Electronic Supplementary Material (ESI) for Faraday Discussions.

Supporting information

Computational Studies on Ground and Excited state Charge Transfer Properties of Peptidomimetics

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Table S1 A comparison of structural parameters of different models studied at neutral state using CAM-B3LYP, wB97XD, M06HF/6-311++G**

Models	r_{C-R}	r_{C-X}	r_{C-N}	$\angle_{N-C-R}$
Ph-UP				
CAM-B3LYP	1.517	1.228	1.371	114
wB97XD	1.514	1.227	1.371	113
M06HF	1.522	1.225	1.364	113
UP-Ph				
CAM-B3LYP	1.512	1.227	1.372	114
wB97XD	1.517	1.226	1.370	113
M06HF	1.520	1.227	1.369	113
Ph-UP-Ph				
CAM-B3LYP	1.513	1.228	1.371	114
wB97XD	1.514	1.227	1.370	113
M06HF	1.522	1.226	1.363	113

Table S2. Structural parameters (bond length (Å) and bond angles (º) of different UP models studied at ionized state using CAM-B3LYP/6-311++G**

Models	r_{C-R}	r_{C-X}	r_{C-N}	$\angle_{N-C-R}$	Models	r_{C-R}	r_{C-X}	r_{C-N}	$\angle_{N-C-R}$
Free UP		1.019	1.361						
Ph-UP	1.520	1.228	1.369	113	Br-UP	1.998	1.225	1.358	113
UP-Ph	1.514	1.227	1.372	114	UP-Br	1.920	1.228	1.359	109
Ph-UP-Ph	1.515	1.229	1.369	113	Br-UP-Br	1.897	1.223	1.365	114
F-UP	1.409	1.225	1.358	111	CN-UP	1.473	1.224	1.360	111
UP-F	1.360	1.225	1.374	107	UP-CN	1.460	1.224	1.368	111
F-UP-F	1.404	1.222	1.368	112	CN-UP-CN	1.478	1.223	1.362	112
Cl-UP	1.829	1.223	1.346	112	NO_2-UP	1.459	1.222	1.360	107
UP-Cl	1.769	1.225	1.374	107	UP-NO_2	1.405	1.221	1.371	107
Cl-UP-Cl	1.829	1.221	1.359	112	NO_2-UP-NO_2	1.459	1.698	1.368	109

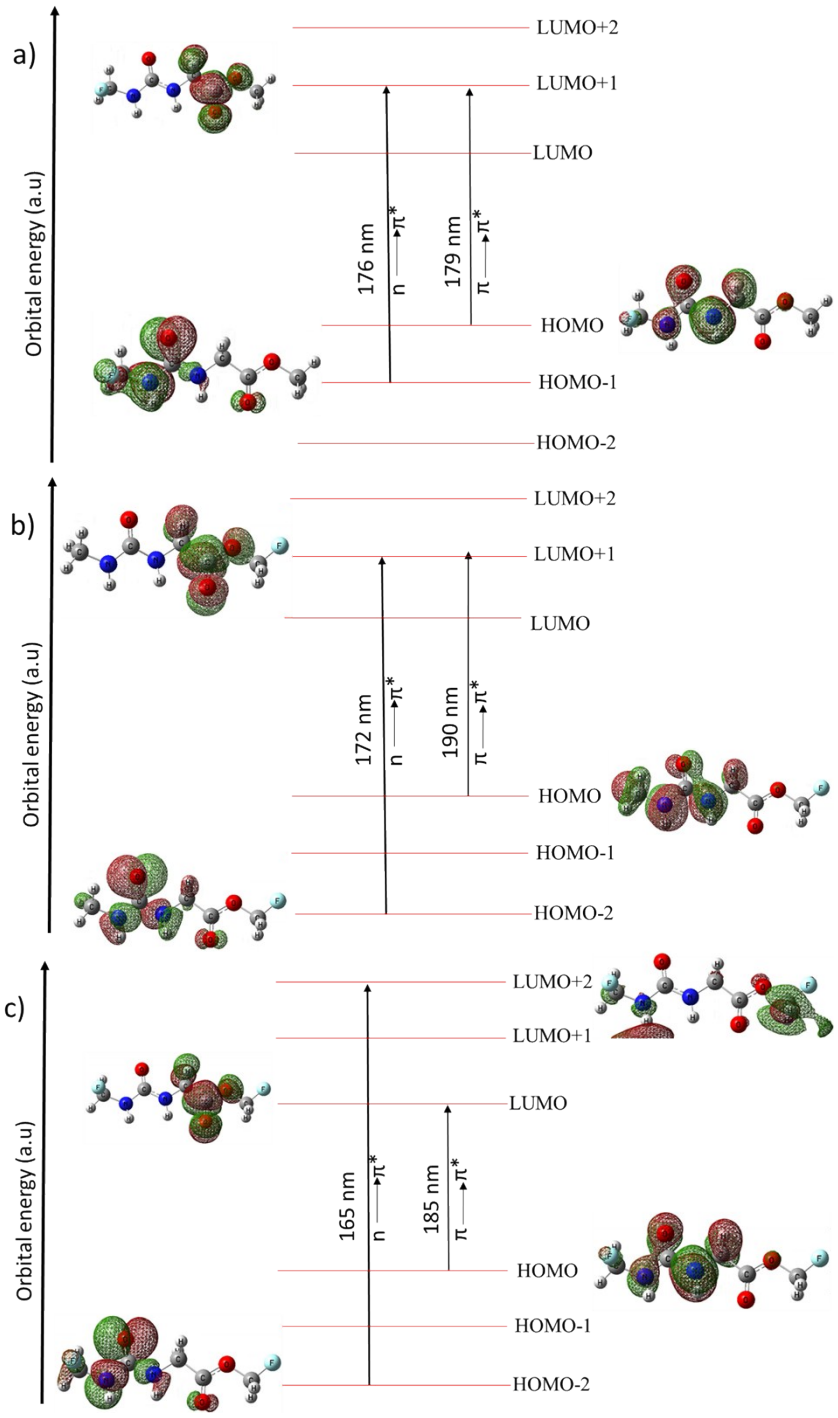

Figure S1 Excitation wavelengths and corresponding orbitals of a) F-UP b) UP-F c) F-UP-F

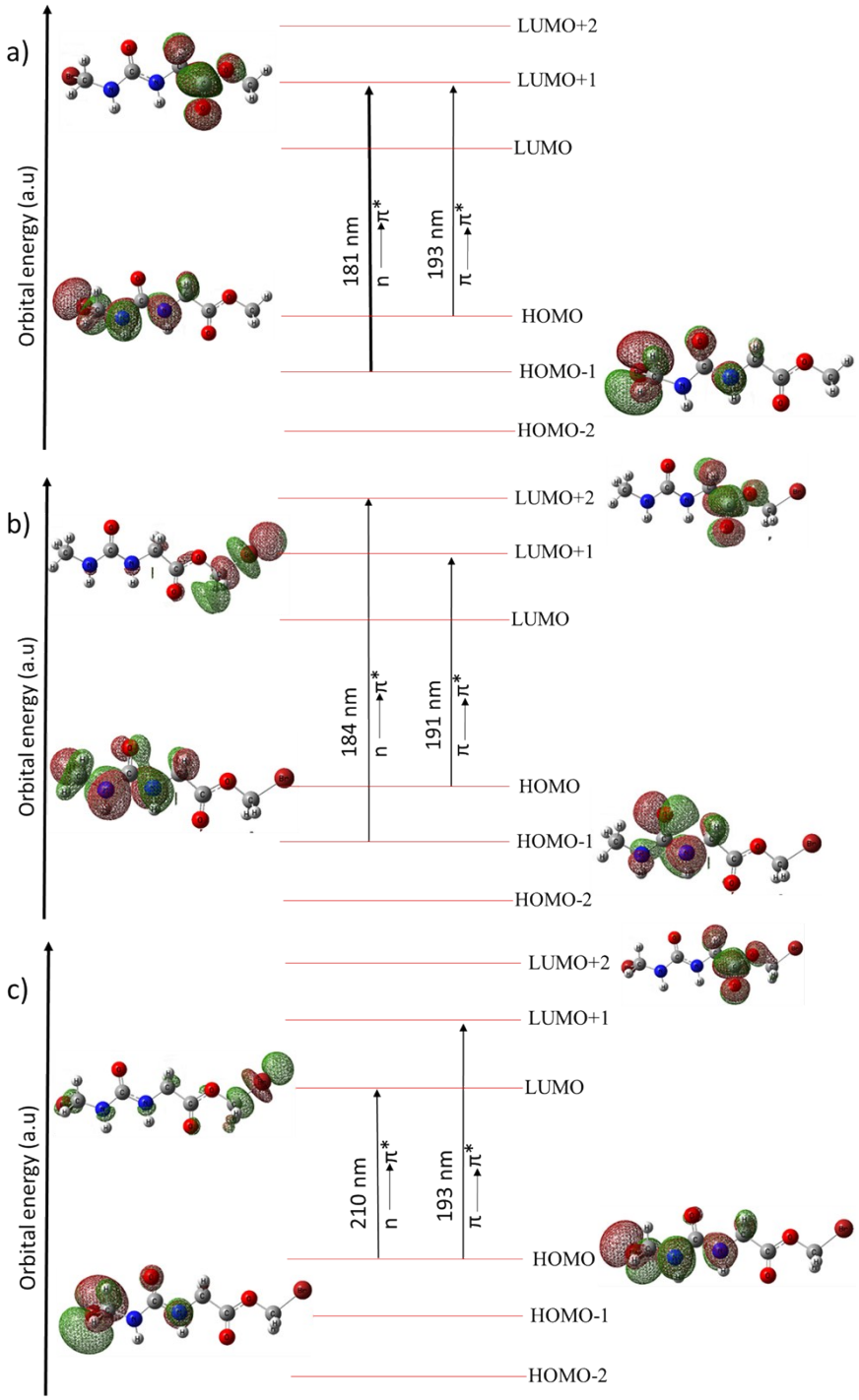

Figure S2 Excitation wavelengths and corresponding orbitals of a) Br-UP b) UP-Br c) Br-UP-Br

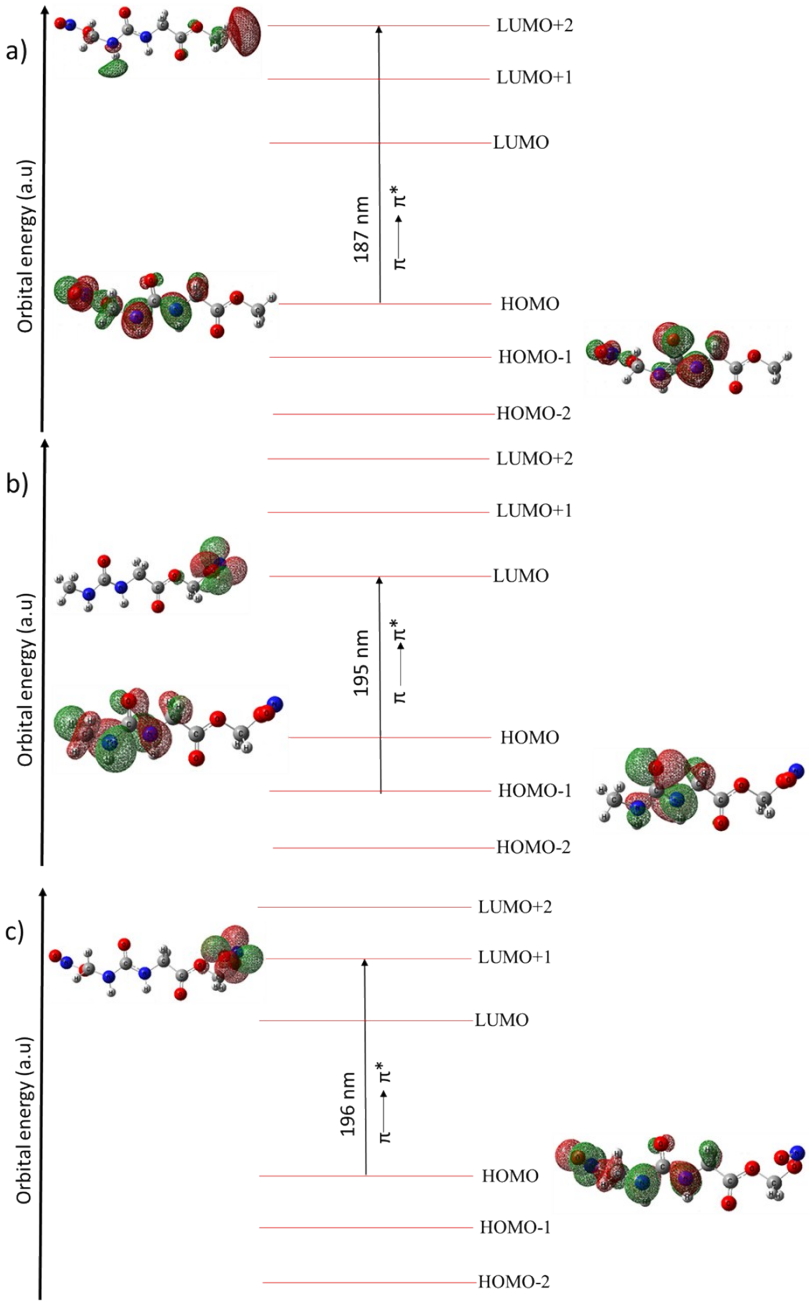

Figure S3 Excitation wavelengths and corresponding orbitals of a) NO_2-UP b) UP-NO_2 c) NO_2-UP-NO_2

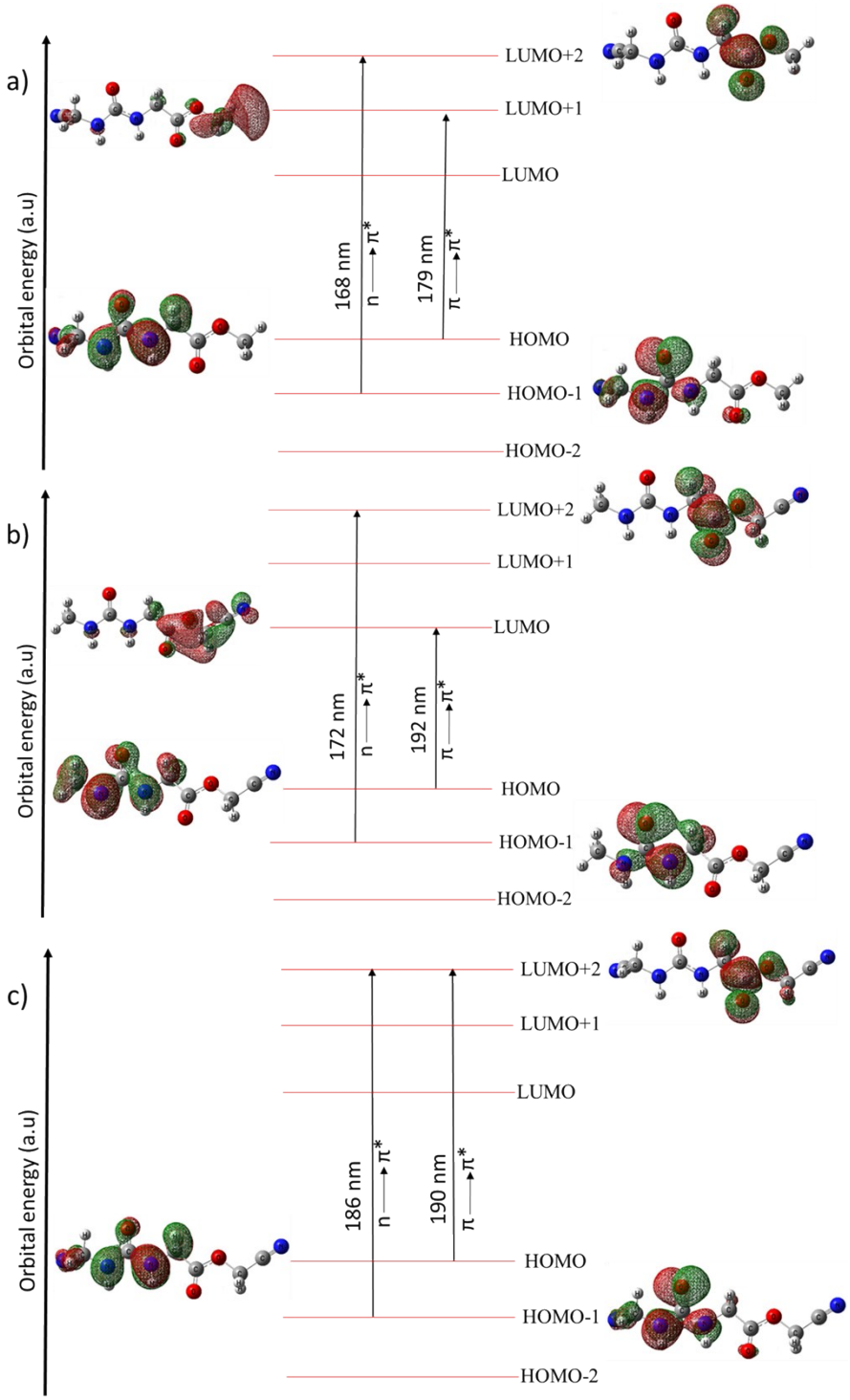

Figure S4 Excitation wavelengths and corresponding orbitals of a) CN-UP b) UP-CN c) CN-UP-CN