Gossipolning ideal va real bog’ uzunliklari farqini empirik usulda o’rganish

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Annotatsiya: Ushbu izlanishimizda Avogadro dasturidagi empirik usullar yordamida gossipolning ayrim geometrik va energetik parametrlarini o’rganish natijalari keltirilgan.

Kalit so’zlar: empirik usul, molekulyar mexanika, geometrik parametr, energetik parametr, hosil bo’lish issiqlik energiyasi, ideal bog’ uzunligi

Empirical study of the difference in ideal and real garden lengths of gossipol

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Abstract: In this research, the results of the study of some geometric and energy parameters of gossipol using the Avogadro program in empirical calculation methods are presented.

Keywords: empirical method, molecular mechanics, geometric parameter, energy parameter, thermal energy of formation, ideal bond length

Kirish: Yangi biologik faol moddalarni sintezi, ular asosida tibbiyotda virus kasalliklarini davolash va profilaktika qilish, turli xil etiologiyali immunotanqisliklar uchun yangi dori vositalarini yaratish muammosi, hozirgi kun bioorganik kimyosining asosiy vazifalaridan biridir. Chunki VICh-infeksiyasini, gepatit B, S va yangi respirator virus infeksiyalarini (parranda grippi) hamda bizga ma’lum virusli kasalliklarning borgan sari keng tarqalmoqda. Tibbiyot amaliyotida qo‘llaniladigan dorivor vositalarning 1/3 qismini o‘simlik moddalaridan ajratib olingan dori preparatlari tashkil qiladi. Gossipol polifunksional birikma bo‘lib, kimyoviy jarayonlar natijasida kerakli mahsulotlar hosil qilish imkoniyatlariga ega bo’lgan keng qo’llaniladigan birikmalardan biri hisoblanadi. U asosida tibbiyot uchun o’ta zarur bo’lgan dori vositalari -megosin, batriden, gazolidon kabi dorilar yaratilgan. Shuningdek go’zadan ajratib olinayotgan gossipol o’zining turli xil kasalliklarga

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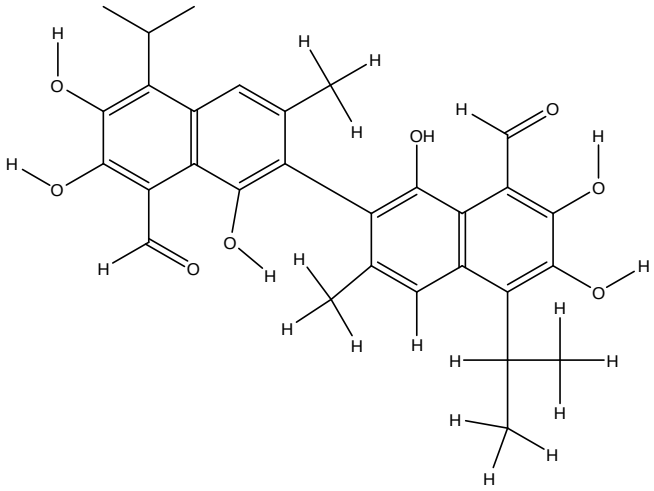
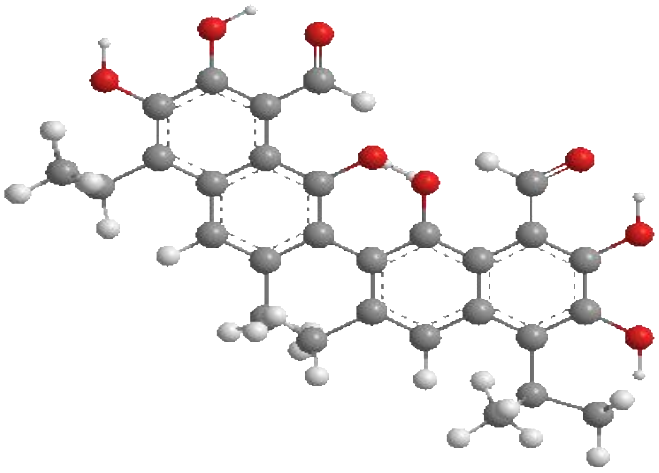
qarshi, shu jumladan o'simtali rakka qarshi, immunosupressiv, parazitlar va turli xil viruslarga qarshi xususiyatlari bilan alohida ahamiyatga egadir [1-5]. Ushbu maqolada Gossipolning epmirik usulda o'rganilgan ayrim geometrik va energetik xarakteristikalari keltirilgan [6].

Olingan natijalar tahlili: Gossipol molekulasining 2D va 3D holatdagi ko'rinishi quyidagi rasmlarda keltirilgan (1-2-rasm):



1-rasm. Gossipol molekulasining 2D holatdagi ko'rinishi.



2-rasm. Gossipol molekulasining 3D holatdagi ko'rinishi

Gossipolning ba'zi geometrik va energetik parametrlarini eksperimental o'rganish uchun Avogadro dasturidan foydalandik. Avogadro empirik usulini o'rganishga mo'ljallangan dastur hisoblanadi. Natijalar Chemical, MMFF94, MMFF94s, UFF metodlarida olindi. Har bir metodda qilingan optimizatsiya natijalari quyidagi jadvallarda keltirilgan (1-jadval):

1-Jadval

Empirik usulda hisoblangan Gossipolning umumiy energiyalari (E_{total})

Chemical	MMFF94	MMFF94S	UFF
206,334 kj/mol	584,339kj/mol	567,279 kj/mol	873,393 kj/mol

Hisoblash natijalari shuni ko'rsatadiki, gassipolning hosil bo'lish issiqlik energiyasi UUF metodida muqobillashtirilganda maksimal qiymatga ega bo'ladi va Chemical metodida muqobillashtirganimizda esa minimal qiymatga ega bo'ldi.

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Demak, gossipol moddasi uchun energetik parametr hisoblashda empirik hisoblash usullaridan Chemical metodi samarali.

2-Jadval

Gossipolning Avogadro dasturi yordamida olingan real bog'uzunliklari (A^0)

T/r	Bog'lar	Chemical	MMFF94	MMFF94S	UFF
1.	C_1-C_2	1,3957	1,38873	1,38812	1,39756
2.	C_1-O_1	1,39431	1,39774	1,3971	1,42743
3.	C_2-C_3	1,39849	1,4288	1,42905	1,45195
4.	C_2-O_2	1,40005	1,42497	1,4267	1,44302
5.	C_3-C_4	1,40464	1,43767	1,43853	1,43657
6.	C_3-C_{15}	1,40026	1,39825	1,39926	1,40875
7.	C_4-C_5	1,39997	1,43146	1,4311	1,44345
8.	C_4-C_7	1,39541	1,41639	1,4159	1,41416
9.	C_5-C_6	1,39587	1,40217	1,40049	1,39673
10.	C_6-C_1	1,39495	1,4072	1,40717	1,38957
11.	C_6-C_{11}	1,40042	1,41545	1,41723	1,41781
12.	C_7-C_8	1,54424	1,53451	1,53462	1,55485
13.	C_7-O_4	1,54681	1,52903	1,52924	1,53843
14.	C_8-C_9	1,54831	1,53725	1,53717	1,53865
15.	C_8-C_{16}	1,5294	1,50799	1,50741	1,51457
16.	C_9-C_{10}	1,39116	1,36994	1,3703	1,35461
17.	C_9-C_{14}	1,39146	1,37819	1,37812	1,35761
18.	C_{10}-C_5	1,51332	1,48399	1,48393	1,51385
19.	C_{10}-H_3	1,08748	1,09809	1,09816	1,0697
20.	C_{11}-C_{12}	1,22006	1,23146	1,23146	1,21765
21.	C_{11}-C_{13}	1,39304	1,38132	1,38124	1,34848
22.	C_{11}-H_4	1,48455	1,49335	1,49017	1,49527
23.	C_{12}-H_5	1,39675	1,39685	1,39534	1,39588
24.	C_{12}-H_6	1,39629	1,40575	1,40564	1,39069
25.	C_{12}-H_7	1,39784	1,41335	1,41453	1,4144
26.	C_{13}-H_8	1,39858	1,43745	1,4405	1,4413
27.	C_{13}-H_9	1,39917	1,44455	1,44451	1,44294
28.	C_{13}-H_{10}	1,39584	1,41667	1,41508	1,40561
29.	C_{14}-H_{11}	1,4029	1,44344	1,44606	1,44372
30.	C_{14}-H_{12}	1,39925	1,40689	1,40687	1,42629
31.	C_{14}-H_{13}	1,39601	1,38491	1,38456	1,39804
32.	O_1-H_{14}	1,39497	1,39043	1,39019	1,4064
33.	O_2-H_{15}	1,39882	1,43461	1,4346	1,43793
34.	C_{15}-H_1	1,39325	1,37657	1,3769	1,35046
35.	C_{15}-O_3	1,51326	1,47841	1,47845	1,50232
36.	O_4-H_{16}	1,08706	1,10415	1,10362	1,08484
37.	C_{16}-C_{17}	1,22001	1,22527	1,22671	1,21968
38.	C_{17}-C_{18}	1,39428	1,37281	1,37285	1,35775
39.	C_{17}-C_{30}	1,39266	1,37531	1,37496	1,35824
40.	C_{18}-C_{19}	1,54537	1,54796	1,54568	1,55369
41.	C_{18}-H_{17}	1,54593	1,54441	1,53733	1,54213
42.	C_{19}-C_{20}	1,54625	1,52998	1,52946	1,54163
43.	C_{19}-C_{22}	1,53016	1,50939	1,50913	1,51183
44.	C_{20}-C_{21}	1,08015	1,08846	1,08801	1,06744
45.	C_{21}-C_{16}	1,09952	1,09507	1,09368	1,09261
46.	C_{21}-O_5	1,10003	1,09517	1,09511	1,10613

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47.	C_{22}-C_{23}	1,09899	1,09537	1,09549	1,11095
48.	C_{22}-C_{27}	1,10032	1,09546	1,09543	1,11133
49.	C_{23}-C_{24}	1,09962	1,09377	1,09348	1,10609
50.	C_{23}-O_{8}	1,10072	1,09632	1,09629	1,11134
51.	C_{24}-C_{25}	1,10029	1,09538	1,09544	1,11098
52.	C_{24}-O_{7}	1,09918	1,09402	1,0943	1,11041
53.	C_{25}-C_{20}	1,09943	1,09404	1,09404	1,10745
54.	C_{25}-C_{26}	1,10009	1,09583	1,09574	1,11049
55.	O_{5}-H_{18}	0,949935	0,979905	0,97995	0,967091
56.	C_{26}-H_{2}	0,950529	0,98642	0,986485	0,959968
57.	C_{26}-O_{6}	0,950615	0,975119	0,974744	0,966464
58.	O_{7}-H_{19}	1,07941	1,08079	1,07858	1,06443
59.	O_{8}-H_{20}	0,950517	0,979822	0.980498	0,964134
60.	C_{27}-C_{28}	0,949226	0,980686	0,980569	0,967185
61.	C_{27}-C_{29}	0,950333	0,971477	0,973197	0,960695
62.	C_{27}-H_{21}	1,09981	1,09603	1,09492	1,09414
63.	C_{28}-H_{22}	1,10007	1,09629	1,0955	1,10114
64.	C_{28}-H_{23}	1,09995	1,09495	1,09618	1,11110
65.	C_{28}-H_{24}	1,10044	1,09567	1,0955	1,11128
66.	C_{29}-H_{25}	1,09974	1,09492	1,0948	1,1015
67.	C_{29}-H_{26}	1,10037	1,09725	1,09736	1,11124
68.	C_{29}-H_{27}	1,09954	1,09414	1,09398	1,11104
69.	C_{30}-H_{28}	1,09933	1,09432	1,09477	1,11043
70.	C_{30}-H_{29}	1,09955	1,09402	1,09387	1,10903

Gossipolning ideal va real bog' uzunliklari nazariy MM usuli bilan o'rganilganda empirik usulning 4 ta metodida sezilarli farqlar kuzatilmadi.

3-jadval

Gossipolning Chemical metodida olingan ideal va real bog'uzunliklari va ularning farqlari (A^0)

T/r	Real bog' uzunligi	Ideal bog' uzunligi	Delta	D/R *100% B.U
1.	1,395	1,395	0,000	0
2.	1,394	1,390	0,004	0,287
3.	1,395	1,395	0,000	0
4.	1,392	1,390	0,002	0,144
5.	1,399	1,395	0,004	0,2859
6.	1,513	1,510	0,003	0,198
7.	1,399	1,395	0,004	0,2859
8.	1,400	1,395	0,005	0,2859
9.	1,402	1,395	0,007	0,357
10.	1,398	1,395	0,003	0,4992
11.	1,542	1,525	0,017	0,2146
12.	1,395	1,395	-0,000	1,1025
13.	1,393	1,390	0,003	0
14.	1,396	1,395	0,001	0,2154
15.	1,482	1,480	0,002	1,1025
16.	1,396	1,395	0,001	0,072
17.	1,530	1,525	0,005	0,1349
18.	1,398	1,395	0,003	0,3268
19.	1,079	1,084	-0,005	0,2146
20.	1,548	1,540	0,008	-0,4634
21.	1,547	1,540	0,007	0,5168

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22.	1,100	1,100	0,000	0,4525
23.	1,097	1,100	-0,003	0
24.	1,101	1,100	0,001	-0,2735
25.	1,100	1,100	0,000	0,0908
26.	1,100	1,100	0,000	0
27.	1,100	1,100	0,000	0
28.	1,097	1,100	-0,003	0
29.	1,100	1,100	-0,000	-0,2735
30.	1,100	1,100	-0,000	0
31.	1,100	1,100	-0,000	0
32.	0,950	0,950	0,000	0
33.	0,950	0,950	0,000	0
34.	1,088	1,089	-0,001	0
35.	1,220	1,220	-0,000	-0,092
36.	1,396	1,395	0,001	0
37.	1,396	1,395	0,001	0,072
38.	1,530	1,525	0,005	0,072
39.	1,397	1,395	0,002	0,327
40.	1,398	1,395	0,003	0,143
41.	1,401	1,395	0,006	0,215
42.	1,399	1,395	0,004	0,4283
43.	1,395	1,395	0,000	0,286
44.	1,393	1,390	0,003	0
45.	1,399	1,395	0,004	0,2154
46.	1,397	1,395	0,002	0,286
47.	1,393	1,390	0,003	0,1432
48.	1,396	1,395	0,001	0,2154
49.	1,394	1,390	0,004	0,0712
50.	1,399	1,395	0,004	0,287
51.	1,513	1,510	0,003	0,287
52.	0,951	0,950	0,001	0,1983
53.	1,088	1,089	-0,001	0,105
54.	1,220	1,220	-0,000	-0,0919
55.	0,949	0,950	-0,001	0
56.	0,950	0,950	0,000	-0,105
57.	1,100	1,100	-0,000	0
58.	1,100	0,950	-0,000	0
59.	1,100	0,950	-0,000	0
60.	1,544	1,525	0,019	0
61.	1,546	1,540	0,006	1,203
62.	1,546	1,540	0,006	0,388
63.	0,951	0,950	0,001	0,388
64.	1,081	1,084	-0,003	0,105
65.	1,100	1,100	-0,000	-0,2775
66.	1,100	1,100	0,000	0
67.	1,100	1,100	-0,000	0
68.	1,100	1,100	0,000	0
69.	1,100	1,100	-0,000	0
70.	1,099	1,100	-0,001	-0,0909

Jami; *10,3402/71=0,14564.* *100-0,14564=99,85%*

Gossipolning Chemical metodida olingan ideal va real bog' uzunliklari 0.14564% ni tashkil qildi.

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Xuddi shunday o'rganish ishlari MMFF94 (99.86%), MMFF94s (93.10%), UFF (93.28%) metodlarida ham olib borildi.

Tajriba qism

Gossipolning ba'zi geometrik va energetik parametrlari empirik hisoblash usullari bilan o'rganildi. O'rganish ishlari Avogadro dasturining Chemical, MMFF94, MMFF94s va UFF kabi empirik usullarida bajarilgan. Bunda gossipol moddasi strukturasi Avogadro dasturida chizilib, har bir usulda 10000 qadam va $10e^{-10}$ energiya qiymatida optimisatsiya qilindi.

Xulosa

Hosil bo'lish issiqlik energiyalari hisoblanganda eng minimal qiymat Chemical usulida kuzatildi. Bog'lar orasidagi masofalarda esa Chemical, MMFF94, MMFF94s va UFF empirik usullarida optimizatsiya qilinganda sezilarli farqlar kuzatilmadi. Real bog'lar uzunliklarining ideal bog'lar uzunligidan katta farq qilmasligi usulning aniqligi yuqoriligidan dalolat beradi. Demak, gossipolni empirik usulda o'rganganimizda Chemical metodi samarali hisoblanadi.

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