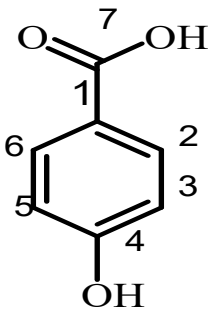
Electronic Supplementary Material (ESI) for RSC Advances.

Phytochemical on-line screening and *in silico* study of *Helianthemum confertum*: antioxidant activity, DFT, MD simulation, ADME/T analysis and xanthine oxidase binding

Yasmine Chemam[a,b,c]*, Samir Benayache[a], Abdeslem Bouzina[c], Eric Marchioni[b] , Omar sekiou[d], Houria Bentoumi[c], , Minjie Zhao[b], Zihad Bouslama[d], Nour-Eddine Aouf[c] and Fadila Benayache[a]

[a]*Unité de Recherche Valorisation des Ressources Naturelles, Molécules Bioactives et Analyses Physicochimiques et Biologiques, Université des Frères Mentouri, Constantine 1, Route d'Aïn El Bey, 25000 Constantine, Algeria.*
[b]*Chimie Analytique des Molécules Bioactives, Institut Pluridisciplinaire Hubert Curien (UMR 7178 CNRS/UDS), 74 route du Rhin, 67400 Illkirch, France.*
[c]*Laboratory of Applied Organic Chemistry, Bioorganic Chemistry Group, Department of Chemistry, Sciences Faculty, Badji Mokhtar Annaba University, Box 12, 23000 Annaba, Algeria*
[d]*Environmental Research Center, Alzon Castle, Boughazi Said Street, PB 2024, Annaba 23000, Algeria.*

Molecule 1: Para-hydroxybenzoic acid



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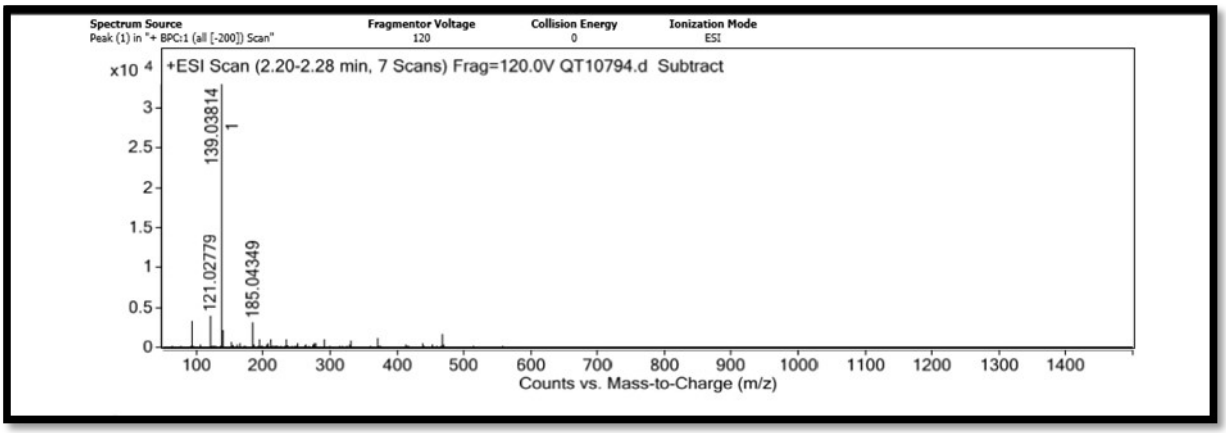


Figure.1.HRESI-MS (+) of para-hydroxybenzoic acid

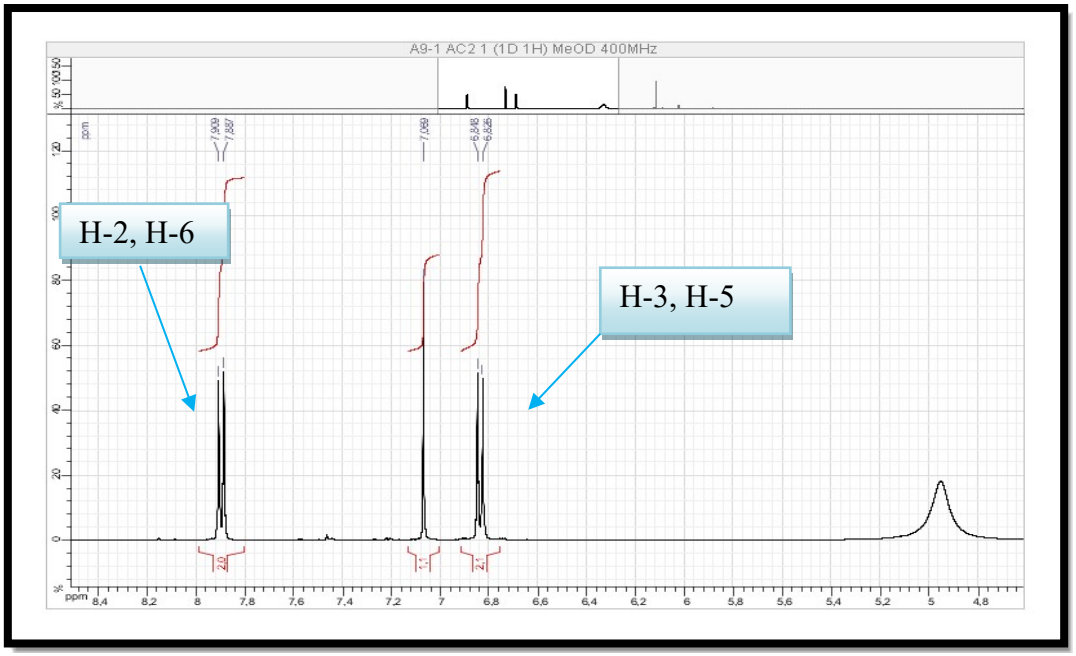


Figure.2. ^{1}H NMR spectrum (400MHz, CD_3OD, δppm) of para-hydroxybenzoic acid

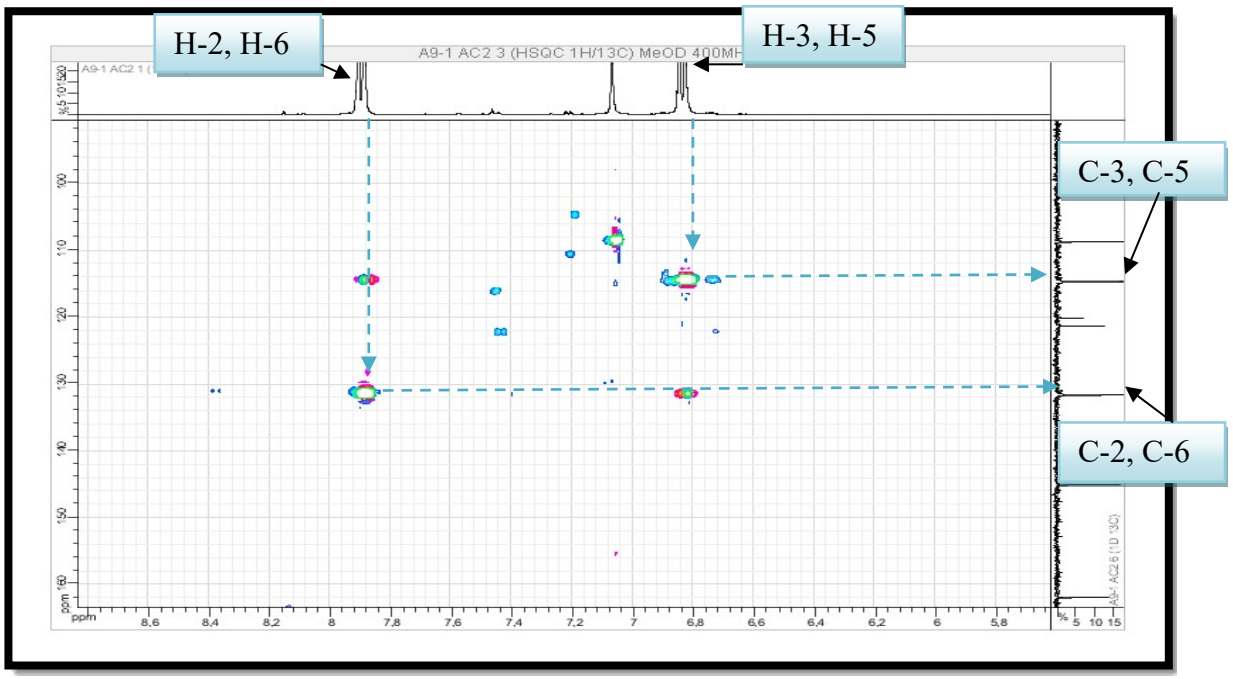


Figure .3.HSQC spectrum (400MHz, CD_3OD, δppm) of para-hydroxybenzoic acid

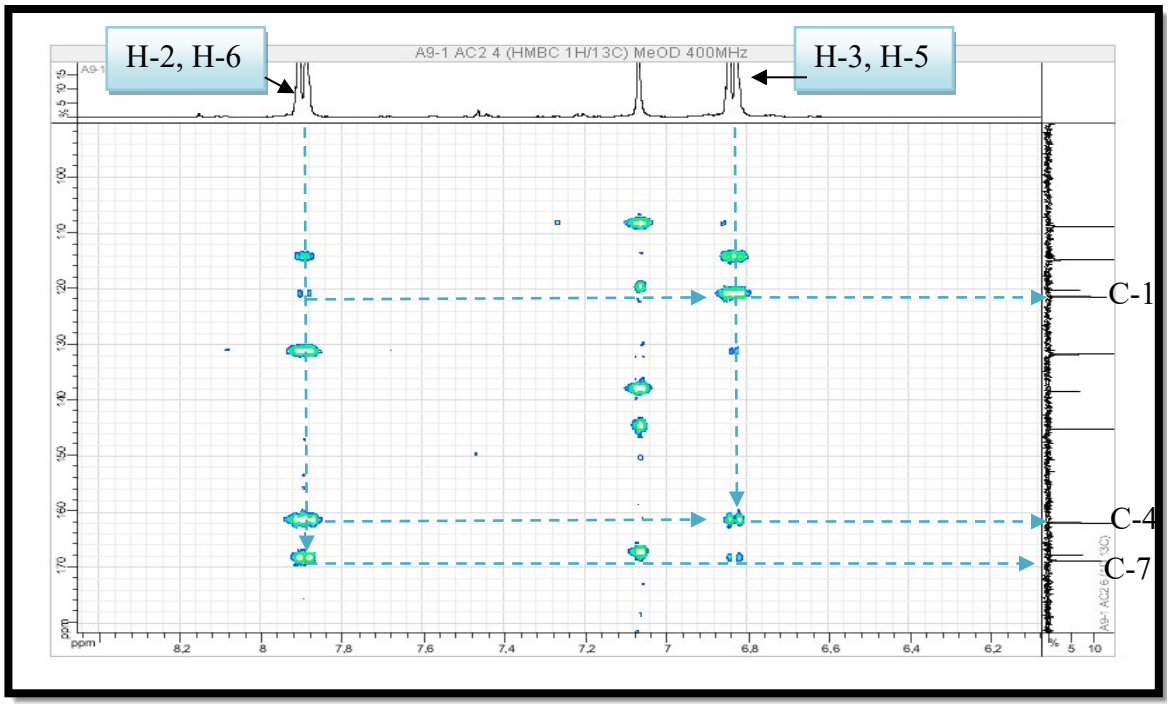


Figure .4.HMBC spectrum (400MHz, CD_3OD, δppm) of para-hydroxybenzoic acid

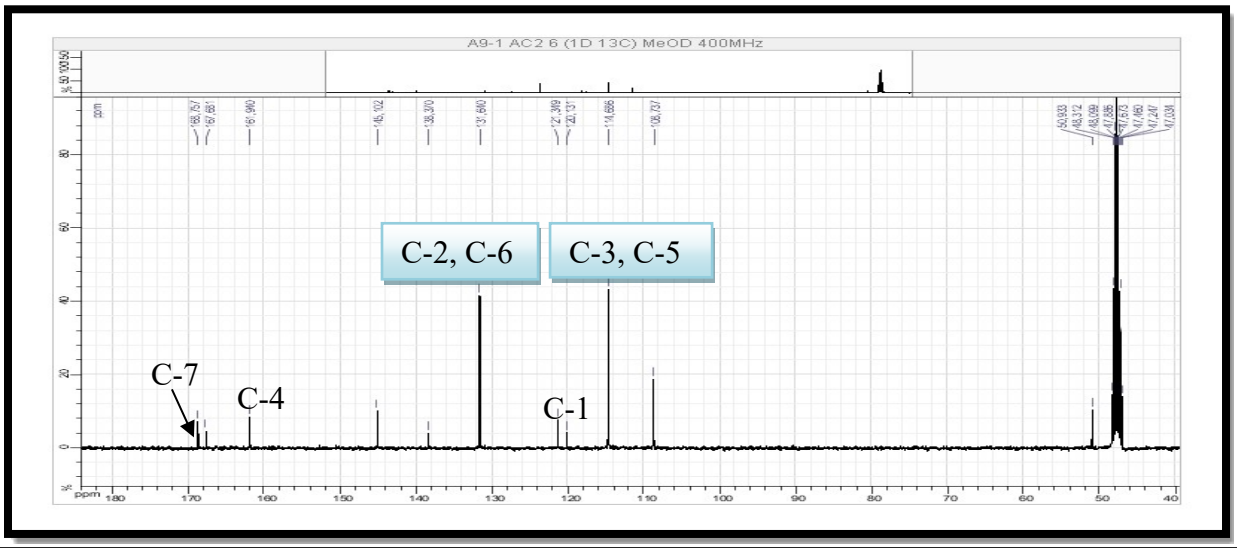


Figure.5. ^{13}C NMR spectrum (100MHz, CD_3OD, δppm) of para-hydroxybenzoic acid

Figure.5. ^{13}C NMR spectrum (100MHz, CD_3OD, δppm) of protocatechuic acid

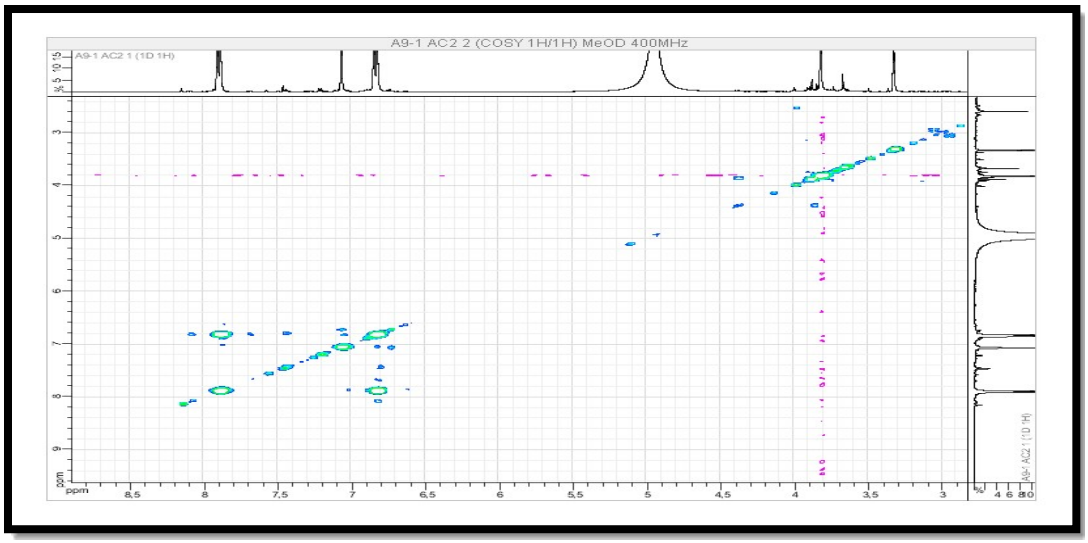
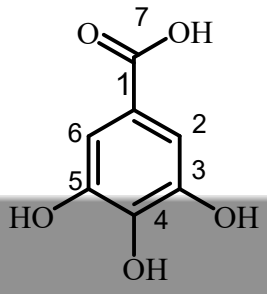


Figure.6. COSY spectrum (400MHz, CD_3OD, δppm) of para-hydroxybenzoic acid

Molecule 2: Methyl gallate



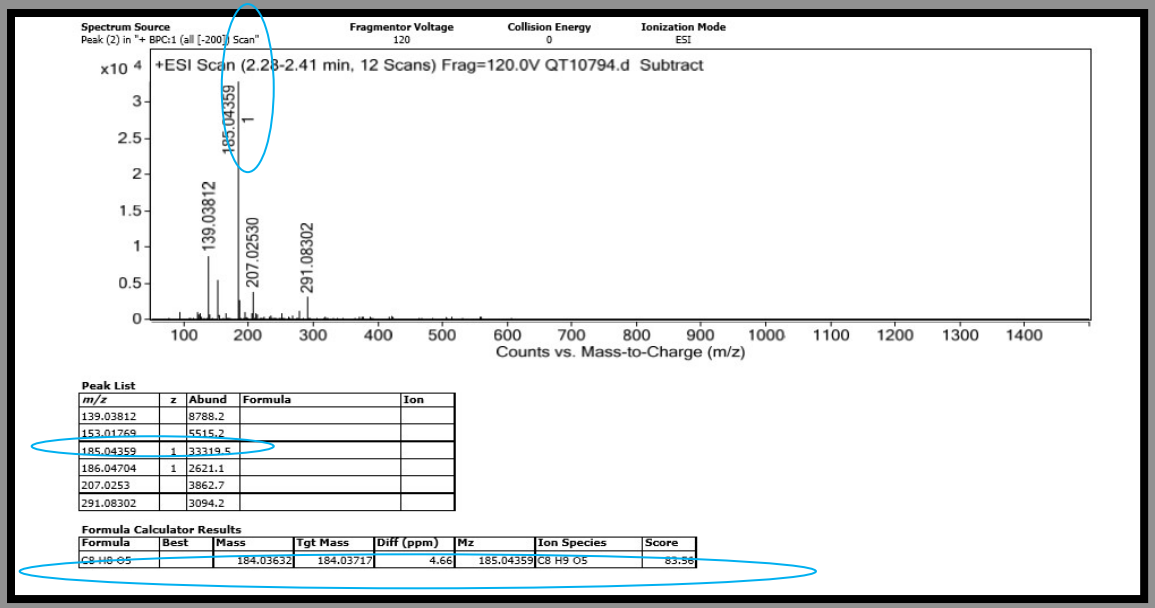


Figure.7.HRESI-MS (+) of methyl gallate

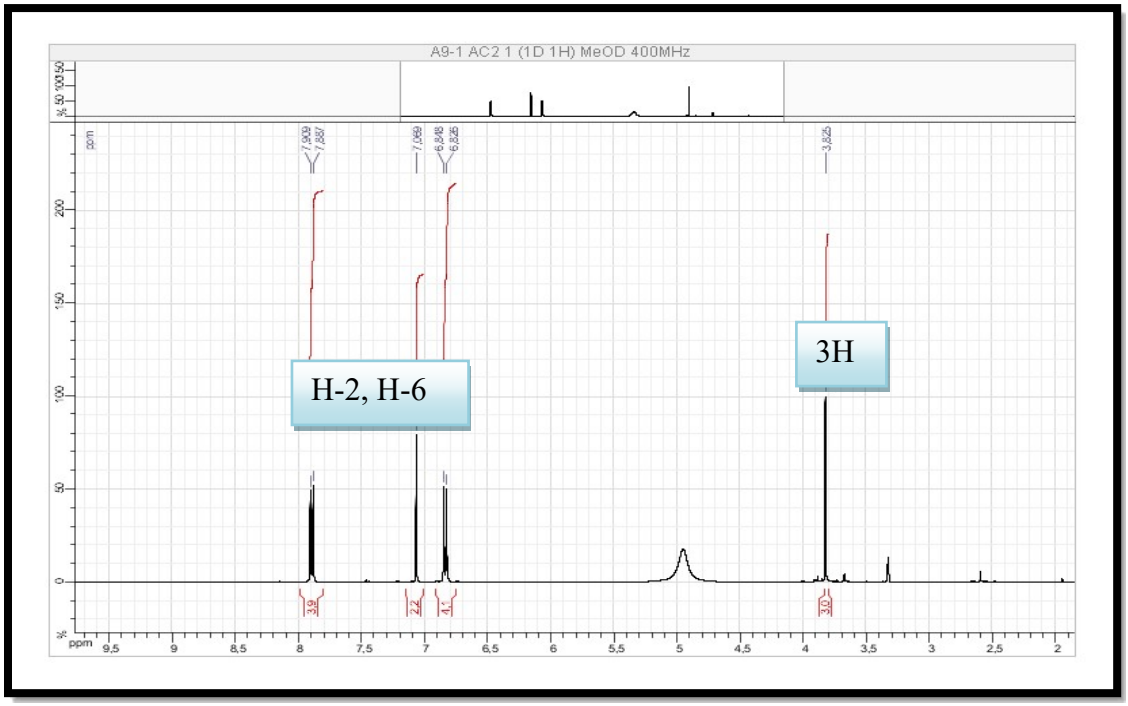


Figure.8. ^{1}H NMR spectrum (spreading out 2) (400MHz, CD_3OD, δppm) of methyl gallate

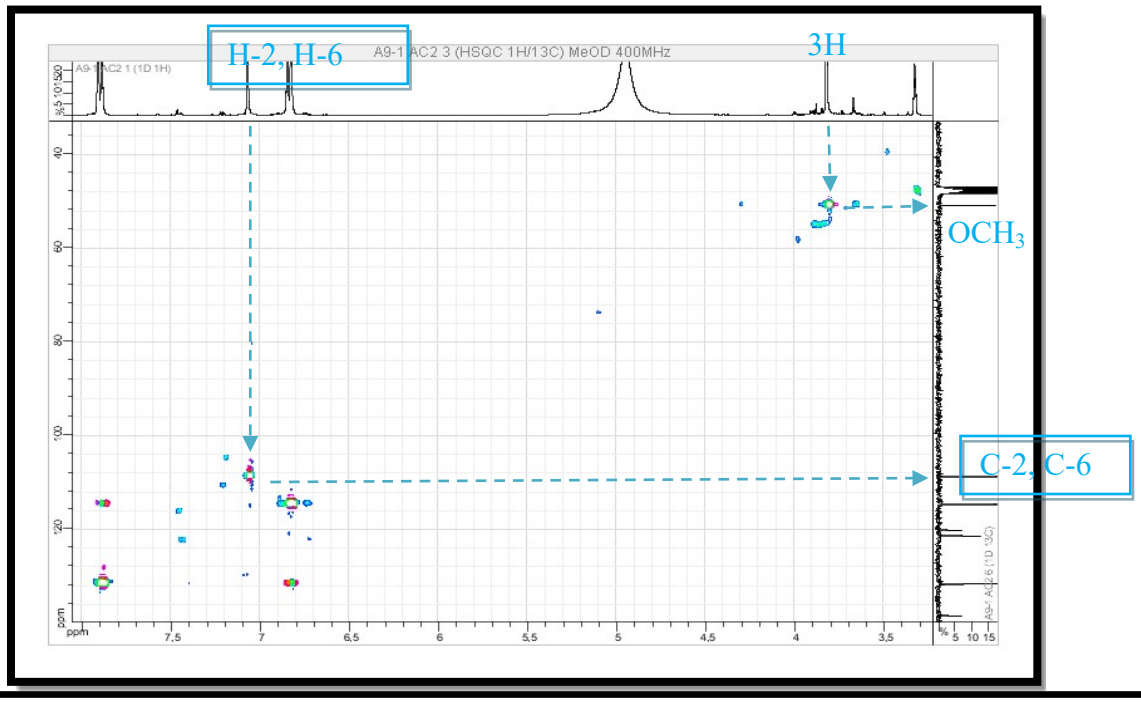


Figure .9.HSQC spectrum (spreading out 2) (400MHz, CD_3OD, δppm) of methyl gallate

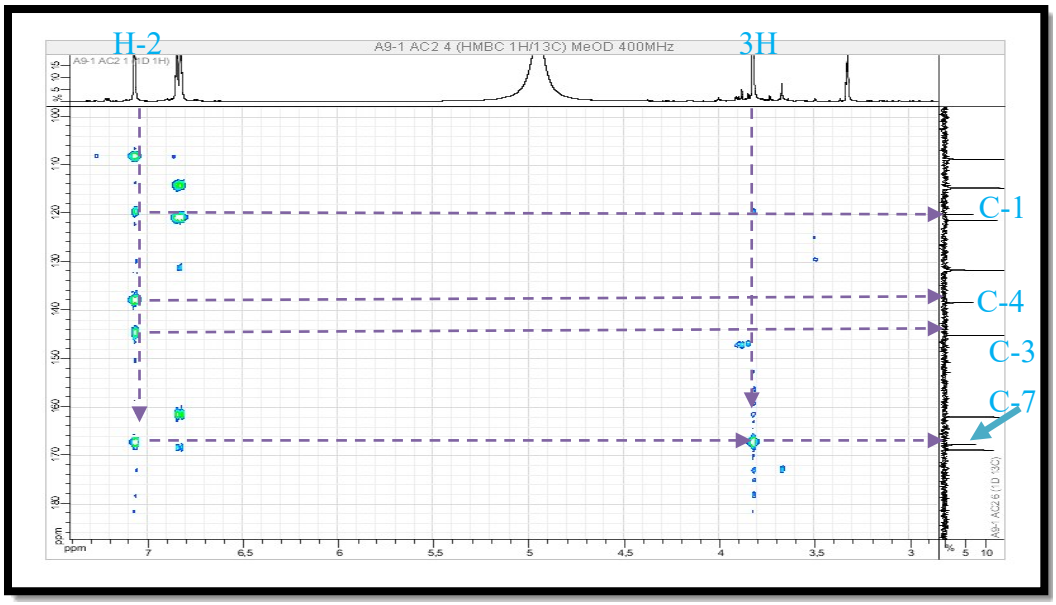


Figure .10.HMBC spectrum (spreading out 2) (400MHz, CD_3OD, δppm) of methyl

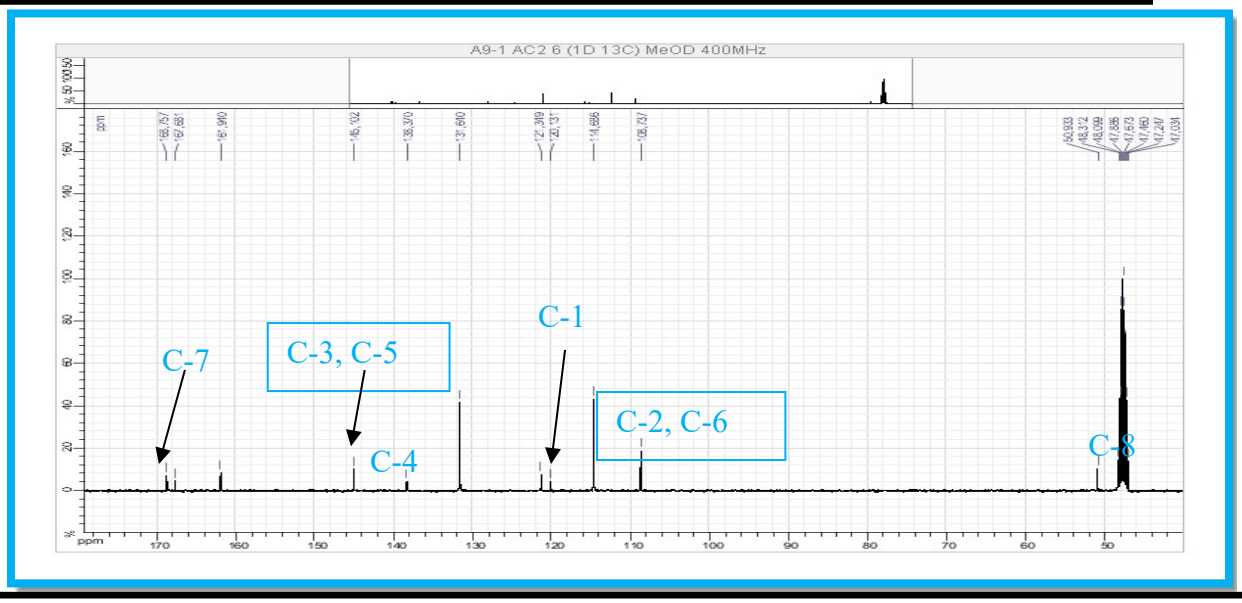
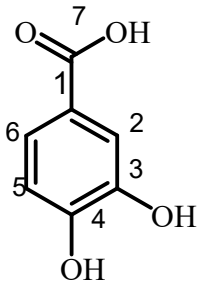


Figure.11. ^{13}C NMR spectrum (spreading out 2) (100MHz, CD_3OD, δppm) of methyl gallate

Molecule 3: Protocatechuic acid



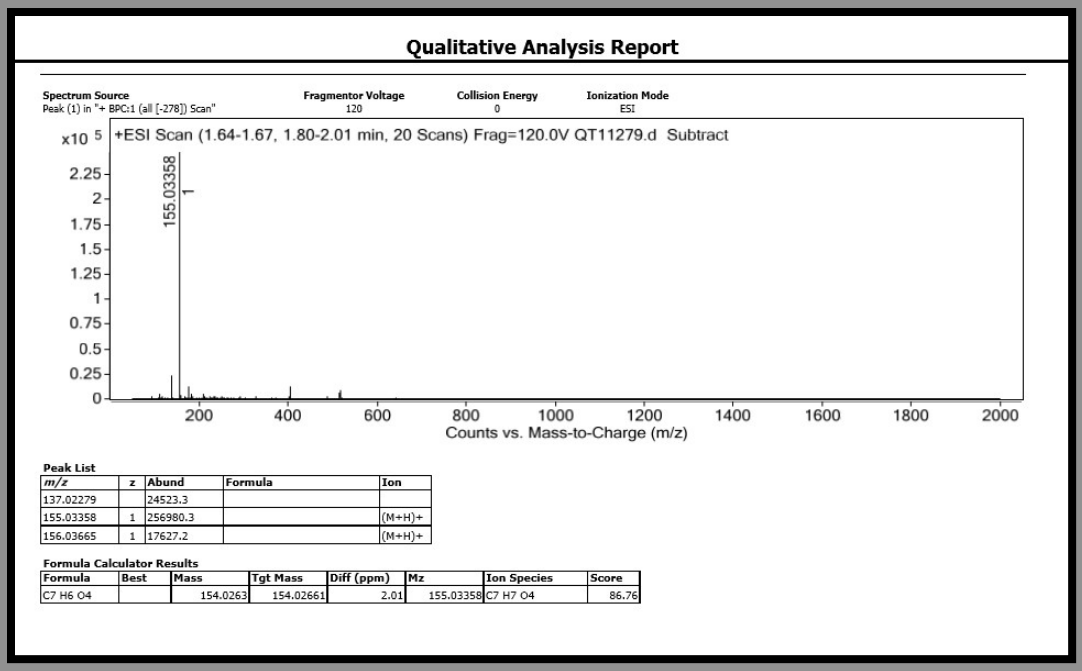


Figure.12.HRESI-MS (+) of Protocatechuic acid

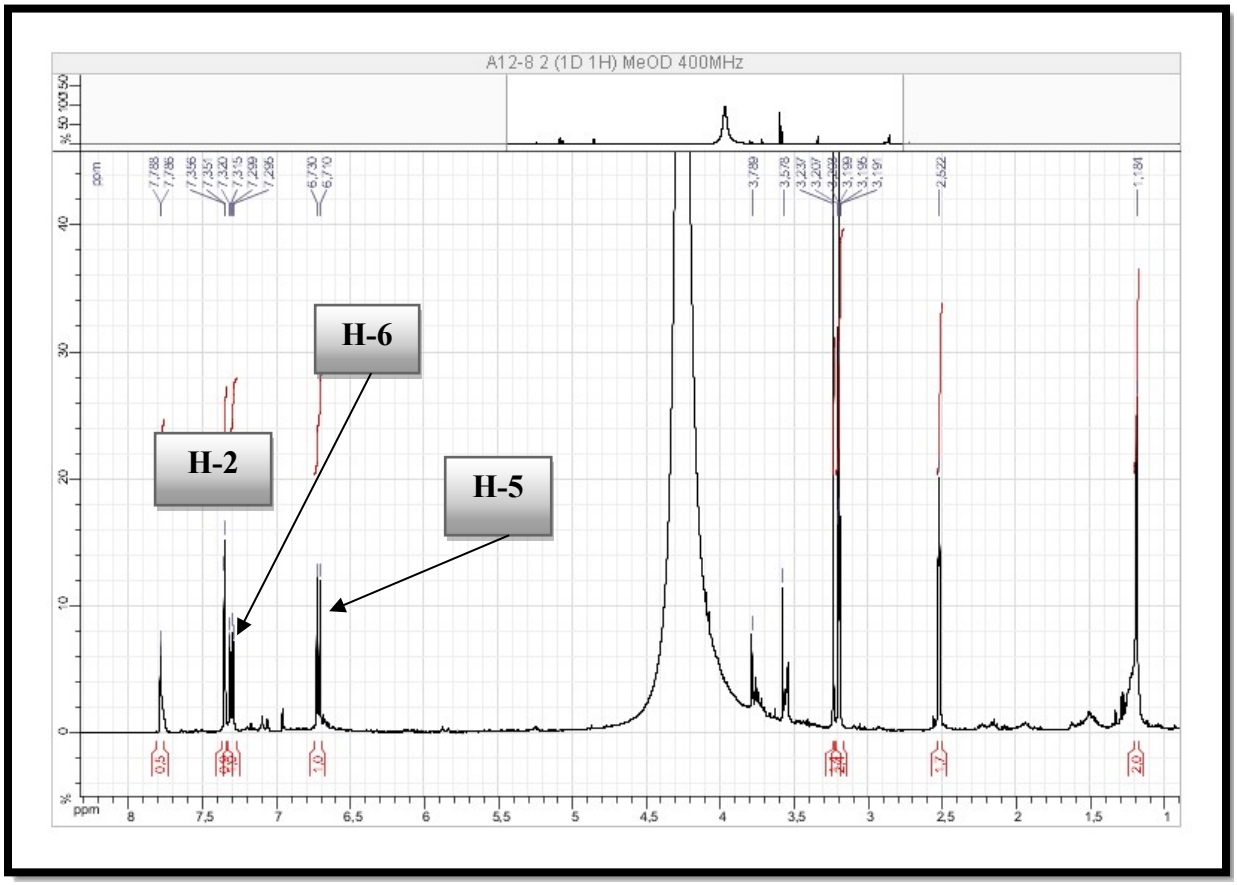


Figure.13. ^{1}H NMR spectrum (400MHz, CD_3OD, δppm) of protocatechuic acid

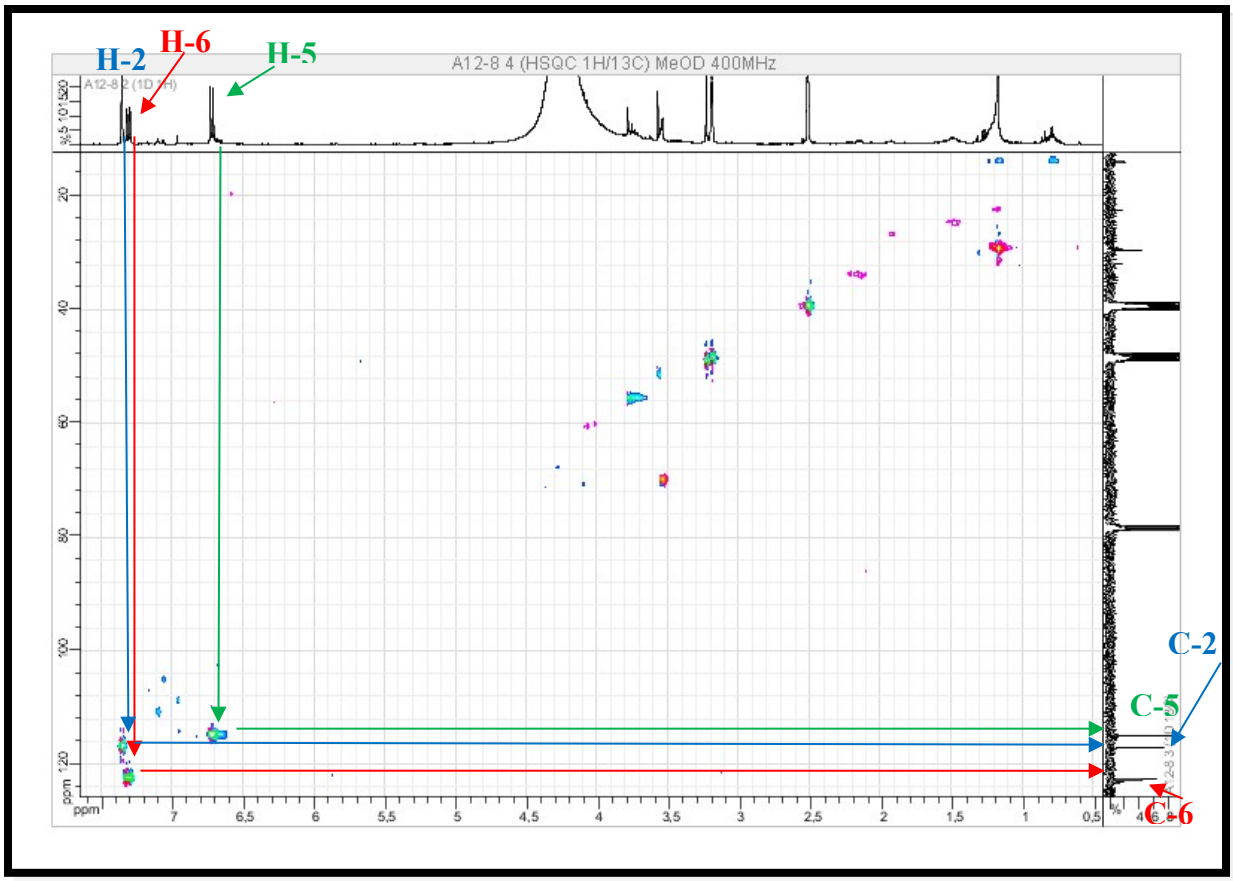


Figure.14. HSQC spectrum (400MHz, CD_3OD, δppm) of protocatechuic acid

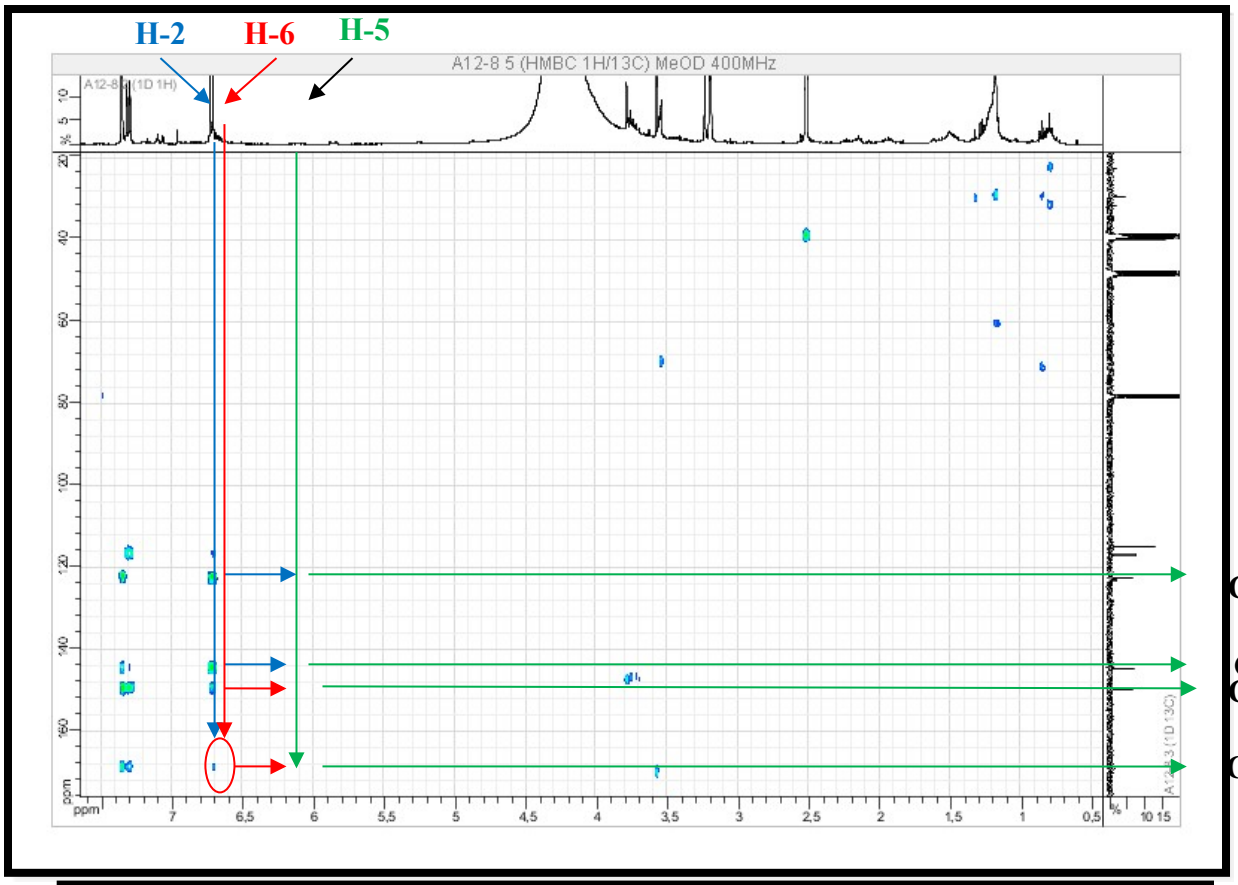


Figure .15.HMBC spectrum (400MHz, CD_3OD, δppm) of protocatechuic acid

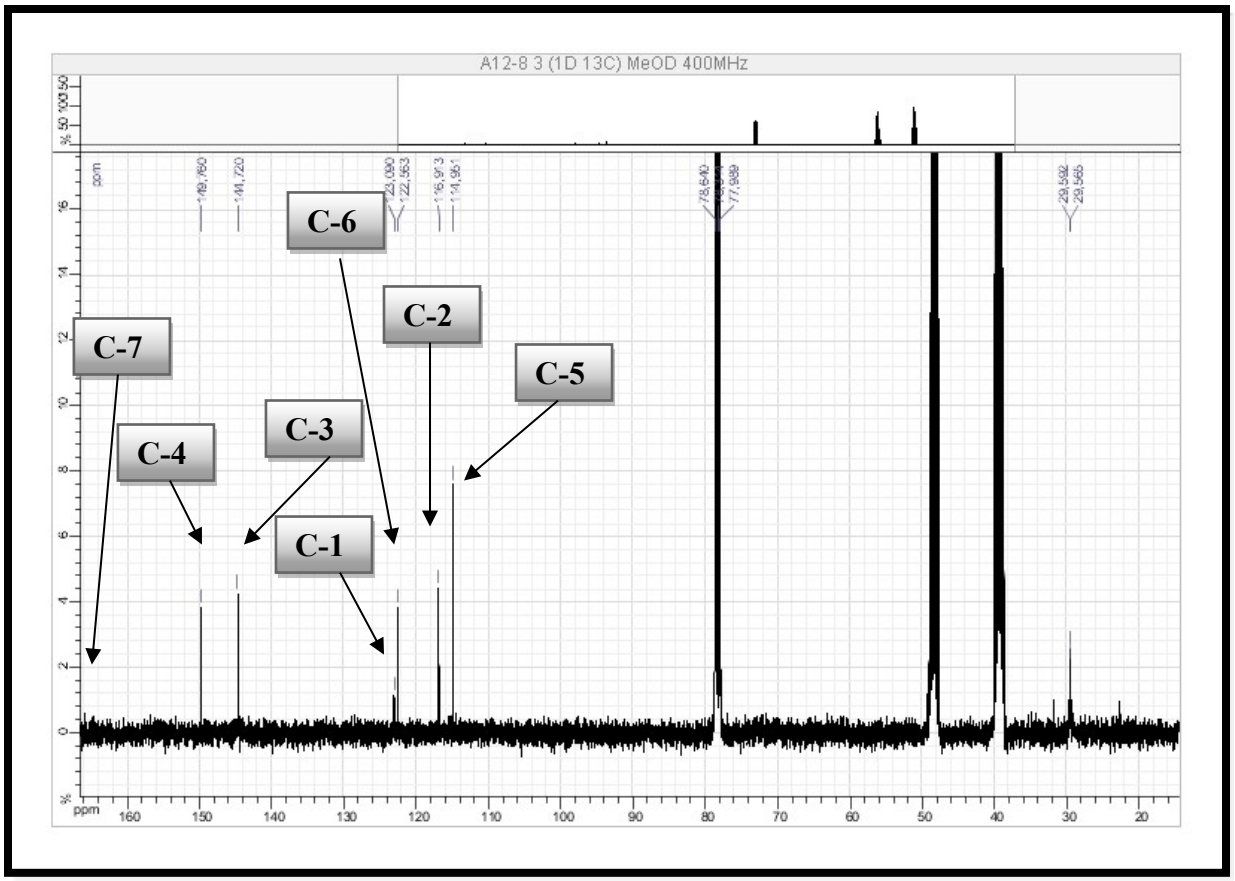
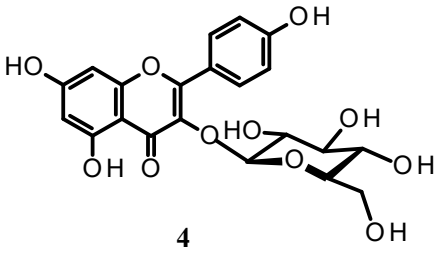


Figure.16. ^{13}C NMR spectrum (100MHz, CD_3OD, δppm) of protocatechuic acid

Molecule 4 : Astragalin



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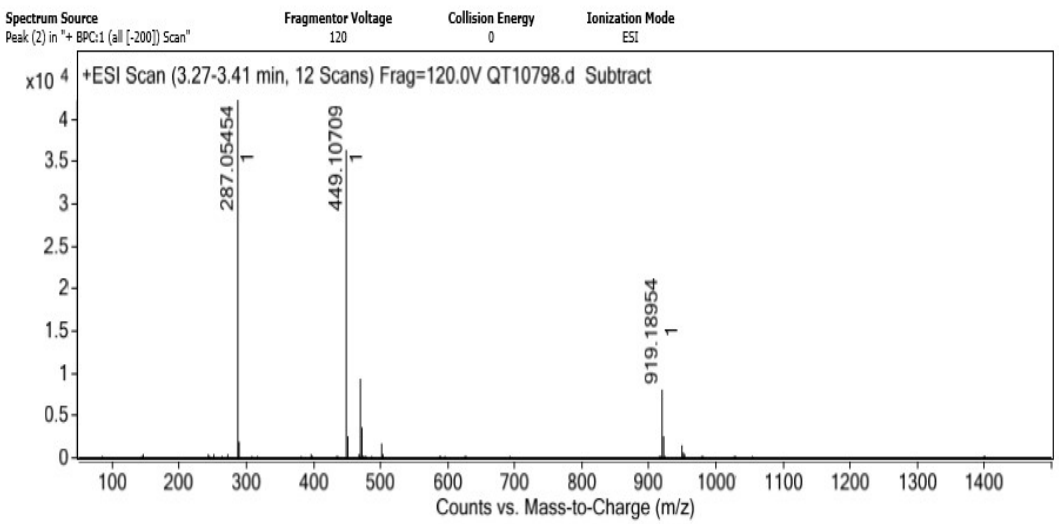


Peak List

m/z	z	Abund	Formula	Ion
287.05454	1	43767.9		(M+H)+
288.0593	1	12794.9		(M+H)+
449.10709	1	36298.9		(M+H)+
450.11158	1	12945.3		(M+H)+
451.11492	1	2487		(M+H)+
471.08895	1	9379.5		
472.09355	1	3573.7		
919.18954	1	8100.6		
920.19365	1	6621.5		
921.19707	1	2599.4		

Figure.17. HRESI-MS (+) of astragalin

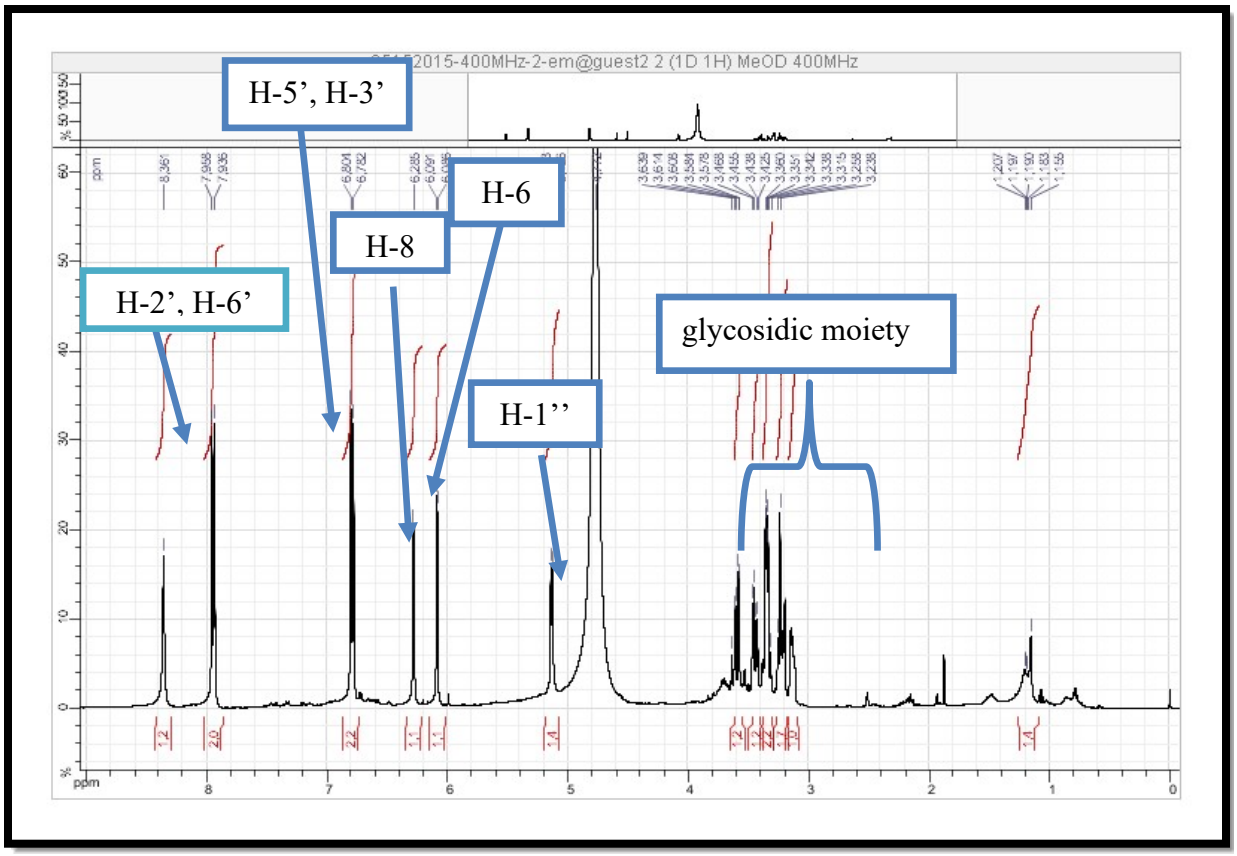


Figure.18. ^{1}H NMR spectrum (400MHz, CD_3OD, δppm) of astragalin

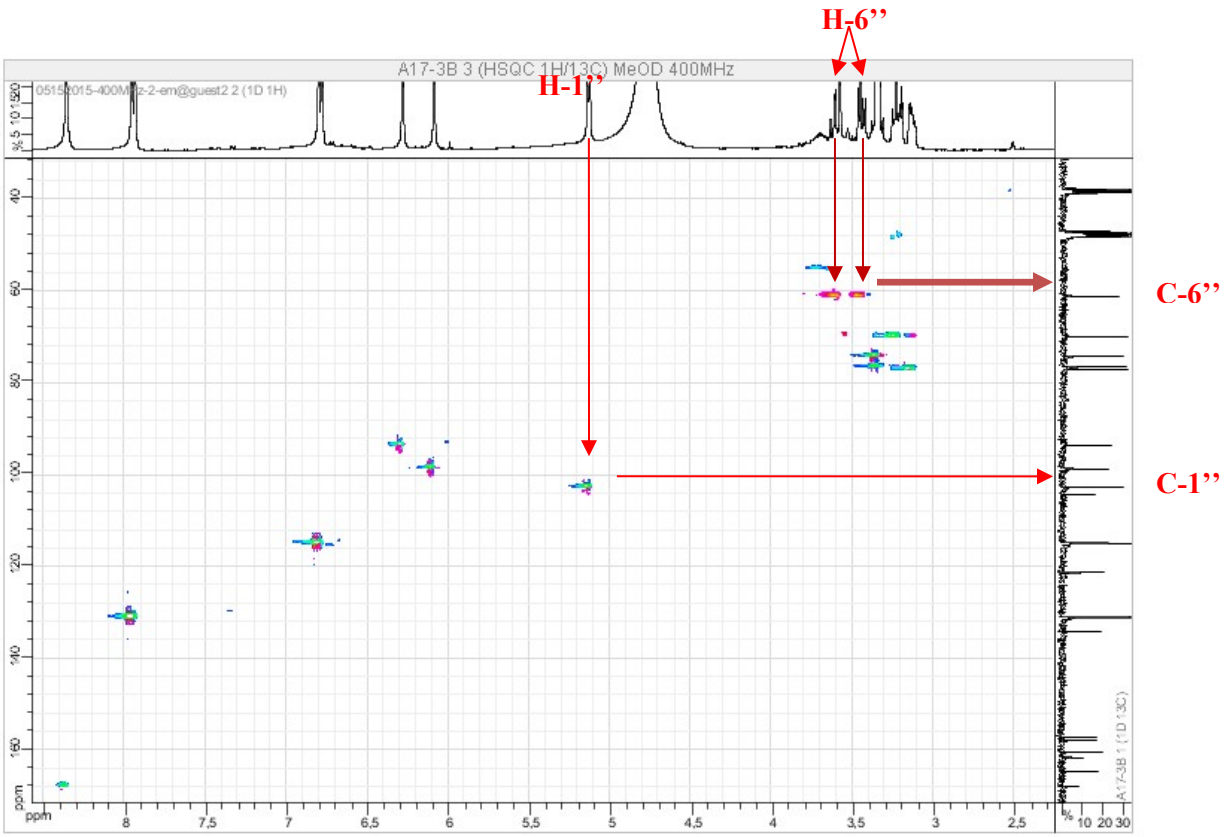


Figure.19. HSQC spectrum (400MHz, CD_3OD, δppm) of astragalin

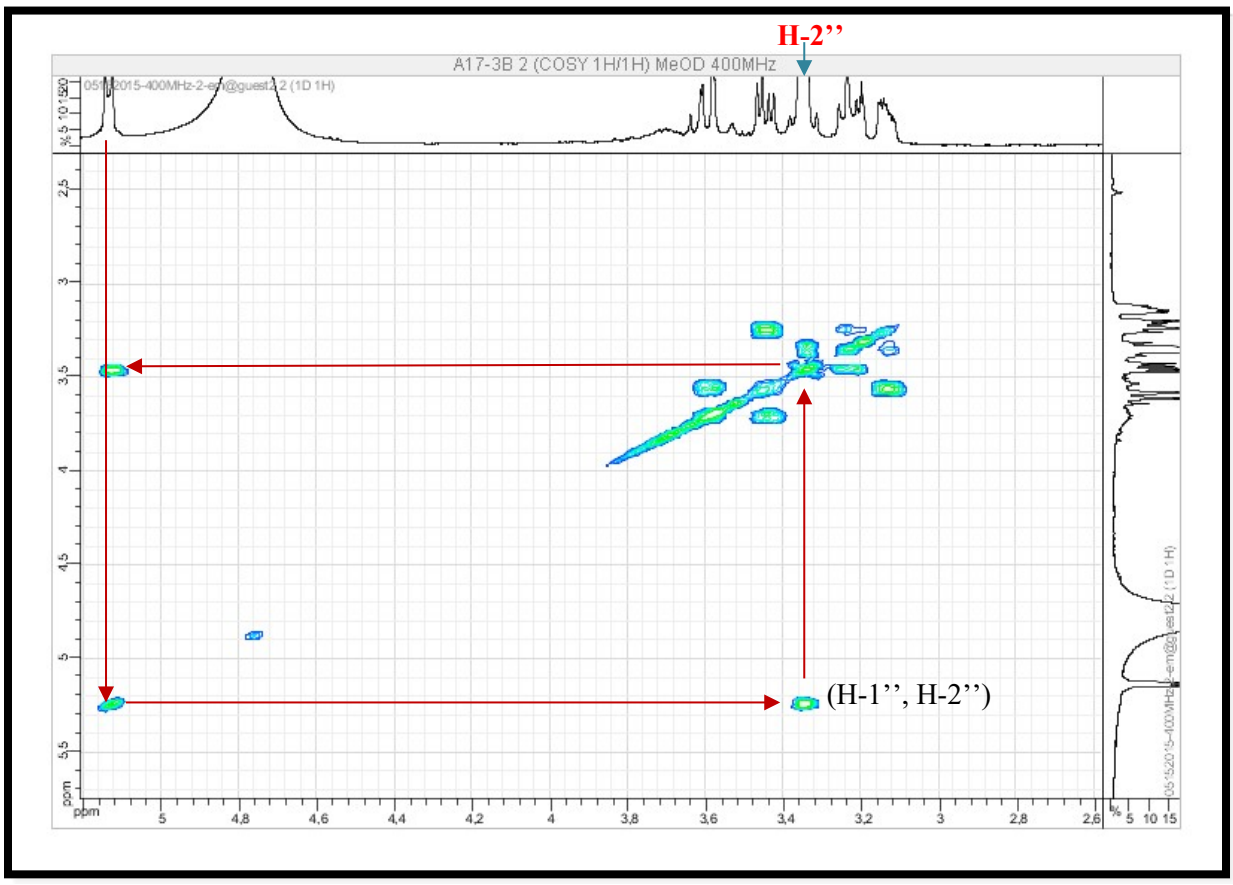


Figure.20. COSY spectrum (400MHz, CD_3OD, δppm) of astragalin

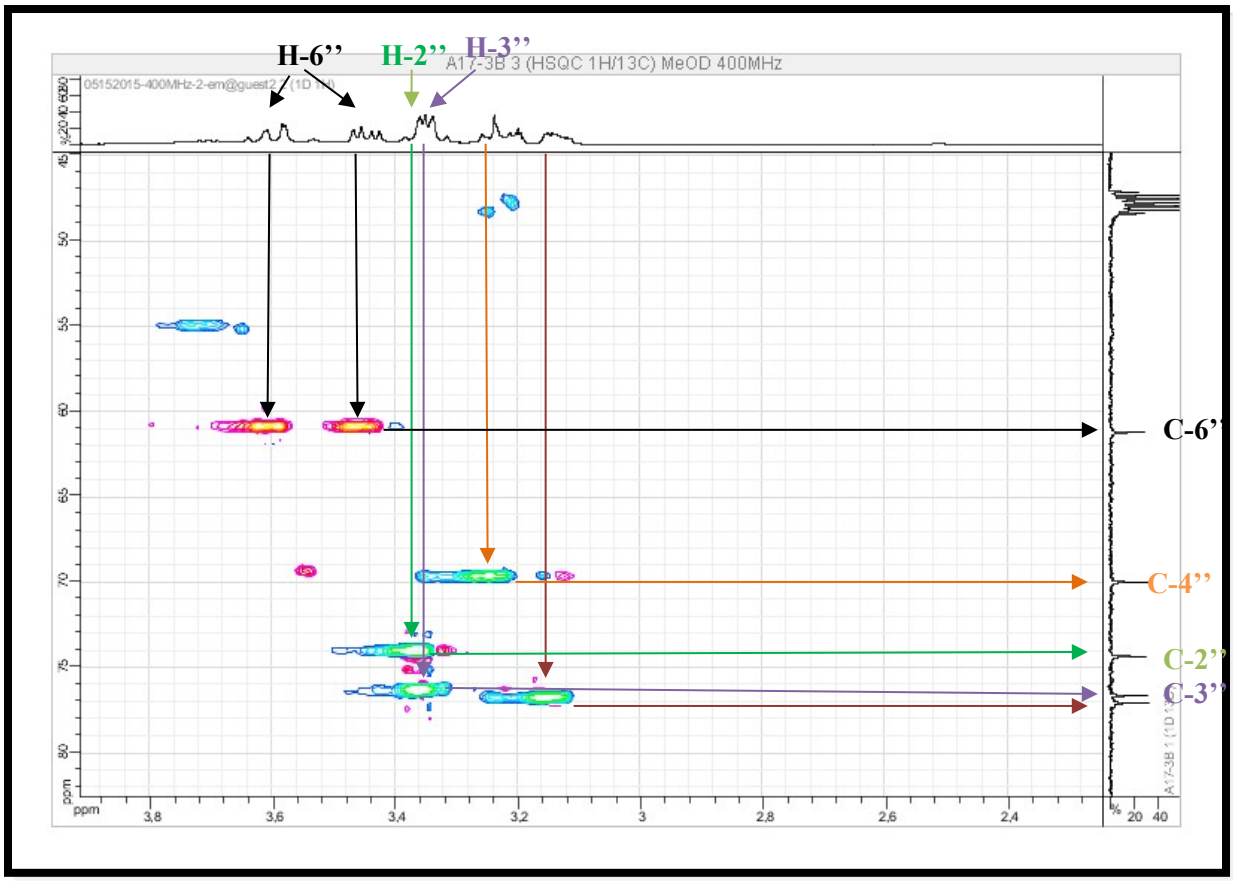


Figure.21. HSQC spectrum (400MHz, CD_3OD, δppm) of astragalin

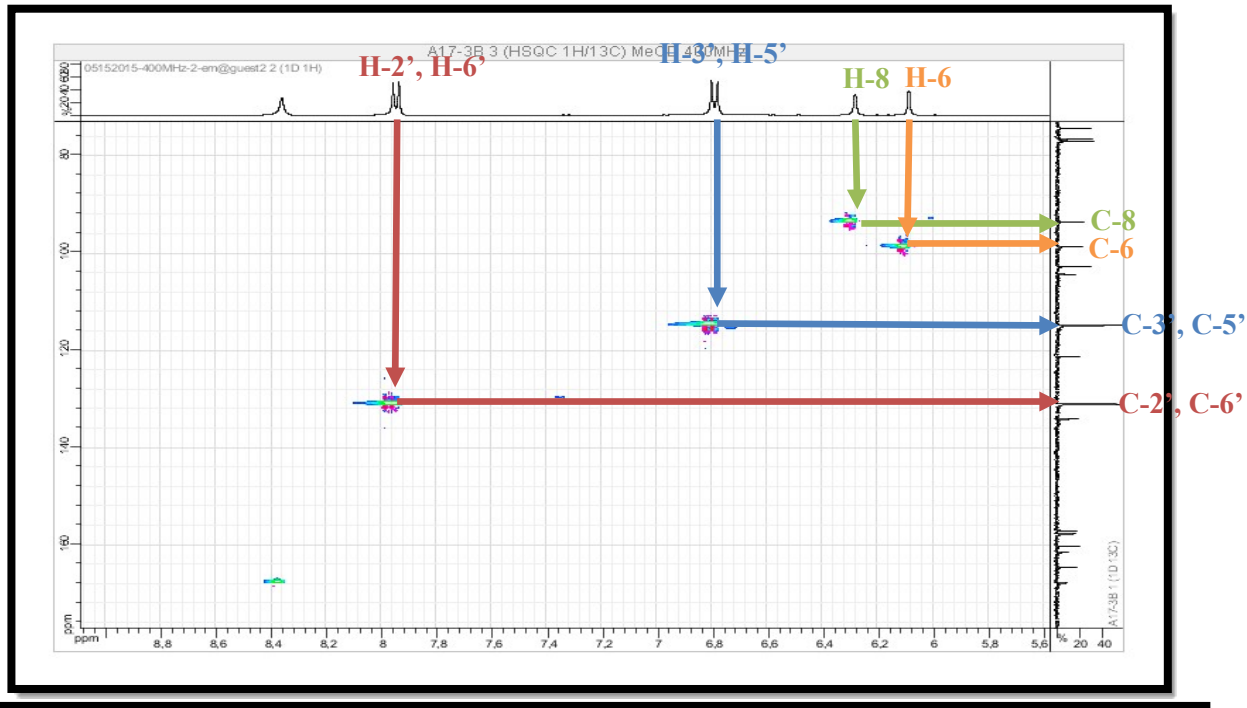


Figure.22. HSQC spectrum (spreading out 1) (400MHz, CD_3OD, δppm) of astragalin

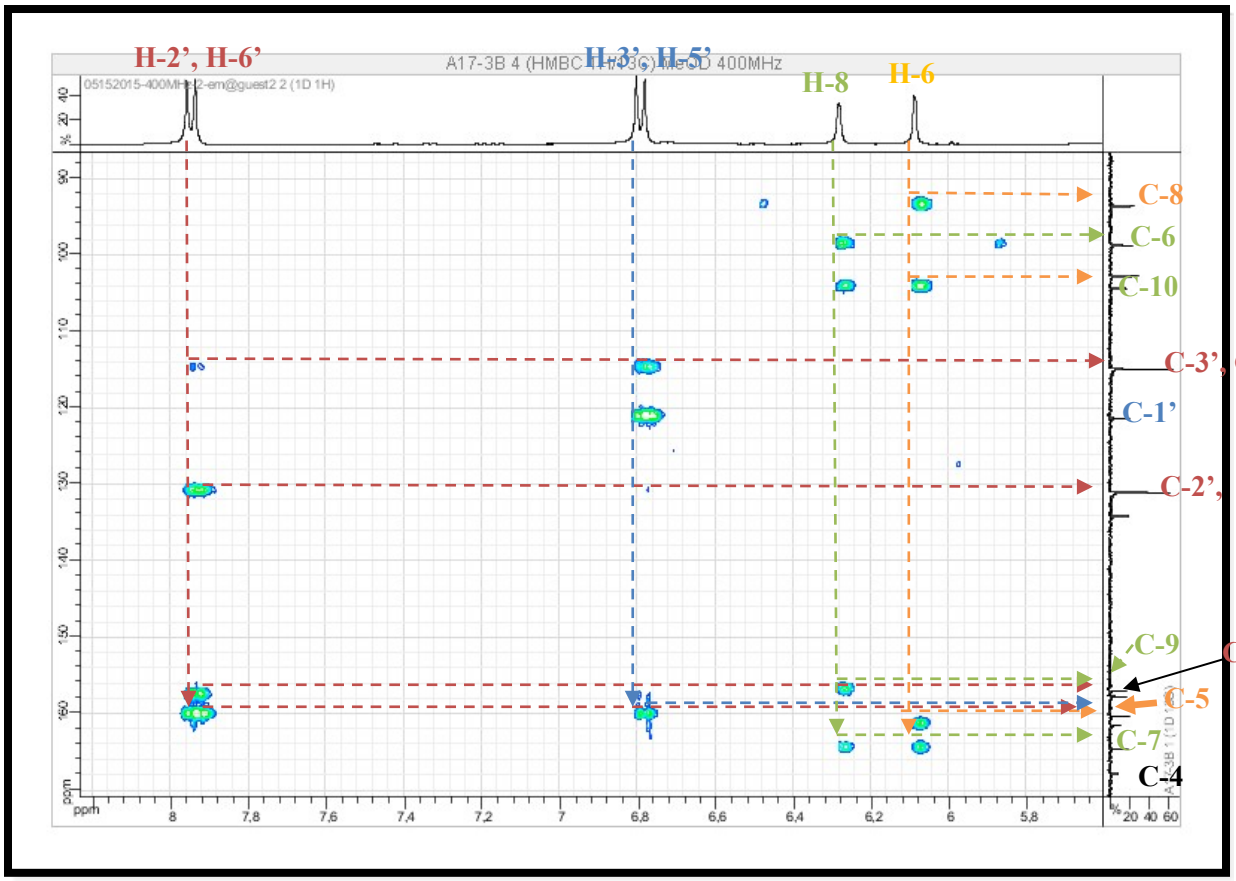


Figure.23. HMBC spectrum (spreading out1) (400MHz, CD_3OD, δppm) of astragalin

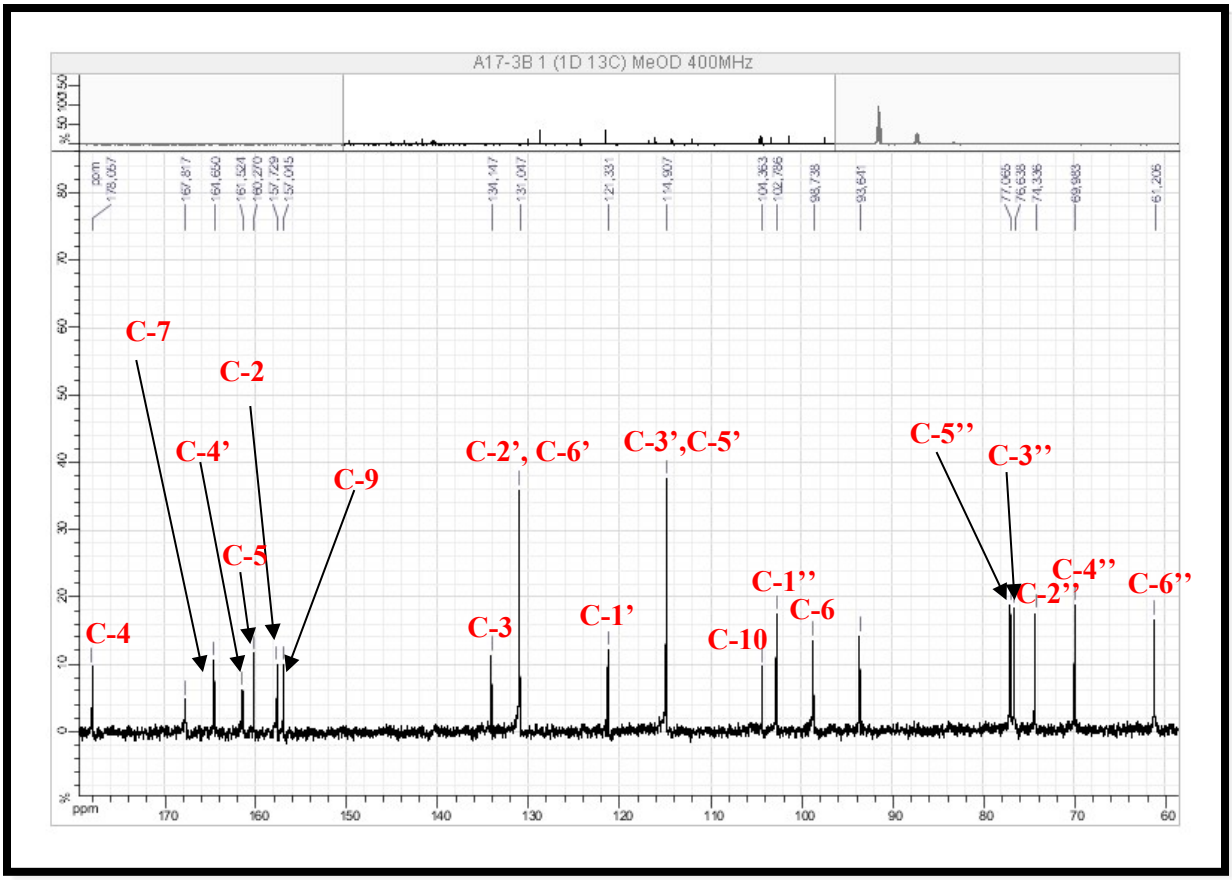
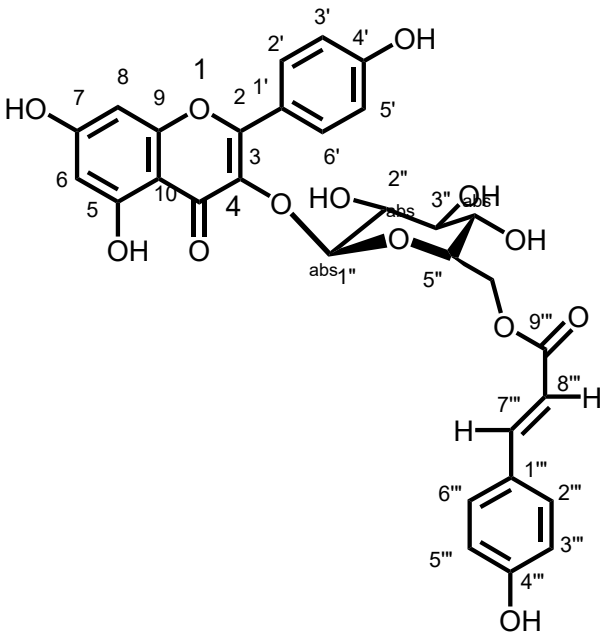


Figure.24. ^{13}C spectrum (100MHz, CD_3OD, δppm) of astragalin

Molecule 5: *Trans*-tiliroside



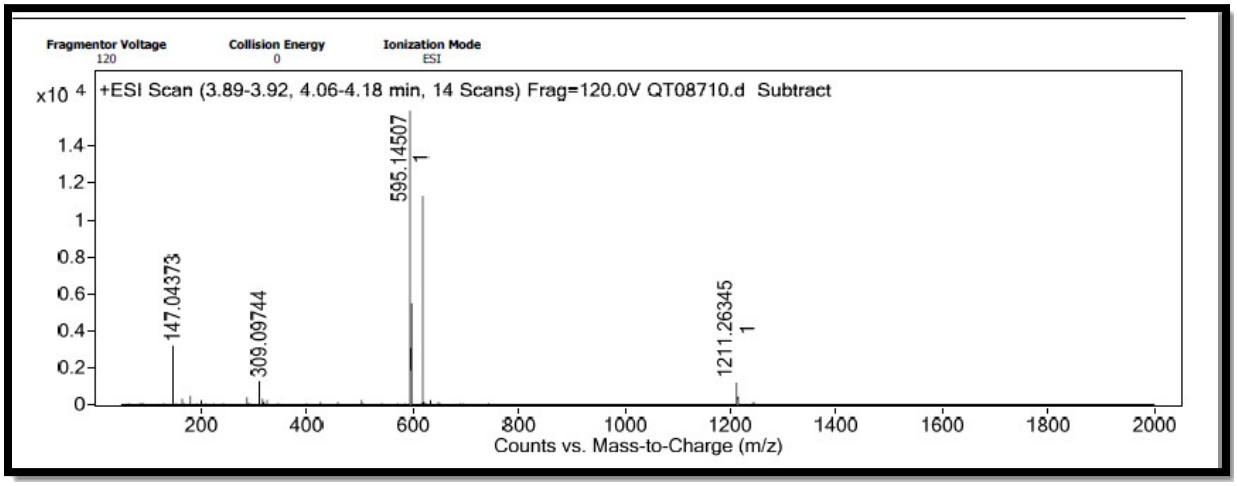


Figure.25.HRESI-MS (+) of *trans*-tiliroside

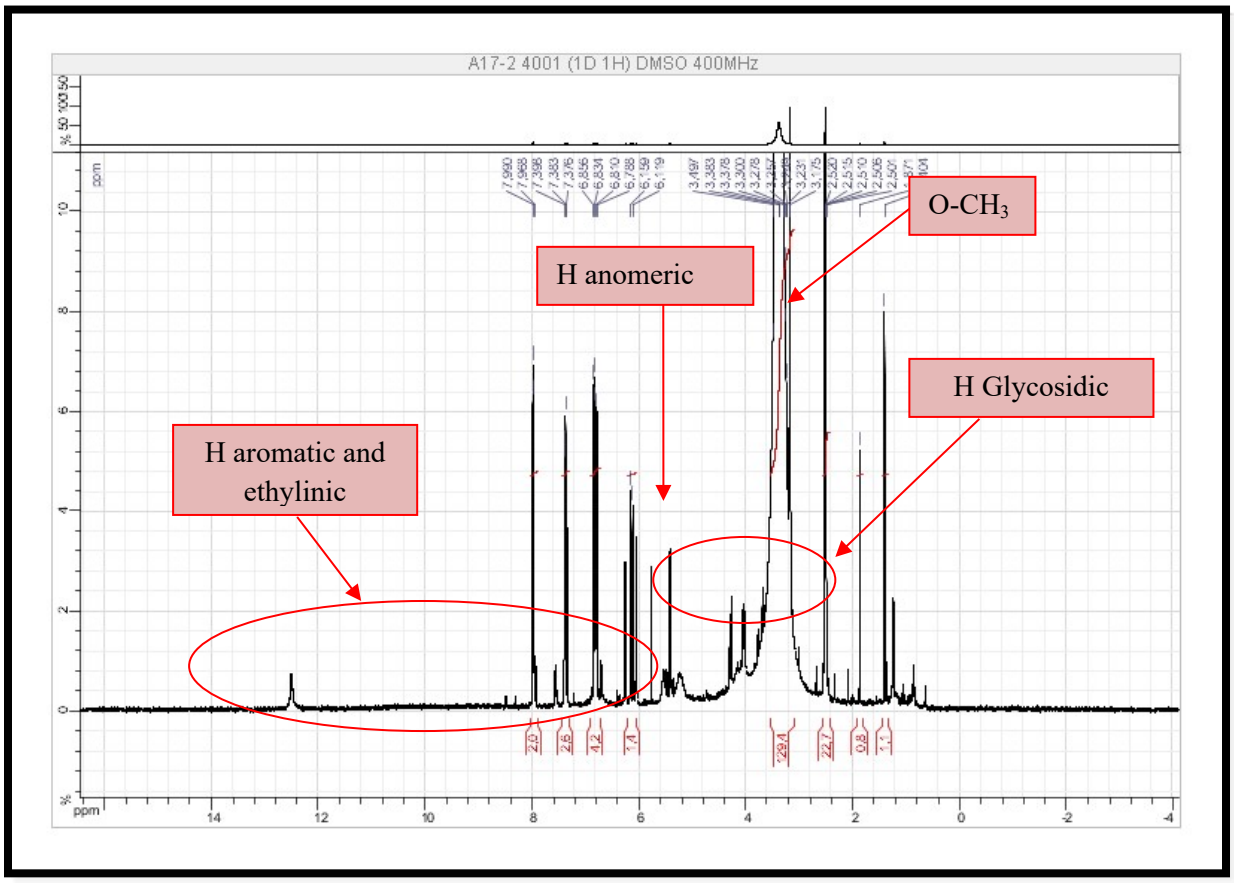


Figure.26. ^{1}H NMR spectrum (400MHz, DMSO-d_6, δppm) of *trans*-tiliroside

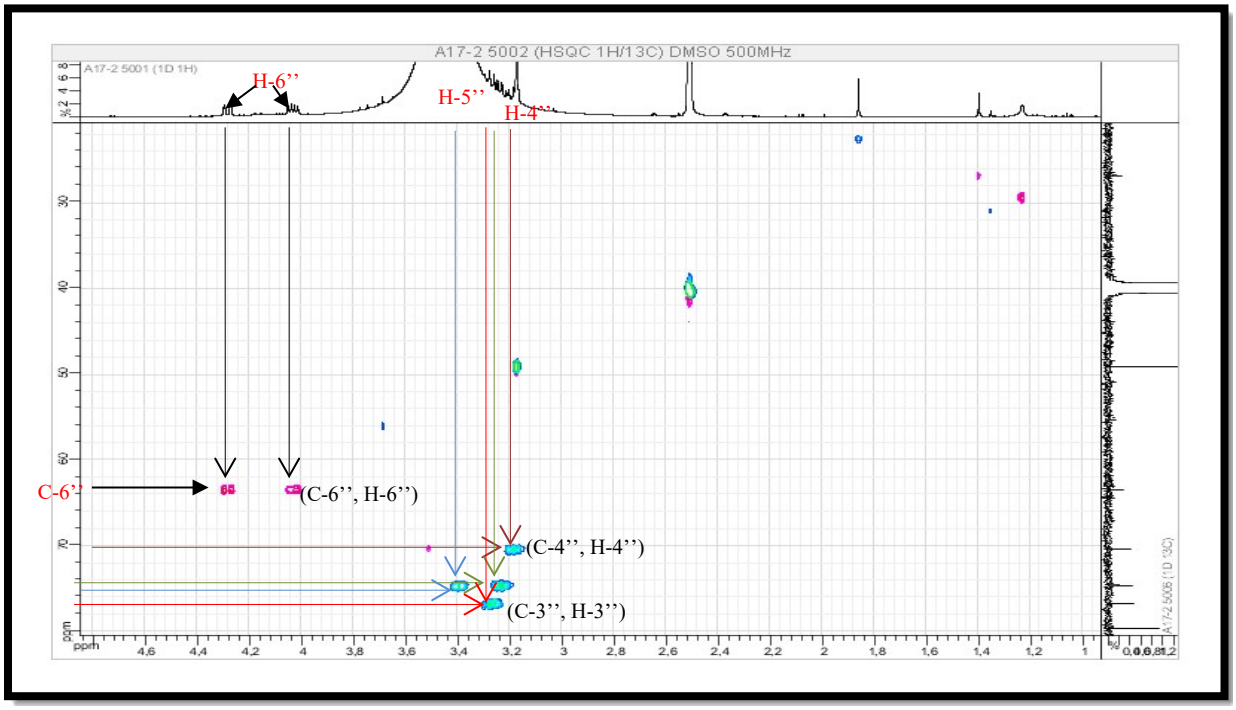


Figure .27. HSQC spectrum (spreading out 1) (500MHz, DMSO-d_6, δppm) of *trans*-tiliroside

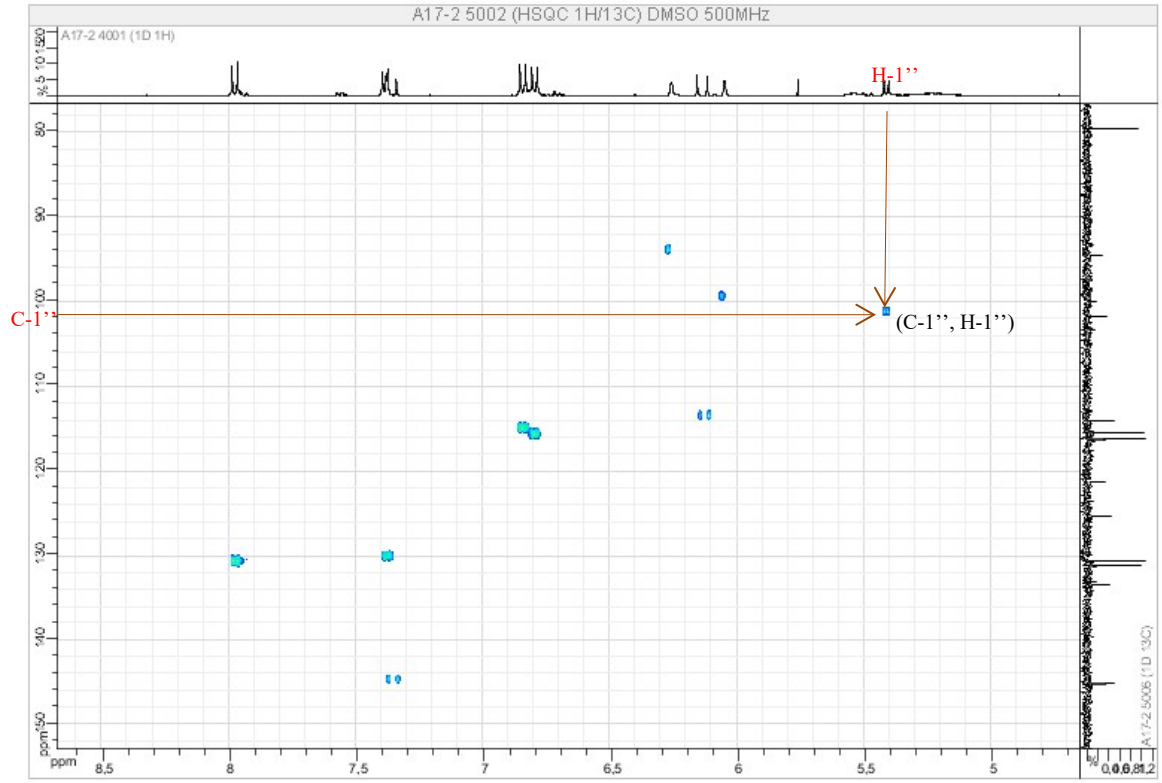


Figure.28. HSQC spectrum (spreading out 2) (500MHz, DMSO-d_6, δppm) of *trans*-

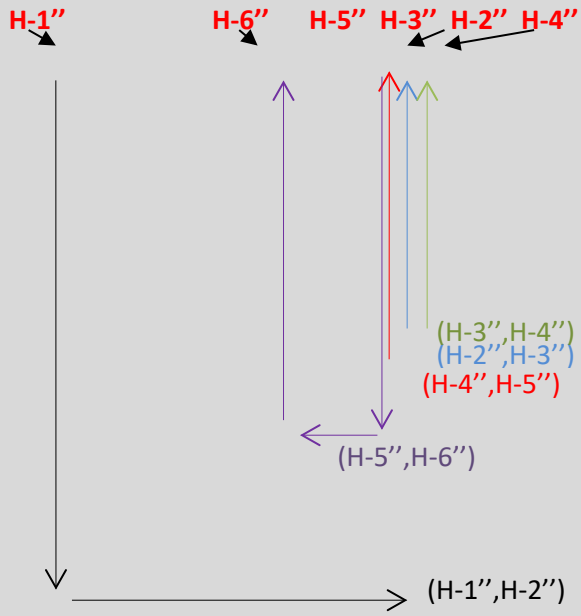


Figure.29. COSY spectrum (spreading out 1) (500MHz, DMSO-d_6, δppm) of *trans*-tiliroside

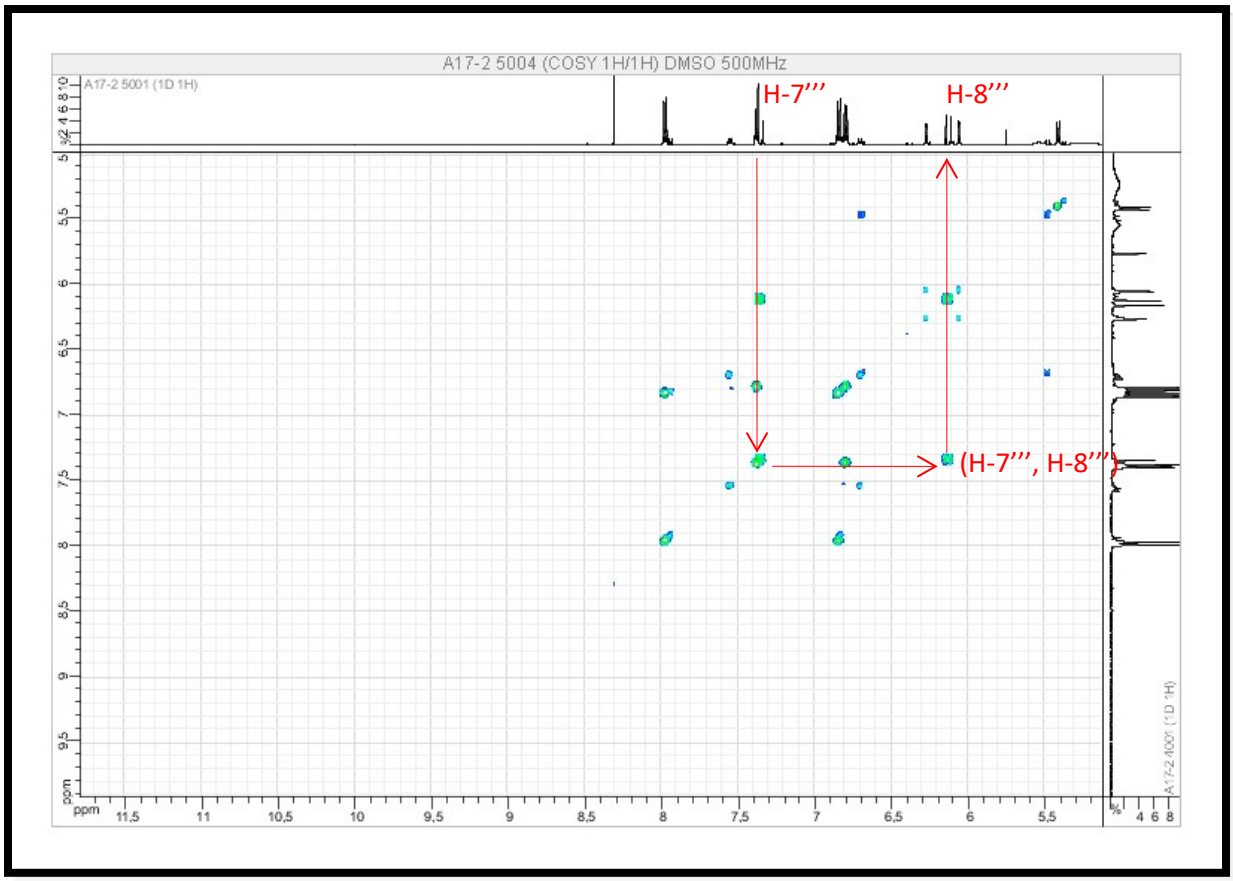


Figure.30. COSY spectrum (spreading out 2) (500MHz, DMSO-d_6, δppm) of *trans*-tiliroside

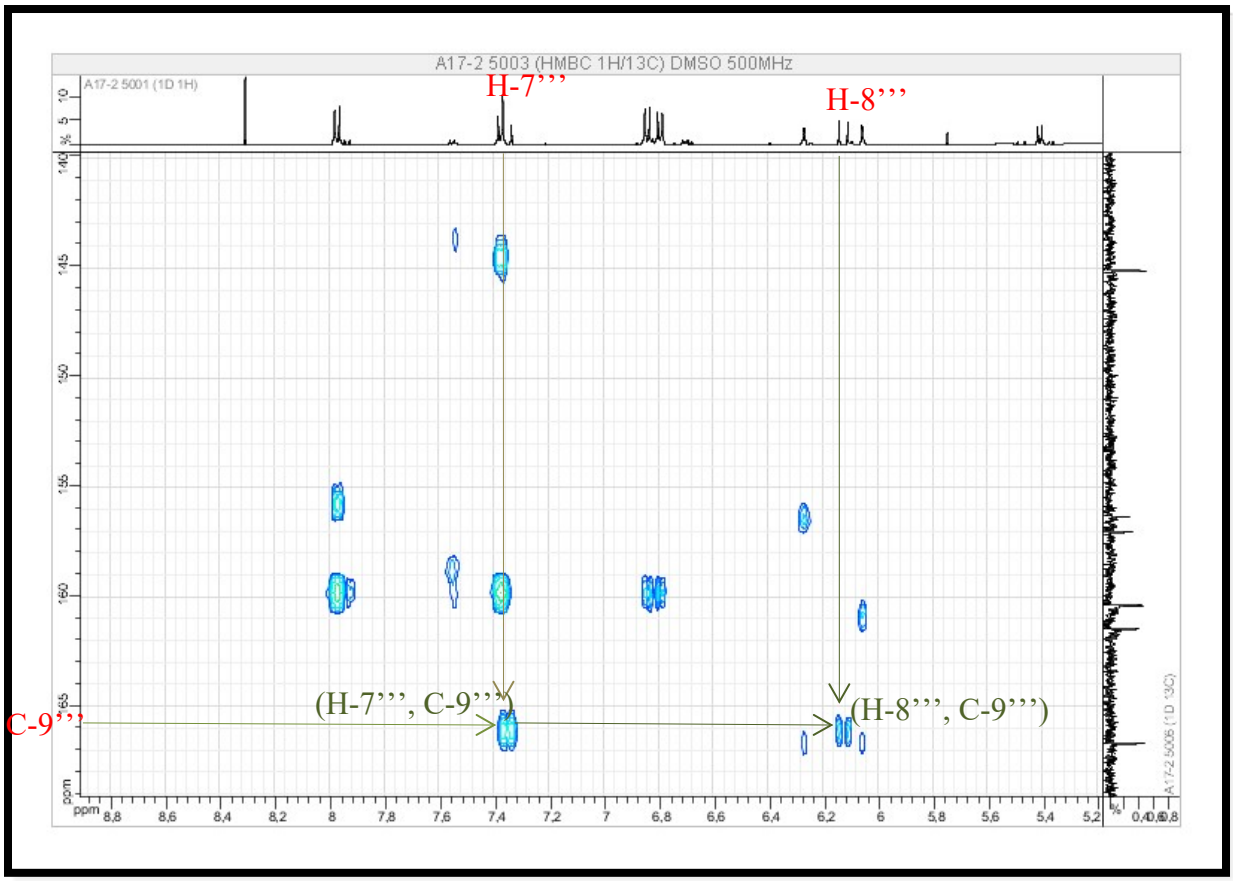


Figure .31. HMBC spectrum (spreading out 1) (500MHz, DMSO-d_6, δppm) of *trans*-tiliroside

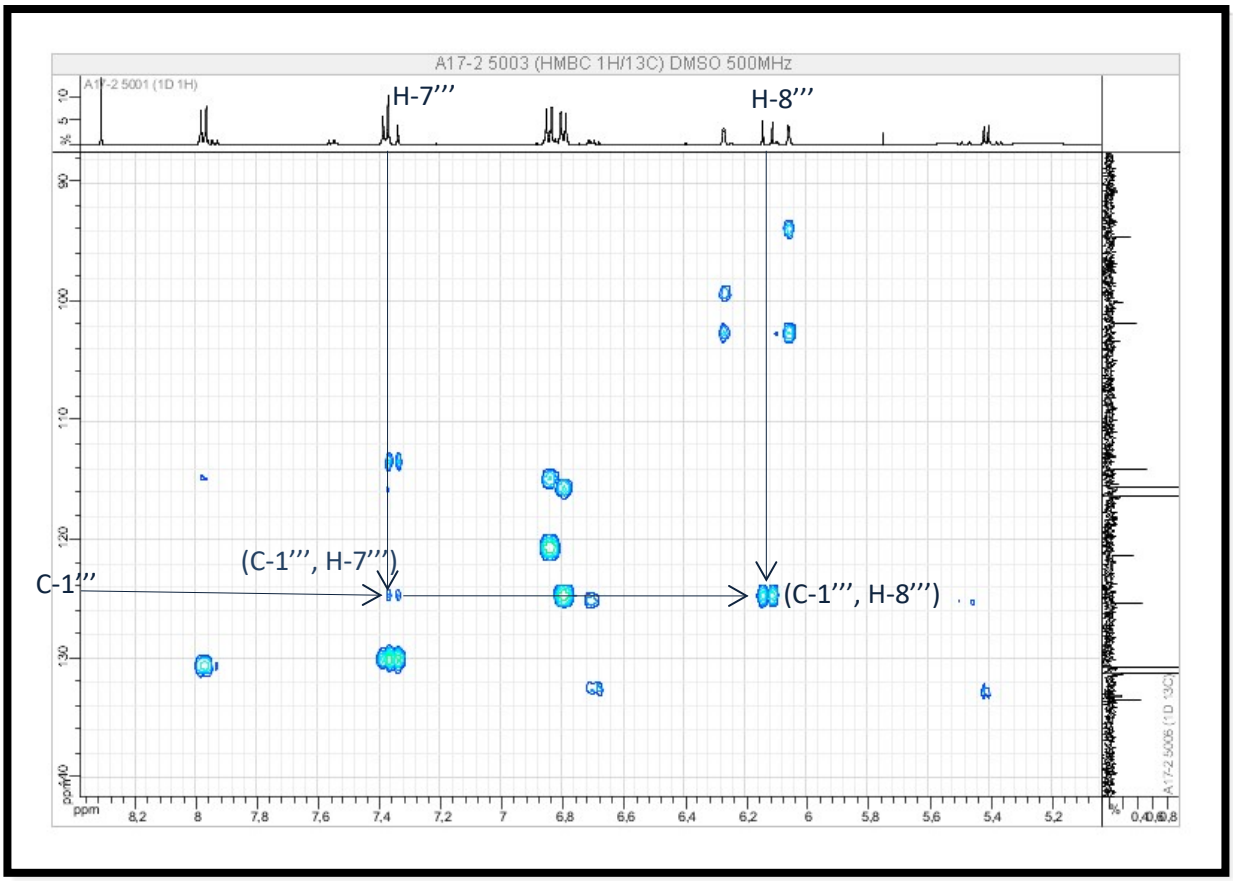


Figure.32. HMBC spectrum (spreading out 2) (500MHz, DMSO-d_6, δppm) of *trans*-tiliroside

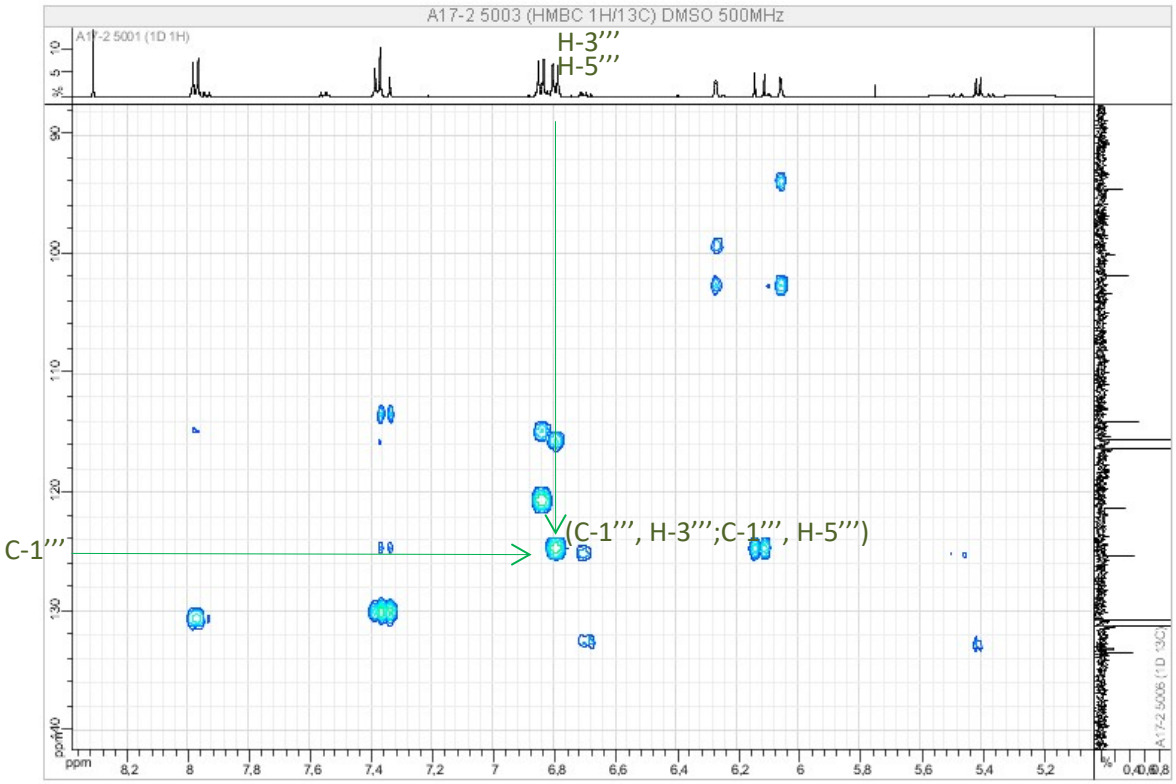


Figure.33. HMBC spectrum (spreading out 3) (500MHz, DMSO-d_6, δppm) of *trans*-tiliroside

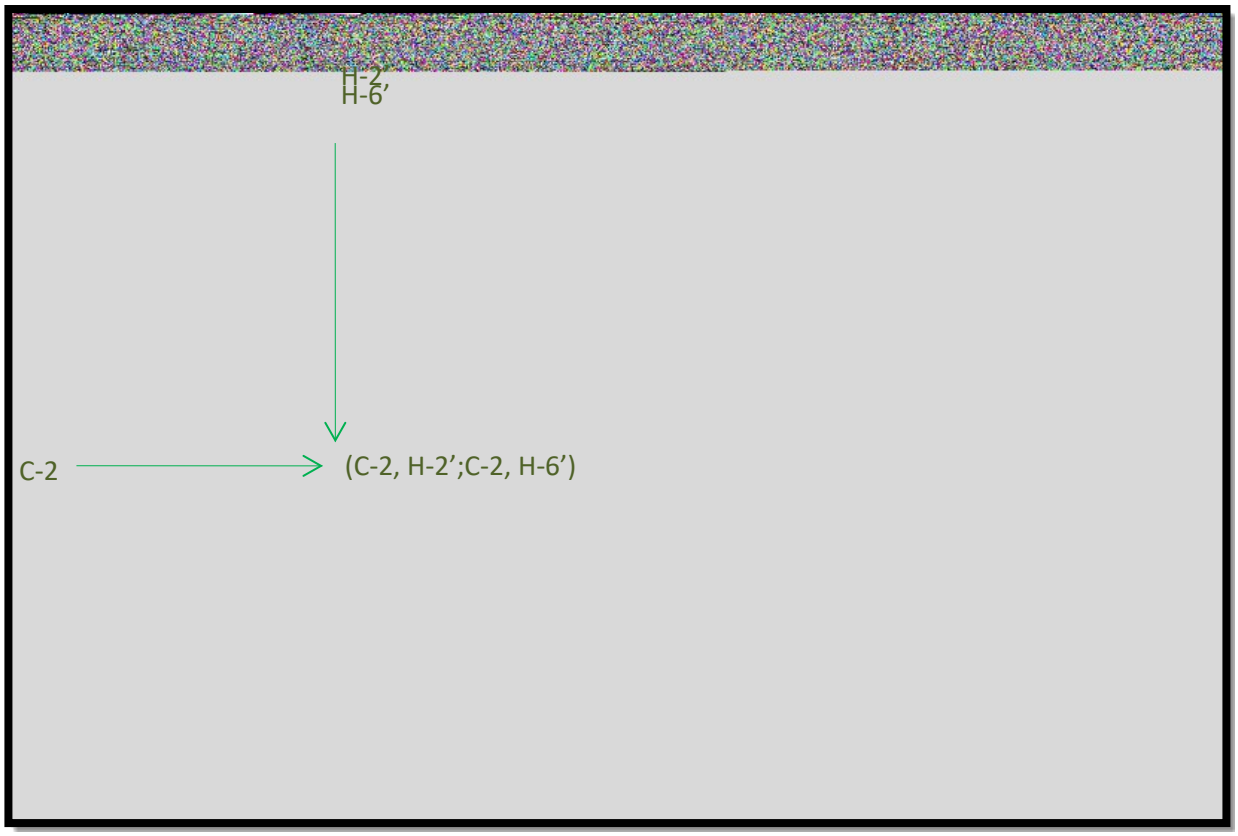


Figure.34. HMBC spectrum (spreading out 4) (500MHz, DMSO-d_6, δppm) of *trans*-tiliroside

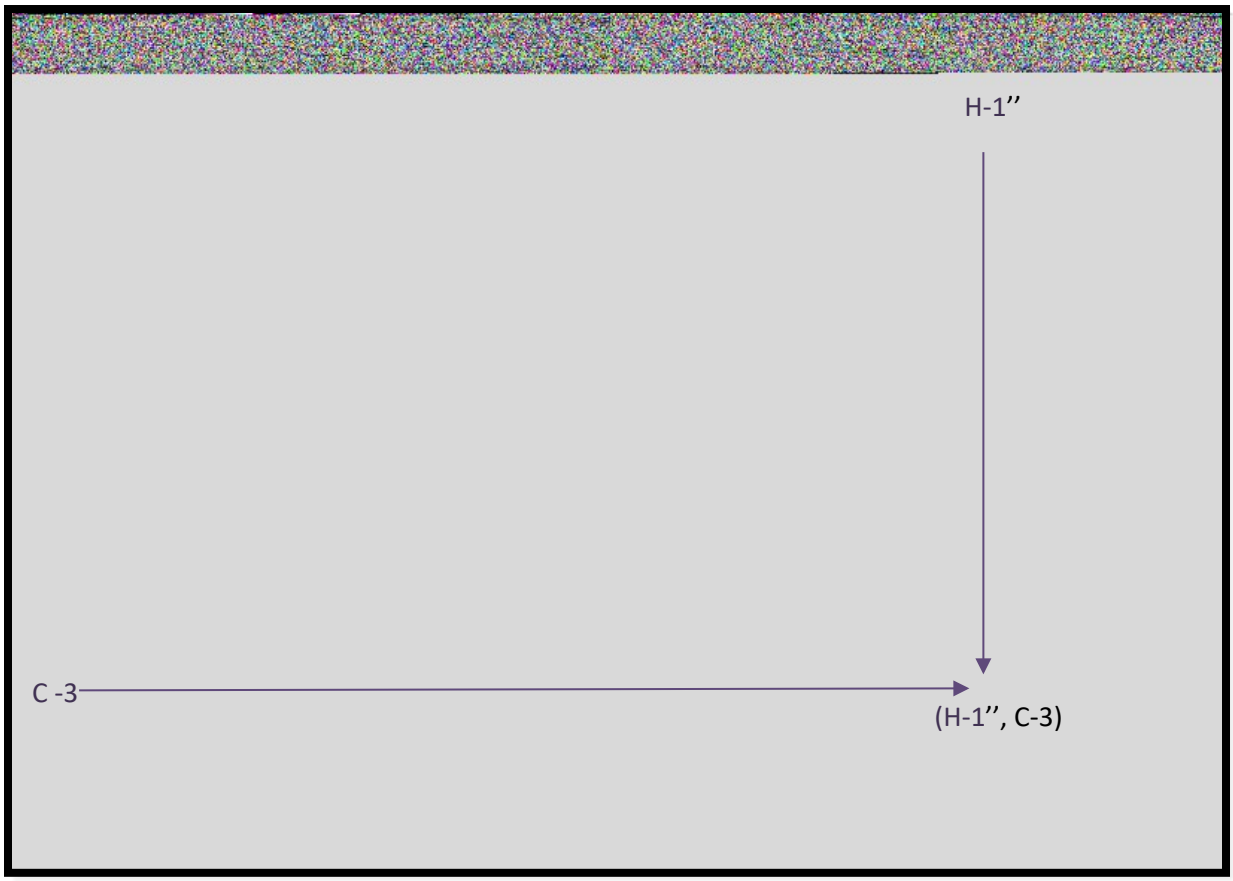


Figure.35.HMBC spectrum (spreading out 5) (500MHz, DMSO-d_6, δppm) of *trans*-tiliroside

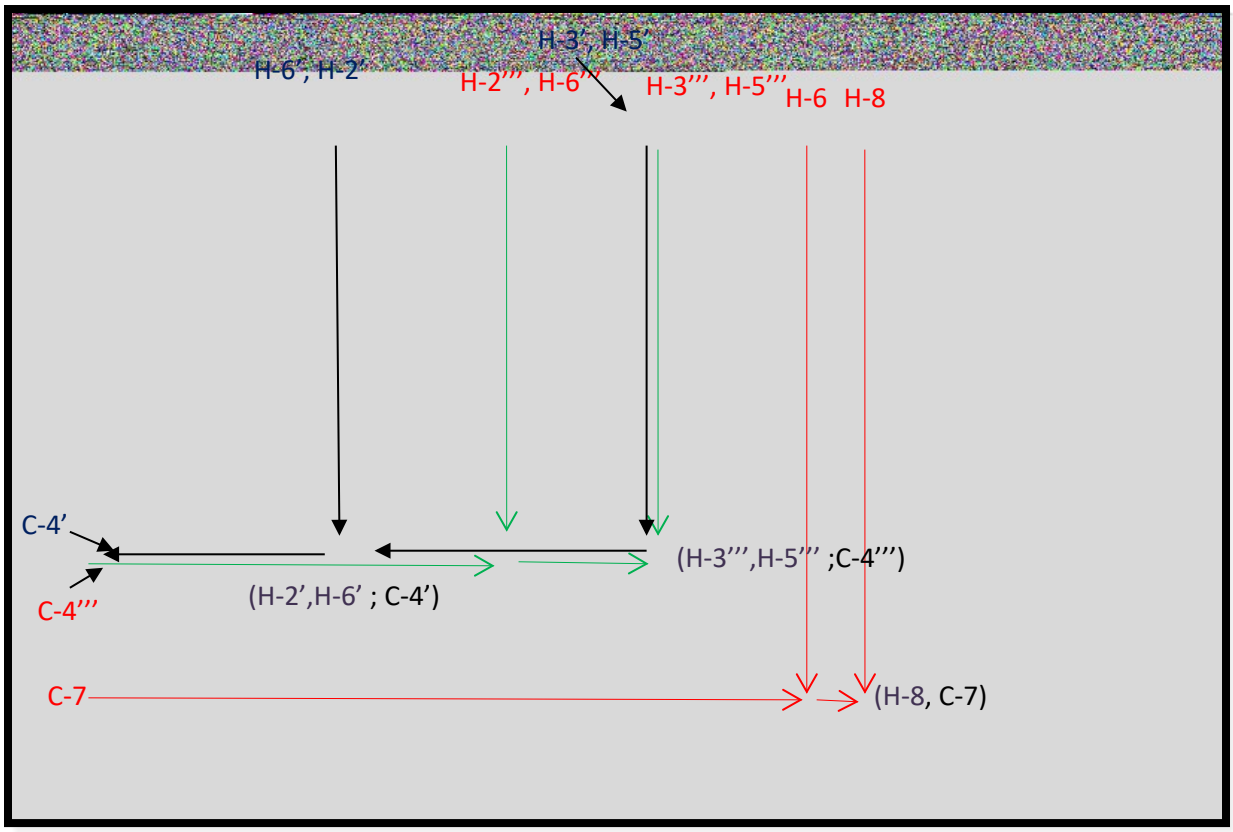


Figure.36.HMBC spectrum (spreading out 6) (500MHz, DMSO-d_6, δppm) of *trans*-tiliroside

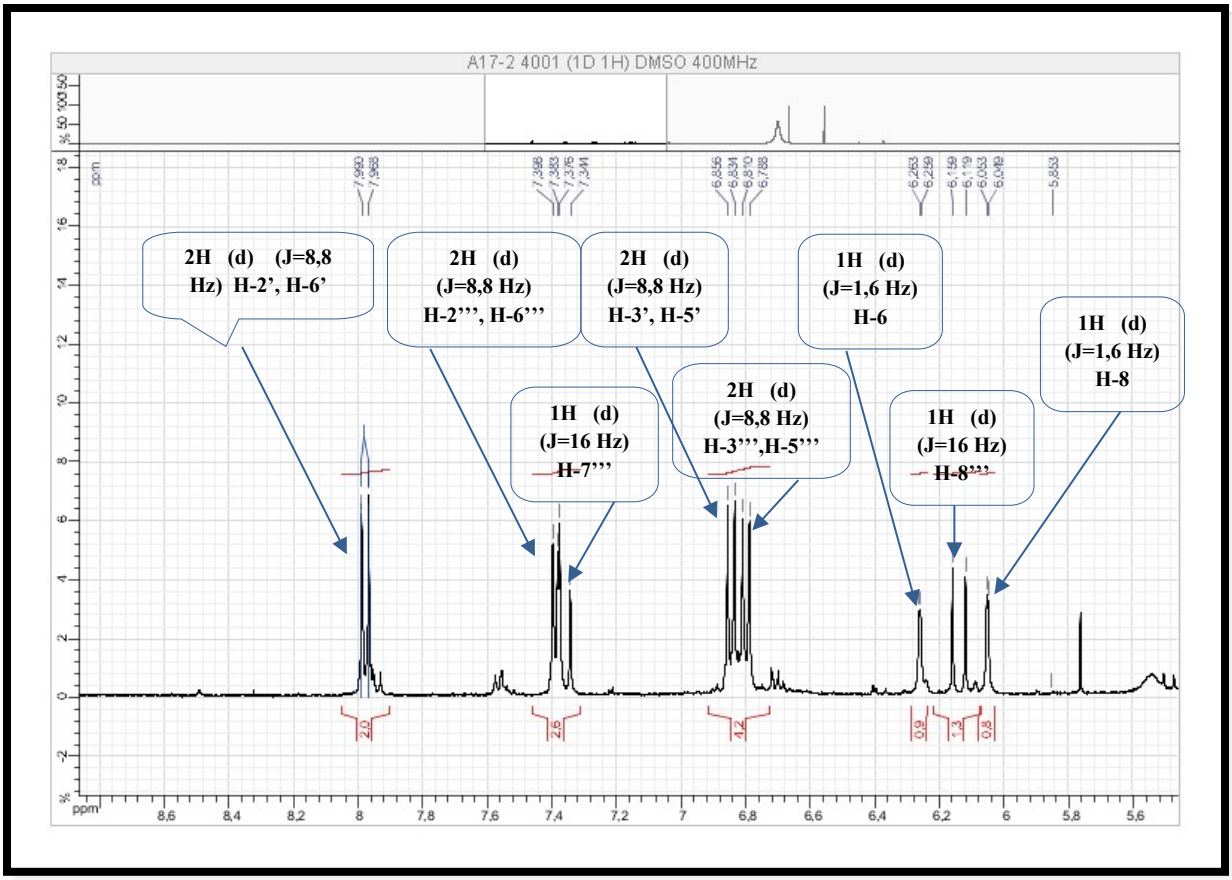


Figure.37.[1]H NMR spectrum (400MHz, DMSO-d_6, δppm) of *trans*-tiliroside

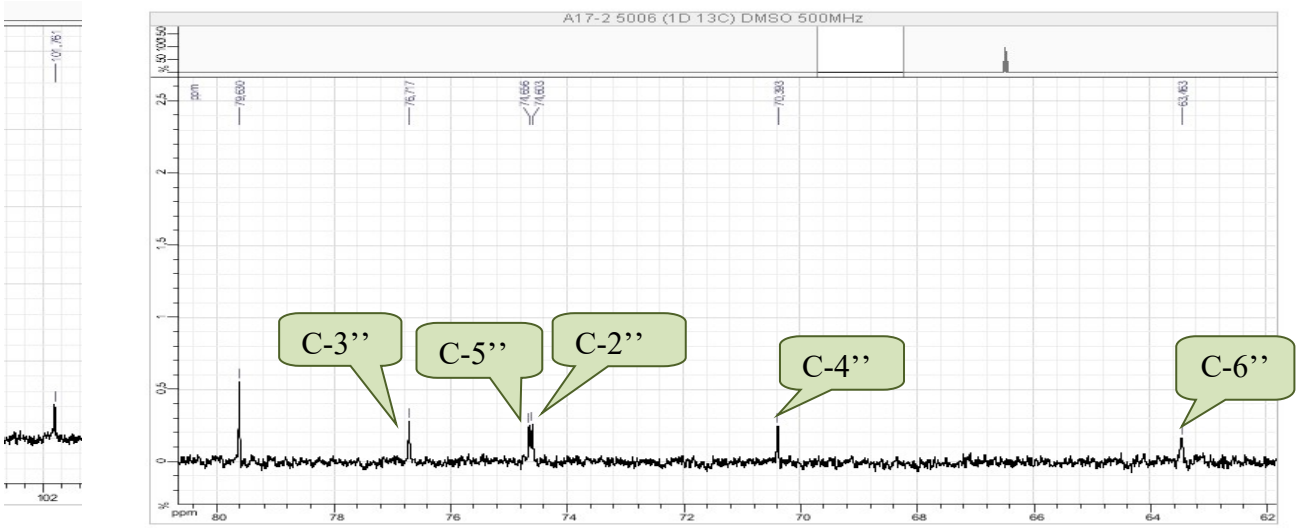


Figure.38. [13]C NMR spectrum (spreading out 1) (125MHz, DMSO-d_6, δppm) of *trans*-tiliroside

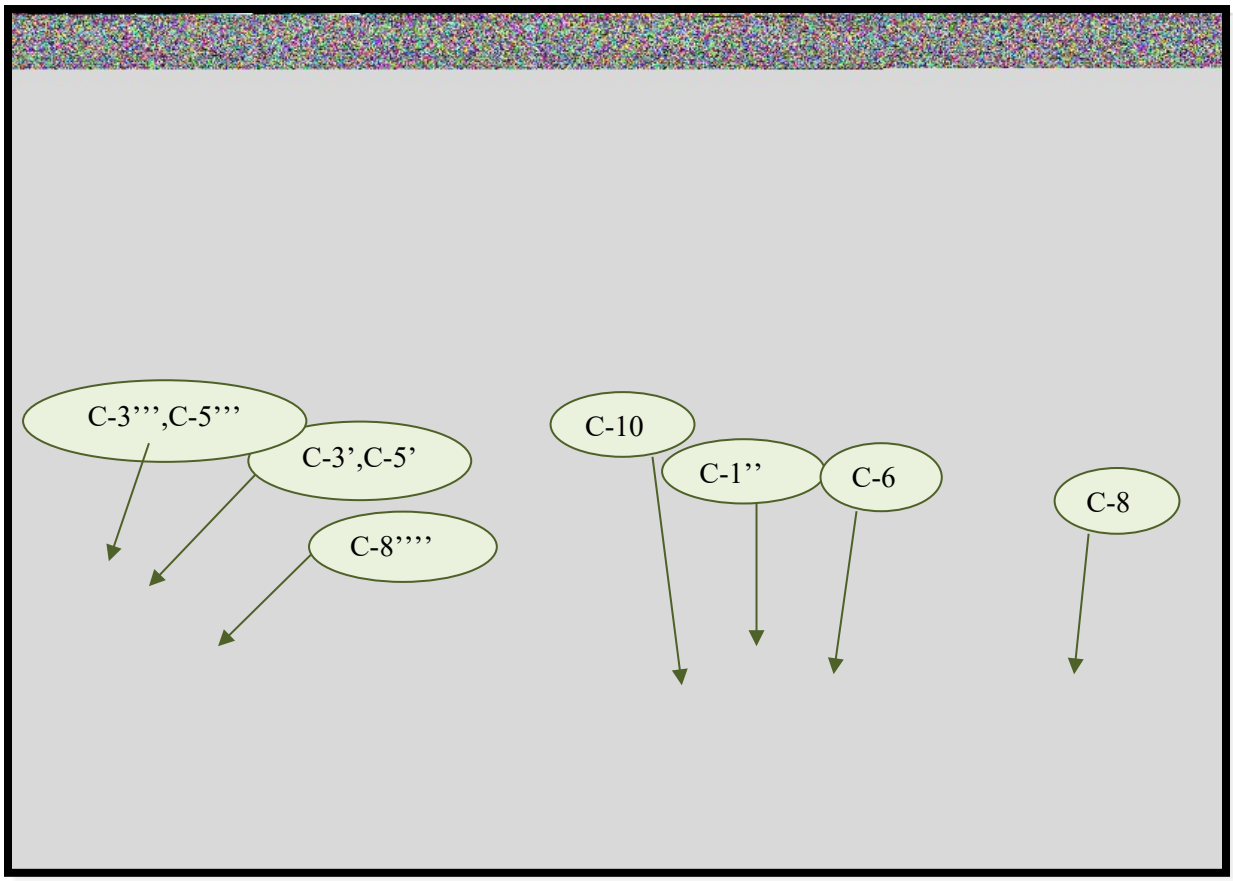


Figure.39. ^{13}C NMR spectrum (spreading out 2) (125MHz, DMSO-d_6, δppm) of *trans*-tiliroside

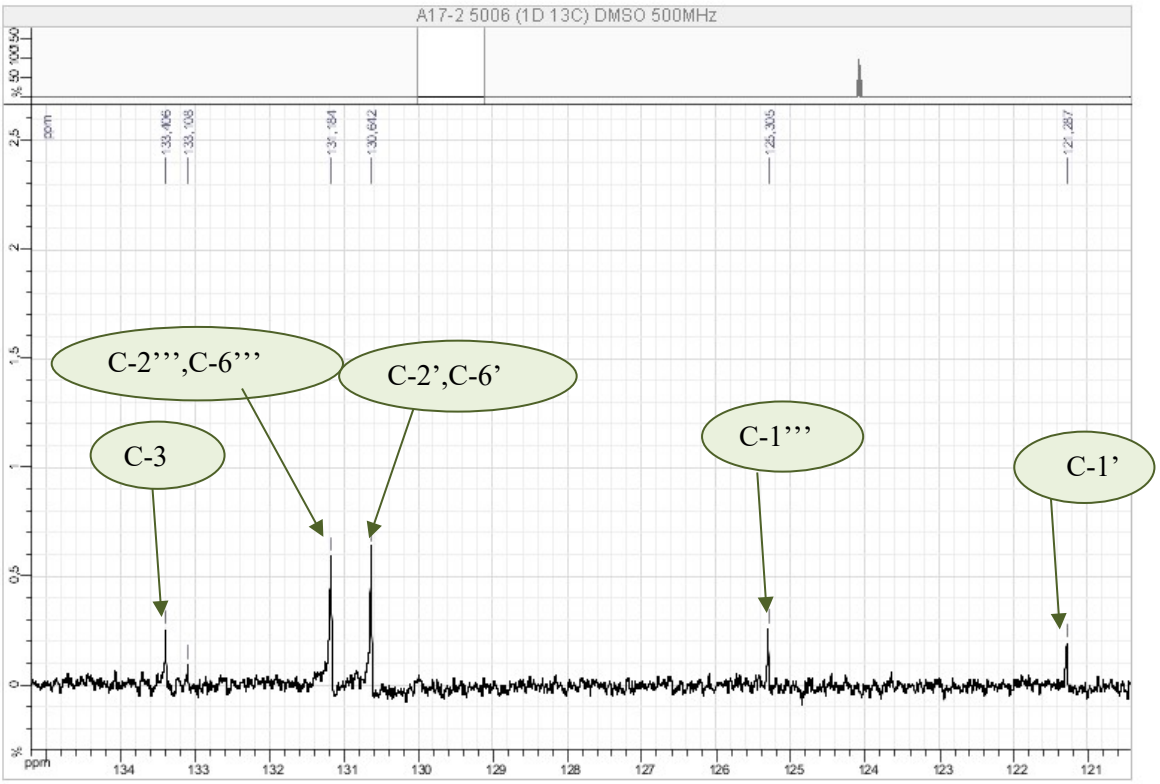


Figure.40. ^{13}C NMR spectrum (spreading out 3) (125MHz, DMSO-d_6, δppm) of *trans*-tiliroside

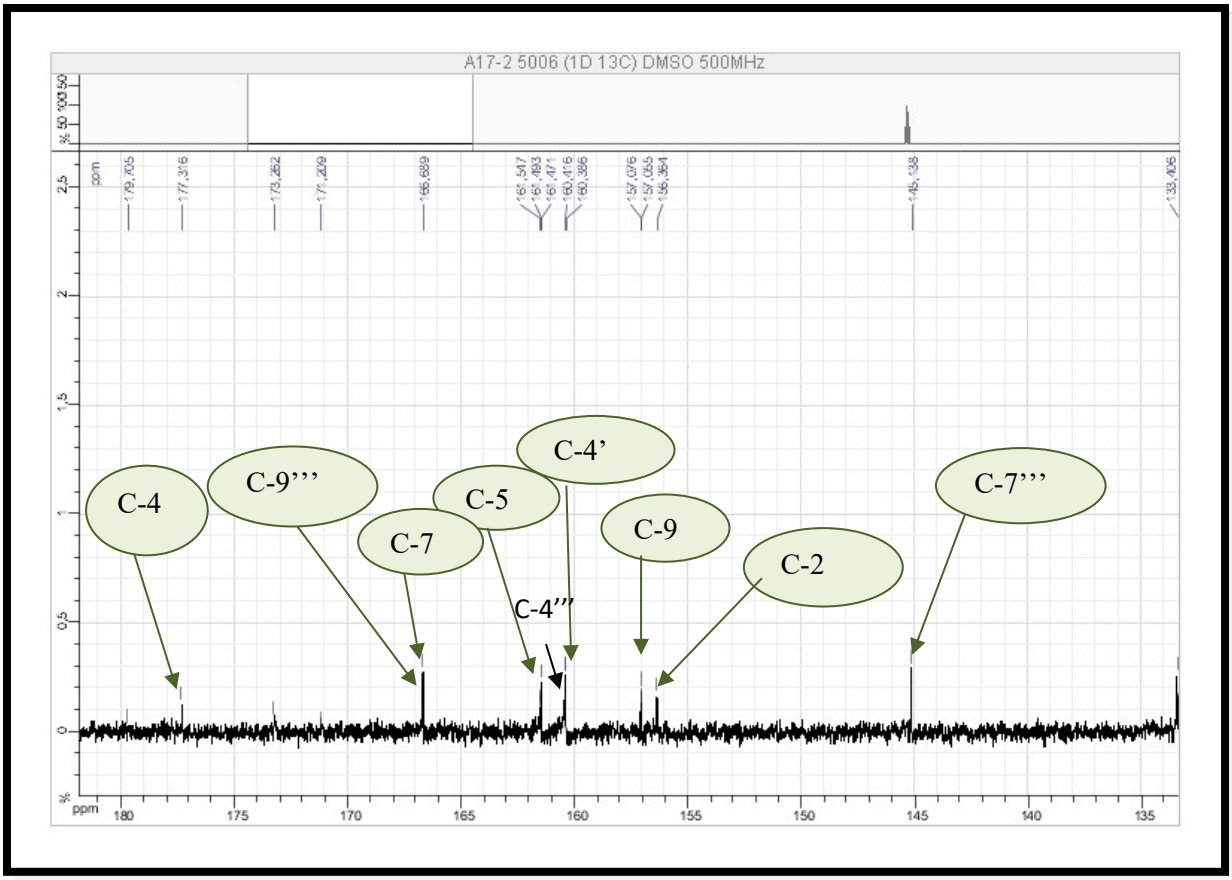
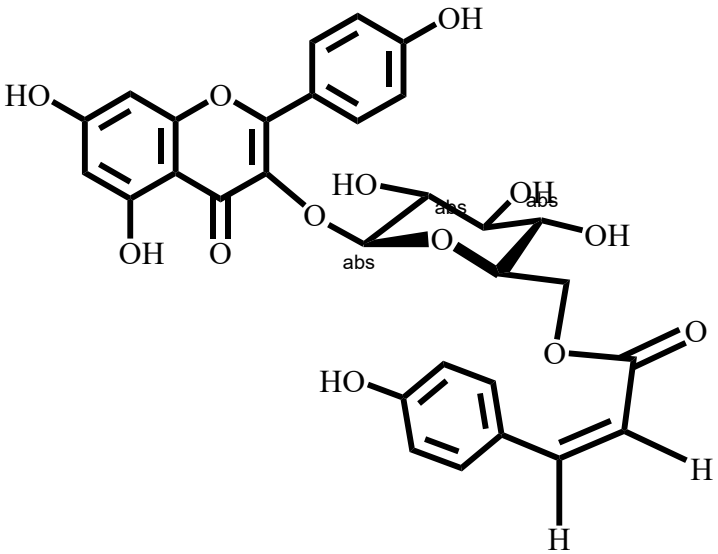


Figure.41.^{13}C NMR spectrum (spreading out 4) (125MHz, DMSO-d_6, δppm) of *trans*-tiliroside

Molecule 5 : *Cis*-tiliroside



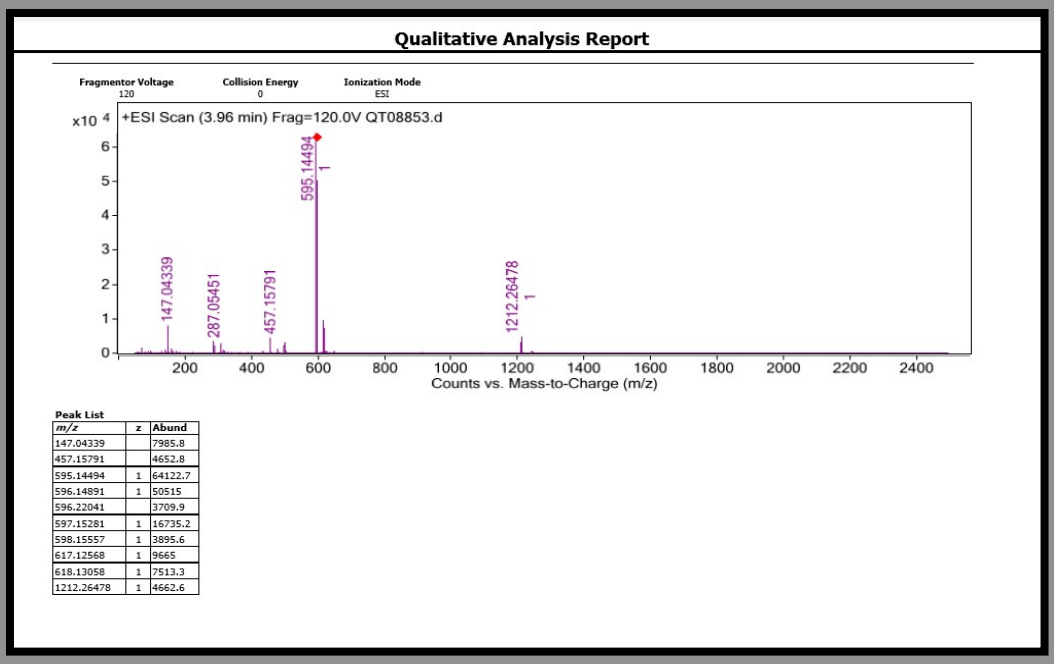


Figure.42.HRESI-MS (+) of *cis*-tiliroside

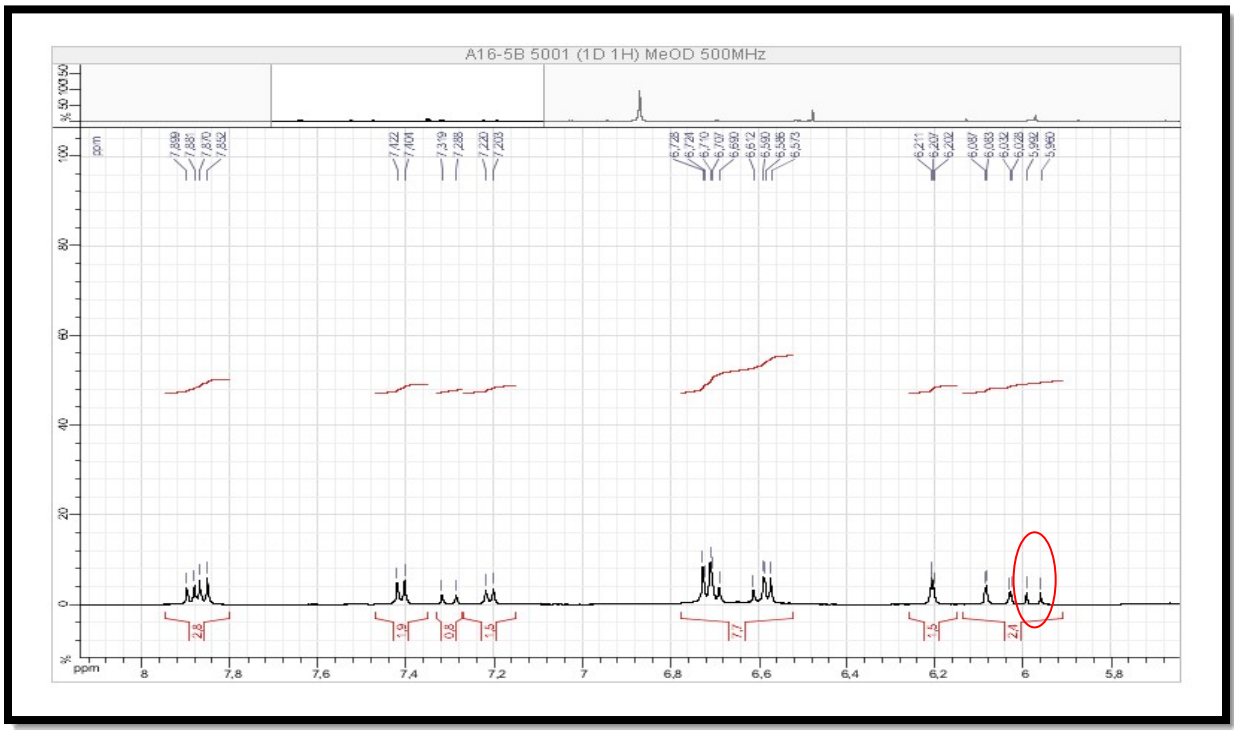


Figure.43. ^{1}H NMR spectrum (spreading out1) (500MHz, CD_3OD, δppm) of *cis*-tiliroside

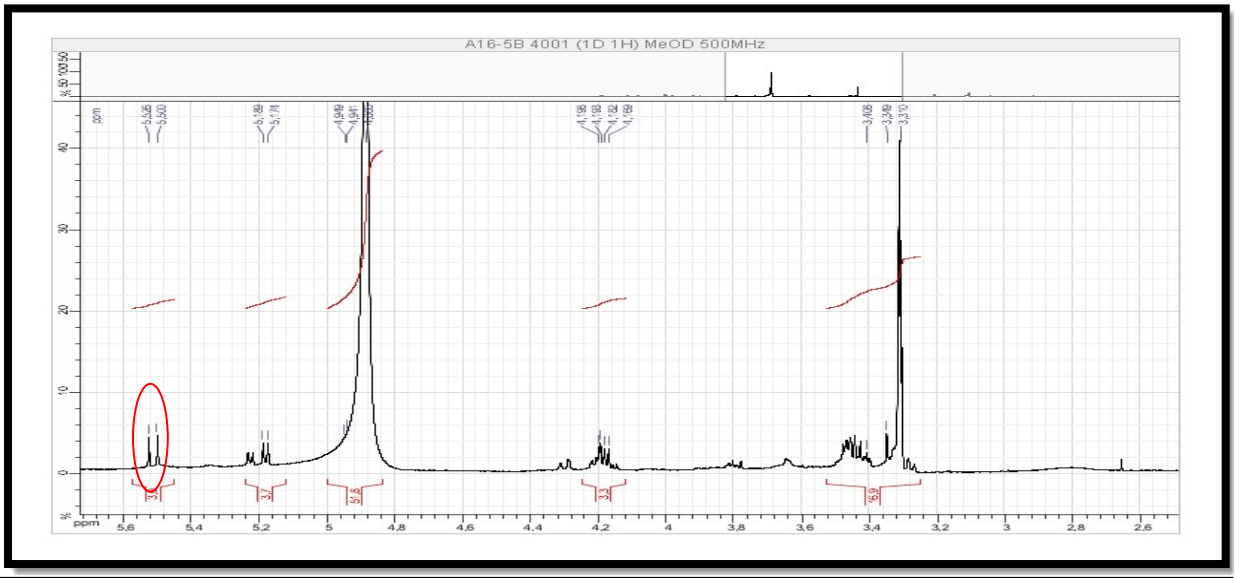


Figure.44. ^{1}H NMR spectrum (spreading out 2) (500MHz, CD_3OD, δppm) of *cis*-tiliroside

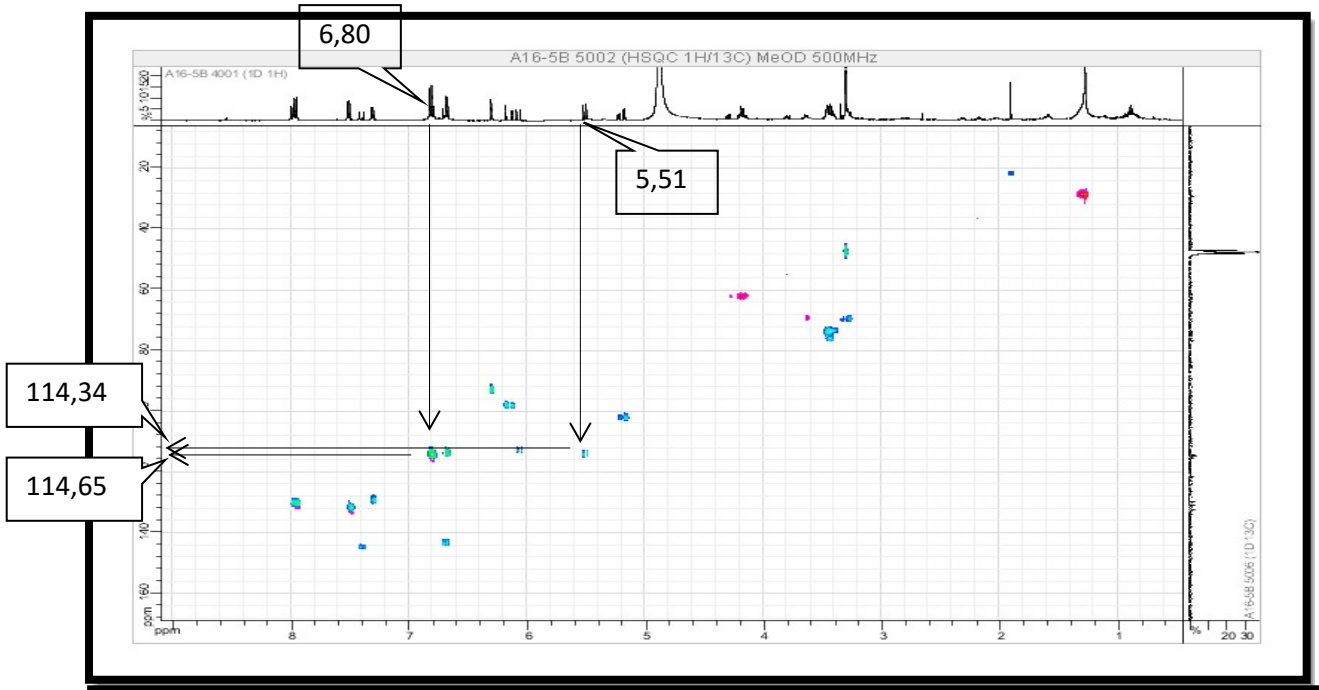
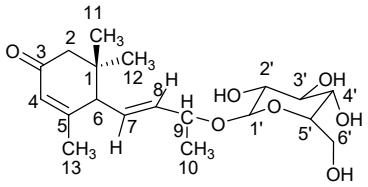


Figure.45. HSQC NMR spectrum (500MHz, CD_3OD, δppm) of *cis*-tiliroside

Molecule 7 : 3-oxo-α-ionol-β-D-glucopyranoside



(7)

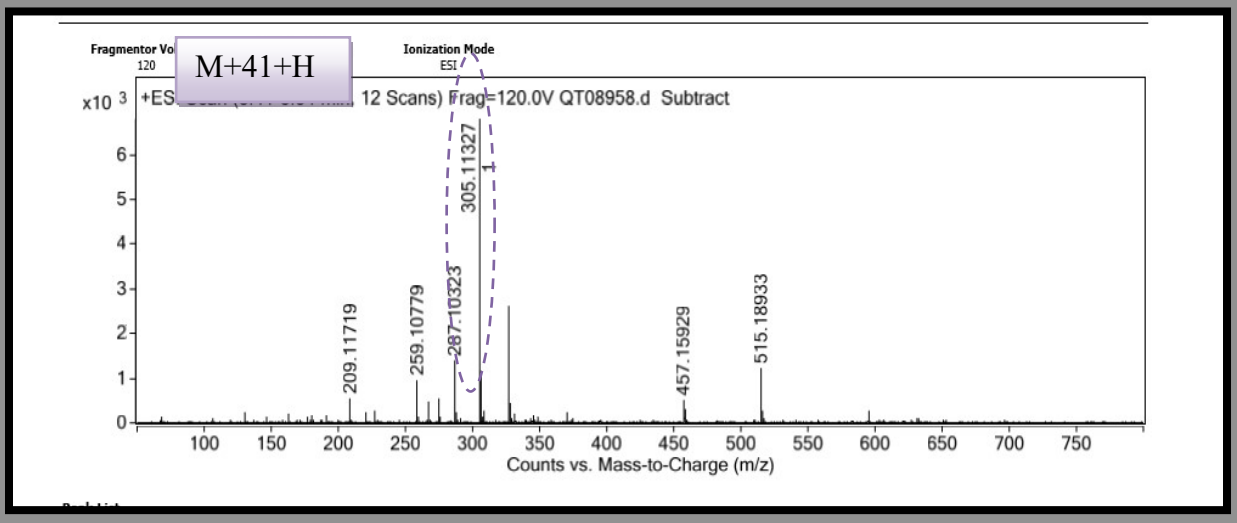


Figure.46.HRESI-MS (+) of 3-oxo-α-ionol-β-D-glucopyranoside

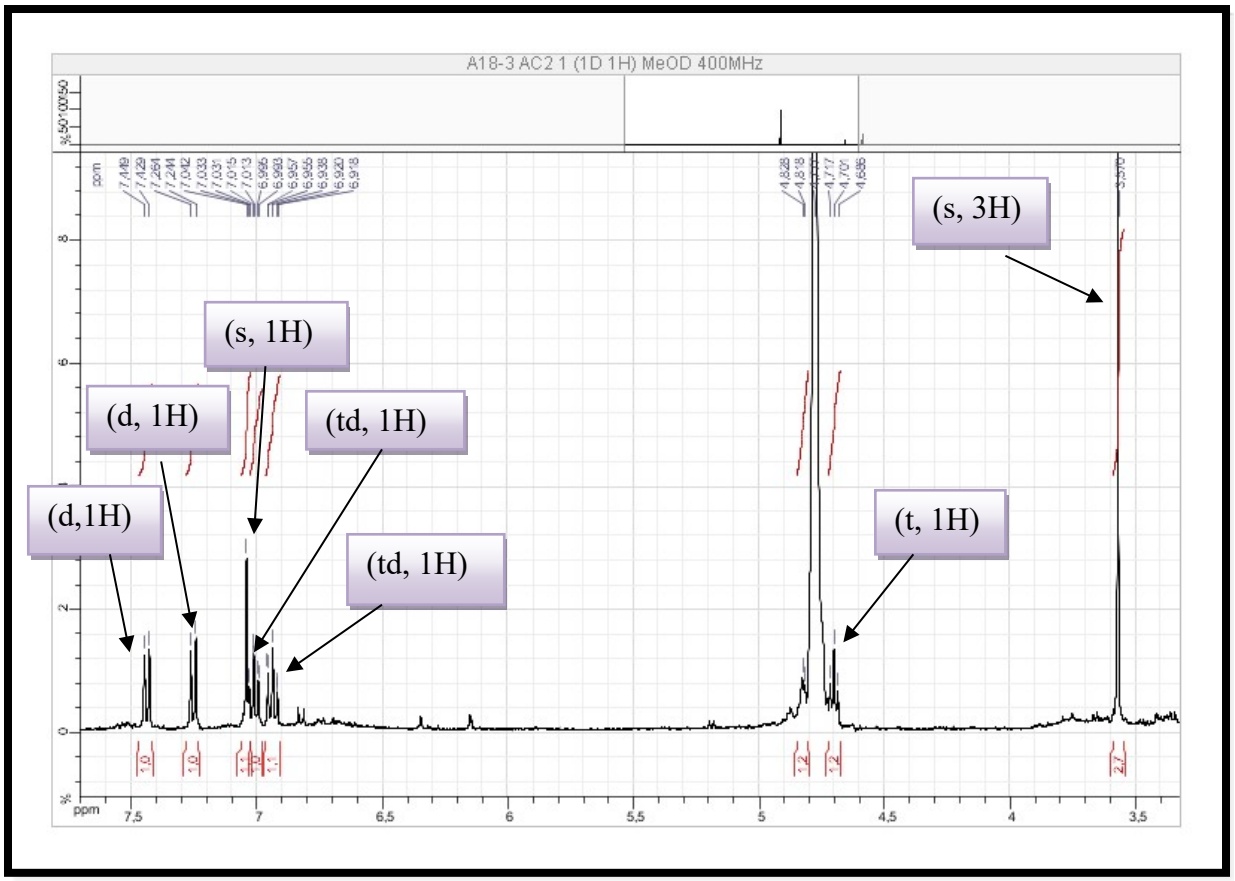


Figure.47-1. ^{1}H NMR spectrum (spreading out1) (400MHz, CD_3OD, δ_{ppm}) of 3-oxo-α-ionol-β-D-glucopyranoside

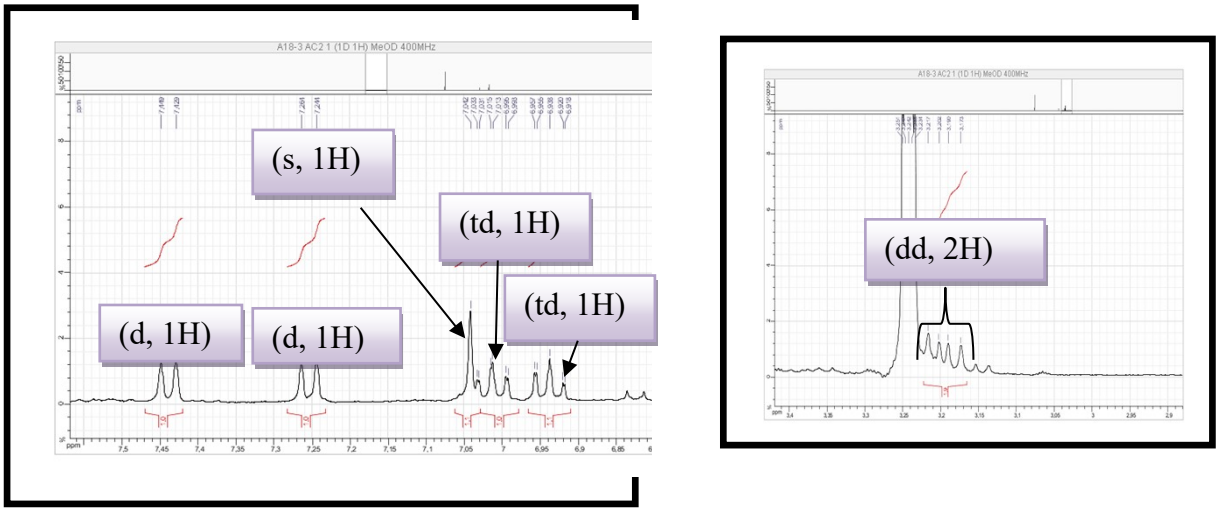


Figure.47-2. ^{1}H NMR spectrum (spreading out2) (400MHz, CD_3OD, δ_{ppm}) of 3-oxo-α-ionol-β-D-glucopyranoside

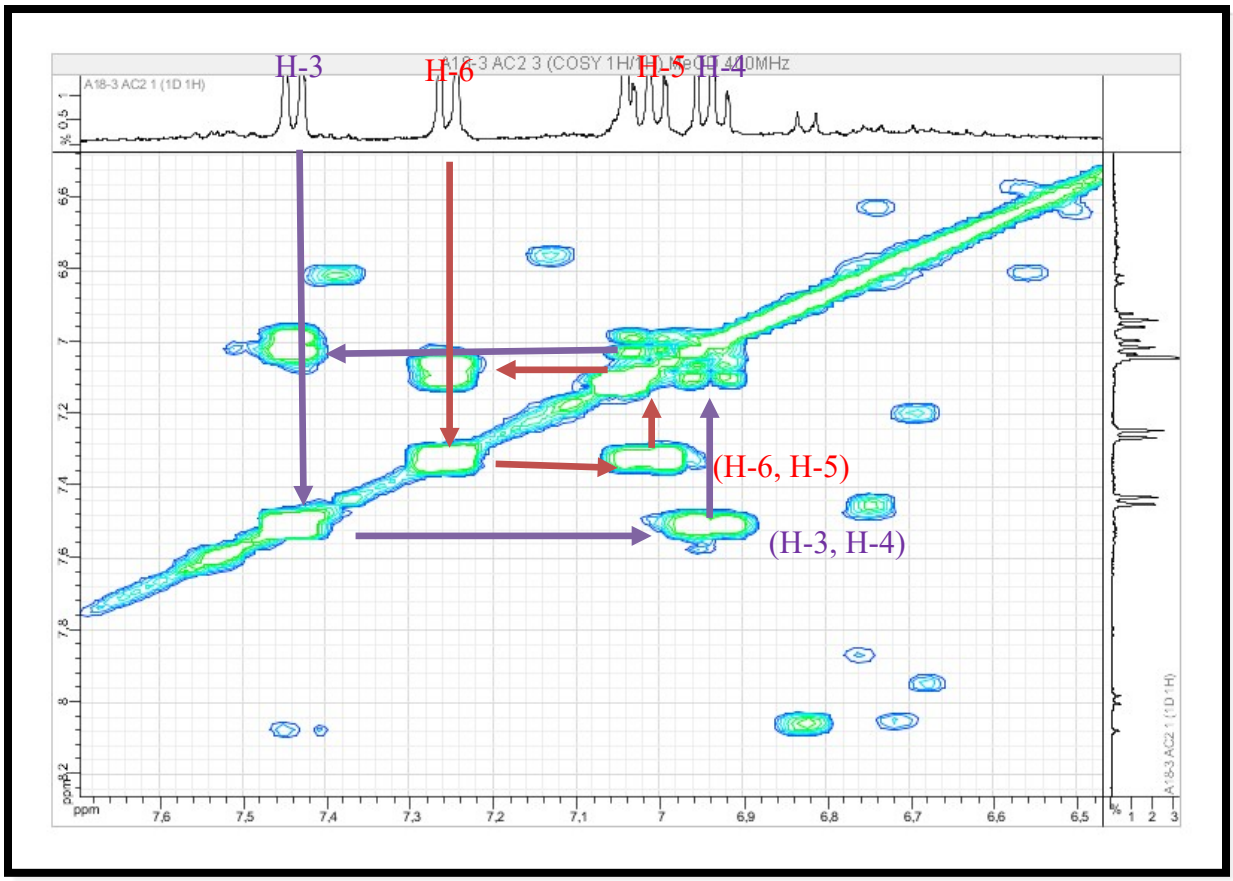


Figure.48-1. COSY spectrum (spreading out 1) (400MHz, CD_3OD, δ_{ppm}) of 3-oxo-α-ionol-β-D-glucopyranoside

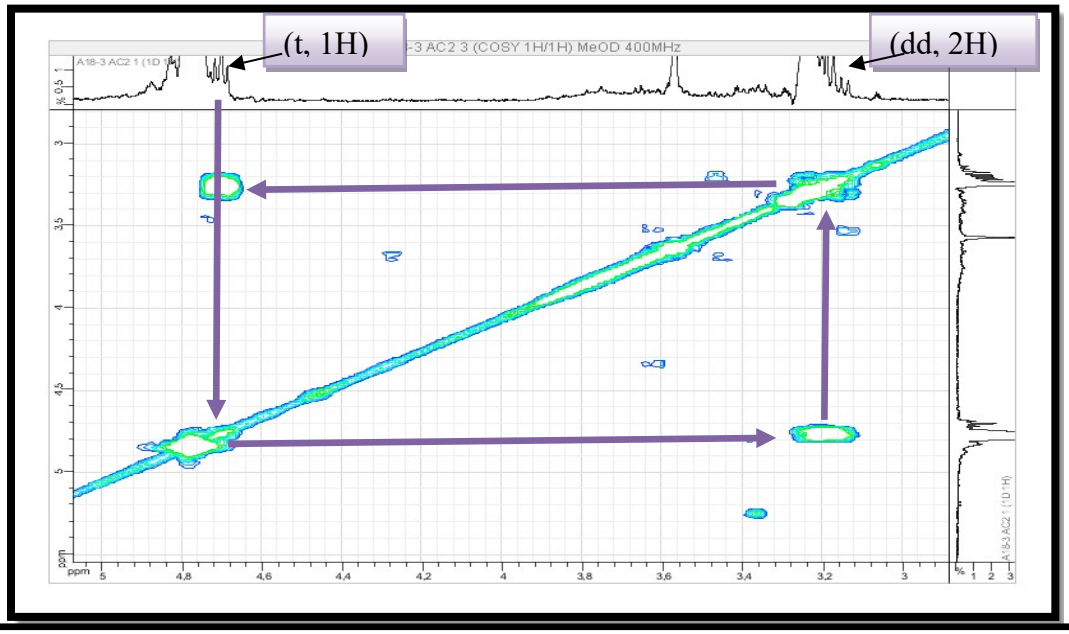


Figure.48-2. COSY spectrum (spreading out 2) (400MHz, CD_3OD, δ_{ppm}) of 3-oxo-α-ionol-β-D-glucopyranoside

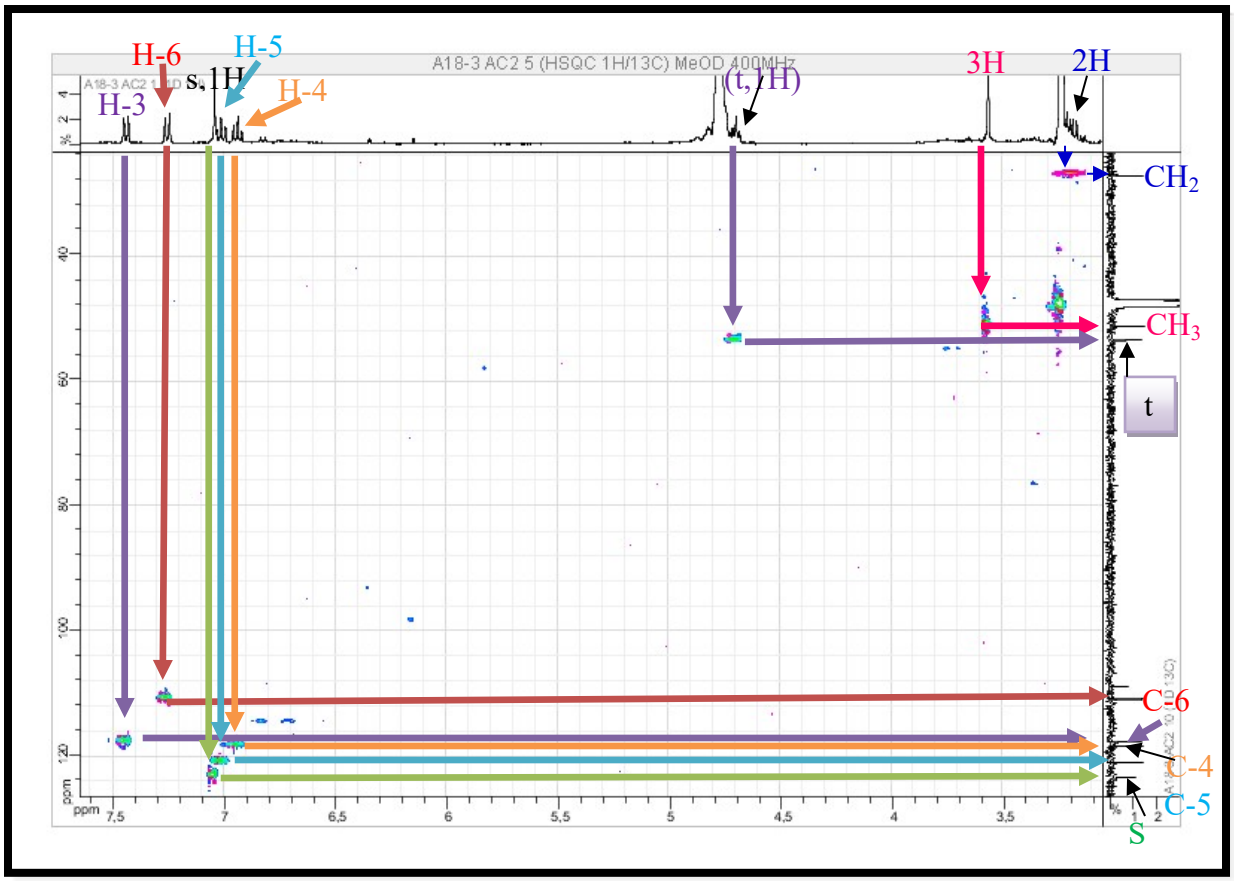


Figure.49. HSQC spectrum (spreading out 1) (400MHz, CD_3OD, δ_{ppm}) of 3-oxo-α-ionol-β-D-glucopyranoside

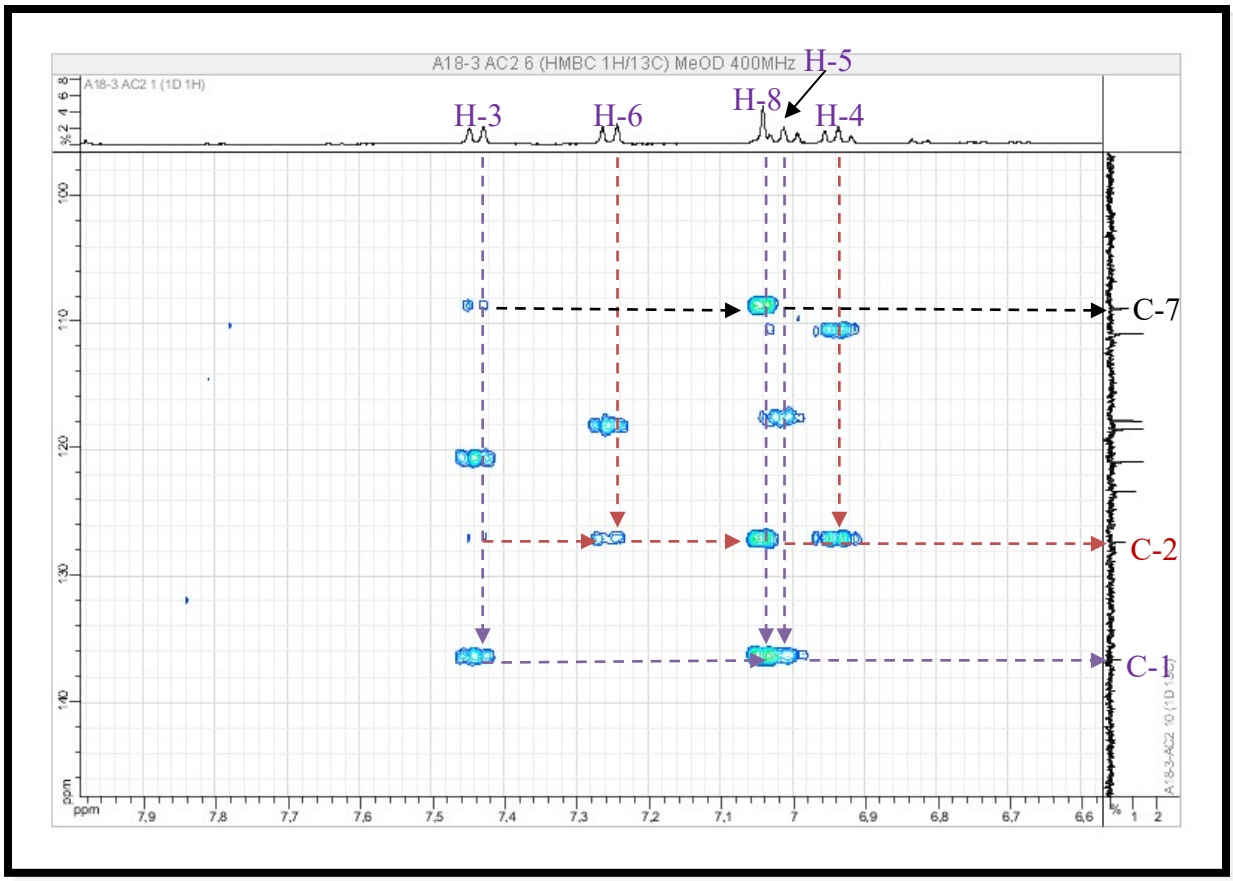


Figure.50-1. HMBC spectrum (spreading out 1) (400MHz, CD_3OD, δ_{ppm}) of 3-oxo-α-ionol-β-D-glucopyranoside

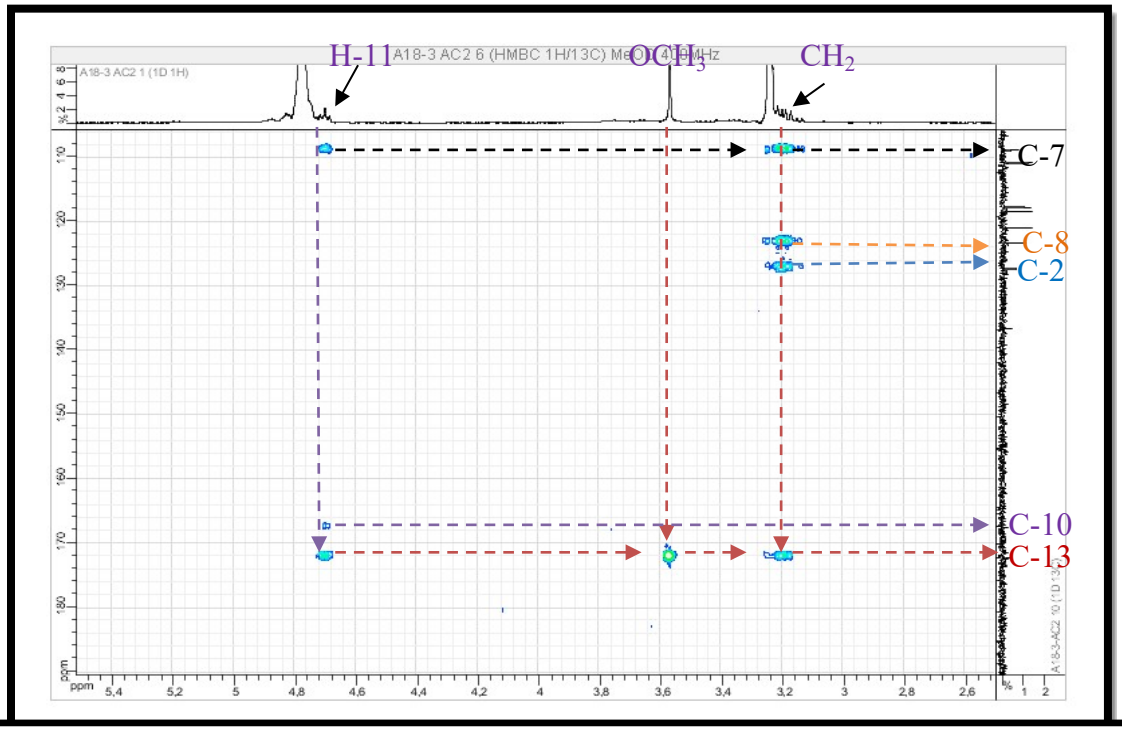


Figure.50-2. HMBC spectrum (spreading out 2) (400MHz, CD_3OD, δ_{ppm}) of 3-oxo-α-ionol-β-D-glucopyranoside

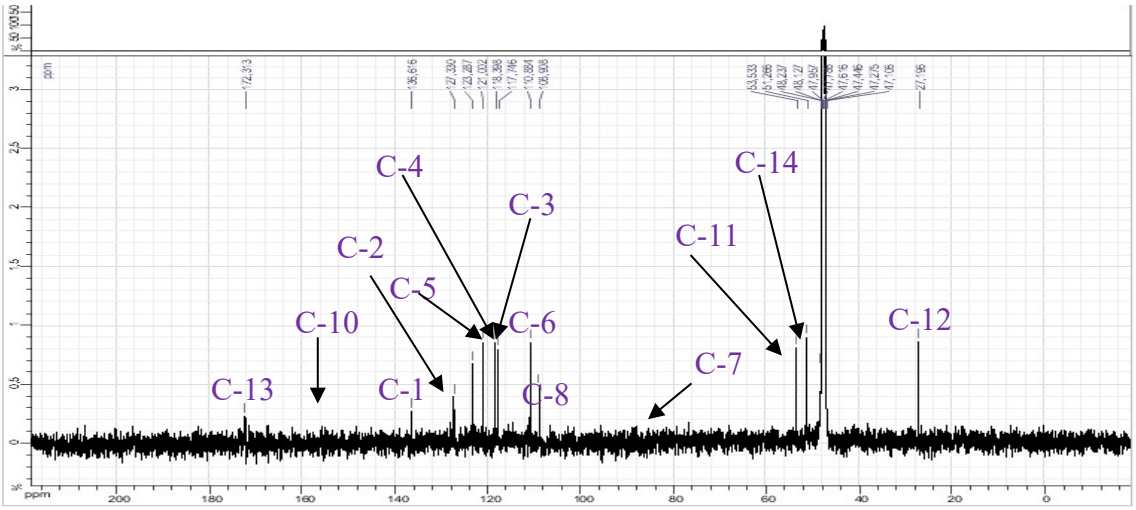


Figure.51. ^{13}C NMR spectrum (100MHz, CD_3OD, δ_{ppm}) of 3-oxo-α-ionol-β-D-glucopyranoside