

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)	
	$\delta_{\text{C}}^{\text{a,b}}$ ppm	$\delta_{\text{H}}^{\text{a,c}}$ ppm (mult., J in Hz)	$\delta_{\text{C}}^{\text{a,b}}$ ppm	$\delta_{\text{C}}^{\text{a,c}}$ (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)	
	$\delta_C^{a,b}$ ppm	$\delta_H^{a,c}$ ppm (mult., J in Hz)	$\delta_C^{a,b}$ ppm	$\delta_C^{a,c}$ (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, ^b150 MHz, ^c600 MHz, ^d125 MHz, ^e500 MHz

Table S2. NMR data of 5-7

Carbon number	5 (Rutin)		6 (Hesperidin)		7 (Neohesperidin)	
	$\delta_C^{a,c}$ ppm	$\delta_H^{a,d}$ ppm (mult., J in Hz)	$\delta_C^{b,e}$ ppm	$\delta_C^{b,f}$ (mult., J in Hz)	$\delta_C^{b,c}$ ppm	$\delta_C^{b,d}$ (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)	
	$\delta_C^{a,c}$ ppm	$\delta_H^{a,d}$ ppm (mult., J in Hz)	$\delta_C^{b,e}$ ppm	$\delta_C^{b,f}$ (mult., J in Hz)	$\delta_C^{b,c}$ ppm	$\delta_C^{b,d}$ (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)	66.0	3.42 (1H, dd, 12.0, 6.0)	62.6	3.78 (1H, m)
		3.83 (1H, dd, 11.0, 1.0)		3.79 (1H, d, 10.4)		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, ^c125 MHz, ^d500 MHz, ^e150 MHz, ^f600 MHz,
*overlap

Full mass spectrum

Spectrum from TRI_MR47_(-)ESI 2021-11-10-10-32-06.wiff2 (sample 1) - TRI_MR47_(-)ESI, ...om 0.143 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)

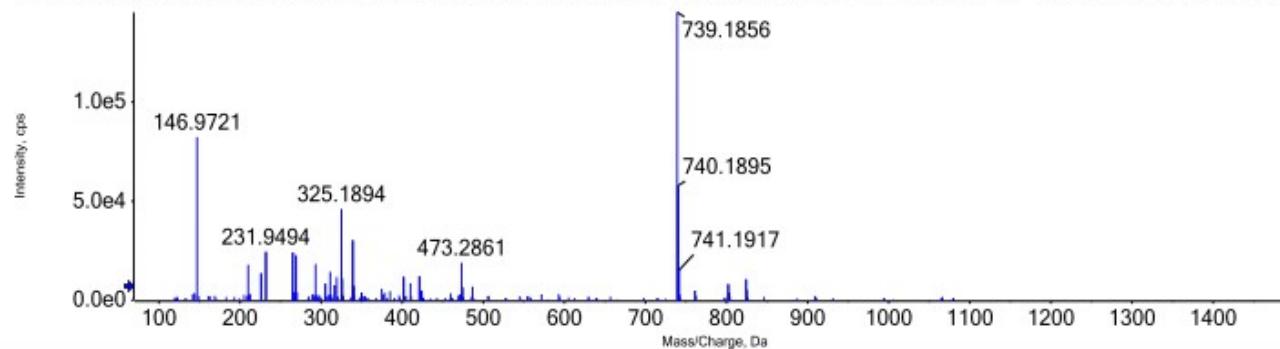


Figure S1. HRESIMS of 1

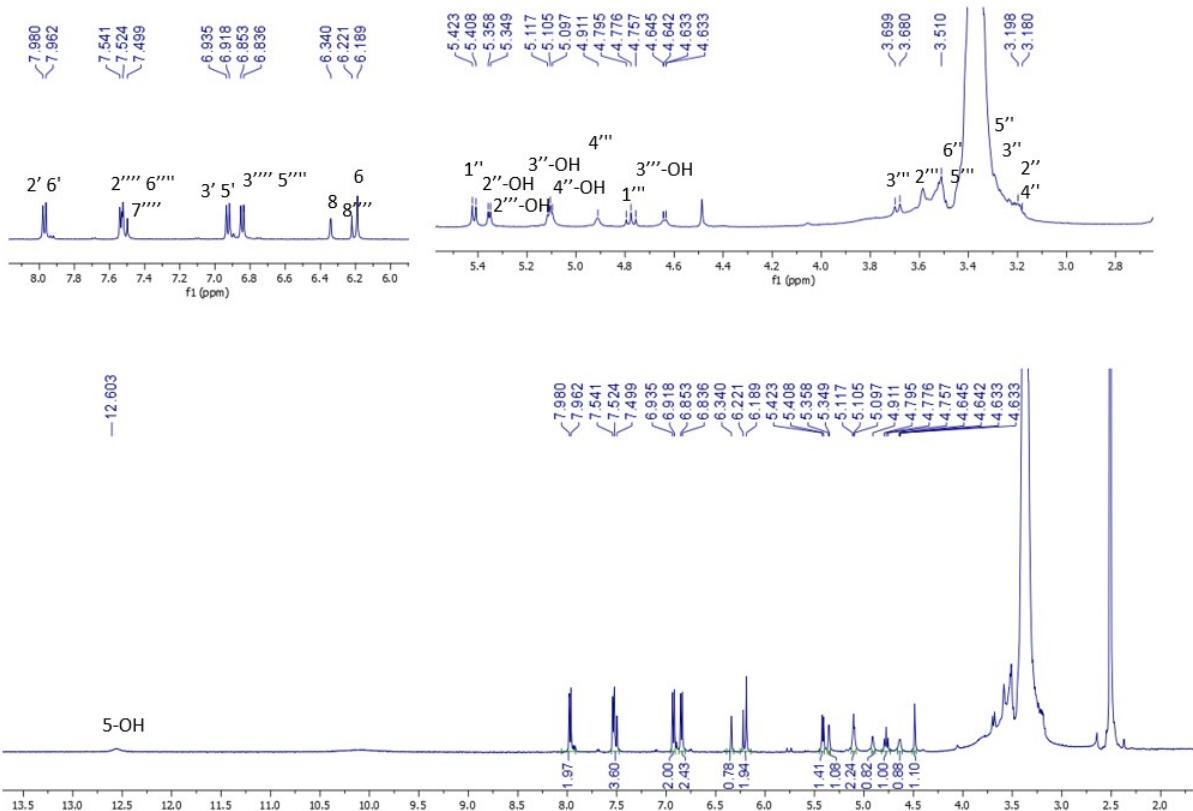
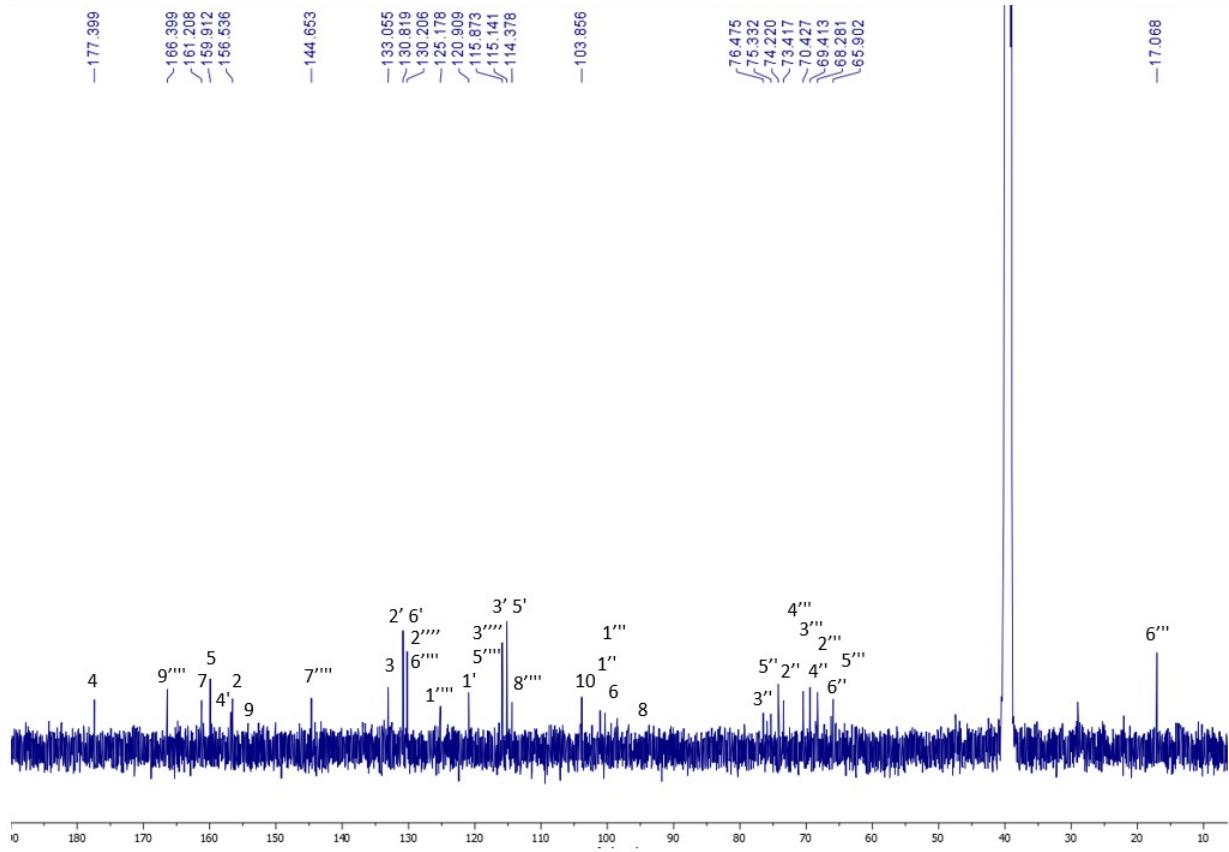


Figure S2. ¹H NMR spectrum of 1



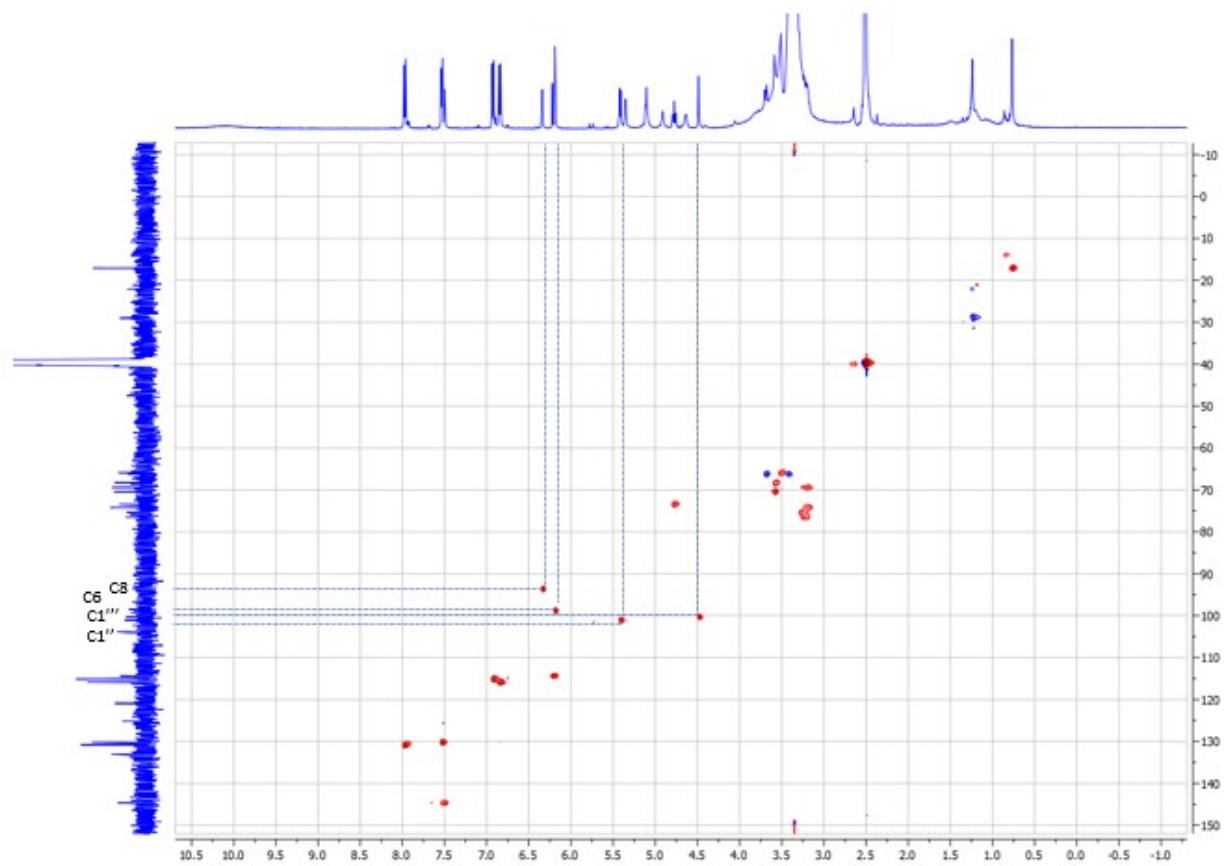


Figure S4. HSQC spectrum of **1**

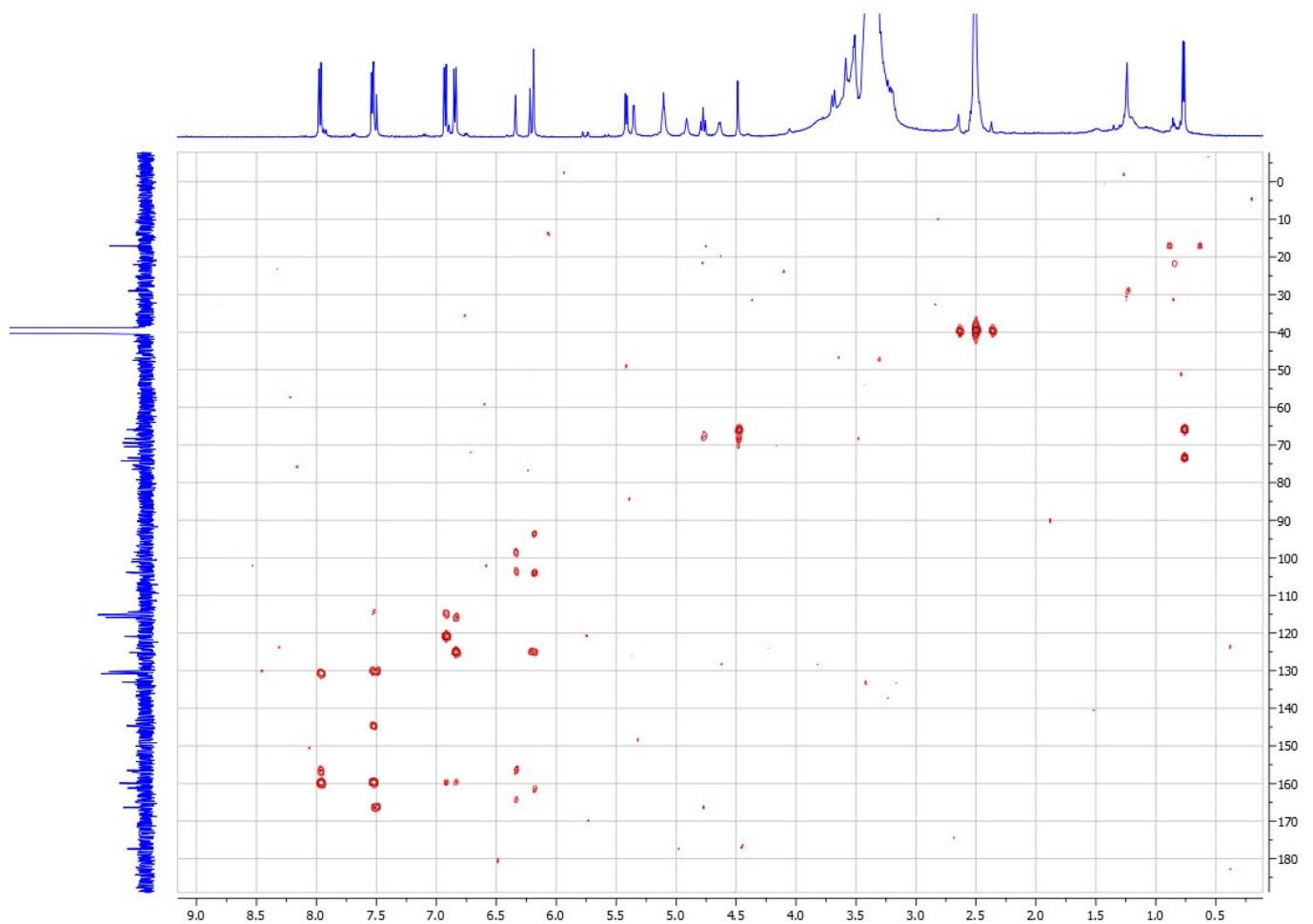


Figure S5. HMBC spectrum of **1**

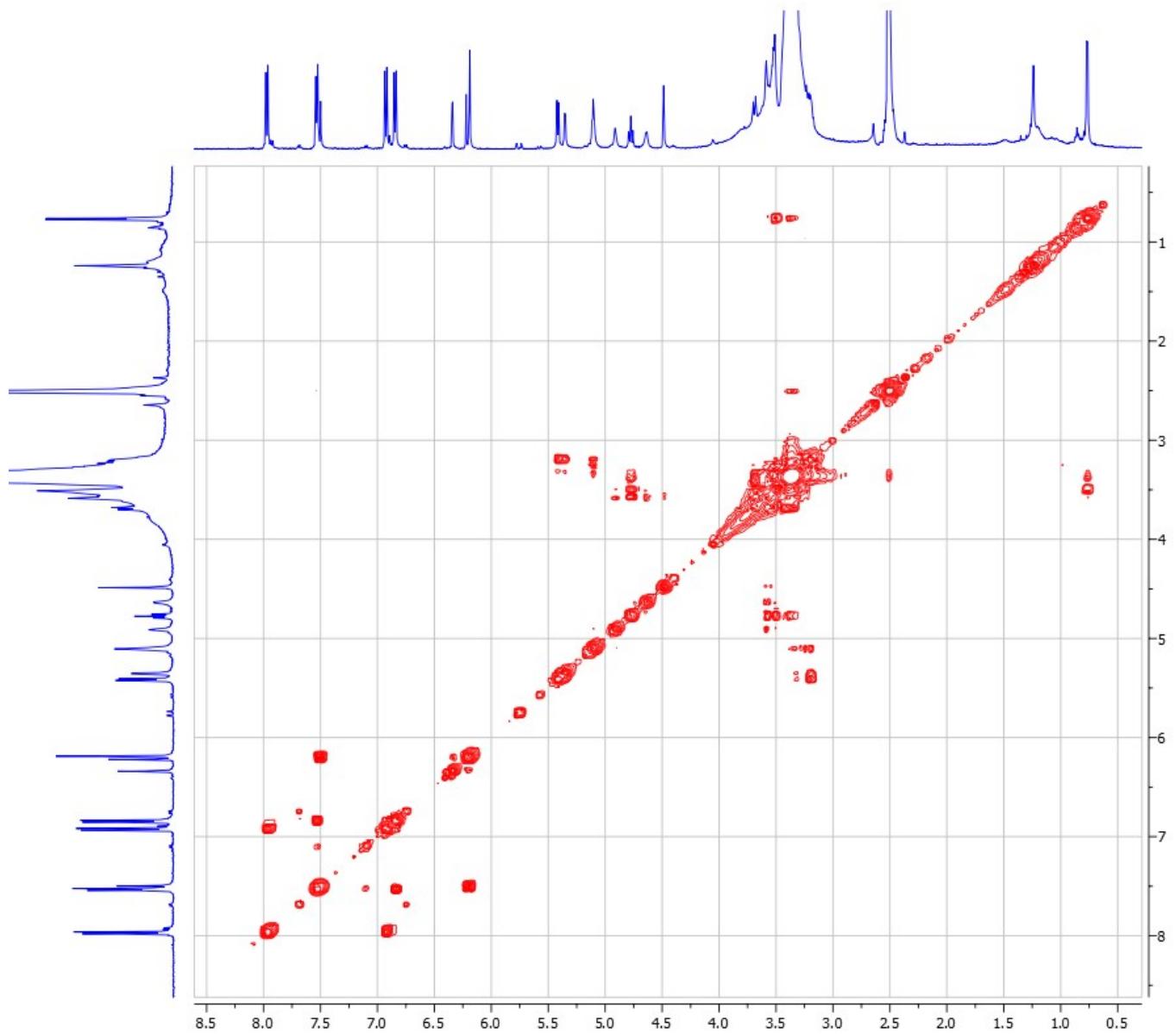


Figure S6. COSY spectrum of 1

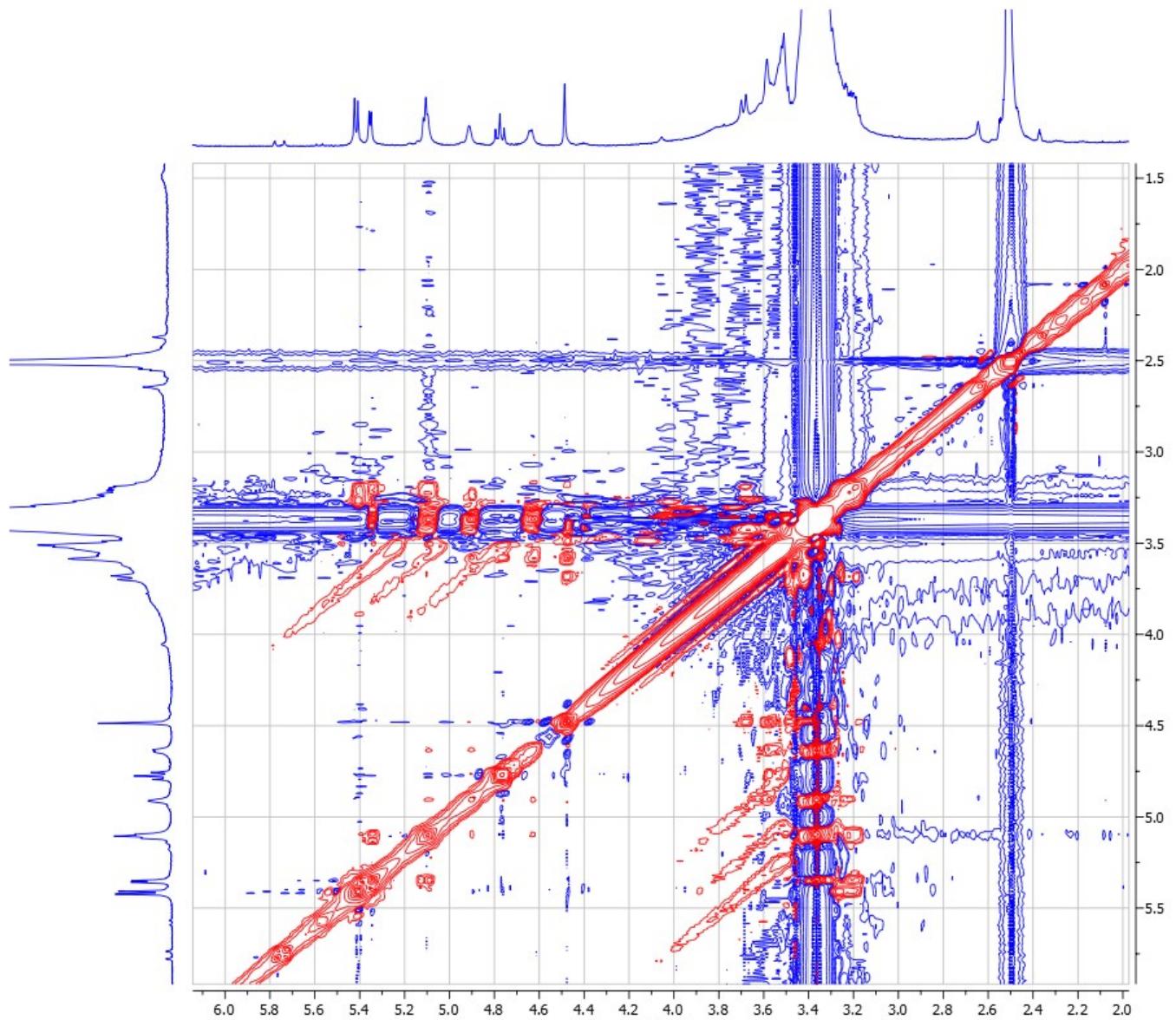


Figure S7. NOESY spectrum of **1**

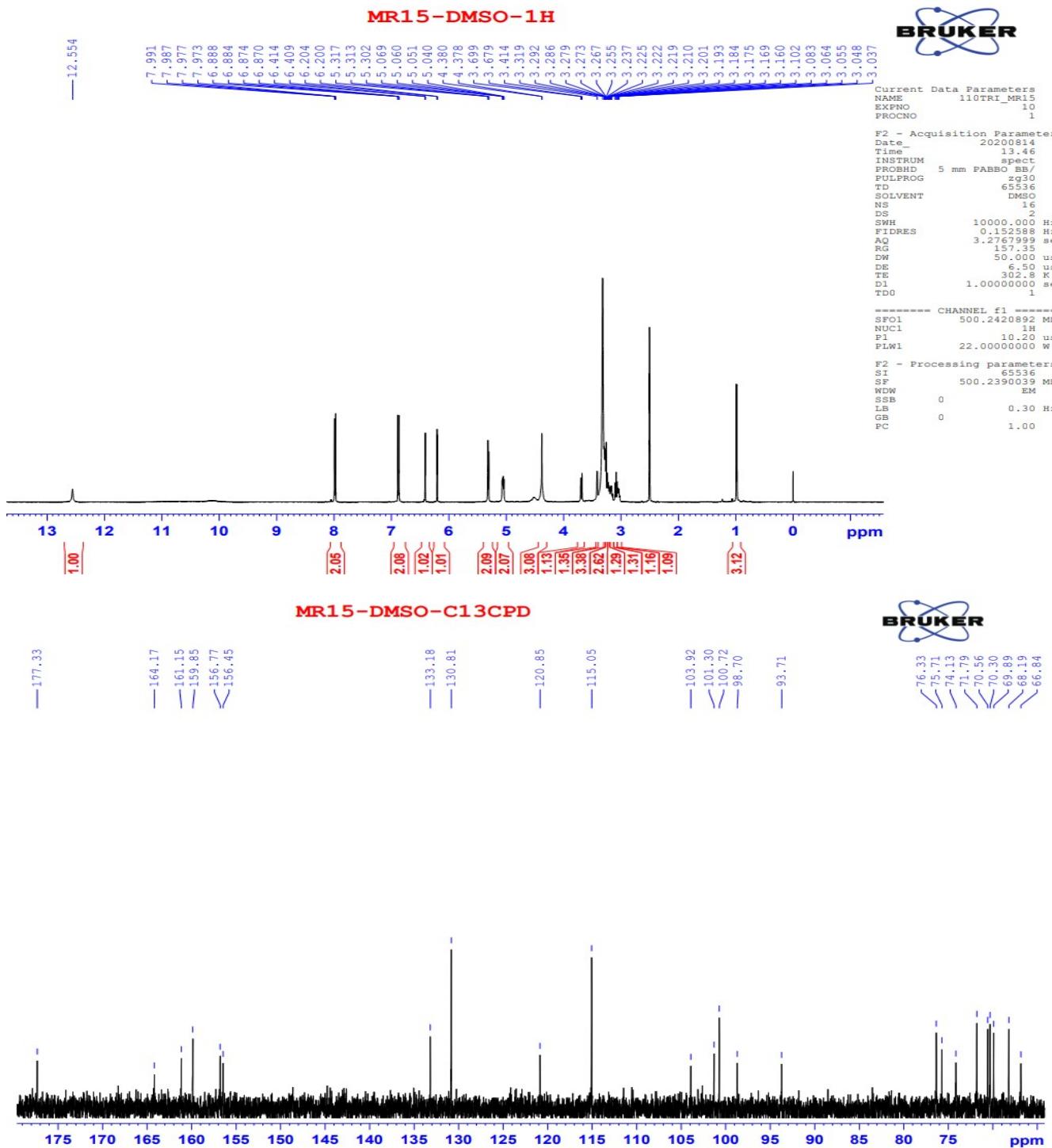


Figure S8. ^1H and ^{13}C NMR spectra of **4**

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
- A SSA	960	947 945 970 975 960 981 993 999 1000 1018 1019 1028 1029	DEEKFICYFDEMGASAENCTARGCINWAEASHASHSGVPPFCYVHNLYLSVSDVQHNGATADISLNSESVTAKA	1029	
- B SSA	960	947 945 970 975 960 981 993 999 995 999 1005 1016 1015 1028 1029	DEEKFICYFDEMGASAENCTARGCINWAEASHASHSGVPPFCYVHNLYLSVSDVQHNGATADISLNSESVTAKA	1029	
- A SSA	1030	1033 1035 1040 1045 1050 1055 1055 1068 1085 1085 1070 1075 1066 1085 1098 1095	FPSTPVPMPPLRLDVTYTHXEMELGKFIYDPMHNSVPLNPIHPSMS83TPGQLYDVLIKENNPFGIEIRK	1099	
- B SSA	1030	1033 1035 1040 1045 1050 1055 1055 1068 1085 1085 1070 1075 1066 1085 1098 1095	FPSTPVPMPPLRLDVTYTHXEMELGKFIYDPMHNSVPLNPIHPSMS83TPGQLYDVLIKENNPFGIEIRK	1099	
- A SSA	1100	1103 1105 1110 1115 1120 1125 1130 1135 1140 1145 1150 1155 1160 1168 1165	STOTIILWDQQLGFTFSDFNFI1STTRLPSSKTYLGFQTEHRSYREDLENHTNGNSFSDRQPPGYYKKNSSYGV	1169	
- B SSA	1100	1103 1105 1110 1115 1120 1125 1130 1135 1140 1145 1150 1155 1160 1168 1165	STOTIILWDQQLGFTFSDFNFI1STTRLPSSKTYLGFQTEHRSYREDLENHTNGNSFSDRQPPGYYKKNSSYGV	1169	
- A SSA	1170	1173 1175 1180 1185 1190 1195 1195 1208 1205 1210 1215 1220 1225 1235 1238 1235	EYTFYNNOLEEDDSARGVLLNNSNAMDDVTFQPLPALTYITRTGQVLDFFVFLQOPTPELVYQQYTELIGRPVHV	1239	
- B SSA	1170	1173 1175 1180 1185 1190 1195 1195 1208 1205 1210 1215 1220 1225 1235 1238 1235	EYTFYNNOLEEDDSARGVLLNNSNAMDDVTFQPLPALTYITRTGQVLDFFVFLQOPTPELVYQQYTELIGRPVHV	1239	
- A SSA	1240	1243 1245 1250 1250 1255 1260 1265 1270 1275 1280 1285 1290 1295 1300 1305	FYNNSLCFOLCRGYQNDESETASLYDENVAQAPIFYDVQYSIDYMERQLOFTLSPKFAFGPFALINHRKADG	1309	
- B SSA	1240	1243 1245 1250 1250 1255 1260 1265 1270 1275 1280 1285 1290 1295 1299 1300 1305	FYNNSLCFOLCRGYQNDESETASLYDENVAQAPIFYDVQYSIDYMERQLOFTLSPKFAFGPFALINHRKADG	1309	
- A SSA	1310	1313 1315 1320 1325 1330 1335 1340 1345 1350 1355 1360 1366 1370 1378 1379	MRRVILLDFPAISGNETQPYPAFTRGVEDDVFIKYPNDGDIUWKGXVNPDFFDVVVNGSLDNDSQVELTRAY	1379	
- B SSA	1310	1313 1315 1320 1325 1330 1335 1340 1345 1350 1355 1360 1365 1370 1378 1379	MRRVILLDFPAISGNETQPYPAFTRGVEDDVFIKYPNDGDIUWKGXVNPDFFDVVVNGSLDNDSQVELTRAY	1379	
- A SSA	1380	1383 1385 1390 1395 1400 1405 1410 1415 1420 1425 1430 1435 1440 1448 1445	VAFDPDFRNBSATAKWWKREIEELYNSPNQPERBLKFDGHNWIDRNNEP83FVNNGAVSFPGCRDASLNHEPTYHP	1449	
- B SSA	1380	1383 1385 1390 1395 1400 1405 1410 1415 1420 1425 1430 1435 1440 1448 1445	VAFDPDFRNBSATAKWWKREIEELYNSPNQPERBLKFDGHNWIDRNNEP83FVNNGAVSFPGCRDASLNHEPTYHP	1449	
- A SSA	1450	1453 1455 1460 1465 1470 1475 1480 1485 1490 1495 1500 1505 1510 1518 1515	LESRDRGLSSEKTLCMESQOILPDSLSVQHYNVHNLYNQHSQTRPTYEAVQEVTOQRGVVIVITSTFPSS80RW	1519	
- B SSA	1450	1453 1455 1460 1465 1470 1475 1480 1485 1490 1495 1500 1505 1510 1518 1515	LESRDRGLSSEKTLCMESQOILPDSLSVQHYNVHNLYNQHSQTRPTYEAVQEVTOQRGVVIVITSTFPSS80RW	1519	
- A SSA	1520	1523 1525 1530 1535 1540 1545 1550 1555 1560 1565 1570 1575 1580 1588 1585	AGHWLGCDNTAAWDLQKESIIGHMRMFESEFLQGSIISYTQGADICOFQDAEYENCVRNMLQGAFYPPSRHMNTG	1589	
- B SSA	1520	1523 1525 1530 1535 1540 1545 1550 1555 1560 1565 1570 1575 1580 1588 1585	AGHWLGCDNTAAWDLQKESIIGHMRMFESEFLQGSIISYTQGADICOFQDAEYENCVRNMLQGAFYPPSRHMNTG	1589	
- A SSA	1590	1593 1595 1600 1605 1610 1615 1620 1625 1630 1635 1640 1645 1650 1655 1655	RKRQDPVENDQAVFVNISRTVLOQTTRYLTLKHAHTEGTVVVRPLLHEFVSDQVTDIDSQPLLGPA	1659	
- B SSA	1590	1593 1595 1600 1605 1610 1615 1620 1625 1630 1635 1640 1645 1650 1655 1655	RKRQDPVENDQAVFVNISRTVLOQTTRYLTLKHAHTEGTVVVRPLLHEFVSDQVTDIDSQPLLGPA	1659	
- A SSA	1660	1663 1665 1670 1675 1680 1685 1690 1695 1700 1705 1710 1715 1720 1725	FLVSPVLEARNHRYTAYFPRAWMDYTTGVDINARGEHLTLPAPLORINLHVGGYILPQEPALNTHL	1729	
- B SSA	1660	1663 1665 1670 1675 1680 1685 1690 1695 1700 1705 1710 1715 1720 1725	FLVSPVLEARNHRYTAYFPRAWMDYTTGVDINARGEHLTLPAPLORINLHVGGYILPQEPALNTHL	1729	
- A SSA	1730	1733 1735 1740 1745 1750 1755 1760 1765 1770 1775 1780 1785 1790 1795 1795	RQRFNGPKIAALDQEGTAGGWLTWDDGSDSIDTYGKGLYIYLAFSFAQRTHOSHII1TQH11GTHPLKLELQYI	1799	
- B SSA	1730	1733 1735 1740 1745 1750 1755 1760 1765 1770 1775 1780 1785 1790 1795 1795	RQRFNGPKIAALDQEGTAGGWLTWDDGSDSIDTYGKGLYIYLAFSFAQRTHOSHII1TQH11GTHPLKLELQYI	1799	
- A SSA	1800	1803 1805 1810 1815 1820 1825 1830 1835 1840 1845	ELNOVSFVTSV18180M1V1TPFNMHDPTVQVLS1D10N1S1H1N1	1849A	
- B SSA	1800	1803 1805 1810 1815 1820 1825 1830 1835 1840 1845	ELNOVSFVTSV18180M1V1TPFNMHDPTVQVLS1D10N1S1H1N1	1849A	

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

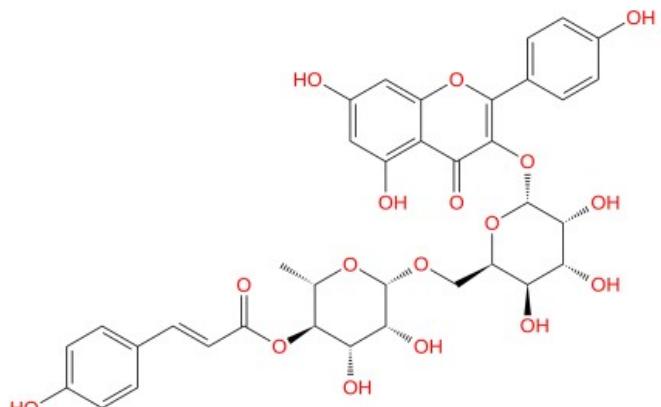
C₃₆H₃₆O₁₇

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 environment.

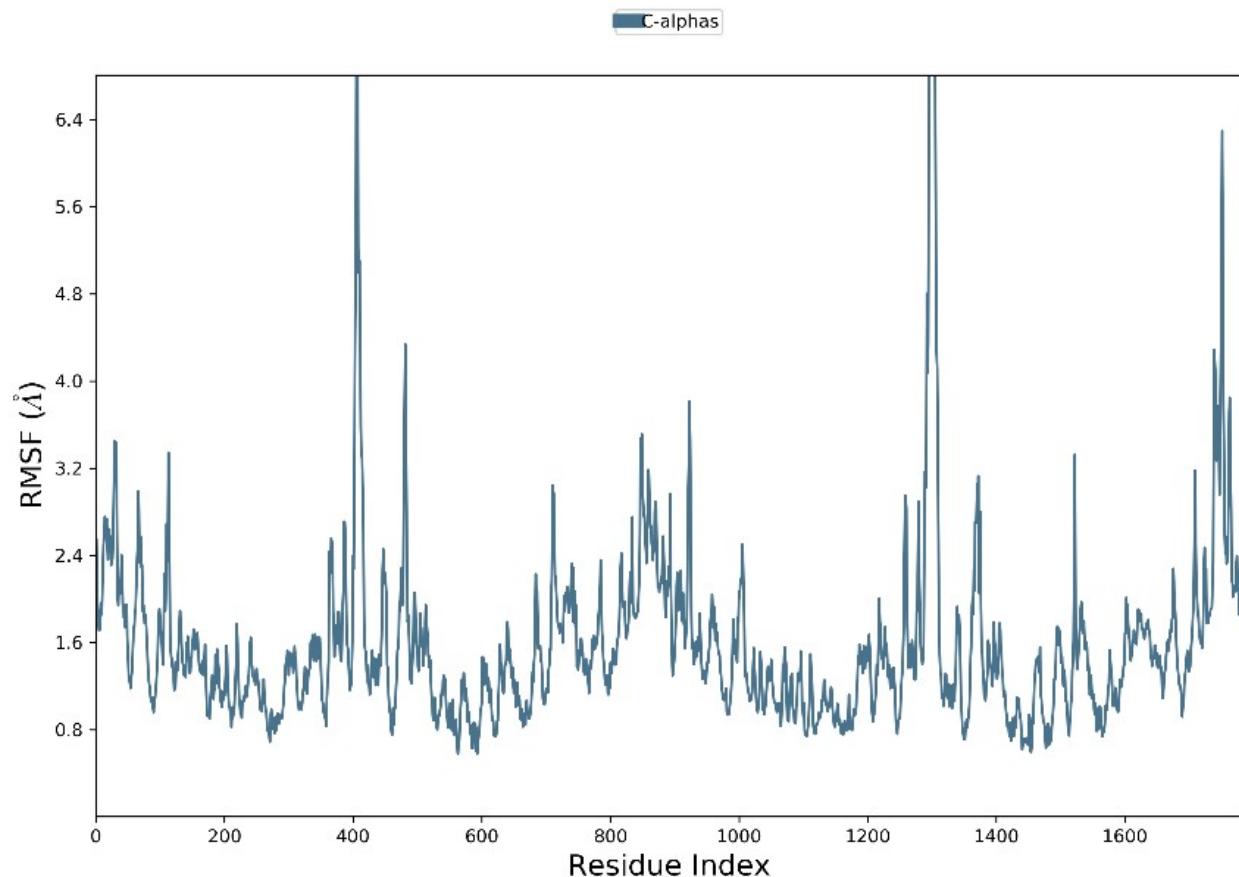


Figure S11. The RMSF (Å) values of 3TOP enzyme

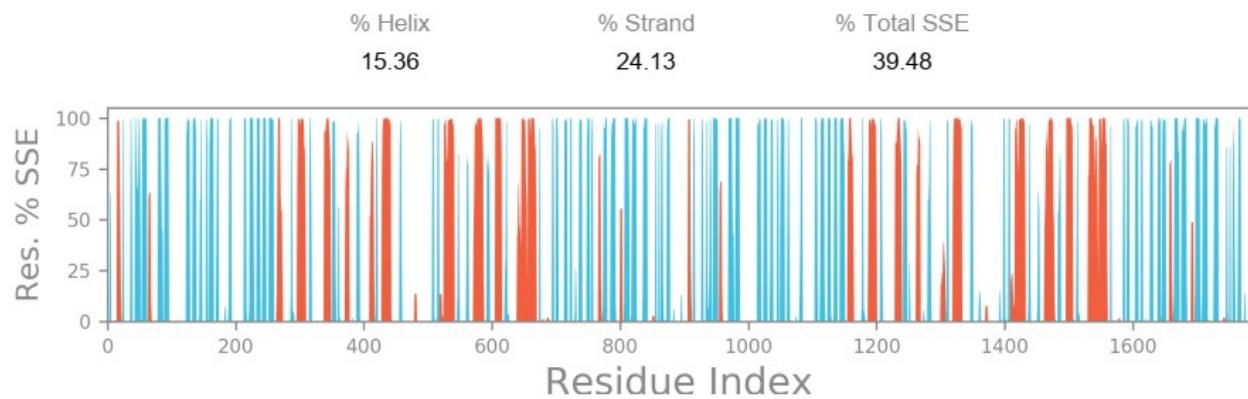


Figure S12. The secondary structure of 3TOP

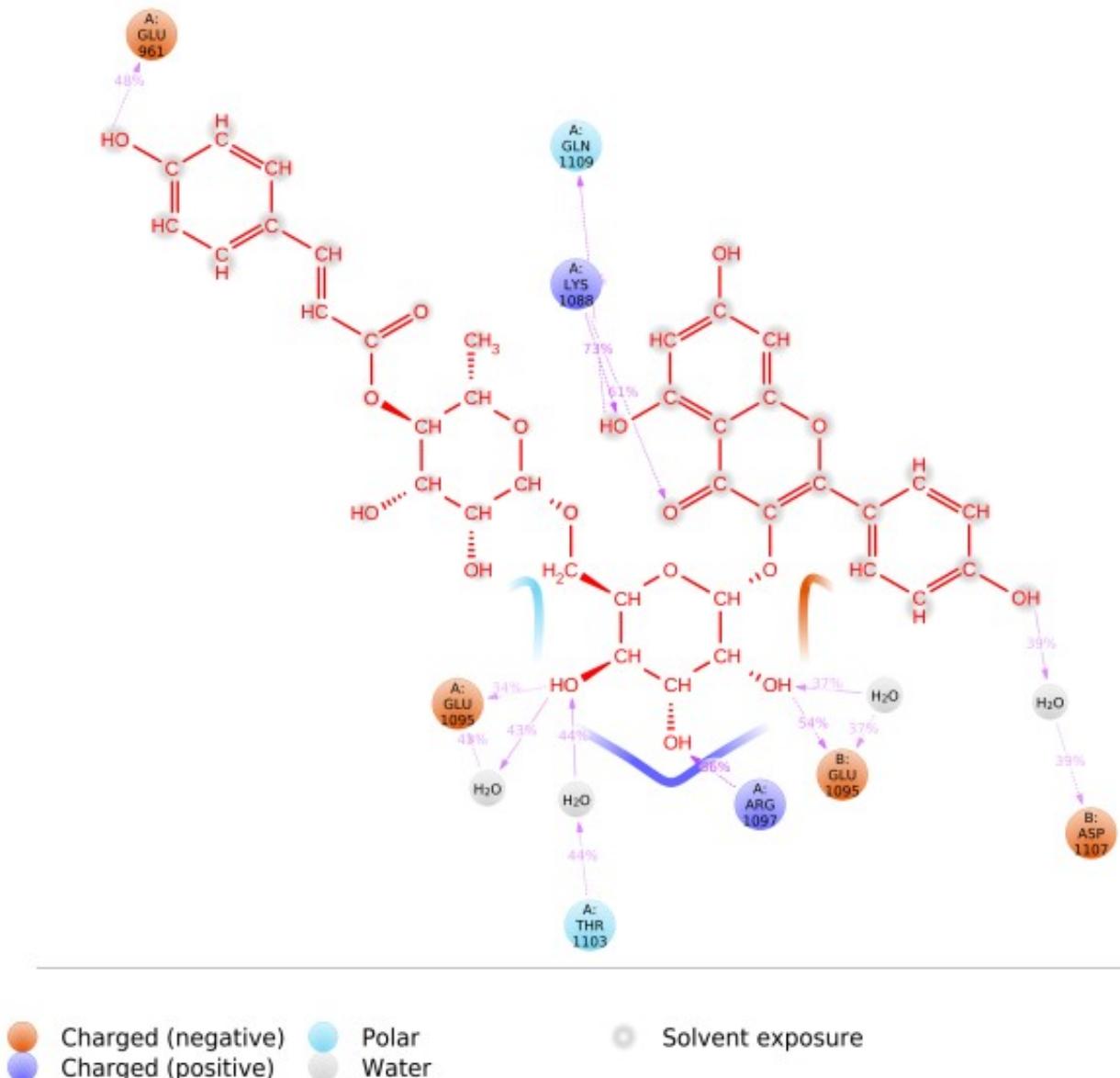


Figure S13. The contacts between pose 472 and 3TOP.

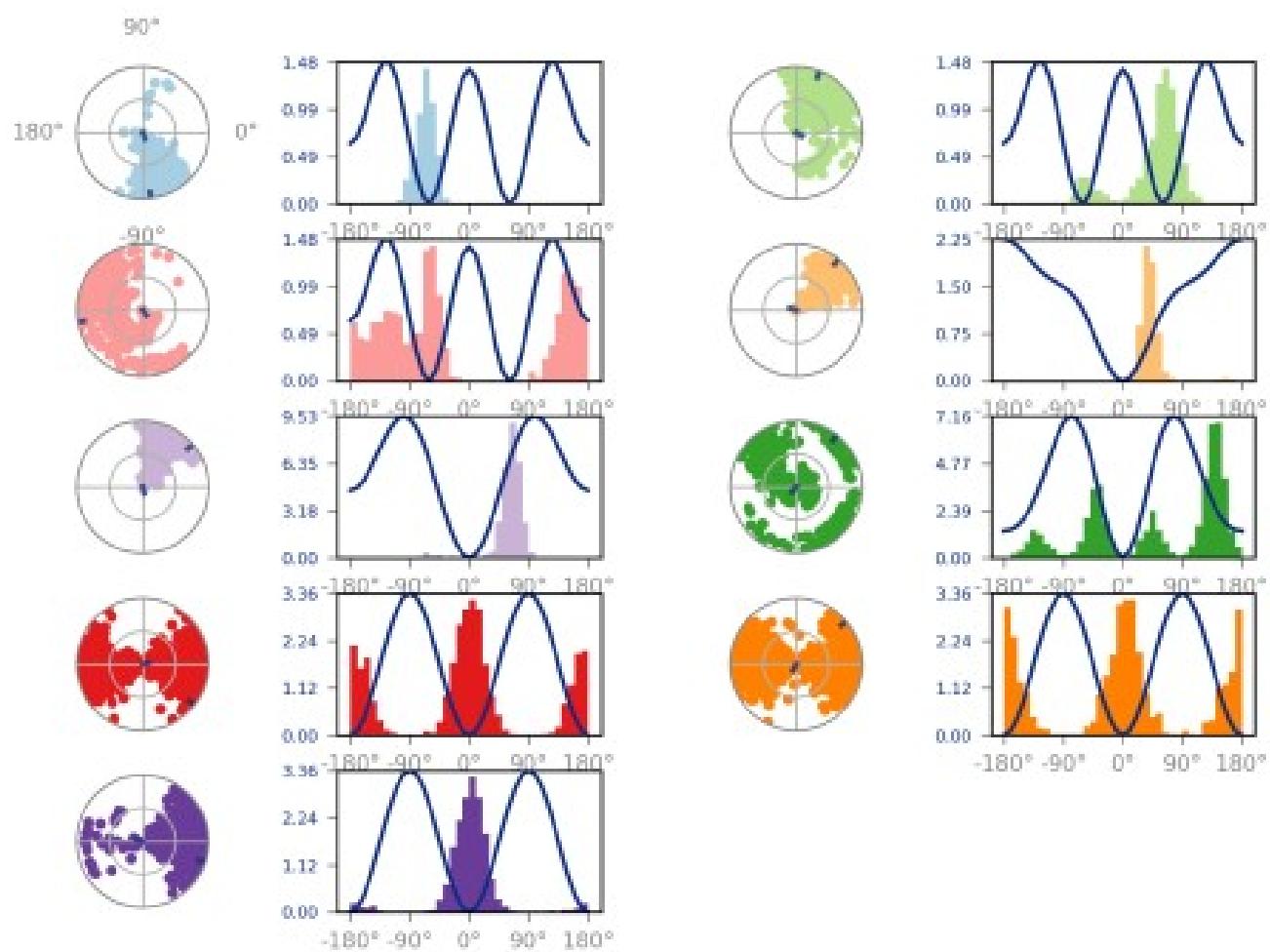
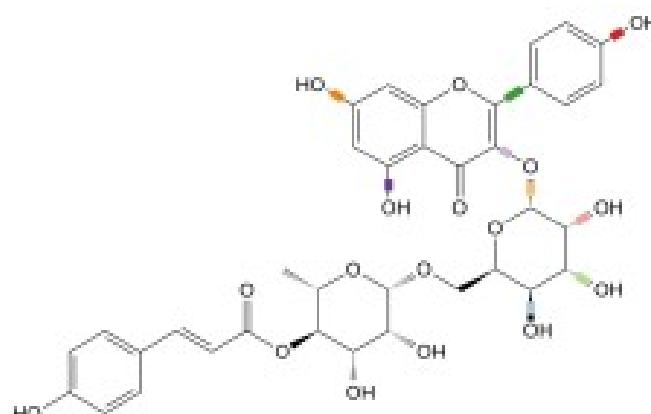


Figure S14. The torsion profile of pose 472.

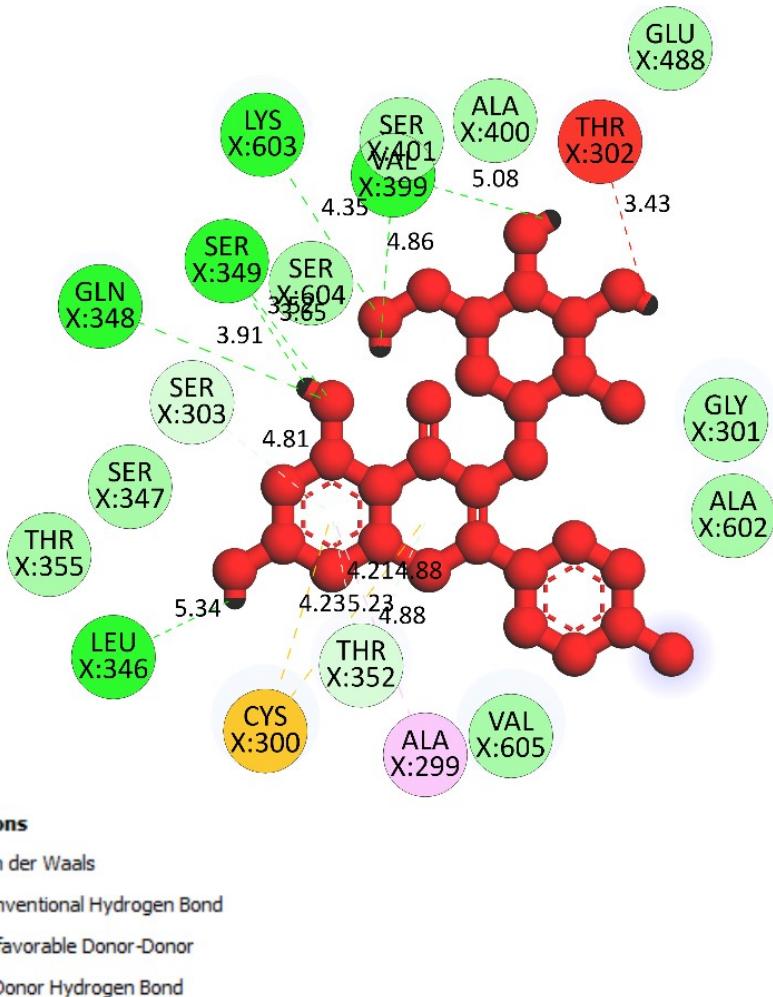
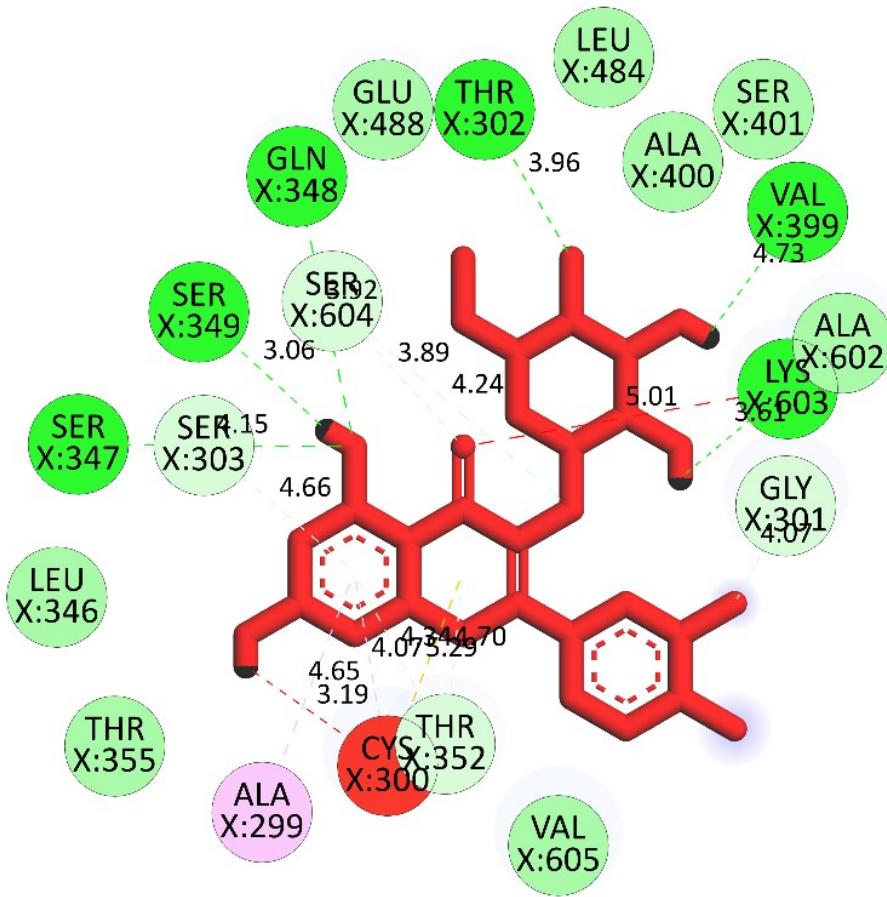


Figure S15. One 2D diagram showed the interactions between pose 305 and 2VF5

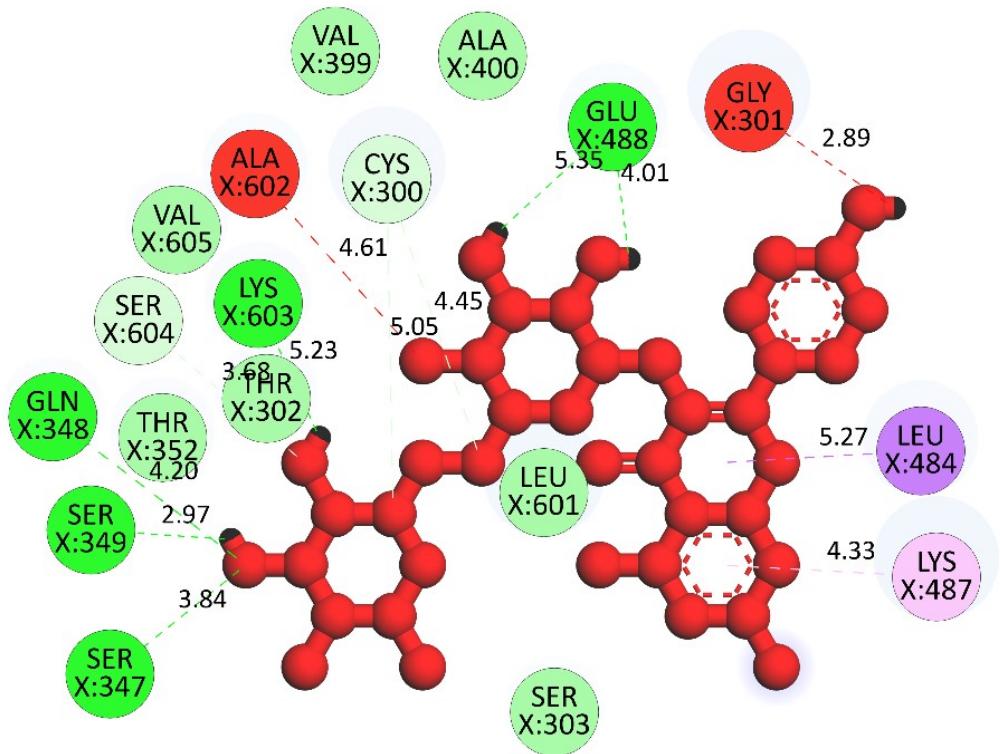


Interactions

- [Green square] van der Waals
- [Green square] Conventional Hydrogen Bond
- [Light green square] Carbon Hydrogen Bond
- [Red square] Unfavorable Donor-Donor
- [Red square] Unfavorable Acceptor-Acceptor

- [Light green square] Pi-Donor Hydrogen Bond
- [Magenta square] Pi-Sigma
- [Yellow square] Pi-Sulfur
- [Pink square] Pi-Alkyl

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



Interactions

- █ van der Waals
- █ Conventional Hydrogen Bond
- █ Carbon Hydrogen Bond
- █ Unfavorable Donor-Donor

- █ Unfavorable Acceptor-Acceptor
- █ Pi-Sigma
- █ Pi-Alkyl

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

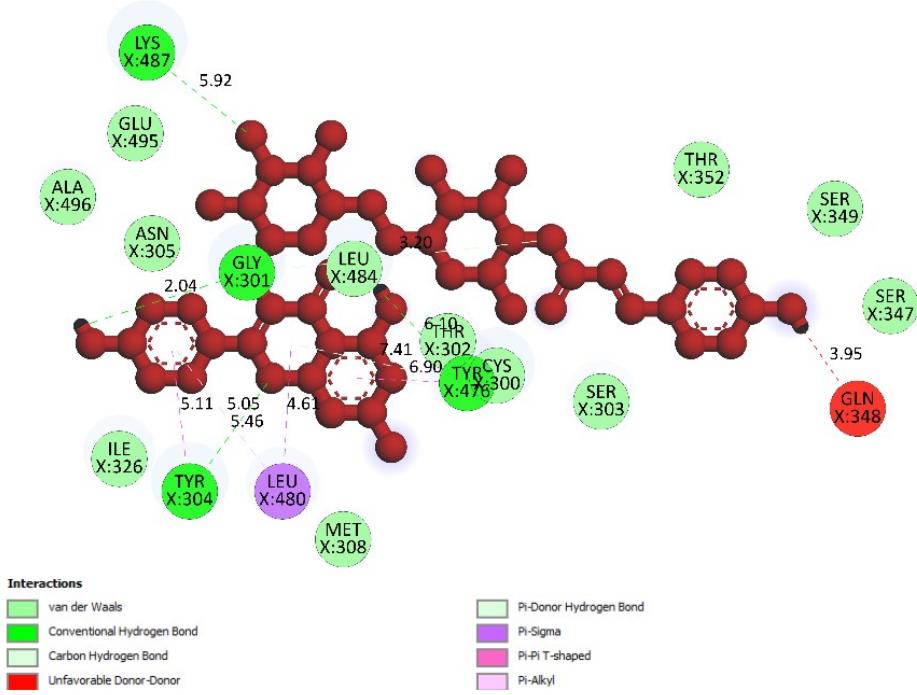
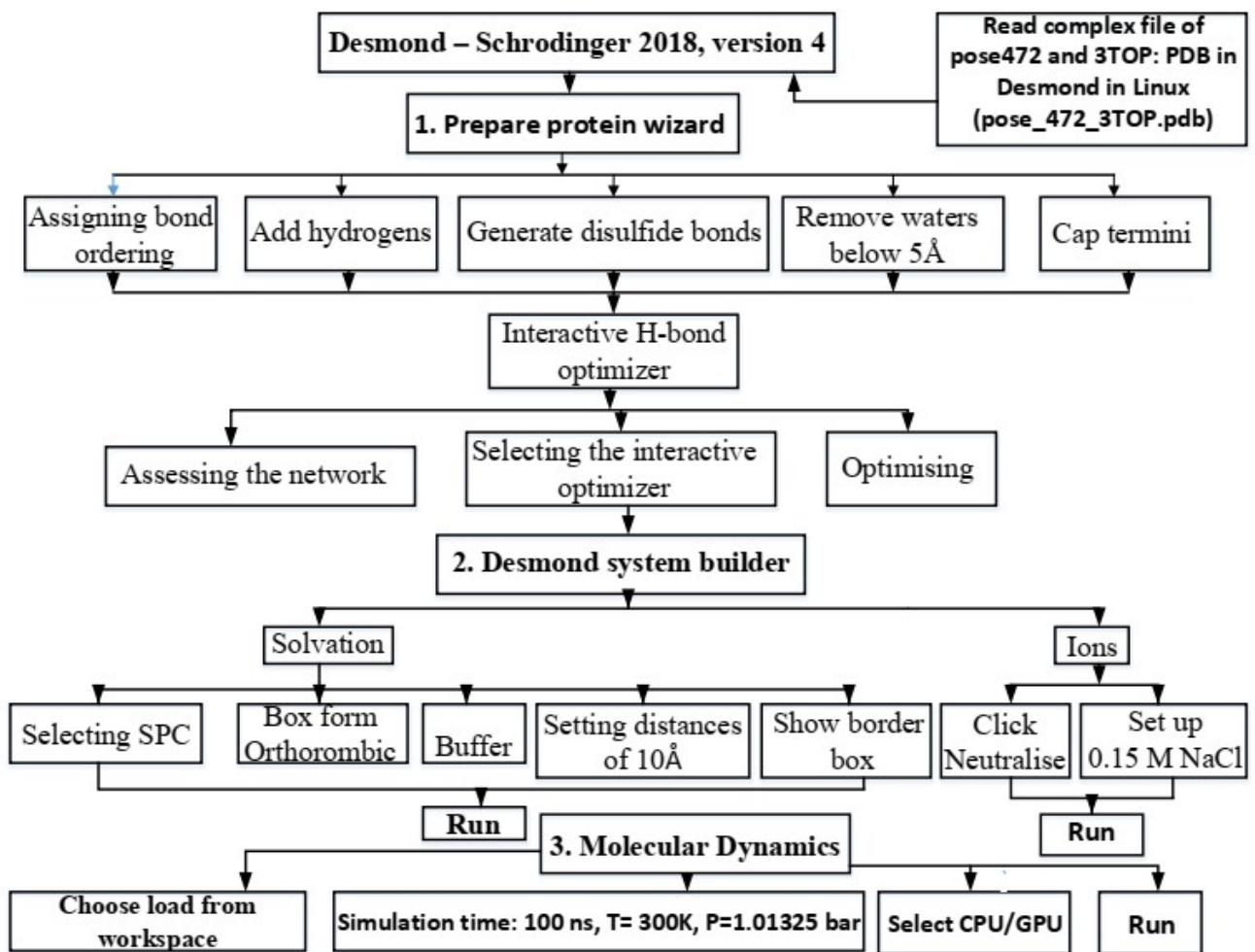


Figure S18. One 2D diagram showed the interactions between pose 43 (compound 1) and 2VF5



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

