Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Antimicrobial and alpha-glucosidase inhibitory flavonoid glycosides from the Plant *Mussaenda recurvata*: *in vitro* and *in silico* approaches

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Table S1. NMR data of **2** and **3**

Carbon number	2 (Astragalin)		3 (Isoquercitrin)	
	δ_C[a,b] ppm	δ_H[a,c] ppm (mult., J in Hz)	δ_C[a,b] ppm	δ_C[a,c] (mult., J in Hz)
2	156.2		156.2	
3	133.2		133.4	
4	177.4		177.5	
5	161.2		161.3	
6	98.7	6.20 (1H, d, 1.8)	98.7	6.20 (1H, d, 1.8)
7	164.2		164.2	
8	93.6	6.42 (1H, d, 1.8)	93.6	6.41 (1H, d, 1.8)
9	156.4		156.4	
10	104.0		104.0	
1'	120.9		121.6	
2'	130.9	8.03 (1H, d, 9.0)	116.3	7.57 (1H, d, 1.8)
3'	115.1	6.88 (1H, d, 9.0)	144.8	
4'	159.9		148.5	
5'	115.1	6.88 (1H, d, 9.0)	115.3	6.85 (1H, d, 9.0)
6'	130.9	8.03 (1H, d, 9.0)	121.2	7.58 (1H, dd, 1.8, 7.8)
5-OH		12.61 (1H, s)		12.63 (1H, s)
1"	100.9	5.45 (1H, d, 7.8)	100.9	5.46 (d, 7.8)

Carbon number	2 (Astragalin)		3 (Isoquercitrin)	
	δ_C[a,b] ppm	δ_H[a,c] ppm (mult., J in Hz)	δ_C[a,b] ppm	δ_C[a,c] (mult., J in Hz)
2"	74.2	3.20 (1H, m)	74.1	3.25 (1H, m)
3"	76,4	3.21 (1H, m)	76.5	3.21 (1H, m)
4"	69.9	3.09 (1H, m)	70.0	3.09 (1H, m)
5"	77.5	3.08 (1H, m)	77,6	3.09 (1H, m)
6"	60.8	3.56 (1H, dd, 11.4, 4.2) 3.33 (1H, m)	61.0	3.58 (d, 11.4) 3.34 (d, 10.8)

[a] Recorded in DMSO-d_6, [b]150 MHz, [c]600 MHz, [d]125 MHz, [e]500 MHz

Table S2. NMR data of **5-7**

Carbon number	5 (Rutin)		6 (Hesperidin)		7 (Neohesperidin)	
	δ_C[a,c] ppm	δ_H[a,d] ppm (mult., J in Hz)	δ_C[b,e] ppm	δ_C[b,f] (mult., J in Hz)	δ_C[b,c] ppm	δ_C[b,d] (mult., J in Hz)
2	159.3		78.3	5.50 (1H, dd, 12.0; 3.0)	78.6	5.51 (1H, dd, 12.0, 3.0)
3	135.6		42.0	3.25 (1H, m) 2.78 (1H, dd, 17.4; 3.0)	42.1	3.24 (1H, m) 2.77 (1H, dd, 17.5; 3.5)
4	179.4		196.9		197.0	
5	162.9		162.9		163.0	
6	99.9	6.23 (1H, d, 2.0)	96.3	6.11 (1H, d, 2.4)	96.4	6.12 (1H, d, 2.0)
7	166.0		165.0		165.1	
8	94.8	6.42 (1H, d, 2.0)	95.5	6.14 (1H, d, 2.4)	95.5	6.13 (1H, d, 2.0)
9	158.5		162.4		162.5	
10	105.6		103.2		103.3	
1'	123.1		130.8		130.4	

Carbon number	5 (Rutin)		6 (Hesperidin)		7 (Neohesperidin)	
	δ_C[a,c] ppm	δ_H[a,d] ppm (mult., J in Hz)	δ_C[b,e] ppm	δ_C[b,f] (mult., J in Hz)	δ_C[b,c] ppm	δ_C[b,d] (mult., J in Hz)
2'	117.7	7.69 (1H, d, 2.5)	114.0	6.93 (1H, d, 2.4)	114.1	6.92 (1H, d, 2.5)
3'	145.8		146.4		146.4	
4'	149.8		147.8		147.9	
5'	116.0	6.90 (1H, d, 8.5)	112.0	6.94 (1H, d, 8.4, 2.4)	112.0	6.94 (1H, d, 8.0, 2.0)
6'	123.5	7.65 (1H, dd, 8.5, 2.0)	117.7	6.89 (1H, d, 8.4)	117.6	6.90 (1H, d, 8.0)
5-OH				12.63 (1H, s)		12.00 (1H, s)
4'-OMe			55.6	3.77 (3H, s)	55.7	3.76 (3H, s)
1"	104.7	5.13 (1H, d, 8.0)	99.3	4.96 (1H, d, 7.8)	99.4	4.96 (1H, d, 7.5)
2"	75.7	3.51 (1H, d, 8.0)	72.9	3.22 (1H, m)	76.2	3.28 (1H, m)
3"	77.2	3.34 (1H, m)	76.2	3.26 (1H, m)	75.8	3.48* (1H)
4"	71.4	3.30 (1H, d, 9.5)	72.0	3.15 (1H, m)	73.0	3.12 (1H, m)
5"	78.1	3.43 (1H, d, 9.0)	75.4	3.53 (1H, m)	75.5	3.51*(1H)
6"	68.5	3.42 (1H, dd, 11.0, 5.0) 3.83 (1H, dd, 11.0,1.0)	66.0	3.42 (1H, dd, 12.0, 6.0) 3.79 (1H, d, 10.4)	62.6	3.78 (1H, m) 3.35 (1H, m)
1"'	102.4	4.54 (1H, d, 1.5)	100.5	4.52 (1H, s)	100.6	4.52 (1H, brs)
2"'	72.1	3.66 (1H, dd, 3.5, 1.5)	69.5	3.13 (1H, m)	70.2	3.62 (1H, brs)
3"'	72.2	3.56 (1H, dd, 9.5, 3.5)	70.6	3.43 (1H, m)	70.7	3.42*(1H)
4"'	73.9	3.31 (1H, d, 8.5)	70.2	3.30 (1H, m)	72.0	3.16 (1H, m)
5"'	69.7	3.47 (1H, m)	68.2	3.63 (1H, m)	69.6	3.13 (1H, m)
6"'	17.8	1.14 (3H, d, 6.0)	17.7	1.08 (3H, d, 6.6)	17.7	1.00 (3H, d, 6.0)

[a] Recorded in MeOD-d_4, [b]Recorded in DMSO-d_6 , [c]125 MHz, [d]500 MHz , [e]150 MHz, [f]600 MHz, [*]overlap

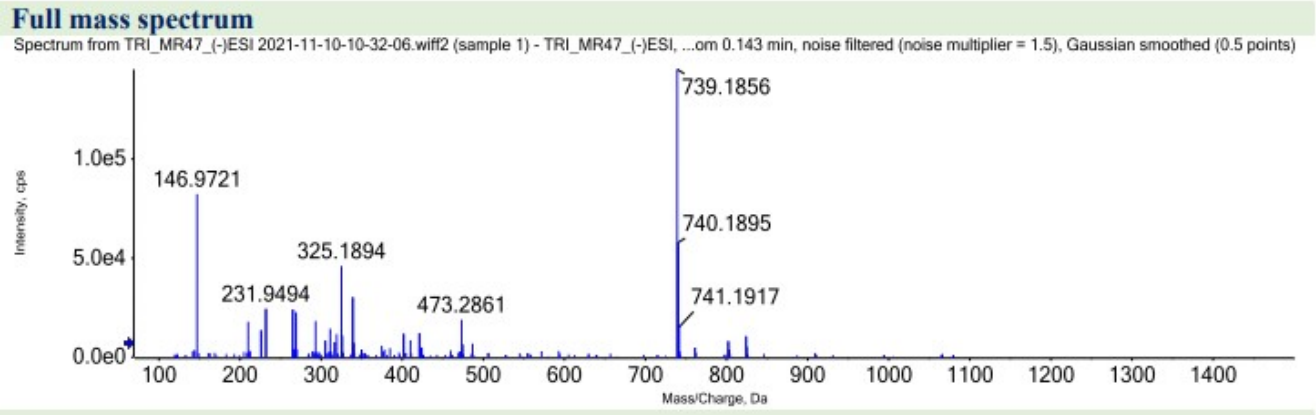


Figure S1. HRESIMS of **1**

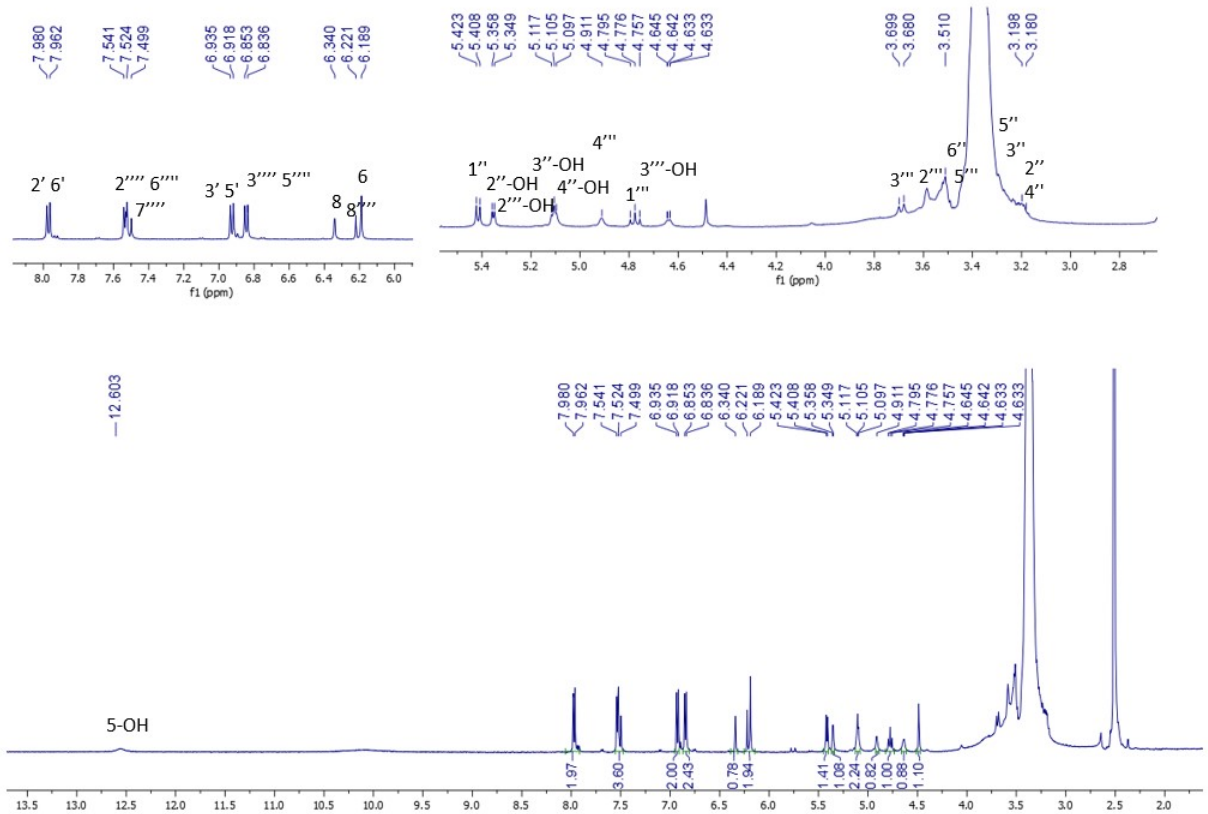


Figure S2. [1]H NMR spectrum of **1**

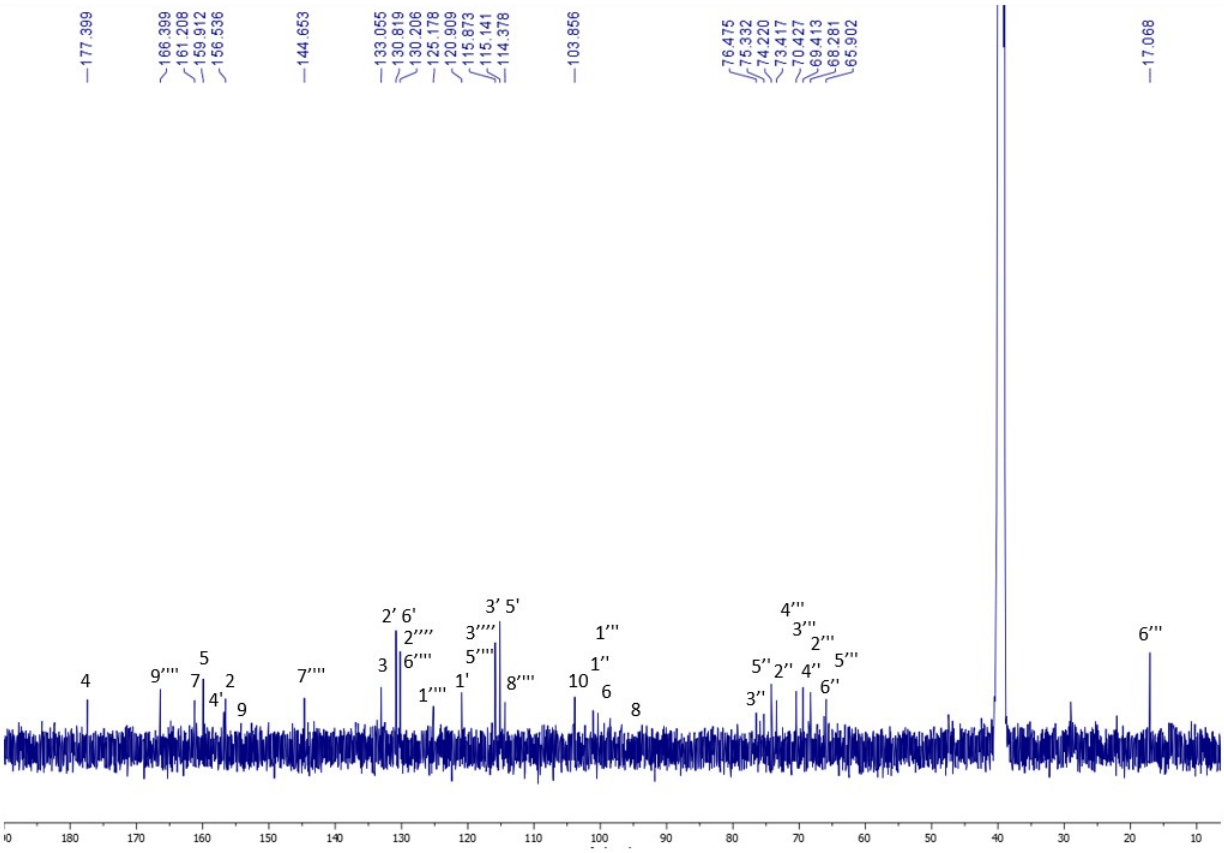


Figure S3. ^{13}C NMR spectrum (JMOD) of **1**

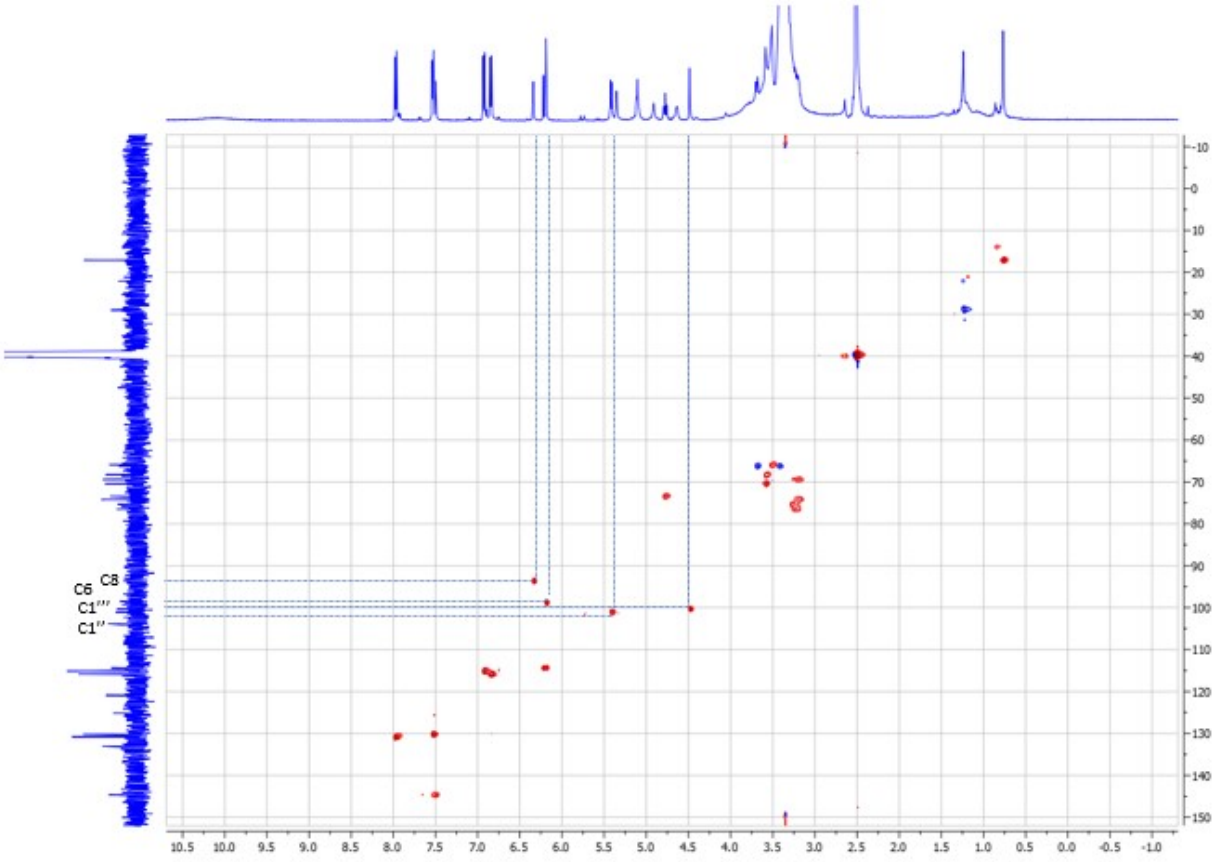


Figure S4. HSQC spectrum of **1**

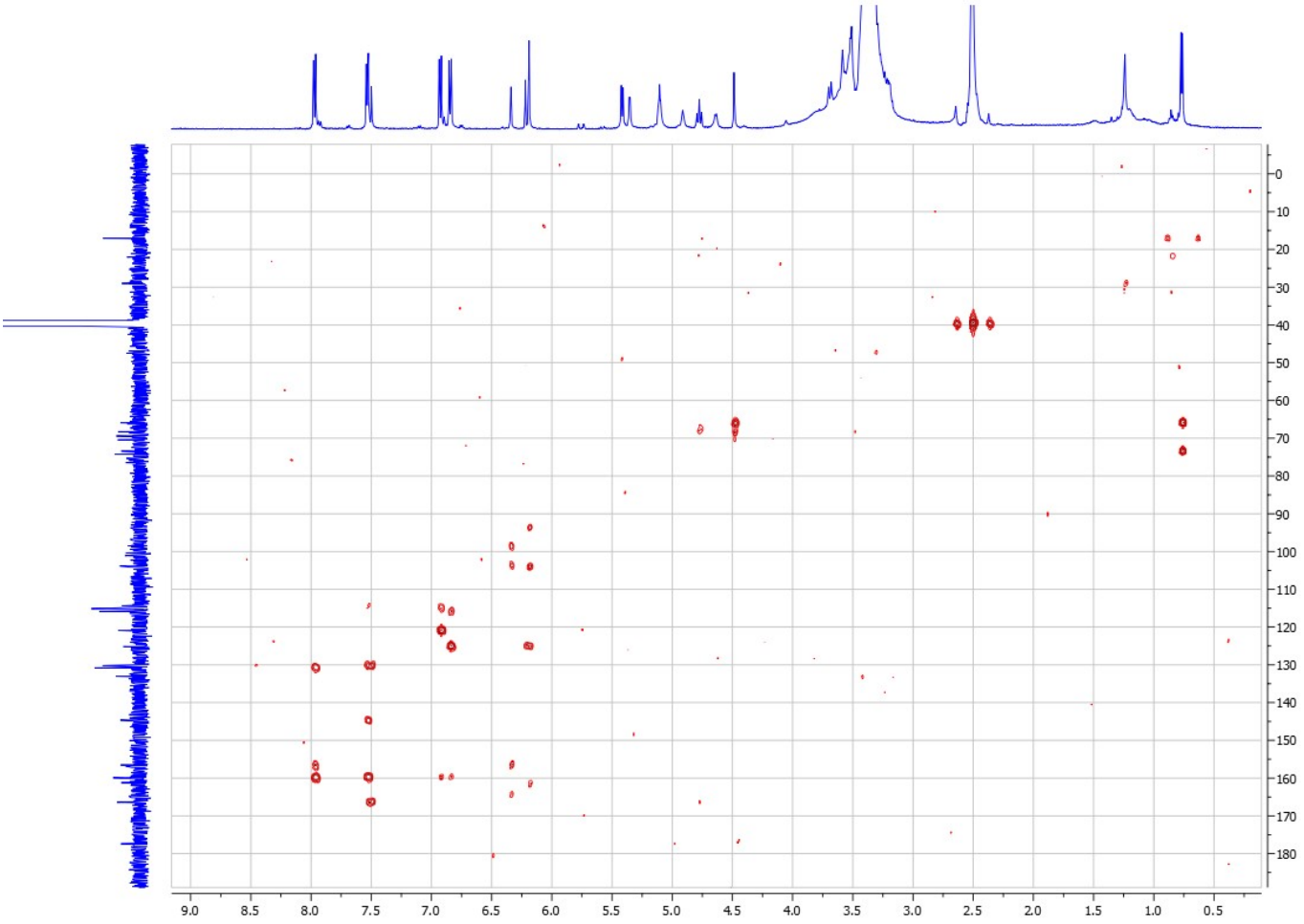


Figure S5. HMBC spectrum of **1**

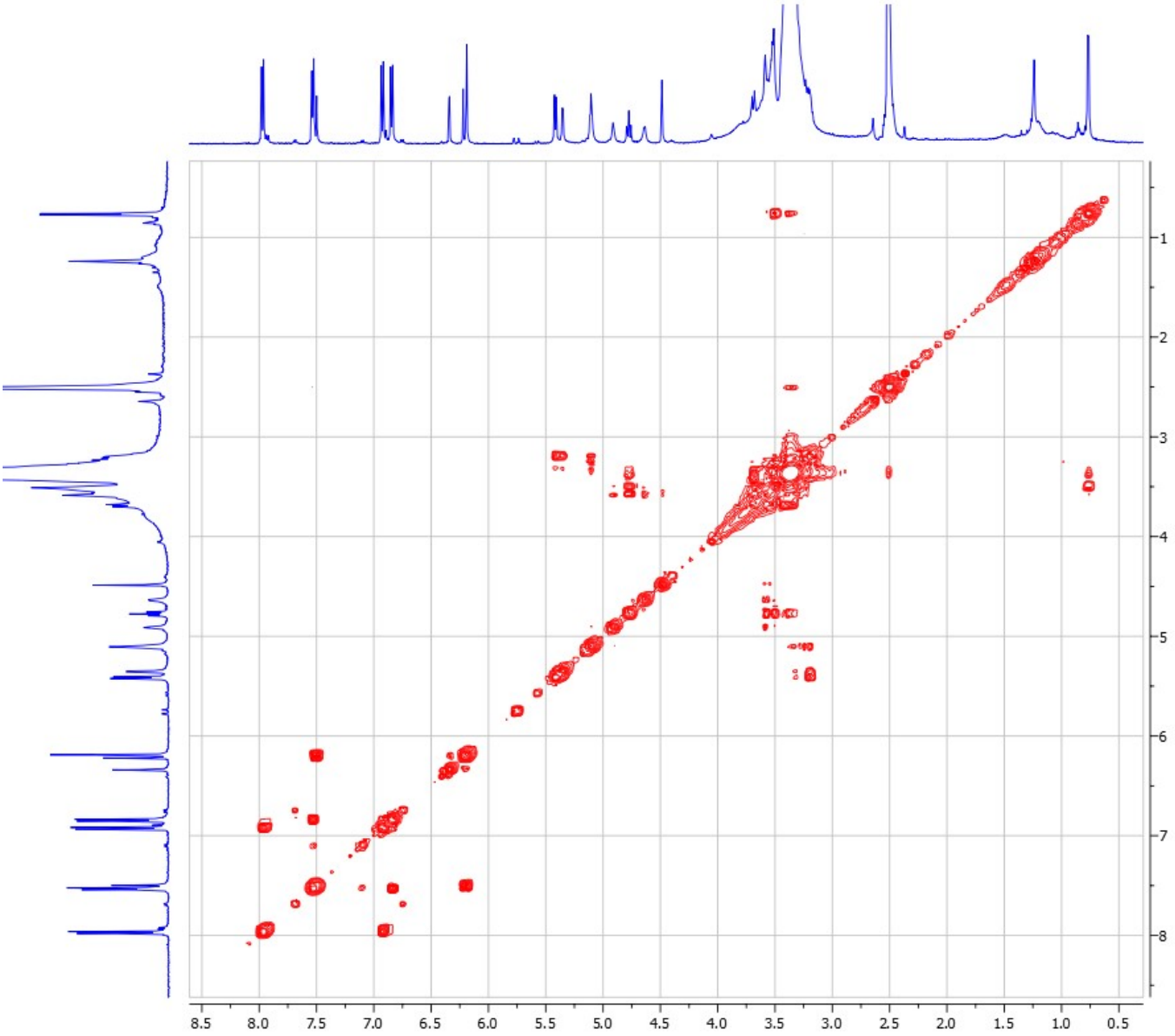


Figure S6. COSY spectrum of **1**

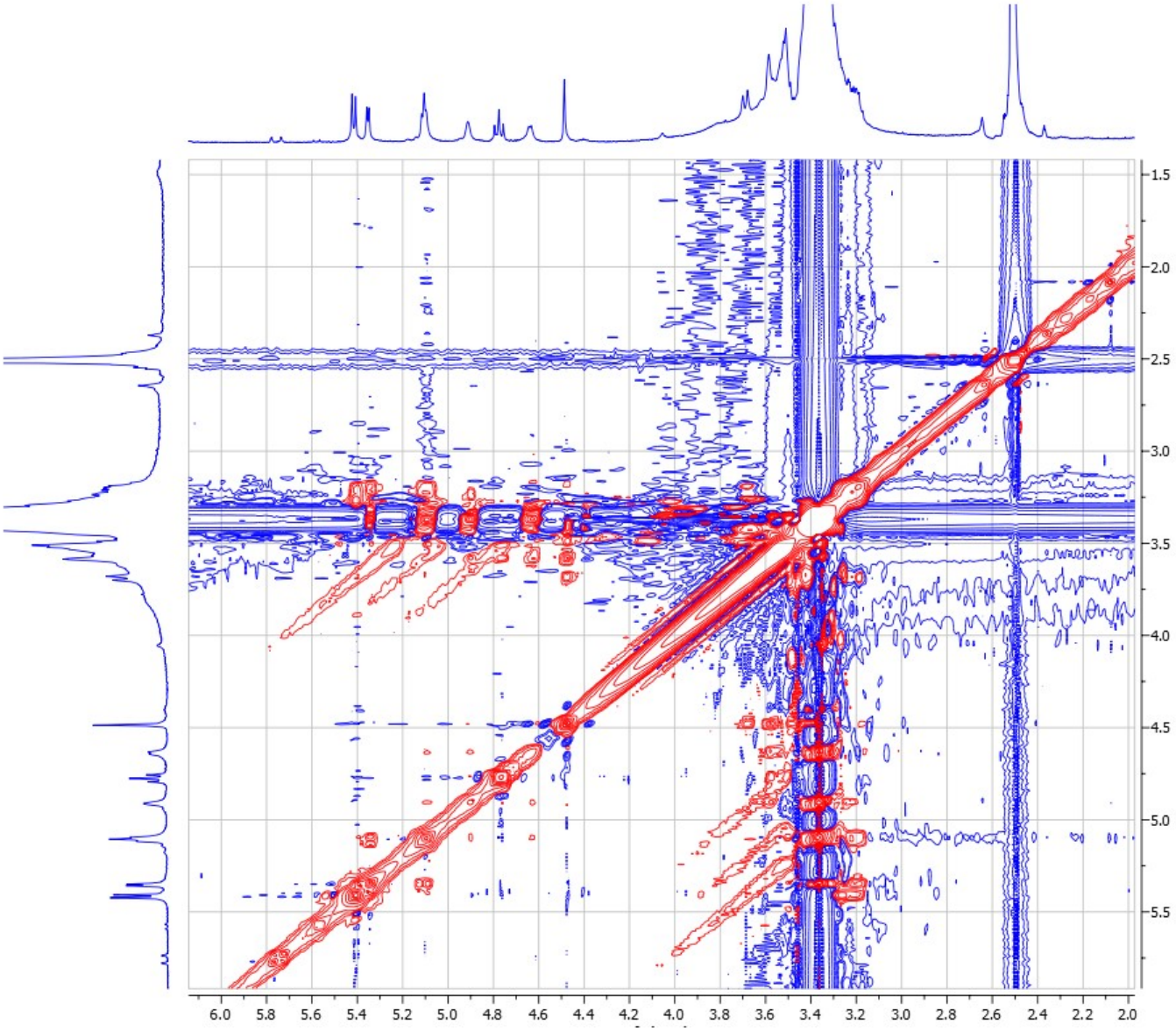


Figure S7. NOESY spectrum of **1**

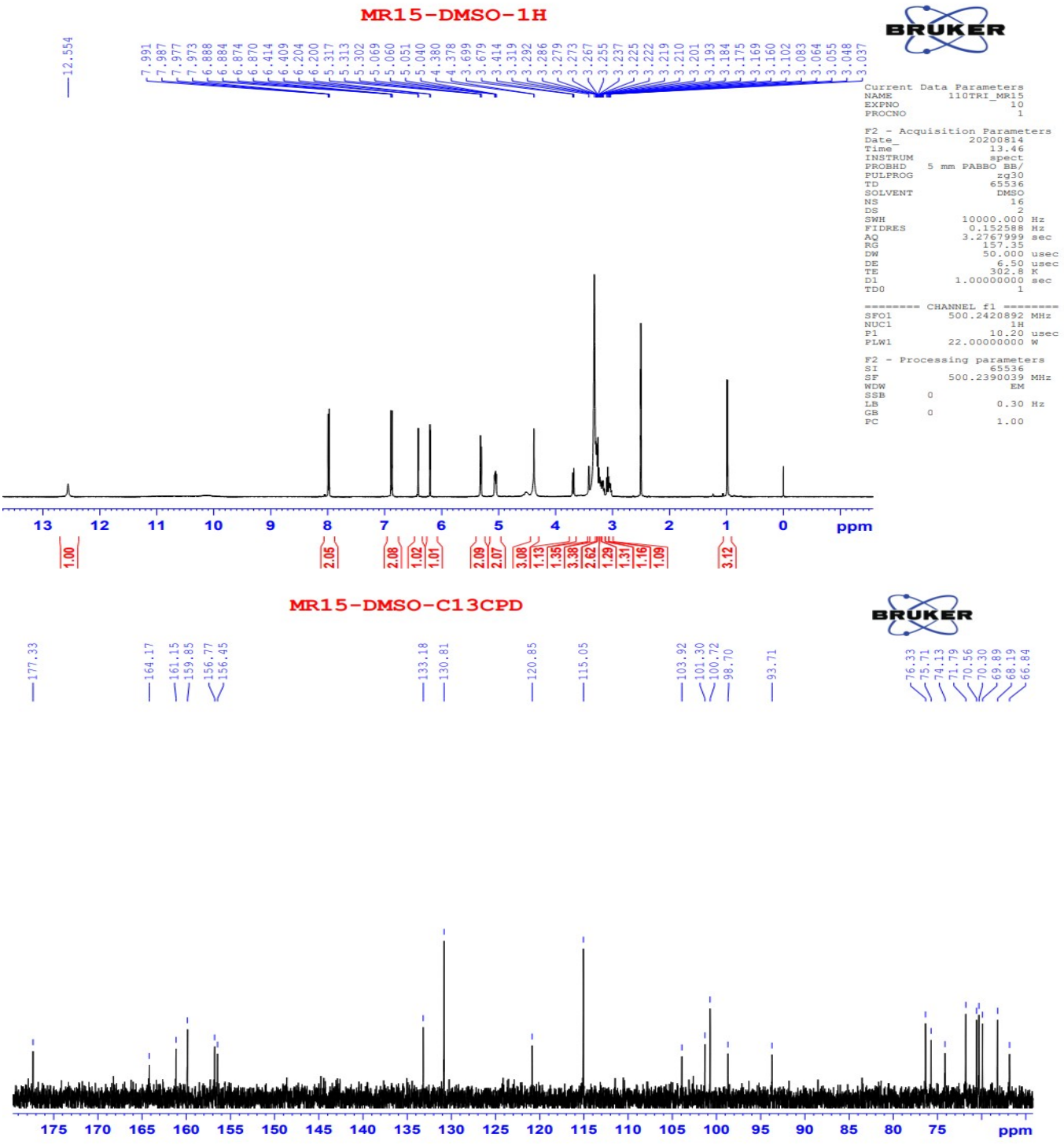


Figure S8. ^{1}H and ^{13}C NMR spectra of **4**

Simulation Details

Jobname: desmond_md_anti-diabetic_20042023
Entry title: Full System

CPU #	Job Type	Ensemble	Temp. [K]	Sim. Time [ns]	# Atoms	# Waters	Charge
1	mdsim	NPT	300.0	100.102	185274	52285	0

Protein Information

Tot. Residues	Prot. Chain(s)	Res. in Chain(s)	# Atoms	# Heavy Atoms	Charge
1784	'A', 'B'	ict_values([892, 892]	27992	14324	-46

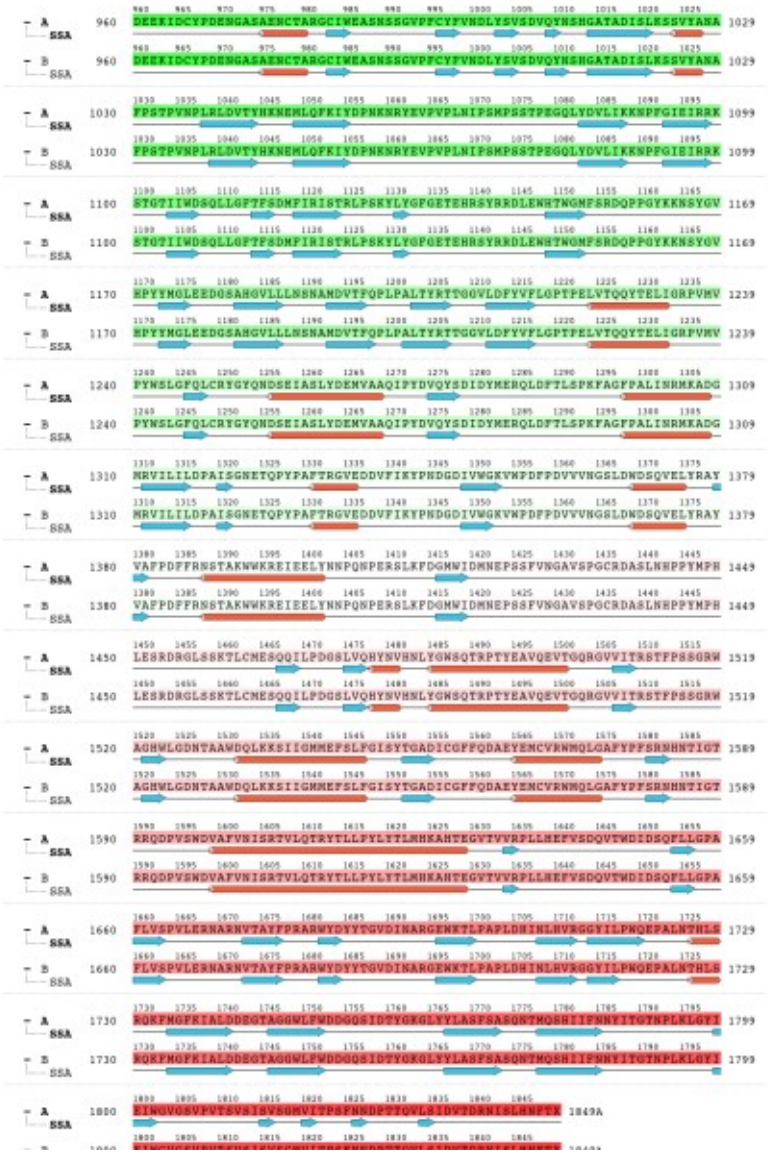
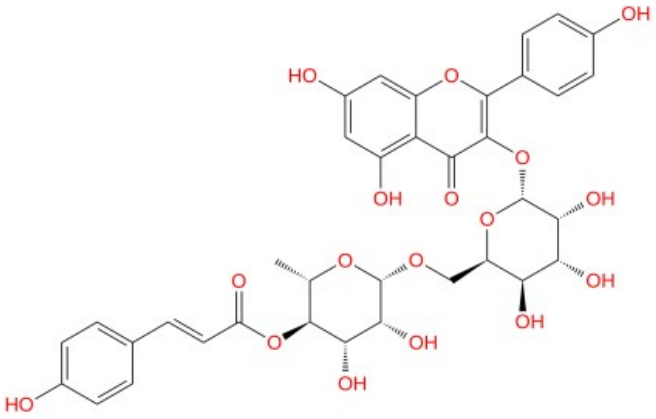


Figure S9. Protein information is indicated Desmond 2018, version 4.

PDB Name	'LIG'
Num. of Atoms	89 (total) 53 (heavy)
Atomic Mass	740.678 au
Charge	0
Mol. Formula	C36H36O17
Num. of Fragments	9
Num. of Rot. Bonds	19



Counter Ion/Salt Information

Figure S10. Ligand information is showed by Desmond 2018 software in Linux or Ubuntu enviroment.

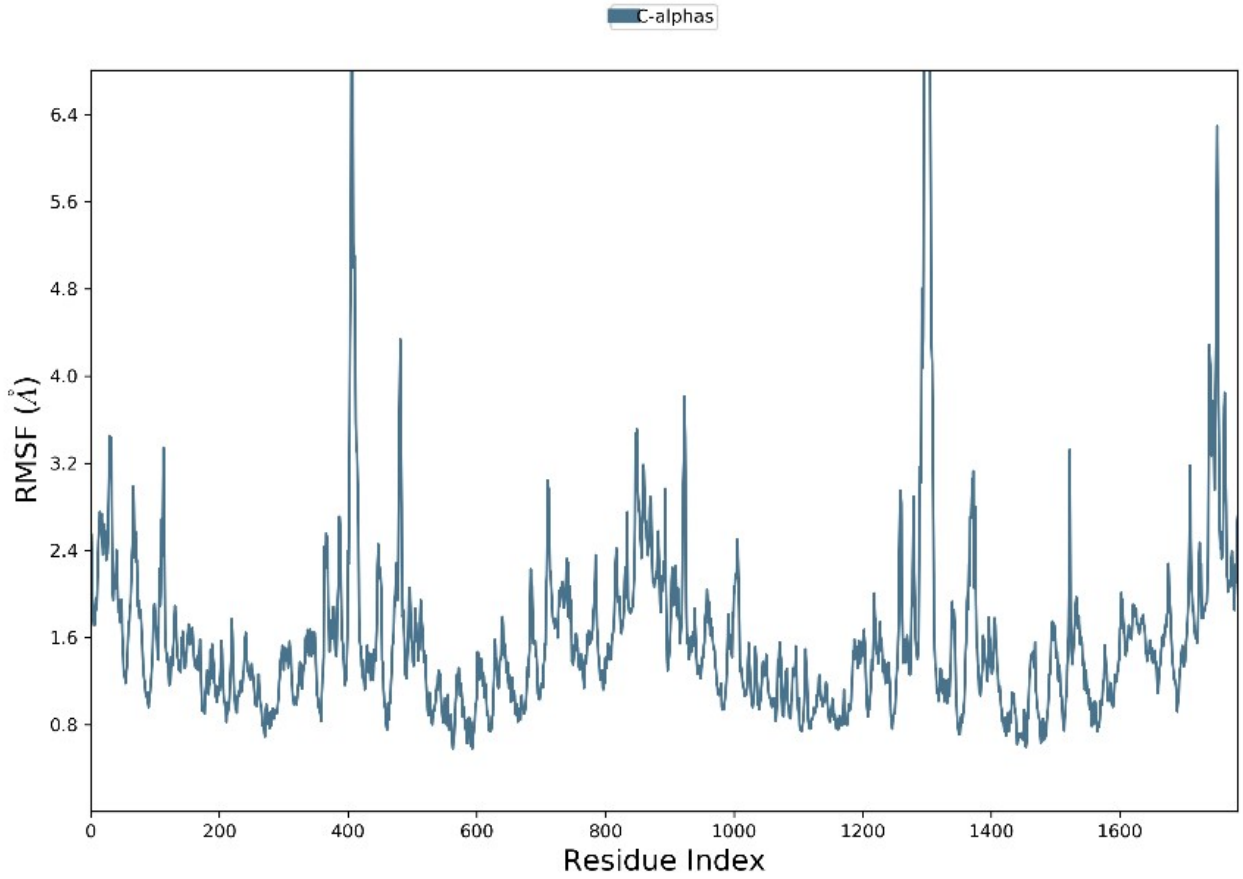


Figure S11. The RMSF (Å) values of 3TOP enzyme

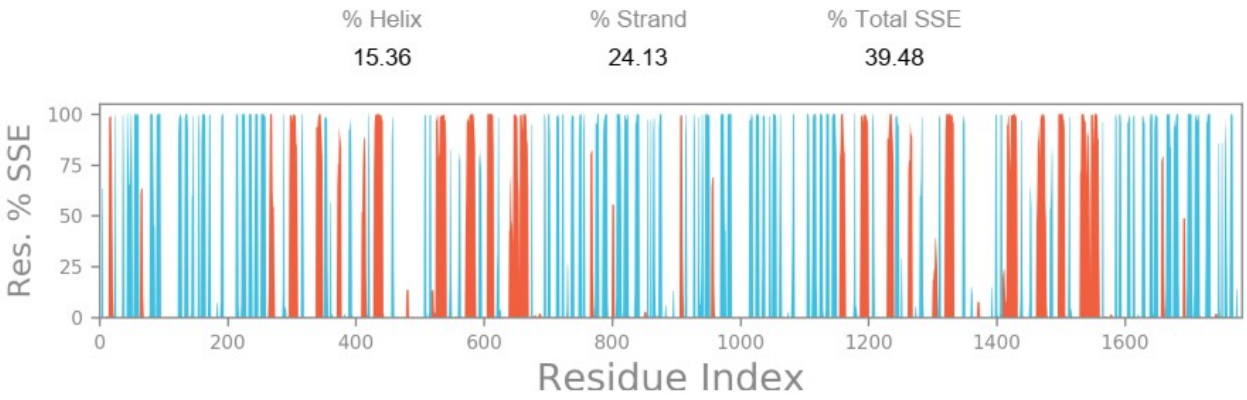


Figure S12. The secondary structure of 3TOP

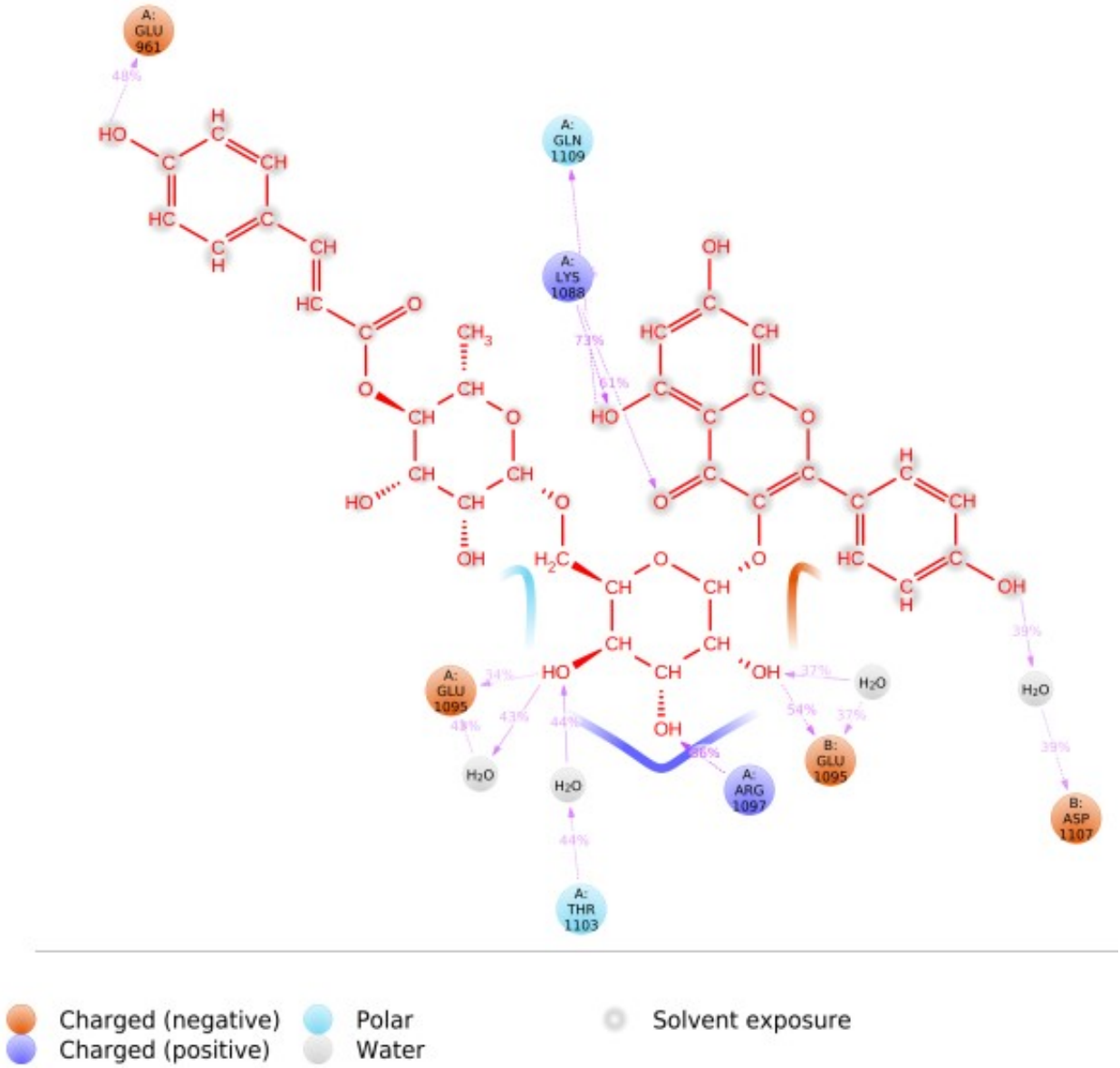


Figure S13. The contacts between pose 472 and 3TOP.

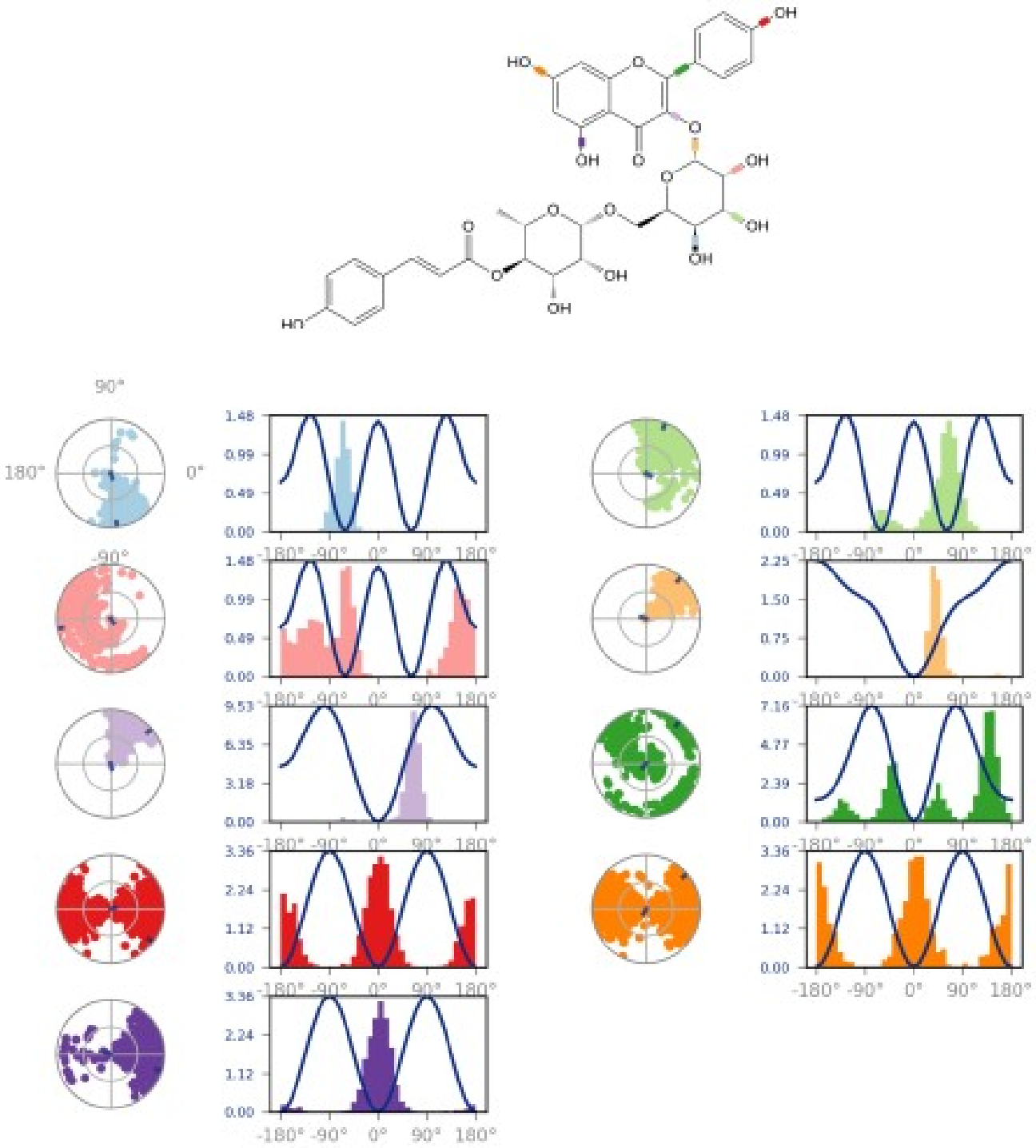


Figure S14. The torsion profile of pose 472.

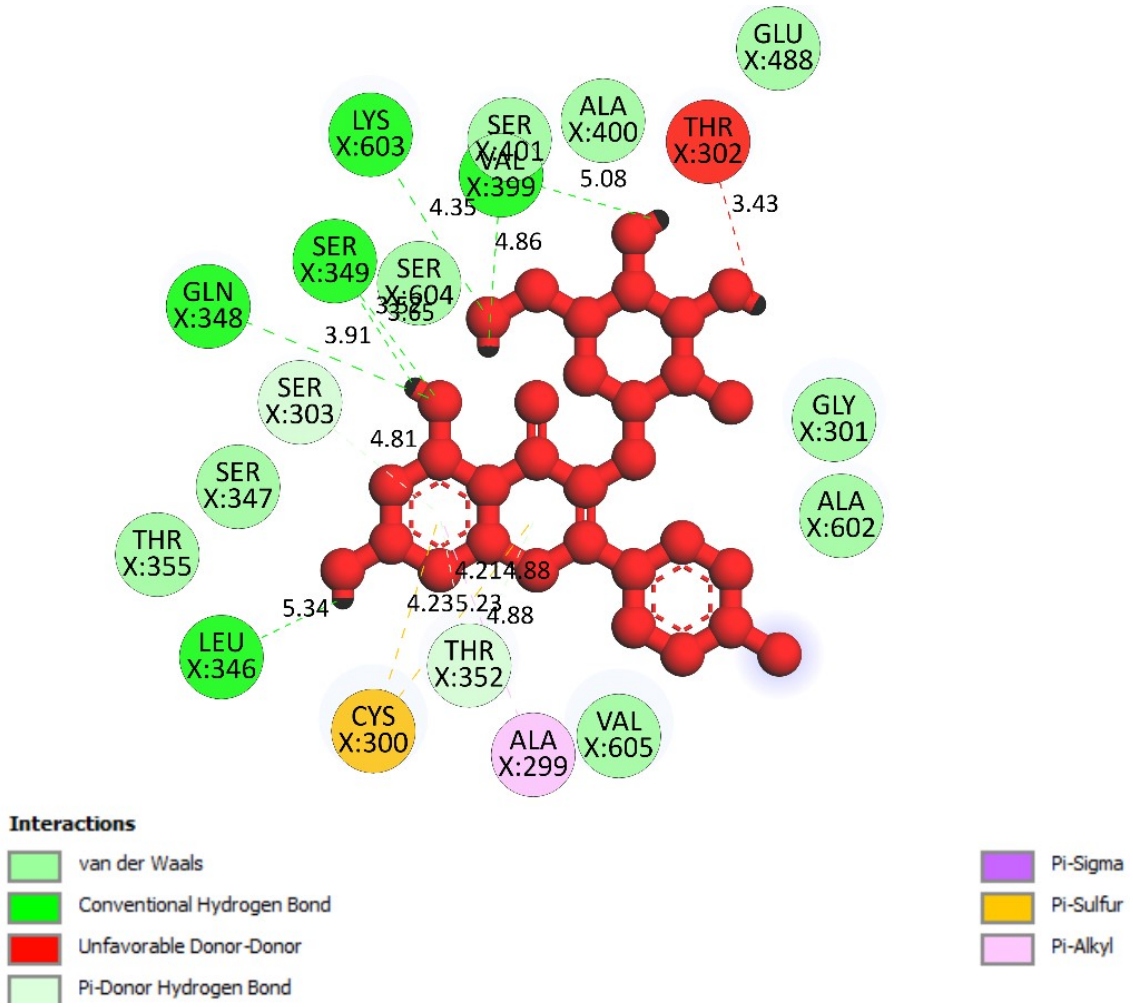


Figure S15. One 2D diagram showed the interactions between pose 305 and 2VF5

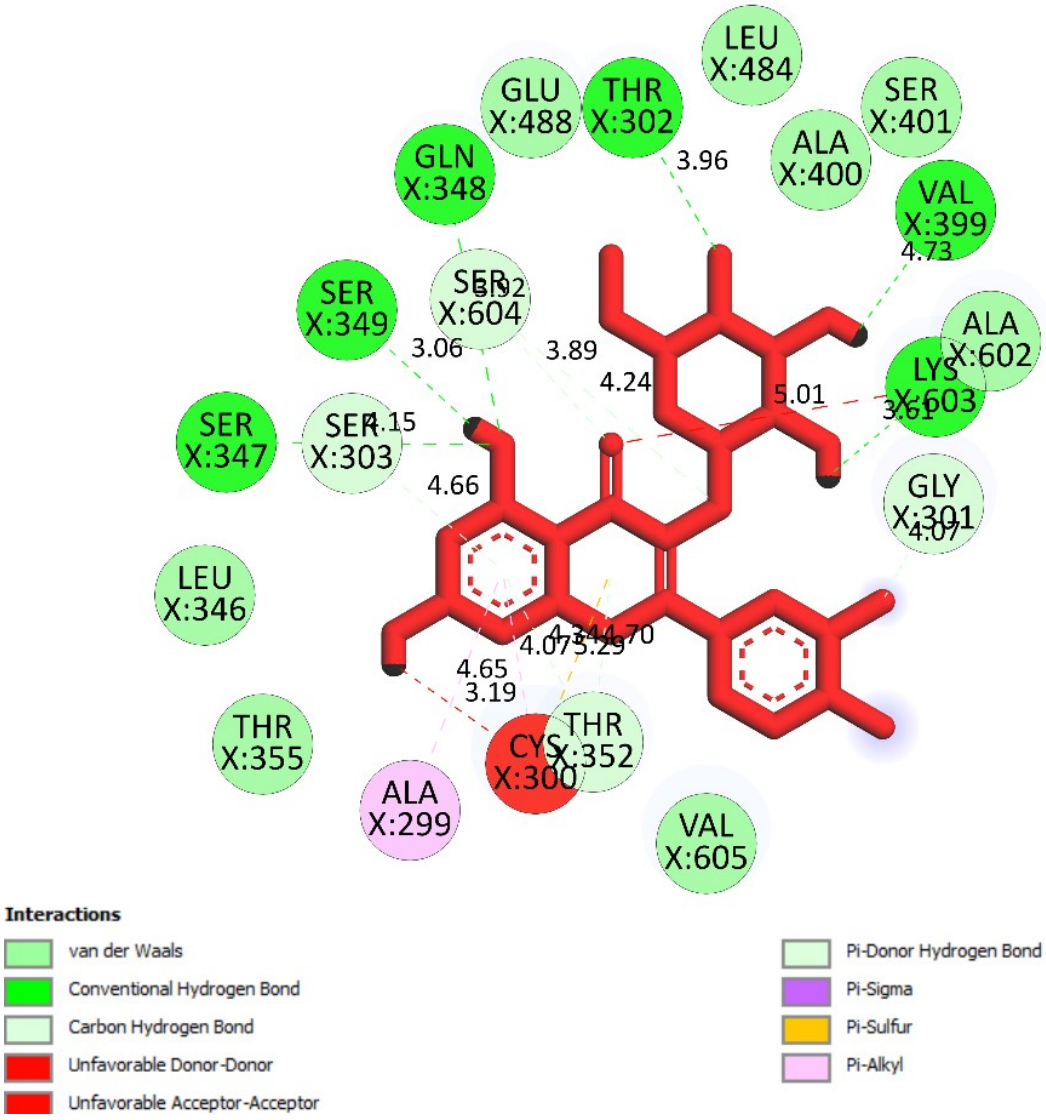


Figure S16. One 2D diagram showed the interactions between pose 387 and 2VF5

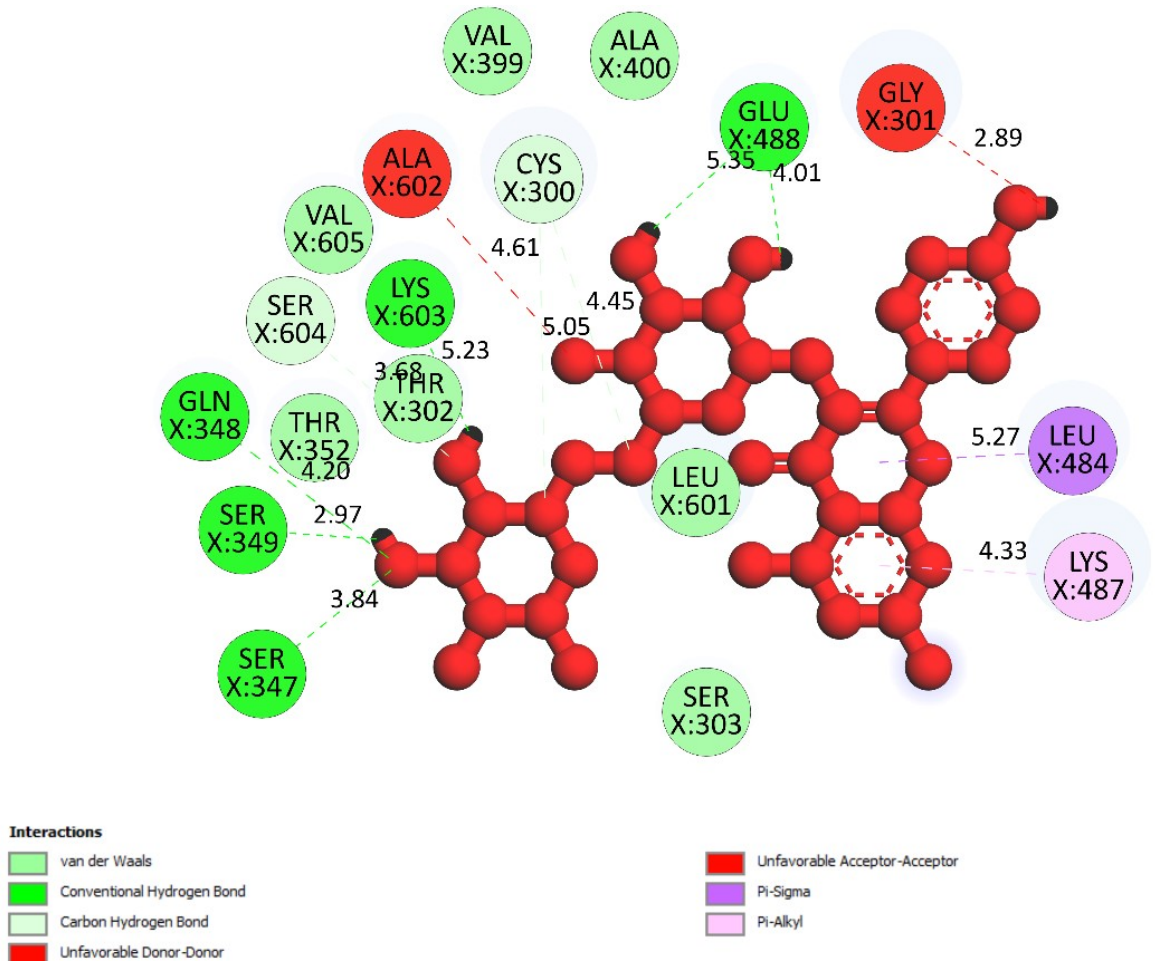


Figure S17. One 2D diagram showed the interactions between pose 136 (compound 4) and 2VF5

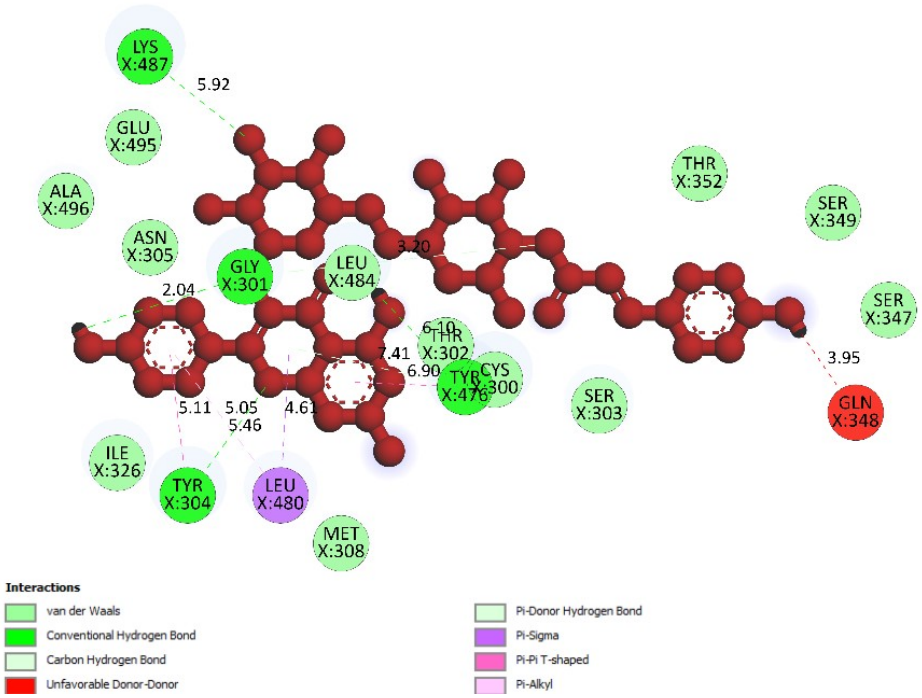
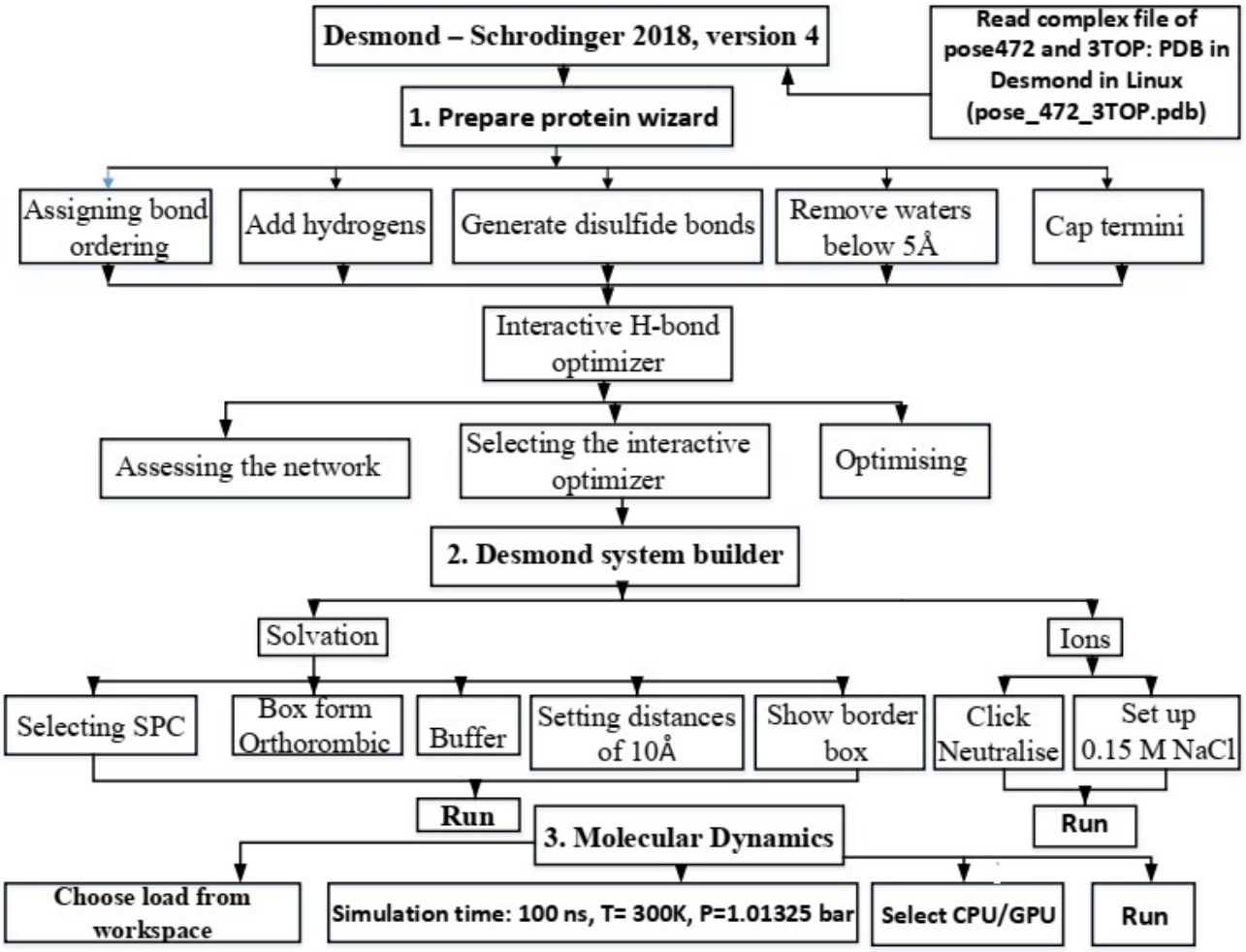


Figure S18. One 2D diagram showed the interactions between pose 43 (compound 1) and 2VF5



Scheme S1. Procedure molecular dynamic of the best docking pose 472 and 3TOP enzyme: PDB.