Supplementary material

5,8-Quinolinedione attached to quinone derivatives: XRD diffraction, Fourier transform infrared spectra and computational analysis

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Figure S1. The XRD pattern of compounds **1-4** in the range of the 2θ angle from 25° to 30°.

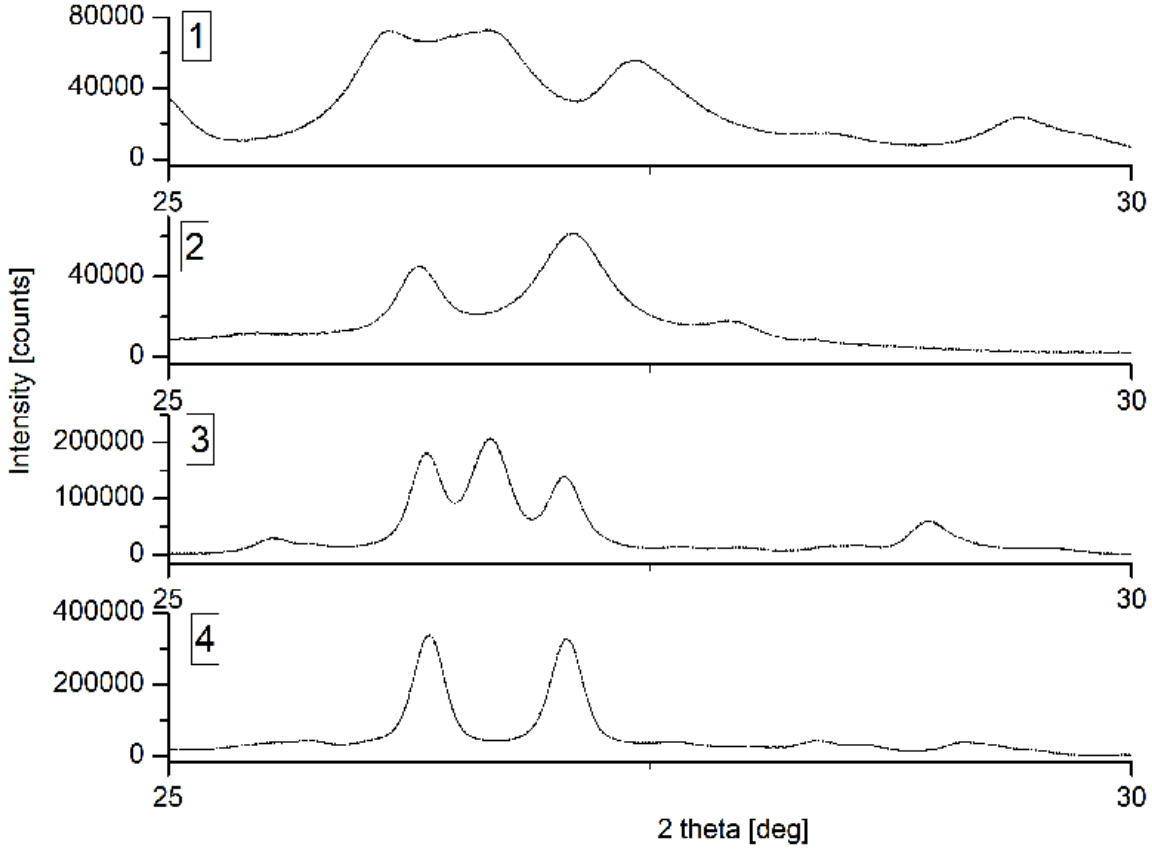

Table S1. Geometric parameters (bond length and angles) for compound **1** (Å, °).

Bond length. bond angles [Å. °]		Bond angles [°]		Bond angles [°]		Bond angles [°]	
C4A-C8A	1.401	C8A-C4-H4	118.95	C4-C3-H3	121.24	Cl-C6-C7-C8	176.15
C4A-C4	1.398	C3-C4-H4	122.58	C2-C3-H3	120.25	Cl-C6-C7-O3	4.65
C4A-C5	1.495	C4A-N1-C2	117.3	C3q-C4q-H4q	121.03	C8A-C8-C7-C6	6.99
C8A-N1	1.339	C4-C3-C2	118.5	C2q-C3q-C4q	119.55	C8A-C8-C7-O3	178.6
C8A-C8	1.503	C4-C3-H3	121.24	C2q-C3q-H3q	119.54	O2-C8-C7-C6	-171.55
C4-C3	1.389	C2-C3-H3	120.25	C4q-C3q-H3q	120.91	O2-C8-C7-O3	0.05
C4-H4	1.085	N1-C2-C3	123.8	C2q-C9q-H9q	111.08	C6-C7-O3-C8q	-141.02
N1-C2	1.335	N1-C2-H2	115.97	C2q-C9q-H9q	109.72	C8-C7-O3-C8q	47.22
C3-C2	1.401	C3-C2-H2	120.23	C2q-C9q-H9q	111.02	C7-O3-C8q-C8Aq	-137.17
C3-H3	1.085	C8A-C5-C6	116.83	H9q-C9q-H9q	108.95	C7-O3-C8q-C7q	48.16
C2-H2	1.088	C8A-C5-O1	120.95	H9q-C9q-H9q	107.08	C8q-C8Aq-C4Aq-C5q	-0.08
C7-C6	1.482	C6-C5-O1	122.21	H9q-C9q-H9q	108.92	C8q-C8Aq-C4Aq-C4q	-179.84
C7-O1	1.222	C5-C6-C7	122.47	C4-C4A-C8A-N1	0.26	N1q-C8Aq-C4Aq-C5q	179.71
C6-C7	1.361	C5-C6-Cl	116.56	C4-C4A-C8A-C8	-178.78	N1q-C8Aq-C4Aq-C4q	-0.06
C6-Cl	1.731	C7-C6-Cl	120.97	C5-C4A-C8A-N1	-179.53	C4Aq-C8Aq-C8q-O3	-175.57
C8-C7	1.509	C4A-C8-C7	116.93	C5-C4A-C8A-C8	1.44	C4Aq-C8Aq-C8q-C7q	-0.91
C8-O2	1.215	C4A-C8-O2	122.61	C8A-C4A-C4-C3	-0.2	N1q-C8Aq-C8q-O3	4.64
C7-O3	1.344	C7-C8-O2	120.44	C8A-C4A-C4-H4	179.81	N1q-C8Aq-C8q-C7q	179.29
O3-C8q	1.390	C6-C7-C8	121.44	C5-C4A-C4-C3	179.59	C4Aq-C8Aq-N1q-C2q	0.1
C8Aq-C4Aq	1.429	C6-C7-O3	119.64	C5-C4A-C4-H4	-0.4	C8q-C8Aq-N1q-C2q	179.88
C8Aq-C8q	1.424	C8-C7-O3	118.39	C8A-C4A-C5-C6	1.82	C8Aq-C4Aq-C5q-C6q	0.46
C8Aq-N1q	1.361	C7-O3-C8q	121.35	C8A-C4A-C5-O1	-179.27	C8Aq-C4Aq-C5q-H5q	-179.72
C4Aq-C5q	1.418	C4Aq-C8Aq-C8q	117.45	C4-C4A-C5-C6	-177.96	C4q-C4Aq-C5q-C6q	-179.79
C16-C4q	1.420	C4Aq-C8Aq-N1q	123.37	C4-C4A-C5-O1	0.95	C4q-C4Aq-C5q-H5q	0.03
C8q-C7q	1.376	C8q-C8Aq-N1q	119.18	C4A-C8A-N1-C2	-0.04	C8Aq-C4Aq-C4q-C3q	-0.01
C5q-C6q	1.376	C8Aq-C4Aq-C5q	120.22	C8-C8A-N1-C2	179.03	C8Aq-C4Aq-C4q-H4q	179.96
C5q-H5q	1.086	C8Aq-C4Aq-C4q	116.44	C4A-C8A-C8-C7	-5.66	C5q-C4Aq-C4q-C3q	-179.76
C7q-C6q	1.413	C5q-C4Aq-C4q	123.34	C4A-C8A-C8-O2	172.86	C5q-C4Aq-C4q-H4q	0.2
C7q-H7q	1.085	O3-C8q-C8Aq	116.67	N1-C8A-C8-C7	175.24	O3-C8q-C7q-C6q	175.9
C6q-H6q	1.085	O3-C8q-C7q	121.41	N1-C8A-C8-O2	-6.25	O3-C8q-C7q-H7q	-3.62
N1q-C2q	1.321	C8Aq-C8q-C7q	121.7	C4A-C4-C3-C2	-0.04	C8Aq-C8q-C7q-C6q	1.5
C2q-C3q	1.427	C4Aq-C5q-C6q	120.15	C4A-C4-C3-H3	-179.98	C8Aq-C8q-C7q-H7q	-178.03
C2q-C9q	1.508	C4Aq-C5q-H5q	119.12	H4-C4-C3-C2	179.94	C4Aq-C5q-C6q-C7q	0.11
C4q-C3q	1.371	C6q-C5q-H5q	120.73	H4-C4-C3-H3	0	C4Aq-C5q-C6q-H6q	179.49
C4q-H4q	1.087	C8q-C7q-C6q	119.91	C8A-N1-C2-C3	-0.23	H5q-C5q-C6q-C7q	-179.7
C3q-H3q	1.086	C8q-C7q-H7q	119.74	C8A-N1-C2-H2	179.85	H5q-C5q-C6q-H6q	-0.33
C9q-H9q	1.096	C6q-C7q-H7q	120.35	C4-C3-C2-N1	0.28	C8q-C7q-C6q-C5q	-1.09
C9q-H9q	1.091	C5q-C6q-C7q	120.56	C4-C3-C2-H2	-179.81	C8q-C7q-C6q-H6q	179.52
C9q-H9q	1.096	C5q-C6q-H6q1	120.36	H3-C3-C2-N1	-179.78	H7q-C7q-C6q-C5q	178.43
C4A-C8A-C4	118.46	C7q-C6q-H6q	119.07	H3-C3-C2-H2	0.13	H7q-C7q-C6q-H6q	-0.95
C4A-C8A-C5	121.97	C8Aq-N1q-C2q	118.52	C4A-C5-C6-C7	-0.56	C8Aq-N1q-C2q-C3q	-0.07
C4-C8A-C5	119.58	N1q-C2q-C3q	122.46	C4A-C5-C6-Cl	179.36	C8Aq-N1q-C2q-C9q	-179.95
C8A-C4A-N1	123.47	N1q-C2q-C9q	117.52	O1-C5-C6-C7	-179.45	N1q-C2q-C3q-C4q	0.01
C8A-C4A-C8	120.02	C3q-C2q-C9q	120.03	O1-C5-C6-Cl	0.47	N1q-C2q-C3q-H3q	-179.94
N1-C4A-C8	116.5	C4A-N1-C2	117.3	C5-C6-C7-C8	-3.94	C9q-C2q-C3q-C4q	179.88
C8A-C4-C3	118.47	C4-C3-C2	118.5	C5-C6-C7-O3	-175.44	C9q-C2q-C3q-H3q	-0.06

Table S2. Geometric parameters (bond length and angles) for compound **2** (Å, °).

Bond length. bond angles [Å, °]		Bond angles [°]		Bond angles [°]		Bond angles [°]	
C4A-C8A	1.402	C3-C4-H4	122.54	C2q-C3q-C4q	118.40	C6-C7-O3-C8q	138.07
C4A-C4	1.398	C8A-N1-C2	117.30	C2q-C3q-H3q	118.77	C8-C7-O3-C8q	-50.14
C4A-C5	1.494	C4-C3-C2	118.52	C4q-C3q-H3q	122.83	C7-O3-C8q-C8Aq	141.26
C8A-N1	1.339	C4-C3-H3	121.23	C2q-C9q-O4	123.71	C7-O3-C8q-C7q	-43.81
C8A-C8	1.503	C2-C3-H3	120.25	C2q-C9q-H9q	113.54	C8q-C8Aq-C4Aq-C5q	0.06
C4-C3	1.389	N1-C2-C3	123.79	O4-C9q-H9q	122.75	C8q-C8Aq-C4Aq-C4q	179.90
C4-H4	1.085	N1-C2-H2	115.97	C4-C4A-C8A-N1	-0.26	N1q-C8Aq-C4Aq-C5q	-179.73
N1-C2	1.335	C3-C2-H2	120.24	C4-C4A-C8A-C8	178.88	N1q-C8Aq-C4Aq-C4q	0.11
C3-C2	1.401	C4A-C5-C6	116.85	C5-C4A-C8A-N1	179.55	C4Aq-C8Aq-C8q-O3	175.92
C3-H3	1.085	C4A-C5-O1	121.12	C5-C4A-C8A-C8	-1.31	C4Aq-C8Aq-C8q-C7q	0.96
C2-H2	1.088	C6-C5-O1	122.02	C8A-C4A-C4-C3	0.17	N1q-C8Aq-C8q-O3	-4.28
C5-C6	1.486	C5-C6-C7	122.22	C8A-C4A-C4-H4	-179.83	N1q-C8Aq-C8q-C7q	-179.25
C5-O1	1.221	C5-C6-Cl	116.61	C5-C4A-C4-C3	-179.65	C4Aq-C8Aq-N1q-C2q	-0.15
C6-C7	1.359	C7-C6-Cl	121.17	C5-C4A-C4-H4	0.35	C8q-C8Aq-N1q-C2q	-179.93
C6-Cl	1.730	C8A-C8-C7	116.89	C8A-C4A-C5-C6	-1.47	C8Aq-C4Aq-C5q-C6q	-0.49
C8-C7	1.508	C8A-C8-O2	122.81	C8A-C4A-C5-O1	179.54	C8Aq-C4Aq-C5q-H5q	179.73
C8-O2	1.215	C7-C8-O2	120.28	C4-C4A-C5-C6	178.34	C4q-C4Aq-C5q-C6q	179.68
C7-O3	1.349	C6-C7-C8	121.75	C4-C4A-C5-O1	-0.65	C4q-C4Aq-C5q-H5q	-0.10
O3-C8q	1.384	C6-C7-O3	119.81	C4A-C8A-N1-C2	0.10	C8Aq-C4Aq-C4q-C3q	-0.02
C8Aq-C4Aq	1.434	C8-C7-O3	117.91	C8-C8A-N1-C2	-179.06	C8Aq-C4Aq-C4q-H4q	180.00
C8Aq-C8q	1.427	C7-O3-C8q	121.09	C4A-C8A-C8-C7	4.94	C5q-C4Aq-C4q-C3q	179.81
C8Aq-N1q	1.355	C4Aq-C8Aq-C8q	117.86	C4A-C8A-C8-O2	-173.77	C5q-C4Aq-C4q-H4q	-0.17
C4Aq-C5q	1.417	C4Aq-C8Aq-N1q	122.90	N1-C8A-C8-C7	-175.86	O3-C8q-C7q-C6q	-176.21
C4Aq-C4q	1.421	C8q-C8Aq-N1q	119.24	N1-C8A-C8-O2	5.43	O3-C8q-C7q-H7q	3.44
C8q-C7q	1.376	C8Aq-C4Aq-C5q	119.88	C4A-C4-C3-C2	0.06	C8Aq-C8q-C7q-C6q	-1.53
C5q-C6q	1.377	C8Aq-C4Aq-C4q	117.02	C4A-C4-C3-H3	-179.97	C8Aq-C8q-C7q-H7q	178.12
C5q-H5q	1.086	C5q-C4Aq-C4q	123.10	H4-C4-C3-C2	-179.94	C4Aq-C5q-C6q-C7q	-0.07
C7q-C6q	1.414	O3-C8q-C8Aq	116.42	H4-C4-C3-H3	0.03	C4Aq-C5q-C6q-H6q	-179.48
C7q-H7q	1.085	O3-C8q-C7q	122.05	C8A-N1-C2-C3	0.15	H5q-C5q-C6q-C7q	179.71
C6q-H6q	1.085	C8Aq-C8q-C7q	121.33	C8A-N1-C2-H2	-179.92	H5q-C5q-C6q-H6q	0.30
N1q-C2q	1.323	C4Aq-C5q-C6q	120.09	C4-C3-C2-N1	-0.23	C8q-C7q-C6q-C5q	1.08
C2q-C3q	1.420	C4Aq-C5q-H5q	119.17	C4-C3-C2-H2	179.83	C8q-C7q-C6q-H6q	-179.50
C2q-C9q	1.492	C6q-C5q-H5q	120.74	H3-C3-C2-N1	179.80	H7q-C7q-C6q-C5q	-178.57
C4q-C3q	1.371	C8q-C7q-C6q	119.90	H3-C3-C2-H2	-0.13	H7q-C7q-C6q-H6q	0.85
C4q-H4q	1.087	C8q-C7q-H7q	119.84	C4A-C5-C6-C7	0.34	C8Aq-N1q-C2q-C3q	0.09
C3q-H3q	1.084	C6q-C7q-H7q	120.26	C4A-C5-C6-Cl	-179.63	C8Aq-N1q-C2q-C9q	-179.95
C9q-O4	1.215	C5q-C6q-C7q	120.93	O1-C5-C6-C7	179.32	N1q-C2q-C3q-C4q	0.00
C9q-H9q	1.108	C5q-C6q-H6q	120.18	O1-C5-C6-Cl	-0.65	N1q-C2q-C3q-H3q	179.97
C8A-C4A-C4	118.44	C7q-C6q-H6q	118.89	C5-C6-C7-C8	3.56	C9q-C2q-C3q-C4q	-179.96
C8A-C4A-C5	122.00	C8Aq-N1q-C2q	117.75	C5-C6-C7-O3	175.03	C9q-C2q-C3q-H3q	0.01
C4-C4A-C5	119.55	N1q-C2q-C3q	124.23	Cl-C6-C7-C8	-176.47	N1q-C2q-C9q-O4	179.82
C4A-C8A-N1	123.48	N1q-C2q-C9q	115.52	Cl-C6-C7-O3	-5.00	N1q-C2q-C9q-H9q	-0.13
C4A-C8A-C8	120.02	C3q-C2q-C9q	120.25	C8A-C8-C7-C6	-6.16	C3q-C2q-C9q-O4	-0.21
N1-C8A-C8	116.50	C4Aq-C4q-C3q	119.70	C8A-C8-C7-O3	-177.79	C3q-C2q-C9q-H9q	179.83
C4A-C4-C3	118.46	C4Aq-C4q-H4q	119.15	O2-C8-C7-C6	172.59	C4Aq-C4q-C3q-C2q	-0.03
C4A-C4-H4	118.99	C3q-C4q-H4q	121.15	O2-C8-C7-O3	0.96	C4Aq-C4q-C3q-H3q	179.99

Table S3. Geometric parameters (bond length and angles) for compound **3** (Å, °).

Bond length. bond angles [Å, °]		Bond angles [°]		Bond angles [°]		Bond angles [°]	
C4A-C8A	1.40	C4A-C4-H4	119.83	C3q-C4q-H4q	121.03	C8A-C8-C7-C6	5.66
C4A-C4	1.39	C3-C4-H4	121.95	C2q-C3q-C4q	119.57	C8A-C8-C7-O3	177.63
C4A-C5	1.50	C8A-C1-N2	123.40	C2q-C3q-H3q	119.53	O2-C8-C7-C6	-173.18
C8A-C1	1.40	C8A-C1-H1	119.24	C4q-C3q-H3q	120.90	O2-C8-C7-O3	-1.21
C8A-C8	1.48	N2-C1-H1	117.36	C2q-C9q-H9q	111.07	C6-C7-O3-C8q	-140.42
C4-C3	1.40	C4-C3-N2	123.96	C2q-C9q-H9q	109.74	C8-C7-O3-C8q	47.49
C4-H4	1.08	C4-C3-H3	120.10	C2q-C9q-H9q	111.02	C7-O3-C8q-C8Aq	-136.70
C1-N2	1.34	N2-C3-H3	115.93	H9q-C9q-H9q	108.95	C7-O3-C8q-C7q	48.59
C1-H1	1.09	C1-N2-C3	117.34	H9q-C9q-H9q	107.08	C8q-C8Aq-C4Aq-C5q	-0.11
C3-N2	1.34	C4A-C5-C6	116.57	H9q-C9q-H9q	108.91	C8q-C8Aq-C4Aq-C4q	-179.90
C3-H3	1.09	C4A-C5-O1	121.05	C4-C4A-C8A-C1	-0.11	N1q-C8Aq-C4Aq-C5q	179.69
C5-C6	1.48	C6-C5-O1	122.37	C4-C4A-C8A-C8	-179.35	N1q-C8Aq-C4Aq-C4q	-0.10
C5-O1	1.22	C5-C6-C7	122.69	C5-C4A-C8A-C1	179.89	C4Aq-C8Aq-C8q-O3	-175.58
C6-C7	1.36	C5-C6-Cl	116.48	C5-C4A-C8A-C8	0.65	C4Aq-C8Aq-C8q-C7q	-0.90
C6-Cl	1.73	C7-C6-Cl	120.84	C8A-C4A-C4-C3	-0.01	N1q-C8Aq-C8q-O3	4.61
C8-C7	1.51	C8A-C8-C7	116.91	C8A-C4A-C4-H4	179.89	N1q-C8Aq-C8q-C7q	179.29
C8-O2	1.22	C8A-C8-O2	122.49	C5-C4A-C4-C3	179.99	C4Aq-C8Aq-N1q-C2q	0.17
C7-O3	1.34	C7-C8-O2	120.59	C5-C4A-C4-H4	-0.11	C8q-C8Aq-N1q-C2q	179.96
O3-C8q	1.39	C6-C7-C8	121.20	C8A-C4A-C5-C6	1.53	C8Aq-C4Aq-C5q-C6q	0.50
C8Aq-C4Aq	1.43	C6-C7-O3	119.72	C8A-C4A-C5-O1	-179.47	C8Aq-C4Aq-C5q-H5q	-179.75
C8Aq-C8q	1.42	C8-C7-O3	118.59	C4-C4A-C5-C6	-178.47	C4q-C4Aq-C5q-C6q	-179.73
C8Aq-N1q	1.36	C7-O3-C8q	121.31	C4-C4A-C5-O1	0.52	C8Aq-C4Aq-C4q-H4q	179.99
C4Aq-C5q	1.42	C4Aq-C8Aq-C8q	117.44	C4A-C8A-C1-N2	0.20	C5q-C4Aq-C4q-C3q	-179.80
C4Aq-C4q	1.42	C4Aq-C8Aq-N1q	123.39	C4A-C8A-C1-H1	-179.81	C5q-C4Aq-C4q-H4q	0.20
C8q-C7q	1.38	C8q-C8Aq-N1q	119.18	C8-C8A-C1-N2	179.45	O3-C8q-C7q-C6q	175.94
C5q-C6q	1.38	C8Aq-C4Aq-C5q	120.21	C8-C8A-C1-H1	-0.56	O3-C8q-C7q-H7q	-3.51
C5q-H5q	1.09	C8Aq-C4Aq-C4q	116.43	C4A-C8A-C8-C7	-4.10	C8Aq-C8q-C7q-C6q	1.51
C7q-C6q	1.41	C5q-C4Aq-C4q	123.36	C4A-C8A-C8-O2	174.71	C8Aq-C8q-C7q-H7q	-177.94
C7q-H7q	1.09	O3-C8q-C8Aq	116.68	C1-C8A-C8-C7	176.67	C4Aq-C5q-C6q-C7q	0.09
C6q-H6q	1.09	O3-C8q-C7q	121.36	C1-C8A-C8-O2	-4.52	C4Aq-C5q-C6q-H6q	179.42
N1q-C2q	1.32	C8Aq-C8q-C7q	121.74	C4A-C4-C3-N2	0.05	H5q-C5q-C6q-C7q	-179.66
C2q-C3q	1.43	C4Aq-C5q-C6q	120.17	C4A-C4-C3-H3	179.96	H5q-C5q-C6q-H6q	-0.33
C2q-C9q	1.51	C4Aq-C5q-H5q	119.11	H4-C4-C3-N2	-179.85	C8q-C7q-C6q-C5q	-1.09
C4q-C3q	1.37	C6q-C5q-H5q	120.72	H4-C4-C3-H3	0.06	C8q-C7q-C6q-H6q	179.57
C4q-H4q	1.09	C8q-C7q-C6q	119.88	C8A-C1-N2-C3	-0.16	H7q-C7q-C6q-C5q	178.36
C3q-H3q	1.09	C8q-C7q-H7q	119.74	H1-C1-N2-C3	179.85	H7q-C7q-C6q-H6q	-0.98
C9q-H9q	1.10	C6q-C7q-H7q	120.38	C4-C3-N2-C1	0.03	C8Aq-N1q-C2q-C3q	-0.12
C9q-H9q	1.09	C5q-C6q-C7q	120.55	H3-C3-N2-C1	-179.88	C8Aq-N1q-C2q-C9q	-179.99
C9q-H9q	1.10	C5q-C6q-H6q	120.35	C4A-C5-C6-C7	0.03	N1q-C2q-C3q-H3q	-179.94
C8A-C4A-C4	118.60	C7q-C6q-H6q	119.09	C4A-C5-C6-Cl	179.80	C9q-C2q-C3q-C4q	179.88
C8A-C4A-C5	121.23	C8Aq-N1q-C2q	118.51	O1-C5-C6-C7	-178.95	C9q-C2q-C3q-H3q	-0.06
C4-C4A-C5	120.17	N1q-C2q-C3q	122.45	O1-C5-C6-Cl	0.82	N1q-C2q-C9q-H9q	-121.34
C4A-C8A-C1	118.48	N1q-C2q-C9q	117.53	C5-C6-C7-C8	-3.68	N1q-C2q-C9q-H9q	-0.80
C4A-C8A-C8	121.17	C3q-C2q-C9q	120.02	C5-C6-C7-O3	-175.56	N1q-C2q-C9q-H9q	119.64
C1-C8A-C8	120.34	C4Aq-C4q-C3q	119.66	Cl-C6-C7-C8	176.55	C3q-C2q-C9q-H9q	58.79
C4A-C4-C3	118.22	C4Aq-C4q-H4q	119.32	Cl-C6-C7-O3	4.67	C3q-C2q-C9q-H9q	179.32

Table S4. Geometric parameters (bond length and angles) for compound **4** (Å, °).

Bond length. bond angles [Å, °]		Bond angles [°]		Bond angles [°]		Bond angles [°]	
C4A-C8A	1.40	C3-C4-H4	121.95	C2q-C3q-C4q	118.45	C6-C7-O3-C8q	147.80
C4A-C4	1.39	C8A-C1-N2	123.35	C2q-C3q-H3q	118.70	C8-C7-O3-C8q	-41.89
C4A-C5	1.50	C8A-C1-H1	119.28	C4q-C3q-H3q	122.85	C7-O3-C8q-C8Aq	-42.70
C8A-C1	1.40	N2-C1-H1	117.36	C2q-C9q-O4	123.68	C7-O3-C8q-C7q	144.56
C8A-C8	1.48	C4-C3-N2	123.99	C2q-C9q-H9q	113.70	C8q-C8Aq-C4Aq-C5q	0.47
C4-C3	1.40	C4-C3-H3	120.08	O4-C9q-H9q	122.63	C8q-C8Aq-C4Aq-C4q	-179.99
C4-H4	1.08	N2-C3-H3	115.93	C4-C4A-C8A-C1	0.24	N1q-C8Aq-C4Aq-C5q	-179.44
C1-N2	1.34	C1-N2-C3	117.34	C4-C4A-C8A-C8	179.00	N1q-C8Aq-C4Aq-C4q	0.10
C1-H1	1.09	C4A-C5-C6	116.56	C5-C4A-C8A-C1	-179.51	C4Aq-C8Aq-C8q-O3	-173.78
C3-N2	1.34	C4A-C5-O1	120.98	C5-C4A-C8A-C8	-0.74	C4Aq-C8Aq-C8q-C7q	-1.34
C3-H3	1.09	C6-C5-O1	122.46	C8A-C4A-C4-C3	0.05	N1q-C8Aq-C8q-O3	6.13
C5-C6	1.48	C5-C6-C7	122.40	C8A-C4A-C4-H4	-179.84	N1q-C8Aq-C8q-C7q	178.57
C5-O1	1.22	C5-C6-Cl	116.64	C5-C4A-C4-C3	179.79	C4Aq-C8Aq-N1q-C2q	0.24
C6-C7	1.36	C7-C6-Cl	120.94	C5-C4A-C4-H4	-0.09	C8q-C8Aq-N1q-C2q	-179.67
C6-Cl	1.73	C8A-C8-C7	116.86	C8A-C4A-C5-C6	-2.19	C8Aq-C4Aq-C5q-C6q	0.34
C8-C7	1.50	C8A-C8-O2	122.77	C8A-C4A-C5-O1	178.70	C8Aq-C4Aq-C5q-H5q	-179.93
C8-O2	1.22	C7-C8-O2	120.35	C4-C4A-C5-C6	178.07	C4q-C4Aq-C5q-C6q	-179.16
C7-O3	1.35	C6-C7-C8	121.47	C4-C4A-C5-O1	-1.04	C4q-C4Aq-C5q-H5q	0.56
O3-C8q	1.38	C6-C7-O3	119.14	C4A-C8A-C1-N2	-0.42	C8Aq-C4Aq-C4q-C3q	-0.32
C8Aq-C4Aq	1.43	C8-C7-O3	118.65	C4A-C8A-C1-H1	179.65	C8Aq-C4Aq-C4q-H4q	179.78
C8Aq-C8q	1.43	C7-O3-C8q	124.11	C8-C8A-C1-N2	-179.20	C5q-C4Aq-C4q-C3q	179.20
C8Aq-N1q	1.35	C4Aq-C8Aq-C8q	118.06	C8-C8A-C1-H1	0.88	C5q-C4Aq-C4q-H4q	-0.70
C4Aq-C5q	1.42	C4Aq-C8Aq-N1q	122.64	C4A-C8A-C8-C7	5.96	O3-C8q-C7q-C6q	174.18
C4Aq-C4q	1.42	C8q-C8Aq-N1q	119.31	C4A-C8A-C8-O2	-172.58	O3-C8q-C7q-H7q	-6.02
C8q-C7q	1.37	C8Aq-C4Aq-C5q	119.86	C1-C8A-C8-C7	-175.29	C8Aq-C8q-C7q-C6q	1.39
C5q-C6q	1.38	C8Aq-C4Aq-C4q	116.90	C1-C8A-C8-O2	6.16	C8Aq-C8q-C7q-H7q	-178.81
C5q-H5q	1.09	C5q-C4Aq-C4q	123.23	C4A-C4-C3-N2	-0.19	C4Aq-C5q-C6q-C7q	-0.33
C7q-C6q	1.41	O3-C8q-C8Aq	121.71	C4A-C4-C3-H3	179.94	C4Aq-C5q-C6q-H6q	179.71
C7q-H7q	1.08	O3-C8q-C7q	116.88	H4-C4-C3-N2	179.70	H5q-C5q-C6q-C7q	179.95
C6q-H6q	1.09	C8Aq-C8q-C7q	121.00	H4-C4-C3-H3	-0.17	H5q-C5q-C6q-H6q	-0.01
N1q-C2q	1.32	C4Aq-C5q-C6q	119.95	C8A-C1-N2-C3	0.29	C8q-C7q-C6q-C5q	-0.54
C2q-C3q	1.42	C4Aq-C5q-H5q	119.20	H1-C1-N2-C3	-179.79	C8q-C7q-C6q-H6q	179.42
C2q-C9q	1.49	C6q-C5q-H5q	120.85	C4-C3-N2-C1	0.03	H7q-C7q-C6q-C5q	179.67
C4q-C3q	1.37	C8q-C7q-C6q	120.09	H3-C3-N2-C1	179.90	H7q-C7q-C6q-H6q	-0.37
C4q-H4q	1.09	C8q-C7q-H7q	118.90	C4A-C5-C6-C7	-0.57	C8Aq-N1q-C2q-C3q	-0.37
C3q-H3q	1.08	C6q-C7q-H7q	121.01	C4A-C5-C6-Cl	-178.75	C8Aq-N1q-C2q-C9q	179.72
C9q-O4	1.21	C5q-C6q-C7q	121.02	O1-C5-C6-C7	178.53	N1q-C2q-C3q-C4q	0.14
C9q-H9q	1.11	C5q-C6q-H6q	120.11	O1-C5-C6-Cl	0.35	N1q-C2q-C3q-H3q	-179.81
C8A-C4A-C4	118.54	C7q-C6q-H6q	118.86	C5-C6-C7-C8	6.13	C9q-C2q-C3q-C4q	-179.94
C8A-C4A-C5	121.25	C8Aq-N1q-C2q	118.33	C5-C6-C7-O3	176.16	C9q-C2q-C3q-H3q	0.10
C4-C4A-C5	120.21	N1q-C2q-C3q	123.77	Cl-C6-C7-C8	-175.77	N1q-C2q-C9q-O4	179.86
C4A-C8A-C1	118.56	N1q-C2q-C9q	115.83	Cl-C6-C7-O3	-5.74	N1q-C2q-C9q-H9q	-0.15
C4A-C8A-C8	120.95	C3q-C2q-C9q	120.39	C8A-C8-C7-C6	-8.75	C3q-C2q-C9q-O4	-0.06
C1-C8A-C8	120.48	C4Aq-C4q-C3q	119.91	C8A-C8-C7-O3	-178.83	C3q-C2q-C9q-H9q	179.93
C4A-C4-C3	118.23	C4Aq-C4q-H4q	119.08	O2-C8-C7-C6	169.83	C4Aq-C4q-C3q-C2q	0.21
C4A-C4-H4	119.82	C3q-C4q-H4q	121.01	O2-C8-C7-O3	-0.25	C4Aq-C4q-C3q-H3q	-179.84

Table S5. The value of local potential minima for nucleophilic regions in compounds **1-4**.

Molecule	Area					
	Oxygen atom at C-5	Oxygen atom at C-8	Oxygen atom at C-6	Nitrogen atom at 5,8-quinolinedione moiety	Nitrogen atom at quinoline moiety	Oxygen atom at carbonyl group
1	-1.96	-1.58 -1.61	-1.20	-2.39	-2.72	
2	-1.74	-1.42 -1.44	-0.93	-2.29	-2.29	-1.74
3	-1.85	-1.47	-1.09	-2.18	-2.61	
4	-1.85	-1.20	-0.82	-2.12	-2.23	-1.77