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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Bond distance and amino acid residues					
Compounds	**Hydrogen bond**		**Hydrophobic bond**		
	Interacting residue of amino acid	**Distance, A°**	**Interacting residue of amino acid**	**Distance, A°**	**Halogen Bond**
1	ALA A: 550	2.75364	Absent	Absent	absent
2			PHE A:519	3.19122	absent
			VAL A:534	4.99707	
	LEU A: 533	3.466	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	

			VAL A:567	4.52352	
			VAL A:567	4.95255	
6	SER A:552	2.54735	VAL A:567	3.58902	absent
			TYR A:564	4.34297	
			ILE A:582	4.87973	
			ILE A:582	4.70961	
			TYR A:532	5.43501	
7	ASN A:530	2.8332	LEU A:540	2.75088	absent
	ILE A:582	2.14612	LEU A:540	3.79922	
	LEU A:533	2.47985	TYR A:532	3.98233	
	VAL A:567	2.75088	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**		
	Interacting residue of amino acid	**Distance, A°**	**Interacting residue of amino acid**	**Distance, A°**	**Halogen Bond**
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**		
	Interacting residue of amino acid	**Distance, A°**	**Interacting residue of amino acid**	**Distance, A°**	**Halogen Bond**
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			
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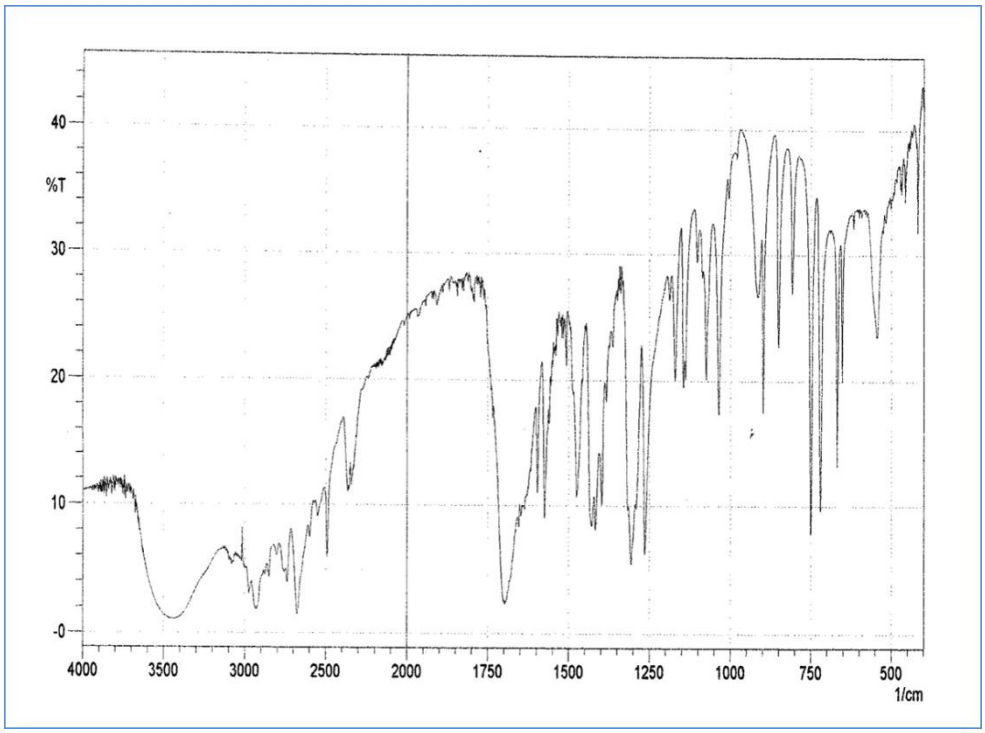

Figure S1: The FTIR spectrum of the compound **2**

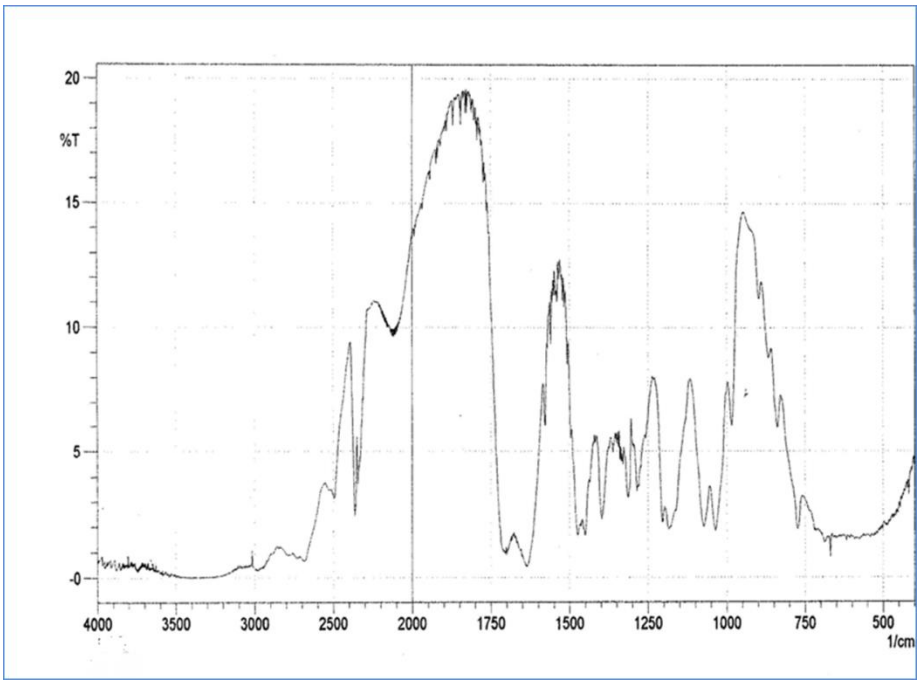

Figure S2: The FTIR spectrum of the compound **3**

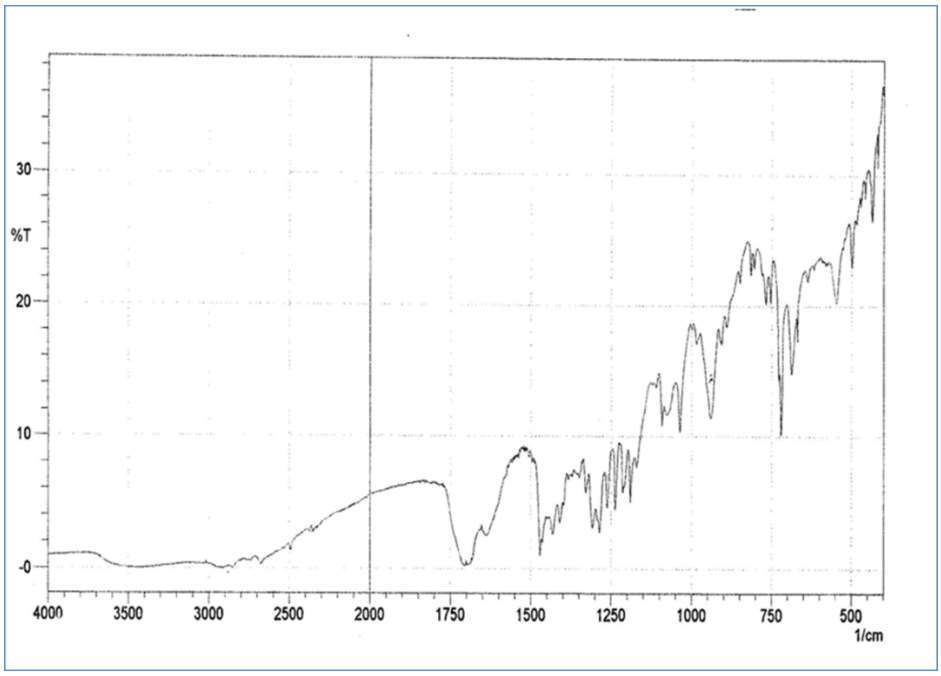

Figure S3: The FTIR spectrum of the compound **4**

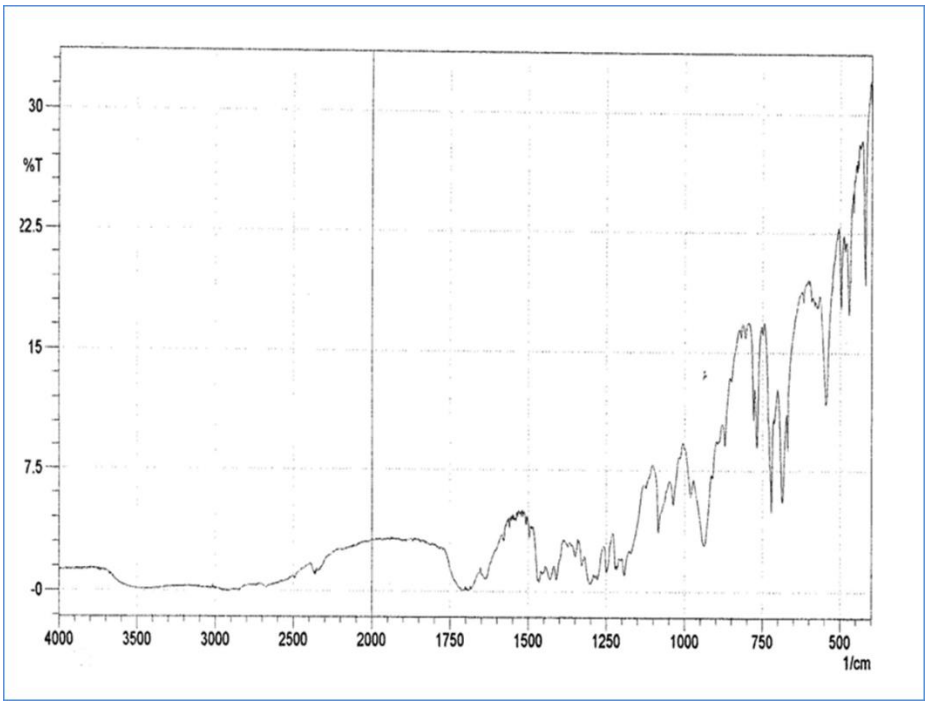

Figure S4: The FTIR spectrum of the compound **5**

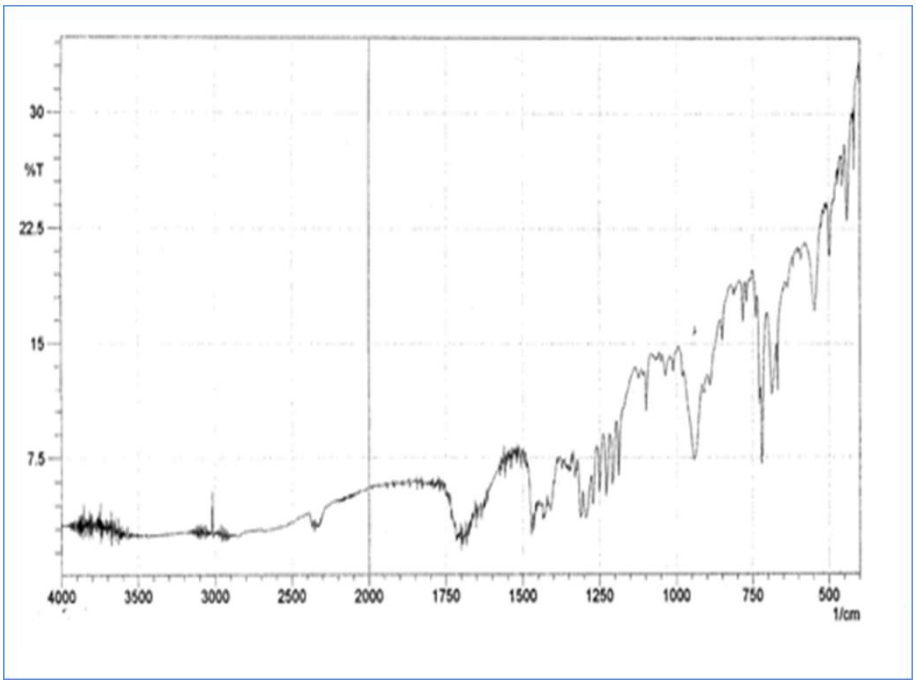

Figure S5: The FTIR spectrum of the compound **6**

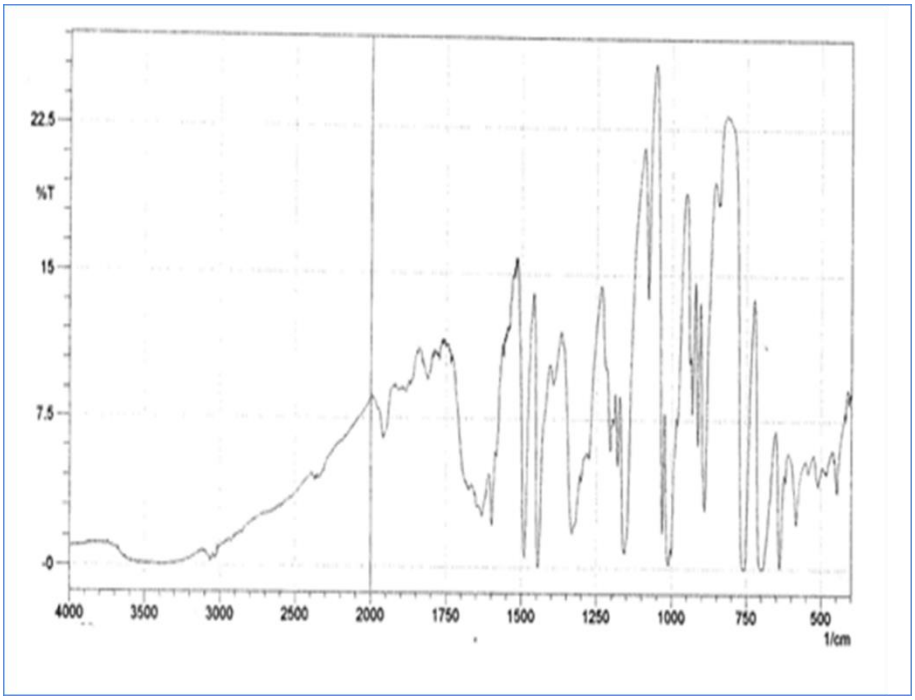

Figure S6: The FTIR spectrum of the compound **7**

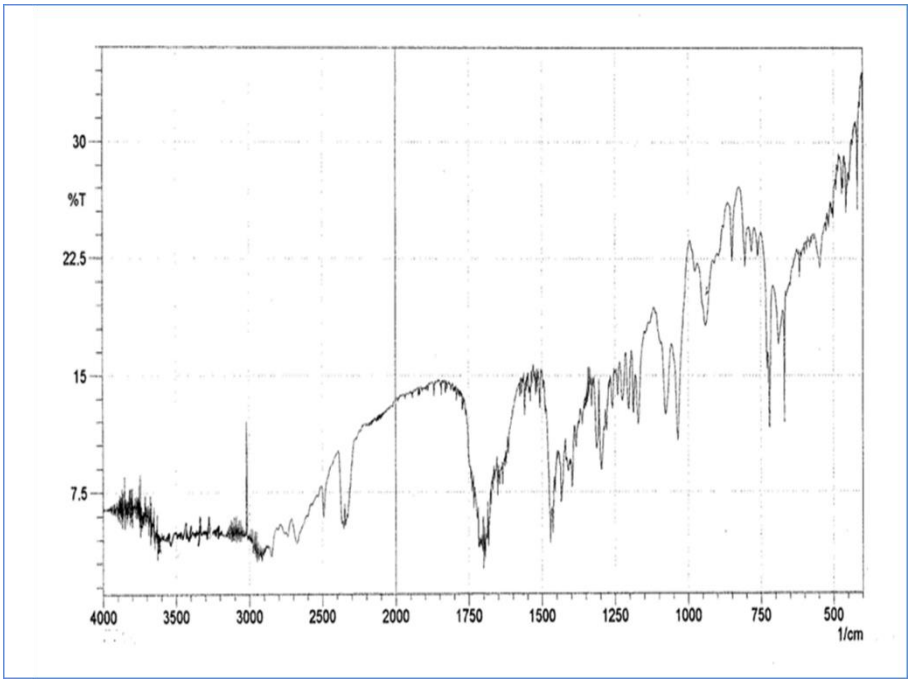

Figure S7: The FTIR spectrum of the compound **8**