

To Supporting Information

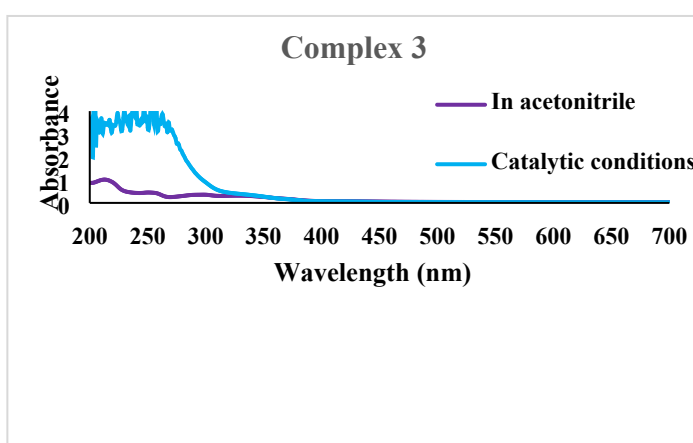
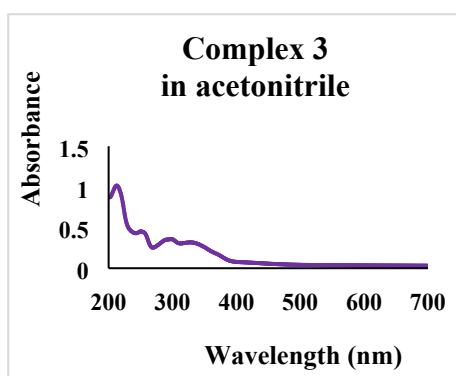
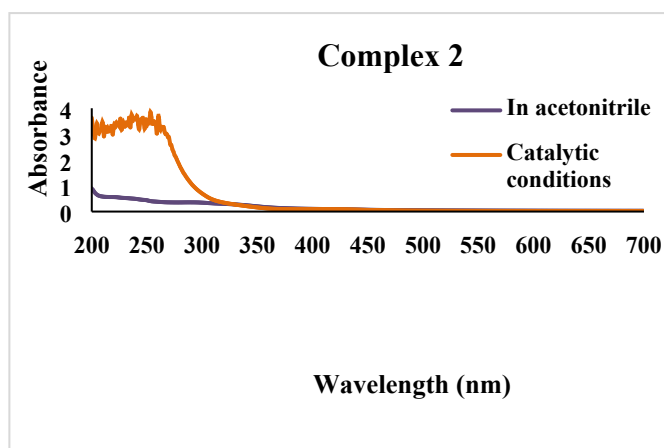
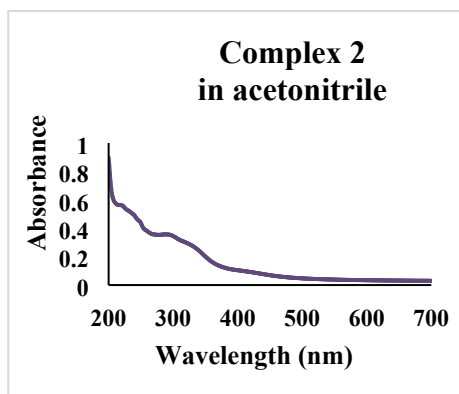
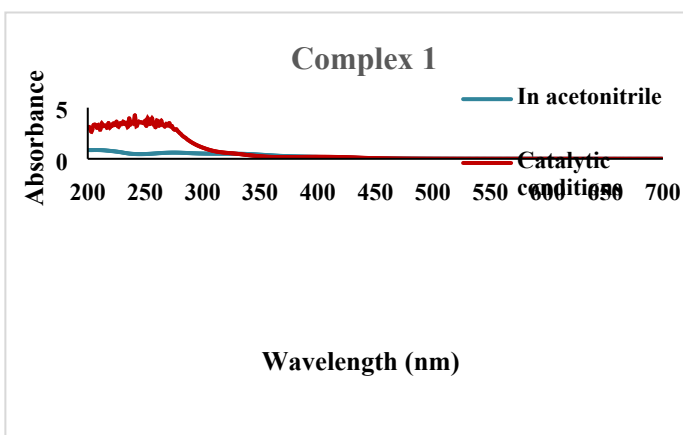
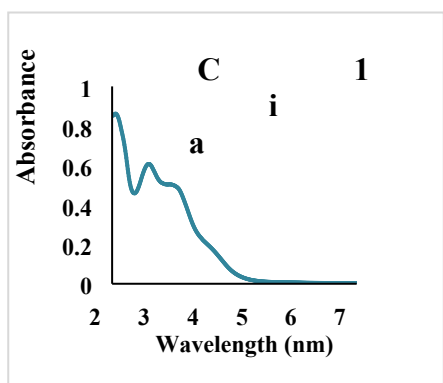


Fig. S1: The UV-vis absorption spectra of 1-3 in CH₃CN and under catalytic conditions.

Table S1T. Cartesian atomic coordinates (Å) of the calculated equilibrium structures.

1'			
C	-0.973682	-2.662417	0.341248
C	0.282157	-2.232596	0.091080
H	1.079584	-2.957852	-0.033127
H	-1.195457	-3.726340	0.410807
C	0.638749	-0.843261	-0.023067
C	3.050670	1.452656	-0.571598
H	3.895225	0.770700	-0.694576
C	3.220603	2.843765	-0.763185
C	2.142091	3.670893	-0.882891
H	2.265800	4.724858	-1.149555
H	4.217916	3.237271	-0.929589
C	-2.236192	2.090263	-1.153251
H	-2.501432	1.022580	-1.197007
H	-1.656168	2.346155	-2.054522
H	-3.157066	2.685266	-1.142404
O	-2.058150	-1.916336	0.530502
N	1.864190	-0.471183	-0.263806
N	1.900531	0.899722	-0.290638
O	-0.323934	0.069103	0.098152
O	0.905503	3.287030	-0.749747
O	0.545265	2.201755	1.760893
O	-1.507600	2.356242	0.013791
V	0.175790	1.905196	0.274746
H	-1.780982	-0.975688	0.479124
2'			
C	7.546403	1.606302	0.069001
H	8.638007	1.699473	0.036639
H	7.248951	3.691084	0.308857
C	6.770756	2.720896	0.219178
C	5.355595	2.655882	0.152052
H	4.764591	3.574674	0.101537
C	2.830833	0.420019	0.123564
C	1.378482	0.210293	0.057302
C	0.856494	-1.082687	0.162879
H	1.540611	-1.917598	0.292252
C	-0.510320	-1.291035	0.098659
H	-0.926814	-2.292229	0.179730
C	6.077625	-1.222560	-2.741142
H	5.810927	-2.249660	-2.484335
H	7.132305	-1.056132	-2.479872
H	5.930998	-1.069788	-3.818544
C	6.185167	-3.134259	1.031608
H	6.346467	-2.757012	2.052090
H	7.098593	-3.633353	0.679791
H	5.370998	-3.872086	1.043167
N	4.693083	1.533839	0.128340
N	3.327643	1.618833	-0.010024
O	7.103303	0.399880	-0.103563
O	3.592369	-0.627122	0.312842
O	5.669561	-0.269881	2.016095
O	5.218460	-0.380248	-1.987845
O	5.859881	-2.095769	0.152249

V	5.473578	-0.405571	0.473663
H	5.434741	0.541836	-2.189315
C	-7.546070	-1.607393	-0.067035
H	-8.637456	-1.701324	-0.029723
H	-7.248708	-3.690464	-0.321868
C	-6.770631	-2.720578	-0.228385
C	-5.355253	-2.655119	-0.167117
H	-4.763443	-3.573783	-0.124154
C	-2.831480	-0.418147	-0.135763
C	-1.379040	-0.208274	-0.071744
C	-0.857056	1.084677	-0.177584
H	-1.541200	1.919625	-0.306611
C	0.509808	1.293006	-0.113607
H	0.926283	2.294220	-0.194589
N	-4.693229	-1.532858	-0.139806
N	-3.327267	-1.617897	-0.006759
O	-7.102647	-0.401946	0.111326
O	-3.594054	0.629534	-0.317444
C	-6.062150	1.204202	2.753787
H	-5.799888	2.233040	2.499321
H	-7.118331	1.036259	2.499546
H	-5.907189	1.047058	3.829391
C	-6.192651	3.140623	-1.002690
H	-6.359625	2.771535	-2.025223
H	-7.104300	3.636406	-0.641714
H	-5.378885	3.878909	-1.013030
O	-5.680691	0.282941	-2.011391
O	-5.206445	0.367363	1.990484
O	-5.861892	2.095485	-0.133380
V	-5.476248	0.407965	-0.469183
H	-5.419653	-0.556159	2.188595

3'

C	-7.649388	-1.091427	0.232460
H	-8.699504	-1.385350	0.330655
H	-8.105129	0.946319	-0.104637
C	-7.315780	0.207119	-0.011695
C	-5.963286	0.642250	-0.030822
H	-5.731320	1.710637	-0.033750
C	-2.823692	-0.583137	-0.066227
C	-1.384980	-0.277909	-0.086832
C	-0.944997	1.049198	-0.097975
H	-1.672119	1.856746	-0.094733
C	0.416532	1.334757	-0.118249
C	1.345984	0.290336	-0.116657
H	2.409033	0.515599	-0.127787
C	0.912697	-1.031262	-0.096842
C	-0.456438	-1.314150	-0.088021
H	-0.790163	-2.348161	-0.076794
C	0.873597	2.732327	-0.139716
C	3.488965	4.831403	-0.466099
H	4.283123	4.092061	-0.600307
C	3.796235	6.218362	-0.478102
H	4.806260	6.529825	-0.724845
H	3.178985	8.210015	-0.006976
C	2.891904	7.155669	-0.076702

C	1.897778	-2.122697	-0.067006
C	2.424804	-5.450706	-0.108683
H	1.388877	-5.788190	-0.199275
C	3.480415	-6.399718	-0.044244
H	3.251954	-7.450045	-0.195011
H	5.516684	-6.804587	0.464267
C	4.743241	-6.042159	0.323544
C	-4.246778	-4.946623	-0.781219
H	-4.414586	-5.942708	-0.351042
H	-3.167474	-4.814319	-0.952051
H	-4.768043	-4.868875	-1.746549
C	-2.256343	6.169684	-0.290703
H	-2.948386	6.803421	0.279223
H	-2.710685	5.174491	-0.413468
H	-2.091383	6.607416	-1.286135
C	6.479410	-1.179674	-0.413025
H	5.867275	-0.297697	-0.655569
H	6.770480	-1.675037	-1.350725
H	7.379105	-0.846514	0.120680
N	-4.951320	-0.174140	-0.027019
N	-3.696881	0.380125	0.018947
N	2.287940	4.367715	-0.281956
N	2.144591	3.003901	-0.229829
N	2.616148	-4.166263	-0.040941
N	1.502545	-3.363851	-0.036935
O	-6.796812	-2.057664	0.424409
O	-5.311548	-2.262304	-1.779398
O	-3.180826	-1.840966	-0.127027
O	0.410337	5.762040	-1.749481
O	1.672774	6.900212	0.305079
O	-0.032909	3.673103	-0.062307
O	4.747154	-3.392738	-1.611423
O	5.125913	-4.826756	0.594105
O	3.165918	-1.797801	-0.056199
O	-4.704225	-2.220730	2.171505
O	-4.697768	-3.972122	0.119301
O	0.763265	5.147374	2.183279
O	-1.053463	6.048162	0.417695
O	4.090045	-2.976999	2.306955
O	5.747023	-2.044032	0.412015
V	-5.046503	-2.264515	-0.240963
V	0.517971	5.500550	-0.214367
V	4.478242	-3.189829	-0.087434
H	-5.555979	-2.556211	2.487995
H	-4.100926	-2.978545	2.208326
H	4.736130	-3.609246	2.654682
H	4.509019	-2.107262	2.398167
H	-0.184213	5.067105	2.372814
H	1.005339	6.041081	2.468082

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C	4.721912	0.203443	1.144091
C	4.046950	0.325710	-0.020551
H	4.590204	0.295463	-0.959243
H	5.802168	0.063992	1.151529
C	2.619864	0.497412	-0.091541

C	-0.082094	1.063470	-2.040547
H	0.425235	1.152041	-3.004468
C	-1.495380	1.184055	-1.964725
C	-2.190817	0.786980	-0.863439
H	-3.284825	0.777644	-0.867491
H	-2.041017	1.497352	-2.849042
C	0.271047	-0.957659	3.262799
H	1.323274	-1.178981	3.027571
H	-0.334708	-1.820929	2.955359
H	0.164117	-0.793276	4.341928
O	4.217120	0.232897	2.372450
N	2.010795	0.599664	-1.244832
N	0.673331	0.806970	-1.009769
O	1.934333	0.533791	1.041407
O	-1.646219	0.334313	0.237456
O	-0.156672	2.385882	1.082008
O	-0.140607	0.196476	2.586393
V	0.038002	0.842826	0.967875
H	3.249569	0.385225	2.289396
O	0.279112	-1.737478	0.457420
O	-1.013976	-2.333868	0.522131
H	-1.577990	-1.528062	0.507828
H	0.515530	-1.848642	-0.481303

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C	-0.063848	-0.241087	-3.757380
C	-0.617467	0.795602	-3.094738
H	-1.223616	1.515257	-3.634970
H	-0.195448	-0.357370	-4.832044
C	-0.480465	0.987493	-1.672736
C	-1.289464	2.811390	1.044773
H	-1.866219	3.579038	0.524565
C	-1.176656	2.835800	2.443906
C	-0.772255	1.715502	3.128216
H	-0.868195	1.676536	4.219453
H	-1.574990	3.682688	2.992824
C	2.845165	-1.572735	-0.561379
H	2.795593	-1.339111	-1.633859
H	2.055012	-2.280796	-0.294808
H	3.817749	-2.024672	-0.330691
O	0.667246	-1.225159	-3.234567
N	-1.145309	1.910658	-1.041570
N	-0.785791	1.868312	0.282321
O	0.347760	0.198966	-0.997338
O	-0.352547	0.632716	2.573915
O	1.666979	1.567320	1.355376
O	2.631037	-0.425643	0.242061
V	0.613078	0.493690	0.880678
H	0.720941	-1.064403	-2.266685
O	0.411434	-1.290400	1.265138
O	1.066480	-1.677579	2.450742
H	0.491442	-1.249007	3.116587
H	3.231936	0.295404	0.006270

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C	-1.350781	3.078010	-1.857090
C	-2.086179	2.089127	-1.308473

H	-3.164024	2.091610	-1.434217
H	-1.818617	3.882885	-2.422414
C	-1.516735	1.000680	-0.550082
C	-2.063320	-1.975063	0.978381
H	-3.134935	-2.080406	0.786871
C	-1.331016	-3.046185	1.545261
C	0.039570	-3.092042	1.550978
H	0.535124	-4.003283	1.907019
H	-1.876670	-3.918373	1.892532
C	3.059140	1.049152	0.499589
H	3.245405	1.208823	1.567682
H	2.428722	1.856068	0.119140
H	3.996520	1.019020	-0.064824
O	-0.025278	3.210224	-1.798301
N	-2.290727	0.058299	-0.080536
N	-1.512361	-0.851145	0.606169
O	-0.195225	0.979687	-0.363793
O	0.843052	-2.162321	1.131716
O	0.407567	0.369037	2.415139
O	2.325449	-0.162939	0.286763
V	0.373456	-0.290060	0.989570
H	0.300411	2.442215	-1.276383
H	2.810139	-0.939269	0.613702

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C	-0.856392	2.195302	-2.328502
C	-1.824558	1.465222	-1.738114
H	-2.859202	1.612876	-2.030127
H	-1.088287	2.919668	-3.108134
C	-1.565385	0.488711	-0.704386
C	-2.927532	-1.766725	1.442027
H	-3.982142	-1.630289	1.185647
C	-2.548360	-2.771309	2.369136
C	-1.254862	-3.178513	2.559813
H	-1.064978	-4.027011	3.228699
H	-3.335855	-3.311671	2.886243
C	2.959703	-0.879970	0.082386
H	2.671105	-0.098512	-0.633630
H	2.912434	-1.868176	-0.383924
H	3.983980	-0.702266	0.426249
O	0.450770	2.146283	-2.060014
N	-2.563606	-0.131202	-0.135029
N	-2.077089	-0.993187	0.827728
O	-0.295339	0.242881	-0.377039
O	-0.193874	-2.681389	1.995363
O	-0.027357	0.100853	2.457401
O	2.069854	-0.917145	1.195905
V	-0.116399	-0.872904	1.224366
H	0.550083	1.489812	-1.332980
O	0.303233	-2.348658	-0.594824
O	1.115714	-3.484722	-0.263193
H	0.843362	-3.561317	0.681437
H	2.263332	-0.196258	1.814632
H	0.801266	-1.945495	-1.326405

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C	0.066868	3.196975	-2.628688
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C	-0.587804	1.201851	-1.348732
C	-1.808801	-1.583976	0.146469
H	-2.877698	-1.430231	-0.024630
C	-1.340118	-2.812081	0.682811
C	-0.027716	-3.190215	0.650292
H	0.251466	-4.195206	0.982749
H	-2.072335	-3.531192	1.037234
O	1.383724	3.014567	-2.584382
N	-1.560387	0.462514	-0.880195
N	-1.014278	-0.617053	-0.220969
O	0.690910	0.858420	-1.179154
O	0.965259	-2.460160	0.212787
O	1.152752	0.073213	1.573347
V	0.956676	-0.524557	0.136814
H	1.538313	2.186071	-2.078098
O	2.953010	-0.769893	-0.559501
O	3.552858	-2.049523	-0.299555
H	2.746489	-2.559920	-0.039177
H	3.521043	-0.182227	-0.026654

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C	0.198033	3.134539	-2.123013
C	-0.758040	2.333508	-1.602184
H	-1.801483	2.542199	-1.814350
H	-0.070983	3.986476	-2.746230
C	-0.472321	1.191766	-0.775926
C	-1.669246	-1.510349	0.872319
H	-2.730432	-1.379072	0.646372
C	-1.218574	-2.660411	1.554572
C	0.112420	-2.957117	1.655472
H	0.429807	-3.903201	2.106529
H	-1.948295	-3.372193	1.926584
O	1.513235	3.024462	-1.977473
N	-1.425650	0.414019	-0.339301
N	-0.862366	-0.574397	0.437637
O	0.802148	0.931658	-0.479903
O	1.083614	-2.209894	1.220851
O	1.185754	0.525944	2.440656
V	1.100745	-0.316579	0.915303
H	1.690459	2.235462	-1.419040
O	2.769364	-0.479836	0.263065
O	3.575517	-1.321408	1.081280
H	3.083327	-2.167049	1.040096
H	1.999797	0.965112	2.734274

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C	0.052570	2.701337	-2.604133
C	-0.754843	1.689658	-2.216047
H	-1.652217	1.474204	-2.786592
H	-0.186654	3.297926	-3.483384
C	-0.499639	0.867071	-1.064706
C	-1.509745	-1.661265	0.924134
H	-2.438972	-1.910743	0.406611
C	-1.149422	-2.340310	2.112610

C	-0.132799	-1.885621	2.898075
H	0.082277	-2.341397	3.868865
H	-1.759174	-3.170493	2.453423
O	1.177416	3.104748	-2.024216
N	-1.327426	-0.068835	-0.693570
N	-0.797517	-0.699590	0.401275
O	0.605566	1.095670	-0.359181
O	0.618827	-0.863510	2.603263
O	2.289253	1.045014	1.622478
V	1.146306	-0.146468	0.972080
H	1.333174	2.532969	-1.240969
O	1.926771	-1.296705	0.268314
H	3.233818	0.830290	1.586579

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C	2.837140	1.699250	-3.166161
C	1.770107	2.020322	-2.406139
H	1.489665	3.064440	-2.317023
H	3.395096	2.478288	-3.684639
C	0.958751	1.077743	-1.664013
C	-2.065653	1.099123	-0.183947
H	-2.321167	1.861346	-0.925467
C	-3.092010	0.652892	0.687999
C	-2.862553	-0.050867	1.833820
H	-3.703372	-0.265992	2.504263
H	-4.104390	0.988337	0.483043
C	1.457594	-2.401257	3.255932
H	1.857608	-1.506440	3.746042
H	2.092961	-2.666492	2.408167
H	1.399437	-3.240530	3.957826
O	3.354647	0.493709	-3.397461
N	-0.018274	1.562735	-0.966309
N	-0.808478	0.732777	-0.172115
O	1.318521	-0.201392	-1.833050
O	-1.711607	-0.492598	2.242209
O	1.216830	0.235040	1.677470
O	0.160141	-2.142486	2.705747
V	-0.050401	-0.588879	1.247188
H	2.819695	-0.159817	-2.901839
O	0.166886	-1.829944	-0.161537
O	1.104780	-2.866807	0.150094
H	0.502085	-3.617881	0.281123
H	-0.471682	-1.889185	3.399223
H	0.818535	-0.859515	-1.268385

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C	-0.253051	3.113195	-2.545064
C	-1.270756	2.414552	-1.999500
H	-2.287217	2.615614	-2.321720
H	-0.432666	3.864117	-3.313218
C	-1.089456	1.406073	-0.980094
C	-2.766116	-0.691713	1.123286
H	-3.774839	-0.419324	0.802515
C	-2.587867	-1.660138	2.139753
C	-1.361790	-2.081355	2.580019
H	-1.311325	-2.843045	3.365949
H	-3.474832	-2.101122	2.584397

C	2.947439	-1.782040	1.205132
H	3.009792	-2.009366	0.139775
H	2.366291	-2.560034	1.714316
H	3.956417	-1.717090	1.627520
O	1.041653	3.005101	-2.245581
N	-2.148724	0.842926	-0.459060
N	-1.791003	-0.073682	0.510269
O	0.152086	1.103014	-0.612031
O	-0.207973	-1.670897	2.151076
O	0.377310	1.078253	2.004821
O	2.297946	-0.512111	1.311173
V	0.145738	-0.301767	0.878238
H	1.108485	2.326574	-1.536827
O	0.528676	-1.441232	-0.462104
O	1.362613	-1.097182	-1.529912
H	1.099450	-0.157392	-1.663224
H	0.618696	1.941986	1.640358
H	2.336840	-0.183664	2.223160

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C	4.836215	0.283291	1.092945
C	4.113989	0.429607	-0.051863
H	4.620685	0.482502	-1.009192
H	5.922882	0.209786	1.067053
C	2.691623	0.523468	-0.039874
C	-0.002762	0.982250	-2.090280
H	0.533727	1.114409	-3.033163
C	-1.382005	1.042512	-2.066537
C	-2.219372	0.818836	-0.934809
H	-3.304702	0.877380	-1.117163
H	-1.890109	1.248413	-3.005365
C	0.340658	-1.045012	3.357776
H	1.436762	-1.142353	3.414996
H	-0.050451	-1.890621	2.776145
H	-0.061292	-1.049505	4.378647
O	4.356676	0.217423	2.317695
N	2.055141	0.696490	-1.221974
N	0.756377	0.762639	-1.010289
O	2.044372	0.452789	1.074249
O	-1.866381	0.533275	0.222326
O	-0.171081	2.118838	1.031440
O	0.002262	0.171097	2.751015
V	0.064022	0.545159	1.032904
H	3.374250	0.302601	2.263471
O	-0.093002	-1.270293	0.539501
H	-0.598261	-1.586341	-0.218924

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C	-7.615263	1.572533	0.058953
H	-8.701637	1.651646	0.176662
H	-7.383621	3.633996	-0.359659
C	-6.878671	2.680189	-0.243836
C	-5.460178	2.644616	-0.279525
H	-4.886961	3.575465	-0.303048
C	-2.906807	0.447695	-0.234778
C	-1.451446	0.250019	-0.186080
C	-0.928693	-1.047474	-0.172209

H	-1.612017	-1.892232	-0.216243
C	0.438736	-1.249363	-0.101203
H	0.853943	-2.254341	-0.086679
C	-4.350014	-1.249713	2.659885
H	-3.353970	-1.159809	2.217019
H	-4.722102	-2.267419	2.484224
H	-4.281209	-1.053876	3.737775
C	-6.240018	-3.198027	-0.736304
H	-6.507791	-2.875935	-1.753190
H	-7.094128	-3.720019	-0.283281
H	-5.397168	-3.901259	-0.792517
N	-4.778996	1.537337	-0.257302
N	-3.411763	1.646745	-0.193826
O	-7.134790	0.385590	0.288022
O	-3.661903	-0.623606	-0.290740
O	-5.855945	-0.398534	-1.909694
O	-5.166718	-0.280566	2.020038
O	-5.887842	-2.108574	0.068070
V	-5.554876	-0.427587	-0.378251
H	-6.072620	-0.347528	2.355743
C	7.482122	-1.512362	0.117484
H	8.573938	-1.593992	0.125415
H	7.195341	-3.589232	0.382660
C	6.711184	-2.625351	0.261448
C	5.295558	-2.578556	0.155533
H	4.717811	-3.504844	0.093626
C	2.757993	-0.358871	0.039112
C	1.307159	-0.154743	-0.041406
C	0.785338	1.143255	-0.058919
H	1.467778	1.988561	-0.017618
C	-0.582171	1.344350	-0.131156
H	-0.998750	2.348658	-0.143530
N	4.625746	-1.463830	0.114938
N	3.264192	-1.559034	-0.052212
O	7.033718	-0.302626	-0.090919
O	3.519401	0.698408	0.186787
O	6.424612	0.367800	-2.703124
H	6.997007	0.230172	-1.918047
C	6.214973	3.214506	0.956852
H	6.304234	2.898384	2.006376
H	7.183079	3.594252	0.604030
H	5.477567	4.024409	0.879655
O	5.518905	0.348286	2.018587
O	5.158801	0.511155	-2.060230
O	5.815581	2.153400	0.137388
V	5.383060	0.491008	0.471732
H	4.709410	-0.314363	-2.317222

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C	-7.437721	1.502480	0.045369
H	-8.523782	1.568468	0.173114
H	-7.244521	3.552984	-0.443898
C	-6.722573	2.611899	-0.302805
C	-5.305535	2.597528	-0.356815
H	-4.748622	3.535928	-0.425612
C	-2.715238	0.446301	-0.264612

C	-1.255037	0.284272	-0.234518
C	-0.701869	-0.997785	-0.153467
H	-1.364870	-1.859307	-0.133243
C	0.671440	-1.161874	-0.102691
H	1.114233	-2.152698	-0.038630
C	-4.109197	-1.173206	2.717330
H	-3.115791	-1.071808	2.270922
H	-4.455306	-2.205039	2.573773
H	-4.045095	-0.942346	3.788461
C	-5.974005	-3.274585	-0.602334
H	-6.233972	-2.995278	-1.633774
H	-6.825908	-3.790321	-0.138442
H	-5.120431	-3.966545	-0.621047
N	-4.605745	1.502059	-0.301900
N	-3.240617	1.637199	-0.266616
O	-6.935730	0.332477	0.307752
O	-3.448292	-0.640353	-0.260401
O	-5.658929	-0.509140	-1.869478
O	-4.950683	-0.245154	2.048917
O	-5.645801	-2.149618	0.163232
V	-5.347888	-0.479858	-0.340461
H	-5.852731	-0.320425	2.393251
C	7.742524	-1.614174	-0.048889
H	8.803746	-1.913119	-0.043615
H	7.218183	-3.678647	0.136515
C	6.798611	-2.678562	0.057112
C	5.421830	-2.565747	0.039031
H	4.798656	-3.462890	0.083519
C	2.962832	-0.195648	-0.069527
C	1.511782	-0.041689	-0.128139
C	0.956505	1.243108	-0.213000
H	1.620844	2.103367	-0.240111
C	-0.414202	1.404553	-0.266607
H	-0.861433	2.393459	-0.333739
N	4.777289	-1.397059	-0.032462
N	3.463243	-1.457668	-0.059988
O	7.511779	-0.399558	-0.176159
O	3.707450	0.831570	-0.023683
C	5.827149	3.256807	0.951589
H	6.227412	2.815413	1.876464
H	6.393422	4.158594	0.685118
H	4.776273	3.539034	1.117099
O	5.922041	0.373720	1.532462
O	5.763787	0.335439	-1.865356
O	5.900840	2.346443	-0.106723
V	5.676456	0.609937	-0.029161
H	6.247964	-0.361040	-2.324698

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C	0.337125	7.694298	0.137821
H	0.263023	8.781531	0.246276
H	2.382076	7.747669	-0.400989
C	1.517194	7.116294	-0.224125
C	1.677618	5.705494	-0.259770
H	2.674622	5.268571	-0.362293
C	-0.126988	2.863519	-0.112236

C	-0.106906	1.393287	-0.132955
C	1.109940	0.703974	-0.154025
H	2.045038	1.257794	-0.158453
C	1.123891	-0.686974	-0.159881
C	-0.080087	-1.396737	-0.147210
H	-0.067286	-2.483423	-0.151409
C	-1.292671	-0.714558	-0.134624
C	-1.303595	0.683334	-0.126096
H	-2.252116	1.213451	-0.115069
C	2.405574	-1.403572	-0.162215
C	4.000410	-4.346957	0.204459
H	3.124557	-4.986590	0.340679
C	5.302343	-4.898931	0.272250
H	5.417527	-5.973207	0.372621
H	7.398363	-4.532626	0.494201
C	6.405110	-4.096749	0.340309
C	-2.554298	-1.469533	-0.125979
C	-5.920287	-1.338360	-0.232866
H	-6.048954	-0.255055	-0.304013
C	-7.056898	-2.191092	-0.212434
H	-8.039356	-1.759270	-0.375187
H	-7.860072	-4.123171	0.222281
C	-6.959548	-3.508290	0.123235
C	-4.213633	5.289597	-0.422550
H	-5.051101	5.773222	0.097752
H	-4.460510	4.227988	-0.572048
H	-4.071934	5.761116	-1.406065
C	6.840646	0.695123	-1.076106
H	7.841797	0.860490	-0.655002
H	6.348325	1.669923	-1.196653
H	6.938125	0.217716	-2.061093
C	-2.472253	-6.108090	-0.559008
H	-1.472702	-5.670751	-0.705148
H	-2.946278	-6.240704	-1.542670
H	-2.358837	-7.085347	-0.071450
N	0.684354	4.872523	-0.157256
N	0.988577	3.534495	-0.140089
N	3.765413	-3.079409	0.012787
N	2.449852	-2.681431	0.072925
N	-4.698853	-1.776698	-0.150772
N	-3.695773	-0.841248	-0.111694
O	-0.752651	7.047085	0.435163
O	-1.460557	5.627889	-1.706636
O	-1.293682	3.458158	-0.056131
O	5.339165	-1.910629	-1.993294
O	6.388882	-2.802512	0.284547
O	3.495472	-0.709273	-0.384451
O	-4.310559	-3.975886	-1.760779
O	-5.848009	-4.126459	0.407112
O	-2.481864	-2.776601	-0.125242
O	-1.147981	5.026590	2.233163
O	-3.059201	5.394449	0.364354
O	5.016949	-0.966067	2.050903
O	6.096622	-0.099536	-0.193168
O	-3.881114	-3.486854	2.182379

O	-3.233585	-5.266271	0.263111
V	-1.362447	5.367448	-0.170871
V	5.164070	-1.591457	-0.477603
V	-4.103155	-3.791448	-0.224714
H	-1.368612	5.912425	2.556914
H	-1.955533	4.503951	2.351871
H	-4.617568	-4.031005	2.498209
H	-3.092132	-4.041294	2.282614
O	3.727070	-0.531592	2.480220
H	5.423090	-0.126088	1.755924
H	3.730942	-0.859850	3.394239

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C	6.443456	-4.346249	0.135587
H	7.417027	-4.837836	0.233249
H	5.435831	-6.129680	-0.393636
C	5.338376	-5.063659	-0.214720
C	4.043227	-4.480599	-0.224991
H	3.156216	-5.114319	-0.306258
C	2.528518	-1.475949	-0.076290
C	1.250443	-0.746150	-0.084172
C	0.040571	-1.441140	-0.081530
H	0.038265	-2.527967	-0.071945
C	-1.165483	-0.740947	-0.091679
C	-1.164428	0.658851	-0.099872
H	-2.104652	1.202490	-0.106004
C	0.040510	1.353401	-0.098246
C	1.246695	0.646957	-0.092574
H	2.187588	1.190975	-0.093046
C	-2.426495	-1.484110	-0.091045
C	-5.813913	-1.039459	-0.165778
H	-5.846575	0.050894	-0.231015
C	-6.984597	-1.769524	-0.104869
H	-7.923989	-1.223408	-0.137257
H	-8.104920	-3.592218	0.102879
C	-7.084921	-3.182396	0.034497
C	0.038885	2.824491	-0.094544
C	1.883510	5.637982	-0.276269
H	2.874100	5.186868	-0.379762
C	1.743073	7.050837	-0.253669
H	2.615462	7.668270	-0.442197
H	0.515679	8.737214	0.213666
C	0.573727	7.648424	0.112574
C	6.568355	0.844012	-0.471527
H	7.353144	1.416554	0.039803
H	5.705221	1.504852	-0.642996
H	6.943325	0.493615	-1.444241
C	-2.970951	-6.294720	-0.408209
H	-3.354966	-7.260061	-0.052820
H	-1.873633	-6.318171	-0.363776
H	-3.292749	-6.123062	-1.445479
C	-4.013429	5.308307	-0.415500
H	-4.279087	4.250550	-0.560178
H	-3.866844	5.774074	-1.400964
H	-4.840460	5.807751	0.106313
N	3.837441	-3.200601	-0.118080

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N	0.879046	4.820190	-0.159680
N	1.164218	3.477709	-0.129007
O	6.445301	-3.079580	0.439429
O	5.577008	-1.764047	-1.703567
O	3.631913	-0.773785	-0.067395
O	-4.301256	-3.824795	-1.565858
O	-6.159061	-4.010198	0.094685
O	-2.412133	-2.751332	-0.031634
O	-1.258515	5.599694	-1.705811
O	-0.522202	7.018513	0.423650
O	-1.120102	3.431706	-0.047146
O	4.953761	-1.679864	2.234839
O	6.179032	-0.230768	0.339488
O	-4.433462	-3.203422	1.833010
O	-3.445205	-5.280038	0.433012
O	-0.937994	5.009873	2.228096
O	-2.854710	5.395764	0.367394
V	5.309380	-1.698911	-0.167480
V	-4.137912	-3.723662	0.021433
V	-1.160367	5.345430	-0.169272
H	5.748125	-2.138814	2.545669
H	5.135360	-0.736405	2.365097
H	-1.112698	5.902132	2.562115
H	-1.761555	4.518708	2.369310
H	-4.082271	-3.899680	2.408851

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C	-2.892714	-2.141051	-4.366147
C	-3.878761	-1.840300	-3.491982
H	-4.911998	-1.867816	-3.821841
H	-3.125881	-2.415538	-5.394090
C	-3.638616	-1.474874	-2.122546
C	-4.926889	-0.389762	0.801720
H	-5.975540	-0.319252	0.503583
C	-4.538544	-0.053187	2.125358
C	-3.311261	-0.381740	2.615513
H	-3.063157	-0.227403	3.669412
H	-5.278593	0.371024	2.796245
O	0.669782	-0.576732	-0.721224
H	0.316333	0.327880	-0.587493
O	-1.585113	-2.148566	-4.136403
N	-4.623941	-1.182540	-1.316478
N	-4.094779	-0.818300	-0.106865
O	-2.382382	-1.439421	-1.693848
O	-2.372112	-0.961999	1.915358
O	-1.781591	0.719195	-0.080604
O	-0.295109	-1.373270	-0.104512
V	-2.024114	-0.821473	0.079681
H	-1.444289	-1.894347	-3.197748
O	-2.063323	-3.145317	0.539432
O	-1.084576	-3.949583	-0.109093
H	-0.439896	-3.253469	-0.368787
H	-1.864548	-3.270642	1.485822

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C	-2.863094	-2.129065	-4.393384
C	-3.840897	-1.846386	-3.480772
H	-4.885299	-1.946715	-3.754405
H	-3.119628	-2.452704	-5.402219
C	-3.512676	-1.424629	-2.164641
C	-4.941502	-0.542593	0.830690
H	-5.992555	-0.557605	0.531643
C	-4.587404	-0.282919	2.142285
C	-3.277848	-0.378776	2.674575
H	-3.180969	-0.223487	3.760771
H	-5.382112	-0.051489	2.846565
O	0.440019	-1.028878	-1.132918
H	0.837087	-0.158308	-0.957724
O	-1.568497	-2.056525	-4.204838
N	-4.541367	-1.162988	-1.301829
N	-4.047060	-0.813749	-0.127348
O	-2.286324	-1.299227	-1.811662
O	-2.219406	-0.653624	2.059787
O	-1.784105	0.976329	-0.128909
O	-0.200829	-1.286349	0.126585
V	-1.956917	-0.577102	0.031220
H	-1.393903	-1.766538	-3.272049
O	-2.320443	-3.000674	0.531720
O	-1.205511	-3.746965	0.043851
H	-0.545615	-3.005800	-0.029950
H	-2.234754	-3.111711	1.495427

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C	-3.115138	-1.758390	-4.756160
C	-3.961728	-1.737190	-3.687679
H	-5.000592	-2.020569	-3.817081
H	-3.473198	-2.044385	-5.744820
C	-3.523772	-1.382532	-2.381353
C	-4.675480	-1.013786	0.794418
H	-5.705744	-1.136329	0.448832
C	-4.533704	-0.683798	2.121470
C	-3.422105	-0.507477	3.034589
H	-3.714829	0.034546	3.958231
H	-5.491241	-0.506289	2.613381
O	0.227969	-1.923661	-1.619653
H	0.636345	-2.346988	-0.838697
O	-1.832059	-1.467401	-4.757839
N	-4.385194	-1.444516	-1.358283
N	-3.779627	-1.145222	-0.212898
O	-2.293492	-0.998734	-2.200347
O	-2.269297	-0.909831	2.947986
O	-1.756390	0.647303	0.248691
O	0.071400	-0.579782	-1.165990
V	-1.567109	-0.752626	-0.411320
H	-1.558568	-1.224984	-3.840489
O	-1.276774	-1.994824	0.772219
H	-1.578012	-1.744422	1.687654

TS1

C	0.076138	0.042797	-3.993091
C	0.891946	-0.637856	-3.160406

H	1.588105	-1.362304	-3.569871
H	0.121675	-0.109125	-5.070264
C	0.883260	-0.479036	-1.728652
C	1.922877	-1.634380	1.264833
H	2.545388	-2.455246	0.901388
C	1.790264	-1.413839	2.658135
C	1.221848	-0.275473	3.154417
H	1.235033	-0.060965	4.227027
H	2.256841	-2.112864	3.344509
C	-2.661594	1.929475	0.281947
H	-3.083281	1.100038	0.863106
H	-2.823949	1.730476	-0.786926
H	-3.170178	2.864388	0.547654
O	-0.851242	0.939565	-3.657442
N	1.624327	-1.216760	-0.956897
N	1.359888	-0.893500	0.351125
O	0.085532	0.458921	-1.206751
O	0.700448	0.657601	2.421096
O	-1.197554	-0.434625	1.073919
O	-1.281308	2.054656	0.544500
V	-0.048119	0.581367	0.715359
H	-0.855008	1.002343	-2.678028
O	1.347058	2.162857	0.568238
O	1.320429	2.886358	-0.673954
H	1.036035	2.186636	-1.291900
H	0.720408	3.251653	1.260858
O	-0.095751	3.941290	1.384903
H	-0.825990	3.135647	0.943349
H	0.073303	4.576856	0.669740

TS2

C	0.878985	-0.007599	-3.625603
C	-0.270477	-0.080671	-2.922302
H	-1.217396	-0.130123	-3.449888
H	0.871907	0.020610	-4.714294
C	-0.317419	-0.111474	-1.480840
C	-2.197715	-0.574346	1.296718
H	-3.163058	-0.761501	0.818263
C	-2.050341	-0.736590	2.693883
C	-0.827355	-0.737910	3.308998
H	-0.764818	-0.959626	4.380230
H	-2.932283	-0.956646	3.287320
O	2.117353	0.031906	-3.132474
N	-1.450892	-0.265685	-0.853218
N	-1.208444	-0.249341	0.506377
O	0.833575	0.008638	-0.813382
O	0.316161	-0.524403	2.728887
O	0.655536	2.017495	1.234418
V	0.628485	0.393253	1.058109
H	2.032867	-0.045717	-2.155447
O	2.500358	-0.026501	1.202634
O	2.960303	0.079232	2.562622
H	2.256577	-0.404718	3.040742
H	3.058187	1.338122	0.806843
O	3.000097	2.380499	0.675140
H	1.928029	2.448874	0.940163

H	3.086840	2.565492	-0.275211
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TS3

C	-0.121727	2.748143	-2.566811
C	-1.097947	2.134651	-1.861320
H	-2.134331	2.394278	-2.050694
H	-0.367124	3.499183	-3.316526
C	-0.847962	1.132350	-0.861438
C	-2.139248	-1.072718	1.345770
H	-3.198600	-0.878476	1.160261
C	-1.743208	-2.090667	2.240397
C	-0.441072	-2.490149	2.332327
H	-0.166780	-3.335332	2.971645
H	-2.501479	-2.622614	2.805665
O	3.269156	-1.413935	1.500032
O	1.188253	2.552695	-2.474347
N	-1.824477	0.521362	-0.249294
N	-1.285864	-0.340308	0.676280
O	0.419895	0.821143	-0.587588
O	0.554552	-1.965517	1.677236
O	0.975990	0.869387	2.311787
O	2.287128	-0.591296	0.372886
V	0.773991	-0.218890	0.958663
H	1.343440	1.864190	-1.791435
H	1.882326	1.130261	2.548468
H	2.629860	-2.144229	1.622480

TS4

C	1.727259	3.589595	-0.653960
C	0.466505	3.155513	-0.862304
H	-0.212935	3.782363	-1.431567
H	2.074494	4.519698	-1.100205
C	-0.083983	1.939539	-0.315353
C	-2.941198	0.200742	0.321501
H	-3.621013	0.966045	-0.063443
C	-3.462924	-1.009866	0.809444
C	-2.682605	-2.082975	1.191807
H	-3.195505	-3.010826	1.481014
H	-4.541632	-1.133012	0.823140
C	2.807590	-1.993451	1.243107
H	3.266286	-1.052461	0.905602
H	2.594119	-2.632256	0.383837
H	3.493860	-2.511854	1.923467
O	2.682966	3.015870	0.081681
N	-1.349955	1.715266	-0.281261
N	-1.663230	0.489374	0.272559
O	0.821121	1.012019	0.161493
O	-1.402108	-2.141100	1.224935
O	-0.170599	-0.052466	2.584370
O	1.559728	-1.766146	1.889500
V	-0.173884	-0.594687	1.090225
H	2.307369	2.225992	0.516502
O	0.492484	-1.522812	-0.594333
O	0.530501	-2.948605	-0.628719
H	-0.217261	-3.161180	-0.035760
H	1.682447	-1.343334	2.752766
H	1.595113	-0.851263	-1.370952

O	2.158566	0.000978	-1.570656
H	1.494667	0.661707	-0.679197
H	1.925640	0.296405	-2.462908

TS5

C	4.449866	2.772431	1.054225
C	3.834195	2.506931	-0.118939
H	4.327244	2.771468	-1.048751
H	5.422988	3.262786	1.076190
C	2.552552	1.842576	-0.211715
C	0.445670	0.844114	-2.734705
H	1.039437	1.360058	-3.493031
C	-0.754115	0.192867	-3.126912
C	-1.558471	-0.505376	-2.281985
H	-2.463221	-0.989314	-2.661523
H	-1.036179	0.251568	-4.173961
C	-1.379762	-0.678844	2.804574
H	-1.891032	0.286436	2.722239
H	-0.412072	-0.528018	3.289940
H	-1.976577	-1.391079	3.385405
O	4.005691	2.490765	2.274758
N	2.117840	1.585466	-1.423412
N	0.930143	0.896681	-1.520380
O	1.946700	1.534014	0.920945
O	-1.353176	-0.681981	-1.000718
O	-0.412410	1.408025	0.878867
O	-1.097022	-1.221288	1.511536
V	0.038238	0.001953	0.062117
H	3.140219	2.033367	2.155066
O	1.391604	-1.223594	0.178823
O	1.647644	-1.304493	1.579049
H	1.153349	-2.114372	1.801960
H	-1.921482	-1.381109	1.022656
H	0.699311	1.706131	1.017251

TS6

C	1.231140	0.436446	-3.627799
C	0.055711	0.711805	-3.012444
H	-0.715688	1.248705	-3.555265
H	1.386148	0.751534	-4.660006
C	-0.219696	0.329007	-1.655465
C	-2.376254	0.009221	0.906311
H	-3.266134	0.493448	0.493737
C	-2.450900	-0.778152	2.068350
C	-1.443162	-1.664108	2.385808
H	-1.602637	-2.380520	3.202660
H	-3.375398	-0.805854	2.636959
C	1.790033	-0.728923	3.809789
H	1.319280	-1.714606	3.838114
H	1.838282	-0.316698	4.824382
H	2.796757	-0.826969	3.386138
O	2.294477	-0.190173	-3.148662
N	-1.343276	0.621234	-1.037811
N	-1.261868	0.108392	0.221842
O	0.712771	-0.370461	-1.030099
O	-0.315460	-1.769671	1.777169
O	1.162544	1.355258	0.956842

O	0.966330	0.092615	2.988290
V	0.692864	-0.400737	0.842592
H	2.151031	-0.463188	-2.209241
O	2.079130	-1.351935	0.857031
O	3.172989	-1.228254	-0.468355
H	3.344929	-2.185423	-0.458522
H	0.981939	1.887127	0.166308
H	1.357439	0.976492	2.864747