5-(2-Carboxyethenyl)-Isatin Derivatives as Anticancer Agents: QSAR, Molecular Docking and, Molecular Dynamic Simulation Analysis

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Table S1. Leverage (*h*) of the external test set molecules for different models. The last row (*h**) is the warning leverage.

Molecular No	MLR	FA-MLR	PCR	GA-MLR	GA-PLS
12	0.23	0.02	0.23	0.1	0.4
15	0.34	0.003	0.14	0.31	0.06
17	0.25	0.001	0.39	0.22	0.36
18	0.55	0.12	0.14	0.21	0.29
20	0.27	0.07	0.14	0.27	0.17
21	0.27	0.003	0.18	0.25	0.29
22	1.03	0.04	0.13	0.097	0.12
23	0.4	0.03	0.22	0.43	0.59
26	0.32	0.07	0.12	0.21	0.24
34	0.14	0.06	0.15	0.18	0.14
37	0.58	0.02	0.20	0.36	0.45
h*	1.04	0.13	0.65	0.65	0.91

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