

Hasil Perhitungan Muatan Atom (q) Menggunakan Metode MM+

Senyawa	Muatan Atom														IC_{50}	LOG IC_{50}
	C1	C2	C3	C4	C5	C6	N7	C8	C9	C10	C11	O12	C13	N14		
6a	-0.108	-0.100	-0.097	0.070	-0.056	-0.086	0.446	-0.022	-0.217	0.208	-0.129	-0.097	0.092	-0.078	101	2.0043
6b	0.170	-0.146	-0.094	0.051	-0.059	-0.185	0.441	-0.032	-0.230	0.207	-0.129	-0.097	0.092	-0.078	101	2.0043
6c	-0.154	0.177	-0.196	0.068	-0.075	-0.082	0.436	-0.036	-0.223	0.208	-0.129	-0.098	0.092	-0.078	10.45	1.0191
6d	-0.178	0.308	-0.220	0.071	-0.082	-0.076	0.433	-0.038	-0.224	0.208	-0.129	-0.097	0.092	-0.078	12.9	1.1106
6e	-0.111	-0.105	-0.104	0.070	-0.054	-0.094	0.432	0.087	-0.253	0.201	-0.130	-0.094	0.091	-0.078	21.2	1.3263
6f	-0.096	-0.104	-0.099	0.054	-0.031	-0.092	0.533	-0.018	-0.193	0.208	-0.125	-0.097	0.092	-0.078	25.69	1.4098
6g	0.179	-0.153	-0.095	0.031	-0.032	-0.186	0.528	-0.026	-0.202	0.208	-0.126	-0.097	0.092	-0.078	55.21	1.742
6h	-0.142	0.171	-0.195	0.053	-0.052	-0.091	0.525	-0.034	-0.196	0.208	-0.125	-0.097	0.092	-0.078	95.1	1.9782
6i	-0.097	-0.112	-0.097	0.060	-0.038	-0.103	0.536	0.073	-0.239	0.193	-0.135	-0.087	0.090	-0.076	11.2	1.0492
6j	-0.108	-0.101	-0.097	0.070	-0.056	-0.086	0.446	-0.022	-0.217	0.208	-0.128	-0.118	0.101	-0.110	101	2.0043
6k	-0.108	-0.101	-0.097	0.070	-0.056	-0.086	0.446	-0.022	-0.217	0.208	-0.128	-0.119	0.102	-0.113	70.14	1.846
6l	-0.108	-0.101	-0.097	0.070	-0.056	-0.086	0.446	-0.022	-0.217	0.207	-0.128	-0.119	0.099	-0.111	15.5	1.1903
6m	0.170	-0.146	-0.094	0.051	-0.059	-0.185	0.441	-0.032	-0.230	0.207	-0.129	-0.119	0.099	-0.111	42.58	1.6292