Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Machine-learning-assisted performance improvements for multi-resonance thermally activated delayed fluorescence molecules

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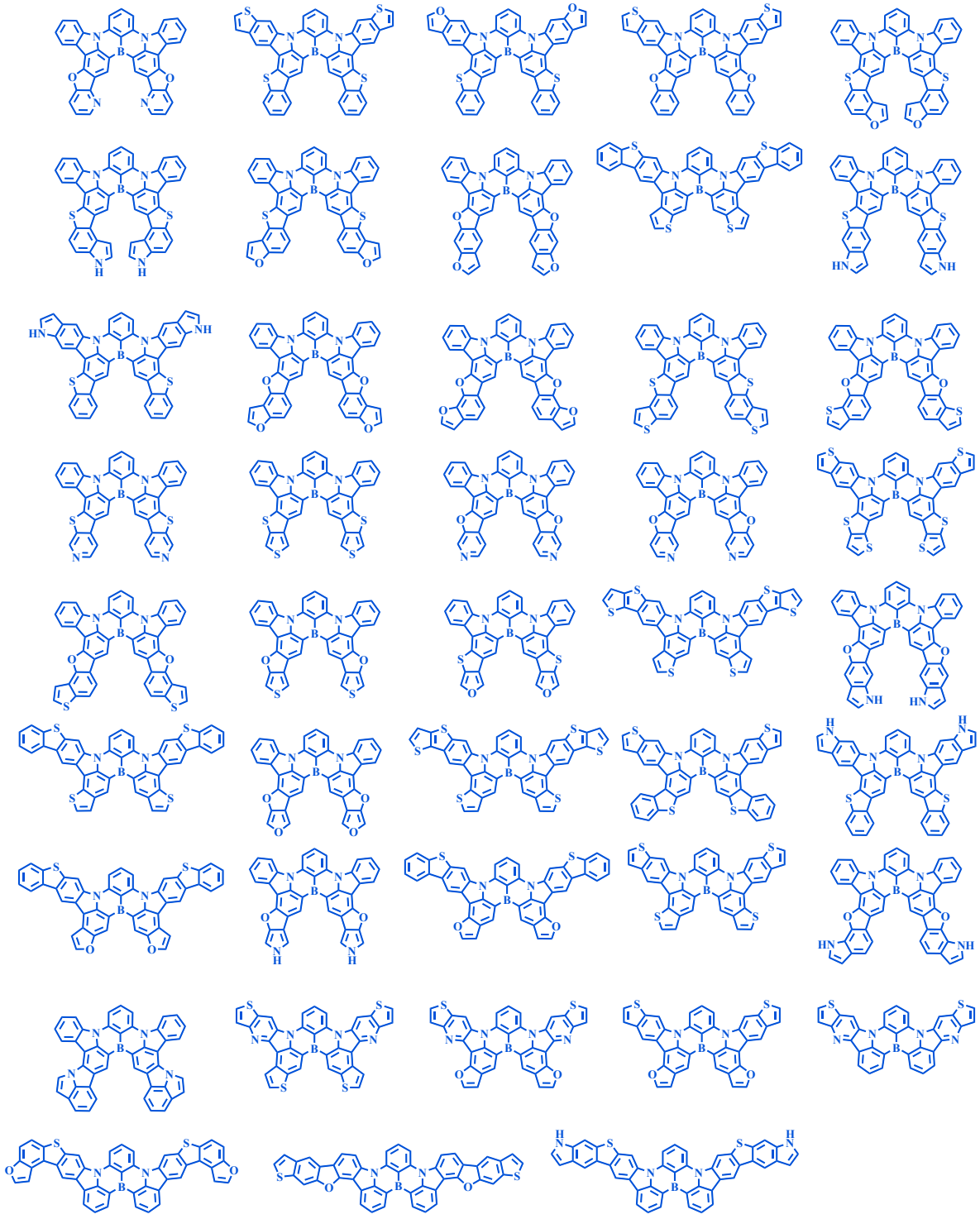

Figure S1. Chemical structure of the suggested molecules based on **Core_1** among the top 100 molecules.

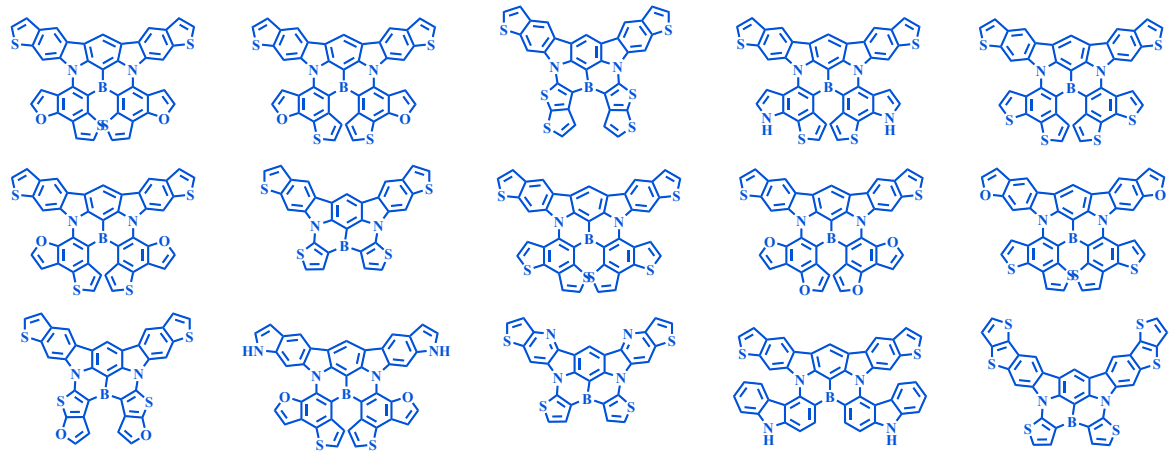

Figure S2. Chemical structure of the suggested molecules based on **Core_2** among the top 100 molecules.

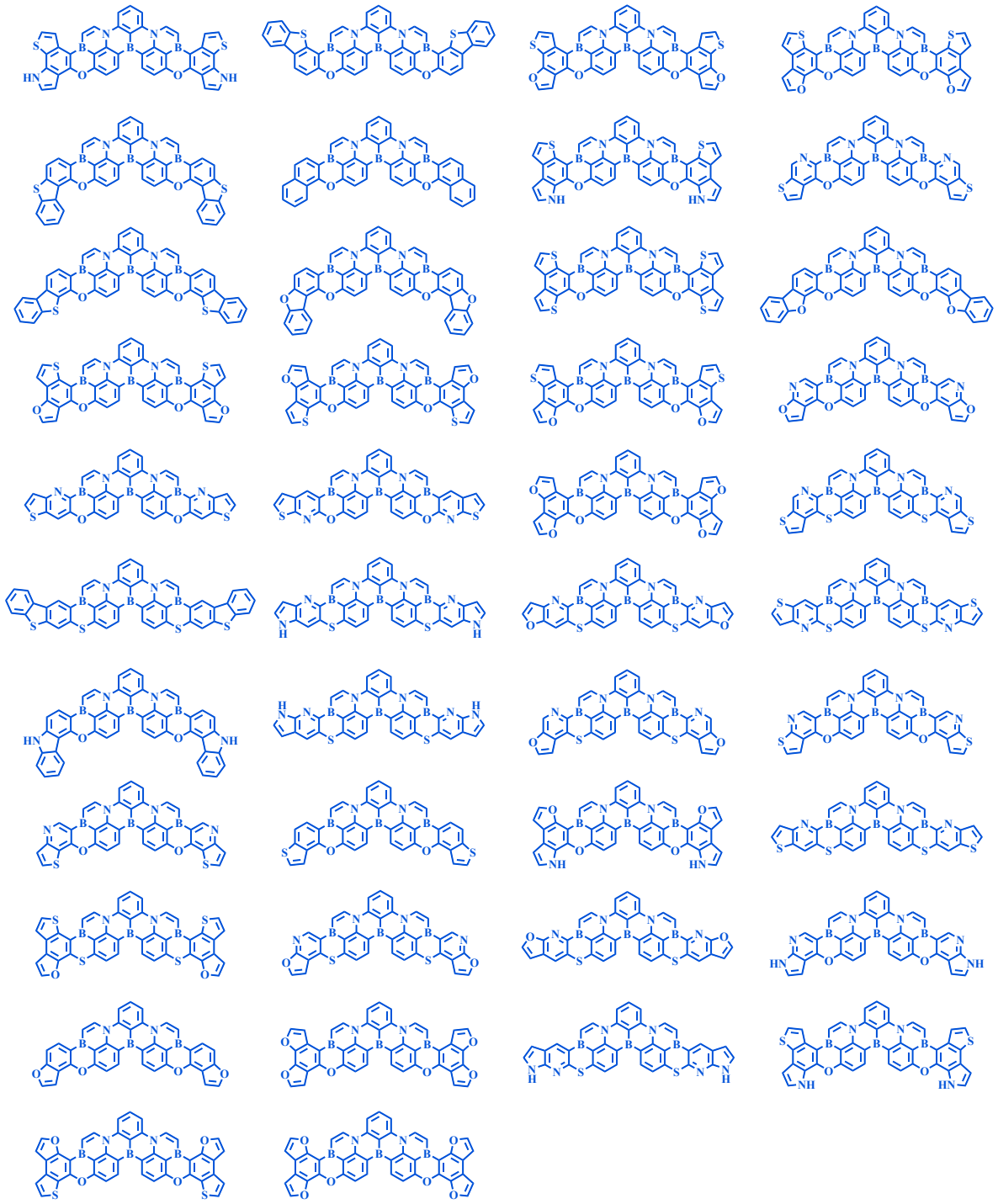

Figure S3. Chemical structure of the suggested molecules based on **Core_3** among the top 100 molecules.

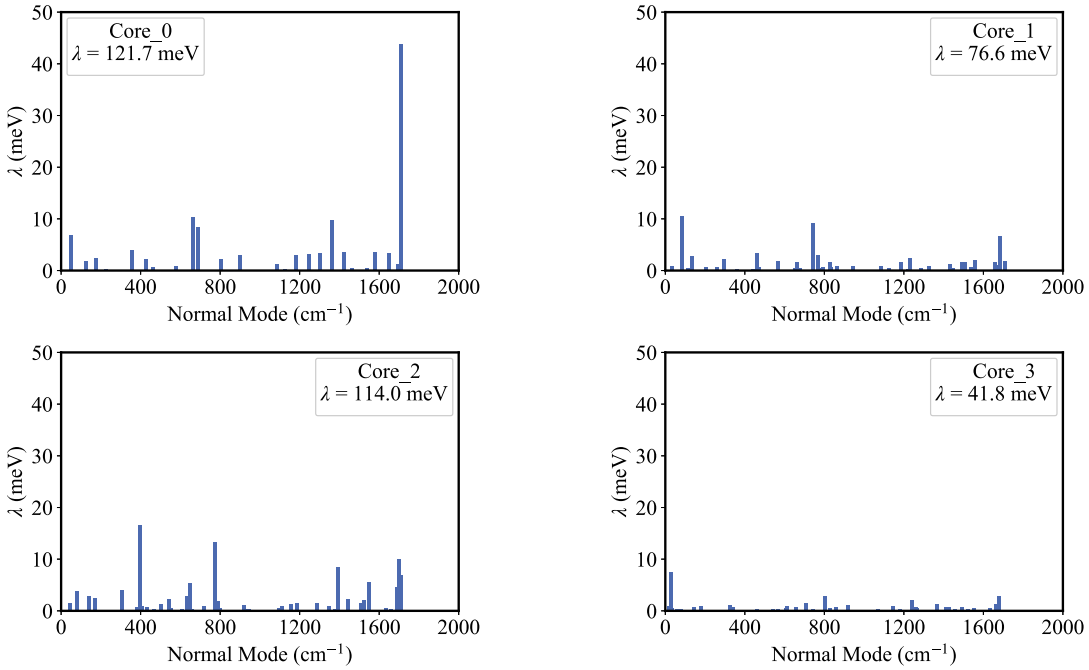

Figure S4. The contribution of the normal modes to λ_{em}, for the four cores.

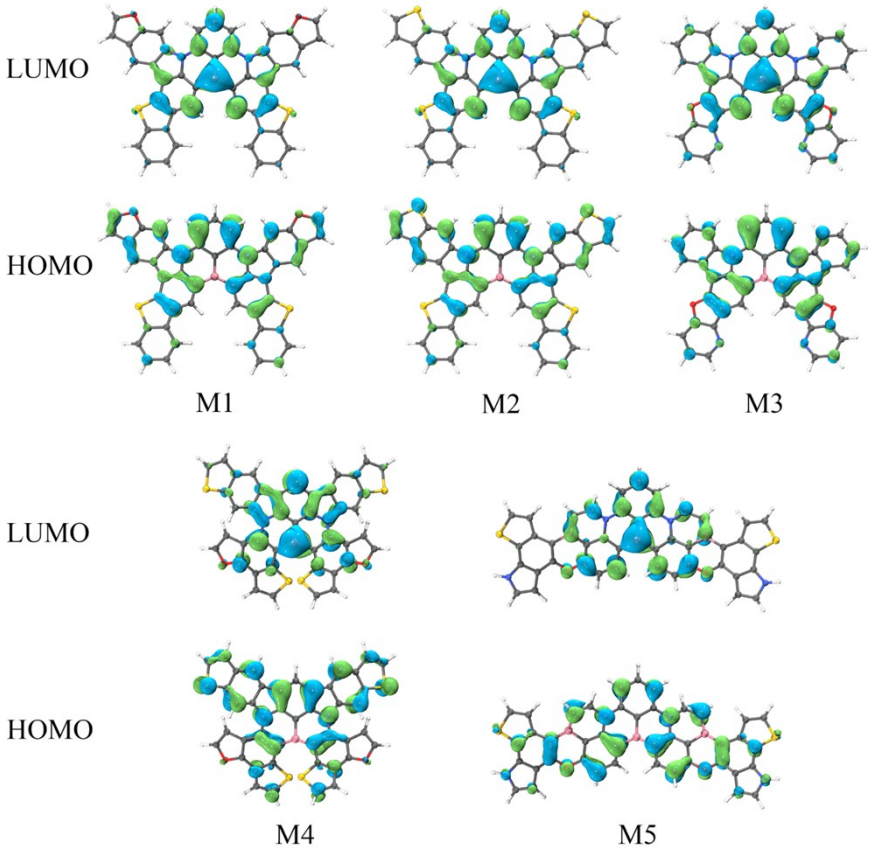

Figure S5. HOMO and LUMO distribution (isovalue = 0.03 au) for the top 5 molecules.

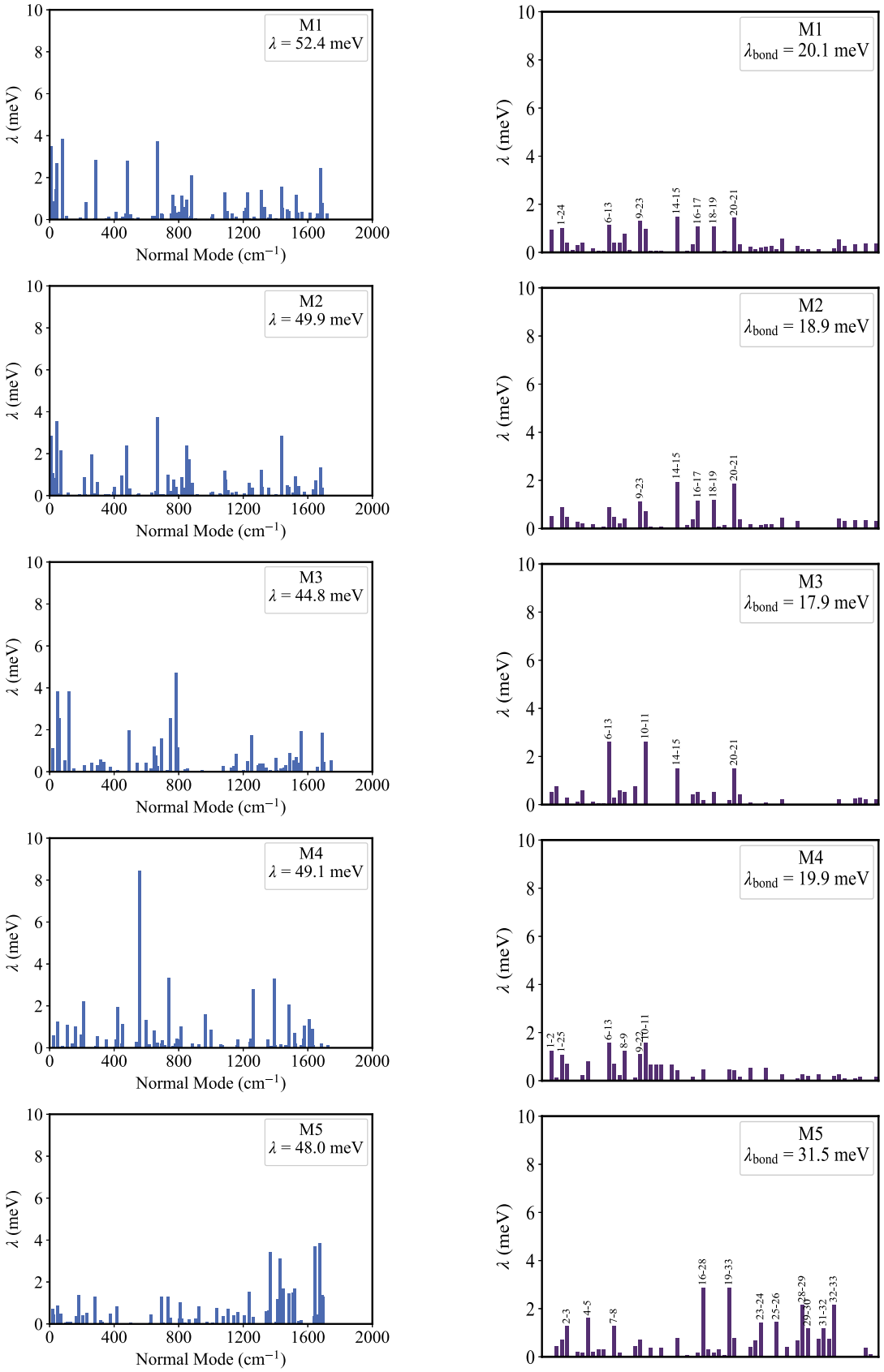

Figure S6. The contribution of the normal modes to λ_{em} (left), and the contribution of each chemical bond to λ_{BL} (right), for **M1**, **M2**, **M3**, **M4**, and **M5**.

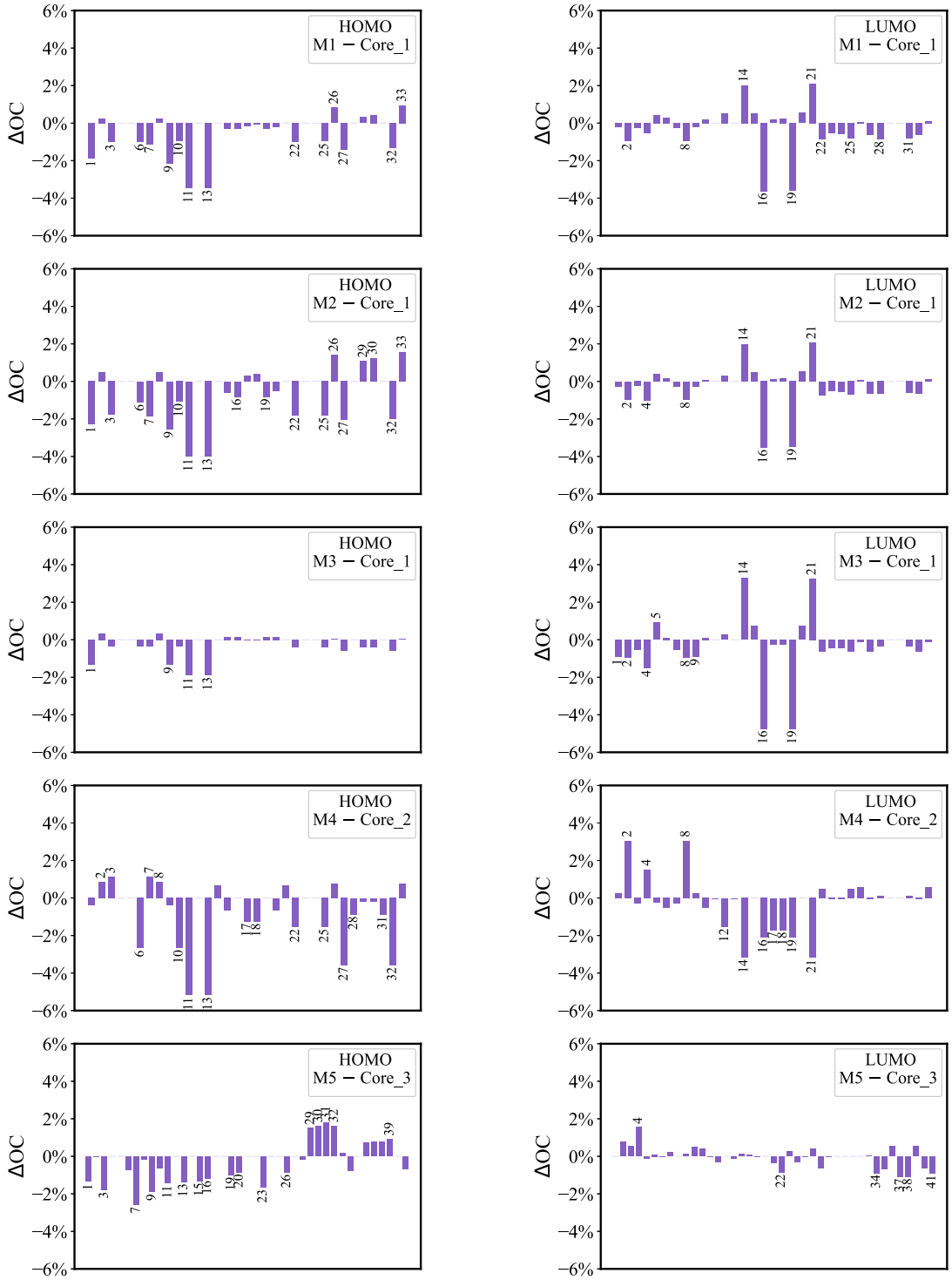

Figure S7. The difference in orbital composition of the top 5 molecules and their respective corresponding core.

Table S1. Calculated f_{osc} at the S_1 geometry and SOC matrix element (cm^{-1}) based on the S_1 and T_1 geometries.

	DABNA-1	M1	M2	M3	M4	M5
$f_{osc}(S_1)$	0.163	0.449	0.471	0.457	0.287	1.037
$SOC(S_1)$	0.044	0.011	0.068	0.006	0.052	0.037
$SOC(T_1)$	0.043	0.008	0.077	0.011	0.095	0.034