

The antimicrobial potentials and pharmacokinetic profiles of novel quinoline-based scaffolds: synthesis and *in silico* mechanistic studies as dual DNA gyrase and DHFR inhibitors

Supplementary Materials

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Summary of docking results

Compound	ΔG, kcal/mol	H-bonding interactions		Hydrophobic interaction	
		Residue	Distance (Å)	Residue	Distance (Å)
1. DNA Gyrase					
15	-10.98	ILE 94	3.51	PRO 79	3.97
				LYS 103	3.98
				ASN 46	3.71
16	-10.96	GLY 101	3.27	PRO 79	3.83
		GLU 50	3.56	LYS 103	3.97
20	-11.21	THR 165	3.10	LYS 103	3.88
		LYS 103	2.84		
		VAL 120	3.40		
21	-10.33	ASP 73	2.94	ILE 78	4.53
				ILE 78	3.99
				PRO 79	3.61
				LYS 103	4.04
22	-10.71	ASP 73	2.90	LYS 103	3.93
RLI	-12.23	3.06	Arg76	-	
		3.15	Arg136		
		3.63 bidirectional	Gly101		
		2.81	Gly101		
2. DHFR					
15	-10.29	SER69	2.99	VAL70	4.15
16	-11.11	SER69	2.80	LEU32	4.02

Compound	ΔG , kcal/mol	H-bonding interactions		Hydrophobic interaction	
		Residue	Distance (Å)	Residue	Distance (Å)
				VAL70	4.57
20	-8.83	-	-	LEU32	4.43
				VAL70	3.90
21	-8.75	TYR162	3.08	GLY157	4.45
22	-8.45	TYR162	2.98	GLY157	3.16
H9G	-11.16	SER69	2.99	VAL70	4.15

Docking Against 4DUH (DNA Gyrase)

Docking details for the Co-crystallized ligand RLI in the active site of DNA Gyrase

Score -12.2316351

Ligand Interactions Report

4DUH: ISOMERASE/ISOMERASE INHIBITOR / 4DUH: ISOMERASE/ISOMERASE INHIBITOR

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
S11 11	O	GLY 101 (A) H-donor	3.63	-1.0
N13 18	O	GLY 101 (A) H-donor	2.81	-4.2
O12 14	NH1	ARG 136 (A) H-acceptor	3.15	-1.7
O12 14	NH2	ARG 136 (A) H-acceptor	3.06	-5.2
O12 14	NH2	ARG 76 (A) ionic	3.64	-1.4
O12 14	NH1	ARG 136 (A) ionic	3.15	-3.5
O12 14	NH2	ARG 136 (A) ionic	3.06	-4.1

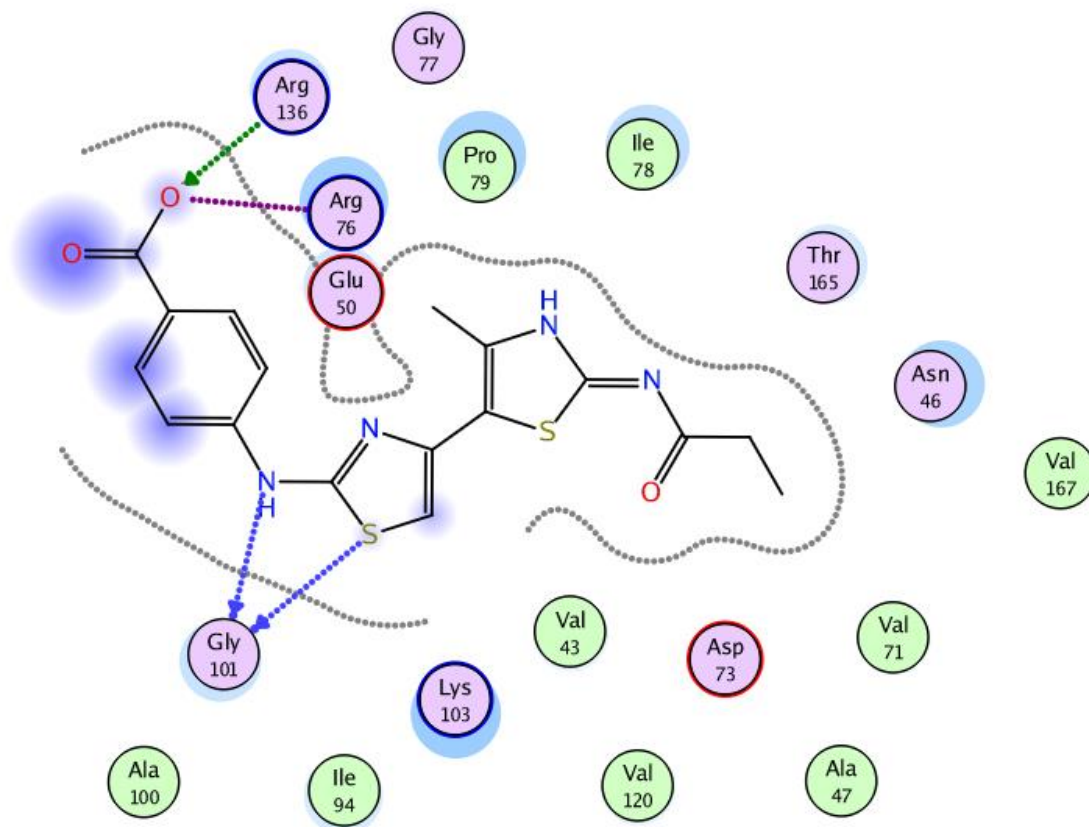


Figure 1: 2D interactions of the co-crystallized ligand, RLI in the active site of DNA Gyrase

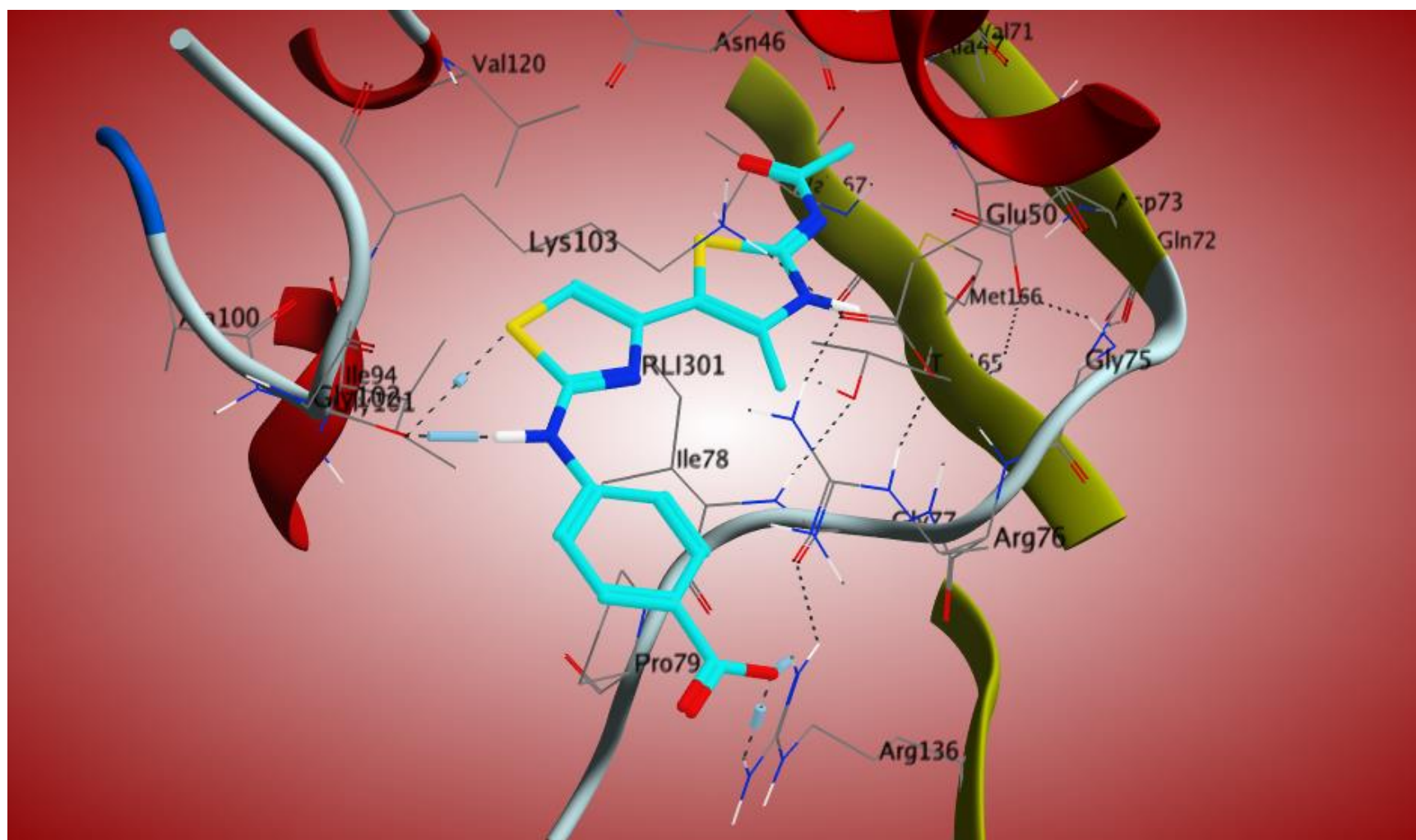


Figure 2: 3D interactions of the co-crystallized ligand, RLI in the active site of DNA Gyrase

Docking details for compound 15 in the active site of DNA Gyrase

Score -10.98

Ligand Interactions Report 1

4DUH: ISOMERASE/ISOMERASE INHIBITOR / 4DUH

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
6-ring	CD PRO 79	(A) pi-H	3.97	-0.7
6-ring	CE LYS 103	(A) pi-H	3.98	-0.7

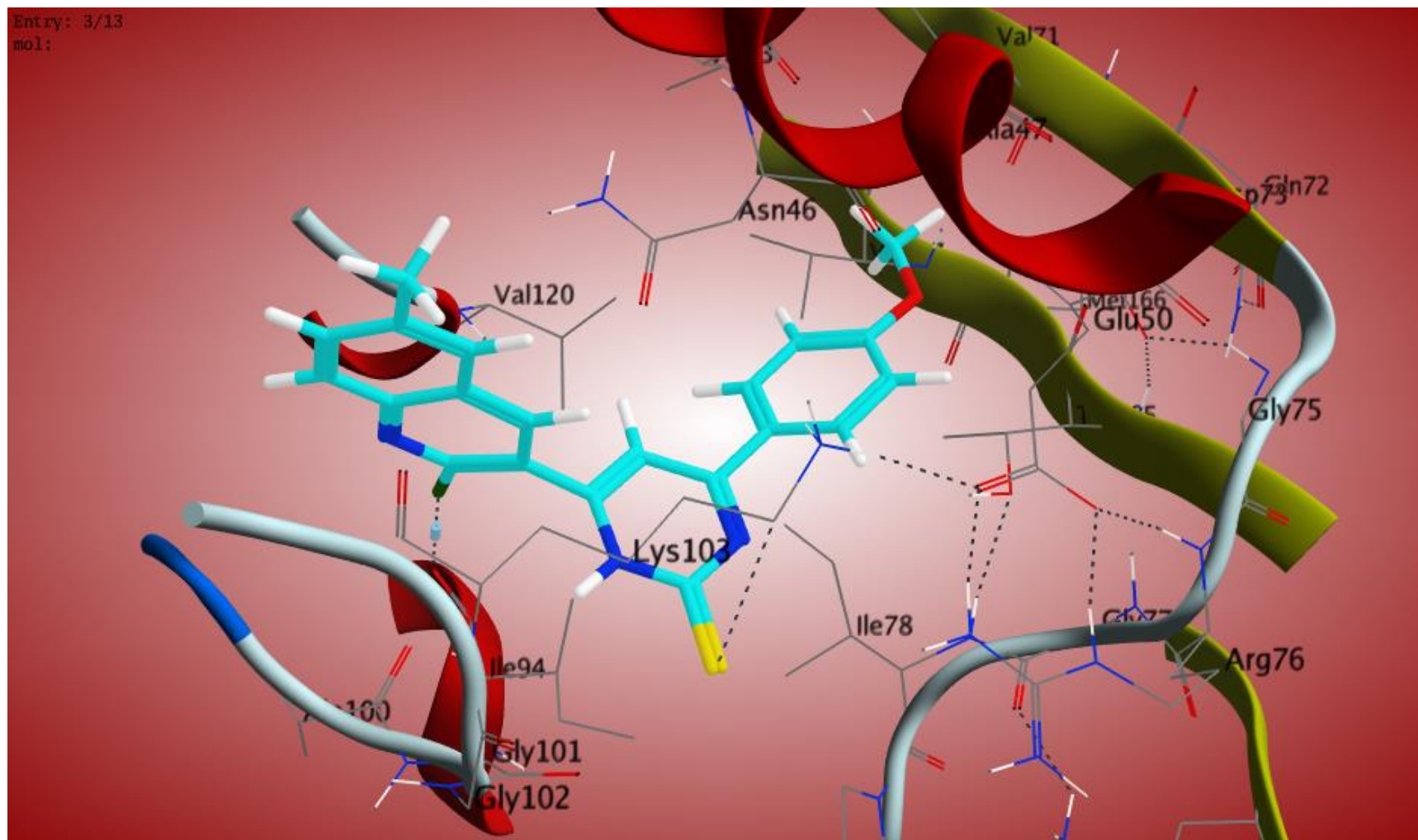


Figure 4: 2D interactions of the quinoline derivative 15 in the active site of DNA Gyrase

Docking details for compound 16 in the active site of DNA Gyrase

Ligand Interactions Report 2

4DUH: ISOMERASE/ISOMERASE INHIBITOR / 4DUH

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
--------	----------	-------------	----------	--------------

C 10	O	GLY 101 (A) H-donor	3.27	-0.7
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quinoline ring serves as a backbone HB acceptor

CL 12	OE2	GLU 50 (A) H-donor	3.56	-0.3
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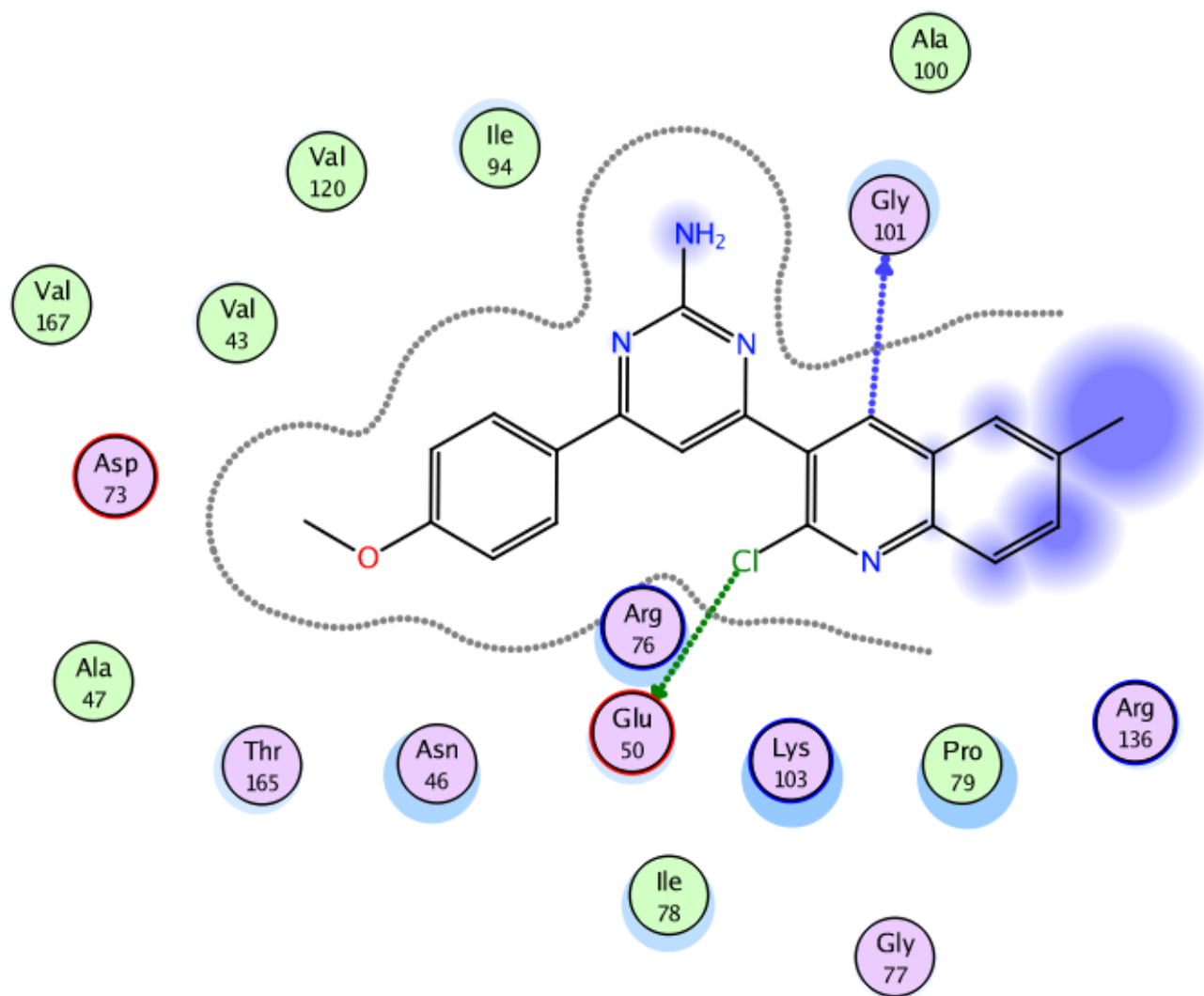


Figure 5: 2D interactions of the quinoline derivative 16 in the active site of DNA Gyrase

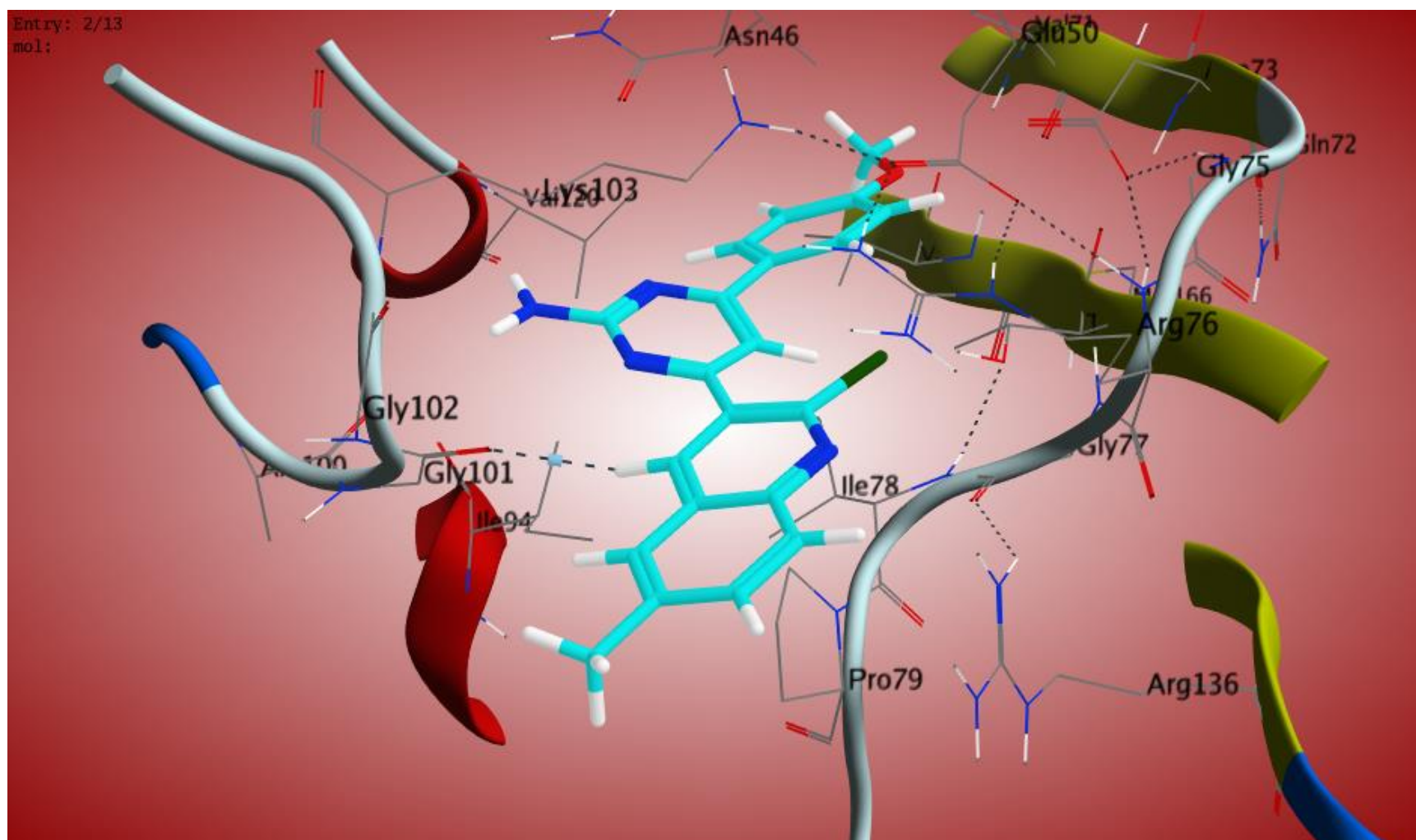


Figure 6: 3D interactions of the quinoline derivative 16

Docking details for compound 20 in the active site of DNA Gyrase

Score -11.2167978

Ligand Interactions Report 1

4DUH: ISOMERASE/ISOMERASE INHIBITOR / 4DUH

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
--------	----------	-------------	----------	--------------

O 20	CB THR 165 (A)	H-acceptor	3.10	-0.8
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6-ring	CE LYS 103 (A)	pi-H	3.88	-0.8
--------	----------------	------	------	------

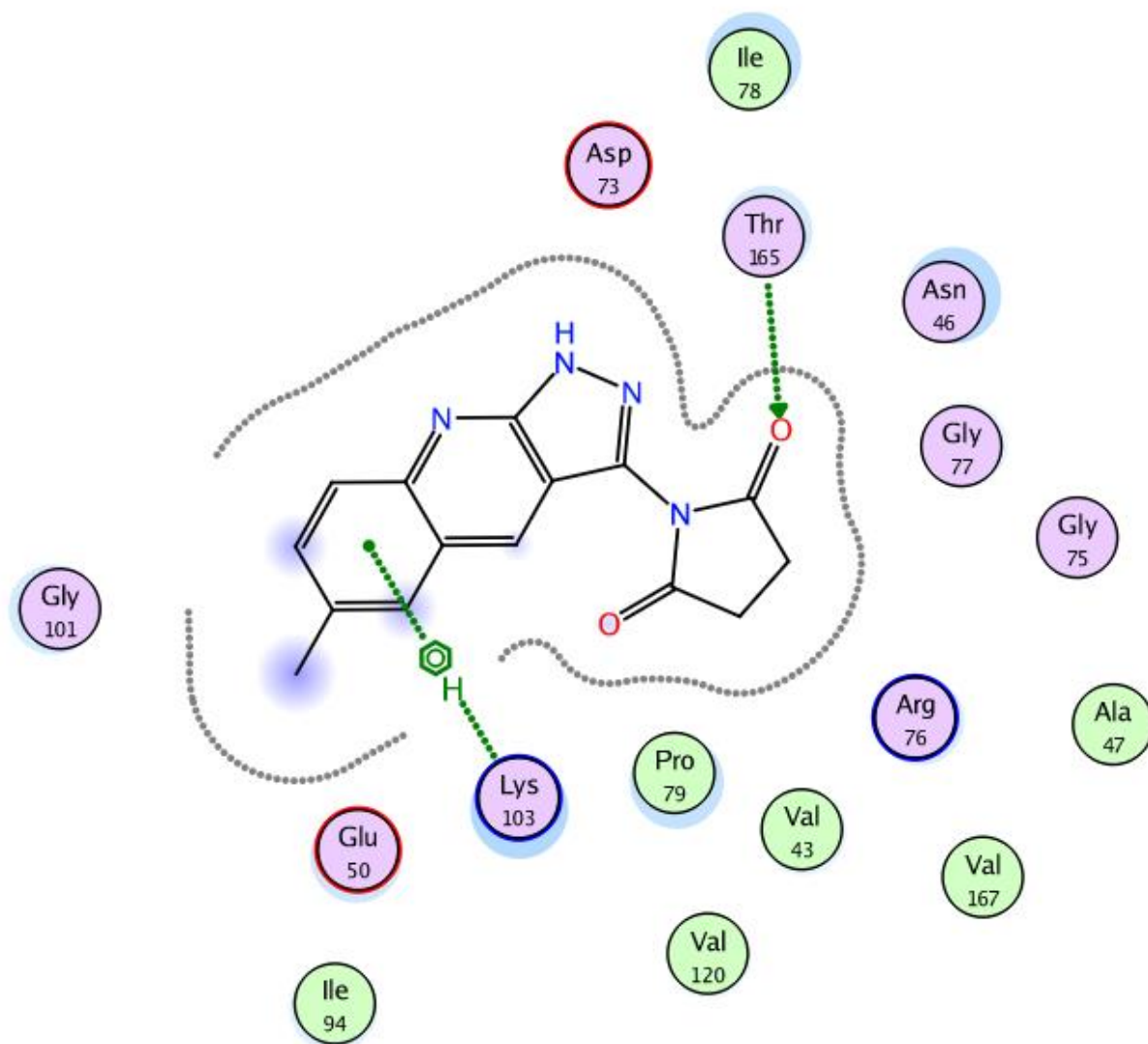


Figure 7: 2D interactions of the quinoline derivative 20 in the active site of DNA Gyrase

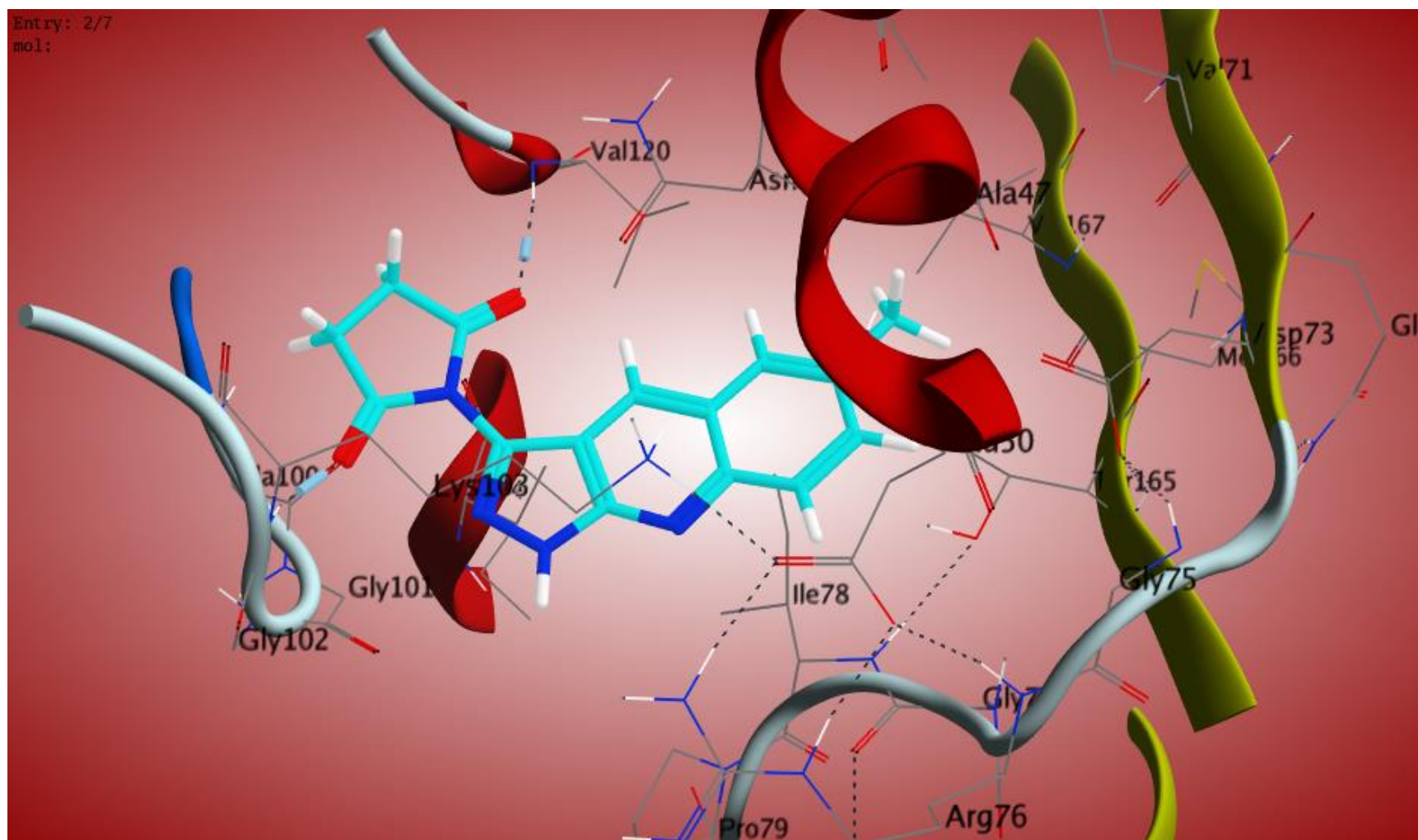


Figure 8: 3D interactions of the quinoline derivative 20

Docking details for compound 21 in the active site of DNA Gyrase

Score -10.3347683

Ligand Interactions Report 1

4DUH: ISOMERASE/ISOMERASE INHIBITOR / 4DUH

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
6-ring	CA ILE 78 (A)	pi-H	4.53	-0.6
6-ring	CA ILE 78 (A)	pi-H	3.99	-0.6
6-ring	CD PRO 79 (A)	pi-H	3.61	-0.7
6-ring	CE LYS 103 (A)	pi-H	4.04	-0.7

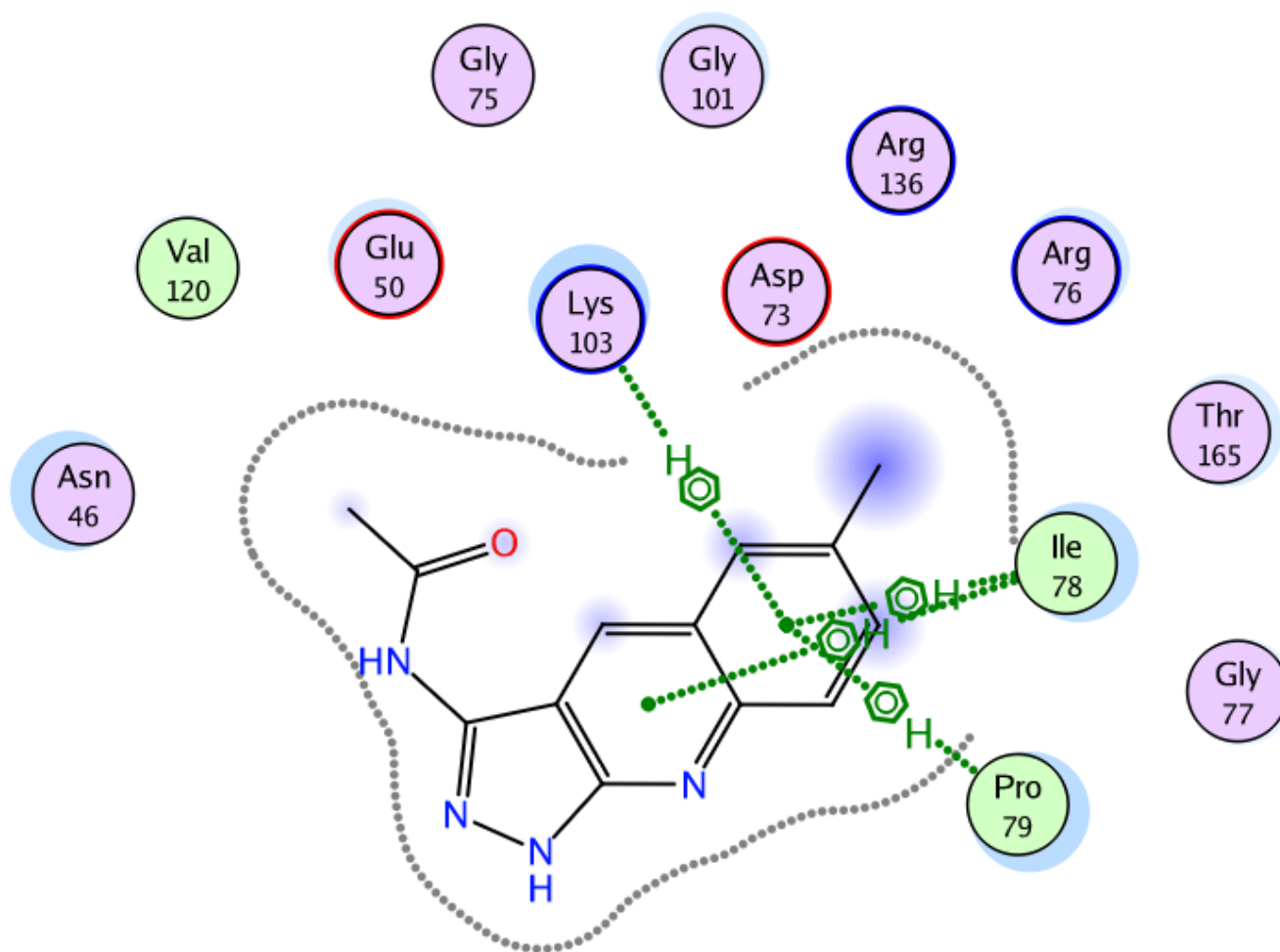


Figure 9: 2D interactions of the quinoline derivative 21 in the active site of DNA Gyrase

Ligand Interactions Report

4DUH: ISOMERASE/ISOMERASE INHIBITOR / 4DUH

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
--------	----------	-------------	----------	--------------

N 15	OD1 ASP 73	(A) H-donor	2.94	-7.2
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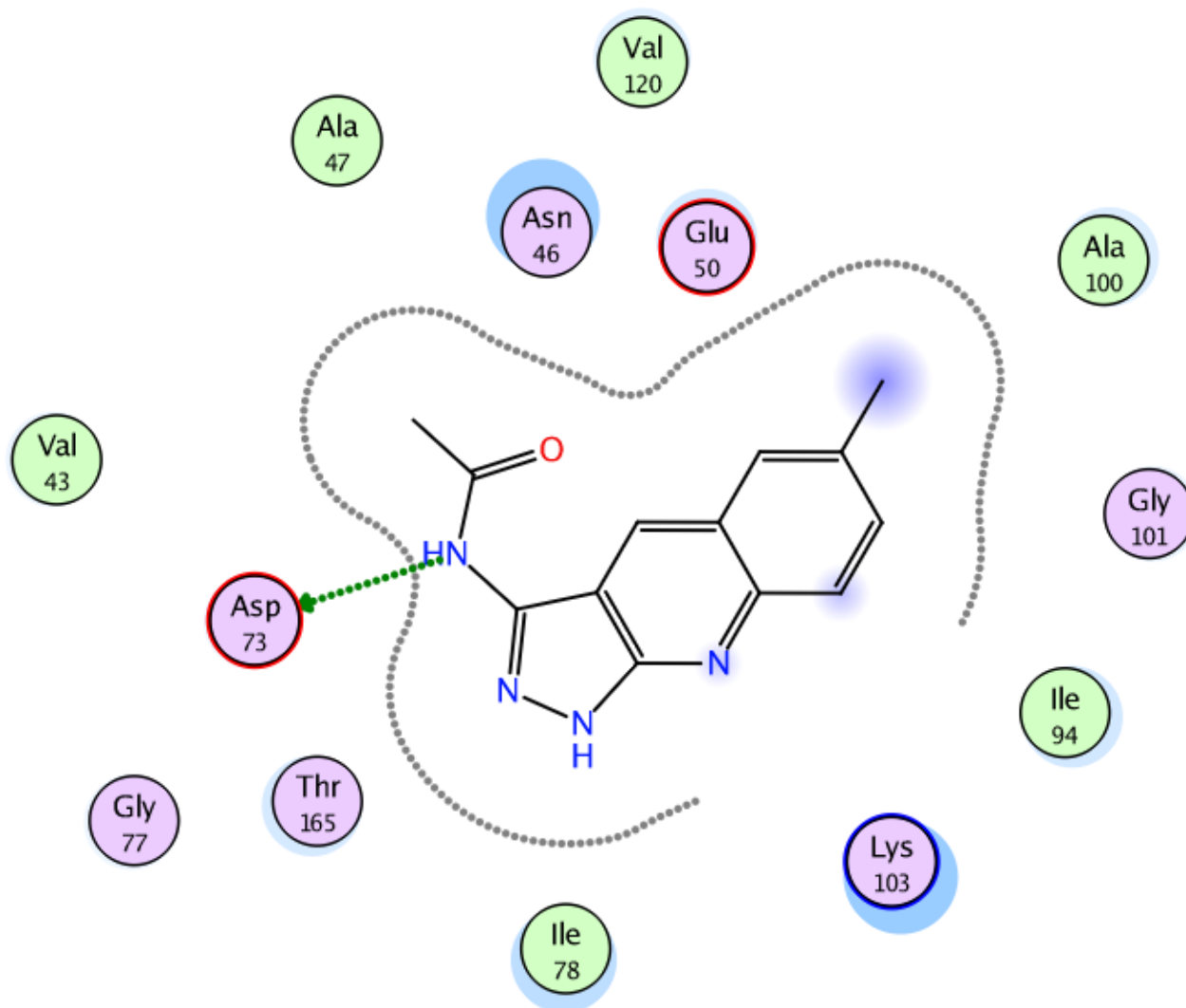


Figure 10: 2D interactions of the quinoline derivative 21, pose 2

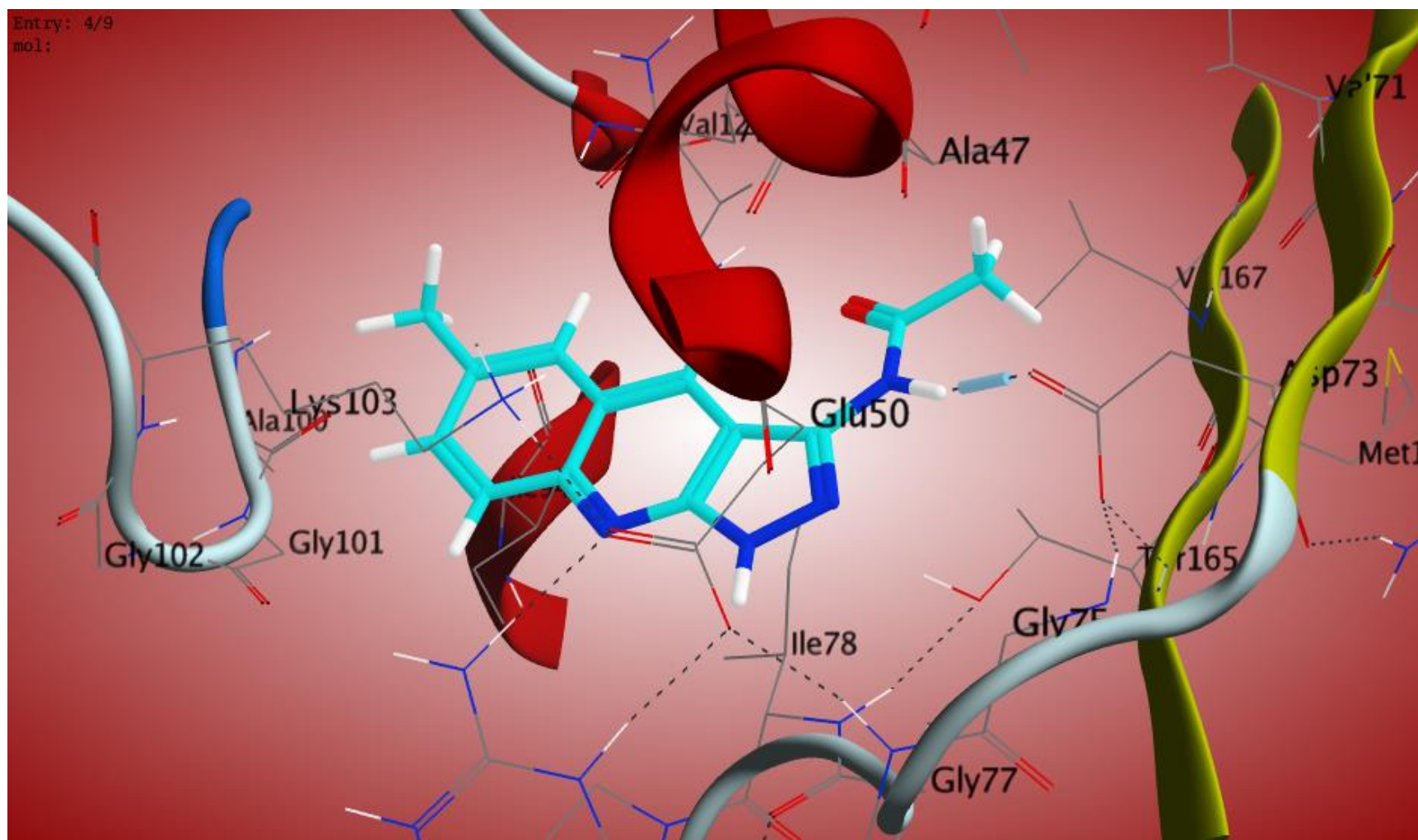


Figure 11: 3D interactions of the quinoline derivative 21

Docking details for compound 22 in the active site of DNA Gyrase

Score -10.7126884

Ligand Interactions Report 1

4DUH: ISOMERASE/ISOMERASE INHIBITOR / 4DUH

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
--------	----------	-------------	----------	--------------

N 15	OD1 ASP 73	(A) H-donor	3.01	-4.4
------	------------	-------------	------	------

6-ring	CE LYS 103	(A) pi-H	3.93	-0.7
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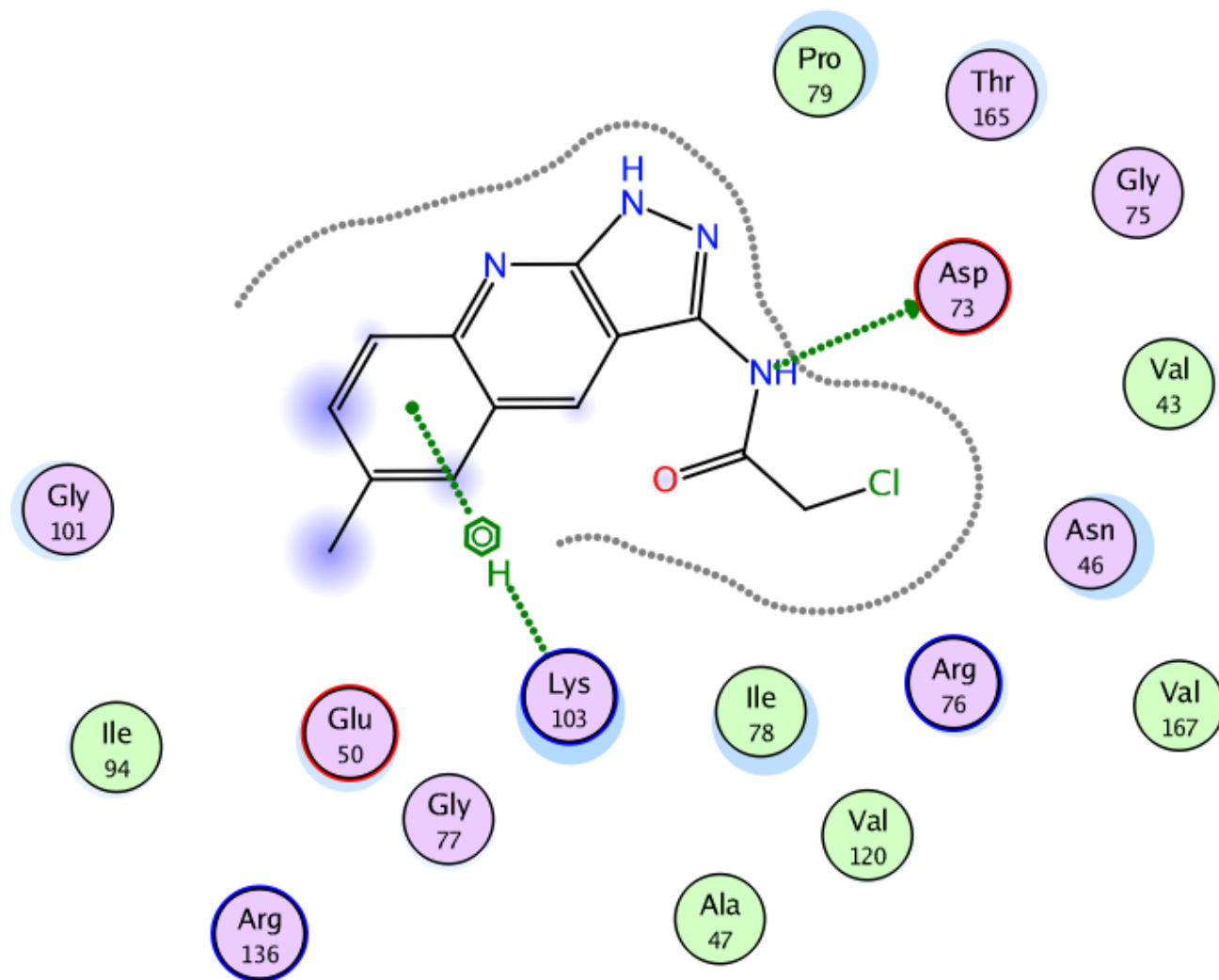


Figure 12: 2D interactions of the quinoline derivative 22, pose 1, in the active site of DNA Gyrase

Ligand Interactions Report 2

4DUH: ISOMERASE/ISOMERASE INHIBITOR / 4DUH

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
--------	----------	-------------	----------	--------------

N 15	OD1 ASP 73	(A) H-donor	2.90	-7.9
------	------------	-------------	------	------

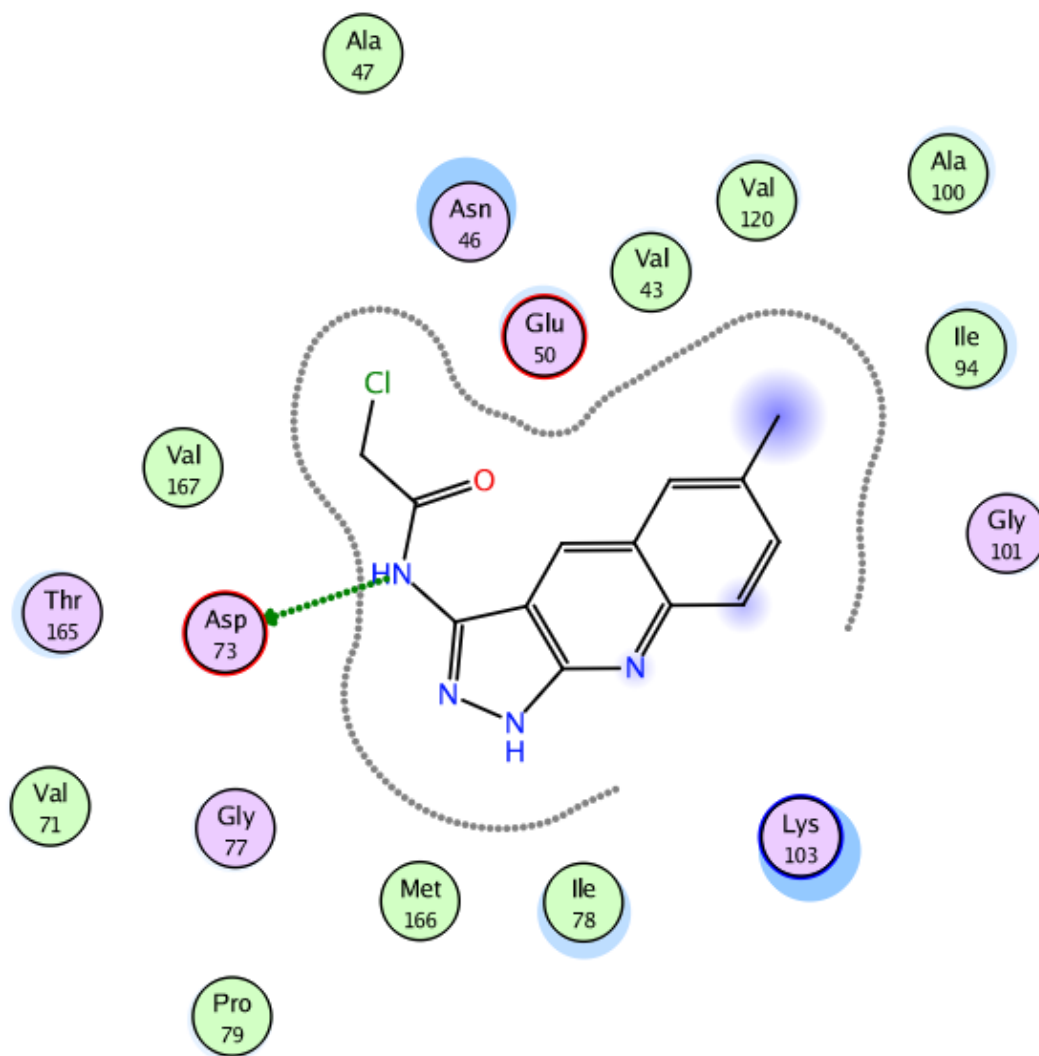


Figure 13: 2D interactions of the quinoline derivative 22, pose 2, in the active site of DNA Gyrase

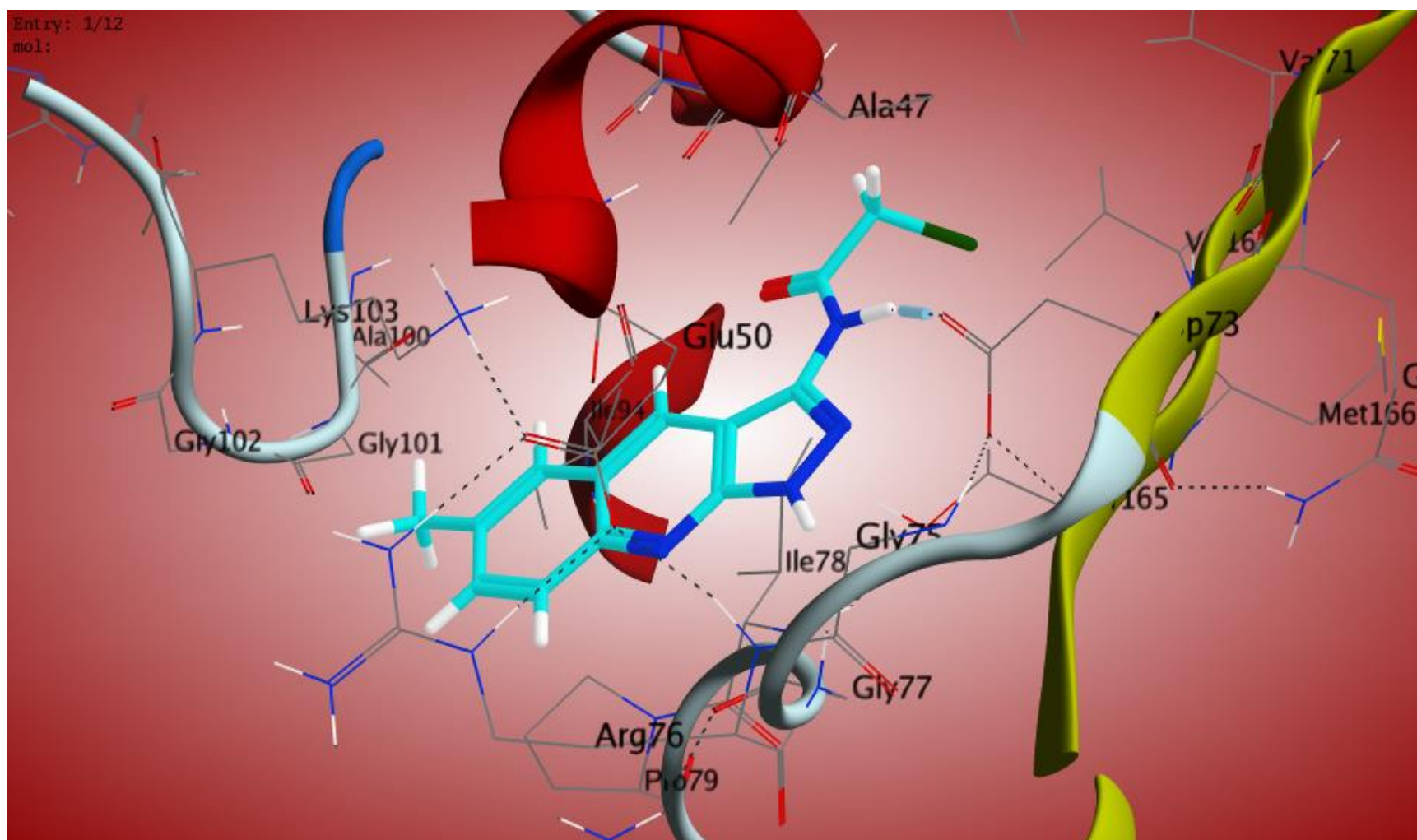


Figure 14: 3D interactions of the quinoline derivative 22 in the active site of DNA Gyrase

Docking Against 6DTH (DHFR)

Docking details for H9G in the active site of DHFR

Score -11.1688385

Ligand Interactions Report

6DTC: ANTIFUNGAL PROTEIN/INHIBITOR / 6DTC: ANTIFUNGAL PROTEIN/INHIBITOR

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
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N12 16	O ILE 10 (A)	H-donor	2.97	-1.6
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N13 19	OD1 ASP 40 (A)	H-donor	2.46	4.5
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N22 31	NH1 ARG 80 (A)	H-acceptor	2.68	-8.6
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N21 30	NH1 ARG 80 (A)	ionic	3.64	-1.4
--------	----------------	-------	------	------

N22 31	NH1 ARG 80 (A)	ionic	2.68	-7.0
--------	----------------	-------	------	------

N22 31	NH2 ARG 80 (A)	ionic	3.17	-3.5
--------	----------------	-------	------	------

N23 32	NH1 ARG 80 (A)	ionic	3.73	-1.1
--------	----------------	-------	------	------

N23 32	NH2 ARG 80 (A)	ionic	3.60	-1.5
--------	----------------	-------	------	------

5-ring	CD2 LEU 77 (A)	pi-H	3.73	-0.6
--------	----------------	------	------	------

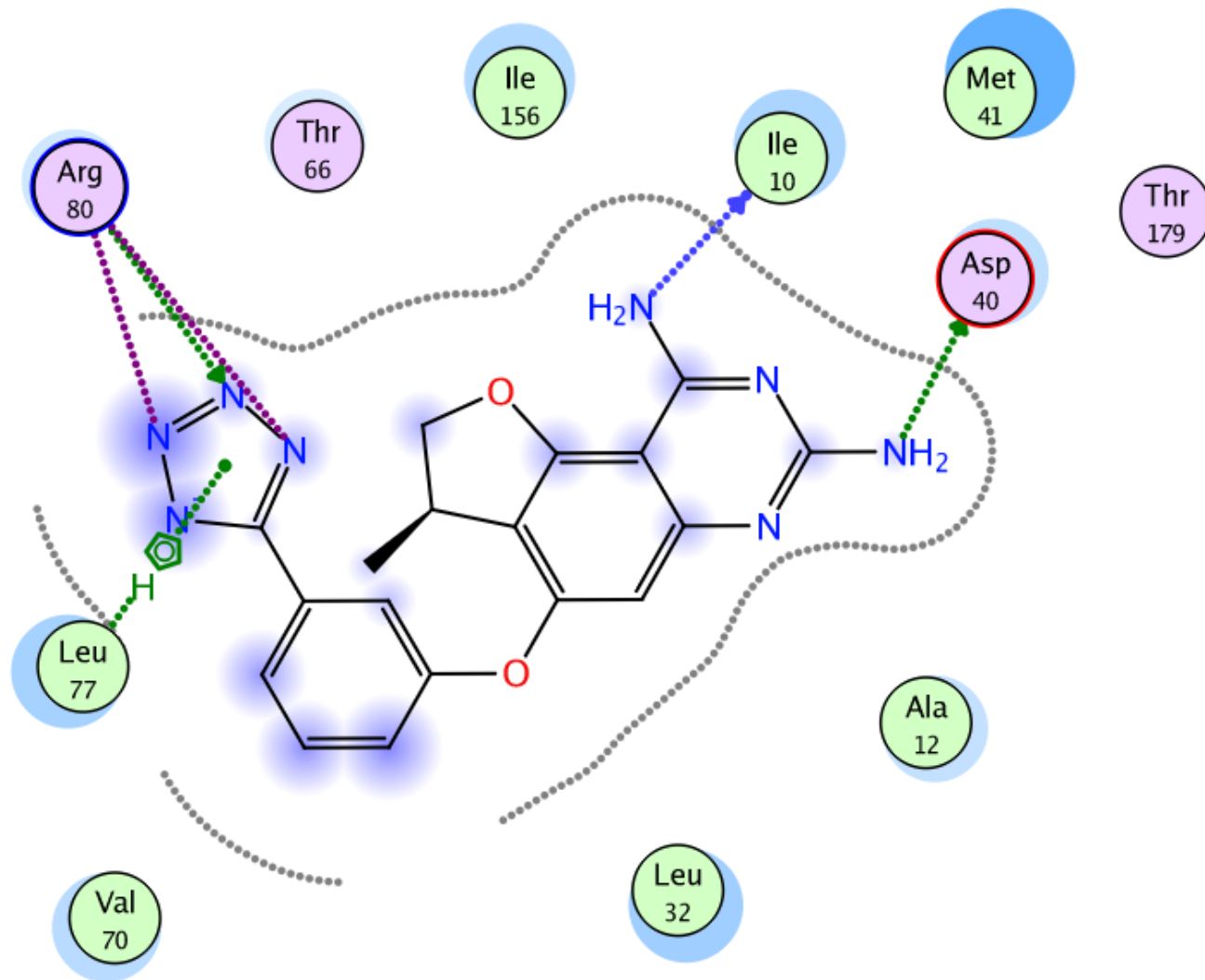


Figure 15: 2D interactions of quinoline derivative 15 in the active site of DHFR

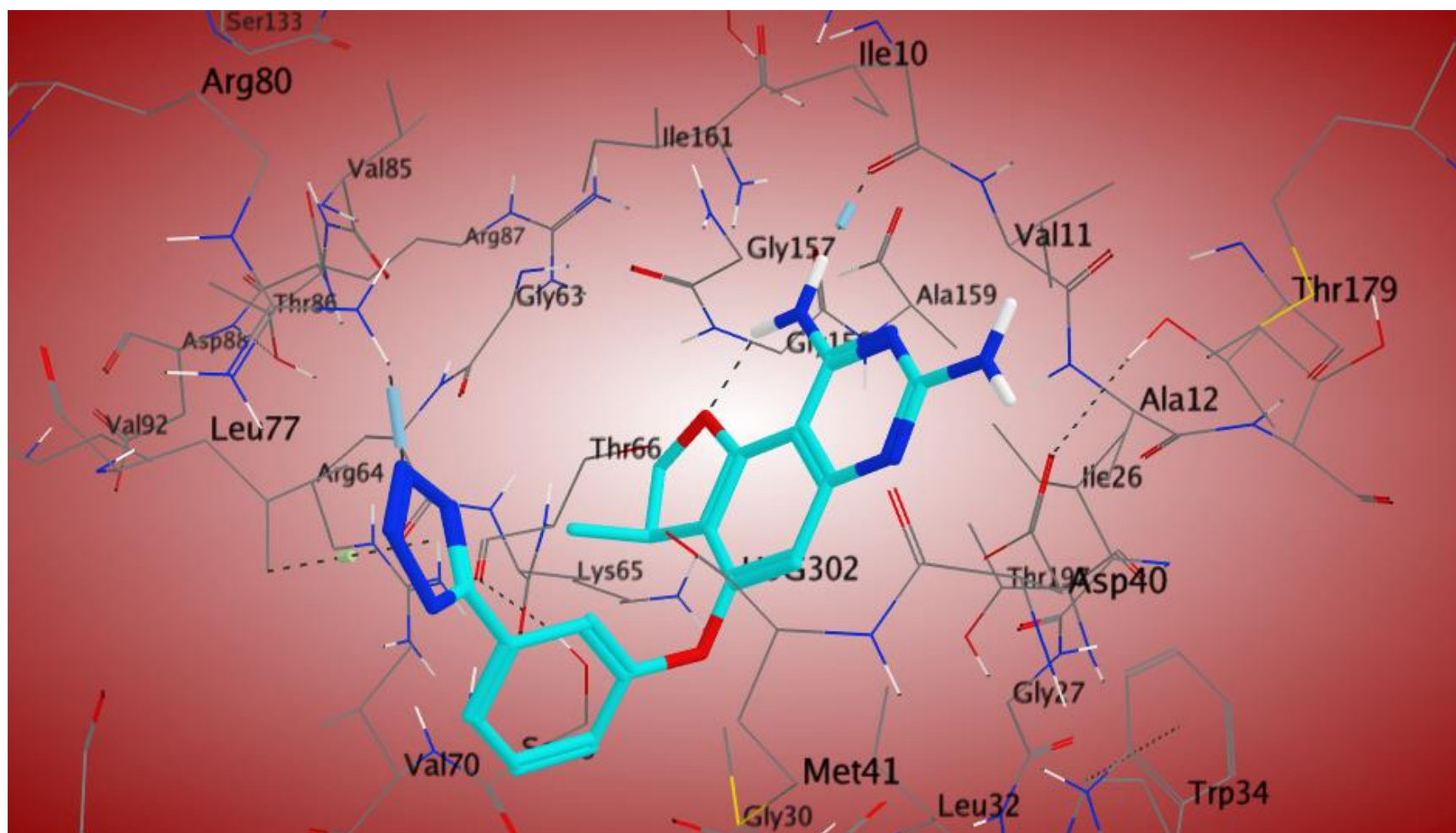


Figure 16: 3D interactions of quinoline derivative 15 in the active site of DHFR

Docking details for H9G redocked in the active site of DHFR

Score -11.16

Ligand Interactions Report

6DTC: ANTIFUNGAL PROTEIN/INHIBITOR / 6DTC

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
N 24	OD1 ASP 40 (A)	H-donor	2.99	-4.5
N 27	O ILE 10 (A)	H-donor	3.02	-2.2
N 27	O ILE 156 (A)	H-donor	2.89	-2.3
6-ring	6-ring PHE 44 (A)	pi-pi	4.00	-0.0

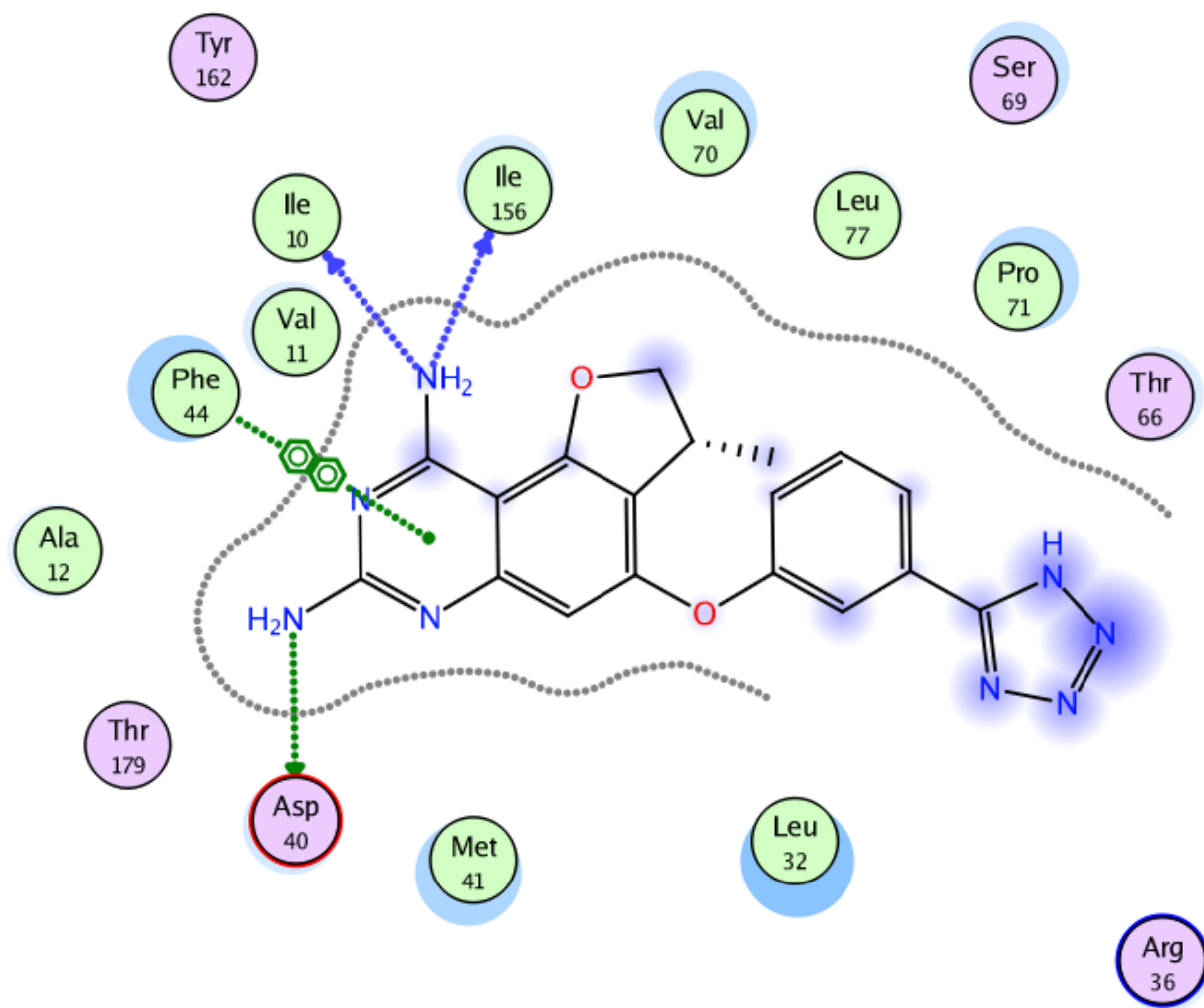


Figure 17: 2D interactions of H9G in the active site of DHFR

Docking details for compound 15 in the active site of DHFR

Score -10.2931118

Ligand Interactions Report

6DTC: ANTIFUNGAL PROTEIN/INHIBITOR / 6DTC

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
N 24	OG SER 69	(A) H-donor	2.99	-1.3
6-ring	CG2 VAL 70	(A) pi-H	4.15	-0.7

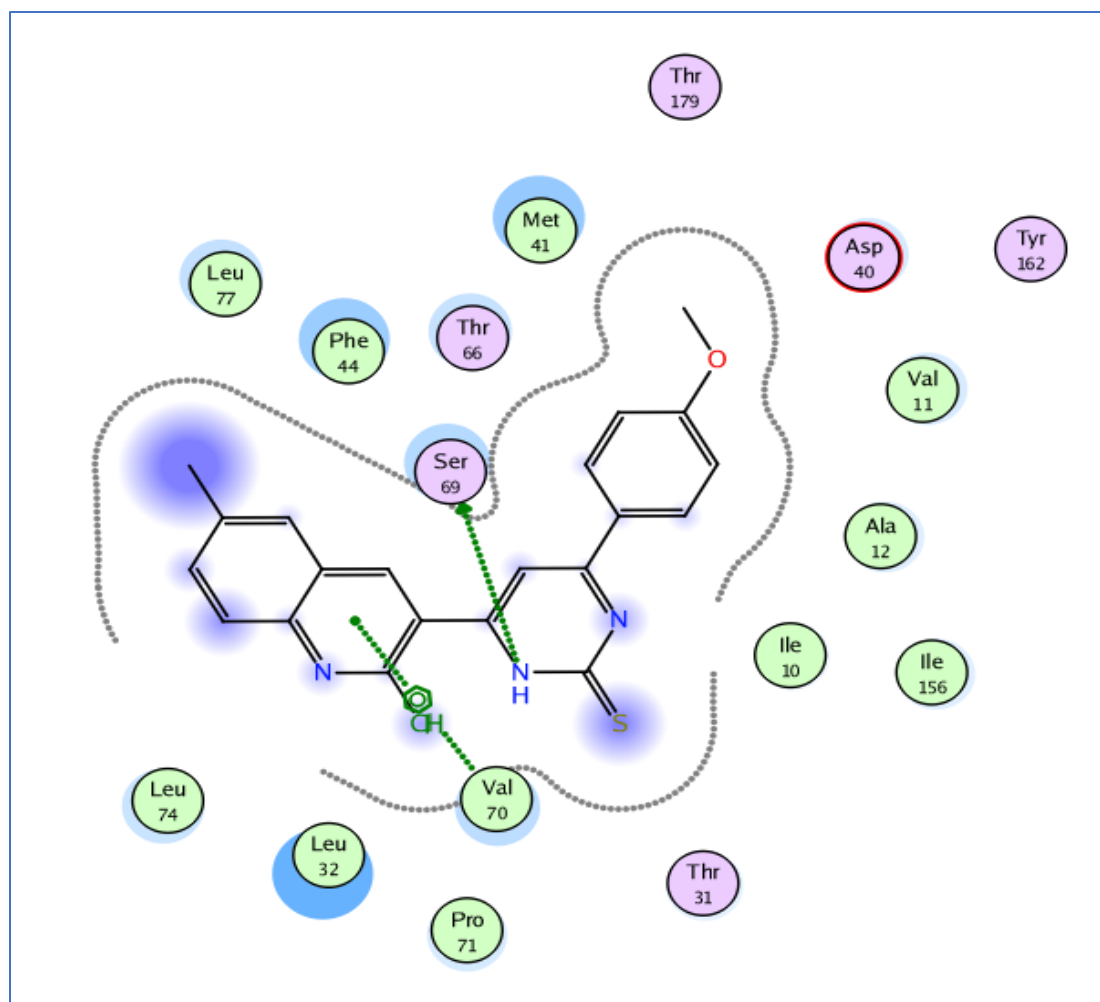


Figure 18: 2D interactions of quinoline derivative 15 in the active site of DHFR

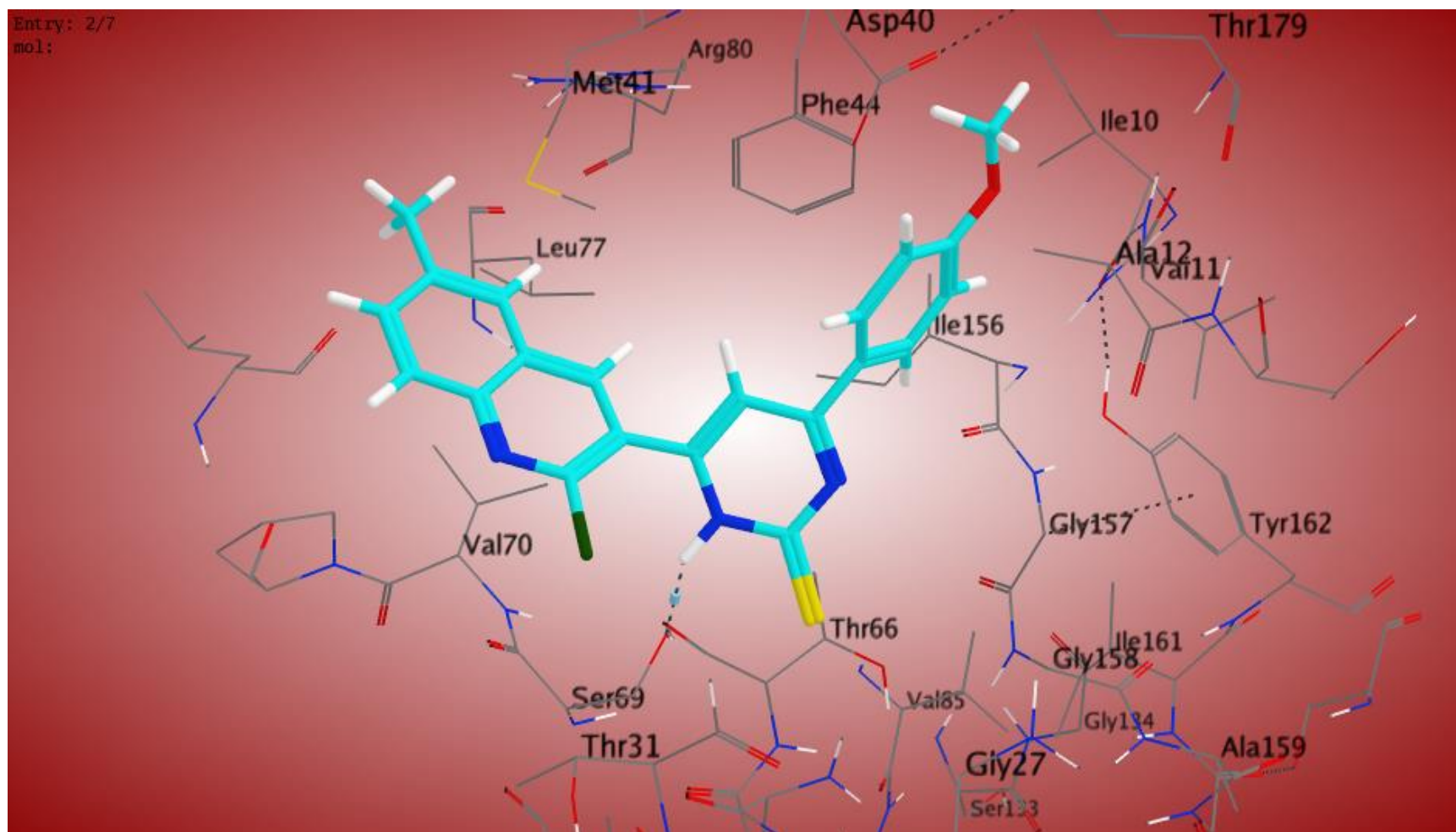


Figure 19: 3D interactions of quinoline derivative 15 in the active site of DHFR

Docking details for compound 16 in the active site of DHFR

Score -11.1149416

Ligand Interactions Report

6DTC: ANTIFUNGAL PROTEIN/INHIBITOR / 6DTC

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
N 26	OG SER 69	(A) H-donor	2.80	-1.5
6-ring	CD2 LEU 32	(A) pi-H	4.02	-0.6
6-ring	CG2 VAL 70	(A) pi-H	4.57	-0.7

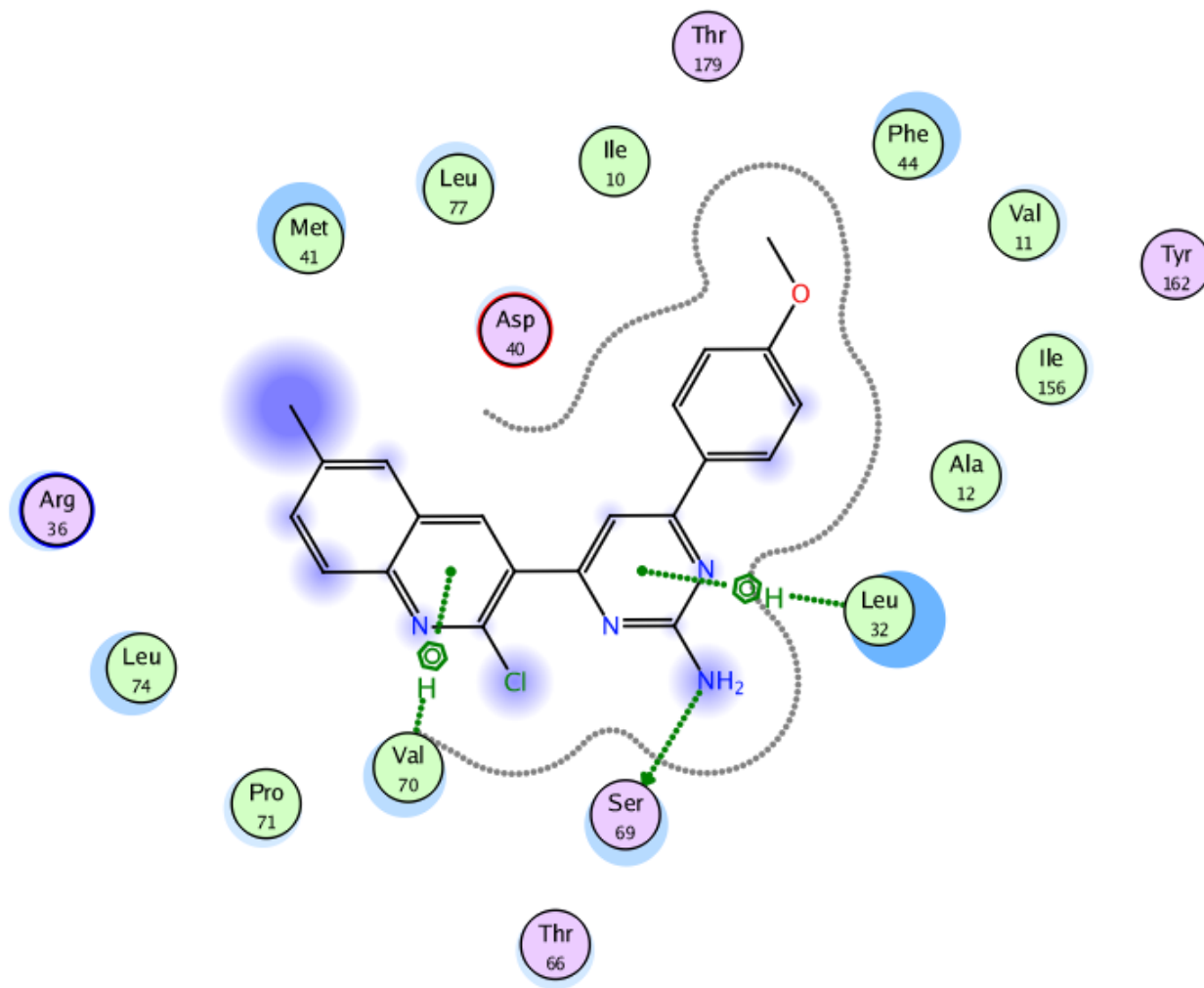


Figure 20: 2D interactions of quinoline derivative 16 in the active site of DHFR

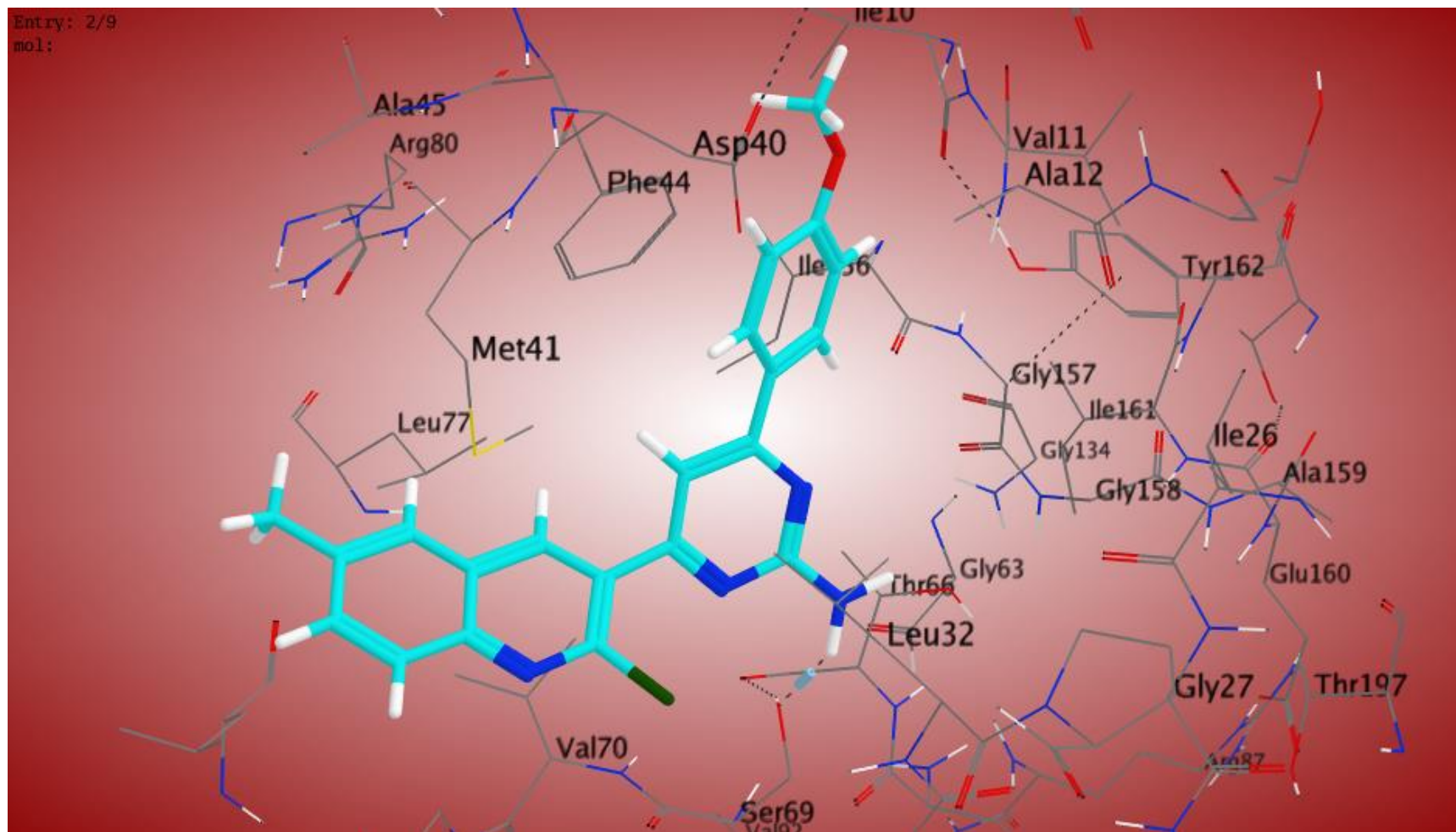


Figure 21: 3D interactions of quinoline derivative 16 in the active site of DHFR

Docking details for compound 20 in the active site of DHFR

Score -8.83793068

Ligand Interactions Report

6DTC: ANTIFUNGAL PROTEIN/INHIBITOR / 6DTC

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
6-ring	CD2 LEU 32	(A) pi-H	4.43	-0.6
5-ring	CG2 VAL 70	(A) pi-H	3.90	-1.4

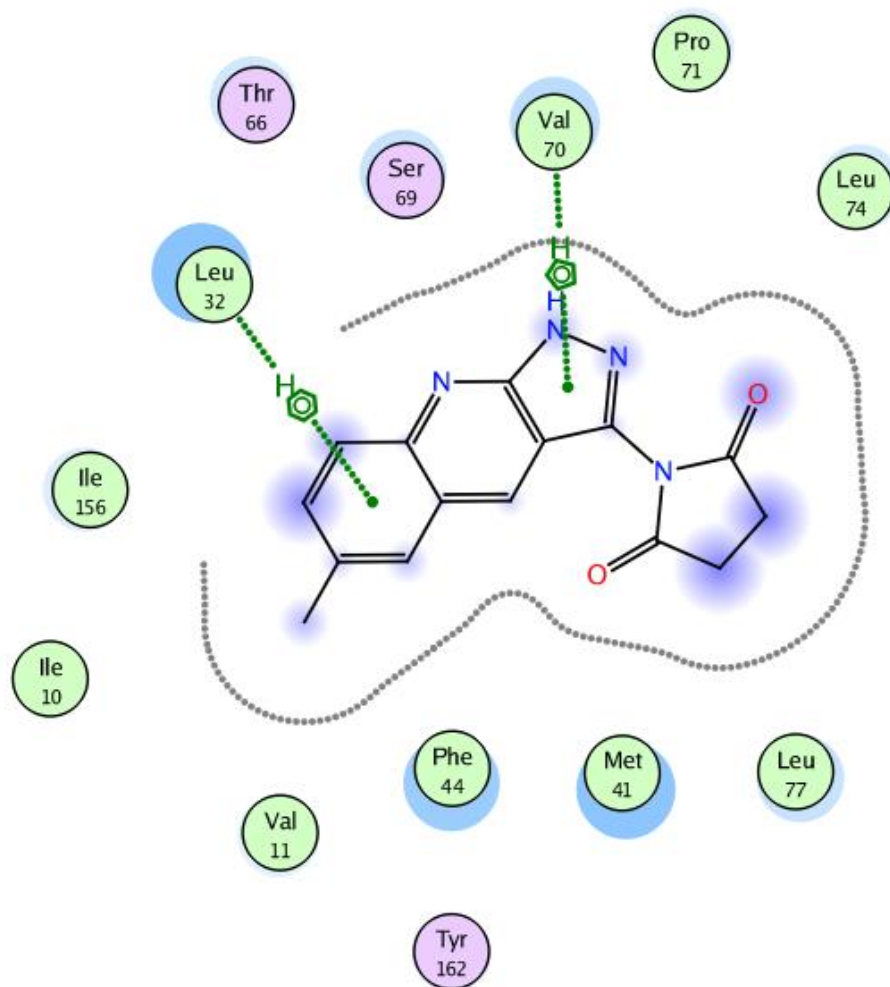


Figure 22: 2D interactions of quinoline derivative 20 in the active site of DHFR

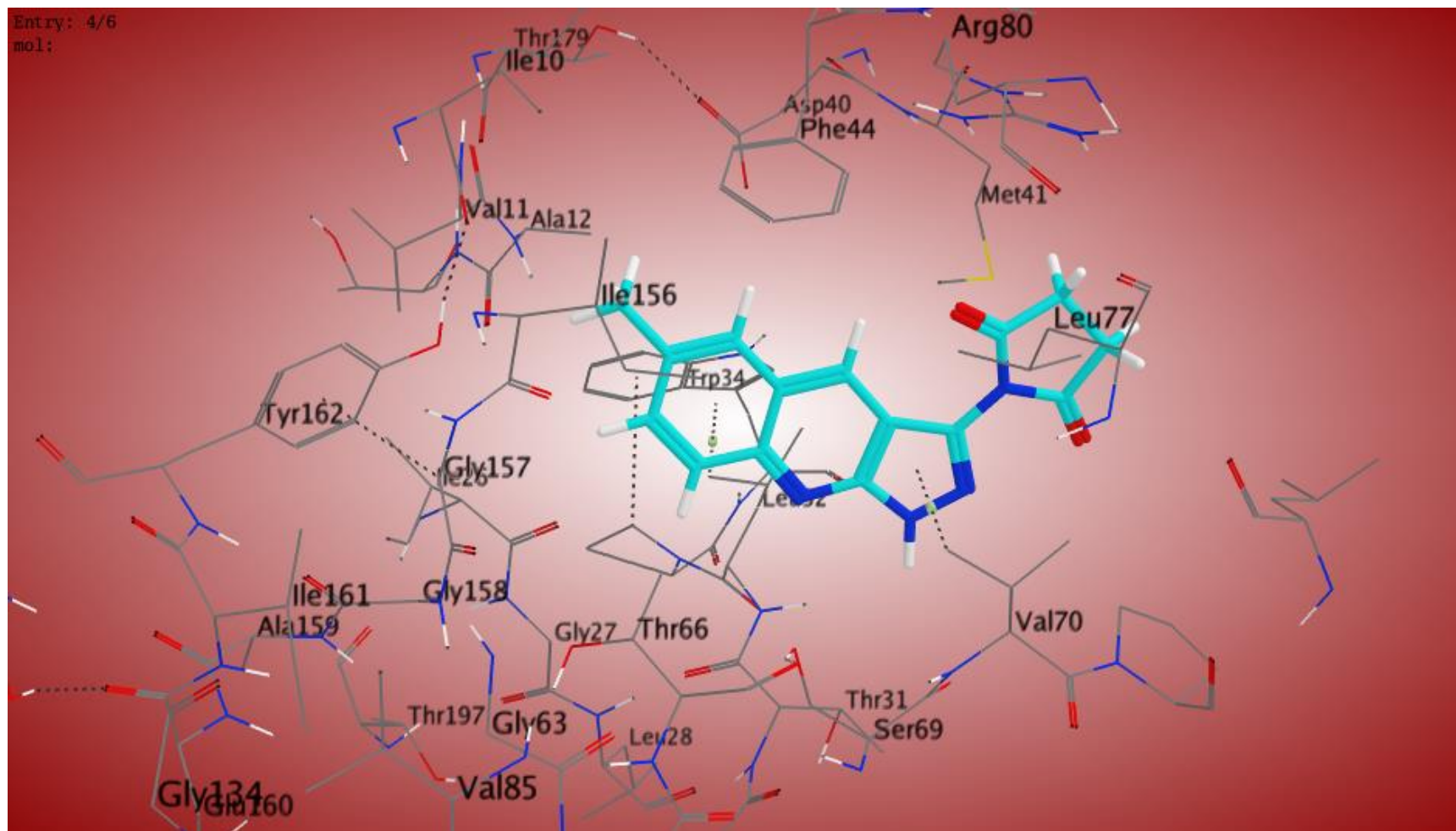


Figure 23: 3D interactions of quinoline derivative 20 in the active site of DHFR

Docking details for compound 21 in the active site of DHFR

Score -8.75586033

Ligand Interactions Report

6DTC: ANTIFUNGAL PROTEIN/INHIBITOR / 6DTC

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
N 12	OH TYR 162 (A)	H-donor	3.08	-0.6
5-ring	CA GLY 157 (A)	pi-H	4.45	-1.0

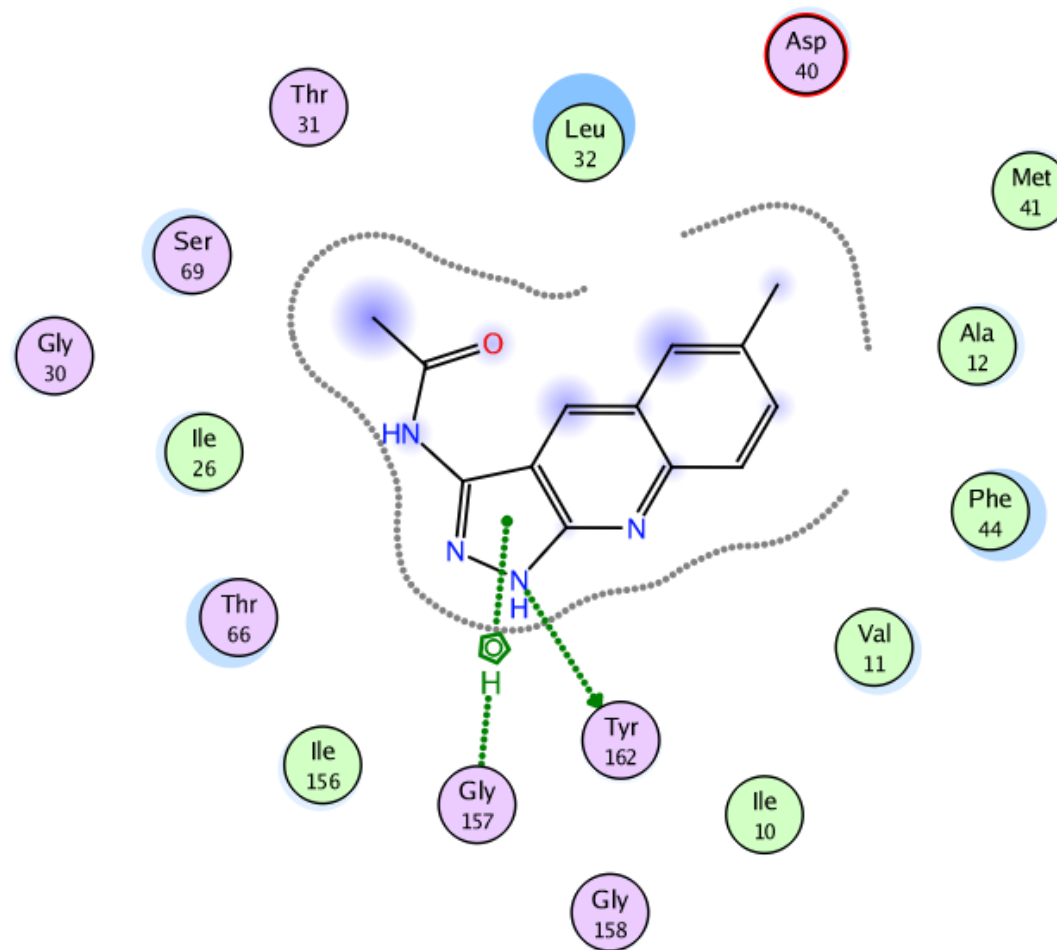


Figure 24: 2D interactions of quinoline derivative 21 in the active site of DHFR

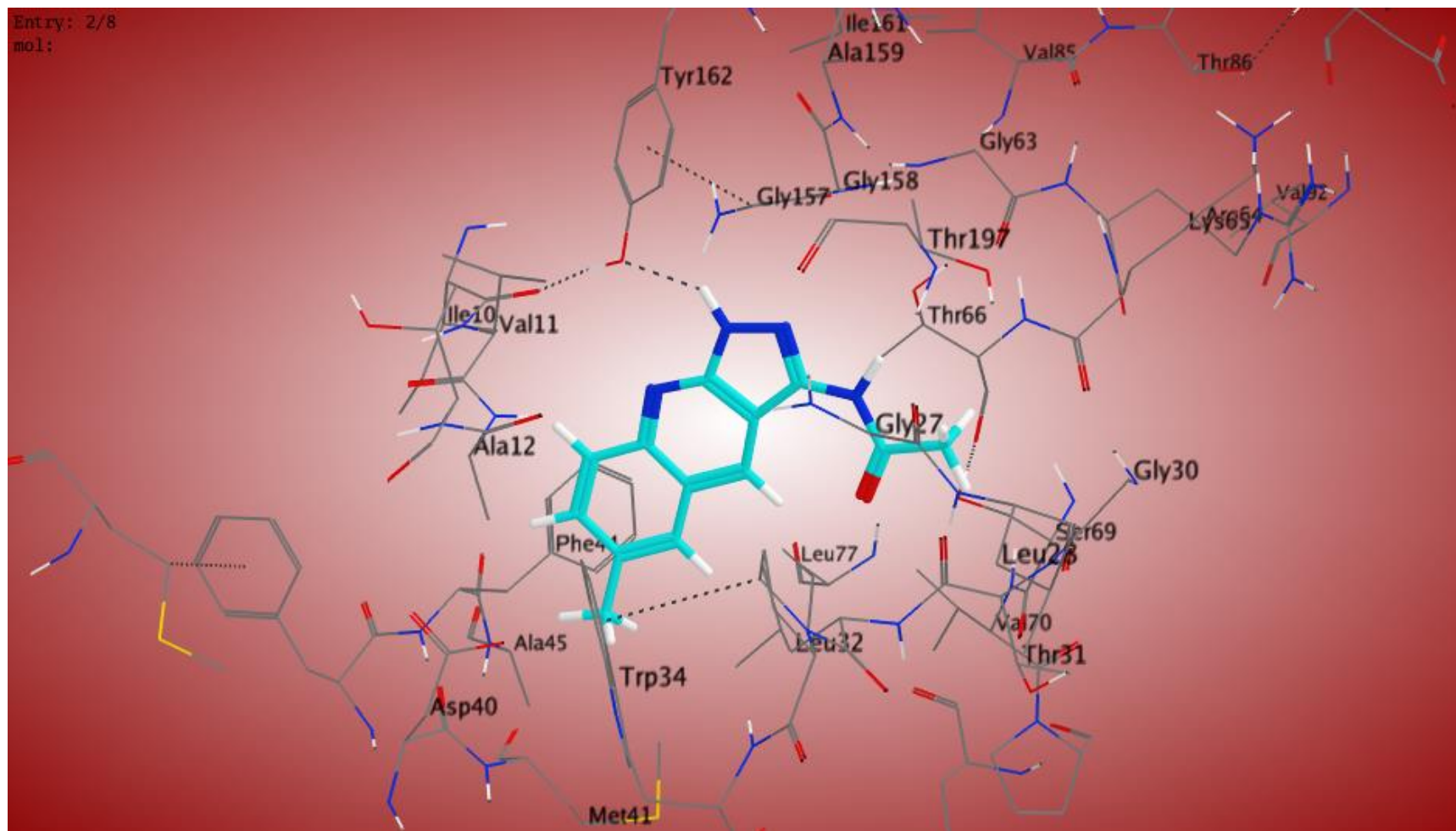


Figure 25: 3D interactions of quinoline derivative 21 in the active site of DHFR

Docking details for compound 21 in the active site of DHFR

Score -8.45339394

Ligand Interactions Report

6DTC: ANTIFUNGAL PROTEIN/INHIBITOR / 6DTC

Ligand	Receptor	Interaction	Distance	E (kcal/mol)
--------	----------	-------------	----------	--------------

N 12	OG SER 69	(A) H-donor	2.98	-1.1
------	-----------	-------------	------	------

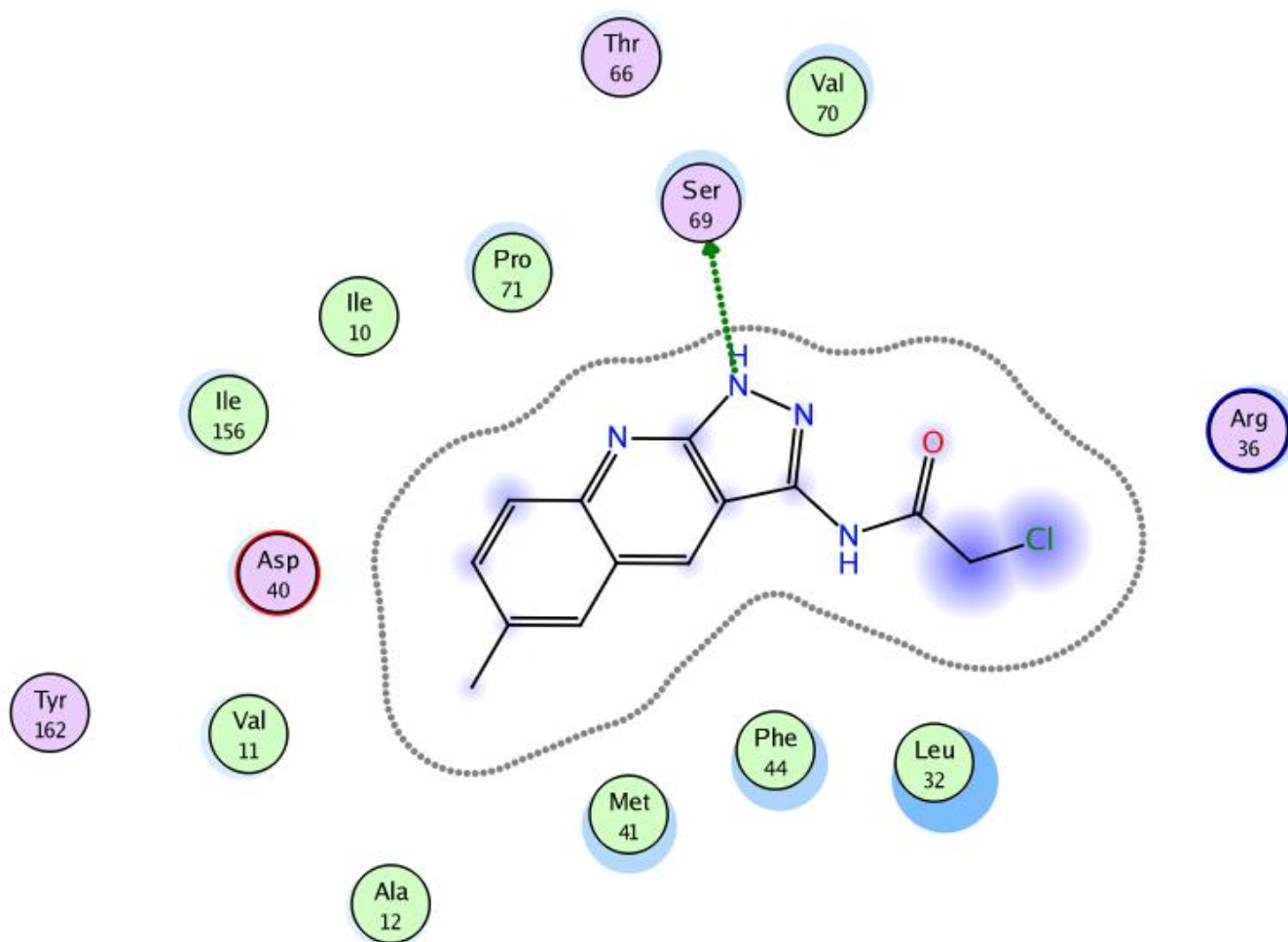


Figure 26: 2D interactions of quinoline derivative 22 in the active site of DHFR

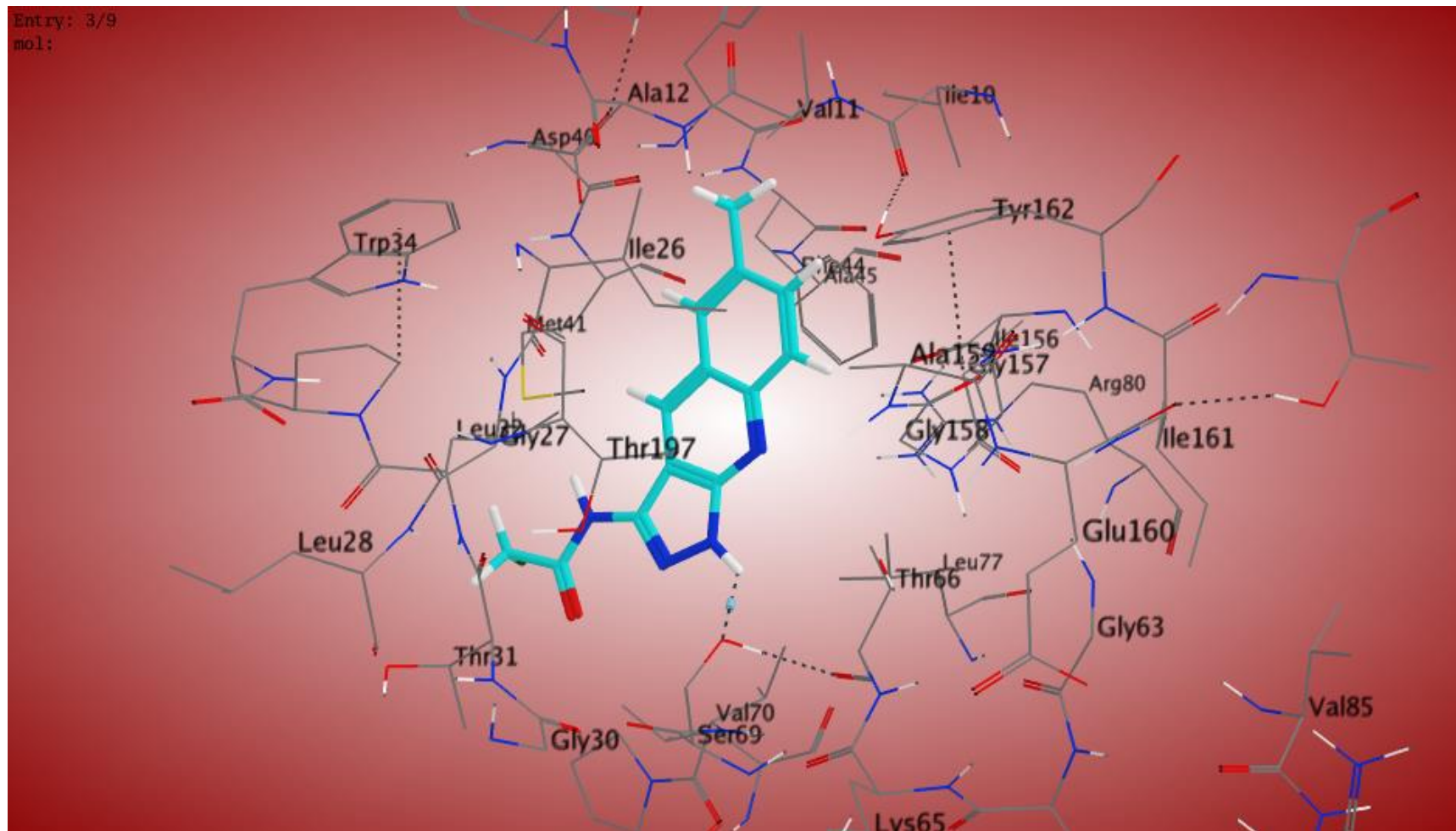
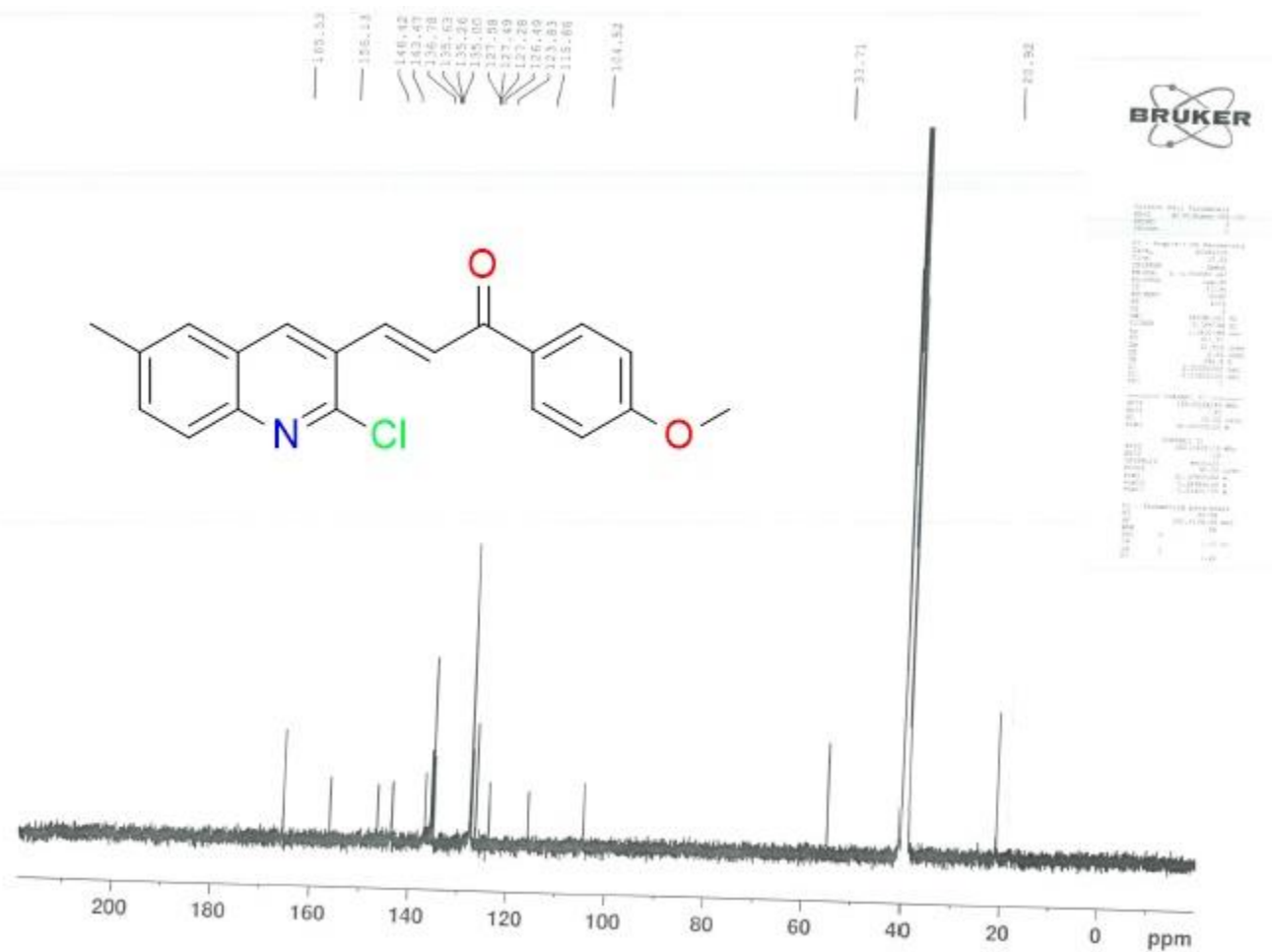


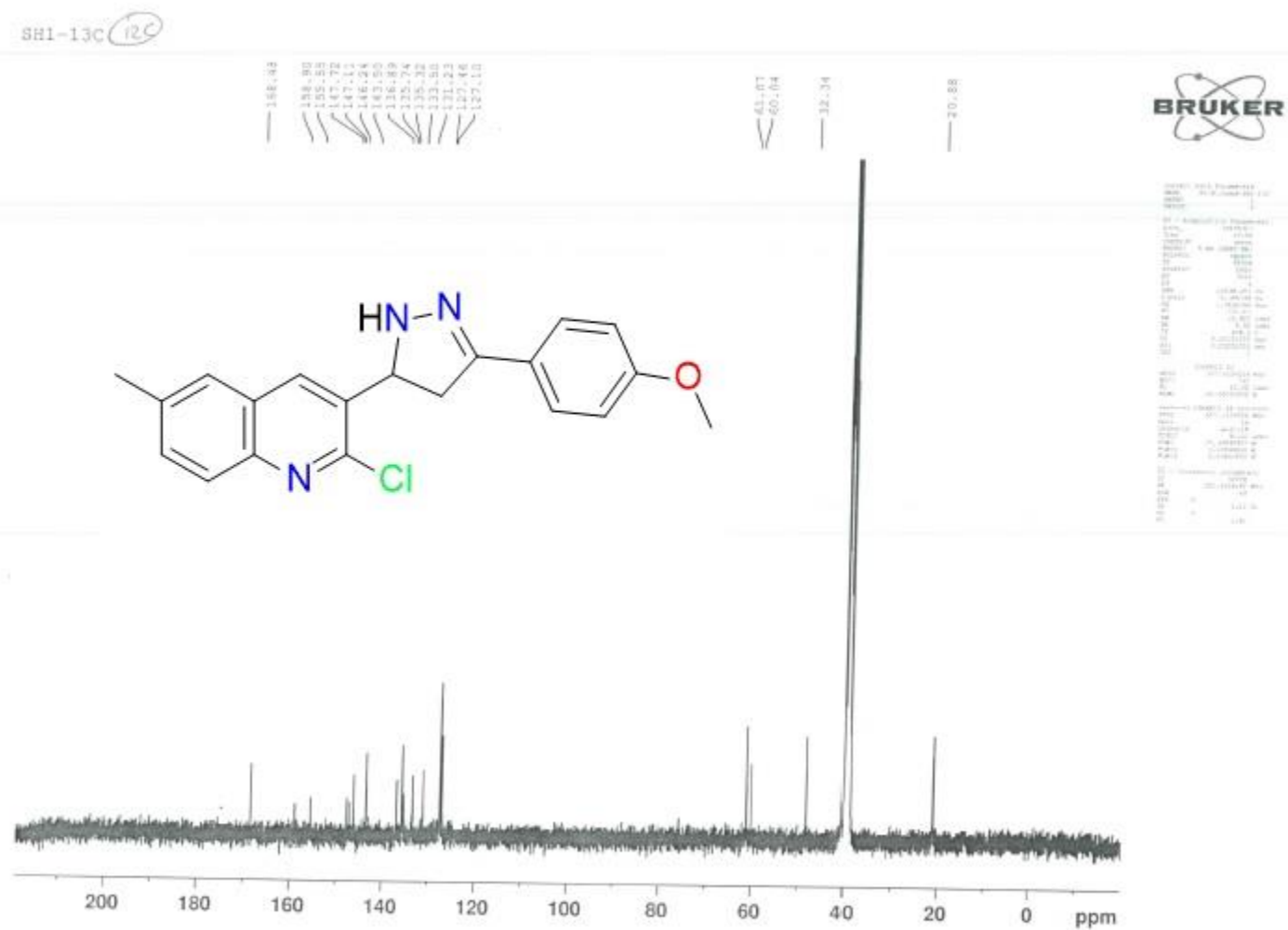
Figure 27: 3D interactions of quinoline derivative 22 in the active site of DHFR

Representative spectral data of new compounds

^{13}C NMR spectrum of compound 12



¹³C NMR spectrum of compound 13

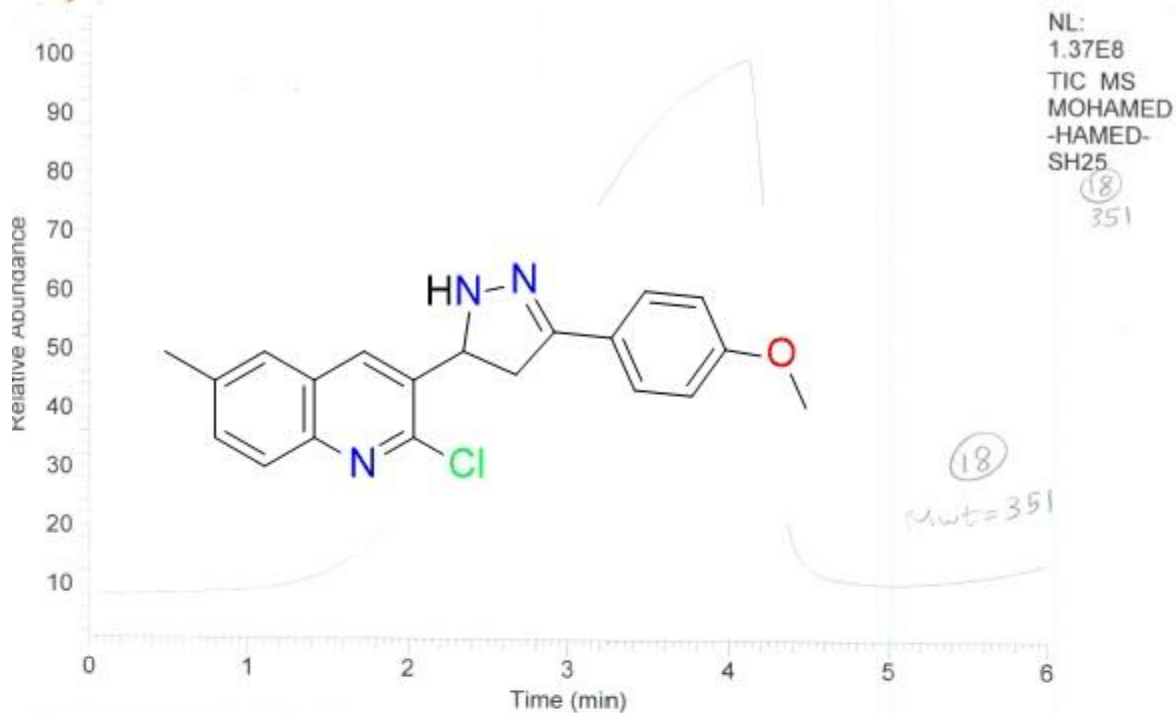


Mass Spectrum of compound 13

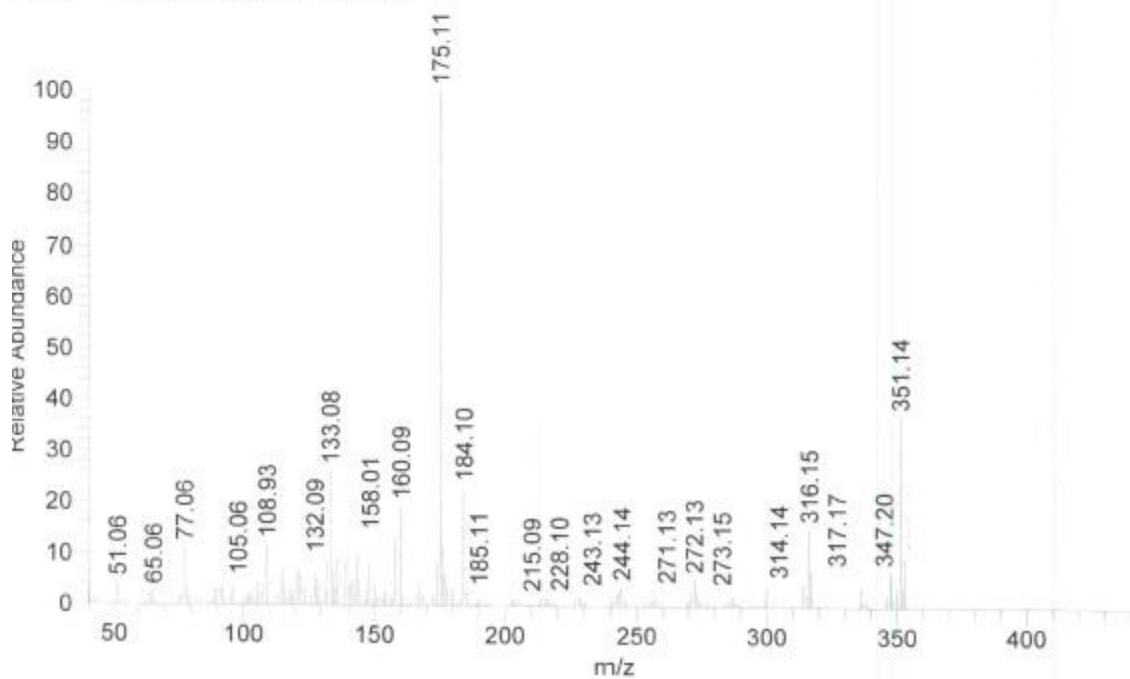
Azhar University C:\Xcalibur\data\SI\MOHAMED-HAMED-SH25

The Regional Center for Mycology & Biotechnology 5/25/2015 10:37:36 AM

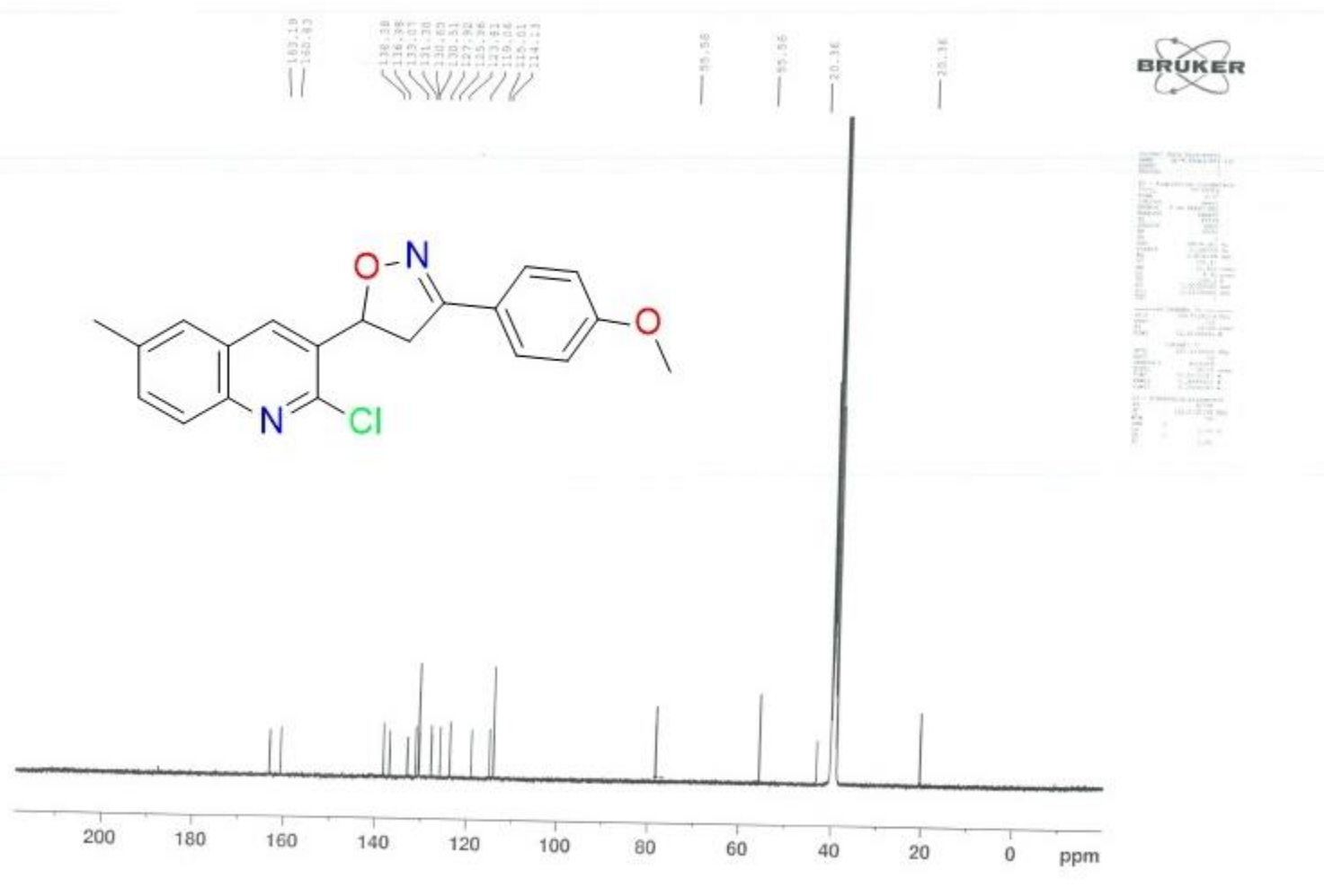
T: 0.00 - 6.00 SM: 15B



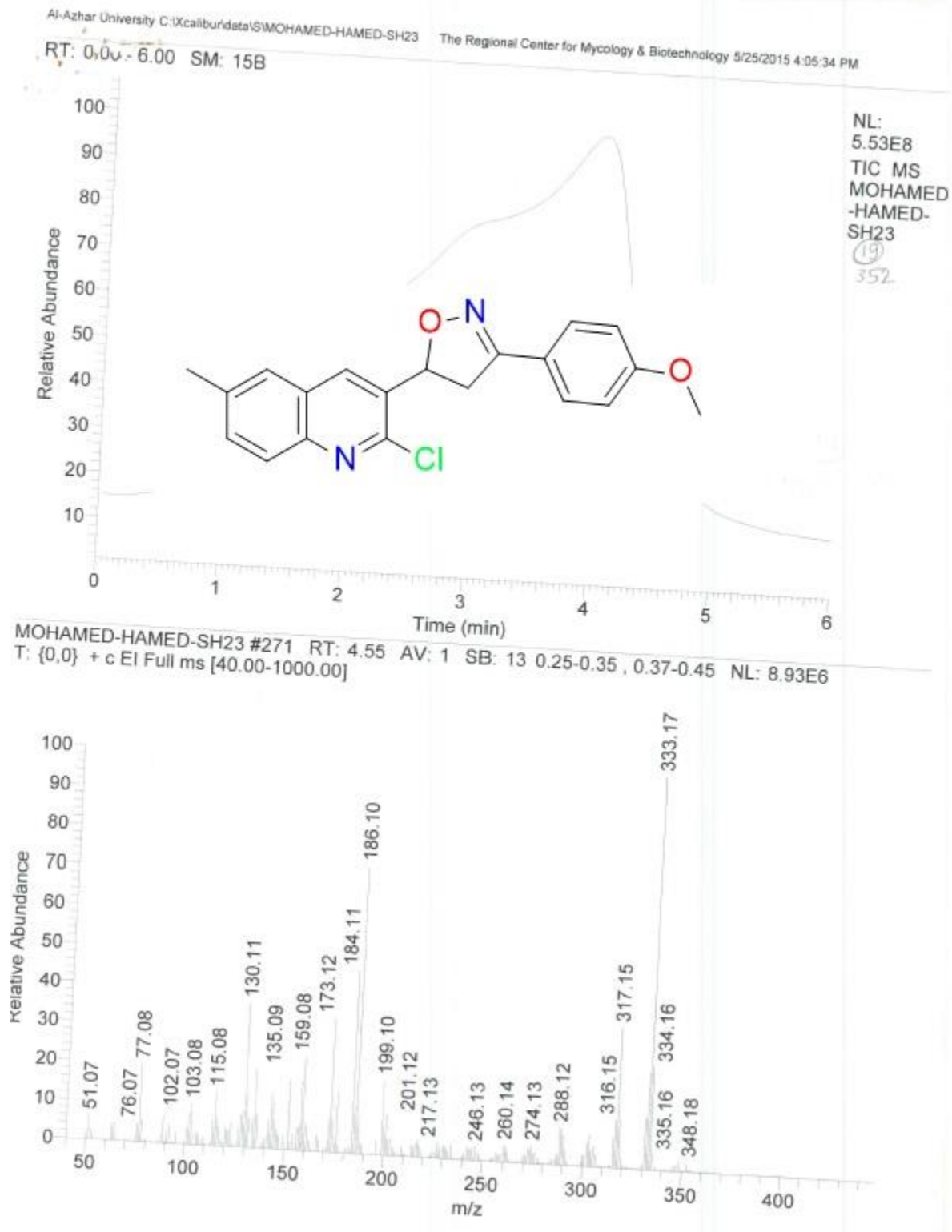
MOHAMED-HAMED-SH25 #206 RT: 3.46 AV: 1 SB: 19 4.17-4.30 , 4.18-4.33 NL: 3.78E6
{0,0} + c EI Full ms [40.00-1000.00]



¹³C NMR spectrum of compound 14



Mass spectrum of compound 14



SH3-13C

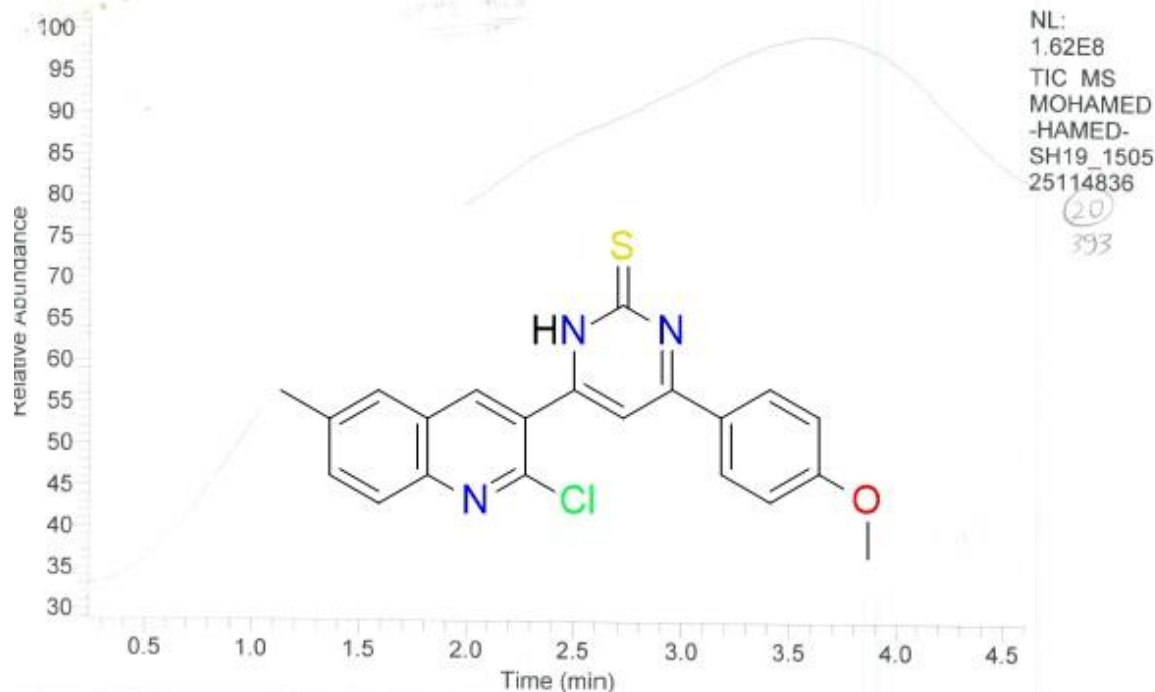
[illegible]

Mass spectrum of compound 15

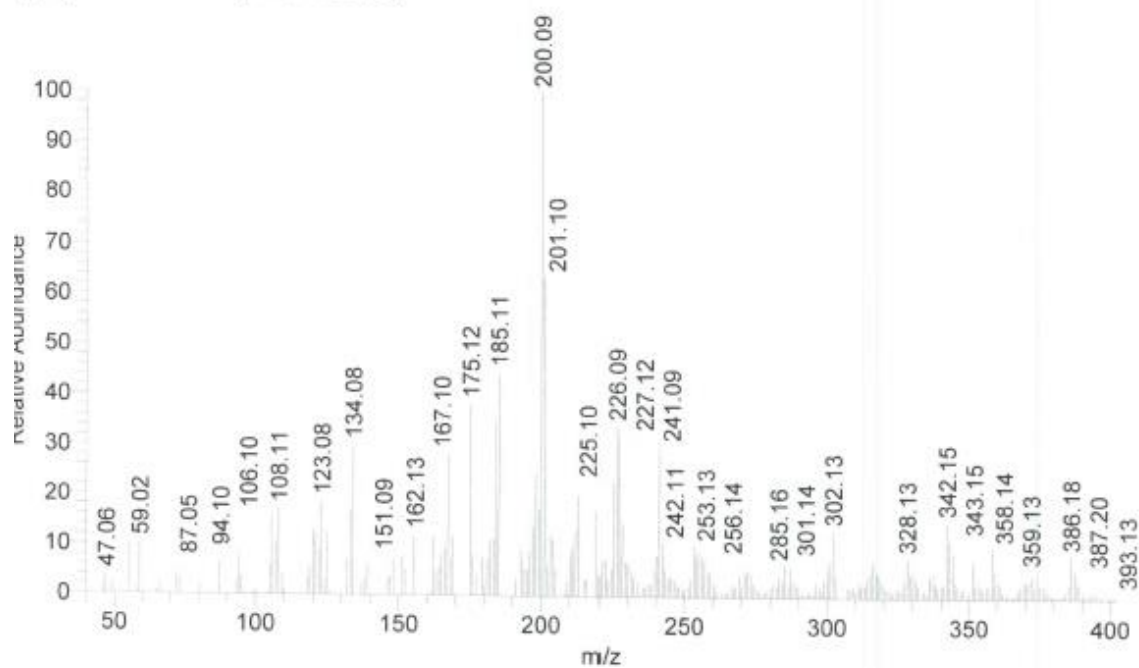
Azhar University MOHAMED-HAMED-SH19_150525114836

The Regional Center for Mycology & Biotechnology 5/25/2015 11:48:36 AM

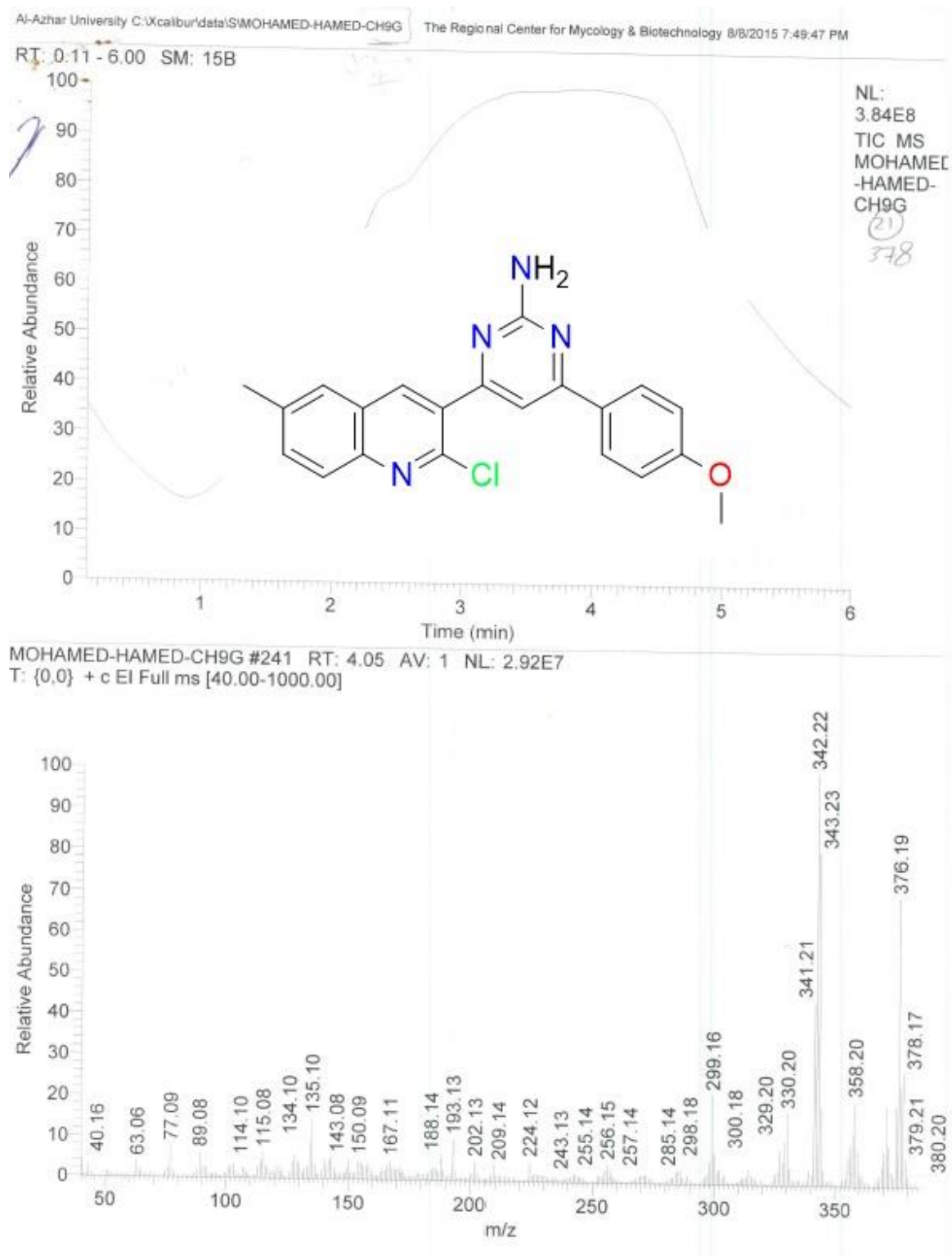
T: 0.24 - 4.62 SM: 15B



OHAMED-HAMED-SH19_150525114836 #363 RT: 6.09 AV: 1 SB: 36 1.34-1.56, 1.29-1.64 NL: {0.0} + c EI Full ms [40.00-1000.00]



Mass spectrum of compound 16

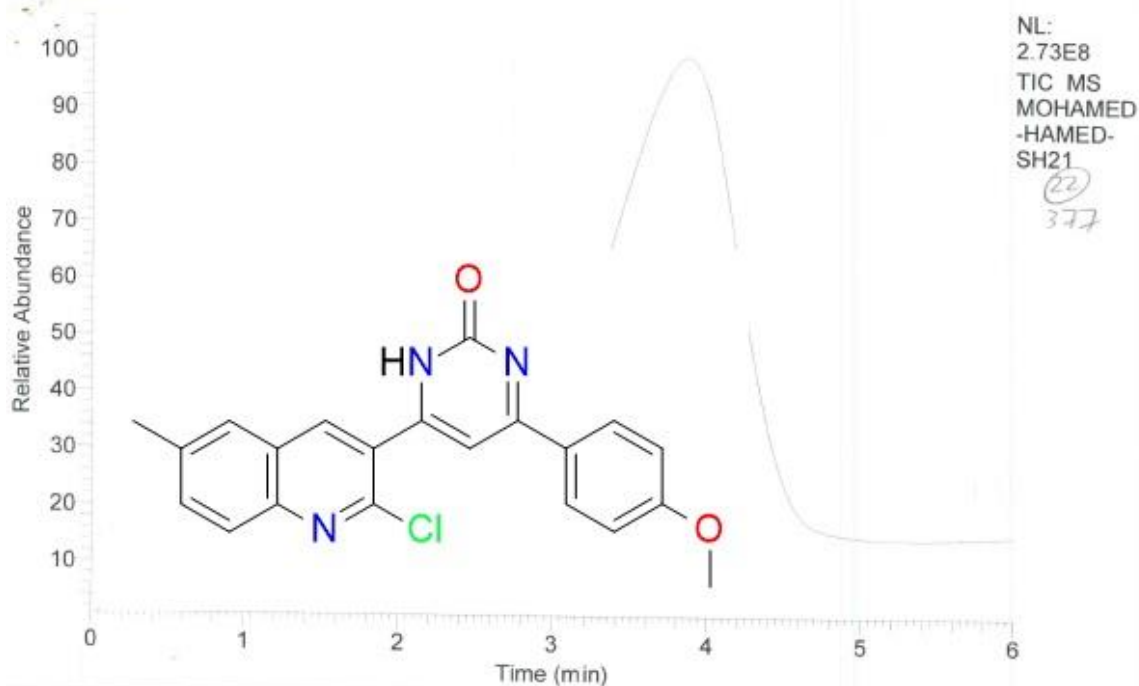


Mass spectrum of compound 17

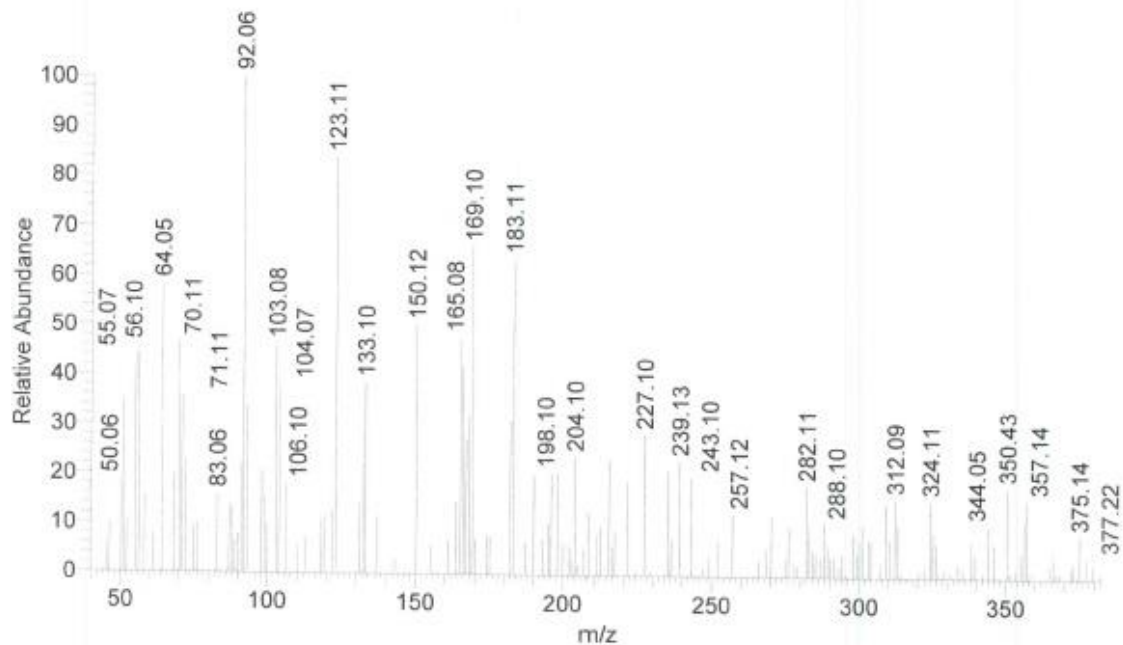
Al-Azhar University C:\Xcalibur\data\SI\MOHAMED-HAMED-SH21

The Regional Center for Mycology & Biotechnology 5/25/2015 12:10:02 PM

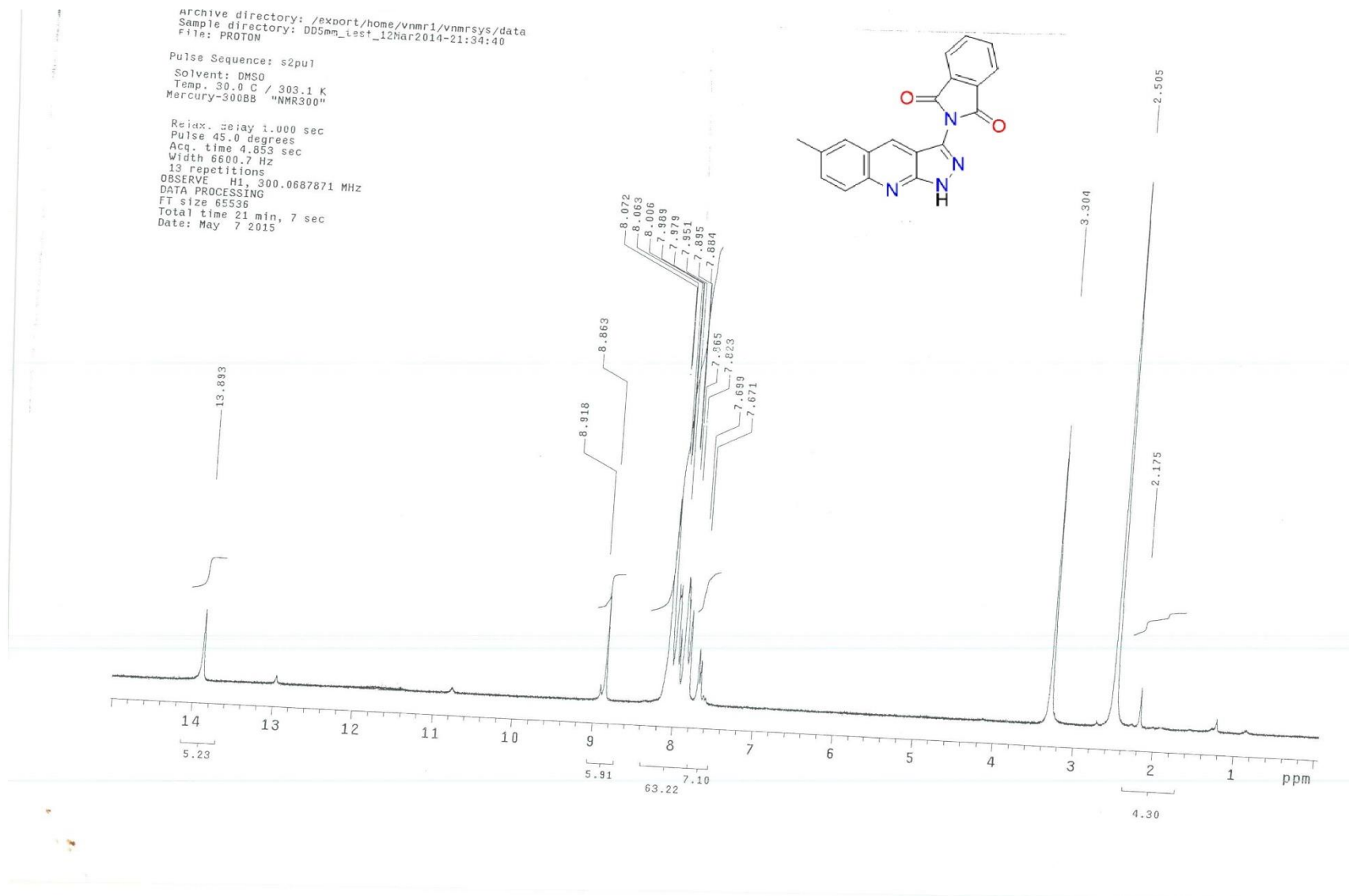
RT: 0.00-6.00 SM: 15B



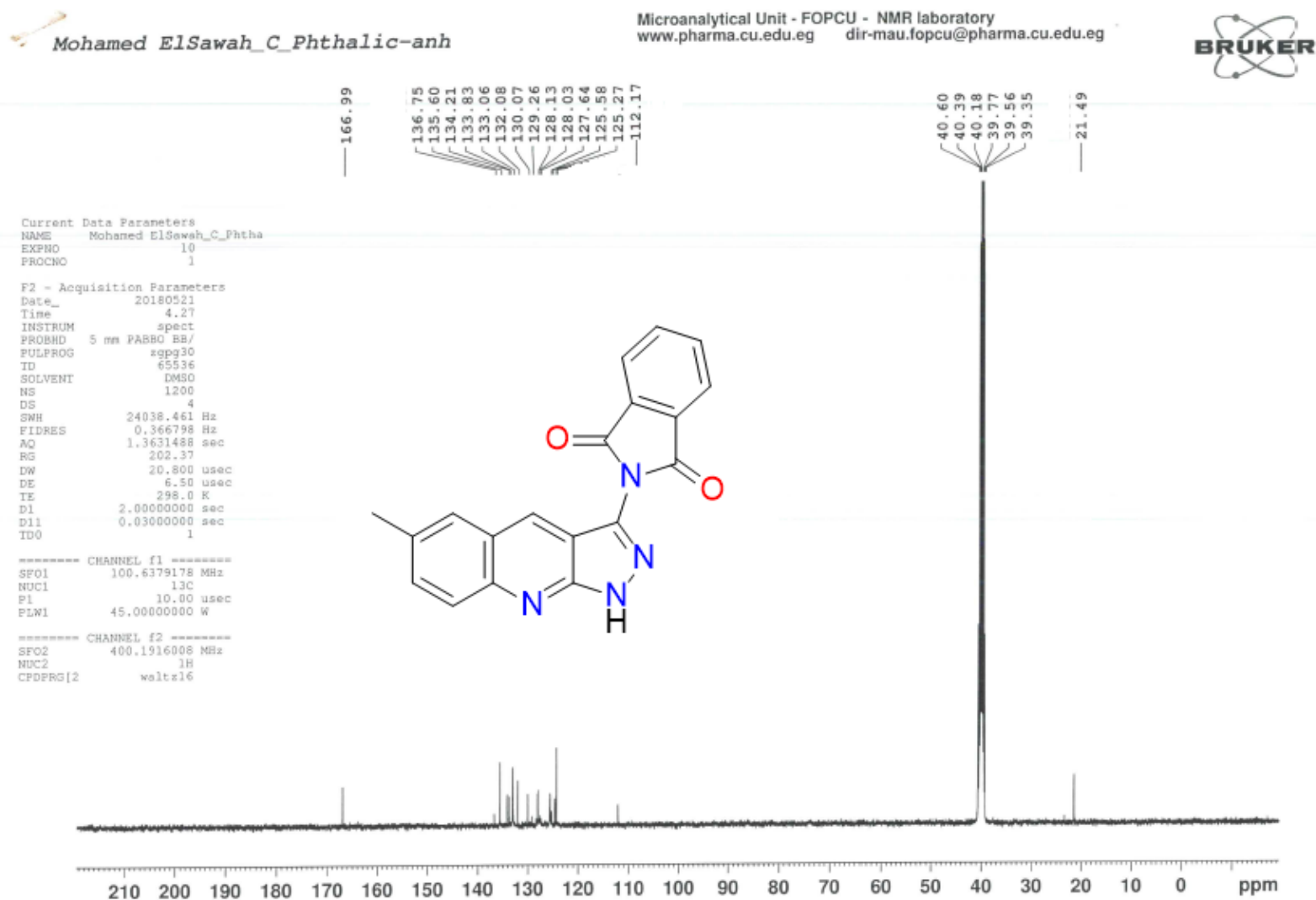
MOHAMED-HAMED-SH21 #323 RT: 5.42 AV: 1 SB: 57 5.32-5.62, 5.07-5.69 NL: 1.21E4
[0,0] + c EI Full ms [40.00-1000.00]



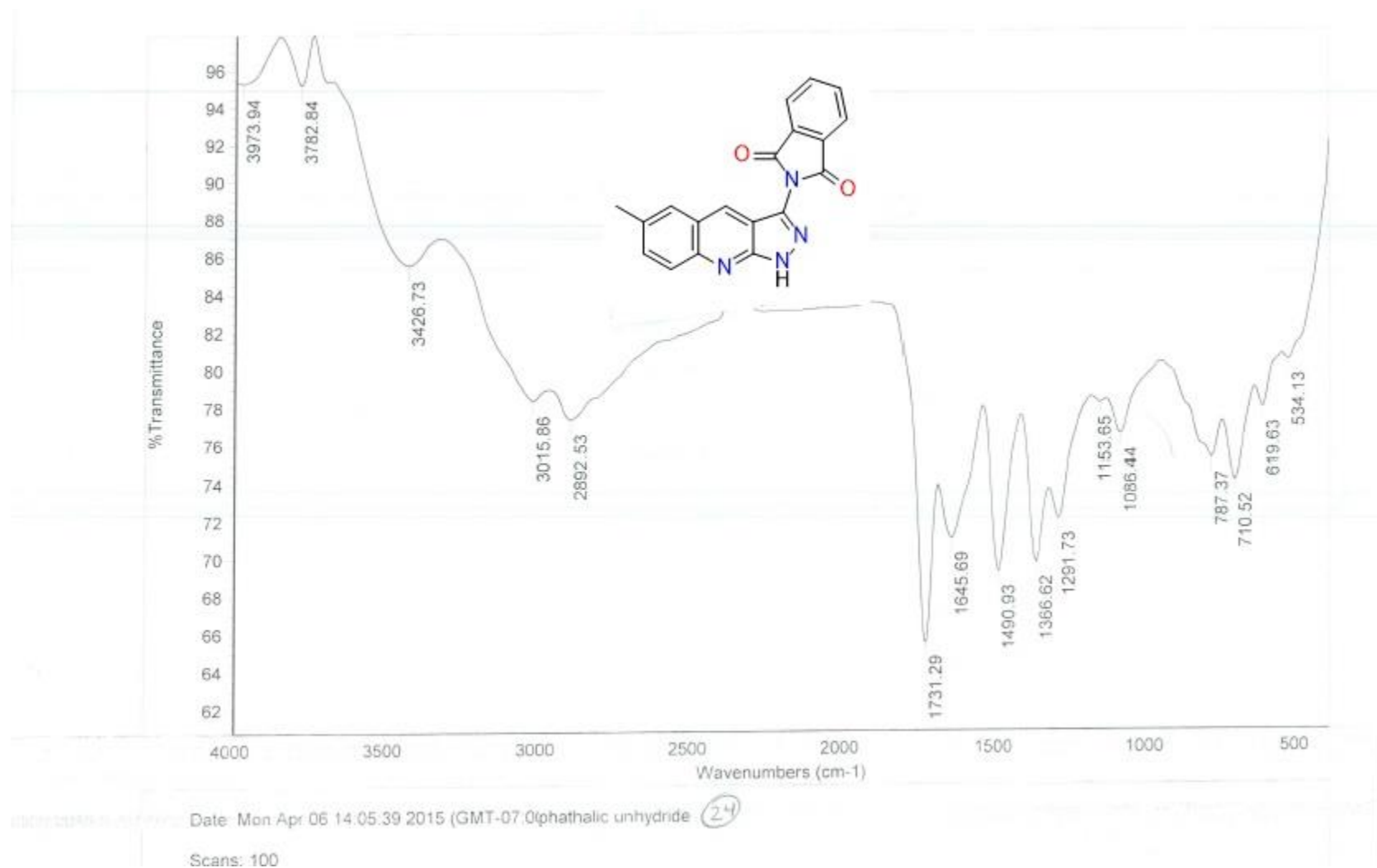
¹H NMR spectrum of compound 18



¹³C NMR spectrum of compound 18



IR spectrum of compound 18

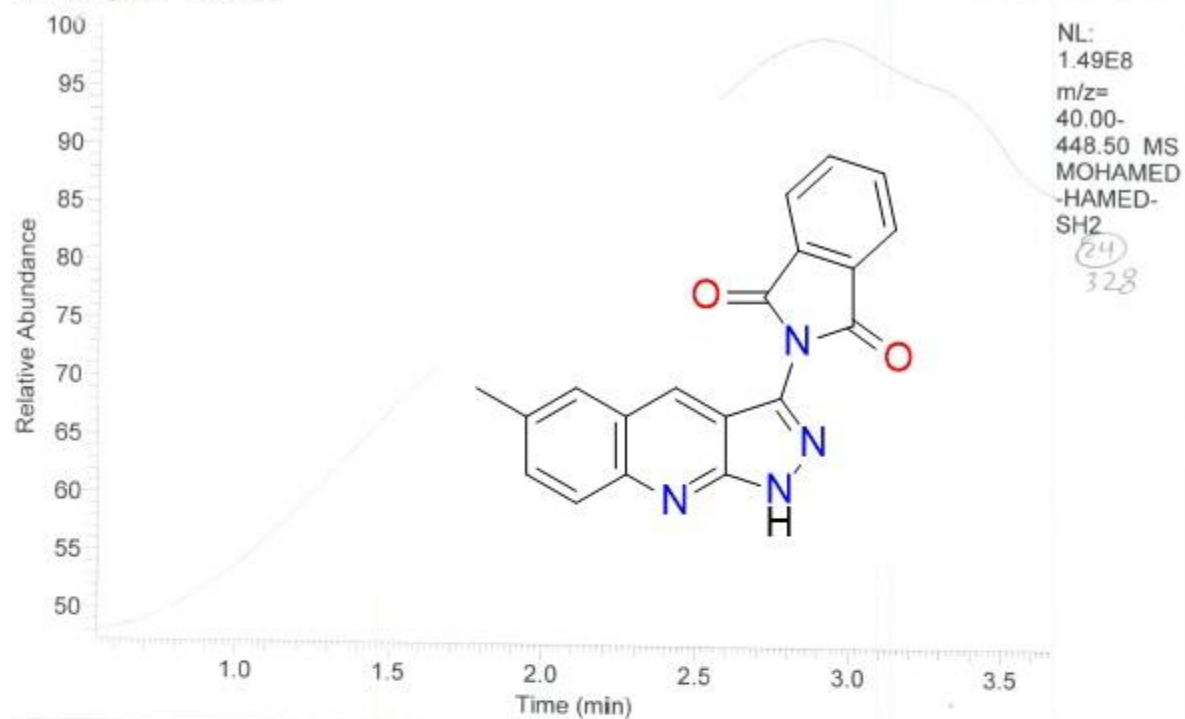


Mass spectrum of compound 18

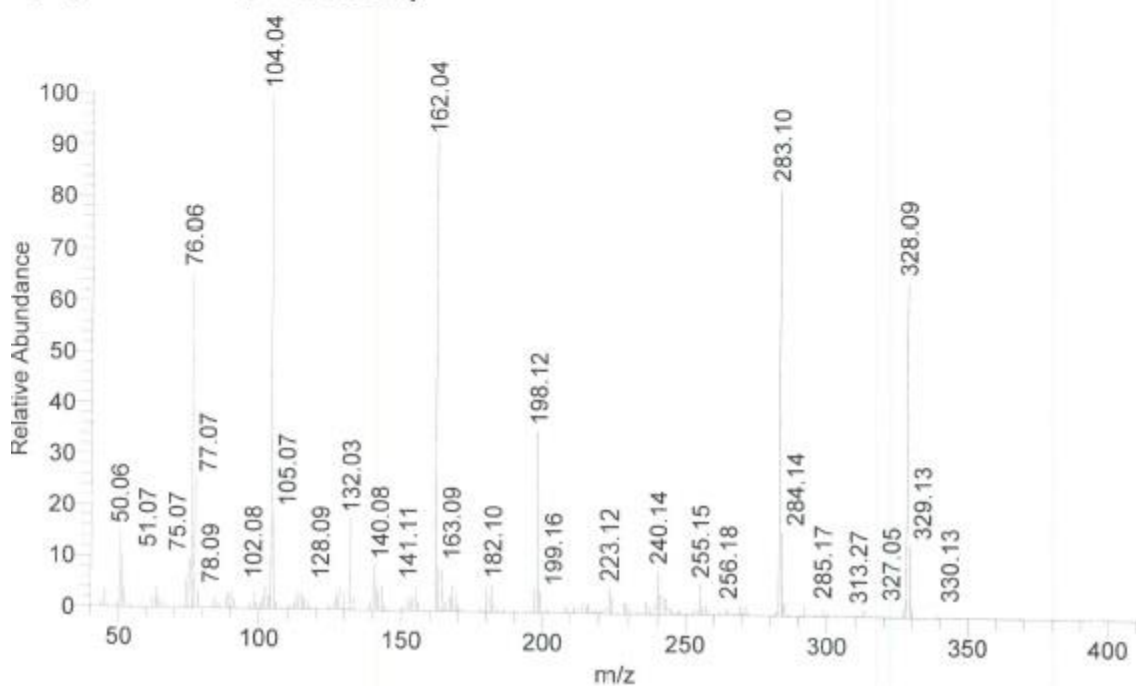
N-Azhar University C:\Xcalibur\data\1\MOHAMED-HAMED-SH2

The Regional Center for Mycology & Biotechnology 5/24/2015 12:14:36 PM

RT: 0.54, 3.67 SM: 15B



MOHAMED-HAMED-SH2 #78-341 RT: 1.32-5.72 AV: 264 SB: 20 0.27-0.39, 0.18-0.37 NL: 7.58E6
: [0,0] + c EI Full ms [40.00-1000.00]



¹³C NMR spectrum of compound 19

Mohamed ElSawah_C_Maliec-anh

www.pharma.cu.edu.eg

dir-mau.fopcu@pharma.cu.edu.eg

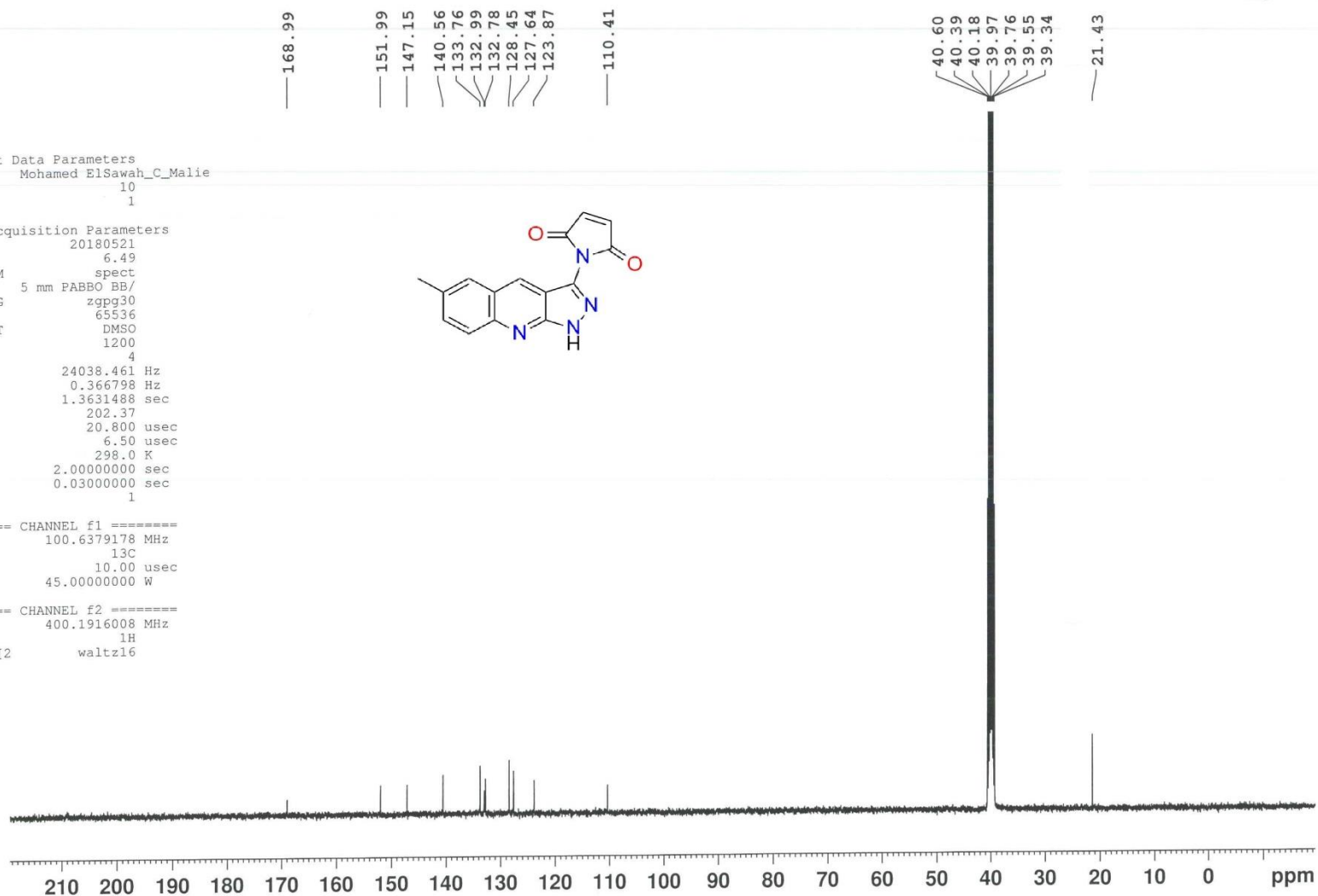
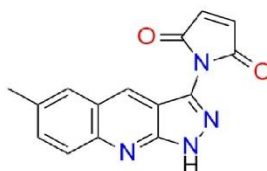


Current Data Parameters
NAME Mohamed ElSawah_C_Malie
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180521
Time 6.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

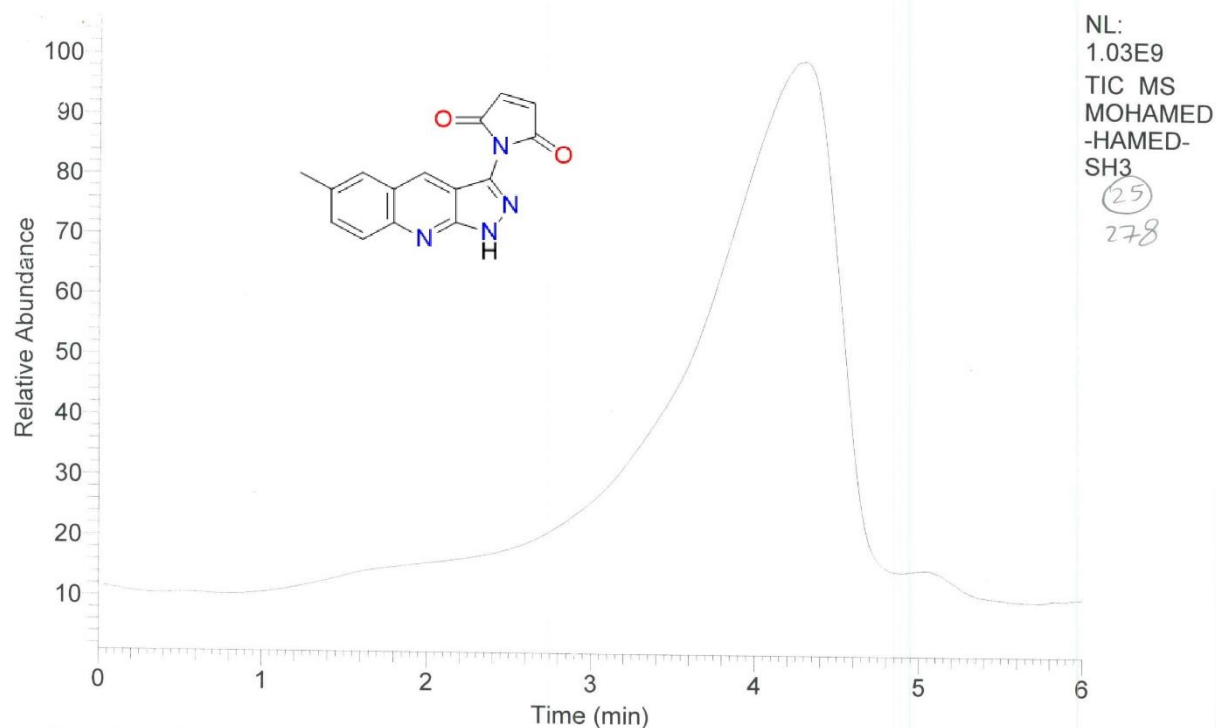
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NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

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NUC2 1H
CPDPRG[2] waltz16

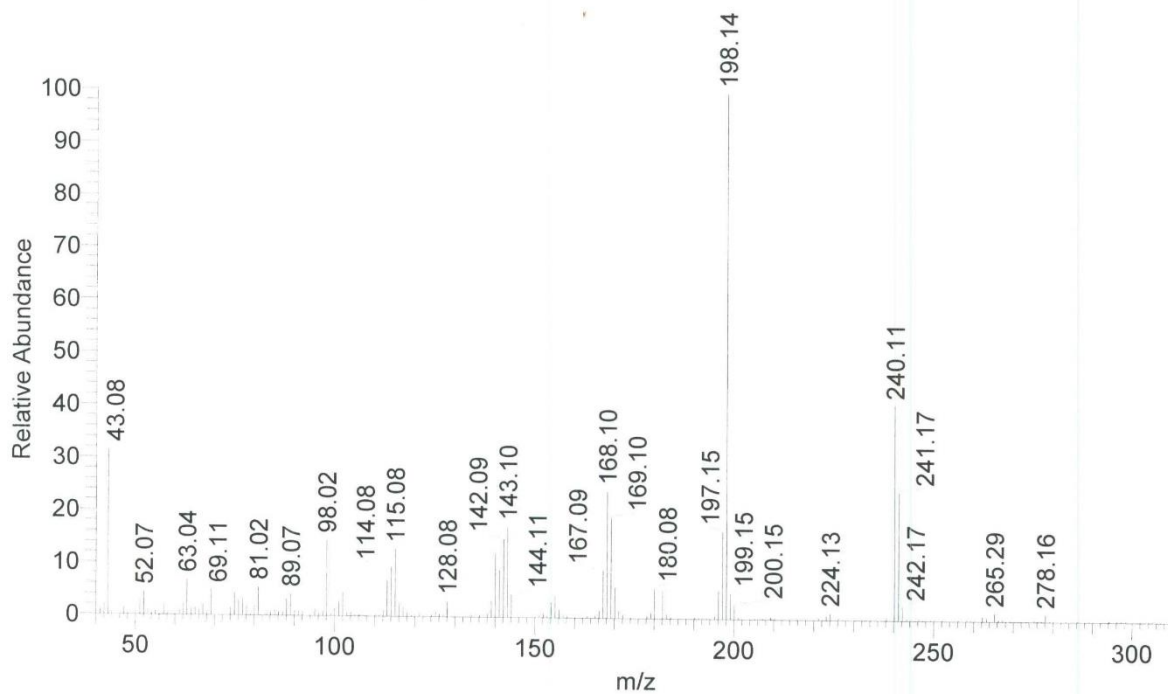


Mass spectrum of compound 19

RT: 0.00 - 6.00 SM: 15B



MOHAMED-HAMED-SH3 #219 RT: 3.68 AV: 1 SB: 22 3.58-3.73, 3.55-3.73 NL: 3.43E6
F: {0,0} + c EI Full ms [40.00-1000.00]



¹H NMR spectrum of compound 19

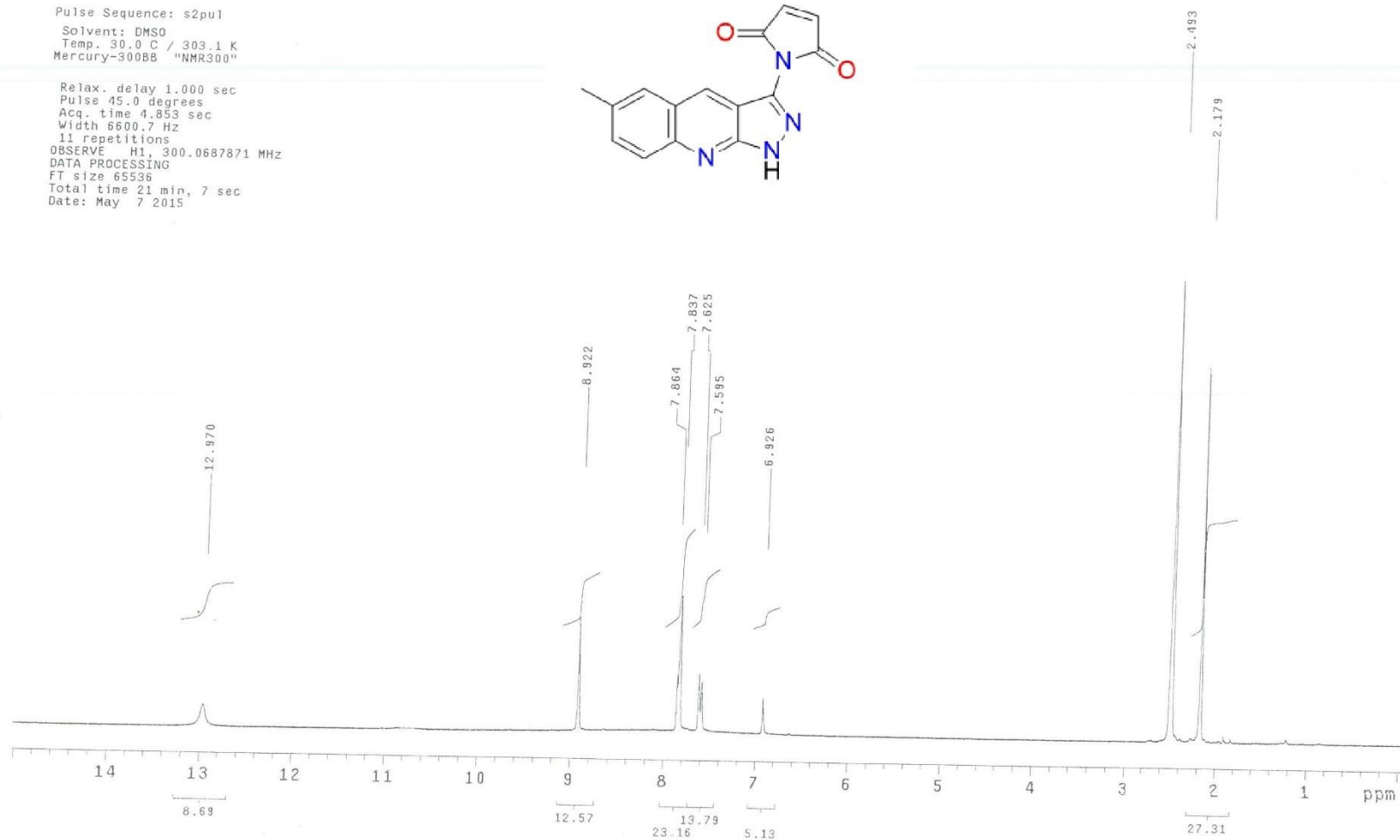
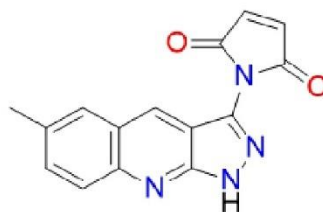
MohammedHamed-maliec-DMSO-H1 (25)

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
11 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 21 min, 7 sec
Date: May 7 2015

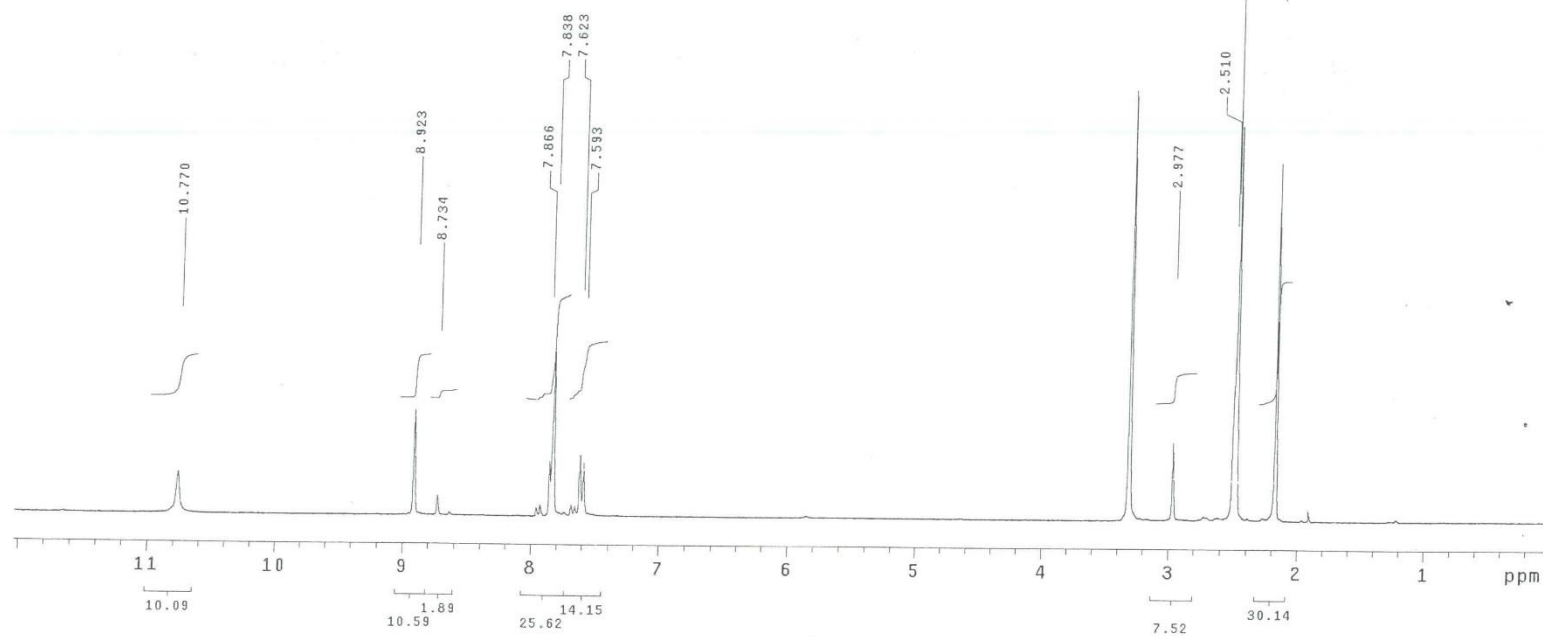
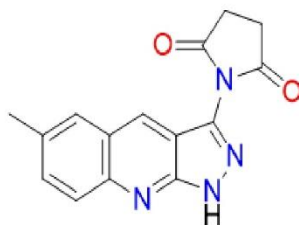


¹H NMR spectrum of compound 20

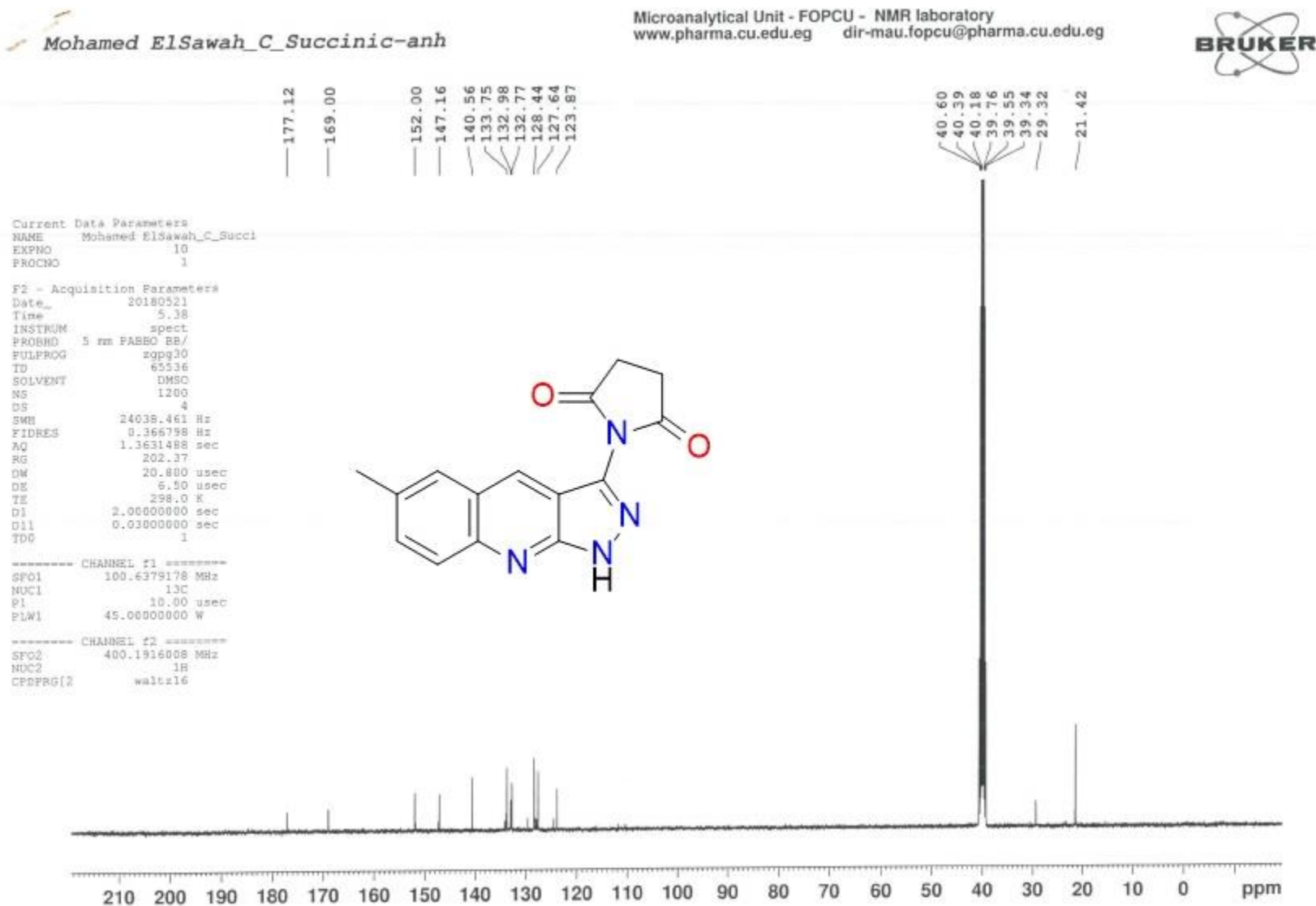
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
9 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 21 min, 7 sec
Date: May 7 2015



¹³C NMR spectrum of compound 20

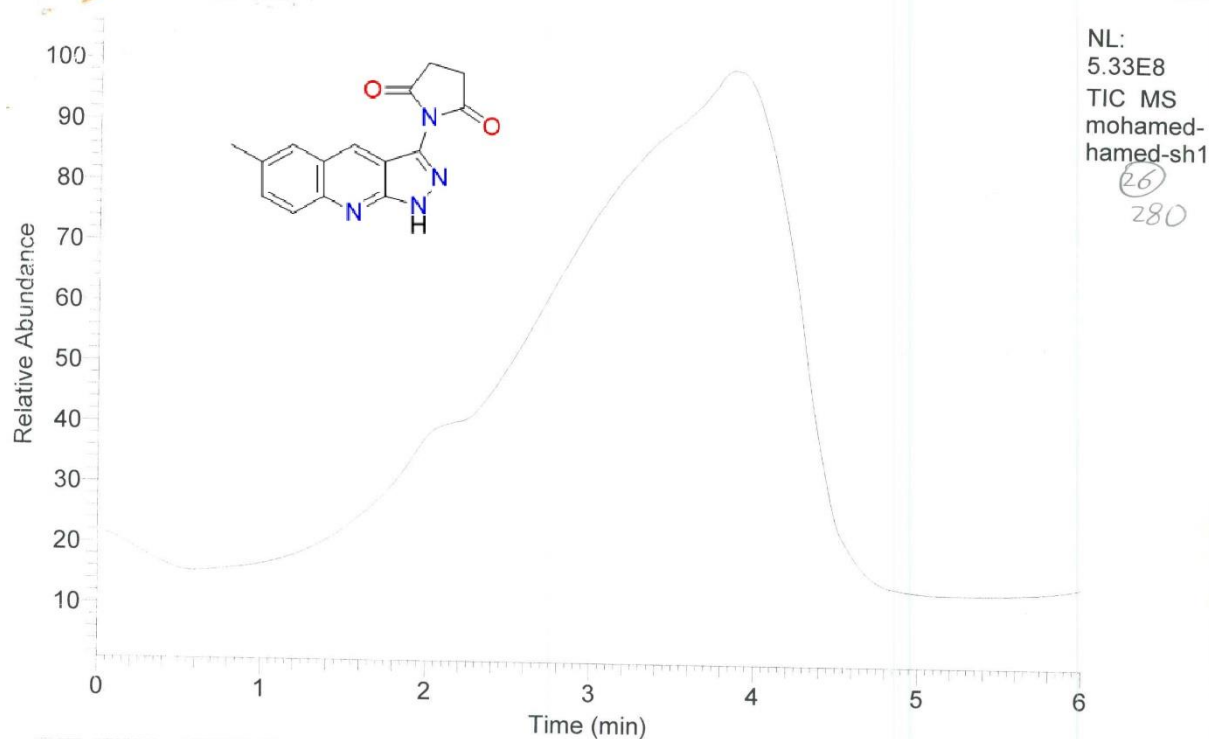


Mass spectrum of compound 20

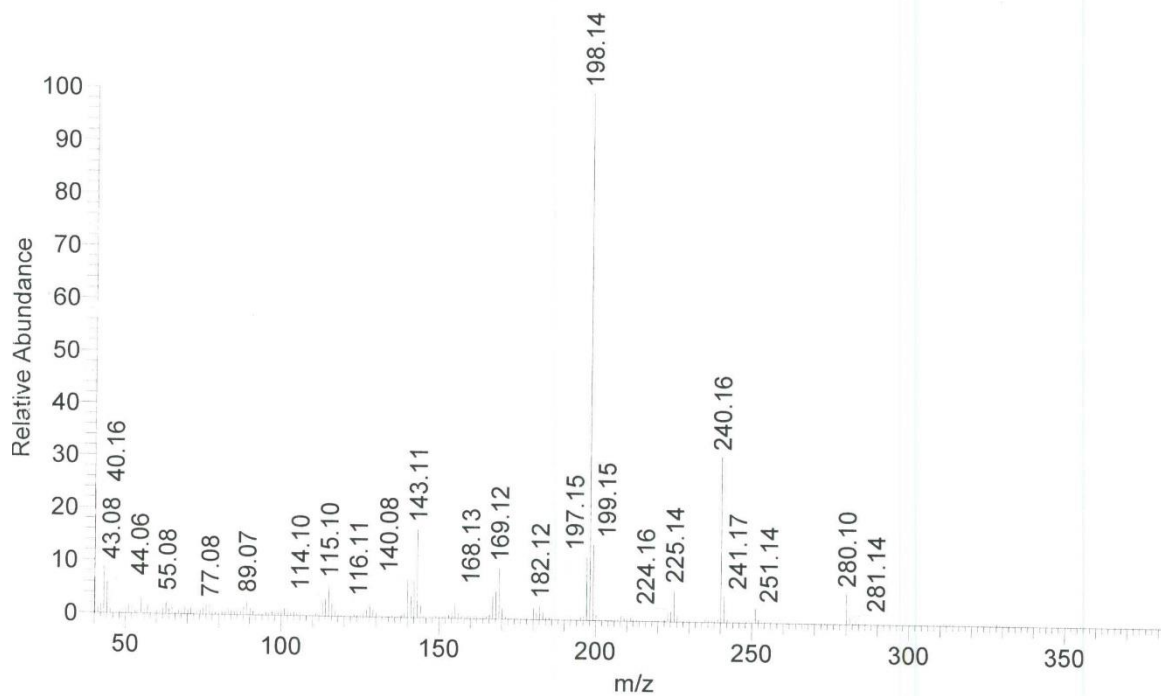
Al-Azhar University C:\Xcalibur\data\1\mohamed-hamed-sh1

The Regional Center for Mycology & Biotechnology 5/24/2015 10:42:14 AM

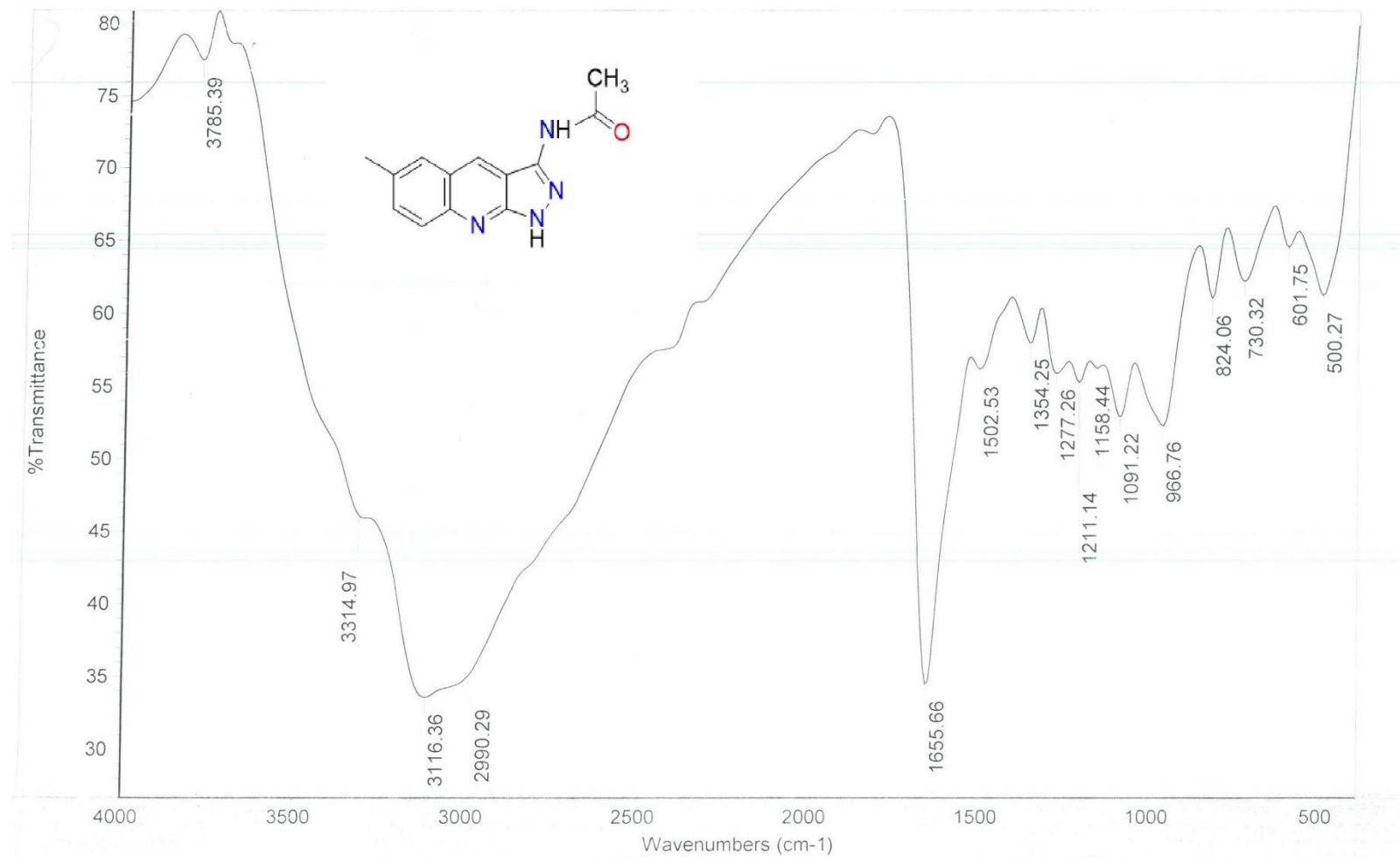
RT: 0.00 - 6.00 SM: 15B



mohamed-hamed-sh1 #176 RT: 2.96 AV: 1 NL: 9.74E7
[0,0] + c EI Full ms [40.00-1000.00]



IR spectrum of compound 21



Date: Wed Apr 08 14:19:29 2015 (GMT-07:00)pyrazolo acetyl cl (27)

Scans: 100

¹H NMR spectrum of compound 21

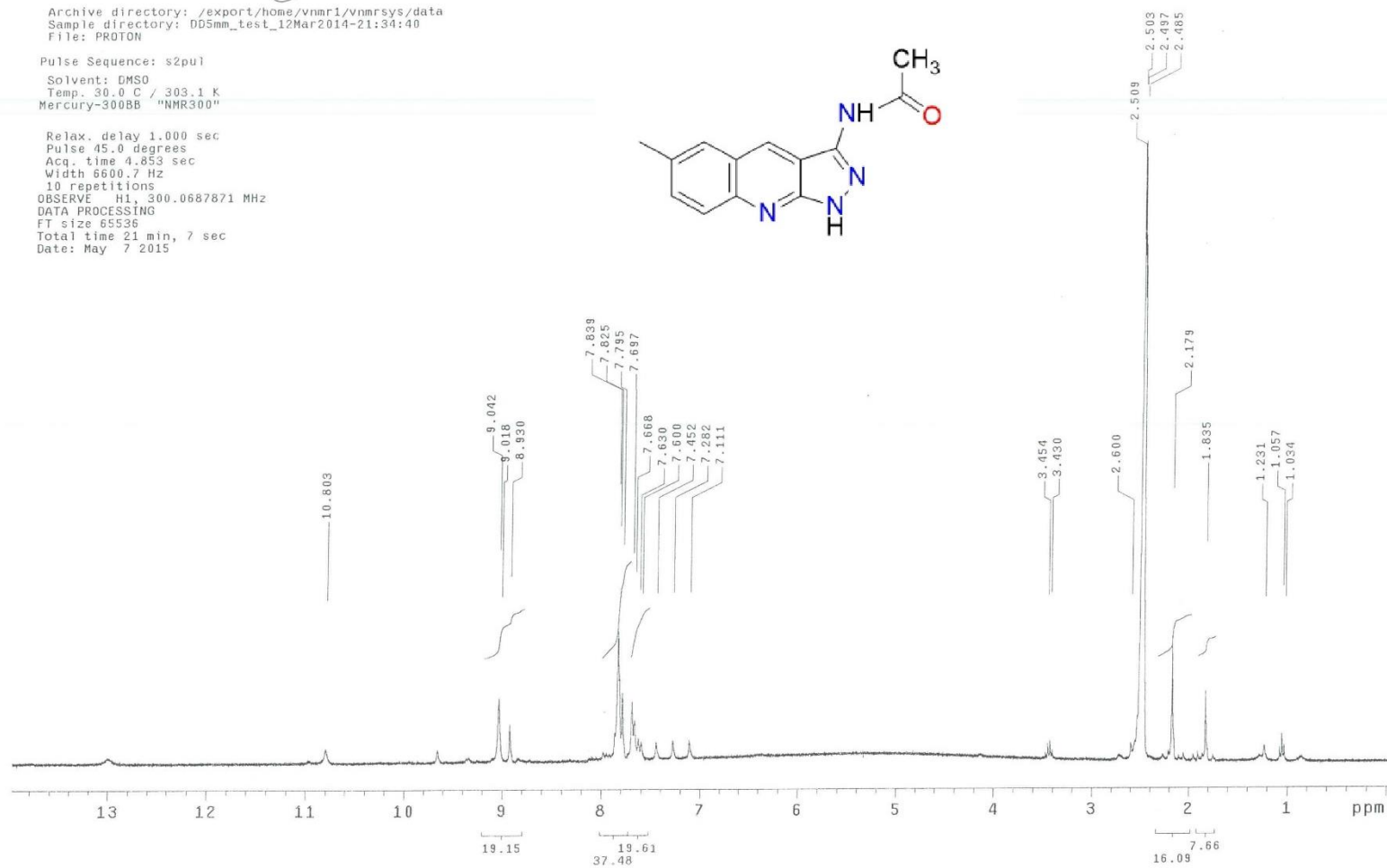
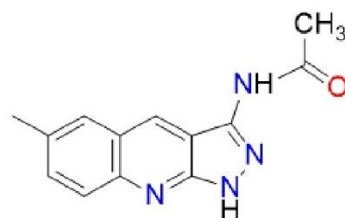
MohammedHamed-Acetyl-DMSO-H1 (27)

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DDSmm_test_12Mar2014-21:34:40
File: PROTON

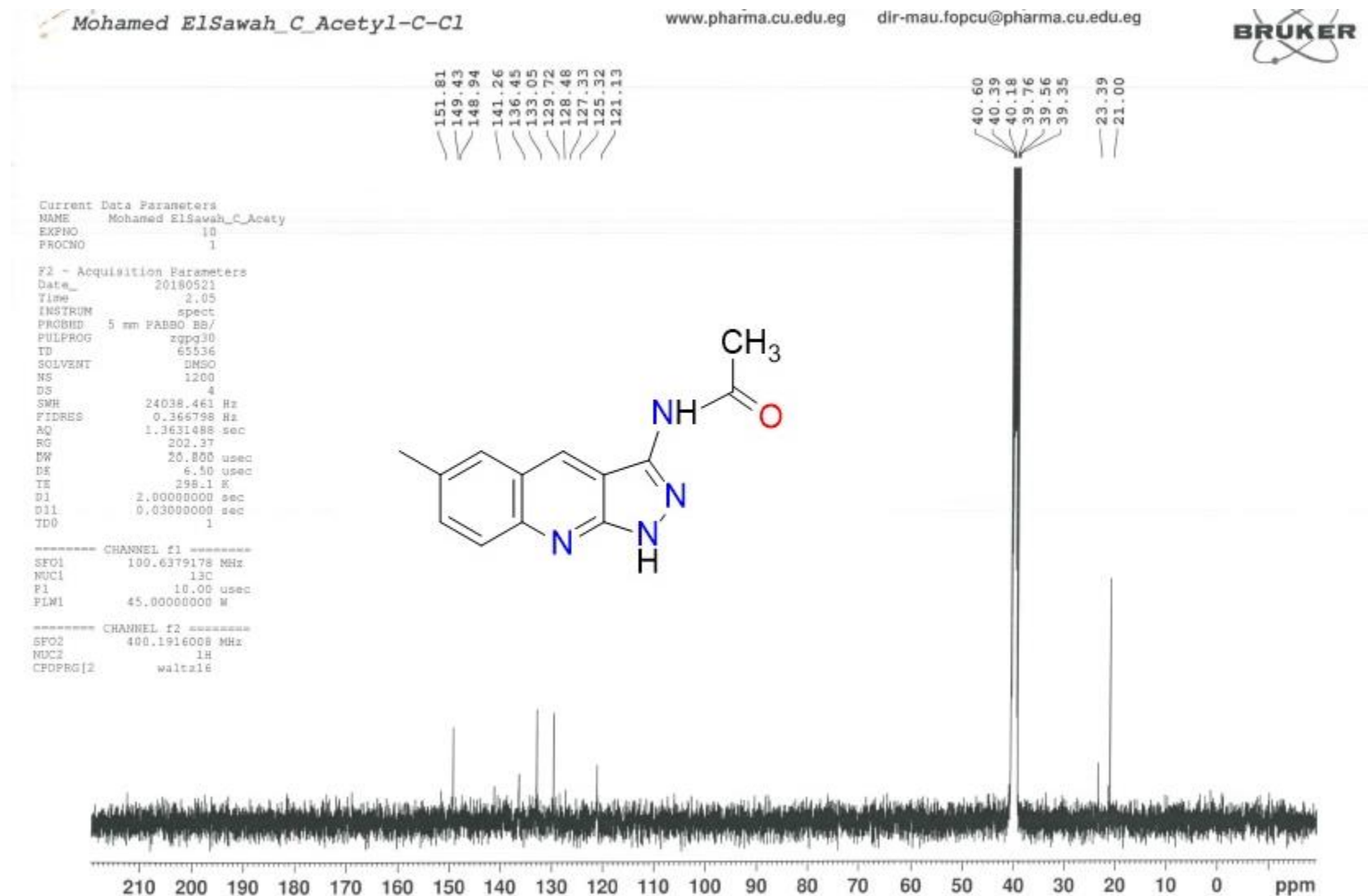
Pulse Sequence: s2pul

Solvent: DMSO
Temp: 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
10 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
F1 size 65536
Total time 21 min, 7 sec
Date: May 7 2015



¹³C NMR spectrum of compound 21

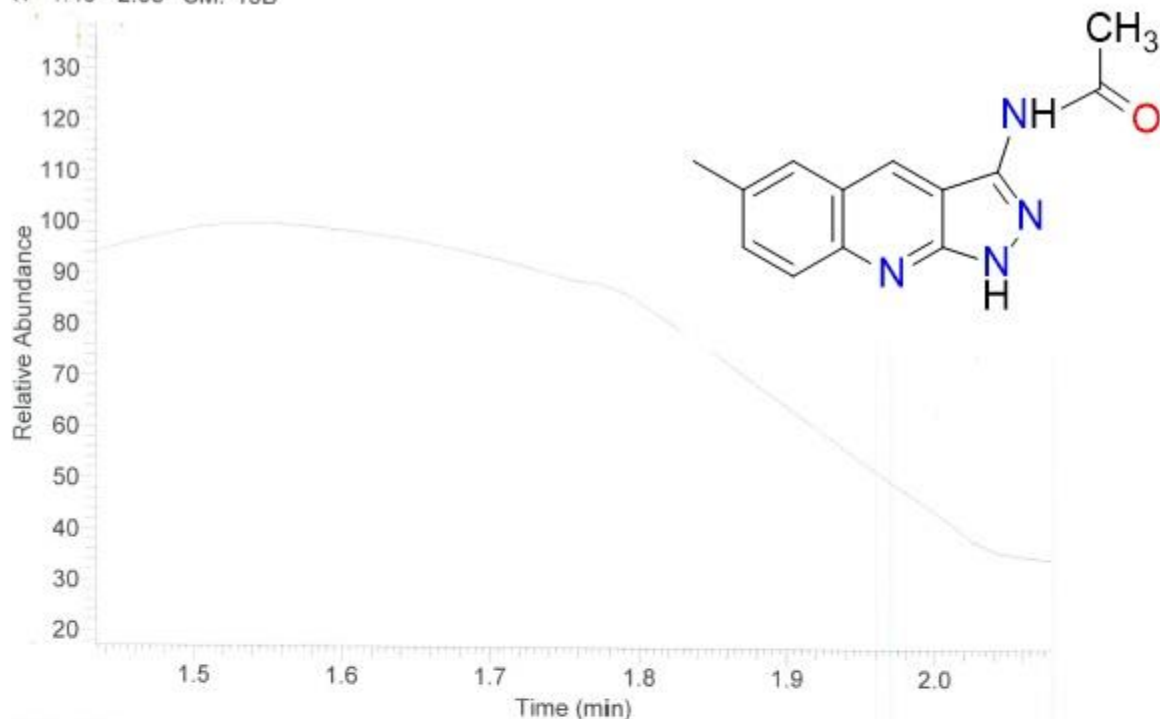


Mass spectrum of compound 21

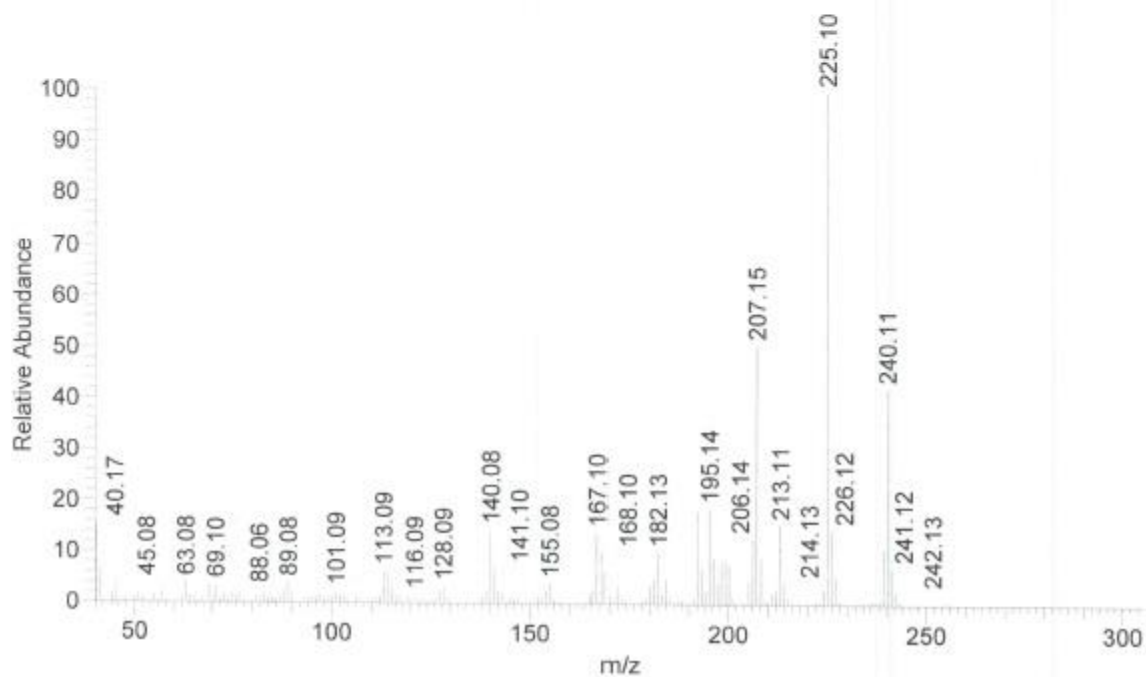
i-Azhr University C:\Xcalibur\data\SMOHAMED-HAMED-SH4

The Regional Center for Mycology & Biotechnology 5/24/2015 11:39:33 AM

RT: 1.43 - 2.08 SM: 15B



MOHAMED-HAMED-SH4 #204 RT: 3.43 AV: 1 SB: 28 5.15-5.22 , 4.92-5.29 NL: 1.41E7
[0,0] + c EI Full ms [40.00-1000.00]



¹H NMR spectrum of compound 22

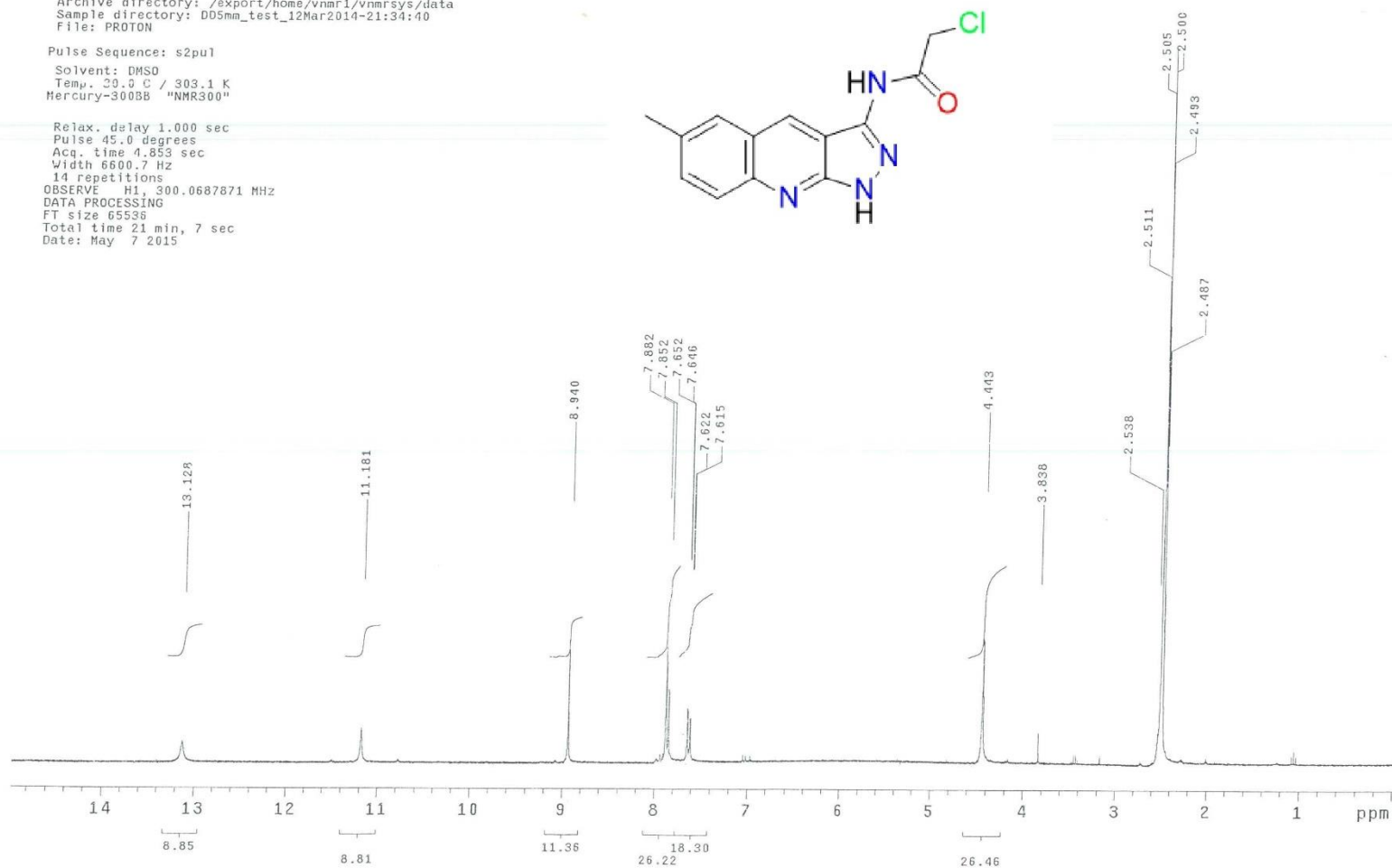
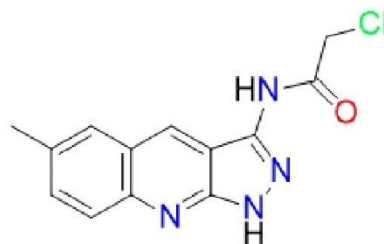
MohammedHamed-CLACL-DMSO-H1 (29)

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

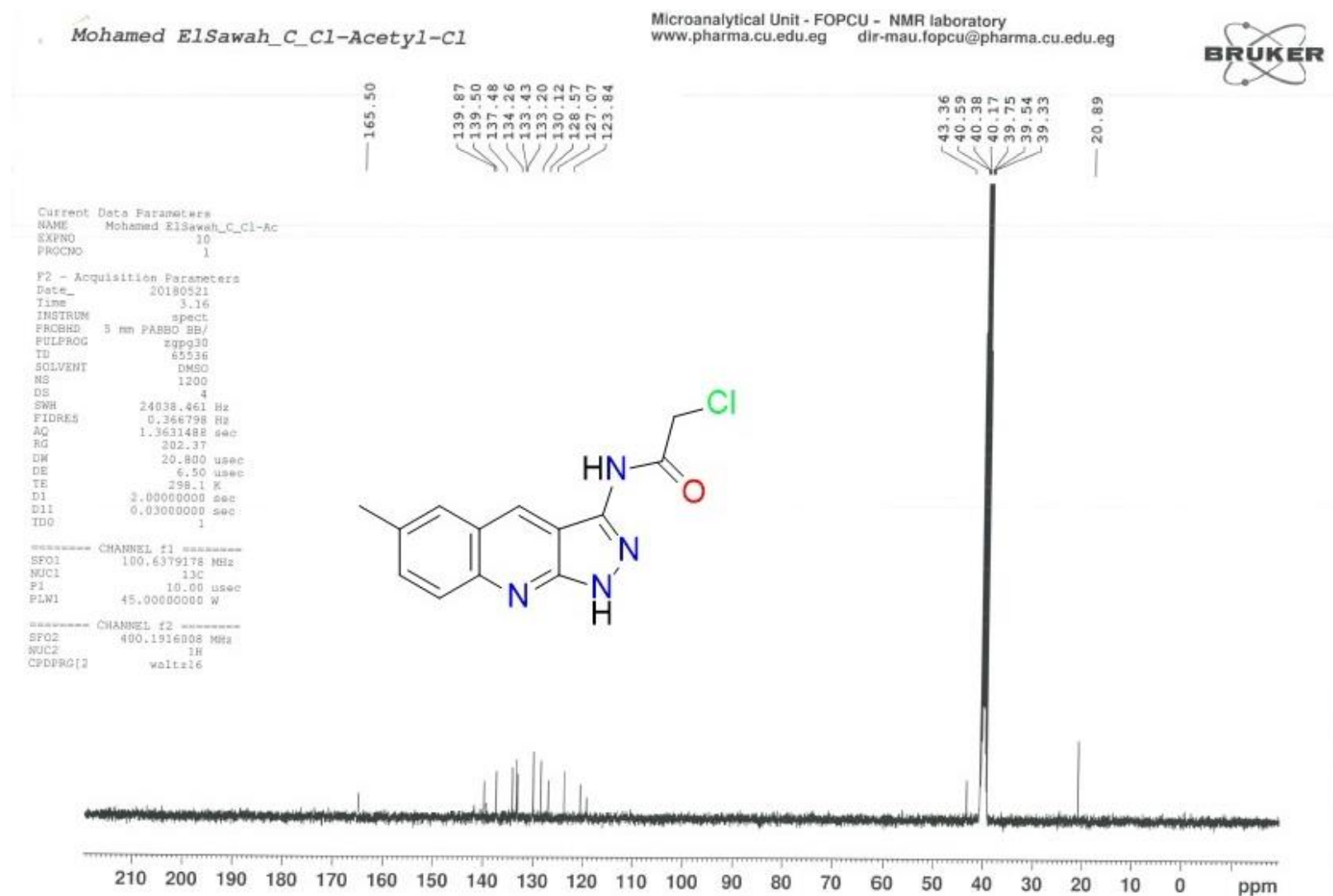
Pulse Sequence: s2pu1

Solvent: DMSO
Temp: 30.0 C / 303.1 K
Mercury-3003B "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
14 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 21 min, 7 sec
Date: May 7 2015



¹³C NMR spectrum of compound 22

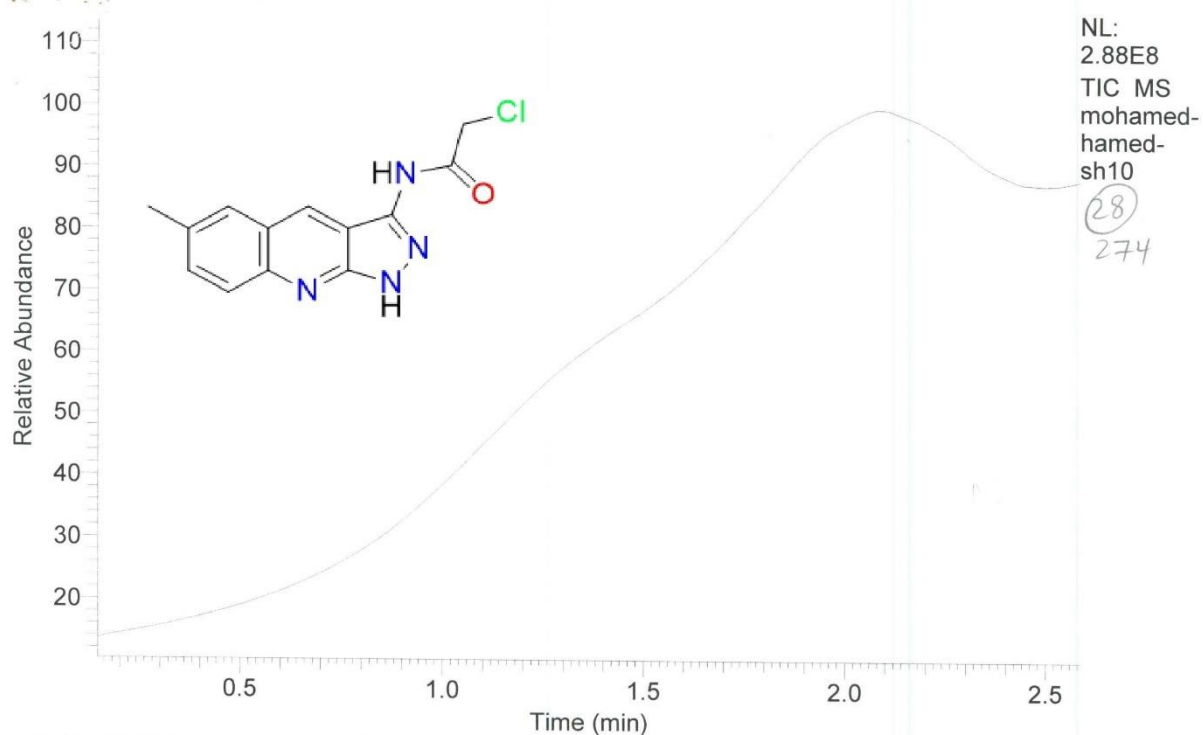


Mass spectrum of compound 22

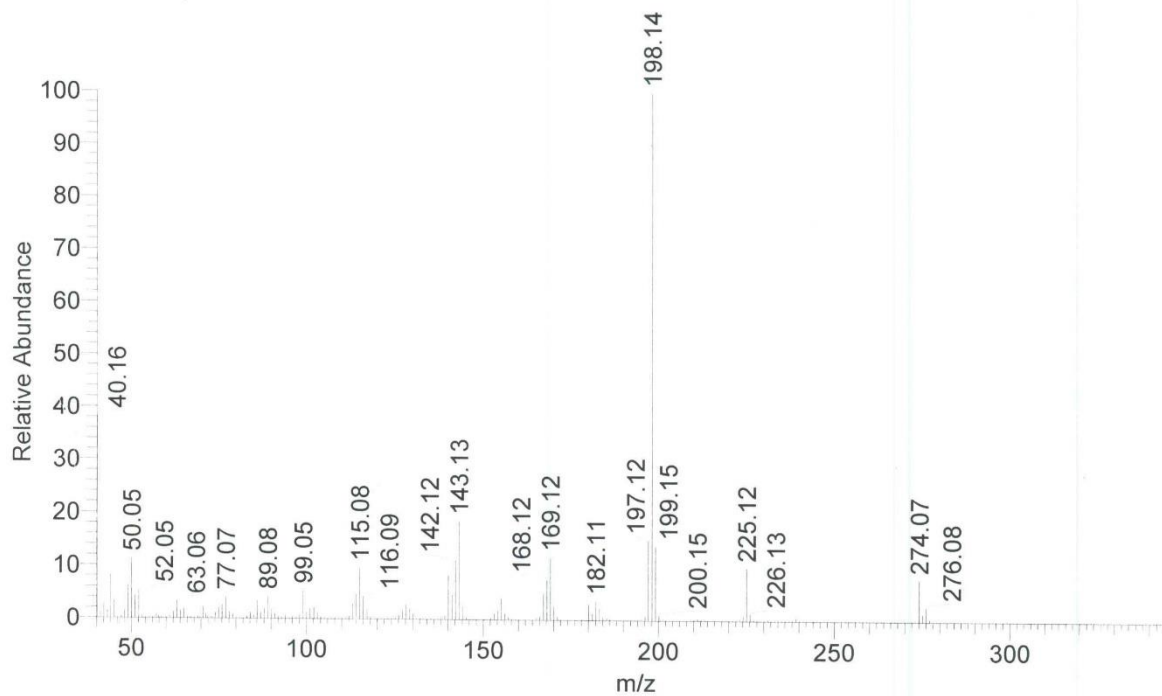
Al-Azhar University C:\Xcalibur\data\S\mohamed-hamed-sh10

The Regional Center for Mycology & Biotechnology 5/24/2015 10:07:39 AM

RT: 0.14 - 2.59 SM: 15B



mohamed-hamed-sh10 #120 RT: 2.03 AV: 1 NL: 6.77E7
F: {0,0} + c EI Full ms [40.00-1000.00]



Elemental analyses data of the new compounds

Al-Azhar University The Regional Center for Mycology and Biotechnology



Requester Data:

Name: Dr. Mohamed Hamed
Authority: Faculty of Pharmacy,
Al-Azhar University

Sample Data:

Ten samples had been submitted for elemental analysis.

Analysis Report:

Sample Code	C%	H%	N%
SH 1 12a	61.98	4.48	10.53
SH 2 12c	64.12	5.43	9.61
SH 3 14a	70.23	5.09	11.94
SH 4 14b	75.18	5.39	9.34
SH 5 15a	62.21	3.81	11.67
SH 6 15b	69.37	4.98	12.31
SH 7 15c	56.89	3.28	10.69
SH 8 15e	66.34	4.78	11.81
SH 9 15f	60.59	3.70	15.03
SH 10 15g	40.18	2.16	7.52

INVESTIGATOR

M. Elanss

DIRECTOR




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Website: <http://www.azhar.edu.eg.htm> * http://www.azhar.edu.eg/pages/fungi_center.htm

Facebook: RCMB AZHAR

P.O. box mail : 11751

Nasr City Cairo, Egypt.

Al-Azhar University
The Regional Center for Mycology and Biotechnology



Requester Data:

Name: Dr. Mohamed Hamed
Authority: Faculty of Pharmacy,
Al-Azhar University

Sample Data:

Ten samples had been submitted for elemental analysis.

Analysis Report:

Sample Code	C%	H%	N%
SH 11 16	69.94	5.38	11.89
SH 12 18	68.41	5.22	12.13
SH 13 20	64.20	4.13	10.88
SH 14 21	67.28	4.62	15.01
SH 15 13	57.51	4.48	20.74
SH 16 24	69.84	3.75	17.19
SH 17 25	64.89	3.67	20.41
SH 18 26	64.37	4.30	20.36
SH 19 27	65.13	5.18	23.60
SH 20 28	57.08	4.11	20.59

INVESTIGATOR

M. Hamed

DIRECTOR

[Signature]



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Facebook: RCMB AZHAR

P.O. box mail : 11751

Nasr City Cairo, Egypt.

Results of the In vitro antimicrobial evaluation study



THE REGIONAL CENTER FOR MYCOLOGY AND BIOTECHNOLOGY

ANTIMICROBIAL ACTIVITY UNIT



REFERRED FROM: Dr.: MOHAMED HAMED

Mean zone of inhibition in mm $\pm$ Standard deviation beyond well diameter (6 mm) produced on a range of environmental and clinically pathogenic microorganisms using (1mg/ml) concentration of tested samples. Results are depicted in the following table:

Sample	SH26	SH27	SH29	SH32	SH31	St.
Tested microorganisms						
FUNGI						Amphotericin B
<i>Aspergillus fumigatus</i> (RCMB 02568)	NA	24.2 $\pm$ 0.58	20.3 $\pm$ 1.2	21.3 $\pm$ 1.5	23.2 $\pm$ 0.58	23.7 $\pm$ 0.63
<i>Syncephalastrum racemosum</i> (RCMB 05922)	NA	22.3 $\pm$ 1.2	19.3 $\pm$ 0.63	20.4 $\pm$ 0.72	21.4 $\pm$ 1.5	19.7 $\pm$ 0.72
<i>Geotricum candidum</i> (RCMB 05097)	NA	27.3 $\pm$ 0.58	22.4 $\pm$ 2.1	23.2 $\pm$ 0.58	24.6 $\pm$ 0.44	28.7 $\pm$ 0.58
<i>Candida albicans</i> (RCMB 05036)	NA	NA	NA	NA	NA	25.4 $\pm$ 0.63
Gram Positive Bacteria:						Ampicillin
<i>Streptococcus pneumoniae</i> (RCMB 010010)	16.3 $\pm$ 1.2	26.8 $\pm$ 1.63	21.3 $\pm$ 0.63	20.6 $\pm$ 2.1	24.3 $\pm$ 2.1	23.8 $\pm$ 0.2
<i>Bacillus subtilis</i> (RCMB 010067)	18.2 $\pm$ 2.1	28.1 $\pm$ 0.58	23.6 $\pm$ 2.1	22.4 $\pm$ 1.5	26.2 $\pm$ 0.58	32.4 $\pm$ 0.58
Gram negative Bacteria:						Gentamicin
<i>Pseudomonas aeruginosa</i> (RCMB 010043)	NA	NA	NA	NA	NA	17.3 $\pm$ 0.63
<i>Escherichia coli</i> (RCMB 010059)	15.4 $\pm$ 0.72	22.3 $\pm$ 1.5	20.3 $\pm$ 1.6	18.3 $\pm$ 0.58	18.6 $\pm$ 0.72	21.3 $\pm$ 0.58

♦ The test was done using the diffusion agar technique, Well diameter: 6.0 mm (100 μ l was tested), RCMB: Regional Center for Mycology and Biotechnology Antimicrobial unit test organisms *NA: No activity, data are expressed in the form of mean $\pm$ SD.
Some of your antimicrobial results are promising, so determination of the Minimum Inhibitory Concentration (MIC) for the tested sample(s) is recommended.

Investigators

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DIRECTOR

Prof. Dr. H.H. Elsheikh

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THE REGIONAL CENTER FOR MYCOLOGY AND BIOTECHNOLOGY

ANTIMICROBIAL ACTIVITY UNIT



REFERRED FROM: Dr.: MOHAMED HAMED

Mean zone of inhibition in mm $\pm$ Standard deviation beyond well diameter (6 mm) produced on a range of environmental and clinically pathogenic microorganisms using (1mg/ml) concentration of tested samples. Results are depicted in the following table:

Sample	SH1 (26)	SH2 (24)	SH3 (25)	SH4 (14a)	SH5 (14b)	St.
Tested microorganisms						
FUNGI						Amphotericin B
<i>Aspergillus fumigatus</i> (RCMB 02568)	14.6 $\pm$ 1.5	16.3 $\pm$ 1.2	16.9 $\pm$ 0.63	20.3 $\pm$ 2.1	13.2 $\pm$ 0.58	23.7 $\pm$ 0.63
<i>Syncephalastrum racemosum</i> (RCMB 05922)	13.4 $\pm$ 0.44	14.2 $\pm$ 0.58	15.2 $\pm$ 1.2	19.2 $\pm$ 0.72	11.3 $\pm$ 1.2	19.7 $\pm$ 0.72
<i>Geotricum candidum</i> (RCMB 05097)	15.4 $\pm$ 1.2	15.9 $\pm$ 2.1	16.3 $\pm$ 0.42	22.3 $\pm$ 1.5	14.1 $\pm$ 0.63	28.7 $\pm$ 0.58
<i>Candida albicans</i> (RCMB 05036)	NA	NA	NA	NA	NA	25.4 $\pm$ 0.63
Gram Positive Bacteria:						Ampicillin
<i>Streptococcus pneumoniae</i> (RCMB 010010)	16.3 $\pm$ 1.5	16.8 $\pm$ 0.58	17.1 $\pm$ 1.5	21.3 $\pm$ 0.63	14.3 $\pm$ 2.1	23.8 $\pm$ 0.2
<i>Bacillus subtilis</i> (RCMB 010067)	18.1 $\pm$ 0.58	19.1 $\pm$ 0.63	19.6 $\pm$ 0.63	22.4 $\pm$ 0.58	16.1 $\pm$ 0.58	32.4 $\pm$ 0.58
Gram negative Bacteria:						Gentamicin
<i>Pseudomonas aeruginosa</i> (RCMB 010043)	NA	NA	NA	NA	NA	17.3 $\pm$ 0.63
<i>Escherichia coli</i> (RCMB 010059)	14.8 $\pm$ 2.1	15.6 $\pm$ 0.63	16.3 $\pm$ 0.72	20.6 $\pm$ 1.2	12.4 $\pm$ 1.5	21.3 $\pm$ 0.58

♦ The test was done using the diffusion agar technique, Well diameter: 6.0 mm (100 μ l was tested), RCMB: Regional Center for Mycology and Biotechnology Antimicrobial unit test organisms *NA: No activity, data are expressed in the form of mean $\pm$ SD.

Some of your antimicrobial results are promising, so determination of the Minimum Inhibitory Concentration (MIC) for the tested sample(s) is recommended.

Investigators

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THE REGIONAL CENTER FOR MYCOLOGY AND BIOTECHNOLOGY

ANTIMICROBIAL ACTIVITY UNIT



REFERRED FROM: Dr.: MOHAMED HAMED

Mean zone of inhibition in mm $\pm$ Standard deviation beyond well diameter (6 mm) produced on a range of environmental and clinically pathogenic microorganisms using (1mg/ml) concentration of tested samples. Results are depicted in the following table:

Sample	SH6	SH7	SH8	SH9	SH10	St.
Tested microorganisms	12C	16	12b	15e	28	
FUNGI						Amphotericin B
<i>Aspergillus fumigatus</i> (RCMB 02568)	17.3 $\pm$ 2.1	NA	NA	NA	22.3 $\pm$ 1.2	23.7 $\pm$ 0.63
<i>Syncephalastrum racemosum</i> (RCMB 05922)	16.4 $\pm$ 0.58	NA	NA	NA	20.7 $\pm$ 0.58	19.7 $\pm$ 0.72
<i>Geotrichum candidum</i> (RCMB 05097)	19.1 $\pm$ 1.5	NA	NA	NA	25.2 $\pm$ 0.63	28.7 $\pm$ 0.58
<i>Candida albicans</i> (RCMB 05036)	NA	NA	NA	NA	NA	25.4 $\pm$ 0.63
Gram Positive Bacteria:						Ampicillin
<i>Streptococcus pneumoniae</i> (RCMB 010010)	18.3 $\pm$ 0.63	13.6 $\pm$ 1.2	15.7 $\pm$ 2.1	17.1 $\pm$ 0.44	22.8 $\pm$ 2.1	23.8 $\pm$ 0.2
<i>Bacillus subtilis</i> (RCMB 010067)	20.4 $\pm$ 0.63	15.2 $\pm$ 1.5	16.1 $\pm$ 0.58	17.9 $\pm$ 0.63	26.8 $\pm$ 0.58	32.4 $\pm$ 0.58
Gram negative Bacteria:						Gentamicin
<i>Pseudomonas aeruginosa</i> (RCMB 010043)	NA	NA	NA	NA	NA	17.3 $\pm$ 0.63
<i>Escherichia coli</i> (RCMB 010059)	17.5 $\pm$ 2.1	12.4 $\pm$ 0.58	15.2 $\pm$ 0.63	16.7 $\pm$ 2.1	23.4 $\pm$ 0.63	21.3 $\pm$ 0.58

The test was done using the diffusion agar technique, Well diameter: 6.0 mm (100 μ l was tested), RCMB: Regional Center for Mycology and Biotechnology Antimicrobial unit test organisms *NA: No activity, data are expressed in the form of mean $\pm$ SD.
Some of your antimicrobial results are promising, so determination of the Minimum Inhibitory Concentration (MIC) for the tested sample(s) is recommended.

Investigators

Dr. MARWA MOSTAFA

DIRECTOR

Prof. Dr. H.H. Elsheikh

CC: H. Shukr



THE REGIONAL CENTER FOR MYCOLOGY AND BIOTECHNOLOGY

ANTIMICROBIAL ACTIVITY UNIT



REFERRED FROM: Dr.: MOHAMED HAMED

Mean zone of inhibition in mm $\pm$ Standard deviation beyond well diameter (6 mm) produced on a range of environmental and clinically pathogenic microorganisms using (1mg/ml) concentration of tested samples. Results are depicted in the following table:

Sample	SH16 (15f)	SH17 (12a)	SH18 (13)	SH19 (20)	SH20	St.
Tested microorganisms						
FUNGI						Amphotericin B
<i>Aspergillus fumigatus</i> (RCMB 02568)	18.3 $\pm$ 1.2	19.3 $\pm$ 0.63	19.5 $\pm$ 1.2	19.8 $\pm$ 1.2	21.3 $\pm$ 1.2	23.7 $\pm$ 0.63
<i>Syncephalastrum racemosum</i> (RCMB 05922)	19.3 $\pm$ 0.58	19.9 $\pm$ 2.1	20.1 $\pm$ 0.63	20.5 $\pm$ 0.25	20.4 $\pm$ 0.58	19.7 $\pm$ 0.72
<i>Geotrichum candidum</i> (RCMB 05097)	20.4 $\pm$ 2.1	20.6 $\pm$ 0.58	21.3 $\pm$ 2.1	21.4 $\pm$ 2.1	21.9 $\pm$ 0.58	28.7 $\pm$ 0.58
<i>Candida albicans</i> (RCMB 05036)	NA	NA	NA	NA	NA	25.4 $\pm$ 0.63
Gram Positive Bacteria:						Ampicillin
<i>Streptococcus pneumoniae</i> (RCMB 010010)	19.3 $\pm$ 0.58	20.3 $\pm$ 0.58	20.7 $\pm$ 0.72	21.3 $\pm$ 0.44	22.4 $\pm$ 0.63	23.8 $\pm$ 0.2
<i>Bacillus subtilis</i> (RCMB 010067)	21.2 $\pm$ 0.72	21.4 $\pm$ 1.2	21.8 $\pm$ 0.63	22.1 $\pm$ 0.63	23.8 $\pm$ 0.63	32.4 $\pm$ 0.58
Gram negative Bacteria:						Gentamicin
<i>Pseudomonas aeruginosa</i> (RCMB 010043)	NA	NA	NA	NA	NA	17.3 $\pm$ 0.63
<i>Escherichia coli</i> (RCMB 010059)	18.3 $\pm$ 0.63	20.3 $\pm$ 0.58	20.9 $\pm$ 0.58	21.2 $\pm$ 0.58	18.9 $\pm$ 0.72	21.3 $\pm$ 0.58

♦ The test was done using the diffusion agar technique, Well diameter: 6.0 mm (100 μ l was tested), RCMB: Regional Center for Mycology and Biotechnology Antimicrobial unit test organisms *NA: No activity, data are expressed in the form of mean $\pm$ SD.

Some of your antimicrobial results are promising, so determination of the Minimum Inhibitory Concentration (MIC) for the tested sample(s) is recommended.

Investigators

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THE REGIONAL CENTER FOR MYCOLOGY AND BIOTECHNOLOGY

ANTIMICROBIAL ACTIVITY UNIT



REFERRED FROM: Dr.: MOHAMED HAMED

Mean zone of inhibition in mm $\pm$ Standard deviation beyond well diameter (6 mm) produced on a range of environmental and clinically pathogenic microorganisms using (1mg/ml) concentration of tested samples. Results are depicted in the following table:

Sample	SH11 (15a)	SH12 (15b)	SH13 (15c)	SH14 (15d)	SH15 (15g)	St.
Tested microorganisms						
FUNGI						Amphotericin B
<i>Aspergillus fumigatus</i> (RCMB 02568)	19.3 $\pm$ 2.1	17.3 $\pm$ 1.2	NA	20.1 $\pm$ 1.2	NA	23.7 $\pm$ 0.63
<i>Syncephalastrum racemosum</i> (RCMB 05922)	17.2 $\pm$ 0.25	16.2 $\pm$ 0.44	NA	18.3 $\pm$ 0.58	NA	19.7 $\pm$ 0.72
<i>Geotricum candidum</i> (RCMB 05097)	19.9 $\pm$ 1.5	18.3 $\pm$ 2.1	NA	20.1 $\pm$ 2.1	NA	28.7 $\pm$ 0.58
<i>Candida albicans</i> (RCMB 05036)	NA	NA	NA	NA	NA	25.4 $\pm$ 0.63
Gram Positive Bacteria:						Ampicillin
<i>Streptococcus pneumoniae</i> (RCMB 010010)	17.4 $\pm$ 0.58	18.1 $\pm$ 0.72	NA	19.3 $\pm$ 0.58	NA	23.8 $\pm$ 0.2
<i>Bacillus subtilis</i> (RCMB 010067)	19.1 $\pm$ 0.63	20.2 $\pm$ 0.58	NA	20.8 $\pm$ 0.67	NA	32.4 $\pm$ 0.58
Gram negative Bacteria:						Gentamicin
<i>Pseudomonas aeruginosa</i> (RCMB 010043)	NA	NA	NA	NA	NA	17.3 $\pm$ 0.63
<i>Escherichia coli</i> (RCMB 010059)	15.2 $\pm$ 0.58	16.6 $\pm$ 0.72	NA	19.2 $\pm$ 0.63	NA	21.3 $\pm$ 0.58

♦ The test was done using the diffusion agar technique, Well diameter: 6.0 mm (100 μ l was tested), RCMB: Regional Center for Mycology and Biotechnology Antimicrobial unit test organisms *NA: No activity, data are expressed in the form of mean $\pm$ SD.
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