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Fig. S1. ¹H NMR spectrum of 9a



Fig. S2. ¹³C NMR spectrum of 9a



Fig. S3. ¹H NMR spectrum of 9b



Fig. S4. ¹³C NMR spectrum of 9b



Fig. S5. ¹H NMR spectrum of 9c



Fig. S6. ¹³C NMR spectrum of 9c



Fig. S7. ¹H NMR spectrum of 20a



Fig. S8. ¹³C NMR spectrum of 20a



Fig. S9. ¹H NMR spectrum of 20b



Fig. S10. ¹³C NMR spectrum of 20b



Fig. S11. ¹H NMR spectrum of 20c



Fig. S12. ¹³C NMR spectrum of 20c



Fig. S13. ¹H NMR spectrum of 21a



Fig. S14. ¹³C NMR spectrum of 21a



Fig. S15. ¹H NMR spectrum of 22a



Fig. S16. ¹³C NMR spectrum of 22a



Fig. S17. ¹H NMR spectrum of 21b



Fig. S18. ¹³C NMR spectrum of 21b



Fig. S19. ¹H NMR spectrum of 22b



Fig. S20. ¹³C NMR spectrum of 22b



Fig. S21. ¹H NMR spectrum of 21c



Fig. S22. ¹³C NMR spectrum of 21c



Fig. S23. ¹H NMR spectrum of 22c



Fig. S24. ¹³C NMR spectrum of 22c



Fig. S25. ¹H NMR spectrum of 1



Fig. S26. ¹³C NMR spectrum of 1



Fig. S27. ¹H NMR spectrum of 2



Fig. S28. ¹³C NMR spectrum of 2



Fig. S29. ¹H NMR spectrum of 3



Fig. S30. ¹³C NMR spectrum of 3



Fig. S31. ¹H NMR spectrum of 19



Fig. S32. ¹³C NMR spectrum of 19



Fig. S33. ¹H NMR spectrum of 24



Fig. S34. ¹³C NMR spectrum of 24



Fig. S35. ¹H NMR spectrum of 25



Fig. S36. ¹³C NMR spectrum of 25



Fig. S37. ¹H NMR spectrum of 26



Fig. S38. ¹³C NMR spectrum of 26



Fig. S39. ¹H NMR spectrum of 10a



Fig. S40. ¹³C NMR spectrum of 10a



Fig. S41. ¹H NMR spectrum of 14



Fig. S42. ¹³C NMR spectrum of 14



Fig. S43. ¹H NMR spectrum of 16



Fig. S44. ¹³C NMR spectrum of 16



Fig. S45. ¹H NMR spectrum of 17



Fig. S46. ¹³C NMR spectrum of 17



Fig. S47. ¹H NMR spectrum of 18



Fig. S48. ¹³C NMR spectrum of 18

Table S1. Cartesian Coordinates of Quercetin Optimized by DFT at the B3LYP/6-31G(d) Level of Theory

C	-4. 56160000	-0. 52860000	0.00010000
С	-3. 79300000	0. 62780000	-0.00010000
С	-2.36890000	0.53540000	0.0000000
С	-1.77370000	-0. 73820000	0.00020000
С	-2. 53230000	-1.90550000	0.00040000
С	-3. 92590000	-1.77980000	0.00040000
0	-0. 42110000	-0. 87290000	0.00020000
С	-1. 52840000	1.69640000	-0.00010000
С	-0. 09470000	1.46980000	-0.00010000
С	0. 43430000	0. 20580000	-0.00010000
0	-4. 39130000	1.82860000	-0.00060000
Н	-3.67490000	2.51510000	-0.00090000
Н	-2. 04110000	-2. 87350000	0.00060000
0	-4. 74010000	-2.86850000	0.00060000
Н	-4. 19950000	-3. 67420000	0.00080000
Н	-5. 64330000	-0. 46890000	0.00010000
С	1.84080000	-0. 19570000	-0. 00010000
С	2.87840000	0.76360000	0.00060000
С	2. 19080000	-1. 55920000	-0. 00100000
С	4. 20160000	0.35750000	0.00060000
Н	2.64050000	1.82060000	0.00140000
С	3. 52400000	-1.95770000	-0. 00110000
Н	1. 41280000	-2. 31190000	-0.00160000
С	4. 54260000	-1.00750000	-0.00030000
0	5.84470000	-1.39410000	-0.00040000
Н	3. 79390000	-3.00890000	-0.00170000
Н	6. 38960000	-0. 58760000	0.00020000
0	5. 27710000	1.21750000	0.00130000
Н	4. 96150000	2. 13380000	0.00150000
0	-1.94630000	2.88700000	-0.00050000
0	0.65030000	2.60620000	-0.00020000
Н	-0. 02890000	3. 32040000	-0.00030000

Table S2. Cartesian Coordinates of **1** Optimized by DFT at the B3LYP/6-31G(d) Level of Theory

C	4.81980000	0.69670000	0.16960000
C	4. 11800000	-0. 45500000	-0. 15970000
C	2.69020000	-0. 45090000	-0. 13750000
C	2. 02420000	0.73760000	0.21540000
C	2.71690000	1.89970000	0.54620000
C	4. 11470000	1.85900000	0.51870000
0	0.66560000	0.79020000	0. 25480000
C	1.92140000	-1.61240000	-0. 48020000
C	0. 47490000	-1. 47150000	-0. 43620000
C	-0. 11630000	-0. 30180000	-0. 05540000
0	4. 78430000	-1.56910000	-0. 49890000
Н	4. 10830000	-2. 26600000	-0. 70550000
Н	2.17030000	2.79730000	0.81780000
0	4.86630000	2.94850000	0.83000000
Н	4. 28070000	3.68910000	1.05310000
Н	5.90310000	0.70190000	0. 15630000
C	-1. 55340000	0.00380000	-0. 01280000
C	-2. 49150000	-0. 85160000	0.61050000
С	-1.98660000	1.19810000	-0. 61630000
C	-3. 83760000	-0. 48710000	0. 52730000
C	-3. 32830000	1.56790000	-0. 66970000
Н	-1.24690000	1.84840000	-1.07310000
С	-4. 25980000	0.69550000	-0. 09440000
0	-5. 58470000	1.00640000	-0. 13820000
Н	-6.06290000	0. 27070000	0. 28460000
0	-4. 86450000	-1.22300000	1.09380000
Н	-4. 59460000	-2. 14930000	1.17630000
0	2. 40910000	-2. 71940000	-0. 83470000
0	-0. 22520000	-2. 56650000	-0. 82580000
Н	0. 47520000	-3. 22210000	-1.04280000
C	-2. 11630000	-2. 08350000	1.39950000
Н	-2. 19010000	-2. 99990000	0.80130000
Н	-1.08490000	-2. 02630000	1.75380000
Н	-2. 75860000	-2. 18710000	2.28290000
С	-3. 79570000	2.83830000	-1.33170000
Н	-4. 50700000	2.62730000	-2. 13900000
Н	-4. 31560000	3. 49000000	-0. 61940000
Н	-2. 95170000	3.39270000	-1.75260000

Table S3. Cartesian Coordinates of **2** Optimized by DFT at the B3LYP/6-31G(d) Level of Theory

С	-4. 67480000	-0. 55150000	0. 15860000
C	-3. 90570000	0.58150000	-0.06990000
C	-2. 48140000	0. 48310000	-0. 09590000
C	-1.88830000	-0. 77710000	0. 10670000
С	-2. 64880000	-1.92110000	0.33490000
С	-4. 04100000	-1.78780000	0.35850000
0	-0. 53550000	-0. 92080000	0.09620000
С	-1.64540000	1.62300000	-0. 33910000
С	-0. 21080000	1.38540000	-0. 35810000
С	0. 30950000	0.14620000	-0. 12180000
0	-4. 50410000	1.76600000	-0. 26680000
Н	-3. 78840000	2.43620000	-0. 42170000
Н	-2. 15720000	-2.87610000	0. 49150000
0	-4. 85610000	-2.85370000	0. 57700000
Н	-4. 31640000	-3.65040000	0.70050000
Н	-5. 75590000	-0. 48550000	0. 18090000
С	1.72340000	-0. 25480000	-0. 15790000
С	2. 73450000	0.46390000	0. 52640000
С	2.06180000	-1. 40070000	-0. 89900000
С	4. 05370000	0.03270000	0.36950000
С	3. 37880000	-1.82670000	-1.01640000
Н	1.27500000	-1.95190000	-1. 40290000
С	4. 38850000	-1.10070000	-0. 38850000
0	5.68530000	-1. 48800000	-0. 50330000
Н	3.64360000	-2. 70120000	-1.60140000
Н	6. 22160000	-0. 83750000	-0. 01580000
0	5. 13480000	0.63960000	0.98390000
Н	4. 92730000	1.56710000	1.16960000
0	-2.06600000	2.79080000	-0. 55770000
0	0. 55150000	2.46840000	-0. 65270000
Н	-0. 10810000	3. 18730000	-0. 77680000
C	2. 45500000	1.62400000	1. 45220000
Н	2. 57550000	2.59280000	0.95260000
Н	1. 42900000	1.59240000	1.82470000
Н	3. 11970000	1.59230000	2.32450000

Table S4. Cartesian Coordinates of **3** Optimized by DFT at the B3LYP/6-31G(d) Level of Theory

C	4. 71070000	0.71710000	0.0000000
С	4. 03450000	-0. 49570000	0. 00000000
С	2.60760000	-0. 51450000	0. 00000000
С	1.91480000	0. 70840000	0. 00000000
С	2. 58030000	1.93160000	0.00010000
С	3.97940000	1.91480000	0.00010000
0	0.55610000	0.73710000	0.00010000
С	1.86020000	-1.73750000	0.0000000
С	0. 41350000	-1.62400000	0. 00000000
С	-0. 21320000	-0. 40510000	0.0000000
0	4. 72440000	-1.64630000	-0. 00010000
Н	4. 06320000	-2.38660000	-0. 00020000
Н	2.01510000	2.85830000	0.00010000
0	4. 70630000	3.06390000	0.00010000
Н	4. 10440000	3.82480000	0.0000000
Н	5.79380000	0.74190000	0.0000000
С	-1.64710000	-0. 11570000	0.0000000
С	-2. 60420000	-1.15260000	0.00010000
С	-2. 10050000	1.21720000	-0. 00010000
C	-3.95260000	-0.83850000	0.00010000
C	-3. 45790000	1.54040000	-0.00010000
Н	-1.37630000	2.02270000	-0. 00020000
C	-4. 38980000	0. 49580000	0.0000000
0	-5. 72080000	0.78200000	0.0000000
Н	-6. 20030000	-0.06500000	0.0000000
0	-4. 96550000	-1.77290000	0.00020000
Н	-4. 58480000	-2.66400000	0.00020000
0	2.37060000	-2.89180000	-0.00010000
0	-0. 24020000	-2.81540000	0.0000000
Н	0. 49330000	-3. 47380000	-0.00010000
C	-3.94240000	2.96800000	-0. 00020000
Н	-4. 56450000	3.17620000	-0. 87870000
Н	-4. 56340000	3.17660000	0.87900000
Н	-3. 10020000	3.66600000	-0.00080000
Н	-2. 28930000	-2. 18900000	0. 00030000