Supporting Information

Controlling charge-transfer properties through a microwave-assisted mono- or bis-annulation of dialkynyl-*N*-(het)arylpyrroles

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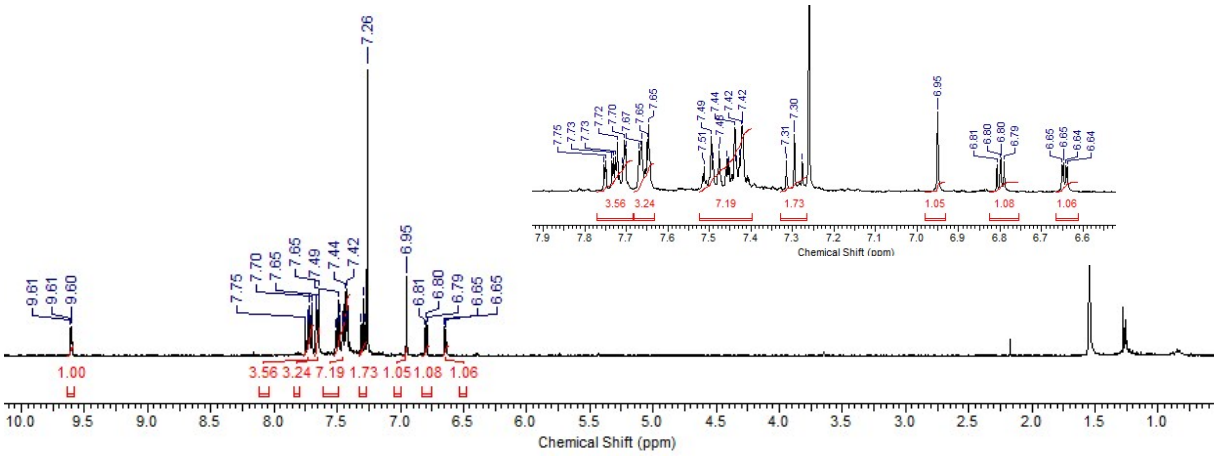
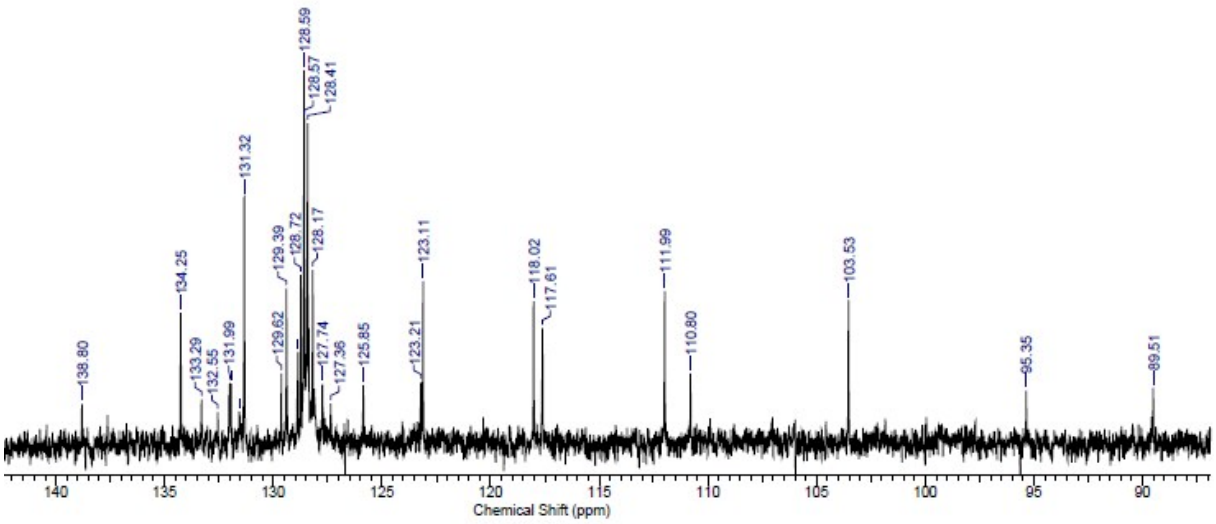
Contents:

1. ^{1}H and ^{13}C RMN spectra



^{1}H NMR of compound **5a**



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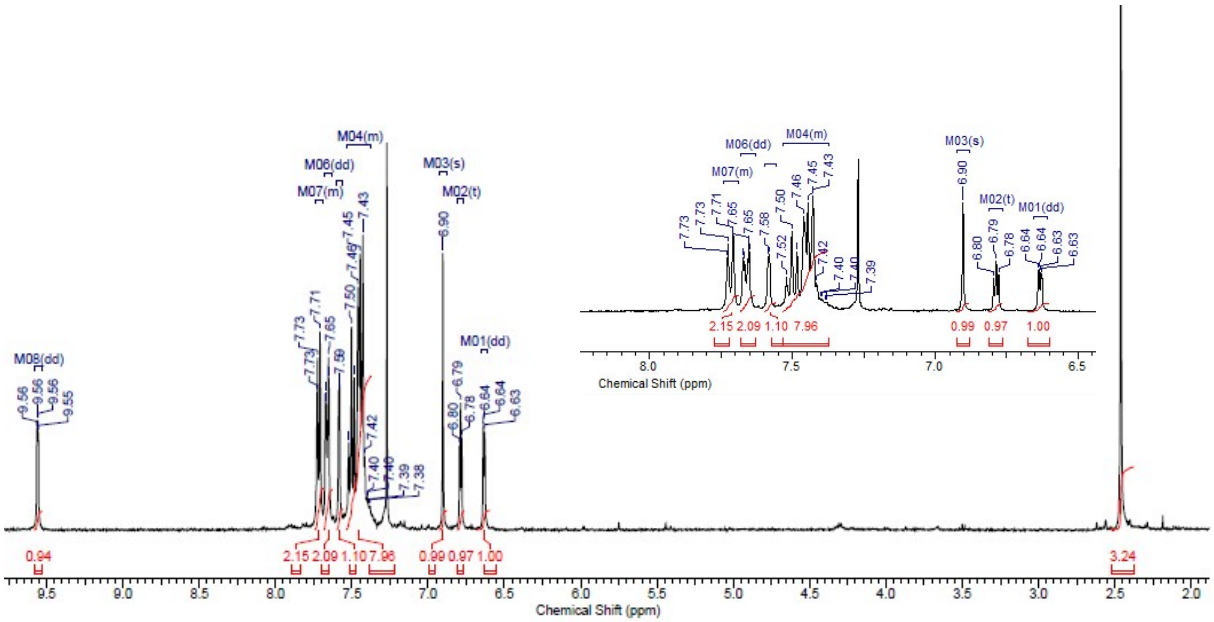

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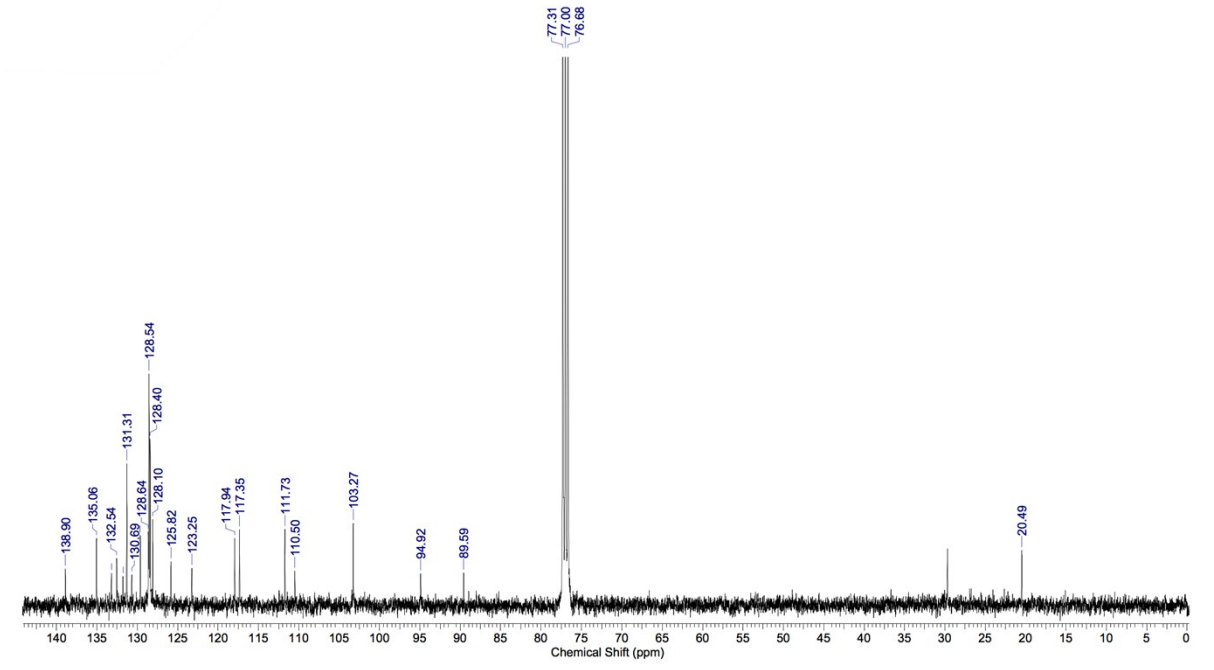

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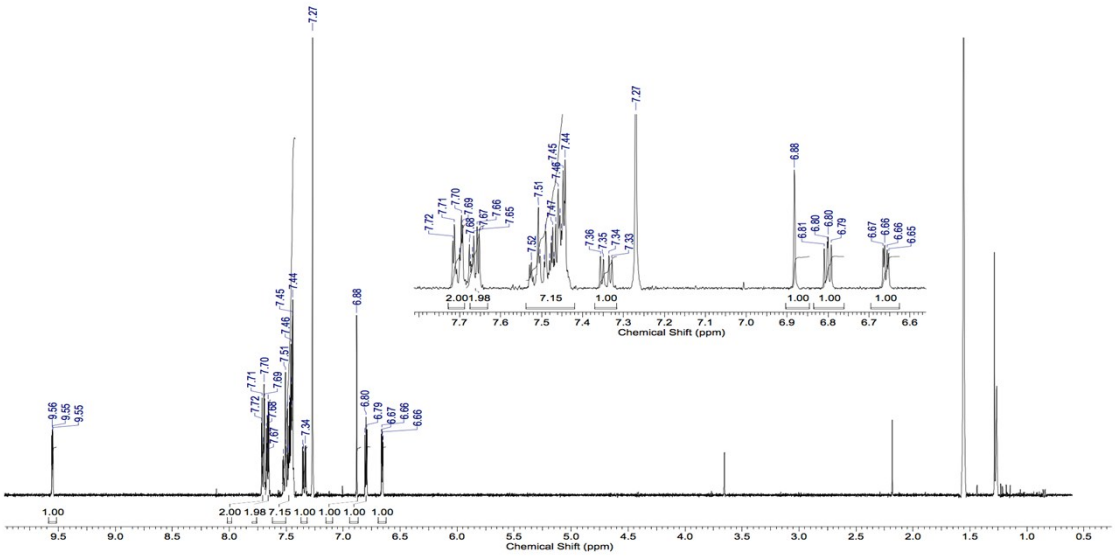

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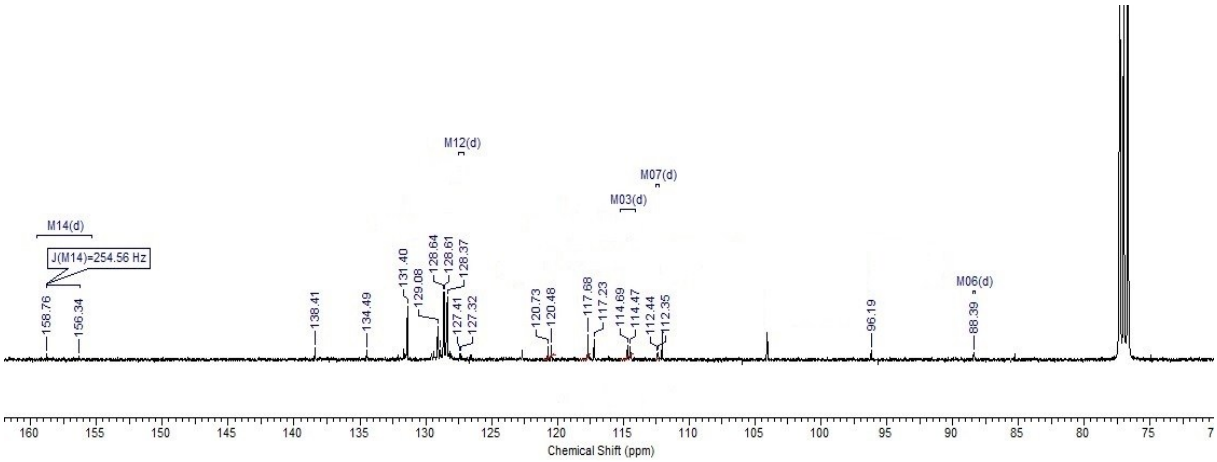

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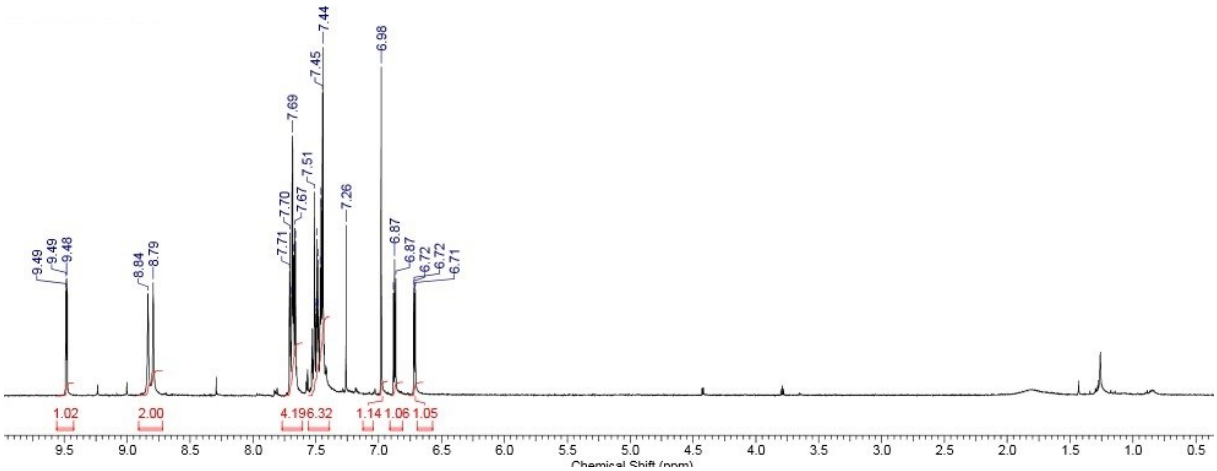

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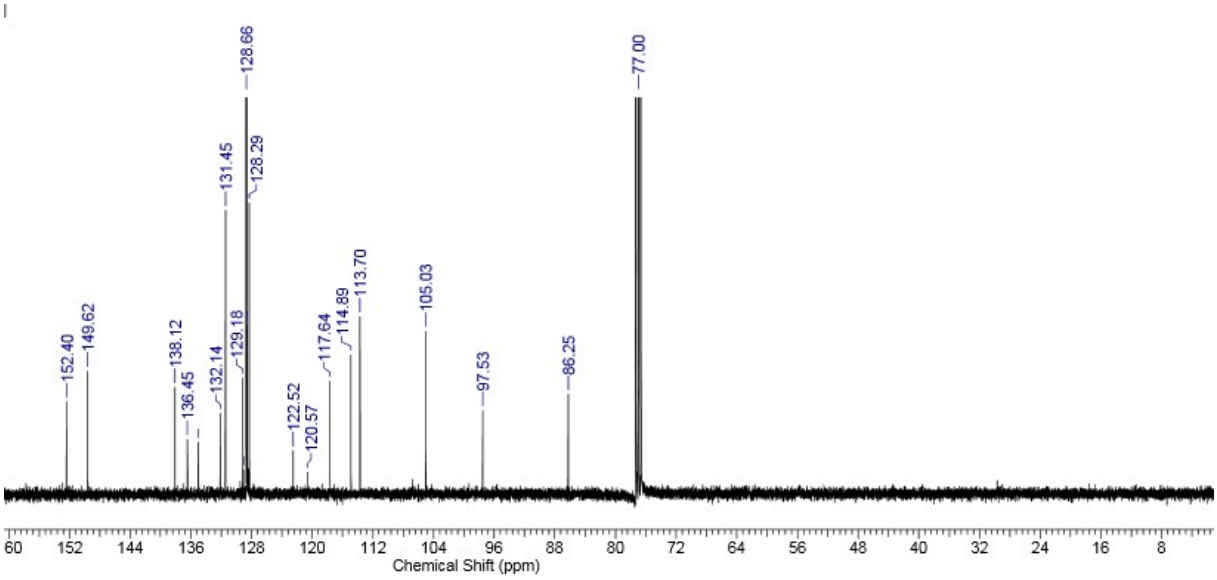

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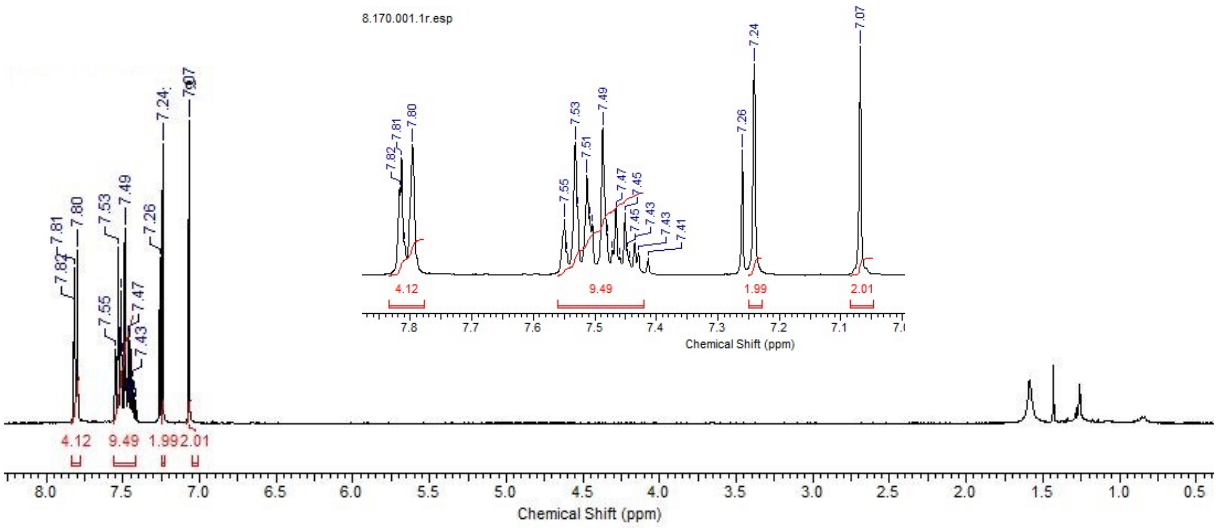

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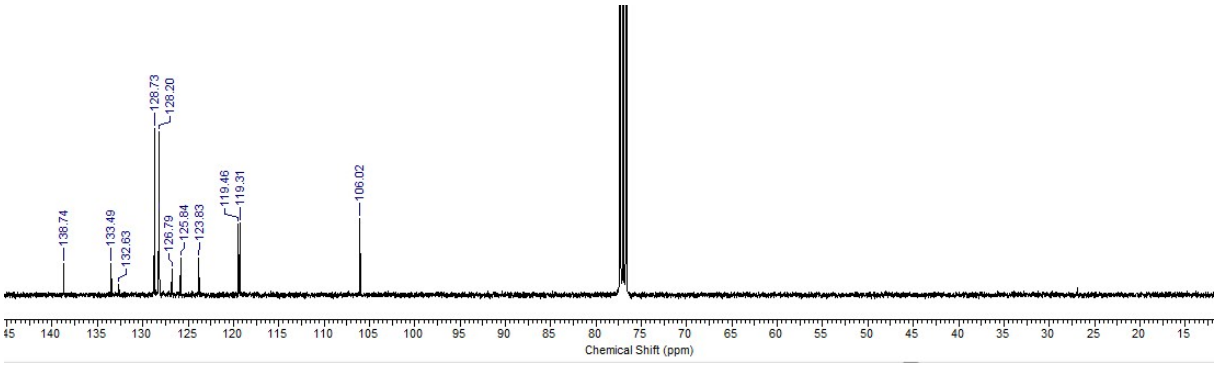
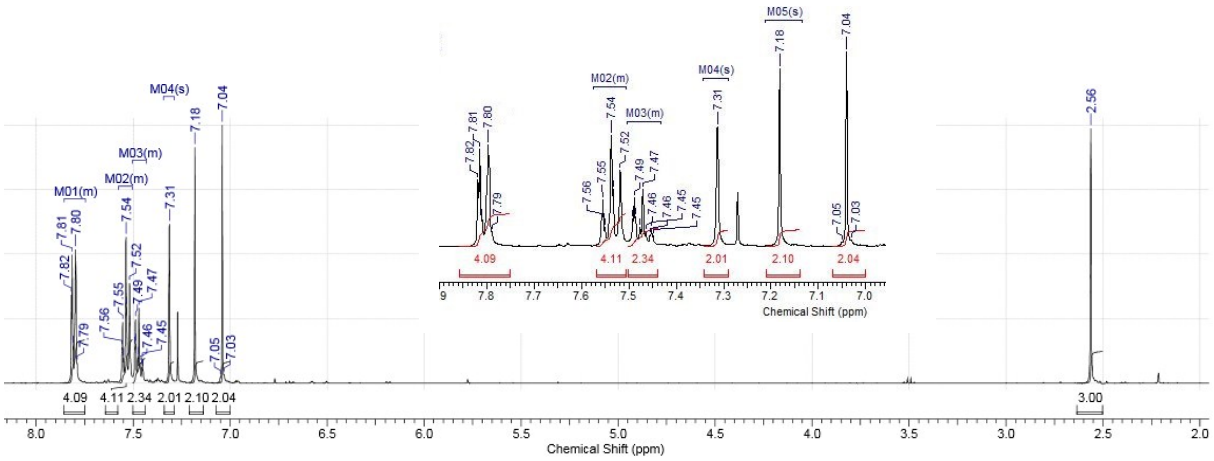


^{13}C NMR of compound **6a**



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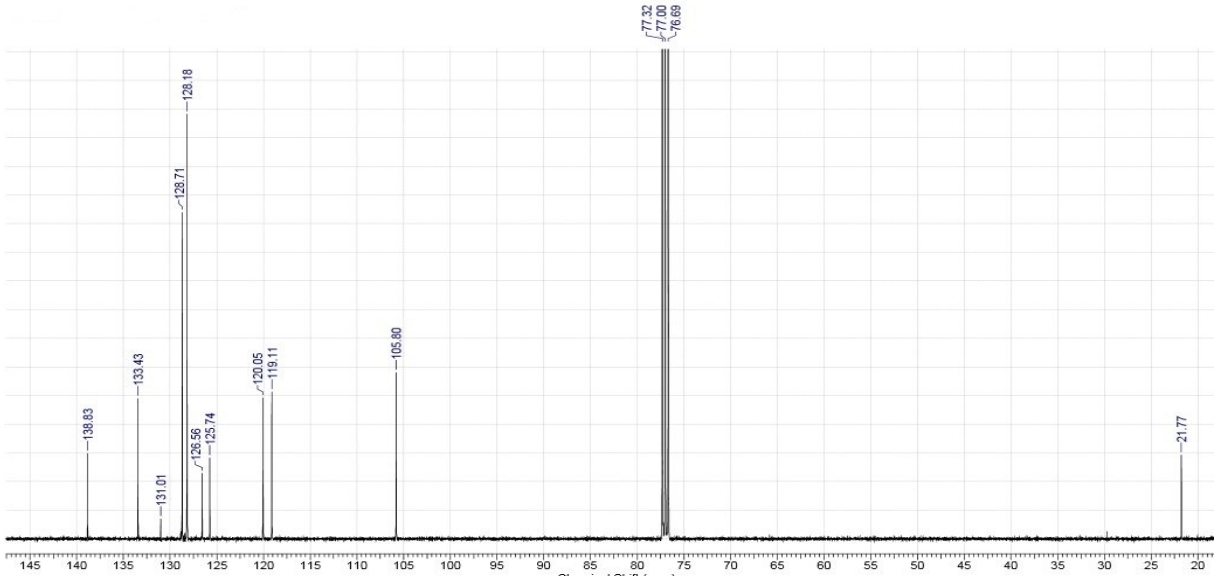

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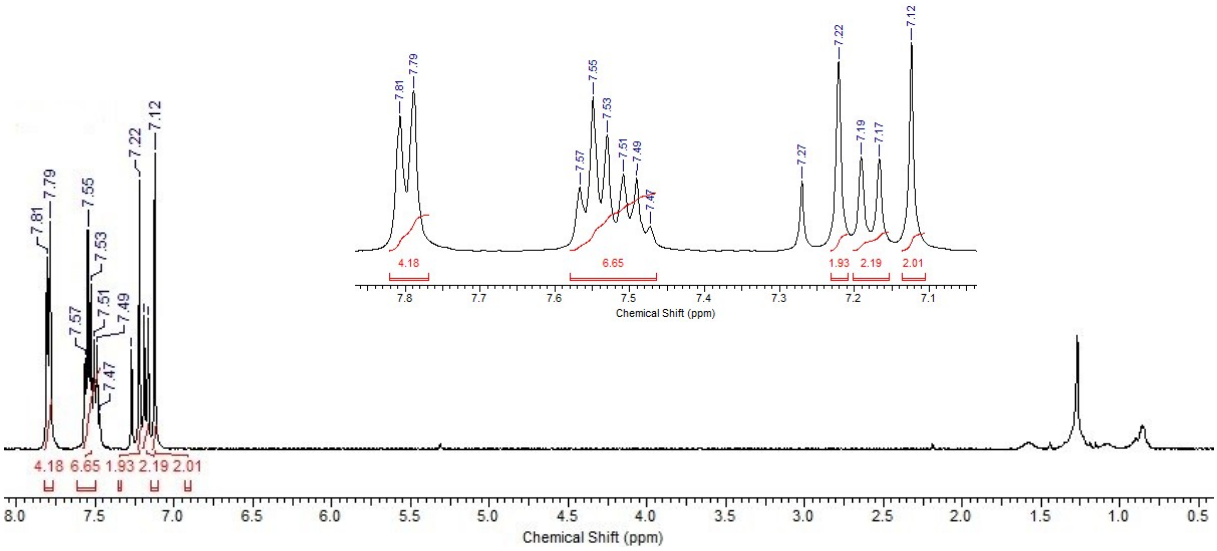

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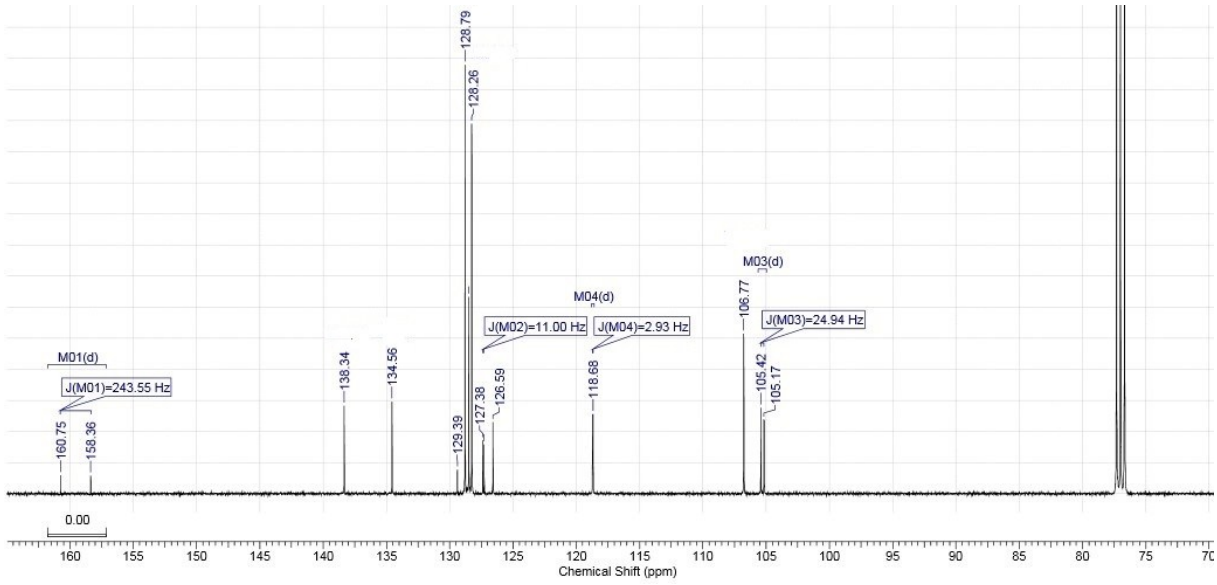

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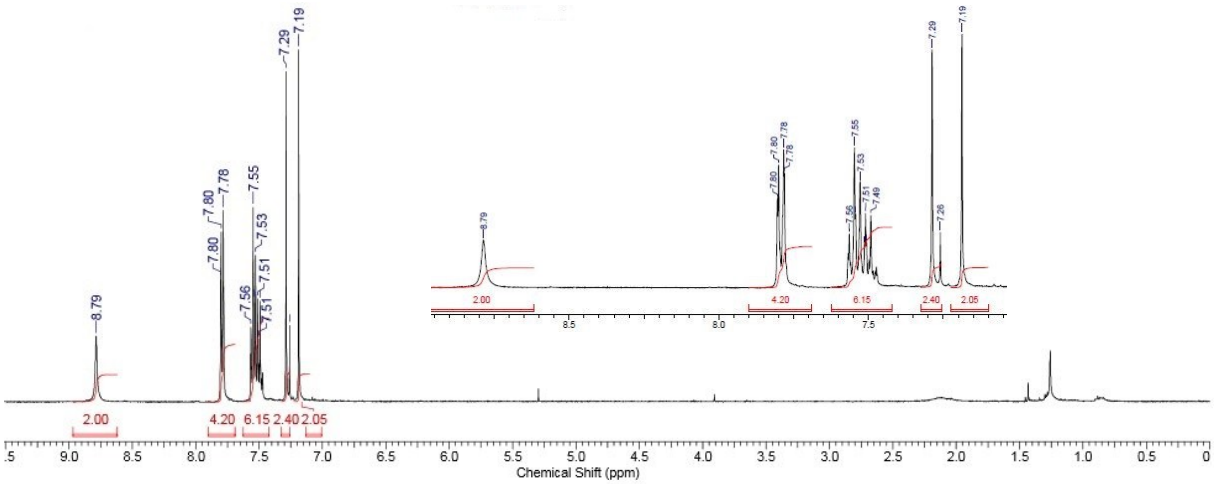

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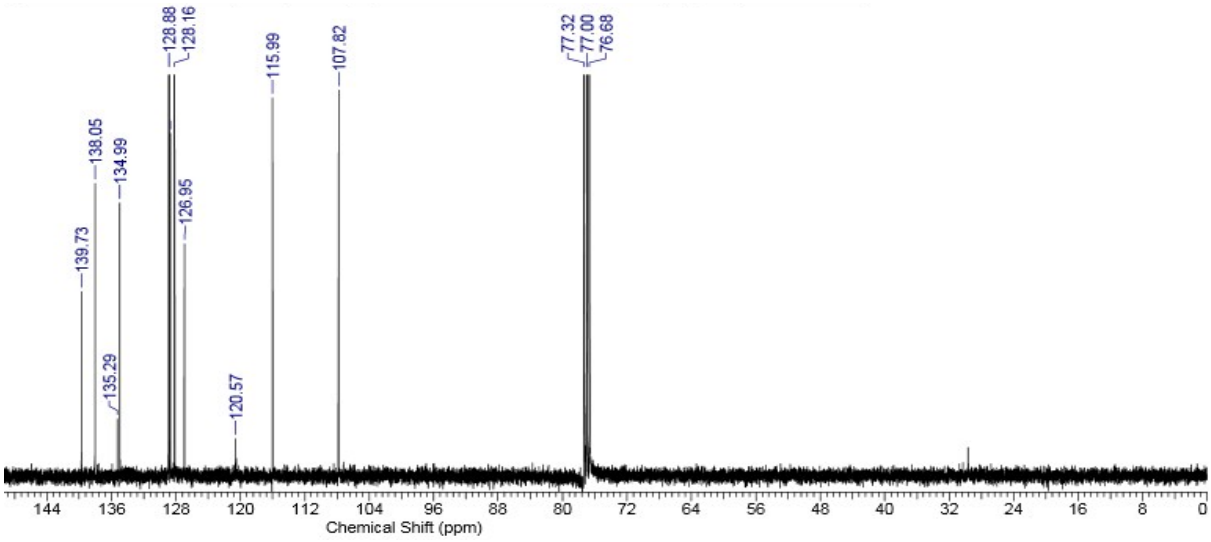

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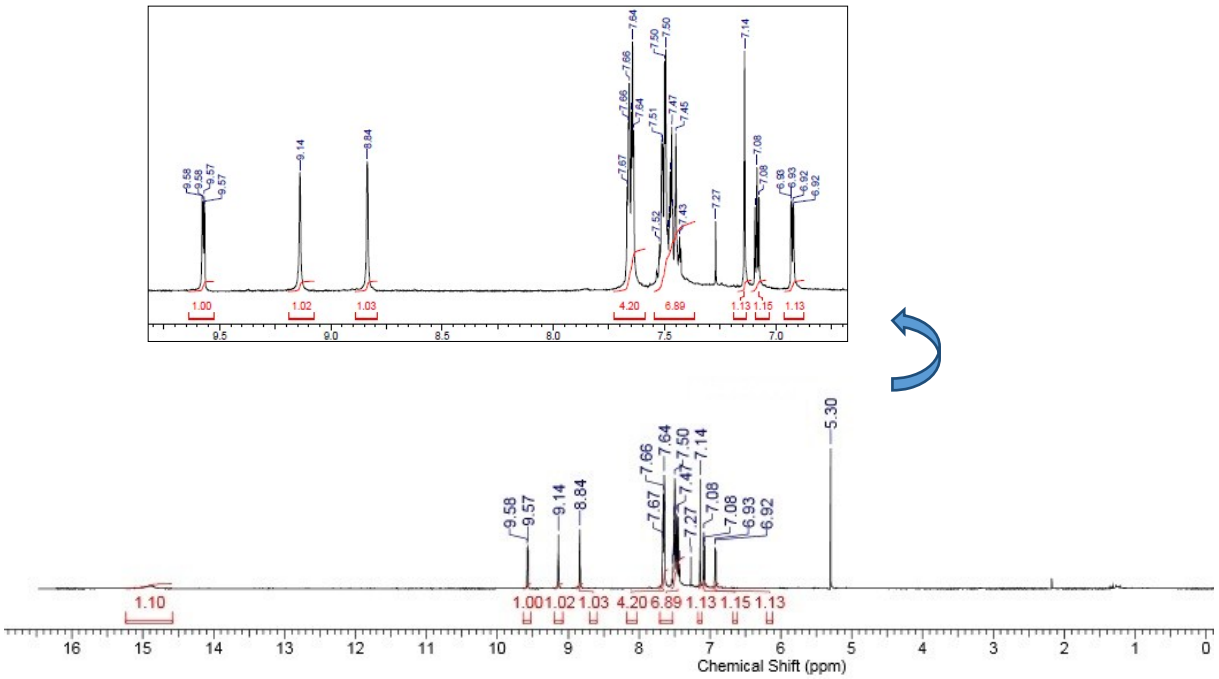

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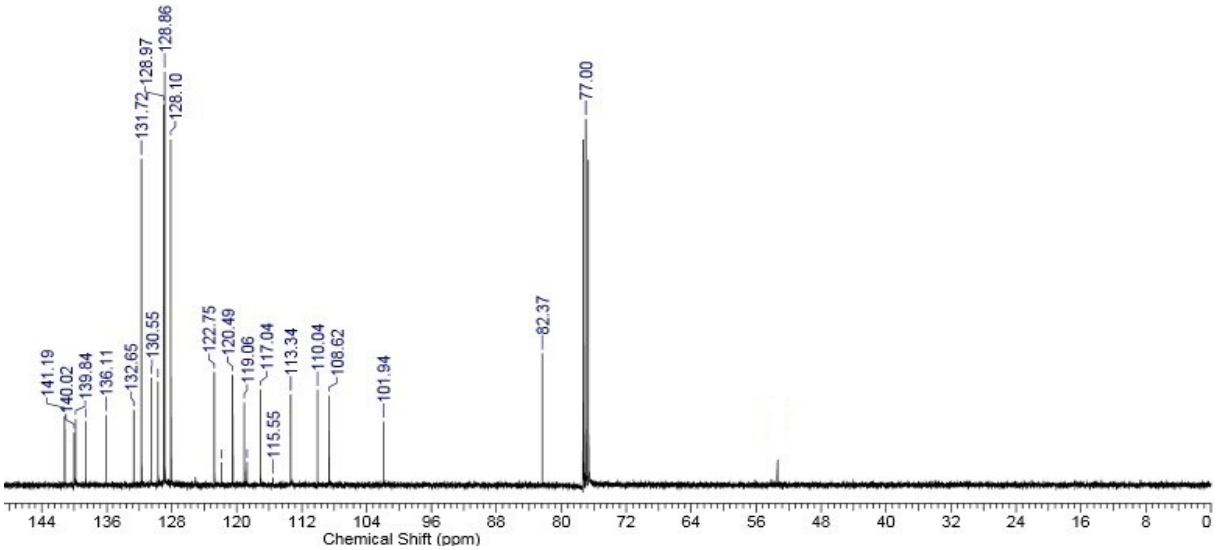

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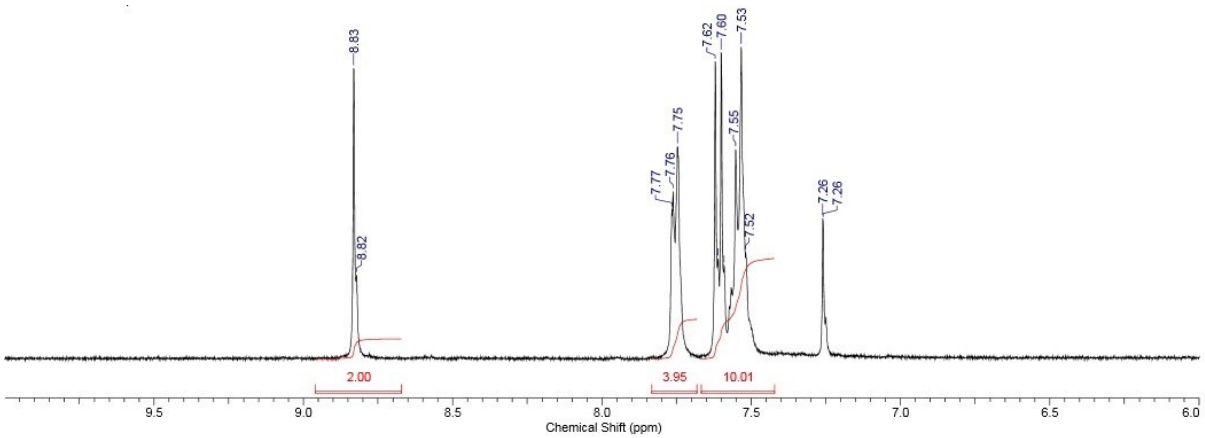
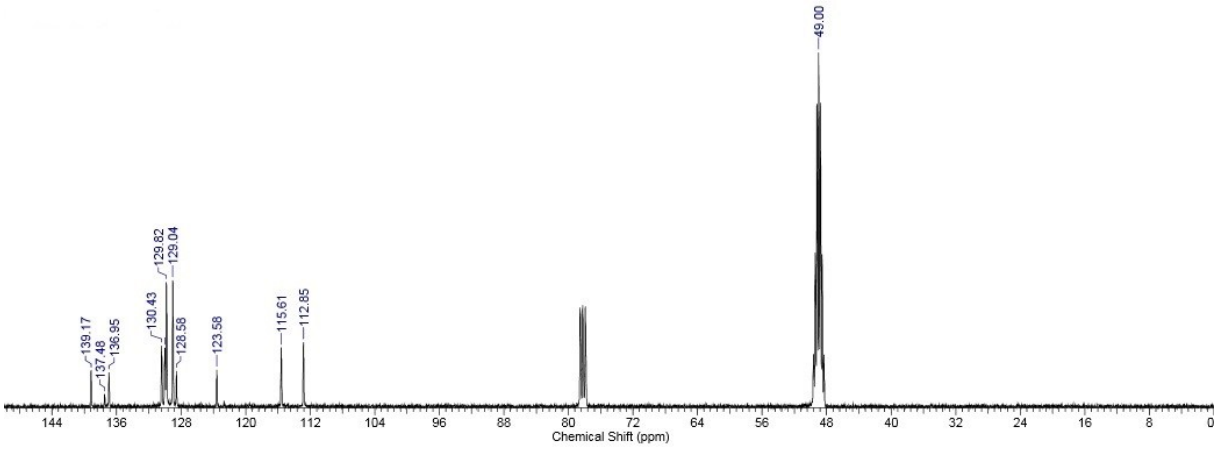


^{1}H NMR of compound **6d**·H^{+}



^{13}C NMR of compound **6d**·H^{+}

2. Computational section

All calculations were performed with Gaussian 09[1] computational package. In order to include electron correlation at a reasonable computational cost, Density Functional Theory (DFT)[2] was used.

Ground-state (S_0) geometries were optimized without symmetry constraints at the PBE1PBE[3] level of theory using 6-31G(d)[4] as basis set. The nature of all the stationary points was checked by computing vibrational frequencies, and all the species were found to be true potential energy minima with no imaginary frequencies (NImag = 0). NBO analysis[5] was performed at the same computational level.

The singlet–singlet ($S_0 \rightarrow S_n$) transition energies were computed at the optimized S_0 geometries by using the time-dependent DFT (TD-DFT) methodology at the PBE1PBE/6-31+G(d,p) level. The electron density reorganization in the excited states was analyzed in terms of NTOs[6] by using a locally developed and free downloadable code NancyEX (see www.nancyex.sourceforge.net/). Additionnally, Φ_S[7] values were also obtained by employing the NancyEX code from post-processing of the attachment and detachment densities. For the convenience of the reader we recall that Φ_S is based on the normalized overlap of the detachment and attachment electronic densities, calculated in the direct space. Values close to 1.0 are indicative of localized transitions, while values close to zero reflect spatially separated charge-transfer states. Therefore, the lower the value of Φ_S, the higher the charge-transfer nature of the state is.

Finally, solvent effects were taken into account in all calculations by means of the Integral Equation Formalism version of the Polarizable Continuum Model (IEF-PCM),[8] employing dichloromethane as solvent.

2.1. Ground-state optimisation

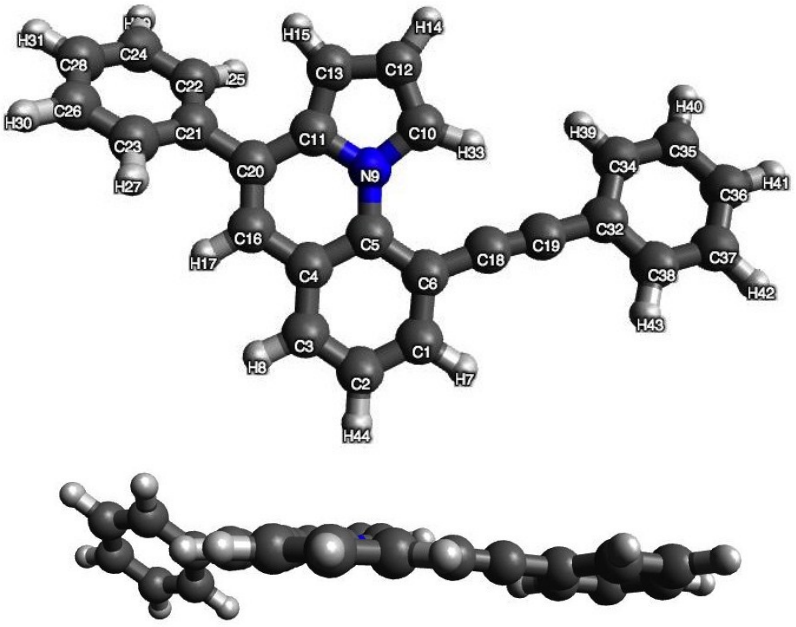


Figure S1. Optimized geometry of **5a**. (Top) Frontal view with atom labeling; (bottom) edge-on view.

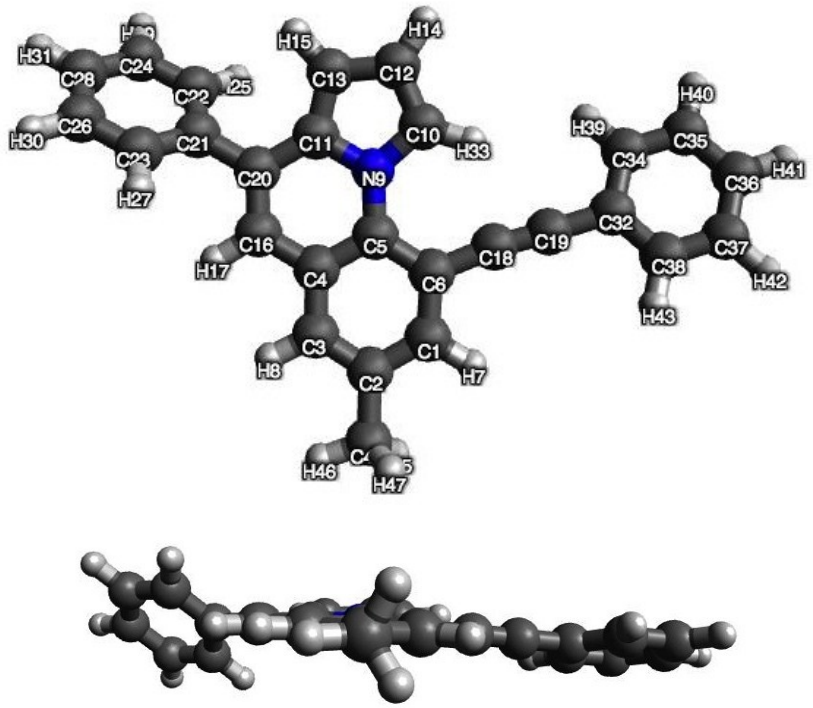


Figure S2. Optimized geometry of **5b**. (Top) Frontal view with atom labeling; (bottom) edge-on view.

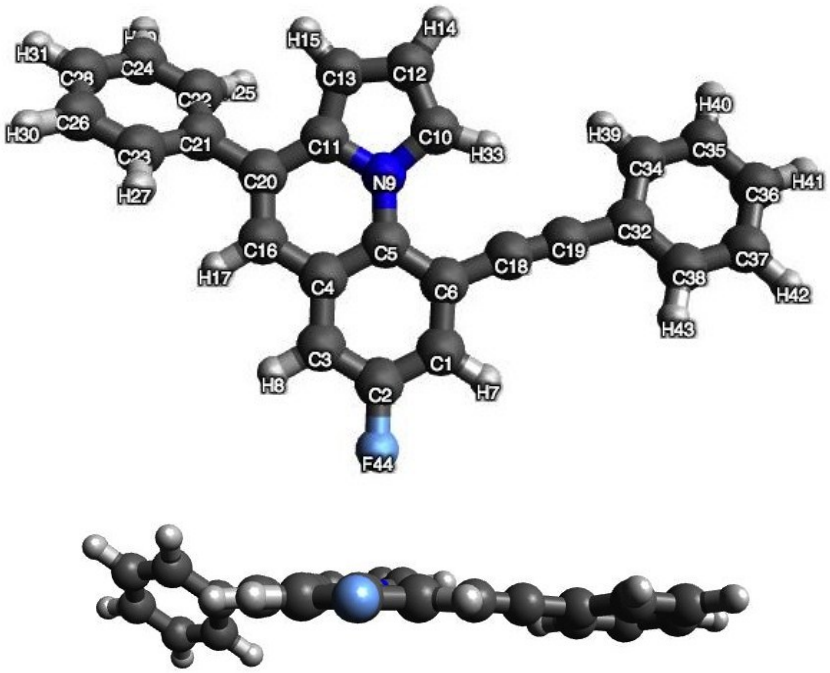


Figure S3. Optimized geometry of **5c**. (Top) Frontal view with atom labeling; (bottom) edge-on view.

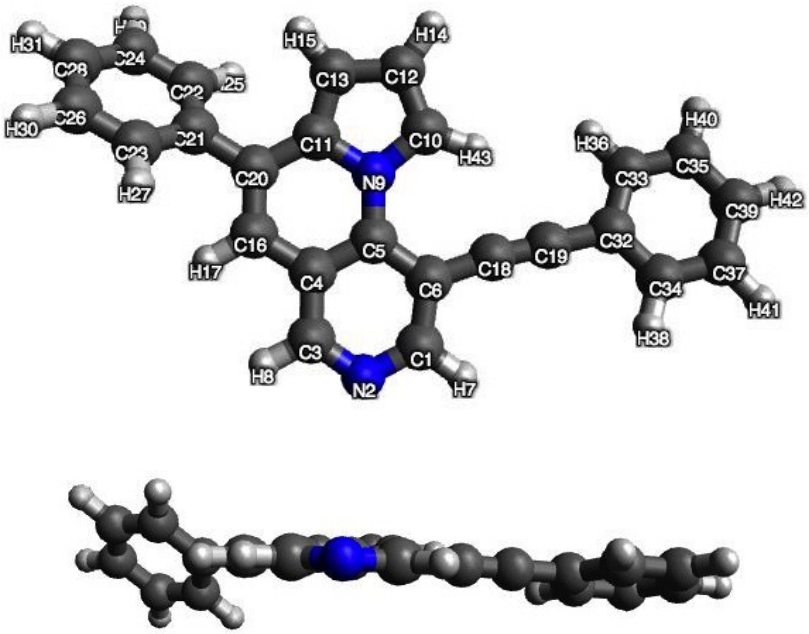
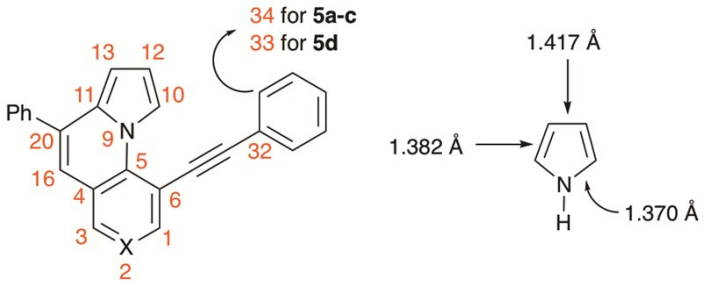


Figure S4. Optimized geometry of **5d**. (Top) Frontal view with atom labeling; (bottom) edge-on view.

Table S1. Selected geometrical parameters of the ground state optimized geometry for mono-annulated compounds **5**. For the sake of comparison, reported bond distances for unsubstituted pyrrole are also depicted.[9] Bond distances are given in [Å] and dihedral angles in [°].



	Geometrical parameter	5a	5b	5c	5d
phenyl or pyridine	$d(C^1–X^2)$	1.390	1.397	1.384	1.332
	$d(X^2–C^3)$[a]	1.382	1.385	1.375	1.326
	$d(C^3–C^4)$	1.405	1.406	1.405	1.403
	$d(C^5–C^6)$	1.421	1.420	1.421	1.417
	$d(C^1–C^6)$	1.404	1.402	1.403	1.404
	$d(N^9–C^5)$	1.397	1.397	1.398	1.387
pyrrole	$d(N^9–C^{10})$	1.376	1.375	1.375	1.377
	$d(C^{10}–C^{12})$	1.375	1.375	1.376	1.373
	$d(C^{12}–C^{13})$	1.409	1.408	1.408	1.411
	$d(C^{13}–C^{11})$	1.385	1.386	1.386	1.383
	$d(C^{11}–C^{20})$	1.431	1.431	1.430	1.433
	$d(C^{20}–C^{16})$	1.361	1.362	1.362	1.362
	$d(C^{16}–C^4)$	1.434	1.434	1.433	1.431
	$\phi(C^{10}–N^9–C^{10}–C^6)$	-6.4	-6.2	-6.8	-4.5
	$\phi(C^5–C^6–C^{32}–C^b)$	-12.5	-11.8	-11.5	-12.9

[a] X = C for **5a-c** and X = N for **5d**. [b] C^{34} for **5a-c** and C^{33} for **5d**.

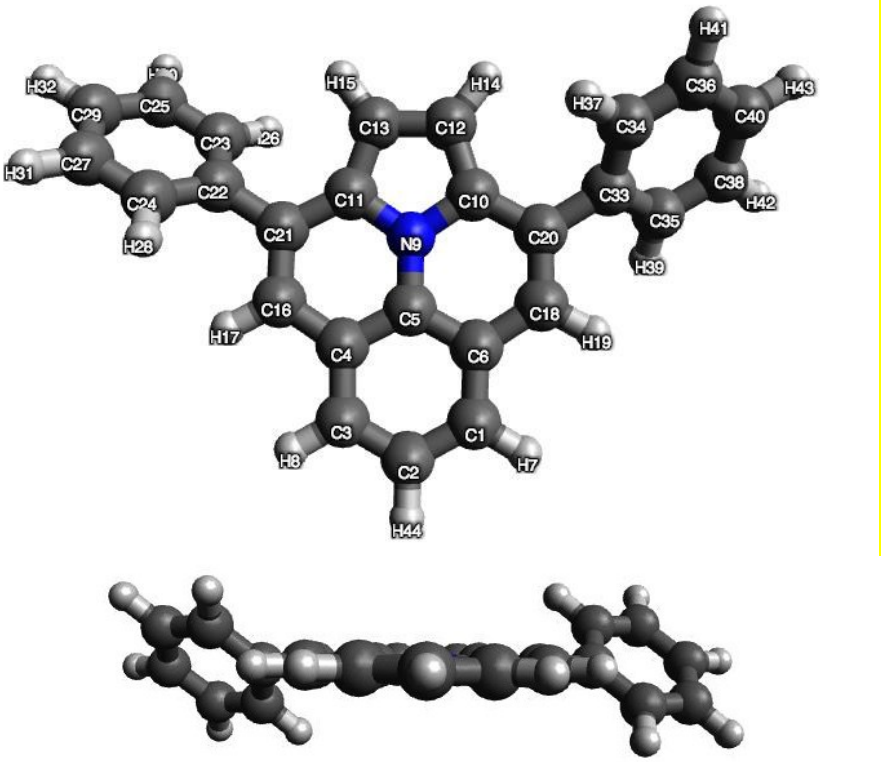


Figure S5. Optimized geometry of **6a**. (Top) Frontal view with atom labeling; (bottom) edge-on view.

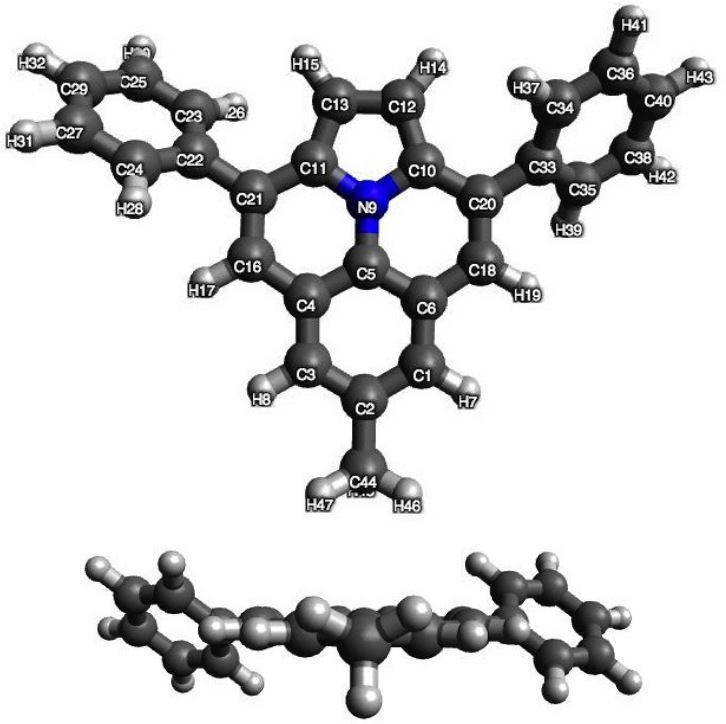


Figure S6. Optimized geometry of **6b**. (Top) Frontal view with atom labeling; (bottom) edge-on view.

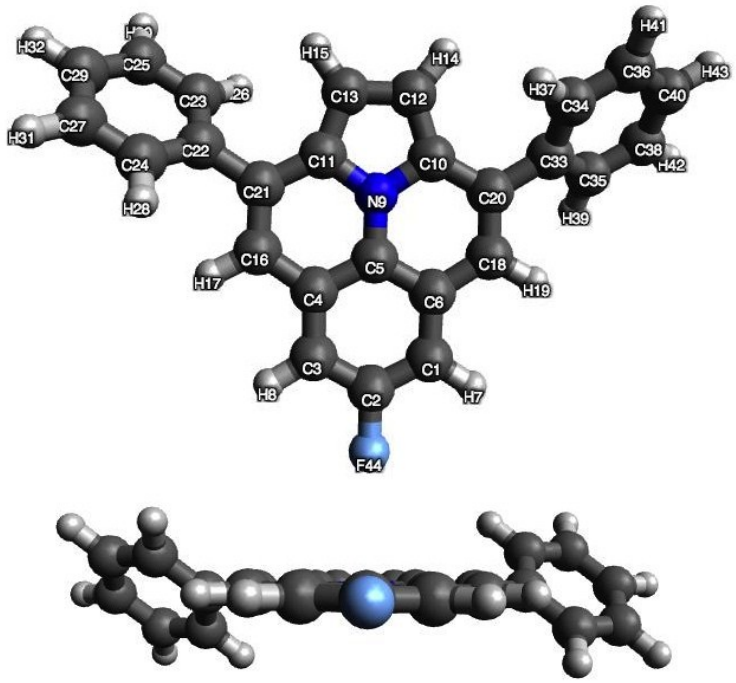


Figure S7. Optimized geometry of **6c**. (Top) Frontal view with atom labeling; (bottom) edge-on view.

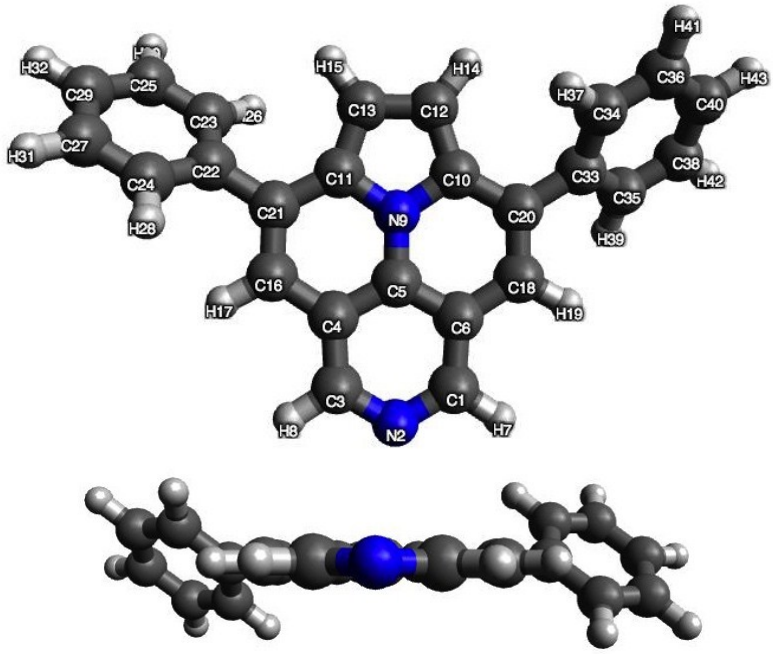
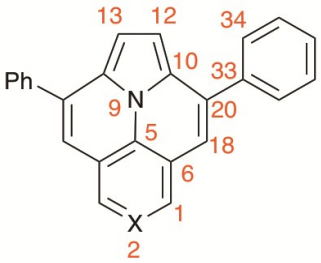


Figure S8. Optimized geometry of **6d**. (Top) Frontal view with atom labeling; (bottom) edge-on view.

Table S2. Selected geometrical parameters of the ground state optimized geometry for bis-annulated compounds **6**. For the sake of comparison, reported bond distances for unsubstituted pyrrole are also depicted.[9] Bond distances are given in [Å] and dihedral angles in [°].

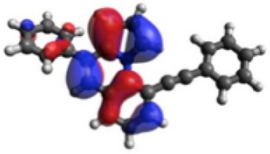
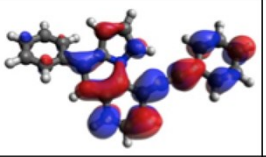
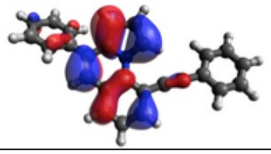
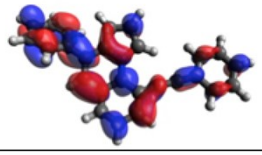
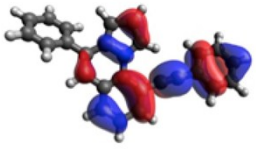
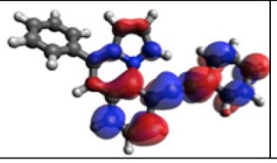
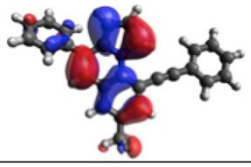
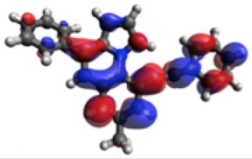
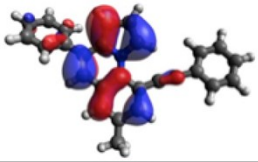
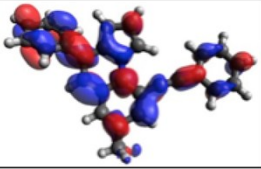
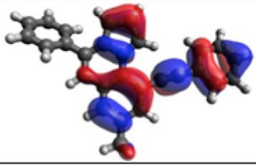
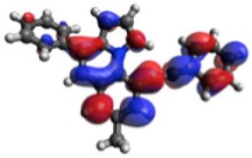
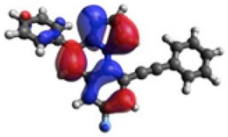
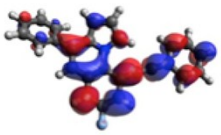
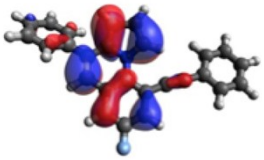
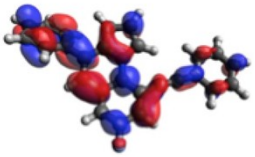


	Geometrical parameter	6a	6b	6c	6d
phenyl or pyridine	$d(C^1–X^2)$	1.392	1.397	1.386	1.333
	$d(C^1–C^6)$	1.403	1.402	1.403	1.404
	$d(C^5–C^6)$	1.413	1.411	1.413	1.407
pyrrole	$d(N^9–C^5)$	1.366	1.366	1.366	1.358
	$d(N^9–C^{10})$	1.386	1.386	1.386	1.387
	$d(C^{10}–C^{12})$	1.398	1.398	1.399	1.396
	$d(C^{12}–C^{13})$	1.400	1.400	1.398	1.403
	$d(C^{10}–C^{20})$	1.432	1.432	1.430	1.434
	$d(C^{20}–C^{18})$	1.371	1.371	1.372	1.372
	$d(C^{18}–C^6)$	1.435	1.436	1.434	1.434
	$\phi(C^1–C^6–C^{18}–C^{20})$	-178.6	-178.6	-179,1	-178.7
	$\phi(C^{12}–C^{10}–C^{20}–C^{18})$	-178.1	-178.2	-178.1	-178.2
	$\phi(C^{18}–C^{20}–C^{33}–C^{34})$	-134.1	-134.2	-134.0	-134.2

[a] X = C for **6a-c** and X = N for **6d**.

2.2. Vertical excited-state transitions

Table S3. Computed excitation energies and oscillator strengths of the first three $S_0 \rightarrow S_n$ transitions for mono-annulated compounds **5**. Also, the associated NTO and the corresponding Φ_s value are reported.

5a					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	392 (3.163)	0.1153			0.63
$S_0 \rightarrow S_2$	352 (3.526)	0.1415			0.75
$S_0 \rightarrow S_3$	336 (3.691)	0.7952			0.89
5b					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	392 (3.161)	0.1267			0.62
$S_0 \rightarrow S_2$	352 (3.522)	0.1157			0.77
$S_0 \rightarrow S_3$	338 (3.663)	0.7644			0.90
5c					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	*402 (3.084)*	*0.1280*			*0.63*
$S_0 \rightarrow S_2$	*350 (3.542)*	*0.0698*			*0.84*

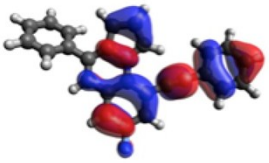
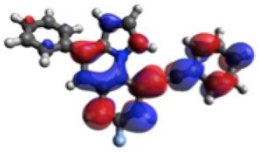
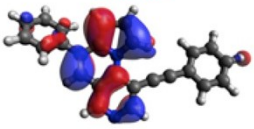
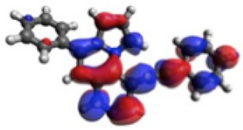
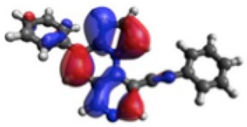
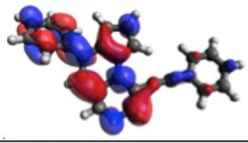
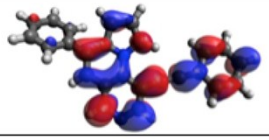
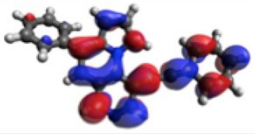
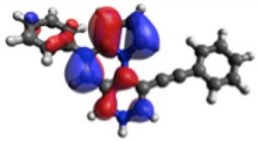
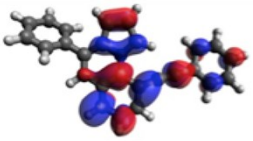
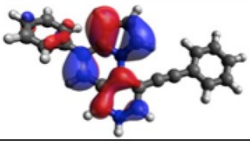
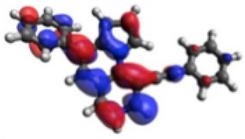
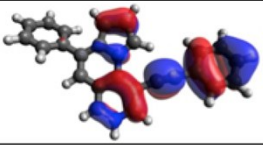
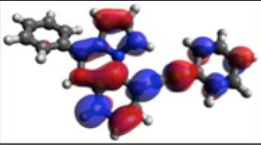
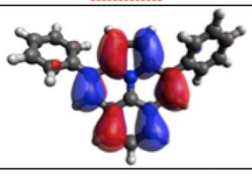
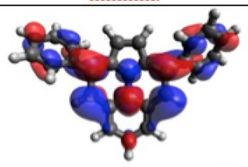
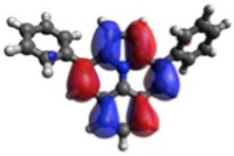
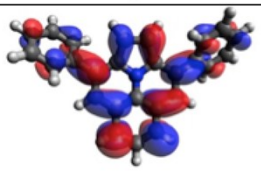
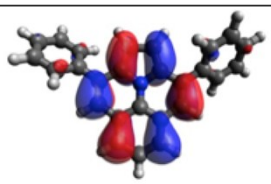
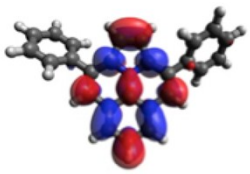
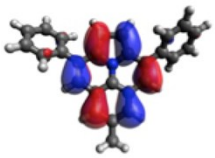
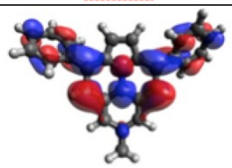
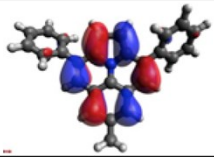
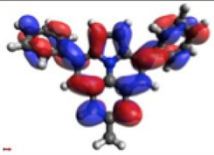
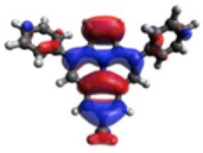
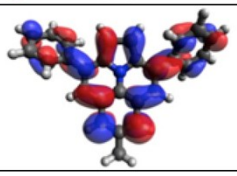
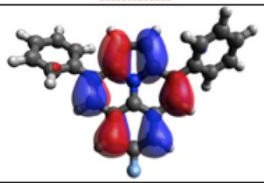
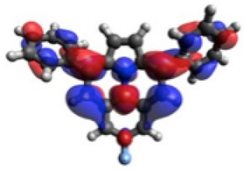
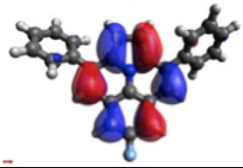
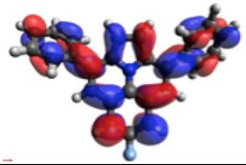
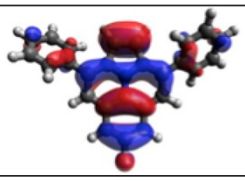
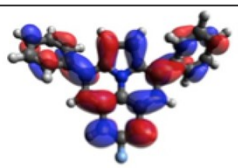
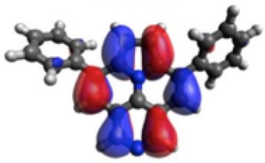
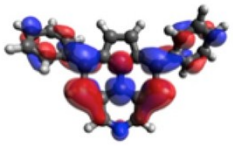
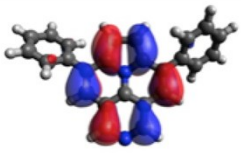
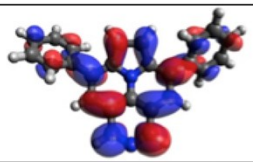
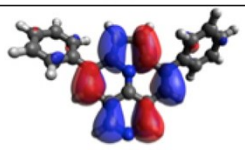
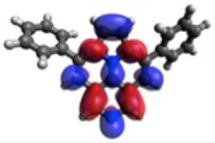
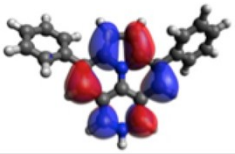
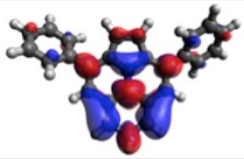
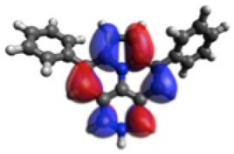
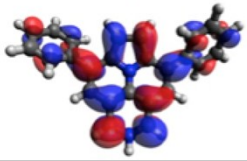
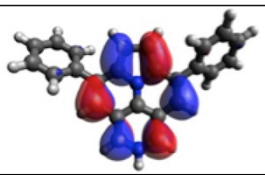
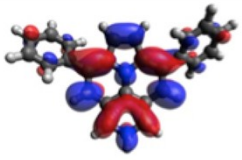
$S_0 \rightarrow S_3$	*343 (3.620)*	*0.7824*			*0.91*
5d					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	*390 (3.175)*	*0.1058*			*0.66*
$S_0 \rightarrow S_2$	*355 (3.493)*	*0.1648*			*0.74*
$S_0 \rightarrow S_3$	*331 (3.744)*	*0.8208*			*0.90*
5d·H^+					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	*447 (2.774)*	*0.0357*			*0.59*
$S_0 \rightarrow S_2$	*407 (3.043)*	*0.1089*			*0.65*
$S_0 \rightarrow S_3$	*361 (3.431)*	*0.8160*			*0.82*

Table S4. Computed excitation energies and oscillator strengths of the first three $S_0 \rightarrow S_n$ transitions for bis-annulated compounds **6**. Also, the associated NTO and the corresponding Φ_s value are reported.

6a					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	418 (2.965)	0.0001			0.59
$S_0 \rightarrow S_2$	376 (3.294)	0.3197			0.81
$S_0 \rightarrow S_3$	313 (3.957)	0.0033			0.97
6b					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	418 (2.965)	0.0001			0.59
$S_0 \rightarrow S_2$	378 (3.279)	0.3324			0.82
$S_0 \rightarrow S_3$	316 (3.919)	0.0271			0.96
6c					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	*410 (3.019)*	*0.0012*			*0.59*
$S_0 \rightarrow S_2$	*378 (3.283)*	*0.3205*			*0.79*

$S_0 \rightarrow S_3$	*314 (3.944)*	*0.1032*			*0.93*
6d					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	*411 (3.175)*	*0.0000*			*0.57*
$S_0 \rightarrow S_2$	*373 (3.493)*	*0.3084*			*0.82*
$S_0 \rightarrow S_3$	*321 (3.863)*	*0.0613*			*0.92*
6d·H$^+$					
Transition	***λ (nm)[E (eV)]***	***f***	***oNTO***	***vNTO***	***Φs***
$S_0 \rightarrow S_1$	*434 (2.859)*	*0.0221*			*0.54*
$S_0 \rightarrow S_2$	*384 (3.229)*	*0.2089*			*0.80*
$S_0 \rightarrow S_3$	*345 (3.606)*	*0.0478*			*0.92*

2.3. Cartesian coordinates of the computed structures at PBE1PBE/6-31G(d)

Compound **5a**

Atomic Number	Coordinates (Å) X	Y	Z
6	1.35902	3.02961	0.12931
6	0.27242	3.89303	0.20455
6	-1.00656	3.37125	0.17828
6	-1.22748	1.98906	0.05482
6	-0.12114	1.10759	-0.04975
6	1.19471	1.63992	0.01341
1	2.37169	3.41759	0.17037
1	-1.8712	4.02513	0.25475
7	-0.40795	-0.25029	-0.20835
6	0.44695	-1.3011	-0.44964
6	-1.72315	-0.75289	-0.18752
6	-0.29557	-2.45162	-0.57693
6	-1.65439	-2.11728	-0.41552
1	0.11198	-3.43395	-0.77689
1	-2.50344	-2.78246	-0.4804
6	-2.56647	1.47656	0.06799
1	-3.38018	2.18431	0.1989
6	2.39847	0.88053	0.00283
6	3.49889	0.36085	0.02713
6	-2.82647	0.14313	-0.02091
6	-4.21136	-0.37371	0.04005
6	-4.54574	-1.46742	0.85034
6	-5.22872	0.2558	-0.6891
6	-5.86087	-1.91479	0.92993
1	-3.772	-1.95458	1.43679
6	-6.54305	-0.19394	-0.61057
1	-4.97921	1.09298	-1.33576
6	-6.86402	-1.28144	0.19897
1	-6.10313	-2.75853	1.57054
1	-7.31711	0.3027	-1.18947
1	-7.88989	-1.63441	0.25905
6	4.76877	-0.28095	0.0518
1	1.50841	-1.14716	-0.52826
6	4.86498	-1.66819	0.25817
6	6.10882	-2.2864	0.27986
6	7.27032	-1.53662	0.09831
6	7.18359	-0.16009	-0.10553
6	5.94461	0.46764	-0.12942
1	3.95972	-2.25016	0.4043
1	6.1723	-3.35899	0.44037
1	8.24098	-2.02411	0.1165
1	8.08615	0.4278	-0.24695
1	5.87309	1.53937	-0.28888
1	0.43284	4.96283	0.29541

Compound **5b**

Atomic Number	Coordinates (Å) X	Y	Z
6	1.3569	2.77136	0.06796
6	0.2881	3.66846	0.12429
6	-0.99063	3.13781	0.10515
6	-1.22888	1.75572	0.00991
6	-0.13722	0.85819	-0.07425
6	1.18162	1.38315	-0.02081
1	2.37592	3.14654	0.10383
1	-1.85207	3.79926	0.16656
7	-0.43861	-0.49994	-0.20272
6	0.40426	-1.56554	-0.41619
6	-1.75959	-0.9851	-0.17519
6	-0.3521	-2.71004	-0.52041
6	-1.707	-2.35568	-0.37237
1	0.04419	-3.70164	-0.6959
1	-2.56387	-3.01182	-0.42532
6	-2.57432	1.2611	0.0309
1	-3.37957	1.98136	0.14494
6	2.38012	0.6147	-0.01783
6	3.47614	0.08618	0.01268
6	-2.85113	-0.0709	-0.03119
6	-4.24303	-0.56791	0.03649
6	-4.59442	-1.64009	0.8681
6	-5.25011	0.05971	-0.70848
6	-5.91563	-2.06822	0.95293
1	-3.82893	-2.1253	1.46683
6	-6.57059	-0.37068	-0.6246
1	-4.98772	0.87996	-1.37153
6	-6.90835	-1.43686	0.20617
1	-6.17082	-2.89533	1.61003
1	-7.33632	0.12422	-1.21595
1	-7.93899	-1.77489	0.27042
6	4.74299	-0.56142	0.04447
1	1.46791	-1.42578	-0.49316
6	4.83347	-1.94798	0.25765
6	6.07489	-2.57085	0.28544
6	7.23978	-1.8265	0.10336
6	7.15882	-0.4506	-0.10709
6	5.9223	0.18166	-0.13719
1	3.92569	-2.52594	0.40404
1	6.13379	-3.64294	0.45108
1	8.20849	-2.31765	0.12628
1	8.06398	0.1332	-0.24892
1	5.8553	1.2529	-0.30193
6	0.53323	5.14854	0.21075
1	1.1759	5.3956	1.06323
1	-0.40462	5.69982	0.32272
1	1.03591	5.51918	-0.69027

Compound **5c**

Atomic Number	Coordinates (Å) X	Y	Z
6	1.36945	2.79741	0.05994
6	0.2767	3.64479	0.11688
6	-1.01095	3.16203	0.10223
6	-1.23435	1.77894	0.00323
6	-0.13401	0.88683	-0.08683
6	1.18583	1.40946	-0.03128
1	2.37339	3.20426	0.09846
1	-1.8513	3.84546	0.16921
7	-0.43096	-0.47214	-0.22289
6	0.41376	-1.53247	-0.45247
6	-1.74935	-0.96379	-0.18716
6	-0.33831	-2.67989	-0.55721
6	-1.69274	-2.3327	-0.39392
1	0.06097	-3.66809	-0.74418
1	-2.54752	-2.9917	-0.44443
6	-2.57666	1.27719	0.02919
1	-3.38516	1.99221	0.1493
6	2.38257	0.63994	-0.02585
6	3.47749	0.11022	0.0103
6	-2.84422	-0.05671	-0.03325
6	-4.23252	-0.56224	0.04189
6	-4.5713	-1.63747	0.87463
6	-5.24729	0.06014	-0.6968
6	-5.88921	-2.07403	0.96668
1	-3.79917	-2.118	1.46856
6	-6.56421	-0.37945	-0.60614
1	-4.99411	0.88277	-1.36044
6	-6.88994	-1.44848	0.22578
1	-6.13543	-2.90314	1.62457
1	-7.33657	0.1107	-1.1927
1	-7.91796	-1.79324	0.29561
6	4.7423	-0.54041	0.04862
1	1.47587	-1.38877	-0.54073
6	4.82674	-1.92754	0.25997
6	6.06633	-2.55345	0.29453
6	7.23392	-1.81126	0.12088
6	7.1584	-0.43477	-0.0878
6	5.9239	0.20088	-0.12439
1	3.91644	-2.50309	0.39973
1	6.12182	-3.62586	0.45877
1	8.2012	-2.30491	0.14907
1	8.06605	0.14662	-0.22291
1	5.86041	1.27252	-0.2875
9	0.48771	4.96664	0.20374

Compound **5d**

Atomic Number	Coordinates (Å) X	Y	Z
6	1.31203	2.98723	0.14741
7	0.29491	3.84487	0.21379
6	-0.92384	3.32447	0.18364
6	-1.20548	1.95419	0.07421
6	-0.11838	1.05308	-0.01095
6	1.1916	1.59196	0.0421
1	2.31291	3.41122	0.18315
1	-1.7573	4.02301	0.24856
7	-0.41974	-0.29431	-0.14129
6	0.42494	-1.36563	-0.32871
6	-1.74794	-0.77082	-0.14554
6	-0.33625	-2.50215	-0.45201
6	-1.69514	-2.13869	-0.34102
1	0.05612	-3.49742	-0.6139
1	-2.55208	-2.79276	-0.41288
6	-2.55607	1.47984	0.07301
1	-3.35594	2.20622	0.18364
6	2.40742	0.85878	0.01861
6	3.51473	0.35388	0.02368
6	-2.83754	0.14985	-0.01282
6	-4.2324	-0.34221	0.01995
6	-4.60675	-1.41698	0.83779
6	-5.21768	0.2939	-0.74628
6	-5.93118	-1.8404	0.88781
1	-3.85859	-1.9072	1.45404
6	-6.54108	-0.13269	-0.69752
1	-4.93614	1.11684	-1.398
6	-6.90245	-1.20185	0.11933
1	-6.20571	-2.66936	1.53454
1	-7.29031	0.3678	-1.30489
1	-7.93548	-1.5365	0.15639
6	4.79716	-0.26251	0.02774
6	4.92385	-1.64751	0.23118
6	5.95387	0.51096	-0.17066
6	6.18021	-2.24004	0.23355
1	4.03323	-2.24829	0.39023
6	7.20547	-0.09153	-0.16609
1	5.8578	1.58107	-0.32771
6	7.32296	-1.46615	0.03522
1	6.26821	-3.31114	0.39198
1	8.09362	0.51462	-0.32054
1	8.30355	-1.9336	0.03829
1	1.49146	-1.22967	-0.37277

Compound **5d**·H^+

Atomic Number	Coordinates (Å) X	Y	Z
6	1.3532	2.99166	0.1253
7	0.28384	3.79835	0.18773
6	-0.97166	3.34102	0.16848
6	-1.22283	1.97936	0.06165
6	-0.11707	1.08231	-0.03462
6	1.20529	1.61311	0.0223
1	2.32686	3.46054	0.16562
1	-1.76492	4.0746	0.23738
7	-0.40935	-0.25045	-0.17465
6	0.43749	-1.32156	-0.38584
6	-1.74377	-0.74003	-0.16643
6	-0.32079	-2.45477	-0.51065
6	-1.68256	-2.09943	-0.37712
1	0.07223	-3.44604	-0.69136
1	-2.53507	-2.75917	-0.44602
6	-2.56892	1.501	0.07246
1	-3.37127	2.22063	0.19433
6	2.41134	0.86961	0.00623
6	3.51515	0.35871	0.02445
6	-2.83692	0.16712	-0.01381
6	-4.2248	-0.33798	0.03285
6	-4.57528	-1.41906	0.85267
6	-5.22206	0.29293	-0.72185
6	-5.89473	-1.85477	0.91587
1	-3.81666	-1.90138	1.46214
6	-6.53901	-0.15016	-0.66189
1	-4.9568	1.11974	-1.37526
6	-6.87904	-1.22461	0.15727
1	-6.15471	-2.68681	1.56409
1	-7.29992	0.34194	-1.26099
1	-7.90784	-1.57021	0.20414
6	4.7905	-0.26726	0.04075
6	4.89951	-1.65491	0.2366
6	5.95257	0.50281	-0.13855
6	6.15118	-2.25551	0.2504
1	4.00282	-2.24985	0.38106
6	7.19852	-0.10958	-0.12357
1	5.86571	1.57436	-0.28952
6	7.30059	-1.48665	0.07037
1	6.23097	-3.32775	0.40289
1	8.09363	0.48916	-0.26353
1	8.27739	-1.96148	0.08205
1	1.50224	-1.18534	-0.4488
1	0.43759	4.79899	0.26053

Compound **6a**

Atomic Number	Coordinates (Å) X	Y	Z
6	-1.213613	3.712191	-0.021293
6	0.000003	4.393692	-0.000006
6	1.213618	3.712189	0.021282
6	1.242522	2.309063	0.022853
6	0.000001	1.637324	-0.000002
6	-1.242520	2.309065	-0.022858
1	-2.151518	4.260670	-0.035957
1	2.151524	4.260667	0.035944
7	0.000000	0.270936	0.000001
6	-1.139383	-0.518853	0.008186
6	1.139382	-0.518855	-0.008182
6	-0.700149	-1.845560	0.000059
6	0.700145	-1.845561	-0.000048
1	-1.341762	-2.715365	-0.010420
1	1.341756	-2.715368	0.010437
6	2.437524	1.514148	0.026072
1	3.394767	2.028232	0.010872
6	-2.437523	1.514152	-0.026075
1	-3.394765	2.028237	-0.010878
6	-2.408871	0.143720	-0.000044
6	2.408871	0.143717	0.000045
6	3.661415	-0.643250	-0.025676
6	3.824187	-1.719212	-0.908984
6	4.726397	-0.302112	0.818350
6	5.019368	-2.430639	-0.947173
1	3.017281	-1.982310	-1.586980
6	5.920510	-1.015159	0.780335
1	4.605755	0.518019	1.521295
6	6.071049	-2.082970	-0.101953
1	5.130889	-3.256167	-1.645006
1	6.732731	-0.740106	1.447789
1	7.002542	-2.641612	-0.130231
6	-3.661416	-0.643245	0.025678
6	-3.824185	-1.719208	0.908986
6	-4.726400	-0.302107	-0.818345
6	-5.019366	-2.430636	0.947176
1	-3.017277	-1.982308	1.586977
6	-5.920512	-1.015153	-0.780328
1	-4.605759	0.518025	-1.521290
6	-6.071049	-2.082965	0.101960
1	-5.130885	-3.256165	1.645009
1	-6.732735	-0.740099	-1.447780
1	-7.002543	-2.641607	0.130239
1	0.000004	5.480239	-0.000008

Compound **6b**

Atomic Number	Coordinates (Å) X	Y	Z
6	1.207314	3.448288	0.010470
6	0.000396	4.151600	-0.009715
6	-1.206435	3.448594	-0.031369
6	-1.238596	2.046510	-0.027279
6	0.000071	1.371314	-0.001587
6	1.239051	2.046396	0.017955
1	2.148248	3.993968	0.019402
1	-2.147100	3.994404	-0.051378
7	-0.000054	0.005242	0.000497
6	1.139202	-0.783506	-0.006219
6	-1.139548	-0.783177	0.010069
6	0.699758	-2.110750	0.005065
6	-0.700464	-2.110582	0.005122
1	1.341188	-2.980692	0.017306
1	-1.342130	-2.980392	-0.003693
6	-2.434900	1.252966	-0.031055
1	-3.391873	1.767703	-0.018437
6	2.435178	1.252491	0.020533
1	3.392240	1.766898	0.002155
6	2.407686	-0.118395	-0.001066
6	-2.407819	-0.117810	-0.001294
6	-3.661731	-0.902666	0.025232
6	-3.826380	-1.977181	0.909992
6	-4.726115	-0.561432	-0.819555
6	-5.022554	-2.686917	0.948949
1	-3.019911	-2.240490	1.588427
6	-5.921284	-1.272677	-0.780743
1	-4.604127	0.257414	-1.523770
6	-6.073609	-2.339002	0.103051
1	-5.135341	-3.511328	1.647917
1	-6.732941	-0.997458	-1.448834
1	-7.005901	-2.896293	0.131911
6	3.661464	-0.903530	-0.025910
6	3.824232	-1.983056	-0.904901
6	4.727688	-0.557451	0.814582
6	5.020377	-2.692914	-0.942461
1	3.016315	-2.250266	-1.580078
6	5.922832	-1.268819	0.777177
1	4.607163	0.265405	1.514356
6	6.073279	-2.340132	-0.100877
1	5.131695	-3.521266	-1.636989
1	6.735949	-0.989740	1.441885
1	7.005551	-2.897513	-0.128643
6	0.000693	5.656288	0.019631
1	0.003959	6.029688	1.051516
1	0.886215	6.065215	-0.477033
1	-0.887082	6.065701	-0.472336

Compound **6c**

Atomic Number	Coordinates (Å) X	Y	Z
6	1.221600	3.468640	0.020520
6	0.000000	4.122380	0.000000
6	-1.221600	3.468640	-0.020520
6	-1.243030	2.065610	-0.021880
6	0.000000	1.393670	0.000000
6	1.243030	2.065610	0.021880
1	2.142640	4.041990	0.033850
1	-2.142640	4.041990	-0.033850
7	0.000000	0.027490	0.000000
6	1.138690	-0.761770	-0.009150
6	-1.138690	-0.761770	0.009150
6	0.699150	-2.090110	-0.000670
6	-0.699150	-2.090110	0.000670
1	1.341340	-2.959450	0.009080
1	-1.341330	-2.959450	-0.009080
6	-2.436960	1.271660	-0.023850
1	-3.394440	1.784530	-0.007670
6	2.436960	1.271660	0.023850
1	3.394440	1.784530	0.007670
6	2.406270	-0.099890	-0.002290
6	-2.406270	-0.099890	0.002280
6	-3.658950	-0.886580	0.028530
6	-3.821870	-1.960290	0.914380
6	-4.722540	-0.547070	-0.817730
6	-5.016840	-2.672000	0.952490
1	-3.015960	-2.221080	1.594420
6	-5.916100	-1.260970	-0.780040
1	-4.601420	0.271700	-1.522150
6	-6.067170	-2.326720	0.104640
1	-5.129220	-3.495750	1.652220
1	-6.727520	-0.987960	-1.449220
1	-6.998470	-2.885640	0.132930
6	3.658950	-0.886580	-0.028530
6	3.821870	-1.960290	-0.914380
6	4.722540	-0.547070	0.817730
6	5.016840	-2.672000	-0.952490
1	3.015960	-2.221080	-1.594420
6	5.916100	-1.260970	0.780040
1	4.601420	0.271700	1.522140
6	6.067170	-2.326720	-0.104640
1	5.129220	-3.495750	-1.652210
1	6.727520	-0.987950	1.449220
1	6.998470	-2.885640	-0.132920
9	0.000000	5.467620	0.000000

Compound **6d**

Atomic Number	Coordinates (Å) X	Y	Z
6	-0.132806	1.141519	3.704447
7	0.000000	0.000000	4.381164
6	0.132806	-1.141519	3.704447
6	0.140863	-1.224107	2.303259
6	0.000000	0.000000	1.624010
6	-0.140863	1.224107	2.303259
1	-0.239885	2.049939	4.295435
1	0.239885	-2.049939	4.295435
7	0.000000	0.000000	0.265714
6	-0.157769	1.131531	-0.519942
6	0.157769	-1.131531	-0.519942
6	-0.091748	0.695263	-1.844737
6	0.091748	-0.695263	-1.844737
1	-0.165550	1.330291	-2.716241
1	0.165550	-1.330291	-2.716241
6	0.296142	-2.417042	1.523250
1	0.437371	-3.361149	2.041876
6	-0.296142	2.417042	1.523250
1	-0.437371	3.361149	2.041876
6	-0.317042	2.388652	0.151271
6	0.317042	-2.388652	0.151271
6	0.505447	-3.629412	-0.631958
6	1.401100	-3.677319	-1.708804
6	-0.192331	-4.793920	-0.286102
6	1.593879	-4.859182	-2.417239
1	1.968504	-2.789936	-1.974485
6	0.000000	-5.974377	-0.996761
1	-0.904006	-4.763952	0.534780
6	0.893127	-6.010902	-2.065539
1	2.299329	-4.881083	-3.243434
1	-0.555418	-6.866001	-0.718923
1	1.041919	-6.932152	-2.621978
6	-0.505447	3.629412	-0.631958
6	-1.401100	3.677319	-1.708804
6	0.192331	4.793920	-0.286102
6	-1.593879	4.859182	-2.417239
1	-1.968504	2.789936	-1.974485
6	0.000000	5.974377	-0.996761
1	0.904006	4.763952	0.534780
6	-0.893127	6.010902	-2.065539
1	-2.299329	4.881083	-3.243434
1	0.555418	6.866001	-0.718923
1	-1.041919	6.932152	-2.621978

Compound **6d**·H^+

Atomic Number	Coordinates (Å) X	Y	Z
6	-1.19302	3.7031	-0.01861
7	-0.00071	4.32135	0.00382
6	1.19172	3.70326	0.02512
6	1.24476	2.30977	0.02547
6	-0.00045	1.63903	0.00177
6	-1.24578	2.30961	-0.02106
1	-2.07154	4.33402	-0.03234
1	2.07013	4.3343	0.03991
7	-0.00035	0.29098	0.00089
6	-1.14448	-0.50064	0.0083
6	1.14392	-0.50044	-0.00755
6	-0.70017	-1.82317	-0.00165
6	0.69981	-1.82306	0.00055
1	-1.33849	-2.69494	-0.01274
1	1.33828	-2.69474	0.01058
6	2.44248	1.53402	0.02689
1	3.39709	2.04965	0.01193
6	-2.44338	1.53365	-0.02347
1	-3.39807	2.0491	-0.00786
6	-2.40986	0.15854	0.00379
6	2.40919	0.15894	-0.00221
6	3.65937	-0.62839	-0.0283
6	3.81958	-1.69773	-0.91948
6	4.71813	-0.29016	0.82404
6	5.0135	-2.41055	-0.95523
1	3.01868	-1.95179	-1.60782
6	5.90843	-1.00862	0.78957
1	4.59657	0.5256	1.53165
6	6.05921	-2.07063	-0.09969
1	5.12843	-3.23037	-1.65857
1	6.71752	-0.74163	1.4634
1	6.98918	-2.6314	-0.12627
6	-3.65989	-0.62904	0.02894
6	-3.81984	-1.69953	0.91878
6	-4.71878	-0.28991	-0.82289
6	-5.01364	-2.41261	0.95372
1	-3.01884	-1.95432	1.60674
6	-5.90895	-1.00862	-0.78923
1	-4.59743	0.52677	-1.52947
6	-6.05947	-2.07178	0.09869
1	-5.12837	-3.23334	1.65603
1	-6.71814	-0.74091	-1.46265
1	-6.98934	-2.63275	0.12463
1	-0.00079	5.33664	0.00472

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