

Inhibitors	E_{HOMO} (eV)	E_{LUMO} (eV)
Fe	-7.9024*	-0.1510*
Thiophene 1	-9.9133	-0.4352
Thiophene 2	-9.2712	-1.2941
Thiophene 3	-8.9479	-1.6624
Thiophene 4	-8.7854	-1.8467
Thiophene 5	-8.6945	-1.9526
Thiophene 6	-8.6412	-2.0168
Thiophene 7	-8.6002	-2.0593
Thiophene 8	-8.5717	-2.0897
Thiophene 9	-8.5553	-2.1095
Thiophene 10	-8.5392	-2.1258

*From ref [24]

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