
Quantum Chemistry Prasad Pdf 13

Inhibitors	$(\text{LUMO})_{\text{Inh}^-}$ $(\text{HOMO})_{\text{Fe}^-}$ (eV)	$(\text{LUMO})_{\text{Fe}^-}$ $(\text{HOMO})_{\text{Inh}^-}$ (eV)
Thiophene 1	7.4959	6.3357
Thiophene 2	6.4224	5.4636
Thiophene 3	5.9622	5.1229
Thiophene 4	5.7089	4.9468
Thiophene 5	5.5502	4.8423
Thiophene 6	5.4430	4.7749
Thiophene 7	5.3668	4.7291
Thiophene 8	5.3099	4.6968
Thiophene 9	5.2667	4.6731
Thiophene 10	5.2329	4.6551

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