Unravelling the antifungal and antiprotozoal activities and LC-MS/MS quantification of steroidal saponins isolated from *Panicum turgidum*

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Supplementary file

Contents

1 List of Supplementary Figures and Tables

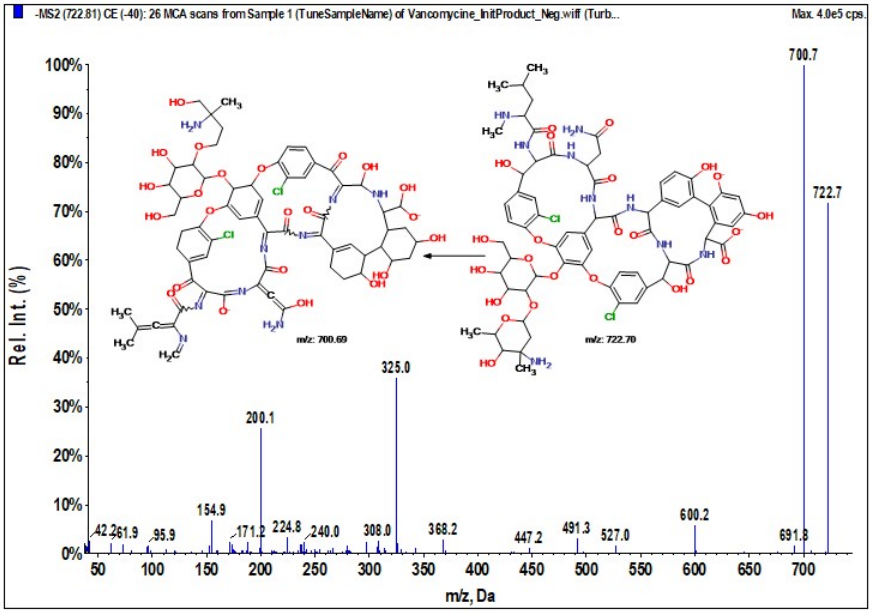


Figure S1: ESI-MS/MS spectrum showing the precursor and the product ions of vancomycin under the negative mode.

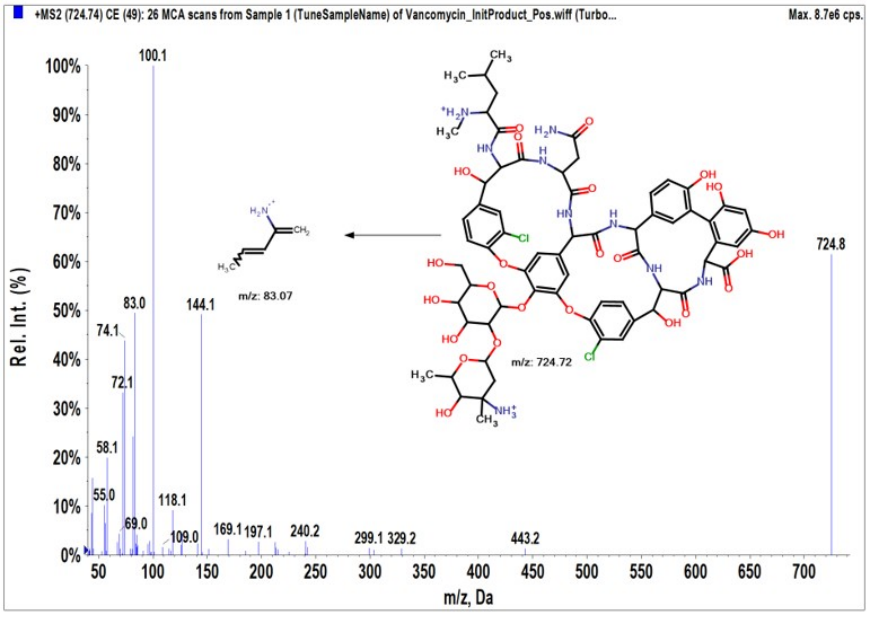


Figure S2: ESI-MS/MS spectrum showing the precursor and the product ions of vancomycin under the positive mode.

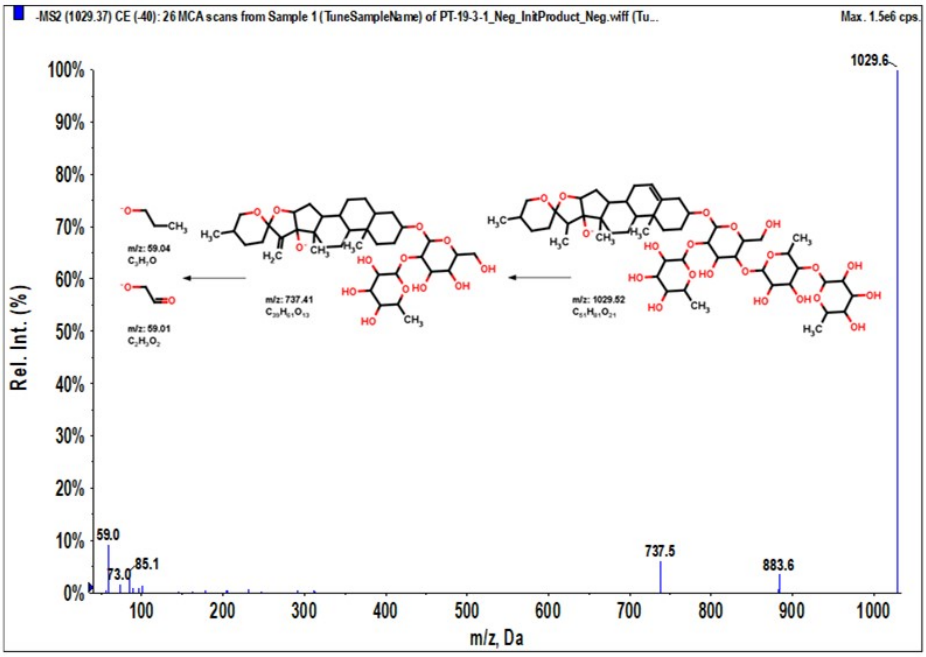


Figure S3: ESI-MS/MS spectrum showing the precursor and the product ions of compound **4** under the negative mode.

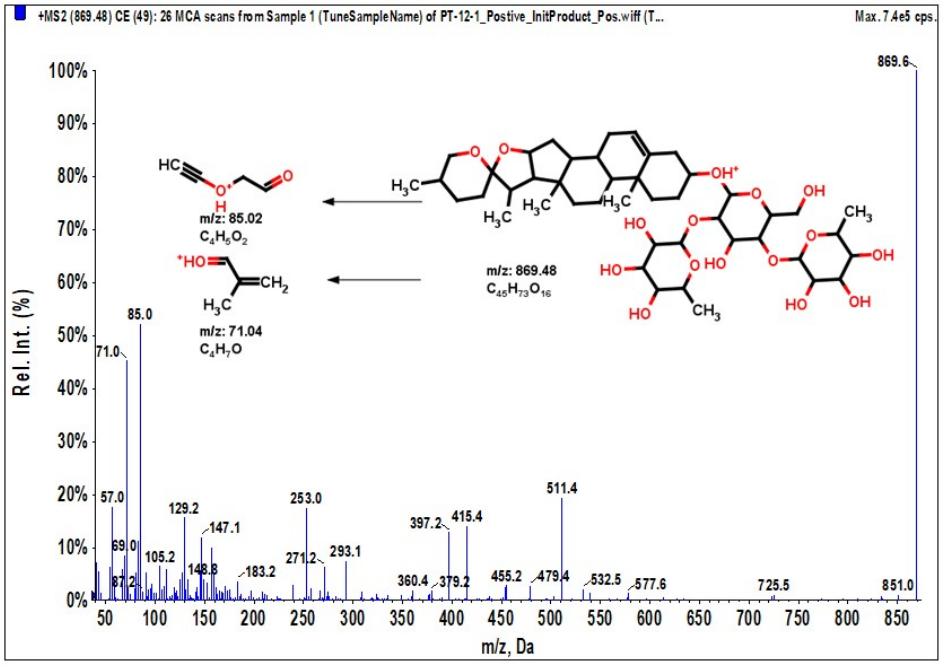


Figure S4: ESI-MS/MS spectrum showing the precursor and the product ions of compound **5** under the positive mode.

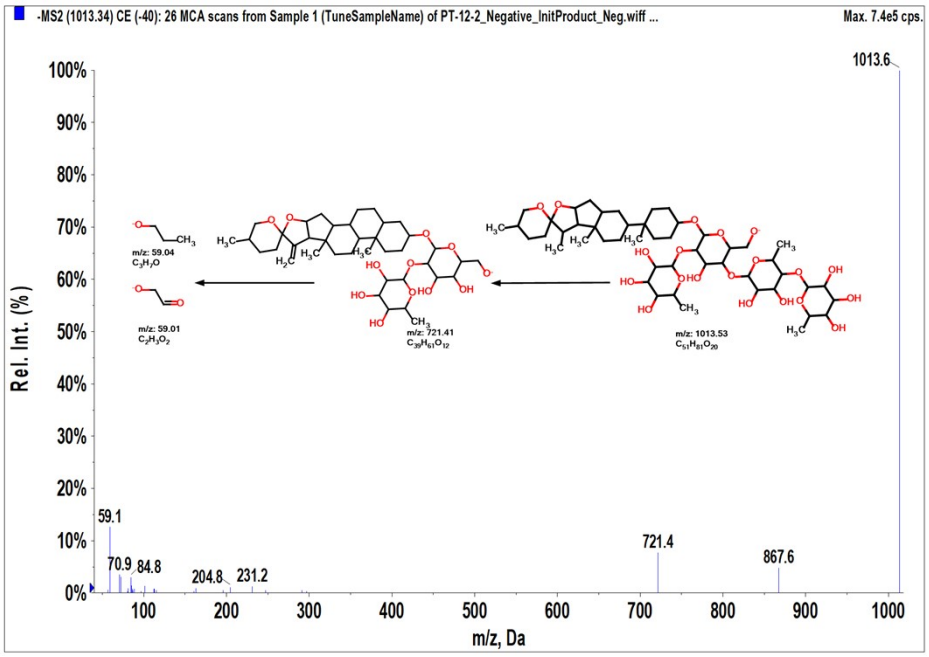


Figure S5: ESI-MS/MS spectrum showing the precursor and the product ions of compound **6** under the negative mode.

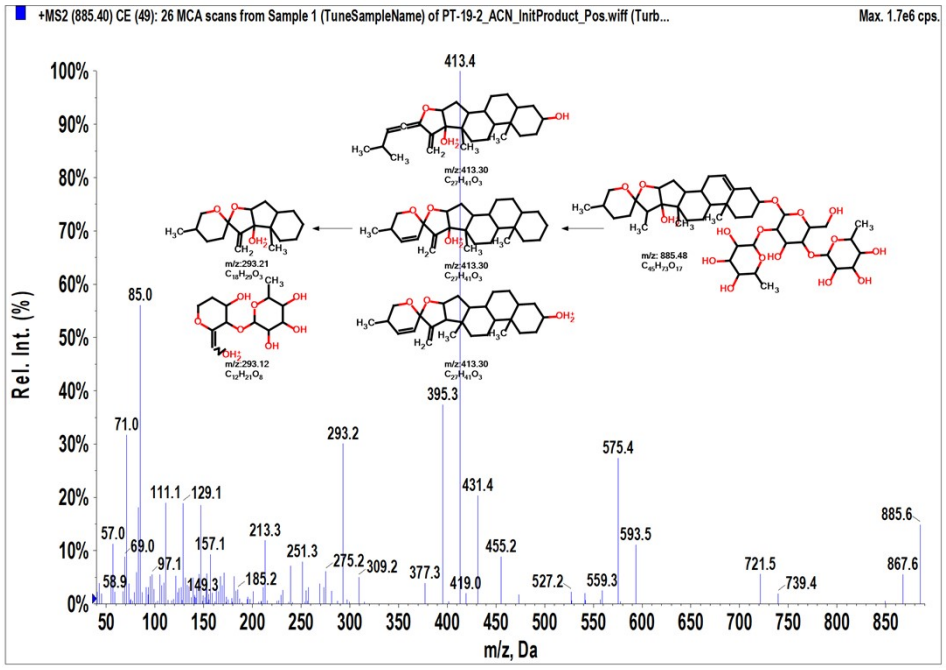


Figure S6: ESI-MS/MS spectrum showing the precursor and the product ions of compound **7** under the positive mode.

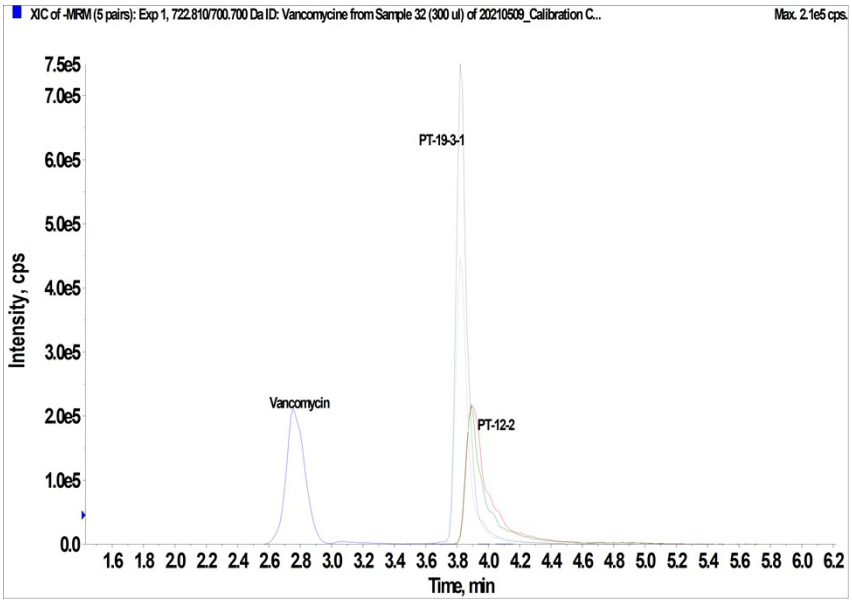


Figure S7: Representative extracted negative ion MRM chromatograms of **4** (m/z: 1029.6/737.5 & 1029.6/59 Da), **6** (m/z: 1013.6/721.4 & 1013.6/59.1 Da), and vancomycin (IS) ((m/z: 722.7/700.7 Da)

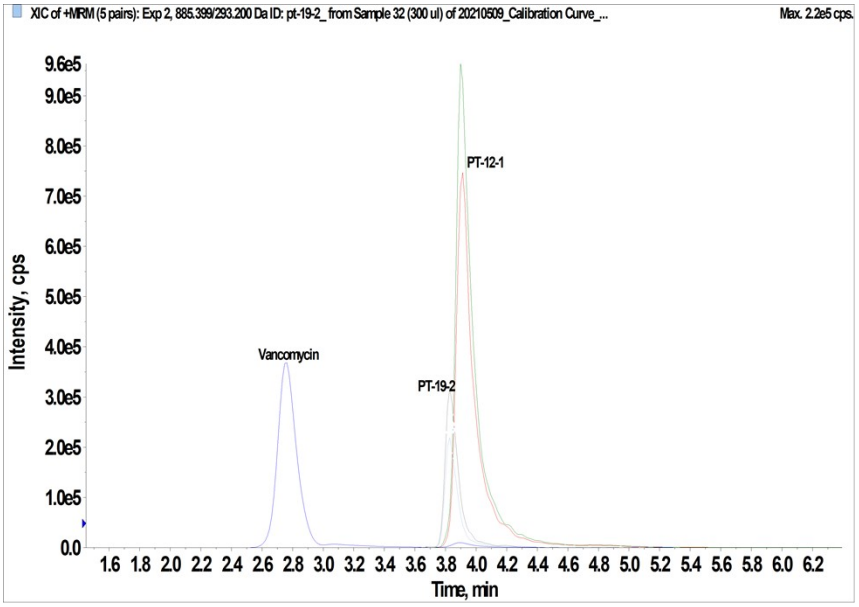


Figure S8: Representative extracted positive ion MRM chromatograms of **7, 5**, and vancomycin (IS)

Table S1: Time programming of the gradient elution using A: 0.01% formic acid in water and B: 0.01% formic acid in methanol

No	Time (min)	Flow (mL/min)	% Aqueous phase (A)	% Organic phase (B)
1	0	0.5	70	30
2	1	0.5	70	30
3	5	0.5	0	100
4	6	0.5	0	100
5	6.5	0.5	70	30
6	8	0.5	70	30

Table S2: Intra-day accuracy and precision of selected compounds

Analyte	Concentration level	Intra-day accuracy and precision (*n=3*)		
		Nominal concentration (ng/mL)	Found concentration (mean ± SD)	% CV
6	LQC	20	19.38 ± 0.26	1.32
	MQC	600	603.82 ± 12.80	2.12
	HQC	800	831.63 ± 41.12	4.94
4	LQC	20	19.45 ± 0.64	3.30
	MQC	600	592.92 ± 23.39	3.94
	HQC	800	837.6 ± 23.69	2.83
5	LQC	20	18.96 ± 0.64	3.38
	MQC	600	605.03 ± 18.78	3.10
	HQC	800	810.40 ± 53.89	6.65
7	LQC	20	21.43 ± 0.76	3.53
	MQC	600	606.8 ± 17.42	2.87
	HQC	800	791.23 ± 55.21	6.98

Table S3: Online PASS-prediction of new saponins as antifungal and antiprotozoal

Comp. #	Antifungal		Antiprotozoal (Leishmania)	
	* Pa %	Pi %	Pa %	Pi %
1.	74.10	0.80	82.50	0.40
2.	72.20	0.90	80.10	0.50
3.	71.30	0.90	73.90	0.70
4.	79.90	0.50	93.00	0.20
5.	85.30	0.30	95.70	0.20
6.	85.30	0.30	95.70	0.20
7.	79.90	0.50	93.00	0.20

* Pa = probability that the compound is active; Pi = probability that the compound is inactive.

Table S4: Docking results of 1YN and the best effective antifungal Turgidosterones (**4, 5, 6, and 7**).

Comp. No	ΔG (kcal/mol)	RMSD (Å)	Residue		Type	Length (Å)
			Name	ID		
1YN	-12.38	1.18	Cys	470	H. bond	4.23
			Tyr	118	Hydrophobic	3.23
			Ala	61	Hydrophobic	3.89
			Tyr	64	Hydrophobic	4.13
			Leu	376	Hydrophobic	4.25
1	-1.80	1.82	Cys	470	H. Bond	3.18
			Met	508	H. Bond	2.41
			His	377	H. Bond	2.96
2	-4.07	1.78	Ser	378	H. Bond	2.78

Comp. No	ΔG (kcal/mol)	RMSD (Å)	Residue		Type	Length (Å)
			Name	ID		
			Tyr	118	H. Bond	2.85
			Arg	381	H. Bond	2.93
			His	468	H. Bond	3.35
			His	468	Hydrophobic	4.49
3	-9.73	1.91	Cys	470	H. Bond	3.48
			Ser	507	H. Bond	3.23
			Ser	378	H. Bond	3.04
			Lys	143	H. Bond	3.54
4	-11.32	1.73	Gly	303	H. bond	2.76
			Cys	470	H. bond	3.39
			Gly	308	H. bond	3.13
			His	377	Hydrophobic	4.04
5	-9.89	1.59	Gly	303	H. bond	2.84
			His	468	H. bond	2.84
			Cys	470	H. bond	3.15
			Gly	472	H. bond	3.29
			Tyr	118	Hydrophobic	4.61
6	-13.43	1.56	His	468	H. bond	2.89
			Cys	470	H. bond	3.28
			Tyr	118	H. bond	2.92
			Gly	472	H. bond	3.29
7	-9.90	1.93	His	468	H. bond	2.81
			Cys	470	H. bond	3.98
			His	468	H. bond	3.30
			His	377	Hydrophobic	4.11

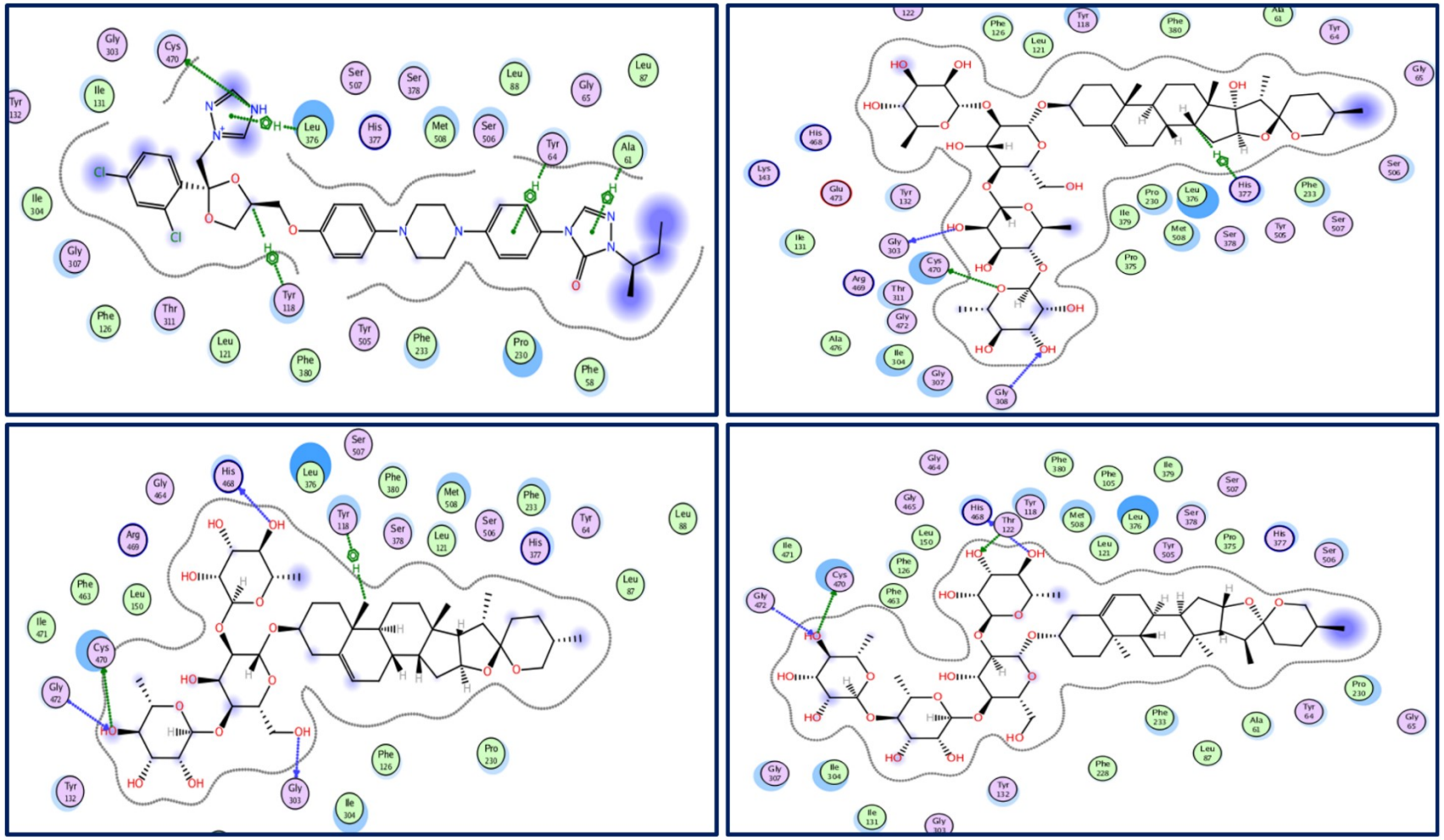


Figure S9: 2D interactions of 1YN (upper left), 4 (upper right), 5 (lower left), and 6 (lower right) with the active site of *C. albicance* oxidoreductase target site.

Table S5: Docking results of FAD and the best effective antitrypanosomal Turgidosterones (4, 5, 6, and 7).

Comp. No	ΔG (kcal/mol)	RMSD (Å)	Residue		Type	Length (Å)
			Name	ID		
FAD	-10.29	1.61	Asp	35	H. bond	2.43
			Asp	327	H. bond	2.47
			Thr	51	H. bond	2.35
			Ser	14	H. bond	3.46
			Gly	127	H. bond	2.78
			Thr	335	H. bond	2.69
			Lys	60	H. bond	2.64
			Gly	15	H. bond	2.58
			Cys	57	Hydrophobic	3.68
			Tyr	198	Hydrophobic	3.98
1	22.17	1.60	Asp	327	H. Bond	3.16
2	13.73	1.60	Asp	327	H. Bond	2.52
			Ala	365	H. Bond	2.44
			Cys	364	H. Bond	3.70
			Gly	13	H. Bond	3.02
			Cys	364	H. Bond	3.26
3	1.48	1.73	Val	55	H. Bond	2.50
			Cys	57	H. Bond	3.25
			Ser	178	H. Bond	2.83
			Gln	439	H. Bond	2.46
4	-4.41	1.67	Val	55	H. bond	2.68

Comp. No	ΔG (kcal/mol)	RMSD (Å)	Residue		Type	Length (Å)
			Name	ID		
			Cys	57	H. bond	3.52
			Asp	327	H. bond	2.67
			Tyr	198	H. bond	2.94
			Gly	56	H. bond	2.84
			Gly	56	H. bond	2.92
			Thr	335	H. bond	2.82
			Arg	290	H. bond	3.21
5	-0.789	1.46	Cys	52	H. bond	3.34
			Cys	57	H. bond	3.10
			Pro	435	H. bond	2.75
			Thr	51	H. bond	3.04
			Lys	60	H. bond	2.63
6	-3.72	1.97	Ala	159	H. bond	2.55
			Thr	160	H. bond	2.48
			Tyr	198	H. bond	2.94
			Gly	15	H. bond	3.17
			Thr	51	H. bond	3.06
			Thr	51	H. bond	2.59
7	4.61	1.61	Cys	57	H. bond	2.90
			Pro	435	H. bond	3.20
			Thr	51	H. bond	2.54
			Lys	60	H. bond	2.56
			Gln	439	H. bond	3.13
			Ser	14	H. bond	2.53

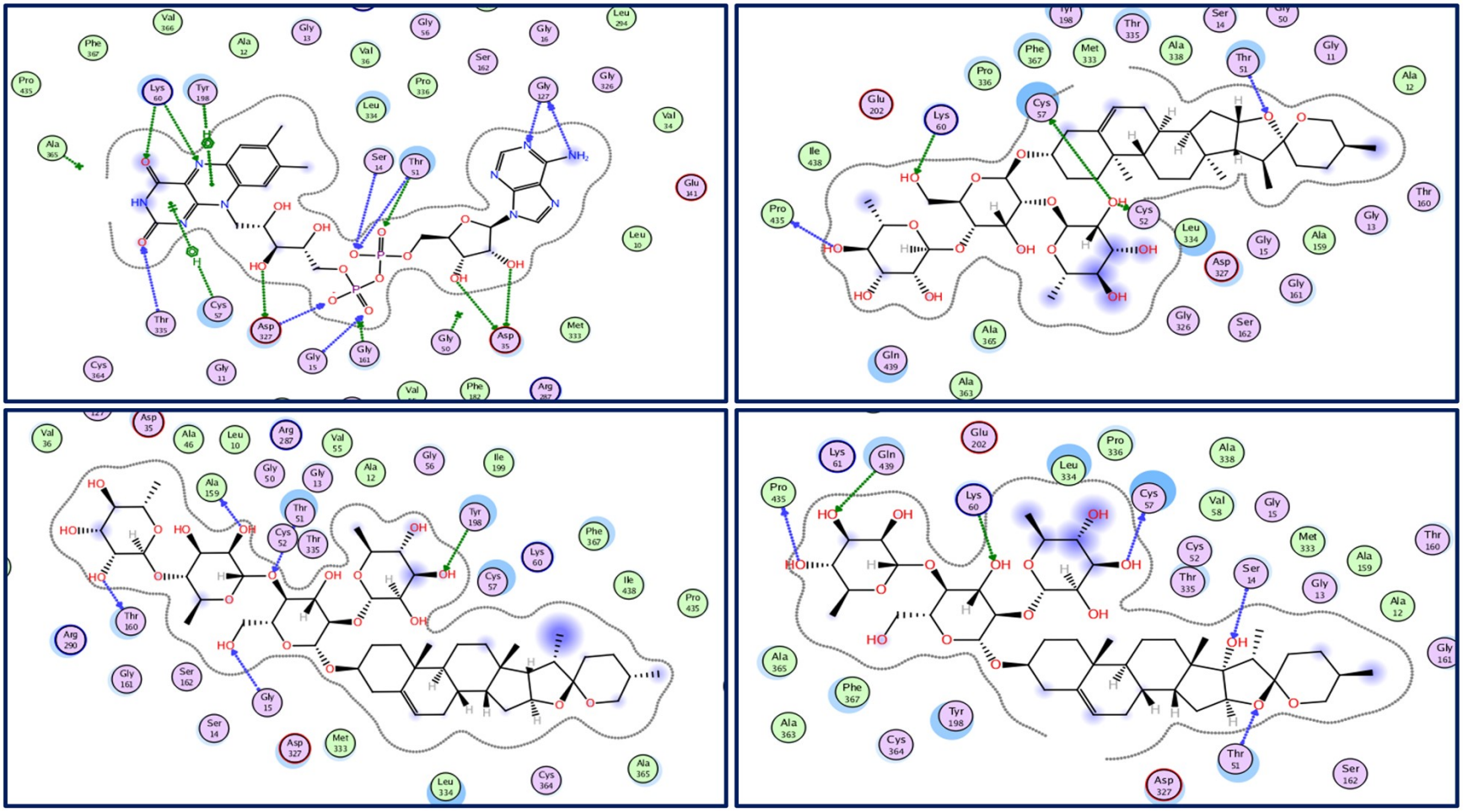


Figure S10: 2D interactions of FAD (upper left), 5 (upper right), 6 (lower left), and 7 (lower right) with the active site of trypanothione reductase

2 Docking files

2.1 Antifungal, 5V5Z

2.1.1 1YN redocked

Score -12.3857269 RNSD 1.18514907

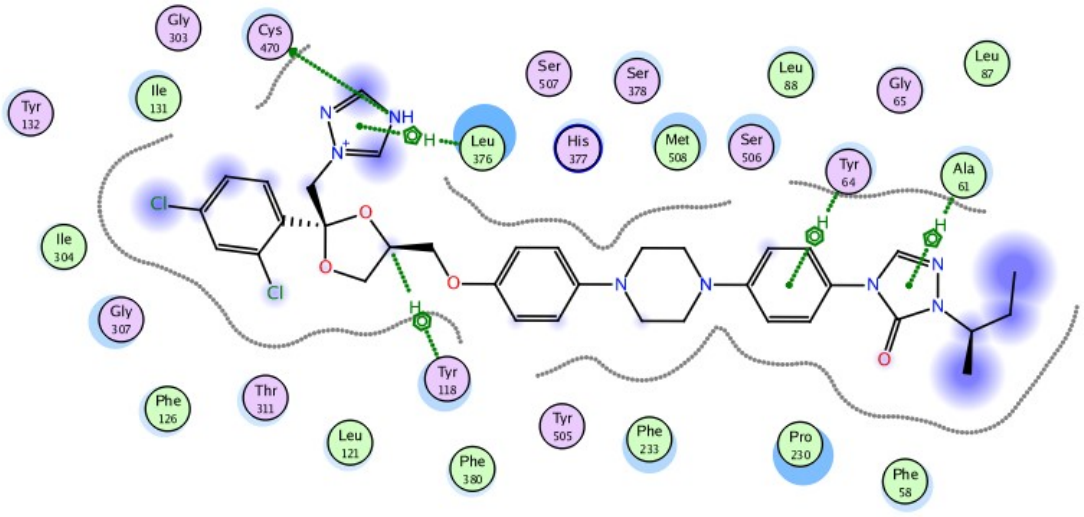
Ligand Interactions Report

Mon Sep 20 09:19:53 2021 (MOE 2014.09)

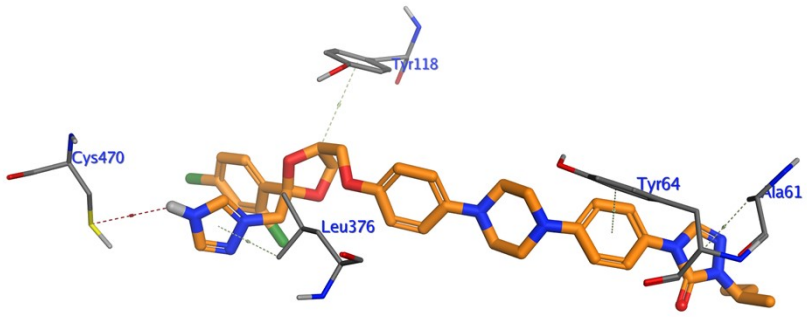
5v5z prepared.pdb: OXIDOREDUCTASE/OXIDOREDUCATSE INHIBITOR / 5v5z prepared.pdb: OXIDOREDUCTASE/OXIDOREDUCATSE INHIBITOR

Ligand Receptor Interaction Distance E (kcal/mol)

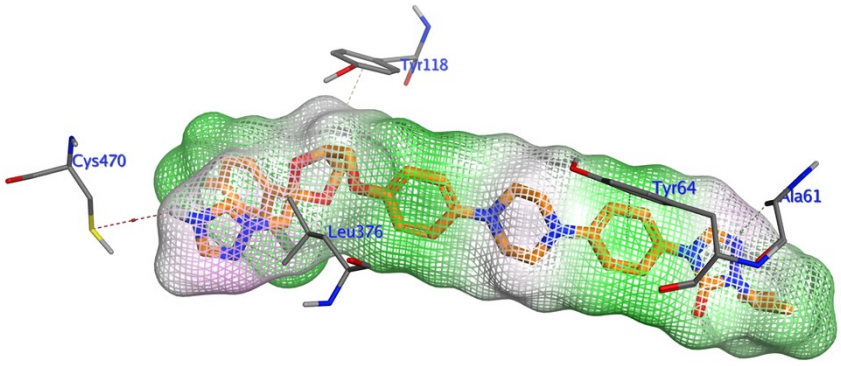
N39	39	SG	CYS	470	H-donor	4.23	-0.7
C31	31	6-ring	TYR	118	Hydrophobic	3.97	-0.7
5-ring	CB	ALA	61	pi-H	3.89	-0.6	
6-ring	CE2	TYR	64	pi-H	4.13	-0.6	
5-ring	CD1	LEU	376	pi-H	4.25	-1.0	



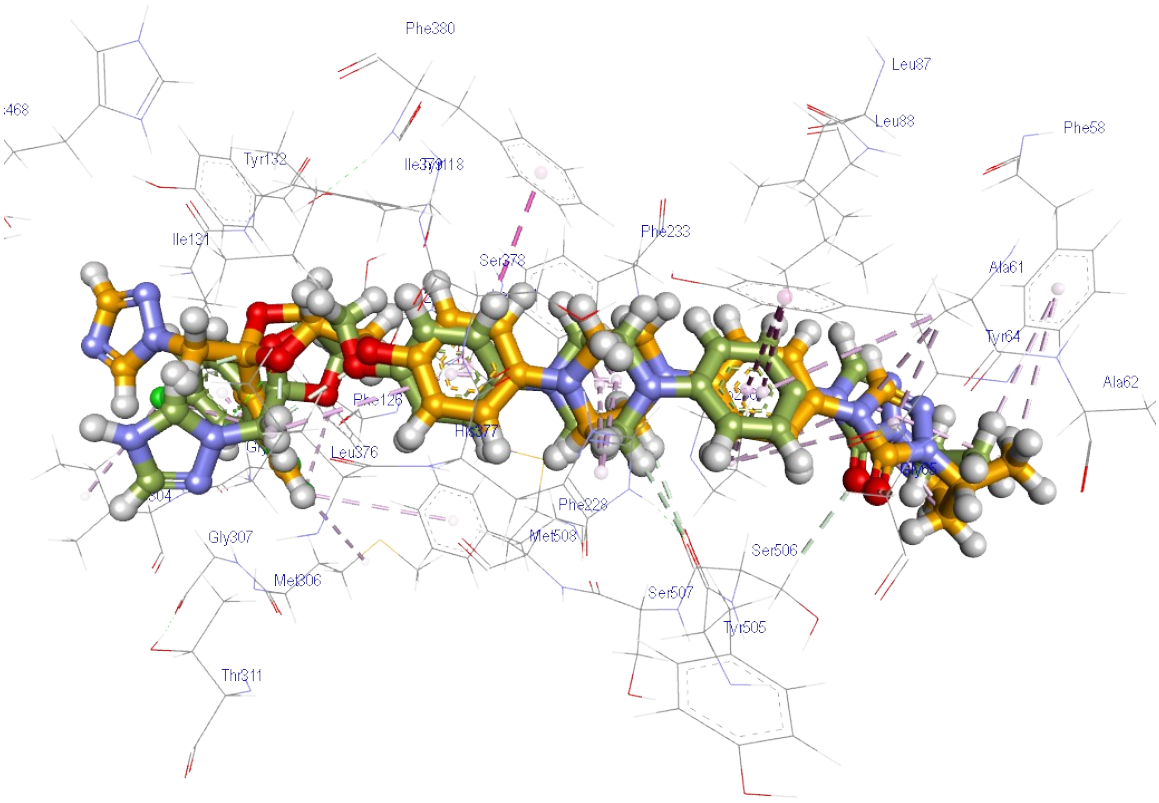
2D interactions of 1YN with Candida albicance oxidoreductases



3D interactions of 1YN with Candida albicance oxidoreductases



Positioning of 1YN with Candida albicance oxidoreductases



Superimposition of the re-docked 1YN conformer (golden) over that of the co-crystalized one (green) with RMSD value of 1.16

2.1.2 Compound #1

Score -1.80028617 RMSD 1.8228012

Ligand Interactions Report

Mon Dec 13 13:30:58 2021 (MOE 2014.09)

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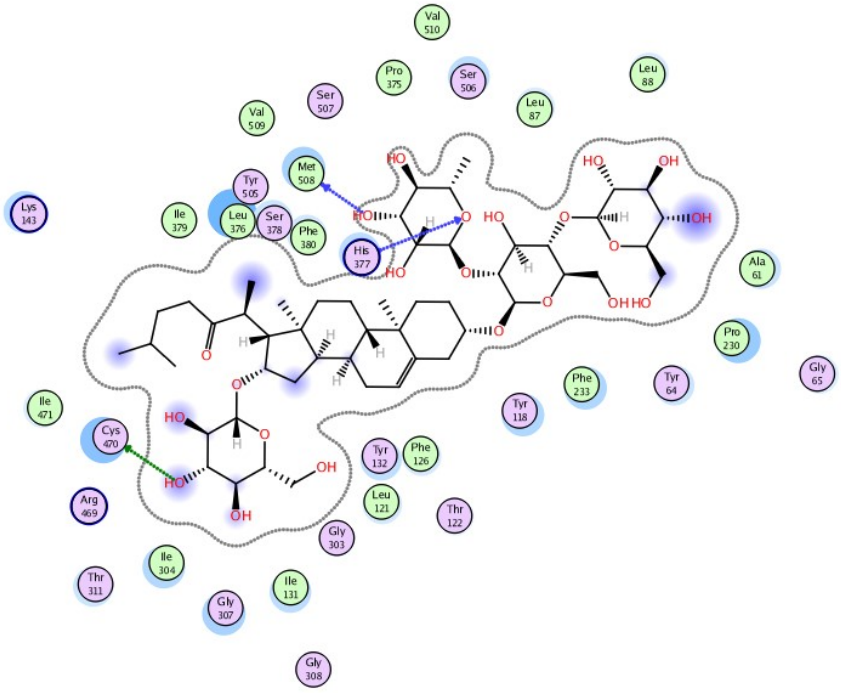
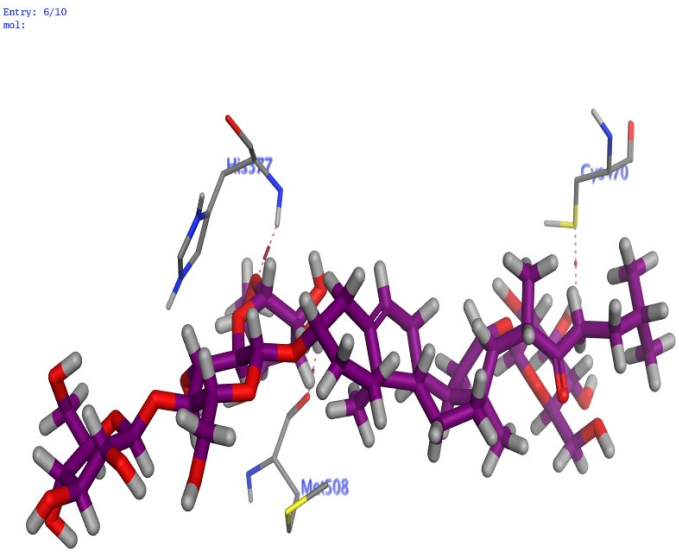
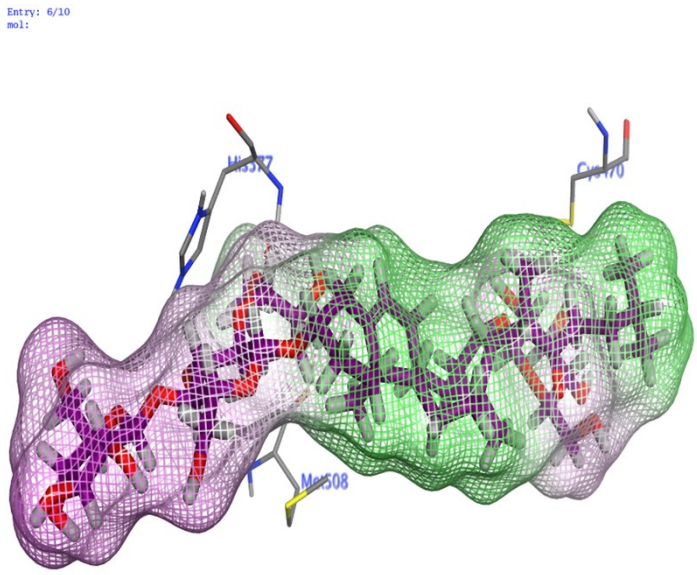
Ligand	Receptor		Interaction		Distance	E	(kcal/ml)
O	38	SG	CYS	470	H-donor	3.18	-1.3
O	48	O	MET	508	H-donor	2.41	1.8
O	46	N	HIS	377	H-acceptor	2.96	-3.0



2D interactions of **1** with *Candida albicance* oxidoreductases



3D interactions of **1** with *Candida albicance* oxidoreductases



Positioning of **1** in *Candida albicance* oxidoreductases

2.1.3 Compound #2

Score -4.07385206 RMSD 1.78011239

Ligand Interactions Report

Tue Dec 14 08:58:21 2021 (MOE 2014.09)

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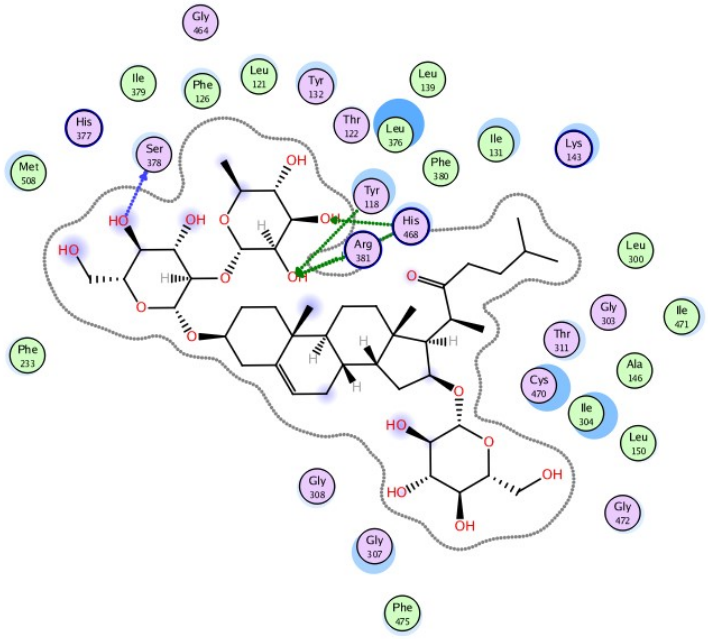
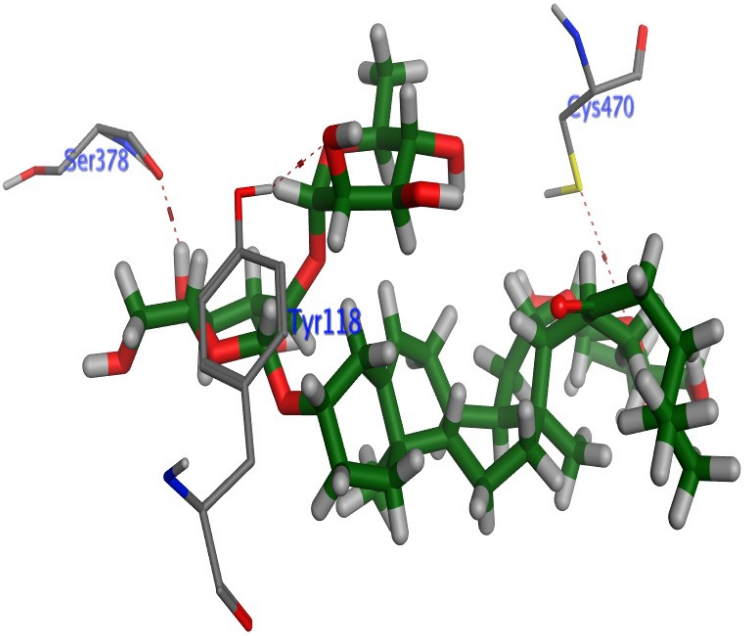
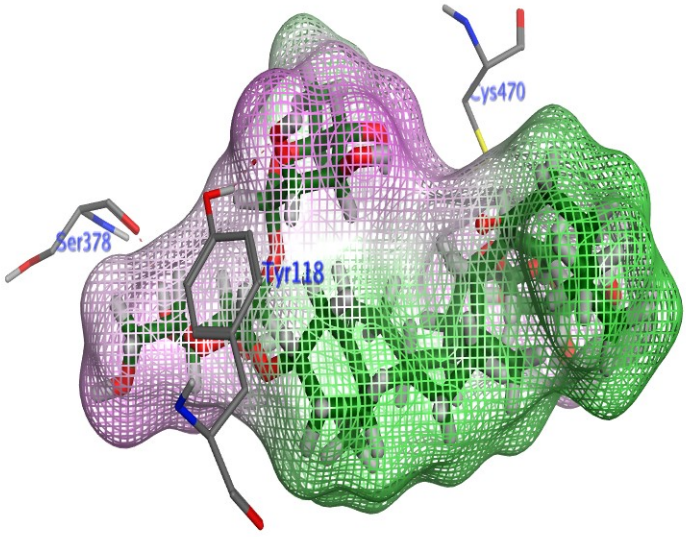
Ligand	Receptor	Interaction	Distance	E (kcal/mol)
O 62	O SER 378	H-donor	2.78	-2.5
O 47	OH TYR 118	H-acceptor	2.85	-1.2
O 47	NH1 ARG 381	H-acceptor	2.93	-2.8
O 48	ND1 HIS 468	H-acceptor	3.35	-0.7
O 47	5-ring HIS 468	H-pi	4.49	-2.3



2D interactions of **2** with *Candida albicance* oxidoreductases



3D interactions of **2** with *Candida albicance* oxidoreductases



Positioning of **2** in *Candida albicance* oxidoreductases

2.1.4 Compound #3

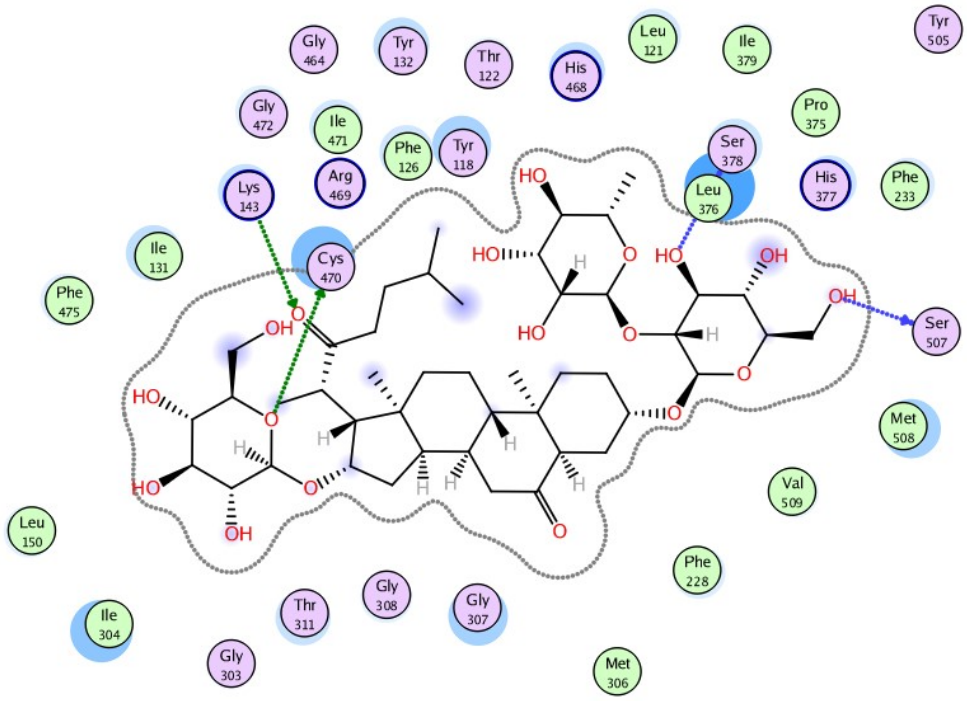
Score -10.7376976 RMSD 1.91103399

Ligand Interactions Report

Tue Dec 14 09:27:57 2021 (MOE 2014.09)

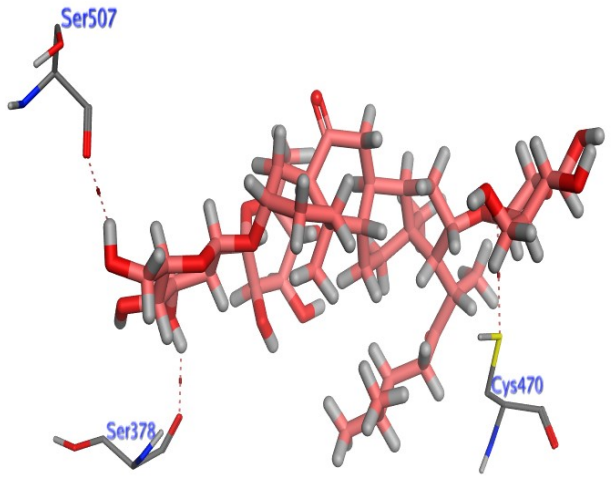
5v5z prepared.pdb: OXIDOREDUCTASE/OXIDOREDUCATSE INHIBITOR / 5v5z prepared.pdb

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
O 33	SG CYS 470	H-donor	3.48	-0.9
O 58	O SER 507	H-donor	3.23	-0.7
O 59	O SER 378	H-donor	3.04	-1.1
O 63	NZ LYS 143	H-acceptor	3.54	-0.8

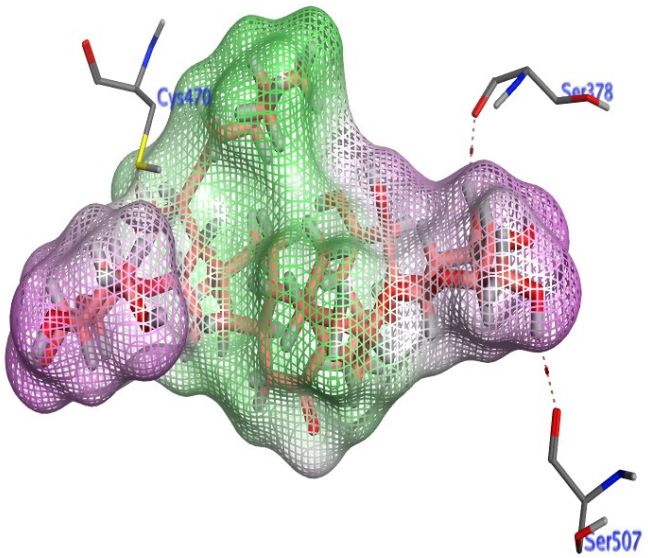


2D interactions of **3** with *Candida albicance* oxidoreductases

Entry: 2/10
mol:



3D interactions of **3** with *Candida albicance* oxidoreductases



Positioning of **3** in *Candida albicance* oxidoreductases

2.1.5 Compound #4

Score -11.3269691 RMSD 1.73269594

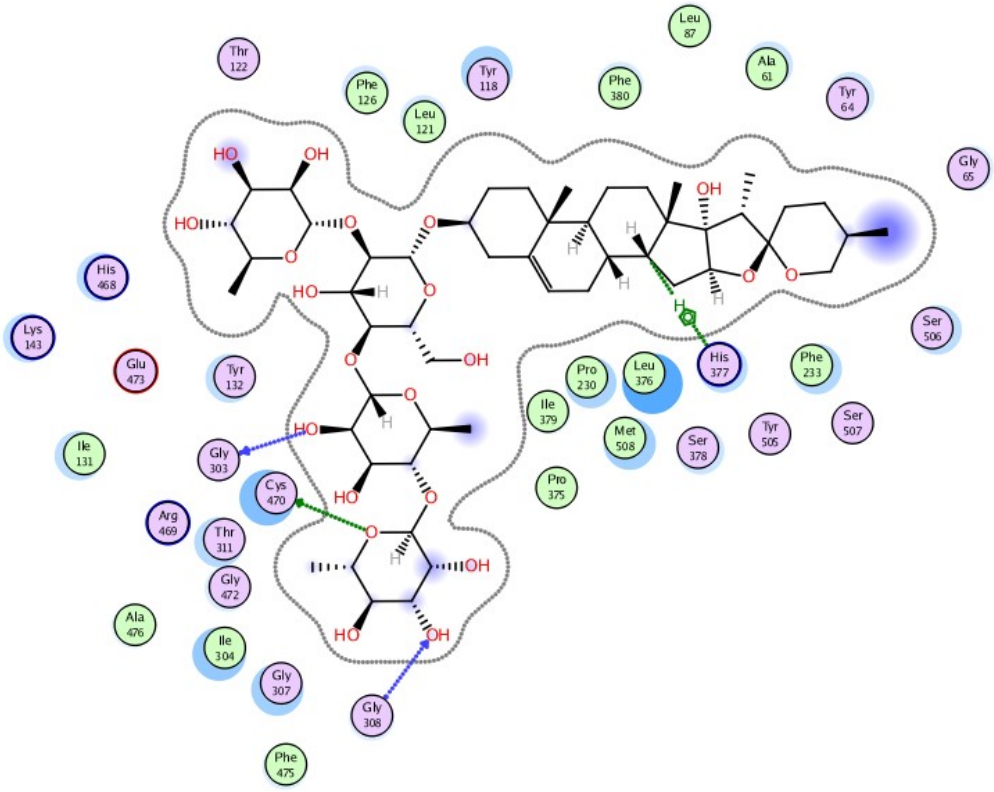
Ligand Interactions Report

Mon Sep 20 22 09:41:19 2021 (MOE 2014.09)

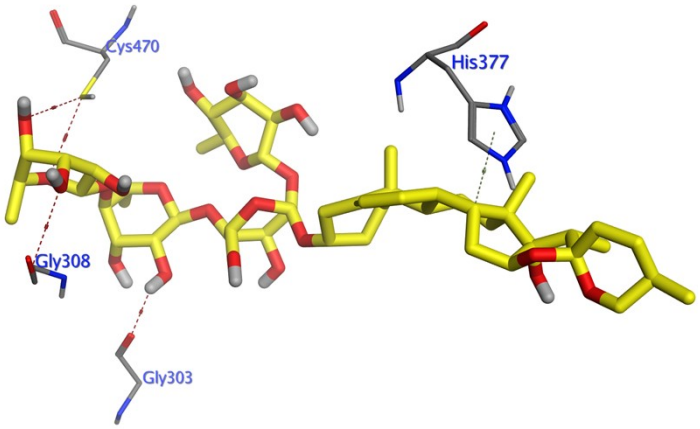
5v5z prepared.pdb: OXIDOREDUCTASE/OXIDOREDUCATSE INHIBITOR / 5v5z prepared.pdb

Ligand Receptor Interaction Distance E (kcal/mol)

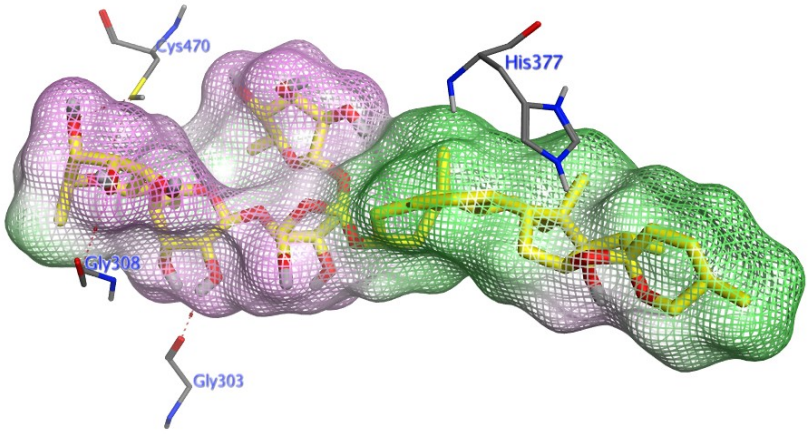
O	57	O	GLY	303	H-donor	2.76	-1.1
O	66	SG	CYS	470	H-donor	3.39	-1.5
O	68	CA	GLY	308	H-acceptor	3.13	-0.5
C	21	5-ring	HIS	377	H-pi	4.04	-0.7



2D interactions of **4** with Candida albicance oxidoreductases



3D interactions of **4** with Candida albicance oxidoreductases



Positioning of **4** with Candida albicance oxidoreductases

2.1.6 Compound #5

Score -9.89089775 RMSD 1.59490478

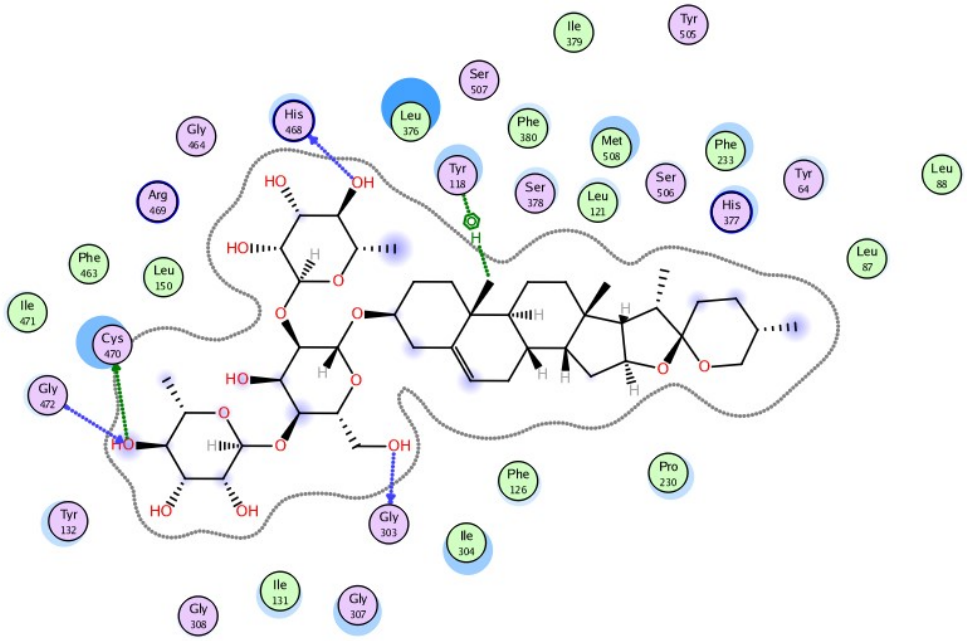
Ligand Interactions Report

Wed Sep 22 12:00:06 2021 (MOE 2014.09)

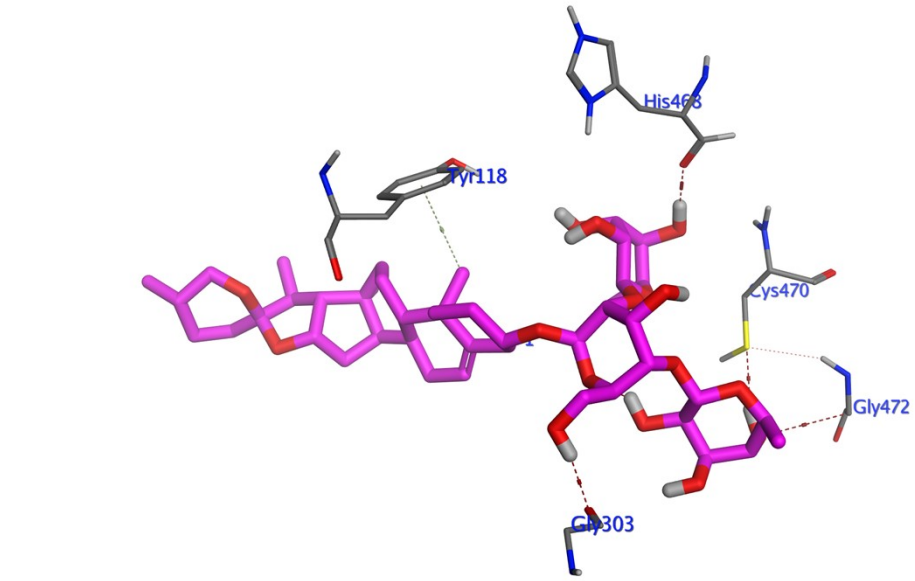
5v5z prepared.pdb: OXIDOREDUCTASE/OXIDOREDUCATSE INHIBITOR / 5v5z prepared.pdb

Ligand Receptor Interaction Distance E (kcal/mol)

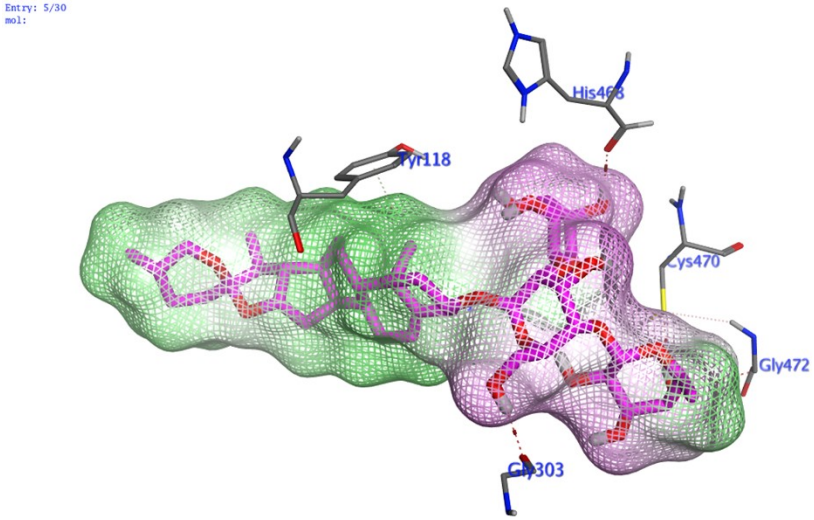
O	36	O	GLY	303	H-donor	2.84	-1.5
O	49	O	HIS	468	H-donor	2.84	-2.7
O	60	SG	CYS	470	H-donor	3.15	-1.4
O	60	CA	GLY	472	H-acceptor	3.29	-0.5
C	27	6-ring	TYR	118	H-pi	4.61	-0.6



2D interactions of **5** with Candida albicance oxidoreductases



3D interactions of **5** with Candida albicance oxidoreductases



Positioning of **5** with Candida albicance oxidoreductases

2.1.7 Compound #6

Score -13.4313364 RMSD 1.56254482

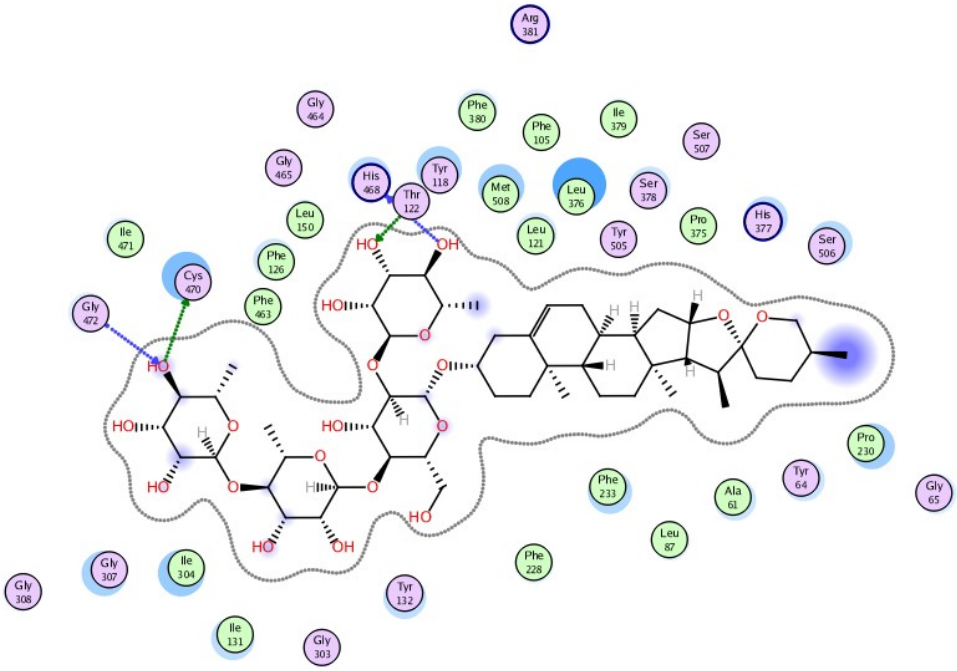
Ligand Interactions Report

Wed Sep 22 12:24:44 2021 (MOE 2014.09)

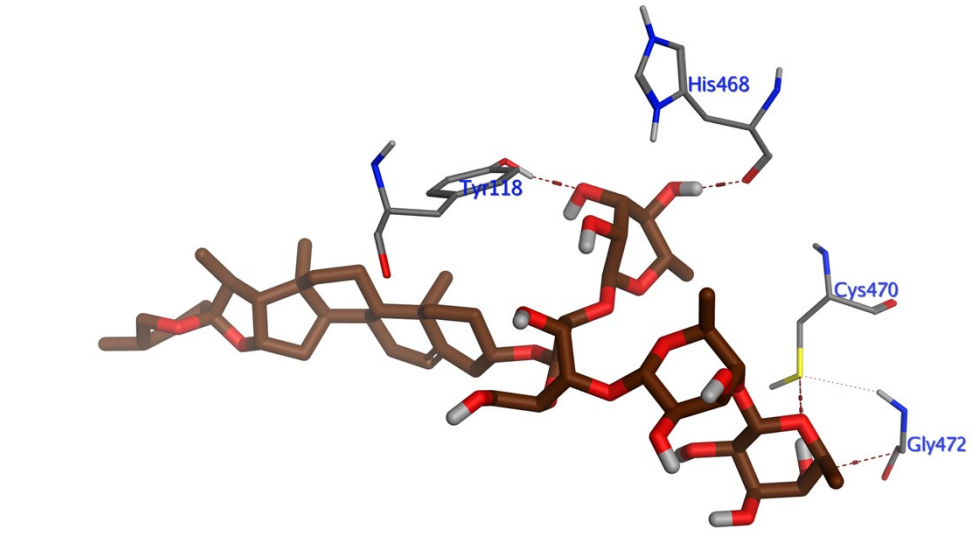
5v5z prepared.pdb: OXIDOREDUCTASE/OXIDOREDUCATSE INHIBITOR / 5v5z prepared.pdb

Ligand Receptor Interaction Distance E (kcal/mol)

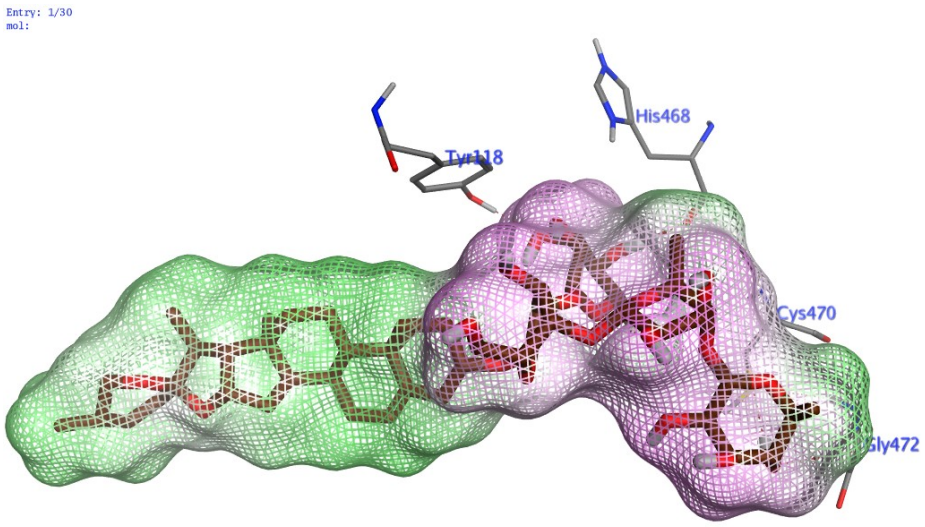
O	9	O	HIS	468	H-donor	2.89	-2.2
O	69	SG	CYS	470	H-donor	3.28	-1.3
O	8	OH	TYR	118	H-acceptor	2.92	-1.4
O	69	CA	GLY	472	H-acceptor	3.29	-0.5



2D interactions of **6** with Candida albicance oxidoreductases



3D interactions of **6** with Candida albicance oxidoreductases



Positioning of **6** with Candida albicance oxidoreductases

2.1.8 Compound #7

Score -9.89949226 RMSD 1.93743289

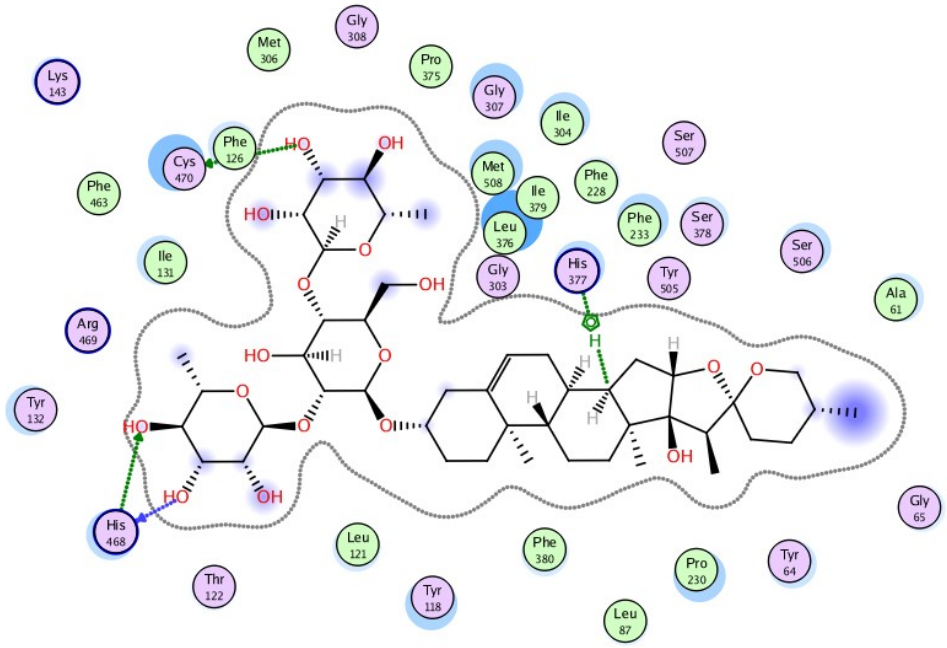
Ligand Interactions Report

Wed Sep 22 13:06:37 2021 (MOE 2014.09)

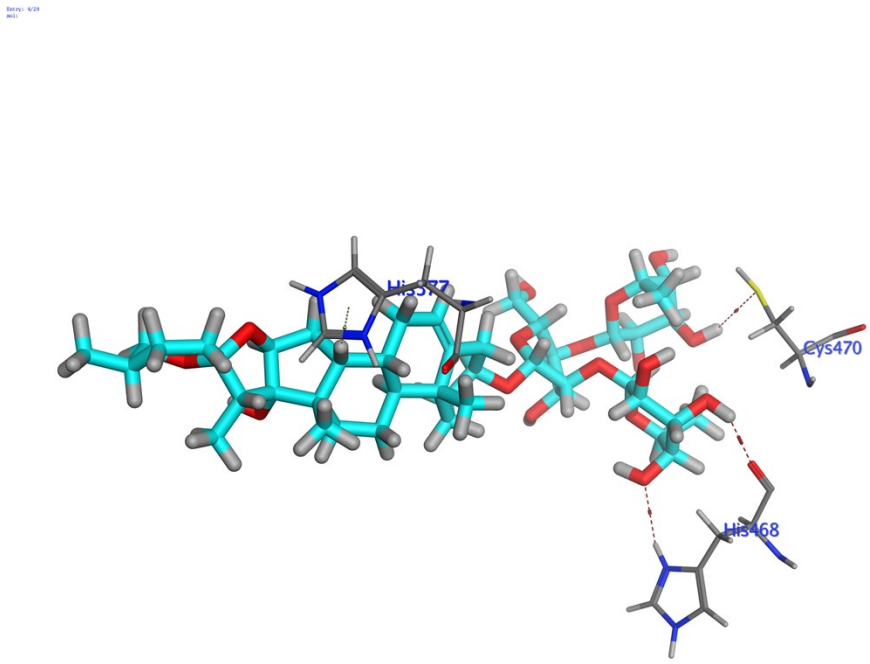
5v5z prepared.pdb: OXIDOREDUCTASE/OXIDOREDUCATSE INHIBITOR / 5v5z prepared.pdb

Ligand Receptor Interaction Distance E (kcal/mol)

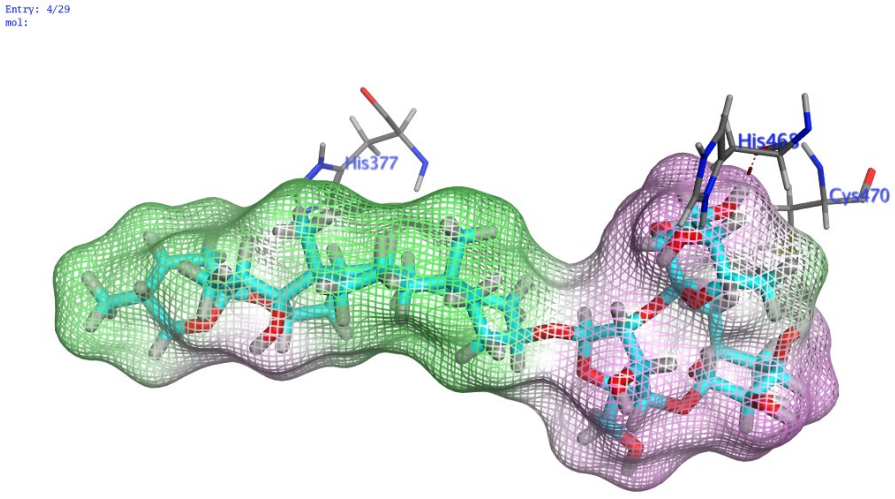
O	8	O	HIS	468	H-donor	2.81	-1.8
O	58	SG	CYS	470	H-donor	3.98	-0.7
O	9	ND1	HIS	468	H-acceptor	3.30	-0.7
C	21	5-ring	HIS	377	H-pi	4.11	-0.8



2D interactions of **7** with Candida albicance oxidoreductases



3D interactions of **7** with Candida albicance oxidoreductases



Positioning of **7** with Candida albicance oxidoreductases

2.2 Antitrypanosomal, 2JK6

2.2.1 FAD Redocked

Score -10.2982645 RMSD 1.61059213

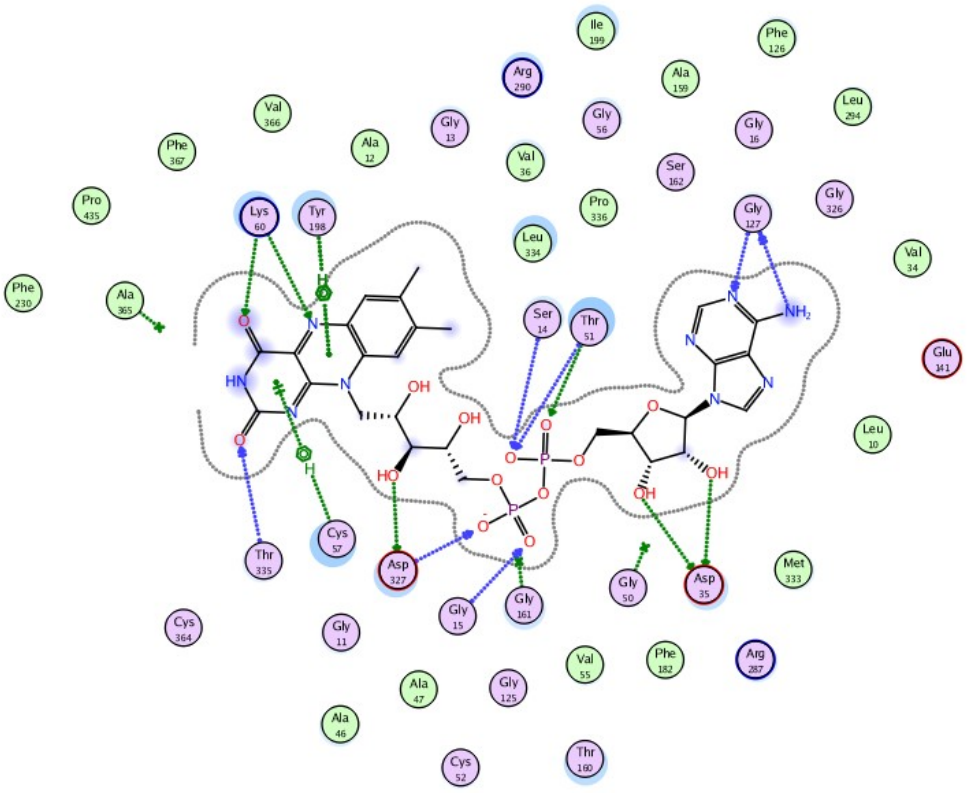
Ligand Interactions Report

Mon Sep 13 10:48:44 2021 (MOE 2014.09)

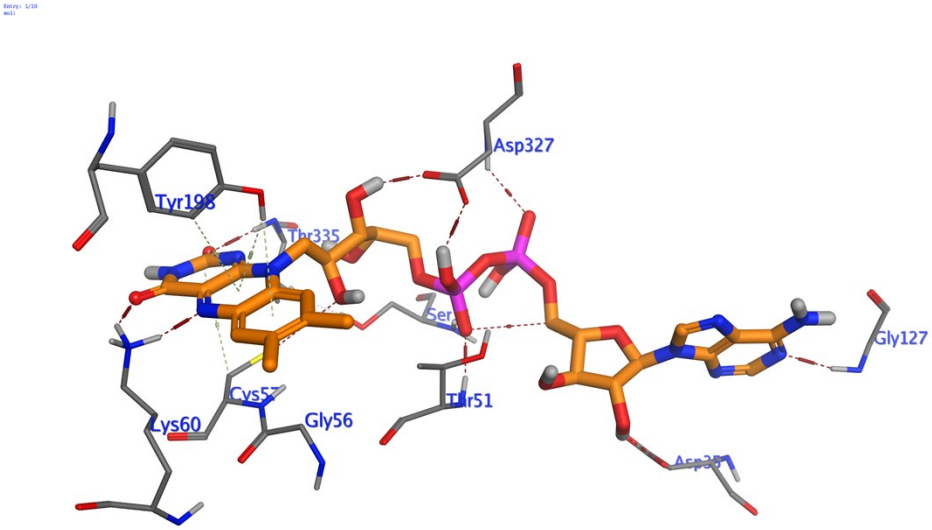
2JK6: *L. Infantum* trypanothione reductase / 2JK6: trypanothione reductase

Ligand Receptor Interaction Distance E (kcal/mol)

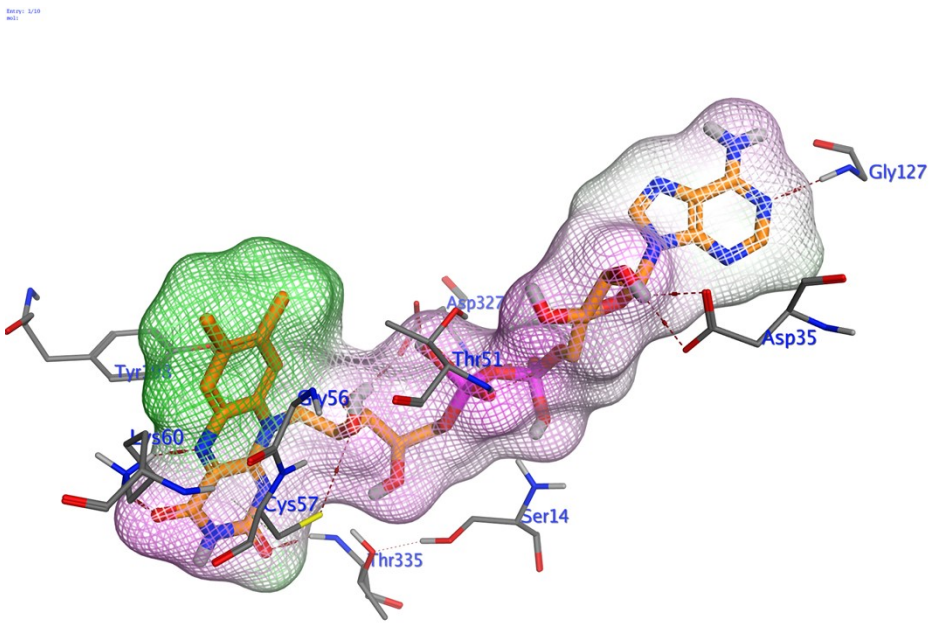
O3B	13	OD2	ASP	35	(A)	H-donor	2.43	5.3
O2B	17	OD1	ASP	35	(A)	H-donor	2.78	-4.5
N6A	27	O	GLY	127	(A)	H-donor	2.85	-3.6
O3'	71	OD1	ASP	327	(A)	H-donor	2.47	2.4
O2A	2	OG1	THR	51	(A)	H-acceptor	2.35	23.6
O1A	3	N	SER	14	(A)	H-acceptor	3.46	-1.7
O1A	3	N	THR	51	(A)	H-acceptor	2.84	-6.5
N1A	30	N	GLY	127	(A)	H-acceptor	2.78	-3.7
O2	37	N	THR	335	(A)	H-acceptor	2.69	-4.7
O4	41	NZ	LYS	60	(A)	H-acceptor	2.64	-3.9
N5	43	NZ	LYS	60	(A)	H-acceptor	2.82	-10.5
O1P	82	N	GLY	15	(A)	H-acceptor	2.58	-2.5
O2P	83	N	ASP	327	(A)	H-acceptor	2.67	-4.0
	6-ring	CB	CYS	57	(A)	pi-H	3.68	-0.8
	6-ring	CE2	TYR	198	(A)	pi-H	3.98	-1.2
	6-ring	OH	TYR	198	(A)	pi-H	4.15	-2.9



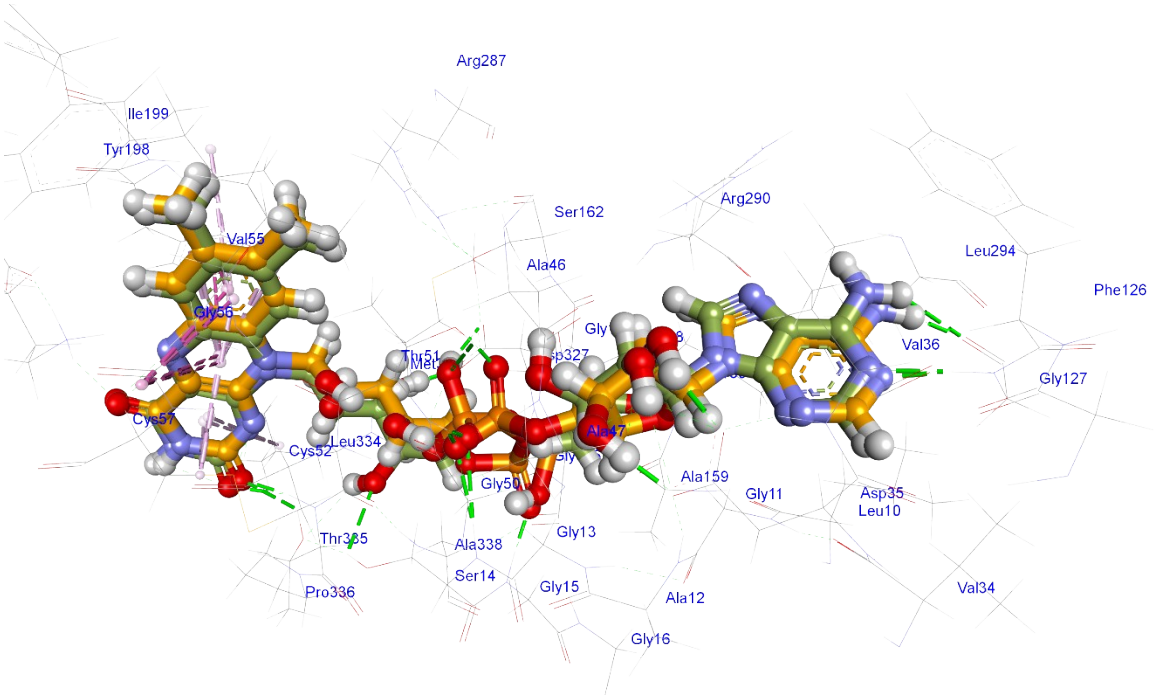
2D interactions of **FAD** with *Leishmania infantum* trypanothione reductase



3D interactions of **FAD** with Leishmania infantum trypanothione reductase



Positioningof **FAD** with *Leishmania infantum* trypanothione reductase



Superimposition of the re-docked **FAD** conformer (golden) over that of the co-crystalized one (green) with RMSD value of 1.61

2.2.2 Compound #1

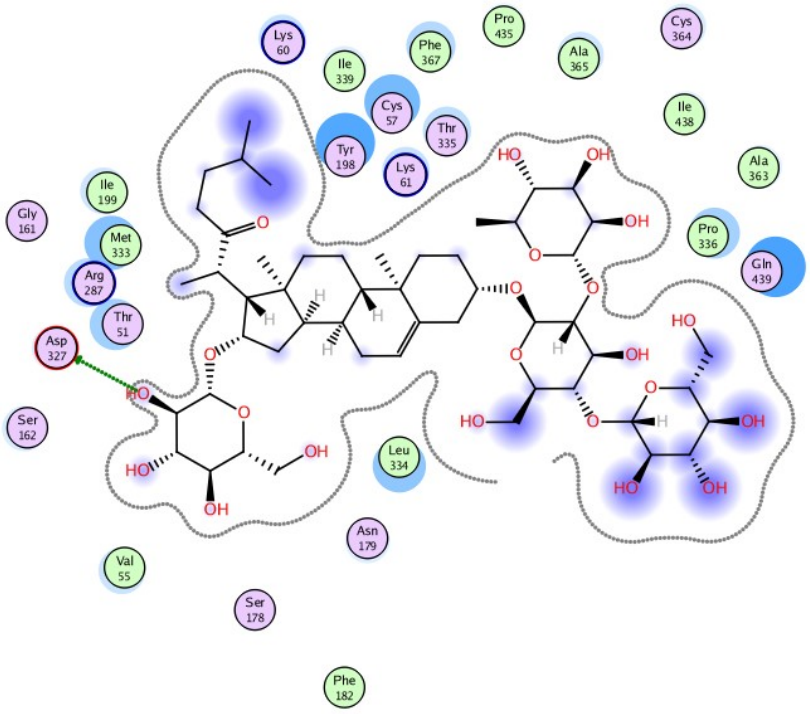
Score 22.1789684 RMSD 1.60361874

Ligand Interactions Report

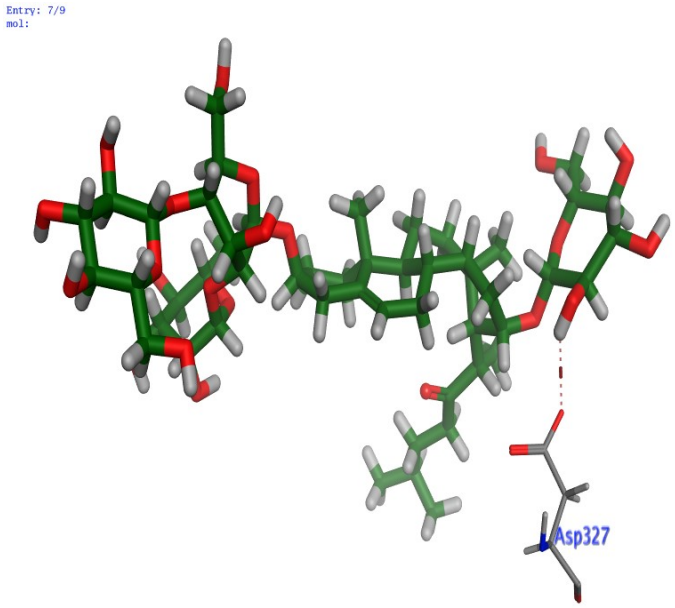
Tue Dec 14 10:03:47 2021 (MOE 2014.09)

2jk6 prepared.pdb: *L. Infantum* trypanothione reductase / 2jk6 prepared.pdb

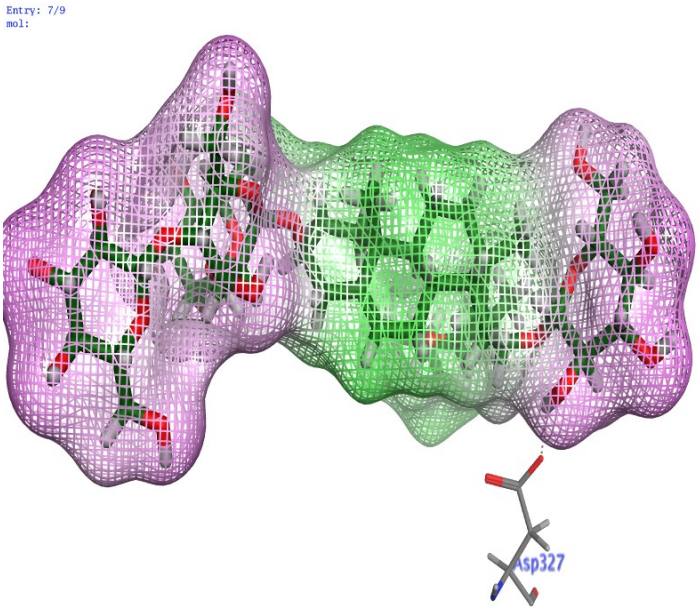
Ligand	Receptor	Interaction	Distance	E (kcal/mol)
O 39	OD2 ASP 327	H-donor	3.16	-1.6



2D interactions of **1** with *Leishmania infantum* trypanothione reductase



3D interactions of **1** with *Leishmania infantum* trypanothione reductase



Positioning of **1** in *Leishmania infantum* trypanothione reductase

2.2.3 Compound #2

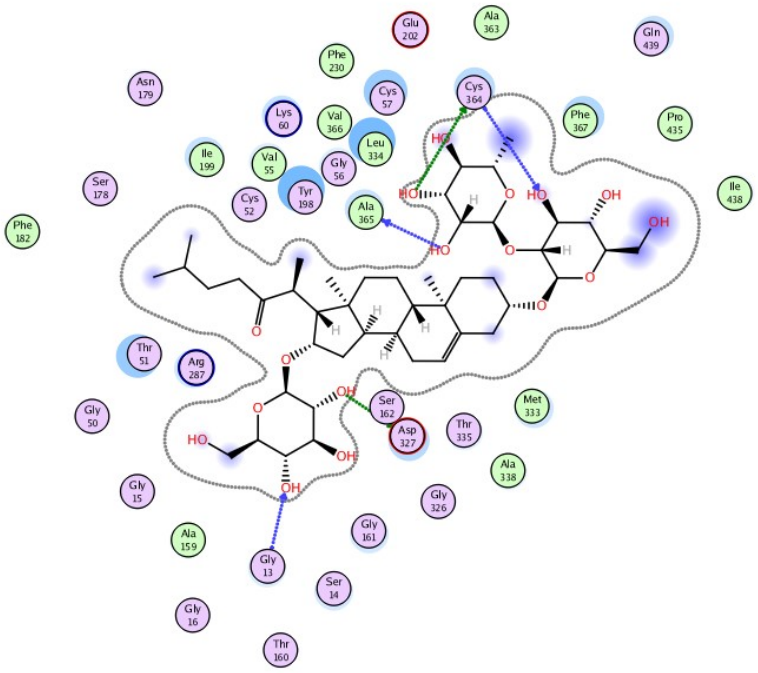
Score 13.7332754 RMSD 1.60623026

Ligand Interactions Report

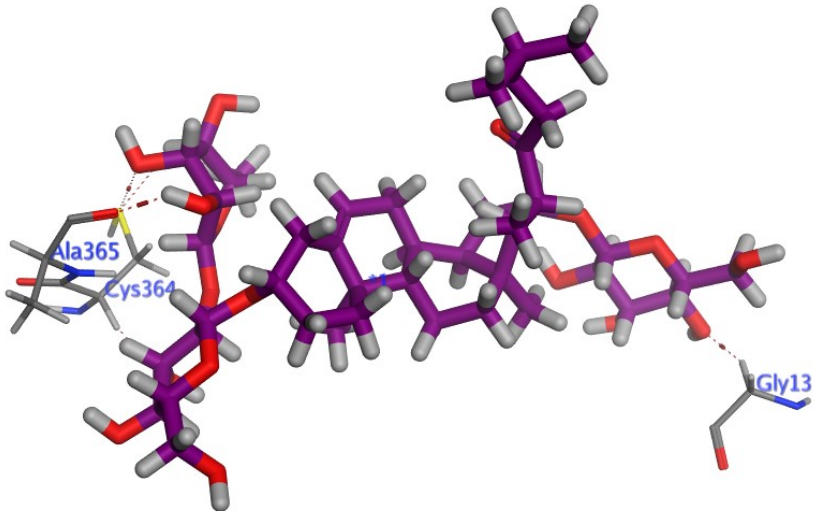
Tue Dec 14 19:44:12 2021 (MOE 2014.09)

2jk6 prepared.pdb: *L. Infantum* trypanothione reductase / 2jk6 prepared.pdb

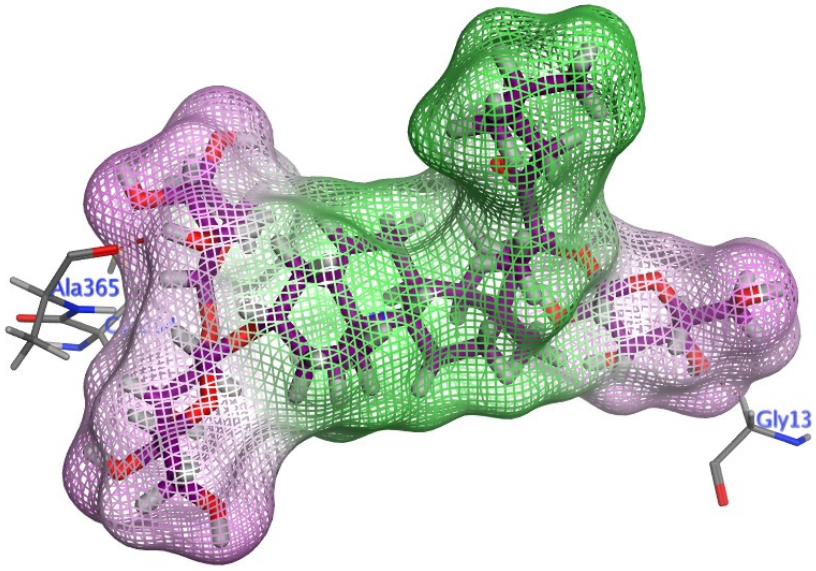
Ligand	Receptor	Interaction	Distance	E (kcal/mol)
O 39	OD1 ASP 327	H-donor	2.52	-1.4
O 47	O ALA 365	H-donor	2.44	-0.2
O 48	SG CYS 364	H-donor	3.70	-1.2
O 40	CA GLY 13	H-acceptor	3.02	-1.0
O 60	CA CYS 364	H-acceptor	3.26	-0.6



2D interactions of **2** with *Leishmania infantum* trypanothione reductase



3D interactions of **2** with *Leishmania infantum* trypanothione reductase



Positioning of **2** in *Leishmania infantum* trypanothione reductase

2.2.4 Compound #3

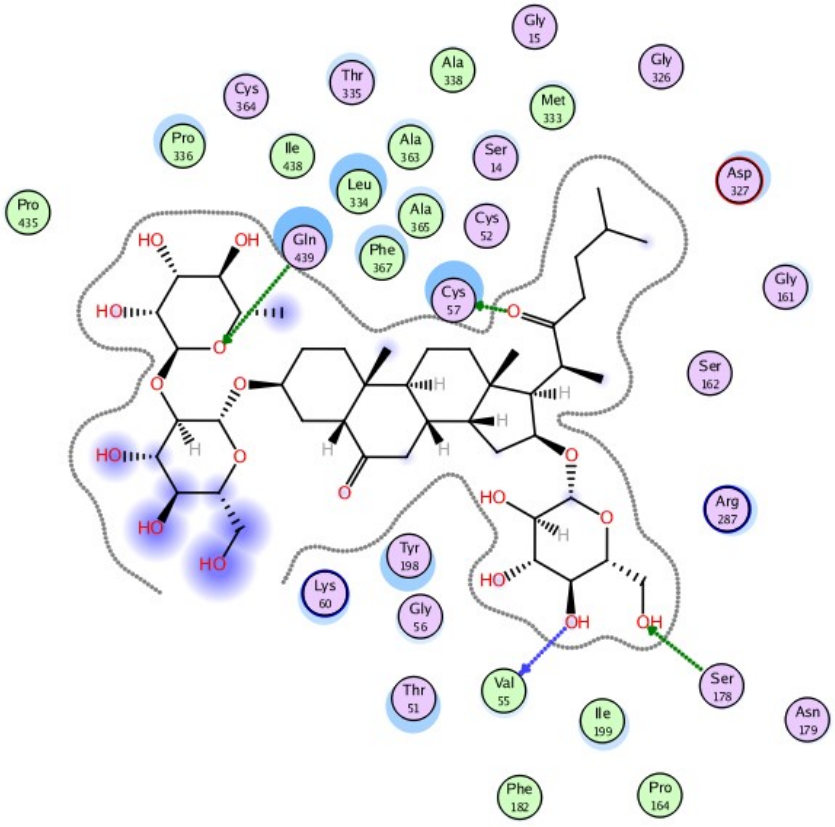
Score 1.48917317 RMSD 1.73117518

Ligand Interactions Report

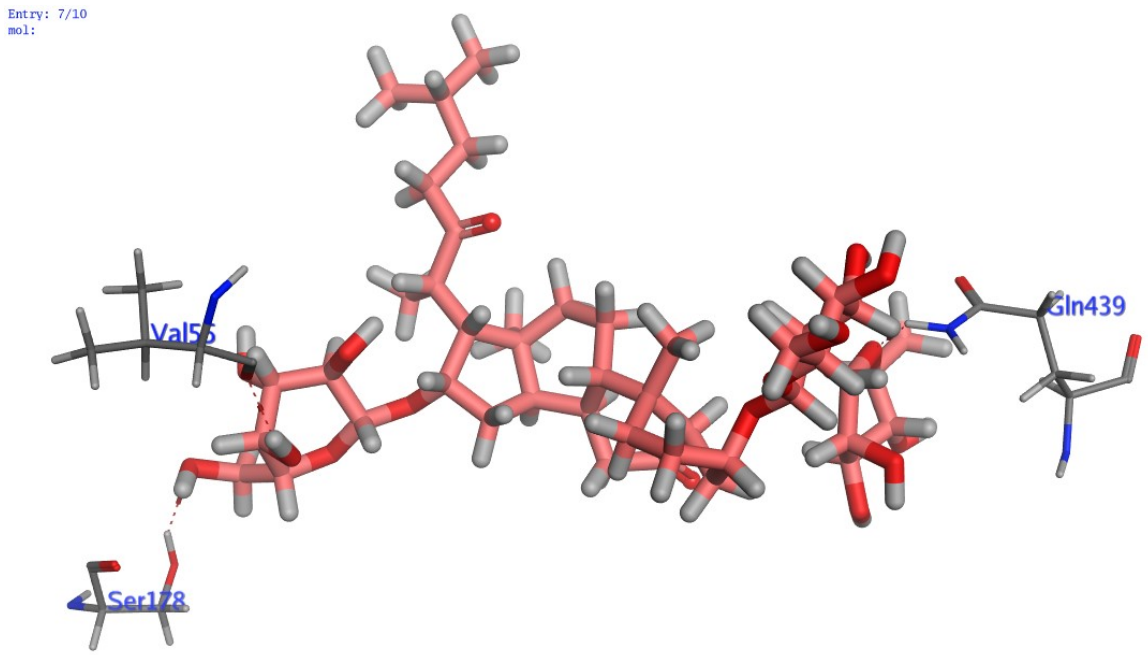
Tue Dec 14 19:44:12 2021 (MOE 2014.09)

2jk6 prepared.pdb: *L. Infantum* trypanothione reductase / 2jk6 prepared.pdb

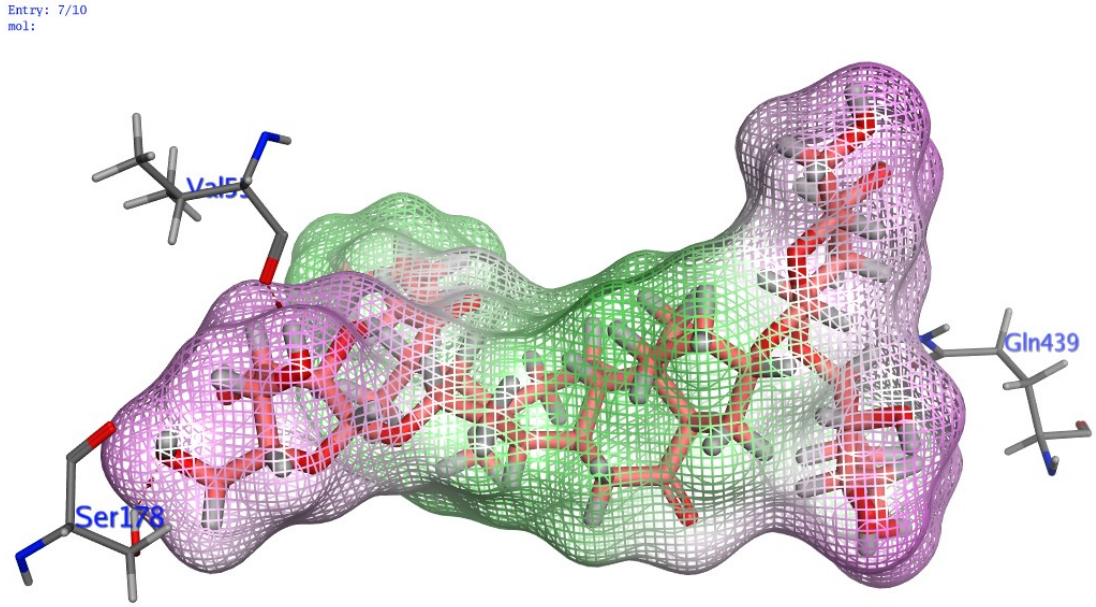
Ligand	Receptor	Interaction	Distance	E (kcal/mol)
O 39	O VAL 55	H-donor	2.50	0.2
O 63	SG CYS 57	H-donor	3.25	-0.4
O 36	OG SER 178	H-acceptor	2.83	0.8
O 45	NE2 GLN 439	H-acceptor	2.46	2.5



2D interactions of **3** with *Leishmania infantum* trypanothione reductase



3D interactions of **3** with *Leishmania infantum* trypanothione reductase



Positioning of **3** in *Leishmania infantum* trypanothione reductase

2.2.5 Compound #4

Score -4.41324139 RMSD 1.67518234

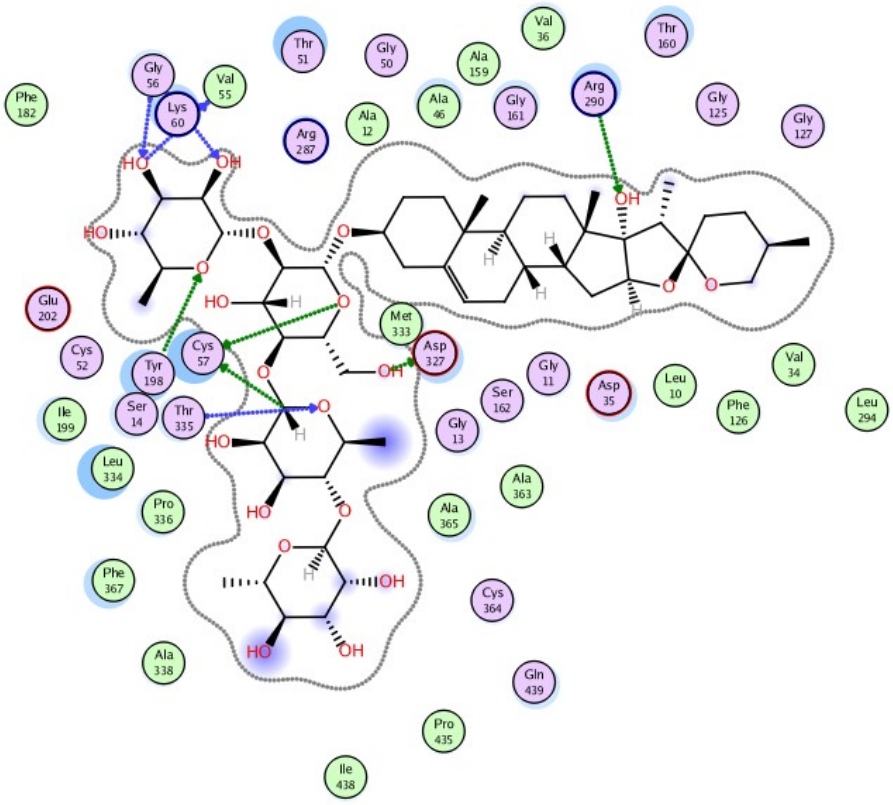
Ligand Interactions Report

Mon Sep 13 12:02:51 2021 (MOE 2014.09)

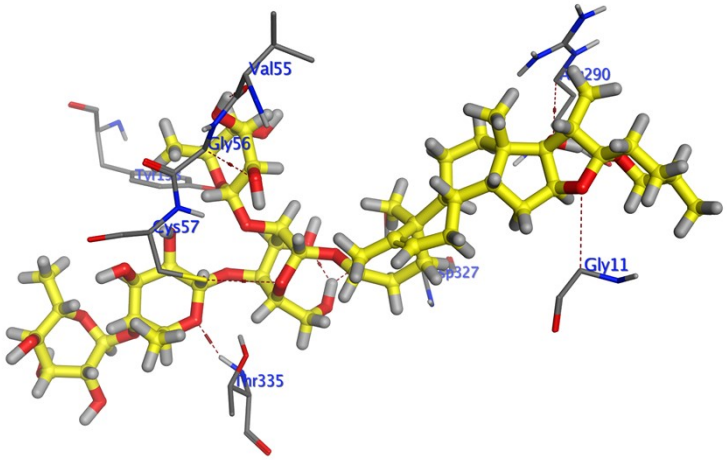
2JK6: *L. Infantum* trypanothione reductase / 2JK6

Ligand Receptor Interaction Distance E (kcal/mol)

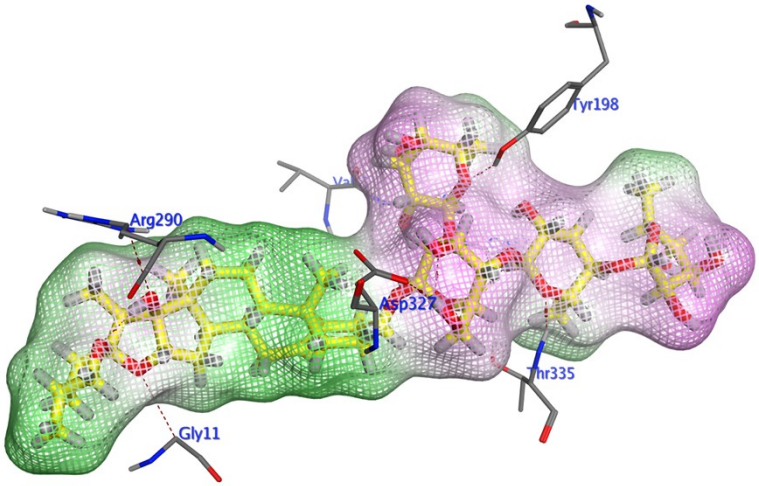
O	8	O	VAL	55	(A)	H-donor	2.68	-2.3
O	42	SG	CYS	57	(A)	H-donor	3.52	-0.7
O	46	OD1	ASP	327	(A)	H-donor	2.67	-1.1
C	55	SG	CYS	57	(A)	H-donor	3.62	-0.9
O	6	OH	TYR	198	(A)	H-acceptor	2.94	-1.6
O	7	CA	GLY	56	(A)	H-acceptor	2.84	-0.9
O	8	CA	GLY	56	(A)	H-acceptor	2.92	-0.3
O	56	N	THR	335	(A)	H-acceptor	2.82	-3.4
O	72	CD	ARG	290	(A)	H-acceptor	3.21	-0.5



2D interactions of **4** with Leishmania infantum trypanothione reductase



3D interactions of **4** with Leishmania infantum trypanothione reductase



Positioning of **4** with Leishmania infantum trypanothione reductase

2.2.6 Compound #5

Score -0.789431393 RMSD 1.46603882

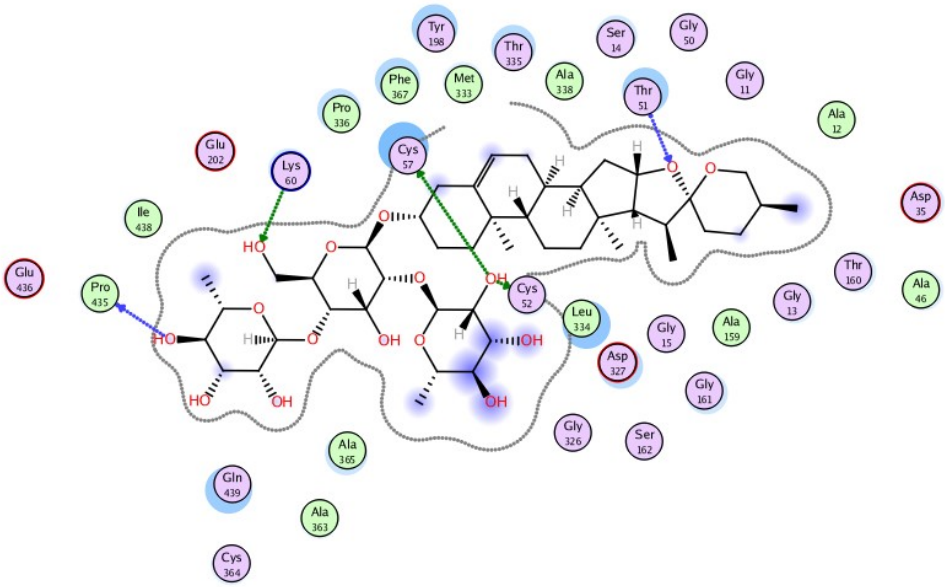
Ligand Interactions Report

Fri Sep 17 14:47:34 2021 (MOE 2014.09)

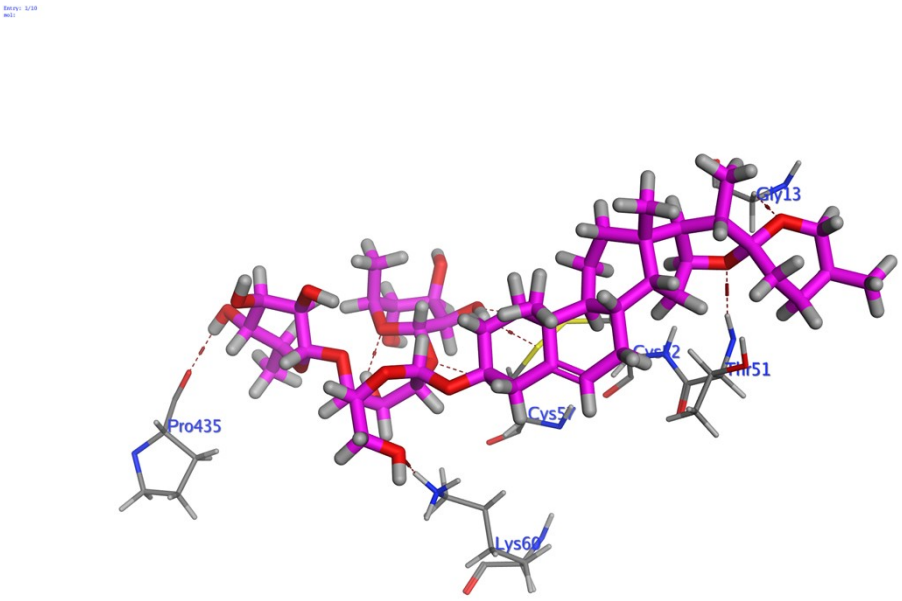
2jk6 prepared.pdb: L *L. Infantum* trypanothione reductase / 2jk6 prepared.pdb

Ligand Receptor Interaction Distance E (kcal/mol)

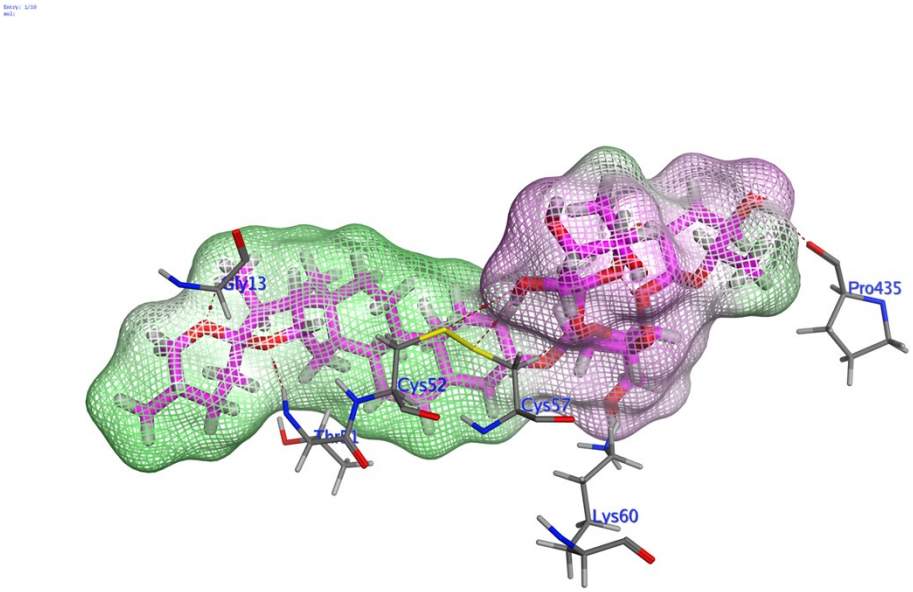
O	47	SG	CYS	52	H-donor	3.34	-0.9
O	47	SG	CYS	57	H-donor	3.10	-1.1
O	60	O	PRO	435	H-donor	2.75	-2.2
O	18	N	THR	51	H-acceptor	3.04	-3.0
O	36	NZ	LYS	60	H-acceptor	2.63	-1.1



2D interactions of **5** with Leishmania infantum trypanothione reductase



3D interactions of **5** with Leishmania infantum trypanothione reductase



Positioning of **5** with Leishmania infantum trypanothione reductase

2.2.7 Compound # 6
2.2.8 Compound #6

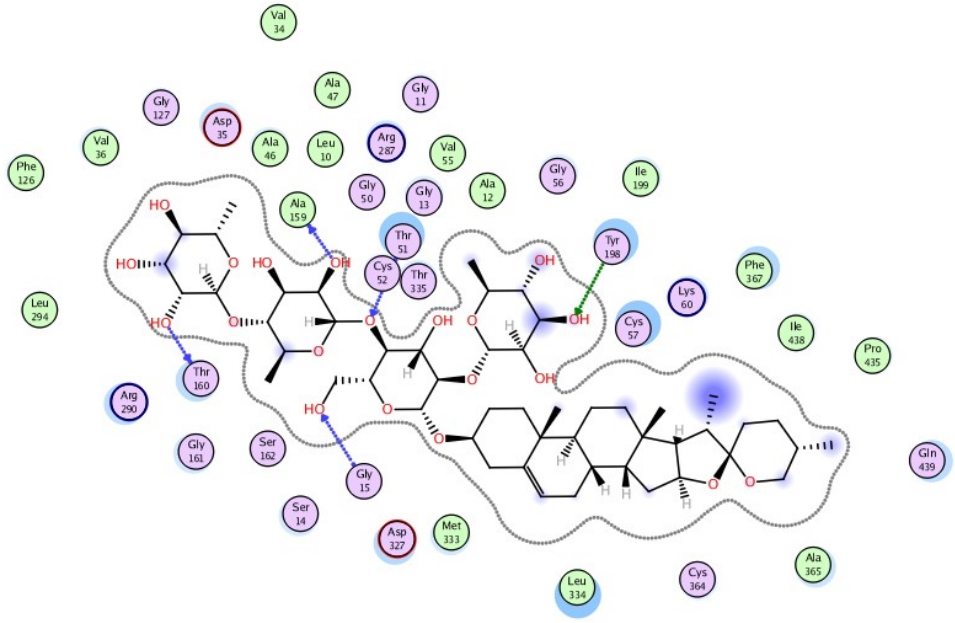
Score -3.72905278 RMSD 1.97958124

Ligand Interactions Report

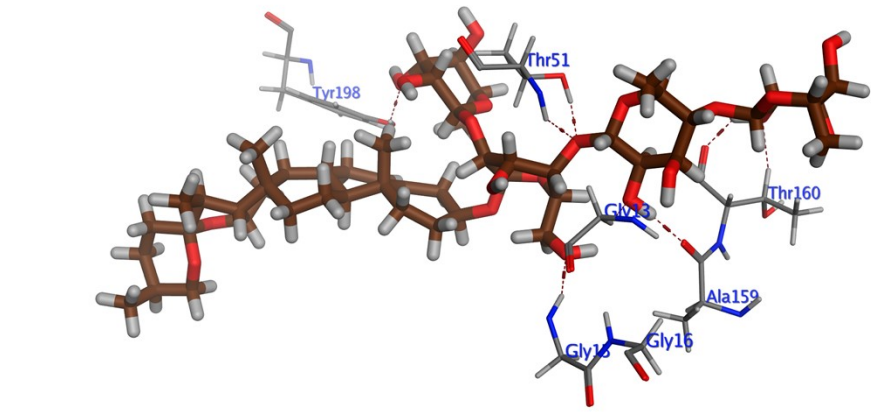
Fri Sep 24 08:16:01 2021 (MOE 2014.09)

2jk6 prepared.pdb: *L. Infantum* trypanothione reductase / 2jk6 prepared.pdb

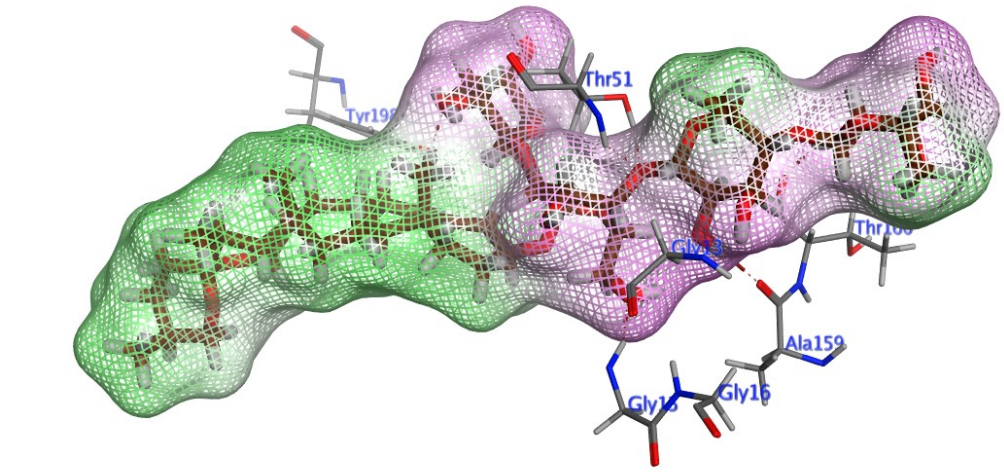
Ligand	Receptor		Interaction	Distance	E (kcal/mol)		
O	57	O	ALA	159	H-donor	2.55	-1.0
O	67	O	THR	160	H-donor	2.48	-0.4
O	8	OH	TYR	198	H-acceptor	2.94	-0.4
O	46	N	GLY	15	H-acceptor	3.17	-1.8
O	60	N	THR	51	H-acceptor	3.06	-1.4
O	60	OG1	THR	51	H-acceptor	2.59	-1.1



2D interactions of **6** with Leishmania infantum trypanothione reductase



3D interactions of **6** with Leishmania infantum trypanothione reductase



Positioning of **6** with Leishmania infantum trypanothione reductase

2.2.9 Compound #7

Score 4.6140976 RMSD 1.61256039

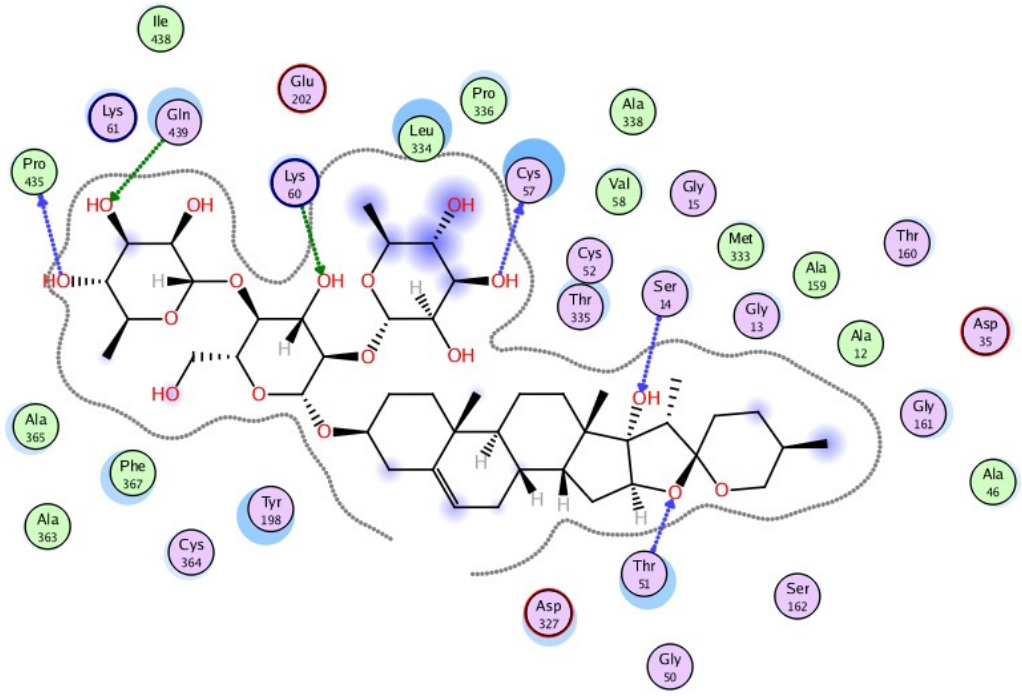
Ligand Interactions Report

Fri Sep 17 19:00:31 2021 (MOE 2014.09)

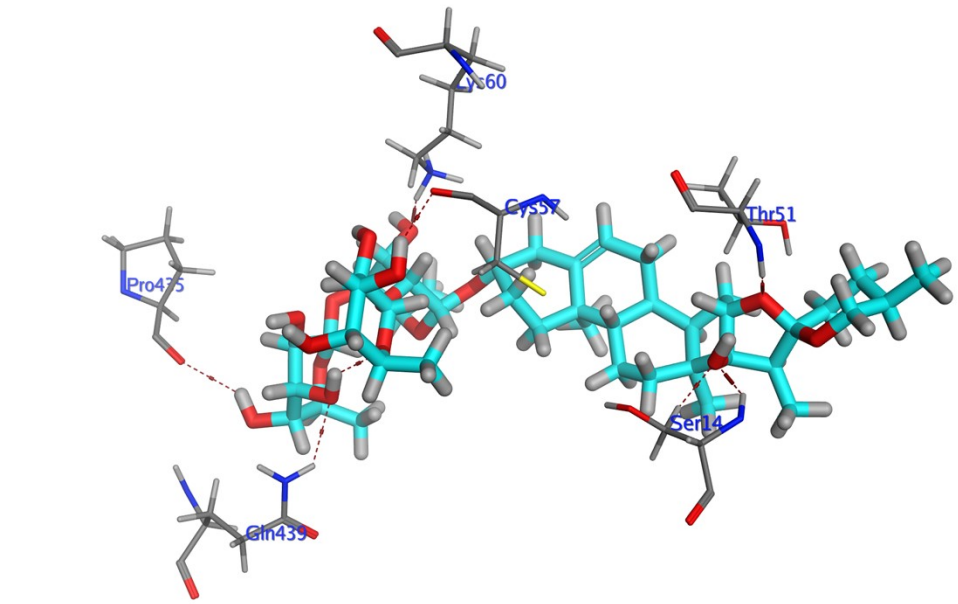
2jk6 prepared.pdb: *L. Infantum* trypanothione reductase / 2jk6 prepared.pdb

Ligand Receptor Interaction Distance E (kcal/mol)

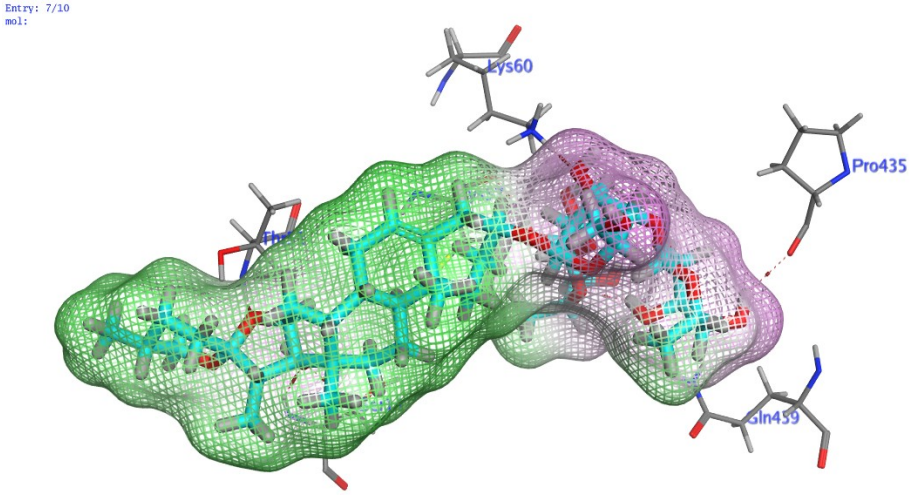
O	8	O	CYS	57	H-donor	2.90	-1.0
O	61	O	PRO	435	H-donor	3.20	-1.0
O	28	N	THR	51	H-acceptor	2.54	-1.9
O	47	NZ	LYS	60	H-acceptor	2.56	-5.7
O	58	NE2	GLN	439	H-acceptor	3.13	-0.7
O	62	N	SER	14	H-acceptor	2.53	1.6



2D interactions of **7** with Leishmania infantum trypanothione reductase



3D interactions of **7** with Leishmania infantum trypanothione reductase



Positioning of **7** with Leishmania infantum trypanothione reductase

3 PASS online predictions

Pa	Pi	
Compound #1		
0,962	0,001	Cholesterol antagonist
0,939	0,002	Proliferative diseases treatment
0,935	0,003	Caspase 3 stimulant
0,915	0,004	Alkenylglycerophosphocholine hydrolase inhibitor
0,900	0,002	Chemopreventive
0,901	0,003	Antihypercholesterolemic
0,883	0,003	Membrane integrity antagonist
0,880	0,003	CYP3A4 inducer
0,878	0,005	Antineoplastic
0,875	0,003	CYP3A inducer
0,870	0,003	Hepatoprotectant
0,868	0,016	CDP-glycerol glycerophosphotransferase inhibitor
0,853	0,005	Respiratory analeptic
0,842	0,004	Anticarcinogenic
0,837	0,004	UDP-glucuronosyltransferase substrate
0,825	0,004	Antiprotozoal (Leishmania)
0,821	0,004	Immunosuppressant
0,816	0,005	Oxidoreductase inhibitor
0,812	0,005	Glyceryl-ether monooxygenase inhibitor
0,786	0,010	Immunostimulant
0,768	0,009	CYP3A5 substrate
0,779	0,021	CYP2H substrate
0,747	0,003	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
0,741	0,008	Antifungal
0,734	0,005	Alkenylglycerophosphoethanolamine hydrolase inhibitor
0,738	0,011	Hypolipemic
0,731	0,021	CYP3A substrate
0,711	0,004	Transcription factor NF kappa B stimulant
0,711	0,004	Transcription factor stimulant
0,716	0,010	Glucan endo-1,3-beta-D-glucosidase inhibitor
0,712	0,006	Anesthetic general
0,726	0,027	Benzoate-CoA ligase inhibitor
0,703	0,010	Analeptic
Compound #2		

Pa	Pi	
0,959	0,001	Cholesterol antagonist
0,929	0,002	Proliferative diseases treatment
0,925	0,004	Alkenylglycerophosphocholine hydrolase inhibitor
0,922	0,002	Chemopreventive
0,920	0,003	Antihypercholesterolemic
0,912	0,003	Caspase 3 stimulant
0,891	0,003	CYP3A4 inducer
0,890	0,003	CYP3A inducer
0,889	0,003	Hepatoprotectant
0,886	0,005	Respiratory analeptic
0,872	0,004	Membrane integrity antagonist
0,873	0,005	Antineoplastic
0,872	0,015	CDP-glycerol glycerophosphotransferase inhibitor
0,857	0,004	UDP-glucuronosyltransferase substrate
0,835	0,004	Oxidoreductase inhibitor
0,825	0,004	Anticarcinogenic
0,818	0,004	Immunosuppressant
0,801	0,005	Antiprotozoal (Leishmania)
0,783	0,007	CYP3A5 substrate
0,780	0,006	Glyceryl-ether monooxygenase inhibitor
0,785	0,020	CYP2H substrate
0,757	0,004	Alkenylglycerophosphoethanolamine hydrolase inhibitor
0,757	0,007	Analeptic
0,753	0,011	Immunostimulant
0,747	0,008	Glucan endo-1,3-beta-D-glucosidase inhibitor
0,727	0,004	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
0,722	0,009	Antifungal
0,736	0,025	Benzoate-CoA ligase inhibitor
0,712	0,003	DELTA14-sterol reductase inhibitor
0,705	0,013	Hypolipemic
Compound #3		
0,949	0,001	Cholesterol antagonist
0,938	0,003	Alkenylglycerophosphocholine hydrolase inhibitor
0,914	0,003	Caspase 3 stimulant
0,893	0,005	Antineoplastic
0,873	0,004	Membrane integrity antagonist
0,871	0,003	Hepatoprotectant
0,878	0,014	CDP-glycerol glycerophosphotransferase inhibitor

Pa	Pi	
0,851	0,005	Respiratory analeptic
0,848	0,005	CYP3A4 inducer
0,834	0,006	Membrane permeability inhibitor
0,823	0,003	Proliferative diseases treatment
0,820	0,002	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
0,820	0,004	Immunosuppressant
0,821	0,005	CYP3A inducer
0,819	0,005	UDP-glucuronosyltransferase substrate
0,818	0,004	Glucan endo-1,3-beta-D-glucosidase inhibitor
0,808	0,005	Glyceryl-ether monooxygenase inhibitor
0,794	0,004	Chemopreventive
0,787	0,004	Alkenylglycerophosphoethanolamine hydrolase inhibitor
0,796	0,018	CYP2H substrate
0,778	0,005	Antihypercholesterolemic
0,739	0,007	Antiprotozoal (Leishmania)
0,736	0,008	Analeptic
0,742	0,025	Benzoate-CoA ligase inhibitor
0,716	0,002	Dementia treatment
0,713	0,009	Antifungal
0,705	0,004	CYP2C9 inducer
Compound #4		
0,984	0,001	Proliferative diseases treatment
0,977	0,000	Cholesterol antagonist
0,963	0,001	Chemopreventive
0,952	0,002	Anticarcinogenic
0,952	0,002	UDP-glucuronosyltransferase substrate
0,942	0,000	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
0,943	0,002	Glyceryl-ether monooxygenase inhibitor
0,942	0,004	Antineoplastic
0,938	0,003	G-protein-coupled receptor kinase inhibitor
0,938	0,003	Beta-adrenergic receptor kinase inhibitor
0,930	0,002	Antiprotozoal (Leishmania)
0,881	0,005	Apoptosis agonist
0,855	0,004	CYP3A inducer
0,864	0,016	CDP-glycerol glycerophosphotransferase inhibitor
0,851	0,004	UGT1A substrate
0,849	0,002	Bilirubin oxidase inhibitor
0,841	0,005	CYP3A4 inducer
0,838	0,005	Hypolipemic

Pa	Pi	
0,832	0,011	CYP3A substrate
0,808	0,008	Respiratory analeptic
0,799	0,005	Antifungal
0,797	0,005	Immunosuppressant
0,795	0,015	CYP3A4 substrate
0,791	0,019	CYP2H substrate
0,764	0,001	Dementia treatment
0,749	0,004	Galactolipase inhibitor
0,747	0,010	CYP3A5 substrate
0,730	0,001	Vascular dementia treatment
0,715	0,002	Beta-glucosidase inhibitor
0,723	0,028	Alkenylglycerophosphocholine hydrolase inhibitor
0,707	0,012	Phosphatase inhibitor
Compound #5		
0,995	0,001	UDP-glucuronosyltransferase substrate
0,991	0,000	Cholesterol antagonist
0,991	0,001	Chemopreventive
0,977	0,000	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
0,976	0,002	UGT1A substrate
0,975	0,001	Beta-adrenergic receptor kinase inhibitor
0,975	0,001	G-protein-coupled receptor kinase inhibitor
0,968	0,001	Glyceryl-ether monooxygenase inhibitor
0,967	0,002	Hypolipemic
0,962	0,001	Beta-glucosidase inhibitor
0,957	0,002	Antiprotozoal (Leishmania)
0,936	0,002	Proliferative diseases treatment
0,922	0,001	Bilirubin oxidase inhibitor
0,908	0,001	Galactolipase inhibitor
0,905	0,001	Neurotrophic factor enhancer
0,892	0,005	Antineoplastic
0,883	0,003	Anticarcinogenic
0,857	0,002	Apoptosis antagonist
0,857	0,005	Respiratory analeptic
0,853	0,003	Antifungal
0,866	0,016	CDP-glycerol glycerophosphotransferase inhibitor
0,844	0,004	CYP3A inducer
0,845	0,012	Alkenylglycerophosphocholine hydrolase inhibitor
0,835	0,006	Apoptosis agonist

Pa	Pi	
0,831	0,005	CYP3A4 inducer
0,821	0,001	Dementia treatment
0,809	0,001	Vascular dementia treatment
0,801	0,005	Immunosuppressant
0,786	0,003	UGT1A4 substrate
0,793	0,018	CYP2H substrate
0,773	0,009	Antiinflammatory
0,772	0,007	Caspase 3 stimulant
0,771	0,017	CYP3A substrate
0,751	0,003	4-Nitrophenylphosphatase inhibitor
0,753	0,005	Phosphatase inhibitor
0,751	0,005	Hepatoprotectant
0,741	0,011	Membrane integrity antagonist
0,730	0,003	Caspase 8 stimulant
0,729	0,012	CYP3A5 substrate
0,717	0,004	Transcription factor NF kappa B stimulant
0,717	0,004	Transcription factor stimulant
0,725	0,013	Oxidoreductase inhibitor
0,714	0,024	CYP3A4 substrate
0,706	0,030	Benzoate-CoA ligase inhibitor
Compound #6		
0,995	0,001	UDP-glucuronosyltransferase substrate
0,991	0,000	Cholesterol antagonist
0,991	0,001	Chemopreventive
0,977	0,000	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
0,976	0,002	UGT1A substrate
0,975	0,001	Beta-adrenergic receptor kinase inhibitor
0,975	0,001	G-protein-coupled receptor kinase inhibitor
0,968	0,001	Glyceryl-ether monooxygenase inhibitor
0,967	0,002	Hypolipemic
0,962	0,001	Beta-glucosidase inhibitor
0,957	0,002	Antiprotozoal (Leishmania)
0,936	0,002	Proliferative diseases treatment
0,922	0,001	Bilirubin oxidase inhibitor
0,908	0,001	Galactolipase inhibitor
0,905	0,001	Neurotrophic factor enhancer
0,892	0,005	Antineoplastic
0,883	0,003	Anticarcinogenic

Pa	Pi	
0,857	0,002	Apoptosis antagonist
0,857	0,005	Respiratory analeptic
0,853	0,003	Antifungal
0,866	0,016	CDP-glycerol glycerophosphotransferase inhibitor
0,844	0,004	CYP3A inducer
0,845	0,012	Alkenylglycerophosphocholine hydrolase inhibitor
0,835	0,006	Apoptosis agonist
0,831	0,005	CYP3A4 inducer
0,821	0,001	Dementia treatment
0,809	0,001	Vascular dementia treatment
0,801	0,005	Immunosuppressant
0,786	0,003	UGT1A4 substrate
0,793	0,018	CYP2H substrate
0,773	0,009	Antiinflammatory
0,772	0,007	Caspase 3 stimulant
0,771	0,017	CYP3A substrate
0,751	0,003	4-Nitrophenylphosphatase inhibitor
0,753	0,005	Phosphatase inhibitor
0,751	0,005	Hepatoprotectant
0,741	0,011	Membrane integrity antagonist
0,730	0,003	Caspase 8 stimulant
0,729	0,012	CYP3A5 substrate
0,717	0,004	Transcription factor NF kappa B stimulant
0,717	0,004	Transcription factor stimulant
0,725	0,013	Oxidoreductase inhibitor
0,714	0,024	CYP3A4 substrate
0,706	0,030	Benzoate-CoA ligase inhibitor
Compound #7		
0,984	0,001	Proliferative diseases treatment
0,977	0,000	Cholesterol antagonist
0,963	0,001	Chemopreventive
0,952	0,002	Anticarcinogenic
0,952	0,002	UDP-glucuronosyltransferase substrate
0,942	0,000	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
0,943	0,002	Glyceryl-ether monooxygenase inhibitor
0,942	0,004	Antineoplastic
0,938	0,003	G-protein-coupled receptor kinase inhibitor
0,938	0,003	Beta-adrenergic receptor kinase inhibitor

Pa	Pi	
0,930	0,002	Antiprotozoal (Leishmania)
0,881	0,005	Apoptosis agonist
0,855	0,004	CYP3A inducer
0,864	0,016	CDP-glycerol glycerophosphotransferase inhibitor
0,851	0,004	UGT1A substrate
0,849	0,002	Bilirubin oxidase inhibitor
0,841	0,005	CYP3A4 inducer
0,838	0,005	Hypolipemic
0,832	0,011	CYP3A substrate
0,808	0,008	Respiratory analeptic
0,799	0,005	Antifungal
0,797	0,005	Immunosuppressant
0,795	0,015	CYP3A4 substrate
0,791	0,019	CYP2H substrate
0,764	0,001	Dementia treatment
0,749	0,004	Galactolipase inhibitor
0,747	0,010	CYP3A5 substrate
0,730	0,001	Vascular dementia treatment
0,715	0,002	Beta-glucosidase inhibitor
0,723	0,028	Alkenylglycerophosphocholine hydrolase inhibitor
0,707	0,012	Phosphatase inhibitor