Biological Evaluation, Molecular Docking Analyses and ADME Profiling of Certain New Quinazolinones as Anti-colorectal Agents

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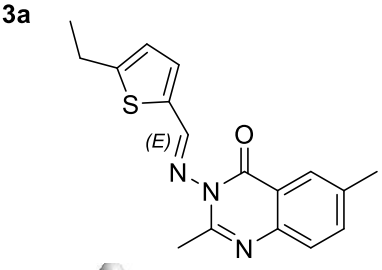
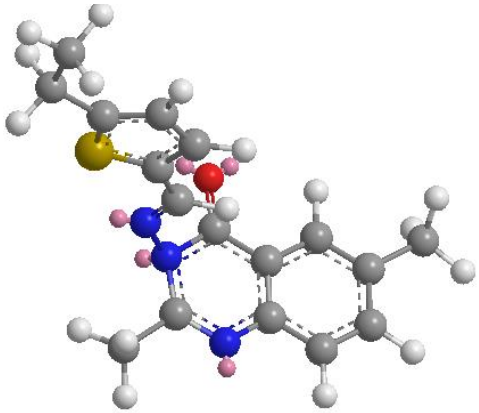
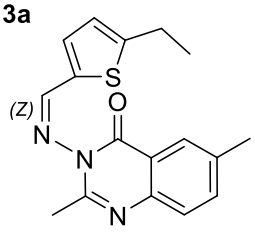
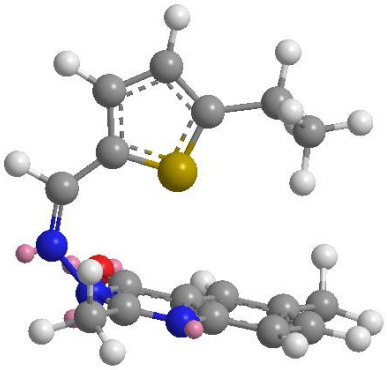
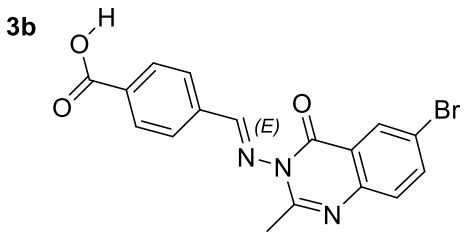
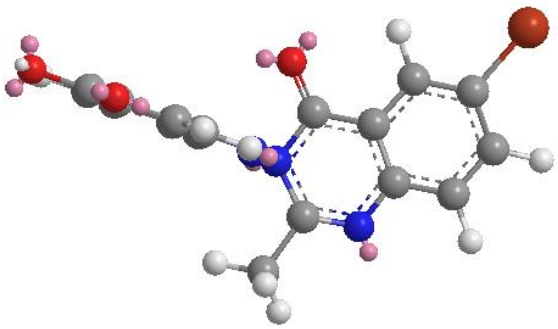
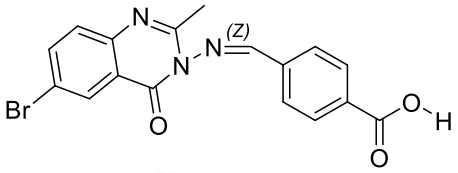
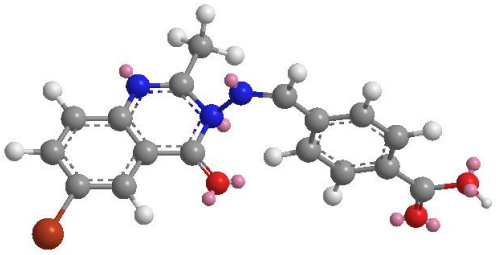
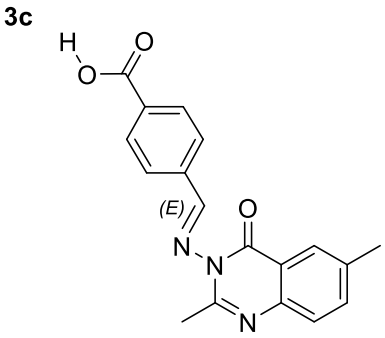
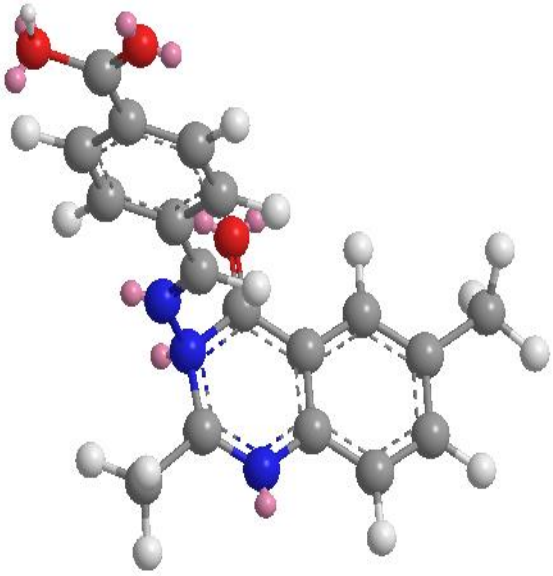
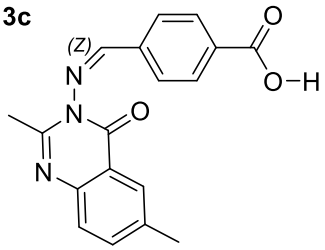
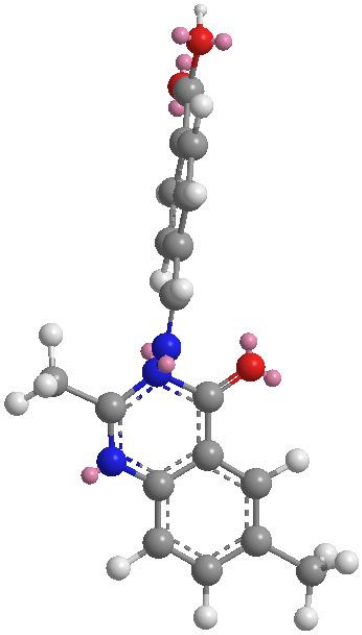
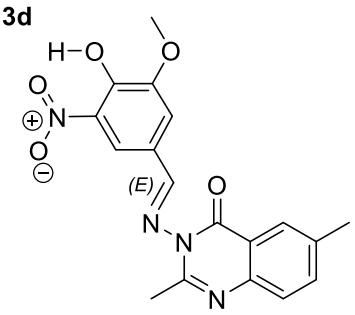
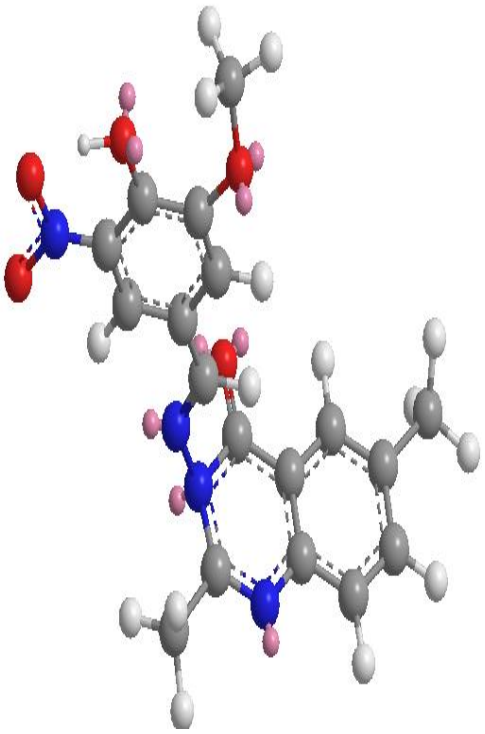
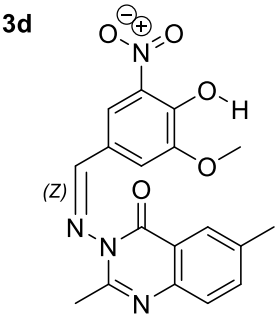
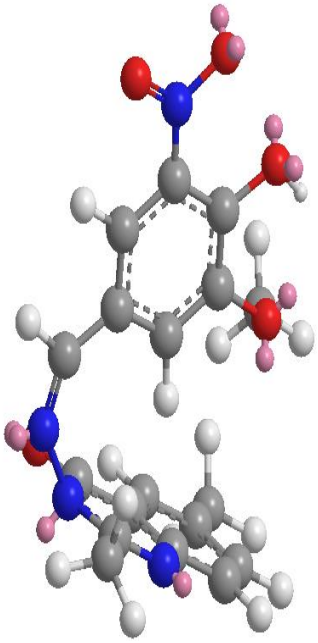
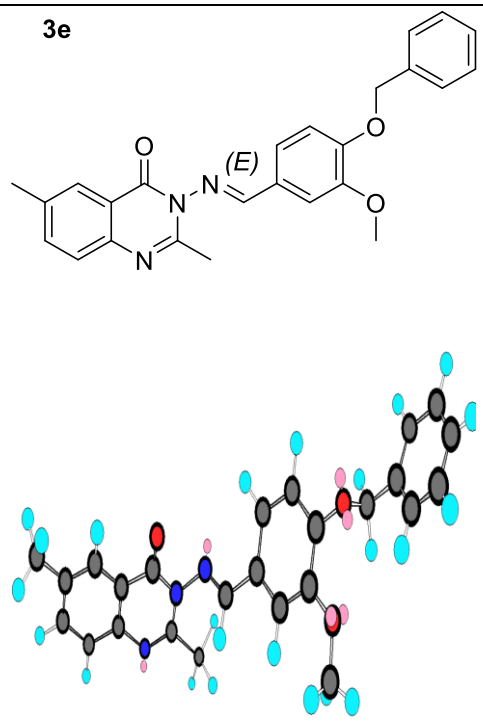
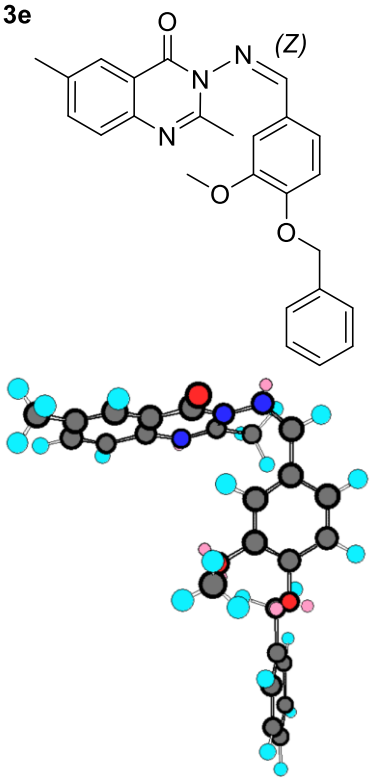
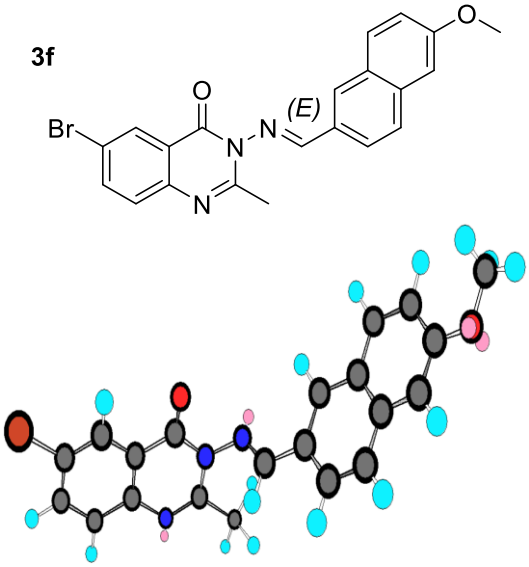
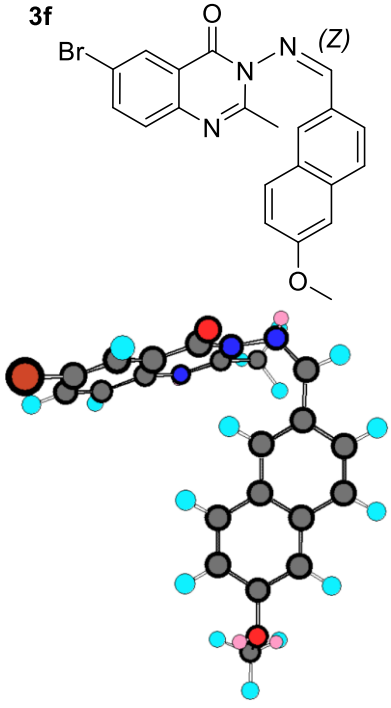
Supplementary information

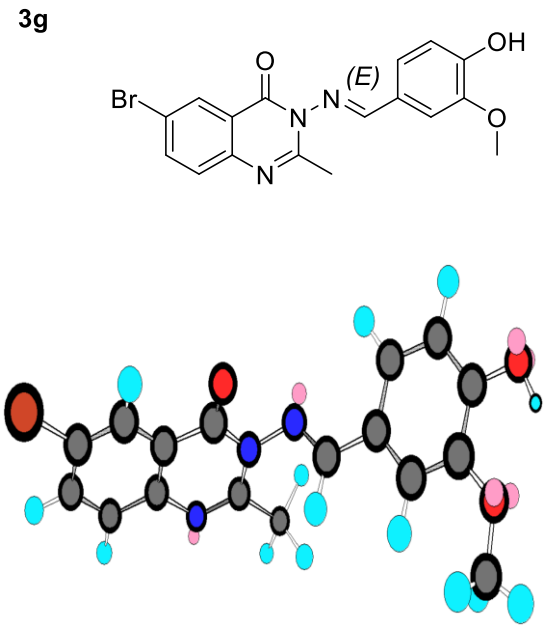
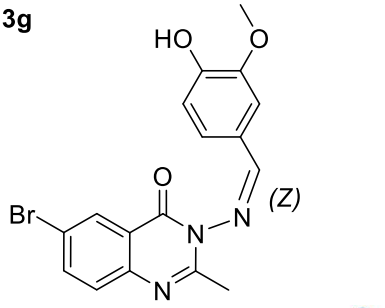
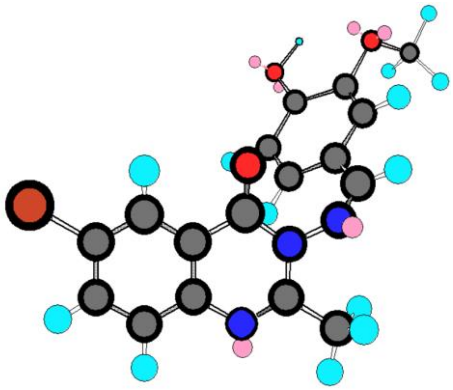
Table S1. The values of the minimized total energies of *E* and *Z* isomers of Schiff bases **3a-g** and compound **5**

2D/ 3D-minimized *E*-isomer	**2D/3D-minimized *Z*-isomer**
3a   Total energy = 28.8470 kcal/mol	**3a**   Total energy = 29.3365 kcal/mol
3b   Total energy = 17.8970 kcal/mol	**3b**   Total energy = 21.5747 kcal/mol

3c   Total energy: 19.1689 kcal/mol	**3c**   Total energy: 20.1828 kcal/mol

3d   Total Energy: 23.3731 kcal/mol	**3d**   Total Energy: 24.3114 kcal/mol

3e  Total energy = 5.9596	3e  Total energy = 8.9264
3f  Total energy = −3.2846	3f  Total energy = −1.0803

3g  Total energy = −2.2141	**3g**   Total energy = 0.3024

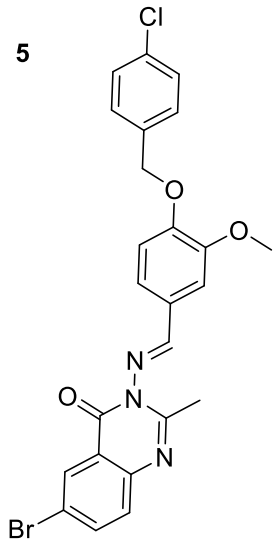
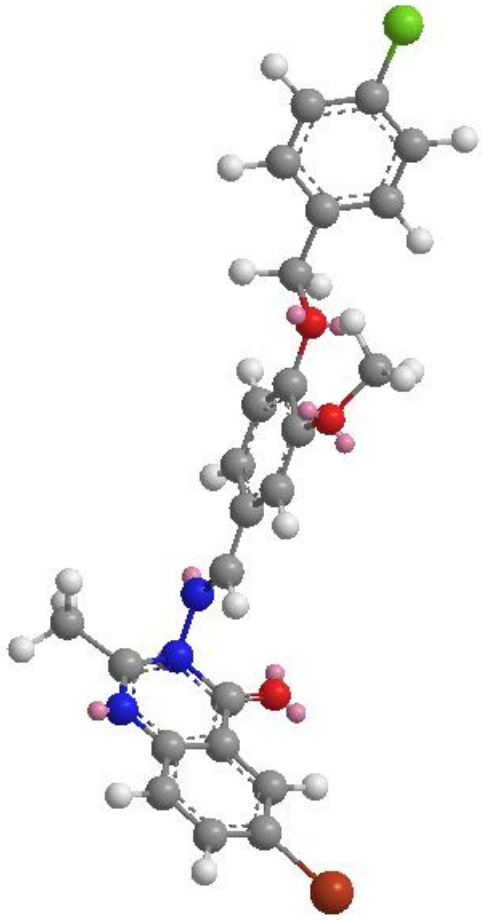
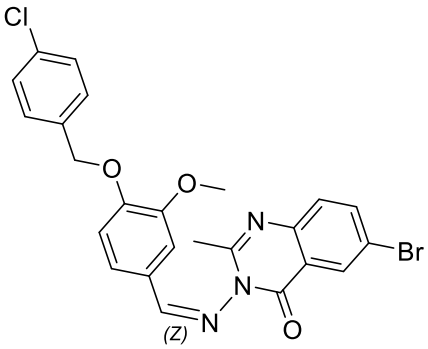
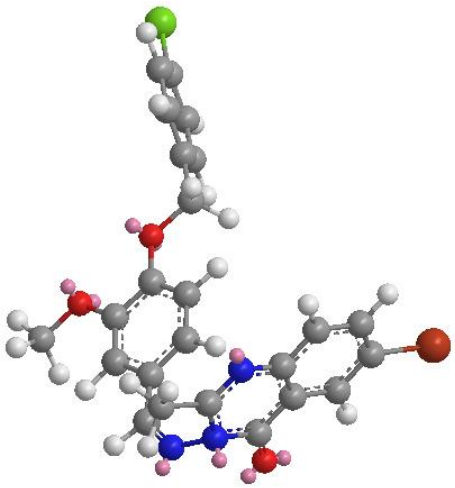
5   Total energy = 29.1194 kcal/mol	**5**   Total energy = 35.5597 kcal/mol

Table S2. The mean IC_{50} values (µg/mL) of the synthesized derivatives against selected proteases. Results are the mean values of two separate determinations ± SD.

Compound #	Cathepsin-B	Collagenase	Thrombin	Elastase	Trypsin
1a	24.00±2.83	27.00±1.41	2.30±0.42	2.30±0.28	2.00±0.00
1c	28.50±2.12	2.50±0.71	14.00±1.41	15.50±2.12	17.50±2.12
3a	36.61±1.83	47.69±1.59	83.65±4.78	34.04±1.83	69.85±3.40
3b	12.94±1.09	24.86±1.47	18.77±0.91	56.06±2.38	82.08±1.09
3c	24.12±1.09	18.52±1.56	37.34±4.39	100.36±5.51	109.85±1.77
3d	39.36±2.69	57.83±2.69	77.24±1.74	34.34±1.36	20.50±1.74
3e	27.93±1.89	53.45±3.07	11.00±1.55	37.97±1.72	44.50±2.056
3f	55.77±1.85	43.57±3.01	21.91±0.83	25.22±1.18	17.17±0.83
3g	13.00±2.83	18.00±1.41	16.50±2.12	14.50±0.71	18.00±1.41
5	23.50±2.12	32.50±2.12	23.00±1.41	26.50±2.12	24.50±2.12
7b	9.00±1.41	12.50±2.12	24.00±4.24	25.50±2.12	28.00±1.41
8	23.00±1.41	24.50±0.71	0.225±0.04	0.20±0.00	0.55±0.07
9	19.50±0.71	4.00±1.41	23.50±2.12	26.00±1.41	21.5±2.12
10	29.50±2.12	28.50±2.12	2.35±0.35	1.80±0.28	1.75±0.35
12	30.50±2.12	34.00±2.83	27.50±3.54	25.00±1.41	23.50±2.12
Cocktail	0.175±0.04	0.15±0.07	0.25±0.07	0.125±0.04	0.215±.04

Table S3. The mean IC_{50} values (μM) of the synthesized derivatives against selected phospholipases. Results are the mean values of two separate determinations ± SD.

Compound #	Mean IC_{50} values (μM)		
	hsPLA$_2$-G-IIA	hsPLA$_2$-G-V	hsPLA$_2$-G-X
1a	22.05±2.23	16.14±0.85	21.84±0.64
1c	31.97± 0.85	26.26±0.57	24.55±0.42
3a	58.61±3.40	71.29±2.73	109.5±5.01
3b	68.10±4.74	33.01±1.37	43.37±1.66
3c	100.83±6.16	93.67±3.52	131.48±5.51
3d	30.13±1.14	65.43±1.71	21.45±2.31
3e	93.72±4.28	70.27±1.89	48.01±2.23
3f	16.81±1.00	34.10±1.00	24.63±2.01
3g	30.27±0.35	22.28±0.92	14.55±0.92
5	49.73±2.12	49.73±0.71	41.15±1.56
7b	127.42±2.12	112.36±1.49	105.90±1.41
8	57.01±0.57	68.02±1.41	78.71±0.99
9	104.21±8.34	151.39±2.12	88.47±2.12
10	13.84±2.12	14.70±0.42	23.43±1.41
12	69.31±2.83	113.20±1.41	77.39±2.12
Oleanolic acid	11.50±0.35	16.42±0.71	16.53±0.64

Table S4. The mean IC_{50} values expressed in (μM) of the synthesized derivatives against α-amylase, α-glucosidase and xanthine oxidase. Results are the mean values of two separate determinations ± SD.

	Mean IC_{50} values μM		
Compound #	**Anti-α-amylase**	**α-Glucosidase**	**Xanthine oxidoreductase**
1a	399.48±4.95	23.61±1.41	159.40±3.54
1c	1093±4.95	59.93±2.12	339.63±4.95
3a	831.73±22.70	37.25±1.83	68.41±1.35
3b	264.11±10.98	16.44±0.54	42.21±2.56
3c	625.51±17.6	93.36±4.39	102.54±4.17
3d	374.64±11.51	54.97±2.88	190.04±7.68
3e	550.21±25.66	57.44±2.56	144.51±5.97
3f	310.22±10.04	12.43±0.83	7.34±0.33
3g	468.8±4.24	25.76±1.41	56.67±4.24
5	357.85±4.95	13.65±1.41	32.18±2.12
7b	440.16±7.07	19.86±1.41	233.32±2.12
8	458.31±9.19	53.44±2.12	137.66±4.95
9	580.00±3.54	62.91±1.41	151.39±4.95
10	430.22±8.49	43.66±2.12	12.78±1.41
12	400.82±6.36	21.03±1.27	28.88±2.12
Quercetin	406.97±2.83	12.57±0.28	-----
Allopurinol	----	----	4.78±0.07

Table S5. The cytotoxic effects of the studied quinazolinone derivatives. Results are expressed as mean values of % of viable cells at 200 µg/mL and IC_{50} values (concentrations required to reduce the viability of cancerous cells by 50% expressed in µM). Results are the mean values of two separate determinations ± SD. ND: Not determined

Compound No.	**LoVo cell line of CRC**			**HCT-116 cell line of CRC**	
	% of Viable cells	**IC_{50} µM**		**% Viable of cells**	**IC_{50} µM**
Positive control Triton X-100 (0.1%)	0.00			0.00	-
Negative control (Assay medium)	99.50± 0.71			100.00±0.00	-
1a	62.9±1.56	1052.80±64.01		48.25±1.06	757.64±19.48
1c	28.0±4.24	339.63±12.10		46.50±2.12	530.85±16.15
3a	89.5±3.54	ND		86.5±2.12	ND
3b	61.9±2.69	651.20±12.82		53.5±2.12	572.22±14.66
3c	32.5±2.12	320.53±13.20		36.0±4.24	459.79±12.11
3d	90.5±3.54	ND		90.0±5.66	ND
3e	76.5±3.54	ND		74.5±2.12	ND
3f	58.0±4.24	681.63±8.38		57.0±2.83	552.95±11.72
3g	16.75±0.35	206.07±7.29		12.75±1.06	284.63±9.11
5	80.0±2.83	ND		93.50±2.12	ND
7b	89.5±3.54	ND		89.00±2.82	ND
8	13.50±0.71	319.04±11.45		28.00±1.41	448.60±11.46
9	63.0±2.83	831.66±19.46		73.50±2.12	1450.99±22.24
10	22.00±1.41	272.62±9.04		4.75± 0.35	230.02±9.04
12	59.5±3.54	607.59±13.07		54.5±2.12	573.13±8.17

Table S6. The studied target proteins, their PDB code and cocrystallized ligands.

Target Protein	**PDB Code**	**Cocrystallized ligand**
Thrombin	1ETR	Amino{[(4*S*)-5-[(2*R*,4*R*)-2-carboxy-4-methylpiperidin-1-yl]-4-({[(3*R*)-3-methyl-1,2,3,4-tetrahydroquinolin-8-yl]sulfonyl}amino)-5-oxopentyl]amino} methaniminium (**MIT**)
Elastase	1EAT	2-[5-Methanesulfonylamino-2-(4-aminophenyl)-6-oxo-1,6-dihydro-1-pyrimidinyl]-*n*-(3,3,3-trifluoro-1-isopropyl-2-oxopropyl)acetamide (**TFI**)
Trypsin	3AAV	3,3'-[ethane-1,2-diylbis(nitrilomethylylidene)] bis(4-hydroxybenzenecarboximidamide) (**A2C**)
$sPLA_2$-G-IIA	1KQU	6-Phenyl-4(*R*)-(7-phenyl-heptanoylamino)-hexanoic acid (**BR4**)
$sPLA_2$-G-X	5G3M	4-Benzylbenzamide (**9JH**)
α-Glucosidase	2JKP	Castanospermine (**CTS**)
Xanthine oxidoreductase	3ETR	2,4-Pteridinediol, Lumazine, (**LUZ)**
α-Amylase	1B2Y	Acarbose (**AC1**)

Table S7. Binding score (S) of the cocrystallized ligands & root square deviation (RMSD) values

Target Protein	S-score (Kcal/mol)	RMSD values (Å)
Thrombin	−15.0807	1.0730
Elastase	−11.4465	0.9243
Trypsin	−14.3302	0.2877
hsPLA$_2$-G-IIA	−13.9194	0.5614
hsPLA$_2$-G-X	−8.9121	0.1342
α-Amylase	−19.7135	1.1470
α-Glucosidase	−15.3919	0.2274
Xanthine oxidoreductase	−12.5689	0.1073

Table S8. Docking results

Comp. No.	Target	S (kcal/mol)	Amino acids	Interacting groups	Type of interaction
8	Thrombin	−10.4683	Ser195	O (C=O)	Conventional H-bond
			Trp215	Benzene	Amide-Pi Stacked
			Cys191	Pyrimidine	Amide-Pi Stacked
			Ala190	Cl	Pi-Alkyl interaction
			Val213	Cl	Pi-Alkyl interaction
			Tyr228	Cl	Pi-Alkyl interaction
8	Elastase	−9.8673	Gln192	O (C=O)	Conventional H-bond
			Gly193	O (C=O)	Conventional H-bond
			Asp194	O (C=O)	Conventional H-bond
			Ser195	O (C=O)	Conventional H-bond
			Val216	S	Conventional H-bond
			Val99	Benzene/Pyrimidine/CH_3	Pi-Alkyl interaction
			His57	CH_3	Alkyl interaction
			Trp172	Cl	Pi-alkyl interaction
			Arg217	Cl/Benzene	Pi-Alkyl interaction
8	Trypsin	−10.1979	Trp193	Benzene/Pyrimidine	Amide-Pi Stacked
			Ser195	Cl	Halogen bond
			Lys202	Cl	Halogen bond
			His40	CH_3	Pi-Alkyl interaction
			Val191	CH_3	Alkyl interaction
Oleanolic acid	hsPLA$_2$-G-IIA	−12.4222	Thr61	O (OH)	Conventional H-bond
			Lys62	O (C=O)	Conventional H-bond
			Thr51	CH_3	Alkyl interaction
			Lys52	CH_3	Alkyl interaction
			His47	CH_3	Pi-Alkyl interaction
			Leu2	CH_3	Alkyl interaction
			Phe5	CH_3	Alkyl interaction
10	hsPLA$_2$-G-IIA	−12.3560	Gly29	NH	Conventional H-bond
			Gly31	O (C=O)	Conventional H-bond
			Lys62	O (C=O)	Conventional H-bond
			Asp48	Pyrimidine	Pi-Anion interaction
			Glu55	Benzene	Pi-Anion interaction
			His47	S	Pi-Cation interaction
			Phe5	S	Pi-Sulfur interaction
			Tyr51	CH_3	Pi-Pi T-Shaped
			Lys52	Benzene	Pi-Alkyl
			Cys44	Benzene	Pi-Alkyl
			Ala17	Benzene	Pi-Alkyl
			Ala18	Benzene	Pi-Alkyl
			Leu2	Pyrimidine	Pi-Alkyl
Oleanolic acid	hsPLA$_2$-G-X	−13.1880	Gly28	O (C=O)	Conventional H-bond
			His46	OH	Conventional H-bond
			Leu5	CH_3	Alkyl interaction
			Ala6	CH_3	Alkyl interaction
			Pro17	CH_3	Pi-Alkyl interaction
			Ile18	CH_3	Alkyl interaction
			Met21	CH_3	Alkyl interaction
			Leu29	CH_3	Alkyl interaction
			Tyr50	CH_3	Pi-Alkyl interaction

3g	hsPLA$_2$-G-X	−11.7267	Leu29	N (Pyrimidine)	Carbon-hydrogen bond
			His46	O (C=O)	Carbon-hydrogen bond
			Lys61	Phenyl/Pyrimidine	Pi-cation interaction
			Asp47	Phenyl/Pyrimidine	Pi-anion interaction
			Leu5	Phenyl	Pi-alkyl interaction
			Leu29	CH_3	Alkyl interaction
Quercetin	α-Glucosidase	−16.1296	Glu194	OH	Conventional H-bond
			Lys467	O (C=O)	Conventional H-bond
			His507	OH	Conventional H-bond
			Glu532	OH	Conventional H-bond
			Glu439	Pyran	Pi-Anion
3f	α-Glucosidase	−14.5846	Glu439	Benzene	Pi-Anion interaction
			Phe401	Pyrimidine	Pi-Pi Stacked
			Trp341	Benzene	Pi-Pi Stacked
			Phe536	CH_3	Pi-Alkyl interaction
			Val471	Benzene	Pi-Alkyl interaction
Allopurinol	Xanthine oxidoreductase	−9.1790	Glu802	NH	Conventional H-bond
			Arg880	O (C=O)	Conventional H-bond
			Thr1010	O (C=O)	Conventional H-bond
			Phe914	Benzene	Pi-Pi Stacked
			Phe1009	Benzene	Pi-Pi Stacked
			Ala1078	Benzene	Pi-Alkyl interaction
			Ala1079	Benzene	Pi-Alkyl interaction
3f	Xanthine oxidoreductase	−14.9338	Arg912	N (Pyrimidine)	Conventional H-bond
			Ser1080	O (C=O)	Conventional H-bond
			Phe914	Benzene	Pi-Pi Stacked
			Phe1009	Benzene	Pi-Pi Stacked
			Ala910	Benzene	Pi-Alkyl interaction
			Ala1079	Benzene	Pi-Alkyl interaction
Quercetin	α-Amylase	−10.2531	Trp59	Benzene	Pi-Pi Stacked
			Trp59	Pyridine	Pi-Pi Stacked
			His305	O (C=O)	Carbon-H bond
3b	α-Amylase	−11.4264	Arg195	O (C=O)	Conventional H-bond
			Arg195	O (OH)	Conventional H-bond
			Trp62	Benzene	Pi-Pi Stacked
			Gln63	Benzene	Pi-donor H-bond
			His305	CH_3	Pi-Alkyl interaction
			Trp59	CH_3	Pi-Alkyl interaction

Table S9. Drug-likeness of the most biologically active compounds

Compound No.	Properties	Comment
1a	• Log P = 1.58 (<5) • Molecular weight = 254.08 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 2 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 4 (≤ 10)	No violation
1c	• Log P = 0.92 (<5) • Molecular weight = 175.19 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 2 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 4 (≤ 10)	No violation
3b	• Log P = 3.05 (<5) • Molecular weight = 386.20 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 1 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 6 (≤ 10)	No violation
3c	• Log P = 2.83 (<5) • Molecular weight = 321.33 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 1 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 6 (≤ 10)	No violation
3d	• Log P = 2.11 (<5) • Molecular weight = 368.34 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 1 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 9 (≤ 10)	No violation
3f	• Log P = 4.32 (<5) • Molecular weight = 388.22 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 1 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 5 (≤ 10)	No violation
3g	• Log P = 2.94 (<5) • Molecular weight = 388.22 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 1 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 5 (≤ 10)	No violation
5	• Log P = 5.09 (>5) • Molecular weight = 512.78 g/mol (> 500) • No of H-bond donor groups (OHs + NHs) = 0 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 6 (≤ 10)	Two violations in log P and molecular weight
8	• Log P = 1.92 (<5) • Molecular weight = 308.74 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 1 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 6 (≤ 10)	No violation
10	• Log P = 3.39 (<5) • Molecular weight = 469.52 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 1 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 8 (≤ 10)	No violation
12	• Log P = 2.35 (<5) • Molecular weight = 432.86 g/mol (<500) • No of H-bond donor groups (OHs + NHs) = 2 (≤ 5) • No of H-bond acceptor atoms (Os + Ns) = 9 (≤ 10)	No violation

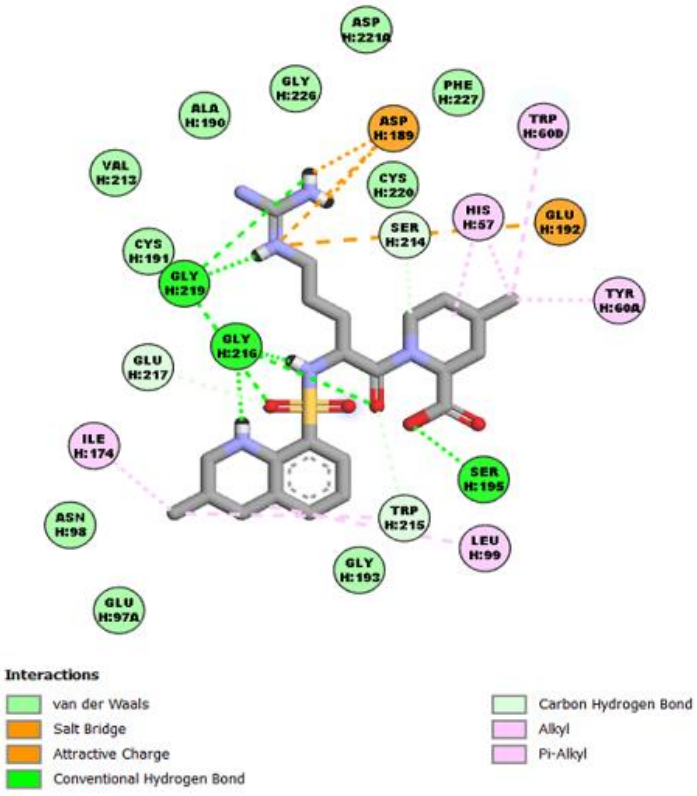


Figure S1. The 2D representation of the interactions of **MIT** within **THR** active site

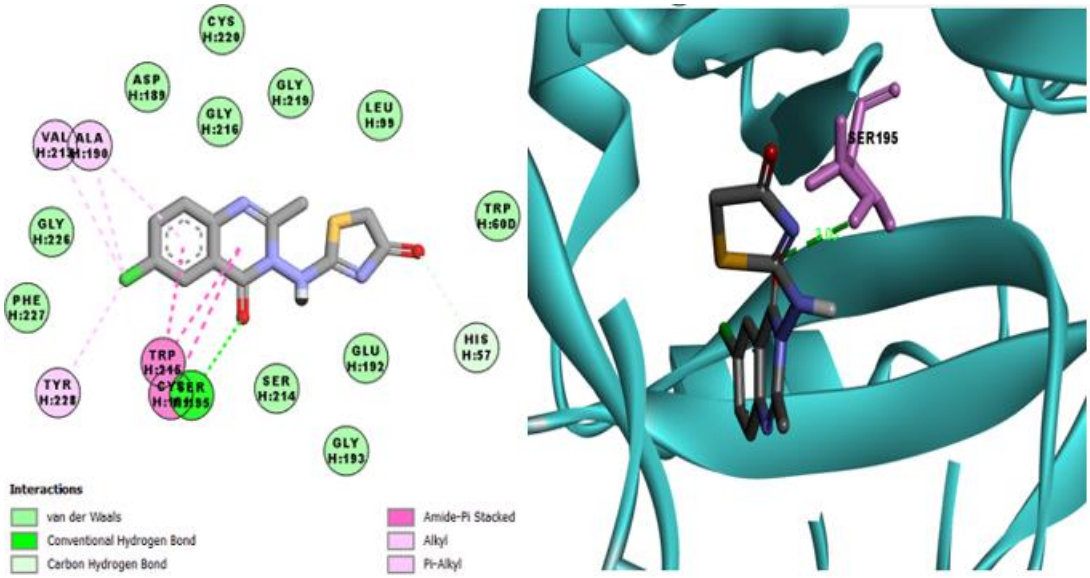


Figure S2. The 2D & 3D representations of the interactions of compound **8** within **Thrombin** active site

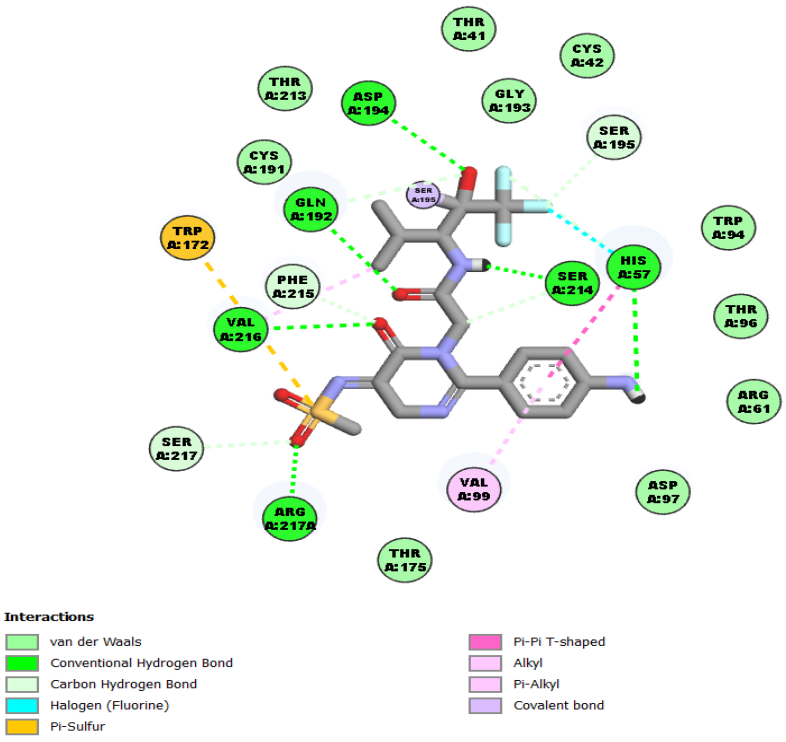


Figure S3. The 2D representation of the interactions of **TFI** within **Elastase** active site

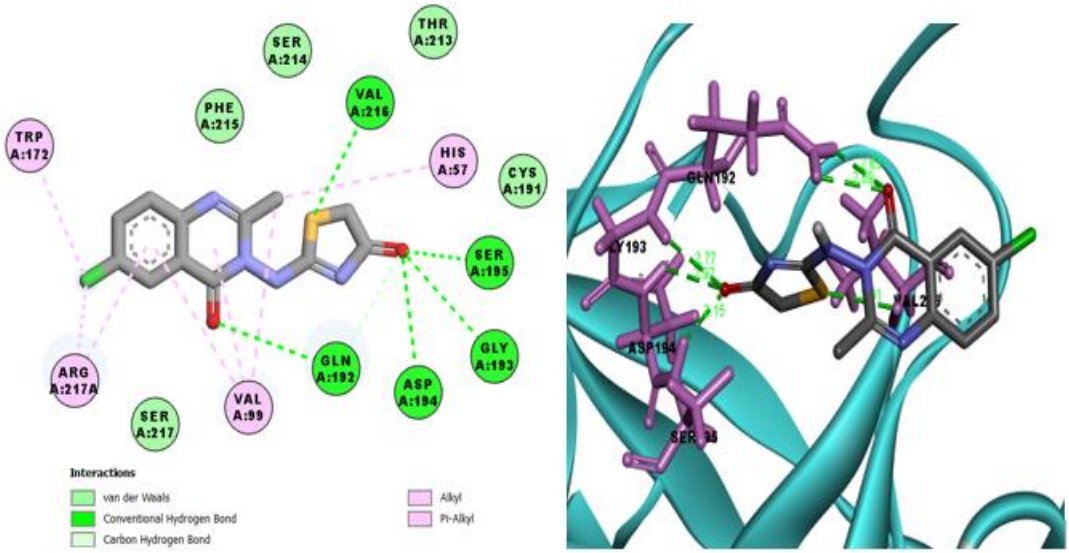


Figure S4. The 2D & 3D representations of the interactions of compound **8** within **Elastase** active site

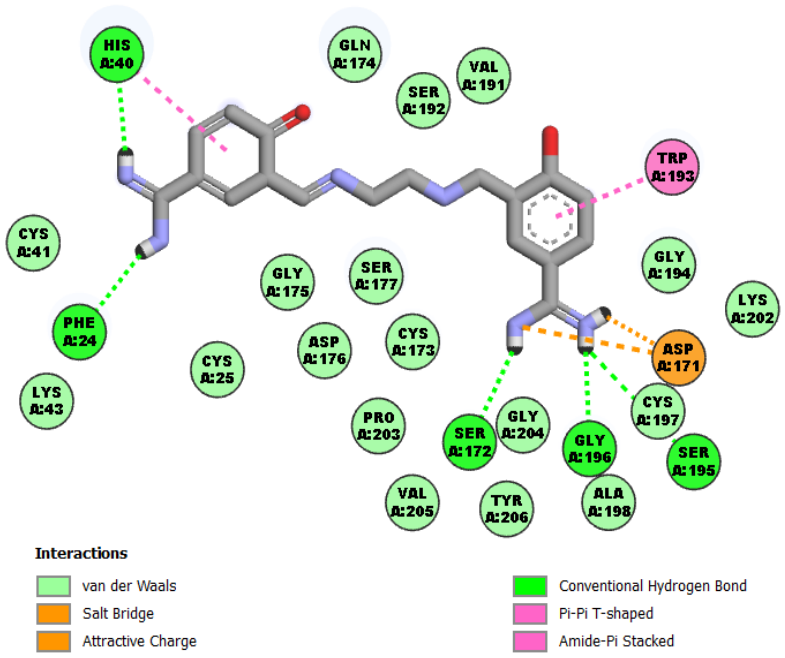


Figure S5. The 2D representations of the interactions of **A2C** within **Trypsin** active site

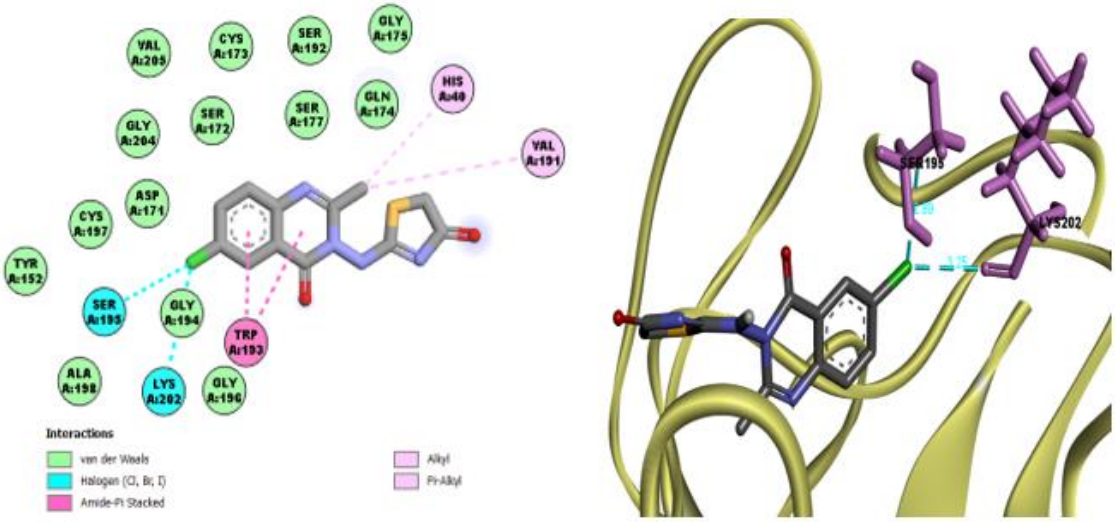


Figure S6. The 2D & 3D representations of the interactions of compound **8** within **Trypsin** active site

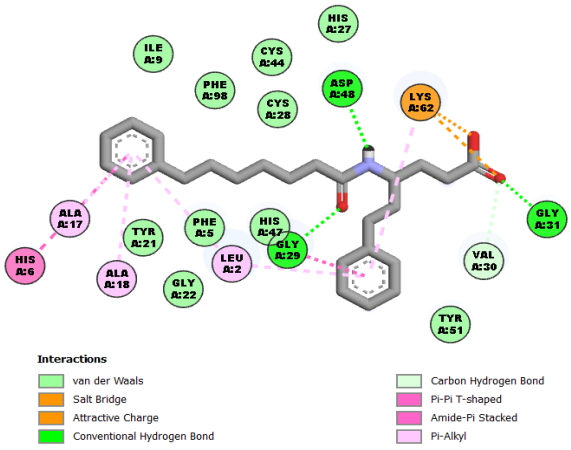


Figure S7. The 2D representation of the interactions of **BR4** within **hsPLA2-G-IIA** active site

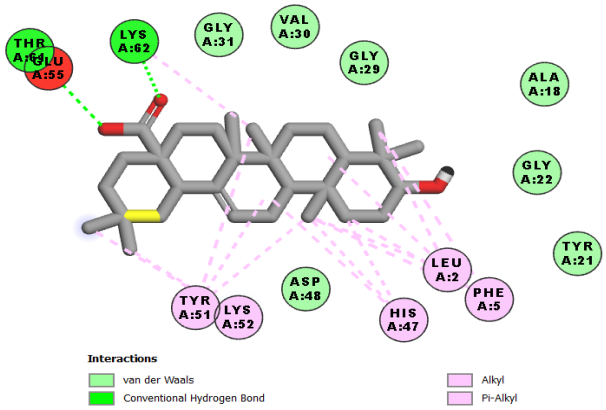


Figure S8. The 2D representation of the interactions of **Oleanolic acid** within **hsPLA2-G-IIA** active site

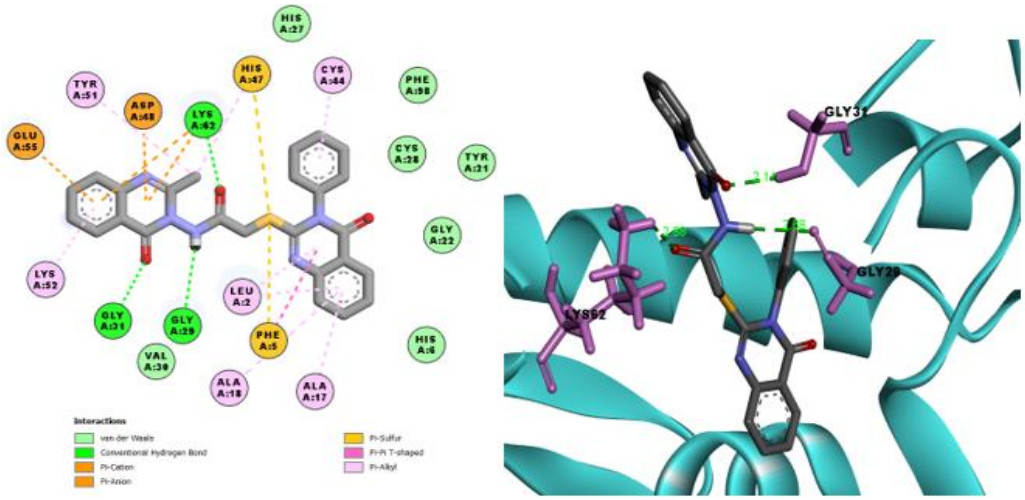


Figure S9. The 2D & 3D representations of the interactions of compound **10** within **hsPLA2-G-IIA** active site

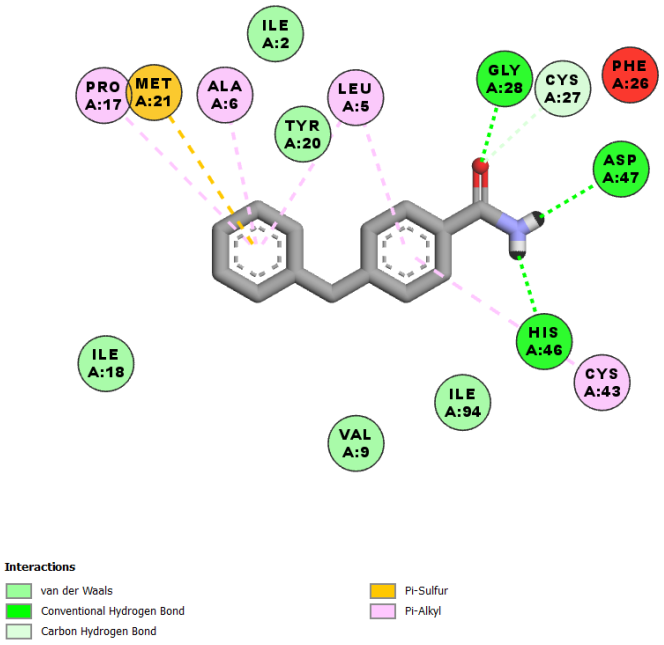


Figure S10. The 2D representation of the interactions of **9JH** within **hsPLA$_2$-G-X** active site

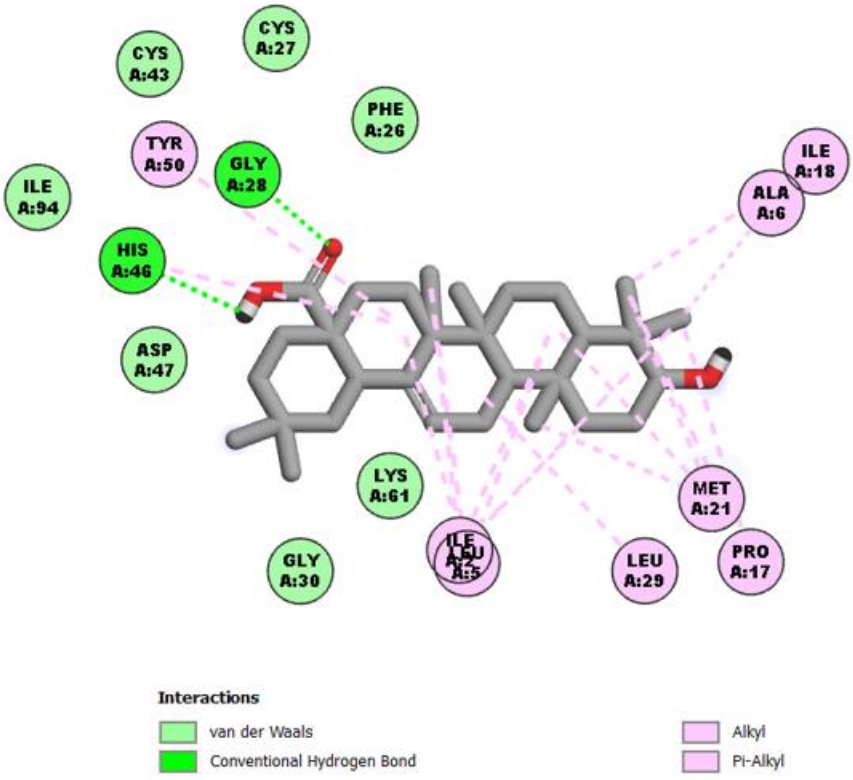


Figure S11. The 2D & 3D representations of the interactions of **Oleanolic acid** within **hsPLA$_2$-G-X** active site

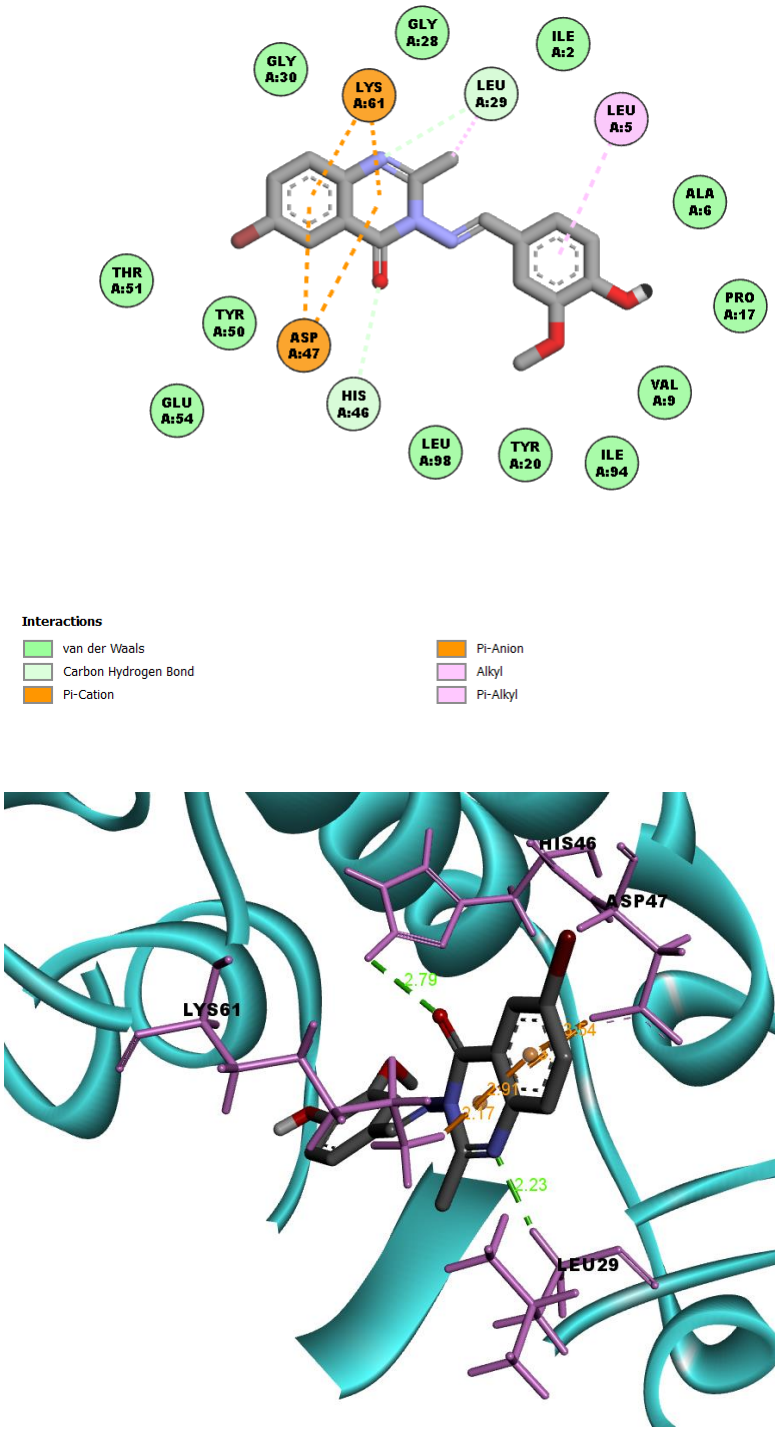


Figure S12. The 2D & 3D representations of the interactions of compound **3g** within **hsPLA$_2$-G-X** active site

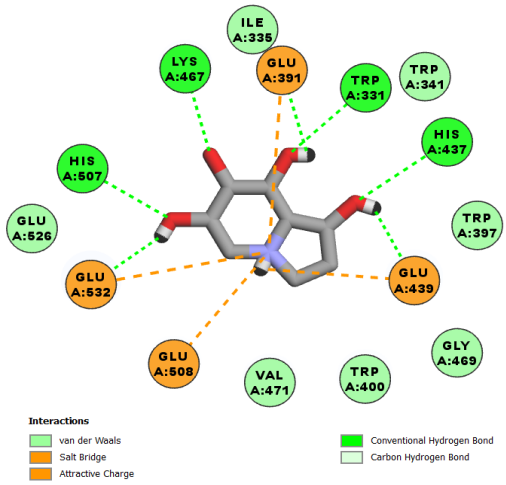


Figure S13. The 2D representation of the interactions of **CTS** within **α-Glucosidase** active site

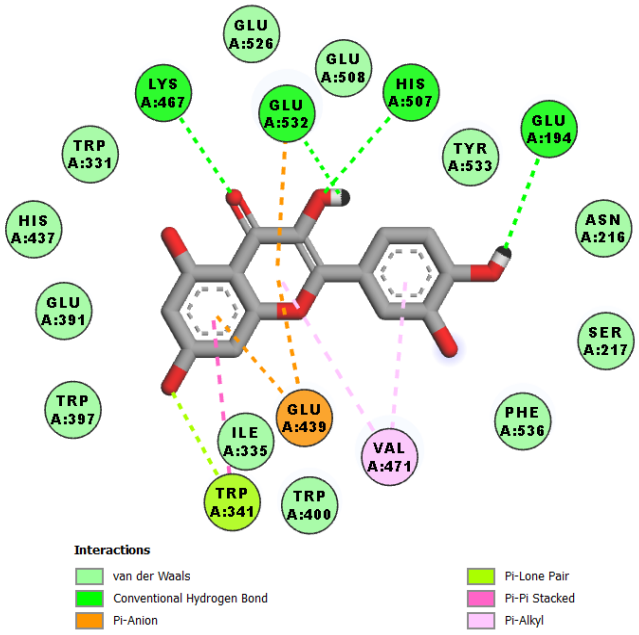


Figure S14. The 2D representation of the interaction of the **Quercetin** within **α-Glucosidase** active site

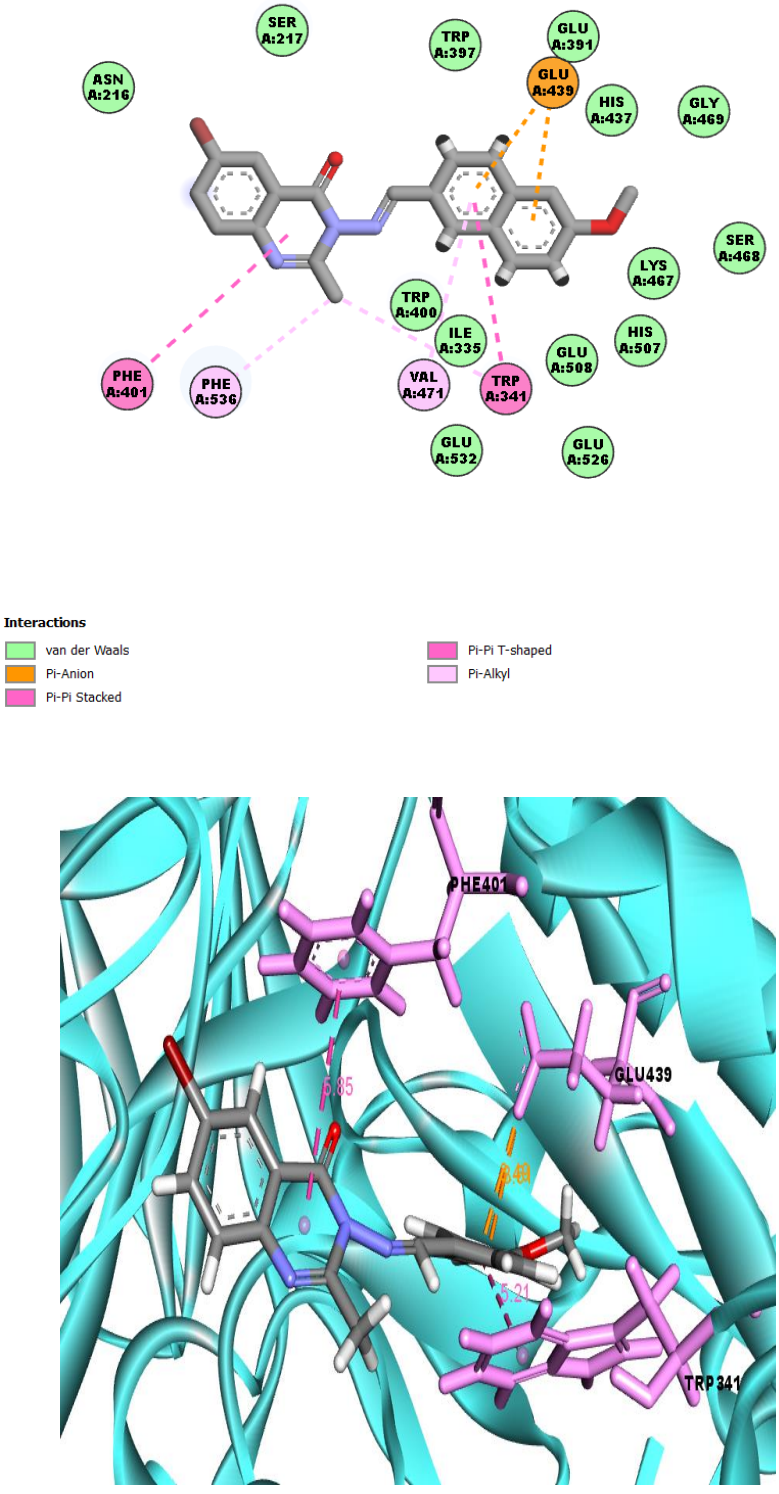


Figure S15. The 2D & 3D representations of the interactions of compound **3f** within **α-Glucosidase** active site

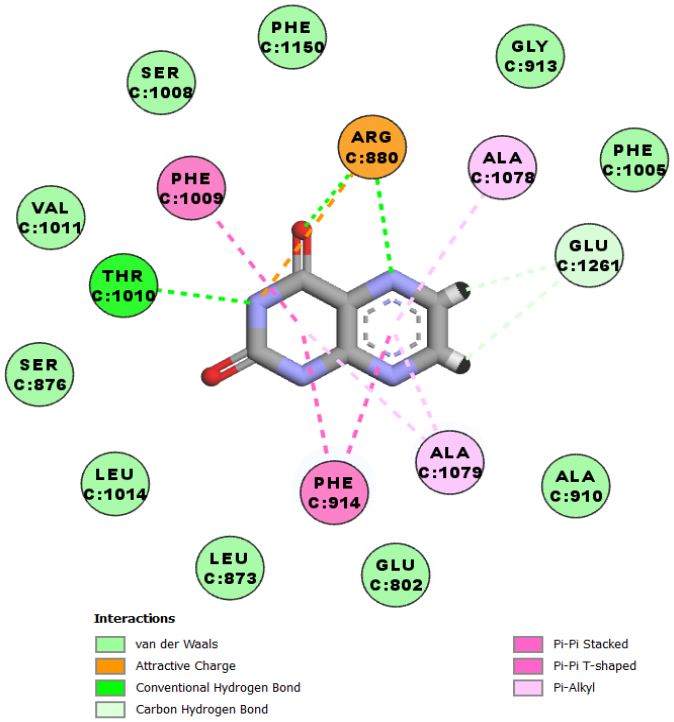


Figure S16. The 2D representation of the interactions of **LUZ** within **Xanthine oxidoreductase** active site

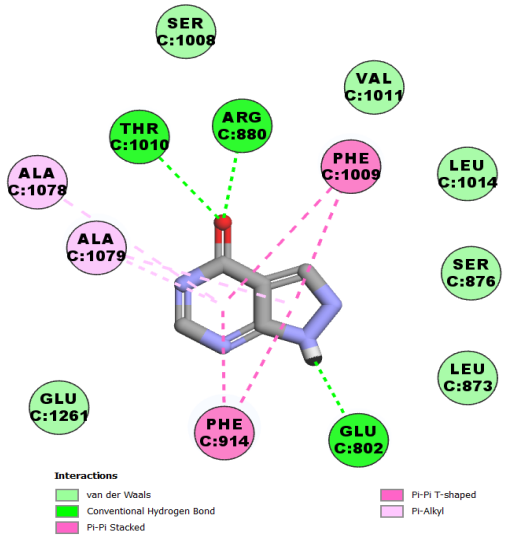


Figure S17. The 2D representations of the interactions of **Allopurinol** within **Xanthine oxidoreductase** active site

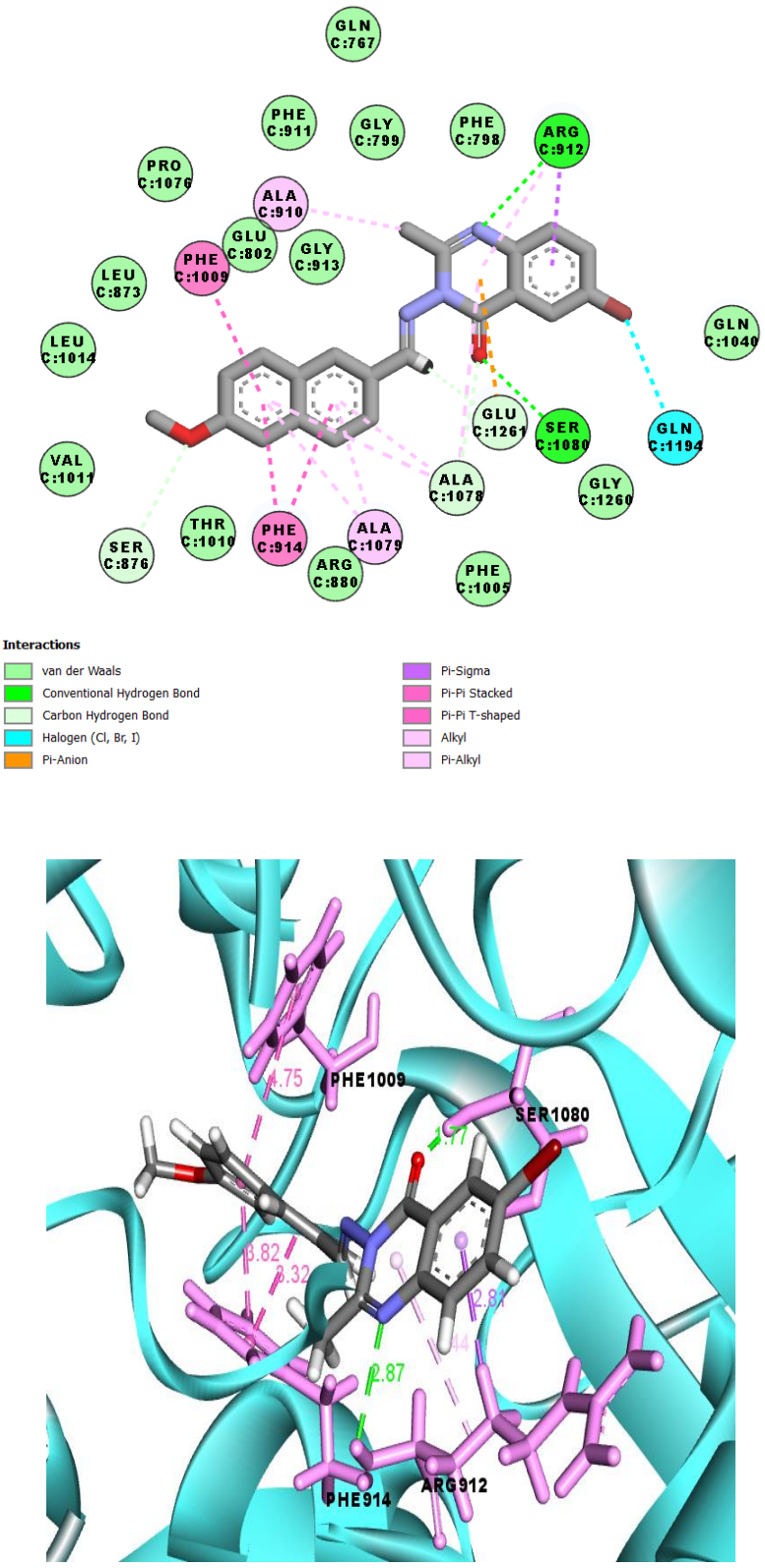


Figure S18. The 2D & 3D representations of the interactions of compound **3f** within **Xanthine oxidoreductase** active site

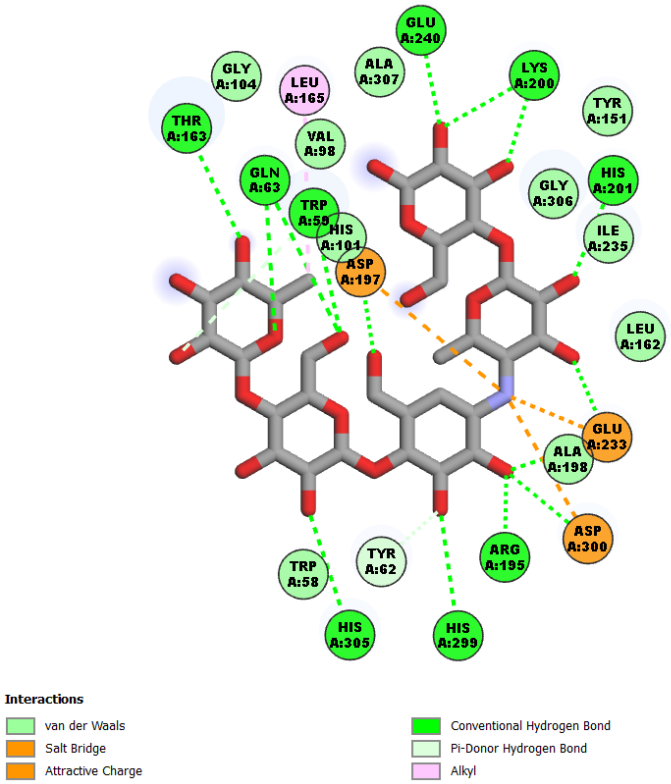


Figure S19. The 2D representations of the interactions of **AC1** within **α-Amylase** active site

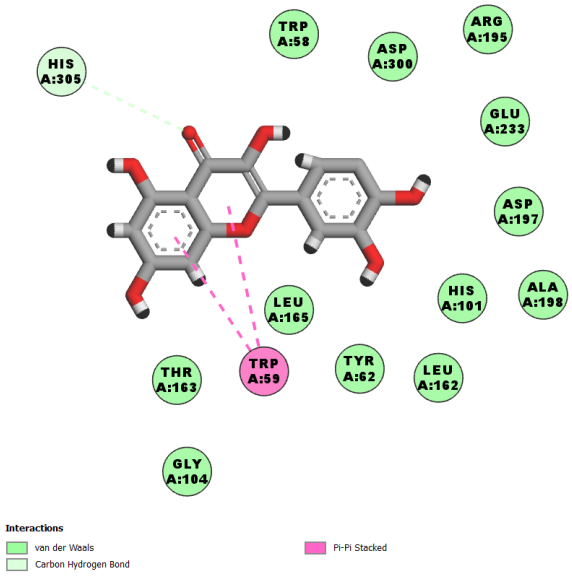


Figure S20. The 2D representations of the interactions of **Quercetin** within **α-Amylase** active site

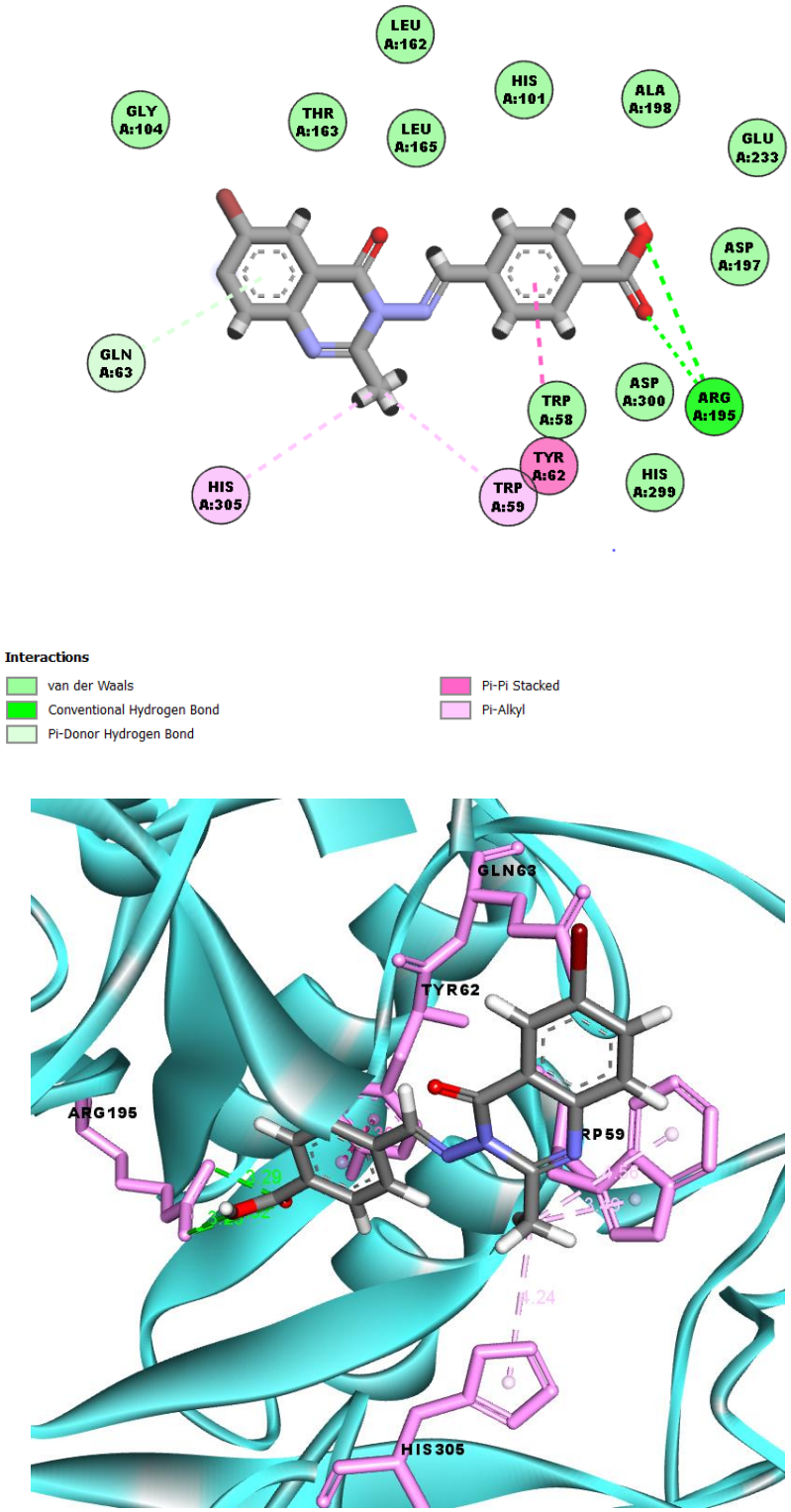
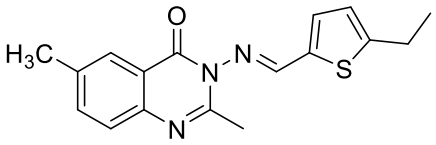


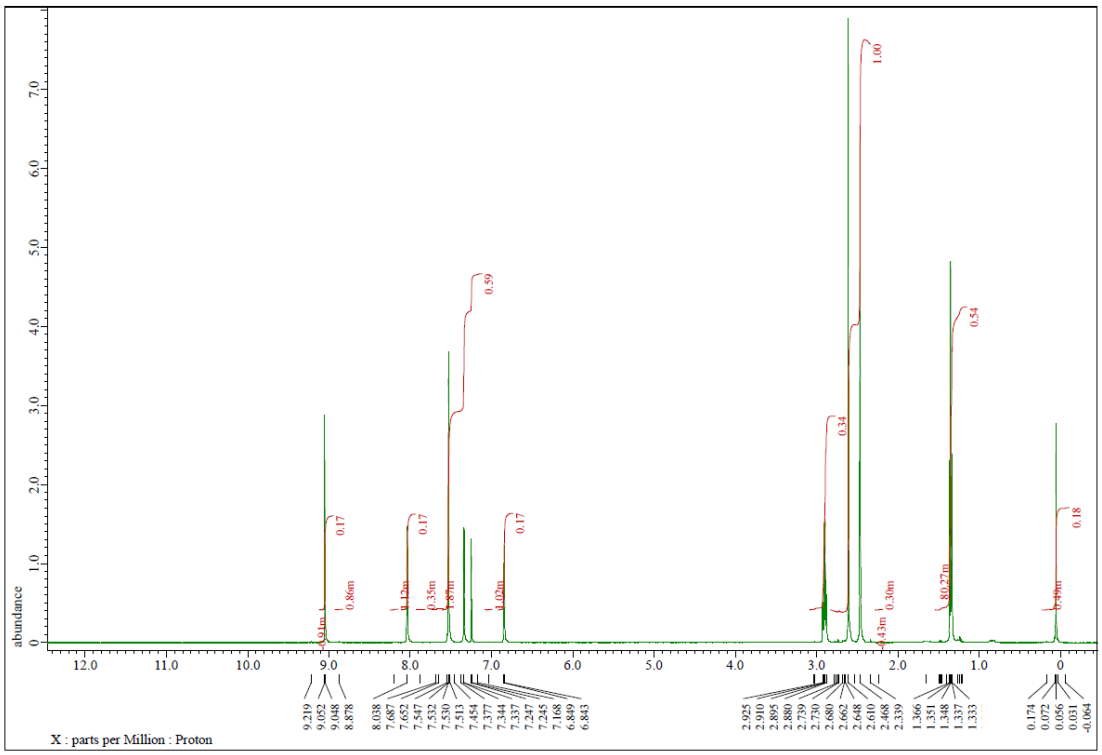
Figure S21. The 2D & 3D representations of the interactions of compound **3b** within **α-Amylase** active site

^{1}H and ^{13}CNMR spectra of selected compounds

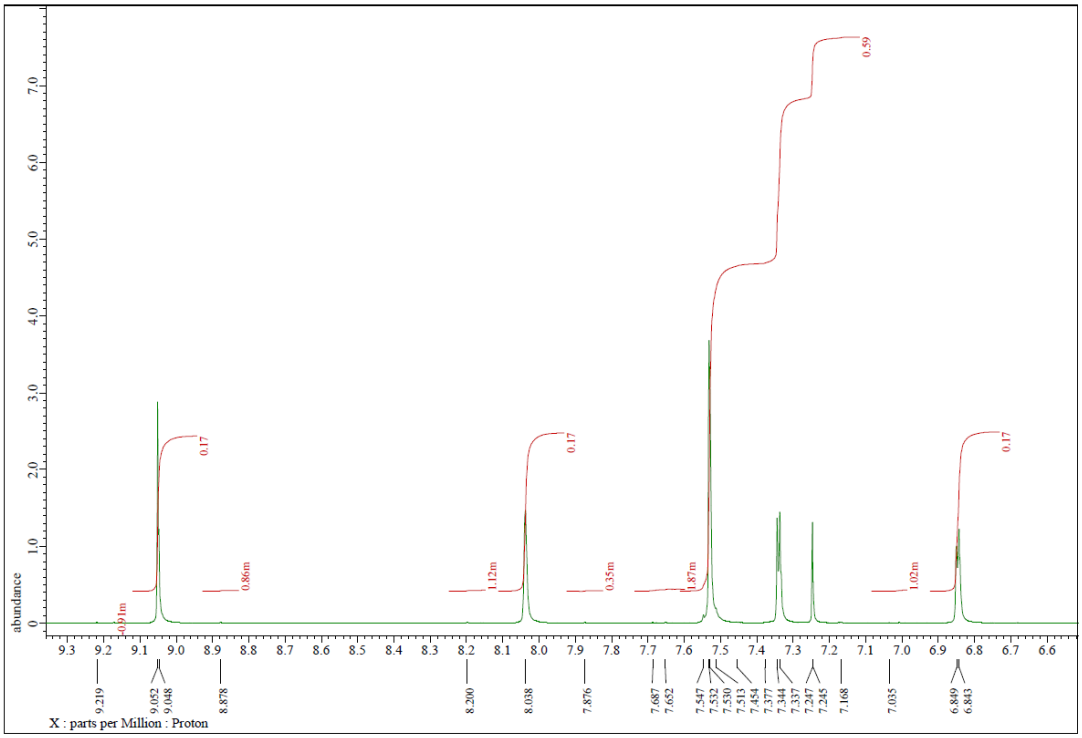
Compound 3a

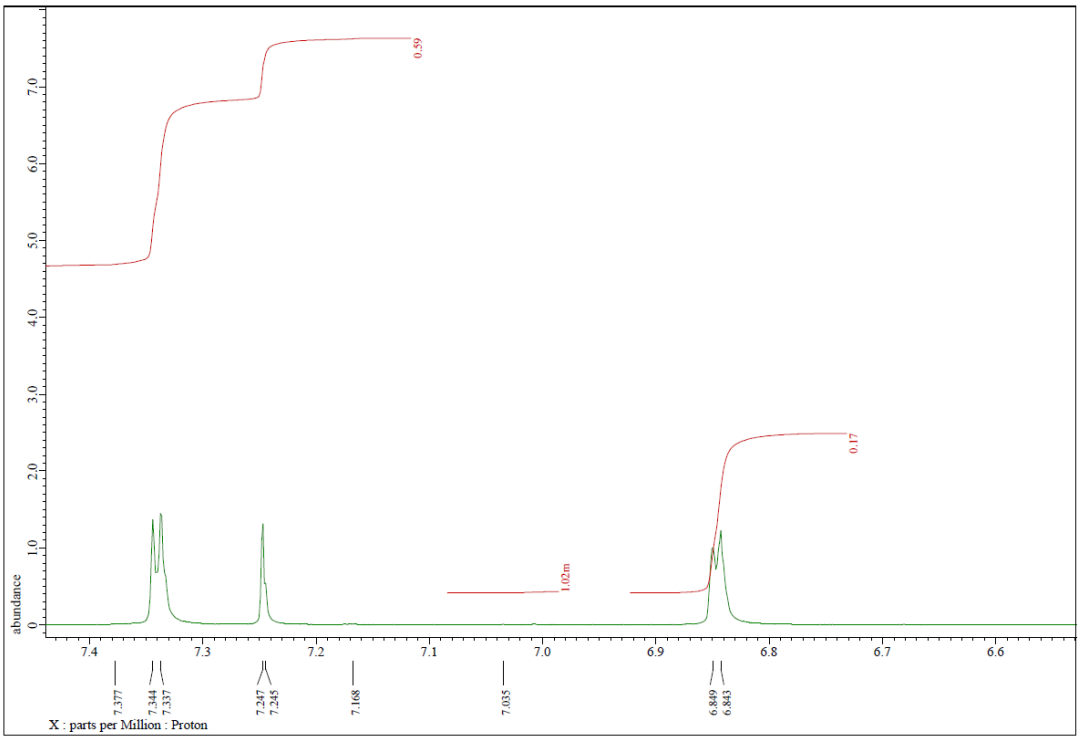


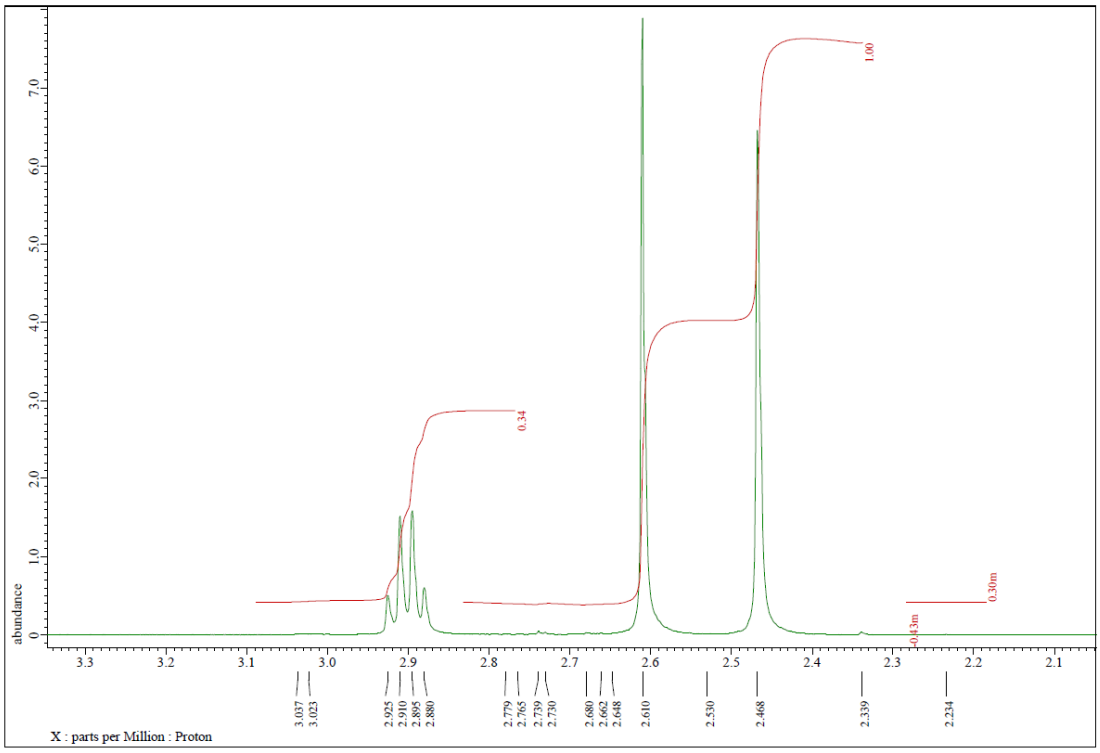
^{1}H-NMR (500 MHz; $CDCl_3$) of compound 3a



Expanded ^{1}H-NMR (500 MHz; $CDCl_3$) of compound 3a






abundance
X : parts per Million : Proton
0.34
1.00
0.30m
0.43m
3.037
3.023
2.925
2.910
2.895
2.880
2.779
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2.730
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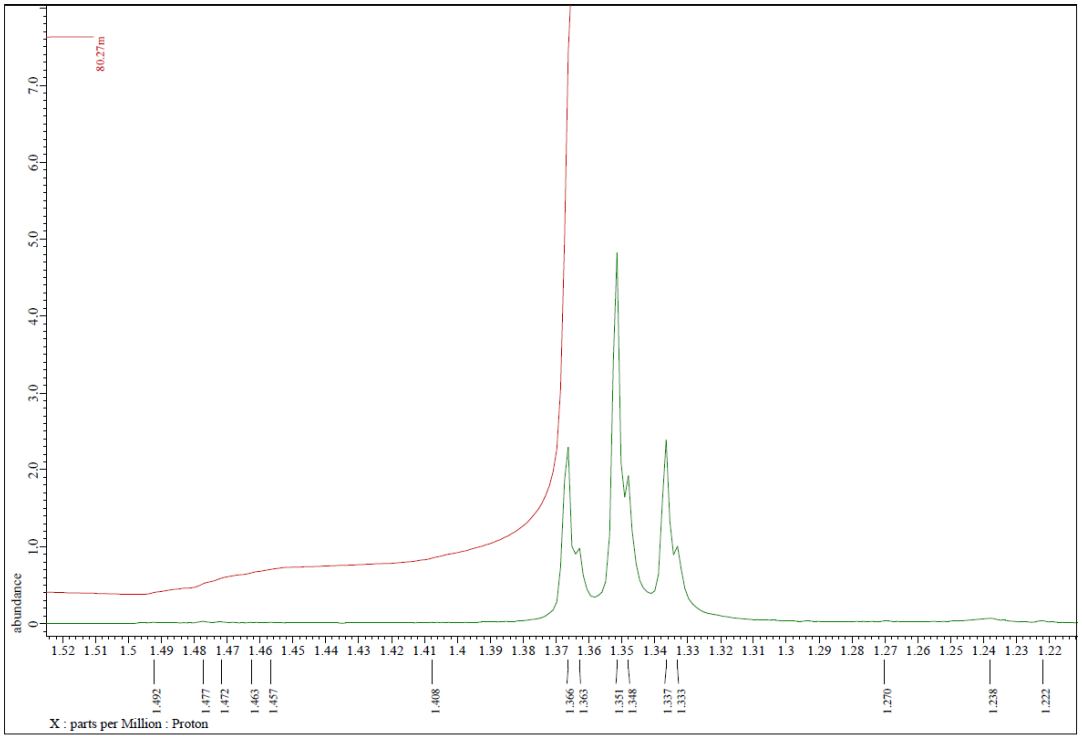
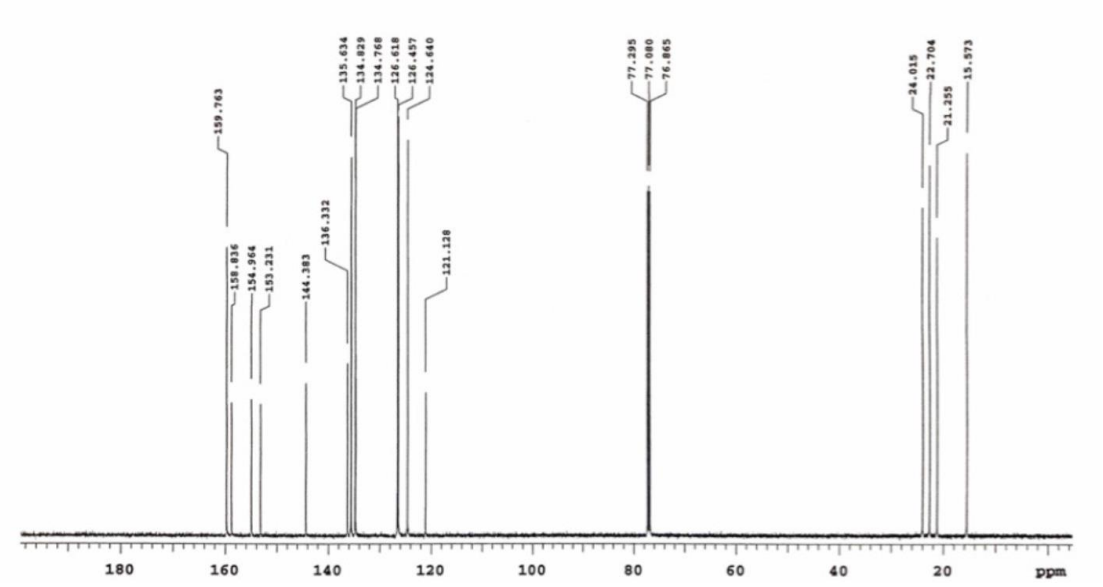
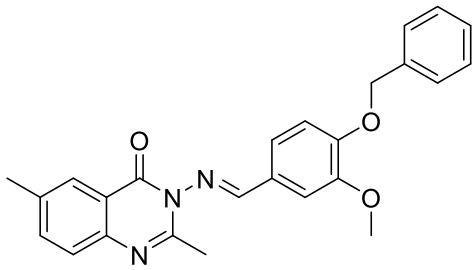
2.648
2.610
2.530
2.468
2.339
2.234


abundance
X : parts per Million : Proton
80.27m
1.492
1.477
1.472
1.463
1.457
1.408
1.366
1.363
1.351
1.348
1.337
1.333
1.270
1.238
1.222

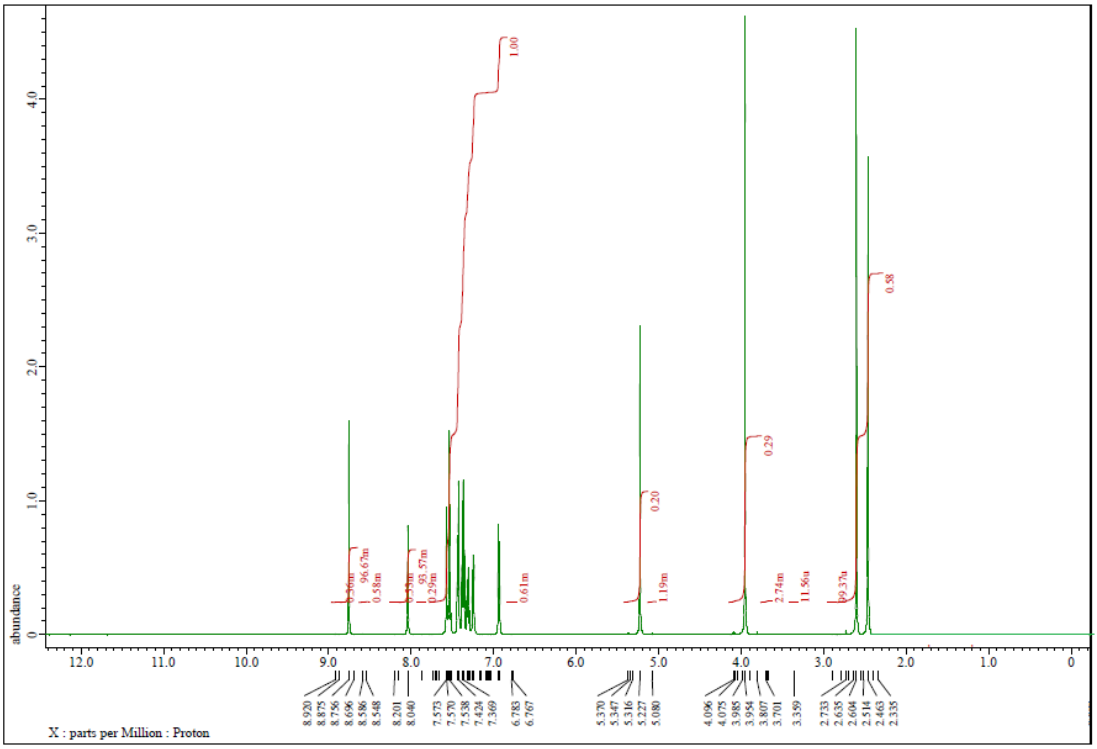
^{13}C-NMR (150 MHz; $CDCl_3$) of compound 3a



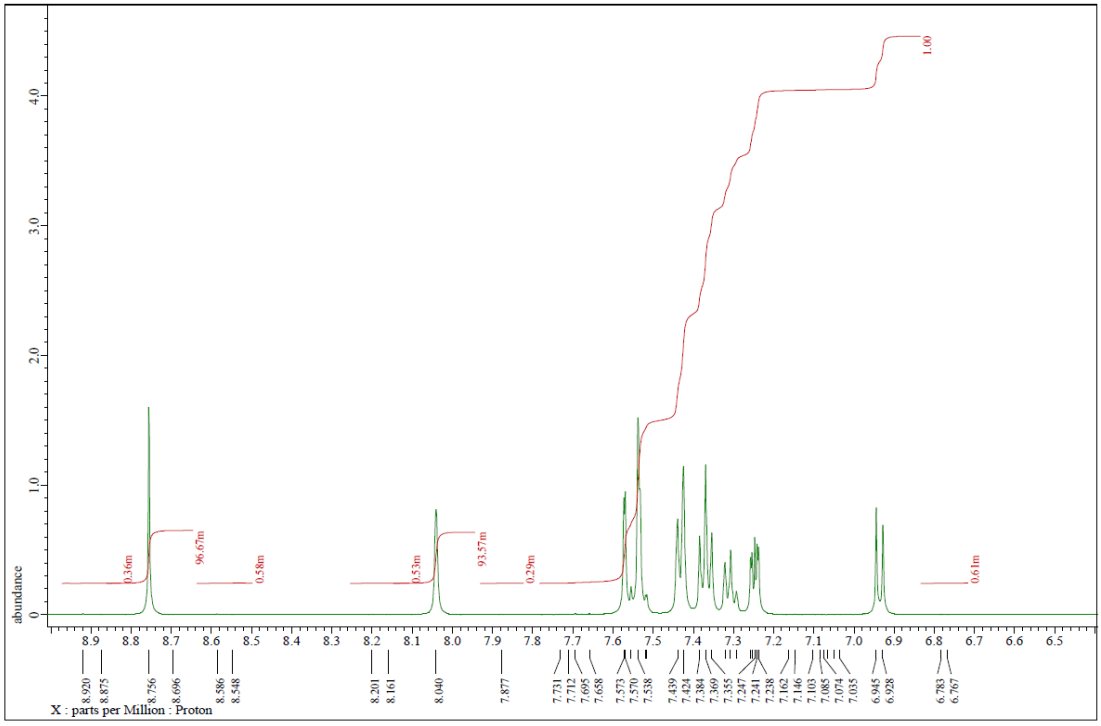
Compound 3e



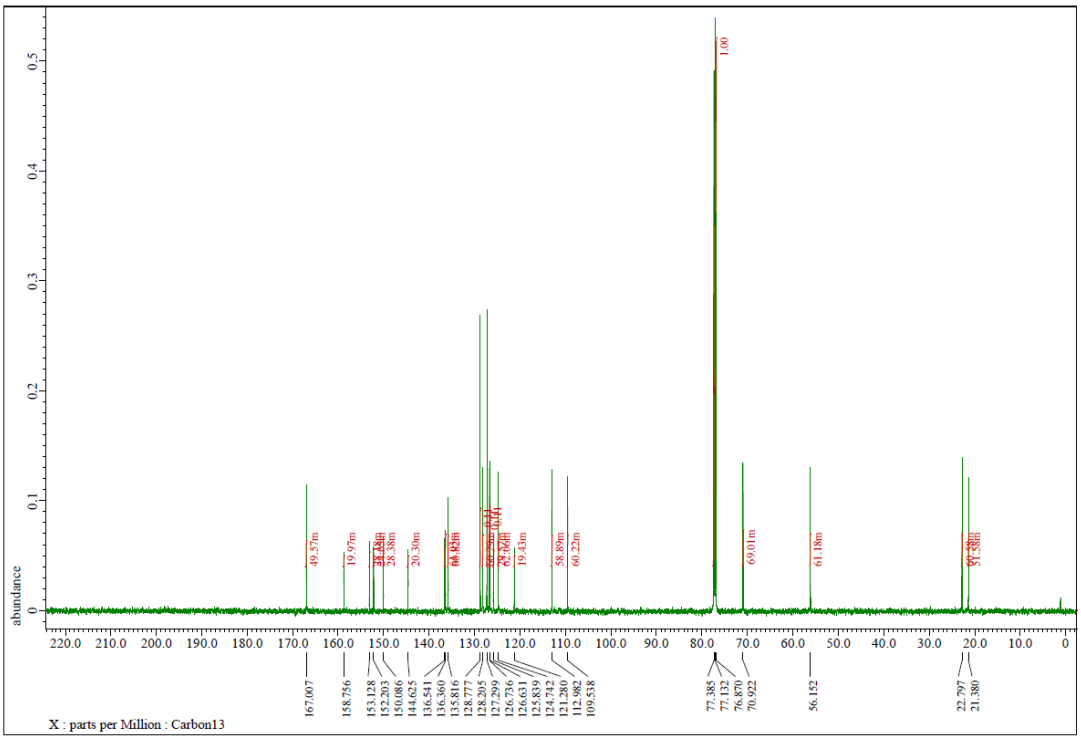
^{1}H-NMR (500 MHz; $CDCl_3$) of compound 3e



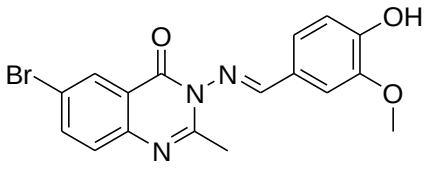
Expanded ^{1}H-NMR (500 MHz; $CDCl_3$) of compound 3e



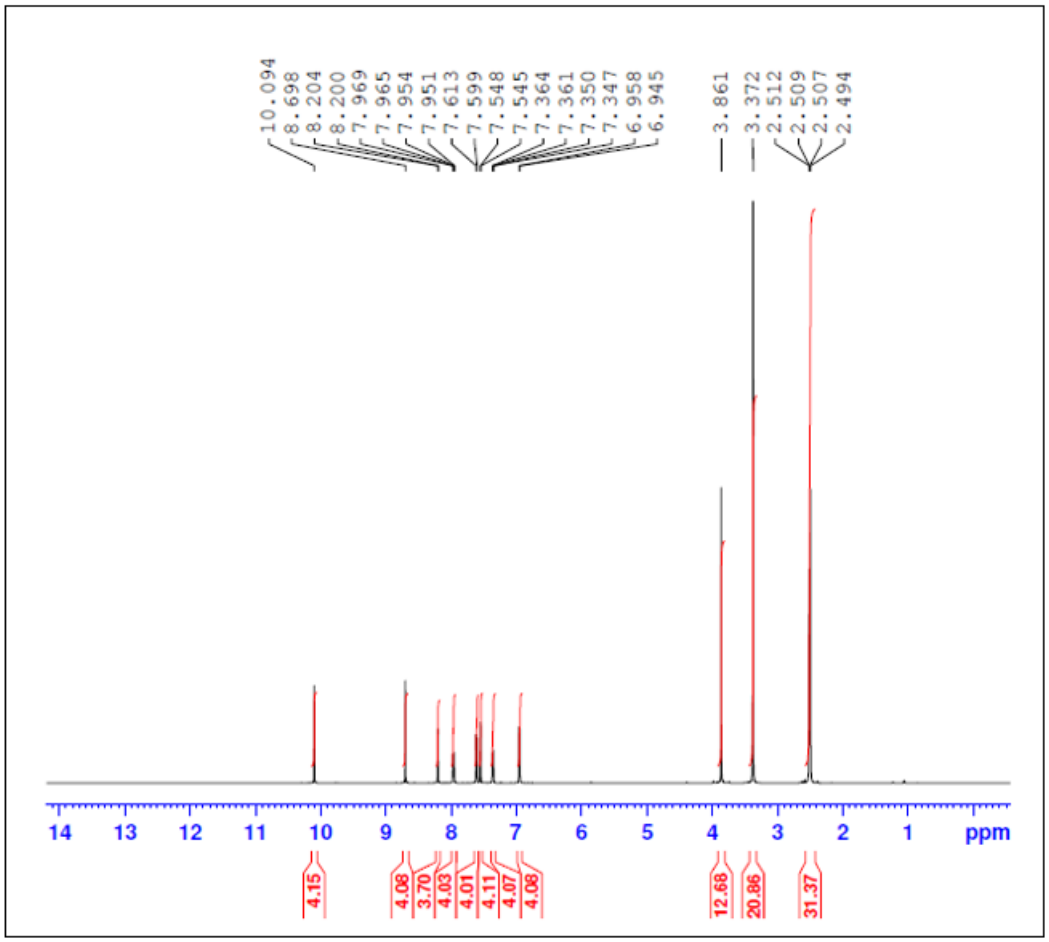
^{13}C-NMR (125 MHz; $CDCl_3$) of compound 3e



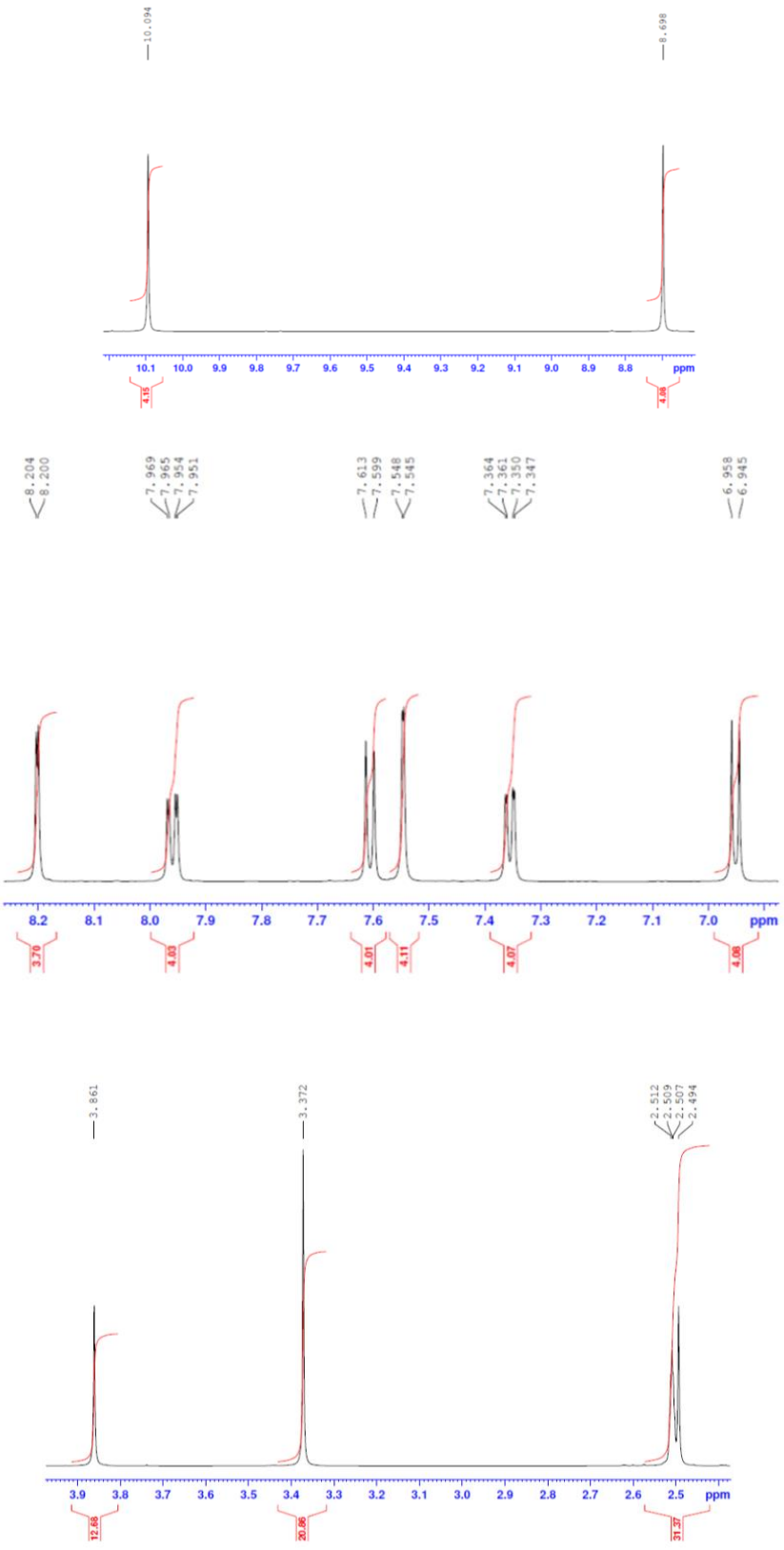
Compound 3g



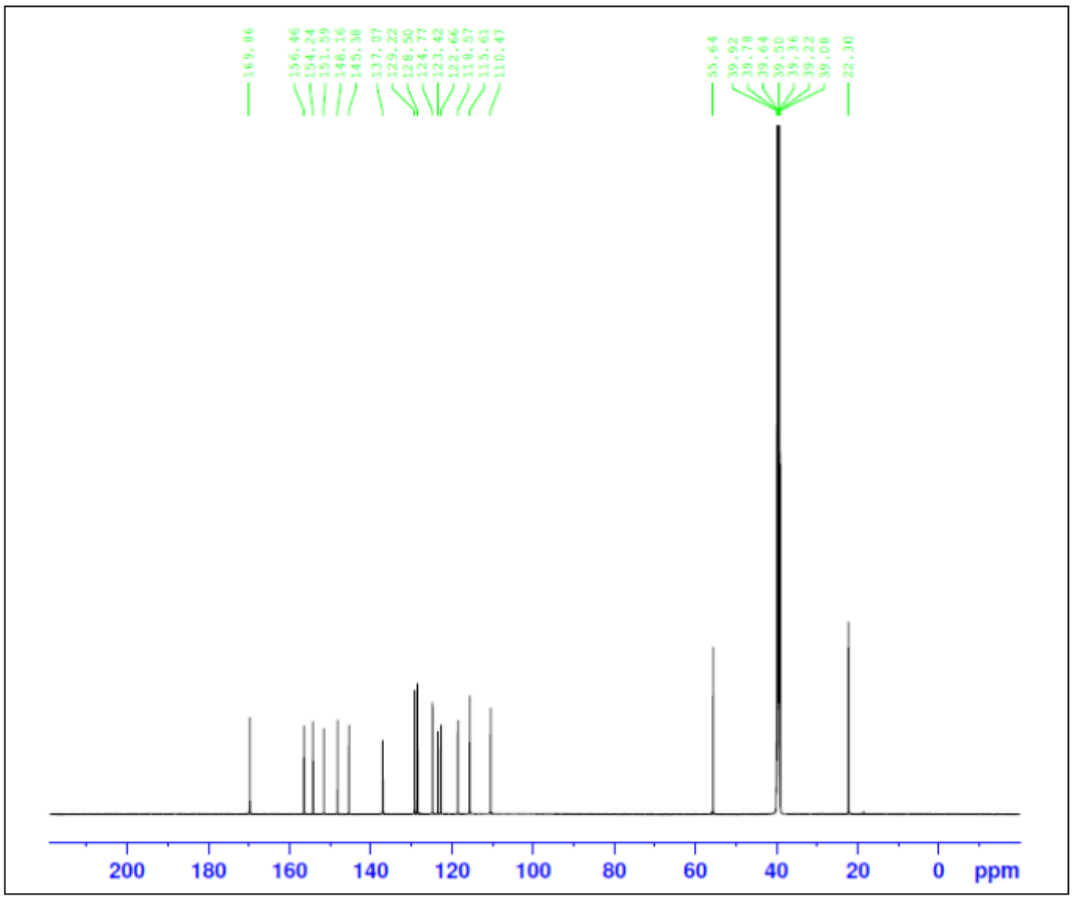
^{1}H-NMR (600 MHz; DMSO-d_6) of compound 3g



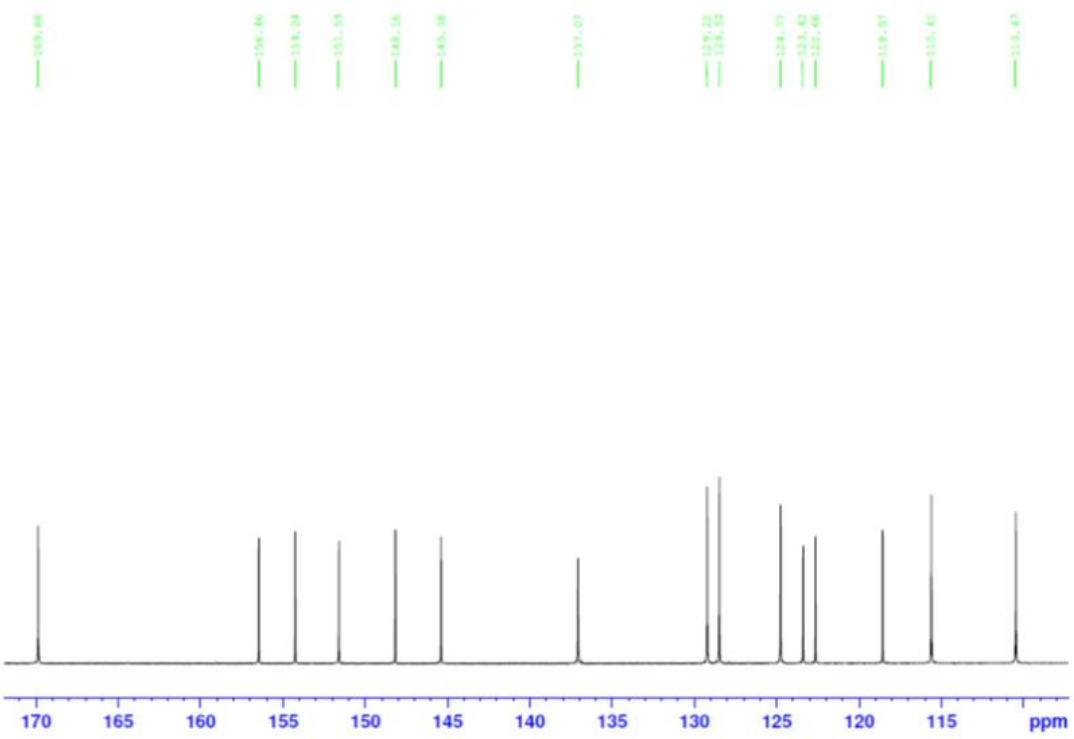
Expanded ^{1}H-NMR spectrum (600 MHz; DMSO-d_6) of compound 3g

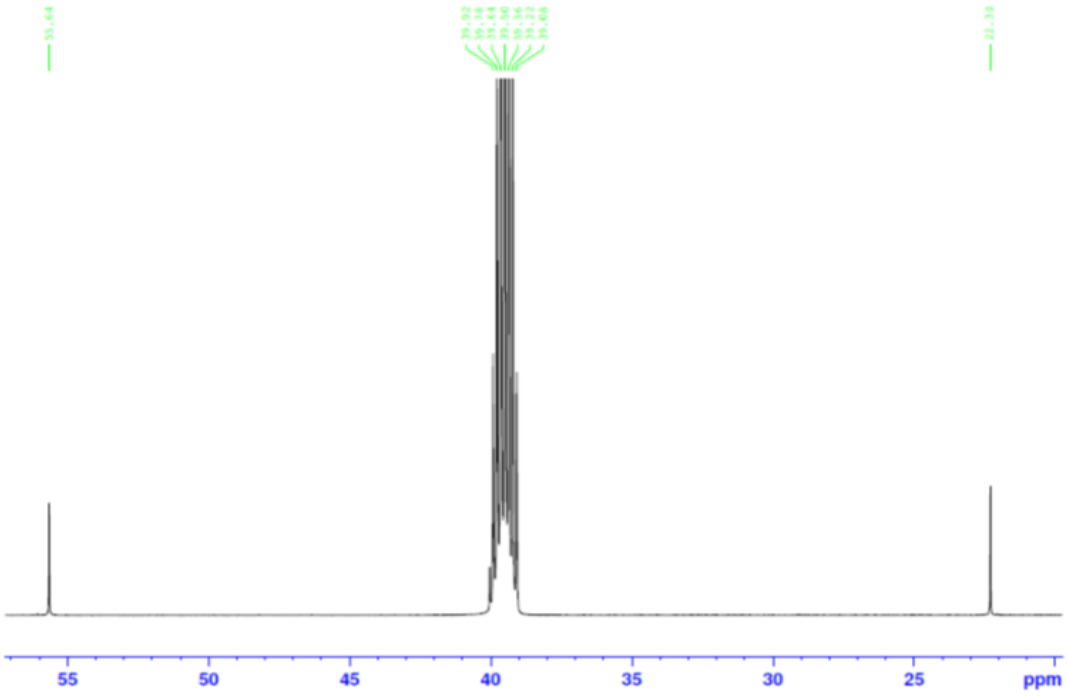


^{13}C-NMR (150 MHz; DMSO-d_6) of compound 3g

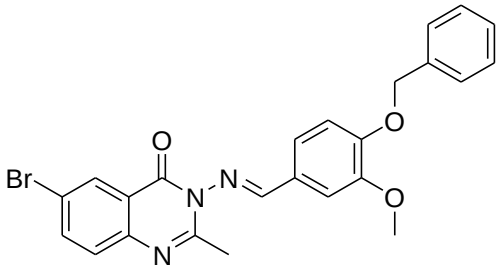


Expanded ^{13}C-NMR (150 MHz; DMSO-d_6) of compound 3g

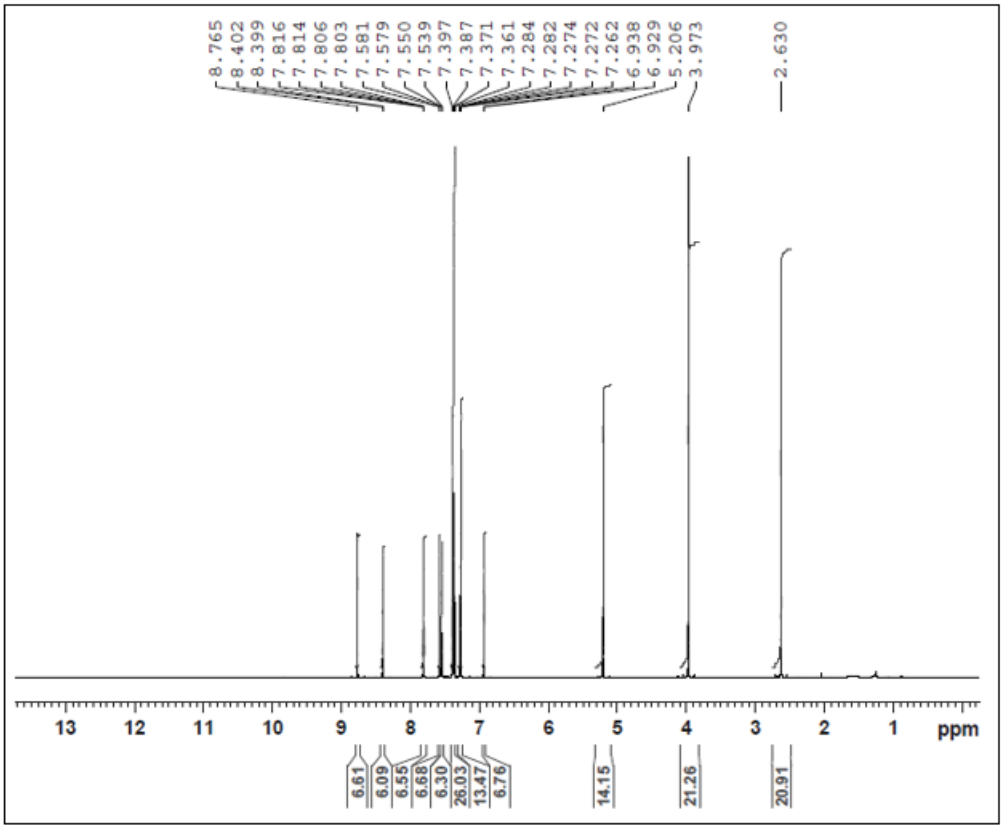




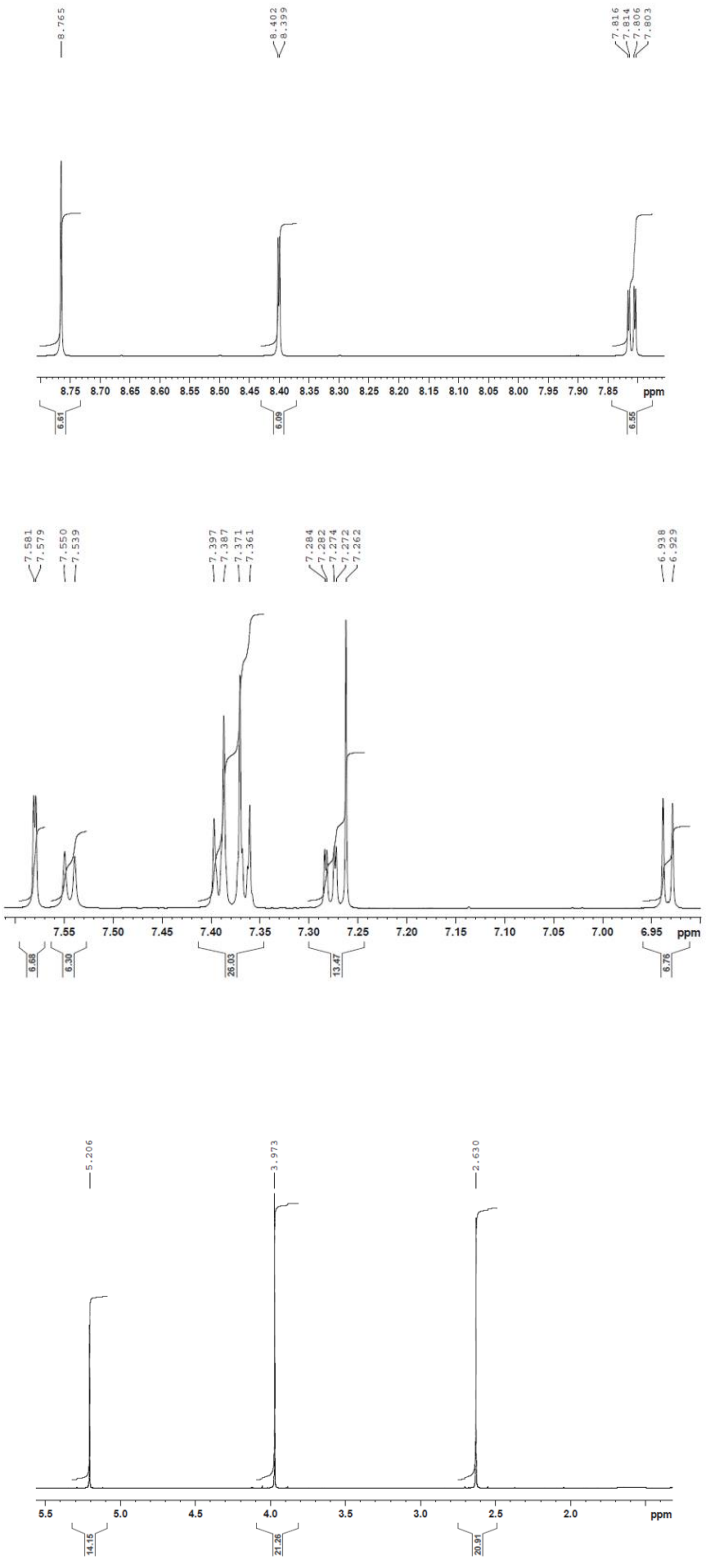
Compound 5



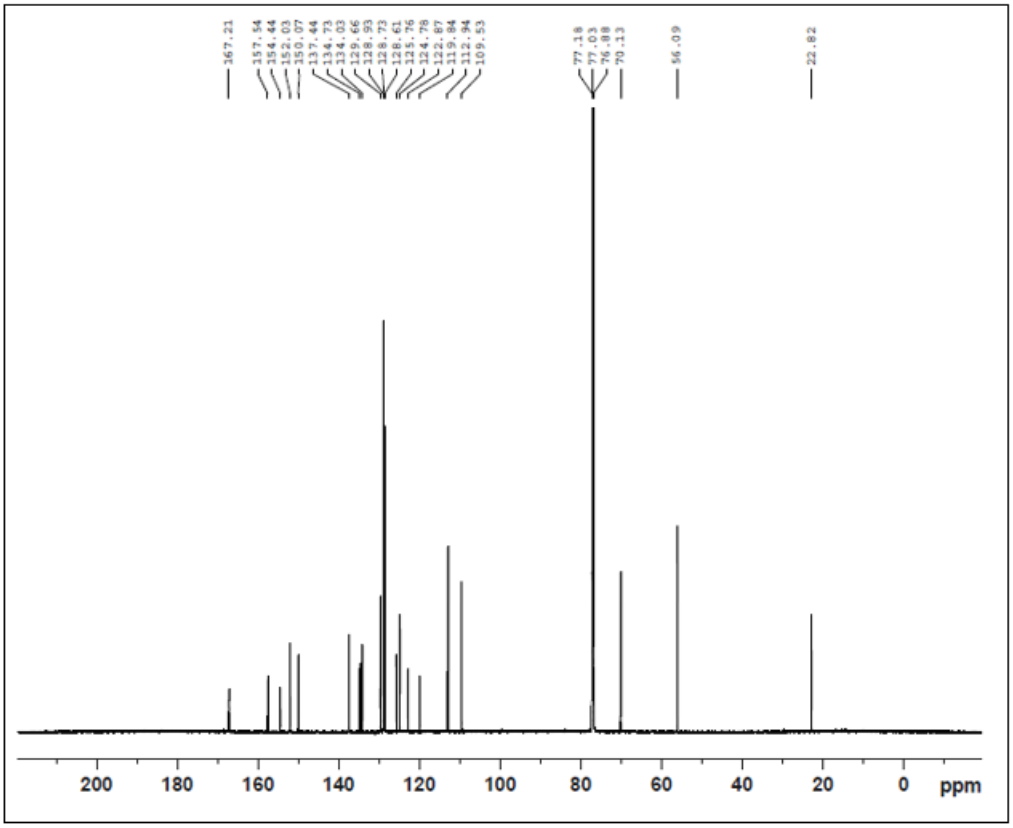
^{1}H-NMR (850 MHz; $CDCl_3$) of compound 5



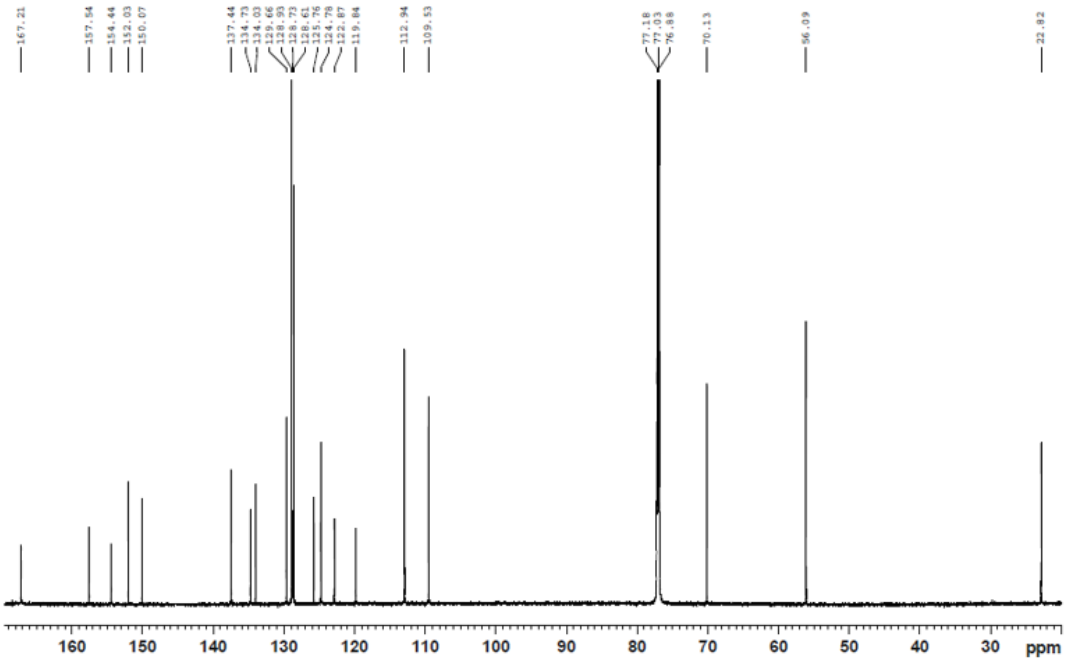
Expanded ^{1}H-NMR (850 MHz; $CDCl_3$) of compound 5



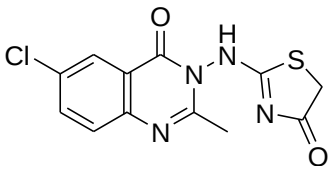
^{13}C-NMR (213 MHz; $CDCl_3$) of compound 5



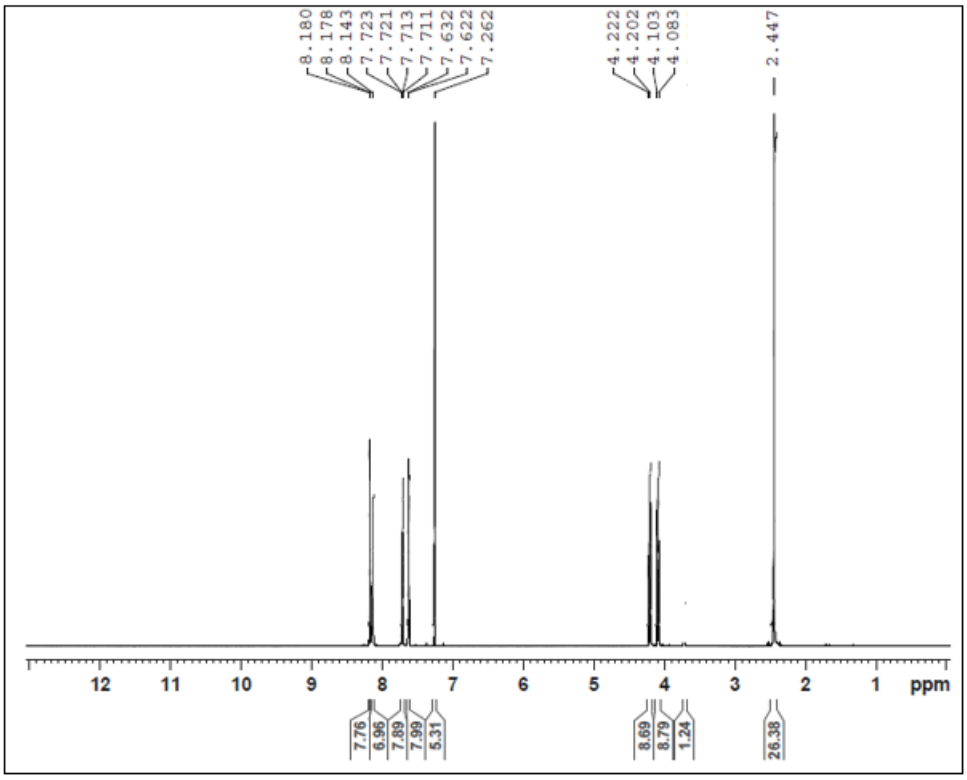
Expanded ^{13}C-NMR (213 MHz; $CDCl_3$) of compound 5



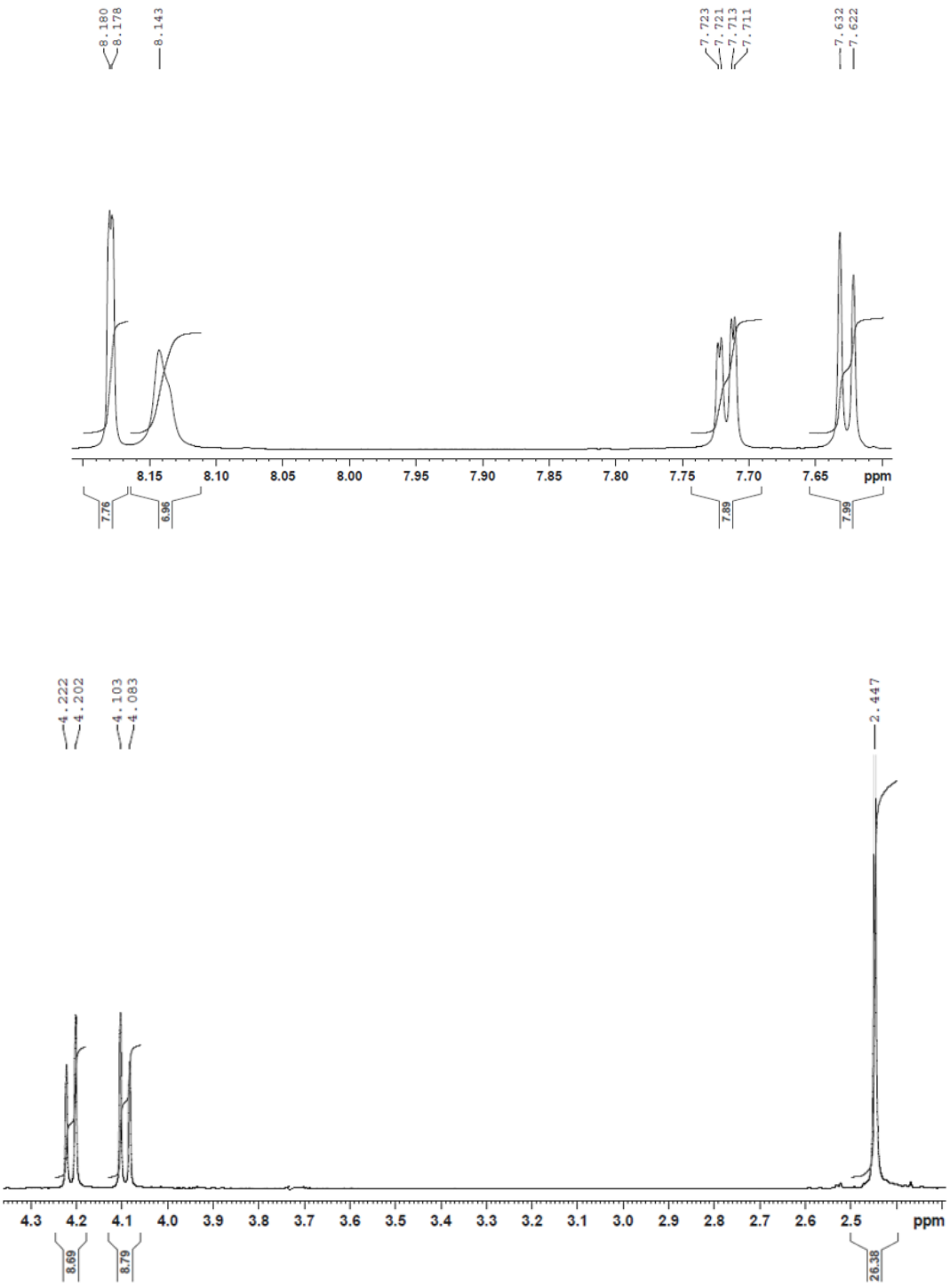
Compound 8



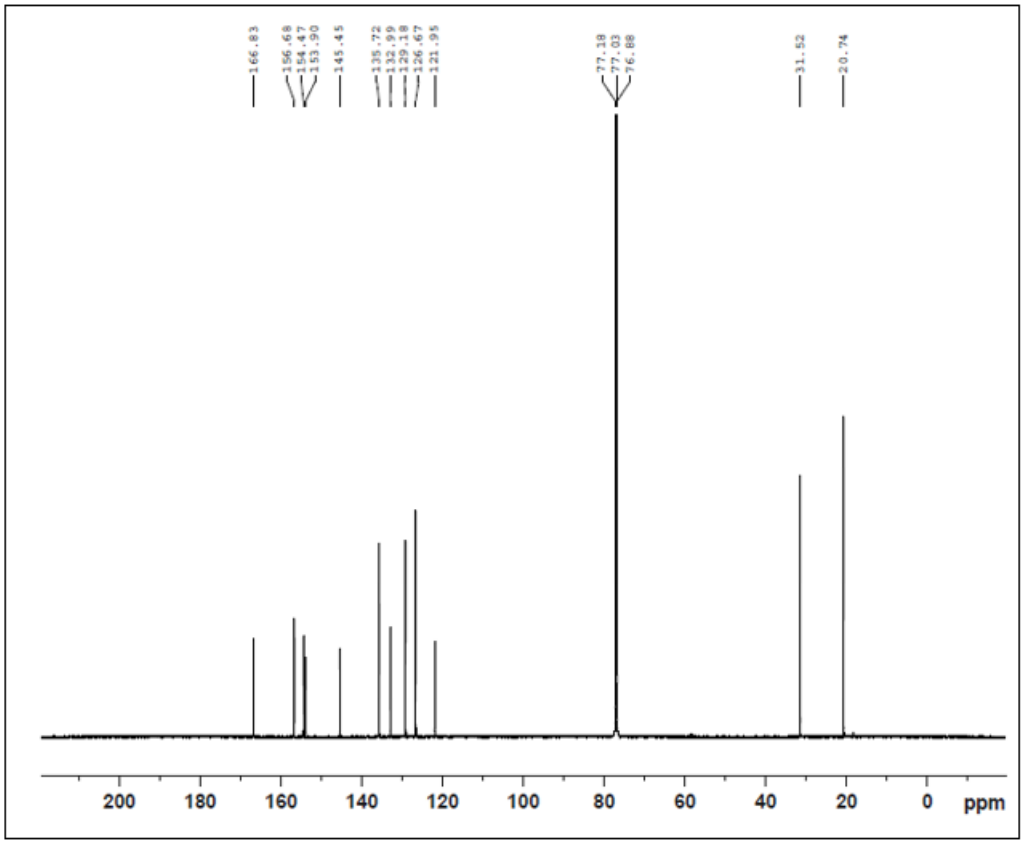
^{1}H-NMR (850 MHz; $CDCl_3$) of compound 8



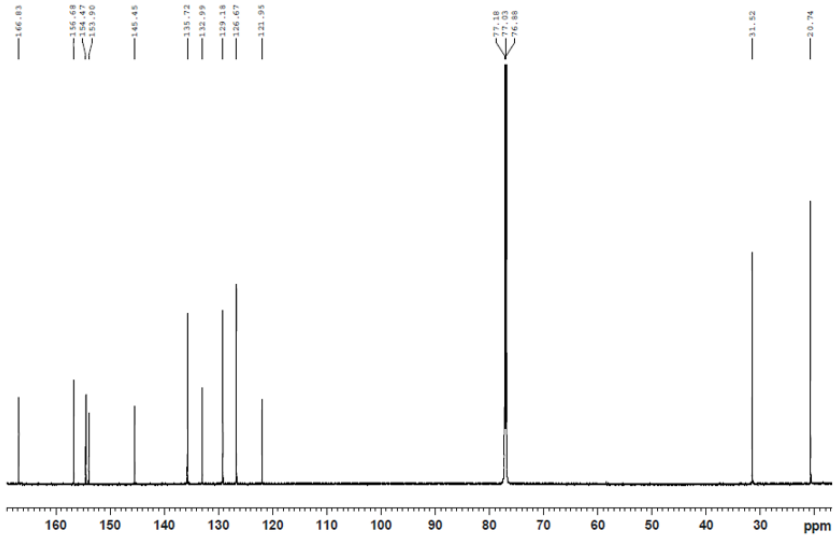
Expanded ^{1}H-NMR (850 MHz; $CDCl_3$) of compound 8



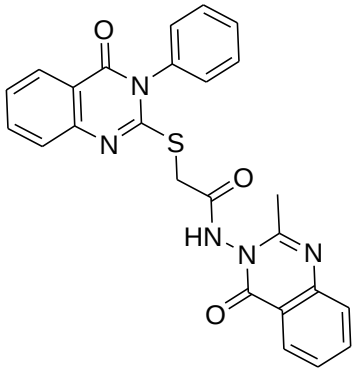
^{13}C-NMR (213 MHz; $CDCl_3$) of compound 8



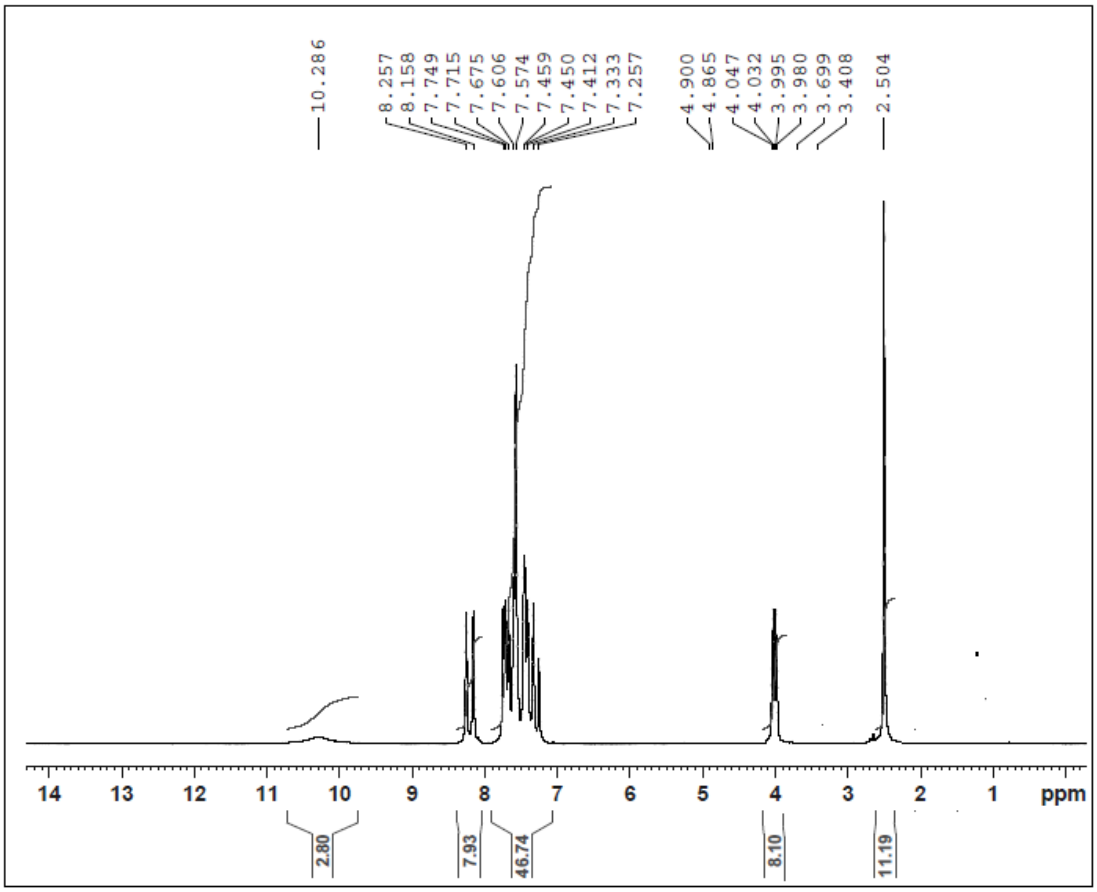
Expanded ^{13}C-NMR (213 MHz; $CDCl_3$) of compound 8



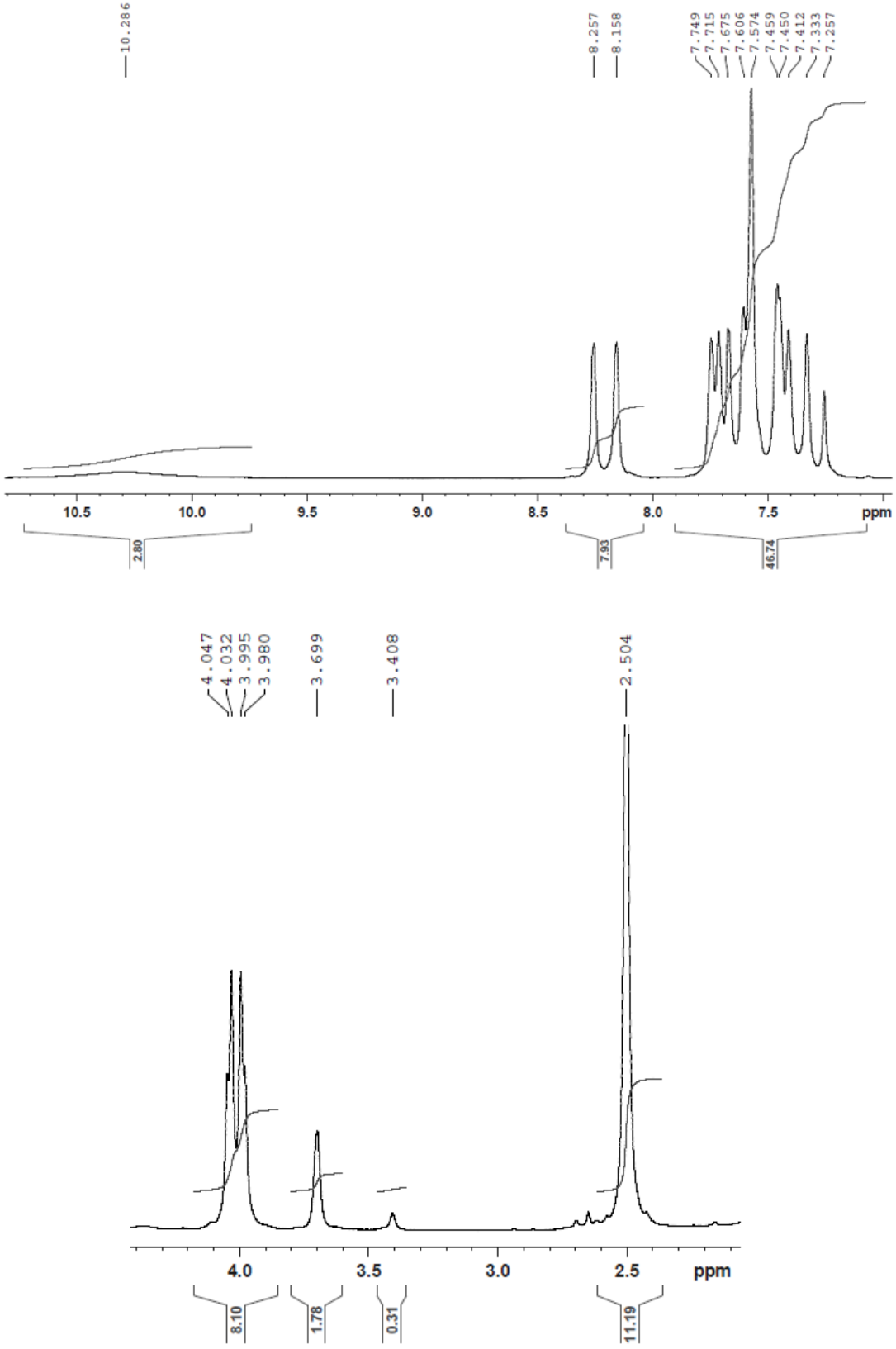
Compound 10



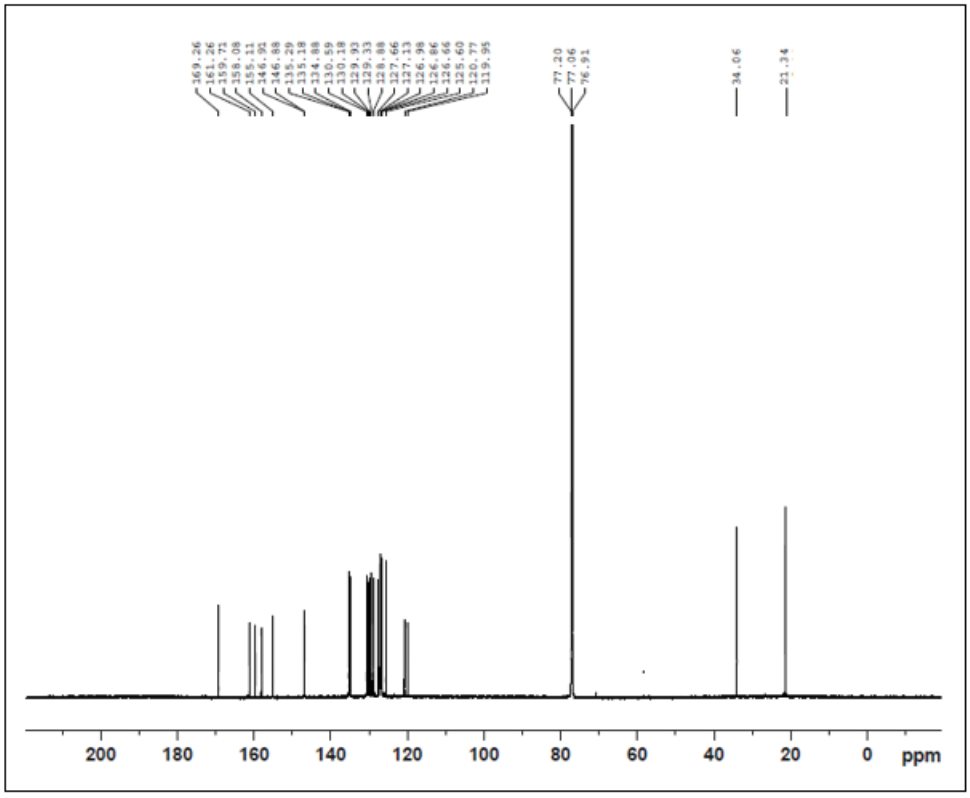
The ^{1}H-NMR (850 MHz; $CDCl_3$) of compound 10



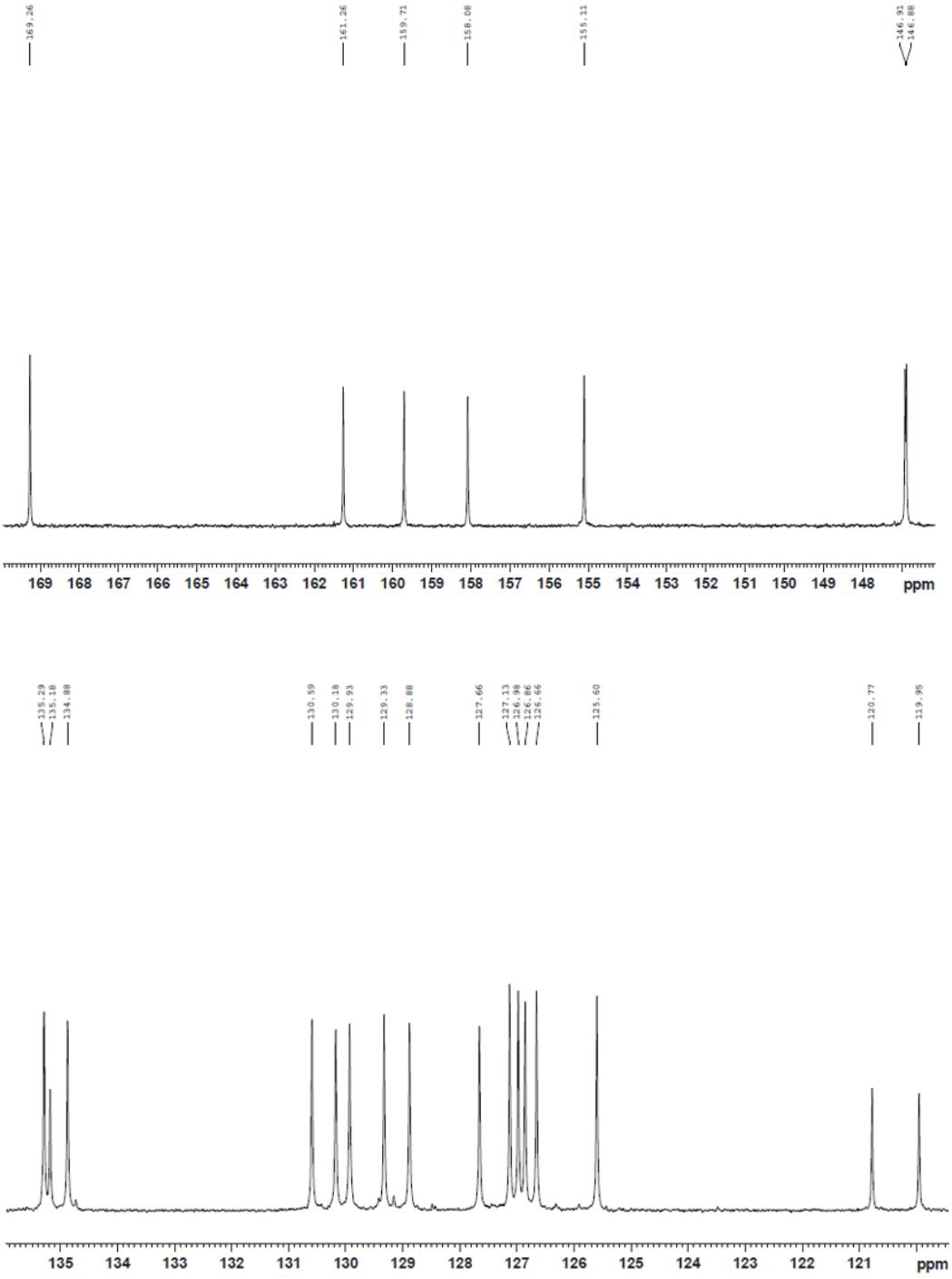
Expanded ^{1}H-NMR (850 MHz; $CDCl_3$) of compound 10



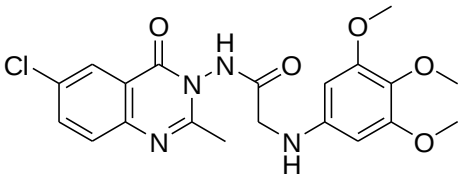
The ^{13}C-NMR (213 MHz; $CDCl_3$) of compound 10



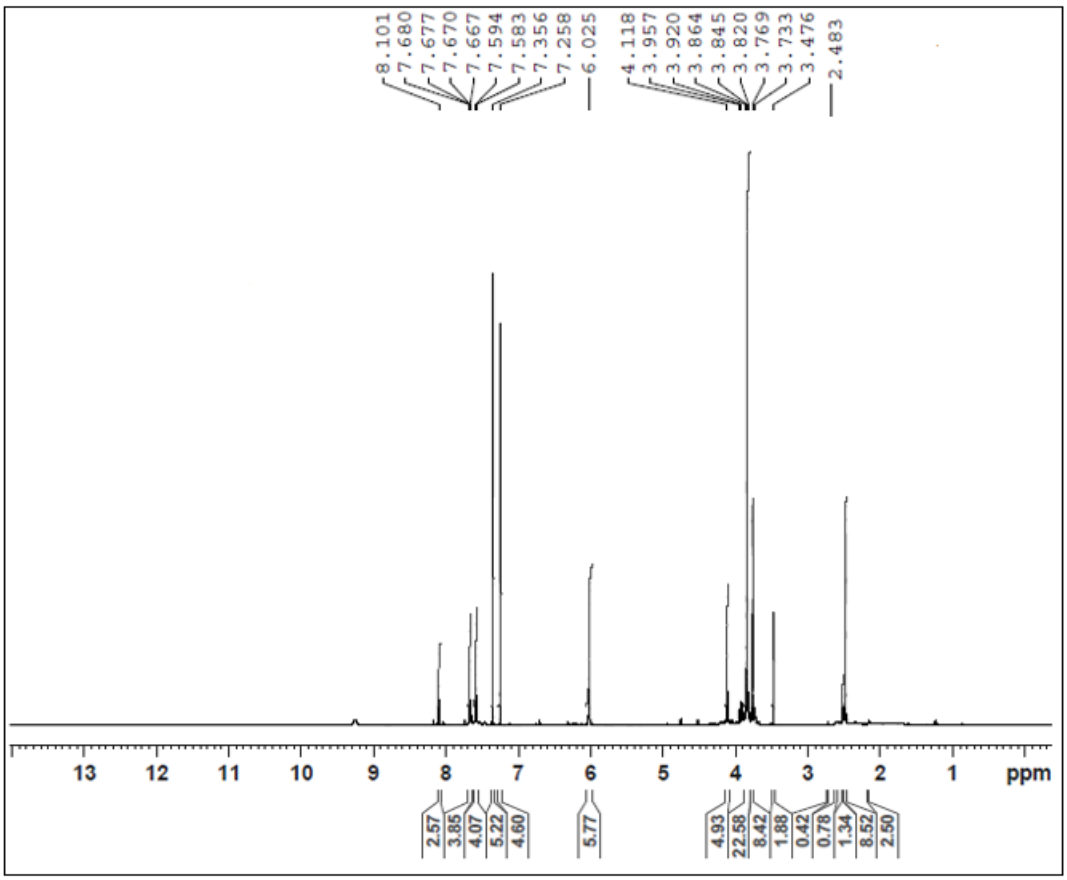
Expanded ^{13}C-NMR (213 MHz; $CDCl_3$) of compound 10



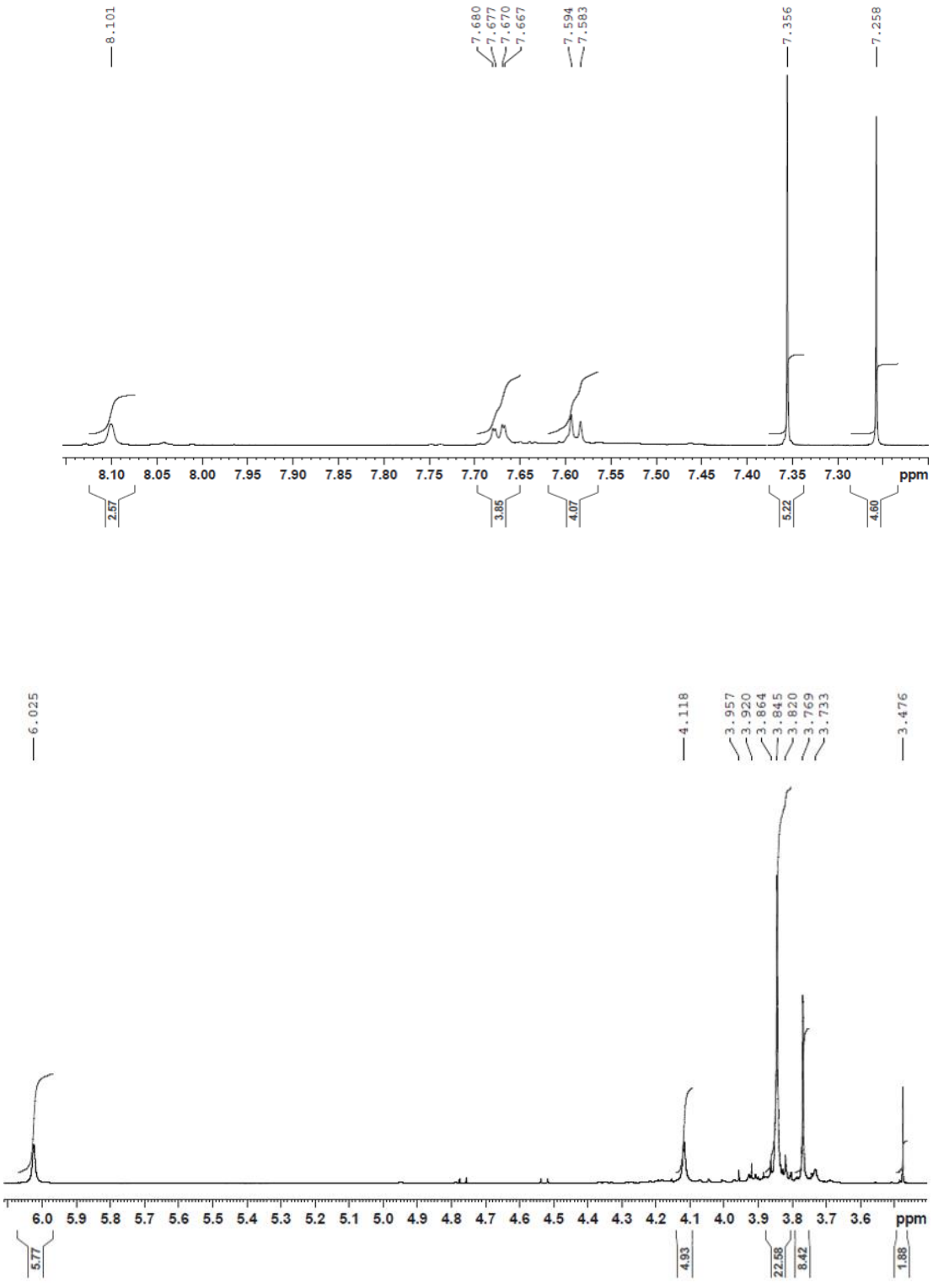
Compound 12



The ^{1}H-NMR (850 MHz; $CDCl_3$) of compound 12



Expanded ^{1}H-NMR (850 MHz; $CDCl_3$) of compound 12



The ^{13}C-NMR (213 MHz; $CDCl_3$) of compound 12