

*Supplementary Materials*

# Bound electron enhanced radiosensitisation of nimorazole upon charge transfer

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TDDFT/ M06-2X/6-311++g(d,p) computational model was used in electronic structure calculations. All electrons have been considered explicitly for carbon, oxygen, nitrogen, hydrogen and potassium atoms with the 6-311++g(d,p) basis set

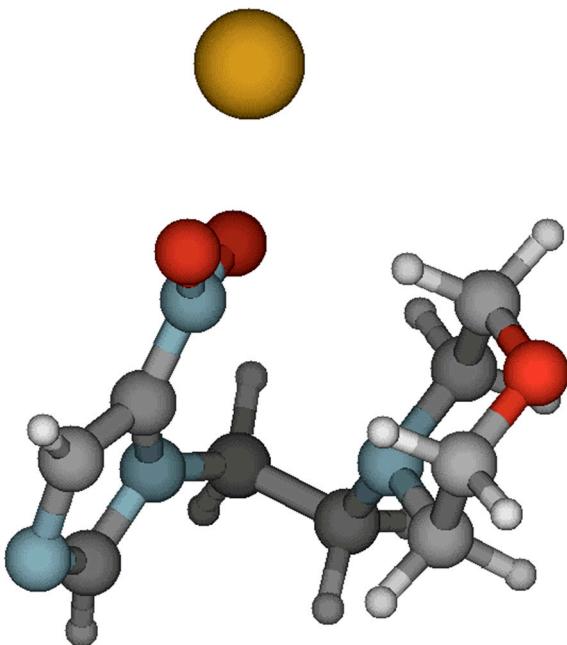
## Figure caption

Figure S1: Fully optimised geometry of nimorazole at the M06-2X/6-311++g(d,p) level of theory. Fully optimized molecular structure of the K + nimorazole collisional system K–O  $\approx$  5.1 Å. K: yellow, O: red, C: grey, N: light blue, and H: white. Cartesian coordinates (in Å).

Figure S2: Energy (in eV) and shape of a selection of the molecular orbitals (TDDFT/ M06-2X/6-311++g(d,p)) for K + NIMO (K: purple, C: grey, N: blue, O: red, and H: white). The straight lines between the K atom and the –NO<sub>2</sub> end in the nitroimidazole ring are just to indicate the spatial mutual position.

Figure S3: Energy (in eV) and shape of a selection of the molecular orbitals (M06-2X/6-311++g(d,p)) for NIMO (C: grey, N: blue, O: red, and H: white).

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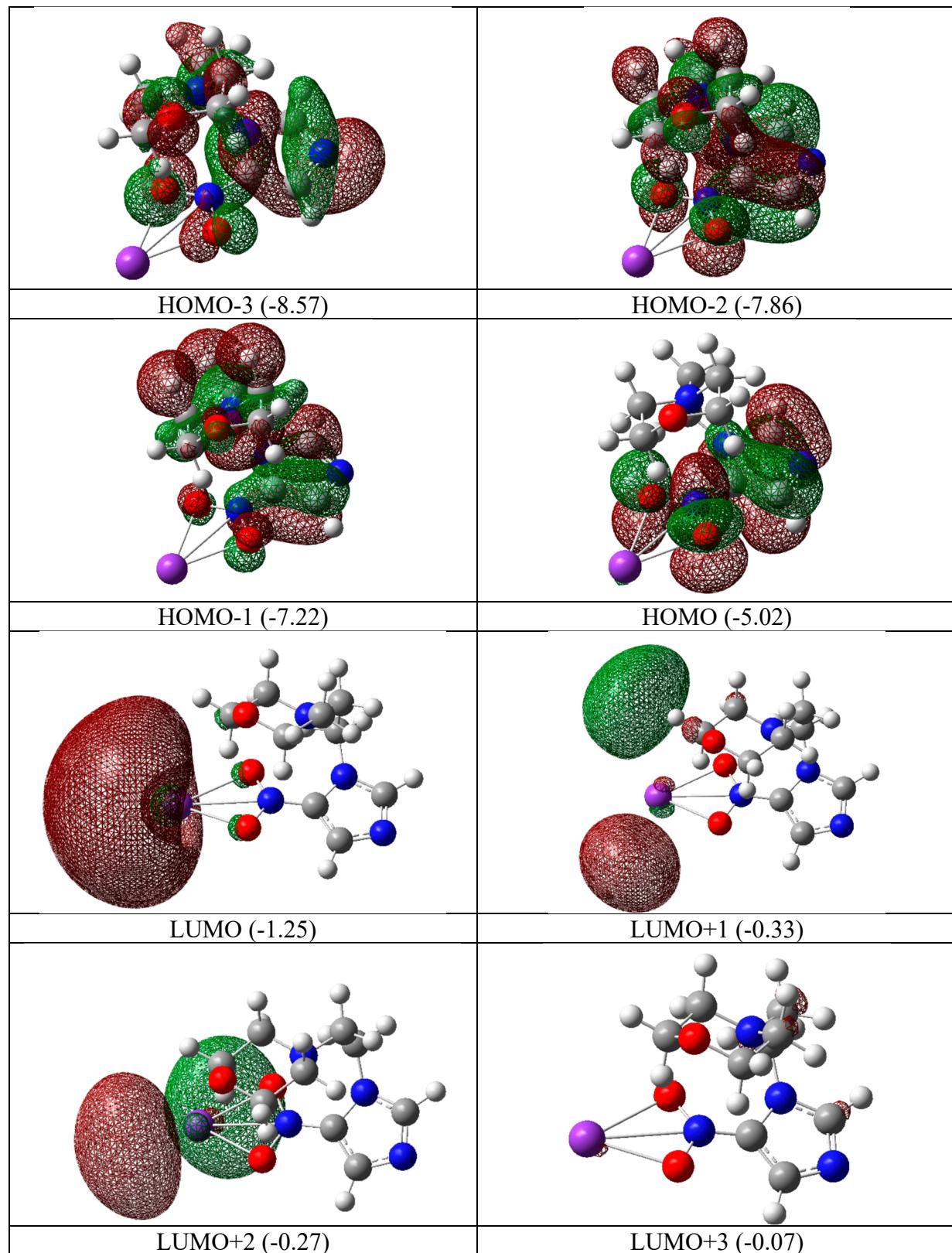


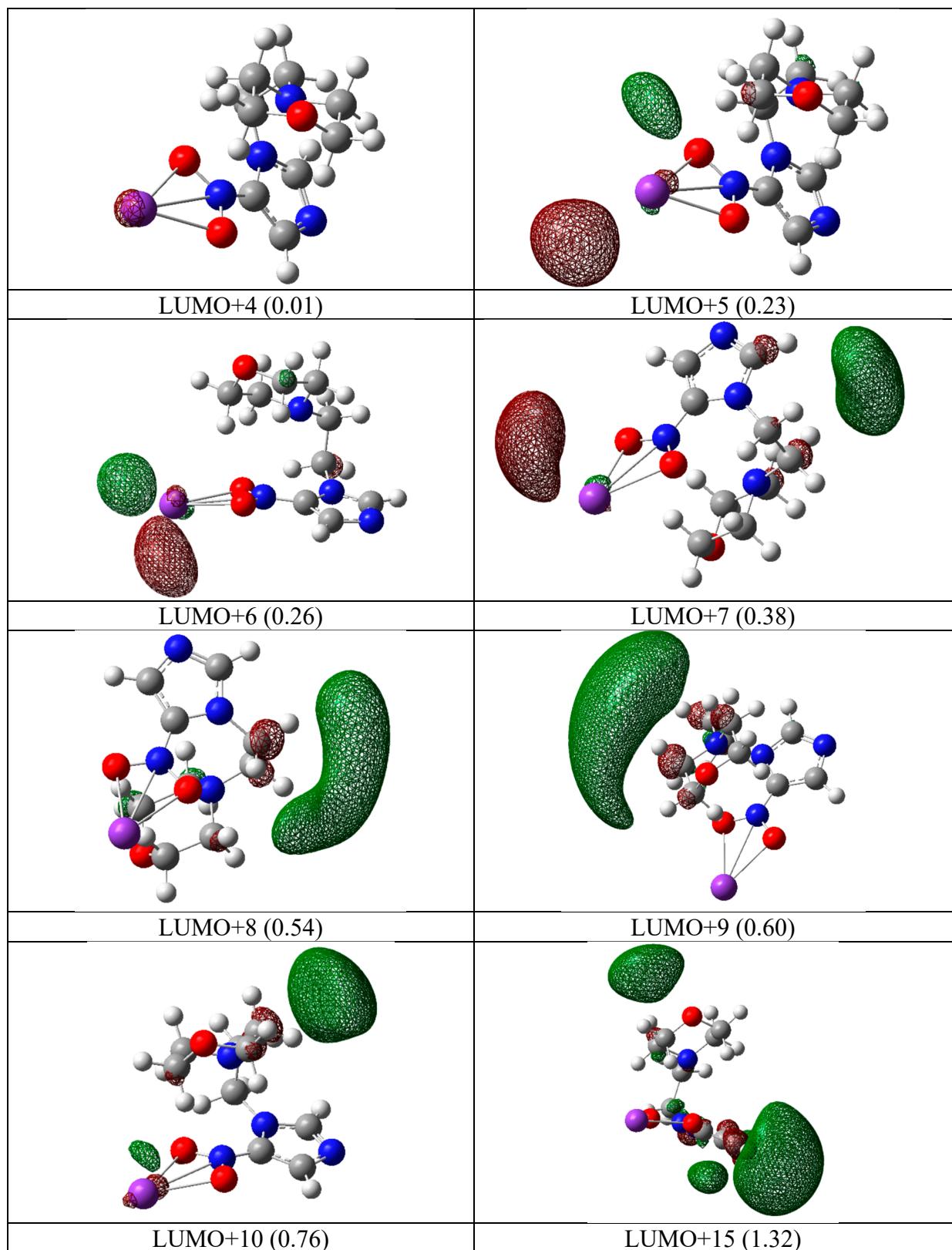
Cartesian coordinates (in Å).

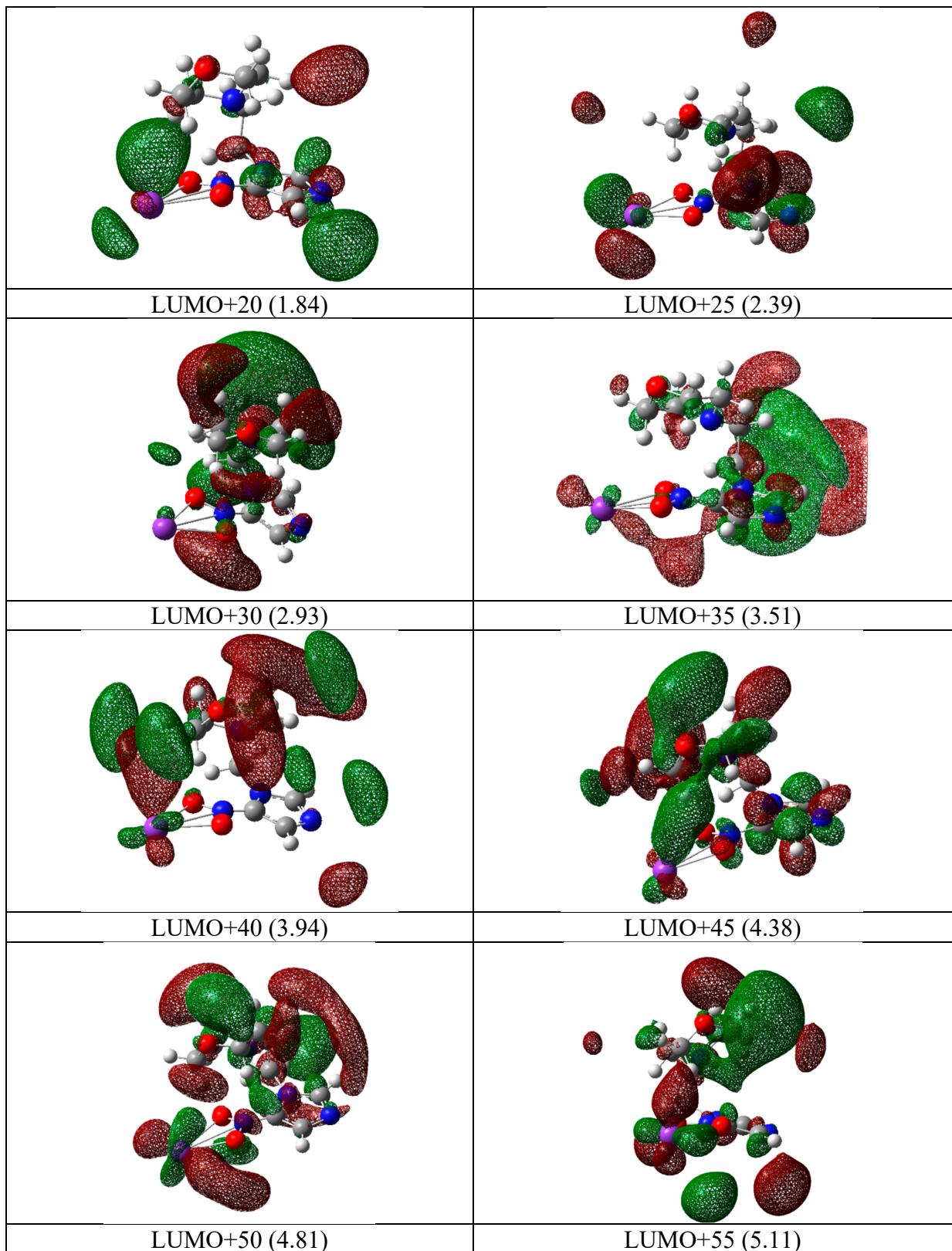
C	-1.420369	0.935288	-0.002623
C	-2.173875	1.301569	1.093023
C	-2.763699	-0.681986	0.585502
N	-1.812232	-0.343711	-0.339432
H	-2.145992	2.245774	1.609137
H	-3.241564	-1.651108	0.562053
N	-0.481321	1.677568	-0.687116
O	-0.095453	2.803273	-0.171942
O	-0.108712	1.352728	-1.894973
C	-1.127140	-1.314816	-1.183171
H	-1.863916	-2.060121	-1.492879
H	-0.752059	-0.795845	-2.061864
C	0.008225	-1.982200	-0.400485
H	0.468590	-2.770692	-1.019343
H	-0.419992	-2.467095	0.481591
N	0.970923	-0.991773	0.034944
O	3.361762	0.290946	0.792860
C	2.007597	-0.717105	-0.945513
H	1.537980	-0.493391	-1.905521
H	2.686518	-1.582196	-1.061822
C	2.803816	0.495525	-0.490399
H	2.127998	1.362282	-0.463349
H	3.640056	0.686577	-1.166570
C	2.340919	0.030164	1.742421
H	2.837580	-0.109915	2.702912

H	1.660440	0.890794	1.799458
C	1.541132	-1.205151	1.354725
H	2.199143	-2.092655	1.383743
H	0.729244	-1.347031	2.073211
N	-3.010278	0.275255	1.441875
K	0.993434	3.583190	-2.269275

Figure S2: Energy (in eV) and shape of a selection of the molecular orbitals (VTZ/6-311G) for K + NIMO (K: purple, C: grey, N: blue, O: red, and H: white). The straight lines between the K atom and the  $-NO_2$  end in the nitroimidazole ring are just to indicate the spatial mutual position.







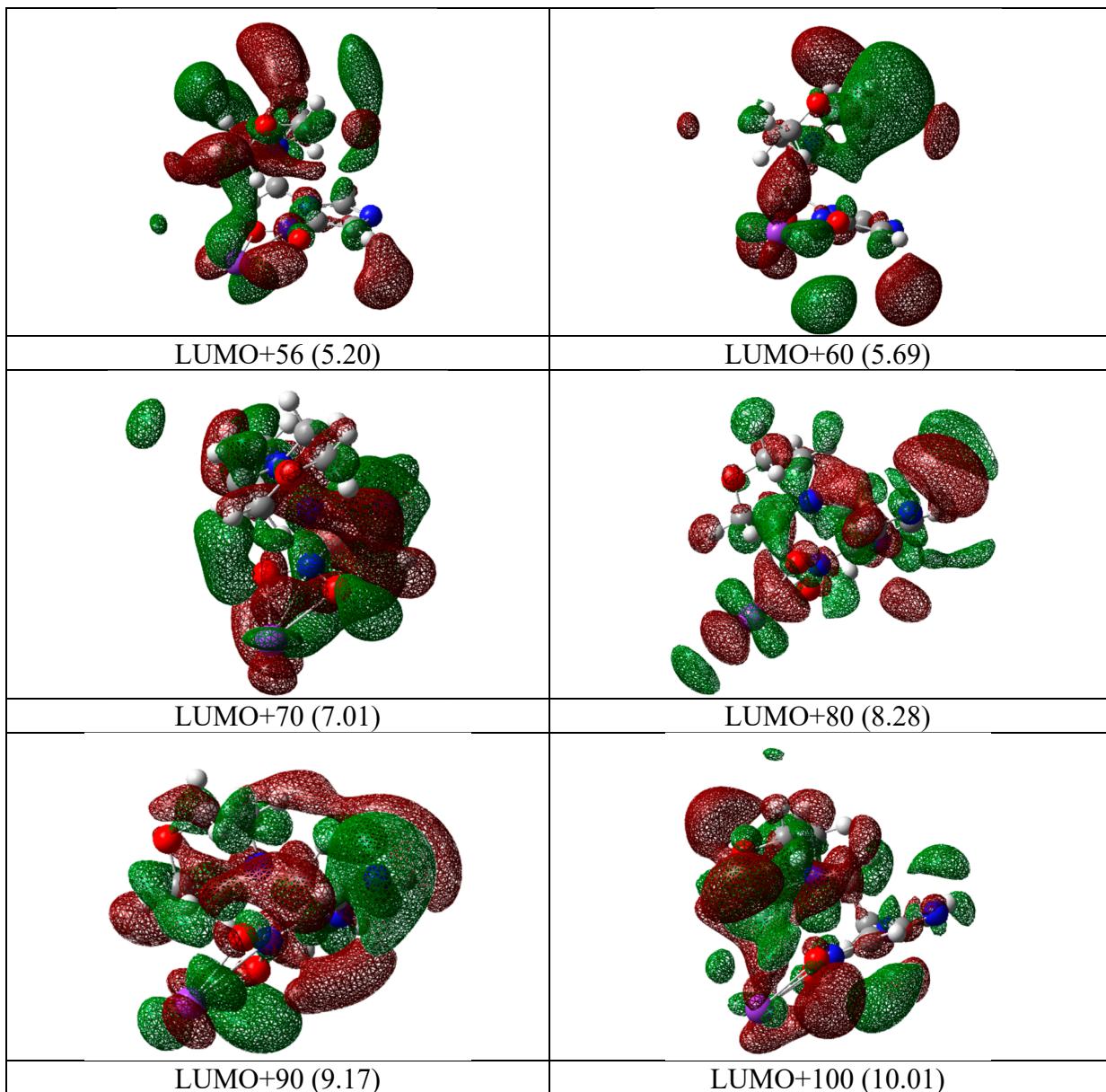


Figure S3: Energy (in eV) and shape of a selection of the molecular orbitals (M06-2X/6-311++g(d,p)) for NIMO (C: grey, N: blue, O: red, and H: white).

