

Supporting Information

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Chemical descriptors, PASS, molecular docking, molecular dynamics and ADMET predictions of glucopyranoside derivatives as inhibitors to bacteria and fungi growth

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Table S1: Ligands Interaction with amino acid residues and their bond distance (1ACZ).

Bond distance and amino acid residues					
Compounds	Hydrogen bond		Hydrophobic bond		Halogen Bond
	Interacting residue of amino acid	Distance, Å	Interacting residue of amino acid	Distance, Å	
1	ALA A: 550	2.75364	Absent	Absent	absent
			PHE A:519	3.19122	absent
2	LEU A: 533	3.466	VAL A:534	4.99707	
			ALA A:550	5.30485	
			ILE A:531	4.7079	
			LEU A:533	5.23879	
			LEU A:551	4.40789	
			ILE A :580	4.99908	
			LEU A:533	3.8786	
			ILE A;549	4.65299	
			ILE A:580	4.49096	
			LEU A:533	5.14417	
			LYS A:578	4.87532	
			ILE A:580	4.20055	
			TRP A:543	4.70904	
			TRP A:590	5.25757	
			TRP A:590	4.35356	
			TRP A:590	5.05673	
			TRP A:590	3.04268	
3	ASN A:530	3.51506	ALA A:550	3.69998	absent
			ALA A:550	5.24843	
			VAL A:565	5.00633	
			VAL A:567	4.68006	
			VAL A:567	4.01376	
			TYR A:564	5.29588	
4	TYR A:564	1.93638	ALA A:550	4.35638	absent
	THR A:566	2.12502	VAL A:567	4.44508	
	THR A:566:	2.58935	VAL A:567	4.86562	
5	SER A:552	3.04882	ALA A:550	5.21977	absent
	TYR A:564	2.14804	ALA A:550	4.01972	
	SER A:552	3.51667	VAL A:565	5.15295	
	SER A:559	3.47739	VAL A:567	4.40437	

6	SER A:552	2.54735	VAL A:567	4.52352	absent
			VAL A:567	4.95255	
			VAL A:567	3.58902	
			TYR A:564	4.34297	
			ILE A:582	4.87973	
			ILE A:582	4.70961	
7	ASN A:530 ILE A:582 LEU A:533 VAL A:567	2.8332 2.14612 2.47985 2.75088	TYR A:532	5.43501	absent
			LEU A:540	2.75088	
			LEU A:540	3.79922	
			TYR A:532	3.98233	
			PHE A:519	3.58676	
			VAL A:588	3.91401	
			VAL A:534	5.32406	
			ILE A:531	4.44201	
			VAL A:517	3.51737	
			VAL A:515	3.3669	
			VAL A:517	4.56067	
			LEU A:569	3.62925	
			PHE A:519 -	4.69319	
			TYR A:532 -	4.08057	
			TRP A:543	5.36939	
			TYR A:577	5.03449	
			PHE A:579	3.98524	
			TRP A:590	4.46769	
			TRP A:590	5.30449	
			TRP A:590	5.02444	
			TYR A:598	4.96477	
			VAL A:517	4.30704	
			ILE A:549	4.96223	
			VAL A:567	4.78427	
			VAL A:517	5.00721	
			LEU A:533	4.44813	
8	ASN A:530	2.36739	TRP A:590		absent
	SER A:552	3.02273	TYR A:598		
	ILE A:582	2.47423			
	ARG A:581	3.60893	LYS A:578		

VAL A:588
LEU A:533
VAL A:534
ILE A:580
TYR A:532
TYR A:532
TRP A:543
TRP A:543
PHE A:579
TRP A:590
TRP A:590
LEU A:551
ARG A:581
ALA A:516
VAL A:517
VAL A:567
VAL A:517
LEU A:540
ILE A:549
LEU A:569

Table S2: Ligands Interaction with amino acid residues and their bond distance for (1KUM)

Bond distance and amino acid residues					
Compounds	Hydrogen bond		Hydrophobic bond		Halogen Bond
	Interacting residue of amino acid	Distance, Å	Interacting residue of amino acid	Distance, Å	
1	A: VAL565	2.7248	Absent		absent
	A: VAL534	2.27443			
2	A: VAL517	1.89265	A: VAL534	3.58556	absent
	A: VAL565	2.54224	A: ILE531	5.21608	
	A: ASP613	3.39578	A: ILE580	4.33617	
			A: PHE519	4.97597	
			A: TRP590	4.07329	
3	A: ASP520	2.18486	A: PHE519	3.73113	absent
	A: VAL565	2.15348	A: VAL534	4.47275	
	A: ASP613	2.7279	A: ILE531	5.1258	
	A: VAL565	3.64716	A: LEU533	4.26524	
	A: VAL534	3.06868	A: ILE580	4.52457	
	A: LYS578	3.20441	A: ILE580	4.59447	
			A: VAL534	2.99401	
			A: ILE580	4.96354	
			A: VAL517	4.2296	
			A: PHE519	3.93351	
			A: TRP590	5.11231	
			A: TRP590	4.66873	
			A: TRP590	3.85049	
4	A: LEU521	2.7454	A: PHE519	5.63086	absent
	A: VAL565	2.63261	A: TYR577	4.06753	
	A: ASP613:	3.19001	A: PHE519	2.8548	
	A: VAL565	3.60765	A: VAL534	3.10617	
	A: VAL565	3.54838	A: ILE580	5.43279	
	A: VAL534	3.13534	A: LEU533	4.64881	
			A: LEU551	5.24115	
			A: ILE580	3.71573	
			A: LEU533	5.2332	
			A: ILE580	4.95833	
			A: TYR532	4.97408	

			A: TRP590	4.7354	
			A: TRP590	3.93073	
5	A: TYR564	2.34602	A: LEU521	3.4506	absent
	A: VAL565	1.90018	A: PHE519	5.62151	
	A:ASP 613	2.7499	A: TRP563	2.93445	
	A: VAL534	2.41218	A: PHE575	5.46902	
			A: TRP563	3.02883	
			A TYR564	3.53967	
			A: VAL534	3.75154	
			A: ILE531	5.3991	
			A: LEU533	4.34781	
			A: LEU551	4.67313	
			A: ILE580	3.82547	
			A: LEU533	4.30978	
			A: ILE580	3.39224	
			A: VAL534	3.63332	
			A: TRP590	4.74196	
			A: TRP590	4.29928	
			A: TRP590	4.38825	
			A: VAL517	5.38347	
			A: VAL611	3.95877	
			A: VAL517	5.20803	
			A: LEU540	4.80898	
6	A:ASP520	2.95909	A:ASP520	4.99728	absent
	A: VAL565	2.57377	A: LEU551	3.62829	
	A: VAL567	2.73184	A: ALA523	3.90088	
	A: VAL534	2.95556	A: VAL534	4.47856	
	A: LYS578	2.6819	A: VAL534	3.26226	
			A: ALA609	2.46501	
			A: ILE531	5.07441	
			A: LEU533	4.61899	
			A: ILE580	4.29997	
			A: ILE580	3.97488	
			A: VAL534	3.61347	
			A: ILE531	4.50368	
			A: VAL517	3.10167	

				A: VAL611	5.25849	
				A: TRP563	4.71681	
				A: TYR577	3.63829	
				A: TRP590	4.80826	
				A: TRP590	5.39299	
				A: TRP590	4.16866	
				A: TRP590	4.30833	
				A: TYR598	3.55815	
				A: ALA609	5.12390	
				A: VAL517	4.38755	
				A: LEU540	5.41700	
				A: VAL567	5.2927	
7	A:ASP520	2.50244	A: LEU551:	3.56426	absent	
	A: VAL565	3.06052	A: PHE575	3.62679		
	A:ASP613	2.96664	A: PHE575	3.08638		
	A: LEU533	3.01789	A: THR518	2.72458		
				A: PHE519	2.68986	
				A: ALA523	4.34033	
				A: VAL534	4.03638	
				A: VAL534	3.78776	
				A: ALA609	2.59136	
				A: ILE531	5.29329	
				A: LEU533	4.80533	
				A: LEU551	4.83136	
				A: ILE580	3.99817	
				A: VAL534	4.23046	
				A: ILE580	4.75912	
				A: LEU521	2.84557	
				A: ILE531	3.93252	
				A: VAL611	4.47417	
				A: TYR556	5.35665	
				A: TRP563	3.69968	
				A: PHE575	3.54884	
				A: TYR577	3.44309	
				A: TRP590	4.97921	
				A: TRP590	4.58886	

			A: TRP590	4.53944	
			A: TRP590	3.86579	
			A: TYR598 -	2.74393	
			A: ILE531	5.02766	
			A: ALA609	5.30085	
			A: VAL517	4.66198	
			A: LEU540	5.14806	
			A: VAL567	5.16166	
8	A:ASP520	1.91333	A: LEU569:	2.81871	absent
	A:ASP613	2.88584	A: VAL611	3.43763	
	A: VAL534	3.42362	A: PHE519	3.7828	
			A: PHE519	3.01664	
			A: VAL534	4.87092	
			A: LEU551	3.9113	
			A: ILE580	4.61175	
			A: LEU533	4.97524	
			A: VAL534	3.2792	
			A: ILE580	4.82099	
			A: TYR532	5.23404	
			A: TRP590	4.6099	
			A: TRP590 -	5.23646	
			A: TRP590	3.78912	
			A: TRP590	4.15056	
			ALA523	4.99816	
			A: LEU551	5.1904	
			A: ILE537	5.17774	
			A: LEU540	5.47988	

Table S3: Ligands Interaction with amino acid residues and their bond distance for (2UU2.)

Bond distance and amino acid residues					
Compounds	Hydrogen bond		Hydrophobic bond		Halogen Bond
	Interacting residue of amino acid	Distance, Å	Interacting residue of amino acid	Distance, Å	
1	A: GLN356	2.31956	Absent	Absent	Absent
	A: GLN356	2.70901			
	A: GLU109	2.29578			
	A: TYR324	2.63322			
	A: GLN356	2.58394			
	A:PRO108	3.43269			
	A: TYR324	3.10169			
2	A: TYR53	2.35358	A: VAL75	4.54005	Absent
	A: ARG132	2.33801	A: VAL75	5.35678	
	A: ARG132	2.56497	A: PHE77	5.14924	
	A: ARG132	2.71932	A: TYR94	4.99462	
	A:ASP89	3.42821	A: TYR94	4.85916	
			A: TYR94	4.38672	
			A: TYR94	4.27703	
			A: TYR98	5.31808	
			A: TYR98	4.81952	
3	A: TYR22	2.8121	A: VAL354	4.30284	Absent
	A: TYR35	2.12918	A: VAL354	3.63212	
	A: ARG74	2.70634	A: LEU20	4.87669	
	A: GLN123	2.29957	A: TYR35	4.3356	
	A: ARG124	1.89278	A: TYR324	4.66877	
	A: ARG124	3.07607			
	A: ARG124	2.59978			
	A: GLU109	4.30280			
4	A: ARG37	2.18127	A: LYS16	4.6457	absent
	A: SER322	2.98214	A: PHE14	5.15836	
	A: GLN356	2.12505	A: PHE14	4.01894	
	A: ARG37	3.39436			
5	A: GLN122	1.80786	A: PHE337	3.76415	absent
	A: GLN122	2.44747	A: PHE120	4.08342	
	A: THR239	2.25729	A: ILE305	4.58736	

	A: LYS290	2.05436	A: ALA341	4.31147	
	A: LYS290	2.63453	A: ILE292	4.21939	
	A: LYS290	2.4393	A: PHE337	4.37256	
			A: ILE305	5.06707	
6	A: TYR35	2.04221	A: GLU109	3.90429	absent
	A: ARG37	2.2881	A: VAL354	3.67753	
	A: ARG37	2.37754	A: VAL354	3.8682	
	A: ARG74	2.34484	A: TYR324	4.38776	
	A: ASP113	2.17497			
	A: GLN123	2.25176			
	A: GLN123	2.56268			
	A: ARG124	2.4942			
	A: ARG124	2.09268			
	A: TYR94	3.63874			
7	A: TYR35	2.43593	A: ASP18	4.87496	absent
	A: TYR35	2.30574	A: GLU109	3.91429	
	A: ARG74	2.39416	A: LYS16	4.55652	
	A: ARG74	5.94430	A: LYS16	5.29258	
	A: ARG124	2.29566	A: ARG37	4.91582	
			A: PHE14	4.90484	
			A: PHE14	3.88307	
8	A: TYR35	1.75002	A: ASP18	4.31537	absent
	A: ARG37	2.25072	A: PHE14	4.16882	
	A: ARG37	2.25098	A: VAL354	4.41241	
	A: ARG74	2.41733			
	A: ARG74	2.63106			

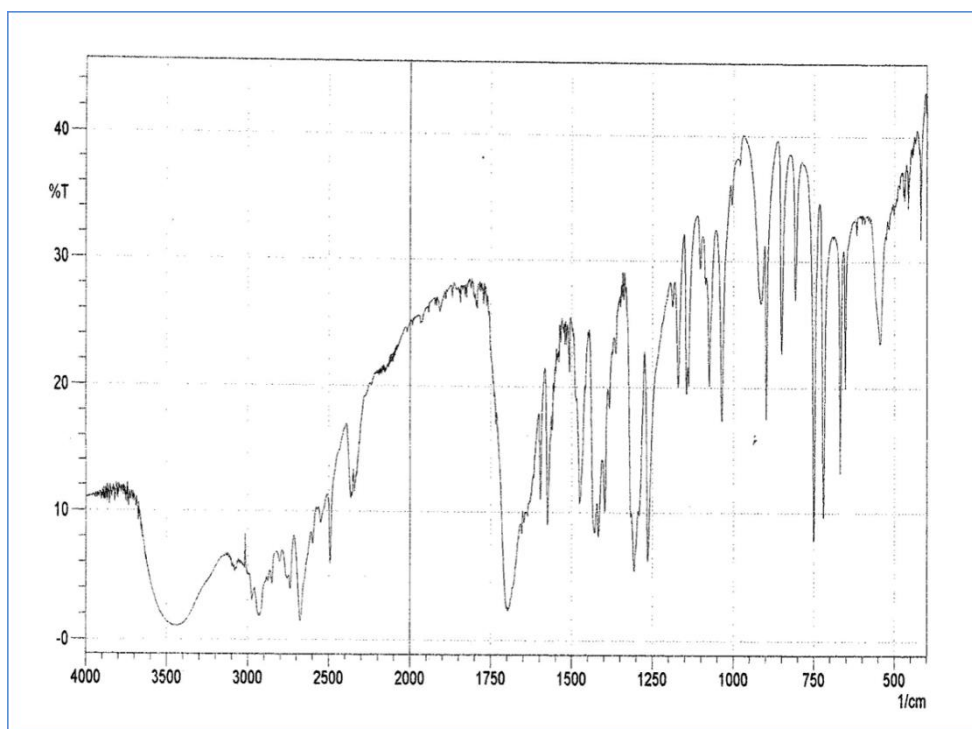


Figure S1: The FTIR spectrum of the compound 2

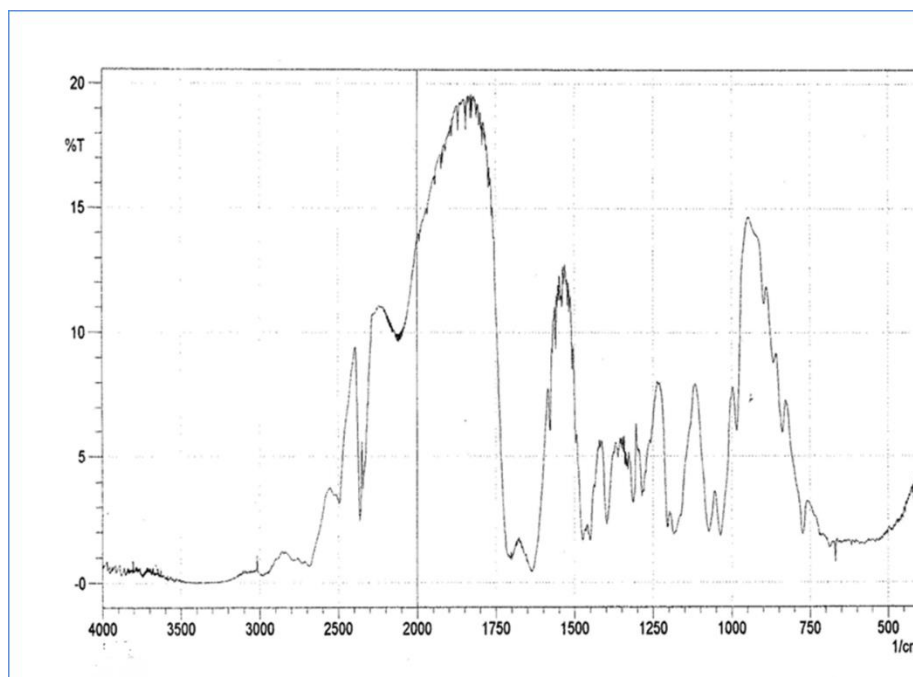


Figure S2: The FTIR spectrum of the compound 3

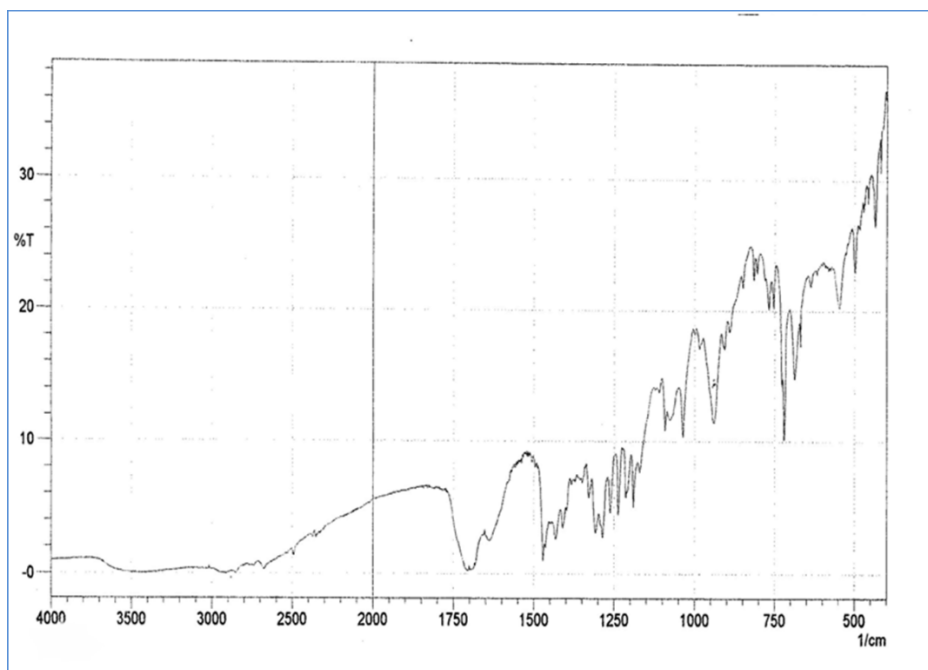


Figure S3: The FTIR spectrum of the compound 4

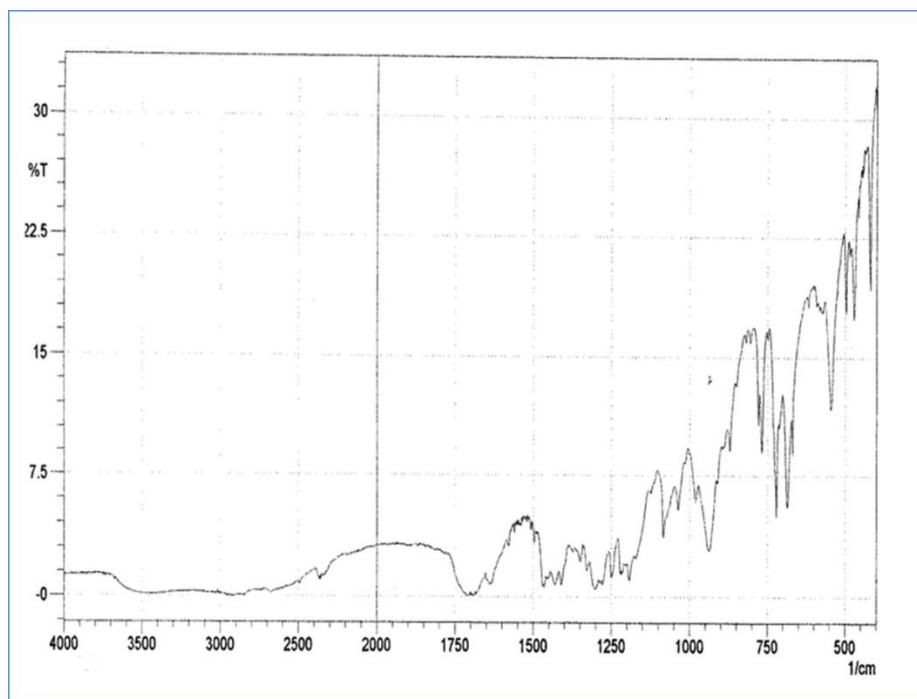


Figure S4: The FTIR spectrum of the compound 5

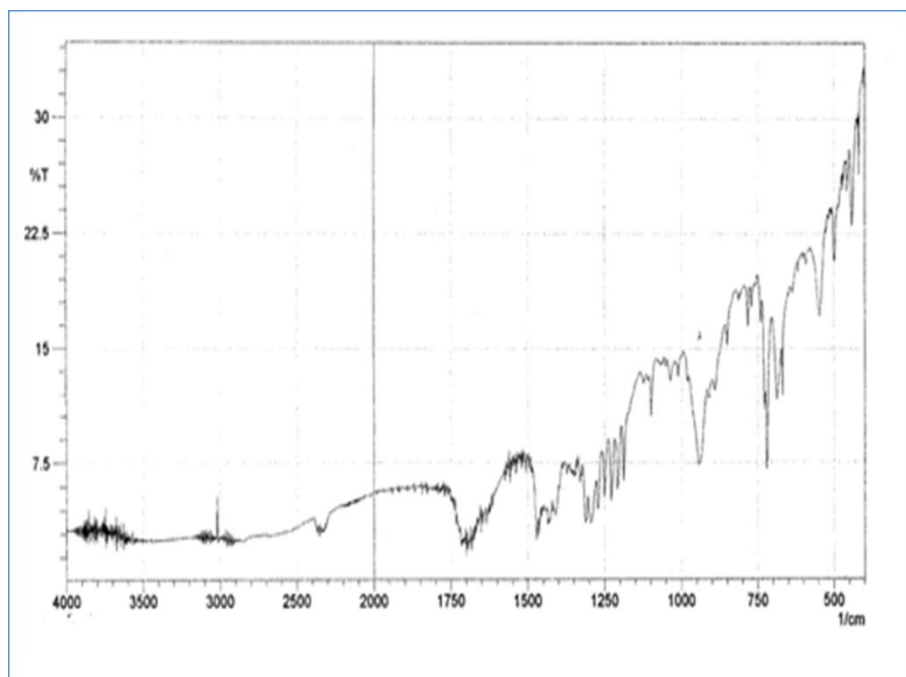


Figure S5: The FTIR spectrum of the compound **6**

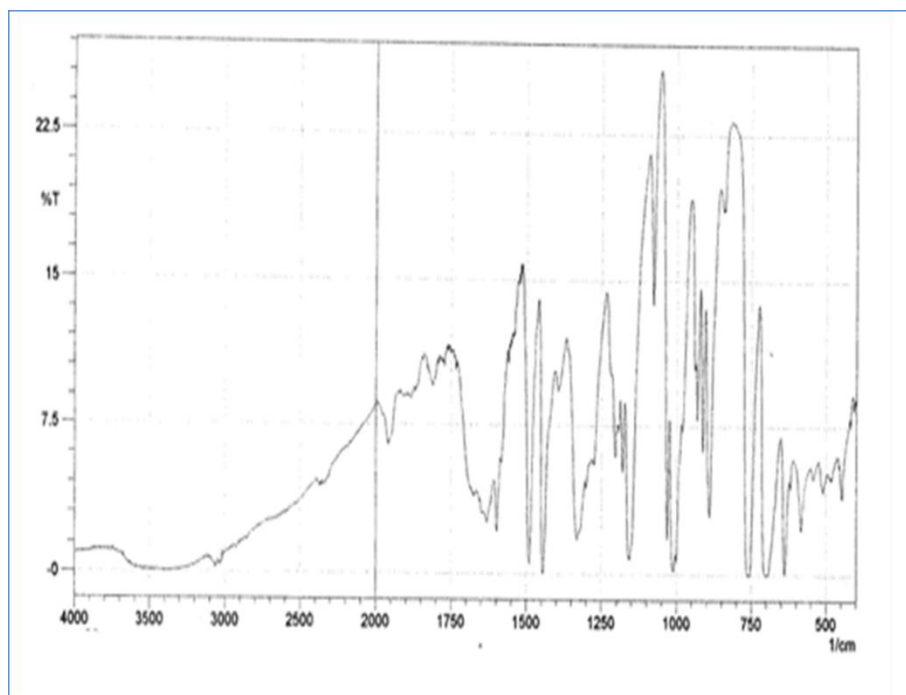


Figure S6: The FTIR spectrum of the compound 7

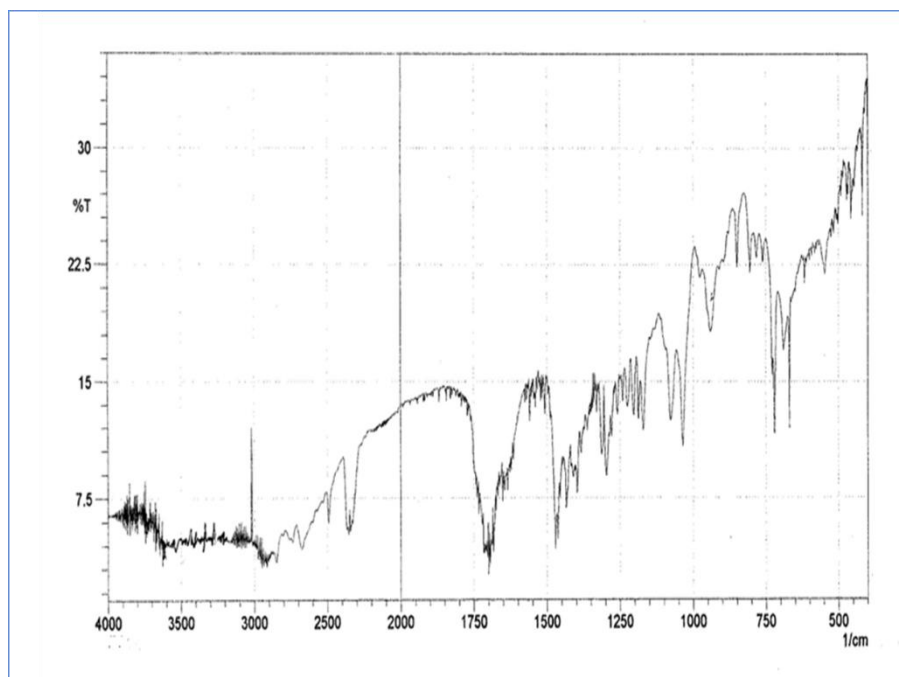


Figure S7: The FTIR spectrum of the compound **8**