Novel Quercetin and Apigenin-Acetamide Derivatives: Design, Synthesis, Characterization, Biological Evaluation and Molecular Docking Studies

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Supporting Information

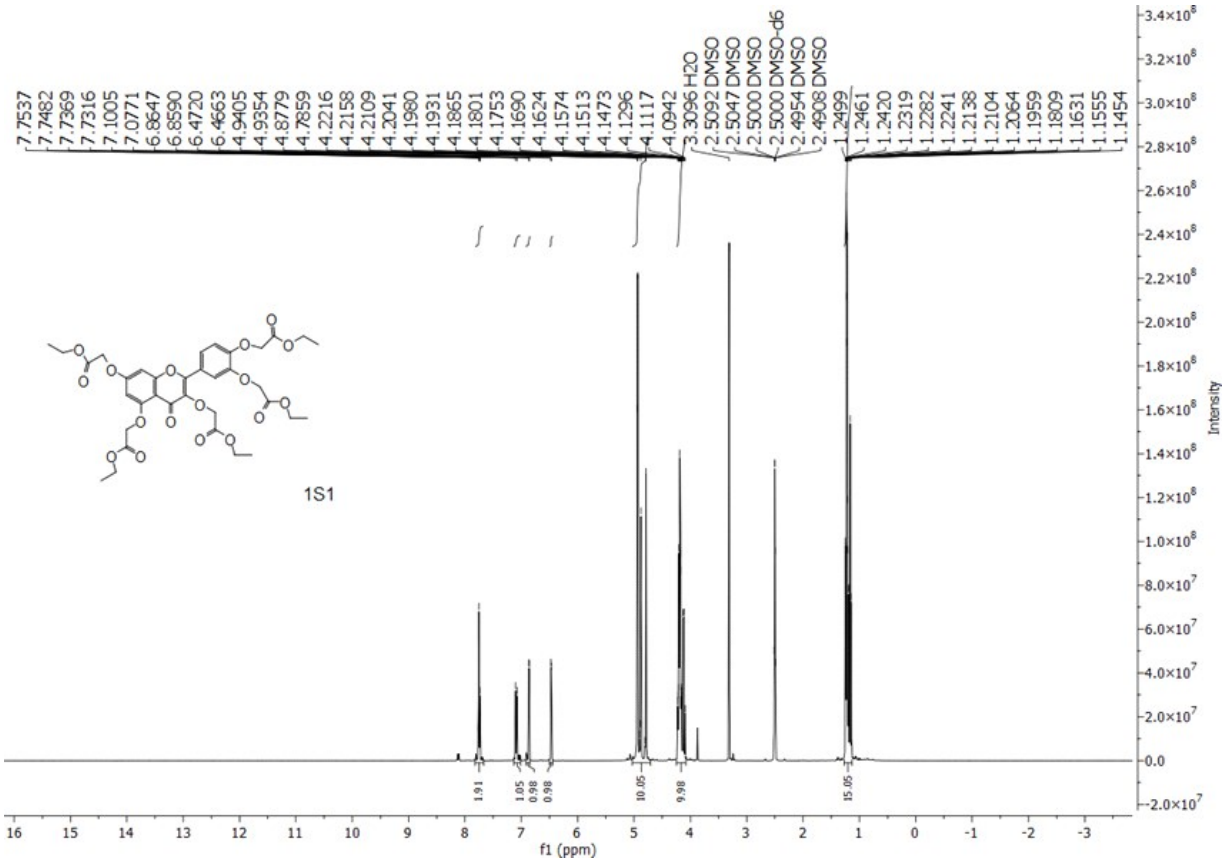

Figure S1: ^{1}H NMR (400 MHz, DMSO-d_6): 1S1.

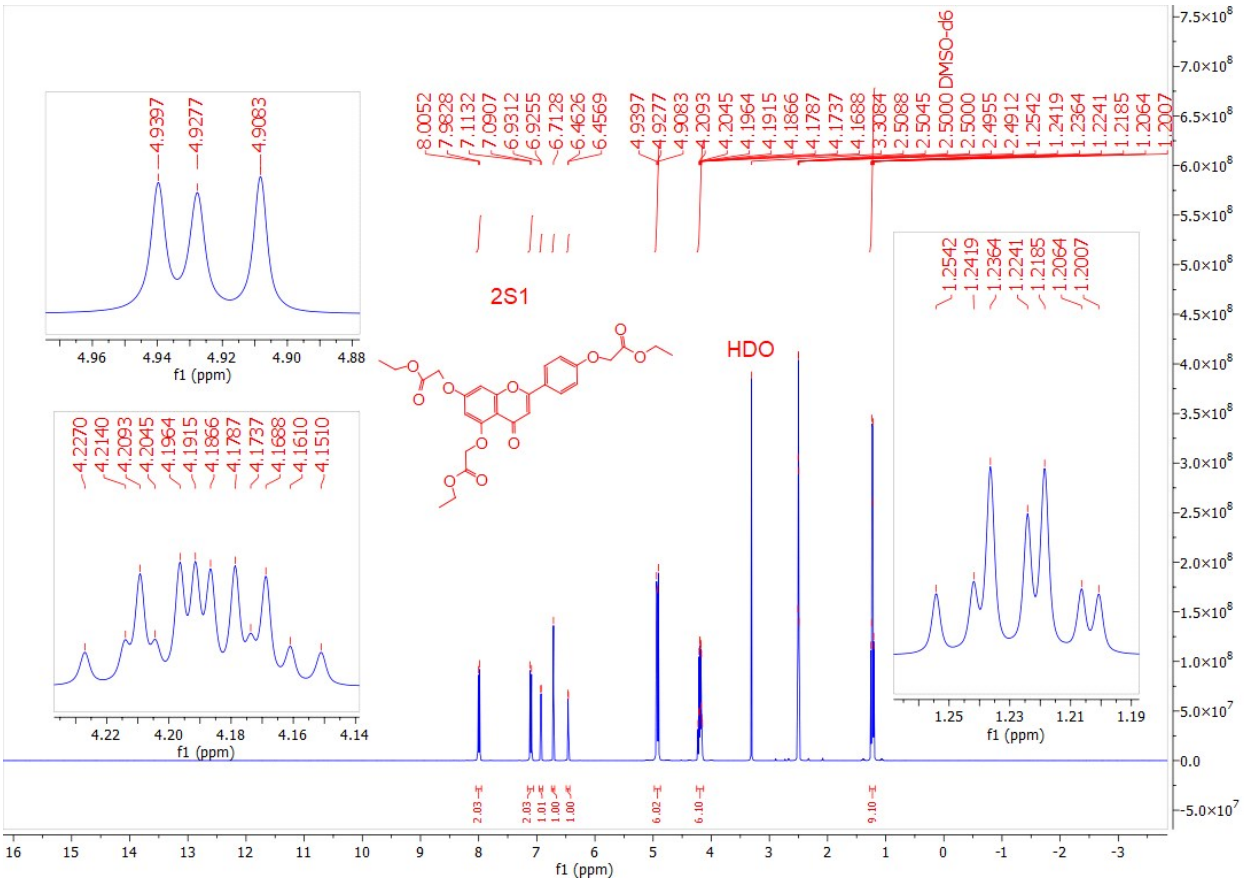

Figure S2: ^{1}H NMR (400 MHz, DMSO-d6): 2S1.

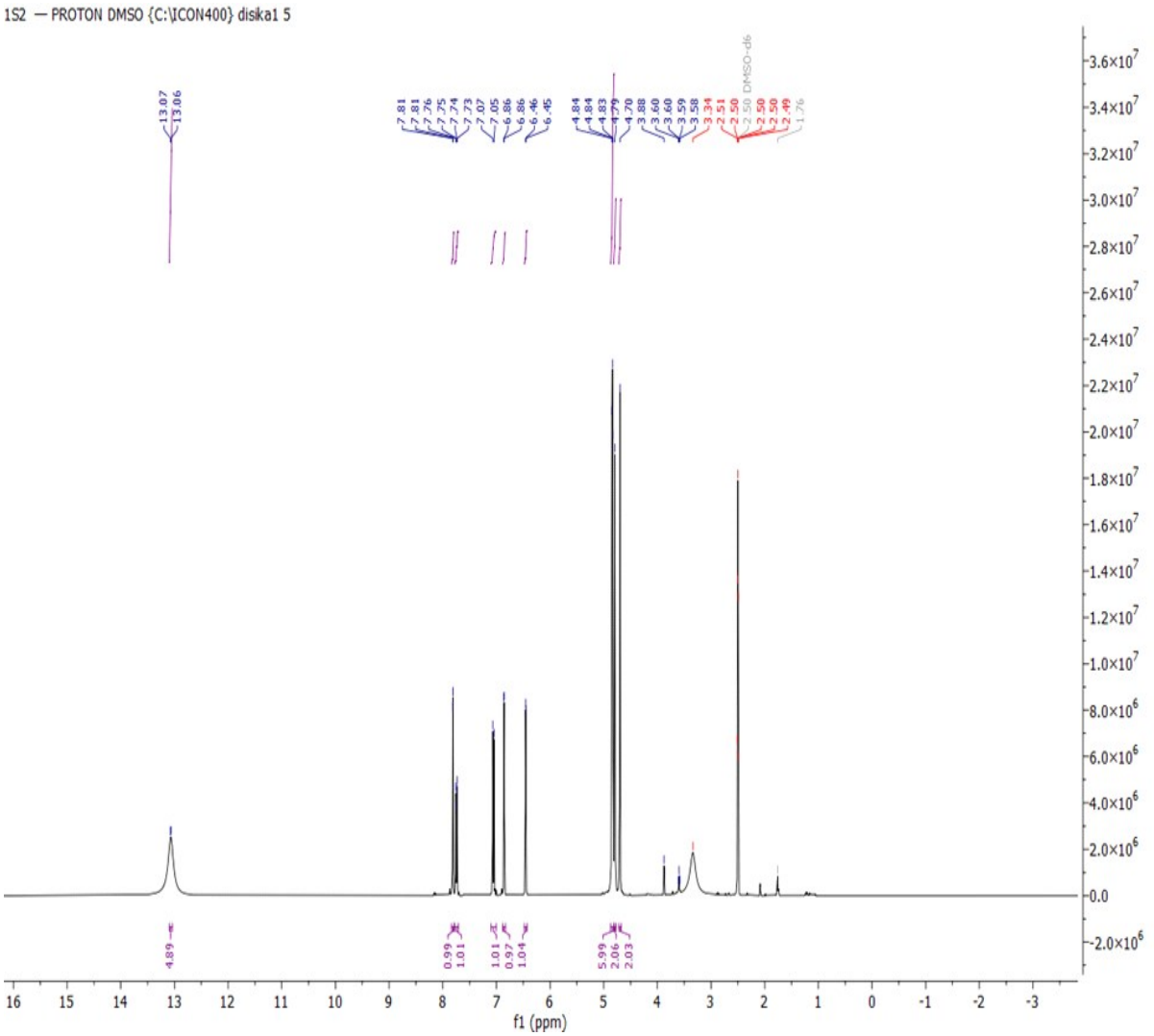

Figure S3: ^{1}H NMR (400 MHz, DMSO-d_6): 1S2.

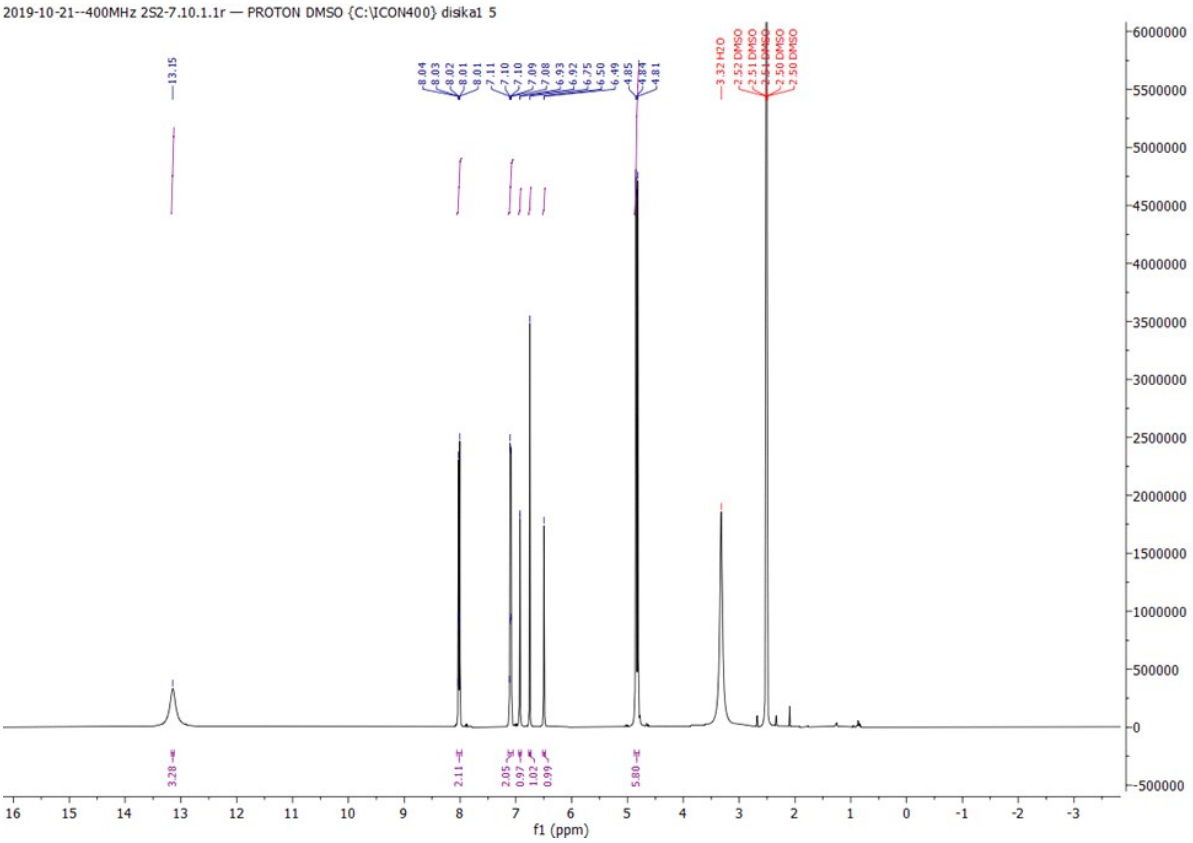

Figure S4: ^{1}H NMR (400 MHz, DMSO-d_6): 2S2.

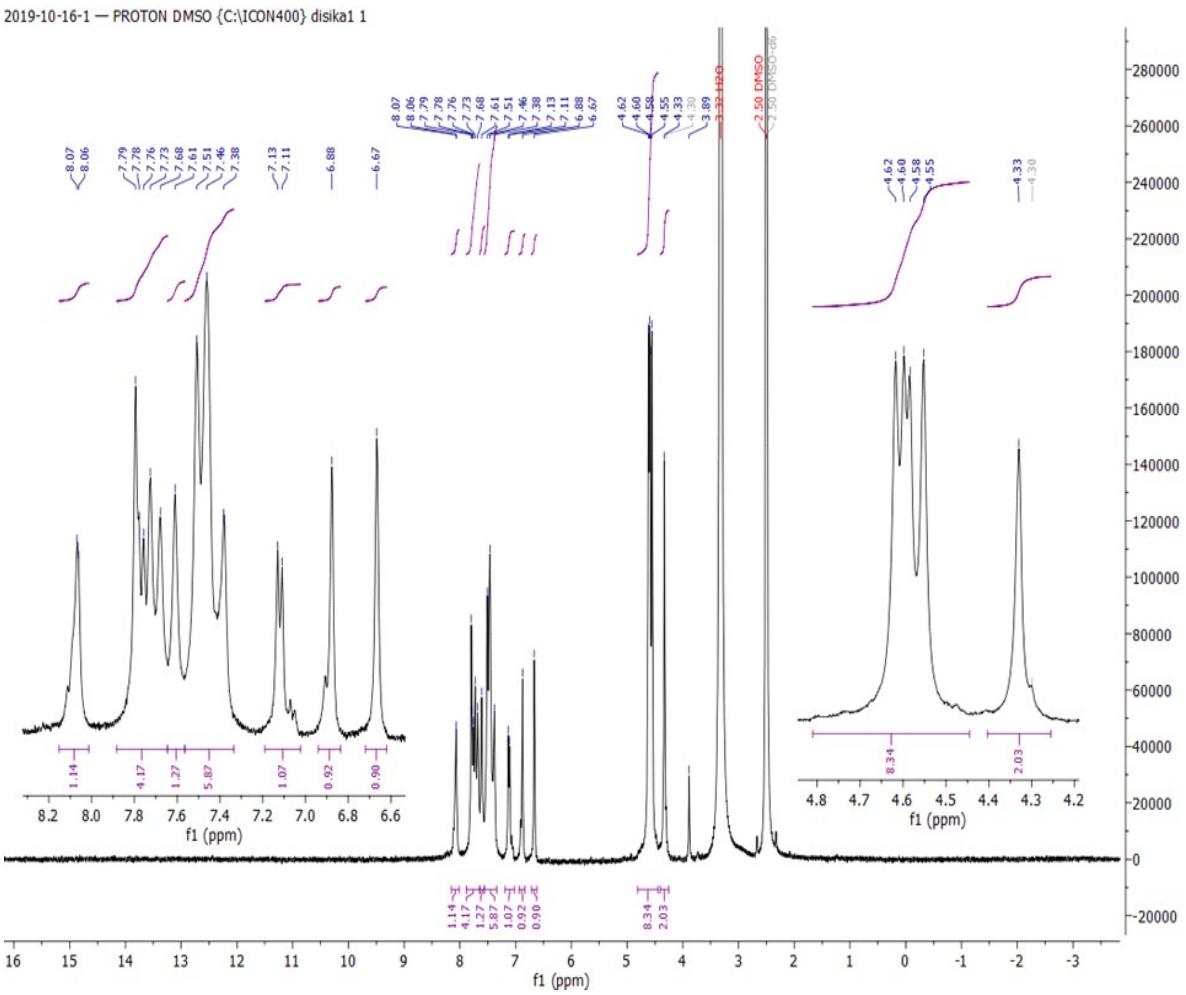

Figure S5: ^{1}H NMR (400 MHz, DMSO-d_6): 1S3

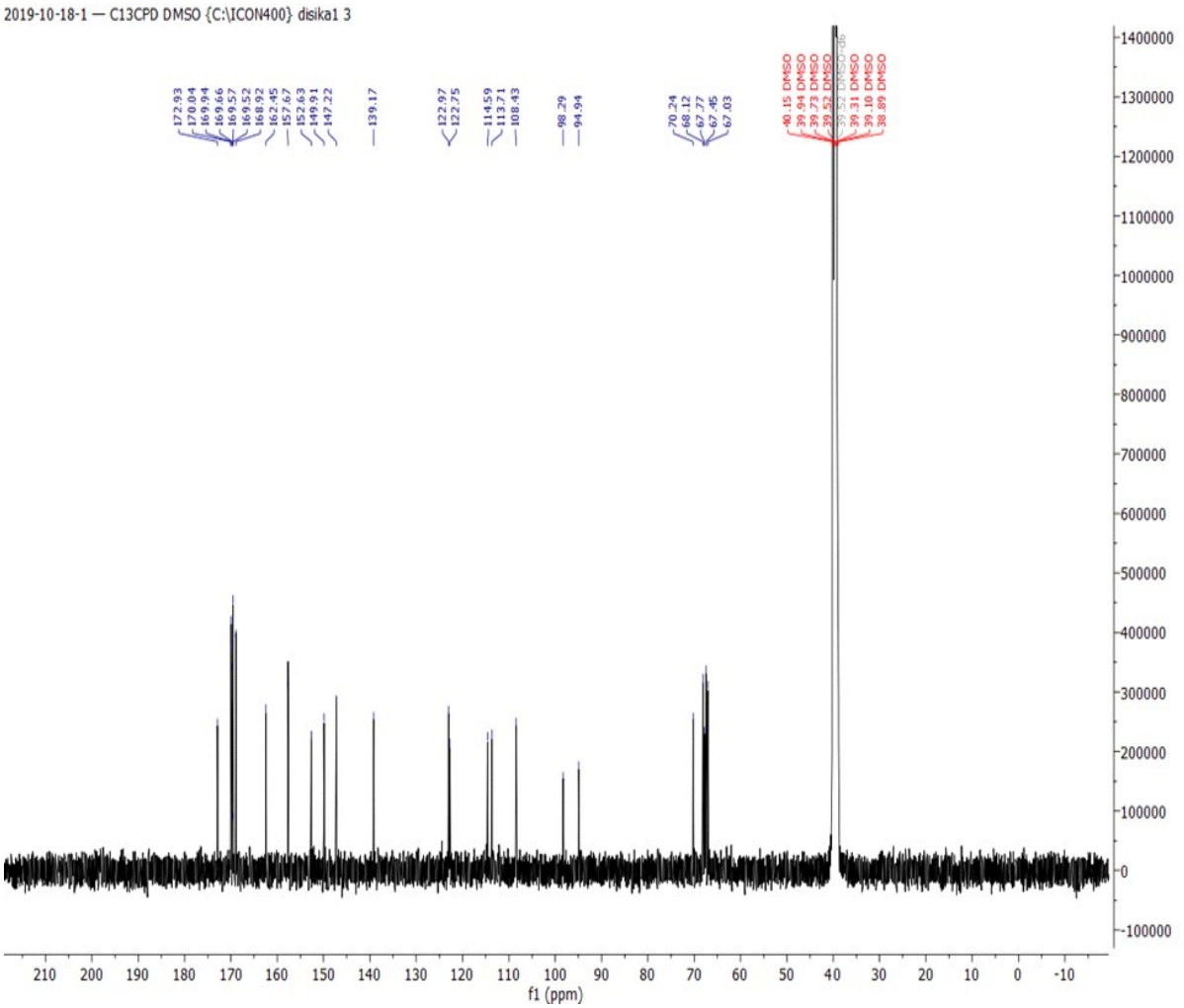

Figure S6: ^{13}C NMR (400 MHz, DMSO-d_6): 1S3

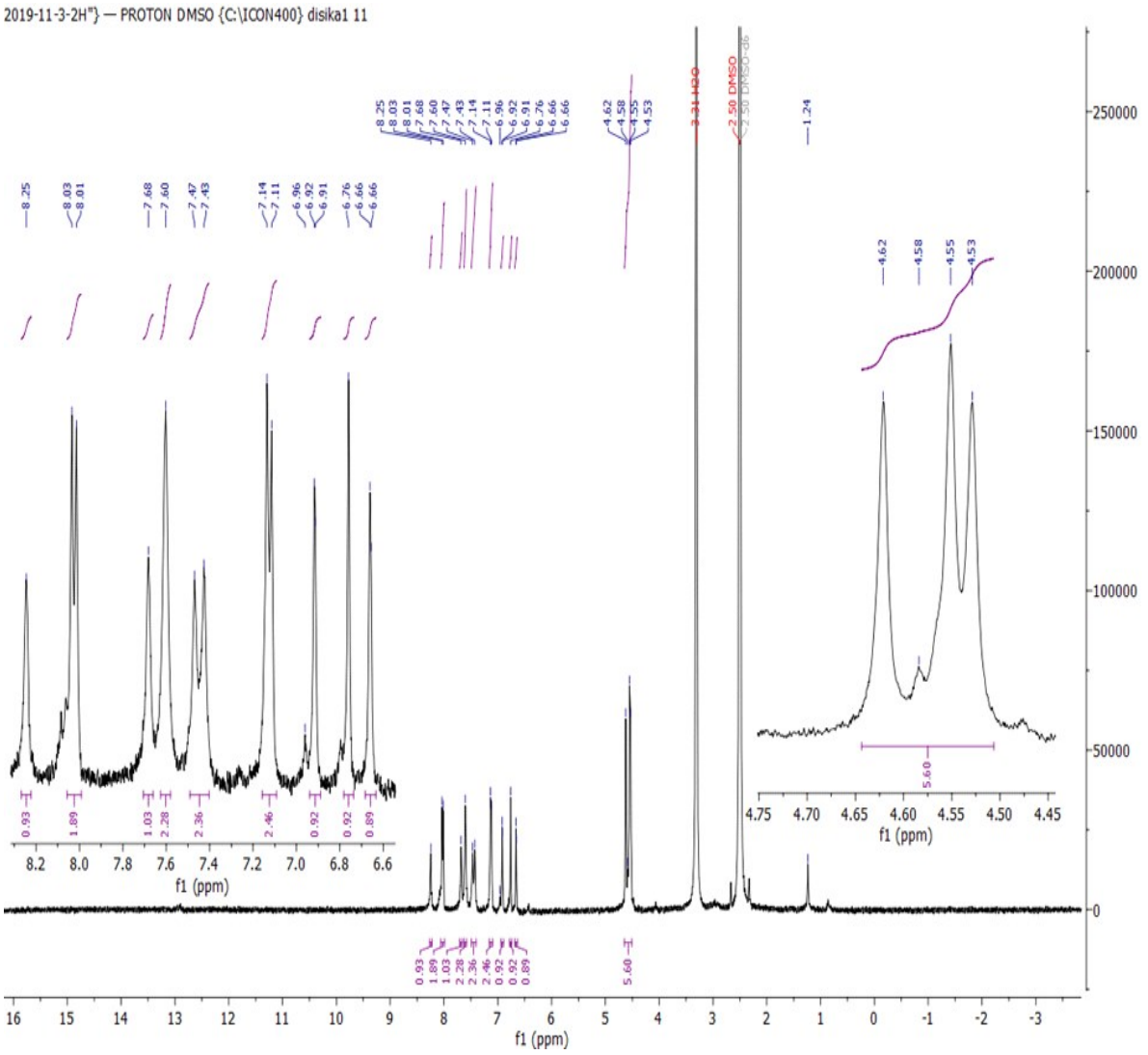

Figure S7: ^{1}H NMR (400 MHz, DMSO-d_6): 2S3

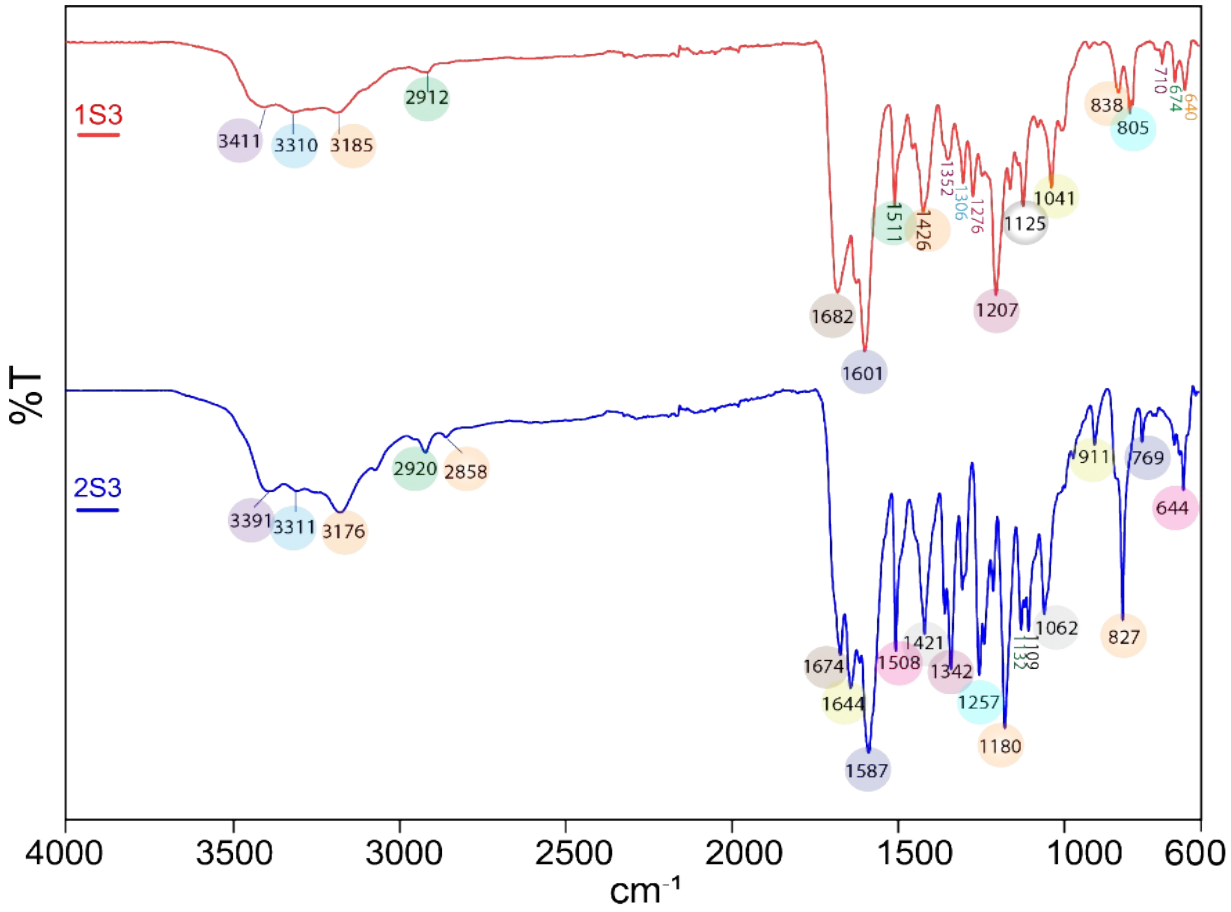

Figure S8. FTIR spectra of 1S3 and 2S3.

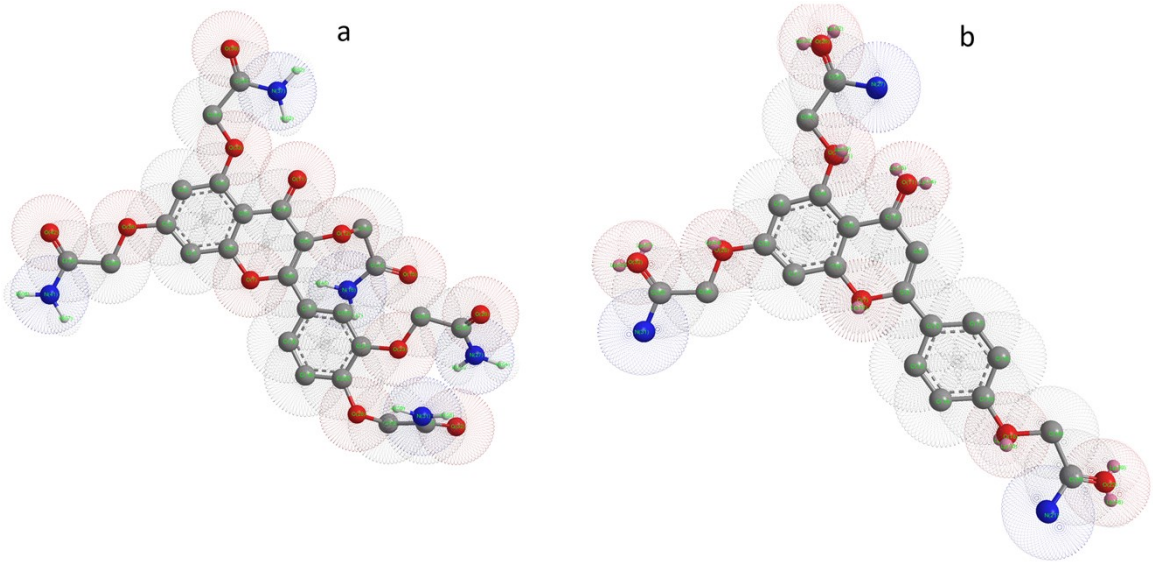

Figure S9. Energy minimized and optimized molecular structures of 1S3 and 2S3

Table S1. Assignments of FTIR bands for 1S3 and 2S3 derivatives.

	Frequency(cm^{-1})	
Assignments	1S3	2S3
Amide N-H Stretch	3411	3391
Amide N-H Stretch	3310	3311
Alkenyl C-H Stretch	3185	3176
Alkyl C-H Stretch	2912	2920
(C=O) Ketone	1682	1674
(C=O) Amide	1601	1587

Table S2. Predicted bond lengths and angles of the 1S3

Atom	Bond at	Bond Length (A°)	Angle atom	Angle (°)	2nd Angle atom	2nd Angle (°)	2nd angle type
C(5)							
C(6)	C(5)	1.401					
C(1)	C(6)	1.395	C(5)	120.582			
C(2)	C(1)	1.395	C(6)	119.909	C(5)	0.002	Dihedral
C(4)	C(5)	1.401	C(6)	119.115	C(1)	0.001	Dihedral
O(7)	C(6)	1.378	C(1)	116.714	C(5)	122.704	Pro-S
C(3)	C(4)	1.396	C(5)	120.277	C(6)	-0.004	Dihedral
C(8)	O(7)	1.375	C(6)	117.952	C(1)	179.997	Dihedral
C(10)	C(5)	1.504	C(4)	120.532	C(6)	120.353	Pro-R
H(43)	C(1)	1.1	C(2)	120.045	C(6)	120.045	Pro-R
Lp(68)	O(7)	0.6	C(6)	107.292	C(8)	107.292	Pro-S
Lp(69)	O(7)	0.6	C(6)	104.501	C(8)	104.501	Pro-R
C(9)	C(10)	1.495	C(5)	112.597	C(4)	180	Dihedral
O(33)	C(4)	1.355	C(3)	119.862	C(5)	119.862	Pro-S
O(38)	C(2)	1.355	C(1)	120.014	C(3)	120.014	Pro-S
H(44)	C(3)	1.1	C(2)	119.927	C(4)	119.927	Pro-S
O(11)	C(10)	1.208	C(5)	123.702	C(9)	123.702	Pro-R
O(12)	C(9)	1.355	C(8)	119.335	C(10)	119.335	Pro-S
C(17)	C(8)	1.337	O(7)	117.468	C(9)	117.468	Pro-R
C(34)	O(33)	1.402	C(4)	110.8	C(3)	0	Dihedral

C(39)	O(38)	1.402	C(2)	110.8	C(1)	0	Dihedral
Lp(84)	O(33)	0.6	C(4)	109.116	C(34)	109.116	Pro-S
Lp(85)	O(33)	0.6	C(4)	108.703	C(34)	108.703	Pro-R
Lp(88)	O(38)	0.6	C(2)	109.116	C(39)	109.116	Pro-S
Lp(89)	O(38)	0.6	C(2)	108.703	C(39)	108.703	Pro-R
C(13)	O(12)	1.402	C(9)	110.8	C(8)	180	Dihedral
C(18)	C(17)	1.395	C(8)	119.999	O(7)	36	Dihedral
C(35)	C(34)	1.509	O(33)	109.5	C(4)	180	Dihedral
C(40)	C(39)	1.509	O(38)	109.5	C(2)	-180	Dihedral
Lp(70)	O(11)	0.6	C(10)	120	C(5)	-180	Dihedral
Lp(71)	O(11)	0.6	C(10)	109	C(5)	0	Dihedral
Lp(72)	O(12)	0.6	C(9)	109.116	C(13)	109.116	Pro-S
Lp(73)	O(12)	0.6	C(9)	108.703	C(13)	108.703	Pro-R
C(14)	C(13)	1.509	O(12)	109.5	C(9)	180	Dihedral
C(19)	C(18)	1.395	C(17)	119.997	C(8)	-179.994	Dihedral
C(22)	C(17)	1.395	C(8)	119.999	C(18)	120.003	Pro-S
N(37)	C(35)	1.369	C(34)	120	O(33)	0	Dihedral
N(41)	C(40)	1.369	C(39)	120	O(38)	-180	Dihedral
H(60)	C(34)	1.113	O(33)	109.442	C(35)	109.442	Pro-S
H(61)	C(34)	1.113	O(33)	109.462	C(35)	109.462	Pro-R
H(64)	C(39)	1.113	O(38)	109.442	C(40)	109.442	Pro-S
H(65)	C(39)	1.113	O(38)	109.462	C(40)	109.462	Pro-R
N(16)	C(14)	1.369	C(13)	120	O(12)	0	Dihedral
C(20)	C(19)	1.395	C(18)	120	C(17)	-0.006	Dihedral
C(21)	C(22)	1.395	C(17)	120	C(8)	179.999	Dihedral
O(36)	C(35)	1.208	C(34)	120	N(37)	120	Pro-R
O(42)	C(40)	1.208	C(39)	120	N(41)	120	Pro-S
H(45)	C(13)	1.113	O(12)	109.442	C(14)	109.442	Pro-S
H(46)	C(13)	1.113	O(12)	109.462	C(14)	109.462	Pro-R
H(49)	C(18)	1.1	C(17)	120.002	C(19)	120.002	Pro-S
H(62)	N(37)	1.012	C(35)	120	C(34)	-180	Dihedral
H(66)	N(41)	1.012	C(40)	120	C(39)	-180	Dihedral

O(15)	C(14)	1.208	C(13)	120	N(16)	120	Pro-R
O(23)	C(21)	1.355	C(20)	120.001	C(22)	120.001	Pro-S
O(28)	C(20)	1.355	C(19)	119.998	C(21)	119.998	Pro-S
H(47)	N(16)	1.012	C(14)	120	C(13)	-180	Dihedral
H(50)	C(19)	1.1	C(18)	120	C(20)	120	Pro-S
H(51)	C(22)	1.1	C(17)	120	C(21)	120	Pro-R
H(63)	N(37)	1.012	C(35)	120	H(62)	120	Pro-S
H(67)	N(41)	1.012	C(40)	120	H(66)	120	Pro-S
Lp(86)	O(36)	0.6	C(35)	120	C(34)	-180	Dihedral
Lp(87)	O(36)	0.6	C(35)	109	C(34)	0	Dihedral
Lp(90)	O(42)	0.6	C(40)	120	C(39)	-180	Dihedral
Lp(91)	O(42)	0.6	C(40)	109	C(39)	0	Dihedral
C(24)	O(23)	1.402	C(21)	110.8	C(20)	-180	Dihedral
C(29)	O(28)	1.402	C(20)	110.8	C(19)	180	Dihedral
H(48)	N(16)	1.012	C(14)	120	H(47)	120	Pro-R
Lp(74)	O(15)	0.6	C(14)	120	C(13)	-180	Dihedral
Lp(75)	O(15)	0.6	C(14)	109	C(13)	0	Dihedral
Lp(76)	O(23)	0.6	C(21)	109.116	C(24)	109.116	Pro-S
Lp(77)	O(23)	0.6	C(21)	108.703	C(24)	108.703	Pro-R
Lp(80)	O(28)	0.6	C(20)	109.116	C(29)	109.116	Pro-S
Lp(81)	O(28)	0.6	C(20)	108.703	C(29)	108.703	Pro-R
C(25)	C(24)	1.509	O(23)	109.5	C(21)	180	Dihedral
C(30)	C(29)	1.509	O(28)	109.5	C(20)	-180	Dihedral
N(27)	C(25)	1.369	C(24)	120	O(23)	0	Dihedral
N(31)	C(30)	1.369	C(29)	120	O(28)	-180	Dihedral
H(52)	C(24)	1.113	O(23)	109.442	C(25)	109.442	Pro-S
H(53)	C(24)	1.113	O(23)	109.462	C(25)	109.462	Pro-R
H(56)	C(29)	1.113	O(28)	109.442	C(30)	109.442	Pro-S
H(57)	C(29)	1.113	O(28)	109.462	C(30)	109.462	Pro-R
O(26)	C(25)	1.208	C(24)	120	N(27)	120	Pro-R
O(32)	C(30)	1.208	C(29)	120	N(31)	120	Pro-R
H(54)	N(27)	1.012	C(25)	120	C(24)	180	Dihedral

H(58)	N(31)	1.012	C(30)	120	C(29)	180	Dihedral
H(55)	N(27)	1.012	C(25)	120	H(54)	120	Pro-R
H(59)	N(31)	1.012	C(30)	120	H(58)	120	Pro-S
Lp(78)	O(26)	0.6	C(25)	120	C(24)	180	Dihedral
Lp(79)	O(26)	0.6	C(25)	109	C(24)	0	Dihedral
Lp(82)	O(32)	0.6	C(30)	120	C(29)	-180	Dihedral
Lp(83)	O(32)	0.6	C(30)	109	C(29)	0	Dihedral

Table S3. Predicted bond lengths and angles of the 2S3

Atom	Bond Atom	Bond Length (Å)	Angle Atom	Angle (°)	2nd Angle Atom	2nd Angle (°)	2nd Angle Type
C(5)							
C(6)	C(5)	1.348					
C(1)	C(6)	1.346	C(5)	118.766			
O(7)	C(6)	1.364	C(1)	117.652	C(5)	123.583	Pro-S
C(4)	C(5)	1.356	C(6)	120.069	C(1)	-0.136	Dihedral
C(10)	C(5)	1.37	C(4)	121.319	C(6)	118.612	Pro-S
C(2)	C(1)	1.344	C(6)	123.674	C(5)	-0.154	Dihedral
C(3)	C(4)	1.346	C(5)	118.048	C(6)	0.371	Dihedral
C(8)	O(7)	1.365	C(6)	117.865	C(1)	-179.967	Dihedral
C(9)	C(10)	1.363	C(5)	117.513	C(4)	-179.906	Dihedral
C(12)	C(8)	1.359	O(7)	118.939	C(9)	122.598	Pro-S
C(13)	C(12)	1.349	C(8)	119.224	O(7)	-0.079	Dihedral
C(17)	C(12)	1.348	C(8)	125.978	C(13)	114.798	Pro-S
C(14)	C(13)	1.342	C(12)	122.446	C(8)	179.982	Dihedral
C(15)	C(14)	1.345	C(13)	122.685	C(12)	0.103	Dihedral
C(16)	C(17)	1.344	C(12)	122.632	C(8)	-179.93	Dihedral
O(18)	C(15)	1.373	C(14)	119.071	C(16)	125.871	Pro-R
O(23)	C(4)	1.365	C(3)	122.747	C(5)	119.201	Pro-R
O(28)	C(2)	1.374	C(1)	125.825	C(3)	118.946	Pro-S
O(11)	C(10)	1.22	C(5)	125.652	C(9)	116.834	Pro-S

C(19)	O(18)	1.413	C(15)	119.24	C(14)	177.045	Dihedral
C(20)	C(19)	1.521	O(18)	110.473	C(15)	-179.202	Dihedral
N(21)	C(20)	1.358	C(19)	114.491	O(18)	-17.396	Dihedral
O(22)	C(20)	1.204	C(19)	124.498	N(21)	121.011	Pro-R
C(24)	O(23)	1.405	C(4)	123.594	C(3)	3.52	Dihedral
C(25)	C(24)	1.525	O(23)	107.659	C(4)	177.255	Dihedral
N(27)	C(25)	1.363	C(24)	114.817	O(23)	-2.171	Dihedral
O(26)	C(25)	1.203	C(24)	124.153	N(27)	121.03	Pro-R
C(29)	O(28)	1.414	C(2)	119.185	C(1)	-1.184	Dihedral
C(30)	C(29)	1.524	O(28)	111.695	C(2)	-179.354	Dihedral
N(31)	C(30)	1.36	C(29)	114.4	O(28)	176.646	Dihedral
O(32)	C(30)	1.204	C(29)	125.427	N(31)	120.173	Pro-S
H(33)	C(1)	1.102	C(2)	120.083	C(6)	116.244	Pro-S
H(34)	C(3)	1.102	C(2)	115.955	C(4)	119.831	Pro-S
H(35)	C(9)	1.101	C(8)	121.536	C(10)	114.5	Pro-S
H(36)	C(13)	1.103	C(12)	121.713	C(14)	115.841	Pro-R
H(37)	C(14)	1.104	C(13)	118.885	C(15)	118.431	Pro-S
H(38)	C(16)	1.102	C(15)	120.433	C(17)	117.184	Pro-S
H(39)	C(17)	1.1	C(12)	122.514	C(16)	114.854	Pro-S
H(40)	C(19)	1.114	O(18)	109.592	C(20)	108.412	Pro-S
H(41)	C(19)	1.114	O(18)	109.558	C(20)	107.561	Pro-R
H(44)	C(24)	1.114	O(23)	109.941	C(25)	108.985	Pro-S
H(45)	C(24)	1.114	O(23)	109.918	C(25)	108.625	Pro-R
H(48)	C(29)	1.115	O(28)	109.122	C(30)	107.797	Pro-S
H(49)	C(29)	1.115	O(28)	109.29	C(30)	107.682	Pro-R
H(42)	N(21)	1.01	C(20)	118.139	C(19)	-179.746	Dihedral
H(43)	N(21)	1.011	C(20)	120.033	H(42)	121.823	Pro-R
H(46)	N(27)	1.009	C(25)	117.97	C(24)	-179.99	Dihedral
H(47)	N(27)	1.015	C(25)	121.527	H(46)	120.503	Pro-R
H(50)	N(31)	1.01	C(30)	117.59	C(29)	179.962	Dihedral
H(51)	N(31)	1.01	C(30)	121.273	H(50)	121.137	Pro-S

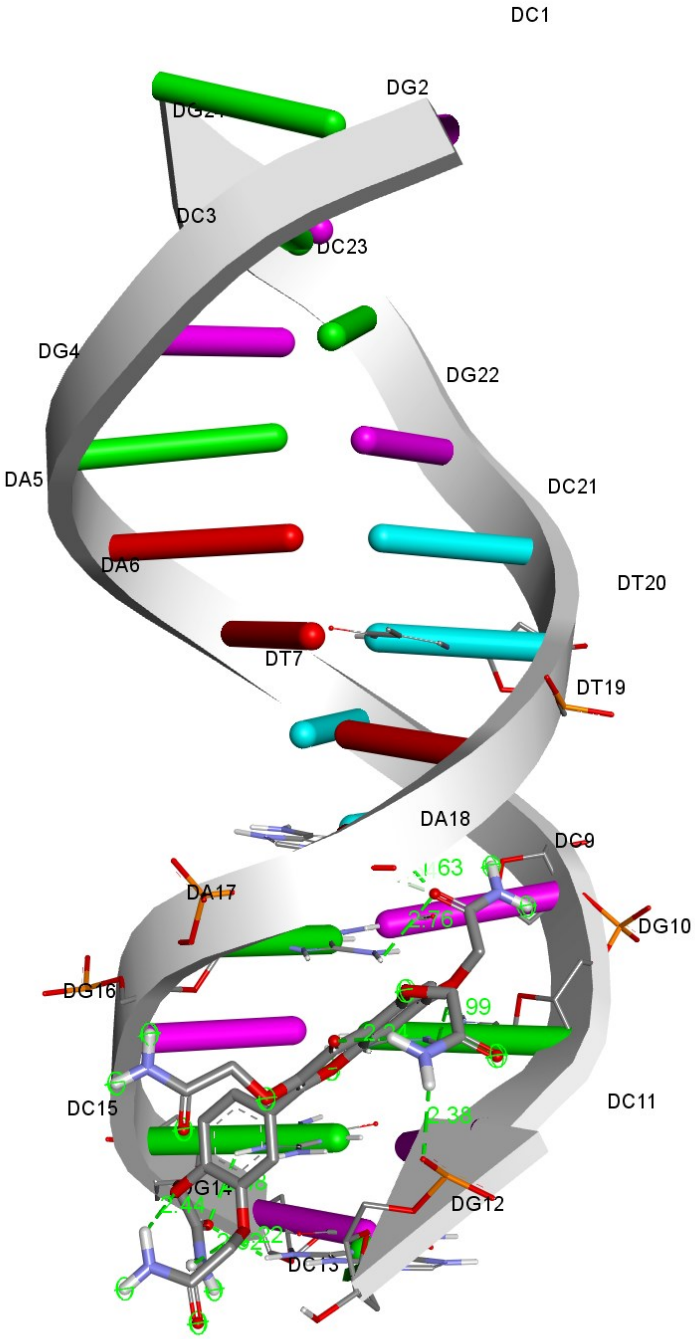

Figure S10. 3D interactions of 1S3 in the active site of DNA with depicting the bond lengths.

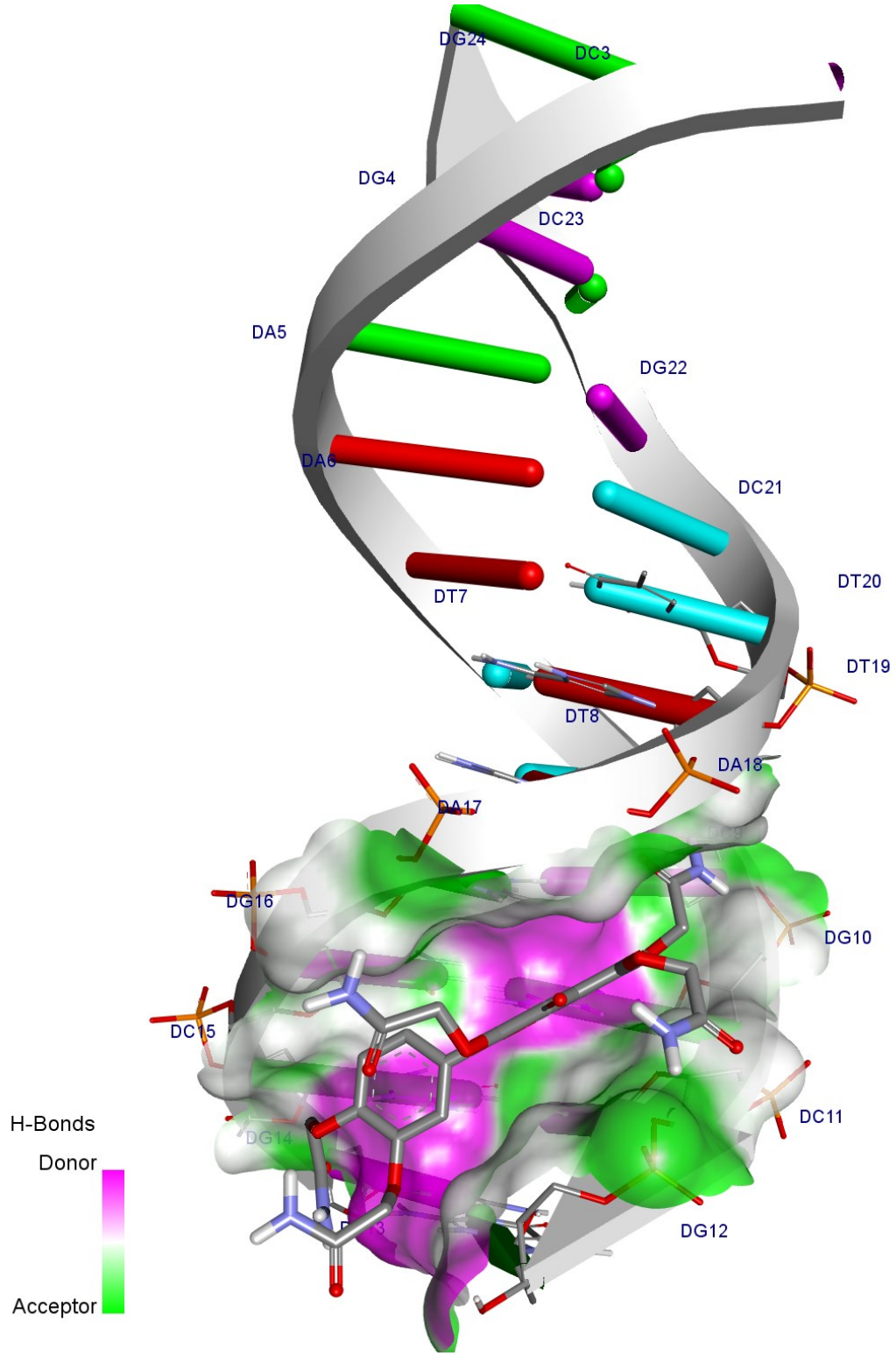

Figure S11. 3D interactions of 1S3 in the active site of DNA with depicting the H-bonds

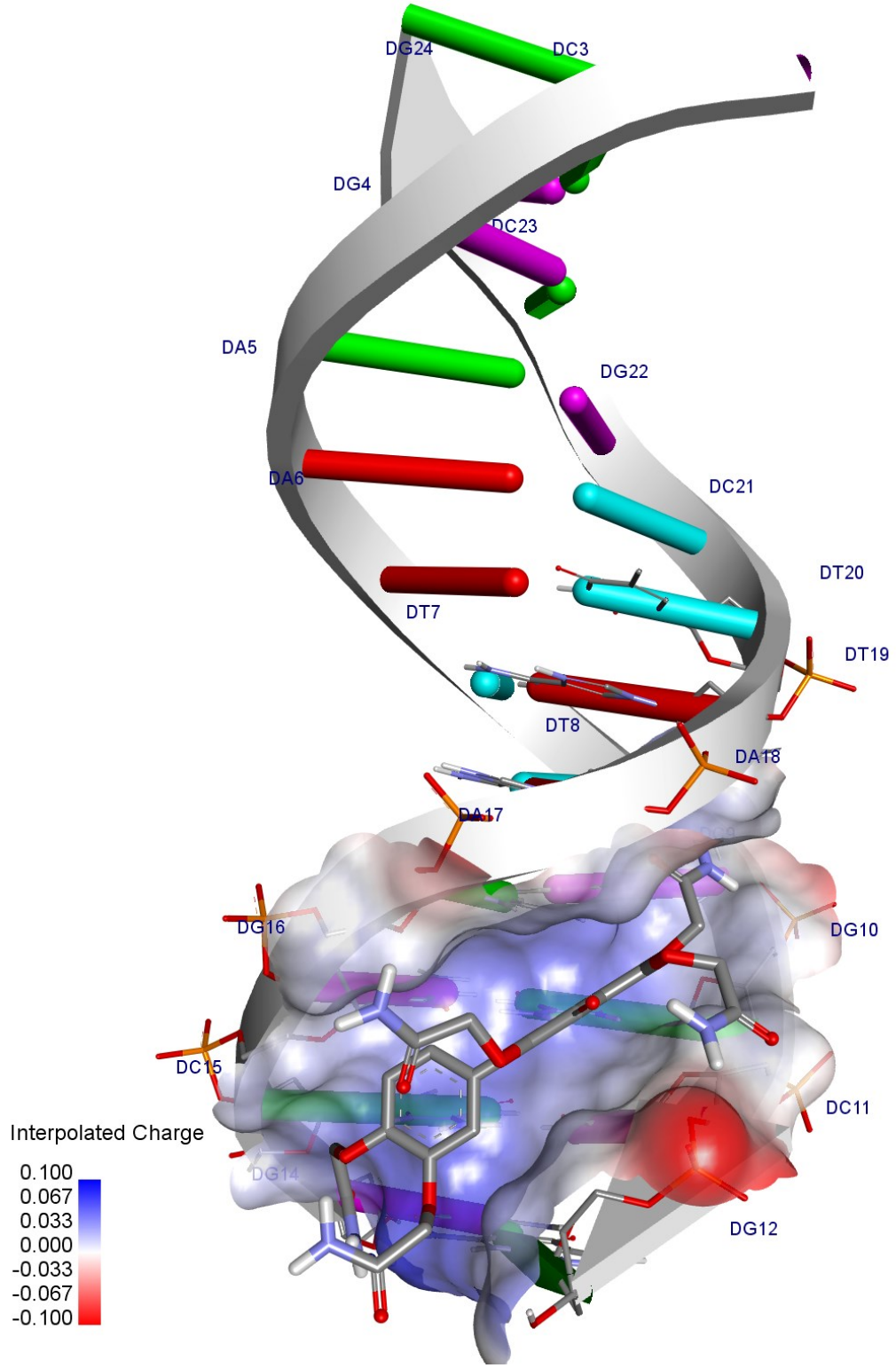

Figure S12. 3D interactions of 1S3 in the active site of DNA with depicting the charge.

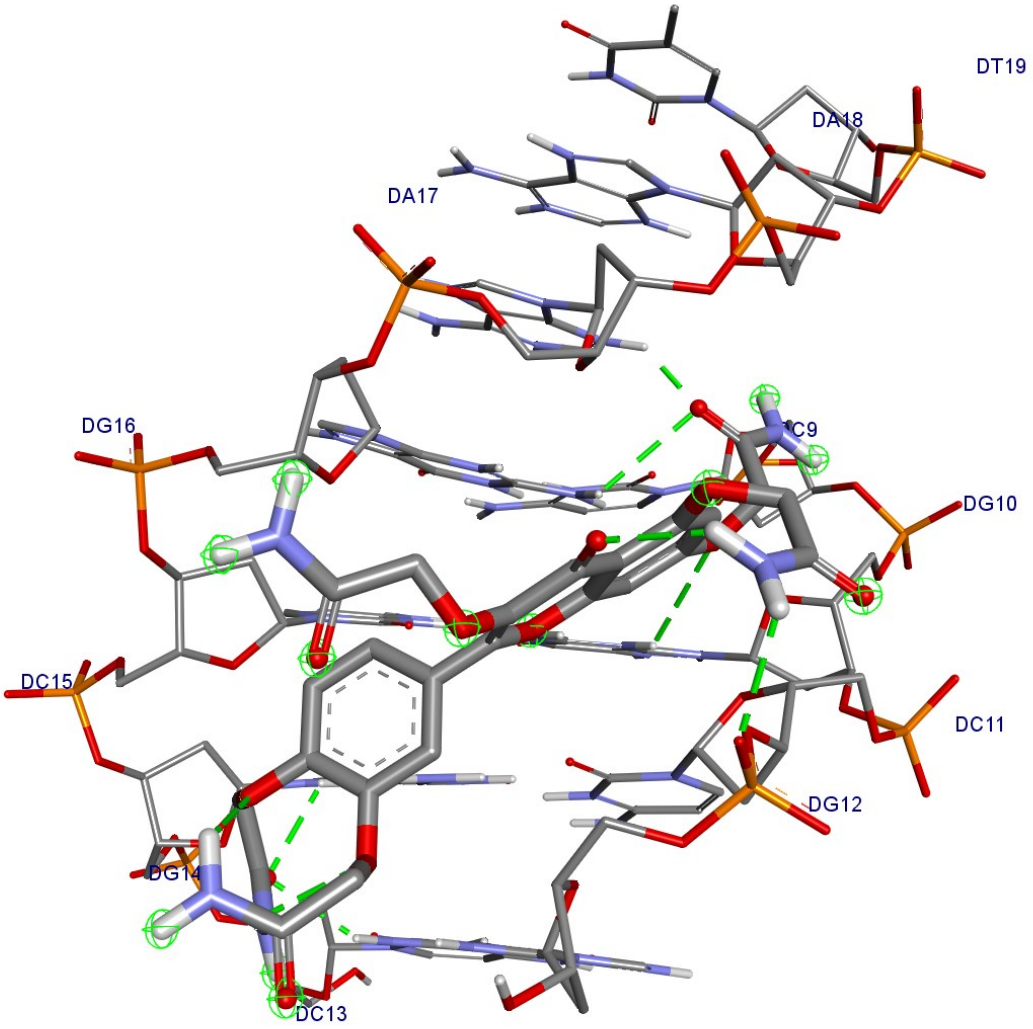

Figure S13. 2D interactions of 1S3 in the active site of DNA with depicting the bonds

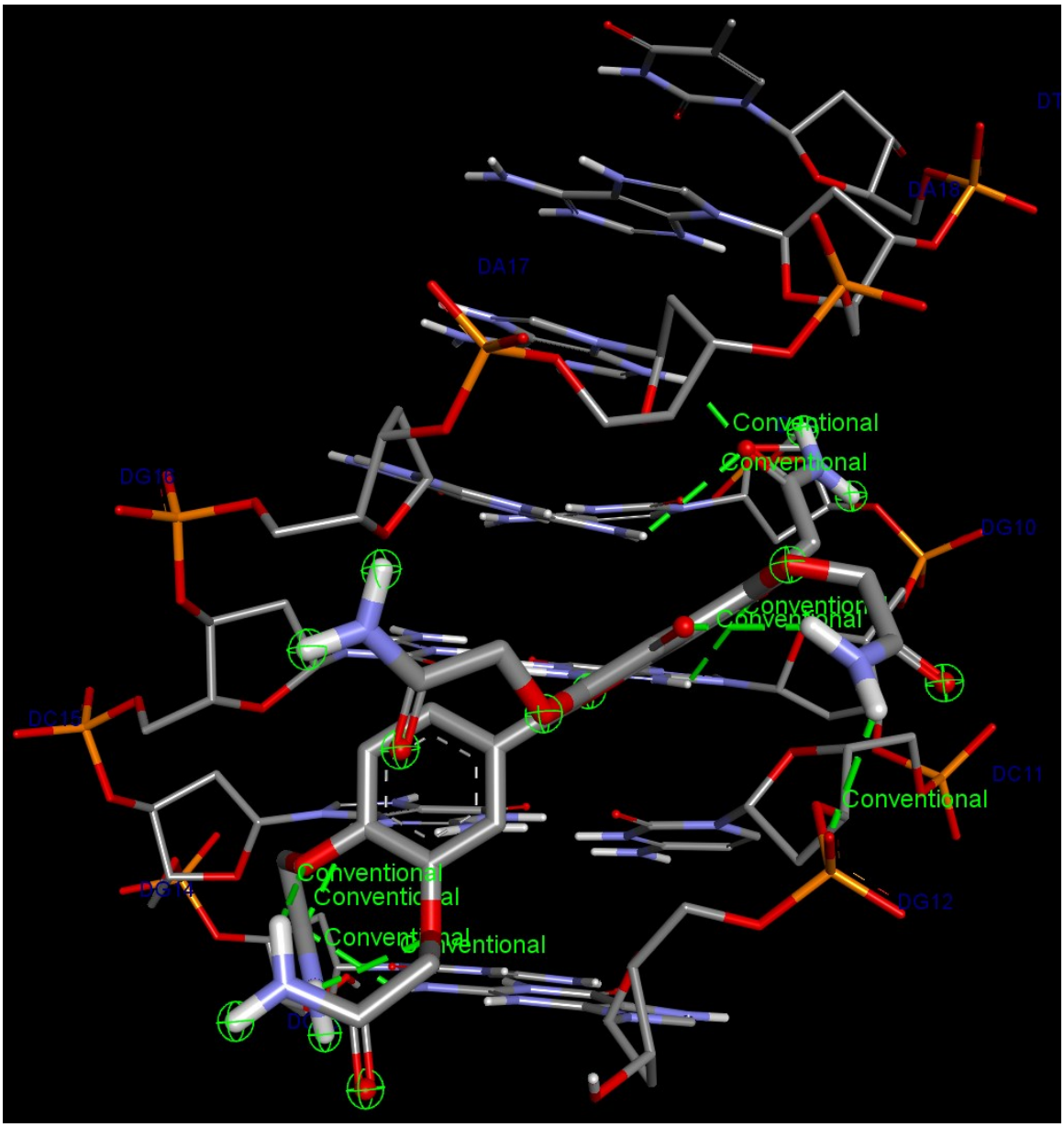

Figure S14. 2D interactions of 1S3 in the active site of DNA with depicting the bond types

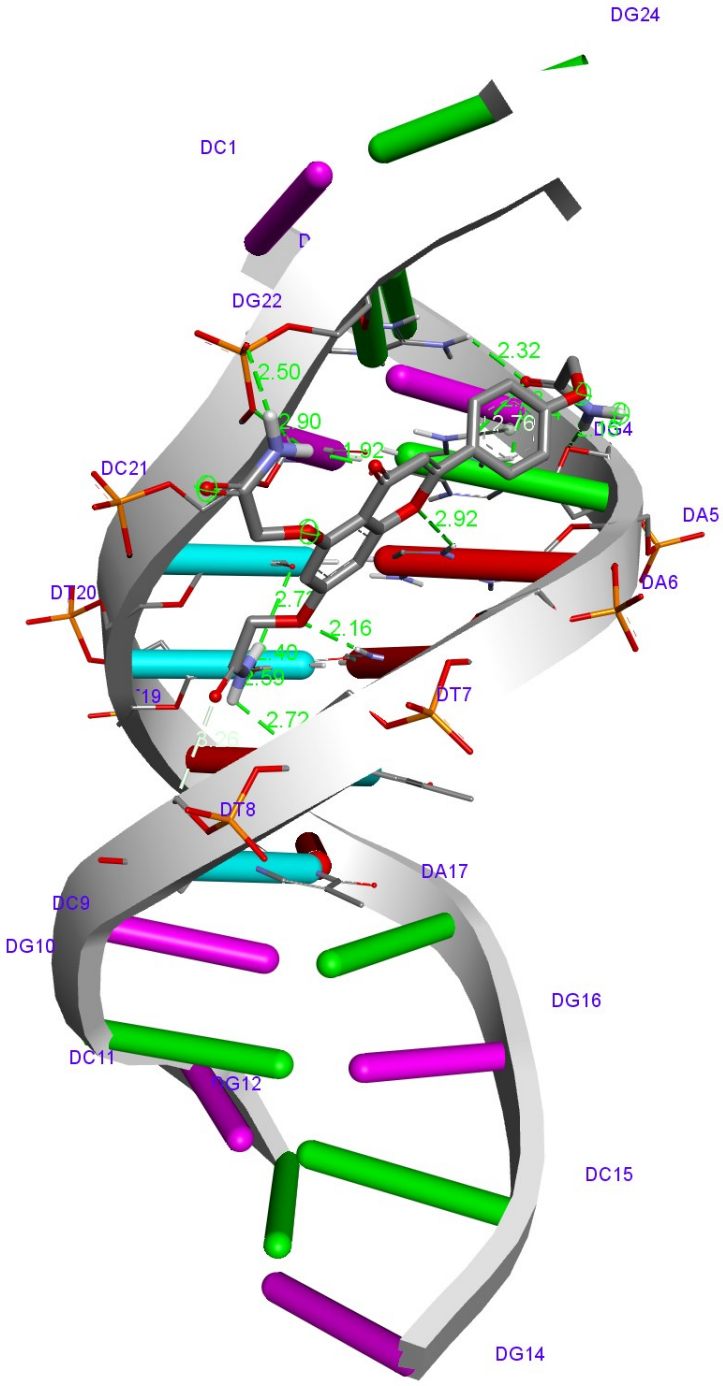

Figure S15. 3D interactions of 2S3 in the active site of DNA with depicting the bond lengths.

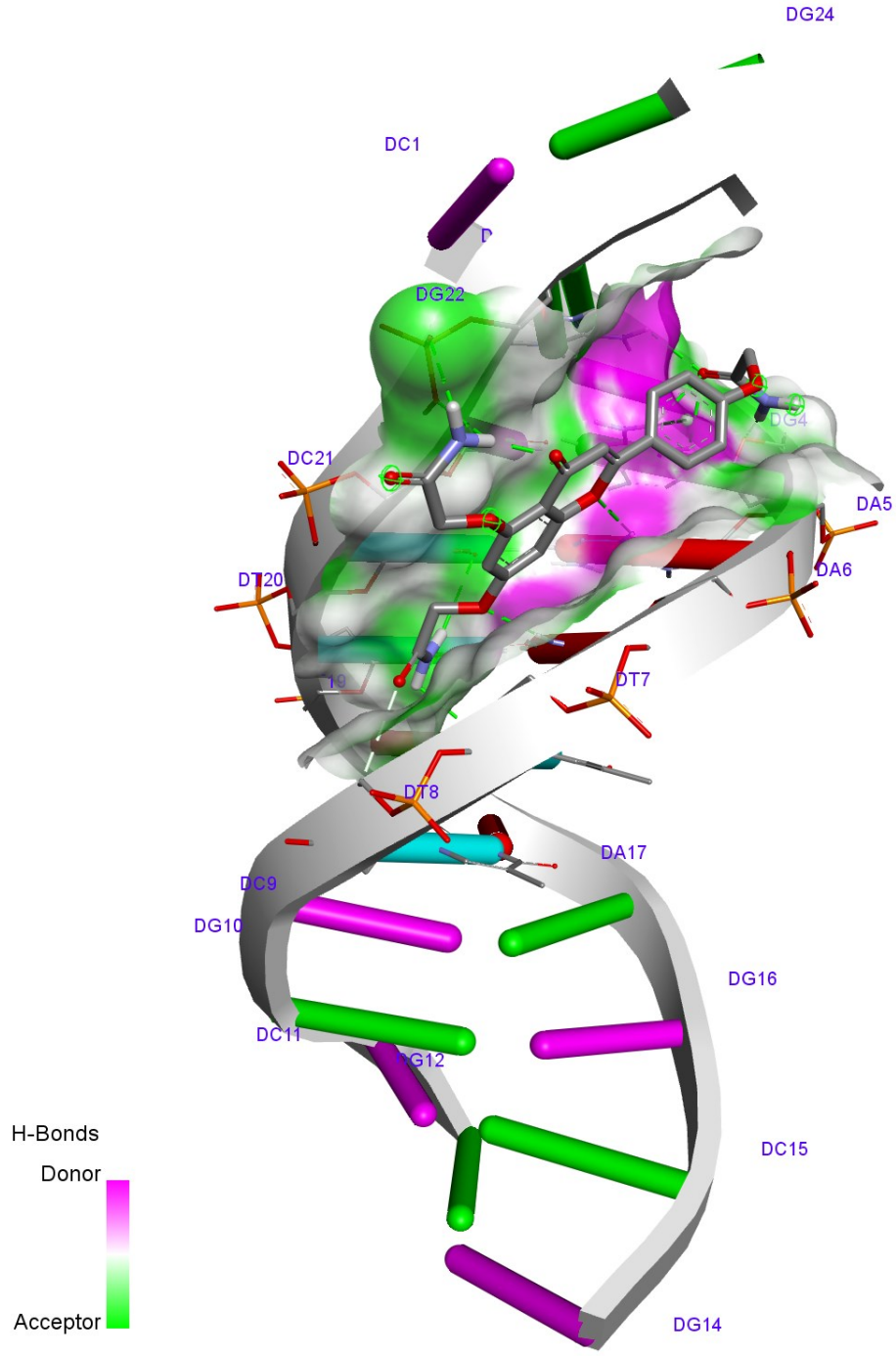

Figure S16. 3D interactions of 2S3 in the active site of DNA with depicting the H-bonds

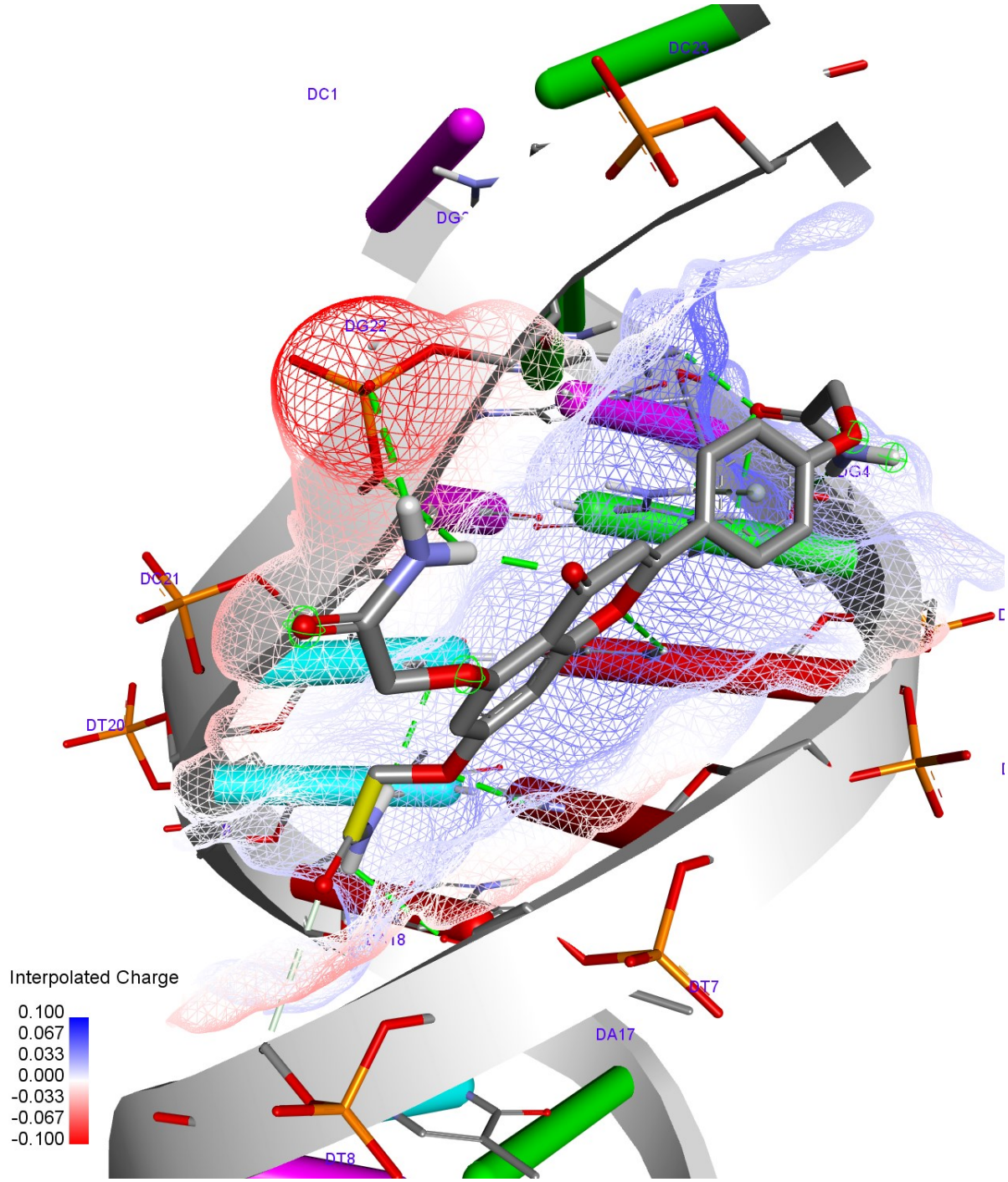

Figure S17. 3D interactions of 2S3 in the active site of DNA with depicting the charge.

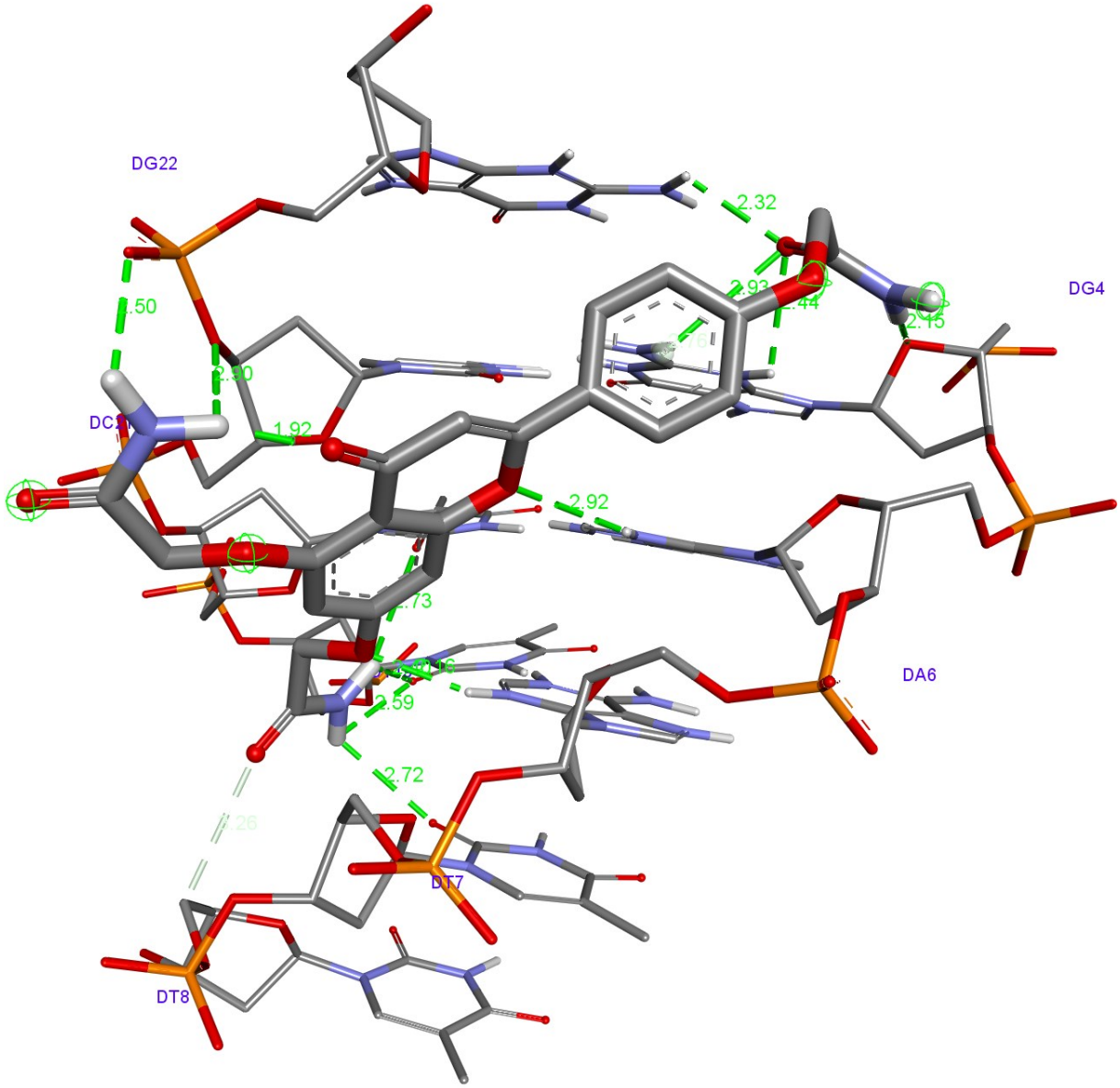

Figure S18. 2D interactions of 2S3 in the active site of DNA with depicting the bonds

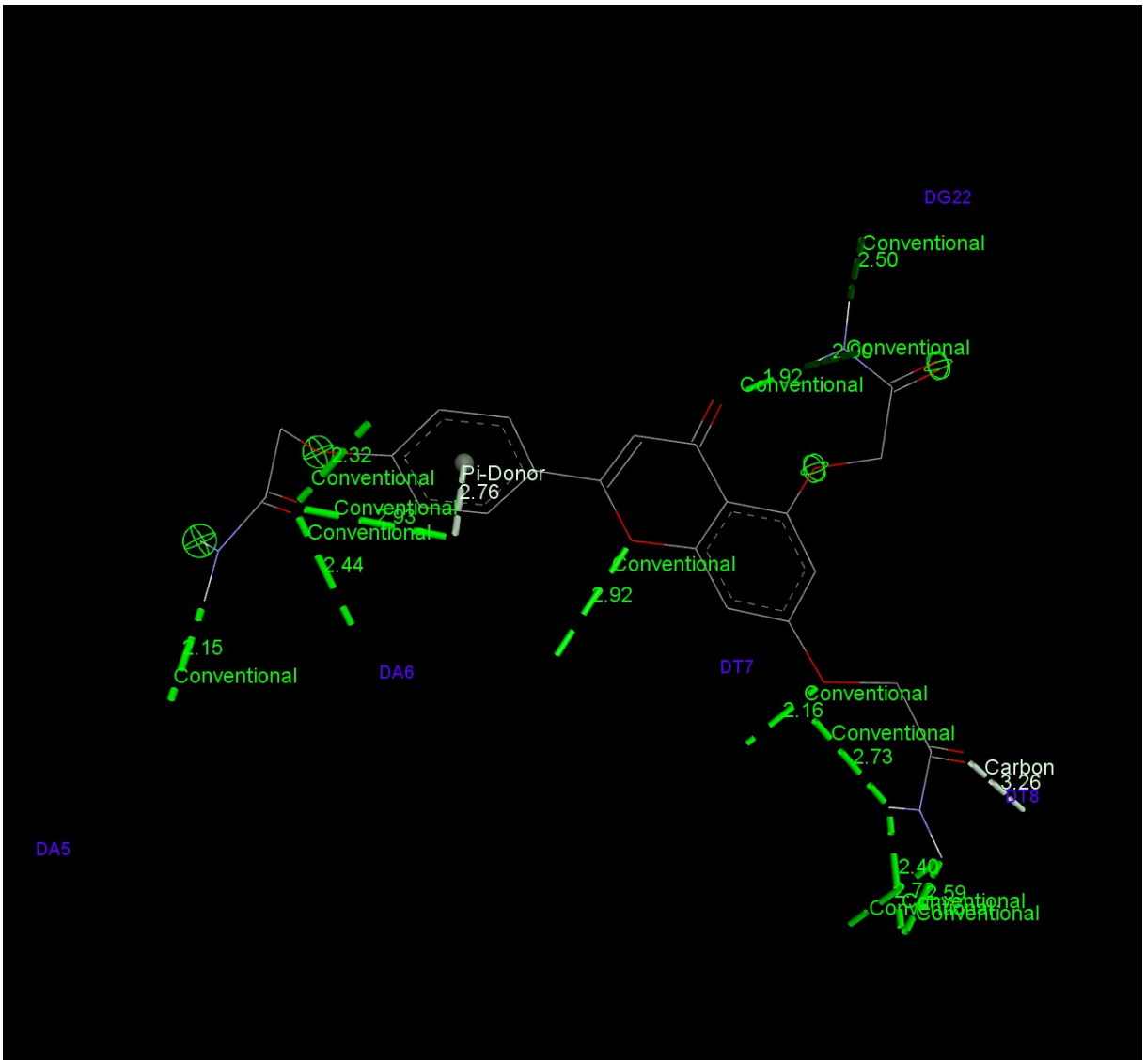

Figure S19. 2D interactions of 2S3 in the active site of DNA with depicting the bond types