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SUPPLEMENTARY MATERIAL TO

Theoretical and experimental prediction of corrosion inhibition efficiency of isatin and its derivatives by DFT calculations and weight loss method – A comparative study

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Table C1. List of software, functional and basis set analysis for computational studies.

Compound s	Functions	Software	Basis set
I-IX	Optimization	Gaussian 09W	B3LYP/6-311G
	Frequency	Gaussian 09W	B3LYP/6-311G
	Dispersion Correction	Gaussian 16	PBE0-GD3BJ/6-31G (d,p)
	IEFPCM Water model	Gaussian 16	B3LYP/6-311G (d,p)

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Table S2. Fukui local parameters of compound I (isatin)

N	Z	f-	f+	f0	Dual-descriptor	Hardness (au)	W- (eV)	W+ (eV)
1	C	0.0001	0.0014	0.0007	0.0013	0	0.0001	0.0014
2	C	0.0019	0.0001	0.001	-0.0018	0.0005	0.002	0.0001
3	C	0.0031	0.004	0.0035	0.0009	0.0008	0.0032	0.0041
4	C	0.005	0.0002	0.0026	-0.0048	0.0013	0.0051	0.0002
5	C	0.0262	0.0003	0.0133	-0.0259	0.007	0.0266	0.0003
6	C	0.0008	0	0.0004	-0.0008	0.0002	0.0008	0
7	N	0.0571	0.1087	0.0829	0.0516	0.0143	0.058	0.1104
8	C	0.0608	0.5624	0.3116	0.5015	0.0111	0.0618	0.5712
9	C	0.1235	0.0136	0.0685	-0.1099	0.0331	0.1254	0.0138
10	O	0.7159	0.3057	0.5108	-0.4102	0.1897	0.7272	0.3106
11	O	0.0015	0.0035	0.0025	0.002	0.0004	0.0015	0.0036
12	H	0	0	0	0	0	0	0
13	H	0.0001	0	0	-0.0001	0	0.0001	0
14	H	0.0004	0	0.0002	-0.0004	0.0001	0.0005	0
15	H	0.0001	0	0	-0.0001	0	0.0001	0
16	H	0.0034	0	0.0017	-0.0034	0.0009	0.0035	0

Table S3. Fukui local parameters of compound II (N-methyl isatin)

N	Z	f-	f+	f0	Dual-descriptor	Hardness (au)	W- (eV)	W+ (eV)
1	C	0.0001	0.0015	0.0008	0.0014	0	0.0001	0.0015
2	C	0.0012	0.0001	0.0007	-0.0012	0.0003	0.0012	0.0001
3	C	0.0017	0.0047	0.0032	0.0031	0.0004	0.0016	0.0047
4	C	0.0032	0.0004	0.0018	-0.0028	0.0009	0.0032	0.0004
5	C	0.0243	0.0004	0.0124	-0.0238	0.0065	0.0239	0.0004
6	C	0.0008	0	0.0004	-0.0008	0.0002	0.0008	0
7	N	0.0575	0.1144	0.0859	0.0569	0.0145	0.0565	**0.1125**
8	C	0.0515	**0.556**	**0.3037**	**0.5045**	0.0097	0.0506	**0.5469**
9	C	0.1026	0.0141	0.0583	-0.0885	0.0273	**0.1009**	0.0139
10	O	**0.7425**	**0.2989**	**0.5207**	**-0.4435**	**0.1959**	**0.7303**	**0.294**
11	O	0.0013	0.0034	0.0023	0.0021	0.0003	0.0013	0.0033
12	C	0.0069	0.0003	0.0036	-0.0066	0.0018	0.0068	0.0003
13	H	0	0	0	0	0	0	0
14	H	0.0001	0	0	-0.0001	0	0.0001	0
15	H	0.0002	0	0.0001	-0.0002	0.0001	0.0002	0
16	H	0	0	0	0	0	0	0
17	H	0.0061	0	0.003	-0.0061	0.0016	0.006	0
18	H	0	0.0029	0.0014	0.0028	0	0	0.0028
19	H	0	0.0029	0.0014	0.0028	0	0	0.0028

Table S4. Fukui local parameters of compound III (N-benzyl isatin)

N	Z	f-	f+	f0	Dual-descriptor	Hardness (au)	W- (eV)	W+ (eV)
1	C	0.0001	0.0015	0.0008	0.0014	0	0.0001	0.0014
2	C	0	0.0001	0.0001	0.0001	0	0	0.0001
3	C	0.0018	0.0047	0.0032	0.0029	0.0004	0.0017	0.0045
4	C	0.0034	0.0005	0.002	-0.003	0.0009	0.0033	0.0004
5	C	0.0018	0.0004	0.0011	-0.0014	0.0005	0.0017	0.0004
6	C	0.0002	0	0.0001	-0.0002	0	0.0002	0
7	N	0.001	**0.1137**	0.0574	**0.1127**	-0.0007	0.001	**0.1099**
8	C	0.0005	**0.555**	**0.2777**	**0.5545**	-0.0045	0.0005	**0.5364**
9	C	0.0001	0.0141	0.0071	0.0141	-0.0001	0.0001	0.0137
10	C	0.0024	0.0008	0.0016	-0.0016	0.0006	0.0023	0.0007
11	C	0.0398	0.0047	0.0223	-0.035	0.0102	0.0384	0.0046
12	O	0	**0.2974**	**0.1487**	**0.2973**	-0.0025	0	**0.2874**
13	O	0	0.0034	0.0017	0.0034	0	0	0.0033
14	C	0.0679	0.0003	0.0341	-0.0676	0.0175	0.0657	0.0003
15	C	0.0623	0.0001	0.0312	-0.0622	0.0161	0.0602	0.0001
16	C	0.0353	0.0002	0.0178	-0.0351	0.0091	0.0341	0.0002
17	C	**0.3899**	0.0002	**0.1951**	-0.3897	**0.1005**	**0.3768**	0.0002
18	C	**0.3916**	0.0005	**0.1961**	-0.3911	**0.1009**	**0.3785**	0.0005
19	H	0	0	0	0	0	0	0
20	H	0	0	0	0	0	0	0
21	H	0.0009	0	0.0005	-0.0009	0.0002	0.0009	0
22	H	0	0	0	0	0	0	0
23	H	0.0001	0.0022	0.0011	0.0021	0	0.0001	0.0021
24	H	0.0001	0.0001	0.0001	0	0	0.0001	0.0001
25	H	0.0001	0	0	-0.0001	0	0.0001	0
26	H	0	0	0	0	0	0	0
27	H	0	0	0	0	0	0	0
28	H	0.0002	0	0.0001	-0.0002	0.0001	0.0002	0
29	H	0.0003	0	0.0001	-0.0002	0.0001	0.0002	0

Table S5. Fukui local parameters of compound IV (N-allyl isatin)

N	Z	f-	f+	f0	Dual-descriptor	Hardness (au)	W- (eV)	W+ (eV)
1	C	0.0001	0.0014	0.0008	0.0013	0	0.0001	0.0014
2	C	0.0009	0.0001	0.0005	-0.0008	0.0002	0.0009	0.0001
3	C	0.002	0.0047	0.0033	0.0027	0.0005	0.002	0.0047
4	C	0.0016	0.0005	0.001	-0.0011	0.0004	0.0016	0.0005
5	C	0.0192	0.0004	0.0098	-0.0188	0.0051	0.0192	0.0004
6	C	0.0009	0	0.0005	-0.0009	0.0002	0.0009	0
7	N	0.063	**0.1126**	0.0878	0.0496	0.016	0.0629	**0.1124**
8	C	0.0471	**0.5554**	**0.3013**	**0.5083**	0.0081	0.047	**0.5545**
9	C	0.0911	0.0141	0.0526	-0.077	0.0243	0.091	0.0141
10	C	0.0074	0.0007	0.0041	-0.0068	0.002	0.0074	0.0007
11	C	0.002	0.0046	0.0033	0.0026	0.0005	0.002	0.0045
12	C	0.001	0.0011	0.001	0	0.0003	0.001	0.0011
13	O	**0.7563**	**0.2986**	**0.5274**	**-0.4577**	**0.2002**	**0.755**	**0.2981**
14	O	0.0012	0.0034	0.0023	0.0022	0.0003	0.0012	0.0034
15	H	0	0	0	0	0	0	0
16	H	0.0001	0	0	-0.0001	0	0.0001	0
17	H	0.0003	0	0.0002	-0.0003	0.0001	0.0003	0
18	H	0	0	0	0	0	0	0
19	H	0.0002	0.0021	0.0012	0.0019	0	0.0002	0.0021
20	H	0.0052	0.0001	0.0026	-0.0051	0.0014	0.0052	0.0001
21	H	0.0002	0	0.0001	-0.0002	0.0001	0.0002	0
22	H	0	0.0001	0.0001	0.0001	0	0	0.0001
23	H	0	0	0	0	0	0	0

Table S6. Fukui local parameters of compound V (N-propargyl isatin)

N	Z	f-	f+	f0	Dual-descriptor	Hardness (au)	W- (eV)	W+ (eV)
1	C	0.0001	0.0013	0.0007	0.0012	0	0.0001	0.0014
2	C	0.0009	0.0001	0.0005	-0.0008	0.0002	0.0009	0.0001
3	C	0.0018	0.0046	0.0032	0.0028	0.0004	0.0018	0.0048
4	C	0.0022	0.0004	0.0013	-0.0018	0.0006	0.0023	0.0004
5	C	0.02	0.0004	0.0102	-0.0196	0.0054	0.0209	0.0004
6	C	0.0009	0	0.0004	-0.0009	0.0002	0.0009	0
7	N	0.0621	**0.1094**	0.0857	0.0474	0.0157	0.0649	**0.1144**
8	C	0.0486	0.551	**0.2998**	**0.5024**	0.0071	0.0508	**0.5759**
9	C	0.0939	0.0139	0.0539	-0.08	0.0254	0.0981	0.0145
10	C	0.009	0.0033	0.0061	-0.0057	0.0024	0.0094	0.0034
11	C	0.0049	0.0084	0.0066	0.0036	0.0012	0.0051	0.0088
12	O	**0.743**	**0.2968**	**0.5199**	**-0.4463**	**0.1988**	**0.7765**	**0.3101**
13	O	0.0012	0.0034	0.0023	0.0022	0.0003	0.0013	0.0036
14	C	0.005	0.0047	0.0048	-0.0003	0.0013	0.0052	0.0049
15	H	0	0	0	0	0	0	0
16	H	0.0001	0	0	-0.0001	0	0.0001	0
17	H	0.0003	0	0.0001	-0.0003	0.0001	0.0003	0
18	H	0	0	0	0	0	0	0
19	H	0	0.0022	0.0011	0.0022	0	0	0.0023
20	H	0.006	0	0.003	-0.006	0.0016	0.0063	0
21	H	0.0001	0.0002	0.0001	0.0001	0	0.0001	0.0002

Table S7. Fukui local parameters of compound VII (5-methyl isatin)

N	Z	f-	f+	f0	Dual-descriptor	Hardness (au)	W- (eV)	W+ (eV)
1	C	0.0003	0.0013	0.0008	0.001	0.0001	0.0003	0.0013
2	C	0.0027	0.0001	0.0014	-0.0026	0.0007	0.0027	0.0001
3	C	0.0035	0.0041	0.0038	0.0006	0.0009	0.0034	0.0041
4	C	0.0051	0.0002	0.0026	-0.0049	0.0014	0.005	0.0002
5	C	0.0271	0.0003	0.0137	-0.0267	0.0072	0.0265	0.0003
6	C	0.0014	0	0.0007	-0.0014	0.0004	0.0014	0
7	N	0.0564	**0.1106**	0.0835	0.0542	0.0142	0.0552	**0.1082**
8	C	0.0608	**0.5619**	**0.3113**	**0.5011**	0.0123	0.0595	0.55
9	C	**0.1263**	0.0135	0.0699	-0.1127	0.0335	**0.1236**	0.0133
10	O	**0.7109**	**0.3042**	**0.5075**	**-0.4067**	**0.187**	**0.6959**	**0.2978**
11	O	0.0015	0.0034	0.0025	0.0019	0.0004	0.0015	0.0033
12	C	0	0	0	0	0	0	0
13	H	0.0001	0	0	-0.0001	0	0.0001	0
14	H	0.0005	0	0.0002	-0.0005	0.0001	0.0005	0
15	H	0.0001	0	0	-0.0001	0	0.0001	0
16	H	0.0035	0	0.0018	-0.0035	0.0009	0.0034	0
17	H	0	0	0	0	0	0	0
18	H	0	0.0001	0.0001	0.0001	0	0	0.0001
19	H	0	0.0001	0.0001	0.0001	0	0	0.0001

Table S8. Fukui local parameters of compound IX (1-methyl-5-methyl isatin)

N	Z	f-	f+	f0	Dual-Descriptor	Hardness(au)	W-(eV)	W+(eV)
1	C	0	0	0	0	0	0	0
2	C	0	0	0	0	0	0	0
3	C	0.0001	0	0.0001	-0.0001	0	0.0001	0
4	C	0.0012	0.0001	0.0007	-0.0011	0.0003	0.0011	0.0001
5	C	0.0015	0.0001	0.0008	-0.0013	0.0004	0.0014	0.0001
6	C	0.0001	0	0.0001	-0.0001	0	0.0001	0
7	N	0.0023	0.0094	0.0058	0.0071	0.0006	0.0022	0.0089
8	C	0.0117	**0.6262**	**0.3189**	**0.6145**	0	0.0111	**0.5943**
9	C	0.0026	0.0055	0.0041	0.0029	0.0007	0.0025	0.0053
10	C	0.0002	0.0002	0.0002	0	0.0001	0.0002	0.0002
11	O	0	0	0	0	0	0	0
12	O	**0.98**	**0.3582**	**0.6691**	**-0.6218**	**0.2569**	**0.93**	**0.3399**
13	O	0.0001	0.0001	0.0001	-0.0001	0	0.0001	0.0001
14	H	0	0	0	0	0	0	0
15	H	0	0	0	0	0	0	0
16	H	0	0	0	0	0	0	0
17	H	0.0001	0	0.0001	-0.0001	0	0.0001	0
18	H	0	0.0001	0	0.0001	0	0	0.0001
19	H	0	0.0001	0	0.0001	0	0	0.0001
20	H	0	0	0	0	0	0	0
21	H	0	0	0	0	0	0	0
22	H	0	0	0	0	0	0	0

Table S9. Calculated global parameters by HOMO and LUMO energies (Grimme's D3)

Compound No	ΔE (eV)	I (eV)	A (eV)	χ (eV)	η (eV)	σ (eV)	ΔN (eV)	ω (eV)	ε (eV)
I	4.3002	6.8316	2.5314	4.6815	2.1501	0.4651	0.5391	5.0966	0.1962
II	4.1527	6.6281	2.4754	4.5517	2.0763	0.4816	0.5895	4.9891	**0.2004**
III	4.1524	6.6123	2.4599	4.5361	2.0762	0.4816	0.5933	4.9552	**0.2018**
IV	4.1541	6.6265	2.4724	4.54945	2.0770	0.4814	0.5899	4.9824	**0.2007**
V	4.2033	6.7454	2.5421	4.6437	2.1016	0.4758	0.5605	5.1303	0.1949
VI	4.4096	**7.5865**	**3.1769**	**5.3817**	2.2048	0.4535	0.3669	**6.5681**	0.1522
VII	4.1453	6.6014	2.4561	4.52875	2.0726	0.4824	0.5961	4.9476	**0.2021**
VIII	4.2336	**7.3465**	**3.1129**	**5.2297**	2.1168	0.4724	0.4181	**6.4601**	0.1547
IX	**4.0494**	6.4521	2.4027	4.4274	**2.0247**	**0.4939**	**0.6353**	4.8406	**0.2065**

Table S10. Calculated global parameters by HOMO and LUMO energies (IEFPCM-Water).

Compound No	ΔE (eV)	I (eV)	A (eV)	χ (eV)	η (eV)	σ (eV)	ΔN (eV)	ω (eV)	ε (eV)
I	3.7114	6.6276	2.9162	4.7719	1.8557	0.5389	0.6003	6.1354	0.1630
II	3.587	6.4825	2.8955	4.689	1.7935	0.5576	0.6443	6.1295	0.1631
III	3.6085	6.5421	2.9336	4.7378	1.8042	0.5542	0.6269	6.2207	0.1607
IV	3.6077	6.5288	2.9211	4.7249	1.8038	0.5544	0.6306	6.1882	0.1616
V	3.669	6.6461	2.9771	4.8116	1.8345	0.5451	0.5965	6.3100	0.1585
VI	3.8738	**7.1372**	**3.2634**	**5.2003**	1.9369	0.5163	0.4646	**6.9810**	0.1432
VII	3.5454	6.4197	2.8743	4.647	1.7727	0.5641	0.6637	6.0909	0.1642
VIII	3.7108	**6.9601**	**3.2493**	**5.1047**	1.8554	0.5389	0.5108	**7.0222**	0.1424
IX	**3.4452**	6.3002	2.8550	4.5776	**1.7226**	**0.5805**	**0.7031**	6.0822	0.1644

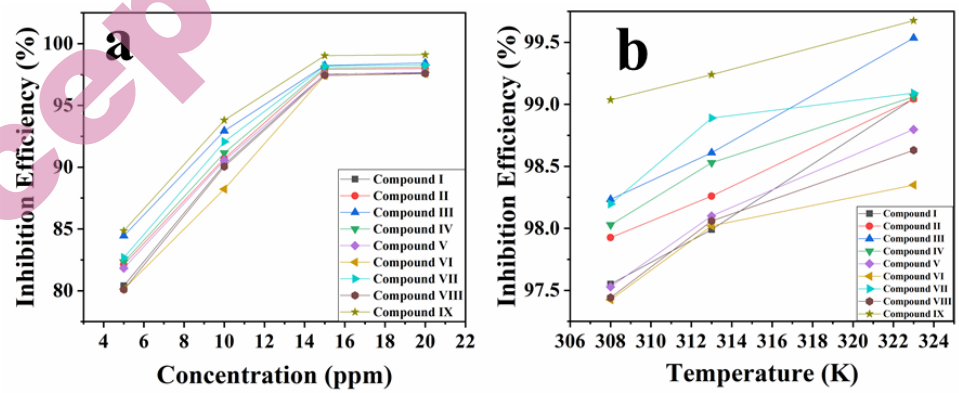


Figure s1. Inhibition efficiency of mild steel immersed in 1 M HCl with (a) different concentrations of compounds I to IX (b) Maximum inhibition efficiency of 15 ppm of compounds I to IX with at 308, 313, 323 K.

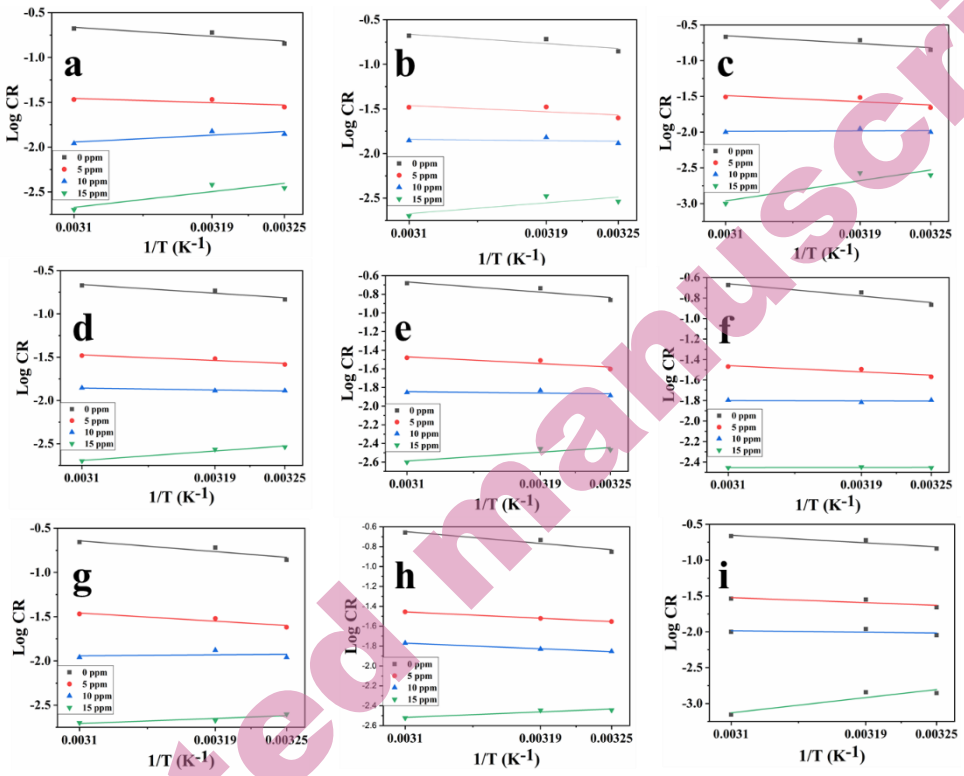


Figure s2. Arrhenius plots of (a) compound I (b) compound II (c) compound III (d) compound IV (e) compound V (f) compound VI (g) compound VII (h) compound VIII (i) compound IX.

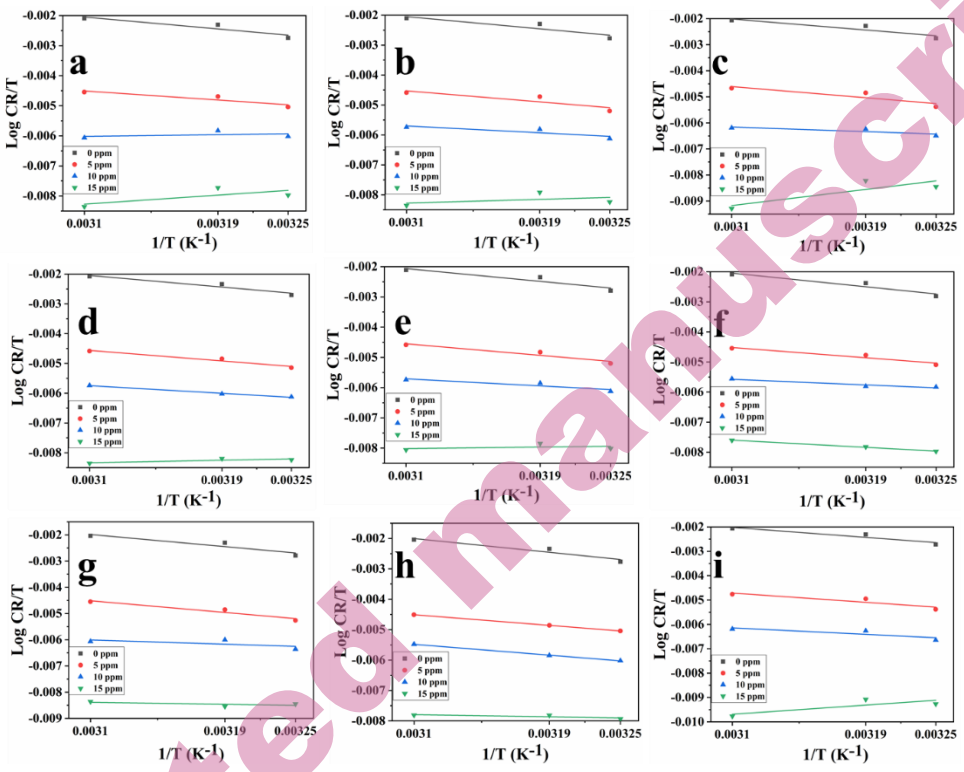


Figure s3. Transition state plots of (a) compound I (b) compound II (c) compound III (d) compound IV (e) compound V (f) compound VI (g) compound VII (h) compound VIII (i) compound IX.

				-ΔS (KJ mol^{-1})
Compound I	0	19.54	76.3703	78.2303
	5	09.31	58.3556	78.333
	10	14.99	10.9885	78.2781
	15	33.97	58.2284	78.088
Compound II	0	20.23	78.6450	78.222
	5	13.21	71.2637	78.2934
	10	2.64	44.1169	78.4006
	15	23.44	24.1465	78.1939
Compound III	0	21.22	81.6032	78.2130
	5	16.63	82.8554	78.2589
	10	12.4	34.3327	78.5424
	15	54.83	119.9951	78.8884
Compound IV	0	19.28	75.3669	78.2188
	5	12.33	63.3572	78.3030
	10	4.40	49.6083	78.3834
	15	21.20	16.9893	78.2149
Compound V	0	21.14	81.6358	78.2149
	5	14.04	73.9118	78.2858
	10	2.99	45.2504	78.3968
	15	18.43	9.8435	78.2436
Compound VI	0	23.14	87.9313	78.1939
	5	11.70	66.0672	78.3088
	10	0.56	36.1804	78.4217
	15	0.19	46.4203	78.4257
Compound VII	0	23.70	89.4248	78.1881
	5	17.97	86.4053	78.2455
	10	2.03	31.0011	78.4466
	15	11.32	14.9500	78.5423
Compound VIII	0	23.07	87.4450	78.1958
	5	12.34	67.8536	78.3030
	10	10.84	69.0043	78.3183
	15	11.27	13.6864	78.5347
Compound IX	0	20.44	79.0375	78.2207
	5	13.55	73.4255	78.2896
	10	4.02	51.4100	78.3853
	15	41.18	72.8778	78.8391

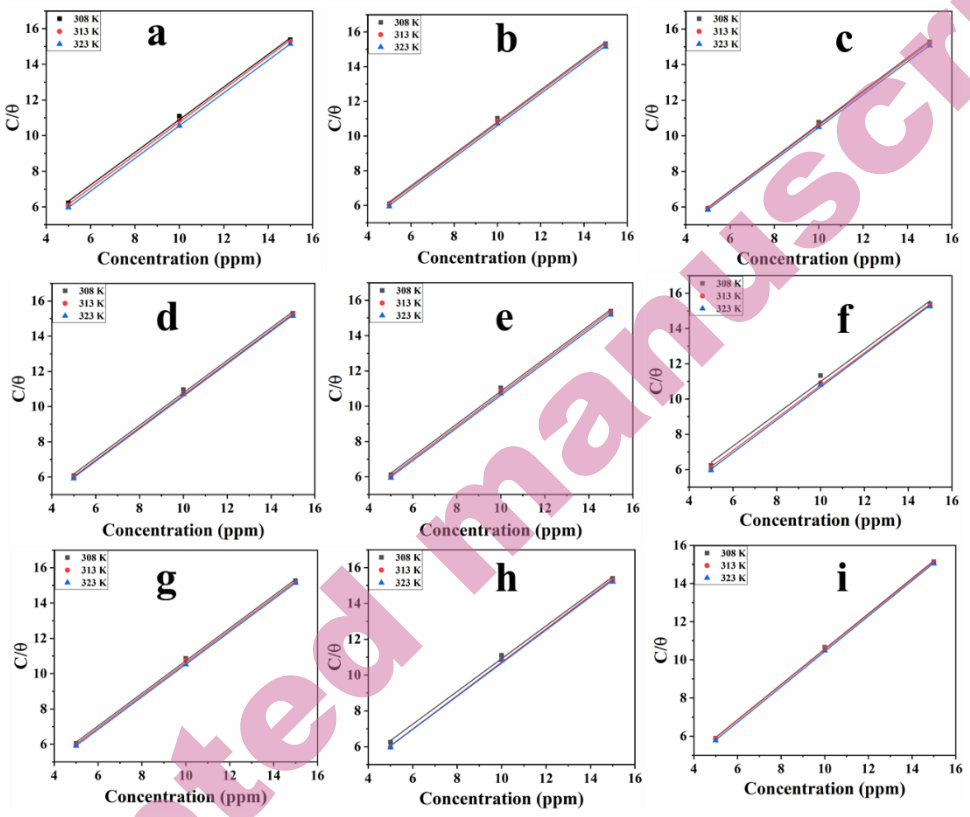


Figure s4. Langmuir adsorption isotherm for mild steel in 1 M HCl containing different concentrations of (a) compound I (b) compound II (c) compound III (d) compound IV (e) compound V (f) compound VI (g) compound VII (h) compound VIII (i) compound IX at 308–323 K.

Table S12. Thermodynamic parameters for Langmuir adsorption of (a) compound I (b) compound II (c) compound III (d) compound IV (e) compound V (f) compound VI (g) compound VII (h) compound VIII (i) compound IX on the mild steel in 1M HCl.

Compound	Temperature	K_{ads}	$-\Delta G$ (KJ mol^{-1})	R^2
Compound I	308	0.5762	8.873	0.998
	313	0.6526	9.341	0.999
	323	0.7267	9.928	1
Compound II	308	0.6322	9.110	0.998
	313	0.6615	9.376	0.999
	323	0.7180	9.896	0.999
Compound III	308	0.7686	9.610	0.999
	313	0.7633	9.748	1
	323	0.8070	10.209	1
Compound IV	308	0.6437	9.156	0.998
	313	0.7087	9.554	0.999
	323	0.7343	9.956	0.999
Compound V	308	0.6351	9.122	0.998
	313	0.6947	9.503	0.999
	323	0.7267	9.928	0.999
Compound VI	308	0.5454	8.732	0.995
	313	0.6449	9.310	0.999
	323	0.7263	9.926	0.999
Compound VII	308	0.6667	9.246	0.999
	313	0.7193	9.594	0.999
	323	0.7678	10.076	1
Compound VIII	308	0.5675	8.834	0.998
	313	0.7175	9.587	0.999
	323	0.7093	9.863	0.998
Compound IX	308	0.7620	9.588	0.999
	313	0.7735	9.783	0.999
	323	0.8597	10.379	0.999

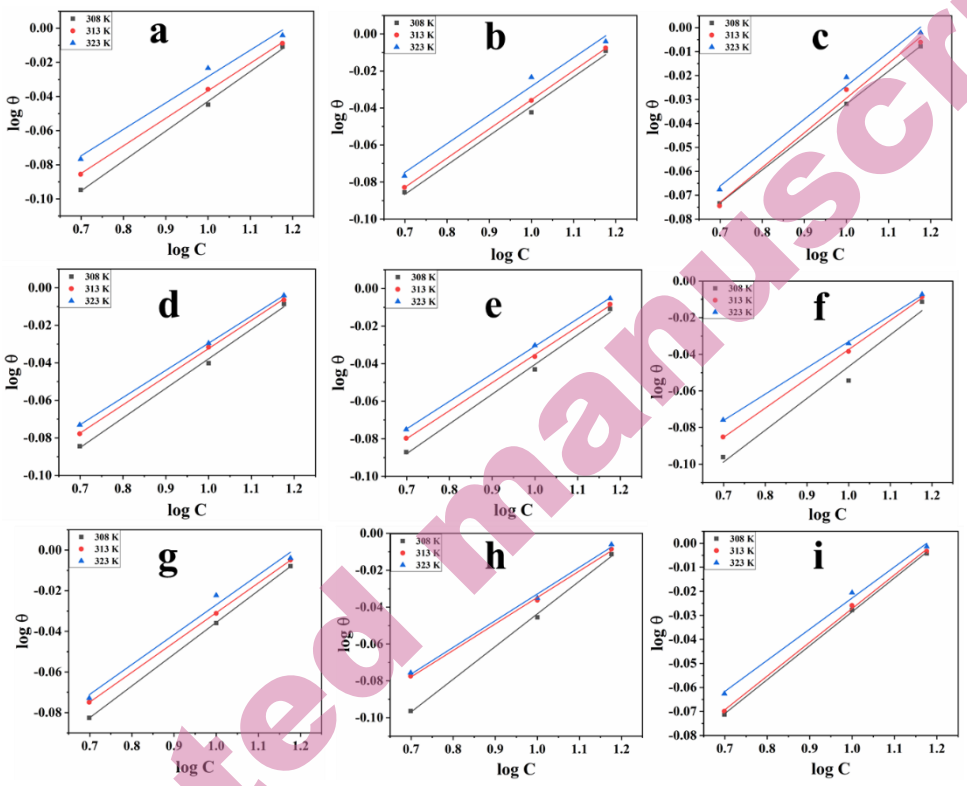


Figure s5. Freundlich adsorption isotherm for mild steel in 1 M HCl containing different concentrations of (a) compound I (b) compound II (c) compound III (d) compound IV (e) compound V (f) compound VI (g) compound VII (h) compound VIII (i) compound IX at 308–323 K.

Table S13. Thermodynamic parameters for Freundlich adsorption of (a) compound I (b) compound II (c) compound III (d) compound IV (e) compound V (f) compound VI (g) compound VII (h) compound VIII (i) compound IX on the mild steel in 1M HCl.

Compound	Temperature	K_{ads}	-ΔG (KJ mol^{-1})	R^2
Compound I	308	0.5530	8.767	0.995
	313	0.5887	9.072	1
	323	0.6147	9.478	0.991
Compound II	308	0.5897	8.932	0.989
	313	0.5974	9.111	0.999
	323	0.6147	9.478	0.991
Compound III	308	0.6427	9.152	0.999
	313	0.6320	9.257	0.995
	323	0.6513	9.634	0.994
Compound IV	308	0.5933	8.947	0.994
	313	0.6170	9.195	1
	323	0.6319	9.553	0.999
Compound V	308	0.5885	8.927	0.993
	313	0.6145	9.184	0.998
	323	0.6265	9.529	0.999
Compound VI	308	0.5483	8.745	0.966
	313	0.5901	9.079	0.998
	323	0.6291	9.541	0.998
Compound VII	308	0.5996	8.975	0.999
	313	0.6258	9.232	0.999
	323	0.6322	9.554	0.991
Compound VIII	308	0.5470	8.739	0.996
	313	0.6260	9.232	0.996
	323	0.6262	9.528	0.994
Compound IX	308	0.6409	9.145	1
	313	0.6446	9.309	0.999
	323	0.6738	9.725	0.9979

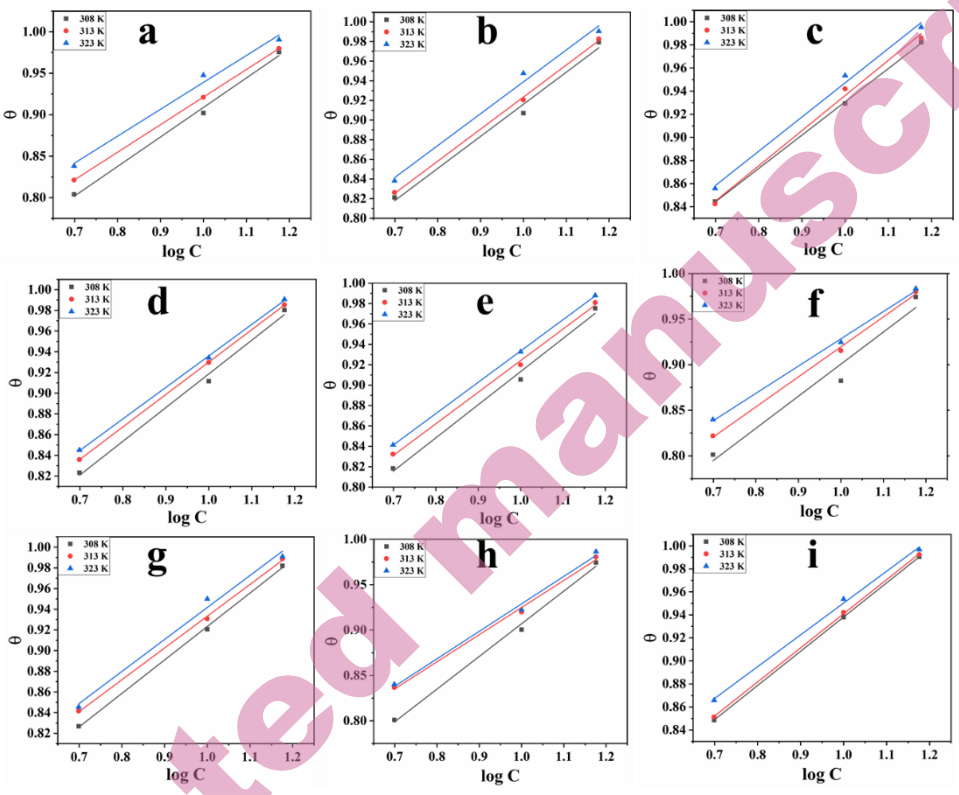


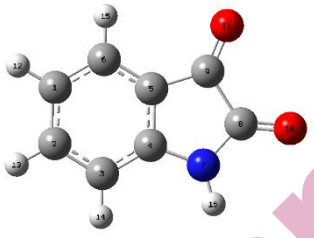
Figure s6. Temkin adsorption isotherm for mild steel in 1 M HCl containing different concentrations of (a) compound I (b) compound II (c) compound III (d) compound IV (e) compound V (f) compound VI (g) compound VII (h) compound VIII (i) compound IX at 308–323 K.

Table S14. Thermodynamic parameters for Temkin adsorption of (a) compound I (b) compound II (c) compound III (d) compound IV (e) compound V (f) compound VI (g) compound VII (h) compound VIII (i) compound IX on the mild steel in 1M HCl.

Compound	Temperature	K_{ads}	-ΔG (KJ mol^{-1})	R^2
Compound I	308	0.8044	9.727	0.998
	313	0.8204	9.936	0.999
	323	0.8327	10.294	0.987
Compound II	308	0.8208	9.779	0.994
	313	0.8244	9.949	0.999
	323	0.8327	10.294	0.987
Compound III	308	0.8440	9.850	1
	313	0.8398	9.997	0.992
	323	0.8489	10.345	0.991
Compound IV	308	0.8224	9.784	0.9972
	313	0.8332	9.976	0.9997
	323	0.8401	10.317	1
Compound V	308	0.8198	9.775	0.996
	313	0.8317	9.972	0.999
	323	0.8376	10.309	0.999
Compound VI	308	0.8022	9.720	0.975
	313	0.8210	9.938	0.999
	323	0.8383	10.312	0.999
Compound VII	308	0.8253	9.793	1
	313	0.8374	9.989	0.999
	323	0.8403	10.318	0.987
Compound VIII	308	0.8017	9.718	0.998
	313	0.8366	9.987	0.998
	323	0.8373	10.308	0.997
Compound IX	308	0.8440	9.850	0.999
	313	0.8458	10.015	0.999
	323	0.8587	10.376	0.996

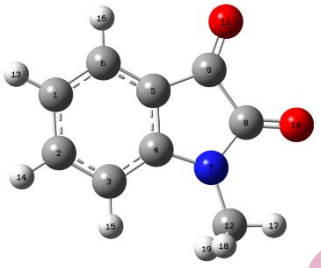
XYZ COORDINATES OF ISATIN AND ITS DERIVATIVES WITHOUT GRIMME D3 OPTIMIZED STRUCTURE

Table S15. Compound I (Isatin)



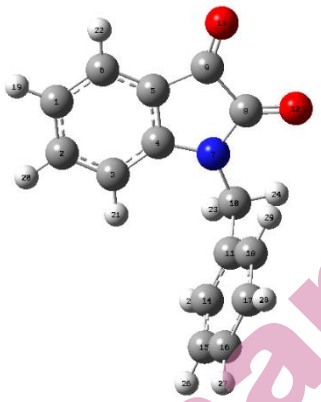
Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.640644	0.809011	0.000021
2	6	2.766522	-0.58669	0.000348
3	6	1.644607	-1.43081	0.000211
4	6	0.392043	-0.83285	-0.000204
5	6	0.252448	0.572535	-0.000556
6	6	1.371801	1.399081	-0.000498
7	7	-0.88501	-1.4355	-0.000097
8	6	-1.90391	-0.49041	-0.000052
9	6	-1.17957	0.886018	0.000056
10	8	-3.11621	-0.71012	-0.000034
11	8	-1.75124	1.979303	0.000577
12	1	3.526544	1.427684	0.000117
13	1	3.753157	-1.03015	0.000742
14	1	1.760525	-2.50565	0.000539
15	1	1.248075	2.473459	-0.000671
16	1	-1.06113	-2.42563	-0.000349

Table S16. Compound II (N-methyl isatin)



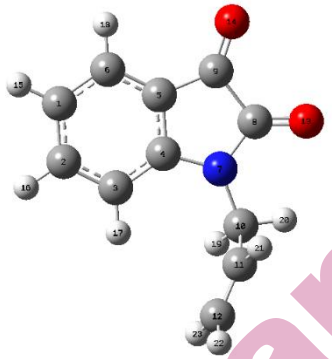
Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.91547	-0.50036	-0.00003
2	6	-2.73683	0.884986	-0.000027
3	6	-1.46363	1.468996	0.000024
4	6	-0.36684	0.618545	0.000069
5	6	-0.53678	-0.77911	0.000103
6	6	-1.80448	-1.34566	0.000013
7	7	0.995994	0.96027	-0.000034
8	6	1.794392	-0.17241	0.000016
9	6	0.800814	-1.38919	-0.000004
10	8	2.999549	-0.20804	0.000038
11	8	1.138564	-2.54519	-0.000074
12	6	1.516712	2.314489	-0.000043
13	1	-3.91613	-0.9146	-0.00007
14	1	-3.60704	1.531928	-0.000067
15	1	-1.35047	2.545812	0.000047
16	1	-1.91412	-2.42408	0.00007
17	1	2.603864	2.248257	-0.001251
18	1	1.188821	2.857761	-0.890845
19	1	1.190825	2.857119	0.891903

Table S17. Compound III (N-Benzyl isatin)



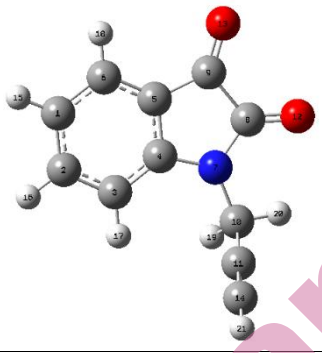
Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	4.332837	-1.34281	-0.221448
2	6	3.312967	-2.30076	-0.162262
3	6	1.960569	-1.94252	-0.046354
4	6	1.650105	-0.58668	0.004998
5	6	2.675205	0.378957	-0.045086
6	6	4.013006	0.01669	-0.160167
7	7	0.36404	0.037754	0.119461
8	6	0.527336	1.419716	0.186885
9	6	2.045898	1.688851	0.053778
10	6	-0.80563	-0.85357	0.310983
11	6	-2.25948	-0.43797	0.099942
12	8	-0.32114	2.305276	0.322701
13	8	2.549169	2.816152	0.061761
14	6	-3.16913	-1.49523	0.306553
15	6	-4.53809	-1.32081	0.12575
16	6	-5.03533	-0.07454	-0.269678
17	6	-4.14516	0.977615	-0.469716
18	6	-2.76466	0.806596	-0.29271
19	1	5.362389	-1.65855	-0.310022
20	1	3.569455	-3.35087	-0.206563
21	1	1.20508	-2.71111	0.002487
22	1	4.774786	0.783467	-0.195422
23	1	-0.63172	-1.6755	-0.387856
24	1	-0.71601	-1.28643	1.313984
25	1	-2.79919	-2.46851	0.610551
26	1	-5.21225	-2.15117	0.290735
27	1	-6.09844	0.069679	-0.408485
28	1	-4.51563	1.951833	-0.760183
29	1	-2.11364	1.660165	-0.389966

Table S18. Compound IV (N-allyl isatin)



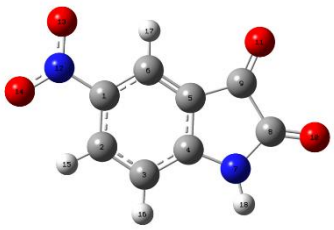
Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.801626	2.579291	0.064102
2	6	0.423958	2.768749	-0.26132
3	6	-0.44739	1.676148	-0.297884
4	6	0.083818	0.407831	-0.161006
5	6	1.449647	0.225369	0.0556
6	6	2.325028	1.296081	0.106175
7	7	-0.65304	-0.80136	-0.106187
8	6	0.397473	-1.82426	-0.25862
9	6	1.721748	-1.22548	0.250797
10	6	-2.10156	-0.98869	0.060763
11	6	-2.76268	0.3448	0.221039
12	6	-4.08707	0.418519	0.388134
13	8	0.246123	-2.93664	-0.704698
14	8	2.704167	-1.77729	0.686066
15	1	2.474079	3.449488	-0.043544
16	1	0.026708	3.786635	-0.388212
17	1	-1.5294	1.822437	-0.432293
18	1	3.400743	1.140816	0.275429
19	1	-2.51462	-1.50159	-0.836487
20	1	-2.29341	-1.60879	0.964892
21	1	-2.1588	1.264083	0.201205
22	1	-4.5729	1.398387	0.505933
23	1	-4.69103	-0.50071	0.407973

Table S19. Compound V (N-Propargyl isatin)



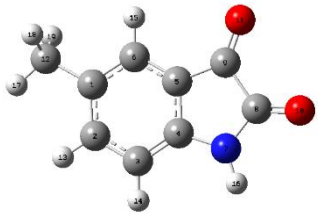
Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.79631	-1.59025	0.10676
2	6	-1.69917	-2.39279	-0.230685
3	6	-0.41451	-1.85451	-0.414055
4	6	-0.26558	-0.48403	-0.250258
5	6	-1.36444	0.334819	0.09193
6	6	-2.63119	-0.21016	0.272549
7	7	0.90283	0.307718	-0.383762
8	6	0.626822	1.650434	-0.136445
9	6	-0.88732	1.715629	0.19122
10	6	2.237973	-0.17476	-0.744217
11	6	2.842946	-1.04537	0.267931
12	8	1.436185	2.580769	-0.187884
13	8	-1.50144	2.749827	0.466374
14	6	3.353456	-1.76287	1.089788
15	1	-3.76974	-2.03978	0.24081
16	1	-1.83913	-3.45857	-0.351771
17	1	0.421613	-2.49256	-0.657931
18	1	-3.46166	0.43123	0.534327
19	1	2.185926	-0.68972	-1.707933
20	1	2.84613	0.72068	-0.887179
21	1	3.80299	-2.38696	1.820974

Table S20. Compound VI (5-nitro isatin)



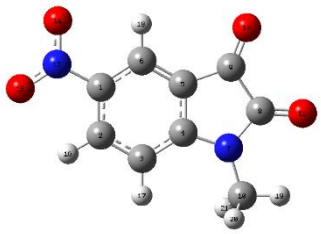
Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.716441	-0.10467	-0.00023
2	6	1.478361	-1.48458	0.000296
3	6	0.172688	-1.97951	0.000585
4	6	-0.87084	-1.05712	0.000561
5	6	-0.61879	0.336584	-0.00027
6	6	0.675877	0.829045	-0.00075
7	7	-2.25216	-1.28792	0.000376
8	6	-2.98198	-0.09594	0.000012
9	6	-1.91384	1.031107	-0.00052
10	8	-4.20539	0.013833	0.000087
11	8	-2.16308	2.236531	-0.00074
12	7	3.097332	0.371653	-0.00028
13	8	3.294797	1.622927	0.002817
14	8	4.027485	-0.48978	-0.00219
15	1	2.323935	-2.1545	0.000288
16	1	-0.00955	-3.04419	0.000917
17	1	0.883257	1.888248	-0.00085
18	1	-2.69181	-2.19328	0.001077

Table S21. compound VII (5-methyl isatin)



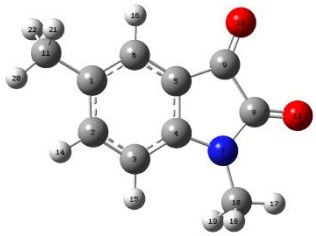
Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.351864	0.210881	-0.000065
2	6	2.193143	-1.18547	0.000274
3	6	0.934023	-1.80883	0.000182
4	6	-0.18656	-0.99428	-0.000242
5	6	-0.05635	0.411034	-0.000597
6	6	1.196223	1.012165	-0.000516
7	7	-1.55658	-1.34379	-0.000009
8	6	-2.37623	-0.22312	-0.000015
9	6	-1.40335	0.990994	0.000037
10	8	-3.60875	-0.20674	0.000005
11	8	-1.75675	2.173151	0.000526
12	6	3.726366	0.841932	0.00013
13	1	3.077616	-1.8097	0.000624
14	1	0.854628	-2.88715	0.00054
15	1	1.268807	2.092528	-0.000701
16	1	-1.91794	-2.28222	-0.000314
17	1	4.510649	0.084858	-0.000974
18	1	3.875408	1.473428	-0.878971
19	1	3.876099	1.471556	0.880476

Table S22. Compound VIII (N-methyl-5-nitro isatin)



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.939666	-0.13322	-0.000256
2	6	1.532261	-1.47219	0.000259
3	6	0.174767	-1.80259	0.000501
4	6	-0.74845	-0.7582	0.000472
5	6	-0.32295	0.593767	-0.000259
6	6	1.021066	0.922575	-0.000754
7	7	-2.14887	-0.8293	0.000138
8	6	-2.71423	0.451956	-0.000358
9	6	-1.52248	1.440188	-0.000377
10	6	-2.94097	-2.05454	0.000643
11	8	-3.91773	0.71095	-0.000449
12	8	-1.62337	2.667367	-0.000207
13	7	3.367635	0.168107	-0.000307
14	8	3.719283	1.385547	0.002726
15	8	4.184888	-0.80177	-0.002165
16	1	2.288511	-2.2416	0.000217
17	1	-0.13459	-2.83675	0.000741
18	1	1.357741	1.948083	-0.000711
19	1	-3.98861	-1.76491	0.001767
20	1	-2.73659	-2.64975	-0.890135
21	1	-2.73453	-2.64988	0.890839

Table S23. Compound IX (N-methyl-5-methyl isatin)



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.579981	0.037445	-0.000077
2	6	2.192296	-1.31228	0.000127
3	6	0.846258	-1.71887	0.000166
4	6	-0.12452	-0.72937	-0.000009
5	6	0.238833	0.634937	-0.000278
6	6	1.572217	1.020047	-0.000324
7	7	-1.53509	-0.85949	0.000171
8	6	-2.14741	0.388913	0.00003
9	6	-0.99453	1.426735	0.000024
10	6	-2.26858	-2.11666	-0.000147
11	6	4.039642	0.433321	0.000047
12	8	-3.36347	0.607383	-0.000038
13	8	-1.14961	2.651084	0.000262
14	1	2.961211	-2.07443	0.000254
15	1	0.591552	-2.76893	0.000345
16	1	1.823313	2.073373	-0.000477
17	1	-3.32895	-1.87646	-0.000078
18	1	-2.03622	-2.70447	-0.889961
19	1	-2.03613	-2.70489	0.889326
20	1	4.68849	-0.44264	-0.000878
21	1	4.290743	1.031729	-0.879091
22	1	4.291068	1.030086	0.880222

XYZ COORDINATES OF ISATIN AND ITS DERIVATIVES WITH GRIMME D3 OPTIMIZED STRUCTURE

Table S24. Compound I (Isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.577738	0.837977	0.17273
2	6	2.742137	-0.55254	0.062287
3	6	1.633569	-1.39159	-0.0841
4	6	0.374899	-0.82129	-0.091509
5	6	0.217201	0.561794	-0.002629
6	6	1.303904	1.40823	0.131142
7	7	-0.84807	-1.50711	-0.296728
8	6	-1.85054	-0.49777	0.089843
9	6	-1.22904	0.895255	-0.122197
10	8	-2.96381	-0.72357	0.500788
11	8	-1.76401	1.958696	-0.327579
12	1	3.460266	1.483424	0.293126
13	1	3.752913	-0.98549	0.091302
14	1	1.760123	-2.47905	-0.190727
15	1	1.168173	2.497558	0.202626
16	1	-1.00168	-2.48804	-0.638308

Table S25. Compound II (N-methyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.873646	-0.51321	-0.096731
2	6	2.719178	0.882516	-0.125675
3	6	1.446582	1.459511	-0.081711
4	6	0.347649	0.623021	-0.035063
5	6	0.506181	-0.76193	0.014676
6	6	1.758659	-1.34982	-0.016313
7	7	-1.00436	1.031247	0.081293
8	6	-1.74101	-0.21067	-0.215567
9	6	-0.83252	-1.40047	0.146056
10	8	-2.86056	-0.28253	-0.663718
11	8	-1.1239	-2.5326	0.450497
12	6	-1.5383	2.359688	0.414475
13	1	3.881835	-0.95111	-0.13772
14	1	3.608042	1.527808	-0.183486
15	1	1.322976	2.552552	-0.084177
16	1	1.872264	-2.44334	0.021268
17	1	-2.65072	2.322735	0.418469
18	1	-1.17407	2.663522	1.42133
19	1	-1.19462	3.098298	-0.343838

Table S26 Compound III (N-Benzyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	4.478806	-0.58664	-0.016213
2	6	3.785344	-1.79913	0.131224
3	6	2.388289	-1.81972	0.177808
4	6	1.710993	-0.61767	0.101015
5	6	2.402572	0.582077	-0.066399
6	6	3.784701	0.619889	-0.126104
7	7	0.303578	-0.45655	0.064503
8	6	0.14081	0.991974	0.284574
9	6	1.421772	1.694003	-0.20332
10	6	-0.73372	-1.47757	-0.141125
11	6	-2.08433	-0.83327	-0.09945
12	8	-0.82715	1.533136	0.763481
13	8	1.584895	2.827283	-0.588482
14	6	-3.23187	-1.60739	-0.271248
15	6	-4.49032	-1.0069	-0.232351
16	6	-4.60112	0.367403	-0.021727
17	6	-3.45363	1.141421	0.150147
18	6	-2.19518	0.541032	0.111261
19	1	5.578449	-0.58754	-0.045376
20	1	4.346957	-2.74158	0.210845
21	1	1.8416	-2.76944	0.273286
22	1	4.320349	1.571801	-0.256173
23	1	-0.58503	-1.9624	-1.13199
24	1	-0.66371	-2.24452	0.662354
25	1	-3.14441	-2.69119	-0.437278
26	1	-5.39535	-1.61734	-0.367964
27	1	-5.59352	0.840828	0.00897
28	1	-3.54101	2.225286	0.316458
29	1	-1.2901	1.151476	0.246787

Table S27. Compound IV (N-allyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.801626	2.579291	-0.064102
2	6	0.423958	2.768749	-0.26132
3	6	-0.44739	1.676148	-0.297884
4	6	0.083818	0.407831	-0.161006
5	6	1.449647	0.225369	0.0556
6	6	2.325028	1.296081	0.106175
7	7	-0.65304	-0.80136	-0.106187
8	6	0.397473	-1.82426	-0.25862
9	6	1.721748	-1.22548	0.250797
10	6	-2.10156	-0.98869	0.060763
11	6	-2.76268	0.3448	0.221039
12	6	-4.08707	0.418519	0.388134
13	8	0.246123	-2.93664	-0.704698
14	8	2.704167	-1.77729	0.686066
15	1	2.474079	3.449488	-0.043544
16	1	0.026708	3.786635	-0.388212
17	1	-1.5294	1.822437	-0.432293
18	1	3.400743	1.140816	0.275429
19	1	-2.51462	-1.50159	-0.836487
20	1	-2.29341	-1.60879	0.964892
21	1	-2.1588	1.264083	0.201205
22	1	-4.5729	1.398387	0.505933
23	1	-4.69103	-0.50071	0.407973

Table S28. Compound V (N-Propargyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.309727	3.003985	-0.109515
2	6	-1.00062	2.528766	-0.282514
3	6	-1.26511	1.156068	-0.292483
4	6	-0.2039	0.281906	-0.153821
5	6	1.092945	0.758154	0.03872
6	6	1.371352	2.113581	0.062824
7	7	-0.29403	-1.13004	-0.073873
8	6	1.109447	-1.55069	-0.236523
9	6	2.010225	-0.39695	0.242267
10	6	-1.48748	-1.96554	0.122002
11	6	-2.66866	-1.1048	0.279402
12	8	1.48663	-2.61357	-0.66929
13	8	3.141938	-0.42199	0.664025
14	6	-3.64252	-0.39508	0.409091
15	1	0.501307	4.087152	-0.109874
16	1	-1.82665	3.243607	-0.411439
17	1	-2.29272	0.781036	-0.40791
18	1	2.398096	2.478496	0.213182
19	1	-1.62608	-2.62676	-0.762494
20	1	-1.35826	-2.58844	1.035379
21	1	-4.51845	0.243241	0.525679

Table S29. Compound VI (5-nitro isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.740137	-0.06979	0.01346
2	6	1.501616	-1.45282	-0.041986
3	6	0.196318	-1.94839	-0.112508
4	6	-0.85014	-1.04599	-0.100418
5	6	-0.60828	0.327342	-0.066413
6	6	0.677553	0.835766	-0.008039
7	7	-2.22472	-1.36418	-0.232329
8	6	-2.88398	-0.10078	0.144957
9	6	-1.90631	1.052155	-0.149373
10	8	-3.99563	0.010554	0.604301
11	8	-2.12953	2.216357	-0.381941
12	7	2.912199	0.353414	0.082582
13	8	3.141206	1.642266	0.134607
14	8	3.913395	-0.49111	0.103109
15	1	2.350079	-2.15276	-0.029757
16	1	0.006915	-3.03008	-0.176022
17	1	0.857089	1.920624	0.020606
18	1	-2.6635	-2.27198	-0.525281

Table S30. Compound VII (5-methyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.29372	0.22116	0.071031
2	6	2.179629	-1.17657	-0.007077
3	6	0.924657	-1.78449	-0.10627
4	6	-0.19774	-0.97843	-0.09965
5	6	-0.07913	0.410252	-0.043053
6	6	1.155512	1.02944	0.04384
7	7	-1.53647	-1.41489	-0.258993
8	6	-2.31093	-0.22051	0.124133
9	6	-1.43484	1.018622	-0.138097
10	8	-3.4351	-0.21476	0.566133
11	8	-1.75669	2.16178	-0.358695
12	6	3.647662	0.849857	0.184401
13	1	3.086582	-1.79891	0.009906
14	1	0.832978	-2.87767	-0.187656
15	1	1.237753	2.125413	0.090057
16	1	-1.88843	-2.35345	-0.571518
17	1	4.426913	0.055199	0.190756
18	1	3.815616	1.526552	-0.683058
19	1	3.706875	1.434836	1.129417

Table S31. compound VIII (N-methyl-5-nitro isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.96287	-0.12005	-0.023243
2	6	-1.54066	-1.45912	-0.060686
3	6	-0.17956	-1.77769	-0.044413
4	6	0.736535	-0.7435	-0.016499
5	6	0.312867	0.584206	0.041773
6	6	-1.03036	0.917369	0.038113
7	7	2.14419	-0.88107	0.071217
8	6	2.619185	0.48034	-0.23549
9	6	1.504305	1.470834	0.148839
10	6	2.932806	-2.08035	0.388364
11	8	3.693946	0.768356	-0.705686
12	8	1.576114	2.638045	0.451735
13	7	-3.18228	0.144811	-0.045036
14	8	-3.58232	1.391802	-0.010331
15	8	-4.06208	-0.82404	-0.102558
16	1	-2.28822	-2.26492	-0.103268
17	1	0.153993	-2.82584	-0.053643
18	1	-1.35367	1.967847	0.082169
19	1	4.016665	-1.82783	0.37026
20	1	2.655248	-2.44912	1.401164
21	1	2.723867	-2.87184	-0.36577

Table S32. Compound IX (N-methyl-5-methyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.523595	-0.03268	-0.051808
2	6	2.162063	1.32401	-0.089697
3	6	0.816924	1.703841	-0.063487
4	6	-0.14472	0.712215	-0.025332
5	6	0.218956	-0.63315	0.033342
6	6	1.545679	-1.02672	0.019928
7	7	-1.54397	0.91352	0.073205
8	6	-2.08248	-0.42578	-0.225831
9	6	-1.01044	-1.46472	0.15242
10	6	-2.27501	2.147999	0.393345
11	6	3.970093	-0.41628	-0.088658
12	8	-3.17301	-0.66606	-0.686577
13	8	-1.13256	-2.62673	0.45925
14	1	2.944838	2.095168	-0.140459
15	1	0.530942	2.765984	-0.072991
16	1	1.821433	-2.09062	0.064448
17	1	-3.36929	1.944705	0.384597
18	1	-1.9728	2.506349	1.402797
19	1	-2.03653	2.927352	-0.36473
20	1	4.596658	0.501867	-0.145081
21	1	4.226574	-0.98358	0.833928
22	1	4.162531	-1.05204	-0.981655

XYZ COORDINATES OF ISATIN AND ITS DERIVATIVES (IEFPCM-WATER MODEL)

Table S33. Compound I (Isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.63772	0.799399	0.000188
2	6	-2.75111	-0.59402	0.000325
3	6	-1.6283	-1.42894	0.000077
4	6	-0.38019	-0.8249	-0.000291
5	6	-0.25483	0.576032	-0.000559
6	6	-1.37663	1.394291	-0.000244
7	7	0.884702	-1.42615	-0.000296
8	6	1.909469	-0.49268	0.000027
9	6	1.178667	0.903473	-0.00009
10	8	3.091773	-0.70864	0.000299
11	8	1.739842	1.968239	0.000278
12	1	-3.53057	1.412233	0.000427
13	1	-3.73675	-1.0457	0.000638
14	1	-1.73489	-2.50719	0.00014
15	1	-1.25401	2.471163	-0.000414
16	1	1.054273	-2.42021	0.000075

Table S34. Compound II (N-methyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.912556	-0.50059	0.000156
2	6	2.734748	0.884936	0.000129
3	6	1.462399	1.470103	-0.000053
4	6	0.365798	0.62016	-0.000212
5	6	0.535623	-0.77684	-0.000215
6	6	1.800975	-1.34474	-0.000021
7	7	-0.99427	0.959523	-0.000289
8	6	-1.79457	-0.17371	0.000001
9	6	-0.8	-1.38973	-0.000064
10	8	-2.99884	-0.2053	0.00023
11	8	-1.13265	-2.54671	0.000036
12	6	-1.51474	2.311928	0.000085
13	1	3.912886	-0.91549	0.00032
14	1	3.605549	1.530974	0.000283
15	1	1.345526	2.546363	-0.000061
16	1	1.904632	-2.42364	-0.000032
17	1	-2.60182	2.243088	-0.000237
18	1	-1.18611	2.854172	0.891383
19	1	-1.18557	2.854832	-0.890589

Table S35. Compound III (N-Benzyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.704825	2.602199	0.433825
2	6	1.477126	2.843612	-0.188295
3	6	0.642082	1.803543	-0.613252
4	6	1.078083	0.50435	-0.398262
5	6	2.309635	0.251249	0.232566
6	6	3.128436	1.290816	0.650399
7	7	0.434532	-0.6977	-0.737317
8	6	1.17676	-1.79512	-0.329843
9	6	2.475847	-1.20489	0.327392
10	6	-0.85939	-0.80151	-1.398178
11	6	-2.01272	-0.35926	-0.519312
12	8	0.872798	-2.95531	-0.452758
13	8	3.368789	-1.86618	0.791147
14	6	-2.92203	0.602139	-0.960362
15	6	-3.98612	0.996634	-0.149767
16	6	-4.1448	0.432554	1.112921
17	6	-3.23913	-0.53026	1.559893
18	6	-2.18051	-0.92445	0.748364
19	1	3.321839	3.434304	0.7497
20	1	1.154571	3.866915	-0.344659
21	1	-0.31448	2.009787	-1.073945
22	1	4.072768	1.068817	1.133801
23	1	-0.83529	-0.21639	-2.322405
24	1	-0.96621	-1.85419	-1.670253
25	1	-2.80011	1.04579	-1.943895
26	1	-4.68563	1.745562	-0.503605
27	1	-4.96891	0.739607	1.746647
28	1	-3.36076	-0.97587	2.540659
29	1	-1.48086	-1.67818	1.093522

Table S36. Compound IV (N-allyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.43887	-2.12443	0.079178
2	6	-1.17051	-2.65432	-0.171829
3	6	-0.03882	-1.84178	-0.308943
4	6	-0.21629	-0.47074	-0.189299
5	6	-1.48952	0.071678	0.064466
6	6	-2.60353	-0.74459	0.200314
7	7	0.747373	0.546705	-0.296444
8	6	0.174471	1.798657	-0.120531
9	6	-1.35207	1.532116	0.133748
10	6	2.163275	0.347929	-0.582074
11	6	2.905975	-0.28158	0.5668
12	6	3.663173	-1.36787	0.462243
13	8	0.741678	2.860915	-0.161959
14	8	-2.1727	2.390397	0.332964
15	1	-3.28965	-2.78686	0.180235
16	1	-1.05342	-3.72863	-0.260568
17	1	0.937898	-2.27104	-0.484482
18	1	-3.57291	-0.30045	0.394706
19	1	2.269916	-0.25278	-1.491289
20	1	2.559684	1.346426	-0.786743
21	1	2.798678	0.225587	1.522511
22	1	4.201831	-1.77076	1.311838
23	1	3.78086	-1.88945	-0.483574

Table S37. Compound V (N-Propargyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.75735	-1.61753	0.097592
2	6	-1.64614	-2.39568	-0.237512
3	6	-0.37472	-1.8375	-0.415846
4	6	-0.25072	-0.46618	-0.250677
5	6	-1.36192	0.325821	0.089933
6	6	-2.61694	-0.23999	0.26594
7	7	0.901323	0.327635	-0.382337
8	6	0.625161	1.665739	-0.133429
9	6	-0.91009	1.719417	0.195853
10	6	2.22734	-0.15419	-0.741957
11	6	2.817912	-1.03204	0.268975
12	8	1.407215	2.579992	-0.176874
13	8	-1.51566	2.72431	0.464573
14	6	3.294965	-1.76302	1.092401
15	1	-3.72427	-2.08738	0.228452
16	1	-1.76638	-3.46618	-0.360286
17	1	0.478562	-2.45827	-0.655359
18	1	-3.45789	0.391509	0.527908
19	1	2.176776	-0.67464	-1.705128
20	1	2.844905	0.737733	-0.877113
21	1	3.7216	-2.39981	1.828657

Table S38. Compound VI (5-nitro isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.712432	-0.10453	0.000098
2	6	1.467465	-1.47939	0.000423
3	6	0.163491	-1.96803	0.000836
4	6	-0.87515	-1.04308	0.000653
5	6	-0.61439	0.342675	0.000235
6	6	0.679734	0.830128	-0.000023
7	7	-2.24562	-1.27851	0.001101
8	6	-2.98624	-0.098	-0.00011
9	6	-1.9082	1.04876	-0.000236
10	8	-4.18053	0.005576	-0.001064
11	8	-2.15677	2.223845	-0.000615
12	7	3.110106	0.370124	-0.000217
13	8	3.293279	1.5796	0.002514
14	8	3.996253	-0.47472	-0.003101
15	1	2.31261	-2.15401	0.000365
16	1	-0.02689	-3.03395	0.001334
17	1	0.88774	1.891536	-0.000168
18	1	-2.67754	-2.19051	-0.00084

Table S39. Compound VII (5-methyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.346811	0.204842	-0.000088
2	6	2.178451	-1.1859	-0.000295
3	6	0.920432	-1.80163	-0.000104
4	6	-0.1954	-0.98311	0.00031
5	6	-0.0531	0.415452	0.000626
6	6	1.199905	1.008538	0.000354
7	7	-1.55314	-1.33431	0.000277
8	6	-2.38141	-0.22443	-0.000053
9	6	-1.39916	1.008384	0.000097
10	8	-3.5837	-0.21067	-0.000317
11	8	-1.74811	2.160448	-0.00032
12	6	3.721324	0.829981	-0.000163
13	1	3.06055	-1.81772	-0.000635
14	1	0.832462	-2.88164	-0.000245
15	1	1.274246	2.091083	0.000514
16	1	-1.90841	-2.27796	-0.000108
17	1	4.506352	0.071422	-0.002784
18	1	3.866068	1.464041	-0.879953
19	1	3.868041	1.459938	0.882261

Table S40. compound VIII (N-methyl-5-nitro isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.933037	-0.1312	0.000066
2	6	1.520412	-1.46443	0.000288
3	6	0.165434	-1.78967	0.000437
4	6	-0.75277	-0.7436	0.000232
5	6	-0.32067	0.599793	-0.000046
6	6	1.021845	0.924427	-0.000098
7	7	-2.14169	-0.82268	-0.000012
8	6	-2.72087	0.446406	-0.000243
9	6	-1.5193	1.455463	-0.000424
10	6	-2.91032	-2.05452	0.000651
11	8	-3.89644	0.694854	-0.000256
12	8	-1.62629	2.652103	-0.000775
13	7	3.377078	0.16791	0.000009
14	8	3.707902	1.345992	0.002757
15	8	4.153779	-0.77898	-0.002779
16	1	2.276134	-2.23796	0.000268
17	1	-0.15185	-2.82398	0.000701
18	1	1.359192	1.952042	-0.000082
19	1	-3.96423	-1.78029	0.000667
20	1	-2.68986	-2.64746	-0.890849
21	1	-2.68956	-2.64671	0.892573

Table S41. compound IX (N-methyl-5-methyl isatin)

Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.571076	0.035221	-0.000115
2	6	2.176228	-1.30765	-0.000133
3	6	0.832869	-1.70839	0.000043
4	6	-0.1332	-0.71651	0.000251
5	6	0.239447	0.639651	0.00028
6	6	1.571428	1.018143	0.000075
7	7	-1.53011	-0.85293	0.000302
8	6	-2.15499	0.384169	-0.000006
9	6	-0.99266	1.441651	0.000069
10	6	-2.24179	-2.11465	-0.000101
11	6	4.029402	0.42645	-0.000099
12	8	-3.34186	0.593602	-0.000249
13	8	-1.15166	2.635082	-0.000077
14	1	2.942387	-2.07606	-0.000335
15	1	0.569912	-2.75869	-0.000009
16	1	1.823922	2.073496	0.000071
17	1	-3.30739	-1.88867	0.000229
18	1	-1.99534	-2.69926	-0.891278
19	1	-1.9949	-2.70004	0.890418
20	1	4.679398	-0.45062	-0.002693
21	1	4.276403	1.028365	-0.879792
22	1	4.277555	1.02395	0.882296