Chapter 9
References

9. References

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Appendix

10.1 Supplementary data of 1,3-dimethylbarbituric acid-based fluorescent emitting theranostics fluorescent probes

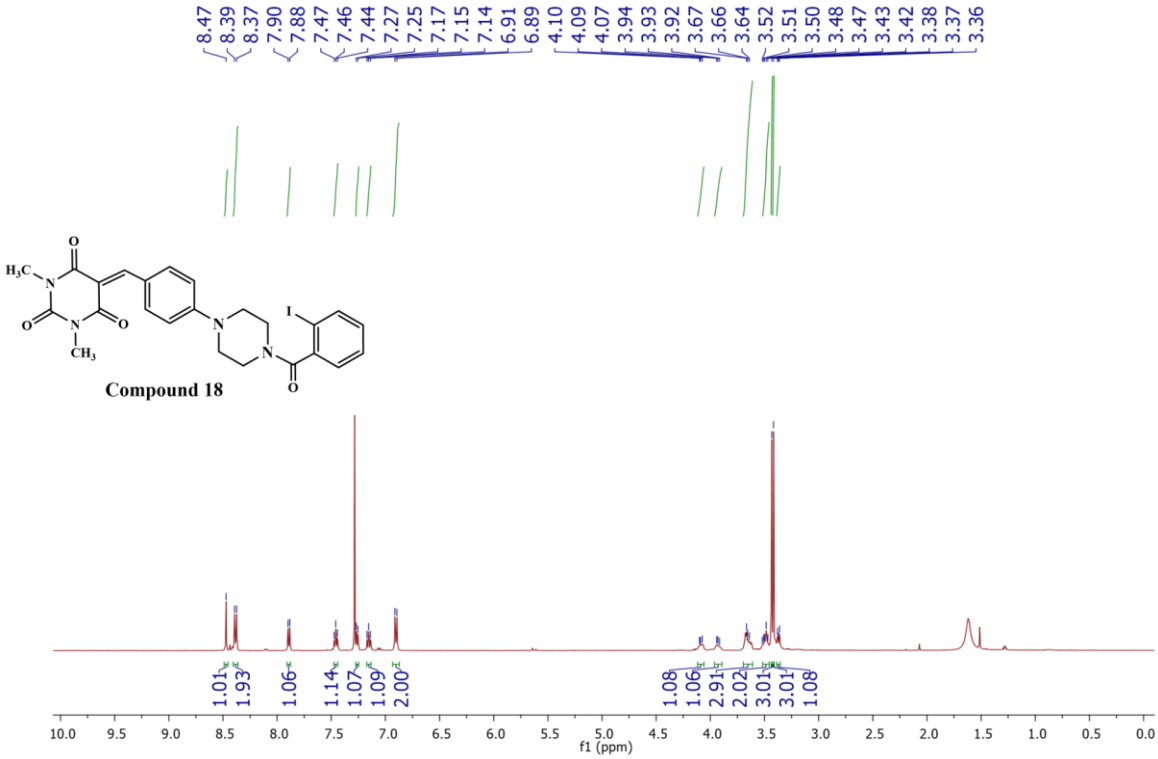

Figure A.1: ^{1}H NMR spectrum of *5-(4-(4-(2-Iodobenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(18)**.

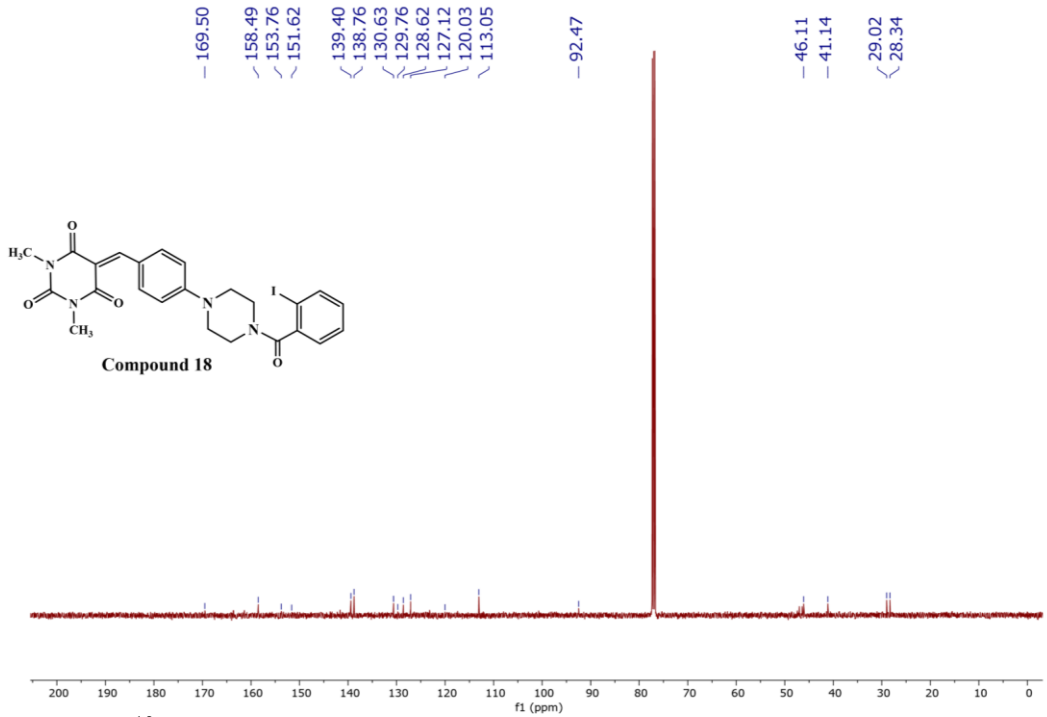

Figure A.2: ^{13}C NMR spectrum of *5-(4-(4-(2-Iodobenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(18).**

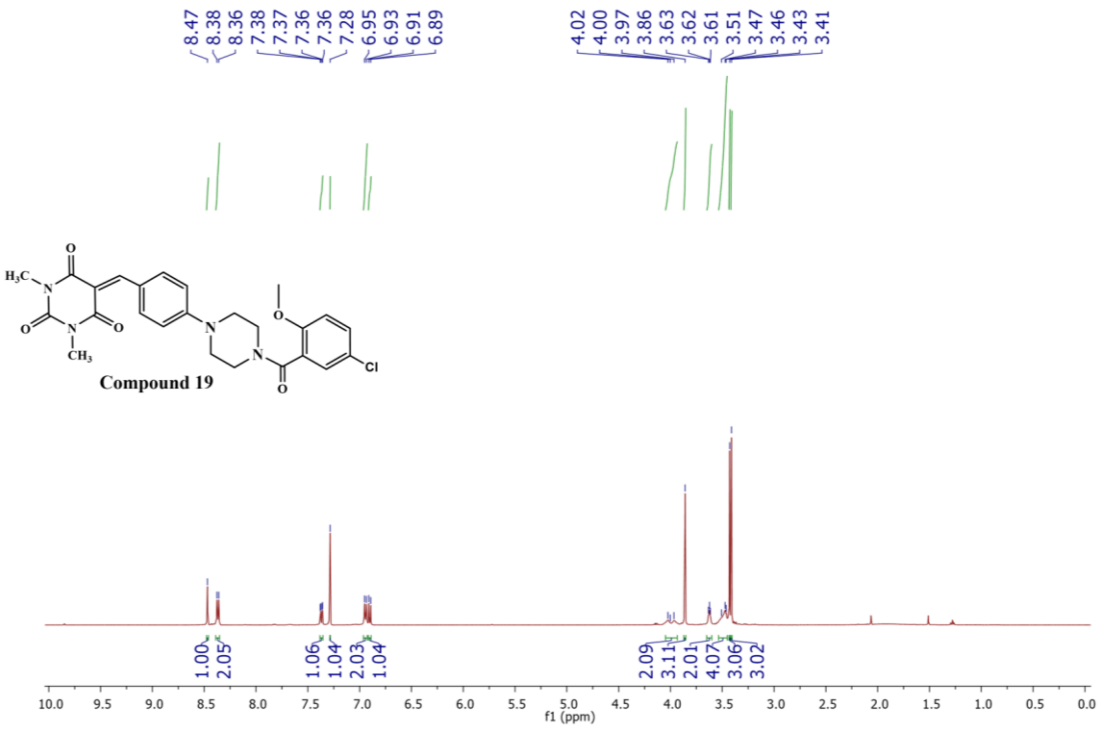

Figure A.3: ^{1}H NMR spectrum of *5-(4-(4-(5-Chloro-2-methoxybenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* (**19**).

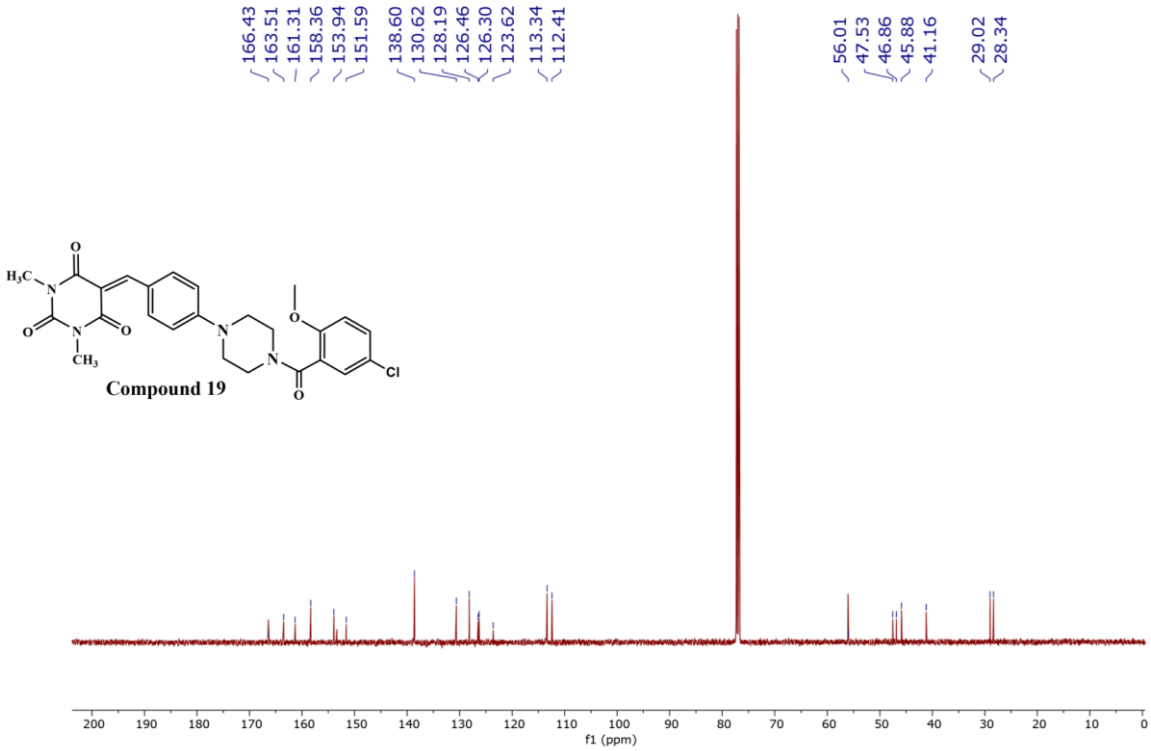

Figure A.4: ^{13}C NMR spectrum of *5-(4-(4-(5-Chloro-2-methoxybenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* (**19**).

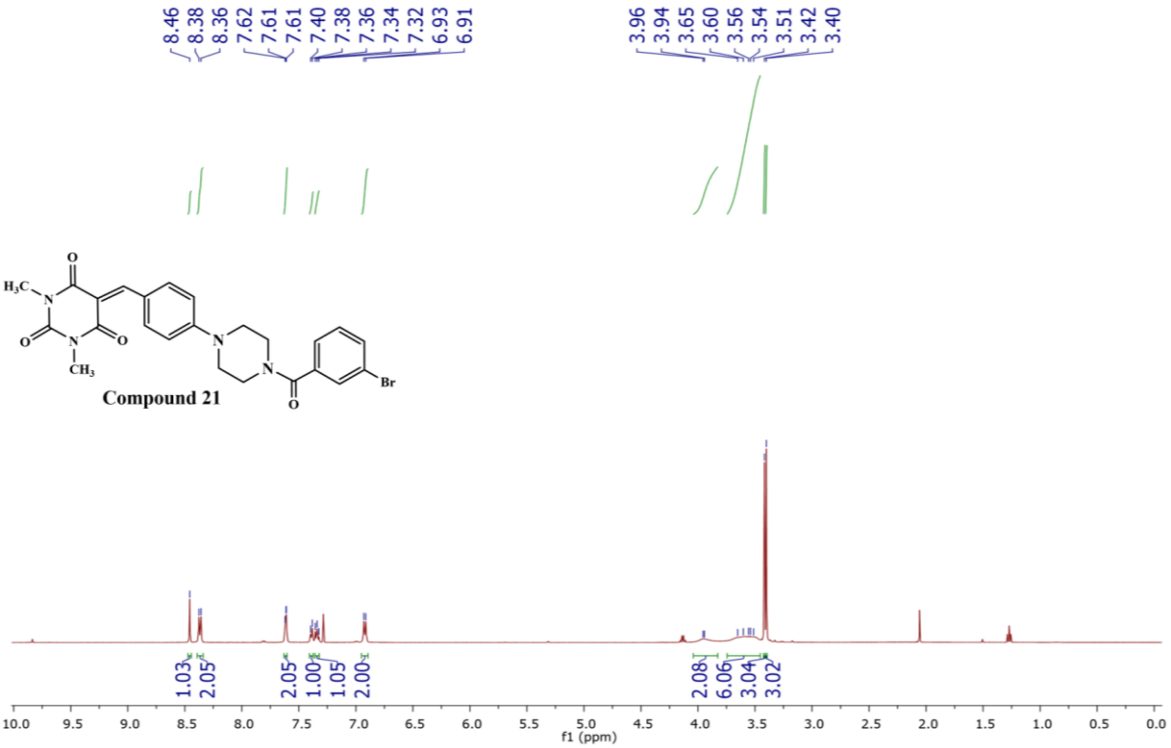

Figure A.5: ^{1}H NMR spectrum of *5-(4-(4-(3-Bromobenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(21).**

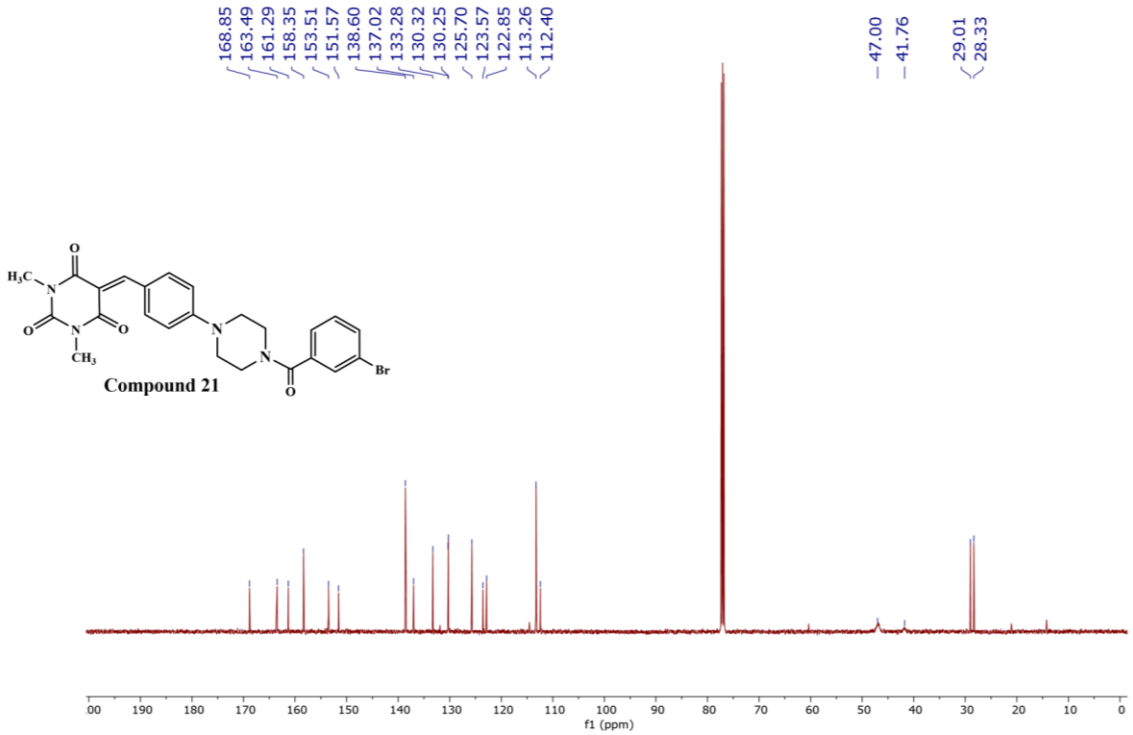

Figure A.6: ^{13}C NMR spectrum of *5-(4-(4-(3-Bromobenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(21).**

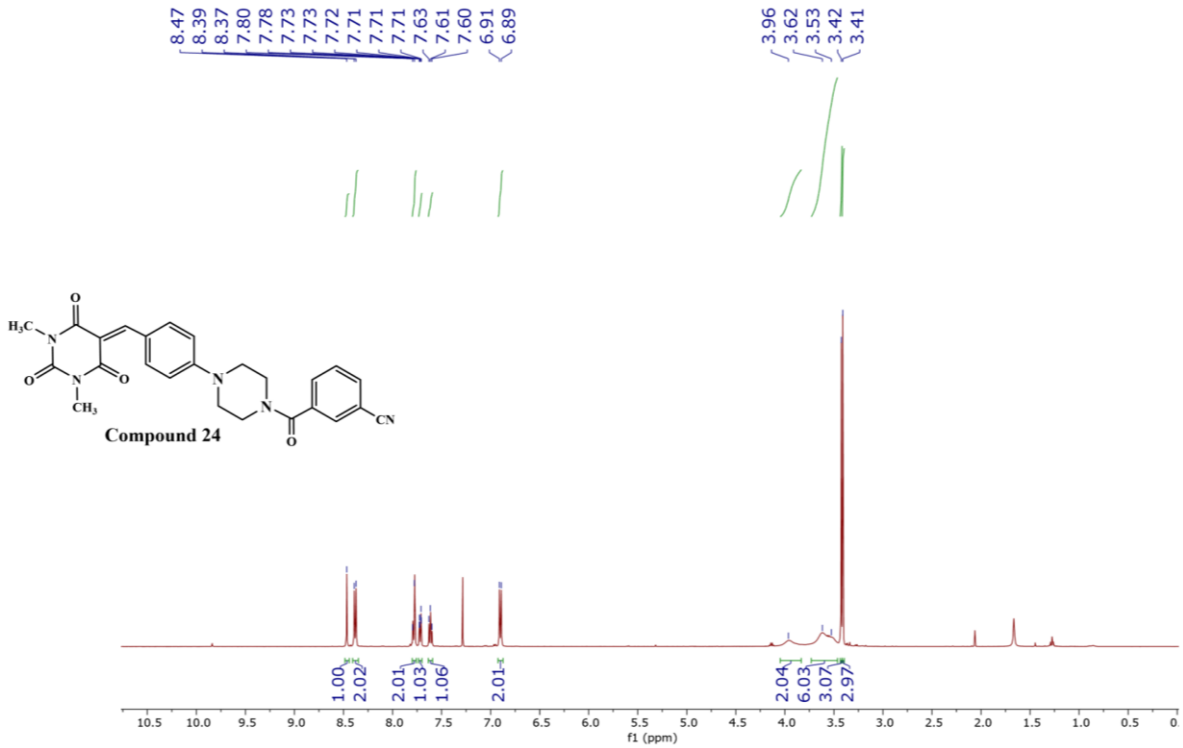

Figure A.7: ^{1}H NMR spectrum of *3-(4-(4-((1,3-Dimethyl-2,4,6-trioxotetrahydropyrimidin-5(2H)-ylidene)methyl)phenyl)piperazine-1-carbonyl)benzonitrile* **(24).**

.

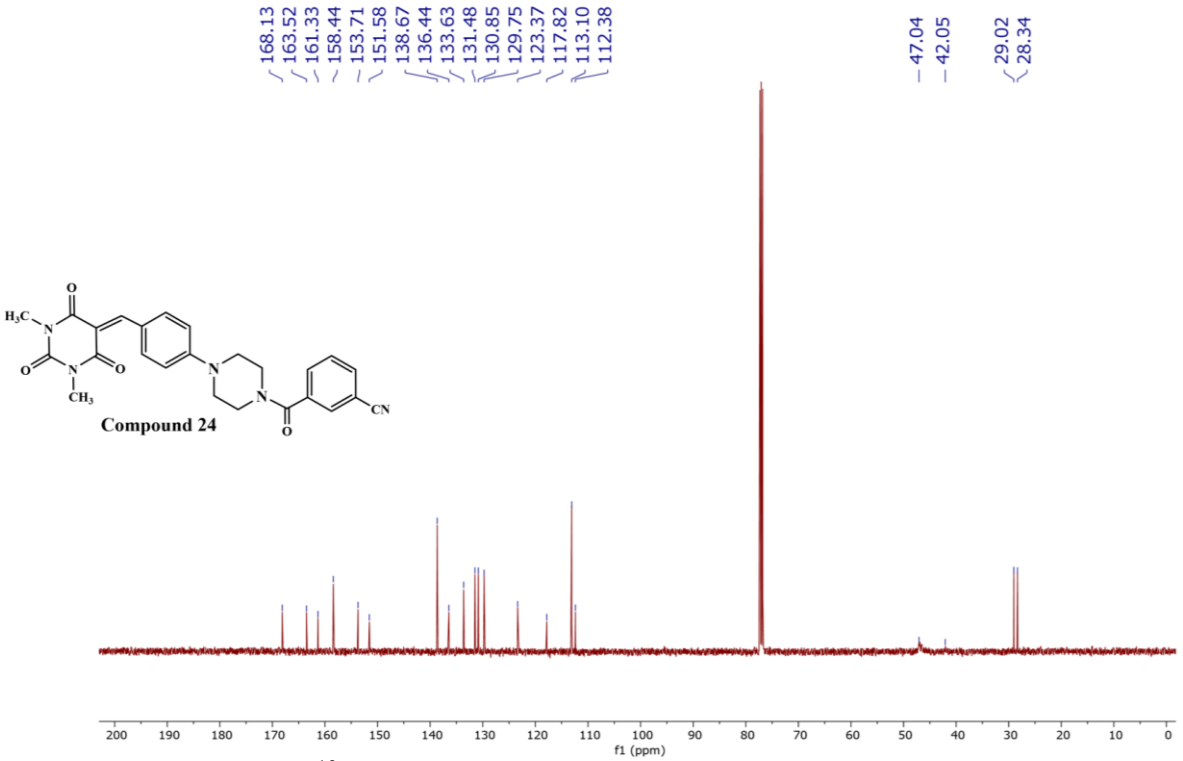

Figure A.8: ^{13}C NMR spectrum of *3-(4-(4-((1,3-Dimethyl-2,4,6-trioxotetrahydropyrimidin-5(2H)-ylidene)methyl)phenyl)piperazine-1-carbonyl)benzonitrile* **(24).**

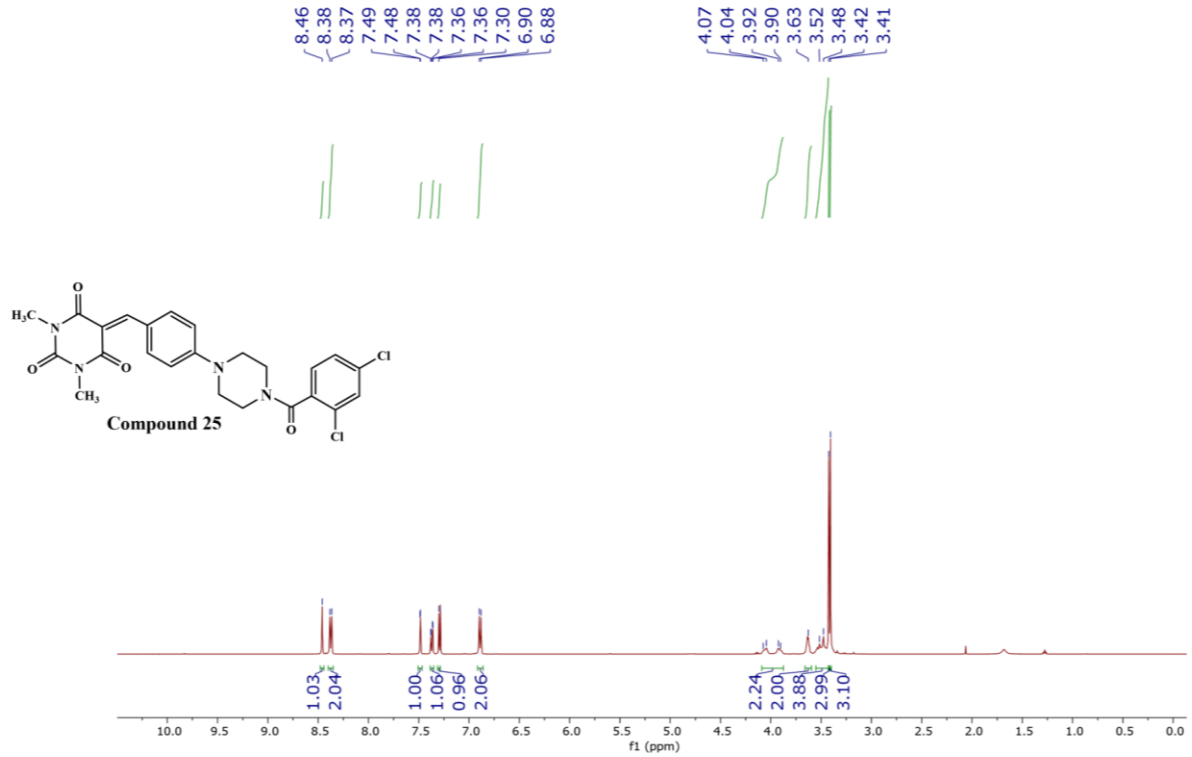

Figure A.9: ^{1}H NMR spectrum of *5-(4-(4-(2,4-Dichlorobenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(25).**

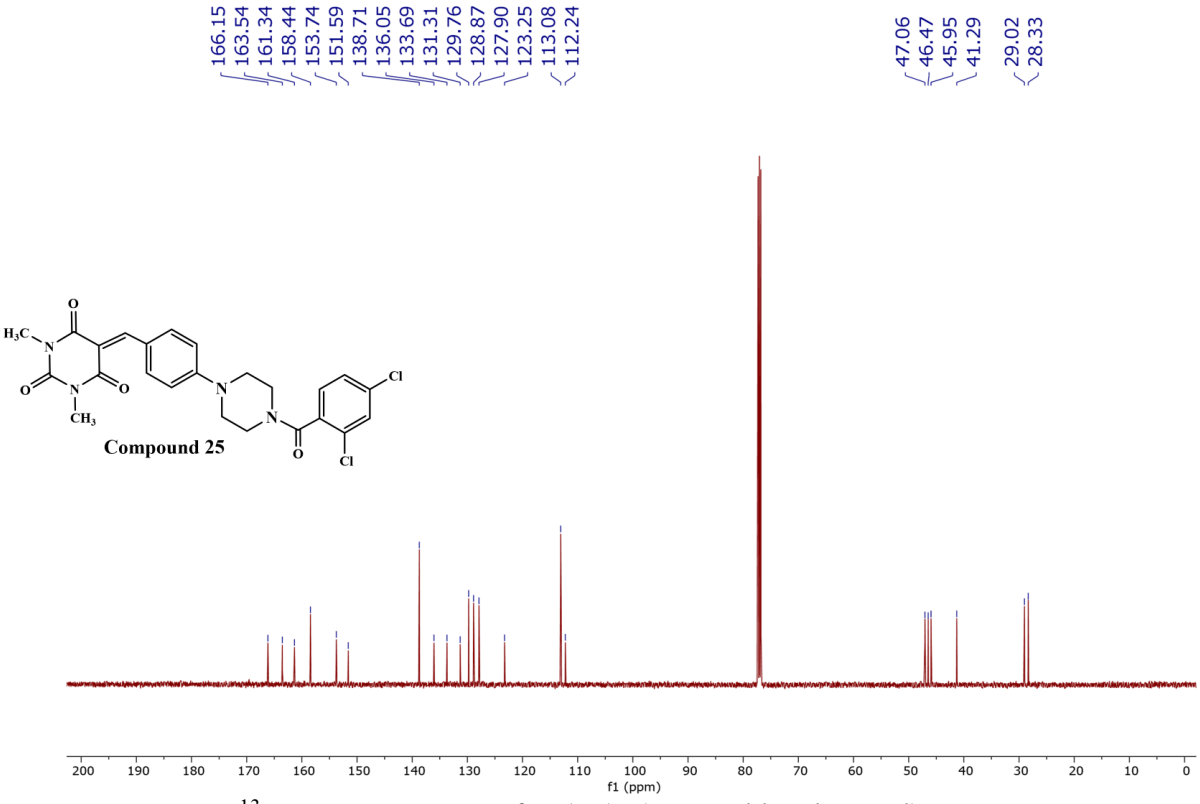

Figure A.10: ^{13}C NMR spectrum of *5-(4-(4-(2,4-Dichlorobenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(25).**

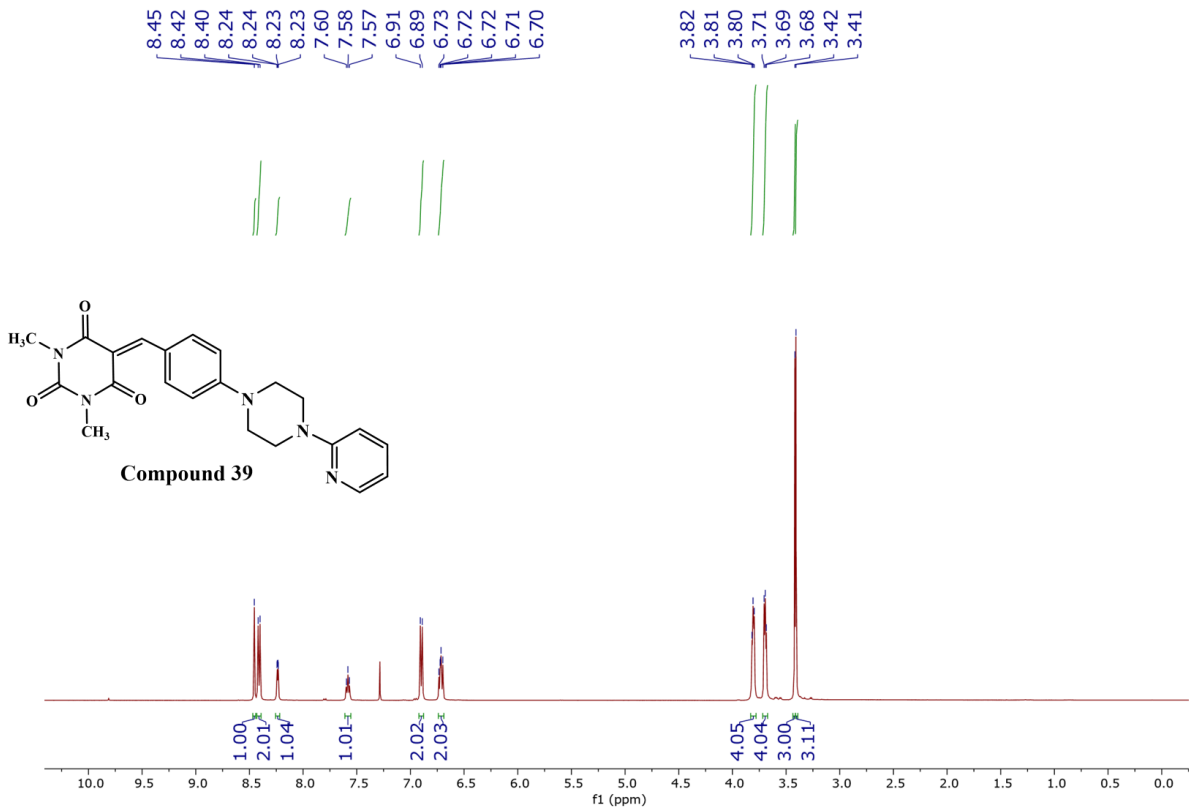

Figure A.11: ^{1}H NMR spectrum of *1,3-Dimethyl-5-(4-(4-(pyridin-2-yl)piperazin-1-yl)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione* **(39).**

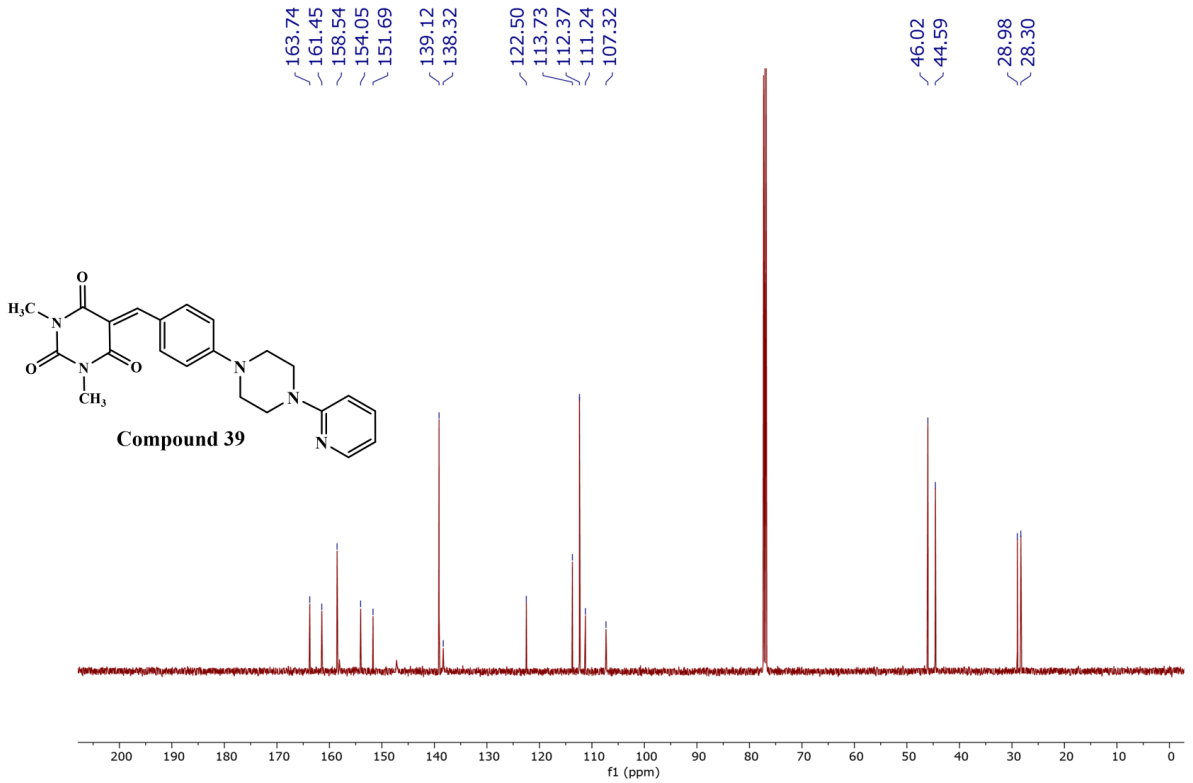

Figure A.12: ^{13}C NMR spectrum of *1,3-Dimethyl-5-(4-(4-(pyridin-2-yl)piperazin-1-yl)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione* **(39).**

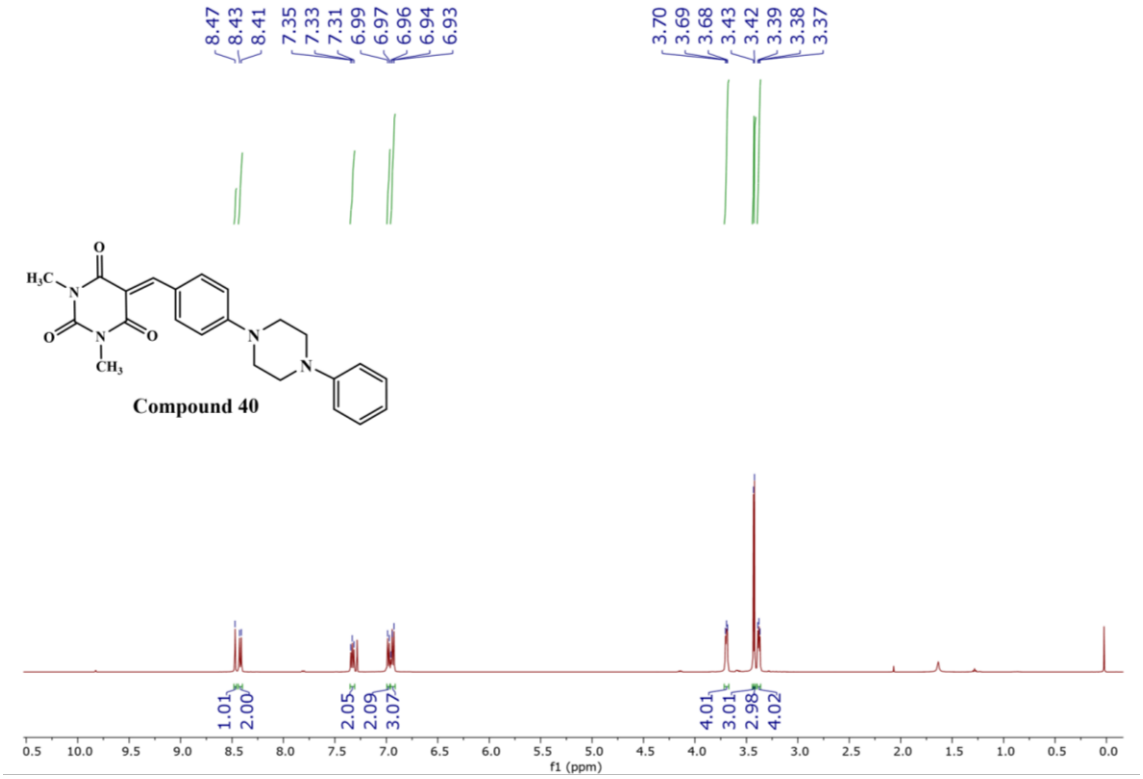

Figure A.13: [1]H NMR spectrum of *1,3-Dimethyl-5-(4-(4-phenylpiperazin-1-yl)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione* **(40).**

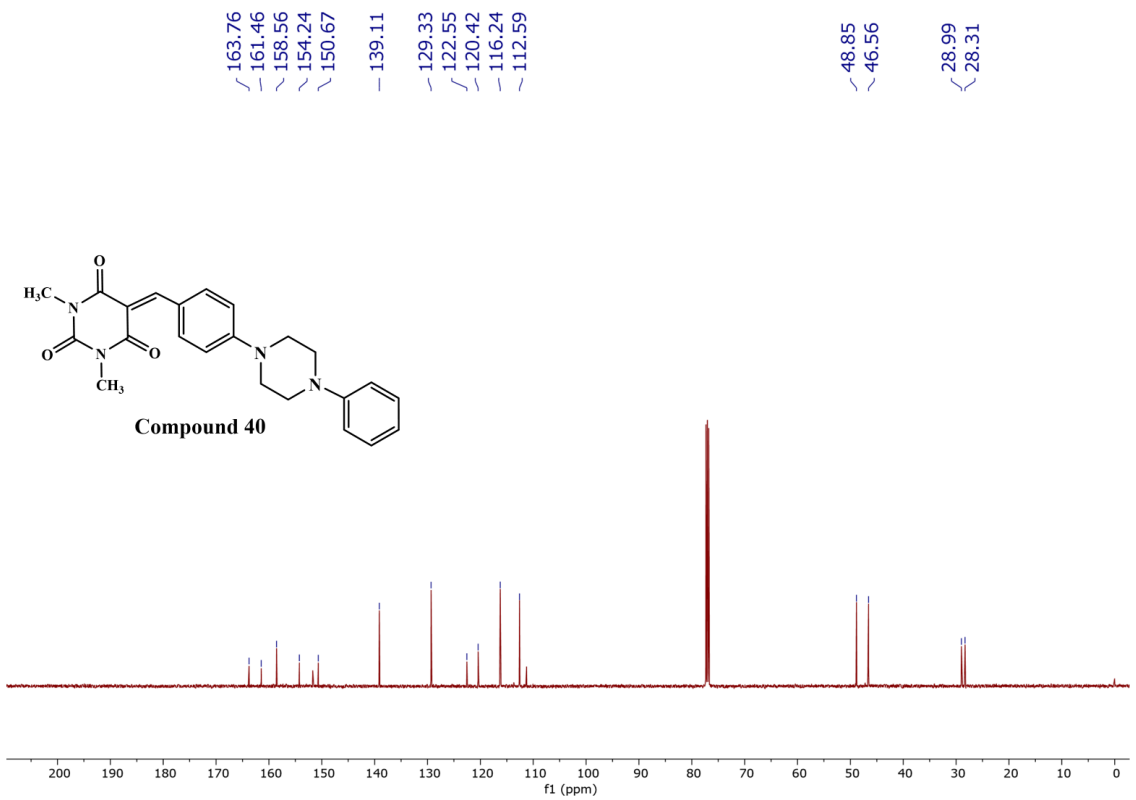

Figure A.14: [13]C NMR spectrum of *1,3-Dimethyl-5-(4-(4-phenylpiperazin-1-yl)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione* **(40)**.

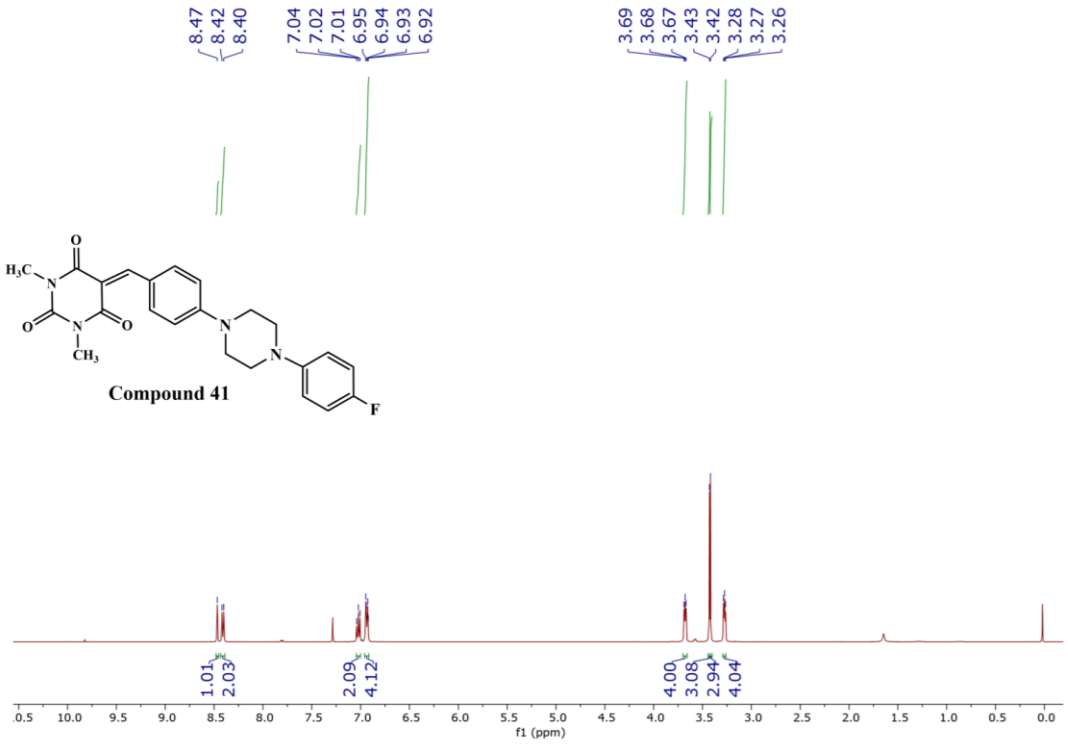

Figure A.15: ^{1}H NMR spectrum of *5-(4-(4-(4-Fluorophenyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(41).**

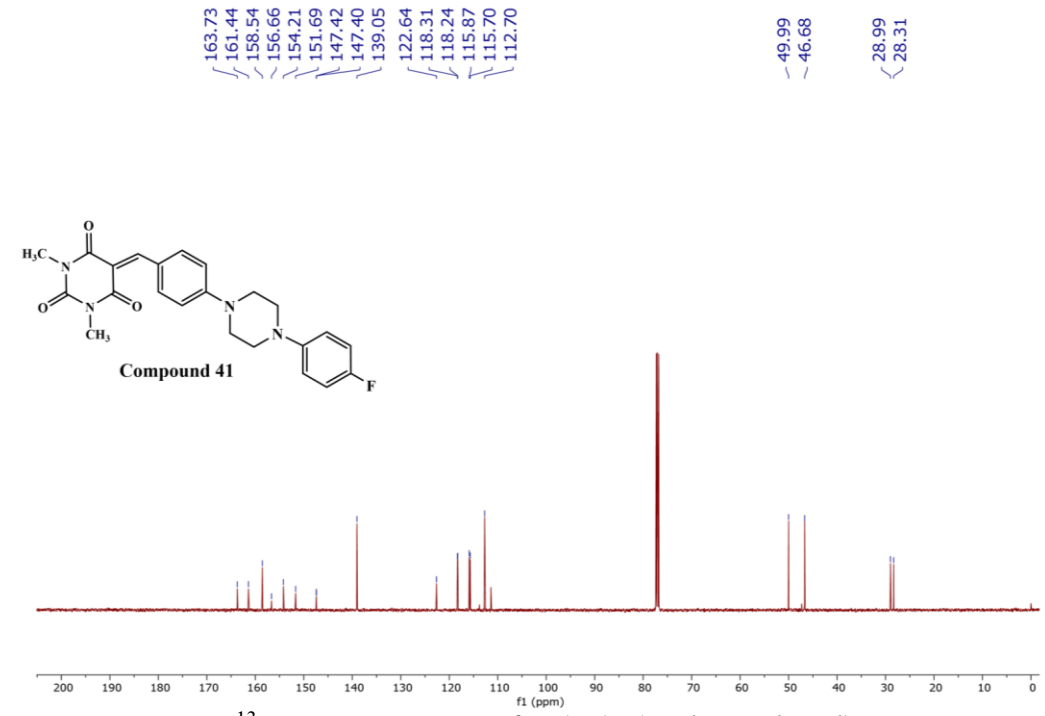

Figure A.16: ^{13}C NMR spectrum of *5-(4-(4-(4-Fluorophenyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(41).**

Table A.1: Purity analysis of lead compounds determined by HPLC.

Compound ID	Retention Time (min)	HPLC Purity (%)
19	4.527	98.98 %
21	4.773	99.29 %
22	4.333	98.06%
23	4.727	99.59 %
25	4.940	99.76%
39	2.293	93.66%
40	5.233	99.37%
41	5.193	96.18%
42	4.532	98.31%
43	4.493	93.59 %

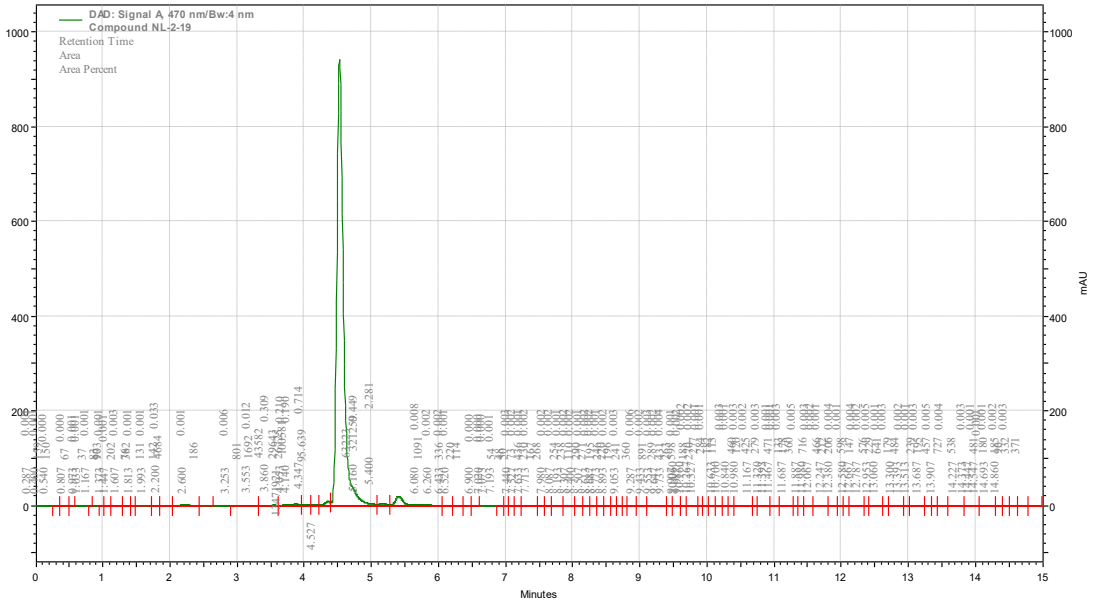

Figure A.17: HPLC chromatogram of *5-(4-(4-(5-Chloro-2-methoxybenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(19).**

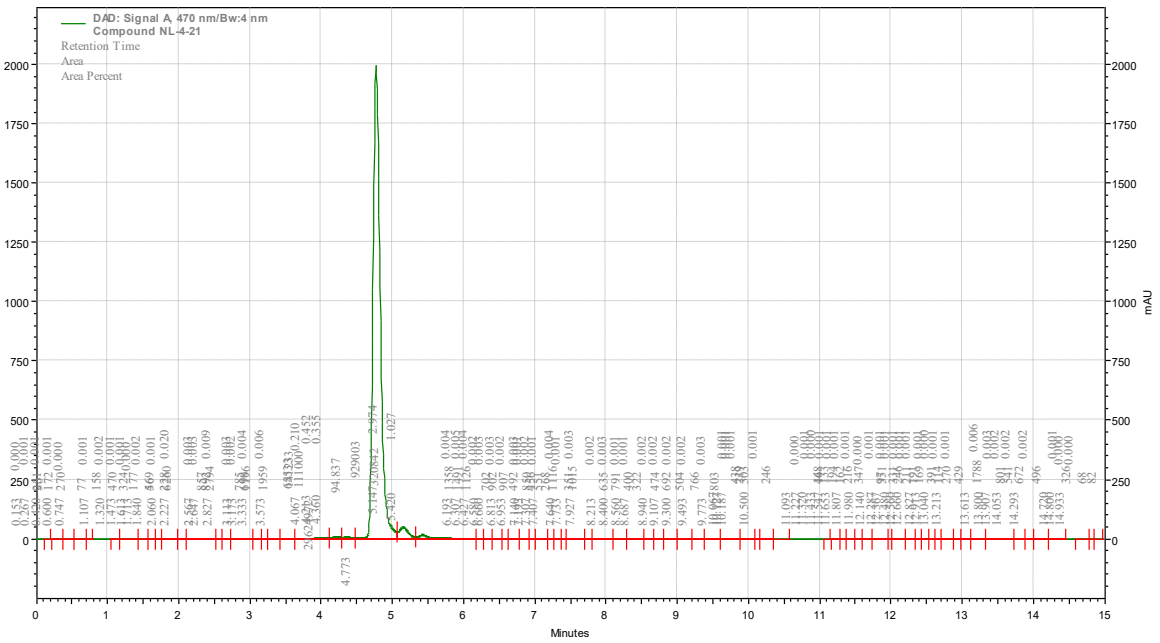

Figure A.18: HPLC chromatogram of *5-(4-(4-(3-Bromobenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(21).**

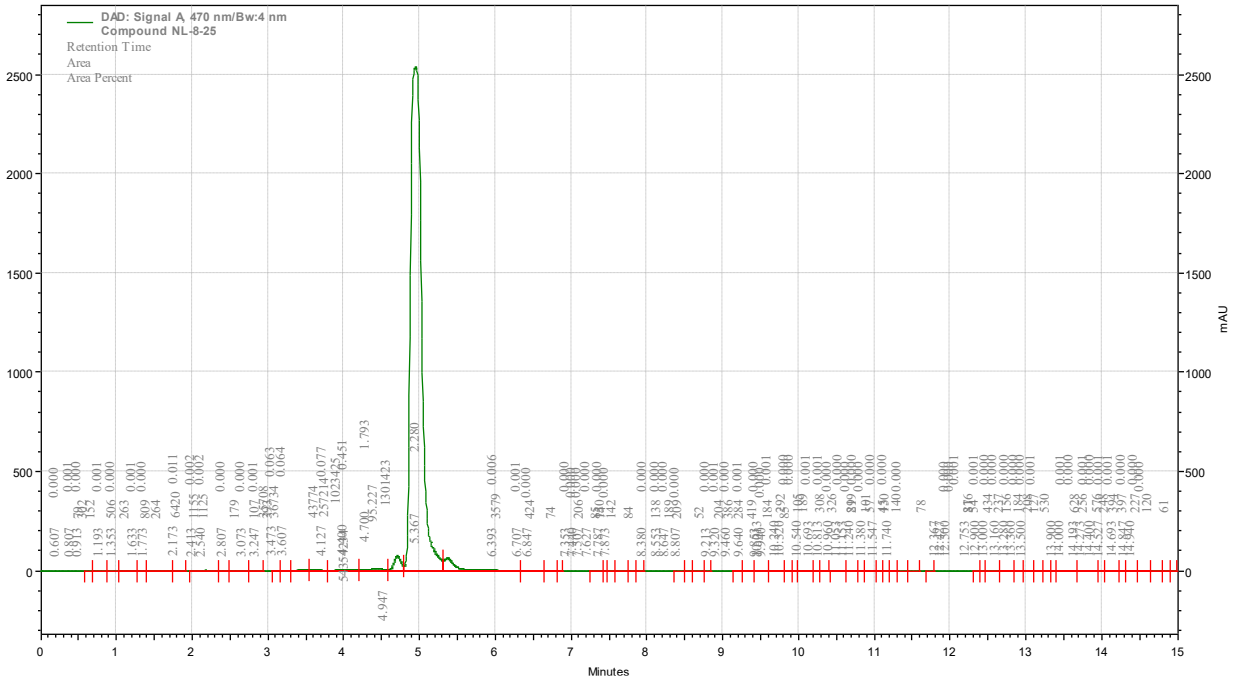

Figure A.19: HPLC chromatogram of *5-(4-(4-(2,4-Dichlorobenzoyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(25).**

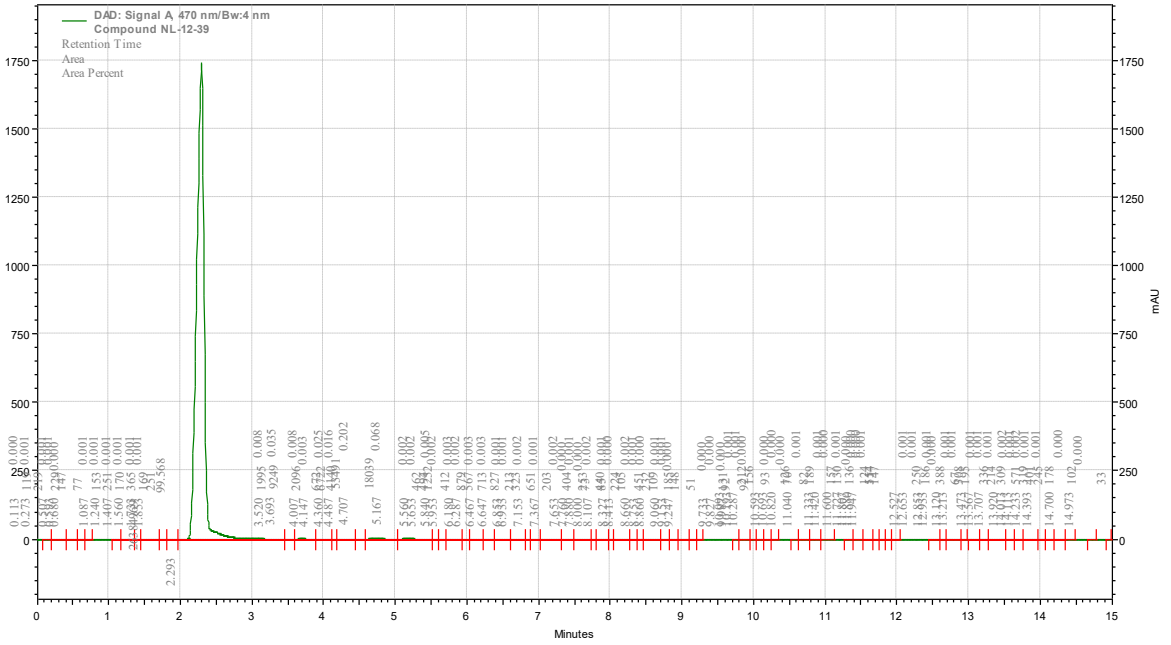

Figure A.20: HPLC chromatogram of *1,3-Dimethyl-5-(4-(4-(pyridin-2-yl)piperazin-1-yl)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione* **(39).**

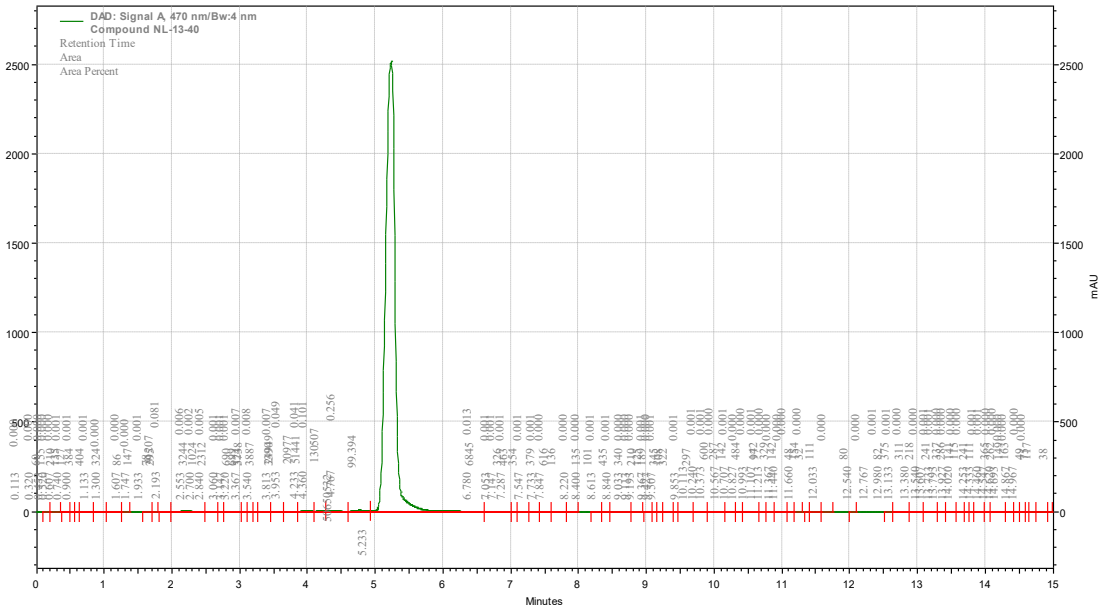

Figure A.21: HPLC chromatogram of *1,3-Dimethyl-5-(4-(4-phenylpiperazin-1-yl)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione* **(40)**.

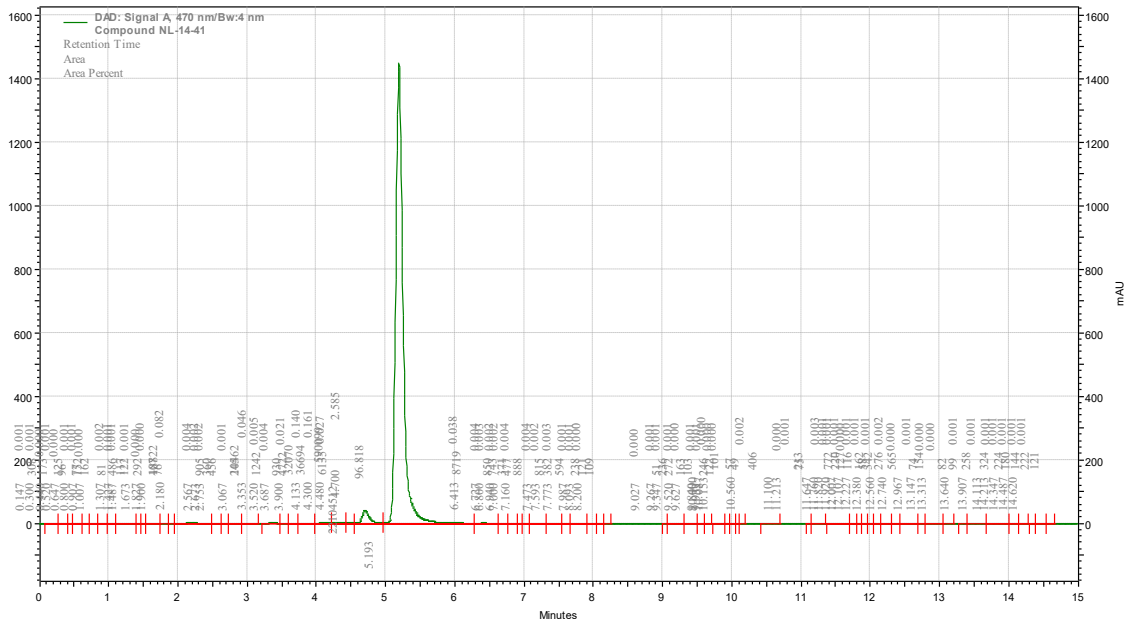

Figure A.22: HPLC chromatogram of *5-(4-(4-(4-Fluorophenyl)piperazin-1-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione* **(41).**

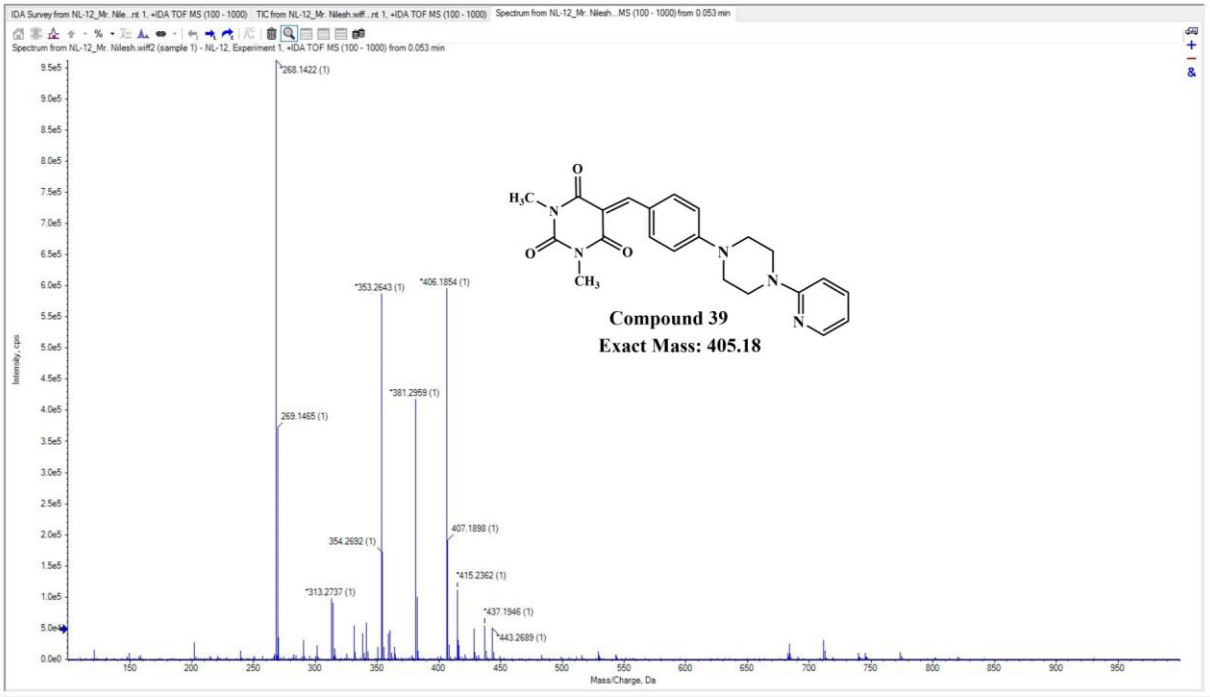

Figure A.23: Mass spectra (HRMS) of *1,3-Dimethyl-5-(4-(4-(pyridin-2-yl)piperazin-1-yl)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione* **(39).**

10.2 Supplementary data of indolium and benzothiazolium based theranostics fluorescent probes

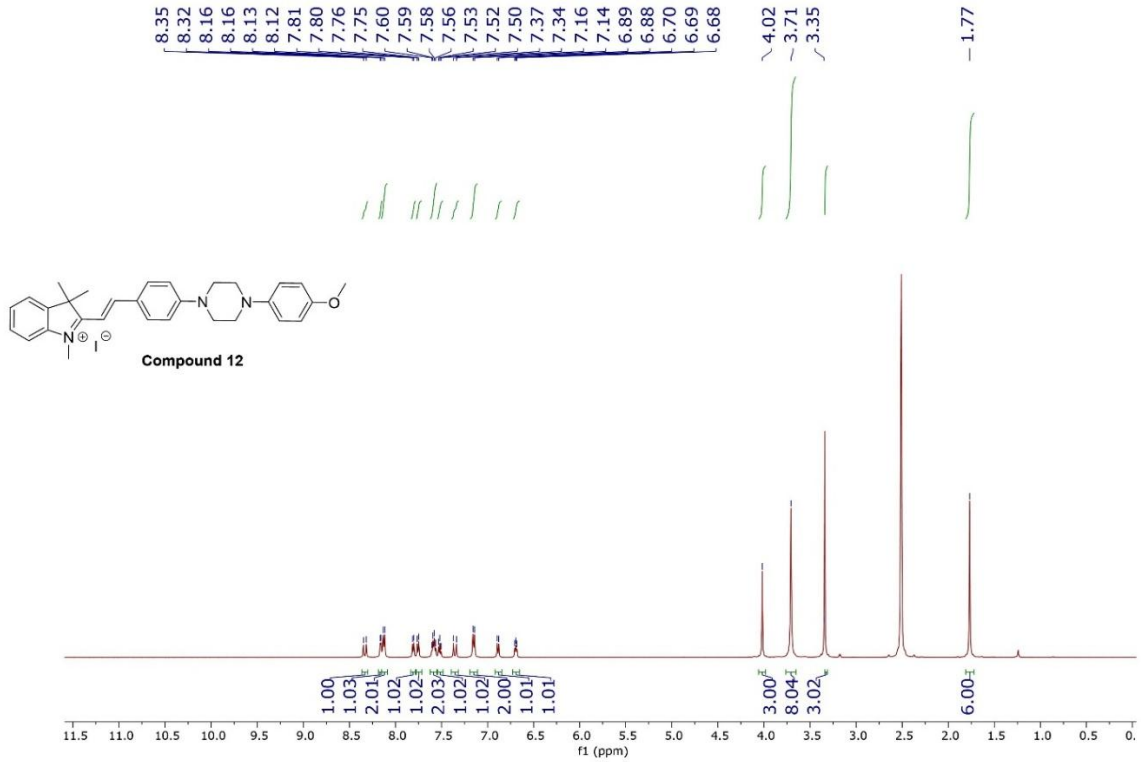

Figure B.1: ^{1}H NMR spectrum of (*E)-1,3,3-trimethyl-2-(4-(4-(pyridin-2-yl)piperazin-1-yl)styryl)-3H-indol-1-ium iodide* **(12).**

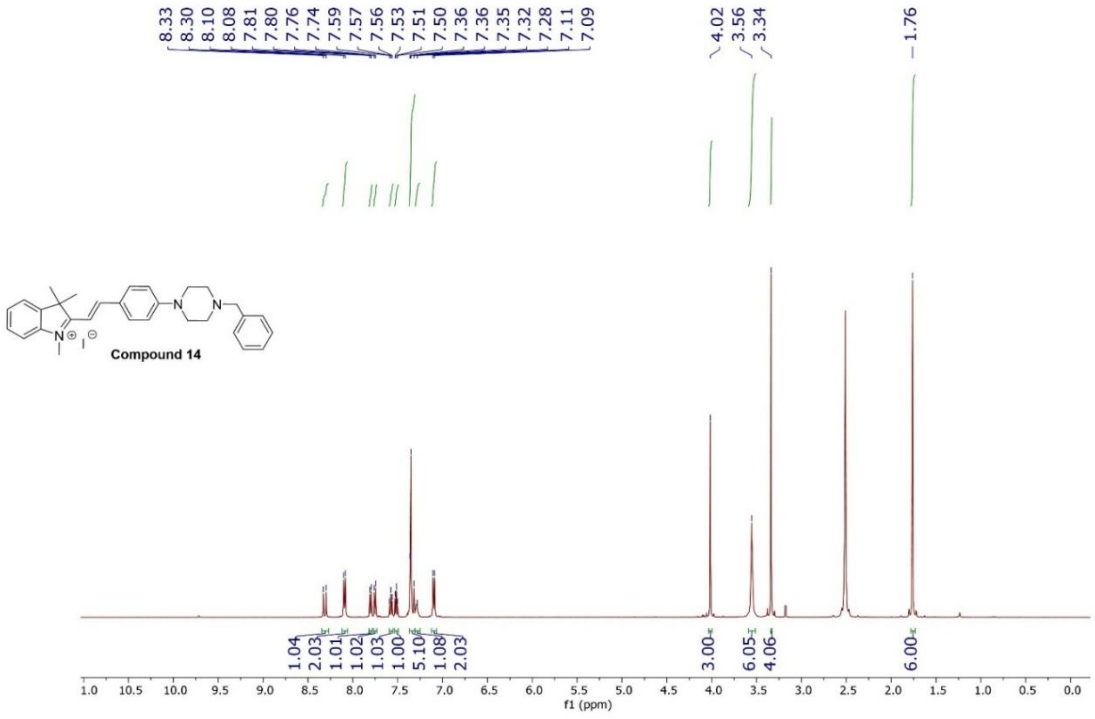

Figure B.2: ^{1}H NMR spectrum of *(E)-2-(4-(4-Benzylpiperazin-1-yl)styryl)-1,3,3-trimethyl-3H-indol-1-ium iodide* ***(14).***

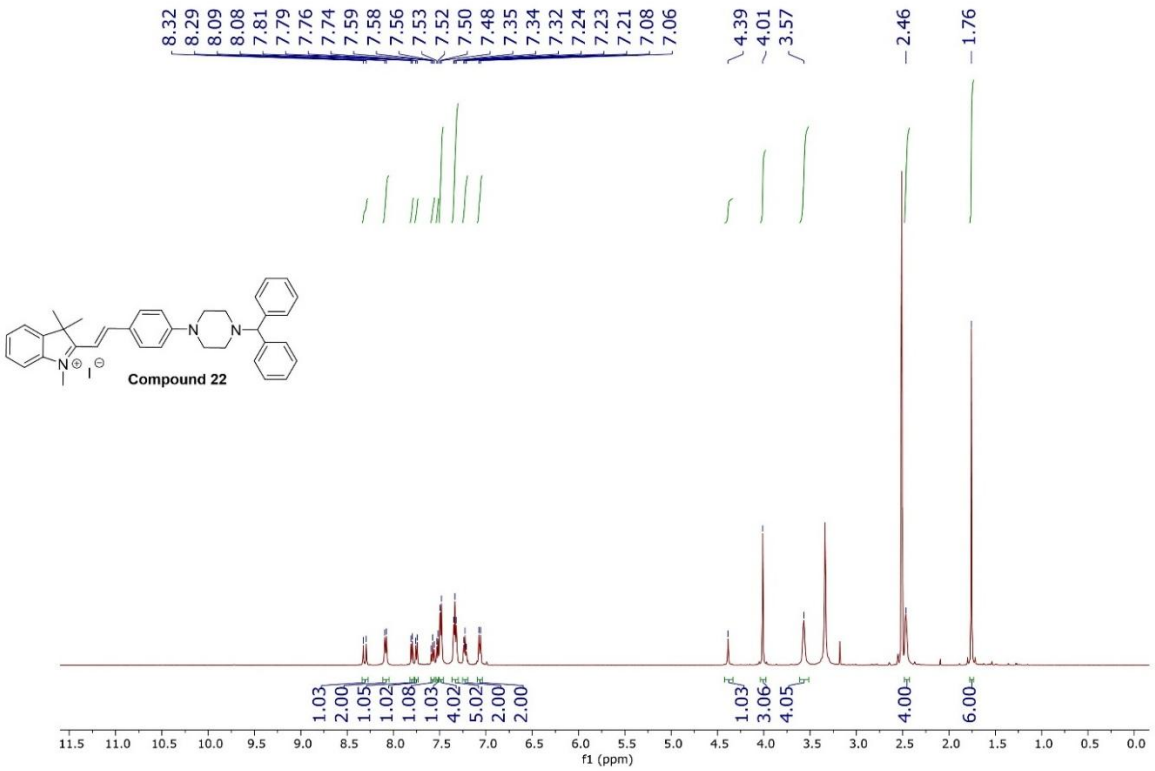

Figure B.3: ^{1}H NMR spectrum of *(E)-2-(4-(4-Benzhydrylpiperazin-1-yl)styryl)-1,3,3-trimethyl-3H-indol-1-ium iodide* **(22)**.

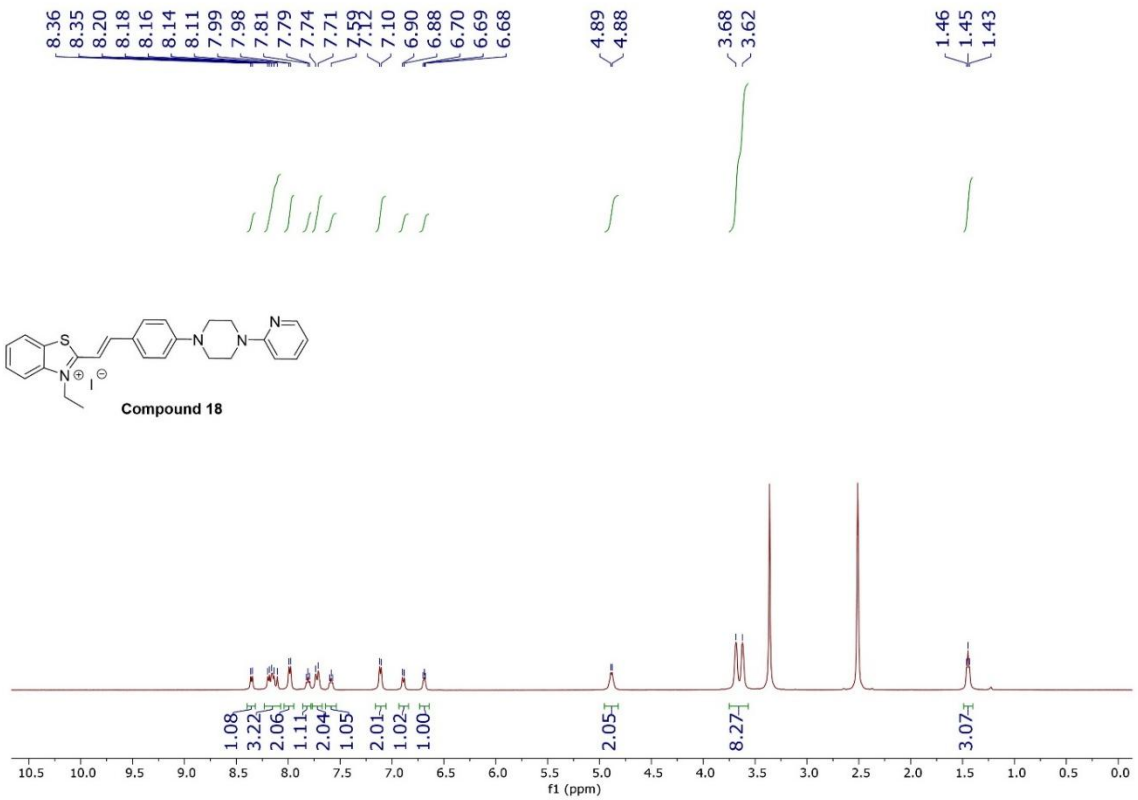

Figure B.4: ^{1}H NMR spectrum of *(E)-3-Ethyl-2-(4-(4-(pyridin-2-yl)piperazin-1-yl)styryl)benzo[d]thiazol-3-ium iodide* **(18).**

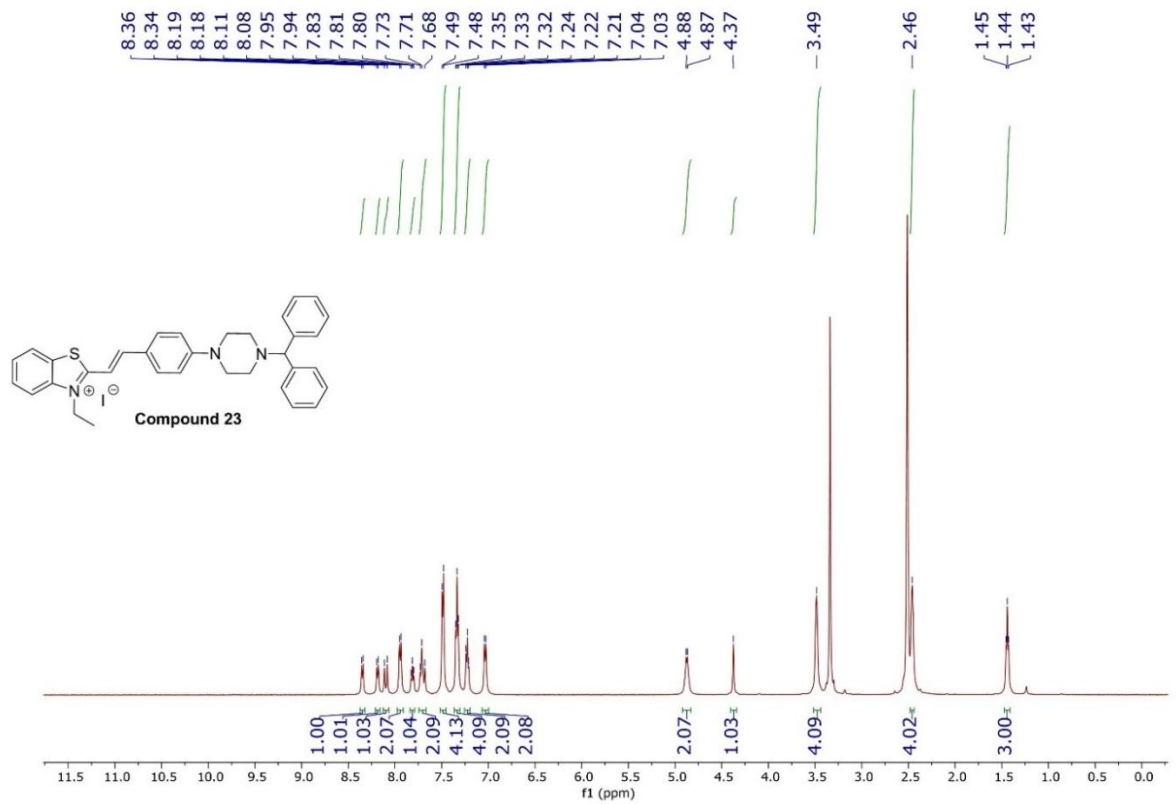

Figure B.5: ^{1}H NMR spectrum of *(E)-2-(4-(4-Benzhydrylpiperazin-1-yl)styryl)-3-ethylbenzo[d]thiazol-3-ium iodide* **(23).**

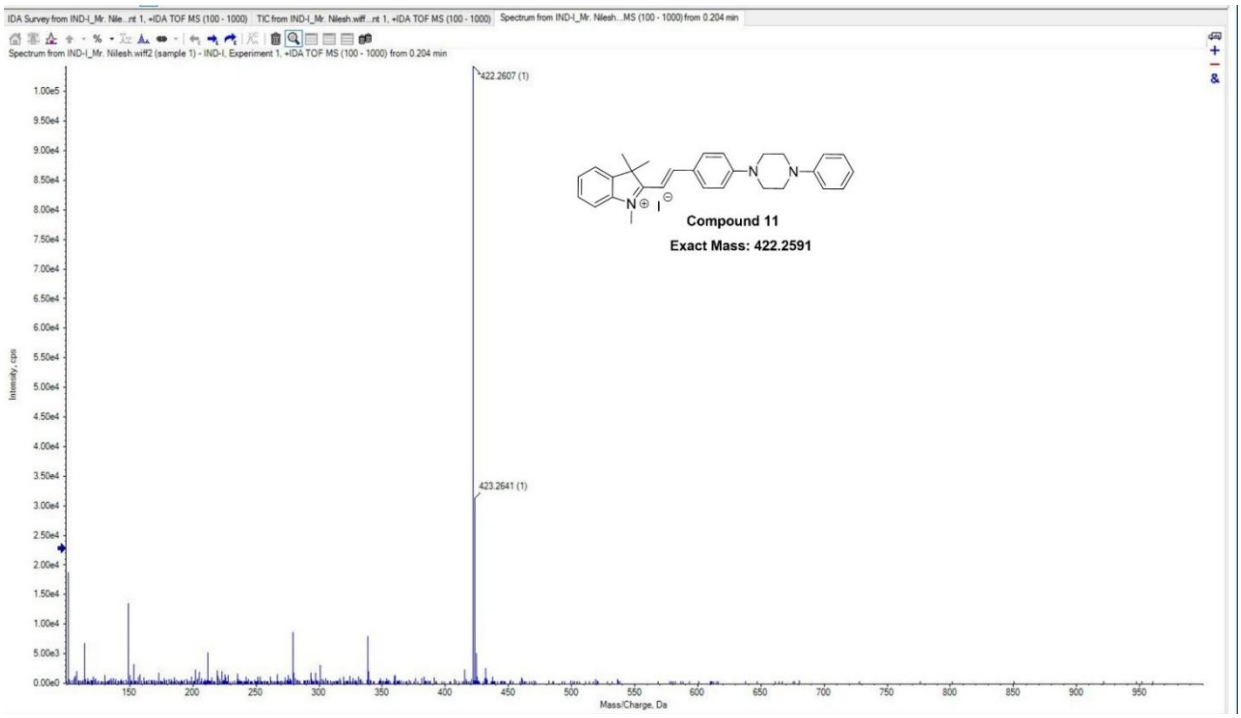

Figure B6: HRMS spectra of *(E)-1,3,3-Trimethyl-2-(4-(4-phenylpiperazin-1-yl)styryl)-3H-indol-1-ium iodide* ***(11)***.

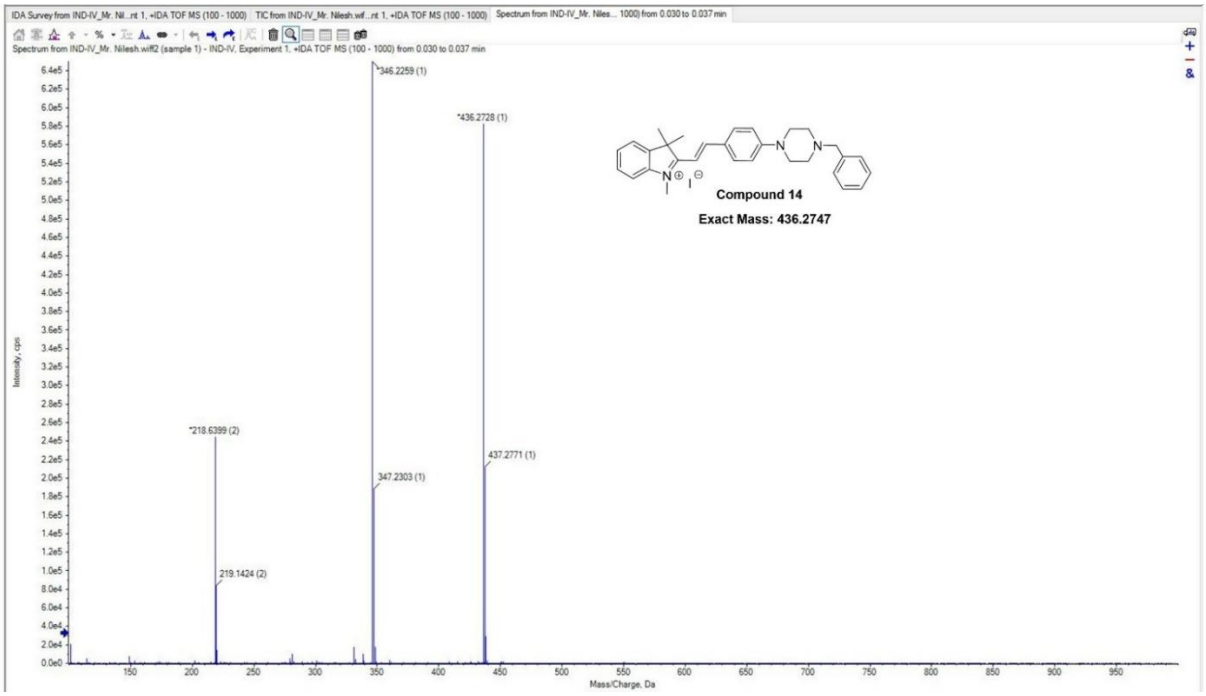

Figure B.7: HRMS spectra of *(E)-2-(4-(4-Benzylpiperazin-1-yl)styryl)-1,3,3-trimethyl-3H-indol-1-ium iodide* **(14).**

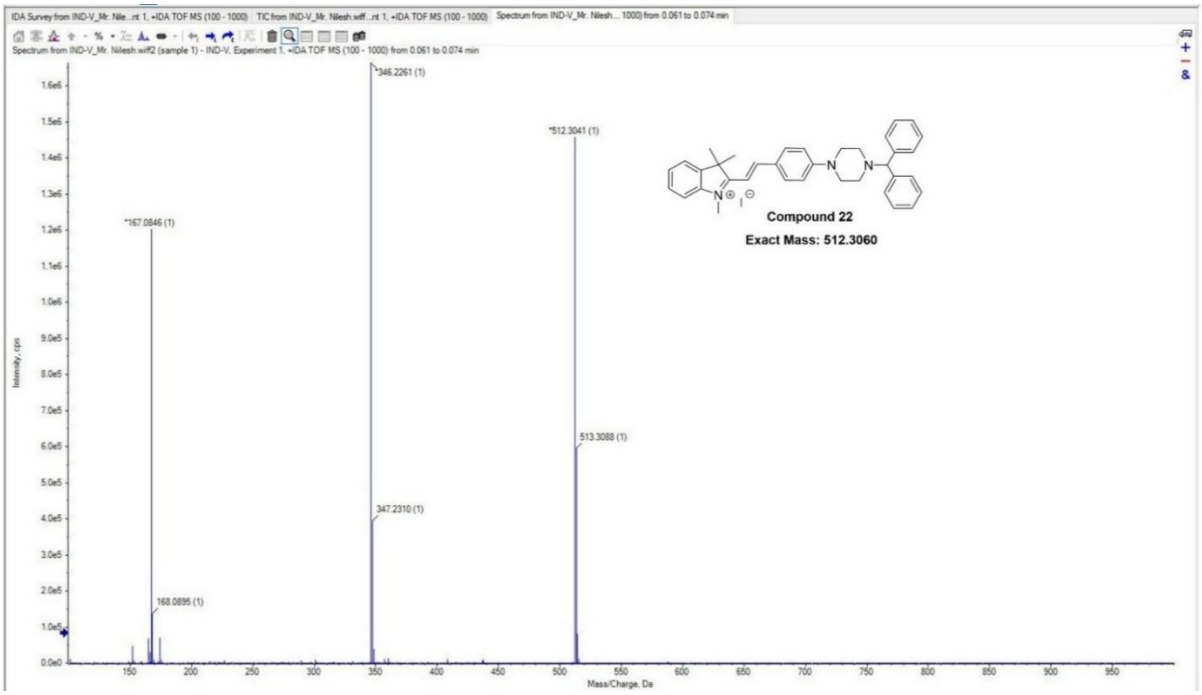

Figure B.8: HRMS spectra of *(E)-2-(4-(4-Benzhydrylpiperazin-1-yl)styryl)-1,3,3-trimethyl-3H-indol-1-ium iodide* **(22).**

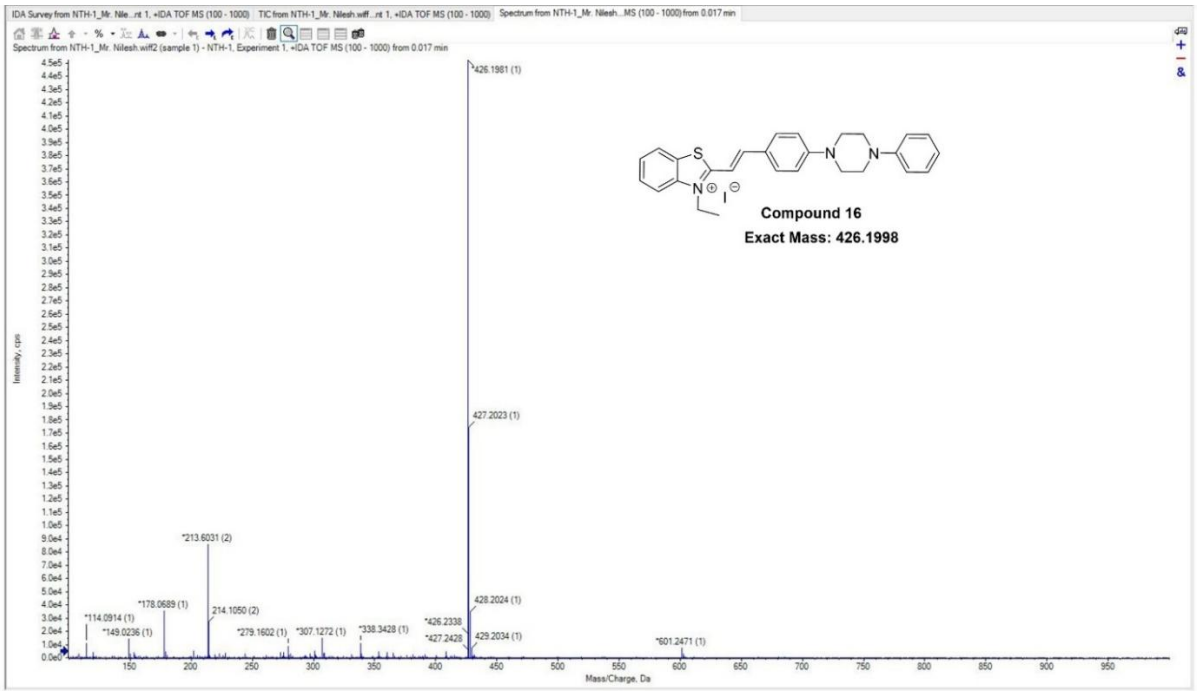

Figure B.9: HRMS spectra of *(E)-3-Ethyl-2-(4-(4-phenylpiperazin-1-yl)styryl)benzo[d]thiazol-3-ium iodide* ***(16).***

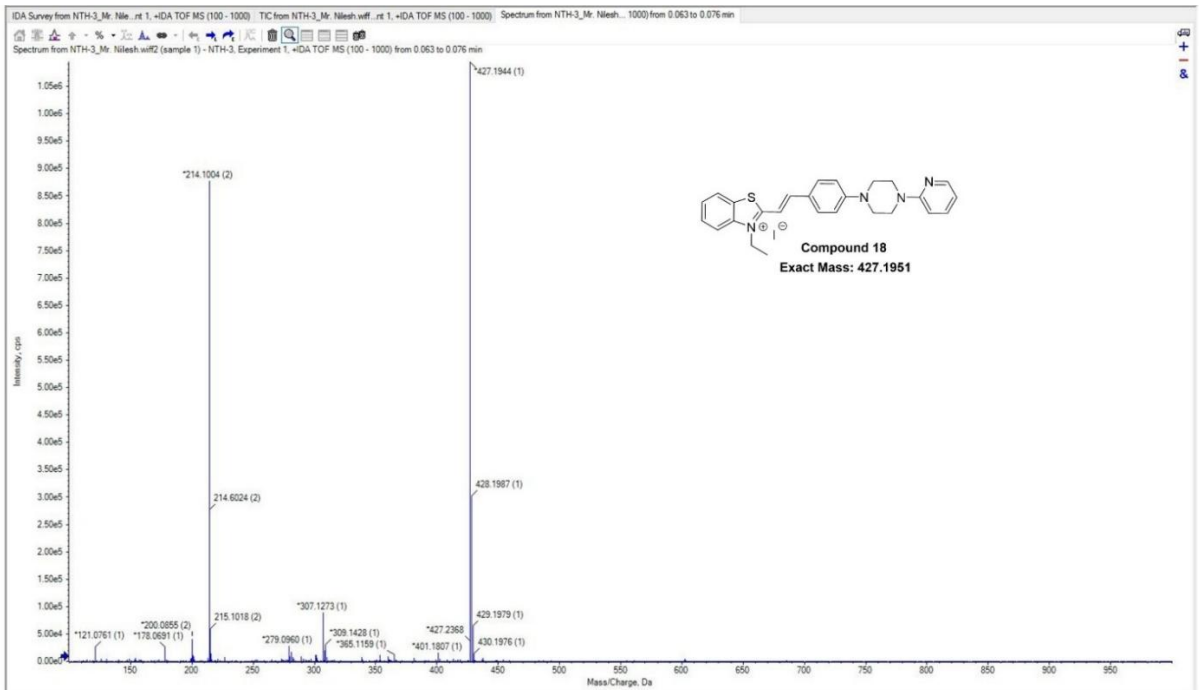

Figure B.10: HRMS spectra of *(E)-3-Ethyl-2-(4-(4-(pyridin-2-yl)piperazin-1-yl)styryl)benzo[d]thiazol-3-ium iodide* **(18).**

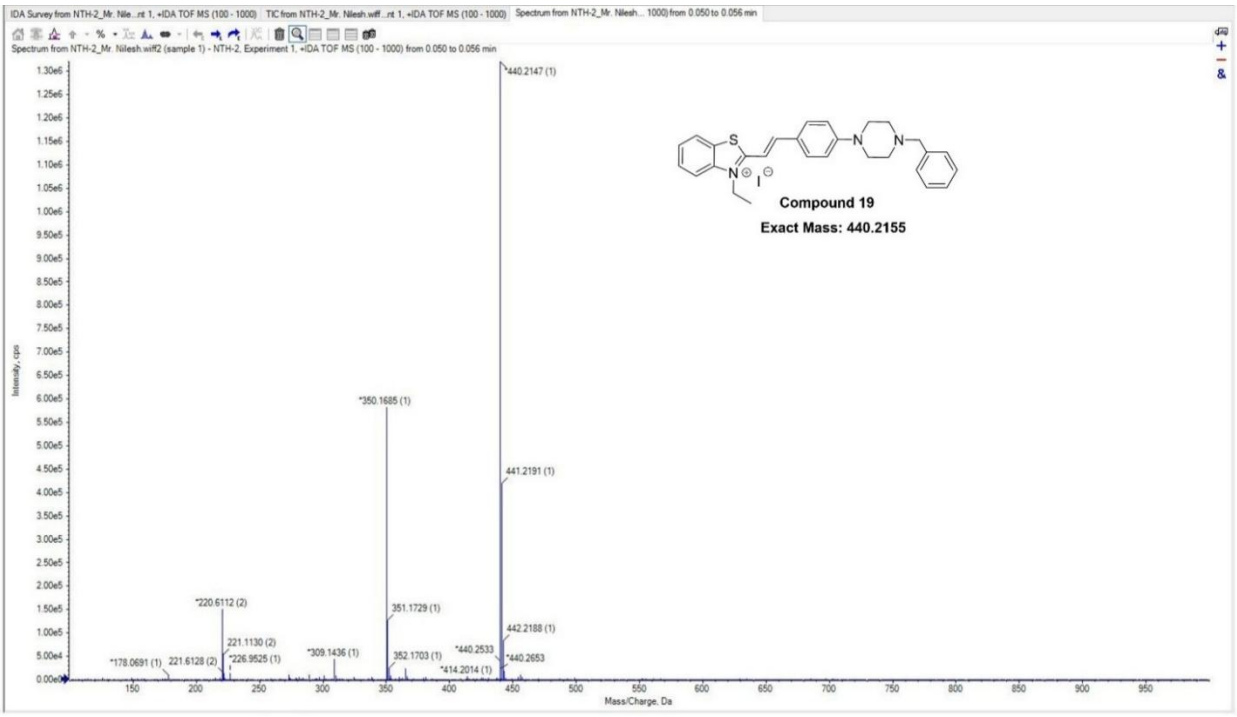

Figure B.11: HRMS spectra of *(E)-2-(4-(4-Benzylpiperazin-1-yl)styryl)-3-ethylbenzo[d]thiazol-3-ium iodide* ***(19)*****.**

10.3 Supplementary data of chalcone derivatives bearing N-aryl piperazine moiety

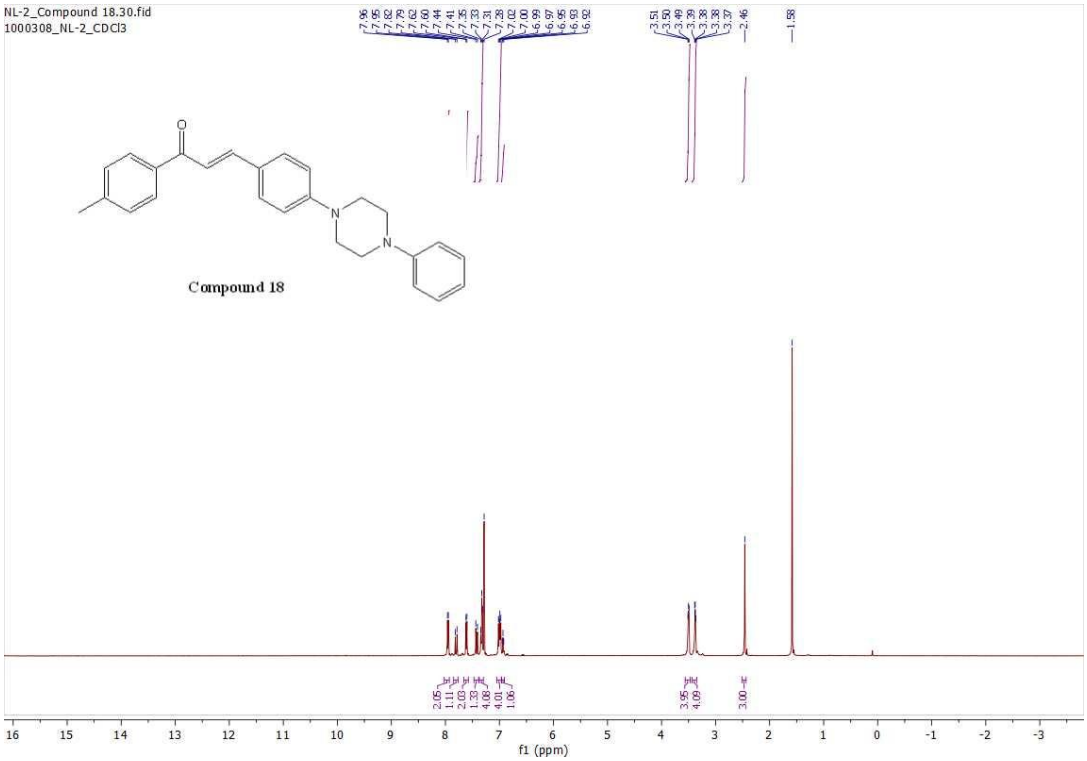

Figure C.1: ^{1}H NMR spectrum of *(E)-3-(4-(4-phenylpiperazin-1-yl)phenyl)-1-(p-tolyl)prop-2-en-1-one* **(18).**

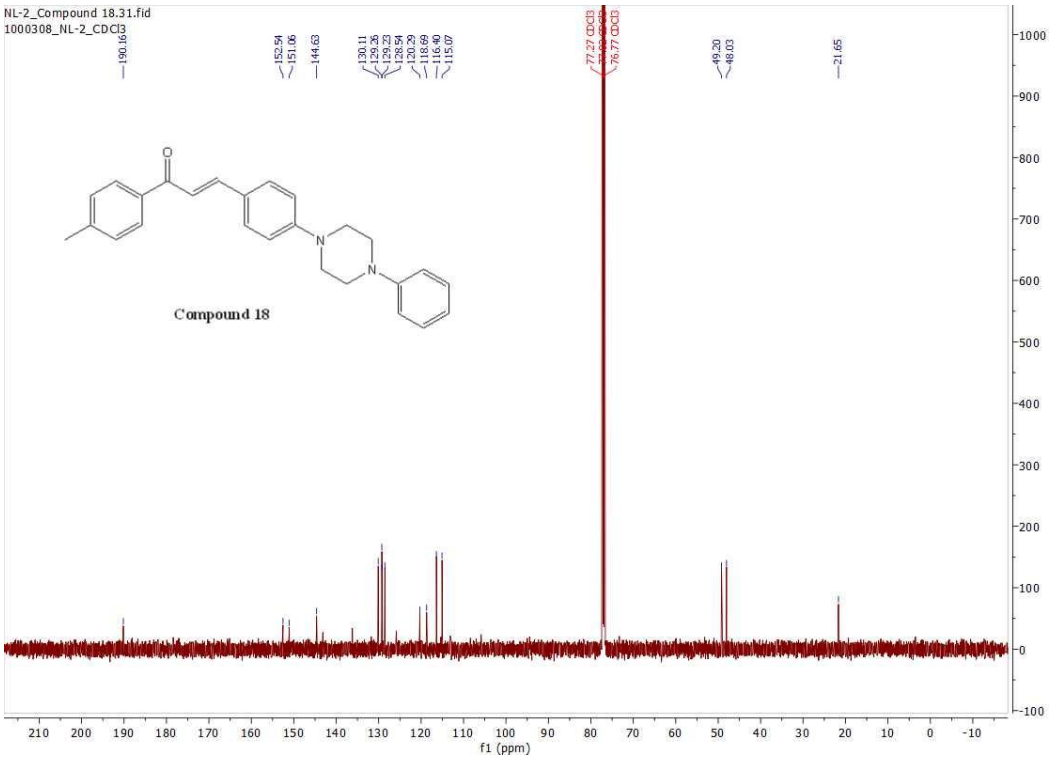

Figure C.2: ^{13}C NMR spectrum of *(E)-3-(4-(4-phenylpiperazin-1-yl)phenyl)-1-(p-tolyl)prop-2-en-1-one* **(18).**

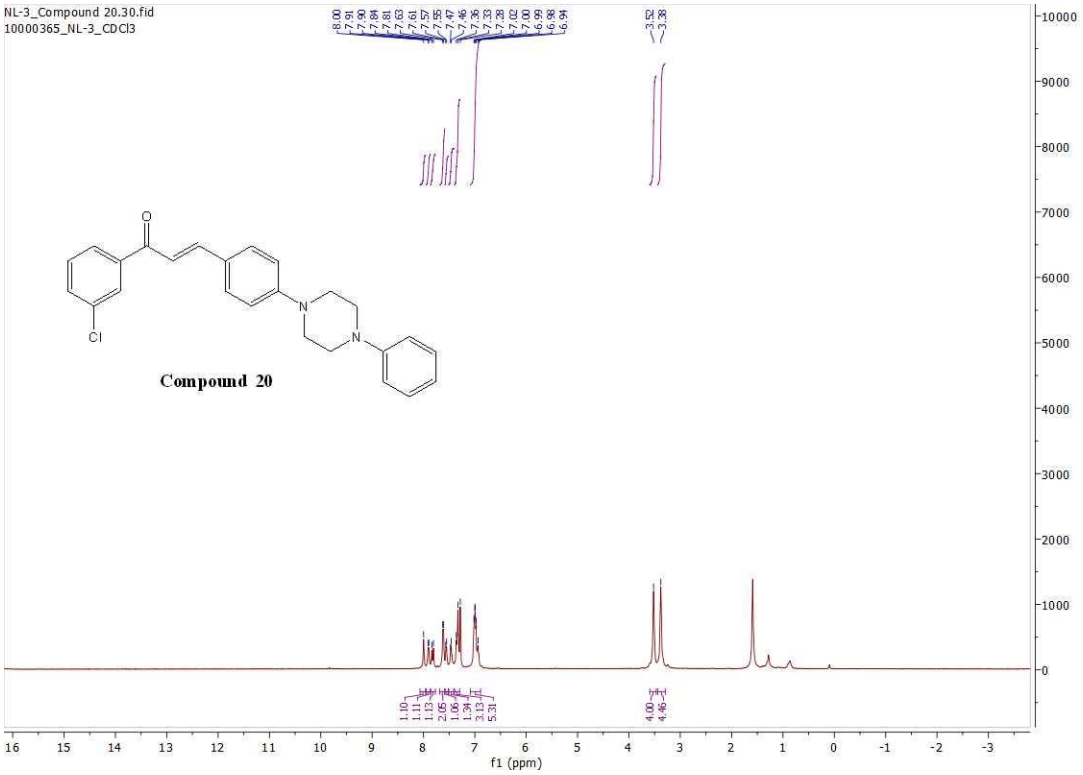

Figure C.3: ^{1}H NMR spectrum of *(E)-1-(3-chlorophenyl)-3-(4-(4-phenylpiperazin-1-yl)phenyl)prop-2-en-1-one* **(20).**

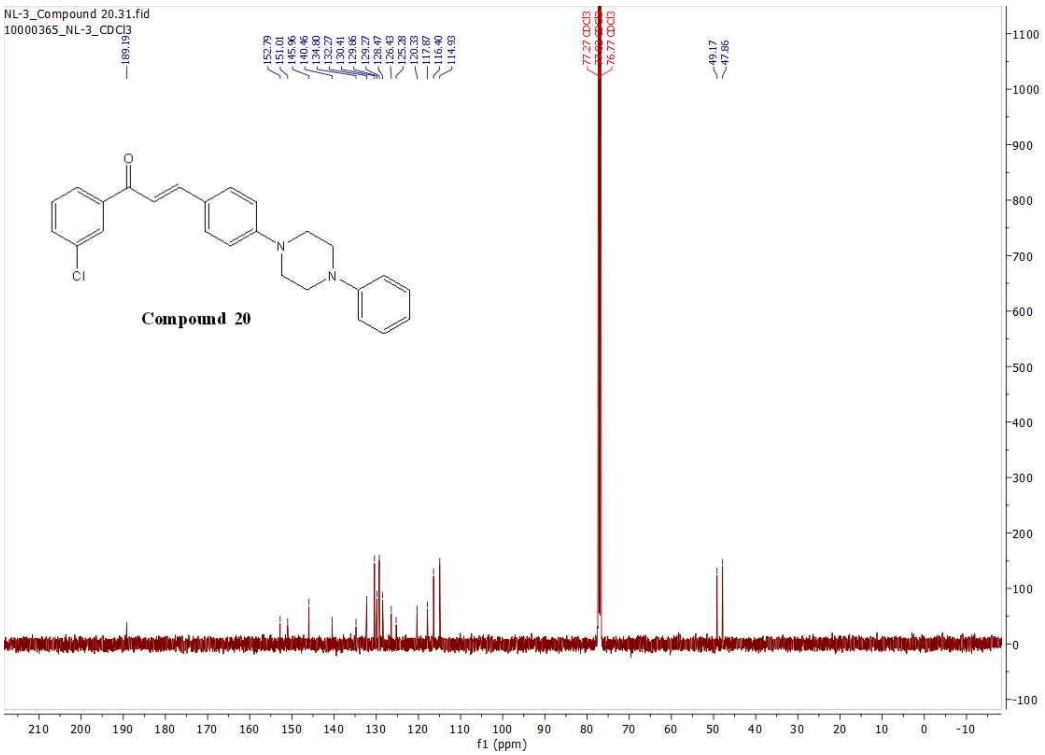

Figure C.4: ^{13}C NMR spectrum of *(E)-1-(3-chlorophenyl)-3-(4-(4-phenylpiperazin-1-yl)phenyl)prop-2-en-1-one* **(20).**

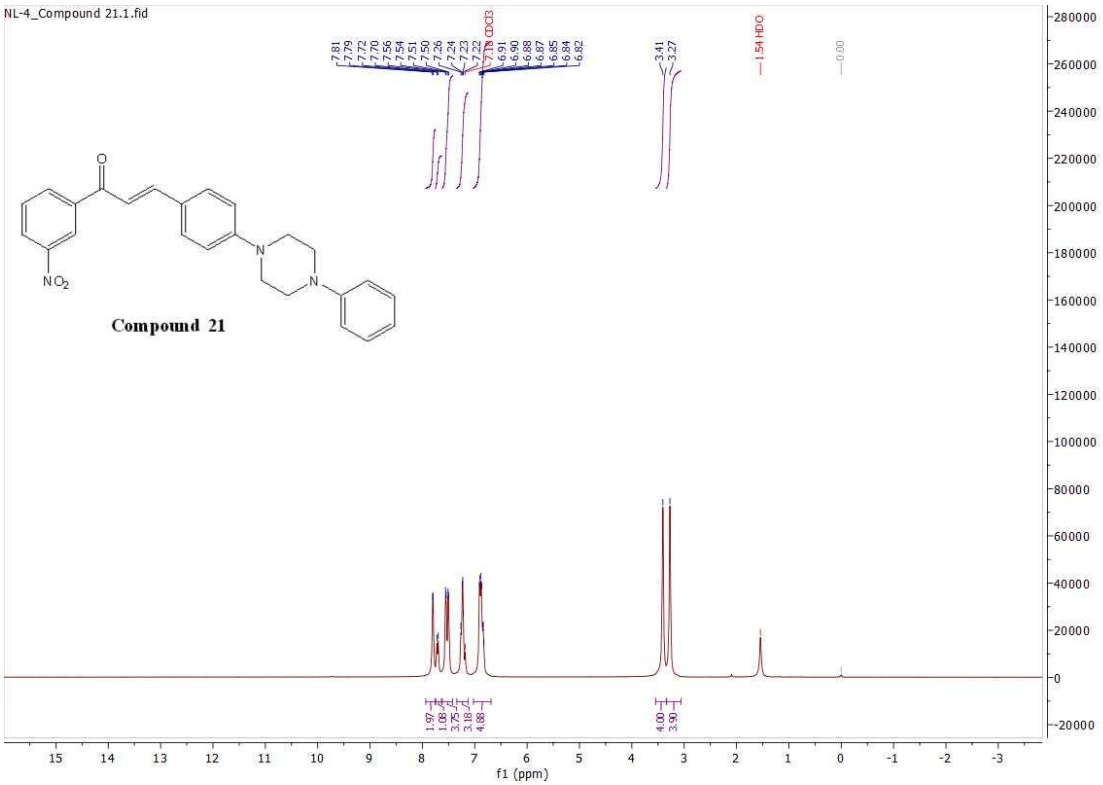

Figure C.5: ^{1}H NMR spectrum of *(E)-1-(3-nitrophenyl)-3-(4-(4-phenylpiperazin-1-yl)phenyl)prop-2-en-1-one* **(21).**

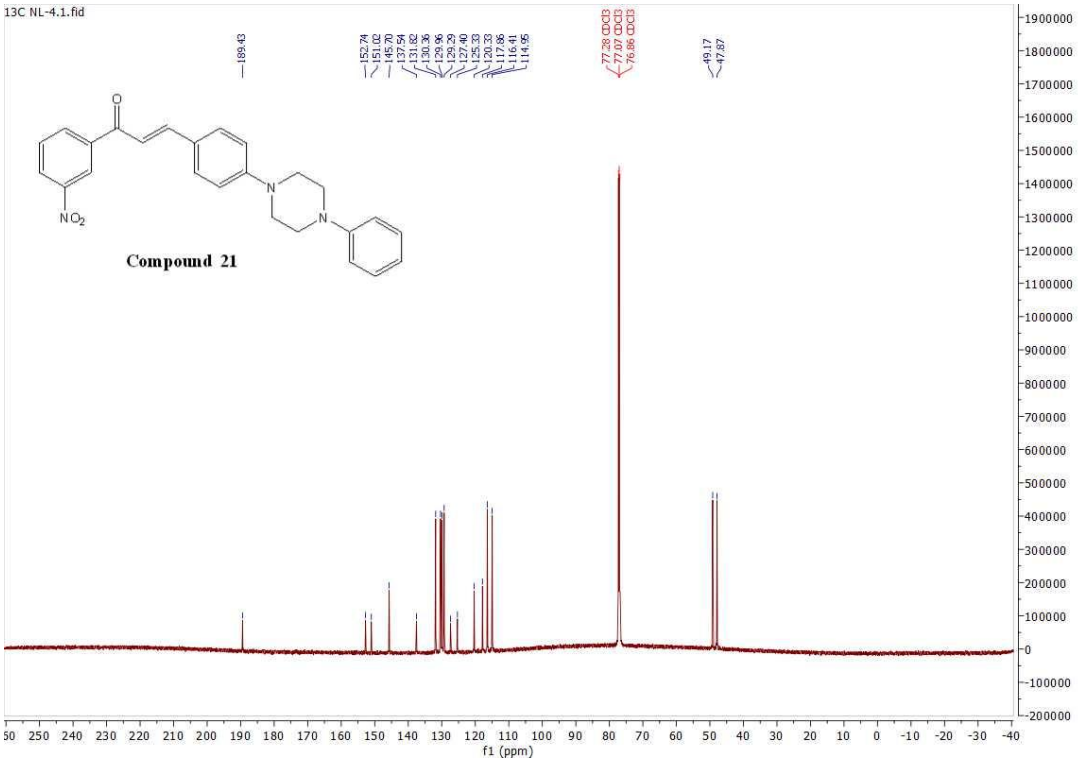

Figure C.6: ^{13}C NMR spectrum of *(E)-1-(3-nitrophenyl)-3-(4-(4-phenylpiperazin-1-yl)phenyl)prop-2-en-1-one* **(21).**

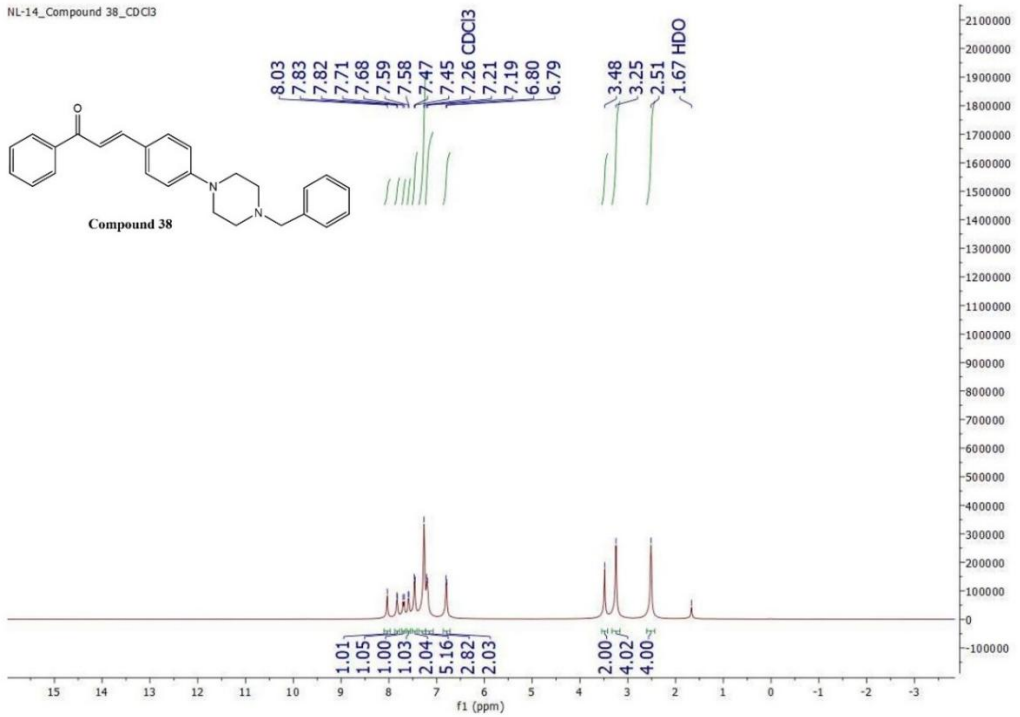

Figure C.7: ^{1}H NMR spectrum of *(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-phenylprop-2-en-1-one* **(38).**

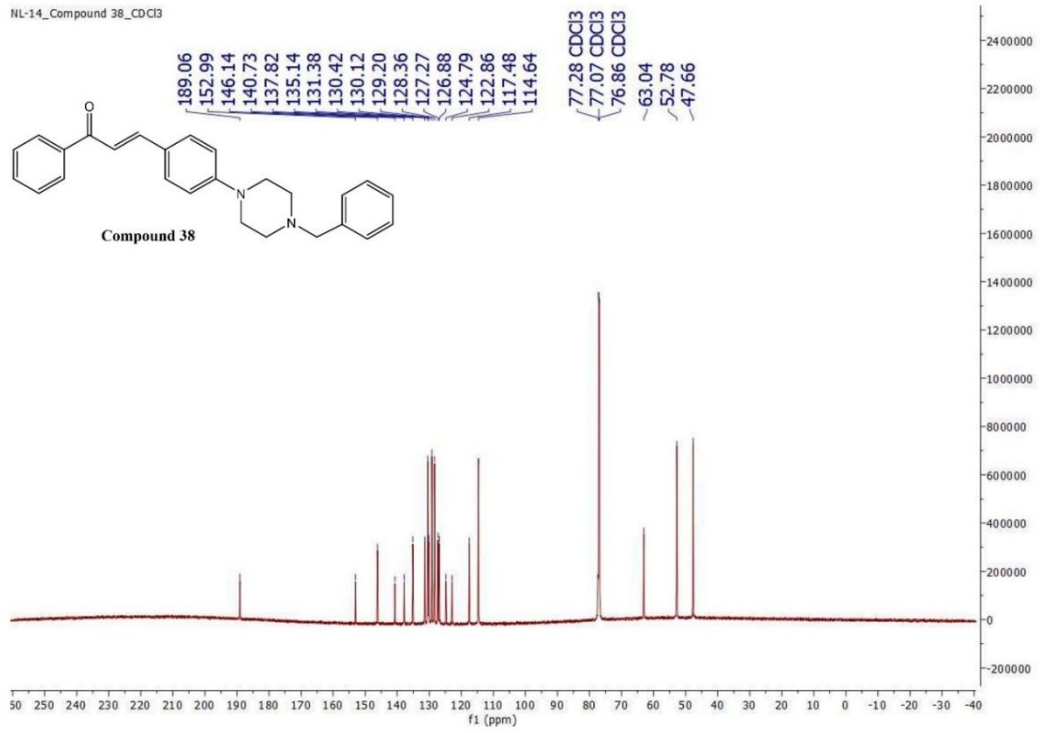

Figure C.8: ^{13}C NMR spectrum of *(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-phenylprop-2-en-1-one* **(38).**

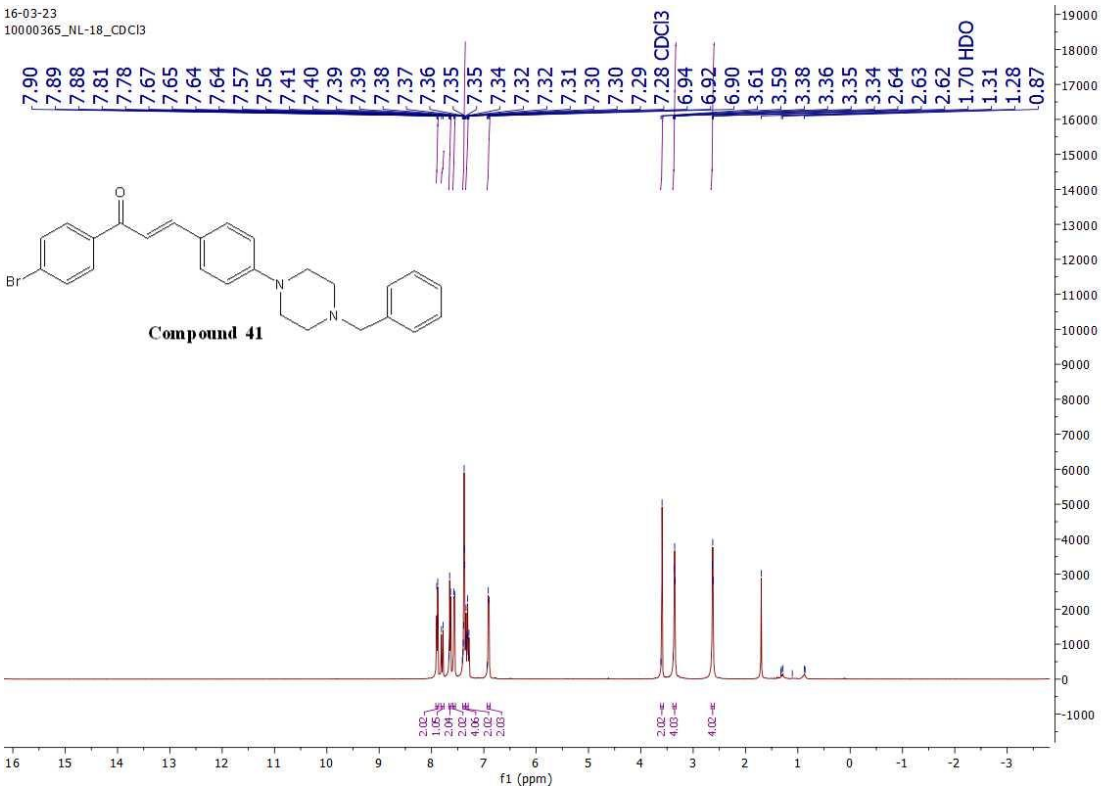

Figure C.9: ^{1}H NMR spectrum of ***(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-(4-bromophenyl)prop-2-en-1-one*** **(41).**

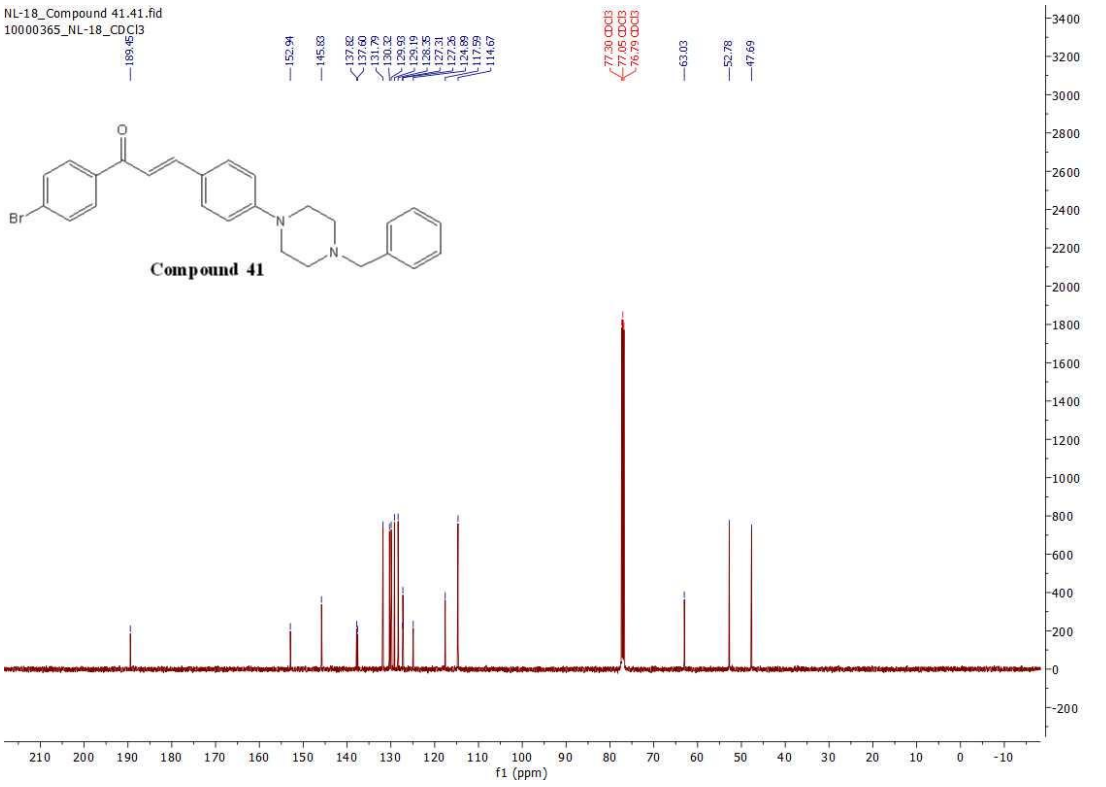

Figure C.10: ^{13}C NMR spectrum of ***(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-(4-bromophenyl)prop-2-en-1-one*** **(41).**

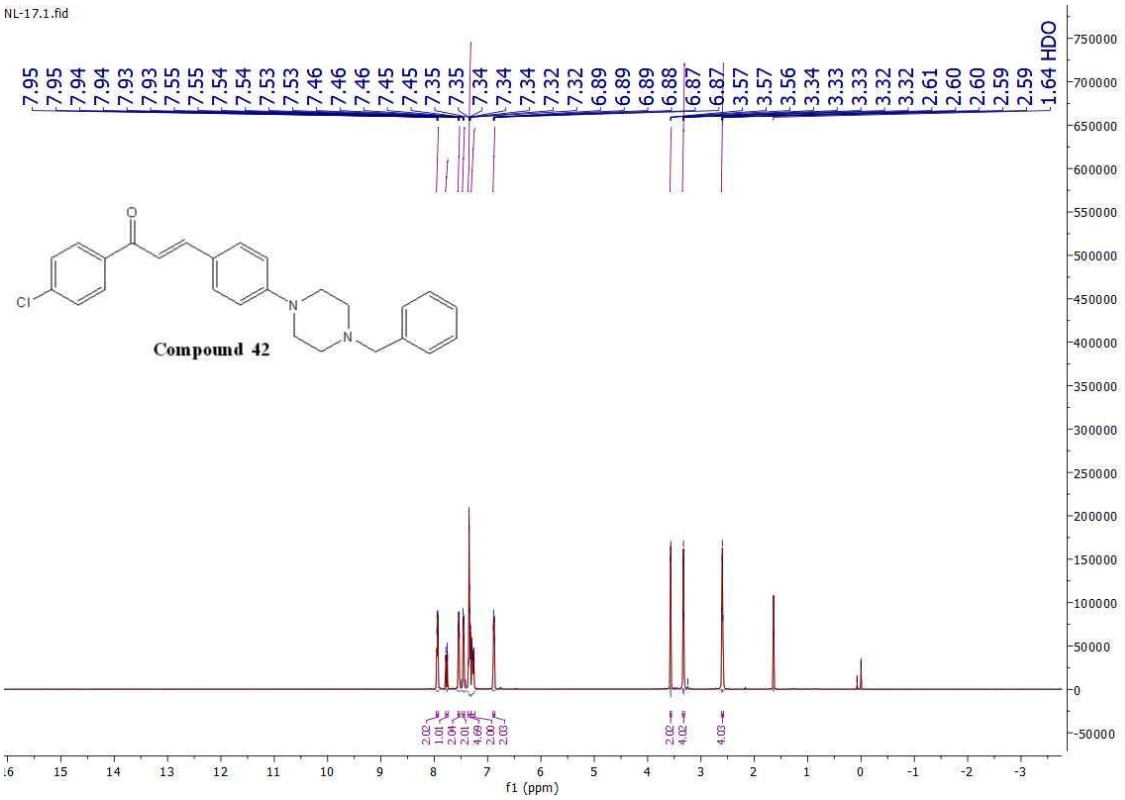

Figure C.11: ^{1}H NMR spectrum of *(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-(4-chlorophenyl)prop-2-en-1-one* **(42).**

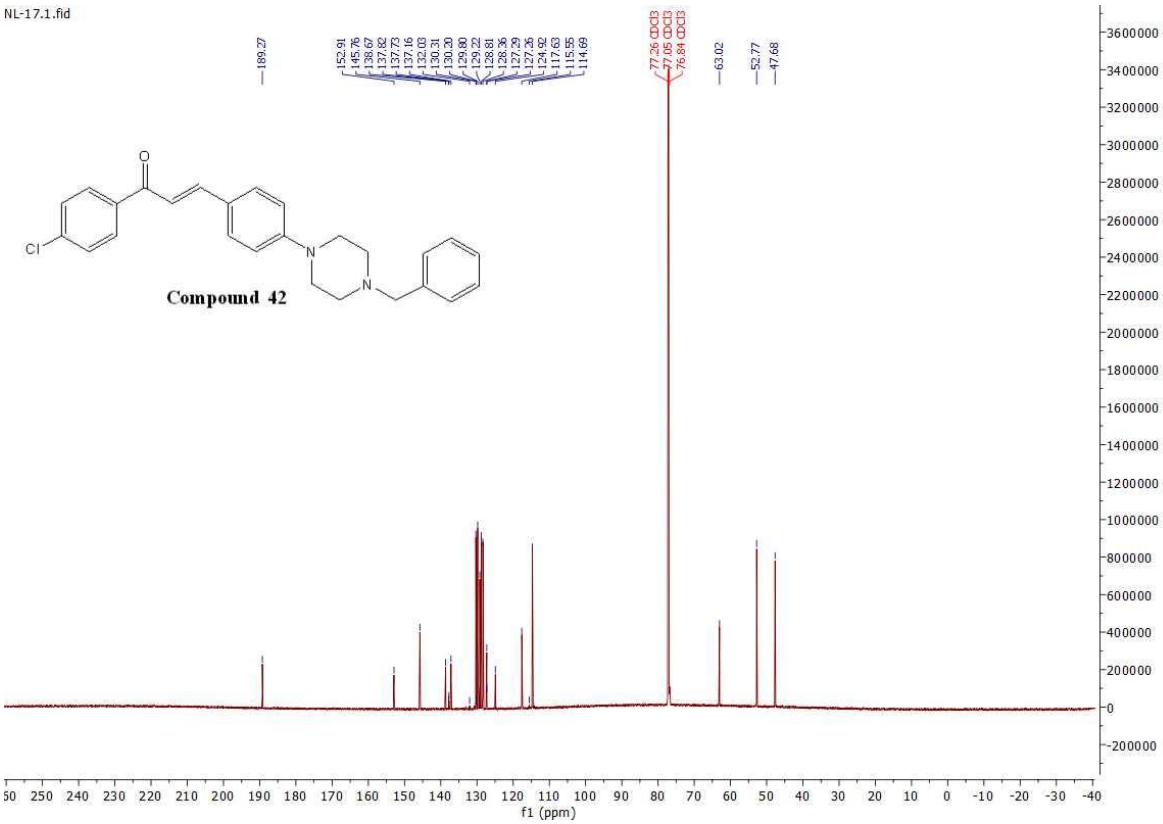

Figure C.12: ^{13}C NMR spectrum of *(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-(4-chlorophenyl)prop-2-en-1-one* **(42).**

Table C.1: Purity analysis of lead compounds determined by HPLC.

Compound ID	Retention Time (min)	HPLC Purity (%)
38	1.907	98.62%
41	1.973	99.74%
42	1.986	99.81%

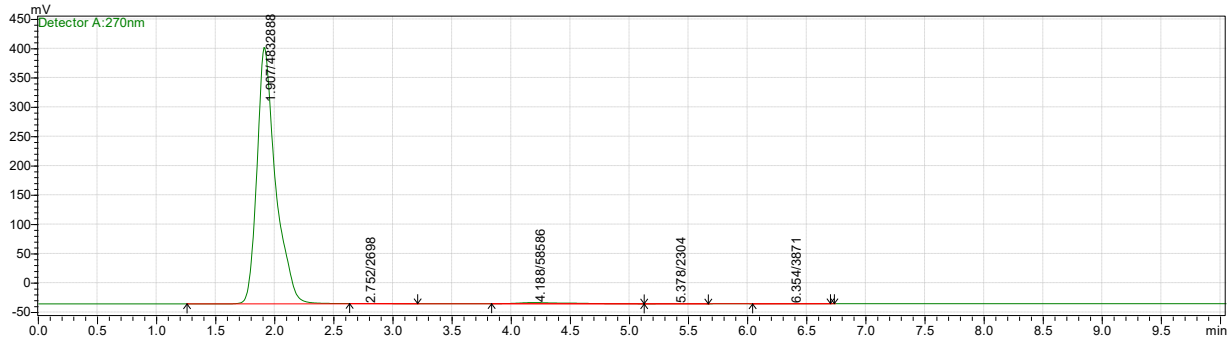

Figure C.13: HPLC chromatogram of the *(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-phenylprop-2-en-1-one* **(38).**

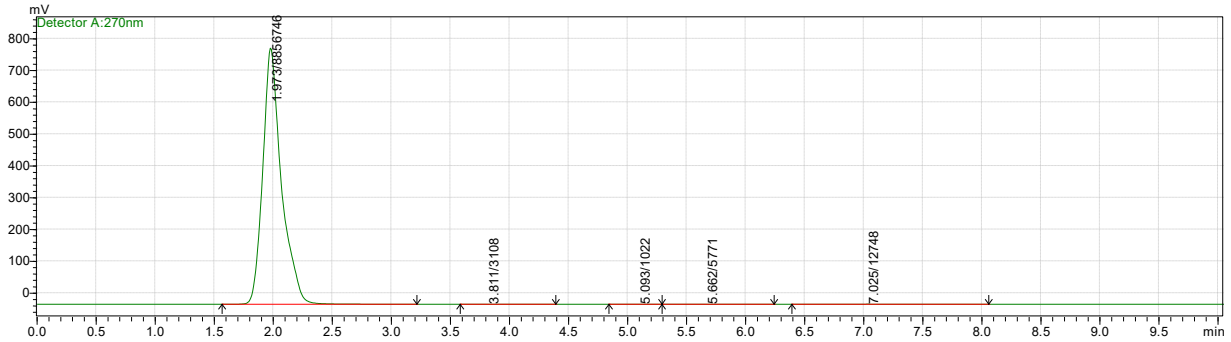

Figure C.14: HPLC chromatogram of the *(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-(4-bromophenyl)prop-2-en-1-one* **(41).**

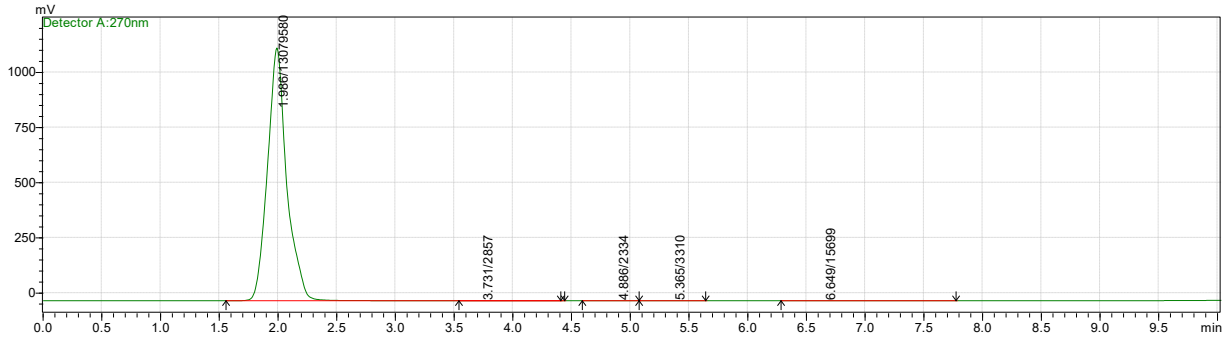

Figure C.15: HPLC chromatogram of the *(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-(4-chlorophenyl)prop-2-en-1-one* **(42).**

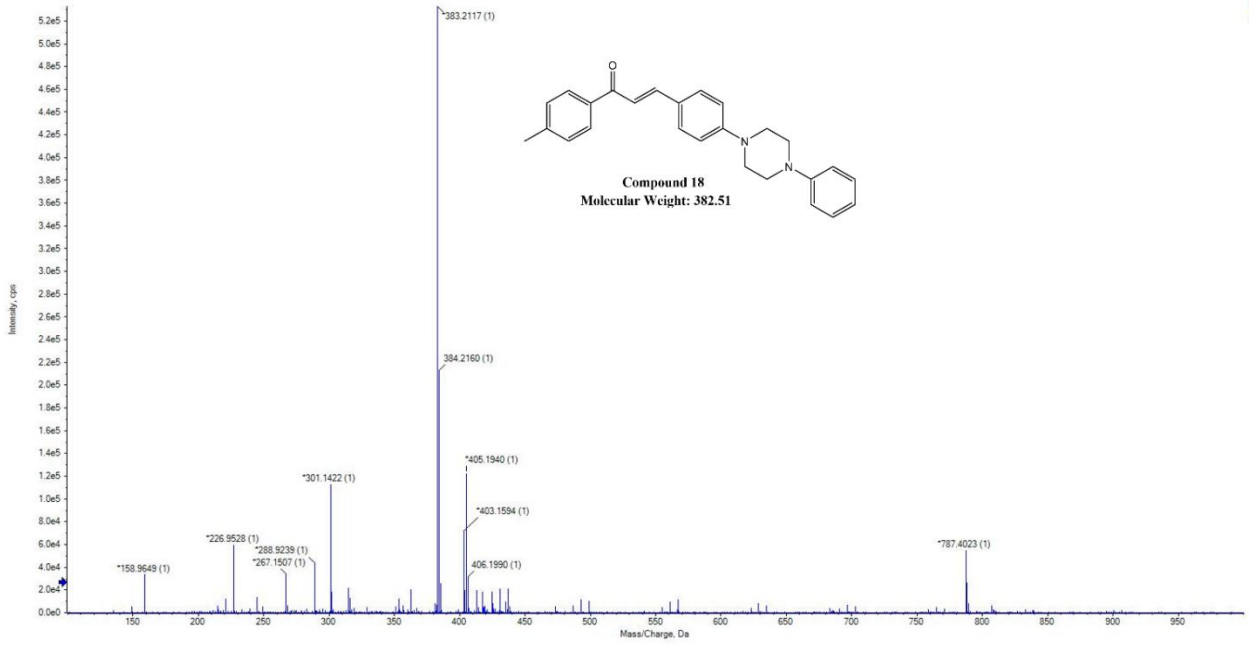

Figure C.16. HRMS of *(E)-3-(4-(4-phenylpiperazin-1-yl)phenyl)-1-(p-tolyl)prop-2-en-1-one* **(18).**

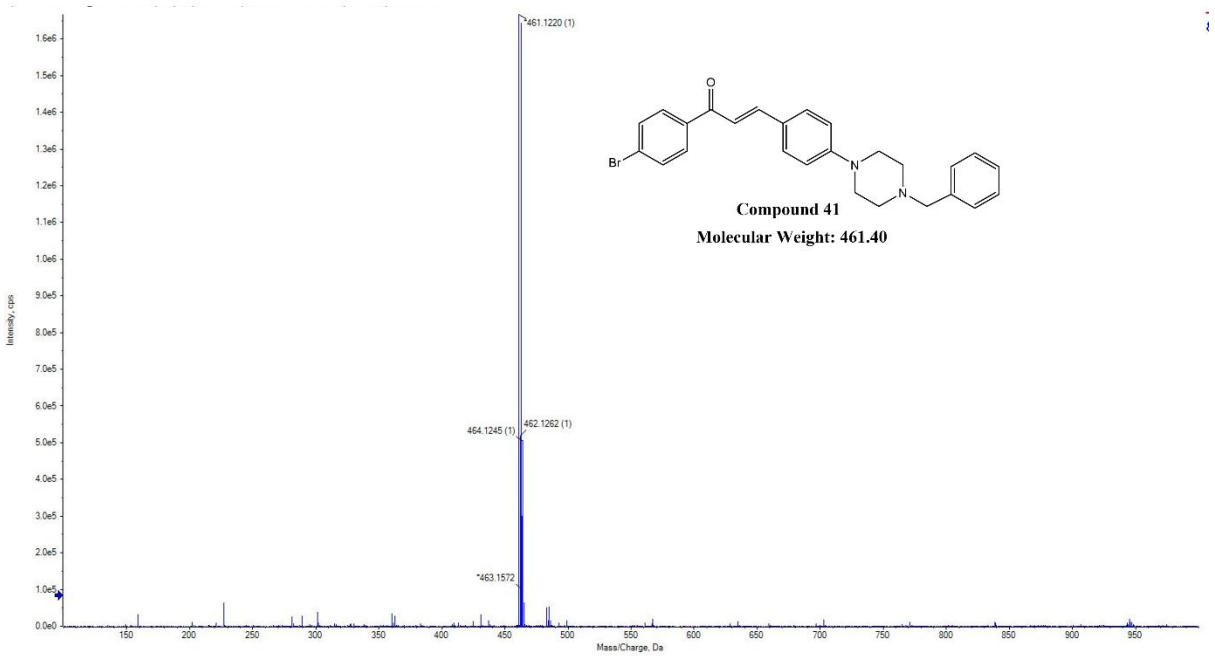

Figure C.17. HRMS of *(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-(4-bromophenyl)prop-2-en-1-one* **(41).**

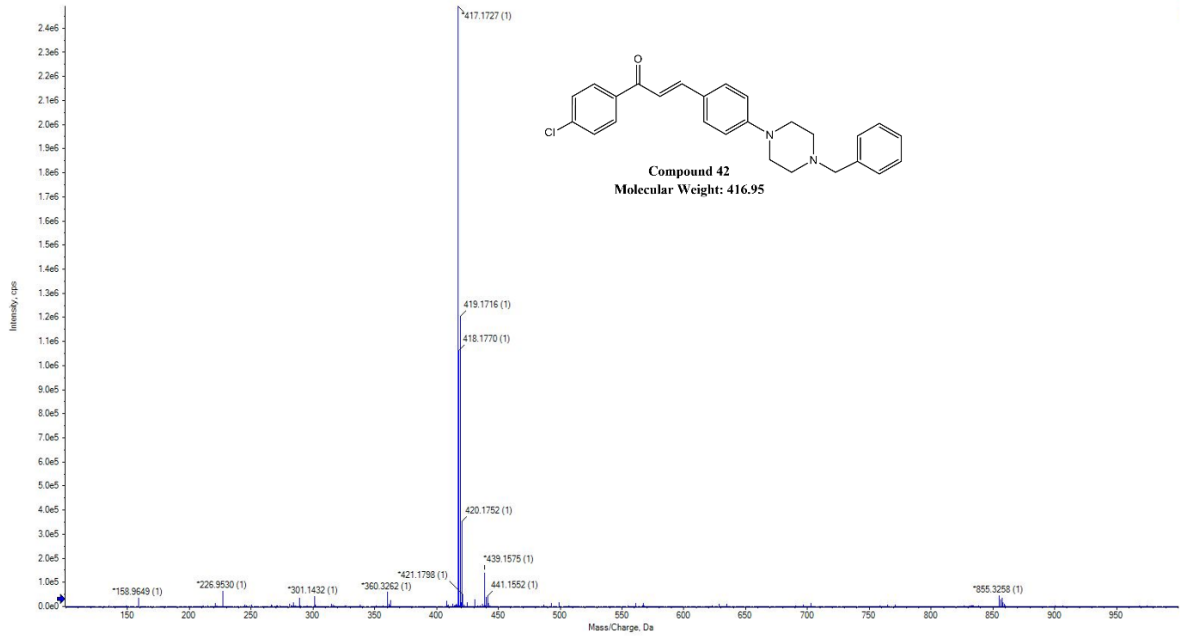

Figure C.18. HRMS of *(E)-3-(4-(4-benzylpiperazin-1-yl)phenyl)-1-(4-chlorophenyl)prop-2-en-1-one* **(42).**

10.4 Supplementary data of pyrazoline analogs

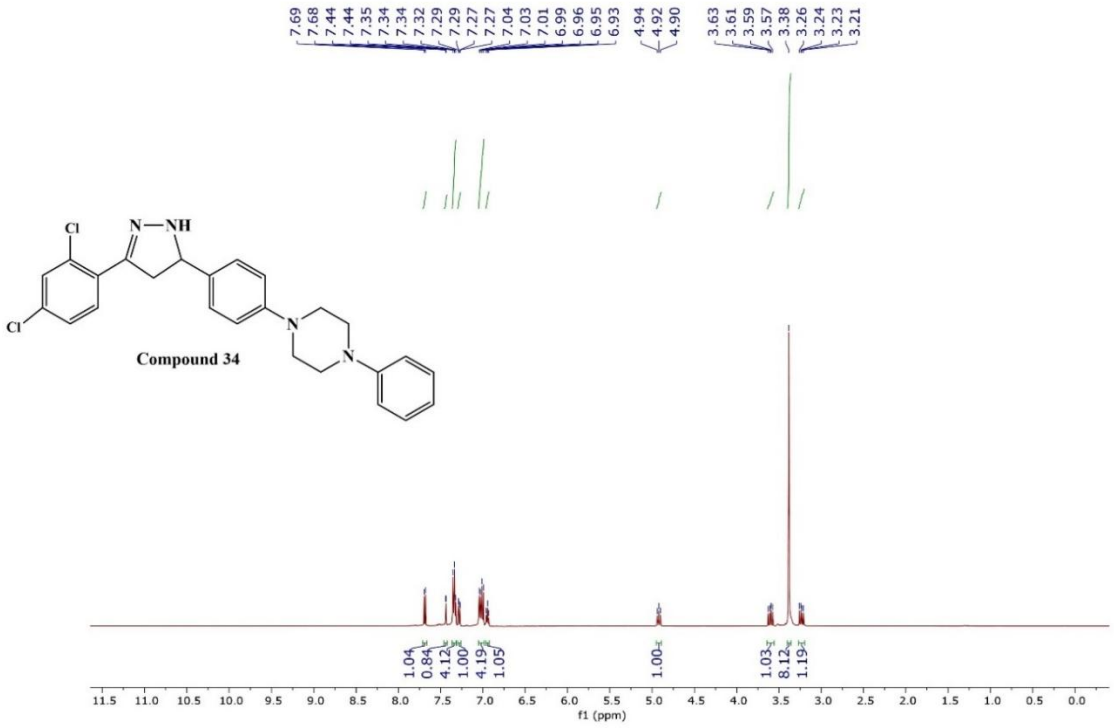

Figure D.1: ^{1}H NMR spectrum of *1-(4-(3-(2,4-Dichlorophenyl)-4,5-dihydro-1H-pyrazol-5-yl)phenyl)-4-phenylpiperazine* ***(34).***

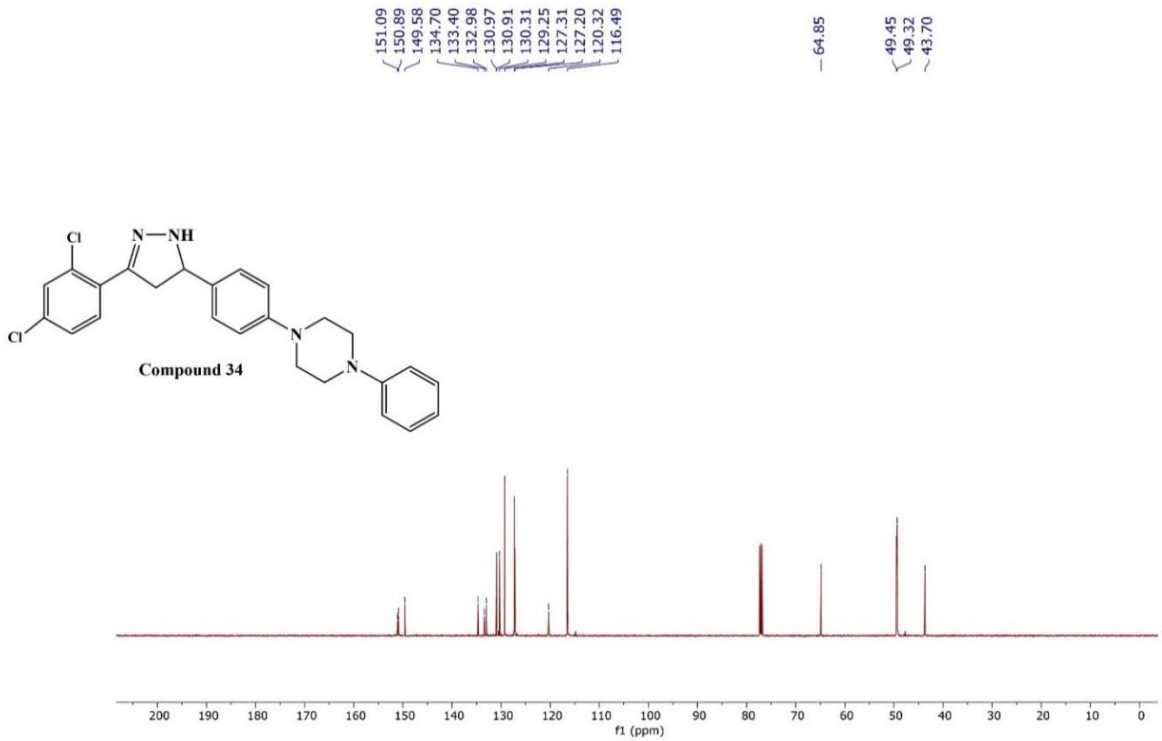

Figure D.2: ^{13}C NMR spectrum of *1-(4-(3-(2,4-Dichlorophenyl)-4,5-dihydro-1H-pyrazol-5-yl)phenyl)-4-phenylpiperazine* ***(34).***

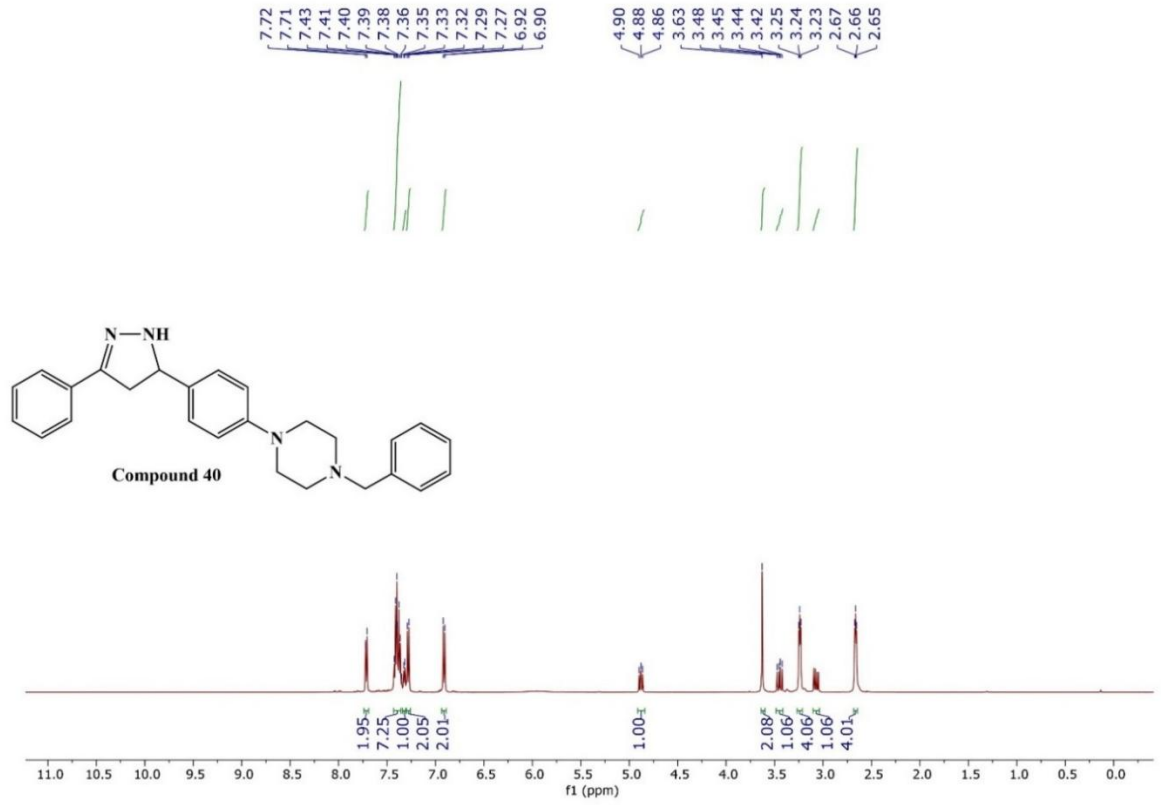

Figure D.3: ^{1}H NMR spectrum of *1-Benzyl-4-(4-(3-phenyl-4,5-dihydro-1H-pyrazol-5-yl)phenyl)piperazine* **(40).**

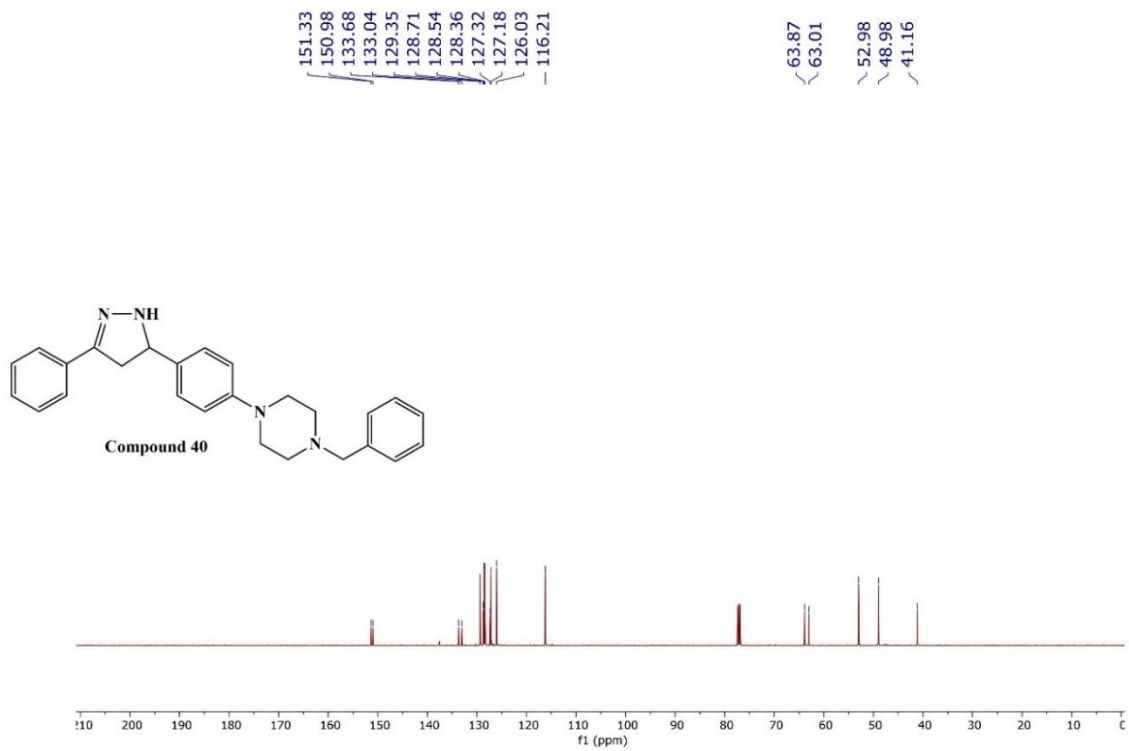

Figure D.4: ^{13}C NMR spectrum of *1-Benzyl-4-(4-(3-phenyl-4,5-dihydro-1H-pyrazol-5-yl)phenyl)piperazine* **(40).**

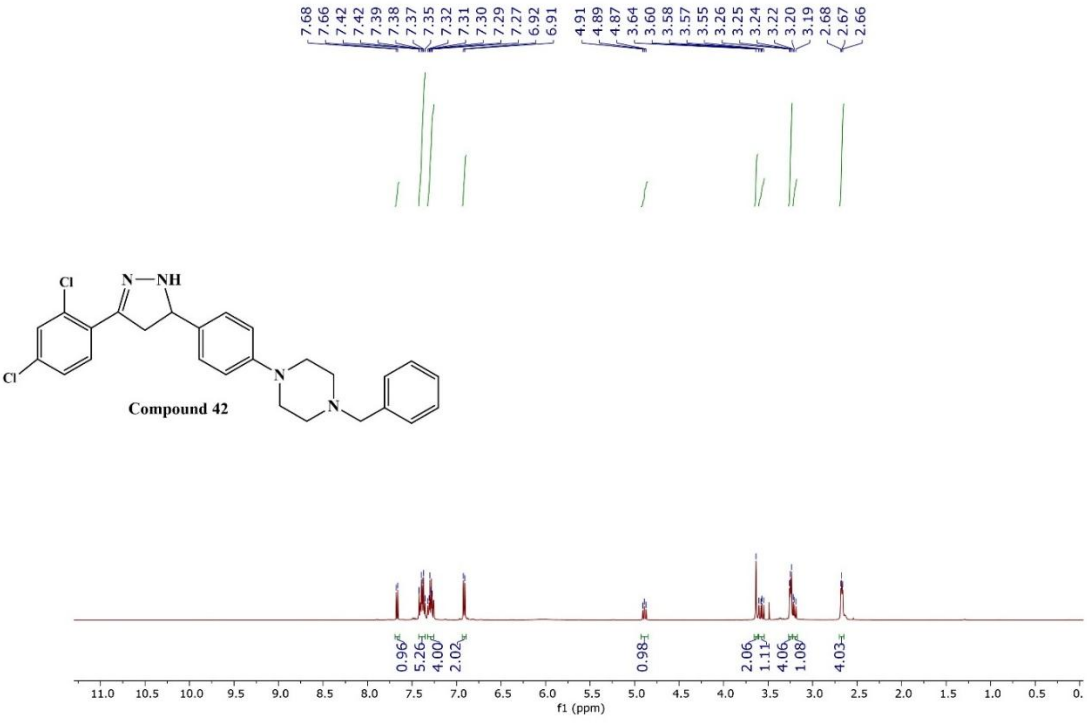

Figure D.5: ^{1}H NMR spectrum of *1-Benzyl-4-(4-(3-(2,4-dichlorophenyl)-4,5-dihydro-1H-pyrazol-5-yl)phenyl)piperazine* ***(42).***

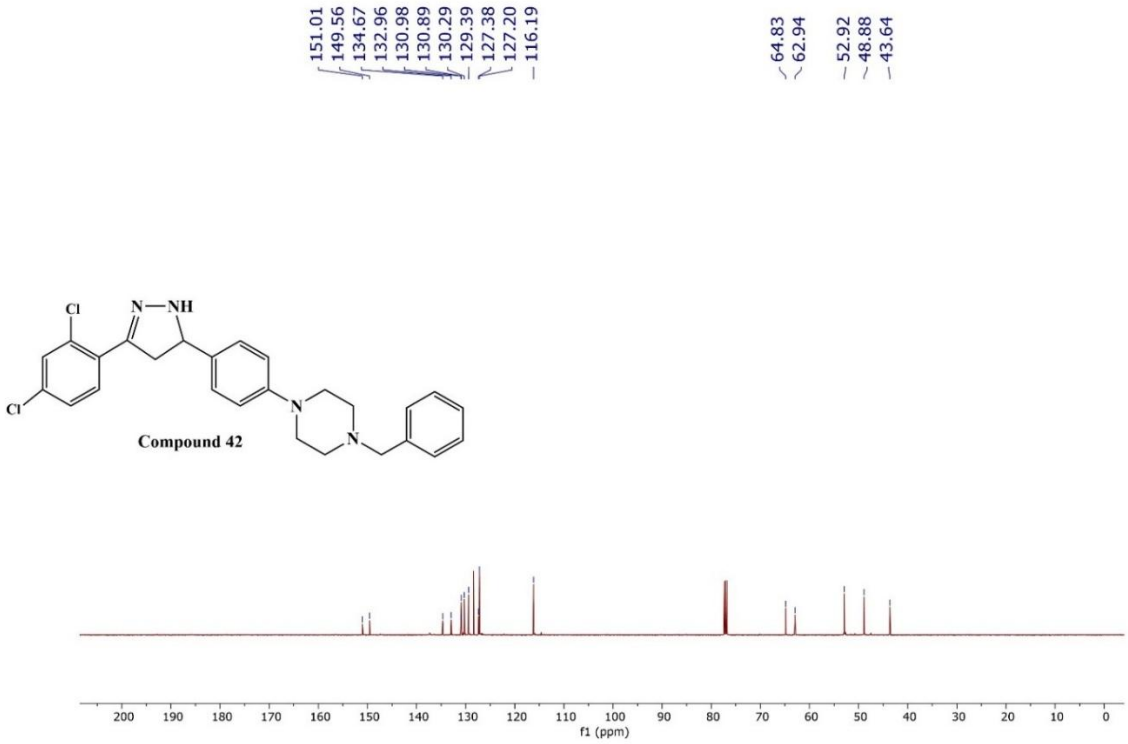

Figure D.6: ^{13}C NMR spectrum of *1-Benzyl-4-(4-(3-(2,4-dichlorophenyl)-4,5-dihydro-1H-pyrazol-5-yl)phenyl)piperazine* **(42).**

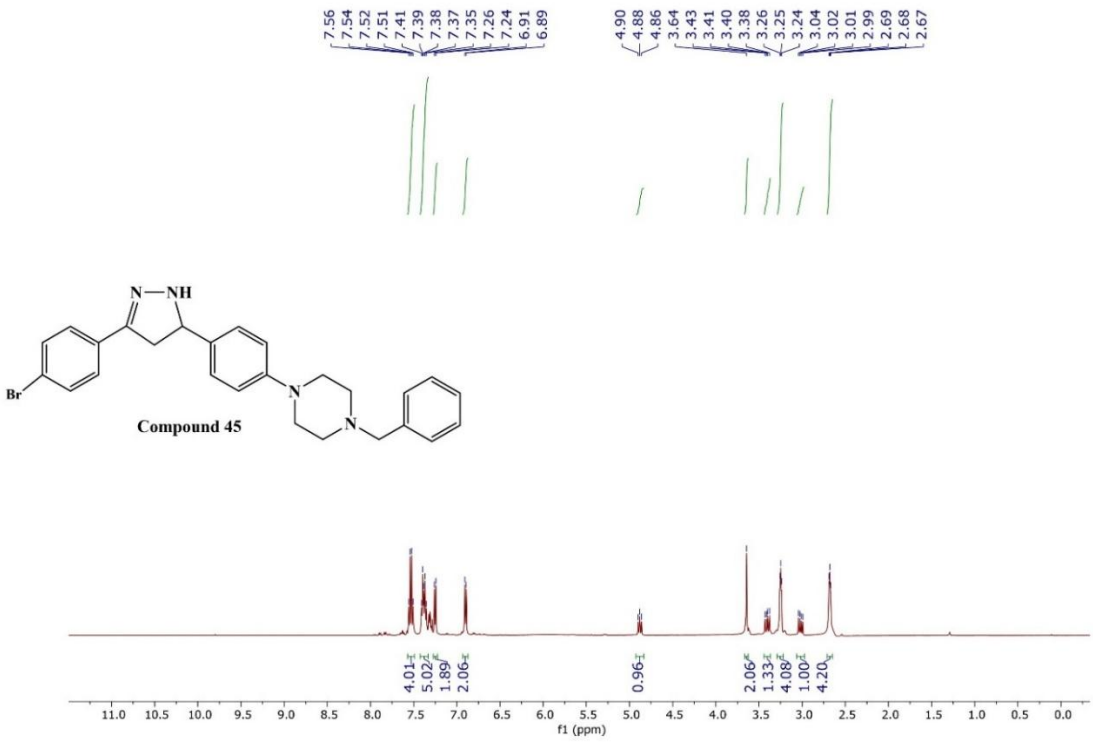

Figure D.7: ^{1}H NMR spectrum of *1-Benzyl-4-(4-(3-(4-bromophenyl)-4,5-dihydro-1H-pyrazol-5-yl)phenyl)piperazine* ***(45).***

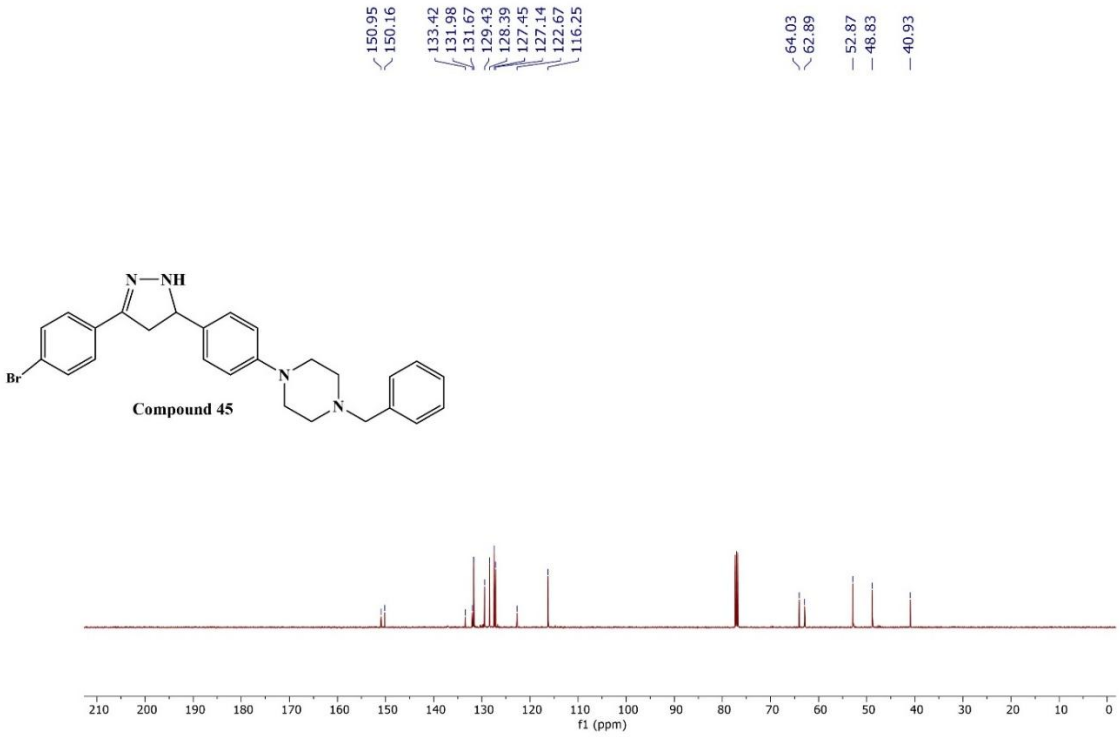

Figure D.8: ^{13}C NMR spectrum of *1-Benzyl-4-(4-(3-(4-bromophenyl)-4,5-dihydro-1H-pyrazol-5-yl)phenyl)piperazine* ***(45).***

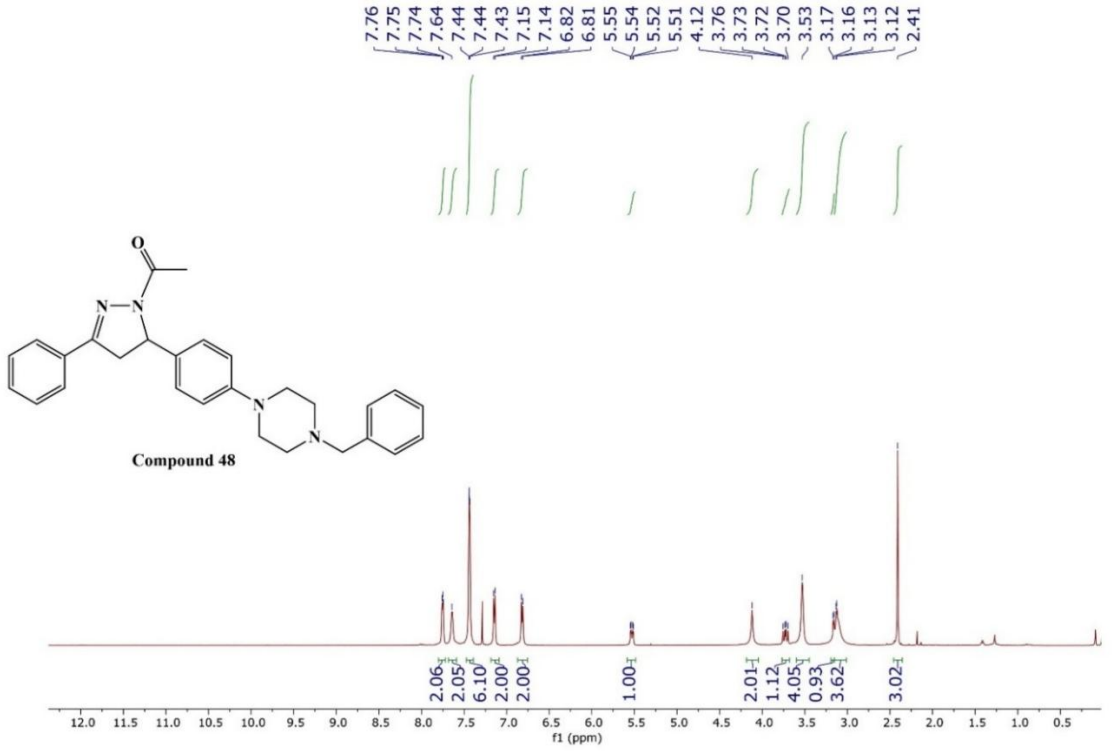

Figure D.9: ^{1}H NMR spectrum of *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-phenyl-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(48).**

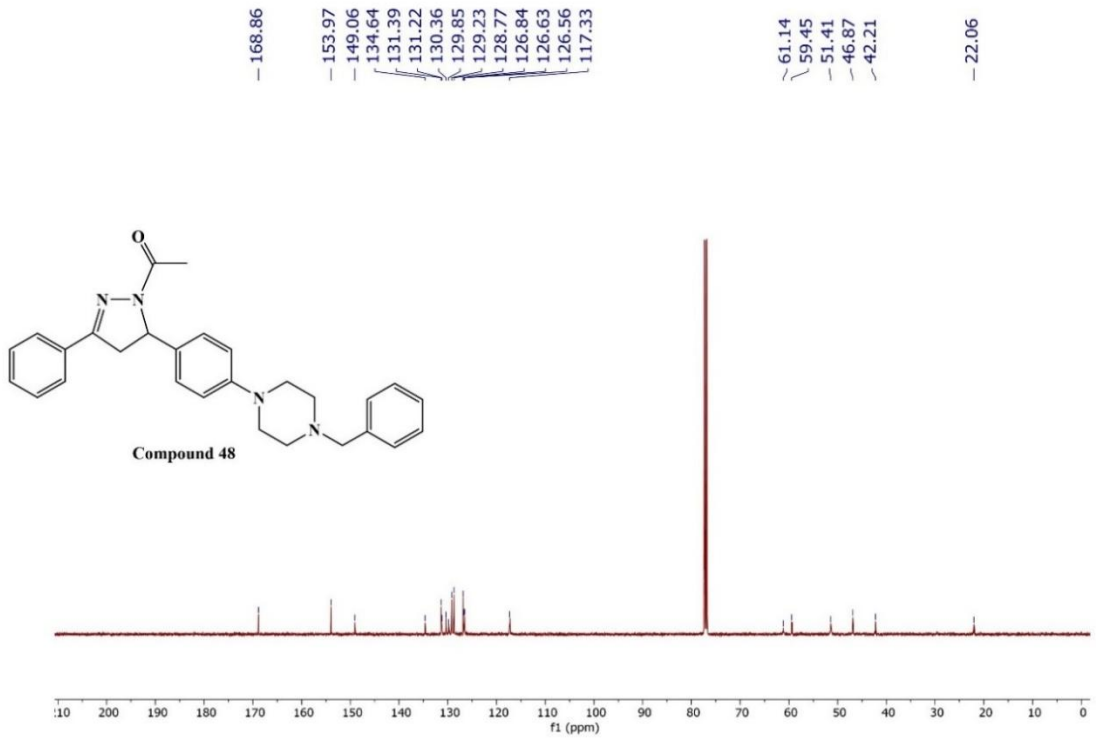

Figure D.10: ^{13}C NMR spectrum of *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-phenyl-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(48).**

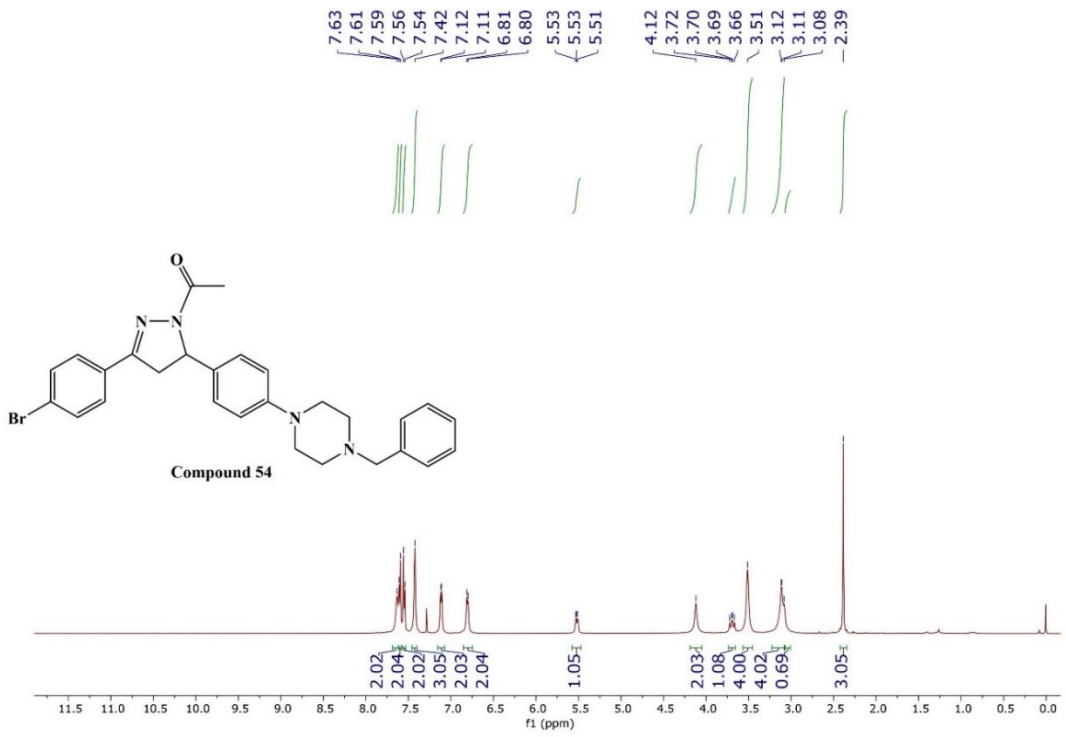

Figure D.11: ^{1}H NMR spectrum of *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-(4-bromophenyl)-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(54).**

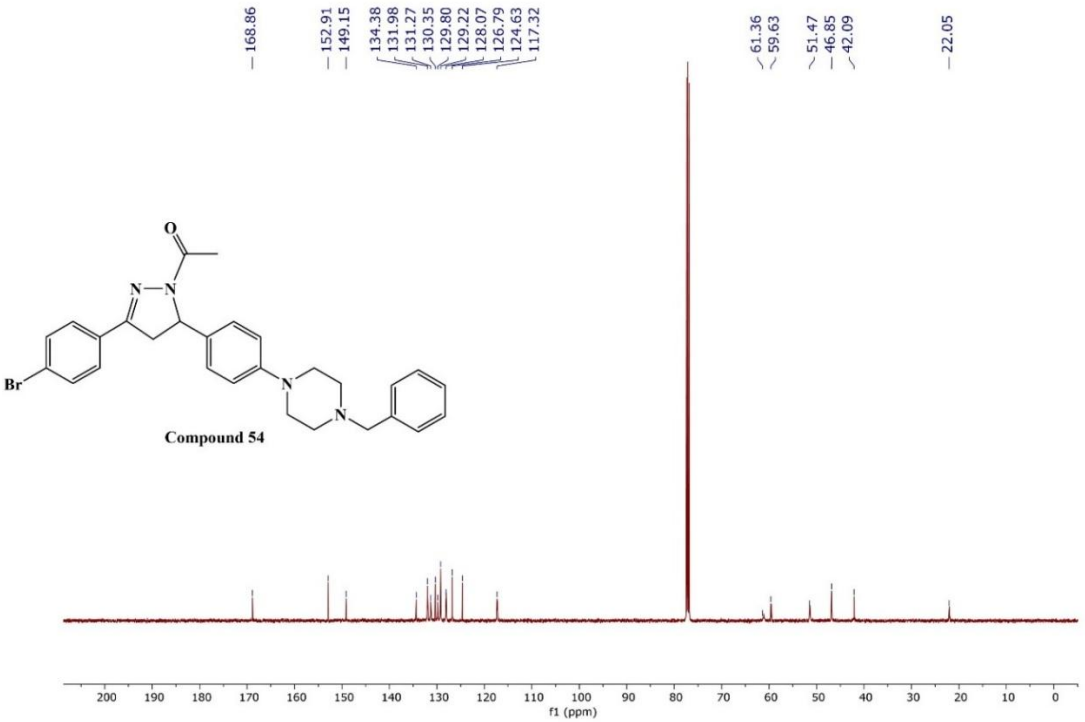

Figure D.12: ^{13}C NMR spectrum of of *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-(4-bromophenyl)-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(54).**

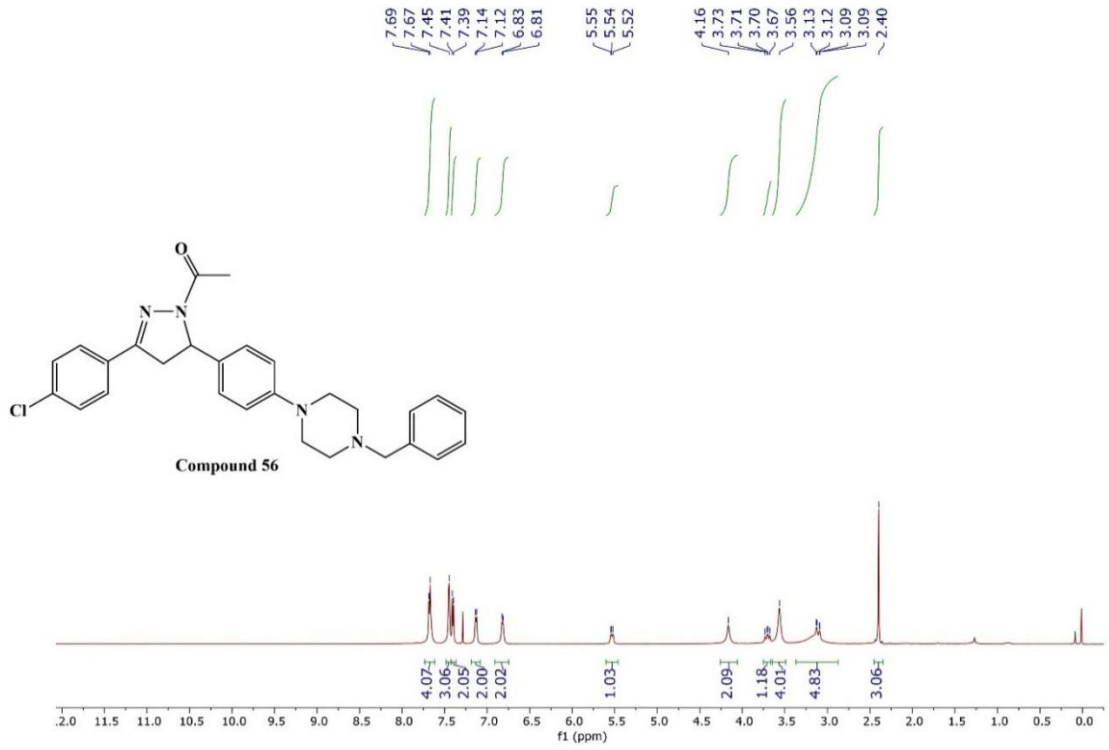

Figure D.13: ^{1}H NMR spectrum of *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-(4-chlorophenyl)-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(56).**

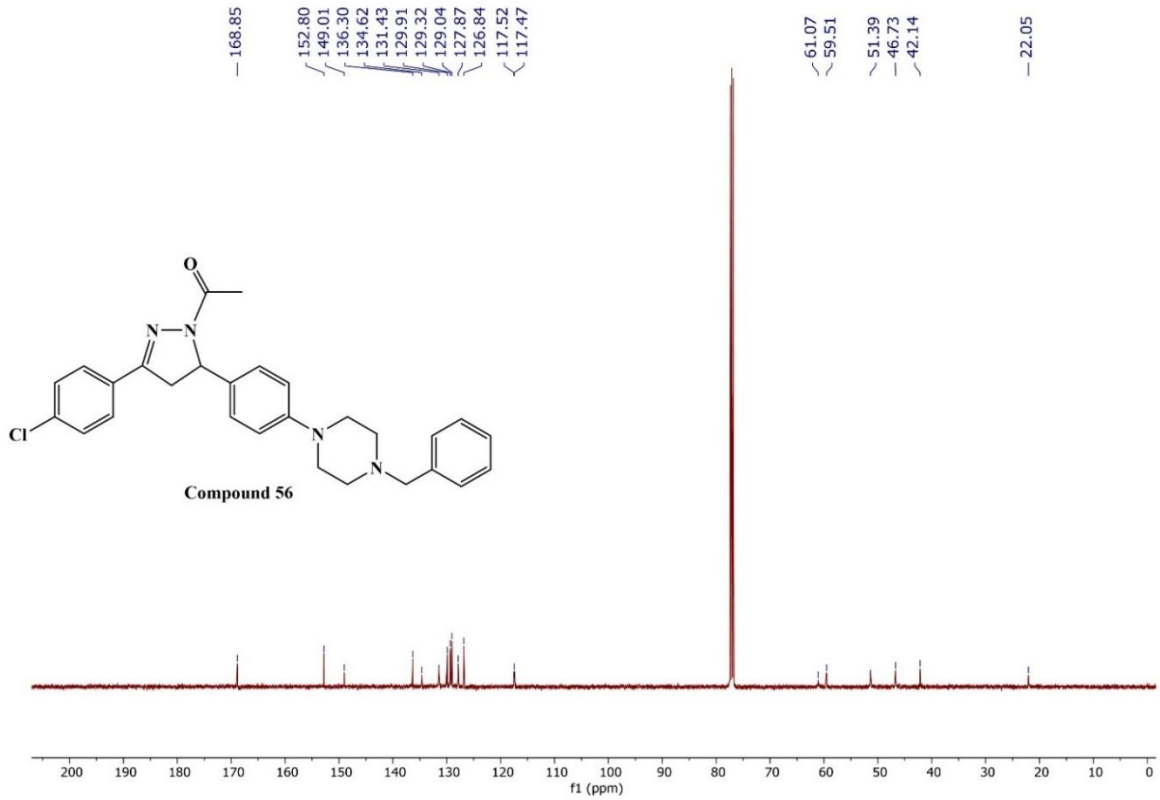

Figure D.14: ^{13}C NMR spectrum of *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-(4-chlorophenyl)-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(56).**

Table D.1: Purity analysis of lead compounds determined by HPLC.

Compound ID	Retention Time (min)	HPLC Purity (%)
34	5.373	96.94
42	6.660	98.07
48	5.153	96.41
54	6.073	97.45
56	5.827	97.87

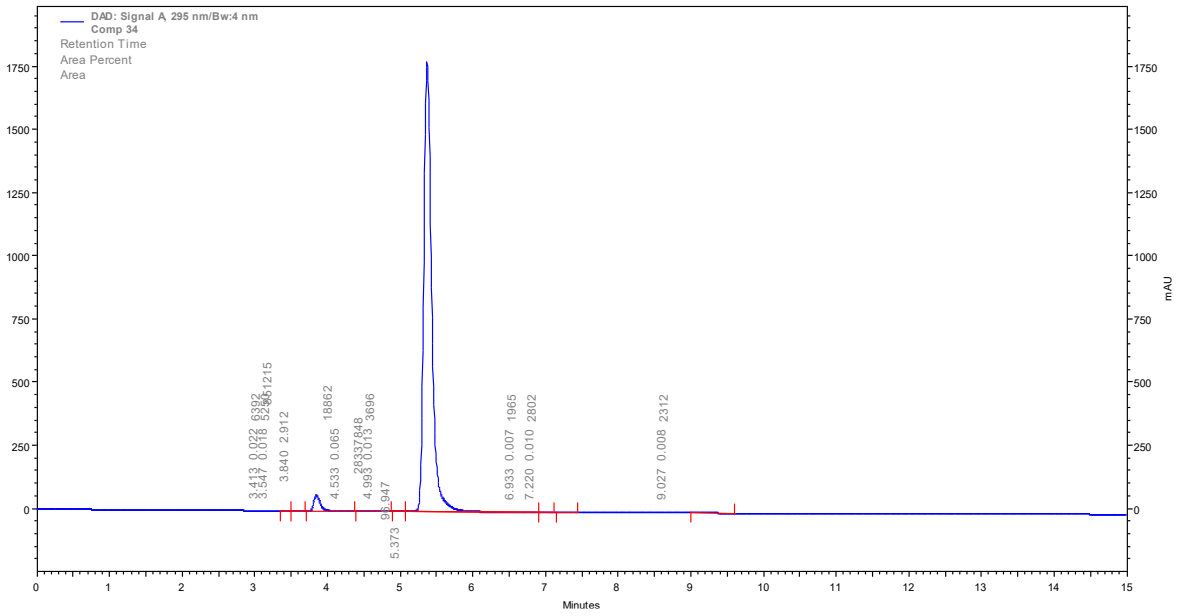

Figure D.15: HPLC chromatogram of the *1-(4-(3-(2,4-Dichlorophenyl)-4,5-dihydro-1H-pyrazol-5-yl)phenyl)-4-phenylpiperazine* ***(34).***

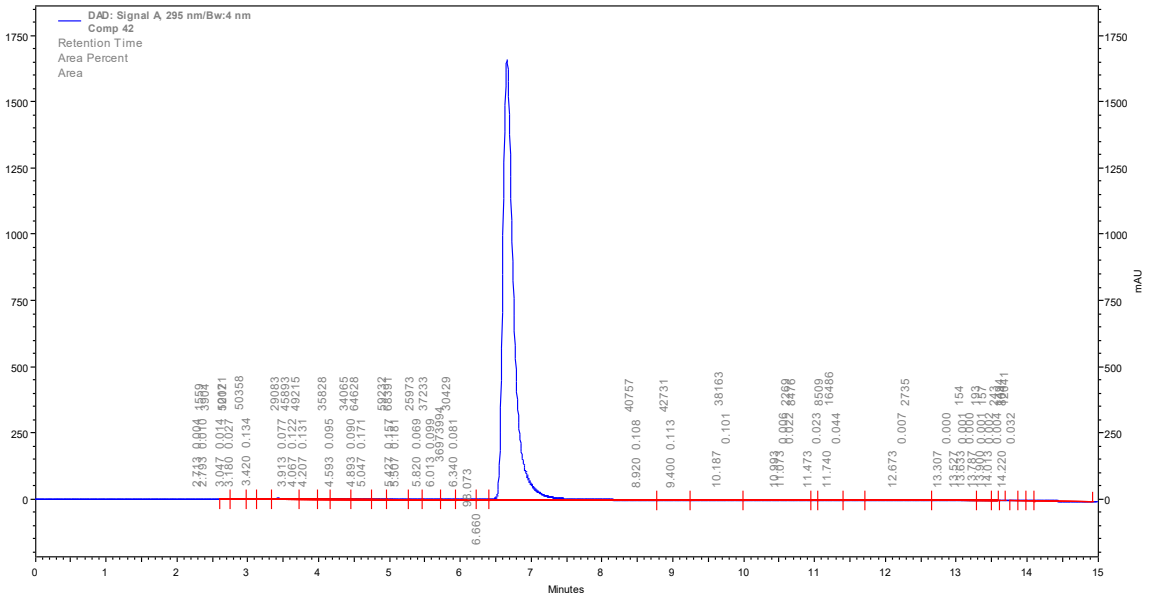

Figure D.16: HPLC chromatogram of the *1-Benzyl-4-(4-(3-(2,4-dichlorophenyl)-4,5-dihydro-1H-pyrazol-5-yl)phenyl)piperazine* **(42).**

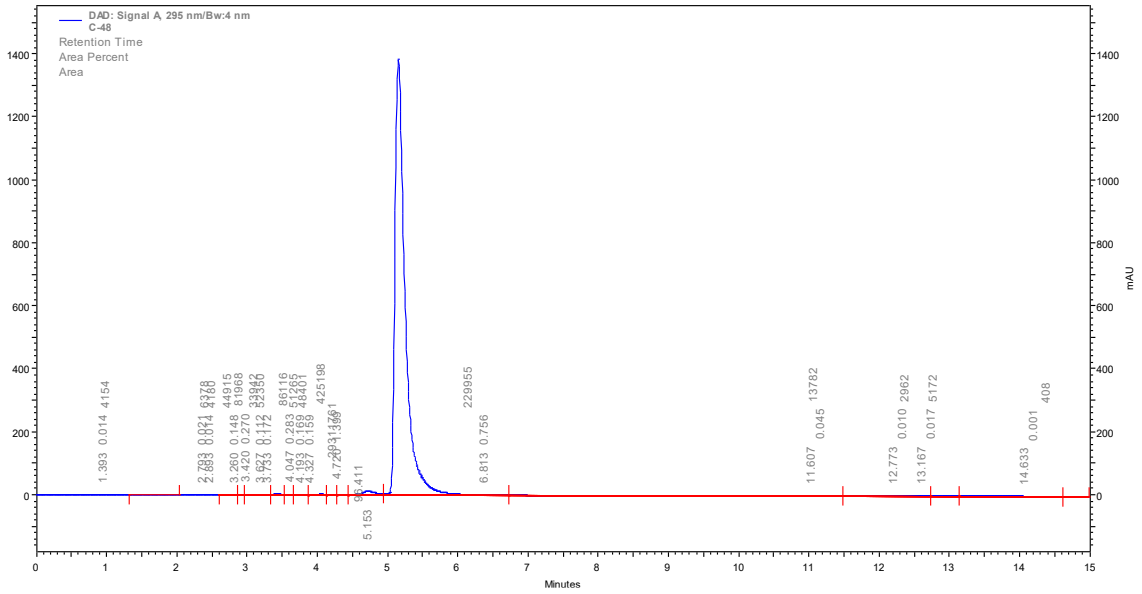

Figure D.17: HPLC chromatogram of the *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-phenyl-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* ***(48).***

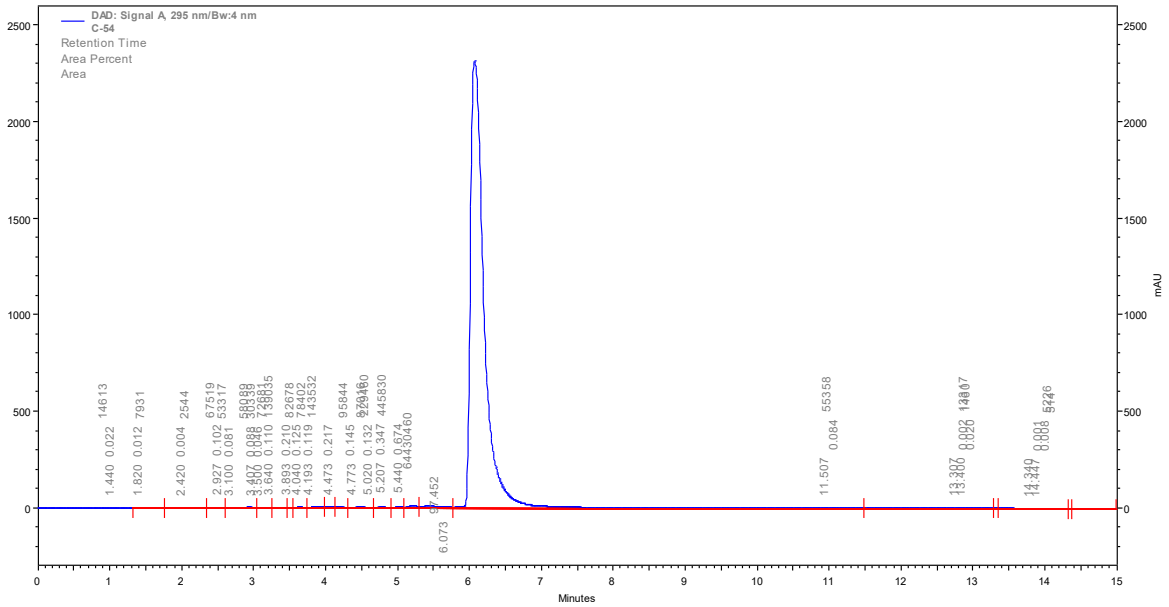

Figure D.18: HPLC chromatogram of the *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-(4-bromophenyl)-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(54).**

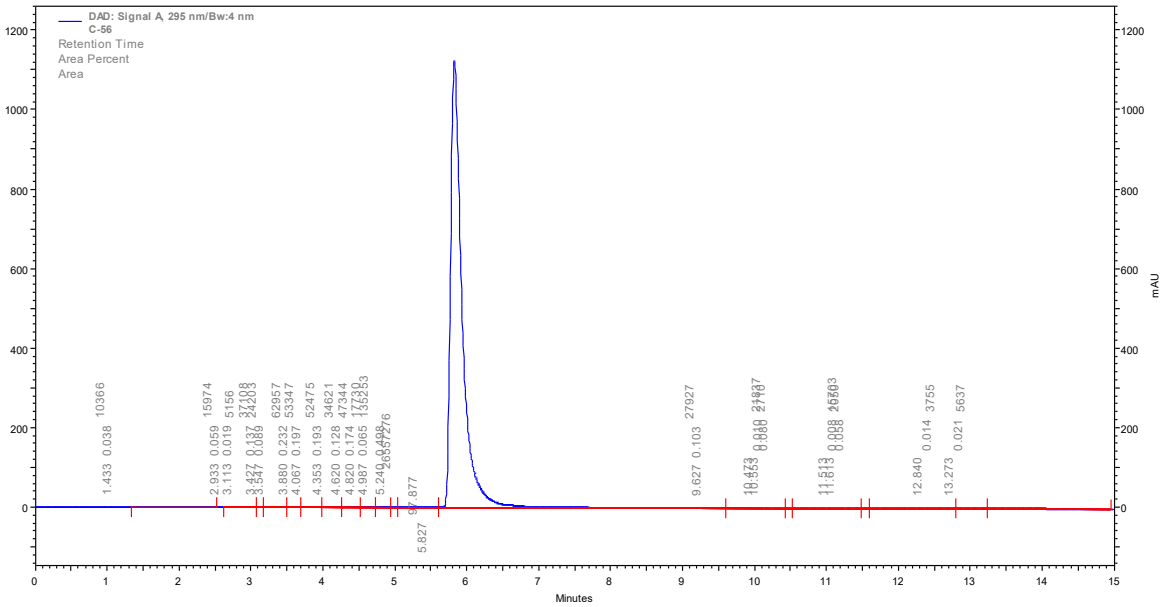

Figure D.19: HPLC chromatogram of the *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-(4-chlorophenyl)-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(56).**

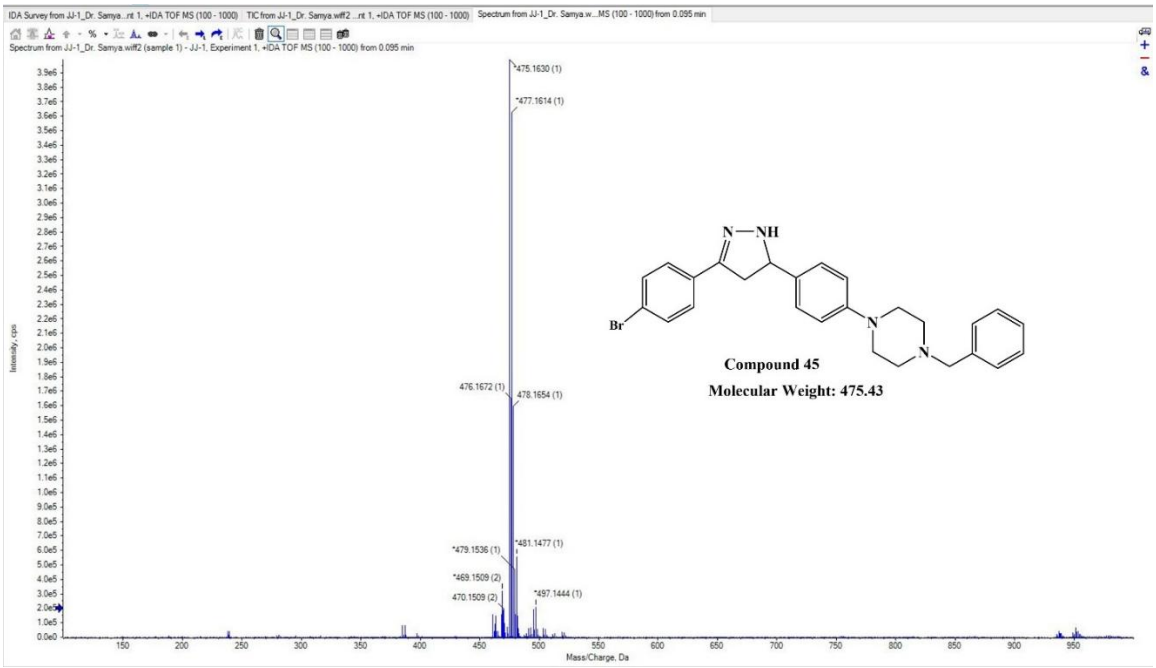

Figure D.20: HRMS of *1-Benzyl-4-(4-(3-(4-bromophenyl)-4,5-dihydro-1H-pyrazol-5-yl)phenyl)piperazine* **(45).**

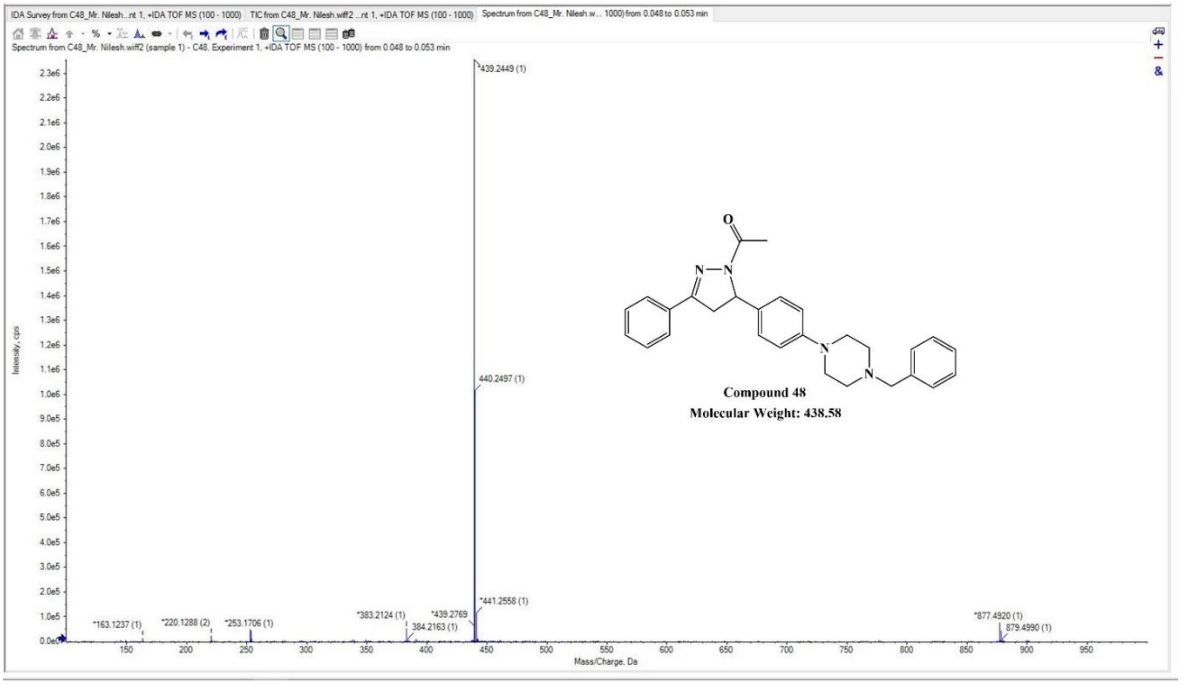

Figure D.21: HRMS of *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-phenyl-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(48).**

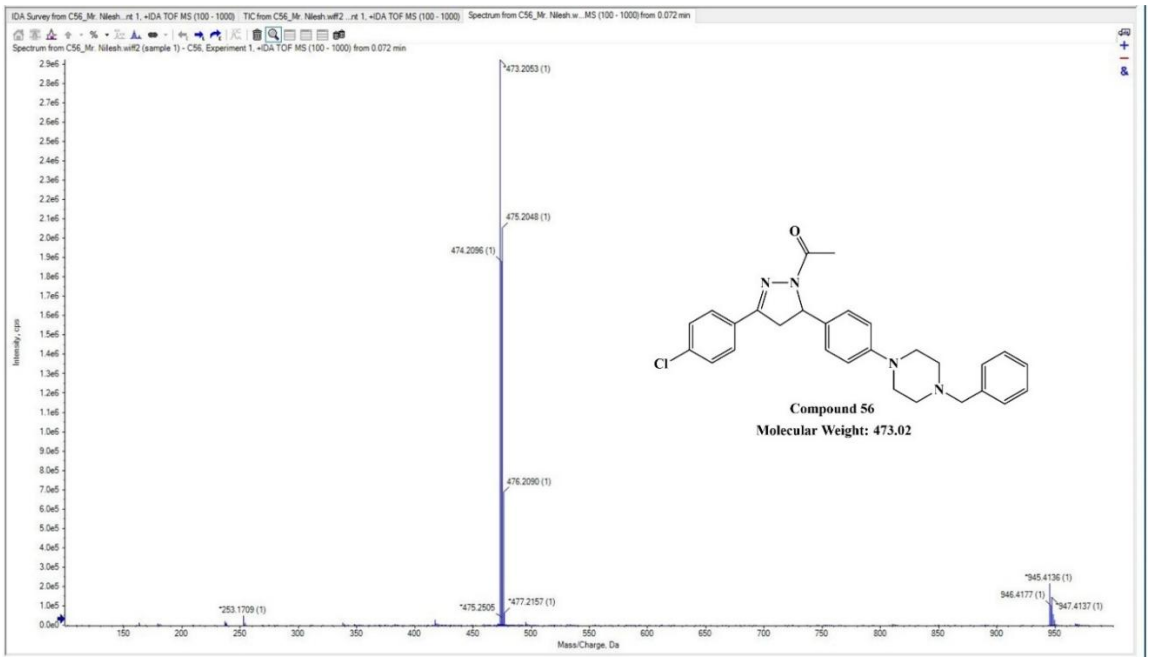

Figure D.22: HRMS of *1-(5-(4-(4-Benzylpiperazin-1-yl)phenyl)-3-(4-chlorophenyl)-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one* **(56).**

10.5 List of Publications

1. **Bajad NG**, Gajendra TA, Sharma K, Tapadia MG, Kumar A, Krishnamurthy S, Singh SK. Development of donor-acceptor architecture type potential theranostic fluorescent probes for Alzheimer's disease. **ACS Chemical Neuroscience**. 2025 March https://doi.org/10.1021/acschemneuro.5c00092
2. **Bajad NG**, Jangra J, Gajendra TA, Kumar A, Krishnamurthy S, Singh SK. Discovery of pyrazoline analogs as multi-targeting cholinesterase, β-secretase and Aβ aggregation inhibitors through lead optimization strategy. **International Journal of Biological Macromolecules**. 2025 Jan 28:140436. https://doi.org/10.1016/j.ijbiomac.2025.140436.
3. **Bajad NG,** Gajendra TA, Kothari M, Mukherjee R, Chowdhury A, Kumar A, Krishnamurthy S, Singh SK. Development of multifunctional fluorescence-emitting potential theranostic agents for Alzheimer's disease. **Talanta**. 2025 Jan 10:127574. https://doi.org/10.1016/j.talanta.2025.127574.
4. **Bajad NG**, Singh RB, Gajendra TA, Gutti G, Kumar A, Krishnamurthy S, Singh SK. Development of multi-targetable chalcone derivatives bearing *N*-aryl piperazine moiety for the treatment of Alzheimer's disease. **Bioorganic Chemistry**. 2024 Jan 2:107082. https://doi.org/10.1016/j.bioorg.2023.107082.
5. **Bajad NG**, Kumar A, Singh SK. Recent Advances in the Development of Near-Infrared Fluorescent Probes for the in Vivo Brain Imaging of Amyloid-β Species in Alzheimer's disease. **ACS Chemical Neuroscience** 2023 Aug 14;14(17):2955-67, https://doi.org/10.1021/acschemneuro.3c00304.
6. **Bajad NG**, Swetha R, Singh R, Ganeshpurkar A, Gutti G, Singh RB, Kumar A, Singh SK. Combined structure and ligand-based design of dual BACE-1/GSK-3β inhibitors for Alzheimer's disease. **Chemical Papers**. 2022 Aug 23:1-8. https://link.springer.com/article/10.1007/s11696-022-02421-8.
7. Jangra J, **Bajad NG**, Kumar A, Singh SK. Integrated pharmacophore-based virtual screening and molecular modeling approaches for the identification of sigma-2 receptor antagonists as novel therapeutics against Alzheimer's disease. **Journal of Biomolecular Structure and Dynamics**. 2024 Dec 22:1-25, https://doi.org/10.1080/07391102.2024.2446666.
8. Jangra J, **Bajad NG,** Singh R, Kumar A, Singh SK. Identification of novel potential cathepsinB inhibitors through pharmacophore-based virtual screening, molecular docking, and dynamics simulation studies for the treatment of Alzheimer's disease. **Molecular Diversity** 2024 Mar 22:1-21, 10.1007/s11030-024-10821-z. https://link.springer.com/article/10.1007/s11030-024-10821-z.
9. Gutti G, Leifeld J, Kakarla R, **Bajad NG**, Ganeshpurkar A, Kumar A, Krishnamurthy S, Klein-Schmidt C, Tapken D, Hollmann M, Singh SK. Discovery of triazole-bridged aryl adamantane analogs as an intriguing class of multifunctional agents for treatment of Alzheimer's disease. **European Journal of Medicinal Chemistry**. 2023 Nov 5; 259:115670, doi.org/10.1016/j.ejmech.2023.115670.
10. Anand A, Ghosh P, Singh R, **Bajad NG**, Kumar A, Singh S.K. Identification of potent Histone Deacetylase 2 (HDAC2) inhibitors through combined structure and ligand-based designs and molecular modelling approach. **Journal of Biomolecular Structure and Dynamic**. 2023 June https://doi.org/10.1080/07391102.2023.2222177.
11. Singh SK, Kumar A, Singh RB, Ghosh P, **Bajad NG**. Recent Applications of Bioinformatics in Target Identification and Drug Discovery for Alzheimer's disease. **Current Topics in Medicinal Chemistry**. 2022 Oct 1;22(26):2153-75. (https://doi.org/10.2174/1568026623666221026091010).

12. Sharma A, Swetha R, **Bajad NG**, Ganeshpurkar A, Singh R, Kumar A, Singh SK. Cathepsin B - A Neuronal Death Mediator in Alzheimer's Disease Leading to Neurodegeneration. **Mini Reviews in Medicinal Chemistry**. **2022** Aug 1;22(15):2012-23. (https://doi.org/10.2174/1389557522666220214095859).
13. **Bajad NG**, Swetha R, Gutti G, Singh M, Kumar A, Singh SK. A systematic review of carbohydrate-based bioactive molecules for Alzheimer's disease. **Future Medicinal Chemistry**. 2021 Jul;13(19):1695-711. https://doi.org/10.4155/fmc-2021-0109.
14. **Bajad NG**, Singh SK, Singh SK, Singh TD, Singh M. Indole: A promising scaffold for the discovery and development of potential anti-tubercular agents. **Current Research in Pharmacology and Drug Discovery**. **2022** Jul 16:100119. https://doi.org/10.1016/j.crphar.2022.100119.
15. **Bajad NG**, Rayala S, Gutti G, Sharma A, Singh M, Kumar A, Singh SK. Systematic review on role of structure-based drug design (SBDD) in the identification of anti-viral leads against SARS-Cov-2. **Current Research in Pharmacology and Drug Discovery**. 2021 Jan 1; 2:100026. (https://doi.org/10.1016/j.crphar.2021.100026).