Old Code	New Code	Description
1/2/1	1/2/1	Performs the following at PBE1PBE/6-31G(d,p): • Ground optimisation (with frequency) • TDA excited states (50/50)
1/2/4	1/2/4	Performs the following at B3LYP/6-31G(d,p), using SBKJC-VDZ-ECP for metals, in MeCN: • Ground optimisation (with frequency) • TD-DFT excited states (50/50) • Optimised triplet (with frequency) • Single point singlet at the same geometry
1/3/5	1/3/5	Performs the following at SCS-CC2/cc-pVDZ: • Ground optimisation • S_1 and S_2 excited states • T_1 and T_2 excited states
1/2/275	1/2/281	Optimisation (with frequency) at PBE1PBE/6-31G(d,p)
1/2/288	1/2/294	Optimisation (with frequency) at B3LYP/6-31G(d,p)
1/2/338	1/2/344	Optimisation (with frequency) at B3LYP/6-31G(d,p), using SBKJC-VDZ-ECP for metals, in MeCN
1/2/809	1/2/820	TDA excited states at PBE1PBE/6-31G(d,p)
1/2/2132	1/2/2203	TD-DFT excited states at B3LYP/6-31G(d,p), using SBKJC-VDZ-ECP for metals, in MeCN
1/2/1277	1/2/1288	TDA excited states (100 singlets) at PBE1PBE/6-31G(d,p)
1/2/1340	1/2/2671	TD-DFT excited states (100 singlets) at B3LYP/6-31G(d,p), using SBKJC-VDZ-ECP for metals, in MeCN