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# GLITSIRRET KISLOTASI VA UNING XOSILALARINI REAKSION FAOLLIGINI HyperChem DASTURI YORDAMIDA KVANT KIMYOVIY HISOB – KITOB QILISH

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**Annotatsiya**
HyperChem dasuri orqali glitsirret kislotasining zaryad qiymatlari va hosil bo'lish issiqligi, IQ spektrlarini nazriy o'rganish natijalari keltirilgan.

**Kalit so'zlar:** MM+, AMPER, IQ sprktr olish, AM1, RM1, PM3 glitsirret kislotasining**.**

## Kirish

HyperChem pragrammasi orqali kimyoviy birikmalarning sturukturasini chizish va uni malekulyar mexanika, yarim empirik, noempirik, hamda DFT usullari bilan hisob kitob qilishimiz mumkin va shu bilan bir qatorda moddaning infraqizil va ultrabinafsha spektrlarini hisoblash mumkin. Yarim empirik, noempirik, hamda malekulyar mexanika usullarida hisob -kitob o'tkazish imkoniyatini beruvchi majmualardan biri HyperChem hisoblanadi.Bu programma boshqa programmalardan farqli ravishda hisoblanishi kerak bo'lgan birikmaning geometriyasini xuddi qalam bilan chizgandek hosil qiladi va hisoblashlarni bevosita kuztib turish imkonini beradi.HyperChem programmasida MM+, AMBER, BIO+ va OPLS MM usullari kiritilgan.

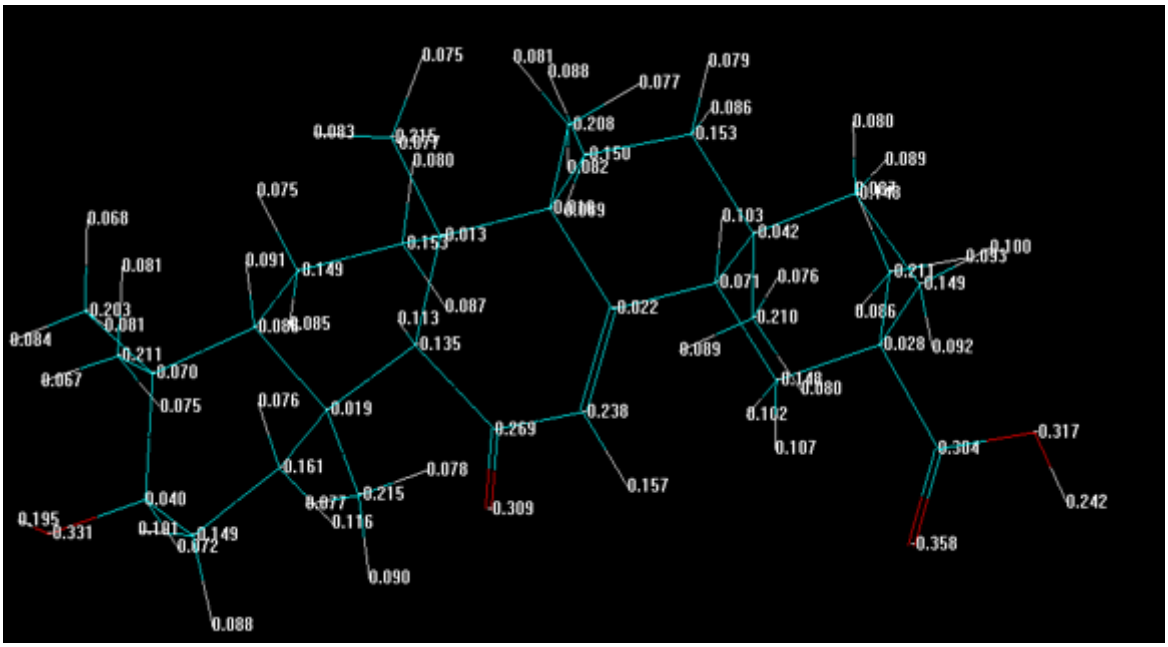
**Olingan natijalar tahlili.**

1-jadval HyperChem dasturida glitsirret kislotasining olingan hosil bo'lish issiqlik energiyalari.

| MM | AMBER | BIO+(CHARMM) | OPLS |
|---|---|---|---|
| 83.421342 kcal/mol | 107.90669 kcal/mol | 135.34904 kcal/mol | 69.039166 kcal/mol |

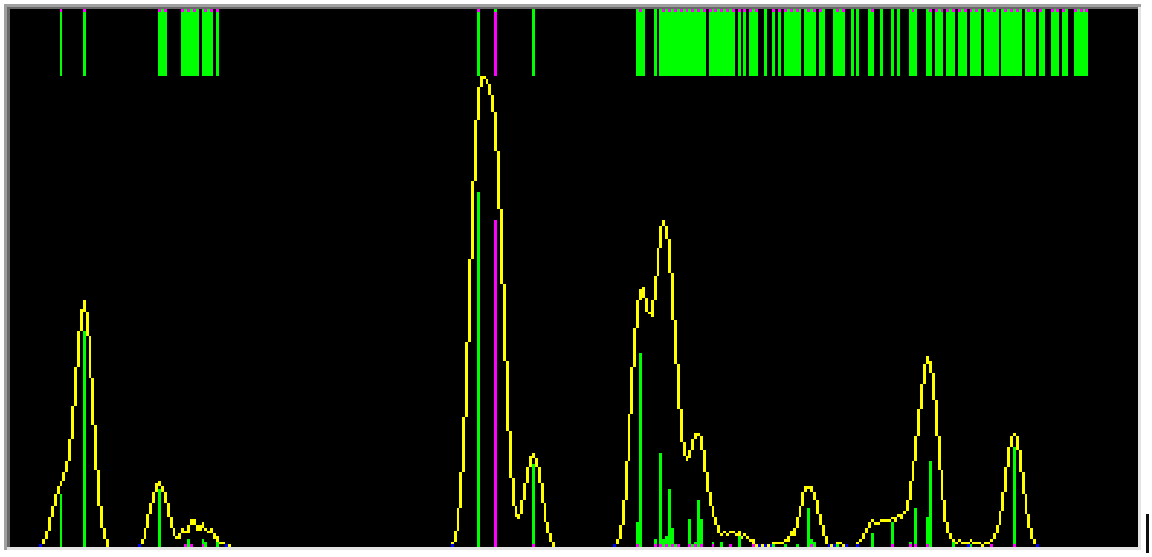
Hisoblash natijalari shuni ko'rsatadiki, glitsirret kislotasining hosil bo'lish issiqlik energiyasi **BIO+ (CHARMM)** metodida optimizatsiya qilinganda eng maksimal qiymatga ega (135.34904 kcal/mol) bo'ldi va **OPLS** metodida optimizatsiya qilinganda eng minimal qiymatga ega (69.039166 kcal/mol) bo'ldi. Bundan shunday xulosaga kelish mumkin, energetik parametr hisoblashda **OPLS** metodi samarali ekan.

**AM1-YARIM EMPERIK USUL**




**1-rasm. Glitsirret kislotasining HyperChem dasturida yarim emperik usullarda olingan tebranish spektri va zaryad qiymatlari.**

Glitsirret kislotasining HyperChem dasturining AM1- yarim emperik usulda hosil bo'lish issiqligi -7969.9 kcal/mol ga ega bo'ldi. 1-rasmda glitsirret kislotasining tebranish spektri va zaryad taqsimoti keltirilgan.

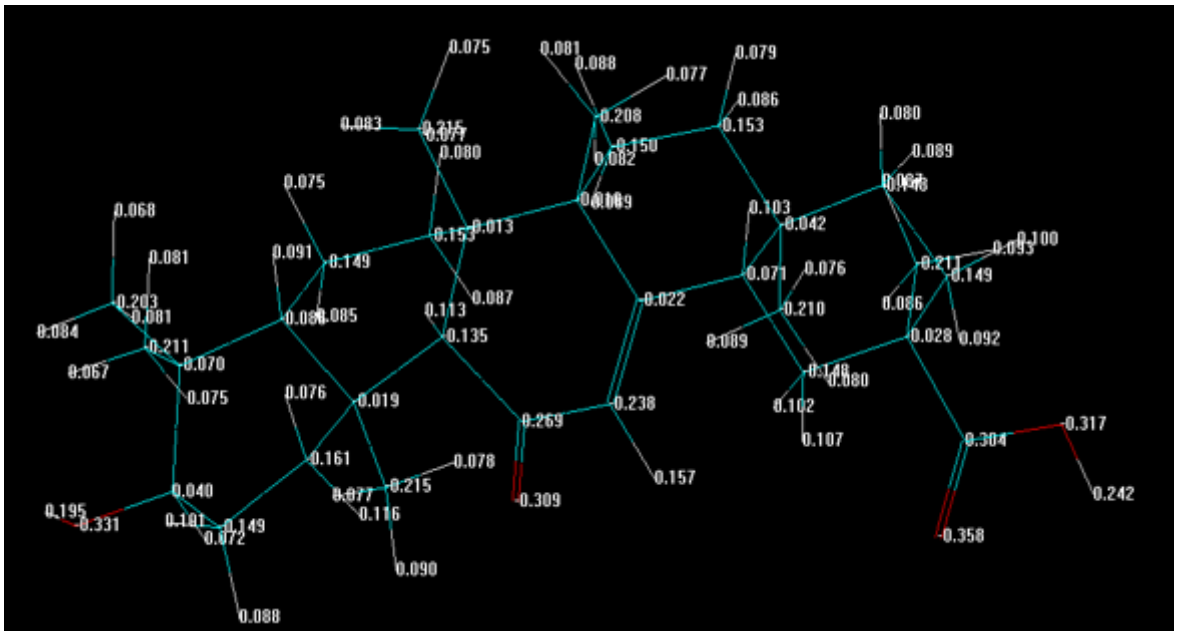


**2-rasm. Glitsirret kislotasining HyperChem dasturidagi AM1 yarim emperik metodida olingan IQ spektri**

HyperChem dasturida glitsirret kislotasiing strukturasini chizilib yarim empirik metodlarda IQ spektrlar olinganda quyidagi natijalar olindi:

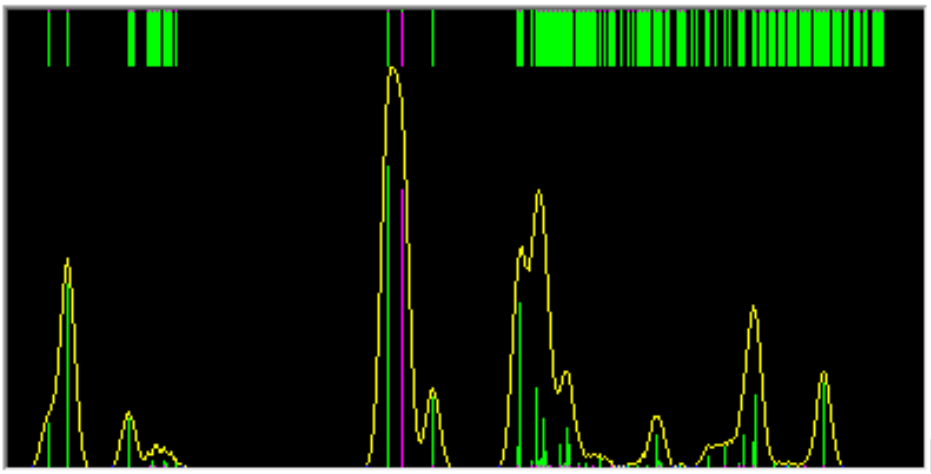
AM1 yarim empirik usulida 3506 $sm^{-1}$ sohada O-H bog'lar valent tebranishlar signal berdi. 3162 $sm^{-1}$ sohada $-CH_3$ bog'lar valent tebranish signal berdi. 1082 $sm^{-1}$ sohada karbaksil gurupposidagi C=O bog'lar valent tebranishlar hosil qiladi. 2024 $sm^{-1}$ sohada halqaga birikkan C=O bog'lar valent tebranishlar signal berdi. 1899 $sm^{-1}$ sohada xalqadagi qo'shbog' tutgan C=C atomlari bog'lar valent tebranish signal berdi. 1537 $sm^{-1}$ sohada COOH gurupposi valent tebranishlar signal berdi. 1462 $sm^{-1}$ sohada halqadagi uglerod atomlari valent tebranishlar signal berdi. 263 $sm^{-1}$ sohada O-H bog'lar defarmatsion tebranish signal berdi. Eng yuqori signal OH funksional gurihidagi O-H bog'lar orasidagi valent tebranishlar ekan.

## RM1-YARIM EMPERIK USUL



**3-rasm. Glitsirret kislotasining HyperChem dasturida yarim emperik usullarda olingan tebranish spektri va zaryad qiymatlari.**

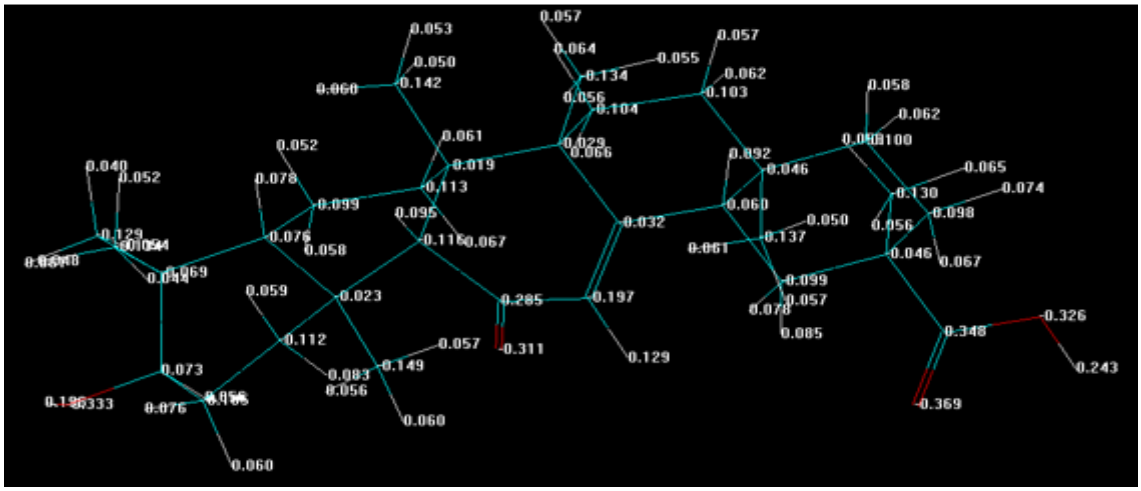
Glitsirret kislotasining HyperChem dasturining RM1- yarim emperik usulda hosil bo'lish issiqligi -6421.9 kcal/mol ga ega bo'ldi.



**4-rasm. Glitsirret kislotasining HyperChem dasturidagi RM1 yarim emperik metodida olingan IQ spektri**

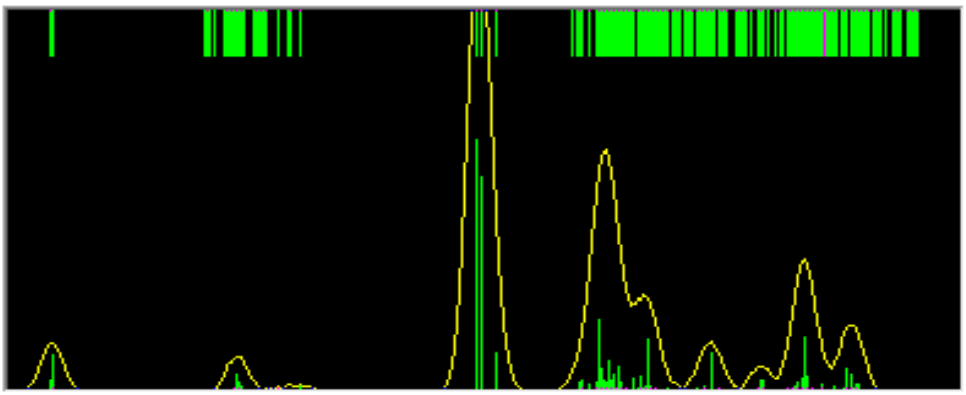
RM1 yarim empirik usulida 3317 $sm^{-1}$ sohada O-H bog'lar, 1491 $sm^{-1}$ sohada $-CH_3$ bog'lar, 2016 $sm^{-1}$ sohada karbaksil gurupposidagi C=O bog'lar, 1984 $sm^{-1}$ sohada halqaga birikkan C=O bog'lar, 1858 $sm^{-1}$ sohada xalqadagi qo'shbog' tutgan C=C atomlari bog'lar, 1557 $sm^{-1}$ sohada COOH gurupposidagi C atomi va OH gurupposidagi O atomi, 3025 $sm^{-1}$ sohada qo'shbog' tutgan C-H atomlari valent tebranish signallar beradi. 529 $sm^{-1}$ sohada halqadagi uglerod atomlari defarmatsion tebranishlar signal berdi.

## PM3-YARIM EMPERIK USUL



**5-rasm. Glitsirret kislotasining HyperChem dasturida yarim emperik usullarda olingan tebranish spektri va zaryad qiymatlari.**

Glitsirret kislotasining HyperChem dasturining PM3- yarim emperik usulda hosil bo'lish issiqligi -7972.3 kcal/mol ga ega bo'ldi.



**6 rasm. Glitsirret kislotasining HyperChem dasturidagi PM3 yarim emperik metodida olingan IQ spektri**

PM31 yarim empirik usulida 3855 $sm^{-1}$ sohada O-H bog'lar, 1426 $sm^{-1}$ sohada $-CH_3$ bog'lar, 1971 $sm^{-1}$ sohada karbaksil gurupposidagi C=O bog'lar, 19841945 $sm^{-1}$ sohada halqaga birikkan C=O bog'lar, 1882 $sm^{-1}$ sohada xalqadagi qo'shbog' tutgan C=C atomlari bog'lar, 3850 $sm^{-1}$ sohada COOH gurupposidagi O atomi va H atomlari valent tebranish signallar beradi. 949, 530, 333 $sm^{-1}$ sohalarda defarmatsion tebranishlar signal berdi.

## Xulosa

HyperChem dasturi yordamida glitsirret kislotasining energiyalari hisoblanganda eng minimal qiymat BIO+(CHARMM) metodida kuzatildi. Zaryad qiymatlari uch xil usulda optimizatsiya qilinganda ham unchalik farq kuzatilmadi. Tebranish spektrlarida esa birozgina siljishlar kuzatildi xolos.Bu shundan dalolat beradiki, HyperChem dasturi aniqliligi jihatdan yuqori o'rinda turadi.

## Foydalanilgan adabiyotlar ro'yxati

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