Density Functional Theory Studies and Molecular Docking on Xanthohumol, 8-Prenylnaringenin and Their Symmetric Substitute Diethanolamine Derivatives as Inhibitors for Colon Cancer-Related Proteins

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S1 Figure: Root-mean-square deviation (RMSD) values (y-axis) along the time frame (x-axis) for atoms of the protein-8Prenylnaringenin derivative complex and protein-Xanthohumol derivative complex.
S1 Table: Bond lenghts of the Xanthohumol and 8-Prenylnaringenin derivatives.
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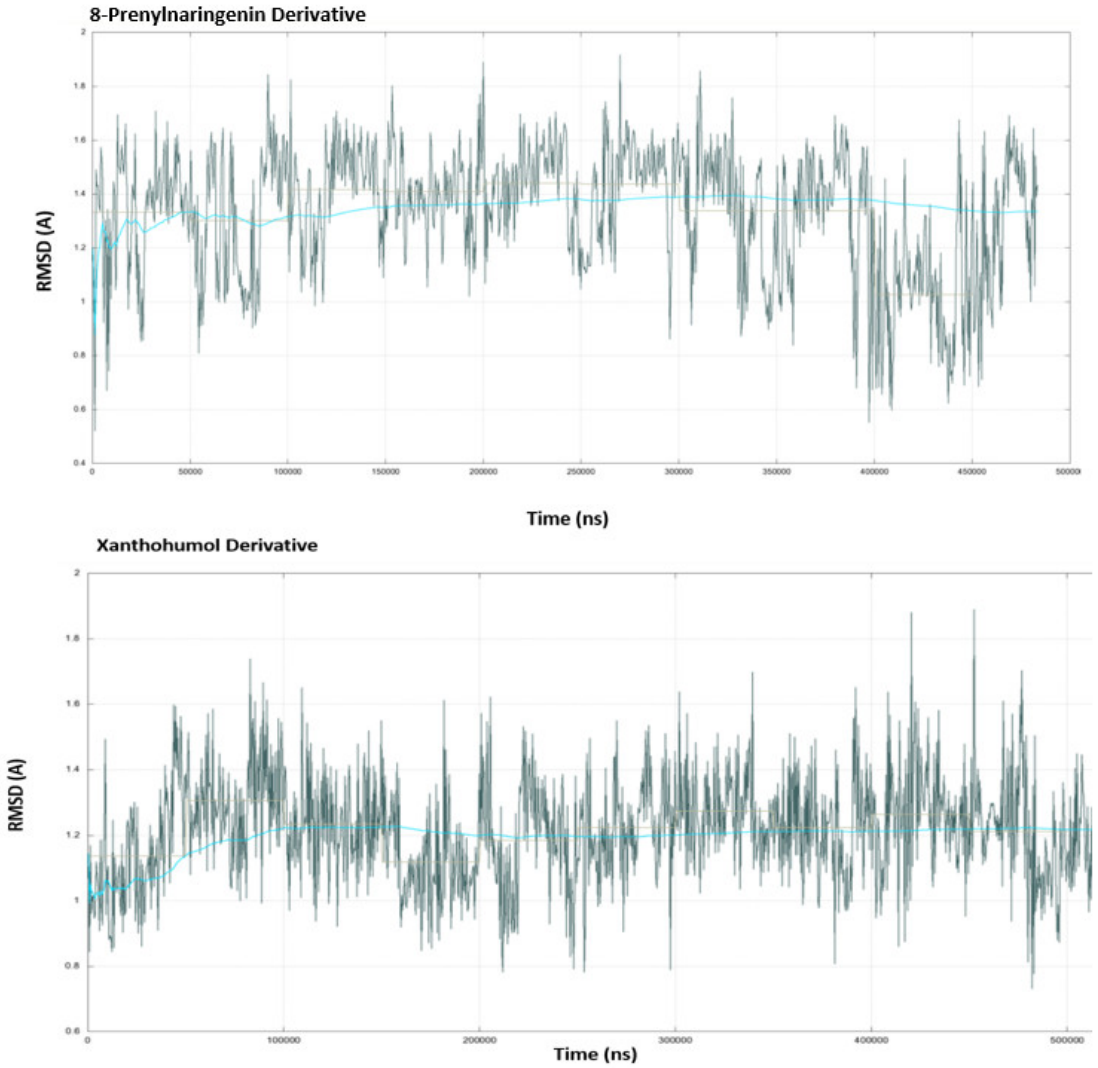

S1 Figure: Root-mean-square deviation (RMSD) values (y-axis) along the time frame (x-axis) for atoms of the protein-8Prenylnaringenin derivative complex and protein-Xanthohumol derivative complex.

S1 Table: Bond lenghts of the Xanthohumol and 8-Prenylnaringenin derivatives.

Atom Xanthohumol Derivative	Bond Length Actual (Å)	Bond Length Optimal (Å)	Bond Angle Actual	Bond Angle Optimal
O(34)-H(67)	0.9602	0.9610	H(67)-O(34)-C(33)	109.2515
C(33)-H(66)	1.1133	1.1110	H(66)-C(33)-H(65)	109.4346
C(33)-H(65)	1.1121	1.1110	H(66)-C(33)-O(34)	107.1432
C(33)-O(34)	1.4146	1.4080	H(66)-C(33)-C(32)	111.2957
C(32)-H(64)	1.1149	1.1130	H(65)-C(33)-O(34)	106.4787
C(32)-H(63)	1.1161	1.1130	H(65)-C(33)-C(32)	112.8275
C(32)-C(33)	1.5297	1.5140	O(34)-C(33)-C(32)	109.3932
O(31)-H(62)	0.9603	0.9610	H(64)-C(32)-H(63)	107.1842
C(30)-H(61)	1.1134	1.1110	H(64)-C(32)-C(33)	108.6036
C(30)-H(60)	1.1124	1.1110	C(33)-C(32)-N(28)	113.8698
C(30)-O(31)	1.4147	1.4080	H(62)-O(31)-C(30)	109.3392
C(29)-H(59)	1.1162	1.1130	H(61)-C(30)-H(60)	109.5652
C(29)-H(58)	1.1155	1.1130	H(61)-C(30)-O(31)	107.1315
C(29)-C(30)	1.5299	1.5140	H(61)-C(30)-C(29)	111.3585
N(28)-C(32)	1.4621	1.4380	H(60)-C(30)-O(31)	106.3492
N(28)-C(29)	1.4619	1.4380	H(60)-C(30)-C(29)	112.7064
C(27)-H(57)	1.1044	1.1130	O(31)-C(30)-C(29)	109.4585
C(27)-H(56)	1.1154	1.1130	H(59)-C(29)-H(58)	107.0890
C(27)-N(28)	1.4638	1.4380	H(59)-C(29)-C(30)	109.1427
O(26)-H(55)	0.9709	0.9720	C(33)-C(32)-N(28)	113.8698
C(25)-C(27)	1.5260	1.4970	H(62)-O(31)-C(30)	109.3392

S2 Table: Bond angles of the Xanthohumol and 8-Prenylnaringenin derivatives.

Atom 8-Prenylnaringenin Derivative	Bond Length Actual (Å)	Bond Length Optimal (Å)	Bond Angle Actual	Bond Angle Optimal
O(33)-H(64)	0.9601	0.9610	H(64)-O(33)-C(32)	109.3757
C(32)-H(63)	1.1131	1.1110	H(63)-C(32)-H(62)	109.4744
C(32)-H(62)	1.1121	1.1110	H(63)-C(32)-O(33)	107.2782
C(31)-H(61)	1.1144	1.1130	H(63)-C(32)-C(31)	111.3428
C(31)-H(60)	1.1157	1.1130	H(62)-C(32)-O(33)	106.5672
O(30)-H(59)	0.9602	0.9610	H(62)-C(32)-C(31)	112.6167
C(29)-H(58)	1.1118	1.1110	O(33)-C(32)-C(31)	109.3117
C(29)-H(57)	1.1117	1.1110	H(61)-C(31)-H(60)	106.4268
C(28)-H(56)	1.1151	1.1130	H(61)-C(31)-C(32)	109.4620
C(28)-H(55)	1.1168	1.1130	H(59)-O(30)-C(29)	109.4713
C(26)-H(54)	1.1070	1.1130	H(58)-C(29)-H(57)	109.0734
C(26)-H(53)	1.1166	1.1130	H(58)-C(29)-O(30)	106.6903
C(25)-H(52)	1.1132	1.1130	H(58)-C(29)-C(28)	112.5453
C(25)-H(51)	1.1081	1.1130	H(57)-C(29)-O(30)	106.5982
C(25)-H(50)	1.1133	1.1130	H(57)-C(29)-C(28)	112.5316
O(24)-H(49)	0.9708	0.9720	O(30)-C(29)-C(28)	109.0664
O(23)-H(48)	0.9642	0.9720	H(56)-C(28)-H(55)	103.8769
O(22)-H(47)	0.9709	0.9720	H(56)-C(28)-C(29)	108.9133
C(20)-H(46)	1.1029	1.1000	H(59)-O(30)-C(29)	109.4713
C(18)-H(45)	1.1028	1.1000	C(31)-N(27)-C(28)	113.6412
C(17)-H(44)	1.1030	1.1000	C(31)-N(27)-C(26)	110.6734

S3 Table: Atomic charges of the Xanthohumol and 8-Prenylnaringenin derivatives.

Atom (Xanthohumol Derivative)	Huckel Charges	Atom (8-Prenylnaringenin Derivative)	Huckel Charges
C(1)	0.253132	C(1)	-0.135827
C(2)	-0.210702	C(2)	0.0544411
C(3)	0.283483	C(3)	-0.106989
C(4)	-0.135689	C(4)	-0.075156
C(5)	0.256933	C(5)	-0.0915145
C(6)	-0.096558	C(6)	0.263514
O(7)	-0.28014	C(7)	-0.218512
O(8)	-0.284228	C(8)	0.274666
O(9)	-0.264119	C(9)	-0.161194
C(10)	0.0907518	C(10)	0.264306
C(11)	-0.0700673	O(11)	-0.230673
C(12)	-0.10036	C(12)	0.207376
C(13)	0.0558938	C(13)	-0.130401
C(14)	-0.135778	C(14)	0.436209
C(15)	-0.139015	O(15)	-0.625994
C(16)	0.392511	C(16)	-0.0392965
C(17)	-0.164622	C(17)	-0.0397658
O(18)	-0.702263	C(18)	-0.118305
C(19)	0.0847444	C(19)	0.243305
C(20)	-0.0304084	C(20)	-0.133341
C(21)	0.0114225	C(21)	0.0534758
C(22)	-0.112686	O(22)	-0.267755
C(23)	0.27799	O(23)	-0.250495
C(24)	-0.128902	O(24)	-0.243384
C(25)	0.0994122	C(25)	-0.14531
O(26)	-0.231647	C(26)	0.00754896
C(27)	-0.000756697	N(27)	-0.115866
N(28)	-0.107473	C(28)	0.0163106
C(29)	0.0153326	C(29)	0.119224
C(30)	0.146912	O(30)	-0.372973