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List of Publications

1. **Singh G**, S. Kumar, S. Panda, P. Kumar, S.Rai ,H. Verma, Y.Singh, S. kumar, S. Srikrishna,Vgm Naidu,G .Modi ; Design, Synthesis, and Biological Evaluation of Ferulic Acid-Piperazine Derivatives Targeting Pathological Hallmarks of Alzheimer's Disease. **ACS Chem Neurosci.** (Accepted).
2. **Singh G**, Shankar G, Panda SR, Kumar S, Rai S, Verma H, Kumar P, Nayak PK, Naidu VGM, Srikrishna S, Kumar S, Modi G. Design, Synthesis, and Biological Evaluation of Ferulic Acid Template-Based Novel Multifunctional Ligands Targeting NLRP3 Inflammasome for the Management of Alzheimer's Disease. **ACS Chem Neurosci.** 2024 Apr 3;15(7):1388-1414
3. **Singh G**, Kesharwani P, Kumar Singh G, Kumar S, Putta A, Modi G. Ferroptosis and its modulators: A raising target for cancer and Alzheimer's disease. **Bioorg Med Chem.** 2024 Jan 15;98:117564.
4. **Singh G**, Thomas J, Wadhawa S, Kashyap A, Rahaman SA, Borkotoky S, Datta A, Singh GK, Mishra I, Rai G, Satija J, Dubey VK, Modi G. Repurposing the in-house generated Alzheimer's disease targeting molecules through computational and preliminary in-vitro studies for the management of SARS-coronavirus-2. **Mol Divers.** 2023 Sep 25.
5. Himanshu Rai, Rishabh Singh, Gauri Shankar, Sanskriti Rai, Prabhat Kumar, Aishwarya S. Nilakhe, Neha Singh, Poonam Bhadoria, Venkatnarayan Ramanathan, **Gourav Singh**, Sarika Gupta, Sairam Krishnamurthy, Saripella Srikrishna, Saroj Kumar, Gyan Modi. Discovery of novel NIRF theranostic probes targeting amyloid-β fibrils and cholinesterases in Alzheimer's disease models. **Nature Communication** (Under revision).
6. Narayanan AC, Venkatesh R, Singh S, **Singh G**, Modi G, Singh S, Kandasamy J. Synthesis of phenylethanoid glycosides from acrylic esters of glucose and aryldiazonium salts via palladium-catalyzed cross-coupling reactions and evaluation of their anti-Alzheimer activity. **Carbohydr Res.** 2023 Oct;532:108920.
7. Singh YP, Kumar N, Priya K, Chauhan BS, Shankar G, Kumar S, Singh GK, Srikrishna S, Garg P, **Singh G**, Rai G, Modi G. Exploration of Neuroprotective Properties of a Naturally Inspired Multifunctional Molecule (F24) against Oxidative

Stress and Amyloid β Induced Neurotoxicity in Alzheimer's Disease Models. **ACS Chem Neurosci.** 2022 Jan 5;13(1):27-42.

8. Singh YP, Shankar G, Jahan S, **Singh G**, Kumar N, Barik A, Upadhyay P, Singh L, Kamble K, Singh GK, Tiwari S, Garg P, Gupta S, Modi G. Further SAR studies on natural template based neuroprotective molecules for the treatment of Alzheimer's disease. **Bioorg Med Chem.** 2021 Sep 15;46:116385.
9. Singh YP, Rai H, **Singh G**, Singh GK, Mishra S, Kumar S, Srikrishna S, Modi G. A review on ferulic acid and analogs based scaffolds for the management of Alzheimer's disease. **Eur J Med Chem.** 2021 Apr 5;215:113278.

PATENT FILED

1. A natural template-based anticholinesterase inhibitors and antioxidants for the treatment Alzheimer's disease. Gyan Modi, Yash Pal Singh, Gauri Shankar, **Gourav Singh**, Atanu Barik, Lovejit Singh. Patent #202111016470 # Indian
2. A multifunctional diaryl ureas-hydroxyamidine based compounds for the treatment of Alzheimer's disease. Gyan Modi, Yash Pal Singh, C. Praveen Kumar, Meenu Yadav, Gauri Shankar, **Gourav Singh**, Saroj Kumar, S. Srikrishna. Patent #202111001482

BOOK CHAPTER:

1. Ferroptosis Modulators: A Potential Therapeutic Target in Alzheimer's Disease, **Gourav Singh**, Nishant Rana, Indubhusan Mishra, Springer Nature, 2023 (accepted)

SEMINARS & WORKSHOPS ATTENDED:

1. Participated in workshop on "Biological Evaluation of Brain Targeting Molecules" Held at **IIT BHU**, November 10-12, 2022.
2. Presented poster at 48th Annual Conference of Indian Immunology Society, Infections, Vaccines & Immuno-Innovations for Human Health, held at Human Genetics Department **BHU** July 8-9, 2022.
3. Participated in SERB Sponsored Workshop on the topic "Role of Artificial Intelligence and Machine Learning in Drug Discovery, held at Institute of Pharmacy, Harischandra PG college, **Varanasi,** December 12-17, 2022.
4. Presented Poster 2nd National Conference on CONTEMPORARY FACETS IN ORGANIC SYNTHESIS (CFOS-2022) in partnership with Royal Society of Chemistry, held at **IIT Roorkee**, December 01-04, 2022.

Figure A1: ^{1}H NMR spectra of (E)-3-(4-hydroxy-3-methoxyphenyl)-N-(2-((8-hydroxyquinolin-5-yl)amino)-2 oxoethyl)acrylamide (12o)

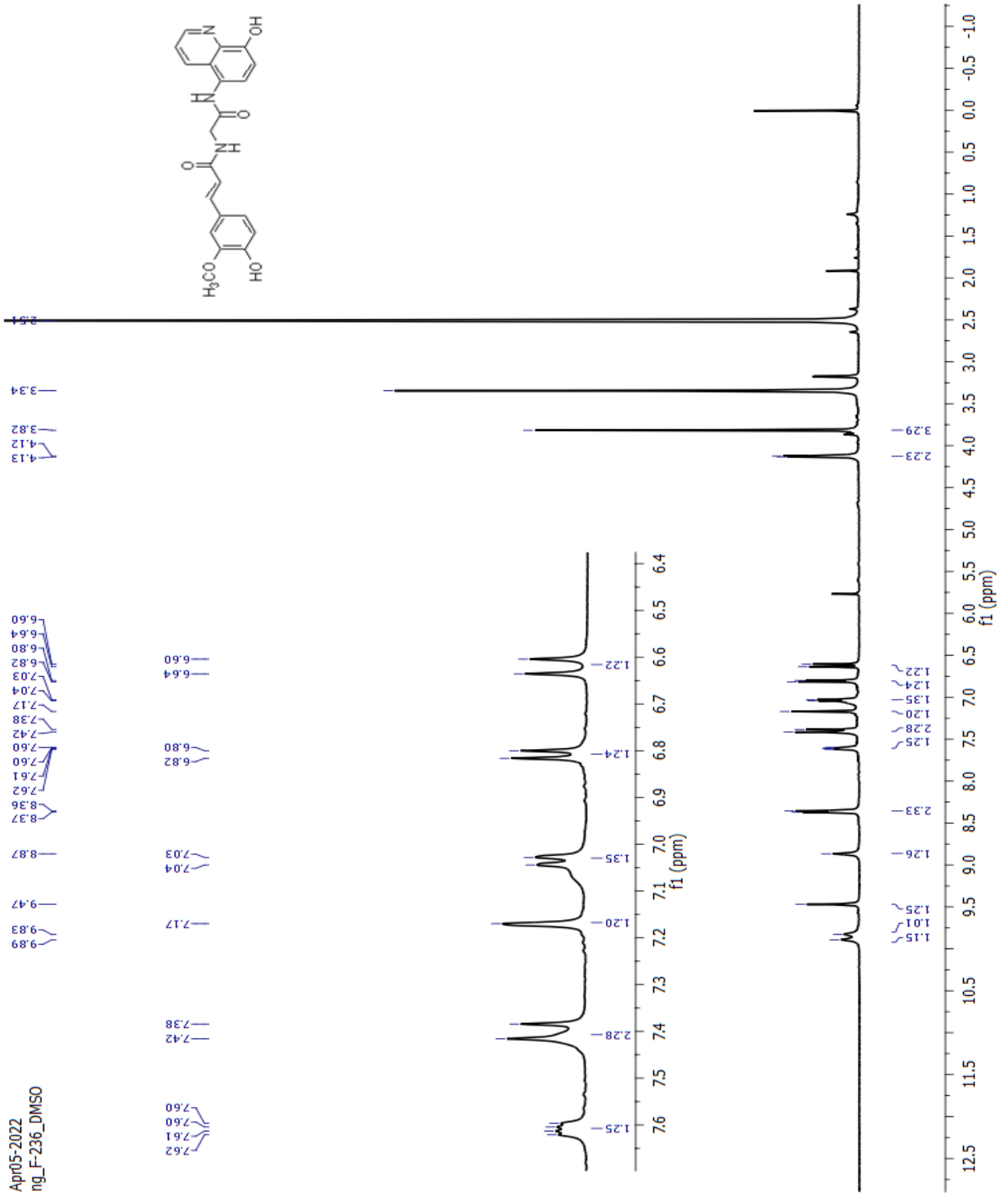


Figure A2: ^{13}C NMR spectra of (E)-3-(4-hydroxy-3-methoxyphenyl)-N-(2-((8-hydroxyquinolin-5-yl)amino)-2 oxoethyl)acrylamide (12o)

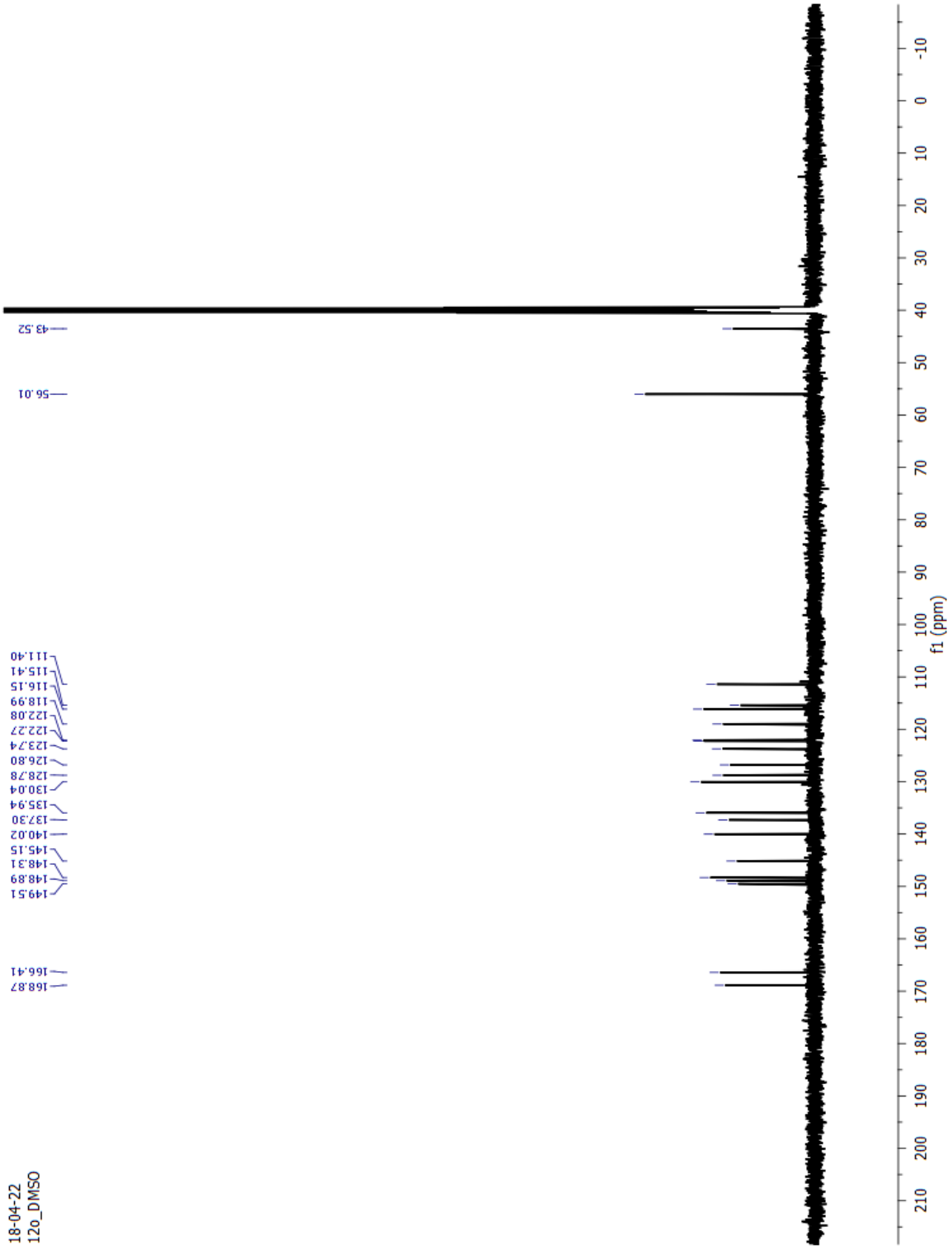
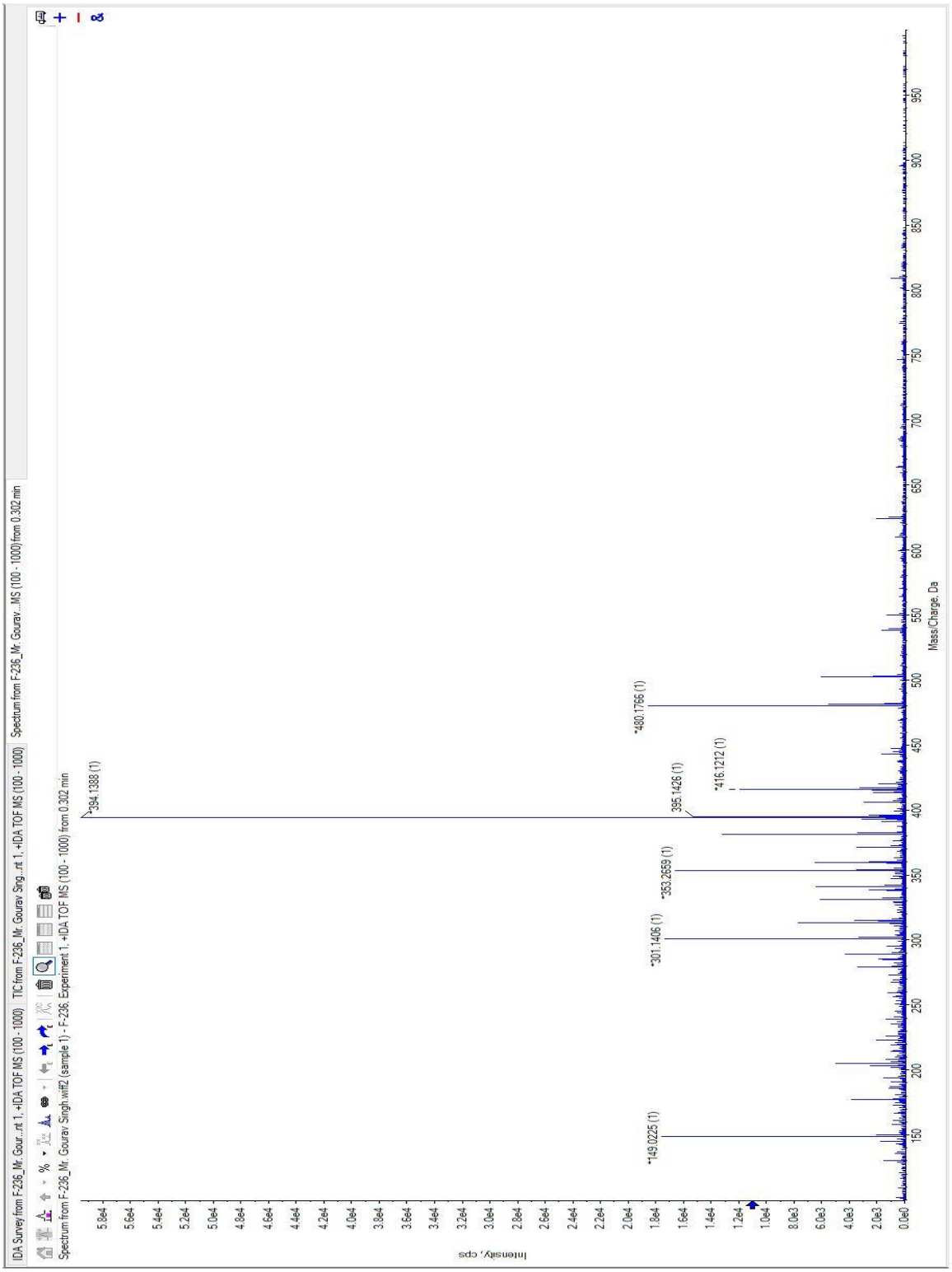


Figure A3: HRMS spectra of (E)-3-(4-hydroxy-3-methoxyphenyl)-N-(2-((8-hydroxyquinolin-5-yl)amino)-2 oxoethyl)acrylamide (12o)



Supplementary data of the second series of compounds

Figure A4: ^{1}H NMR Spctra of (E)-3-(4-hydroxy-3-methoxyphenyl)-1-(4-((8-hydroxyquinolin -5-yl) methyl) piperazin-1-yl)prop-2-en-1-one (13a)

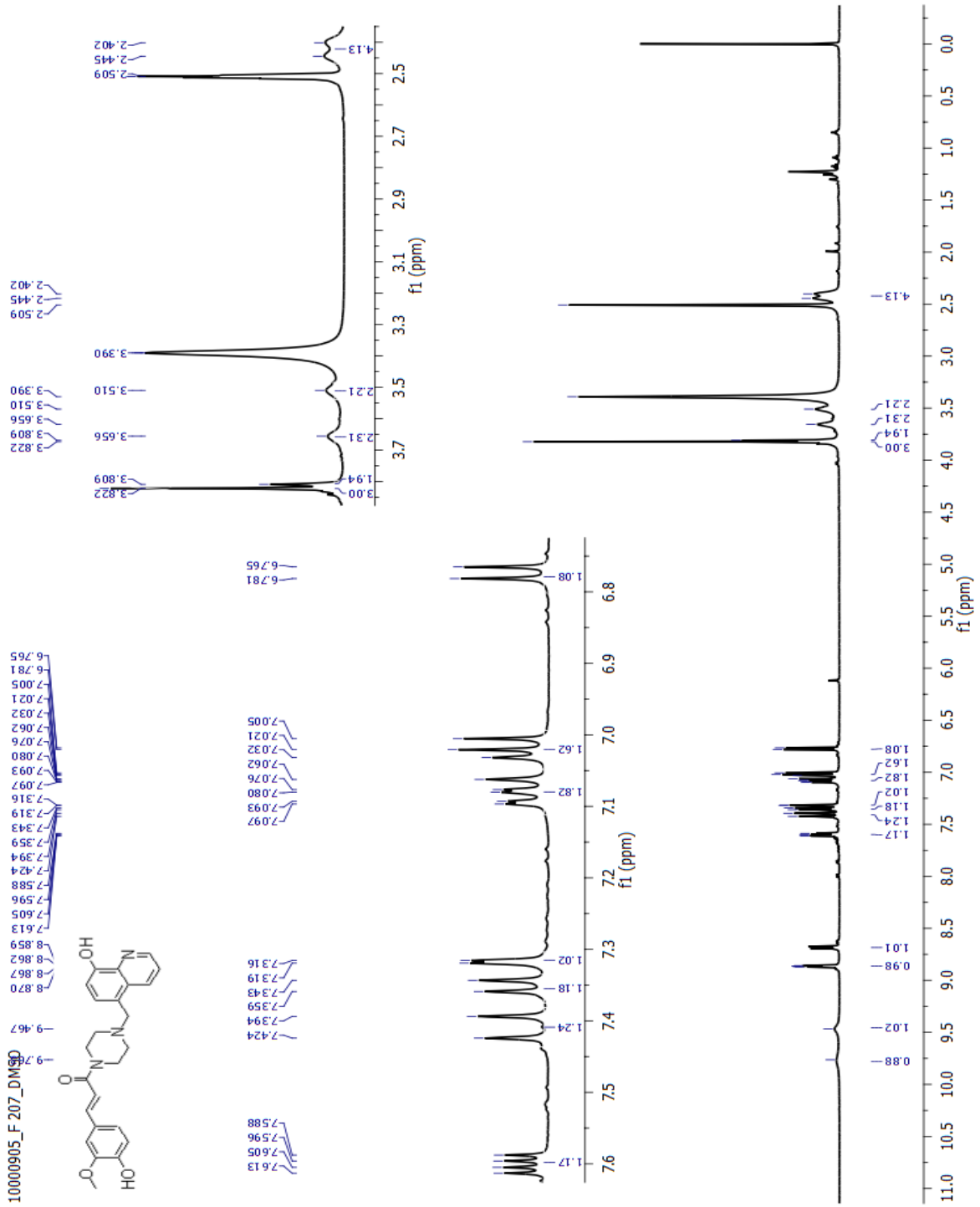


Figure A5: ^{13}C NMR Spectra of (E)-3-(4-hydroxy-3-methoxyphenyl)-1-(4-((8-hydroxyquinolin-5-yl)methyl) piperazin-1-yl)prop-2-en-1-one (13a)

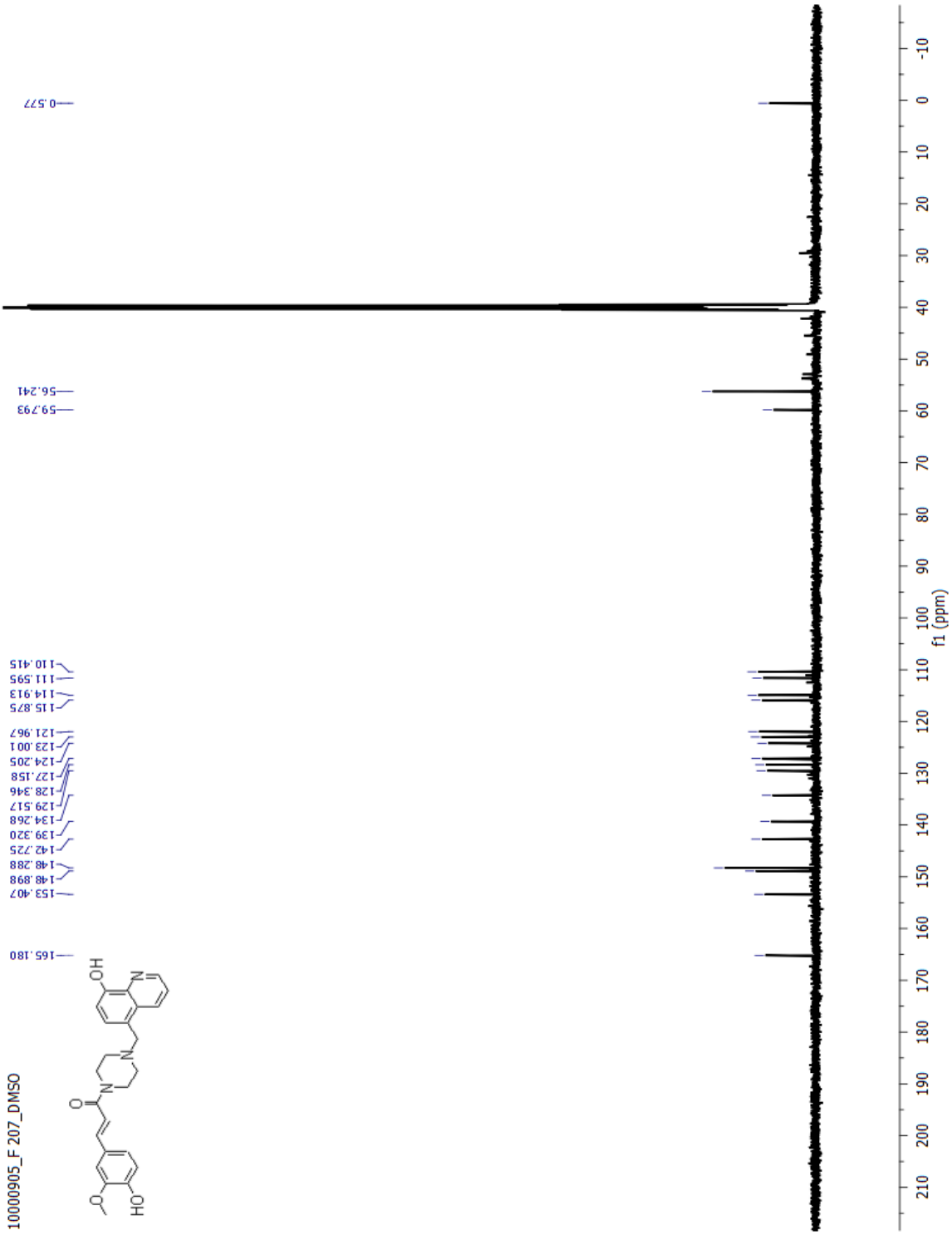


Figure A6: HRMS spectra of (E)-3-(4-hydroxy-3-methoxyphenyl)-1-(4-((8-hydroxyquinolin-5-yl)methyl) piperazin-1-yl)prop-2-en-1-one (13a)