.51894	-3.40339	0.04518

[Compound 6] _TS

N	1.26576	0.27578	-0.26475
H	1.75120	1.35258	0.00649
C	-0.08448	0.24739	-0.19059
C	-0.84464	-0.93808	-0.00021
C	-0.78233	1.48005	-0.33788
C	-2.22433	-0.88662	0.02907
C	-2.15920	1.51606	-0.28721
H	-0.20333	2.38484	-0.48411
C	-2.89880	0.33677	-0.10972
H	-2.79813	-1.79533	0.16537
H	-2.69494	2.45229	-0.39419
C	-4.37713	0.43574	-0.08012
O	-4.99290	1.47516	-0.20034
O	-4.97249	-0.75579	0.09597
C	-6.40918	-0.73771	0.13701
H	-6.72711	-0.07946	0.94988
H	-6.78008	-0.31066	-0.79851
C	-6.87923	-2.15827	0.33894
H	-7.97137	-2.18202	0.37486
H	-6.55036	-2.80135	-0.48071
H	-6.49765	-2.56912	1.27656
H	-0.34493	-1.89163	0.11687
C	4.26490	3.22903	0.50399
H	5.07155	3.51322	-0.17525
H	4.60448	2.44262	1.18663
H	3.93472	4.09722	1.08246
O	3.22047	2.76104	-0.32072
O	2.14478	2.42439	0.49536
C	2.04456	-0.92564	-0.06600
H	1.78014	-1.64569	-0.85419
H	1.78528	-1.40395	0.89100
C	3.54022	-0.64867	-0.11240
C	4.36809	-1.92698	-0.02237
H	3.80337	0.02418	0.71112
H	3.77432	-0.11204	-1.03819
C	5.87305	-1.67092	-0.04210
H	4.10892	-2.47214	0.89549
H	4.10619	-2.59269	-0.85588
C	6.69883	-2.95067	0.02819
H	6.13166	-1.11676	-0.95276
H	6.13811	-1.01653	0.79746
H	7.77083	-2.73620	0.01221
H	6.48622	-3.50969	0.94509
H	6.47979	-3.60946	-0.81809

[Compound 7] _TS

N	1.36262	0.15127	-0.21881
H	1.87638	1.22433	0.02084
C	0.01060	0.16955	-0.16766
C	-0.79076	-0.97903	0.07260
C	-0.64401	1.41407	-0.39174
C	-2.16829	-0.88191	0.07694
C	-2.01960	1.49704	-0.36501
H	-0.03378	2.29086	-0.57617
C	-2.80002	0.35335	-0.13694
H	-2.77348	-1.76313	0.25229
H	-2.52260	2.44303	-0.52955

C	-4.27470	0.50147	-0.13443
O	-4.85389	1.55335	-0.31318
O	-4.91113	-0.66031	0.08925
C	-6.34695	-0.59416	0.10974
H	-6.65290	0.10487	0.89264
H	-6.69198	-0.19160	-0.84627
C	-6.86585	-1.98990	0.35932
H	-7.95850	-1.97663	0.38252
H	-6.54923	-2.67404	-0.43138
H	-6.50856	-2.37706	1.31640
H	-0.32477	-1.94061	0.24846
C	4.43471	3.04066	0.51263
H	5.26836	3.26635	-0.15564
H	4.72853	2.27501	1.23869
H	4.11918	3.94439	1.04278
O	3.39715	2.57066	-0.31986
O	2.29188	2.29832	0.47962
C	2.09482	-1.06299	0.05963
H	1.80770	-1.82213	-0.68234
H	1.81523	-1.46924	1.04412
C	3.59980	-0.84327	0.00523
C	4.37308	-2.14732	0.22171
H	3.88215	-0.11270	0.77061
H	3.87028	-0.40498	-0.96009
C	5.85653	-1.93946	0.24919
H	4.05731	-2.59404	1.17503
H	4.11861	-2.86923	-0.56309
H	6.22887	-1.26830	1.02326
C	6.72699	-2.49873	-0.59109
H	7.79167	-2.30403	-0.51894
H	6.40296	-3.17243	-1.37984

[Compound 8] _TS

N	-2.02956	0.39425	-0.45005
H	-2.70508	-0.56778	-0.09509
C	-0.69438	0.18663	-0.32937
C	0.25556	1.21480	-0.09314
C	-0.22191	-1.14769	-0.47050
C	1.60322	0.91882	-0.01840
C	1.12423	-1.42947	-0.37528
H	-0.94611	-1.93469	-0.64724
C	2.05443	-0.40264	-0.15448
H	2.32321	1.70977	0.15337
H	1.48858	-2.44517	-0.47794
C	3.48997	-0.76342	-0.07469
O	3.91559	-1.89431	-0.19167
O	4.27943	0.30130	0.14377
C	5.68783	0.02932	0.23718
H	5.85173	-0.69203	1.04205
H	6.01650	-0.43565	-0.69604
C	6.39003	1.34053	0.49721
H	7.46697	1.17136	0.57564
H	6.21368	2.04898	-0.31552
H	6.04604	1.79143	1.43093
H	-0.06896	2.24114	0.02577
C	-5.51574	-1.55274	0.76704
H	-6.43577	-1.70901	0.19972
H	-5.53772	-0.57845	1.26549
H	-5.38828	-2.34822	1.50696
O	-4.47290	-1.59704	-0.18544
O	-3.26628	-1.47529	0.48862
C	-2.57801	1.71841	-0.25073
C	-4.05762	1.74864	-0.48474
H	-2.09523	2.39688	-0.97059
H	-2.34572	2.10757	0.75140
C	-4.92569	2.35792	0.32044
H	-4.40300	1.25290	-1.38912
H	-5.98457	2.39118	0.08832
H	-4.60769	2.84808	1.23668

[Compound 9] _TS

N	-2.09991	0.52583	-0.34674
H	-2.77855	-0.45089	0.00730
C	-0.76516	0.28857	-0.25835

C	0.20825	1.27132	0.06044	C	0.38591	-1.74304	-0.73293
C	-0.32163	-1.03569	-0.52777	C	1.83531	0.30555	0.49546
C	1.55054	0.94387	0.08854	C	1.75953	-1.72001	-0.83504
C	1.01956	-1.35098	-0.47791	H	-0.19416	-2.52703	-1.20748
H	-1.06362	-1.78878	-0.76569	C	2.50229	-0.69596	-0.22600
C	1.97296	-0.36738	-0.17616	H	2.41027	1.10082	0.95413
H	2.28832	1.70163	0.32295	H	2.29004	-2.48419	-1.39139
H	1.36138	-2.35975	-0.67899	C	3.97633	-0.71518	-0.38178
C	3.40202	-0.76182	-0.15112	O	4.58396	-1.56256	-1.00372
O	3.80100	-1.88693	-0.37100	O	4.57607	0.31118	0.24300
O	4.21670	0.26453	0.14305	C	6.00882	0.35967	0.13580
C	5.62053	-0.04277	0.18888	H	6.42090	-0.56785	0.54197
H	5.78265	-0.82199	0.93830	H	6.27843	0.40611	-0.92262
H	5.92101	-0.44835	-0.78073	C	6.48356	1.57418	0.89694
C	6.35710	1.23155	0.52537	H	7.57271	1.64273	0.83634
H	7.43093	1.03334	0.57184	H	6.05987	2.49030	0.47899
H	6.18377	1.99803	-0.23356	H	6.20323	1.51189	1.95098
H	6.04006	1.62462	1.49410	H	-0.03833	1.07795	1.16737
H	-0.08934	2.28918	0.28037	C	-4.64114	-3.58765	0.84731
C	-5.56093	-1.51590	0.74632	H	-5.70771	-3.39758	0.71023
H	-6.43538	-1.75750	0.13880	H	-4.32761	-3.28738	1.85275
H	-5.64911	-0.50439	1.15409	H	-4.42541	-4.64962	0.69769
H	-5.45179	-2.24001	1.55882	O	-3.98839	-2.80989	-0.13447
O	-4.45824	-1.59702	-0.13466	O	-2.61899	-3.04021	-0.02063
O	-3.30271	-1.36286	0.58940	C	-2.42215	0.07242	0.90203
C	-2.59467	1.84371	-0.00378	C	-2.65935	1.43781	0.28219
C	-4.03369	1.97588	-0.20366	C	-2.74261	2.56620	1.10067
H	-2.09246	2.58993	-0.63385	C	-2.83809	1.58516	-1.09511
H	-2.35386	2.10446	1.03837	C	-3.00520	3.82124	0.55562
C	-5.21883	2.14132	-0.35905	H	-2.60189	2.46450	2.17364
H	-6.26495	2.27794	-0.50974	C	-3.09501	2.83989	-1.64124
				H	-2.77010	0.71353	-1.73753
[Compound 10] _TS				C	-3.18071	3.96161	-0.81879
				H	-3.06659	4.68855	1.20484
N	-1.65241	-0.81968	0.06268	H	-3.22888	2.94108	-2.71327
H	-2.15411	-1.91999	-0.11667	H	-3.37970	4.93846	-1.24663
C	-0.30217	-0.74293	0.00914	H	-1.95769	0.19869	1.88892
C	0.45975	0.28546	0.62330	H	-3.38814	-0.41790	1.06016

[Compound 11] _TS

N	-1.33566	-1.26852	0.08644
H	-1.69776	-2.40604	-0.16754
C	-0.00820	-1.01538	0.01387
C	0.63490	0.05391	0.69100
C	0.77977	-1.86244	-0.81423
C	1.99337	0.25736	0.54208
C	2.13658	-1.65827	-0.93721
H	0.28983	-2.67618	-1.33772
C	2.76132	-0.59600	-0.26441
H	2.47645	1.08291	1.05051
H	2.74368	-2.30624	-1.55890
C	4.22160	-0.41828	-0.44537
O	4.91416	-1.13744	-1.13635
O	4.70524	0.63025	0.24086
C	6.11762	0.86451	0.11252
H	6.65172	-0.02775	0.44981
H	6.35244	1.01059	-0.94509
C	6.45756	2.07842	0.94356
H	7.52797	2.28636	0.86868
H	5.91304	2.95874	0.59429
H	6.21401	1.91509	1.99594
H	0.05553	0.73461	1.30185
C	-3.93176	-4.43818	0.70934
H	-5.01694	-4.37191	0.60654
H	-3.62958	-4.17201	1.72779
H	-3.59271	-5.45268	0.47976
O	-3.40571	-3.51984	-0.22574
O	-2.01563	-3.58271	-0.15061
C	-2.19082	-0.54422	1.00268
C	-2.61272	0.81855	0.48582
C	-2.75202	1.89128	1.36484
C	-2.90929	1.02102	-0.86475
C	-3.18261	3.13625	0.90863
H	-2.52480	1.75843	2.41954
C	-3.33270	2.26551	-1.31578
H	-2.80209	0.19823	-1.56407
C	-3.47862	3.34698	-0.43887
H	-3.28374	3.95639	1.61361
H	-3.55519	2.40041	-2.37067
H	-1.71986	-0.42928	1.98774
H	-3.08093	-1.16623	1.14077
C	-3.93536	4.68897	-0.94177
H	-4.01369	5.41348	-0.12848
H	-3.23854	5.09212	-1.68310
H	-4.91542	4.61871	-1.42335

[Compound 12] _TS

N	1.34562	1.23005	0.08966
H	1.72461	2.36697	-0.15502
C	0.01452	0.99402	0.01915
C	-0.64157	-0.06831	0.69454
C	-0.76347	1.85260	-0.80647
C	-2.00257	-0.25487	0.54608
C	-2.12275	1.66545	-0.92912
H	-0.26393	2.66121	-1.32884
C	-2.76008	0.60951	-0.25832
H	-2.49572	-1.07532	1.05306
H	-2.72223	2.32199	-1.54920
C	-4.22294	0.44974	-0.43951
O	-4.90598	1.18007	-1.12795
O	-4.71818	-0.59513	0.24291
C	-6.13352	-0.81349	0.11384
H	-6.65735	0.08330	0.45509
H	-6.36964	-0.95238	-0.94439
C	-6.48653	-2.02713	0.93965
H	-7.55918	-2.22276	0.86404
H	-5.95209	-2.91195	0.58630
H	-6.24115	-1.87113	1.99270
H	-0.07156	-0.75688	1.30542
C	4.00042	4.35157	0.72983
H	5.08378	4.26003	0.62828
H	3.69109	4.09874	1.74942

H	3.68434	5.37159	0.49277
O	3.45460	3.43887	-0.20021
O	2.06681	3.53313	-0.12761
C	2.19288	0.48995	0.99959
C	2.61128	-0.86723	0.46437
C	2.76858	-1.94526	1.33735
C	2.88564	-1.05309	-0.89303
C	3.19626	-3.18843	0.87662
H	2.55678	-1.81897	2.39541
C	3.30825	-2.28872	-1.37355
H	2.76214	-0.22366	-1.58100
C	3.45675	-3.33424	-0.47572
H	3.32081	-4.03183	1.54529
H	3.52120	-2.44647	-2.42419
H	1.71873	0.36286	1.98150
H	3.08579	1.10518	1.14992
F	3.86437	-4.53542	-0.93479

[Compound 13] _TS

N	0.92303	1.62802	0.07526
H	1.13965	2.79753	-0.21968
C	-0.35844	1.19707	0.00372
C	-0.86056	0.07676	0.71645
C	-1.24237	1.89860	-0.86261
C	-2.17672	-0.31511	0.56333
C	-2.55723	1.50771	-0.98930
H	-0.86057	2.75197	-1.41247
C	-3.04149	0.39573	-0.28207
H	-2.55036	-1.17978	1.09824
H	-3.23795	2.04381	-1.64056
C	-4.46170	0.01326	-0.47033
O	-5.23395	0.60444	-1.19691
O	-4.80731	-1.06358	0.25286
C	-6.17208	-1.49677	0.11998
H	-6.82939	-0.67217	0.40803
H	-6.36531	-1.72237	-0.93208
C	-6.35613	-2.70674	1.00401
H	-7.38571	-3.06509	0.92566
H	-5.68848	-3.51773	0.70411
H	-6.15795	-2.46319	2.05036
H	-0.20480	-0.49637	1.35983
C	3.05965	5.14065	0.63548
H	4.14756	5.21107	0.57399
H	2.75119	4.89525	1.65715
H	2.60291	6.08688	0.33138
O	2.69592	4.10940	-0.25926
O	1.30765	3.99885	-0.24177
C	1.85048	1.06398	1.03033
C	2.47932	-0.23803	0.56990
C	2.85886	-1.19789	1.50955
C	2.72937	-0.48578	-0.78100
C	3.48042	-2.38066	1.11907
H	2.66982	-1.02596	2.56560
C	3.34532	-1.66509	-1.18825
H	2.43516	0.24913	-1.52260
C	3.71811	-2.60516	-0.23265
H	3.77173	-3.12246	1.85325
H	3.53515	-1.85455	-2.23814
H	1.38043	0.91215	2.01093
H	2.64079	1.81013	1.16340
Cl	4.48692	-4.08484	-0.73508

[SRS8-71]_TS

C	1.73050	-0.97479	-0.11829
C	2.18969	0.35764	-0.19310
C	1.28301	1.37861	-0.41888
C	-0.08642	1.12512	-0.60575
C	-0.56064	-0.23706	-0.50599
C	0.39206	-1.25777	-0.26456
H	2.43809	-1.77241	0.06942
H	1.65178	2.39801	-0.47370
H	0.05189	-2.28167	-0.17675
N	-0.93797	2.12638	-0.94065
H	-0.55203	3.05752	-0.87848

H	-1.96522	2.05963	-0.70943	C	0.52703	-1.13999	-0.23528
N	-1.87461	-0.49588	-0.64123	H	2.53452	-1.79020	0.09119
H	-2.54821	0.29866	-0.63066	H	2.02945	2.41889	-0.48578
C	3.61522	0.72139	-0.02829	H	0.12388	-2.13962	-0.13901
O	4.04506	1.85607	-0.08928	N	-0.57164	2.31988	-0.94251
O	4.39689	-0.34758	0.20169	H	-0.12000	3.22175	-0.89156
C	5.79639	-0.07472	0.37728	H	-1.59768	2.33158	-0.69884
H	6.17444	0.41088	-0.52637	N	-1.68702	-0.22391	-0.61630
H	5.91484	0.62951	1.20503	H	-2.29535	0.61910	-0.61563
C	6.48810	-1.38970	0.64695	C	3.87861	0.61767	-0.03416
H	6.35780	-2.08117	-0.18877	O	4.38314	1.72094	-0.10148
H	7.55879	-1.22012	0.78679	O	4.58952	-0.50074	0.19214
H	6.09565	-1.86115	1.55096	C	6.00548	-0.32091	0.35375
C	-4.57872	2.67180	1.32717	H	6.40369	0.15194	-0.54796
H	-4.90944	2.47375	2.34945	H	6.17895	0.36264	1.18917
H	-5.44113	2.85856	0.67953	C	6.61417	-1.68126	0.59739
H	-3.91278	3.54196	1.30960	H	6.42785	-2.35127	-0.24516
O	-3.88969	1.51341	0.91341	H	7.69540	-1.58308	0.72397
O	-3.46913	1.70067	-0.39844	H	6.20429	-2.13882	1.50083
C	-2.45712	-1.80386	-0.50889	C	-4.11988	3.17014	1.35839
C	-2.71210	-2.40152	0.90252	H	-4.47235	2.99835	2.37813
C	-3.96874	-1.90733	-0.77780	H	-4.95531	3.45645	0.71183
H	-1.90537	-2.51651	-1.13227	H	-3.36306	3.96270	1.35092
C	-4.05066	-2.94722	0.36191	O	-3.56010	1.94799	0.93249
H	-2.86827	-1.59797	1.62640	O	-3.12381	2.09925	-0.37719
H	-1.98059	-3.10963	1.29945	C	-2.38542	-1.47942	-0.45023
H	-4.46969	-0.97577	-0.50225	C	-2.67983	-1.87488	1.00575
H	-4.28263	-2.20103	-1.78155	C	-3.78296	-1.43902	-1.07900
H	-4.91674	-2.89882	1.02395	H	-1.80075	-2.27309	-0.93145
H	-3.95175	-3.96988	-0.01186	C	-3.73901	-2.97109	0.86009
				H	-3.08749	-0.99774	1.51963
[SRS8-73]_TS				H	-1.79052	-2.19802	1.55344
				C	-4.54572	-2.60057	-0.41285
C	1.88227	-0.94721	-0.09886	H	-3.74783	-1.51252	-2.16862
C	2.43141	0.34956	-0.18778	H	-4.24582	-0.47829	-0.83188
C	1.59382	1.42693	-0.41944	H	-3.25476	-3.94451	0.73023
C	0.21017	1.26500	-0.59898	H	-4.37080	-3.05120	1.74794
C	-0.35763	-0.06041	-0.48269	H	-4.62224	-3.45993	-1.08449

H	-5.56860	-2.30359	-0.16948

[SRS8-48]_TS

C	2.21465	-0.95977	-0.17673
C	2.96388	0.23590	-0.17627
C	2.31246	1.44460	-0.34966
C	0.92427	1.51683	-0.55317
C	0.14984	0.29473	-0.52146
C	0.84904	-0.92544	-0.33786
H	2.72140	-1.90629	-0.03704
H	2.90095	2.35670	-0.34943
H	0.29298	-1.85352	-0.31517
N	0.32850	2.70196	-0.83899
H	0.91751	3.51462	-0.72674
H	-0.68880	2.86489	-0.61058
N	-1.18641	0.35463	-0.67072
H	-1.65106	1.28470	-0.63211
C	4.43137	0.25962	0.01252
O	5.10595	1.27013	0.02257
O	4.95056	-0.96969	0.17665
C	6.37263	-1.02774	0.37053
H	6.86271	-0.56822	-0.49197
H	6.63046	-0.43432	1.25185
C	6.75341	-2.47998	0.53296
H	6.48633	-3.05781	-0.35493
H	7.83301	-2.56252	0.68265
H	6.25369	-2.92289	1.39765
C	-2.08755	-0.77861	-0.54696
C	-2.36648	-1.12364	0.92292
C	-3.39325	-0.47153	-1.28117
H	-1.62228	-1.64446	-1.03547
C	-3.35748	-2.27945	1.04177
H	-2.77026	-0.22786	1.40942
H	-1.42878	-1.36508	1.43414
C	-4.38371	-1.62688	-1.14989
H	-3.82658	0.44384	-0.86038
H	-3.17927	-0.26515	-2.33476
C	-4.67086	-1.99170	0.30949
H	-3.55509	-2.48894	2.09909
H	-2.91166	-3.19412	0.62426
H	-5.31740	-1.36861	-1.66182
H	-3.98580	-2.51342	-1.66480
H	-5.13132	-1.11427	0.78723
C	-3.09800	4.02896	1.40761
H	-3.51186	3.88643	2.40867
H	-3.84792	4.47665	0.74789
H	-2.21698	4.67920	1.45465
O	-2.74084	2.74377	0.95094
O	-2.23815	2.86197	-0.33856
C	-5.64468	-3.16057	0.41631
H	-5.86574	-3.40068	1.46079
H	-6.59224	-2.93625	-0.08284
H	-5.22811	-4.06010	-0.05062

[SRS13-10]_TS

C	2.85319	-1.05887	-0.17688
C	3.80008	-0.01355	-0.13593
C	3.37209	1.29526	-0.27666
C	2.02120	1.61531	-0.48949
C	1.04498	0.54729	-0.50395
C	1.51697	-0.78107	-0.34849
H	3.18440	-2.08309	-0.06073
H	4.11137	2.08944	-0.24546
H	0.80580	-1.59671	-0.35614
N	1.64733	2.89432	-0.74589
H	2.36671	3.58842	-0.60339
H	0.67025	3.22707	-0.53520
N	-0.25681	0.84433	-0.66952
H	-0.55403	1.84026	-0.61851
C	5.24745	-0.25210	0.05780
O	6.08803	0.62430	0.09983
O	5.54307	-1.55751	0.18508
C	6.93237	-1.86899	0.37509
H	7.49834	-1.47784	-0.47458

H	7.28714	-1.35548	1.27268	H	-5.09910	-2.49289	2.23598
C	7.05238	-3.36958	0.49444	H	-5.93211	-0.93183	2.17526
H	6.68906	-3.86536	-0.40875				
H	8.10054	-3.64453	0.63762	**[SRS8-90]_TS**			
H	6.48134	-3.74277	1.34777				
C	-1.34557	-0.11692	-0.62527	C	-2.29359	-0.91723	-0.32571
C	-1.74771	-0.46442	0.81271	C	-2.92455	0.24737	0.15844
C	-2.54604	0.44717	-1.38285	C	-2.14813	1.30309	0.60431
H	-1.02045	-1.03183	-1.13736	C	-0.74461	1.24121	0.61118
C	-2.93871	-1.42245	0.84242	C	-0.09500	0.07138	0.05963
H	-2.00220	0.46934	1.32813	C	-0.92040	-0.99812	-0.37129
H	-0.89522	-0.89791	1.34620	H	-2.89772	-1.74728	-0.66962
C	-3.73577	-0.51113	-1.33886	H	-2.64594	2.18909	0.98569
H	-2.82296	1.40915	-0.93503	H	-0.45985	-1.89971	-0.75274
H	-2.26004	0.65182	-2.41967	N	-0.01575	2.22728	1.19166
C	-4.15533	-0.85241	0.09818	H	-0.53986	3.05108	1.44982
H	-3.18573	-1.63782	1.88547	H	0.98218	2.41664	0.90139
H	-2.64468	-2.37773	0.38749	N	1.24756	0.03627	-0.03213
H	-4.56471	-0.05762	-1.88835	H	1.78567	0.89738	0.17911
H	-3.47316	-1.43293	-1.87471	C	-4.39569	0.39586	0.21327
H	-4.41000	0.10026	0.58956	O	-4.97119	1.38330	0.62569
C	-1.62122	4.77518	1.39380	O	-5.04124	-0.68908	-0.24927
H	-2.10900	4.69909	2.36845	C	-6.47578	-0.61952	-0.23156
H	-2.24642	5.34683	0.70068	H	-6.80583	-0.45361	0.79746
H	-0.64736	5.26679	1.49864	H	-6.79213	0.24378	-0.82306
O	-1.46011	3.45057	0.93818	C	-7.00332	-1.91766	-0.79466
O	-0.87156	3.48934	-0.31867	H	-6.67523	-2.76875	-0.19337
C	-5.43913	-1.73088	0.20178	H	-8.09622	-1.90082	-0.79617
C	-6.60750	-1.02662	-0.50505	H	-6.66219	-2.06740	-1.82168
C	-5.25202	-3.12019	-0.42258	C	3.26459	4.23156	-0.73757
C	-5.82997	-1.90233	1.67775	H	3.53655	4.52518	-1.75405
H	-6.73899	-0.00533	-0.13162	H	4.13760	4.28911	-0.07981
H	-6.46837	-0.97524	-1.58781	H	2.47493	4.88847	-0.35542
H	-7.54128	-1.56857	-0.32494	O	2.80209	2.90261	-0.83145
H	-4.46531	-3.69167	0.07835	O	2.47320	2.46339	0.44220
H	-6.17805	-3.69767	-0.33643	C	2.01736	-1.08817	-0.55085
H	-5.00382	-3.06058	-1.48606	C	2.16589	-2.19364	0.51440
H	-6.79142	-2.41944	1.75724	H	1.45947	-1.51764	-1.39246

C	3.33623	-0.53357	-1.10543
C	3.30489	-2.01130	1.52231
H	2.30144	-3.15338	0.00053
H	1.20984	-2.26951	1.04224
H	3.71696	0.23282	-0.42093
H	3.10467	-0.00321	-2.03395
C	4.43949	-1.56908	-1.34378
C	4.64222	-2.57977	1.03790
H	3.40989	-0.95309	1.79240
H	3.03234	-2.52970	2.44783
C	5.31214	-1.82928	-0.11247
H	4.01770	-2.51016	-1.72085
H	5.08836	-1.19482	-2.14273
H	5.34290	-2.61345	1.88035
H	4.47938	-3.62476	0.73991
H	5.67591	-0.86050	0.25406
H	6.20311	-2.39123	-0.41683

[SRS8-70]_TS

C	2.52640	-0.92719	0.34306
C	3.17651	0.22001	-0.15725
C	2.41742	1.28484	-0.61126
C	1.01315	1.24846	-0.61166
C	0.34438	0.09612	-0.04617
C	1.15228	-0.98255	0.39514
H	3.11674	-1.76391	0.69470
H	2.92962	2.15773	-1.00367
H	0.67729	-1.87056	0.79047
N	0.29948	2.24252	-1.19797
H	0.83778	3.05415	-1.46544
H	-0.69194	2.45447	-0.90127
N	-0.99836	0.08729	0.04891
H	-1.51951	0.95792	-0.16649
C	4.64973	0.34154	-0.21942
O	5.24106	1.31523	-0.64211
O	5.27792	-0.75118	0.24877
C	6.71337	-0.70684	0.22454
H	7.04170	-0.54755	-0.80605
H	7.04738	0.15134	0.81384
C	7.22078	-2.01342	0.78659
H	6.87574	-2.85915	0.18722
H	8.31381	-2.01534	0.78367
H	6.88131	-2.15667	1.81508
C	-2.91230	4.32580	0.75233
H	-3.17250	4.62627	1.76990
H	-3.78513	4.40987	0.09722
H	-2.10460	4.95950	0.36861
O	-2.48915	2.98362	0.84362
O	-2.17870	2.53500	-0.43120
C	-1.79297	-1.01051	0.58559
C	-1.99165	-2.10948	-0.47846
H	-1.23377	-1.46230	1.41546
C	-3.08084	-0.41941	1.16607
C	-2.96966	-1.81606	-1.62355
H	-2.28587	-3.03945	0.02146
H	-1.00299	-2.30955	-0.90523
H	-3.52454	0.24640	0.42022
H	-2.80373	0.23156	1.99962
C	-4.09986	-1.48134	1.60714
C	-4.44169	-2.22588	-1.43103
H	-2.91680	-0.75518	-1.89971
H	-2.60198	-2.36072	-2.49991
C	-5.43460	-1.42005	0.85663
H	-3.67060	-2.48147	1.48859
H	-4.30205	-1.38363	2.67850
C	-5.35608	-1.25877	-0.66554
H	-4.86449	-2.34223	-2.43520
H	-4.48632	-3.22601	-0.97782
H	-6.02799	-0.58497	1.24927
H	-6.00350	-2.32860	1.09029
H	-5.06912	-0.23158	-0.92080
H	-6.37698	-1.37197	-1.04821

[SRS8-94]_TS

C	3.22731	-1.23653	0.01997	H	-3.32408	-1.84492	-0.75136
C	4.13252	-0.16663	-0.14623	H	-3.31842	-1.45550	0.96077
C	3.64608	1.10145	-0.41257	H	-5.01340	0.33936	0.56438
C	2.27044	1.35421	-0.55003	H	-5.01124	-0.02879	-1.15032
C	1.34026	0.26511	-0.34382	C	-5.95092	-1.53738	0.06806
C	1.87152	-1.02116	-0.07341	C	-7.37401	-0.99697	-0.04372
H	3.60747	-2.22811	0.23067	H	-5.81244	-1.98975	1.05931
H	4.35495	1.91324	-0.54178	H	-5.81471	-2.35038	-0.65776
H	1.19070	-1.85030	0.07036	C	-8.44880	-2.05947	0.17161
N	1.82638	2.57613	-0.93191	H	-7.51378	-0.18843	0.68631
H	2.52516	3.30505	-0.94264	H	-7.51190	-0.53878	-1.03234
H	0.84937	2.90015	-0.69307	C	-9.86704	-1.51015	0.06043
N	0.01770	0.49343	-0.40678	H	-8.31016	-2.86588	-0.55953
H	-0.33008	1.47634	-0.46020	H	-8.30980	-2.51827	1.15865
C	5.59922	-0.33822	-0.04299	H	-10.61430	-2.29298	0.21769
O	6.40627	0.55949	-0.18003	H	-10.04664	-0.72605	0.80290
O	5.95232	-1.60753	0.22320	H	-10.04570	-1.07444	-0.92781
C	7.36280	-1.85441	0.33952				
H	7.84764	-1.56243	-0.59583	**[SRS8-80]_TS**			
H	7.76533	-1.21885	1.13277				
C	7.54653	-3.32283	0.64005	C	2.21468	-0.95850	-0.17258
H	7.13713	-3.94201	-0.16154	C	2.95881	0.24021	-0.17706
H	8.61176	-3.54803	0.73627	C	2.30223	1.44558	-0.35457
H	7.05325	-3.59676	1.57555	C	0.91382	1.51097	-0.55772
C	-1.36959	4.62171	1.15945	C	0.14488	0.28590	-0.52213
H	-1.75969	4.68120	2.17828	C	0.84878	-0.93051	-0.33337
H	-2.10034	5.02297	0.45002	H	2.72537	-1.90242	-0.02971
H	-0.43496	5.18888	1.08176	H	2.88693	2.36011	-0.35792
O	-1.14032	3.25288	0.91377	H	0.29680	-1.86097	-0.30751
O	-0.67018	3.11686	-0.38814	N	0.31259	2.69298	-0.84689
C	-0.97915	-0.52682	-0.15635	H	0.89788	3.50856	-0.73666
C	-2.38616	0.04062	-0.28325	H	-0.70395	2.85217	-0.61759
H	-0.83788	-0.94944	0.84920	N	-1.19175	0.33992	-0.67393
H	-0.84444	-1.35050	-0.87048	H	-1.66037	1.26753	-0.63481
C	-3.45519	-1.01994	-0.03814	C	4.42640	0.27078	0.01058
H	-2.50553	0.86777	0.42489	O	5.09652	1.28429	0.01689
H	-2.51068	0.46952	-1.28420	O	4.95084	-0.95570	0.17809
C	-4.87680	-0.47665	-0.15702	C	6.37342	-1.00742	0.37032

H	6.86045	-0.54826	-0.49409	C	0.38447	0.36091	-0.52537
H	6.62990	-0.41050	1.24968	C	1.06549	-0.87309	-0.36967
C	6.76030	-2.45764	0.53620	H	2.92149	-1.88716	-0.07625
H	6.49435	-3.03897	-0.34973	H	3.16355	2.37923	-0.27307
H	7.84043	-2.53537	0.68462	H	0.49837	-1.79483	-0.37906
H	6.26357	-2.90023	1.40277	N	0.60226	2.77178	-0.78123
C	-2.08787	-0.79645	-0.54641	H	1.20058	3.57483	-0.65094
C	-2.37046	-1.13415	0.92500	H	-0.42404	2.94134	-0.58343
C	-3.39291	-0.49858	-1.28649	N	-0.94990	0.44526	-0.67853
H	-1.61847	-1.66337	-1.02820	H	-1.40228	1.38758	-0.64559
C	-3.35752	-2.29251	1.04454	C	4.66108	0.25256	0.04849
H	-2.77412	-0.23577	1.40670	O	5.34758	1.25363	0.09127
H	-1.43474	-1.37417	1.43975	O	5.16035	-0.98730	0.18474
C	-4.37664	-1.65816	-1.14984	C	6.58027	-1.07186	0.39041
H	-3.82863	0.42025	-0.87596	H	7.08463	-0.59676	-0.45517
H	-3.17779	-0.30236	-2.34142	H	6.83740	-0.50569	1.28959
C	-4.66407	-1.99830	0.31112	C	6.93812	-2.53324	0.51766
H	-3.55941	-2.49844	2.10250	H	6.67182	-3.08345	-0.38780
H	-2.92877	-3.21053	0.62248	H	8.01486	-2.63524	0.67527
H	-5.31112	-1.40896	-1.66628	H	6.42393	-2.99153	1.36566
H	-3.97980	-2.55783	-1.63714	C	-1.86249	-0.67909	-0.60098
H	-5.11580	-1.10508	0.77997	C	-2.14985	-1.07622	0.85626
C	-3.09580	4.01815	1.41214	C	-3.16563	-0.32363	-1.32114
H	-3.50934	3.87889	2.41376	H	-1.40877	-1.53247	-1.12279
H	-3.84054	4.47845	0.75529	C	-3.12716	-2.24819	0.92526
H	-2.20522	4.65523	1.45892	H	-2.56551	-0.20521	1.37262
O	-2.75831	2.72907	0.95099	H	-1.21904	-1.33781	1.36747
O	-2.25746	2.84291	-0.33885	C	-4.15694	-1.48493	-1.26569
N	-5.53719	-3.16518	0.37794	H	-3.60023	0.56600	-0.85377
H	-5.75780	-3.39702	1.34034	H	-2.95311	-0.06670	-2.36259
H	-6.41637	-2.98574	-0.09483	C	-4.39428	-1.94441	0.15647
				H	-3.39602	-2.48232	1.95838
[SRS8-52]_TS				H	-2.68434	-3.14937	0.48755
				H	-5.11827	-1.20563	-1.70382
C	2.42869	-0.93052	-0.19540	H	-3.77608	-2.34405	-1.82814
C	3.19419	0.25467	-0.15518	C	-3.07051	3.97022	1.31011
C	2.56255	1.47587	-0.30311	H	-3.50513	3.77483	2.29317
C	1.17634	1.57364	-0.51927	H	-3.84627	4.30244	0.61313

H	-2.29403	4.73954	1.38752
O	-2.51390	2.74650	0.88574
O	-1.96901	2.93209	-0.38327
F	-5.10359	-0.97278	0.82995
F	-5.20488	-3.05638	0.14890