B3LYP transition state coordinates for concerted reaction mechanism between 6-substituted 4-quinazolinones and MoCo.

6-Nitro-4-Quinazolinone

30

Mo	2.630849	-0.361921	-0.074386
S	4.715700	-0.259218	1.112403
C	5.688300	0.899957	0.194576
H	6.744813	0.967746	0.478730
C	5.166178	1.707661	-0.745093
H	5.774551	2.446932	-1.277167
S	3.463049	1.618371	-1.218265
S	1.450004	-0.778006	1.830611
O	0.703207	0.526110	-0.606543
H	0.678002	1.501379	-0.628569
C	-0.550491	0.121789	0.005958
H	0.094540	-0.265018	1.221905
N	-1.384348	1.137348	0.210934
O	2.666970	-1.742541	-1.038864
C	-2.328120	-1.467944	-0.598978
C	-3.254166	-0.378792	-0.211527
C	-2.713981	0.893751	0.166078
N	-0.991999	-1.092151	-0.537577
H	-0.303473	-1.824795	-0.708961
O	-2.663913	-2.583620	-0.955301
C	-3.633910	1.934183	0.493972
C	-4.630841	-0.592914	-0.248227
C	-4.995495	1.717111	0.458267
C	-5.494133	0.448653	0.088693
H	-3.220928	2.903854	0.778892
H	-5.707114	2.503159	0.711073
N	-6.933861	0.231354	0.054038
H	-5.018830	-1.567737	-0.543534
O	-7.665129	1.173425	0.350581
O	-7.345720	-0.877924	-0.269009

6-Trifluoromethyl-4-Quinazolinone

31

Mo	3.012876	-0.363487	-0.083521
S	5.111903	-0.248844	1.084527
C	6.046076	0.968588	0.203006
H	7.101809	1.056989	0.484920
C	5.497007	1.791982	-0.707332
H	6.081791	2.566146	-1.215984
S	3.794958	1.669562	-1.175386
S	1.862343	-0.866018	1.818048
O	1.075413	0.511301	-0.561794
H	1.036916	1.486128	-0.561694
C	-0.176644	0.078436	0.061282
H	0.487236	-0.347689	1.235022
N	-1.009106	1.082627	0.306383
O	3.068908	-1.714295	-1.089227
C	-1.956070	-1.474079	-0.641145
C	-2.880993	-0.398522	-0.222796
C	-2.343726	0.843896	0.230344
N	-0.620136	-1.115886	-0.527273
H	0.066829	-1.843839	-0.721352
O	-2.293364	-2.569827	-1.058829
C	-3.266449	1.865285	0.596109
C	-4.262919	-0.599022	-0.304240
C	-4.629258	1.653113	0.513279
C	-5.144608	0.415278	0.060683
H	-2.858750	2.817539	0.941563
H	-5.320682	2.451765	0.794969
C	-6.628241	0.211810	0.007677
H	-4.620645	-1.564098	-0.667283
F	-7.175976	0.078388	1.239452
F	-6.976313	-0.885565	-0.688712
F	-7.262792	1.261882	-0.563539

6-Cloro-4-Quinazolinone

28

Mo	2.457426	-0.386202	-0.106356
S	4.549862	-0.272528	1.079712
C	5.477252	0.975451	0.235350
H	6.527569	1.074069	0.534065
C	4.929045	1.808094	-0.667166
H	5.509500	2.600479	-1.152362
S	3.235665	1.669438	-1.161045
S	1.302316	-0.919331	1.782582
O	0.521921	0.484112	-0.586313
H	0.488104	1.458890	-0.598723
C	-0.737491	0.068671	0.052549
H	-0.075496	-0.372384	1.201793
N	-1.548778	1.086653	0.302359
O	2.533969	-1.722135	-1.130809
C	-2.552420	-1.446226	-0.649827
C	-3.455274	-0.357358	-0.215689
C	-2.891542	0.872331	0.236624
N	-1.210653	-1.114305	-0.541960
H	-0.540357	-1.856458	-0.738741
O	-2.914562	-2.532994	-1.072285
C	-3.791954	1.904624	0.617725
C	-4.843158	-0.542814	-0.276485
C	-5.163354	1.716246	0.558989
C	-5.689072	0.487733	0.112349
H	-3.367314	2.849464	0.963786
H	-5.847334	2.513394	0.858859
Cl	-7.433716	0.271260	0.049345
H	-5.226847	-1.500173	-0.633191

4-Quinazolinone

28

Mo	1.810359	-0.409713	-0.116091
S	3.906837	-0.301327	1.067087
C	4.834599	0.948807	0.226628
H	5.884735	1.046916	0.526360
C	4.287201	1.783489	-0.674605
H	4.868302	2.577142	-1.157102
S	2.594278	1.646428	-1.169610
S	0.661040	-0.947457	1.773994
O	-0.118312	0.470053	-0.586353
H	-0.140635	1.445083	-0.607132
C	-1.384140	0.082472	0.073411
H	-0.717426	-0.377767	1.202318
N	-2.160645	1.122663	0.336579
O	1.886663	-1.742776	-1.144085
C	-3.253249	-1.366983	-0.626603
C	-4.117755	-0.252801	-0.184698
C	-3.512355	0.954416	0.276049
N	-1.899238	-1.082232	-0.520807
H	-1.256280	-1.846523	-0.722073
O	-3.648991	-2.441099	-1.053778
C	-4.372614	2.014840	0.670386
C	-5.513259	-0.381147	-0.239075
C	-5.750623	1.868385	0.612453
C	-6.335752	0.668212	0.158646
H	-3.909019	2.939309	1.022187
H	-6.392784	2.697639	0.925954
H	-7.423547	0.566281	0.119595
H	-5.921317	-1.327217	-0.603768

6-Methyl-4-Quinazolinone

31

Mo	2.096020	-0.396125	-0.116815
S	4.172423	-0.272156	1.100750
C	5.091142	1.007528	0.296306
H	6.134480	1.119029	0.614633
C	4.543293	1.847660	-0.599646
H	5.117655	2.659493	-1.059425
S	2.860263	1.691028	-1.122080
S	0.934603	-0.976707	1.751314
O	0.156464	0.453874	-0.602841
H	0.116536	1.428212	-0.623725
C	-1.108806	0.045655	0.049150
H	-0.450539	-0.409477	1.171041
N	-1.900833	1.076630	0.307920
O	2.214226	-1.710196	-1.165578
C	-2.957962	-1.433388	-0.643103
C	-3.837776	-0.332122	-0.200566
C	-3.249294	0.885066	0.247816
N	-1.608370	-1.121224	-0.557334
H	-0.955810	-1.879498	-0.750148
O	-3.338002	-2.518279	-1.058191
C	-4.132360	1.929863	0.633880
C	-5.231555	-0.486351	-0.243107
C	-5.505128	1.753960	0.583490
C	-6.090907	0.539648	0.147807
H	-3.690120	2.868852	0.974841
H	-6.158772	2.577323	0.892540
C	-7.591837	0.376083	0.119600
H	-5.619036	-1.445441	-0.598194
H	-8.077726	1.161999	-0.485497
H	-7.880703	-0.598147	-0.303920
H	-8.028850	0.440089	1.132639

6-Methoxy-4-Quinazolinone

32

Mo	2.393195	-0.368533	-0.100980
S	4.495626	-0.185299	1.064017
C	5.387036	1.069708	0.192445
H	6.436146	1.200031	0.483603
C	4.813516	1.871877	-0.722082
H	5.372196	2.669785	-1.223711
S	3.120928	1.684192	-1.202243
S	1.268082	-0.893636	1.806665
O	0.442800	0.444542	-0.585617
H	0.378159	1.416267	-0.631359
C	-0.812220	0.016020	0.081426
H	-0.136814	-0.379730	1.214910
N	-1.641454	1.023858	0.299118
O	2.493626	-1.719599	-1.103433
C	-2.596870	-1.543951	-0.611601
C	-3.524455	-0.458409	-0.218392
C	-2.984051	0.788017	0.218301
N	-1.263567	-1.190594	-0.488286
H	-0.580404	-1.927953	-0.655724
O	-2.936520	-2.646564	-1.012996
C	-3.906516	1.805623	0.562755
C	-4.903962	-0.663514	-0.296784
C	-5.279466	1.597215	0.486078
C	-5.792335	0.354402	0.055897
H	-3.504941	2.764813	0.897267
H	-5.952242	2.409555	0.765935
O	-7.127567	0.066346	-0.046148
H	-5.279486	-1.629695	-0.638977
C	-8.064807	1.047496	0.308145
H	-7.984521	1.953806	-0.323079
H	-9.060291	0.604150	0.158601
H	-7.971332	1.354735	1.368026

6-Amino-4-Quinazolinone

30

Mo	2.103966	-0.400245	-0.120567
S	4.208164	-0.269566	1.050908
C	5.110219	1.005312	0.220164
H	6.159537	1.119568	0.517499
C	4.545122	1.838738	-0.671475
H	5.110811	2.647372	-1.147581
S	2.852800	1.676968	-1.161395
S	0.975706	-0.966554	1.774455
O	0.162825	0.448764	-0.578558
H	0.121700	1.422378	-0.609298
C	-1.099588	0.044393	0.098573
H	-0.422102	-0.402338	1.206466
N	-1.889737	1.074328	0.353800
O	2.197584	-1.723142	-1.160993
C	-2.950705	-1.423966	-0.622570
C	-3.831770	-0.318591	-0.187903
C	-3.240953	0.889645	0.278479
N	-1.603799	-1.128800	-0.496519
H	-0.951850	-1.886895	-0.691528
O	-3.336309	-2.499895	-1.058036
C	-4.125317	1.933377	0.657586
C	-5.222240	-0.467928	-0.266909
C	-5.499334	1.773177	0.582396
C	-6.080306	0.566719	0.117219
H	-3.686550	2.867748	1.015237
H	-6.156298	2.592701	0.893282
N	-7.474816	0.409772	0.101191
H	-5.609105	-1.420000	-0.641192
H	-7.991738	1.269930	-0.055206
H	-7.800712	-0.325453	-0.518895

B3LYP-D3 transition state coordinates for concerted reaction mechanism between 6-substituted 4-quinazolinones and MoCo.

6-Nitro-4-Quinazolinone

30

Mo	2.611675	-0.342779	-0.059616
S	4.713538	-0.297010	1.106602
C	5.701677	0.841623	0.176838
H	6.763888	0.883508	0.445101
C	5.187736	1.664907	-0.754847
H	5.810010	2.388728	-1.292543
S	3.476132	1.621301	-1.208773
S	1.426796	-0.738096	1.844450
O	0.701816	0.578993	-0.594513
H	0.677115	1.554125	-0.602393
C	-0.552316	0.166768	0.011443
H	0.070550	-0.209005	1.228339
N	-1.397072	1.175986	0.208610
O	2.607295	-1.720241	-1.027782
C	-2.304247	-1.447424	-0.592823
C	-3.244330	-0.367993	-0.209885
C	-2.722439	0.914269	0.162085
N	-0.974177	-1.053091	-0.535924
H	-0.272455	-1.774730	-0.700729
O	-2.627604	-2.568653	-0.943068
C	-3.657631	1.942472	0.485292
C	-4.617045	-0.602528	-0.246295
C	-5.015837	1.705090	0.450366
C	-5.496091	0.427648	0.086051
H	-3.259432	2.919379	0.766479
H	-5.738231	2.482251	0.700094
N	-6.933038	0.188110	0.052108
H	-4.989049	-1.584564	-0.538293
O	-7.679443	1.120085	0.344126
O	-7.328083	-0.928924	-0.265791

6-Trifluoromethyl-4-Quinazolinone

31

Mo	2.992266	-0.341636	-0.065740
S	5.114225	-0.292057	1.070870
C	6.064929	0.903303	0.173840
H	7.128672	0.961671	0.433365
C	5.522272	1.746300	-0.723407
H	6.121807	2.504177	-1.239932
S	3.807781	1.676789	-1.161451
S	1.843005	-0.822699	1.838703
O	1.071115	0.569432	-0.540083
H	1.032382	1.543699	-0.523382
C	-0.179898	0.126446	0.077832
H	0.464938	-0.288506	1.252324
N	-1.024842	1.123082	0.314673
O	2.998957	-1.689139	-1.076511
C	-1.930922	-1.450702	-0.633347
C	-2.872007	-0.386556	-0.219761
C	-2.354824	0.865655	0.231913
N	-0.601414	-1.073701	-0.516191
H	0.100277	-1.788860	-0.705858
O	-2.253738	-2.551046	-1.050496
C	-3.293445	1.875030	0.591111
C	-4.250087	-0.607683	-0.305779
C	-4.652612	1.642369	0.503443
C	-5.146055	0.395732	0.052699
H	-2.900661	2.833919	0.935437
H	-5.359652	2.429439	0.778663
C	-6.626113	0.172852	-0.001038
H	-4.594489	-1.578209	-0.667342
F	-7.170206	0.026987	1.231498
F	-6.960843	-0.925856	-0.702806
F	-7.273421	1.219312	-0.566087

6-Cloro-4-Quinazolinone

28

Mo	2.434197	-0.358296	-0.082812
S	4.553227	-0.315349	1.065421
C	5.501617	0.903173	0.198289
H	6.562008	0.967114	0.470286
C	4.961035	1.755507	-0.691437
H	5.559392	2.526963	-1.189048
S	3.252057	1.676948	-1.148898
S	1.282032	-0.865998	1.811399
O	0.517405	0.555574	-0.555119
H	0.483093	1.529921	-0.547560
C	-0.740603	0.124885	0.075163
H	-0.099089	-0.300903	1.227518
N	-1.570853	1.130701	0.315996
O	2.452257	-1.693292	-1.110031
C	-2.516098	-1.423414	-0.647650
C	-3.442714	-0.352154	-0.217559
C	-2.907770	0.889210	0.239319
N	-1.182972	-1.066682	-0.526831
H	-0.492257	-1.790905	-0.720710
O	-2.856370	-2.514746	-1.076357
C	-3.832261	1.901530	0.616253
C	-4.825243	-0.567091	-0.287599
C	-5.198962	1.683640	0.549516
C	-5.695511	0.444634	0.097770
H	-3.430032	2.854529	0.966655
H	-5.902646	2.464283	0.846975
Cl	-7.434945	0.189751	0.024469
H	-5.186688	-1.531529	-0.648281

4-Quinazolinone

28

Mo	1.786094	-0.376605	-0.090088
S	3.912581	-0.350250	1.048775
C	4.864241	0.866587	0.183206
H	5.926070	0.923887	0.451375
C	4.324912	1.725488	-0.701123
H	4.925731	2.496169	-1.197150
S	2.613620	1.659911	-1.150399
S	0.642368	-0.886619	1.806828
O	-0.121687	0.552638	-0.547574
H	-0.147051	1.527272	-0.545142
C	-1.386508	0.144501	0.100426
H	-0.741621	-0.301439	1.230816
N	-2.185646	1.171242	0.354004
O	1.798108	-1.706827	-1.123532
C	-3.212069	-1.343319	-0.625377
C	-4.104689	-0.249180	-0.186978
C	-3.531707	0.972019	0.279953
N	-1.866895	-1.028649	-0.507644
H	-1.200542	-1.773784	-0.705334
O	-3.582601	-2.423585	-1.059720
C	-4.420543	2.010626	0.669073
C	-5.495722	-0.411528	-0.252186
C	-5.794287	1.830343	0.601113
C	-6.346797	0.616785	0.141350
H	-3.982360	2.945322	1.026454
H	-6.458786	2.642856	0.911926
H	-7.431479	0.488258	0.094575
H	-5.876662	-1.367019	-0.621757

6-Methyl-4-Quinazolinone

31

Mo	2.071810	-0.374131	-0.052425
S	4.198511	-0.317282	1.085227
C	5.143896	0.889145	0.198520
H	6.205393	0.956562	0.465741
C	4.600231	1.729355	-0.701016
H	5.197460	2.494127	-1.210368
S	2.889377	1.647130	-1.149747
S	0.930090	-0.860771	1.851939
O	0.159542	0.531612	-0.529215
H	0.122454	1.505607	-0.543011
C	-1.104763	0.117942	0.121117
H	-0.459471	-0.297579	1.259383
N	-1.919552	1.137995	0.350515
O	2.090488	-1.720330	-1.064653
C	-2.905621	-1.404748	-0.598605
C	-3.815394	-0.314570	-0.187948
C	-3.261815	0.917755	0.264717
N	-1.565926	-1.072705	-0.468040
H	-0.888226	-1.811808	-0.649251
O	-3.258225	-2.496171	-1.020732
C	-4.173920	1.946607	0.624629
C	-5.203860	-0.495529	-0.266940
C	-5.541422	1.743046	0.542042
C	-6.091525	0.516118	0.096581
H	-3.758176	2.895822	0.970559
H	-6.219771	2.553628	0.830840
C	-7.587935	0.326144	0.034522
H	-5.563182	-1.463574	-0.627397
H	-8.074702	1.122486	-0.555802
H	-7.852974	-0.640077	-0.422110
H	-8.042772	0.353869	1.041403

6-Methoxy-4-Quinazolinone

32

Mo	2.368812	-0.339521	-0.068148
S	4.496212	-0.236082	1.066008
C	5.421708	0.974239	0.163888
H	6.482234	1.061837	0.429320
C	4.864115	1.794655	-0.745443
H	5.449164	2.562276	-1.264613
S	3.154102	1.680444	-1.191559
S	1.237139	-0.819378	1.843831
O	0.441457	0.522042	-0.560064
H	0.380064	1.494006	-0.592550
C	-0.816056	0.087437	0.096360
H	-0.167552	-0.289174	1.237422
N	-1.660043	1.087575	0.297883
O	2.405036	-1.697517	-1.064242
C	-2.565583	-1.502081	-0.611395
C	-3.512854	-0.429388	-0.227428
C	-2.997045	0.828608	0.207321
N	-1.240098	-1.127888	-0.477037
H	-0.539402	-1.850420	-0.637497
O	-2.887038	-2.609565	-1.014236
C	-3.939588	1.830455	0.543469
C	-4.887494	-0.659904	-0.311184
C	-5.308163	1.596223	0.462882
C	-5.795932	0.342085	0.035391
H	-3.557055	2.797834	0.876759
H	-5.996186	2.397191	0.737652
O	-7.124728	0.026877	-0.070520
H	-5.244095	-1.633893	-0.651133
C	-8.081693	0.975520	0.320078
H	-8.039353	1.895974	-0.295124
H	-9.067916	0.508104	0.181840
H	-7.974687	1.266390	1.383850

6-Amino-4-Quinazolinone

30

Mo	2.078195	-0.371530	-0.093105
S	4.211850	-0.321535	1.036384
C	5.140910	0.918738	0.179799
H	6.201932	0.992874	0.447598
C	4.586156	1.774622	-0.698066
H	5.173464	2.559519	-1.188171
S	2.875636	1.682631	-1.146116
S	0.951116	-0.904659	1.808407
O	0.159474	0.529898	-0.544131
H	0.119946	1.503545	-0.554160
C	-1.103281	0.111691	0.120438
H	-0.449096	-0.322894	1.233821
N	-1.911880	1.130627	0.366107
O	2.105325	-1.695760	-1.134649
C	-2.915415	-1.389446	-0.623413
C	-3.820427	-0.302217	-0.189558
C	-3.257752	0.918273	0.281253
N	-1.576603	-1.068575	-0.487015
H	-0.903642	-1.808741	-0.680338
O	-3.279380	-2.469865	-1.066389
C	-4.166316	1.941647	0.658297
C	-5.206383	-0.481847	-0.274919
C	-5.536289	1.750930	0.578292
C	-6.088694	0.532656	0.108675
H	-3.749529	2.884329	1.020402
H	-6.212483	2.554540	0.889518
N	-7.479656	0.344471	0.087987
H	-5.570073	-1.441564	-0.653074
H	-8.014972	1.192760	-0.071747
H	-7.786950	-0.397599	-0.533496

B3LYP transition state coordinates for concerted reaction mechanism between 6-substituted 4-quinazolinones and deprotonated MoCo.

6-Nitro-4-Quinazolinone

29

Mo	2.589388	-0.413949	-0.042533
S	4.655561	0.097008	1.213221
C	5.563169	1.180179	0.155749
H	6.597424	1.398561	0.454701
C	5.016861	1.773323	-0.926155
H	5.599100	2.478592	-1.534400
S	3.343110	1.519931	-1.414935
S	1.554071	-0.964743	1.894222
O	0.770055	0.124476	-0.562014
C	-0.430792	-0.150056	-0.002352
H	0.056230	-0.582235	1.159301
N	-1.257575	0.916566	0.302158
O	2.918027	-1.847691	-0.878473
C	-2.392199	-1.558570	-0.720676
C	-3.234328	-0.438549	-0.244694
C	-2.567104	0.763274	0.228571
N	-1.049893	-1.297615	-0.620160
H	-0.419150	-2.040923	-0.908852
O	-2.822590	-2.615351	-1.179884
C	-3.436013	1.849658	0.632551
C	-4.615259	-0.532256	-0.291634
C	-4.801622	1.744835	0.585501
C	-5.417943	0.545415	0.124046
H	-2.946722	2.761194	0.984953
H	-5.449405	2.565155	0.897164
H	-5.074824	-1.449010	-0.661615
N	-6.838509	0.449235	0.077775
O	-7.516873	1.425130	0.444470
O	-7.361777	-0.600993	-0.325502

6-Trifluoromethyl-4-Quinazolinone

30

Mo	2.933508	-0.373377	-0.090434
S	5.091568	-0.161175	1.111033
C	6.013167	1.022188	0.180451
H	7.067957	1.148549	0.461678
C	5.459453	1.788401	-0.782722
H	6.057458	2.544773	-1.309664
S	3.759121	1.687064	-1.233500
S	1.944570	-1.126035	1.797789
O	1.142149	0.357168	-0.443879
C	-0.062450	-0.023584	0.070508
H	0.429281	-0.570113	1.163635
N	-0.935995	0.971662	0.456101
O	3.111114	-1.699378	-1.128751
C	-1.949142	-1.422435	-0.849010
C	-2.844058	-0.391842	-0.286007
C	-2.241261	0.774551	0.323074
N	-0.622358	-1.127290	-0.680062
H	0.045283	-1.814151	-1.022638
O	-2.329342	-2.441118	-1.430432
C	-3.168756	1.774734	0.800275
C	-4.226279	-0.536486	-0.380130
C	-4.531058	1.612281	0.700426
C	-5.096021	0.446590	0.108316
H	-2.734733	2.671883	1.249536
H	-5.198513	2.395020	1.075751
H	-4.604321	-1.443239	-0.858633
C	-6.566511	0.267979	0.081573
F	-7.237885	1.418606	-0.212752
F	-6.982052	-0.654972	-0.816800
F	-7.100853	-0.132968	1.278541

6-Cloro-4-Quinazolinone

27

Mo	2.366986	-0.390097	-0.054577
S	4.566738	-0.168675	1.073990
C	5.472407	0.982401	0.088489
H	6.535035	1.108474	0.339463
C	4.899681	1.726440	-0.881195
H	5.490349	2.463993	-1.442412
S	3.188201	1.625734	-1.286715
S	1.419680	-1.078104	1.876849
O	0.587604	0.368537	-0.385248
C	-0.618386	0.003090	0.159929
H	-0.116539	-0.508880	1.249902
N	-1.486094	1.009626	0.513397
O	2.486985	-1.748866	-1.059268
C	-2.507969	-1.399554	-0.757118
C	-3.398912	-0.341413	-0.243361
C	-2.795847	0.824954	0.357344
N	-1.182737	-1.123466	-0.556952
H	-0.516946	-1.823681	-0.875673
O	-2.892395	-2.426032	-1.324592
C	-3.717480	1.841003	0.800702
C	-4.786656	-0.471611	-0.376469
C	-5.085677	1.701317	0.667735
C	-5.626521	0.537166	0.077820
H	-3.284410	2.736275	1.254940
H	-5.761759	2.487356	1.017500
H	-5.172956	-1.378363	-0.847585
Cl	-7.392129	0.382887	-0.079989

4-Quinazolinone

27

Mo	1.680278	-0.346459	0.062100
S	3.893510	-0.141995	1.175935
C	4.831149	0.930247	0.133209
H	5.899755	1.030179	0.371000
C	4.277848	1.648243	-0.867212
H	4.891142	2.337069	-1.465264
S	2.561400	1.589633	-1.260242
S	0.716713	-0.925760	2.018970
O	-0.073807	0.441680	-0.312627
C	-1.296198	0.105136	0.232477
H	-0.818821	-0.347241	1.345954
N	-2.166011	1.131161	0.512205
O	1.761968	-1.749218	-0.884448
C	-3.169344	-1.335119	-0.656509
C	-4.068193	-0.251068	-0.219387
C	-3.475296	0.943110	0.334460
N	-1.847080	-1.054734	-0.439128
H	-1.177239	-1.772417	-0.706579
O	-3.541263	-2.390095	-1.180849
C	-4.400752	1.983816	0.703971
C	-5.454732	-0.374571	-0.373338
C	-5.766122	1.834987	0.544492
C	-6.321904	0.649670	0.004054
H	-3.969195	2.898154	1.121307
H	-6.432484	2.654011	0.844633
H	-5.823404	-1.309745	-0.806941
H	-7.405151	0.545561	-0.116568

6-Methyl-4-Quinazolinone

30

Mo	2.001547	-0.390780	-0.046210
S	4.225418	-0.185764	1.042867
C	5.121932	0.958192	0.040499
H	6.190421	1.075115	0.270864
C	4.537672	1.707236	-0.918678
H	5.125185	2.439397	-1.490551
S	2.818350	1.622097	-1.292929
S	1.081075	-1.081584	1.896080
O	0.227953	0.384960	-0.349364
C	-0.979294	0.016492	0.206399
H	-0.469643	-0.496778	1.283890
N	-1.843445	1.021287	0.564782
O	2.094889	-1.747441	-1.057188
C	-2.869882	-1.372391	-0.729323
C	-3.760271	-0.313131	-0.217397
C	-3.156233	0.843476	0.398732
N	-1.544772	-1.107432	-0.513976
H	-0.880350	-1.807961	-0.834782
O	-3.252798	-2.394402	-1.308136
C	-4.079431	1.853016	0.842824
C	-5.146863	-0.425951	-0.361606
C	-5.446852	1.710184	0.689023
C	-6.026969	0.565960	0.083121
H	-3.649693	2.742737	1.311785
H	-6.108996	2.509654	1.048188
H	-5.516898	-1.335057	-0.848854
C	-7.523519	0.428517	-0.080241
H	-8.052765	1.307009	0.327820
H	-7.827085	0.331726	-1.140975
H	-7.927883	-0.462718	0.438284

6-Methoxy-4-Quinazolinone

31

Mo	2.319664	-0.382061	-0.048308
S	4.550897	-0.114277	1.012674
C	5.415630	1.028504	-0.018539
H	6.483201	1.172233	0.200936
C	4.808367	1.746172	-0.987381
H	5.376029	2.478939	-1.578255
S	3.088144	1.617545	-1.345366
S	1.429099	-1.042890	1.918224
O	0.531885	0.358822	-0.354757
C	-0.665052	-0.028094	0.216914
H	-0.139559	-0.494743	1.303783
N	-1.558362	0.960318	0.539787
O	2.423299	-1.759096	-1.030834
C	-2.510224	-1.501923	-0.683909
C	-3.433881	-0.449757	-0.213608
C	-2.866596	0.741351	0.369366
N	-1.196322	-1.192644	-0.468105
H	-0.509824	-1.883925	-0.761966
O	-2.864228	-2.551380	-1.230096
C	-3.818063	1.737151	0.772009
C	-4.814282	-0.609975	-0.369100
C	-5.186792	1.565552	0.615181
C	-5.703270	0.381787	0.040400
H	-3.416932	2.653026	1.214699
H	-5.857679	2.363159	0.945899
H	-5.183114	-1.531860	-0.825814
O	-7.060635	0.132280	-0.148668
C	-7.966243	1.133673	0.183269
H	-8.973591	0.760213	-0.066566
H	-7.951989	1.390692	1.264273
H	-7.795039	2.075055	-0.381341

6-Amino-4-Quinazolinone

29

Mo	2.005094	-0.412113	-0.065620
S	4.230741	-0.199088	1.021954
C	5.111707	0.973914	0.039831
H	6.178295	1.102339	0.273417
C	4.517970	1.730441	-0.907767
H	5.096170	2.480176	-1.466405
S	2.800207	1.628432	-1.284812
S	1.100774	-1.138764	1.870921
O	0.225221	0.352844	-0.353515
C	-0.980463	-0.011887	0.219858
H	-0.460269	-0.545037	1.275717
N	-1.827904	0.996155	0.602631
O	2.112922	-1.751757	-1.098608
C	-2.899514	-1.351864	-0.735648
C	-3.768580	-0.287607	-0.204916
C	-3.145790	0.841744	0.432290
N	-1.570130	-1.117238	-0.511945
H	-0.919201	-1.822913	-0.848110
O	-3.302729	-2.354476	-1.336887
C	-4.051492	1.859419	0.895327
C	-5.160235	-0.366024	-0.371503
C	-5.421414	1.750207	0.740874
C	-6.010892	0.634256	0.093039
H	-3.605882	2.728771	1.387161
H	-6.077693	2.539734	1.128824
H	-5.548485	-1.249271	-0.891655
N	-7.438269	0.548613	-0.023129
H	-7.815621	1.387471	-0.468638
H	-7.688403	-0.237007	-0.622744

B3LYP-D3 transition state coordinates for concerted reaction mechanism between 6-substituted 4-quinazolinones and deprotonated MoCo.

6-Nitro-4-Quinazolinone

29

Mo	2.508772	-0.308738	-0.028494
S	4.710903	-0.165125	1.098409
C	5.687735	0.848773	0.031382
H	6.760464	0.907337	0.262023
C	5.160022	1.572552	-0.978621
H	5.797704	2.223490	-1.592386
S	3.439098	1.576870	-1.365675
S	1.503439	-0.832098	1.927812
O	0.761221	0.507786	-0.421167
C	-0.443047	0.144522	0.083903
H	0.009954	-0.274863	1.252644
N	-1.353104	1.152274	0.343397
O	2.549204	-1.725691	-0.950898
C	-2.258024	-1.424875	-0.664525
C	-3.198379	-0.371388	-0.216047
C	-2.644197	0.890846	0.244473
N	-0.945661	-1.047975	-0.557747
H	-0.244902	-1.740922	-0.813770
O	-2.597326	-2.518453	-1.112842
C	-3.608058	1.907597	0.609935
C	-4.564456	-0.583683	-0.282684
C	-4.959131	1.685845	0.544022
C	-5.462959	0.429361	0.099122
H	-3.204312	2.864264	0.951028
H	-5.679047	2.454370	0.828070
H	-4.936435	-1.543210	-0.642588
N	-6.870047	0.210441	0.033369
O	-7.636002	1.130770	0.370916
O	-7.294388	-0.887878	-0.357334

6-Trifluoromethyl-4-Quinazolinone

30

Mo	2.880629	-0.285075	-0.073201
S	5.096441	-0.175097	1.043472
C	6.027083	0.976560	0.079228
H	7.097697	1.056912	0.314877
C	5.467660	1.772378	-0.857366
H	6.078481	2.504620	-1.404023
S	3.747039	1.746547	-1.243047
S	1.908325	-1.015268	1.829710
O	1.119955	0.533422	-0.377222
C	-0.084332	0.114883	0.110263
H	0.386530	-0.416464	1.210099
N	-0.996672	1.084036	0.471543
O	2.949808	-1.612706	-1.121374
C	-1.896469	-1.357891	-0.833244
C	-2.837626	-0.368246	-0.270068
C	-2.291264	0.828545	0.333626
N	-0.585512	-1.008271	-0.654228
H	0.117127	-1.663582	-0.990221
O	-2.232881	-2.387184	-1.422451
C	-3.264103	1.787806	0.804730
C	-4.210923	-0.580350	-0.359848
C	-4.617059	1.557321	0.711941
C	-5.123530	0.361094	0.129869
H	-2.872302	2.706842	1.248589
H	-5.323681	2.305879	1.085503
H	-4.548690	-1.505324	-0.833245
C	-6.583357	0.115243	0.114337
F	-7.304789	1.212324	-0.261172
F	-6.952708	-0.887635	-0.715664
F	-7.101775	-0.218275	1.339064

6-Cloro-4-Quinazolinone

27

Mo	2.341479	-0.324405	-0.081974
S	4.575913	-0.178446	1.000153
C	5.463910	1.011632	0.042680
H	6.535100	1.116982	0.266489
C	4.872181	1.806448	-0.875027
H	5.457507	2.562599	-1.417300
S	3.148009	1.742544	-1.239071
S	1.420975	-1.095584	1.829831
O	0.565533	0.464124	-0.349919
C	-0.631853	0.050720	0.179756
H	-0.128976	-0.493893	1.248327
N	-1.521460	1.023860	0.569814
O	2.426551	-1.635263	-1.151034
C	-2.483866	-1.370938	-0.777027
C	-3.399915	-0.358738	-0.215312
C	-2.826507	0.805145	0.419143
N	-1.166000	-1.061498	-0.582468
H	-0.480606	-1.730619	-0.925813
O	-2.846135	-2.386602	-1.377303
C	-3.774132	1.776194	0.906246
C	-4.783660	-0.528418	-0.338681
C	-5.138850	1.597421	0.783229
C	-5.649616	0.437139	0.159295
H	-3.364588	2.668581	1.387219
H	-5.836500	2.347848	1.167045
H	-5.147838	-1.429667	-0.837031
Cl	-7.411365	0.231066	0.015007

4-Quinazolinone

27

Mo	1.694780	-0.374575	-0.021689
S	3.941374	-0.271647	1.049088
C	4.868942	0.845333	0.041648
H	5.945301	0.916546	0.254779
C	4.303467	1.627397	-0.903536
H	4.916112	2.337754	-1.477129
S	2.576406	1.618826	-1.258529
S	0.745295	-1.050279	1.910981
O	-0.046778	0.466998	-0.326336
C	-1.266498	0.100368	0.202963
H	-0.792286	-0.417275	1.287863
N	-2.133778	1.108433	0.545996
O	1.731696	-1.724790	-1.043226
C	-3.138602	-1.289180	-0.760537
C	-4.036711	-0.235732	-0.251286
C	-3.443733	0.925565	0.369058
N	-1.816201	-1.019685	-0.534611
H	-1.143933	-1.716786	-0.846768
O	-3.513428	-2.309824	-1.347010
C	-4.370327	1.936482	0.810801
C	-5.423618	-0.356122	-0.402014
C	-5.736673	1.790677	0.654384
C	-6.292174	0.638694	0.045374
H	-3.939852	2.825115	1.281455
H	-6.404114	2.585479	1.011872
H	-5.790905	-1.264622	-0.890202
H	-7.375972	0.537260	-0.072693

6-Methyl-4-Quinazolinone

30

Mo	1.967401	-0.358685	-0.034633
S	4.223681	-0.221135	1.009616
C	5.122985	0.909928	-0.007759
H	6.200149	0.998518	0.194548
C	4.535182	1.682133	-0.947387
H	5.130304	2.401966	-1.527526
S	2.804763	1.645165	-1.284140
S	1.050358	-1.045746	1.910383
O	0.211440	0.460764	-0.316886
C	-0.996488	0.077365	0.226937
H	-0.500959	-0.432525	1.307537
N	-1.874729	1.072504	0.576952
O	2.008608	-1.709135	-1.055845
C	-2.856666	-1.341880	-0.717842
C	-3.765355	-0.295529	-0.210284
C	-3.183387	0.872345	0.405920
N	-1.537282	-1.054547	-0.500660
H	-0.857705	-1.744065	-0.814023
O	-3.223331	-2.370110	-1.296167
C	-4.125199	1.864261	0.851279
C	-5.149334	-0.432914	-0.357224
C	-5.489517	1.696971	0.695616
C	-6.046824	0.543094	0.086324
H	-3.712213	2.758250	1.327220
H	-6.166983	2.482219	1.057660
H	-5.503477	-1.348659	-0.843774
C	-7.537720	0.392073	-0.108335
H	-8.101902	1.112968	0.509400
H	-7.850484	0.559628	-1.159214
H	-7.890255	-0.620041	0.163226

6-Methoxy-4-Quinazolinone

31

Mo	2.275627	-0.342786	-0.007768
S	4.538799	-0.151678	1.013098
C	5.410136	0.981468	-0.026132
H	6.486907	1.092239	0.167199
C	4.801726	1.729137	-0.972440
H	5.379856	2.451365	-1.566674
S	3.069889	1.656223	-1.295500
S	1.385835	-1.023572	1.951012
O	0.507695	0.450116	-0.289816
C	-0.693306	0.031889	0.252810
H	-0.192008	-0.442382	1.341071
N	-1.610009	1.000273	0.570513
O	2.324947	-1.704446	-1.013909
C	-2.485358	-1.456327	-0.724082
C	-3.439471	-0.433868	-0.247061
C	-2.909618	0.756888	0.371197
N	-1.184146	-1.132793	-0.463094
H	-0.474798	-1.799729	-0.759995
O	-2.809046	-2.495166	-1.307898
C	-3.890327	1.720565	0.780984
C	-4.812573	-0.623222	-0.427271
C	-5.252439	1.519312	0.601418
C	-5.731434	0.336555	-0.007526
H	-3.518141	2.634444	1.252201
H	-5.946286	2.292547	0.941853
H	-5.153077	-1.542884	-0.909548
O	-7.078591	0.057225	-0.224917
C	-8.019008	0.997971	0.181629
H	-9.014776	0.598935	-0.075501
H	-7.994709	1.189453	1.276478
H	-7.897857	1.979370	-0.326325

6-Amino-4-Quinazolinone

29

Mo	1.981939	-0.369339	-0.021721
S	4.247981	-0.217130	1.002647
C	5.134237	0.913888	-0.026128
H	6.212423	1.008936	0.168062
C	4.536106	1.678551	-0.965565
H	5.124167	2.398346	-1.553111
S	2.803565	1.631724	-1.289934
S	1.084420	-1.051300	1.933260
O	0.224812	0.446964	-0.296971
C	-0.982857	0.062643	0.261049
H	-0.479831	-0.437715	1.334325
N	-1.861701	1.057126	0.604483
O	2.019130	-1.723866	-1.038492
C	-2.841086	-1.350482	-0.702833
C	-3.749292	-0.301529	-0.205498
C	-3.171335	0.859699	0.416848
N	-1.524212	-1.074860	-0.460003
H	-0.843867	-1.764332	-0.771804
O	-3.207893	-2.373376	-1.292959
C	-4.114368	1.857821	0.845330
C	-5.134473	-0.427173	-0.390912
C	-5.478028	1.702118	0.674034
C	-6.022684	0.555195	0.041419
H	-3.703480	2.750500	1.325483
H	-6.164884	2.477939	1.035870
H	-5.486388	-1.332429	-0.898957
N	-7.444966	0.423680	-0.092449
H	-7.841273	1.248214	-0.547812
H	-7.664721	-0.372849	-0.689474

B3LYP transition state coordinates for an initial proton transfer (TS1)and a subsequent concerted reaction with deprotonated MoCo for 6-substituted 4-quinazolinones.

6-Nitro-4-Quinazolinone (TS1)

30

Mo	2.161874	-0.023999	0.245984
S	2.928290	0.135158	-2.099798
C	4.024527	1.488189	-2.211012
H	4.500093	1.650955	-3.184571
C	4.237646	2.321242	-1.170352
H	4.894765	3.193738	-1.257415
S	3.439891	2.101675	0.364514
S	3.349693	-1.492762	1.278894
O	1.055610	0.749063	1.496869
H	0.172126	0.143667	1.599991
C	-0.347635	-1.789807	0.469234
H	0.387571	-2.432983	0.972267
N	-0.913363	-0.823875	1.253266
O	0.794912	-0.969798	-0.503929
C	-2.413984	-2.087597	-0.857830
C	-2.935226	-0.919832	-0.118501
C	-2.130764	-0.332883	0.907100
N	-1.163472	-2.495284	-0.416446
H	-0.738794	-3.247351	-0.951575
O	-3.003564	-2.684677	-1.743619
C	-2.662012	0.793645	1.602433
C	-4.201702	-0.416620	-0.417549
C	-3.913012	1.290616	1.300371
C	-4.686406	0.679614	0.290293
H	-2.048396	1.257373	2.377559
H	-4.325648	2.152289	1.825048
H	-4.795362	-0.884890	-1.202483
N	-6.011002	1.207052	-0.013815
O	-6.406928	2.174118	0.631317
O	-6.665746	0.659824	-0.894226

6-Nitro-4-Quinazolinone (TS2)

30

Mo	2.313474	0.359727	-0.070262
S	3.387831	0.131944	-2.258842
C	5.072861	0.556781	-1.950358
H	5.703721	0.699042	-2.835480
C	5.571611	0.682684	-0.706469
H	6.628833	0.917164	-0.535617
S	4.596110	0.390667	0.737671
S	1.603132	-0.852237	1.729072
O	1.653956	1.907514	0.147967
H	-0.482298	1.122467	0.257625
C	-0.351931	-0.839475	-0.333569
H	0.267791	-1.235788	0.947504
N	-1.077061	0.325699	0.015901
O	0.786187	-0.655928	-0.947817
C	-2.559702	-1.974159	-0.698168
C	-3.211070	-0.762334	-0.128800
C	-2.419608	0.370943	0.206641
N	-1.187327	-1.876370	-0.808452
H	-0.703007	-2.691785	-1.174638
O	-3.167310	-2.970641	-1.051591
C	-3.058620	1.529223	0.720623
C	-4.591885	-0.731853	0.044278
C	-4.431188	1.549858	0.888879
C	-5.197253	0.418867	0.551607
H	-2.454026	2.400732	0.982286
H	-4.939899	2.429517	1.283480
N	-6.643500	0.455991	0.732263
H	-5.184098	-1.606733	-0.223315
O	-7.140600	1.487914	1.174351
O	-7.287824	-0.542707	0.433614

6-Trifluoromethyl-4-Quinazolinone (TS1)

31

Mo	2.450616	-0.148680	0.215749
S	3.144278	0.142035	-2.151536
C	4.157191	1.562702	-2.224305
H	4.622568	1.780518	-3.192396
C	4.313382	2.386524	-1.165980
H	4.911914	3.302024	-1.237387
S	3.515793	2.098044	0.359531
S	3.830697	-1.535911	1.127561
O	1.360601	0.480132	1.537453
H	0.431007	-0.167844	1.621547
C	-0.018838	-2.015967	0.539283
H	0.762174	-2.623058	1.010893
N	-0.566171	-1.041102	1.304637
O	1.138416	-1.163266	-0.521690
C	-2.077555	-2.313890	-0.782039
C	-2.575209	-1.111208	-0.084323
C	-1.772980	-0.512197	0.925792
N	-0.834926	-2.733399	-0.324792
H	-0.410511	-3.489523	-0.854408
O	-2.675630	-2.924704	-1.652737
C	-2.269043	0.650644	1.566412
C	-3.822531	-0.575872	-0.419561
C	-3.502577	1.176957	1.218387
C	-4.295316	0.565716	0.225269
H	-1.651094	1.128739	2.329075
H	-3.867896	2.077082	1.716429
C	-5.634475	1.123697	-0.158590
H	-4.399953	-1.077789	-1.199315
F	-5.976749	2.197895	0.581456
F	-5.678016	1.510927	-1.451637
F	-6.625080	0.215509	-0.009538

6-Trifluoromethyl-4-Quinazolinone (TS2)

31

Mo	2.629290	0.373155	0.079125
S	3.820791	1.171901	-1.908101
C	5.479348	1.400653	-1.348659
H	6.152376	1.924057	-2.037877
C	5.910394	0.949253	-0.156046
H	6.952535	1.076641	0.159761
S	4.868481	0.041661	0.945150
S	1.876740	-1.533502	1.075758
O	1.913529	1.644828	0.946730
H	-0.143954	0.910408	0.607157
C	0.007140	-0.560781	-0.815950
H	0.575725	-1.512527	0.133169
N	-0.729613	0.317625	0.012991
O	1.161953	-0.125068	-1.248909
C	-2.182602	-1.434721	-1.662662
C	-2.838513	-0.674792	-0.564033
C	-2.066517	0.199026	0.243779
N	-0.817807	-1.246113	-1.741070
H	-0.324368	-1.783189	-2.449008
O	-2.780844	-2.159790	-2.441993
C	-2.713915	0.942351	1.258905
C	-4.212985	-0.796679	-0.352452
C	-4.078874	0.805947	1.455980
C	-4.843953	-0.065641	0.656093
H	-2.126278	1.619418	1.883255
H	-4.569326	1.384741	2.241792
C	-6.306936	-0.243203	0.932888
H	-4.769306	-1.472697	-1.004399
F	-6.872458	0.888015	1.407969
F	-6.997871	-0.603385	-0.165634
F	-6.543425	-1.198424	1.862113

6-Cloro-4-Quinazolinone (TS1)

28

Mo	1.939895	-0.130730	0.158022
S	2.837057	-0.022911	-2.177071
C	4.003379	1.274700	-2.230764
H	4.547333	1.404588	-3.174036
C	4.192283	2.117095	-1.191445
H	4.896231	2.955219	-1.259006
S	3.284501	1.982060	0.293096
S	3.060677	-1.650225	1.235874
O	0.877368	0.673497	1.375132
H	-0.203096	0.004452	1.496639
C	-0.679576	-1.817398	0.601634
H	0.158019	-2.363577	1.043855
N	-1.131700	-0.729751	1.240575
O	0.617801	-1.034219	-0.655875
C	-2.779812	-2.121754	-0.635067
C	-3.192235	-0.828129	-0.054981
C	-2.325476	-0.161393	0.843301
N	-1.528942	-2.547196	-0.187003
H	-1.158967	-3.377395	-0.641508
O	-3.435256	-2.793769	-1.411396
C	-2.714039	1.098444	1.351294
C	-4.427304	-0.264663	-0.413640
C	-3.931659	1.655253	0.988222
C	-4.790986	0.966841	0.111180
H	-2.032662	1.628740	2.019763
H	-4.230494	2.631285	1.375656
H	-5.068938	-0.808598	-1.108248
Cl	-6.331645	1.688897	-0.323810

6-Cloro-4-Quinazolinone (TS2)

28

Mo	2.177593	0.024684	0.316339
S	3.419598	1.347947	-1.336305
C	5.106863	1.153328	-0.856944
H	5.829049	1.809749	-1.356743
C	5.501190	0.241827	0.051967
H	6.558978	0.117129	0.312472
S	4.372461	-0.876788	0.824674
S	1.191967	-2.010287	0.634731
O	1.693231	0.976275	1.631505
H	-0.679735	0.645091	1.073586
C	-0.557683	-0.260243	-0.760375
H	-0.094354	-1.524417	-0.176974
N	-1.268960	0.356830	0.292321
O	0.642864	0.194695	-1.007110
C	-2.759482	-0.586856	-1.919476
C	-3.419327	-0.138122	-0.663518
C	-2.631331	0.330681	0.415931
N	-1.382202	-0.539832	-1.878113
H	-0.891900	-0.869995	-2.705029
O	-3.365505	-0.957757	-2.912944
C	-3.284541	0.778145	1.586321
C	-4.815349	-0.157321	-0.571160
C	-4.672166	0.756134	1.669252
C	-5.438405	0.286778	0.590752
H	-2.690138	1.141109	2.428509
H	-5.172929	1.101055	2.576357
Cl	-7.191244	0.266248	0.717483
H	-5.383975	-0.522225	-1.427959

4-Quinazolinone (TS1)

28

Mo	1.402359	-0.091929	0.165501
S	2.456544	-0.617980	-2.052411
C	3.808295	0.466811	-2.259735
H	4.427846	0.312944	-3.151547
C	4.056112	1.482981	-1.403727
H	4.884570	2.180594	-1.576560
S	3.043111	1.804760	-0.019486
S	2.216596	-1.493959	1.623838
O	0.432921	1.089671	1.107686
H	-0.799581	0.585236	1.310601
C	-1.460806	-1.294630	0.805591
H	-0.682022	-1.814555	1.369641
N	-1.766692	-0.039733	1.146093
O	0.016495	-0.958856	-0.564805
C	-3.558261	-1.597365	-0.431578
C	-3.802669	-0.165154	-0.179109
C	-2.867397	0.578017	0.579267
N	-2.376007	-2.065060	0.152656
H	-2.115434	-3.018767	-0.082495
O	-4.281926	-2.345266	-1.064176
C	-3.077327	1.960229	0.768771
C	-4.940379	0.465122	-0.710739
C	-4.203646	2.567020	0.228300
C	-5.146847	1.823876	-0.507802
H	-2.332868	2.531961	1.326635
H	-4.354159	3.640557	0.374173
H	-5.636986	-0.144845	-1.290279
H	-6.028149	2.317131	-0.925666

4-Quinazolinone (TS2)

28

Mo	1.600568	-0.007529	0.171977
S	2.789345	1.309441	-1.525778
C	4.493938	1.067806	-1.136931
H	5.205493	1.713844	-1.664968
C	4.912525	0.135111	-0.260843
H	5.979218	-0.017528	-0.057254
S	3.798289	-0.966661	0.555658
S	0.584624	-2.020609	0.507599
O	1.201619	0.932396	1.524341
H	-1.153196	0.673881	1.120553
C	-1.194844	-0.194482	-0.734169
H	-0.740743	-1.473231	-0.220769
N	-1.807087	0.422481	0.378579
O	0.001542	0.232337	-1.057608
C	-3.484270	-0.421231	-1.734637
C	-4.036524	0.008811	-0.423719
C	-3.157283	0.427523	0.605680
N	-2.105573	-0.416948	-1.795700
H	-1.688377	-0.740407	-2.664074
O	-4.168888	-0.746696	-2.693356
C	-3.702761	0.861024	1.834819
C	-5.420962	0.027904	-0.216174
C	-5.081789	0.871693	2.017986
C	-5.954277	0.454796	0.998258
H	-3.029912	1.183084	2.633806
H	-5.487218	1.208485	2.976854
H	-7.035401	0.466822	1.156937
H	-6.056298	-0.300590	-1.042141

6-Methyl-4-Quinazolinone (TS1)

31

Mo	1.689662	-0.163487	0.182695
S	2.565334	0.032572	-2.163612
C	3.738451	1.325453	-2.175434
H	4.278191	1.488483	-3.116277
C	3.936372	2.130219	-1.108015
H	4.643264	2.967739	-1.152003
S	3.034736	1.950571	0.376546
S	2.828704	-1.728972	1.174249
O	0.664288	0.597549	1.450323
H	-0.506493	0.011285	1.514359
C	-1.080194	-1.717108	0.542535
H	-0.298908	-2.342087	0.980080
N	-1.455927	-0.616843	1.201466
O	0.350771	-1.011302	-0.657465
C	-3.150076	-1.787495	-0.776975
C	-3.475844	-0.489086	-0.156856
C	-2.587901	0.068250	0.793041
N	-1.957885	-2.339659	-0.301226
H	-1.637797	-3.173324	-0.786189
O	-3.824812	-2.372013	-1.606398
C	-2.890511	1.330688	1.339662
C	-4.643414	0.196107	-0.523884
C	-4.049894	1.993009	0.955891
C	-4.955029	1.441413	0.022808
H	-2.192942	1.777245	2.051368
H	-4.265093	2.975485	1.387895
C	-6.208411	2.179590	-0.386464
H	-5.294226	-0.279405	-1.262880
H	-6.337174	3.107510	0.191952
H	-6.183168	2.455207	-1.455097
H	-7.110112	1.561873	-0.235982

6-Methyl-4-Quinazolinone (TS2)

31

Mo	1.845042	0.344185	0.034033
S	3.067614	0.374730	-2.101877
C	4.762411	0.476348	-1.625241
H	5.479032	0.668658	-2.435003
C	5.172010	0.310530	-0.352491
H	6.236825	0.347766	-0.085790
S	4.057860	-0.069561	0.963252
S	0.874075	-1.088396	1.534829
O	1.361424	1.918604	0.511567
H	-0.975380	1.321343	0.328239
C	-0.917943	-0.506072	-0.599818
H	-0.454031	-1.172619	0.588905
N	-1.591555	0.632991	-0.107122
O	0.269800	-0.315165	-1.113888
C	-3.165760	-1.425395	-1.240790
C	-3.775908	-0.316454	-0.461467
C	-2.948138	0.692338	0.088635
N	-1.786512	-1.381769	-1.299656
H	-1.328118	-2.145614	-1.790065
O	-3.804668	-2.306332	-1.797125
C	-3.555923	1.745160	0.802633
C	-5.163448	-0.256465	-0.295875
C	-4.940267	1.779072	0.952417
C	-5.777553	0.783775	0.411058
H	-2.930269	2.530660	1.237442
H	-5.388025	2.607471	1.513820
C	-7.279483	0.830686	0.584950
H	-5.752940	-1.060579	-0.747795
H	-7.592781	1.733712	1.138342
H	-7.804322	0.838026	-0.389438
H	-7.654905	-0.048150	1.144065

6-Methoxy-4-Quinazolinone (TS1)

32

Mo	1.929954	-0.071922	0.148673
S	2.853430	0.118043	-2.180134
C	3.958668	1.469537	-2.196262
H	4.511150	1.639175	-3.128580
C	4.092012	2.306171	-1.143178
H	4.757475	3.176909	-1.191951
S	3.167898	2.113317	0.325459
S	3.114649	-1.565188	1.206557
O	0.849688	0.668404	1.378611
H	-0.274638	-0.049681	1.483039
C	-0.673290	-1.855815	0.592685
H	0.198537	-2.358721	1.017353
N	-1.147285	-0.771585	1.206333
O	0.659765	-1.010375	-0.692378
C	-2.754700	-2.211257	-0.660486
C	-3.194916	-0.913224	-0.108967
C	-2.347242	-0.217808	0.785499
N	-1.495452	-2.604829	-0.199466
H	-1.105494	-3.432378	-0.641800
O	-3.389176	-2.911300	-1.428672
C	-2.752633	1.043888	1.254630
C	-4.424686	-0.368838	-0.495826
C	-3.971861	1.586668	0.859432
C	-4.823652	0.879274	-0.015357
H	-2.085021	1.598476	1.917354
H	-4.252163	2.571985	1.233467
O	-6.035915	1.339201	-0.442082
H	-5.060329	-0.922780	-1.188324
C	-6.461717	2.618688	-0.045533
H	-7.437739	2.787761	-0.522796
H	-6.587022	2.696781	1.051428
H	-5.763809	3.411276	-0.375322

6-Methoxy-4-Quinazolinone (TS2)

32

Mo	2.181252	0.348554	-0.031115
S	3.512281	-1.206187	-1.389528
C	5.181447	-0.720641	-1.084828
H	5.941890	-1.174210	-1.731634
C	5.518650	0.138864	-0.104874
H	6.565910	0.402137	0.086557
S	4.327381	0.835102	0.998246
S	1.113135	0.542947	1.976170
O	1.724710	1.705780	-0.934313
H	-0.715596	1.077465	-0.688213
C	-0.541354	-0.799468	0.101170
H	-0.141353	-0.279238	1.395413
N	-1.278089	0.252552	-0.482957
O	0.678132	-0.985831	-0.337647
C	-2.705287	-2.036123	0.375445
C	-3.401088	-0.761390	0.045063
C	-2.646078	0.361547	-0.375857
N	-1.331401	-1.961945	0.295949
H	-0.814861	-2.794181	0.567068
O	-3.281406	-3.068159	0.685127
C	-3.334608	1.544773	-0.696892
C	-4.791459	-0.690364	0.134051
C	-4.726686	1.608983	-0.604535
C	-5.469257	0.490280	-0.186551
H	-2.770855	2.423847	-1.019805
H	-5.222882	2.546765	-0.858725
O	-6.832767	0.465311	-0.067533
H	-5.343471	-1.574562	0.457494
C	-7.561905	1.627442	-0.360426
H	-8.621883	1.388453	-0.190195
H	-7.281632	2.474848	0.294806
H	-7.437489	1.946994	-1.413499

6-Amino-4-Quinazolinone (TS1)

30

Mo	1.679825	-0.121686	0.140055
S	2.713996	-0.203631	-2.154266
C	3.993719	0.983375	-2.192351
H	4.598473	1.022975	-3.106825
C	4.204108	1.854124	-1.179932
H	4.986452	2.620366	-1.245834
S	3.210236	1.876570	0.254734
S	2.607158	-1.691422	1.345099
O	0.670481	0.830832	1.267132
H	-0.562529	0.176142	1.433608
C	-1.095371	-1.612788	0.620057
H	-0.261040	-2.166596	1.057551
N	-1.463229	-0.458905	1.176466
O	0.340922	-0.949247	-0.708541
C	-3.205397	-1.818863	-0.617753
C	-3.524504	-0.467385	-0.118451
C	-2.615350	0.182373	0.742979
N	-1.987152	-2.311106	-0.137994
H	-1.678772	-3.190051	-0.544145
O	-3.901747	-2.486842	-1.361709
C	-2.905836	1.494887	1.164047
C	-4.704274	0.171099	-0.529450
C	-4.071776	2.118784	0.747827
C	-4.998562	1.470131	-0.105952
H	-2.188695	2.015184	1.802528
H	-4.280348	3.140428	1.080832
N	-6.189338	2.106333	-0.468721
H	-5.371661	-0.375329	-1.200672
H	-6.143137	3.120339	-0.481659
H	-6.620788	1.745506	-1.313580

6-Amino-4-Quinazolinone (TS2)

30

Mo	1.866534	0.344856	-0.082866
S	3.061178	-0.175253	-2.165672
C	4.763999	0.028088	-1.748743
H	5.471658	0.010708	-2.586300
C	5.186381	0.174652	-0.478662
H	6.252747	0.267711	-0.239731
S	4.080370	0.138295	0.898536
S	0.906708	-0.636464	1.736519
O	1.419194	1.978025	-0.021945
H	-0.962531	1.378432	0.002435
C	-0.894948	-0.614629	-0.447805
H	-0.416649	-0.957863	0.864418
N	-1.574081	0.605986	-0.260446
O	0.293312	-0.554866	-1.002201
C	-3.133083	-1.688682	-0.810178
C	-3.747733	-0.435460	-0.297001
C	-2.929748	0.686212	-0.033526
N	-1.758939	-1.642457	-0.907752
H	-1.294947	-2.496301	-1.205062
O	-3.770508	-2.682658	-1.129076
C	-3.547528	1.865192	0.429663
C	-5.132758	-0.370542	-0.107950
C	-4.925060	1.914219	0.617383
C	-5.749433	0.798947	0.351677
H	-2.934064	2.744243	0.643914
H	-5.379101	2.838765	0.988375
N	-7.131015	0.851616	0.599909
H	-5.711510	-1.269806	-0.335333
H	-7.539777	1.774817	0.488986
H	-7.667808	0.158895	0.086832

B3LYP-D3 transition state coordinates for an initial proton transfer (TS1)and a subsequent concerted reaction with deprotonated MoCo for 6-substituted 4-quinazolinones.

6-Nitro-4-Quinazolinone (TS1)

30

Mo	2.120486	-0.002835	0.246495
S	2.871916	0.146484	-2.104527
C	3.978272	1.492257	-2.224961
H	4.443307	1.655599	-3.203712
C	4.216452	2.318071	-1.183109
H	4.883578	3.182428	-1.276988
S	3.446160	2.094847	0.366407
S	3.271409	-1.489160	1.291526
O	1.013596	0.785555	1.489278
H	0.164986	0.147359	1.625607
C	-0.337897	-1.802703	0.478523
H	0.409018	-2.442776	0.970345
N	-0.913526	-0.859034	1.287094
O	0.751760	-0.952746	-0.499884
C	-2.396727	-2.092610	-0.856761
C	-2.917126	-0.927591	-0.112459
C	-2.122485	-0.358289	0.930823
N	-1.154710	-2.513870	-0.405140
H	-0.720549	-3.249198	-0.955269
O	-2.981702	-2.674924	-1.755613
C	-2.652116	0.767827	1.627898
C	-4.173149	-0.409549	-0.426151
C	-3.892963	1.280320	1.311221
C	-4.657815	0.685500	0.284193
H	-2.042345	1.220206	2.412751
H	-4.303457	2.142960	1.835942
H	-4.758128	-0.865633	-1.224671
N	-5.972627	1.228388	-0.036118
O	-6.371172	2.192976	0.611858
O	-6.618468	0.696003	-0.932574

6-Nitro-4-Quinazolinone (TS2)

30

Mo	2.307592	0.354675	-0.066725
S	3.388641	0.108936	-2.250702
C	5.071791	0.544955	-1.939417
H	5.706852	0.681637	-2.822745
C	5.566258	0.686757	-0.694696
H	6.622277	0.929016	-0.525755
S	4.588842	0.406383	0.752552
S	1.572379	-0.837370	1.735729
O	1.646093	1.903657	0.129612
H	-0.479927	1.128588	0.230062
C	-0.353837	-0.837630	-0.348328
H	0.241739	-1.228808	0.939768
N	-1.076111	0.334121	-0.013595
O	0.789791	-0.664412	-0.955540
C	-2.558967	-1.975189	-0.699603
C	-3.206693	-0.761246	-0.130114
C	-2.415860	0.376606	0.190574
N	-1.188655	-1.873502	-0.825764
H	-0.701710	-2.690340	-1.184274
O	-3.168988	-2.974492	-1.040712
C	-3.052956	1.536117	0.703216
C	-4.585388	-0.734496	0.055686
C	-4.423964	1.553510	0.884111
C	-5.189713	0.417639	0.561206
H	-2.447693	2.410533	0.953262
H	-4.931144	2.434443	1.277768
N	-6.635394	0.450276	0.754355
H	-5.176172	-1.613554	-0.201233
O	-7.133196	1.482137	1.196147
O	-7.278586	-0.552226	0.465534

6-Trifluoromethyl-4-Quinazolinone (TS1)

31

Mo	2.380161	-0.138772	0.166978
S	3.130128	0.235896	-2.190647
C	4.135263	1.665259	-2.193491
H	4.618362	1.922376	-3.143857
C	4.272378	2.452856	-1.103602
H	4.871147	3.371083	-1.138959
S	3.451741	2.114640	0.400947
S	3.740946	-1.576331	1.053915
O	1.311145	0.448119	1.501984
H	0.324371	-0.320631	1.612209
C	-0.056936	-2.102283	0.578809
H	0.813638	-2.633686	0.973707
N	-0.568917	-1.105519	1.317415
O	1.114704	-1.129729	-0.642214
C	-2.126539	-2.401832	-0.701366
C	-2.594086	-1.170311	-0.033201
C	-1.768163	-0.545535	0.934558
N	-0.868755	-2.817436	-0.263316
H	-0.449100	-3.575620	-0.793801
O	-2.744615	-3.030464	-1.541238
C	-2.195095	0.669329	1.513831
C	-3.826879	-0.608888	-0.382077
C	-3.415653	1.220061	1.153445
C	-4.244665	0.580134	0.210976
H	-1.536181	1.168902	2.226494
H	-3.739035	2.163362	1.596907
C	-5.574034	1.161692	-0.180481
H	-4.430871	-1.121300	-1.134137
F	-5.826634	2.331363	0.440538
F	-5.655097	1.391359	-1.507350
F	-6.596450	0.329544	0.119601

6-Trifluoromethyl-4-Quinazolinone (TS2)

31

Mo	2.628210	0.391128	0.090349
S	3.821300	1.157277	-1.909102
C	5.487642	1.364243	-1.360568
H	6.166696	1.869471	-2.057784
C	5.918458	0.918093	-0.165056
H	6.964996	1.033487	0.141580
S	4.869117	0.038590	0.954352
S	1.841165	-1.496642	1.099141
O	1.934056	1.679749	0.947859
H	-0.160605	0.943614	0.608699
C	0.003416	-0.522585	-0.816741
H	0.548449	-1.473264	0.143078
N	-0.741116	0.364202	-0.001448
O	1.163265	-0.093569	-1.240826
C	-2.171833	-1.420313	-1.663914
C	-2.834124	-0.666635	-0.564478
C	-2.073044	0.217762	0.242116
N	-0.812015	-1.205580	-1.752004
H	-0.308387	-1.745829	-2.449869
O	-2.763192	-2.158616	-2.436033
C	-2.726622	0.946292	1.264004
C	-4.206485	-0.805832	-0.352354
C	-4.089805	0.792444	1.462158
C	-4.843952	-0.083063	0.656705
H	-2.144979	1.627426	1.889622
H	-4.589199	1.361027	2.249980
C	-6.306117	-0.271690	0.927977
H	-4.757365	-1.486816	-1.003495
F	-6.892657	0.870770	1.350665
F	-6.980386	-0.688880	-0.161138
F	-6.535038	-1.189842	1.896039

6-Cloro-4-Quinazolinone (TS1)

28

Mo	1.896359	-0.120210	0.144797
S	2.797300	0.014563	-2.195182
C	3.960663	1.317170	-2.231335
H	4.505615	1.462158	-3.172267
C	4.150148	2.147285	-1.181053
H	4.854522	2.986008	-1.242187
S	3.246012	1.995193	0.305797
S	3.015997	-1.660295	1.199882
O	0.849057	0.667275	1.381420
H	-0.232526	-0.058134	1.533917
C	-0.696084	-1.868133	0.642123
H	0.171571	-2.394479	1.050064
N	-1.138860	-0.782254	1.282775
O	0.583768	-1.016394	-0.679084
C	-2.786249	-2.147815	-0.607641
C	-3.181999	-0.845051	-0.036863
C	-2.314552	-0.188225	0.865724
N	-1.542261	-2.590131	-0.149116
H	-1.169780	-3.412765	-0.615089
O	-3.443199	-2.810536	-1.389347
C	-2.667691	1.090674	1.346437
C	-4.395202	-0.254056	-0.422753
C	-3.863834	1.675185	0.956430
C	-4.731067	0.994936	0.079792
H	-1.973558	1.613326	2.007699
H	-4.139691	2.667241	1.319065
H	-5.040727	-0.787907	-1.121430
Cl	-6.244395	1.751837	-0.388695

6-Cloro-4-Quinazolinone (TS2)

28

Mo	2.172111	0.032090	0.313888
S	3.428080	1.321209	-1.354871
C	5.112866	1.125211	-0.860931
H	5.842835	1.769479	-1.365756
C	5.498187	0.226040	0.065155
H	6.554958	0.103126	0.331668
S	4.361225	-0.876852	0.851819
S	1.161319	-1.986980	0.646140
O	1.687189	1.002214	1.614418
H	-0.678436	0.677381	1.061402
C	-0.558560	-0.234388	-0.767788
H	-0.118103	-1.494955	-0.180246
N	-1.268848	0.393358	0.279687
O	0.643693	0.216984	-1.013437
C	-2.755788	-0.581547	-1.922240
C	-3.414673	-0.138645	-0.663188
C	-2.629114	0.345581	0.411295
N	-1.379446	-0.517633	-1.886855
H	-0.884832	-0.849351	-2.710137
O	-3.363037	-0.961938	-2.911365
C	-3.282453	0.786158	1.583767
C	-4.809285	-0.178429	-0.564535
C	-4.669121	0.743566	1.673436
C	-5.433272	0.259759	0.599351
H	-2.688156	1.159913	2.421271
H	-5.172144	1.082957	2.581308
Cl	-7.185319	0.213469	0.733382
H	-5.377307	-0.553913	-1.417091

4-Quinazolinone (TS1)

28

Mo	1.354103	-0.077578	0.163173
S	2.380752	-0.574484	-2.076266
C	3.733146	0.512465	-2.282162
H	4.343542	0.371407	-3.182696
C	3.993886	1.516276	-1.414281
H	4.823370	2.212628	-1.589068
S	2.998557	1.823346	-0.012281
S	2.187843	-1.488934	1.600970
O	0.392182	1.092385	1.127540
H	-0.820144	0.546024	1.372789
C	-1.475574	-1.331434	0.862715
H	-0.685416	-1.851169	1.412129
N	-1.782003	-0.081317	1.216181
O	-0.032341	-0.950278	-0.554002
C	-3.549034	-1.614482	-0.411788
C	-3.778110	-0.178163	-0.169324
C	-2.854395	0.552728	0.613168
N	-2.387316	-2.097892	0.202853
H	-2.119416	-3.045574	-0.047324
O	-4.266141	-2.352258	-1.062873
C	-3.034595	1.941076	0.779470
C	-4.882749	0.470498	-0.745884
C	-4.127756	2.566902	0.193994
C	-5.063935	1.835984	-0.563825
H	-2.289101	2.500814	1.347938
H	-4.255773	3.645959	0.318467
H	-5.571294	-0.130692	-1.343940
H	-5.918604	2.344577	-1.017036

4-Quinazolinone (TS2)

28

Mo	1.526270	0.099437	0.235047
S	2.759322	1.238517	-1.555535
C	4.455005	1.056296	-1.095742
H	5.179624	1.639378	-1.677119
C	4.853852	0.236425	-0.104159
H	5.916187	0.117677	0.141781
S	3.724047	-0.771646	0.809834
S	0.506838	-1.874296	0.748132
O	1.056837	1.180424	1.453153
H	-1.225194	0.834432	1.004275
C	-1.217395	-0.210457	-0.756375
H	-0.791341	-1.426897	-0.101950
N	-1.859850	0.511515	0.273177
O	-0.013124	0.184760	-1.088440
C	-3.475581	-0.588173	-1.770226
C	-4.059206	-0.067829	-0.505864
C	-3.210658	0.477191	0.489421
N	-2.097237	-0.537821	-1.816608
H	-1.652310	-0.931762	-2.640636
O	-4.136564	-1.019914	-2.703232
C	-3.786092	0.991154	1.672322
C	-5.445328	-0.090052	-0.311477
C	-5.166261	0.957933	1.844034
C	-6.009137	0.417366	0.857508
H	-3.134340	1.408031	2.444501
H	-5.595936	1.357371	2.767594
H	-7.091391	0.396658	1.006755
H	-6.056401	-0.516237	-1.110701

6-Methyl-4-Quinazolinone (TS1)

31

Mo	1.584888	-0.193687	0.280317
S	2.630821	0.005792	-1.996412
C	3.900116	1.201413	-1.884843
H	4.512582	1.351757	-2.782730
C	4.093524	1.951658	-0.776456
H	4.869080	2.727416	-0.748288
S	3.088781	1.798678	0.644828
S	2.533670	-1.868447	1.301492
O	0.541777	0.610652	1.504896
H	-0.634776	-0.029842	1.559551
C	-1.208254	-1.726479	0.547126
H	-0.414248	-2.351942	0.963823
N	-1.570785	-0.629258	1.210989
O	0.264244	-0.936221	-0.665516
C	-3.228613	-1.711960	-0.840767
C	-3.514871	-0.399522	-0.234265
C	-2.645460	0.113845	0.751848
N	-2.070290	-2.312170	-0.329591
H	-1.759898	-3.149497	-0.814384
O	-3.897438	-2.267825	-1.693126
C	-2.886049	1.402620	1.270378
C	-4.621523	0.352814	-0.663889
C	-3.978329	2.130208	0.823138
C	-4.874725	1.619913	-0.145839
H	-2.184074	1.814046	1.998712
H	-4.147229	3.134247	1.225940
H	-5.264241	-0.087726	-1.430467
C	-6.049873	2.448881	-0.604543
H	-6.711482	2.711390	0.239383
H	-5.715346	3.398466	-1.057328
H	-6.653909	1.913808	-1.352869

6-Methyl-4-Quinazolinone (TS2)

31

Mo	1.824478	0.345856	0.027584
S	3.063027	0.316476	-2.092707
C	4.756551	0.428749	-1.603214
H	5.481953	0.601458	-2.407539
C	5.152871	0.293689	-0.322816
H	6.214106	0.338119	-0.049166
S	4.021974	-0.052311	0.991704
S	0.820773	-1.029358	1.544123
O	1.357811	1.917758	0.452365
H	-0.971199	1.348106	0.286580
C	-0.920348	-0.485766	-0.619837
H	-0.481448	-1.134854	0.593488
N	-1.589198	0.667881	-0.155980
O	0.279816	-0.314038	-1.117118
C	-3.158477	-1.413186	-1.255508
C	-3.767545	-0.304476	-0.473845
C	-2.942263	0.716113	0.058556
N	-1.781998	-1.360866	-1.326392
H	-1.318798	-2.128008	-1.804935
O	-3.799433	-2.299552	-1.801360
C	-3.550466	1.766582	0.774652
C	-5.152369	-0.258050	-0.289632
C	-4.932415	1.786840	0.944074
C	-5.765844	0.779482	0.420406
H	-2.926711	2.559657	1.195102
H	-5.380840	2.612384	1.506383
C	-7.263061	0.802540	0.621467
H	-5.738684	-1.070051	-0.729015
H	-7.593850	1.736725	1.102251
H	-7.801388	0.710605	-0.337339
H	-7.598864	-0.035017	1.258414

6-Methoxy-4-Quinazolinone (TS1)

32

Mo	1.868007	-0.025370	0.130904
S	2.807531	0.152206	-2.196895
C	3.939950	1.483048	-2.200162
H	4.502034	1.646952	-3.128131
C	4.085770	2.313553	-1.142818
H	4.771280	3.169190	-1.187748
S	3.152237	2.136852	0.323495
S	3.020536	-1.539565	1.198101
O	0.795036	0.724003	1.355560
H	-0.311259	-0.078498	1.512481
C	-0.670029	-1.875412	0.612217
H	0.226052	-2.358471	1.011616
N	-1.153494	-0.804973	1.243107
O	0.601195	-0.959277	-0.718757
C	-2.744303	-2.228448	-0.647194
C	-3.187265	-0.933611	-0.090722
C	-2.347583	-0.244093	0.814031
N	-1.487013	-2.626253	-0.180000
H	-1.085056	-3.437523	-0.641097
O	-3.372366	-2.920711	-1.426894
C	-2.741738	1.023528	1.273179
C	-4.406899	-0.379655	-0.493708
C	-3.951107	1.576408	0.861965
C	-4.799997	0.872693	-0.019574
H	-2.069987	1.575118	1.934180
H	-4.223717	2.567305	1.226118
O	-6.002398	1.340707	-0.463405
H	-5.037764	-0.927043	-1.195497
C	-6.429862	2.619385	-0.063505
H	-7.404081	2.790737	-0.543865
H	-6.558988	2.693395	1.033767
H	-5.730237	3.413673	-0.387341

6-Methoxy-4-Quinazolinone (TS2)

32

Mo	2.164996	0.342863	-0.019731
S	3.492182	-1.210685	-1.384641
C	5.161825	-0.708581	-1.102129
H	5.919896	-1.161395	-1.752661
C	5.504382	0.163363	-0.134035
H	6.552772	0.434933	0.040066
S	4.322411	0.864141	0.978517
S	1.102074	0.536323	1.987118
O	1.682045	1.687324	-0.927628
H	-0.699496	1.065346	-0.661961
C	-0.540823	-0.814803	0.122993
H	-0.154272	-0.307144	1.406732
N	-1.268808	0.244403	-0.459557
O	0.678386	-1.007633	-0.319037
C	-2.709483	-2.043124	0.383281
C	-3.396778	-0.763284	0.055137
C	-2.635415	0.358139	-0.358417
N	-1.335386	-1.975072	0.310251
H	-0.821038	-2.808776	0.579595
O	-3.292984	-3.072927	0.686784
C	-3.317248	1.545708	-0.677191
C	-4.787057	-0.687674	0.136381
C	-4.709570	1.614722	-0.592781
C	-5.458530	0.496175	-0.184262
H	-2.746910	2.423174	-0.992511
H	-5.200234	2.555578	-0.845440
O	-6.822715	0.473117	-0.073378
H	-5.344992	-1.570610	0.452731
C	-7.549126	1.631704	-0.388550
H	-8.611810	1.392401	-0.235560
H	-7.282437	2.485756	0.264715
H	-7.405926	1.943681	-1.442068

6-Amino-4-Quinazolinone (TS1)

30

Mo	1.617043	-0.140330	0.155732
S	2.538200	-0.077942	-2.188386
C	3.822660	1.106932	-2.209490
H	4.389032	1.200561	-3.144668
C	4.081793	1.915408	-1.156653
H	4.865746	2.681077	-1.213343
S	3.151908	1.857057	0.321343
S	2.613111	-1.754620	1.235136
O	0.638326	0.736747	1.369590
H	-0.582348	0.065644	1.536391
C	-1.125630	-1.685448	0.660066
H	-0.292927	-2.258251	1.077032
N	-1.488894	-0.552929	1.261036
O	0.259827	-0.947618	-0.682581
C	-3.202207	-1.809287	-0.635841
C	-3.496681	-0.461451	-0.112378
C	-2.602747	0.136225	0.800134
N	-2.014586	-2.349885	-0.130489
H	-1.703149	-3.210109	-0.572352
O	-3.891814	-2.434699	-1.421652
C	-2.856566	1.451796	1.232192
C	-4.630870	0.230034	-0.562035
C	-3.977674	2.129290	0.777864
C	-4.891163	1.532636	-0.127149
H	-2.142008	1.932318	1.903832
H	-4.158200	3.154169	1.117100
N	-6.037562	2.223710	-0.531754
H	-5.286708	-0.276696	-1.274558
H	-5.943757	3.234616	-0.540458
H	-6.449827	1.885868	-1.395613

6-Amino-4-Quinazolinone (TS2)

30

Mo	1.850993	0.338542	-0.082472
S	3.054077	-0.220691	-2.150647
C	4.754294	0.016146	-1.735228
H	5.465316	-0.012626	-2.569945
C	5.173081	0.201957	-0.468310
H	6.238480	0.316705	-0.233561
S	4.066846	0.187605	0.911584
S	0.872640	-0.596062	1.751783
O	1.387557	1.967620	-0.068607
H	-0.951734	1.373321	-0.059190
C	-0.897216	-0.630958	-0.454568
H	-0.444999	-0.942327	0.872544
N	-1.568213	0.600110	-0.308377
O	0.296467	-0.595908	-0.998032
C	-3.134397	-1.710376	-0.772927
C	-3.740630	-0.443225	-0.283636
C	-2.919960	0.685829	-0.063140
N	-1.762623	-1.664831	-0.896618
H	-1.298758	-2.527572	-1.165987
O	-3.777085	-2.712387	-1.053886
C	-3.531791	1.877405	0.374016
C	-5.122723	-0.373896	-0.077829
C	-4.906888	1.931541	0.578045
C	-5.734007	0.808383	0.355676
H	-2.914858	2.761669	0.553947
H	-5.357317	2.866290	0.927186
N	-7.112624	0.867870	0.619547
H	-5.703656	-1.279563	-0.271910
H	-7.524530	1.786165	0.482331
H	-7.654888	0.157938	0.136606

B3LYP transition state coordinates for an initial proton transfer and subsequent stepwise reaction for negatively charged xanthine

Xanthine (TS1)

25

Mo	0.184551	-0.180201	1.922863
S	-0.250152	-0.790108	4.384172
C	-0.187562	0.700637	5.304267
H	-0.263234	0.605635	6.397368
C	-0.119657	1.918442	4.722028
H	-0.130845	2.835464	5.328063
S	-0.091075	2.126919	2.983021
S	-0.704298	-2.209669	1.553127
O	-0.330200	0.741756	0.472538
O	1.871144	-0.383663	1.786186
H	-0.188980	0.544403	-0.830472
N	-0.168632	1.609817	-3.710867
C	-0.081080	0.377414	-3.224039
C	0.034157	-0.820397	-3.954297
C	0.072624	-0.821208	-5.383163
N	-0.021835	0.493961	-5.829441
C	-0.142822	1.713481	-5.067184
N	0.088425	-1.856668	-3.030091
C	0.012322	-1.322480	-1.801762
N	-0.086405	0.004774	-1.874829
O	0.170075	-1.789014	-6.146694
O	-0.213599	2.757179	-5.713617
H	-0.006033	0.629201	-6.835299
H	0.166950	-2.840062	-3.253182
H	-0.002453	-1.875124	-0.851109

Xanthine (TS2)

25

Mo	0.234442	-0.404568	1.865050
S	-0.568794	-0.042970	4.265700
C	-0.031085	1.561164	4.731468
H	-0.194782	1.845644	5.780592
C	0.491401	2.443783	3.852487
H	0.771137	3.457468	4.171427
S	0.690558	2.077841	2.148071
S	-1.368460	-1.959026	1.743571
O	0.177947	0.102600	0.113239
O	1.722566	-1.195267	2.103411
H	-2.019009	0.869880	-1.566910
N	-1.152816	1.254526	-4.150066
C	-0.780419	0.371797	-3.232206
C	0.214119	-0.606317	-3.299336
C	0.966508	-0.770173	-4.496082
N	0.550280	0.192581	-5.434514
C	-0.465487	1.188425	-5.328458
N	0.172222	-1.324345	-2.091348
C	-0.704265	-0.738828	-1.229345
N	-1.372230	0.209879	-1.977712
O	1.852486	-1.592575	-4.760130
O	-0.658369	1.914382	-6.306532
H	1.032037	0.168803	-6.326974
H	0.857063	-2.004807	-1.792666
H	-1.227176	-1.339056	-0.452623

Xanthine (TS3)

25

Mo	0.187205	-0.432620	1.989746
S	-1.029182	-0.040812	4.104827
C	-0.196646	1.320009	4.861422
H	-0.492632	1.560256	5.892135
C	0.708598	2.078431	4.208954
H	1.174661	2.944230	4.698971
S	1.176722	1.781601	2.533717
S	-1.691066	-1.327129	1.064074
O	0.548489	0.103110	0.097528
O	1.285637	-1.671561	2.333330
H	-1.326305	1.488746	-1.425428
N	-0.961802	1.416865	-4.142048
C	-0.464922	0.648202	-3.178864
C	0.372418	-0.473161	-3.296811
C	0.777869	-0.920096	-4.584336
N	0.245306	-0.061351	-5.565841
C	-0.601349	1.073228	-5.412885
N	0.582434	-0.981455	-2.013979
C	-0.098908	-0.228445	-1.047267
N	-0.703613	0.801015	-1.826720
O	1.490302	-1.887266	-4.890974
O	-0.952340	1.667239	-6.436597
H	0.484172	-0.291874	-6.524360
H	1.248856	-1.697523	-1.763586
H	-1.070201	-0.938391	-0.470322

B3LYP-D3 transition state coordinates for an initial proton transfer and subsequent stepwise reaction for negatively charged xanthine.

Xanthine (TS1)

25

Mo	0.139972	-0.173149	1.903244
S	-0.237558	-0.798060	4.377295
C	-0.158155	0.691476	5.300426
H	-0.211684	0.594824	6.394879
C	-0.102162	1.912423	4.721537
H	-0.101377	2.825552	5.333933
S	-0.106566	2.131360	2.981967
S	-0.773665	-2.190533	1.528404
O	-0.388314	0.763474	0.468299
O	1.821998	-0.386258	1.733891
H	-0.214463	0.552763	-0.835613
N	-0.177407	1.609313	-3.706366
C	-0.080492	0.378627	-3.217612
C	0.049531	-0.819736	-3.944514
C	0.091572	-0.824603	-5.372662
N	-0.013415	0.488623	-5.823364
C	-0.147238	1.709881	-5.063516
N	0.108576	-1.853618	-3.018219
C	0.021955	-1.318985	-1.790605
N	-0.088344	0.007513	-1.868212
O	0.199073	-1.794673	-6.131876
O	-0.224038	2.751320	-5.712618
H	0.004538	0.620041	-6.829464
H	0.196217	-2.836094	-3.241406
H	0.002833	-1.870996	-0.840244

Xanthine (TS2)

25

Mo	0.231277	-0.406748	1.845457
S	-0.492654	-0.065605	4.284974
C	0.007087	1.559661	4.720430
H	-0.127519	1.847467	5.773166
C	0.468238	2.454636	3.818664
H	0.725782	3.478240	4.125153
S	0.622066	2.087172	2.108204
S	-1.358717	-1.975776	1.749802
O	0.151330	0.097893	0.094650
O	1.733899	-1.175390	2.058189
H	-2.027450	0.868095	-1.560958
N	-1.142195	1.263814	-4.137585
C	-0.790461	0.367112	-3.225273
C	0.196027	-0.619305	-3.290929
C	0.968039	-0.773100	-4.475933
N	0.562348	0.193195	-5.415797
C	-0.434229	1.209250	-5.304944
N	0.141021	-1.344707	-2.088701
C	-0.738376	-0.756649	-1.232577
N	-1.403753	0.192789	-1.982268
O	1.858496	-1.593561	-4.730375
O	-0.597176	1.957231	-6.271735
H	1.070207	0.187475	-6.293810
H	0.829648	-2.016853	-1.780664
H	-1.263057	-1.355493	-0.457026

Xanthine (TS3)

25

Mo	0.180647	-0.433223	1.984454
S	-1.033327	-0.044827	4.106788
C	-0.197283	1.318484	4.858616
H	-0.488618	1.561353	5.890357
C	0.707181	2.077020	4.203000
H	1.173613	2.942457	4.693938
S	1.173640	1.779737	2.525453
S	-1.696806	-1.317971	1.044521
O	0.555918	0.102006	0.097209
O	1.275081	-1.674543	2.327974
H	-1.319565	1.487499	-1.414266
N	-0.963484	1.417000	-4.137277
C	-0.463258	0.649991	-3.174235
C	0.374369	-0.471709	-3.293404
C	0.777602	-0.920089	-4.580482
N	0.241829	-0.063688	-5.562598
C	-0.605978	1.071066	-5.408844
N	0.587780	-0.980264	-2.012102
C	-0.091105	-0.226342	-1.046754
N	-0.697230	0.803675	-1.821776
O	1.490913	-1.887203	-4.885174
O	-0.960374	1.662957	-6.432801
H	0.479199	-0.295969	-6.520956
H	1.259938	-1.689559	-1.759413
H	-1.066975	-0.936609	-0.477541

B3LYP transition state coordinates for a concerted reaction mechanism for 6-substituted quinazolines.

6-Nitro-quinazoline (C2 - Secondary SOM)

29

Mo	2.571973	-0.475361	-0.158768
S	4.487019	-0.283196	1.286800
C	5.414857	1.065432	0.618499
H	6.414165	1.213691	1.044334
C	4.916475	1.913058	-0.299460
H	5.492540	2.767824	-0.670601
S	3.304258	1.703188	-0.993433
S	1.266036	-1.224211	1.540501
O	0.641593	0.397754	-0.727116
H	0.628023	1.364272	-0.589938
C	-0.638757	-0.079782	-0.250774
H	-0.083383	-0.708511	0.867275
N	-1.430679	0.952520	0.135640
O	2.916875	-1.717503	-1.236280
C	-2.358121	-1.367749	-1.026050
C	-3.311457	-0.474551	-0.413819
C	-2.751314	0.744870	0.117901
N	-1.080264	-1.165481	-1.005130
C	-3.661543	1.732640	0.617521
C	-4.692215	-0.691903	-0.410724
C	-5.017994	1.502546	0.623436
C	-5.536717	0.284563	0.113946
H	-3.239439	2.660665	1.008444
H	-5.721277	2.237470	1.015421
N	-6.970230	0.059467	0.125722
H	-5.122128	-1.608156	-0.818499
O	-7.691762	0.943559	0.584437
O	-7.395892	-1.002923	-0.323974
H	-2.727379	-2.245516	-1.577353

6-Nitro-quinazoline (C4 - Primary SOM)

29

Mo	1.635282	-0.348848	0.139681
S	3.783515	-0.593002	1.187408
C	4.943868	-0.450255	-0.140293
H	5.983775	-0.693446	0.107163
C	4.605096	-0.002449	-1.362373
H	5.345708	0.117692	-2.160451
S	2.935656	0.401164	-1.784511
S	0.734417	0.611894	1.988406
O	0.151334	0.978474	-0.793733
H	0.599041	1.715582	-1.255001
C	-0.953019	1.608637	-0.092768
H	-0.413784	1.348171	1.164696
N	-0.960076	2.948266	-0.302115
O	1.000563	-1.892574	-0.071352
C	-3.392592	1.705011	0.021741
N	-3.325867	3.065883	0.028032
C	-2.122649	3.585573	-0.180157
C	-2.228586	0.878124	-0.115452
C	-2.349563	-0.517470	-0.201244
C	-4.663860	1.071681	0.105962
C	-4.780414	-0.300511	0.035799
C	-3.619862	-1.084268	-0.130169
H	-5.539176	1.715850	0.211592
H	-5.745921	-0.802679	0.092385
N	-3.768513	-2.538457	-0.239266
H	-1.478799	-1.165040	-0.320052
H	-2.075627	4.679678	-0.279488
O	-4.896343	-3.007720	-0.106665
O	-2.769900	-3.206503	-0.461229

6-Amino-quinazoline (C2 - Secondary SOM)

29

Mo	2.024134	-0.475000	-0.178297
S	4.010634	-0.302413	1.189835
C	4.845934	1.138191	0.595034
H	5.852266	1.307080	0.997392
C	4.276268	2.023550	-0.242886
H	4.799665	2.930355	-0.567101
S	2.652034	1.784330	-0.898502
S	0.827518	-1.372579	1.522034
O	0.067608	0.334610	-0.647205
H	0.014491	1.298001	-0.505141
C	-1.208476	-0.190141	-0.108595
H	-0.601471	-0.833133	0.900689
N	-1.983141	0.829638	0.329879
O	2.357907	-1.631945	-1.352377
C	-2.966743	-1.383022	-0.973903
C	-3.906037	-0.495290	-0.341054
C	-3.318256	0.661634	0.267829
N	-1.682352	-1.226420	-0.919552
C	-4.212739	1.641965	0.792038
C	-5.304640	-0.660449	-0.392512
C	-5.579717	1.454773	0.742084
C	-6.159702	0.296105	0.150922
H	-3.779759	2.536227	1.246334
H	-6.244417	2.212009	1.172169
N	-7.554611	0.122467	0.174734
H	-5.715997	-1.554988	-0.873885
H	-3.349611	-2.221810	-1.577133
H	-8.079335	0.991822	0.138379
H	-7.899730	-0.528621	-0.524510

6-Amino-quinazoline (C4 - Primary SOM)

29

Mo	1.425142	-0.363953	0.133825
S	3.607465	-0.433024	1.154528
C	4.718032	0.106285	-0.112694
H	5.786148	0.006746	0.114566
C	4.300200	0.673390	-1.258671
H	5.005971	1.039728	-2.012567
S	2.584521	0.854006	-1.643925
S	0.402613	0.138968	2.087928
O	-0.223330	0.834649	-0.616232
H	0.072118	1.694214	-0.973236
C	-1.451941	1.177343	0.156212
H	-0.887262	0.838421	1.322168
N	-1.686296	2.507734	0.091593
O	1.037072	-1.944100	-0.319723
C	-3.868966	0.840949	-0.042412
N	-4.058477	2.195940	0.058611
C	-2.960028	2.925508	0.095829
C	-2.573426	0.245427	-0.047436
C	-2.417436	-1.141850	-0.196364
C	-4.986513	-0.020356	-0.190876
C	-4.825714	-1.386144	-0.334295
C	-3.532046	-1.972859	-0.345087
H	-5.978592	0.437988	-0.193537
H	-5.703710	-2.032185	-0.441067
N	-3.388670	-3.356795	-0.450135
H	-1.416565	-1.579744	-0.212202
H	-3.095522	4.017214	0.115829
H	-4.104363	-3.830519	-0.991225
H	-2.453859	-3.671096	-0.691522

B3LYP-D3 transition state coordinates for a concerted reaction mechanism for 6-substituted quinazolines.

6-Nitro-quinazoline (C2 - Secondary SOM)

29

Mo	2.551986	-0.440548	-0.243693
S	4.489977	-0.419247	1.188018
C	5.429847	0.975612	0.638508
H	6.437034	1.069789	1.061931
C	4.933621	1.915591	-0.187140
H	5.521331	2.792526	-0.480910
S	3.309176	1.797612	-0.879893
S	1.246906	-1.327495	1.388250
O	0.632422	0.500170	-0.725463
H	0.619185	1.447610	-0.491181
C	-0.643551	-0.020528	-0.290058
H	-0.100742	-0.739304	0.771786
N	-1.439590	0.970528	0.185861
O	2.856919	-1.580587	-1.437595
C	-2.350913	-1.256136	-1.163001
C	-3.306766	-0.431310	-0.464389
C	-2.756767	0.745413	0.166266
N	-1.075804	-1.041327	-1.136097
C	-3.673953	1.671515	0.760928
C	-4.683572	-0.667143	-0.468547
C	-5.027054	1.422248	0.759673
C	-5.535707	0.247427	0.147946
H	-3.259774	2.566947	1.228747
H	-5.734630	2.109879	1.223178
N	-6.966773	0.002602	0.150719
H	-5.103595	-1.549668	-0.953835
O	-7.696097	0.832439	0.691737
O	-7.383032	-1.021162	-0.388970
H	-2.717258	-2.085601	-1.786262

6-Nitro-quinazoline (C4 - Primary SOM)

29

Mo	1.625056	-0.313900	0.170229
S	3.754976	-0.616984	1.245294
C	4.932286	-0.487579	-0.070996
H	5.964266	-0.757990	0.182279
C	4.617545	-0.018971	-1.292520
H	5.371053	0.089213	-2.080530
S	2.961669	0.427632	-1.731530
S	0.707068	0.645850	2.009574
O	0.163522	1.027354	-0.782102
H	0.611571	1.773361	-1.227233
C	-0.951002	1.641442	-0.086644
H	-0.430603	1.391022	1.174008
N	-0.980230	2.982011	-0.289934
O	0.963720	-1.842264	-0.063566
C	-3.388107	1.686056	0.039282
N	-3.347109	3.048425	0.059536
C	-2.155640	3.593511	-0.155079
C	-2.209155	0.885604	-0.114965
C	-2.294558	-0.509973	-0.217403
C	-4.643913	1.023234	0.123325
C	-4.728133	-0.350994	0.037568
C	-3.550963	-1.106704	-0.144189
H	-5.534250	1.644228	0.241458
H	-5.682264	-0.874567	0.093802
N	-3.665596	-2.563251	-0.273835
H	-1.408169	-1.133098	-0.348111
H	-2.131805	4.688933	-0.245580
O	-4.779778	-3.062885	-0.135068
O	-2.653590	-3.202757	-0.518122

6-Amino-quinazoline (C2 - Secondary SOM)

29

Mo	2.006298	-0.460468	-0.213695
S	4.014112	-0.353254	1.135444
C	4.848009	1.107800	0.586996
H	5.860296	1.258003	0.982355
C	4.272043	2.029096	-0.207972
H	4.797410	2.945933	-0.499968
S	2.637817	1.824348	-0.853810
S	0.823412	-1.419507	1.457253
O	0.054021	0.376136	-0.640611
H	-0.005224	1.331539	-0.455146
C	-1.217892	-0.176252	-0.117884
H	-0.623144	-0.849127	0.861947
N	-1.995711	0.826543	0.356500
O	2.323665	-1.570566	-1.435205
C	-2.967476	-1.339187	-1.035786
C	-3.910601	-0.480744	-0.368444
C	-3.329130	0.654899	0.285754
N	-1.684154	-1.181838	-0.973033
C	-4.229251	1.609000	0.847237
C	-5.307681	-0.651325	-0.427879
C	-5.595262	1.416253	0.788881
C	-6.168637	0.278756	0.151471
H	-3.801229	2.486231	1.337999
H	-6.264242	2.151835	1.248919
N	-7.563254	0.097035	0.166481
H	-5.713114	-1.528430	-0.944769
H	-3.348343	-2.153119	-1.673376
H	-8.092054	0.964737	0.157311
H	-7.903376	-0.530237	-0.556648

6-Amino-quinazoline (C4 - Primary SOM)

29

Mo	1.434738	-0.341271	0.184978
S	3.603667	-0.425049	1.240475
C	4.737904	0.069626	-0.026004
H	5.802197	-0.042928	0.213913
C	4.343212	0.618214	-1.189928
H	5.065957	0.954643	-1.942024
S	2.634361	0.819032	-1.602628
S	0.378971	0.223218	2.103454
O	-0.198080	0.831664	-0.632172
H	0.090416	1.682781	-1.013105
C	-1.439834	1.190971	0.113127
H	-0.891747	0.913158	1.295969
N	-1.694961	2.512501	-0.019894
O	1.034884	-1.926212	-0.237967
C	-3.845466	0.796354	-0.103936
N	-4.061458	2.151505	-0.082131
C	-2.977311	2.903499	-0.062115
C	-2.539267	0.228674	-0.054005
C	-2.349192	-1.159452	-0.112782
C	-4.941920	-0.096536	-0.218542
C	-4.748983	-1.464986	-0.274600
C	-3.442817	-2.022622	-0.227556
H	-5.943726	0.337669	-0.264320
H	-5.610811	-2.135985	-0.355762
N	-3.266211	-3.406554	-0.243261
H	-1.339186	-1.573069	-0.085817
H	-3.133865	3.991759	-0.101179
H	-3.959747	-3.930372	-0.766737
H	-2.319699	-3.712189	-0.447466

B3LYP transition state coordinates for a concerted reaction mechanism for quinazoline.

Quinazoline (C2 - Secondary SOM)

27

Mo	1.697606	-0.479248	-0.267274
S	3.674845	-0.414661	1.118775
C	4.524318	1.055564	0.627261
H	5.529050	1.189247	1.046269
C	3.963298	2.001419	-0.148028
H	4.492856	2.925685	-0.405417
S	2.341707	1.817216	-0.828150
S	0.489254	-1.477271	1.366420
O	-0.258053	0.375277	-0.679042
H	-0.296718	1.325907	-0.462109
C	-1.531460	-0.169757	-0.183744
H	-0.925027	-0.901135	0.791951
N	-2.294011	0.820908	0.335785
O	2.034131	-1.558890	-1.511720
C	-3.300297	-1.298644	-1.098479
C	-4.226130	-0.453738	-0.391730
C	-3.629411	0.661067	0.290671
N	-2.014661	-1.149322	-1.055437
C	-4.504733	1.604277	0.909868
C	-5.625903	-0.609601	-0.424337
C	-5.874747	1.420778	0.870255
C	-6.452216	0.310812	0.205230
H	-4.052723	2.457677	1.420705
H	-6.528610	2.148997	1.360906
H	-7.538350	0.188607	0.185146
H	-6.050578	-1.465980	-0.959681
H	-3.696344	-2.094901	-1.748705

Quinazoline (C4 - Primary SOM)

27

Mo	1.411628	-0.492726	0.178350
S	3.558889	-0.331779	1.258995
C	4.666187	0.204559	-0.011854
H	5.731345	0.196126	0.248171
C	4.243354	0.666926	-1.201977
H	4.942814	1.034183	-1.961102
S	2.530896	0.697909	-1.640499
S	0.302009	0.060284	2.071014
O	-0.305137	0.534131	-0.682827
H	-0.052993	1.389770	-1.081474
C	-1.558536	0.839497	0.042901
H	-0.998768	0.608698	1.245374
N	-1.869778	2.150263	-0.094109
O	1.149042	-2.119217	-0.182685
C	-3.954453	0.351153	-0.092306
N	-4.219639	1.696878	-0.048809
C	-3.164225	2.489344	-0.083935
C	-2.623186	-0.164403	-0.108915
C	-2.399044	-1.552247	-0.204864
C	-5.032800	-0.568839	-0.162416
C	-4.796343	-1.930882	-0.251886
C	-3.476253	-2.427704	-0.279763
H	-6.044728	-0.156826	-0.151967
H	-5.639009	-2.627245	-0.307127
H	-3.296439	-3.503301	-0.358793
H	-1.377480	-1.939056	-0.225486
H	-3.365018	3.570450	-0.125367

Quinazoline (C5)

27

Mo	1.494417	-0.532449	0.242112
S	3.639823	-0.182010	1.275312
C	4.696834	0.359547	-0.036649
H	5.763284	0.432032	0.207825
C	4.233220	0.728363	-1.244289
H	4.898331	1.097551	-2.032784
S	2.513321	0.636073	-1.648388
S	0.338761	0.045937	2.124834
O	-0.308062	0.318728	-0.617716
H	-0.234913	0.788524	-1.463542
C	-1.548219	0.767804	0.080385
H	-0.956987	0.486169	1.290931
C	-1.804247	2.167077	0.000555
O	1.361896	-2.187923	-0.039844
C	-4.022621	0.411643	-0.141614
C	-4.222015	1.814749	-0.093197
C	-3.113531	2.656681	-0.038277
C	-2.693033	-0.123394	-0.099074
C	-2.577796	-1.525156	-0.202374
N	-5.092316	-0.428453	-0.261326
C	-4.837350	-1.716829	-0.338532
N	-3.631227	-2.324836	-0.324881
H	-5.705440	-2.385717	-0.428876
H	-1.586980	-1.995867	-0.190245
H	-3.264484	3.741170	-0.027738
H	-5.243825	2.195266	-0.132495
H	-0.953619	2.851076	0.063919

Quinazoline (C6)

27

Mo	1.824616	-0.489189	-0.197677
S	3.812354	-0.309151	1.153714
C	4.598871	1.183379	0.618533
H	5.599149	1.369635	1.027360
C	3.999089	2.077713	-0.187409
H	4.487890	3.014465	-0.477944
S	2.380668	1.802773	-0.846235
S	0.629260	-1.510308	1.459700
O	-0.161937	0.232447	-0.629383
H	-0.272217	1.151427	-0.920233
C	-1.469611	-0.268915	-0.082506
H	-0.771763	-0.999349	0.865945
C	-2.296868	0.726020	0.498006
O	2.177099	-1.583843	-1.428109
C	-3.468301	-1.319406	-1.074653
C	-4.319345	-0.378238	-0.407356
C	-3.699267	0.655650	0.375448
C	-2.109800	-1.242702	-0.954737
C	-4.612406	1.563020	0.988141
N	-5.662658	-0.462046	-0.529862
N	-5.921492	1.466795	0.859811
C	-6.385561	0.446968	0.099595
H	-4.222021	2.386257	1.603585
H	-7.476620	0.375577	0.001491
H	-3.944454	-2.084826	-1.692293
H	-1.841515	1.504698	1.118397
H	-1.455989	-1.948765	-1.474786

Quinazoline (C7)

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   27

Mo     1.769732    -0.446242    -0.207783
 S     3.787076    -0.275899     1.099236
 C     4.589734     1.187528     0.510506
 H     5.606024     1.358538     0.885093
 C     3.985308     2.081503    -0.292396
 H     4.485079     3.001491    -0.615558
 S     2.342716     1.829865    -0.897744
 S     0.599905    -1.435337     1.479798
 O    -0.212711     0.302998    -0.604454
 H    -0.314033     1.249989    -0.792580
 C    -1.504626    -0.229181    -0.062137
 H    -0.806526    -0.926314     0.903931
 C    -2.369662     0.747400     0.499636
 O     2.073994    -1.563511    -1.430602
 C    -3.445233    -1.355858    -1.063470
 C    -4.328473    -0.426608    -0.423191
 C    -3.764918     0.642020     0.360318
 C    -2.093147    -1.244225    -0.925825
 N    -4.596286     1.551556     0.957384
 C    -5.729337    -0.462180    -0.514661
 C    -5.889793     1.388624     0.783364
 N    -6.523795     0.424233     0.075560
 H    -3.872160    -2.153304    -1.680807
 H    -1.966961     1.554677     1.116703
 H    -1.408458    -1.937556    -1.421906
 H    -6.212018    -1.257690    -1.101650
 H    -6.545964     2.124146     1.271087
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Quinazoline (C8)

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   27

Mo     1.520135    -0.617317     0.295320
 S     3.623825    -0.011024     1.302940
 C     4.631642     0.545293    -0.040490
 H     5.686529     0.726880     0.198241
 C     4.143466     0.798326    -1.268586
 H     4.778782     1.178386    -2.076436
 S     2.442644     0.526243    -1.669812
 S     0.334467    -0.062976     2.167488
 O    -0.322837     0.149018    -0.579812
 H    -0.221410     0.625835    -1.419303
 C    -1.533423     0.645017     0.109550
 H    -0.975937     0.311109     1.327763
 C    -1.715869     2.059626     0.047468
 O     1.565098    -2.285543     0.095895
 C    -4.021255     0.452234    -0.090573
 C    -4.146632     1.864416    -0.018795
 C    -2.989951     2.636774     0.031489
 C    -2.733108    -0.177185    -0.080967
 N    -2.612451    -1.512663    -0.199826
 C    -5.118455    -0.441713    -0.220402
 N    -4.985331    -1.749387    -0.330165
 C    -3.717557    -2.223267    -0.319124
 H    -3.070117     3.728329     0.054972
 H    -5.138684     2.323703    -0.036640
 H    -0.823400     2.688184     0.109736
 H    -3.603487    -3.310039    -0.417778
 H    -6.140029    -0.034082    -0.237336
```


B3LYP-D3 transition state coordinates for a concerted reaction mechanism for quinazoline.

Quinazoline (C2 - Secondary SOM)

27

Mo	1.682035	-0.472099	-0.257936
S	3.666883	-0.431946	1.122447
C	4.535842	1.024581	0.618384
H	5.545376	1.145211	1.030297
C	3.988179	1.974433	-0.162695
H	4.534169	2.887517	-0.426677
S	2.358775	1.815089	-0.833678
S	0.461589	-1.457869	1.374156
O	-0.256169	0.419888	-0.660868
H	-0.295805	1.366261	-0.427580
C	-1.531200	-0.130921	-0.181728
H	-0.949259	-0.862373	0.797184
N	-2.303166	0.854415	0.336351
O	1.994928	-1.555968	-1.503415
C	-3.280557	-1.275916	-1.108091
C	-4.216014	-0.449417	-0.391689
C	-3.635428	0.676218	0.288558
N	-1.997449	-1.108821	-1.066074
C	-4.525606	1.607370	0.904585
C	-5.612408	-0.630491	-0.418440
C	-5.892529	1.400478	0.868828
C	-6.452988	0.276806	0.211837
H	-4.086939	2.469979	1.411564
H	-6.557155	2.118167	1.360441
H	-7.536749	0.134930	0.196481
H	-6.023266	-1.495522	-0.950580
H	-3.668002	-2.069708	-1.766271

Quinazoline (C4 - Primary SOM)

27

Mo	1.292885	-0.404064	-0.012691
S	3.457353	-0.549488	1.040406
C	4.551646	0.283563	-0.074421
H	5.620935	0.202159	0.155063
C	4.118733	1.037018	-1.102177
H	4.815442	1.577453	-1.752902
S	2.400443	1.198170	-1.493835
S	0.204133	-0.330946	1.970944
O	-0.434557	0.800318	-0.580609
H	-0.192607	1.729602	-0.759290
C	-1.675335	0.913619	0.212168
H	-1.104739	0.405180	1.325292
N	-1.997305	2.215190	0.401057
O	1.016206	-1.887291	-0.764648
C	-4.066002	0.435078	0.016491
N	-4.341768	1.727264	0.388360
C	-3.294969	2.520899	0.521412
C	-2.730954	-0.040083	-0.153305
C	-2.489686	-1.358844	-0.583426
C	-5.135097	-0.460886	-0.243282
C	-4.883384	-1.758050	-0.660792
C	-3.558527	-2.209986	-0.839490
H	-6.151671	-0.083308	-0.109025
H	-5.718650	-2.436741	-0.860524
H	-3.369303	-3.232364	-1.177689
H	-1.463886	-1.708722	-0.717107
H	-3.507474	3.576910	0.745511

Quinazoline (C5)

27

Mo	1.343962	-0.383074	0.034142
S	3.538950	-0.424981	1.025905
C	4.582993	0.345693	-0.180616
H	5.661935	0.279191	0.004673
C	4.101167	1.031598	-1.233794
H	4.765288	1.531745	-1.947938
S	2.362711	1.177976	-1.542106
S	0.252345	-0.239523	2.036246
O	-0.456152	0.673238	-0.541689
H	-0.497216	1.193575	-1.358629
C	-1.695127	0.896254	0.248802
H	-1.063936	0.373959	1.364084
C	-2.015436	2.261082	0.494067
O	1.113822	-1.904157	-0.651402
C	-4.150749	0.463275	0.001124
C	-4.415186	1.804159	0.379111
C	-3.347420	2.672699	0.599927
C	-2.796006	0.007783	-0.108054
C	-2.607560	-1.322695	-0.536231
N	-5.180002	-0.385889	-0.289670
C	-4.859497	-1.604518	-0.670374
N	-3.623527	-2.130122	-0.821769
H	-5.694089	-2.283023	-0.898677
H	-1.592890	-1.723401	-0.652153
H	-3.551698	3.715715	0.863071
H	-5.454923	2.126482	0.453063
H	-1.191375	2.952518	0.687241

Quinazoline (C6)

27

Mo	1.771957	-0.417512	-0.156688
S	3.828201	-0.296355	1.098127
C	4.657759	1.134690	0.463302
H	5.693877	1.275988	0.794218
C	4.052657	2.041244	-0.326438
H	4.572997	2.939954	-0.677239
S	2.373085	1.849763	-0.852835
S	0.591799	-1.390837	1.539826
O	-0.206867	0.326227	-0.549772
H	-0.367886	1.147020	-1.039638
C	-1.510587	-0.205246	-0.027484
H	-0.812501	-0.898616	0.940281
C	-2.376151	0.770898	0.525195
O	2.042334	-1.534267	-1.386803
C	-3.449615	-1.318550	-1.064750
C	-4.341860	-0.396905	-0.424912
C	-3.770975	0.660617	0.365768
C	-2.097738	-1.208471	-0.901999
C	-4.723298	1.548807	0.946685
N	-5.679019	-0.514000	-0.585526
N	-6.025540	1.417462	0.784488
C	-6.441587	0.380452	0.018002
H	-4.369223	2.385658	1.565610
H	-7.527187	0.281095	-0.110517
H	-3.888781	-2.098582	-1.691432
H	-1.951440	1.569463	1.140577
H	-1.403528	-1.896506	-1.393017

Quinazoline (C7)

27

Mo	1.756916	-0.433385	-0.214115
S	3.785382	-0.326260	1.085886
C	4.612076	1.132129	0.512760
H	5.634311	1.279648	0.881880
C	4.020147	2.050730	-0.272692
H	4.538170	2.964909	-0.584313
S	2.367958	1.841120	-0.874067
S	0.565809	-1.422268	1.463856
O	-0.216111	0.351641	-0.603623
H	-0.315812	1.300648	-0.779906
C	-1.505177	-0.185663	-0.080390
H	-0.825970	-0.894705	0.889321
C	-2.378272	0.775542	0.491854
O	2.032278	-1.538964	-1.453096
C	-3.425487	-1.336001	-1.083980
C	-4.319689	-0.427261	-0.428851
C	-3.771732	0.646278	0.360611
C	-2.075286	-1.201814	-0.952848
N	-4.616347	1.533459	0.972403
C	-5.720187	-0.491440	-0.508897
C	-5.908012	1.343816	0.807980
N	-6.528308	0.372485	0.096904
H	-3.844002	-2.133925	-1.706247
H	-1.979398	1.580683	1.113561
H	-1.373625	-1.873815	-1.454161
H	-6.190196	-1.291912	-1.099225
H	-6.575071	2.060435	1.308623

Quinazoline (C8)

27

Mo	1.389014	-0.490600	0.046820
S	3.545610	-0.172137	1.080304
C	4.522433	0.641930	-0.152238
H	5.592472	0.736998	0.069484
C	3.996797	1.176250	-1.270598
H	4.615958	1.709045	-2.001494
S	2.269888	1.057374	-1.638157
S	0.257076	-0.335147	2.025416
O	-0.467182	0.433889	-0.595404
H	-0.464948	0.971913	-1.402124
C	-1.661197	0.764748	0.204171
H	-1.075205	0.195702	1.315542
C	-1.854169	2.158763	0.441573
O	1.390647	-2.074359	-0.513704
C	-4.147115	0.577105	0.031876
C	-4.283859	1.938498	0.409121
C	-3.133491	2.704250	0.585937
C	-2.852500	-0.017329	-0.128592
N	-2.714900	-1.291902	-0.539152
C	-5.236561	-0.287684	-0.261492
N	-5.088880	-1.537654	-0.656949
C	-3.814709	-1.978992	-0.783987
H	-3.225070	3.764718	0.841580
H	-5.280974	2.373311	0.518013
H	-0.960784	2.767385	0.603317
H	-3.690220	-3.014988	-1.122619
H	-6.263295	0.094257	-0.161830

B3LYP transition state coordinates for a concerted reaction mechanism for phthalazine.

Phthalazine (C4 - Primary SOM)

27

Mo	1.322472	-0.418817	0.067171
S	3.477544	-0.499787	1.139049
C	4.581632	0.251478	-0.020346
H	5.649205	0.173104	0.217090
C	4.155675	0.943777	-1.092218
H	4.855552	1.437312	-1.775643
S	2.440079	1.097023	-1.491525
S	0.229690	-0.222226	2.034167
O	-0.408399	0.732425	-0.600888
H	-0.187463	1.653797	-0.846711
C	-1.655165	0.889385	0.175617
H	-1.104083	0.490182	1.307058
N	-1.959220	2.222213	0.220400
O	1.058944	-1.945866	-0.602226
C	-4.040127	0.379638	0.009631
C	-4.212902	1.769978	0.311573
N	-3.213155	2.630634	0.348687
C	-2.709000	-0.091326	-0.143717
C	-2.470710	-1.428398	-0.513836
C	-5.116099	-0.515789	-0.205989
C	-4.868780	-1.833270	-0.560352
C	-3.544408	-2.289619	-0.721125
H	-5.218586	2.185282	0.444539
H	-6.141929	-0.150279	-0.096419
H	-5.704030	-2.521709	-0.721689
H	-3.356779	-3.328192	-1.007035
H	-1.446774	-1.788220	-0.637222

Phthalazine (C5)

27

Mo	1.368096	-0.470465	-0.012011
S	3.550562	-0.333410	0.992134
C	4.545192	0.522583	-0.196373
H	5.621834	0.547730	0.009963
C	4.024851	1.163366	-1.258426
H	4.651683	1.720425	-1.963587
S	2.288100	1.146650	-1.595840
S	0.278944	-0.408012	1.999139
O	-0.481392	0.526273	-0.563945
H	-0.457354	1.156900	-1.301253
C	-1.685590	0.789266	0.264873
H	-1.046180	0.179908	1.354681
C	-1.910277	2.159406	0.589115
O	1.240638	-2.003910	-0.694706
C	-4.157888	0.550622	0.061016
C	-4.333816	1.882095	0.509883
C	-3.203648	2.663133	0.749768
C	-2.855648	0.002143	-0.104230
C	-2.786723	-1.321620	-0.606251
C	-5.228633	-0.323710	-0.294572
N	-5.080322	-1.545390	-0.753081
N	-3.840112	-2.056754	-0.921817
H	-5.341255	2.287747	0.631094
H	-6.264708	0.026271	-0.192507
H	-1.811936	-1.795749	-0.765916
H	-1.038472	2.785455	0.798251
H	-3.323908	3.703581	1.068142

Phthalazine (C6)

27

Mo	1.812397	-0.458167	-0.108917
S	3.812305	-0.266601	1.220299
C	4.653012	1.151744	0.576659
H	5.667128	1.319657	0.958429
C	4.078651	2.019901	-0.275139
H	4.601607	2.913388	-0.633879
S	2.439237	1.771544	-0.892461
S	0.589976	-1.341934	1.607478
O	-0.156218	0.280941	-0.592233
H	-0.254952	1.193755	-0.905864
C	-1.466849	-0.205686	-0.060643
H	-0.789083	-0.862405	0.968980
C	-2.335458	0.804933	0.432824
O	2.117809	-1.635875	-1.272786
C	-3.405680	-1.373919	-1.027245
C	-4.289466	-0.411296	-0.445781
C	-3.726799	0.684111	0.277642
C	-2.052333	-1.256686	-0.878201
C	-4.688149	1.606787	0.802308
N	-5.989836	1.495622	0.662825
C	-5.698304	-0.444013	-0.544882
N	-6.516784	0.453342	-0.022587
H	-6.183137	-1.265446	-1.089486
H	-4.342288	2.479891	1.370997
H	-3.824913	-2.200519	-1.609572
H	-1.916713	1.636141	1.008674
H	-1.365158	-1.977337	-1.330312

B3LYP-D3 transition state coordinates for a concerted reaction mechanism for phthalazine.

Phthalazine (C4 - Primary SOM)

```
   27

Mo     1.296672    -0.404408     0.028623
 S     3.458990    -0.561973     1.083237
 C     4.563408     0.238347    -0.044883
 H     5.631960     0.142987     0.182819
 C     4.138541     0.983030    -1.082382
 H     4.841524     1.502927    -1.743131
 S     2.421914     1.166940    -1.470224
 S     0.205377    -0.283275     1.999849
 O    -0.424618     0.788271    -0.593621
 H    -0.207424     1.720679    -0.796345
 C    -1.667732     0.906702     0.191798
 H    -1.128794     0.474545     1.302003
 N    -1.985213     2.235102     0.285389
 O     1.011031    -1.897163    -0.705104
 C    -4.043576     0.370288     0.030035
 C    -4.230968     1.745270     0.390705
 N    -3.242764     2.619318     0.446168
 C    -2.709033    -0.073479    -0.161652
 C    -2.451628    -1.387761    -0.590684
 C    -5.108191    -0.532272    -0.208221
 C    -4.843815    -1.829692    -0.621603
 C    -3.514560    -2.257064    -0.819979
 H    -6.137978    -0.188573    -0.069263
 H    -5.669937    -2.524692    -0.800819
 H    -1.423724    -1.723279    -0.741484
 H    -5.240535     2.139158     0.554978
 H    -3.314007    -3.279309    -1.152100
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Phthalazine (C5)

```
   27

Mo     1.796246    -0.434948    -0.088344
 S     3.825667    -0.289358     1.206664
 C     4.682372     1.111173     0.541177
 H     5.709955     1.257000     0.895643
 C     4.106966     1.992968    -0.296964
 H     4.644587     2.873024    -0.667866
 S     2.445736     1.787962    -0.875059
 S     0.577067    -1.308733     1.630981
 O    -0.165594     0.322363    -0.564018
 H    -0.277058     1.234592    -0.873814
 C    -1.471854    -0.180302    -0.031736
 H    -0.805427    -0.821471     0.994939
 C    -2.355624     0.820019     0.454369
 O     2.064682    -1.610574    -1.261666
 C    -3.382596    -1.371310    -1.023630
 C    -4.282788    -0.416596    -0.453105
 C    -3.742410     0.682977     0.281520
 C    -2.033411    -1.238855    -0.856292
 C    -4.721001     1.593050     0.796316
 N    -6.019819     1.468257     0.639296
 C    -5.689559    -0.463700    -0.571665
 N    -6.525847     0.422926    -0.057807
 H    -6.156671    -1.288291    -1.126836
 H    -4.391092     2.466504     1.373863
 H    -3.787235    -2.201049    -1.611623
 H    -1.949635     1.652300     1.037128
 H    -1.325661    -1.948049    -1.294344
```

Phthalazine (C6)

27

Mo	1.340202	-0.410533	-0.003682
S	3.548251	-0.431564	0.958556
C	4.563209	0.386916	-0.241685
H	5.645348	0.336886	-0.070455
C	4.056060	1.087614	-1.272851
H	4.700803	1.617916	-1.982936
S	2.311584	1.204701	-1.555746
S	0.268584	-0.340830	2.014443
O	-0.476377	0.652132	-0.520452
H	-0.525151	1.194549	-1.322957
C	-1.695049	0.867410	0.298593
H	-1.056207	0.272339	1.379091
C	-1.973812	2.227533	0.622031
O	1.127833	-1.918075	-0.721699
C	-4.150524	0.533013	0.058771
C	-4.384420	1.853483	0.512498
C	-3.288090	2.677841	0.769212
C	-2.826340	0.037559	-0.091133
C	-2.691203	-1.280976	-0.592086
C	-5.178834	-0.382901	-0.317376
N	-4.972773	-1.596771	-0.775737
N	-3.709808	-2.058357	-0.923492
H	-5.408080	2.218449	0.623985
H	-6.229621	-0.074552	-0.232386
H	-1.693763	-1.712194	-0.735323
H	-1.125009	2.881669	0.837148
H	-3.454780	3.711282	1.089209

B3LYP transition state coordinates for a concerted reaction mechanism for quinoline.

Quinoline (C2 - Primary SOM)

28

Mo	1.706406	-0.440282	-0.155144
S	3.762010	-0.322424	1.108013
C	4.571724	1.136246	0.521356
H	5.600597	1.284911	0.870557
C	3.958198	2.055102	-0.246203
H	4.464971	2.973183	-0.564613
S	2.296818	1.845600	-0.812003
S	0.592133	-1.423180	1.548887
O	-0.262677	0.346849	-0.533661
H	-0.362352	1.301236	-0.356211
C	-1.535509	-0.255187	0.007999
H	-0.880723	-0.883759	0.978633
N	-2.348729	0.713650	0.466328
O	1.959636	-1.551884	-1.396053
C	-3.394070	-1.442877	-1.016870
C	-4.290254	-0.491838	-0.414168
C	-3.686522	0.594861	0.312386
C	-2.050370	-1.321471	-0.856034
C	-4.550936	1.580537	0.872793
C	-5.925365	1.484224	0.738725
C	-5.693598	-0.558792	-0.537084
C	-6.511287	0.409293	0.032549
H	-6.132402	-1.392041	-1.096795
H	-4.084607	2.404853	1.417734
H	-3.810777	-2.257958	-1.618280
H	-1.338493	-2.024054	-1.295602
H	-7.598315	0.343826	-0.066497
H	-6.567209	2.249303	1.187109

Quinoline (C3)

28

Mo	1.799930	-0.521845	-0.166161
S	3.700346	-0.078906	1.246698
C	4.437328	1.387590	0.584505
H	5.407037	1.669239	1.012096
C	3.831407	2.159446	-0.335615
H	4.286253	3.085178	-0.705407
S	2.262010	1.725806	-1.025547
S	0.590990	-1.471045	1.527072
O	-0.203402	0.064779	-0.715036
H	-0.319072	0.945743	-1.106048
C	-1.514141	-0.361955	-0.100217
H	-0.807627	-1.075930	0.847530
C	-2.285395	0.678086	0.468057
O	2.288871	-1.697555	-1.267776
N	-3.544956	-1.351680	-1.045195
C	-4.302347	-0.396446	-0.410497
C	-3.692163	0.655728	0.358913
C	-2.249744	-1.315776	-0.924087
C	-4.545231	1.627519	0.963392
C	-5.917674	1.555931	0.819121
C	-5.709615	-0.439437	-0.541230
C	-6.512013	0.516378	0.061815
H	-6.131697	-1.253611	-1.135887
H	-4.091142	2.431238	1.551275
H	-1.660221	-2.077454	-1.453000
H	-7.599499	0.471898	-0.044738
H	-6.553095	2.309214	1.295190
H	-1.788433	1.459907	1.050899

Quinoline (C4)

28

Mo	1.361969	-0.436476	0.008357
S	3.544788	-0.360207	1.021501
C	4.574373	0.427169	-0.183925
H	5.651066	0.414011	0.023480
C	4.080693	1.066730	-1.259589
H	4.731163	1.580043	-1.976477
S	2.345067	1.117852	-1.600157
S	0.265962	-0.305233	2.009930
O	-0.452127	0.585701	-0.572113
H	-0.417421	1.235531	-1.291590
C	-1.694383	0.810479	0.221910
H	-1.052756	0.279961	1.343420
C	-2.026116	2.168342	0.462732
O	1.187394	-1.979651	-0.645716
C	-4.138120	0.460540	-0.025614
N	-4.411717	1.755299	0.311585
C	-3.372999	2.549392	0.530366
C	-2.807926	-0.068731	-0.123727
C	-2.612771	-1.413501	-0.517103
C	-5.227138	-0.406807	-0.324266
C	-5.013110	-1.718322	-0.703341
C	-3.697674	-2.226955	-0.804889
H	-5.864878	-2.367359	-0.929901
H	-3.533733	-3.264131	-1.110227
H	-1.595369	-1.804581	-0.594094
H	-3.605795	3.593942	0.783618
H	-1.230659	2.887603	0.675345
H	-6.231940	0.015540	-0.245631

Quinoline (C5)

28

Mo	1.387803	-0.412637	0.072368
S	3.580734	-0.440799	1.065926
C	4.626726	0.342094	-0.128829
H	5.704307	0.284396	0.066306
C	4.146144	1.027032	-1.182425
H	4.808643	1.537891	-1.890296
S	2.410442	1.154946	-1.500672
S	0.297276	-0.301215	2.074357
O	-0.399143	0.662496	-0.485853
H	-0.419367	1.227659	-1.273315
C	-1.659890	0.867208	0.306039
H	-1.038761	0.330560	1.388728
C	-1.981189	2.231160	0.555251
O	1.168632	-1.933299	-0.624235
C	-4.112438	0.454315	-0.038631
C	-4.373274	1.801120	0.338604
C	-3.313501	2.657734	0.611831
C	-2.755937	-0.016304	-0.099058
C	-2.532173	-1.344566	-0.518976
N	-5.164686	-0.351373	-0.365238
C	-4.914313	-1.587231	-0.748872
C	-3.617869	-2.139918	-0.851182
H	-5.786405	-2.207226	-1.003209
H	-3.482105	-3.172440	-1.182475
H	-1.511700	-1.731440	-0.583237
H	-3.518293	3.700174	0.877245
H	-1.163321	2.917104	0.791977
H	-5.413241	2.130082	0.373206

Quinoline (C6)

28

Mo	1.807188	-0.497754	-0.186788
S	3.778106	-0.222532	1.176938
C	4.552367	1.250658	0.574372
H	5.549923	1.465196	0.976284
C	3.945437	2.102780	-0.271321
H	4.425514	3.030392	-0.602964
S	2.329362	1.782560	-0.914664
S	0.618818	-1.488452	1.492822
O	-0.182099	0.172218	-0.652428
H	-0.309307	1.067057	-1.004499
C	-1.494602	-0.311431	-0.074693
H	-0.791683	-1.010081	0.872759
C	-2.299269	0.707043	0.495752
O	2.195863	-1.627048	-1.374409
C	-3.518179	-1.324167	-1.038008
C	-4.350827	-0.347890	-0.396134
C	-3.705439	0.685740	0.377124
C	-2.158397	-1.290832	-0.919801
C	-4.563537	1.649444	0.982250
C	-5.930192	1.549125	0.813787
N	-5.691794	-0.424310	-0.550633
C	-6.450838	0.487986	0.033484
H	-4.017889	-2.088002	-1.639194
H	-1.526870	-2.028595	-1.422696
H	-7.535988	0.397042	-0.109498
H	-6.609948	2.273353	1.272154
H	-1.818473	1.484715	1.097726
H	-4.126301	2.456028	1.579134

Quinoline (C7)

28

Mo	1.786845	-0.449288	-0.123299
S	3.810262	-0.258736	1.176056
C	4.619374	1.185984	0.551043
H	5.638651	1.359457	0.916641
C	4.017638	2.063499	-0.272223
H	4.522325	2.972919	-0.617599
S	2.367269	1.814820	-0.857379
S	0.614104	-1.406503	1.583339
O	-0.190549	0.271817	-0.548866
H	-0.323793	1.183859	-0.850824
C	-1.496704	-0.261804	-0.007001
H	-0.804532	-0.915892	0.970841
C	-2.376949	0.724740	0.505888
O	2.095942	-1.588871	-1.324329
C	-3.418261	-1.408054	-1.020902
C	-4.324580	-0.468455	-0.427695
C	-3.774648	0.621440	0.344201
C	-2.068483	-1.293992	-0.858835
N	-4.584105	1.566796	0.914071
C	-5.887506	1.454733	0.758850
C	-5.723411	-0.543026	-0.563080
C	-6.524697	0.422161	0.030298
H	-6.162750	-1.363356	-1.140962
H	-3.829335	-2.221858	-1.627656
H	-1.376365	-2.002197	-1.322670
H	-7.614123	0.393987	-0.050913
H	-6.503873	2.231827	1.234450
H	-1.989648	1.546428	1.113641

Quinoline (C8)

28

Mo	1.413124	-0.555794	0.098787
S	3.550003	-0.202580	1.158347
C	4.533683	0.628515	-0.055536
H	5.596767	0.744574	0.188092
C	4.018927	1.150561	-1.183884
H	4.639091	1.695615	-1.904609
S	2.304256	0.990993	-1.584500
S	0.267065	-0.420267	2.073809
O	-0.435028	0.381922	-0.546296
H	-0.377428	0.994246	-1.296500
C	-1.647031	0.702157	0.242460
H	-1.063322	0.114872	1.357643
C	-1.835805	2.091579	0.498794
O	1.438412	-2.140381	-0.462300
C	-4.137558	0.525043	0.006001
C	-4.262438	1.887766	0.391115
C	-3.115172	2.643285	0.612529
C	-2.836855	-0.078798	-0.119845
N	-2.665282	-1.350841	-0.525292
C	-5.250269	-0.298757	-0.315994
C	-5.049970	-1.601035	-0.728765
C	-3.723584	-2.083154	-0.821706
H	-5.890609	-2.252316	-0.983953
H	-3.534320	-3.113321	-1.150398
H	-3.209270	3.700967	0.879489
H	-0.947384	2.697776	0.695734
H	-5.257395	2.333666	0.474669
H	-6.259795	0.118374	-0.238805

B3LYP-D3 transition state coordinates for a concerted reaction mechanism for quinoline.

Quinoline (C2 - Primary SOM)

28

Mo	1.696958	-0.424504	-0.207922
S	3.791051	-0.375017	1.003127
C	4.601264	1.094907	0.442420
H	5.640781	1.222612	0.768363
C	3.979055	2.045515	-0.279347
H	4.490429	2.967465	-0.579491
S	2.300378	1.873927	-0.810154
S	0.608161	-1.442154	1.489275
O	-0.266752	0.397411	-0.526207
H	-0.363341	1.344069	-0.310987
C	-1.532383	-0.222240	0.015486
H	-0.879776	-0.868361	0.962294
N	-2.345903	0.733664	0.501037
O	1.902692	-1.498620	-1.489531
C	-3.385288	-1.393456	-1.035390
C	-4.283019	-0.459458	-0.407682
C	-3.682788	0.612193	0.344919
C	-2.042652	-1.270674	-0.873083
C	-4.551004	1.579603	0.930455
C	-5.925415	1.480558	0.795431
C	-5.685802	-0.529396	-0.530847
C	-6.507512	0.420934	0.063221
H	-6.121042	-1.350700	-1.110604
H	-4.087803	2.392256	1.495277
H	-3.801465	-2.195170	-1.654790
H	-1.322082	-1.954673	-1.327257
H	-7.594339	0.353251	-0.036574
H	-6.569946	2.231483	1.263501

Quinoline (C3)

28

Mo	1.782842	-0.494883	-0.186358
S	3.680167	-0.009718	1.224865
C	4.391677	1.463359	0.547221
H	5.356085	1.767754	0.971795
C	3.775431	2.214295	-0.384407
H	4.217842	3.142907	-0.762696
S	2.211278	1.750273	-1.069989
S	0.577625	-1.435342	1.511642
O	-0.223951	0.035107	-0.773272
H	-0.362225	0.883205	-1.223993
C	-1.527859	-0.371388	-0.129798
H	-0.825159	-1.063737	0.821270
C	-2.279651	0.688923	0.427170
O	2.294066	-1.676846	-1.269584
N	-3.577325	-1.366603	-1.023801
C	-4.317029	-0.400541	-0.384082
C	-3.687192	0.665200	0.352605
C	-2.279871	-1.331947	-0.928916
C	-4.523462	1.649026	0.960741
C	-5.899118	1.575930	0.853222
C	-5.727236	-0.443832	-0.477554
C	-6.513088	0.522851	0.130398
H	-6.165877	-1.267264	-1.046923
H	-4.052583	2.461938	1.522122
H	-1.697750	-2.099303	-1.457246
H	-7.602968	0.477226	0.053168
H	-6.522236	2.337162	1.332846
H	-1.762217	1.475605	0.984308

Quinoline (C4)

28

Mo	1.329858	-0.398270	0.020622
S	3.522425	-0.447190	1.018589
C	4.573646	0.323533	-0.181957
H	5.651586	0.256361	0.009286
C	4.098426	1.010763	-1.237220
H	4.766840	1.511000	-1.947385
S	2.362088	1.156311	-1.555982
S	0.234587	-0.264831	2.021246
O	-0.458934	0.671354	-0.542408
H	-0.501111	1.201366	-1.353086
C	-1.708656	0.877417	0.240478
H	-1.072618	0.355549	1.360143
C	-2.064148	2.230876	0.472778
O	1.095997	-1.918733	-0.667364
C	-4.141149	0.478566	-0.016691
N	-4.440971	1.767763	0.320080
C	-3.418410	2.583758	0.539433
C	-2.800531	-0.023363	-0.109639
C	-2.570109	-1.363578	-0.496274
C	-5.209236	-0.413977	-0.316488
C	-4.962740	-1.721438	-0.691639
C	-3.635671	-2.201713	-0.785947
H	-5.798822	-2.389669	-0.920921
H	-3.447885	-3.236480	-1.085498
H	-1.542907	-1.729751	-0.566732
H	-3.673779	3.623793	0.789331
H	-1.278063	2.961736	0.677530
H	-6.224349	-0.016052	-0.242399

Quinoline (C5)

28

Mo	1.323978	-0.390513	0.020831
S	3.530332	-0.483192	0.987912
C	4.576224	0.284277	-0.218935
H	5.655639	0.200631	-0.042833
C	4.096451	0.989495	-1.260491
H	4.762767	1.487945	-1.974036
S	2.358194	1.167041	-1.551370
S	0.249944	-0.240309	2.028585
O	-0.459073	0.687546	-0.539827
H	-0.531459	1.161932	-1.381793
C	-1.717162	0.888192	0.253034
H	-1.087312	0.394028	1.345790
C	-2.067684	2.251138	0.460867
O	1.062991	-1.906796	-0.671639
C	-4.157806	0.397999	-0.048861
C	-4.449625	1.749755	0.286048
C	-3.410218	2.643001	0.522196
C	-2.790199	-0.036333	-0.111499
C	-2.528160	-1.372048	-0.480294
N	-5.190259	-0.448977	-0.332110
C	-4.905957	-1.691455	-0.669386
C	-3.594386	-2.210849	-0.765599
H	-5.761714	-2.346441	-0.888861
H	-3.432555	-3.251733	-1.056496
H	-1.496759	-1.728953	-0.542125
H	-3.641682	3.687408	0.756023
H	-1.260786	2.960665	0.661144
H	-5.497335	2.053129	0.322453

Quinoline (C6)

28

Mo	1.756101	-0.437129	-0.221664
S	3.801880	-0.290470	1.053246
C	4.592847	1.183886	0.470846
H	5.618821	1.349390	0.821891
C	3.970067	2.093081	-0.302025
H	4.466218	3.017673	-0.619218
S	2.306607	1.861698	-0.862516
S	0.595664	-1.468237	1.452323
O	-0.232385	0.269578	-0.612375
H	-0.398666	1.122941	-1.040709
C	-1.533703	-0.264643	-0.066187
H	-0.825861	-0.976342	0.865339
C	-2.370524	0.712679	0.526890
O	2.066378	-1.520712	-1.472295
C	-3.513321	-1.310792	-1.079100
C	-4.380743	-0.384982	-0.407988
C	-3.773829	0.644891	0.403000
C	-2.156312	-1.235757	-0.949851
C	-4.665518	1.555474	1.040514
C	-6.027347	1.415610	0.860726
N	-5.717789	-0.501234	-0.570800
C	-6.508747	0.365836	0.039775
H	-3.984238	-2.068668	-1.710285
H	-1.490001	-1.931116	-1.467961
H	-7.589680	0.243658	-0.111025
H	-6.733347	2.098802	1.341724
H	-1.912798	1.485178	1.152126
H	-4.256857	2.354021	1.667621

Quinoline (C7)

28

Mo	1.746586	-0.437292	-0.208881
S	3.797026	-0.293272	1.060527
C	4.594054	1.174450	0.470714
H	5.618637	1.339463	0.825970
C	3.977680	2.080410	-0.311019
H	4.477991	3.001393	-0.631997
S	2.320114	1.845674	-0.886064
S	0.595062	-1.440602	1.483056
O	-0.231916	0.301815	-0.591323
H	-0.370915	1.226041	-0.850213
C	-1.528104	-0.246795	-0.041149
H	-0.830383	-0.927075	0.908620
C	-2.398561	0.722765	0.516215
O	2.030869	-1.541033	-1.448074
C	-3.458559	-1.360529	-1.068131
C	-4.356324	-0.438682	-0.434788
C	-3.797279	0.628125	0.364143
C	-2.107311	-1.255189	-0.914192
N	-4.599632	1.553766	0.974954
C	-5.904680	1.448482	0.826793
C	-5.756053	-0.505472	-0.562088
C	-6.550399	0.440765	0.070602
H	-6.201724	-1.305711	-1.162742
H	-3.878857	-2.153779	-1.695455
H	-1.414739	-1.945814	-1.402806
H	-7.640464	0.418677	-0.003876
H	-6.515874	2.208812	1.334933
H	-1.996924	1.524887	1.140092

Quinoline (C8)

28

Mo	1.364036	-0.498454	0.031145
S	3.526470	-0.177048	1.056839
C	4.499348	0.637712	-0.178442
H	5.569448	0.736847	0.041912
C	3.971411	1.166298	-1.298593
H	4.588901	1.699228	-2.030994
S	2.244892	1.040810	-1.665565
S	0.246609	-0.343955	2.018099
O	-0.486987	0.434103	-0.597490
H	-0.472848	1.006688	-1.379737
C	-1.684459	0.756908	0.210562
H	-1.097184	0.190894	1.310805
C	-1.874471	2.148919	0.452683
O	1.362328	-2.082952	-0.528184
C	-4.174273	0.560389	0.014052
C	-4.301344	1.925352	0.390230
C	-3.155095	2.692352	0.582134
C	-2.871791	-0.034473	-0.128442
N	-2.692097	-1.308139	-0.523828
C	-5.285404	-0.276392	-0.278525
C	-5.078473	-1.581332	-0.680855
C	-3.749100	-2.053089	-0.793808
H	-5.917201	-2.243770	-0.913382
H	-3.556341	-3.084614	-1.115719
H	-3.252843	3.752006	0.839843
H	-0.982304	2.755999	0.626663
H	-5.297806	2.364939	0.487689
H	-6.297201	0.132358	-0.187952

B3LYP transition state coordinates for a concerted reaction mechanism for 2-amino-9-methylpurine (Famciclovir).

Famcilcovir (C6 - Primary SOM)

29

Mo	-1.686402	0.548674	0.091247
S	-3.777076	0.117812	1.223347
C	-4.751174	-0.785663	0.056488
H	-5.797038	-0.957028	0.339017
C	-4.246169	-1.299209	-1.079798
H	-4.858669	-1.887693	-1.772240
S	-2.562019	-1.041639	-1.554125
S	-0.520852	0.451899	2.043652
O	0.178551	-0.327549	-0.617290
H	0.008245	-1.240075	-0.923152
O	-1.764639	2.131358	-0.469388
N	4.611131	1.101151	-0.253263
N	2.495508	1.868807	-0.352616
N	4.172205	-1.255850	0.160702
N	1.818379	-1.746422	0.244675
N	3.393340	-3.426382	0.400359
C	6.054715	1.075385	-0.274316
C	3.790143	0.009940	-0.050076
C	3.763160	2.184387	-0.432652
C	2.481503	0.513727	-0.127861
C	1.436023	-0.442509	0.150763
C	3.113793	-2.077880	0.277091
H	4.158233	3.186042	-0.612864
H	0.820292	-0.029985	1.319135
H	4.332869	-3.639224	0.712419
H	2.642973	-3.980116	0.795911
H	6.482304	1.707273	0.522862
H	6.369117	0.035195	-0.109310
H	6.450927	1.418009	-1.245304

Famcilcovir (C8 - Secondary SOM)

29

Mo	1.972241	-0.612695	-0.044133
S	3.905047	0.107022	1.194857
C	4.693143	1.298060	0.148625
H	5.689088	1.632249	0.463212
C	4.090299	1.822853	-0.933483
H	4.574826	2.588073	-1.550711
S	2.468886	1.321079	-1.437370
S	0.726304	-0.928462	1.853800
O	-0.070505	-0.320254	-0.839910
H	-0.193757	-0.747050	-1.705427
O	2.405652	-2.071740	-0.768528
N	-1.992590	0.698249	0.224630
N	-2.170686	-1.417608	-0.629242
N	-4.347155	1.247046	0.332629
N	-5.773914	-0.534222	-0.438758
N	-6.654766	1.491452	0.264737
C	-1.382748	1.886104	0.783034
C	-3.324527	0.452130	0.060360
C	-1.320902	-0.517197	-0.109447
C	-3.416177	-0.873917	-0.468130
C	-4.717429	-1.320988	-0.702663
C	-5.545228	0.694193	0.051172
H	-0.654087	-0.920035	1.030900
H	-4.915857	-2.324652	-1.097277
H	-6.518345	2.259939	0.910309
H	-7.531158	0.989187	0.338114
H	-0.858325	1.642594	1.721184
H	-0.643955	2.307205	0.082337
H	-2.181005	2.616703	0.972230

B3LYP-D3 transition state coordinates for a concerted reaction mechanism for 2-amino-9-methylpurine (Famciclovir).

Famcilcovir (C6 - Primary SOM)

29

Mo	-1.630241	0.531564	-0.042663
S	-3.748303	0.243000	1.091700
C	-4.724339	-0.739320	-0.009848
H	-5.777256	-0.868092	0.269953
C	-4.214670	-1.357421	-1.091736
H	-4.833125	-1.992933	-1.736136
S	-2.519818	-1.174552	-1.565887
S	-0.493406	0.573539	1.924812
O	0.220079	-0.434090	-0.649720
H	0.053049	-1.373496	-0.859783
O	-1.671613	2.060207	-0.738123
N	4.619449	1.087867	-0.385263
N	2.491490	1.813929	-0.524840
N	4.218944	-1.242047	0.195848
N	1.872105	-1.760482	0.333204
N	3.474334	-3.399308	0.605294
C	6.062634	1.084915	-0.415417
C	3.817196	0.000024	-0.103807
C	3.754313	2.144849	-0.631019
C	2.501246	0.477506	-0.209151
C	1.471055	-0.471404	0.140574
C	3.172815	-2.068308	0.381154
H	4.134570	3.136348	-0.884017
H	0.860143	0.016176	1.252989
H	4.416441	-3.574872	0.932983
H	2.737392	-3.933638	1.050017
H	6.481739	1.792846	0.319776
H	6.398692	0.069173	-0.162776
H	6.445128	1.348745	-1.416197

Famcilcovir (C8 - Secondary SOM)

29

Mo	1.957273	-0.644921	-0.033893
S	3.843576	0.181632	1.221796
C	4.538809	1.450593	0.199382
H	5.507208	1.852700	0.521367
C	3.899214	1.954115	-0.872520
H	4.329271	2.765200	-1.471579
S	2.321022	1.339926	-1.396840
S	0.704103	-1.032647	1.843268
O	-0.074818	-0.476614	-0.876994
H	-0.189176	-0.952892	-1.716843
O	2.475750	-2.074693	-0.759631
N	-1.935287	0.616249	0.187075
N	-2.215197	-1.500067	-0.640666
N	-4.260264	1.269245	0.322228
N	-5.774712	-0.457260	-0.410114
N	-6.555150	1.615607	0.277146
C	-1.251328	1.776215	0.716673
C	-3.277054	0.427402	0.045708
C	-1.324312	-0.629482	-0.140296
C	-3.433810	-0.899353	-0.469952
C	-4.756623	-1.292518	-0.678399
C	-5.485271	0.766377	0.060661
H	-0.671430	-1.046599	1.006663
H	-5.003122	-2.290962	-1.058366
H	-6.376360	2.385123	0.911220
H	-7.452780	1.155644	0.369850
H	-0.794691	1.539746	1.691178
H	-0.443891	2.084198	0.032813
H	-1.988584	2.583350	0.826116

B3LYP transition state coordinates for a concerted reaction mechanism for 4-methylacridine (DACA).

DACA (C1)

37

Mo	2.083549	-0.420906	0.126182
S	4.287855	-0.584075	1.076038
C	5.388348	-0.253037	-0.270284
H	6.452438	-0.429243	-0.072655
C	4.972658	0.245828	-1.448480
H	5.673963	0.480876	-2.256869
S	3.262987	0.559205	-1.777972
S	1.139540	0.352941	2.053025
O	0.465251	0.789374	-0.662042
H	0.549565	1.210568	-1.531216
C	-0.676286	1.403156	0.075954
H	-0.091620	1.066242	1.251315
C	-0.771290	2.812627	-0.047114
O	1.581053	-2.002499	-0.182530
C	-3.207580	1.335655	-0.023732
C	-3.233621	2.773040	-0.015508
C	-2.019916	3.452634	-0.039605
C	-1.932069	0.638674	-0.026918
C	-1.940099	-0.748438	-0.088545
N	-4.375415	0.673061	-0.062960
C	-3.164800	-1.448641	-0.132610
C	-4.378080	-0.669570	-0.109108
H	-0.999264	-1.305443	-0.101921
C	-3.244486	-2.870523	-0.185313
C	-5.628704	-1.366335	-0.143579
C	-4.467162	-3.505486	-0.213111
C	-5.668850	-2.741165	-0.193611
C	-4.557887	3.485041	-0.018790
H	0.152341	3.397395	-0.047319
H	-2.036107	4.548143	-0.053413
H	-2.313202	-3.444191	-0.197619
H	-4.520347	-4.597051	-0.250696
H	-6.633317	-3.258069	-0.217007
H	-6.538402	-0.761183	-0.127186
H	-4.421147	4.577760	0.008138
H	-5.152837	3.227465	-0.912526
H	-5.178094	3.186569	0.843884

DACA (C2)

37

Mo	2.737805	-0.542695	0.050531
S	4.912593	-0.183955	1.013934
C	5.876951	0.474022	-0.315622
H	6.957065	0.542059	-0.138905
C	5.328297	0.930624	-1.456608
H	5.938557	1.370281	-2.253747
S	3.583713	0.876272	-1.747121
S	1.647326	-0.206089	2.027085
O	0.804104	0.169075	-0.639477
H	0.594895	0.087064	-1.582854
C	-0.470395	0.281965	0.132626
H	0.229341	0.015606	1.283237
C	-0.938676	1.657661	0.272378
O	2.718571	-2.165539	-0.403310
C	-2.813097	-0.416295	-0.130319
C	-3.264553	0.949161	0.114995
C	-2.261229	1.990204	0.304153
C	-1.430348	-0.709101	-0.168101
C	-3.817794	-1.382452	-0.325621
N	-4.546234	1.293571	0.161269
C	-5.501177	0.355248	-0.022604
H	-0.169160	2.424024	0.405405
C	-5.174785	-1.029190	-0.275492
H	-3.534958	-2.423363	-0.512891
C	-6.244516	-1.961123	-0.458498
C	-6.872718	0.739449	0.033776
C	-7.557636	-1.551258	-0.397676
C	-7.878100	-0.186460	-0.148428
C	-2.726078	3.405649	0.516387
H	-1.095338	-1.735287	-0.344801
H	-5.998186	-3.010627	-0.648375
H	-8.363892	-2.276893	-0.540983
H	-8.926234	0.122702	-0.102298
H	-7.086937	1.793558	0.226997
H	-3.354717	3.743578	-0.323466
H	-3.361223	3.478536	1.414275
H	-1.872952	4.091744	0.626406

DACA (C3)

37

Mo	2.734332	-0.471633	-0.031511
S	4.816901	0.026146	1.070247
C	5.696916	1.045863	-0.077431
H	6.748363	1.242784	0.163718
C	5.112286	1.610089	-1.150091
H	5.662847	2.270329	-1.829476
S	3.407956	1.331522	-1.535671
S	1.565553	-0.621552	1.927118
O	0.752298	0.129143	-0.676376
H	0.637666	0.580642	-1.527197
C	-0.502974	0.262050	0.122949
H	0.162303	-0.256521	1.207679
C	-0.785808	1.648020	0.475258
O	2.946588	-1.986674	-0.734051
C	-2.916520	-0.136333	-0.136325
C	-3.176537	1.229475	0.313366
C	-2.062389	2.094417	0.597641
C	-1.571017	-0.588642	-0.279960
C	-1.265488	-1.997730	-0.703111
N	-3.935843	-0.973066	-0.425299
C	-4.493952	1.644901	0.443884
C	-5.559688	0.767179	0.150995
C	-6.931561	1.124848	0.269646
C	-5.203641	-0.562410	-0.292257
H	0.070606	2.292115	0.692410
H	-2.263739	3.122993	0.913447
C	-6.270190	-1.470690	-0.597959
C	-7.587125	-1.089664	-0.471681
C	-7.928822	0.220966	-0.033048
H	-5.989567	-2.472420	-0.931800
H	-8.384501	-1.800045	-0.710946
H	-8.980365	0.505493	0.062728
H	-7.182047	2.135696	0.608296
H	-4.709031	2.665237	0.780783
H	-2.189319	-2.519729	-0.979845
H	-0.556368	-2.030377	-1.546239
H	-0.774229	-2.543450	0.124547

DACA (C5)

37

Mo	0.415961	1.851330	0.163900
S	0.606930	4.063395	1.092902
C	0.525695	5.152019	-0.300079
H	0.751681	6.205773	-0.096939
C	0.146218	4.745843	-1.525547
H	0.062381	5.444348	-2.365769
S	-0.244932	3.056230	-1.867841
S	-0.579911	1.014208	2.037513
O	-0.946749	0.391397	-0.697259
H	-1.324357	0.557045	-1.574851
C	-1.722310	-0.653224	-0.008368
H	-1.359616	-0.145137	1.197957
C	-3.132623	-0.564557	-0.178283
O	1.990405	1.272545	0.027151
C	-1.984892	-3.164323	-0.036367
C	-3.401013	-2.990156	-0.052699
C	-3.937235	-1.713187	-0.145898
C	-1.115089	-2.001652	-0.080876
N	0.202130	-2.089000	-0.140828
C	-1.349499	-4.414864	-0.025933
C	0.807701	-3.291777	-0.139333
C	0.050609	-4.518805	-0.066838
C	2.246071	-3.336081	-0.202514
C	0.748970	-5.765601	-0.050039
C	2.865435	-4.572478	-0.178018
C	2.122534	-5.784405	-0.101727
H	-3.584760	0.430430	-0.216000
H	-5.024315	-1.589870	-0.191874
H	3.958004	-4.621490	-0.219179
H	2.658751	-6.738342	-0.085064
H	0.174080	-6.695300	0.006207
C	3.017489	-2.049316	-0.297183
H	-4.047139	-3.871811	-0.030518
H	-1.956142	-5.326241	0.004751
H	4.102293	-2.235301	-0.273593
H	2.771587	-1.506621	-1.224410
H	2.747712	-1.349914	0.508554

DACA (C6)

37

Mo	2.806216	-0.520851	0.080659
S	4.991379	-0.163186	1.021247
C	5.963487	0.417720	-0.337848
H	7.045177	0.473276	-0.166597
C	5.419620	0.834394	-1.496258
H	6.035222	1.226927	-2.313564
S	3.673438	0.799739	-1.779682
S	1.738996	-0.065139	2.047119
O	0.884239	0.207972	-0.628667
H	0.652395	0.088784	-1.562718
C	-0.352169	0.496217	0.149074
H	0.334711	0.198305	1.311643
C	-0.648921	1.923437	0.252611
O	2.752066	-2.160865	-0.300080
C	-2.774299	0.050395	-0.047301
C	-3.047602	1.468050	0.157404
C	-1.931735	2.371280	0.292598
C	-1.429357	-0.386857	-0.096947
N	-3.773369	-0.842894	-0.199003
C	-4.371180	1.881231	0.197065
C	-5.422301	0.949657	0.046445
H	0.199823	2.605288	0.349503
C	-5.049016	-0.432807	-0.152803
C	-6.095622	-1.417510	-0.307239
C	-6.797480	1.313802	0.082076
C	-7.413890	-1.006255	-0.264424
C	-7.775351	0.355890	-0.070929
H	-2.138415	3.438879	0.420831
H	-1.238538	-1.452319	-0.244055
H	-8.206351	-1.752694	-0.382498
H	-8.832710	0.634052	-0.043586
H	-7.061042	2.365575	0.233261
C	-5.708353	-2.857004	-0.505625
H	-4.606370	2.941050	0.346583
H	-6.595810	-3.500687	-0.609539
H	-5.071905	-2.975124	-1.397783
H	-5.099205	-3.219543	0.338643

DACA (C7)

37

Mo	2.887383	-0.473755	0.031864
S	5.059402	-0.121166	1.004416
C	6.004303	0.629298	-0.289867
H	7.082944	0.713674	-0.111336
C	5.441851	1.132914	-1.403864
H	6.038606	1.629695	-2.177328
S	3.698384	1.051408	-1.692866
S	1.798353	-0.260719	2.026330
O	0.943251	0.248850	-0.612843
H	0.734848	0.235942	-1.559919
C	-0.331224	0.303328	0.166082
H	0.375588	-0.022988	1.297876
C	-0.817851	1.662146	0.393598
O	2.892928	-2.072604	-0.501124
C	-2.672262	-0.411138	-0.153537
C	-3.142444	0.925768	0.182578
C	-2.148119	1.941869	0.438078
C	-1.282930	-0.676567	-0.200491
C	-3.666086	-1.370566	-0.423308
N	-4.429471	1.254020	0.249453
C	-5.372819	0.322845	-0.002116
H	-0.066880	2.434980	0.579287
C	-5.026827	-1.035649	-0.354145
H	-3.373436	-2.392639	-0.684841
C	-6.076974	-1.971592	-0.612448
C	-6.757250	0.704479	0.084895
C	-7.391892	-1.580987	-0.525590
C	-7.729713	-0.243268	-0.175338
H	-2.513757	2.947660	0.658812
H	-0.931759	-1.683871	-0.443311
H	-5.813142	-2.999524	-0.879699
H	-8.192175	-2.299784	-0.725858
H	-8.785260	0.039917	-0.110407
C	-7.101751	2.121343	0.458046
H	-8.191841	2.273443	0.484360
H	-6.681267	2.383647	1.442605
H	-6.657984	2.836010	-0.253994

DACA (C8)

37

Mo	2.152679	-0.413484	0.155685
S	4.354792	-0.677847	1.083773
C	5.453599	-0.484641	-0.291038
H	6.506432	-0.723446	-0.098888
C	5.054365	-0.010479	-1.484895
H	5.756916	0.139629	-2.312221
S	3.363800	0.398186	-1.808210
S	1.289771	0.475808	2.067905
O	0.615654	0.884973	-0.655277
H	0.764060	1.329629	-1.504308
C	-0.479933	1.578153	0.079981
H	0.089546	1.230965	1.261128
C	-0.489296	2.992035	-0.056766
O	1.533594	-1.964799	-0.084091
C	-3.007793	1.645656	0.006463
C	-2.932867	3.070992	0.012859
C	-1.698794	3.703249	-0.035367
C	-1.774666	0.879310	-0.008220
C	-1.862848	-0.505040	-0.076858
N	-4.212526	1.049995	-0.024456
C	-3.124951	-1.133765	-0.117238
C	-4.293457	-0.288546	-0.079243
H	-0.957070	-1.116743	-0.101532
C	-3.275608	-2.549168	-0.187414
C	-5.600857	-0.902046	-0.109191
C	-4.532010	-3.108714	-0.215896
C	-5.687832	-2.278174	-0.176149
H	-3.870811	3.628708	0.021038
H	0.468781	3.518809	-0.065789
H	-1.658683	4.797344	-0.056365
H	-2.376697	-3.171575	-0.214078
H	-4.652553	-4.194504	-0.267937
H	-6.677091	-2.747606	-0.199224
C	-6.818069	-0.019359	-0.067618
H	-7.744840	-0.613187	-0.100645
H	-6.824076	0.601936	0.843111
H	-6.818344	0.691789	-0.910190

DACA (C9 - Primary SOM)

37

Mo	1.993667	-0.529154	0.088718
S	3.955339	0.363334	1.152500
C	4.812790	1.214352	-0.141455
H	5.826485	1.555292	0.100536
C	4.250344	1.497949	-1.330249
H	4.784244	2.059402	-2.104749
S	2.607687	0.976235	-1.733555
S	0.736892	-0.370526	1.993980
O	-0.005192	-0.188895	-0.736674
H	-0.070281	0.322809	-1.559638
C	-1.293210	-0.164199	-0.039029
H	-0.627181	-0.293308	1.202348
C	-1.968475	1.114412	-0.032694
O	2.336486	-2.139130	-0.270400
C	-3.538383	-1.192217	-0.113315
N	-4.155141	-0.001994	0.035494
C	-3.407430	1.116047	0.050233
C	-2.110412	-1.345938	-0.213222
C	-1.254989	2.340205	-0.043667
C	-4.089392	2.386086	0.133308
C	-3.349290	3.553551	0.113905
C	-1.934841	3.540940	0.020550
C	-1.550088	-2.632481	-0.413152
C	-4.341213	-2.372691	-0.205374
C	-2.363026	-3.748013	-0.508560
C	-3.770648	-3.612592	-0.397959
C	-5.590877	2.391228	0.226473
H	-0.164217	2.327766	-0.104850
H	-1.381808	4.483935	0.010113
H	-3.871517	4.514566	0.171422
H	-5.422957	-2.239955	-0.126315
H	-4.406739	-4.500527	-0.469306
H	-1.918728	-4.734781	-0.664123
H	-0.464791	-2.733525	-0.487856
H	-5.985004	3.418282	0.280497
H	-6.041775	1.878441	-0.639206
H	-5.932861	1.829462	1.111578

B3LYP-D3 transition state coordinates for a concerted reaction mechanism for 4-methylacridine (DACA).

DACA (C1)

37

Mo	2.024479	-0.368735	0.128654
S	4.216194	-0.652626	1.079736
C	5.327484	-0.407230	-0.278636
H	6.379754	-0.651090	-0.088406
C	4.937304	0.110327	-1.458439
H	5.649377	0.290631	-2.271942
S	3.249938	0.539925	-1.780814
S	1.107132	0.457205	2.044067
O	0.453376	0.893236	-0.671793
H	0.454661	1.202234	-1.590230
C	-0.705455	1.478577	0.052847
H	-0.123939	1.174493	1.232021
C	-0.847375	2.882270	-0.085784
O	1.433221	-1.921703	-0.173018
C	-3.229412	1.317196	-0.022286
C	-3.304793	2.752347	-0.007415
C	-2.117461	3.476718	-0.056596
C	-1.930614	0.668419	-0.042581
C	-1.882237	-0.716667	-0.112006
N	-4.372571	0.612358	-0.054022
C	-3.080122	-1.460912	-0.152093
C	-4.322644	-0.729128	-0.112617
H	-0.922334	-1.238760	-0.135927
C	-3.102135	-2.883580	-0.222134
C	-5.544640	-1.474571	-0.145009
C	-4.299173	-3.566031	-0.251143
C	-5.529994	-2.849627	-0.212176
C	-4.655720	3.410972	0.016508
H	0.058961	3.492315	-0.102926
H	-2.175158	4.570738	-0.073270
H	-2.147311	-3.416989	-0.248182
H	-4.309622	-4.658245	-0.303201
H	-6.473392	-3.403977	-0.235950
H	-6.477698	-0.906570	-0.114909
H	-4.566183	4.508678	0.042405
H	-5.256642	3.125689	-0.864696
H	-5.243552	3.083100	0.891213

DACA (C2)

37

Mo	2.735001	-0.547545	0.055480
S	4.922204	-0.181724	0.998767
C	5.865320	0.483431	-0.344532
H	6.947580	0.558527	-0.182815
C	5.301240	0.937648	-1.479853
H	5.902587	1.379590	-2.282817
S	3.552401	0.873874	-1.752843
S	1.644764	-0.206874	2.030066
O	0.805784	0.148800	-0.637827
H	0.598501	0.097395	-1.583545
C	-0.465981	0.266514	0.136806
H	0.221570	0.004621	1.281537
C	-0.925542	1.644789	0.271167
O	2.716574	-2.170227	-0.395384
C	-2.807307	-0.424806	-0.130301
C	-3.252582	0.943963	0.112969
C	-2.246047	1.981893	0.300374
C	-1.426800	-0.723269	-0.165623
C	-3.816157	-1.386347	-0.325431
N	-4.532170	1.294872	0.159559
C	-5.491037	0.360578	-0.022840
H	-0.148128	2.402827	0.404177
C	-5.170965	-1.025932	-0.275387
H	-3.538301	-2.428744	-0.511632
C	-6.244646	-1.952951	-0.457984
C	-6.860357	0.751210	0.034407
C	-7.555981	-1.536956	-0.396441
C	-7.870140	-0.170453	-0.147019
C	-2.711102	3.397224	0.509800
H	-1.088524	-1.748548	-0.339002
H	-6.002438	-3.003382	-0.648051
H	-8.365710	-2.258752	-0.539454
H	-8.916799	0.143379	-0.099947
H	-7.069597	1.806346	0.227666
H	-3.339457	3.730354	-0.332127
H	-3.349888	3.466837	1.405282
H	-1.860226	4.085961	0.621590

DACA (C3)

37

Mo	2.708876	-0.476041	-0.044910
S	4.819387	-0.048340	1.042561
C	5.699614	0.987037	-0.092735
H	6.758056	1.161201	0.136175
C	5.109797	1.590219	-1.142143
H	5.664596	2.258625	-1.810408
S	3.394660	1.352308	-1.512126
S	1.543616	-0.630026	1.914401
O	0.742801	0.163512	-0.678308
H	0.616677	0.596314	-1.536849
C	-0.509144	0.292992	0.124083
H	0.143829	-0.231146	1.203253
C	-0.794740	1.677229	0.474266
O	2.883967	-1.981454	-0.776751
C	-2.914701	-0.125414	-0.135933
C	-3.182020	1.240971	0.311533
C	-2.074223	2.114873	0.596522
C	-1.567972	-0.567067	-0.275940
C	-1.229848	-1.973557	-0.677441
N	-3.927513	-0.970262	-0.423487
C	-4.501776	1.648189	0.441158
C	-5.561350	0.762969	0.148697
C	-6.934951	1.113469	0.266525
C	-5.197308	-0.566122	-0.291898
H	0.063128	2.320495	0.687069
H	-2.284195	3.141904	0.911850
C	-6.258636	-1.480552	-0.596843
C	-7.577766	-1.105857	-0.472415
C	-7.927087	0.203563	-0.035637
H	-5.972366	-2.481208	-0.929144
H	-8.371181	-1.820948	-0.710885
H	-8.980274	0.482436	0.058886
H	-7.190543	2.123502	0.603874
H	-4.724500	2.667208	0.776846
H	-2.134013	-2.522229	-0.967763
H	-0.497752	-1.997183	-1.500823
H	-0.741253	-2.492639	0.169177

DACA (C5)

37

Mo	0.342441	1.902102	0.265972
S	0.625293	4.092573	1.220437
C	0.725731	5.153528	-0.192984
H	1.054518	6.182406	-0.002733
C	0.348971	4.759530	-1.425196
H	0.377465	5.449721	-2.276732
S	-0.224341	3.121139	-1.768503
S	-0.849332	1.128351	2.009772
O	-0.720735	0.250174	-0.781481
H	0.058688	-0.366188	-0.891576
C	-1.671799	-0.632042	-0.126198
H	-1.520701	-0.171300	1.046061
C	-3.067854	-0.531689	-0.460469
O	1.885533	1.215664	0.209470
C	-1.985850	-3.149049	0.042265
C	-3.389240	-2.933820	-0.016328
C	-3.881641	-1.653128	-0.310948
C	-1.116776	-2.005869	-0.111508
N	0.189872	-2.077244	-0.262812
C	-1.327308	-4.388520	0.139391
C	0.826497	-3.267528	-0.173585
C	0.075988	-4.477344	0.063295
C	2.252536	-3.300527	-0.303085
C	0.793470	-5.708344	0.173492
C	2.891627	-4.523128	-0.177961
C	2.164577	-5.722625	0.058905
H	-3.487129	0.457818	-0.653615
H	-4.962480	-1.526066	-0.435021
H	3.981728	-4.567134	-0.260801
H	2.710482	-6.666573	0.151155
H	0.234660	-6.631892	0.353324
C	2.995898	-2.018194	-0.564472
H	-4.068808	-3.783591	0.086556
H	-1.915526	-5.305278	0.252103
H	4.084830	-2.176167	-0.536652
H	2.732575	-1.609081	-1.554925
H	2.724763	-1.227895	0.153420

DACA (C6)

37

Mo	2.814589	-0.528286	0.077616
S	5.010537	-0.119008	0.985337
C	5.932220	0.528068	-0.381002
H	7.015287	0.617371	-0.232753
C	5.350812	0.951716	-1.519451
H	5.937289	1.385172	-2.337770
S	3.600064	0.860108	-1.770050
S	1.752102	-0.143085	2.058057
O	0.876777	0.146272	-0.603857
H	0.650880	0.119297	-1.546224
C	-0.350933	0.427756	0.192070
H	0.329562	0.101260	1.332215
C	-0.625061	1.855696	0.332321
O	2.804667	-2.160511	-0.333527
C	-2.774876	0.018555	-0.026530
C	-3.028001	1.435447	0.213624
C	-1.901130	2.320297	0.378256
C	-1.437343	-0.436420	-0.078841
N	-3.785581	-0.855273	-0.209704
C	-4.344980	1.867707	0.256414
C	-5.408396	0.956181	0.073045
H	0.237668	2.515776	0.451800
C	-5.054513	-0.425667	-0.162216
C	-6.113742	-1.388950	-0.354119
C	-6.777943	1.339706	0.108667
C	-7.426157	-0.960246	-0.309335
C	-7.768885	0.401143	-0.078594
H	-2.095207	3.386508	0.534460
H	-1.252950	-1.498040	-0.255757
H	-8.228446	-1.691209	-0.454220
H	-8.822078	0.694484	-0.051881
H	-7.026726	2.390780	0.287304
C	-5.740497	-2.825598	-0.593527
H	-4.565427	2.926127	0.432875
H	-6.631749	-3.459088	-0.724642
H	-5.096344	-2.918521	-1.483192
H	-5.140053	-3.217285	0.243909

DACA (C7)

37

Mo	2.882944	-0.475511	0.038428
S	5.063572	-0.130569	1.004962
C	6.000088	0.626306	-0.293783
H	7.080327	0.710418	-0.123307
C	5.431873	1.134938	-1.403571
H	6.026986	1.633995	-2.177194
S	3.685395	1.054871	-1.685637
S	1.787046	-0.257261	2.027226
O	0.947003	0.240882	-0.618898
H	0.742502	0.239934	-1.566694
C	-0.327567	0.298076	0.157430
H	0.363909	-0.024550	1.290133
C	-0.807811	1.658638	0.381725
O	2.883082	-2.072711	-0.497142
C	-2.665286	-0.414611	-0.162096
C	-3.132332	0.924487	0.174315
C	-2.137039	1.940946	0.426742
C	-1.277648	-0.682335	-0.209849
C	-3.660360	-1.372932	-0.429774
N	-4.418284	1.254519	0.244980
C	-5.362826	0.323657	-0.003262
H	-0.049817	2.424672	0.565498
C	-5.019906	-1.035521	-0.356564
H	-3.369200	-2.395322	-0.691584
C	-6.072330	-1.969587	-0.611233
C	-6.745581	0.707028	0.089456
C	-7.386437	-1.576677	-0.518939
C	-7.721185	-0.238386	-0.166868
H	-2.501987	2.947238	0.646299
H	-0.921313	-1.687774	-0.451347
H	-5.810791	-2.997816	-0.879622
H	-8.188584	-2.294416	-0.715496
H	-8.775366	0.046301	-0.097584
C	-7.080493	2.125242	0.464986
H	-8.169089	2.286659	0.498855
H	-6.649041	2.382258	1.446161
H	-6.633648	2.835262	-0.249750

DACA (C8)

37

Mo	2.133452	-0.374207	0.162163
S	4.320861	-0.744107	1.094530
C	5.423203	-0.602461	-0.286018
H	6.462832	-0.900186	-0.103276
C	5.044702	-0.099549	-1.475862
H	5.752836	0.015569	-2.304456
S	3.378845	0.412218	-1.788876
S	1.279820	0.530676	2.071556
O	0.626244	0.955501	-0.645373
H	0.670314	1.288517	-1.554514
C	-0.474184	1.641639	0.082731
H	0.091554	1.302277	1.263657
C	-0.493468	3.054159	-0.057904
O	1.459486	-1.899268	-0.095606
C	-2.999603	1.682669	0.014233
C	-2.937742	3.108398	0.020917
C	-1.709393	3.753506	-0.031206
C	-1.759120	0.929734	-0.001375
C	-1.826790	-0.455533	-0.064015
N	-4.197644	1.073764	-0.017400
C	-3.081465	-1.097839	-0.104028
C	-4.260291	-0.265881	-0.070631
H	-0.912891	-1.054836	-0.085715
C	-3.214669	-2.514852	-0.172177
C	-5.559513	-0.894922	-0.104427
C	-4.464634	-3.088928	-0.204523
C	-5.630662	-2.271827	-0.169982
H	-3.880872	3.657397	0.031357
H	0.463355	3.581720	-0.076716
H	-1.681239	4.847900	-0.053318
H	-2.307449	-3.125277	-0.195213
H	-4.572557	-4.176046	-0.256058
H	-6.614275	-2.752690	-0.196346
C	-6.783722	-0.022123	-0.067768
H	-7.707748	-0.620175	-0.104162
H	-6.793624	0.599538	0.842687
H	-6.781912	0.689456	-0.909951

DACA (C9 - Primary SOM)

37

Mo	1.983760	-0.538562	0.081780
S	3.966104	0.318552	1.146745
C	4.807689	1.197475	-0.140599
H	5.828429	1.525552	0.090562
C	4.227607	1.517808	-1.312564
H	4.755357	2.095378	-2.079733
S	2.571236	1.023368	-1.701565
S	0.723012	-0.396236	1.982240
O	-0.008522	-0.220676	-0.746520
H	-0.095245	0.226169	-1.603896
C	-1.292355	-0.179603	-0.045118
H	-0.639205	-0.316530	1.188406
C	-1.942047	1.108566	-0.033410
O	2.316668	-2.143936	-0.304550
C	-3.549442	-1.171039	-0.117081
N	-4.146741	0.029061	0.031990
C	-3.379126	1.134597	0.055108
C	-2.124388	-1.346630	-0.218451
C	-1.199053	2.315175	-0.040657
C	-4.033819	2.416903	0.147947
C	-3.268815	3.568780	0.133893
C	-1.854511	3.528864	0.034701
C	-1.574923	-2.637923	-0.409768
C	-4.366259	-2.341710	-0.209133
C	-2.401360	-3.743722	-0.501990
C	-3.808212	-3.588754	-0.396388
C	-5.534674	2.447850	0.241777
H	-0.109367	2.273263	-0.111450
H	-1.283440	4.460990	0.027357
H	-3.770959	4.539854	0.200256
H	-5.446821	-2.197719	-0.132965
H	-4.454793	-4.469130	-0.466797
H	-1.970325	-4.737305	-0.650947
H	-0.489685	-2.745565	-0.479410
H	-5.911996	3.477744	0.342826
H	-5.991803	1.983076	-0.647870
H	-5.885298	1.848925	1.098265

B3LYP-D3 transition state coordinates for a concerted reaction mechanism for phenanthridine.

Phenanthridine (C1)

34

Mo	1.923798	-0.544243	0.029059
S	3.784232	0.561489	1.086476
C	4.463598	1.597652	-0.177906
H	5.428913	2.065998	0.049215
C	3.814611	1.859999	-1.326893
H	4.229921	2.534460	-2.084411
S	2.236168	1.147679	-1.694724
S	0.723089	-0.656250	1.975424
O	-0.121658	-0.559770	-0.717916
H	-0.208621	-0.706466	-1.673539
C	-1.279534	-1.254151	-0.027173
H	-0.634647	-1.019313	1.179065
C	-2.564978	-0.568242	-0.084646
O	2.495745	-2.056864	-0.454066
C	-2.428238	-3.396930	-0.402833
C	-3.669787	-2.764389	-0.399730
C	-3.747353	-1.360444	-0.256556
C	-1.255905	-2.661820	-0.265666
N	-5.012359	-0.804427	-0.318316
C	-2.724614	0.860328	0.082099
C	-4.048583	1.394671	0.000269
C	-5.137044	0.481453	-0.207734
C	-1.664013	1.772781	0.339392
C	-4.275870	2.782659	0.143009
C	-3.221579	3.648180	0.377400
C	-1.913669	3.128209	0.482804
H	-0.275813	-3.147171	-0.282260
H	-2.366213	-4.481799	-0.532729
H	-4.605148	-3.310864	-0.529760
H	-5.301879	3.157396	0.068503
H	-3.397266	4.722262	0.485504
H	-0.645072	1.410048	0.442224
H	-1.074208	3.800527	0.680062
H	-6.154966	0.897425	-0.268530

Phenanthridine (C2)

34

Mo	2.414936	-0.469047	0.116532
S	4.622307	-0.212245	1.042052
C	5.619405	0.328548	-0.316466
H	6.701972	0.343873	-0.141962
C	5.095258	0.761556	-1.477702
H	5.726059	1.130359	-2.294521
S	3.349628	0.784121	-1.764134
S	1.377509	0.033318	2.092212
O	0.566959	0.407582	-0.578306
H	0.429285	0.614796	-1.515272
C	-0.664928	0.774796	0.195694
H	0.012223	0.442297	1.356827
C	-0.934884	2.194383	0.238043
O	2.263969	-2.106537	-0.250432
C	-3.092277	0.369029	-0.017607
C	-3.341150	1.778555	0.121736
C	-2.224284	2.659692	0.234954
C	-1.770018	-0.095985	-0.027008
C	-4.257828	-0.497619	-0.154694
N	-4.593312	2.324052	0.131222
C	-5.629771	1.538788	0.012485
C	-5.547668	0.111758	-0.135603
C	-6.708015	-0.691977	-0.259635
C	-4.184990	-1.904102	-0.297190
C	-5.333181	-2.673041	-0.415993
C	-6.607110	-2.065129	-0.399165
H	-0.083067	2.873590	0.329751
H	-2.442184	3.727772	0.313425
H	-6.625375	2.005979	0.025040
H	-1.546878	-1.158644	-0.141766
H	-7.688286	-0.205148	-0.242328
H	-7.507362	-2.678913	-0.493221
H	-5.248796	-3.758208	-0.521917
H	-3.211367	-2.397479	-0.305436

Phenanthridine (C3)

34

Mo	2.693200	-0.426734	-0.007862
S	4.709611	0.175557	1.167652
C	5.510243	1.354830	0.119317
H	6.531457	1.635241	0.404089
C	4.895986	1.933369	-0.928769
H	5.393400	2.691310	-1.544507
S	3.236229	1.521818	-1.380005
S	1.527001	-0.826858	1.916896
O	0.685538	0.061823	-0.614256
H	0.508339	0.478816	-1.471535
C	-0.609693	-0.091092	0.138031
H	0.113356	-0.597776	1.195238
C	-1.183109	1.163786	0.572384
O	3.048501	-1.860389	-0.817215
C	-2.893851	-0.853938	-0.388770
C	-3.453842	0.364207	0.129270
C	-2.541620	1.357118	0.592930
C	-1.504432	-1.046040	-0.416370
N	-3.690544	-1.871238	-0.890771
C	-4.885454	0.516187	0.134684
C	-4.978566	-1.721312	-0.877745
C	-5.671794	-0.560313	-0.381458
C	-5.577429	1.662085	0.616846
C	-7.081785	-0.471792	-0.401036
C	-6.960331	1.727165	0.587482
C	-7.728604	0.656362	0.076592
H	-0.499205	1.935988	0.934311
H	-2.925561	2.307452	0.971749
H	-1.119257	-1.983043	-0.823674
H	-5.013890	2.505203	1.020798
H	-7.464571	2.621577	0.965762
H	-8.819766	0.721939	0.059441
H	-7.655290	-1.314058	-0.801621
H	-5.585727	-2.547853	-1.279494

Phenanthridine (C4)

34

Mo	2.213154	-0.555478	0.152438
S	4.400201	-0.266527	1.121297
C	5.405604	0.351576	-0.196828
H	6.482557	0.400405	0.004890
C	4.894793	0.800636	-1.357937
H	5.531340	1.215501	-2.147667
S	3.158633	0.754741	-1.691631
S	1.154728	-0.133786	2.134808
O	0.395420	0.419048	-0.529254
H	0.418341	0.875159	-1.384704
C	-0.742055	0.941926	0.265624
H	-0.161121	0.423721	1.407859
C	-0.766829	2.366722	0.377666
O	2.111598	-2.184114	-0.254285
C	-3.242926	1.004323	0.129090
C	-3.202503	2.398495	0.358987
C	-1.971406	3.053799	0.463984
C	-2.018546	0.267700	0.031043
N	-1.975085	-1.067982	-0.226565
C	-4.479874	0.257112	-0.050296
C	-4.389578	-1.141542	-0.315079
C	-3.084118	-1.732419	-0.392923
C	-5.771907	0.836503	0.022043
C	-5.568569	-1.907238	-0.494643
C	-6.815718	-1.314327	-0.416297
C	-6.913401	0.070570	-0.155552
H	0.189664	2.886975	0.473442
H	-1.953897	4.138283	0.611606
H	-4.125227	2.976315	0.424846
H	-3.002766	-2.809041	-0.599932
H	-5.875174	1.904099	0.223813
H	-7.898039	0.543144	-0.092019
H	-7.722258	-1.910330	-0.554806
H	-5.472240	-2.978691	-0.695877

Phenanthridine (C6 - Primary SOM)

34

Mo	2.017612	-0.357218	0.053682
S	4.084457	0.245423	1.140406
C	4.980352	1.173636	-0.068431
H	6.017164	1.418834	0.190762
C	4.421738	1.623981	-1.206312
H	4.982909	2.234246	-1.922726
S	2.748953	1.254125	-1.640469
S	0.858518	-0.298344	1.986416
O	0.082238	0.251009	-0.722300
H	0.093977	1.159744	-1.079578
C	-1.205148	0.212800	0.047287
H	-0.593473	0.016670	1.193478
N	-1.787991	1.418891	-0.009571
O	2.179192	-1.953600	-0.471248
C	-3.411626	-0.925046	-0.145761
C	-4.018966	0.393536	0.034733
C	-3.137027	1.527199	0.045377
C	-1.996054	-1.023836	-0.198407
C	-1.378046	-2.270406	-0.416299
C	-4.166726	-2.109843	-0.312574
C	-2.146316	-3.418205	-0.578798
C	-3.547346	-3.335201	-0.520442
C	-3.709962	2.829684	0.118216
C	-5.407477	0.611710	0.139913
C	-5.941383	1.892829	0.233321
C	-5.079072	3.008023	0.212629
H	-6.087461	-0.243509	0.148555
H	-7.022672	2.031603	0.319130
H	-5.493199	4.019037	0.279250
H	-3.019372	3.676183	0.113450
H	-0.289423	-2.336971	-0.461122
H	-1.655961	-4.380214	-0.750417
H	-4.155867	-4.235923	-0.645897
H	-5.257188	-2.063264	-0.289796

Phenanthridine (C7)

34

Mo	2.176416	-0.500583	0.145175
S	4.397491	-0.401163	1.070029
C	5.418000	0.170556	-0.258703
H	6.499779	0.130263	-0.083815
C	4.915829	0.687847	-1.394443
H	5.562087	1.073159	-2.191035
S	3.173125	0.783946	-1.682493
S	1.168600	-0.037370	2.143634
O	0.388902	0.534675	-0.511234
H	0.396467	0.988336	-1.368726
C	-0.756861	1.049151	0.300061
H	-0.135741	0.558522	1.439948
C	-0.810431	2.471510	0.404365
O	1.909786	-2.106504	-0.286308
C	-3.252143	1.047604	0.148656
C	-3.248776	2.442547	0.373866
C	-2.033743	3.127204	0.483272
C	-2.013191	0.346389	0.074734
C	-2.028598	-1.061005	-0.182845
C	-4.462644	0.261124	-0.049114
C	-4.325069	-1.139400	-0.300608
N	-3.109802	-1.775409	-0.366221
C	-5.767972	0.810157	-0.007976
C	-5.489686	-1.926951	-0.496952
C	-6.751204	-1.362368	-0.448479
C	-6.890591	0.020273	-0.201729
H	0.132183	3.016495	0.500042
H	-2.043680	4.212170	0.628121
H	-4.184833	2.998478	0.432748
H	-5.897740	1.877601	0.181880
H	-7.886434	0.471246	-0.162778
H	-7.639102	-1.982724	-0.601920
H	-5.338313	-2.992198	-0.686222
H	-1.069303	-1.590010	-0.238913

Phenanthridine (C8)

34

Mo	2.679781	-0.487219	-0.070960
S	4.710076	0.092588	1.089256
C	5.510045	1.274783	0.043532
H	6.535328	1.546026	0.322213
C	4.891149	1.865338	-0.994922
H	5.387598	2.624846	-1.609304
S	3.225563	1.464946	-1.435467
S	1.527392	-0.889855	1.862853
O	0.670178	0.027748	-0.655476
H	0.500241	0.519272	-1.474054
C	-0.617832	-0.114598	0.112579
H	0.111880	-0.636493	1.157183
C	-1.176542	1.142913	0.559437
O	3.013301	-1.919999	-0.891285
C	-2.916035	-0.837511	-0.387401
C	-3.459099	0.375060	0.141171
C	-2.532951	1.357146	0.598025
C	-1.530939	-1.054799	-0.438530
C	-3.848619	-1.825463	-0.879934
C	-4.894590	0.525470	0.156951
N	-5.141837	-1.704242	-0.872314
C	-5.692377	-0.546124	-0.361386
C	-5.569448	1.671164	0.656374
C	-7.102740	-0.434829	-0.360917
C	-6.952546	1.756057	0.644821
C	-7.731776	0.696489	0.132819
H	-0.479313	1.905560	0.917105
H	-2.898836	2.311439	0.983614
H	-1.138174	-1.986944	-0.854959
H	-4.989956	2.503359	1.061593
H	-7.442115	2.652403	1.037059
H	-8.822868	0.770094	0.126940
H	-7.666753	-1.278457	-0.766044
H	-3.433720	-2.757792	-1.291364

Phenanthridine (C9)

34

Mo	2.395510	-0.517034	0.084379
S	4.604754	-0.246395	1.000535
C	5.586573	0.322452	-0.357288
H	6.669619	0.349260	-0.187867
C	5.052057	0.760783	-1.511617
H	5.673604	1.145590	-2.327997
S	3.304886	0.761316	-1.788491
S	1.363913	-0.046986	2.071922
O	0.540024	0.358291	-0.583902
H	0.394778	0.562681	-1.520693
C	-0.681179	0.725262	0.197892
H	0.003969	0.364326	1.359423
C	-0.926460	2.148371	0.274540
O	2.258261	-2.151202	-0.300524
C	-3.111246	0.358723	-0.003930
C	-3.332385	1.765237	0.155882
C	-2.208071	2.632655	0.283681
C	-1.798572	-0.129000	-0.028044
C	-4.303258	-0.472896	-0.146994
C	-4.669922	2.256385	0.156632
N	-5.747540	1.527022	0.023281
C	-5.582574	0.167951	-0.126197
C	-6.752203	-0.623027	-0.263496
C	-4.256848	-1.878962	-0.297402
C	-5.415581	-2.630079	-0.429183
C	-6.675629	-1.996698	-0.413420
H	-0.062662	2.810624	0.374703
H	-2.384739	3.708914	0.382080
H	-1.591481	-1.192237	-0.163299
H	-7.709752	-0.097161	-0.242816
H	-7.588357	-2.591080	-0.515821
H	-5.348867	-3.715621	-0.543196
H	-3.290497	-2.387363	-0.304065
H	-4.817017	3.341039	0.275874

Phenanthridine (C10)

34

Mo	1.934600	-0.566206	0.018875
S	3.801306	0.521280	1.080081
C	4.490023	1.555059	-0.181098
H	5.458553	2.015277	0.048654
C	3.844901	1.823426	-1.330764
H	4.266002	2.496979	-2.085752
S	2.262277	1.123518	-1.704405
S	0.737020	-0.680345	1.968134
O	-0.118687	-0.552922	-0.721398
H	-0.218816	-0.660955	-1.680932
C	-1.270353	-1.247255	-0.039143
H	-0.624352	-1.021534	1.175659
C	-2.558375	-0.564843	-0.079944
O	2.492739	-2.081264	-0.471825
C	-2.423574	-3.397365	-0.402253
C	-3.666565	-2.767096	-0.372608
C	-3.731427	-1.362812	-0.228941
C	-1.252661	-2.655614	-0.285954
C	-5.006467	-0.691994	-0.260062
C	-2.739119	0.863398	0.078307
C	-4.073414	1.386962	0.017185
N	-5.184776	0.588753	-0.157082
C	-1.680210	1.783712	0.308345
C	-4.294473	2.777852	0.154125
C	-3.239481	3.648418	0.365713
C	-1.927110	3.140015	0.450084
H	-0.271996	-3.139119	-0.320808
H	-2.358524	-4.481424	-0.535961
H	-4.592860	-3.336761	-0.483197
H	-5.904230	-1.316370	-0.388005
H	-5.329119	3.123703	0.093562
H	-3.421483	4.721864	0.472333
H	-0.658311	1.423241	0.389693
H	-1.086416	3.816195	0.626876

B3LYP-D3 transition state coordinates for a concerted reaction mechanism for phenanthridine.

Phenanthridine (C1)

34

Mo	1.914437	-0.603514	0.015486
S	3.780861	0.506716	1.069230
C	4.414954	1.589127	-0.181807
H	5.375498	2.071280	0.037763
C	3.739605	1.869795	-1.312007
H	4.129963	2.571813	-2.057978
S	2.167918	1.134682	-1.670644
S	0.724319	-0.758084	1.964565
O	-0.118233	-0.614003	-0.725245
H	-0.239243	-0.696046	-1.684229
C	-1.298358	-1.265428	-0.034000
H	-0.649033	-1.072677	1.165171
C	-2.544685	-0.514824	-0.078272
O	2.493006	-2.100573	-0.502605
C	-2.551773	-3.341022	-0.429067
C	-3.760501	-2.645517	-0.413664
C	-3.766855	-1.240907	-0.256316
C	-1.342846	-2.669456	-0.287726
N	-4.999959	-0.615769	-0.306983
C	-2.620339	0.917099	0.100969
C	-3.912786	1.524964	0.027181
C	-5.051315	0.674499	-0.183821
C	-1.508814	1.765857	0.359742
C	-4.061618	2.922278	0.181694
C	-2.958454	3.724605	0.418335
C	-1.681113	3.131538	0.514840
H	-0.385282	-3.196757	-0.311966
H	-2.547627	-4.426162	-0.570600
H	-4.722086	-3.143862	-0.546274
H	-5.064776	3.355967	0.114398
H	-3.073131	4.805873	0.536050
H	-0.511109	1.350091	0.454769
H	-0.802903	3.752612	0.710575
H	-6.044825	1.146855	-0.236249

Phenanthridine (C2)

34

Mo	2.391809	-0.546878	0.059384
S	4.611552	-0.270938	0.963080
C	5.563964	0.376565	-0.382157
H	6.648698	0.421817	-0.225564
C	5.006440	0.849694	-1.512535
H	5.612438	1.281247	-2.317512
S	3.255369	0.820272	-1.774147
S	1.365121	-0.154191	2.063298
O	0.520413	0.301672	-0.584593
H	0.383982	0.585090	-1.501605
C	-0.689849	0.668613	0.225612
H	-0.015445	0.273720	1.357714
C	-0.909689	2.092835	0.331155
O	2.282817	-2.169235	-0.379061
C	-3.126853	0.351102	0.008690
C	-3.327291	1.763488	0.197766
C	-2.181510	2.601614	0.347329
C	-1.821730	-0.157421	-0.022544
C	-4.321122	-0.470173	-0.152204
N	-4.559605	2.351791	0.222609
C	-5.622053	1.607712	0.071814
C	-5.588943	0.183765	-0.119212
C	-6.776570	-0.574358	-0.269202
C	-4.297141	-1.874485	-0.328726
C	-5.471472	-2.598394	-0.473163
C	-6.723488	-1.946042	-0.445762
H	-0.030768	2.732050	0.447537
H	-2.363174	3.672677	0.466968
H	-6.600818	2.108751	0.094804
H	-1.628224	-1.220151	-0.179731
H	-7.739268	-0.053877	-0.242200
H	-7.644551	-2.524807	-0.559524
H	-5.425663	-3.682772	-0.607258
H	-3.341195	-2.400821	-0.346038

Phenanthridine (C3)

34

Mo	2.694282	-0.440720	-0.007423
S	4.682949	0.202284	1.201326
C	5.460306	1.415973	0.172986
H	6.469826	1.724281	0.471369
C	4.843083	1.987981	-0.877839
H	5.328764	2.765465	-1.478761
S	3.200094	1.533459	-1.356852
S	1.504511	-0.863695	1.897190
O	0.687276	-0.016200	-0.665183
H	0.520899	0.450553	-1.498509
C	-0.607062	-0.141062	0.086732
H	0.096674	-0.651474	1.156941
C	-1.154735	1.126749	0.513368
O	3.094158	-1.862643	-0.815064
C	-2.901068	-0.880981	-0.409422
C	-3.438760	0.350011	0.104960
C	-2.509372	1.337458	0.547328
C	-1.514923	-1.089940	-0.453244
N	-3.715971	-1.895055	-0.888217
C	-4.867618	0.518541	0.129819
C	-5.002206	-1.730306	-0.855141
C	-5.673690	-0.555310	-0.361529
C	-5.539660	1.677849	0.608114
C	-7.082701	-0.451192	-0.362126
C	-6.921919	1.759224	0.595588
C	-7.709682	0.691086	0.108521
H	-0.450451	1.887533	0.859398
H	-2.877956	2.295445	0.921476
H	-1.138077	-2.032536	-0.854352
H	-4.960878	2.519229	0.993244
H	-7.410658	2.664164	0.968928
H	-8.800105	0.769200	0.105564
H	-7.671412	-1.291727	-0.743747
H	-5.625377	-2.554246	-1.237060

Phenanthridine (C4)

34

Mo	2.139983	-0.512530	0.108800
S	4.365835	-0.306869	1.021999
C	5.373819	0.169280	-0.354156
H	6.457424	0.157507	-0.183361
C	4.862347	0.586839	-1.527724
H	5.506275	0.913250	-2.352734
S	3.117865	0.646656	-1.819565
S	1.131986	0.072851	2.074946
O	0.363594	0.489638	-0.602577
H	0.300916	0.782765	-1.524014
C	-0.772726	1.041907	0.169030
H	-0.185374	0.608597	1.328343
C	-0.826136	2.469667	0.196455
O	1.937306	-2.150534	-0.207187
C	-3.272724	1.034129	0.059043
C	-3.262837	2.439335	0.211187
C	-2.046174	3.130159	0.259870
C	-2.031636	0.324962	-0.014919
N	-1.949000	-1.019528	-0.203951
C	-4.489289	0.243937	-0.062441
C	-4.360778	-1.164074	-0.255602
C	-3.040364	-1.722704	-0.322039
C	-5.796347	0.788805	0.000046
C	-5.518776	-1.971749	-0.377343
C	-6.781757	-1.411640	-0.310407
C	-6.916916	-0.018404	-0.119271
H	0.122219	3.009877	0.247217
H	-2.055360	4.221421	0.345589
H	-4.198347	2.998125	0.258811
H	-2.930206	-2.805382	-0.476265
H	-5.928073	1.861917	0.149045
H	-7.914207	0.427721	-0.063777
H	-7.671964	-2.039998	-0.403949
H	-5.393332	-3.048897	-0.524914

Phenanthridine (C6 - Primary SOM)

34

Mo	2.002787	-0.354736	0.033589
S	4.088413	0.173905	1.129466
C	4.995146	1.121929	-0.057834
H	6.037289	1.343327	0.202341
C	4.441021	1.612595	-1.181906
H	5.011930	2.232843	-1.882144
S	2.759475	1.283443	-1.621818
S	0.839371	-0.312215	1.962021
O	0.073002	0.279184	-0.743552
H	0.079795	1.191665	-1.090602
C	-1.210344	0.235718	0.028046
H	-0.612404	0.040345	1.170935
N	-1.799237	1.439373	-0.031239
O	2.132210	-1.940950	-0.528195
C	-3.407021	-0.919732	-0.144660
C	-4.021741	0.395866	0.033657
C	-3.148069	1.536864	0.032090
C	-1.992029	-1.006719	-0.208558
C	-1.362945	-2.248144	-0.415875
C	-4.152803	-2.111879	-0.300361
C	-2.121094	-3.404360	-0.564233
C	-3.523281	-3.333371	-0.501451
C	-3.731021	2.834861	0.103075
C	-5.410602	0.603772	0.151302
C	-5.953997	1.880845	0.243757
C	-5.100882	3.003093	0.208990
H	-6.083223	-0.256971	0.172036
H	-7.035598	2.011396	0.339763
H	-5.522448	4.011066	0.274681
H	-3.047558	3.687108	0.088354
H	-0.274465	-2.304269	-0.465278
H	-1.622384	-4.363217	-0.729221
H	-4.124469	-4.240223	-0.618177
H	-5.243465	-2.074829	-0.272549

Phenanthridine (C7)

34

Mo	2.123539	-0.464295	0.143716
S	4.354885	-0.526423	1.054956
C	5.397286	0.010663	-0.273543
H	6.476637	-0.097193	-0.111250
C	4.918523	0.580642	-1.394924
H	5.583503	0.941290	-2.188053
S	3.182013	0.791760	-1.667881
S	1.134872	0.019108	2.145916
O	0.392199	0.656081	-0.501426
H	0.362917	1.066972	-1.379203
C	-0.764521	1.142538	0.306541
H	-0.153584	0.658408	1.442714
C	-0.848951	2.562289	0.416924
O	1.758749	-2.042564	-0.315336
C	-3.255598	1.077340	0.156823
C	-3.286018	2.470488	0.392780
C	-2.088240	3.186050	0.503359
C	-1.999891	0.409870	0.073332
C	-1.971662	-0.994295	-0.197781
C	-4.443336	0.259165	-0.044175
C	-4.265201	-1.134145	-0.314474
N	-3.033115	-1.736180	-0.390107
C	-5.763643	0.769252	0.010834
C	-5.407567	-1.951655	-0.518669
C	-6.684748	-1.424356	-0.458445
C	-6.863605	-0.050075	-0.190300
H	0.083668	3.123208	0.513997
H	-2.126251	4.269409	0.655218
H	-4.235498	3.002565	0.457706
H	-5.923514	1.829519	0.217034
H	-7.872064	0.370444	-0.140101
H	-7.554541	-2.068354	-0.617501
H	-5.227162	-3.009449	-0.723351
H	-0.997271	-1.494506	-0.259312

Phenanthridine (C8)

34

Mo	2.688434	-0.503473	-0.057335
S	4.699641	0.146391	1.107969
C	5.474325	1.331470	0.044385
H	6.488951	1.639021	0.325594
C	4.846185	1.892058	-1.005994
H	5.328220	2.654907	-1.628069
S	3.196626	1.433791	-1.457989
S	1.518441	-0.867515	1.874067
O	0.679432	-0.061524	-0.699054
H	0.523216	0.455103	-1.504771
C	-0.606590	-0.150950	0.074460
H	0.109764	-0.646777	1.150381
C	-1.138636	1.131576	0.476415
O	3.054560	-1.951015	-0.835468
C	-2.913695	-0.861600	-0.378497
C	-3.433816	0.377045	0.110875
C	-2.491244	1.365076	0.520177
C	-1.532829	-1.099243	-0.435407
C	-3.863910	-1.856919	-0.819735
C	-4.866565	0.546005	0.137078
N	-5.155422	-1.720720	-0.798354
C	-5.684219	-0.536135	-0.326793
C	-5.521339	1.720437	0.594725
C	-7.093145	-0.409529	-0.308861
C	-6.903359	1.822181	0.596737
C	-7.701825	0.749044	0.145857
H	-0.421304	1.892056	0.796254
H	-2.842538	2.337202	0.872840
H	-1.149038	-2.047647	-0.821211
H	-4.926908	2.563251	0.953278
H	-7.377119	2.740926	0.954968
H	-8.791998	0.835099	0.152102
H	-7.672839	-1.262903	-0.668914
H	-3.465298	-2.809418	-1.199734

Phenanthridine (C9)

34

Mo	2.390762	-0.512045	0.090080
S	4.606992	-0.254766	1.003498
C	5.583662	0.322405	-0.356517
H	6.668297	0.344827	-0.195077
C	5.043936	0.773179	-1.504506
H	5.664999	1.161978	-2.319677
S	3.294108	0.783256	-1.775079
S	1.354184	-0.043975	2.074299
O	0.537102	0.351672	-0.587913
H	0.386422	0.547718	-1.525463
C	-0.681760	0.720805	0.194206
H	-0.007453	0.363681	1.357611
C	-0.920850	2.144728	0.268861
O	2.249670	-2.143258	-0.302722
C	-3.107709	0.354733	-0.006511
C	-3.325770	1.762120	0.153270
C	-2.201398	2.630632	0.278984
C	-1.796913	-0.134760	-0.030714
C	-4.300703	-0.474372	-0.147763
C	-4.662351	2.255550	0.155881
N	-5.741879	1.528323	0.024437
C	-5.579369	0.169128	-0.125785
C	-6.750561	-0.619864	-0.261211
C	-4.256737	-1.880518	-0.297401
C	-5.416762	-2.629950	-0.427500
C	-6.675711	-1.993838	-0.410554
H	-0.051101	2.799049	0.366396
H	-2.378150	3.706900	0.376912
H	-1.583727	-1.196684	-0.163927
H	-7.707721	-0.093279	-0.240162
H	-7.589526	-2.586614	-0.512346
H	-5.352342	-3.715769	-0.540017
H	-3.291149	-2.390199	-0.304987
H	-4.807384	3.340350	0.275980

Phenanthridine (C10)

34

Mo	1.901397	-0.590176	0.008435
S	3.780544	0.492031	1.064788
C	4.424727	1.571618	-0.183845
H	5.392050	2.040307	0.034707
C	3.747895	1.868104	-1.309134
H	4.144526	2.568543	-2.053180
S	2.165489	1.155258	-1.666651
S	0.714236	-0.749740	1.958533
O	-0.136538	-0.591607	-0.727046
H	-0.266334	-0.649890	-1.686643
C	-1.312499	-1.235836	-0.036286
H	-0.657849	-1.051274	1.166993
C	-2.558467	-0.483029	-0.060814
O	2.467169	-2.088366	-0.519559
C	-2.582793	-3.309833	-0.429005
C	-3.789277	-2.610975	-0.388372
C	-3.775861	-1.207445	-0.221412
C	-1.371411	-2.639015	-0.297606
C	-5.008161	-0.459822	-0.234790
C	-2.648557	0.950212	0.119425
C	-3.949624	1.554292	0.076968
N	-5.107774	0.827332	-0.103412
C	-1.532889	1.799421	0.352693
C	-4.083863	2.953666	0.239066
C	-2.974389	3.754308	0.450782
C	-1.694744	3.165645	0.515350
H	-0.416217	-3.169563	-0.341638
H	-2.580587	-4.393514	-0.580083
H	-4.745505	-3.126671	-0.509740
H	-5.943296	-1.025016	-0.369801
H	-5.095098	3.364910	0.192480
H	-3.089197	4.835206	0.573994
H	-0.533903	1.380518	0.418886
H	-0.811069	3.784646	0.691229

