Electronic Supplementary Information of "X-ray Circular Dichroism Signals: A Unique Probe of Local Molecular Chirality"

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Molecular coordinates (unit: angstrom)

1. *o*-CPEO-1 (∠C1-C2-C3-C4 = 120°, see the main text for full explanation)

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	2.81028867	-0.30808352	-1.12932941
C	0.84702944	-0.11414310	-2.52429853
C	3.61208882	-0.38483982	-2.26794556
C	1.64883653	-0.19190014	-3.66336356
H	-0.24269633	-0.00737061	-2.62542410
C	3.03118405	-0.32709165	-3.53539628
H	4.70195827	-0.49116982	-2.16707418
H	1.19071325	-0.14636649	-4.66212477
H	3.66357184	-0.38769006	-4.43300969
Cl	3.54256434	-0.38028526	0.46946990

2. *o*-CPEO-2 (∠C1-C2-C3-C4 = 60°)

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	2.42150514	0.78184194	-1.47695727
C	1.23577662	-1.20368451	-2.17672233
C	3.22278648	0.70509192	-2.61593901
C	2.03786991	-1.28116519	-3.31560468
H	0.45263782	-1.95594907	-2.00374646
C	3.03117930	-0.32693308	-3.53541038
H	4.00574834	1.45754546	-2.78937751
H	1.88661870	-2.09464799	-4.04006518
H	3.66312203	-0.38727576	-4.43335441
Cl	2.66240982	2.08364929	-0.31727518

3. *o*-CPEO-3 (∠C1-C2-C3-C4 = 0°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	1.43973396	0.87888202	-2.17455590
C	2.21725558	-1.30058398	-1.47933892
C	2.24073391	0.80158634	-3.31369866
C	3.01930532	-1.37763319	-2.61828121
H	2.20799773	-2.12915958	-0.75649332
C	3.03106412	-0.32686417	-3.53549612
H	2.24982376	1.62989371	-4.03696956
H	3.64207262	-2.26711596	-2.79279628
H	3.66258762	-0.38755824	-4.43371137
Cl	0.44230489	2.30169757	-1.89467886

4. *o*-CPEO-4 (∠C1-C2-C3-C4 = 300°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	0.84674631	-0.11400336	-2.52452668
C	2.80998736	-0.30794203	-1.12953171
C	1.64798368	-0.19185098	-3.66346487
C	3.61170735	-0.38483614	-2.26871662
H	3.26802349	-0.35379163	-0.13091782
C	3.03095369	-0.32695383	-3.53556776
H	1.19010911	-0.14647333	-4.66225827
H	4.70162108	-0.49130242	-2.16758697
H	3.66250302	-0.38825502	-4.43372361
Cl	-0.89764552	0.05581128	-2.68533746

5. *o*-CPEO-5 (∠C1-C2-C3-C4 = 240°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	1.23552984	-1.20392883	-2.17689882
C	2.42124018	0.78159938	-1.47710792
C	2.03728602	-1.28178273	-3.31547143
C	3.22267398	0.70442891	-2.61647550
H	2.57268934	1.59478683	-0.75259546
C	3.03095844	-0.32711240	-3.53555365
H	1.88631904	-2.09518861	-4.03995493
H	4.00571563	1.45697909	-2.78964656
H	3.66295283	-0.38866932	-4.43337889
Cl	-0.01749099	-2.40812328	-1.89859238

6. *o*-CPEO-6 (∠C1-C2-C3-C4 =180°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	2.21730102	-1.30096891	-1.47930018
C	1.43976122	0.87849885	-2.17449133
C	3.01933859	-1.37827715	-2.61771178
C	2.24123858	0.80089691	-3.31379897
H	0.81732944	1.76799734	-1.99984860
C	3.03107361	-0.32718131	-3.53546791
H	3.64224362	-2.26753685	-2.79236289
H	2.25026171	1.62944705	-4.03691546
H	3.66348724	-0.38838685	-4.43302193
Cl	2.20261394	-2.62617155	-0.32118870

7. *m*-CPEO-1 (∠C1-C2-C3-C4 =120°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847

H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	2.81028867	-0.30808352	-1.12932941
C	0.84702944	-0.11414310	-2.52429853
C	3.61208882	-0.38483982	-2.26794556
C	1.64883653	-0.19190014	-3.66336356
H	-0.24269633	-0.00737061	-2.62542410
C	3.03118405	-0.32709165	-3.53539628
H	1.19071325	-0.14636649	-4.66212477
H	3.66357184	-0.38769006	-4.43300969
Cl	5.35638707	-0.55501729	-2.10650441
H	3.25547899	-0.35197890	-0.15733210

8. *m*-CPEO-2 (∠C1-C2-C3-C4 =60°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	2.42150514	0.78184194	-1.47695727
C	1.23577662	-1.20368451	-2.17672233
C	3.22278648	0.70509192	-2.61593901
C	2.03786991	-1.28116519	-3.31560468
H	0.45263782	-1.95594907	-2.00374646
C	3.03117930	-0.32693308	-3.53541038
H	1.88661870	-2.09464799	-4.04006518
H	3.66312203	-0.38727576	-4.43335441
Cl	4.47588978	1.90936771	-2.89352132
H	2.56796423	1.57328163	-0.77192327

9. *m*-CPEO-3 (∠C1-C2-C3-C4 = 0°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178

H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	1.43973396	0.87888202	-2.17455590
C	2.21725558	-1.30058398	-1.47933892
C	2.24073391	0.80158634	-3.31369866
C	3.01930532	-1.37763319	-2.61828121
H	2.20799773	-2.12915958	-0.75649332
C	3.03106412	-0.32686417	-3.53549612
H	3.64207262	-2.26711596	-2.79279628
H	3.66258762	-0.38755824	-4.43371137
Cl	2.25528190	2.12726355	-4.47126865
H	0.83334243	1.74388919	-2.00440338

10. *m*-CPEO-4 (∠C1-C2-C3-C4 = 300°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	0.84674631	-0.11400336	-2.52452668
C	2.80998736	-0.30794203	-1.12953171
C	1.64798368	-0.19185098	-3.66346487
C	3.61170735	-0.38483614	-2.26871662
H	3.26802349	-0.35379163	-0.13091782
C	3.03095369	-0.32695383	-3.53556776
H	4.70162108	-0.49130242	-2.16758697
H	3.66250302	-0.38825502	-4.43372361
Cl	0.91517131	-0.11922562	-5.26199907
H	-0.21376462	-0.01076378	-2.62229232

11. *m*-CPEO-5 (∠C1-C2-C3-C4 = 240°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641

H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	1.23552984	-1.20392883	-2.17689882
C	2.42124018	0.78159938	-1.47710792
C	2.03728602	-1.28178273	-3.31547143
C	3.22267398	0.70442891	-2.61647550
H	2.57268934	1.59478683	-0.75259546
C	3.03095844	-0.32711240	-3.53555365
H	4.00571563	1.45697909	-2.78964656
H	3.66295283	-0.38866932	-4.43337889
Cl	1.79566860	-2.58361064	-4.47498216
H	0.47375014	-1.93602431	-2.00770115

12. *m*-CPEO-6 (∠C1-C2-C3-C4 =180°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	2.21730102	-1.30096891	-1.47930018
C	1.43976122	0.87849885	-2.17449133
C	3.01933859	-1.37827715	-2.61771178
C	2.24123858	0.80089691	-3.31379897
H	0.81732944	1.76799734	-1.99984860
C	3.03107361	-0.32718131	-3.53546791
H	2.25026171	1.62944705	-4.03691546
H	3.66348724	-0.38838685	-4.43302193
Cl	4.01627649	-2.80150648	-2.89723483
H	2.20837194	-2.10663187	-0.77522104

13. *p*-CPEO-1 (∠C1-C2-C3-C4 =120°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000

C	1.42766302	-0.17238329	-1.25740435
C	2.81028867	-0.30808352	-1.12932941
C	0.84702944	-0.11414310	-2.52429853
C	3.61208882	-0.38483982	-2.26794556
C	1.64883653	-0.19190014	-3.66336356
H	-0.24269633	-0.00737061	-2.62542410
C	3.03118405	-0.32709165	-3.53539628
H	1.19071325	-0.14636649	-4.66212477
H	3.25547899	-0.35197890	-0.15733210
H	4.67254288	-0.48829999	-2.16979668
Cl	4.04329886	-0.42407731	-4.97199553

14. *p*-CPEO-2 (∠C1-C2-C3-C4 =60°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	2.42150514	0.78184194	-1.47695727
C	1.23577662	-1.20368451	-2.17672233
C	3.22278648	0.70509192	-2.61593901
C	2.03786991	-1.28116519	-3.31560468
H	0.45263782	-1.95594907	-2.00374646
C	3.03117930	-0.32693308	-3.53541038
H	1.88661870	-2.09464799	-4.04006518
H	2.56796423	1.57328163	-0.77192327
H	3.98461633	1.43723687	-2.78469644
Cl	4.04258180	-0.42350946	-4.97253878

15. *m*-CPEO-3 (∠C1-C2-C3-C4 = 0°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	1.43973396	0.87888202	-2.17455590

C	2.21725558	-1.30058398	-1.47933892
C	2.24073391	0.80158634	-3.31369866
C	3.01930532	-1.37763319	-2.61828121
H	2.20799773	-2.12915958	-0.75649332
C	3.03106412	-0.32686417	-3.53549612
H	3.64207262	-2.26711596	-2.79279628
H	0.83334243	1.74388919	-2.00440338
H	2.24957842	1.60753783	-4.01744860
Cl	4.04179566	-0.42400294	-4.97305860

16. *m*-CPEO-4 (∠C1-C2-C3-C4 = 300°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	0.84674631	-0.11400336	-2.52452668
C	2.80998736	-0.30794203	-1.12953171
C	1.64798368	-0.19185098	-3.66346487
C	3.61170735	-0.38483614	-2.26871662
H	3.26802349	-0.35379163	-0.13091782
C	3.03095369	-0.32695383	-3.53556776
H	4.70162108	-0.49130242	-2.16758697
H	-0.21376462	-0.01076378	-2.62229232
H	1.20246706	-0.14769807	-4.63530100
Cl	4.04172658	-0.42506428	-4.97303517

17. *m*-CPEO-5 (∠C1-C2-C3-C4 = 240°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	1.23552984	-1.20392883	-2.17689882
C	2.42124018	0.78159938	-1.47710792
C	2.03728602	-1.28178273	-3.31547143

C	3.22267398	0.70442891	-2.61647550
H	2.57268934	1.59478683	-0.75259546
C	3.03095844	-0.32711240	-3.53555365
H	4.00571563	1.45697909	-2.78964656
H	0.47375014	-1.93602431	-2.00770115
H	1.89039361	-2.07323493	-4.02040124
Cl	4.04244365	-0.42563213	-4.97249192

18. *m*-CPEO-6 (∠C1-C2-C3-C4 =180°）

C	0.54264952	-0.08702873	0.00000000
C	-0.21953722	1.25113021	0.00140847
H	0.48052568	2.06033413	0.00238599
H	-0.83425965	1.31238108	-0.87224178
H	-0.83444898	1.31043412	0.87505982
O	-0.39294828	-1.16848843	-0.00130641
H	0.08176204	-2.00290400	-0.00218473
H	1.15737218	-0.14828047	0.87365000
C	1.42766302	-0.17238329	-1.25740435
C	2.21730102	-1.30096891	-1.47930018
C	1.43976122	0.87849885	-2.17449133
C	3.01933859	-1.37827715	-2.61771178
C	2.24123858	0.80089691	-3.31379897
H	0.81732944	1.76799734	-1.99984860
C	3.03107361	-0.32718131	-3.53546791
H	2.25026171	1.62944705	-4.03691546
H	2.20837194	-2.10663187	-0.77522104
H	3.62543152	-2.24353589	-2.78764908
Cl	4.04322979	-0.42513864	-4.97197210

19. 1CHHC (compound a in Fig. 3 in the main text)

C	3.14702200	-2.44591700	0.73942700
C	2.26775800	-3.08521800	1.58758300
C	1.06676100	-2.44299800	1.94644000
C	2.85277800	-1.16634800	0.20866300
C	0.74096700	-1.21170300	1.41188700
C	1.59493700	-0.54690100	0.49599400
H	2.51080700	-4.06127900	1.99862700
H	0.39057600	-2.91429200	2.65452500
H	4.10123200	-2.90296800	0.48738800
C	3.83550600	-0.45871600	-0.55156900
C	1.29630100	0.76414700	-0.07042200
C	2.38612100	1.49552800	-0.61800600
C	3.62824300	0.84085500	-0.89815500
H	4.40865600	1.41482200	-1.39193000

H	4.77577700	-0.95387200	-0.78131500
C	2.27278200	2.89904700	-0.83638800
C	1.15121600	3.56639500	-0.43856900
C	-0.00000800	1.42159600	0.00000400
C	-0.00001600	2.85074900	0.00000300
H	3.12741000	3.43444200	-1.24216300
H	1.10020000	4.65134800	-0.48502900
C	-1.15125300	3.56638400	0.43857200
C	-1.29631100	0.76413500	0.07042500
C	-2.38614000	1.49550500	0.61800400
C	-2.27281600	2.89902500	0.83638700
H	-3.12744800	3.43441300	1.24215800
H	-1.10024800	4.65133700	0.48503000
C	-3.62825800	0.84082200	0.89814600
C	-3.83550700	-0.45875100	0.55155900
C	-1.59493100	-0.54691600	-0.49599100
C	-2.85276800	-1.16637500	-0.20866800
H	-4.40868000	1.41478100	1.39191600
H	-4.77577400	-0.95391600	0.78129900
C	-3.14699600	-2.44594700	-0.73943300
C	-2.26772100	-3.08524100	-1.58758200
C	-0.74094700	-1.21171100	-1.41187700
C	-1.06672600	-2.44301000	-1.94643000
H	-4.10120300	-2.90300600	-0.48740000
H	-2.51075700	-4.06130400	-1.99862700
H	0.17863100	-0.73341500	-1.72278400
H	-0.39053000	-2.91429800	-2.65451000
Cl	-0.75462599	-0.43382075	1.91755568

20. 2CHHC (compound b in Fig. 3 in the main text)

C	3.14702200	-2.44591700	0.73942700
C	2.26775800	-3.08521800	1.58758300
C	1.06676100	-2.44299800	1.94644000
C	2.85277800	-1.16634800	0.20866300
C	0.74096700	-1.21170300	1.41188700
C	1.59493700	-0.54690100	0.49599400
H	2.51080700	-4.06127900	1.99862700
H	4.10123200	-2.90296800	0.48738800
H	-0.17861200	-0.73341500	1.72280200
C	3.83550600	-0.45871600	-0.55156900
C	1.29630100	0.76414700	-0.07042200
C	2.38612100	1.49552800	-0.61800600
C	3.62824300	0.84085500	-0.89815500
H	4.40865600	1.41482200	-1.39193000

H	4.77577700	-0.95387200	-0.78131500
C	2.27278200	2.89904700	-0.83638800
C	1.15121600	3.56639500	-0.43856900
C	-0.00000800	1.42159600	0.00000400
C	-0.00001600	2.85074900	0.00000300
H	3.12741000	3.43444200	-1.24216300
H	1.10020000	4.65134800	-0.48502900
C	-1.15125300	3.56638400	0.43857200
C	-1.29631100	0.76413500	0.07042500
C	-2.38614000	1.49550500	0.61800400
C	-2.27281600	2.89902500	0.83638700
H	-3.12744800	3.43441300	1.24215800
H	-1.10024800	4.65133700	0.48503000
C	-3.62825800	0.84082200	0.89814600
C	-3.83550700	-0.45875100	0.55155900
C	-1.59493100	-0.54691600	-0.49599100
C	-2.85276800	-1.16637500	-0.20866800
H	-4.40868000	1.41478100	1.39191600
H	-4.77577400	-0.95391600	0.78129900
C	-3.14699600	-2.44594700	-0.73943300
C	-2.26772100	-3.08524100	-1.58758200
C	-0.74094700	-1.21171100	-1.41187700
C	-1.06672600	-2.44301000	-1.94643000
H	-4.10120300	-2.90300600	-0.48740000
H	-2.51075700	-4.06130400	-1.99862700
H	0.17863100	-0.73341500	-1.72278400
H	-0.39053000	-2.91429800	-2.65451000
Cl	-0.02846354	-3.20635826	3.09333333

21. 3CHHC (compound c in Fig. 3 in the main text)

C	3.14702200	-2.44591700	0.73942700
C	2.26775800	-3.08521800	1.58758300
C	1.06676100	-2.44299800	1.94644000
C	2.85277800	-1.16634800	0.20866300
C	0.74096700	-1.21170300	1.41188700
C	1.59493700	-0.54690100	0.49599400
H	0.39057600	-2.91429200	2.65452500
H	4.10123200	-2.90296800	0.48738800
H	-0.17861200	-0.73341500	1.72280200
C	3.83550600	-0.45871600	-0.55156900
C	1.29630100	0.76414700	-0.07042200
C	2.38612100	1.49552800	-0.61800600
C	3.62824300	0.84085500	-0.89815500
H	4.40865600	1.41482200	-1.39193000

H	4.77577700	-0.95387200	-0.78131500
C	2.27278200	2.89904700	-0.83638800
C	1.15121600	3.56639500	-0.43856900
C	-0.00000800	1.42159600	0.00000400
C	-0.00001600	2.85074900	0.00000300
H	3.12741000	3.43444200	-1.24216300
H	1.10020000	4.65134800	-0.48502900
C	-1.15125300	3.56638400	0.43857200
C	-1.29631100	0.76413500	0.07042500
C	-2.38614000	1.49550500	0.61800400
C	-2.27281600	2.89902500	0.83638700
H	-3.12744800	3.43441300	1.24215800
H	-1.10024800	4.65133700	0.48503000
C	-3.62825800	0.84082200	0.89814600
C	-3.83550700	-0.45875100	0.55155900
C	-1.59493100	-0.54691600	-0.49599100
C	-2.85276800	-1.16637500	-0.20866800
H	-4.40868000	1.41478100	1.39191600
H	-4.77577400	-0.95391600	0.78129900
C	-3.14699600	-2.44594700	-0.73943300
C	-2.26772100	-3.08524100	-1.58758200
C	-0.74094700	-1.21171100	-1.41187700
C	-1.06672600	-2.44301000	-1.94643000
H	-4.10120300	-2.90300600	-0.48740000
H	-2.51075700	-4.06130400	-1.99862700
H	0.17863100	-0.73341500	-1.72278400
H	-0.39053000	-2.91429800	-2.65451000
Cl	2.66142781	-4.66615745	2.25335663

22. 4CHHC (compound d in Fig. 3 in the main text)

C	3.14702200	-2.44591700	0.73942700
C	2.26775800	-3.08521800	1.58758300
C	1.06676100	-2.44299800	1.94644000
C	2.85277800	-1.16634800	0.20866300
C	0.74096700	-1.21170300	1.41188700
C	1.59493700	-0.54690100	0.49599400
H	2.51080700	-4.06127900	1.99862700
H	0.39057600	-2.91429200	2.65452500
H	-0.17861200	-0.73341500	1.72280200
C	3.83550600	-0.45871600	-0.55156900
C	1.29630100	0.76414700	-0.07042200
C	2.38612100	1.49552800	-0.61800600
C	3.62824300	0.84085500	-0.89815500
H	4.40865600	1.41482200	-1.39193000

H	4.77577700	-0.95387200	-0.78131500
C	2.27278200	2.89904700	-0.83638800
C	1.15121600	3.56639500	-0.43856900
C	-0.00000800	1.42159600	0.00000400
C	-0.00001600	2.85074900	0.00000300
H	3.12741000	3.43444200	-1.24216300
H	1.10020000	4.65134800	-0.48502900
C	-1.15125300	3.56638400	0.43857200
C	-1.29631100	0.76413500	0.07042500
C	-2.38614000	1.49550500	0.61800400
C	-2.27281600	2.89902500	0.83638700
H	-3.12744800	3.43441300	1.24215800
H	-1.10024800	4.65133700	0.48503000
C	-3.62825800	0.84082200	0.89814600
C	-3.83550700	-0.45875100	0.55155900
C	-1.59493100	-0.54691600	-0.49599100
C	-2.85276800	-1.16637500	-0.20866800
H	-4.40868000	1.41478100	1.39191600
H	-4.77577400	-0.95391600	0.78129900
C	-3.14699600	-2.44594700	-0.73943300
C	-2.26772100	-3.08524100	-1.58758200
C	-0.74094700	-1.21171100	-1.41187700
C	-1.06672600	-2.44301000	-1.94643000
H	-4.10120300	-2.90300600	-0.48740000
H	-2.51075700	-4.06130400	-1.99862700
H	0.17863100	-0.73341500	-1.72278400
H	-0.39053000	-2.91429800	-2.65451000
Cl	4.69112408	-3.18551667	0.33157763

23. 5CHHC (compound e in Fig. 3 in the main text)

C	3.14702200	-2.44591700	0.73942700
C	2.26775800	-3.08521800	1.58758300
C	1.06676100	-2.44299800	1.94644000
C	2.85277800	-1.16634800	0.20866300
C	0.74096700	-1.21170300	1.41188700
C	1.59493700	-0.54690100	0.49599400
H	2.51080700	-4.06127900	1.99862700
H	0.39057600	-2.91429200	2.65452500
H	4.10123200	-2.90296800	0.48738800
H	-0.17861200	-0.73341500	1.72280200
C	3.83550600	-0.45871600	-0.55156900
C	1.29630100	0.76414700	-0.07042200
C	2.38612100	1.49552800	-0.61800600
C	3.62824300	0.84085500	-0.89815500

H	4.40865600	1.41482200	-1.39193000
C	2.27278200	2.89904700	-0.83638800
C	1.15121600	3.56639500	-0.43856900
C	-0.00000800	1.42159600	0.00000400
C	-0.00001600	2.85074900	0.00000300
H	3.12741000	3.43444200	-1.24216300
H	1.10020000	4.65134800	-0.48502900
C	-1.15125300	3.56638400	0.43857200
C	-1.29631100	0.76413500	0.07042500
C	-2.38614000	1.49550500	0.61800400
C	-2.27281600	2.89902500	0.83638700
H	-3.12744800	3.43441300	1.24215800
H	-1.10024800	4.65133700	0.48503000
C	-3.62825800	0.84082200	0.89814600
C	-3.83550700	-0.45875100	0.55155900
C	-1.59493100	-0.54691600	-0.49599100
C	-2.85276800	-1.16637500	-0.20866800
H	-4.40868000	1.41478100	1.39191600
H	-4.77577400	-0.95391600	0.78129900
C	-3.14699600	-2.44594700	-0.73943300
C	-2.26772100	-3.08524100	-1.58758200
C	-0.74094700	-1.21171100	-1.41187700
C	-1.06672600	-2.44301000	-1.94643000
H	-4.10120300	-2.90300600	-0.48740000
H	-2.51075700	-4.06130400	-1.99862700
H	0.17863100	-0.73341500	-1.72278400
H	-0.39053000	-2.91429800	-2.65451000
Cl	5.35760780	-1.26026985	-0.92347965

24. 6CHHC (compound f in Fig. 3 in the main text)

C	3.14702200	-2.44591700	0.73942700
C	2.26775800	-3.08521800	1.58758300
C	1.06676100	-2.44299800	1.94644000
C	2.85277800	-1.16634800	0.20866300
C	0.74096700	-1.21170300	1.41188700
C	1.59493700	-0.54690100	0.49599400
H	2.51080700	-4.06127900	1.99862700
H	0.39057600	-2.91429200	2.65452500
H	4.10123200	-2.90296800	0.48738800
H	-0.17861200	-0.73341500	1.72280200
C	3.83550600	-0.45871600	-0.55156900
C	1.29630100	0.76414700	-0.07042200
C	2.38612100	1.49552800	-0.61800600
C	3.62824300	0.84085500	-0.89815500

H	4.77577700	-0.95387200	-0.78131500
C	2.27278200	2.89904700	-0.83638800
C	1.15121600	3.56639500	-0.43856900
C	-0.00000800	1.42159600	0.00000400
C	-0.00001600	2.85074900	0.00000300
H	3.12741000	3.43444200	-1.24216300
H	1.10020000	4.65134800	-0.48502900
C	-1.15125300	3.56638400	0.43857200
C	-1.29631100	0.76413500	0.07042500
C	-2.38614000	1.49550500	0.61800400
C	-2.27281600	2.89902500	0.83638700
H	-3.12744800	3.43441300	1.24215800
H	-1.10024800	4.65133700	0.48503000
C	-3.62825800	0.84082200	0.89814600
C	-3.83550700	-0.45875100	0.55155900
C	-1.59493100	-0.54691600	-0.49599100
C	-2.85276800	-1.16637500	-0.20866800
H	-4.40868000	1.41478100	1.39191600
H	-4.77577400	-0.95391600	0.78129900
C	-3.14699600	-2.44594700	-0.73943300
C	-2.26772100	-3.08524100	-1.58758200
C	-0.74094700	-1.21171100	-1.41187700
C	-1.06672600	-2.44301000	-1.94643000
H	-4.10120300	-2.90300600	-0.48740000
H	-2.51075700	-4.06130400	-1.99862700
H	0.17863100	-0.73341500	-1.72278400
H	-0.39053000	-2.91429800	-2.65451000
Cl	4.89144846	1.76989930	-1.69739755

25. 7CHHC (compound g in Fig. 3 in the main text)

C	3.14702200	-2.44591700	0.73942700
C	2.26775800	-3.08521800	1.58758300
C	1.06676100	-2.44299800	1.94644000
C	2.85277800	-1.16634800	0.20866300
C	0.74096700	-1.21170300	1.41188700
C	1.59493700	-0.54690100	0.49599400
H	2.51080700	-4.06127900	1.99862700
H	4.10123200	-2.90296800	0.48738800
H	-0.17861200	-0.73341500	1.72280200
C	3.83550600	-0.45871600	-0.55156900
C	1.29630100	0.76414700	-0.07042200
C	2.38612100	1.49552800	-0.61800600
C	3.62824300	0.84085500	-0.89815500
H	4.40865600	1.41482200	-1.39193000

H	4.77577700	-0.95387200	-0.78131500
C	2.27278200	2.89904700	-0.83638800
C	1.15121600	3.56639500	-0.43856900
C	-0.00000800	1.42159600	0.00000400
C	-0.00001600	2.85074900	0.00000300
H	1.10020000	4.65134800	-0.48502900
C	-1.15125300	3.56638400	0.43857200
C	-1.29631100	0.76413500	0.07042500
C	-2.38614000	1.49550500	0.61800400
C	-2.27281600	2.89902500	0.83638700
H	-3.12744800	3.43441300	1.24215800
H	-1.10024800	4.65133700	0.48503000
C	-3.62825800	0.84082200	0.89814600
C	-3.83550700	-0.45875100	0.55155900
C	-1.59493100	-0.54691600	-0.49599100
C	-2.85276800	-1.16637500	-0.20866800
H	-4.40868000	1.41478100	1.39191600
H	-4.77577400	-0.95391600	0.78129900
C	-3.14699600	-2.44594700	-0.73943300
C	-2.26772100	-3.08524100	-1.58758200
C	-0.74094700	-1.21171100	-1.41187700
C	-1.06672600	-2.44301000	-1.94643000
H	-4.10120300	-2.90300600	-0.48740000
H	-2.51075700	-4.06130400	-1.99862700
H	0.17863100	-0.73341500	-1.72278400
H	-0.39053000	-2.91429800	-2.65451000
Cl	3.65646936	3.76587946	-1.49335891
H	0.39057808	-2.91429055	2.65452282

26. 8CHHC (compound h in Fig. 3 in the main text)

C	3.14702200	-2.44591700	0.73942700
C	2.26775800	-3.08521800	1.58758300
C	1.06676100	-2.44299800	1.94644000
C	2.85277800	-1.16634800	0.20866300
C	0.74096700	-1.21170300	1.41188700
C	1.59493700	-0.54690100	0.49599400
H	2.51080700	-4.06127900	1.99862700
H	0.39057600	-2.91429200	2.65452500
H	4.10123200	-2.90296800	0.48738800
H	-0.17861200	-0.73341500	1.72280200
C	3.83550600	-0.45871600	-0.55156900
C	1.29630100	0.76414700	-0.07042200
C	2.38612100	1.49552800	-0.61800600
C	3.62824300	0.84085500	-0.89815500

H	4.40865600	1.41482200	-1.39193000
H	4.77577700	-0.95387200	-0.78131500
C	2.27278200	2.89904700	-0.83638800
C	1.15121600	3.56639500	-0.43856900
C	-0.00000800	1.42159600	0.00000400
C	-0.00001600	2.85074900	0.00000300
C	-1.15125300	3.56638400	0.43857200
C	-1.29631100	0.76413500	0.07042500
C	-2.38614000	1.49550500	0.61800400
C	-2.27281600	2.89902500	0.83638700
H	-3.12744800	3.43441300	1.24215800
H	-1.10024800	4.65133700	0.48503000
C	-3.62825800	0.84082200	0.89814600
C	-3.83550700	-0.45875100	0.55155900
C	-1.59493100	-0.54691600	-0.49599100
C	-2.85276800	-1.16637500	-0.20866800
H	-4.40868000	1.41478100	1.39191600
H	-4.77577400	-0.95391600	0.78129900
C	-3.14699600	-2.44594700	-0.73943300
C	-2.26772100	-3.08524100	-1.58758200
C	-0.74094700	-1.21171100	-1.41187700
C	-1.06672600	-2.44301000	-1.94643000
H	-4.10120300	-2.90300600	-0.48740000
H	-2.51075700	-4.06130400	-1.99862700
H	0.17863100	-0.73341500	-1.72278400
H	-0.39053000	-2.91429800	-2.65451000
Cl	1.06862521	5.32284638	-0.51378399
H	3.12736618	3.43441455	-1.24214219

27. B2CTA (compound a in Fig. 4 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
Br	-0.25510332	-2.38133280	1.51491303
H	0.19205600	-2.16452200	-0.86772800
C	0.96300800	-0.38088800	0.00000000
Cl	2.63879301	0.18888792	0.00000000
C	0.00000000	0.54341400	0.00000000
H	-1.03174687	0.22419870	0.00000000
C	0.24789500	1.97634600	0.00000000
H	1.30364400	2.22723400	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71732200	2.75165700	0.00000000

C	-0.21429549	4.42943607	0.00000000
H	0.82734296	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347761	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000
H	-2.65469260	7.65403606	0.00000000
H	-1.29120766	8.90770237	0.00000000

28. B3CTA (compound b in Fig. 4 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
Br	-0.25510332	-2.38133280	1.51491303
H	0.19205600	-2.16452200	-0.86772800
C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000
C	0.00000000	0.54341400	0.00000000
Cl	-1.68136526	0.02321129	0.00000000
C	0.24789500	1.97634600	0.00000000
H	1.30364400	2.22723400	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71732200	2.75165700	0.00000000
C	-0.21429549	4.42943607	0.00000000
H	0.82734296	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347761	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000
H	-2.65469260	7.65403606	0.00000000
H	-1.29120766	8.90770237	0.00000000

29. B4CTA (compound c in Fig. 4 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
Br	-0.25510332	-2.38133280	1.51491303
H	0.19205600	-2.16452200	-0.86772800
C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000

C	0.00000000	0.54341400	0.00000000
H	-1.03174686	0.22419870	0.00000000
C	0.24789500	1.97634600	0.00000000
Cl	1.96020949	2.38326010	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71732200	2.75165700	0.00000000
C	-0.21429549	4.42943607	0.00000000
H	0.82734296	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347761	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000
H	-2.65469260	7.65403606	0.00000000
H	-1.29120766	8.90770237	0.00000000

30. B5CTA (compound d in Fig. 4 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
Br	-0.25510332	-2.38133280	1.51491303
H	0.19205600	-2.16452200	-0.86772800
C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000
C	0.00000000	0.54341400	0.00000000
H	-1.03174686	0.22419870	0.00000000
H	1.29863344	2.22604329	0.00000000
C	0.24789500	1.97634600	0.00000000
C	-0.65593500	2.95412100	0.00000000
Cl	-2.38476248	2.62433994	0.00000000
C	-0.21429549	4.42943607	0.00000000
H	0.82734296	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347761	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000
H	-2.65469260	7.65403606	0.00000000
H	-1.29120766	8.90770237	0.00000000

31. B6CTA (compound e in Fig. 4 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900

N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
Br	-0.25510332	-2.38133280	1.51491303
H	0.19205600	-2.16452200	-0.86772800
C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000
C	0.00000000	0.54341400	0.00000000
H	-1.03174686	0.22419870	0.00000000
C	0.24789500	1.97634600	0.00000000
H	1.29863344	2.22604329	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71680641	2.75175535	0.00000000
C	-0.21429549	4.42943607	0.00000000
Cl	1.49905375	4.83197103	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347761	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000
H	-2.65469260	7.65403606	0.00000000
H	-1.29120766	8.90770237	0.00000000

32. B7CTA (compound f in Fig. 4 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
Br	-0.25510332	-2.38133280	1.51491303
H	0.19205600	-2.16452200	-0.86772800
C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000
C	0.00000000	0.54341400	0.00000000
H	-1.03174686	0.22419870	0.00000000
C	0.24789500	1.97634600	0.00000000
H	1.29863344	2.22604329	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71680641	2.75175535	0.00000000
C	-0.21429549	4.42943607	0.00000000
H	0.82734297	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
Cl	-2.85611417	5.02647706	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000

H	-2.65469260	7.65403606	0.00000000
H	-1.29120766	8.90770237	0.00000000

33. B8CTA (compound g in Fig. 4 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
Br	-0.25510332	-2.38133280	1.51491303
H	0.19205600	-2.16452200	-0.86772800
C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000
C	0.00000000	0.54341400	0.00000000
H	-1.03174686	0.22419870	0.00000000
C	0.24789500	1.97634600	0.00000000
H	1.29863344	2.22604329	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71680641	2.75175535	0.00000000
C	-0.21429549	4.42943607	0.00000000
H	0.82734297	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347762	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
Cl	1.02570422	7.28383846	0.00000000
C	-1.61021975	7.88636438	0.00000000
H	-2.65469260	7.65403606	0.00000000
H	-1.29120766	8.90770237	0.00000000

34. B9CTA (compound h in Fig. 4 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
Br	-0.25510332	-2.38133280	1.51491303
H	0.19205600	-2.16452200	-0.86772800
C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000
C	0.00000000	0.54341400	0.00000000
H	-1.03174686	0.22419870	0.00000000
C	0.24789500	1.97634600	0.00000000
H	1.29863344	2.22604329	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71680641	2.75175535	0.00000000
C	-0.21429549	4.42943607	0.00000000

H	0.82734297	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347762	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000
Cl	-3.32823118	7.50421686	0.00000000
H	-1.29120766	8.90770237	0.00000000

35. B10CTA (compound i in Fig. 4 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
Br	-0.25510332	-2.38133280	1.51491303
H	0.19205600	-2.16452200	-0.86772800
C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000
C	0.00000000	0.54341400	0.00000000
H	-1.03174687	0.22419870	0.00000000
C	0.24789500	1.97634600	0.00000000
H	1.30364400	2.22723400	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71732200	2.75165700	0.00000000
C	-0.21429549	4.42943607	0.00000000
H	0.82734296	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347761	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000
H	-2.65469260	7.65403606	0.00000000
Cl	-1.08548958	9.56632219	0.00000000

36. Modified B3CTA (see panel e in Fig. 8 in the main text)

H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
C	-0.05233977	-2.28302036	-1.22144820
H	0.47217017	-2.02870514	-2.11872915
H	-0.22661991	-3.33845184	-1.19714150
H	-0.98893962	-1.76621292	-1.19714216
Br	-0.25510332	-2.38133280	1.51491303

C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000
C	0.00000000	0.54341400	0.00000000
Cl	-1.68136526	0.02321129	0.00000000
C	0.24789500	1.97634600	0.00000000
H	1.30364400	2.22723400	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71732200	2.75165700	0.00000000
C	-0.21429549	4.42943607	0.00000000
H	0.82734296	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347761	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000
H	-2.65469260	7.65403606	0.00000000
H	-1.29120766	8.90770237	0.00000000

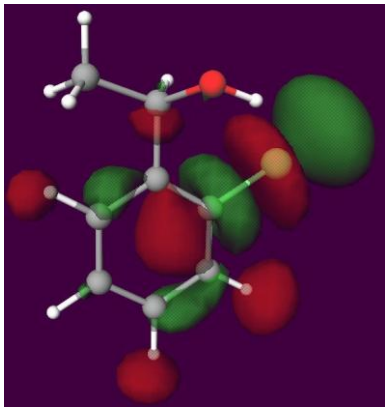
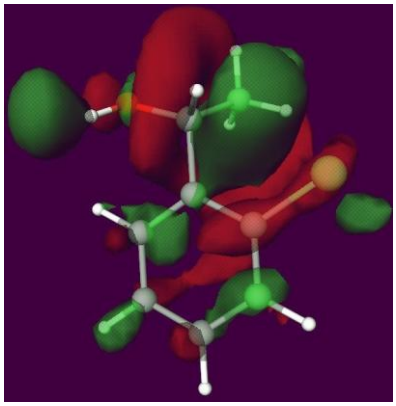
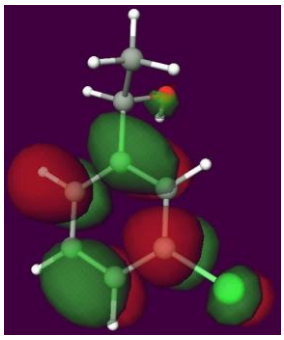
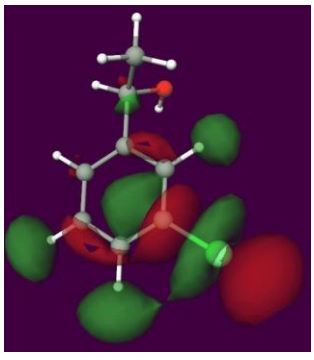
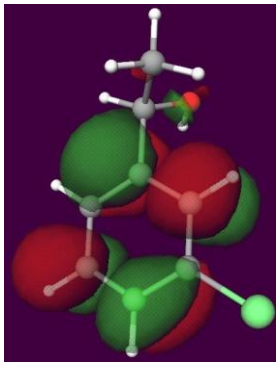
37. Modified B4CTA (see panel g in Fig. 8 in the main text)

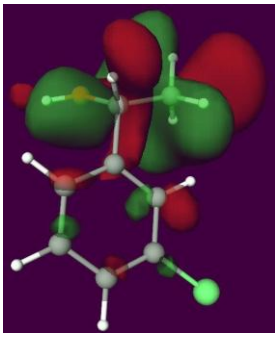
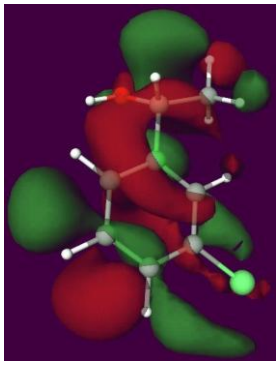
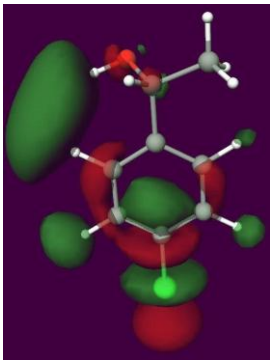
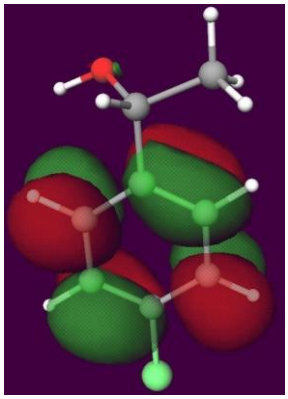
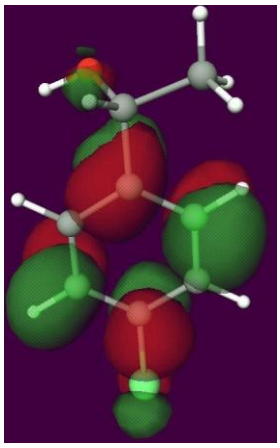
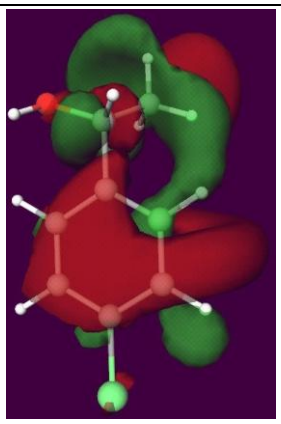
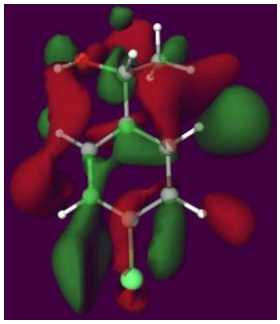
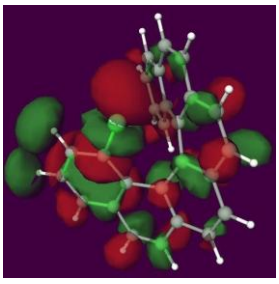
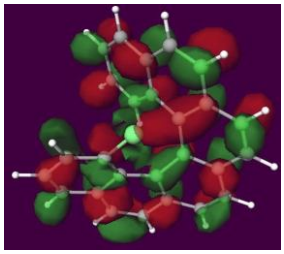
H	2.18834000	-3.15829800	0.81220900
H	2.18834000	-3.15829800	-0.81220900
N	2.08808900	-2.56689600	0.00000000
C	0.79159500	-1.87382800	0.00000000
C	-0.05233977	-2.28302036	-1.22144820
H	0.47217016	-2.02870514	-2.11872915
H	-0.22661991	-3.33845184	-1.19714149
H	-0.98893963	-1.76621292	-1.19714216
Br	-0.25510332	-2.38133280	1.51491303
C	0.96300800	-0.38088800	0.00000000
H	1.98552089	-0.03322812	0.00000000
C	0.00000000	0.54341400	0.00000000
H	-1.03174686	0.22419870	0.00000000
C	0.24789500	1.97634600	0.00000000
Cl	1.96020949	2.38326010	0.00000000
C	-0.65593500	2.95412100	0.00000000
H	-1.71732200	2.75165700	0.00000000
C	-0.21429549	4.42943607	0.00000000
H	0.82734296	4.67415903	0.00000000
C	-1.14040355	5.41882523	0.00000000
H	-2.18347761	5.18029538	0.00000000
C	-0.69000640	6.89149030	0.00000000
H	0.35306767	7.13002015	0.00000000
C	-1.61021975	7.88636438	0.00000000
H	-2.65469260	7.65403606	0.00000000

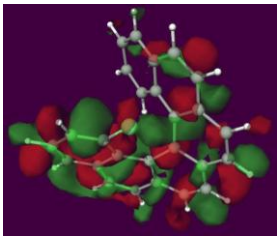
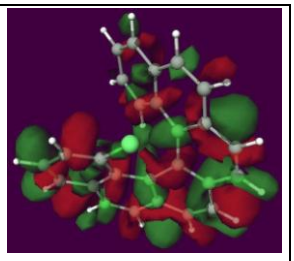
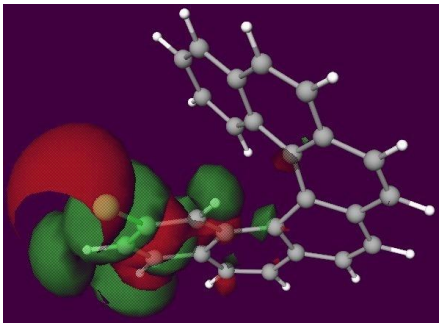
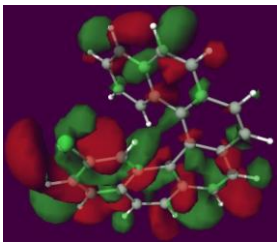
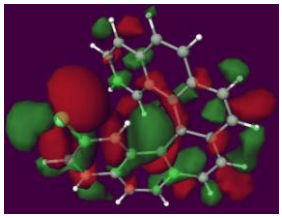
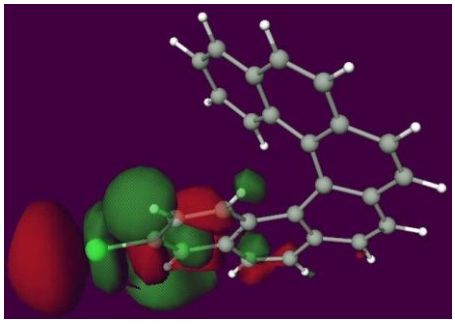
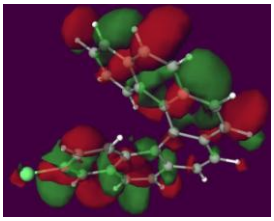
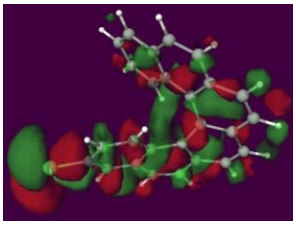
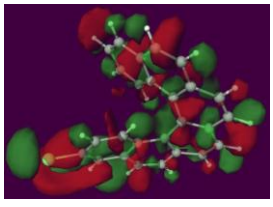
H	-1.29120766	8.90770237	0.00000000

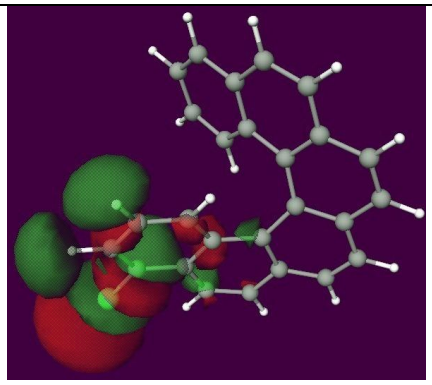
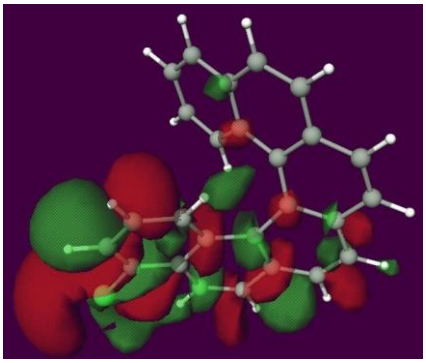
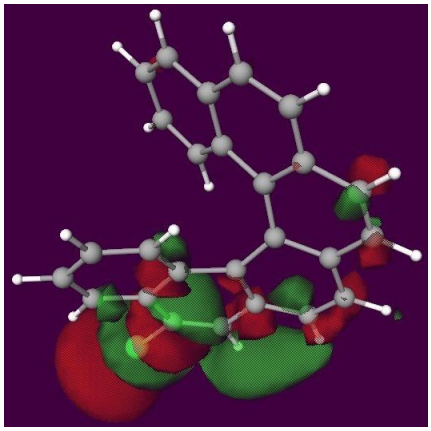
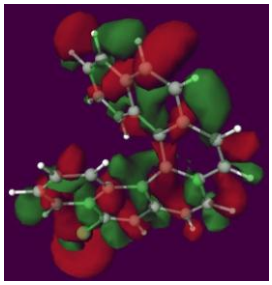
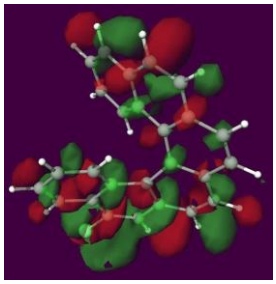
More representative MOs involved in the studied core excitatons

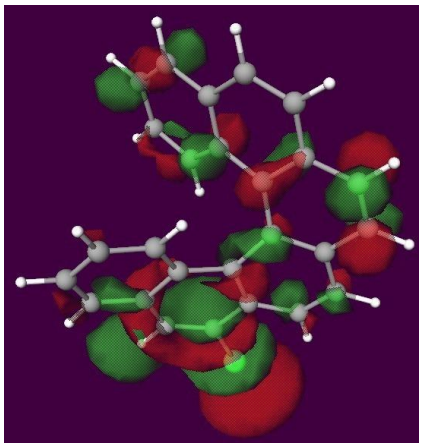
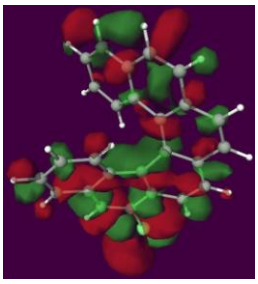
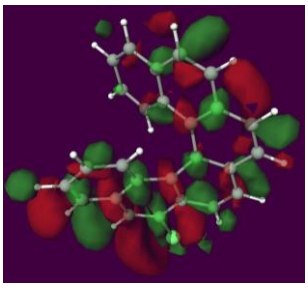
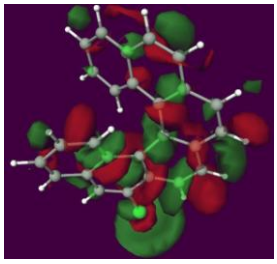
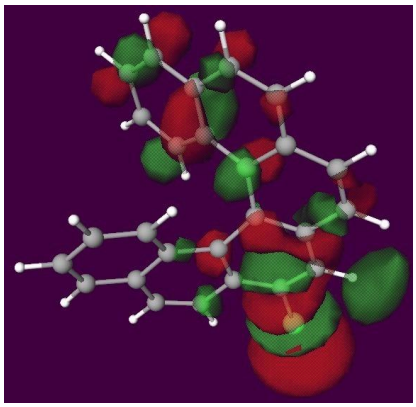
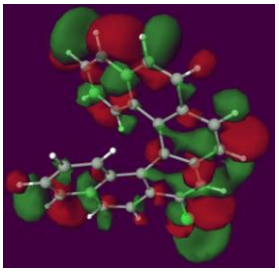
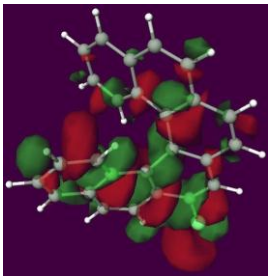
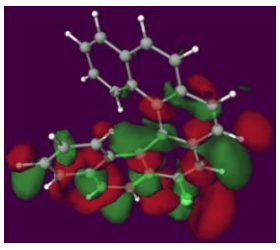
Excitation energies (eV) are in red and CI-type coefficients are in blue.

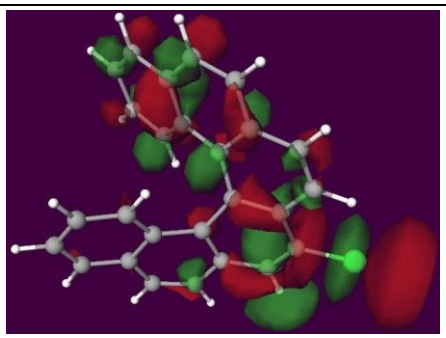
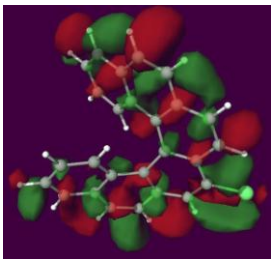
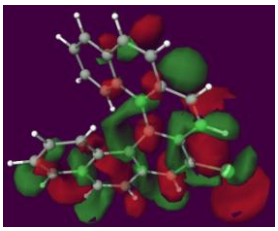
o-CEPO-6: 194.9065	 -0.9474		
o-CEPO-2: 199.9064	 0.8823		
m-CEPO-4: 194.7569	 0.6811	 -0.4809	 0.4760

m-CEPO-3: 200.7211	 0.5752		 -0.4668
p-CEPO-3: 194.7453	 -0.5802	 -0.5073	 0.4770
p-CEPO-2: 200.8824	 0.6036		 0.5388
1CHHC: 194.8319	 0.5464		 0.4951

1CHHC: 201.6729	 0.6287		 -0.4126
2CHHC: 194.8527	 -0.8810		
2CHHC: 202.0326	 0.5810		 -0.5127
3CHHC: 194.8375	 -0.7367		
3CHHC: 201.7024	 -0.5855	 0.3452	 0.5582

4CHHC: 194.9096	 0.7680		
4CHHC: 301.2355	 -0.7580		
5CHHC: 194.8874	 -0.9222		
5CHHC: 201.5336	 -0.5922		 0.4119

6CHHC: 194.8752	 -0.8046		
6CHHC: 201.8369	 -0.5647	 0.4629	 -0.4049
7CHHC: 194.8938	 -0.8505		
7CHHC: 202.2022	 0.5201	 0.4976	 0.4798

8CHHC: 194.9189	 0.8270		
8CHHC: 201.9711	 -0.6330		 -0.5015

Calculated electric and magnetic transition dipole magnitudes and the angles between the two types of dipoles

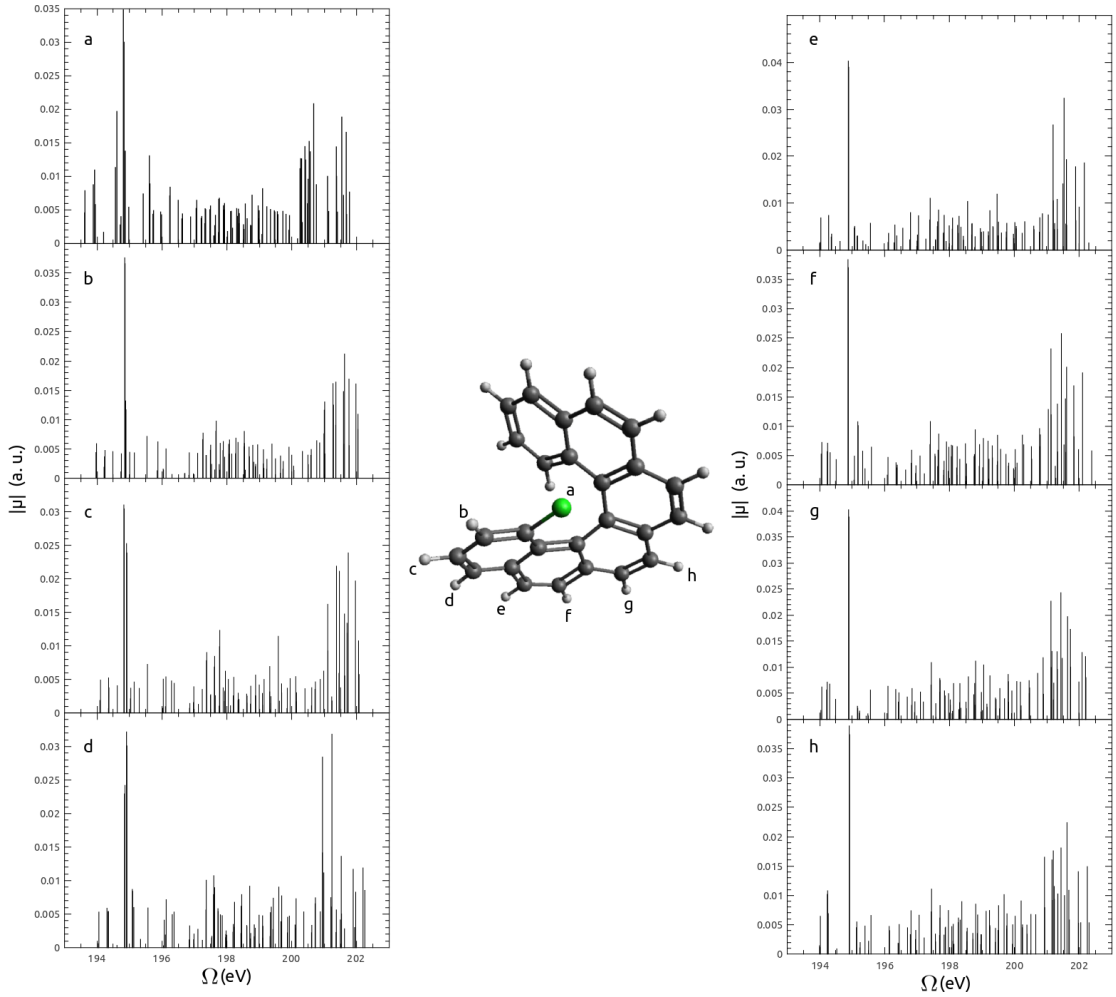


Figure S1. Magnitudes of the calculated electric transition dipoles of nCHHCs. Panels a to h correspond to nCHHCs with the Cl atom at the positions a to h labeled in the molecular structure in the middle.

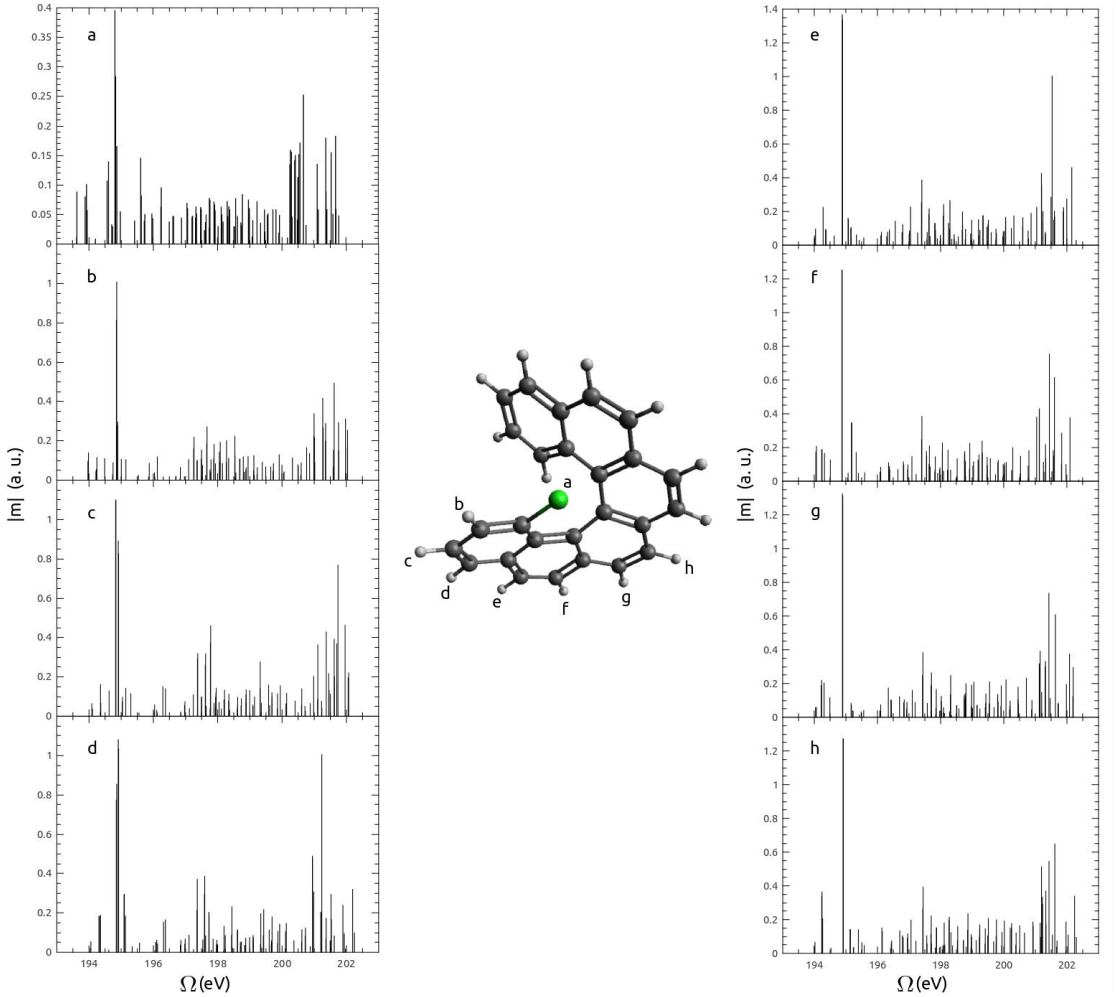


Figure S2. Magnitudes of the calculated magnetic transition dipoles of nCHHCs. Panels a to h correspond to nCHHCs with the Cl atom at the positions a to h labeled in the molecular structure in the middle.

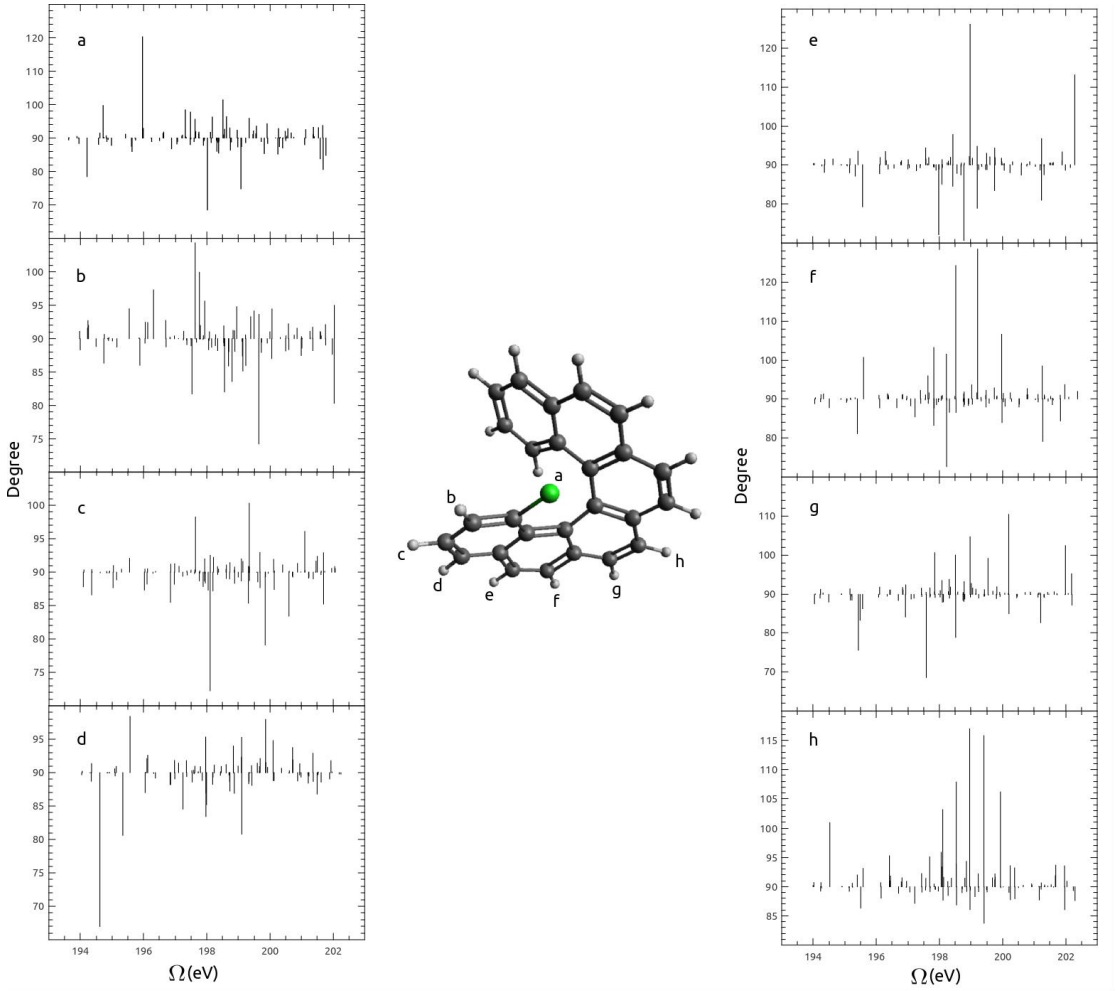


Figure S3. Angles between the calculated electric and magnetic transition dipoles of nCHHCs. Panels a to h correspond to nCHHCs with the Cl atom at the positions a to h labeled in the molecular structure in the middle.

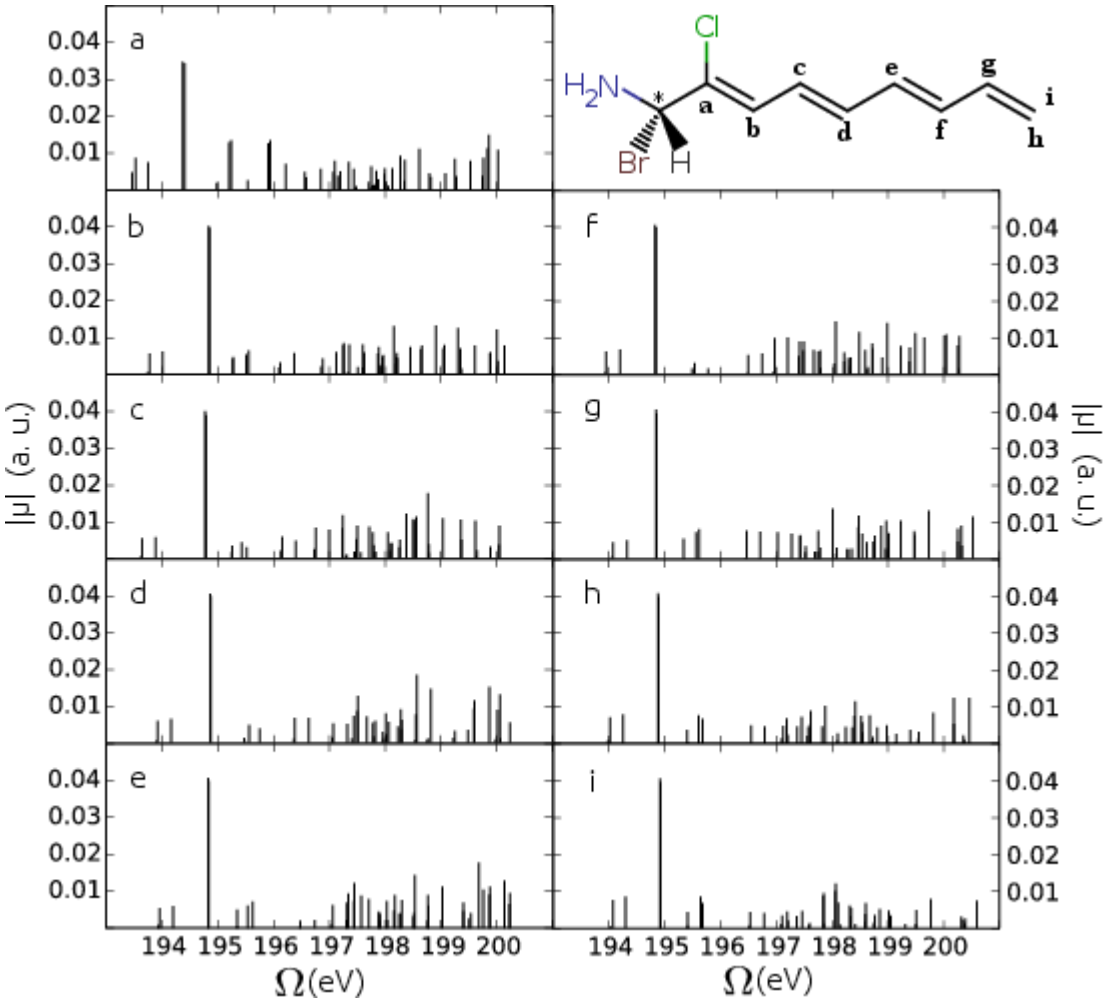


Figure S4. Magnitudes of the calculated electric transition dipoles of BnCTAs. Panels a to i correspond to BnCTAs with the Cl atom at the positions a to i labeled in the molecular structure on top right.

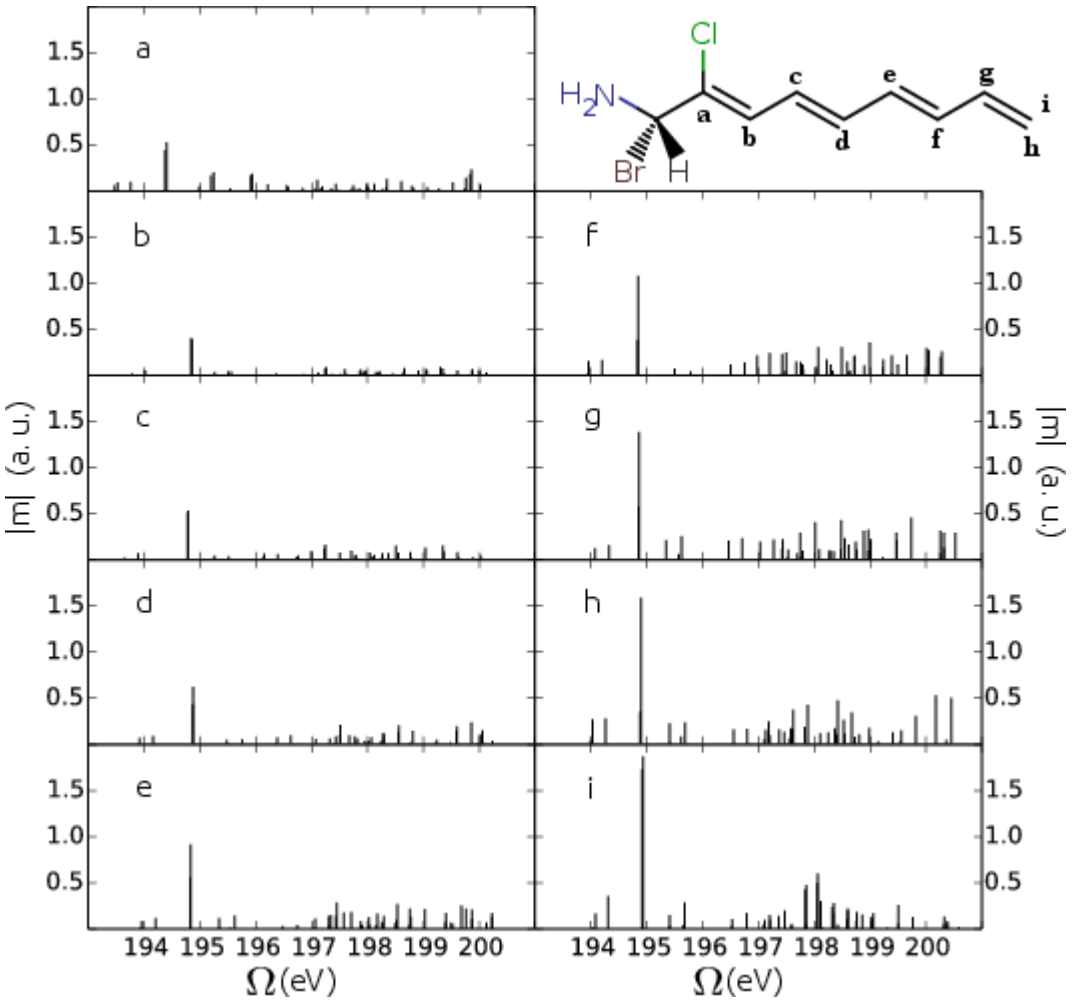


Figure S5. Magnitudes of the calculated magnetic transition dipoles of BnCTAs. Panels a to i correspond to BnCTAs with the Cl atom at the positions a to i labeled in the molecular structure on top right.

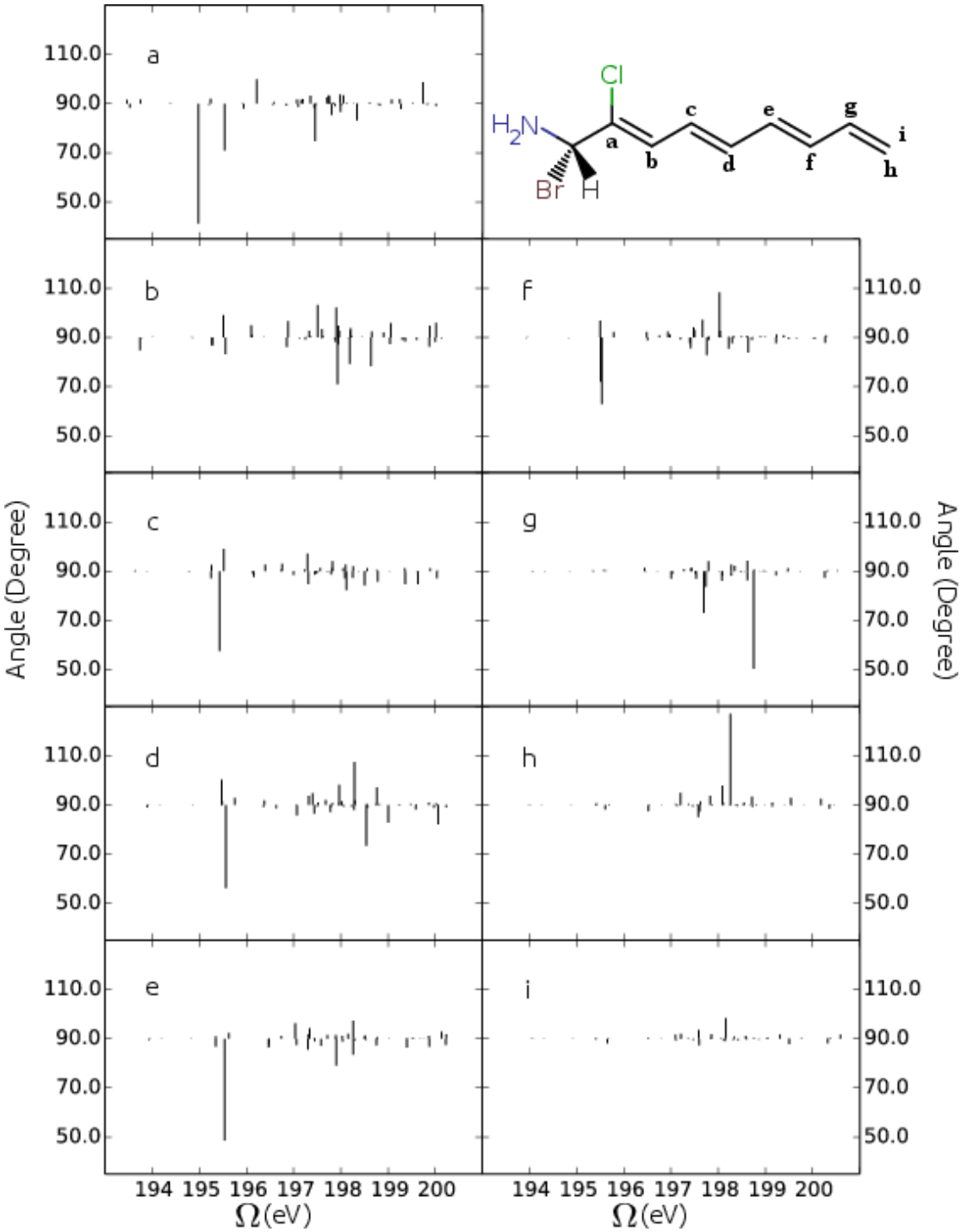


Figure S6. Angles between the calculated electric and magnetic transition dipoles of BnCTAs. Panels a to i correspond to BnCTAs with the Cl atom at the positions a to i labeled in the molecular structure on top right.