PAPER DETAILS

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SEMI-EMPIRICAL DETERMINATION OF DIABETES, CHOLESTEROL AND BLOOD PRESSURE DRUG ACTIVE COMPOUNDS AND THEIR BINARY INTERACTION

DİYABET, KOLESTROL VE TANSİYON İLAÇ MOLEKÜLLERİNİN İKİLİ ETKİLEŞİMLERİNİN SEMİEMPİRİK YÖNTEMLE BELİRLENMESİ

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ABSTRACT

In this study, enthalpy (ΔH), heat formation (ΔH_f), entropy (ΔS), HOMO and LUMO values and dipole moments, possible H-bonds values belong to diabetes (D), cholesterol (K) and blood pressure (T) drugs (Table 1), and the binary interactions of the molecules have been calculated by MOPAC2012 packet program [1, 2] at the Restricted Hartree-Fock level using both PM6 and PM7 semi-empirical SCF-MO methods.Product stabilities were calculated for products formed the binary interaction by using ΔG and ΔG_f values.

The most stable products were K2-D1 both for PM6 and PM7at T=298 K, at T=310 K, K2-D1 for PM6 and K2-D1, K3-D1 for PM7 using ΔG_f values; D1-T3 was at T=298K and 310K for PM6 and PM7, K3-D1 and D1-T3 were both at T=298K and 310K for PM6 and PM7 by ΔG values, have been calculated.

Table 1. Name and abbreviations of drug compounds

Drug Active Compound Name	Drug Active Compound IUPAC Name	Abbreviation
Acarbose	(2R,3R,4R,5S,6R)-5-{[(2R,3R,4R,5S,6R)-5-{[(2R,3R,4S,5S,6R)-3,4-dihydroxy-6-methyl-5-{[(1S,4S,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}oxan-2-yl]oxy}-3,4-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-6-(hydroxymethyl)oxane-2,3,4-triol	**D1**
Metformin	1-carbamimidamido-N,N-dimethylmethanimidamide	**D2**
Gliclazide	3-[(3aR,6aS)-octahydrocyclopenta[c]pyrrol-2-yl]-1-(4-methylbenzenesulfonyl)urea	**D3**
Gemfibrozil	5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoic acid	**K1**
Ezetimibe	(3R,4S)-1-(4-fluorophenyl)-3-[(3S)-3-(4-fluorophenyl)-3-hydroxypropyl]-4-(4-hydroxyphenyl)azetidin-2-one	**K2**
Fenofibrate	propan-2-yl2-{4-[(4-chlorophenyl)carbonyl]phenoxy}-2-methylpropanoate	**K3**
Atenolol	2-(4-{2-hydroxy-3-[(propan-2-yl)amino]propoxy}phenyl)acetamide	**T1**
Metoprolol	{2-hydroxy-3-[4-(2-methoxyethyl)phenoxy]propyl}(propan-2-yl)amine	**T2**
Carvedilol	[3-(9H-carbazol-4-yloxy)-2-hydroxypropyl][2-(2-methoxyphenoxy)ethyl]amine	**T3**

Keywords

Diabetes (D), cholesterol (K) and blood pressure (T) drugs, MOPAC2012 packet program.

ÖZET

Bu çalışmada, Diyabet , Kolestrol ve Tansiyon ilaç moleküllerinin ikili etkileşimleri teorik hesaplama yöntemlerinden Mopac 2012 programları kullanılarak moleküllerin entalpi (ΔH), oluşum ısıları (ΔH_f), entropi (ΔS), en yüksek dolu orbital (HOMO), en düşük boş orbital (LUMO) değerleri ve dipol momentleri, PM6 ve PM7 semiempirik SCF-MO yöntemi ile hesaplanmıştır. Bu değerlerden yararlanılarak ürün kararlılıkları ve Gibss Serbert Enerji (ΔG ve ΔG_f) değerleri hesaplanmıştır.

ΔG_f için en kararlı ürün 298 K'de PM6 ve PM7 için K2-D2, 310 K'de PM6 için K2-D1, PM7 için K3-D1, ΔG için en kararlı ürün 298 K ve 310 K' de PM6 ve PM7 için D1-T3, 298 K ve 310 K'de PM6 ve PM7 için K3-D1 ve D1-T3 olarak hesaplanmıştır.

Tablo 1. İlaç bileşiklerinin isimleri ve kısaltmaları.

İlaç Aktif Bileşiğinin Adı	İlaç Aktif Bileşiğinin IUPAC İsmi	Kısaltma
Acarbose	(2R,3R,4R,5S,6R)-5-{[(2R,3R,4R,5S,6R)-5-{[(2R,3R,4S,5S,6R)-3,4-dihydroxy-6-methyl-5-{[(1S,4S,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}oxan-2-yl]oxy}-3,4-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-6-(hydroxymethyl)oxane-2,3,4-triol	**D1**
Metformin	1-carbamimidamido-N,N-dimethylmethanimidamide	**D2**
Gliclazide	3-[(3aR,6aS)-octahydrocyclopenta[c]pyrrol-2-yl]-1-(4-methylbenzenesulfonyl)urea	**D3**
Gemfibrozil	5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoic acid	**K1**
Ezetimibe	(3R,4S)-1-(4-fluorophenyl)-3-[(3S)-3-(4-fluorophenyl)-3-hydroxypropyl]-4-(4-hydroxyphenyl)azetidin-2-one	**K2**
Fenofibrate	propan-2-yl2-{4-[(4-chlorophenyl)carbonyl]phenoxy}-2-methylpropanoate	**K3**
Atenolol	2-(4-{2-hydroxy-3-[(propan-2-yl)amino]propoxy}phenyl)acetamide	**T1**
Metoprolol	{2-hydroxy-3-[4-(2-methoxyethyl)phenoxy]propyl}(propan-2-yl)amine	**T2**
Carvedilol	[3-(9H-carbazol-4-yloxy)-2-hydroxypropyl][2-(2-methoxyphenoxy)ethyl]amine	**T3**

Anahtar Kelimeler

Diabet (D), Kolestrol (K) Tansiyon (T) ilaçları MOPAC2012 paket programı.

Kaynaklar / References

[1] http://www.drugbank

[2] *J. Stewart MOPAC2012, Stewart Computational Chemistry,* Version 14.128W,(2012).