Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Theoretical Insight into the Mechanism of Ferroptosis Suppression via Inactivation of Lipid Peroxide Radical by Liproxstatin-1

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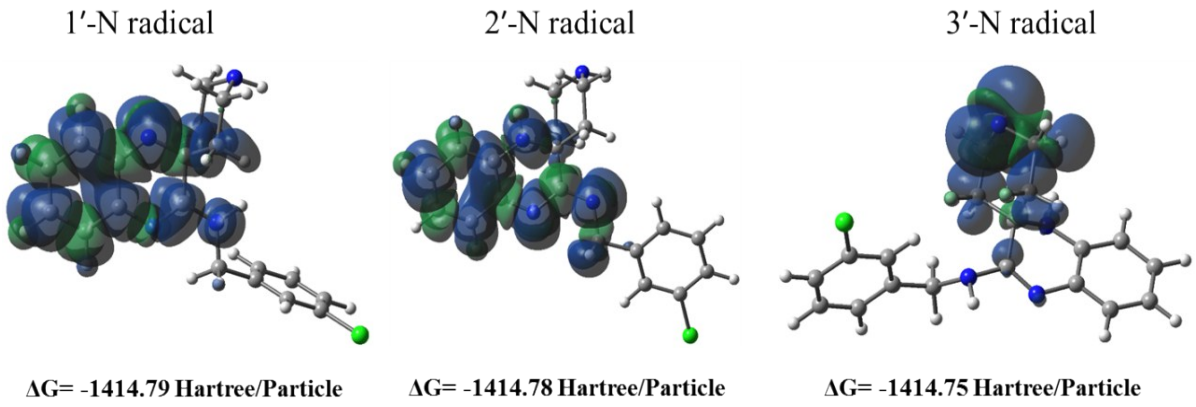

Figure S1 Spin density of the 1′, 2′, 3′-N radicals of liproxstatin-1; in blue the α spin density and in green the β spin density, isovalue = 0.0004

COORDINATES OF THE STATIONARY POINTS

[Liproxstatin-1]

reactant complex (1′-NH)

C	-4.88871	-2.08853	-0.96679
C	-4.40535	-0.94325	-0.35973
C	-3.03444	-0.62936	-0.4421
C	-2.13459	-1.5346	-1.07014
C	-2.65125	-2.67605	-1.69473
C	-4.01419	-2.94457	-1.65255
H	-5.94741	-2.31887	-0.91885
H	-5.06666	-0.26029	0.16145
H	-1.95789	-3.35554	-2.17602
H	-4.39972	-3.83467	-2.13713
C	-0.32359	-0.23959	-0.51391
N	-2.55437	0.53186	0.0958
H	-2.8669	0.76688	1.02323
N	-0.76646	-1.37004	-0.96706
N	1.00634	-0.09207	-0.31074
C	-1.22707	0.97504	-0.30338
C	-0.71378	1.98803	0.7352
C	-1.34726	1.69899	-1.67558
C	-1.57529	3.25884	0.75801
H	0.30449	2.2972	0.46848
H	-0.68263	1.52565	1.72722
C	-2.17592	2.98098	-1.55946
H	-0.33435	1.93627	-2.02749
H	-1.79353	1.01448	-2.40285
H	-1.14677	3.97387	1.46583
H	-2.57861	3.02446	1.12452
H	-2.19243	3.49811	-2.52346
H	-3.21234	2.72002	-1.32059
N	-1.7021	3.90357	-0.53969
H	-0.81316	4.30616	-0.81904
H	1.33435	0.72771	0.17048
C	1.94393	-1.18665	-0.48619

H	1.8423	-1.91574	0.32782
H	1.671	-1.71017	-1.40629
C	3.35478	-0.66219	-0.55602
C	4.25009	-0.90453	0.48605
C	3.7787	0.08404	-1.66065
C	5.54848	-0.40566	0.413
C	5.07705	0.57799	-1.71962
C	5.97524	0.33702	-0.68144
H	5.40141	1.15119	-2.58152
H	6.98969	0.71523	-0.72029
H	3.08716	0.27106	-2.47606
H	3.94333	-1.48197	1.35142
Cl	6.65381	-0.71914	1.72099
C	-3.32869	-1.22903	3.53887
H	-4.09513	-1.98803	3.70648
H	-3.02255	-0.7788	4.48579
H	-2.46451	-1.66974	3.0346
O	-3.93036	-0.24763	2.70951
O	-3.02648	0.75605	2.49481

transition state (1′-NH)

C	5.49809	-2.11075	-0.33594
C	4.99902	-0.90952	-0.83422
C	3.64536	-0.60229	-0.69315
C	2.77689	-1.51502	-0.06094
C	3.29534	-2.71203	0.43586
C	4.64909	-3.0103	0.30852
H	6.55277	-2.33874	-0.4483
H	5.66038	-0.20785	-1.33594
H	2.60907	-3.40515	0.91076
H	5.03817	-3.94362	0.70053
C	0.99233	-0.06923	-0.24569
N	3.06553	0.5535	-1.20866
H	3.44189	0.95165	-2.22094
N	1.40754	-1.26572	-0.00457
N	-0.34534	0.1951	-0.19121
C	1.94098	1.11509	-0.46136

C	1.34559	2.26784	-1.28314
C	2.35721	1.66269	0.92873
C	2.28627	3.48048	-1.33177
H	0.41549	2.61019	-0.81407
H	1.11287	1.91816	-2.29502
C	3.26402	2.88788	0.79783
H	1.45145	1.92868	1.48722
H	2.86345	0.87012	1.48993
H	1.7966	4.30257	-1.86144
H	3.18495	3.24749	-1.91791
H	3.49416	3.29397	1.78671
H	4.22706	2.59138	0.36204
N	2.71204	3.9555	-0.02552
H	1.93402	4.39662	0.45369
H	-0.67684	1.0221	-0.65926
C	-1.30437	-0.88393	-0.04023
H	-1.31687	-1.52765	-0.9287
H	-0.95884	-1.51276	0.7853
C	-2.68176	-0.33936	0.23795
C	-3.74446	-0.64748	-0.61168
C	-2.91575	0.47119	1.35404
C	-5.01726	-0.15347	-0.33722
C	-4.19095	0.96067	1.61389
C	-5.25633	0.65192	0.76954
H	-4.36578	1.58427	2.48423
H	-6.25357	1.02695	0.96572
H	-2.09248	0.71125	2.01905
H	-3.58655	-1.27214	-1.48409
Cl	-6.33153	-0.55016	-1.4096
C	3.88157	-0.63514	-4.81691
H	4.63306	-1.39572	-5.02625
H	3.65276	-0.05339	-5.71034
H	2.97655	-1.0812	-4.40346
O	4.47394	0.22925	-3.8306
O	3.65832	1.19473	-3.49332

product complex (1′-NH)

C	-4.88871	-2.08363	-0.96189
C	-4.41025	-0.94325	-0.35973
C	-3.02464	-0.61466	-0.4372
C	-2.12479	-1.5395	-1.07504
C	-2.65125	-2.67605	-1.69473
C	-4.00929	-2.94457	-1.65255
H	-5.94741	-2.31397	-0.91885
H	-5.06176	-0.26029	0.17125
H	-1.95789	-3.36044	-2.17602
H	-4.39972	-3.83467	-2.13713
C	-0.32359	-0.23469	-0.51391
N	-2.56417	0.52696	0.0909
H	-2.9159	0.73258	1.50343
N	-0.76646	-1.37494	-0.96706
N	1.00144	-0.09207	-0.31074
C	-1.22707	0.97014	-0.29848
C	-0.71378	1.98803	0.7352
C	-1.34726	1.69899	-1.67558
C	-1.57529	3.25884	0.75801
H	0.30449	2.2972	0.46848
H	-0.68753	1.52565	1.72722
C	-2.17592	2.98098	-1.55946
H	-0.33435	1.93627	-2.01769
H	-1.79353	1.01448	-2.40775
H	-1.14677	3.97387	1.46583
H	-2.57861	3.01955	1.12452
H	-2.18753	3.49811	-2.52346
H	-3.21234	2.72002	-1.32059
N	-1.7021	3.90357	-0.53969
H	-0.81316	4.30616	-0.81904
H	1.32945	0.72771	0.17048
C	1.94393	-1.18665	-0.48619
H	1.8423	-1.91084	0.32782
H	1.671	-1.71017	-1.40629
C	3.35478	-0.66219	-0.55602
C	4.25009	-0.90453	0.48605
C	3.7787	0.08404	-1.66065
C	5.54848	-0.40566	0.413

C	5.07705	0.57799	-1.71962
C	5.97524	0.33702	-0.68144
H	5.40141	1.15119	-2.58152
H	6.98969	0.71523	-0.72029
H	3.08716	0.27106	-2.47606
H	3.94333	-1.48197	1.35142
Cl	6.65381	-0.71914	1.72099
C	-3.32869	-1.22413	3.53397
H	-4.09023	-1.98803	3.71138
H	-3.01765	-0.7837	4.49069
H	-2.45471	-1.67464	3.0444
O	-3.94506	-0.26723	2.71441
O	-3.00688	0.77075	2.46051

reactant complex (2′-NH)

C	5.14607	-2.7437	0.22446
C	4.92203	-1.38224	0.10243
C	3.62789	-0.90755	-0.15451
C	2.55418	-1.82948	-0.31928
C	2.81439	-3.20701	-0.1869
C	4.09016	-3.66275	0.08786
H	6.14859	-3.10034	0.43208
H	5.74268	-0.67727	0.21039
H	1.98389	-3.89129	-0.31814
H	4.2796	-4.72476	0.1907
C	1.02538	-0.12387	-0.69593
N	3.34613	0.41259	-0.32962
H	4.10309	1.0664	-0.21466
N	1.29796	-1.41162	-0.64866
N	-0.17198	0.28657	-1.12213
C	1.99638	0.95901	-0.20817
C	1.94189	2.25508	-1.03566
C	1.65318	1.27168	1.27278
C	2.76128	3.37902	-0.39019
H	0.9094	2.5986	-1.10971
H	2.29603	2.04451	-2.05042
C	2.48584	2.43843	1.8102

H	0.59028	1.52909	1.33717
H	1.8132	0.37105	1.87509
H	2.62566	4.29848	-0.9662
H	3.83821	3.16587	-0.42988
H	2.16489	2.68036	2.82721
H	3.54252	2.14791	1.8875
N	2.41288	3.64282	0.99758
H	1.47298	4.02656	1.04067
H	-0.51454	1.19376	-0.86679
C	-1.17868	-0.66911	-1.55669
H	-1.69067	-0.23024	-2.4161
H	-0.66872	-1.57726	-1.88362
C	-2.19813	-1.00973	-0.49153
C	-3.55404	-0.79727	-0.74169
C	-1.80869	-1.56206	0.7325
C	-4.49698	-1.13703	0.22365
C	-2.76297	-1.8913	1.68896
C	-4.11918	-1.68227	1.44464
H	-2.45381	-2.32099	2.63606
H	-4.86868	-1.93762	2.18408
H	-0.7567	-1.7413	0.92283
H	-3.87766	-0.36217	-1.68142
Cl	-6.18804	-0.86174	-0.10569
C	-3.32865	2.69832	0.26256
H	-4.30632	2.77466	-0.21507
H	-3.08205	3.63161	0.77718
H	-3.31484	1.86556	0.96803
O	-2.40288	2.46792	-0.78325
O	-1.14329	2.38884	-0.22929

transition state (2′-NH)

C	5.19813	-2.07204	-0.31598
C	4.69906	-0.87081	-0.81427
C	3.3454	-0.56358	-0.6732
C	2.47693	-1.47631	-0.04099
C	2.99538	-2.67332	0.45582
C	4.34913	-2.97159	0.32848

H	6.25281	-2.30003	-0.42835
H	5.36042	-0.16914	-1.31599
H	2.30911	-3.36644	0.93071
H	4.73821	-3.90491	0.72048
C	0.69237	-0.03052	-0.22574
N	2.76557	0.59221	-1.18871
H	3.43368	1.27811	-1.50673
N	1.10758	-1.22701	0.01538
N	-0.6453	0.23381	-0.17125
C	1.64102	1.1538	-0.44141
C	1.04563	2.30655	-1.26319
C	2.05725	1.7014	0.94868
C	1.98631	3.51919	-1.31181
H	0.11553	2.6489	-0.79412
H	0.81292	1.95687	-2.27507
C	2.96406	2.92659	0.81778
H	1.15149	1.96739	1.50717
H	2.56349	0.90883	1.50988
H	1.49664	4.34128	-1.84148
H	2.88499	3.2862	-1.89795
H	3.1942	3.33268	1.80666
H	3.92711	2.63009	0.38199
N	2.41209	3.99421	-0.00556
H	1.63406	4.43533	0.47364
H	-1.05779	1.20206	-0.63476
C	-1.60433	-0.84522	-0.02028
H	-1.61683	-1.48894	-0.90874
H	-1.2588	-1.47405	0.80525
C	-2.98172	-0.30065	0.25791
C	-4.04442	-0.60877	-0.59173
C	-3.21571	0.5099	1.37399
C	-5.31722	-0.11476	-0.31727
C	-4.49091	0.99938	1.63384
C	-5.55628	0.69063	0.78949
H	-4.66574	1.62298	2.50418
H	-6.55353	1.06566	0.98567
H	-2.39244	0.74996	2.039
H	-3.88651	-1.23343	-1.46413

Cl	-6.63149	-0.51144	-1.38965
C	-3.29301	1.7946	-2.79469
H	-3.44642	1.34247	-3.77402
H	-3.58626	2.84483	-2.79721
H	-3.82939	1.24506	-2.02055
O	-1.87884	1.70076	-2.54529
O	-1.56557	2.21659	-1.38472

product complex (2′-NH)

C	5.14607	-2.7386	0.22446
C	4.92713	-1.38224	0.10243
C	3.62789	-0.89735	-0.15451
C	2.54398	-1.82438	-0.31928
C	2.81949	-3.21211	-0.1869
C	4.08506	-3.66275	0.08786
H	6.14859	-3.10034	0.43208
H	5.74268	-0.67727	0.21039
H	1.98389	-3.89129	-0.31814
H	4.2796	-4.72476	0.1907
C	1.01008	-0.10857	-0.70613
N	3.34613	0.40749	-0.32452
H	4.10309	1.0664	-0.21466
N	1.30816	-1.42692	-0.64356
N	-0.16178	0.28657	-1.11703
C	1.99128	0.95901	-0.20817
C	1.94189	2.25508	-1.03566
C	1.65318	1.27168	1.27278
C	2.76128	3.37902	-0.39019
H	0.9043	2.5884	-1.10461
H	2.29603	2.04451	-2.05042
C	2.48584	2.43843	1.8102
H	0.59028	1.52909	1.32187
H	1.8132	0.37105	1.88019
H	2.62566	4.29848	-0.9662
H	3.84331	3.16587	-0.42988
H	2.16489	2.68036	2.82721
H	3.54252	2.14791	1.8875

N	2.41288	3.64282	0.99758
H	1.47298	4.02146	1.04067
H	-0.75934	1.57626	-0.64749
C	-1.17358	-0.67421	-1.55669
H	-1.68557	-0.21494	-2.4059
H	-0.68402	-1.59256	-1.88872
C	-2.19813	-1.00973	-0.49153
C	-3.55404	-0.79727	-0.74169
C	-1.80869	-1.56206	0.7325
C	-4.49698	-1.13703	0.22365
C	-2.76297	-1.8913	1.68896
C	-4.11918	-1.68227	1.44464
H	-2.45381	-2.32099	2.63606
H	-4.86868	-1.93762	2.18408
H	-0.7567	-1.7413	0.92793
H	-3.87766	-0.35707	-1.67632
Cl	-6.18804	-0.86174	-0.10569
C	-3.31845	2.69832	0.25746
H	-4.30632	2.77976	-0.20997
H	-3.08715	3.63161	0.78738
H	-3.31994	1.86556	0.97823
O	-2.42328	2.46792	-0.79345
O	-1.11269	2.36844	-0.22929

reactant complex (3′-NH)

C	-6.08017	-1.17035	-0.31193
C	-5.19486	-0.34726	0.37942
C	-3.82127	-0.58574	0.30844
C	-3.33643	-1.67234	-0.44692
C	-4.23771	-2.48564	-1.13489
C	-5.60512	-2.23462	-1.07903
H	-7.14562	-0.9743	-0.25341
H	-5.56833	0.48115	0.97554
H	-3.83984	-3.32176	-1.69989
H	-6.29746	-2.87052	-1.61924
C	-1.13315	-1.1314	0.01376
N	-2.87357	0.1572	0.99972

H	-3.23236	1.00169	1.4199
N	-1.97906	-1.9919	-0.42957
N	0.22077	-1.45677	-0.08211
H	0.275	-2.29634	-0.65188
C	1.02872	-1.64841	1.12444
H	0.66268	-2.50198	1.71231
H	0.93932	-0.76933	1.7632
C	2.48317	-1.86698	0.78322
C	3.108	-1.08532	-0.1919
C	3.22486	-2.83338	1.46439
C	4.45706	-1.28056	-0.46368
C	4.57743	-3.01229	1.18499
H	2.74183	-3.45177	2.21478
C	5.20638	-2.23706	0.21633
H	5.14611	-3.76697	1.71769
H	6.25604	-2.37191	-0.01538
C	-1.55948	0.29763	0.37034
C	-0.6388	1.06974	1.31699
C	-1.60709	1.07767	-0.97043
C	-1.03299	2.55037	1.44543
H	0.37822	1.04674	0.9193
H	-0.64612	0.61071	2.31235
C	-1.98988	2.54632	-0.75964
H	-0.62062	1.02259	-1.44025
H	-2.32716	0.60432	-1.6474
H	-0.29845	3.06914	2.06441
H	-2.00068	2.65695	1.95919
H	-1.97759	3.08299	-1.71138
H	-3.02164	2.60407	-0.37908
N	-1.13661	3.24587	0.17806
H	-0.22398	3.43864	-0.22469
H	2.54282	-0.33645	-0.7346
Cl	5.22976	-0.30635	-1.68408
C	2.06502	5.2159	0.05316
H	2.68746	5.59862	0.86395
H	1.11569	5.75358	0.0202
H	2.58698	5.31422	-0.90016
O	1.85674	3.84356	0.3517

O	1.11644	3.27037	-0.66095

transition state (3′-NH)

C	5.78051	-0.82003	0.25856
C	4.87885	-0.00155	-0.41657
C	3.50647	-0.23497	-0.30699
C	3.04145	-1.3123	0.47361
C	3.95872	-2.1218	1.14421
C	5.32492	-1.87623	1.04832
H	6.84438	-0.62662	0.16943
H	5.23784	0.82068	-1.02965
H	3.5737	-2.95058	1.72873
H	6.03031	-2.50891	1.5753
C	0.83041	-0.77077	0.06503
N	2.54629	0.50335	-0.98453
H	2.89707	1.35204	-1.40304
N	1.68197	-1.62671	0.50388
N	-0.52521	-1.08203	0.21234
H	-0.57278	-1.8906	0.82482
C	-1.35463	-1.31096	-0.96819
H	-1.19236	-2.32319	-1.36439
H	-1.04289	-0.62973	-1.76081
C	-2.82917	-1.11154	-0.69995
C	-3.2671	-0.33082	0.36938
C	-3.77255	-1.68864	-1.55475
C	-4.63072	-0.13199	0.5625
C	-5.13199	-1.47802	-1.35007
H	-3.44128	-2.30859	-2.38267
C	-5.57623	-0.69518	-0.28668
H	-5.85718	-1.93115	-2.01758
H	-6.63293	-0.53003	-0.11465
C	1.24163	0.64956	-0.33457
C	0.30196	1.38896	-1.29614
C	1.31603	1.46545	0.98738
C	0.67809	2.86918	-1.45675
H	-0.71699	1.33935	-0.89946
H	0.31771	0.90201	-2.27745

C	1.67184	2.93103	0.73458
H	0.34151	1.40034	1.48529
H	2.05316	1.00503	1.65356
H	-0.06402	3.36317	-2.09036
H	1.63327	2.96854	-1.99058
H	1.66708	3.48512	1.6774
H	2.69615	3.0029	0.34559
N	0.78991	3.60393	-0.20836
H	-0.20844	3.97487	0.395
H	-2.54274	0.10559	1.04662
Cl	-5.16297	0.84607	1.90445
C	-0.79931	6.62236	1.57204
H	-0.64827	7.64075	1.21552
H	0.0866	6.25225	2.08894
H	-1.67753	6.55808	2.21516
O	-1.02107	5.83059	0.39103
O	-1.21759	4.57282	0.69193

product complex (3′-NH)

C	-6.08017	-1.17035	-0.31193
C	-5.19486	-0.34726	0.37942
C	-3.82127	-0.58574	0.30844
C	-3.33643	-1.67234	-0.44692
C	-4.23771	-2.48564	-1.13489
C	-5.60512	-2.23462	-1.07903
H	-7.14562	-0.9743	-0.25341
H	-5.56833	0.48115	0.97554
H	-3.83984	-3.32176	-1.69989
H	-6.29746	-2.87052	-1.61924
C	-1.13315	-1.1314	0.01376
N	-2.87357	0.1572	0.99972
H	-3.23236	1.00169	1.4199
N	-1.97906	-1.9919	-0.42957
N	0.22077	-1.45677	-0.08211
H	0.275	-2.29634	-0.65188
C	1.02872	-1.64841	1.12444
H	0.66268	-2.50198	1.71231

H	0.93932	-0.76933	1.7632
C	2.48317	-1.86698	0.78322
C	3.108	-1.08532	-0.1919
C	3.22486	-2.83338	1.46439
C	4.45706	-1.28056	-0.46368
C	4.57743	-3.01229	1.18499
H	2.74183	-3.45177	2.21478
C	5.20638	-2.23706	0.21633
H	5.14611	-3.76697	1.71769
H	6.25604	-2.37191	-0.01538
C	-1.55948	0.29763	0.37034
C	-0.6388	1.06974	1.31699
C	-1.60709	1.07767	-0.97043
C	-1.03719	2.55037	1.44543
H	0.37822	1.05094	0.9193
H	-0.64612	0.61911	2.31235
C	-1.99408	2.54632	-0.75964
H	-0.62062	1.02259	-1.44025
H	-2.32716	0.61272	-1.6474
H	-0.29845	3.06914	2.06021
H	-2.00488	2.65275	1.96339
H	-1.97339	3.08299	-1.71138
H	-3.02584	2.59987	-0.37908
N	-1.14501	3.23747	0.18226
H	0.17082	3.45124	-0.36329
H	2.54282	-0.33645	-0.7346
Cl	5.22976	-0.30635	-1.68408
C	2.06502	5.2117	0.05316
H	2.68746	5.59862	0.86395
H	1.11569	5.76198	0.0202
H	2.58698	5.31842	-0.90436
O	1.86094	3.84776	0.3643
O	1.09544	3.27037	-0.66935

reactant complex (UQH_2)

C	-0.88843	4.59508	-0.88448
C	-1.18658	3.32985	-0.45229

C	-0.15339	2.33692	-0.37494
C	1.16773	2.66608	-0.85055
C	1.42856	3.97305	-1.28599
C	0.42727	4.92825	-1.29088
H	-1.66548	5.351	-0.91168
H	-2.17881	3.03951	-0.11902
H	2.42495	4.20223	-1.6406
H	0.64212	5.93715	-1.63351
C	1.87774	0.51882	-0.47194
N	-0.40541	1.12616	0.10499
N	2.1204	1.70061	-0.97911
N	2.74831	-0.47845	-0.71289
C	0.7063	0.24672	0.45911
C	0.22399	-1.21817	0.48003
C	1.20113	0.63134	1.89759
C	-0.72571	-1.5247	1.64792
H	1.08743	-1.88004	0.6031
H	-0.26052	-1.45386	-0.47278
C	0.17755	0.2597	2.97352
H	2.13703	0.08834	2.07903
H	1.42898	1.6997	1.92213
H	-0.94452	-2.5963	1.65552
H	-1.67767	-1.00999	1.50056
H	0.58535	0.50421	3.95705
H	-0.73121	0.85693	2.84174
N	-0.20675	-1.14169	2.95135
H	0.58435	-1.72556	3.20857
H	2.58034	-1.36632	-0.26654
C	3.97552	-0.33075	-1.47449
H	4.02667	-1.13574	-2.21347
H	3.89295	0.61638	-2.01341
C	5.20908	-0.34448	-0.6014
C	6.14365	-1.3727	-0.71973
C	5.4227	0.67161	0.33635
C	7.27388	-1.37741	0.09442
C	6.55426	0.65177	1.14345
C	7.49166	-0.37436	1.03063
H	6.7183	1.44399	1.86617

H	8.37675	-0.39499	1.65498
H	4.70153	1.47785	0.42253
H	6.00072	-2.16839	-1.4433
Cl	8.4305	-2.66989	-0.06566
H	-6.69014	-2.68896	-1.46357
O	-6.97839	-2.2454	-0.65676
C	-5.9357	-1.43803	-0.27979
C	-6.07327	-0.57148	0.80288
C	-4.97952	0.23679	1.16996
C	-3.77119	0.18638	0.44307
C	-3.66858	-0.68789	-0.64198
C	-4.74466	-1.50812	-0.98984
C	-7.37197	-0.51502	1.56122
H	-8.12144	-1.15462	1.09593
H	-7.24228	-0.84383	2.59816
H	-7.76671	0.50532	1.59789
C	-5.10191	1.17715	2.3377
H	-4.14248	1.65963	2.5241
H	-5.84825	1.9622	2.15597
H	-5.41036	0.65345	3.24877
O	-2.74621	0.99712	0.78278
H	-1.84228	0.88728	0.44275
O	-2.49387	-0.75309	-1.37835
C	-2.54024	0.01151	-2.57698
H	-1.56837	-0.10526	-3.06236
H	-2.713	1.07023	-2.35612
H	-3.32712	-0.35618	-3.24306
O	-4.70978	-2.36957	-2.07055
C	-3.81846	-3.47406	-1.92539
H	-3.92766	-4.08085	-2.82719
H	-4.08644	-4.0722	-1.04763
H	-2.78729	-3.12577	-1.83262

transition state (UQH_2)

C	-1.03543	4.44221	-0.68901
C	-1.26176	3.15498	-0.26315
C	-0.19749	2.20894	-0.27544

C	1.0769	2.59041	-0.81202
C	1.26593	3.90832	-1.23937
C	0.23191	4.82772	-1.17108
H	-1.84111	5.16798	-0.65505
H	-2.22046	2.83367	0.12922
H	2.23666	4.17694	-1.64162
H	0.39251	5.84573	-1.51007
C	1.89836	0.46944	-0.50698
N	-0.38506	0.96717	0.18471
N	2.07421	1.66652	-0.98484
N	2.82362	-0.4763	-0.77795
C	0.75031	0.09072	0.43037
C	0.29314	-1.37946	0.31195
C	1.26594	0.34462	1.88311
C	-0.628	-1.80994	1.46317
H	1.16805	-2.04088	0.34265
H	-0.20525	-1.5278	-0.64947
C	0.26176	-0.14243	2.93083
H	2.21773	-0.1895	2.00783
H	1.47483	1.41366	1.99965
H	-0.83436	-2.88092	1.37169
H	-1.58657	-1.29318	1.38779
H	0.66866	0.0259	3.93322
H	-0.66411	0.43784	2.85493
N	-0.0892	-1.54608	2.78848
H	0.73654	-2.11956	2.94559
H	2.73906	-1.36967	-0.32354
C	4.04321	-0.22684	-1.52527
H	4.14227	-0.99317	-2.30091
H	3.90746	0.73822	-2.01615
C	5.26975	-0.21649	-0.6429
C	6.23627	-1.21207	-0.76985
C	5.43803	0.78387	0.31945
C	7.35413	-1.19968	0.05943
C	6.5581	0.78198	1.14094
C	7.52754	-0.21141	1.0194
H	6.68743	1.563	1.88307
H	8.4047	-0.21873	1.65552

H	4.69014	1.56522	0.41115
H	6.12755	-1.99578	-1.51242
Cl	8.55276	-2.4522	-0.1115
H	-6.82388	-2.23338	-1.69727
O	-7.11192	-1.86762	-0.84444
C	-6.02355	-1.21372	-0.35309
C	-6.10429	-0.48079	0.83597
C	-4.96328	0.16889	1.31666
C	-3.72755	0.11863	0.61016
C	-3.6852	-0.62931	-0.59301
C	-4.81725	-1.29028	-1.05338
C	-7.4094	-0.41407	1.5786
H	-8.19542	-0.93936	1.03522
H	-7.32561	-0.86467	2.57444
H	-7.73042	0.62304	1.72665
C	-5.01996	0.95464	2.5947
H	-4.03849	1.3731	2.81637
H	-5.74205	1.77803	2.53159
H	-5.32961	0.32788	3.43943
O	-2.67922	0.76543	1.06402
H	-1.49875	0.71975	0.53397
O	-2.50437	-0.70239	-1.29923
C	-2.50223	0.0835	-2.48494
H	-1.51764	-0.04074	-2.93994
H	-2.65936	1.14202	-2.2516
H	-3.27465	-0.25608	-3.18157
O	-4.83603	-2.01531	-2.2302
C	-4.06239	-3.21028	-2.18658
H	-4.20458	-3.70466	-3.14918
H	-4.40759	-3.86858	-1.38145
H	-3.00429	-2.98068	-2.04028

product complex (UQH_2)

C	-0.88343	4.60008	-0.88448
C	-1.18158	3.32485	-0.45229
C	-0.15339	2.35192	-0.37494
C	1.15773	2.67108	-0.85055

C	1.42356	3.97305	-1.28599
C	0.42227	4.93325	-1.29088
H	-1.66548	5.351	-0.91668
H	-2.17881	3.04951	-0.12902
H	2.42495	4.19723	-1.6406
H	0.64212	5.93715	-1.63351
C	1.87774	0.52382	-0.47694
N	-0.40541	1.11616	0.09999
N	2.1204	1.69561	-0.97911
N	2.74831	-0.48345	-0.71289
C	0.7013	0.24672	0.46911
C	0.22399	-1.21817	0.48003
C	1.20113	0.62634	1.89759
C	-0.72571	-1.5247	1.64792
H	1.08743	-1.88504	0.6031
H	-0.25552	-1.45386	-0.47278
C	0.17755	0.2597	2.97352
H	2.14203	0.09334	2.08903
H	1.42398	1.6997	1.91713
H	-0.94452	-2.5963	1.65552
H	-1.67767	-1.00999	1.50556
H	0.58035	0.50421	3.96205
H	-0.73121	0.85693	2.84174
N	-0.20675	-1.14169	2.95135
H	0.58435	-1.72556	3.20357
H	2.59034	-1.36632	-0.26154
C	3.97552	-0.33075	-1.47449
H	4.03167	-1.13574	-2.21347
H	3.89295	0.61638	-2.00841
C	5.20908	-0.34448	-0.6014
C	6.14365	-1.3727	-0.71973
C	5.4227	0.67161	0.33635
C	7.27388	-1.37741	0.09442
C	6.55426	0.65177	1.14345
C	7.49166	-0.37436	1.03063
H	6.7183	1.44399	1.86617
H	8.37675	-0.39499	1.65498
H	4.70153	1.47785	0.42253

H	6.00072	-2.16839	-1.4433
Cl	8.4305	-2.66989	-0.06566
H	-6.68514	-2.69396	-1.46357
O	-6.97339	-2.2404	-0.65676
C	-5.9407	-1.44303	-0.27979
C	-6.07327	-0.56648	0.80788
C	-4.99452	0.23679	1.17496
C	-3.75619	0.20638	0.45307
C	-3.66358	-0.69789	-0.65198
C	-4.73466	-1.50812	-0.99484
C	-7.37197	-0.51502	1.56122
H	-8.12144	-1.15462	1.09593
H	-7.24228	-0.84383	2.59816
H	-7.76671	0.50532	1.59789
C	-5.10191	1.17715	2.3377
H	-4.14248	1.65963	2.5191
H	-5.84825	1.9572	2.15097
H	-5.41036	0.65345	3.24877
O	-2.78121	0.98212	0.78278
H	-1.35728	0.91228	0.34275
O	-2.49887	-0.75309	-1.37335
C	-2.54024	0.01151	-2.57698
H	-1.56837	-0.10526	-3.05736
H	-2.708	1.07023	-2.35612
H	-3.32712	-0.35618	-3.24306
O	-4.70978	-2.36957	-2.07055
C	-3.81846	-3.47406	-1.92539
H	-3.92766	-4.07585	-2.82719
H	-4.08644	-4.0722	-1.04763
H	-2.78729	-3.12577	-1.83262

[Liproxstatin-2]

transition state (1′-NH)

C	-5.37114	-1.55779	0.72715
C	-4.66552	-0.39596	1.03197
C	-3.28952	-0.33405	0.80925

C	-2.60785	-1.4534	0.28965
C	-3.3319	-2.60786	-0.01286
C	-4.70717	-2.6632	0.19588
H	-6.44131	-1.59449	0.90155
H	-5.18257	0.46623	1.44522
H	-2.78745	-3.46171	-0.4021
H	-5.25658	-3.56678	-0.04484
C	-0.61244	-0.30379	0.20786
N	-2.51015	0.77238	1.13518
H	-2.65277	1.19587	2.20301
N	-1.22191	-1.43908	0.1542
N	0.74392	-0.26185	0.06698
C	-1.35245	1.03615	0.28269
C	-0.53935	2.17586	0.91542
C	-1.74879	1.45502	-1.15717
C	-1.27485	3.5203	0.82635
H	0.40376	2.29767	0.36972
H	-0.30609	1.92981	1.9571
C	-2.44015	2.82013	-1.17156
H	-0.84266	1.49014	-1.77412
H	-2.40512	0.69061	-1.58662
H	-0.63696	4.31422	1.22499
H	-2.1698	3.514	1.46297
H	-2.65192	3.12363	-2.20061
H	-3.41518	2.74752	-0.67247
N	-1.68469	3.88299	-0.52052
H	-0.87001	4.11862	-1.07766
H	1.21646	0.54996	0.42856
C	1.51845	-1.49158	0.04494
H	1.54633	-1.95156	1.04091
H	0.99643	-2.19146	-0.60829
C	2.9126	-1.24318	-0.46724
C	3.9173	-0.67317	0.32235
C	3.25128	-1.58317	-1.78094
C	5.20297	-0.45151	-0.16235
C	4.52964	-1.37032	-2.2856
C	5.50785	-0.80316	-1.4731
H	5.95141	-0.01059	0.4853

H	4.76138	-1.64795	-3.30793
H	6.50942	-0.63418	-1.85338
H	2.48722	-2.02559	-2.41234
Cl	3.57323	-0.21175	1.97464
C	-4.47877	0.54231	4.75708
H	-5.51642	0.82556	4.9306
H	-3.89526	0.60822	5.67586
H	-4.41171	-0.45751	4.32712
O	-3.97293	1.49839	3.80793
O	-2.72015	1.26103	3.51578

[Liproxstatin-3]

transition state (1′-NH)

C	-4.90617	-2.08887	0.38093
C	-4.32984	-0.90385	0.83269
C	-2.98022	-0.645	0.59061
C	-2.19132	-1.59051	-0.09598
C	-2.78809	-2.76992	-0.54618
C	-4.13815	-3.02024	-0.31771
H	-5.95712	-2.27895	0.57163
H	-4.92773	-0.17638	1.37581
H	-2.16332	-3.48762	-1.06732
H	-4.58704	-3.94088	-0.67437
C	-0.3455	-0.21118	-0.04114
N	-2.32618	0.49369	1.05273
H	-2.62337	0.88915	2.08462
N	-0.82487	-1.38877	-0.26823
N	0.99823	-0.02151	-0.09898
C	-1.23212	1.00979	0.23368
C	-0.54236	2.13638	1.01791
C	-1.71655	1.57526	-1.12658
C	-1.43256	3.38214	1.12724
H	0.37204	2.44698	0.49881
H	-0.2566	1.77098	2.00946
C	-2.56507	2.83452	-0.93719
H	-0.84132	1.80952	-1.74627

H	-2.28778	0.80335	-1.653
H	-0.88142	4.18403	1.62668
H	-2.30154	3.1802	1.76776
H	-2.84269	3.25258	-1.90874
H	-3.50838	2.57231	-0.44087
N	-1.9219	3.87781	-0.14925
H	-1.15932	4.29019	-0.67647
H	1.35823	0.91685	-0.1178
C	1.89893	-1.08071	-0.52499
H	1.6353	-1.98287	0.03287
H	1.73235	-1.31687	-1.58351
C	3.33201	-0.67567	-0.29591
C	3.90137	-0.71447	0.99193
C	4.10107	-0.23763	-1.3762
C	5.22712	-0.30206	1.14686
C	5.42294	0.16761	-1.20719
C	5.98627	0.13627	0.06387
H	5.67414	-0.33006	2.13644
H	6.00444	0.50134	-2.06001
H	7.01457	0.44784	0.21537
H	3.65484	-0.22133	-2.3669
C	3.11744	-1.21001	2.17668
H	2.14603	-0.71523	2.25537
H	2.92254	-2.28511	2.09913
H	3.66584	-1.04073	3.10539
C	-3.0849	-0.85391	4.57609
H	-3.89577	-1.54649	4.79939
H	-2.70817	-0.38469	5.48543
H	-2.27977	-1.35345	4.03643
O	-3.66391	0.15579	3.72984
O	-2.77808	1.05621	3.38974

[Liproxstatin-4]

transition state (1′-NH)

C	5.73854	-0.90214	-0.4608
C	4.75228	-0.04163	-0.93506

C	3.40418	-0.3463	-0.73215
C	3.0457	-1.53601	-0.0682
C	4.04777	-2.38595	0.4026
C	5.39047	-2.07095	0.21811
H	6.78302	-0.65439	-0.61874
H	5.02573	0.86857	-1.46207
H	3.74641	-3.3006	0.90209
H	6.16126	-2.73711	0.5896
C	0.79024	-1.02431	-0.18932
N	2.3609	0.42276	-1.21556
H	2.41262	0.94393	-2.24585
N	1.70756	-1.89603	0.05335
N	-0.5083	-1.50041	-0.26153
H	-0.47184	-2.50869	-0.16592
C	-1.63087	-0.91811	0.45584
H	-1.37648	0.08652	0.7978
H	-1.8208	-1.48747	1.37541
C	-2.9044	-0.86247	-0.35907
C	-4.09859	-0.40451	0.20735
C	-2.941	-1.26432	-1.69527
C	-5.28495	-0.34822	-0.51525
C	-4.11916	-1.21575	-2.43543
H	-2.01756	-1.61262	-2.1449
C	-5.29347	-0.75841	-1.8454
H	-4.1171	-1.53525	-3.47189
H	-6.21692	-0.71773	-2.4127
C	1.10545	0.45696	-0.4654
C	0.07156	1.15946	-1.36023
C	1.25689	1.21334	0.87781
C	0.36216	2.65234	-1.53396
H	-0.92697	1.06214	-0.9311
H	0.04856	0.65293	-2.32925
C	1.54529	2.69924	0.67439
H	0.33656	1.10075	1.46413
H	2.05549	0.74066	1.45858
H	-0.43824	3.10127	-2.13261
H	1.2821	2.81121	-2.11509
H	1.60972	3.19401	1.64975

H	2.53206	2.8257	0.20794
C	0.48666	3.38327	-0.19425
H	-0.48006	3.29127	0.32412
C	0.7832	4.86669	-0.38656
H	0.00959	5.3532	-0.98836
H	0.83823	5.38885	0.57333
H	1.74168	5.01039	-0.89769
H	-6.18703	0.01369	-0.03612
Cl	-4.11671	0.12506	1.87395
C	3.6321	-0.34975	-4.84508
H	4.65095	-0.69645	-5.0148
H	3.21274	0.09309	-5.74897
H	2.99812	-1.15856	-4.48054
O	3.73517	0.66318	-3.82811
O	2.56244	1.16244	-3.53389

[Liproxstatin-5]

transition state (1′-NH)

C	-5.57227	-1.35522	0.0012
C	-4.75106	-0.34863	0.50284
C	-3.36628	-0.4318	0.343
C	-2.80379	-1.54689	-0.31036
C	-3.64152	-2.54536	-0.8081
C	-5.02255	-2.45164	-0.66383
H	-6.64713	-1.27792	0.12778
H	-5.18291	0.50435	1.01949
H	-3.18167	-3.39787	-1.2966
H	-5.6653	-3.23181	-1.0562
C	-0.66036	-0.69545	-0.1159
N	-2.47699	0.5024	0.85331
H	-2.73403	0.98802	1.86255
N	-1.41912	-1.7001	-0.37881
N	0.71184	-0.86893	-0.31021
H	0.82422	-1.75487	-0.79436
C	1.64177	-0.81772	0.81789
H	1.53029	-1.7084	1.45319

H	1.3911	0.03524	1.44877
C	3.0789	-0.70005	0.36761
C	3.42527	-0.08681	-0.83668
C	4.10605	-1.18231	1.18293
C	4.76149	0.04708	-1.20787
C	5.4391	-1.04121	0.81205
H	3.86131	-1.68107	2.11711
C	5.79296	-0.4202	-0.39032
H	6.21763	-1.42996	1.46255
C	-1.23095	0.70903	0.11089
C	-0.3486	1.67683	0.91109
C	-1.4685	1.30721	-1.30544
C	-0.9068	3.1029	0.95365
H	0.63718	1.71391	0.43665
H	-0.22572	1.29861	1.93095
C	-2.03951	2.72272	-1.25702
H	-0.50778	1.3101	-1.83345
H	-2.13832	0.64442	-1.86209
H	-0.2057	3.73848	1.50442
H	-1.84271	3.13544	1.52791
H	-2.1658	3.09819	-2.27773
H	-3.04574	2.69994	-0.81815
H	2.63786	0.27459	-1.48975
C	-1.14634	3.65934	-0.44748
H	-1.58794	4.65979	-0.38969
H	-0.18165	3.77123	-0.96004
H	5.00497	0.5213	-2.15465
C	7.23613	-0.24928	-0.77873
H	7.66806	0.63894	-0.30494
H	7.83779	-1.10774	-0.46927
H	7.34716	-0.13103	-1.85905
C	-3.4397	-0.47124	4.54171
H	-4.33442	-1.03682	4.79986
H	-3.04701	0.05935	5.40962
H	-2.67788	-1.11911	4.10709
O	-3.86221	0.48715	3.55488
O	-2.8641	1.23526	3.16089

[Liproxstatin-6]

transition state (1′-NH)

C	2.93184	2.55222	0.40971
C	1.77967	3.33454	-0.18893
C	0.65235	1.26847	-0.36191
N	3.07052	1.32588	-0.35777
H	4.14533	0.70859	-0.03818
N	0.57877	2.54668	-0.35859
N	-0.52197	0.55228	-0.41545
H	-0.4813	-0.3854	-0.77829
C	-1.7816	1.2477	-0.59142
H	-1.80591	1.7897	-1.54575
H	-1.85781	2.0049	0.19298
C	-2.93082	0.2783	-0.52877
C	-3.40137	-0.26431	0.67403
C	-3.57035	-0.12574	-1.70531
C	-4.45868	-1.16928	0.70529
C	-4.62783	-1.03034	-1.69408
H	-3.22551	0.29029	-2.64739
C	-5.07151	-1.55401	-0.48342
H	-5.10346	-1.32059	-2.62446
H	-5.8962	-2.25805	-0.45699
C	1.92641	0.41876	-0.24205
C	1.90217	-0.36257	1.09774
C	2.02924	-0.59232	-1.40439
C	3.08498	-1.32035	1.24015
H	0.96648	-0.92803	1.1633
H	1.88378	0.34647	1.93175
C	3.22925	-1.5273	-1.25532
H	1.12974	-1.21909	-1.44331
H	2.08463	-0.03572	-2.34419
H	2.99028	-1.87439	2.18106
H	4.02609	-0.75717	1.32465
H	3.24615	-2.22981	-2.09643
H	4.16491	-0.95635	-1.32618
C	3.19561	-2.29823	0.06694

H	2.28403	-2.91564	0.06543
C	4.39724	-3.22568	0.2131
H	4.35078	-3.79407	1.14701
H	4.45006	-3.94182	-0.61265
H	5.33283	-2.65539	0.21766
H	-4.79633	-1.56197	1.65718
Cl	-2.676	0.19892	2.18975
H	3.86316	3.1208	0.33112
H	2.74129	2.37804	1.48328
H	2.07684	3.73319	-1.16769
H	1.53672	4.19724	0.44196
C	7.48923	0.21154	0.32181
H	8.26743	0.97406	0.3218
H	7.54448	-0.40534	-0.57563
H	7.54448	-0.40534	1.21925
O	6.24413	0.93306	0.32181
O	5.22181	0.11698	0.32181