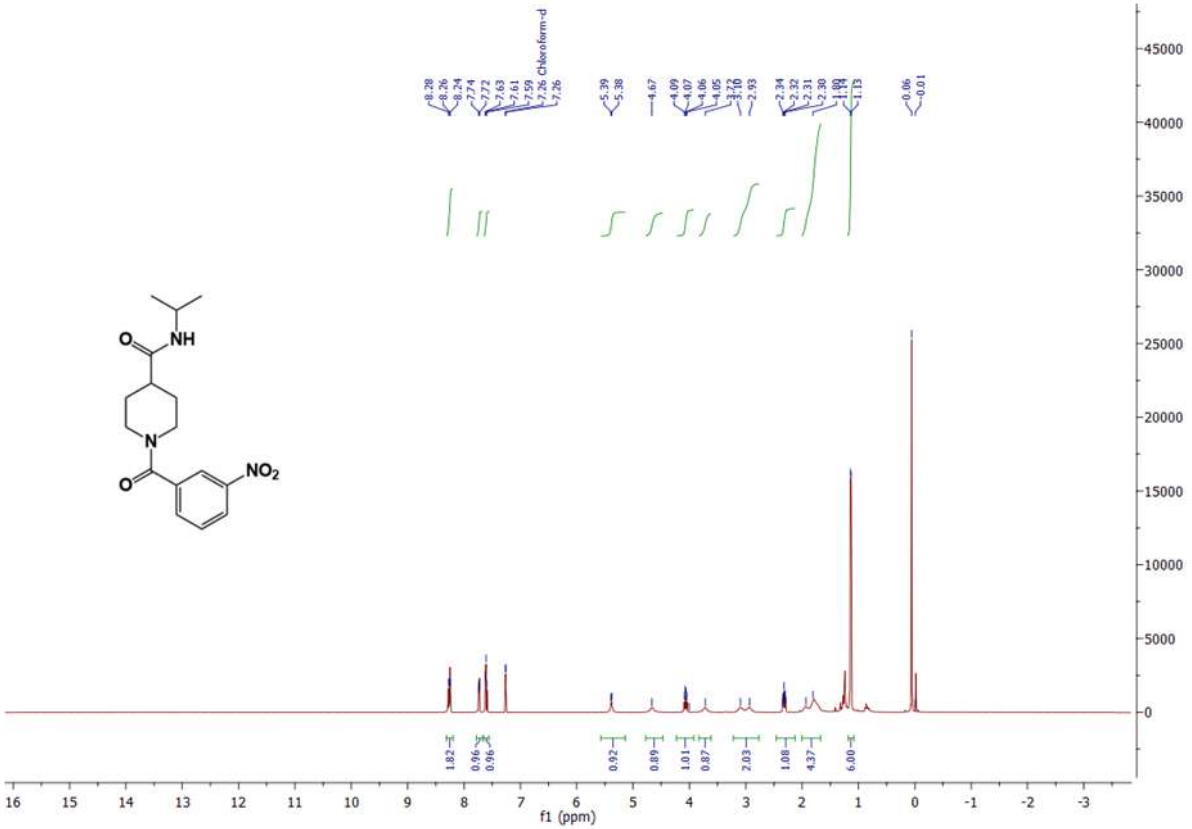
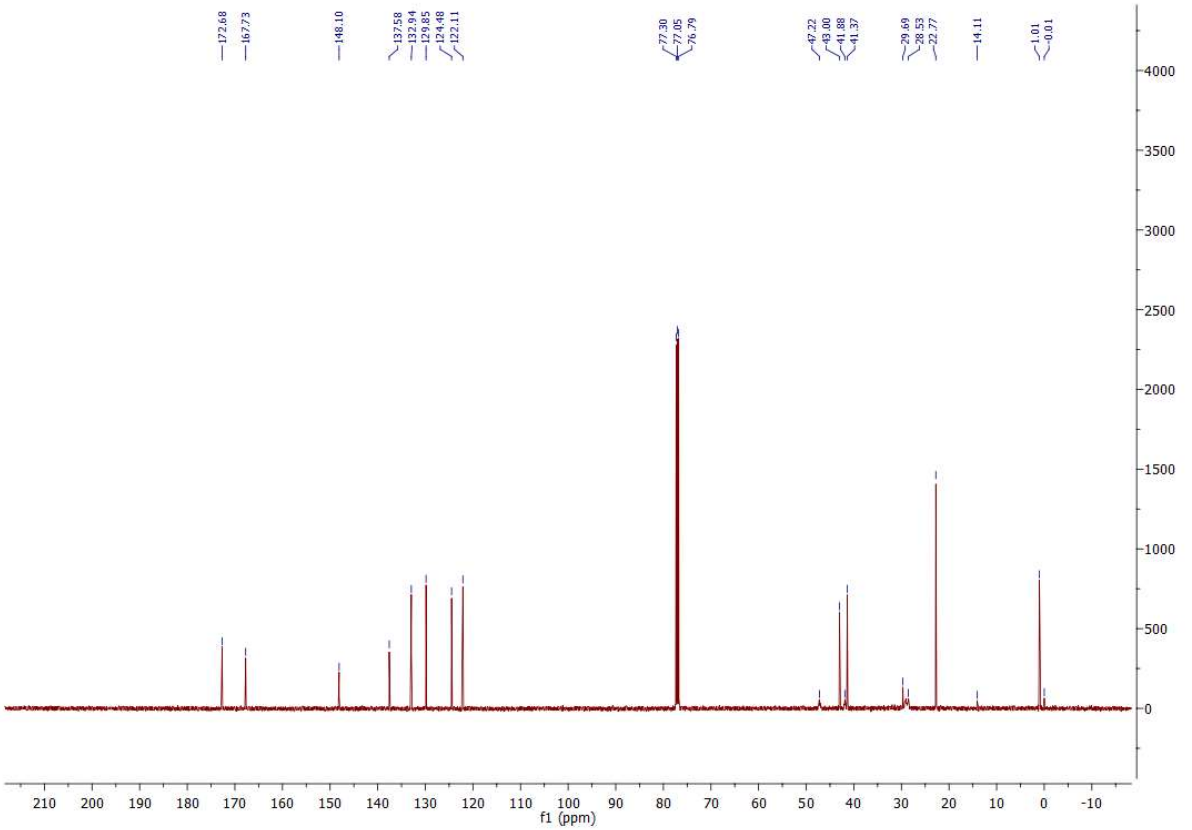
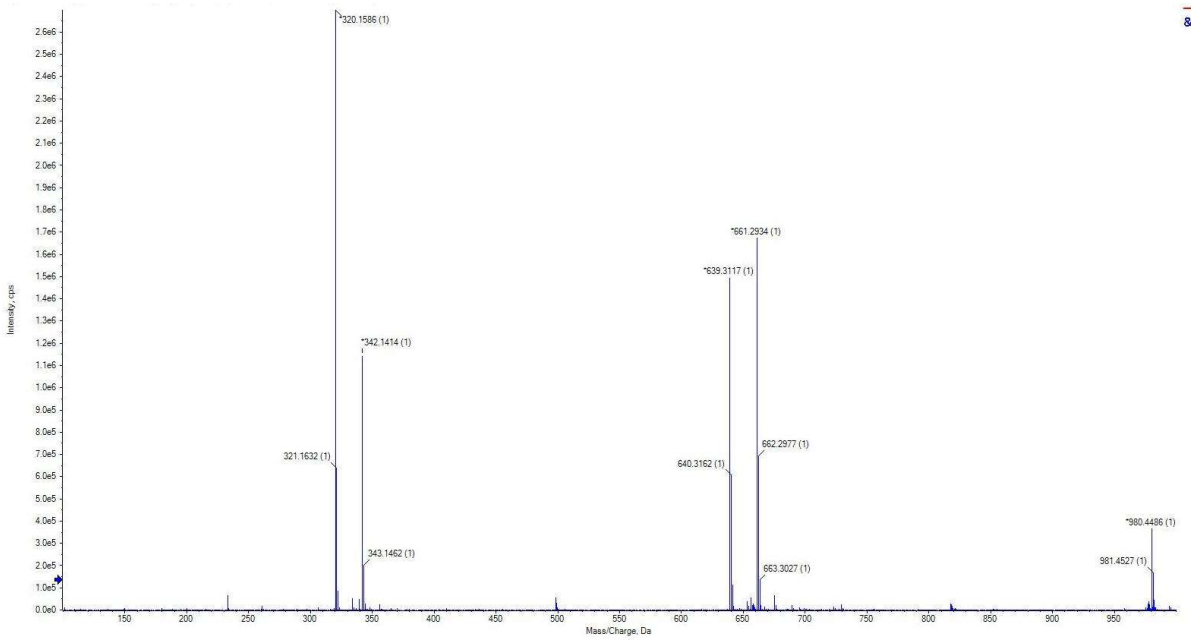
Annexure-I

^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A1

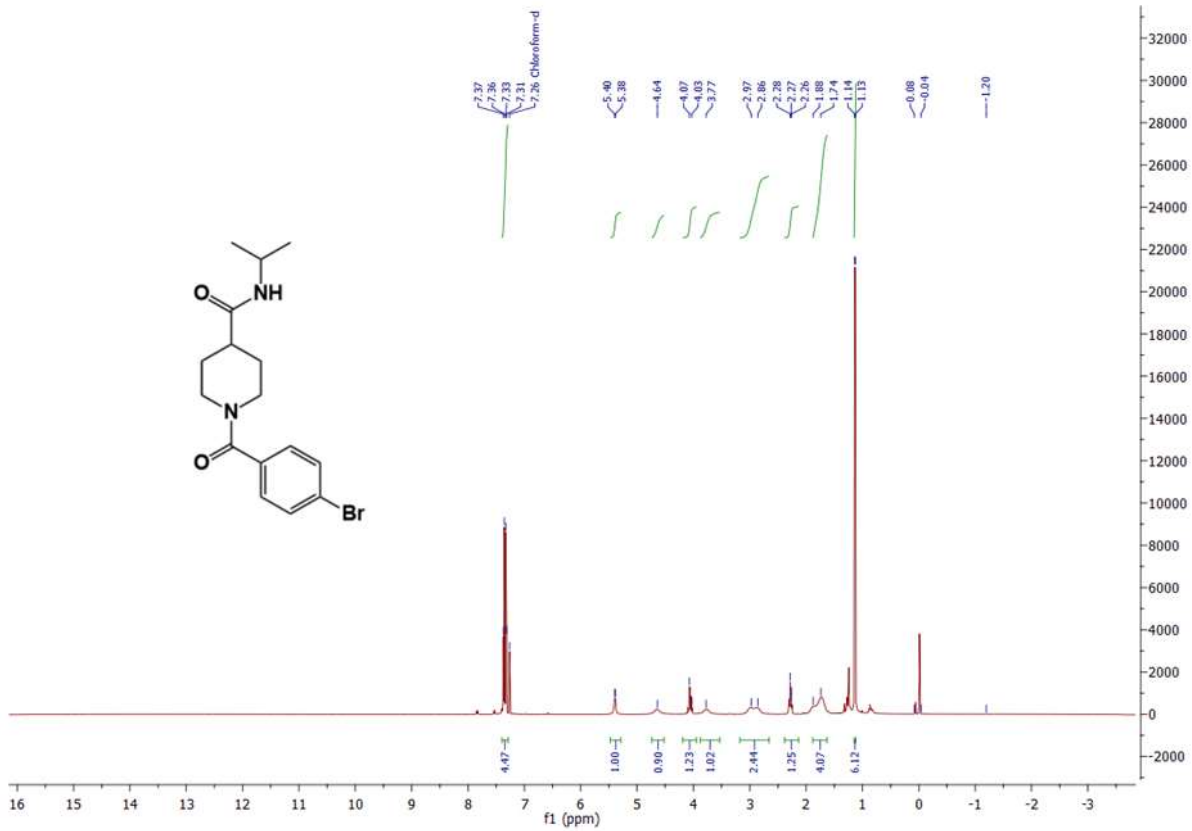


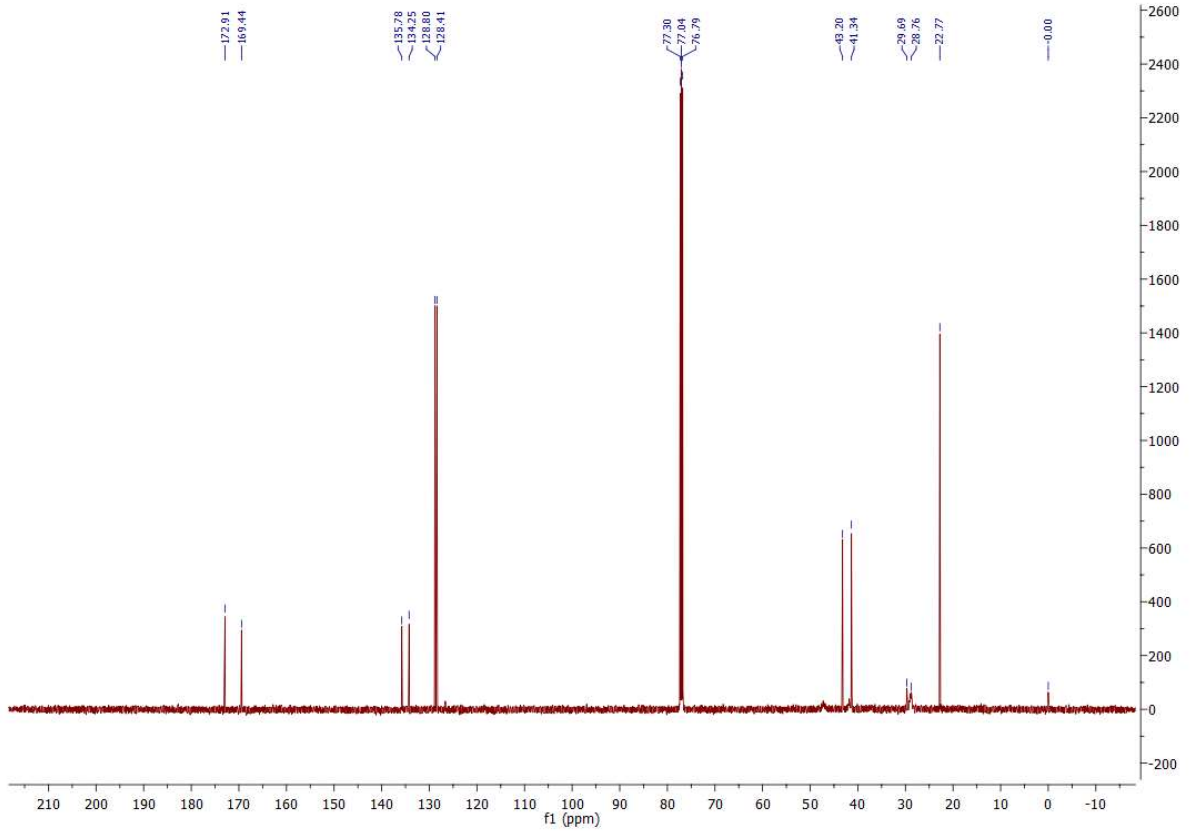


HRMS spectra of compound A1

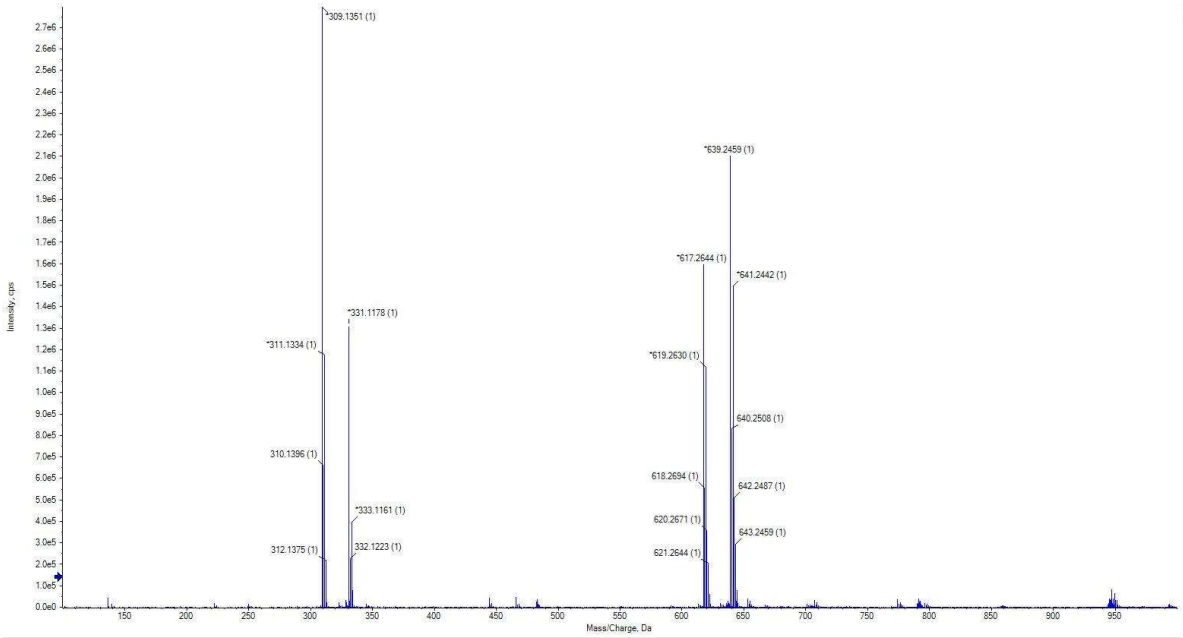


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A2

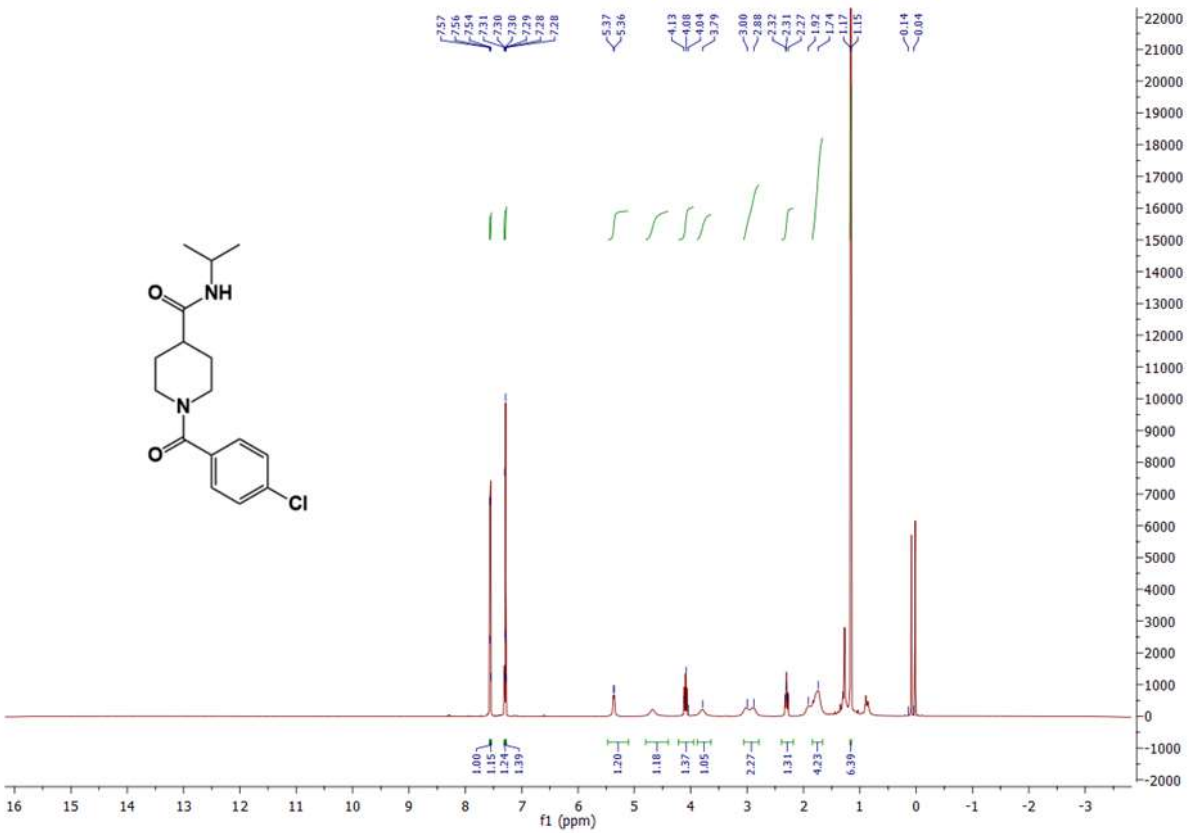


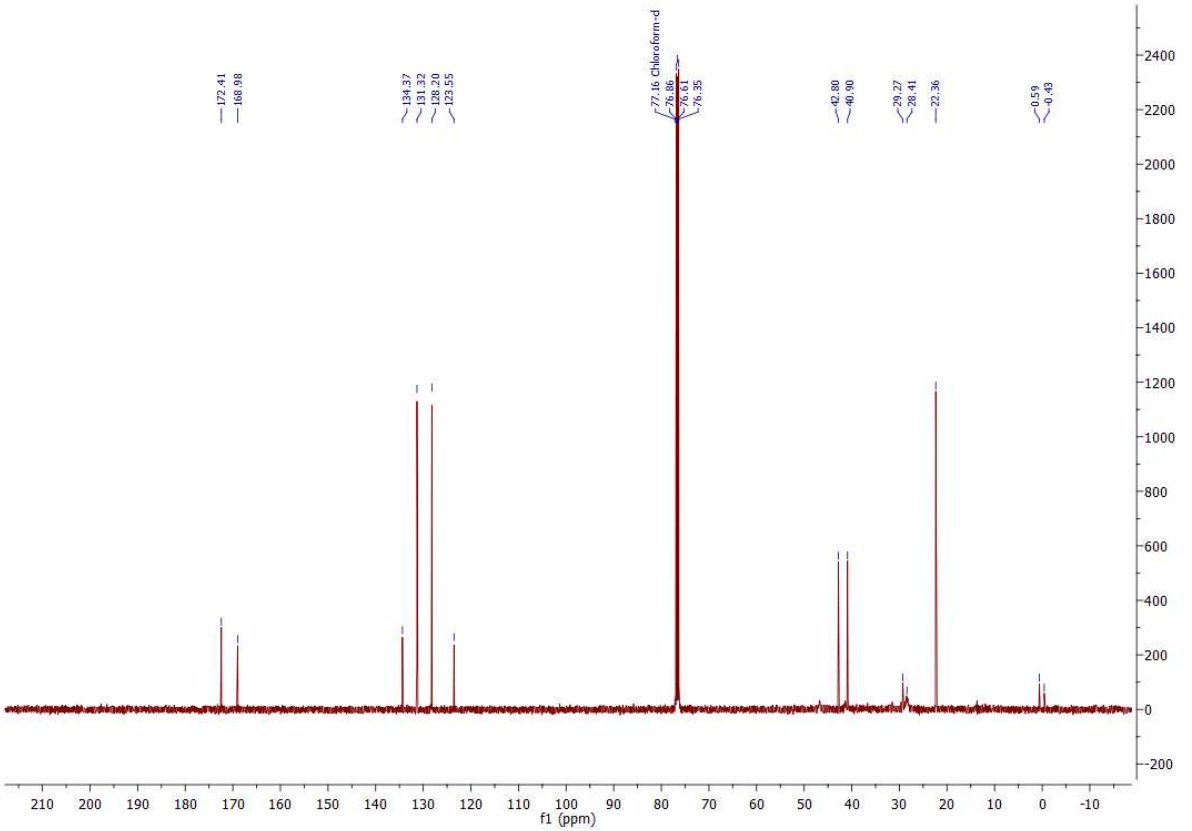


HRMS spectra of compound A2

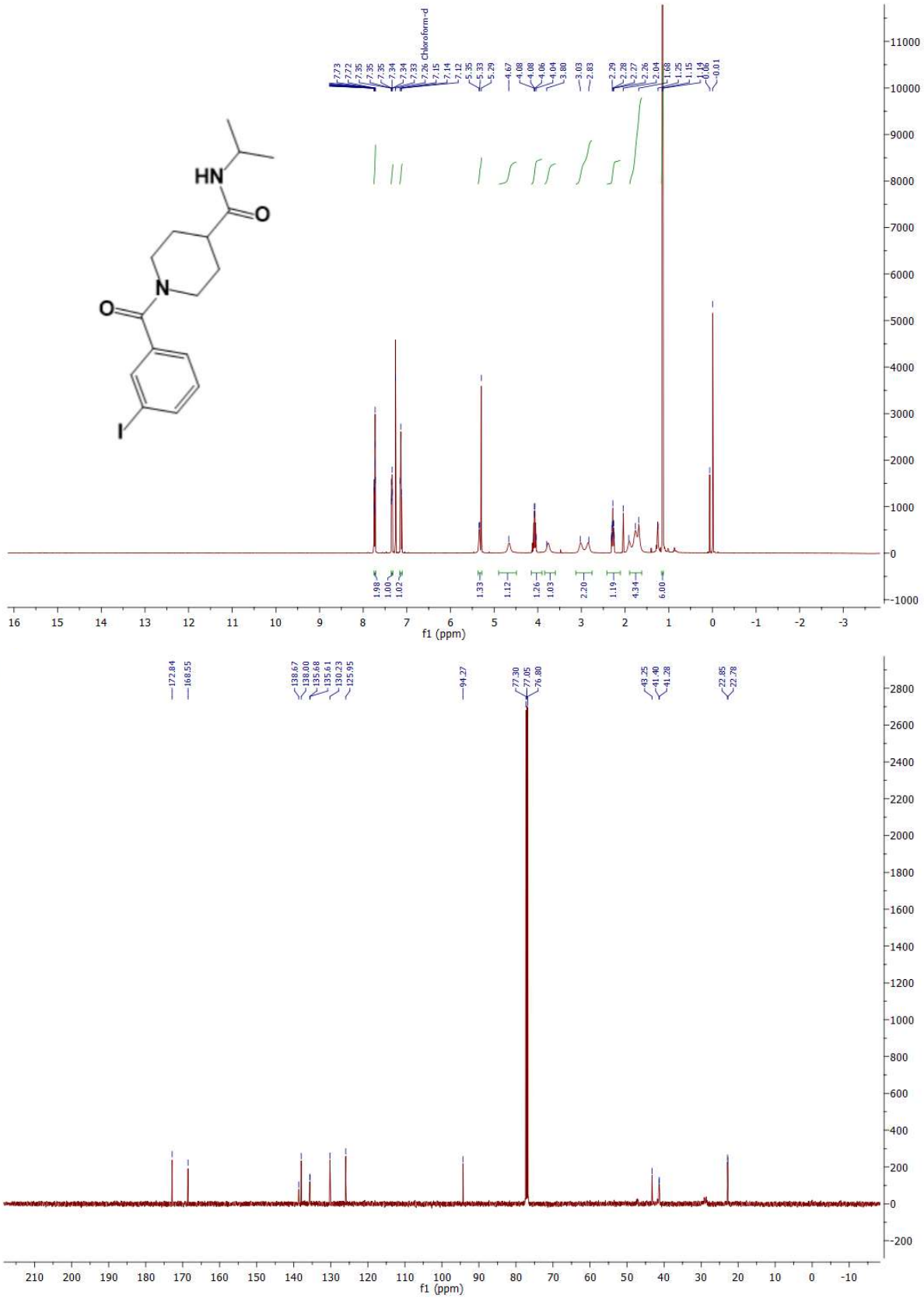


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A3

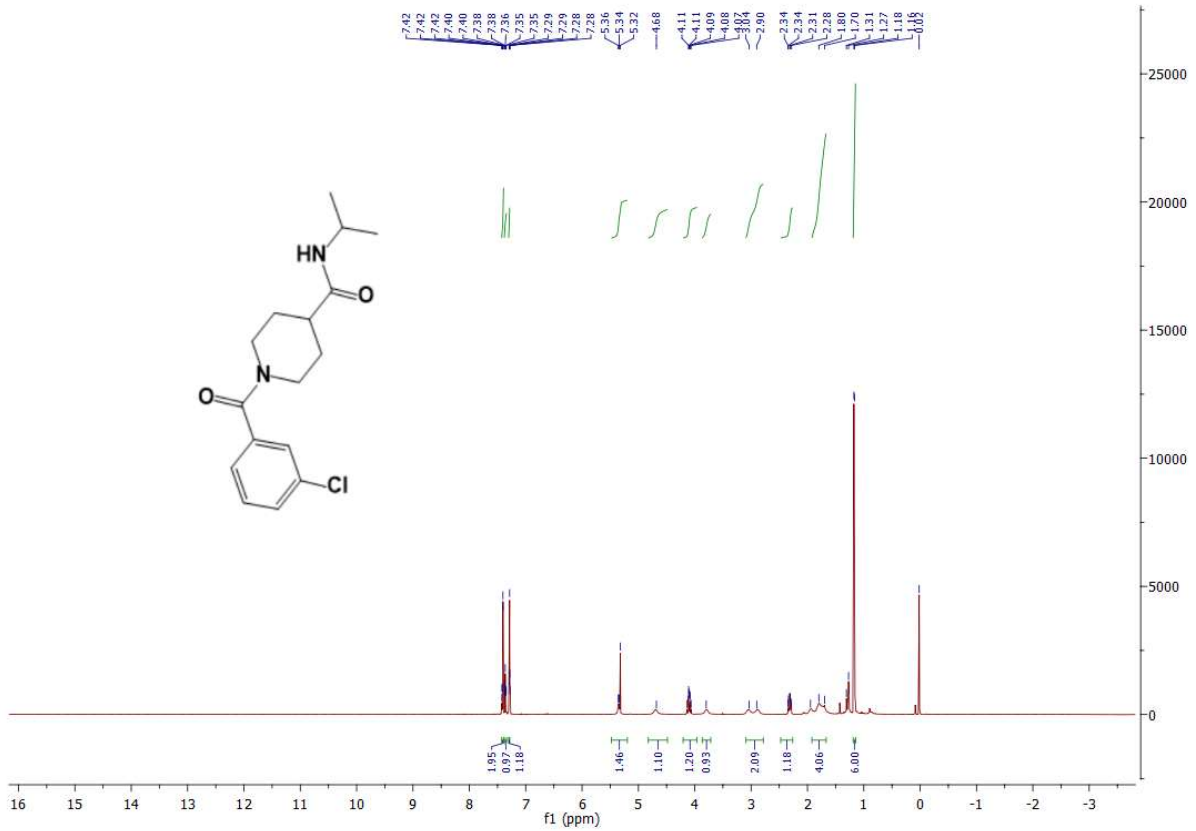


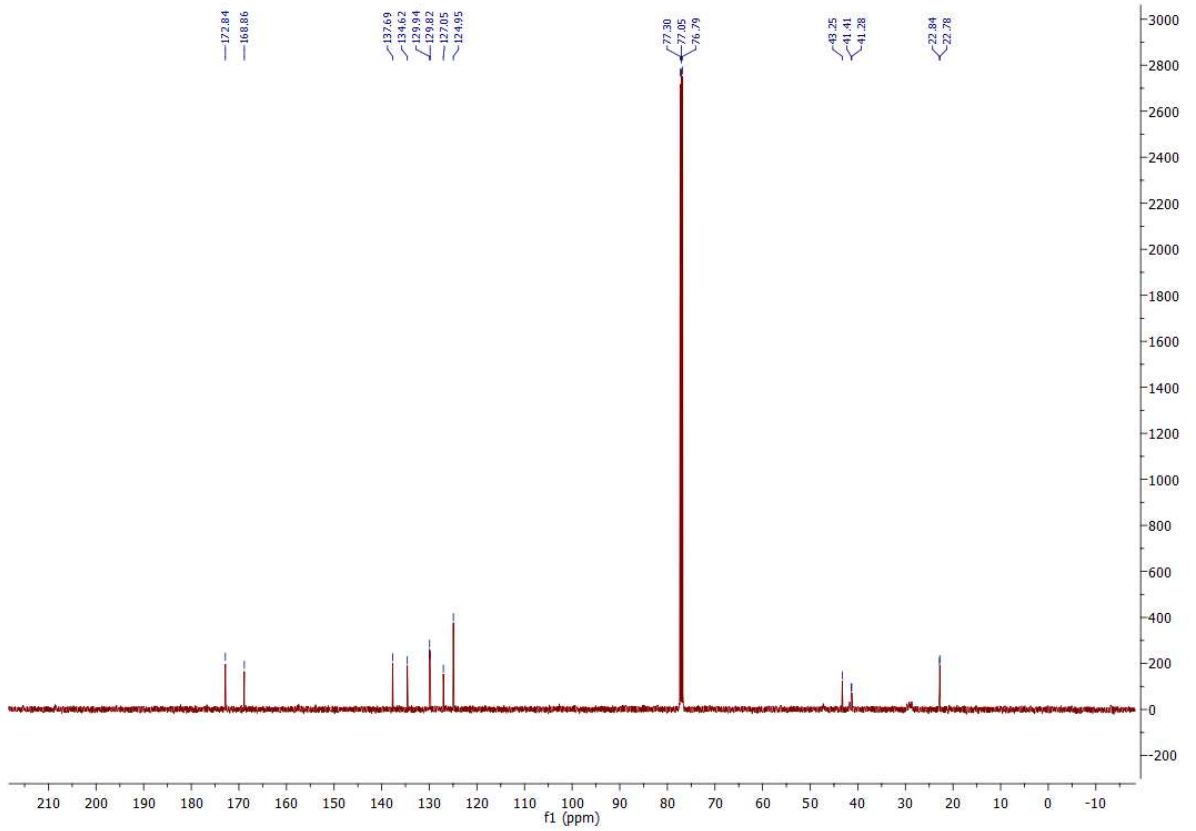


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A4

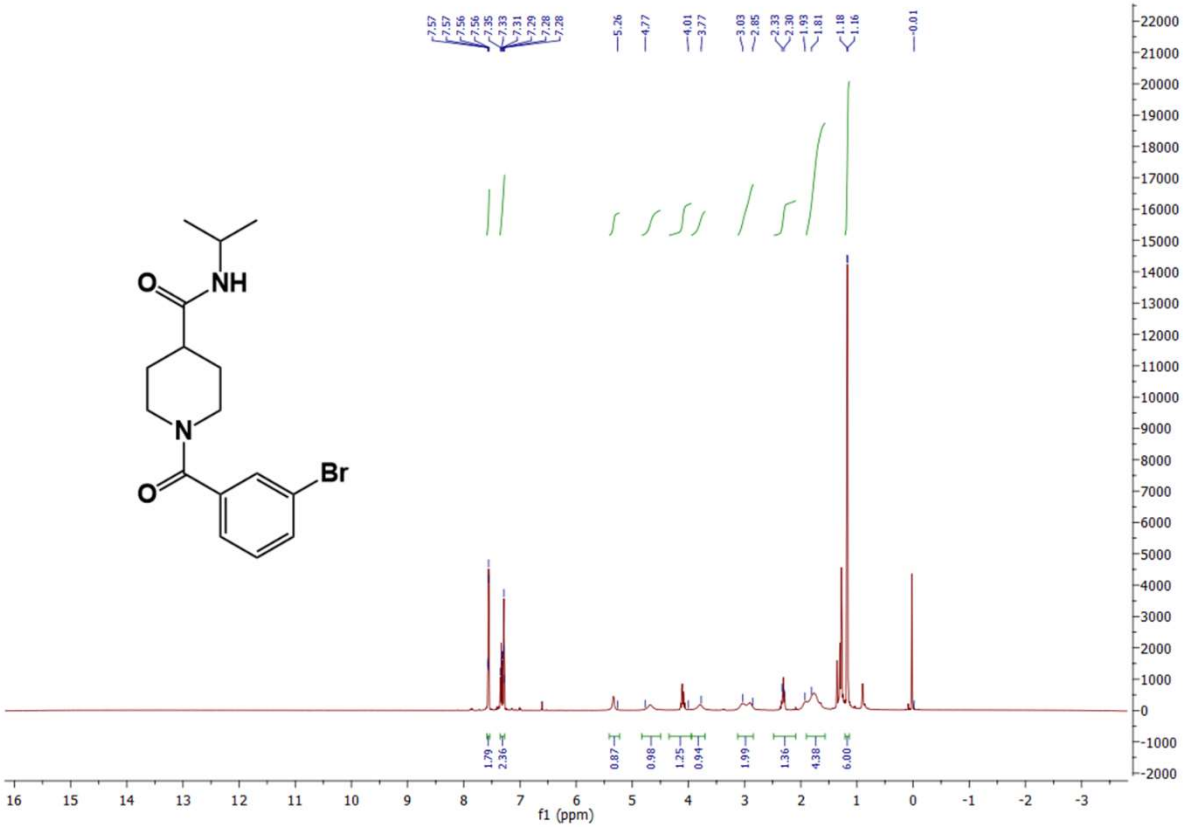


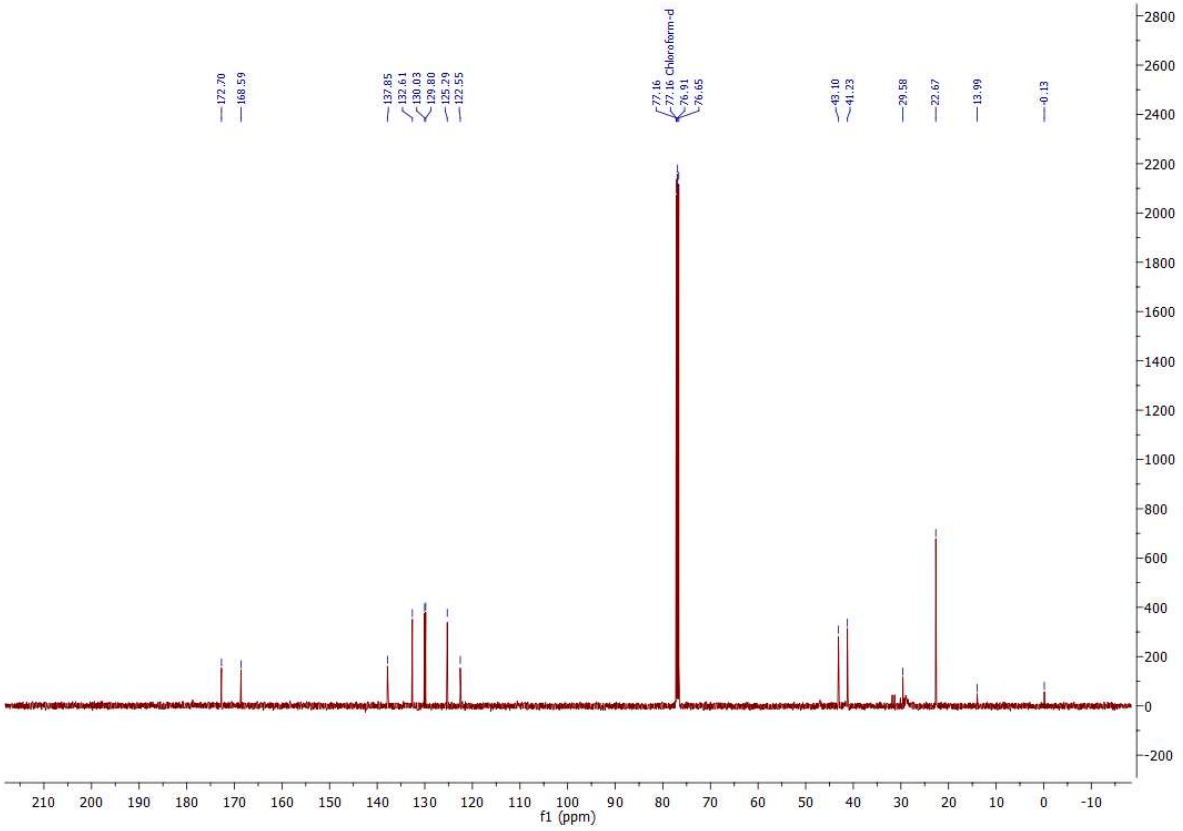
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A5



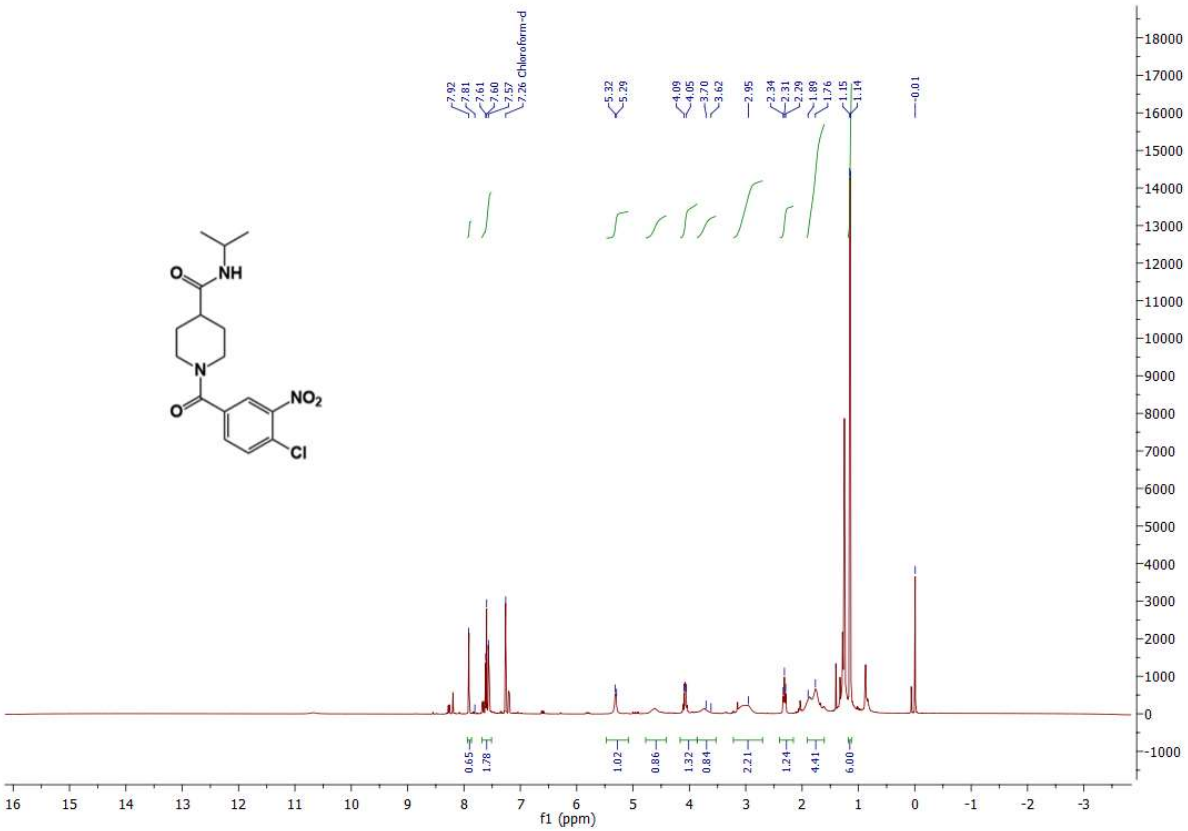


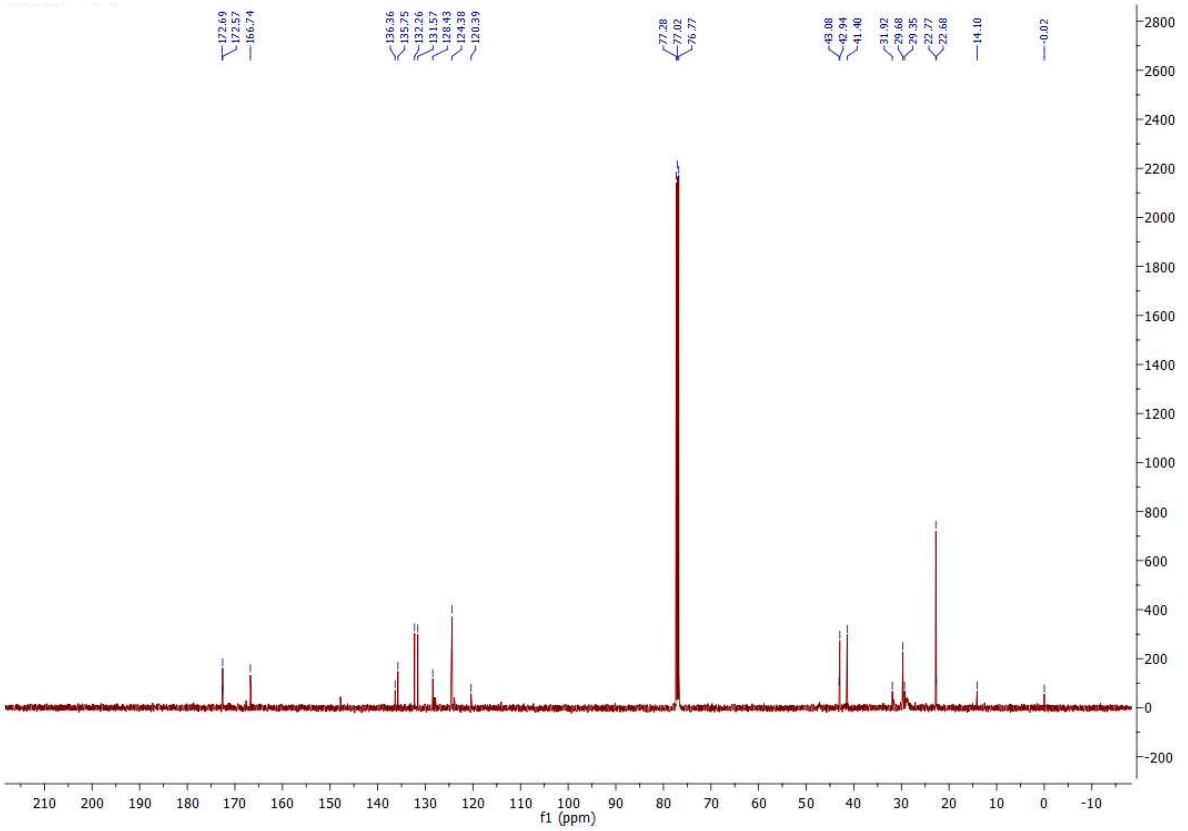
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A6



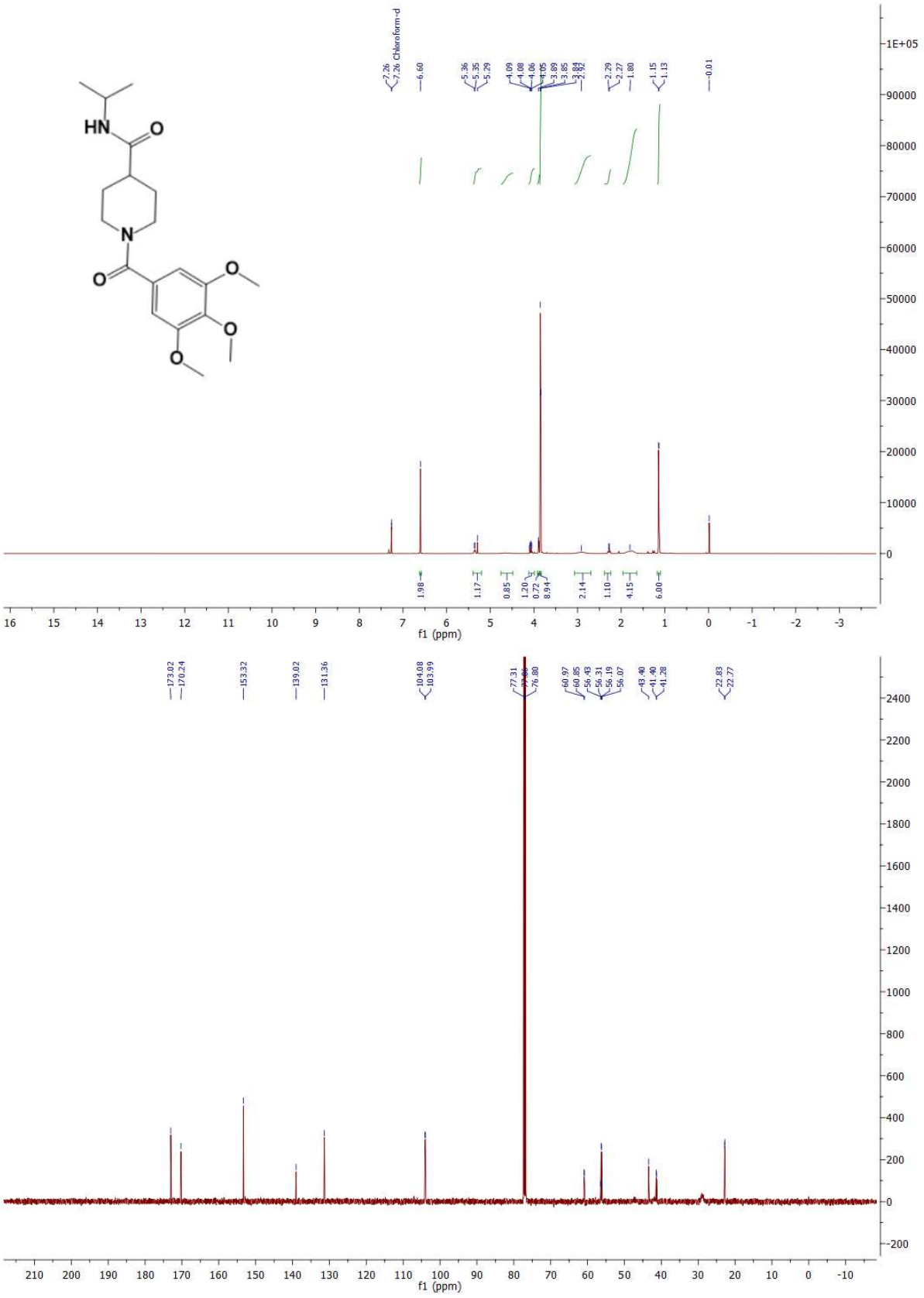


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A7

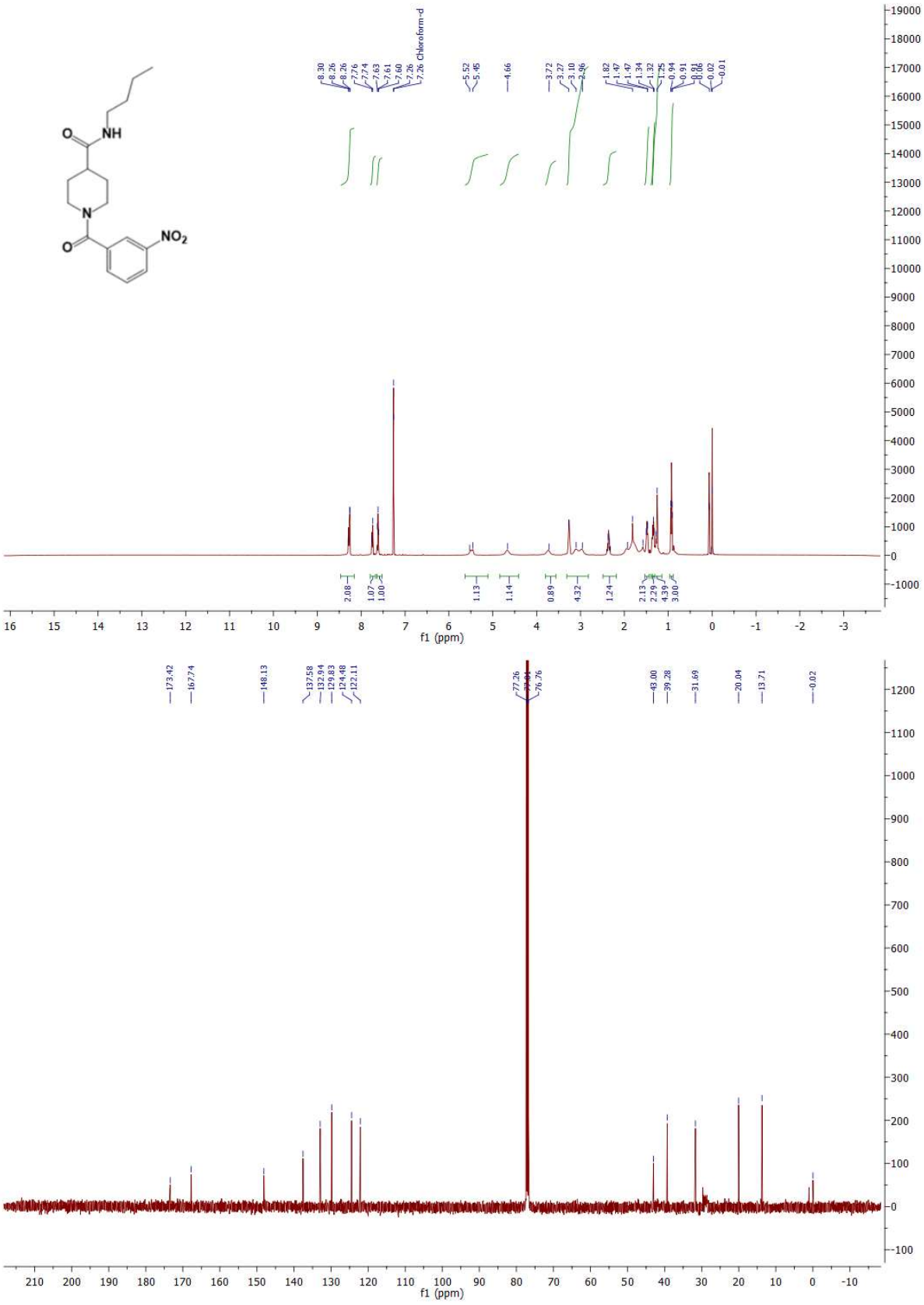




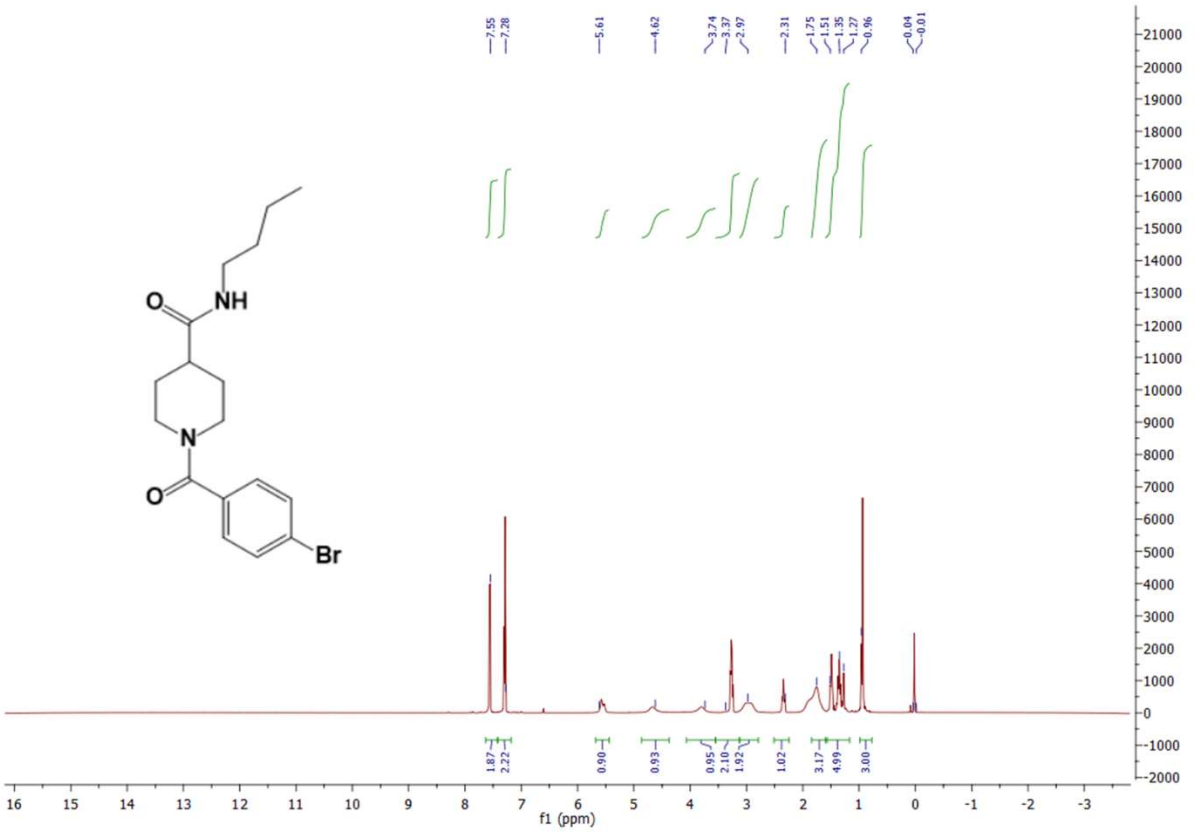
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A8

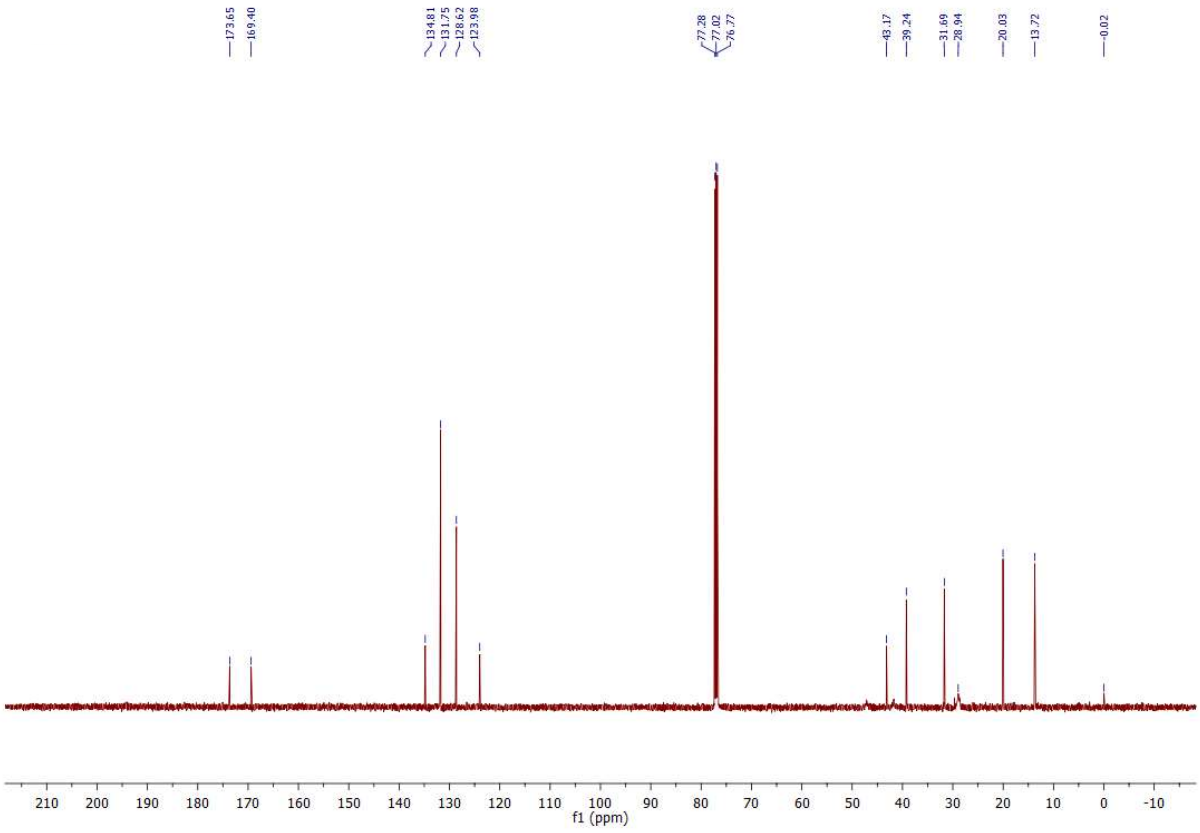


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A9

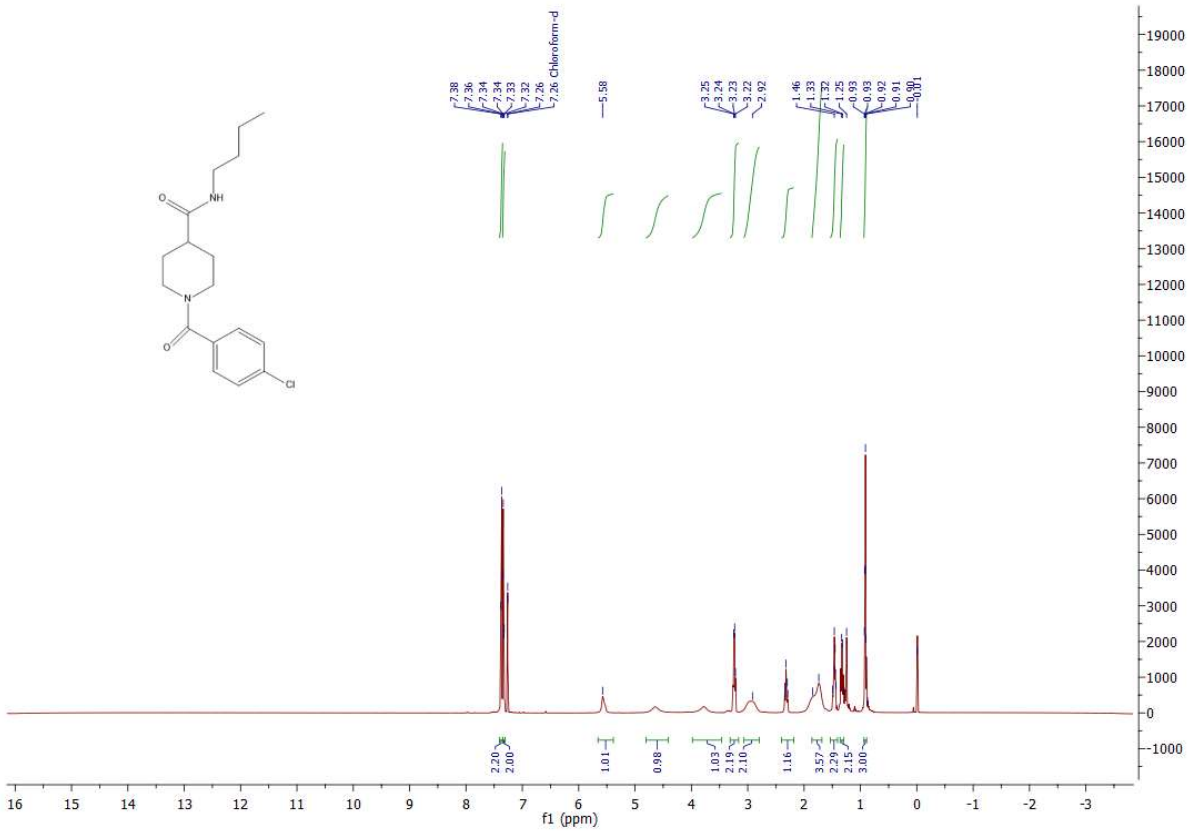


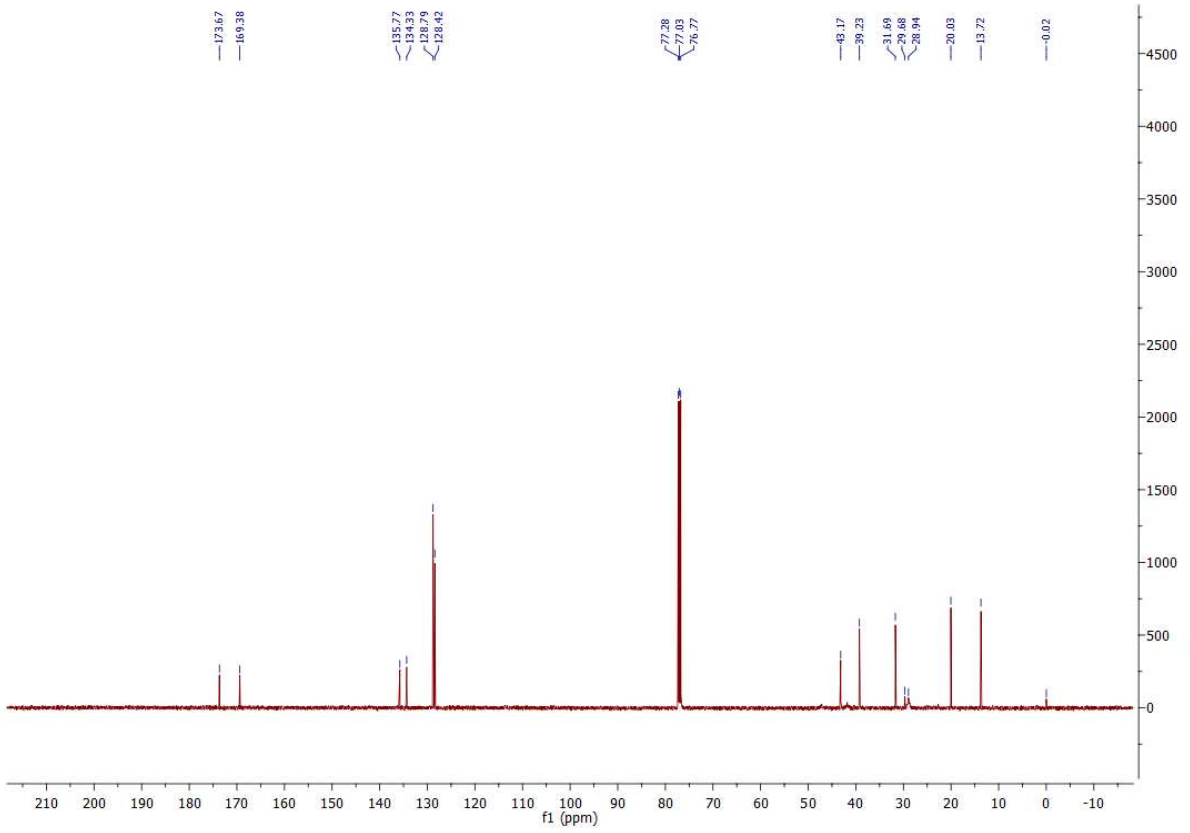
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A10



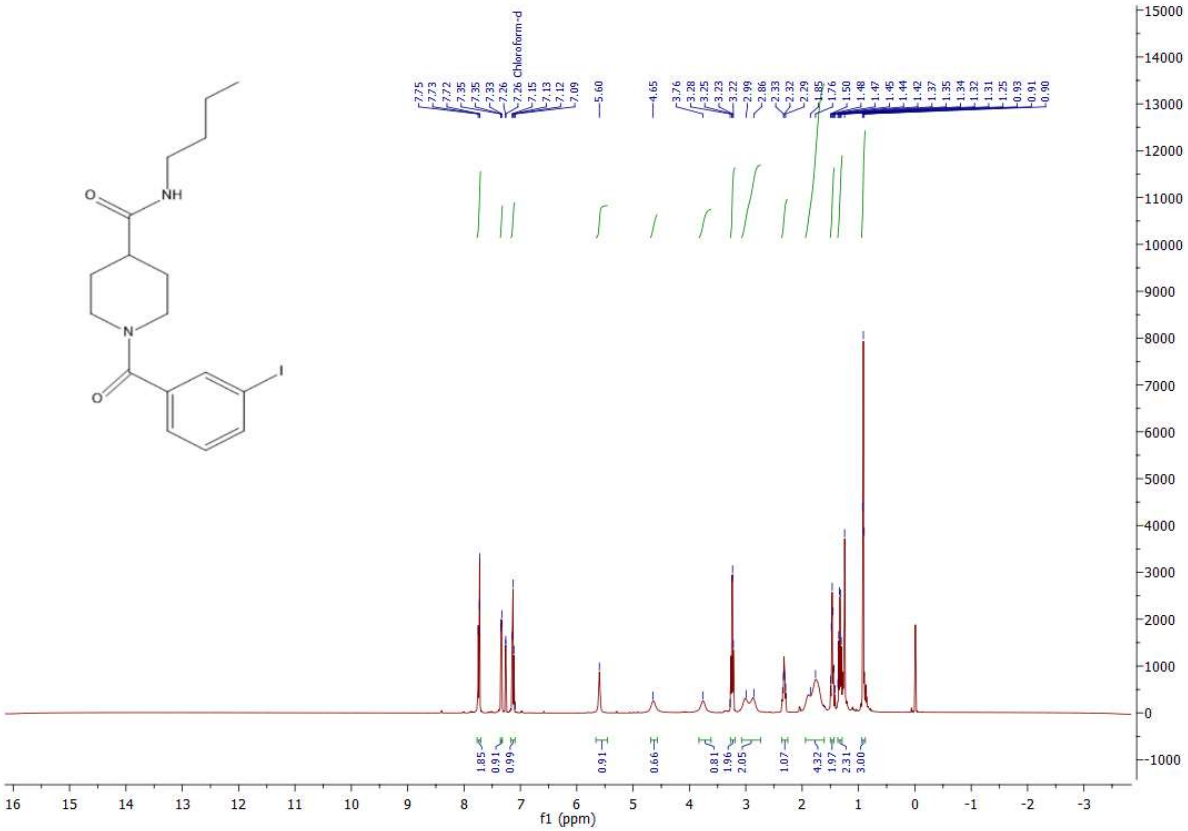


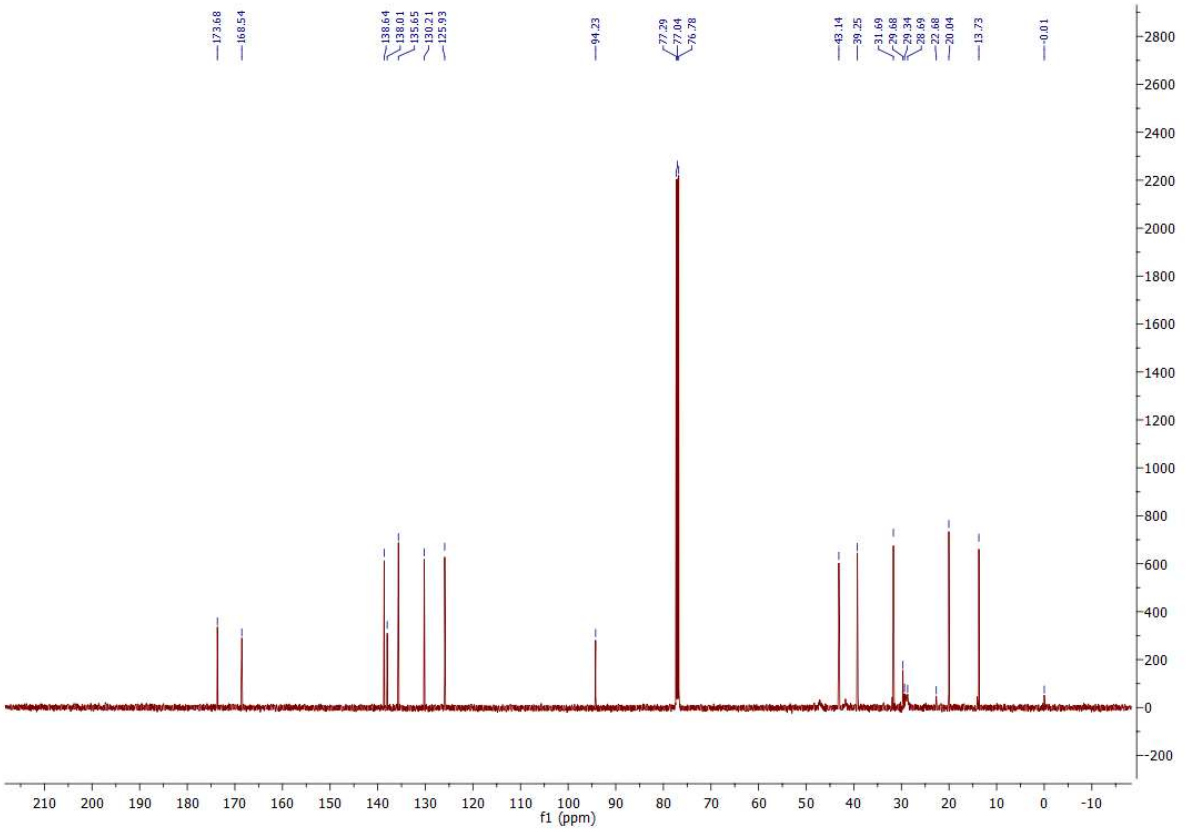
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A11



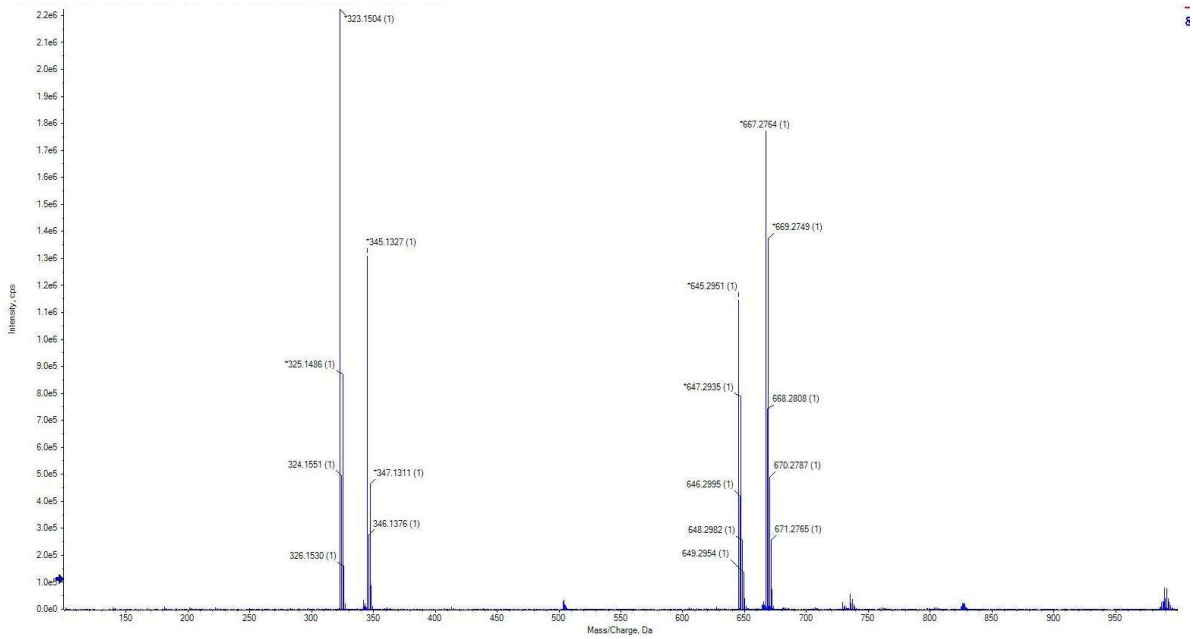


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A12

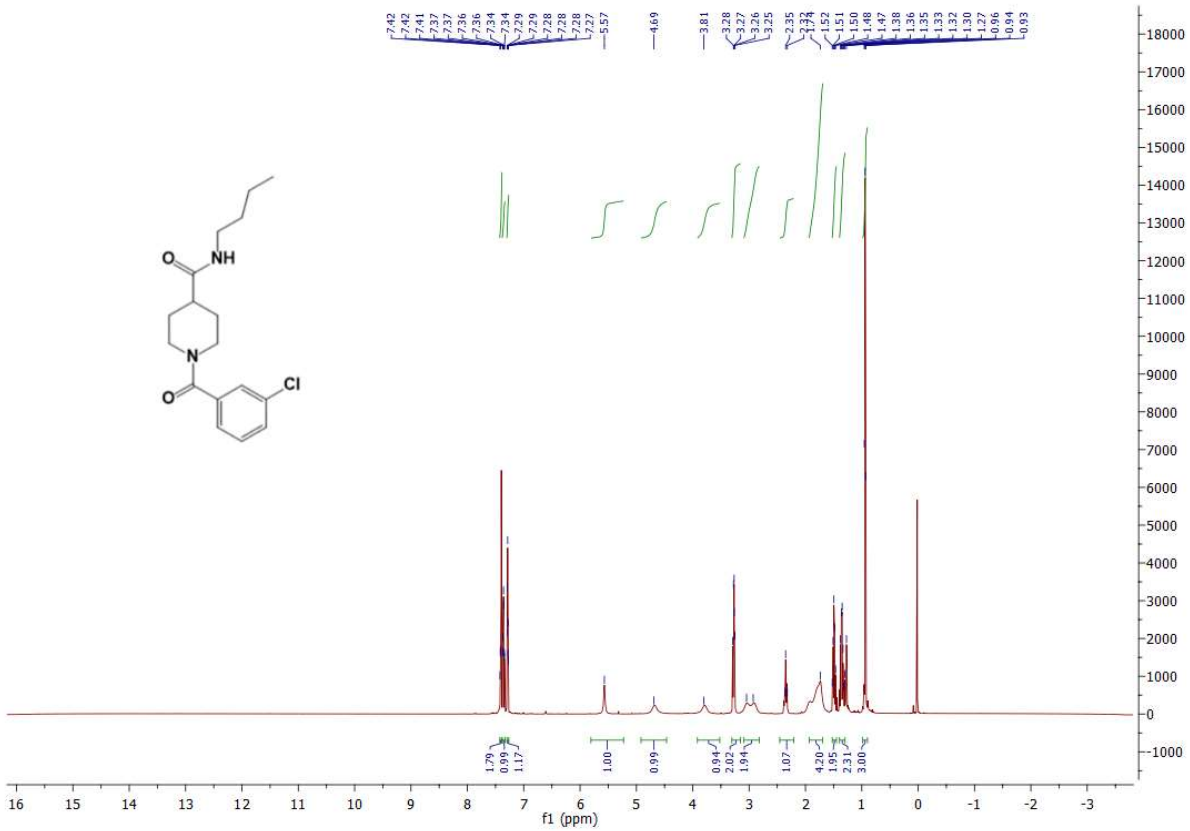


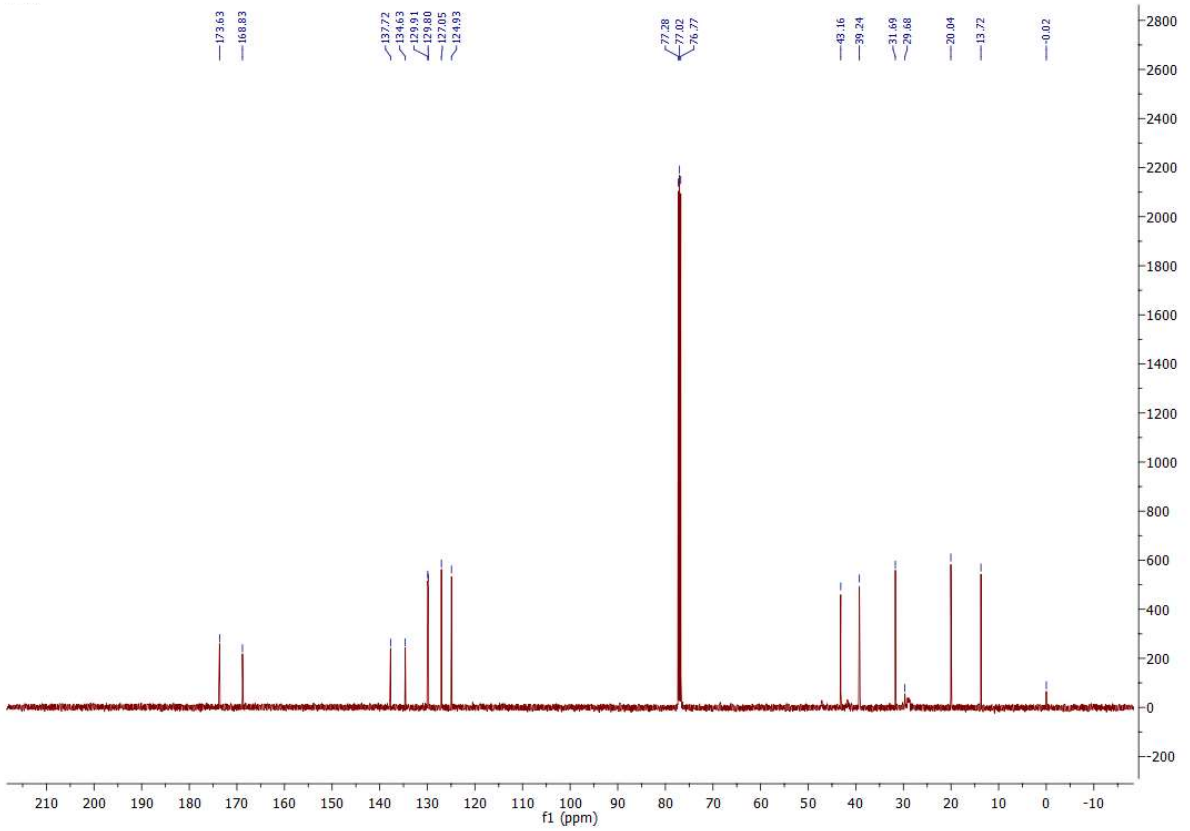


HRMS spectra of compound A12

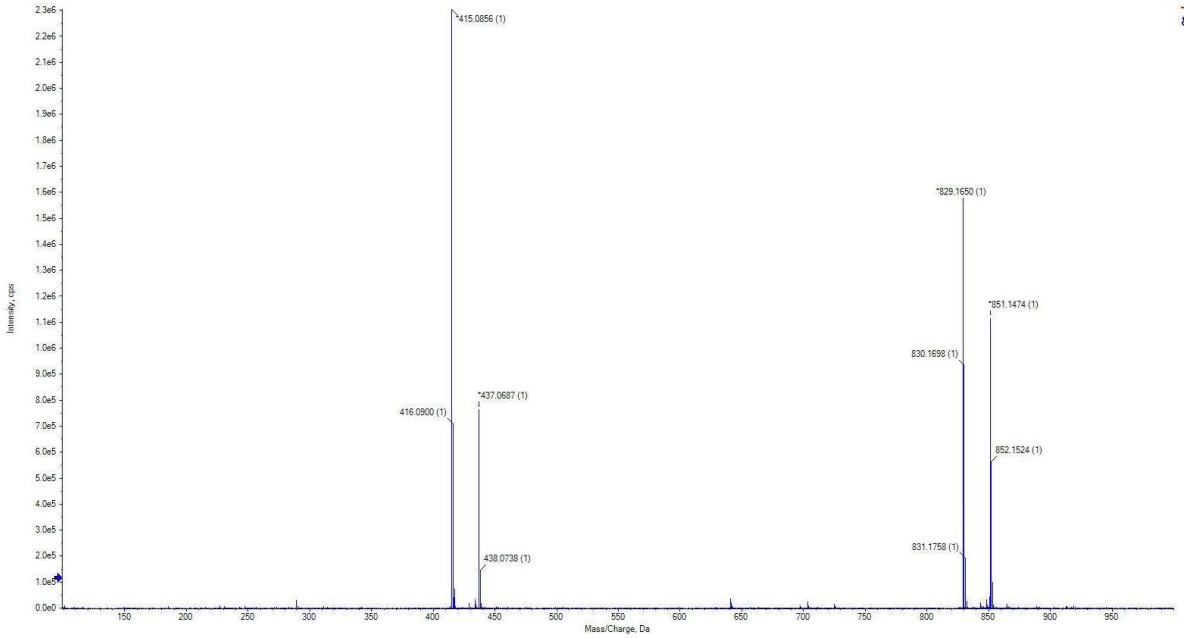


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A13

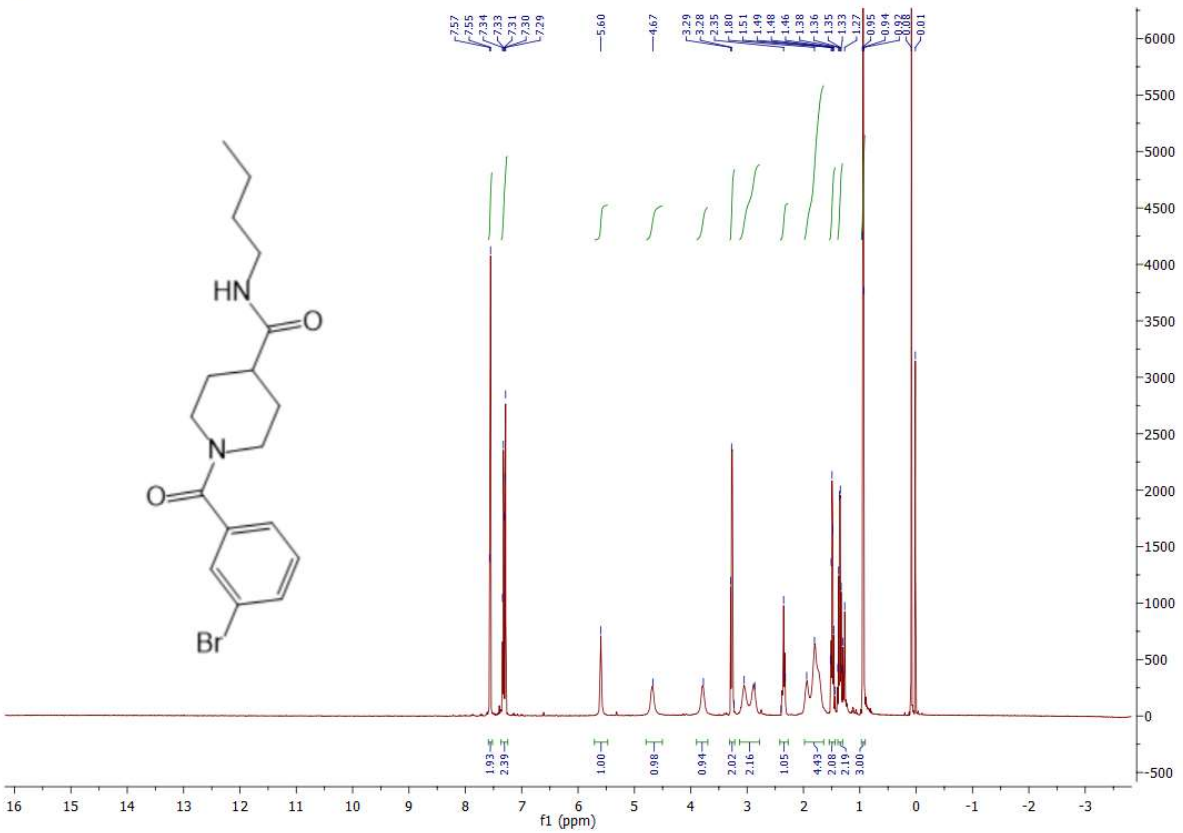


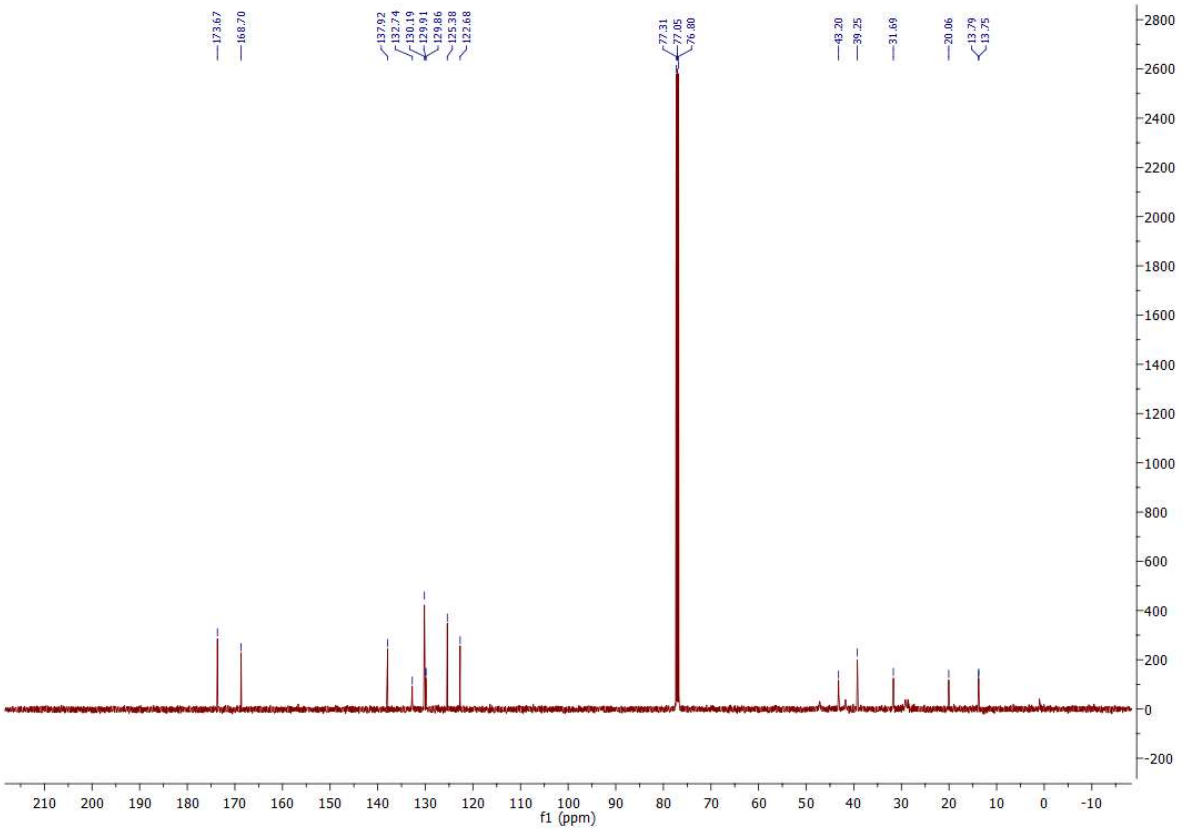


HRMS spectra of compound A13

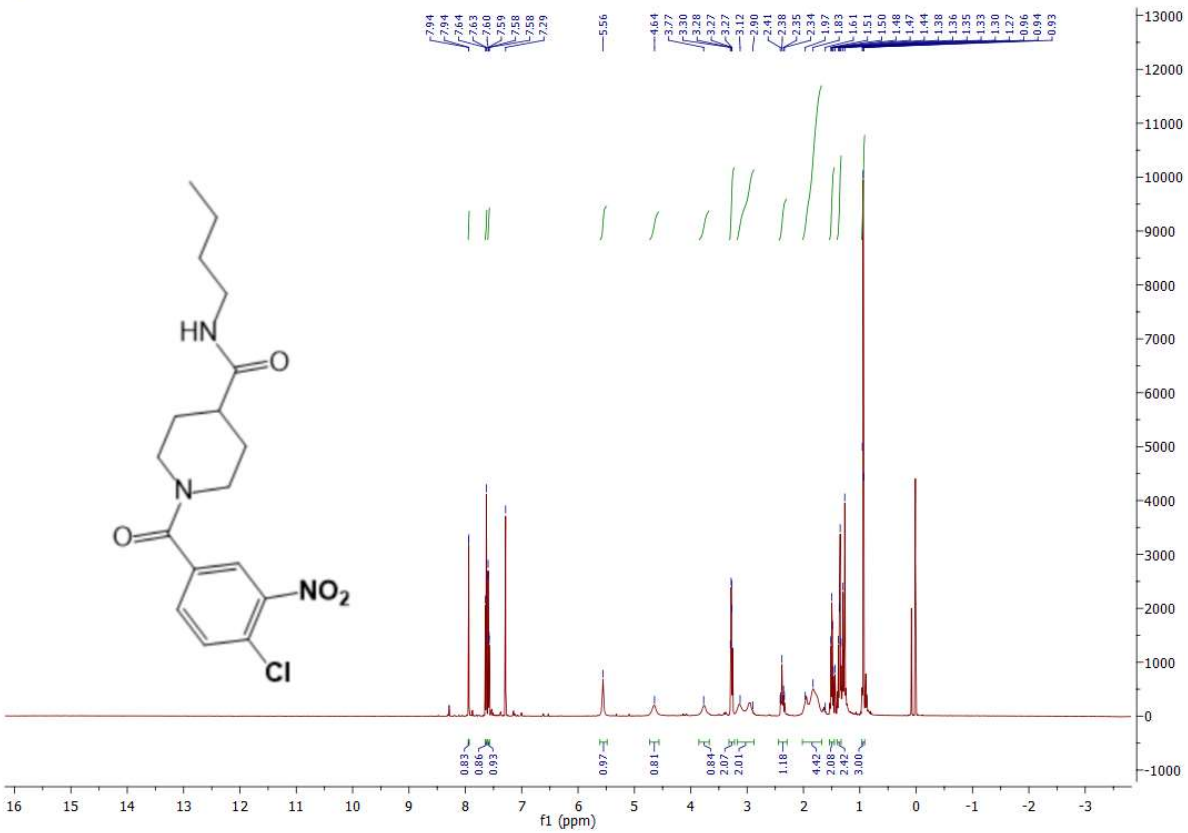


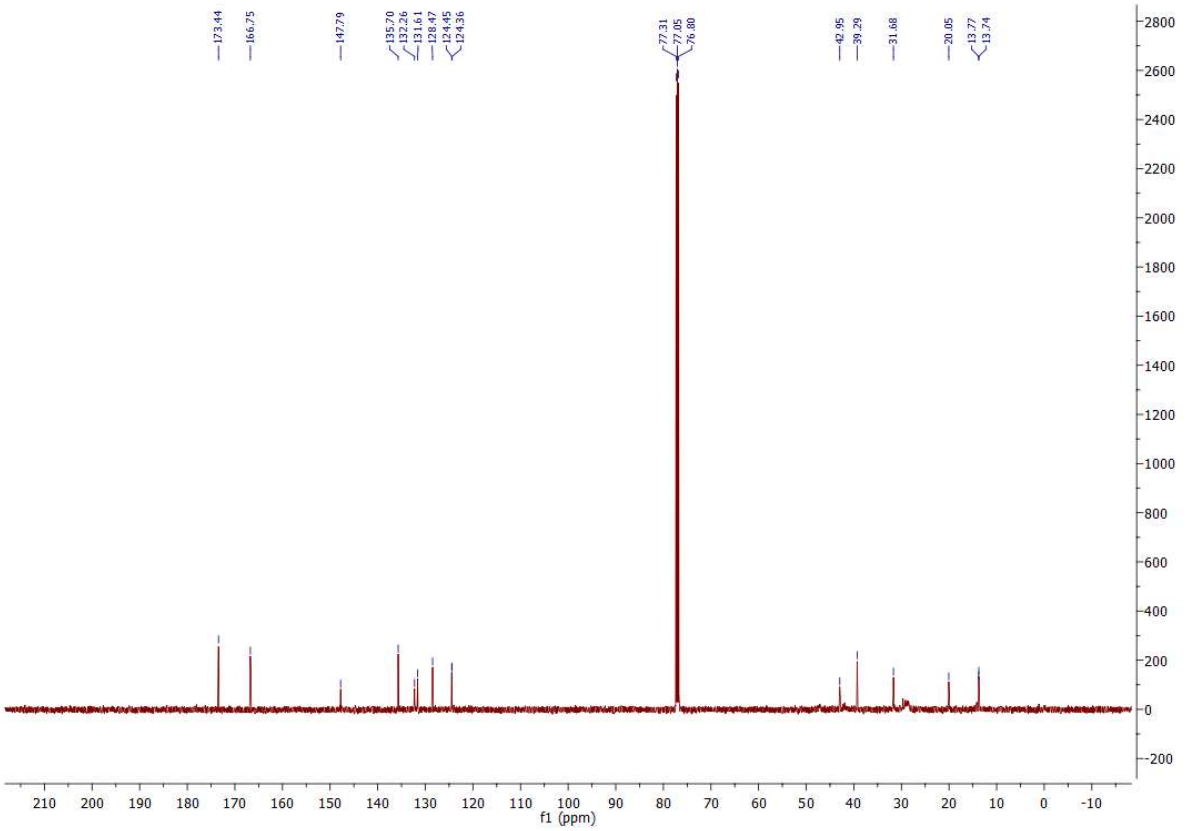
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A14



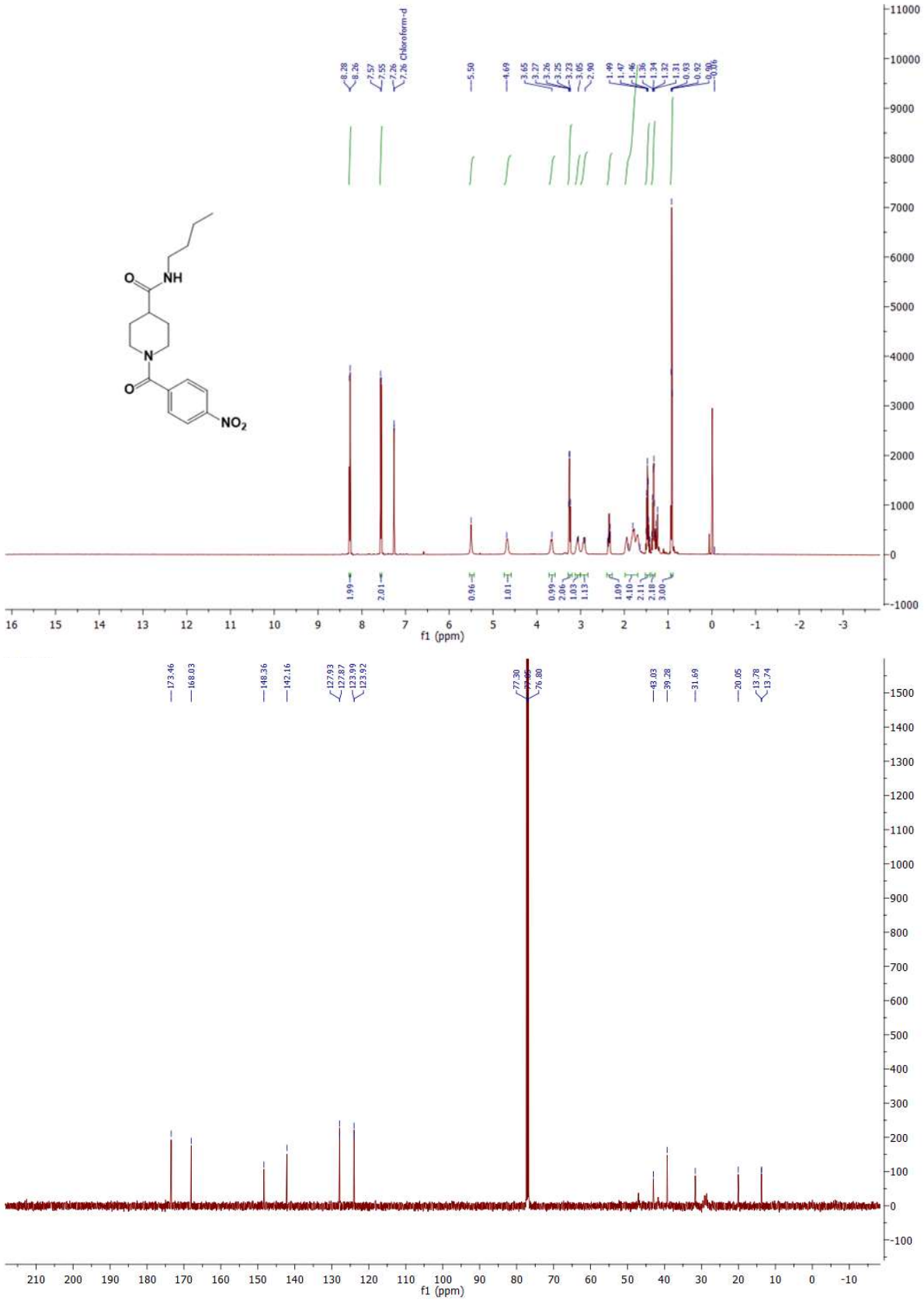


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A15

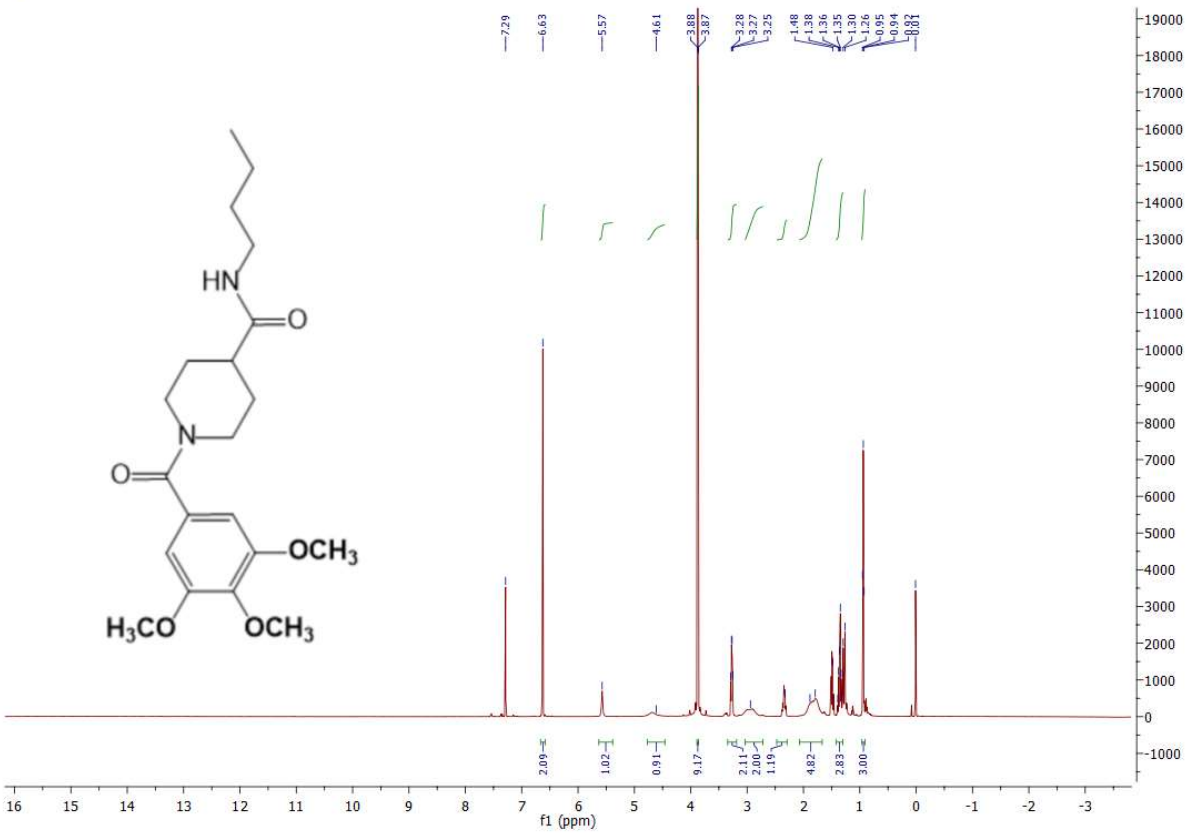


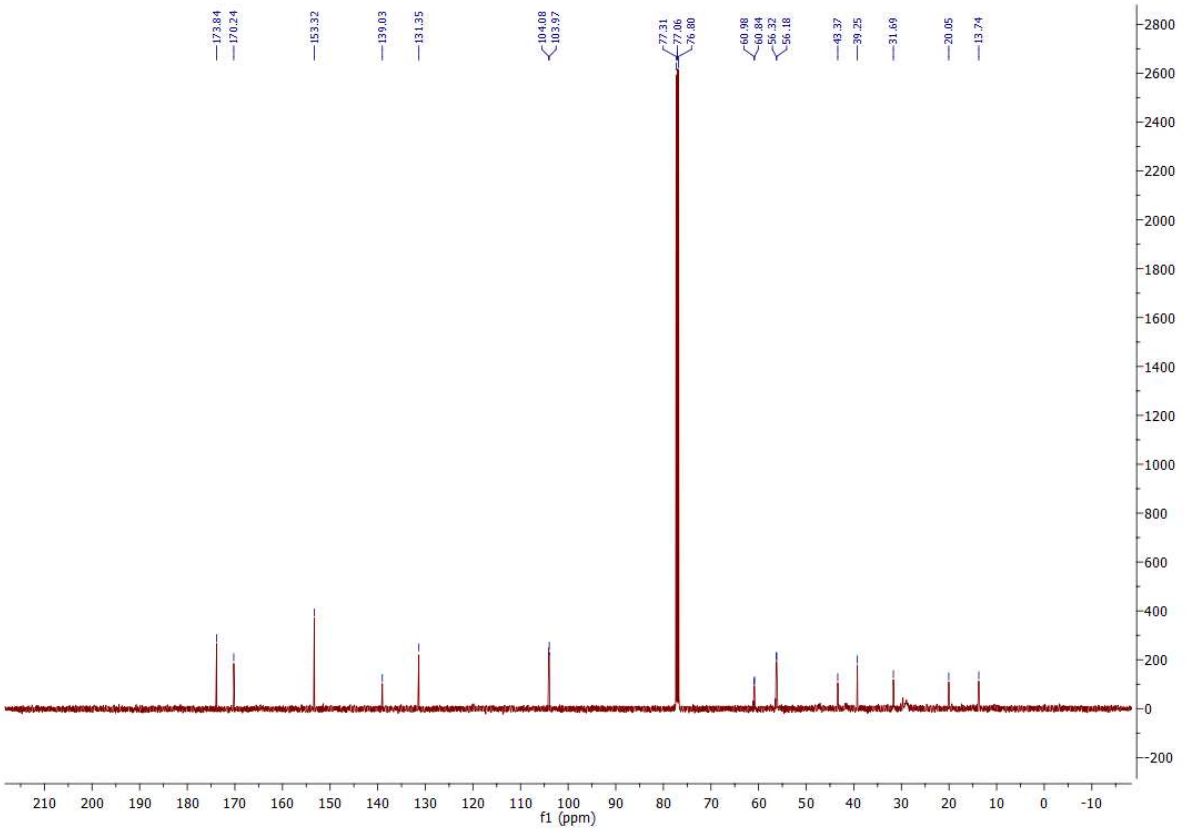


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A16

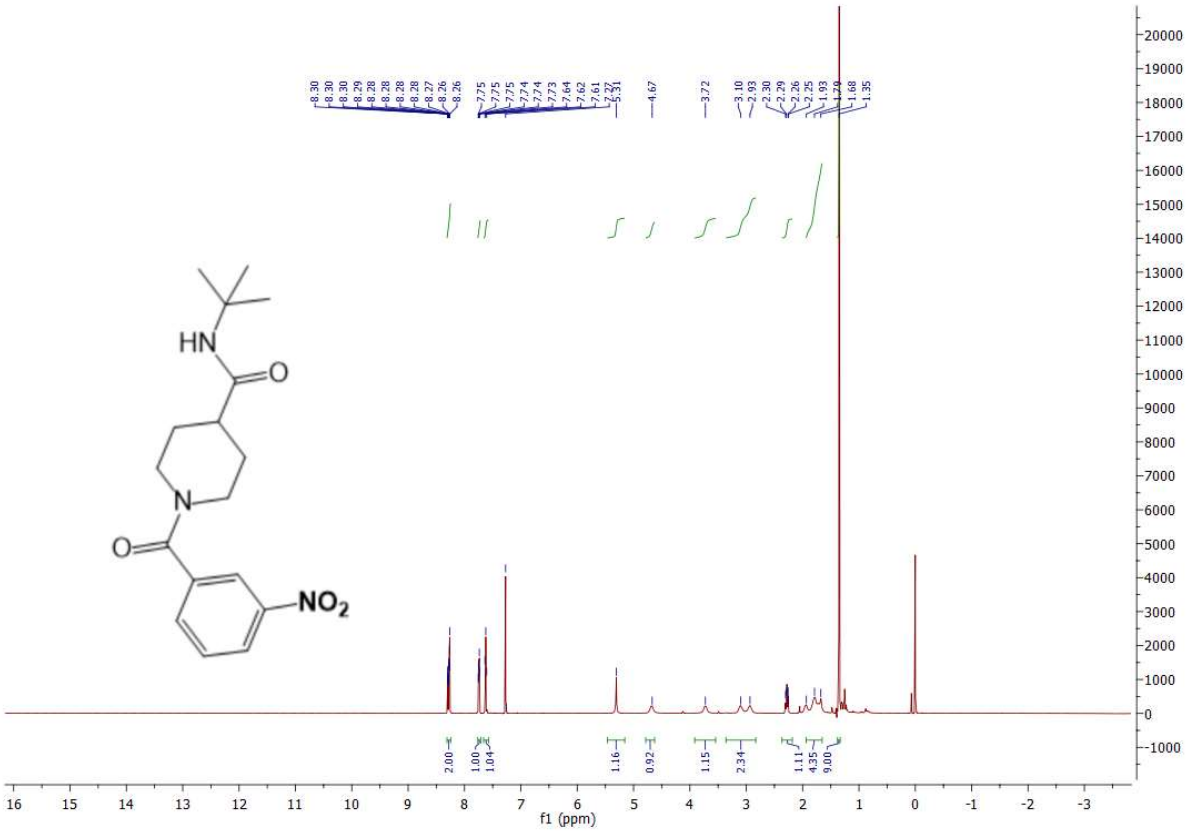


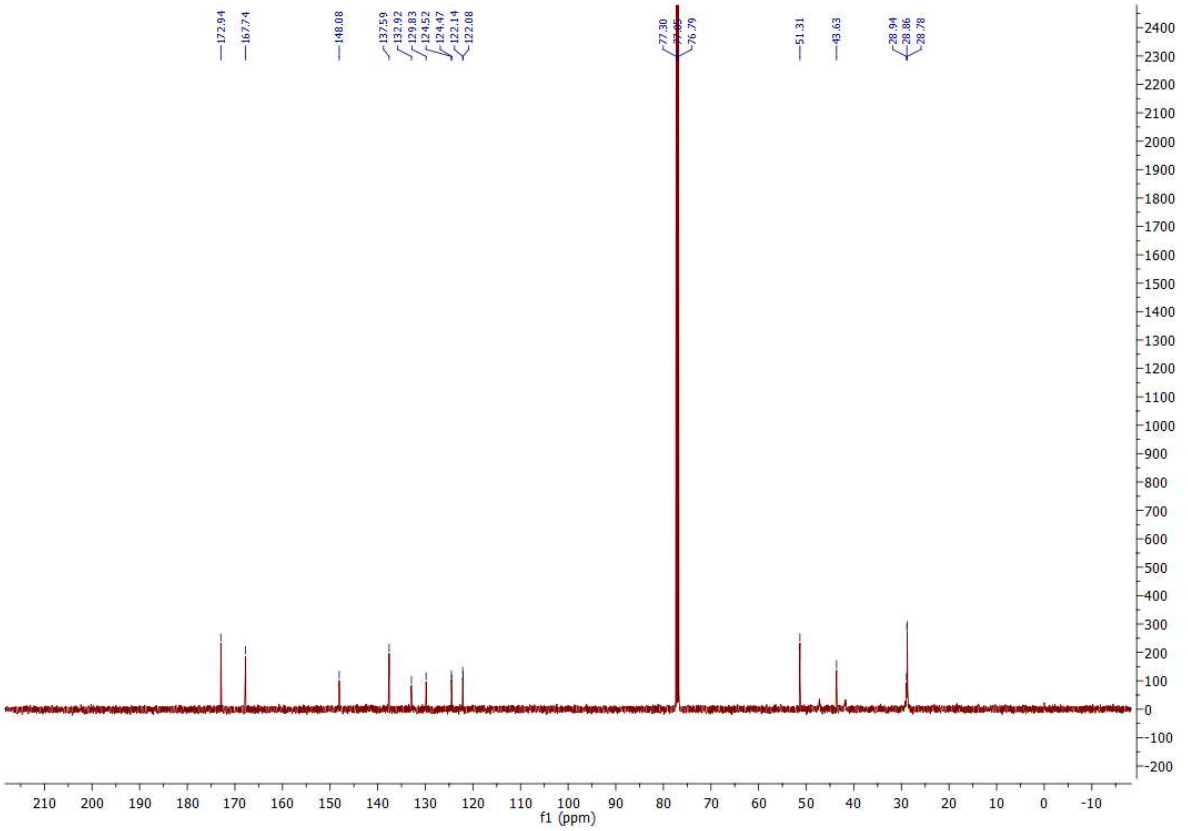
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A17



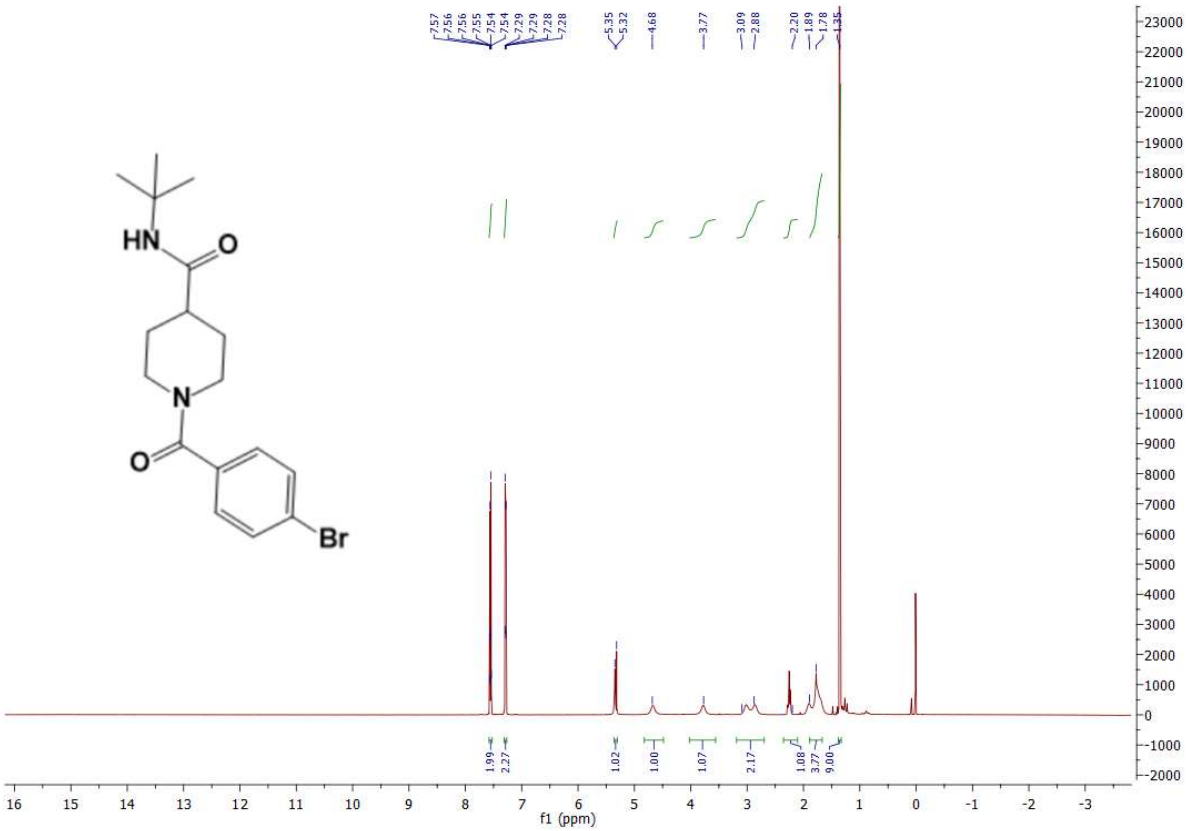


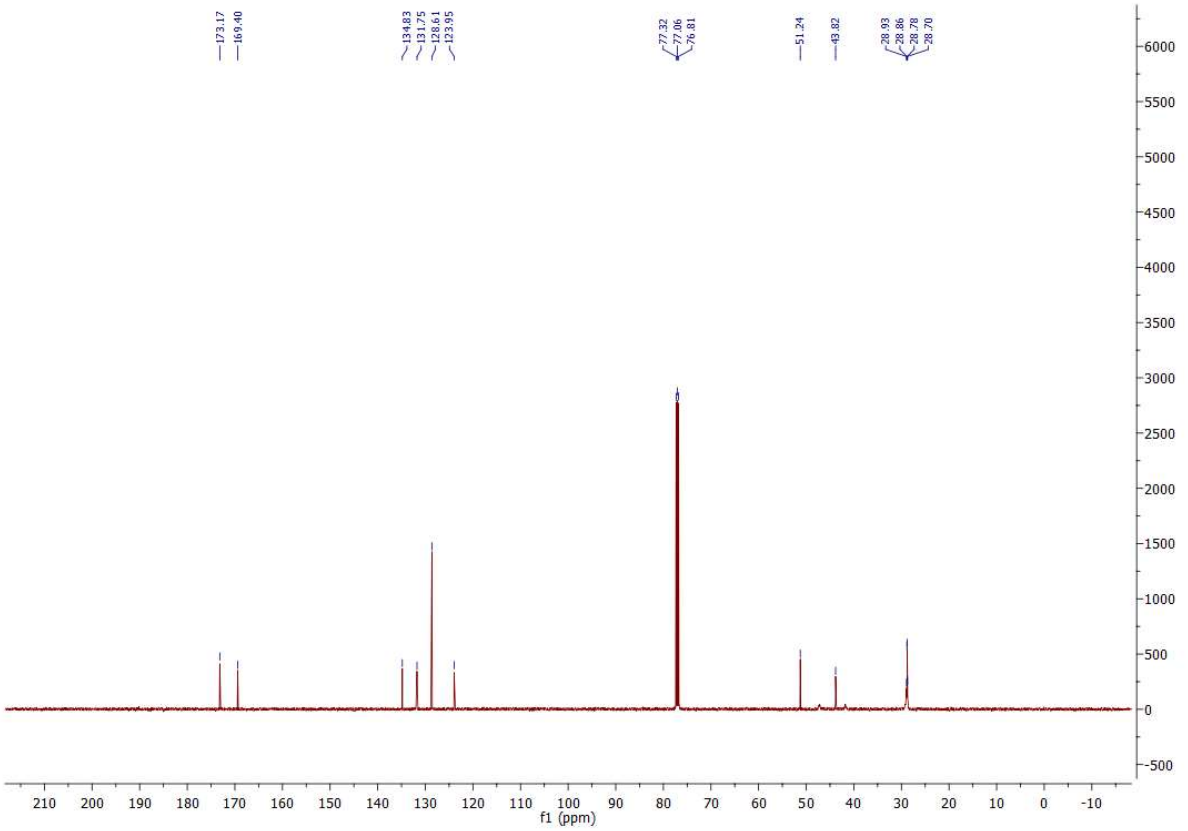
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A18



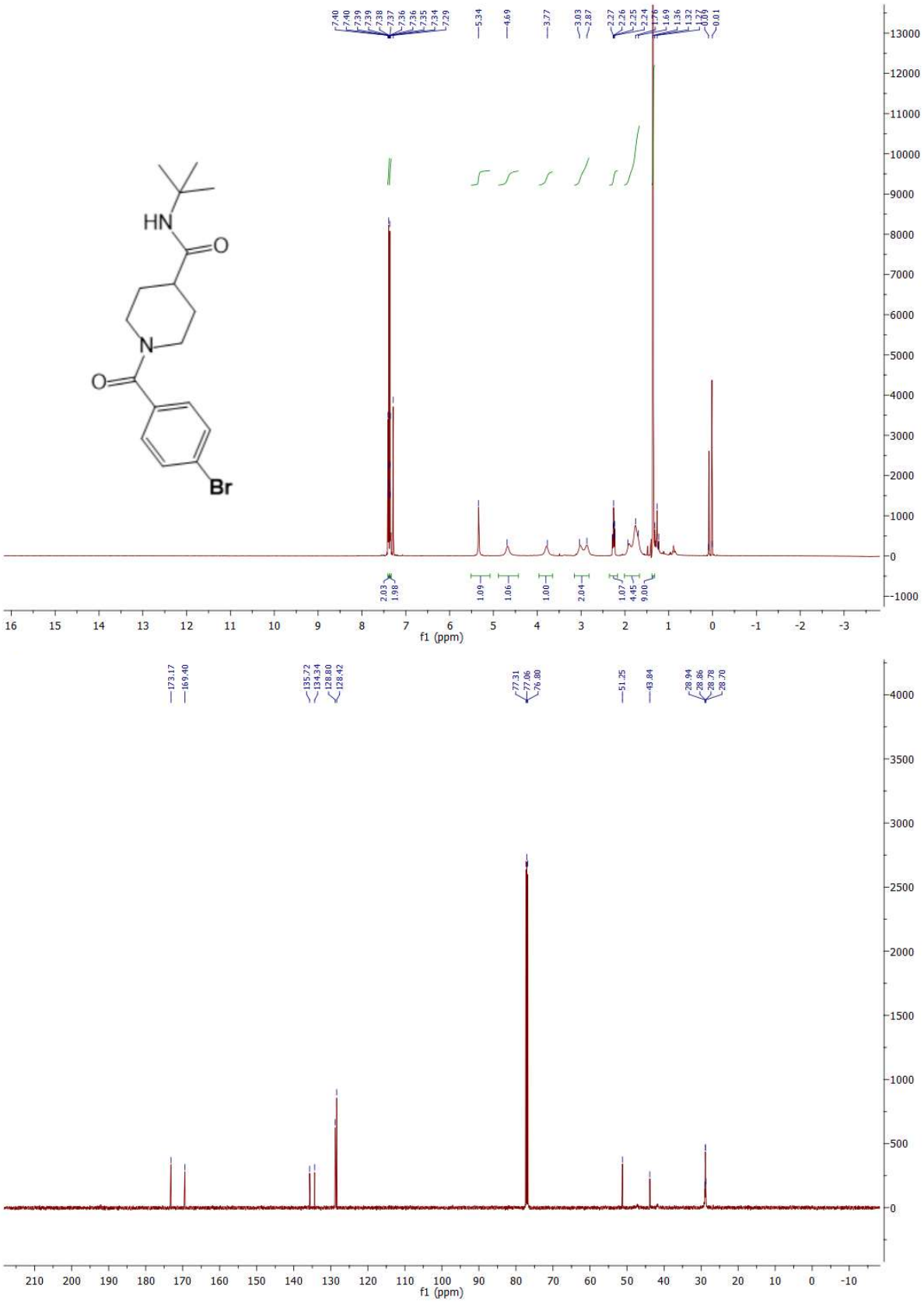


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A19

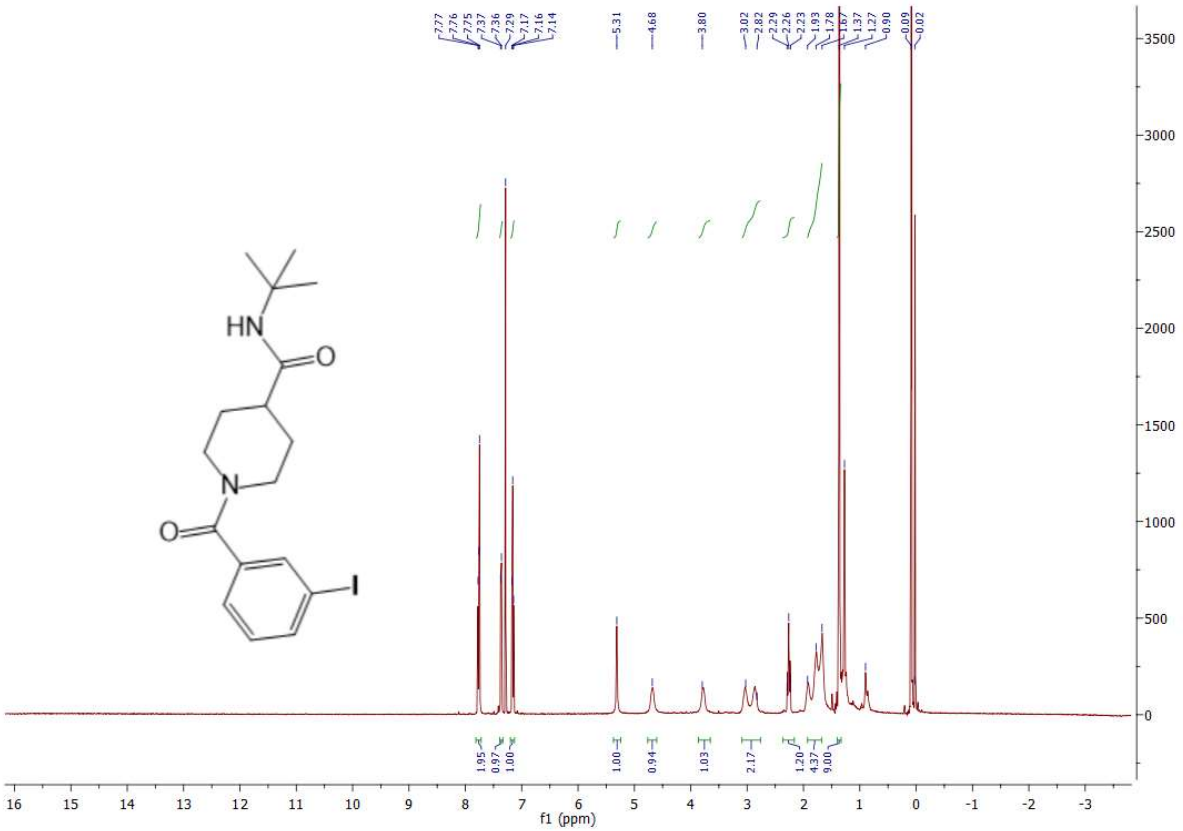


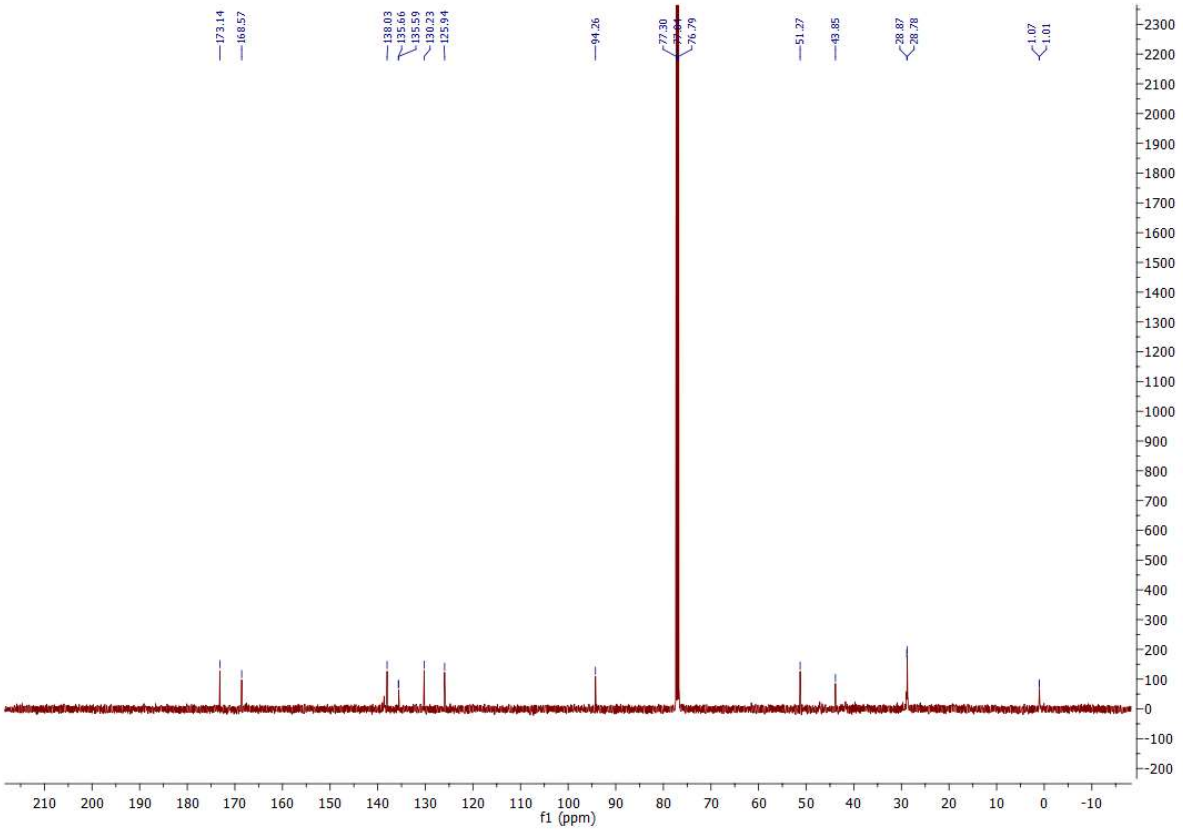


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A20

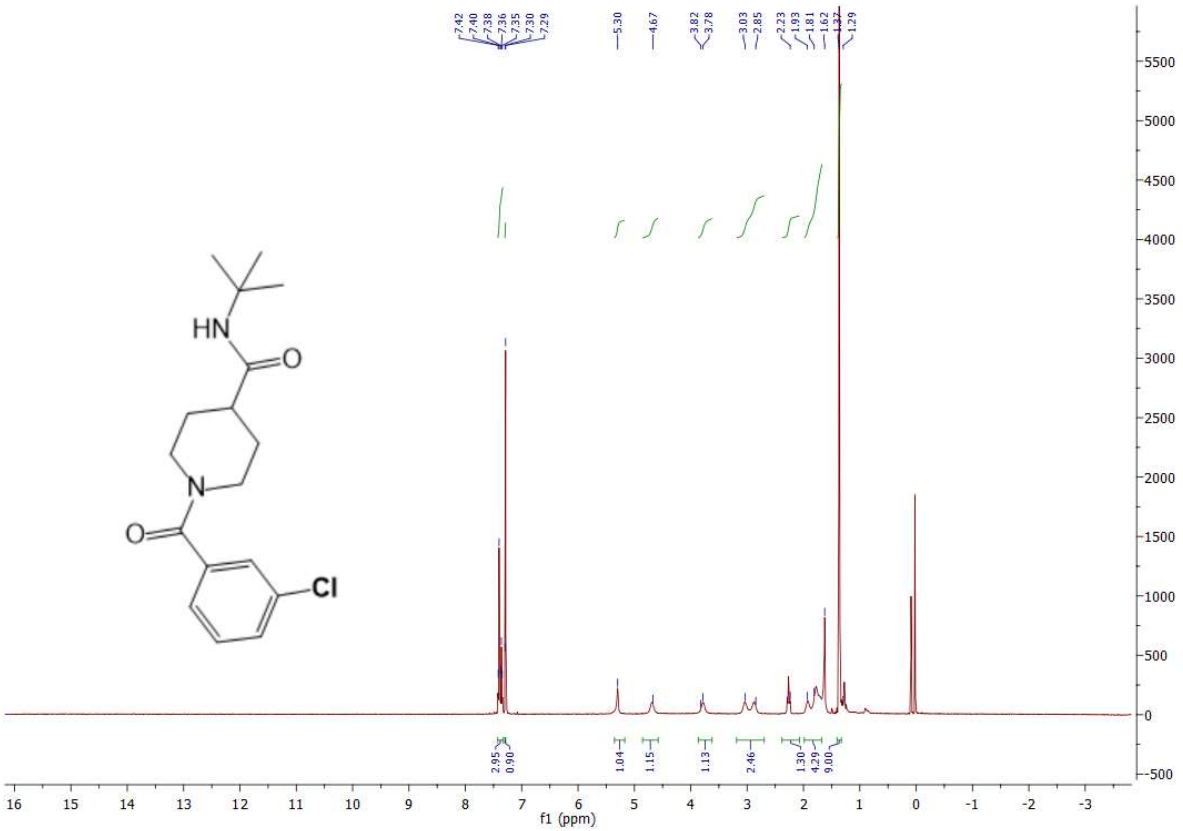


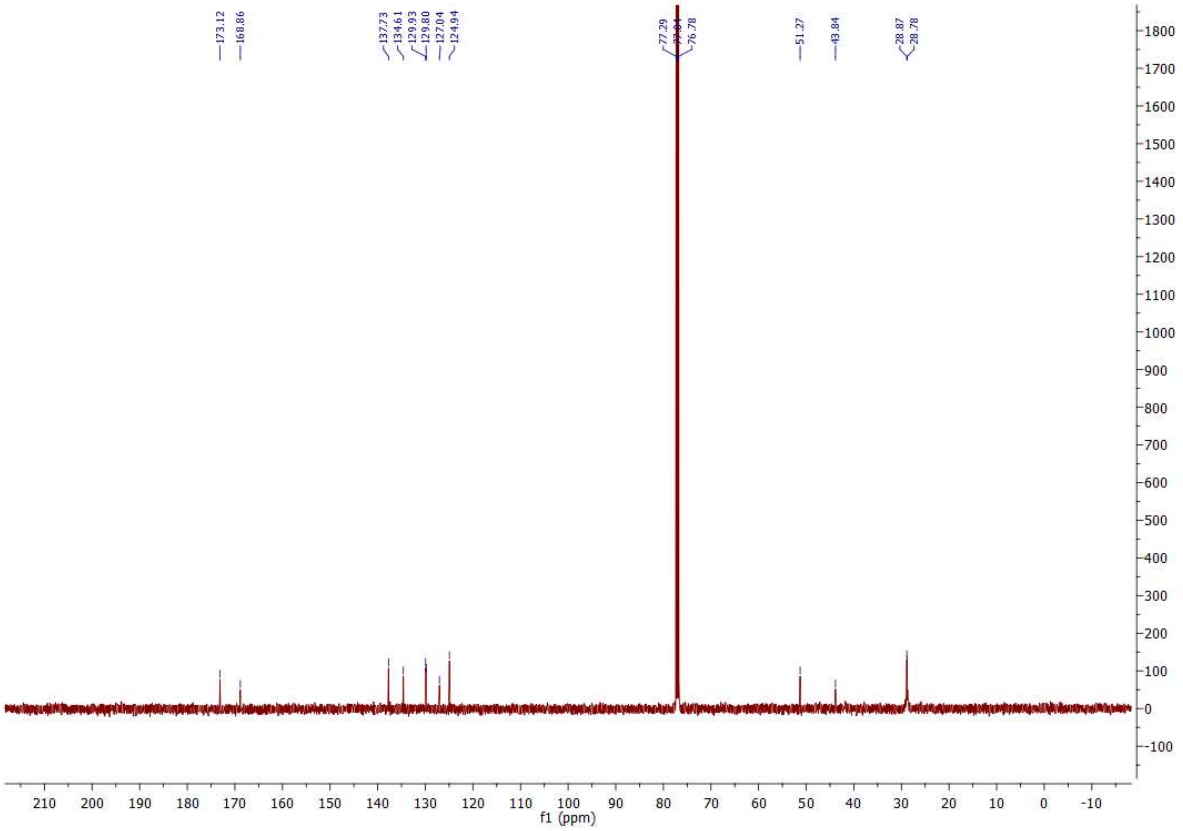
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A21



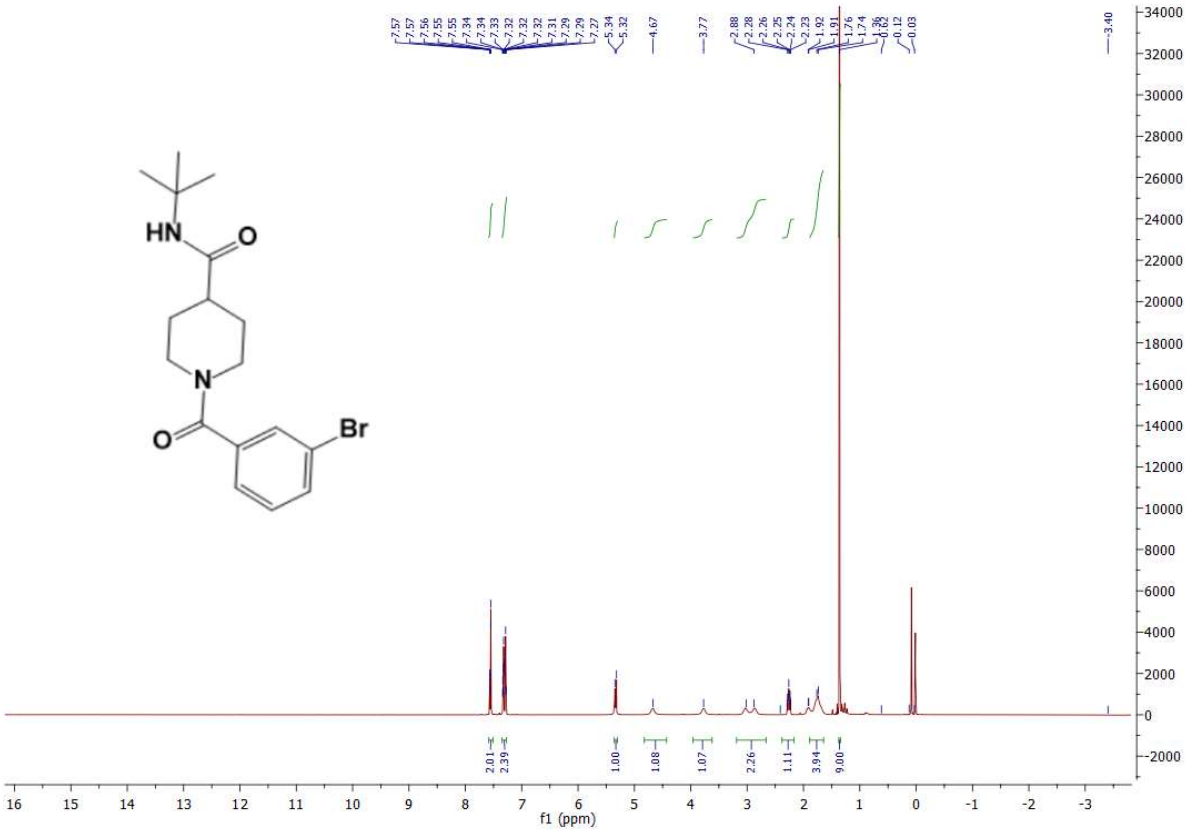


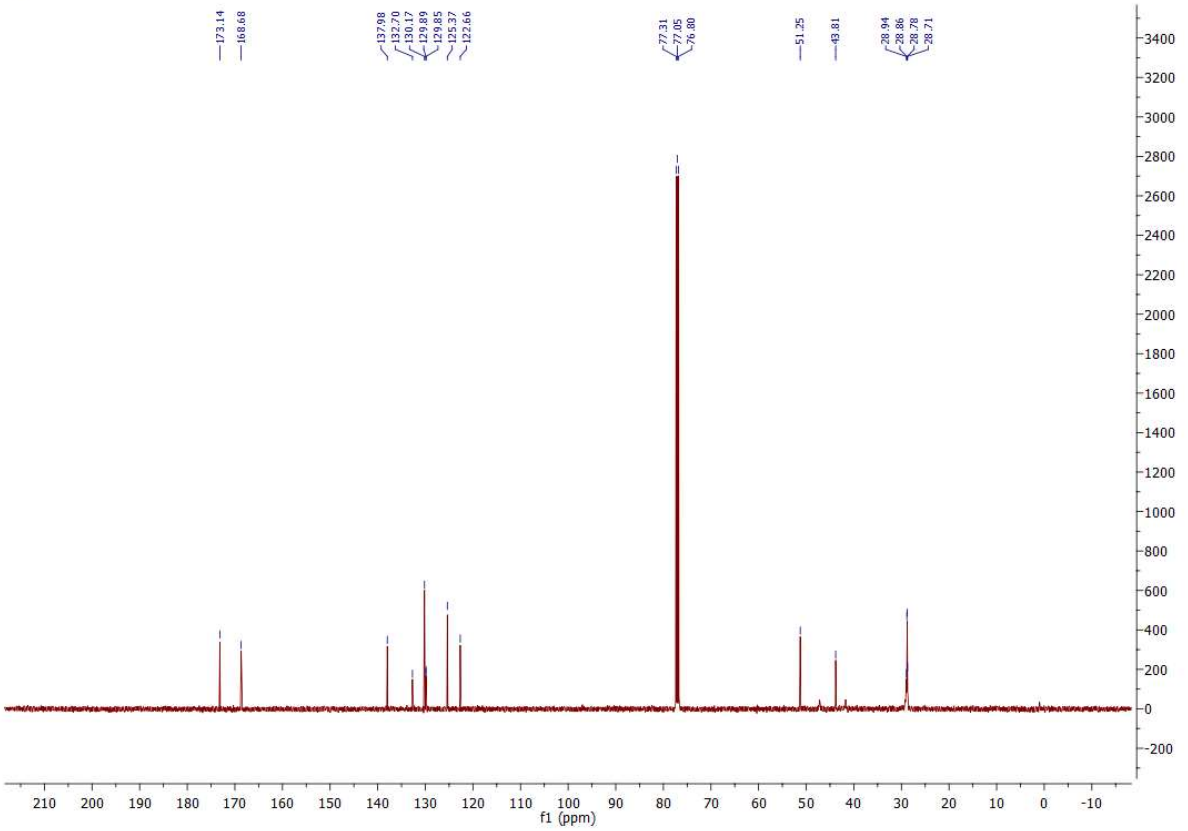
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A22



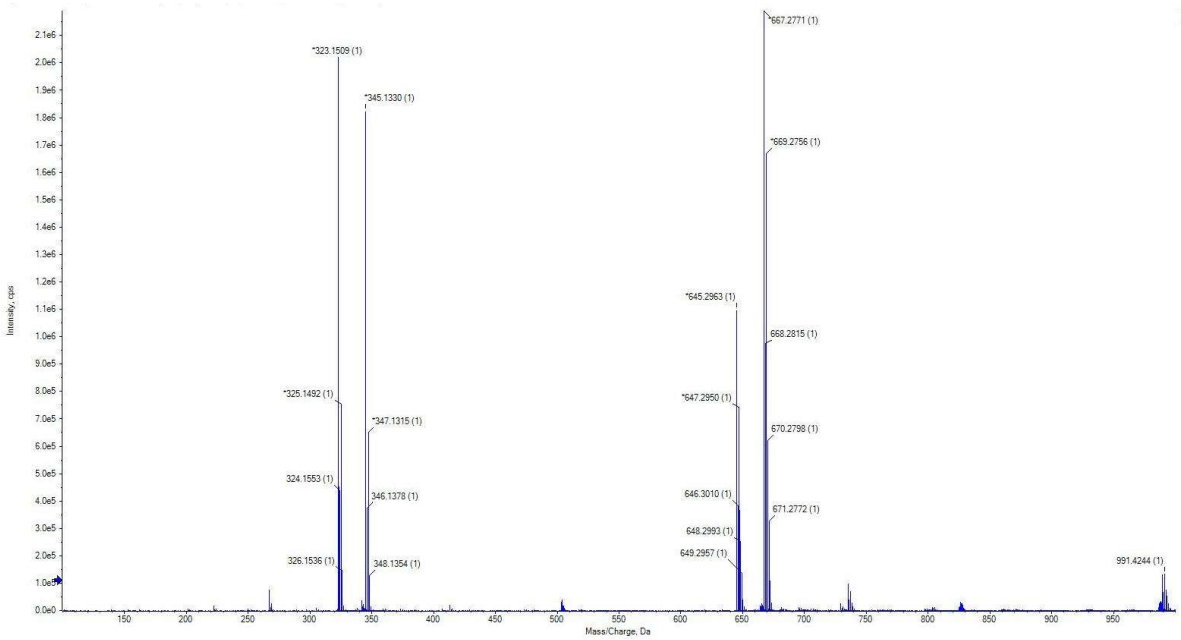


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A23

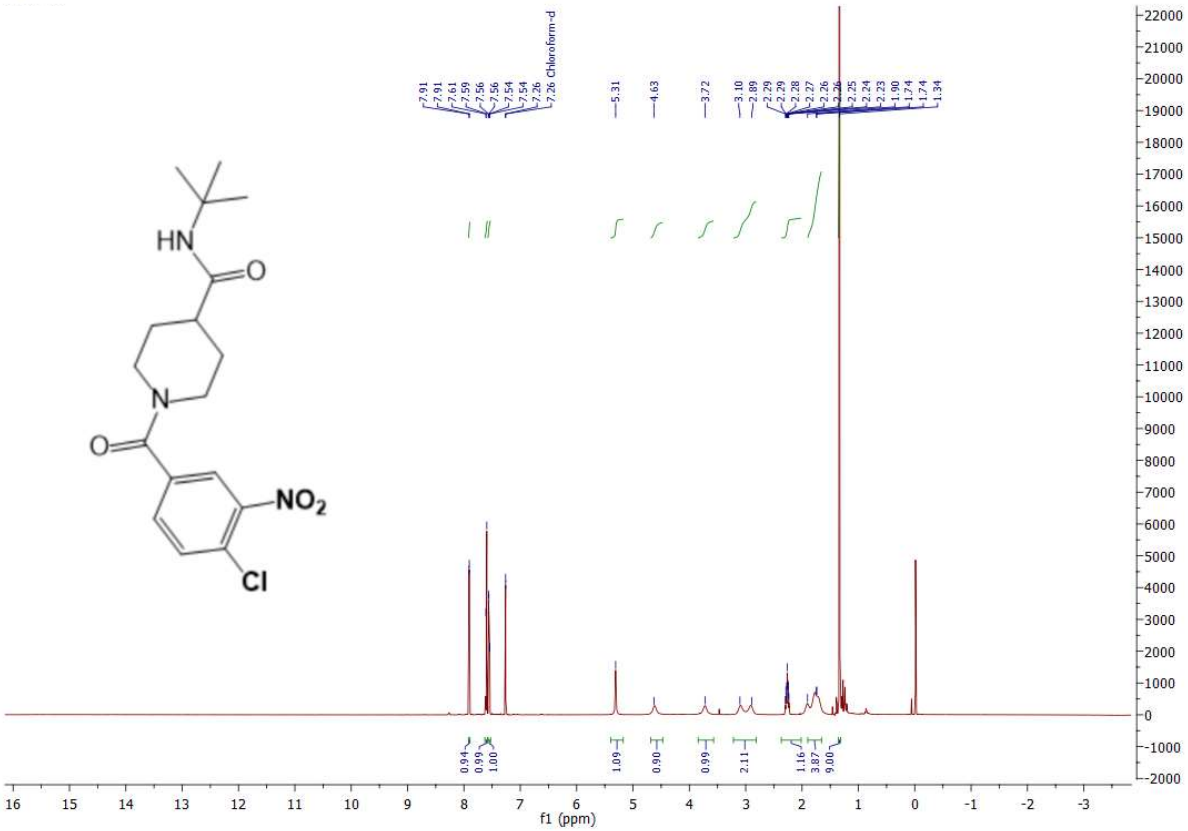


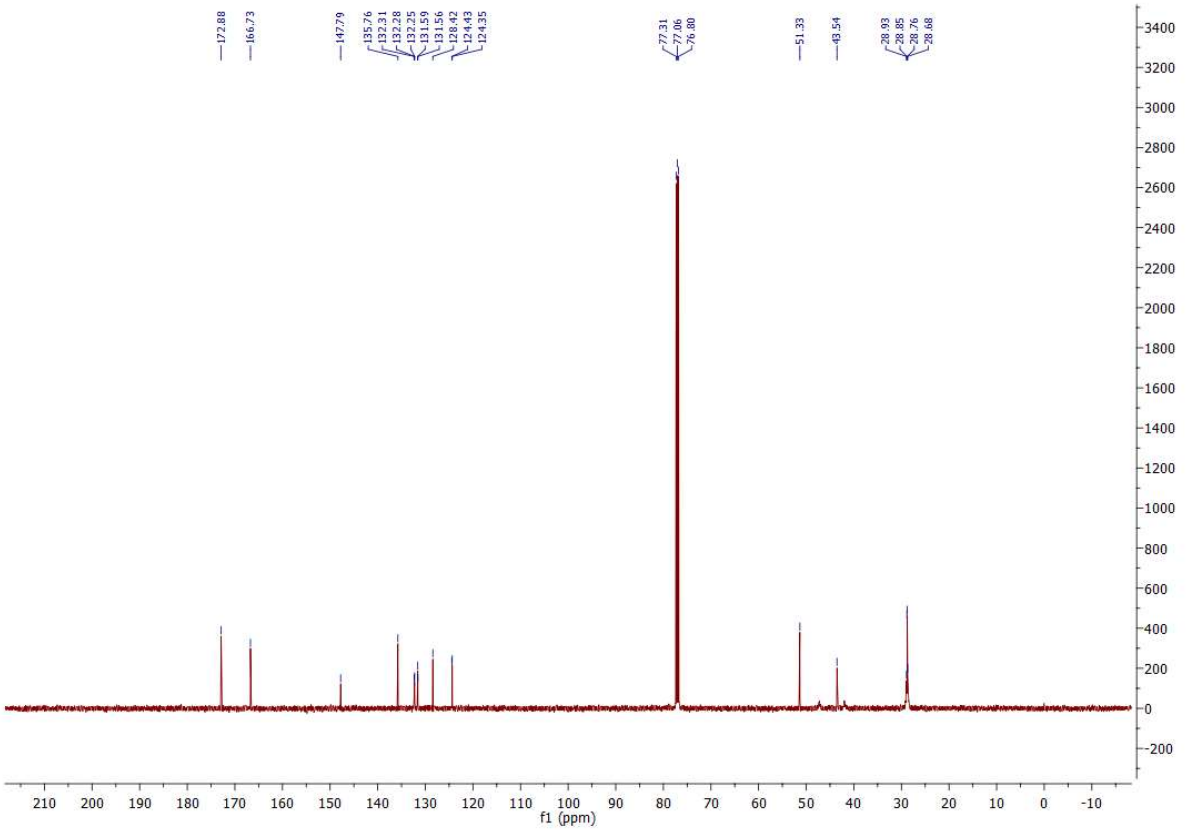


HRMS spectra of compound A23

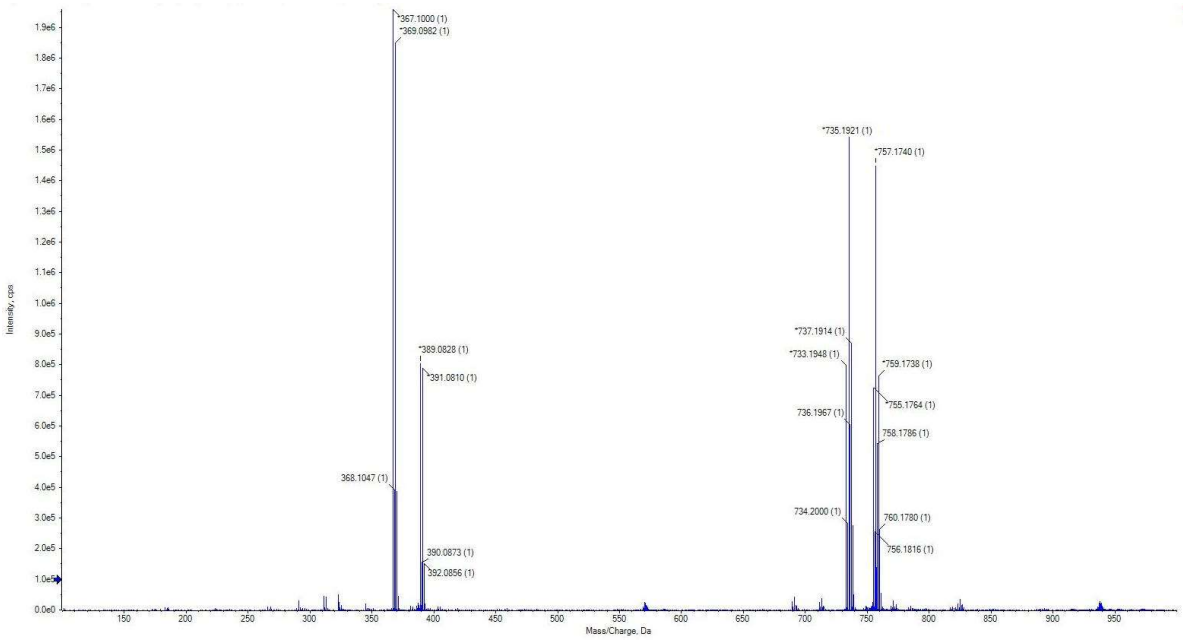


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A24

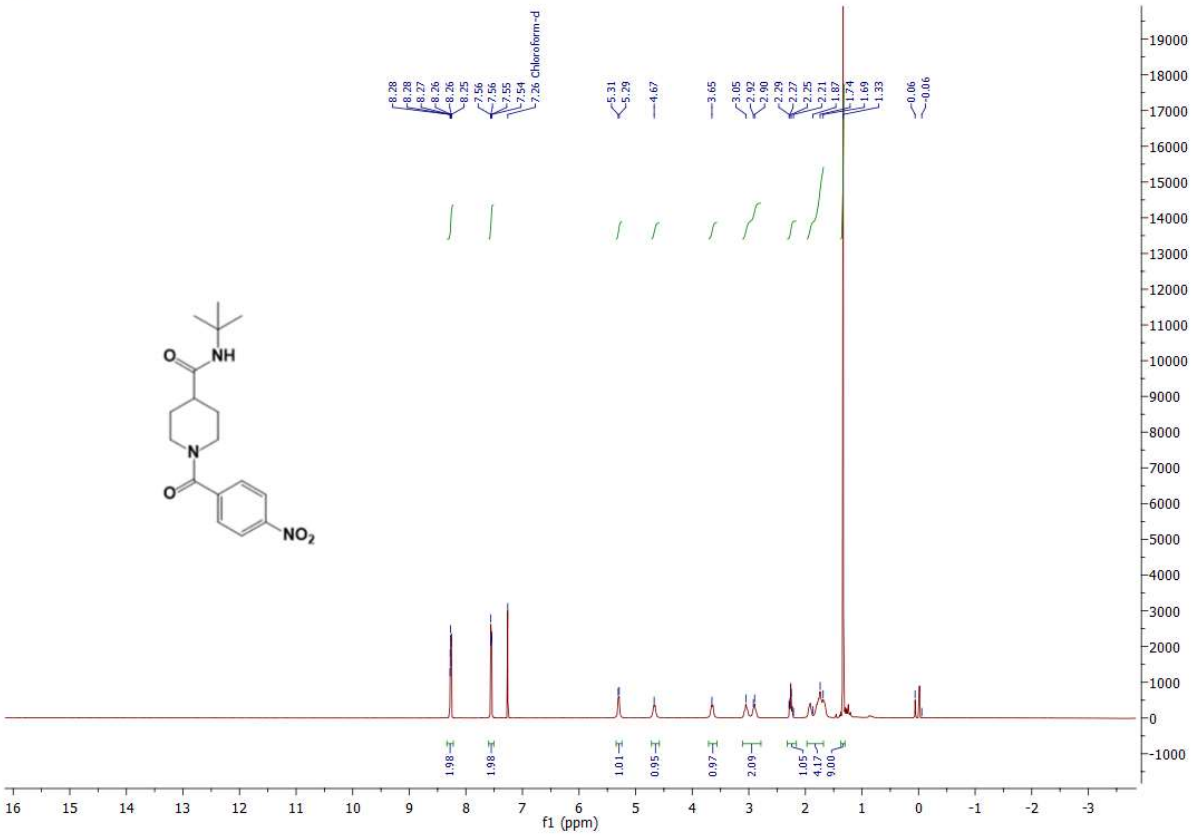


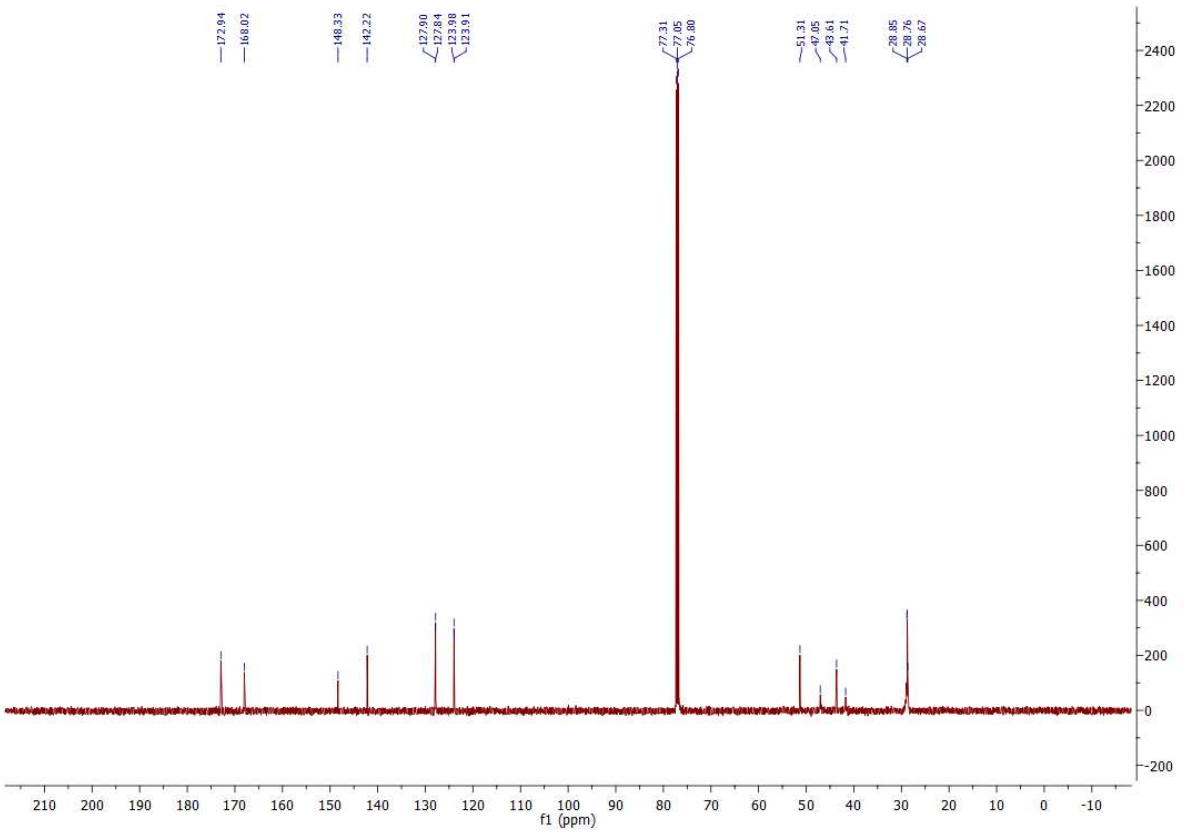


HRMS spectra of compound A24

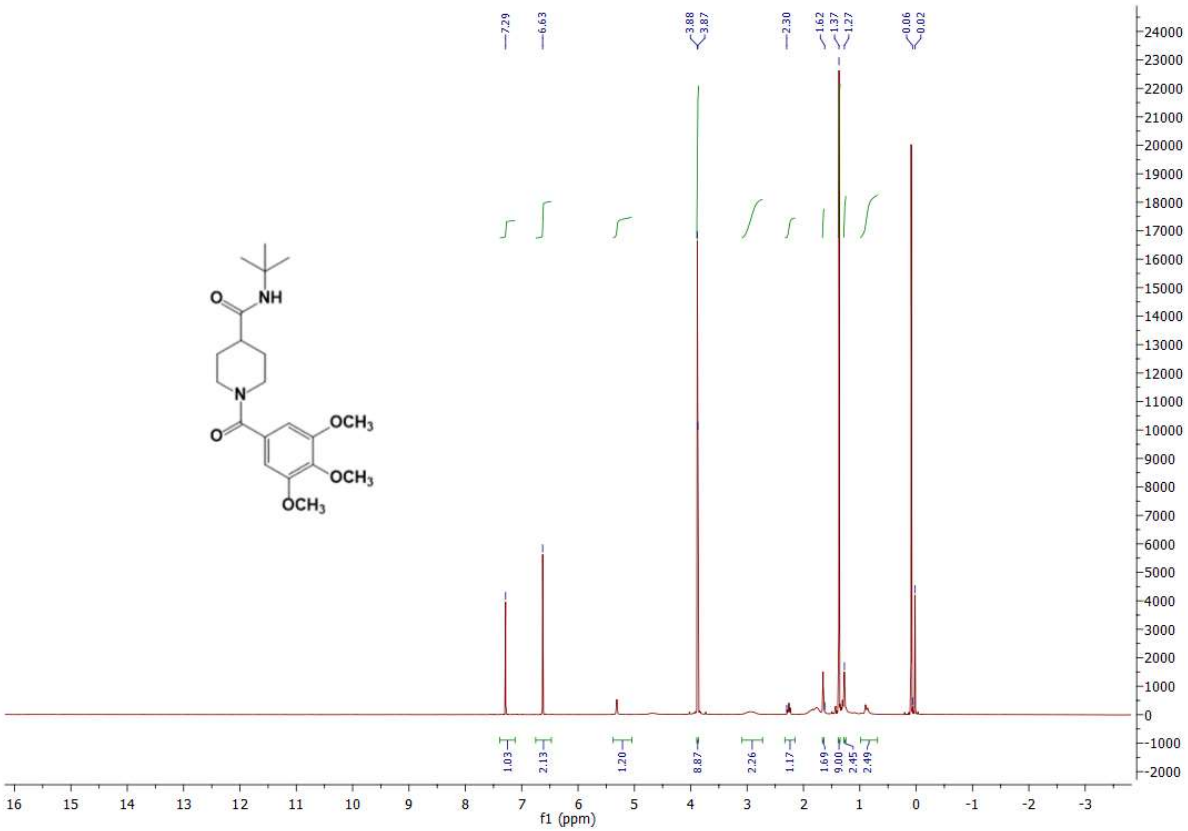


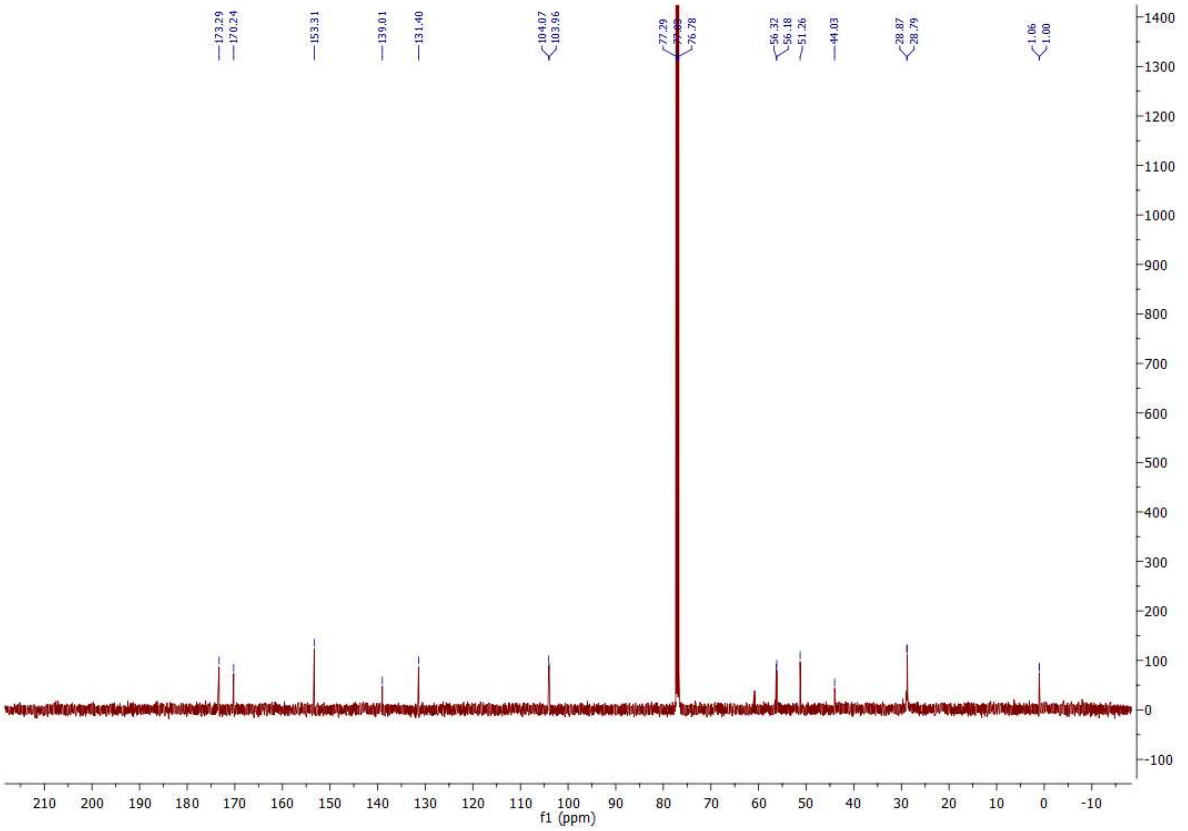
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A25



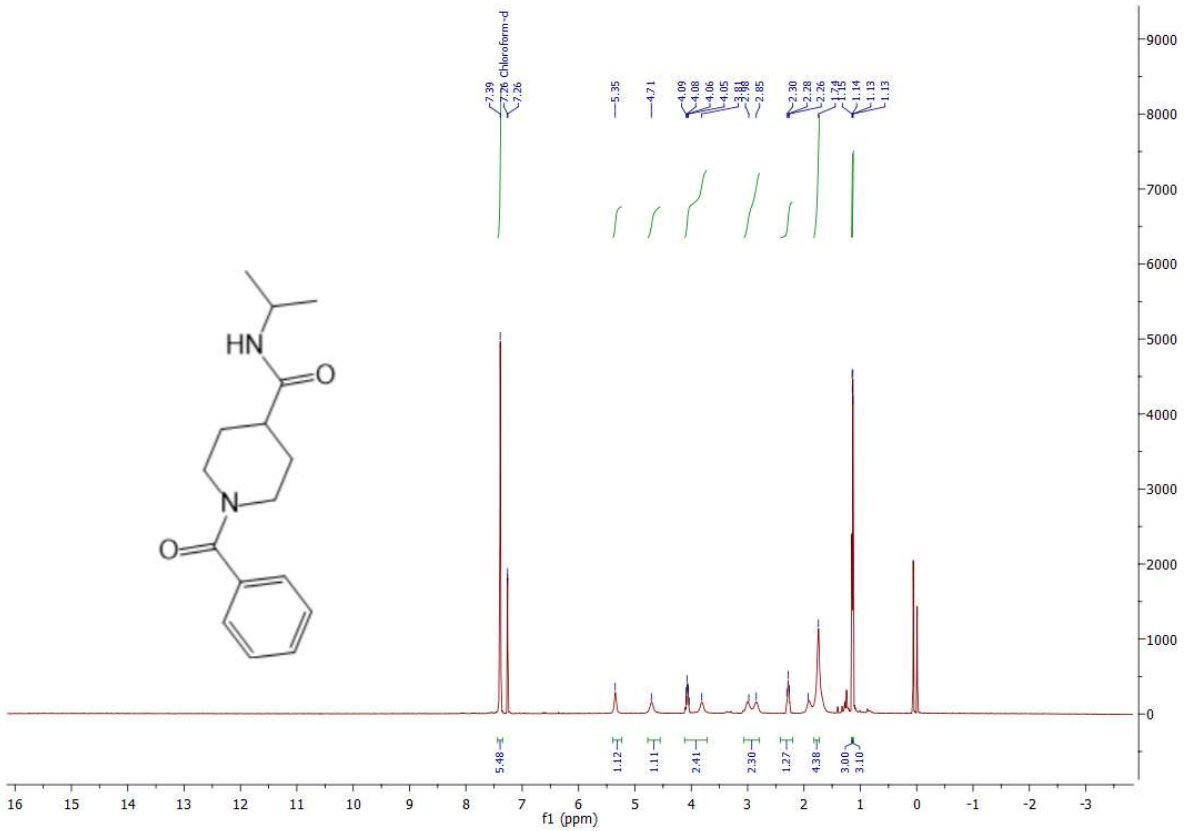


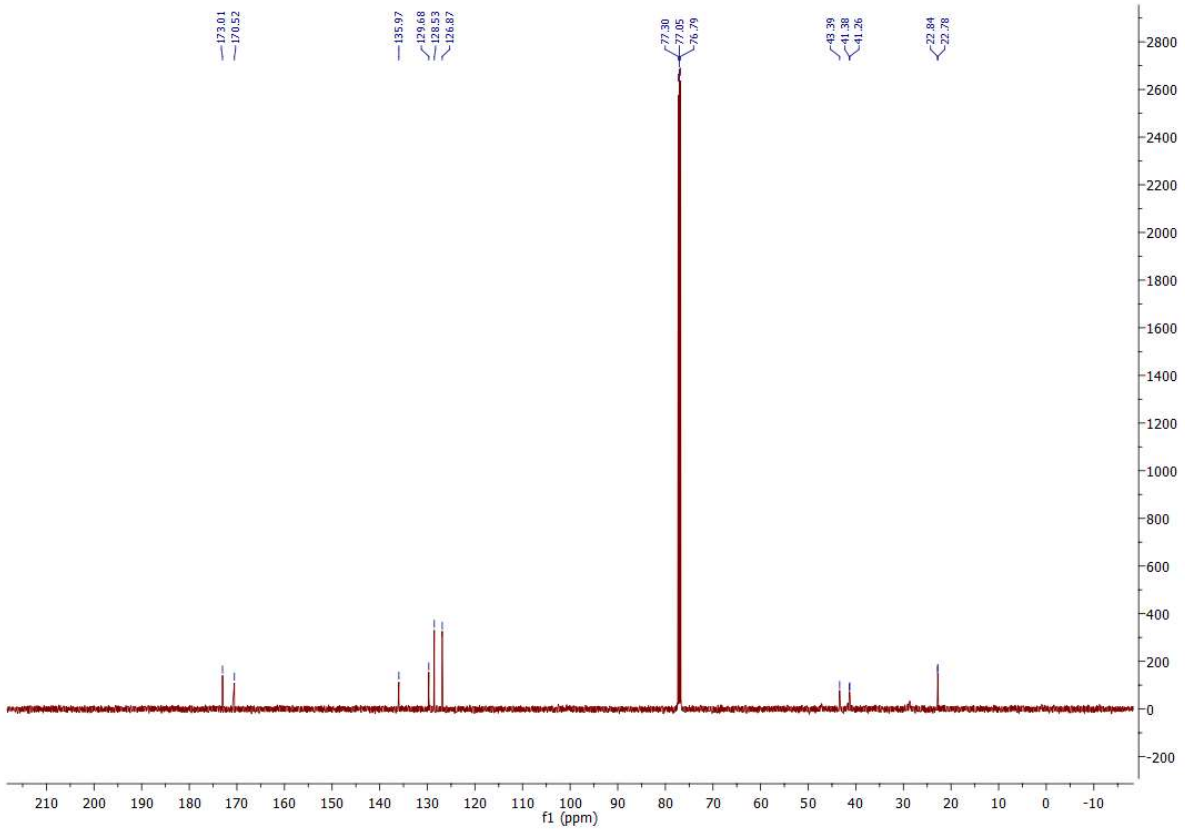
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A26



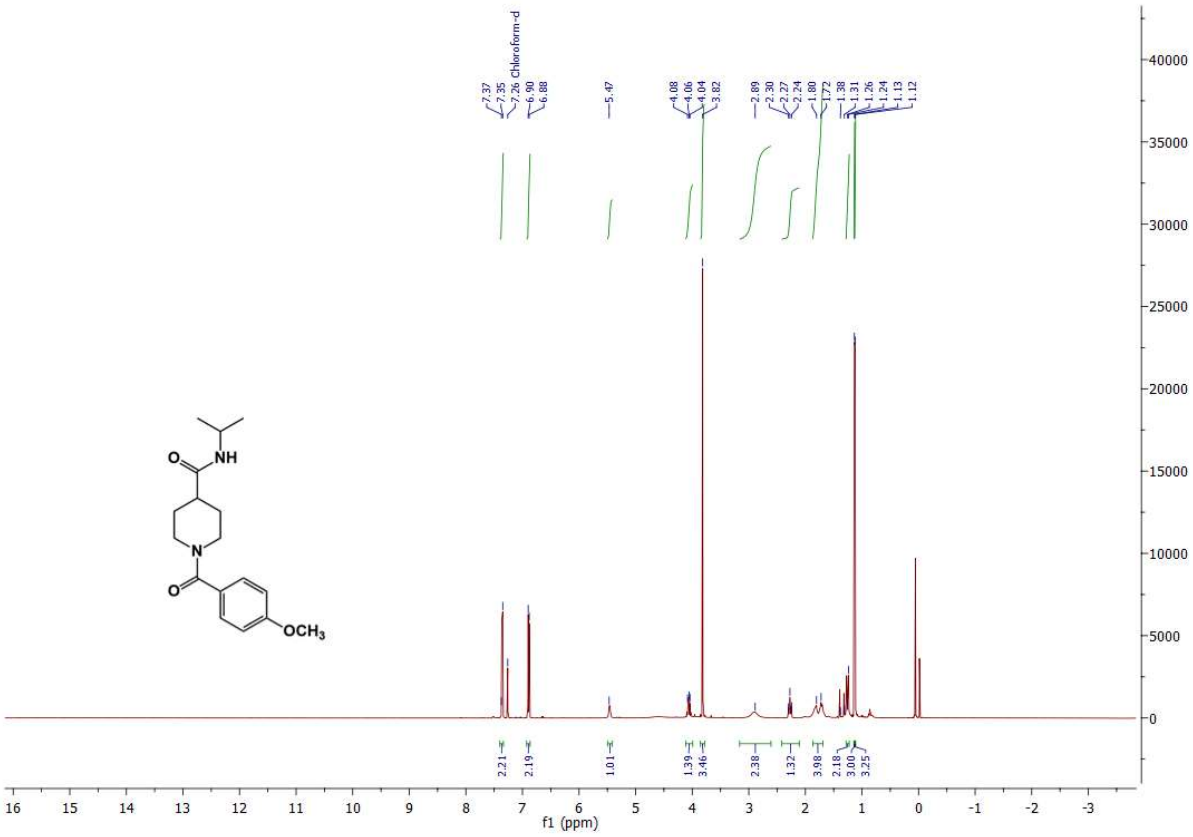


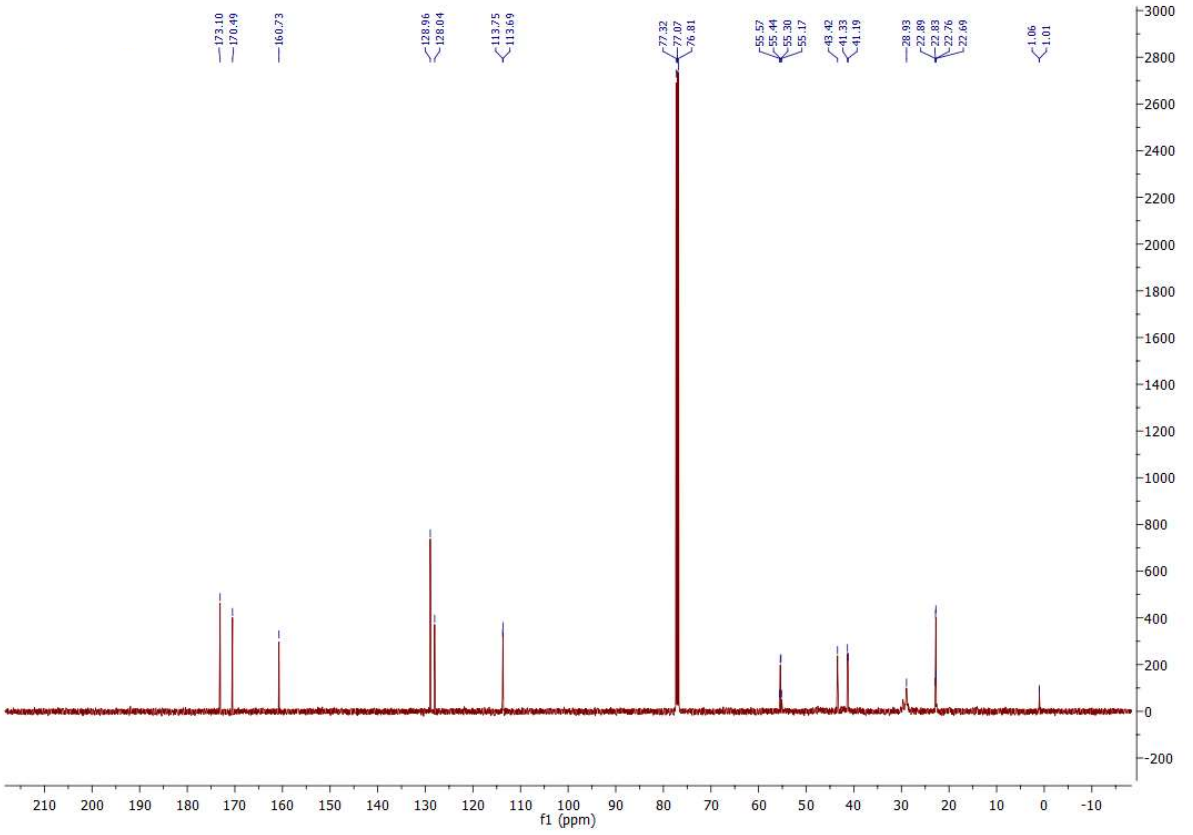
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A27



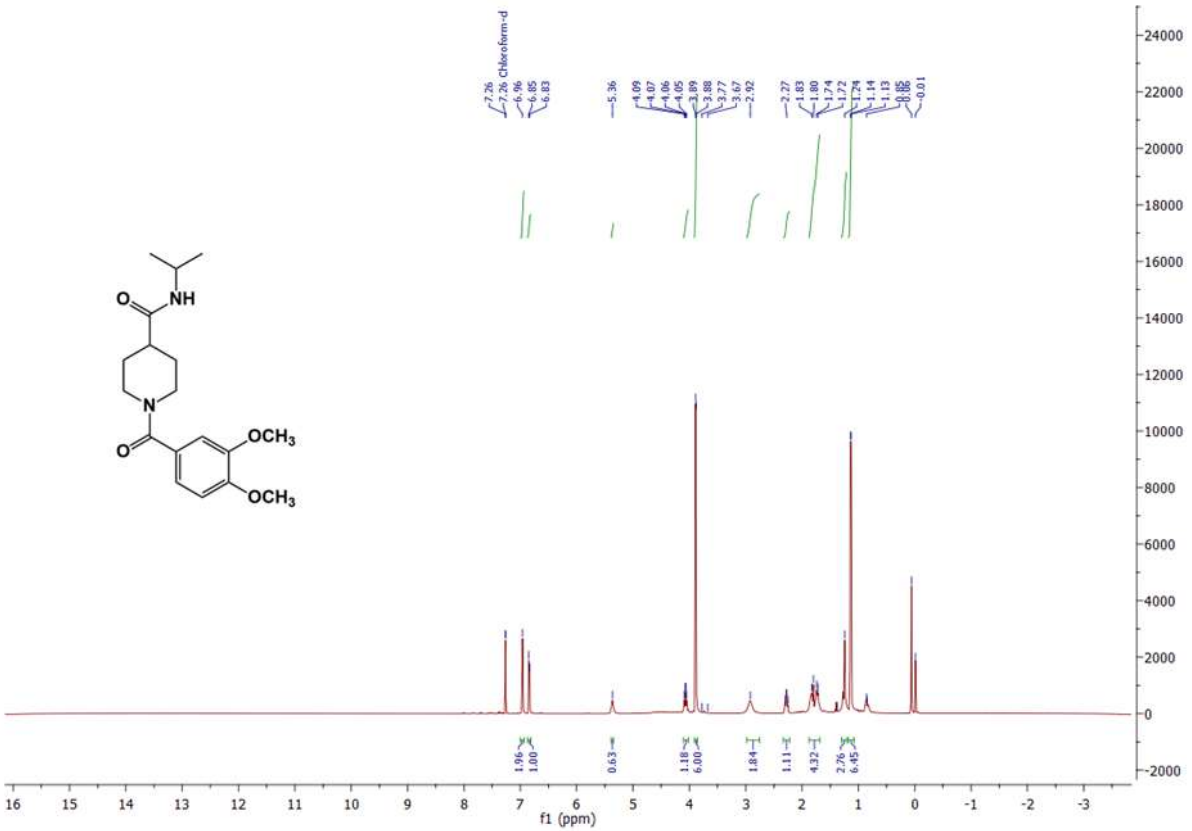


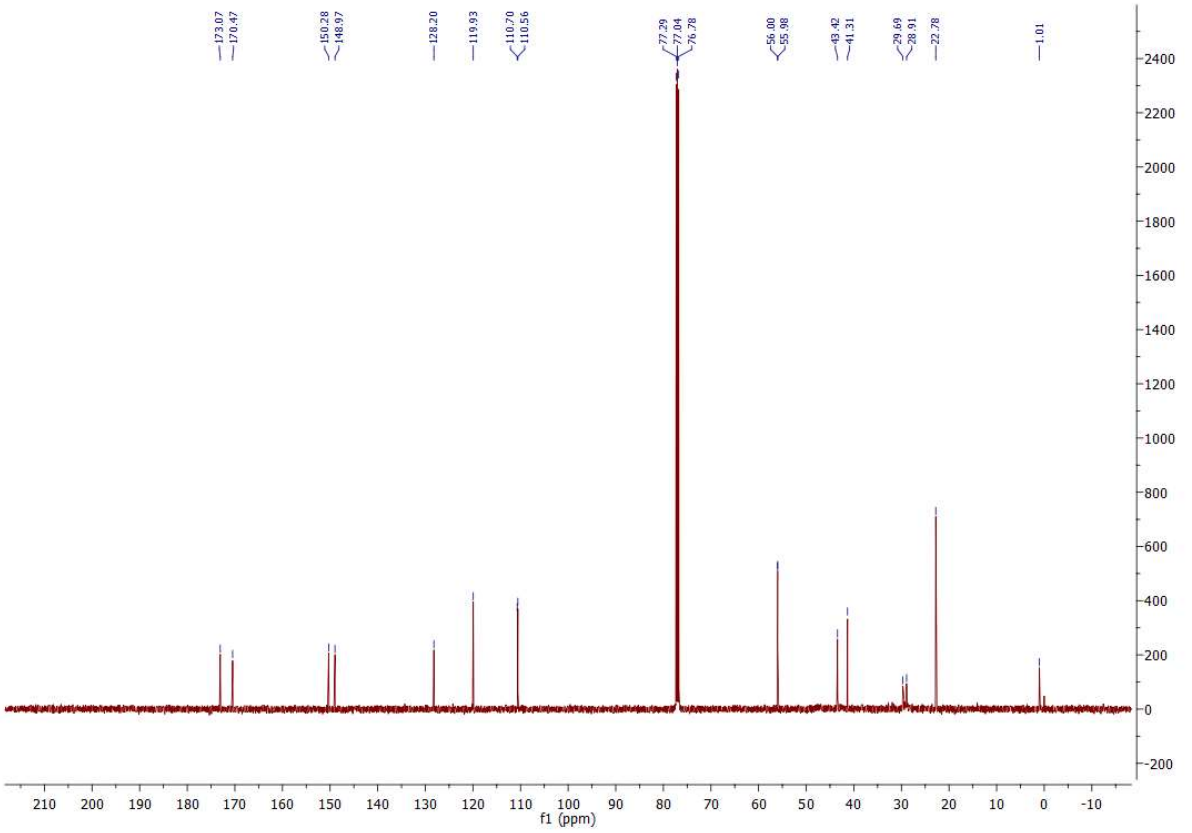
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A28



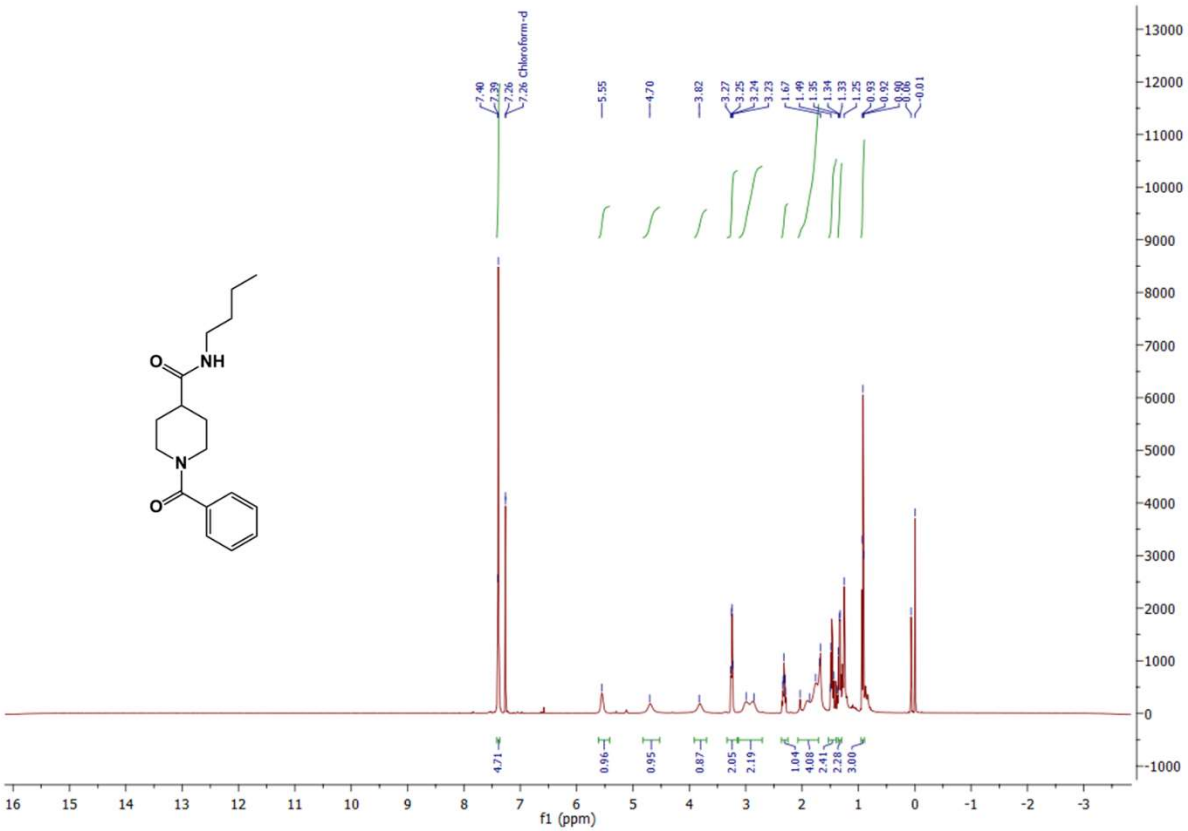


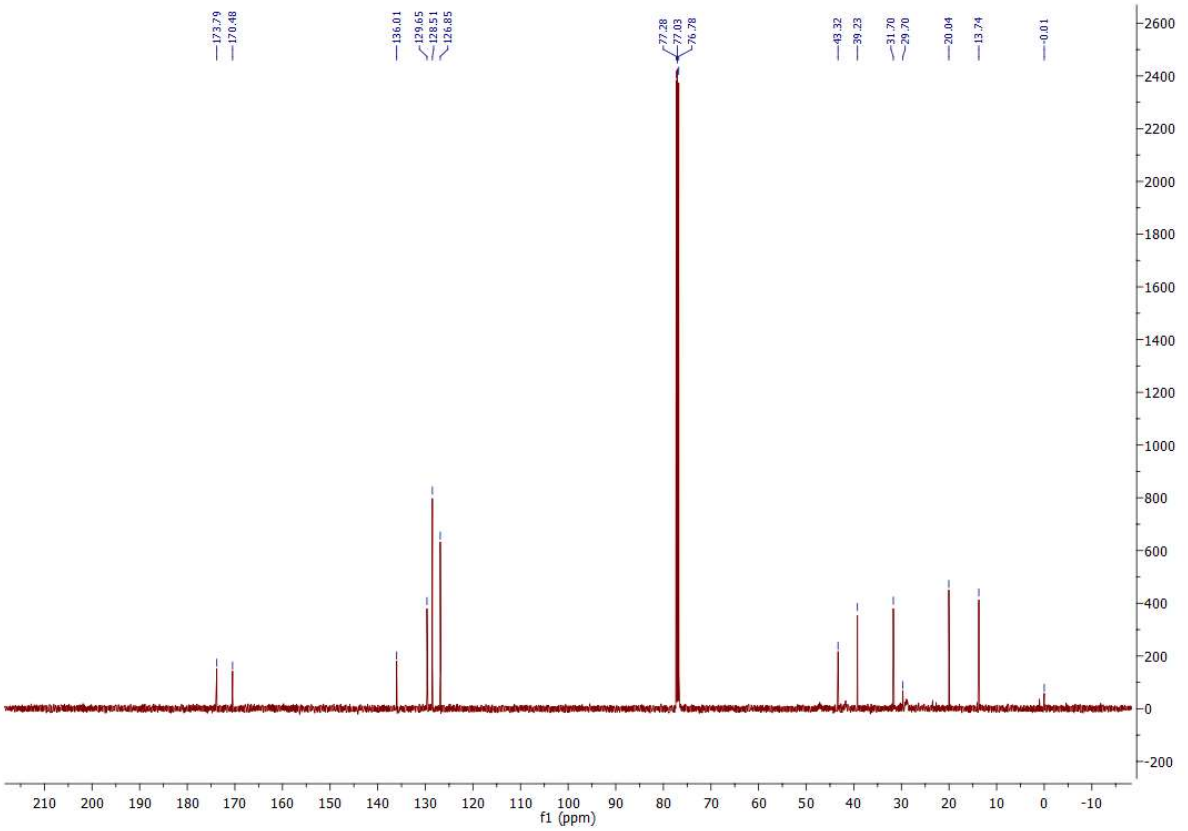
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A29



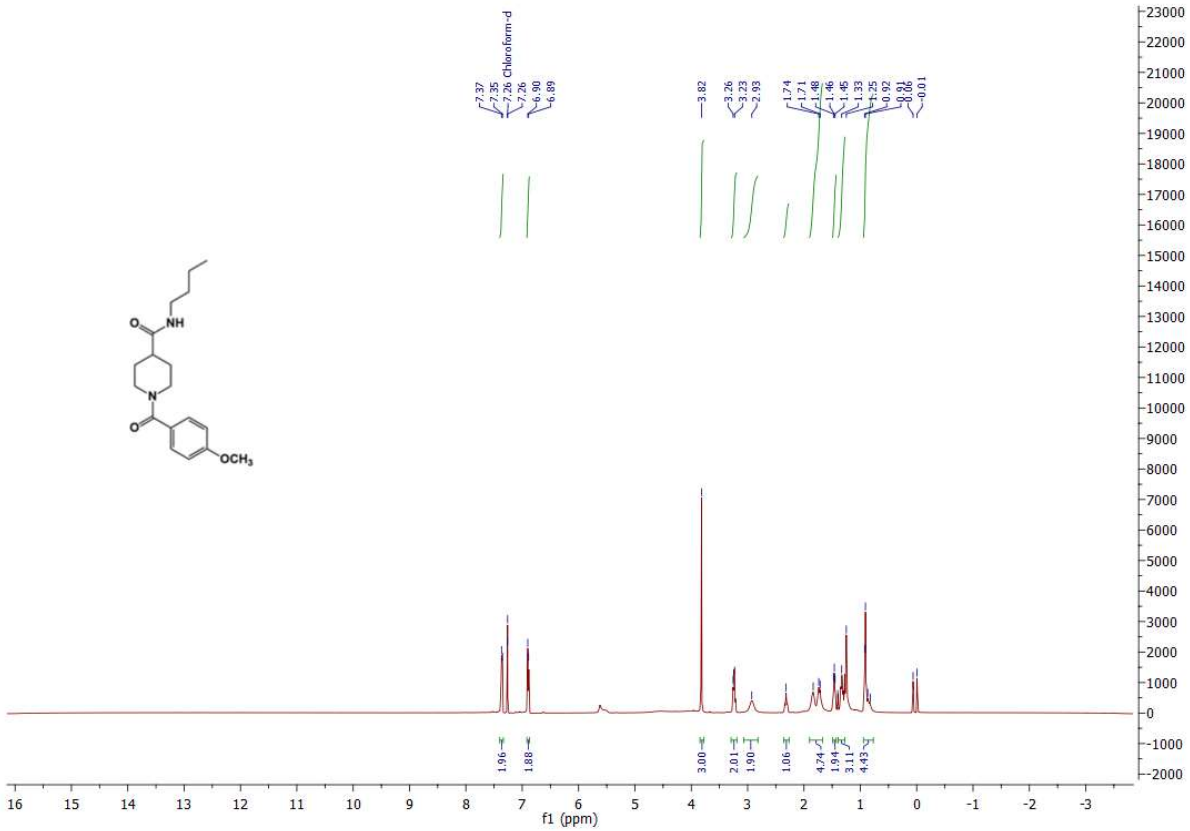


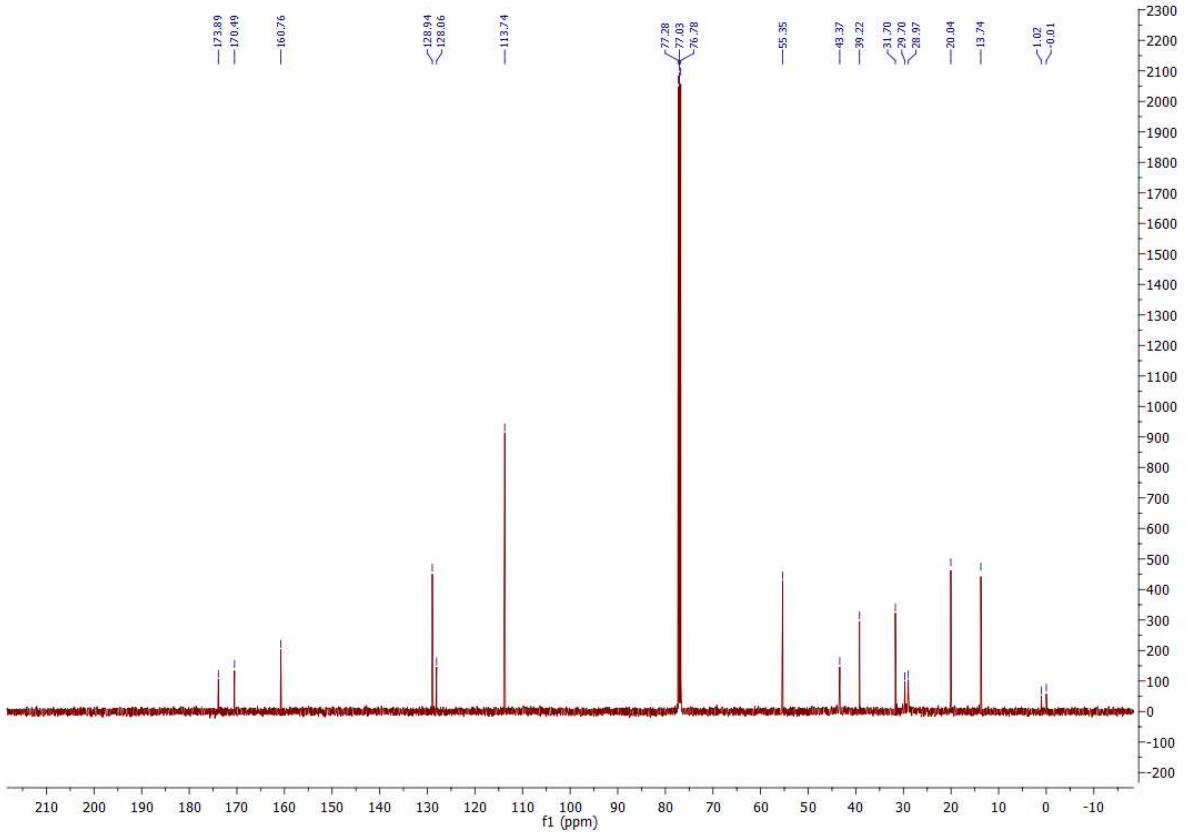
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A30



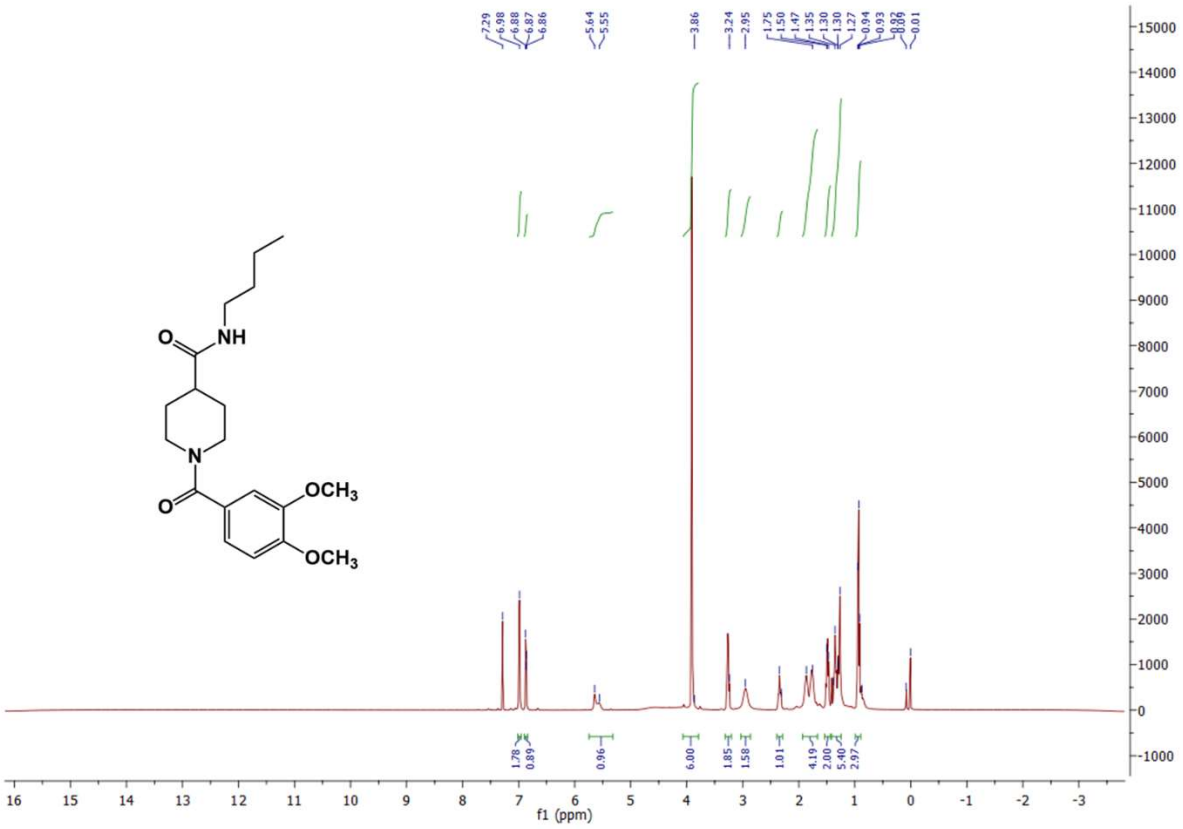


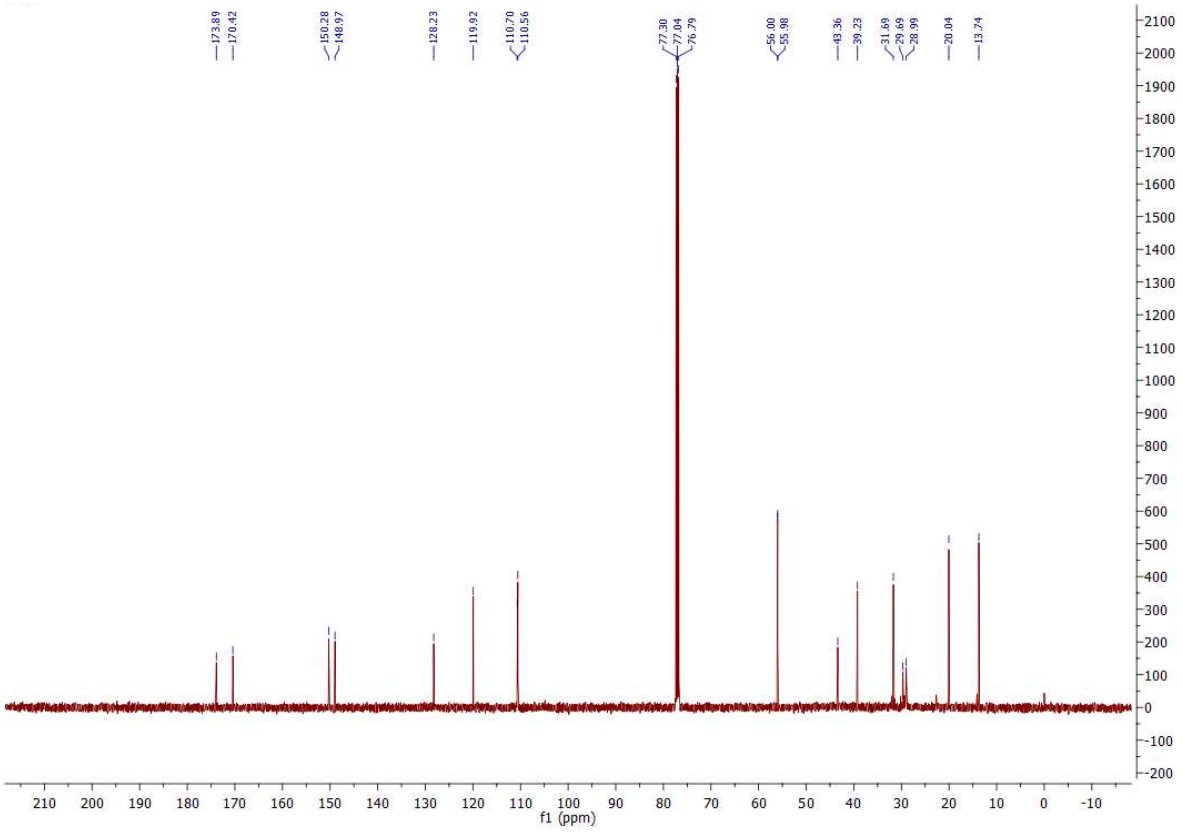
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A31



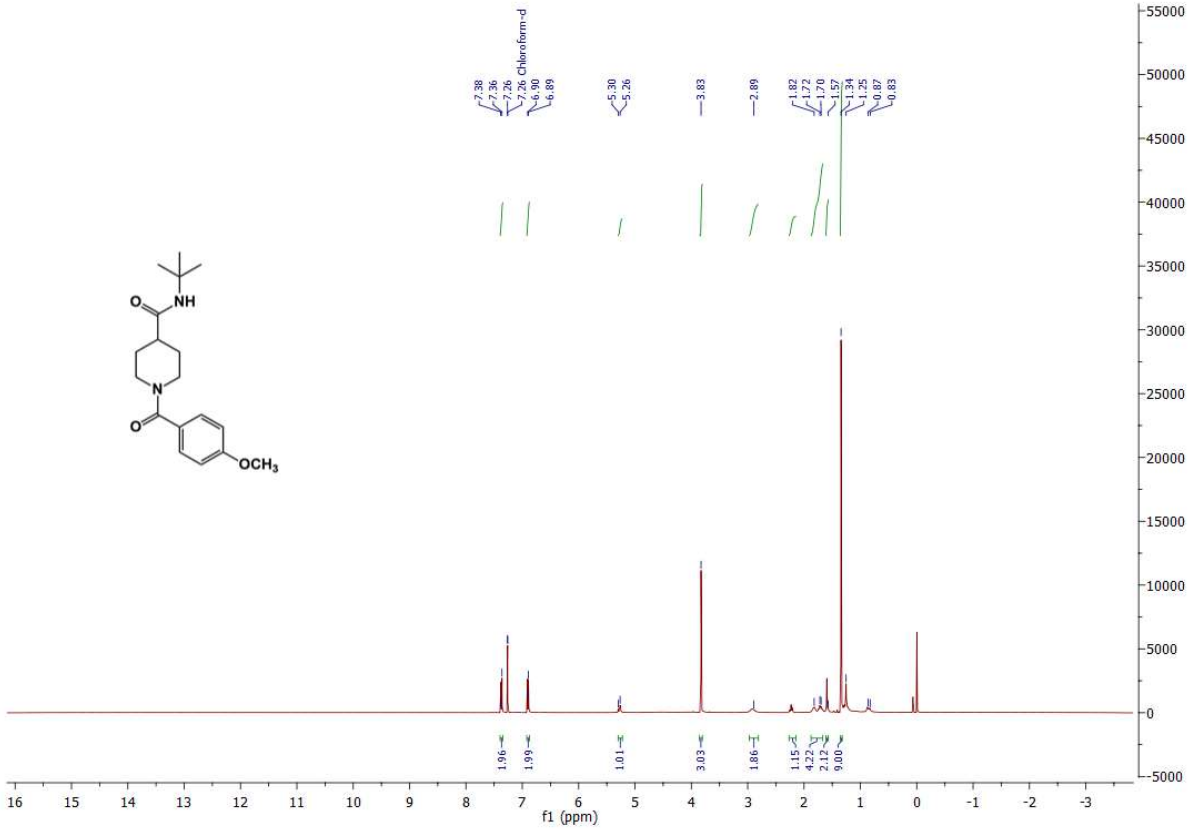


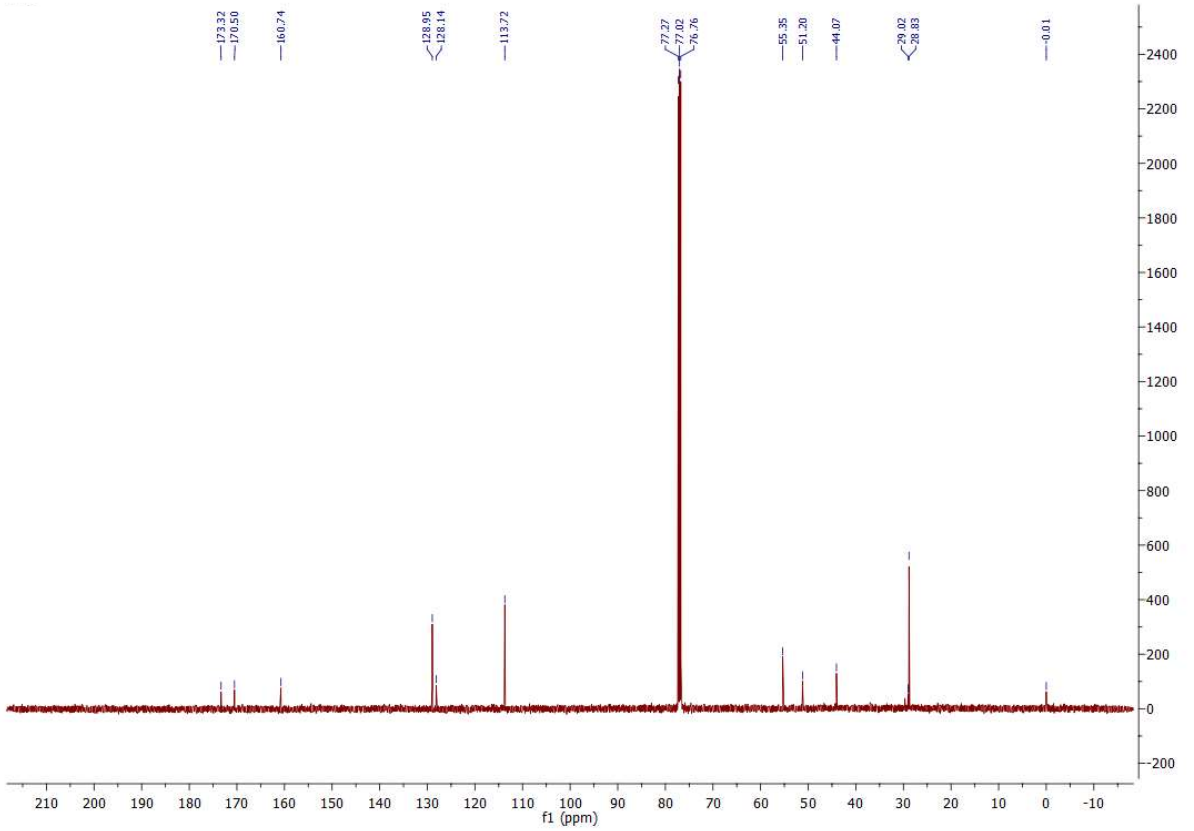
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A32



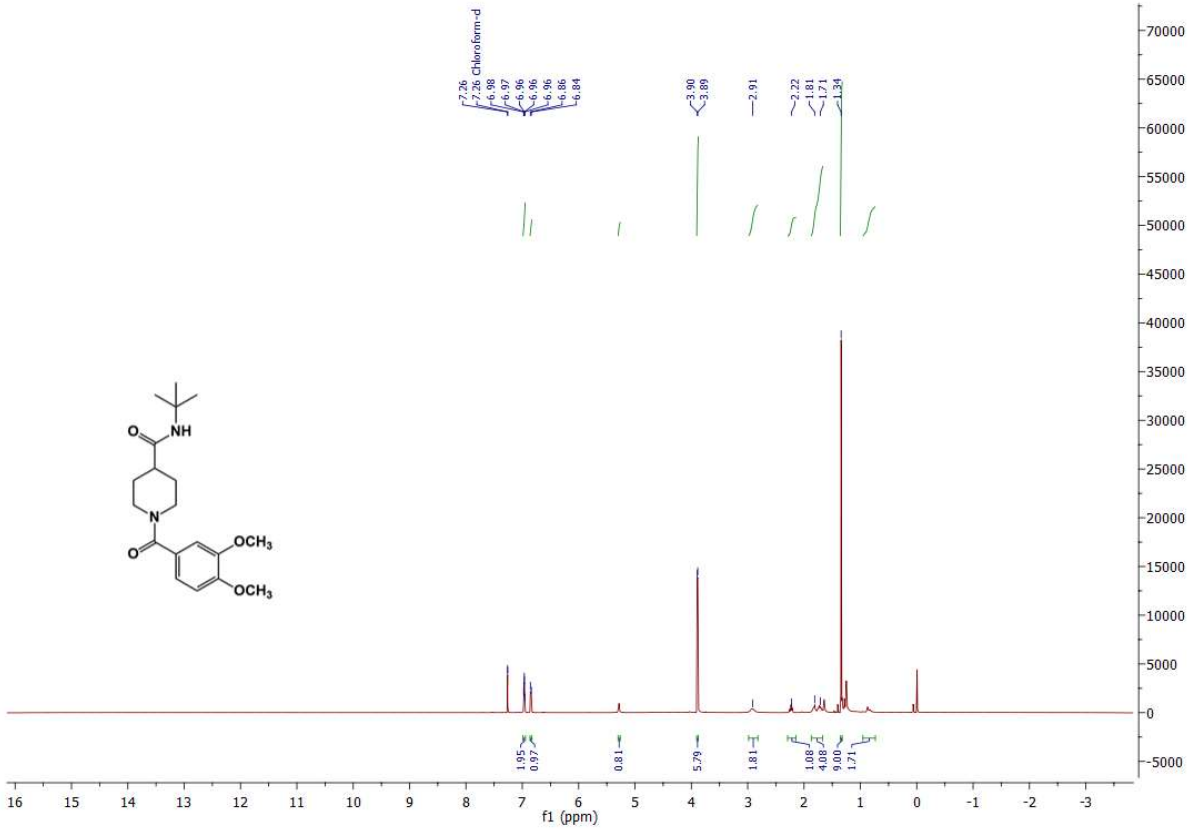


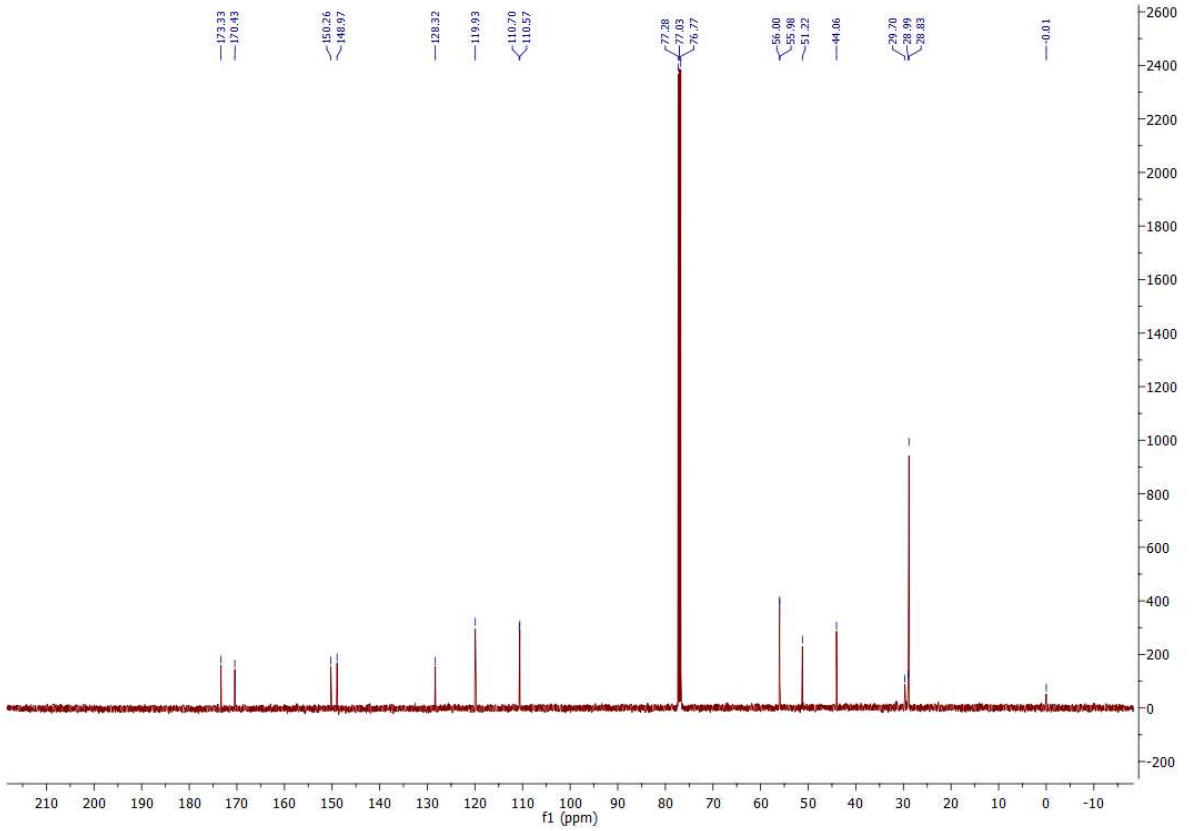
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A33



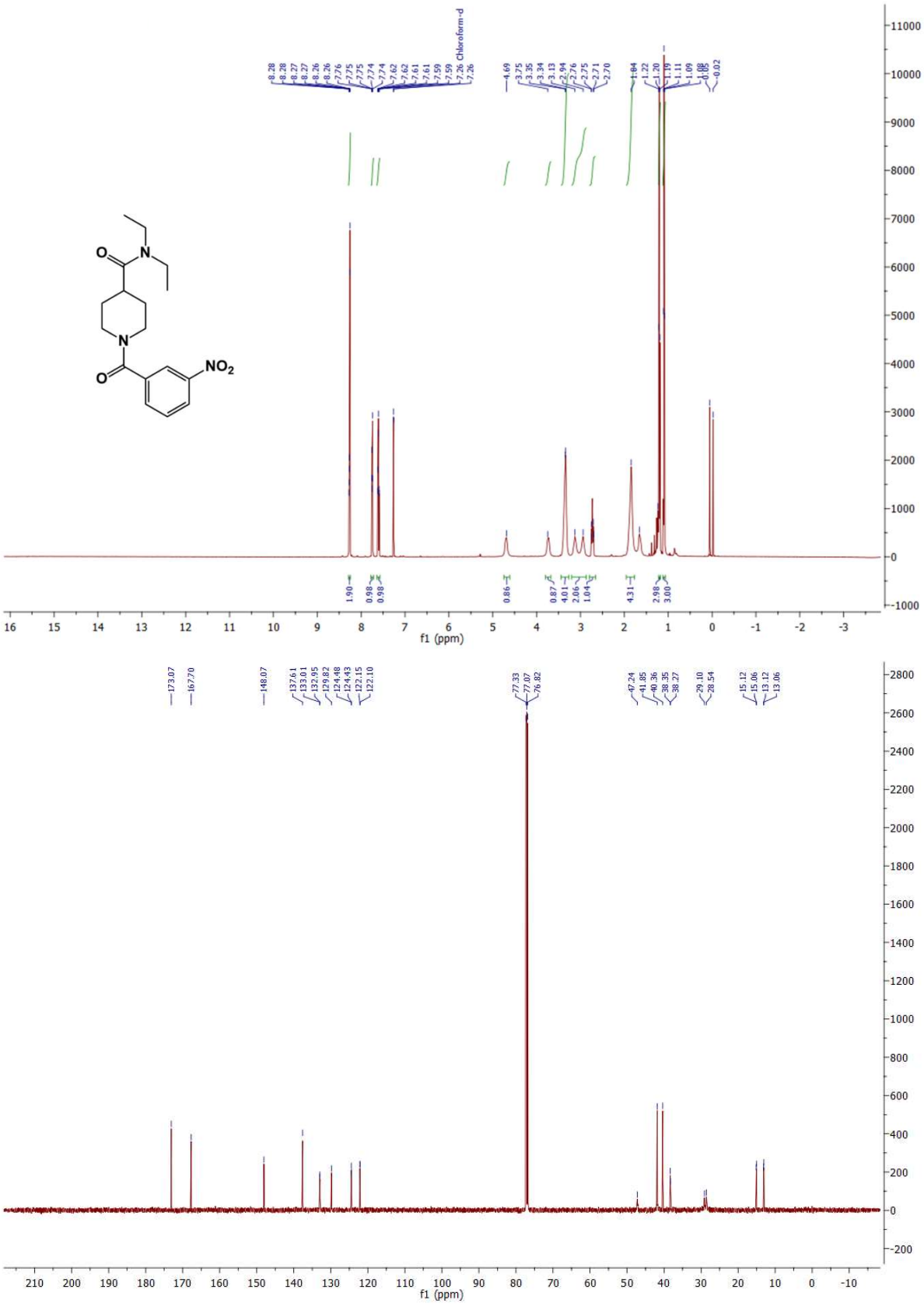


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A34

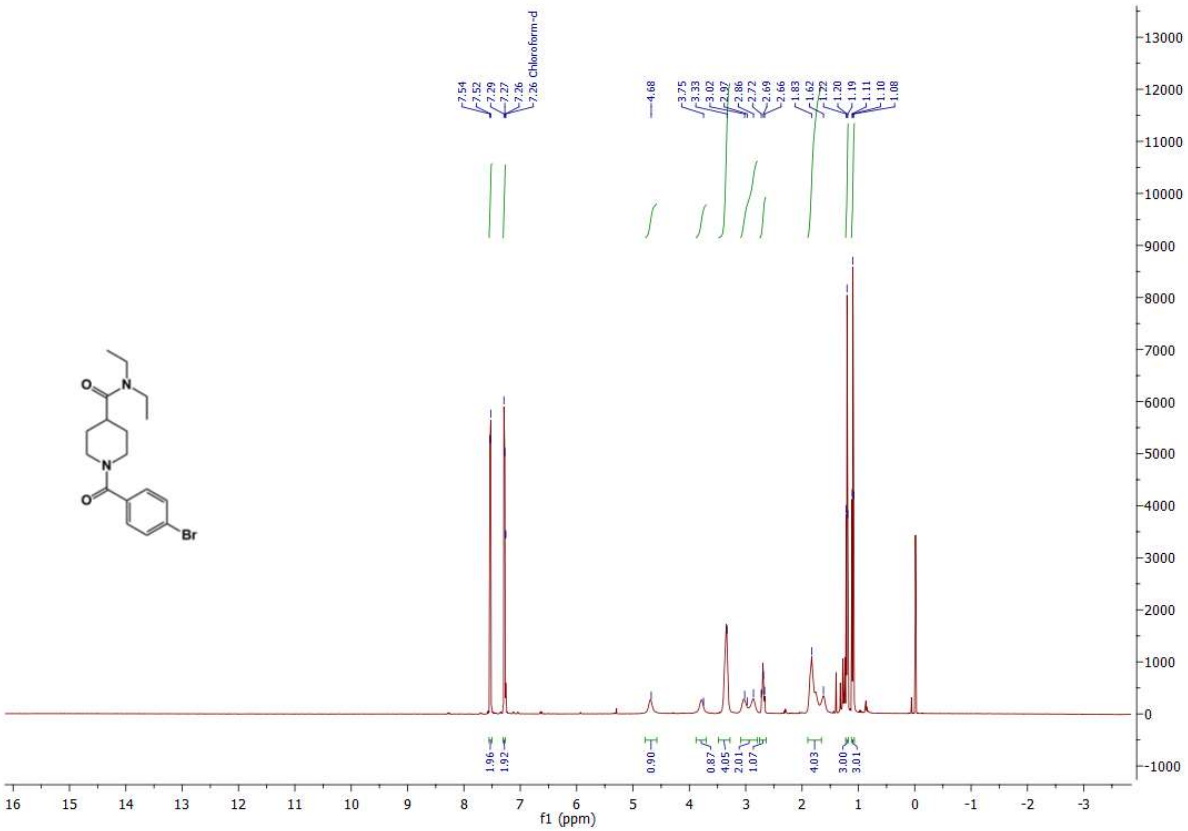


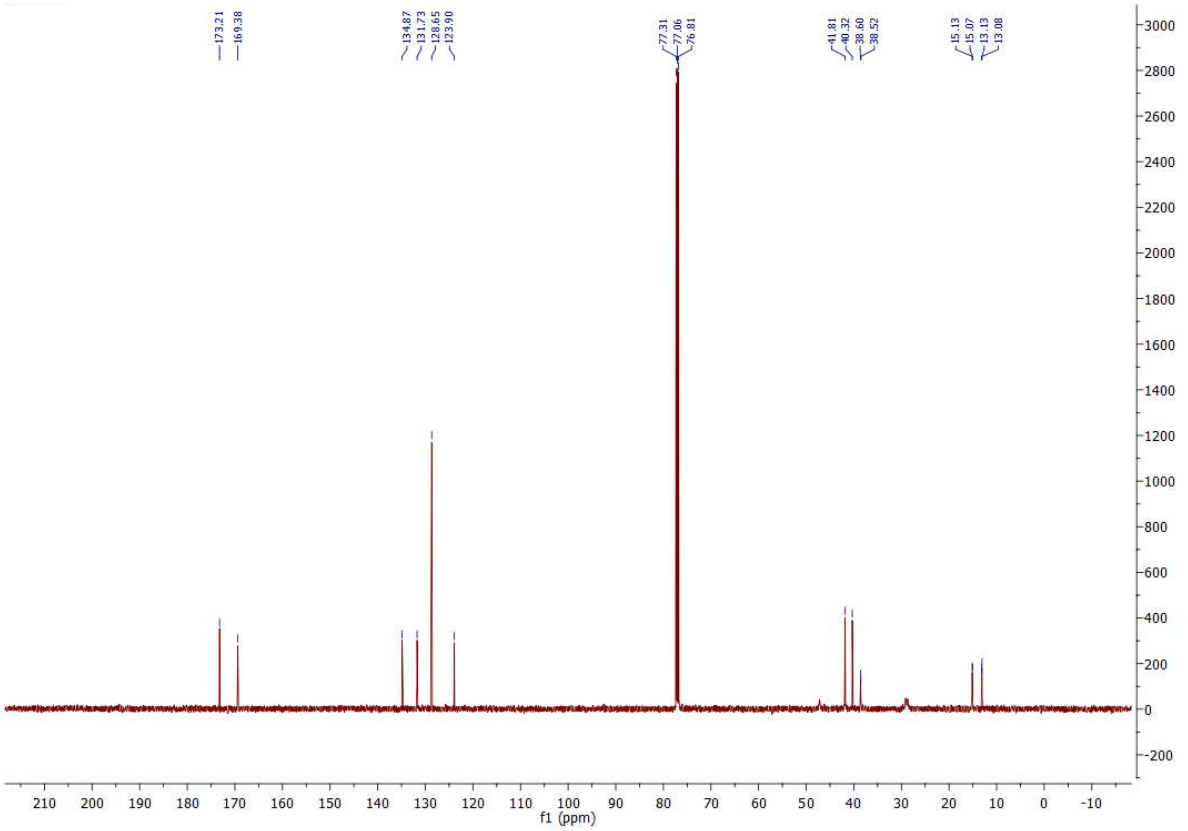


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A35

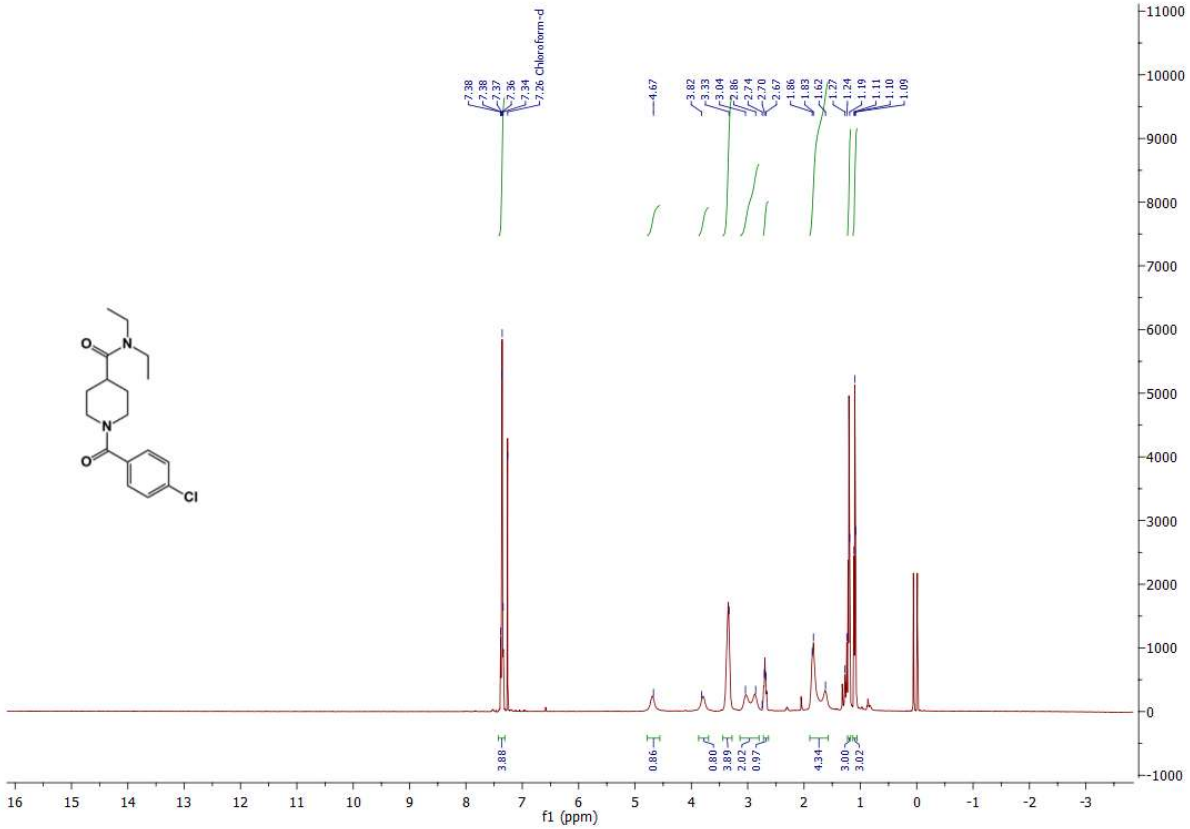


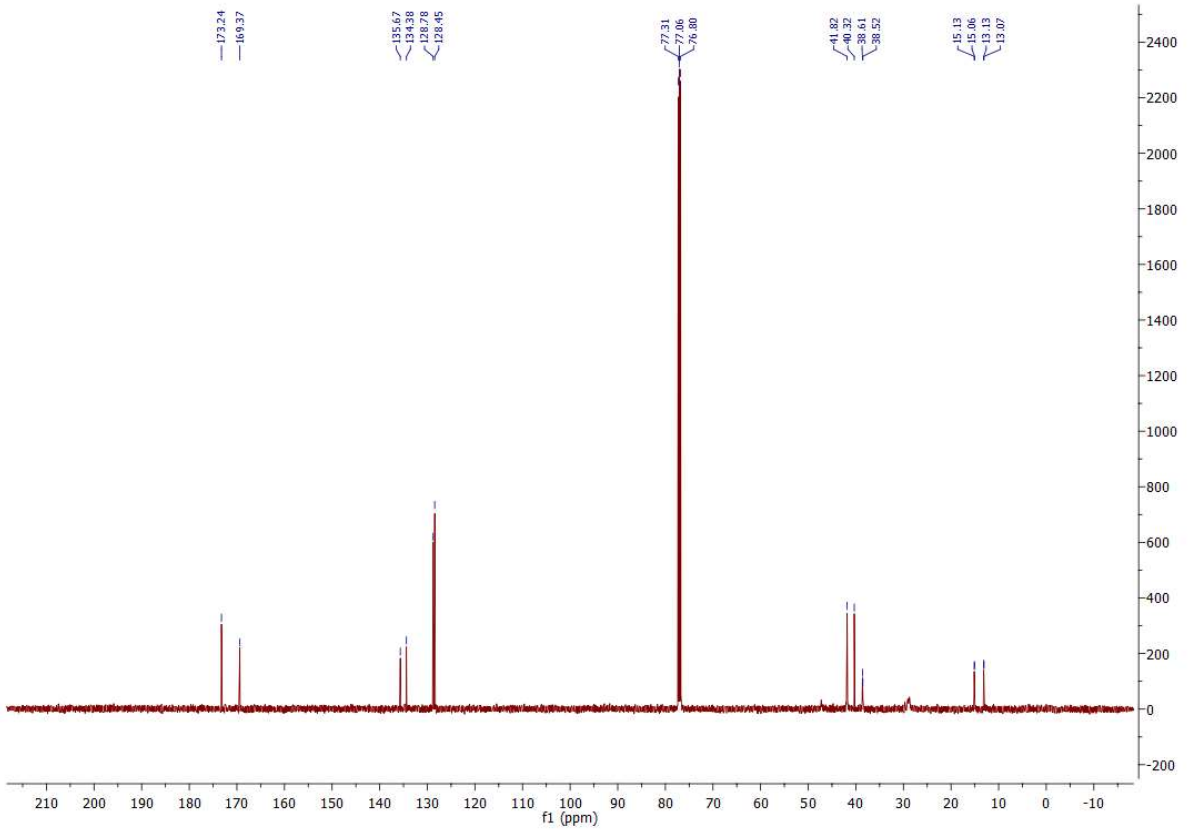
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A36



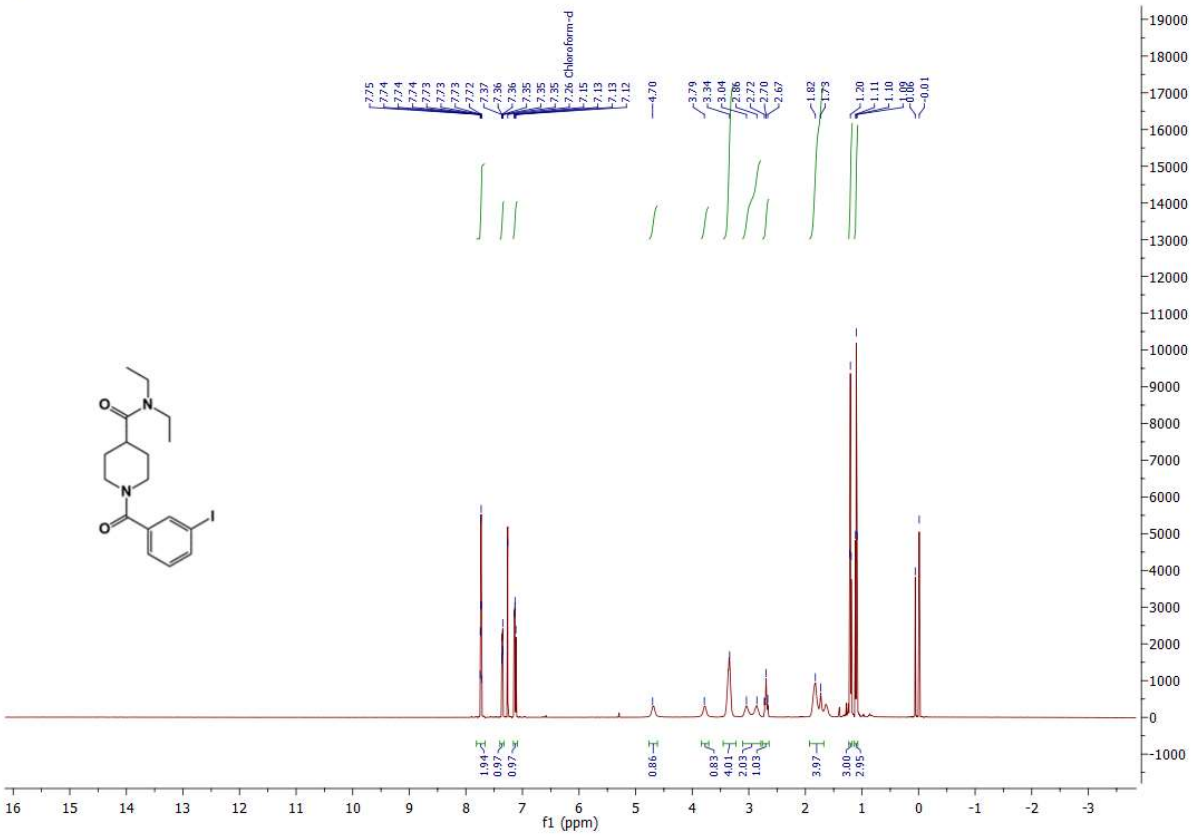


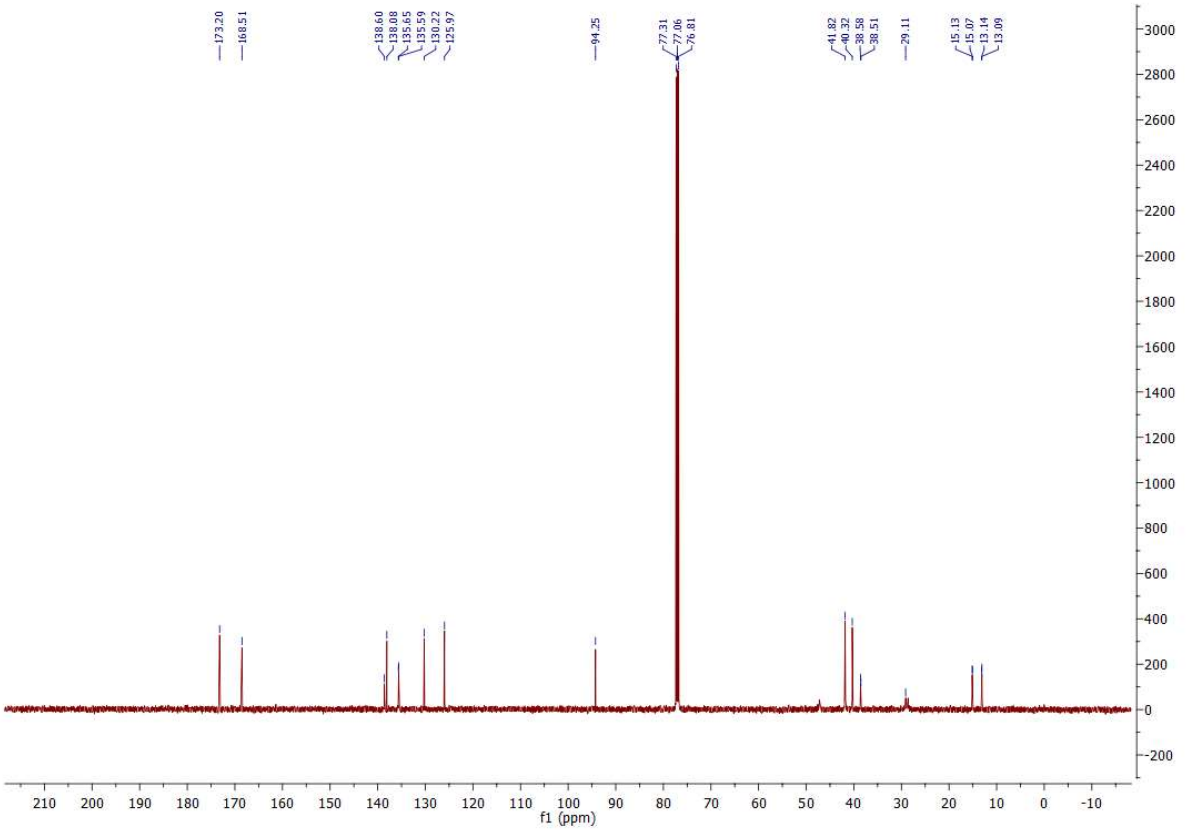
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A37



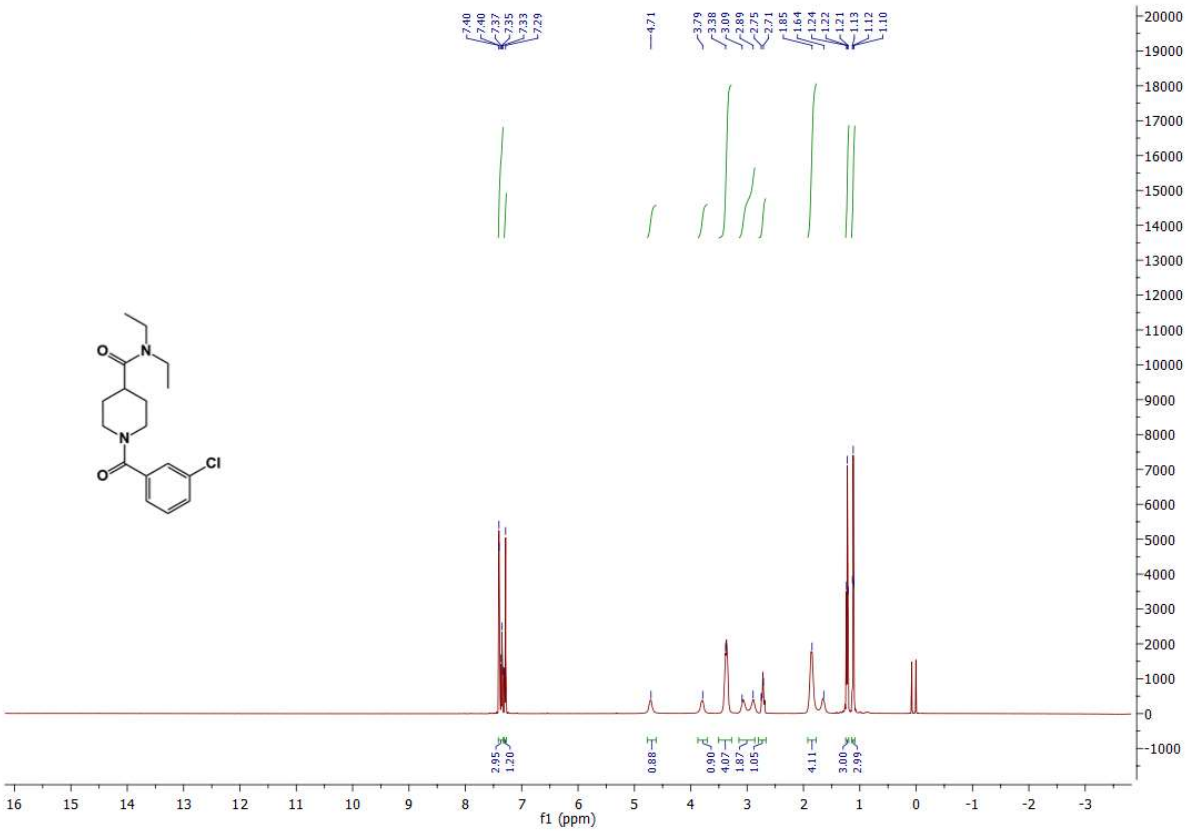


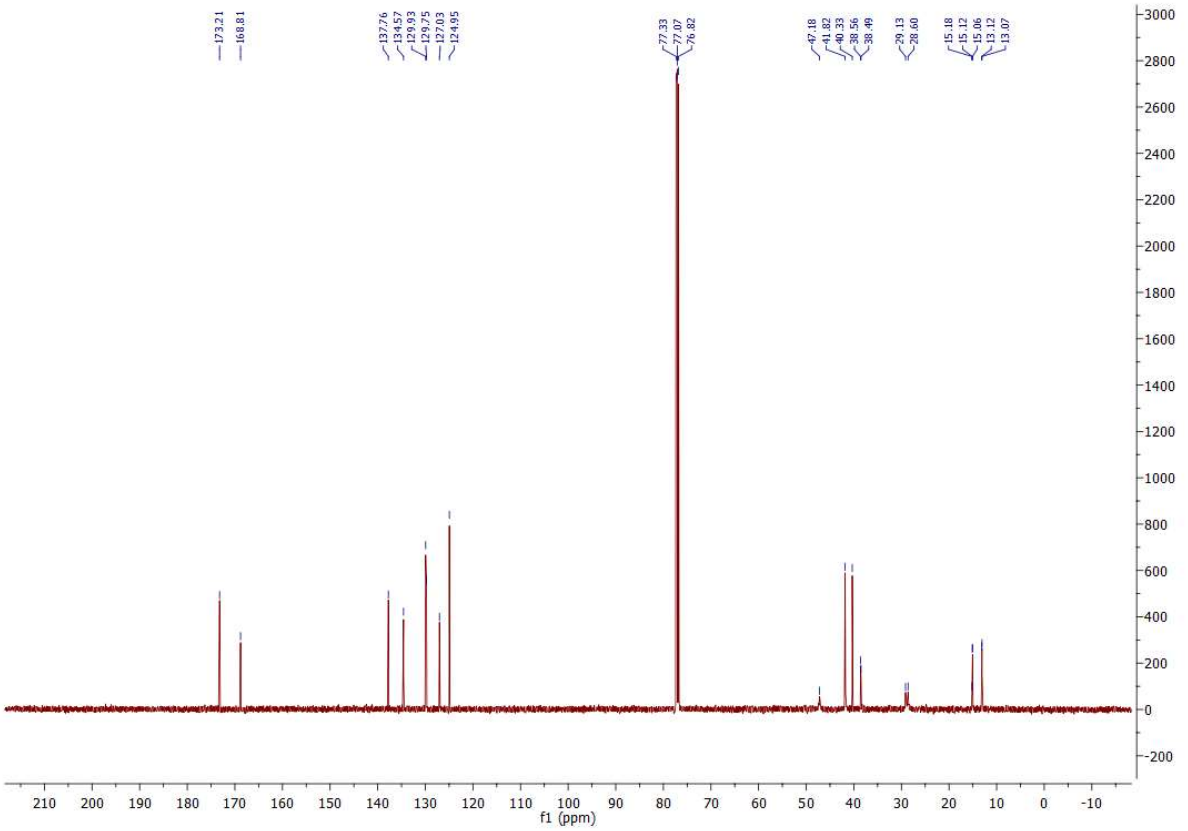
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A38



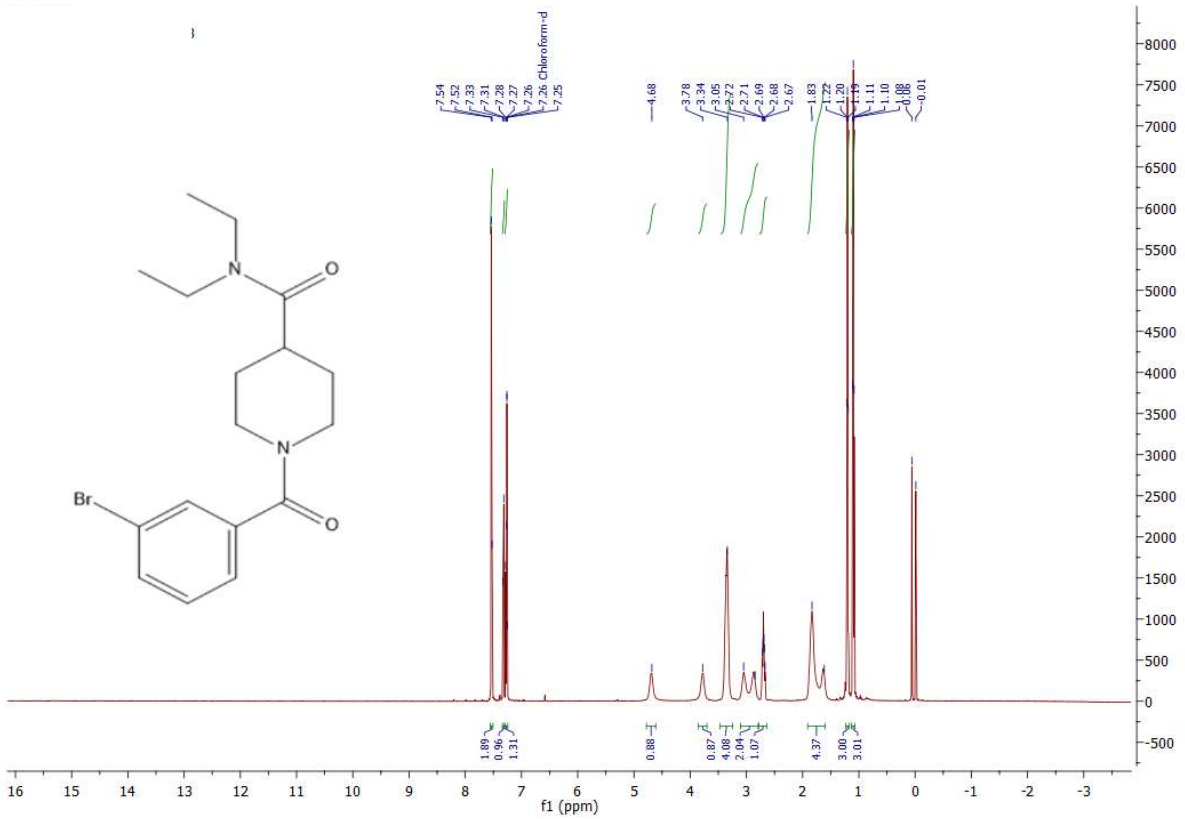


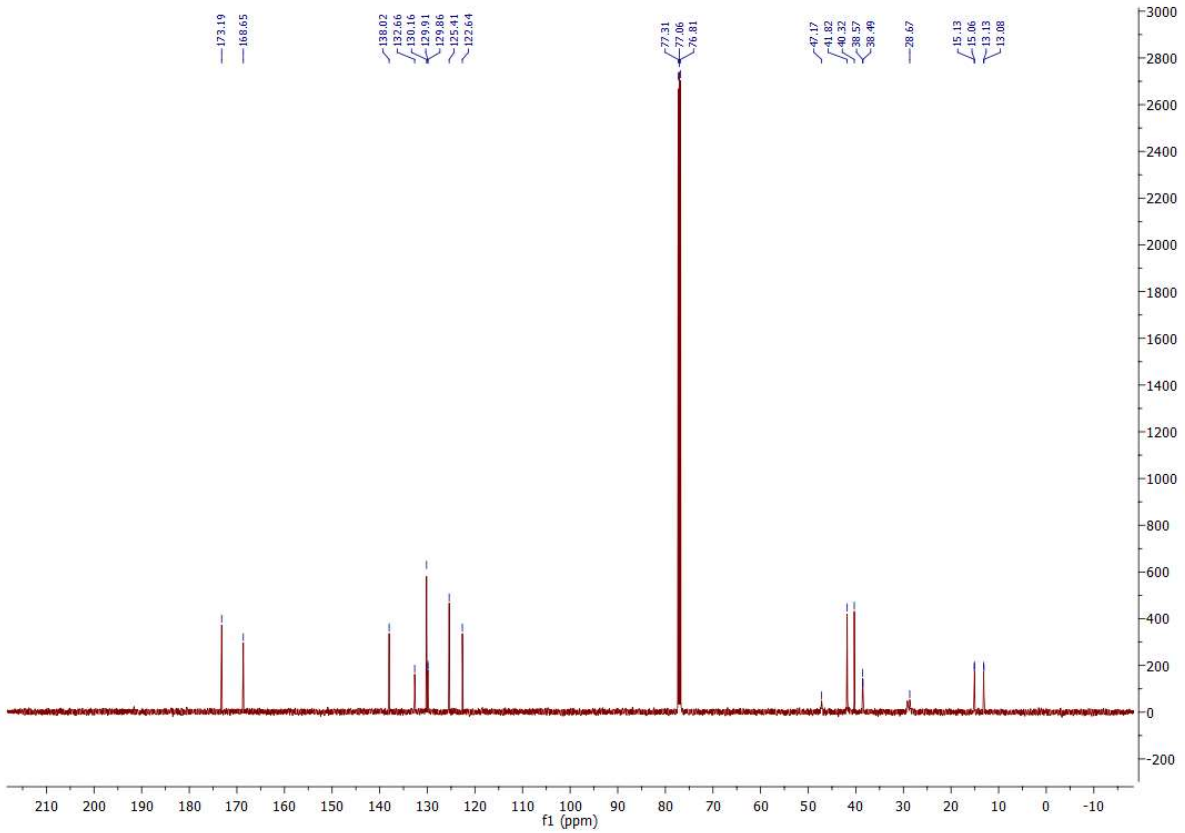
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A39



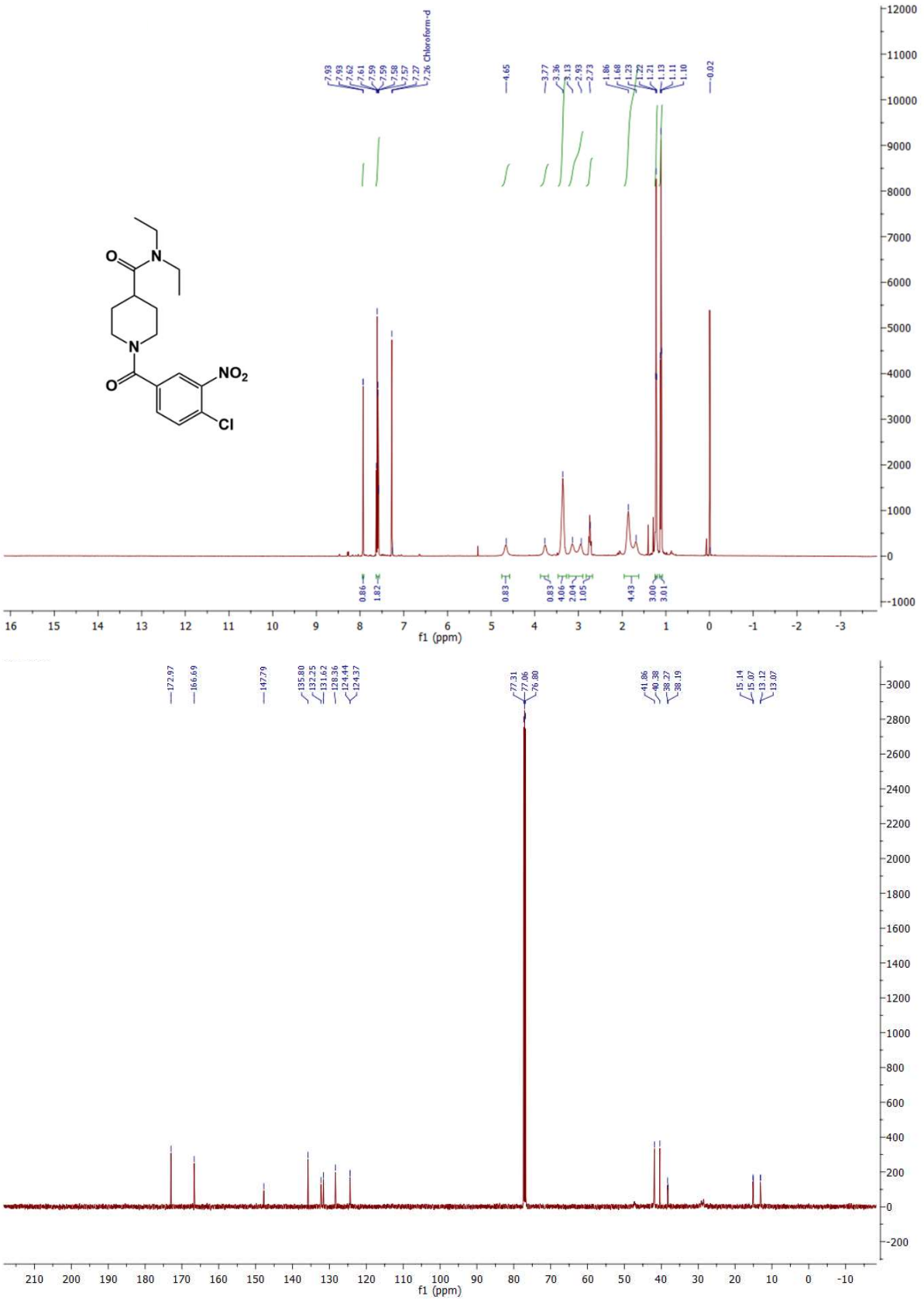


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A40

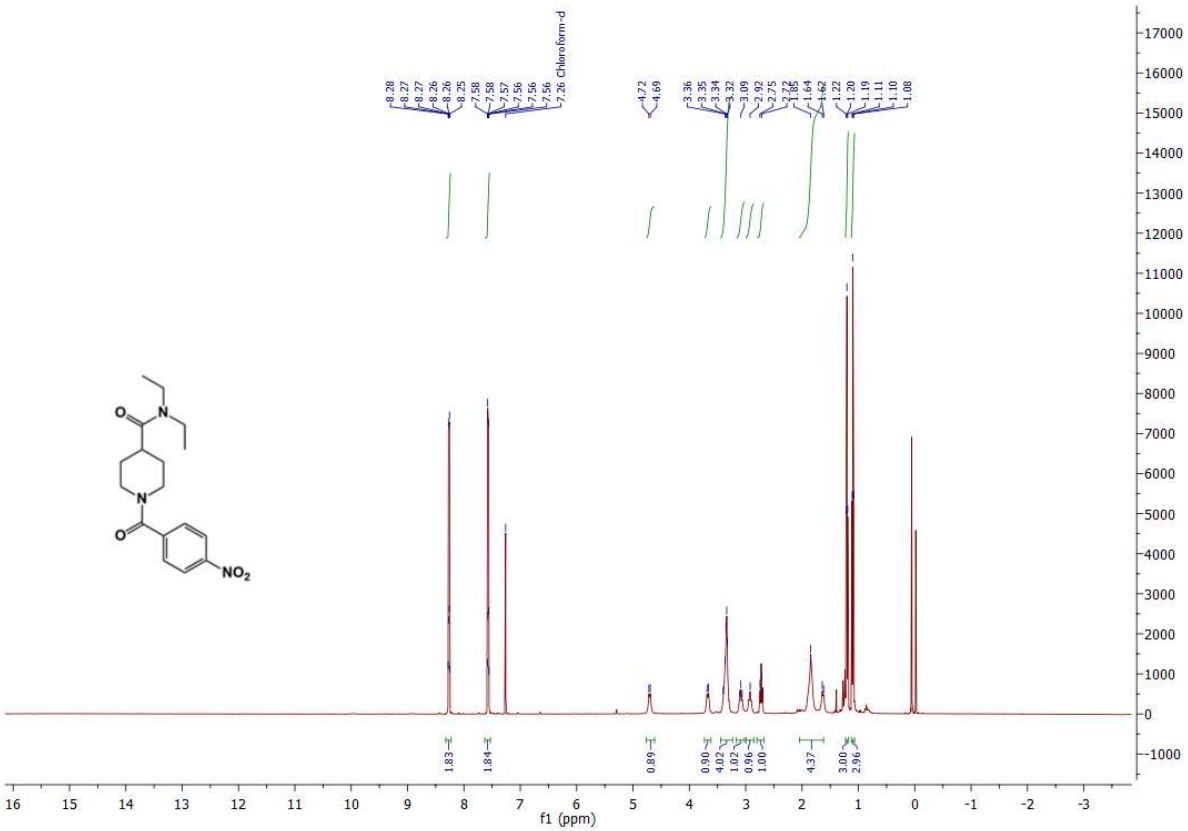


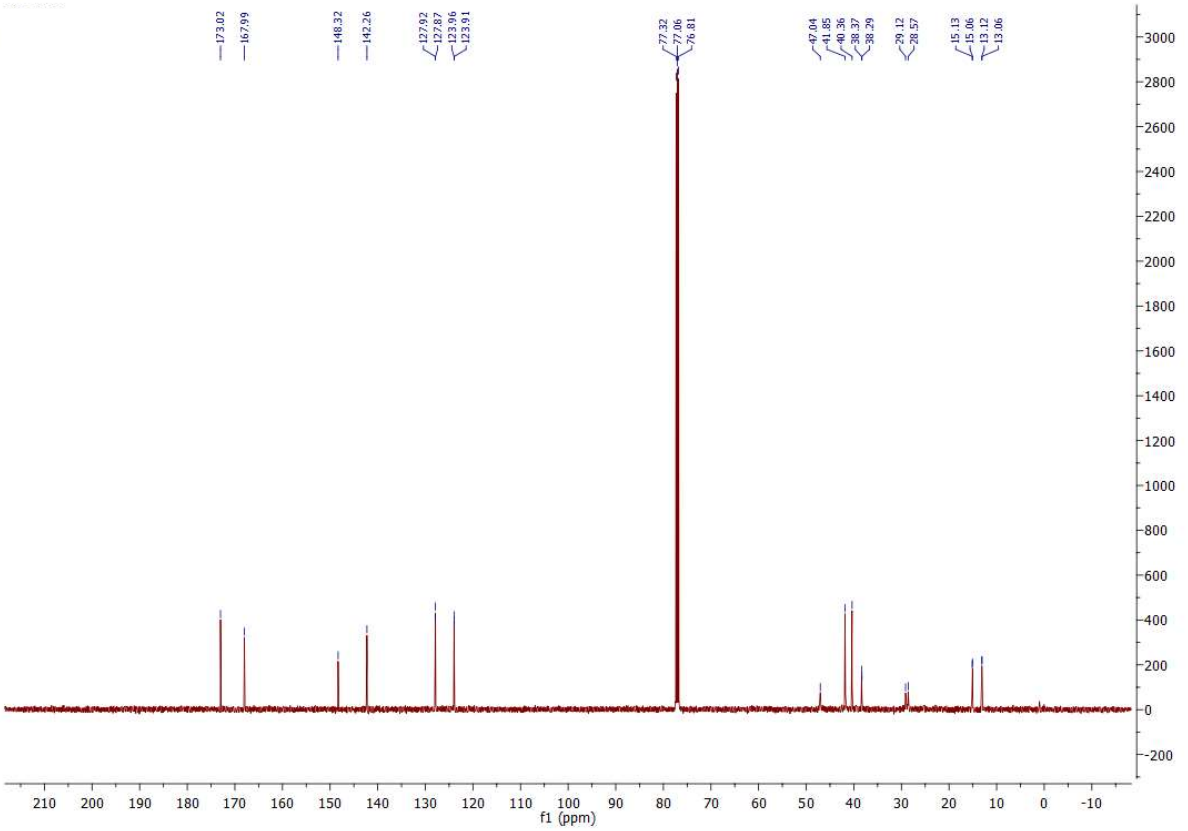


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A41

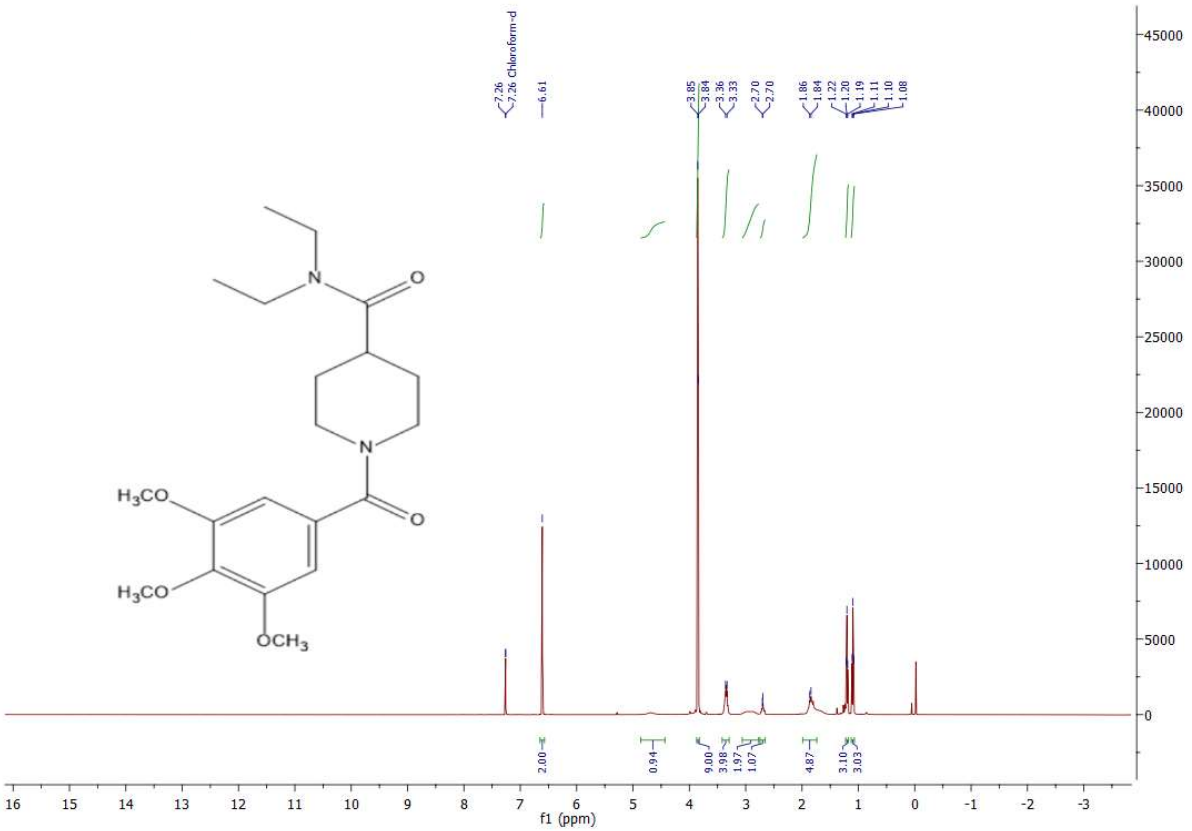


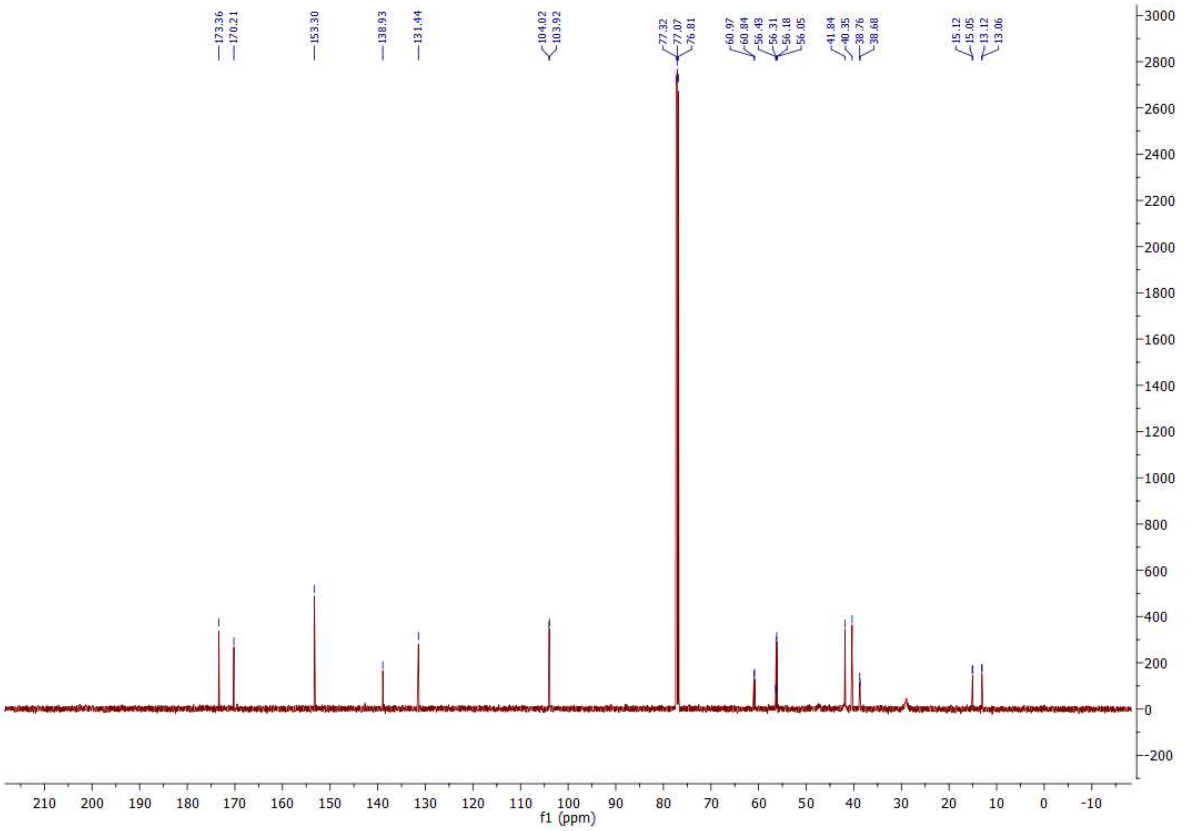
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A42



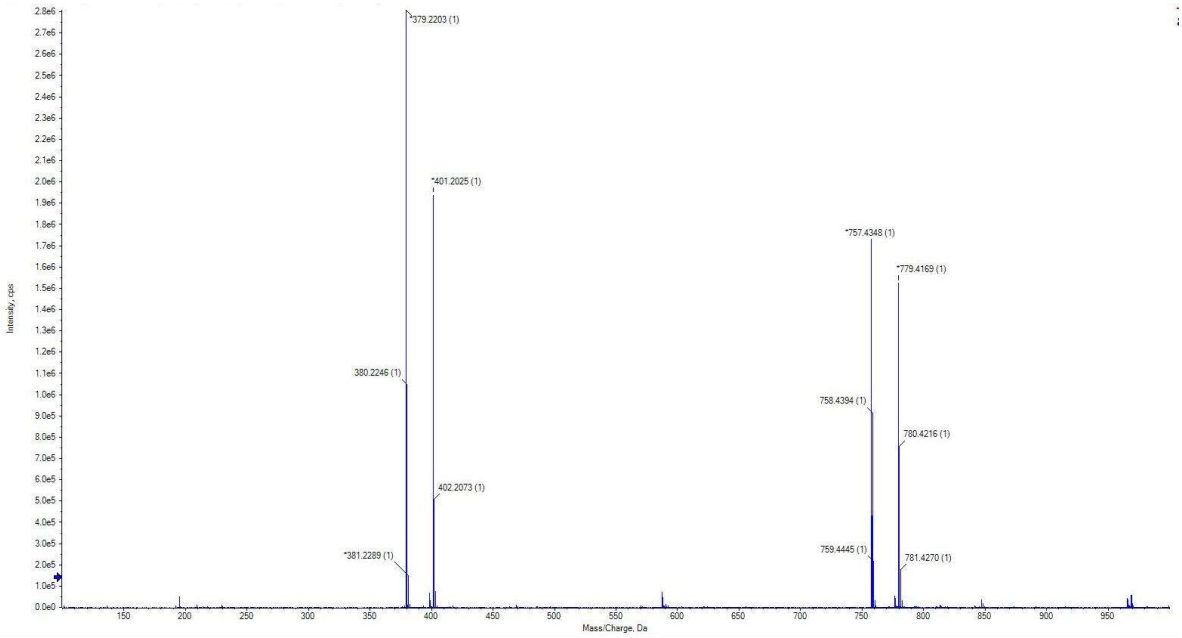


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A43

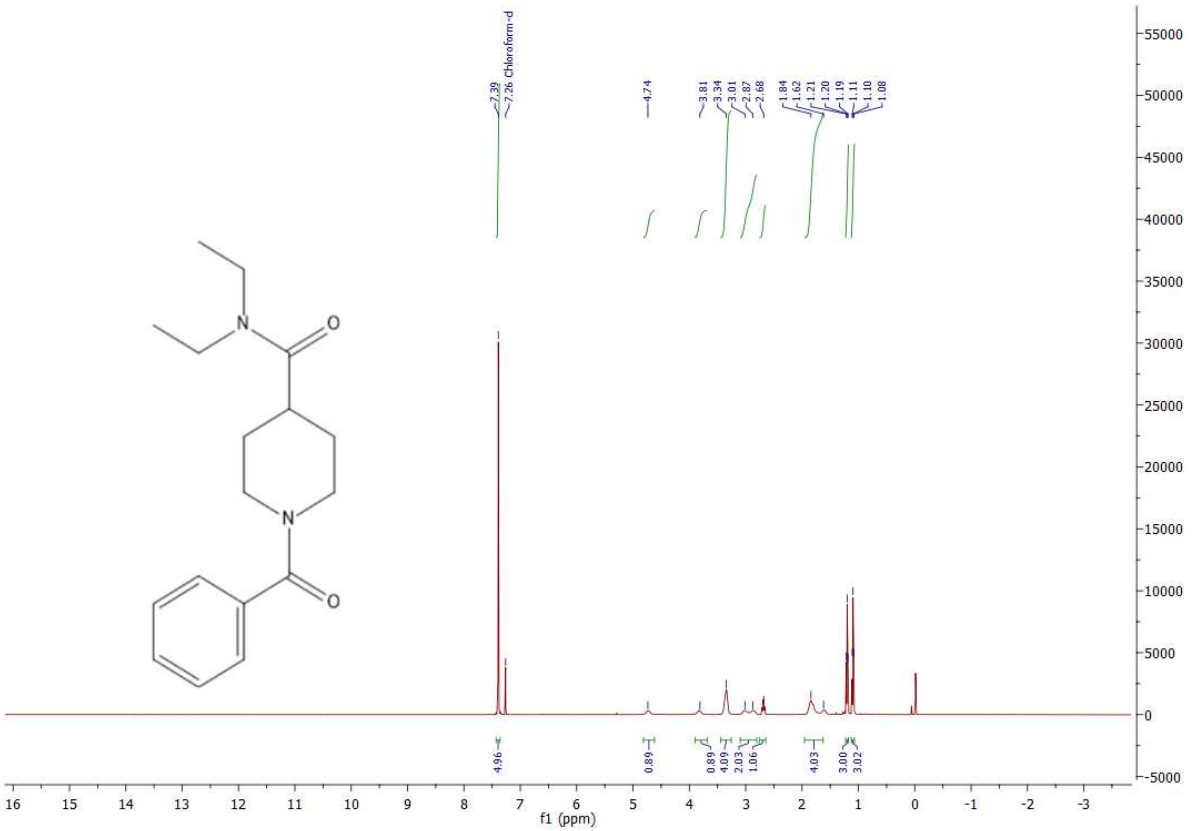


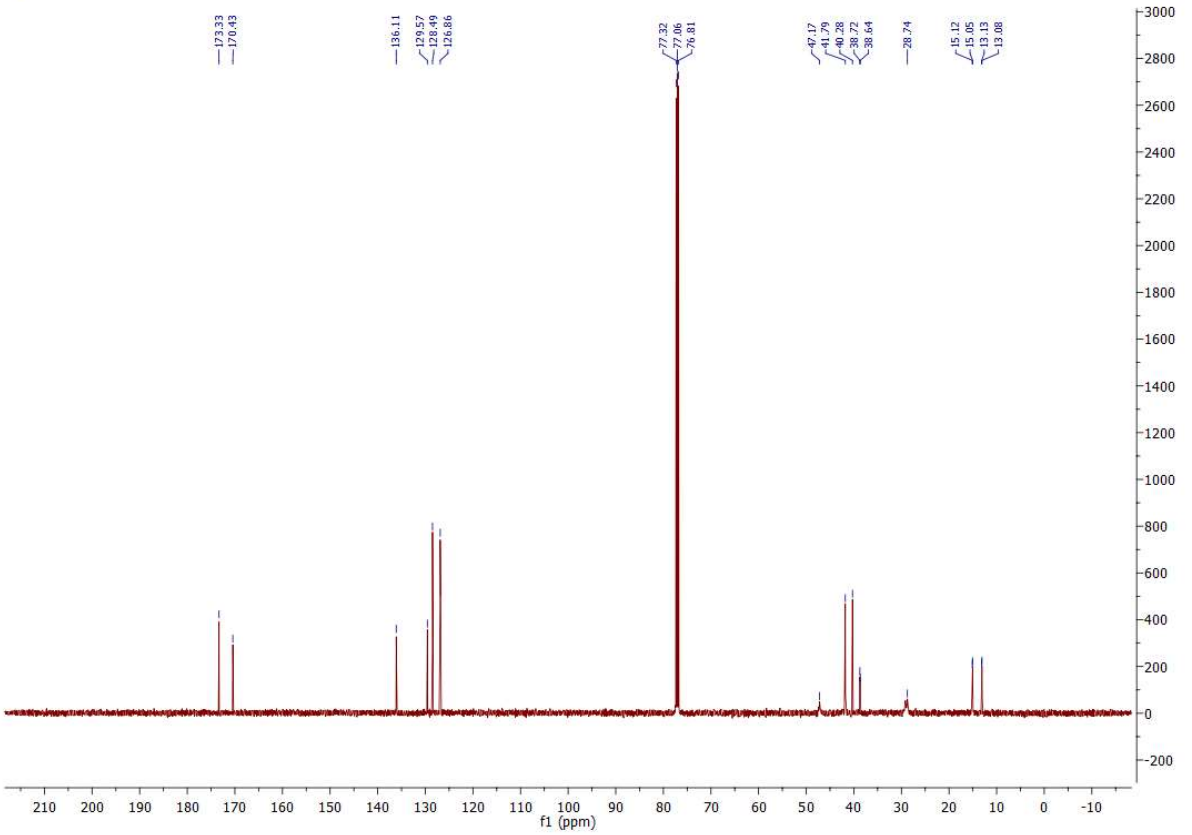


HRMS spectra of compound A43

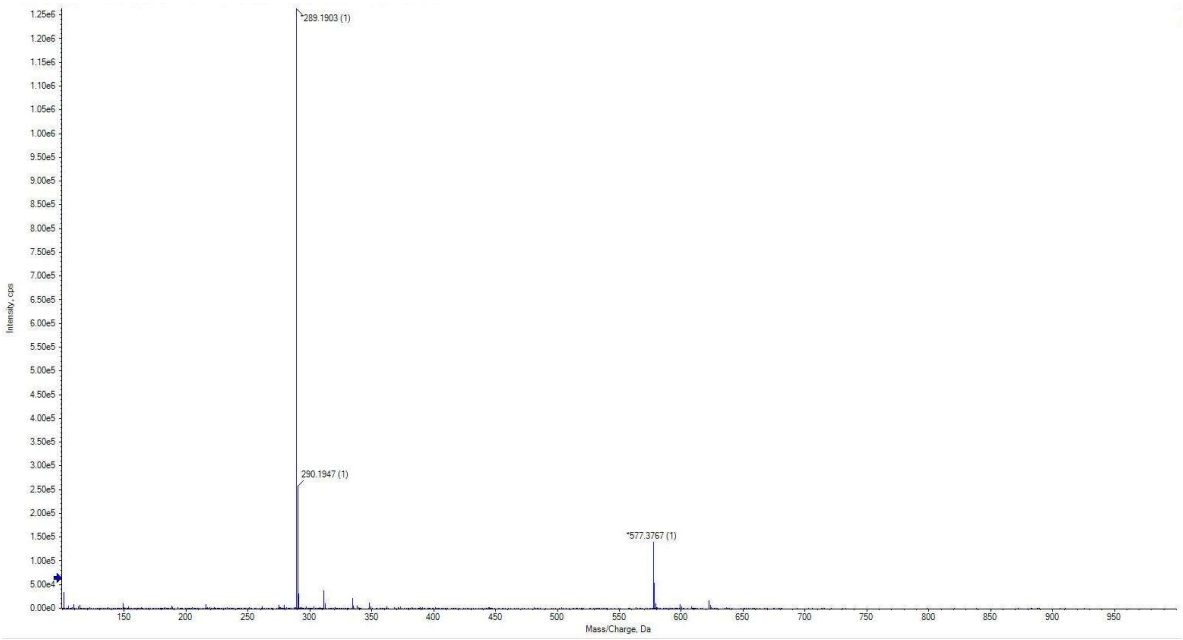


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A44

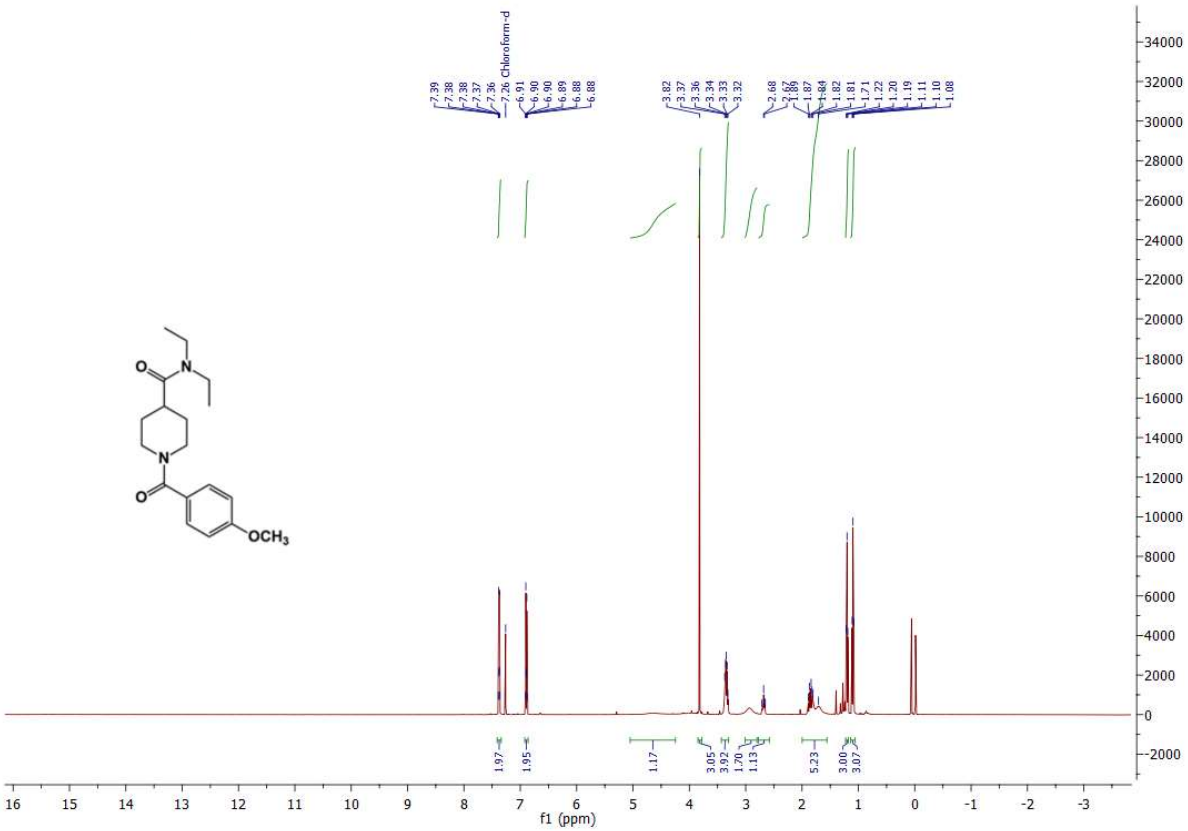


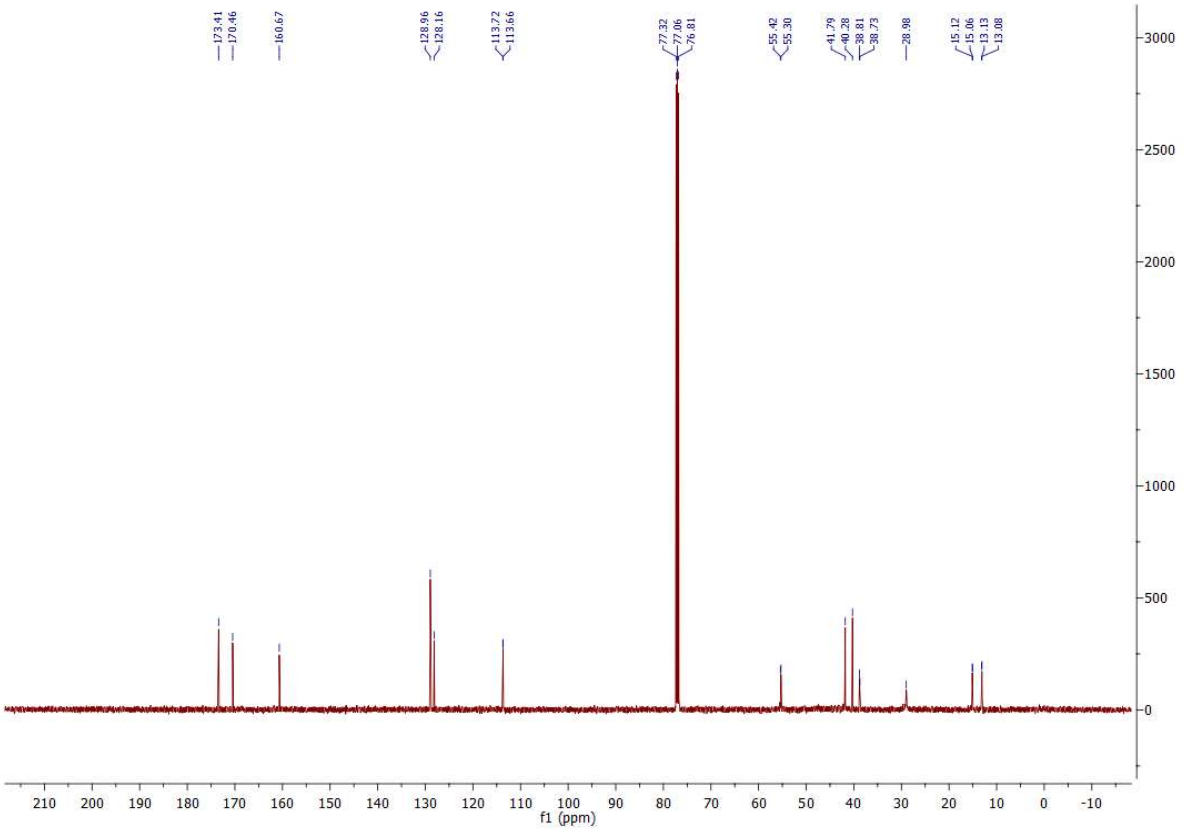


HRMS spectra of compound A44

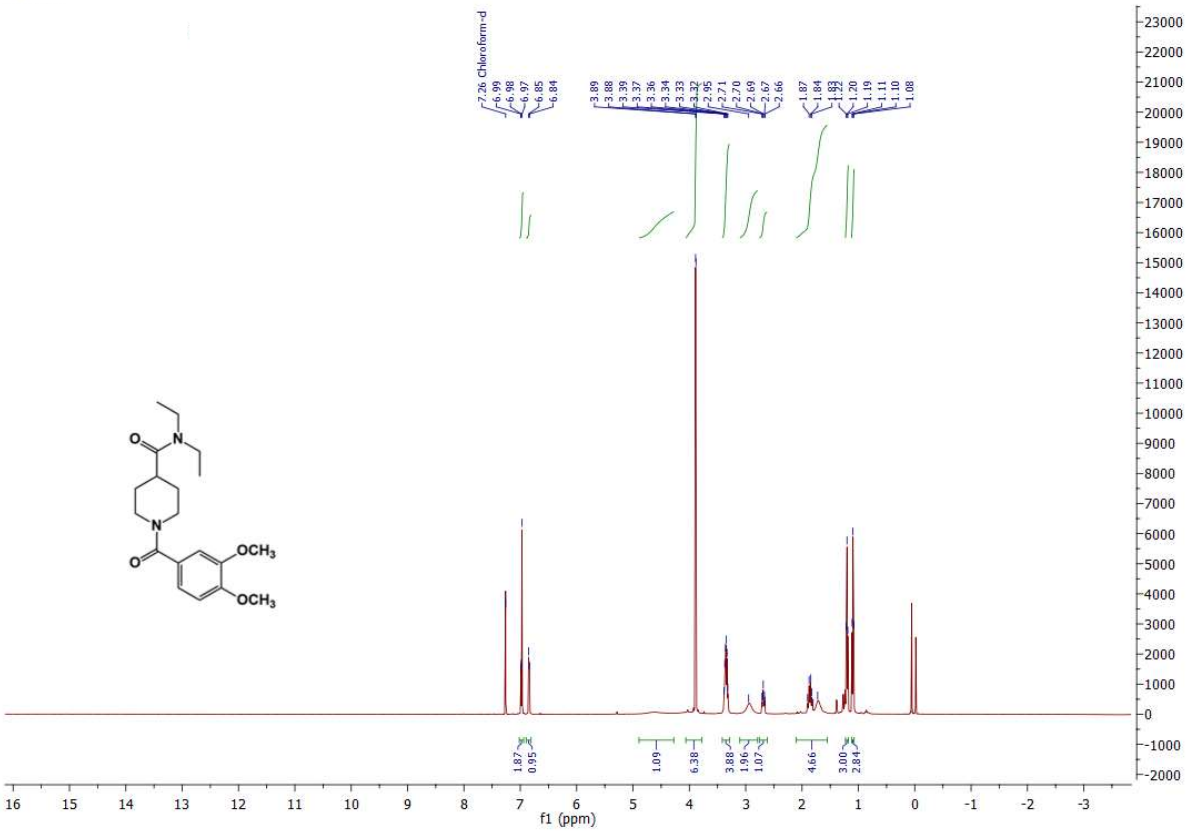


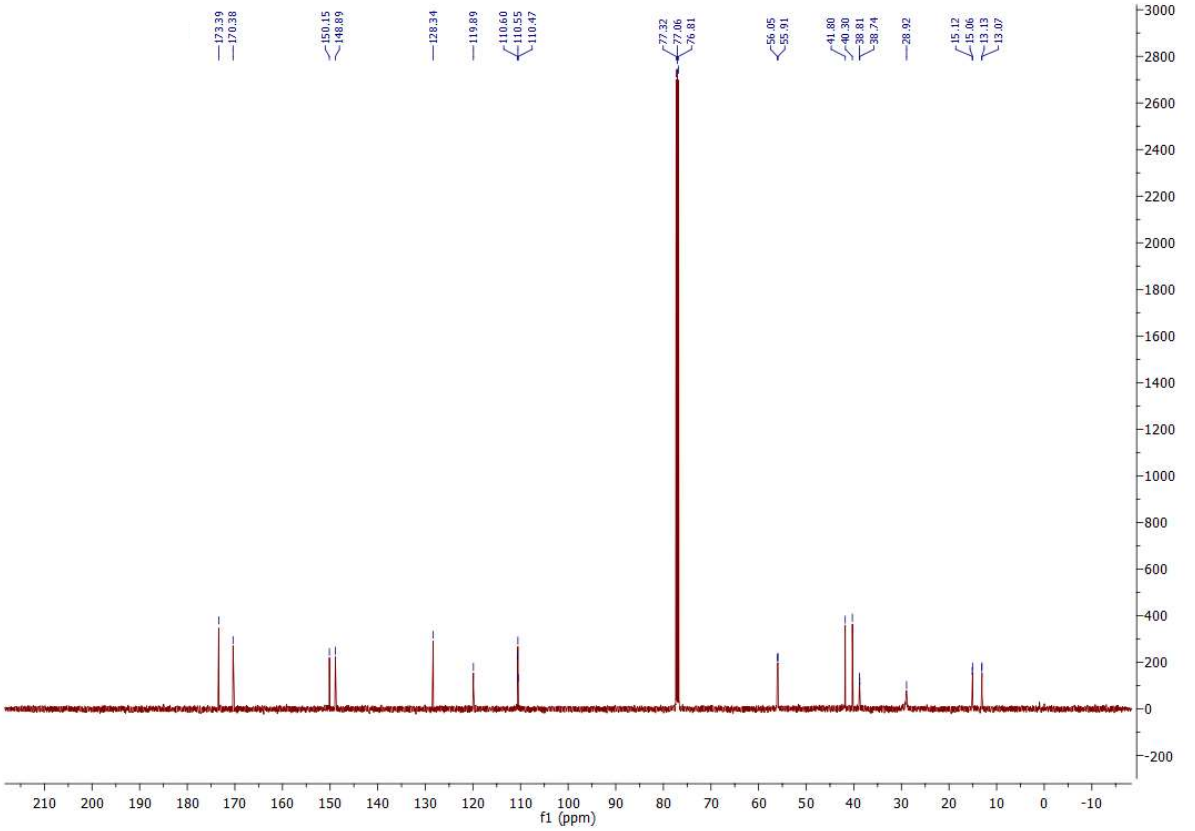
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A45



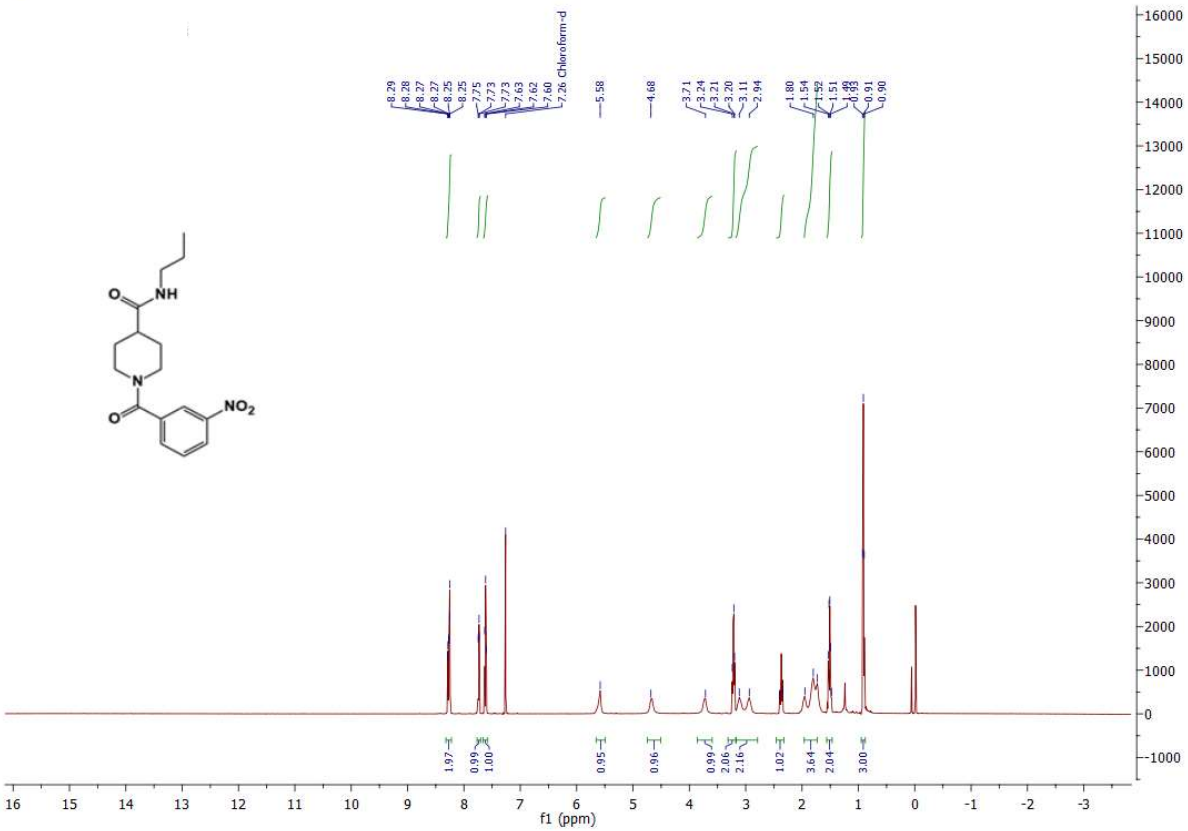


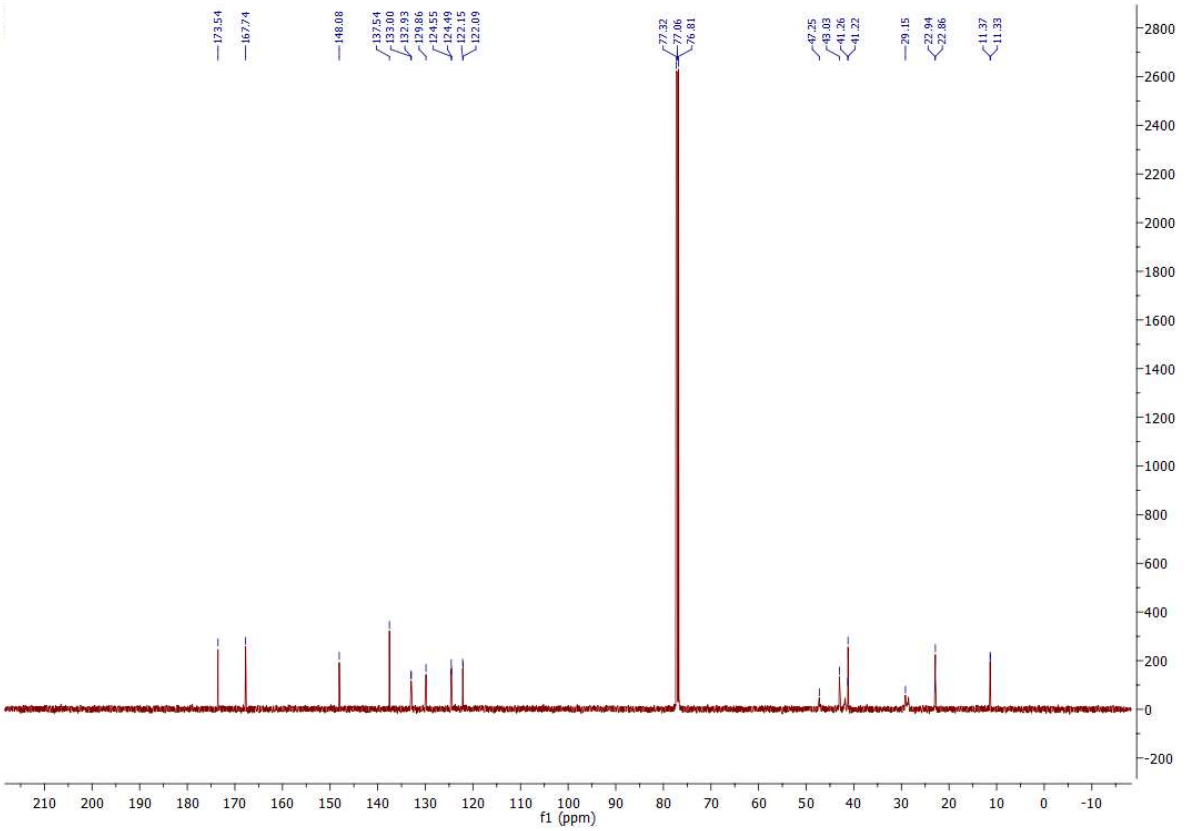
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A46



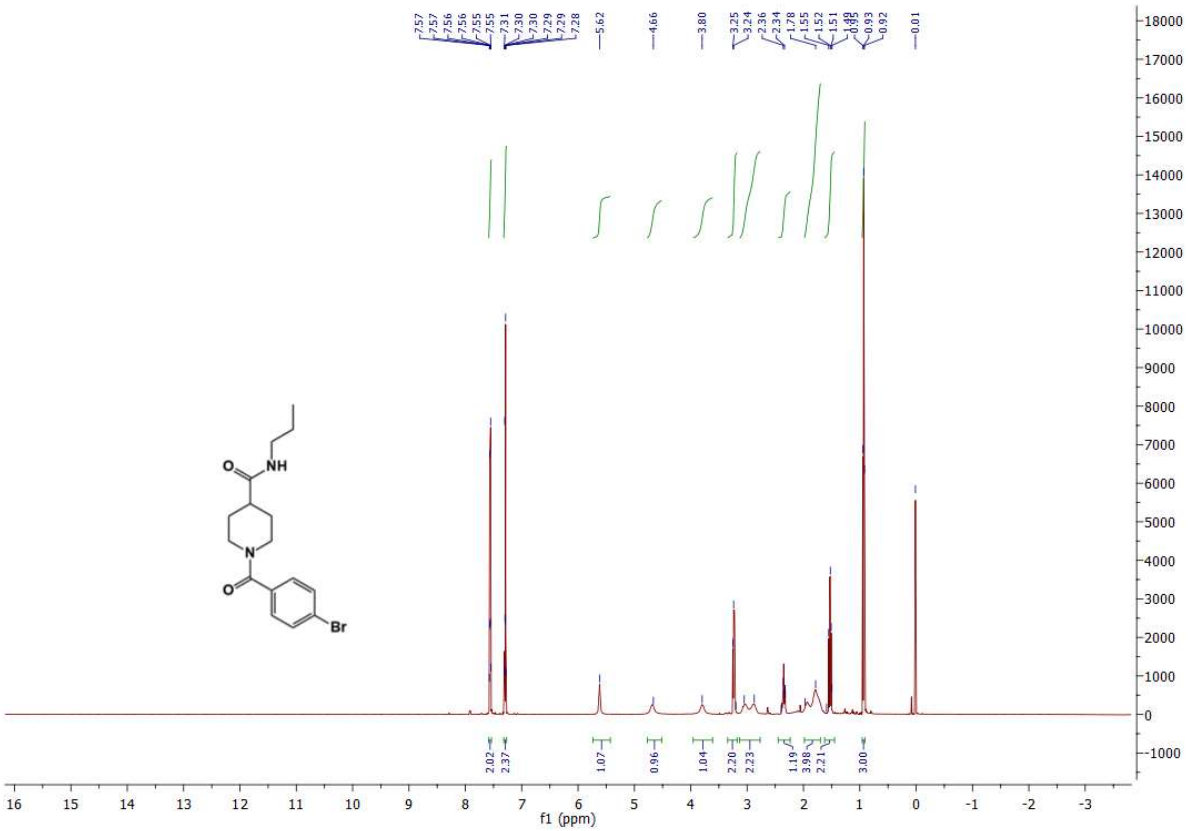


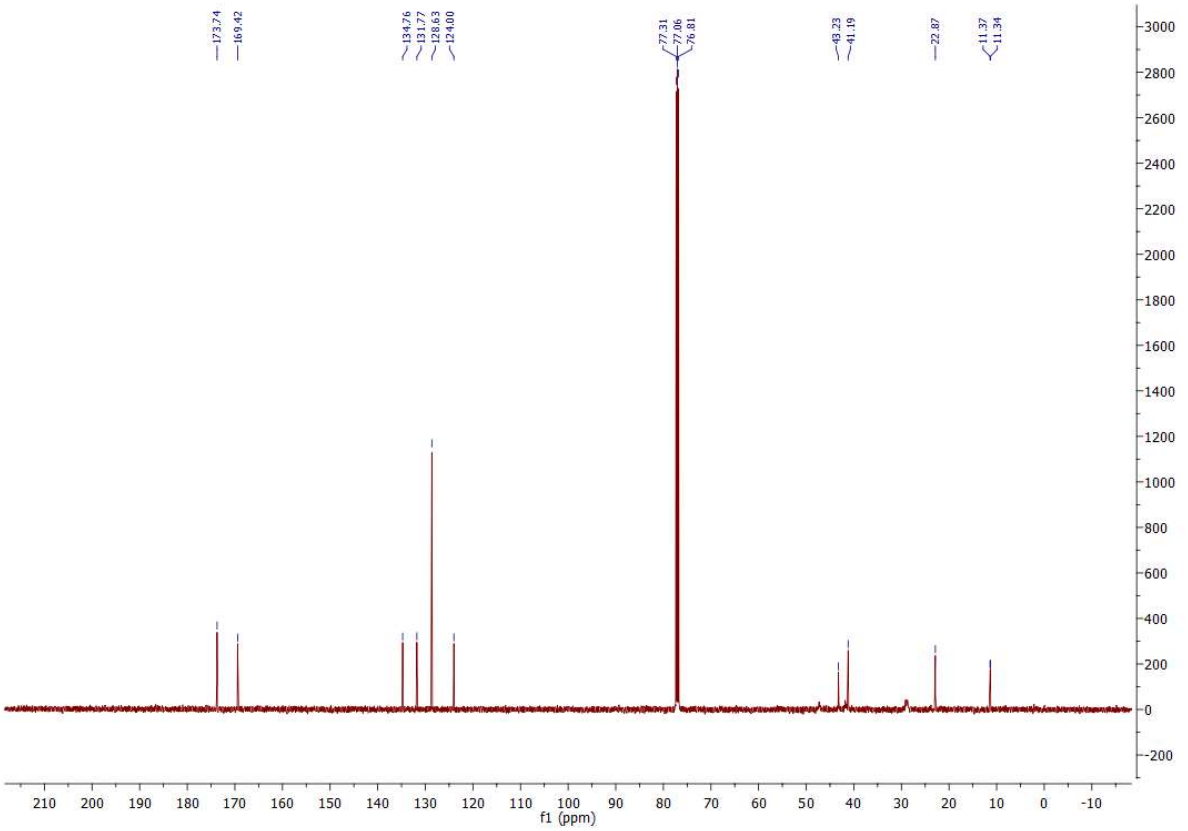
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A47



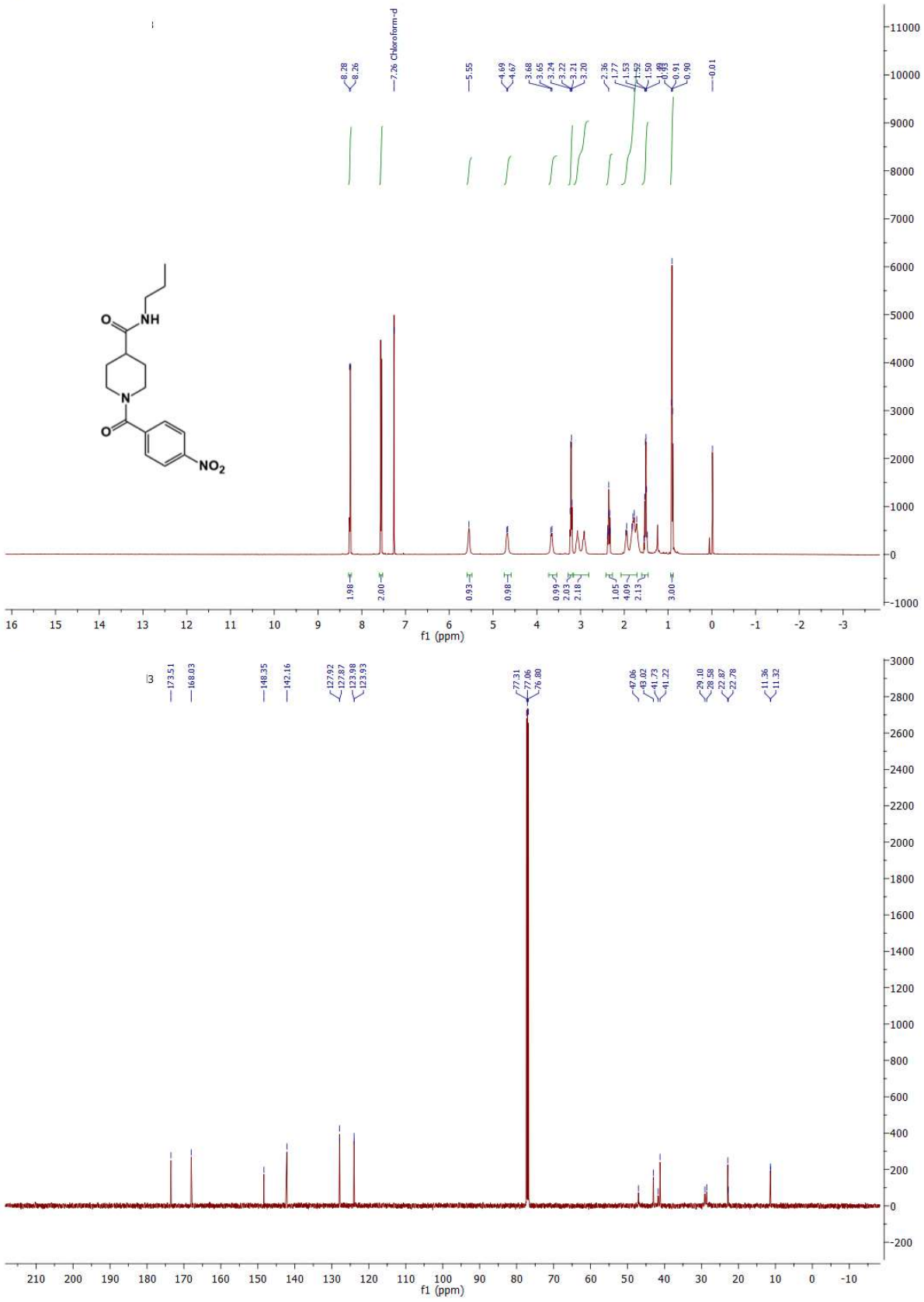


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A48

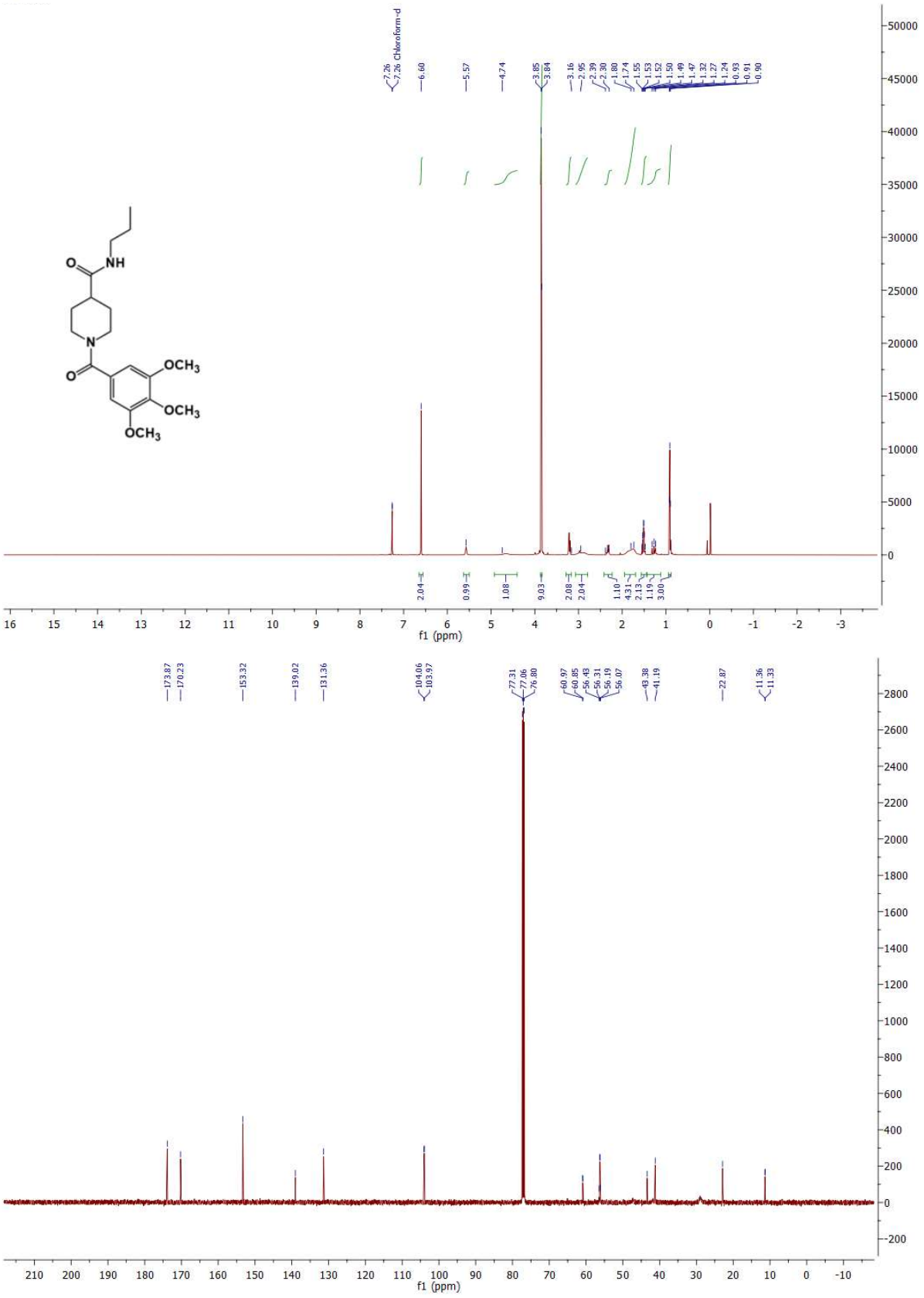




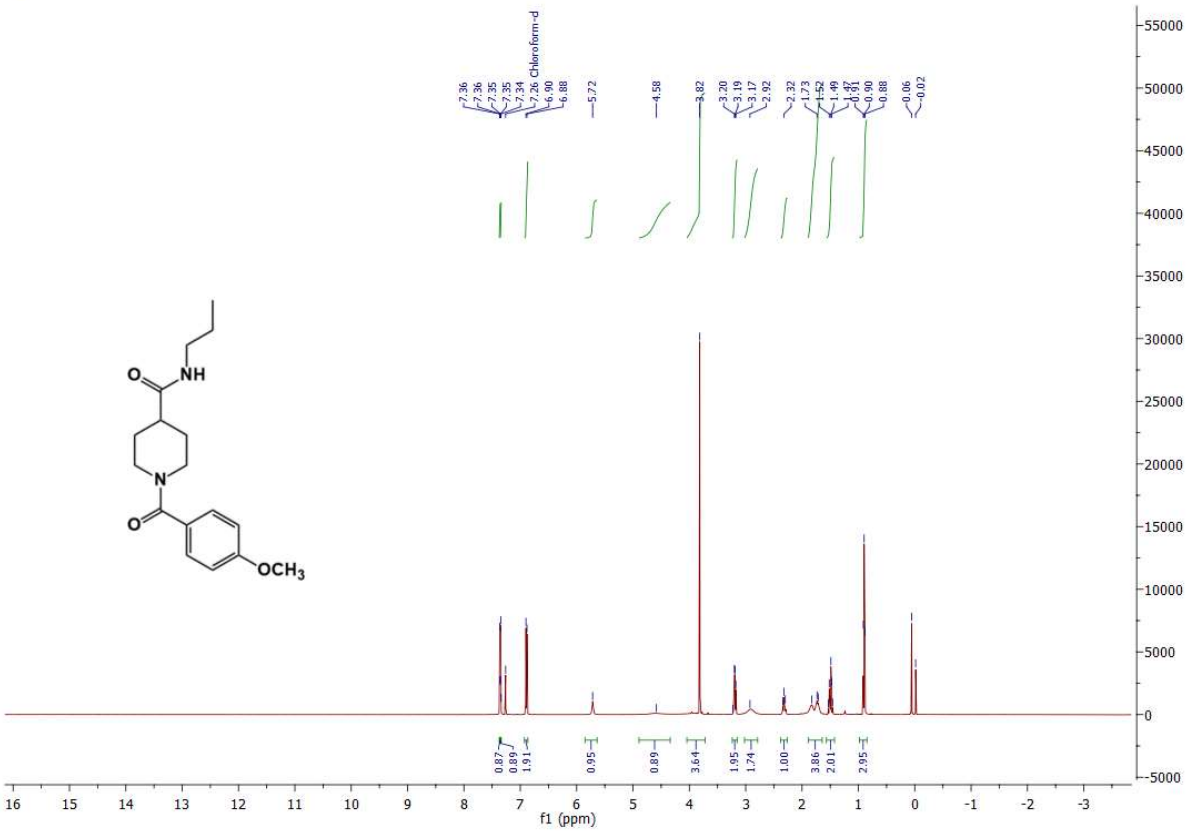
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A49

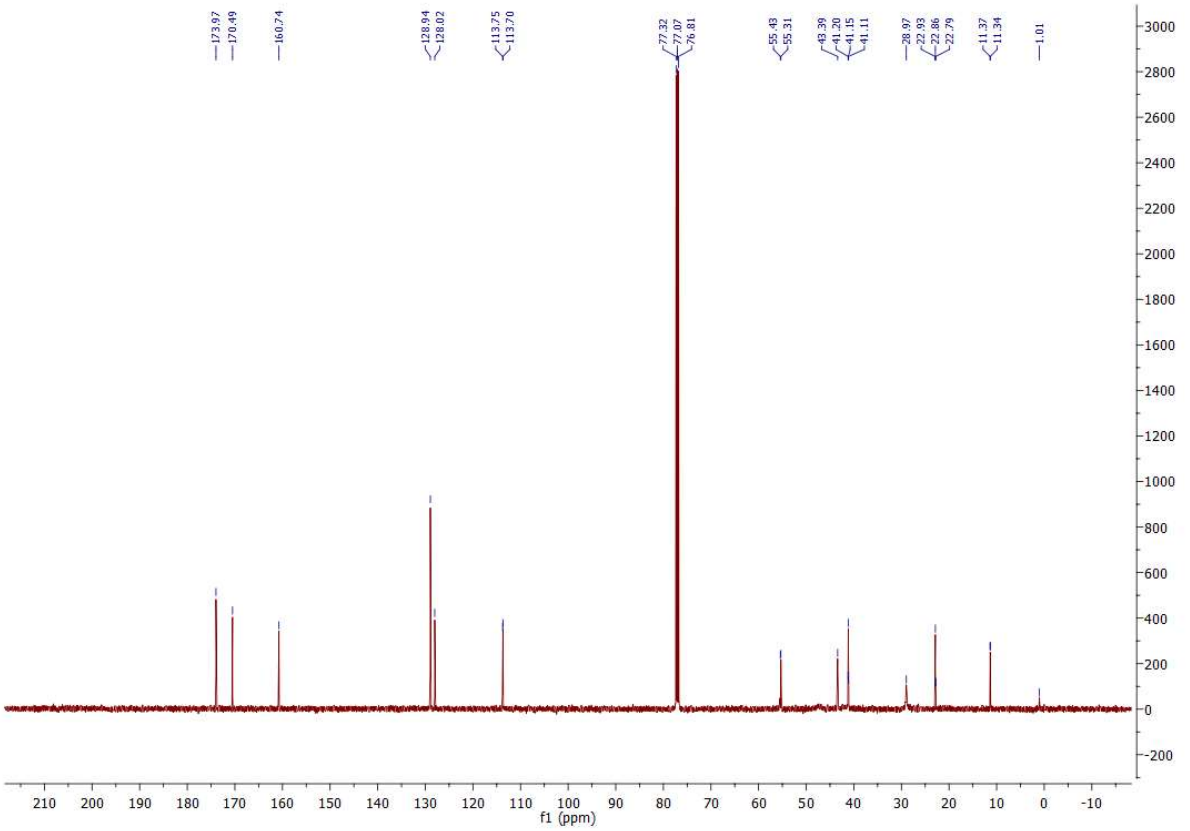


^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A50

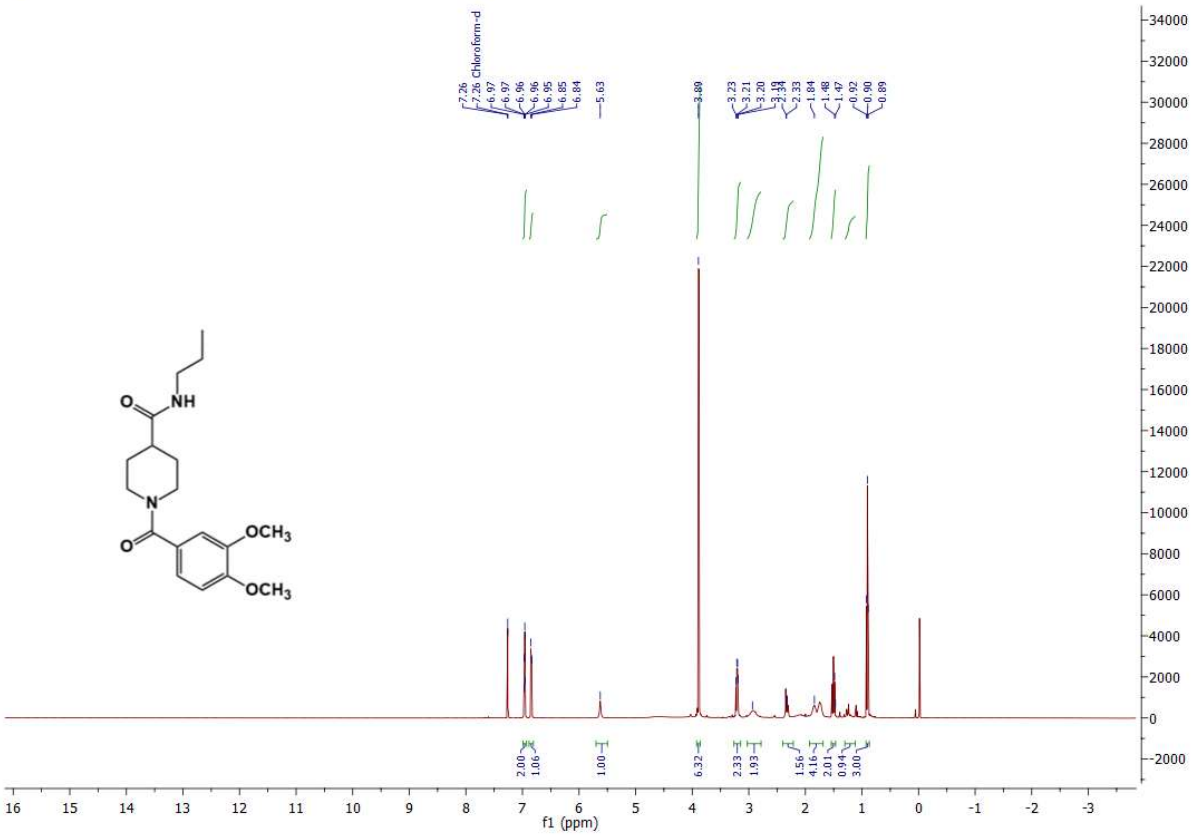


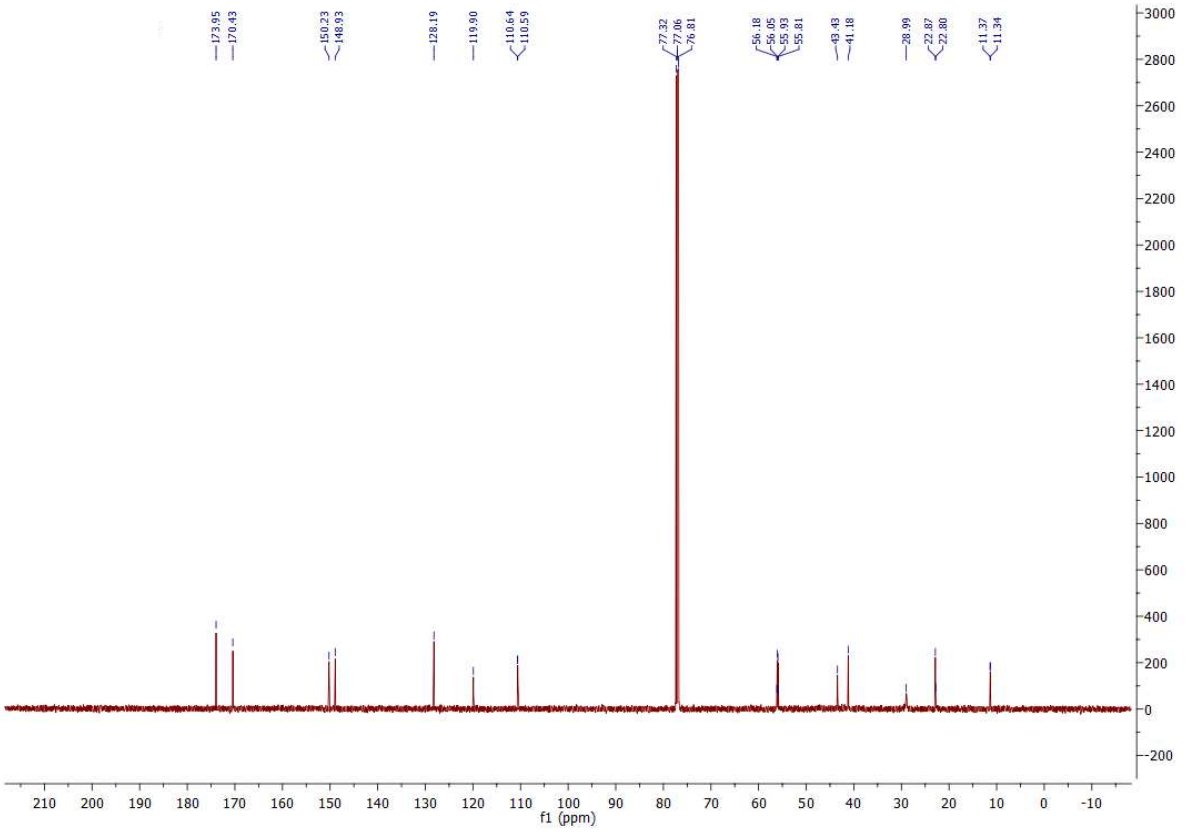
^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A51





^{1}H, $^{13}C\{1H\}$ NMR spectra of compound A52





Annexure-II

List of Publications

From Thesis

1. **Baidya AT**, Das B, Devi B, Långström B, Ågren H, Darreh-Shori T, Kumar R. *Mechanistic insight into the inhibition of choline acetyltransferase by proton pump inhibitors.* ACS Chemical Neuroscience. 2023 Feb 7;14(4):749-65.

2. **Baidya AT,** Goswami AK, Das B, Darreh-Shori T, Kumar R. *AI-Enabled Ultra-large Virtual Screening Identifies Potential Inhibitors of Choline Acetyltransferase for Theranostic Purposes.* ACS Chemical Neuroscience. 2024 Oct 31;15(22):4156-70.

3. **Baidya AT**, Dante D, Das B, Wang L, Darreh-Shori T, and Kumar R. *Discovery and characterization of novel pyridone and furan substituted ligands of choline acetyltransferase.* European Journal of Pharmacology. 2025 Apr 17:177638

4. **Baidya AT**, Devi B, Dante D, Das B, Darreh-Shori T, and Kumar R. *Piperidine scaffold Exploration, design and synthesis of novel derivatives for ChAT inhibitory activity.* (Manuscript Under preparation)

Other than thesis

1. **Baidya AT**, Deshwal S, Das B, Mathew AT, Devi B, Sandhir R, Kumar R. *Catalyzing a Cure: Discovery and development of LRRK2 inhibitors for the treatment of Parkinson's disease.* Bioorganic Chemistry. 2024 Feb 1;143:106972.
2. **Baidya AT**, Kumar A, Kumar R, Darreh-Shori T. *Allosteric binding sites of Aβ peptides on the acetylcholine synthesizing enzyme ChAT as deduced by in silico molecular modeling.* International Journal of Molecular Sciences. 2022 May 28;23(11):6073.
3. Darreh-Shori T, **Baidya AT**, Brouwer M, Kumar A, Kumar R. *Repurposing Duloxetine as a Potent Butyrylcholinesterase Inhibitor: Potential Cholinergic Enhancing Benefits*

for Elderly Individuals with Depression and Cognitive Impairment. ACS omega. 2024 Aug 21;9(35):37299-309.

4. Das B, Mathew AT, **Baidya AT**, Devi B, Salmon RR, Kumar R. *Artificial intelligence assisted identification of potential tau aggregation inhibitors: ligand-and structure-based virtual screening, in silico ADME, and molecular dynamics study.* Molecular Diversity. 2024 Aug;28(4):2013-31.
5. Das B, **Baidya AT**, Chakrabarti S, Chouhan D, Thakur B, Darreh-Shori T, Chen G, Tiwari V, Kumar R. *Synthesis and biological evaluation of Halogen-Substituted novel α-Ketoamides as potential protein aggregation modulators in Alzheimer's disease.* Bioorganic Chemistry. 2024 Jun 1;147:107373.
6. Das B, **Baidya AT**, Devi B, Rom T, Paul AK, Thakur B, Darreh-Shori T, Kumar R. *Synthesis, single crystal X-ray, DFT, spectroscopic, molecular docking studies and in vitro biological evaluation of compound N-benzyl-4-(4-chlorophenyl)-2-oxobutanamide.* Journal of Molecular Structure. 2023 Mar 15;1276:134782.
7. Mathew AT, **Baidya AT**, Das B, Devi B, Kumar R. *N-glycosylation induced changes in tau protein dynamics reveal its role in tau misfolding and aggregation: A microsecond long molecular dynamics study.* Proteins: Structure, Function, and Bioinformatics. 2023 Feb;91(2):147-60.
8. Nag S, **Baidya AT**, Mandal A, Mathew AT, Das B, Devi B, Kumar R. *Deep learning tools for advancing drug discovery and development.* 3 Biotech. 2022 May;12(5):110.
9. Das B, **Baidya AT**, Mathew AT, Yadav AK, Kumar R. *Structural modification aimed for improving solubility of lead compounds in early phase drug discovery.* Bioorganic & Medicinal Chemistry. 2022 Feb 15;56:116614.
10. Dante D, Jangra J, **Baidya AT**, Kumar R, Darreh-Shori T. *Micellar Choline-Acetyltransferase Complexes Exhibit Ultra-Boosted Catalytic Rate for Acetylcholine*

Synthesis—Mechanistic Insights for Development of Acetylcholine-Enhancing Micellar Nanotherapeutics. International Journal of Molecular Sciences. 2024 Dec 19;25(24):13602.

11. Brown LD, Girgis AS, Patel S, Samir N, Said MF, **Baidya AT**, Kumar R, Moore J, Khadanga A, Sakhuja R, Panda SS. *Novel isatin conjugates endowed with analgesic and anti-inflammatory properties: design, synthesis and biological evaluation.* Future Medicinal Chemistry. 2024 Dec 16:1-5.
12. Chauhan M, Prajapati C, Mirza S, Barot R, Yadav R, Barmade M, Kakadiya D, Vijayvargia R, Haobam B, **Baidya AT**, Kumar R. *Design, synthesis, biological evaluation and molecular dynamics of some novel 3-phenylpyrazolo [1, 5-a] pyrimidine-2, 7 (1 H, 4 H)-dione based compounds as anti-tubercular agents.* Journal of Biomolecular Structure and Dynamics. 2024 Nov 21;42(17):9031-49.
13. Saklani M, Jha CB, **Baidya AT**, Singh S, Kumar R, Mathur R, Tiwari AK, Varshney R. *Laminin mimetic angiogenic and collagen peptide hydrogel for enhance dermal wound healing.* Biomaterials Advances. 2024 Apr 1;158:213761.
14. Devi B, Vasishta SS, Das B, **Baidya AT**, Rampa RS, Mahapatra MK, Kumar R. *Integrated use of ligand and structure-based virtual screening, molecular dynamics, free energy calculation and ADME prediction for the identification of potential PTP1B inhibitors.* Molecular Diversity. 2024 Apr;28(2):649-69.
15. Mukhopadhyay A, Devi B, **Baidya AT**, Yadav ML, Kumar R, Mohapatra B. *Implication of TITIN Variations in Dilated Cardiomyopathy: Integrating Whole Exome Sequencing With Molecular Dynamics Simulation Study.* bioRxiv. 2024:2024-11.
16. Dahiya L, Kumar R, **Baidya AT**, Kumar S, Kumar R, Pawar SV, Yadav AK. *Design, synthesis, biological evaluations and in silico studies of N-substituted 2, 4-*

thiazolidinedione derivatives as potential a-glucosidase inhibitors. Journal of Biomolecular Structure and Dynamics. 2023 Dec 5:1-8.

17. Akhilesh, **Baidya AT**, Uniyal A, Das B, Kumar R, Tiwari V. *Structure-based virtual screening and molecular dynamics simulation for the identification of sphingosine kinase-2 inhibitors as potential analgesics.* Journal of Biomolecular Structure and Dynamics. 2022 Dec 19;40(23):12472-90.
18. Deshwal S, **Baidya AT**, Kumar R, Sandhir R. *Structure-based virtual screening for identification of potential non-steroidal LXR modulators against neurodegenerative conditions.* The Journal of Steroid Biochemistry and Molecular Biology. 2022 Oct 1;223:106150.
19. Poonia N, Lal K, Kumar A, Kumar A, Sahu S, **Baidya AT**, Kumar R. *Urea-thiazole/benzothiazole hybrids with a triazole linker: synthesis, antimicrobial potential, pharmacokinetic profile and in silico mechanistic studies.* Molecular Diversity. 2022 Oct 1:1-7.

Book chapter

1. Devi B, **Baidya AT**, Kumar R. *Community Benchmarking Exercises for Docking and Scoring*. Computational Drug Discovery: Methods and Applications. 2024 Apr 1;2:471-94.
2. Das B, **Baidya AT**, Kumar R. *Polyphenol: Development of Polyphenol-Inspired Derivatives Targeting Pathological Factors of AD.* InNatural Product-based Synthetic Drug Molecules in Alzheimer's Disease: Therapeutic & Theranostic Agents 2023 Dec 15 (pp. 245-266). Singapore: Springer Nature Singapore.

Patent application

1. Rajnish Kumar, **Anurag TK Baidya** and Bhanuranjan Das. "An amide linkage-based heterocyclic derivative and a method of preparation thereof". 2024 Oct; Application No. 202411036401

2. Rajnish Kumar, Bhanuranjan Das and **Anurag TK Baidya.** "Piperazine, Piperidine, and Indole-Substituted 1,2-Dicarbonyl Compounds as amyloid aggregation modulators: synthesis and application thereof". 2023 Oct; Application No. 202311080715

Workshop/Conference presentation

1. Hands-on training program on "Advanced Equipment Handling and Applications in Molecular Biology". **JSS AHER & DST-STUTI sponsored, University of Mysore**, Mysuru, 25 April to 01 May 2022.
2. "*Understanding the Mechanism of Choline Acetyltransferase Inhibition by Proton Pump Inhibitors*" **International Society for Molecular and Cellular Mechanisms (ISMND)** NextGen 2023 International Virtual Conference. August 23-24, 2023.
3. "*Deep Learning Guided Ultra-Large Scale Virtual Screening for the Identification of Potential Choline Acetyltransferase Ligands*" **AI-SPARK Conference**, NIPER Mohali, October 9-11, 2023.
4. "*Structure-based discovery of choline acetyltransferase ligands as potential theranostic agents for Alzheimer's disease*" **10th Congress of the European Academy of Neurology –** Helsinki, 29 June to 02 July 2024.
5. "*Discovery of novel Diagnostic/Therapeutic agents for Alzheimer's Disease*" **Research and Innovation Day**, Indian Institute of Technology (BHU), Varanasi, September 05, 2024.

6. "*AI-enabled ultra large virtual screening identifies potential inhibitors of Choline Acetyltransferase for theranostic purpose*" **International Conference on Emerging Trends in Translational Bioinformatics (ET2B-2024),** Birla Institute of Technology Mesra, Ranchi, December 5th-7th, 2024.