

Supporting Information

Use of Molecular Electrostatic potential for Quantitative Assessment of Inductive Effect

Cherumuttathu H. Suresh,^{a*} P. Alexander,^a Periya S. Vijayalakshmi,^a

Shridhar R. Gadre^b

^aComputational Modeling and Simulation Section, National Institute for Interdisciplinary Science and Technology (CSIR), Trivandrum 695 019

^bDepartment of Chemistry, University of Pune, Pune 411007

E-mail: sureshch@gmail.com

Contents

1. Table S1. Total energy of 4-substituted bicyclooctane carboxylic acids, 4-substituted bicyclooctane carboxylates, and 4-substituted bicyclooctane quinuclidines at B3LYP/6-31G(d,p) level. (Page S2)
2. Table S2. Cartesian coordinates of the optimized geometries of 4-substituted bicyclooctane carboxylic acids at B3LYP/6-31G(d,p) level (Pages S2, S13)
3. Table S3. Cartesian coordinates of the optimized geometries of 4-substituted bicyclooctane carboxylates at B3LYP/6-31G(d,p) level (Pages S13, S23)
4. Table S4. Cartesian coordinates of the optimized geometries of 4-substituted 4-substituted Quinuclidines at B3LYP/6-31G(d,p) level. (Pages S23, S32)
5. Table S5. Comparison of V_{\min} values at three different levels of theory. (Pages 33)

1. Table S1. Total energy of 4-substituted bicyclooctane carboxylic acids, 4-substituted bicyclooctane carboxylates, and 4-substituted quinuclidines at B3LYP/6-31G(d,p) level.

Substituents	Model (i), 4-substituted Bicyclooctane carboxylic acids	Model (ii), 4-substituted Bicyclooctane carboxylates	Model (iii), 4-substituted quinuclidines
	SCF Energy (in a.u.)	SCF Energy (in a.u.)	SCF Energy (in a.u.)
NO ₂	-706.381959388	-705.818042366	-533.830675856
CN	-594.118885134	-593.554349182	-421.567277157
Cl	-961.479971177	-960.911871323	-788.928278234
Br	-3072.99071096	-3072.42302568	-2900.43879082
CF ₃	-838.920990850	-838.351132059	-666.369405551
F	-601.118041329	-600.546163546	-428.565960500
CHO	-615.196060493	-614.625764911	-442.644595515
CH ₂ Cl	-1000.79161546	-1000.21937613	-828.240302029
COOH	-690.450760428	-689.877878103	-517.899187013
COCH ₃	-654.521040827	-653.948733426	-481.969794172
CONH ₂	-670.581877248	-670.008553573	-498.029765033
OH	-577.098158315	-576.523191572	-404.546409316
OCH ₃	-616.399898607	-615.824445279	-443.848206919
C ₆ H ₅	-732.933609032	-732.358593415	-560.382243678
NH ₂	-557.231979610	-556.655086348	-384.680150292
H	-501.880559166	-501.301710829	-329.328291955
CH ₃	-541.199206457	-540.621147692	-368.647438177
CH ₂ CH ₃	-580.512452957	-579.934315084	-407.960834158
CH(CH ₃) ₂	-619.825025707	-619.246978958	-447.273138422
C(CH ₃) ₃	-659.136732534	-658.558546842	-486.583709125

2. Table S2. Cartesian coordinates of the optimized geometries of 4-substituted bicyclooctane carboxylic acids at B3LYP/6-31G(d,p) level

Substituents	Atomic number followed by Cartesian coordinates in Angstrom unit			
NO ₂	6	1.282624579	0.052689650	-0.029056064
	6	0.773309998	-1.185840706	-0.815238299
	6	0.714151156	1.329911858	-0.680366364
	6	-0.839632841	1.274351951	-0.703229996
	6	-0.782858472	-1.242070551	-0.784935493
	6	-1.304708733	-0.024107199	-0.017561276
	6	0.759129635	-0.046500392	1.428351526
	6	-0.796159871	-0.051805394	1.435892831
	7	-2.831948670	-0.021893650	0.018248148

	8	-3.433333742	-0.926594655	-0.553536865
	8	-3.369059344	0.901564042	0.626731075
	6	2.802445980	0.096542039	-0.040116927
	8	3.483163189	0.990517150	-0.493619713
	8	3.351736198	-1.006388763	0.530975393
	1	1.201429209	-2.092775897	-0.381590243
	1	1.131364025	-1.127958769	-1.848682836
	1	1.116371375	1.431204321	-1.691595511
	1	1.064168568	2.204431767	-0.124850376
	1	-1.216464722	1.291469776	-1.731334077
	1	-1.279603506	2.127519558	-0.182503708
	1	-1.134651803	-2.157553013	-0.302665573
	1	-1.197455088	-1.243279721	-1.795631759
	1	1.137827925	0.800617131	2.009995641
	1	1.152983561	-0.953630320	1.893208868
	1	-1.198051471	0.813133761	1.967686862
	1	-1.178915363	-0.947415663	1.936432066
	1	4.314784815	-0.884323447	0.476955392
CN	6	-0.458097632	-0.692309365	1.255956691
	6	1.096322436	-0.715894795	1.266888964
	6	1.643058845	-0.005714585	-0.000111656
	6	1.095830831	-0.732197159	-1.257657996
	6	-0.458017726	-0.683533490	-1.260786492
	6	-0.972477497	0.060257413	0.000189975
	6	-0.408929128	1.494976529	0.005163712
	6	1.143704967	1.464031302	-0.009595042
	6	3.110854185	-0.040353469	-0.000062443
	7	4.272091324	-0.068185018	0.000076202
	6	-2.492827547	0.102079350	0.000025930
	8	-3.175138637	1.103462096	0.000021167
	8	-3.041247268	-1.140444706	-0.000105835
	1	-0.837871210	-0.196522672	2.155760160
	1	-0.861564063	-1.708087850	1.259109000
	1	1.489830281	-0.214487181	2.156249120
	1	1.470159175	-1.744048089	1.291996837
	1	1.504384772	-0.255848204	-2.153875760
	1	1.453576347	-1.766445517	-1.257932110
	1	-0.877421388	-1.692560201	-1.282583832
	1	-0.821757233	-0.168451406	-2.156449678
	1	-0.797739995	2.037969538	-0.860599902
	1	-0.781423873	2.024664434	0.886376655
	1	1.538767005	1.969144745	-0.896398213
	1	1.555405396	1.987523600	0.858702272
	1	-4.004430296	-1.007741869	-0.000285227
CI	6	-1.075698812	0.061526910	-0.000319623
	6	-0.558868326	-0.684552156	1.259675749
	6	-0.558722802	-0.689280355	-1.257338902
	6	0.999971430	-0.720665328	-1.254181302
	6	0.999812148	-0.715951417	1.256842005
	6	1.514785751	-0.003279311	0.000022225
	6	-0.509860163	1.496206867	-0.002900421
	6	1.047193091	1.457346206	-0.002780297
	17	3.354922903	-0.047735492	0.000237601
	6	-2.595409086	0.102713304	0.000030163

	8	-3.279402431	1.103220791	0.000227546
	8	-3.144293425	-1.140181705	0.000102660
	1	-0.928892342	-0.178273465	2.157716529
	1	-0.967515931	-1.698119738	1.274477366
	1	-0.967345536	-1.702901383	-1.268402940
	1	-0.928586478	-0.186451370	-2.157384734
	1	1.403925234	-0.229376112	-2.143840443
	1	1.369316512	-1.750215121	-1.259926579
	1	1.403631011	-0.221299280	2.144702472
	1	1.369154584	-1.745466284	1.266509015
	1	-0.888023983	2.032257599	-0.877761120
	1	-0.888142519	2.035436896	0.869932472
	1	1.453151947	1.968299649	0.875078720
	1	1.453178406	1.964866876	-0.882617909
	1	-4.107194401	-1.005956425	0.000539761
Br	6	1.634109928	0.061432187	-0.000830808
	6	1.113183611	-0.689473505	-1.256654676
	6	1.075819993	1.499606301	-0.006252758
	6	-0.482708078	1.469054782	-0.005406075
	6	-0.446965859	-0.711532787	-1.253589152
	6	-0.950165268	0.010751294	-0.000113244
	6	1.113528635	-0.679565190	1.261228355
	6	-0.446574268	-0.702641022	1.258284013
	35	-2.953376327	-0.028186097	0.000379420
	6	3.153971018	0.094552862	-0.000056622
	8	3.843287886	1.091414847	0.000856738
	8	3.696284034	-1.151201292	0.000452976
	1	1.515372608	-1.705718194	-1.265126804
	1	1.485908019	-0.190894872	-2.157916028
	1	1.456076710	2.031710430	-0.882668710
	1	1.457035579	2.038716736	0.865400598
	1	-0.886108891	1.978066673	-0.885388681
	1	-0.885347405	1.984282919	0.871305157
	1	-0.822316044	-1.738727212	-1.259054495
	1	-0.847659930	-0.219813879	-2.144342632
	1	1.485993216	-0.173222997	2.158257348
	1	1.516411383	-1.695438926	1.278005920
	1	-0.847533986	-0.205075234	2.145670338
	1	-0.821322250	-1.729985204	1.270719678
	1	4.659885641	-1.022201638	0.001728293
CF ₃	6	-1.049669641	-0.726832360	1.229584614
	6	0.497421851	-0.610015424	1.309273416
	6	1.042500348	0.007178819	0.000791120
	6	0.535441649	1.464011723	-0.110981169
	6	-1.007630213	1.496871513	0.053688736
	6	-1.572730659	0.063557892	0.000339732
	6	-1.046938557	-0.634613699	-1.282727239
	6	0.494776494	-0.803082568	-1.196775095
	6	2.563443605	-0.023100704	0.000058739
	9	3.080803797	0.558089906	-1.109101538
	9	3.044553567	-1.289467899	0.040882118
	9	3.084496925	0.629819882	1.066434505
	6	-3.091830263	0.097631086	-0.000816520
	8	-3.781944072	1.094071316	-0.001136144

	8	-3.634114703	-1.148483967	-0.000238659
	1	-1.507392086	-0.334719956	2.144119319
	1	-1.361132257	-1.771597586	1.144657486
	1	0.949527080	-1.593188123	1.470366612
	1	0.797025076	0.018464053	2.153399501
	1	1.019875374	2.080818607	0.651647915
	1	0.833679068	1.871071796	-1.081990729
	1	-1.290678127	1.956966260	1.005566951
	1	-1.472962756	2.103943124	-0.726945075
	1	-1.535097690	-1.604987188	-1.402811316
	1	-1.320690944	-0.029194180	-2.154066264
	1	0.764342031	-1.856113543	-1.070357826
	1	0.972251009	-0.462633739	-2.120211620
	1	-4.597676093	-1.019143522	-0.000936115
F	6	0.739181240	0.062202140	-0.000297927
	6	0.228221976	-0.692859181	-1.259771001
	6	0.228457460	-0.689356027	1.261450080
	6	-1.327419962	-0.729206778	1.253890783
	6	-1.327623166	-0.734060921	-1.251018938
	6	-1.845861792	-0.022022770	0.000103719
	6	0.163092428	1.494817776	-0.002168568
	6	-1.391037122	1.438329692	-0.002781885
	9	-3.246892955	-0.065919610	0.000313273
	6	2.258096161	0.113975254	-0.000090489
	8	2.936427838	1.118629903	0.000153991
	8	2.816645393	-1.125110208	0.000060855
	1	0.647566371	-1.702080629	-1.271826717
	1	0.595937722	-0.185984107	-2.158472723
	1	0.597283419	-0.180675930	2.158667460
	1	0.646936650	-1.698918266	1.275539954
	1	-1.742810344	-0.234570516	2.137597739
	1	-1.697306921	-1.759612251	1.258505209
	1	-1.696611583	-1.764809830	-1.251000946
	1	-1.744033802	-0.243572350	-2.136545205
	1	0.539216800	2.035573953	0.870652682
	1	0.539941243	2.033657273	-0.875869311
	1	-1.808373818	1.936920496	-0.883628108
	1	-1.809231614	1.940709406	0.875494654
	1	3.778286928	-0.982438730	0.000456151
CHO	6	-0.511098437	1.503927563	-0.146093667
	6	1.042796158	1.518760930	-0.123885157
	6	1.586537952	0.085474826	0.116282996
	6	0.995560738	-0.435701792	1.451713643
	6	-0.555506463	-0.513462801	1.354969988
	6	-1.028793599	0.058471440	-0.006306734
	6	-0.421190165	-0.811430868	-1.142136486
	6	1.129326163	-0.828860379	-1.031628401
	6	3.094819585	0.143849427	0.232523129
	8	3.877271120	-0.436162706	-0.488333761
	6	-2.546082887	0.041013354	-0.088676878
	8	-3.260029781	1.000393185	-0.288361912
	8	-3.057016221	-1.205435610	0.086828991
	1	-0.922460722	2.112862407	0.664596353
	1	-0.892973378	1.936622041	-1.074556847

	1	1.411624763	2.190176261	0.660474062
	1	1.438441349	1.897666128	-1.072608946
	1	1.412950881	-1.424008569	1.674212568
	1	1.299419606	0.226375677	2.270920772
	1	-0.899311334	-1.546244280	1.453063045
	1	-1.018805907	0.053846960	2.170061705
	1	-0.735047837	-0.402775855	-2.109228546
	1	-0.829313355	-1.823727895	-1.079753368
	1	1.498931071	-1.843509070	-0.853123156
	1	1.594922766	-0.498099198	-1.964688014
	1	3.463303166	0.788569882	1.065943429
	1	-4.021699466	-1.110360980	0.013043161
CH ₂ Cl	6	0.741371505	-1.265176546	-0.720103342
	6	-0.786671723	-1.014033258	-0.851428731
	6	-1.172288476	0.347634527	-0.232652778
	6	-0.383557724	1.455015709	-0.978498476
	6	1.148292934	1.215323816	-0.853232167
	6	1.417122914	-0.067777551	-0.024476564
	6	0.788041234	0.120026396	1.381284914
	6	-0.741319116	0.367732150	1.250004506
	6	-2.658893422	0.659864979	-0.403957507
	17	-3.782493358	-0.530432987	0.406943655
	6	2.912420125	-0.310591590	0.098609005
	8	3.507233345	-1.299184652	-0.273217918
	8	3.556832599	0.728759094	0.693208967
	1	0.943247334	-2.174188758	-0.146339735
	1	1.202170586	-1.418909417	-1.700281956
	1	-1.352256367	-1.808913578	-0.357048061
	1	-1.089675441	-1.026999158	-1.905518060
	1	-0.649326414	2.435416049	-0.565538076
	1	-0.681880869	1.467182553	-2.033319128
	1	1.601043759	1.106925032	-1.845020930
	1	1.637883491	2.066551989	-0.373113882
	1	1.278598598	0.955106196	1.888583330
	1	0.982187371	-0.774311730	1.983654256
	1	-1.010502587	1.335735982	1.689809009
	1	-1.303300592	-0.391840936	1.800464734
	1	-2.942035530	0.653742398	-1.458555905
	1	-2.908039596	1.632454662	0.025504756
	1	4.494631524	0.474705331	0.725461791
COOH	6	-1.309558642	0.053047373	-0.030987032
	6	-0.775504496	-0.047394173	1.422192961
	6	-0.815360539	-1.192925860	-0.814806490
	6	0.727930403	-1.318000607	-0.692713128
	6	0.775678595	0.044631338	1.422179732
	6	1.309559172	-0.052858986	-0.031314593
	6	-0.728008721	1.319491299	-0.689950293
	6	0.815277458	1.194676907	-0.812498219
	6	2.827681914	-0.111898763	-0.034526699
	8	3.505989778	-0.991046856	-0.521244882
	8	3.386723810	0.960088400	0.586664949
	6	-2.827694614	0.111807215	-0.034389642
	8	-3.506116781	0.990783326	-0.521257053
	8	-3.386613212	-0.960310125	0.586693524

	1	-1.112821654	-0.989481550	1.862877487
	1	-1.203347477	0.757550041	2.029903289
	1	-1.114029766	-1.092831983	-1.864620067
	1	-1.309639077	-2.088607567	-0.429471259
	1	1.189610035	-1.463262408	-1.672789081
	1	1.002949111	-2.192654398	-0.094707381
	1	1.203611536	-0.761544800	2.028192459
	1	1.113082009	0.985837635	1.864693094
	1	-1.189856103	1.466694651	-1.669648943
	1	-1.002914714	2.192967671	-0.090154870
	1	1.309602035	2.089574374	-0.425428874
	1	1.113794811	1.096765358	-1.862566330
	1	4.348089114	0.827658089	0.529075118
	1	-4.348001800	-0.828234363	0.528678235
COCH ₃	6	-0.803857284	1.502771839	-0.149323236
	6	0.735278558	1.488421082	-0.342439065
	6	1.304903999	0.087784155	-0.028640131
	6	0.767970070	-0.348599217	1.364881478
	6	-0.772605663	-0.544885346	1.307712343
	6	-1.325980071	0.059201176	-0.009798246
	6	-0.780190890	-0.784726468	-1.192808912
	6	0.765288200	-0.911287674	-1.082115086
	6	2.839316405	0.123953420	0.023682799
	8	3.439877019	1.171924932	0.180836800
	6	3.603830418	-1.185527433	-0.103375834
	6	-2.845165930	0.040184133	-0.003043298
	8	-3.571967598	1.000810706	-0.136456820
	8	-3.343646665	-1.212602258	0.176327151
	1	-1.084125959	2.070822449	0.744047554
	1	-1.303842470	1.993715503	-0.988378744
	1	0.999785689	1.754118333	-1.372425429
	1	1.224892928	2.226863061	0.295568248
	1	1.035145313	0.420085772	2.097702537
	1	1.251148058	-1.276222063	1.690895939
	1	-1.036864610	-1.605157583	1.356961282
	1	-1.247128956	-0.060194970	2.167869323
	1	-1.059657332	-0.297323529	-2.133653781
	1	-1.249883853	-1.772032041	-1.193013703
	1	1.039034237	-1.934146549	-0.802087186
	1	1.228132552	-0.716166263	-2.056143072
	1	3.175069844	-1.976939526	0.518879989
	1	3.567563785	-1.539729579	-1.140179059
	1	4.644898283	-1.016095461	0.174097198
	1	-4.310996964	-1.116405242	0.165802345
CONH ₂	6	-0.758911085	1.339479912	-0.668383145
	6	0.786517204	1.249111254	-0.777958291
	6	1.313331676	0.002974505	-0.023050432
	6	0.761454840	0.044723944	1.426148561
	6	-0.787912644	-0.057985655	1.422059609
	6	-1.316630038	0.051105293	-0.032514238
	6	-0.793198066	-1.172073630	-0.831281895
	6	0.756847294	-1.258837532	-0.717565937
	6	2.845722095	0.092481133	0.060198675
	8	3.395772741	1.091295782	0.508918227

	7	3.566268888	-0.989015874	-0.358849380
	6	-2.835979942	0.075414637	-0.038306612
	8	-3.533622885	0.963391524	-0.478792166
	8	-3.372586840	-1.039171294	0.527004447
	1	-1.060346321	2.196718479	-0.058106837
	1	-1.217412479	1.490928323	-1.649464536
	1	1.096508178	1.186605367	-1.828175630
	1	1.269834894	2.135134419	-0.360822682
	1	1.195945345	-0.776323133	2.008144050
	1	1.100462719	0.973334235	1.892191260
	1	-1.122025634	-1.005195997	1.854993804
	1	-1.225415756	0.740335905	2.031698788
	1	-1.261323078	-2.085200195	-0.454824670
	1	-1.095510149	-1.068820036	-1.879476719
	1	1.035794614	-2.151548968	-0.143380576
	1	1.194458886	-1.364472424	-1.717396606
	1	3.146421775	-1.817552926	-0.743184466
	1	4.571146850	-0.932142020	-0.292537650
	1	-4.336374718	-0.921184347	0.479162061
OH	6	-0.748656688	0.061331114	-0.000234955
	6	-0.237429661	-0.688720485	1.260689653
	6	-0.237296308	-0.692371279	-1.258844941
	6	1.317868313	-0.724900334	-1.251659772
	6	1.317747131	-0.720400211	1.254262266
	6	1.863767563	-0.012936267	0.000054505
	6	-0.173177488	1.492871462	-0.002223074
	6	1.379598955	1.442758906	-0.002576035
	8	3.288169310	0.025650280	0.000065089
	6	-2.267639873	0.110219683	0.000030163
	8	-2.949763105	1.112370795	0.000157695
	8	-2.824738630	-1.130332129	-0.000009525
	1	-0.653968886	-1.699368596	1.274292154
	1	-0.609334373	-0.181170181	2.157595876
	1	-0.654383761	-1.702816186	-1.270011110
	1	-0.608491923	-0.186994835	-2.157276253
	1	1.680329857	-1.761281276	-1.261700910
	1	1.731190670	-0.235623579	-2.139343494
	1	1.730433417	-0.227461020	2.140220341
	1	1.680779128	-1.756525031	1.268464854
	1	-0.552614509	2.030558940	-0.875897887
	1	-0.552190638	2.032785718	0.870251036
	1	1.795174549	1.945621229	-0.881770696
	1	1.795697377	1.948994205	0.874429949
	1	3.605638617	-0.887961541	0.001754752
	1	-3.786288617	-0.987384420	0.000297927
OCH ₃	6	0.654328727	1.535763395	0.028576101
	6	-0.887404846	1.620896902	-0.117978480
	6	-1.518518038	0.224776503	0.008502291
	6	-1.048544081	-0.635731851	-1.181966599
	6	0.504314914	-0.613604833	-1.270509595
	6	1.094872491	0.058149700	-0.000556694
	6	0.511745621	-0.663512069	1.245060932
	6	-1.022231271	-0.417938899	1.320647022
	8	-2.928973848	0.456840836	0.014329062

	6	-3.785068334	-0.669230358	-0.020742161
	6	2.610628752	-0.041594390	-0.006992548
	8	3.387767348	0.888768007	-0.022118551
	8	3.043287246	-1.331038476	0.008391164
	1	1.160787338	2.084428125	-0.769884104
	1	0.988887284	1.989864680	0.966682477
	1	-1.174292471	2.042655403	-1.087097819
	1	-1.326159991	2.267534566	0.648001884
	1	-1.498774964	-0.245475801	-2.100849025
	1	-1.402443008	-1.665603912	-1.063494397
	1	0.832512761	-0.052986518	-2.153105278
	1	0.903347369	-1.626102418	-1.371768720
	1	1.003902159	-0.293836780	2.151271679
	1	0.738298043	-1.731494947	1.178756610
	1	-1.541518727	-1.363961768	1.504547229
	1	-1.276035264	0.250257975	2.150330273
	1	-3.624433935	-1.356499839	0.821643460
	1	-4.803776873	-0.279264826	0.047020044
	1	-3.695909906	-1.240613197	-0.954939505
	1	4.014217959	-1.283313038	0.003827539
C ₆ H ₅	6	2.135547177	-0.037594868	-0.049054731
	6	1.635805412	1.426888351	-0.132165722
	6	1.559170492	-0.825363576	-1.240389884
	6	0.011169873	-0.884835161	-1.137034159
	6	0.086437399	1.451535840	-0.251209965
	6	-0.514070826	0.046447475	-0.007649257
	6	1.595827659	-0.652447502	1.268305572
	6	0.055170962	-0.465111347	1.344615577
	6	-2.046326834	0.042201886	0.008906053
	6	-2.740598389	-1.157111144	0.246744768
	6	-4.132882252	-1.204650311	0.256957889
	6	-4.877467451	-0.046425249	0.026685350
	6	-4.209033504	1.151349462	-0.214983549
	6	-2.812391866	1.193148644	-0.224341520
	6	3.653624410	-0.082736863	-0.074154666
	8	4.337405555	-0.672627147	-0.883271443
	8	4.209238296	0.633842159	0.939522455
	1	2.092878028	1.924701265	-0.994573293
	1	1.969655930	1.970453400	0.756313883
	1	1.993518649	-1.828821226	-1.258339576
	1	1.873443040	-0.343713323	-2.171963038
	1	-0.318395367	-1.910571174	-0.941118454
	1	-0.450980198	-0.591474641	-2.085600253
	1	-0.210073843	1.806447083	-1.244679924
	1	-0.325228104	2.162378580	0.473014080
	1	2.088008539	-0.181898329	2.123713186
	1	1.858224960	-1.716522935	1.296493785
	1	-0.422277624	-1.409140805	1.621659975
	1	-0.208812813	0.253621426	2.128955216
	1	-2.186475195	-2.073838760	0.425518305
	1	-4.636736782	-2.148701465	0.444863967
	1	-5.962961862	-0.079572912	0.034880718
	1	-4.771729369	2.062541354	-0.398278906
	1	-2.325929805	2.141815811	-0.419397312
	1	5.170826913	0.540800627	0.831137429

NH ₂	6	-0.759273571	0.061126852	0.000945111
	6	-0.247839635	-0.667870373	1.272623658
	6	-0.247523717	-0.712450910	-1.244279866
	6	1.306628588	-0.750041016	-1.241375212
	6	1.307026529	-0.699812040	1.261450080
	6	1.869790129	-0.016620928	-0.008631939
	6	-0.183658902	1.491526294	-0.024641139
	6	1.368678854	1.440255368	-0.038716724
	7	3.334012464	-0.018083045	-0.086530005
	6	-2.277935545	0.111217712	0.000645596
	8	-2.959599452	1.113891650	-0.014287786
	8	-2.836907061	-1.128414391	0.020356920
	1	-0.664091518	-1.678478795	1.302931226
	1	-0.619976656	-0.146497430	2.161808127
	1	-0.667684631	-1.721850162	-1.240007818
	1	-0.618719860	-0.220268972	-2.150238196
	1	1.663453865	-1.787982501	-1.235409268
	1	1.717864399	-0.282162601	-2.140949018
	1	1.670902564	-1.734258310	1.299555605
	1	1.710941702	-0.192858119	2.146486858
	1	-0.569208979	2.017416294	-0.902898098
	1	-0.556555292	2.043748154	0.842969832
	1	1.779355325	1.978034394	0.825454595
	1	1.776113585	1.927490029	-0.930043303
	1	3.718076082	0.456757755	0.729496767
	1	3.676313943	-0.976933170	-0.038293382
	1	-3.798181876	-0.983381724	0.018174063
	H	6	-0.425535239	0.061077638
6		0.075736906	-0.697322791	1.260020773
6		0.075807287	-0.697647176	-1.259875778
6		1.631737098	-0.758962415	-1.253814582
6		1.631714343	-0.757479131	1.254720004
6		2.181887229	-0.054340683	0.000043393
6		0.165949456	1.486165728	-0.000206379
6		1.719992750	1.414909366	-0.000836100
6		-1.943293378	0.129757966	-0.000028576
8		-2.612789912	1.140924670	0.000010054
8		-2.518264568	-1.102929744	-0.000008467
1		-0.289659984	-0.184218242	2.156904241
1		-0.358189496	-1.700958244	1.272852262
1		-0.288761441	-0.184163737	-2.156884662
1		-0.358862610	-1.700952953	-1.273042766
1		2.037334525	-0.282186414	-2.153206351
1		1.972007594	-1.800704452	-1.271174241
1		1.972740504	-1.798937000	1.273859816
1		2.036582035	-0.278989654	2.153536028
1		3.277262438	-0.100708251	0.000084139
1		-0.208032806	2.029314844	-0.873220779
1		-0.207320533	2.029165616	0.873210725
1		2.128039210	1.928101758	-0.879151798
1	2.128803871	1.929466506	0.876320170	
1	-3.477482471	-0.945139142	0.000049743	
CH ₃	6	-0.771844177	0.062413281	-0.000067206

	6	-0.258233206	-0.721205089	1.237538148
	6	-0.255485717	-0.654951568	-1.276281331
	6	1.291243289	-0.795074529	-1.208765193
	6	1.293978077	-0.655653787	1.288512734
	6	1.864532753	-0.020508793	-0.000069322
	6	-0.194147724	1.491092368	0.038418797
	6	1.353365523	1.436444763	-0.081766881
	6	3.394851443	-0.065961415	0.001551548
	6	-2.289973798	0.111508230	-0.000406408
	8	-2.972924135	1.113604836	0.000297927
	8	-2.848183828	-1.128867896	-0.000085727
	1	-0.608243738	-1.755711685	1.177015617
	1	-0.693670409	-0.295094105	2.148393484
	1	-0.554144890	-0.072550730	-2.155636862
	1	-0.735632048	-1.632985956	-1.367200862
	1	1.748271453	-0.421061045	-2.132499116
	1	1.577477908	-1.850869926	-1.126840088
	1	1.712781652	-1.660667218	1.418639007
	1	1.625214459	-0.067506612	2.152972455
	1	-0.636244094	2.084394787	-0.766782067
	1	-0.501175835	1.973690378	0.971817613
	1	1.820300944	2.032265536	0.711457115
	1	1.682279875	1.875635421	-1.031635810
	1	3.804762195	0.454868063	0.874514617
	1	3.805793561	0.412130650	-0.894982135
	1	3.760841542	-1.098865662	0.026888025
	1	-3.809470285	-0.984187131	0.000199500
CH ₂ CH ₃	6	-1.118503959	0.064686098	-0.014618522
	6	-0.532722207	-0.466983047	1.320403072
	6	-0.746426206	-0.941686261	-1.135648773
	6	0.785939342	-1.192474472	-1.115904641
	6	1.020000260	-0.443064235	1.255591559
	6	1.507330172	-0.183156713	-0.189739678
	6	-0.469812558	1.425640551	-0.336739297
	6	1.049082254	1.235631522	-0.601795714
	6	3.032752386	-0.369102719	-0.331763972
	6	3.923418022	0.473992000	0.589577011
	6	-2.626368071	0.210662288	0.090284518
	8	-3.260410259	1.229683570	-0.083754471
	8	-3.237929222	-0.960077287	0.415640154
	1	-0.906080570	-1.480228889	1.495707323
	1	-0.892420388	0.147661620	2.153255564
	1	-1.061208351	-0.529223817	-2.101331634
	1	-1.298935938	-1.874514624	-0.994316113
	1	1.196161779	-1.116740211	-2.129851642
	1	1.002285523	-2.210758081	-0.769635391
	1	1.428690729	-1.394223298	1.618227203
	1	1.410816709	0.336330772	1.918547462
	1	-0.970547059	1.875444917	-1.198465817
	1	-0.641346421	2.108558608	0.501950021
	1	1.620624905	1.992498925	-0.054857689
	1	1.275996634	1.385939557	-1.664761462
	1	3.305768158	-0.162897162	-1.376083631
	1	3.263844619	-1.430843951	-0.167031624
	1	3.767003811	1.547729680	0.445251325

	1	4.979659515	0.269726406	0.386558159
	1	3.745989653	0.251174510	1.646357207
	1	-4.187722478	-0.757355833	0.457522416
CH(CH ₃) ₂	6	1.399474853	0.062074608	-0.014201001
	6	0.921962766	-0.996162942	-1.042090764
	6	0.767230280	-0.287833794	1.360129466
	6	-0.760855282	-0.513963403	1.190156675
	6	-0.600636286	-0.818970586	-1.286545253
	6	-1.248440258	0.042781864	-0.170503556
	6	0.875327434	1.440318341	-0.458942728
	6	-0.670078629	1.473926388	-0.323846422
	6	-2.803255092	0.043047511	-0.310350285
	6	-3.452846624	-1.320119433	-0.008169438
	6	-3.505570141	1.128246112	0.526560468
	6	2.914449520	0.070741473	0.079050614
	8	3.638530687	1.024031003	-0.114880147
	8	3.417817207	-1.148491905	0.411881937
	1	1.148023583	-1.996204753	-0.659697230
	1	1.476873376	-0.886139583	-1.980562273
	1	0.963325377	0.534778590	2.057974026
	1	1.246836321	-1.178060742	1.776142690
	1	-1.300753662	-0.037463103	2.015717635
	1	-0.987769132	-1.584104795	1.247022063
	1	-0.778278972	-0.330977085	-2.252920807
	1	-1.077228663	-1.801995115	-1.344318708
	1	1.342486697	2.225904721	0.140880742
	1	1.186252935	1.622829457	-1.493266758
	1	-0.952305261	2.076052308	0.546042657
	1	-1.116712165	1.963154988	-1.198057292
	1	-3.005974429	0.274519165	-1.367430525
	1	-4.519407603	-1.291241172	-0.254591408
	1	-3.008983860	-2.138849772	-0.581441440
	1	-3.372293146	-1.574502345	1.054295709
	1	-3.199109837	2.138440189	0.243949124
	1	-3.309127904	1.005045711	1.597762860
	1	-4.590107271	1.065451294	0.388127170
	1	4.382890456	-1.035468111	0.440873441
C(CH ₃) ₃	6	1.631420121	0.064622596	-0.008529808
	6	1.097614158	-0.690051895	1.237137561
	6	1.054698412	1.491971861	0.007447641
	6	-0.471148730	1.434415898	-0.267482695
	6	-0.432684424	-0.458985591	1.354941942
	6	-1.031264856	0.008205422	-0.001007024
	6	1.090827989	-0.664313772	-1.265449073
	6	-0.430806373	-0.917981766	-1.095285778
	6	-2.613118531	-0.023042494	0.003232744
	6	-3.184693991	0.643573199	1.275742629
	6	-3.192126814	0.727734078	-1.217814654
	6	-3.146440297	-1.473713129	-0.043263944
	6	3.148421007	0.096814565	-0.001117622
	8	3.843487386	1.090580334	0.009790308
	8	3.691098097	-1.150616551	0.004069902
	1	1.605471914	-0.335884146	2.141224720
	1	1.333157831	-1.754536912	1.141117291

1	1.565489398	2.109122182	-0.736650715
1	1.264028761	1.952033799	0.979376910
1	-0.668602225	1.710793004	-1.308503992
1	-0.985351321	2.176918783	0.351147735
1	-0.631591568	0.300218129	2.117958913
1	-0.916969450	-1.379033265	1.697975801
1	1.286710885	-0.042440545	-2.147004923
1	1.624415401	-1.606773690	-1.415290903
1	-0.937647051	-0.767714478	-2.053771300
1	-0.598211596	-1.963429102	-0.816324170
1	-2.941829151	0.078331991	2.180145706
1	-4.276902603	0.695367481	1.208358785
1	-2.819080667	1.666426783	1.409806510
1	-4.280766656	0.608326290	-1.244225361
1	-2.983173240	1.800517652	-1.176818234
1	-2.801036781	0.344788082	-2.165824582
1	-2.745694895	-2.090355969	0.767649389
1	-2.910298124	-1.968428768	-0.989824986
1	-4.237015339	-1.471267801	0.059458885
1	4.654022886	-1.018180949	0.017821631

3. Table S3. Cartesian coordinates of the optimized geometries of 4-substituted bicyclooctane carboxylates at B3LYP/6-31G(d,p) level

Substituents	Atomic number followed by Cartesian coordinates in Angstrom unit			
NO ₂	6	-1.337797657	0.045672759	0.000079906
	6	-0.790520429	1.481409483	-0.000198441
	6	-0.792986925	-0.684353715	1.245980642
	6	0.765264916	-0.703979311	1.257262172
	6	0.770626011	1.484703612	-0.001315005
	6	1.267882759	0.033994876	-0.000266176
	6	-0.793202829	-0.684776527	-1.245671073
	6	0.765027315	-0.705931975	-1.256426601
	7	2.797263747	-0.019214955	-0.000028576
	8	3.434350292	1.034436745	0.001109685
	8	3.325808100	-1.133226199	-0.000839804
	6	-2.920099016	-0.023457898	0.000097369
	8	-3.519861631	1.077490077	-0.000802762
	8	-3.375942882	-1.195647419	0.000995382
	1	-1.183935138	2.012025565	0.871234248
	1	-1.185359684	2.012221361	-0.870837365
	1	-1.208344497	-1.695236251	1.248065071
	1	-1.166981358	-0.183792255	2.146912317
	1	1.165371071	-1.722187777	1.249425586
	1	1.168775269	-0.204796358	2.147353121
	1	1.176731449	2.003270327	0.873483780
	1	1.175476769	2.001418736	-0.877849492
	1	-1.209504454	-1.695277527	-1.247959235
	1	-1.166450064	-0.183750979	-2.146662016
	1	1.169277458	-0.208995379	-2.147441494
	1	1.164100517	-1.724507690	-1.246478068

CN	6	-0.469160611	1.474309512	-0.000513302
	6	1.088344560	1.465268519	-0.001511330
	6	1.607849507	-0.001779623	-0.000060326
	6	1.066571033	-0.732951237	-1.260019185
	6	-0.489294218	-0.693237542	-1.246130399
	6	-1.024750684	0.042134151	-0.000065618
	6	-0.489288926	-0.692384509	1.246524107
	6	1.066616542	-0.730472570	1.261343186
	6	3.076905348	-0.015460972	-0.000034397
	7	4.240348626	-0.025442313	0.000237601
	6	-2.608440605	-0.010508402	0.000045509
	8	-3.196658159	1.096867489	0.000112715
	8	-3.077371553	-1.177414616	0.000064030
	1	-0.861434414	2.006518417	-0.871724266
	1	-0.860306737	2.006594619	0.871163867
	1	1.496944540	1.981847116	0.875768768
	1	1.495776116	1.979554720	-0.880682178
	1	1.446213375	-1.762182994	-1.259459845
	1	1.476571216	-0.248804326	-2.154594383
	1	-0.920705441	-1.697533409	-1.248904875
	1	-0.858826629	-0.186797981	-2.146148185
	1	-0.859875458	-0.186132276	2.146201102
	1	-0.919621686	-1.697144464	1.249317633
	1	1.475626634	-0.243645377	2.154921414
	1	1.447323060	-1.759302682	1.263593248
Cl	6	-1.132664213	0.042395564	-0.000358782
	6	-0.574258388	1.474729679	-0.003195701
	6	-0.593662259	-0.690367814	1.247654959
	6	0.968205449	-0.722567721	1.255195734
	6	0.989291046	1.457384307	-0.002716796
	6	1.464576355	0.000080964	0.000033338
	6	-0.593473872	-0.695389706	-1.245254611
	6	0.968424529	-0.727307032	-1.252492168
	17	3.344193835	-0.019018101	0.000244480
	6	-2.715286254	-0.010826967	0.000000000
	8	-3.304807172	1.096311324	0.000355607
	8	-3.184723625	-1.177899343	0.000209025
	1	-0.962023601	2.007208465	-0.876193697
	1	-0.962725290	2.010892067	0.867201388
	1	-1.019429807	-1.696975127	1.252982186
	1	-0.961992379	-0.184444201	2.148377079
	1	1.352917309	-1.748931866	1.254282904
	1	1.379573555	-0.228469102	2.142594230
	1	1.399482791	1.968226093	0.876071457
	1	1.399959579	1.965061084	-0.883111631
	1	-1.019142464	-1.702041999	-1.246515640
	1	-0.961733082	-0.193279344	-2.148138950
	1	1.379809568	-0.236425282	-2.141664995
	1	1.353344355	-1.753587568	-1.247751798
	Br	6	-1.694137150	0.042222524
6		-1.139087367	1.476530469	-0.003108387
6		-1.153748751	-0.690127568	1.247988869
6		0.409406975	-0.718327952	1.256234509
6		0.425695050	1.463156043	-0.002962334

	6	0.894401098	0.005980761	-0.000046568
	6	-1.153489455	-0.694797557	-1.246065310
	6	0.409675268	-0.723322856	-1.253557402
	35	2.940018835	-0.011193157	0.000214317
	6	-3.276304627	-0.014499457	-0.000010054
	8	-3.867731112	1.091476760	0.000593737
	8	-3.742842107	-1.182657705	0.000414875
	1	-1.527670158	2.008156221	-0.876249260
	1	-1.528085033	2.011331814	0.867862859
	1	-1.523001757	-0.185291943	2.148867097
	1	-1.576342823	-1.698025544	1.252054009
	1	0.797084873	-1.743204581	1.255707978
	1	0.819126164	-0.223092132	2.143379529
	1	0.834940097	1.974956699	0.875302562
	1	0.835003069	1.971414915	-0.883251334
	1	-1.576411616	-1.702562181	-1.246608775
	1	-1.522181003	-0.193241773	-2.149016855
	1	0.819848491	-0.231835199	-2.142566713
	1	0.797147316	-1.748277274	-1.248695321
CF ₃	6	1.088864212	-0.690828198	-1.245094799
	6	-0.467918103	-0.722996883	-1.255645006
	6	-1.006813163	0.004297448	0.000001058
	6	-0.485467208	1.464065699	0.000059268
	6	1.072929627	1.474706395	-0.000881609
	6	1.628976380	0.042848540	-0.000254005
	6	1.088996507	-0.689662950	1.245375792
	6	-0.467747708	-0.723111186	1.255500540
	6	-2.524238979	-0.008509170	0.000090489
	9	-3.056070581	0.614034525	1.087347061
	9	-3.039470291	-1.268343672	-0.000002646
	9	-3.056172183	0.614232967	-1.087005213
	6	3.211192541	-0.013006118	-0.000078847
	8	3.803735062	1.092782770	0.000265647
	8	3.679589021	-1.180743141	0.000242892
	1	1.459949758	-0.187055162	-2.146163002
	1	1.515720278	-1.697130705	-1.248750355
	1	-0.846815893	-1.752072004	-1.259936104
	1	-0.872575183	-0.237070878	-2.151298667
	1	-0.887842476	1.982845673	0.878494030
	1	-0.888916705	1.983352625	-0.877589137
	1	1.465309265	2.008159396	0.869681112
	1	1.464140313	2.007003144	-0.872703244
	1	1.459465561	-0.184397633	2.145867192
	1	1.516610883	-1.695636838	1.250423085
	1	-0.845789818	-1.752496404	1.259146043
	1	-0.873077372	-0.237954075	2.151270620
F	6	-0.793461597	0.043212085	-0.000197383
	6	-0.229686210	1.475272085	-0.000936644
	6	-0.256446703	-0.693943465	1.248452429
	6	1.302747602	-0.727969033	1.249748384
	6	1.330813576	1.445132795	-0.000808054
	6	1.809112020	-0.008322371	0.000075143
	6	-0.256256729	-0.695346843	-1.247897851
	6	1.302938635	-0.729438558	-1.248832907

	9	3.227569519	-0.025942385	0.000185212
	6	-2.375824340	-0.005518790	-0.000130178
	8	-2.964461003	1.102385220	0.000152403
	8	-2.850498978	-1.170862344	0.000111656
	1	-0.618734148	2.010813220	0.869729797
	1	-0.618534119	2.009871284	-0.872282019
	1	-0.688514106	-1.697864674	1.252550906
	1	-0.625586994	-0.187733038	2.148828467
	1	1.691483326	-1.754490344	1.244518525
	1	1.723656773	-0.234057214	2.134724835
	1	1.750970786	1.949640859	0.878931131
	1	1.751072917	1.948593617	-0.881098641
	1	-0.688409329	-1.699233656	-1.250976604
	1	-0.625157302	-0.190126506	-2.148931657
	1	1.724047306	-0.236613140	-2.134318427
	1	1.691639962	-1.755968336	-1.242293864
CHO	6	-0.586814177	-0.614701818	1.306748182
	6	0.968226616	-0.683307002	1.347895417
	6	1.552142489	0.062790585	0.115559082
	6	0.986800209	1.513984576	0.120095189
	6	-0.563046180	1.480769179	-0.047156572
	6	-1.082893505	0.036123227	0.000238659
	6	-0.461645236	-0.743689830	-1.180540466
	6	1.093594528	-0.656995251	-1.163318922
	6	3.049037286	0.133701924	0.252271495
	8	3.875744973	-0.306757701	-0.523582787
	6	-2.660570914	-0.058829164	-0.080405837
	8	-3.269754471	1.022453526	-0.266594206
	8	-3.109552409	-1.227487484	0.042913100
	1	-0.961476961	-0.034704502	2.160148627
	1	-1.038920464	-1.607345731	1.375535933
	1	1.322123956	-1.722695787	1.328009995
	1	1.364800514	-0.237257678	2.271048303
	1	1.461896072	2.086335280	-0.688189721
	1	1.276116228	2.007057120	1.058915955
	1	-0.865718104	1.935907651	-0.994597106
	1	-1.057995187	2.065385682	0.733975194
	1	-0.853157553	-0.337526183	-2.121202769
	1	-0.811630897	-1.778141921	-1.118765902
	1	1.558741859	-1.649547616	-1.202367970
	1	1.477789382	-0.111846374	-2.034246247
	1	3.386941302	0.659636904	1.181530028
CH ₂ Cl	6	-1.182508477	1.188777639	-0.857156016
	6	0.344754215	1.484318370	-0.917310240
	6	1.131597392	0.339899543	-0.219759374
	6	0.723832454	-0.996824413	-0.882613675
	6	-0.796110129	-1.270614372	-0.672135012
	6	-1.476618312	-0.064082306	-0.008153034
	6	-0.834964968	0.151697654	1.378762855
	6	0.708977390	0.319898231	1.265704136
	6	2.610397502	0.658488589	-0.406709758
	17	3.784241230	-0.533279960	0.374475984
	6	-3.042957040	-0.232767609	0.153939249
	8	-3.528140080	-1.317878367	-0.246919396

	8	-3.610974311	0.761490295	0.676375309
	1	-1.575418880	1.034811931	-1.870226171
	1	-1.741046596	2.022170422	-0.423144416
	1	0.584299526	2.435422928	-0.420333956
	1	0.687828822	1.583552334	-1.957194864
	1	1.335243318	-1.805950186	-0.466225265
	1	0.971876881	-0.944057504	-1.953126550
	1	-0.954271154	-2.155335231	-0.047487837
	1	-1.299013727	-1.486591187	-1.619131037
	1	-1.074629344	-0.704359790	2.021321622
	1	-1.309481382	1.025563501	1.833922495
	1	1.045308691	1.250656452	1.745840942
	1	1.236194567	-0.495393515	1.774442972
	1	2.868371940	1.623320534	0.035561240
	1	2.887153499	0.660302080	-1.463376710
COOH	6	1.364450198	0.035649084	-0.018953012
	6	0.788826533	1.247851813	-0.767393796
	6	0.856624722	-1.245606513	-0.714239000
	6	-0.695928938	-1.254043186	-0.817433855
	6	-0.766511658	1.264829406	-0.677523624
	6	-1.274791697	-0.058845568	-0.031895100
	6	0.805566526	0.037824002	1.417961131
	6	-0.741878457	-0.123607339	1.426942856
	6	-2.787682464	-0.093767563	-0.049071135
	8	-3.497238774	-0.915009377	-0.598884180
	8	-3.354709645	0.943228283	0.640247320
	6	2.946770608	0.023146213	0.023746300
	8	3.523933650	0.957103311	-0.584168290
	8	3.433096671	-0.942815525	0.666854352
	1	1.122968628	1.212429746	-1.808883944
	1	1.219187868	2.162547917	-0.349750707
	1	1.231810863	-2.103866393	-0.149538082
	1	1.301540549	-1.312470705	-1.714615780
	1	-1.125568475	-2.182893195	-0.424140328
	1	-1.030911366	-1.186300032	-1.859475935
	1	-1.221590862	1.377729901	-1.671060788
	1	-1.124704858	2.107733092	-0.075609904
	1	1.301977649	-0.767081582	1.966188232
	1	1.086559645	0.978805399	1.908515320
	1	-1.224602939	0.655726813	2.026460991
	1	-1.038846379	-1.086763908	1.864020509
	1	-4.311148309	0.803767324	0.542651689
COCH ₃	6	-0.888666405	1.419535433	-0.225709443
	6	0.662942145	1.482648287	-0.318550416
	6	1.270859910	0.097037878	-0.012081646
	6	0.763935094	-0.909388457	-1.093804082
	6	-0.794163815	-0.891378438	-1.156860843
	6	-1.377588082	-0.030540936	-0.026822936
	6	-0.807694348	-0.531284433	1.314647740
	6	0.740944459	-0.377504995	1.367715751
	6	2.795211598	0.145684613	-0.059705481
	8	3.408073466	1.095033890	-0.525263454
	6	3.581635666	-1.044717600	0.488111507

	6	-2.959167643	-0.059033956	0.022155593
	8	-3.528498862	-0.714515230	-0.884286405
	8	-3.453371039	0.596030328	0.975813960
	1	-1.339028523	1.828740262	-1.138525910
	1	-1.272470196	2.018427022	0.605324797
	1	1.081172621	2.217145780	0.381159493
	1	0.996084094	1.798998913	-1.313000940
	1	1.130816855	-1.916296342	-0.853205179
	1	1.204906433	-0.642217976	-2.063323478
	1	-1.204106317	-1.902909216	-1.083838087
	1	-1.142500560	-0.499362344	-2.117126517
	1	-1.084485800	-1.585227180	1.449019602
	1	-1.301099744	0.029135441	2.112842827
	1	1.040915991	0.354250830	2.130972969
	1	1.212859438	-1.327544319	1.646974227
	1	3.594279298	-1.001597063	1.583534342
	1	4.609298413	-0.987181746	0.123748629
	1	3.134234294	-2.003102049	0.210756481
CONH ₂	6	0.842446476	-0.815782822	-1.171213188
	6	-0.710091838	-0.759778936	-1.252437133
	6	-1.280309428	-0.004034447	-0.024184988
	6	-0.749361023	1.450691802	-0.052215507
	6	0.806362409	1.461862205	-0.157662011
	6	1.370589184	0.041806590	-0.001971185
	6	0.817248114	-0.563432480	1.304312908
	6	-0.731727250	-0.696521087	1.255272465
	6	-2.806679398	-0.136143548	-0.017757072
	8	-3.379346021	-1.218998423	-0.110425533
	7	-3.533987488	1.022035476	0.104971833
	6	2.952787882	0.003540196	0.017588793
	8	3.534589163	1.107734144	-0.118409760
	8	3.434746645	-1.148890904	0.165003287
	1	1.282678555	-0.455305163	-2.109206321
	1	1.206471739	-1.837365322	-1.029373048
	1	-1.159271774	-1.757400290	-1.280189305
	1	-1.039763443	-0.244271922	-2.165413412
	1	-1.066637180	1.969764941	0.865874741
	1	-1.199622069	1.992762455	-0.895825644
	1	1.254009319	2.109099427	0.601357026
	1	1.130350121	1.869191100	-1.120407939
	1	1.115808330	0.073760429	2.147164205
	1	1.303812836	-1.531296081	1.452314260
	1	-1.054620623	-1.743118854	1.238386948
	1	-1.198602873	-0.242214481	2.140762219
	1	-3.093961260	1.904112565	0.305426820
	1	-4.530252032	0.926032139	0.226574648
OH	6	-0.802291977	0.043009939	-0.001778565
	6	-0.264841042	-0.671558209	1.258490921
	6	-0.265685609	-0.716890707	-1.235653219
	6	1.292185224	-0.756813955	-1.241803317
	6	1.292289472	-0.710598790	1.253253125
	6	1.826512426	-0.015716564	-0.011109547
	6	-0.237504275	1.473526330	-0.028477144
	6	1.321021151	1.438943009	-0.037205394

	8	3.264103916	-0.068640639	-0.068428968
	6	-2.384941006	-0.002726321	0.004278927
	8	-2.972163707	1.106404321	-0.008482182
	8	-2.863051063	-1.166649564	0.023606068
	1	-0.699589257	-1.674269719	1.282818258
	1	-0.631841340	-0.148228898	2.150367315
	1	-0.701222827	-1.719503261	-1.222321656
	1	-0.635927646	-0.226432299	-2.144660138
	1	1.676328219	-1.784924915	-1.220247810
	1	1.711069234	-0.285651996	-2.140082755
	1	1.679620230	-1.737540797	1.272529994
	1	1.708799593	-0.203216235	2.137714158
	1	-0.629683355	1.993990146	-0.907144745
	1	-0.623612633	2.024430538	0.834168556
	1	1.737711721	1.969280744	0.834082301
	1	1.739196063	1.930567724	-0.925232553
	1	3.577574760	0.405545039	0.714469192
OCH ₃	6	0.730858340	-0.922743832	-1.136951078
	6	-0.814991173	-1.084724459	-1.189431173
	6	-1.476718327	-0.137250057	-0.177409319
	6	-1.021169742	1.305407247	-0.476516704
	6	0.526302758	1.423130134	-0.304247813
	6	1.144787135	0.046361748	-0.009446343
	6	0.539866629	-0.487678640	1.307103789
	6	-1.017521594	-0.534598670	1.236944411
	8	-2.899856928	-0.314538723	-0.379735477
	6	-3.769485652	0.344209163	0.508904469
	6	2.722088298	0.082386018	0.118251536
	8	3.262853470	1.209003323	0.000925531
	8	3.243499342	-1.042914693	0.332369351
	1	1.105939704	-0.537849406	-2.093937441
	1	1.238410232	-1.874495044	-0.960284195
	1	-1.129265837	-2.109660355	-0.953459396
	1	-1.219413827	-0.857725411	-2.183833543
	1	-1.538398169	2.006624253	0.191479612
	1	-1.337792365	1.557214124	-1.497092180
	1	0.784898980	2.109532823	0.507859344
	1	0.995226298	1.840544090	-1.199870782
	1	0.860971913	0.154587491	2.136291200
	1	0.969017736	-1.475708657	1.494480161
	1	-1.407455904	-1.536253413	1.462484517
	1	-1.455812650	0.148262236	1.976258475
	1	-3.693304766	-0.027954847	1.541987578
	1	-4.787309935	0.149027955	0.152849673
	1	-3.621772173	1.434466169	0.533100040
C ₆ H ₅	6	2.191955884	-0.031094455	-0.028986213
	6	1.624376771	-0.992124261	-1.082579174
	6	1.631342331	-0.432326700	1.349680861
	6	0.076153898	-0.385608286	1.366392279
	6	0.066991194	-0.943500810	-1.095431302
	6	-0.475976943	0.047405815	-0.022376789
	6	1.676266305	1.386434867	-0.342990467
	6	0.120318502	1.441458718	-0.333694940
	6	-2.007747167	0.036856666	-0.011129127

	6	-2.782462130	1.183646208	-0.245402774
	6	-4.179432387	1.142269309	-0.225706797
	6	-4.848012916	-0.052820885	0.030441450
	6	-4.098117953	-1.207188774	0.267064116
	6	-2.705951038	-1.158241466	0.245784311
	6	3.773767225	-0.020260609	0.024983516
	8	4.361775226	-0.781687932	-0.780835957
	8	4.249830424	0.765732180	0.885021961
	1	1.987335213	-2.003076649	-0.872357691
	1	2.038386530	-0.730275187	-2.060931597
	1	2.068188205	0.239434713	2.093634751
	1	1.980815220	-1.443351585	1.595704890
	1	-0.296496954	0.318951003	2.122456390
	1	-0.340723472	-1.364561855	1.634221056
	1	-0.353853418	-1.940339511	-0.913385332
	1	-0.316072279	-0.631165051	-2.076562435
	1	2.057814214	1.696423195	-1.324188806
	1	2.112524262	2.069352924	0.391028649
	1	-0.236284521	2.161883270	0.415312593
	1	-0.258813184	1.790013484	-1.303978468
	1	-2.292401664	2.128976912	-0.447139429
	1	-4.743731130	2.053184971	-0.412054978
	1	-5.934394228	-0.086820524	0.046345873
	1	-4.599549380	-2.150831933	0.469227288
	1	-2.146428119	-2.069585233	0.432883923
NH ₂	6	0.812737936	0.042145264	-0.000186270
	6	0.249956344	1.472718276	-0.027208707
	6	0.275622499	-0.715606394	-1.233955089
	6	-1.281414880	-0.741414897	-1.245438764
	6	-1.308529393	1.450052027	-0.036123756
	6	-1.833558950	0.000355607	-0.013810997
	6	0.272379172	-0.670655432	1.258394082
	6	-1.283822107	-0.699697738	1.250517807
	7	-3.310133341	0.019066256	-0.081312847
	6	2.395274779	-0.009555354	0.005517731
	8	2.987837408	1.096716144	-0.010387749
	8	2.868962502	-1.175707491	0.026598036
	1	0.645095113	1.991452212	-0.905817568
	1	0.638845000	2.022624985	0.835124251
	1	0.704580986	-1.721226791	-1.218237466
	1	0.652120999	-0.228944303	-2.142598464
	1	-1.662400273	-1.774468373	-1.235122983
	1	-1.693546059	-0.270069313	-2.146328105
	1	-1.721029937	1.949386854	-0.921961708
	1	-1.718420564	1.985018475	0.834689267
	1	0.704166640	-1.674867689	1.283433162
	1	0.640479629	-0.148682402	2.150921364
	1	-1.699716265	-0.198917728	2.138076644
	1	-1.666783978	-1.731683863	1.272598787
	1	-3.658236190	0.473924265	0.764340973
	1	-3.640497639	-0.945128030	-0.015843038
H	6	-0.478315378	0.041907663	0.000066147
	6	0.054892085	-0.697223305	-1.248330718
	6	0.091374623	1.471769461	0.000440805

	6	1.650643013	1.439152034	-0.000402704
	6	1.612731168	-0.741160892	-1.252022258
	6	2.151028786	-0.020787141	-0.000046568
	6	0.054936536	-0.697854085	1.248056604
	6	1.612816894	-0.740587264	1.252298489
	6	-2.059917694	0.001657912	0.000012171
	8	-2.543907439	-1.160678328	-0.000037042
	8	-2.645334842	1.112433767	-0.000030163
	1	-0.314301123	-0.187892320	-2.147961675
	1	-0.385753810	-1.698054120	-1.253803998
	1	-0.298822159	2.007041245	0.871601497
	1	-0.299859876	2.007935025	-0.869684817
	1	2.057425798	1.959960345	-0.879138039
	1	2.058412184	1.960834016	0.877355241
	1	2.021513184	-0.262340680	-2.153039131
	1	1.980650117	-1.777195223	-1.260928312
	1	3.251006250	-0.039931715	-0.000075143
	1	-0.314989053	-0.189609500	2.147993426
	1	-0.384935173	-1.699027277	1.252521802
	1	1.981545485	-1.776324727	1.262215271
	1	2.020912568	-0.260686471	2.153052360
CH ₃	6	0.824848687	0.042337884	-0.000048155
	6	0.261398215	1.472738914	-0.000508539
	6	0.286336751	-0.693605850	-1.245899148
	6	-1.269926971	-0.727283219	-1.248500584
	6	-1.296242955	1.446479551	0.000260884
	6	-1.830271172	-0.007011069	0.000014288
	6	0.286351568	-0.692878760	1.246242055
	6	-1.269887282	-0.727609192	1.248324897
	6	-3.362076851	-0.025340711	0.000024342
	6	2.406503920	-0.006709438	0.000043922
	8	2.997399112	1.100840552	0.000027517
	8	2.883047084	-1.171862489	0.000031751
	1	0.652626364	2.006963985	-0.871738024
	1	0.653593700	2.007951429	0.869656241
	1	0.719234433	-1.697697983	-1.251006238
	1	0.657219622	-0.188055836	-2.146795368
	1	-1.644855402	-1.761399282	-1.259015336
	1	-1.676519781	-0.246328305	-2.150078913
	1	-1.701893830	1.971302730	-0.877333545
	1	-1.701019629	1.970559765	0.878703585
	1	0.719917601	-1.696679846	1.252367282
	1	0.656579847	-0.186273567	2.146820240
	1	-1.677106638	-0.247451748	2.150045046
	1	-1.644102912	-1.761989315	1.258105151
	1	-3.765791995	0.481808477	0.886020518
	1	-3.747858178	-1.053059021	0.000021696
	1	-3.765795699	0.481814827	-0.885966542
CH ₂ CH ₃	6	1.173554798	0.049392346	-0.007169293
	6	0.539372907	1.389463878	-0.409871592
	6	0.784564539	-1.005861702	-1.062543465
	6	-0.760663720	-1.146677356	-1.164477291
	6	-1.011619680	1.257976561	-0.514299960
	6	-1.472857979	-0.183242439	-0.182646586

	6	0.564342665	-0.393875622	1.339222202
	6	-0.984336359	-0.532177155	1.243241091
	6	-2.999987847	-0.356451149	-0.335358673
	6	-3.897947133	0.507167180	0.561149080
	6	2.749678012	0.115663859	0.124128578
	8	3.279261140	1.233354473	-0.090605729
	8	3.284344946	-0.980695091	0.435725605
	1	0.976078549	1.717243145	-1.358400115
	1	0.827038951	2.150628199	0.321784747
	1	1.266912248	-1.947207702	-0.785146634
	1	1.205534037	-0.712933520	-2.033086290
	1	-1.081410751	-2.175450317	-0.942319686
	1	-1.111678631	-0.934086746	-2.185106214
	1	-1.364358122	1.516754819	-1.523859553
	1	-1.503184069	1.964304890	0.168182055
	1	1.043324277	-1.334520992	1.625088515
	1	0.832315378	0.340267850	2.109938173
	1	-1.475084757	0.126591898	1.971910755
	1	-1.308384927	-1.554623272	1.488670324
	1	-3.244932354	-1.414445807	-0.158481178
	1	-3.264163184	-0.161130239	-1.385490815
	1	-3.717846948	0.314404842	1.623694133
	1	-4.956648242	0.298454910	0.364392512
	1	-3.736967181	1.576203120	0.389022538
CH(CH ₃) ₂	6	-1.451670251	-0.005932606	0.048552013
	6	-0.784757689	-0.012154143	1.433291396
	6	-0.955389306	1.242301272	-0.710284458
	6	0.596480128	1.332622833	-0.659882971
	6	0.754158544	-0.220675380	1.298482963
	6	1.211499452	-0.004540341	-0.168790609
	6	-0.952181962	-1.236453335	-0.734278413
	6	0.568649109	-1.123440125	-1.031821022
	6	2.764265841	-0.003857702	-0.340910272
	6	3.460120694	-1.244064491	0.251027928
	6	3.462021499	1.257751660	0.201641403
	6	-3.031953328	-0.001221341	0.106484221
	8	-3.546623712	0.035093448	1.251064448
	8	-3.585757957	-0.024027293	-1.023875425
	1	-1.243529493	-0.791999480	2.047683645
	1	-1.010508937	0.931992263	1.941669862
	1	-1.398966843	2.141548576	-0.265064884
	1	-1.330901419	1.188581315	-1.736597803
	1	0.903138344	2.140117152	0.016560073
	1	1.012352061	1.583407869	-1.647539918
	1	1.298789885	0.459917472	1.967980026
	1	1.027263747	-1.237203179	1.611911472
	1	-1.544650927	-1.310868885	-1.650271531
	1	-1.157269897	-2.141578739	-0.146527593
	1	1.066029685	-2.084414896	-0.849597248
	1	0.745760501	-0.885863882	-2.091318542
	1	2.944348564	-0.021518993	-1.428057833
	1	3.021974633	-2.179322836	-0.107632536
	1	4.523455809	-1.251114719	-0.019028685
	1	3.401022709	-1.248838199	1.345083369
	1	3.116835475	2.167598385	-0.295886284

	1	4.546639593	1.188511993	0.050856050
	1	3.289814522	1.380501732	1.277195749
C(CH ₃) ₃	6	-1.686282572	0.041281646	-0.007935013
	6	-1.125778030	-0.735430432	-1.215583642
	6	-1.134141147	-0.642075098	1.260329812
	6	0.402194818	-0.425139414	1.370602942
	6	0.402471578	-0.968444638	-1.059712367
	6	0.995810510	0.004250352	-0.000951990
	6	-1.113204778	1.464890686	-0.053151092
	6	0.419407896	1.416963103	-0.316686125
	6	2.580173014	-0.008443552	0.001850004
	6	3.151736303	0.711385676	1.245255669
	6	3.152952352	0.701058253	-1.246816742
	6	3.136246755	-1.451669722	0.009637905
	6	-3.265886185	-0.012276912	-0.003154426
	8	-3.738298591	-1.179221228	0.003089866
	8	-3.859829438	1.093837420	0.005208692
	1	-1.672594873	-1.679481057	-1.288947188
	1	-1.334139984	-0.170255371	-2.134384045
	1	-1.395764262	-1.704136483	1.221271239
	1	-1.633326746	-0.232668653	2.147242523
	1	0.895082679	-1.336349828	1.735645813
	1	0.615266450	0.355582769	2.111178565
	1	0.591527558	-2.001019207	-0.740377710
	1	0.911906282	-0.848612979	-2.025135931
	1	-1.635375720	2.039710531	-0.823099756
	1	-1.333332989	1.971549856	0.893735393
	1	0.935556801	2.185327939	0.274518106
	1	0.623241151	1.655687131	-1.368241224
	1	2.911302503	0.178409993	2.169646830
	1	2.769466066	1.732429474	1.339660361
	1	4.245236637	0.773662959	1.175002627
	1	2.924573739	1.770665705	-1.246407159
	1	2.759417520	0.276045841	-2.175455079
	1	4.245012795	0.595524963	-1.272220954
	1	2.740171872	-2.038496599	0.844349927
	1	4.229098318	-1.432953252	0.108445352
	1	2.898493767	-1.985641846	-0.914930530

4. Table S4. Cartesian coordinates of the optimized geometries of 4-substituted 4-substituted quinuclidines at B3LYP/6-31G(d,p) level

Substituents	Atomic number followed by Cartesian coordinates in Angstrom unit			
NO ₂	7	2.142357688	-0.016548960	0.000218021
	6	1.664827609	1.374419369	-0.001860058
	6	1.637432632	-0.703990424	-1.196731174
	6	0.072476116	-0.710803581	-1.254352226
	6	0.100775457	1.467165090	-0.001682784
	6	-0.427646656	0.030404408	-0.000247655
	6	1.637075438	-0.700549714	1.198972768
	6	0.072089287	-0.708015875	1.255709565

	7	-1.954643701	0.003946604	-0.000114302
	8	-2.558851934	1.072267626	0.000000529
	8	-2.487770200	-1.103820878	0.000048684
	1	2.079333207	1.873706570	-0.883187833
	1	2.079713685	1.876577356	0.877655284
	1	2.024884572	-1.727576389	-1.190223881
	1	2.052821956	-0.204802708	-2.077512837
	1	-0.331730634	-1.725698868	-1.259509058
	1	-0.294795649	-0.202686528	-2.152479261
	1	-0.271404427	2.000702230	-0.880143476
	1	-0.271121318	2.002331567	0.875886774
	1	2.051668879	-0.198332987	2.078414026
	1	2.025051263	-1.723948350	1.195946933
	1	-0.331618977	-1.723115425	1.262598395
	1	-0.296001115	-0.198288536	2.152585626
CN	6	-1.364245936	-0.314602754	1.349308850
	6	0.195824687	-0.331433765	1.418165923
	6	0.737557724	0.000116948	0.000069851
	6	0.196089805	1.394147626	-0.421905083
	6	-1.364026327	1.325861006	-0.402481632
	7	-1.854823409	0.000095252	0.000028046
	6	-1.364099883	-1.011510670	-0.946953691
	6	0.196137960	-1.062325973	-0.996493678
	6	2.204045468	-0.000011642	0.000099485
	7	3.365713886	-0.000248184	0.000131236
	1	-1.774755716	-1.286898743	1.640556895
	1	-1.774093715	0.428742053	2.040841912
	1	0.573788479	-1.309527950	1.732592460
	1	0.574535148	0.405486300	2.133659072
	1	0.575061679	1.645986253	-1.417557898
	1	0.573800650	2.154927235	0.268682869
	1	-1.773413723	1.551992203	-1.392415628
	1	-1.775115027	2.064638484	0.293187480
	1	-1.775138311	-0.778446721	-1.934599525
	1	-1.773474049	-1.981870400	-0.647781746
	1	0.575198736	-2.050329002	-0.716327662
	1	0.573677351	-0.845070137	-2.000809653
CI	7	1.947324121	-0.000109540	-0.000098956
	6	1.450059435	-0.350111076	1.338393511
	6	1.450021335	1.334179143	-0.366368460
	6	-0.117709129	1.393970351	-0.383876818
	6	-0.117511217	-0.363843226	1.399179043
	6	-0.628838259	0.000078318	0.000142349
	6	1.450035622	-0.984303021	-0.972206559
	6	-0.117453007	-1.029254512	-1.014800035
	17	-2.470514259	-0.000229663	-0.000112186
	1	1.857401560	0.372962538	2.052255736
	1	1.855135623	-1.331438005	1.605467152
	1	1.856904134	1.590589333	-1.349775584
	1	1.855554203	2.056428828	0.349376578
	1	-0.496397893	1.666040484	-1.373770597
	1	-0.497668448	2.135269888	0.325722885
	1	-0.495799394	0.357556600	2.129824654
	1	-0.497923511	-1.348892387	1.686009516

	1	1.856735855	-1.964256735	-0.702563762
	1	1.855458422	-0.725858674	-1.955692001
	1	-0.496052341	-2.022673140	-0.755524880
	1	-0.497500170	-0.785354072	-2.011508030
Br	7	-2.467361421	0.000118007	-0.000181508
	6	-1.971348239	-0.022980051	1.383833432
	6	-1.970909022	-1.186860430	-0.711813251
	6	-0.401756130	-1.240575625	-0.743371795
	6	-0.402005902	-0.023362646	1.445824430
	6	0.101856037	-0.000164574	-0.000010584
	6	-1.970693118	1.209965897	-0.672273656
	6	-0.401368243	1.263936155	-0.702471156
	35	2.107628314	-0.000044980	0.000075143
	1	-2.376589001	-0.912613792	1.876500097
	1	-2.377304449	0.849485592	1.905951456
	1	-2.376502745	-1.169137226	-1.728486045
	1	-2.376647740	-2.075005595	-0.216793865
	1	-0.022828177	-1.239958075	-1.769732766
	1	-0.023643639	-2.145105176	-0.257727841
	1	-0.022967351	-0.912434401	1.958555379
	1	-0.024087619	0.849550152	1.986360468
	1	-2.375928588	2.081760543	-0.148646948
	1	-2.376315946	1.225676111	-1.689040114
	1	-0.022878978	1.296719215	-1.728550075
	1	-0.022417536	2.152065445	-0.188062186
CF ₃	6	-1.909908644	-0.958897222	-0.998120368
	6	-0.348988691	-1.005119796	-1.044292142
	6	0.189597329	0.000675759	0.000218021
	6	-0.349375520	-0.401144930	1.393244849
	6	-1.910239380	-0.385390265	1.328991089
	7	-2.406033482	-0.000072497	-0.000292635
	6	-1.910116610	1.343598498	-0.331135839
	6	-0.349376578	1.407760710	-0.348502907
	6	1.710643246	0.000118536	0.000071968
	9	2.218095653	0.871604143	0.904687775
	9	2.217275957	0.347215948	-1.207606295
	9	2.216503358	-1.219891145	0.302700499
	1	-2.319497126	-1.944294052	-0.753054680
	1	-2.318467877	-0.674254896	-1.973282911
	1	0.027814615	-0.739768627	-2.036987914
	1	0.025960907	-2.007500570	-0.815357364
	1	0.027547380	-1.393369735	1.660013684
	1	0.024757558	0.298410988	2.147217652
	1	-2.321384172	0.318022297	2.060461688
	1	-2.317699511	-1.373132939	1.568251174
	1	-2.320517909	1.625000142	-1.306441259
	1	-2.318663143	2.044913931	0.403824684
	1	0.025433846	1.711106806	-1.330978150
	1	0.026664183	2.135403241	0.377497587
F	7	-1.607806644	0.000857796	0.000029634
	6	-1.110432419	-0.737339174	-1.172770557
	6	-1.108911563	1.384900782	-0.052094854
	6	0.455573985	1.441503698	-0.055290556

	6	0.454635754	-0.768937406	-1.220422439
	6	0.966225797	0.000023813	-0.000081493
	6	-1.110130788	-0.646884261	1.225002997
	6	0.454878117	-0.673119811	1.275771204
	9	2.366698679	-0.000491076	-0.000157695
	1	-1.518550318	-0.261869712	-2.070158332
	1	-1.519373188	-1.751838108	-1.131990041
	1	-1.516836842	1.924227122	0.808574899
	1	-1.517664475	1.857868295	-0.950560034
	1	0.843646121	1.995648058	0.805662307
	1	0.842188767	1.927254016	-0.957237193
	1	0.842571362	-0.301111380	-2.131226445
	1	0.840767926	-1.793111287	-1.189193573
	1	-1.517992036	-1.661939360	1.260350979
	1	-1.519235073	-0.105710564	2.084000550
	1	0.841789767	-0.135738198	2.147882299
	1	0.842014138	-1.696148023	1.324416881
CHO	6	1.507946664	-0.556991864	-1.196123678
	6	-0.031236804	-0.822778545	-1.252771044
	6	-0.677534207	-0.170861809	-0.000224900
	6	-0.358454085	1.334104529	-0.002264879
	6	1.194634573	1.500866272	-0.000909127
	7	1.893598872	0.203654923	0.000158224
	6	1.507409020	-0.555304846	1.197330202
	6	-0.032087192	-0.819081184	1.254756517
	6	-2.164716485	-0.447977117	-0.000042863
	8	-3.035918982	0.394297377	0.000019050
	1	1.833636210	0.007301059	-2.076166081
	1	2.065787328	-1.499628527	-1.192551202
	1	-0.247952350	-1.897777255	-1.269657090
	1	-0.471682670	-0.392727308	-2.159399841
	1	-0.815684924	1.807045583	0.872728644
	1	-0.813745490	1.804160508	-0.879844491
	1	1.527252637	2.060810416	0.879577256
	1	1.528856044	2.060366965	-0.881066890
	1	1.834135224	0.009323574	2.076774106
	1	2.064052155	-1.498650607	1.194359930
	1	-0.250052655	-1.893751804	1.275592871
	1	-0.472202851	-0.385087047	2.159657551
	1	-2.426004102	-1.533203765	0.000237071
CH ₂ Cl	7	-2.245438241	-0.440980864	-0.000003704
	6	-1.557042141	-0.942766312	-1.198814544
	6	-2.207200951	1.026438760	0.000350845
	6	-0.742971737	1.574538329	-0.000436042
	6	-0.066189490	-0.480226237	-1.255643418
	6	0.235257388	0.369904951	0.000007938
	6	-1.556857459	-0.943353698	1.198454704
	6	-0.066449316	-0.479519256	1.256086869
	6	1.656781469	0.929513596	0.000008996
	17	2.969827390	-0.340178949	0.000000000
	1	-2.109011584	-0.591083049	-2.077135534
	1	-1.625797083	-2.035679259	-1.193407940
	1	-2.752216476	1.380518136	0.881823614
	1	-2.753357911	1.381058956	-0.880198510

	1	-0.559618170	2.201617073	0.880499083
	1	-0.560123535	2.200428541	-0.882321569
	1	0.125863750	0.116919067	-2.155808315
	1	0.612470277	-1.337579107	-1.292718635
	1	-1.624603259	-2.036324326	1.191788129
	1	-2.109316919	-0.593172770	2.077066212
	1	0.124370941	0.118583859	2.155881342
	1	0.612890444	-1.336273627	1.294458040
	1	1.838743300	1.536867259	0.889164890
	1	1.838748062	1.536849267	-0.889158539
COOH	7	2.174770853	-0.055240813	0.000027517
	6	1.651094401	-0.725413107	1.198642033
	6	1.735063718	1.349382935	-0.001439891
	6	0.180130348	1.480095536	0.001185357
	6	0.089694485	-0.697218014	1.254788797
	6	-0.422756000	0.060575978	-0.000055564
	6	1.651019258	-0.727914527	-1.197154515
	6	0.089811963	-0.695067966	-1.256009609
	6	-1.939385933	0.130202475	-0.000011113
	8	-2.606260923	1.142651905	0.000066147
	8	-2.513093448	-1.102227525	-0.000035455
	1	2.080167190	-0.231410269	2.076709017
	1	2.018726537	-1.757166393	1.196880931
	1	2.166356935	1.835071339	-0.883302135
	1	2.169619312	1.838278682	0.877036676
	1	-0.179731878	2.031019324	-0.873150928
	1	-0.176948405	2.028048523	0.878552769
	1	-0.262049103	-0.188413030	2.159648026
	1	-0.328508474	-1.707733301	1.270229660
	1	2.015466276	-1.760781203	-1.190872123
	1	2.083049090	-0.238599671	-2.076392569
	1	-0.258818476	-0.182279866	-2.159844879
	1	-0.331279775	-1.704316932	-1.275564296
	1	-3.472648437	-0.946285869	-0.000037042
COCH ₃	6	1.793295970	1.261063781	-0.345384465
	6	0.243985108	1.423981581	-0.406309700
	6	-0.412164517	0.078131962	-0.027575426
	6	0.090281872	-0.315607661	1.392136752
	6	1.649683615	-0.427065090	1.348249966
	7	2.192122575	-0.107542576	0.021443320
	6	1.644781317	-1.049608256	-0.963485718
	6	0.082633673	-1.004529234	-1.020955954
	6	-1.940794074	0.209530907	-0.008332425
	8	-2.478638188	1.302452850	-0.000008996
	6	-2.781397426	-1.058423820	0.007697412
	1	2.230995936	1.945037017	0.389782966
	1	2.251346505	1.496683655	-1.312081759
	1	-0.086802003	1.719009539	-1.407981377
	1	-0.110150890	2.202847939	0.273754504
	1	-0.356361189	-1.265908399	1.705492235
	1	-0.231452604	0.443728882	2.113403755
	1	1.972649486	-1.440382371	1.610666318
	1	2.105187749	0.254579237	2.074243051
	1	1.993513357	-2.054488335	-0.701450373

	1	2.075564407	-0.804583844	-1.939983904
	1	-0.263551966	-0.764281176	-2.033322303
	1	-0.339114773	-1.981812719	-0.763032317
	1	-2.784303138	-1.510098299	-0.991395055
	1	-3.806358723	-0.801076986	0.277865682
	1	-2.388750553	-1.810927627	0.697760420
CONH ₂	6	-1.737823907	1.346124261	-0.025186191
	6	-0.184187021	1.467823916	-0.054148062
	6	0.424663155	0.050238500	-0.004144516
	6	-0.099744620	-0.743686126	-1.230112733
	6	-1.663043753	-0.751142763	-1.181218342
	7	-2.183505453	-0.057168077	0.003947662
	6	-1.657743514	-0.703683501	1.213671196
	6	-0.096180611	-0.653490510	1.277538127
	6	1.959084027	0.149422192	-0.002580268
	8	2.554902684	1.218531159	-0.000640834
	7	2.636276915	-1.039584052	0.006505176
	1	-2.185496747	1.822255724	-0.904265492
	1	-2.154748373	1.847071491	0.855253624
	1	0.193067673	2.052246211	0.789442495
	1	0.164648738	1.978157163	-0.956674148
	1	0.286752684	-1.770053447	-1.219969463
	1	0.265422079	-0.279461680	-2.152965046
	1	-2.080268792	-0.263224935	-2.068340079
	1	-2.045041992	-1.777860928	-1.168665729
	1	-2.013047936	-1.739993004	1.223926651
	1	-2.097104037	-0.204208442	2.083543341
	1	0.246760643	-0.101986214	2.160043850
	1	0.319873888	-1.664502695	1.358388473
	1	2.176579581	-1.933613139	-0.024457514
	1	3.643834631	-1.005447886	-0.006216245
OH	7	1.618927304	-0.009698231	-0.000047626
	6	1.118014470	-0.697641355	1.200850818
	6	1.127240676	1.378152185	-0.002666524
	6	-0.433378704	1.447405611	-0.002148460
	6	-0.444946519	-0.712194259	1.250862831
	6	-0.978002108	0.012823552	0.000032809
	6	1.117906518	-0.702222972	-1.198252558
	6	-0.445067171	-0.715953005	-1.248646108
	8	-2.398915519	0.103711332	-0.000002117
	1	1.531605120	-0.190088935	2.078426197
	1	1.520611463	-1.715848763	1.199447440
	1	1.540777350	1.879500532	-0.883885817
	1	1.541568999	1.883220648	0.876051348
	1	-0.817165033	1.971946739	-0.883425433
	1	-0.816460698	1.974353437	0.878003483
	1	-0.828716443	-0.208802759	2.144466459
	1	-0.829540372	-1.740702631	1.268108188
	1	1.519775892	-1.720706081	-1.192433725
	1	1.532085613	-0.198683302	-2.077852040
	1	-0.828266113	-0.214776641	-2.143744132
	1	-0.830249999	-1.744291511	-1.263200069
	1	-2.747798375	-0.799140727	0.000192091

OCH ₃	6	-1.732197165	1.180823047	-0.037836173
	6	-0.213993459	1.540740307	-0.070040313
	6	0.605343847	0.241045529	0.000290518
	6	0.231322955	-0.630625819	-1.216137691
	6	-1.313837570	-0.883185716	-1.178712159
	7	-1.947626281	-0.274451430	-0.000178862
	6	-1.327289255	-0.819501351	1.216335603
	6	0.206058446	-0.511055045	1.286502390
	8	1.970788370	0.662768046	-0.001676963
	6	2.971315965	-0.337748967	0.001135614
	1	-2.248022743	1.577201149	-0.918785057
	1	-2.220166852	1.615558562	0.840908158
	1	0.070719777	2.180479088	0.771723524
	1	0.057050070	2.076765639	-0.985702166
	1	0.774418624	-1.581402287	-1.187274776
	1	0.532251769	-0.112623206	-2.133467510
	1	-1.532135885	-1.956181490	-1.164556138
	1	-1.795743415	-0.470382482	-2.071146835
	1	-1.508206490	-1.899499727	1.230549833
	1	-1.848077457	-0.396849599	2.081914534
	1	0.452533333	0.112676653	2.152627960
	1	0.778797566	-1.439651048	1.381643696
	1	3.928234064	0.189604737	0.028772955
	1	2.949150847	-0.964099563	-0.901391001
	1	2.915928041	-0.995535338	0.879620120
	C ₆ H ₅	7	-3.024694074	-0.039004597
6		-2.505508750	-0.713673839	1.198253087
6		-2.505616702	-0.714521051	-1.197673638
6		-0.945570951	-0.690768401	-1.256686956
6		-0.945472524	-0.689932830	1.257056851
6		-0.393898906	0.040920747	-0.000057680
6		-2.563068418	1.354955171	-0.000427575
6		-1.004940405	1.462989352	-0.000500073
6		1.137817870	0.038441023	-0.000065089
6		1.897326396	1.216881714	-0.000073026
6		3.294093979	1.182237538	-0.000001058
6		3.969410933	-0.035978232	0.000067735
6		3.231334615	-1.220942091	0.000021167
6		1.838672919	-1.180431985	-0.000030163
1		-2.879538109	-1.743427365	1.192550144
1		-2.937077139	-0.221117243	2.076492054
1		-2.937309448	-0.222585710	-2.076197303
1		-2.879553455	-1.744306857	-1.191266889
1		-0.590138468	-0.174963991	-2.156065496
1		-0.545365310	-1.708644015	-1.302414749
1		-0.545237779	-1.707785160	1.303377852
1		-0.589964369	-0.173584955	2.156092484
1		-2.986643584	1.851178436	0.879573023
1		-2.986736190	1.850419067	-0.880802831
1		-0.659391365	2.016118751	-0.881217706
1		-0.659426820	2.016541035	0.879977314
1		1.403938992	2.181995710	-0.000215375
1		3.851684342	2.114795491	0.000043922
1		5.055115428	-0.064144749	0.000115361
1		3.740738627	-2.180646837	0.000026459

	1	1.290283890	-2.117871069	0.000006350
NH ₂	7	-1.632253575	-0.000004233	0.010701022
	6	-1.137513064	-1.198636212	-0.684729960
	6	-1.137514123	1.198966418	-0.684147336
	6	0.423411121	1.246595546	-0.729999486
	6	0.423420647	-1.246670689	-0.729862429
	6	0.979945776	0.000003704	-0.013000297
	6	-1.128311201	-0.000334969	1.392136223
	6	0.433482952	0.000076202	1.436266960
	7	2.442238202	0.000008467	-0.109700560
	1	-1.555961562	-1.196738582	-1.696949727
	1	-1.543884678	-2.077148763	-0.172115959
	1	-1.543380372	2.077207502	-0.170663367
	1	-1.556470630	1.197964686	-1.696158078
	1	0.803944598	2.151466945	-0.238267877
	1	0.799672550	1.259697445	-1.758097216
	1	0.800151985	-1.260229798	-1.757781297
	1	0.803503264	-2.151462183	-0.237630219
	1	-1.536070847	-0.880904433	1.900324185
	1	-1.536570920	0.879621178	1.900983011
	1	0.814529730	0.881806680	1.967592139
1	0.814982177	-0.881274328	1.967895358	
1	2.812066422	-0.813208375	0.381904046	
1	2.812067481	0.813177683	0.381981305	
H	7	1.293746826	0.002934288	0.003333287
	6	0.795570368	-0.317614831	1.351719252
	6	0.796218081	1.330437331	-0.396257449
	6	-0.765030491	1.384651011	-0.418270694
	6	-0.765536384	-0.334283385	1.406912968
	6	-1.294497729	-0.003199935	-0.003233273
	6	0.803339748	-1.007251322	-0.949481042
	6	-0.757452143	-1.055501703	-0.994322993
	1	1.206516190	0.423973637	2.045362673
	1	1.210678169	-1.289692799	1.639403818
	1	1.212675813	1.561190362	-1.382879325
	1	1.206412471	2.066259354	0.304029263
	1	-1.136046714	1.644007660	-1.416890605
	1	-1.142386258	2.150902313	0.269212575
	1	-1.141903119	0.398986945	2.129837884
	1	-1.138126910	-1.314875286	1.725666059
	1	-2.389811024	-0.006008278	-0.005973882
	1	1.219319634	-1.976479671	-0.653477810
	1	1.218891529	-0.768344728	-1.934531261
	1	-1.129248374	-0.843454559	-2.003719070
1	-1.128872129	-2.050429546	-0.721780305	
CH ₃	7	-1.647871712	0.000845625	-0.000040217
	6	-1.149033253	1.384509720	-0.007427003
	6	-1.150262003	-0.685298825	1.202331986
	6	0.410385953	-0.716623472	1.251903723
	6	0.411049012	1.442168873	-0.006116231
	6	0.969944855	-0.000185212	0.000044451
	6	-1.150189505	-0.698022363	-1.195046802
	6	0.410398653	-0.727421334	-1.245578996

	6	2.500080979	0.000179920	-0.000055034
	1	-1.561772986	1.895343569	0.869522888
	1	-1.559952087	1.885188129	-0.891051406
	1	-1.563457357	-1.699968154	1.205677973
	1	-1.560814117	-0.170158003	2.077727683
	1	0.782171600	-1.748457194	1.280093524
	1	0.785282104	-0.221492429	2.156317384
	1	0.783924235	1.983326166	0.872412725
	1	0.785735080	1.976841628	-0.887829775
	1	-1.562312747	-0.193376184	-2.075834816
	1	-1.561826433	-1.713273257	-1.186590021
	1	0.783879784	-1.758794672	-1.265960258
	1	0.783889839	-0.238790704	-2.154121298
	1	2.894882662	0.508222888	-0.887610696
	1	2.896096594	-1.021954512	0.004073606
	1	2.895130317	0.515582685	0.883116394
CH ₂ CH ₃	7	1.977203056	-0.314299006	-0.000015346
	6	1.333598106	-0.873147753	1.197937169
	6	1.804645235	1.145952912	-0.000093135
	6	0.298199317	1.551618075	-0.000622842
	6	-0.194340345	-0.550126847	1.250857010
	6	-0.581002223	0.275756381	0.000012171
	6	1.333543072	-0.873297510	-1.197861496
	6	-0.194622925	-0.551197902	-1.250197655
	6	-2.069018484	0.682566683	-0.000014288
	6	-3.101316294	-0.452032731	0.000026988
	1	1.849914232	-0.470006766	2.076185131
	1	1.504313333	-1.955383491	1.196621105
	1	2.320040062	1.545835226	-0.880365730
	1	2.319409283	1.545804533	0.880563643
	1	0.055981661	2.159949657	-0.881014502
	1	0.055666801	2.161106967	0.878875567
	1	-0.443924148	0.018071403	2.155862821
	1	-0.780005677	-1.475191121	1.287410987
	1	1.504927178	-1.955427942	-1.196908448
	1	1.849309911	-0.469589245	-2.076172431
	1	-0.445070875	0.015837746	-2.155696130
	1	-0.779788186	-1.476637892	-1.285384767
	1	-2.246695566	1.321165616	-0.876556183
	1	-2.246697683	1.321362999	0.876378380
	1	-4.115941701	-0.040505343	0.000159812
	1	-3.009915212	-1.091521740	0.883695843
	1	-3.010060207	-1.091324357	-0.883803795
CH(CH ₃) ₂	7	-2.264079039	-0.000626546	0.172991218
	6	-1.588501729	-0.061786736	1.477255971
	6	-1.847133934	1.223183157	-0.525081946
	6	-0.295846595	1.314302716	-0.666960188
	6	-0.033360921	-0.150867905	1.337804536
	6	0.352211381	0.000429163	-0.155237850
	6	-1.859774920	-1.161848338	-0.630935917
	6	-0.327928495	-1.160867773	-0.928961665
	6	1.894078306	0.000569395	-0.404134253
	6	2.612491986	-1.254114096	0.126299792
	6	2.617629238	1.251728565	0.127413181

	1	-1.979963245	-0.928062063	2.022105333
	1	-1.879261873	0.829453587	2.044401158
	1	-2.238240901	2.082861232	0.030448859
	1	-2.333692306	1.229482483	-1.506778770
	1	0.082214036	2.164871534	-0.091225395
	1	-0.006833795	1.486036080	-1.711698426
	1	0.326687045	-1.111907765	1.720930452
	1	0.449450875	0.629106022	1.937335371
	1	-2.439989198	-1.151840538	-1.560416176
	1	-2.150658892	-2.065147552	-0.083147504
	1	0.110424475	-2.121715542	-0.642185696
	1	-0.138647085	-1.035979826	-2.002649073
	1	2.014827559	0.003501566	-1.498394485
	1	2.178822763	-2.182854565	-0.253924645
	1	3.664943511	-1.238290638	-0.176107013
	1	2.590966643	-1.298282934	1.220729362
	1	2.246957509	2.175173028	-0.324717448
	1	3.688052153	1.187074218	-0.095084156
	1	2.519311810	1.346532257	1.214669224
C(CH ₃) ₃	7	-2.489705930	0.000924473	0.000151345
	6	-1.986021266	-0.731281682	-1.168259321
	6	-1.985786311	-0.646509075	1.217473863
	6	-0.424347765	-0.678740732	1.270420693
	6	-0.424361524	-0.761346359	-1.222324302
	6	0.162891341	-0.000180449	0.000374657
	6	-1.984367058	1.378193461	-0.049080661
	6	-0.423166642	1.439348359	-0.047506888
	6	1.751169228	-0.000523356	-0.000060855
	6	2.318995466	0.671310025	-1.272308268
	6	2.320596757	0.766176688	1.216981729
	6	2.321451907	-1.437353890	0.054406830
	1	-2.393421600	-1.747765030	-1.129304996
	1	-2.397713757	-0.257150509	-2.066173098
	1	-2.396959150	-1.661538244	1.253168456
	1	-2.393804196	-0.107017632	2.079564457
	1	-0.075172274	-1.713395497	1.340344587
	1	-0.070675326	-0.164373566	2.169311860
	1	-0.075090252	-0.305458042	-2.153877877
	1	-0.071910426	-1.797401856	-1.225823751
	1	-2.395909792	1.918447448	0.810805910
	1	-2.391617106	1.853741241	-0.948338019
	1	-0.069121132	1.959948703	-0.942593800
	1	-0.074178479	2.017728508	0.813457088
	1	3.413891770	0.659945943	-1.236778779
	1	2.020699309	0.149330645	-2.185940197
	1	2.009850647	1.716432975	-1.363874983
	1	3.415570320	0.744479892	1.185970354
	1	2.019924065	1.817700567	1.223801765
	1	2.016201303	0.321623878	2.168975833
	1	3.416229675	-1.397598920	0.055087352
	1	2.021220549	-2.038002347	-0.809089259
	1	2.017603622	-1.970710051	0.959541230

5. Table S5. Comparison of V_{\min} values at three different levels of theory

	B3LYP/6-31G(d,p)	B3LYP/6-311++G(d,p)	BPW91/6-311++G(d,p)
Acid (Model (i))	V_{\min} (in kcal/mol)	V_{\min} (in kcal/mol)	V_{\min} (in kcal/mol)
X = CN	-40.41	-38.97	-36.83
X = CHO	-43.67	-42.11	-39.97
X = CH ₃	-47.88	-47.00	-44.99
Anion (Model (ii))			
X = CN	-173.95	-170.18	-165.73
X = CHO	-177.40	-173.76	-168.36
X = CH ₃	-182.04	-178.21	-173.44
Qunuclidines (Model iii)			
X = CN	-54.09	-53.84	-51.52
X = CHO	-58.99	-58.73	-56.60
X = CH ₃	-64.26	-65.89	-62.88