References

References

1. Verpoorte, R., *Exploration of nature's chemodiversity: the role of secondary metabolites as leads in drug development.* Drug Discov. Today, 1998. **3**(5): p. 232-238.
2. Newman, D.J. and Cragg, G.M., *Natural Products as Sources of New Drugs over the Nearly Four Decades from 01/1981 to 09/2019.* J. Nat. Prod., 2020. **83**(3): p. 770-803.
3. Atanasov, A.G., Zotchev, S.B., Dirsch, V.M., Orhan, I.E., Banach, M., Rollinger, J.M., Barreca, D., et al., *Natural products in drug discovery: advances and opportunities.* Nat. Rev. Drug Discov., 2021. **20**(3): p. 200-216.
4. Wang, S., Fang, K., Dong, G., Chen, S., Liu, N., Miao, Z., Yao, J., et al., *Scaffold Diversity Inspired by the Natural Product Evodiamine: Discovery of Highly Potent and Multitargeting Antitumor Agents.* J. Med. Chem., 2015. **58**(16): p. 6678-6696.
5. Barnes, E. C., Kumar, R., and Davis, R.A., *The use of isolated natural products as scaffolds for the generation of chemically diverse screening libraries for drug discovery.* Nat. Prod. Rep., 2016. **33**(3): p. 372-381.
6. Schuman, M. C., Van Dam, N. M., Beran, F., and Harpole, W.S., *How does plant chemical diversity contribute to biodiversity at higher trophic levels?* Curr. Opin. Insect Sci., 2016. **14**: p. 46-55.
7. Hong, J., *Role of natural product diversity in chemical biology.* Curr Opin Chem Biol, 2011. **15**(3): p. 350-354.
8. Lautie, E., Russo, O., Ducrot, P., and Boutin, J.A., *Unraveling Plant Natural Chemical Diversity for Drug Discovery Purposes.* Front. Pharmacol., 2020. **11**.
9. Wilson, D.M., Driedger, D.J., Liu, D.Y., Keerthisinghe, S., Hermann, A., Bieniossek, C., Linington, R.G., et al., *Targeted sampling of natural product space to identify bioactive natural product-like polyketide macrolides.* Nat. Commun., 2024. **15**(1): p. 2534.
10. Zhang, Q.W., Lin, L.-G., and Ye, W.C., *Techniques for extraction and isolation of natural products: a comprehensive review.* Chin. Med, 2018. **13**(1): p. 20.
11. Abdelmohsen, U.R., Sayed, A.M., and Elmaidomy, A.H., *Natural Products' Extraction and Isolation-Between Conventional and Modern Techniques.* Front. Nat. Prod, 2022. **1**.

12. Nasim, N., Sandeep, I.S., and Mohanty, S., *Plant-derived natural products for drug discovery: current approaches and prospects.* The Nucleus, 2022. **65**(3): p. 399-411.
13. Ito, T. and Masubuchi, M., *Dereplication of microbial extracts and related analytical technologies.* J. Antibiot., 2014. **67**(5): p. 353-360.
14. Hubert, J., Nuzillard, J.-M., and Renault, J.-H., *Dereplication strategies in natural product research: How many tools and methodologies behind the same concept?* Phytochem. Rev., 2017. **16**(1): p. 55-95.
15. Michel, C.G., Nesseem, D.I., El-Alfy, T.S., El-Dine, N.S., Fahmy, S.M., and Ezzat, S.M., *Formulation of herbal drugs.* Planta Med, 2013. **79**(13): p. PN64.
16. Potterat, O. and Hamburger, M., *Concepts and technologies for tracking bioactive compounds in natural product extracts: generation of libraries, and hyphenation of analytical processes with bioassays.* Nat. Prod. Rep., 2013. **30**(4): p. 546-564.
17. Johansen, K.T., Wubshet, S.G., and Nyberg, N.T., *HPLC–NMR Revisited: Using Time-Slice High-Performance Liquid Chromatography–Solid-Phase Extraction–Nuclear Magnetic Resonance with Database-Assisted Dereplication.* Anal. Chem., 2013. **85**(6): p. 3183-3189.
18. Hasada, K., Yoshida, T., Yamazaki, T., Sugimoto, N., Nishimura, T., Nagatsu, A., and Mizukami, H., *Quantitative determination of atractylon in Atractylodis Rhizoma and Atractylodis Lanceae Rhizoma by 1H-NMR spectroscopy.* J. Nat. Med., 2010. **64**(2): p. 161-166.
19. Nielsen, K.F. and Smedsgaard, J., *Fungal metabolite screening: database of 474 mycotoxins and fungal metabolites for dereplication by standardised liquid chromatography–UV–mass spectrometry methodology.* J. Chromatogr. A, 2003. **1002**(1): p. 111-136.
20. Carnevale Neto, F., Pilon, A.C., Selegato, D.M., Freire, R.T., Gu, H., Raftery, D., Lopes, N.P., et al., *Dereplication of Natural Products Using GC-TOF Mass Spectrometry: Improved Metabolite Identification by Spectral Deconvolution Ratio Analysis.* Front. Mol. Biosci., 2016. **3**.
21. Spring, O., Buschmann, H., Vogler, B., Schilling, E.E., Spraul, M., and Hoffmann, M., *Sesquiterpene lactone chemistry of Zaluzania grayana from on-line LC-NMR measurements.* Phytochemistry, 1995. **39**(3): p. 609-612.
22. Corcoran, O. and Spraul, M., *LC–NMR–MS in drug discovery.* Drug Discov Today, 2003. **8**(14): p. 624-631.

23. Konishi, Y., Kiyota, T., Draghici, C., Gao, J.-M., Yeboah, F., Acoca, S., Jarussophon, S., et al., *Molecular Formula Analysis by an MS/MS/MS Technique To Expedite Dereplication of Natural Products.* Anal. Chem., 2007. **79**(3): p. 1187-1197.
24. Ridder, L., van der Hooft, J.J.J., Verhoeven, S., de Vos, R.C.H., Bino, R.J., and Vervoort, J., *Automatic Chemical Structure Annotation of an LC–MSn Based Metabolic Profile from Green Tea.* Anal. Chem., 2013. **85**(12): p. 6033-6040.
25. Gaudencio, S.P., Bayram, E., Lukić Bilela, L., Cueto, M., Díaz-Marrero, A.R., Haznedaroglu, B.Z., Jimenez, C., et al. *Advanced Methods for Natural Products Discovery: Bioactivity Screening, Dereplication, Metabolomics Profiling, Genomic Sequencing, Databases and Informatic Tools, and Structure Elucidation*. Mari. Drugs, 2023. **21**.
26. Banerjee, P., Erehman, J., Gohlke, B.-O., Wilhelm, T., Preissner, R., and Dunkel, M., *Super Natural II—a database of natural products.* Nucleic Acids Res., 2015. **43**(D1): p. D935-D939.
27. Chassagne, F., Cabanac, G., Hubert, G., David, B., and Marti, G., *The landscape of natural product diversity and their pharmacological relevance from a focus on the Dictionary of Natural Products®.* Phytochem. Rev., 2019. **18**(3): p. 601-622.
28. Wang, M., Carver, J.J., Phelan, V.V., Sanchez, L.M., Garg, N., Peng, Y., Nguyen, D.D., et al., *Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking.* Nat. Biotechnol., 2016. **34**(8): p. 828-837.
29. Gotthardt, M., Kanawati, B., Schmidt, F., Asam, S., Hammerl, R., Frank, O., Hofmann, T., et al., *Comprehensive Analysis of the Alternaria Mycobolome Using Mass Spectrometry Based Metabolomics.* Mol. Nutr. Food Res., 2020. **64**(3): p. 1900558.
30. Guijas, C., Montenegro-Burke, J.R., Domingo-Almenara, X., Palermo, A., Warth, B., Hermann, G., Koellensperger, G., et al., *METLIN: A Technology Platform for Identifying Knowns and Unknowns.* Anal. Chem., 2018. **90**(5): p. 3156-3164.
31. Baker, D.D., Chu, M., Oza, U., and Rajgarhia, V., *The value of natural products to future pharmaceutical discovery.* Nat. Prod. Rep., 2007. **24**(6): p. 1225-1244.
32. Tsugawa, H., Rai, A., Saito, K., and Nakabayashi, R., *Metabolomics and complementary techniques to investigate the plant phytochemical cosmos.* Nat. Prod. Rep., 2021. **38**(10): p. 1729-1759.

33. Lang, G., Mayhudin, N.A., Mitova, M.I., Sun, L., van der Sar, S., Blunt, J.W., Cole, A.L.J., et al., *Evolving Trends in the Dereplication of Natural Product Extracts: New Methodology for Rapid, Small-Scale Investigation of Natural Product Extracts.* J. Nat. Prod., 2008. **71**(9): p. 1595-1599.
34. Tawfike, A.F., Viegelmann, C., and Edrada-Ebel, R., *Metabolomics and Dereplication Strategies in Natural Products*, in *Metabolomics Tools for Natural Product Discovery: Methods and Protocols*. 2013, Humana Press: Totowa, NJ. p. 227-244.
35. Gaudencio, S.P. and Pereira, F., *Dereplication: racing to speed up the natural products discovery process.* Nat. Prod. Rep., 2015. **32**(6): p. 779-810.
36. Yang, J.Y., Sanchez, L.M., Rath, C.M., Liu, X., Boudreau, P.D., Bruns, N., Glukhov, E., et al., *Molecular Networking as a Dereplication Strategy.* J.Nat Prod., 2013. **76**(9): p. 1686-1699.
37. Corley, D.G. and Durley, R.C., *Strategies for Database Dereplication of Natural Products.* J. Nat. Prod., 1994. **57**(11): p. 1484-1490.
38. Sashidhara, K.V. and Rosaiah, J.N., *Various Dereplication Strategies Using LC-MS for Rapid Natural Product Lead Identification and Drug Discovery.* Nat. Prod. Commun, 2007. **2**(2): p. 1934578X0700200218.
39. Cuthbertson, D.J., Johnson, S.R., Piljac-Zegarac, J., Kappel, J., Schäfer, S., Wüst, M., Ketchum, R.E.B., et al., *Accurate mass–time tag library for LC/MS-based metabolite profiling of medicinal plants.* Phytochemistry, 2013. **91**: p. 187-197.
40. Whittle, M., Willett, P., Klaffke, W., and van Noort, P., *Evaluation of Similarity Measures for Searching the Dictionary of Natural Products Database.* J. Chem. Inf. Comput. Sci., 2003. **43**(2): p. 449-457.
41. Kushwaha, M., Qayum, A., Sharma, N., Abrol, V., Choudhary, P., Murtaza, M., Singh, S.K., et al., *LC–PDA–MS/MS-Based Dereplication Guided Isolation of a New Optical Isomer of 19,20-Epoxycytochalasin-N and Its Cytotoxic Activity.* ACS Omega, 2022. **7**(33): p. 29135-29141.
42. Sorokina, M. and Steinbeck, C., *Review on natural products databases: where to find data in 2020.* J. Cheminform., 2020. **12**(1): p. 20.
43. Chervin, J., Stierhof, M., Tong, M.H., Peace, D., Hansen, K.O., Urgast, D.S., Andersen, J.H., et al., *Targeted Dereplication of Microbial Natural Products by High-Resolution MS and Predicted LC Retention Time.* J. Nat. Prod., 2017. **80**(5): p. 1370-1377.

44. Perez de Souza, L., Alseekh, S., Scossa, F., and Fernie, A.R., *Ultra-high-performance liquid chromatography high-resolution mass spectrometry variants for metabolomics research.* Nat. Methods, 2021. **18**(7): p. 733-746.

45. Wolfender, J.-L., Marti, G., Thomas, A., and Bertrand, S., *Current approaches and challenges for the metabolite profiling of complex natural extracts.* J. Chromatogr. A, 2015. **1382**: p. 136-164.

46. Allard, P.-M., Péresse, T., Bisson, J., Gindro, K., Marcourt, L., Pham, V.C., Roussi, F., et al., *Integration of Molecular Networking and In-Silico MS/MS Fragmentation for Natural Products Dereplication.* Anal. Chem., 2016. **88**(6): p. 3317-3323.

47. Mahrous, E.A. and Farag, M.A., *Two dimensional NMR spectroscopic approaches for exploring plant metabolome: A review.* J. Adv. Res, 2015. **6**(1): p. 3-15.

48. Buevich, A.V., Williamson, R.T., and Martin, G.E., *NMR Structure Elucidation of Small Organic Molecules and Natural Products: Choosing ADEQUATE vs HMBC.* J. Nat. Prod., 2014. **77**(8): p. 1942-1947.

49. Kwan, E.E. and Huang, S.G., *Structural Elucidation with NMR Spectroscopy: Practical Strategies for Organic Chemists.* Eur. J. Org. Chem., 2008. **2008**(16): p. 2671-2688.

50. Li, X.-C., Ferreira, D., and Ding, Y., *Determination of Absolute Configuration of Natural Products: Theoretical Calculation of Electronic Circular Dichroism as a Tool.* Curr. Org. Chem., 2010. **14**(16): p. 1678-1697.

51. Mazzeo, G., Cimmino, A., Masi, M., Longhi, G., Maddau, L., Memo, M., Evidente, A., et al., *Importance and Difficulties in the Use of Chiroptical Methods to Assign the Absolute Configuration of Natural Products: The Case of Phytotoxic Pyrones and Furanones Produced by Diplodia corticola.* J. Nat. Prod., 2017. **80**(9): p. 2406-2415.

52. Hosoi, S., Serata, J., Kiuchi, F., Sakushima, A., and Ohta, T., *Advanced Method for Assignment of Absolute Configuration Utilizing an Induced CD and Computational Technique: Its Application to Natural Products Possessing a Secondary Alcohol.* J. Nat. Prod., 2004. **67**(9): p. 1568-1570.

53. Neuhaus, G.F., Adpressa, D.A., Bruhn, T., and Loesgen, S., *Polyketides from Marine-Derived Aspergillus porosus: Challenges and Opportunities for Determining Absolute Configuration.* J. Nat. Prod., 2019. **82**(10): p. 2780-2789.

54. Bodare, S., Ravikanth, G., Ismail, S.A., Patel, M.K., Spanu, I., Vasudeva, R., Shaanker, R.U., et al., *Fine- and local- scale genetic structure of Dysoxylum malabaricum, a late-successional canopy tree species in disturbed forest patches in the Western Ghats, India.* Conserv. Genet., 2017. **18**(1): p. 1-15.
55. Nugroho, A.E., Momota, T., Sugiura, R., Hanzawa, M., Yajima, E., Nagakura, Y., Yasuda, N., et al., *Dysotriflorins A–M, triterpenoids from Dysoxylum densiflorum.* Tetrahedron, 2014. **70**(51): p. 9661-9667.
56. Adesanya, S.A., Païs, M., Sévenet, T., and Cosson, J.P., *Apotirucallane Triterpenes from Dysoxylum roseum.* J. Nat. Prod., 1991. **54**(6): p. 1588-1594.
57. Aladesanmi, A.J., Kelley, C.J., and Leary, J.D., *The Constituents of Dysoxylum lenticellare. I. Phenylethylisoquinoline, Homoerythrina, and Dibenzazecine Alkaloids.* J. Nat. Prod., 1983. **46**(1): p. 127-131.
58. Kashiwada, Y., Fujioka, T., Chang, J.J., Chen, I.S., Mihashi, K., and Lee, K.H., *Anti-tumor agents. 136. Cumingianosides A-F, potent antileukemic new triterpene glucosides, and cumindysosides A and B, trisnor- and tetranortriterpene glucosides with a 14,18-cycloapoeuphane-type skeleton from Dysoxylum cumingianum.* J. Org. Chem, 1992. **57**(25): p. 6946-6953.
59. Sofian, F.F., Subarnas, A., Hakozaki, M., Uesugi, S., Koseki, T., and Shiono, Y., *Bidysoxyphenols A–C, dimeric sesquiterpene phenols from the leaves of Dysoxylum parasiticum (Osbeck) Kosterm.* Fitoterapia, 2022. **158**: p. 105157.
60. Singh, S., Garg, H.S., and Khanna, N.M., *Dysobinin, a new tetranortriterpene from Dysoxylum binectariferum.* Phytochem., 1976. **15**(12): p. 2001-2002.
61. Huang, H.-L., Wang, C.-M., Wang, Z.-H., Yao, M.-J., Han, G.-T., Yuan, J.-C., Gao, K., et al., *Tirucallane-Type Triterpenoids from Dysoxylum lenticellatum.* J. Nat. Prod., 2011. **74**(10): p. 2235-2242.
62. Aalbersberg, W. and Singh, Y., *Dammarane triterpenoids from Dysoxylum richii.* Phytochemistry, 1991. **30**(3): p. 921-926.
63. Luo, X.-D., Wu, S.-H., Ma, Y.-B., and Wu, D.-G., *Tirucallane triterpenoids from Dysoxylum hainanense.* Phytochemistry, 2000. **54**(8): p. 801-805.
64. Mohamad, K., Martin, M.-T., Litaudon, M., Gaspard, C., Sévenet, T., and Païs, M., *Tirucallane triterpenes from Dysoxylum macranthum.* Phytochemistry, 1999. **52**(8): p. 1461-1468.

65. Zhou, B., Shen, Y., Wu, Y., Leng, Y., and Yue, J.-M., *Limonoids with 11β-Hydroxysteroid Dehydrogenase Type 1 Inhibitory Activities from Dysoxylum mollissimum.* J. Nat. Prod., 2015. **78**(8): p. 2116-2122.

66. Chen, J.L., Kernan, M.R., Jolad, S.D., Stoddart, C.A., Bogan, M., and Cooper, R., *Dysoxylins A−D, Tetranortriterpenoids with Potent Anti-RSV Activity from Dysoxylum gaudichaudianum.* J. Nat. Prod., 2007. **70**(2): p. 312-315.

67. Lakshmi, V., Pandey, K., and Agarwal, S.K., *Bioactivity of the compounds in genus Dysoxylum.* Acta Ecol. Sin., 2009. **29**(1): p. 30-44.

68. Lakshmi, V., Pandey, K., Kapil, A., Singh, N., Samant, M., and Dube, A., *In vitro and in vivo leishmanicidal activity of Dysoxylum binectariferum and its fractions against Leishmania donovani.* Phytomedicine, 2007. **14**(1): p. 36-42.

69. Jiang, K., Chen, L.-L., Wang, S.-F., Wang, Y., Li, Y., and Gao, K., *Anti-inflammatory Terpenoids from the Leaves and Twigs of Dysoxylum gotadhora.* J. Nat. Prod., 2015. **78**(5): p. 1037-1044.

70. Kumar, V., Gupta, M., Gandhi, S.G., Bharate, S.S., Kumar, A., Vishwakarma, R.A., and Bharate, S.B., *Anti-inflammatory chromone alkaloids and glycoside from Dysoxylum binectariferum.* Tetrahedron Lett., 2017. **58**(42): p. 3974-3978.

71. Yan, H.J., Wang, J.S., and Kong, L.Y., *Cytotoxic Dammarane-Type Triterpenoids from the Stem Bark of Dysoxylum binecteriferum.* J. Nat. Prod., 2014. **77**(2): p. 234-242.

72. Dharmayani, N.K.T., Juliawaty, L.D., and Syah, Y.M., *Three Tetracyclic Triterpenoic Acids from Dysoxylum densiflorum and Their Antibacterial Activities.* Nat. Prod. Commun., 2016. **11**(8): p. 1934578X1601100812.

73. Hu, J., Song, Y., Li, H., Mao, X., Zhao, Y., Shi, X., and Yang, B., *Antibacterial and cytotoxic triterpenoids from the ethanol extract of Dysoxylum densiflorum (Blume) Miq.* Phytochem. Lett., 2014. **10**: p. 219-223.

74. Hu, J., Song, Y., Li, H., Yang, B., Mao, X., Zhao, Y., and Shi, X., *Cytotoxic and anti-inflammatory tirucallane triterpenoids from Dysoxylum binectariferum.* Fitoterapia, 2014. **99**: p. 86-91.

75. Naini, A.A., Mayanti, T., and Supratman, U., *Triterpenoids from Dysoxylum genus and their biological activities.* Arch. Pharm. Res., 2022. **45**(2): p. 63-89.

76. Wang, J.-N., Zhang, Z.-Y., Sun, P., Cao, D.-H., Xiao, Y.-D., Shi, X.-C., Xiao, C.-F., et al., *Four new steroids from the leaves and twigs of Dysoxylum pallens and their cytotoxic activities.* Fitoterapia, 2020. **146**: p. 104696.

77. Jain, S.K., Meena, S., Gupta, A.P., Kushwaha, M., Uma Shaanker, R., Jaglan, S., Bharate, S.B., et al., *Dysoxylum binectariferum bark as a new source of anticancer drug camptothecin: Bioactivity-guided isolation and LCMS-based quantification.* Bioorg. Med. Chem. Lett., 2014. **24**(14): p. 3146-3149.

78. Jain, S.K., Meena, S., Qazi, A.K., Hussain, A., Bhola, S.K., Kshirsagar, R., Pari, K., et al., *Isolation and biological evaluation of chromone alkaloid dysoline, a new regioisomer of rohitukine from Dysoxylum binectariferum.* Tetrahedron Lett., 2013. **54**(52): p. 7140-7143.

79. Kumar, V., Guru, S.K., Jain, S.K., Joshi, P., Gandhi, S.G., Bharate, S.B., Bhushan, S., et al., *A chromatography-free isolation of rohitukine from leaves of Dysoxylum binectariferum: Evaluation for in vitro cytotoxicity, Cdk inhibition and physicochemical properties.* Bioorg. Med. Chem. Lett., 2016. **26**(15): p. 3457-3463.

80. Bharate, S.B., Kumar, V., Jain, S.K., Mintoo, M.J., Guru, S.K., Nuthakki, V.K., Sharma, M., et al., *Discovery and Preclinical Development of IIIM-290, an Orally Active Potent Cyclin-Dependent Kinase Inhibitor.* J. Med. Chem, 2018. **61**(4): p. 1664-1687.

81. Cragg, G.M., Grothaus, P.G., and Newman, D.J., *Impact of Natural Products on Developing New Anti-Cancer Agents.* Chem. Rev., 2009. **109**(7): p. 3012-3043.

82. Goel, B., Tripathi, N., Bhardwaj, N., and Jain, K.S., *Small Molecule CDK Inhibitors for the Therapeutic Management of Cancer.* Curr. Top. Med. Chem., 2020. **20**(17): p. 1535-1563.

83. K Jain, S., B Bharate, S., and a Vishwakarma, R., *Cyclin-dependent kinase inhibition by flavoalkaloids.* Mini Rev Med Chem 2012. **12**(7): p. 632-649.

84. Hisham, A., Ajitha Bai, M.D., Fujimoto, Y., Hara, N., and Shimada, H., *Complete 1H and 13C NMR Spectral Assignment of Cabraleadiol, a Dammarane Triterpene from Dysoxylum malabaricum Bedd.* Magn. Reson. Chem., 1996. **34**(2): p. 146-150.

85. Hisham, A., Ajitha Bai, M.D., JayaKumar, G., Nair, M.S., and Fujimoto, Y., *Triterpenoids from Dysoxylum malabaricum.* Phytochemistry, 2001. **56**(4): p. 331-334.

86. Jayakumar, G., Ajithabai, M., Santhosh, B., Veena, C., and Nair, M.S., *Microwave assisted acetylation and deacetylation studies on the triterpenes isolated from*

Dysoxylum malabaricum and Dysoxylum beddomei. Indian J. Chem., 2003. **42B(02)**: p. 429-431.

87. Guru, S.K., Pathania, A.S., Kumar, S., Ramesh, D., Kumar, M., Rana, S., Kumar, A., et al., *Secalonic Acid-D Represses HIF1α/VEGF-Mediated Angiogenesis by Regulating the Akt/mTOR/p70S6K Signaling Cascade.* Cancer Res., 2015. **75**(14): p. 2886-2896.
88. Hisham, A., Jayakumar, G., Ajitha Bai, M.D., and Fujimoto, Y., *Beddomeilactone: A New Triterpene from Dysoxylum Beddomei.* Nat. Prod. Res., 2004. **18**(4): p. 329-334.
89. Bogseth, R., Edgcomb, E., Jones, C.M., Chess, E.K., and Hu, P., *Acetonitrile Adduct Formation as a Sensitive Means for Simple Alcohol Detection by LC-MS.* J. Am. Soc. Mass Spectrom., 2014. **25**(11): p. 1987-1990.
90. Bhardwaj, N., Swathilaxmi, S., Tripathi, N., Kumar, S., Lal, U.R., G, R., Guru, S.K., et al., *Mahamanalactone A, a new triterpenoid from Dysoxylum malabaricum bark: a case study for rapid identification of new metabolites via LC-HRMS profiling and database mining strategy.* Nat. Prod. Res., 2024: p. 1-6.
91. Bhardwaj, N., Sharma, V.K., Tripathi, N., Pimpre, K., Sonti, R., Ravikanth, G., Koch, B., et al., *Isolation of cytotoxic cycloartane triterpenoids from Dysoxylum malabaricum.* New J. Chem., 2024.
92. Singh, C.P., Sharma, A., Sharma, K., Darshani, P., Katare, A., Kumar, D., and Bharitkar, Y.P., *Two new cycloartane type triterpenes from Dysoxyllum binectariferum.* Nat. Prod. Res., 2023: p. 1-8.
93. Bhardwaj, N., Sharma, A., Tripathi, N., Goel, B., Ravikanth, G., Kumar Guru, S., and Jain, S.K., *New cycloartane triterpenoids from Dysoxylum malabaricum and their cytotoxic evaluation.* Steroids, 2023. **200**: p. 109315.
94. Bhardwaj, N., Gupta, P., Tripathi, N., Chakrabarty, S., Verma, A., Kumari, S., Gautam, V., et al., *New ring-A modified cycloartane triterpenoids from Dysoxylum malabaricum bark: Isolation, structure elucidation and their cytotoxicity.* Steroids, 2024. **205**: p. 109390.
95. Yan, X.-J., Gong, L.-H., Zheng, F.-Y., Cheng, K.-J., Chen, Z.-S., and Shi, Z., *Triterpenoids as reversal agents for anticancer drug resistance treatment.* Drug Discov. Today, 2014. **19**(4): p. 482-488.
96. Zhou, M., Zhang, R.-H., Wang, M., Xu, G.-B., and Liao, S.-G., *Prodrugs of triterpenoids and their derivatives.* Eur. J. Med. Chem., 2017. **131**: p. 222-236.

97. Liby, K.T., Yore, M.M., and Sporn, M.B., *Triterpenoids and rexinoids as multifunctional agents for the prevention and treatment of cancer.* Nat. Rev. Cancer, 2007. **7**(5): p. 357-369.

98. Xu, G.-B., Xiao, Y.-H., Zhang, Q.-Y., Zhou, M., and Liao, S.-G., *Hepatoprotective natural triterpenoids.* Eur. J. Med. Chem., 2018. **145**: p. 691-716.

99. Goossens, J.F. and Bailly, C., *Ursodeoxycholic acid and cancer: From chemoprevention to chemotherapy.* Pharmacol. Ther., 2019. **203**: p. 107396.

100. Lombrea, A., Scurtu, A.D., Avram, S., Pavel, I.Z., Turks, M., Lugiņina, J., Peipiņš, U., et al. *Anticancer Potential of Betulonic Acid Derivatives*. International Journal of Molecular Sciences, 2021. **22**.

101. Eastman, R.T. and Fidock, D.A., *Artemisinin-based combination therapies: a vital tool in efforts to eliminate malaria.* Nature Reviews Microbiology, 2009. **7**(12): p. 864-874.

102. Vuddanda, P.R., Singh, S., and Velaga, S., *Boswellic acid – Medicinal use of an ancient herbal remedy.* J. Herb. Med., 2016. **6**(4): p. 163-170.

103. Hussain, H., Al-Harrasi, A., Csuk, R., Shamraiz, U., Green, I.R., Ahmed, I., Khan, I.A., et al., *Therapeutic potential of boswellic acids: a patent review (1990-2015).* Expert Opin. Ther. Pat., 2017. **27**(1): p. 81-90.

104. Pastorino, G., Cornara, L., Soares, S., Rodrigues, F., and Oliveira, M.B.P.P., *Liquorice (Glycyrrhiza glabra): A phytochemical and pharmacological review.* Phytother. Res., 2018. **32**(12): p. 2323-2339.

105. Lynch, D.R., Chin, M.P., Boesch, S., Delatycki, M.B., Giunti, P., Goldsberry, A., Hoyle, J.C., et al., *Efficacy of Omaveloxolone in Friedreich's Ataxia: Delayed-Start Analysis of the MOXIe Extension.* Mov Disord, 2023. **38**(2): p. 313-320.

106. Keam, S.J., *Vamorolone: First Approval.* Drugs, 2024. **84**(1): p. 111-117.

107. Sun, Y., Wang, C., Li, X., Lu, J., and Wang, M., *Recent advances in drug delivery of celastrol for enhancing efficiency and reducing the toxicity.* Front. pharmacol., 2024. **15**.

108. Srivastava, V., Negi, A.S., Kumar, J.K., Gupta, M.M., and Khanuja, S.P.S., *Plant-based anticancer molecules: A chemical and biological profile of some important leads.* Bioorg. Med. Chem. , 2005. **13**(21): p. 5892-5908.

109. Pattabiraman, V.R. and Bode, J.W., *Rethinking amide bond synthesis.* Nature, 2011. **480**(7378): p. 471-479.

110. Li, J., Gu, A., Nong, X.-M., Zhai, S., Yue, Z.-Y., Li, M.-Y., and Liu, Y., *Six-Membered Aromatic Nitrogen Heterocyclic Anti-Tumor Agents: Synthesis and Applications.* Chem. Rec., 2023. **23**(12): p. e202300293.

111. Jana, R., Begam, H.M., and Dinda, E., *The emergence of the C–H functionalization strategy in medicinal chemistry and drug discovery.* Chem. Commun., 2021. **57**(83): p. 10842-10866.

112. Rankovic, Z., *CNS Drug Design: Balancing Physicochemical Properties for Optimal Brain Exposure.* J. Med. Chem., 2015. **58**(6): p. 2584-2608.

113. Subbaiah, M.A.M. and Meanwell, N.A., *Bioisosteres of the Phenyl Ring: Recent Strategic Applications in Lead Optimization and Drug Design.* J. Med. Chem., 2021. **64**(19): p. 14046-14128.

114. Noriega, S., Cardoso-Ortiz, J., López-Luna, A., Cuevas-Flores, M.D., and Flores De La Torre, J.A. *The Diverse Biological Activity of Recently Synthesized Nitro Compounds*. Pharmaceuticals, 2022. **15**, DOI: 10.3390/ph15060717.

115. Onoue, S., Yamada, S., and Chan, H.-K., *Nanodrugs: pharmacokinetics and safety.* Int. J. Nanomed., 2014. **9**: p. 1025-1037.

116. Wu, W. and Jiang, H., *Haloalkynes: A Powerful and Versatile Building Block in Organic Synthesis.* Acc. Chem. Res., 2014. **47**(8): p. 2483-2504.

117. Pavlinac, J., Zupan, M., Laali, K.K., and Stavber, S., *Halogenation of organic compounds in ionic liquids.* Tetrahedron, 2009. **65**(29): p. 5625-5662.

118. Chung, W.-j. and Vanderwal, C.D., *Stereoselective Halogenation in Natural Product Synthesis.* Angew. Chem., 2016. **55**(14): p. 4396-4434.

119. Mo, F., Yan, J.M., Qiu, D., Li, F., Zhang, Y., and Wang, J., *Gold-Catalyzed Halogenation of Aromatics by N-Halosuccinimides.* Angew. Chem, 2010. **49**(11): p. 2028-2032.

120. Scheide, M.R., Nicoleti, C.R., Martins, G.M., and Braga, A.L., *Electrohalogenation of organic compounds.* Org. Biomol. Chem., 2021. **19**(12): p. 2578-2602.

121. Fuchigami, T. and Inagi, S., *Recent Advances in Electrochemical Systems for Selective Fluorination of Organic Compounds.* Acc. Chem. Res., 2020. **53**(2): p. 322-334.

122. Nigst, T.A., Antipova, A., and Mayr, H., *Nucleophilic Reactivities of Hydrazines and Amines: The Futile Search for the α-Effect in Hydrazine Reactivities.* J. Org. Chem., 2012. **77**(18): p. 8142-8155.

123. Rosamilia, A.E., Aricò, F., and Tundo, P., *Insight into the Hard−Soft Acid−Base Properties of Differently Substituted Phenylhydrazines in Reactions with Dimethyl Carbonate.* J. Phys. Chem. B, 2008. **112**(46): p. 14525-14529.

124. Smith, P.A.S. and DeWall, G.L., *Hydrazines as ambident nucleophiles: the site of benzylation of N-benzyl-N-phenylhydrazines.* J. Am. Chem. Soc., 1977. **99**(17): p. 5751-5760.

125. Bhardwaj, N., Tripathi, N., Kumar, S., and Jain, S.K., *Synthesis of amides directly from carboxylic acids and hydrazines.* Org. Biomol. Chem., 2023. **21**(37): p. 7572-7579.

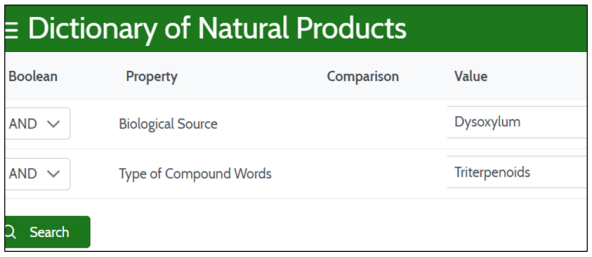
126. Bhardwaj, N., Singh, A.K., Tripathi, N., Goel, B., Indra, A., and Jain, S.K., *Ni–NiO heterojunctions: a versatile nanocatalyst for regioselective halogenation and oxidative esterification of aromatics.* New J. Chem., 2021. **45**(31): p. 14177-14183.

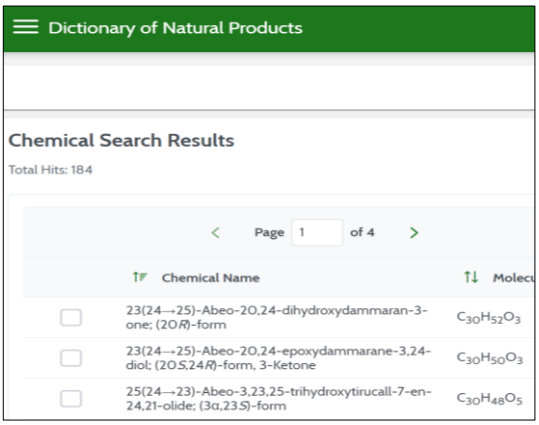
Appendix

APPENDIX

DNP-database search results

Figure A.1. DNP-Database search for phytoconstituents present in *Dysoxylum* genus

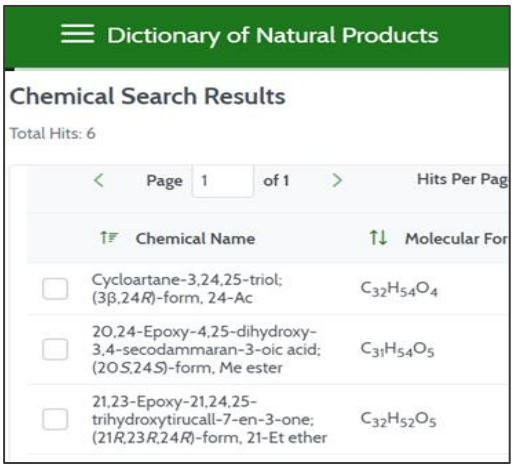




Search Query
Biological source: *Dysoxylum*
Type of compound: Triterpenoid

Total hits: 184

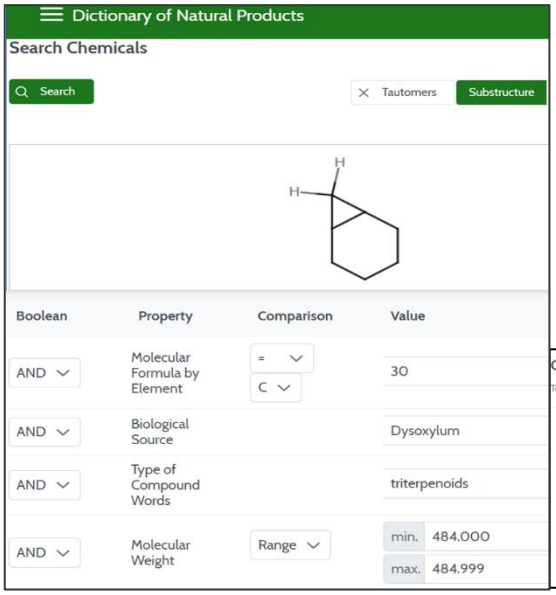
Figure A.2. DNP-Database search for phytoconstituents present in *D.malabaricum*

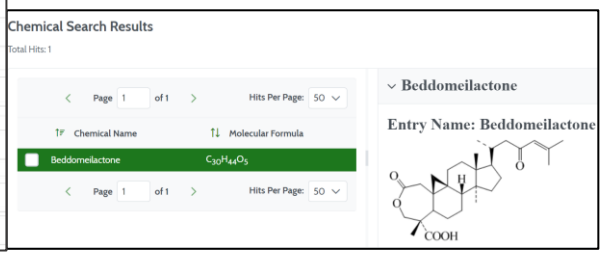


Search Query
Biological source: *Dysoxylum malabaricum*

Total hits: 6

Figure A.3. DNP-Database search for identification of compound **1**



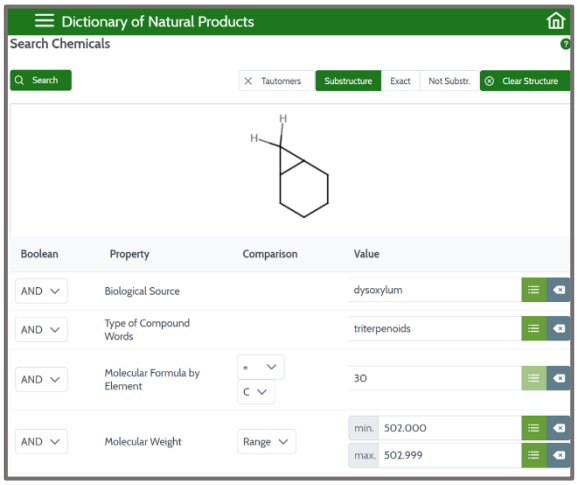


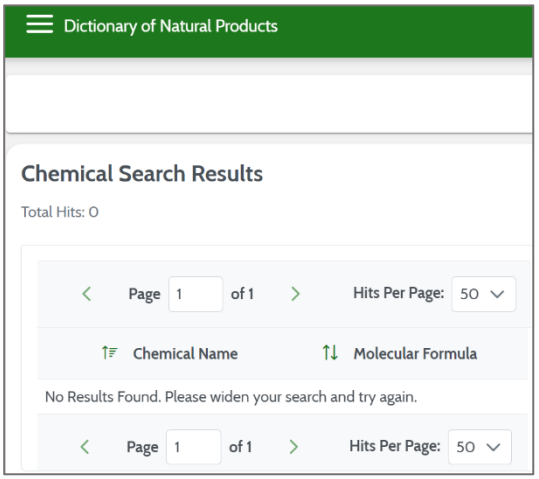
Search Query

Biological source: *Dysoxylum*
Type of compound: Triterpenoid
Substructure: Cyclopropane ring
Molecular weight: 484
Carbon atom: 30

Total Hits: 1

Figure A.4. DNP-Database search for identification of compound **3**



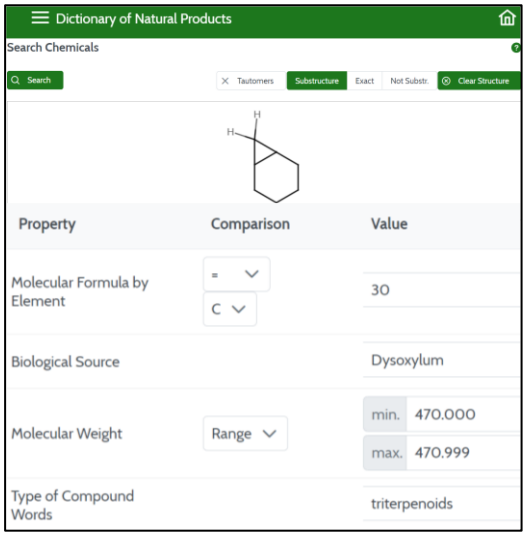


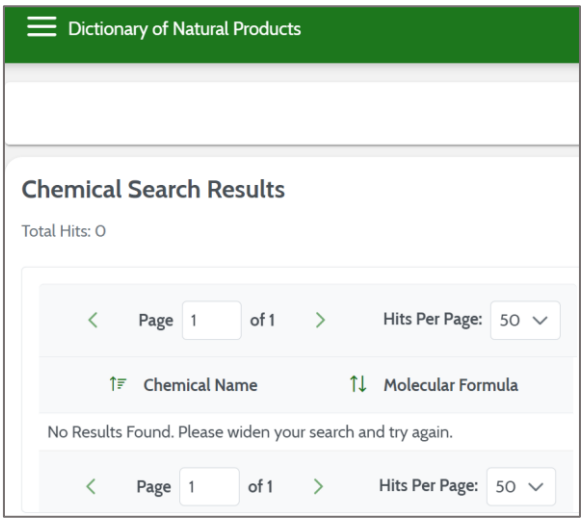
Search Query

Biological source: Dysoxylum
Type of compound: Triterpenoid
Substructure: Cyclopropane ring
Molecular weight: 502
Carbon atom: 30

Total Hits: 0

Figure A.5. DNP-Database search for identification of compound **4**





Search Query
Biological Source: Dysoxylum
Type of Compound: Triterpenoid
Mol weight: 470 Da
Substructure: Cyclopropane

Total Hits: 0

Spectral data of isolated compounds from *Dysoxylum malabaricum*.

Figure A.6. ^{13}C NMR spectrum of compound **1** in $CDCl_3$ [91]

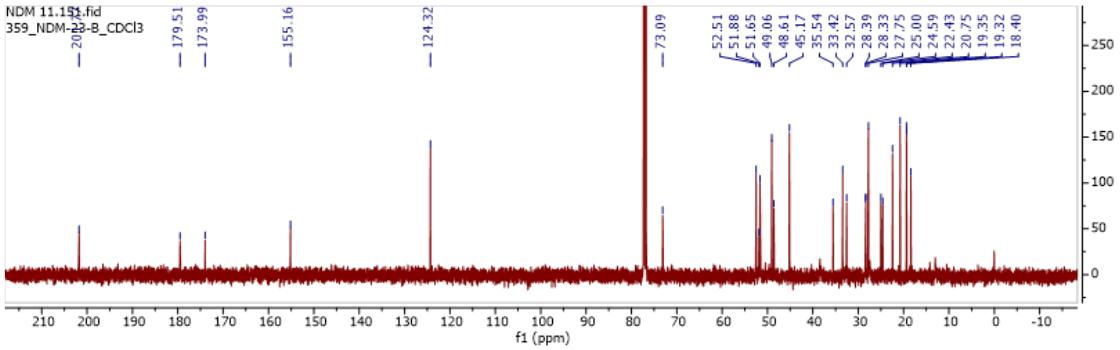


Figure A.7. HSQC NMR spectrum of compound **1** in $CDCl_3$ [91]

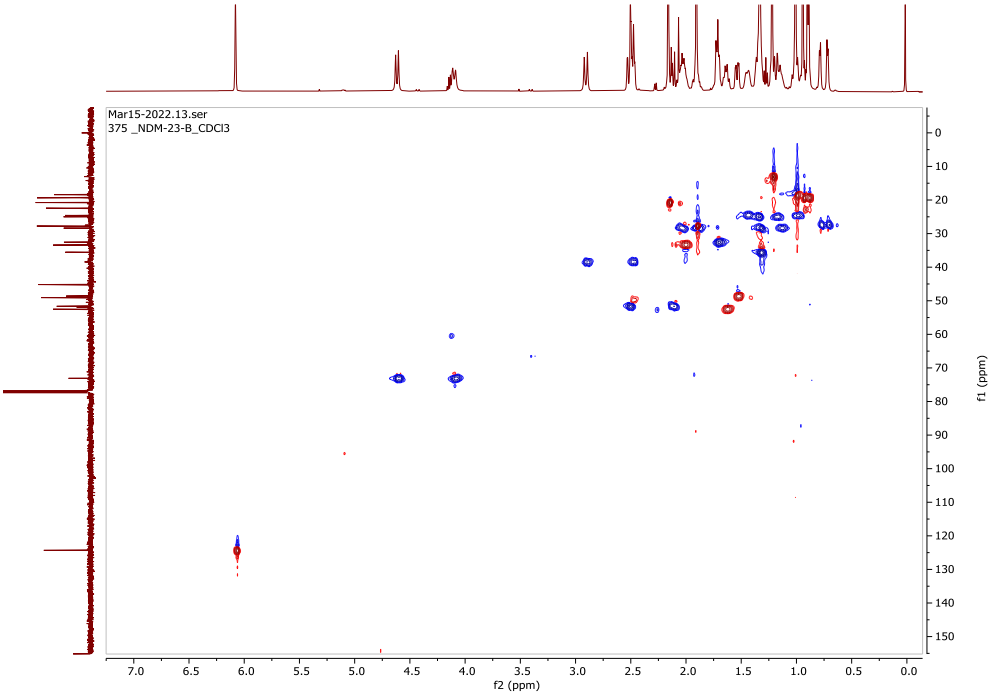


Figure A.8. HMBC NMR spectrum of compound **1** in $CDCl_3$ [91]

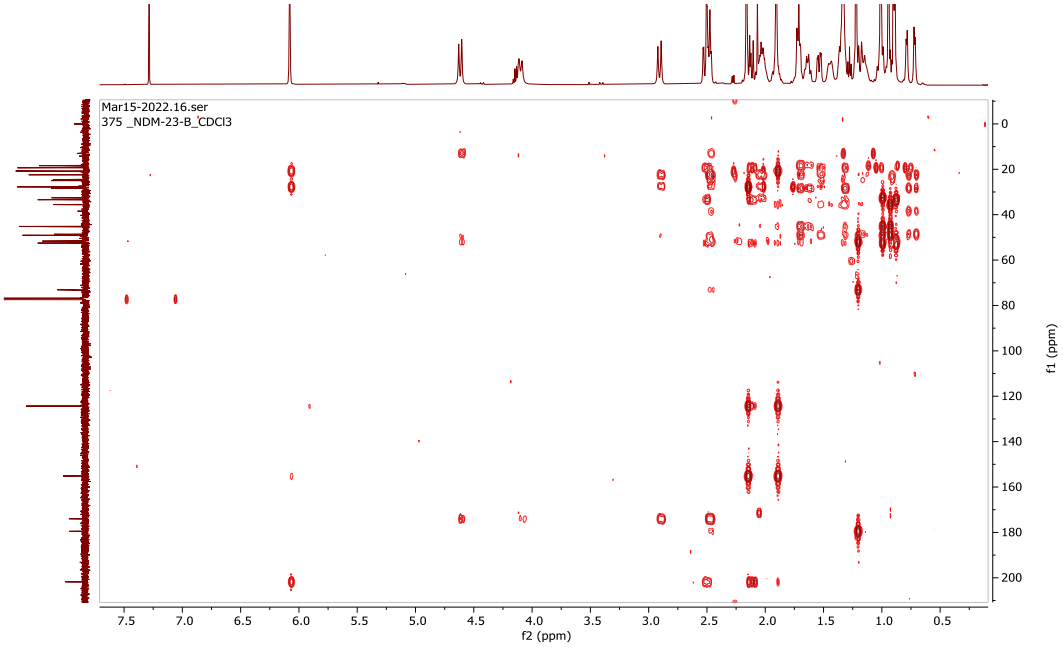


Figure A.9. COSY and NOESY NMR spectrum of compound **1** in $CDCl_3$ [91]

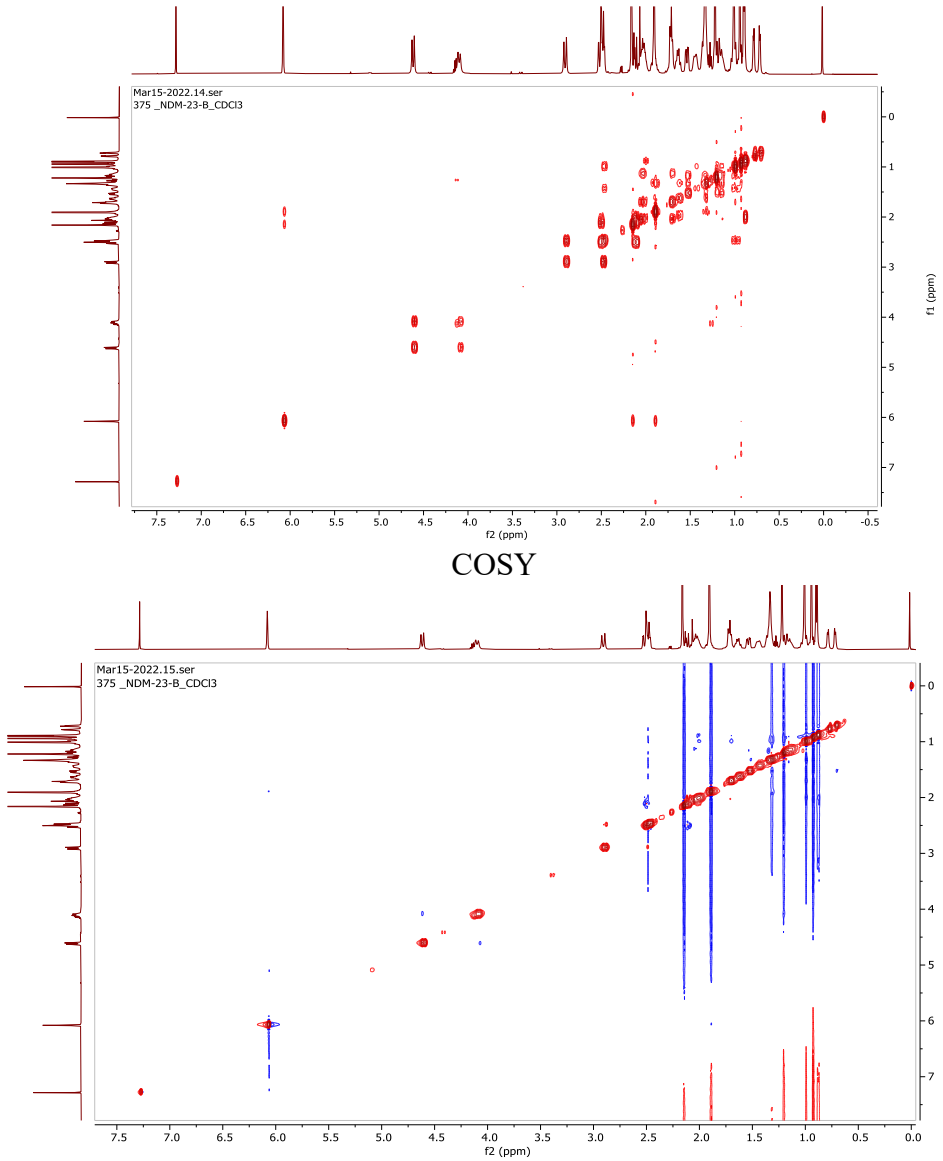


Figure A.10. HRESIMS spectrum of compound **1** [91]

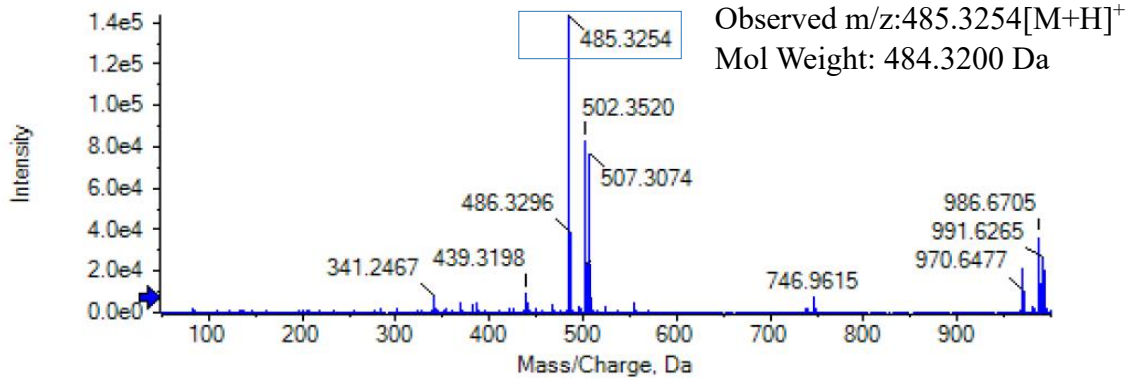


Figure A.11 Stereochemistry of compound **1** [91]

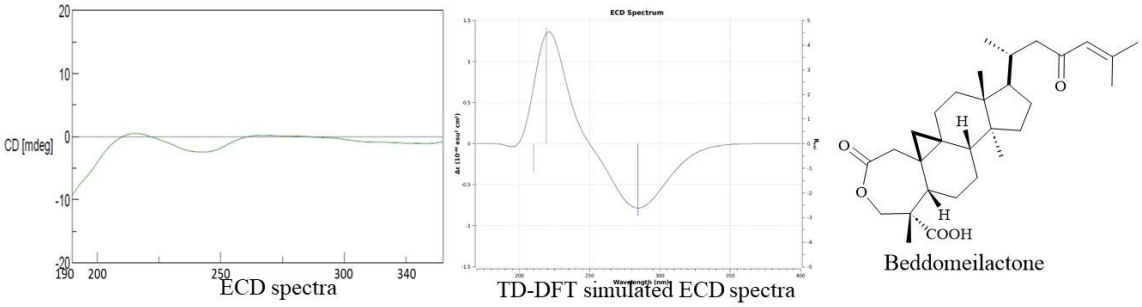


Figure A.12: ^{1}H NMR spectrum of compound **2** in $CDCl_3$ [91]

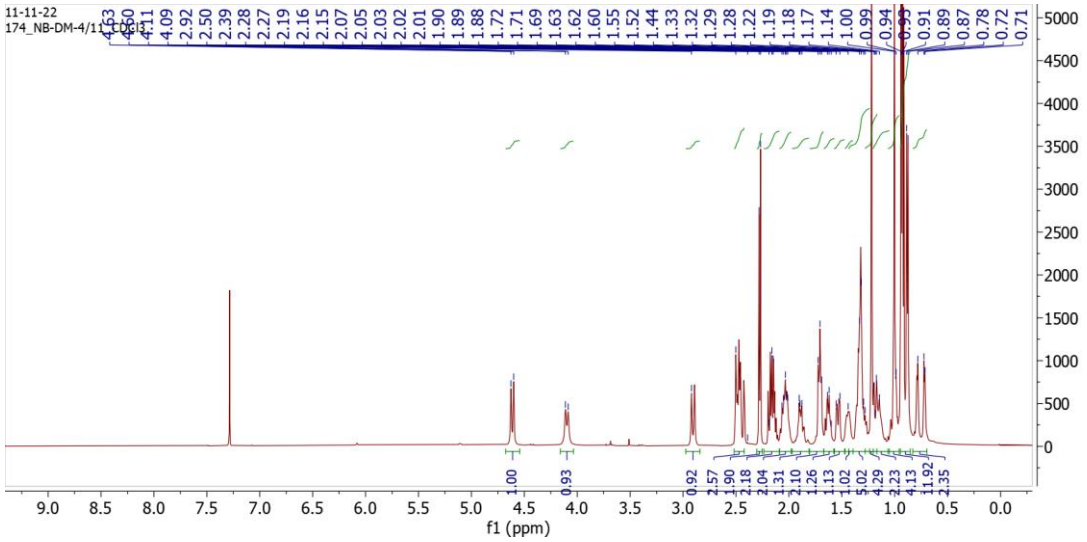


Figure A.13: ^{13}C NMR spectrum of compound **2** in $CDCl_3$ [91]

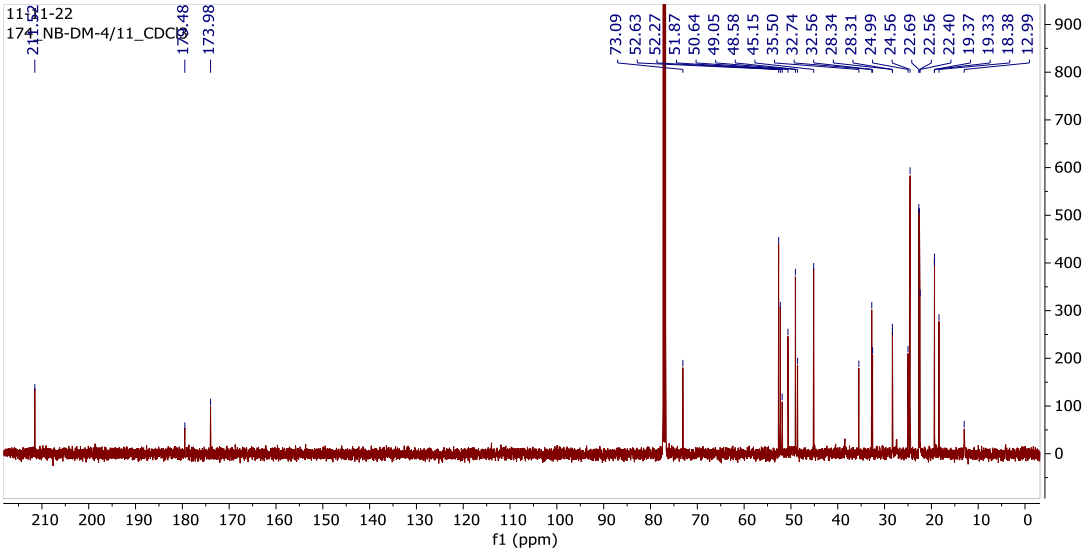
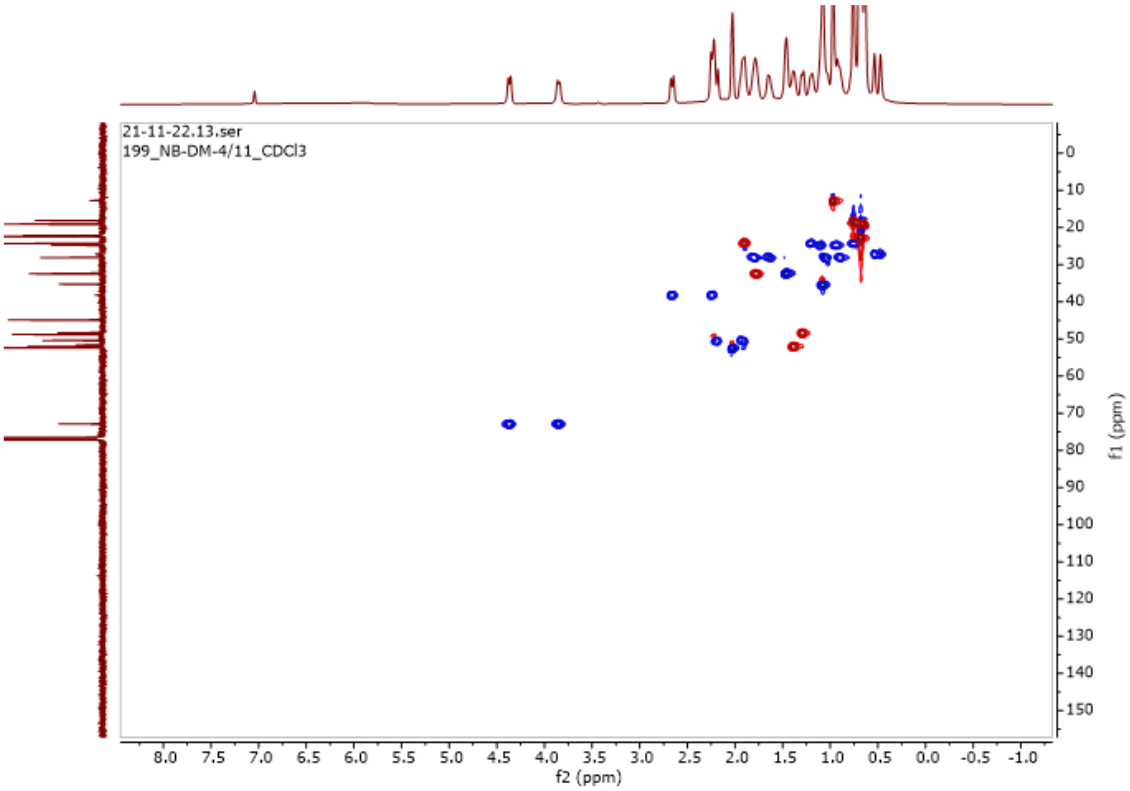
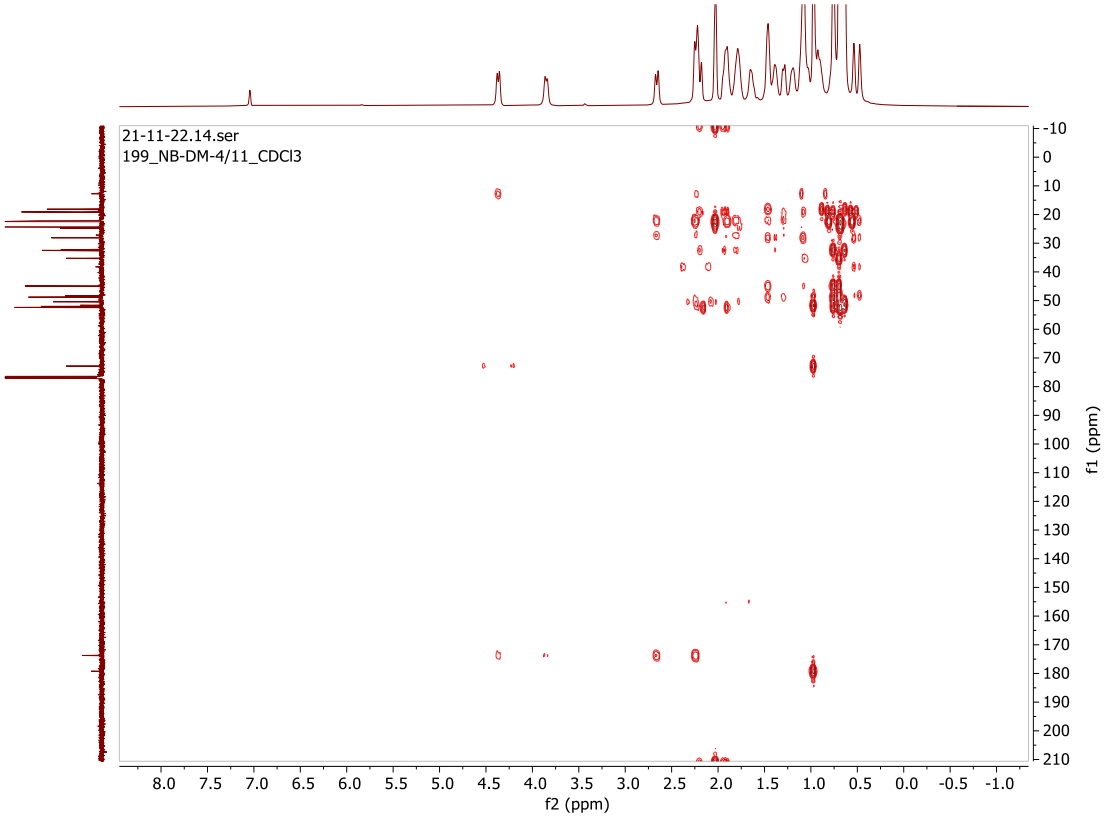


Figure A.14: HSQC and HMBC NMR spectra of compound **2** in $CDCl_3$ [91]

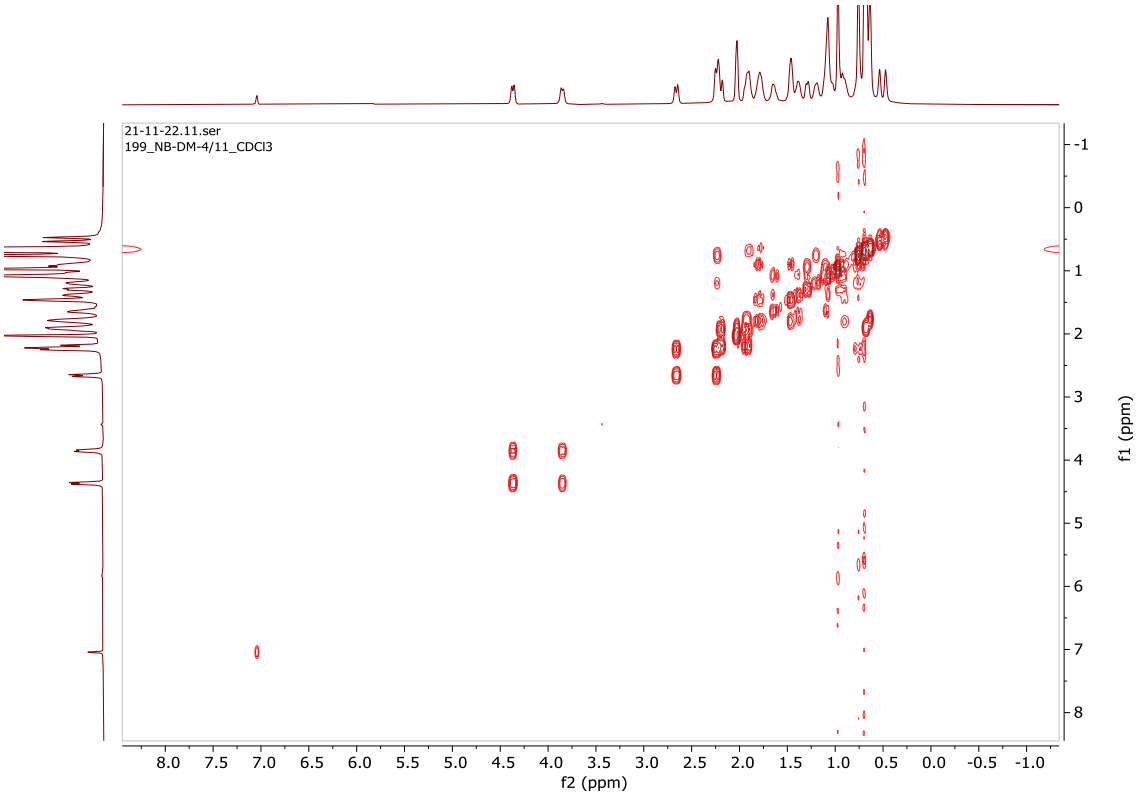


HSQC

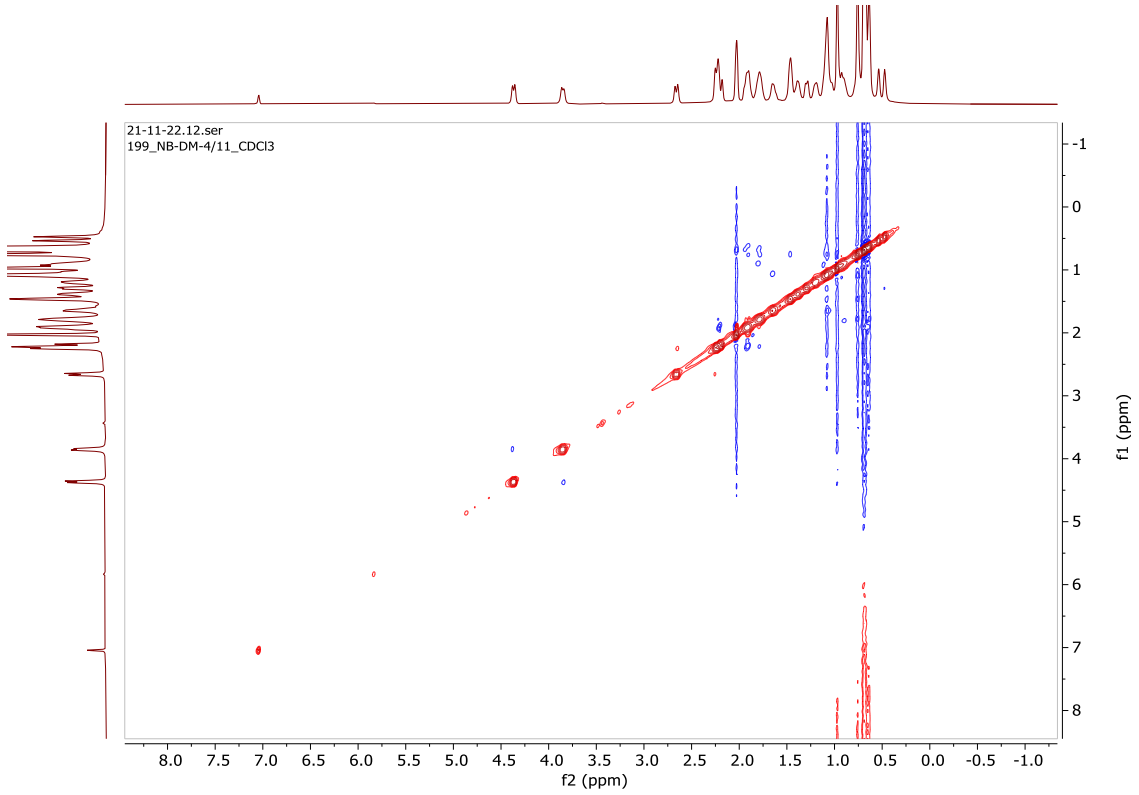


HMBC

Figure A.15: ^{1}H-^{1}H COSY and NOESY NMR spectra of compound **2** in $CDCl_3$ [91]



COSY



NOESY

Figure A.16: HRESIMS spectrum of compound **2** [91]

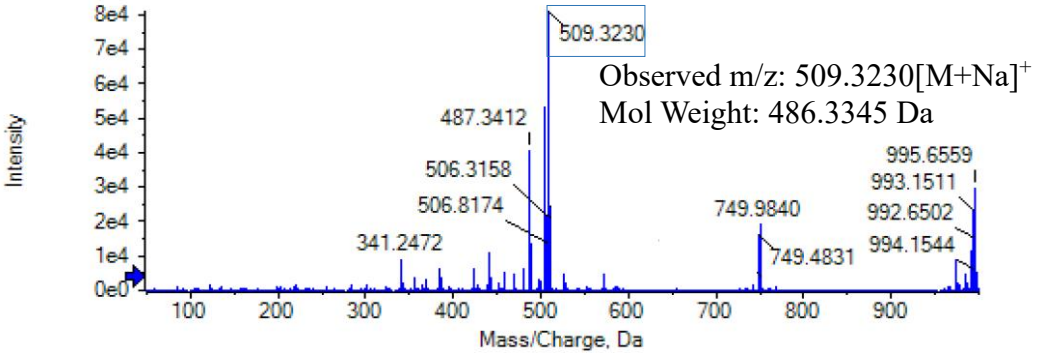
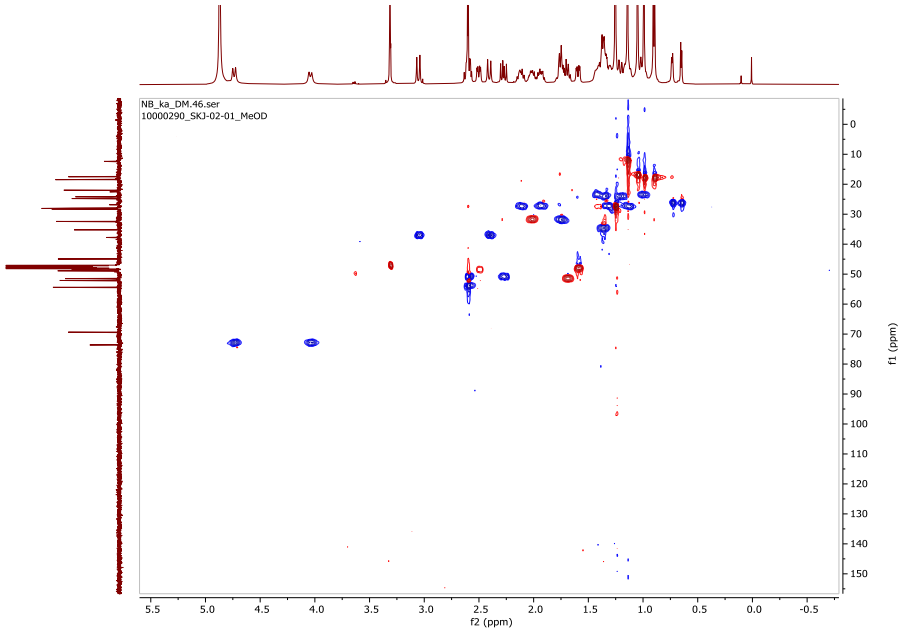
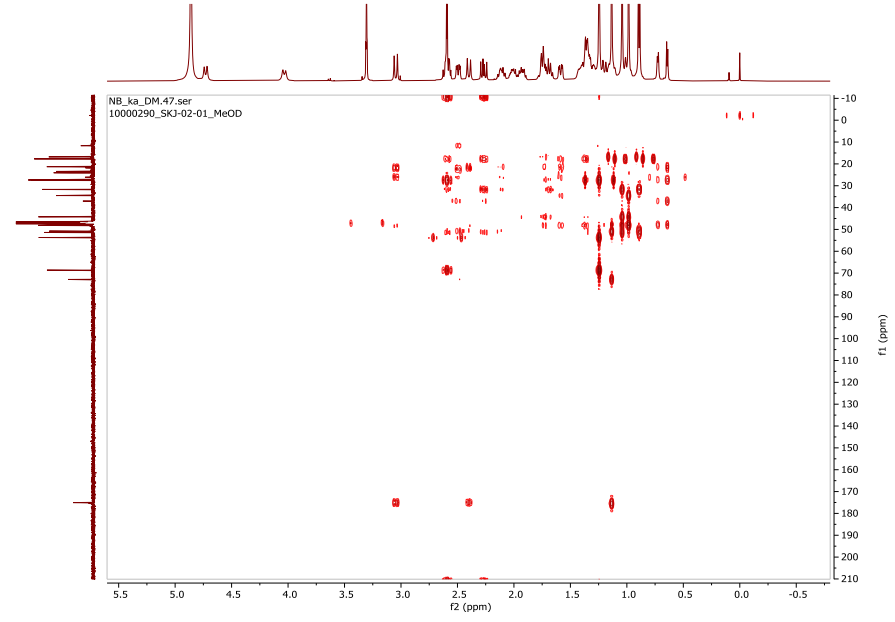


Figure A.17: HSQC and HMBC NMR spectrum of compound **3** in CD_3OD [91]

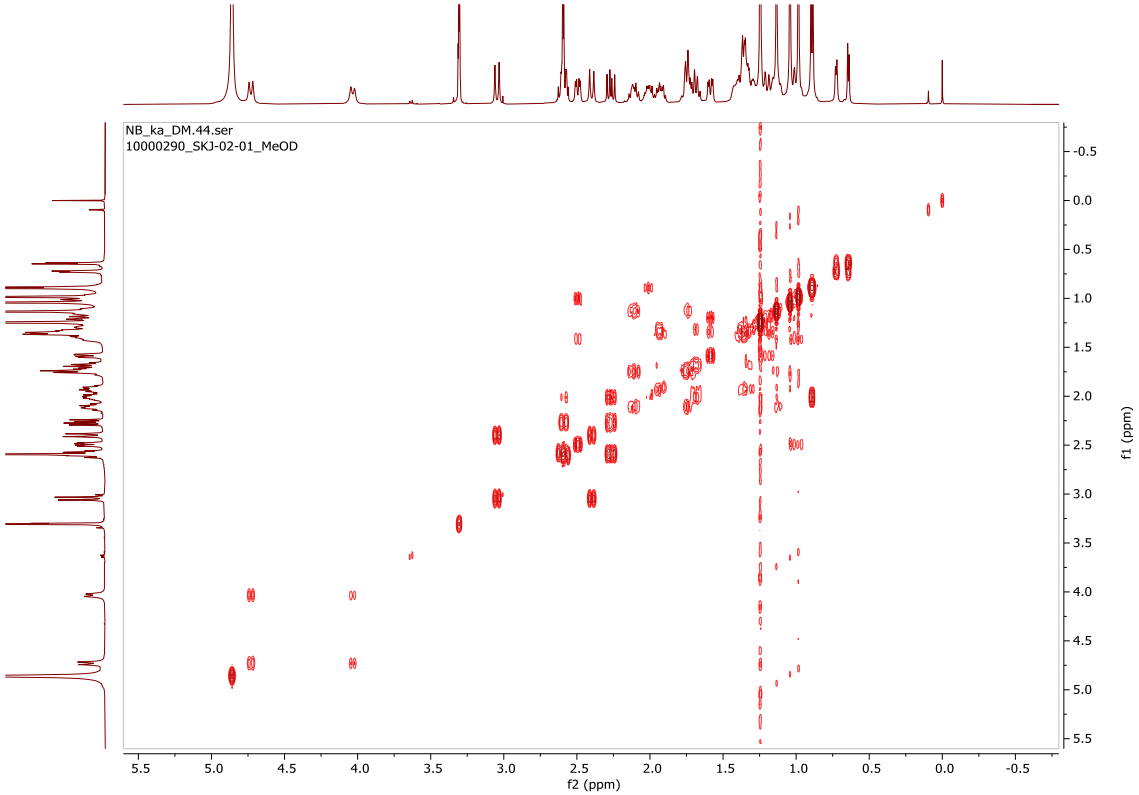


HSQC

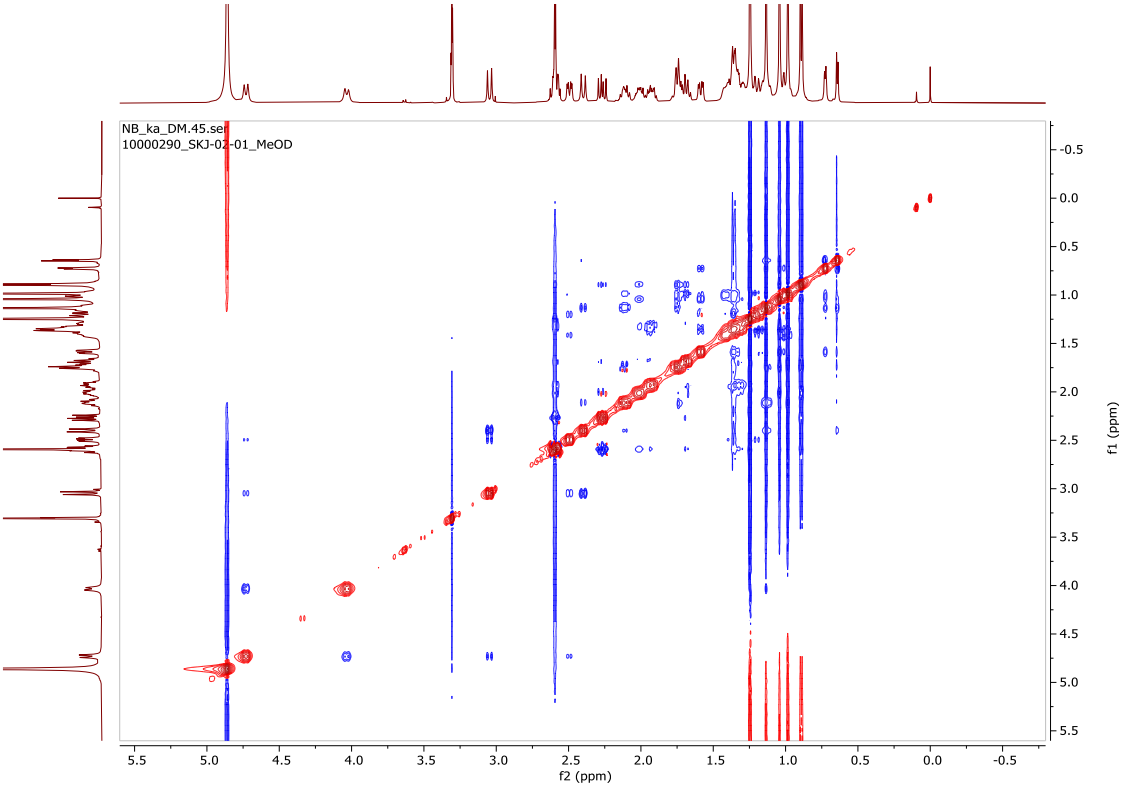


HMBC

Figure A.18: ^{1}H-^{1}H COSY and NOESY NMR spectrum of compound **3** in CD_3OD [91]



COSY



NOSEY

Figure A.19: HRMS mass spectrum of compound **3** [91]

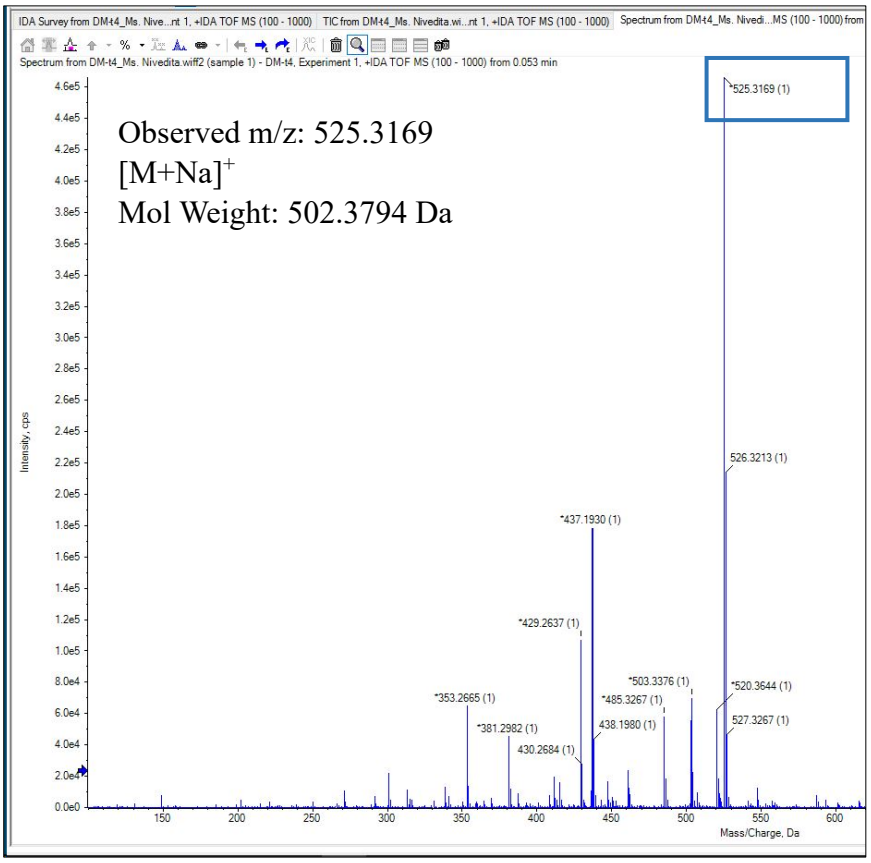


Figure A.20: HSQC NMR spectrum of compound **4** in CD_3OD [90]

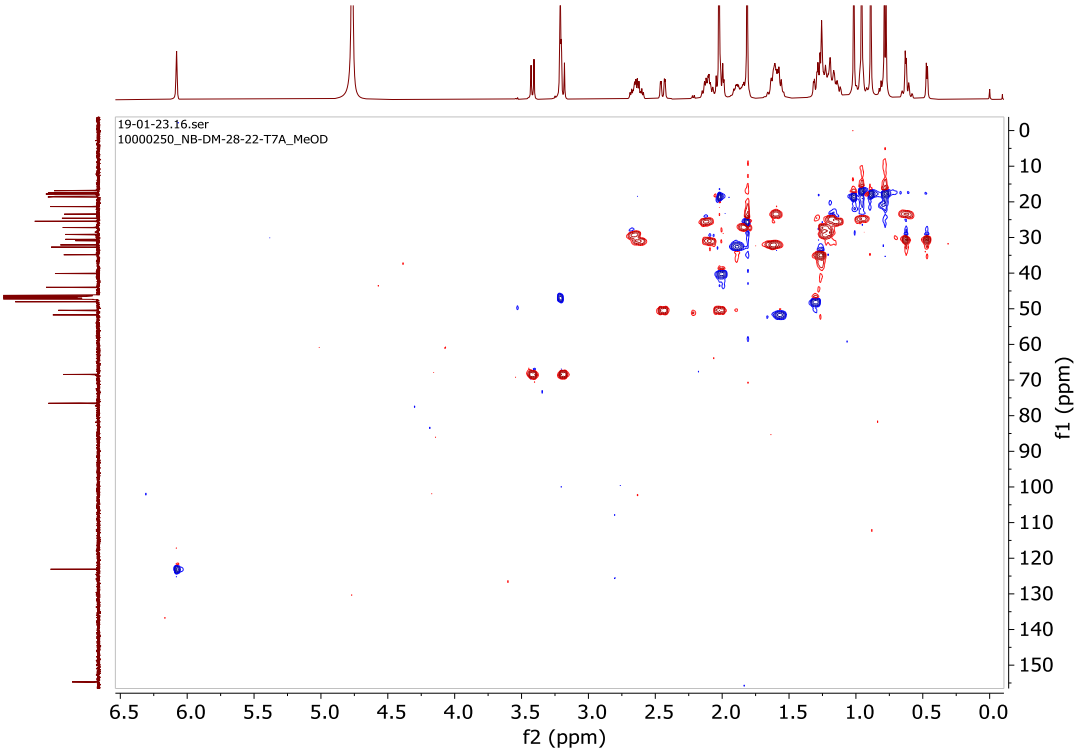
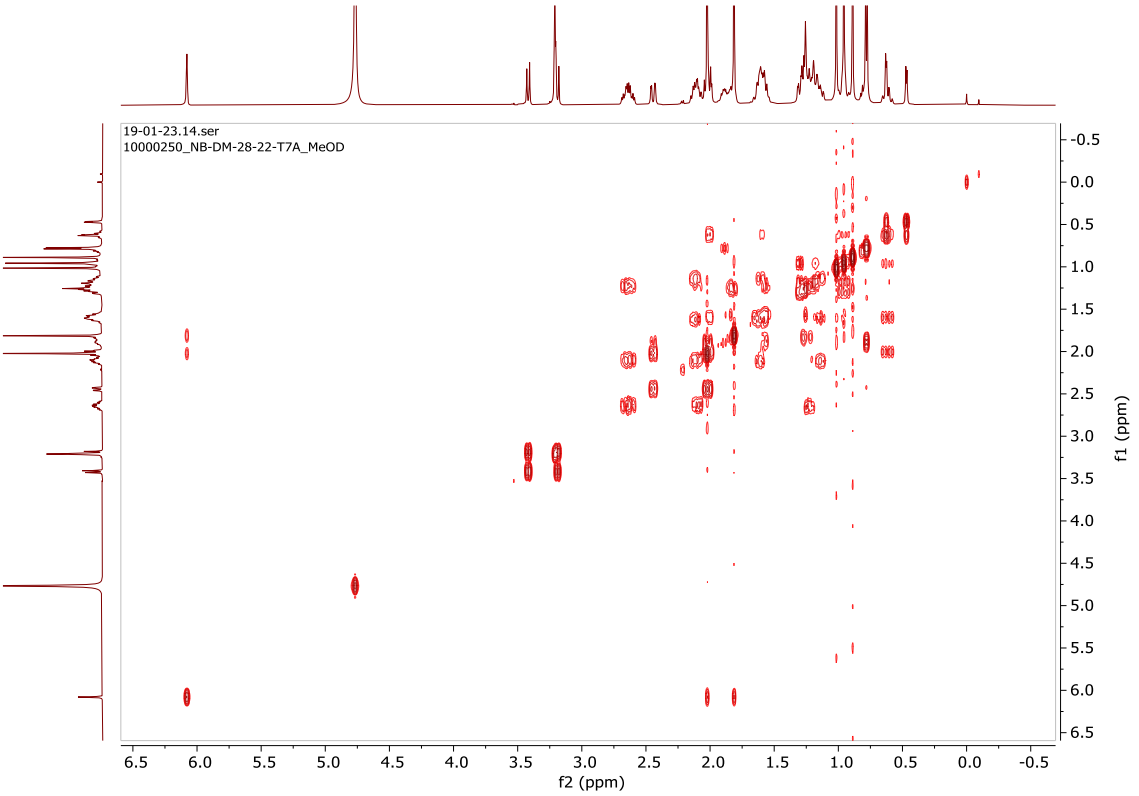
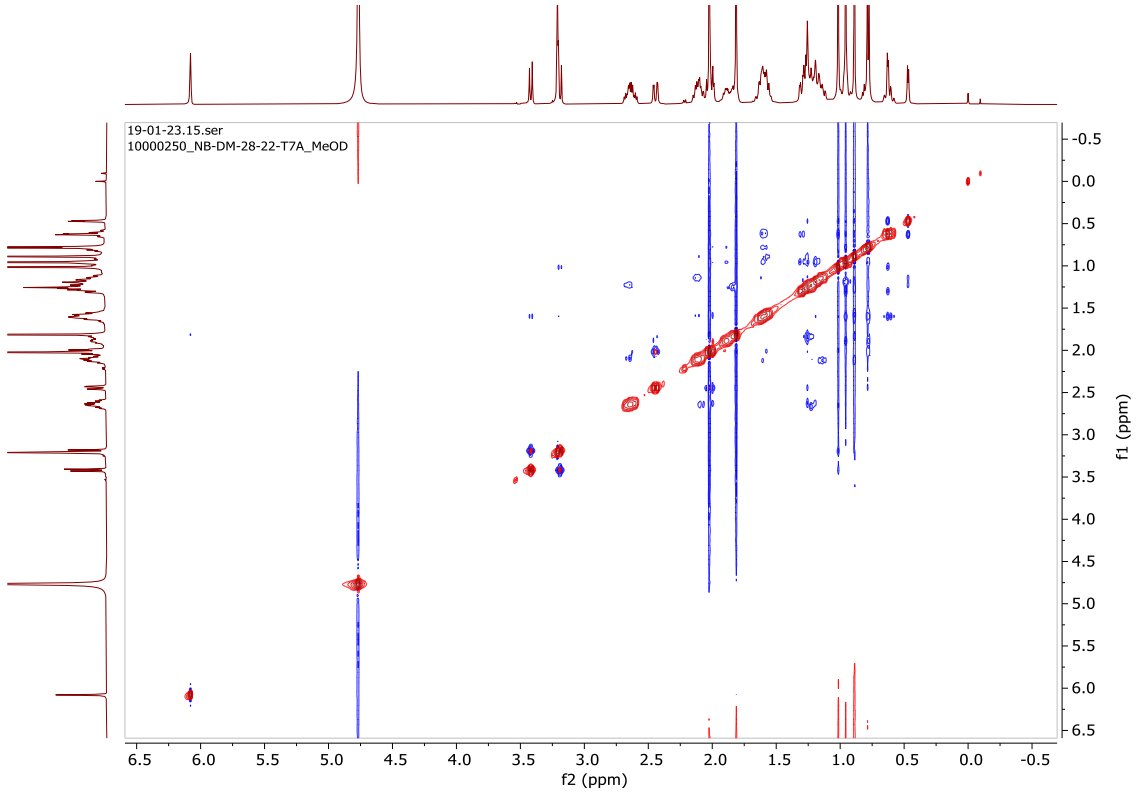


Figure A.21: ^{1}H-^{1}H COSY and NOESY NMR spectrum of compound **4** in CD_3OD [90]



COSY



NOESY

Figure A.22: HRESIMS spectrum of compound **4** [90]

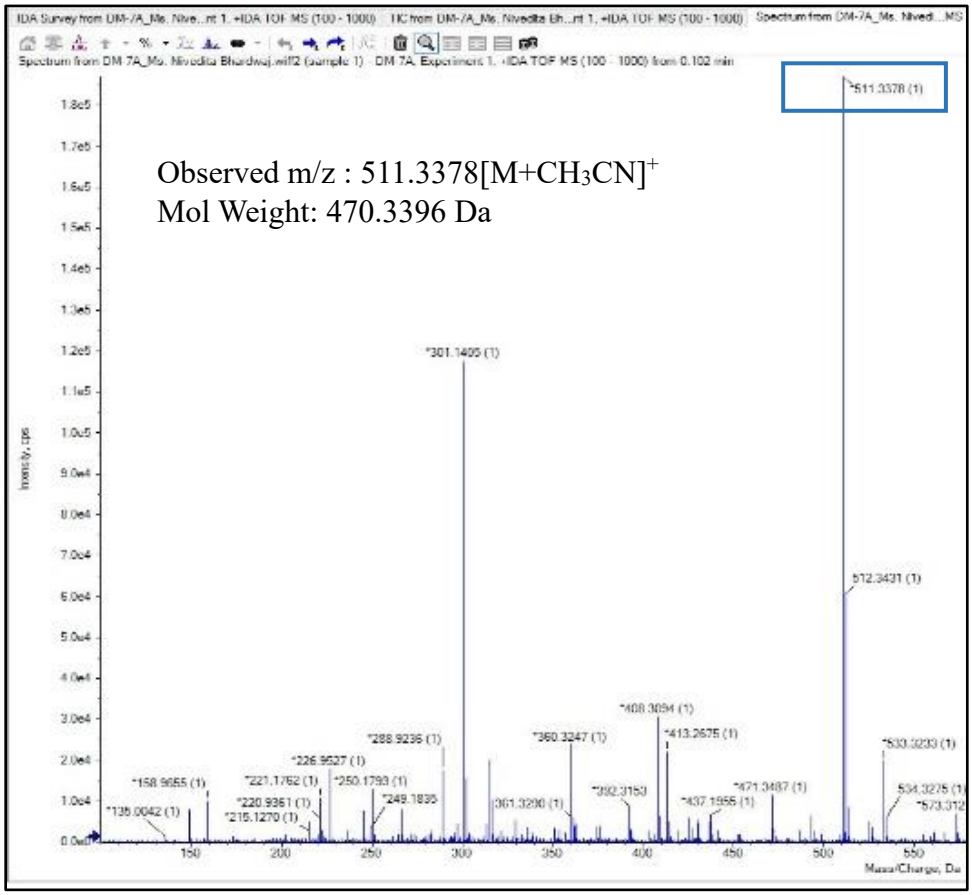


Figure A.23: DEPT-135 NMR spectrum of compound **5** in CD_3OD [91]

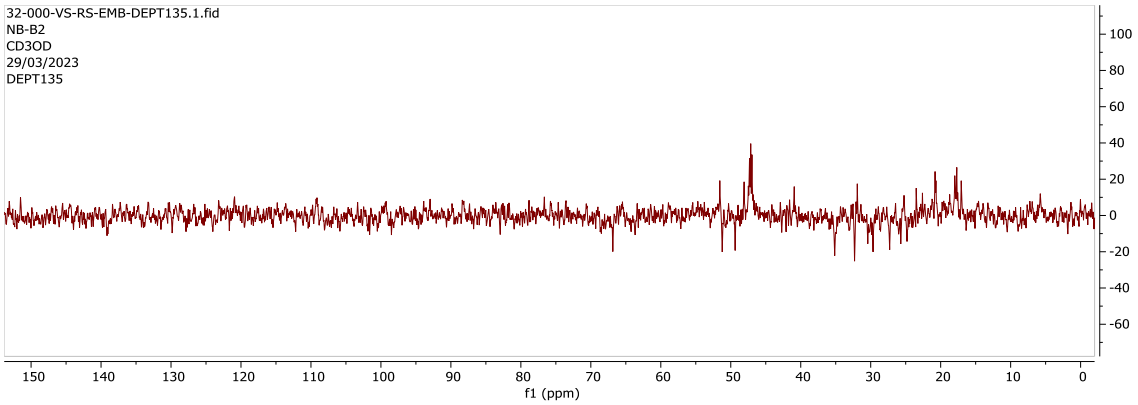
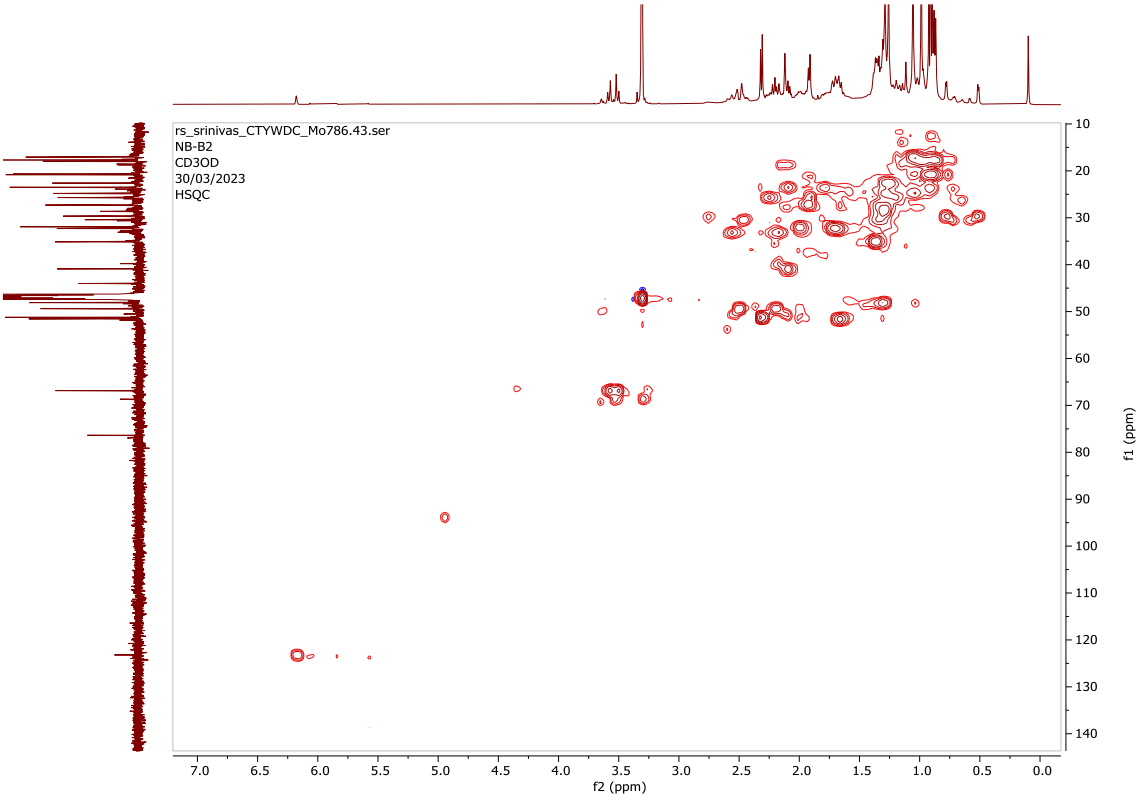
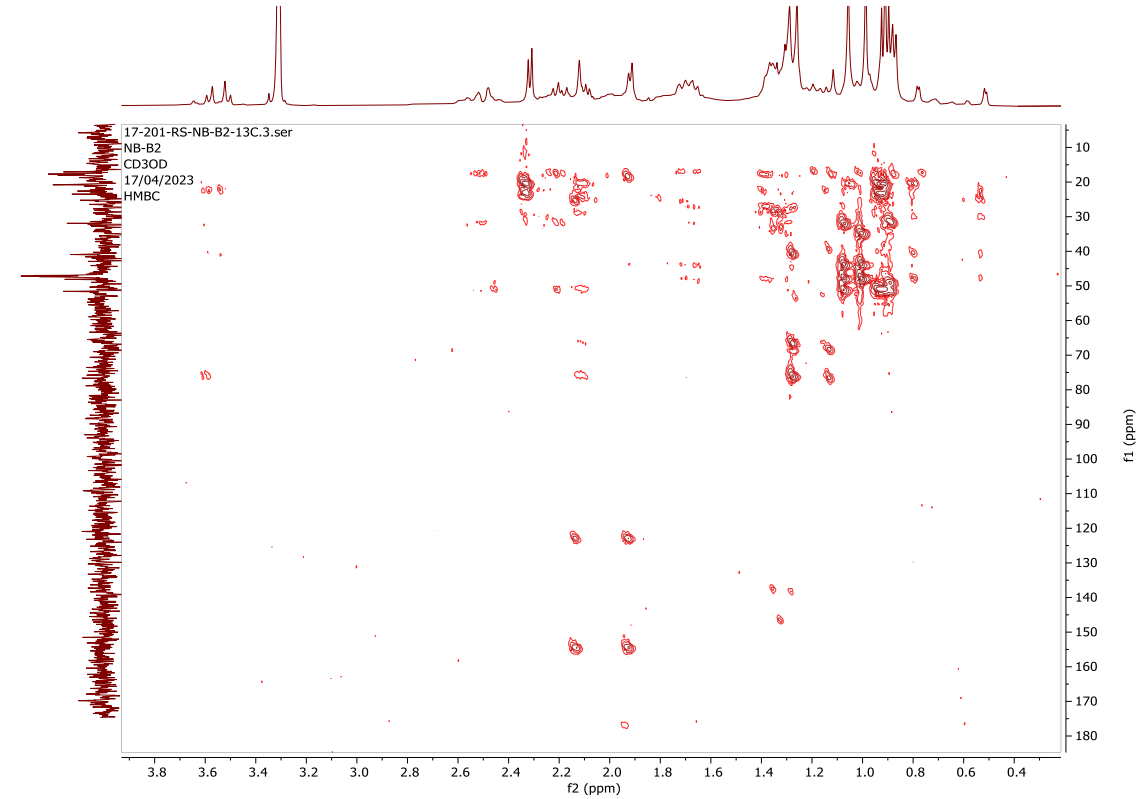


Figure A.24: HSQC and HMBC NMR spectrum of compound **5** in CD_3OD [91]



HSQC



HMBC

Figure A.25: ^{1}H-^{1}H COSY NMR spectrum of compound **5** in CD_3OD [91]

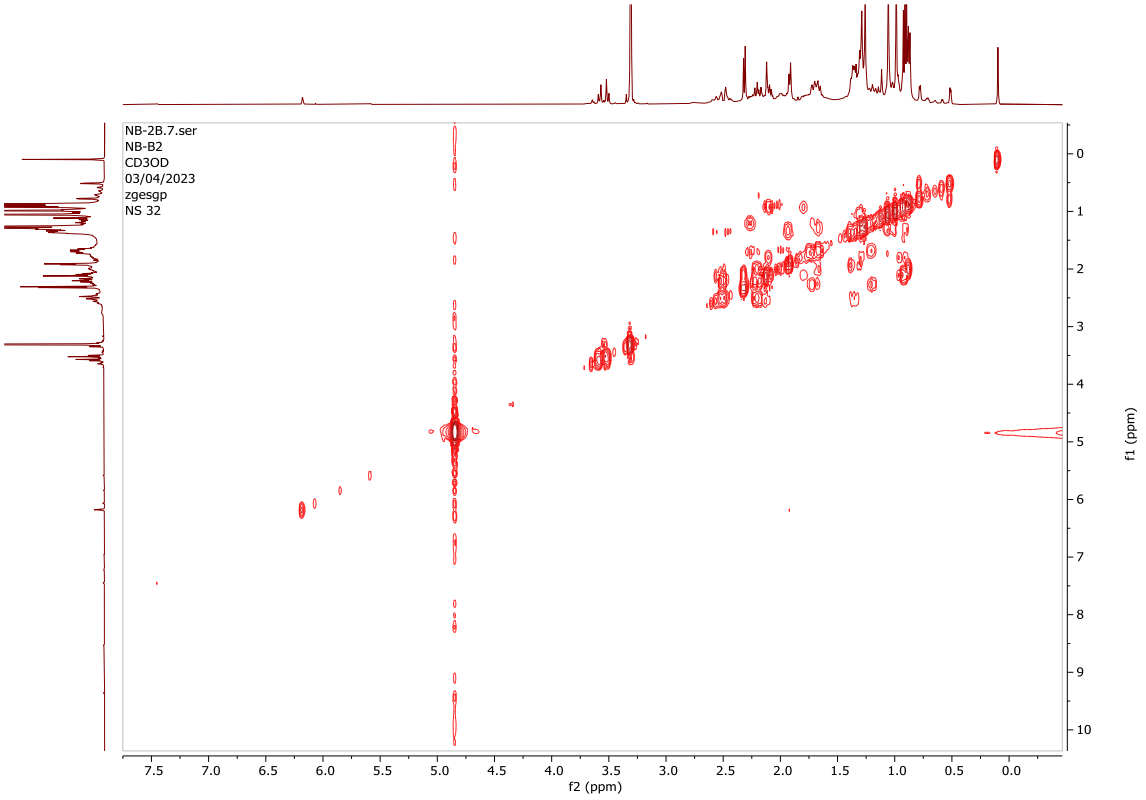
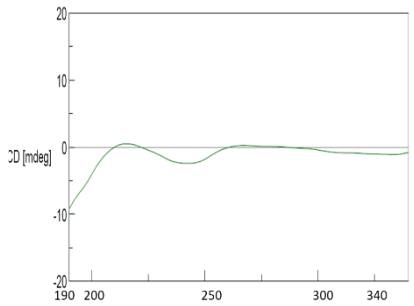
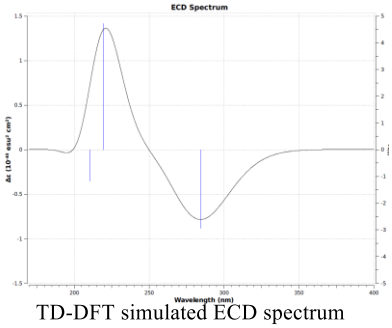


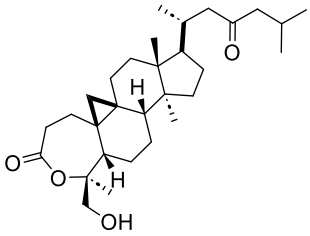
Figure A.26. Stereochemistry of compound **5** [91]



ECD spectrum



TD-DFT simulated ECD spectrum



Dihydromahamanlactone A

Figure A.27: HRESIMS spectrum of compound **5** [91]

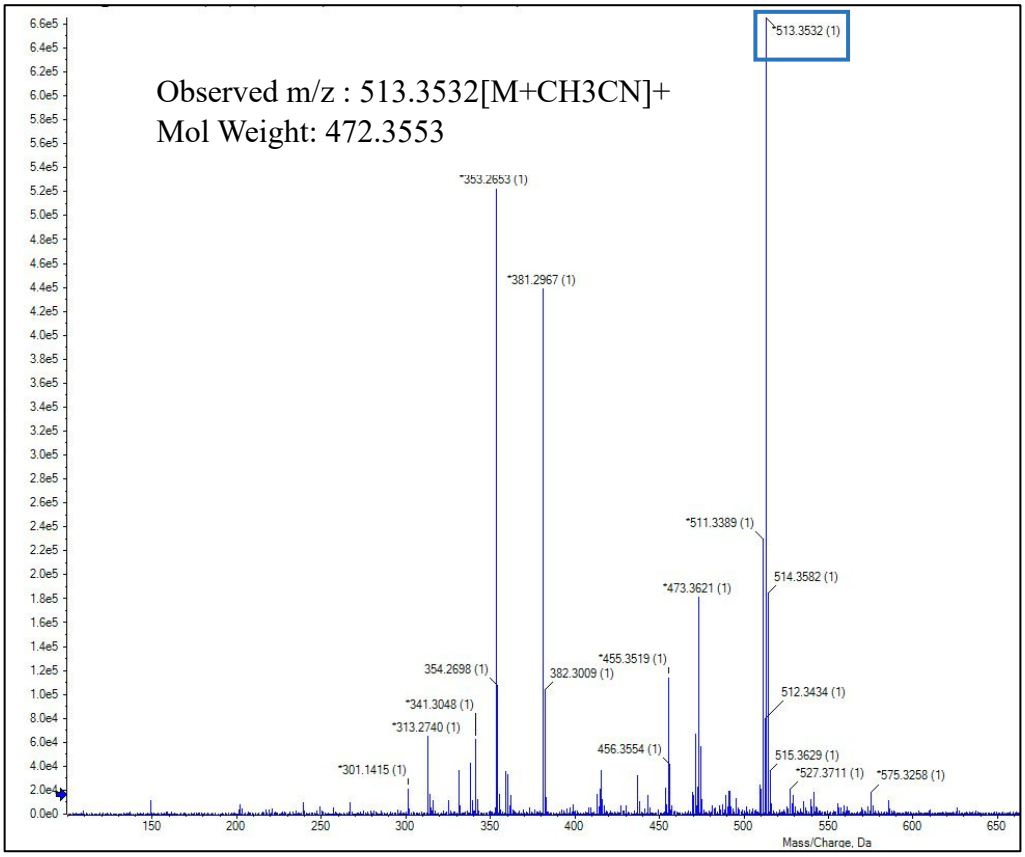


Figure A.28: ^{13}C NMR spectrum of compound **6** in CD_3OD [93]

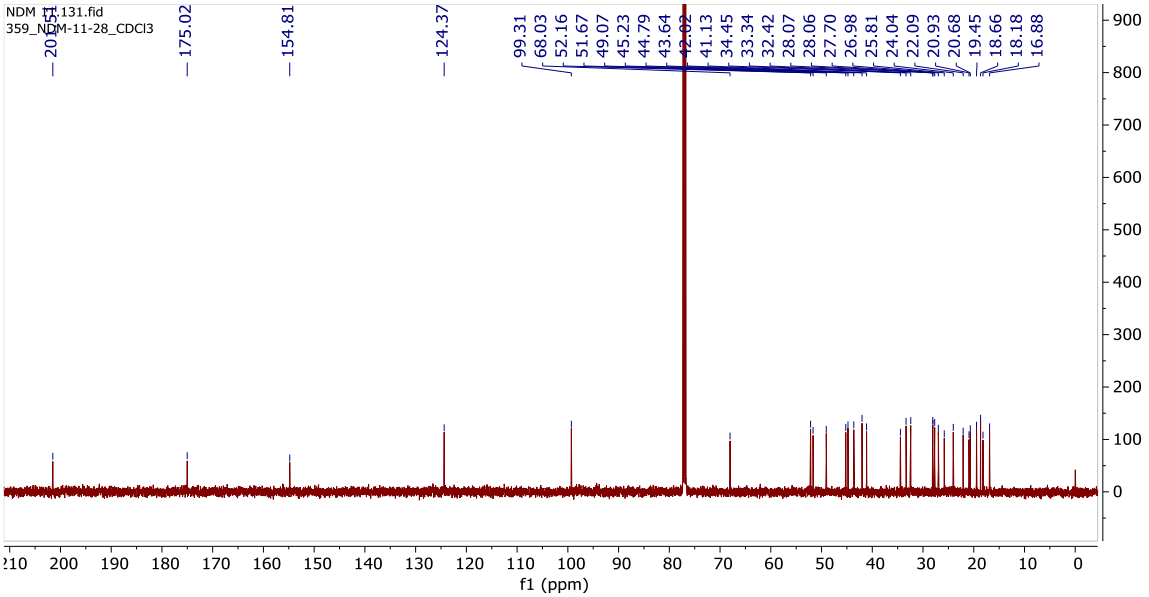
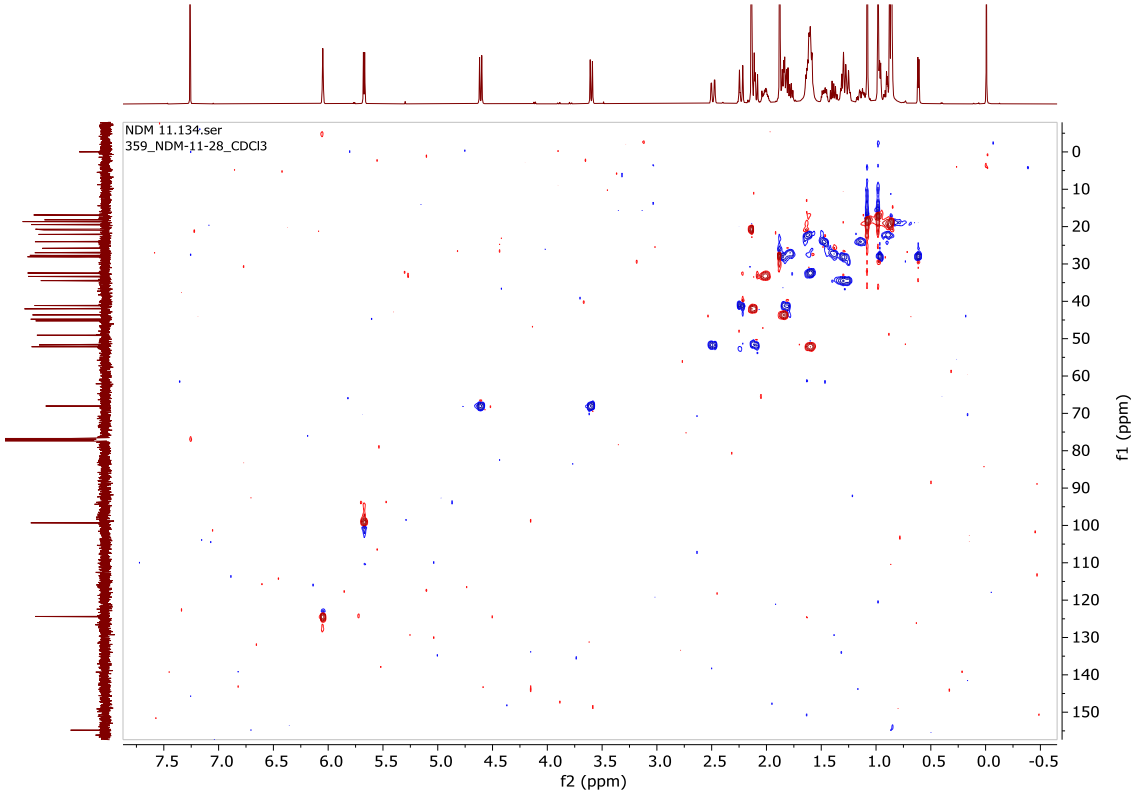
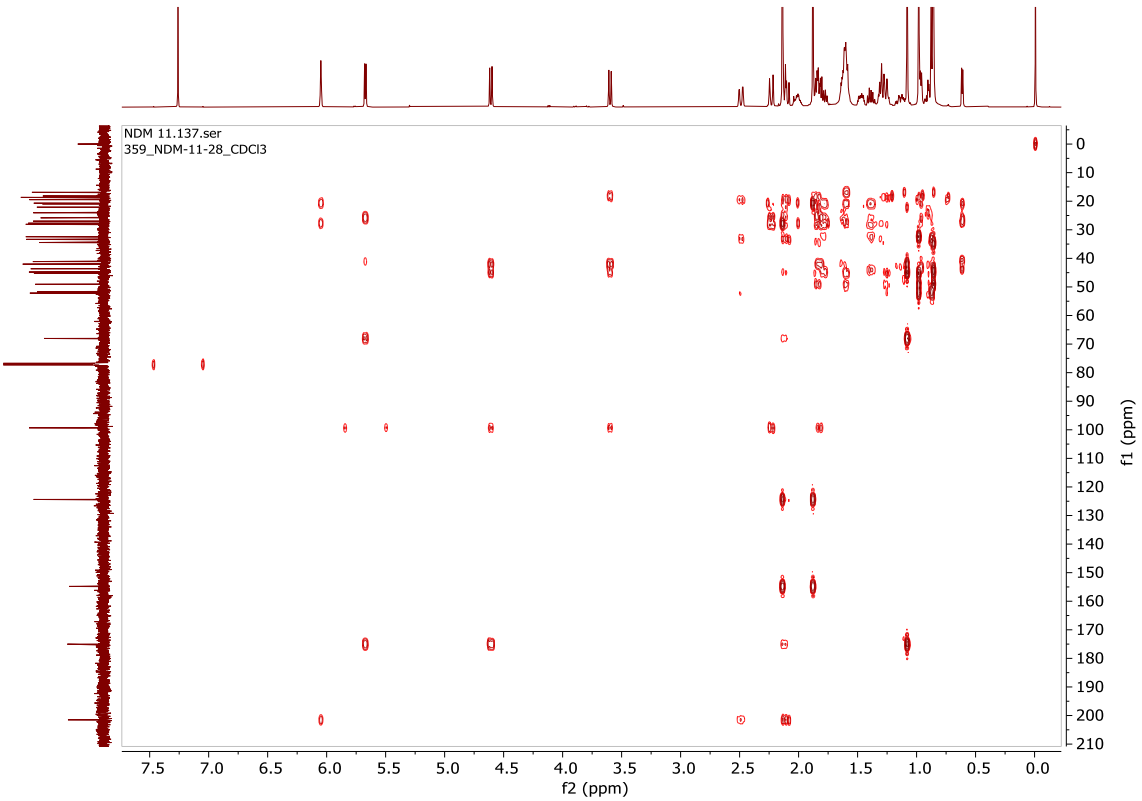


Figure A.29: HSQC and HMBC NMR spectrum of compound **6** in $CDCl_3$[93]

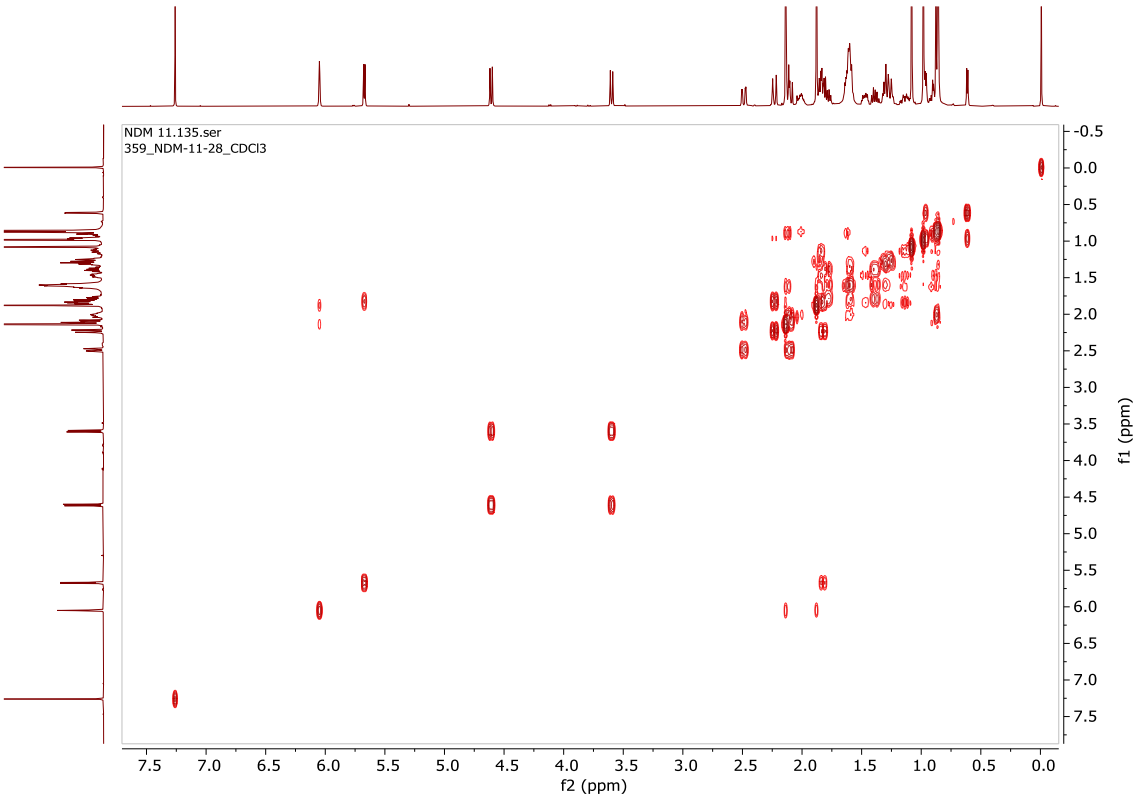


HSQC

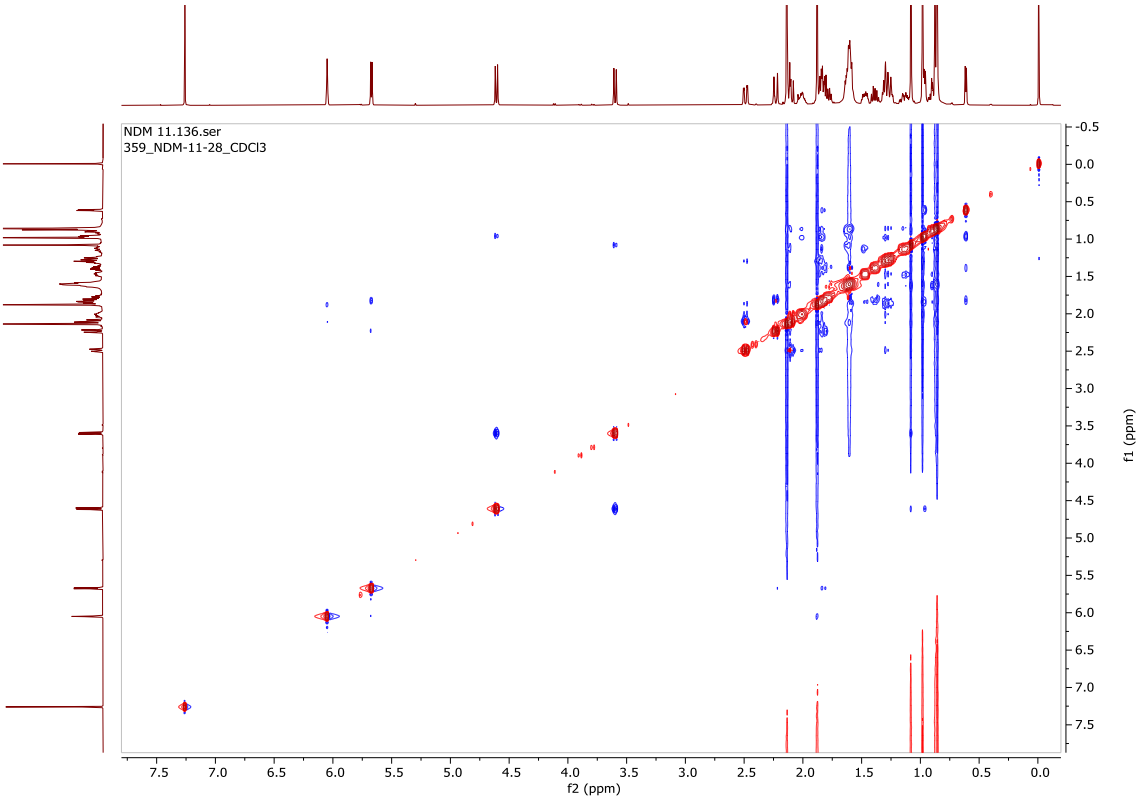


HMBC

Figure A.30: ^{1}H-^{1}H COSY and NOESY NMR spectra of compound **6** in $CDCl_3$ [93]



COSY



NOESY

Figure A.31: HRESIMS spectrum of compound **6** [93]

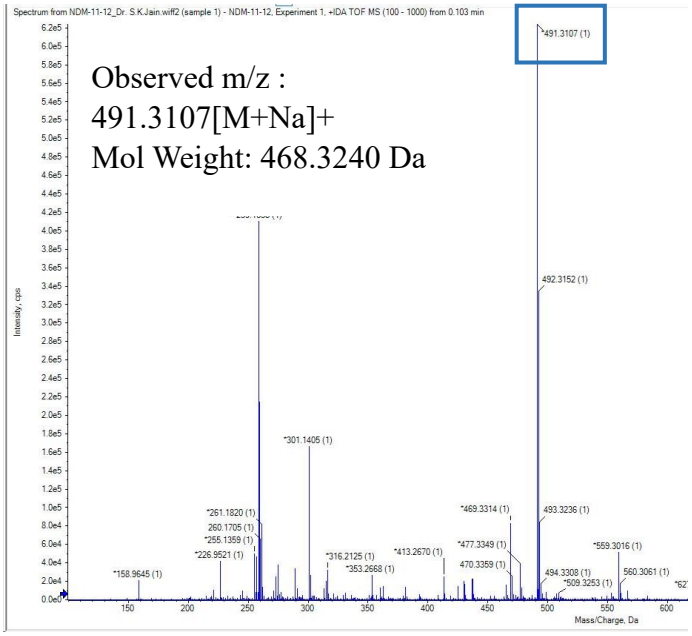


Figure A.32. ^{1}H NMR spectrum of compound **7** in $CDCl_3$ [93]

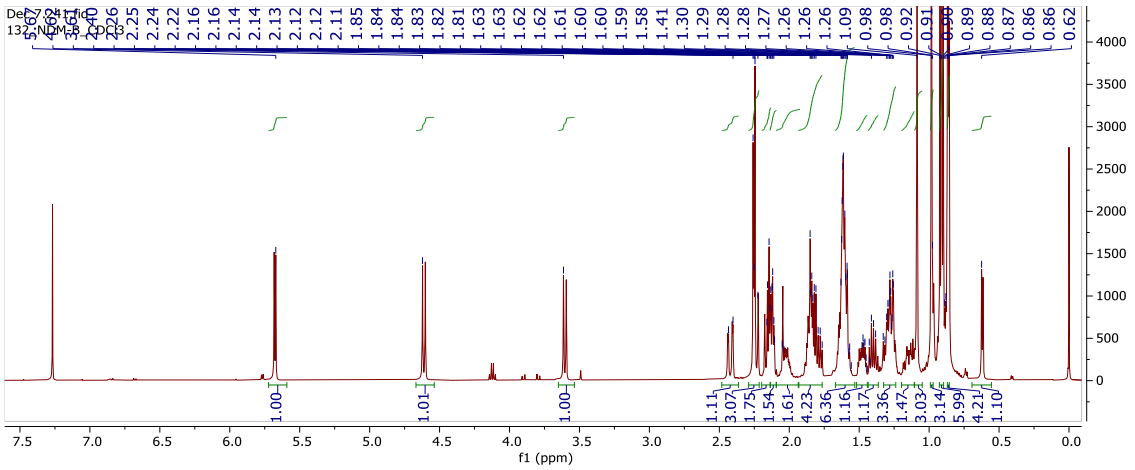


Figure A.33. HSQC spectrum of compound **7** in $CDCl_3$ [93]

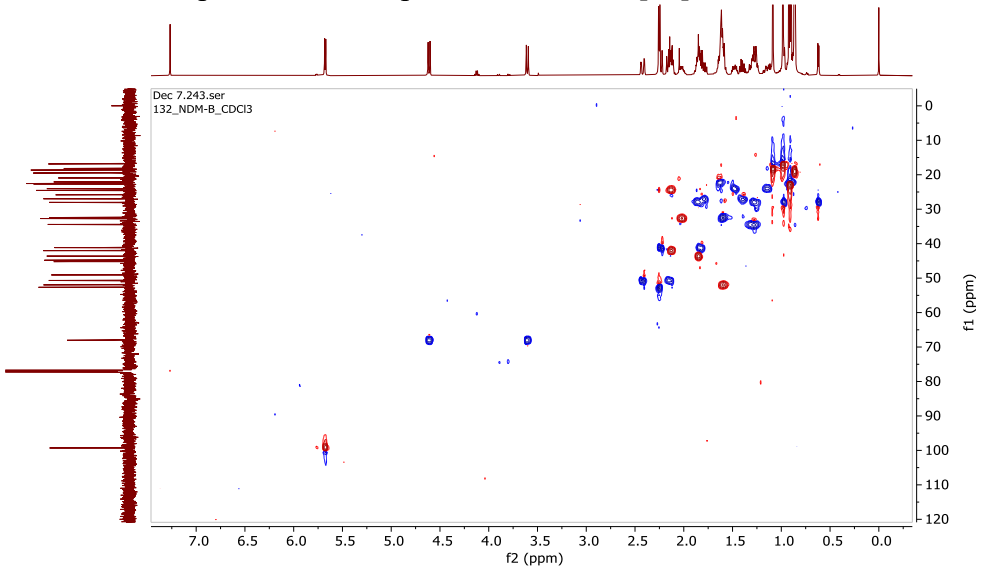
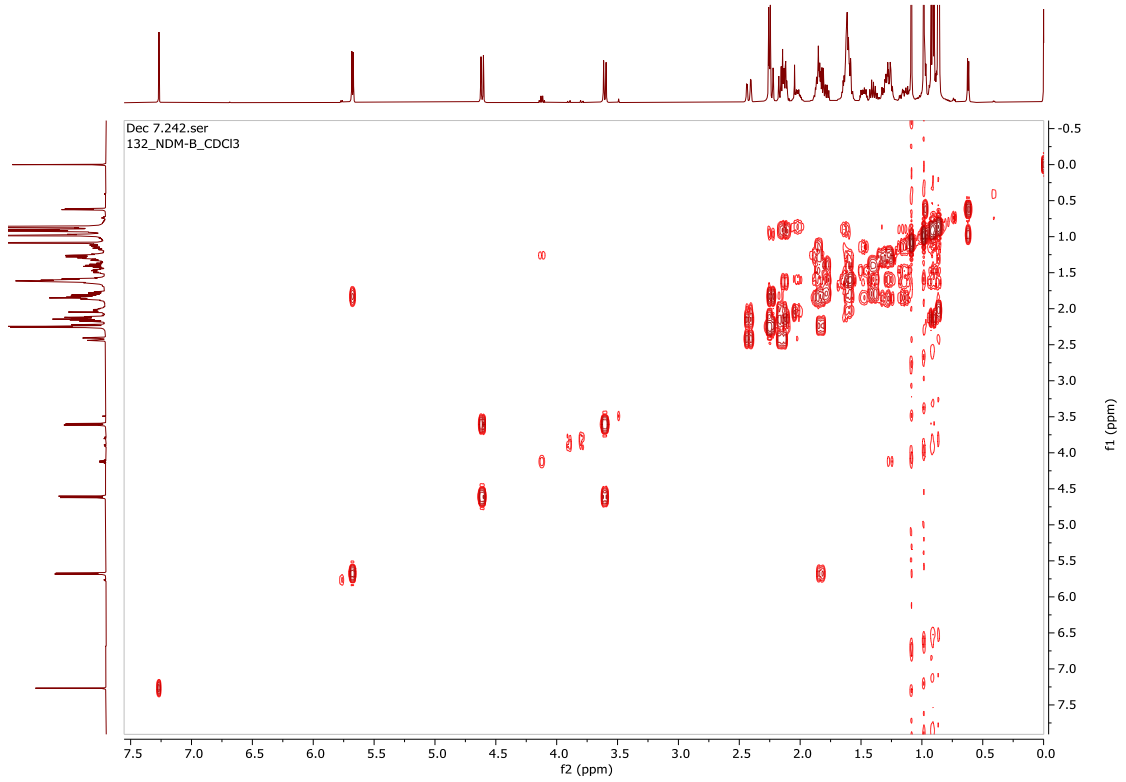
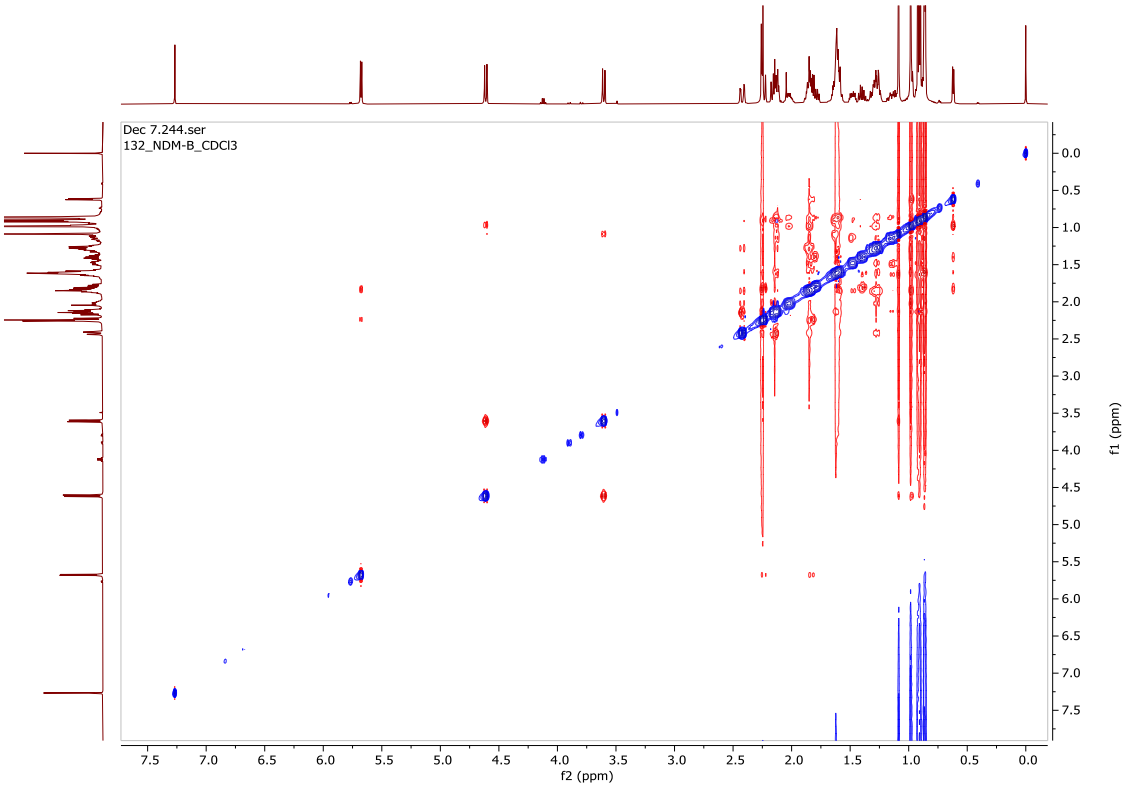


Figure A.34. ^{1}H-^{1}H COSY and NOESY spectrum of compound **7** in $CDCl_3$ [93]



COSY



NOESY

Figure A.35: HRMS spectrum of compound **7** in $CDCl_3$ [93]

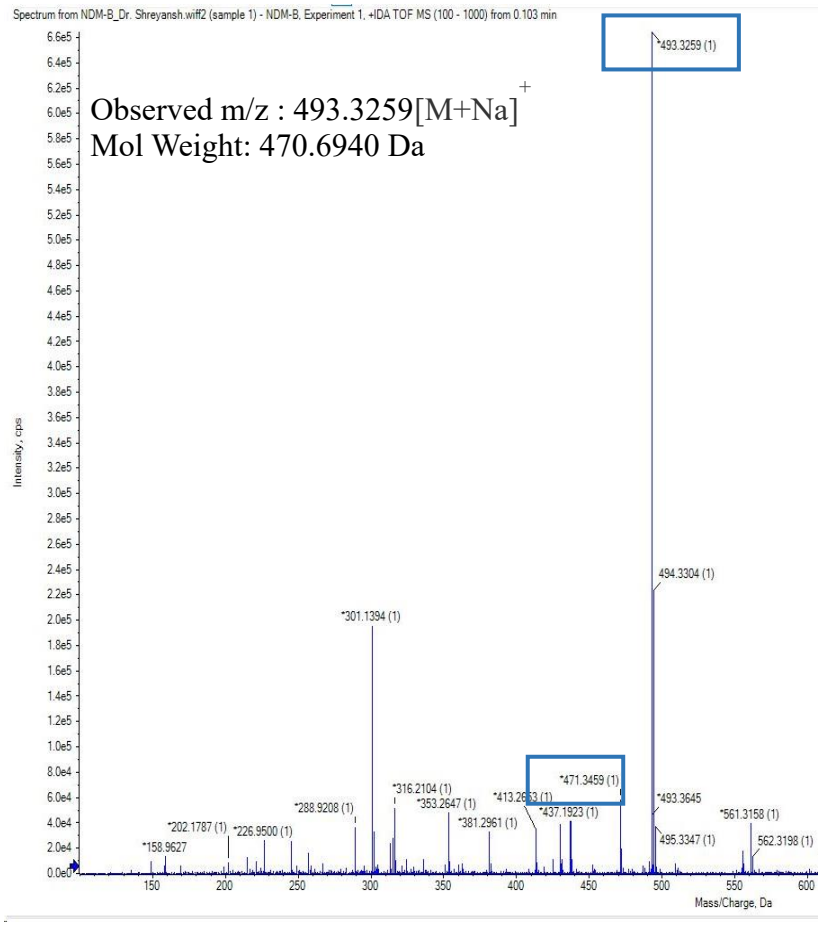


Figure A.36: DEPT-135 NMR spectrum of compound **8** in CD_3OD [93]

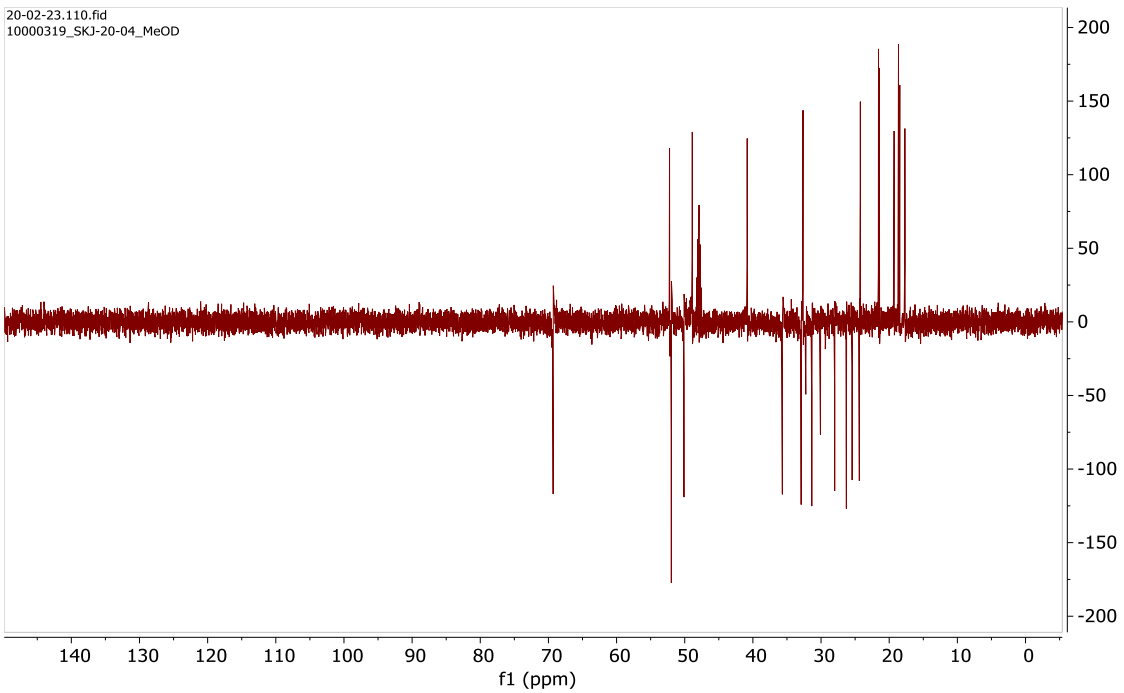
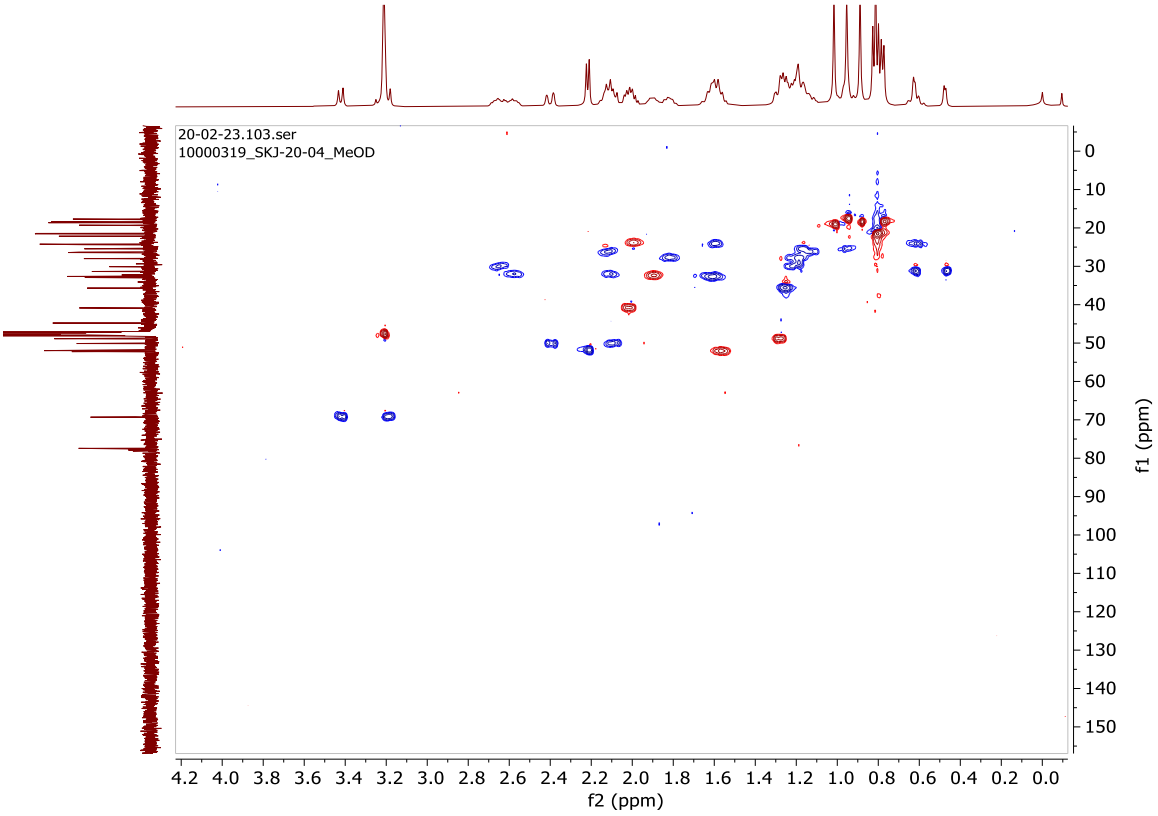
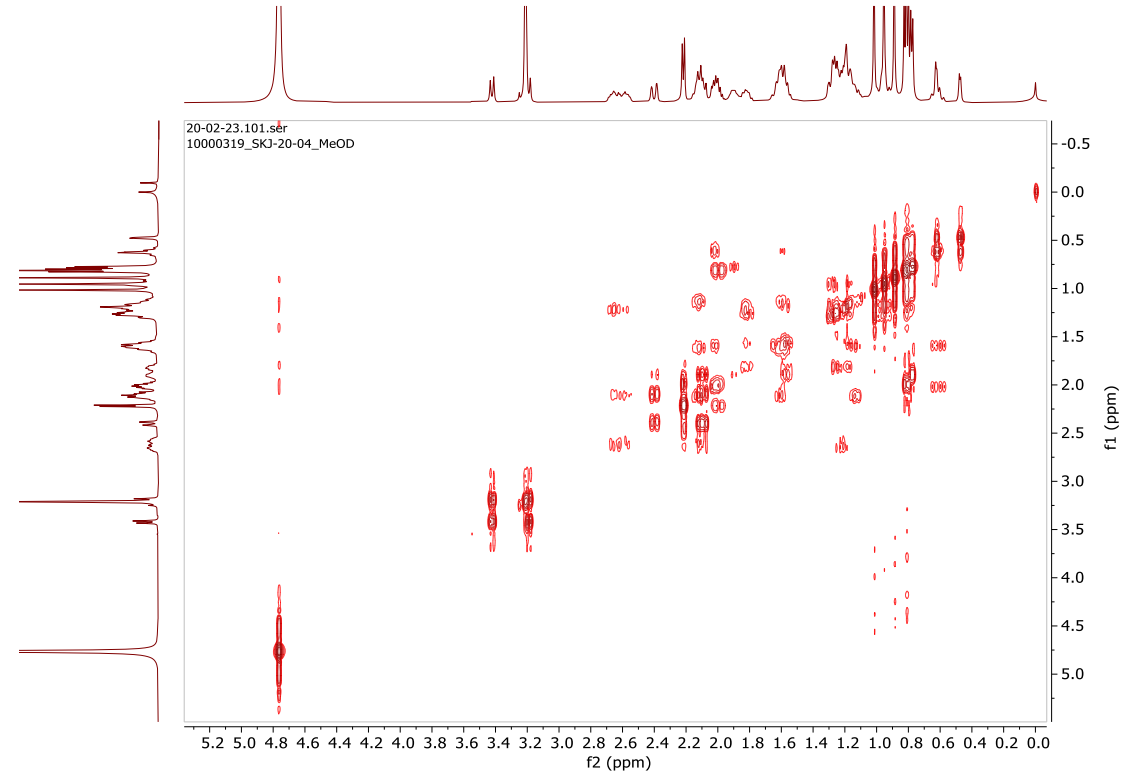


Figure A.37: HSQC and COSY NMR spectra of compound **8** in CD_3OD [93]



HSQC



COSY

Figure A.37: NOESY NMR spectra of compound **8** CD_3OD [93]

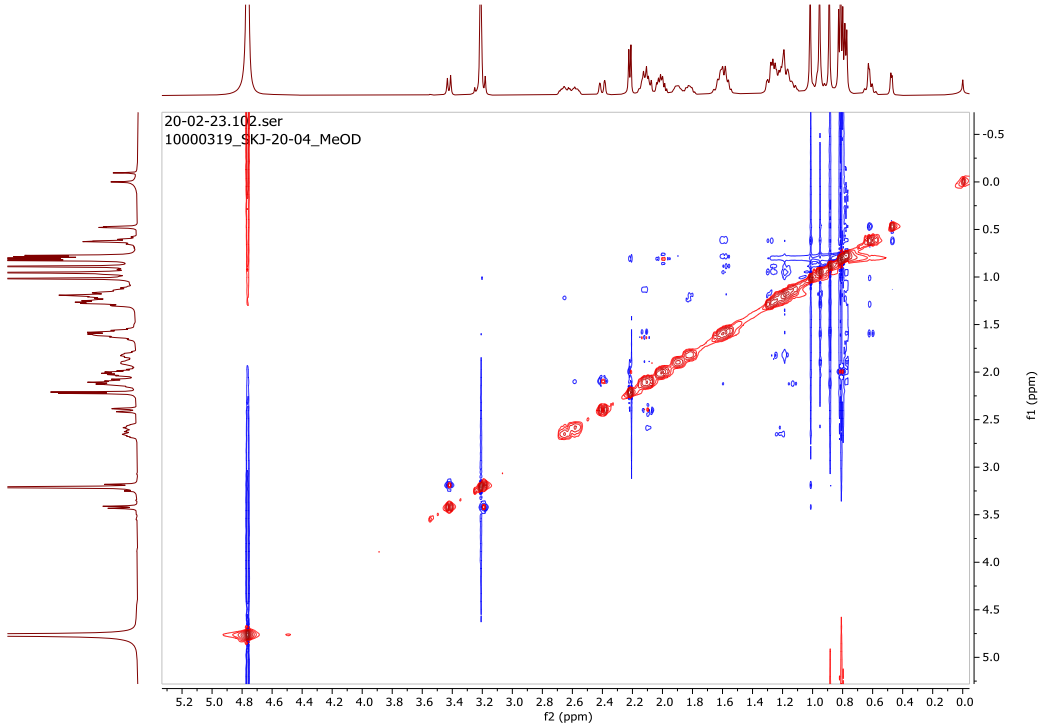


Figure A.38: HRMS spectrum of compound **8** [93]

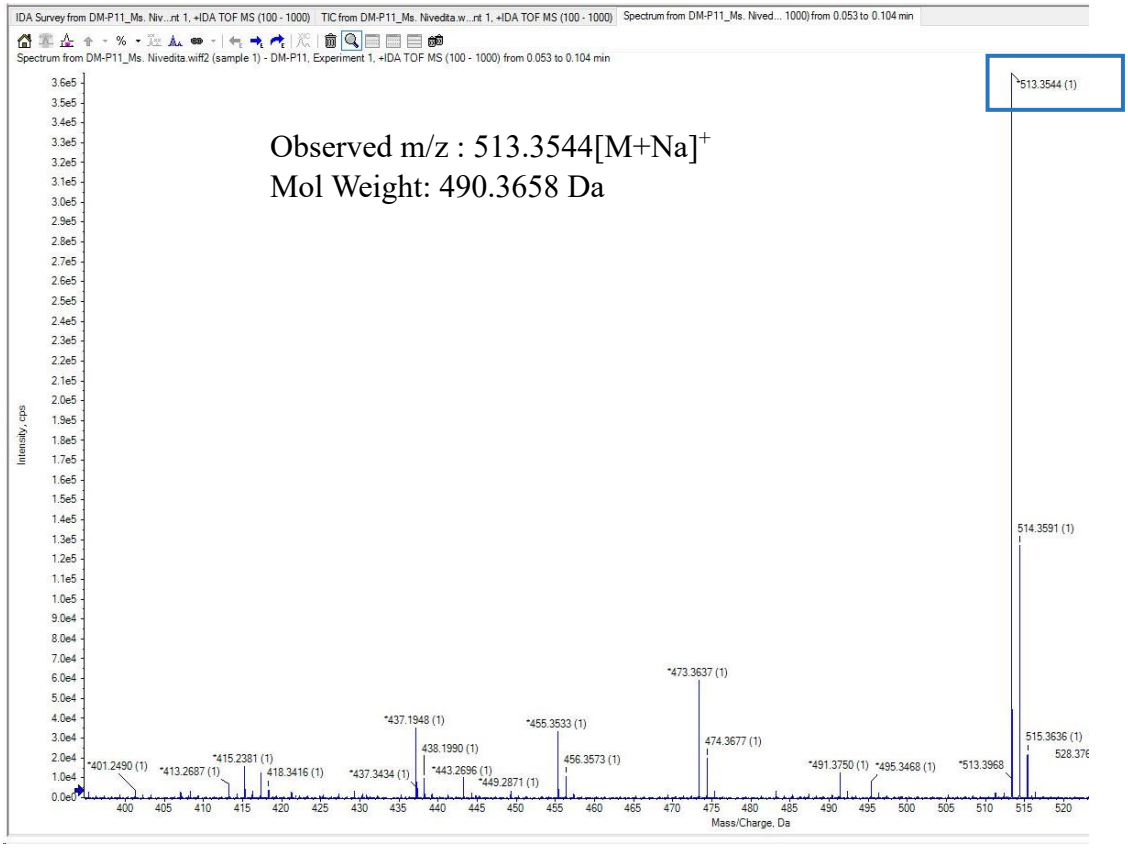


Figure A.39: ^{13}C NMR spectrum of compound **9** in CD_3OD [94]

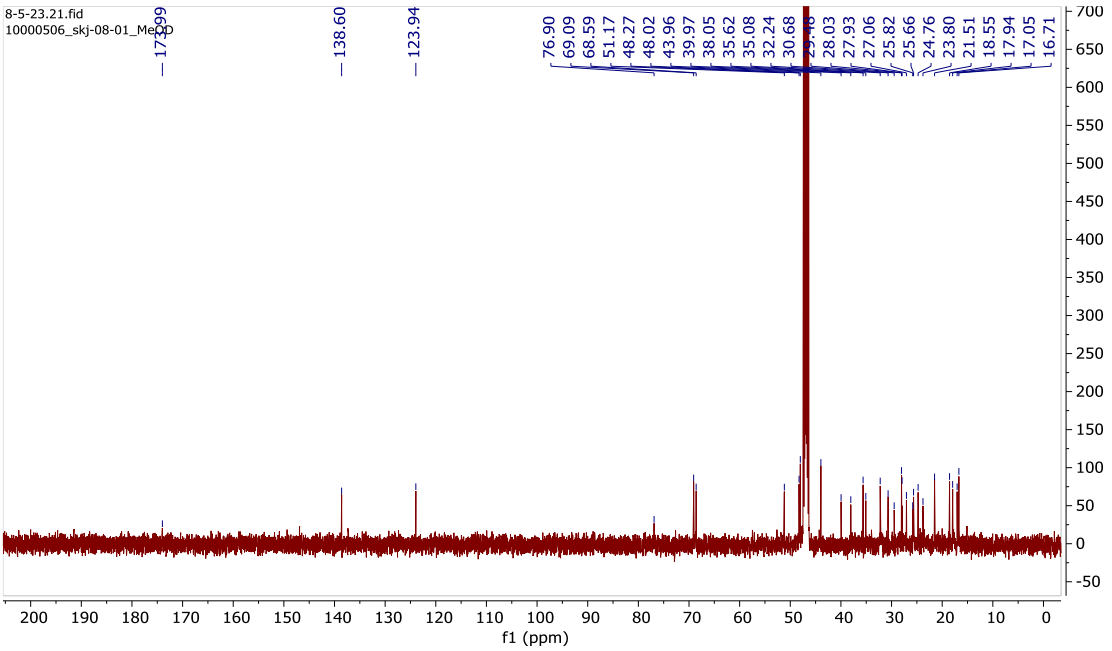


Figure A.40: HSQC NMR spectrum of compound **9** in CD_3OD [94]

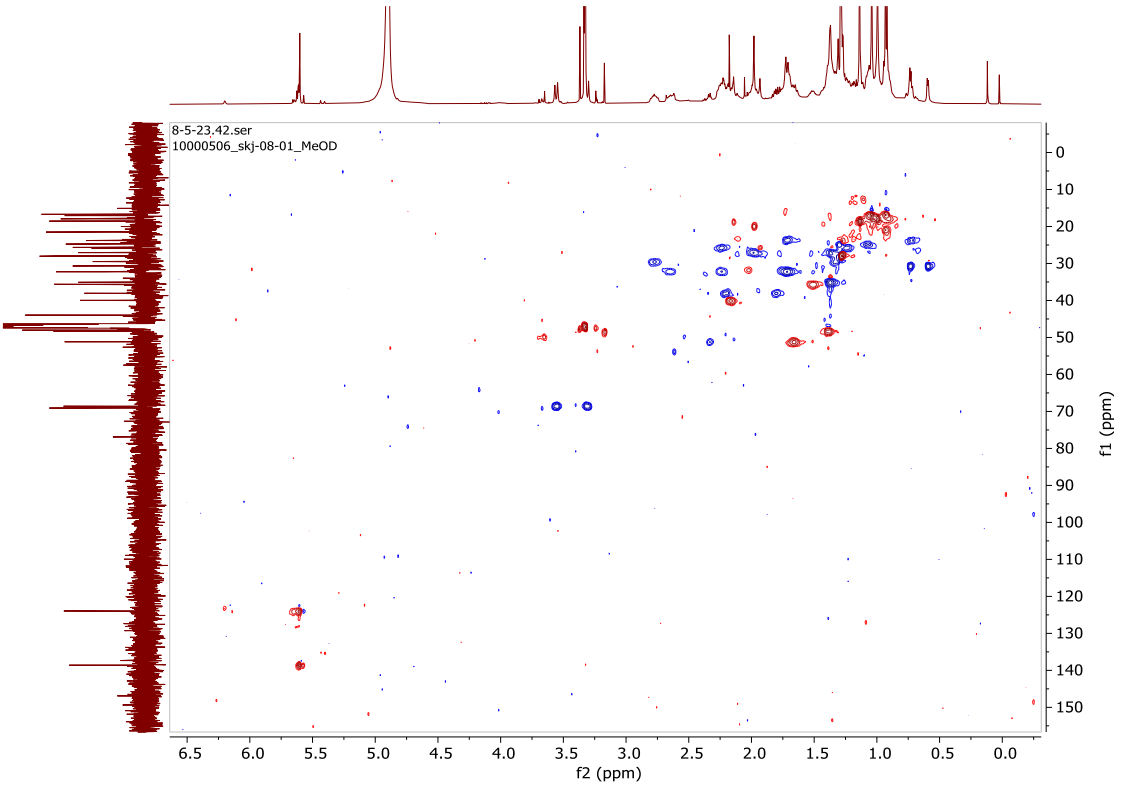
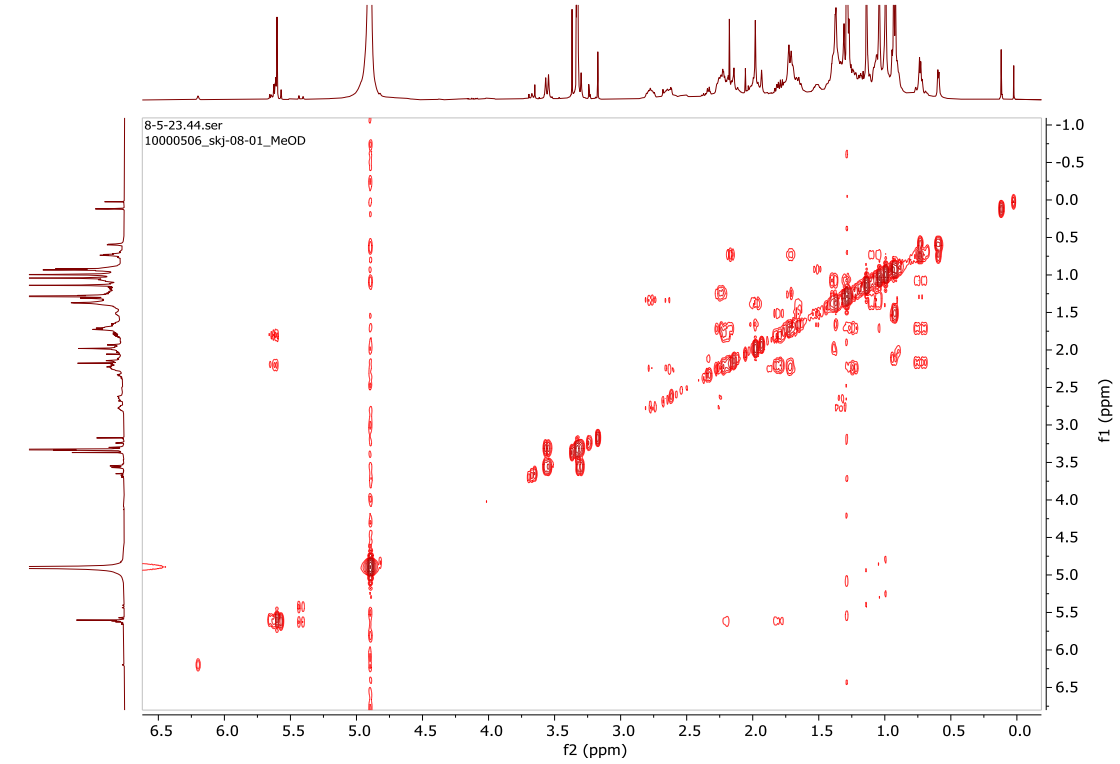
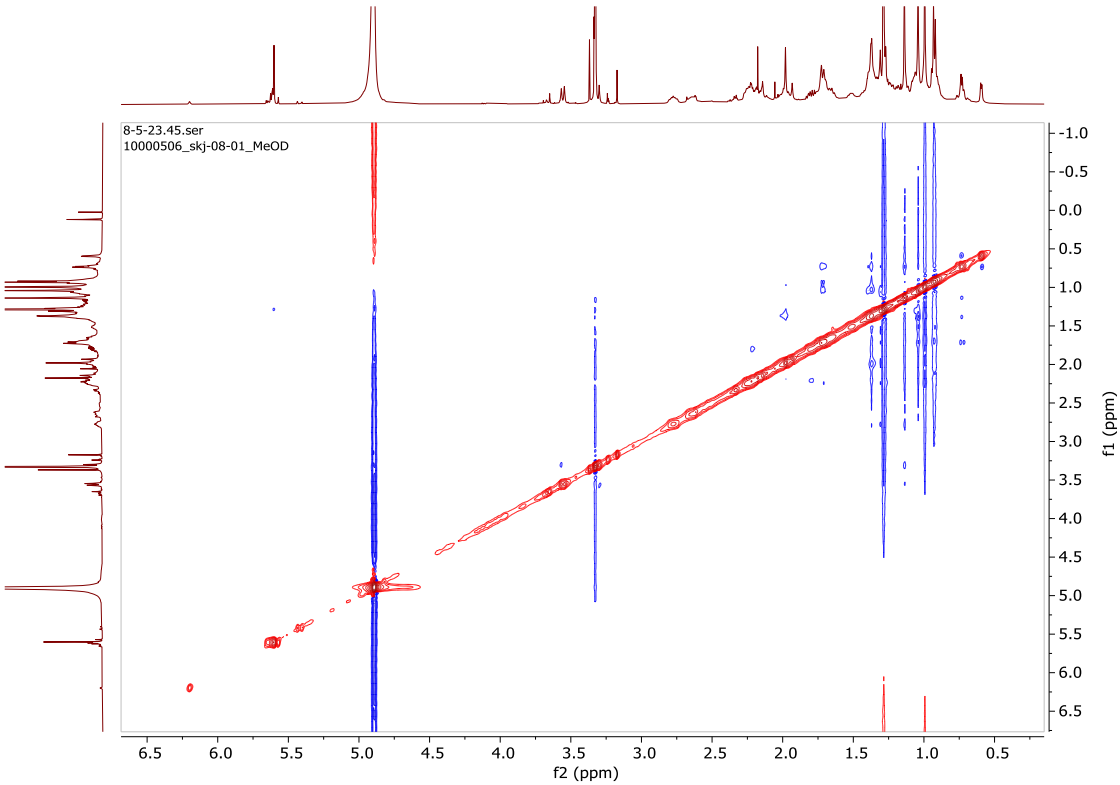


Figure A.41: ^{1}H-^{1}H COSY and NOESY NMR spectra of compound **9** in CD_3OD [94]



COSY



NOESY

Figure A.42: HRMS spectrum of compound **9** [94]

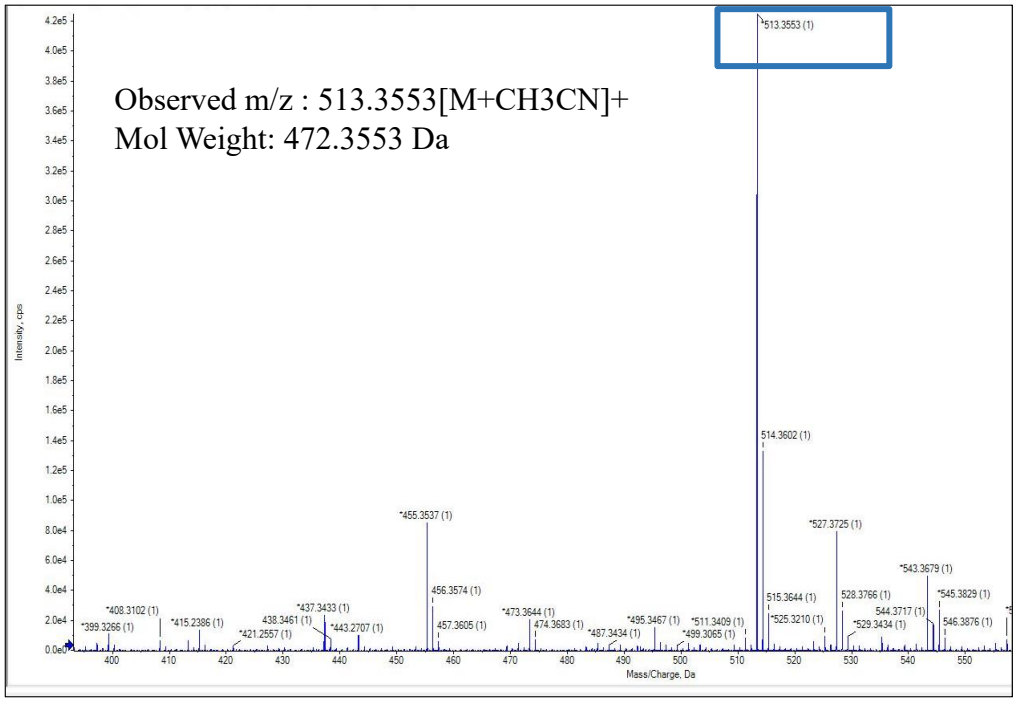


Figure A.43:^{13}C NMR spectrum of compound **10** in CD_3OD [94]

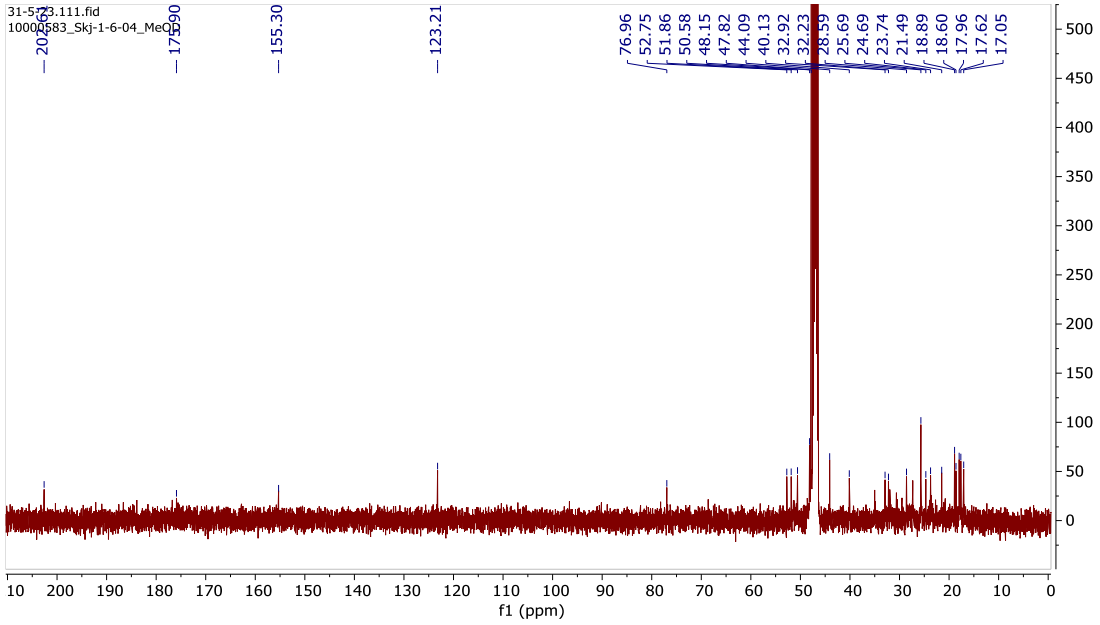
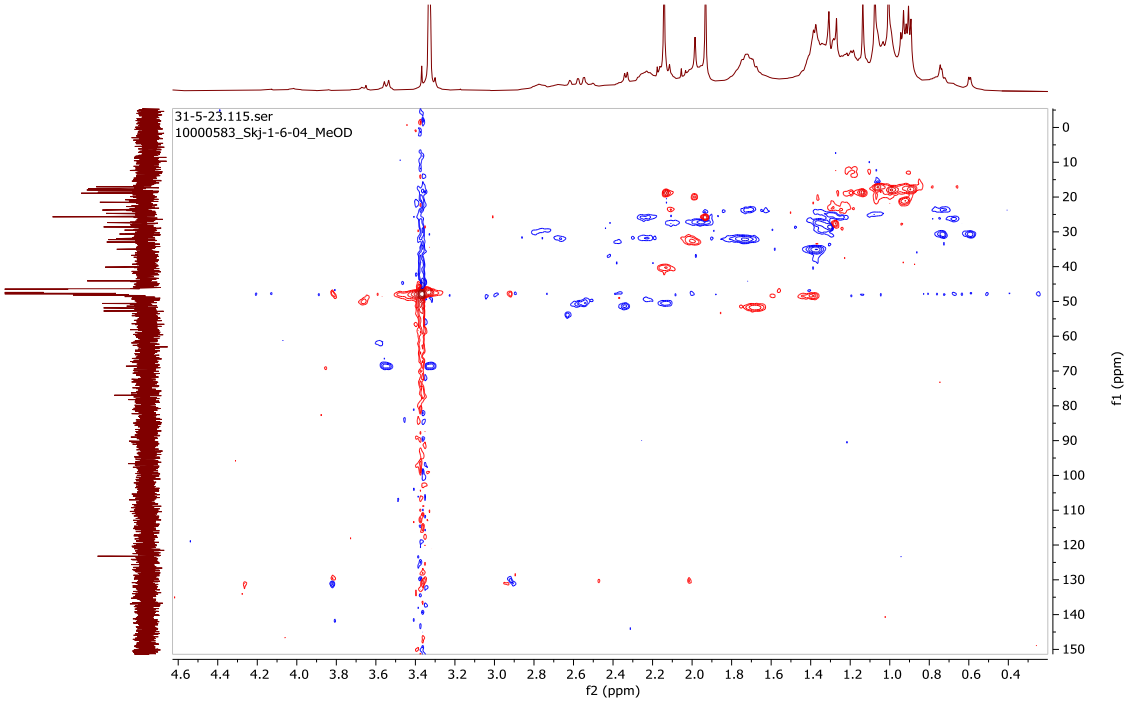
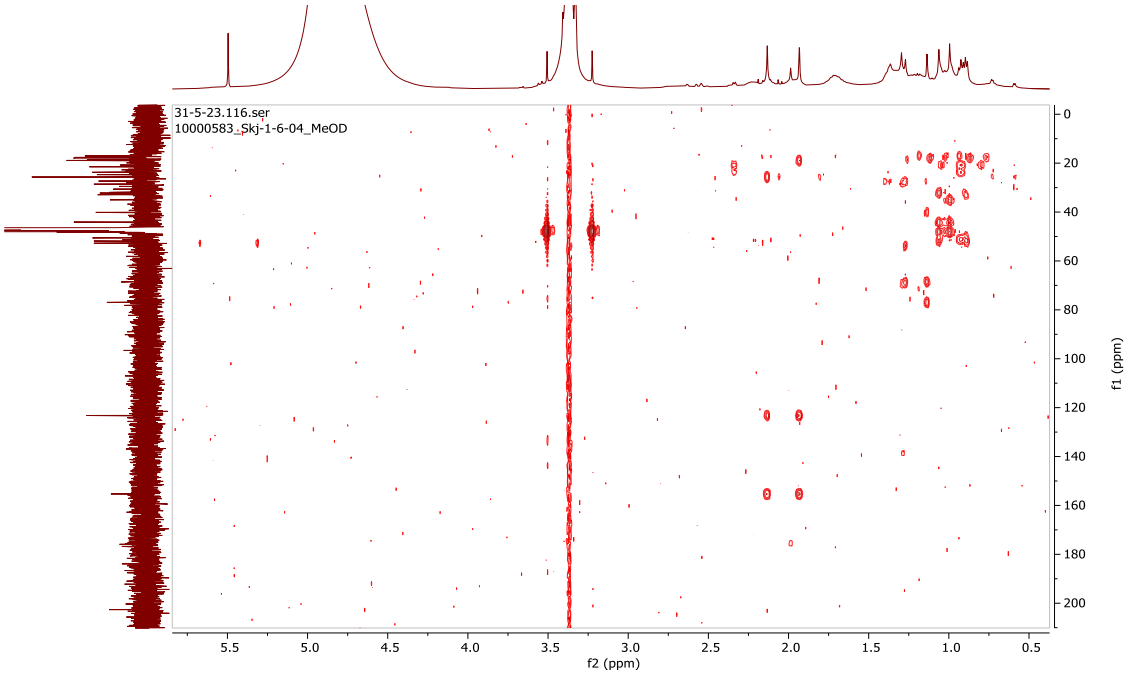


Figure A.44: HSQC and HMBC NMR spectrum of compound **10** in CD_3OD [94]

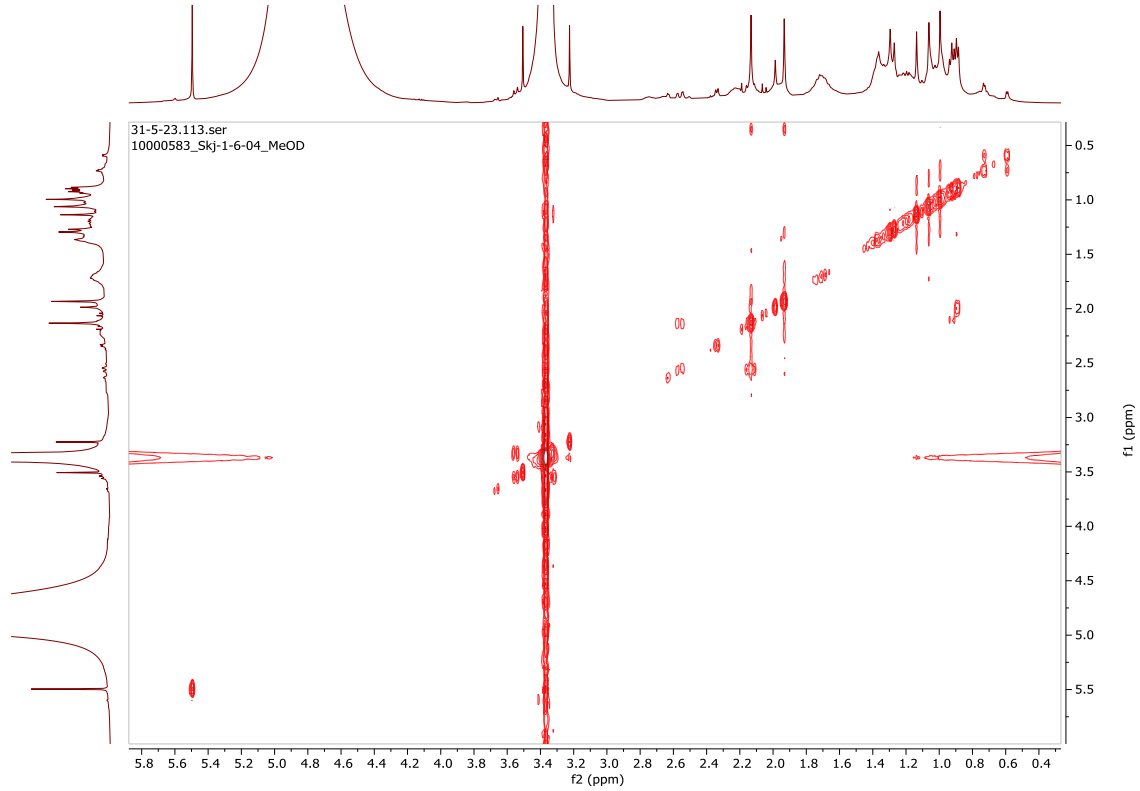


HSQC

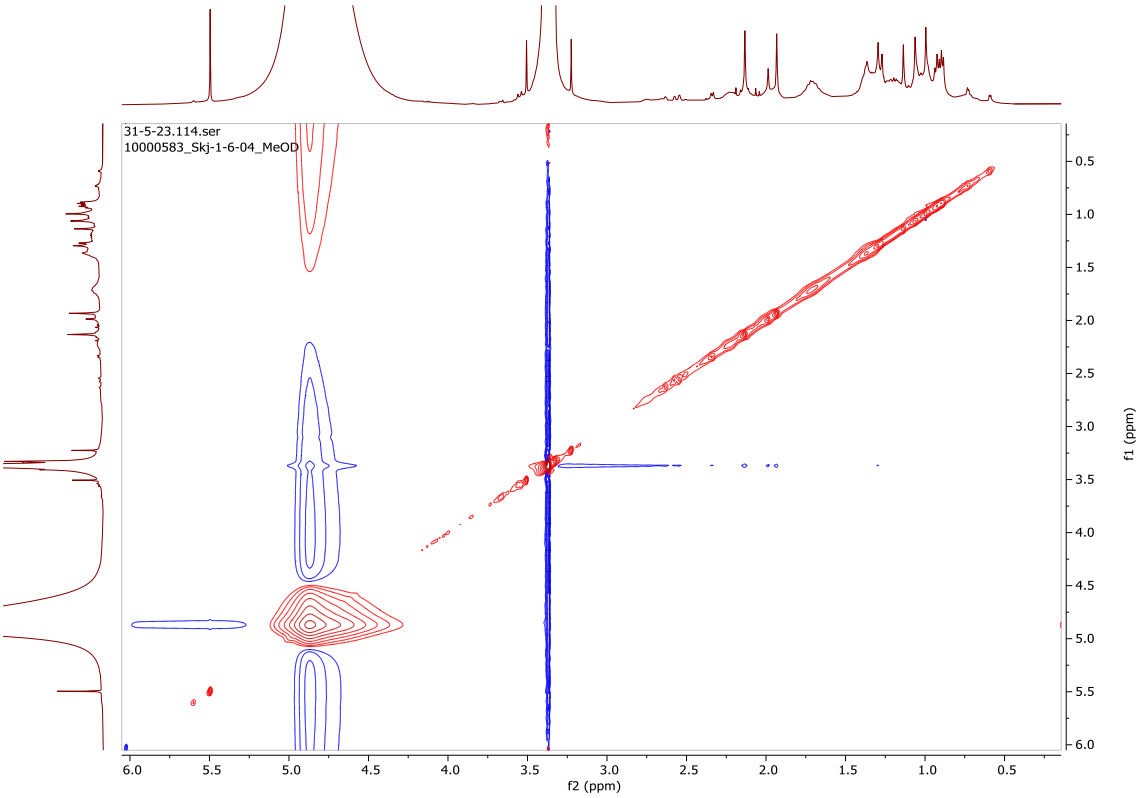


HMBC

Figure A.45: ^{1}H-^{1}H COSY and NOESY spectra of compound **10** in CD_3OD [94]

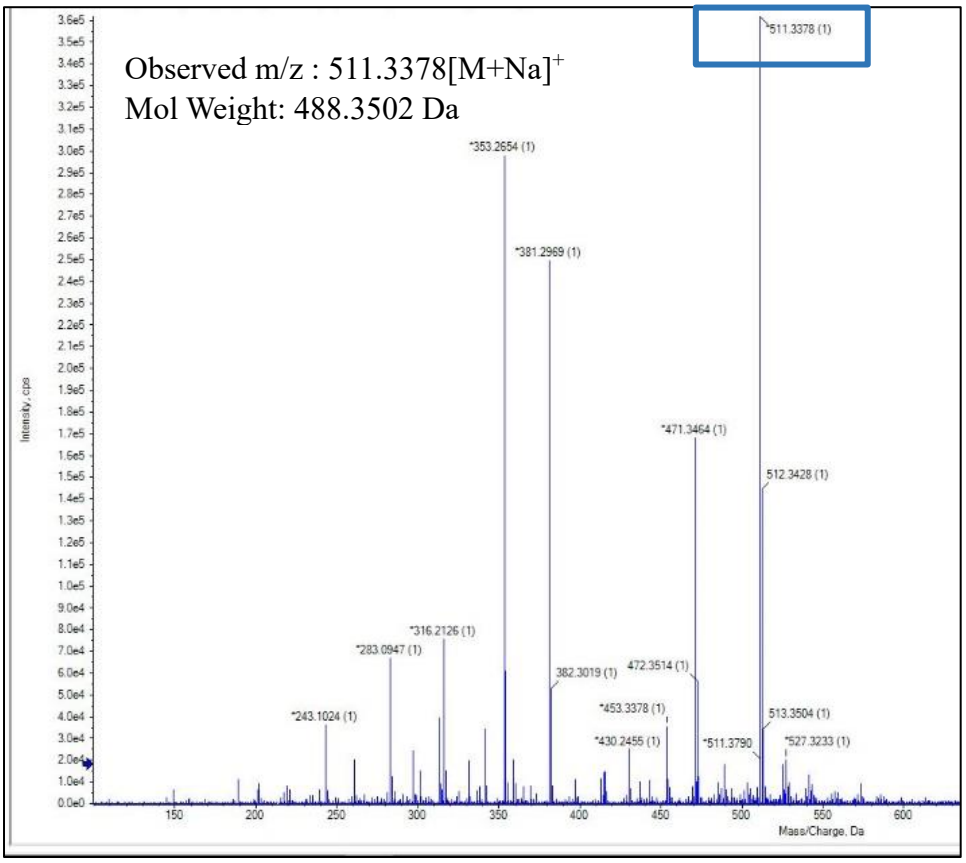


COSY



NOESY

Figure A.46: HRMS spectrum of compound **10** [94]



Spectral information of synthesized derivatives from series 1 and 2 [125-126].

1. *N-phenylacetamide (1c).* Yield 92%; white needles; mp 157°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (t, J =7.4 Hz, 2H), 7.33 (t, J = 7.3 Hz, 1H), 7.12 (d, J = 7.4 Hz, 2H), 2.19 (s,3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.5, 137.9, 129.0, 124.3, 119.9, 24.5. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for C_8H_9NO 136.1586; found 136.1582 .

2. *N-(4-chlorophenyl)acetamide (2c).* Yield 90%; white needles; mp 178°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, J = 8.8 Hz, 2H), 7.30 (d, J = 9.1 Hz, 2H), 2.20 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.3, 136.4, 129.2, 129.0, 121.0, 24.5. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for C_8H_8ClNO 170.0392; found 170.0388 .

3. *N-(4-bromophenyl)acetamide (3c).* Yield 88%; white needles; mp 166°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.44 (m, 1H), 7.43 (d, J = 3.4 Hz, 2H), 7.41 (d, J = 2.7 Hz, 1H), 7.33 (s, 1H), 2.19 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ168.3, 136.9, 131.9, 121.3, 116.8, 24.6. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for C_8H_8BrNO 213.9870; found 213.9868.

4. *N-phenylstearamide (4c).* Yield 88%; off white crystal; mp 96°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48(s, 1H), 7.24 (m, 2H) 6.93 (m, 1H), 6.84 (d, J=8.6 Hz, 2H), 6.72 (m, 2H),

2.26 (m, 2H), 1.69 (m, 6H), 1.28 (m, 22H), 0.91 (s,3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.3, 148.0, 129.1, 121.2, 113.5, 112.4, 34.5, 31.9, 31.1, 29.7, 29.6, 29.5, 29.3, 25.5, 24.6, 22.7, 14.2. HRMS (ESI) *m/z*: $[M+K]^+$ calcd for $C_{24}H_{41}NO$ 398.3292; found 398.3287

5. *N-(4-chlorophenyl)stearamide (5c).*Yield 90%; off white crystal; mp 57℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, J=8.9 Hz, 2H), 7.30 (d, J = 8.7 Hz, 2H), 2.38 (m, 2H), 1.76 (m, 2H), 1.64 (m,6H), 1.24 (m, 22H), 0.90 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 171.5, 136.5, 129.1, 128.9, 120.9, 37.8, 31.9, 29.7, 29.6, 29.7, 29.6, 29.5, 29.4, 29.3, 29.2, 25.5, 22.7, 14.1. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{40}ClNO$ 394.2879; found 394.2878.

6. *N-(4-bromophenyl)stearamide (6c).* Yield 82%; off white crystal; mp 113℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, J = 8.9 Hz, 2H), 7.15 (d, J = 8.7 Hz, 2H), 2.36 (m,2H), 2.07 (m, 2H), 1.75 (m,6H), 1.27 (m, 22H), 0.89 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.4, 132.0, 121.3, 116.7, 37.9, 31.9, 29.7, 29.7, 29.6, 29.5, 29.3, 29.3, 25.5, 22.7, 14.1. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{40}BrNO$ 438.2359; found 438.2355.

7. *N-phenyloleamide (7c).* Yield 82%; brownish semisolid; mp 41℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51(d, J = 8.6 Hz, 2H), 7.34 (d, J = 8.4 Hz, 2H), 7.12 (t,1H), 5.38 (m, 2H), 2.37 (t, 2H) 2.04 (m, 2H), 1.75 (m, 2H), 1.62 (m, 6H), 1.34 (m, 6H), 1.29 (m, 10H), 0.90 (t, J=6.4Hz 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.4, 137.9, 130.1 129.7, 128.9, 124.2, 119.7, 37.7, 31.9, 29.7, 29.7, 29.6, 29.3, 29.3, 29.3, 29.2, 29.1, 27.2, 27.1, 25.6, 22.7, 14.12. HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{24}H_{39}NO$ 380.2918; found 380.2917.

8. *N-(4-bromophenyl)oleamide (8c).* Yield 85%; orange semisolid; mp 121℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (s, 4H), 7.23 (s, 1H), 5.37 (m, 2H), 2.38 (t, 2H), 2.04 (m, 4H), 1.75 (m, 2H), 1.35-1.27 (m, 20H), 0.89 (t, J=6.4Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$) δ171.4, 137.0, 131.9, 130.1, 129.7, 121.2, 37.9, 31.9, 31.5, 29.8, 29.5, 29.4, 29.2, 29.1, 27.2, 25.5, 22.5, 14.1. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{39}BrNO$ 437.2192; found 436.2189.

9. *N-(2-amino-4-nitrophenyl)oleomide (9c).* Yield 64%; red solid; mp 126 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.11 (s,1H), 8.60 (s,1H), 7.86 (d, J=8.9Hz,1H), 7.83 (d, J=8.9Hz,1H), 5.37 (d, J=8.5Hz,1H), 5.36 (d, J=8.5Hz,1H), 2.35 (t, 2H), 2.08 (m, 2H), 1.68 (m,6H), 1.33 (m, 6H), 1.28 (m, 10H), 0.89 (t, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 179.70, 130.72, 130.03, 129.73, 128.89, 128.06, 127.90, 119.12, 33.98, 31.94, 29.78, 29.69, 29.54, 29.34, 29.16, 29.08, 29.04, 27.23, 24.68, 22.70, 14.0. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{39}N_3O_3$ 437.1929; found 437.1926.

10. *N-phenylbenzamide (10c).* Yield 90%; white solid; mp 163 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90(d, J=7.8 Hz, 2H), 7.68(d, J = 8.2 Hz,2H), 7.59 7.56(m, 3H), 7.50 7.49(m, 2H) 7.41-7.38 (m,1H), 7.20- 7.16 (m,1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.7, 137.9, 135.0, 131.8, 129.1, 128.8, 127.0, 124.5, 120.2. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{13}H_{11}NO$ for 198.0919; found 198.0918

11. *N-(4-bromophenyl)-benzamide (11c).* Yield: 88%, white powder; mp 204 ℃; ^{1}H NMR (500 MHz, DMSO-d6) δ 10.38 (s, 1H), 7.95-7.94 (m, 2H), 7.84–7.72 (m, 2H), 7.68– 7.52 (m, 5H); ^{13}C NMR (125 MHz, DMSO-d6) δ 166.1, 139.0, 135.1, 132.2, 131.9, 128.9, 128.1, 122.72, 115.8. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{13}H_{10}BrNO$ 276.0021; found 276.0019.

12. *N-(4-chlorophenyl)-benzamide (12c).* Yield 91%; pale yellow powder; mp 195℃; ^{1}H NMR (500 MHz, DMSO- d6) δ 10.39 (s, 1H), 8.05 – 7.90 (m, 2H), 7.90 – 7.74 (m, 2H), 7.70 – 7.48 (m, 3H), 7.54 – 7.31 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d6) δ 166.2, 138.6, 135.1, 132.2, 129.0, 128.9, 128.1, 127.8, 122.4. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{13}H_{10}ClNO$ 232.0538; found 232.0534.

13. *N-phenylcinnamamide (13c).* Yields 85%; yellow crystals; mp 146 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.65(s, 1H), 7.78(dd, J=7.15Hz, 2H), 7.73(dd, J=7.84Hz, 2H), 7.43(m,2H), 7.34(m,2H), 7.29(m,1H) 7.13(d,1H, J=16 Hz), 6.77(d,1H, J=16 Hz), 6.73(m,1H); ^{13}C NMR (125 MHz, CDCl3) δ 164.8, 142.2, 138.2, 134.6, 129.9, 129.1, 128.8, 127.9, 124.5, 121.2, 120.4, 119.9. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}NO$ 224.1075; found 224.1073.

14. *N-(4-chlorophenyl)cinnamamide (14c).* Yields 86%; transparent crystals; mp 186 ℃, ^{1}H NMR (500 MHz, DMSO-d6) δ 10.37(s, 1H), 7.75(d, J=15.8, 1H), 7.65(d, J=8Hz, 2H) 7.64-7.61(m, 2H), 7.45(m, 1H) 7.38(m, 2H), 7.13(d, J=8.8Hz, 2H), 6.85 (d, J=15.8 Hz,1H); ^{13}C NMR (125 MHz, DMSO-d6) δ 164.1, 141.0, 138.7, 135.1, 130.3, 129.5, 129.2, 128.9, 128.2, 127.4, 122.4, 121.2. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{12}ClNO$ 259.1338; found 259.1334.

15. *N,2-diphenylacetamide (15c).* Yields 80%; off white powder; mp 118 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44(d, J = 8.4 Hz, 2H), 7.42(m, 2H), 7.37(d, 2H), 7.32(m, 2H), 7.30(m, 1H) 7.11 (m, 1H), 3.75(s, 2H); ^{13}C NMR (125MHz, $CDCl_3$) δ 169.2, 137.7, 134.5, 129.5, 129.2, 129.2, 128.9, 127.7, 124.5, 119.9, 44.8. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{13}NO$ 212.1075; found 212.1074.

16. *3-(3,4-dihydroxyphenyl)-N-phenylacrylamide (16c).* Yields 75%; pale yellow powder; mp 235 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.89(s,1H), 8.37(s,1H), 8.08(s,1H),

7.58(d, J=8.4Hz, 2H), 7.38(m, 2H)), 7.37(d, J=8.9,1H), 7.35 (d, J=8.9Hz,1H),7.32(m,1H) 7.20(s,1H), 7.14(d, J=8.2Hz, 1H), 7.13(d, J=8.2Hz,1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.0, 159.5, 137.0, 136.8, 129.8, 129.1, 125.3, 124.8, 120.1, 118.8. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}NO_3$ 255.1076; found 255.1072.

17. *4-amino-N-phenylbenzamide (17c).* Yields 78%; brown solid; mp 135 °C; ^{1}H NMR (500 MHz, DMSO-d6) δ 9.76(s, 1H), 7.76-7.72(m, 4H), 7.32(t, J = 7.8 Hz, 2H), 7.05(t, J = 7.3 Hz, 1H), 6.62 (d, J=8.5Hz, 2H),5.79(s, 2H); ^{13}C NMR (125 MHz, DMSO-d6) δ 165.7, 152.4, 140.2, 129.8, 128.8, 123.3, 121.7, 120.5, 113.1. HRMS (ESI) *m/z*: $[M+H]^+$ 214.1288 calcd for $C_{13}H_{12}N_2O$ 213.1259; found 213.1255

18. *3-chloro-4-nitro-N-phenylbenzamide (18c).* Yields 64%; red crystals; mp 197 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36(1H, s), 8.29(1H, s), 8.03(d,1H) 7.66(d, 2H, J=8.6Hz), 7.61(d,1H, J=8.4Hz) 7.39-7.35(2H, m), 7.22-7.19 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.6, 147.7, 137.0, 134.6, 132.5, 131.7, 130.5, 129.2, 125.4, 124.2, 120.7. HRMS (ESI) *m/z*: $[M+Na]^+$calcd for $C_{13}H_9ClN_2O_3Na$ 299.0112; found 299.0109.

19. *2-amino-N-(4-chlorophenyl)acetamide (19c).* Yields 70%; pale yellow powder; mp 215 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.45(s, 2H) 7.61(d, 2H, J=8.2Hz), 7.28 (d, 2H, J=8.4Hz), 3.42(m, 2H) 13C NMR (125 MHz, $CDCl_3$) δ 168.26, 146.55, 145.94, 135.52, 129.23, 121.04, 107.05, 47.44. HRMS (ESI) *m/z*: $[M+H]^+$calcd for $C_8H_9ClN_2O$ 185.1159; found 185.1158.

20. *4-methoxy-N-phenylbenzamide (20c).* Yield 83%; white powder; mp 140-160°C; ^{1}H NMR (500 MHz, DMSO-d6) δ 10.12(s,1H), 7.95(d, J=8.4 Hz, 2H), 7.68(d, J=8.2Hz, 2H), 7.58(d, J=8.6 Hz, 2H), 7.50(m,1H), 6.94(d, J=8.4 Hz, 2H), 3.74(s, 3H); ^{13}C NMR (125 MHz, DMSO-d6) δ 165.6, 156.0, 135.5, 132.7, 131.8, 128.8, 128.0, 122.4, 122.3, 114.2, 55.7. HRMS (ESI) *m/z*: $[M+Na]^+$calcd for $C_{14}H_{13}NO_2Na$ 250.0775 found 250.0772.

21. *2-fluoro-N-(4-methoxyphenyl)benzamide (21c).* Yield 70%; brown powder, mp 178–188 °C; ^{1}H NMR (125 MHz, $CDCl_3$) δ 8.42(d, J=8.0 Hz,1H), 8.19 8.14(m, 1H), 7.60 7.57(m, 2H) 7.54-7.51(m,1H) 7.33-7.29(m,1H), 7.18(m,1H), 6.93-6.91(d, J=8.2Hz,2H) 3.83(s,3H);13C NMR (125 MHz, $CDCl_3$) δ 161.4, 161.1, 159.4, 156.8, 133.5, 133.5(d, J=2.8 Hz), 132.2, 132.2, 132.2, 130.8(d, J=3.0 Hz), 125.1(d, J=8.9 Hz),125.0, 122.5, 122.2 (d, J=7.8 Hz),121.5, 121.4, 116.1, 115.9(d, J=22.0 Hz),114.2(d, J=22.0 Hz), 55.5. HRMS (ESI) *m/z*: $[M+Na]^+$calcd for $C_{14}H_{12}FNO_2Na$ 268.0677; found 268.0674.

22. *N-(4-ethoxyphenyl)benzamide (22c).* Yield 78%; white solid; mp 170-175°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89(d, J = 7.6 Hz, 2H,), 7.50(d, J=8.4 Hz, 2H) 7.54(m, 3H), 6.93, (d, J=8.6 Hz, 2H), 4.07(m,2H), 1.42(t, J = 6.6 Hz, 3H);^{13}C NMR (125 MHz, $CDCl_3$)

δ 165.6, 156.0, 135.1, 131.7, 130.9, 128.8, 126.9, 122.0, 114.9, 63.7, 14.8. HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{15}NO_2Na$ 264.0933; found 264.0931.

23. *N-(4-ethoxyphenyl)-2-fluorobenzamide (23c).* Yield 67%; white needles; mp 182-192°C; ^1H NMR (500 MHz, $CDCl_3$) δ 8.39(d, J = 8.0 Hz,1H), 8.20(m, 1H), 7.58 7.52(m, 3H),7.34(m,1H), 7.21(m,1H), 6.93(d, J=8.6 Hz, 2H),4.05(m,2H),1.42(t, J = 6.6 Hz, 3H); ^{13}C NMR (125 MHz, CDCl3) δ 161.4, 161.1, 159.4, 156.2, 133.6(d, J=2.8 Hz),133.3, 132.3, 132.2, 130.7(d, J=3.0 Hz),125.1(d, J=8.9 Hz),125.0,122.3(d, J=7.8 Hz),121.5, 121.4, 116.2, 115.9(d, J=22.0 Hz),114.8(d, J=22.0 Hz), 63.7, 14.8. HRMS $[M+Na]^+$ *m/z* calcd for $C_{15}H_{14}FNO_2Na$ 282.0835; found 282.0831.

24. *N-butylbenzamide (24c).* Yield 69%; yellow liquid; mp 140-150 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 7.79(d, J=8.2Hz, 2H), 7.41-7.32(m,1H),7.29(m,2H), 3.37(m,2H), 1.55(m, 2H), 1.34(m,2H), 0.86 (t, J = 7.28 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.78, 134.84, 131.10, 128.30, 127.05, 39.85, 31.67, 20.16, 13.77. HRMS (ESI) *m/z*: $[M+Na]^+$calcd for $C_{11}H_{15}NONa$ 200.0984; found 200.0982.

25. *N-butyl-4-chlorobenzamide (25c).* Yield 80%; brown liquid; mp 155-165 °C; ^1H NMR ($CDCl_3$, 500 MHz) δ 7.72-7.70 (d, J=8.2Hz, 2H), 7.41-7.39 (d, J=8.2Hz 2H), 6.20 (s,1H), 3.47-3.30 (m,2H), 1.64-1.53 (m,2H), 1.46-1.34 (m,2H), 0.98-0.93 (m,3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 166.46, 137.51, 133.24, 128.76, 128.29, 39.39, 31.24, 19.97, 13.62. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{11}H_{14}ClNO$ 211.1747; Found 211.1744.

26. 4,6a,6b,8a,11,12,14b-heptamethyl-14-oxo-4-(phenylcarbamoyl)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-icosahydropicen-3-ylacetate(26c). Yields 72%; white crystalline solid; mp 284 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 7.48 (2H, d, J=8.0 Hz), 7.36 (2H, J = 8.5, d,), 7.20 (s, 1H), 7.18 – 7.13 (m, 1H), 5.58 (s, 1H), 5.45 (s, 1H), 2.48 (s, 3H), 2.13 (s, 3H), 1.97 – 1.86 (m, 3H), 1.81 (d, J=3.2 Hz, 1H), 1.67 (s, 3H), 1.61 – 1.42 (m, 7H), 1.35 (d, J=44.5 Hz, 10H), 1.22 (d, J=6.1 Hz, 6H), 1.06 (s, 1H), 0.97 (s, 3H), 0.84 (d, J = 7.2 Hz, 3H); 13C NMR (125 MHz, CDCl3) δ 198.8, 173.5, 170.2, 164.6, 137.4, 130.9, 129.1, 124.6, 120.6, 73.5, 60.4, 59.0, 50.6, 47.4, 45.0, 43.8, 40.9, 39.4, 39.3, 37.5, 34.9, 34.0, 33.3, 30.9, 28.9, 27.5, 27.2, 24.4, 23.8, 21.4, 21.1, 20.5, 19.6, 18.4, 17.4, 13.5. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{38}H_{53}NO$ 588.4059; found 588.4056.

27.4-((4-chlorophenyl)carbamoyl)-4,6a,6b,8a,11,12,14b-heptamethyl-14-oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-icosahydropicen-3-yl acetate (27c). Yields 70%; white crystalline solid; mp 291°C; ^1H NMR (500 MHz, $CDCl_3$) 7.44(2H, d, J=8.0), 7.32 (2H, d, J=8.5 Hz), 7.20 (s, 1H), 5.58 (s, 1H), 5.43 (s, 1H), 3.51

(s, 1H), 2.47 (s, 3H), 2.13 (s, 3H), 1.92- 1.82 (m, 3H), 1.80 (d, J=3.2 Hz, 1H), 1.67 (s, 3H), 1.66-1.42 (m, 7H), 1.34 (d, J=44.5Hz, 10H), 1.22 (d, J=6.1 Hz, 6H),1.06 (s, 1H),0.97(s, 3H), 0.82 (d, J=7.2Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.8, 173.6, 170.1, 164.8, 135.9, 130.6, 129.6, 129.1, 121.8, 73.3, 60.3, 59.0, 50.6, 47.5, 45.0, 43.8, 40.9, 39.4, 39.3, 37.5, 34.9, 34.0, 33.2, 30.9, 28.9, 27.5, 27.2, 24.4, 23.8, 21.4, 21.1, 20.5, 19.6, 18.4, 17.4, 13.5. HRMS (ESI) *m/z*: [M+H]+ calcd for $C_{38}H_{52}ClNO_4$ 622.366; found 622.3657.

28.1-cyclopropyl-6-fluoro-4-oxo-N-phenyl-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxamide (28c). Yields 64%; green powder; mp 271°C; ^{1}H NMR (500 MHz, $CDCl_3$) 10.10(1H, s), 9.08 (s, 1H), 8.93(s, 1H), 7.84-7.67 (m, 5H), 7.49 (d, 1H, J = 12.98 Hz), 3.92;2.04 (m, 8H), 7.15 (s, 1H), 2.04 (m, 4H),1.64-1.44(m,2H), 1.20 (m,2H), ^{13}C NMR (125 MHz, $CDCl_3$) δ: 173.6, 162.6, 159.8, 147.5, 139.4, 130.4, 130.0, 128.5, 124.6, 120.0, 114.2, 106.3, 52.9, 45.7, 41.2, 8.7. HRMS (ESI) *m/z*: $[M+H]^+$, calcd for $C_{23}H_{23}FN_4O_2$ 406.1849; found 406.1845.

29. N, N-dimethylformamide (29c). Yields 75%; yellow liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04(s,1H), 3.00 (s, 6H). ^{13}C NMR (500 MHz, $CDCl_3$) δ 164.1, 31.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for C_3H_7NO 74.0969; found 74.0963

30. N-phenylbenzohydrazide (30). Yields 82%; white solid; ^{1}H NMR (500 MHz, d6-DMSO) δ: 11.57(s 2H), 7.58-7.56 (m,2H), 7.48-7.37(m,8H), 7.25-7.22 (m, 1H) ^{13}C NMR (500 MHz, d6-DMSO) δ 165.8, 132.7, 130.8, 129.2, 129.0, 128.3, 127.7

31. *1-phenylthiourea (31).* Yields 75%; White crystal;^{1}H NMR (500 MHz, DMSO-d6) δ 9.68 (s, 1H), 7.40(d, J= 8.5, 2H), 7.31(m,2H) 7.12(m, 1H), ^{13}C NMR (500 MHz, DMSO-d6) δ 181.5, 139.6, 129.2, 124.8, 123.5.

Figure A.43: ^{1}H NMR spectrum of beddomeilactone amide (**32**)

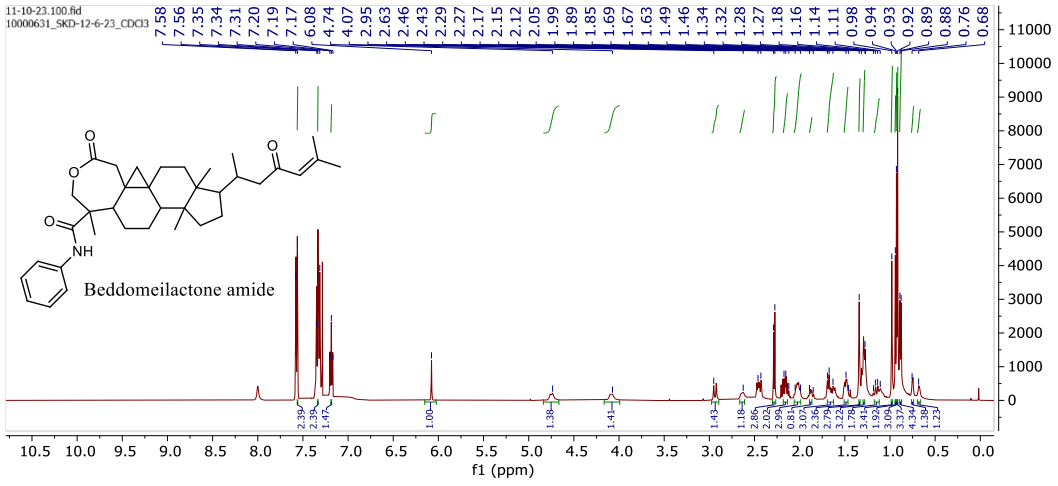


Figure A.43: ^{13}C NMR spectrum of beddomeilactone amide (**32**)

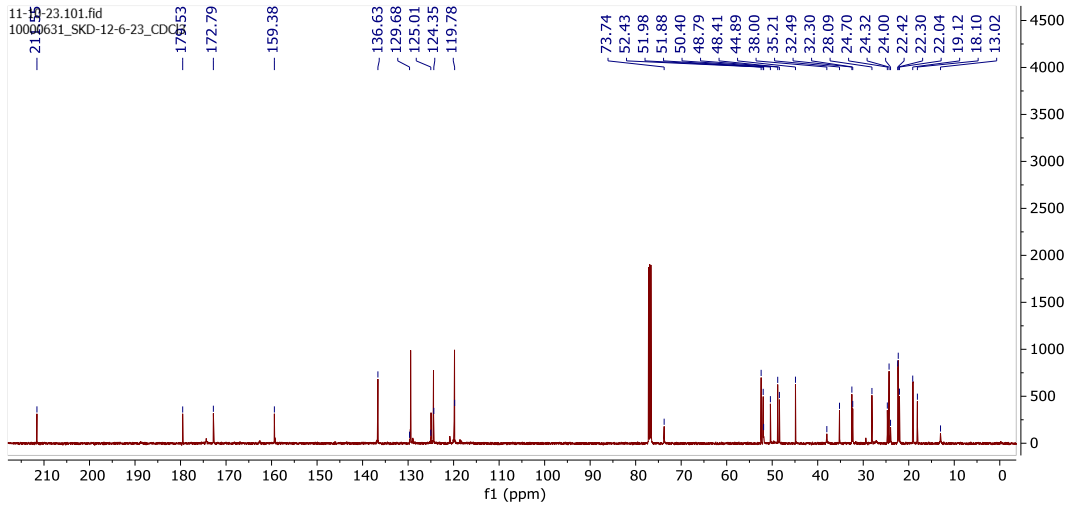
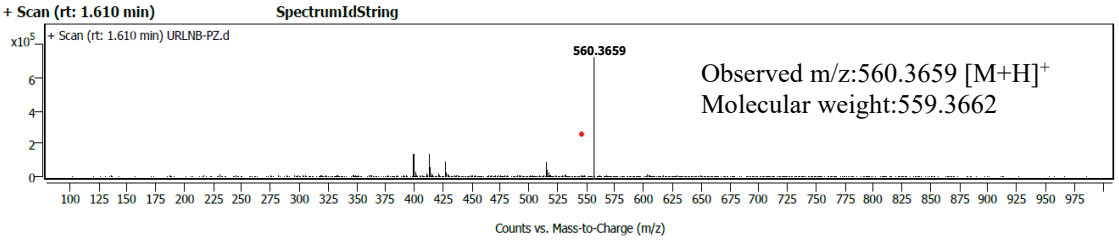


Figure A.44: HRMS spectrum of beddomeilactone amide (**32**)



37. *4-bromo-phenol (1i):* ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.4 (s, 1H, OH), 6.75 (d, 2H, ArH), 7.34 (d, 2H, ArH); ^{13}C NMR (500 MHz,$CDCl_3$) δ 154.5, 132.8, 117.7, 112.5.

38. 4-Bromoanisole (2i): ^{1}H NMR(500 MHz, $CDCl_3$) δ 3.81 (s, 3H, OCH3), 7.35 (d, 2H, ArH), 6.80 (d, 2H, ArH); ^{13}C NMR (500 MHz, $CDCl_3$) δ 159.1, 132.4, 116.4, 113.8, 55.7.

39. *Methyl benzoate (3c):* ^{1}H NMR (500 MHz, MeOD) δ: 8.02 (m, 2H), 7.61 (m, 1H), 5.47 (m, 1H). Mass (GCMS) m/z 136.0 (15%), 105.0 (60%), 92 (10%), 77 (30%), 51.0 (8%).

40. *4-Bromo methylbenzoate (7e):* ^{1}H NMR (500 MHz, MeOD) δ 7.53 (d, J= 8.4, 2H), 7.35 (d, J= 8.4, 2H), 3.90 (s, 3H). Mass m/z 216.0 (30%), 185.1 (100%), 157.1 (30%), 75.1 (30%).

41. *Methyl 3-bromo-4-methoxybenzoate (7f):* ^{1}H-NMR (500 MHz, MeOD): 8.24 (d, J= 2.1 Hz, 1H), 8.00 (dd, J= 2.1, 8.2 Hz, 1H), 6.93 (d, J= 8.2 Hz, 1H), 3.96 (s, 3H). Mass m/z 246.0 (40%), 213.2 (100%), 187.1 (10%), 119.1 (8%), 78.1 (15%), 65.1 (25%).

Figure A.45: ^{1}H NMR spectrum of brominated beddomeilactone (**42**)

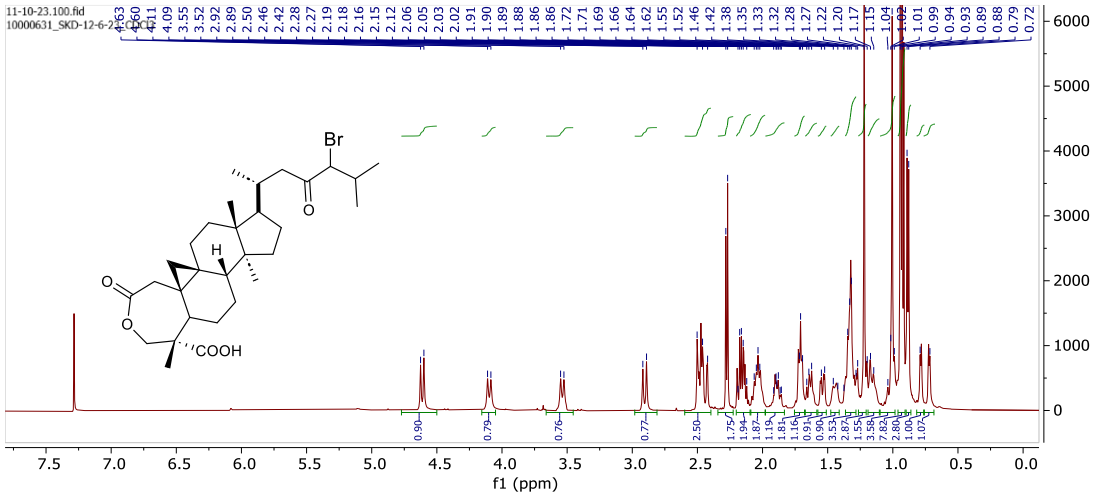


Figure A.46: ^{13}C NMR spectrum of brominated beddomeilactone (**42**)

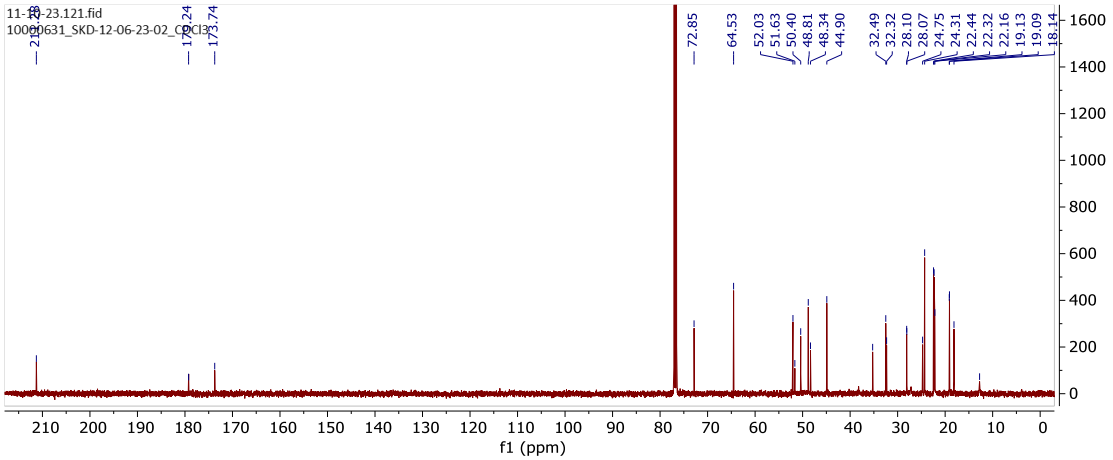
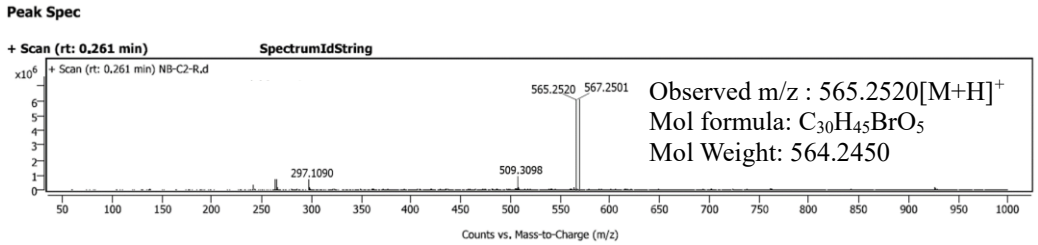


Figure A.47: HRMS spectrum of brominated beddomeilactone amide (**42**)



List of Publications (Thesis work)

1. **Bhardwaj, N**., Singh, A.K., Tripathi, N., Goel, B., Indra, A., and Jain, S.K., Ni–NiO heterojunctions: a versatile nanocatalyst for regioselective halogenation and oxidative esterification of aromatics. New J. Chem., 2021. 45(31): p. 14177-14183.
2. **Bhardwaj, N**., Tripathi, N., Kumar, S., and Jain, S.K., Synthesis of amides directly from carboxylic acids and hydrazines. Org. Biomol. Chem., 2023. 21(37): p. 7572-7579.
3. **Bhardwaj, N**., Swathilaxmi, S., Tripathi, N., Kumar, S., Lal, U.R., G, R., Guru, S.K., et al., Mahamanalactone A, a new triterpenoid from *Dysoxylum malabaricum* bark: a case study for rapid identification of new metabolites via LC-HRMS profiling and database mining strategy. Nat. Prod. Res., 2024: p. 1-6.
4. **Bhardwaj, N**., Sharma, V.K., Tripathi, N., Pimpre, K., Sonti, R., Ravikanth, G., Koch, B., et al., Isolation of cytotoxic cycloartane triterpenoids from *Dysoxylum malabaricum*. New J. Chem., 2024.
5. **Bhardwaj, N**., Sharma, A., Tripathi, N., Goel, B., Ravikanth, G., Kumar Guru, S., and Jain, S.K., New cycloartane triterpenoids from *Dysoxylum malabaricum* and their cytotoxic evaluation. Steroids, 2023. 200: p. 109315.
6. **Bhardwaj, N**., Gupta, P., Tripathi, N., Chakrabarty, S., Verma, A., Kumari, S., Gautam, V., et al., New ring-A modified cycloartane triterpenoids from *Dysoxylum malabaricum* bark: Isolation, structure elucidation and their cytotoxicity. Steroids, 2024. 205: p. 109390.