

Supplementary Data to Article Titled:
Free Radical Scavenging Activity Evaluation of Hydrazones by
Quantitative Structure Activity Relationship

Ikechukwu Ogadimma Alisi ^{1*}, Adamu Uzairu ², Stephen Eyije Abechi², Sulaiman Ola Idris ²

¹Department of Applied Chemistry, Federal University Dutsinma, Katsina State, Nigeria.

²Department of Chemistry, Ahmadu Bello University Zaria, Kaduna State, Nigeria.

***Email:** ikeogadialisi@gmail.com, ialisi@fudutsinma.edu.ng , Tel: +234 7064888876

Table S1. Training Set Predicted Activities /Residual values for Hydrazone Antioxidant Models.

Comp No	Actual values for pIC50	Equation 1: predicted values	Equation 1: residual values	Equation 2: predicted values	Equation 2: residual values	Equation 3: predicted values	Equation 3: residual values	Equation 4: predicted values	Equation 4: residual values	Equation 5: predicted values	Equation 5: residual values
2	4.67985	4.80569	-0.12580	4.80967	-0.12980	4.76695	-0.08710	4.77504	-0.09520	4.73028	-0.05043
3	5.54212	4.98673	0.55539	5.05950	0.48262	5.05339	0.48873	5.00806	0.53406	5.01574	0.52638
4	4.81901	4.80569	0.01332	4.77628	0.04273	4.83385	-0.01480	4.76504	0.05397	4.68896	0.13005
5	4.99183	5.16920	-0.17740	5.13785	-0.14600	5.06035	-0.06850	5.10557	-0.11370	5.08472	-0.09289
6	4.91542	5.16920	-0.25380	5.13487	-0.21940	5.15226	-0.23680	5.14623	-0.23080	5.16968	-0.25426
7	4.62599	4.98673	-0.3607	4.90005	-0.27410	5.02081	-0.39480	4.94340	-0.31740	4.89921	-0.27322
8	6.01773	5.30505	0.71268	5.34373	0.67400	5.36545	0.65228	5.33579	0.68194	5.32505	0.69268
9	6.14874	6.06934	0.07940	6.11065	0.03809	6.16437	-0.01560	6.10379	0.04495	6.03416	0.11458
10	6.16749	6.20891	-0.04140	6.17133	-0.00380	6.12260	0.04490	6.17312	-0.00560	6.17932	-0.01183
11	4.83327	4.80569	0.02758	4.77329	0.05998	4.75066	0.08261	4.76904	0.06423	4.69825	0.13503
12	4.88506	5.16920	-0.28410	5.13487	-0.24980	4.93004	-0.04500	5.11091	-0.22590	5.15065	-0.26559
13	4.84558	5.16920	-0.32360	5.13237	-0.28680	5.08129	-0.23570	5.15023	-0.30470	5.12465	-0.27907
14	4.77937	4.98673	-0.20740	4.89656	-0.11720	4.94926	-0.16990	4.94740	-0.16800	4.90107	-0.12170
15	5.97062	5.30505	0.66557	5.34024	0.63038	5.35439	0.61622	5.33779	0.63283	5.37287	0.59775
16	6.09152	6.06934	0.02218	6.10616	-0.01460	6.15449	-0.06300	6.10446	-0.01290	6.11077	-0.01925
17	6.14874	6.20891	-0.06020	6.16834	-0.01960	6.11503	0.03371	6.17512	-0.02640	6.23225	-0.08351
18	4.99557	5.11404	-0.11850	5.22424	-0.22870	5.17150	-0.17590	5.11700	-0.12140	5.26055	-0.26498
19	4.82194	4.59769	0.22425	4.74868	0.07326	4.54899	0.27295	4.55227	0.26968	4.59385	0.22810
20	5.18161	5.31759	-0.13600	5.30200	-0.12040	5.38604	-0.20440	5.34144	-0.15980	5.27133	-0.08972
21	5.67321	5.55661	0.11660	5.53053	0.14268	5.63808	0.03513	5.61693	0.05628	5.59298	0.08024
22	5.29055	5.17259	0.11796	5.21422	0.07633	5.31649	-0.02590	5.25158	0.03897	5.34943	-0.05888
23	5.27688	5.56909	-0.29220	5.64000	-0.36310	5.69187	-0.41500	5.63313	-0.35620	5.52623	-0.24935
24	4.63209	5.27418	-0.64210	5.32202	-0.68990	5.33939	-0.70730	5.30236	-0.6703	5.20162	-0.56953
26	5.35701	5.56909	-0.21210	5.55181	-0.19480	5.55400	-0.19700	5.58114	-0.2241	5.55548	-0.19847
27	4.69928	4.87161	-0.17230	4.87365	-0.17440	4.85693	-0.15760	4.87471	-0.1754	4.75937	-0.06009
28	5.17150	5.26923	-0.09770	5.30578	-0.13430	5.25512	-0.08360	5.26767	-0.09620	5.17053	0.00098
29	4.92363	4.96094	-0.03730	4.97690	-0.0533	4.91219	0.01145	4.92425	-0.00060	4.87648	0.04715
30	5.67988	5.28164	0.39824	5.20209	0.47778	5.18772	0.49216	5.22151	0.45836	5.26210	0.41777
32	4.34336	4.78854	-0.4452	4.58262	-0.2393	4.61821	-0.27480	4.60909	-0.26570	4.61396	-0.27060
33	5.03664	5.00324	0.03340	4.74336	0.29327	4.86891	0.16773	4.89305	0.14359	4.65506	0.38158
34	4.82971	4.53393	0.29579	4.94408	-0.1144	4.70799	0.12172	4.72894	0.10078	4.87031	-0.04060
35	5.66869	5.4053	0.26339	5.61781	0.05089	5.59175	0.07695	5.55595	0.11275	5.61665	0.05204
36	5.07905	4.69623	0.38281	4.83072	0.24833	4.85743	0.22162	4.83598	0.24306	4.69854	0.38051
37	5.43345	5.14235	0.29110	5.21586	0.21759	5.29089	0.14256	5.25234	0.18111	5.28555	0.14790
38	5.43863	5.36657	0.07207	5.39944	0.03919	5.49858	-0.0599	5.45064	-0.01200	5.49678	-0.05815
39	5.48078	5.42855	0.05223	5.32744	0.15334	5.22721	0.25357	5.36758	0.11320	5.48421	-0.00343
44	5.01345	5.21669	-0.20320	5.14348	-0.13000	5.09694	-0.0835	5.22090	-0.20750	5.15676	-0.14332
47	4.98999	4.87369	0.11630	4.8719	0.11810	4.84334	0.14665	4.91591	0.07409	4.84794	0.14206
48	4.96929	4.89725	0.07204	4.82509	0.14421	4.83013	0.13916	4.91747	0.05183	4.85437	0.11492
49	4.74641	4.87369	-0.12730	4.73537	0.01104	4.82705	-0.08060	4.86525	-0.11880	4.87951	-0.13310
51	4.65472	4.82896	-0.17420	4.89741	-0.24270	4.71460	-0.05990	4.49861	0.15611	5.03530	-0.38058
54	4.17605	4.26535	-0.08930	4.11175	0.06430	4.12318	0.05287	4.28861	-0.11260	4.20024	-0.02419

56	4.00784	4.11366	-0.10580	4.11753	-0.10970	4.13225	-0.12440	4.12970	-0.12190	4.08254	-0.07470
57	4.18197	4.11366	0.06832	4.13298	0.04899	4.14737	0.03460	4.11570	0.06627	4.21069	-0.02871
58	4.71108	4.43592	0.27517	4.43937	0.27171	4.48849	0.22259	4.43842	0.27266	4.39338	0.31770
59	3.99534	4.18909	-0.19380	4.10489	-0.10960	4.25710	-0.26180	4.20727	-0.21190	4.27904	-0.28370
60	3.91204	4.11366	-0.20160	4.11554	-0.20350	4.14446	-0.23240	4.11103	-0.19900	4.09833	-0.18629
61	4.66314	4.43592	0.22723	4.45282	0.21032	4.49780	0.16534	4.45975	0.20339	4.60045	0.06269

Average Activity for Training Set: 5.052023708

Table S2: Test Set Predicted Activities /Residual Values for the Various Models.

Comp No	Actual values for pIC50	Equation 1: predicted values	Equation 1: residual values	Equation 2: predicted values	Equation 2: residual values	Equation 3: predicted values	Equation 3: residual values	Equation 4: predicted values	Equation 4: residual values	Equation 5: predicted values	Equation 5: residual values
1	4.66959	4.80569	-0.13610	4.81266	-0.14310	4.60698	0.06261	4.73305	-0.06350	4.75628	-0.08670
25	5.80432	5.48229	0.32203	5.42857	0.37575	5.51036	0.29395	5.45860	0.34572	5.52962	0.27470
31	5.36955	5.26923	0.10032	5.20912	0.16043	5.08584	0.28371	5.21767	0.15188	5.22206	0.14749
40	5.11418	5.48801	-0.37380	5.36589	-0.25170	5.50012	-0.38590	5.52050	-0.40630	5.56447	-0.45029
41	5.05556	5.48801	-0.43250	5.41622	-0.36070	5.31979	-0.26420	5.47584	-0.42030	5.58072	-0.52516
42	5.07198	5.21669	-0.14470	5.13750	-0.06550	5.10857	-0.03660	5.22290	-0.15090	5.13680	-0.06481
43	5.09688	5.21669	-0.11980	5.11857	-0.02170	5.16500	-0.06810	5.24490	-0.14800	5.19901	-0.10214
45	5.06763	5.21669	-0.14910	5.12305	-0.05540	5.04051	0.02712	5.21290	-0.14530	5.22873	-0.16109
46	5.06908	5.21669	-0.14760	5.09814	-0.02910	5.20979	-0.14070	5.23690	-0.16780	5.22826	-0.15918
50	4.92538	4.95559	-0.03020	4.95499	-0.02960	4.94201	-0.01660	4.91826	0.00712	4.96948	-0.04411
52	4.34298	4.68397	-0.34100	4.67391	-0.33090	4.51459	-0.17160	4.55373	-0.21080	4.66299	-0.32001
53	4.22939	4.44118	-0.21180	4.44666	-0.21730	4.28387	-0.05450	4.45057	-0.22120	4.35189	-0.12250
55	4.58503	4.43592	0.14911	4.43538	0.14965	4.50478	0.08025	4.45442	0.13061	4.38316	0.20186

Table S3. Standard Residuals and Leverage values for Hydrazone Antioxidants Training Set.

Comp No	Standard Residual	Leverage
2	-0.34232	0.04081
3	1.92094	0.01858
4	-0.05830	0.01919
5	-0.26932	0.09759
6	-0.93087	0.06924
7	-1.55184	0.01780
8	2.56377	0.06799
9	-0.06144	0.26151
10	0.17646	0.25926
11	0.32471	0.04844
12	-0.17682	0.18833
13	-0.92646	0.08853
14	-0.66774	0.02909
15	2.42204	0.06537
16	-0.24750	0.25898
17	0.13249	0.26119
18	-0.69145	0.10164
19	1.07283	0.13664
20	-0.80348	0.10365
21	0.13809	0.11541
22	-0.10196	0.06019
23	-1.63106	0.11938
24	-2.78000	0.04530
26	-0.77425	0.08007
27	-0.61963	0.02336
28	-0.32864	0.05317
29	0.04499	0.02856
30	1.93440	0.07035
32	-1.08029	0.16209
33	0.65925	0.14356
34	0.47842	0.09166
35	0.30244	0.15611
36	0.87105	0.08548
37	0.56033	0.09547
38	-0.23561	0.13827
39	0.99664	0.27373
44	-0.32817	0.06256
47	0.57642	0.02846
48	0.54698	0.03297
49	-0.31695	0.03067
51	-0.23536	0.06583
54	0.20782	0.16172
56	-0.48895	0.11076
57	0.13600	0.10972
58	0.87487	0.14284

59	-1.02884	0.12356
60	-0.91352	0.10986
61	0.64986	0.14506

Table S4. Standard Residuals and Leverage values for Hydrazone Antioxidants Test Set.

Comp No	Standard Residual	Leverage
1	0.33458	0.51630
25	1.57085	0.32147
31	1.51613	0.17030
40	-2.06241	0.28505
41	-1.41203	0.25448
42	-0.19554	0.09335
43	-0.36405	0.10384
45	0.14493	0.14162
46	-0.75196	0.14476
50	-0.08888	0.33926
52	-0.91709	0.41725
53	-0.29113	0.39309
55	0.42882	0.81925