Electronic Supplementary Information (ESI) for

***N*-Annulated Perylene Substituted Zinc-Porphyrins with Different Linking Modes and Electron Acceptors for Dye Sensitized Solar Cells**

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1. Experimental Section

1.1 General

All reagents and starting materials were obtained from commercial suppliers and used without further purification unless otherwise noted. Anhydrous dichloromethane (DCM) and *N*, *N*-dimethylformamide (DMF) were distilled from CaH_2. Anhydrous toluene and THF were distilled from sodium-benzophenone immediately prior to use. The ^{1}H NMR and ^{13}C NMR spectra were recorded in solution of $CDCl_3$ or THF-d_8 on Bruker DPX 400 or DRX 500 NMR spectrometers with tetramethylsilane (TMS) as the internal standard. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, m = multiplet. MALDI-TOF mass spectra (MS) were recorded on a Bruker Autoflex instrument using anthracene-1,8,9-triol as matrix. The solvents used for UV-vis PL measurements are of HPLC grade (Merck). The electrochemical measurements were carried out in anhydrous methylene chloride with 0.1 M tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) as the supporting electrolyte at room temperature under the protection of nitrogen. A gold stick was used as working electrode, platinum wire was used as counting electrode, and Ag/AgCl (3M KCl solution) was used as reference electrode. The potential was externally calibrated against the ferrocene/ferrocenium couple. Steady-state UV-vis absorption were recorded on a Shimadzu UV-1700 and UV-3600 spectrometer.

1.2 Cell fabrication

A 2.1-μm-thick, transparent layer of 22-nm-sized TiO_2 particles was first screen-printed on FTO glass (Nippon Sheet Glass, Solar, 4 mm thick) and further coated with a 5.0-μm-thick

second layer of scattering titania particles (WER4-O, Dyesol) to produce a bilayer titania film, which was used later as the negative electrode of a DSC. The preparation procedures of TiO_2 nanocrystals and paste for screen-printing were reported in a previous paper.[1] The film thickness was monitored with a bench-top Ambios XP-1 stylus profilometer. After sintering at 500 ^{o}C and cooling to 80 ^{o}C, a circular titania electrode (~0.28 cm^2) was stained by immersing it overnight into a solution of 150 μM dye dissolved in a binary solvent of tetrahydrofuran and ethanol (volume ratio, 1/4). The dye-coated titania electrode was then rinsed with acetonitrile and dried by air flow, and was further assembled with a thermally platinized FTO positive electrode by a 25-μm-thick Surlyn (DuPont) hot-melt gasket and sealed up by heating. The internal space was perfused with an electrolyte with the aid of a vacuum-back-filling system. Our cobalt electrolyte is composed of 0.25 M tris(2,2′-bipyridine)cobalt(II) di[bis(trifluoromethanesulfonyl)imide], 0.05 M tris(2,2′-bipyridine)cobalt(III) tris[bis(trifluoromethanesulfonyl)imide], 0.5 M TBP and 0.1 M LiTFSI in acetonitrile.

1.3 Transient photovoltage decay and charge extraction measurements

Transient photoelectrical experiments were measured with an Autolab-PGSTAT302N electrochemical workstation.[2] The steady and perturbing lights on the photoanode side of a testing cell were supplied with white and red light-emitting diodes, respectively. We used the red light to generate a photovoltage perturbation near the open-circuit photovoltage of a testing cell under a certain white light and measured the voltage decay process thereafter. The modulated photovoltage by the red pulse of a testing cell was below 5 mV. The electron

lifetime can be obtained by fitting a stretched exponential function to the photovoltage decay. The electron density was estimated by the charge extraction method. A testing cell was first kept at open circuit under white light and subsequently the white light was turned off upon switching the cell from open circuit to short circuit to record the resulting current transient, and the electron density was obtained by current integration.

2. Differential pulse voltammograms of WW-6 – WW-9

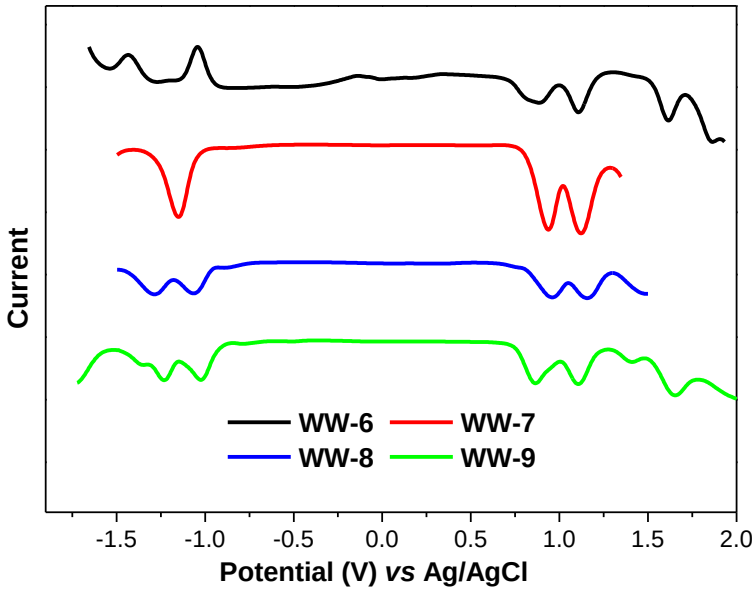

Fig. S1. Differential pulse voltammograms recorded with 0.1 M Bu_4NPF_6 as supporting electrolyte (**WW-6** in dry DCM, **WW-7** to **WW-9** in dry THF).

3. TD-DFT calculations of WW-7 – WW-9

Time-dependent DFT (TD-DFT) calculations have been performed at the B3LYP/6-31G* level of theory,[6-10] as implemented in the Gaussian 09 program package.[11] The geometries of **WW-7** – **WW-9** were fully optimized in gas phase using the default convergence criteria without any constraints and confirmed by frequency calculations. UV-vis-NIR absorption spectra were generated assuming an average UV-vis width of 4000 cm^{-1} at half-height using

the SWizard program.[12]

Table S1. Energy levels of compound **WW-7**

	Hartree	eV
LUMO+5	-0.01572	-0.43
LUMO+4	-0.03244	-0.88
LUMO+3	-0.05369	-1.46
LUMO+2	-0.06185	-1.68
LUMO+1	-0.07467	-2.03
LUMO	-0.092	-2.50
HOMO	-0.1741	-4.74
HOMO-1	-0.1743	-4.74
HOMO-2	-0.18724	-5.10
HOMO-3	-0.20283	-5.52
HOMO-4	-0.21586	-5.87
HOMO-5	-0.21607	-5.88
HOMO-6	-0.22097	-6.01
HOMO-7	-0.22269	-6.06
HOMO-8	-0.22309	-6.07
HOMO-9	-0.22723	-6.18

Table S2. Selected TD-DFT (B3LYP/6-31G*) calculated energies, oscillator strength and compositions of major electronic transitions of **WW-7**

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
624.8	0.9960	H-1->L+0(+82%) H-2->L+1(+13%)
590.0	0.0009	H-2->L+0(+51%) H-1->L+1(46%)
460.2	0.5758	H-3->L+0(+74%) H-2->L+1(16%)
442.4	0.3343	H-0->L+2(+56%) H-1->L+2(+36%)
419.9	0.8675	H-1->L+3(+32%) H-2->L+1(29%)
		H-3->L+0(20%) H-1->L+0(+5%)
402.8	0.0392	H-0->L+3(+91%)
390.2	0.0420	H-2->L+2(+60%) H-3->L+1(29%)
367.0	0.0398	H-3->L+2(+78%) H-0->L+10(+5%)
336.6	0.1253	H-18->L+0(+56%) H-11->L+1(+30%)
		H-15->L+0(+10%)

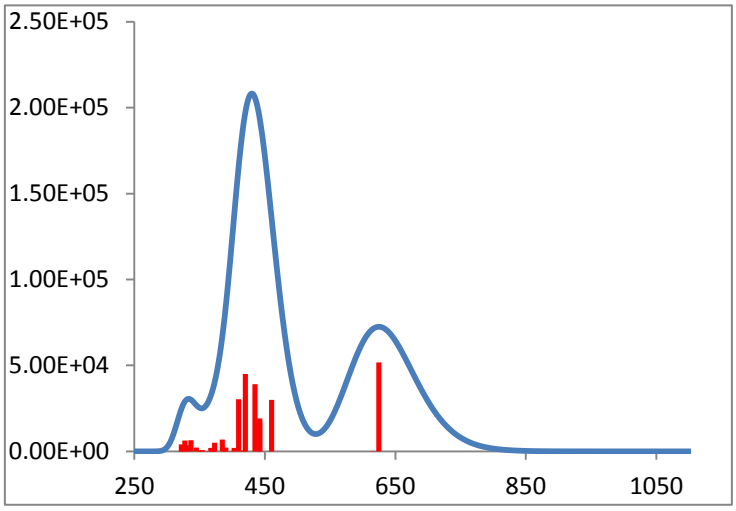

Fig. S2. Calculated absorption spectrum for **WW-7**

Table S3. Energy levels of compound **WW-8**

	Hartree	eV
LUMO+5	-0.03742	-1.02
LUMO+4	-0.05061	-1.38
LUMO+3	-0.06156	-1.68
LUMO+2	-0.07432	-2.02
LUMO+1	-0.08196	-2.23
LUMO	-0.10074	-2.74
HOMO	-0.17369	-4.73
HOMO-1	-0.17426	-4.74
HOMO-2	-0.18689	-5.09
HOMO-3	-0.20197	-5.50
HOMO-4	-0.21524	-5.86
HOMO-5	-0.21575	-5.87
HOMO-6	-0.21646	-5.89
HOMO-7	-0.22222	-6.05
HOMO-8	-0.22333	-6.08
HOMO-9	-0.22715	-6.18

Table S4. Selected TD-DFT (B3LYP/6-31G*) calculated energies, oscillator strength and compositions of major electronic transitions of **WW-8**

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
704.8	1.2325	H-0->L+0(+96%)
571.3	0.1186	H-0->L+1(+85%) H-2->L+2(13%)
453.4	1.4146	H-2->L+2(+30%) H-5->L+0(+30%)
		H-0->L+3(12%) H-4->L+0(+11%)

440.3	0.4348	H-1->L+3(+84%)	H-0->L+3(8%)
423.2	0.6725	H-2->L+1(+45%)	H-0->L+2(36%)
		H-2->L+0(8%)	
409.5	0.3637	H-0->L+4(+48%)	H-3->L+1(+23%)
		H-2->L+2(12%)	
386.2	0.0475	H-2->L+3(+87%)	
370.7	0.0612	H-5->L+1(+40%)	H-0->L+5(+16%)
		H-4->L+2(9%)	H-7->L+2(+6%)

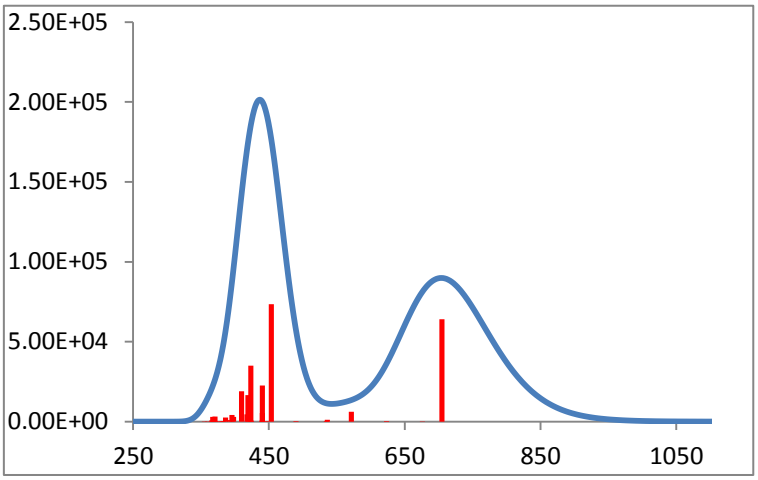

Fig. S3. Calculated absorption spectrum for **WW-8**

Table S5. Energy levels of compound **WW-9**

	Hartree	eV
LUMO+5	-0.02753	-0.75
LUMO+4	-0.04842	-1.32
LUMO+3	-0.06026	-1.64
LUMO+2	-0.07132	-1.94
LUMO+1	-0.07985	-2.17
LUMO	-0.09805	-2.67
HOMO	-0.16353	-4.45
HOMO-1	-0.18253	-4.97
HOMO-2	-0.18386	-5.00
HOMO-3	-0.20789	-5.66
HOMO-4	-0.21178	-5.76
HOMO-5	-0.21406	-5.82
HOMO-6	-0.21456	-5.84
HOMO-7	-0.22076	-6.01
HOMO-8	-0.22118	-6.02
HOMO-9	-0.22976	-6.25

Table S6. Selected TD-DFT (B3LYP/6-31G*) calculated energies, oscillator strength and compositions of major electronic transitions of **WW-9**

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
782.1	1.2840	H-0->L+0(+98%)
616.7	0.5161	H-0->L+1(+81%) H-1->L+0(10%) H-2->L+2(+6%)
502.1	0.2970	H-1->L+1(+77%) H-2->L+2(+16%)
492.8	0.4510	H-0->L+3(+86%) H-2->L+2(10%)
453.6	0.2584	H-4->L+0(+59%) H-3->L+0(+25%) H-2->L+2(6%)
428.1	0.3426	H-0->L+4(+84%) H-2->L+2(+7%)
400.6	0.4906	H-2->L+2(+28%) H-10->L+0(+16%) H-4->L+0(+10%) H-0->L+4(9%) H-1->L+1(7%) H-4->L+1(+6%)
392.4	0.1778	H-11->L+0(+36%) H-2->L+3(+26%) H-12->L+0(+10%) H-1->L+2(8%) H-10->L+0(6%)
376.1	0.0862	H-4->L+1(+36%) H-10->L+0(+12%) H-14->L+0(10%) H-6->L+1(+7%) H-2->L+2(7%)
356.8	0.0820	H-4->L+2(+40%) H-3->L+2(23%) H-2->L+4(+21%)

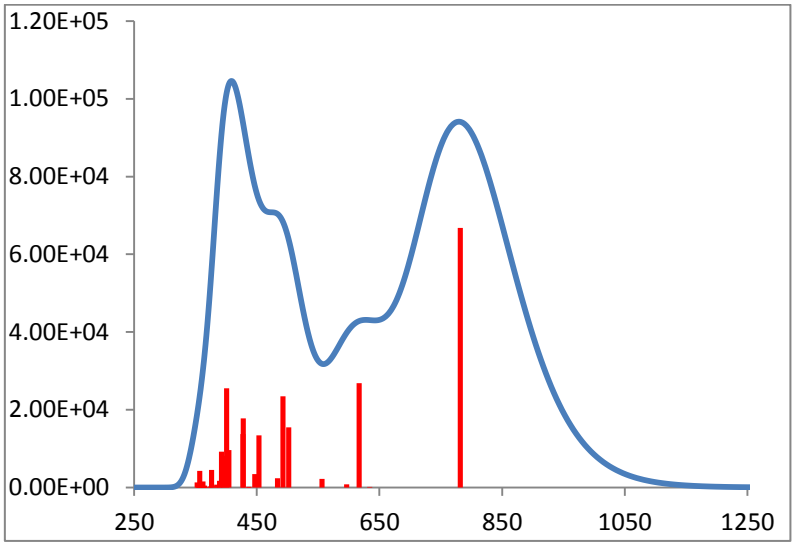

Fig. S4. Calculated absorption spectrum for **WW-9**

4. References

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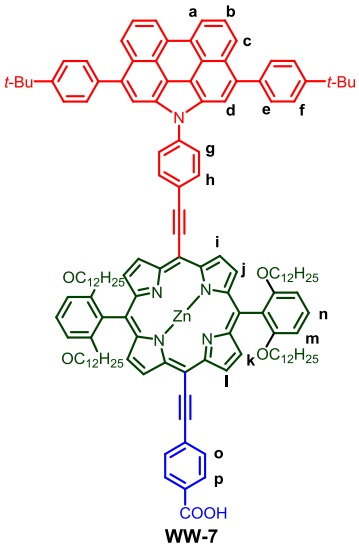
5. NMR and HR mass spectra



WW-7

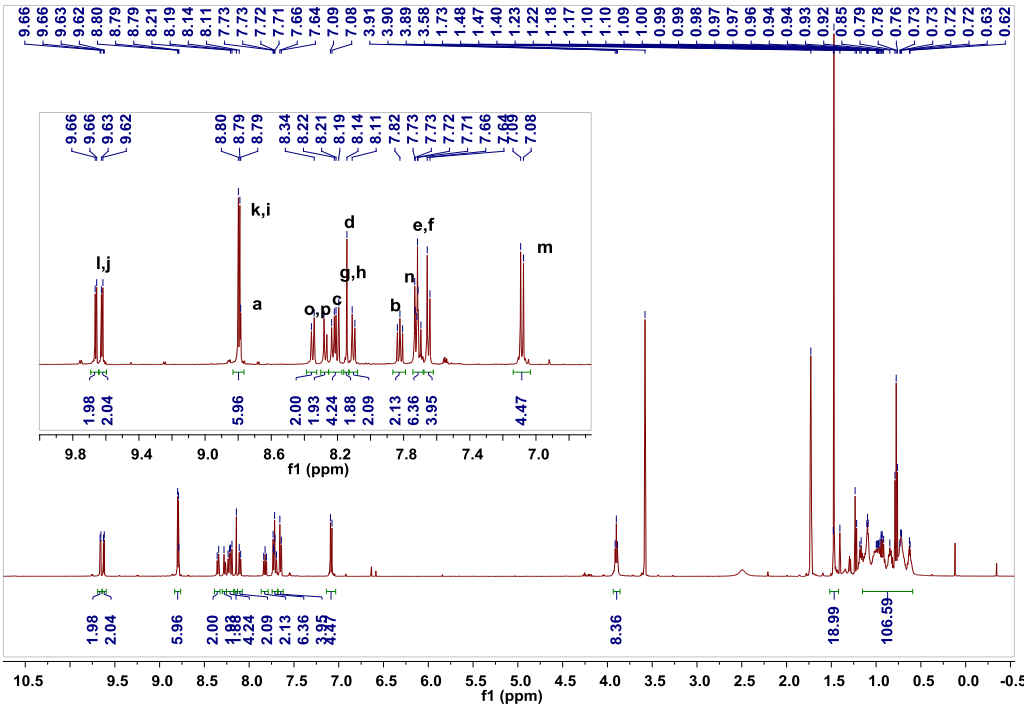


Fig. S5. ^{1}H NMR spectrum (500 MHz) of compound **WW-7** in d_8-THF at 298 K.

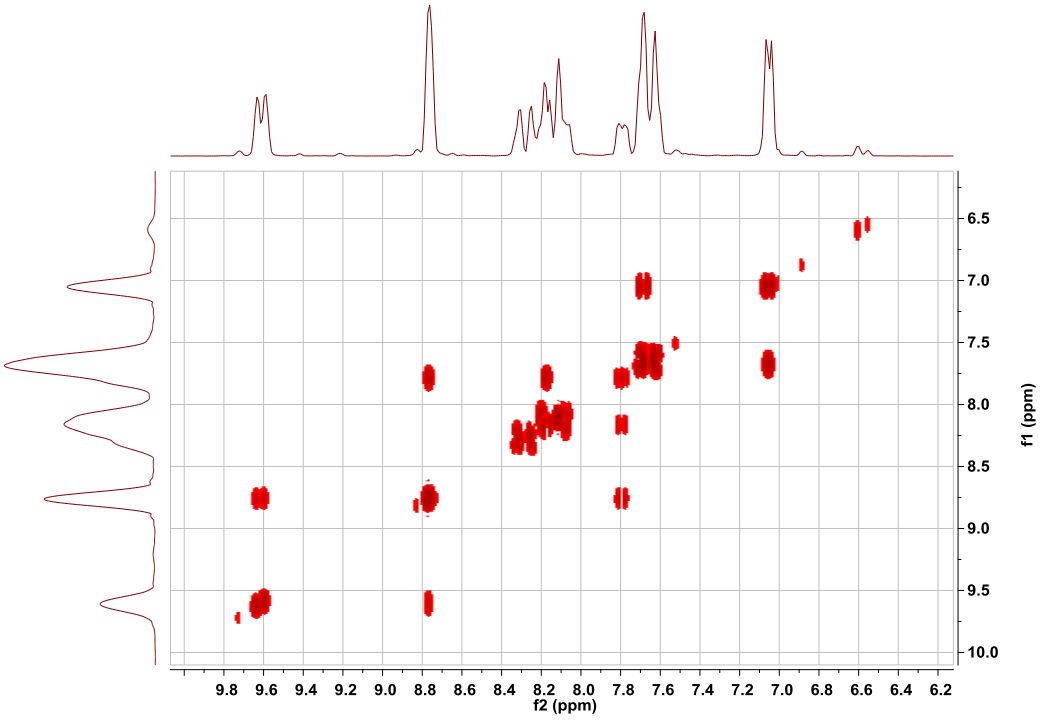


Fig. S6. COSY spectrum of compound **WW-7** in d_8-THF at 298 K.

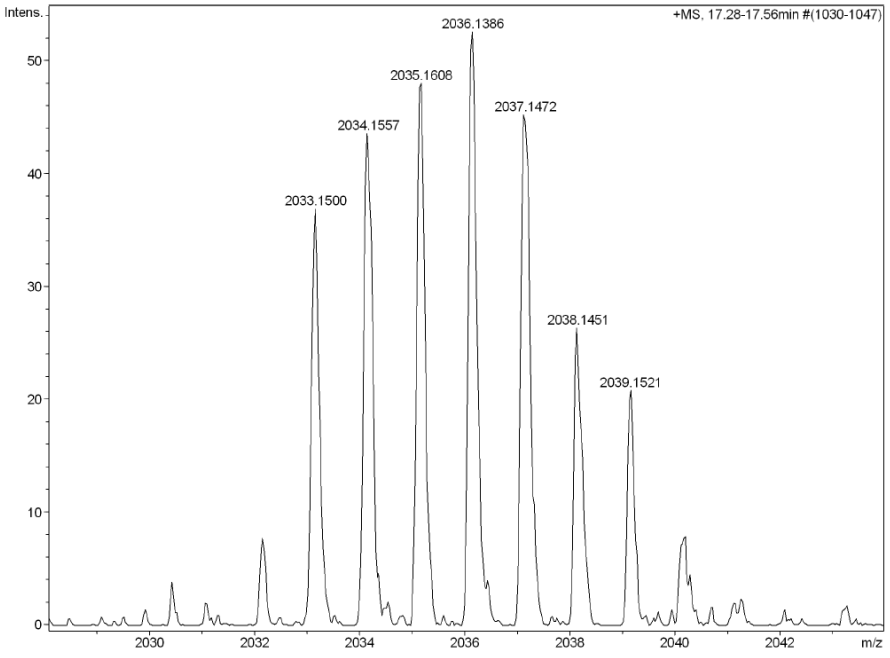
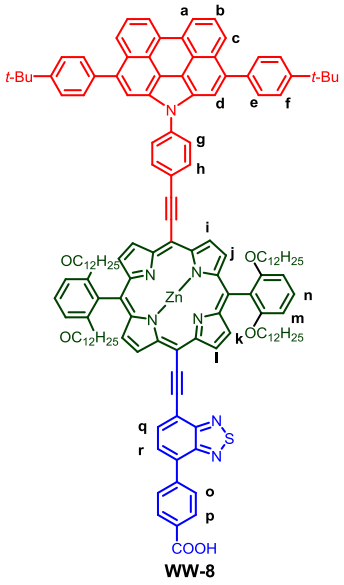


Fig. S7. HRMS spectrum (APCI) of compound **WW-7**.



WW-8

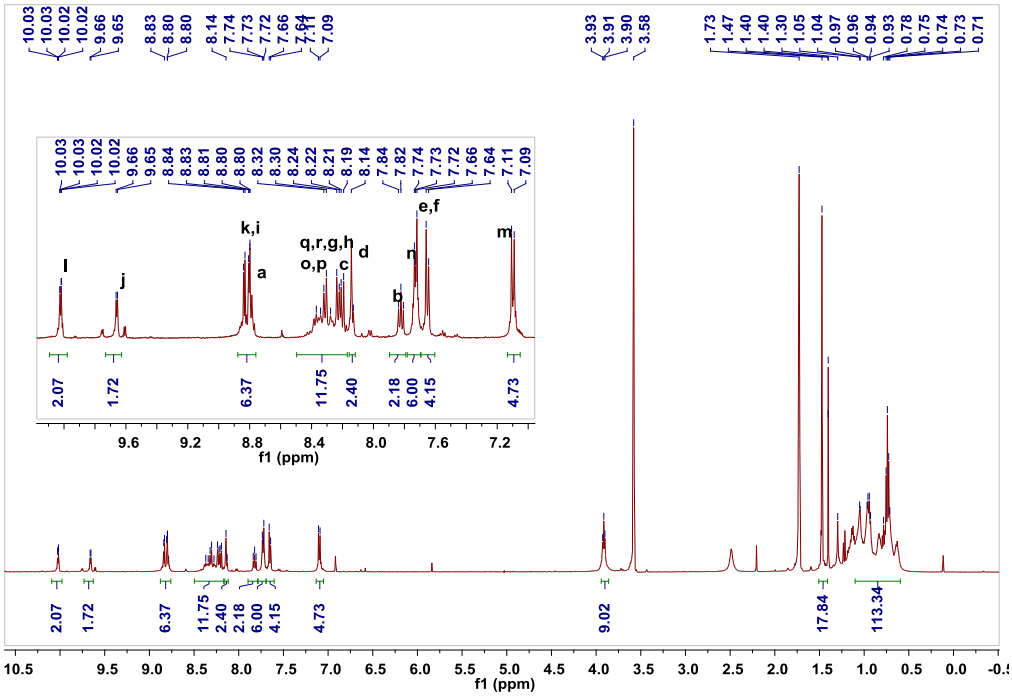


Fig. S8. ^{1}H NMR spectrum (500 MHz) of compound **WW-8** in d_8-THF at 298 K.

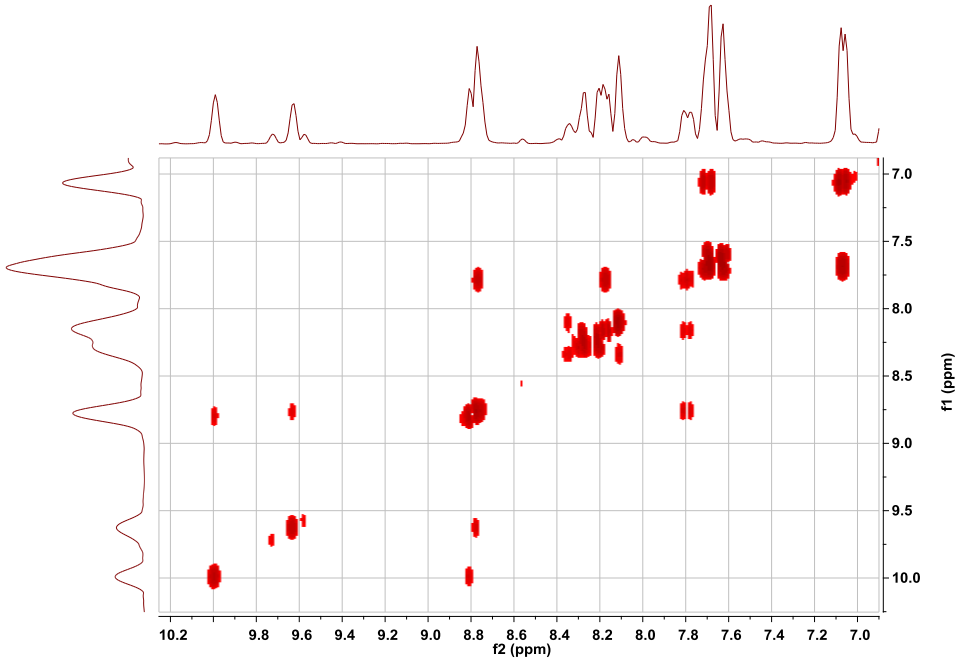


Fig. S9. COSY spectrum of compound **WW-8** in d_8-THF at 298 K.

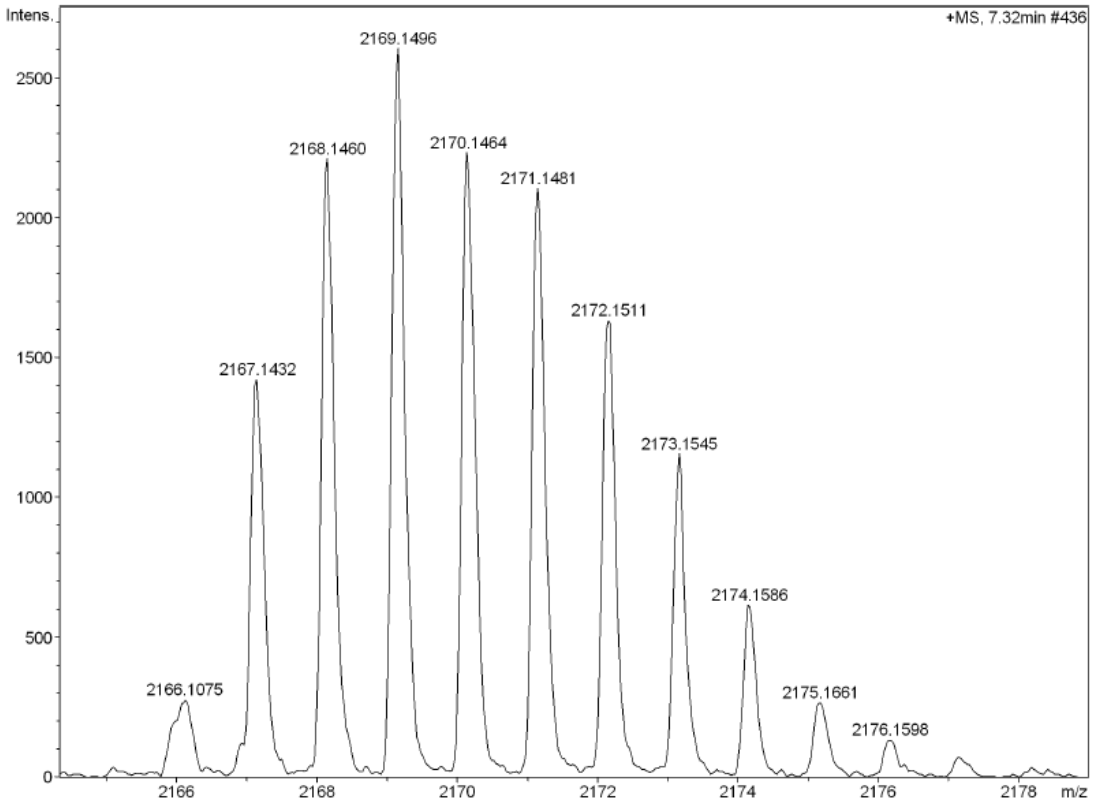


Fig. S10. HRMS spectrum (APCI) of compound **WW-8**.

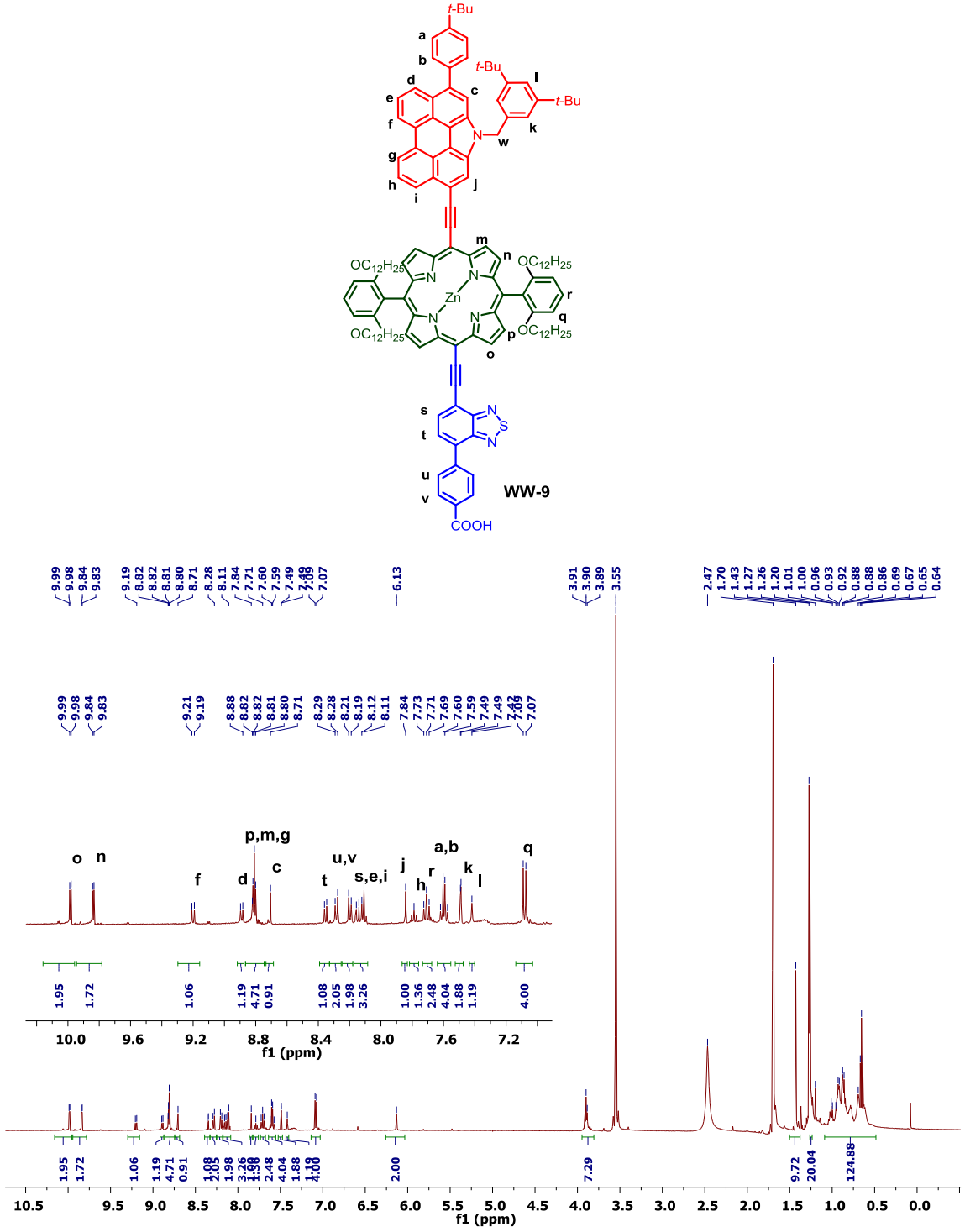


Fig. S11. ^{1}H NMR spectrum (500 MHz) of compound **WW-9** in d_8-THF at 298 K.

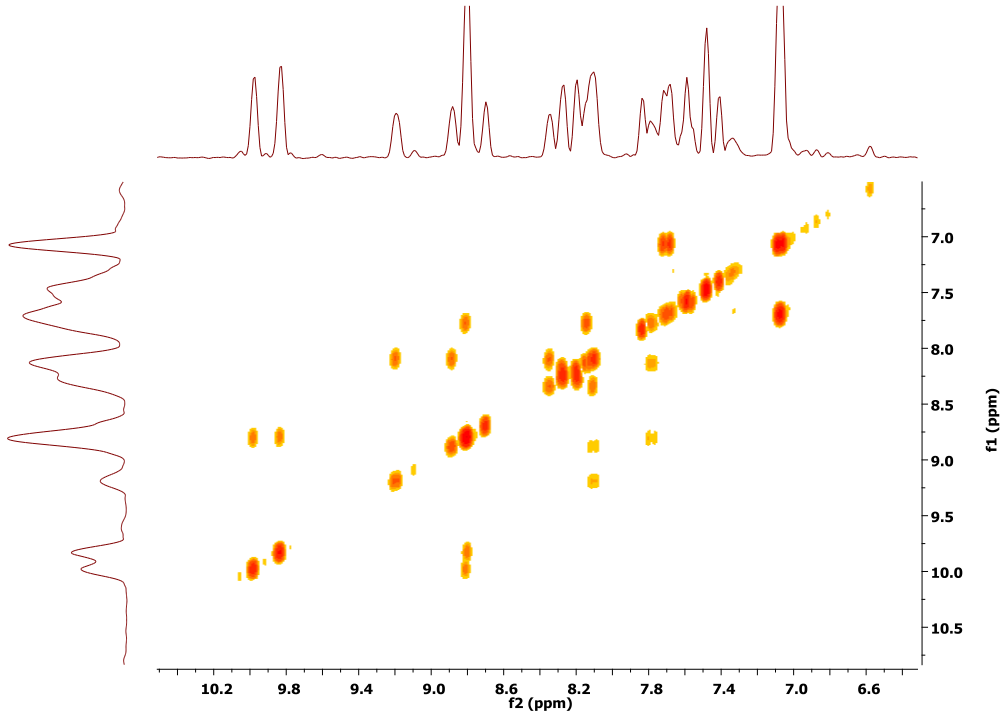


Fig. S12. COSY spectrum of compound **WW-9** in d_8-THF at 298 K.

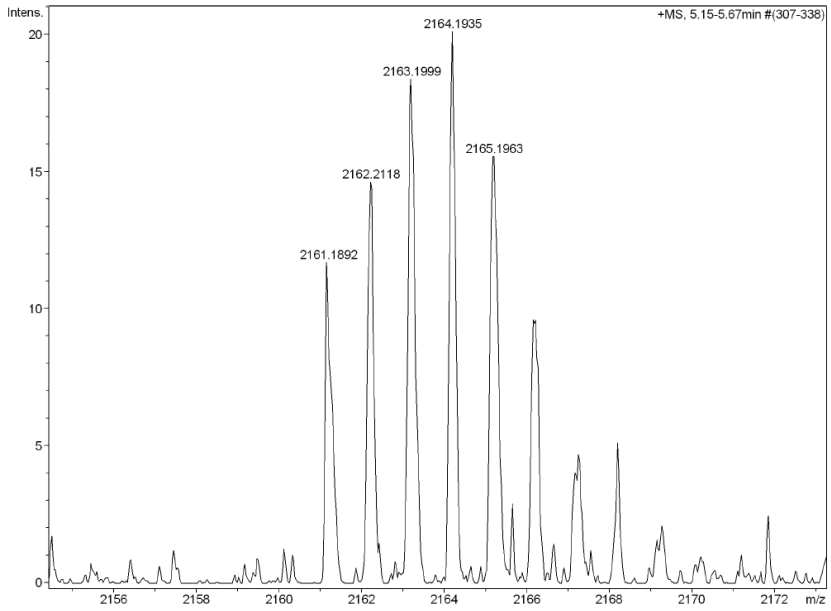


Fig. S13. HRMS spectrum (APCI) of compound **WW-9**.

6. Appendix: Cartesian coordinates of WW-7 – WW-9

WW-7:

C	-7.46988833	2.07327921	1.43719969
H	-7.92427537	1.52997533	2.25344207
C	-8.03386316	3.04238592	0.66203975
H	-9.03483664	3.44549030	0.71971974
C	-7.03005477	3.45595113	-0.28965029
C	-7.21746982	4.45170422	-1.28572976
C	-6.24646222	4.86789963	-2.23563936
C	-6.45885556	5.88024188	-3.24285731
H	-7.37879136	6.42960899	-3.38339864
C	-5.29747919	5.98697233	-3.94860633
H	-5.08571527	6.64320562	-4.78077631
C	-4.36477358	5.04096555	-3.37909777
C	-3.04593376	4.84216656	-3.82564641
C	-2.12465536	3.92299258	-3.28707212
C	-0.77137777	3.73628301	-3.75776206
H	-0.31653652	4.28102947	-4.57278864
C	-0.20804482	2.76482445	-2.98420928
H	0.79303691	2.36194114	-3.04179081
C	-1.21130906	2.35072949	-2.03339854
C	-1.02328886	1.35614813	-1.03677049
C	-1.99247001	0.94376066	-0.08403178
C	-6.11562569	1.88678702	0.96743069
N	-5.88027982	2.74417176	-0.08551089
N	-4.97485905	4.37522624	-2.33821340
C	-5.19420313	0.97168541	1.50764769
C	-3.87323153	0.77347686	1.06097311
C	-2.94138447	-0.17248798	1.63060982
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H	-13.88462817	6.26264970	0.15487345

C	-14.70005348	8.16890459	-1.48671410
O	-14.84324191	9.12328555	-2.44454874
H	-15.75249998	9.46011539	-2.34108272
O	-15.60268027	7.88982355	-0.72059257
C	-5.66045896	0.12873716	2.65804391
C	-6.53489261	-1.44423371	4.80188343
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C	-6.21077488	-1.14739110	2.43283520
C	-6.65007995	-1.93919292	3.50440030
C	-5.99434572	-0.18574022	5.05822817
H	-7.07523211	-2.92095510	3.33623795
H	-5.91645284	0.17170572	6.07757054
C	-2.57779520	5.68649226	-4.97426010
C	-1.70010568	7.26202925	-7.11494200
C	-2.02695182	6.96196548	-4.74665335
C	-2.67981851	5.21788861	-6.29768457
C	-2.24094380	6.00414667	-7.37365538
C	-1.58606617	7.75505702	-5.81662456
H	-2.31815833	5.64828222	-8.39360277
H	-1.16086864	8.73648762	-5.64662955
C	1.33486641	0.16994785	-0.95544485
C	0.24624577	0.71755214	-0.99035852
H	-1.35936130	7.87371481	-7.94617902
H	-6.87466716	-2.05478331	5.63434771
O	-5.01279989	1.84130159	4.11596552
O	-6.27730924	-1.53030137	1.12680885
O	-3.22462513	3.97635359	-6.43526896
O	-1.96157410	7.34311222	-3.44001652
C	-1.42504684	8.62404544	-3.11339861
H	-0.38809258	8.69667380	-3.47126283
H	-2.00995499	9.41139107	-3.60994504
C	-3.35802120	3.41531224	-7.74025361
H	-2.37133982	3.34996914	-8.22055933
H	-3.99412928	4.06210370	-8.36125602
C	-4.88068435	2.40515407	5.41987810
H	-4.24368739	1.76064837	6.04236994
H	-5.86759603	2.46983274	5.89974640
C	-6.81539846	-2.81115413	0.80227030
H	-6.23044308	-3.59846038	1.29884506
H	-7.85189286	-2.88246975	1.16165364
C	-4.26437225	3.78426027	5.25809263
H	-4.14423587	4.25960735	6.23774011
H	-4.90301813	4.42009697	4.63716456
H	-3.28157376	3.71321131	4.78176370

C	-6.75273848	-2.95986804	-0.70838466
H	-5.71838868	-2.88857038	-1.05871207
H	-7.33698874	-2.17375718	-1.19668653
H	-7.15724908	-3.93295961	-1.00762921
C	-3.97656149	2.03691088	-7.58099422
H	-3.33887607	1.39883561	-6.96136793
H	-4.09769080	1.56363564	-8.56152146
H	-4.95914199	2.10868391	-7.10435099
C	-1.48993380	8.77113418	-1.60266924
H	-0.90578128	7.98495501	-1.11434296
H	-2.52471372	8.69862499	-1.25388662
H	-1.08668798	9.74425960	-1.30181586
C	2.60495731	-0.46608694	-0.92028028
C	5.13141595	-1.72685554	-0.85234847
C	3.55233159	-0.24963151	-1.94347313
C	2.95589530	-1.33226060	0.13696232
C	4.20196220	-1.94510180	0.17585596
C	4.79125753	-0.87705503	-1.91583954
H	3.29723992	0.40325439	-2.77226191
H	2.24506495	-1.50446360	0.93905058
H	4.47029205	-2.57948422	1.01424462
H	5.49324265	-0.72917129	-2.72980169
N	6.39765017	-2.35581284	-0.81695837
C	6.64812400	-3.70627049	-0.45014469
C	8.01543631	-3.89797699	-0.55689623
C	6.52574049	-6.05337973	0.17391786
C	8.73072281	-5.05971760	-0.30416605
C	5.87837103	-4.83713493	-0.08550097
C	7.97628635	-6.19849807	0.09407540
C	10.15875832	-5.00925280	-0.44747720
H	4.79520787	-4.80309217	-0.03423550
H	8.23930448	-8.25804423	0.75042644
C	10.82902359	-6.19468667	-0.14889958
H	11.91097045	-6.25576960	-0.22593461
C	10.11593512	-7.33578634	0.27463770
H	10.67680490	-8.23495999	0.51644474
C	8.73181451	-7.35621163	0.40332575
C	7.64094154	-1.74509629	-1.13733121
C	8.61357789	-2.71673124	-0.97091367
C	9.46152490	-0.24731121	-1.73349258
C	9.98436774	-2.58200920	-1.13947371
C	8.09167112	-0.46023308	-1.52463928
C	10.45463767	-1.29869854	-1.53536609
C	10.80599485	-3.72947113	-0.87292869

H	7.40713865	0.36500843	-1.68862016
H	12.30622373	-0.21690513	-1.91456393
C	12.17690567	-3.52888890	-1.02809156
H	12.88066182	-4.33697791	-0.84903799
C	12.67987012	-2.26581368	-1.40441590
H	13.75621030	-2.14519750	-1.49663852
C	11.86076343	-1.16977339	-1.65003530
C	5.67242350	-7.21988991	0.53250972
C	3.96179777	-9.41972530	1.18197498
C	5.75666587	-8.44072257	-0.16053176
C	4.71511744	-7.12685060	1.55222232
C	3.88043610	-8.20079927	1.86806116
C	4.92279881	-9.50790501	0.15911882
H	6.46894215	-8.54456244	-0.97422443
H	4.63337063	-6.20340450	2.11975398
C	9.88264823	1.11225462	-2.17222626
C	10.60406039	3.73909347	-3.04592288
C	9.47170659	2.25500170	-1.47196235
C	10.66446142	1.30994304	-3.32430244
C	11.01330967	2.58969770	-3.74514584
C	9.82398534	3.53680297	-1.89973296
H	8.87919651	2.13841124	-0.56820207
H	10.98223051	0.45052474	-3.90803922
N	-2.36115522	3.06466433	-2.23671353
N	-3.26445976	1.43809718	0.02019300
Zn	-4.12034564	2.90548535	-1.16010557
H	-0.86143139	-0.61919297	1.06174123
H	3.16285304	-8.07224782	2.67108199
H	5.01993676	-10.42701551	-0.41267126
H	11.61083450	2.69091561	-4.64735192
H	9.48206926	4.38383359	-1.31488735
C	11.01128832	5.13451160	-3.55164973
C	12.55483247	5.24232993	-3.58205988
H	13.00330458	4.48731181	-4.23629292
H	12.97676750	5.10833791	-2.57940058
H	12.86139517	6.22870034	-3.95165795
C	10.45600432	5.34613704	-4.98060745
H	10.83897397	4.59722111	-5.68179750
H	10.74288205	6.33510026	-5.35906113
H	9.36181484	5.28289509	-4.98912945
C	10.46979097	6.26391597	-2.65470730
H	10.85132200	6.18927414	-1.62994927
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C	3.05830371	-10.62497787	1.49750072
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H	4.62666304	-12.11966441	1.09642791
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C	2.22710392	-10.98541319	0.24259876
H	2.86599797	-11.24447154	-0.60830541
H	1.59184689	-10.14524964	-0.06034180
H	1.57881658	-11.84630123	0.44801817
C	2.08156895	-10.33785507	2.65388557
H	2.60934309	-10.09957958	3.58445976
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WW-8:

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C	-7.13060046	3.43692936	-0.25331143
C	-7.32660215	4.42119538	-1.25996760
C	-6.36082050	4.84065833	-2.21507288
C	-6.58722607	5.84475801	-3.22991370
H	-7.51268374	6.38626090	-3.37408754
C	-5.42642836	5.95413090	-3.93608023
H	-5.22095581	6.60562699	-4.77359123
C	-4.48346045	5.02052450	-3.36106646
C	-3.16484882	4.82759163	-3.80759464
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H	-0.43340707	4.27872940	-4.55632080
C	-0.30978232	2.77679402	-2.95505995
H	0.69400581	2.38058668	-3.01196349
C	-1.30747204	2.36402943	-1.99818611
C	-1.11057174	1.37974916	-0.99336543
C	-2.07407079	0.96958426	-0.03340521
C	-6.20228063	1.88963015	1.01967555
N	-5.97532027	2.73833270	-0.04285488
N	-5.08610931	4.35763111	-2.31330005
C	-5.27226473	0.98838397	1.56678181
C	-3.95018988	0.79642661	1.11854648
C	-3.01013488	-0.13701553	1.69434398
H	-3.21478868	-0.78659846	2.53348244

C	-1.85174507	-0.03051768	0.98221543
C	-8.59710995	5.04538784	-1.32518591
C	-9.67979274	5.60143712	-1.40884244
C	-14.79408632	8.34044459	-1.95205051
C	-17.32228138	9.59062129	-2.07834285
C	-15.97502436	7.62282653	-1.67195194
C	-14.91226388	9.69733184	-2.31018667
C	-16.15749695	10.31427181	-2.36906799
C	-17.21888364	8.23637448	-1.73212376
H	-15.91527697	6.56519838	-1.43354219
H	-14.02173170	10.26861646	-2.54073520
H	-16.23005636	11.36219453	-2.63832890
H	-18.12679929	7.67994529	-1.52382577
C	-18.67465284	10.19950285	-2.12854913
O	-18.65640644	11.51286606	-2.47682141
H	-19.58975175	11.79550921	-2.47473282
O	-19.71305032	9.61421630	-1.88771933
C	-5.72863180	0.15292757	2.72657639
C	-6.58311040	-1.40677773	4.88814223
C	-5.62147722	0.63532956	4.04459317
C	-6.27208800	-1.12846180	2.51508517
C	-6.70149269	-1.91362580	3.59553846
C	-6.04897280	-0.14286606	5.13096791
H	-7.12123720	-2.89943945	3.43783583
H	-5.96830856	0.22390409	6.14678920
C	-2.70432936	5.66481403	-4.96445190
C	-1.84318989	7.22792335	-7.12069368
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H	-2.45865511	5.60131202	-8.38430058
H	-1.30517410	8.71628712	-5.66596182
C	1.25350432	0.20558532	-0.91083412
C	0.16249147	0.74841469	-0.94597241
H	-1.50894421	7.83483594	-7.95804730
H	-6.91506752	-2.01216802	5.72750783
O	-5.08358274	1.88153479	4.16662738
O	-6.34222283	-1.52310809	1.21278084
O	-3.34911759	3.94036215	-6.40929525
O	-2.08990725	7.33585752	-3.44541665
C	-1.56546236	8.62484879	-3.13134752
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H	-2.15881829	9.40180688	-3.63411571

C	-3.49308344	3.37195594	-7.70992387
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H	-4.13453540	4.01507224	-8.32918439
C	-4.94351303	2.45521625	5.46535205
H	-4.30036939	1.81691107	6.08791003
H	-5.92709359	2.52086024	5.95196858
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H	-6.27668565	-3.58901892	1.40438899
H	-7.90476741	-2.88869663	1.26514289
C	-4.33202053	3.83468849	5.28901711
H	-4.20641047	4.31772138	6.26421453
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C	-6.81031180	-2.97424585	-0.60730164
H	-5.77761351	-2.89749280	-0.96128751
H	-7.40257396	-2.19781855	-1.10141411
H	-7.20734344	-3.95356082	-0.89607693
C	-4.10983901	1.99430676	-7.53774086
H	-3.46703759	1.36002203	-6.91947985
H	-4.23853716	1.51526857	-8.51450760
H	-5.08863331	2.06868291	-7.05379154
C	-1.62964371	8.78506186	-1.62191738
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H	-1.23522405	9.76467282	-1.33052684
C	2.52537303	-0.42685325	-0.87599907
C	5.05357588	-1.68437636	-0.81058516
C	3.46259149	-0.22758500	-1.91197188
C	2.88774626	-1.27326433	0.19328404
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C	4.70225463	-0.85357800	-1.88548265
H	3.19862463	0.41004201	-2.74980849
H	2.18507732	-1.43152425	1.00537169
H	4.41190341	-2.50294538	1.07802930
H	5.39579641	-0.71988470	-2.70905711
N	6.31970676	-2.31339486	-0.77732553
C	6.57332316	-3.65665186	-0.38652414
C	7.93880049	-3.85265932	-0.50774167
C	6.45632688	-5.99043537	0.28679692
C	8.65585699	-5.01029135	-0.24143790
C	5.80711996	-4.77870442	0.01133965
C	7.90540326	-6.13954238	0.19007366
C	10.08184669	-4.96528131	-0.40543395
H	4.72482289	-4.74199365	0.07654455

H	8.17436988	-8.18581556	0.88430977
C	10.75445838	-6.14557119	-0.09214617
H	11.83514919	-6.21006218	-0.18282788
C	10.04566837	-7.27664766	0.36423785
H	10.60853770	-8.17169531	0.61647635
C	8.66343401	-7.29206810	0.51231820
C	7.55946412	-1.71134076	-1.12679970
C	8.53287593	-2.68105157	-0.95384786
C	9.37393088	-0.22934734	-1.77828829
C	9.90142228	-2.55229751	-1.14400905
C	8.00681284	-0.43529529	-1.54612572
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C	10.72498871	-3.69557078	-0.86577664
H	7.32146432	0.38785762	-1.71707461
H	12.21558773	-0.20768964	-2.00014916
C	12.09386733	-3.50065959	-1.04433714
H	12.79882144	-4.30625793	-0.85889756
C	12.59341849	-2.24644830	-1.45347152
H	13.66852568	-2.12975620	-1.56340627
C	11.77259393	-1.15417879	-1.70984500
C	5.60626824	-7.14758927	0.68169001
C	3.90060639	-9.32949285	1.40074621
C	5.67876960	-8.38294065	0.01349468
C	4.66339363	-7.03107920	1.71236383
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C	4.84743531	-9.44138114	0.36707391
H	6.37949648	-8.50546677	-0.80760047
H	4.59131643	-6.09568179	2.26133273
C	9.79191682	1.11969709	-2.25125488
C	10.51098457	3.72482923	-3.18885194
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H	8.82028411	2.18216322	-0.65133684
H	10.85820295	0.41800564	-3.99205741
N	-2.46296071	3.06847390	-2.20470628
N	-3.34939584	1.45574267	0.06989871
Zn	-4.21884146	2.90573103	-1.12343873
H	-0.92852603	-0.57422971	1.12339919
H	3.12478550	-7.94953363	2.87206516
H	4.93522765	-10.37268081	-0.18622975
H	11.48432002	2.64021381	-4.78656964
H	9.42201457	4.40959752	-1.45222554

C	10.91802755	5.10787051	-3.72783970
C	12.46150688	5.20531264	-3.78641354
H	12.89435894	4.43595468	-4.43448605
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H	12.76731306	6.18293883	-4.17919135
C	10.34037147	5.29660859	-5.15112057
H	10.70708009	4.53245555	-5.84449331
H	10.62733471	6.27651960	-5.55220639
H	9.24583009	5.24051984	-5.14057774
C	10.39875210	6.25736243	-2.84335717
H	10.79730682	6.19954876	-1.82401941
H	9.30441948	6.26384787	-2.78319904
H	10.71162392	7.21878885	-3.26637794
C	2.99913776	-10.52563674	1.75420305
C	3.87787560	-11.73060858	2.16735755
H	4.48562417	-11.48929836	3.04703673
H	4.55834281	-12.03278297	1.36434553
H	3.24895459	-12.59480250	2.41458952
C	2.15060316	-10.91134160	0.51865256
H	2.77740653	-11.19240690	-0.33426719
H	1.51452950	-10.07581285	0.20480810
H	1.50182549	-11.76468723	0.75208731
C	2.03844890	-10.21126228	2.91693795
H	2.57900505	-9.95396429	3.83504442
H	1.42017884	-11.09004487	3.13307925
H	1.36198503	-9.38371150	2.67451754
C	-10.91459112	6.26812182	-1.54235357
C	-13.47920940	7.67329528	-1.83817693
C	-12.01359416	6.01351051	-0.73222503
C	-11.09826976	7.27790118	-2.55585896
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C	-13.24550604	6.69584658	-0.88283694
H	-11.92295615	5.26884762	0.05208129
H	-14.04127311	6.44976699	-0.18637865
N	-10.16957560	7.65743615	-3.43571132
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WW-9:

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C	-7.94359049	2.91863931	0.55359486
H	-8.94496514	3.32519165	0.54082526

C	-6.86837874	3.34513644	-0.31022955
C	-6.97749895	4.35806193	-1.30193697
C	-5.93608744	4.79168465	-2.16770093
C	-6.07644456	5.81929590	-3.17485357
H	-6.98524404	6.36918896	-3.38010783
C	-4.86279764	5.93688247	-3.78401166
H	-4.58890545	6.60536971	-4.58791585
C	-3.97194231	4.98660132	-3.15562308
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