Complex ferrocenoyl 17β-hydroxy-estra-1,3,5(10)-trien-3-olate	Torsion angle Cp and ester (-CO_2) group (^{0}) **a**(^{0})	Torsion angle between ester group and phenyl ring (^{0}) **b**(^{0})	Energy
1	0^0 (co-planar)	0^0	-7.11118 x 10^4 eV/-1.139337 x 10^{-17} KJ
2	87.0^0	117^0	-7.110954 x 10^4 eV/-1.1393 10^{-17} KJ
3	0^0	62.6^0	-7.110951 x 10^4/ -1.39300 10^{-17} KJ
4	90^0	62.6^0	-7.110990 x 10^4 eV/-1.139306 10^{-17} KJ
5	-144.1^0	62.6^0	-7.110981 x 10^4 eV/-1.139305 10^{-17} KJ
6	180^0	62.6^0	-7.110973 x 10^4 eV/-1.139304 x 10^{-17} KJ
7	7.7^0	62.7^0	-7.110815 x 10^4 eV/-1.139279 x 10^{-17} KJ
8	180 (co-planar)	62.7^0	-7.110822 x 10^4 eV/-1.139280 x 10^{-17} KJ
9	-90	90^0	-7.110811 x 10^4 eV/-

Table 1. Simple point energies for nine conformations at different a and b torsion angles of ferrocenoyl 17β-hydroxy-estra-1,3,5(10)-trien-3-olate.