ISSN: 2458-8989

Natural and Engineering Sciences

NESciences, 2026, 11 (2): 253-263 doi: 10.28978/nesciences.262023

Comparative DFT Analysis of Amoxicillin and Ampicillin: Electronic Properties, Molecular Stability, and Biological Activity

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Abstract

This study is based on a theoretical analysis using electronic density functional theory (B3LYP/ 6-31G (d, p)) to compare the properties and efficacy of two important antibiotics: ampicillin and amoxicillin. The research aims to optimize the molecular geometry of these molecules and analyze their electronic and thermal stability to identify the active sites most susceptible to nucleophilic or electrophilic attack. The (6-31G) base set was used to analyze the HOMO and LUMO energy levels, which provide a clear indication of the efficacy of both antibiotics. Additionally, thermodynamic functions, vibrational frequencies, and chemical stability were calculated. The density functional theory (DFT) calculations showed a high degree of structural similarity between the two antibiotics, which explains the convergence of their infrared spectra and several physical. The theoretical and computational chemistry results in this research showed higher thermodynamic values for amoxicillin and a larger energy gap for ampicillin, indicating that ampicillin is more chemically stable and less reactive compared to amoxicillin. The lower stability (smaller gap) of amoxicillin may explain its easier reaction with bacterial cells (along with the additional hydroxyl group that distinguishes it from ampicillin and increases its polarity, which may reflect the nature and mechanism of the interaction of each of the two antibiotics with bacterial targets)

Keyword:
Amoxicillin, Ampicillin, DFT

Available online: 02/06/2026

Introduction

The discovery of penicillin in 1928 by Alexander Fleming is considered one of the most important discoveries in human history. It was a serendipitous discovery; been contaminated he found that a green mold of Penicillium killed bacteria that had with it **(Gaynes, R. 2017)**. It was then developed by Howard Florey and Norman Heatley into a drug suitable for human use **(Shama, G. 2009)**, overcoming many deadly bacterial infections. However, bacteria developed mechanisms to resist penicillin **(Kholhring, L. 2021)**. Fleming, Florey, and Chain were awarded the Nobel Prize in 1945. Research efforts continued, leading to the development of the first semi-synthetic antibiotic, ampicillin, which was discovered in 1958 and entered clinical use in 1961 **(Rolinson, G. N et al 2007)**. It represented a significant generation of aminopenicillins that were able to combat many Gram-negative and Gram-positive bacteria **(Agersø, H.et al 1998)**. Ampicillin and Amoxicillin are both antibiotics belonging to the aminopenicillin group. Aminopenicillin is

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a Beta-lactam antibiotic **(Reeves, D. S.et al 1979)**. It was named so because it contains a chemical ring called a Beta-lactam ring. Bacteria contain structural enzymes called penicillin-binding proteins (PBPs**) (Akalin, H. E. 1999**). The beta-lactam ring binds to these enzymes in bacteria, preventing them from strengthening the bacterial cell wall, thus resulting in a fragile and incomplete cell wall. In humans, however, there is no cell wall but rather a plasma membrane; therefore, aminopenicillins are bactericidal **(Biczak, R., et al 2025).** Both amoxicillin and ampicillin share the same central penicillin nucleus and beta-lactam ring, which attack bacterial cell walls **(Biczak, R. et at (2025)**. The only difference is that amoxicillin has an additional chemical group attached to its aromatic ring This slight structural change gives amoxicillin a much higher absorption rate in the body and different antibacterial activity characteristics compared to ampicillin **(Premalath, R. 2019**). Despite the significant similarity in chemical structure between the two antibiotics, there is a fundamental difference that affects their antibacterial activity and absorption rate. Ampicillin contains the penicillin nucleus, while amoxicillin has the same structure but with the addition of a group to the aromatic ring **(Marie, -L. R et al 2019)**. This small substitution makes amoxicillin more stable in acidic environments, granting it a significantly higher absorption rate in the human digestive system and allowing for better bioavailability compared to ampicillin, and its absorption is impaired, causing it to remain in the intestines and leading to diarrhea and gastrointestinal disturbances **(Riveliño, R. C et al 2023)**. Although the two antibiotics are similar in their antibacterial activity, their pharmacokinetics differ significantly. Studies have shown that amoxicillin is characterized by excellent and rapid absorption in the gastrointestinal tract, reaching up to 90% absorption **(Argaman, N. et at 1998)**
, making it suitable for oral use against respiratory and ear infections. Ampicillin, on the other hand, is poorly absorbed, with absorption rates between 30-50%. It is less effective orally and its absorption is affected by the presence of food in the stomach **(Pawłowska, B.et at 2024).** To combat bacteria that produce a Beta-lactamase, amoxicillin is combined with clavulanic acid, which protects it from degradation, thus broadening its spectrum of activity against a large number of bacteria. Physicians prefer it because it is readily available and easy to administer **(Yadav R., et at 2018)**. Therefore, in this study, we attempted to employ density function theory to determine the differences in electron configuration and kinetic energy of the two antibiotics and the resulting differences in their biological activity **(Perdew, J. et at 2005).** Given the challenges associated with traditional laboratory experiments in monitoring the chemical reactivity of drugs Contemporary studies have increasingly focused on computational chemistry and its relationship to molecular modeling **(Nidaa A. J., 2026)**. The significance of this study lies in its application of density function theory to perform a precise comparison between two important drugs, amoxicillin and ampicillin, providing unprecedented insights into drug efficacy and enhancing the effectiveness of these two antibiotics.

Density function theory (DFT)

As a fundamental tool in physical and chemical research, density function theory is used to study and model complex biological molecules that are difficult to manipulate experimentally. It has proven highly efficient in studying complex molecules**,** replacing the wave function (which depends on a constant) with electron density **(Sholl, D. S.et at 2009)** et at which depends on three coordinates and is based on the Kohn-Sham principle. This principle states that electron density is the identifier that determines all the properties of a system in its steady state **(Kohn, W. D., 1996)**. This is achieved by transforming the electronic system into a virtual state and summing all the electrons to solve the Schrödinger equation **(Virtamo, J. 1976)**. The computer then solves the Kuhn-Sham equation iteratively (self-referencing), comparing the density to previous values until a similar state is reached, indicating that the compound has reached a stable state. Density function theory is not merely a computational tool; it is an identifier that determines most of the properties of complex systems**(Malykhanov, Y .et at 2003)**. Quantum computing is the dream of solving the problem of complex systems and turning it into an accessible reality**.** Digital quantum doping (DFD) is a revolution in computational cost, making the study and synthesis of proteins and drugs easier than ever before, after being a major challenge for chemists and physicists using complex wave functions **(Jasim, N. A. 2026a)**. This theory won the Nobel Prize in Chemistry, confirming its fundamental importance in science. It is currently used in battery design and understanding complex.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{eff}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

$V_{eff} = V_{ex} + V_H + V_x$

$$\rho(\mathbf{r}) = \sum_i^N |\varphi_i(\mathbf{r})|^2.$$

(∇^2) Laplacian operator, $(\hbar)$ Reduced Planck constant, (m) : mass of electron ,Veff: potential effective potential acting on the electrons , V_{ex} external potential , V_H : Hartree potential V_{xc} Exchange -Correlation, ψ_i Kohn-Sham Orbitals, ρ(r): electron density , r: position vector ,
$_i\mathcal{E}$: The orbital energy eigenvalue
$_i\mathcal{E}$: The orbital energy eigenvalue

Theoretical framework, computational methodology, and software used

The theoretical framework of this study is based on the Hohenberg–Kohn theorems, which prove that the ground-state energy of an interacting electron system is entirely determined by its electron density. To overcome the complex multi-electron interactions, the system is simplified into a single electron moving within an effective potential using the Kohn–Sham

The theory is based on Kohn-Sham equations **(Jasim, N. A. 2026b)**.

The calculations were performed using a freely available software free
(ORCA, GAMESS, CP2K, Caussin, Chemchrft (free) and ACD/hem Sketch

To obtain accurate and stable energies, the molecular geometries were fully optimized using the [B3LYP] functional combined with the6-31G (d,p) basis set. Long-range dispersion corrections, specifically Dispersion corrections such as ( ) were used, and the electronic properties were calculated based on the optimized structures. The electronic properties and their effect on biological activity were evaluated

Results And Discussion

Angles and lengths of Bonds

Comparing the bonds between amoxicillin and ampicillin using bond theory is an important and precise study for identifying structural differences and their impact on biological activity. The beta-lactam ring is the most important in both antibiotics and is the source of their biological activity. The bond lengths (C-N) and (C-O) are similar, meaning that the antibiotics are similarly susceptible to nucleophilic attack by bacterial enzymes. However, the presence of the hydroxide group in amoxicillin makes it more effective against bacteria. Furthermore, the (OH) group allows for hydrogen bonding with its molecules, which facilitates its solubility and rapid absorption compared to ampicillin. **Fig1, 2, Table1, 2**

$C_{16}H_{19}N_3O_5S$ Amoxicillin
Molar Mass: 365.4

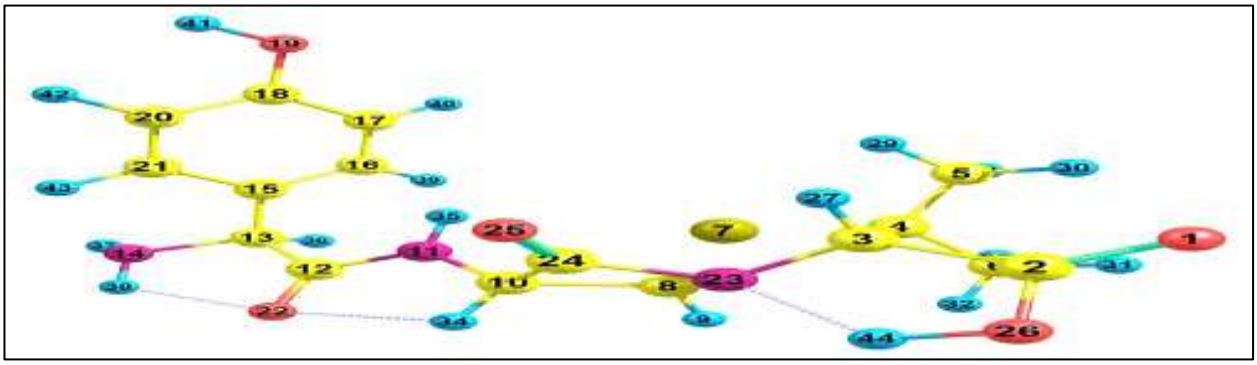

Figure 1. (2*S*,5*R*,6*R*)- 6-{[(2*R*)-2-amino- 2-(4-hydroxyphenyl)- acetyl]amino}- 3,3-dimethyl- 7-oxo- 4-thia- 1-azabicyclo[3.2.0]heptane- 2-carboxylic acid (Amoxicillin) $C_{16}H_{19}N_3O_4S$ Ampicillin

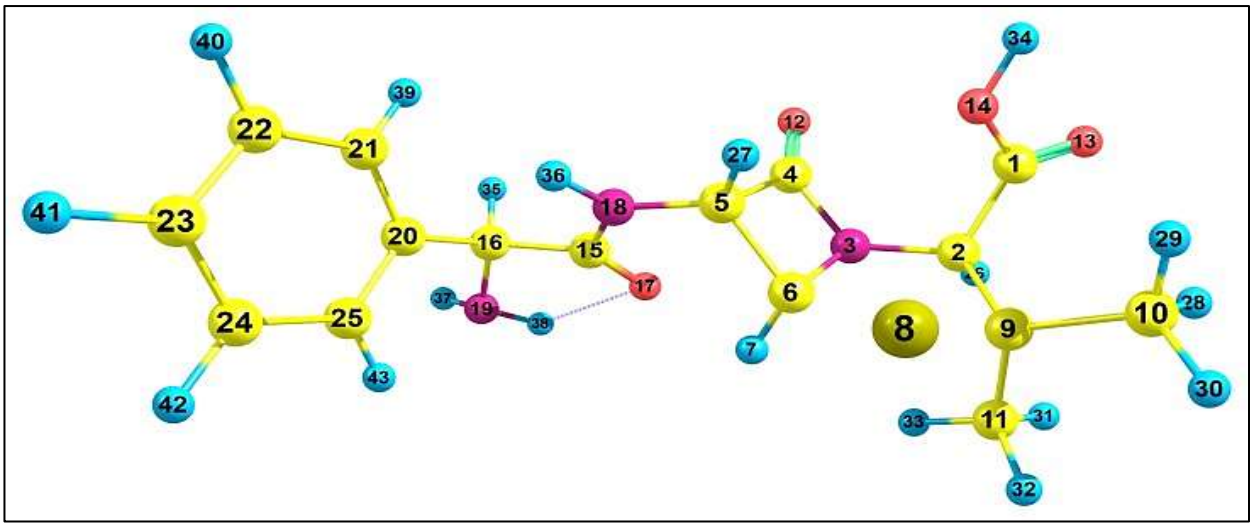

Figure 2. (2S,5R,6R)-6-([(2R)-2-Amino-2-phenylacetyl]amino)-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid (Ampicillin)

Table 1. Geometric Paramedic of important values of bond lengths in angstrom of Amoxicillin and Ampicillin

Type of Chemical bond	**Ampicillin**	**Amoxicillin**	**Significance Of Comparison and influence**
C-C (Aromatic ring)	1.391	1.394	It remains constant due to the similarity of the benzene ring.
N-C(Amine group)	1.468	1.465	Aliphatic nitrogen atom bond
H-N (Amino group)	1.013	1.011	Fixed bonds in the amino acid structure
C=O (B- Lactam ring)	1.216	1.214	Almost identical
N-C (B- Lactam ring)	1.364	1.366	The structural scope is similar in B- Lactam
N-H (Amide grope)	1.11	1.11	Stability of the Amid Group
S-C(Th1azolidine)	1.814	1.812	The connection of the sulfur ring in the five-membered ring
O-H	————	0.962	A unique property of amoxicillin
C-O(Carboxylic grope)	1.223	1.22	Terminal carboxyl group bond
CH_3-C (Methyl grope)	1.525	1.527	The methyl group attached to the thiazolidine ring
C-O (Phenol in benzen ring	————	1.366	A unique feature found only in amoxicillin

Table 2. Geometric Paramedic of important values of Angles in angstrom of Amoxicillin and Ampicillin

Type of Angles	**Ampicillin**	**Amoxicillin**	**Significance Of Comparison and influence**
-CN=O (B- Lactam)	93.5	93..7	Deviation from natural hybridization due to ring tension
-CN-C (Amino nitrogen)	123.5	123.2	Stable angles reflect the spatial shape of the ring.
-CC-C (Inter benzene ring)	120 .0	120.0	Perfect and flat in both compound
-SC-C (Sulfur angles in the ring thiazolidine)	94.8	95.1	

			Closely aligned annular tension angles in both compounds
-CN-C (Thiazolidine)	104,1	104.2	Slight curvature due to annular tension
-H-OH Phenol in benzen ring	———	109.5	This bond is characteristic of amoxicillin and determines its polarity.
-C-CO (Carboxyl grope)	126.2	126.3	Geometrically fixed angles through hybridization
-N=CO (Carbonyl)	132.1	132.0	

Charge and Electron density

Density function theory calculations show a marked increase in electron density on the oxygen atom of the phenolic hydroxyl group and within the nucleus of the beta-lactam ring in amoxicillin compared to ampicillin. The hydroxyl group acts as an electron donor via resonance, enriching the electron density of the pi cloud in the phenolic ring and influencing the electronic environment of the adjacent beta-lactam ring. From a biopharmaceutical perspective, biological activity is closely linked to electron density, as the electron effect of the hydroxyl group not only increases polarity but also contributes to improving the hydrophilic-lipophilic (HLB) balance of the compound. This optimal hydrophilicity significantly enhances intestinal absorption and acid stability in the gastrointestinal tract, resulting in superior bioavailability and higher serum concentrations of amoxicillin compared to ampicillin. Furthermore, the abundance of electron density affects the molecular boundary orbitals (HOMO/LUMO), increasing the efficiency of nucleophilic-electrophilic interactions necessary for binding to penicillin-binding proteins (PBPs) in the bacterial cell wall. This thermodynamic and kinetic preference accelerates the inhibition of cell wall synthesis, thus explaining the faster clinically observed bacterial lysis **Table 3, 4**

Table 3. Charge and Electronic Density of Amoxicillin atoms

Atom	Charge	Electronic Density	Atom	Charge	Electronic Density
O1	-0.4782	6.4782	N23	-0.5810	5.581
C2	0.709	3.291	C24	0.6398	3.3602
C3	- 0.1295	4.1295	O25	-0.4364	6.4364
C4	- 0.3349	4.3349	O26	-0.5562	6.5562
C5	- 0.5347	4.5347	H27	0.2706	0.7294
C6	-0.5291	4.5291	H28	0.2056	0.7944
S7	0.2922	5.7078	H29	0.2079	0.7921
C8	-0.2803	4.2803	H30	0.2389	0.7611
H9	0.2500	0.75	H31	0.2314	0.7686
C10	- 0.0911	4.0911	H32	0.1952	0.8048
N11	-0.7156	5.7156	H33	0.216	0.784
C12	0.7256	3.2744	H34	0.2819	0.7181
C13	-0.2095	4.2095	H35	0.3677	0.6323
N14	- 0.6699	5.6699	H36	0.2082	0.7258
C15	0.0173	3.9827	H37	0.2742	0.7258
C16	- 0.234	4.234	H38	0.2955	0.7045
C17	- 0.1792	4.1792	H39	0.1884	0.8116
C18	0.2875	3.7125	H40	0.2048	0.7952
O19	-0.5990	6.599	H41	0.3564	0.6436
C20	-0.2144	4.2144	H42	0.181	8190
C21	-0.1677	41,677	H43	0.2188	0.7812
O22	-0.5041	6.5041	H44	0.3812	0.6188

Table 4. Charge and Electronic Density of Amoxicillin atoms

Atom	Charge	Electronic Density	Atom	Charge	Electronic Density
C1	0.6661	3.3339	C23	-0.1864	4.1864
C2	-0.0533	4.0533	C24	0.1846 -	4.1846
N3	-0.5930	5.593	C25	-0.1711	4.1711
C4	0.7058	3.2942	H26	0.2577	0.7423
C5	-0.1191	4.1191	H27	0.2672	0.7328
C6	-0.2292	4.2292	H28	0.2153	0.7847
H7	0.2674	3.7326	H29	0.215	0.785
S8	0.289	3.711	H30	0.2104	0.7896
C9	-0.3418	4.3418	H31	0.198	0.802
C10	-0.5395	4.5395	H32	0.2119	0.7881
C11	-0.5082	4.5082	H33	0.2149	0.7851
O12	-0.4733	6.4733	H34	0.3731	0.6269
O13	-0.4722	6.4722	H35	0.2119	0.7881
O14	-0.5443	6.5443	H36	0.3489	0.6511
C15	0.7369	3.2631	H37	0.2729	0.7271
C16	- 0.2058	4.2058	H38	0.2961	0.7039
O17	-0.5075	6.5075	H39	0.1851	0.8149
N18	- 0.7346	5.7346	H40	0.1889	0.8111
N19	-0.6716	5.6716	H41	0.1887	0.8113
C20	0.0257	3.9743	H42	0.1903	0.8097
C21	-0.2356	4.2356	H43	0.2162	0.7838
C22	-0.1826	4.1826			

Thermodynamic functions

Based on the data obtained in this study, we observed significant differences between amoxicillin and ampicillin. Most of the thermodynamic properties of amoxicillin were found to be higher. The higher free energy value of amoxicillin (765.9 KJ/mol) compared to ampicillin (758.0 KJ/mol) reflects its thermodynamic stability, its ability to react, and its high efficacy against bacterial targets. While the high entropy (a measure of randomness) of amoxicillin indicates greater flexibility and more vibrational and rotational patterns, which facilitates its interaction with bacterial bio-binding sites (PBPs), we also observed a high thermal energy of amoxicillin, reaching (970.1 KJ/mol) in amoxicillin compared to (958.0 KJ/mol) in ampicillin .As is known from density function theory calculations, the higher the thermal energy with a smaller energy gap, the greater the molecule's ability to transfer electrons and the higher its biological activity. This interpretation supports the idea that amoxicillin possesses energetic dynamics that facilitate the donation or acceptance of electrons to form chemical bonds and enhance its biological activity within the body. Finally, the high (H^0 , G^0 ,S^0) values of amoxicillin indicate that it is a molecule with higher bioavailability and a large energy reserve, giving it a greater ability to bind to and target bacteria compared to ampicillin. **Table 5**

Table 5. Thermodynamic functions of Amoxicillin and Ampicillin

Comp.	S^0	E^0 (thermal)	H^0	G^0	A^0	Cv
	J /mol .K	KJ /mol	KJ /mol	KJ/mol	KJ /mol	J /mol
Amoxicillin	694	970.1	972.5	765.9	763.5	376
Ampicillin	679.6	958.0	960.5	758.0	755.6	362

Physical properties

The energy gap is the difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). It is a key indicator in density functional theory (DFT) for assessing biological stability and activity. The smaller this gap, the greater the chemical activity and reactivity, facilitating the donation or acceptance of electrons to form bonds with bacterial receptors. The only structural difference between amoxicillin and ampicillin lies in the hydroxyl group (-OH) attached to the para position of the benzene ring in amoxicillin, while ampicillin lacks this group. This group plays a crucial role in the electronic properties and biological activity of the compound. The presence of the hydroxyl group in amoxicillin increases resonance due to its electron-donating effect, leading to a lower energy level at the LUMO (making it more electronegative (-0.9469), thus bringing it closer to the HOMO. The presence of a hydroxyl group in amoxicillin also reduces its energy gap, making it more chemically active, more charge-transferring, and more polar, thus facilitating its penetration of bacterial membranes. These electronic and thermodynamic properties explain amoxicillin's rapid absorption into the body and its superior pharmacological efficacy compared to ampicillin.

Table 6. Physical properties of Amoxicillin and Ampicillin

Comp.	E^0 HOMO (ev)	E^0 LUMO (ev)	Energy gap (LUMO - HOMO) (ev)	IP (ev)
Amoxicillin	-5.8632	-0.9469	4.9163	5.8632
Ampicillin	-5.877	-0.3796	5.4974	5.877

IR Spectra

Density function theory is a powerful tool for interpreting the infrared spectra of drugs such as amoxicillin and ampicillin based on their structural composition, as studies have shown good agreement between theoretically calculated and experimentally determined frequencies

The beta-lactam ring exhibits sharp bands at high wavenumbers (1800 Cm^{-1}-1580 Cm^{-1}), which are specific to the carbonyl group in the tetrameric ring and constitute the signature region of the two antibodies. The amine and hydroxyl groups exhibit vibrational bands above 3000 Cm^{-1} (3540 Cm^{-1} – 3061 Cm^{-1}) as a result of vibrations of (-NH) and (-OH) which are affected by hydrogen bonds . While we observe the vibrational bands of the carboxyl group in both antagonists between (1793Cm^{-1} - 1660 Cm^{-1}) .The difference between amoxicillin and ampicillin lies in the presence of a hydroxyl group in amoxicillin on the aromatic ring, which leads to a slight shift in the The difference between amoxicillin and ampicillin lies in the presence of a hydroxyl group in amoxicillin on the aromatic ring, which leads to a slight shift in the vibrational bands compared to ampicillin, through the difference in electron density and the extension of the resonance outside the aromatic ring bands compared to ampicillin, through the difference in electron density and

Table 7. TR Spectra of Amoxicillin

Frequency Cm^{-1}	Frequency	IR intensities	Frequency Cm^{-1}	IR intensities	Frequency Cm^{-1}
0.1969	16.7129	33.0291	684.7259	0.5208	1314.539
0.7089	22.5244	90.0338	716.6316	5.1595	1320.668
0.0182	35.7057	67.0521	722.0078	25.6175	1340.009
1.0134	49.8724	1.9686	742.3224	356.7194	1359.33
1.7345	63.6695	9.2345	763.3707	58.7446	1364.113
0.7471	72.2103	3.4436	780.5949	33.8193	1367.465
1.7968	75.0183	30.4308	790.1141	2.464	1372.18
3.4634	85.2283	28.7825	810.8371	12.5658	1393.996
0.9718	120.9123	12.0177	827.1941	29.2847	1455.394
4.1866	133.3347	22.1857	846.4739	23.4762	1474.939
8.0049	150.0621	1.8347	854.9006	39.5768	1478.462
5.0843	178.4896	3.2972	864.2918	418.6253	1530.438
5.9453	201.6777	34.7033	867.3142	1.539	1542.052
0.9432	204.8601	57.9846	888.3869	54.7486	1561.268

3.5341	226.8516	6.4037	904.1366	9.5193	1561.763
3.3792	236.8073	60.321	907.5843	12.5018	1566.024
0.2513	259.4831	23.7145	962.1497	15.149	1582.068
7.1115	302.186	25.013	975.7247	17.2502	1614.286
26.4376	302.4376	3.7574	982.9515	75.354	1652.009
14.8084	305.6681	1.4664	1001.484	153	1656.173
5.4144	313.8981	106.8517	1007.339	63.8492	1730.448
1.0924	332.4902	21.8959	1023.665	235.3422	1793.495
8.7301	358.9143	2.1228	1026.326	201	1868.393
8.7779	364.8916	0.4175	1048.978	44.9116	2913.362
22.2272	369.4264	1.8626	1075.649	9.9341	3057.249
29.6951	371.1557	4.4518	1091.058	6.6765	3066.047
138.6575	381.2884	105.1436	1129.823	3.3731	3085.476
14.8364	404.8543	96.8405	1136.755	34.1659	3107.825
38.0444	409.5874	13.6345	1177.179	5.9384	3129.676
1.6753	452.287	18.1216	1185.719	8.3762	3132.281
15.587	457.726	32.2137	1187.774	10.649	3136.393
2.488	488.2733	156.6516	1190.111	6.7396	3149.533
9.6523	494.9707	66.5705	1199.648	13.1857	3173.781
3.6084	518.8744	65.3944	1205.091	10.4053	3179.358
11.0415	546.481	19.4664	1219.296	7.5555	3188.181
16.2196	567.4753	20.1313	1224.317	1.6639	3228.975
16.7776	573.4468	43.9096	1237.421	3.43	3233.101
20.2388	599.689	145.0765	1245.83	195.7421	3243.469
49.8842	614.1497	2.5565	1253.005	17.6369	3422.154
5.6598	621.2902	12.6293	1256.203	29.6192	3522.991
38.9151	663.5218	44.8125	1296.751	78.5385	3525.098
6.5017	674.6435	67.0882	1298.712	13.602	3540.776

Table 8. TR Spectra of Ampicillin

Frequency	**IR intensities**	**Frequency Cm^{-1}**	**IR intensities**	**Frequency Cm^{-1}**
15.4209	34.3864	721.1581	46.6838	1315.404
22.7878	54.9455	742.2866	6.0769	1345.64
37.5143	63.6154	746.3823	13.4084	1351.052
42.7664	77.0762	754.2973	57.9802	1361.334
63.266	10.2863	777.3245	23.3291	1369.59
69.8166	27.4999	799.6828	7.9902	1387.325
78.9454	7.8906	812.3256	5.0641	1401.288
81.9804	9.446	850.1275	17.9235	1458.051
119.5442	9.9609	854.0222	11.3773	1474.842
143.036	11.2496	869.7961	11.5808	1508.531
169.332	0.2075	888.4089	5.379	1541.939
184.1831	15.0145	895.7539	18.6505	1542.693
211.8525	12.7821	919.2447	0.3562	1551.543
221.5173	7.2797	946.2265	297.712	1552.749
236.3104	5.7788	961.8471	9.7079	1560.835

256.6104	8.1242	977.7485	11.0107	1577.786
276.2604	1.2444	985.9971	1.1995	1615.534
282.6333	22.3664	997.853	6.8551	1632.001
307.7427	1.0193	1018.675	148.8371	1652.954
317.5053	1.1112	1033.215	40.7552	1728.43
324.795	1.4662	1044.616	190.5072	1788.565
334.5156	6.7628	1061.608	309	1859.567
348.8543	51.4045	1066.003	38.3107	2926.639
373.9324	68.0185	1073.177	14.6104	3046.262
381.919	11.4615	1085.083	12	3061.101
402.3357	12.9076	1113.108	11.2327	3101.502
417.8962	68.861	1123.624	13.4012	3115.74
428.2843	23.0225	1134.935	6.5101	3127.151
437.7285	45.668	1177.689	1.698	3135.82
474.4968	12.9671	1187.583	8.8407	3142.368
496.9576	38.45	1199.206	12.5896	3146.05
546.9607	28.4437	1210.89	7.2233	3168.894
549.6672	11.3709	1225.419	0.4148	3191.154
556.0313	7.8392	1227.162	3.9463	3200.423
574.708	3.5784	1231.315	17.0484	3201.076
599.8091	11.495	1241.096	14.8538	3215.993
630.2019	6.0676	1247.971	6.4689	3229.223
634.5173	13.8736	1250.088	26.9903	3410.269
651.4016	181.6883	1274.441	26.3916	3477.61
658.7788	43.4403	1279.627	9.918	3532.167
693.3003	8.6015	1307.262	107.7742	3537.197

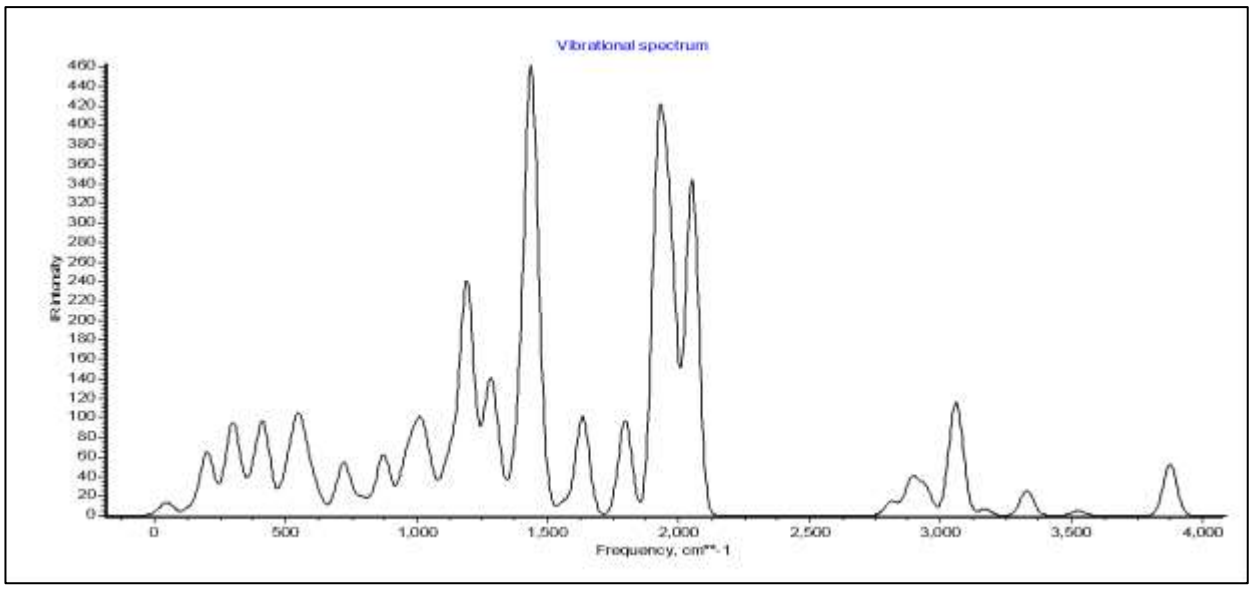

Fig 3. Vibrational Spectra of Amoxicillin

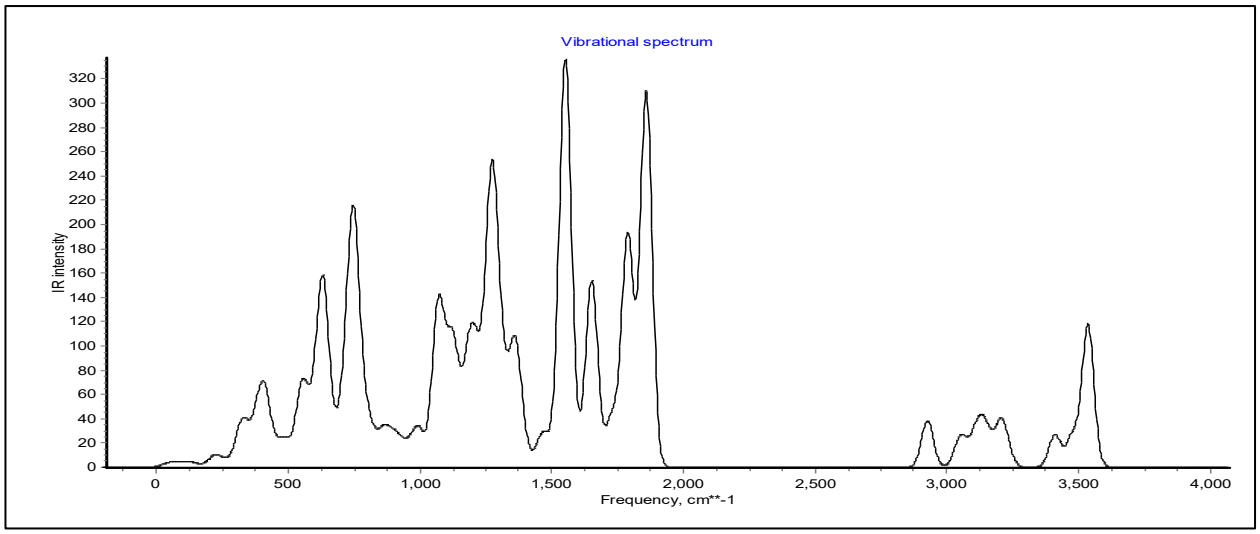

Fig 4. Vibrational Spectra of Ampicillin

Recommendations

1)This study saves time and cost by allowing for a comparison between the important penicillin compounds amoxicillin and ampicillin, which are large biological compounds that are difficult to study experimentally.

2)Comparing penicillin antibiotics is a crucial topic, as they are large molecules. The aim is to improve biological activity and reduce side effects by adding electron-donating groups to the benzene ring, which extends the ring's resonance and increases activity and efficacy against bacteria

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