

**Title**

**Novel rhodanine-thiazole hybrids as potential antidiabetic agents: A structure-based drug design approach**

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### Spectral Data of Synthesized Derivatives (3a-3b):

**(Z)-4-((4-oxo-2-thioxothiazolidin-5-ylidene) methyl) benzaldehyde (3a):** Orange powder; yield: 90 %, m.p.: >300°C. FTIR (KBr, cm<sup>-1</sup>): 3018.73 (N-H), 2861.52 (C-H str of -CHO), 1724.44 (C=O), 1663.68 (C=C). <sup>1</sup>H NMR [400.MHz, δ ppm, DMSO-d<sub>6</sub>] δ: 7.65-7.77 (m, 3H, Ar-H), 7.99-8.09 (m, 2H, Ar-H), 10.11 (s, 1H, -CHO), 13.96 (s, 1H, -NH). **(Z)-2-(5-(4-formylbenzylidene)-4-oxo-2-thioxothiazolidin-3-yl) acetic acid (3b):** Yellow solid powder, yield: 86%, m.p.: >300°C. FTIR (KBR, cm<sup>-1</sup>): 3029.34 (-OH str of -COOH), 3010.05 (N-H), 2848.98 (C-H str of -CHO), 1603.88 (C=O), 1508.40 (C=C). <sup>1</sup>H NMR [400 MHz, δ ppm, DMSO-d<sub>6</sub>] δ: 4.68 (s,2H, -CH<sub>2</sub>), 7.80-7.84 (m, 3H, Ar-H), 7.92-8.01 (m, 2H, Ar-H), 8.03 (s, 1H, -OH),10.03 (s, 1H, -CHO).

### Spectral Data of Synthesized Analogs (6a-6f):

**2-hydrazinyl-4-phenylthiazole (6a):** These analogs were synthesized by general procedure, Orange solid powder; yield: 86 %, m.p.: 168-170°C. FTIR (KBr, cm<sup>-1</sup>): 3337.96 (N-H), 1633.78 (C=O), 1549.87 (C=C). **2-hydrazinyl-4-(p-tolyl) thiazole (6b):** Orange solid powder; yield: 88 %, m.p.: 168-170°C. FTIR (KBr, cm<sup>-1</sup>): 3354.35 (N-H), 1639.56 (C=O), 1552.62 (C=C). **4-(4-fluorophenyl)-2-hydrazinylthiazole (6c):** Dark purple solid powder; yield: 82 %, m.p.: 175-177°C. FTIR (KBr, cm<sup>-1</sup>): 3186.54 (N-H), 1600.02 (C=O), 1558.55 (C=C). **2-hydrazinyl-4-(4-methoxyphenyl) thiazole (6d):** Brown solid powder; yield: 93 %, m.p.: 169-171°C. FTIR (KBr, cm<sup>-1</sup>): 3472.02 (N-H), 2841.27(-OCH<sub>3</sub>), 1630.88 (C=O), 1558.56 (C=C). **4-(4-chlorophenyl)-2-hydrazinylthiazole (6e):** Red solid powder; yield: 86 %, m.p.: 178-180°C. FTIR (KBr, cm<sup>-1</sup>): 3407.40 (N-H), 1537.33 (C=O), 1523.83 (C=C). **4-(4-bromophenyl)-2-hydrazinylthiazole (6f):** Brown solid powder; yield: 91 %, m.p.: 168-170°C. FTIR (KBr, cm<sup>-1</sup>): 3400.65 (N-H), 1608 (C=O), 1545.05 (C=C).

table. S1: Toxicity results on normal mouse fibroblast L929 cell lines.

Comp	Percent survival L929 cell lines	
	125 ug/ml	250 ug/ml
7a	89.38	83.53
7b	88.37	82.09
7c	82.22	78.17
7d	76.31	77.84
7e	91.25	85.22
7f	90.17	84.12
7g	88.85	82.42
7h	86.24	80.08
7i	81.89	76.12
7j	87.07	81.84
7k	86.01	80.18
7l	89.26	83.19

table. S2: Enrichment analysis of modulated proteins by the compounds 7a-7l.

Pathway (KEGG ID)	OGC/BGC	Strength	FDR	Proteins
MAPK signaling pathway (hsa04010)	0.0594	1.24	5.17E-14	MAPK1,MAPK14,FLT3,PDGFRB,KDR,EGFR, KIT,DUSP16,INSR,CASP3,MET,PLA2G4A,GRB2,MAPK8,FGFR1,TNF,FGFR2
Insulin resistance (hsa04931)	0.1038	1.48	1.26E-11	PYGM,PYGL,CPT1A,INSR,GYS1,PRKCD,MT

PPAR signaling pathway (hsa03320)	0.0430	1.1	4.35E-11	OR,PTPN1,MAPK8,PPARA,TNF,GLUT MAPK1,FLT3,PDGFRB,KDR,EGFR,KIT,INSR, GLUT,MET,GYS1,HSP90AA1,PTK2,MTOR,C PT1A,PPARG,PPARA
Insulin signaling pathway (hsa04910)	0.0758	1.35	1.42E-09	PYGM,MAPK1,PYGL,GCK,INSR,GYS1,MTOR, PTPN1, AMY2A, GAA
Starch and sucrose metabolism (hsa00500)	0.1250	1.57	2.20E-09	MAPK1, AMY2A, GAA, SERPINE1,CASP3,PRKCD,SELE,MAPK8,TNF ,GLUT
Type II diabetes mellitus (hsa04930)	0.1556	1.66	1.06E-08	MAPK1,AMY2A, GCK,INSR,PRKCD,MTOR,MAPK8,TNF, GAA
Glycogen metabolism (hsa04922)	0.0700	1.31	8.93E-07	PYGM,PYGL,GCK,GAA, CPT1A,GYS1,PPARA, , AMY2A
Adipocytokine signaling pathway (hsa04920)	0.0735	1.33	3.25E-05	CPT1A,MTOR,MAPK8,PPARA,TNF
FoxO signaling pathway (hsa04068)	0.0476	1.15	3.59E-05	MAPK1,MAPK14,EGFR,INSR,GRB2,MAPK8
AGE-RAGE signaling pathway in diabetic complications (hsa04933)	0.0938	1.44	3.86E-05	PYGM,PYGL,GCK,GYS1
AMPK signaling pathway (hsa04152)	0.0417	1.09	0.00027	CPT1A,PPARG,INSR,GYS1,MTOR
mTOR signaling pathway (hsa04150)	0.0333	0.99	0.00071	MAPK1,INSR,MTOR,GRB2,TNF
JAK-STAT signaling pathway (hsa04630)	0.0253	0.87	0.0068	PDGFRB,EGFR,MTOR,GRB2
PI3K-Akt signaling pathway (hsa04151)	0.0400	1.07	0.0071	GRB2,FGFR1,FGFR2
Insulin secretion (hsa04911)	0.0366	1.03	0.009	GCK,CCKAR,GLP1R
Pancreatic secretion (hsa04972)	0.0309	0.96	0.0131	CA2,CCKAR,PLA2G2A
Glycolysis / Gluconeogenesis (hsa00010)	0.0313	0.96	0.0489	GAA, GCK,LDHA, , AMY2A

Were, OGC: Observed gene count, BGC: Background gene count, FDR: False discovery rate

**table. S3: Binding affinity and interactions of compounds (7a-7l) in  $\alpha$ -amylase binding pocket (PDB ID: 4W93) using Glide module of Schrodinger's.**

Compounds	Docking Score (XP)	Glide Energy (Kcal/mol)	Amino Acids
<b>7a</b>	-4.82	-45.98	<b>ASP197, TRP58, TYR62</b>
<b>7b</b>	-6.15	-52.49	<b>HIE201, ASP197, HIE299, TYR151</b>
<b>7c</b>	-6.13	-53.42	<b>HIE201, ASP197, HIE299, TYR151</b>
<b>7d</b>	-5.76	-53.56	<b>HIE201, TYR151, ASP197, HIE299</b>
<b>7e</b>	<b>-6.21</b>	-52.90	<b>HIE201, ASP197, HIE299, TYR151</b>
<b>7f</b>	<b>-6.25</b>	-51.53	<b>HIE201, ASP197, HIE299, TYR151</b>
<b>7g</b>	-6.02	-52.80	<b>HIE201, LYS200, TRP59, TYR151</b>

7h	-6.22	-58.47	<i>HIE201, LYS200, ASP197, HIE299, TYR151</i>
7i	-5.73	-55.24	<i>ASP356, ARG195, ASP197, HIE201, TYR15</i>
7j	-5.02	-50.79	<i>GLU233, ARG195, ASP356</i>
7k	-5.81	-49.26	<i>ASP197, ARG195, ASP356</i>
7l	-5.45	-55.17	<i>ASP197, ARG195, HIE201, TYR151, ASP356</i>
Acarbose	-10.15	-63.80	<i>ARG195, ASP197, LYS200, HIE201, GLU240, TYR151, ILE235, GLU233, HIE299</i>

table. S4: Binding affinity and interactions of compounds (7a-l) in  $\alpha$ -glucosidase binding pocket (PDB ID: 3A47) using Glide module of Schrodinger's.

Compounds	Docking Score (XP)	Glide Energy (Kcal/mol)	Amino Acids
7a	-5.21	-58.93	<i>HIE239, LYS155, PHE157, ASH214</i>
7b	-4.28	-56.99	<i>GLU276, HIE279, HIE239, HIS245</i>
7c	-4.76	-62.21	<i>GLU276, ASH214, HIE279, HIS245, HIE239, ASN241</i>
7d	-5.27	-47.02	<i>HIE239, PHE157, LYS155</i>
7e	-5.73	-55.21	<i>HIE239, LYS155, PHE157, ASH214</i>
7f	-5.83	-50.71	<i>HIE239, PHE157, LYS155, ASH214</i>
7g	<b>-6.35</b>	-54.17	<i>HIE239, PHE157, GLU304, GLY306, PRO317</i>
7h	-5.56	-58.04	<i>GLN350, GLU276, HIE279, PRO309,</i>
7i	-5.83	-50.71	<i>HIE239, PHE157</i>
7j	-4.71	-57.09	<i>ARG439, PHE157, HIE239, ASN241, ASN246</i>
7k	<b>-6.45</b>	-54.29	<i>HIE239, PHE157, GLU304, GLY306, PRO317</i>
7l	-4.954	-54.75	<i>ARG439, PHE157, HIE239, ASN241</i>
Acarbose	-9.83	-58.14	<i>GLU304, PHE157, ASP408, HIE239</i>

table. S5: Binding affinity and interactions of compounds (7a-l) in PPAR- $\gamma$  binding pocket (PDB ID: 5Y2O) using Glide module of Schrodinger's.

Compounds	Docking Score (XP)	Glide Energy (Kcal/mol)	Amino Acids
7a	-8.02	-57.40	<i>HIE323, SER289, TYR473</i>
7b	-7.6	-52.75	<i>CYS285, ARG288</i>
7c	-7.17	-55.67	<i>CYS285, ARG288</i>
7d	-7.17	-52.53	<i>TYR327, CYS285</i>

<b>7e</b>	<b>-8.23</b>	-60.74	<b>HIE323, SER289, TYR473, GLU259</b>
<b>7f</b>	<b>-8.65</b>	-55.22	<b>HIE323, SER289, TYR473, GLU259</b>
<b>7g</b>	-7.3	-50.39	TYR327, HIE449
<b>7h</b>	-7.17	-56.71	CYS285, ARG288
<b>7i</b>	-7.6	-52.75	CYS285
<b>7j</b>	-7.12	-54.88	TYR327
<b>7l</b>	-6.94	-55.07	TYR327
<b>7k</b>	-7.12	-55.77	TYR327, CYS285
<b>Pioglitazone</b>	<b>-10.57</b>	<b>-59.11</b>	<b>HIE323, SER289, TYR473</b>

table. S6: MM/GBSA Calculation of synthesized compounds (7a-l).

Comp	Prime Energy Kcal/mol	Complex Energy Kcal/mol	MMGBSA dG Bind Kcal/mol	MMGBSA dG Bind Hbond Kcal/mol	MMGBSA dG Bind vdW Kcal/mol
<b><math>\alpha</math>-amylase binding pocket (PDB ID: 4W93)</b>					
<b>7a</b>	-20694.2	-20694.1	-42.9	-1.24	-48.7
<b>7b</b>	-20705.9	-20705.8	-53.0	-1.46	-47.7
<b>7c</b>	-20703.1	-20703.0	-51.5	-1.44	-48.24
<b>7d</b>	-20709.7	-20709.7	-51.4	-1.46	-48.5
<b>7e</b>	-20705.3	-20705.3	-61.2	-1.45	-47.6
<b>7f</b>	-20705.0	-20704.9	-61.7	-1.45	-46.24
<b>7g</b>	-20710.1	-20710.1	-50.8	-1.74	-52.6
<b>7h</b>	-20732.5	-20732.4	-59.1	-2.91	-52.94
<b>7i</b>	-20723.7	-20723.7	-50.0	-2.30	-57.9
<b>7j</b>	-20735.4	-20735.3	-48.4	-0.09	-54.1
<b>7k</b>	-20720.6	-20720.6	-48.1	-1.40	-52.4
<b>7l</b>	-20720.6	-20720.5	-41.2	-1.26	-55.1
<b><math>\alpha</math>-glucosidase binding pocket (PDB ID: 3A47)</b>					
<b>7a</b>	-24384.2	-24384.2	-44.2	-1.63	-55.1
<b>7b</b>	-24374.8	-24374.8	-40.1	-1.16	-59.4
<b>7c</b>	-24390.0	-24389.9	-39.2	-1.46	-58.9
<b>7d</b>	-24398.8	-24398.7	-48.2	-1.64	-53.8

<b>7e</b>	-24388.2	-24388.2	-57.9	-1.52	-50.9
<b>7f</b>	-24383.1	-24383.1	-58.0	-1.0	-56.8
<b>7g</b>	-24406.4	-24406.4	-62.1	-1.85	-51.2
<b>7h</b>	-24405.1	-24405.0	-33.3	-1.94	-60.0
<b>7i</b>	-24392.1	-24392.6	-46.1	-1.38	-62.1
<b>7j</b>	-24407.2	-24407.2	-42.1	-1.44	-55.6
<b>7k</b>	-24403.3	-24403.3	-42.9	-0.80	-55.8
<b>7l</b>	-24413.7	-24413.7	-63.2	-1.86	-50.9

**PPAR- $\gamma$  binding pocket (PDB ID: 5Y2O)**

<b>7a</b>	-10934.5	-10934.5	-70.0	-0.94	-55.3
<b>7b</b>	-10922.1	-10922.1	-60.0	-0.001	-61.1
<b>7c</b>	-10891.3	-10891.3	-62.8	-1.8	-58.2
<b>7d</b>	-10913.8	-10913.8	-69.2	-0.45	-62.1
<b>7e</b>	-10915.2	-10915.2	-69.6	-1.8	-57.1
<b>7f</b>	10905.2	10905.2	-70.7	-0.24	-63.9
<b>7g</b>	-10927.5	-10927.5	-60.9	0	-55.6
<b>7h</b>	-10880.3	-10880.3	-69.1	-0.001	-67.0
<b>7i</b>	-10919.3	-10919.3	-62.1	-0.004	-60.1
<b>7j</b>	-10911.17	-10911.17	-64.7	-0.77	-67.6
<b>7k</b>	-10936.6	-10936.6	-65.0	0	-61.7
<b>7l</b>	-10889.7	-10889.7	-64.9	-0.001	-62.8

**table. S7: Final Energy of Geometry optimized structures.**

<b>Compound</b>	<b>ESP mean (kcal/mol)</b>	<b>Gas Phase Energy (eV)</b>	<b>Final Energy</b>
<b>7a</b>	-42.41	-2259.39221	-2259.39221
<b>7b</b>	-42.6	-2298.673487	-2298.673487
<b>7c</b>	-40.29	-2358.58469	-2358.58469
<b>7d</b>	-42.92	-2373.878607	-2373.878607
<b>7g</b>	-43.52	-2487.283448	-2487.283448
<b>7h</b>	-41.35	-2526.555163	-2526.555163
<b>7i</b>	-41.92	-2586.515849	-2586.515849
<b>7j</b>	-43.06	-2601.812524	-2601.812524
<b>7k</b>	-40.88	-2371.6723	-2371.6723
<b>7l</b>	-39.8	-5060.56535	-5060.56535

**table. S8: Calculated quantum chemical parameters of synthesized compounds Molecular electrostatic Potential Surface.**

Quantum chemical parameters	7a	7b	7c	7d	7g	7h
$E_{\text{HOMO}}$ (eV)	-0.20284	-0.19976	-0.20404	-0.1935	-0.20191	-0.1994
$E_{\text{LUMO}}$ (eV)	-0.10954	-0.10893	-0.11062	-0.1086	-0.10699	-0.1067
$\Delta E_{\text{GAP}}$ (eV)	0.0933	0.09083	0.09342	0.0849	0.09491	0.0927
Hardness ( $\eta$ )	0.0466	0.04541	0.04671	0.0424	0.047458	0.04635
dipole moment ( $\mu$ )	-0.2576	-0.25422	-0.2593	-0.2478	-0.255	-0.2527
excitation binding energy ( $\omega$ )	0.001547	0.00147	0.00157	0.00130	0.001543	0.00148
Softness ( $\sigma$ )	21.46	22.02	21.40	23.58	21.08	21.57
Quantum chemical parameters	7i	7j	7k	7l		
$E_{\text{HOMO}}$ (eV)	-0.20333	-0.193729	-0.20667	-0.2054		
$E_{\text{LUMO}}$ (eV)	-0.10778	-0.109387	-0.10831	-0.10913		
$\Delta E_{\text{GAP}}$ (eV)	0.095556	0.084342	0.098362	0.0962		
Hardness ( $\eta$ )	0.04777	0.042171	0.049181	0.0481		
dipole moment ( $\mu$ )	-0.257	-0.248	-0.260	-0.259		
excitation binding energy ( $\omega$ )	0.001547	0.001296	0.001664	0.0016131		
Softness ( $\sigma$ )	20.92	23.71	20.33	20.79		

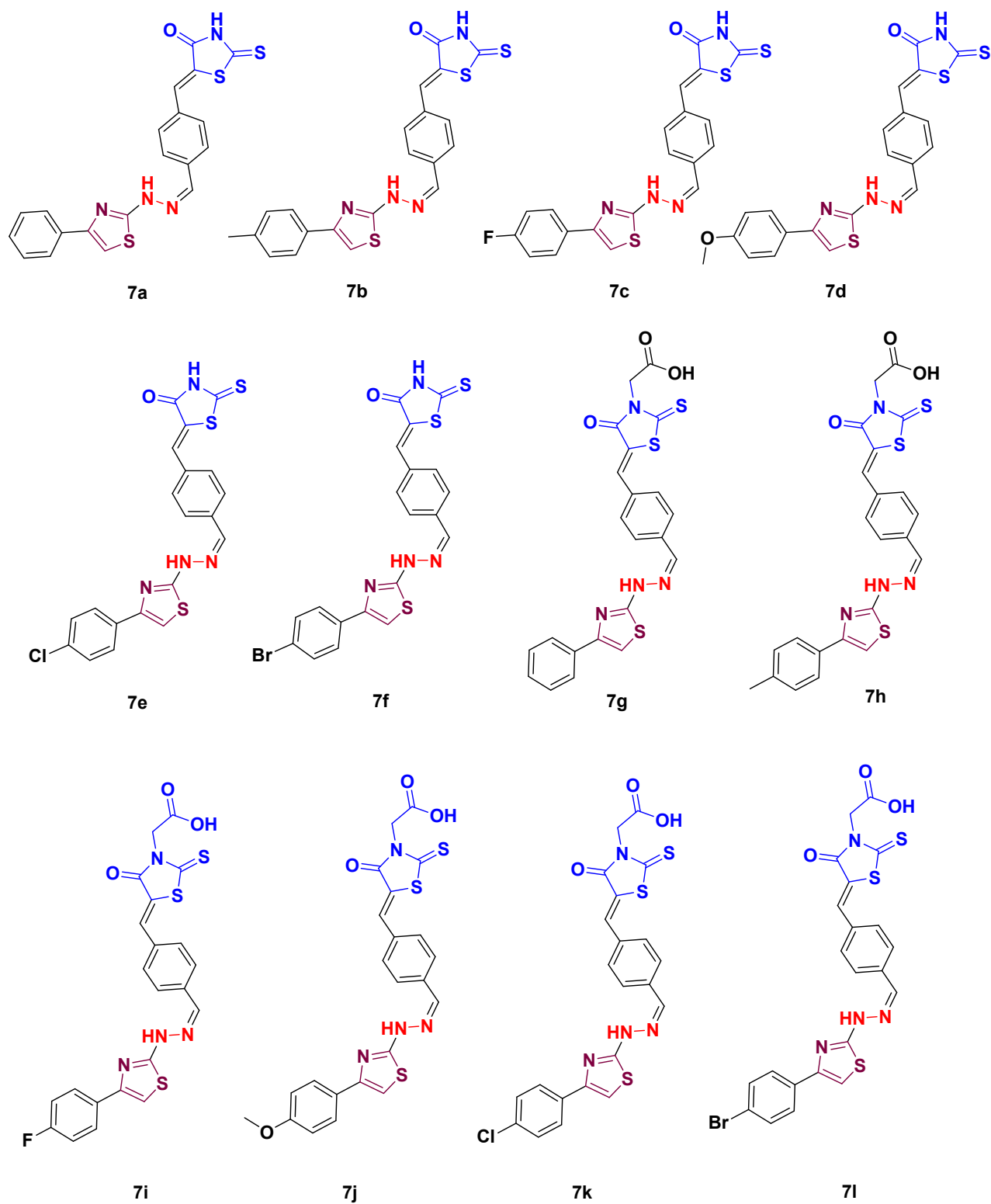
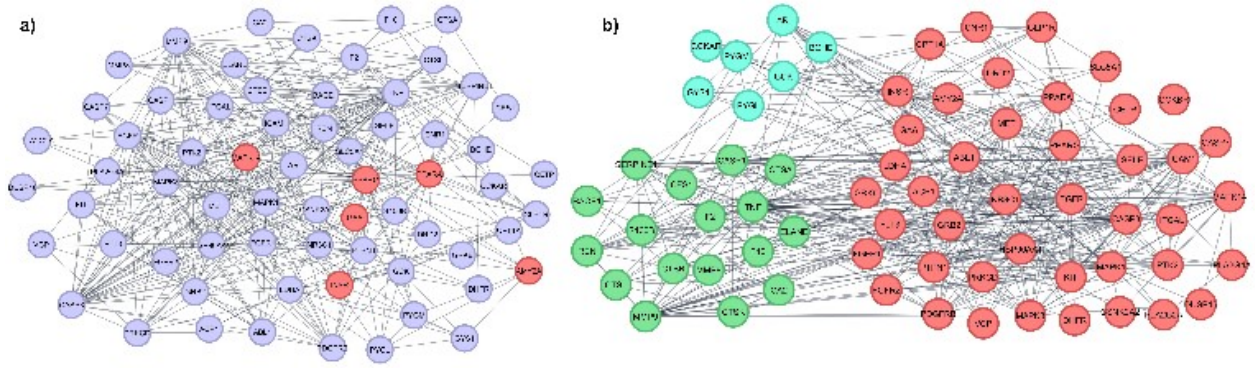
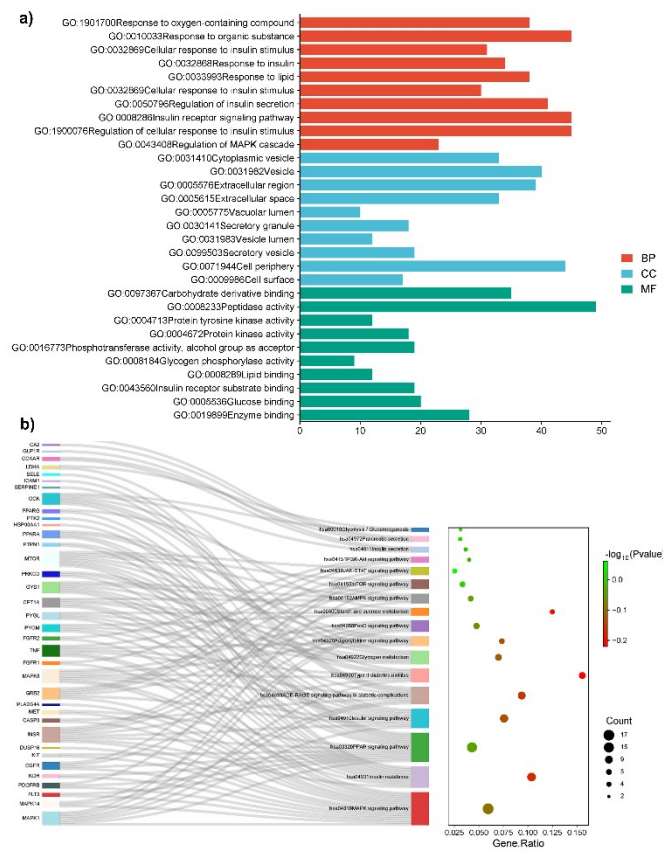


Figure S1. Chemical structures of synthesized compounds (7a-7l).





**Fig. S2:** (a) STRING identified Protein-protein interaction and (b) The cluster analysis where cluster 1: red; cluster 2: green; cluster 3: blue.



**Figure S3.** a) The Gene ontology for the top 10 modulated proteins by biological processes (orange), Molecular function (blue), and cellular components (green), b) Bubble plot represents KEGG enrichment pathways related to GeneCount.

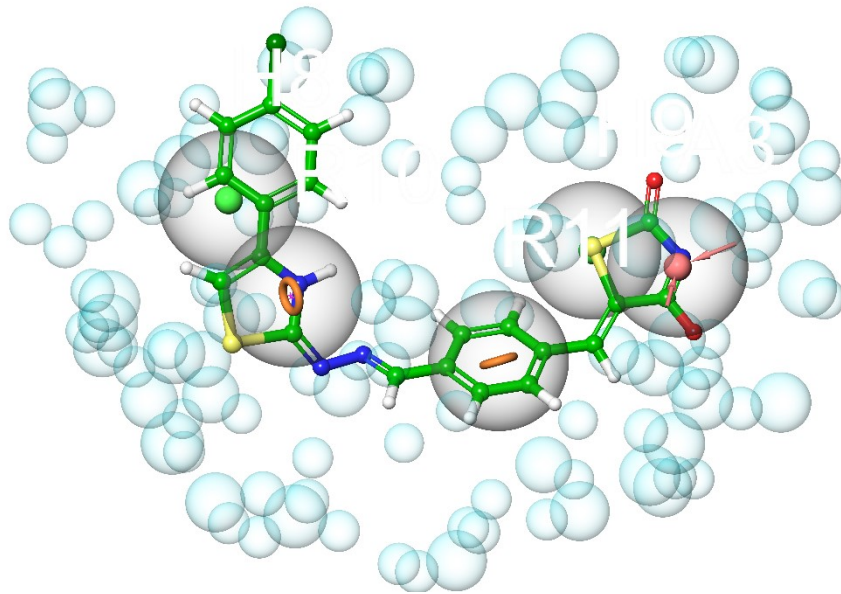
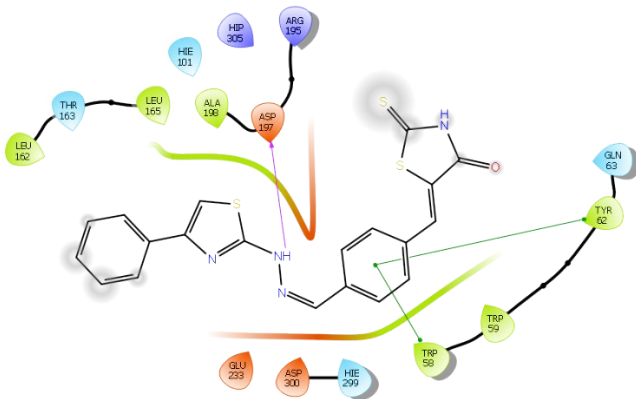
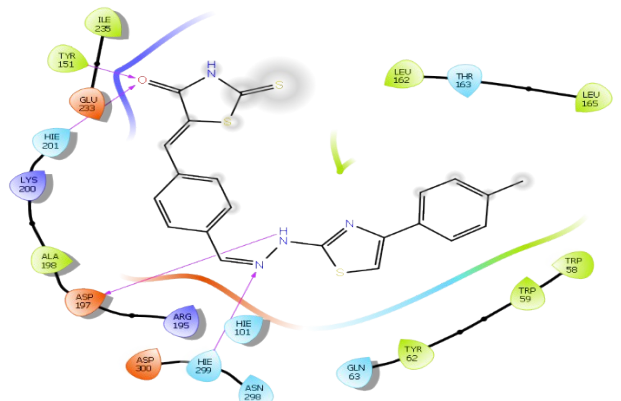


Figure S4. Designed compound 7e based on e-pharmacophore modelling

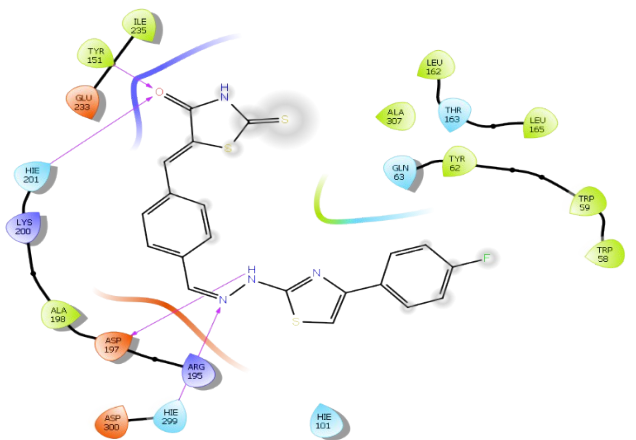
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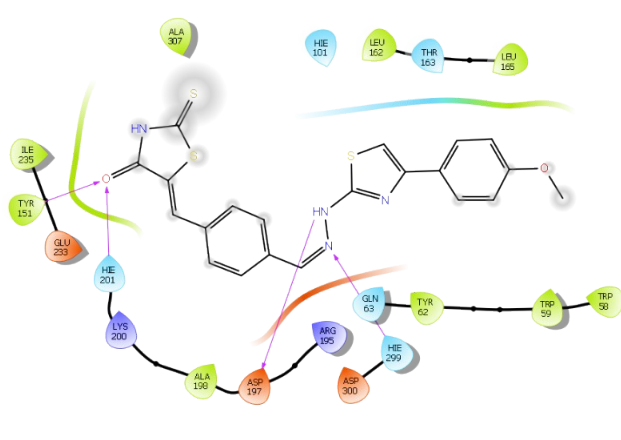
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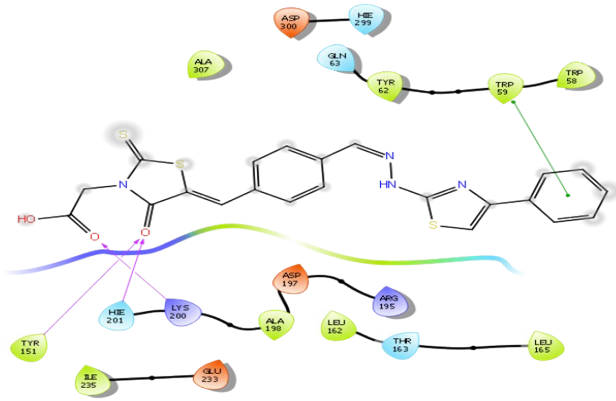
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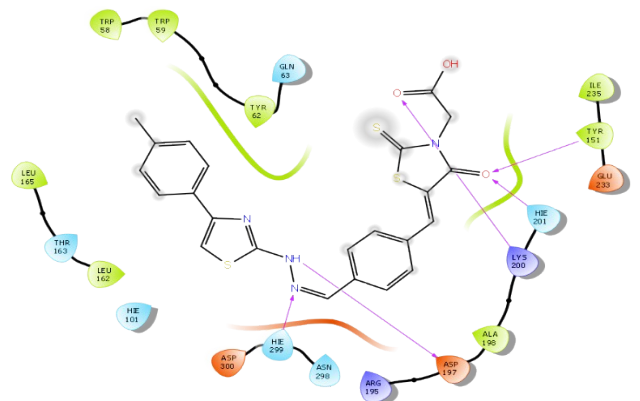
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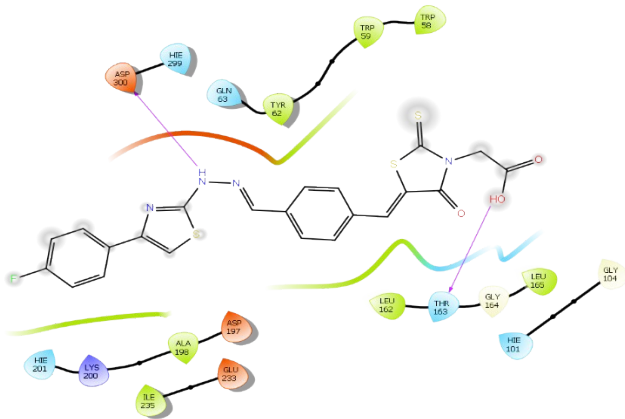
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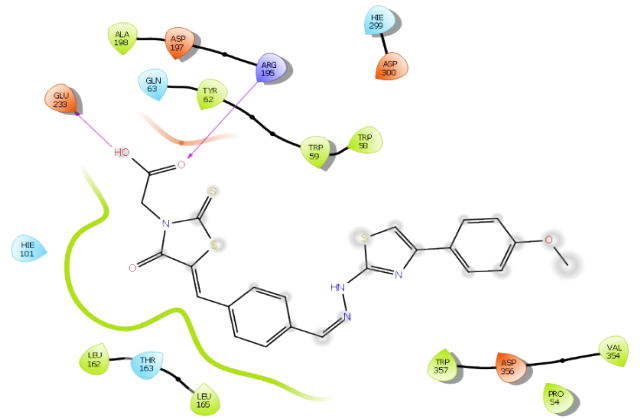
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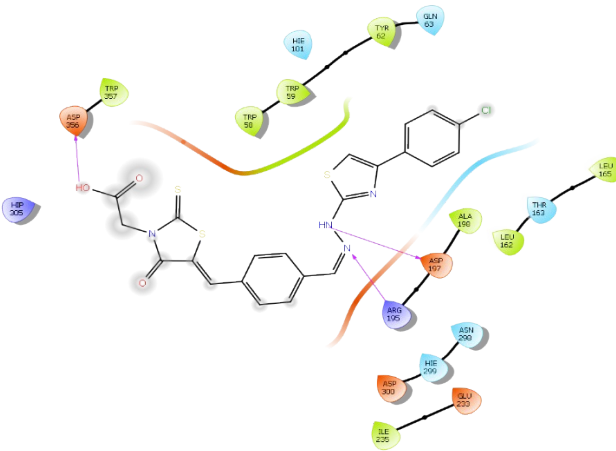
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7j



7k



7l

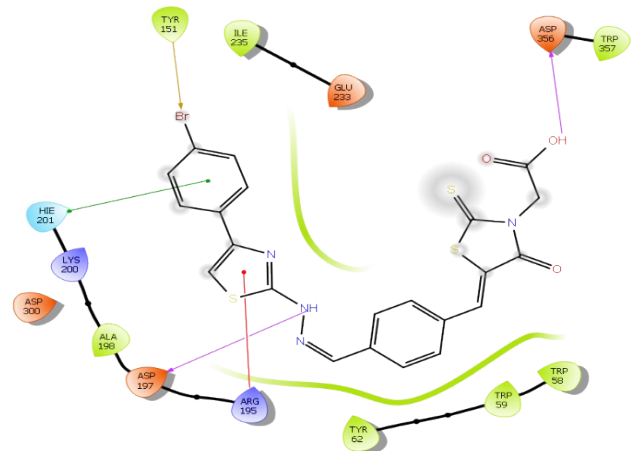
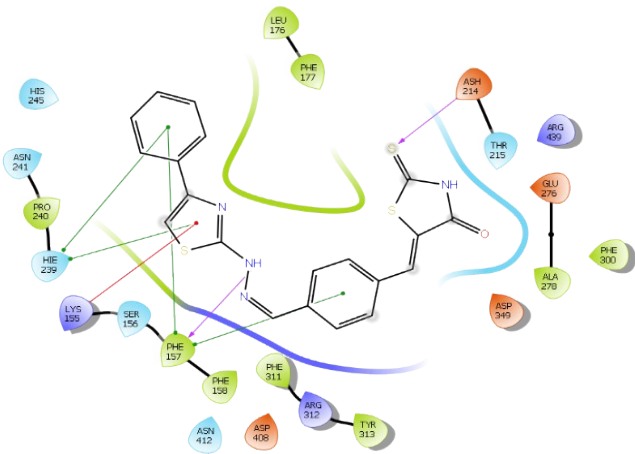
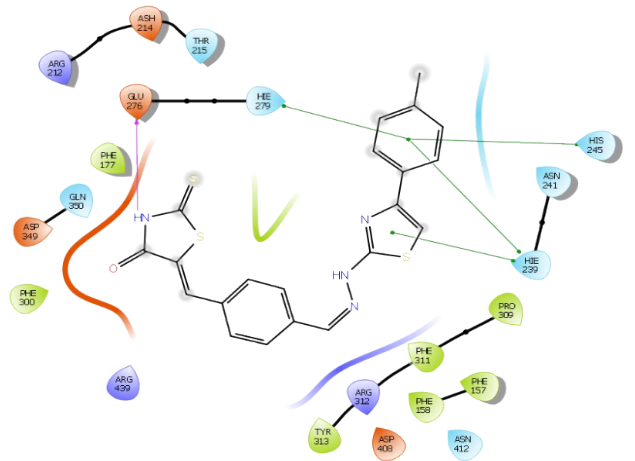
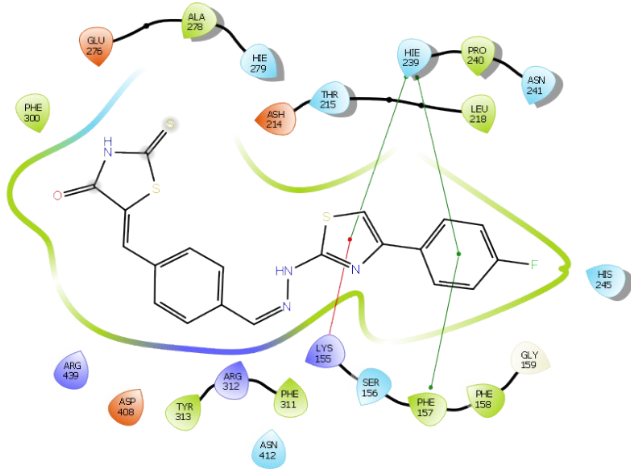
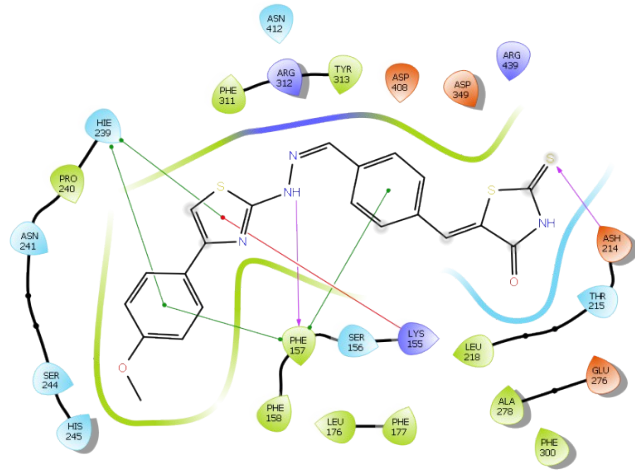
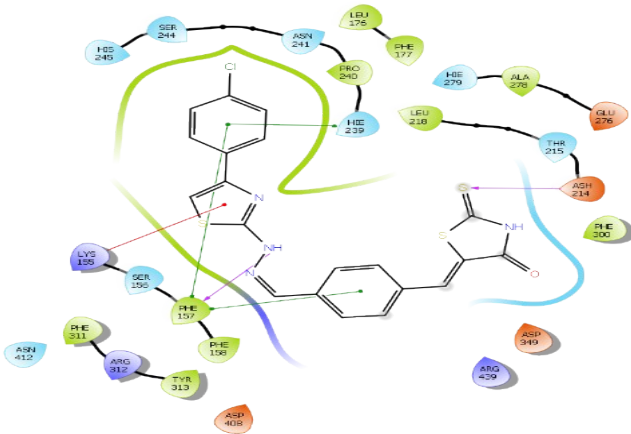
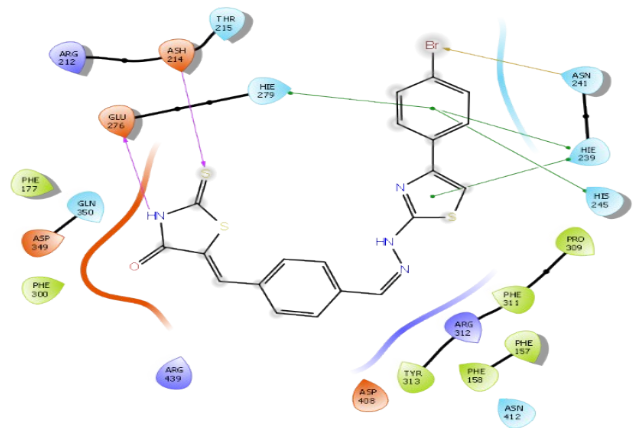
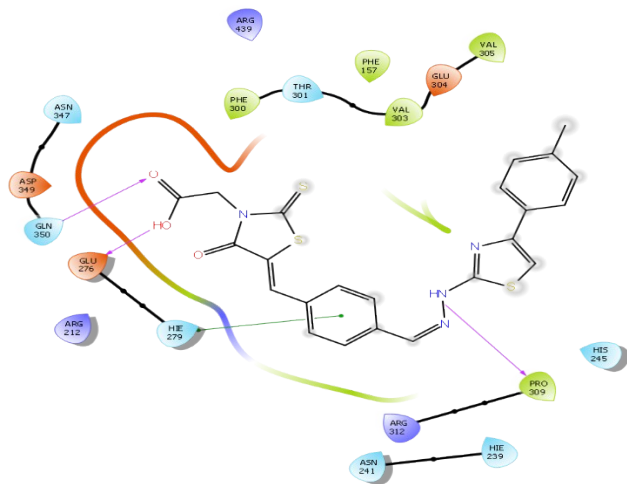


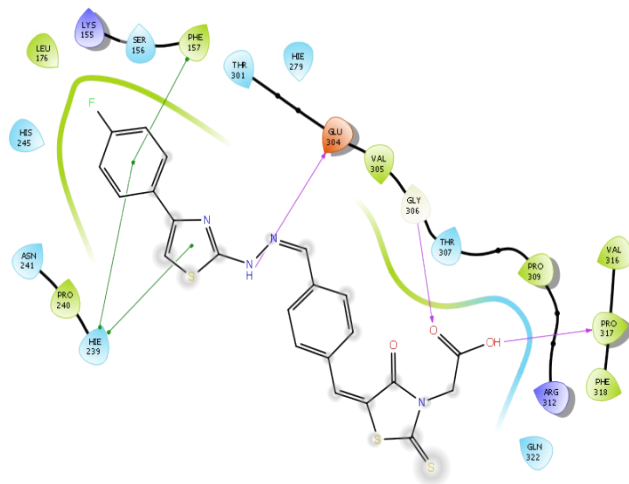
Figure S5: 2D binding orientation of synthesized derivatives in  $\alpha$ -amylase binding pocket (PDB ID: 4W93).

**7a****7b****7c****7d****7e****7f**

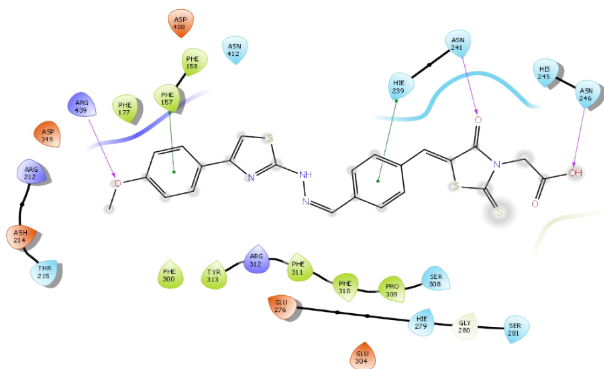
7h



7i



7j



7l

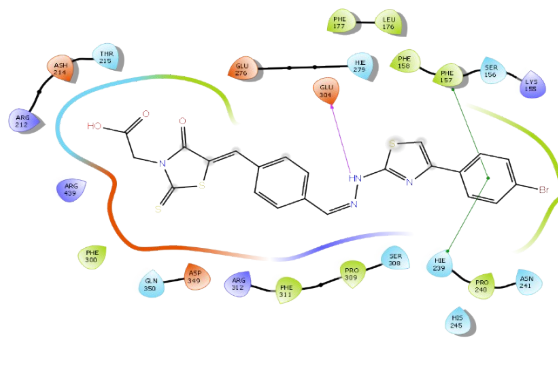
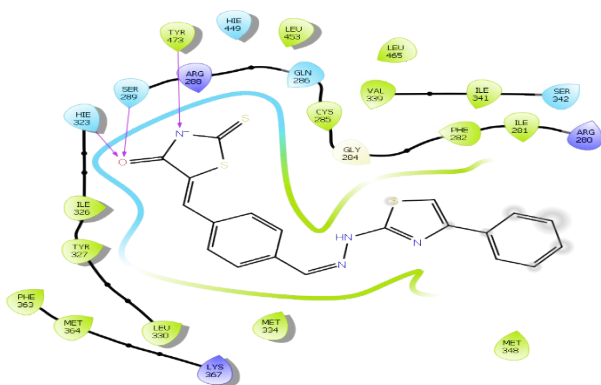
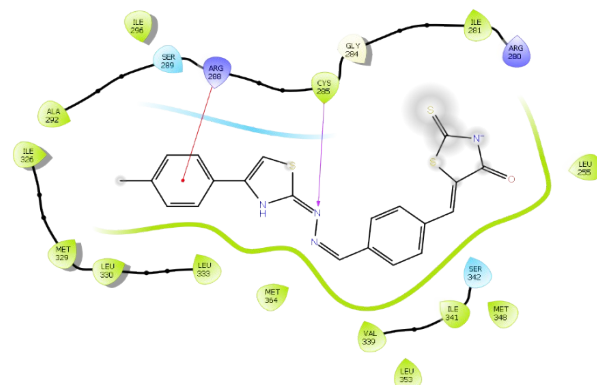


Figure S6: 2D binding orientation of synthesized derivatives in  $\alpha$ -glucosidase binding pocket (PDB ID: 3A47).

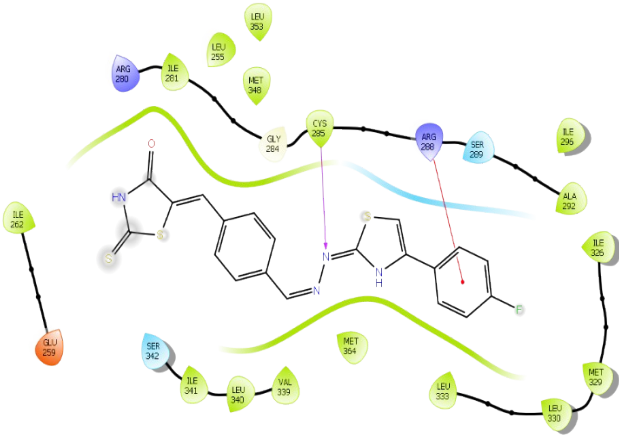
7a



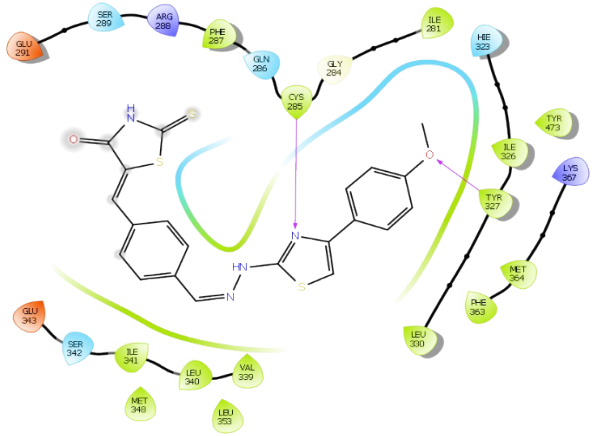
7b



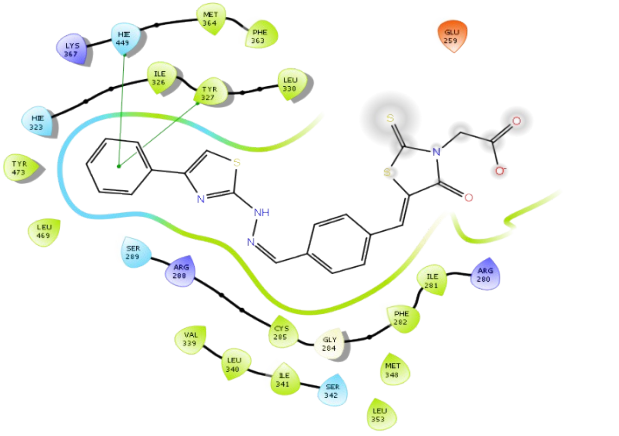
7c



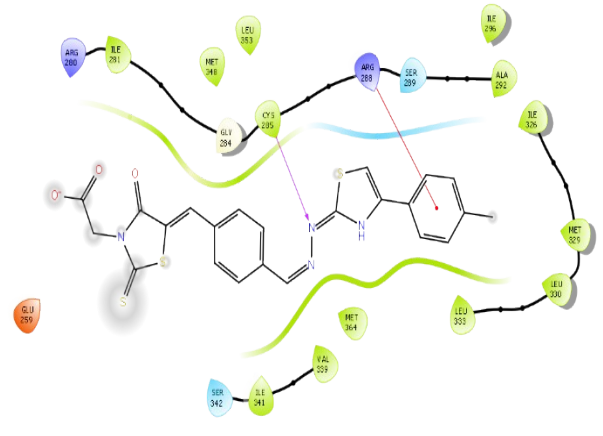
7d



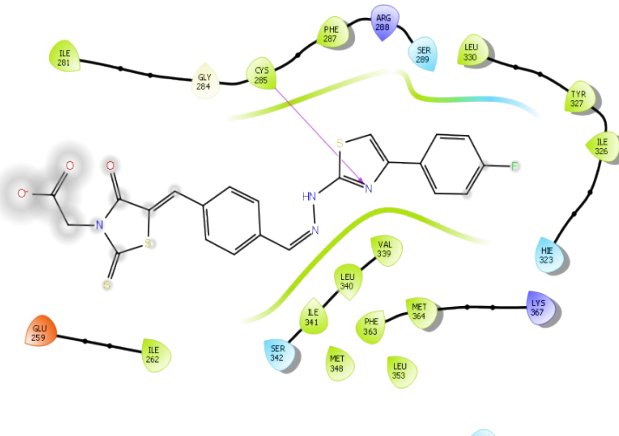
7g



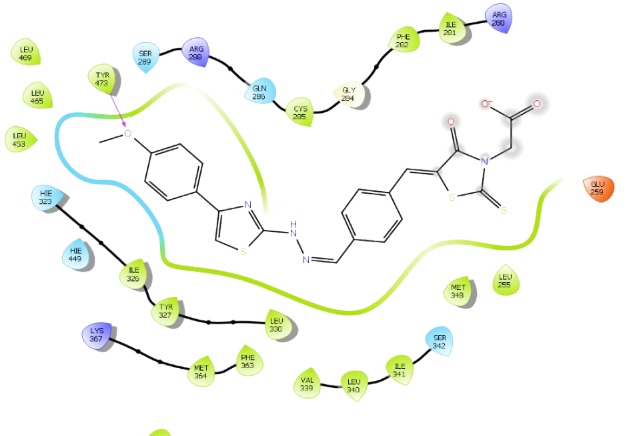
7h



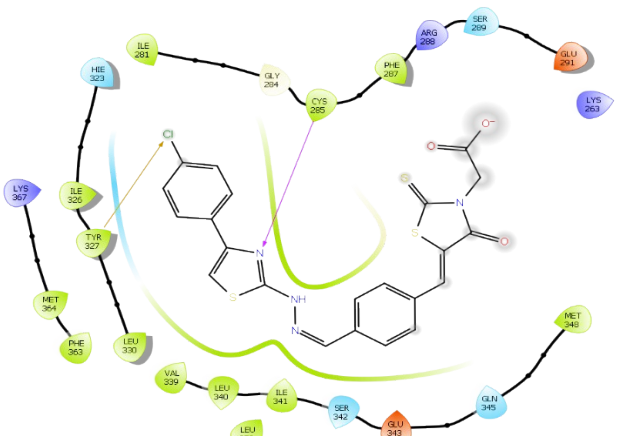
7i



7j



7k



7l

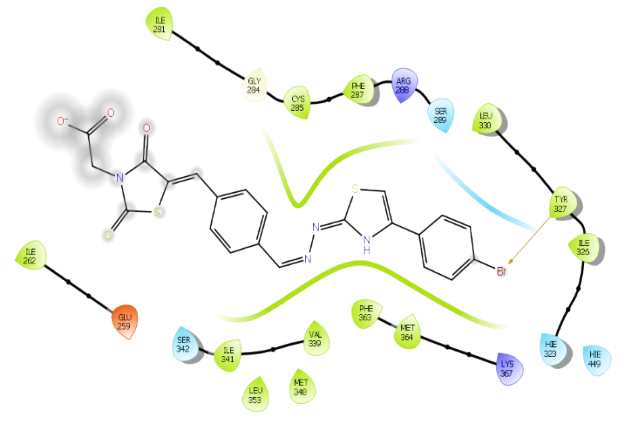


Figure S7: 2D binding orientation of synthesized derivatives in PPAR-gamma binding pocket (PDB ID: 5Y2O).

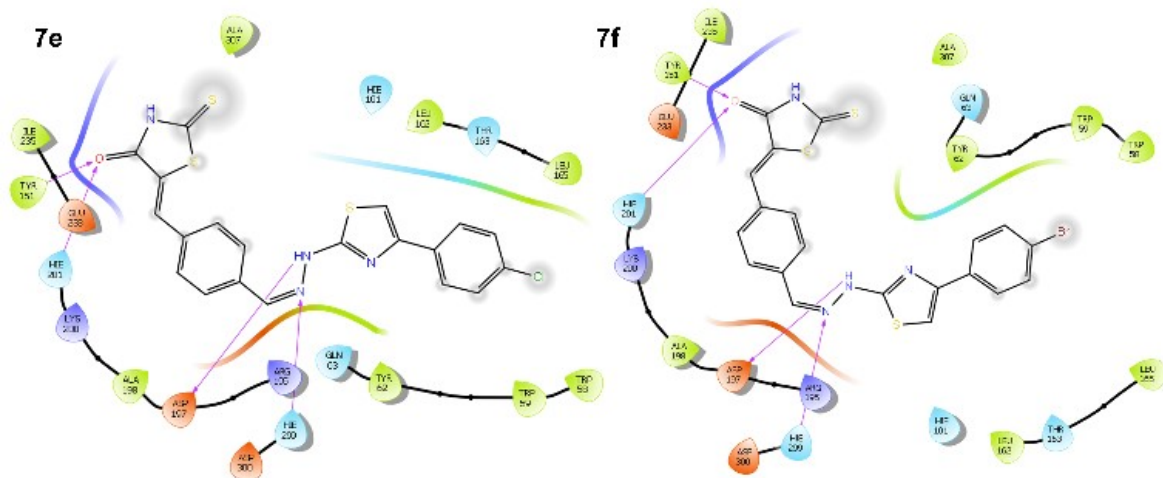


Fig. S8. 2D binding orientation of 7e and 7f in  $\alpha$ -amylase binding pocket (PDB ID: 4W93).

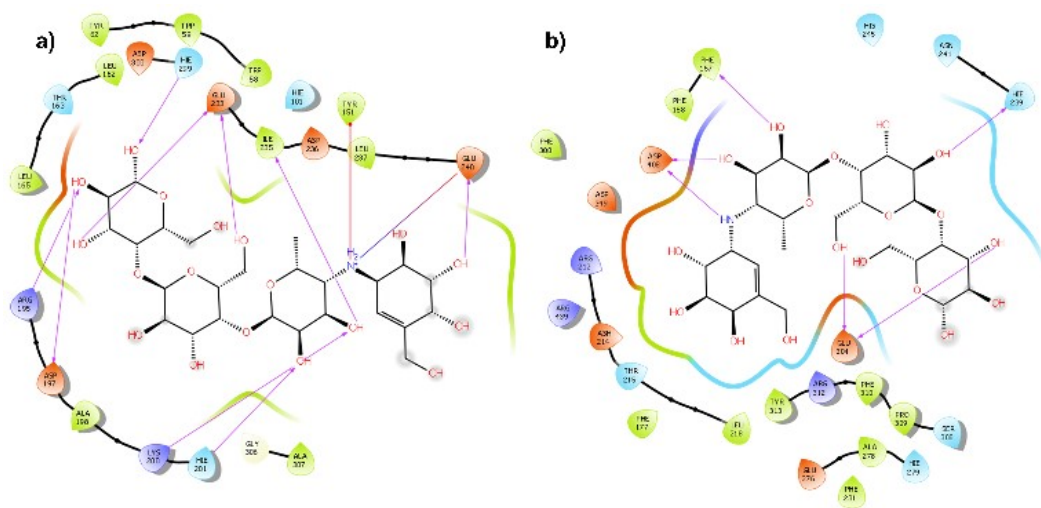


Fig. S9. 2D binding orientation of acarbose in a)  $\alpha$ -amylase, b)  $\alpha$ -glucosidase binding pocket.

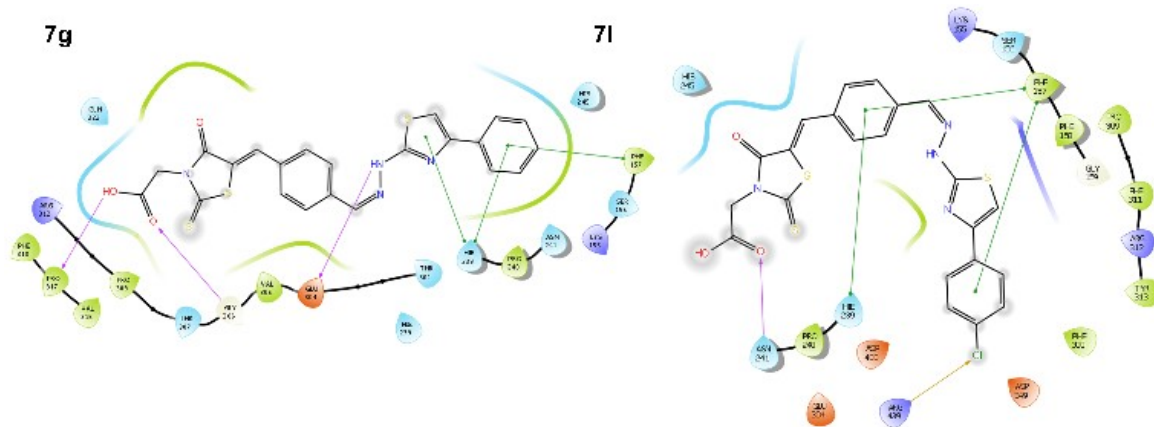


Fig. S10. 2D binding orientation of 7g and 7l in  $\alpha$ -glucosidase binding pocket (PDB ID: 3A47).

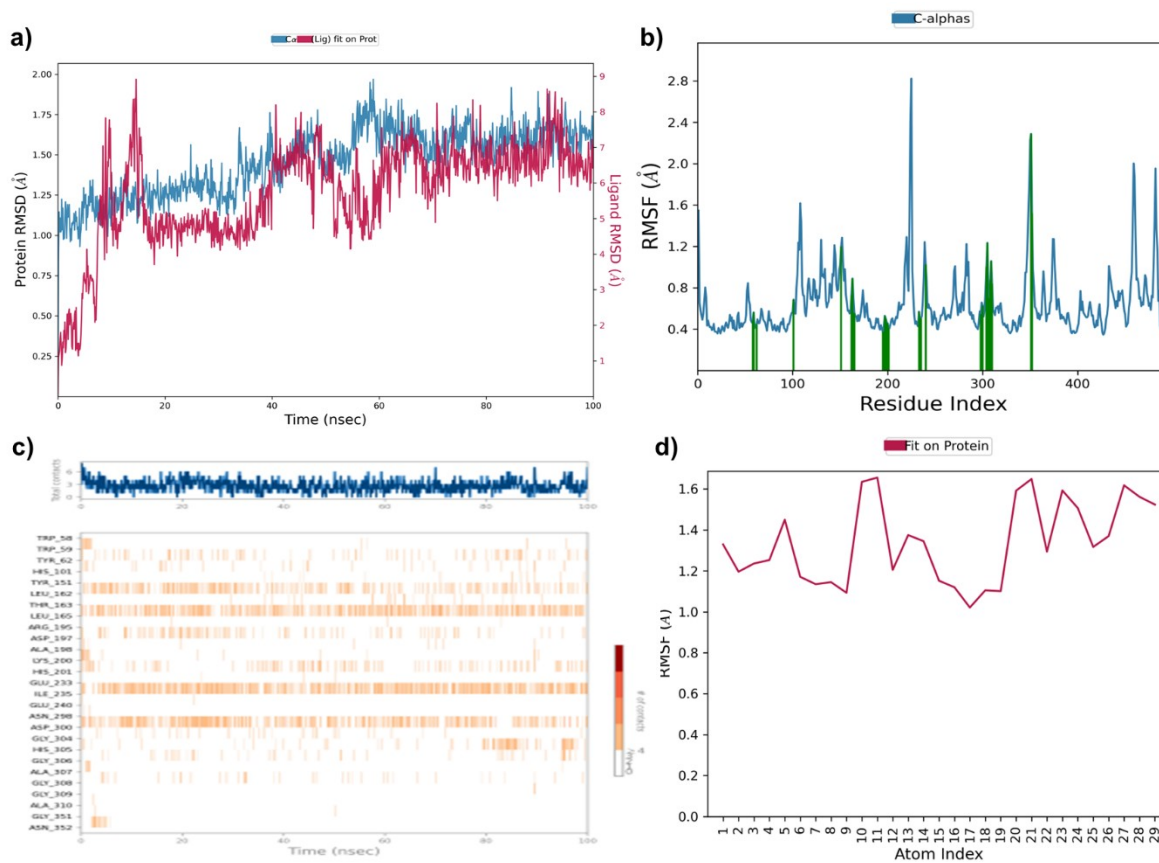
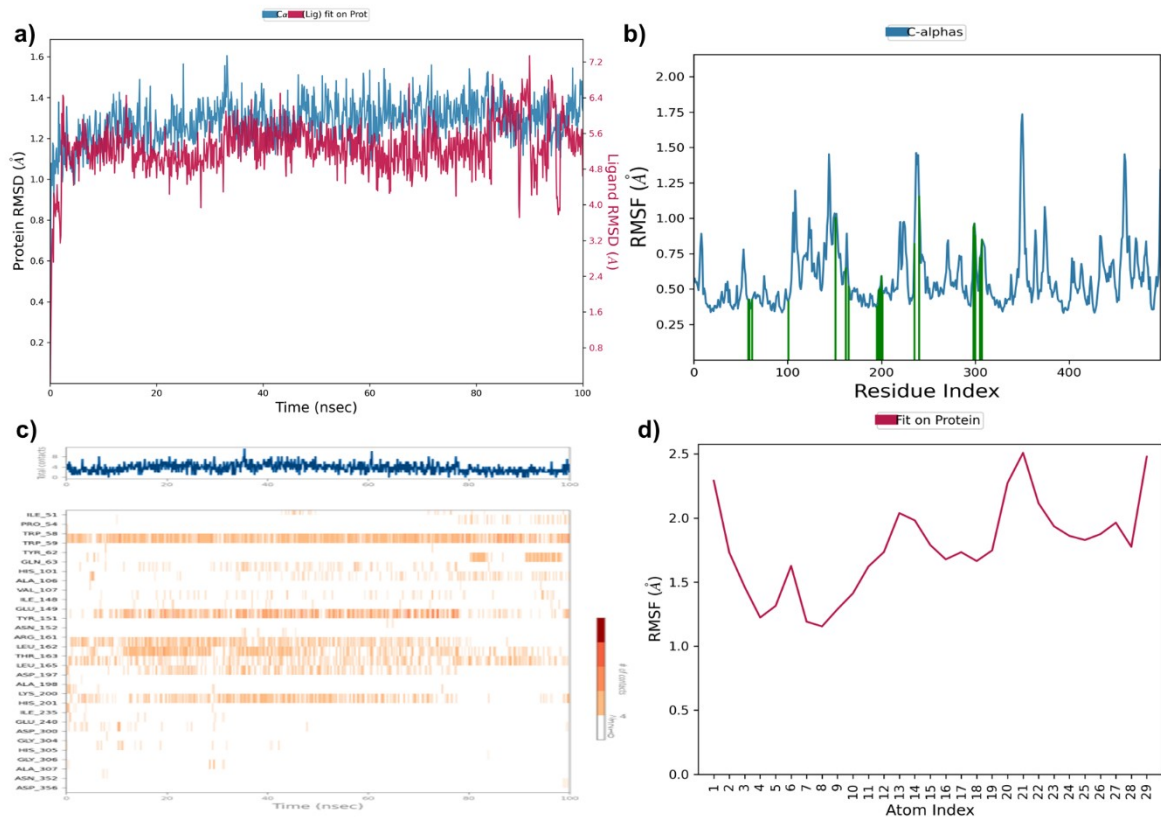


Figure S11. (a) Protein Ligand RMSD Plot of 7e, (b) Protein RMSF Plot, (c) Protein Ligand Contacts timeline, (d) Ligand RMSF plot over period of 100 ns within  $\alpha$ -amylase protein





**Figure S12. (a) Protein Ligand RMSD Plot of 7f, (b) Protein RMSF Plot, (c) Protein Ligand Contacts timeline, (d) Ligand RMSF plot over period of 100 ns within  $\alpha$ -amylase protein**

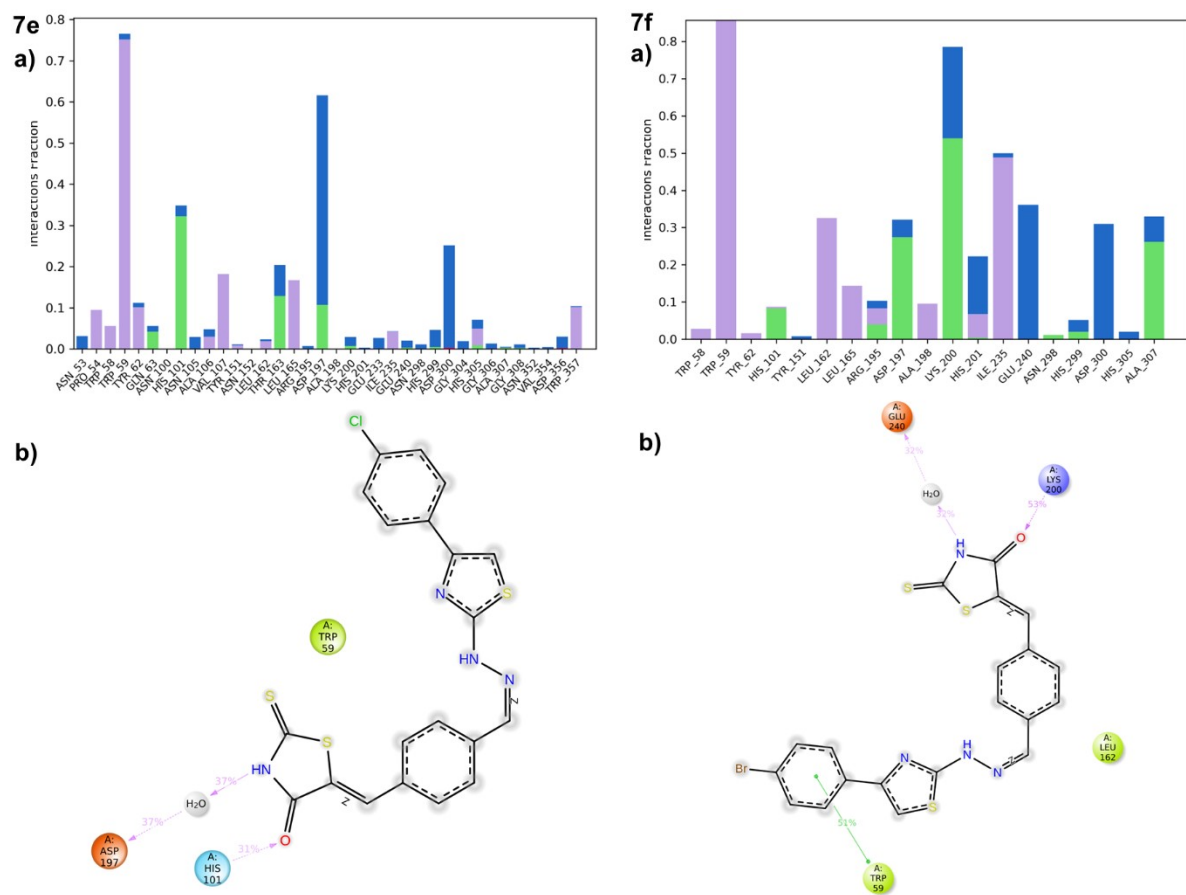
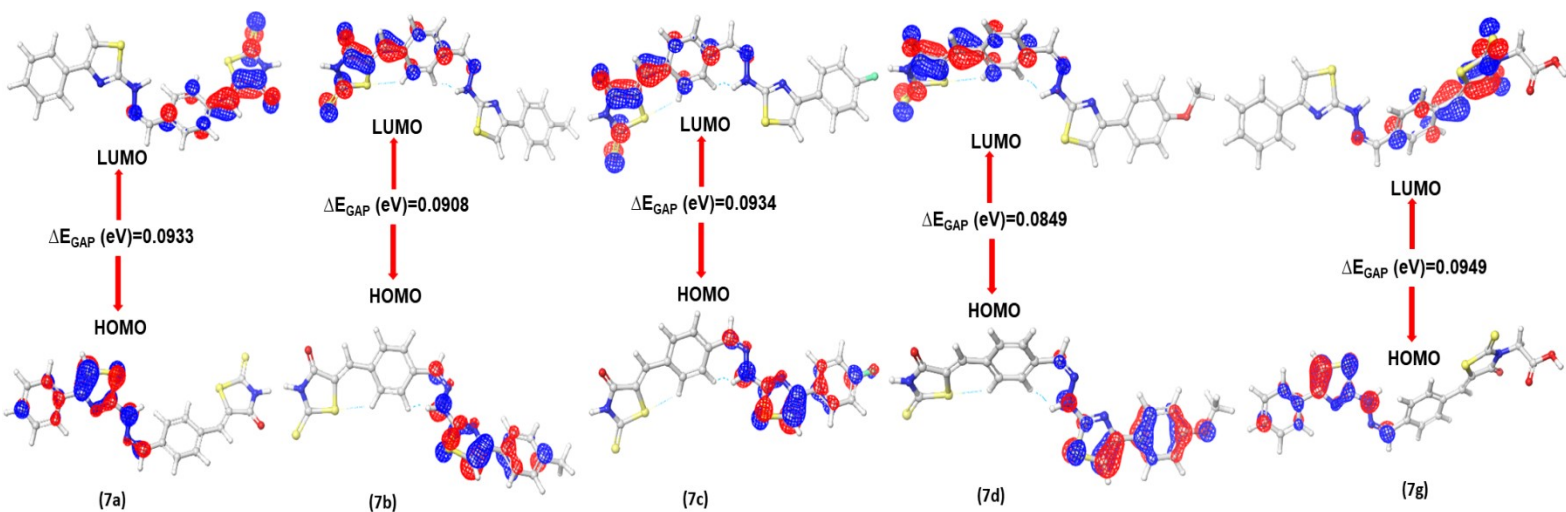


Figure S13. a) Protein ligand contacts of compound **7e** and **7f** with the respective amino acids of the protein  
(b) Ligand protein contacts of **7e** and **7f** with the respective amino acids of the  $\alpha$ -amylase protein.



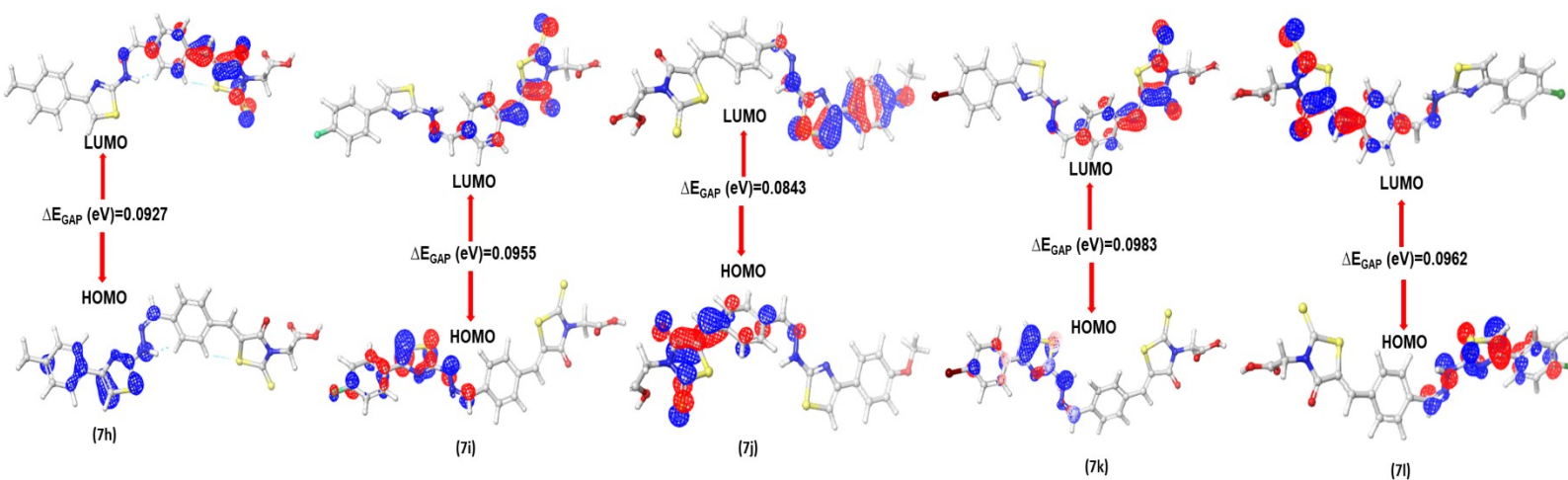


Figure S14. Contours of HOMO and LUMO of synthesized compounds

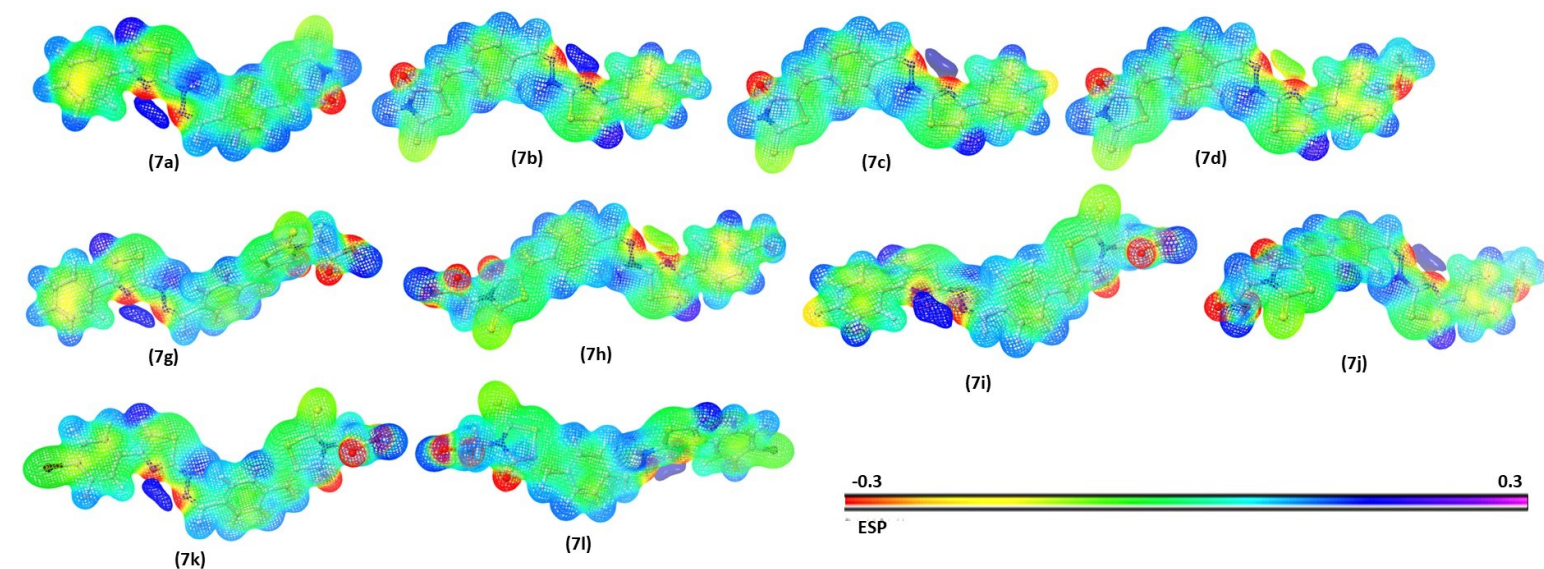


Figure S15. MEP map of synthesized compounds

**table. S9: Pharmacokinetic prediction:**

In the Qikprop module of Schrodinger's, the synthetic derivatives (**7a-l**) were predicted for the ADME prediction. The development of the pharmacokinetic profile of synthetic derivatives as bioactives depends heavily on adsorption, distribution, metabolism, and excretion.

**QPP MDCK:** apparent MDCK permeability (nm/sec) (<25 poor, >500 great).

**QPlog Kh<sub>sa</sub>:** prediction of binding to human serum albumin (-1.5 to 1.5).

**QPlog BB:** predicted brain/blood partition coefficient (-3.0 to 1.2).

**QPlogPo/w:** octanol/water partition coefficient (<5).

**QPlogS:** Aqueous solubility (-6.5 to 0.5).

**QPlogHERG:** IC<sub>50</sub> value for blockage of HERG K<sup>+</sup> channels (<5).

**QPPCaco:** apparent Caco-2 permeability (nm/sec) (<25 poor, >500 great).

**PSA:** Polar surface area (7-200).

**HOA:** Percent human oral absorption (>80% is high <25% is poor).

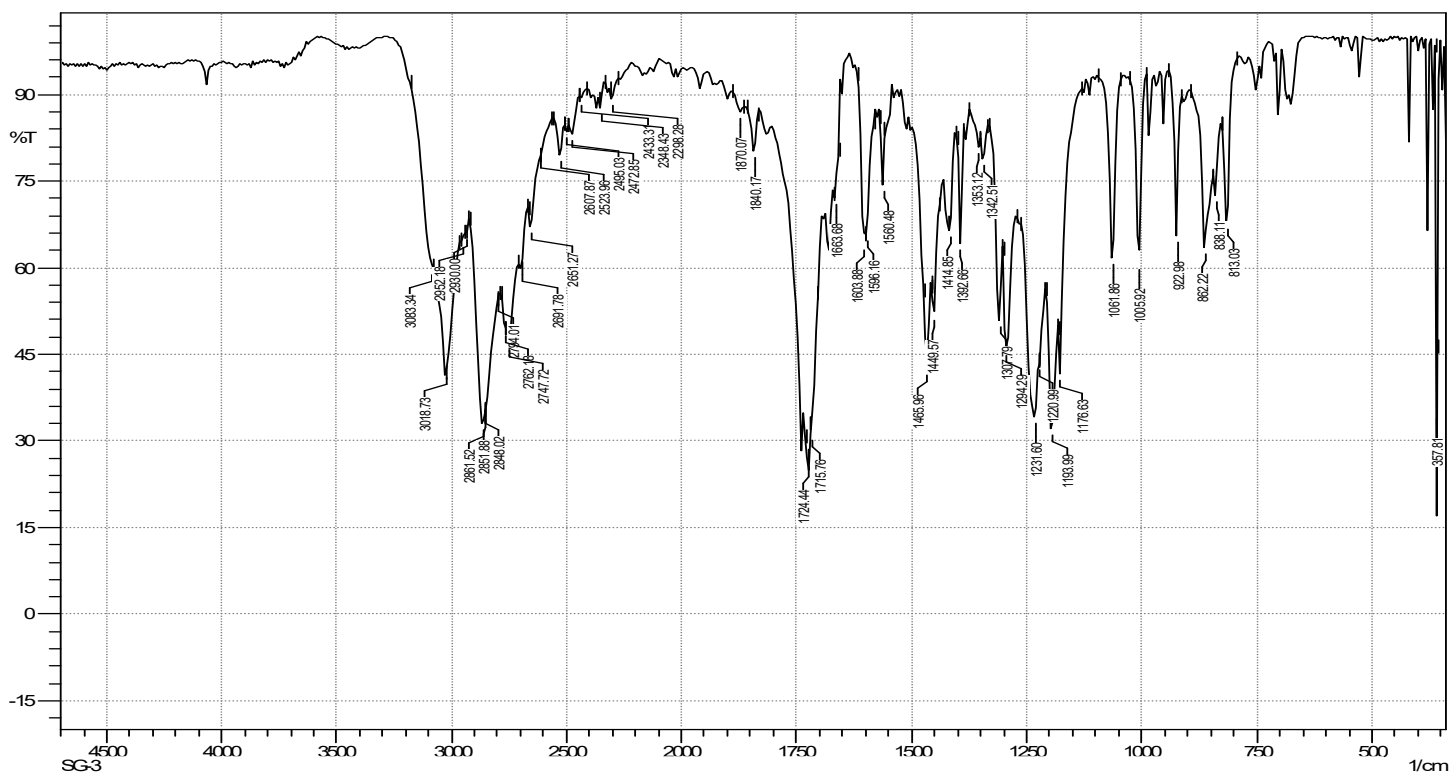
**CNS:** Predicted central nervous system activity (-2.0 to + 2.0).

**ROF:** Rule of five violations (<1).

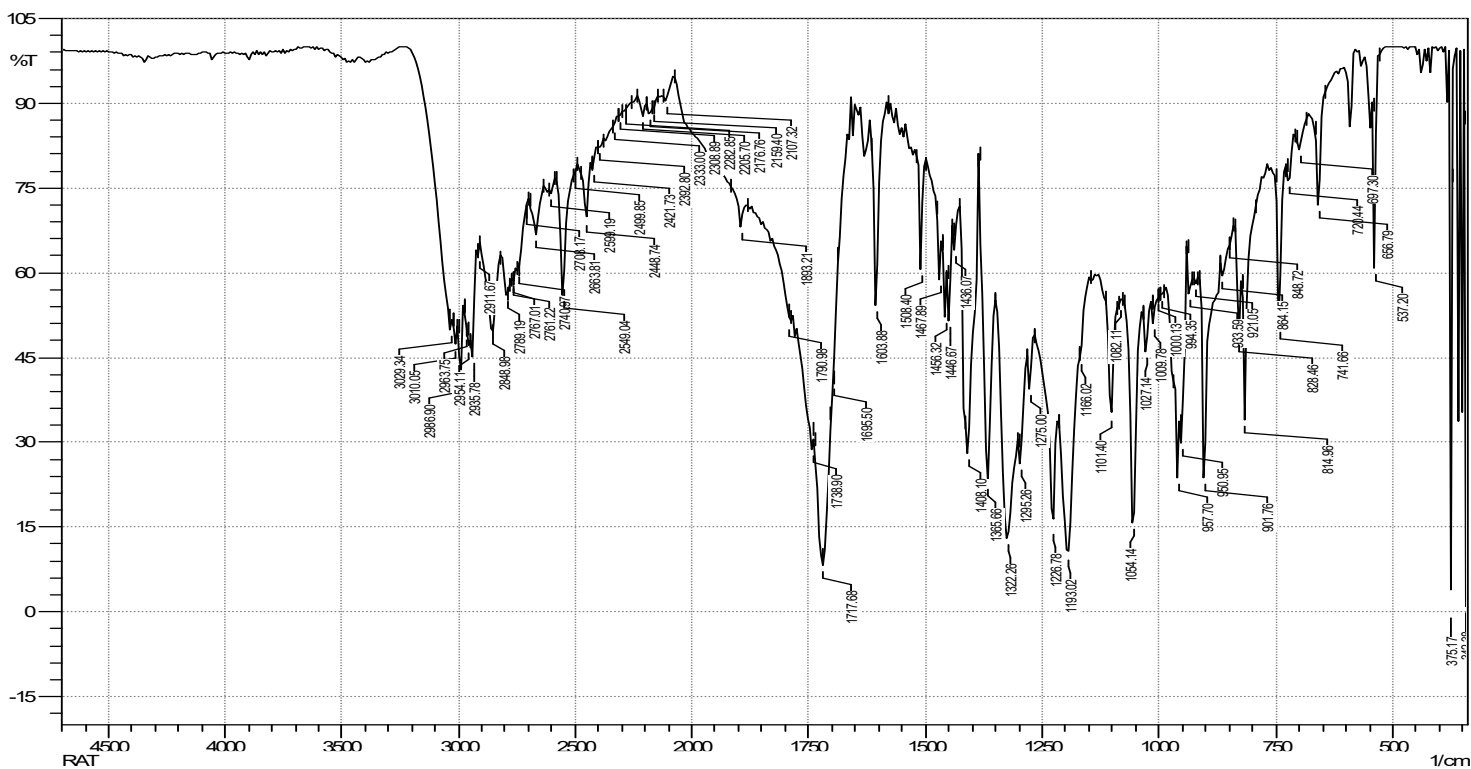
**ROT:** Rule of three violations (<1)

**SASA:** Solvent accessible surface area

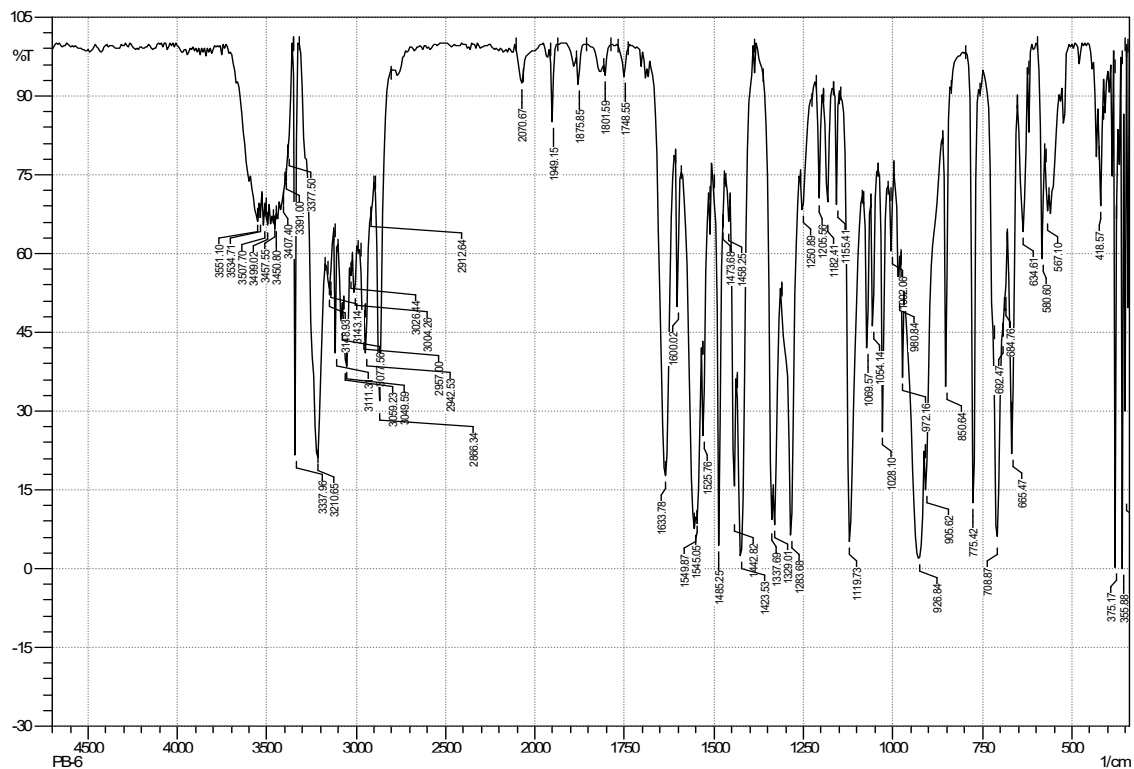
<b>QikProp Parameters</b>	<b>QPlog Po/W</b>	<b>QP logS</b>	<b>PSA</b>	<b>QPlog HERG</b>	<b>QPP Caco</b>	<b>QPP MDCK</b>	<b>QP log Khsa</b>	<b>QPlog BB</b>	<b>HOA</b>	<b>CNS</b>	<b>RoF</b>	<b>RoT</b>	<b>SASA</b>	<b>HBA</b>	<b>HBD</b>
<b>7a</b>	4.4	-6.3	87.0	-6.89	954.4	3572.3	0.37	-0.5	1	0	0	1	703.9	3	2
<b>7b</b>	4.74	-6.9	87.0	-6.7	957.6	3590.7	0.5	-0.5	1	0	0	1	736.3	3	2
<b>7c</b>	5.0	-7.2	87.0	-6.8	955.9	9494.4	0.5	-0.3	1	0	2	1	733.0	4	2
<b>7d</b>	4.53	-6.6	95.2	-6.7	952.6	3564.3	0.3	-0.6	1	0	0	1	741.1	4	2
<b>7e</b>	4.92	-7.1	87.0	-6.7	955.1	8819.1	0.4	-0.4	1	0	0	1	727.9	3	2
<b>7f</b>	4.67	-6.7	87.0	-5.5	954.5	6448.1	0.4	-0.4	1	0	0	1	712.8	3	2
<b>7g</b>	4.63	-6.8	122.5	-5.4	52.4	161.4	0.1	-1.6	1	-2	0	1	792.4	5	2
<b>7h</b>	4.9	-7.3	122.5	-5.4	52.5	162.9	0.3	-1.6	1	-2	0	1	825.7	5	2
<b>7i</b>	5.1	-7.6	122.3	-5.3	52.4	428.0	0.2	-1.4	1	-2	2	1	821.5	6	2
<b>7j</b>	4.7	-7.0	129.8	-5.4	55.7	171.6	0.1	-1.6	1	-2	1	1	827.7	5	2
<b>7k</b>	5.0	-7.5	122.5	-5.4	52.4	398.1	0.2	-1.4	1	-2	2	1	816.4	5	2
<b>7l</b>	4.8	-7.1	122.5	-5.3	52.4	291.3	0.2	-1.5	1	-2	0	1	801.3	5	2



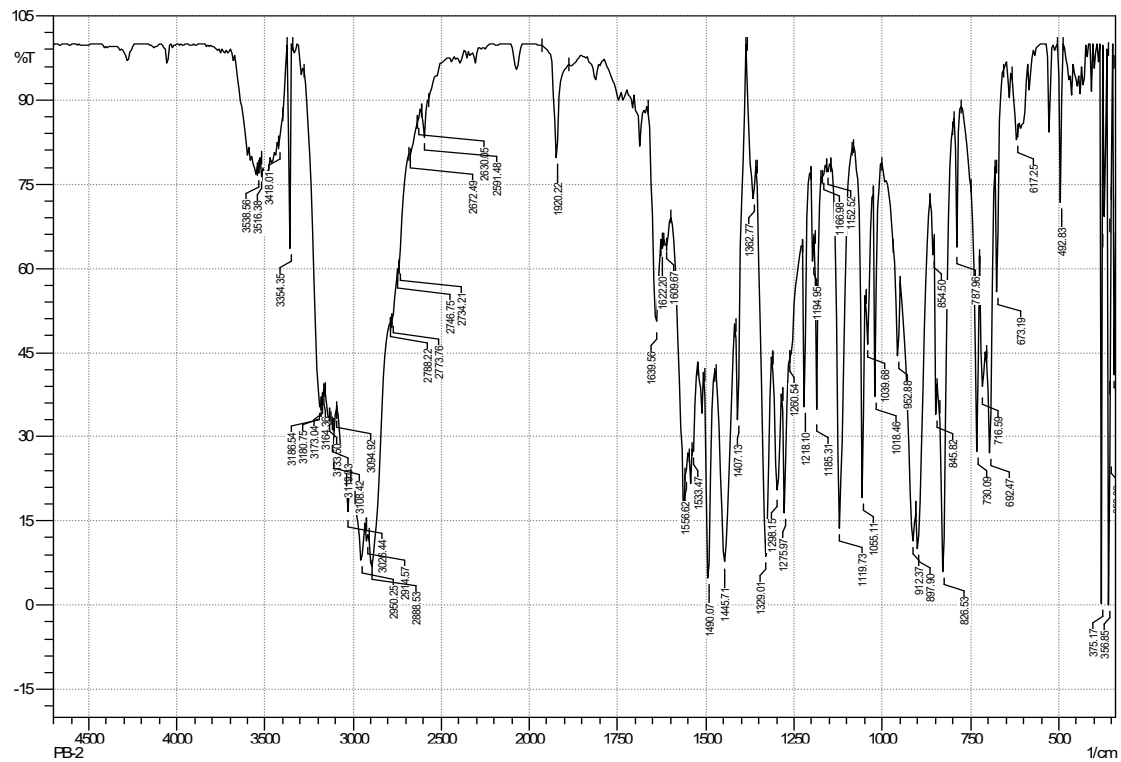
FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 3a



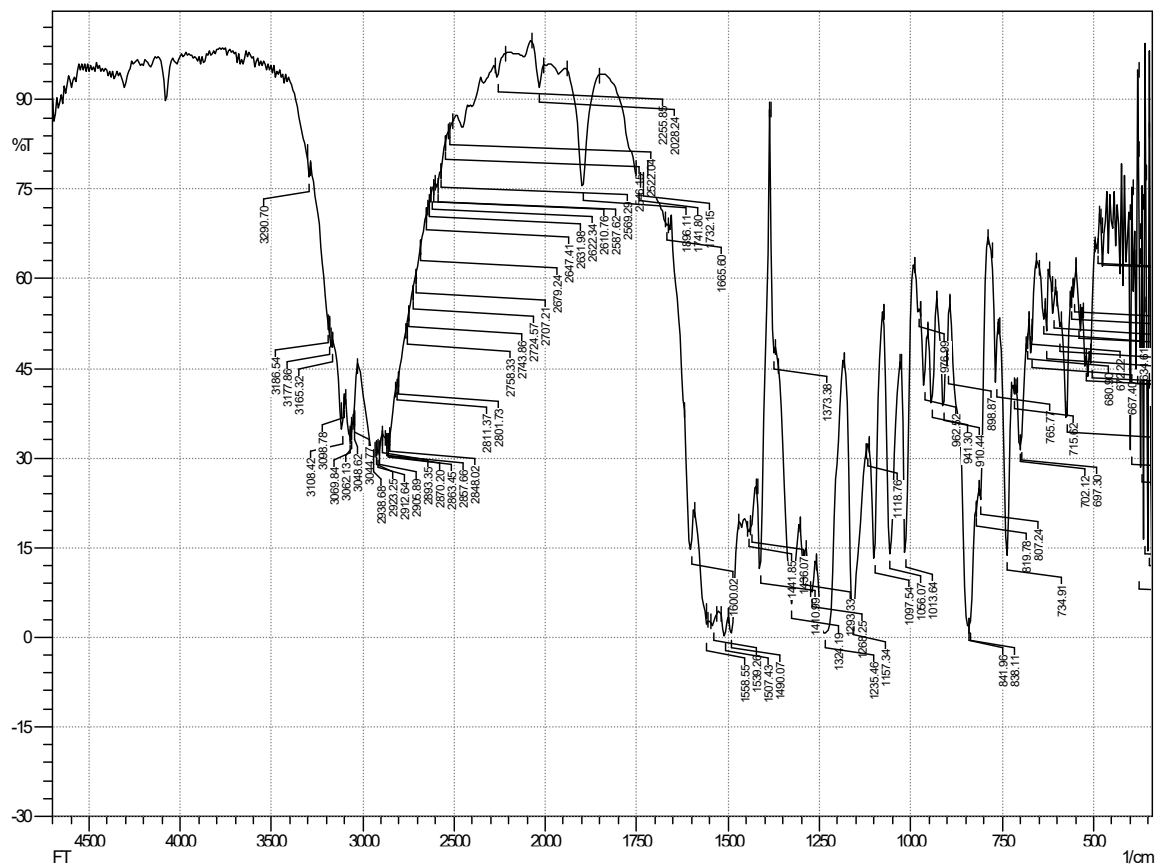
FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 3b



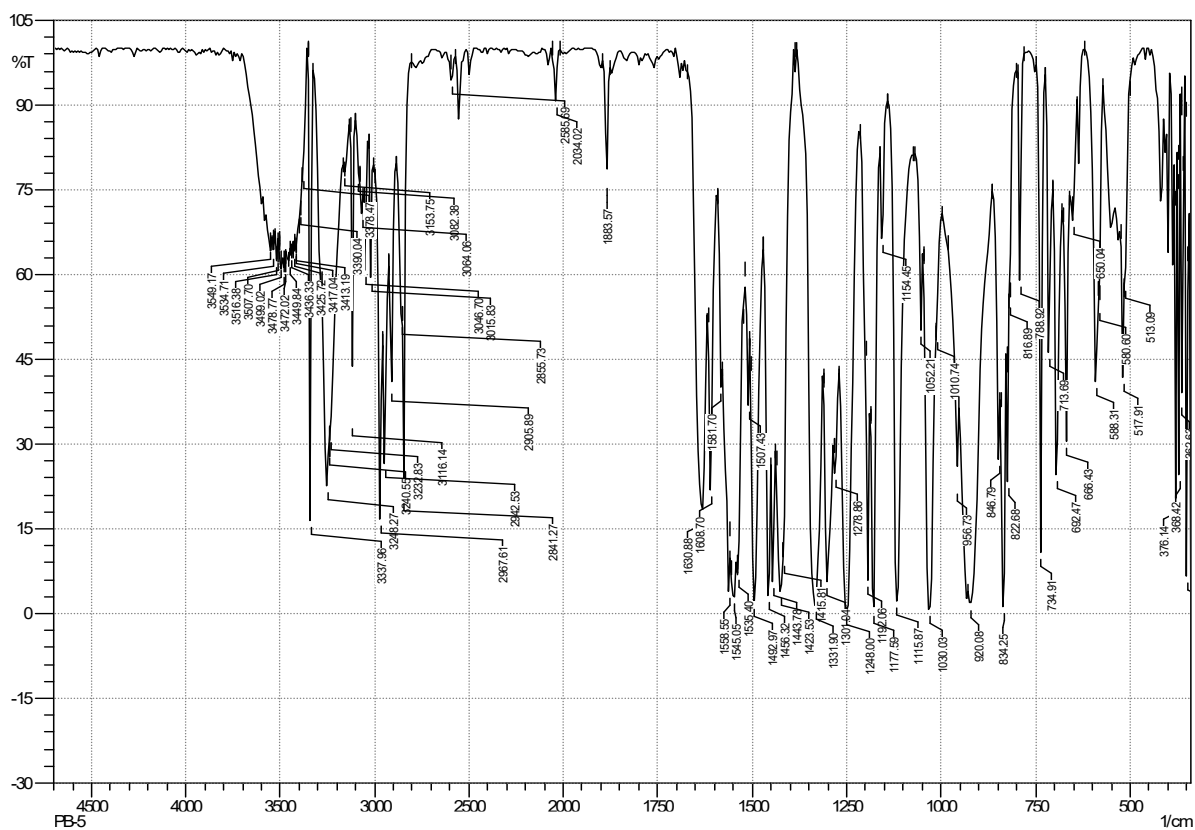
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 6a



FTIR (KBr, cm<sup>-1</sup>) spectra of compound 6b

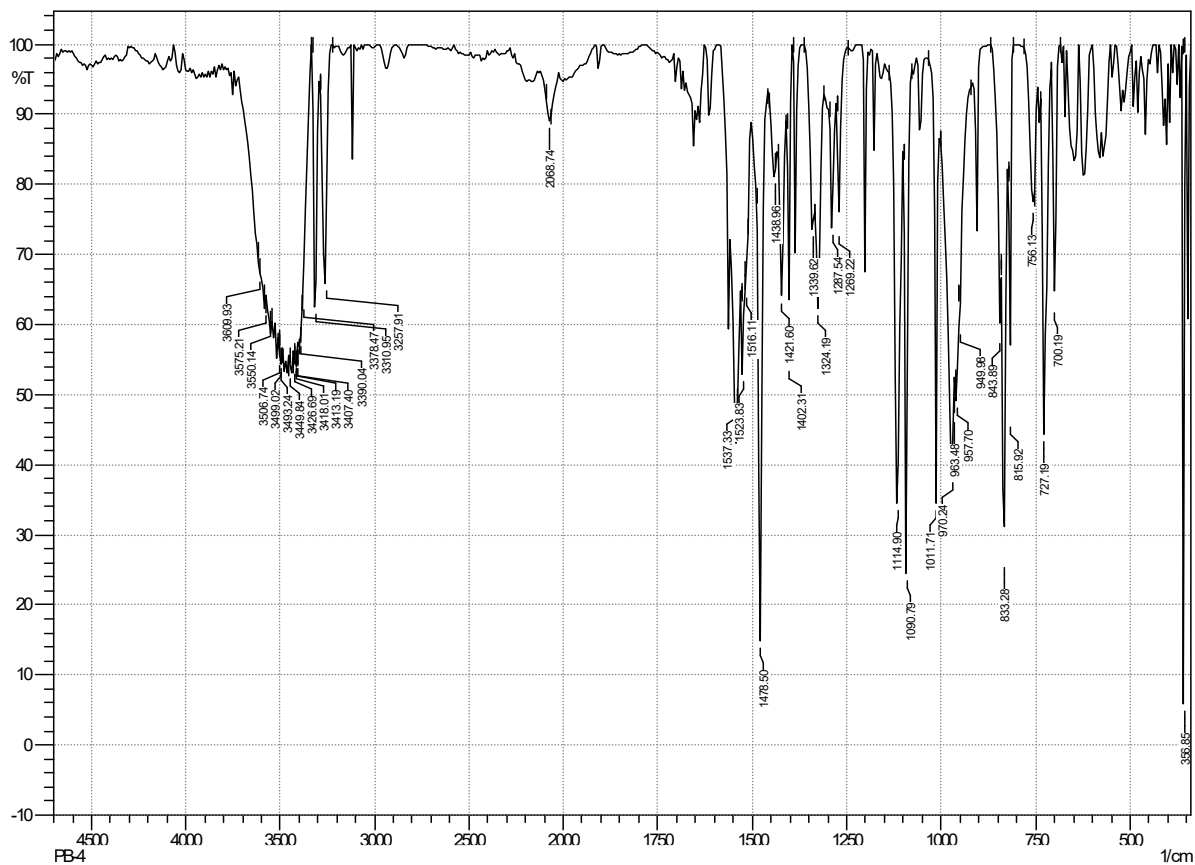


FTIR (KBr, cm<sup>-1</sup>) spectra of compound 6c

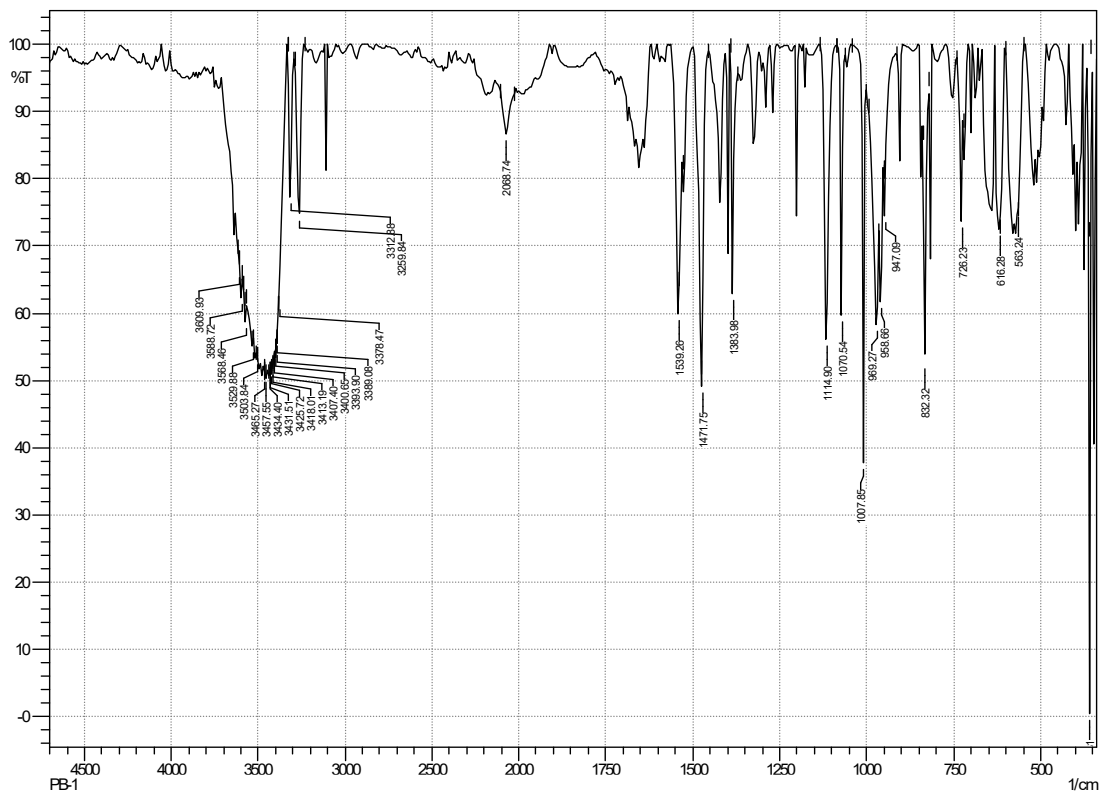


FTIR (KBr, cm<sup>-1</sup>) spectra of compound 6d

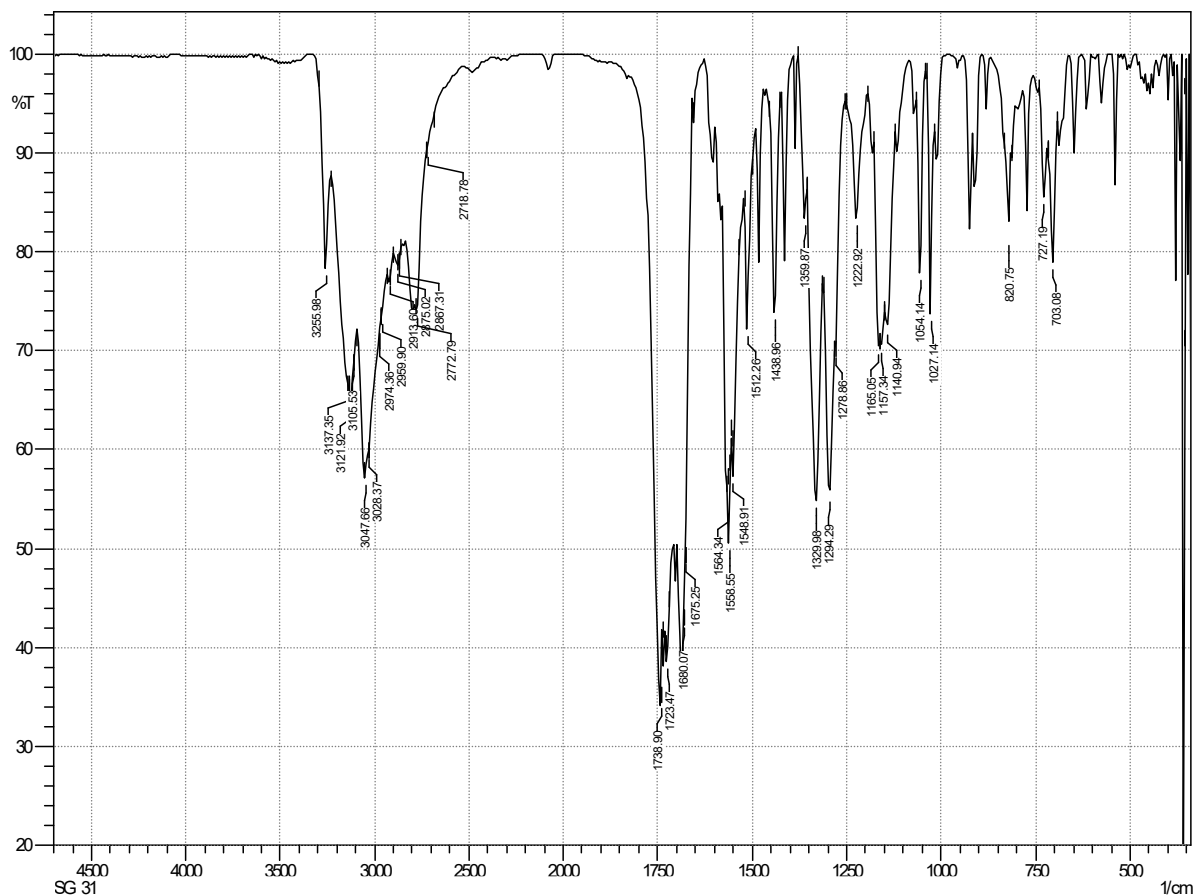




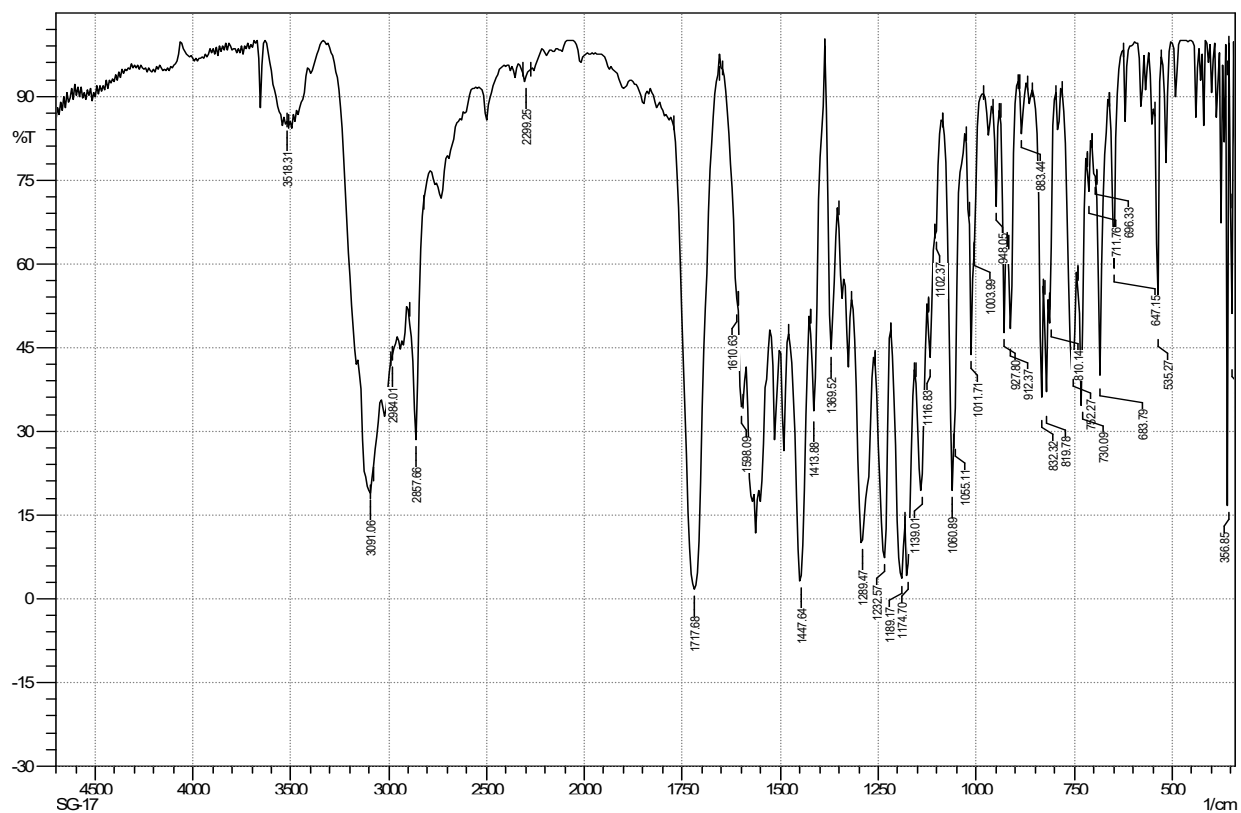
FTIR ( $\text{KBr}$ ,  $\text{cm}^{-1}$ ) spectra of compound 6e



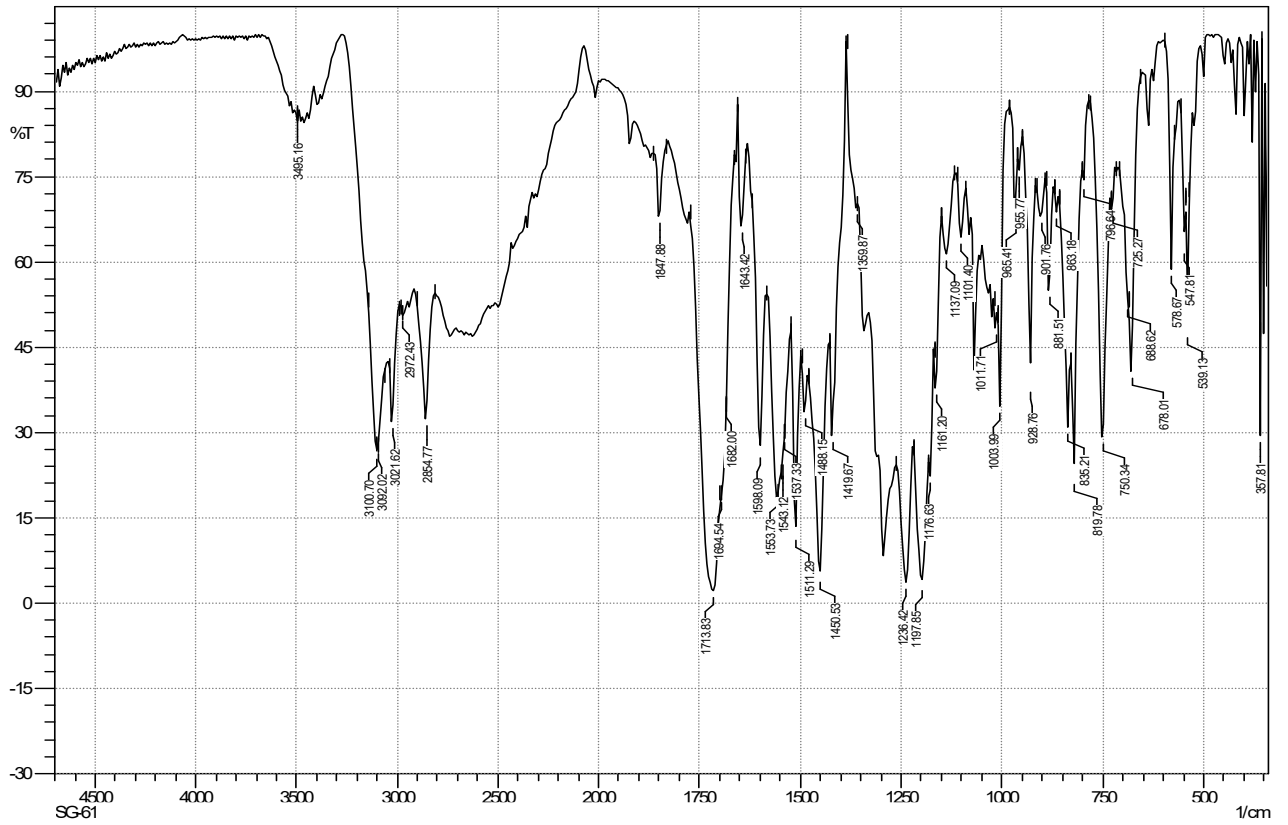
FTIR ( $\text{KBr}$ ,  $\text{cm}^{-1}$ ) spectra of compound 6f



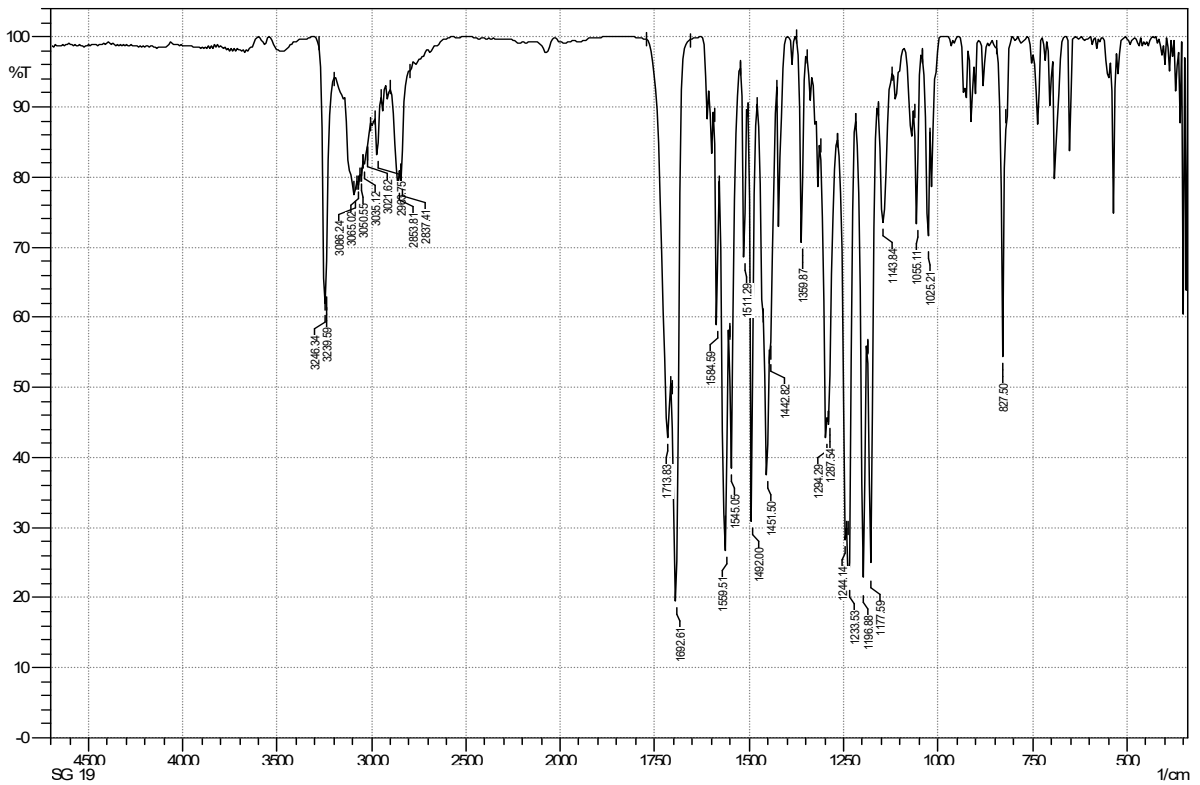
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 7a



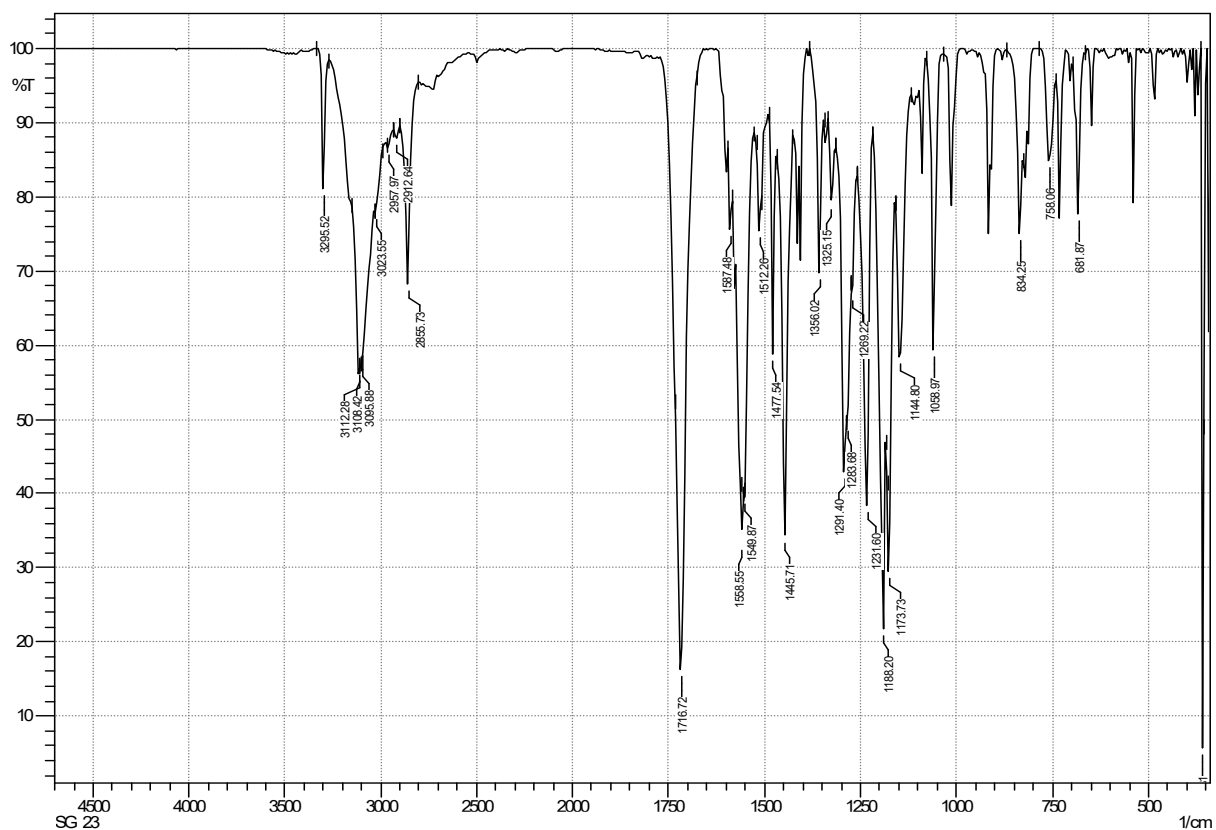
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 7b



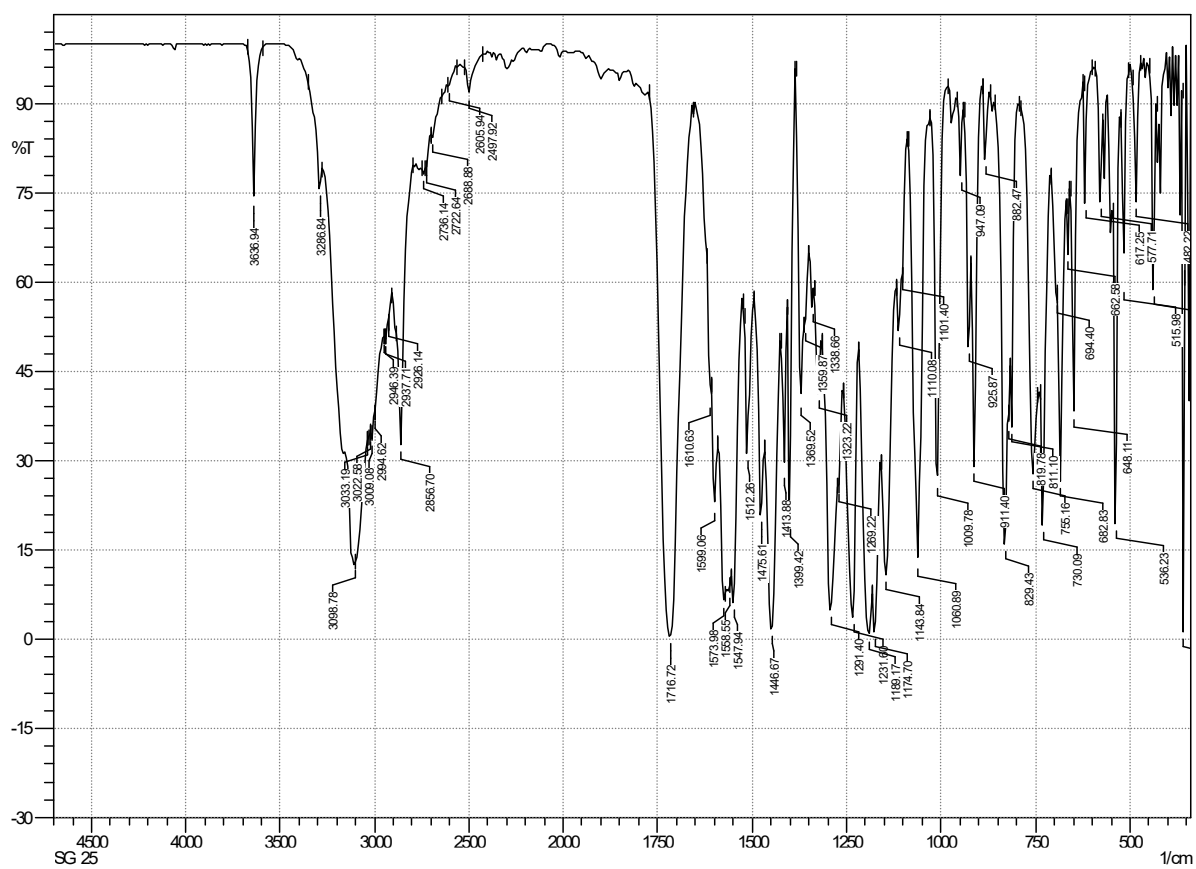
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 7c



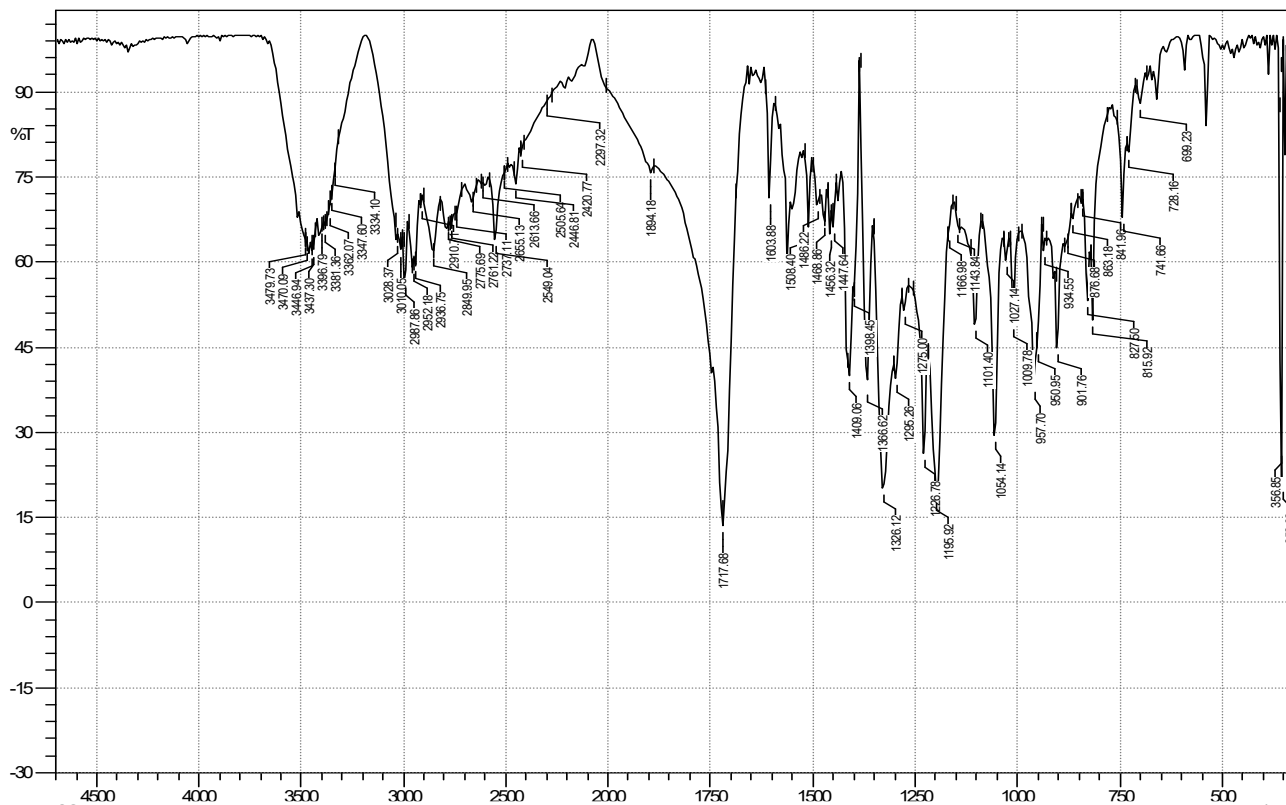
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 7d



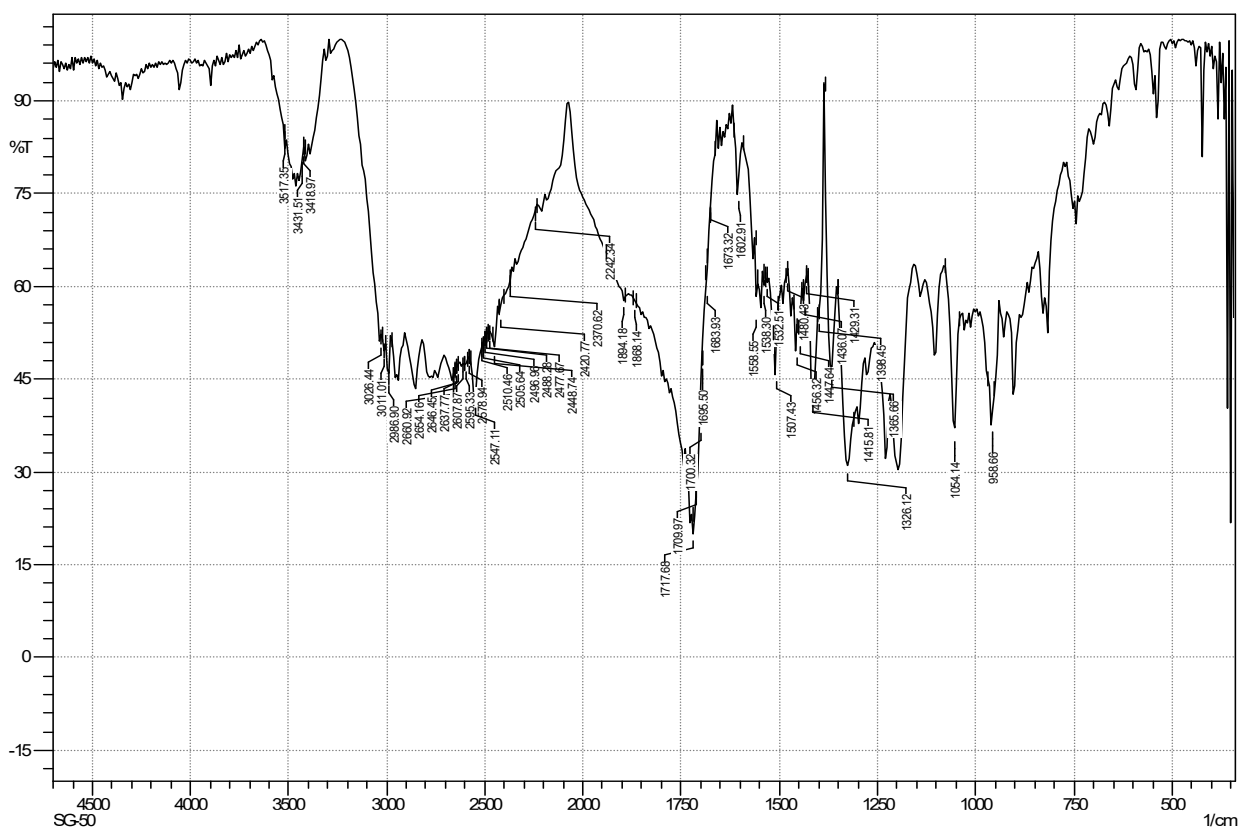
FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 7e



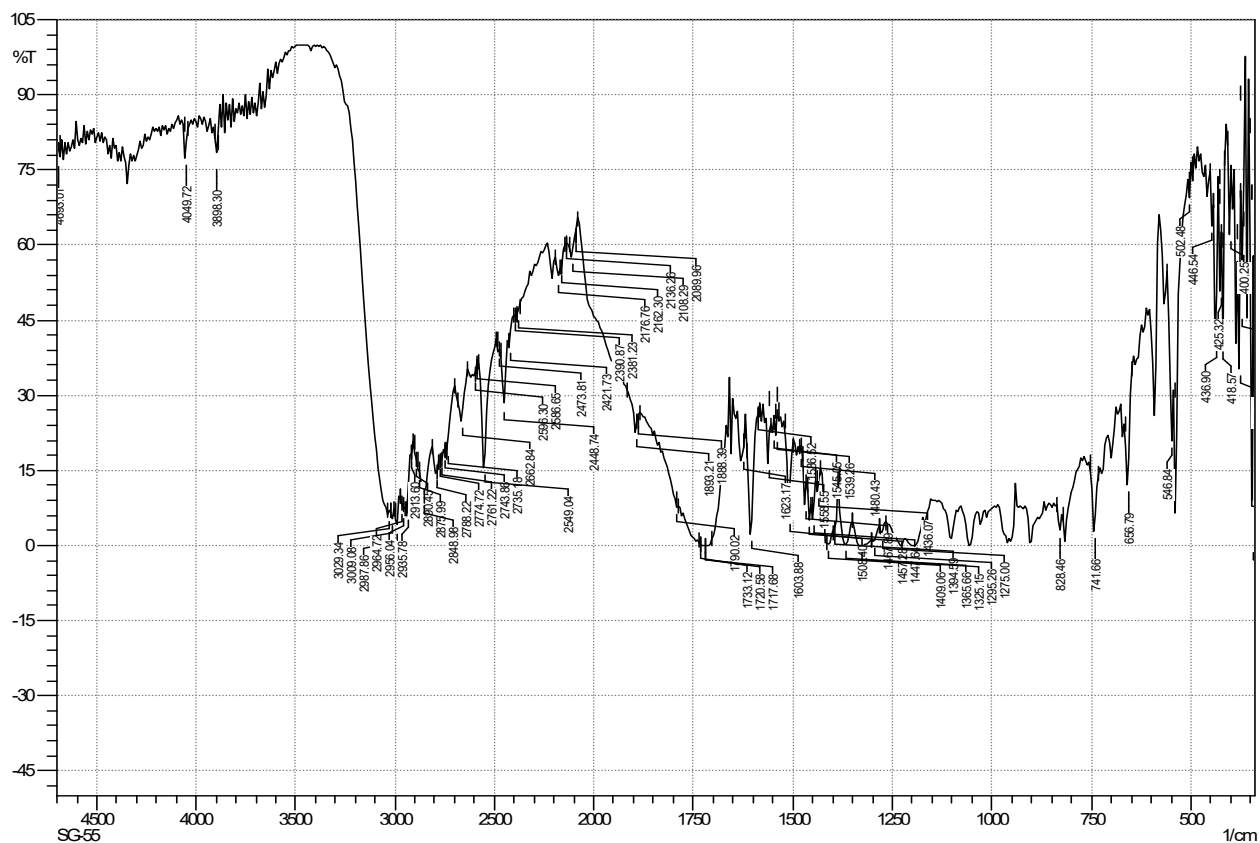
FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 7f



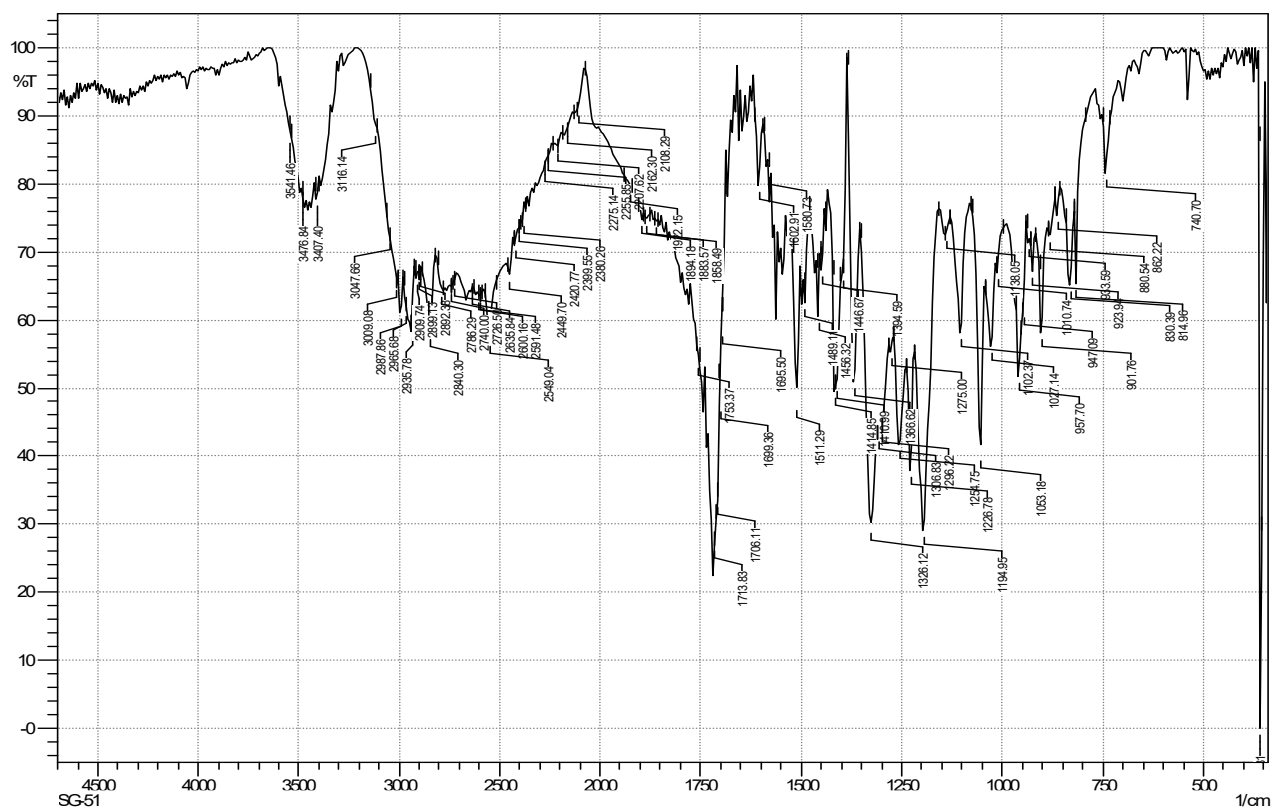
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 7g



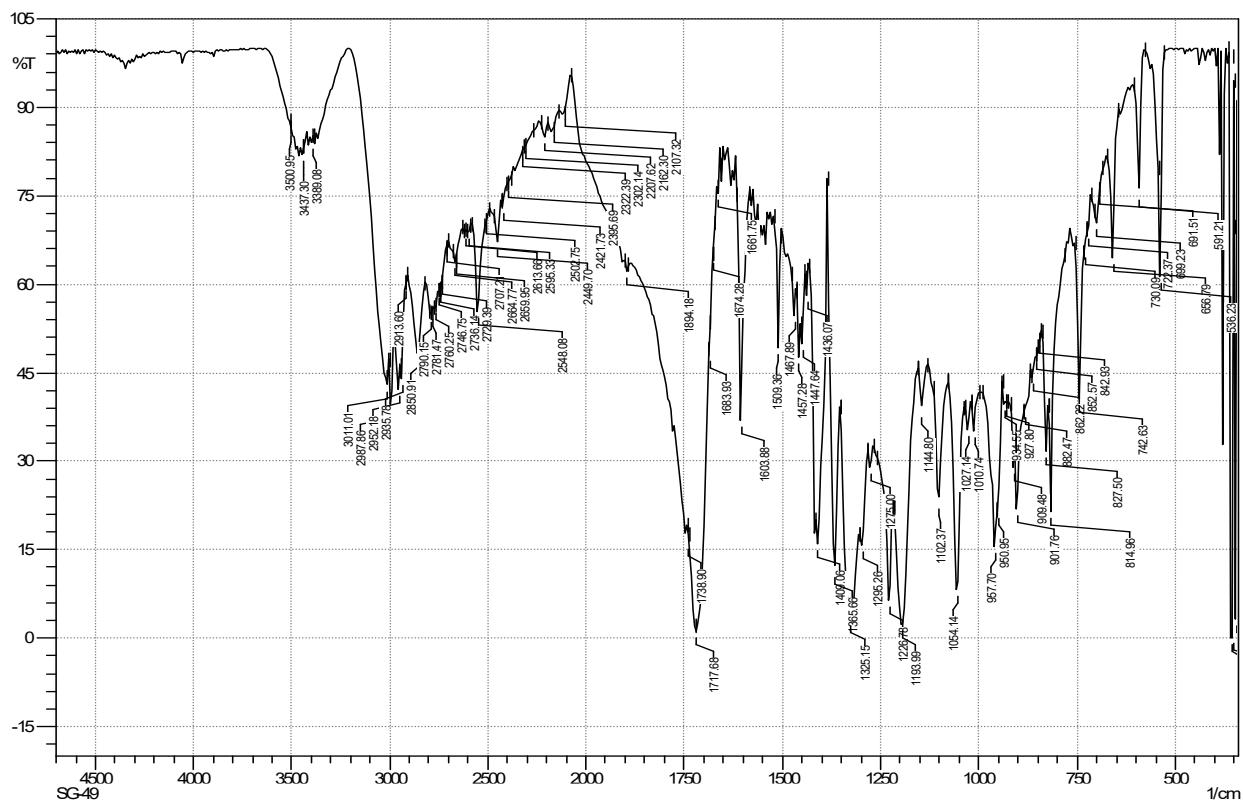
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 7h



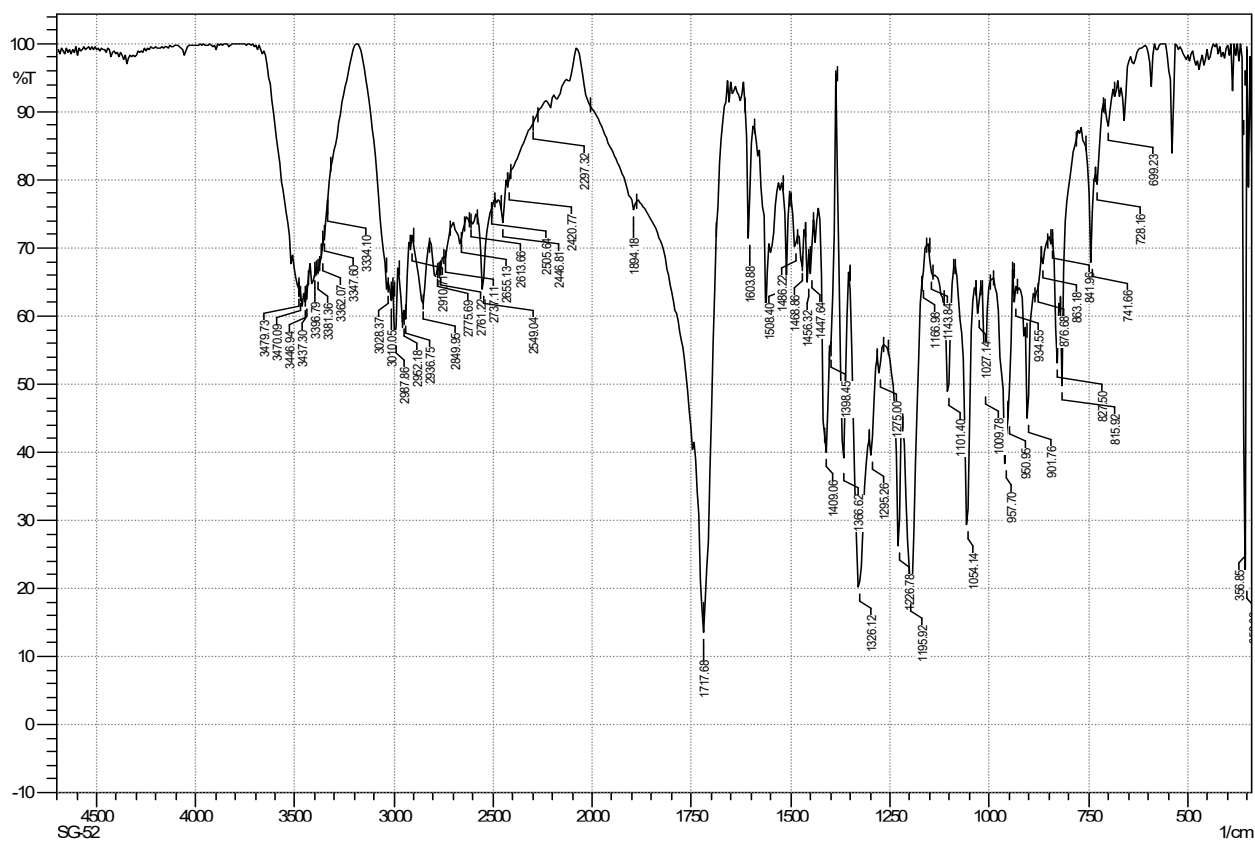
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 7i



FTIR (KBr, cm<sup>-1</sup>) spectra of compound 7j



FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 7k



FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 7l