

SUPPORTING INFORMATION

Chromeno-carbonitriles as Corrosion Inhibitors for Mild Steel in Acidic Solution: Electrochemical, Surface and Computational Studies

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Table S11 Mulliken charges of INH-1, INH-2 and INH-3 molecules

INH-1

Atoms	qN	qN+1	qN-1	fk+	fk-
C1	-0.049	-0.160	-0.0586	-0.111	0.009
C2	-0.062	-0.198	-0.2035	-0.136	0.142
C3	-0.047	-0.544	-0.3984	-0.497	0.351
C4	-0.028	0.120	0.0836	0.148	-0.112
C5	0.011	0.286	0.3709	0.274	-0.359
C6	-0.070	-0.368	-0.3827	-0.297	0.312
C7	0.182	0.221	0.2972	0.039	-0.115

C8	0.191	0.121	0.1189	-0.070	0.072
C9	0.015	0.258	0.1236	0.243	-0.108
C10	-0.208	-0.415	-0.1805	-0.207	-0.028
O11	-0.200	-0.562	-0.3124	-0.362	0.113
C12	-0.087	0.486	0.6290	0.572	-0.716
C13	0.300	0.743	0.7054	0.443	-0.405
O14	-0.241	-0.349	-0.2632	-0.108	0.022
C15	0.154	0.123	0.0128	-0.031	0.141
C16	-0.060	0.797	0.9004	0.858	-0.961
C17	-0.116	-0.930	-0.7422	-0.815	0.627
C18	0.056	0.222	0.0333	0.166	0.023
C19	-0.130	-0.544	-0.3702	-0.414	0.240
C20	0.189	-0.206	-0.3654	-0.395	0.554
O21	-0.236	-0.347	-0.2771	-0.111	0.041
N22	-0.415	-0.652	-0.5280	-0.237	0.113
C23	-0.172	-0.413	-0.3158	-0.241	0.144
C24	-0.177	-0.534	-0.4627	-0.357	0.286
C25	0.050	-0.081	-0.1351	-0.130	0.185
N26	-0.215	-0.574	-0.3953	-0.359	0.180

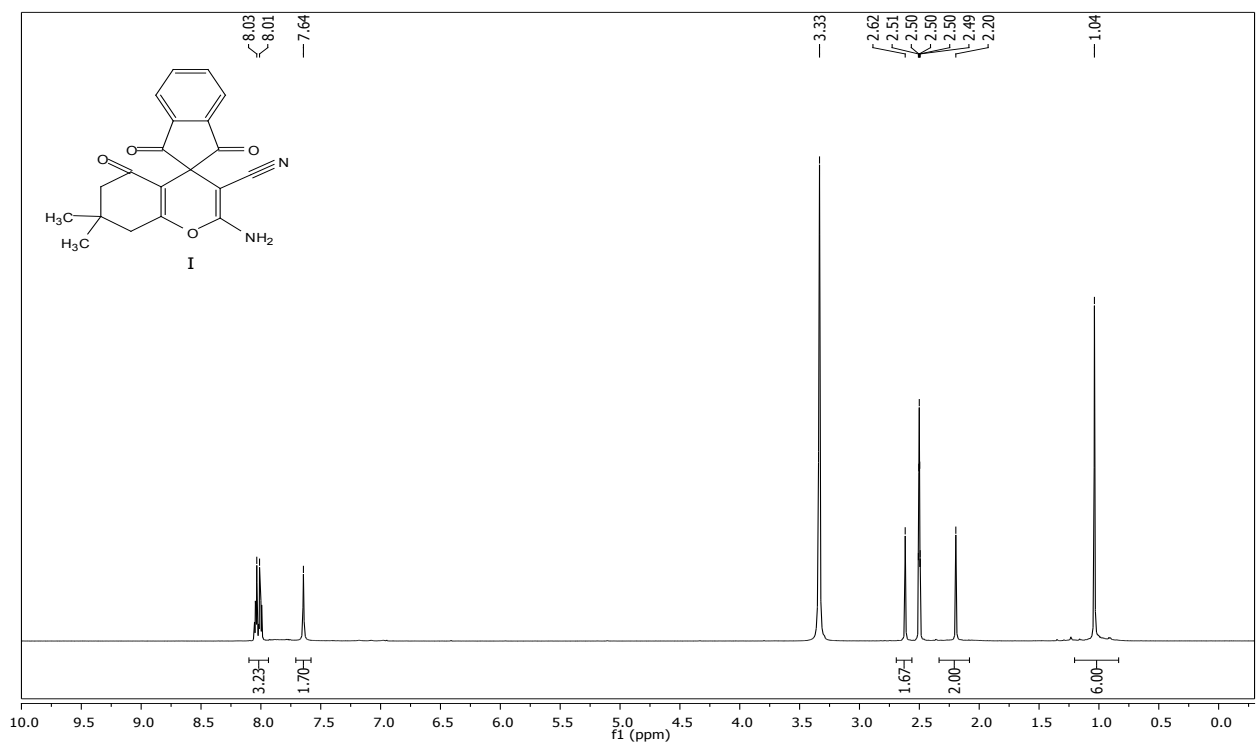
INH-2

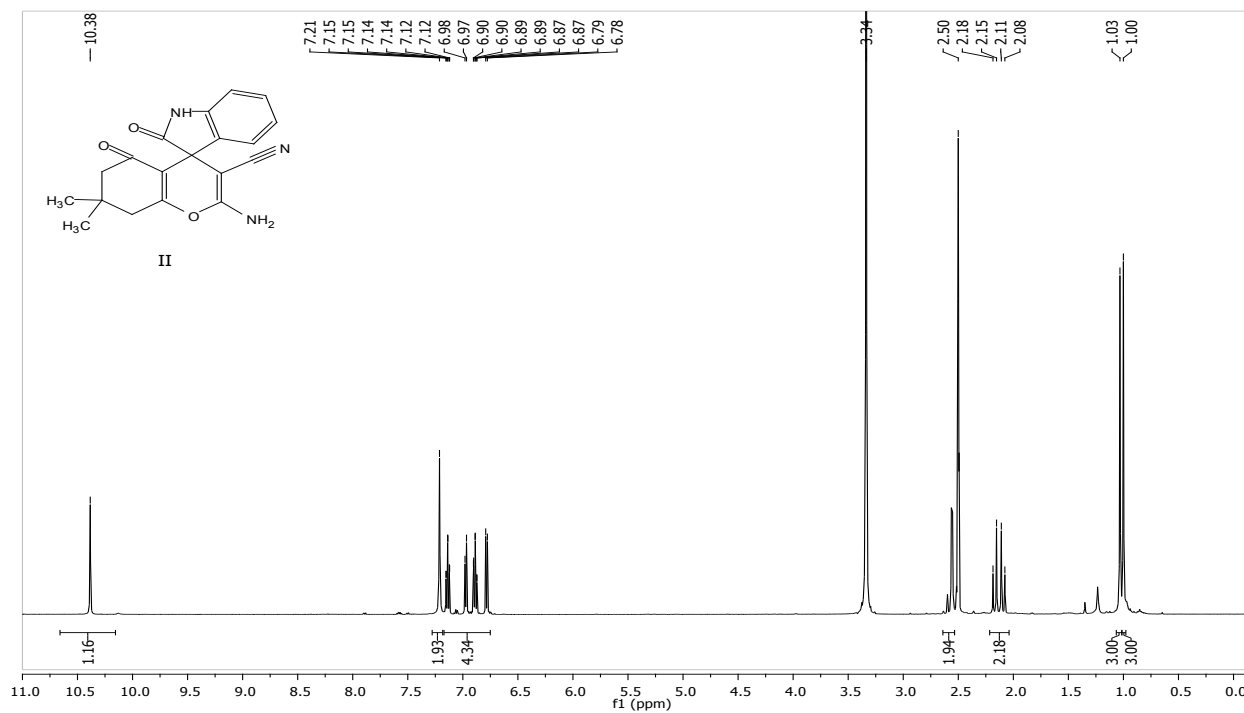
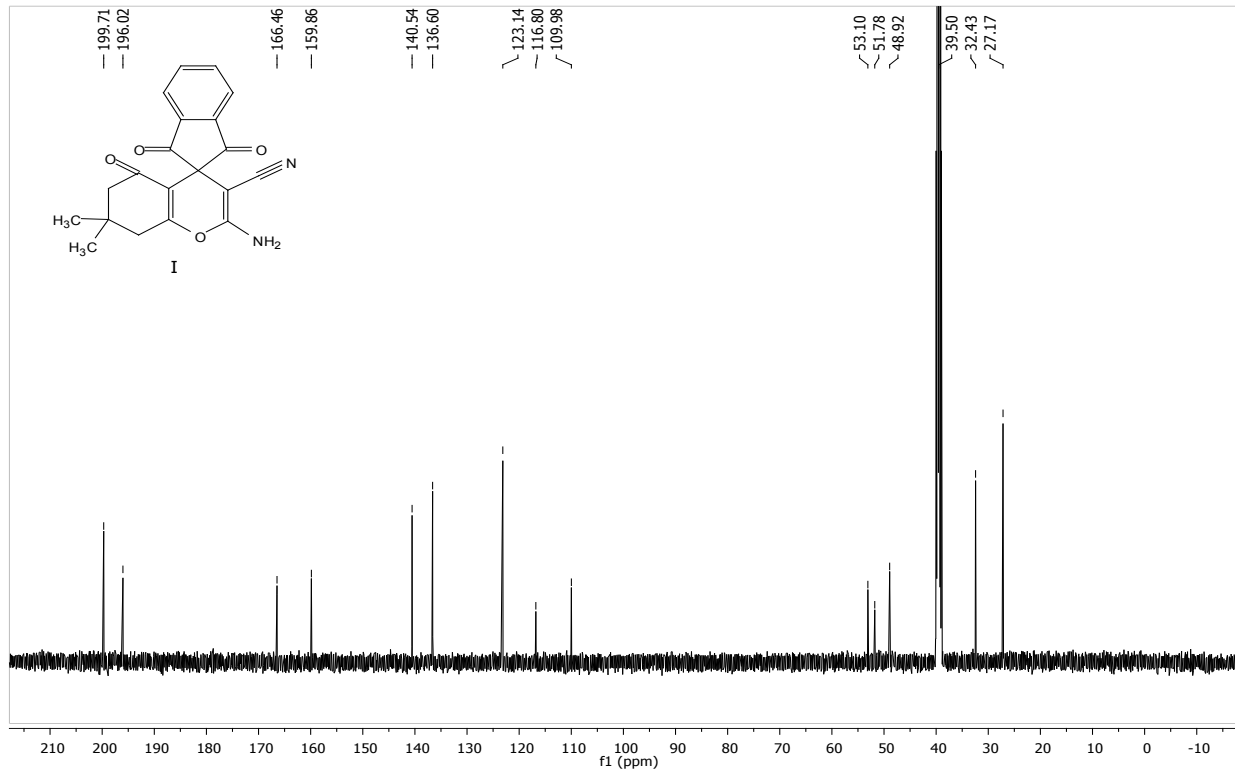
Atoms	qN	qN+1	qN-1	fk+	fk-
C1	-0.074	-0.159	-0.110	-0.085	0.036
C2	-0.048	-0.244	-0.201	-0.196	0.153
C3	-0.084	-0.474	-0.412	-0.390	0.328
C4	0.126	-0.369	-0.360	-0.495	0.486
C5	-0.016	0.904	0.975	0.920	-0.991
C6	-0.057	-0.497	-0.508	-0.439	0.451
N7	-0.363	-0.331	-0.234	0.032	-0.128
C8	0.316	0.136	0.111	-0.180	0.205
O9	-0.281	-0.460	-0.324	-0.180	0.043
C10	0.020	0.163	-0.068	0.143	0.087
C11	-0.083	0.447	0.783	0.530	-0.866
C12	0.299	0.778	0.742	0.480	-0.443
O13	-0.242	-0.378	-0.297	-0.137	0.056
C14	0.154	0.104	-0.027	-0.049	0.181
C15	-0.057	0.620	0.780	0.677	-0.837
C16	-0.115	-0.925	-0.649	-0.809	0.533
C17	0.056	0.428	0.093	0.372	-0.037
C18	-0.130	-0.608	-0.362	-0.478	0.232
C19	0.190	-0.029	-0.239	-0.219	0.429
O20	-0.233	-0.480	-0.312	-0.247	0.079

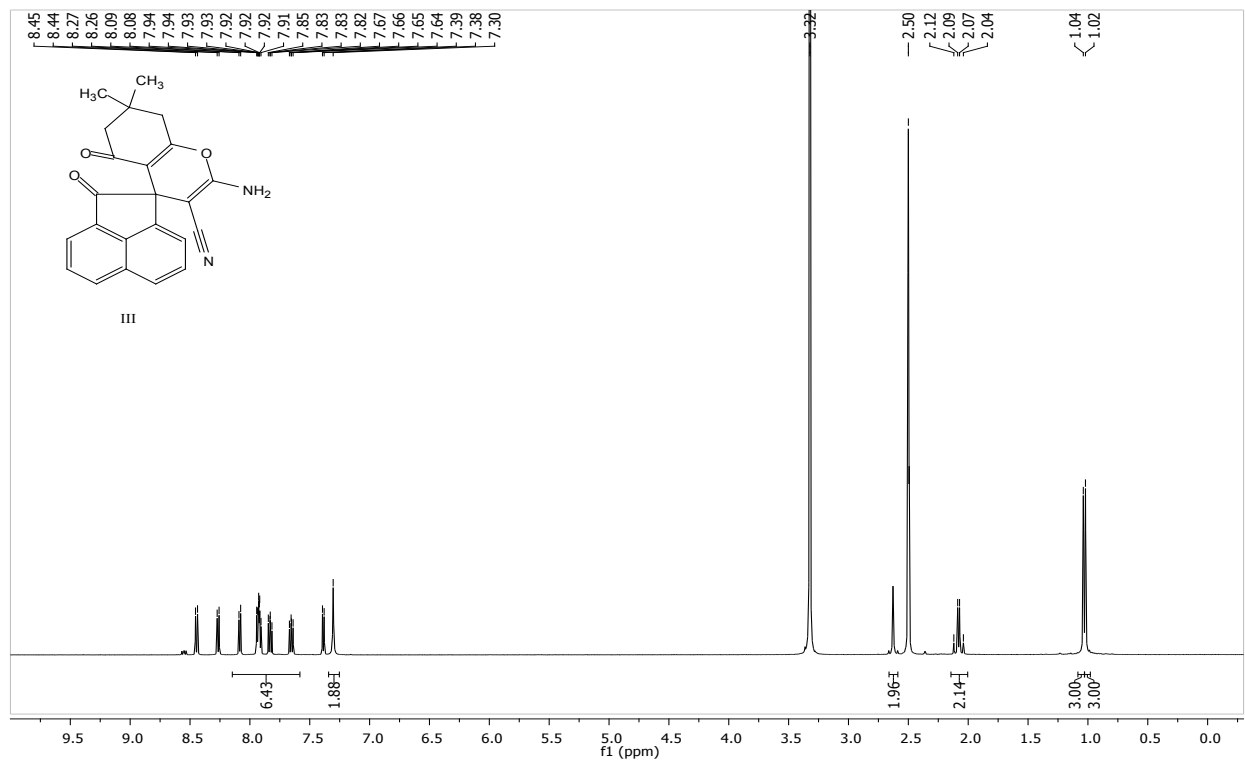
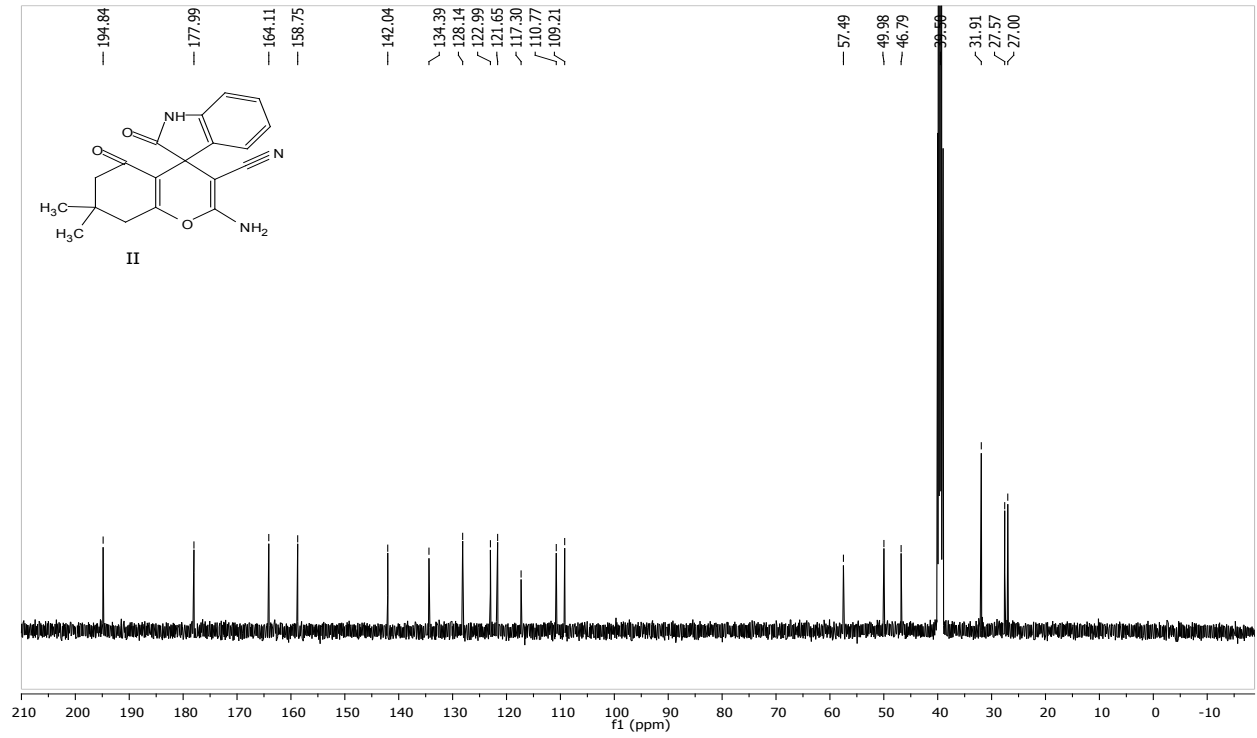
N21	-0.415	-0.681	-0.545	-0.266	0.130
C22	-0.172	-0.467	-0.335	-0.295	0.163
C23	-0.177	-0.577	-0.463	-0.400	0.287
C24	0.053	0.061	-0.047	0.008	0.100
N25	-0.217	-0.632	-0.431	-0.414	0.214

INH-3

Atoms	qN	qN+1	qN-1	fk+	fk-
C1	-0.088	-0.129	-0.060	-0.041	-0.028
C2	-0.057	-0.053	-0.069	0.004	0.012
C3	-0.585	-0.628	-0.526	-0.043	-0.060
C4	0.204	0.219	0.212	0.015	-0.008
C5	-0.181	-0.181	-0.188	-0.001	0.007
C6	0.578	0.547	0.614	-0.031	-0.035
C7	0.056	-0.034	0.118	-0.090	-0.062
C8	-0.345	-0.326	-0.329	0.019	-0.016
C9	-0.366	-0.452	-0.354	-0.086	-0.012
C10	0.127	0.146	0.170	0.018	-0.043
C11	0.468	0.526	0.405	0.058	0.063
O12	-0.259	-0.264	-0.199	-0.005	-0.061
C13	0.469	0.392	0.477	-0.078	-0.008
C14	0.400	0.133	0.504	-0.267	-0.104
C15	0.629	0.704	0.591	0.075	0.038
O16	-0.499	-0.579	-0.472	-0.080	-0.027
C17	-0.417	-0.333	-0.538	0.084	0.121
C18	0.777	0.819	0.877	0.042	-0.100
C19	-0.804	-0.900	-0.708	-0.096	-0.096
C20	0.297	0.372	0.181	0.074	0.116
C21	-0.210	-0.220	-0.178	-0.010	-0.032
C22	-0.156	-0.200	-0.181	-0.044	0.026
O23	-0.443	-0.464	-0.338	-0.021	-0.106
N24	-0.548	-0.587	-0.518	-0.040	-0.030
C25	-0.444	-0.489	-0.402	-0.045	-0.042
C26	-0.532	-0.564	-0.486	-0.031	-0.046
C27	-0.621	-0.553	-0.633	0.068	0.013
N28	-0.511	-0.639	-0.442	-0.128	-0.070







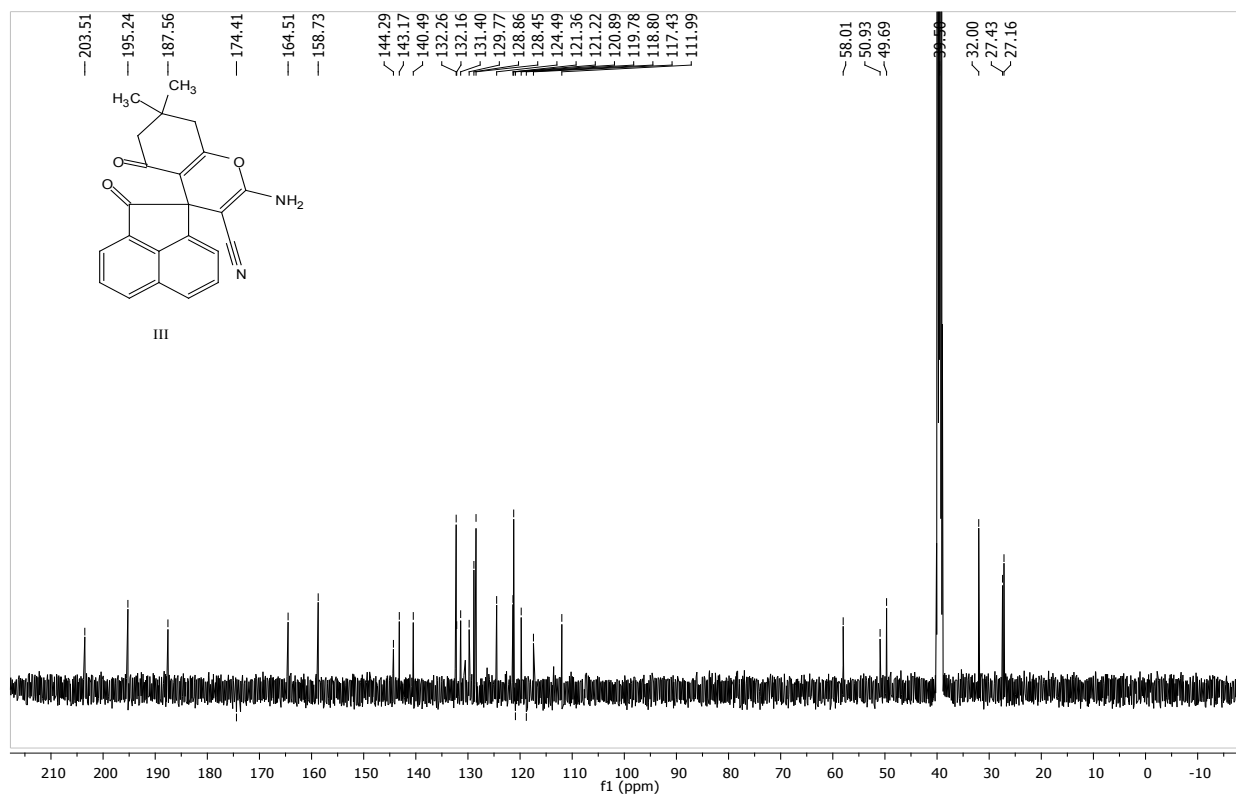


Fig. S1 ^1H and ^{13}C NMR spectra of INH-1, INH-2 and INH-3 molecules.