KEMPFEROLNING ATOMLARI ZARYAD QIYMATLARI VA AYRIM ENERGETIK PARAMETRLARINI HYPERCHEM DASTURIDA O'RGANISH

Dilnoza Birodar qizi Ismatova
O'zbekiston Milliy universiteti
Sunnatillo Shuhratjon o'g'li Salimov
O'zbekiston Milliy universiteti
Asadbek Tajikulovich Sarabekov
O'zbekiston Milliy universiteti
Hamza Sayidmurudovich Toshov
O'zbekiston Milliy universiteti

Annotatsiya. Ushbu izlanishda Hyperchem dasturi orqali kempferol molekulasining hosil bo'lish issiqligi, atomlari zaryadi, zaryad taqsimoti, dipol momenti (Debye), ESP va zaryad zichligining 2D va 3D holati, HOMO – LUMO (2D va 3D holati), UB spektrlari o'rganildi, IQ spektrlari olinib amaliy spektrlar bilan taqqoslab ko'rildi.

Kalit so'zlar: Kempferol, Hyperchem dasturi, hosil bo'lish issiqligi, dipol momenti, zaryad taqsimoti, zaryad zichligi, , HOMO va LUMO, IQ, UB

Abstract. In this study, the heat of formation of the kaempferol molecule, atomic charge, charge distribution, dipole moment (Debye), ESP and charge density in 2D and 3D states, HOMO - LUMO (2D and 3D states), UV spectra were studied using the Hyperchem program, and IR spectra were obtained and compared with practical spectra.

Keywords: Kaempferol, Hyperchem program, heat of formation, dipole moment, charge distribution, charge density, , HOMO and LUMO, IR, UV

Абстрактный. В данном исследовании с помощью программы Hyperchem были изучены теплота образования молекулы кемпферола, заряд атомов, распределение заряда, дипольный момент (Дебай), 2D и 3D состояние ESP и плотность заряда, HOMO-LUMO (2D и 3D состояние), УФ-спектры, получены ИК-спектры и сопоставлены с практическими спектрами.

Ключевые слова: Кемпферол, программа Hyperchem, теплота образования, дипольный момент, распределение заряда, плотность заряда, ВЗМО и НСМО, ИК, УФ.

Kirish: Zamonaviy hisoblash kimyosi organik birikmalarning tuzilishi, fizik-kimyoviy xossalari va reaktivligini chuqur o'rganish imkoniyatini beradi. Flavonoidlar sog'liq uchun yuqori samarali ta'sir ko'rsatadigan o'simliklardan olingan birikmalar toifasidir. Eng mashhur flavonoidlardan biri kempferol bo'lib, uni turli xil o'tlar va o'simliklar oilalaridan topish mumkin. Antikarsinogen va

ISSN 3030-3907

yallig'lanishga qarshi ta'siridan tashqari, kempferol va uning birikmalari ham antibakterial, antifungal va antiprotozoal ta'sir ko'rsatadi. Ushbu birikmalar asosida dori vositalari va davolash sxemalarini ishlab chiqish ko'plab patogenlarning paydo bo'ladigan qarshiligi, shuningdek, turli dori terapiyalari o'rtasidagi murakkab molekulyar o'zaro ta'sirlar sharoitida tobora muhim ahamiyat kasb etmoqda[1-2].

Turli manbalar tufayli kempferolning mikroblarga qarshi faolligining ba'zi molekulyar mexanizmlari yaxshi ma'lum, boshqalari esa hali ham tahlil qilinmoqda. Shu sababdan uning biologik faolligi va fizik-kimyoviy xususiyatlarini o‘rganish katta ahamiyat kasb etadi. Kempferolning kvant-kimyoviy parametrlarini tahlil qilish orqali uning molekulyar tuzilishi, energetik xususiyatlari va reaktiv markazlari haqida muhim ma’lumot olish mumkin[3-5].

Ushbu tadqiqotda Kempferol molekulasining hisoblash usullari yordamida olingan kvant-kimyoviy ko‘rsatkichlari tahlil qilinadi. Hisob-kitoblar CNDO, INDO, MNDO, AM1, RM1 va PM3 kabi yarim empirik usullar asosida HyperChem dasturida amalga oshirildi. Tadqiqot davomida Kempferolning hosil bo‘lish issiqligi, atom zaryadi qiymati va zaryad taqsimoti, dipol momenti, infraqizil (IQ) spektri, ultrabinafsha (UB) spektri hamda HOMO va LUMO orbitallarining xususiyatlari o‘rganildi.

Natijalar Kempferolning molekulyar xususiyatlarini batafsil tushunishga, uning elektron tuzilishini tahlil qilishga va kimyoviy faolligini oldindan bashorat qilishga yordam beradi. Ushbu tadqiqot natijalari Kempferol va boshqa flavonoidlarning fizik-kimyoviy xossalarini modellashtirish, farmakologik faolligini baholash va kelajakdagi tadqiqotlar uchun muhim ilmiy asos yaratadi.

Olingan natijalar tahlili: Kempferolning ayrim fizik – kimyoviy doimiyliklarini o’rganish bilan bir qatorda, tuzilishini o’rganish maqsadida Hyperchem dasturi yordamida turli kvant kimyoviy hisob kitob ishlari olib borildi. Kempferolning hosil bo’lish energiyasi Hyperchem dasturida o’rganilganda quyidagicha natija olindi. (1 – jadval)

1 – jadval

Kempferolning Hyperchem (CNDO, INDO, MNDO, AM1, RM1, PM3) dasturida hisoblangan hosil bo’lish issiqliklari (kkal/mol)

№	Energiya turlari	Hyperchem					
		CNDO	INDO	MNDO	AM1	RM1	PM3
1.	Bog‘lanish	-100980.56	-10538.046	-3640.164	-3613.098	-2356.786	-3623.8145
2.	Atom energiyasi	-130117,817	-124978.474	-88411.00	-88157.59	-88157.59	-81525.985

ISSN 3030-3907

3.	Elektron energiyasi	-645736.252	-639446.223	-547032.475	-550713.41	-554889.74	-541485.804
4.	Yadrolararo ta'sir	504637.875	503929.70	454981.3	458942.727	464375.36	456336.005
5.	O'zaro ta'sir issiqligi	-7538.836	-7096.322	-198.44	-171.374	1084.937	-182.0905
6.	Qiyalik	0.104799	0.09687	0.10476	0.0962938	0.08495	0.09071
7.	Umumiy energiya	-141098.377	-135516.52	-92051.172	-91770.689	-90514.377	-85159.799

Yuqoridagi jadvalga asoslanib Hyperchem dasturining CNDO kuch maydonlari kempferol moddasining hosil bo'lish issiqligini hisoblash uchun qulay ekanligi aniqlandi.

2 – jadval

Kempferolning Hyperchem (CNDO, INDO, MNDO, AM1, RM1, PM3) dasturida hisoblangan atom zaryad qiymatlari

№	Atomlar	Hyperchem					
		CNDO	INDO	MNDO	AM1	RM1	PM3
1	(C) 1	0.246102	0.302904	0.206161	0.178784	0.198049	0.207051
2	(C) 2	-0.145382	-0.164023	-0.178699	-0.242956	-0.222921	-0.257241
3	(C) 3	0.254778	0.321553	0.258848	0.219019	0.252408	0.262713
4	(C) 4	-0.173600	-0.216366	-0.322295	-0.313653	-0.355387	-0.375726
5	(C) 5	0.235214	0.285720	0.228334	0.184360	0.202005	0.199605
6	(C) 6	-0.155836	-0.172922	-0.227411	-0.298418	-0.278444	-0.308200
7	(C) 7	0.275826	0.342682	0.327619	0.309506	0.334021	0.415411
8	(C) 8	0.028649	0.044753	-0.059227	-0.097005	-0.081358	-0.064051
9	(C) 9	0.159447	0.195606	0.136423	0.102426	0.112663	0.019416
10	(O) 10	-0.191979	-0.234441	-0.185598	-0.124981	-0.131197	-0.081736
11	(C) 11	-0.010492	-0.018168	-0.081558	-0.087311	-0.107156	-0.108469
12	(C) 12	0.035894	-0.018168	0.019861	-0.059232	-0.018398	-0.024249

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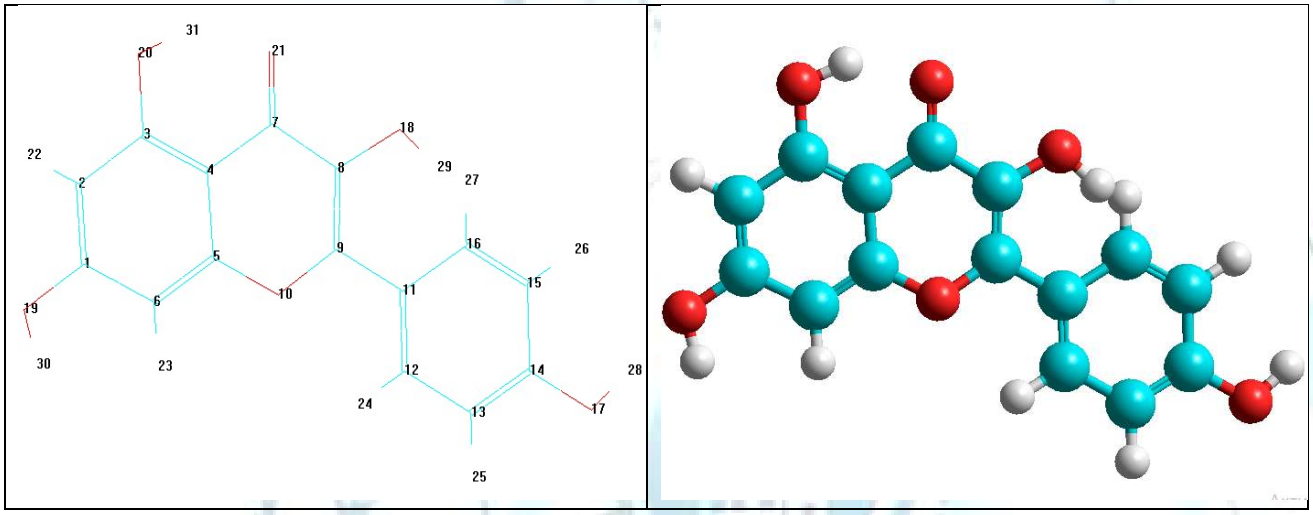
13	(C) 13	-0.043189	-0.037807	-0.097586	-0.168428	-0.141852	-0.146870
14	(C) 14	0.190656	0.239277	0.132136	0.100960	0.117504	0.119684
15	(C) 15	-0.053651	-0.052070	-0.155076	-0.225196	-0.201096	-0.198906
16	(C) 16	0.030411	0.056201	0.026884	-0.044037	0.001299	-0.042773
17	(O)17	-0.233978	-0.281611	-0.244288	-0.246764	-0.256047	-0.220280
18	(O) 18	-0.234130	-0.278417	-0.239476	-0.246305	-0.246384	-0.190976
19	(O)19	-0.234371	-0.283722	-0.236248	-0.235635	-0.246612	-0.218456
20	(O) 20	-0.334881	-0.413800	-0.243612	-0.244138	-0.270646	-0.248792
21	(O) 21	-0.368844	-0.412030	-0.356849	-0.362793	-0.376441	-0.350255
22	(H) 22	0.026921	0.016956	0.100081	0.177781	0.147455	0.148576
23	(H) 23	0.017868	0.008672	0.085838	0.160006	0.131000	0.136528
24	(H) 24	-0.005019	-0.025471	0.064846	0.147355	0.113611	0.113756
25	(H) 25	0.014177	0.000717	0.079797	0.154870	0.124554	0.127734
26	(H) 26	0.006862	-0.006173	0.064911	0.139585	0.109722	0.117057
27	(H) 27	-0.004328	-0.023867	0.061848	0.162011	0.121199	0.113761
28	(H) 28	0.136496	0.156233	0.196035	0.222135	0.222225	0.200952
29	(H) 29	0.138705	0.153685	0.206802	0.244455	0.238631	0.197972
30	(H) 30	0.135796	0.153780	0.202573	0.228766	0.228386	0.202659
31	(H) 31	0.255877	0.280457	0.228928	0.264830	0.279208	0.254106

Yuqoridagi nazariy ma’lumotlar asosida elektropozitiv atomlar (musbat qiymatli) elektronni yo’qotishga moyil va elektrofil markaz bo’lib, CNDO usulida maksimal musbat qiymatli [C (7)] 0.275826; INDO usulida [C (7)] 0.342682; MNDO usulida [C (7)] 0.327619; AM1 usulida [C (7)] 0.309506; RM1 usulida [C (7)] 0.334021; PM3 usulida [C (7)] 0.415411 bo’lgan >C=O guruhi nukleofil hujumning eng ehtimolli markazidir. Elektro manfiy atomlar elektronni tortishga moyil va nukleofil markaz bo’lib, CNDO usulida maksimal manfiy qiymatli [O (21)] -0.368844; INDO usulida [O (20)] -0.413800 ; MNDO usulida [O (21)] -

ISSN 3030-3907

0.356849; AM1 usulida [O (21)] -0.362793; RM1 usulida [O (21)] -0.376441; PM3 usulida [C (4)] -0.375726 bo'lgan atomlar elektrofil hujumning eng ehtimolli markazidir.

1 – rasm. Kempferol moddasining raqamlanishi va3D holati.



3 – jadval

Kempferolning Hyperchem (CNDO, INDO, MNDO, AM1, RM1, PM3) dasturida hisoblangan dipol moment qiymatlari

Usullar	Dipol moment			
CNDO	Dipole (Debyes)	x	y	z	Total
	Point-Chg.	2.040	-4.103	-1.654	4.871
	sp Hybrid	1.602	-2.136	-1.538	3.081
	pd Hybrid	0.000	0.000	0.000	0.000
	Sum	3.641	-6.238	-3.192	7.897
INDO	Dipole (Debyes)	x	y	z	Total
	Point-Chg.	2.693	-4.729	-1.922	5.772
	sp Hybrid	1.338	-1.878	-1.345	2.669
	pd Hybrid	0.000	0.000	0.000	0.000
	Sum	4.031	-6.607	-3.267	8.401
MNDO	Dipole (Debyes)	x	y	z	Total
	Point-Chg.	-0.271	-2.490	-1.340	2.841
	sp Hybrid	0.993	0.442	-0.931	1.431
	pd Hybrid	0.000	0.000	0.000	0.000
	Sum	0.722	-2.048	-2.272	3.143
AM1	Dipole (Debyes)	x	y	z	Total
	Point-Chg.	0.012	-2.741	-0.684	2.826
	sp Hybrid	1.092	0.442	-0.254	1.205

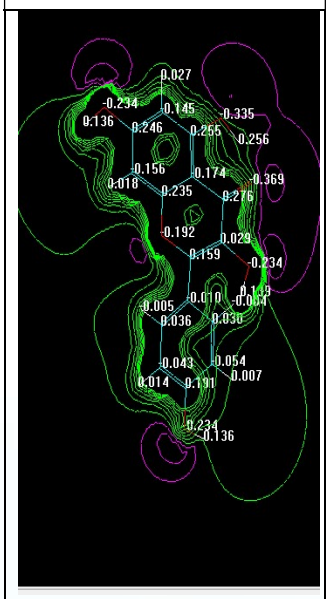
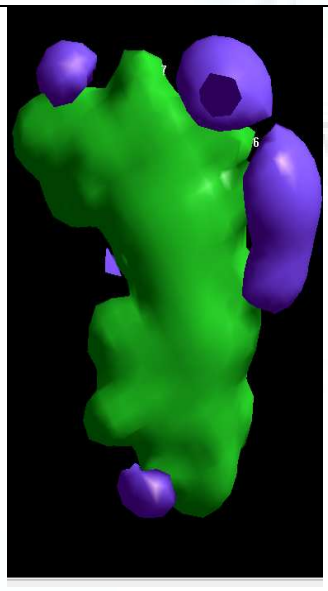
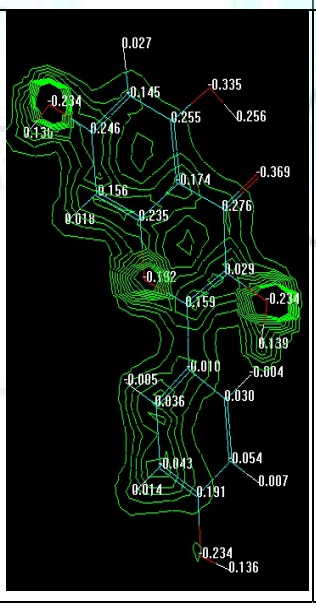
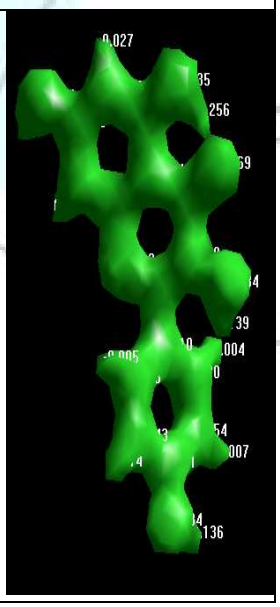
ISSN 3030-3907

	pd Hybrid	0.000	0.000	0.000	0.000
	Sum	1.104	-2.300	-0.939	**2.718**
RM1	Dipole (Debyes)	x	y	z	Total
	Point-Chg.	0.446	-2.721	-0.857	2.887
	sp Hybrid	1.019	0.311	-0.360	1.125
	pd Hybrid	0.000	0.000	0.000	0.000
	Sum	1.465	-2.409	-1.217	**3.071**
PM3	Dipole (Debyes)	x	y	z	Total
	Point-Chg.	1.168	-3.392	-1.148	3.767
	sp Hybrid	1.486	-0.860	-0.867	1.924
	pd Hybrid	0.000	0.000	0.000	0.000
	Sum	2.654	-4.252	-2.015	5.402

Kempferol flavanoidlar sinfiga nansub modda bo'lib, polar funksional guruhlar (- OH va - C=O) mavjudligi sababli o'rtacha qutblikka ega bo'lishi kerak. 3 – jadvalga asoslangan holda AM1 va RM1 o'rtacha 2.718 debye va 3.071 debye qiymatlarni eng maqbul variant deb qarash mumkin.

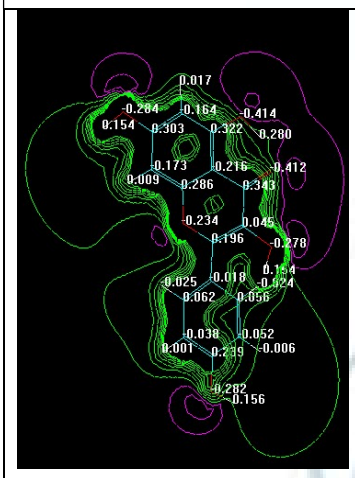
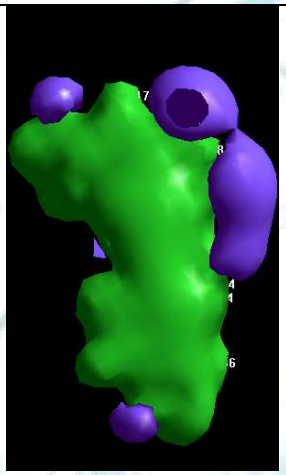
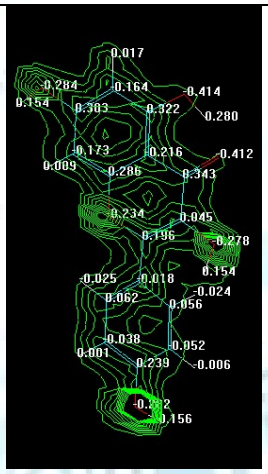
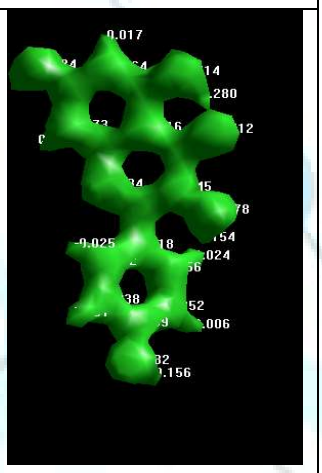
Quyidagi jadvallarda HyperChem dasturida CNDO, INDO, MNDO, AM1, RM1, PM3 yarimempirik usullar yordamida kempferolning 2D va 3D formatda olingan "Elektrostatik potensial" (Electrostatic potential) hamda " Umumiy zaryad zichligi" (Total Charge Density) qiymatlarini ko'rish mumkin.

2 – rasm. Kempferolning Hyperchem (CNDO) dasturida olingan " Elektrostatik potensiali" va " Umumiy zaryad zichligi "

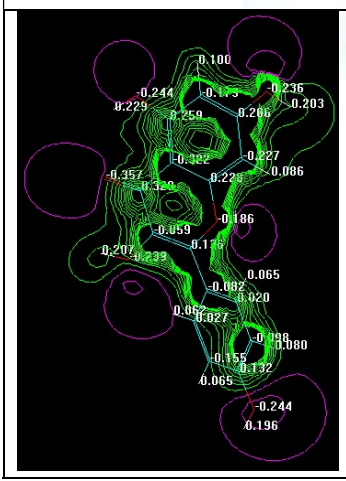
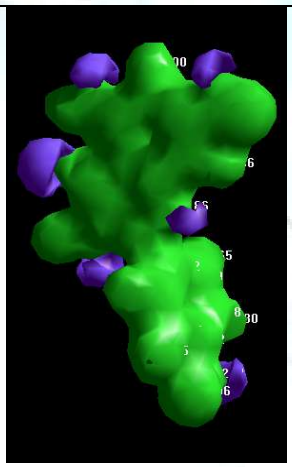
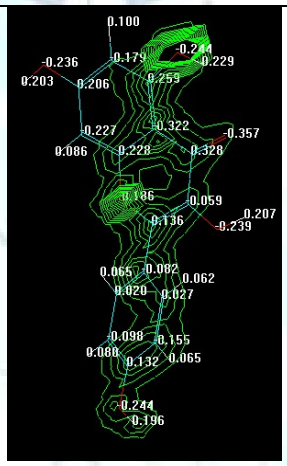
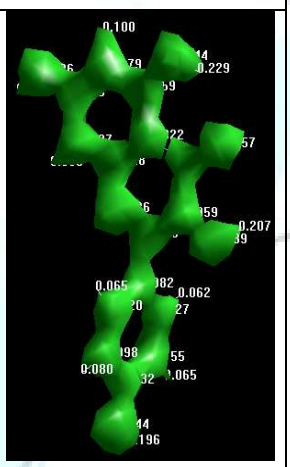
Elektrostatik potensial		Umumiy zaryad zichligi	
2D	3D	2D	3D
			

ISSN 3030-3907

3 – rasm. Kempferolning Hyperchem (INDO) dasturida olingan “Elektrostatik potensiali” va “Umumiy zaryad zichligi”

Elektrostatik potensial		Umumiy zaryad zichligi	
2D	3D	2D	3D
			

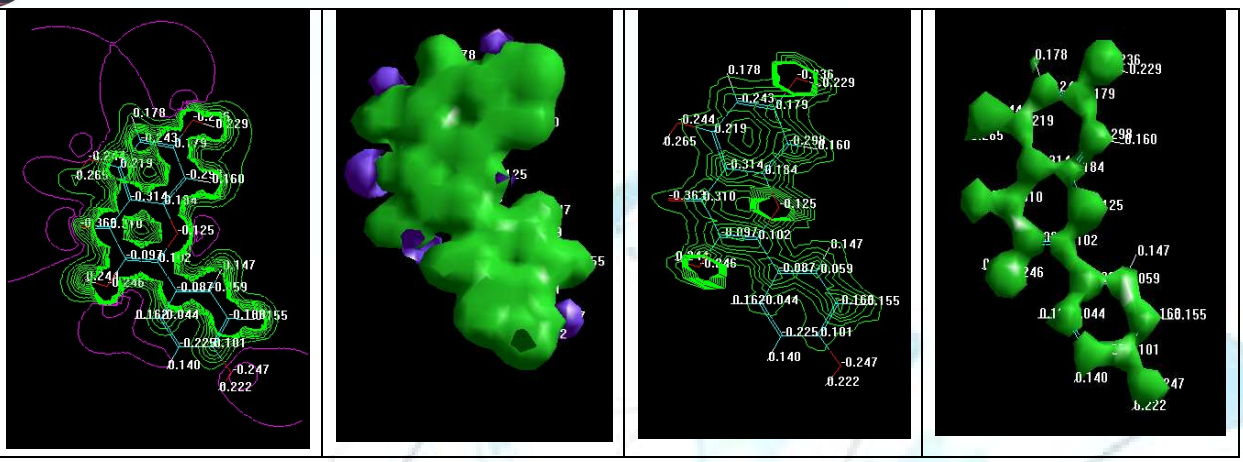
4 – rasm. Kempferolning Hyperchem (MNDO) dasturida olingan “Elektrostatik potensiali” va “Umumiy zaryad zichligi”

Elektrostatik potensial		Umumiy zaryad zichligi	
2D	3D	2D	3D
			

5 – rasm. Kempferolning Hyperchem (AM1) dasturida olingan “Elektrostatik potensiali” va “Umumiy zaryad zichligi”

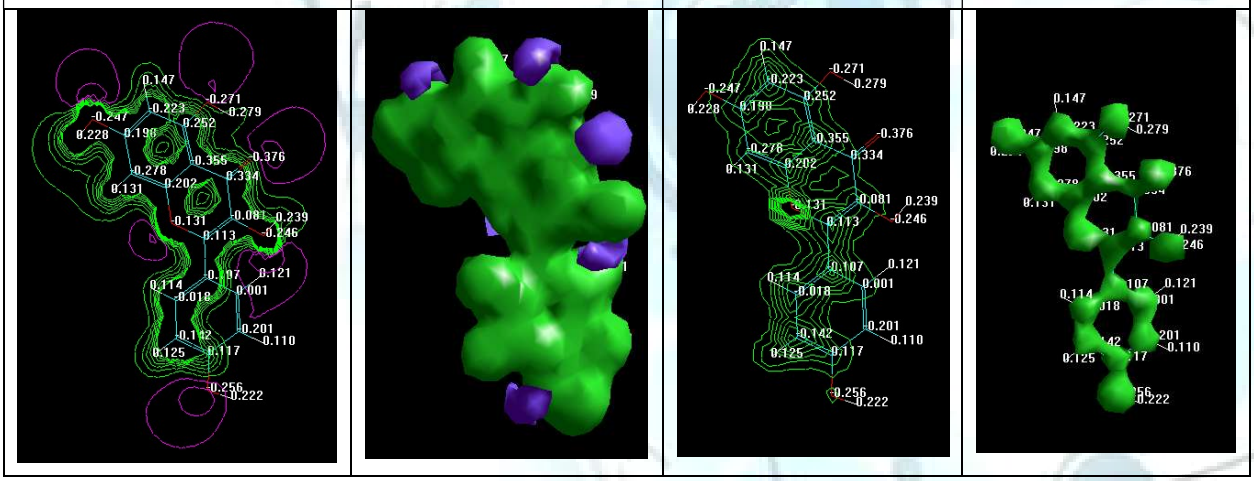
Elektrostatik potensial		Umumiy zaryad zichligi	
2D	3D	2D	3D

ISSN 3030-3907



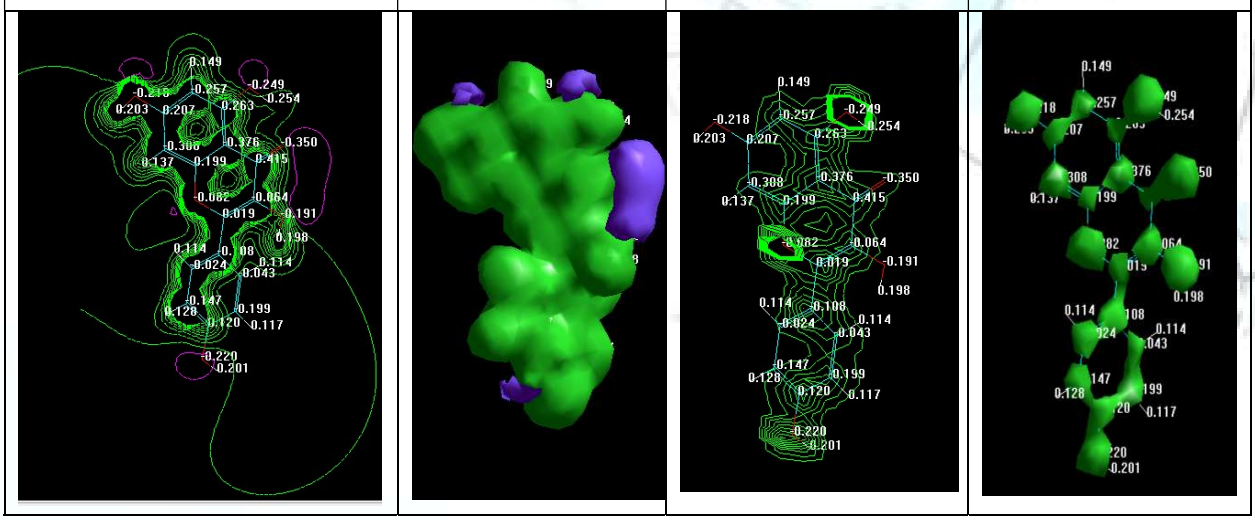
6 – rasm. Kempferolning Hyperchem (RM1) dasturida olingan "Elektrostatik potensiali" va "Umumiy zaryad zichligi"

Elektrostatik potensial		Umumiy zaryad zichligi	
2D	3D	2D	3D



7 – rasm. Kempferolning Hyperchem (PM3) dasturida olingan "Elektrostatik potensiali" va "Umumiy zaryad zichligi"

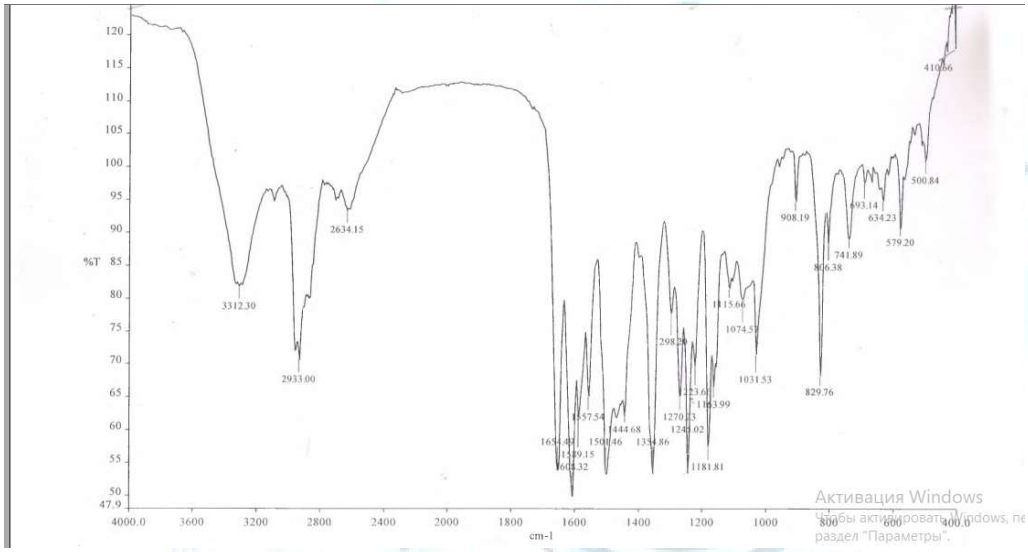
Elektrostatik potensial		Umumiy zaryad zichligi	
2D	3D	2D	3D



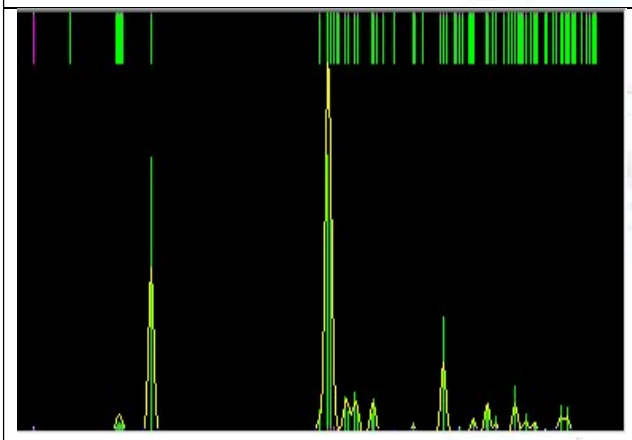
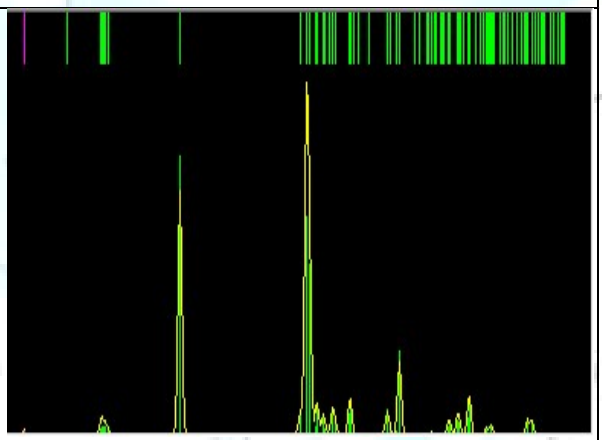
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Izlanishlar davomida kempferolning CNDO, INDO, MNDO, AM1, RM1, PM3 yarimempirik usullar orqali nazariy hisoblangan IQ spektrlari olindi, amaliy hisoblangan IQ spektrlari solishtirildi va usullar orasidagi farqlar jadval shaklida o'zaro taqqoslandi.

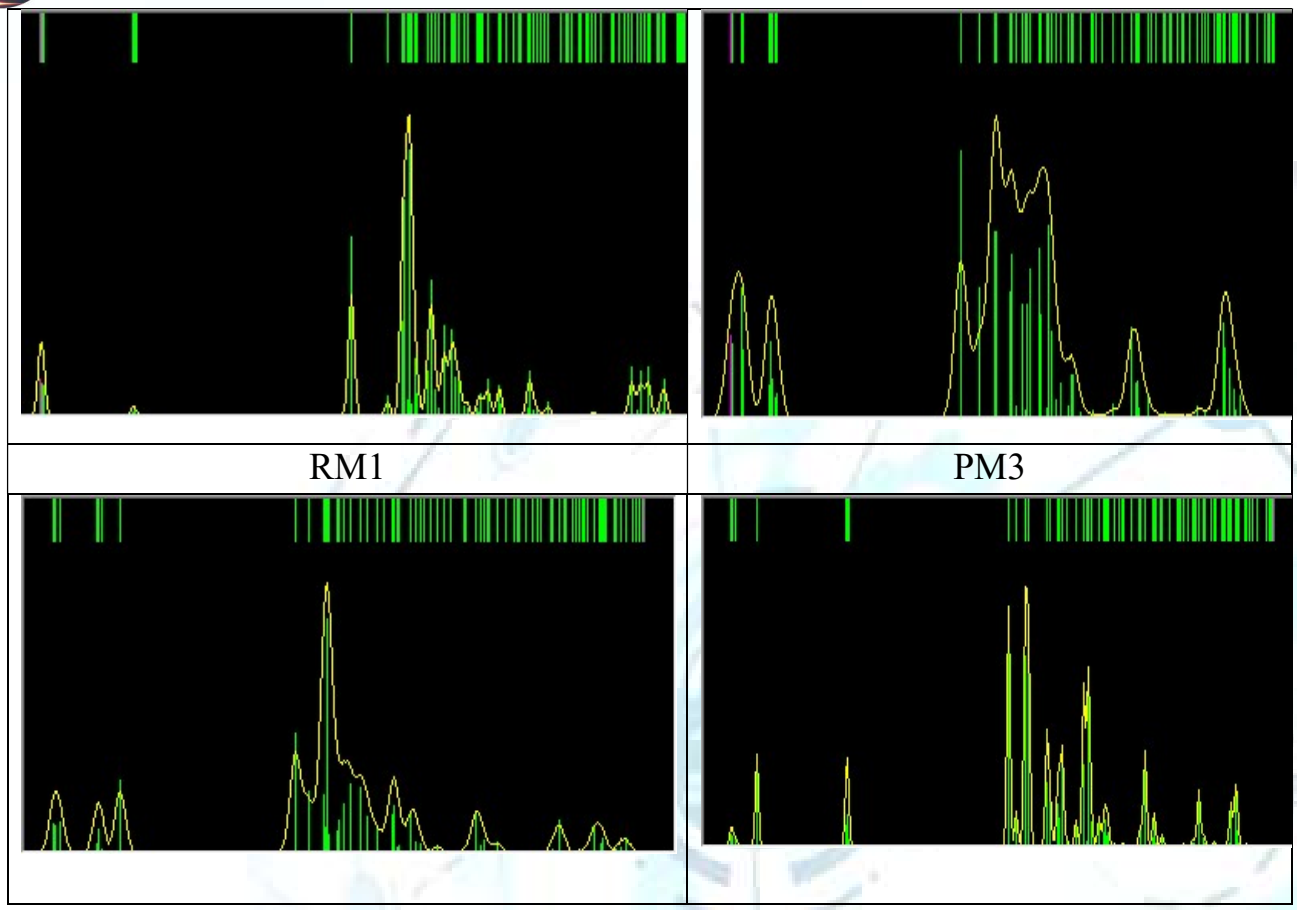
8 – rasm. Kempferolning amaliy tadqiqotlar natijasida olingan IQ qiymati



9 – rasm. Kempferolning Hyperchem (CNDO, INDO, MNDO, AM1, RM1, PM3) dasturida olingan IQ qiymatlari

CNDO	INDO
	
MNDO	AM1

ISSN 3030-3907



4 - jadval

Noemperik usullarda olingan IQ spektrlaring qiymatlari								
N	Bog‘	Real	CNDO	INDO	MNDO	AM1	**RM1**	PM3
1	O-H	3312	5078	4999	3982	3440	3281	3857
2	C-H (ar.hal)	2933	4624	4603	3407	3201	3044	3067
3	C=O	1654	2690	2639	2077	2004	1952	1912
4	C=C (C halqa)	1589	2613	2582	1848	1891	1882	1862
5	C= C (ar.hal)	1608	2583	2546	1757	1792	1796	1796

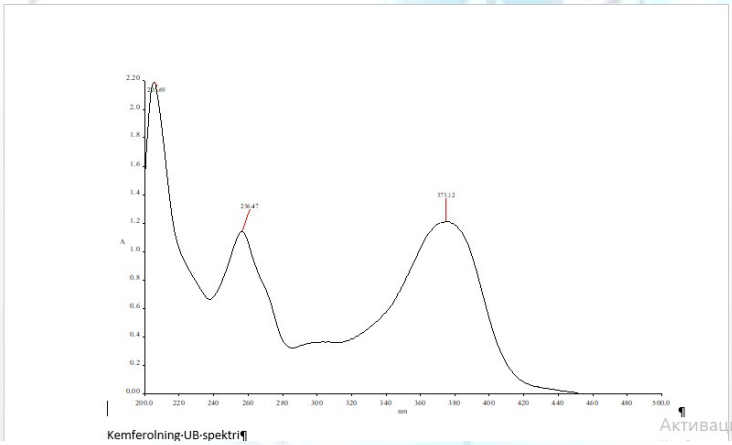
8 – rasmda (amaliy) fenollik –OH guruhlari mavjud va ular 3600 – 3200 cm^{-1} oralig’ida , vodorod bog’lanish va kombinatsion modlar sababli 2600 – 2000 cm^{-1} sohada zaif signal kuzatilgan. Aromatik C – H bog’larida 1300 – 1000 cm^{-1} oralig’ida deformatsion, 2850 – 2950 cm^{-1} oralig’ida 2933 cm^{-1} valent tebranish kuzatilgan. C=O bog’lari 1654 cm^{-1} da valent tebranish, aromatik halqadagi C=C bog’lar 1550 – 1600 cm^{-1}, C halqadagi konyugatsiyalangan C=C bog’i 1550 – 1620

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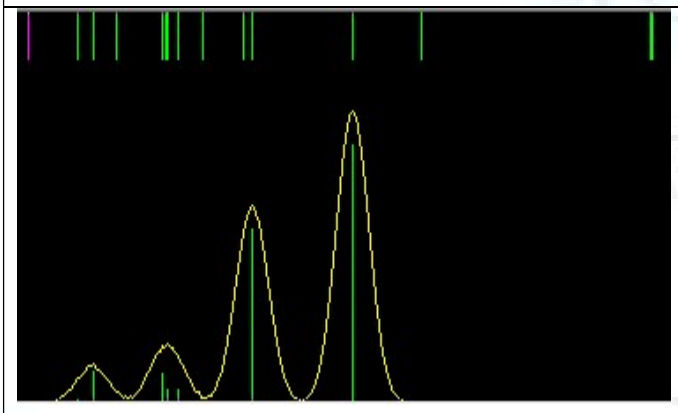
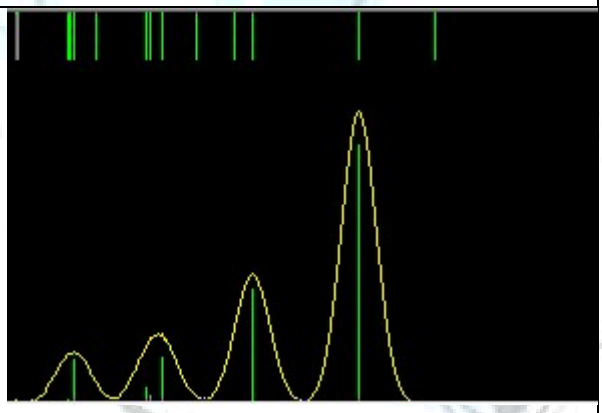
cm^{-1} sohada valent tebranish kuzatilgan. C –O bog'i 1270 – 1015 cm^{-1} sohada deformatsion tebranish kuzatilgan va 4 – jadvalda spektrdagi chastotalar keltirilgan. 9 – rasmda (nazariy) keltirilgan IQ qiymatlari solishtirilganda (4 – jadval) Hyperchem dasturining RM1 kuch maydonlari yordamida hisoblangan nazariy qiymatlarga yaqin ekanligi aniqlandi. Bu natija tajribaviy va nazariy ma'lumotlar o'rtasidagi moslikni tasdiqlab, RM1yondashuvining ushbu birikma uchun vibratsion spektrlarni modellashtirishda boshqa usularga qaraganda yuqori aniqlikka ega ekanligini ko'rsatadi.

Kempferolning CNDO, INDO, MNDO, AM1, RM1, PM3 yarimempirik usullar orqali nazariy hisoblangan UB spektrlari olindi va amaliy hisoblangan UB spektrlari bilan solishtirildi.

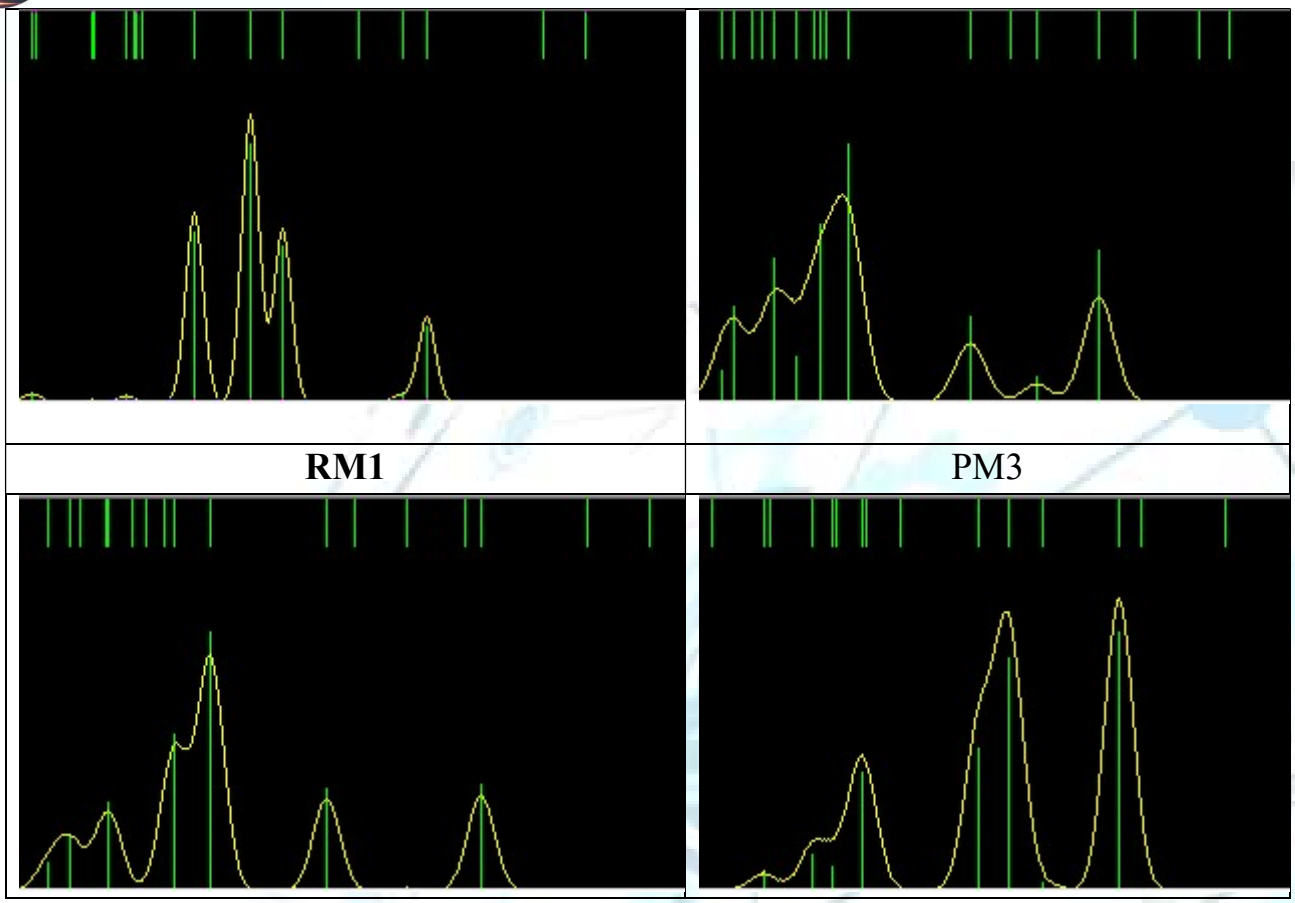
10 – rasm. Kempferolning amaliy tadqiqotlar natijasida olingan UB qiymati



11 – rasm. Kempferolning Hyperchem (CNDO, INDO, MNDO, AM1, RM1, PM3) dasturida olingan UB qiymatlari

CNDO	INDO
	
MNDO	AM1

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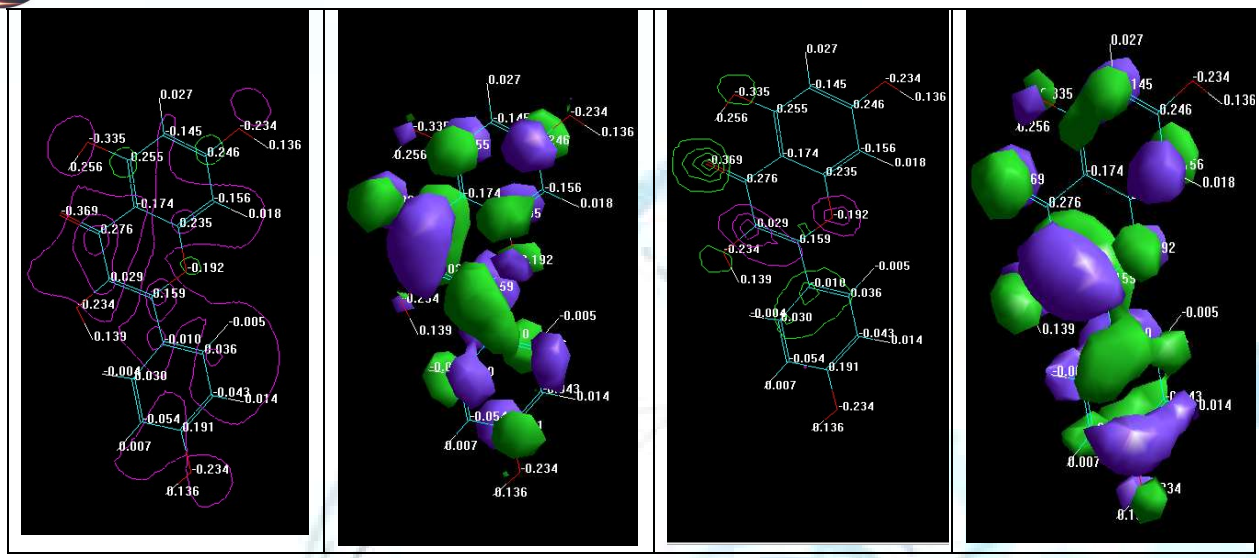
10 – rasmda (amaliy) kempferolning UB spektri bo'yicha 3 ta asosiy singish cho'qqilariga ega ekanligi ko'rsatilgan. 205.69 nm da to'liq konyugatsiyalangan tizimga ega bo'lgan benzol va flovon yadrolarining asosiy π → π o'tishlari, 256.47 nm da flavon yadro tizimining konyugatsiyalangan uglerod – oksigen (C=O) guruhlari, 375.12 nmda (to'lqin uzunligi eng uzun) n → π o'tishlari kuzatilgan. 11 – rasmda (nazariy) Hyperchemning CNDO, INDO, MNDO, AM1, RM1, PM3 usullarida UB spektrlari berilgan, bunga ko'ra mos ravishda π → π o'tishlar 141.24 nm, 149.13 nm, 264.18 nm, 245.55 nm, 246.8 nm, 265.01 nm, n → π o'tishlari 161.05 nm, 170.12 nm, 332.87 nm, 341.44 nm, 336.6 nm, 298.52 nmda o'tishlar kuzatilgan (to'lqin uzuniklarining o'rtacha qiymati olindi). Amaliy va nazariy hisob kitoblar taqooslanganda RM1 usuli eng maqbul usul deb olindi.

Tadqiqot davomida HyperChem hisoblash dasturi yordamida kempferolning CNDO, INDO, MNDO, AM1, RM1, PM3 yarimempirik usullar orqali HOMO va LUMO energiyalarining qiymatlari va 2D va 3D holatlari aniqlandi.

12 – rasmKempferolning CNDO yarimempirik usul orqali hisoblangan LUMO va HOMO energiyalari qiymati hamda 2D, 3D holatlari

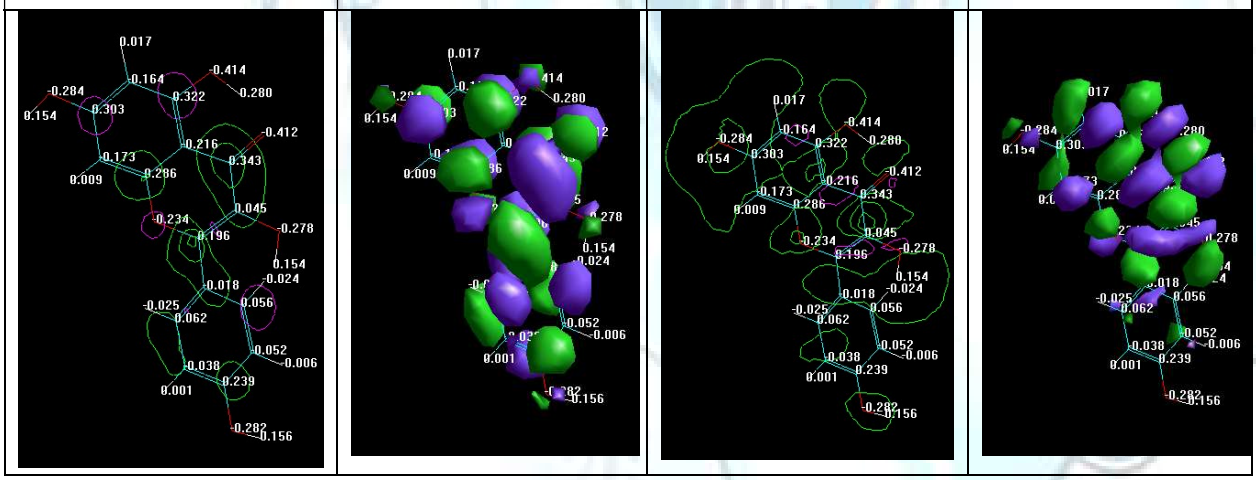
LUMO (1.12372)		HOMO (-10.86457)	
2D	3D	2D	3D

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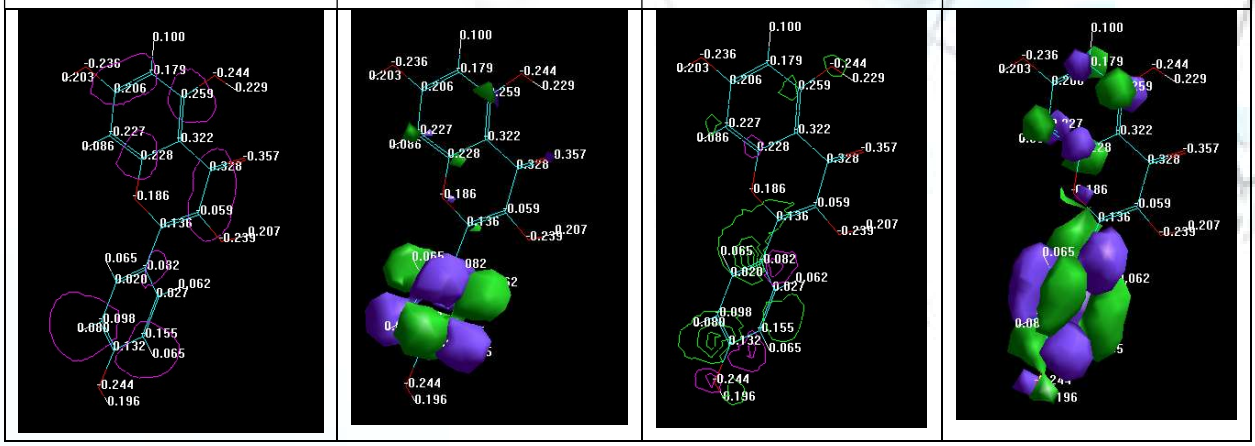
13 – rasm. Kempferolning INDO yarimempirik usul orqali hisoblangan LUMO va HOMO energiyalari qiymati hamda 2D, 3D holatlari

LUMO (1.451411)		HOMO (-10.16178)	
2D	3D	2D	3D



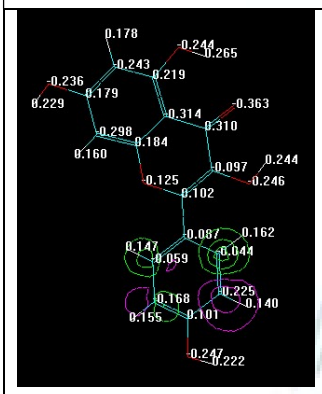
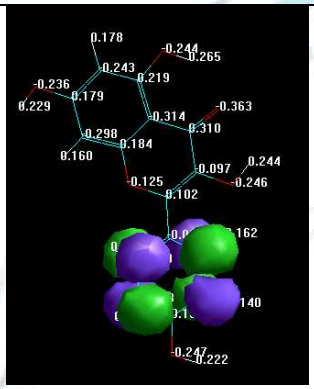
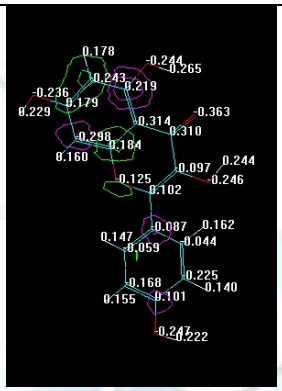
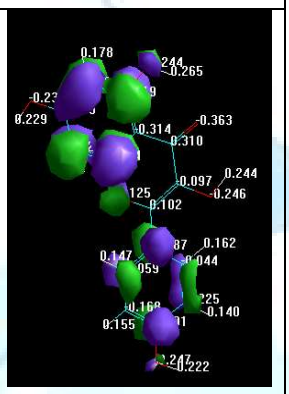
14 – rasm. Kempferolning MNDO yarimempirik usul orqali hisoblangan LUMO va HOMO energiyalari qiymati hamda 2D, 3D holatlari

LUMO (0.08456084)		HOMO (-0.08605517)	
2D	3D	2D	3D

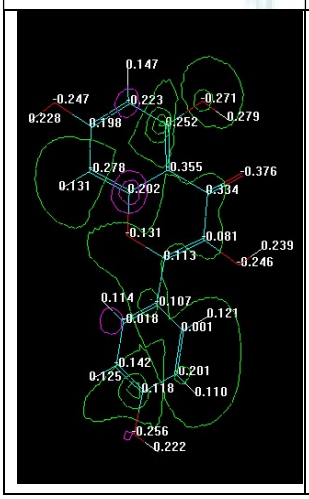
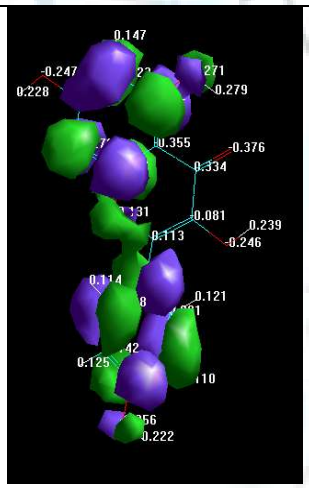
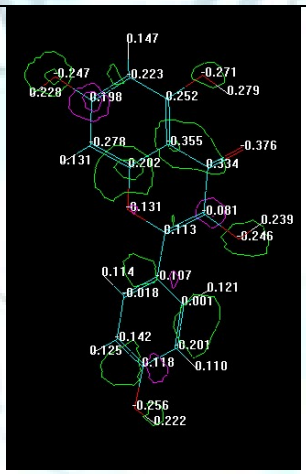
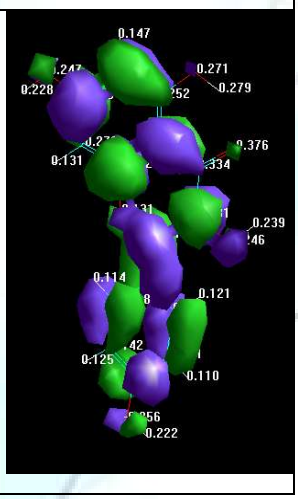


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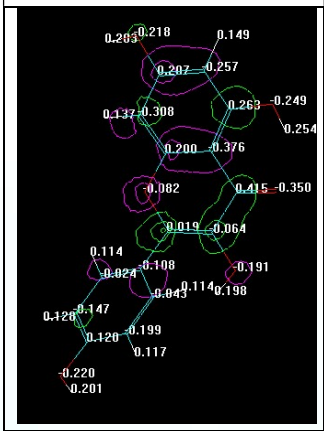
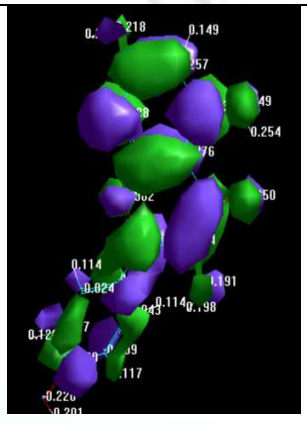
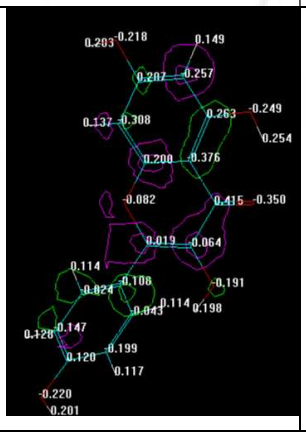
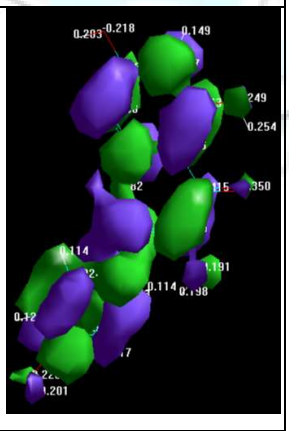
15 – rasm. Kempferolning AM1 yarimempirik usul orqali hisoblangan LUMO va HOMO energiyalari qiymati hamda 2D, 3D holatlari

LUMO (0.1907745)		HOMO (-0.02426674)	
2D	3D	2D	3D
			

16 – rasm. Kempferolning RM1 yarimempirik usul orqali hisoblangan LUMO va HOMO energiyalari qiymati hamda 2D, 3D holatlari

LUMO (0.1218344)		HOMO (-0.3546111)	
2D	3D	2D	3D
			

17 – rasm. Kempferolning PM3 yarimempirik usul orqali hisoblangan LUMO va HOMO energiyalari qiymati hamda 2D, 3D holatlari

LUMO (0.2948135)		HOMO (-0.05800036)	
2D	3D	2D	3D
			

ISSN 3030-3907

5 – jadval

Nomi	LUMO (eV)	HOMO (eV)	ΔE (eV) = LUMO - HOMO
CNDO	1.12372	-10.86457	11.98829
INDO	1.451411	-10.16178	11.61319
MNDO	0.08456084	-0.08605517	0.17062
AM1	0.1907745	-0.02426674	0.21504
RM1	0.1218344	-0.3546111	0.47645
PM3	0.2948135	-0.05800036	**0.35281386**

5 – jadvalda keltirilgan kempferol molekulasi uchun turli usullar orqali hisoblangan. HOMO va LUMO energetik qiymatlari hamda ularning farqlari (ΔE) keltirilgan. (moddaning kimyoviy reaktivligi va barqarorligi haqida ma'lumot beradi. CNDO va INDO usullari juda katta ΔE berayotganligi sababli (≈12 eV) real eksperimental natijalarga mos kelmaydi. MNDO, AM1, PM3 usullari realistik ΔE (0.17 – 0.47 eV oralig'ida), PM3 usuli esa RM1 ga yaqin, lekin biroz past ΔE beradi. Eng maqbul usul sifatida PM3 barqarorlik va reaktivlik o'rtasida yaxshi balans beradi.

Tajriba qism: Hyperchem dasturida dastlab "File" bo'limidan "Start log" ni belgilab bajarilayotgan amallar yozib olinishi uchun bloknot ochildi, "File" bo'limidan " Open" ni belgilab moddaning Chemofficeda chizib olingan sturukturasi chiqarib olindi, " Build" --> " Add H &Model build", " Display" bo'limidan " Labels" --> "Symbol" --> " None" orqali molekuladagi element belgilari chiqarildi. " Setup " bo'limidan "Molecular mechanics" dan MM+ni tanlab olindi va " Compute" --> " Geometry Optimization" orqali optimizatsiya qilib olindi. Shundan so'ng yarimempirik usullar tanlashdan oldin " Display" bo'limidan " Labels" --> "Symbol" --> "Charge" orqali molekula zaryad qiymatlari keltirildi va " Setup" bo'limidan " Semi-empirical " da CNDO, INDO, MNDO, AM1, RM1, PM3 usullarini birma – bir tanlash orqali (" Compute " --> " Geometry Optimization ") atom zaryad zichligi, (" Compute " --> " Plot Molecular Graphs " --> " Electrostatic Potential " 2D, 3D; " Total Charge Density " 2D, 3D) zaryad taqsimoti, (" Compute " --> " Vibration, Rotation Analysis " --> " Vibrational Spectrum ") IQ spektri, (" Compute" --> " Single Point Cl " --> " Electronic Spectrum ") UB spektri, (" Compute " --> " Orbitals " 2D, 3D) LUMO, HOMO qiymatlari olindi. Saqlangan bloknotdan moddaning dipol momenti va hosil bo'lish issiqliklari qiymatlarini olishda foydalanildi.

Xulosa: Hyperchem dasturidagi CNDO yarimempirik usulida kempferol moddasining hosil bo'lish issiqligini hisoblash uchun qulay ekanligi aniqlandi, atom

ISSN 3030-3907

zaryad qiymati, elektrostatik potensial hamda umumiy zaryad zichligi orqali olingan natijalar umumlashtirilganda >C=O guruhning elektrofil markaz ekanligi va nukleofil hujum bo'lish ehtimoli, shu guruhdagi >O esa nukleofil markaz va elektrofil hujum bo'lish ehtimolligi yuqori ko'rsatkichni berdi. Yarimempirik usullardan olingan dipol moment (Debye) molekula tarkibida polyar funksional guruhlar (- OH va - C=O) mavjudligi sababli o'rtacha qutbli qiymatga ega bo'lgan AM1 va RM1 qiymatlarni eng maqbul variant deb qabul qilindi. IQ spektrlari tahlil qilinganda CNDO, INDO, MNDO yarimempirik usullari orqali olingan qiymatlar amalda olingan qiymatlardan keskin farq qilishi va RM1 usulida olingan qiymatlar amaliy natijalarda olingan qiymatlarga nisbatan yaqin chiqishi sababli eng maqbul variant deb qabul qilindi. UB spektrlari tahlili natijada amaliy qiymatlar va RM1 usulida olingan qiymatlar juda ham yaqin keldi. LUMO va HOMO energiyalarining farqi Bandgap molekulyar tarmoqli oralig'ini o'rganish natijasida CNDO yarimempirik usulida katta diapozon hosil bo'ldi va nazariy jihatdan izolyatorlar sifatida qo'lash mumkinligi o'rganildi, PM3 usulida esa o'rtacha diapozon hosil bo'lganligi sababli yarimo'tkazgichlar sifatida qo'llash mumkinligi aniqlandi.

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ISSN 3030-3907