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ORIGINAL ARTICLE

Increasing the efficiency of some antibiotics on penetrating bacteria cell membrane

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By this work, it has been concluded that through halogenated functionalizing of Sulfonamide, Triclosan, Baxdela, Ticarcillin, Ampicillin, and Clavulanic acid we are able to control the treatment of those antibiotics against Gram-positive or negative bacteria of various ecologies. The efficiency of Sulfonamide, Triclosan, Baxdela, Ticarcillin, Ampicillin and Clavulanic acid in viewpoint of NMR shielding and S-NICS methods have been studied as a drug delivery approach. We exhibit some halogenated compounds of those antibiotics, specific chemical derived produced, which are primarily against “gram positive” bacteria (due to higher percentage of “peptidoglycan protein” in the cell membranes). Since Gram-positive bacteria which made of peptidoglycan has a very thick cell wall, some of the antibiotics can penetrate gram (+) and some others cannot. In this work, a list of antibiotics and their halogenated deviated have been set-upped due to the Gram-positive bacteria. A list of halogenated compounds had been reported based on mechanism of the S-layer with two different attachments; for gram (+) it is attached to the peptidoglycan and for gram (-) directly to the outer layers of bacteria.
Key words: Sulfonamide; Triclosan; Baxdela; Ticarcillin; Ampicillin and Clavulanic acid; NMR and S-NICS

Introduction

Antibiotic molecules are able for stopping or killing the growth of, microorganisms, including both fungus and bacteria which are called "bacteriostatic" and "bactericidal" respectively (Genc, 2008). Antibiotics are specific chemical compound which is produced through living organisms and can inhibit the life processes of the various organisms and tissues. The first antibiotics were extracted from “micro-tissues” but some are now received from especial plants or animals. Over 2,000 antibiotics have been known and characterized up to now, but only a few of them are used in high quality medicines (Boxall, 2004).

Although sulfonamides (Lakshmi, 2013), groups were the first antimicrobial (Epand, 2010), to be developed for several of techniques, recently Triclosan, Baxdela, Ticarcillin are extensively applied for antibacterial agents in the modern drug deliveries. Therefor those of them within sulfonamide-based compounds are most important for the second antimicrobial agents and in adition, those are widely used in human and veterinary medicine for preventing of bacterial (Epand, 2010) infectious diseases. An important but often disregarded aspect of antibiotic use is the fate of antibiotic residues entering the environment (Boxall, 2004). In this study increasing the efficiency of those antibiotics on penetrating to bacteria’s cell membrane to control both gram positive and negative treatment has been investigated through halogenated functionalizing. Penicillin which was discovered and characterized by Alexander Fleming in September 1928 has been used in the treatment towards bacteria invasion. Fleming who was working at St. In recent decades; pharmaceutical antibiotics were recognized and sensitized as emerging soil pollutants while the compounds such as sulfonamides and tetracycline reach agricultural land mostly through infected dung from medicated chattels used as muck (Ghosh, 2011).

As an important antibiotic sulfonamide can be mentioned, this is commonly used drug in primary care practice. Reaction to Sulfonamide (Owa, 1999) Antibiotic is relatively common as compared to other antimicrobials (Chohan, 2008). The hypersensitivities reaction, consisting of fever and non-urticarial rash, usually develop seven up to fourteen days after the medication initiation. The term “sulfa” refers to a derivative of an antimicrobial agent (Epand, 2010), “sulfanilamide”. In this work a list of antibiotics has been reported based on mechanism of the S-layer with two different attachments; for gram (+) it is attached to the peptidoglycan and for gram (-) directly to the outer layers of bacteria. By this work, it has been concluded that through halogenated functionalizing of Sulfonamide (Narasaiah, 2008), Triclosan, Baxdela Ticarcillin, Ampicillin and Clavulanic acid we are able to control the treatment of those antibiotics against Gram-positive or negative bacteria. We exhibit some

compounds of those antibiotics, specific chemical derived produced, which are primarily against "gram positive" bacteria (due to higher percentage of "peptidoglycan protein" in the cell membranes). Since Gram-positive bacteria which made of peptidoglycan has a very thick cell wall, some of the antibiotics can penetrate gram (+) and some others cannot. In this work, a list of antibiotics and their halogenated deviated have been set-upped due to the Gram-positive bacteria. We have exhibited the especial properties of those antibiotics in view point of NMR shielding and S-NICS methods (Derakhshandeh, Monajjemi, 2017) for delivering in cell membrane (Monajjemi, 2015) via QM/MM and ab-initio methods. In eukaryotic cell's phospholipids, the prokaryotic plasma consists of mainly one kind of phospholipid. For bacterial (Epand, 2010) cells the phospholipids are to a huge extended phosphate-dyl-ethanolamine (PE) (Fig. 1). The residual lipids are negatively charged at physiologically situations, where phosphate-dyl-glycerol (PG), or its derivatives as the same DPG (di-phosphate-idyl-glycerol) or CL, "Cardiolipine" are prevailing. In addition, the lipid structures also based on whether the bacterium belongs to the class of Gram (-) or Gram (+) bacteria (Fig. 1). The bacterial membrane (Goldfine, 1984) shortcoming sterol and have followed other means of strengthening their combination.

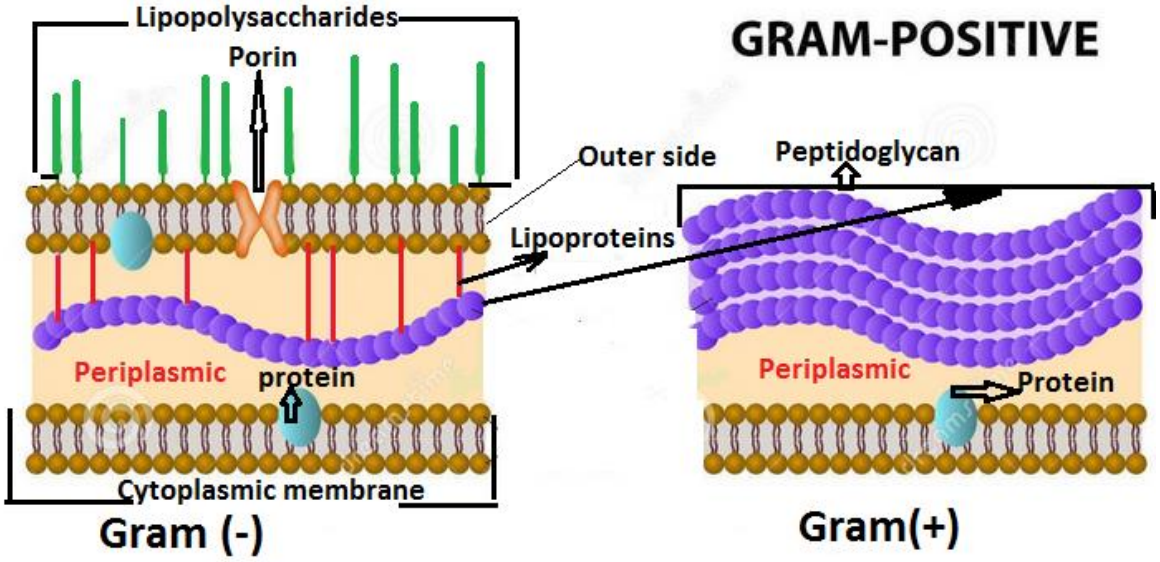


Fig. 1. Representation of the cell membranes of Gram (+) and Gram (-) for bacteria Gram(+) such as Mycobacterium and Nocardia is included of peptidoglycan, Polysaccharides, Ribitol, Glycerol and Glycolipids and Gram(-) Such as E Coli is included of LPS, Lipoprotein, Porins and peptidoglycan

Bacteria with single membrane are known as Gram (+) including a thick peptidoglycan Layers with attached proteins and different glycol-polymers like poly-saccharides and teichoic[31]. Those layers encase their cytoplasmic of membrane and take up the crystal violet stain used in the Gram staining method, as is known by the names. In gram (-) Bacteria's cell, the cytoplasmic region is restricted by considerable thin peptidoglycan layers over-layed by an asymmetrical phospholipids bilayer and lipo-poly-saccharides containing some proteins. In common, higher molecules of PE are placed in the cell membranes (Monajjemi, 2015 Cell membrane...) of Gram (-), while the cytoplasmic of Gram (+) is rich in PG. The lipid compound of various Gram (-) and Gram (+) are discussed in result section based on halogenated functionalizing of mentioned antibiotics.

Methods

(S-NICS method and NMR shielding):

The study of net components of a membrane can help understanding of basic biological membrane structures, interaction and mechanisms with proteins insertion and the environment of other components (Boxall, 2004). Although, precise structure of a bilayer that is in the biological pertaining fluid phase is not able for obtaining experimental data, fluctuation of this kind of bilayer indicates correct structure. Molecular modeling is a strong tool for guiding the interpretation of experimental section. The credit of simulation, in other words, might be measured against existing experimental results. There are several techniques such as deuterium NMR quadrupol splitting that can give certain results of electrostatics surfaces per lipid membrane thickness (Haque, 1984). The absence of experimental data is reversed in molecular modeling of lipid membranes (Seelig, 1974), due to force field parameterization. Tight level ab-initio estimation which is needed for definition and parameterization of force fields, presently allows evaluation of those heavy atoms for gaining accurate results. The mentioned method clearly has been discussed in our previous work (Derakhshandeh, 2017; Monajjemi, 2015) Cell membrane) about a statistical approach in NMR shielding and nucleus independent chemical shifts S-NICS which was based on the treatment of asymmetry (η) and skew (κ) parameters. In this work, we have investigated this method via computing the statistical nucleus-independent chemical shifts in view point of probes motions in the sphere of de-shielding and shielding spaces of some hereto rings in sensitive antibiotics-Ecoli complexes.

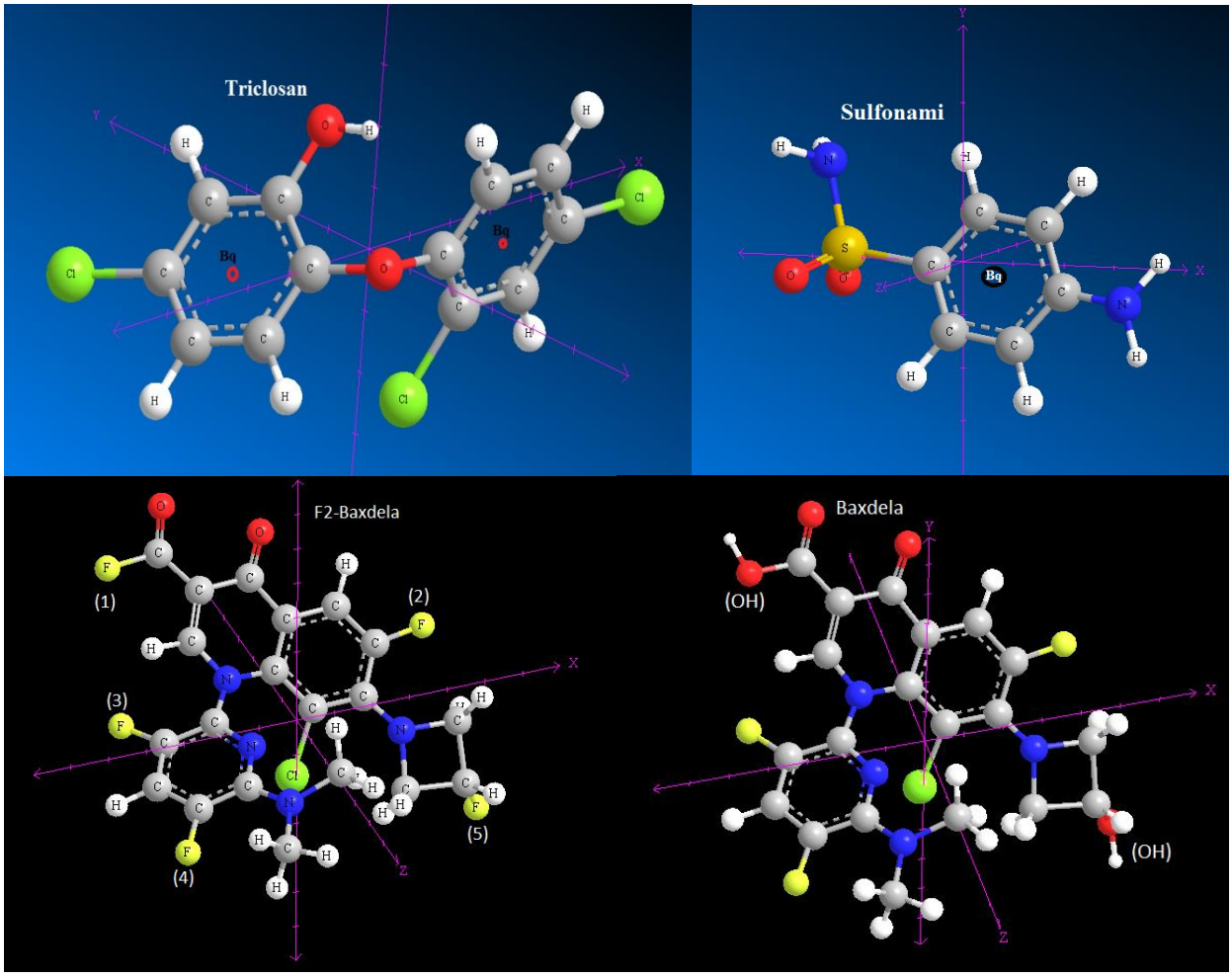
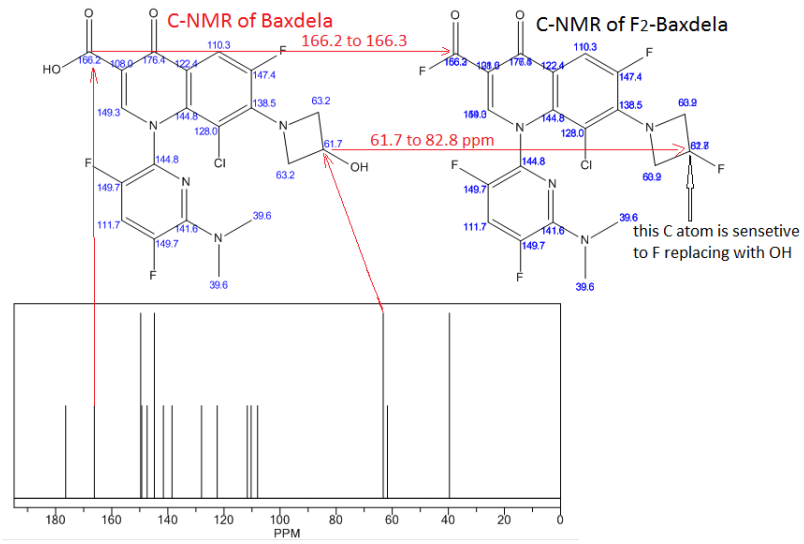


Fig. 2. Optimized (B3LYP-D3/TZP) structures of Triclosan, Sulfonamid, Baxdela and Floriated of Baxdela through two F atoms (number 1 & 5) instead of two (OH) groups, Using "Bq" inside the rings for S-NICS calculations

The NMR (Monajjemi, 2014) parameters including isotropic shielding (σ_{iso}), anisotropic shielding (σ_{aniso}) and chemical shift (δ) were also evaluated after the optimized geometries of all antibiotics structures. The default gauges-including atomic orbital (GIAO) orbitals were used to obtain molecular magnetic susceptibilities, NMR shielding with Gaussian 09 in all calculations (Berlin, 1978).



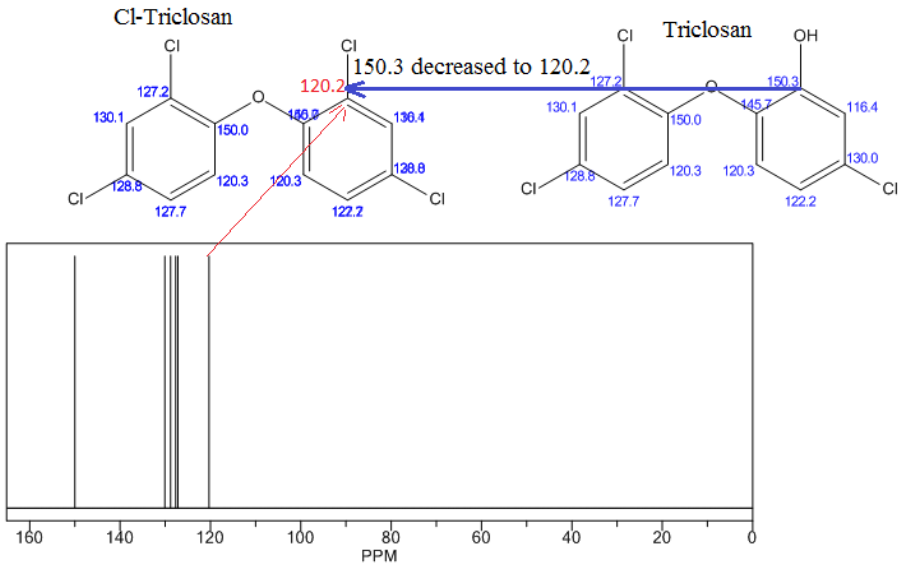


Fig. 3. NMR Shielding Changing of F_2-Baxdela compare to Baxdela and Cl-Triclosan compare to Triclosan

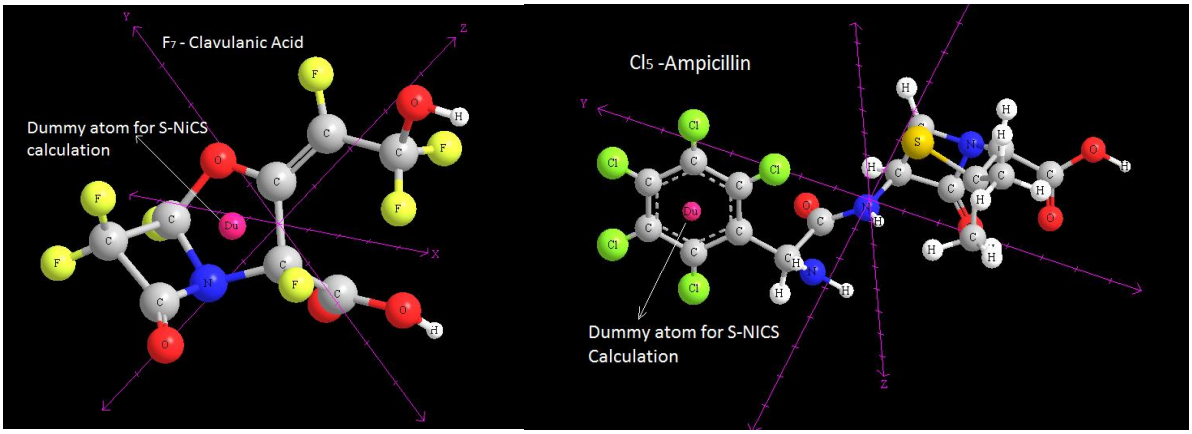


Fig. 4. F7-Clavulanic Acid and Cl5-Ampicillin for S-NICS calculations including dummy atoms

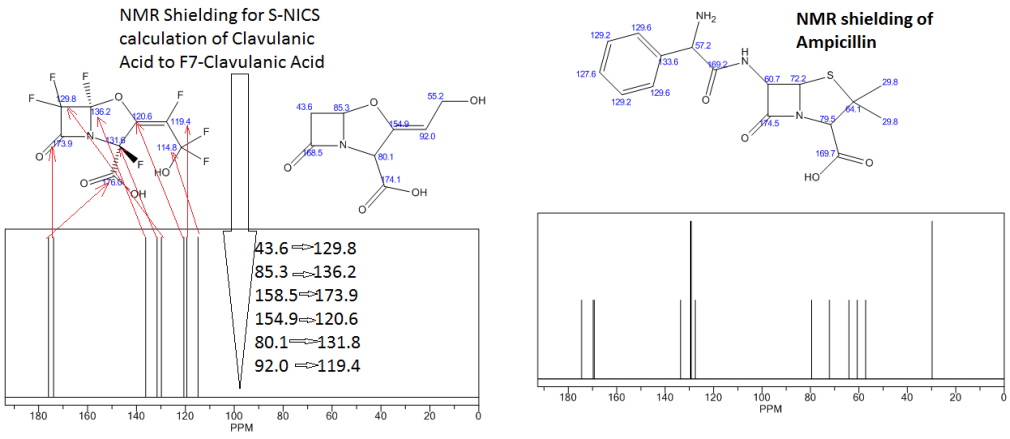


Fig. 5. NMR Shielding Changing of F_7-Clavulanic acid compare to Clavulanic acid and Ampicillin

The positive and negative value of this function correspond to the relationships between $\nabla^2\rho$ (density of electrons) and valence shell electron pair repulsion (Monajjemi, 2015) (VSEPR) model, chemical bond type, electron localization and chemical reactivity respectively, which have been built by Bader (Bader, 1990).
Becke (Becke and Edgecombe,1990) noted that spherically averaged like-spin conditional pair probability has direct correlation with the Fermi hole and then suggested electron localization function (ELF). Savin et al (1971) have reinterpreted the ELF in view point of kinetic energies (see also Lu, 2012), which makes ELF also explaining for Kohn-Sham DFT wave-function.

They show which $D(\mathbf{r})$ reveals the excess kinetic energies densities caused by Pauli repulsion (Monajjemi, 2015), while D_0can be considered as Thomas-Fermi kinetic energies density. Localized orbital locator (LOL) is another function for locating high localization regions likewise ELF, defined by Schmider and Becke (see Lu, 2012)

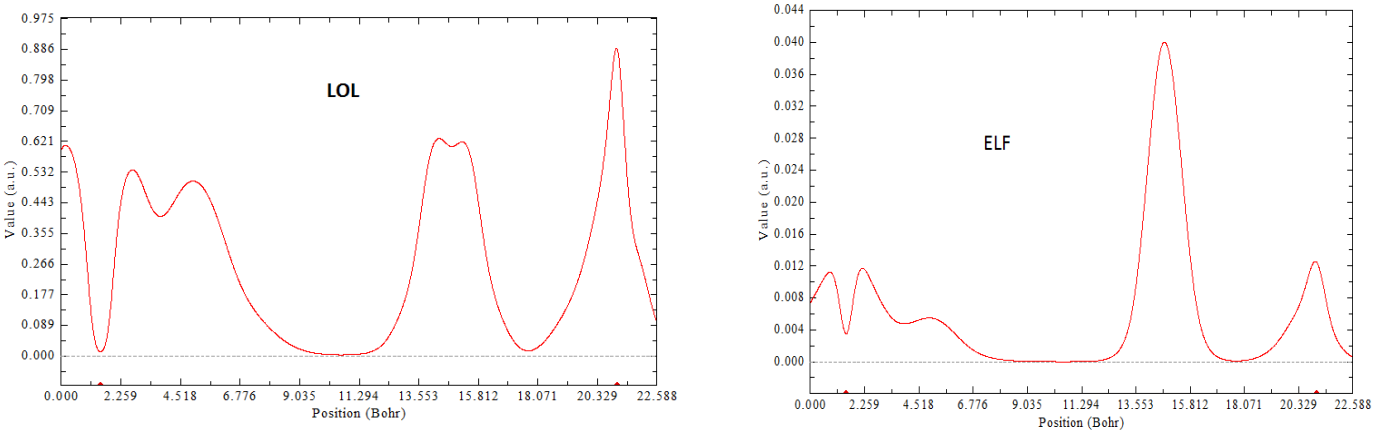


Fig. 6. "ElF" profile and LOL curves of Triclosan in water

Computational details

By this work we have modeled a narrow of membrane thickness (Haque, 1984) including di-palmitoyl-phosphatidyl-choline or $(DPPC)_n$ through QM/MM calculation using charm force fields. Each segment was designed of 60 lipid molecules surrounding with water molecules. In this investigation, differences in force fields are accomplished by comparing the several energies through using AMBER, OPLS and CHARMM force fields. We have investigated density functional theory with the van der Waals densities functional for modeling the exchange-correlation of DPPC units in membrane.

Tight & post-HF ab-initio calculation has applied to model the exchange-correlation energies of the hetero rings of the antibiotics structures. The double ζ-basis set with polarization orbitals (DZP) were used for the hetero rings. The charges and electrostatic potential-derived charges of the halogens were also estimated using Merz-Kollman-Singh, chelp[56], or chelpG[57]. Calculations were performed using packages of Gaussian 09 and GAMESS. The ONIOM methods including 3 levels from high calculation (H), medium (M), and low (L) have been accomplished in this study. The B3LYP-D3/TZP, CAM-B_3LYP and M06 methods are used for high layer of the model and the semi empirical methods of "Pm3MM" including pseudo=CEP and "Pm6" are used for the medium and low layers, respectively. In the calculations, we also have mainly focused on getting the optimized results for each item from "advanced DFT" methods including the "m06-L", "m062x", "m06-L", and "m06-HF" which are novel Meta hybrid DFTB. SPSS "Statistical Package for the Social Sciences" has applied for editing and analyzing all sorts of our S-NICS data of the heterocyclic antibiotics in this work. The semi empirical methods have been used to treat the non-bonded interactions between two parts of upper lateral phospholipids side (P_+) and downer lateral phospholipids side (P_-). The interaction (Monajjemi, 2010; 2012) energy for membrane as a capacitor (Monajjemi, M, 2014) was calculated in all items according to the equation:

$$E_S(eV) = \{E_C - \left(\sum_{i=1}^{60}(DPPC_+)_i + \sum_{i=1}^{40}(DPPC_-)_i\right) + \sum Antibiotics\ moleculs\}\ + E_{BSSE}$$

Where the "ΔE_S" is the stabilities energy of membrane-antibiotics system (Haque, 1984).

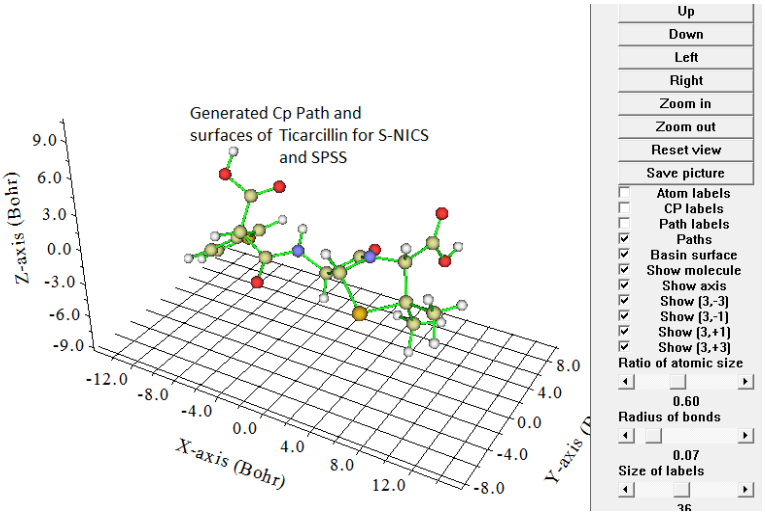


Fig. 7. Generated CP path and surfaces of Ticarcillin for S-NICS and SPSS Calculations

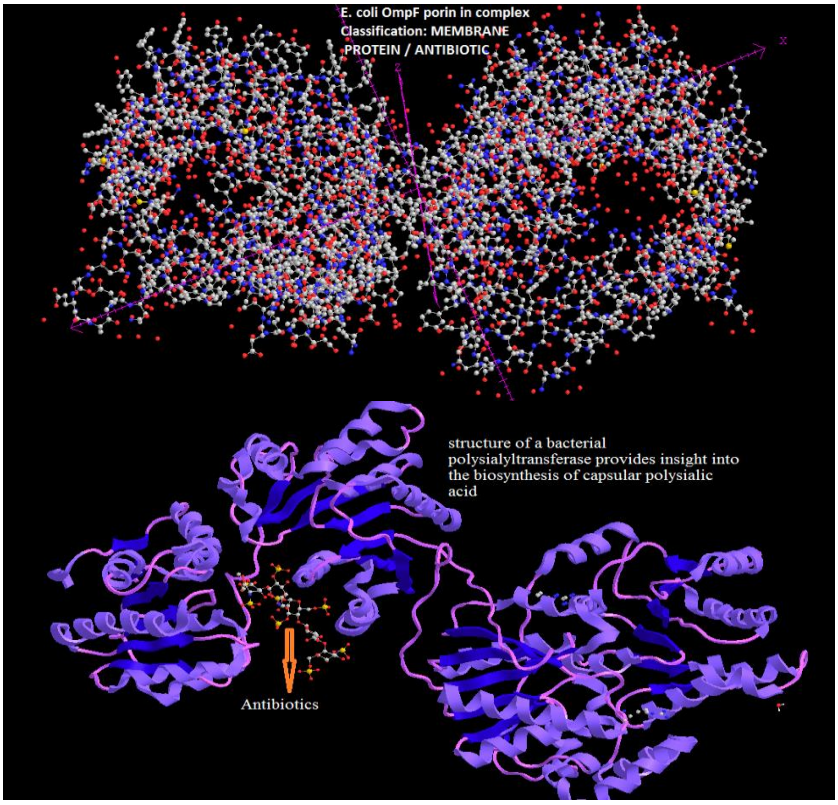


Fig. 8. Molecular Dynamic optimization on simulation of Membrane /protein/antibiotics

Result and Discussion

In this work, we have modeled and simulated those mentioned antibiotic's properties through QM/MM calculations based on specific chemical derived produced, which are primarily against "gram positive" bacteria. Since Gram-positive bacteria which made of peptidoglycan has a very thick cell wall, some of the antibiotics can penetrate gram (+) and some others cannot. The data and results are listed in 7 figures and 5 tables. By this investigation, we have exhibited a statistical method by computing of nucleus-independent chemical shifts in point of probes (BQ) motions around the center of shielding and de-shielding spaces of antibiotic's hetero-rings. In the previous works, it has been exhibited that S-NICS approach is a suitable method for calculation of the aromaticity (Monajjemi, 2012) in non-benzene rings such as those halogenated antibiotics which are important index for Membrane /Protein / Antibiotics interactions (Monajjemi, 2010; 2013) – see Fig. 8.

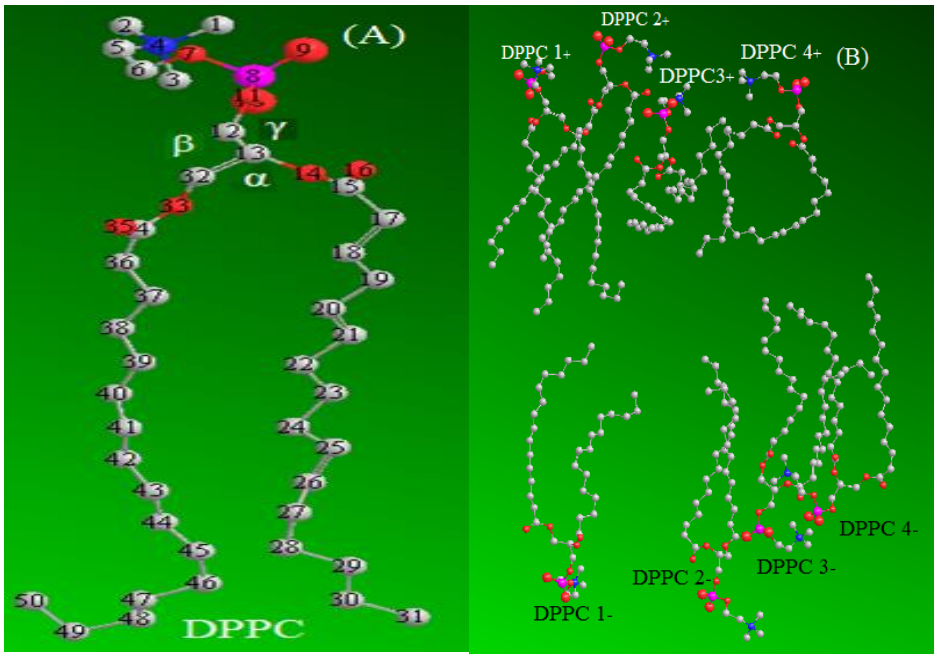


Fig. 9. Membrane simulation including 120 molecules of DPPC phospholipids.

Table1. S-NICS, Charge (ESP), isotropy, span and aromaticity of some atoms of Baxdela in gas phase and solvent media

Cl_3-Triclosan gas phase							Cl_3-Triclosan in water						
Atom	**Charge**	**σiso**	**S-NICS**	**η**	**Δδ**	**Ω**	**atom**	**charge**	**σiso**	**S-NICS**	**η**	**Δδ**	**Ω**
14 Cl	0.20	50.9	52.5	0.87	-137.6	-91.7	**14 Cl**	0.242	120.2	110.5	0.28	36.13	24.09
16 Cl	-0.35	159.	162.0	0.98	-11.98	-7.93	**16 Cl**	0.13	25.7	23.6	0.59	13.3	8.87
14 Cl	0.168	26.0	28.05	0.13	-6.2	7.37	**14 Cl**	-0.45	168.5	144.5	8.6	29.7	-13.4
17 O	0.18	29.3	9.37	0.70	-11.0	-7.3	**17 O**	0.13	29.7	30.1	0.53	10.15	6.7
13 O	0.15	30.1	34.56	0.83	-4.19	3.04	**13 O**	-0.19	130.3	129.7	5.9	9.53	-26.9
1 C	0.16	25.9	12.3	0.18	-7.2	8.24	**1 C**	0.242	120.2	122.1	0.28	36.13	24.09
5 C	0.17	28.6	11.68	0.80	-10.5	7.7	**5 C**	-0.69	245.2	250.4	0.58	50.4	33.6

Table 2. S-NICS, Charge (ESP), isotropy, span and aromaticity of some atoms of Cl_6-Ampicillin in gas phase and solvent media

F_3-Baxdela in gas phase							F_3-Baxdela in water						
atom	**charge**	**σiso**	**S-NICS**	**η**	**Δδ**	**Ω**	**atom**	**charge**	**σ-iso**	**S-NICS**	**η**	**Δδ**	**Ω**
22 Cl	-0.34	157.3	150.9	0.8	-22.9	15.3	**22 Cl**	-0.4	167.0	154.5	0.1	-120.6	113.7
20 F	0.17	29.1	27.7	0.9	-7.8	-5.2	**20 F**	-0.25	160.5	162.4	0.0	-112.1	108.1
21 F	0.181	29.7	26.13	0.3	-9.3	-6.2	**21 F**	-0.44	141.1	149.9	0.1	-125.7	117.1
23 F	-0.13	114.2	26.6	0.5	-20.1	9.9	**23 F**	-0.45	168.3	162.9	0.1	-120.7	113.8
10 N	-0.36	157.2	156.3	0.8	-5.8	4.2	**10 N**	-0.67	248.3	246.93	0.1	-240.6	227.0
15 N	-0.33	156.1	157.2	0.8	-16.3	11.4	**15 N**	0.32	65.27	63.7	0.2	93.78	62.5
24 O	-0.16	66.4	126.8	0.7	144.8	96.5	**24 O**	0.23	67.9	67.0	0.4	97.0	64.6
27 O	-0.21	147.0	145.1	0.5	-19.6	-13.0	**27 O**	0.13	78.2	79.2	0.2	139.2	92.8
1 C	0.14	30.7	27.1	0.5	-9.2	-6.1	**1 C**	0.16	30.1	29.9	0.7	-6.0	4.6
11 C	0.15	29.6	30.8	0.4	-2.7	2.5	**11 C**	0.12	30.0	6.8	0.8	-7.4	-4.9

Based on the data presented in Tables 1-2, isotropy and asymmetry (η) have been calculated for Cl_3-Triclosan, F_3-Baxdela, Cl_6-Ampicillin, and F7-Clavulanic acid. Gram (+) such as Mycobacterium and Nocardia includes the peptidoglycan, Polysaccharides, Ribitol, Glycerol and Glycolipids and Gram (-) such as E Coli including LPS, Lipoprotein, Porins and peptidoglycan. The Molecular Dynamic optimization of those antibiotics with E-coli [gram (-) classification] membrane /protein / antibiotics, have been calculated through the QM/MM simulation with CHARMM force fields and anisotropy has been yielded from the equation (4). We have modeled a section of membrane (Haque, 1984) systems including di-palmitoyl-phosphatidyl -choline $(DPPC)_n$ via those mentioned methods using Monte Carlo (Fig. 2) (Elsagh et al., 2016). Each system was combined of sixty lipids surrounding with water (Seelig, 1974). Thermodynamic averages were calculated from those methods, as the minimum-energy structures which indicate the resistance of membrane /protein/antibiotics. E Coli which includes LPS, Lipoprotein, Porins and peptidoglycan (Figs 8, 9), is some famous bacteria in Gram (-) groups. By this work, through halogenation of antibiotics (Table 3), we exhibited that by changing the aromaticity (total S-NICS value) (Monajjemi, 2012) the bacterial (Epand, 2010) resistance might change due to a relation between S-NICS and resistance. This study is also focused on the electron density of Halogens which is replaced with hydrogen of Ampicillin, Clavulanic acid, Imipeneme, Penicillin, and Ticarcillin in point of view in S-NICS method. The largest

electron localization is located on halogen atoms which indicate the suitable changing of aromaticity and consequently the resistance.

Table 3. The relation between resistance and S-NICS for E-coli

Class of antibiotics	Antibiotics	Halogenated antibiotics	S-NICS (+) increasing aromaticity (-) decreasing aromaticity	Resistance based ΔG interaction (-) decreasing (+) increasing
Penicillin	Ampicillin	Cl_6-Ampicillin	+	-
	Amoxicillin Clavulanic acid Ticarcillin	F_7-Clavulanic acid	+	+
Carbapenems	imipenem	F_3-imipenem	-	+
Quinolones	Triclosan Norfloxacin Ofloxacin	Cl_3-Triclosan	-	+
sulfonamides	Sulfonamide	Cl_2F_2Sulfonamide	+	-
Fluoroquinolone	Baxdela	F_3-Baxdela	-	+

Conclusions

A good result of the theoretical analysis of antibiotics- S-NICS methods is the stable model for drug designing. In this work, a relation between aromaticity and resistance of antibiotics has been exhibited. This resistance is due to membrane potential changing with different compositions of antibiotics-lipids interaction or further affects the interactions with antimicrobial peptides (Epand, 2010).

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