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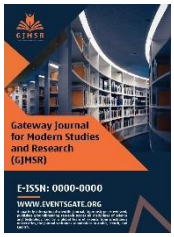

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Exploring Polymer-Saccharide Interactions: A Computational Approach for Biosensing Technology

Eman A.M. AL-Jawadi
College of Environmental Science, University of Mosul, Mosul, Iraq
Email: emanaljawadi@uomosul.edu.iq

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Abstract: The study employed semi-empirical methods and the molecular mechanics (MM2) force field to calculate the steric energy and heat of formation of glucose in various conformations. The appropriate geometric interactions were confirmed, revealing that Poly-Pyrrole (ppy) interacts specifically with the ß-form of glucose. This finding aligns well with previous studies that used modified pyrrole electrodes to determine glucose experimentally. These results suggest that the molecular docking approach is a suitable method for theoretical studies in biosensor development.

Keywords: Molecular Docking, Semi-Empirical Methods, Carbohydrate-Polymer Interactions, Theoretical Studies.

1. Introduction:

Glucose is the principal sugar in blood; it is the main form of carbohydrate utilized by cells. In this work, we study glucose in three forms: the straight-chain structural formula (D-Glucose) and the cyclic forms represented by β-Glucose and α-Glucose. (Jamdade,2026; Khwaiter,2025) As is well known from the literature, molecular recognition is a central phenomenon in biochemistry. The highly specific recognition of, for example, enzymes and their substrate, protein receptors and signal ligands, or antigens and antibodies in biological systems is crucial to the functioning of complex life forms. (Al-Jawadi et al., 2012; Alzeer,2025; Krishna,2026; Pedrotti et al.,2026).

Current research focuses on finding the best methods to detect compounds in the body, such as drugs, substrates, or enzymes, by modifying biosensors. (Feng etl,2026; Rowaiye et al.,2025) Much work has been done to develop different biosensors, specifically glucose biosensors. (Al-Jawadi et al.,2021; Kim et al.,2019). Such studies require numerous experiments modified with different polymers. (Chanbey et al.,2002)

However, these methods have obvious limitations as they depend on the substrate, enzyme, and the polymer used. Therefore, in the present work, we aim to establish a link between theoretical and experimental measurements by using the molecular mechanics (MM2) and semi-empirical methods to study the reaction between Poly Pyrrole (ppy) and glucose via its three structures (D-Glucose, ß-Glucose, and α -Glucose), by using the docking method. (Rastelli et al.,2003; Roomi et al.,2025; Su Tok et al.,2026). This approach is applied here as a

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tool for substrate -polymer design, complementing other structure –based methods such as de novo design.
In this study, we compared the steric energies of different glucose formulas to identify the most stable conformation and subsequently compared these theoretical results with experimental data reported in the literature. (Naghib et al.,2023; Njagi et al.,2007)

The novelty of this study lies in providing a systematic computational comparison of different glucose isomers interacting with a polypyrrole matrix. While experimental biosensors are commonplace, this work offers a molecular-level understanding of the spatial and electronic factors that prioritize α-form interactions, which are crucial for the rational design of more sensitive glucose biosensors.

2. **Methodology**:

Computational Scheme.

The theoretical calculations for this study were performed using ChemOffice software (version 9.0; Cambridge Soft). Although this is an older version, the applied MM2 force field and semi-empirical methods remain robust and reliable for calculating the spatial energy of small organic molecules. For molecular docking, a constraint-based approach with a specific interaction distance of 2 angstroms was used to evaluate spatial impedance under identical geometric conditions systematically.

3. **Results and discussion**

3.1. Polymer Model

The conformation of five Pyrrole rings in poly (pyrrole) can be modeled as shown in Figure 1. This structure was used for theoretical calculation in this work.

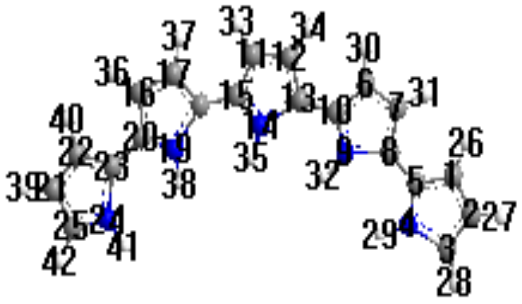

Figure 1: Structure of polypyrrole

3.2. Analysis with Docking Results

Docking analysis was performed to elucidate the interaction mode of the polymer-substrate system. As described, glucose has different structures; we selected the most prevalent formulas from the literature, such as the ß-D-Glucose form (Figure 2). This was used to study the interaction model between ppy and β-D-Glucose by testing four design models, with and without docking (set distance = 2 Å), using molecular mechanics (MM2) to evaluate the steric energy. Table 1 summarizes the energetic results comparing the same system with and without docking. It was found that docking analysis yielded the lowest steric energy compared to the same model without docking.

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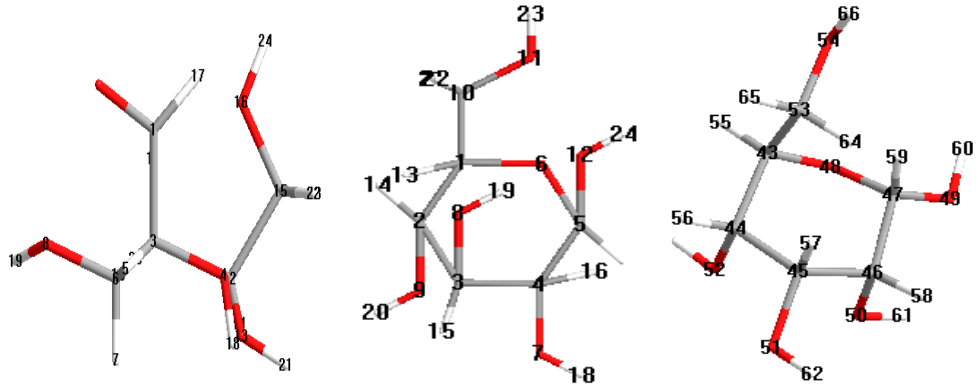
Table 1. The steric energy (Kcal/mol) of the model (ppy-β-D-Glucose) module

Atom for the system (ppy- ß-D-Glucose)	Steric Energy (Kcal/mol)
ß-D-Glucose	92.79
ppy	34.86
N9,C1,H32,O6 (by docking)	220.94
N9,C1,H32,O6 (without docking)	253.78
N14,H19,H35,O8 (by docking)	133.43
N14,H19, H35,O8 (without docking)	238.43
N19,H23,H38,O11 ((by docking)	143.84
N19,H23,H38,O11 (without docking)	264.04
N9,H19,O8,H32 (by docking)	68.24
N9,H19,O8,H32 (without docking)	164.68



1.D- Glucose 2 .ß-D-Glucose 3. α -D-Glucose.

Figure 2. The different structure of glucose

3.3. Detection of optimal bond length

To determine the optimal bond length, a sample of the ppy- ß-D-Glucose model was tested using the specific atoms (N19, H19, O8, H38). Table .2 present the relationship between the bond length and the calculated steric energy. It was found that the optimal H-bond length is 2 Å, as it corresponds to the most stable conformation. (Figure .3) illustrates the correlation between bond length and steric energy.

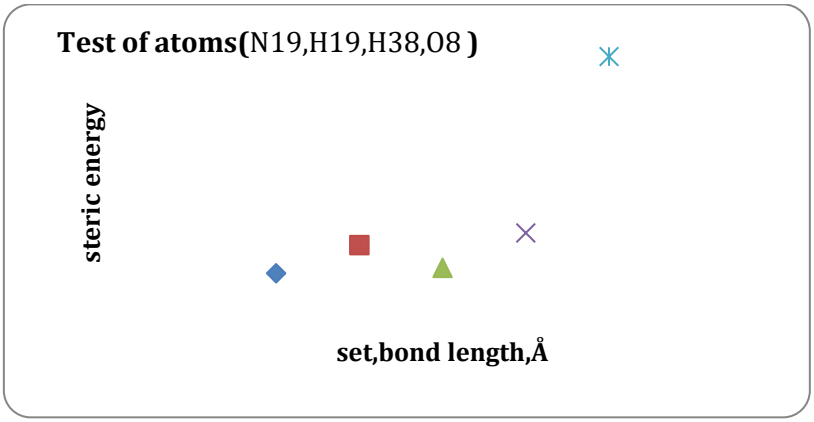


Figure 3. Steric energy (Kcal/mol) as a function of bond length for the ß -D-Glucose-ppy model(Atoms (N_{19}, H_{19}, O_8, H_{38})

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Table 2. Calculating Steric energy (Kcal/mol) values for different bond lengths (Å)in the (ß -D-Glucose-ppy model

Distance of Bond length(Å)	Steric Energy (Kcal/mol)
2	68.102
3	101.34
4	74.54
5	115.35
6	323.43

3.4. Analysis results for the (ppy- Glucose) system

Geometry optimization via docking was performed in two steps. First, the molecular mechanics (MM2) method (Keating, 2026; Pagadala et al., 2008) was used to obtain an initial optimized geometry. These results served as the starting point for the semi-empirical (AM1) calculations for the three modules:
1-D-Glucose-ppy, 2-ß-D-Glucose-ppy and 3- α D--Glucose –ppy
The first model, representing the straight-chain reaction (D-Glucose-ppy), is shown in Figure .4. An AM1 Calculation followed the MM2 analysis to determine the Heat of Formation (ΔHf) and the energy levels of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). As shown in Table .3, the Heat of Formation (ΔHf) and steric energy for this model were slightly higher than those of the free substrates.

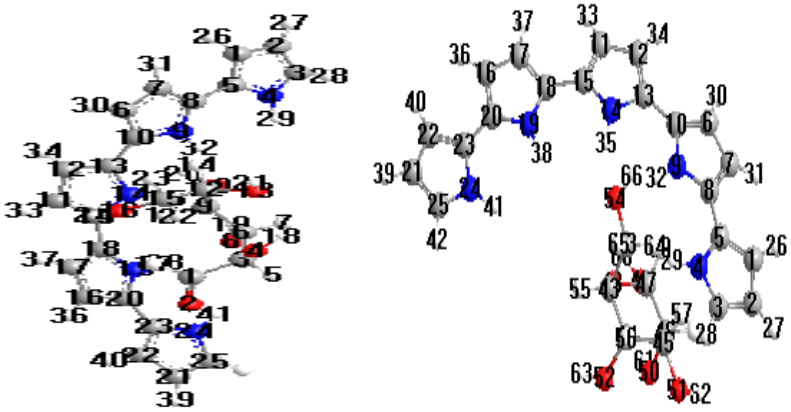

Figure 4 . Geometric shape of (D-Glucose-ppy) model

Figure 5.Geometric shape of (α -D-Glucose-ppy) model

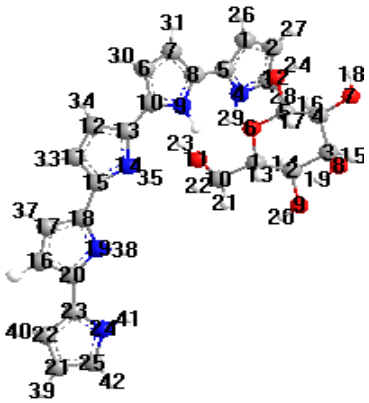

Figure 6. The geometric shape of (ppy- ß-D-Glucose) model

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The second model (α -D-Glucose –ppy) is described in Figure .5. Similar to the first model, MM2 and AM1 calculations were performed, and the results are summarized in Table 4. In this case, the heat of formation and the steric energy were higher than those of the individual free substrate.

Table 3. Value of calculated parameters for the(D-Glucose-ppy) model.

Atom for the system (ppy- D-GLU)	Steric Energy (Kcal/mol)	HOMO	LUMO	H.F.(KJ)	Total Energy(EV)
D-Glucose	9.26	-10.36	0.87	-1178.05	-2857.53
ppy	34.86	-7.52	-0.25	868.15	-3824.22
O4,H32,N9.H18.	67.13	-8.20	-0.68	-195.18	-6680.56
O4,H35,N9,H18.	61.10	-8.12	-0.59	-303.60	-6681.68
O4,H35,N14,H18.	261.55	2.69	5.87	-153437.84	-1657.09
O10,H35,N14,H20	49.70	-8.06	-0.49	-327.93	-6681.93
O10,H35,N9,H20.	53.89	-8.01	-0.52	-314.57	-6681.79
O10,H32,N9,H20	723.08	-6.56	-0.78	2793.10	-6649.59
O10,H38,N19,H20	63.13	-8.05	-0.50	-344.86	-6682.11
O4,H38,N19,H18.	728.39	-6.41	-0.65	3043.55	-6646.99
O16,H38,N19,H24	67.55	-8.16	-0.59	-244.45	-6681.07
O16.H32,N9,H24.	66.65	-8.20	-0.61	-187.28	-6680.48
C15,H35,N14,H22	82.34	-8.19	-0.69	-46.19	-6679.01
O16,H35.N14,H24	66.96	-8.24	-5.41	-9984.02	-6782.01
O13,H35,N9,H21.	57.01	-8.09	-0.56	-355.31	-6682.22
O13,H35,N14,H21	53.17	-8.10	-0.59	-368.97	-6682.36
O2, H35, C 1, N14.	56.79	-7.95	-0.42	-393.48	-6682.61
O8,H35,N14,H19.	59.48	-8.05	-0.51	-341.84	-6682.08
O8,H35,N9,H19.	73.21	-8.23	-0.65	61.59	-6677.89
O8,H32,N9,H19.	689.10	-7.99	-1.21	2523.65	-6652.45
O8,H38,N19,H19.	53.39	-7.95	-0.43	-356.00	-6682.22

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Table 4. Value of calculated parameters for the (α -D-Glucose-ppy) model.

Atom for the system (ppy- α D-GLU.)	Steric Energy (Kcal/mol)	HOMO	LUMO	H.F.(KJ)	Total Energy(EV)
α – D- glu	13.67	-10.51	2.175	-1264.55	-2858.43
ppy	34.86	-7.52	-0.248	868.15	-3824.22
O50,H38,N19,H61	84.20	-8.21	-0.59	-185.32	-6680.46
O52,H32,N9,H63	709.21	-6.62	-0.69	2877.14	-6648.72
O52,H38,N19,H63	58.56	-8.01	-0.45	-366.63	-6682.33
O52,H35,N14,H63	815.03	-7.15	-1.42	3177.23	-6645.60
O52,H35,N9,H63	76.56	-8.07	-0.52	-115.89	-6679.74
O50,H32,N9,H61	70.46	-8.22	-0.59	-181.89	-6680.42
O50,H35,N9,H61.	68.38	-8.21	-0.62	-246.75	-6681.10
O50,H35,N14,H61	84.88	-8.29	-0.67	-118.26	-6679.76
O54,H32,N9,H66.	80.59	-8.16	-0.50	-249.18	-6681.12
O54,H35,N9,H66.	55.90	-8.19	-0.61	-403.45	-6682.72
O54,H35,N14,H66	100.19	-8.32	-0.67	-36.01	-6678.91
O54,H38,N19,H66.	59.21	-8.14	-0.54	-432.87	-6683.02
O51,H32,N9,H62.	75.46	-8.195	-0.58	-205.84	-6680.67
O51,H35,N9,H62.	73.76	-8.128	-0.48	-232.92	-6680.95
O51,H35,N14,H62	62.88	-8.149	-0.56	-280.52	-6681.44
O51,H38,N19,H62	77.29	-8.255	-0.58	-283.07	-6681.47
O48,H35,N9,C47	133.59	-8.288	-0.67	76.48	-6677.74

The third model (ß -D-Glucose –ppy), shown in Figure .6, was analyzed using the same computational approach. The results are presented in Table 5.

Table 5. Value of calculated parameters for the (ß -D-Glucose-ppy) model.

Atom for the system (ppy- D-B-GLU)	Steric energy (Kcal/mol)	HOMO(ev)	LUMO(ev)	H.F.(KJ)	Total Energy(EV)
D-B-GLU	92.79	-8.45	0.25	-622.91	-2851.77
ppy	34.86	-7.52	-0.25	868.15	-3824.22
N9,C1,H32,O6	220.94	-7.96	-1.81	1057.82	-6667.57

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N14,H19,H35,O8	133.43	-8.14	-0.68	377.49	-6674.62
N19,H23,H38,O11	143.84	-8.11	-0.56	283.23	-6675.59
C16,H18,,H36,O7	615.16	-7.88	-1.73	2920.06	-6648.27
N9,H19,O8,H32	65.24	-8.04	-0.42	-378.24	-6682.45
N9,H23,H32,O11	68.54	-8.12	-0.54	-339.83	-6682.06
N19,H19,H38,O8	68.10	-8.18	-0.59	-349.93	-6682.16
N9,H18,H38,O6	155.91	-8.19	-1.01	528.29	-6673.06
N14,C1,H35,O6	254.12	-8.25	-0.79	1130.79	-6666.81
N14,H23,H35,O8	152.47	-8.17	-0.62	574.10	-6672.58

In this final model, it was observed that the heat of formation and the steric energy for certain atomic interaction were significantly lower than those of the free substrate. This indicates a higher degree of stability and more favorable interaction. These theoretical results are in good agreement with experimental data reported in the literature (Njagi et al.,2007). Both methods confirm that the β-conformation of glucose yields optimal results when used with modified ppy electrodes for the development of a glucose biosensor.

4. Conclusions

The results obtained from our theoretical investigations suggest that the Molecular Mechanics (MM2) and Semi-empirical methods are appropriate tools for studying molecular species that are challenging to analyze experimentally. Through Docking analysis, we obtained crucial information regarding the system's geometric parameters, energy profiles, heat of formation, and overall stability, all of which confirm the viability of the proposed system. In the present work, the (ß -D-Glucose –ppy) model demonstrated lower steric energy and a more favorable heat of formation compared to other glucose isomers. From a chemical perspective, lower steric hindrance indicates a more stable, compact spatial arrangement that minimizes the distance between the polymer's redox center and the substrate. Consequently, this facilitates more efficient electron transfer and enhances the redox interaction potential within the biosensor interface. These findings provide a significant theoretical foundation, demonstrating the feasibility of computationally designing and optimizing biosensors before proceeding to practical implementation.

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