Supporting Information

Synthesis of Optically Active Folded Cyclic Dimer and Trimer

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Computational methods

Density-functional theory (DFT) and time-dependent-DFT (TD-DFT) calculations [1-5] were carried out by the Gaussian 16 program package [6], with the 6-31G(d) [7-9] basis set for C and H atoms. Optimized geometries and their molecular orbitals in the ground and S_1 states were determined by DFT and TD-DFT calculation with the MN15 functional [10]. Cartesian coordinates of optimized structures are given in Tables S1–S4.

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[6] Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

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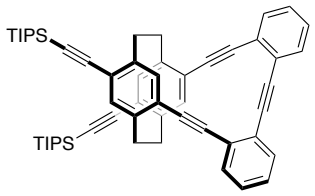


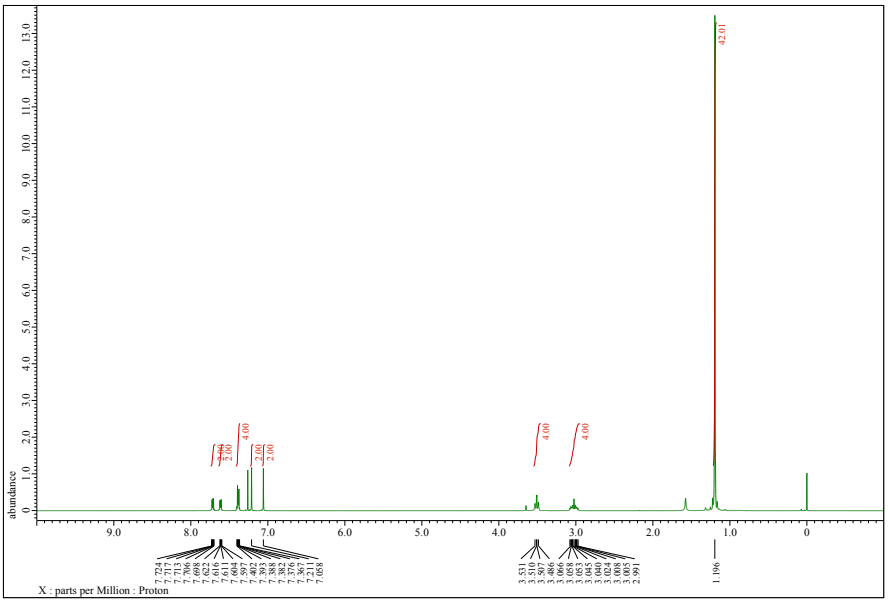


Figure S1. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of (S_p)-**3**.

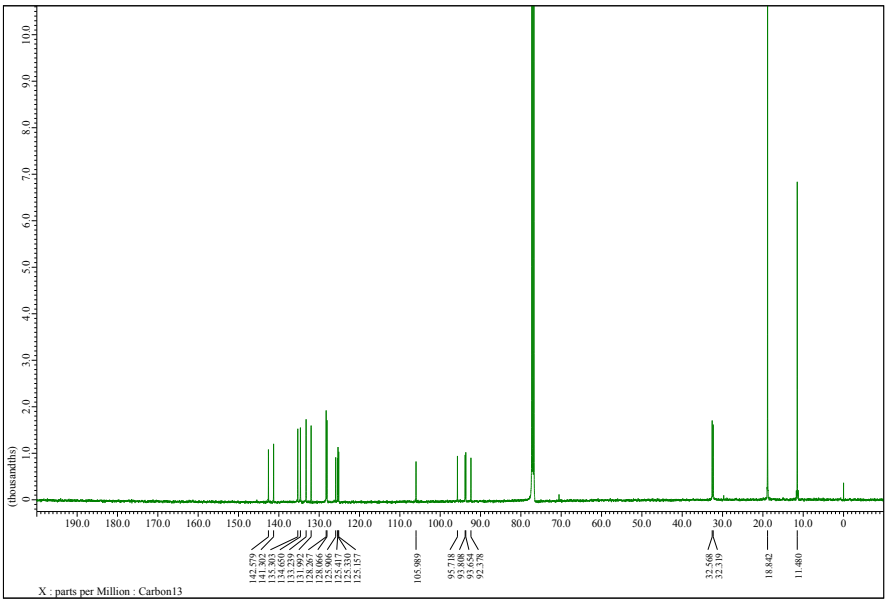


Figure S2. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) spectrum of (S_p)-**3**.

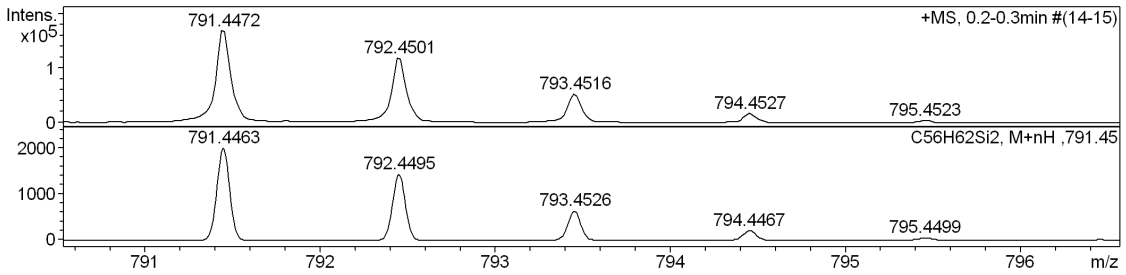


Figure S3. HRMS (APCI) spectra of (S_p)-**3**; upper and lower indicate experimental and theoretical mass spectra, respectively.

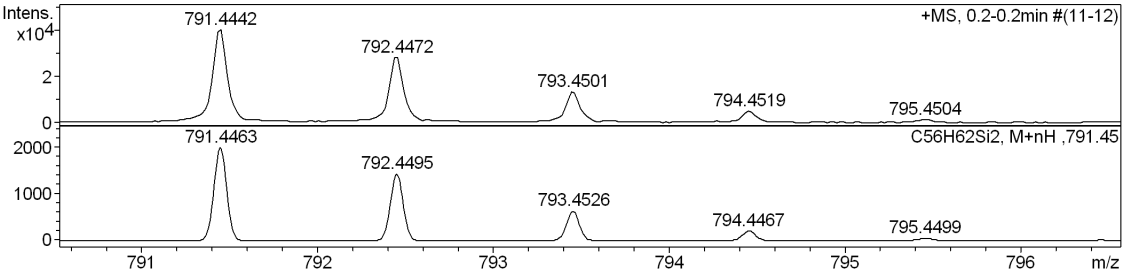
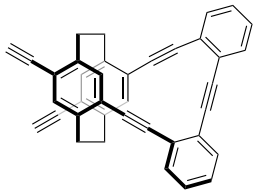


Figure S4. HRMS (APCI) spectra of (R_p)-**3**; upper and lower indicate experimental and theoretical mass spectra, respectively.



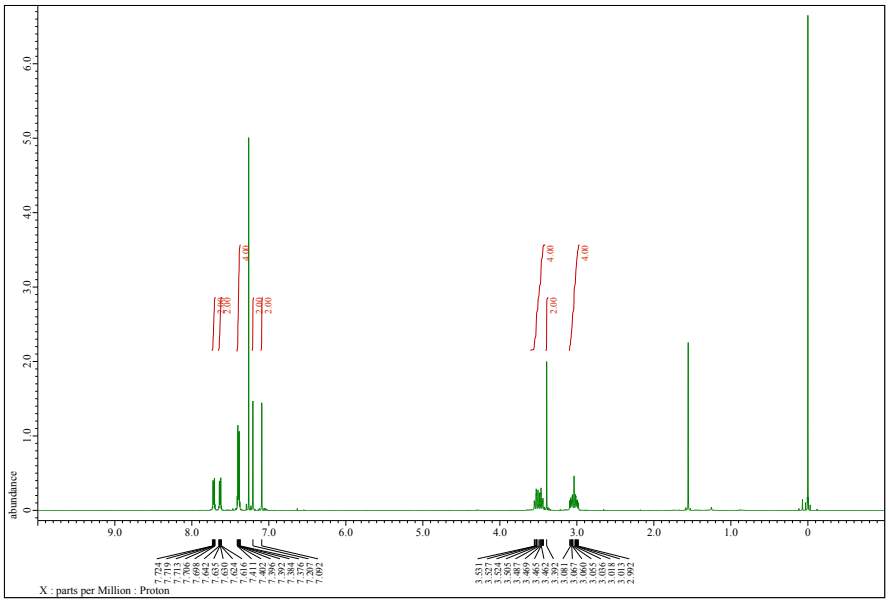


Figure S5. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of (S_p)-**4**.

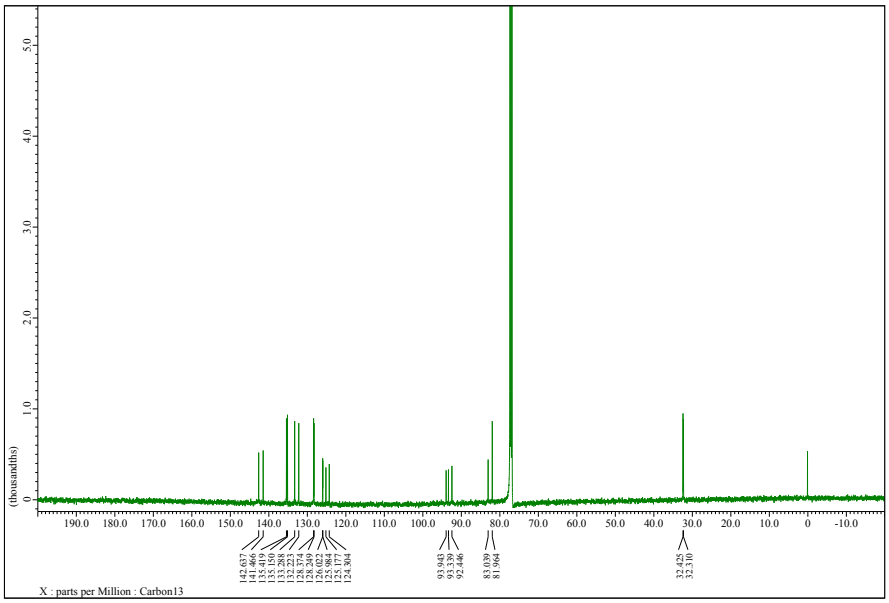


Figure S6. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) spectrum of (S_p)-**4**.

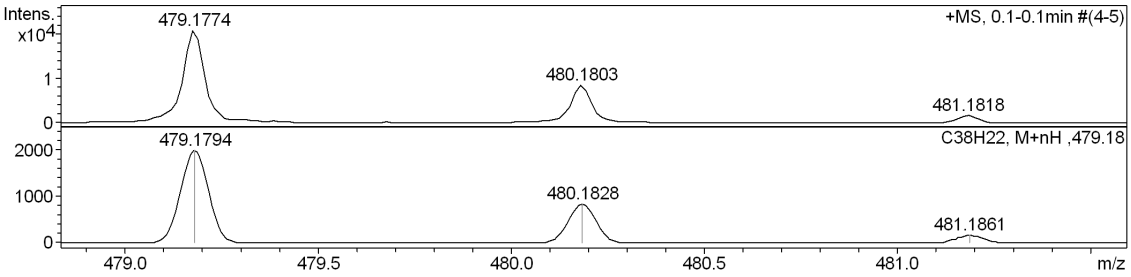


Figure S7. HRMS (APCI) spectra of (S_p)-**4**; upper and lower indicate experimental and theoretical mass spectra, respectively.

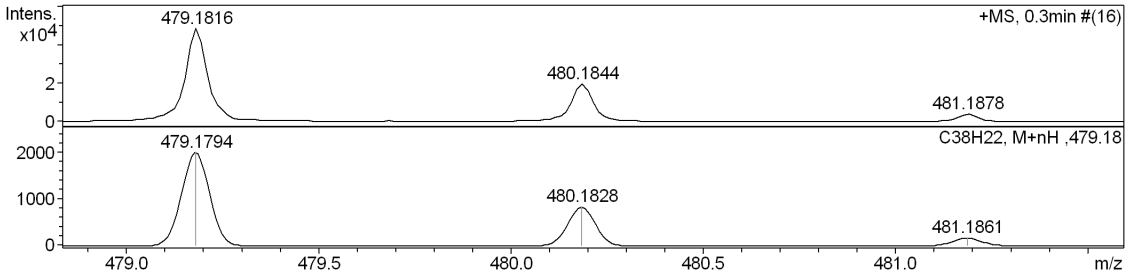
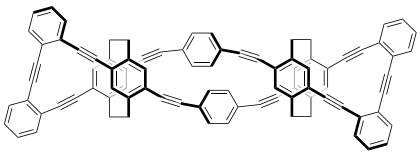


Figure S8. HRMS (APCI) spectra of (R_p)-**4**; upper and lower indicate experimental and theoretical mass spectra, respectively.



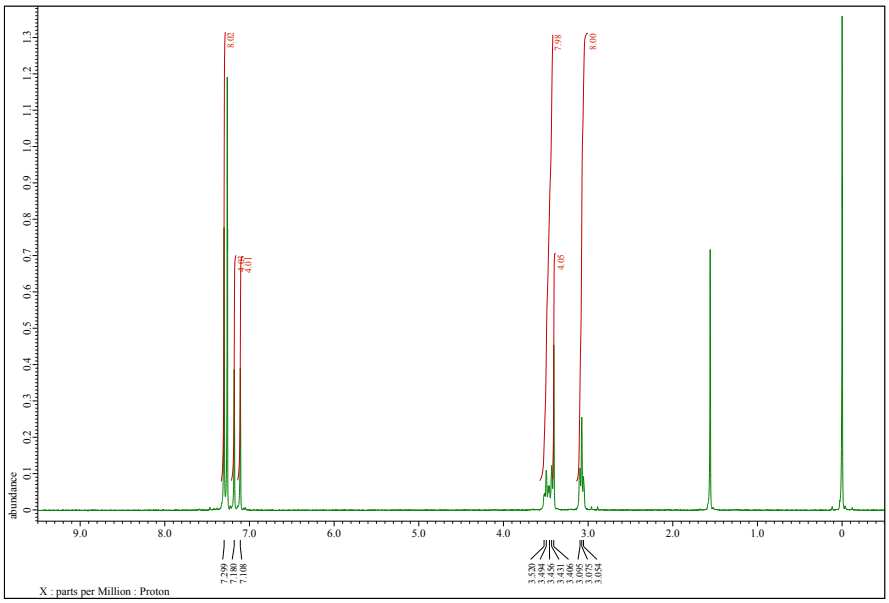


Figure S9. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of (S_p)-**6**.

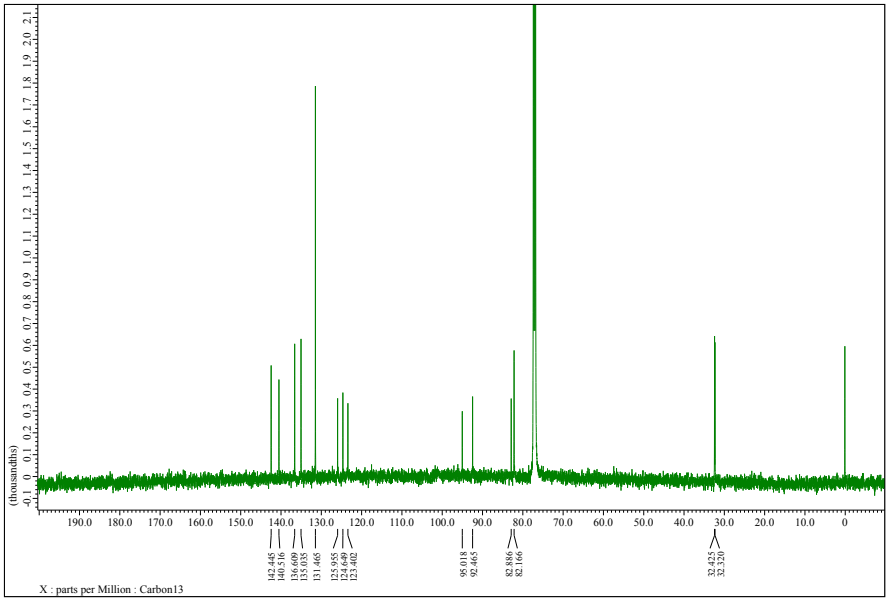


Figure S10. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) spectrum of (S_p)-**6**.

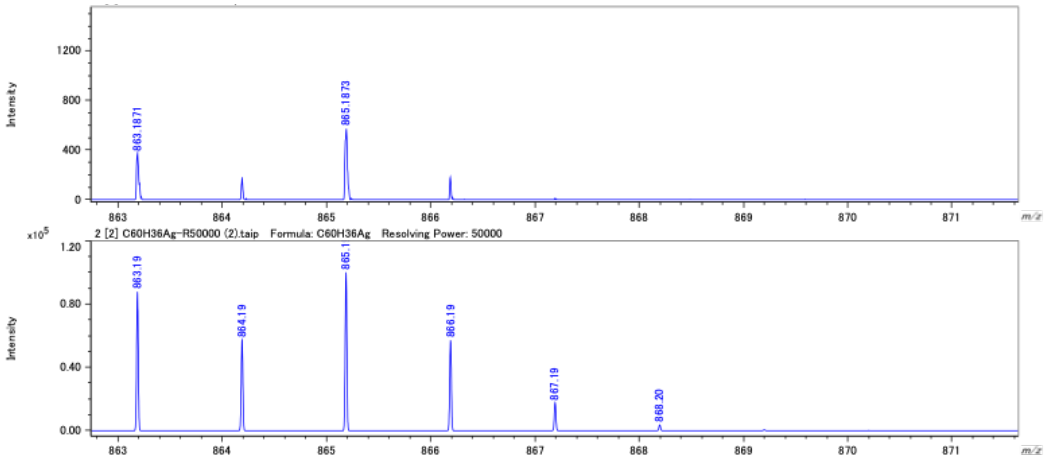


Figure S11. HRMS (MALDI) spectra of (S_p)-**6**; upper and lower indicate experimental and theoretical mass spectra, respectively.

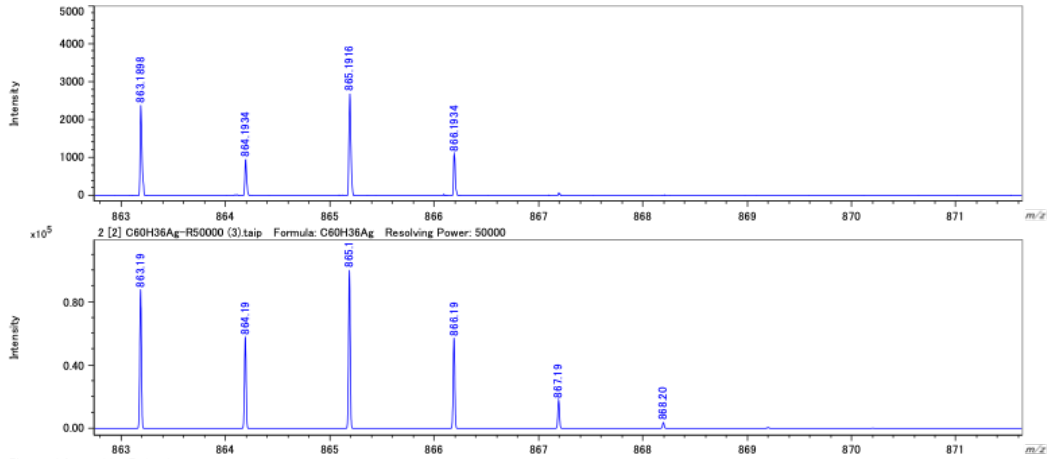
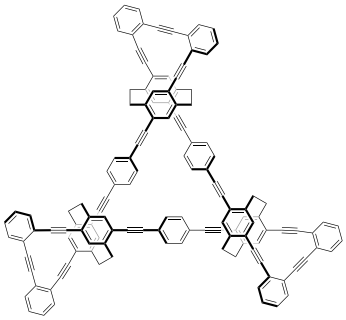


Figure S12. HRMS (MALDI) spectra of (R_p)-**6**; upper and lower indicate experimental and theoretical mass spectra, respectively.



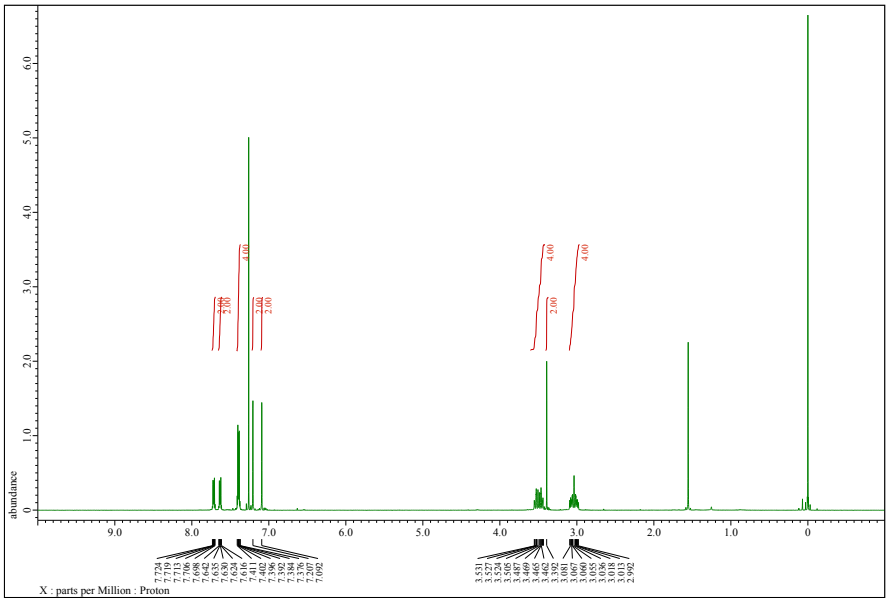


Figure S13. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of (S_p)-**7**.

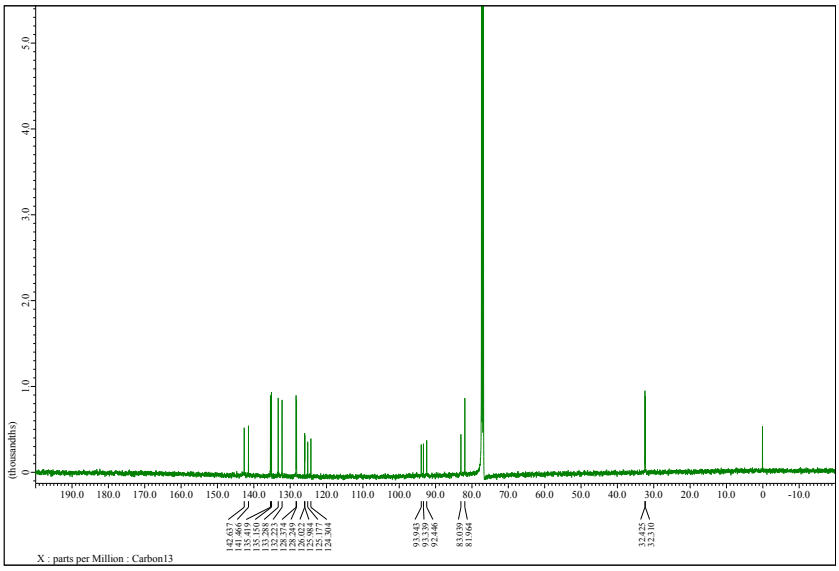


Figure S14. ^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz) spectrum of (S_p)-**7**.

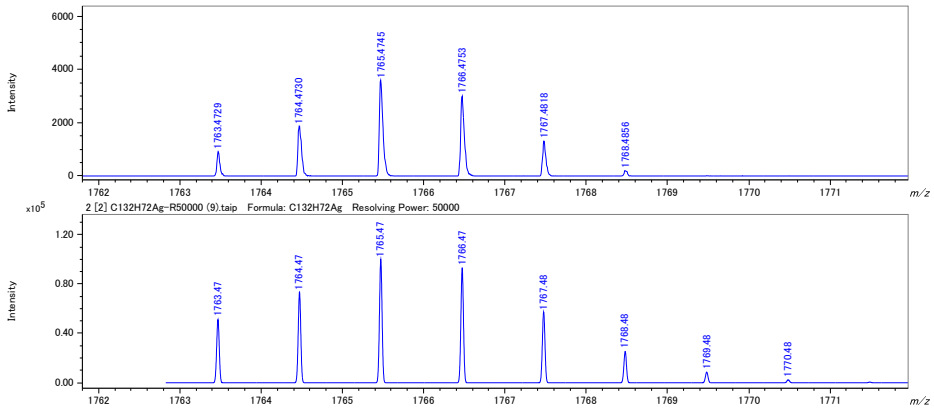


Figure S15. HRMS (MALDI) spectra of (S_p)-**7**; upper and lower indicate experimental and theoretical mass spectra, respectively.

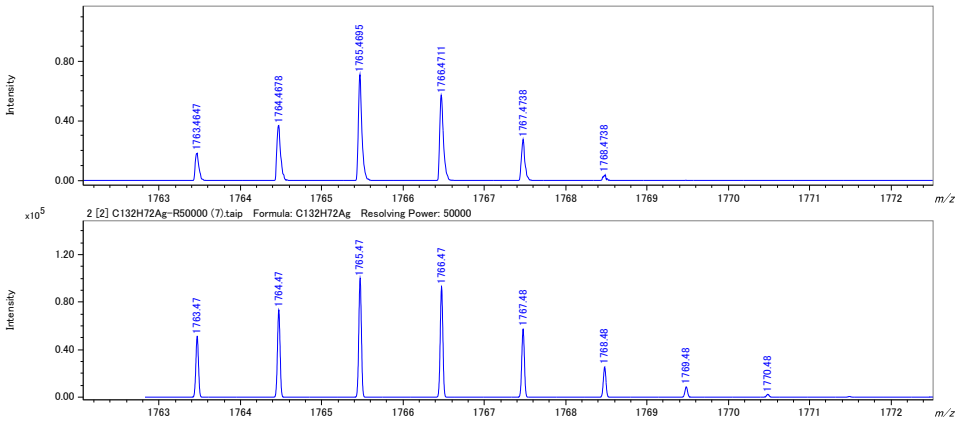


Figure S16. HRMS (MALDI) spectra of (R_p)-**7**; upper and lower indicate experimental and theoretical mass spectra, respectively.

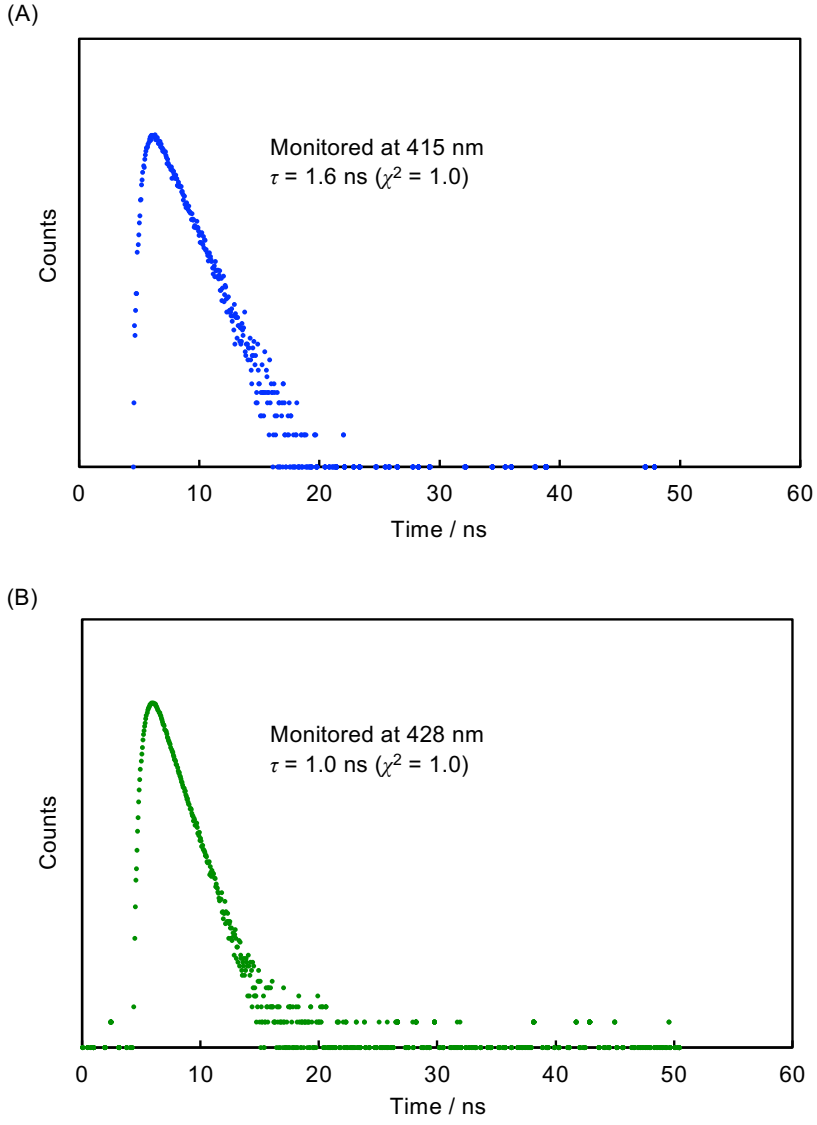


Figure S17. PL decay curves and the data of (A) (S_p)-**6** and (B) (S_p)-**7** in $CHCl_3$. The decay curves were fitted with a single exponential function.

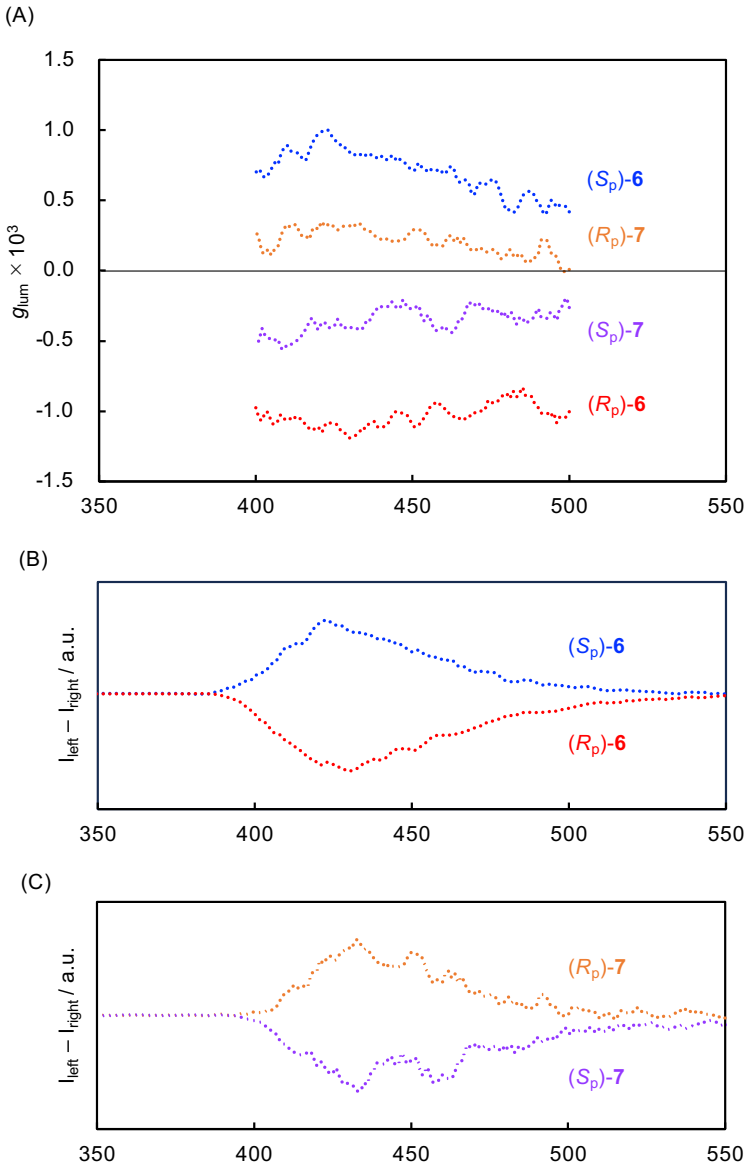
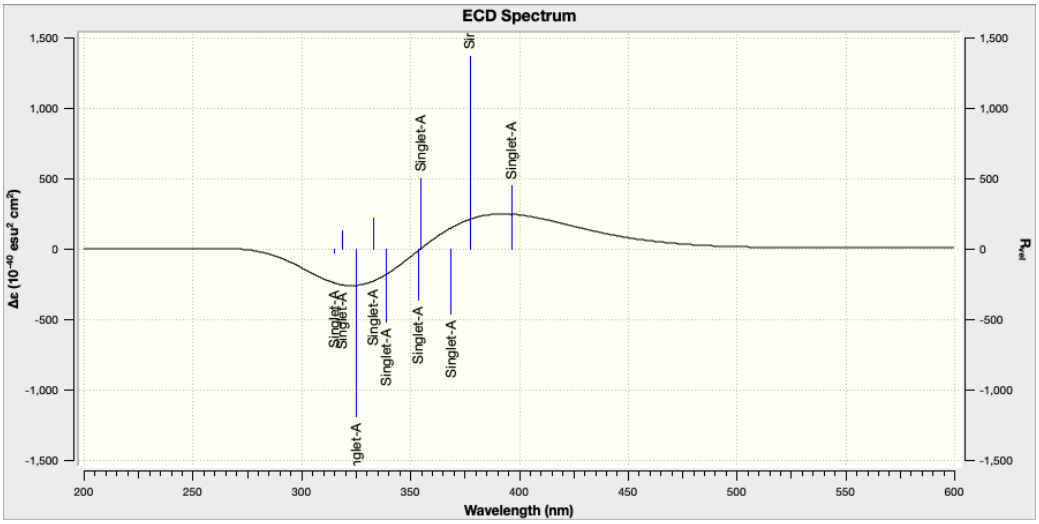


Figure S18. (A) The g_{lum} charts of **6** and **7** with the CPL spectra of (B) **6** and (C) **7** in $CHCl_3$ (1.0×10^{-5} M) excited at 300 nm.

(A)



(B)

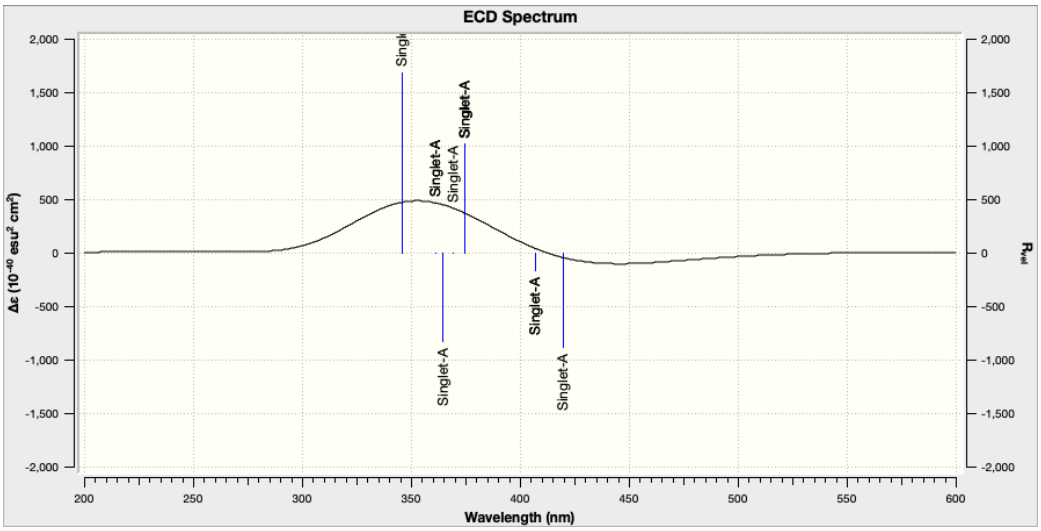


Figure S19. Calculated ECD spectrum of (A) (S_p)-**6** and (B) (S_p)-**7** simulated using TD-DFT calculation (TD-MN15/6-31G(d)//MN15/6-31G(d)).

Table S1. Cartesian coordinate of (S_p)-**6** in the ground state (TD-MN15/6-31G(d)).

atom	x	y	z
C	5.219175	-1.227128	-1.324986
C	-2.831549	2.227834	-0.690421
C	3.955595	-1.834561	-1.035434
C	-1.446275	2.312284	-0.335084
C	-0.399553	-2.770788	1.041687
H	-0.746589	-3.06038	2.029519
C	-1.335604	-2.338332	0.085558
C	-3.832914	-1.754375	0.736629
C	7.610024	-1.10228	-1.282332
H	8.581278	-1.531192	-1.044206
C	-3.977258	1.910872	-0.956755
C	5.179775	0.106672	-1.773978
H	4.204112	0.572072	-1.89942
C	1.416502	-2.348429	-0.51217
C	-2.70828	-2.114726	0.436964
C	1.306091	2.196819	0.241963
C	2.808573	-2.155349	-0.779989
C	7.567378	0.244098	-1.686104
C	0.95873	-2.780277	0.745301
H	1.682251	-3.078979	1.499572
C	-5.085446	-1.159591	1.103928
C	6.45079	-1.799326	-0.946118
C	-5.235683	1.309506	-1.281907
C	5.102883	1.140036	1.133637
C	6.344799	1.73973	0.837107
C	6.525224	-2.930391	0.053325
H	7.551572	-3.313194	0.069532
H	5.862006	-3.758197	-0.223542
C	-5.046831	0.164107	1.580748
H	-4.075871	0.64907	1.667538
C	-6.472748	1.862598	-0.895107
C	6.321839	0.899213	-1.806578
C	7.494247	1.067676	1.248041
H	8.469272	1.518767	1.075426
C	6.220287	-0.962975	1.686429
C	3.845536	1.723797	0.785464
C	5.06591	-0.1963	1.577207
H	4.093763	-0.682186	1.641327
C	2.701513	2.03974	0.509021
C	-6.326552	-1.747627	0.783169
C	-6.322725	-0.811356	-1.827977
C	7.45614	-0.279682	1.648983
C	-7.572894	-0.167157	-1.696135
C	-6.549983	2.953799	0.14783
H	-7.58196	3.318294	0.19594
H	-5.904423	3.802891	-0.105231
C	-5.186364	-0.013019	-1.760914
H	-4.206066	-0.469047	-1.890315
C	0.473502	-1.976647	-1.488902
H	0.825042	-1.648363	-2.462649
C	-7.626295	1.167371	-1.255285
H	-8.601651	1.581463	-1.008029
C	6.461448	2.872736	-0.155704
H	7.476004	3.282224	-0.098769
H	5.758767	3.682834	0.071613
C	6.190065	2.39651	-1.645871
H	5.169509	2.683765	-1.922763
H	6.881022	2.937166	-2.303125
C	-7.43772	0.247091	1.649754
C	-0.881258	-1.973866	-1.194931
H	-1.602765	-1.63646	-1.935029
C	-0.604156	3.382304	-0.678063
H	-1.018642	4.245919	-1.190413
C	-0.900878	1.200214	0.33461
H	-1.560492	0.380259	0.606106
C	-6.180228	-2.312555	-1.719534
H	-5.157673	-2.582395	-2.007323
H	-6.867238	-2.834603	-2.395624
C	-7.477008	-1.087386	1.210277
H	-8.451957	-1.53242	1.022376
C	-6.202817	0.929363	1.706187
C	6.135412	-2.462869	1.519193
H	5.103936	-2.774016	1.721453
H	6.788937	-2.988046	2.225474
C	-6.445225	-2.845627	-0.247886
H	-7.459317	-3.257712	-0.202539
H	-5.740777	-3.662663	-0.053746
C	0.452812	1.13821	0.612755
H	0.873261	0.262911	1.101877
C	0.755953	3.325468	-0.39038
H	1.407562	4.148426	-0.670434
C	-6.12537	2.434871	1.58664
H	-5.091507	2.743167	1.777493
H	-6.765685	2.932186	2.324725
C	-8.669894	0.956405	1.785936
C	-9.733902	1.546073	1.829285
C	8.6876	-0.993605	1.760307
C	9.750805	-1.586301	1.782426
C	8.786872	0.986466	-1.716311
C	9.8353	1.603217	-1.668262

C	-8.787737	-0.916135	-1.749562
C	-9.832882	-1.539417	-1.717192
C	-10.985037	2.23046	1.880164
C	-12.123538	1.702487	1.219156
C	-11.102067	3.437112	2.589608
C	-13.342922	2.394873	1.302128
C	-12.316172	4.110457	2.655326
H	-10.222431	3.830797	3.091283
C	-13.440569	3.586412	2.011444
H	-14.209285	1.981194	0.793714
H	-12.388141	5.042065	3.210075
H	-14.392328	4.108394	2.061511
C	-11.066145	-2.255946	-1.675676
C	-12.16446	-1.755054	-0.930759
C	-11.20683	-3.465893	-2.374983
C	-13.36957	-2.476547	-0.922329
C	-12.405836	-4.168488	-2.349565
H	-10.358196	-3.838909	-2.941626
C	-13.491232	-3.671076	-1.622925
H	-14.20513	-2.083238	-0.350169
H	-12.496665	-5.102285	-2.897852
H	-14.431095	-4.216065	-1.601776
C	-12.056396	0.486502	0.469782
C	-12.069853	-0.537034	-0.187635
C	11.070178	2.315964	-1.612252
C	12.171888	1.793046	-0.887852
C	11.208532	3.544926	-2.278118
C	13.377882	2.51282	-0.865811
C	12.408523	4.245221	-2.23976
H	10.357203	3.93451	-2.829375
C	13.497221	3.726384	-1.533312
H	14.216083	2.102683	-0.30956
H	12.497526	5.193892	-2.762196
H	14.437905	4.269473	-1.502097
C	11.001807	-2.271972	1.81004
C	12.138823	-1.724574	1.162274
C	11.121088	-3.498962	2.483415
C	13.358652	-2.418492	1.22208
C	12.335536	-4.173503	2.526402
H	10.242854	-3.90755	2.975551
C	13.458394	-3.630393	1.895719
H	14.223684	-1.989607	0.724088
H	12.409057	-5.120985	3.053396
H	14.410419	-4.153264	1.928276
C	12.080143	0.554569	-0.179096
C	12.069352	-0.487413	0.448704

Table S2. Cartesian coordinate of (S_p)-**6** in the S_1 state (TD-MN15/6-31G(d)).

atom	x	y	z
C	5.21876	-1.281031	-1.469605
C	-2.856091	2.390252	-0.848631
C	3.963628	-1.923135	-1.223429
C	-1.489565	2.438988	-0.526214
C	-0.289669	-2.704487	1.028702
H	-0.587103	-2.84692	2.063642
C	-1.271624	-2.400419	0.06845
C	-3.723341	-1.682827	0.75901
C	7.604974	-1.113999	-1.330765
H	8.573343	-1.531255	-1.061922
C	-4.006046	2.013959	-1.079566
C	5.1708	0.065297	-1.886048
H	4.19227	0.518714	-2.033314
C	1.450187	-2.500485	-0.653219
C	-2.621562	-2.105313	0.453556
C	1.267974	2.241748	0.089142
C	2.828107	-2.290245	-0.976688
C	7.554067	0.238716	-1.719033
C	1.05223	-2.760948	0.671263
H	1.813202	-2.946997	1.425567
C	-4.966549	-1.063092	1.116603
C	6.446586	-1.839759	-1.060519
C	-5.225966	1.362987	-1.342819
C	4.976111	1.077138	1.006352
C	6.252081	1.685943	0.770367
C	6.498706	-2.987788	-0.079726
H	7.532345	-3.345183	-0.013905
H	5.871769	-3.826675	-0.403741
C	-4.933965	0.284715	1.525456
H	-3.966973	0.784132	1.56604
C	-6.488227	1.897854	-0.966408
C	6.301994	0.874576	-1.873264
C	7.375367	1.006928	1.193191
H	8.359188	1.447946	1.046096
C	6.072922	-1.051009	1.552037
C	3.764749	1.679932	0.667002
C	4.931022	-0.29675	1.400174
H	3.957756	-0.785138	1.396253
C	2.61951	2.05452	0.3856
C	-6.207795	-1.677359	0.847467
C	-6.255971	-0.819782	-1.777419
C	7.325946	-0.361772	1.579052
C	-7.531612	-0.203201	-1.659903
C	-6.563635	3.013568	0.04792
H	-7.605571	3.340585	0.133576
H	-5.961016	3.879781	-0.250903
C	-5.144839	0.002783	-1.743561
H	-4.151461	-0.432059	-1.849602
C	0.460241	-2.27901	-1.629036
H	0.762352	-2.089144	-2.654822
C	-7.618083	1.153742	-1.268066
H	-8.601454	1.539879	-1.007096
C	6.389993	2.83132	-0.201274
H	7.405229	3.234978	-0.120917
H	5.685084	3.641727	0.020577
C	6.143319	2.36798	-1.699344
H	5.12229	2.642721	-1.987506
H	6.834854	2.926781	-2.340744
C	-7.325794	0.339849	1.648755
C	-0.879567	-2.234791	-1.27338
H	-1.637712	-2.00941	-2.01988
C	-0.674694	3.602093	-0.485272
H	-1.119503	4.569506	-0.700934
C	-0.892077	1.178268	-0.234564
H	-1.531283	0.300124	-0.247502
C	-6.080562	-2.313952	-1.627923
H	-5.051863	-2.567846	-1.909236
H	-6.755829	-2.869134	-2.289599
C	-7.35813	-1.012016	1.26355
H	-8.330816	-1.475563	1.112088
C	-6.099074	1.039241	1.647284
C	6.017518	-2.548541	1.366182
H	4.980292	-2.875336	1.505622
H	6.637786	-3.072688	2.103082
C	-6.332483	-2.810484	-0.142972
H	-7.345113	-3.223447	-0.076798
H	-5.62298	-3.618939	0.067836
C	0.435867	1.08029	0.084603
H	0.878953	0.117073	0.325125
C	0.671845	3.503055	-0.206088
H	1.295932	4.392323	-0.197292
C	-6.054308	2.541849	1.476107
H	-5.017791	2.87301	1.604666
H	-6.665053	3.050868	2.231372
C	-8.565601	1.035498	1.785962
C	-9.639919	1.60684	1.82586
C	8.535203	-1.060337	1.733486
C	9.614224	-1.642939	1.785642
C	8.761738	0.999174	-1.694882
C	9.796818	1.631977	-1.588155
C	-8.716902	-0.979697	-1.669645

C	-9.751725	-1.624654	-1.594367
C	-10.899826	2.275551	1.869109
C	-12.038775	1.713573	1.236313
C	-11.024475	3.502228	2.54186
C	-13.265603	2.394472	1.311022
C	-12.245828	4.163287	2.599439
H	-10.144599	3.921515	3.021932
C	-13.370315	3.606239	1.983879
H	-14.132059	1.955059	0.824846
H	-12.323279	5.11082	3.125745
H	-14.327746	4.118341	2.027654
C	-10.967734	-2.352459	-1.501487
C	-12.072522	-1.820653	-0.781745
C	-11.097729	-3.607455	-2.125795
C	-13.270868	-2.551988	-0.732295
C	-12.289139	-4.316402	-2.057943
H	-10.246056	-4.005339	-2.670574
C	-13.381667	-3.78569	-1.362496
H	-14.109398	-2.135207	-0.181376
H	-12.371832	-5.282041	-2.549529
H	-14.316381	-4.337295	-1.309831
C	-11.967188	0.475378	0.526051
C	-11.982632	-0.571387	-0.09513
C	11.010318	2.37067	-1.459843
C	12.081565	1.871202	-0.672543
C	11.15789	3.603746	-2.116014
C	13.268429	2.620061	-0.584179
C	12.337091	4.331766	-2.010107
H	10.330357	3.974048	-2.714802
C	13.396487	3.836339	-1.243579
H	14.083373	2.228754	0.018255
H	12.433462	5.283041	-2.526412
H	14.321149	4.400981	-1.159564
C	10.865594	-2.292445	1.850842
C	12.036638	-1.669075	1.325656
C	10.980554	-3.566884	2.449276
C	13.273628	-2.324884	1.452445
C	12.209939	-4.19619	2.552239
H	10.081874	-4.036475	2.83975
C	13.364636	-3.570949	2.058138
H	14.159169	-1.838909	1.052223
H	12.278674	-5.173734	3.022073
H	14.330007	-4.062608	2.141593
C	11.982404	0.631241	0.026872
C	11.972375	-0.418112	0.646725

Table S3. Cartesian coordinate of (S_p)-**7** in the ground state (MN15/6-31G(d)).

atom	x	y	z
C	5.645152	7.194323	1.658074
C	5.444349	5.796838	1.687073
C	4.130192	5.337312	1.646262
C	3.32606	7.541392	0.98561
C	4.57706	8.046849	1.325473
H	3.937351	4.267908	1.707323
H	4.801005	9.09625	1.144126
C	3.803161	6.984713	-1.687613
C	5.06827	7.611627	-1.659545
C	6.211571	6.862991	-1.326962
C	6.121903	5.517043	-0.985745
C	3.776543	5.592826	-1.645509
H	7.138847	7.403297	-1.146822
H	2.820563	5.07611	-1.705543
C	7.136992	4.916406	-0.040754
H	8.034662	5.544219	-0.049916
H	7.429326	3.904516	-0.345198
C	6.586654	4.835993	1.445098
H	7.42631	5.026759	2.123881
H	6.22866	3.817341	1.631329
C	2.533796	7.770225	-1.445289
H	1.677653	7.112325	-1.631335
H	2.452948	8.627282	-2.124327
C	2.438843	8.318367	0.040465
H	2.75606	9.366879	0.049279
H	1.38633	8.281125	0.345151
C	5.183712	9.034293	-1.699879
C	5.320873	10.243069	-1.655059
C	6.961026	7.747268	1.697167
C	8.06747	8.25283	1.651439
C	5.496338	11.657948	-1.600927
C	4.559172	12.511303	-2.20633
C	6.767738	13.616035	-0.915338
C	4.722624	13.891015	-2.16842
H	3.704866	12.068406	-2.710689
H	7.630755	14.036089	-0.406447
H	3.988167	14.535534	-2.643828
C	9.358811	8.8568	1.595501
C	10.460158	8.230332	2.201662
C	9.545862	10.095787	0.930599
C	11.721676	8.812341	2.162634
H	10.303143	7.281743	2.707533
C	10.827478	10.670394	0.906859
H	12.561849	8.313967	2.638612
H	10.959975	11.620383	0.396765
C	4.913673	4.847555	-1.285104
C	3.067027	6.184868	1.286283
C	5.831589	14.44494	-1.522742
C	11.905334	10.037323	1.515123
C	6.617683	12.219534	-0.93802
C	7.595027	11.399788	-0.291167
C	8.463356	10.770602	0.283749
H	12.889392	10.497168	1.483627
H	5.964542	15.522985	-1.491962
C	4.776176	3.456133	-0.992933
C	1.787519	5.620001	0.996041
C	0.706634	5.140871	0.703373
C	4.659679	2.28015	-0.697804
C	3.407507	-8.491934	1.659839
C	2.295405	-7.622082	1.689609
C	2.551329	-6.253347	1.654246
C	4.864706	-6.651001	0.997436
C	4.67945	-7.988816	1.332104
H	1.719475	-5.554157	1.715432
H	5.478295	-8.704851	1.149156
C	4.148317	-6.775526	-1.677817
C	4.062417	-8.184839	-1.656104
C	2.843345	-8.805295	-1.329022
C	1.719718	-8.059038	-0.987565
C	2.954113	-6.059922	-1.636428
H	2.850196	-9.879079	-1.152345
H	2.98174	-4.973336	-1.692155
C	0.691961	-8.644061	-0.046598
H	0.789087	-9.735086	-0.060262
H	-0.33052	-8.392382	-0.351855
C	0.893794	-8.133072	1.441972
H	0.639726	-8.959009	2.116813
H	0.188359	-7.316103	1.630392
C	5.461277	-6.067057	-1.430125
H	5.317611	-4.99617	-1.611783
H	6.245906	-6.420973	-2.109311
C	5.981733	-6.264267	0.055636
H	6.733385	-7.061138	0.062078
H	6.472811	-5.334152	0.365155
C	5.239344	-8.992384	-1.69703
C	6.220709	-9.711346	-1.652886
C	3.232047	-9.908617	1.693479
C	3.120296	-11.119793	1.642888
C	7.361571	-10.566353	-1.598655
C	8.569083	-10.174042	-2.19943
C	8.428318	-12.644891	-0.918807
C	9.685537	-11.00101	-2.161974
H	8.609912	-9.21059	-2.699902
H	8.363206	-13.604661	-0.41401
H	10.610826	-10.681518	-2.633778

C	3.003507	-12.540319	1.579088	C	-9.129442	0.572465	-1.654365
C	1.910801	-13.18837	2.178205	C	-9.053439	1.939122	-1.330106
C	3.988021	-13.314579	0.913115	C	-7.843401	2.536428	-0.991276
C	1.789426	-14.572154	2.131162	C	-6.735224	0.464162	-1.638889
H	1.163801	-12.583695	2.684908	H	-9.984919	2.473307	-1.153124
C	3.850258	-14.712211	0.881471	H	-5.809421	-0.105278	-1.695317
H	0.937935	-15.056325	2.601661	C	-7.832599	3.721023	-0.052741
H	4.610474	-15.296265	0.370431	H	-8.825581	4.183464	-0.06537
C	1.740849	-6.676741	-1.281625	H	-7.102905	4.479144	-0.360695
C	3.816524	-5.752156	1.298493	C	-7.489051	3.293313	1.436012
C	9.614144	-12.241313	-1.521637	H	-8.074811	3.928767	2.110746
C	2.763452	-15.336503	1.482704	H	-6.428121	3.494256	1.621814
C	7.29069	-11.821078	-0.940821	C	-7.998865	-1.700271	-1.425619
C	6.09214	-12.264437	-0.298613	H	-7.000826	-2.113378	-1.609088
C	5.112857	-12.707007	0.271929	H	-8.700246	-2.202845	-2.102128
H	2.67379	-16.418789	1.444887	C	-8.426267	-2.048799	0.061944
H	10.483858	-12.892074	-1.491326	H	-9.492565	-2.299611	0.071979
C	0.60207	-5.865665	-0.988702	H	-7.866846	-2.939382	0.371673
C	3.965726	-4.360917	1.011441	C	-10.418689	-0.04015	-1.692424
C	4.093756	-3.185518	0.71888	C	-11.533252	-0.527538	-1.645312
C	-0.359513	-5.179301	-0.692655	C	-10.19756	2.160159	1.691994
C	4.235902	-1.808525	0.368214	C	-11.189499	2.863839	1.639454
C	5.512396	-1.245474	0.183773	C	-12.84507	-1.08561	-1.587943
C	3.101981	-0.993651	0.19055	C	-13.111846	-2.329067	-2.184188
C	5.650878	0.089237	-0.166318	C	-15.177755	-0.963617	-0.906369
H	6.389796	-1.871453	0.321233	C	-14.387259	-2.879953	-2.143793
C	3.240428	0.339872	-0.162886	H	-12.299265	-2.849436	-2.683509
H	2.115179	-1.425952	0.334886	H	-15.974931	-0.424253	-0.402572
C	4.517244	0.903398	-0.346153	H	-14.575359	-3.842299	-2.612129
H	6.637986	0.520881	-0.307195	C	-12.358746	3.679055	1.577713
H	2.363583	0.966687	-0.302976	C	-12.367781	4.949849	2.176034
C	-1.481001	-4.367297	-0.342769	C	-13.524603	3.217113	0.914813
C	-1.332259	-2.97821	-0.170053	C	-13.502827	5.750704	2.13129
C	-2.751365	-4.942678	-0.154082	H	-11.468222	5.291578	2.680417
C	-2.418046	-2.190844	0.181476	C	-14.663391	4.039072	0.885452
H	-0.35223	-2.531594	-0.316841	H	-13.491937	6.730428	2.601229
C	-3.838083	-4.154646	0.194183	H	-15.551826	3.675358	0.376903
H	-2.8699	-6.014536	-0.286822	C	-6.659046	1.823778	-1.286249
C	-3.689154	-2.766071	0.367983	C	-6.894204	-0.429378	1.297464
H	-2.300408	-1.118894	0.317499	C	-15.423919	-2.193874	-1.504927
H	-4.817614	-4.602142	0.338428	C	-14.654946	5.29281	1.485944
C	-9.059435	1.298455	1.659781	C	-13.894456	-0.392737	-0.931426
C	-7.749221	1.824792	1.686713	C	-13.676105	0.868435	-0.293229
C	-6.693195	0.917287	1.650183	C	-13.566527	1.938651	0.275068
C	-8.198114	-0.886494	1.000545	H	-15.545435	5.914536	1.44996
C	-9.262107	-0.054925	1.335501	H	-16.423105	-2.61976	-1.472411
H	-5.67115	1.28686	1.70848	C	-5.385985	2.403476	-0.997489
H	-10.282427	-0.387749	1.155569	C	-5.764584	-1.255238	1.01018
C	-7.953635	-0.209492	-1.676499	C	-4.810191	-1.953449	0.718022

C	-4.310489	2.894766	-0.705079
C	-0.557315	4.57482	0.354864
C	-1.687374	5.396472	0.186303
C	-0.692177	3.186885	0.16355
C	-2.912807	4.848123	-0.161384
H	-1.58697	6.46821	0.334004
C	-1.916525	2.639006	-0.187312
H	0.178978	2.55034	0.295268
C	-3.047135	3.460663	-0.354562
H	-3.783392	5.485333	-0.290278
H	-2.017729	1.567324	-0.338019

Table S4. Cartesian coordinate of (S_p)-**7** in the S_1 state (TD-MN15/6-31G(d)).

atom	x	y	z
C	-9.118809	0.18091	1.688508
C	-7.867816	0.829004	1.784205
C	-6.72618	0.041434	1.655009
C	-8.045273	-1.819215	0.795297
C	-9.18622	-1.140894	1.211916
H	-5.74614	0.502422	1.762873
H	-10.168793	-1.550888	0.986714
C	-7.868785	-0.820631	-1.784177
C	-9.119079	-0.171211	-1.688412
C	-9.18506	1.150667	-1.211809
C	-8.043367	1.82778	-0.795268
C	-6.726304	-0.034274	-1.655054
H	-10.167184	1.561698	-0.986541
H	-5.746762	-0.496304	-1.762984
C	-8.153259	2.892372	0.271795
H	-9.189684	3.245532	0.305078
H	-7.509304	3.753494	0.05791
C	-7.758577	2.335289	1.703769
H	-8.401623	2.827194	2.443177
H	-6.722461	2.620188	1.917236
C	-7.761144	-2.32703	-1.703748
H	-6.725339	-2.61303	-1.917256
H	-8.40474	-2.818252	-2.443132
C	-8.156365	-2.883689	-0.27176
H	-9.193173	-3.235727	-0.304995
H	-7.513333	-3.745507	-0.057906
C	-10.338198	-0.904561	-1.808719
C	-11.396748	-1.505614	-1.827545
C	-10.337131	0.915565	1.8089
C	-11.395033	1.517756	1.827807
C	-12.644503	-2.197107	-1.842848
C	-12.786651	-3.386233	-2.576954
C	-14.974213	-2.389848	-1.167391
C	-13.999257	-4.064711	-2.607064
H	-11.927909	-3.761945	-3.126296
H	-15.819602	-1.994182	-0.611521
H	-14.090962	-4.982349	-3.181842
C	-12.642046	2.210582	1.843185
C	-12.782881	3.399864	2.577292
C	-13.75381	1.707231	1.120026
C	-13.994763	4.079632	2.607482
H	-11.923703	3.774667	3.126575
C	-14.971595	2.405799	1.167882
H	-14.085454	4.997369	3.182263
H	-15.817442	2.011033	0.61207
C	-6.79118	1.278237	-1.153448
C	-6.792479	-1.271005	1.153396
C	-15.097101	-3.563641	-1.901917
C	-15.093186	3.579725	1.902411
C	-13.755681	-1.692576	-1.119614
C	-13.664262	-0.495469	-0.342377
C	-13.663708	0.510024	0.34279
H	-16.043228	4.106734	1.924521
H	-16.047704	-4.08964	-1.923965
C	-5.586259	1.953142	-0.788634
C	-5.588313	-1.947197	0.788487
C	-4.572444	-2.519906	0.435596
C	-4.569734	2.524754	-0.435854
C	5.066071	7.541095	1.612354
C	4.951137	6.13323	1.601592
C	3.672495	5.591596	1.698722
C	2.660477	7.767302	1.260867
C	3.914691	8.336576	1.458885
H	3.552364	4.510269	1.727107
H	4.050432	9.405111	1.303847
C	2.794178	7.36024	-1.46636
C	4.023714	8.074053	-1.565141
C	5.250196	7.378562	-1.415602
C	5.284899	6.025081	-1.14191
C	2.847576	5.979781	-1.48581
H	6.156048	7.973329	-1.315857
H	1.924429	5.406243	-1.434765
C	6.445288	5.441866	-0.37271
H	7.298577	6.122535	-0.464722
H	6.747404	4.464456	-0.768612
C	6.103904	5.257346	1.166087
H	7.01452	5.471455	1.737935
H	5.833179	4.210169	1.343715
C	1.530384	8.061229	-1.025804
H	0.690233	7.366734	-1.137474
H	1.32219	8.944849	-1.640862
C	1.609046	8.529528	0.487613
H	1.862798	9.595027	0.513587
H	0.61257	8.408975	0.928724
C	4.050982	9.485737	-1.552957
C	4.128185	10.703966	-1.465626
C	6.341615	8.173327	1.506689
C	7.403724	8.74349	1.334072
C	4.239058	12.113042	-1.366862
C	3.168042	12.941941	-1.757376
C	5.523367	14.113543	-0.828509
C	3.275697	14.323021	-1.689959
H	2.258598	12.473497	-2.12333
H	6.441557	14.560503	-0.457673
H	2.440978	14.945816	-2.000285

C	8.645222	9.415095	1.127042	C	5.058043	-7.546366	-1.612291
C	9.845629	8.82962	1.561968	C	3.905791	-8.340646	-1.459138
C	8.684844	10.678676	0.481658	C	2.652137	-7.770066	-1.261331
C	11.062787	9.474047	1.374444	C	3.666539	-5.595391	-1.698788
H	9.801331	7.862259	2.054586	H	4.040369	-9.409338	-1.304155
C	9.924988	11.316551	0.307298	H	3.547555	-4.513936	-1.727106
H	11.980882	9.006055	1.719275	C	1.599737	-8.531254	-0.48837
H	9.944435	12.284352	-0.185846	H	1.852385	-9.597014	-0.51438
C	4.074854	5.279576	-1.313084	H	0.603486	-8.409629	-0.929698
C	2.522569	6.383896	1.514638	C	1.521219	-8.063013	1.025069
C	4.459525	14.912605	-1.228602	H	1.311967	-8.94647	1.640002
C	11.102042	10.722665	0.747115	H	0.681767	-7.367654	1.13661
C	5.435	12.712145	-0.880122	C	6.098175	-5.263735	-1.165624
C	6.532847	11.923309	-0.421988	H	5.828595	-4.216264	-1.343261
C	7.497739	11.31652	0.006893	H	7.008704	-5.478776	-1.73726
H	12.051009	11.231236	0.600012	C	6.438983	-5.448693	0.373248
H	4.547222	15.99445	-1.177416	H	7.291547	-6.130247	0.46543
C	4.057902	3.902964	-1.06757	H	6.742007	-4.471618	0.769282
C	1.263162	5.740345	1.323892	C	6.332906	-8.17994	-1.506425
C	0.20861	5.180714	1.07885	C	7.394394	-8.751211	-1.333653
C	4.0462	2.705614	-0.767651	C	4.040231	-9.49017	1.552657
C	-1.003789	4.511633	0.736482	C	4.116161	-10.708473	1.465265
C	-2.183997	5.240573	0.496117	C	8.635129	-9.424164	-1.126423
C	-1.030886	3.110067	0.598208	C	9.836263	-8.839979	-1.561074
C	-3.349696	4.591292	0.119324	C	9.912663	-11.327032	-0.306467
H	-2.167294	6.321742	0.604169	C	11.052683	-9.485732	-1.373308
C	-2.195664	2.462123	0.217807	H	9.793124	-7.872555	-2.05367
H	-0.122593	2.544617	0.790341	H	9.930952	-12.294869	0.18665
C	-3.373409	3.191956	-0.032881	H	11.971358	-9.018723	-1.71793
H	-4.256988	5.157756	-0.071296	C	4.22557	-12.11766	1.366405
H	-2.213042	1.380964	0.106959	C	3.153616	-12.945471	1.756644
C	4.039922	1.359804	-0.396796	C	5.420979	-12.717966	0.879846
C	2.814332	0.655772	-0.198567	C	3.259845	-14.326659	1.689131
C	5.264283	0.657456	-0.186458	H	2.244593	-12.476111	2.122468
C	2.813468	-0.658632	0.198428	C	5.507896	-14.119449	0.828126
H	1.879428	1.185837	-0.362377	H	2.424418	-14.948609	1.999249
C	5.263415	-0.663369	0.186834	H	6.425691	-14.567334	0.45743
H	6.200065	1.189904	-0.335617	C	2.515741	-6.386491	-1.514999
C	4.038135	-1.364191	0.396912	C	4.068498	-5.284024	1.313103
H	1.877864	-1.187523	0.362042	C	11.090456	-10.734405	-0.746004
H	6.198497	-1.196992	0.336191	C	4.443144	-14.917437	1.227948
C	4.014418	-8.078456	1.564939	C	8.673248	-10.687811	-0.481082
C	2.785642	-7.36337	1.465964	C	7.485358	-11.324413	-0.006609
C	2.840464	-5.982965	1.485539	C	6.519744	-11.930231	0.422016
C	5.277809	-6.030761	1.142131	H	4.529722	-15.999368	1.176685
C	5.241651	-7.384225	1.415718	H	12.038841	-11.244003	-0.598707
H	1.917923	-5.408465	1.434364	C	1.256993	-5.741607	-1.32441
H	6.146907	-7.979925	1.316143	C	4.053037	-3.907378	1.067654
C	4.944589	-6.138381	-1.601442	C	4.042712	-2.710013	0.767753

C	0.203029	-5.180839	-1.079434
C	-3.376856	-3.188342	0.032492
C	-3.354652	-4.587687	-0.11987
C	-2.198329	-2.459756	-0.218149
C	-2.189661	-5.238188	-0.496744
H	-4.262553	-5.15319	0.070705
C	-1.034258	-3.108918	-0.598638
H	-2.214535	-1.37859	-0.107184
C	-1.008667	-4.5105	-0.737045
H	-2.174127	-6.319363	-0.604902
H	-0.125357	-2.544432	-0.790731