YURAK KASSALIGIDA ISHLATILADIGAN BISOPROLOL TABLETKASINING KIMYOVIY TUZILISHI VA TEBRANISH SPEKTRINING KVANT KIMYOVIY HISOBLARI

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Annotatsiya: Ushbu maqolada yurak kasalligini davolashda qo`llaniladigan bisoprolol tabletkasining kimyoviy tarkibidagi moddalarning strukturasi va IQ spektirining kvant kimyoviy hisob-kitobi ko`rib chiqiladi.

Аннотация: В этой статье будет рассмотрена структура вещества и квантово-химический расчет спектров IQ химического состава таблетки Бисопролол, используемой для лечения сердечных заболеваний.

Abstract: In this article, the structure of the substance and the quantum chemical calculation of the IQ spectra of the chemical composition of the Bisoprolol tablet used for the treatment of heart diseases will be considered.

Kalit so`zlar: Bisoprolol (B), a-reseptor, kvant kimyoviy hisob-kitob, struktura optimizatsiyasi, IQ spektr, xavfsizlik.

Ключевые слова: бисопролол состояние, а-рецепторь, квантово-химический расчет, оптимизация структуры, ИК-спектр, безопасность.

Key words: bisoprolol deficiency state, a-reseptor, quantum chemical calculation, structure optimization, IR spectrum, safety.

Hozirda sog'liqni saqlash sohasining eng dolzarb muammolaridan biri yurak kassaligi hisoblanadi.

Hozirgi vaqtda ushbu kasalliklar butun dunyo bo'ylab aholining o'limi va nogironligining asosiy sabablaridan biri bo'lib kelmoqda. Asosiy arteriyalarning (koronar, miya) aterosklerotik shikastlanishi natijasida kelib chiqqan yurak-qon tomir kasalliklari butun dunyo bo'ylab o'limning asosiy sababidir: boshqa hech qanday sababsiz, har yili yurak-qon tomir kasalliklaridan ko'p odamlar vafot etmaydi.

JSST hisob-kitoblariga ko'ra, 2016-yilda 17,9 million kishi yurak-qon tomir kasalliklaridan vafot etgan, bu butun dunyo bo'ylab o'lim holatlarining 31 foizini tashkil qilgan. Ushbu o'limlarning 85% insult tufayli sodir bo'lgan.

Yurak kasalliklarini shartli ravishda shikastlanish o'chog'iga ko'ra uch katta guruhga ajratish mumkin:

1. Yurakning klapan apparatiga ta'sir qiluvchi kasalliklar. Turli xil orttirilgan va tug'ma yurak nuqsonlarini o'z ichiga oladi.

2. Yurakning qon tomirlariga ta'sir qiladigan kasalliklri va ularning oqibatlari. Bunga yurak ishemik kasalligi, miokard infarkti, stenokardiya va boshqalar kiradi.

3. Bevosita yurak qobig'i to'qimalariga ta'sir qiladigan kasalliklar, ularga perikardit, endokardit, miokardit kiradi.

Preparatning savdo nomi: Bisoprolol/Bisoprolol

Ta'sir etuvchi modda (XPN): bisoprolol

Dori shakli: plyonka qobiq bilan qoplangan tabletkalar

Tarkibi:

Bir tabletka quyidagilarni saqlaydi:

faol modda: 2,5 mg, 5 mg yoki 10 mg bisoprolol fumarati;

yordamchi moddalar: kalsiy gidrofosfati (suvsiz), mikrokristall sellyuloza, makkajo'xori kraxmali (oldindan jelatinlangan), natriy kroskarmelloza, suvsiz kolloid kremniy dioksidi, magniy stearati, laktoza monogidrati, gipromelloza, titan dioksidi (Ye171), makrogol 4000, temir oksidi (Ye172)

Bisoprolol-bu yurak amaliyotida keng qo'llaniladigan b-bloklovchi vosita. Bisoprololni tayinlash uchun ko'rsatmalar arterial gipertenziya, koroner yurak kasalligi, yurak etishmovchiligi, yurak ritmining buzilishi hisoblanadi. Bisoprolol asosiy sog'liqni saqlash tizimi uchun zarur bo'lgan JSSTning eng muhim dorilar ro'yxatiga kiritilgan.

Kimyoviy formulasi: $C_{18}H_{31}NO_4$

Molekulyar massasi : 325,443 g/mol
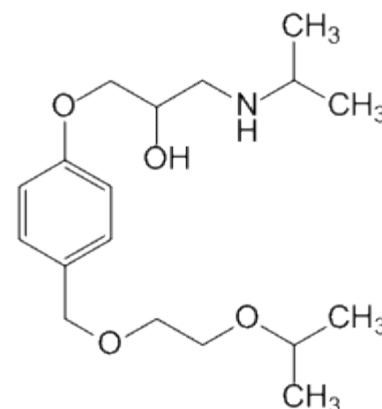
Selektiv Beta1-adrenoblokadaning g'oyasi 1967 yilda adrenoreseptorlarning ikkita subtipasi ochilgandan keyin paydo bo'ldi: b1-adrenoreseptorlar va B2-adrenoreseptorlar. Bisoprolol selektiv Beta1-blokerlar guruhiga kiradi. Bugungi kunda taniqli selektiv Beta1-blokerlar orasida u yuqori selektivlik va harakat kuchi bilan ajralib turadi.

Beta-1 retseptorlari - asosan yurakda joylashgan. Beta-1 retseptorlarini blokirovka qilish yurak tezligini, yurak chiqishini, kontraktillikni va yurak kislorodiga bo'lgan talabni kamaytiradi.

Beta-2 retseptorlari - o'pka, qon tomirlari va boshqa organlarning silliq mushaklarida joylashgan. Beta-2 retseptorlarini blokirovka qilish silliq mushaklarning kengayishini (bo'shashishini) oldini oladi.

Alfa-1 retseptorlari - arteriya va tomirlarning silliq mushaklarida joylashgan. Alfa-1 retseptorlarini blokirovka qilish tomirlarning kengayishiga olib keladi.

Yuqoridagi ma'lumotlardan kelib-chiqgan holda bisoprolol tabletkasining afzalliklari va xususiyatlarini chuqurroq o'rganish uchun biz uning strukturasi va IQ spektrining kvant kimyoviy hisobini o'tkazdik. Hisob-kitoblar 3-21.G asosli DFT/B3LYP usuli (Becke, Li, Yang, Parr) yordamida Gauss 09W dasturiy paketida amalga oshirildi. Tebranish spektri hisob-kitoblari, shuningdek, 3-21G asosli Frequency DFT/B3LYP usuli (Becke, Lee, Yang, Parr) yordamida Gauss 09W dasturiy paketi yordamida hisoblab chiqilgan. Ushbu dasturning eksperimental hisoblangan spektrdan o'ziga xos xususiyati shundaki, u hatto tebranish, valentlik yoki deformatsiyaning turini aniqlay oladi. IQ spektri natijalarining ayrim parametrlari quyidagi jadvalda keltirilgan.

Bog`langan atomlar	Bog` uzunligi	Bog`langan atomlar	Bog` uzunligi	Burchak hosil qiluvchi atomlar	Bog`lar orasidagi burchak (A)	Burchak hosil qiluvchi atomlar	Bog`lar orasidagi burchak (A)	Burchak hosil qiluvchi atomlar	Bog`lar orasidagi burchak (A)
R(1,2)	1.4014	R(12,13)	1.4014	A(2,1,6)	120.0	A(11,10,15)	120.0	A(8,20,10)	21.513
R(1,6)	1.4014	R(12,24)	1.54	A(2,1,7)	120.0	A(11,10,22)	120.0	A(6,22,23)	109.471
R(1,7)	1.07	R(13,14)	1.4012	A(6,1,7)	120.0	A(15,10,20)	120.0	A(12,24,25)	140.6
R(2,1)	1.4014	R(13,17)	1.07	A(1,2,3)	120.0	A(10,11,12)	120.0	A(12,24,30)	81.8419
R(2,8)	1.07	R(14,15)	1.4014	A(1,2,8)	120.0	A(10,11,16)	120.0	A(12,24,31)	83.9594
R(2,22)	1.2402	R(14,19)	2.1	A(1,2,22)	90.698	A(12,11,17)	120.0	A(25,24,30)	82.4855
R(3,4)	1.4014	R(15,18)	1.43	A(3,2,8)	120.0	A(11,12,13)	120.0	A(25,24,31)	83.553
R(3,18)	1.43	R(22,23)	0.95	A(3,2,20)	145.21	A(11,12,24)	120.0	A(30,24,31)	137.3202
R(4,5)	1.4014	R(24,25)	1.54	A(2,3,4)	120.0	A(13,12,24)	120.0	A(24,25,26)	139.4362
R(4,9)	1.07	R(24,30)	1.07	A(2,3,18)	120.0	A(12,13,14)	120.0	A(24,25,27)	84.8021
R(5,6)	1.4014	R(24,31)	1.07	A(4,3,18)	120.0	A(12,13,17)	120.0	A(24,25,32)	84.6216
R(5,21)	2.1	R(25,26)	1.52	A(3,4,5)	120.0	A(14,13,17)	120.0	A(26,25,27)	82.6756
R(6,22)	1.43	R(25,27)	1.47	A(3,4,9)	120.0	A(13,14,12)	120.0	A(26,25,32)	79.2348
R(7,20)	2.0022	R(25,32)	1.07	A(5,4,9)	120.0	A(13,14,19)	120.0	A(27,25,32)	137.5901
R(8,20)	0.6862	R(26,28)	1.2584	A(4,5,6)	120.0	A(15,14,18)	120.0	A(25,26,28)	120.0
R(10,11)	1.4014	R(26,29)	1.41	A(4,5,21)	120.0	A(10,15,14)	120.0	A(25,26,29)	120.0
R(10,15)	1.4014	R(27,33)	1.0	A(6,5,21)	120.0	A(10,15,18)	120.0	A(28,26,29)	120.0
R(10,20)	2.1	R(27,34)	1.0	A(1,6,5)	120.0	A(14,15,16)	120.0	A(25,27,33)	109.4712
R(11,12)	1.4014	R(29,34)	1.3308	A(1,6,22)	120.0	A(3,18,15)	109.47	A(25,27,34)	109.4712
R(11,16)	1.07	R(29,35)	0.96	A(5,6,22)	120.0	A(2,20,10)	81.005	A(33,27,34)	109.4712

Bog`langan atomlar		Bog`langan atomlar		Bog`langan atomlar		Bog`langan atomlar		Bog`langan atomlar	
D(6,1,2,3)	-0.0001	D(2,3,4,9)	-180.0	D(11,10,15,14)	-0.0001	D(13,12,24,25)	-88.4542	D(31,24,25,26)	-137.9985
D(6,1,2,8)	179.9999	D(18,3,4,5)	-180.0	D(11,10,15,18)	179.9999	D(13,12,24,30)	-20.9531	D(31,24,25,27)	-65.644
D(6,1,2,20)	-162.8391	D(18,3,4,9)	0.0	D(20,10,15,14)	179.9999	D(13,12,24,31)	-160.5927	D(31,24,25,32)	155.485
D(7,1,2,3)	-180.0	D(4,3,18,15)	150.0	D(20,10,15,18)	-0.0001	D(12,13,14,15)	-0.0001	D(24,25,26,28)	-88.4171
D(7,1,2,8)	0.0	D(2,3,18,15)	-30.0	D(11,10,20,2)	147.7267	D(12,13,14,19)	180.0	D(24,25,26,29)	91.5829
D(7,1,2,20)	17.161	D(3,4,5,6)	0.0	D(11,10,20,8)	147.7269	D(17,13,14,15)	-179.9998	D(27,25,26,28)	-161.5221
D(2,1,6,5)	0.0001	D(3,4,5,21)	179.9999	D(15,10,20,2)	-32.2733	D(17,13,14,19)	0.0002	D(27,25,26,29)	18.4779
D(2,1,6,22)	-179.9999	D(9,4,5,6)	179.9999	D(15,10,20,8)	-32.2731	D(13,14,15,10)	0.0001	D(32,25,26,28)	-20.0608
D(7,1,6,5)	180.0	D(9,4,5,21)	-0.0001	D(10,11,12,13)	0.0	D(13,14,15,18)	-179.9999	D(32,25,26,29)	159.9392
D(7,1,6,22)	0.0	D(4,5,6,1)	0.0	D(10,11,12,24)	180.0	D(19,14,15,10)	-179.9999	D(24,25,27,33)	-52.4989
D(1,2,3,4)	0.0	D(4,5,6,22)	180.0	D(16,11,12,13)	-179.9998	D(19,14,15,18)	0.0001	D(24,25,27,34)	-172.4989
D(1,2,3,18)	-179.9999	D(21,5,6,1)	-180.0	D(16,11,12,24)	0.0002	D(10,15,18,3)	30.0	D(26,25,27,33)	88.8339
D(8,2,3,4)	-180.0	D(21,5,6,22)	0.0	D(11,12,13,14)	0.0	D(14,15,18,3)	-150.0	D(26,25,27,34)	-31.1661
D(8,2,3,18)	0.0	D(1,6,22,23)	30.0	D(11,12,13,17)	179.9998	D(12,24,25,26)	149.7244	D(32,25,27,33)	23.665
D(20,2,3,4)	148.8554	D(5,6,22,23)	-150.0	D(24,12,13,14)	-180.0	D(12,24,25,27)	-137.9211	D(32,25,27,34)	-96.335
D(20,2,3,18)	-31.1446	D(15,10,11,12)	0.0001	D(24,12,13,17)	-0.0002	D(12,24,25,32)	83.2079	D(25,26,29,35)	150.0
D(1,2,20,10)	-152.4543	D(15,10,11,16)	179.9999	D(11,12,24,25)	91.5458	D(30,24,25,26)	82.4361	D(28,26,29,35)	-30.0
D(3,2,20,10)	54.1574	D(20,10,11,12)	-179.9999	D(11,12,24,30)	159.0469	D(30,24,25,27)	154.7906		
D(2,3,4,5)	0.0	D(20,10,11,16)	-0.0002	D(11,12,24,31)	19.4073	D(30,24,25,32)	15.9196		

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