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Appendix

Spectral data of isolated compounds

S1. MS data of Pinifolic acid (Mass 336)

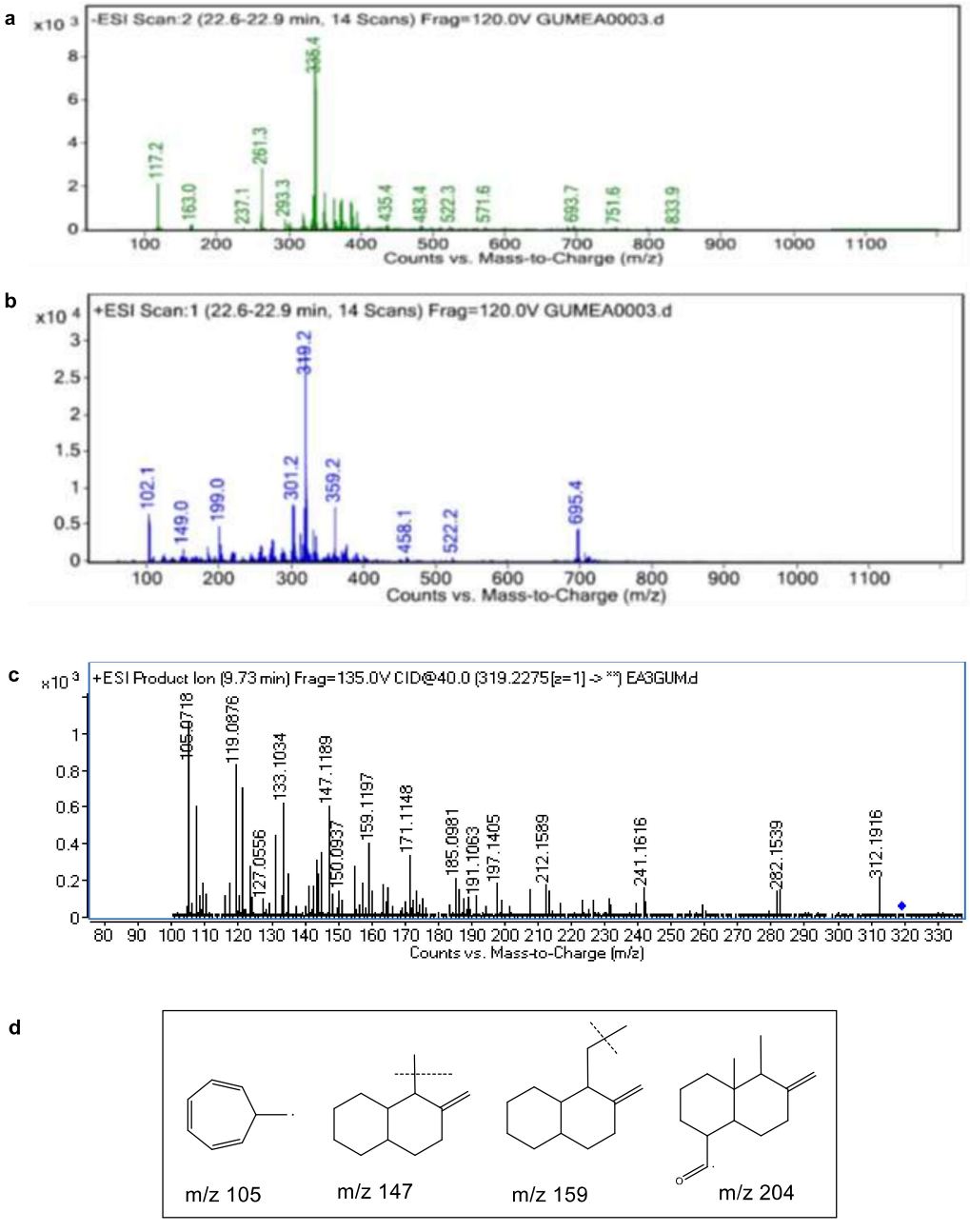


Figure S1. a) -ve ESI scan b) +ve ESI scan c) MS/MS spectrum d) fragments of pinifolic acid

S2. MS data of Dehydropinifolic acid (Mass 334)

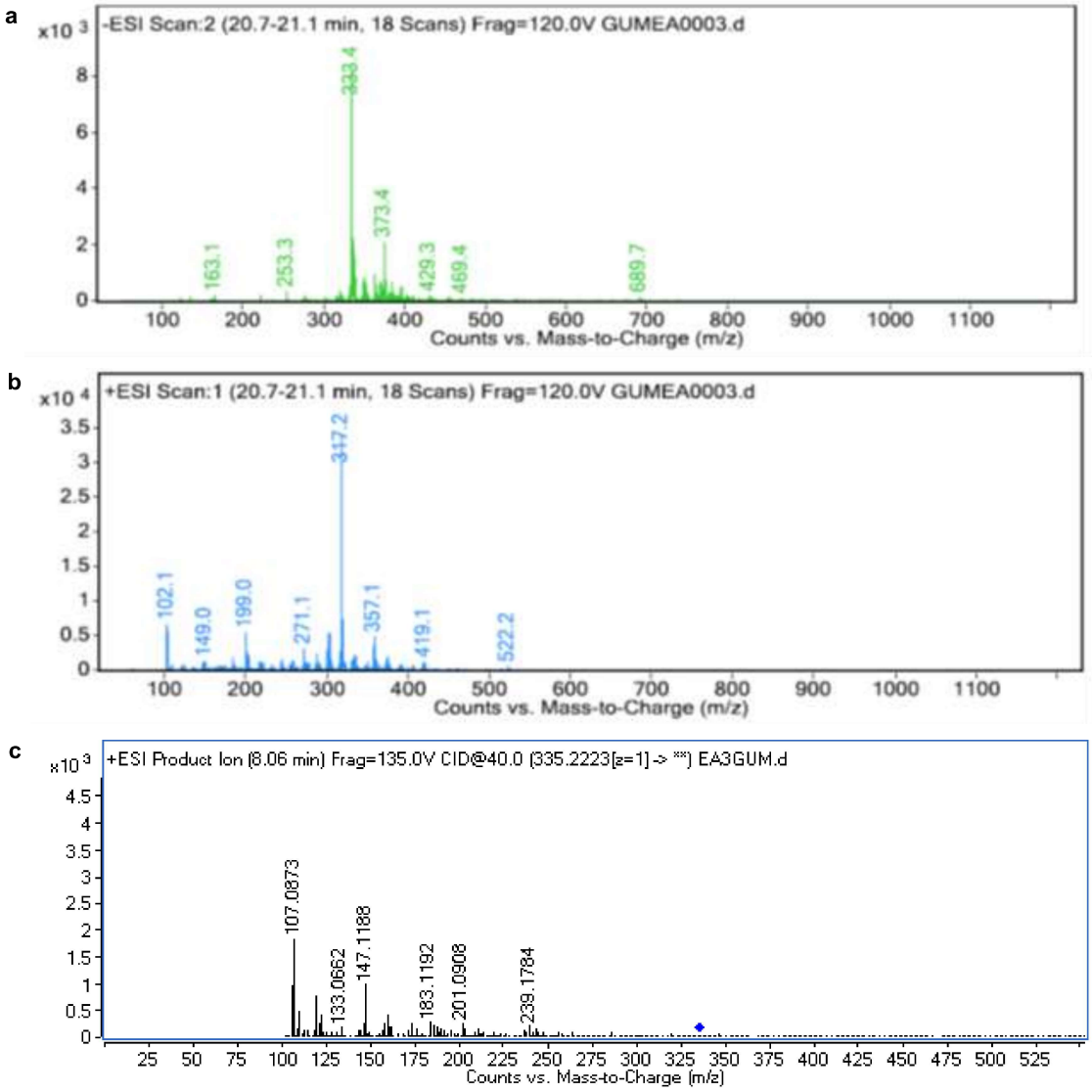


Figure S2. a) -ve ESI scan b) +ve ESI scan c) HRMS MS/MS spectrum of dehydropinifolic acid

S3. MS and NMR data of Dehydropinifolic acid methylester (agathic acid methylester) (348)

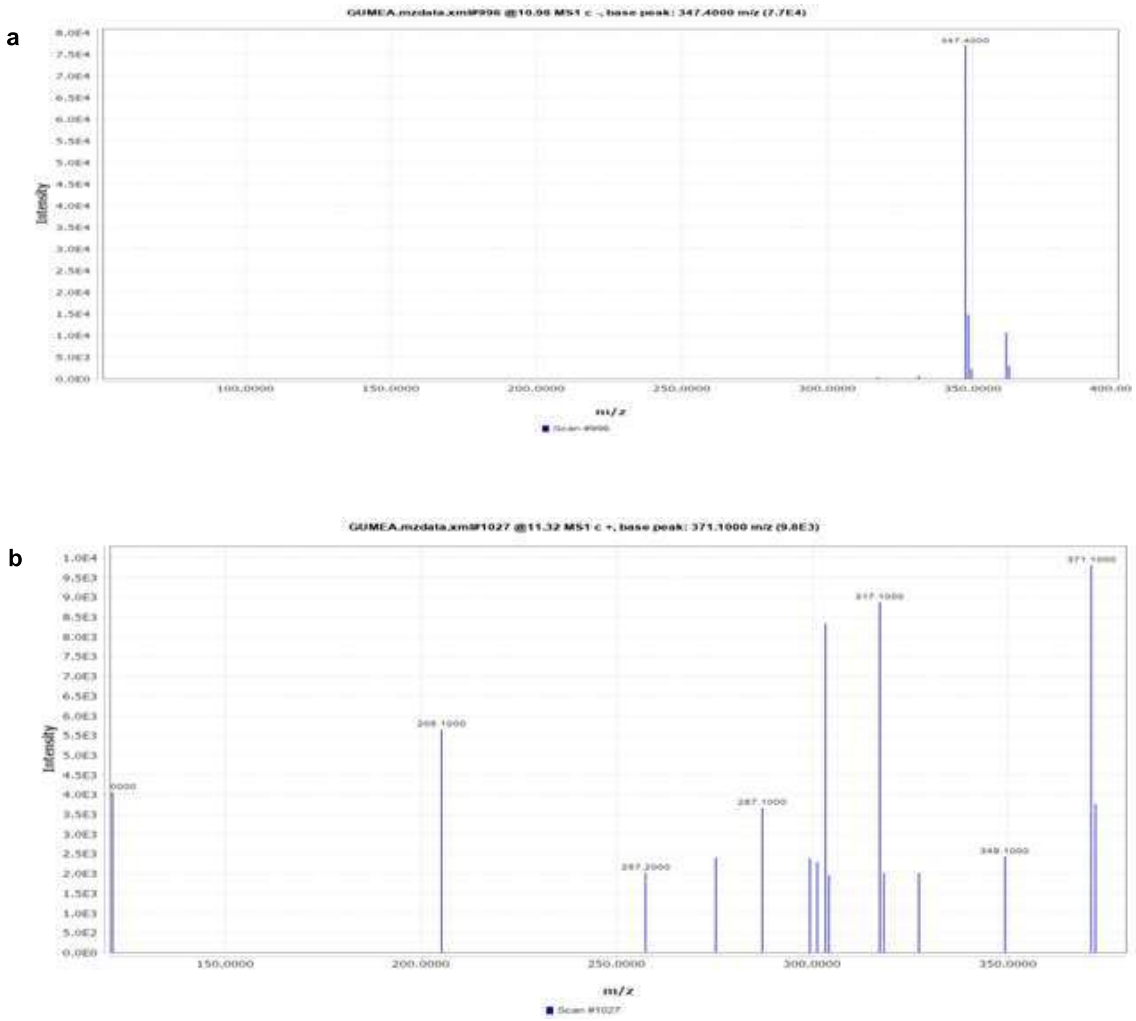


Figure S3. a) -ve HRMS spectrum, b) +ve HRMS spectrum of dehydropinifolic acid methylester

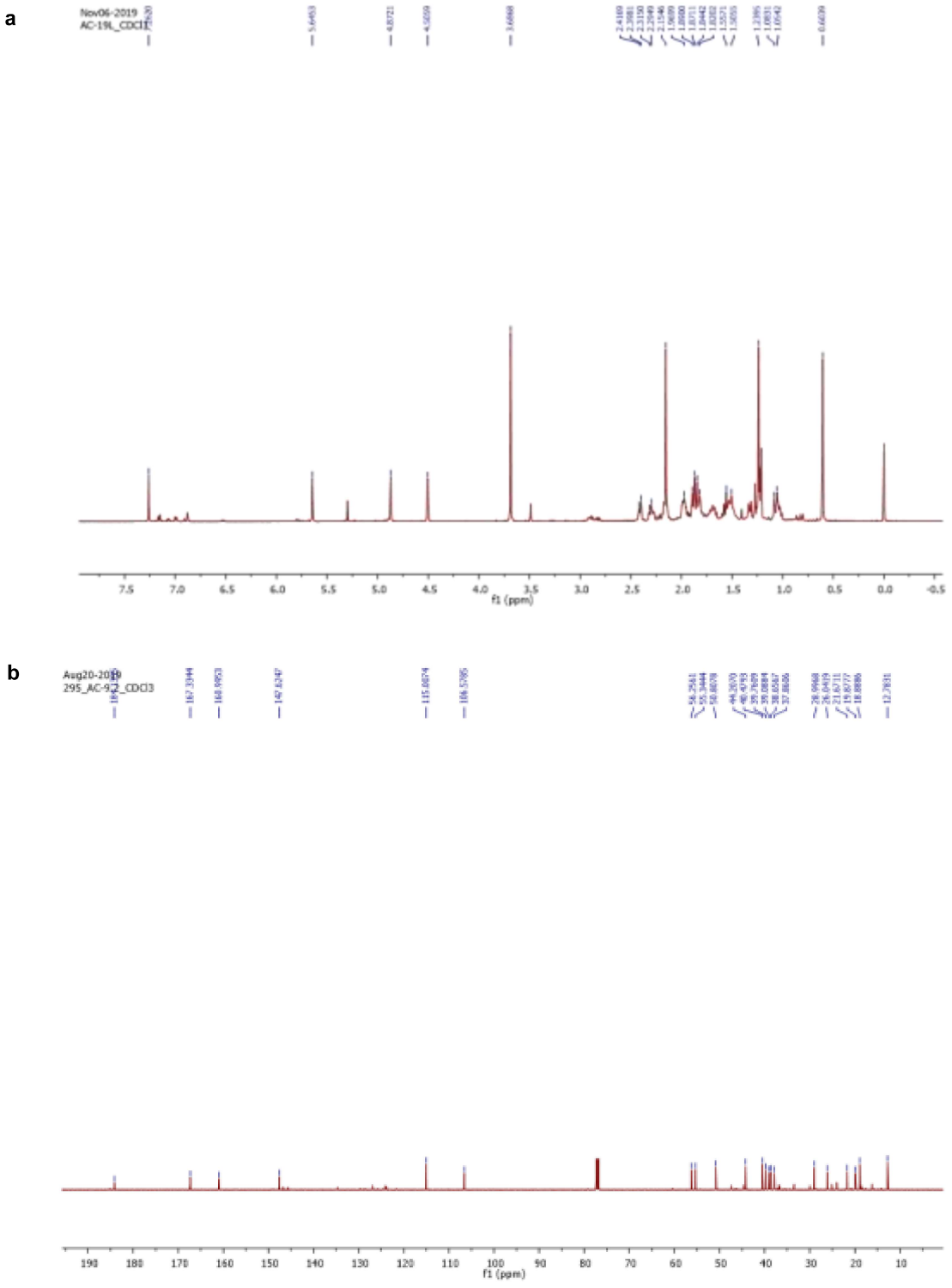


Figure S4. a) ^{1}H-NMR; b) ^{13}C-NMR spectra of dehydropinifolic acid methylester

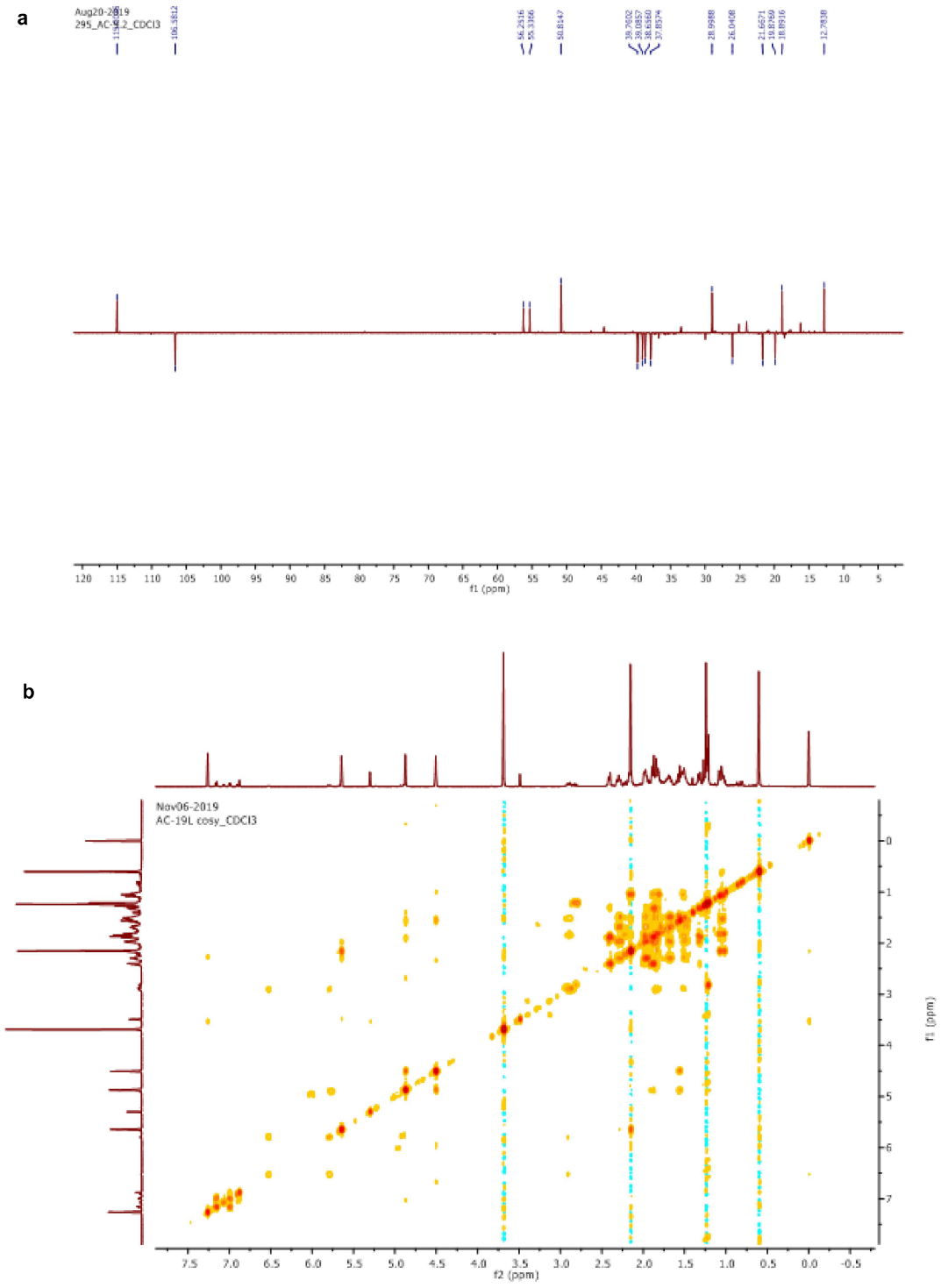


Figure S5. a) DEPT 135; b) ^{1}H-^{1}H COSY spectrum of dehydropinifolic acid methylester

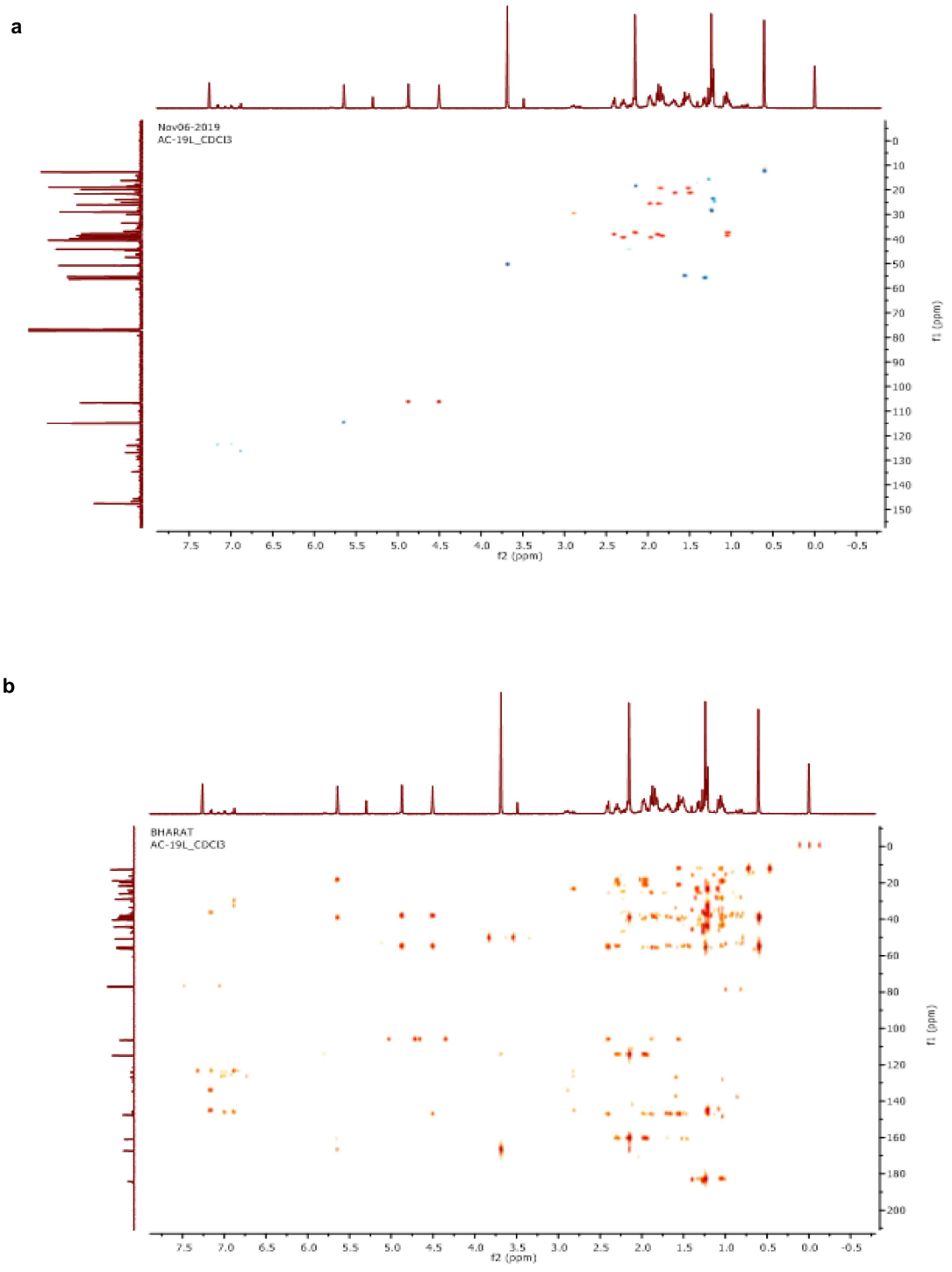


Figure S6. a) HSQC and b) HMBC spectrum of dehydropinifolic acid methylester

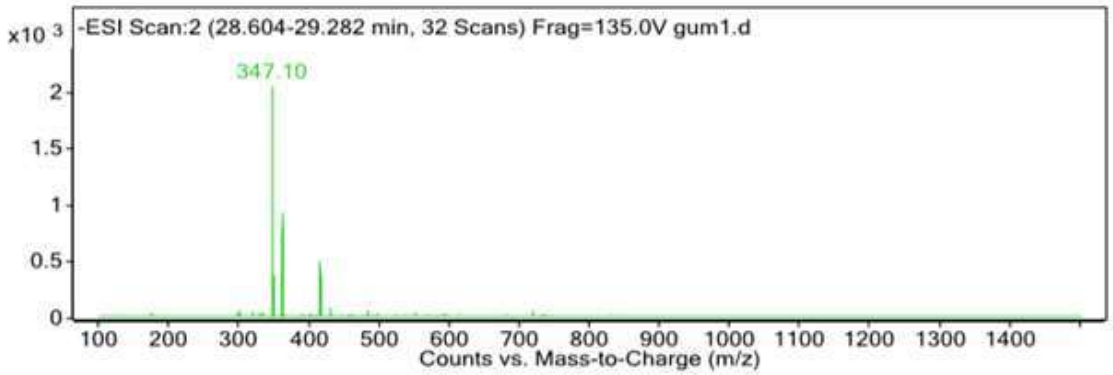


Figure S7. -ve ESI MS spectrum of dehydropinifolic acid methylester

S4. MS data of Isocupressic acid

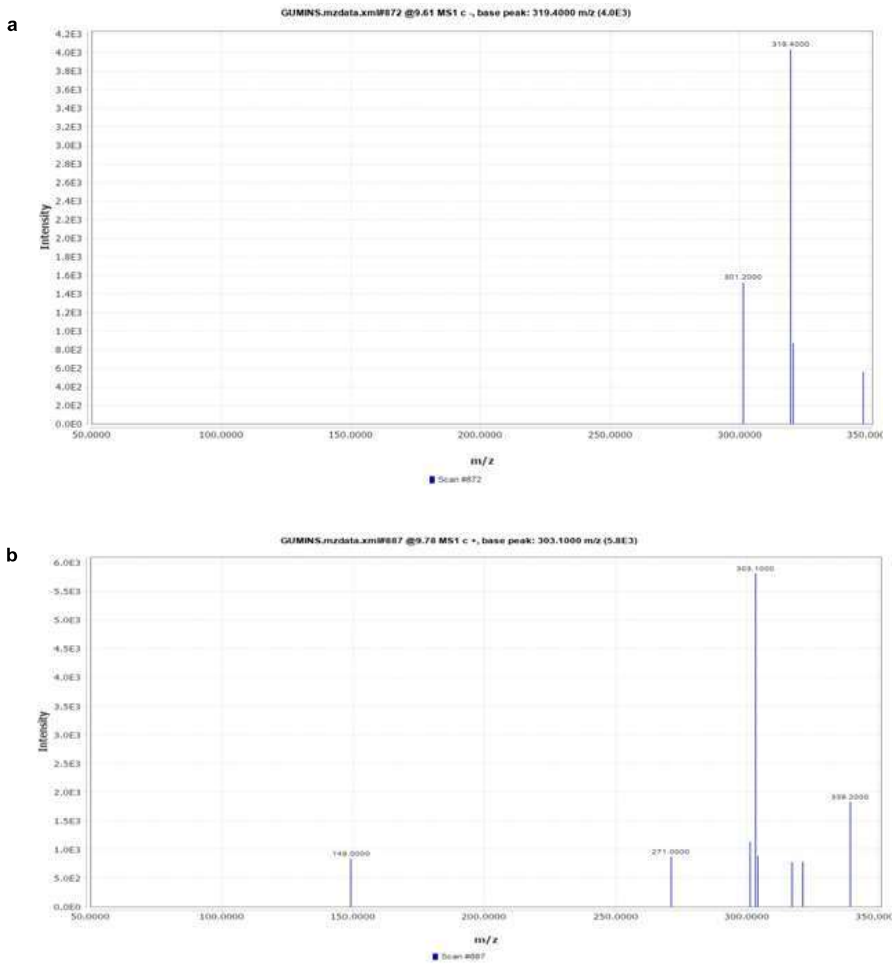


Figure S8. a) -ve HRMS spectrum, b) +ve HRMS spectrum of isocupressic acid

S5. MS data of Manool (290): Method 2

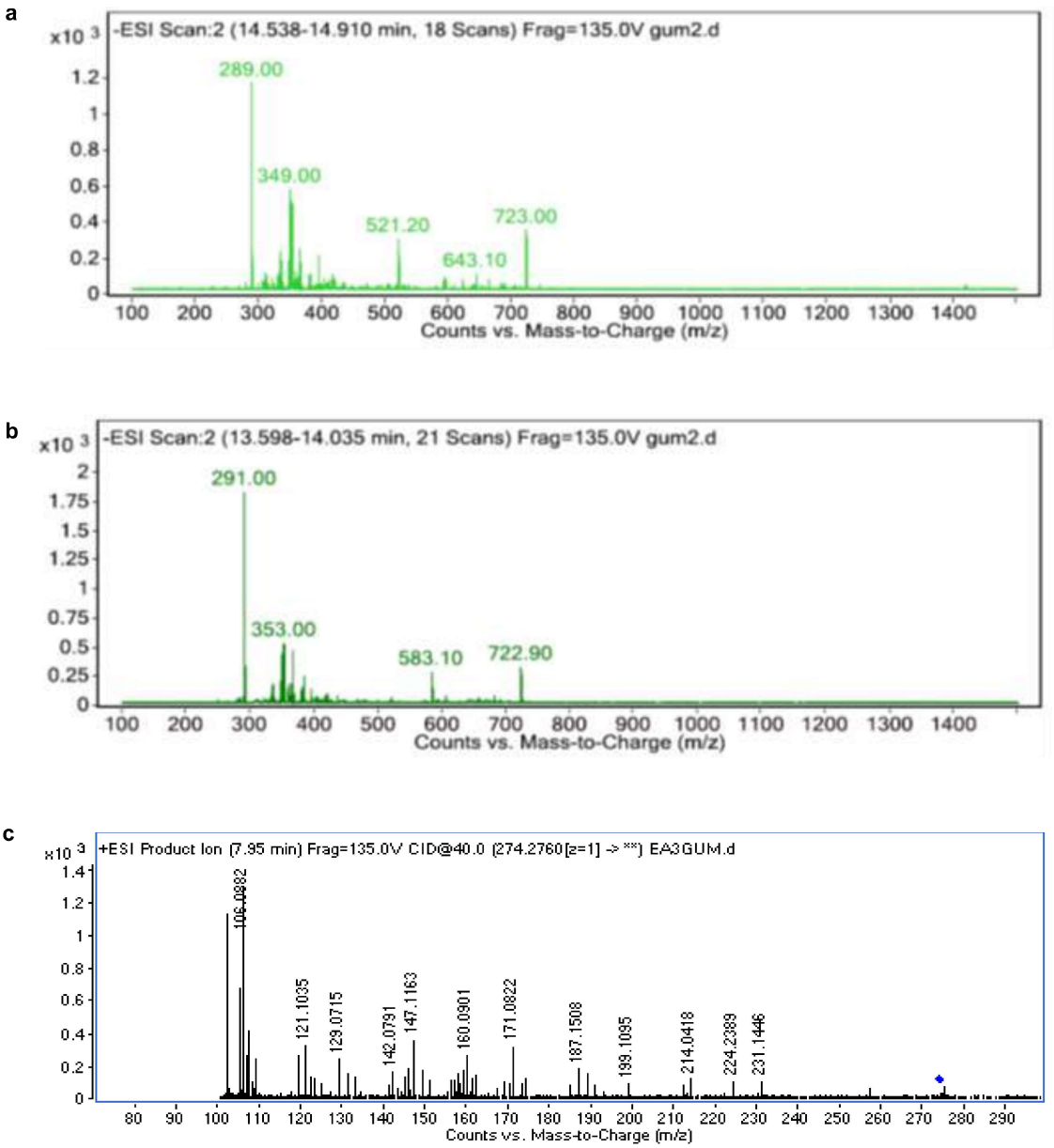


Figure S9. a) -ve ESI scan at 14.5min b) -ve ESI scan at 13.5 min c) MS/MS spectrum of manool

S6. MS data of Imbricataloic acid (320)

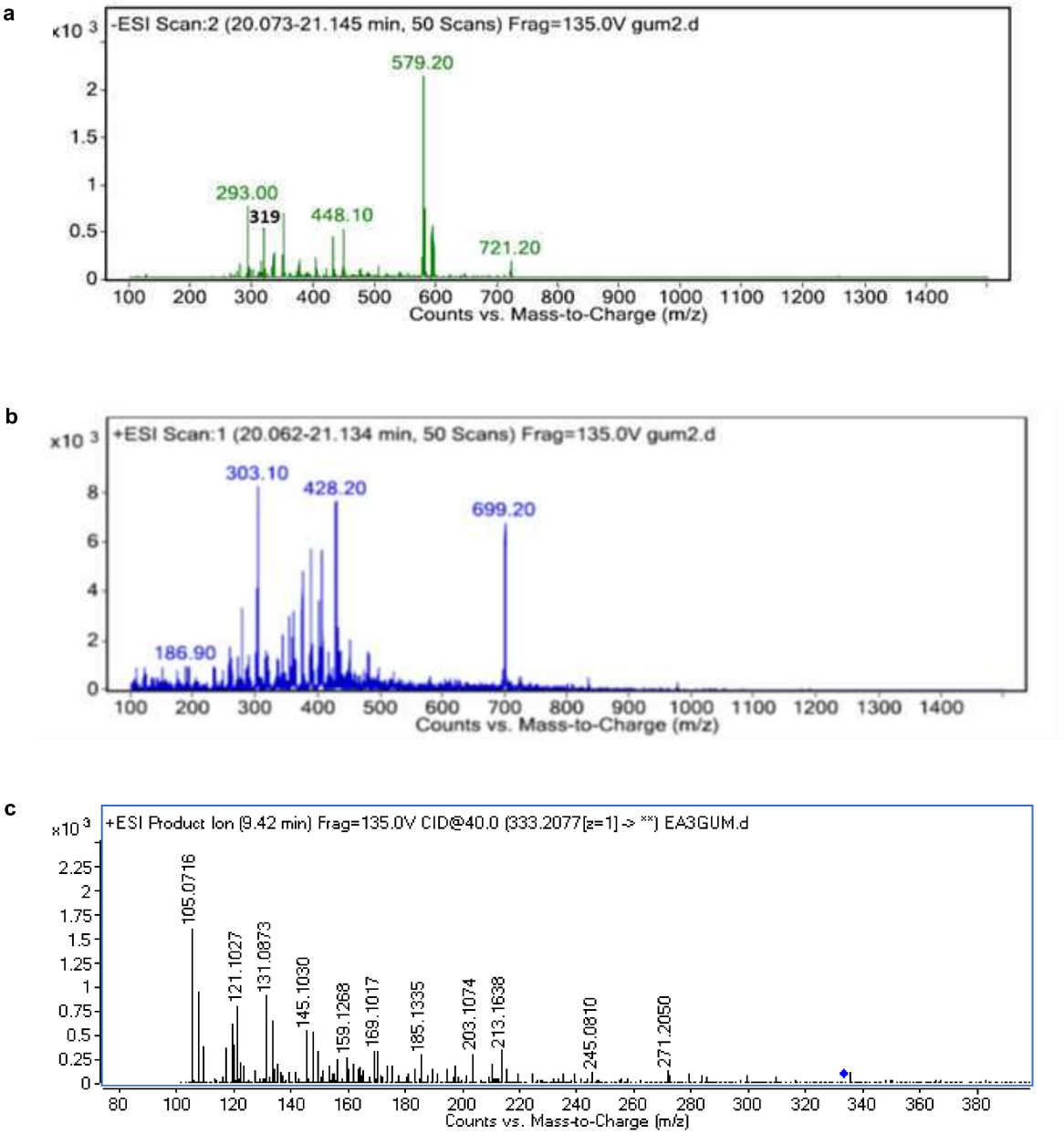


Figure S10. a) -ve ESI scan b) +ve ESI scan c) MS/MS spectrum of imbricataloic acid

S7. MS data of Trans-communic acid (302)

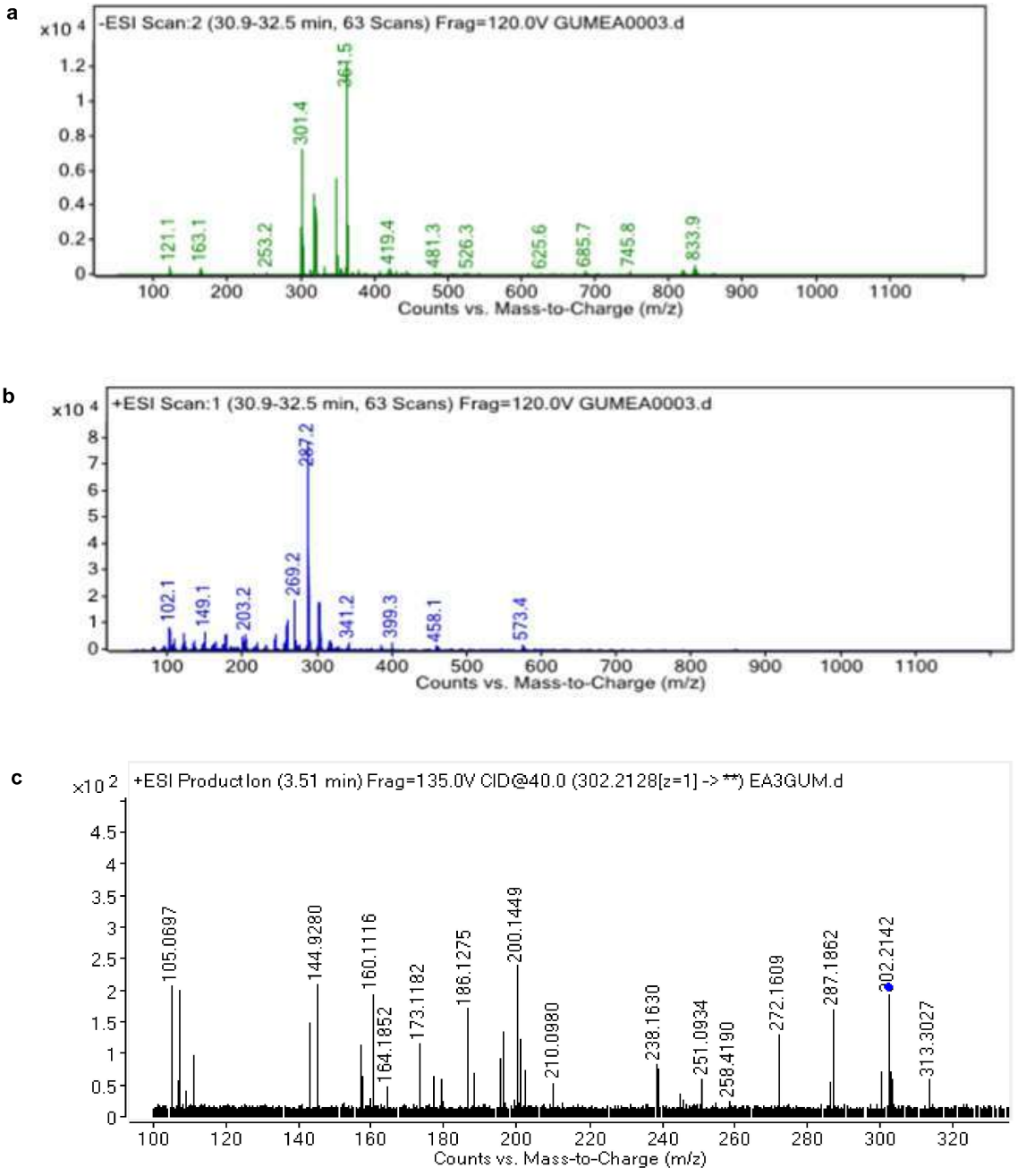


Figure S11. a) -ve ESI scan b) +ve ESI scan c) MS/MS spectrum of trans-communic acid

S8. MS data of Cupressic acid (320)

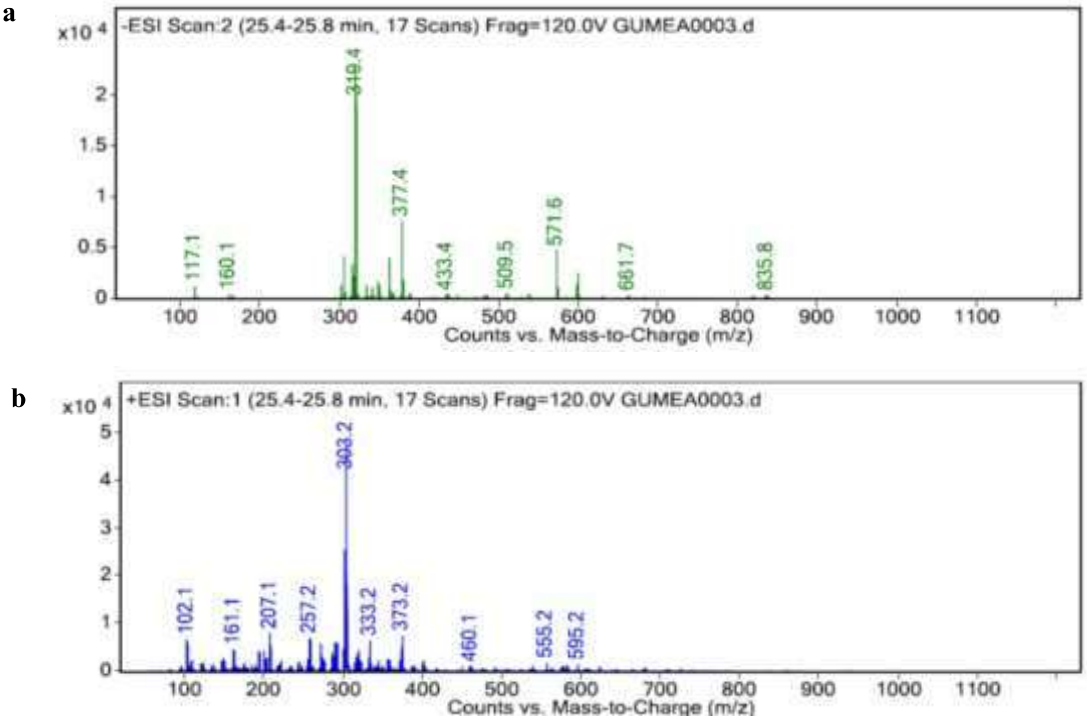


Figure S12. a) -ve ESI b) +ve ESI MS spectra of cupressic acid

S9. NMR and MS data of Abietic acid

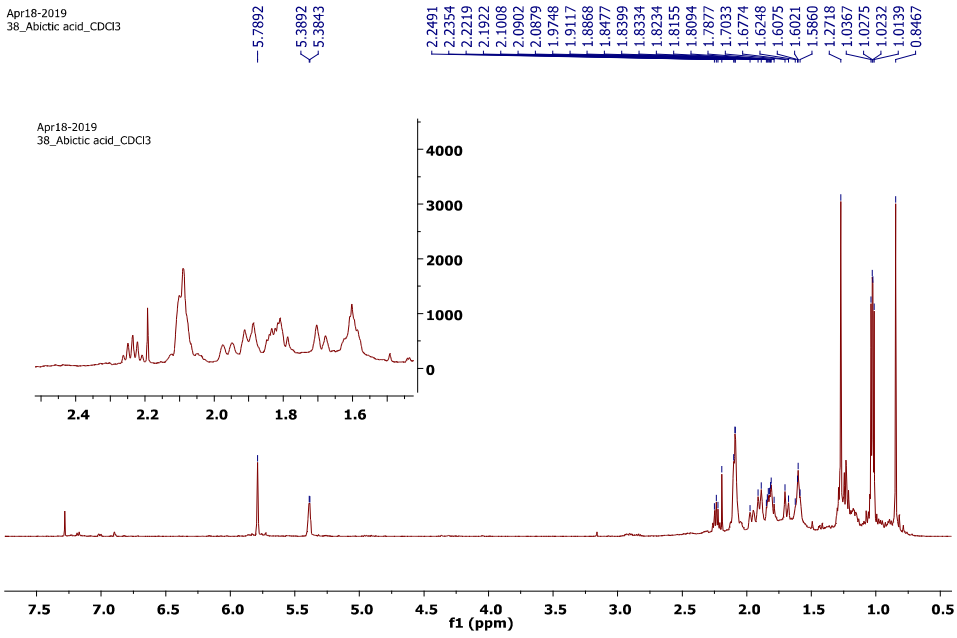


Figure S13. ^{1}H NMR spectrum of Abietic acid

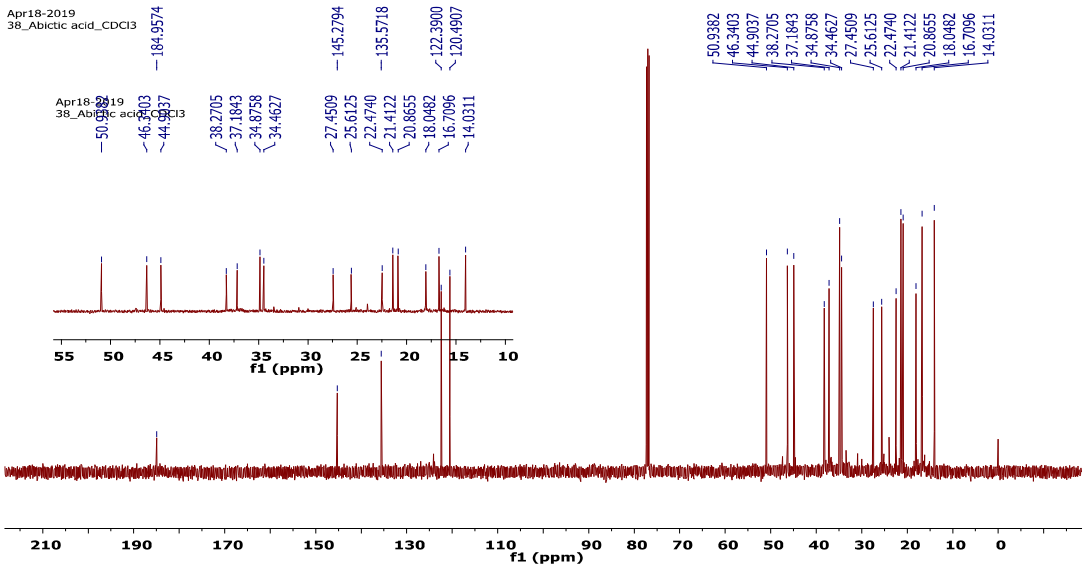


Figure S14. ^{13}C NMR spectrum of Abietic acid

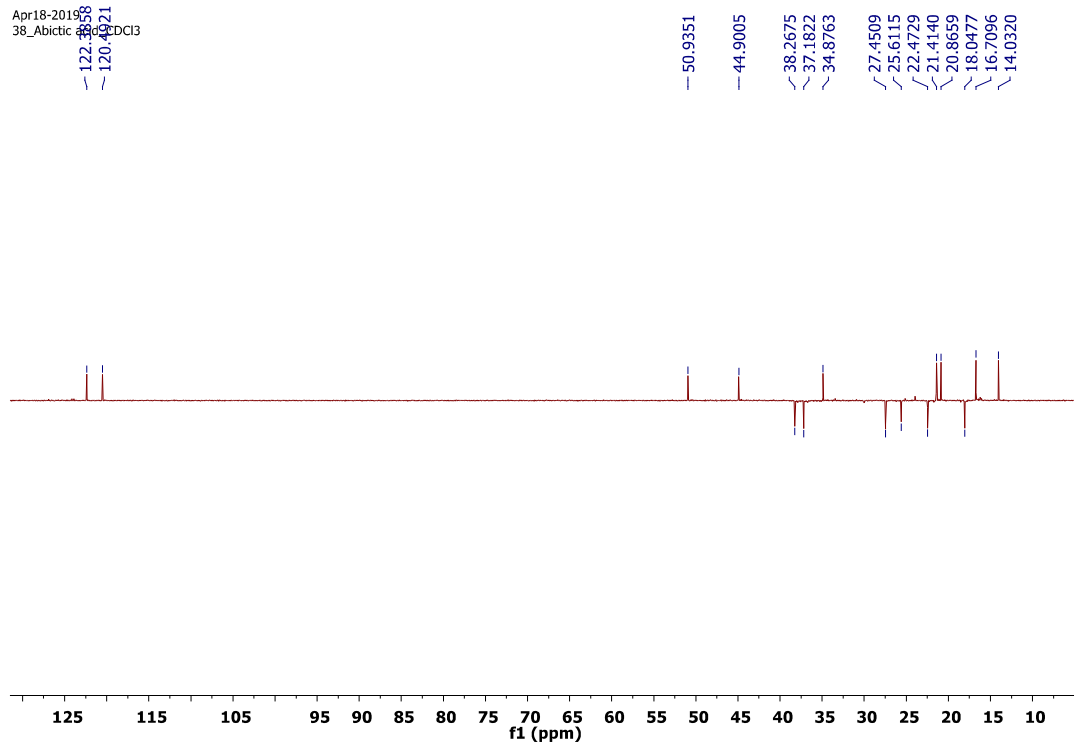


Figure S15. DEPT-135 NMR spectrum of Abietic acid

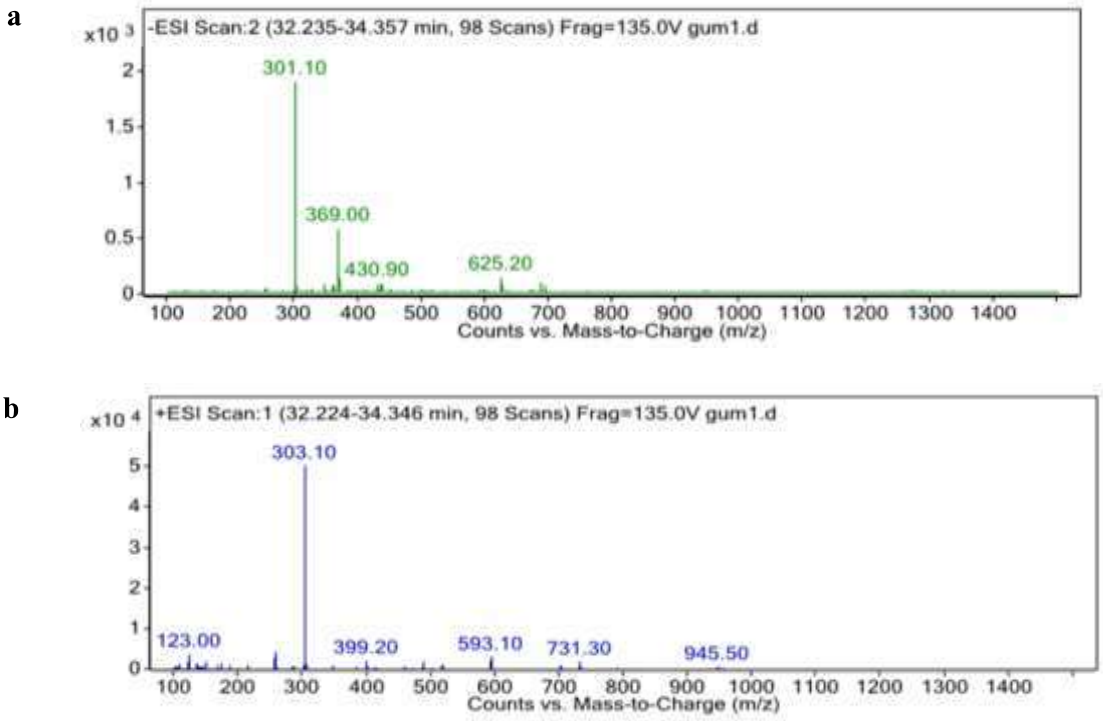


Figure S16. a) -ve ESI; b) +ve ESI MS spectra of Abietic acid

S10. MS and NMR data of 7-Ketodehydroabietic acid

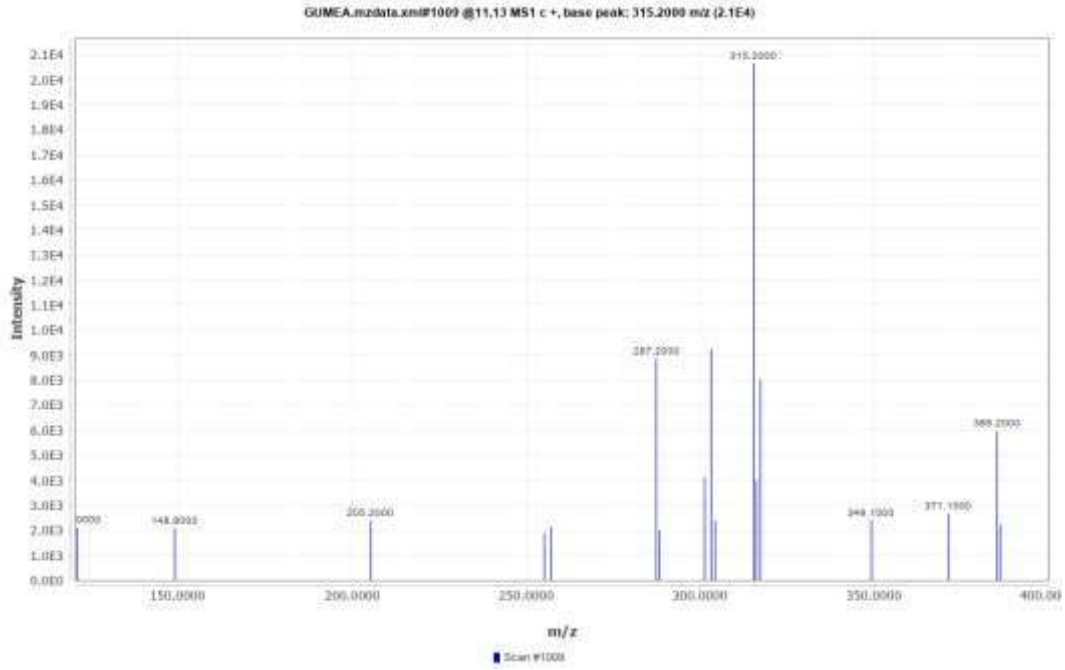


Figure S17. MS spectra of 7-ketodehydroabietic acid

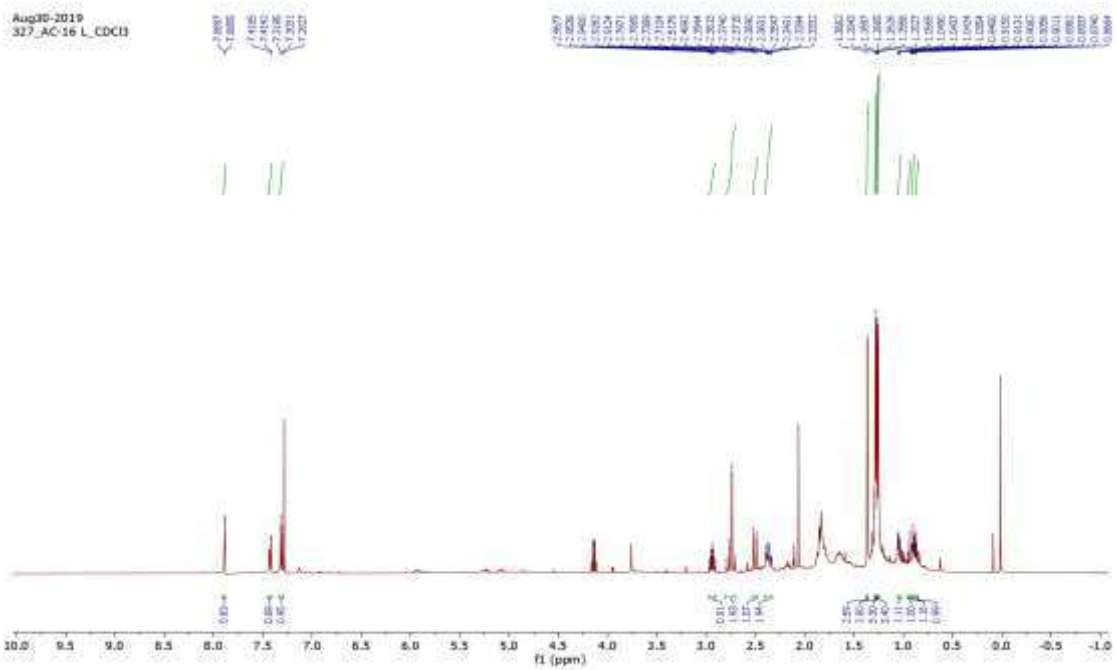


Figure S18. ^{1}H NMR spectrum of 7-ketodehydroabietic acid

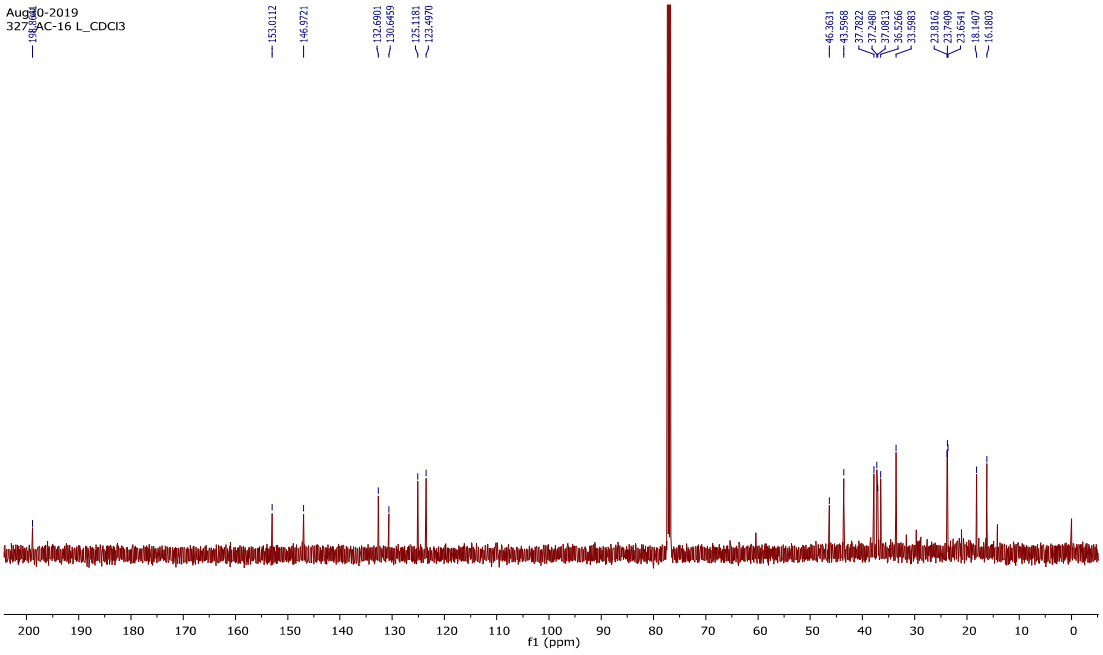


Figure S19. ^{13}C NMR spectrum of 7-ketodehydroabietic acid

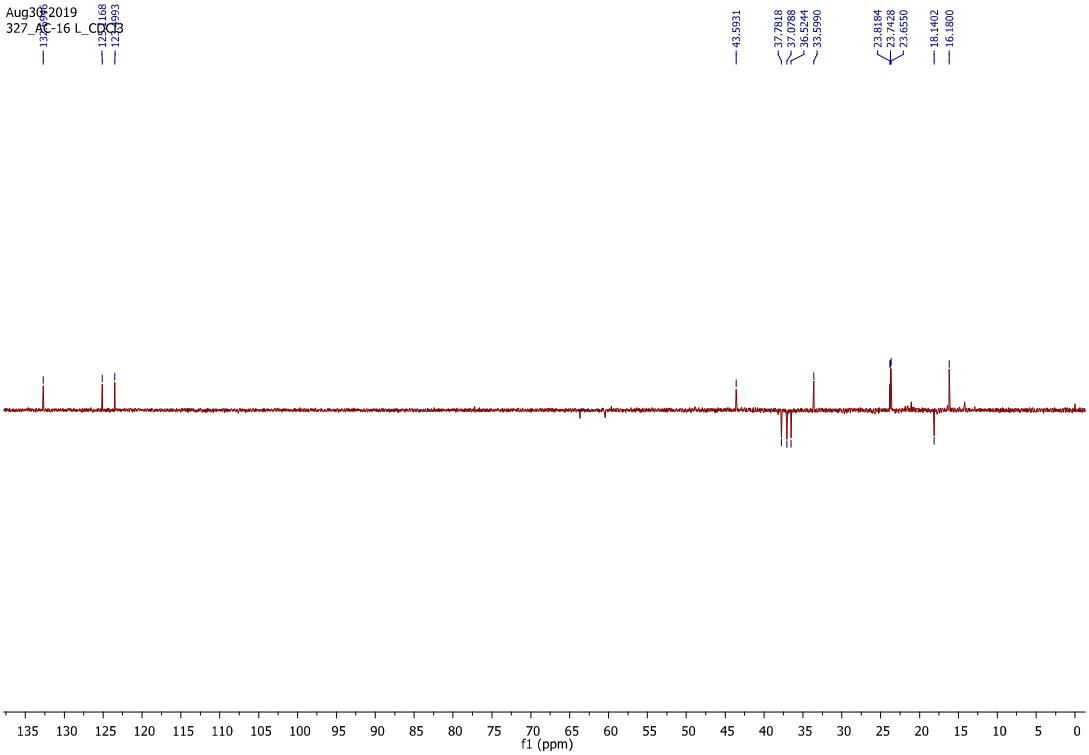


Figure S20. DEPT-135 NMR spectrum of 7-ketodehydroabietic acid

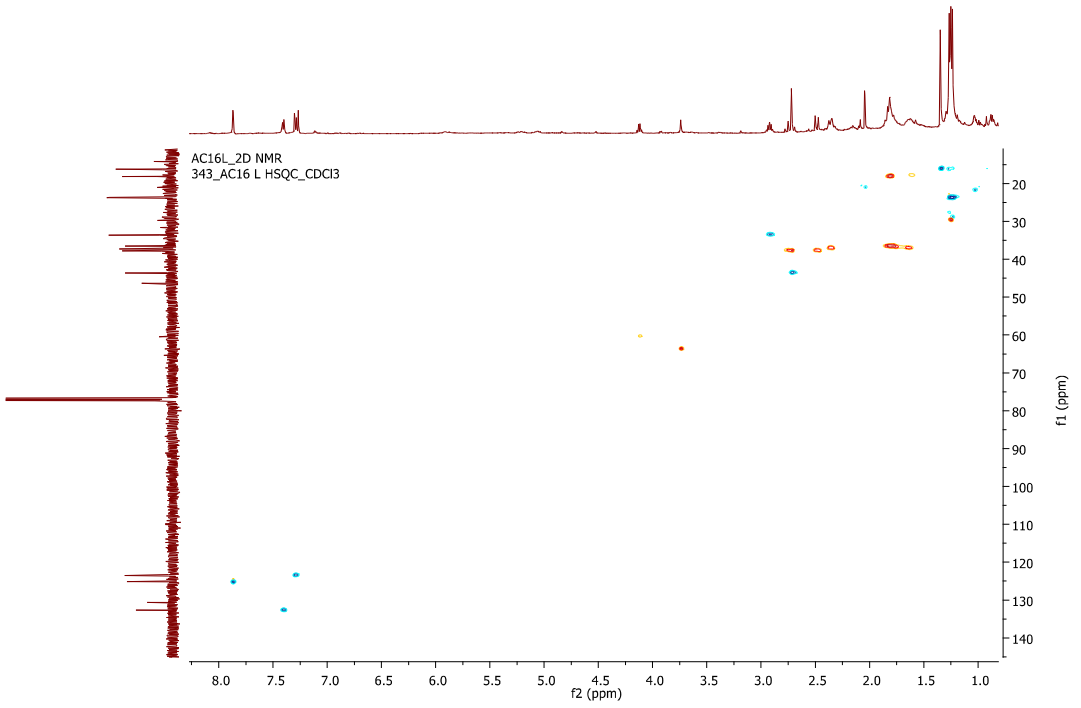


Figure S21. HSQC NMR spectrum of 7-ketodehydroabietic acid

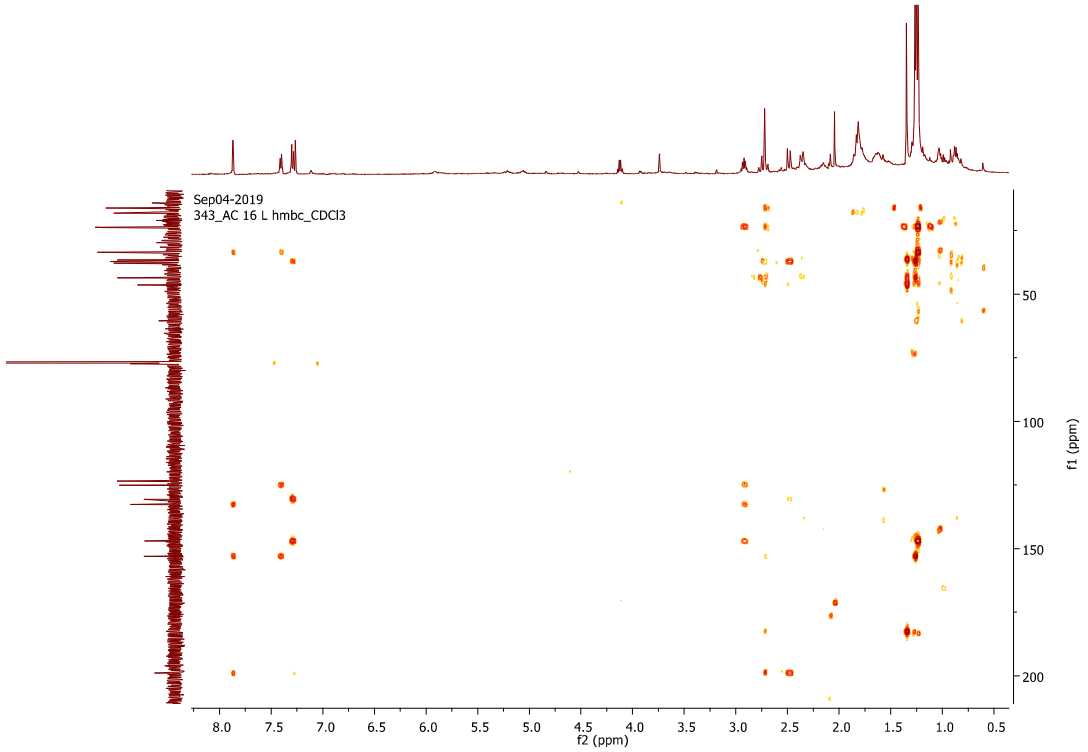


Figure S22. HMBC NMR spectrum of 7-ketodehydroabietic acid

S11. MS and NMR data of Sandaracopimarinol acetate

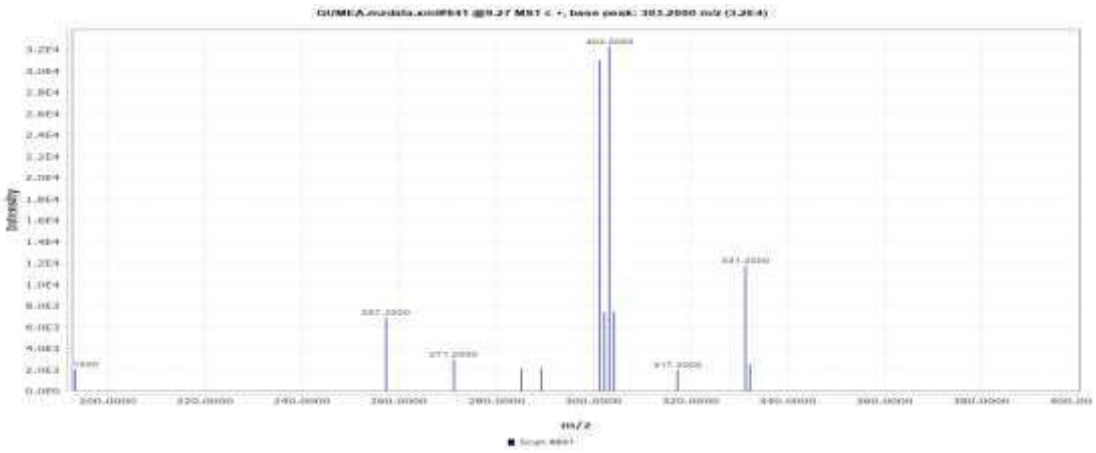


Figure S23. MS spectra of sandaracopimarinol acetate

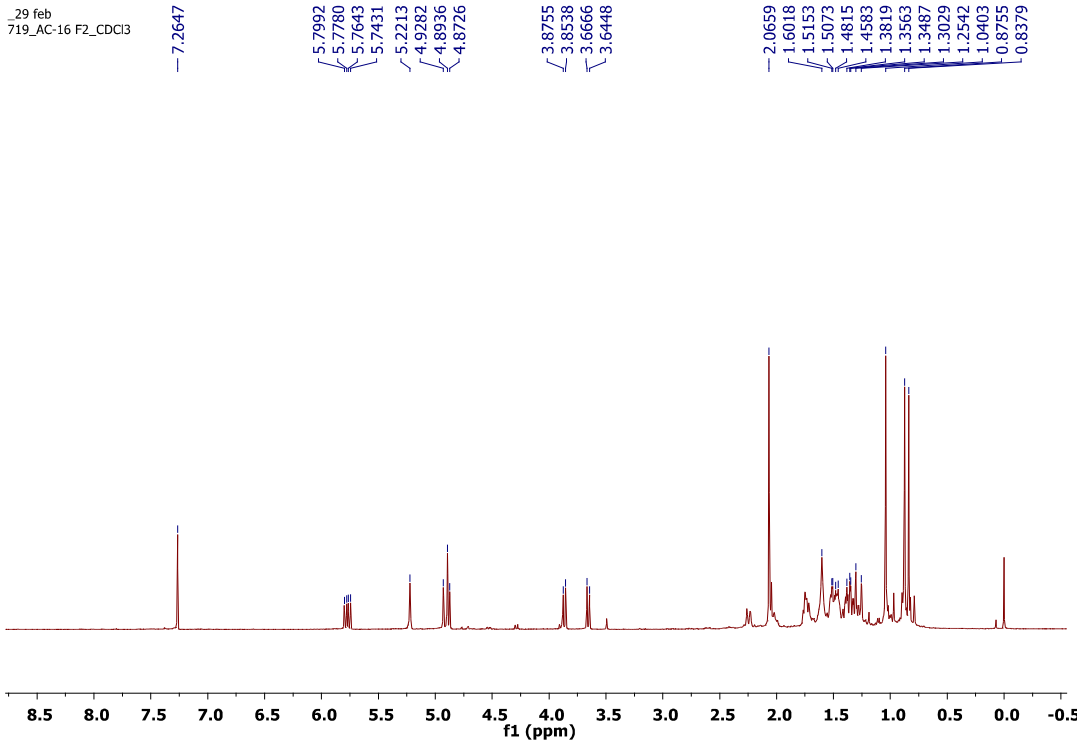


Figure S24. ^{1}H-NMR spectrum of sandaracopimarinol acetate

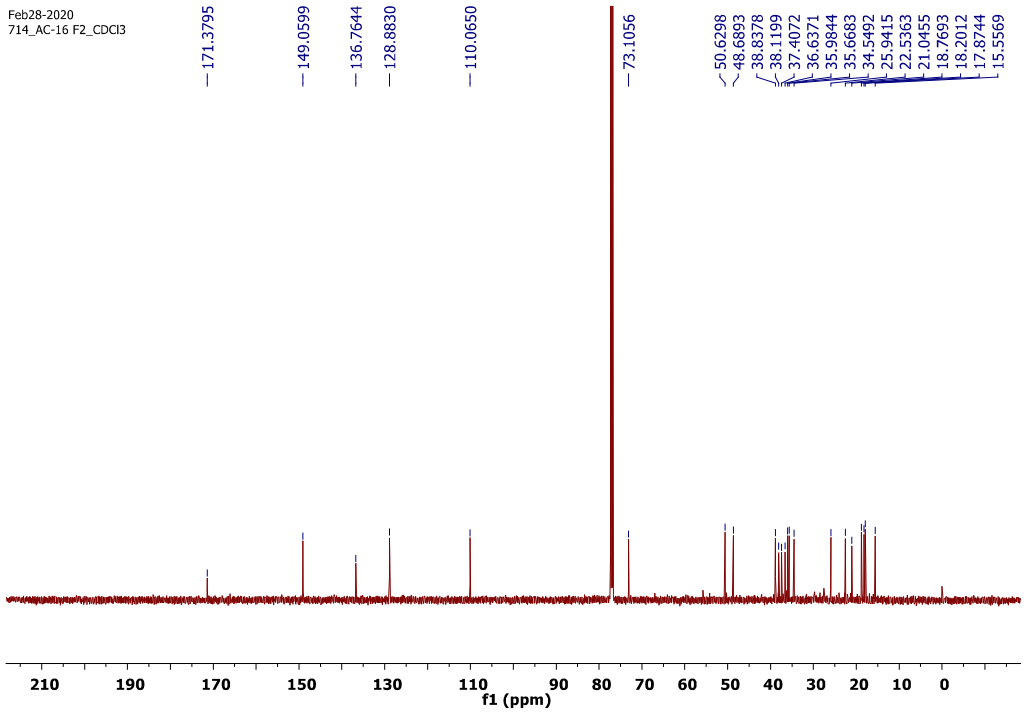


Figure S25. ^{13}C-NMR spectrum of sandaracopimarinol acetate

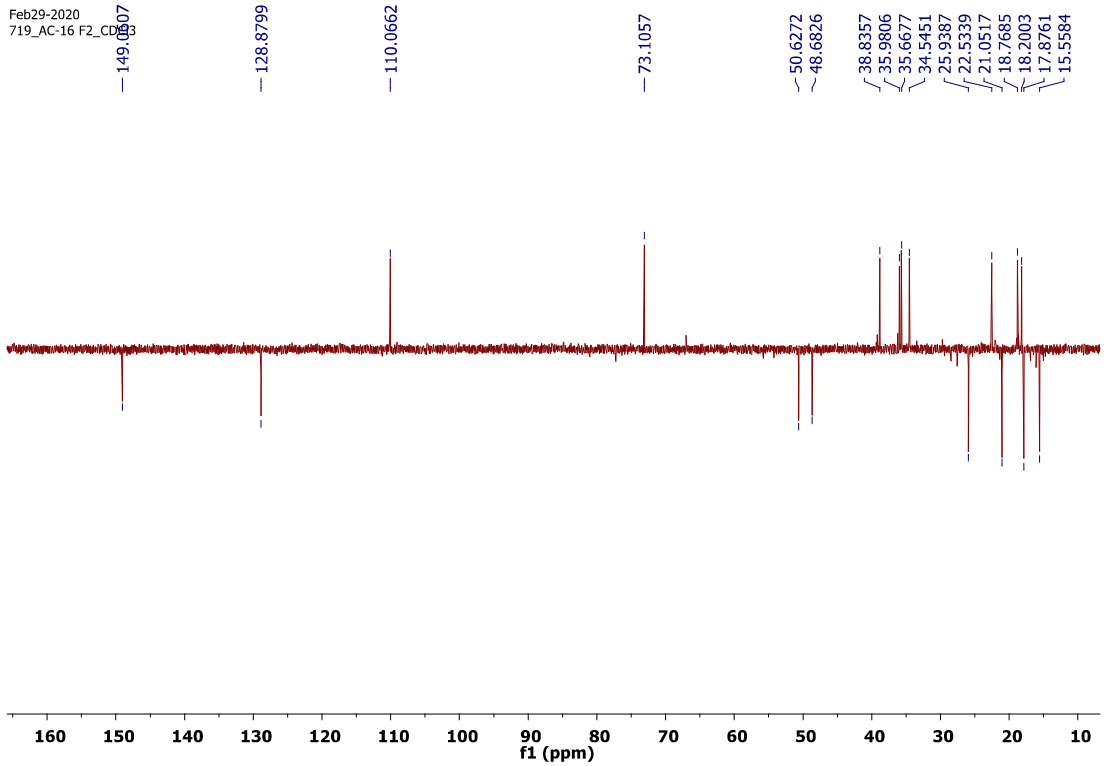


Figure S26. DEPT-135 NMR spectrum of sandaracopimarinol acetate

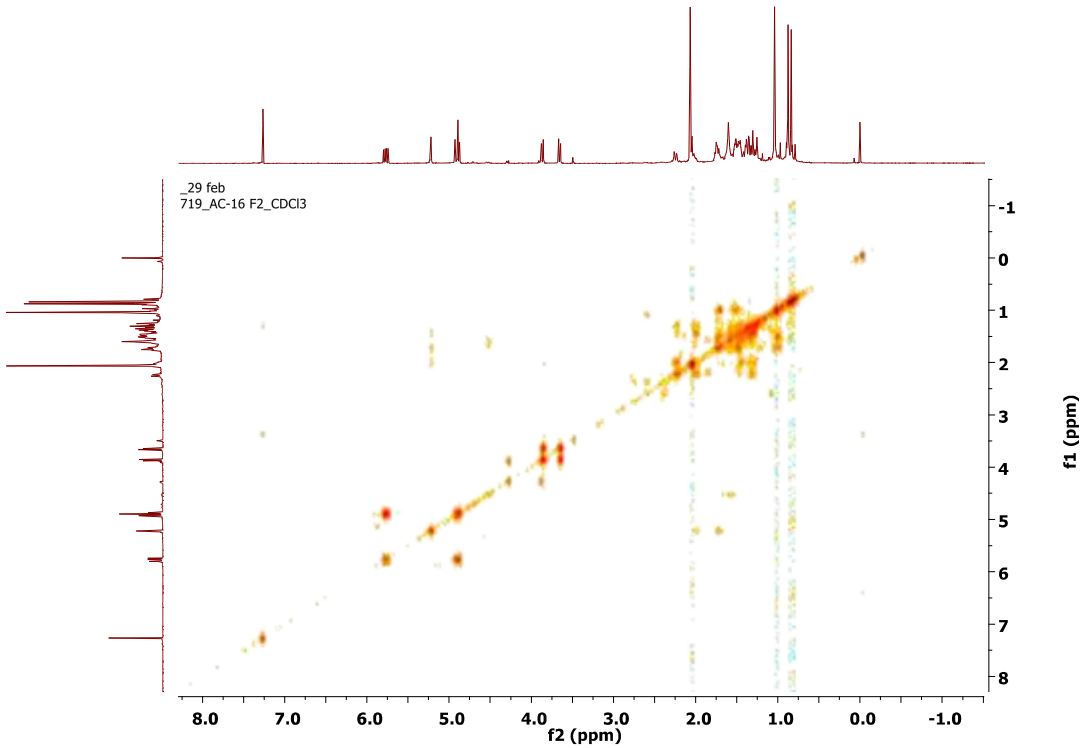


Figure S27. ^{1}H-^{1}H COSY NMR spectrum of sandaracopimarinol acetate

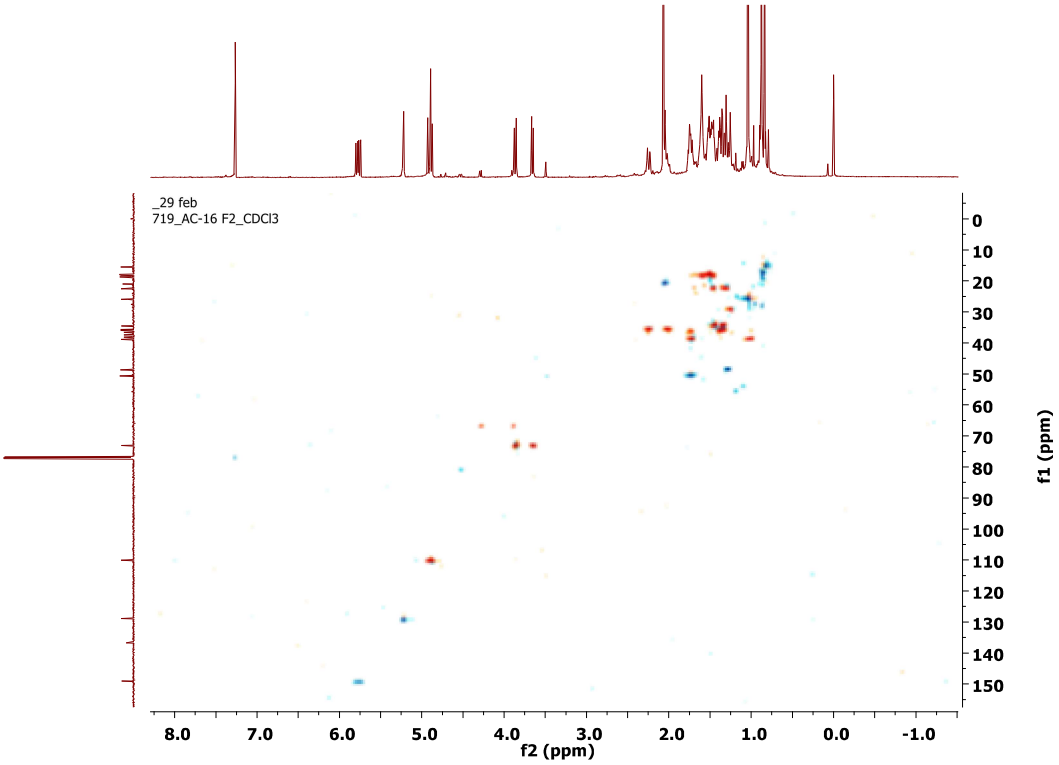


Figure S28. HSQC spectrum of sandaracopimarinol acetate

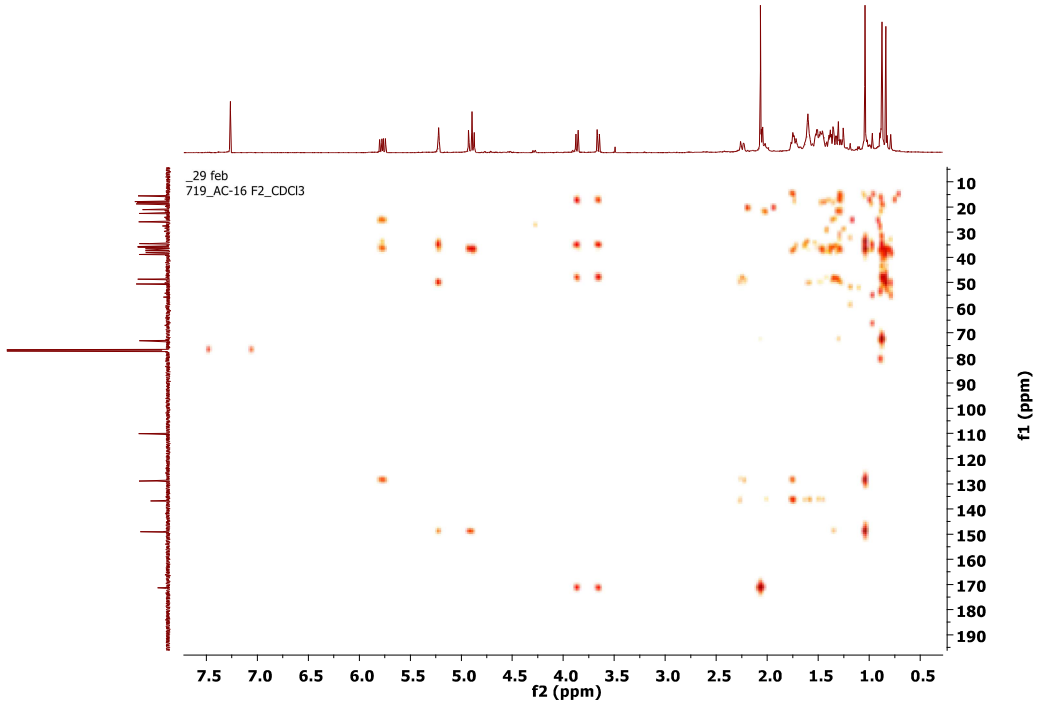


Figure S29. HMBC spectrum of sandaracopimarinol acetate

S12. MS data of Sandaracopimarinol

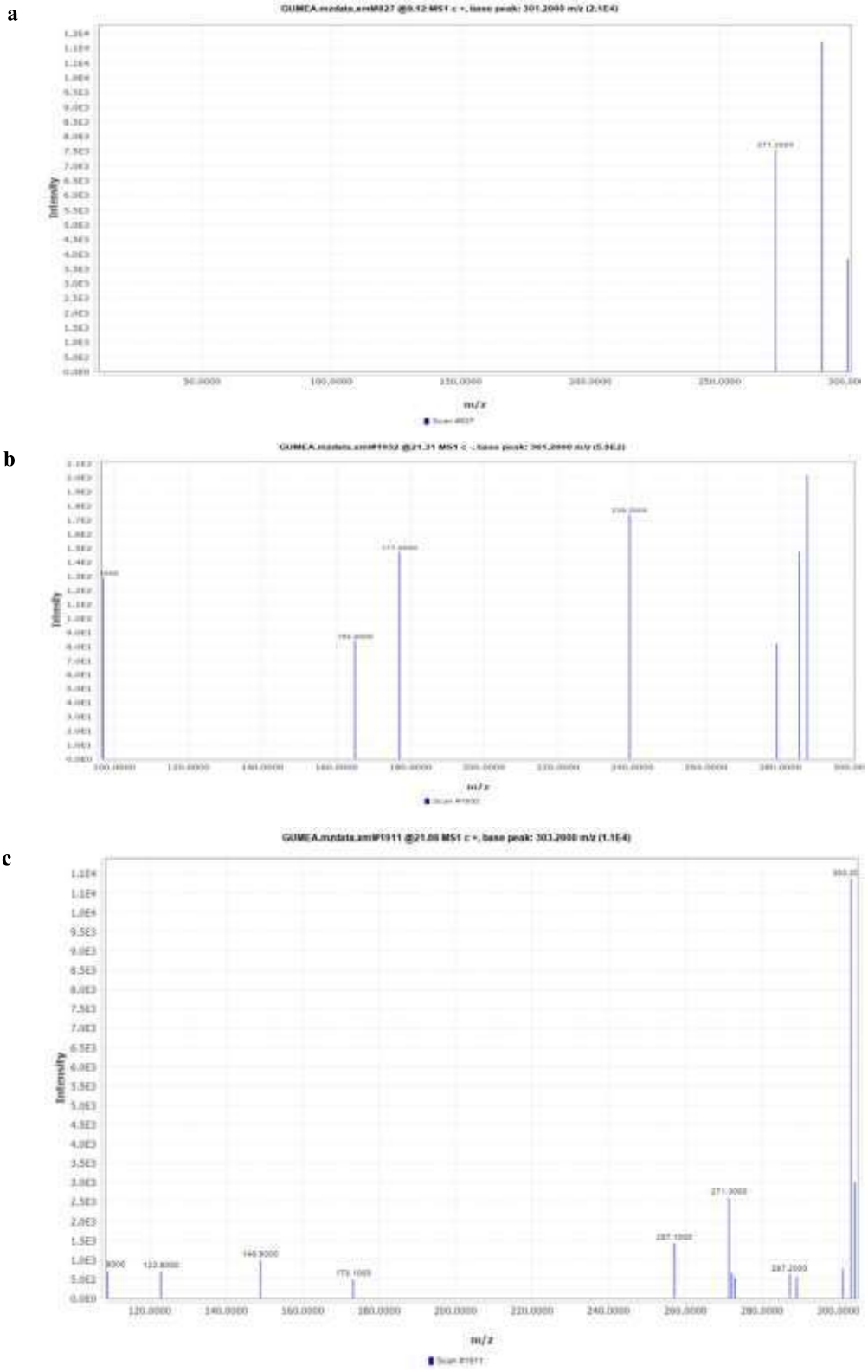
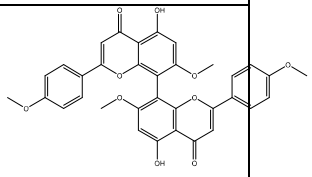


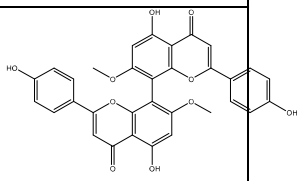
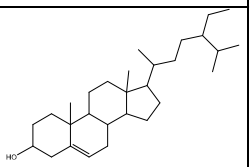
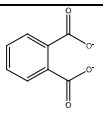
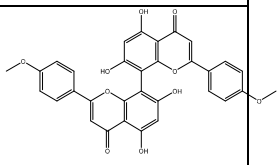
Figure S30. MS data of Sandaracopimarinol

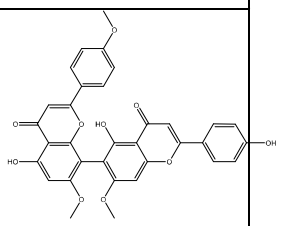
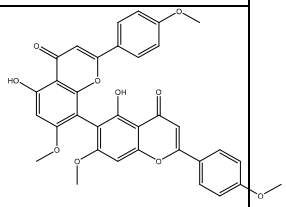
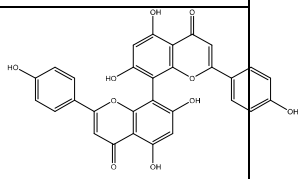
Table 1: List of all the top 20 screened genes

SI no	Compound code	Top genes
1	AC1	APP, PIK3R1, VRK2, CSNK2A1, CA10, PPARG, TOP1, CYP19A1, EDNRB, CDK17, VEGFA, DAPK1, CXCL12, GSK3B, AHR, CDK18, ESR1, PLK1, PYGL, CDK6
2	AC2	APP, EGFR, VRK2, CSNK2A1, NTRK2, CYP19A1 CA10, CHEK1, PPARG, ESR1, DAPK1, VEGFA, NEK6, KIT, PIM1, BCL2, CDK6, TPN1, GSK3B, ABCG2
3	AC3	APP, GRIN2A, ESR1, SRC, CYP27A1, PRKCE, RORA, EPHA4, MAPK3, IGF1R, AVPR1A, EPHA1, AGTR1, CYP19A1, SCD, EPHB2, NR3C1, PRKCH, TACR1, RXRG
4	AC4	PPARG, ESR1, PRL, CYP19A1, FN1, RGS6, PPARGC1A, AHR, NR3C1, MED1, GSN, HAAO, NR1H4, AR, NR1H3, FGF12, NCOA1, FGF9, DPF3, NCOR1
5	AC5	APP, EGFR, CYP19A1, NTRK2, GPR35, DAPK1, VRK2, ESR1, OPRD1, CA10, ADRA2C, CHEK1, CSNK2A1, ADRA2A, HTR1D, PIK3CA, AHR, CHRM2, DRD5, XDH
6	AC6	PIK3R1, APP, CSNK2A1, TOP1, DAPK1, PPARG, ABCB1, PYGL, HIF1A, CTSK, VEGFA, SYK, ESR1, PIK3CG, PTPN1, AHR, XDH, OPRD1, PTGS1, PDE5A
7	AC7	APP, EGFR, PIK3R1, TOP1, DAPK1, CSNK2A1, KDR, CYP19A1, PTPN1, VEGFA, PPARG, SYK, IGF1, ESR1, ABCB1, AHR, KIT, SRC, CTSK, PYGL

Table 2: Metabolites selected for network pharmacology

Sl no		Cannonical SMILES	Formula and (pubchem ID)	Structure
AC1	Cuppresuflavone-4',4''',7,7'' tetramethoxy or WB1: Identified by LC-HRMS and Database mining Isolation and characterization by 2DNMR Networkpharmacology	O=C1C=C(OC2=C1C(O)=CC(OC)=C2C=3C(OC)=CC(O)=C4C(=O)C=C(OC43)C=5C=CC(OC)=CC5)C=6C=CC(OC)=CC6	$C_{34}H_{26}O_{10}$	

	In-vitro cytotoxicity			
AC2	Cuppresuflavone-7,7''-dimethoxy: Identified by LC-HRMS and Database mining Isolation and characterization by NMR Networkpharmacology In-vitro cytotoxicity	COC1=C(C2=C(C(=C1)O)C(=O)C=C(O2)C3=CC=C(C=C3)O)C4=C(C=C(C5=C4OC(=CC5=O)C6=CC=C(C=C6)O)O)OC	$C_{32}H_{22}O_{10}$ 5316884	
AC3	beta-sitosterol: A very common phytoconstituents - Identified by LC-HRMS and Database mining Isolation and characterization by NMR Network pharmacology	CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C	$C_{29}H_{50}O$ 222284	
AC4	Phathalate Identified by LC-HRMS and Database mining Isolation and characterization by NMR	C1=CC=C(C(=C1)C(=O)[O-])C(=O)[O-]	$C_8H_4O_4$	
AC5	Cuppresuflavone-4',4'''-dimethoxy or W11 Identified by LC-HRMS and Database mining	COC1=CC=C(C=C1)C2=CC(=O)C3=C(O2)C(=C(C=C3O)O)C4=C(C=C(C5=C4OC(=CC5=O)C6=CC=C(C=C6)OC)O)O	$C_{32}H_{22}O_{10}$ 14015870	

	Isolation and characterization by NMR Networkpharmacology In-vitro cytotoxicity			
AC6	Agathisflavone 4'",7,7"-trimethyl ether Identified by LC-HRMS and Database mining Networkpharmacology	COC1=CC=C(C=C1)C2=CC(=O)C3=C(O2)C(=C(C=C3O)OC)C4=C(C=C5C(=C4O)C(=O)C=C(O5)C6=CC=C(C=C6)O)OC	$C_{33}H_{24}O_{10}$ 101423563	
AC7	Agathisflavone 4',4'",7,7"-tetramethyl ether Identified by LC-HRMS and Database mining Networkpharmacology	COC1=CC=C(C=C1)C2=CC(=O)C3=C(C(=C(C=C3O2)OC)C4=C(C=C(C5=C4OC(=CC5=O)C6=CC=C(C=C6)OC)O)OC)O	$C_{34}H_{26}O_{10}$ 101921612	
AC8	Cupressuflavone Identified by LC-HRMS and Database mining Isolation and characterization: No Networkpharmacology: Rejected in ADME analysis	C1=CC(=CC=C1C2=CC(=O)C3=C(O2)C(=C(C=C3O)O)C4=C(C=C(C5=C4OC(=CC5=O)C6=CC=C(C=C6)O)O)O)O	$C_{30}H_{18}O_{10}$ 5281609	

List of Publications

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List of publications from thesis

1. **Sahu B**, Bhardwaj N, Chatterjee E, Dey B, Tripathi N, Goel B, Kushwaha M, Kumar B, Singh B, Guru SK, Jain SK. LC-MS-DNP based dereplication of Araucaria cunninghamii Mudie gum-resin: identification of new cytotoxic labdane diterpene. **Nat Prod Res. 2022** Dec;36(24):6207-6214. doi: 10.1080/14786419.2021.2024530. Epub 2022 Jan 4. PMID: 36463507.
2. **Sahu B**, Chakrabarty S, Saini V, Kandpal M, Goel B, Kumari S, Ahmed I, Jha HC, Jain SK. Exploring the cytotoxic potential of biflavones of Araucaria cunninghamii: Precise identification combined by LC-HRMS-metabolomics and database mining, targeted isolation, network pharmacology, in vitro cytotoxicity, and docking studies. **Chem Biol Drug Des. 2024** Jun;103(6):e14564. doi: 10.1111/cbdd.14564. PMID: 38845574.

List of publications from other work

3. Bhardwaj, N., Goel, B., Tripathi, N., **Sahu, B**. and Jain, S.K., 2022. A comprehensive review on chemistry and pharmacology of marine bioactives as antimetastatic agents. ***European Journal of Medicinal Chemistry Reports***, *4*, p.100023.
4. Ganeshpurkar A, Singh R, Kumar D, Gutti G, Gore P, **Sahu B**, Kumar A, Singh SK. Identification of sulfonamide-based butyrylcholinesterase inhibitors using

machine learning. **Future Med Chem**. 2022 Jul;14(14):1049-1070. doi: 10.4155/fmc-2021-0325. Epub 2022 Jun 16. PMID: 35707942.

5. Goel B, Sharma A, Tripathi N, Bhardwaj N, **Sahu B**, Kaur G, Singh B, Jain SK. *In-vitro* antitumor activity of compounds from *Glycyrrhiza glabra* against C6 glioma cancer cells: identification of natural lead for further evaluation. **Nat Prod Res**. **2021** Dec;35(23):5489-5492. doi: 10.1080/14786419.2020.1786830. Epub 2020 Jul 1. PMID: 32608261.