Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information-1

Effect of Alkyl Substituents in BODIPYs: A Comparative DFT Computational Investigation

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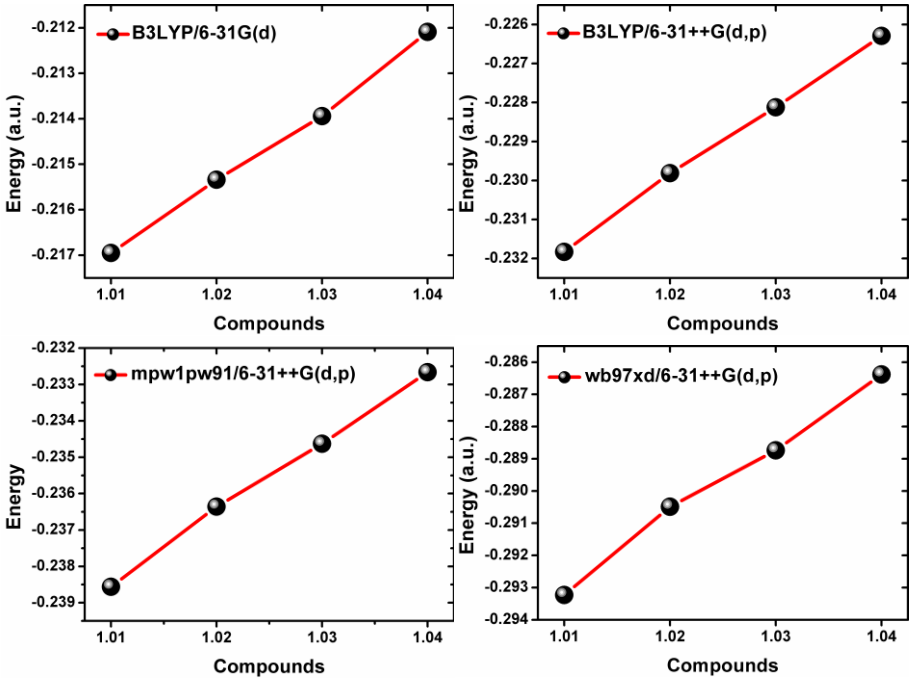
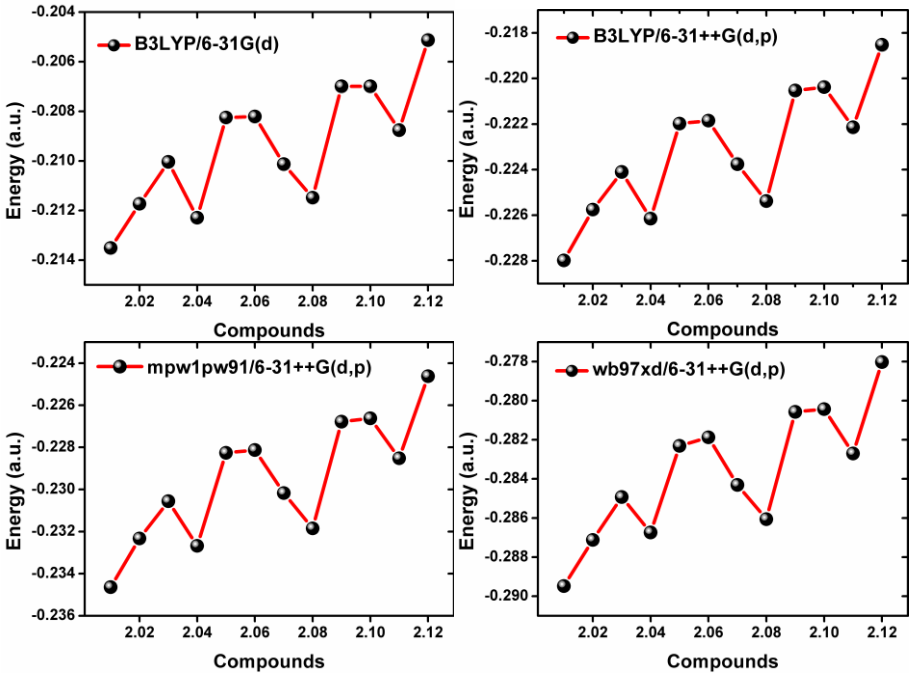


Figure S1-1: Comparison of the HOMO energies in series **1** as obtained from different computational methodologies.



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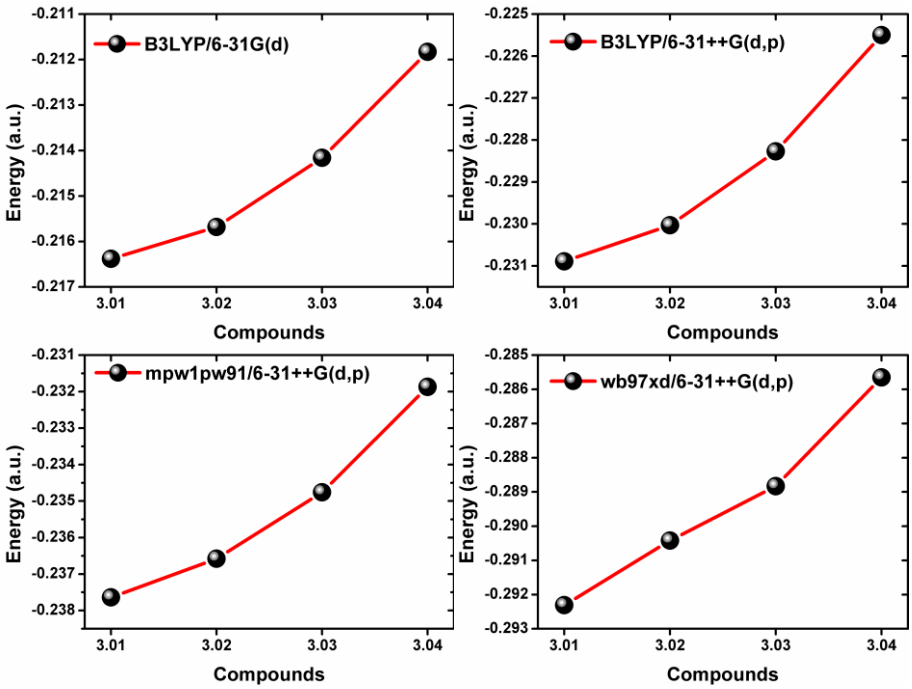

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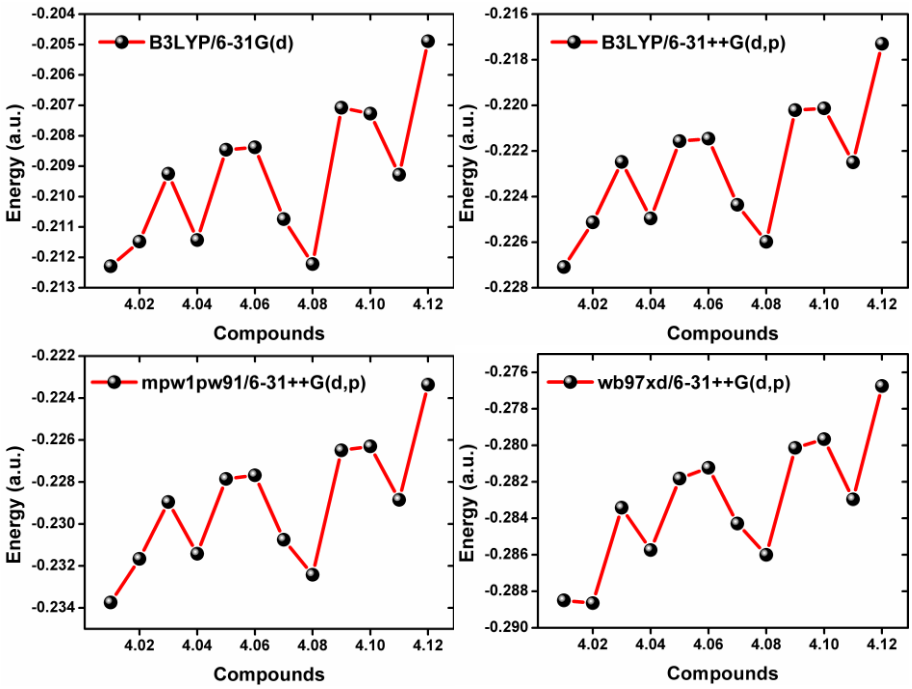

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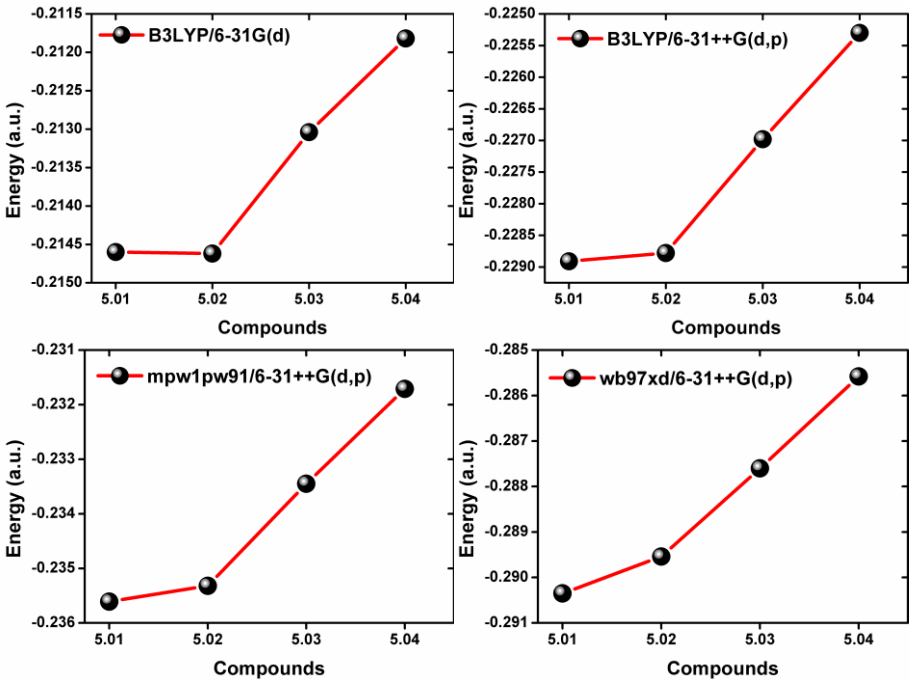

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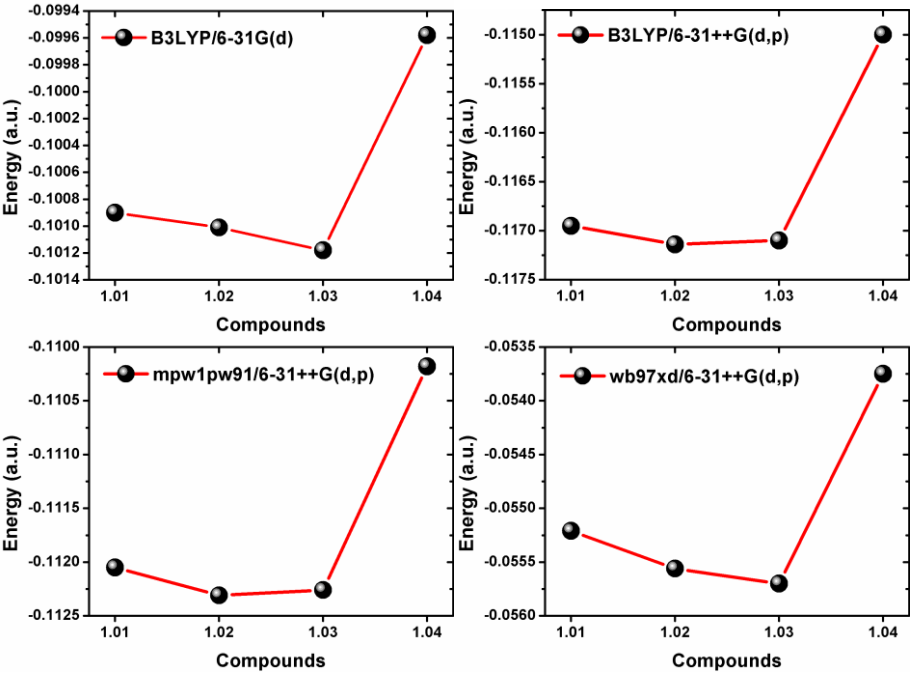

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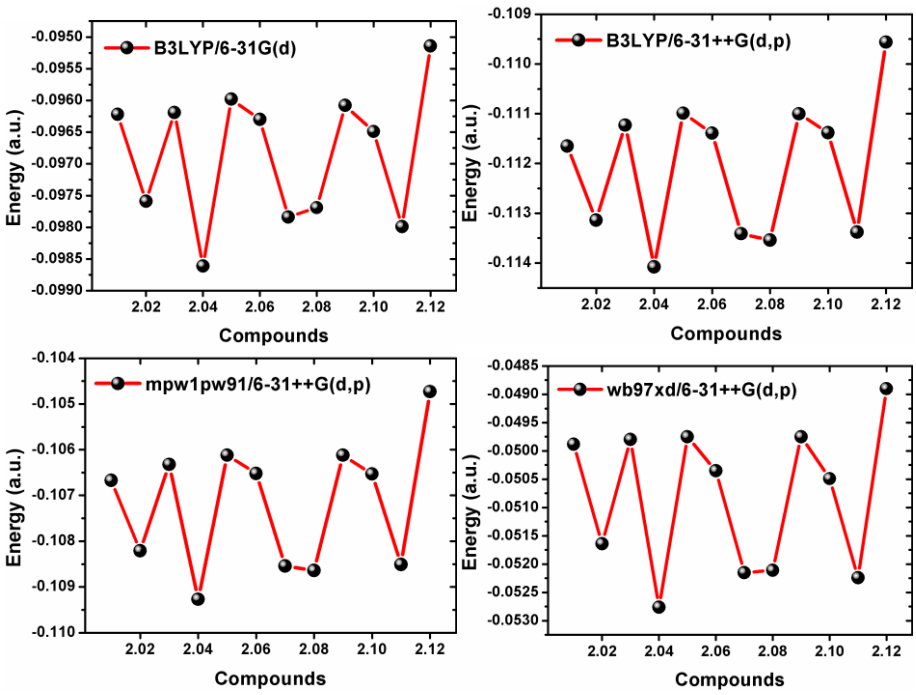

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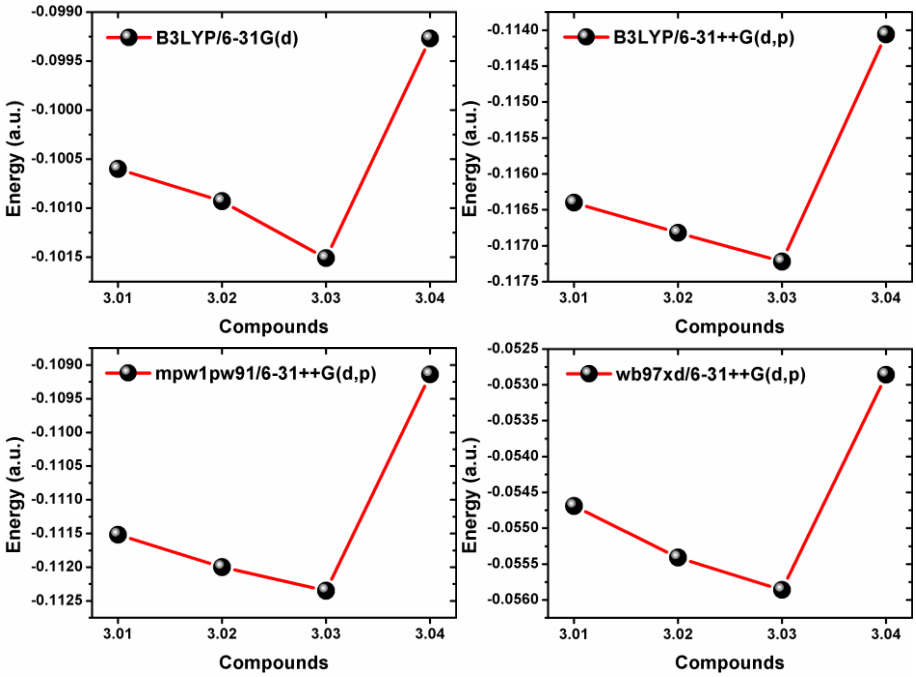

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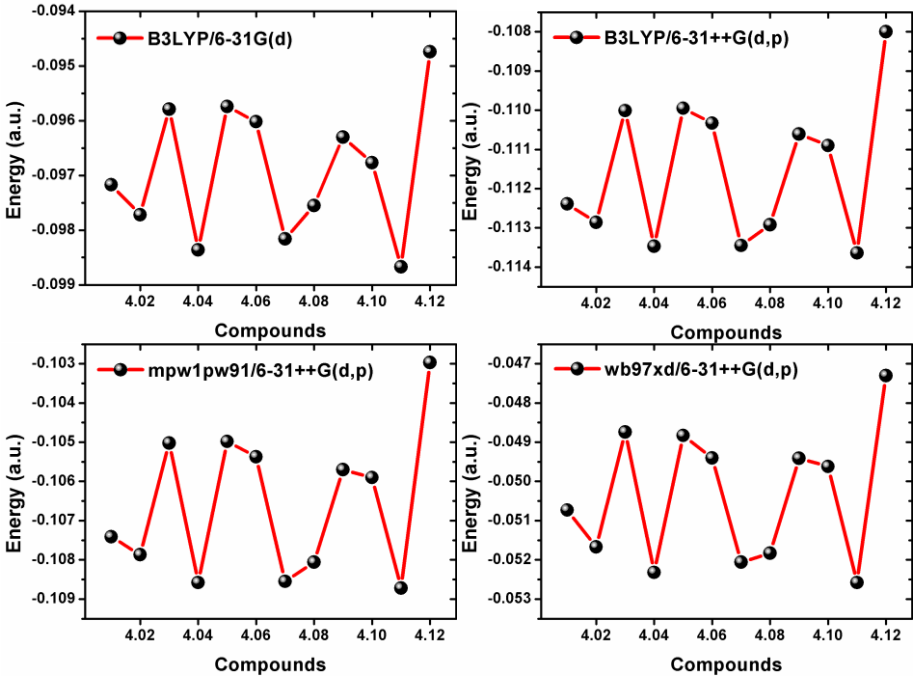

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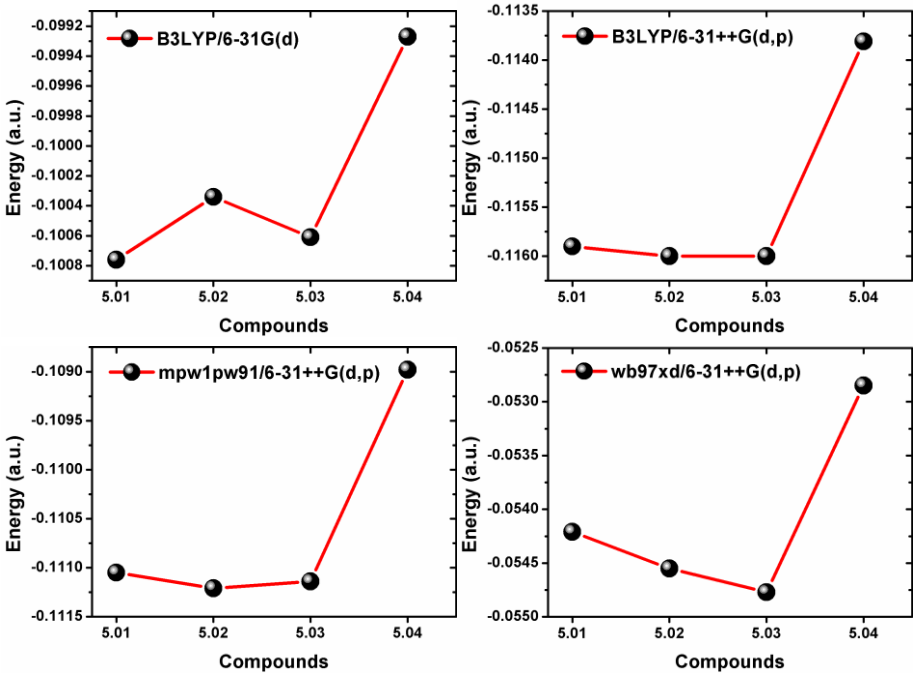

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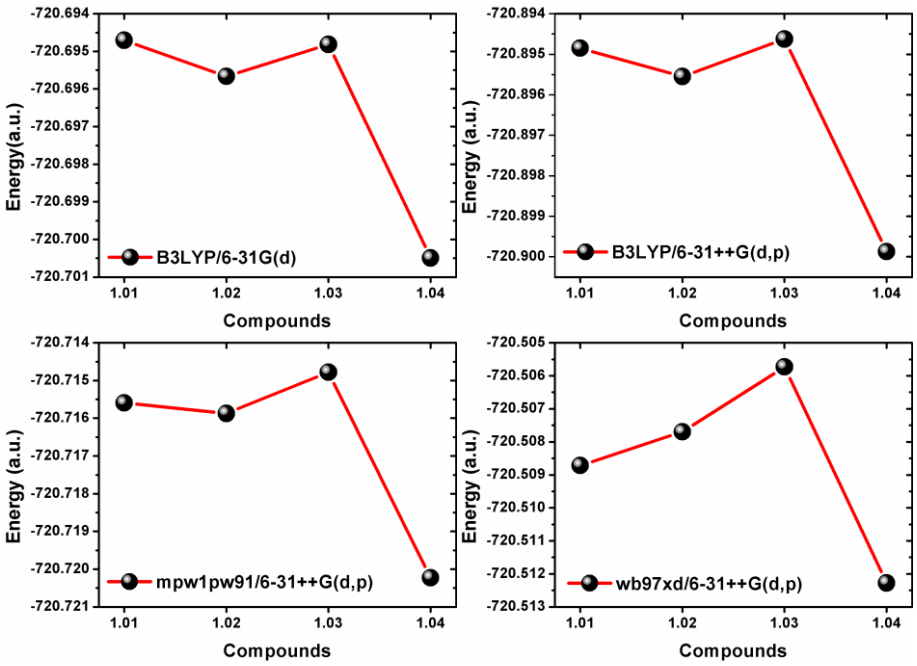

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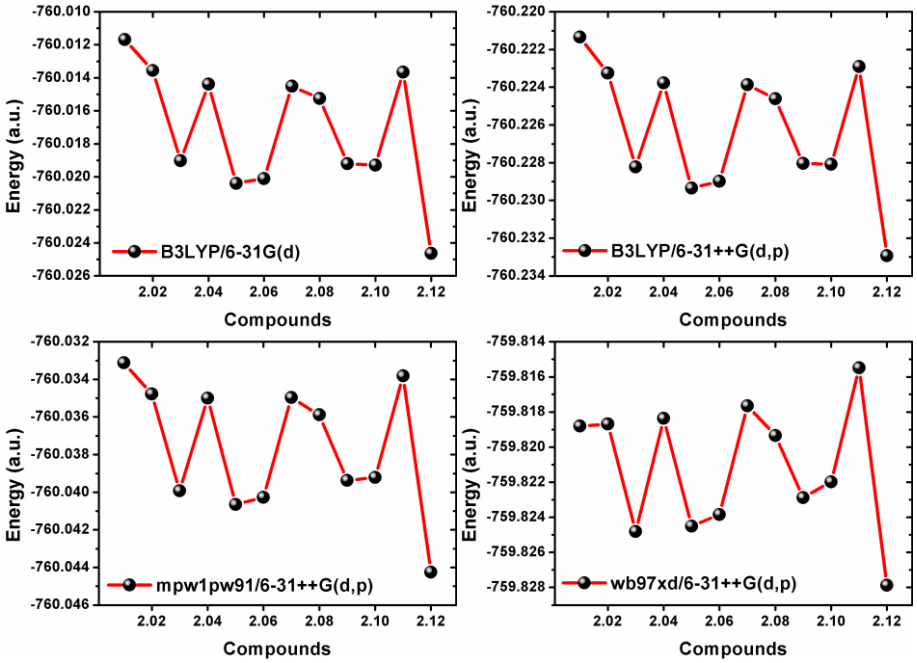

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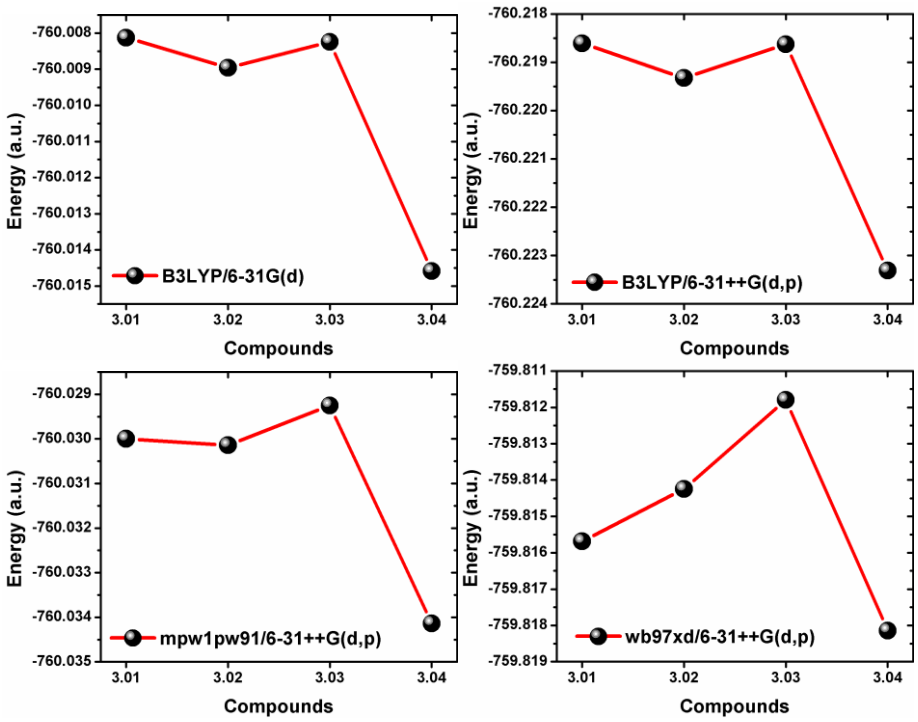

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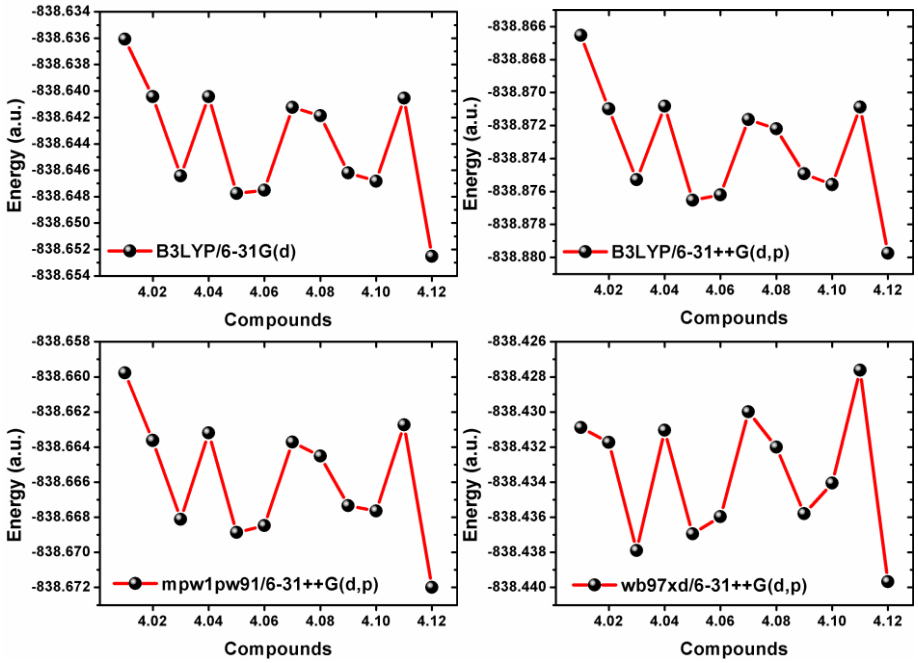

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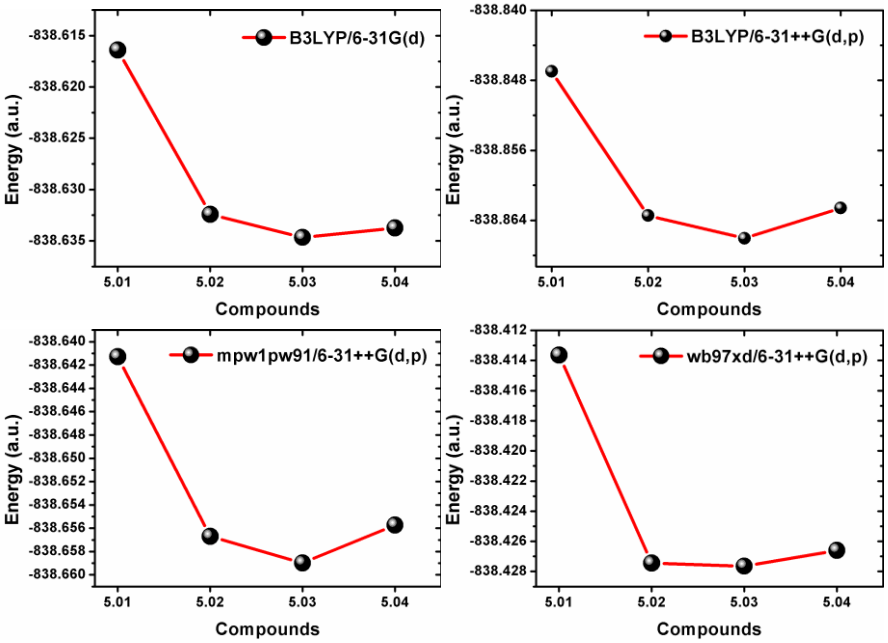

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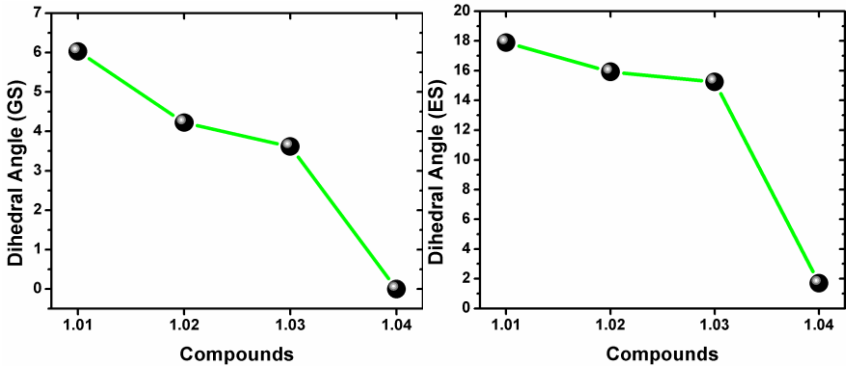

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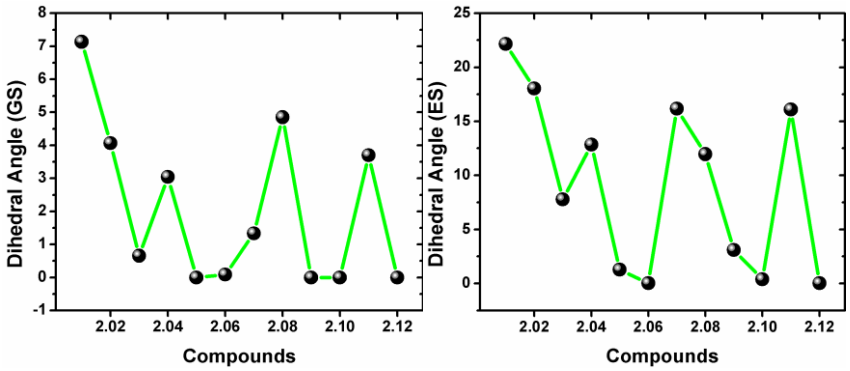

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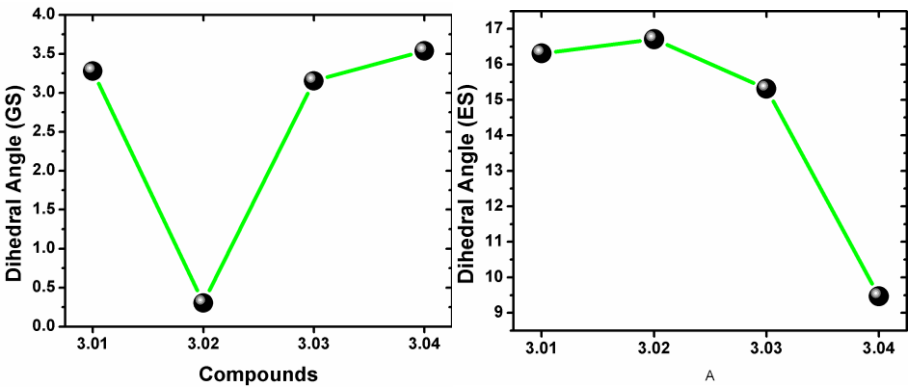

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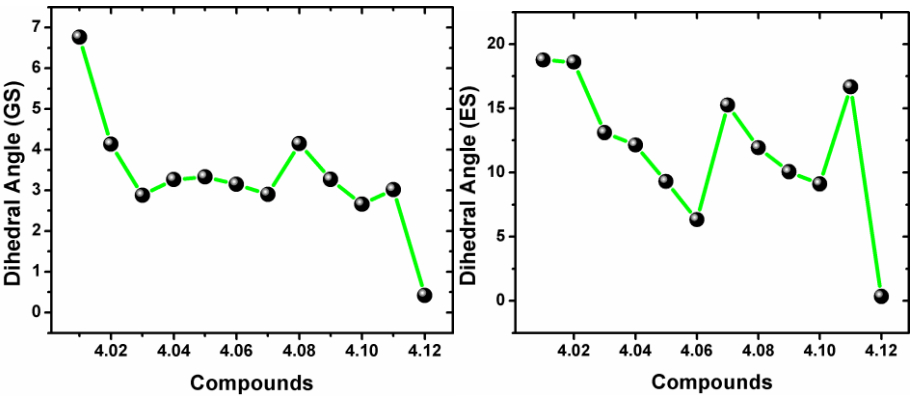

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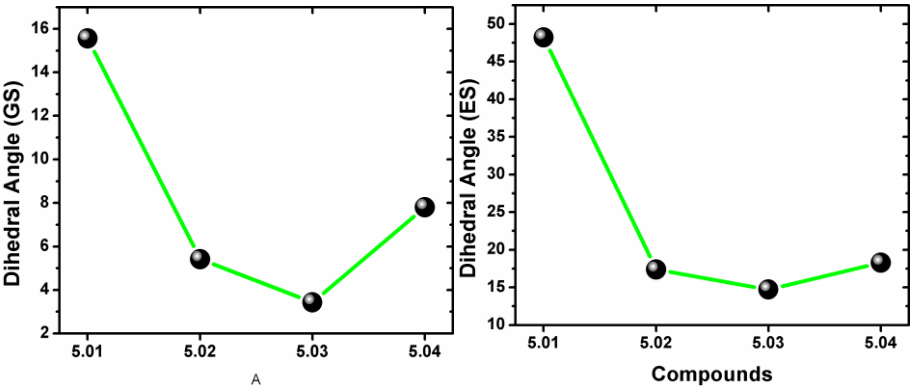

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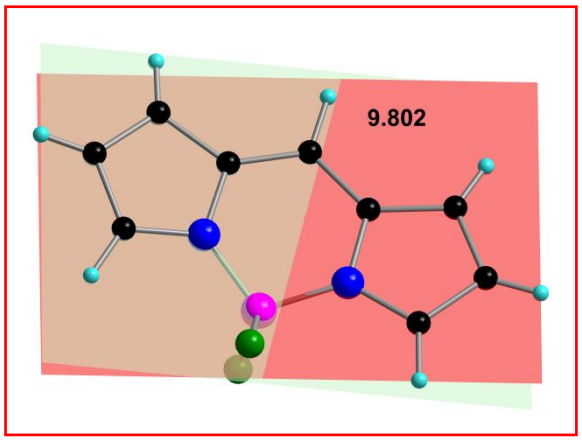

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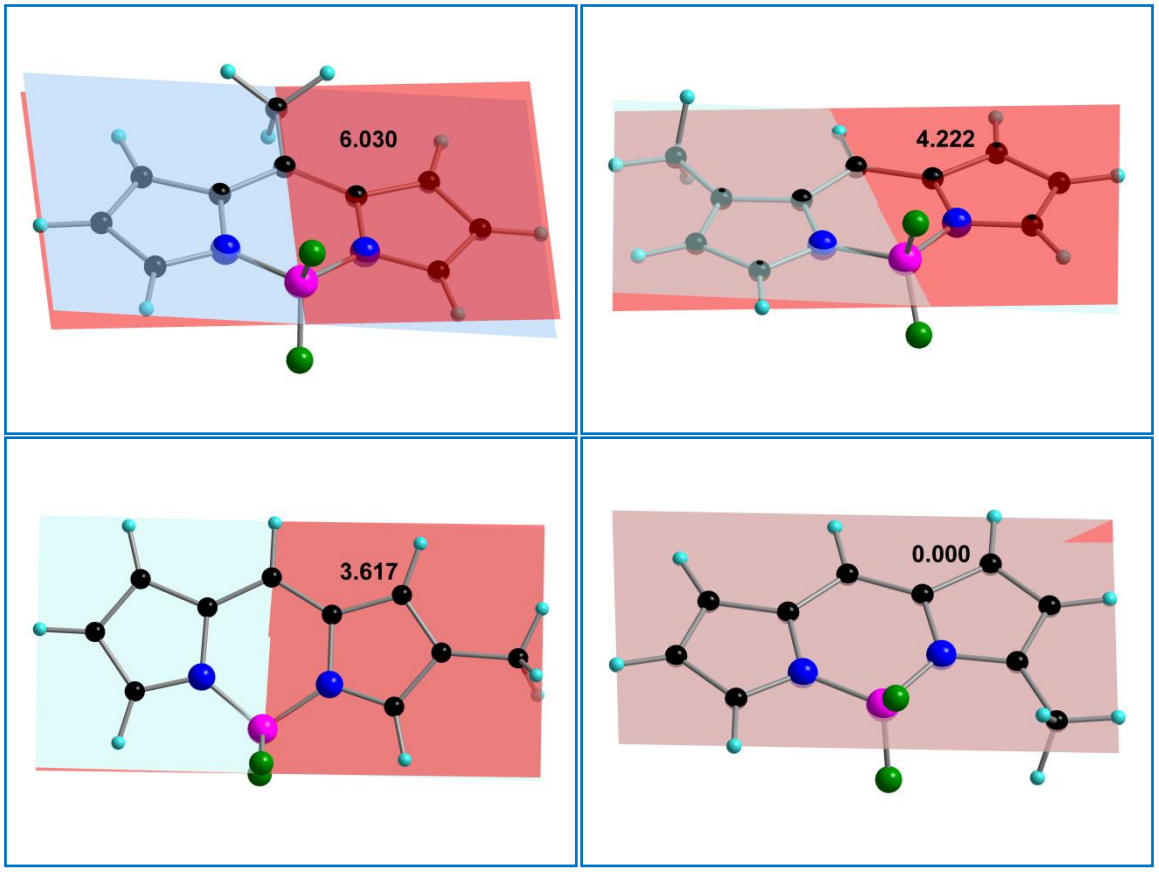

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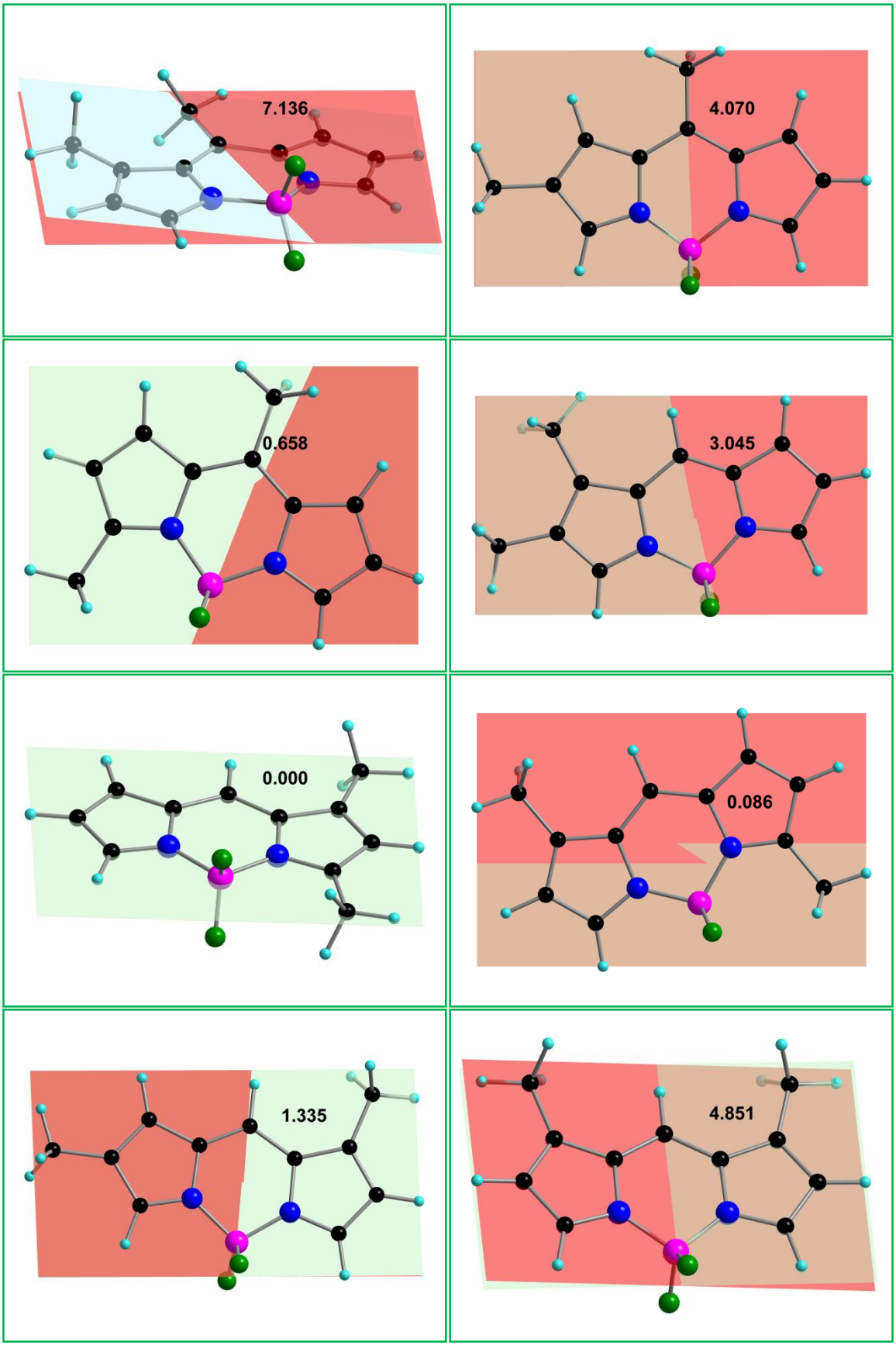
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3.045
0.000
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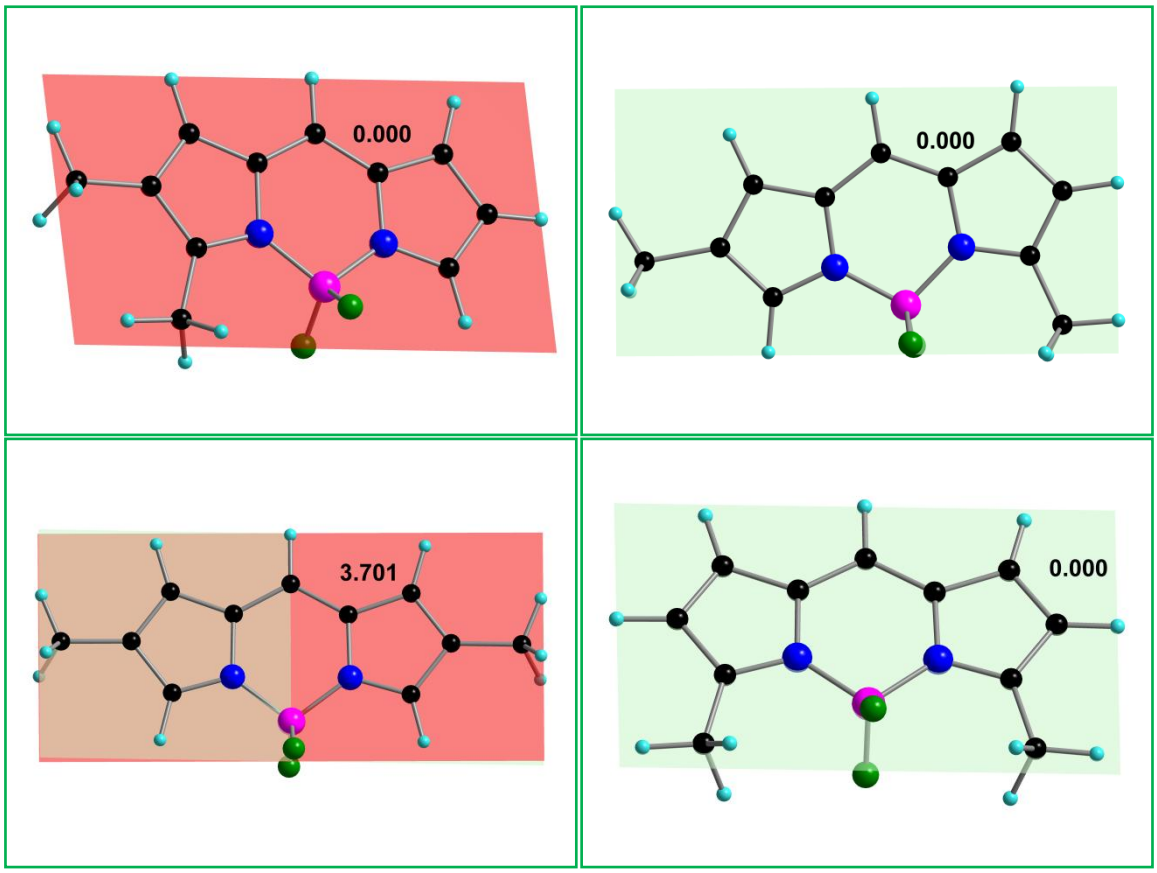
1.335
4.851



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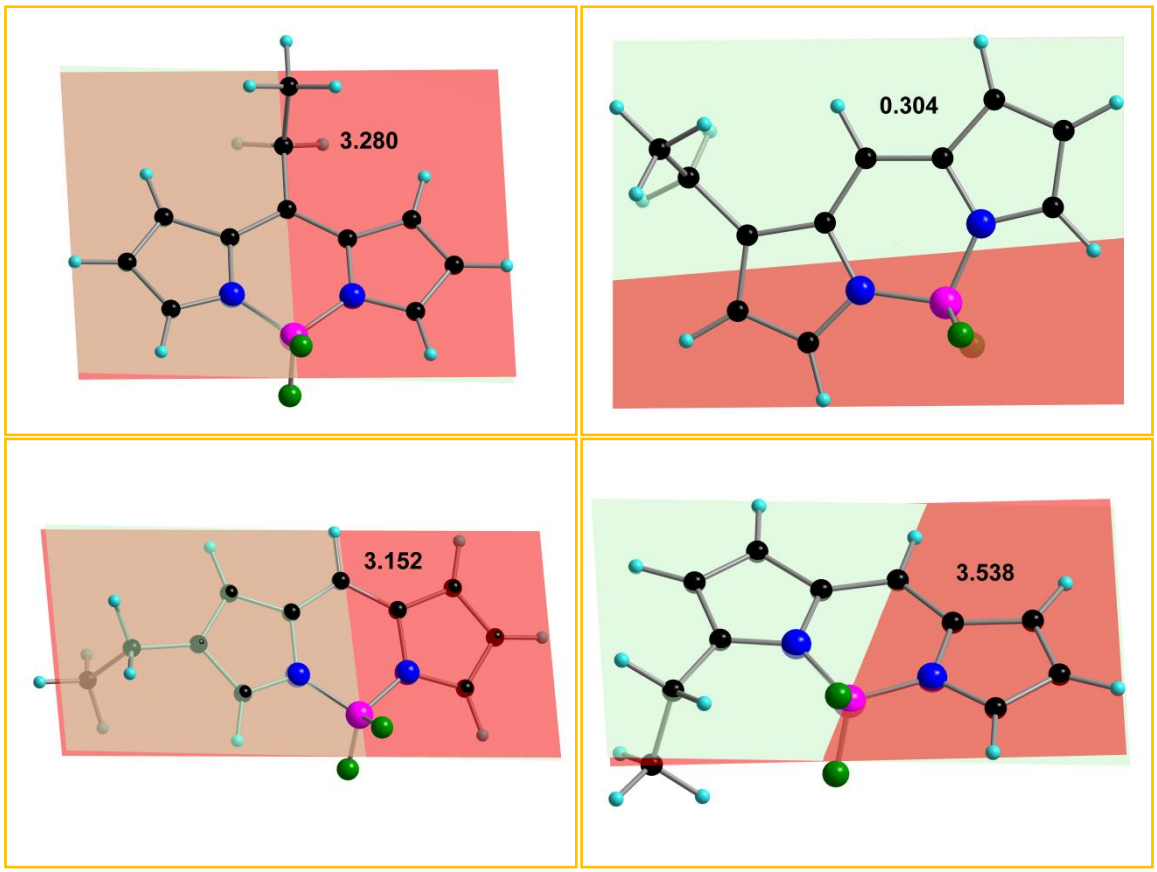

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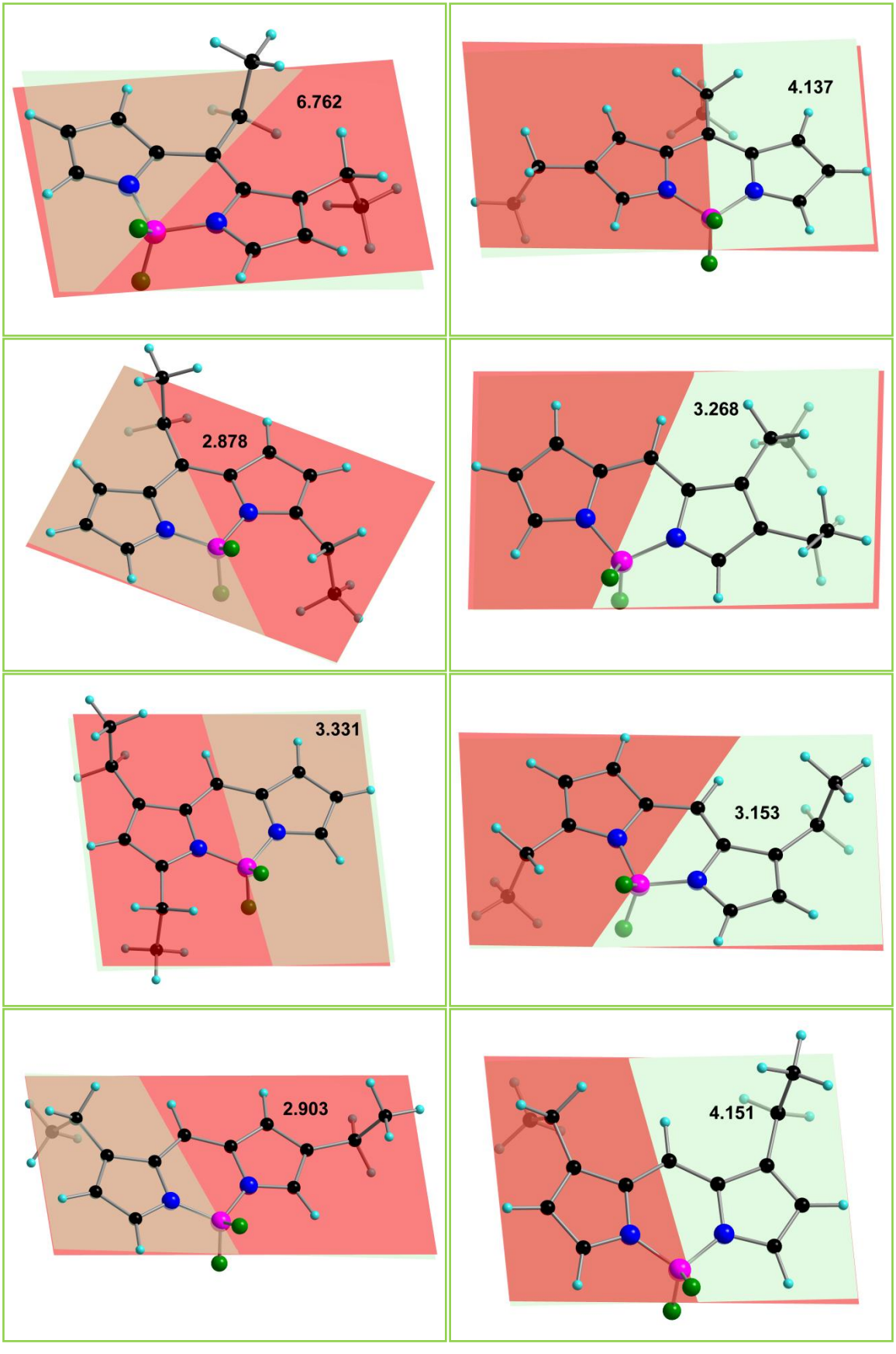
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3.153
2.903
4.151

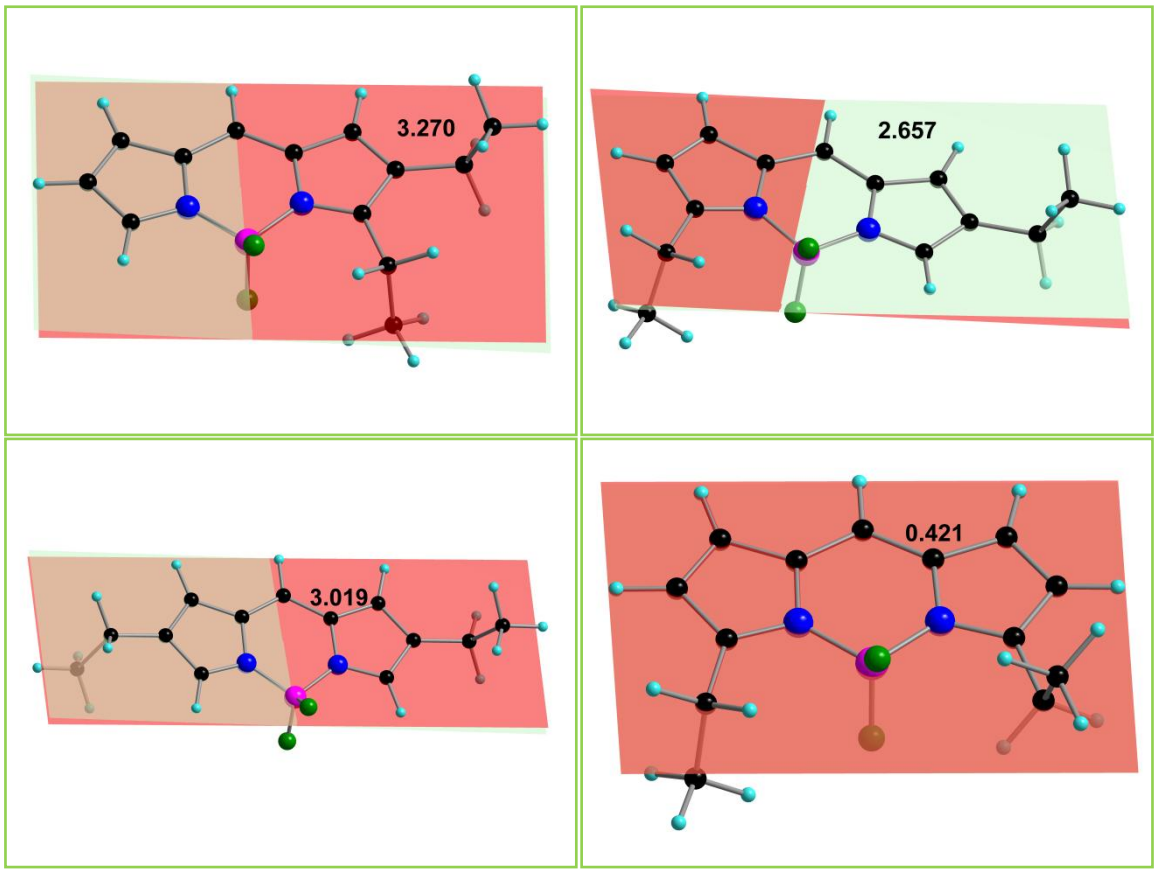
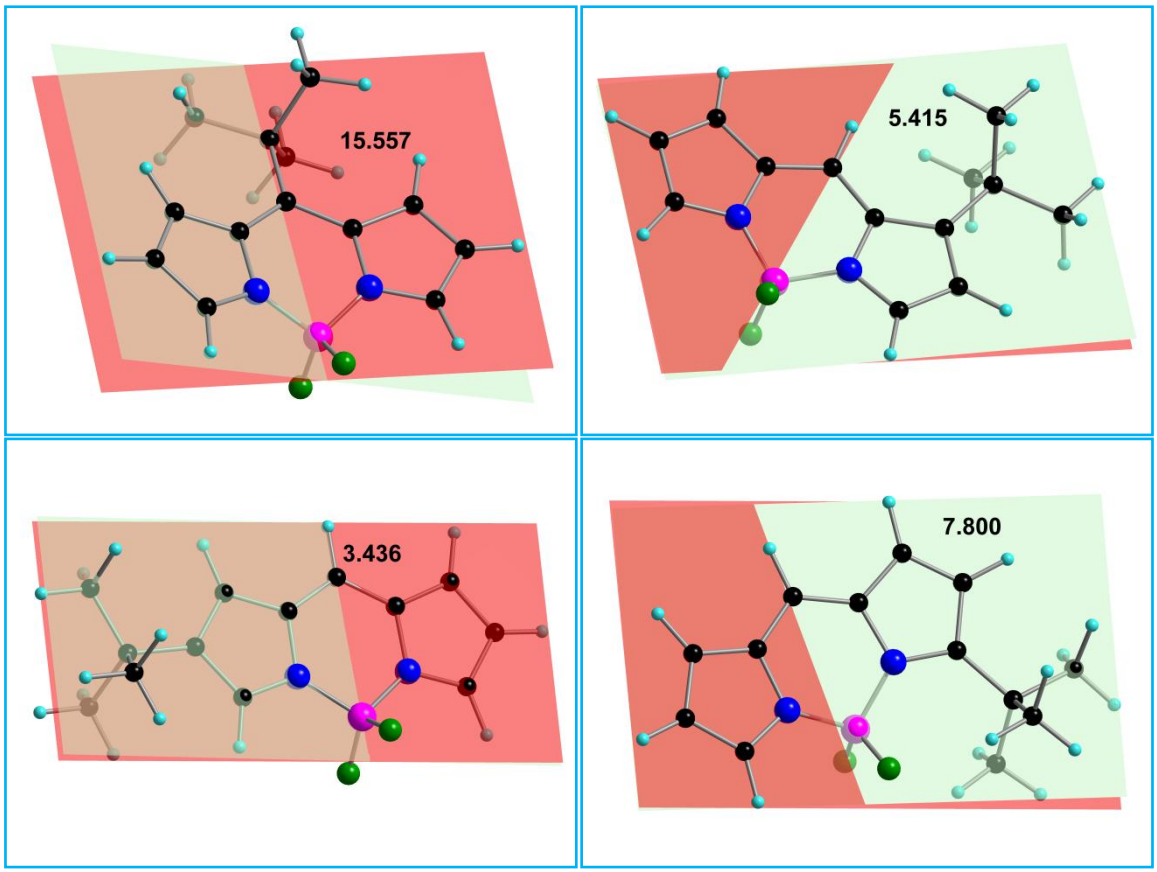


Figure S1-25: Dihedral arrangements between the two pyrrolic units in the DFT B3LYP/6-31G(d) optimised ground state structure of **4.01** to **4.12** respectively.



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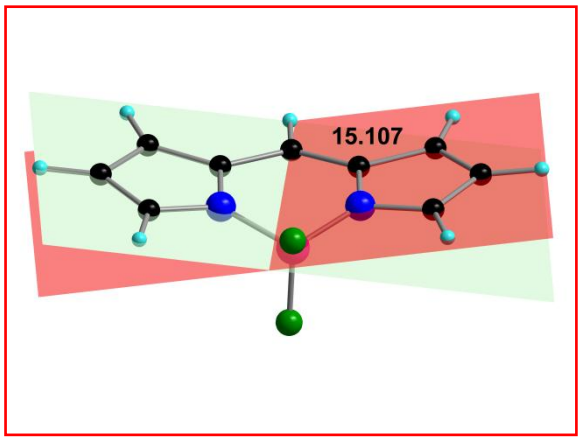

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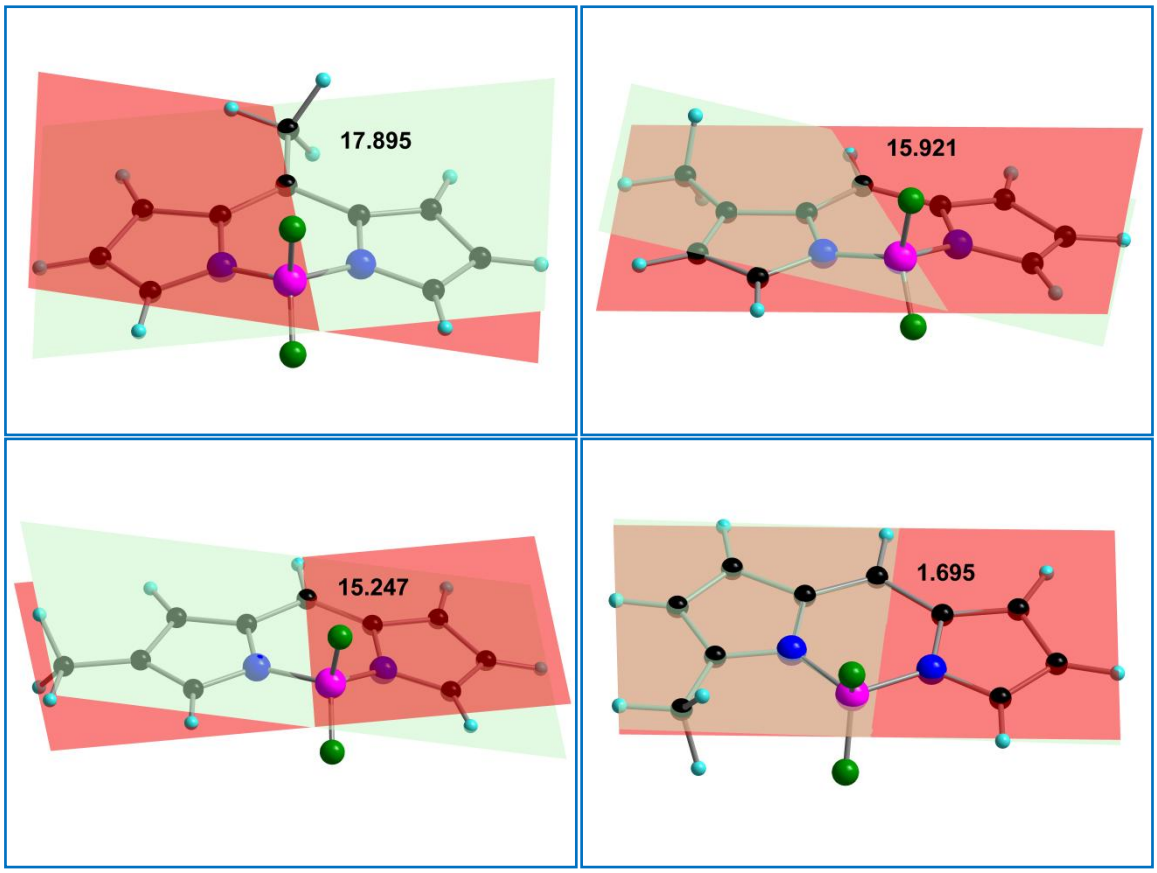
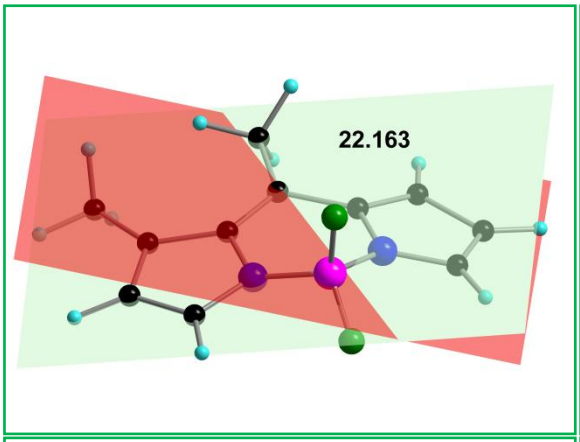


Figure S1-28: Dihedral arrangements between the two pyrrolic units in the DFT B3LYP/6-31G(d) optimised excited state structure of **1.01** to **1.04** respectively.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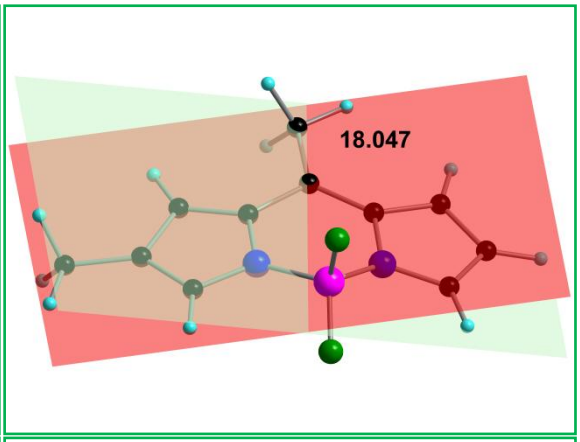
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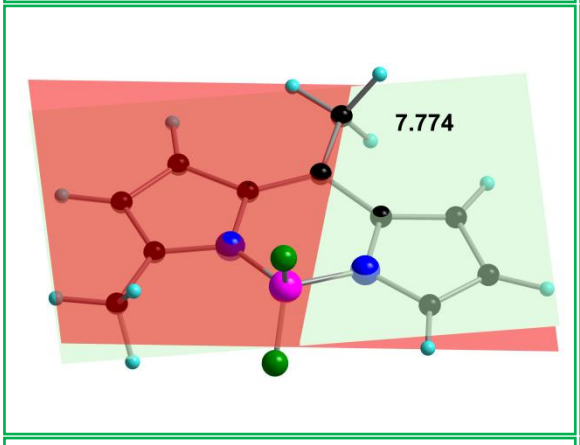
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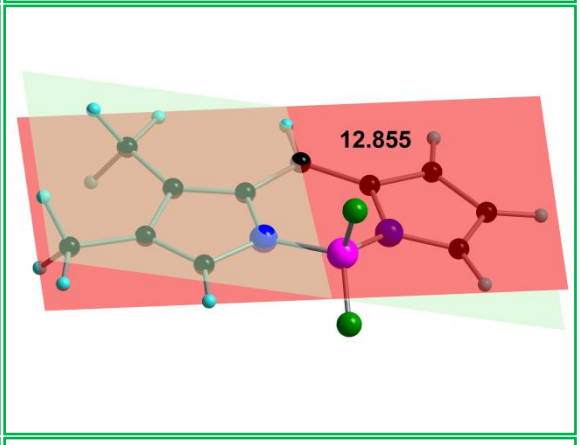
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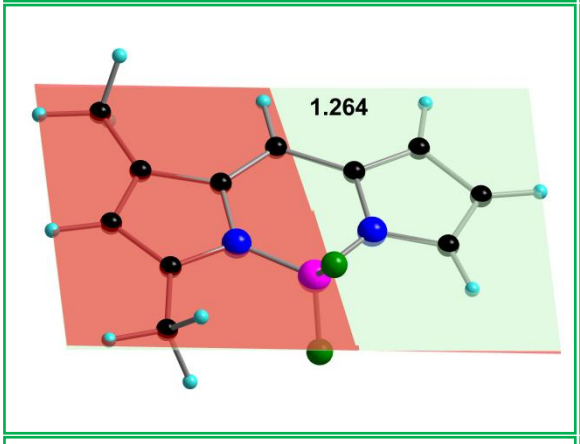
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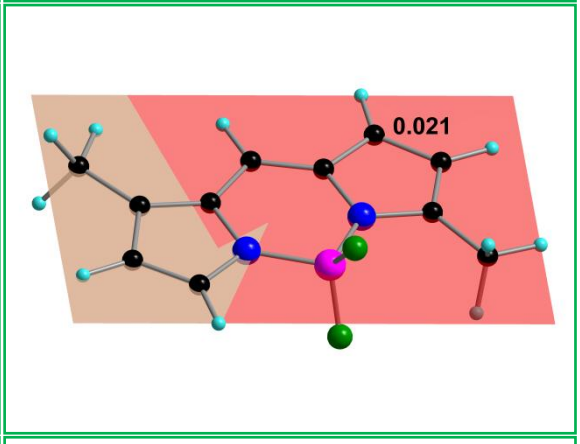
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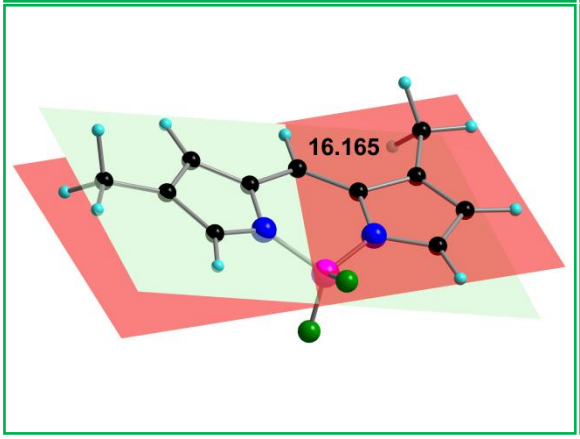
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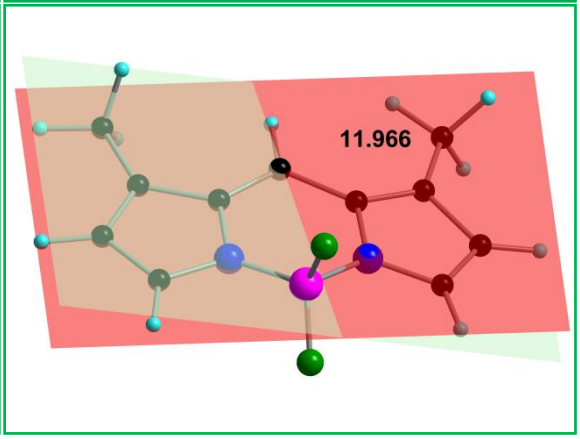
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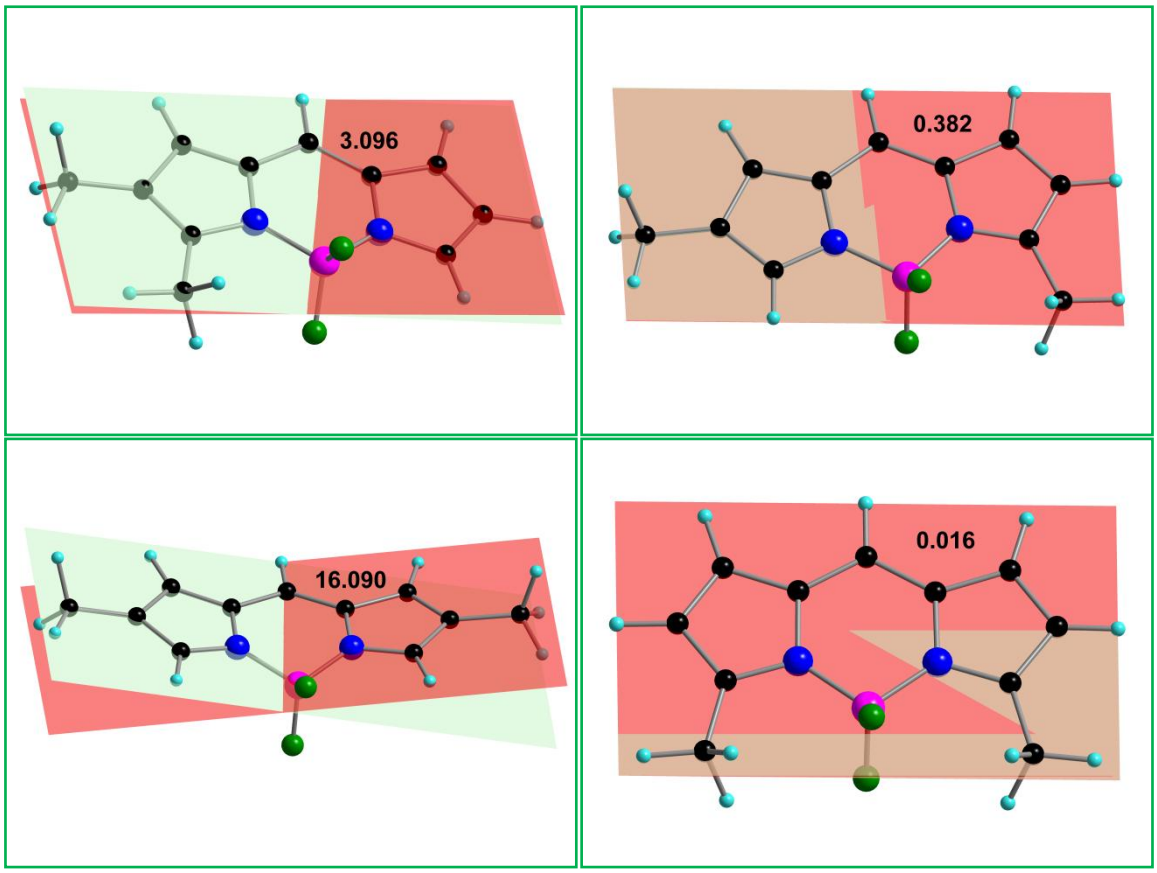


Figure S1-29: Dihedral arrangements between the two pyrrolic units in the DFT B3LYP/6-31G(d) optimised excited state structure of **2.01** to **2.12** respectively.

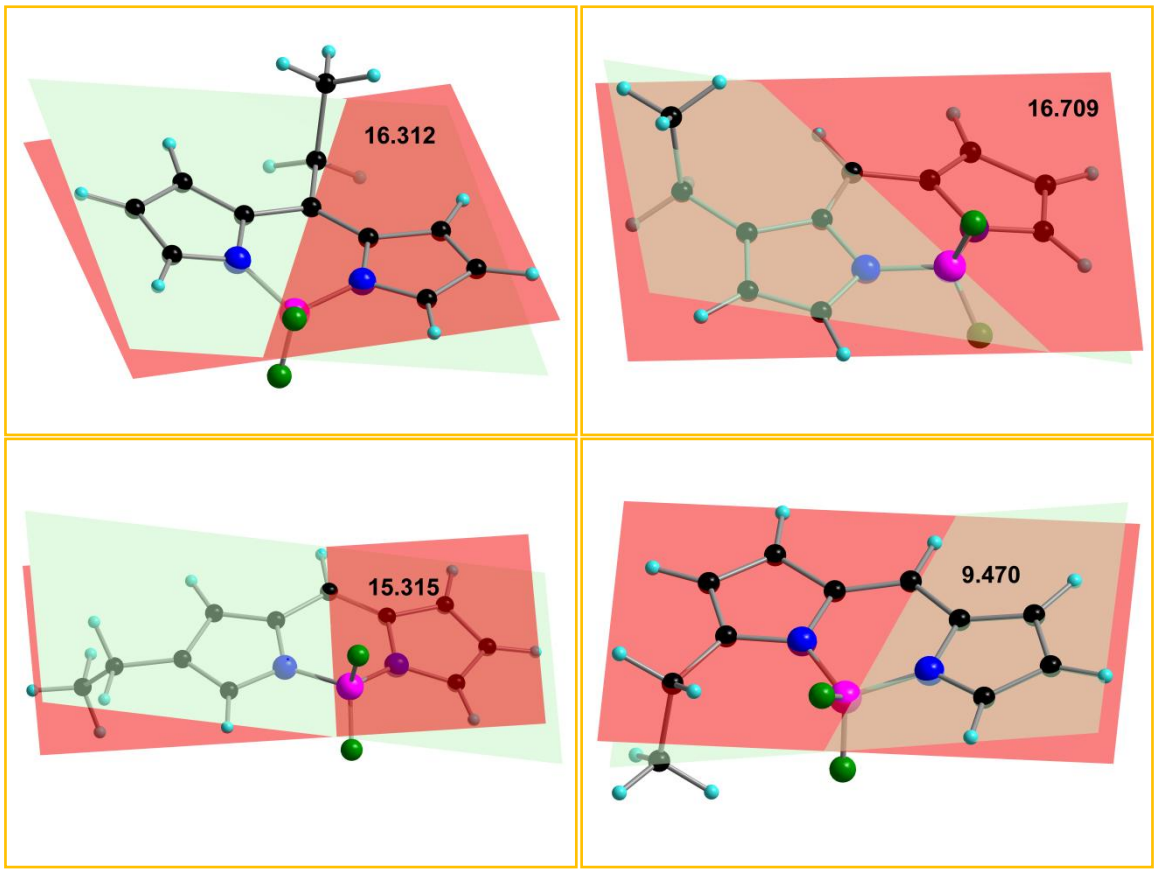
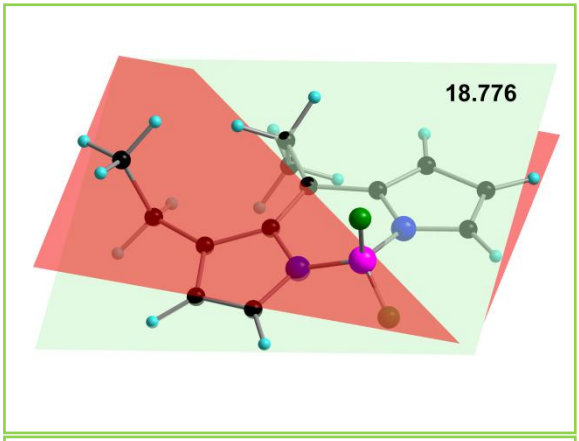


Figure S1-30: Dihedral arrangements between the two pyrrolic units in the DFT B3LYP/6-31G(d) optimised excited state structure of **3.01** to **3.04** respectively.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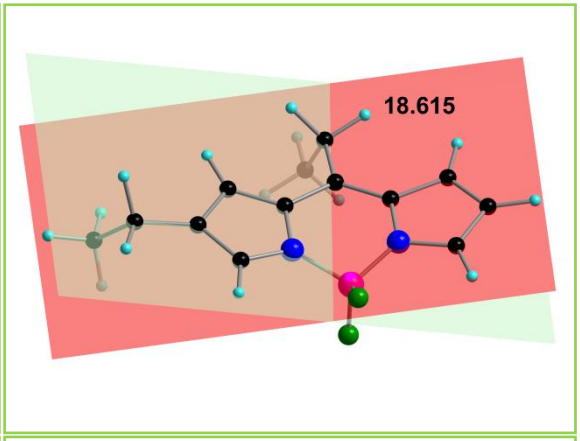
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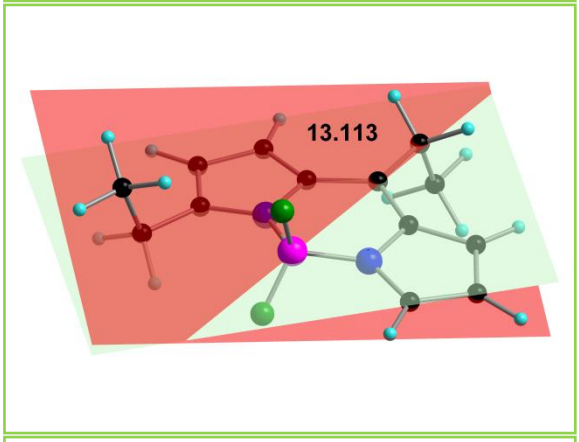
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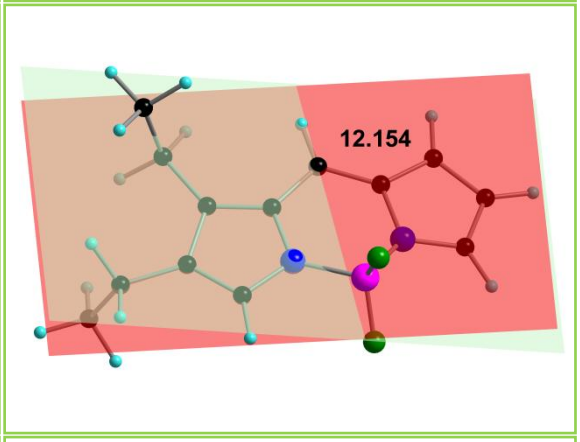
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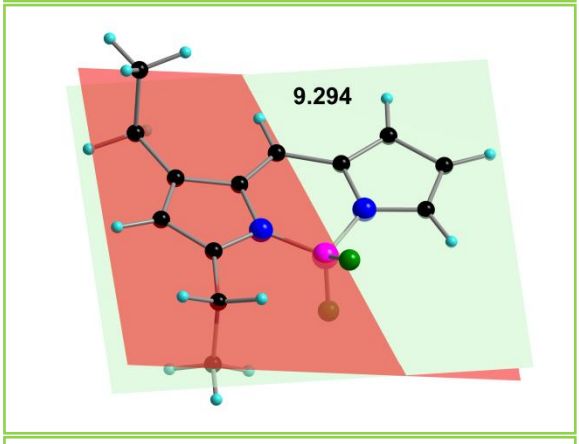
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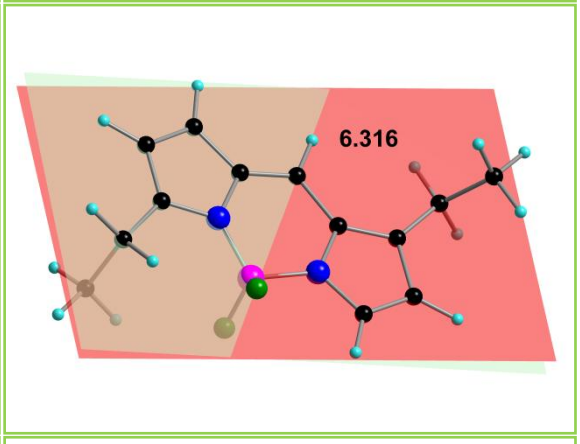
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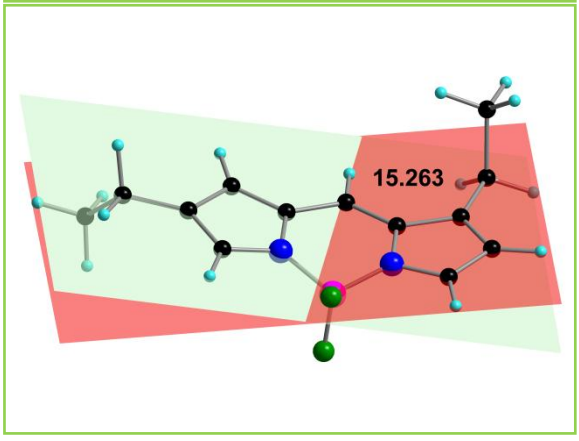
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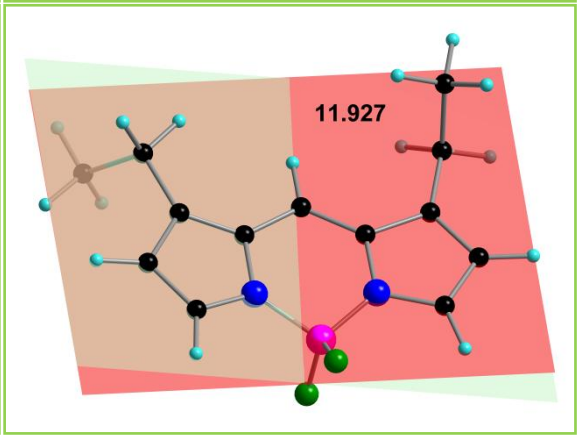
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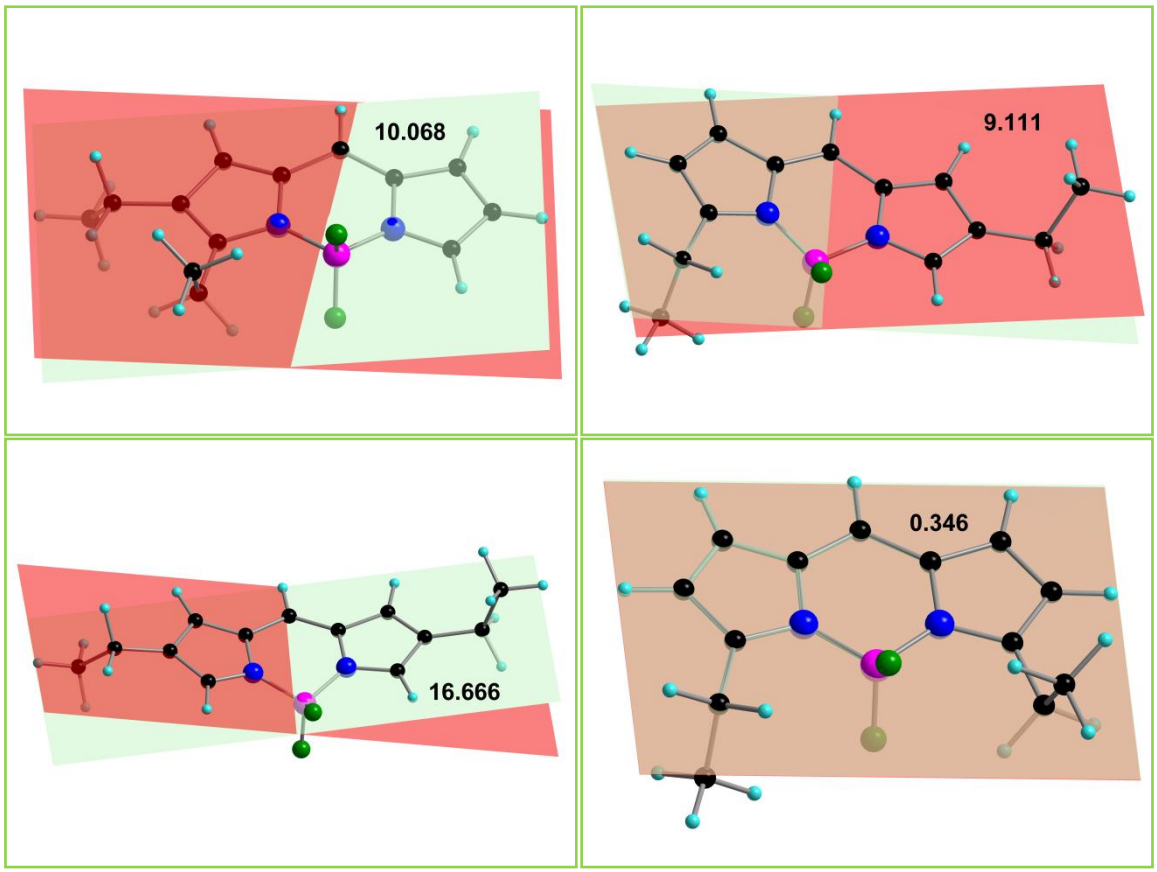

Figure S1-31: Dihedral arrangements between the two pyrrolic units in the DFT B3LYP/6-31G(d) optimised excited state structure of **4.01** to **4.12** respectively.

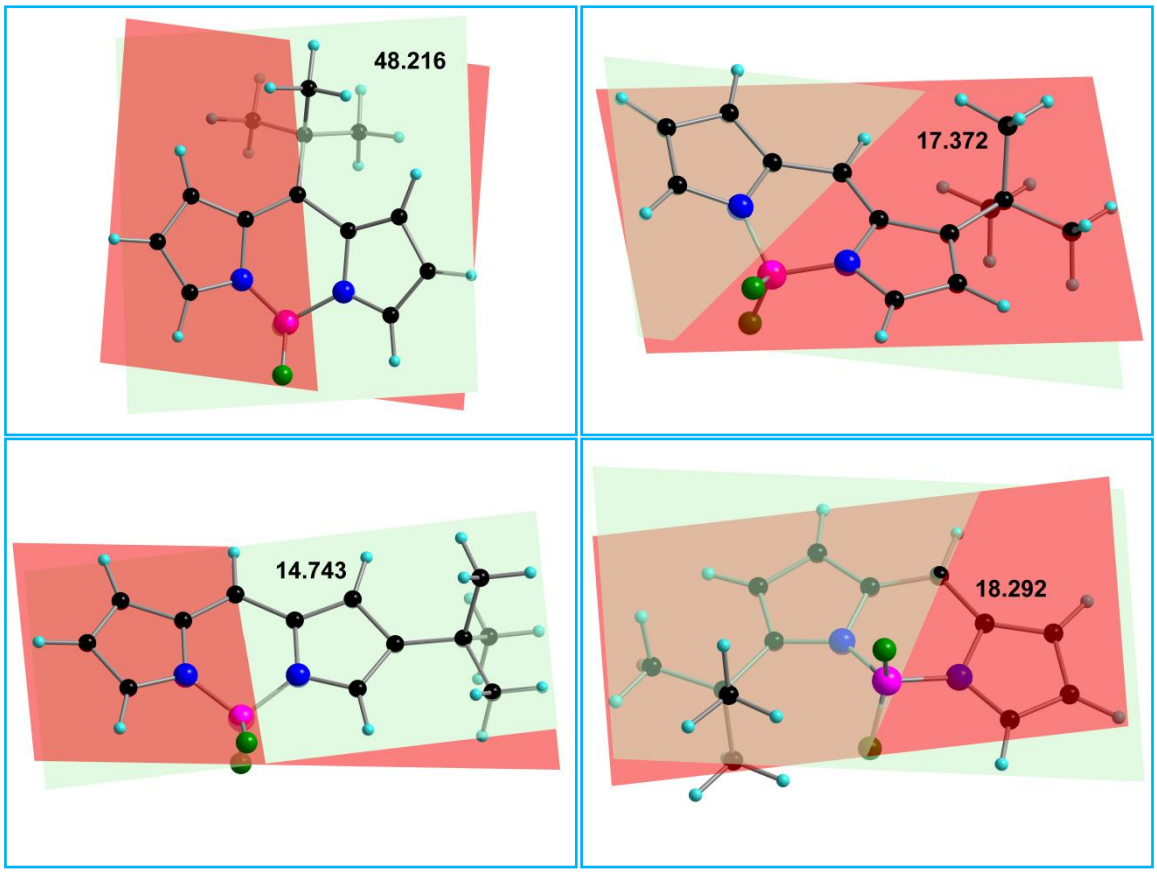

Figure S1-32: Dihedral arrangements between the two pyrrolic units in the DFT B3LYP/6-31G(d) optimised excited state structure of **5.01** to **5.04** respectively.

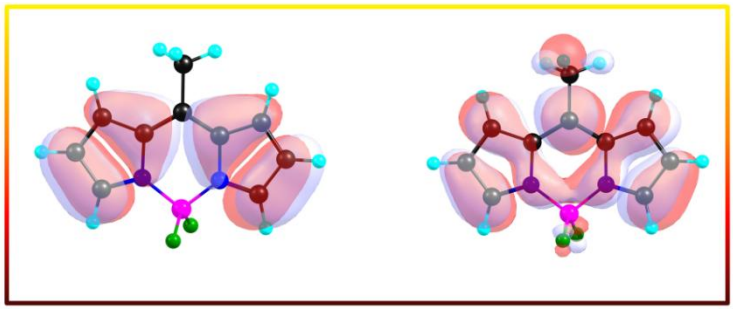

Figure S1-33: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **1.01** (isovalue = 0.02).

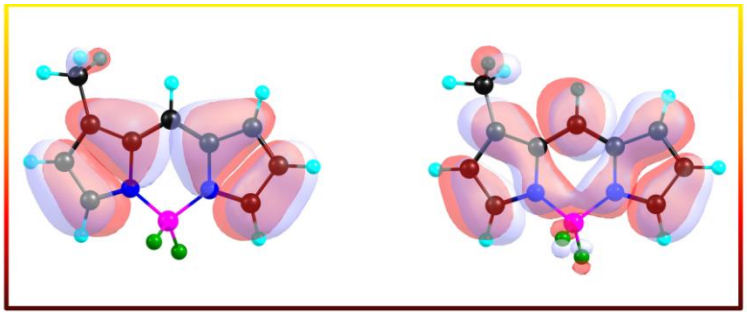

Figure S1-34: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **1.02** (isovalue = 0.02).

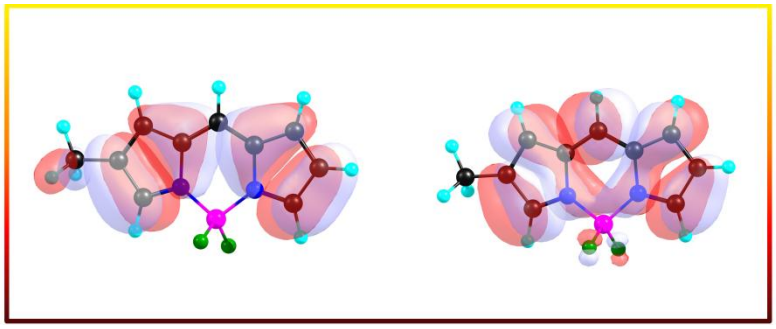

Figure S1-35: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **1.03** (isovalue = 0.02).

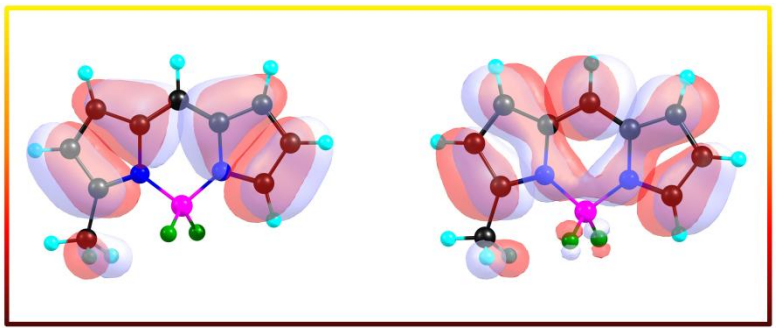

Figure S1-36: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **1.04** (isovalue = 0.02).

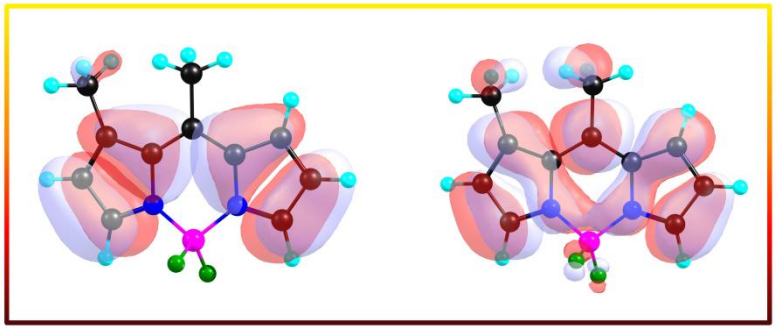

Figure S1-37: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.01** (isovalue = 0.02).

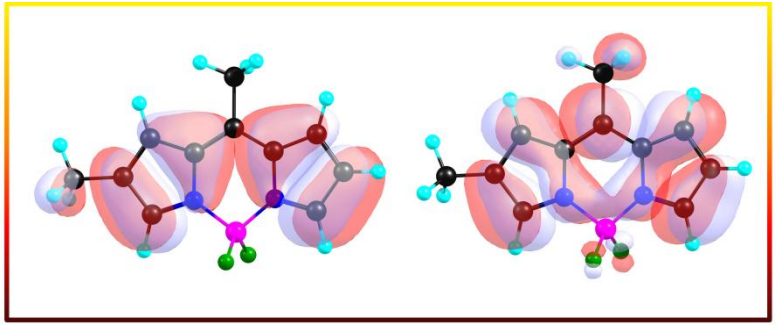

Figure S1-38: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.02** (isovalue = 0.02).

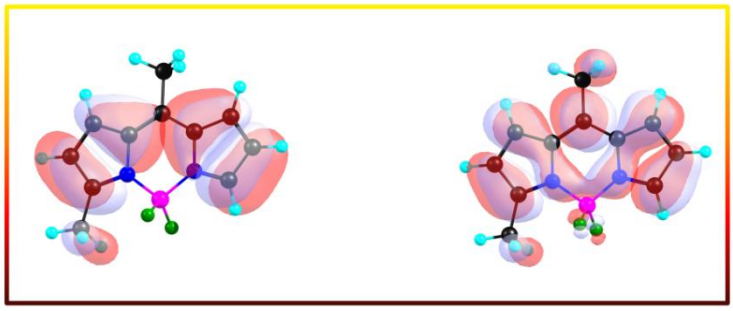

Figure S1-39: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.03** (isovalue = 0.02).

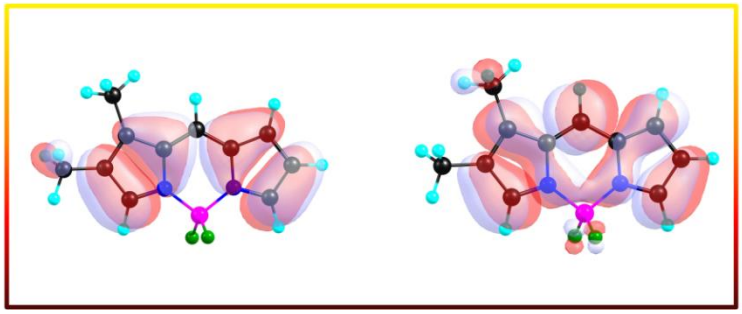

Figure S1-40: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.04** (isovalue = 0.02).

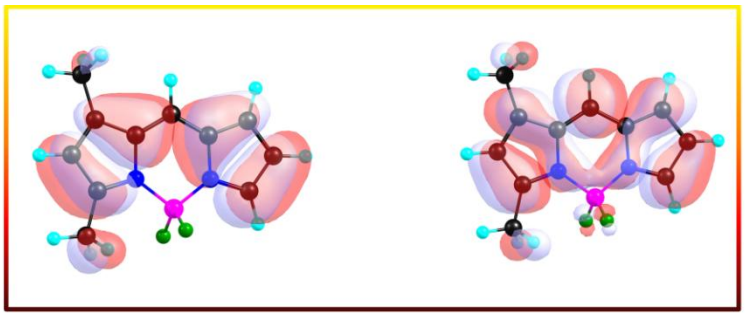

Figure S1-41: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.05** (isovalue = 0.02).

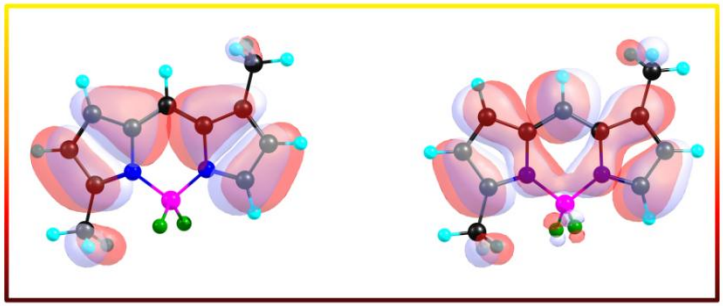

Figure S1-42: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.06** (isovalue = 0.02).

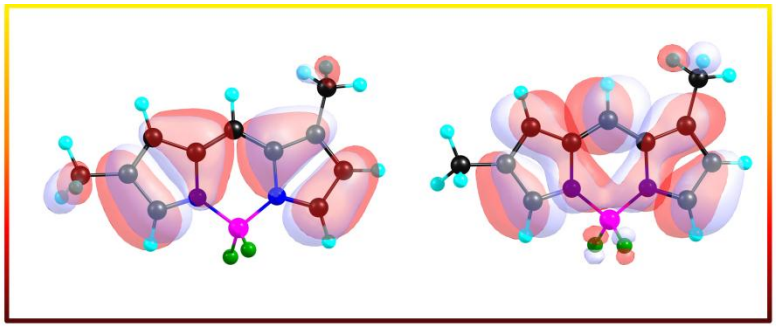

Figure S1-43: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.07** (isovalue = 0.02).

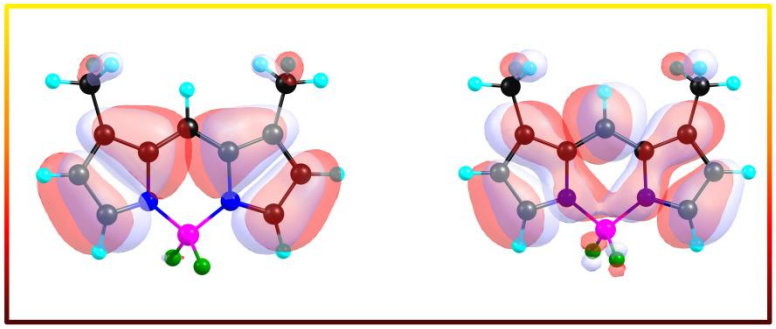

Figure S1-44: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.08** (isovalue = 0.02).

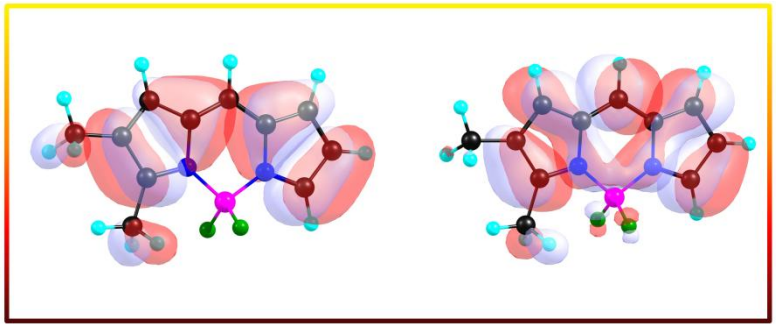

Figure S1-45: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.09** (isovalue = 0.02).

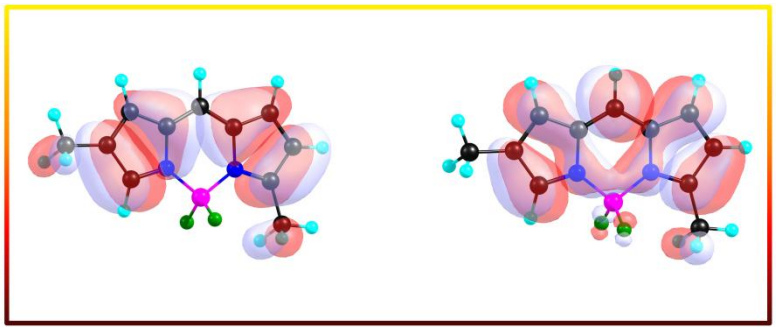

Figure S1-46: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.10** (isovalue = 0.02).

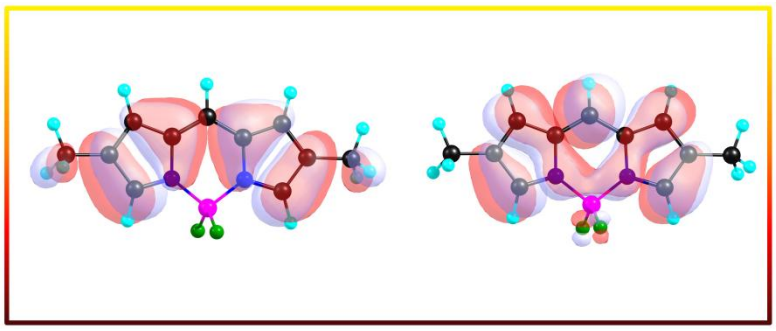

Figure S1-47: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.11** (isovalue = 0.02).

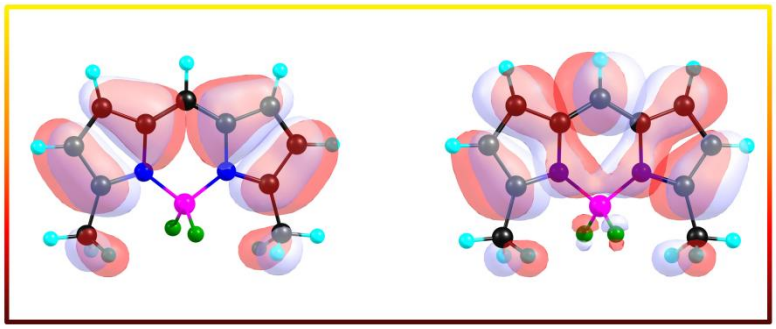

Figure S1-48: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **2.12** (isovalue = 0.02).

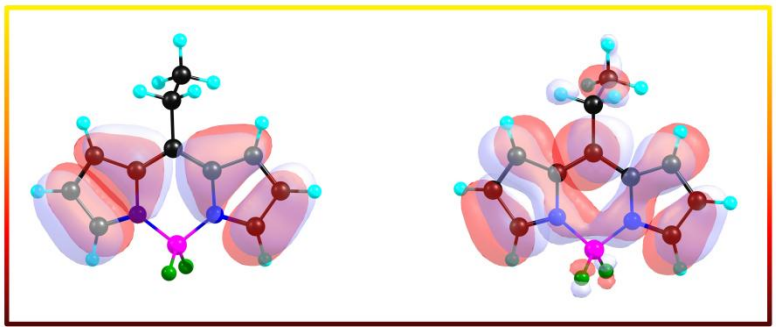

Figure S1-49: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **3.01** (isovalue = 0.02).

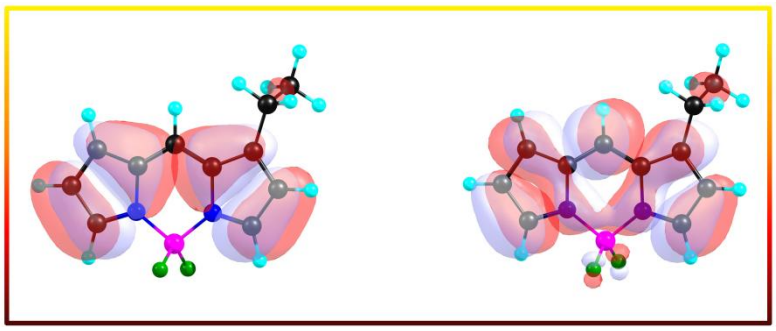

Figure S1-50: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **3.02** (isovalue = 0.02).

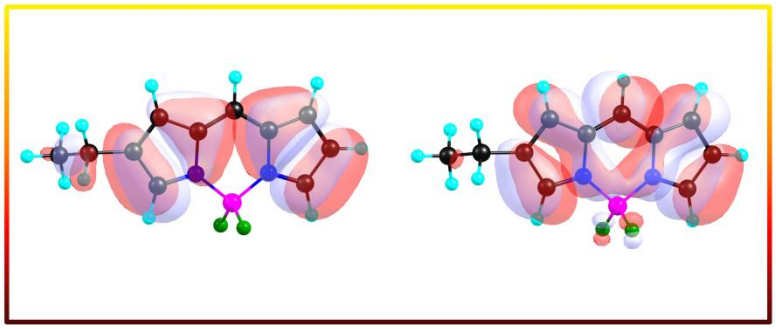

Figure S1-51: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **3.03** (isovalue = 0.02).

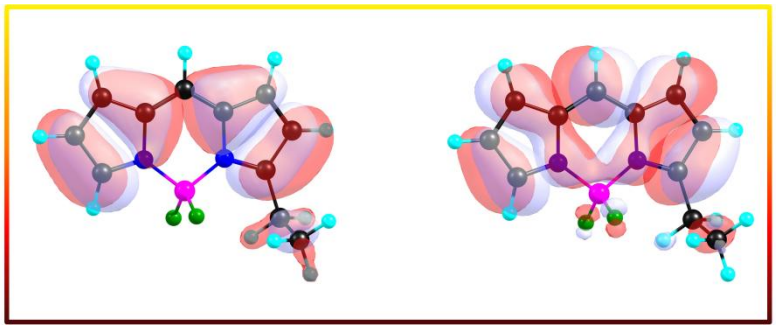

Figure S1-52: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **3.04** (isovalue = 0.02).

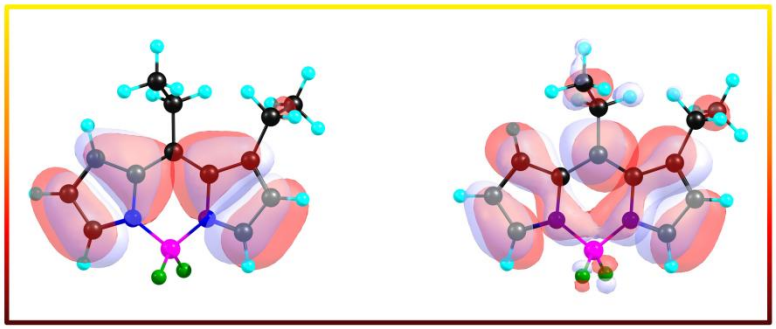

Figure S1-53: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.01** (isovalue = 0.02).

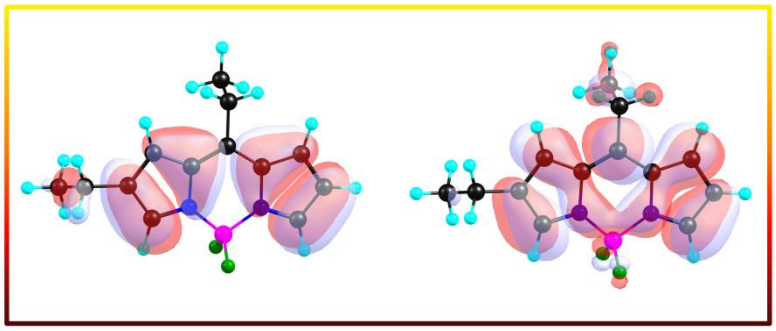

Figure S1-54: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.02** (isovalue = 0.02).

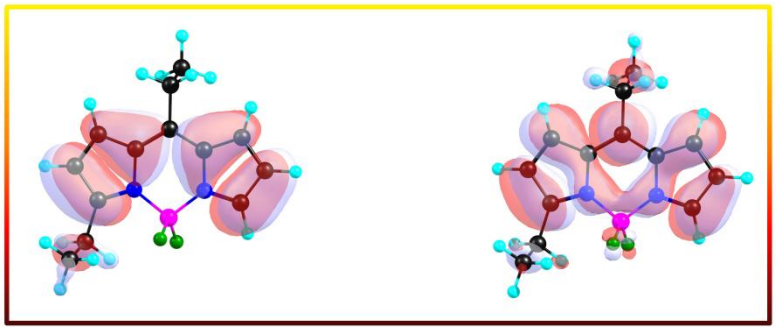

Figure S1-55: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.03** (isovalue = 0.02).

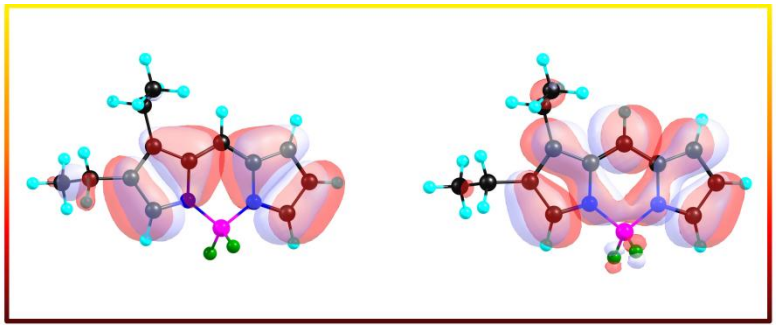

Figure S1-56: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.04** (isovalue = 0.02).

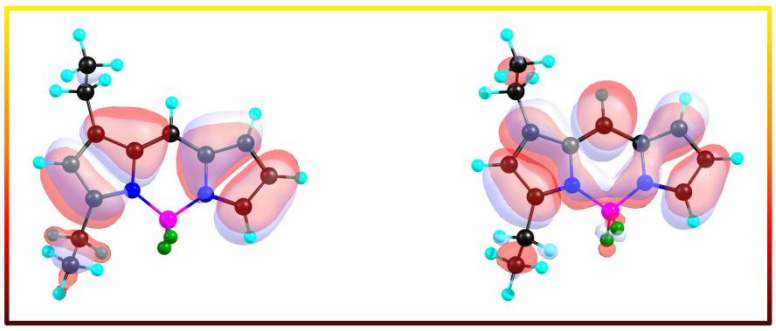

Figure S1-57: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.05** (isovalue = 0.02).

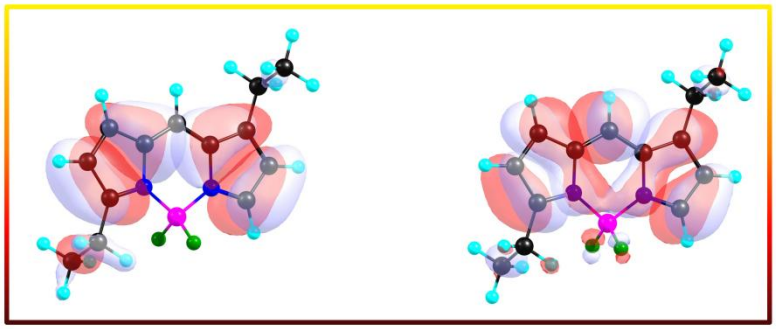

Figure S1-58: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.06** (isovalue = 0.02).

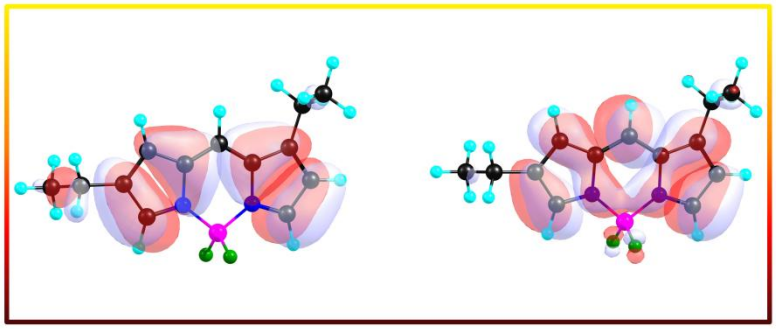

Figure S1-59: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.07** (isovalue = 0.02).

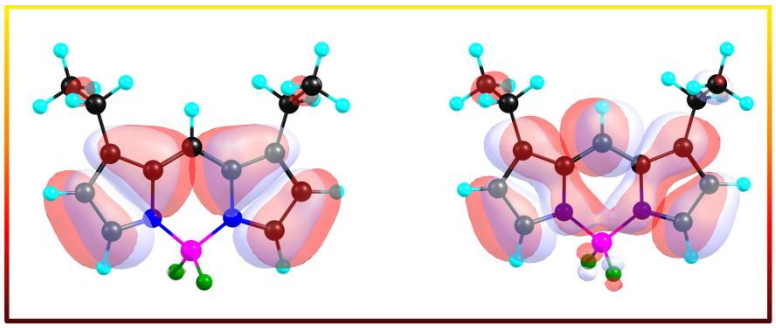

Figure S1-60: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.08** (isovalue = 0.02).

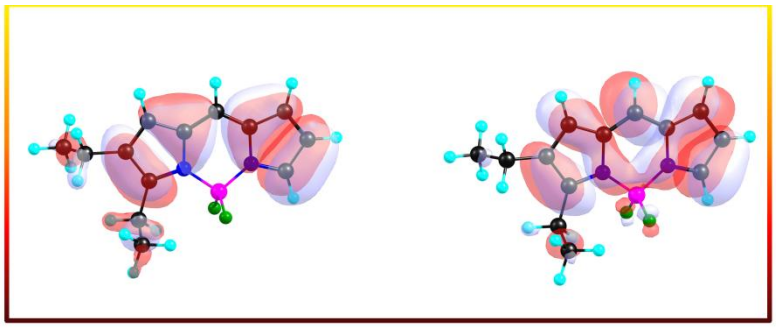

Figure S1-61: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.09** (isovalue = 0.02).

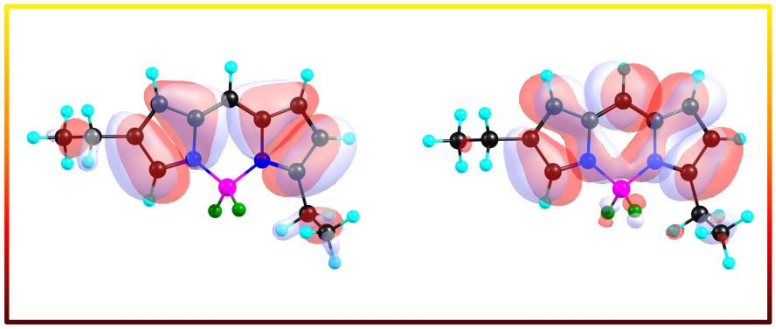

Figure S1-62: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.10** (isovalue = 0.02).

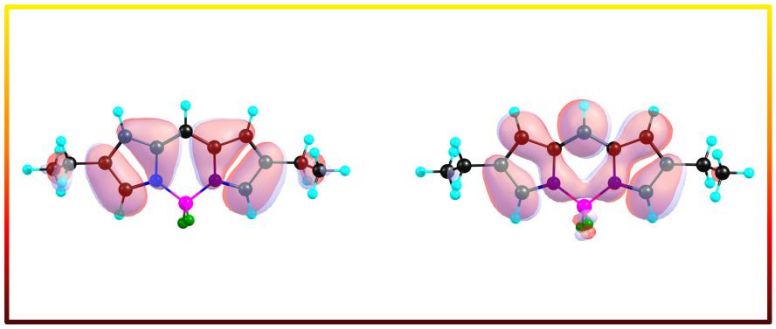

Figure S1-63: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.11** (isovalue = 0.02).

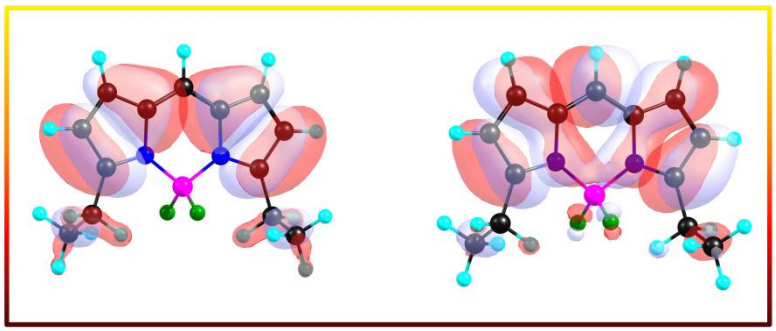

Figure S1-64: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **4.12** (isovalue = 0.02).

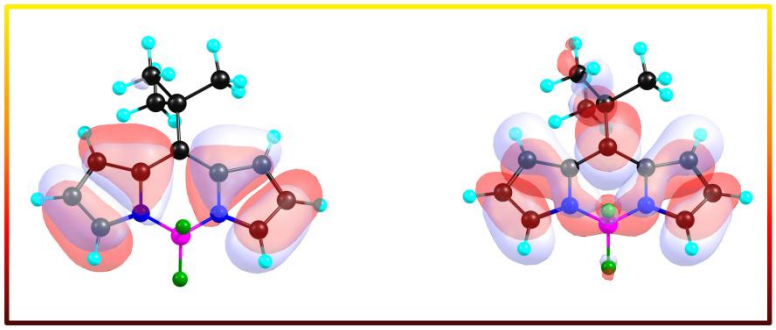

Figure S1-65: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **5.01** (isovalue = 0.02).

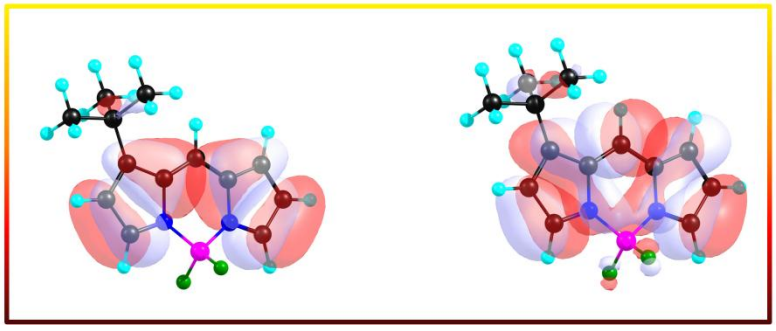

Figure S1-66: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **5.02** (isovalue = 0.02).

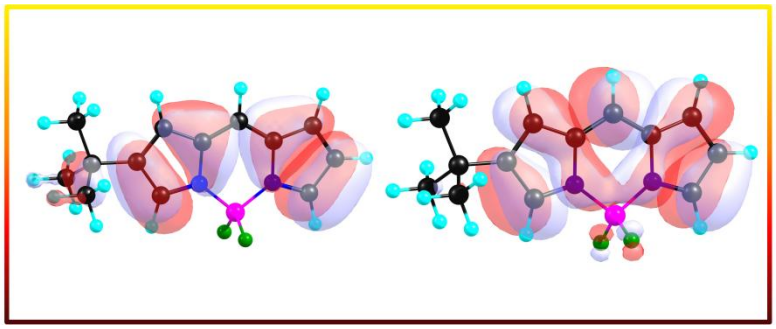

Figure S1-67: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **5.03** (isovalue = 0.02).

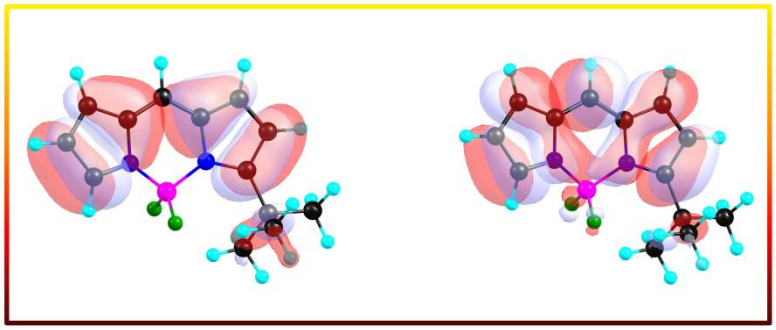

Figure S1-68: HOMO (left) and LUMO (right) of DFT B3LYP/6-31G(d) optimized structure of **5.04** (isovalue = 0.02).

	Total Energy (a.u.)	∠Py-Py(°)	HOMO energy (a.u.)	LUMO energy (a.u.)
BODIPY	-681.37581583	9.802	-0.21938	-0.10462
1.01	-720.69470700	6.030	-0.21695	-0.10090
1.02	-720.69566423	4.222	-0.21534	-0.10101
1.03	-720.69481774	3.617	-0.21394	-0.10118
1.04	-720.70049457	0.000	-0.21209	-0.09958
2.01	-760.01168284	7.136	-0.21351	-0.09622
2.02	-760.01356071	4.070	-0.21173	-0.09759
2.03	-760.01901832	0.658	-0.21004	-0.09619
2.04	-760.01438542	3.045	-0.21229	-0.09861
2.05	-760.02038937	0.000	-0.20825	-0.09598
2.06	-760.02010014	0.086	-0.20821	-0.09630
2.07	-760.01451069	1.335	-0.21013	-0.09784
2.08	-760.01525336	4.851	-0.21148	-0.09769
2.09	-760.01920422	0.000	-0.20699	-0.09608
2.10	-760.01928348	0.000	-0.20699	-0.09649
2.11	-760.01365768	3.701	-0.20876	-0.09799
2.12	-760.02463922	0.000	-0.20513	-0.09514
3.01	-760.00812569	3.280	-0.21638	-0.10060
3.02	-760.00896145	0.304	-0.21568	-0.10093
3.03	-760.00824258	3.152	-0.21416	-0.10151
3.04	-760.01458625	3.538	-0.21183	-0.09927
4.01	-838.63607551	6.762	-0.21229	-0.09717
4.02	-838.64042420	4.137	-0.21148	-0.09772
4.03	-838.64643273	2.878	-0.20925	-0.09579
4.04	-838.64041481	3.268	-0.21143	-0.09836
4.05	-838.64775725	3.331	-0.20846	-0.09574
4.06	-838.64750560	3.153	-0.20838	-0.09602
4.07	-838.64124866	2.903	-0.21074	-0.09816
4.08	-838.64187436	4.151	-0.21222	-0.09755
4.09	-838.64619149	3.270	-0.20708	-0.09630
4.10	-838.64682560	2.657	-0.20727	-0.09677
4.11	-838.64053829	3.019	-0.20928	-0.09867
4.12	-838.65252493	0.421	-0.20489	-0.09474
5.01	-838.61639323	15.557	-0.21460	-0.10076
5.02	-838.63241574	5.415	-0.21462	-0.10034
5.03	-838.63466759	3.436	-0.21304	-0.10061
5.04	-838.63374252	7.800	-0.21182	-0.09927

Table S1-1: Computationally obtained data for the model BODIPY systems based on ground state B3LYP/6-31G(d) level of computations.

Tabular contents of properties of the model BODIPY dye systems:

Compound **BODIPY**

	Total Energy	**HOMO energy**	**LUMO energy**
B3LYP/6-31G(d)	-681.37581583	-0.21938	-0.10462
B3LYP/6-31++G(d,p)	-681.26667659	-0.22530	-0.11618
mpw1pw91/6-31++G(d,p)	-681.39543499	-0.24103	-0.11632
wb97xd/6-31++G(d,p)	-681.19566438	-0.29497	-0.05946

Compound **1.01**

B3LYP/6-31G(d)	-720.69470700	-0.21695	-0.10090
B3LYP/6-31++G(d,p)	-720.89485029	-0.23183	-0.11695
mpw1pw91/6-31++G(d,p)	-720.71559381	-0.23856	-0.11205
wb97xd/6-31++G(d,p)	-720.50871551	-0.29323	-0.05521

Compound **1.02**

B3LYP/6-31G(d)	-720.69566423	-0.21534	-0.10101
B3LYP/6-31++G(d,p)	-720.89554958	-0.22981	-0.11714
mpw1pw91/6-31++G(d,p)	-720.71587167	-0.23636	-0.11231
wb97xd/6-31++G(d,p)	-720.50769694	-0.29049	-0.05556

Compound **1.03**

B3LYP/6-31G(d)	-720.69481774	-0.21394	-0.10118
B3LYP/6-31++G(d,p)	-720.89462456	-0.22812	-0.11710
mpw1pw91/6-31++G(d,p)	-720.71477904	-0.23463	-0.11226
wb97xd/6-31++G(d,p)	-720.50573162	-0.28874	-0.05570

Compound **1.04**

B3LYP/6-31G(d)	-720.70049457	-0.21209	-0.09958
B3LYP/6-31++G(d,p)	-720.89987239	-0.22629	-0.11500

mpw1pw91/6-31++G(d,p)	-720.72022834	-0.23266	-0.11018
wb97xd/6-31++G(d,p)	-720.51227658	-0.28638	-0.05375

Compound **2.01**

B3LYP/6-31G(d)	-760.01168284	-0.21351	-0.09622
B3LYP/6-31++G(d,p)	-760.22133822	-0.22798	-0.11165
mpw1pw91/6-31++G(d,p)	-760.03312358	-0.23464	-0.10667
wb97xd/6-31++G(d,p)	-759.81880897	-0.28948	-0.04988

Compound **2.02**

B3LYP/6-31G(d)	-760.01356071	-0.21173	-0.09759
B3LYP/6-31++G(d,p)	-760.22325744	-0.22575	-0.11314
mpw1pw91/6-31++G(d,p)	-760.03476957	-0.23233	-0.10821
wb97xd/6-31++G(d,p)	-759.81868995	-0.28712	-0.05164

Compound **2.03**

B3LYP/6-31G(d)	-760.01901832	-0.21004	-0.09619
B3LYP/6-31++G(d,p)	-760.22822505	-0.22410	-0.11123
mpw1pw91/6-31++G(d,p)	-760.03993235	-0.23056	-0.10632
wb97xd/6-31++G(d,p)	-759.82480619	-0.28493	-0.04980

Compound **2.04**

B3LYP/6-31G(d)	-760.01438542	-0.21229	-0.09861
B3LYP/6-31++G(d,p)	-760.22377080	-0.22615	-0.11408
mpw1pw91/6-31++G(d,p)	-760.03498961	-0.23268	-0.10927
wb97xd/6-31++G(d,p)	-759.81836911	-0.28674	-0.05276

Compound **2.05**

B3LYP/6-31G(d)	-760.02038937	-0.20825	-0.09598

B3LYP/6-31++G(d,p)	-760.22935066	-0.22198	-0.11099
mpw1pw91/6-31++G(d,p)	-760.04065560	-0.22826	-0.10612
wb97xd/6-31++G(d,p)	-759.82450027	-0.28231	-0.04975

Compound **2.06**

B3LYP/6-31G(d)	-760.02010014	-0.20821	-0.09630
B3LYP/6-31++G(d,p)	-760.22898113	-0.22185	-0.11139
mpw1pw91/6-31++G(d,p)	-760.04026932	-0.22813	-0.10652
wb97xd/6-31++G(d,p)	-759.82383889	-0.28187	-0.05035

Compound **2.07**

B3LYP/6-31G(d)	-760.01451069	-0.21013	-0.09784
B3LYP/6-31++G(d,p)	-760.22386553	-0.22376	-0.11341
mpw1pw91/6-31++G(d,p)	-760.03497013	-0.23017	-0.10854
wb97xd/6-31++G(d,p)	-759.81764957	-0.28431	-0.05215

Compound **2.08**

B3LYP/6-31G(d)	-760.01525336	-0.21148	-0.09769
B3LYP/6-31++G(d,p)	-760.22460896	-0.22538	-0.11354
mpw1pw91/6-31++G(d,p)	-760.03588934	-0.23185	-0.10864
wb97xd/6-31++G(d,p)	-759.81933699	-0.28606	-0.05211

Compound **2.09**

B3LYP/6-31G(d)	-760.01920422	-0.20699	-0.09608
B3LYP/6-31++G(d,p)	-760.22803464	-0.22053	-0.11100
mpw1pw91/6-31++G(d,p)	-760.03936920	-0.22678	-0.10612
wb97xd/6-31++G(d,p)	-759.82288714	-0.28057	-0.04975

Compound **2.10**

B3LYP/6-31G(d)	-760.01928348	-0.20699	-0.09649
B3LYP/6-31++G(d,p)	-760.22808879	-0.22038	-0.11138
mpw1pw91/6-31++G(d,p)	-760.03920939	-0.22662	-0.10653
wb97xd/6-31++G(d,p)	-759.82197608	-0.28043	-0.05049

Compound **2.11**

B3LYP/6-31G(d)	-760.01365768	-0.20876	-0.09799
B3LYP/6-31++G(d,p)	-760.22290104	-0.22214	-0.11338
mpw1pw91/6-31++G(d,p)	-760.03381861	-0.22852	-0.10851
wb97xd/6-31++G(d,p)	-759.81548510	-0.28270	-0.05224

Compound **2.12**

B3LYP/6-31G(d)	-760.02463922	-0.20513	-0.09514
B3LYP/6-31++G(d,p)	-760.23293660	-0.21852	-0.10956
mpw1pw91/6-31++G(d,p)	-760.04424590	-0.22462	-0.10473
wb97xd/6-31++G(d,p)	-759.82787705	-0.27802	-0.04890

Compound **3.01**

B3LYP/6-31G(d)	-760.00812569	-0.21638	-0.10060
B3LYP/6-31++G(d,p)	-760.21860738	-0.23089	-0.11640
mpw1pw91/6-31++G(d,p)	-760.02999611	-0.23764	-0.11152
wb97xd/6-31++G(d,p)	-759.81568507	-0.29231	-0.05469

Compound **3.02**

B3LYP/6-31G(d)	-760.00896145	-0.21568	-0.10093
B3LYP/6-31++G(d,p)	-760.21932590	-0.23003	-0.11682
mpw1pw91/6-31++G(d,p)	-760.03014269	-0.23658	-0.11200
wb97xd/6-31++G(d,p)	-759.81424339	-0.29042	-0.05541

Compound **3.03**

B3LYP/6-31G(d)	-760.00824258	-0.21416	-0.10151
B3LYP/6-31++G(d,p)	-760.21862760	-0.22827	-0.11722
mpw1pw91/6-31++G(d,p)	-760.02924994	-0.23476	-0.11235
wb97xd/6-31++G(d,p)	-759.81179377	-0.28883	-0.05586

Compound **3.04**

B3LYP/6-31G(d)	-760.01458625	-0.21183	-0.09927
B3LYP/6-31++G(d,p)	-760.22331059	-0.22550	-0.11406
mpw1pw91/6-31++G(d,p)	-760.03413831	-0.23187	-0.10914
wb97xd/6-31++G(d,p)	-759.81814288	-0.28565	-0.05286

Compound **4.01**

B3LYP/6-31G(d)	-838.63607551	-0.21229	-0.09717
B3LYP/6-31++G(d,p)	-838.86653376	-0.22709	-0.11239
mpw1pw91/6-31++G(d,p)	-838.65976792	-0.23374	-0.10741
wb97xd/6-31++G(d,p)	-838.43088467	-0.28850	-0.05073

Compound **4.02**

B3LYP/6-31G(d)	-838.64042420	-0.21148	-0.09772
B3LYP/6-31++G(d,p)	-838.87098321	-0.22513	-0.11286
mpw1pw91/6-31++G(d,p)	-838.66362283	-0.23166	-0.10787
wb97xd/6-31++G(d,p)	-838.43173634	-0.28865	-0.05167

Compound **4.03**

B3LYP/6-31G(d)	-838.64643273	-0.20925	-0.09579
B3LYP/6-31++G(d,p)	-838.87528255	-0.22248	-0.11001
mpw1pw91/6-31++G(d,p)	-838.66811312	-0.22895	-0.10502
wb97xd/6-31++G(d,p)	-838.43789071	-0.28342	-0.04874

Compound **4.04**

B3LYP/6-31G(d)	-838.64041481	-0.21143	-0.09836
B3LYP/6-31++G(d,p)	-838.87081872	-0.22496	-0.11347
mpw1pw91/6-31++G(d,p)	-838.66319771	-0.23142	-0.10858
wb97xd/6-31++G(d,p)	-838.43104316	-0.28574	-0.05232

Compound **4.05**

B3LYP/6-31G(d)	-838.64775725	-0.20846	-0.09574
B3LYP/6-31++G(d,p)	-838.87653314	-0.22157	-0.10995
mpw1pw91/6-31++G(d,p)	-838.66887128	-0.22785	-0.10498
wb97xd/6-31++G(d,p)	-838.43694677	-0.28182	-0.04883

Compound **4.06**

B3LYP/6-31G(d)	-838.64750560	-0.20838	-0.09602
B3LYP/6-31++G(d,p)	-838.87620791	-0.22146	-0.11033
mpw1pw91/6-31++G(d,p)	-838.66847760	-0.22768	-0.10537
wb97xd/6-31++G(d,p)	-838.43595855	-0.28123	-0.04940

Compound **4.07**

B3LYP/6-31G(d)	-838.64124866	-0.21074	-0.09816
B3LYP/6-31++G(d,p)	-838.87163249	-0.22436	-0.11345
mpw1pw91/6-31++G(d,p)	-838.66371363	-0.23075	-0.10855
wb97xd/6-31++G(d,p)	-838.42999260	-0.28429	-0.05206

Compound **4.08**

B3LYP/6-31G(d)	-838.64187436	-0.21222	-0.09755
B3LYP/6-31++G(d,p)	-838.87220079	-0.22598	-0.11292
mpw1pw91/6-31++G(d,p)	-838.66451109	-0.23242	-0.10806

wb97xd/6-31++G(d,p)	-838.43199723	-0.28600	-0.05183

Compound **4.09**

B3LYP/6-31G(d)	-838.64619149	-0.20708	-0.09630
B3LYP/6-31++G(d,p)	-838.87493086	-0.22021	-0.11061
mpw1pw91/6-31++G(d,p)	-838.66733261	-0.22649	-0.10570
wb97xd/6-31++G(d,p)	-838.43579651	-0.28014	-0.04941

Compound **4.10**

B3LYP/6-31G(d)	-838.64682560	-0.20727	-0.09677
B3LYP/6-31++G(d,p)	-838.87558395	-0.22013	-0.11090
mpw1pw91/6-31++G(d,p)	-838.66763929	-0.22630	-0.10590
wb97xd/6-31++G(d,p)	-838.43405198	-0.27966	-0.04962

Compound **4.11**

B3LYP/6-31G(d)	-838.64053829	-0.20928	-0.09867
B3LYP/6-31++G(d,p)	-838.87088395	-0.22250	-0.11364
mpw1pw91/6-31++G(d,p)	-838.66272957	-0.22885	-0.10872
wb97xd/6-31++G(d,p)	-838.42762167	-0.28296	-0.05258

Compound **4.12**

B3LYP/6-31G(d)	-838.65252493	-0.20489	-0.09474
B3LYP/6-31++G(d,p)	-838.87973813	-0.21730	-0.10800
mpw1pw91/6-31++G(d,p)	-838.67199098	-0.22336	-0.10297
wb97xd/6-31++G(d,p)	-838.43967539	-0.27675	-0.04730

Compound **5.01**

B3LYP/6-31G(d)	-838.61639323	-0.21460	-0.10076
B3LYP/6-31++G(d,p)	-838.84698078	-0.22891	-0.11590

mpw1pw91/6-31++G(d,p)	-838.64129378	-0.23561	-0.11105
wb97xd/6-31++G(d,p)	-838.41363750	-0.29035	-0.05421

Compound **5.02**

B3LYP/6-31G(d)	-838.63241574	-0.21462	-0.10034
B3LYP/6-31++G(d,p)	-838.86346710	-0.22878	-0.11600
mpw1pw91/6-31++G(d,p)	-838.65670777	-0.23532	-0.11121
wb97xd/6-31++G(d,p)	-838.42744818	-0.28954	-0.05455

Compound **5.03**

B3LYP/6-31G(d)	-838.63466759	-0.21304	-0.10061
B3LYP/6-31++G(d,p)	-838.86604905	-0.22698	-0.11600
mpw1pw91/6-31++G(d,p)	-838.65898209	-0.23345	-0.11114
wb97xd/6-31++G(d,p)	-838.42764520	-0.28760	-0.05477

Compound **5.04**

B3LYP/6-31G(d)	-838.63374252	-0.21182	-0.09927
B3LYP/6-31++G(d,p)	-838.86259843	-0.22530	-0.11381
mpw1pw91/6-31++G(d,p)	-838.65574048	-0.23171	-0.10898
wb97xd/6-31++G(d,p)	-838.42659625	-0.28558	-0.05285

Table S1-2: Dihedral arrangements between the neighbouring pyrrolic units in the model **BODIPY** Dyes

	Ground state B3LYP/6-31G(d)	**Excited state B3LYP/6-31G(d)**
BODIPY	9.802	15.107
1.01	6.030	17.895
1.02	4.222	15.921
1.03	3.617	15.247
1.04	0.000	1.695
2.01	7.136	22.163
2.02	4.070	18.047
2.03	0.658	7.774
2.04	3.045	12.855
2.05	0.000	1.264
2.06	0.086	0.021
2.07	1.335	16.165
2.08	4.851	11.966
2.09	0.000	3.096
2.10	0.000	0.382
2.11	3.701	16.090
2.12	0.000	0.016
3.01	3.280	16.312
3.02	0.304	16.709
3.03	3.152	15.315
3.04	3.538	9.470
4.01	6.762	18.776
4.02	4.137	18.615
4.03	2.878	13.113
4.04	3.268	12.154
4.05	3.331	9.294
4.06	3.153	6.316

4.07	2.903	15.263
4.08	4.151	11.927
4.09	3.270	10.068
4.10	2.657	9.111
4.11	3.019	16.666
4.12	0.421	0.346
5.01	15.557	48.216
5.02	5.415	17.372
5.03	3.436	14.743
5.04	7.800	18.292