Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Nitroimidazolic radiosensitizers investigated by electrospray ionization time-of-flight mass spectrometry and density functional theory

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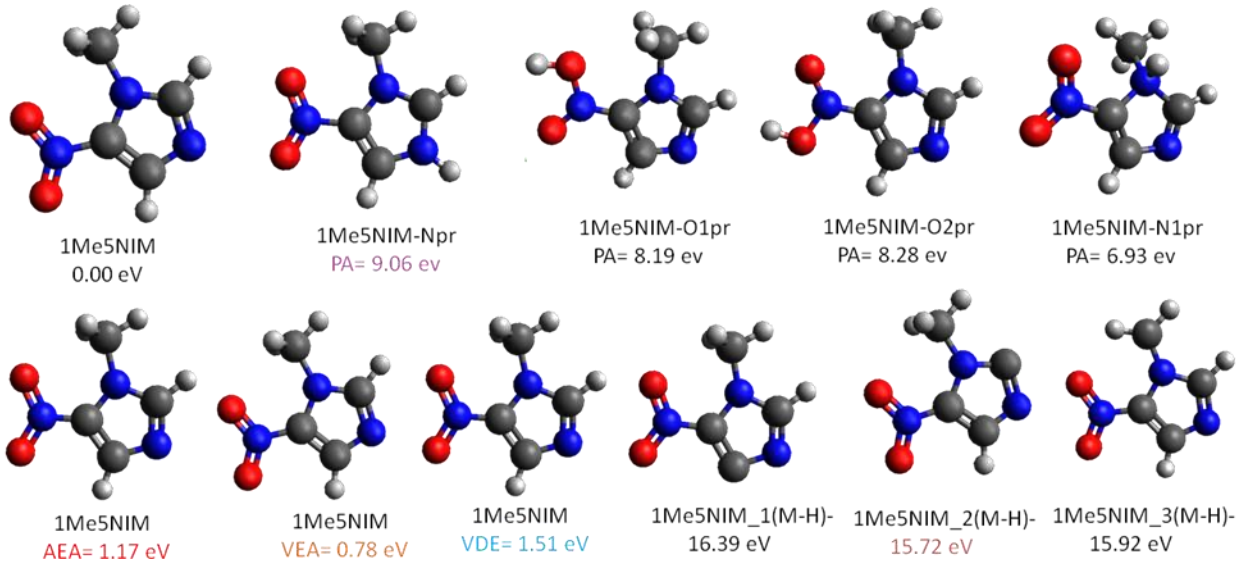

Figure S1. M062x/6-311+G(d,p) calculated minimum energy structure of 1-methyl-5-nitroimidazole, Proton affinity (PA), Adiabatic electron affinity (AEA), Vertical electron affinity (VEA) and Vertical detachment energy (VDE) of the corresponding neutral 1-methyl-5-nitroimidazole, their energies in eV.

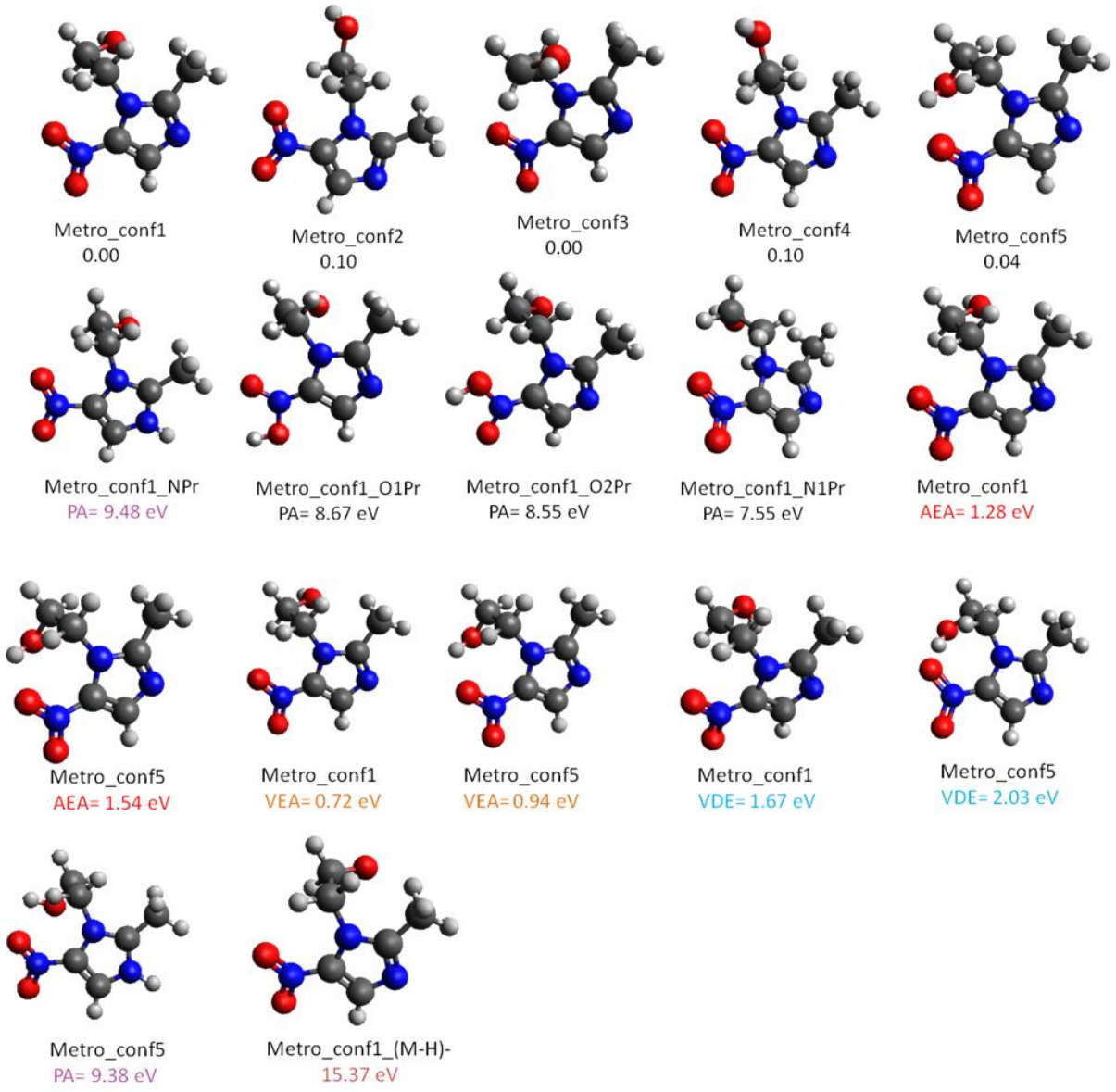

Figure S2. M062x/6-311+G(d,p) calculated minimum energy structures for the tautomer of Metronidazole neutral, Proton affinity (PA), Adiabatic electron affinity (AEA), Vertical electron affinity (VEA) and Vertical detachment energy (VDE) of the corresponding neutral Metronidazole.

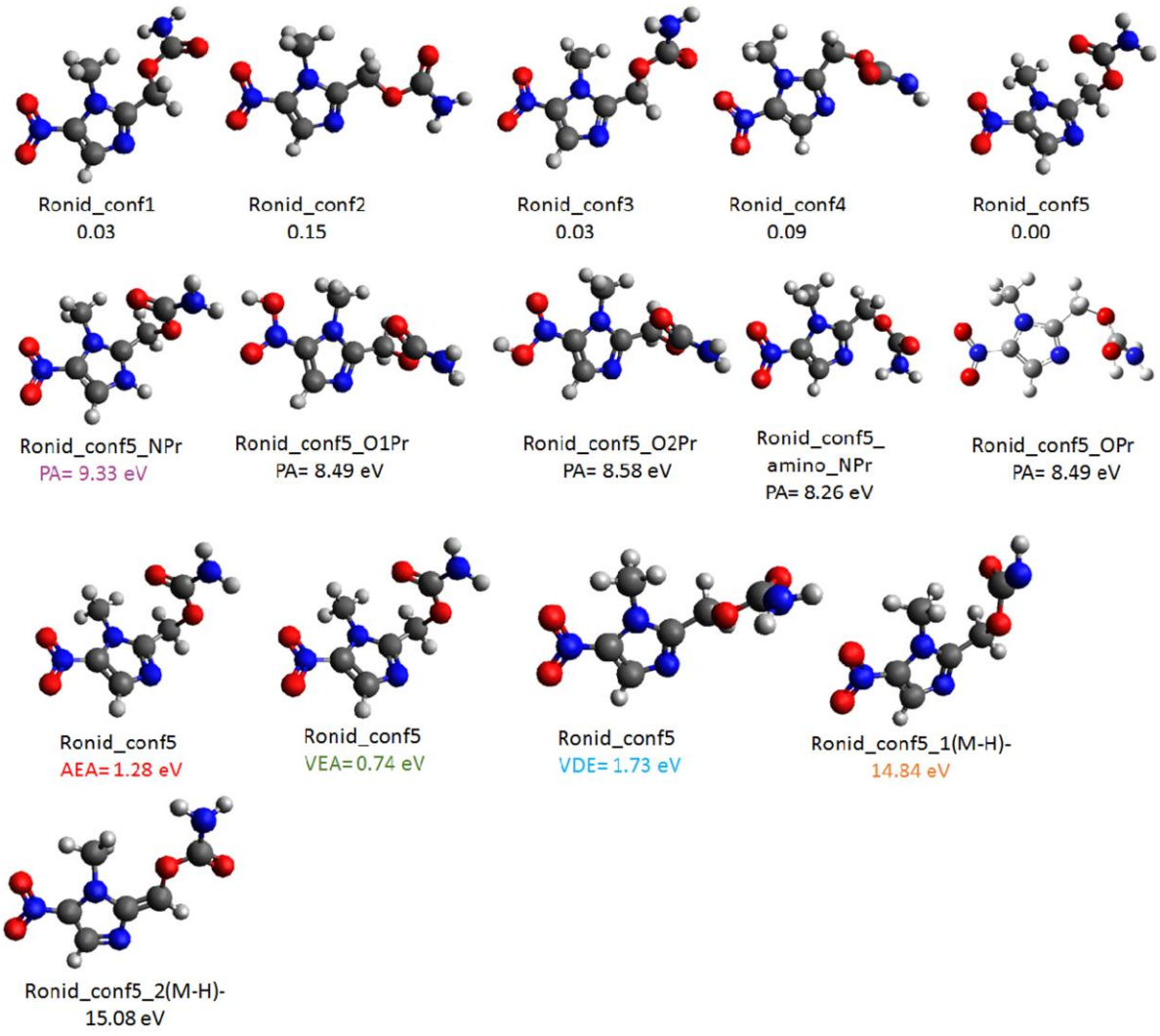

Figure S3. M062x/6-311+G(d,p) calculated minimum energy structures for the tautomer of Ronidazole neutral, Proton affinity (PA), Adiabatic electron affinity (AEA), Vertical electron affinity (VEA) and Vertical detachment energy (VDE) of the corresponding neutral Metronidazole.

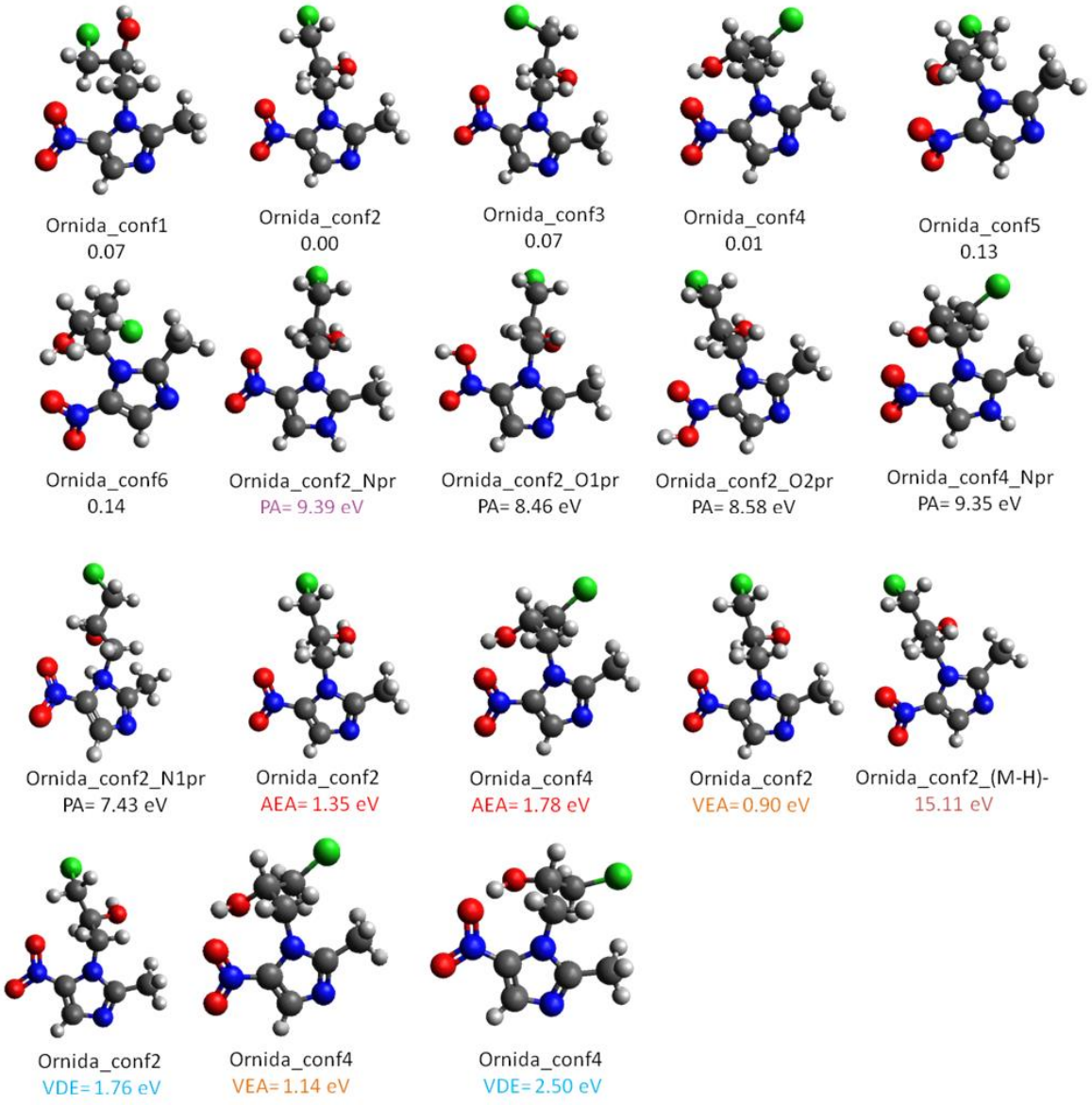

Figure S4. M062x/6-311+G(d,p) calculated minimum energy structures for the tautomer of Ornidazole neutral, Proton affinity (PA), Adiabatic electron affinity (AEA), Vertical electron affinity (VEA) and Vertical detachment energy (VDE) of the corresponding neutral Metronidazole.

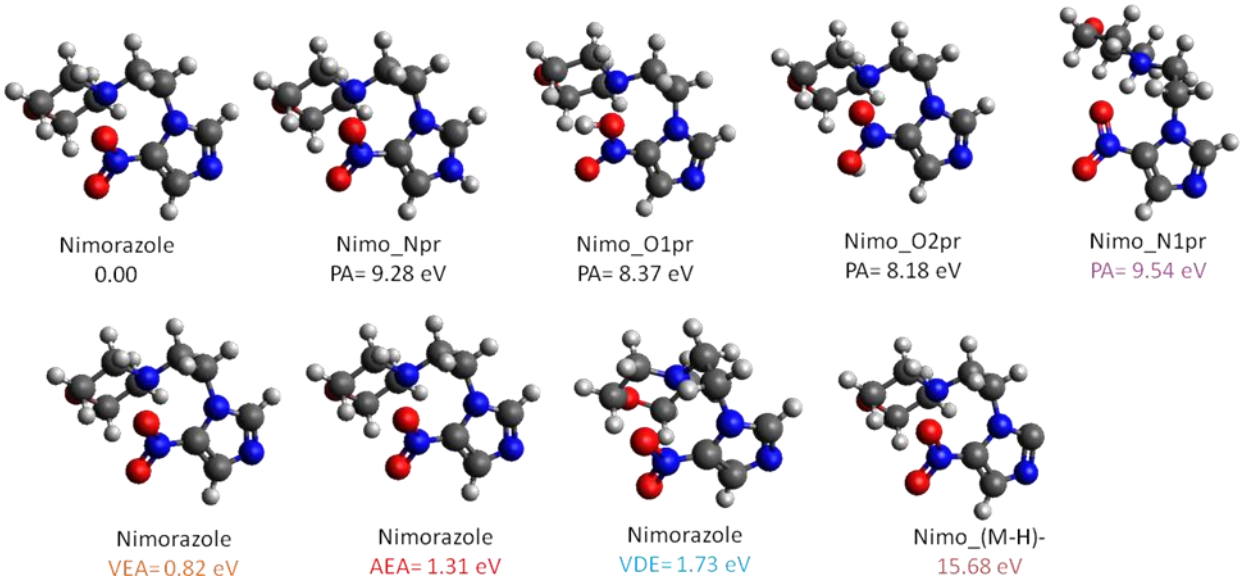

Figure S5. M062x/6-311+G(d,p) calculated minimum energy structure of Nimorazole neutral, Proton affinity (PA), Adiabatic electron affinity (AEA), Vertical electron affinity (VEA) and Vertical detachment energy (VDE) of the corresponding neutral Nimorazole.

	Positive ion mode	Negative ion mode
Capillary (kV)	2.98	-3.41
Cone (V)	34	-54
Extractor (V)	22	-41
RF Lens (V)	3.05	-5.25
Source Temperature (°C)	88	89
Desolvation Temperature (°C)	148	151
Collision	4	-5.3
Ion energy	2	2
Steering	-1.09	2.03
Entrance	-69	69.3
Prefilter	-2.8	-0.4

Table S1. Details of the positive and negative ion mode ESI source and MS settings.