

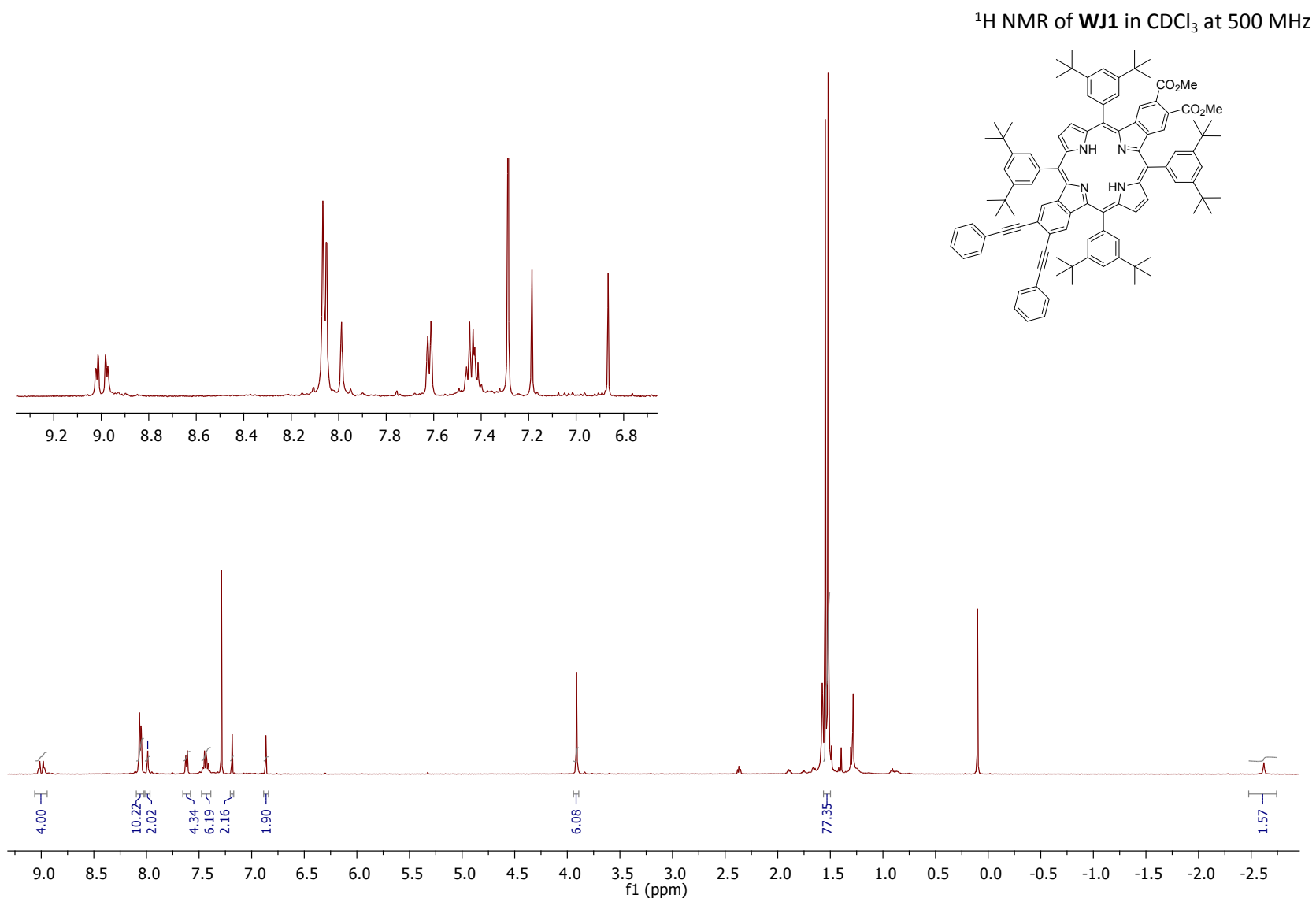
Electronic Supplemental Information

Investigation of the push-pull effects on β -functionalized benzoporphyrins bearing ethynylphenyl bridge

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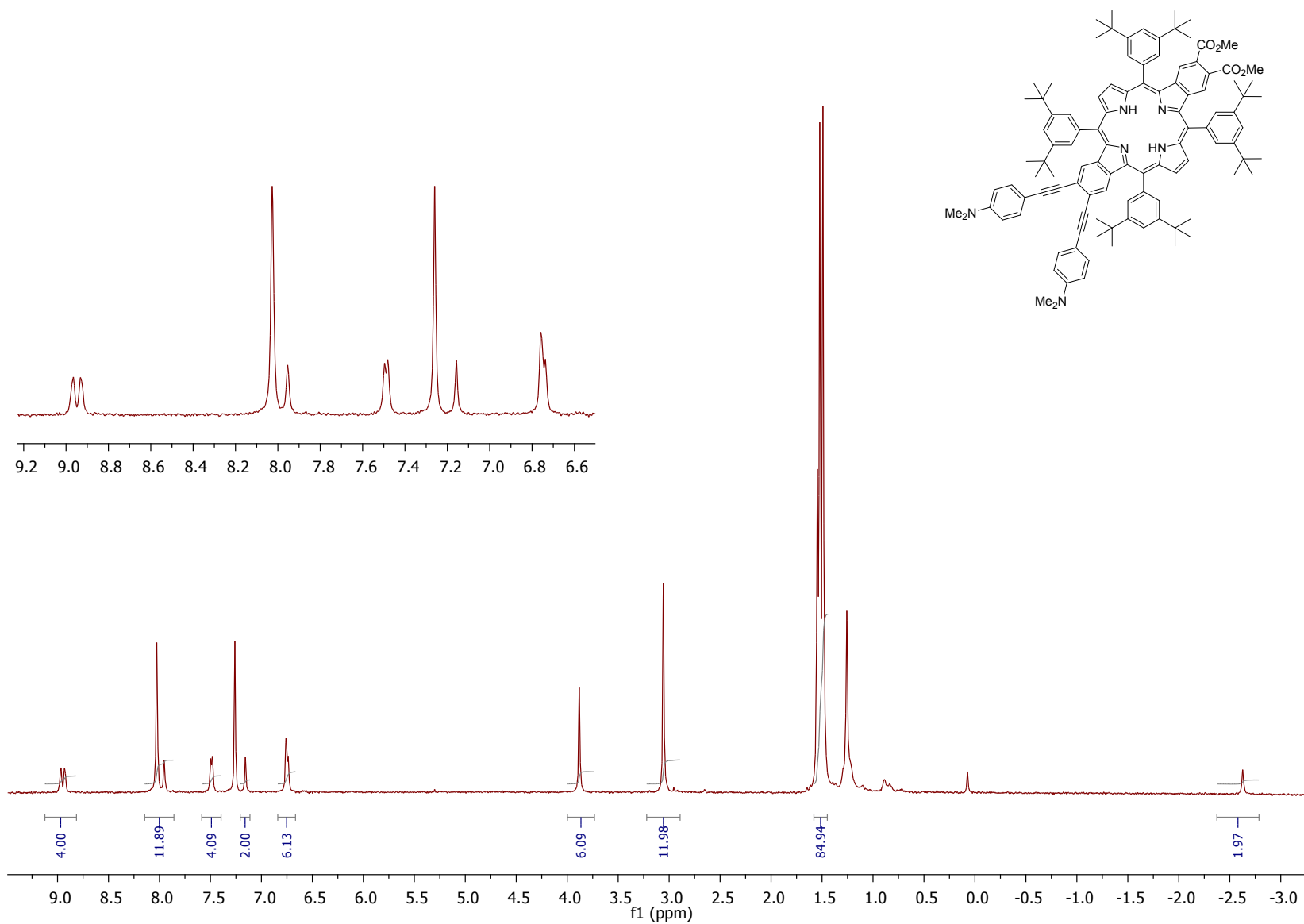
Figure S1. ^1H and ^{13}C NMR characterization of compounds



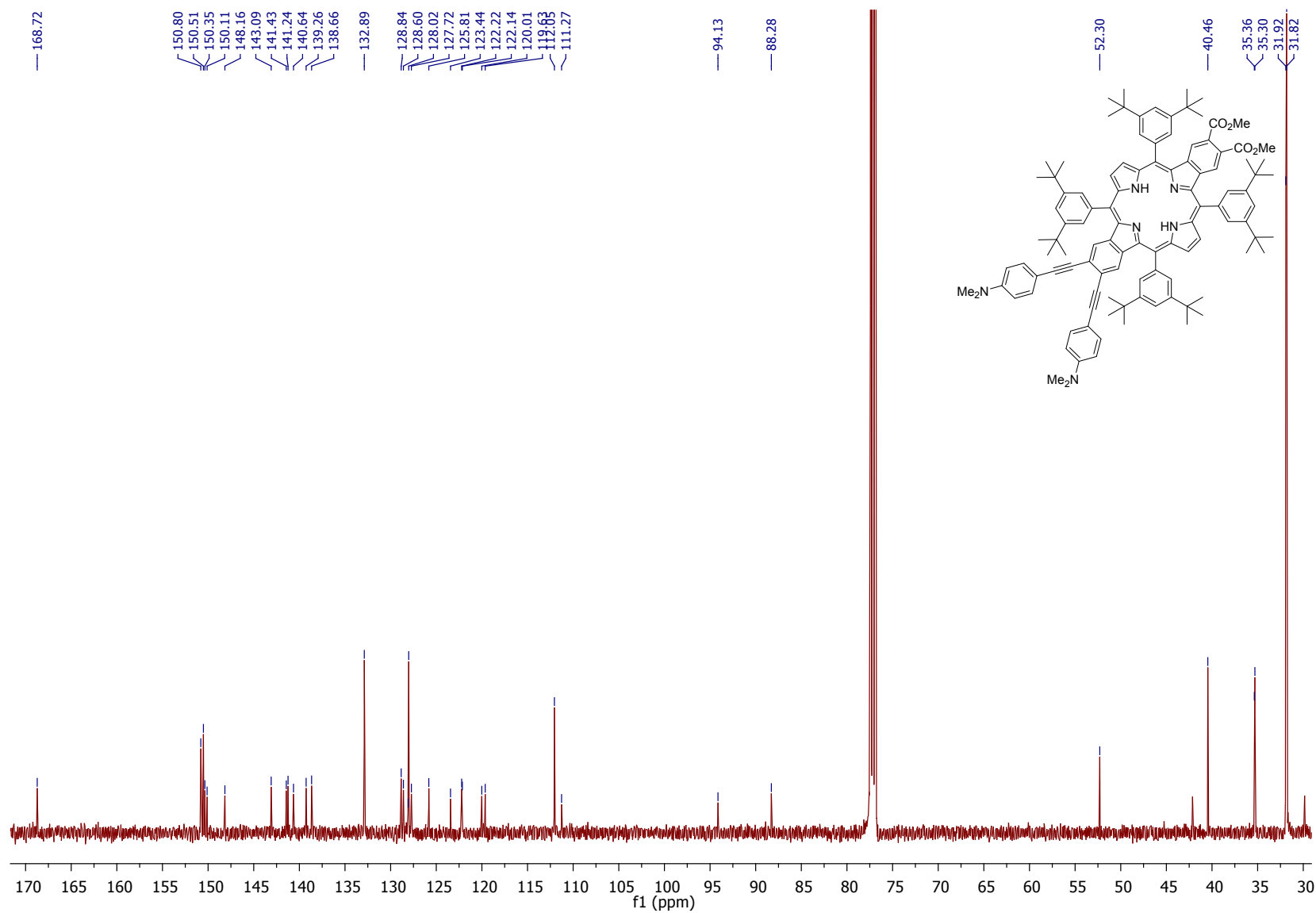
The chemical structure shows a central macrocyclic phthalocyanine core. It features four tert-butylphenyl groups attached to the nitrogen atoms of the ring. Additionally, there are two ethyl ester groups (CO₂Me) attached to the ring. The structure is highly symmetrical and complex, with multiple tert-butyl groups providing steric bulk.



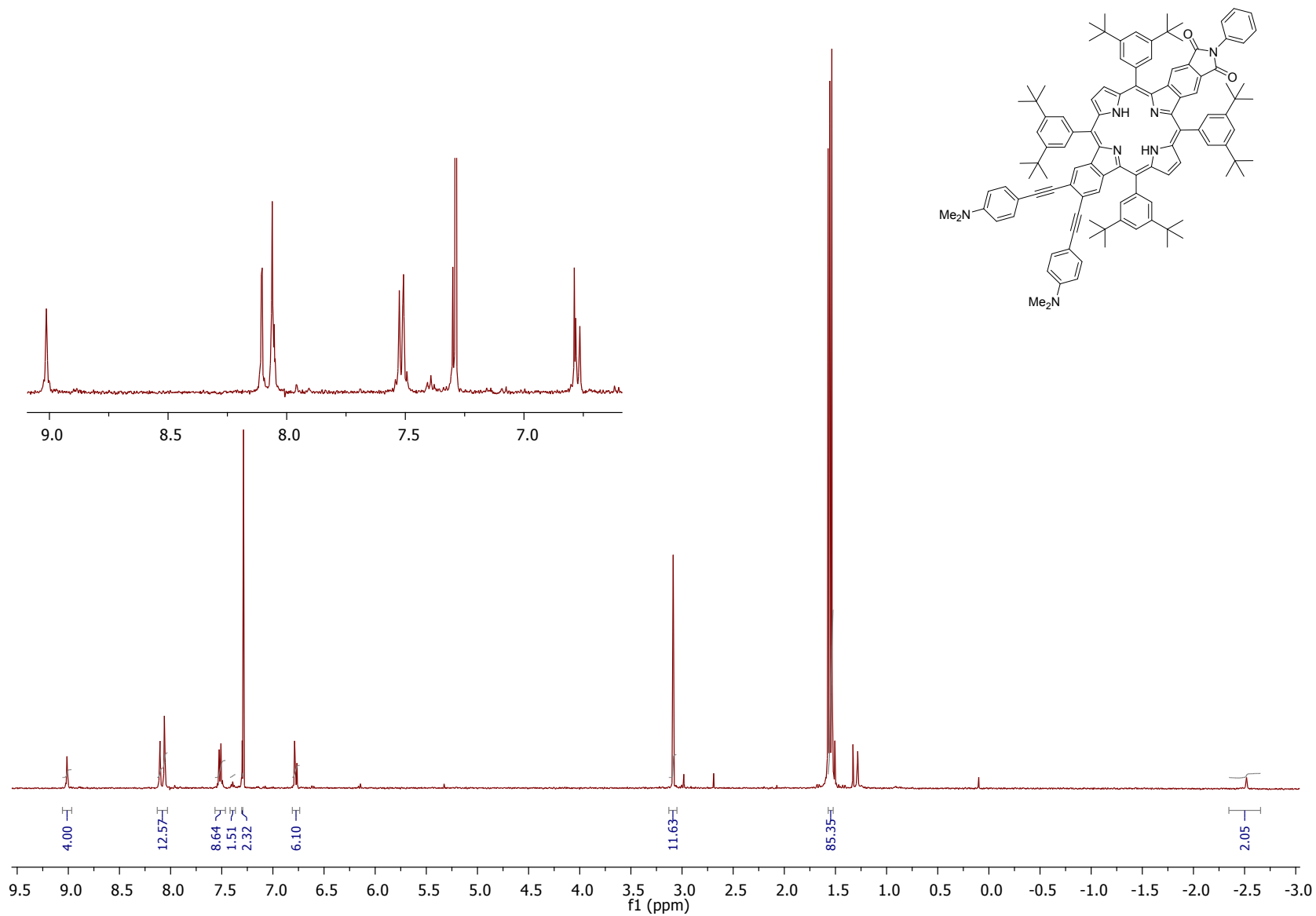
^1H NMR of **WJ2** in CDCl_3 at 500 MHz



¹³C NMR of **WJ2** in CDCl₃ at 126 MHz



^1H NMR of **WJ3** in CDCl_3 at 500 MHz



¹³C NMR of **WJ3** in CDCl₃ at 500 MHz

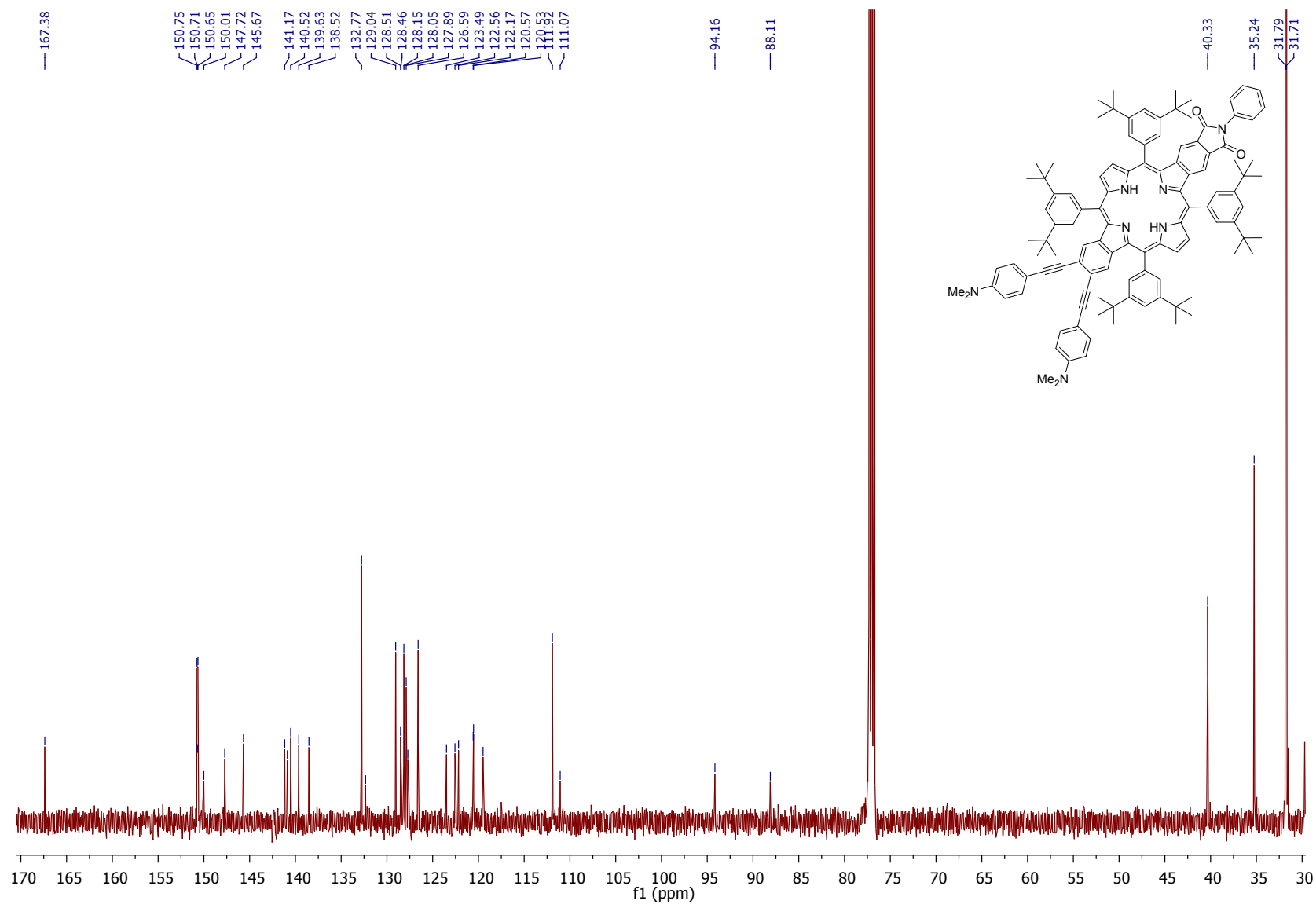
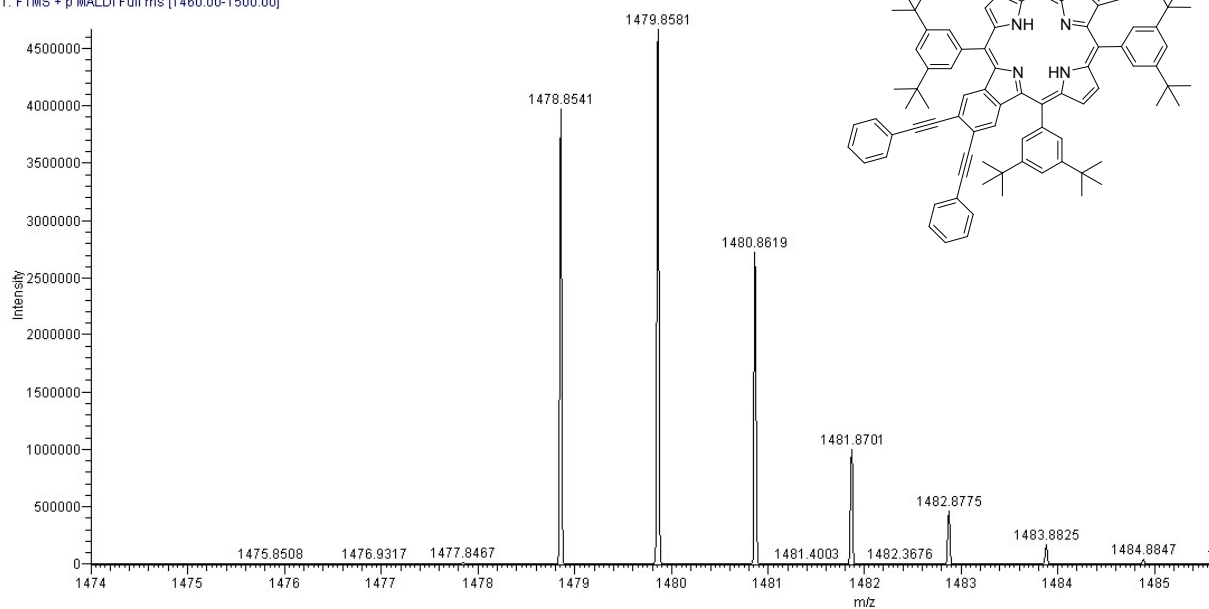


Figure S2. MS characterization of compounds

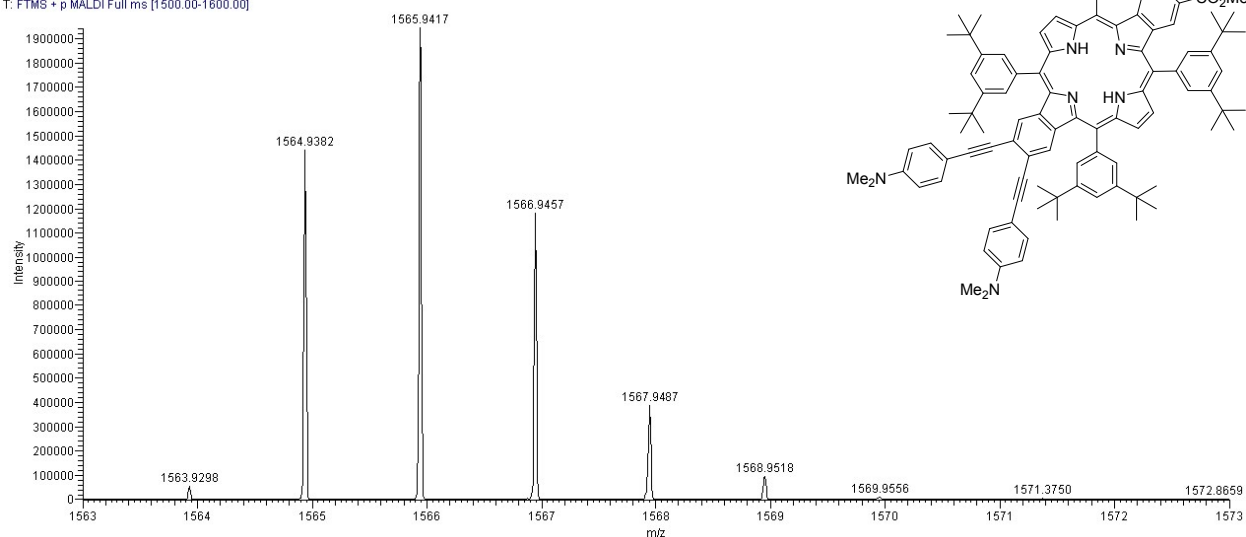
HRMS MALDI-IMS spectra of **WJ1 [M]⁺**

RA_120116_WJ2-122_01_E9 #1-31 RT: 0.00-0.93 AV: 31 NL: 4.67E6
T: FTMS + p MALDI Full ms [1460.00-1500.00]



HRMS MALDI-IMS spectra of **WJ2 [M]⁺**

RA_120116_WJ3-40_02_E2 #1-30 RT: 0.00-0.93 AV: 30 NL: 1.94E6
T: FTMS + p MALDI Full ms [1500.00-1600.00]



HRMS MALDI-IMS spectra of **WJ3** [M]⁺

RA_120116_W2-112_01_E7 #1-31 RT: 0.00-0.93 AV: 31 NL: 1.84E8
T: FTMS + p MALDI Full ms [1550.00-1650.00]

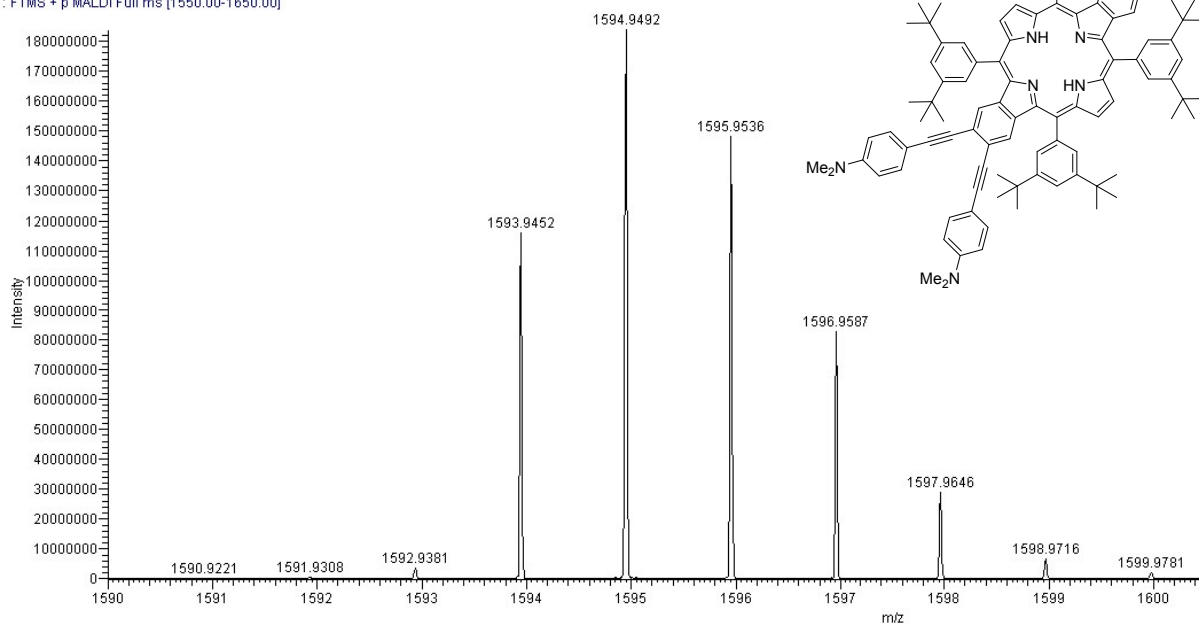
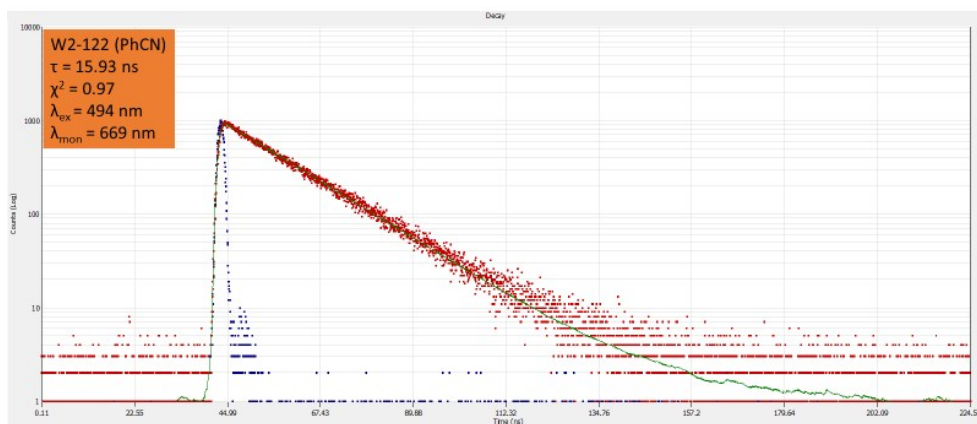


Table S1. Fluorescence Lifetime (τ) of WJ1 – WJ3 in toluene and benzonitrile

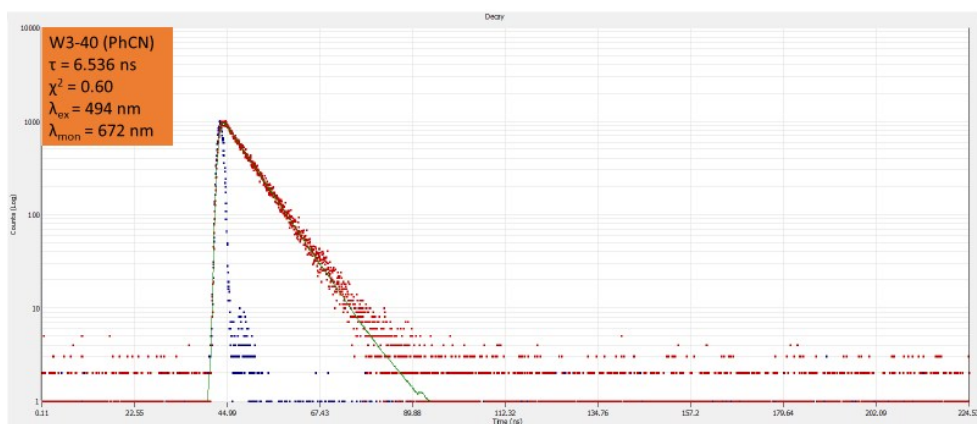
	WJ1	WJ2	WJ3
Toluene	16.75 ns	16.88 ns	14.51 ns
Benzonitrile	15.93 ns	6.54 ns	2.54 ns

Figure S3. Fluorescence decay curves in benzonitrile and toluene

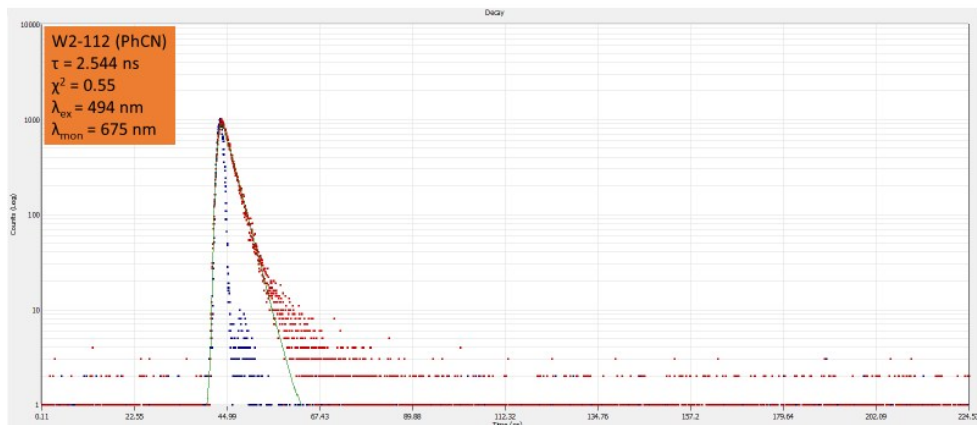
Lifetime decay of **WJ1** in benzonitrile



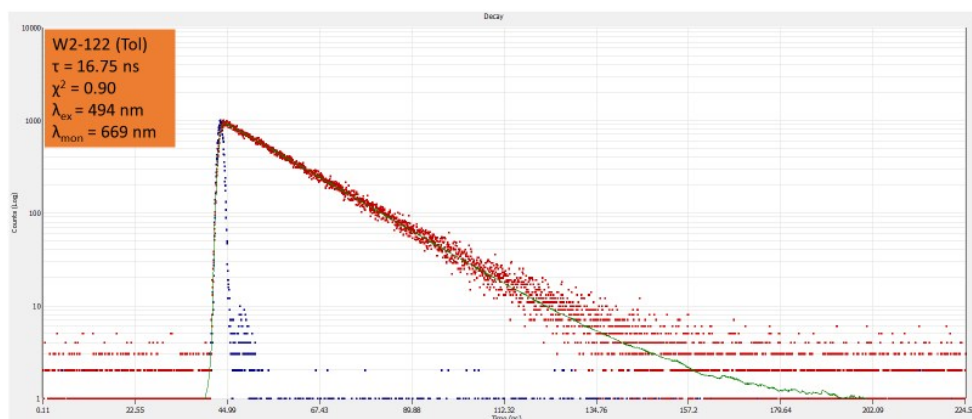
Lifetime decay of **WJ2** in benzonitrile



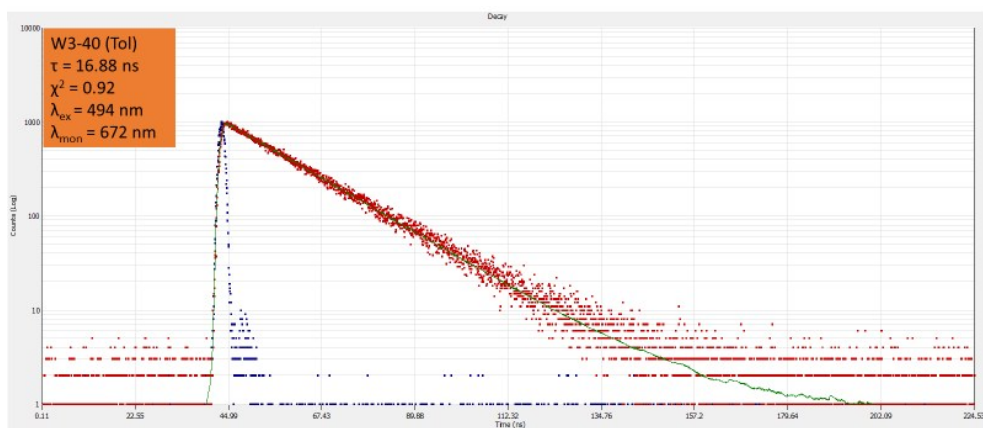
Lifetime decay of **WJ3** in benzonitrile



Lifetime decay of **WJ1** in toluene



Lifetime decay of **WJ2** in toluene



Lifetime decay of **WJ3** in toluene

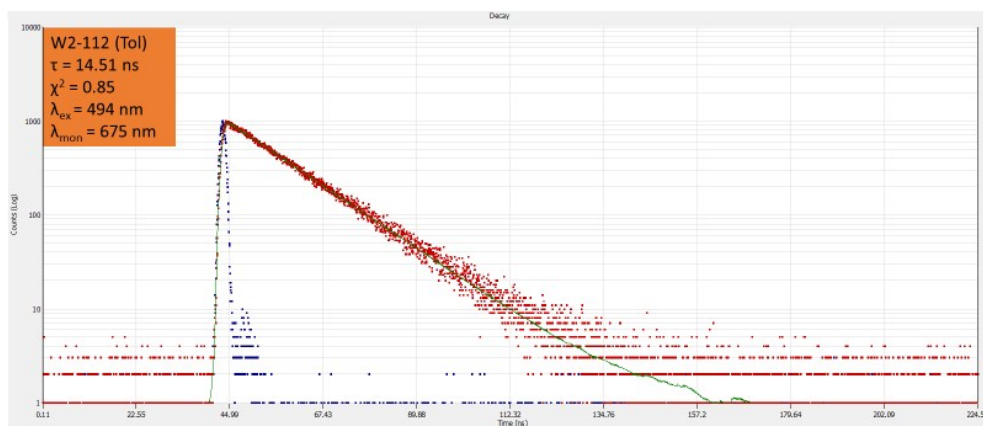
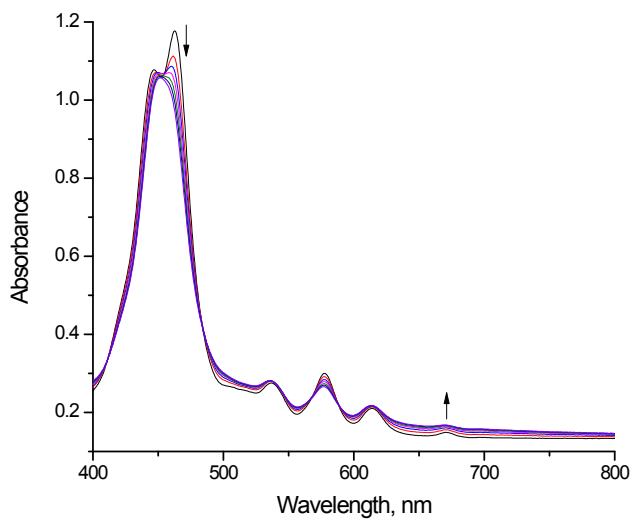


Figure S4. Spectroelectrochemistry in benzonitrile

(a) Spectroelectrochemistry of WJ3 – 1st Oxidation



(b) Spectroelectrochemistry of WJ3 – 1st Reduction

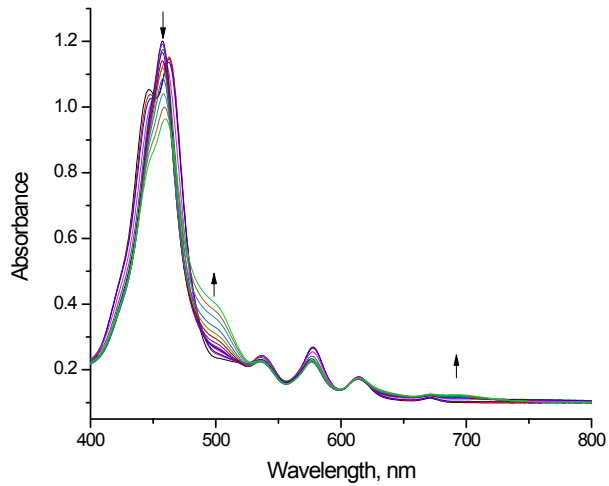
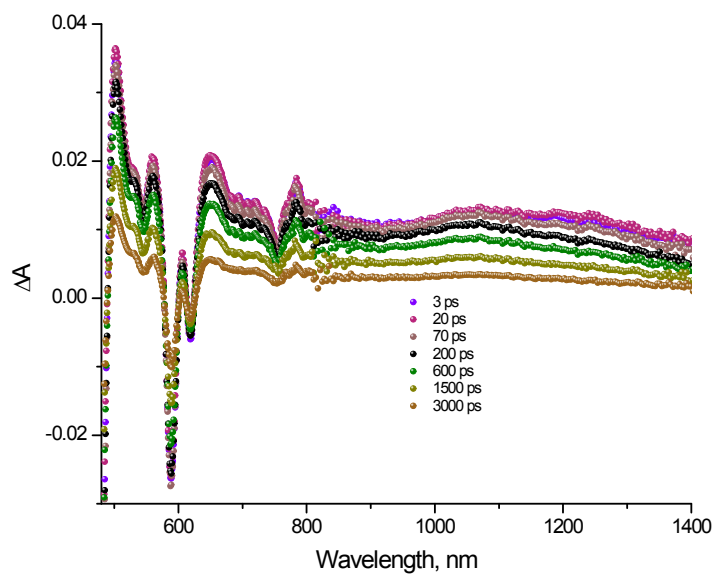
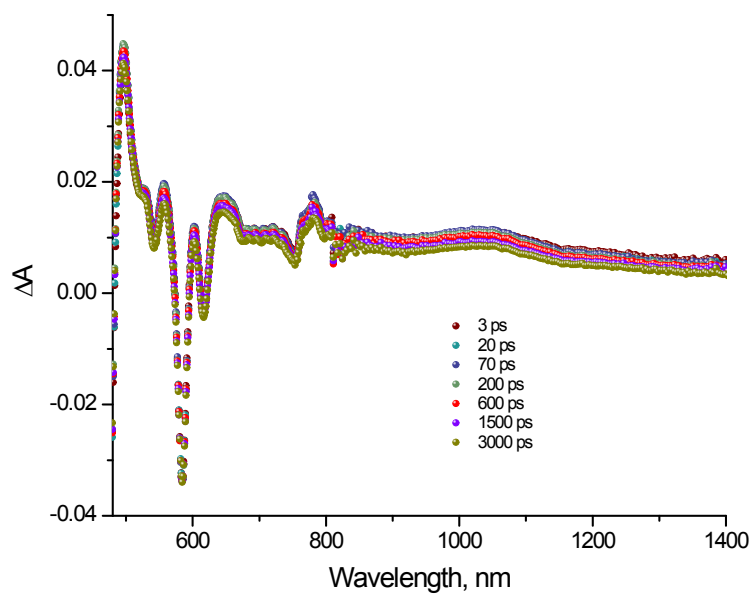


Figure S5. Femtosecond transient spectra

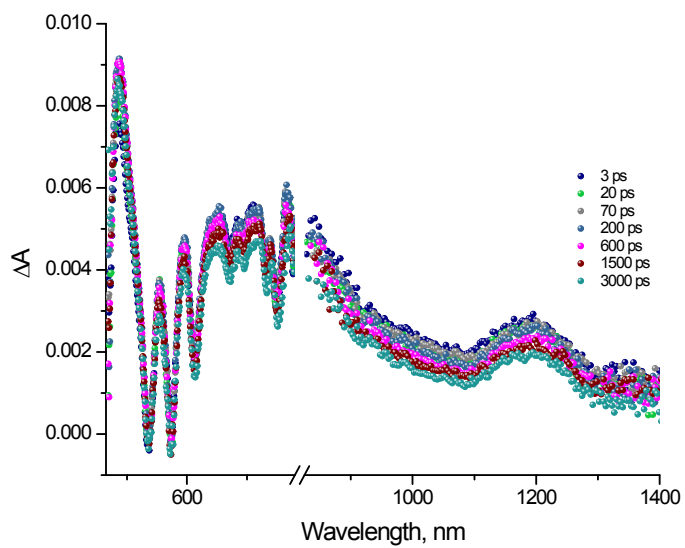
(a) Transient spectra of WJ1 in benzonitrile



(b) Transient spectra of WH1 in toluene



(c) Transient spectra in of WJ2 benzonitrile



(d) Transient spectra of WJ2 in toluene

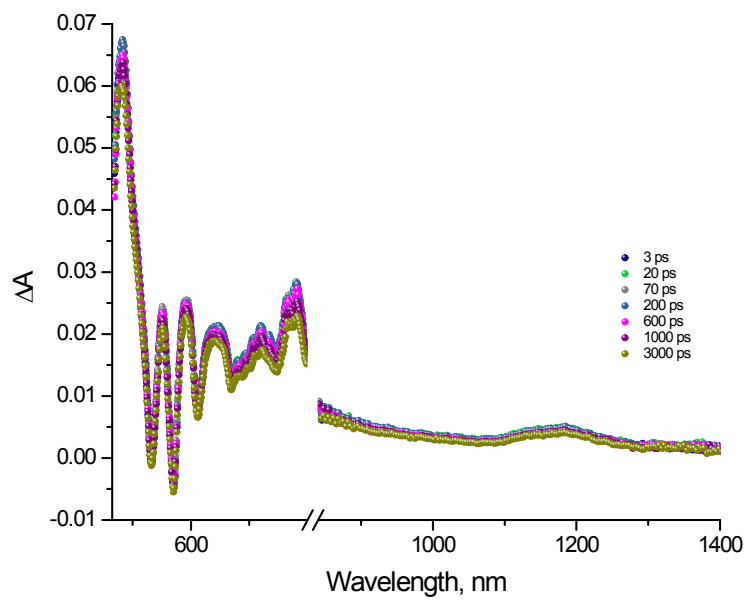
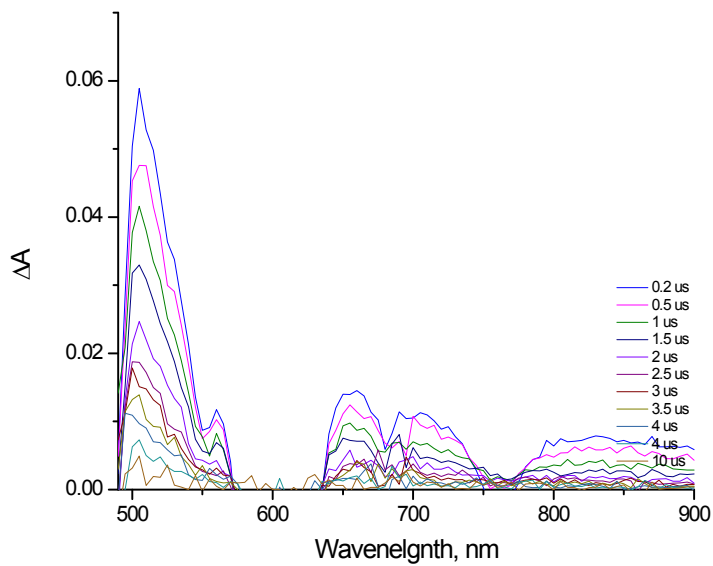
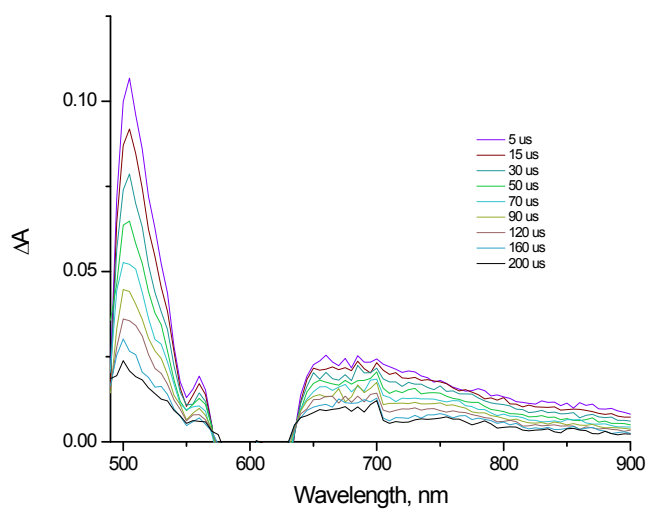


Figure S6. Nanosecond transient absorption spectra

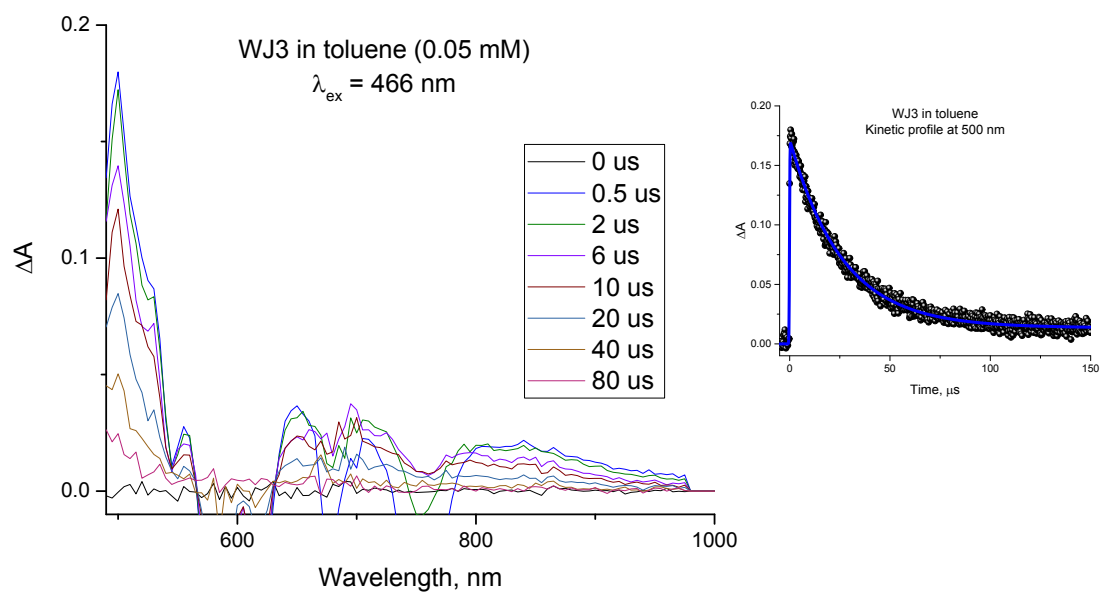
(a) Nanosecond transient spectra of WJ1 in benzonitrile



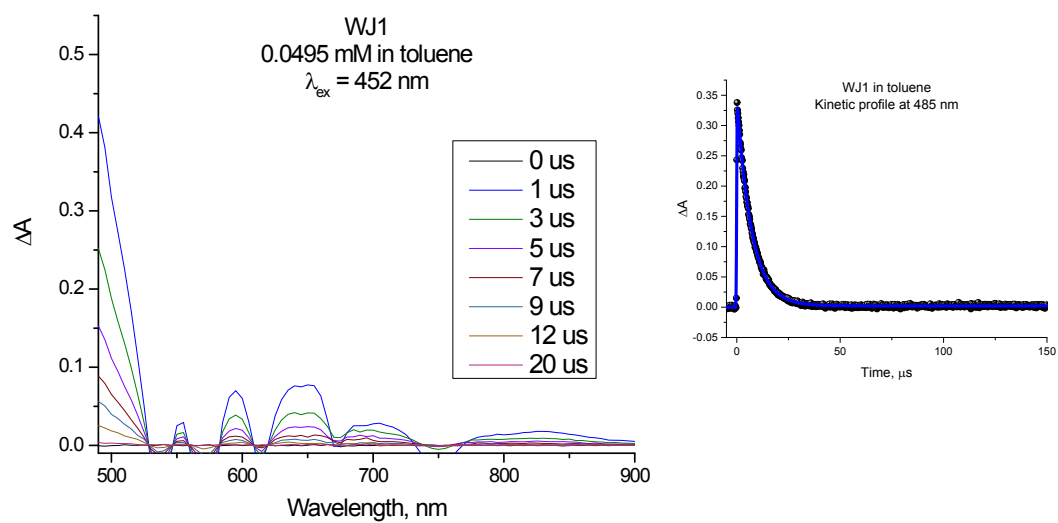
(b) Nanosecond transient spectra of WJ2 in benzonitrile



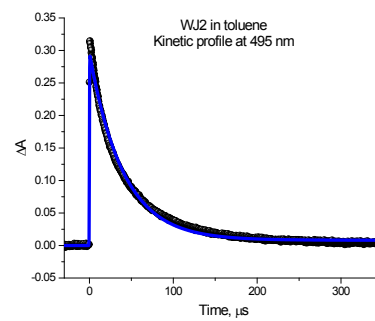
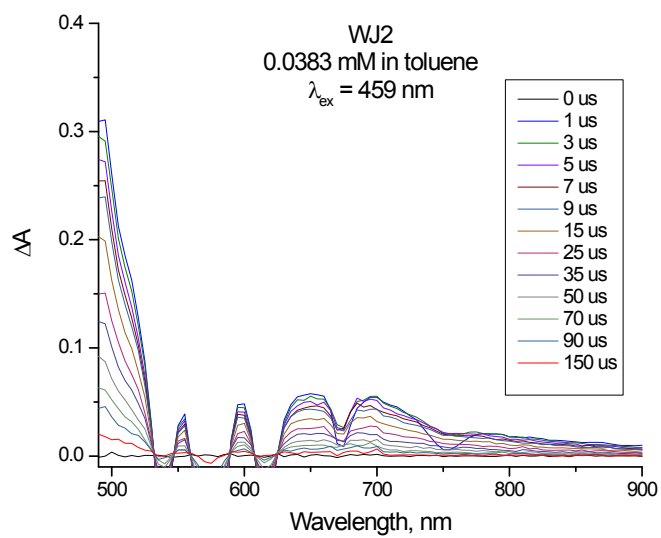
(c) Nanosecond transient spectra of WJ3 in toluene.



(d) Nanosecond transient spectra of WJ1 in toluene.



(e) Nanosecond transient spectra of WJ2 in toluene.



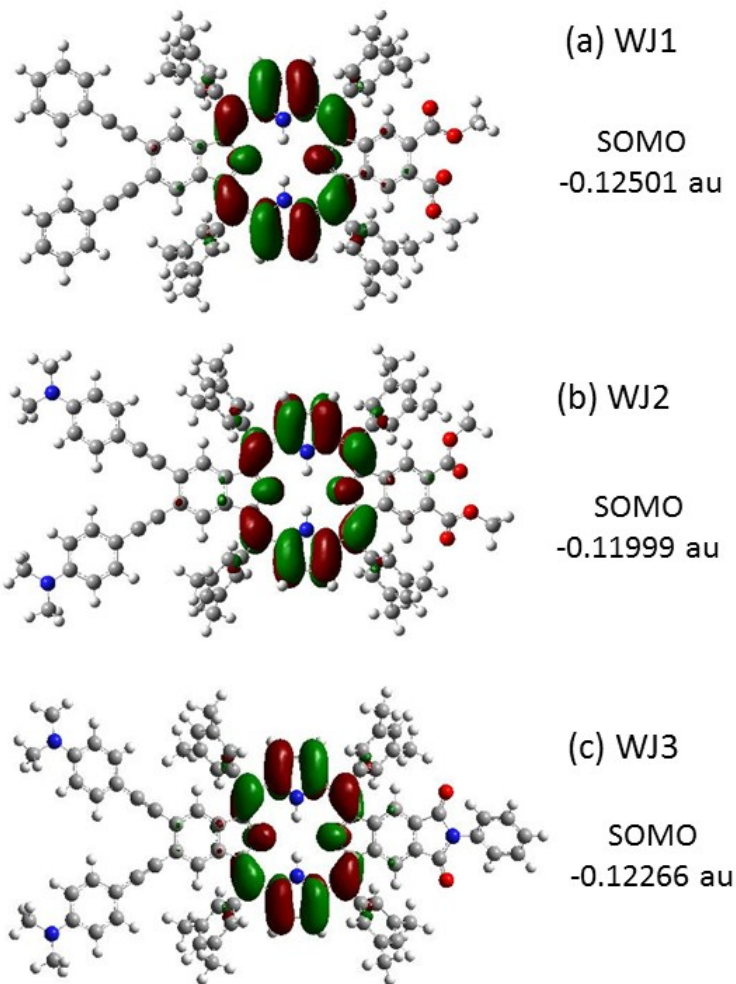


Figure S7. SOMO orbitals of the investigated compounds.

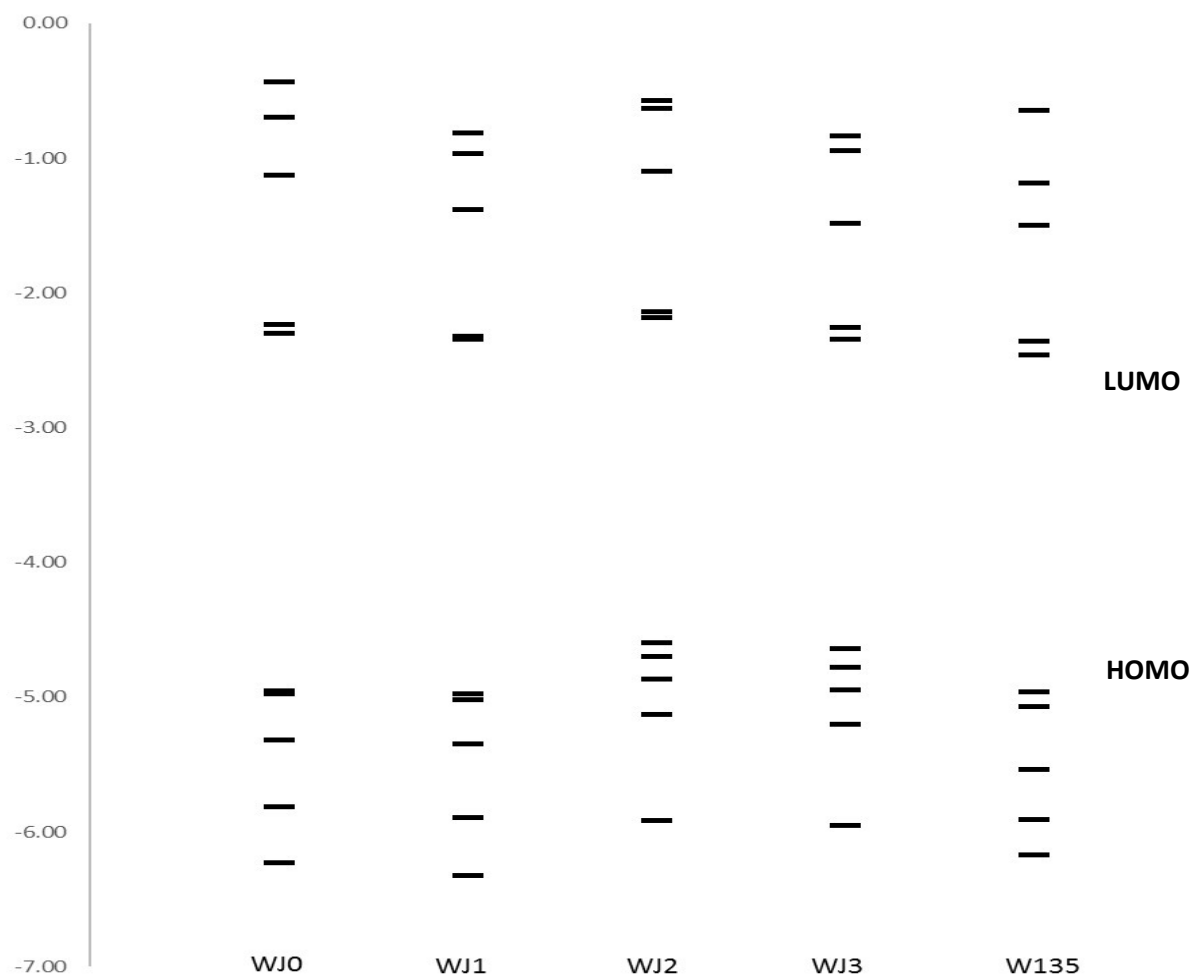
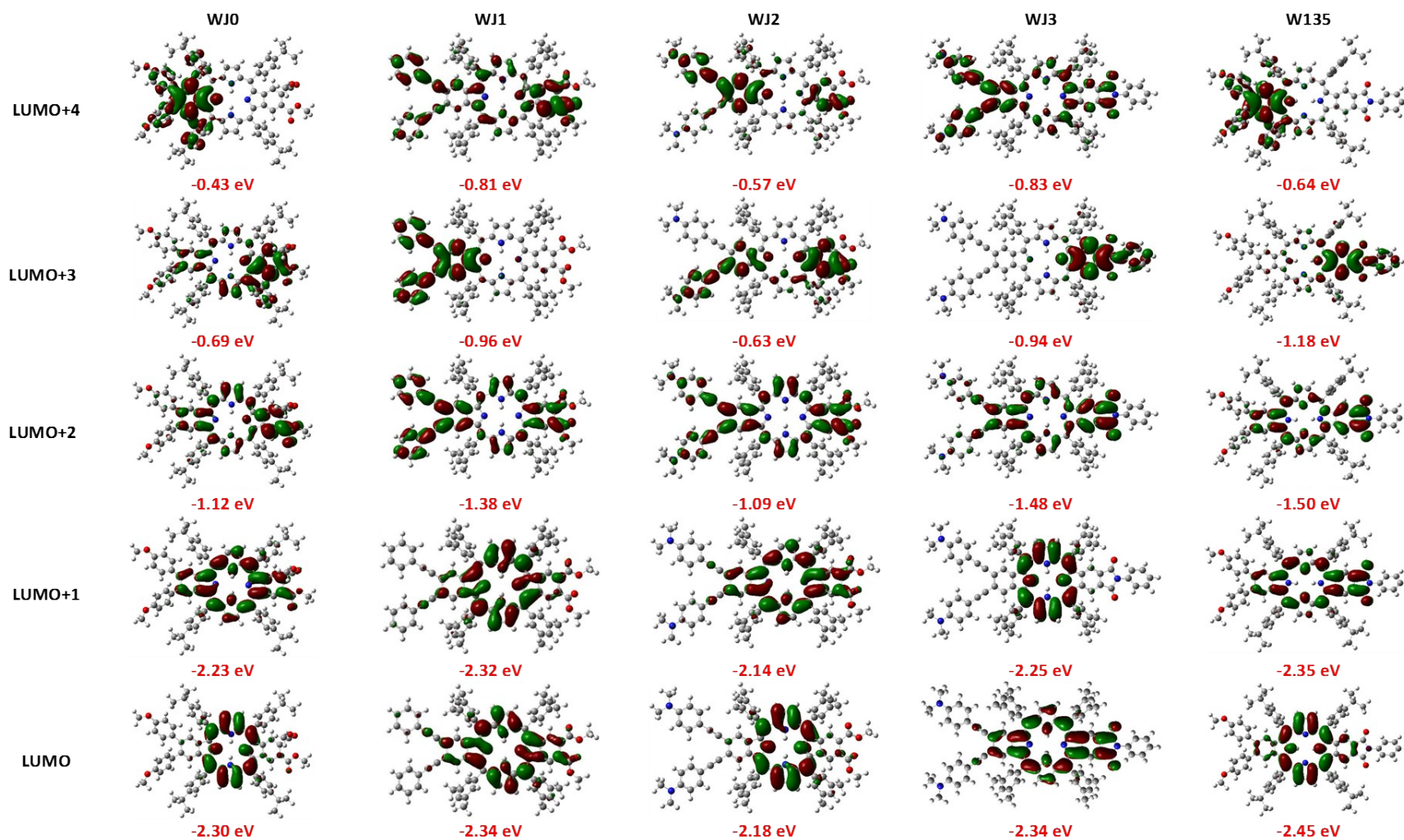


Figure S8. Calculated molecular orbital energy levels from (HOMO - 4 to LUMO + 4) of **WJ0**, **WJ1**, **WJ2**, **WJ3** and **W135** obtained by B3LYP/6-31G(d) level calculations



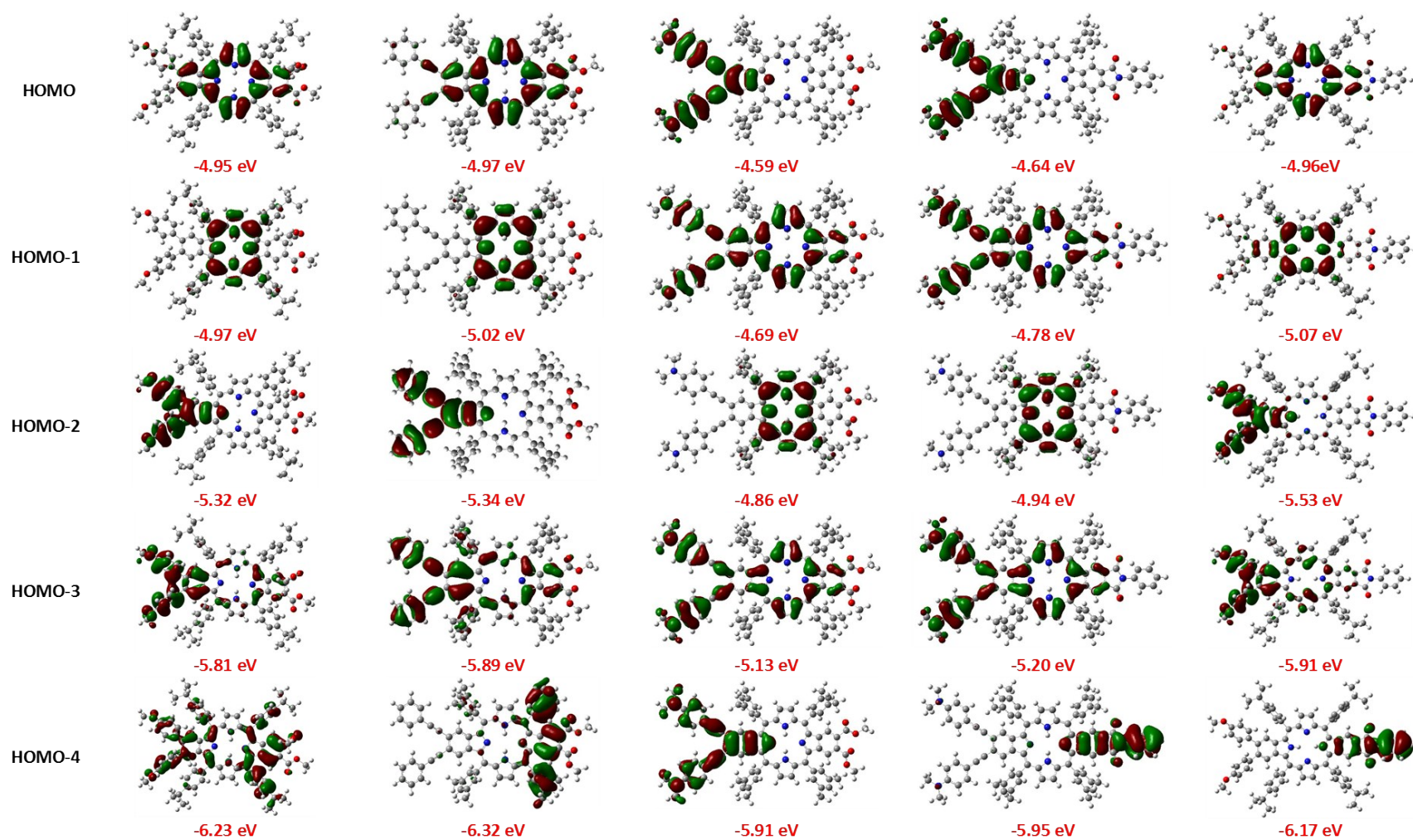


Figure S9. Orbital isodensity surface of **WJ0**, **WJ1**, **WJ2**, **WJ3**, and **W135** obtained by B3LYP/6-31G(d) level calculations

Table S2. Atom coordinates for optimized (*in vacuo*) structures WJ1 – WJ3Atom coordinates of the optimized structure of **WJ1**

	X	Y	Z
C	3.58977	0.70277	0.04531
C	3.58480	-0.71824	-0.01470
C	2.20286	-1.15718	0.10891
N	1.44970	-0.00778	0.19710
C	2.21058	1.13976	0.20273
C	-1.42524	4.19678	0.48611
C	-0.07624	4.18781	0.57840
C	0.33947	2.80185	0.38675
N	-0.74248	1.98380	0.21452
C	-1.82962	2.81494	0.24911
C	1.70676	2.43789	0.35272
C	-5.07452	-0.69724	-0.17482
C	-5.06059	0.72133	-0.25144
C	-3.69096	1.15960	-0.04244
N	-2.94657	0.00853	0.08469
C	-3.70695	-1.13811	0.04495
C	-3.18723	2.46278	0.07441
C	-0.09071	-4.20677	0.40361
C	-1.44250	-4.20028	0.42362
C	-1.84824	-2.80548	0.28387
N	-0.75734	-1.98135	0.20710
C	0.32481	-2.81473	0.26077
C	1.69166	-2.45878	0.17490
C	-3.20965	-2.44046	0.19418
C	2.69588	3.55892	0.50194
C	-4.16802	3.59990	0.03809
C	-4.20520	-3.56444	0.26698
C	2.67229	-3.59807	0.17593
C	3.33186	3.77030	1.73067
C	4.26408	4.80227	1.89631
C	4.52764	5.62181	0.78853
C	3.90343	5.44949	-0.45568
C	2.98087	4.40230	-0.57844
C	2.96729	-4.27491	-1.01302
C	3.88752	-5.33129	-1.03535
C	4.49057	-5.69175	0.17888
C	4.21059	-5.04677	1.39269
C	3.28840	-3.99289	1.36873
C	-4.56885	-4.26764	-0.88682
C	-5.51106	-5.30297	-0.83549
C	-6.05332	-5.62473	0.41733
C	-5.70077	-4.95554	1.59814
C	-4.76806	-3.91486	1.49926

C	-4.95379	3.89241	1.15871
C	-5.88090	4.94154	1.13868
C	-5.98066	5.69697	-0.03880
C	-5.20431	5.44244	-1.17845
C	-4.29370	4.37917	-1.11790
C	-6.28571	-1.39242	-0.33189
C	-7.45980	-0.69373	-0.58243
C	-7.43410	0.72052	-0.72174
C	-6.24627	1.41775	-0.54125
C	-8.71272	-1.50940	-0.61479
C	-8.61245	1.53417	-1.15172
O	-8.85923	2.65649	-0.75760
O	-9.33558	0.91047	-2.10824
O	-9.73289	-0.89209	0.02246
O	-8.79980	-2.62691	-1.08234
C	4.78596	-1.41634	-0.20018
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C	3.87717	7.84825	-1.23022
C	3.47683	6.04068	-2.91035
C	5.00111	5.05214	3.22603
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H	2.39196	6.11025	-2.77261
H	3.71357	5.02941	-3.25963
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H	5.19963	6.66983	4.68244
H	3.59919	6.58831	3.92027
H	6.89446	5.66586	2.27888
H	6.78574	3.93241	2.61201
H	7.06743	5.07857	3.93851
H	4.82760	3.01319	4.02798
H	3.52546	4.10194	4.54980
H	5.14511	4.25958	5.24062
H	-1.93274	0.00591	0.19897
H	0.43159	-0.00793	0.25855

Atom coordinates of the optimized structure of **WJ2**

	X	Y	Z
C	2.81142	0.70677	0.17997
C	2.80744	-0.71512	0.15825
C	1.42559	-1.15126	0.29310
N	0.66968	-0.00132	0.33880
C	1.43121	1.14595	0.32455
C	-2.21224	4.19764	0.57139
C	-0.86433	4.18984	0.68330
C	-0.44295	2.80755	0.47914
N	-1.52043	1.99041	0.28002
C	-2.60988	2.81931	0.30581

C	0.92566	2.44471	0.46004
C	-5.82565	-0.69448	-0.29312
C	-5.81340	0.72563	-0.34401
C	-4.45636	1.16398	-0.06752
N	-3.71489	0.01264	0.07454
C	-4.46979	-1.13530	-0.01240
C	-3.96112	2.46679	0.08942
C	-0.87913	-4.19174	0.61711
C	-2.22981	-4.18762	0.55112
C	-2.62612	-2.79927	0.34122
N	-1.53180	-1.97685	0.30030
C	-0.45471	-2.80591	0.44298
C	0.91518	-2.45045	0.40222
C	-3.97965	-2.43690	0.16648
C	1.91308	3.56533	0.61940
C	-4.94580	3.60009	0.04988
C	-4.97584	-3.56255	0.18531
C	1.89857	-3.58071	0.51617
C	2.56014	3.75654	1.84575
C	3.49219	4.78661	2.02128
C	3.74425	5.62646	0.92616
C	3.10930	5.47474	-0.31516
C	2.18722	4.42839	-0.44820
C	2.17215	-4.40016	-0.58533
C	3.08901	-5.45546	-0.49285
C	3.71686	-5.66326	0.74401
C	3.46471	-4.86846	1.87208
C	2.54049	-3.82543	1.73567
C	-5.27294	-4.26625	-0.98714
C	-6.21622	-5.30199	-0.98978
C	-6.82697	-5.62592	0.23053
C	-6.54157	-4.95709	1.42949
C	-5.60742	-3.91418	1.38358
C	-5.77925	3.85018	1.14615
C	-6.71091	4.89509	1.12422
C	-6.76680	5.69048	-0.02948
C	-5.94335	5.47849	-1.14453
C	-5.02930	4.41833	-1.08300
C	-7.02475	-1.39042	-0.52339
C	-8.18858	-0.69115	-0.81628
C	-8.16266	0.72617	-0.92485
C	-6.98749	1.42343	-0.67556
C	-9.43423	-1.51049	-0.92477
C	-9.32339	1.54421	-1.39160
O	-9.59630	2.65553	-0.98347
O	-9.99659	0.94030	-2.39667
O	-10.48819	-0.90834	-0.32829
O	-9.49390	-2.62021	-1.41496

C	4.00633	-1.41669	-0.02260
C	5.21389	-0.72555	-0.16280
C	5.21996	0.71156	-0.12745
C	4.01614	1.40585	0.02977
C	6.43702	1.43350	-0.24670
C	7.47495	2.06532	-0.33041
C	8.69563	2.78514	-0.42791
C	9.93927	2.13395	-0.30256
C	8.71322	4.17705	-0.64616
C	9.90390	4.88115	-0.74422
C	11.13499	2.82978	-0.39742
C	11.15398	4.22584	-0.63328
C	6.41880	-1.45148	-0.35768
C	7.43873	-2.09176	-0.53989
C	8.63565	-2.82342	-0.76314
C	8.70186	-4.21201	-0.53380
C	9.80243	-2.18932	-1.23517
C	10.97266	-2.89836	-1.46067
C	9.86784	-4.92934	-0.75528
C	11.04421	-4.29140	-1.21745
C	-11.72308	-1.63684	-0.38975
C	-11.12555	1.66940	-2.90026
N	12.34650	4.92046	-0.75748
N	12.21829	-5.00001	-1.41832
C	13.60239	4.25101	-0.46627
C	12.32920	6.37069	-0.83930
C	12.20464	-6.45038	-1.33419
C	13.34899	-4.34906	-2.05714
C	-6.07532	6.39213	-2.37849
C	-5.09821	6.00130	-3.50339
C	-5.77830	7.85506	-1.97167
C	-7.51515	6.29773	-2.93700
C	-7.66882	5.17860	2.29655
C	-7.38597	6.58926	2.86477
C	-9.12977	5.10786	1.78964
C	-7.50924	4.15886	3.44057
C	3.42024	-6.37553	-1.68396
C	4.93581	-6.30397	-1.98833
C	3.03676	-7.83202	-1.32975
C	2.65835	-5.97692	-2.96253
C	4.20258	-5.15891	3.19316
C	3.82324	-4.16369	4.30615
C	5.72961	-5.05988	2.96086
C	3.84774	-6.58364	3.68030
C	-6.61127	-6.06443	-2.26858
C	-5.87649	-5.53505	-3.51480
C	-6.26541	-7.56352	-2.10569
C	-8.13300	-5.90665	-2.50434

C	-7.25555	-5.37845	2.72859
C	-6.82081	-4.53046	3.93912
C	-8.78430	-5.21570	2.55295
C	-6.93035	-6.85916	3.03819
C	3.44002	6.44150	-1.46892
C	4.95147	6.36402	-1.79239
C	3.07996	7.88662	-1.04959
C	2.66022	6.10785	-2.75525
C	4.24397	5.01098	3.34718
C	3.92875	6.42525	3.88901
C	5.76619	4.88173	3.09891
C	3.84555	3.98555	4.42554
H	-2.88097	5.04012	0.66717
H	-0.21127	5.02537	0.88705
H	-0.22523	-5.03793	0.76691
H	-2.90114	-5.02958	0.63337
H	2.32940	3.07552	2.65680
H	4.46430	6.43062	1.04512
H	1.67140	4.26086	-1.38643
H	1.66095	-4.19181	-1.51797
H	4.43038	-6.47706	0.83251
H	2.31088	-3.17736	2.57360
H	-4.77023	-3.97424	-1.90197
H	-7.56008	-6.42681	0.24556
H	-5.35742	-3.35539	2.27821
H	-5.69697	3.20237	2.01122
H	-7.48727	6.50208	-0.06311
H	-4.37128	4.20456	-1.91736
H	-7.07743	-2.46724	-0.46897
H	-6.99928	2.49859	-0.77602
H	4.02737	-2.49474	-0.07375
H	4.04689	2.48487	0.02782
H	9.95687	1.06414	-0.11565
H	7.77023	4.70810	-0.73817
H	9.85986	5.95118	-0.90778
H	12.06257	2.28146	-0.28503
H	7.81592	-4.72969	-0.17769
H	9.77645	-1.12276	-1.43882
H	11.83720	-2.36279	-1.83435
H	9.86143	-5.99650	-0.56855
H	-12.45027	-1.02400	0.14397
H	-11.61728	-2.61365	0.08950
H	-12.03093	-1.78350	-1.42885
H	-11.54373	1.04838	-3.69311
H	-10.81107	2.63864	-3.29619
H	-11.86176	1.83263	-2.10825
H	13.75612	3.39164	-1.13083
H	13.66104	3.89112	0.57303

H	14.42594	4.94778	-0.63280
H	13.35129	6.73435	-0.96036
H	11.90043	6.84286	0.05879
H	11.75189	6.71005	-1.70822
H	11.89215	-6.78569	-0.33753
H	13.21411	-6.82801	-1.50717
H	11.53277	-6.91283	-2.07441
H	13.68492	-3.48161	-1.47575
H	13.12113	-4.00578	-3.07868
H	14.18245	-5.05191	-2.11113
H	-5.27644	4.98155	-3.86290
H	-4.05351	6.07148	-3.18006
H	-5.22696	6.67871	-4.35525
H	-4.75828	7.95432	-1.58288
H	-6.46668	8.21153	-1.19834
H	-5.87786	8.51995	-2.83859
H	-7.75571	5.26898	-3.22788
H	-7.62336	6.93794	-3.82141
H	-8.26090	6.61571	-2.20124
H	-6.36334	6.65917	3.25366
H	-8.07786	6.81635	3.68531
H	-7.50718	7.36615	2.10229
H	-9.34218	5.88931	1.05221
H	-9.82666	5.24525	2.62594
H	-9.33746	4.14409	1.31349
H	-6.49989	4.17518	3.86748
H	-7.72504	3.13753	3.10730
H	-8.21130	4.39894	4.24711
H	5.23923	-5.28096	-2.23757
H	5.18419	-6.94993	-2.83947
H	5.53962	-6.63321	-1.13588
H	3.57572	-8.19247	-0.44712
H	3.27483	-8.50352	-2.16398
H	1.96367	-7.91535	-1.12274
H	2.90490	-4.95864	-3.28345
H	1.57260	-6.04039	-2.82860
H	2.93004	-6.65566	-3.77895
H	2.75436	-4.20542	4.54451
H	4.07362	-3.13241	4.03355
H	4.37498	-4.40700	5.22125
H	6.00790	-4.06646	2.59163
H	6.07918	-5.79735	2.23021
H	6.27041	-5.24022	3.89804
H	2.77122	-6.67805	3.86346
H	4.37257	-6.80914	4.61695
H	4.13010	-7.34753	2.94804
H	-6.10727	-4.48099	-3.70540
H	-6.18993	-6.10632	-4.39593

H	-4.78895	-5.63804	-3.42527
H	-5.18870	-7.70556	-1.95578
H	-6.55969	-8.12193	-3.00292
H	-6.78380	-8.01064	-1.25076
H	-8.41708	-4.85092	-2.56403
H	-8.71751	-6.35877	-1.69589
H	-8.42393	-6.40181	-3.43929
H	-5.74676	-4.62034	4.13678
H	-7.35130	-4.87006	4.83600
H	-7.05524	-3.46918	3.79915
H	-9.04435	-4.17279	2.33888
H	-9.30711	-5.51699	3.46920
H	-9.16904	-5.82911	1.73173
H	-5.85285	-7.00219	3.17905
H	-7.25263	-7.52578	2.23142
H	-7.43843	-7.17748	3.95690
H	5.23552	5.34929	-2.09401
H	5.56773	6.64333	-0.93091
H	5.20104	7.04600	-2.61463
H	3.63238	8.20294	-0.15854
H	2.01022	7.97532	-0.82806
H	3.31873	8.58903	-1.85773
H	2.89278	5.10256	-3.12385
H	2.92953	6.81956	-3.54395
H	1.57684	6.17546	-2.60544
H	2.85636	6.54010	4.08474
H	4.22512	7.20862	3.18338
H	4.46634	6.60277	4.82871
H	6.12929	5.63420	2.39083
H	6.01693	3.89561	2.69242
H	6.31794	5.01534	4.03760
H	2.77833	4.04206	4.66849
H	4.40490	4.18427	5.34678
H	4.07284	2.95941	4.11601
H	-2.70691	0.01056	0.23212
H	-0.34854	-0.00054	0.39110

Atom coordinates of the optimized structure of **WJ3**

	X	Y	Z
C	3.10041	0.71774	0.19524
C	3.10064	-0.70390	0.21093
C	1.72346	-1.14020	0.39089
N	0.96495	0.00844	0.42293
C	1.72281	1.15686	0.36720
C	-1.92549	4.18982	0.72467
C	-0.57482	4.18933	0.79256
C	-0.15233	2.81036	0.56621
N	-1.22940	1.98849	0.39537

C	-2.32341	2.81146	0.45763
C	1.21780	2.45491	0.50302
C	-5.51141	-0.71570	-0.23422
C	-5.51357	0.71582	-0.23331
C	-4.16326	1.15126	0.07062
N	-3.41525	0.00289	0.19545
C	-4.16041	-1.14745	0.07155
C	-3.67419	2.45527	0.25806
C	-0.57100	-4.17179	0.84325
C	-1.92081	-4.17644	0.76036
C	-2.31920	-2.80157	0.47658
N	-1.22662	-1.97680	0.41612
C	-0.14938	-2.79429	0.60609
C	1.22022	-2.43653	0.54881
C	-3.66932	-2.44966	0.26555
C	2.20465	3.58135	0.61692
C	-4.66924	3.58007	0.25645
C	-4.66147	-3.57707	0.26314
C	2.20926	-3.55703	0.69803
C	2.89379	3.78809	1.81767
C	3.82888	4.82207	1.94833
C	4.04148	5.64849	0.83485
C	3.36340	5.48143	-0.38139
C	2.43840	4.43300	-0.46936
C	2.45997	-4.43244	-0.36537
C	3.38587	-5.47655	-0.24075
C	4.04492	-5.61604	0.98947
C	3.81569	-4.76456	2.08052
C	2.88273	-3.73419	1.91225
C	-4.77035	-4.41440	-0.85342
C	-5.70772	-5.45525	-0.88996
C	-6.52790	-5.62839	0.23428
C	-6.44364	-4.81587	1.37448
C	-5.48874	-3.79166	1.37187
C	-5.49401	3.79447	1.36709
C	-6.45191	4.81591	1.37056
C	-6.54166	5.62600	0.22903
C	-5.72411	5.45308	-0.89715
C	-4.78376	4.41494	-0.86146
C	4.29554	-1.40711	0.01409
C	5.49624	-0.71633	-0.18013
C	5.49834	0.72120	-0.18303
C	4.29699	1.41638	-0.00826
C	6.70835	1.44308	-0.35866
C	7.74024	2.07649	-0.49132
C	8.95338	2.79889	-0.64555
C	10.20401	2.15810	-0.53697
C	8.95620	4.18384	-0.90517

C	10.13916	4.89105	-1.05759
C	11.39224	2.85712	-0.68608
C	11.39598	4.24599	-0.96218
C	6.69694	-1.44396	-0.39242
C	7.71237	-2.08700	-0.58975
C	8.90250	-2.82360	-0.83136
C	8.97361	-4.20790	-0.57825
C	10.05662	-2.19977	-1.34636
C	11.21946	-2.91448	-1.59076
C	10.13227	-4.93088	-0.81829
C	11.29604	-4.30322	-1.32471
N	12.57988	4.94338	-1.13792
N	12.46248	-5.01721	-1.54600
C	13.84811	4.28795	-0.86898
C	12.55114	6.39050	-1.26157
C	12.45179	-6.46531	-1.42876
C	13.57926	-4.37816	-2.22037
C	-5.89337	6.38153	-2.11542
C	-4.91666	6.03592	-3.25529
C	-5.63310	7.84558	-1.68773
C	-7.33558	6.25505	-2.66156
C	-7.40670	5.05715	2.55536
C	-7.16985	6.47384	3.12988
C	-8.86985	4.93862	2.06366
C	-7.19901	4.03760	3.69154
C	3.69711	-6.45276	-1.39193
C	5.20345	-6.37936	-1.73912
C	3.34181	-7.89407	-0.95559
C	2.89749	-6.12790	-2.66828
C	4.59083	-4.97807	3.39474
C	4.21756	-3.93915	4.46918
C	6.10902	-4.85926	3.11828
C	4.27921	-6.38508	3.95736
C	-5.87098	-6.38641	-2.10694
C	-4.89368	-6.03848	-3.24558
C	-5.60500	-7.84851	-1.67603
C	-7.31272	-6.26710	-2.65591
C	-7.40152	-5.05694	2.55681
C	-7.19840	-4.03593	3.69252
C	-8.86319	-4.94023	2.06018
C	-7.16548	-6.47275	3.13374
C	3.65469	6.43341	-1.55787
C	5.15367	6.34668	-1.93330
C	3.31436	7.88471	-1.14333
C	2.82854	6.08754	-2.81160
C	4.62580	5.06463	3.24440
C	4.32342	6.48389	3.78069
C	6.13908	4.93878	2.94494

C	4.27040	4.05032	4.34792
C	-6.69193	1.43831	-0.52846
C	-6.68721	-1.44168	-0.53083
C	-7.82550	0.69914	-0.78430
C	-7.82334	-0.70589	-0.78496
C	-9.19937	1.16869	-1.09008
C	-9.19594	-1.17958	-1.09045
N	-9.97988	-0.00673	-1.27050
O	-9.60854	2.31009	-1.16783
O	-9.60135	-2.32253	-1.16677
C	-11.37353	-0.00704	-1.57326
C	-11.89207	0.92970	-2.47600
C	-13.25623	0.92999	-2.76268
C	-14.10599	-0.00428	-2.16876
C	-13.58206	-0.94000	-1.27571
C	-12.22225	-0.94267	-0.96868
H	-0.05183	0.00924	0.49553
H	-2.59584	5.02766	0.84675
H	0.08023	5.02700	0.98076
H	-2.40938	0.00397	0.36561
H	0.08395	-5.00596	1.04672
H	-2.59050	-5.01468	0.88341
H	2.69430	3.11595	2.64419
H	4.76545	6.45351	0.91823
H	1.89062	4.25429	-1.38722
H	1.92504	-4.27514	-1.29466
H	4.76597	-6.42017	1.10231
H	2.67024	-3.04340	2.71996
H	-4.11706	-4.22822	-1.69794
H	-7.26784	-6.42274	0.21888
H	-5.38650	-3.13051	2.22465
H	-5.38756	3.13529	2.22088
H	-7.28392	6.41818	0.21438
H	-4.13236	4.22900	-1.70748
H	4.31847	-2.48625	-0.00954
H	4.32291	2.49516	-0.04047
H	10.23337	1.09438	-0.31928
H	8.00777	4.70689	-0.98641
H	10.08396	5.95542	-1.25185
H	12.32602	2.31735	-0.58421
H	8.09731	-4.71759	-0.18837
H	10.02625	-1.13704	-1.56861
H	12.07416	-2.38718	-1.99736
H	10.13016	-5.99437	-0.61156
H	14.66197	4.98508	-1.07652
H	13.98730	3.41372	-1.51720
H	13.93980	3.95357	0.17634
H	11.95261	6.70152	-2.12681

H	13.56785	6.75678	-1.41533
H	12.13912	6.88530	-0.36797
H	13.45466	-6.84761	-1.62763
H	11.75528	-6.94308	-2.13554
H	12.17296	-6.77841	-0.41492
H	13.93194	-3.50423	-1.65881
H	13.32712	-4.04751	-3.24027
H	14.40896	-5.08438	-2.28597
H	-5.07165	6.72409	-4.09392
H	-5.07153	5.01830	-3.63121
H	-3.87103	6.12886	-2.94056
H	-5.75898	8.52023	-2.54346
H	-4.61274	7.96760	-1.30631
H	-6.32438	8.17130	-0.90346
H	-7.46863	6.90279	-3.53688
H	-8.08250	6.54576	-1.91576
H	-7.55329	5.22424	-2.96255
H	-7.33437	7.25139	2.37639
H	-6.14431	6.58021	3.50212
H	-7.85588	6.66715	3.96371
H	-9.11300	5.70182	1.31722
H	-9.56364	5.06433	2.90400
H	-9.05726	3.96140	1.60509
H	-7.38286	3.01070	3.35584
H	-7.89967	4.24842	4.50728
H	-6.18585	4.08672	4.10658
H	5.43854	-7.06525	-2.56231
H	5.83303	-6.65697	-0.88686
H	5.48685	-5.36700	-2.04828
H	3.56826	-8.60294	-1.76158
H	2.27536	-7.98037	-0.71766
H	3.90716	-8.20393	-0.07036
H	3.15430	-6.84545	-3.45578
H	3.12501	-5.12549	-3.04773
H	1.81645	-6.19390	-2.50155
H	4.44425	-2.91750	4.14462
H	4.79256	-4.13104	5.38216
H	3.15476	-3.98755	4.73222
H	6.45514	-5.62185	2.41221
H	6.67695	-4.98609	4.04819
H	6.35685	-3.87821	2.69776
H	4.55846	-7.17722	3.25450
H	3.21020	-6.49253	4.17432
H	4.83357	-6.55533	4.88859
H	-5.04464	-6.72835	-4.08353
H	-3.84818	-6.12693	-2.92905
H	-5.05204	-5.02200	-3.62312
H	-5.72641	-8.52527	-2.53072

H	-6.29633	-8.17579	-0.89241
H	-4.58481	-7.96539	-1.29253
H	-7.44112	-6.91652	-3.53064
H	-7.53499	-5.23784	-2.95865
H	-8.05977	-6.56056	-1.91128
H	-7.38269	-3.00957	3.35541
H	-6.18622	-4.08317	4.11009
H	-7.90074	-4.24698	4.50679
H	-9.10335	-5.70497	1.31438
H	-9.04854	-3.96393	1.59863
H	-9.55974	-5.06429	2.89855
H	-7.32660	-7.25137	2.38066
H	-7.85404	-6.66577	3.96557
H	-6.14111	-6.57758	3.50954
H	5.37722	7.02038	-2.76967
H	5.42288	5.32810	-2.23564
H	5.80036	6.63035	-1.09590
H	3.52606	8.57637	-1.96808
H	3.89943	8.21006	-0.27674
H	2.25357	7.97992	-0.88460
H	3.07149	6.78939	-3.61747
H	1.75141	6.16048	-2.62398
H	3.04475	5.07741	-3.17694
H	4.59389	7.26042	3.05728
H	4.89121	6.67341	4.70000
H	3.25771	6.59760	4.01052
H	6.47430	5.68402	2.21577
H	6.38027	3.94875	2.54222
H	6.72225	5.08644	3.86229
H	4.49208	3.02160	4.04283
H	3.21213	4.10480	4.62777
H	4.86066	4.26247	5.24656
H	-6.72493	2.51716	-0.56258
H	-6.71667	-2.52060	-0.56609
H	-11.23489	1.65700	-2.93568
H	-13.65251	1.66345	-3.45964
H	-15.16761	-0.00331	-2.40016
H	-14.23372	-1.67268	-0.80742
H	-11.81717	-1.67143	-0.27826