

SYNTHESIS OF HEXAHYDROQUINOLINE-3-CARBOXAMIDE DERIVATIVES AND THEIR HIV-1 ANTIVIRAL ACTIVITY

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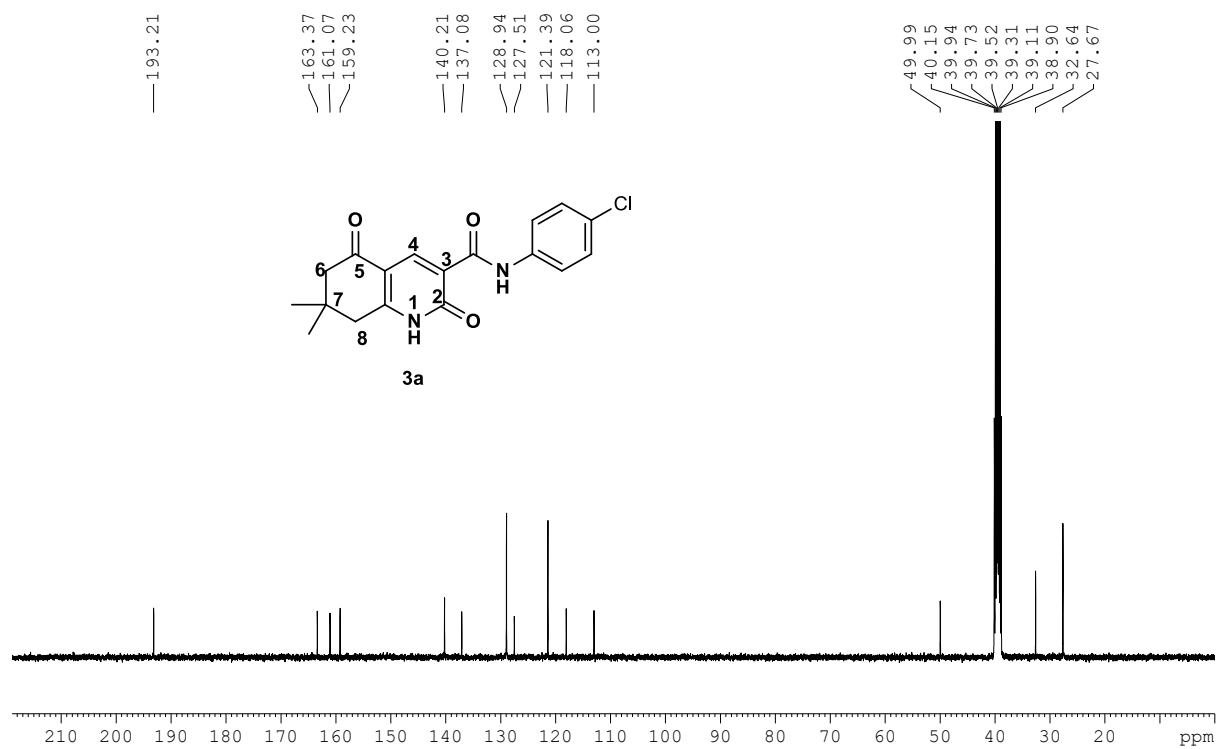
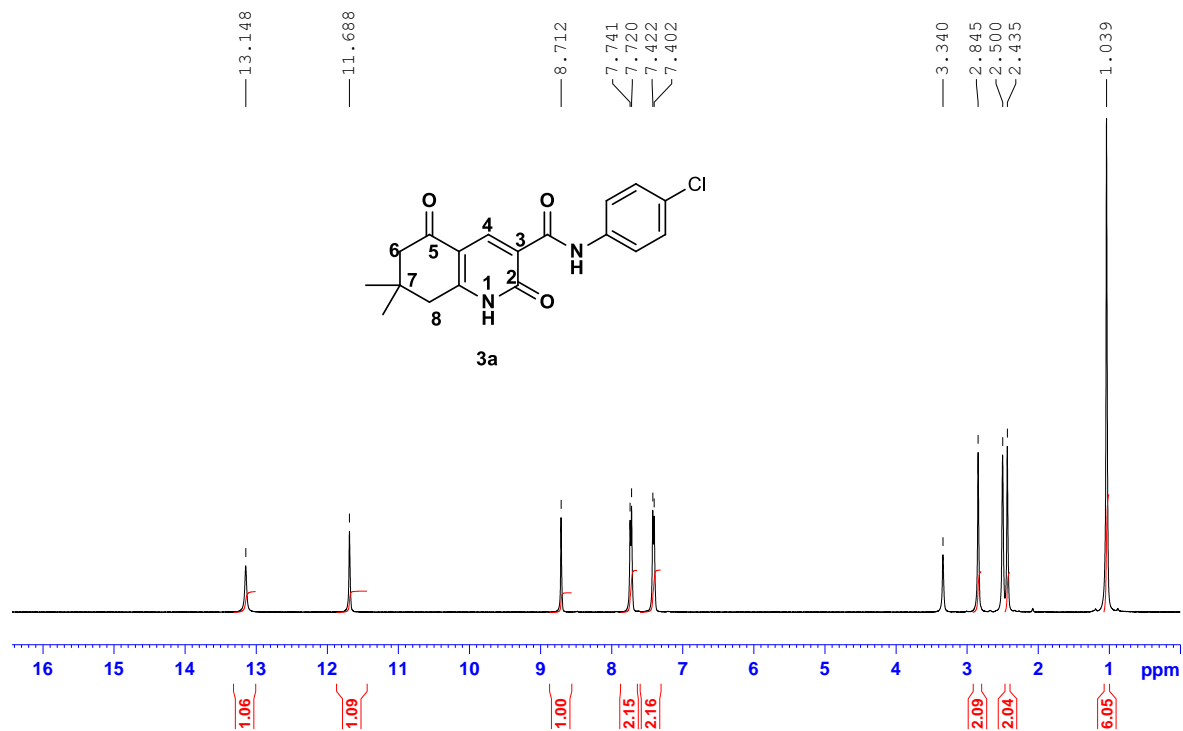
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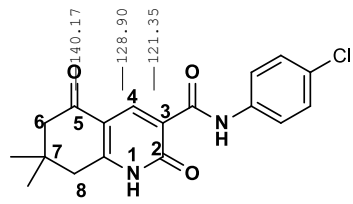
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Table of Contents

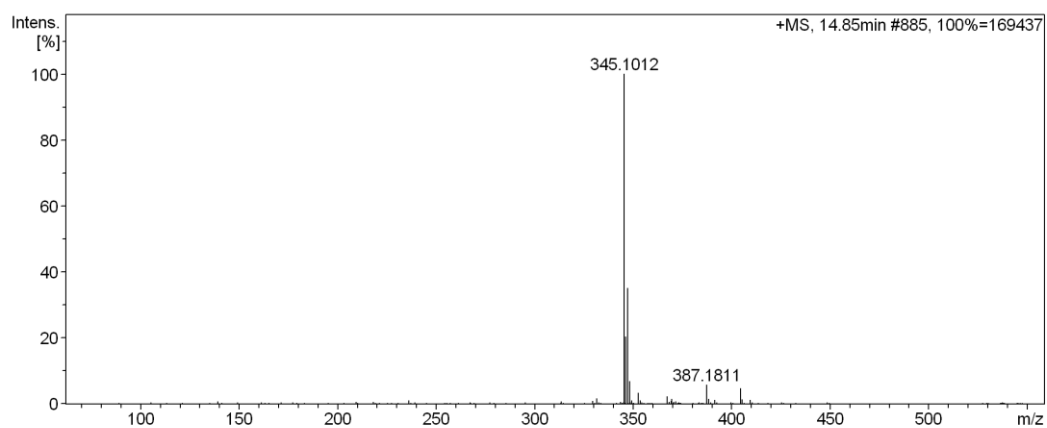
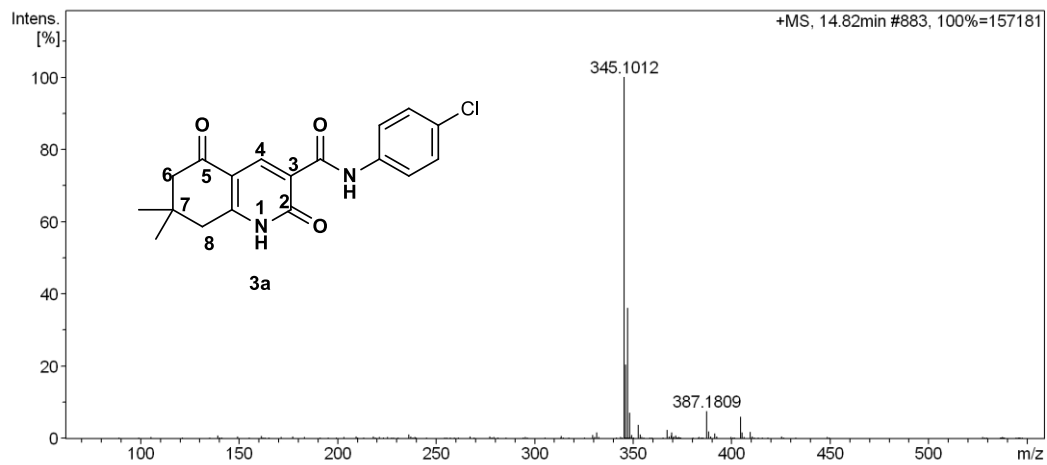
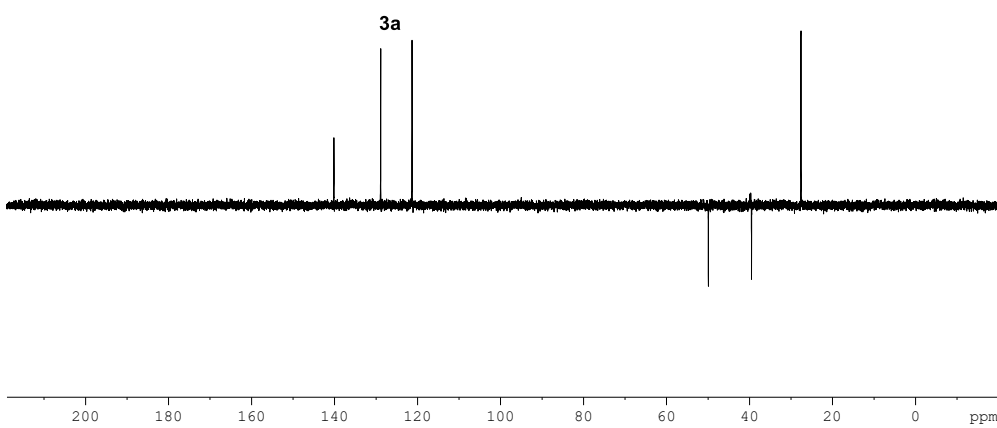
¹ H NMR, ¹³ C NMR spectra and HRMS for compounds 3a-m	2
¹ H NMR, ¹³ C NMR spectra and HRMS for compounds 9a-d	29
¹ H NMR, ¹³ C NMR spectra for compounds 4a-b and 6a-b	37
¹ H NMR, ¹³ C NMR spectra for compounds 8a-b	41
Virtual Screening: Molecular docking and ADME-results.....	43
Antiviral activity graph.....	45

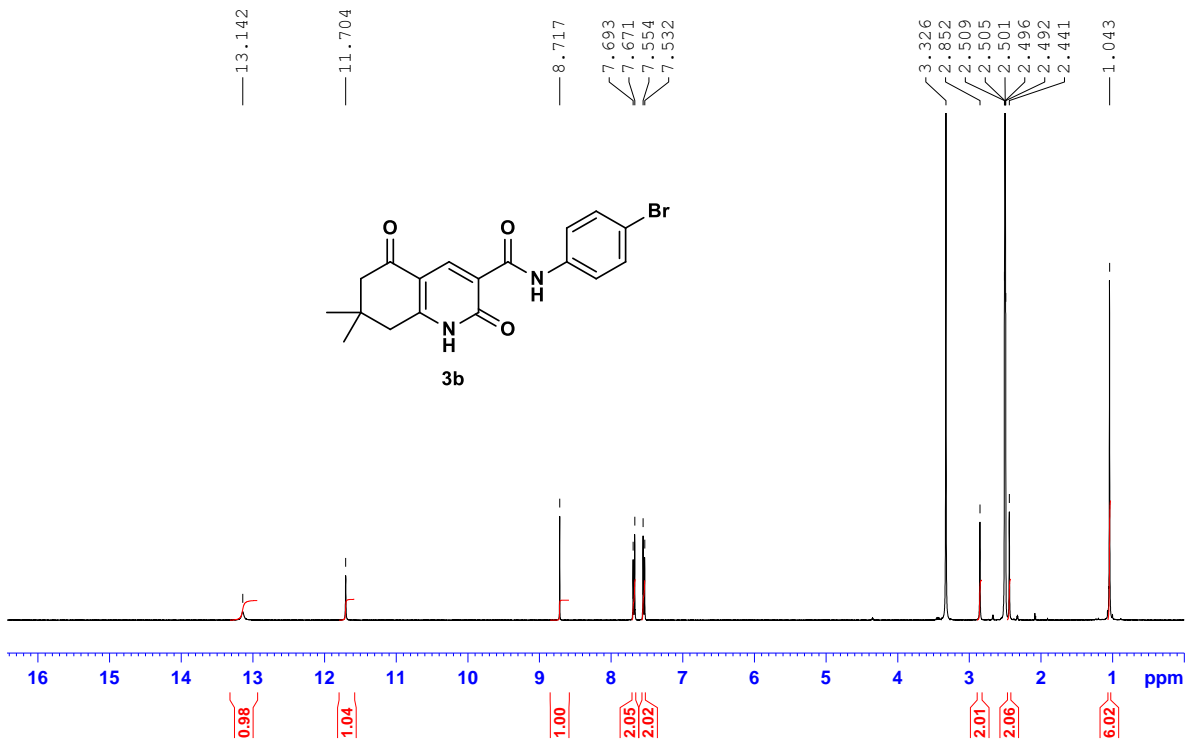
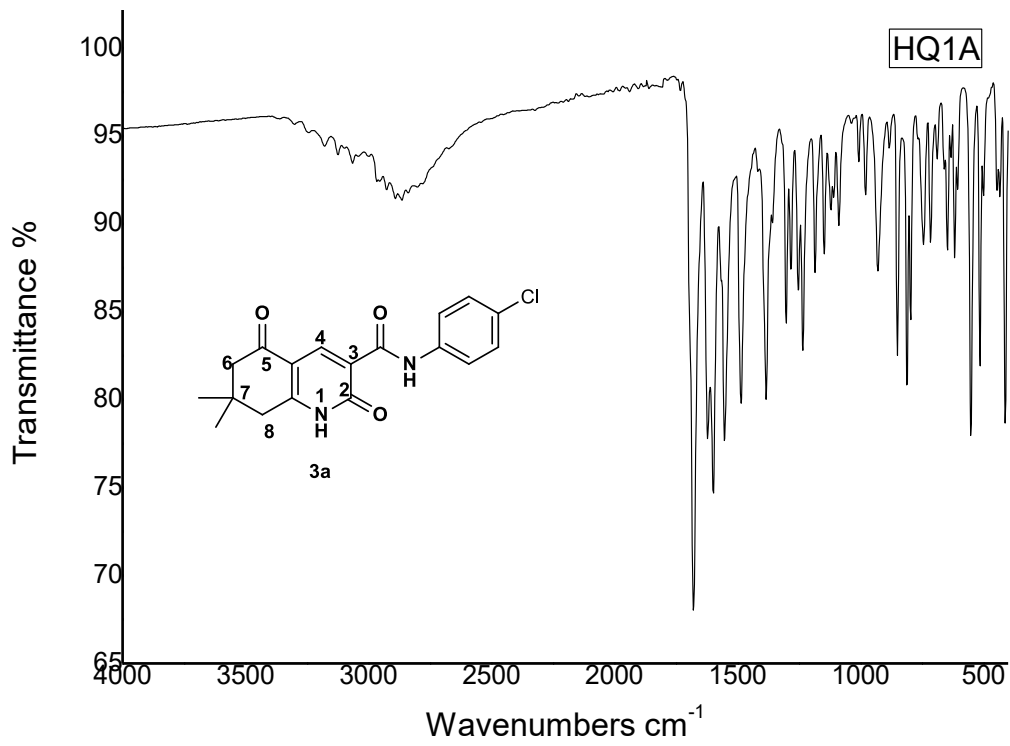
Supplementary data

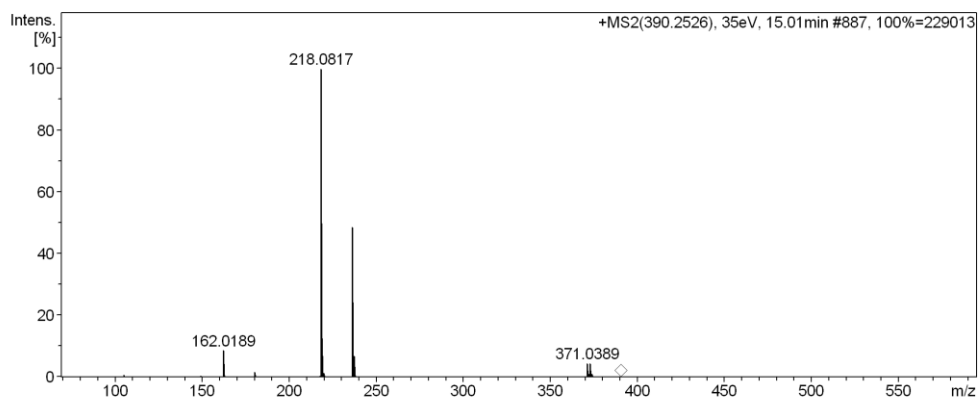
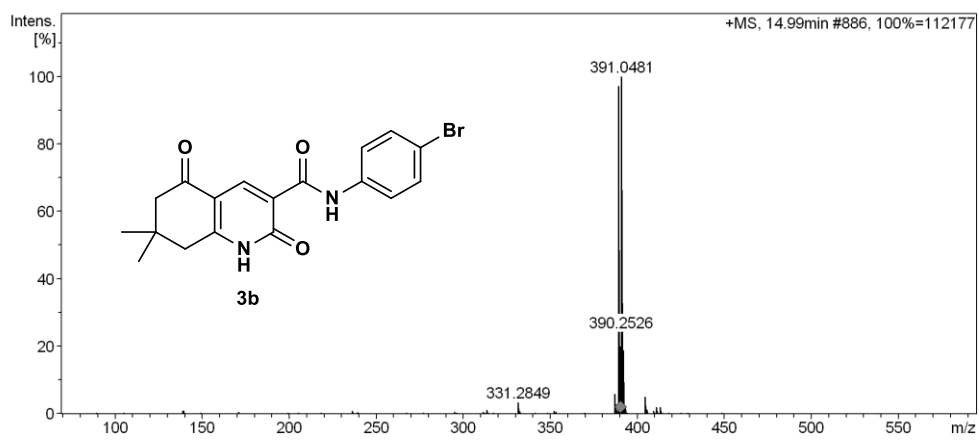
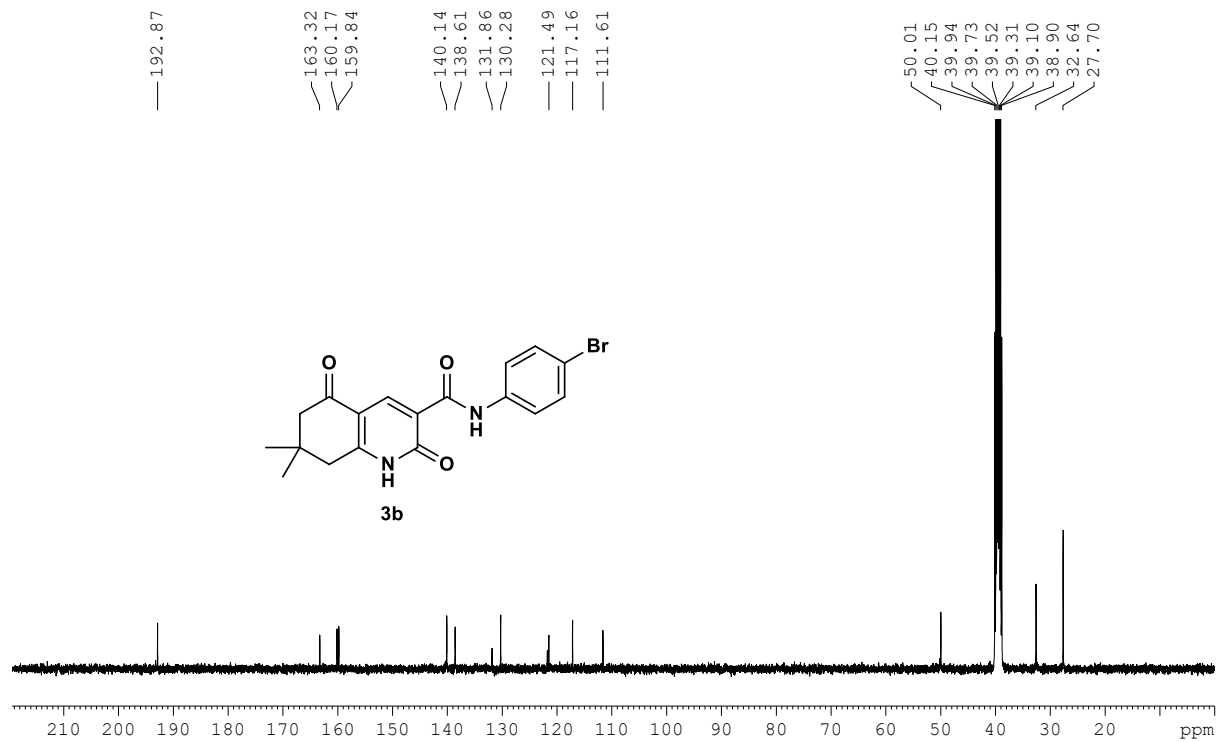


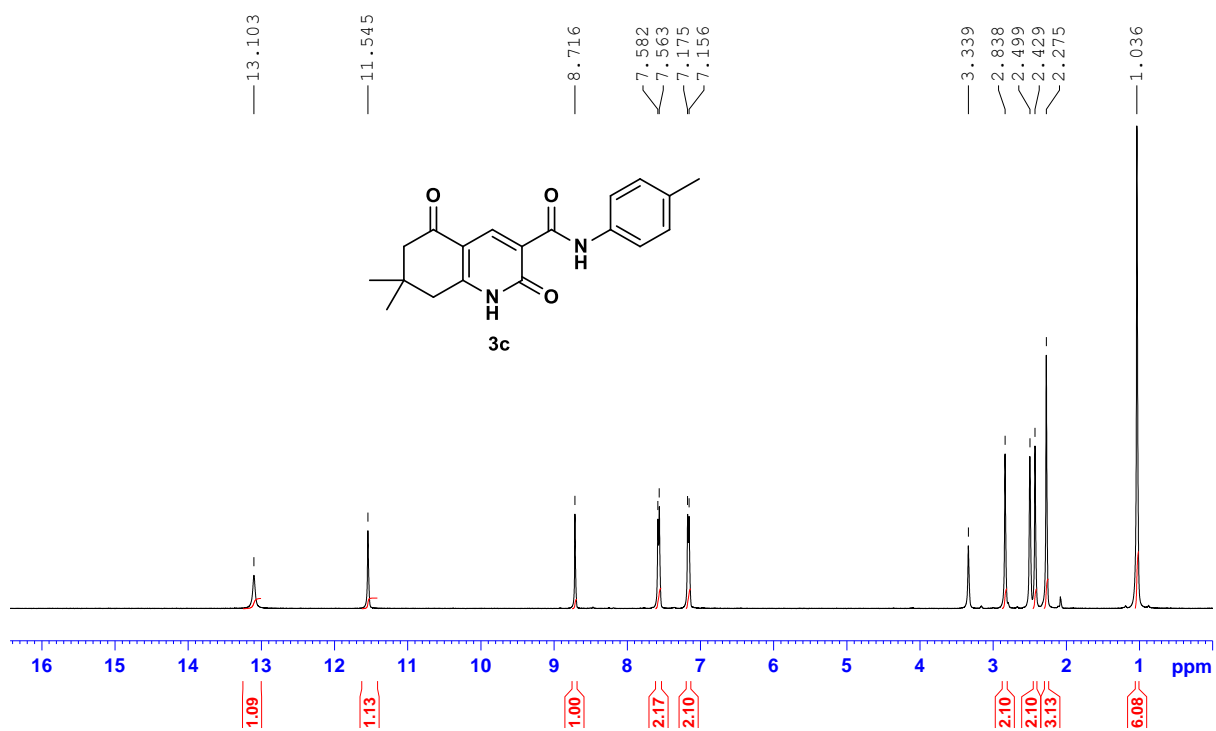
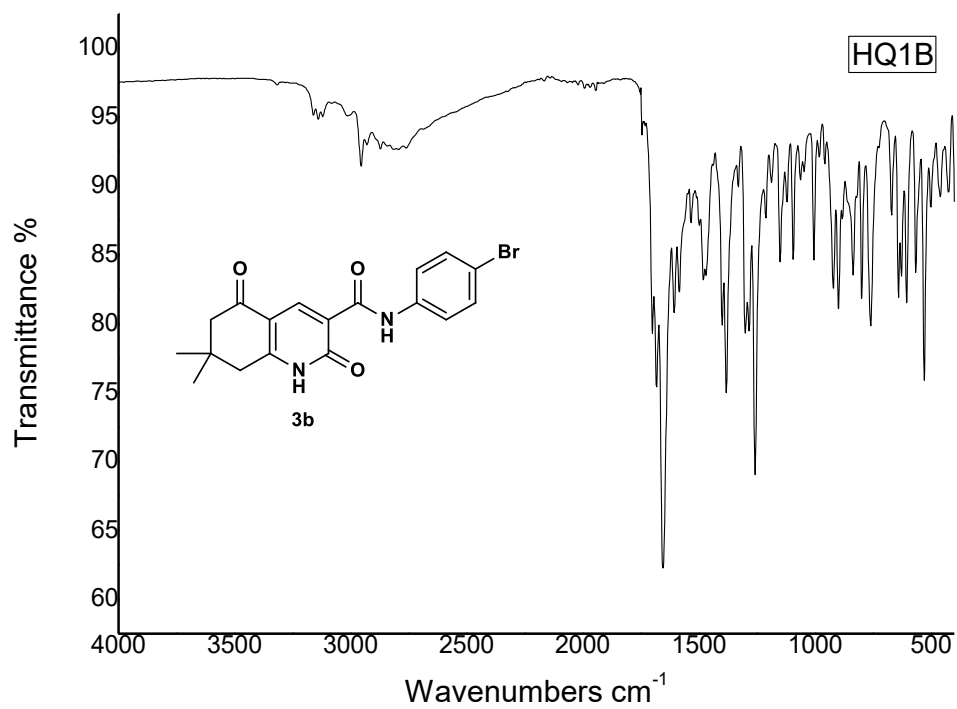


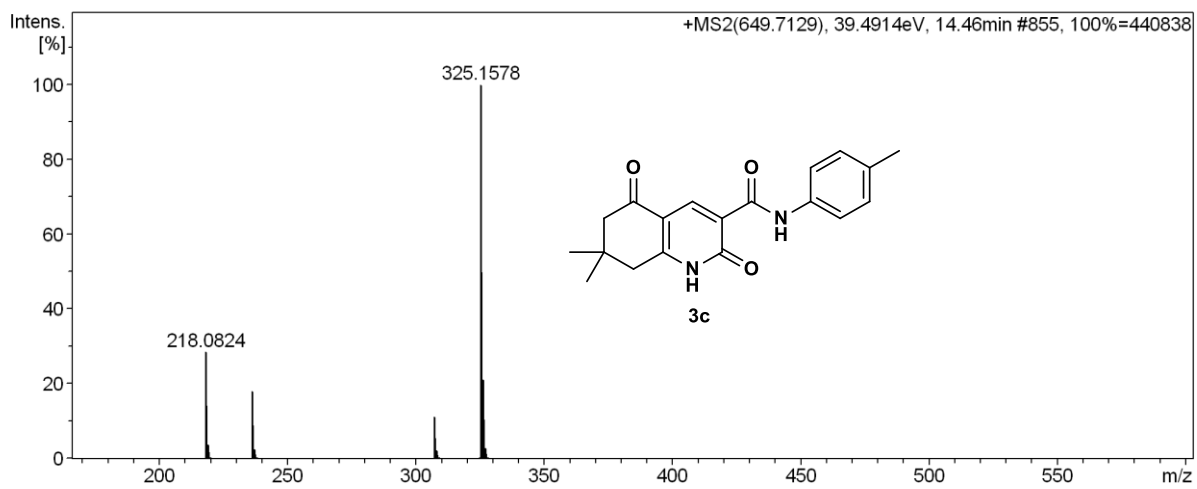
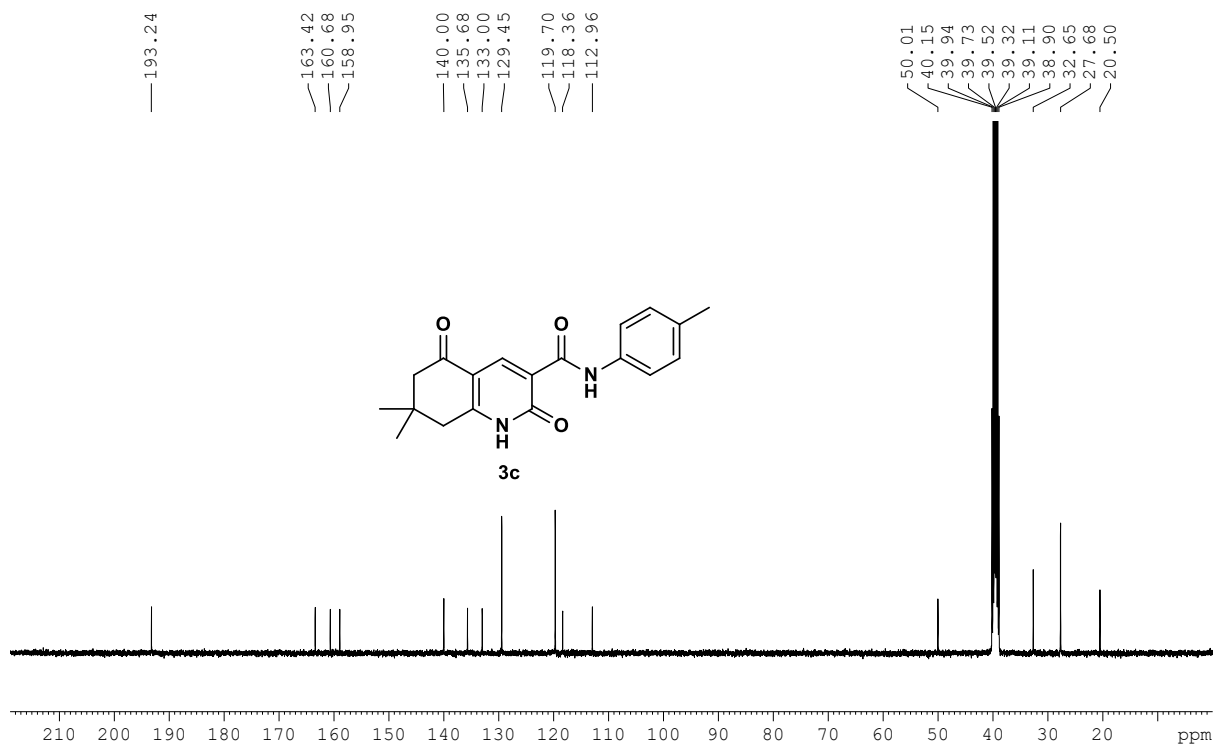
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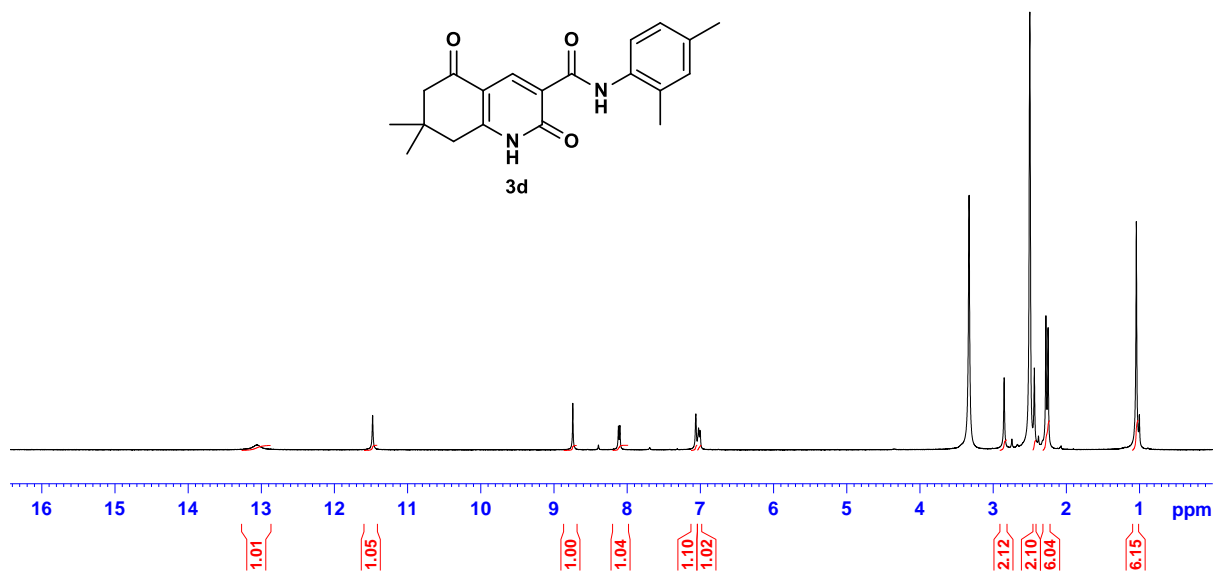
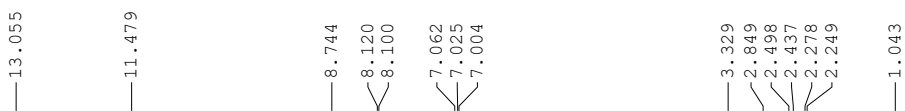
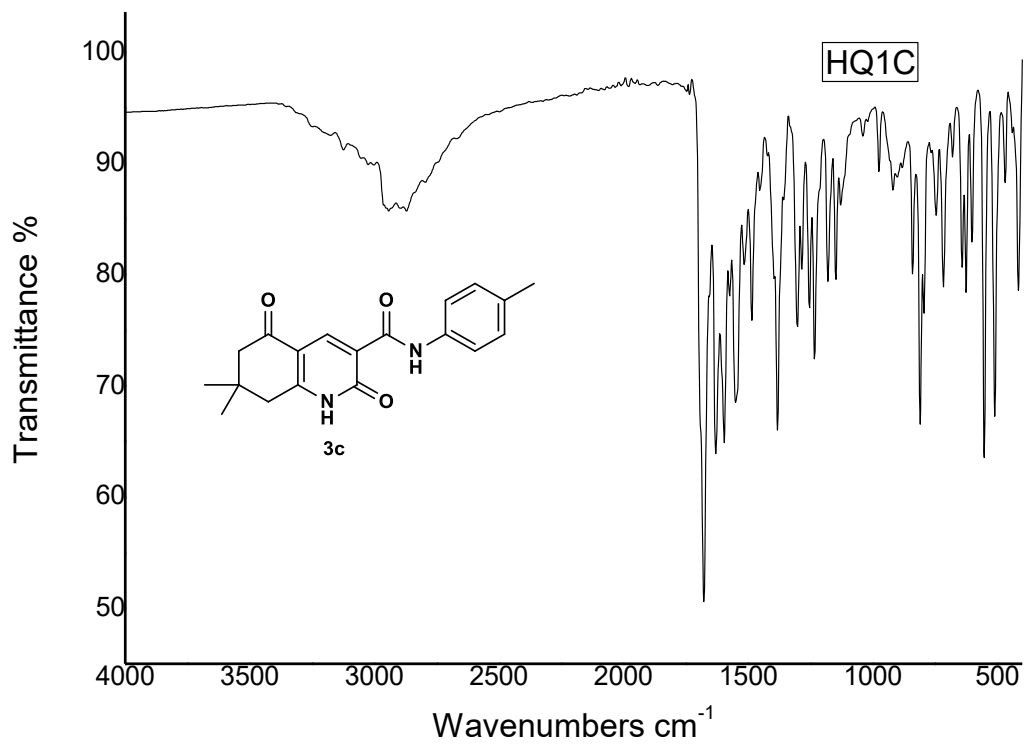


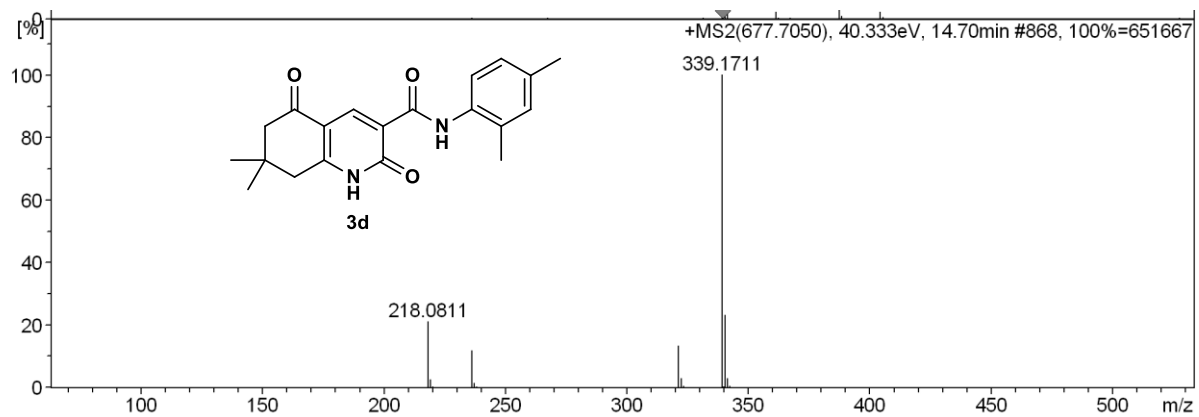
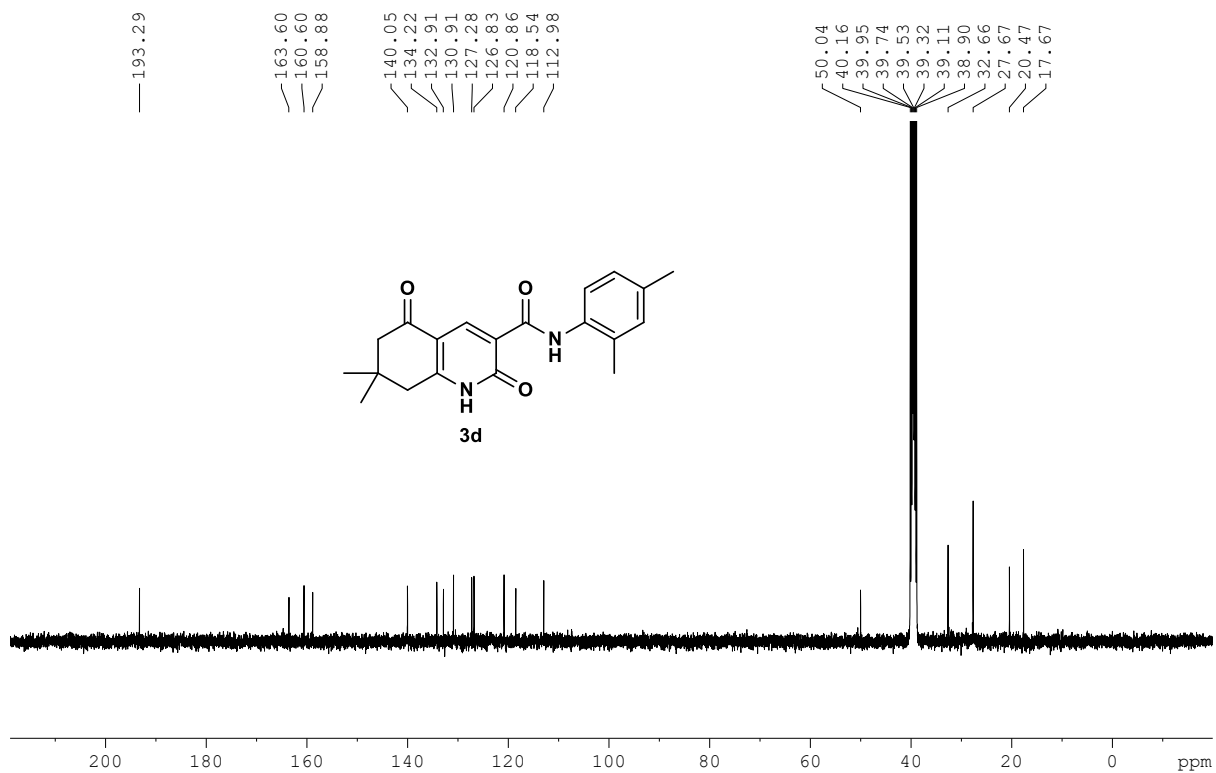


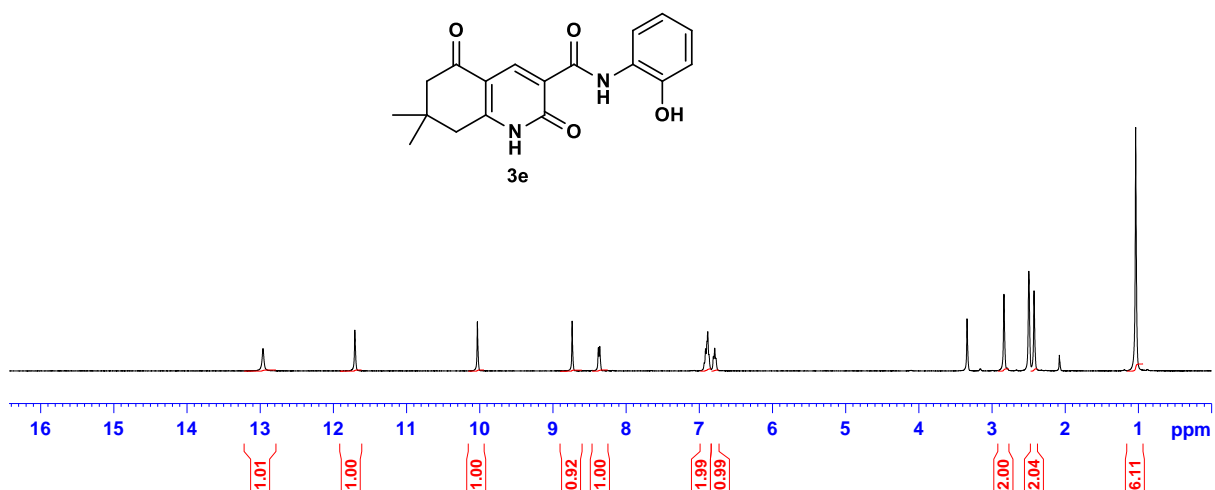
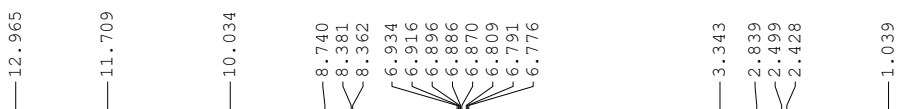
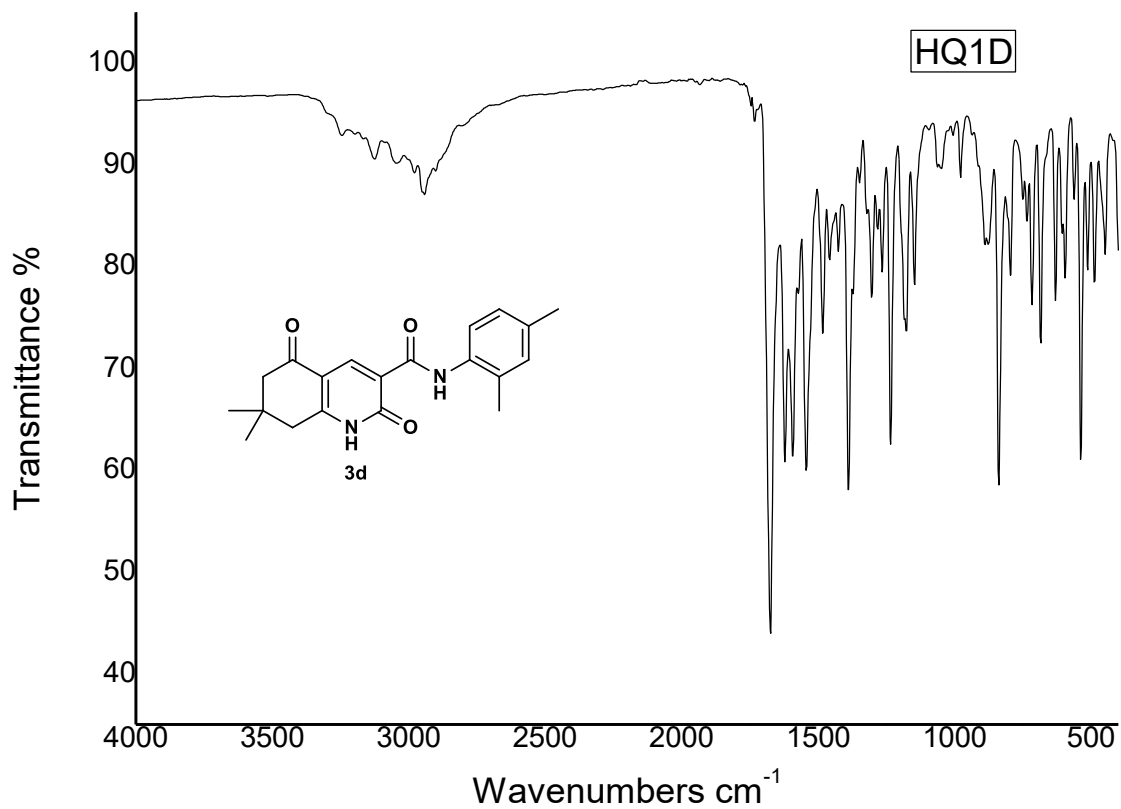


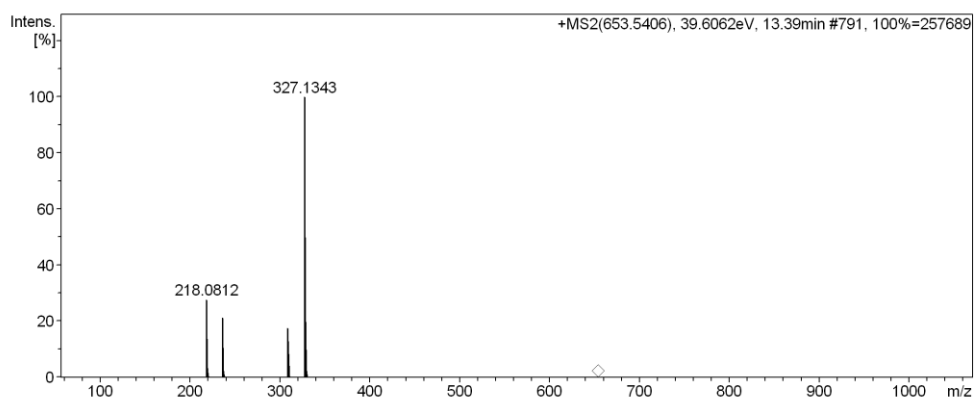
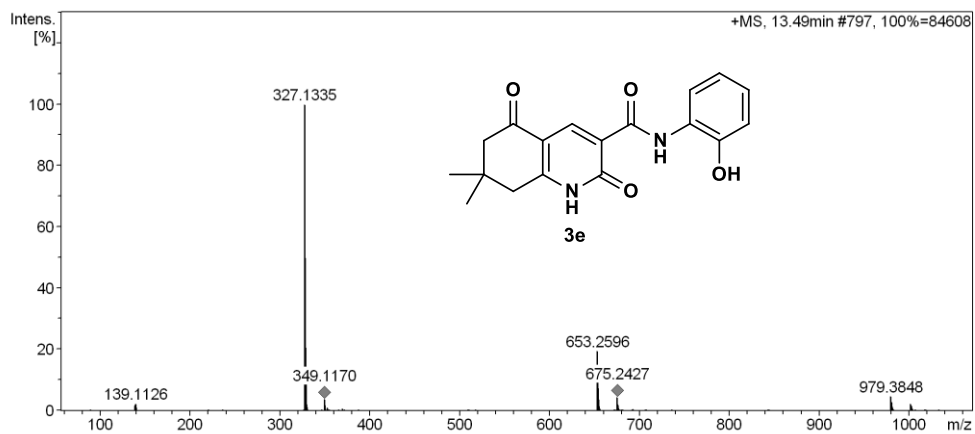
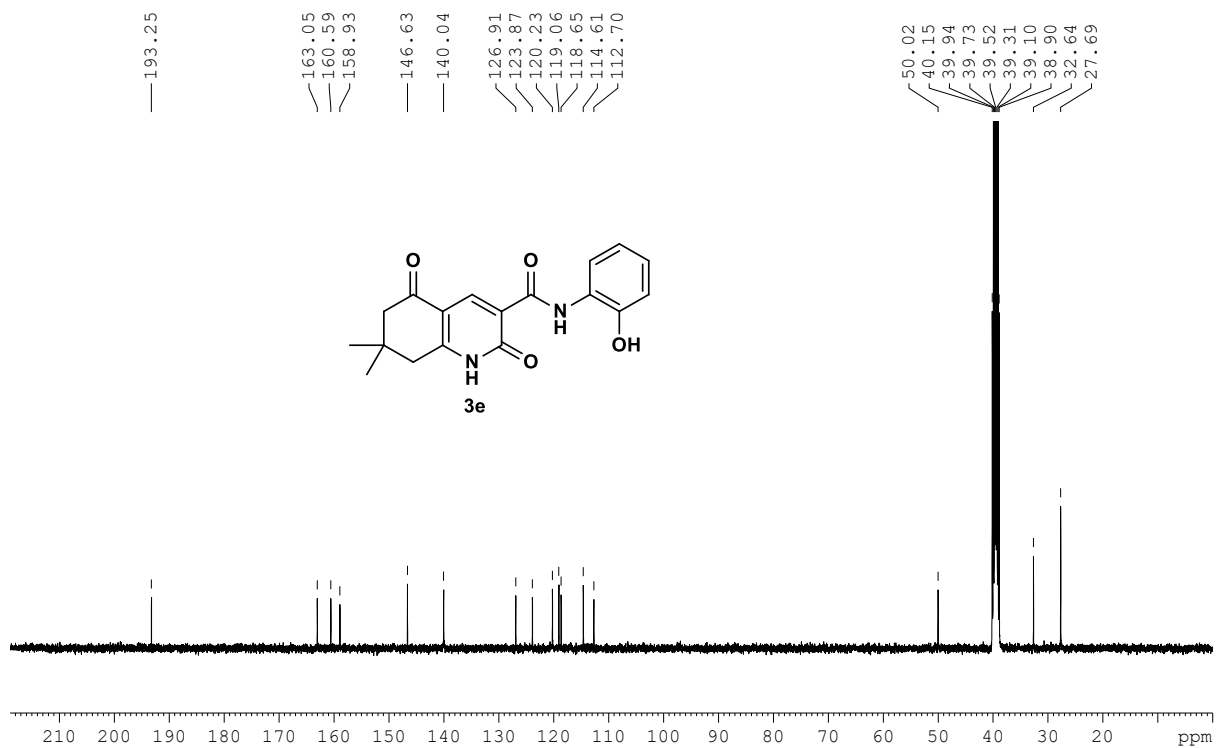


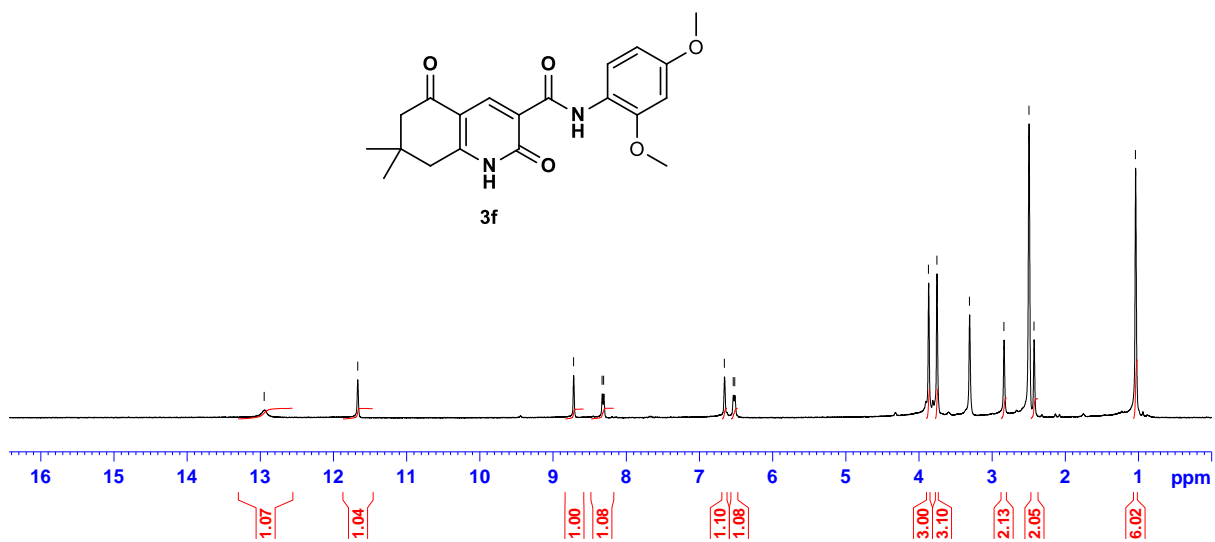
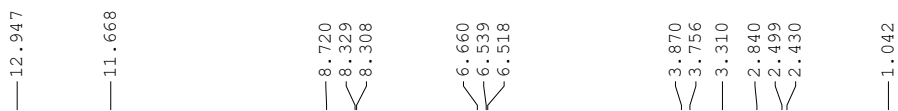
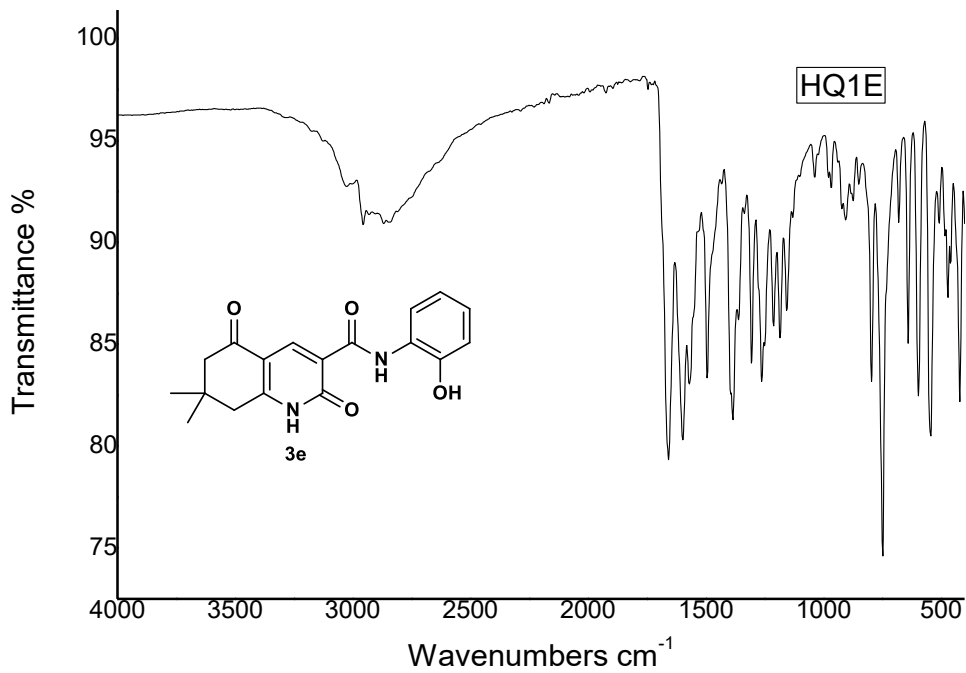


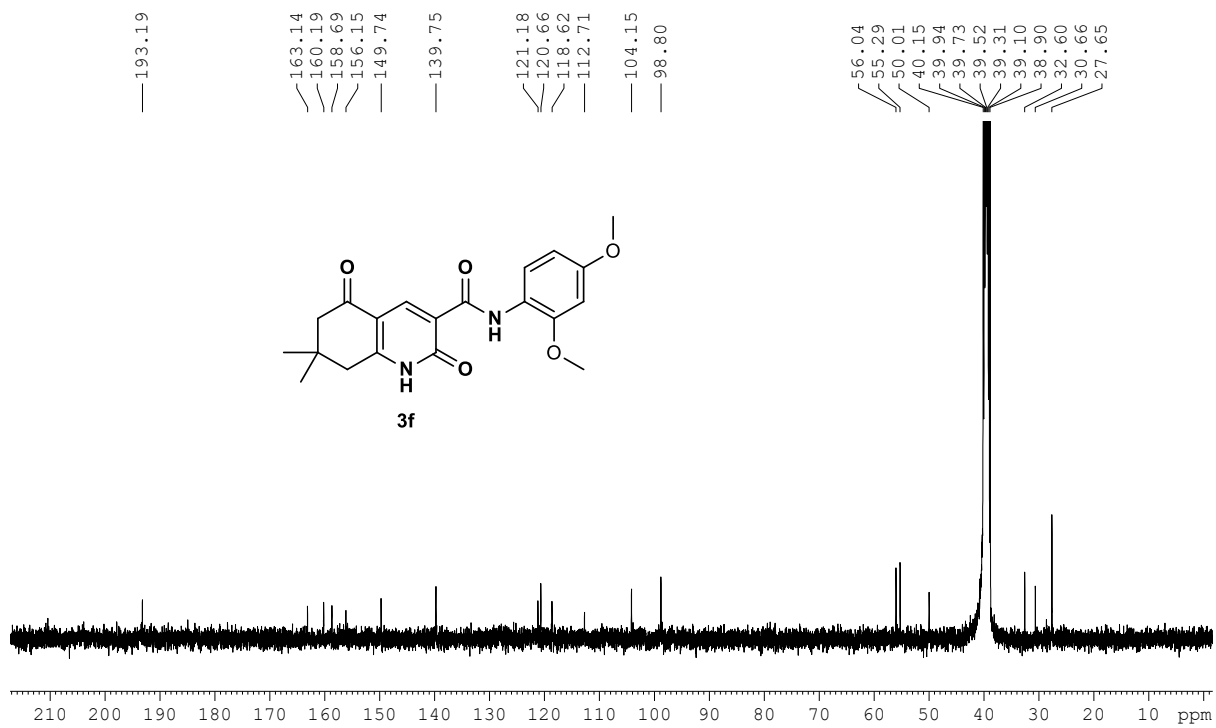


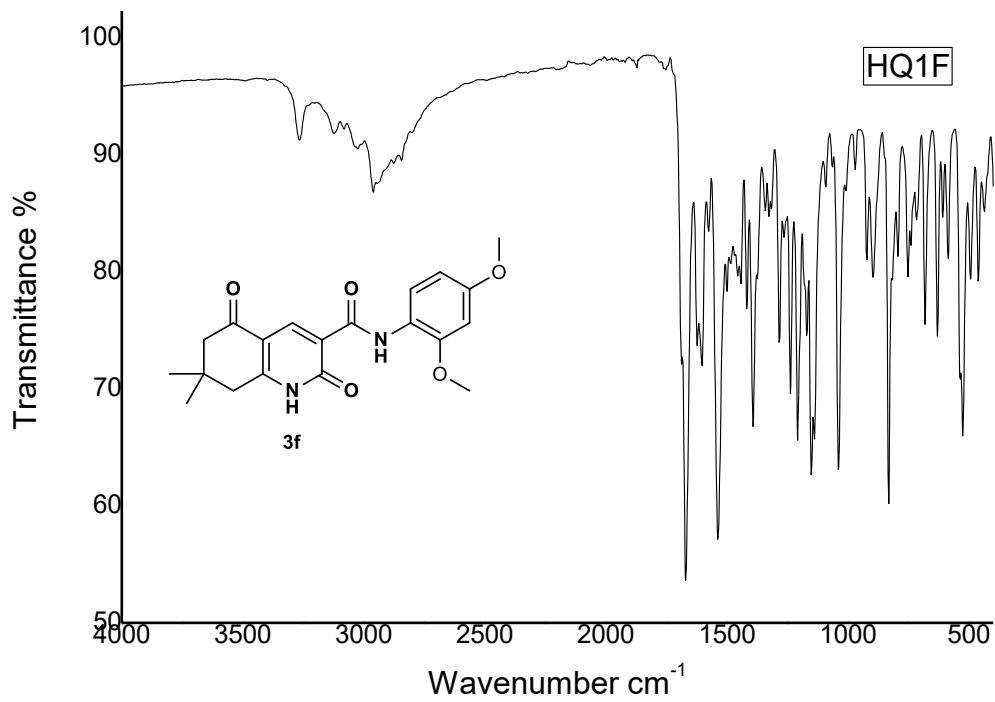
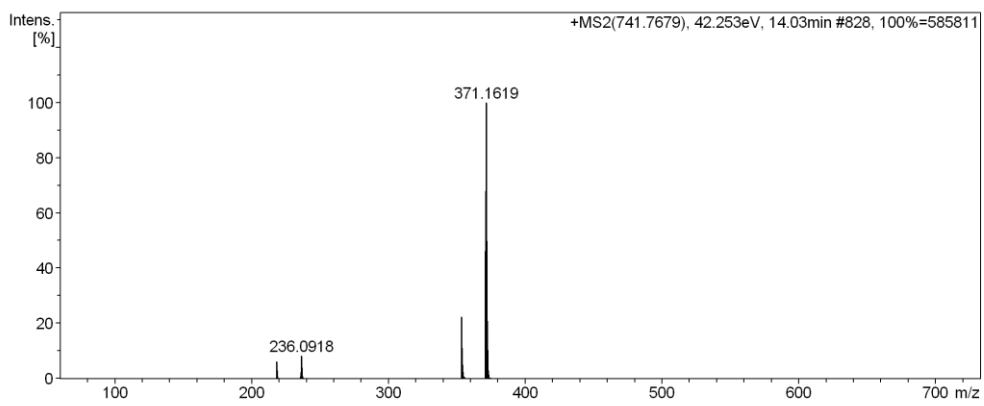
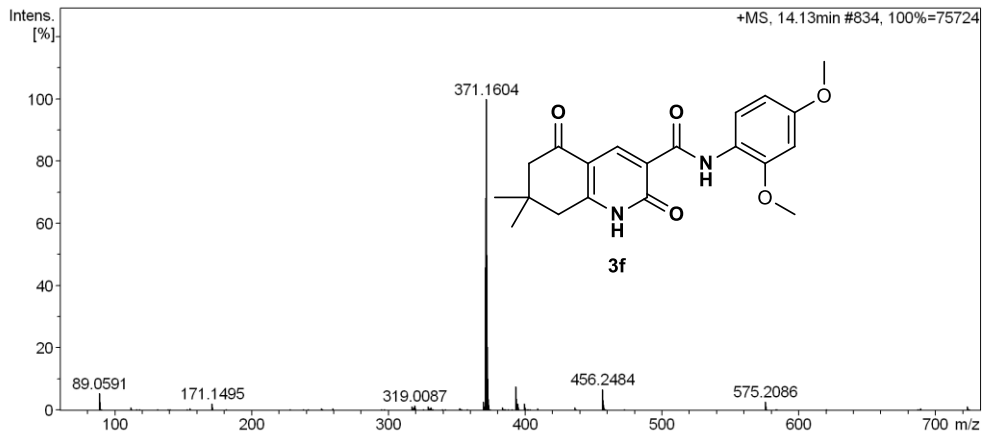


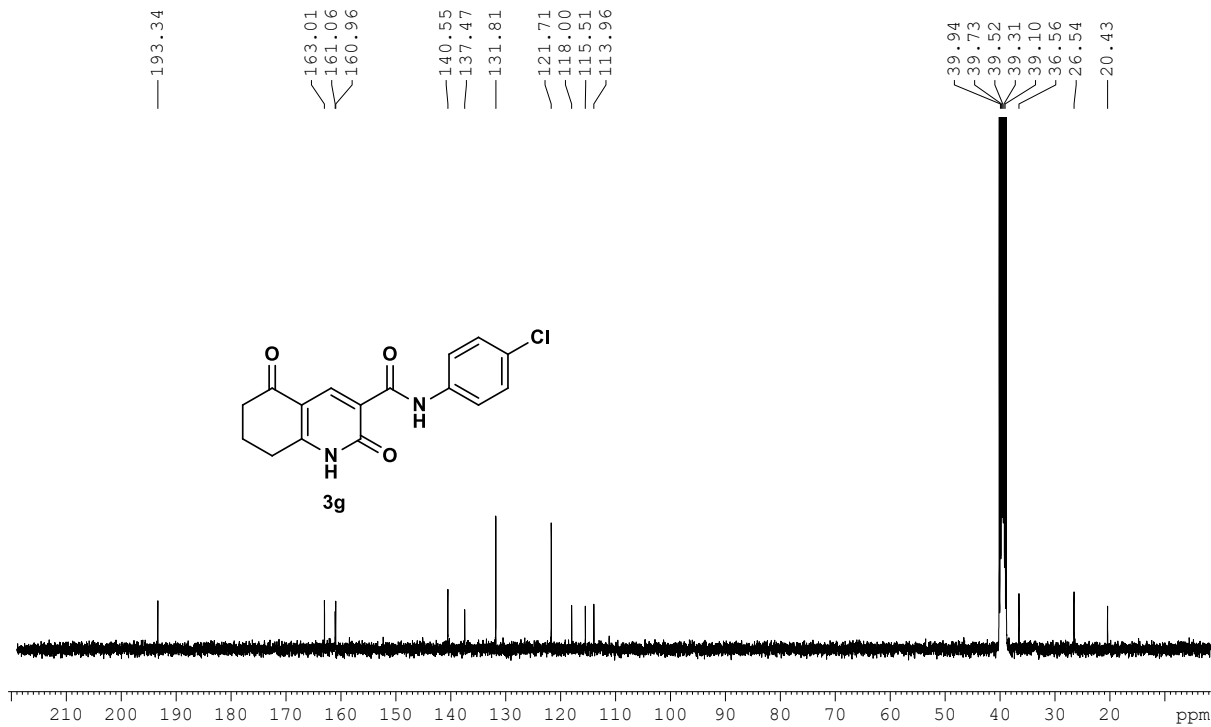
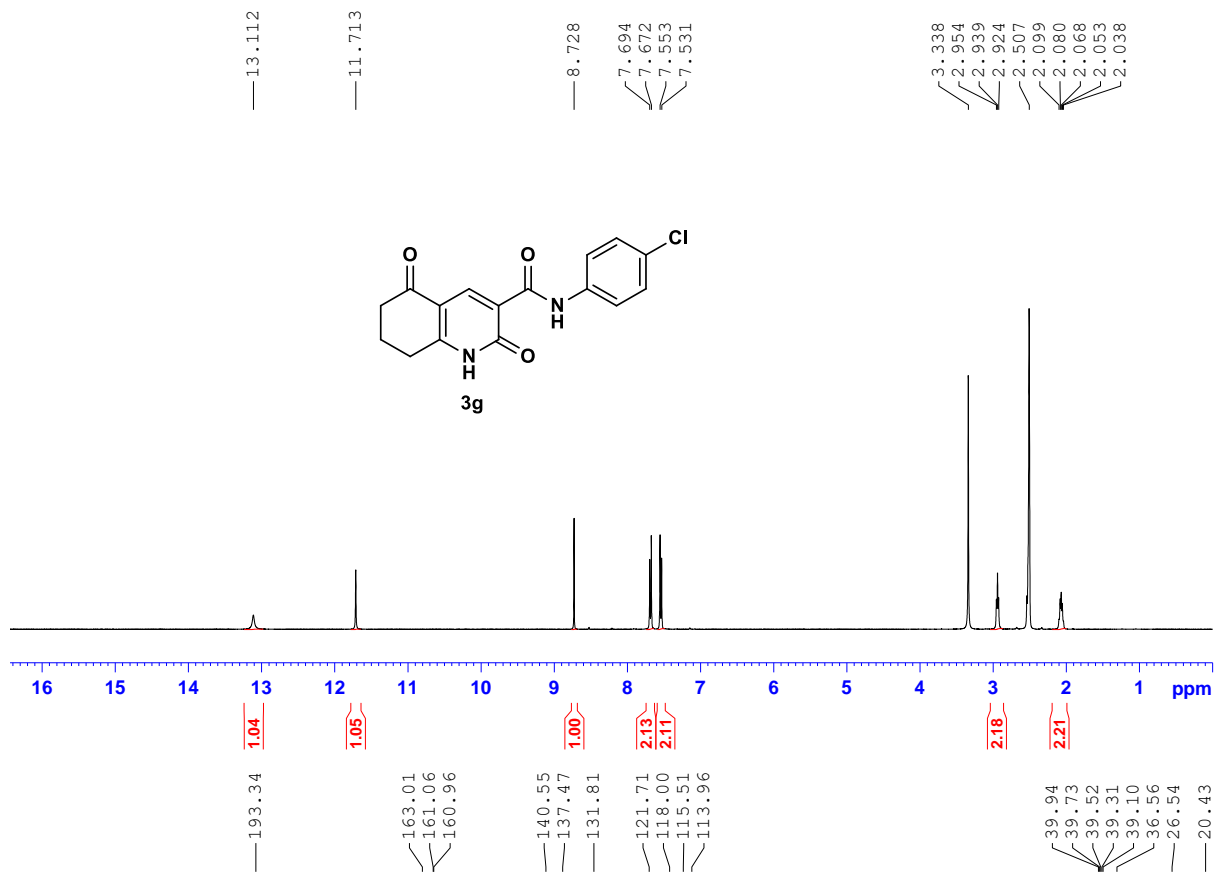


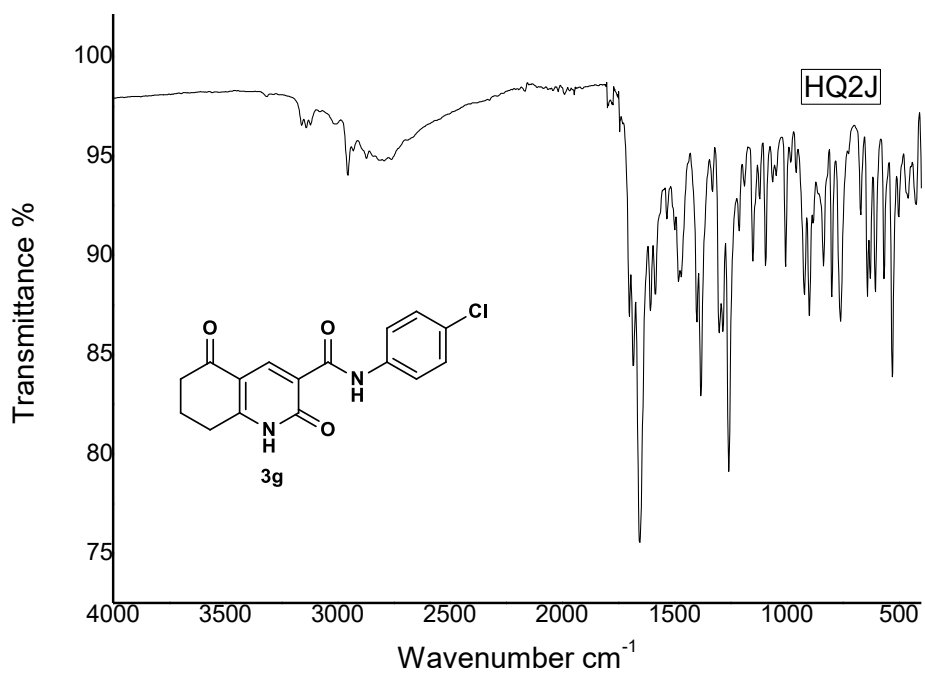
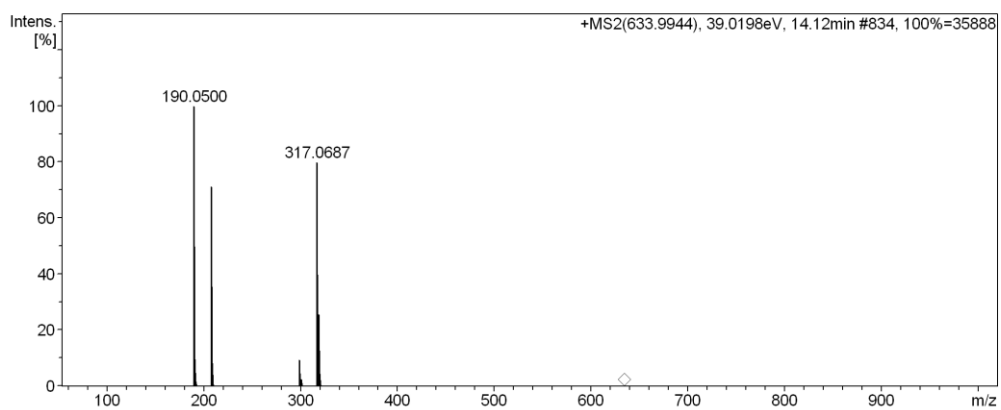
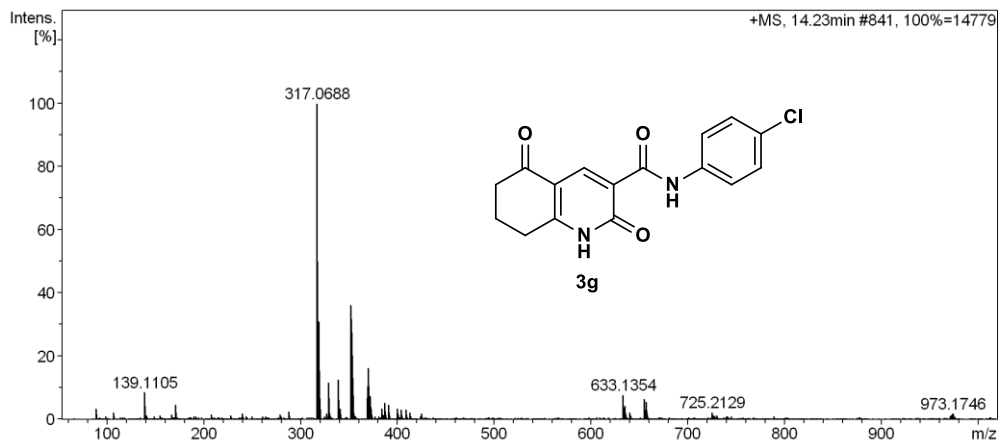


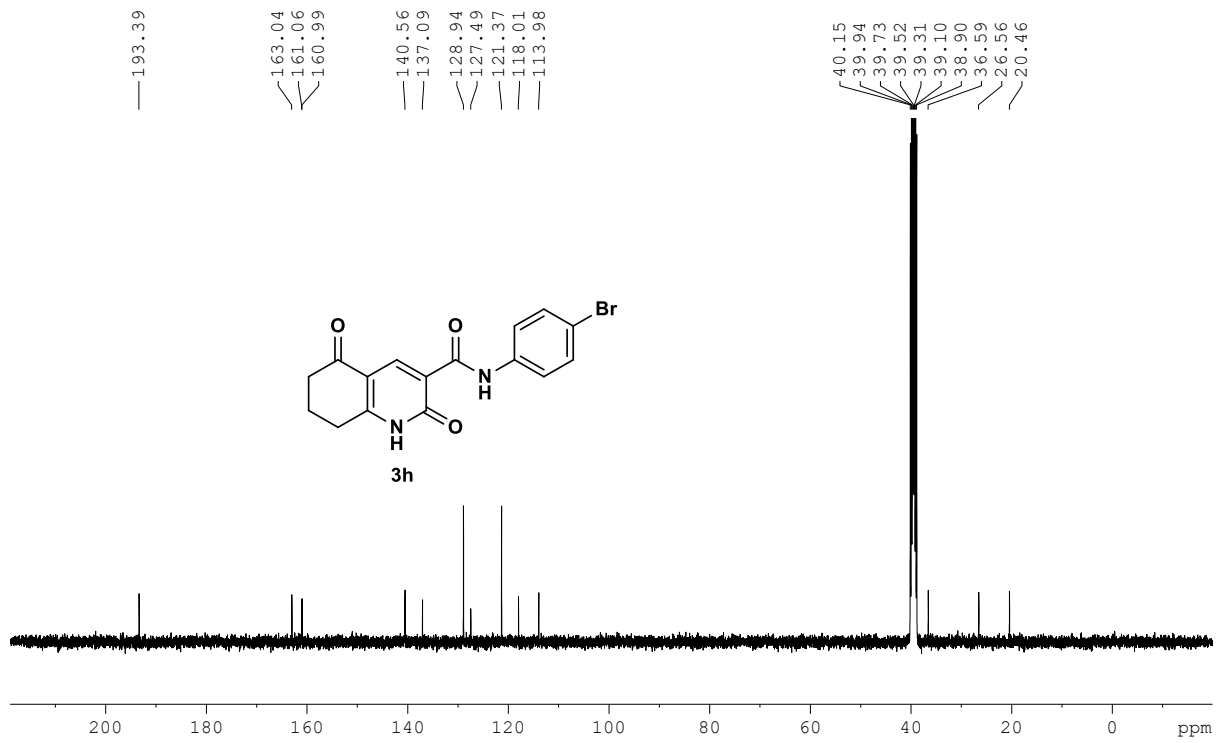
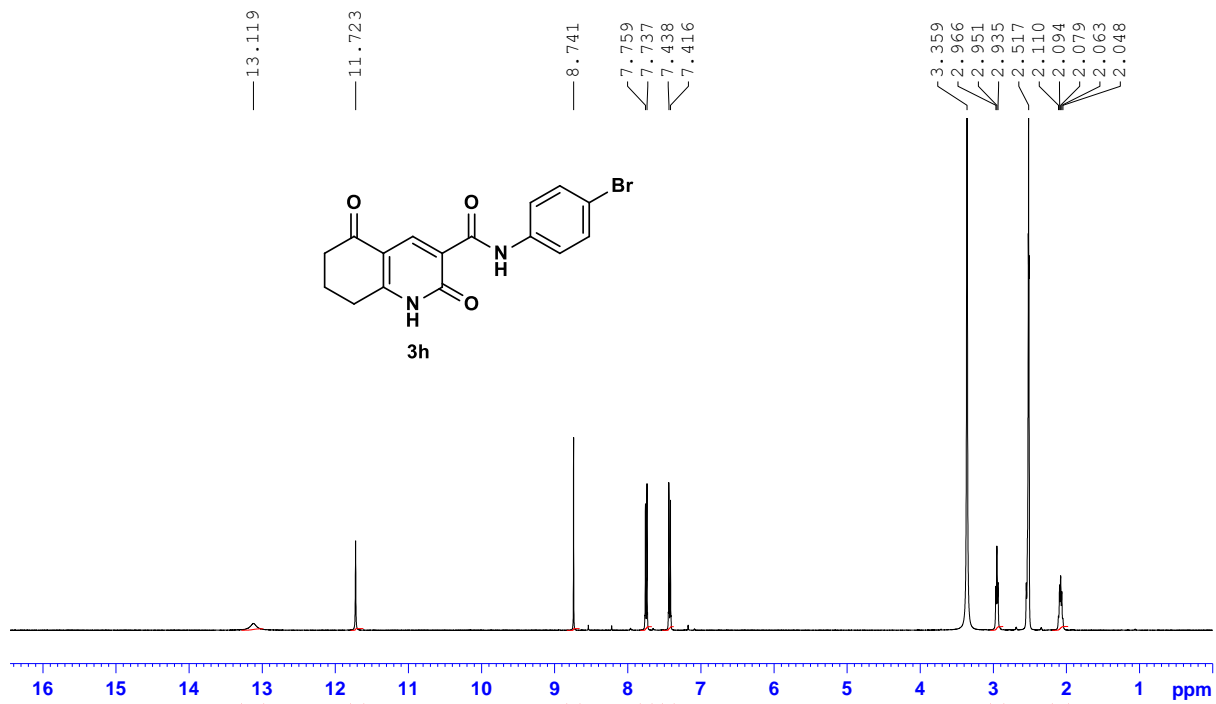


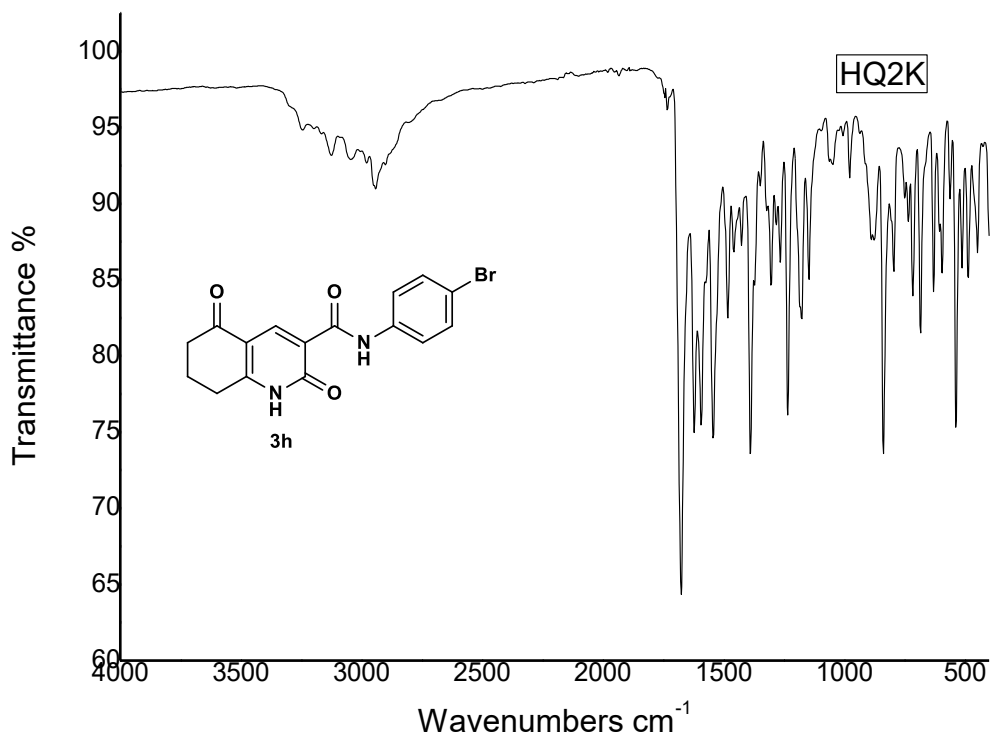
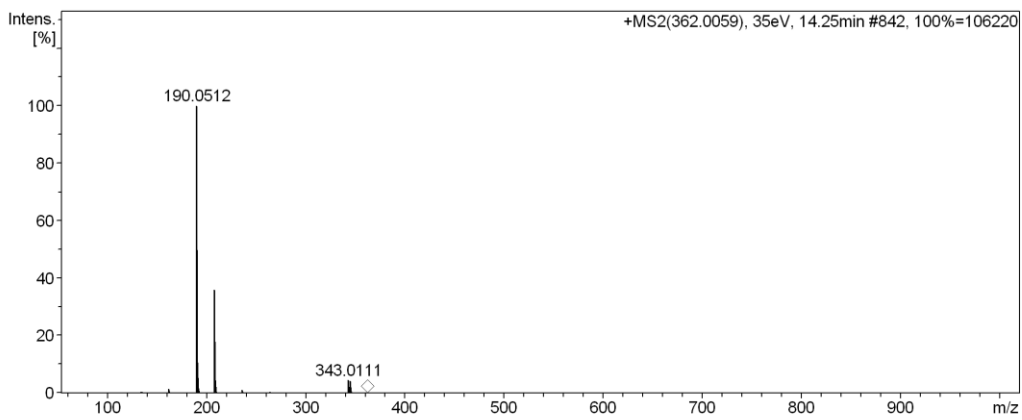
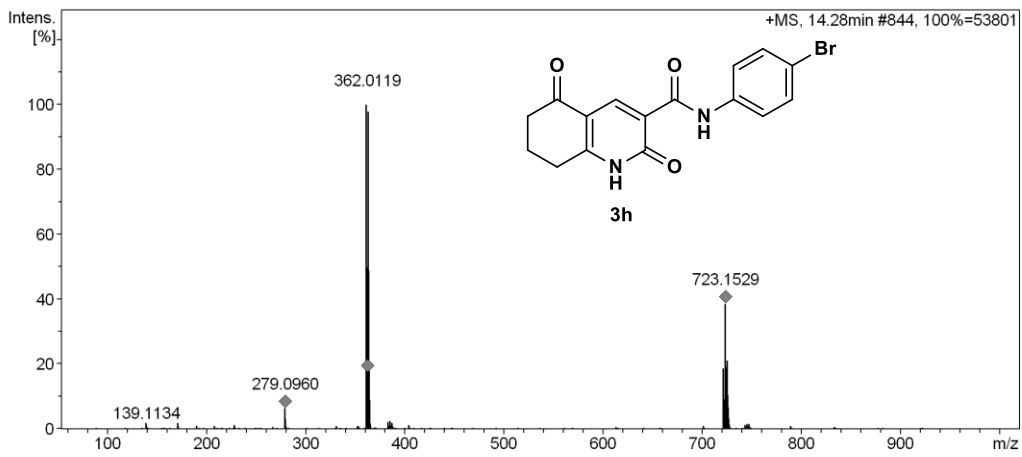


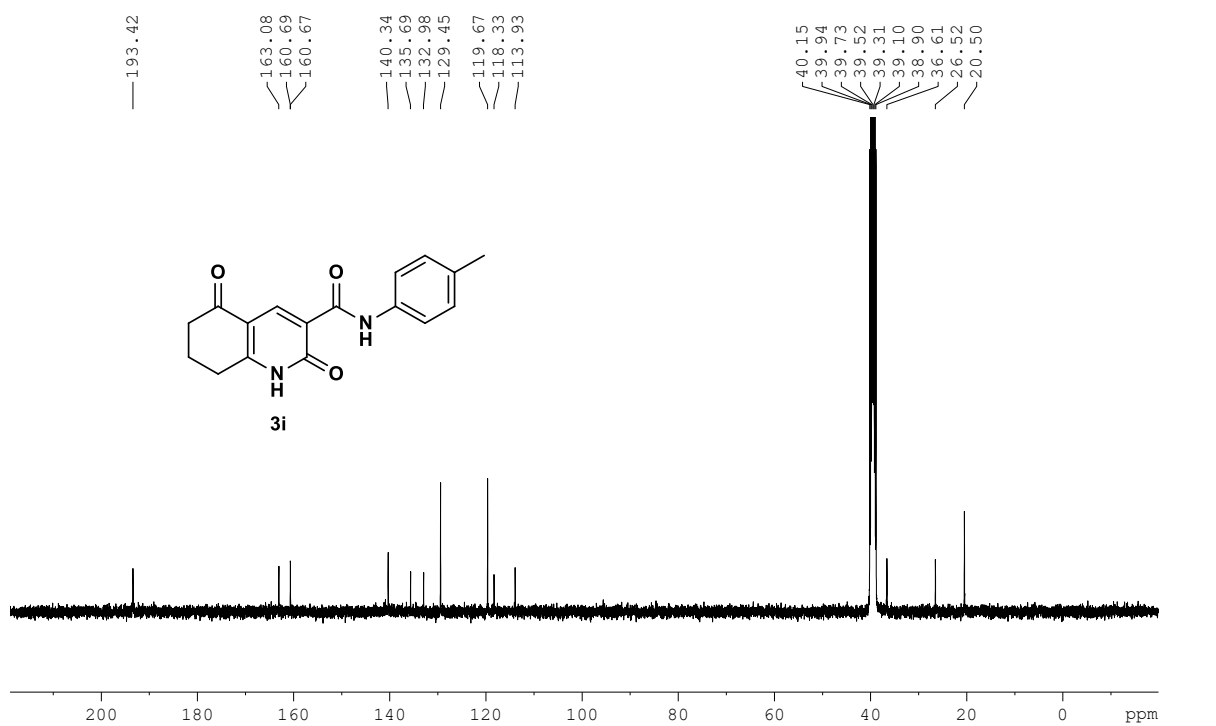
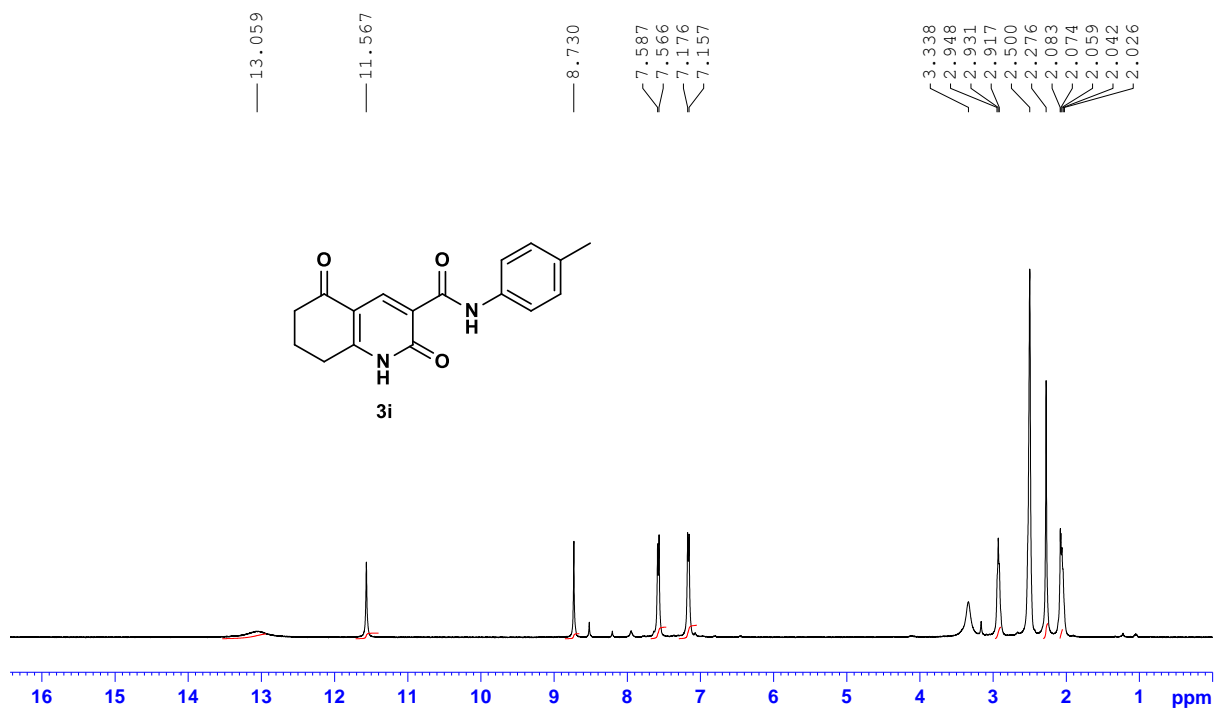


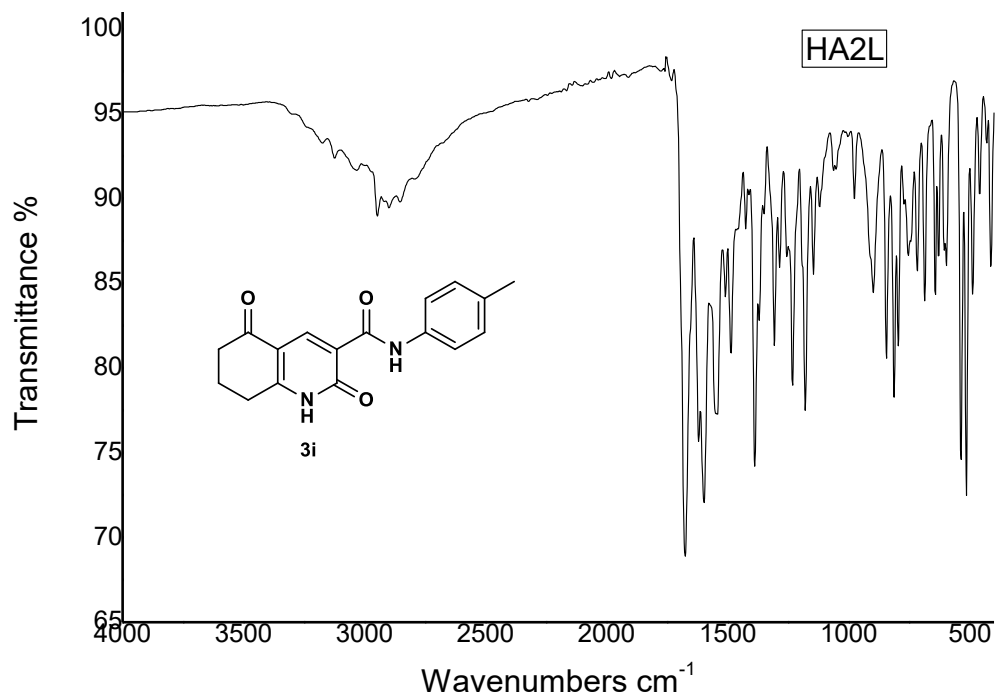
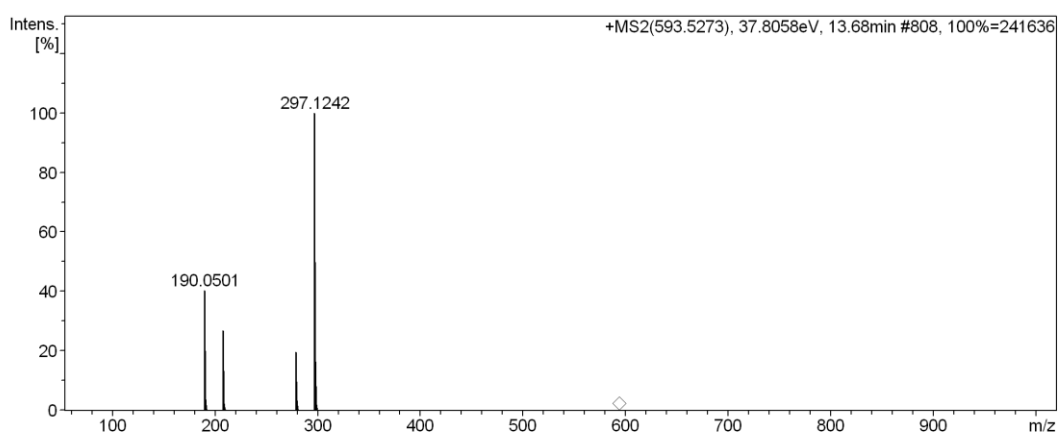
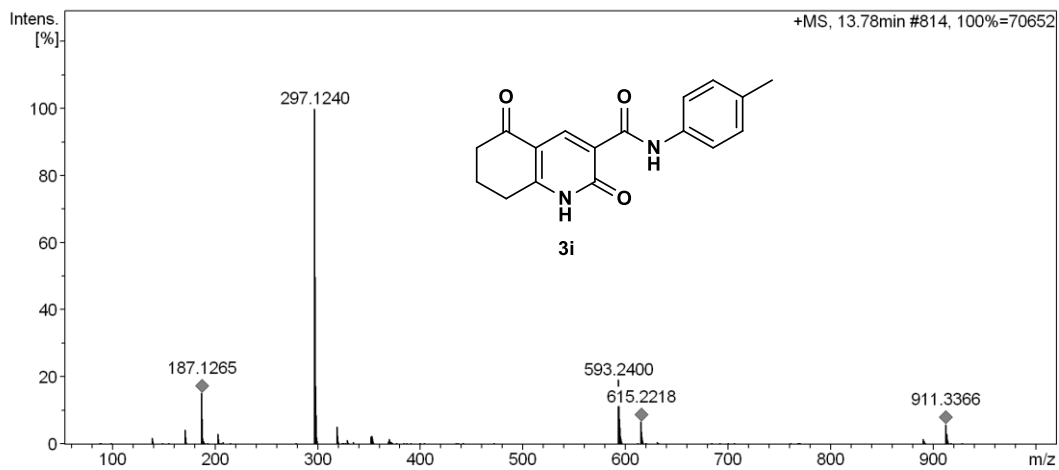


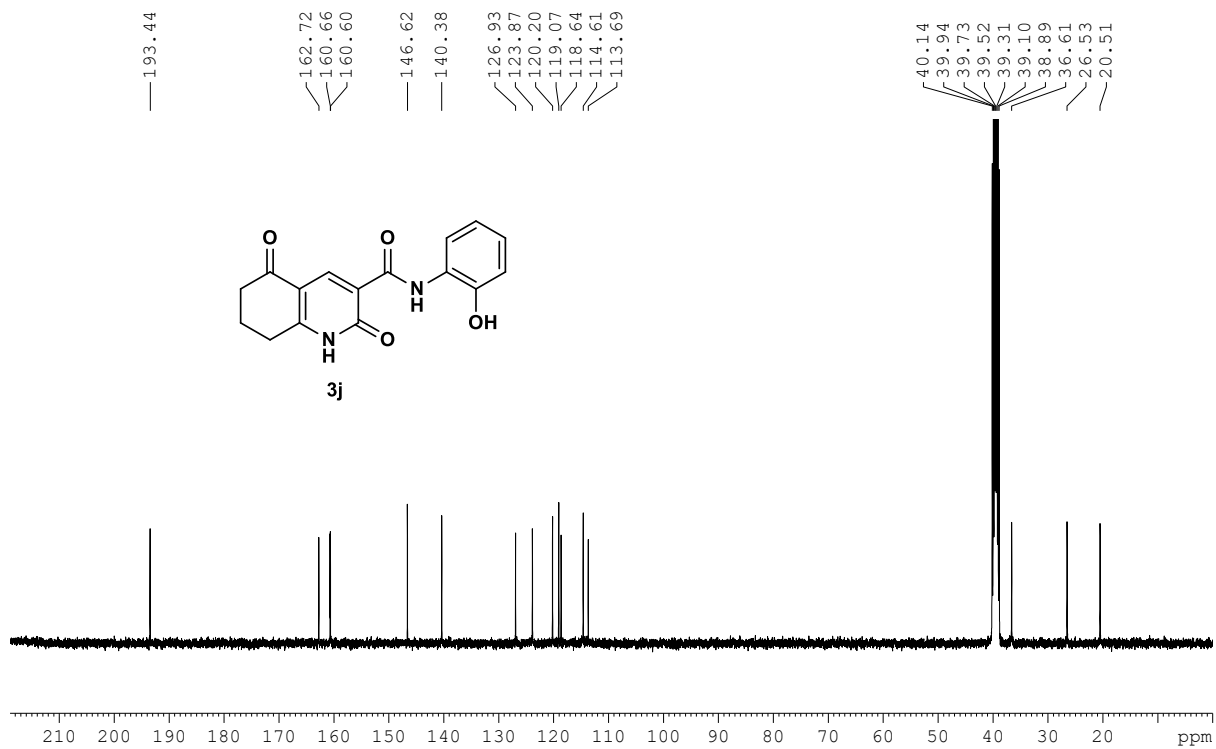
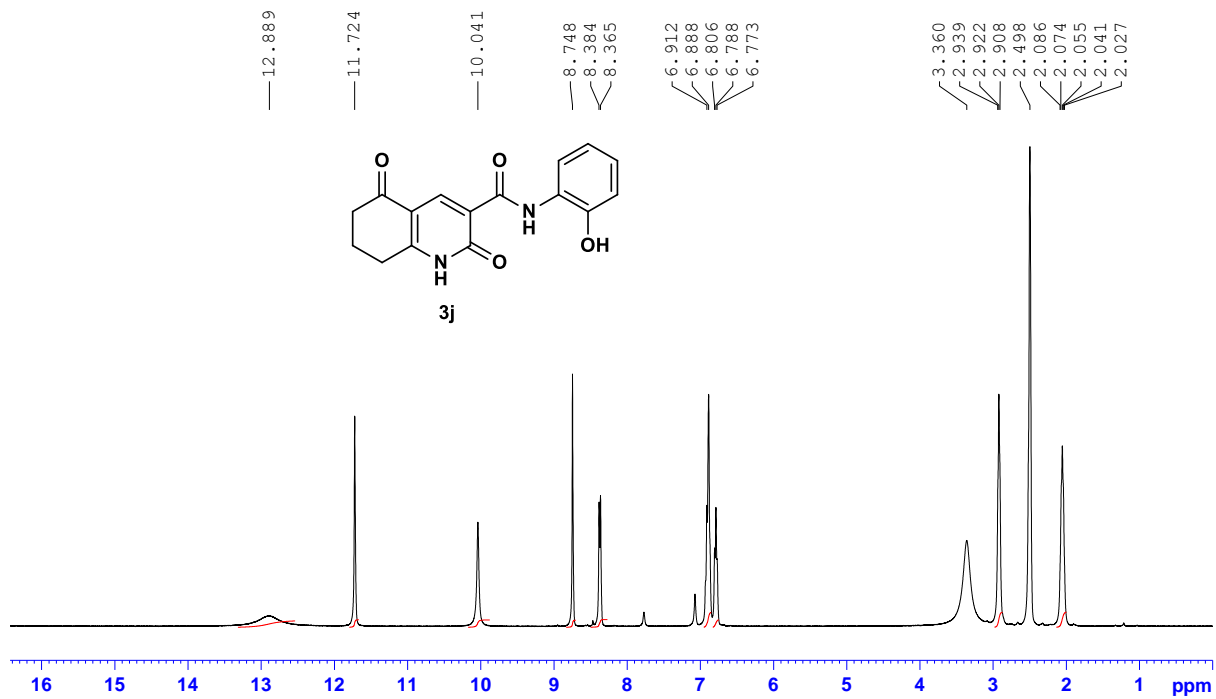


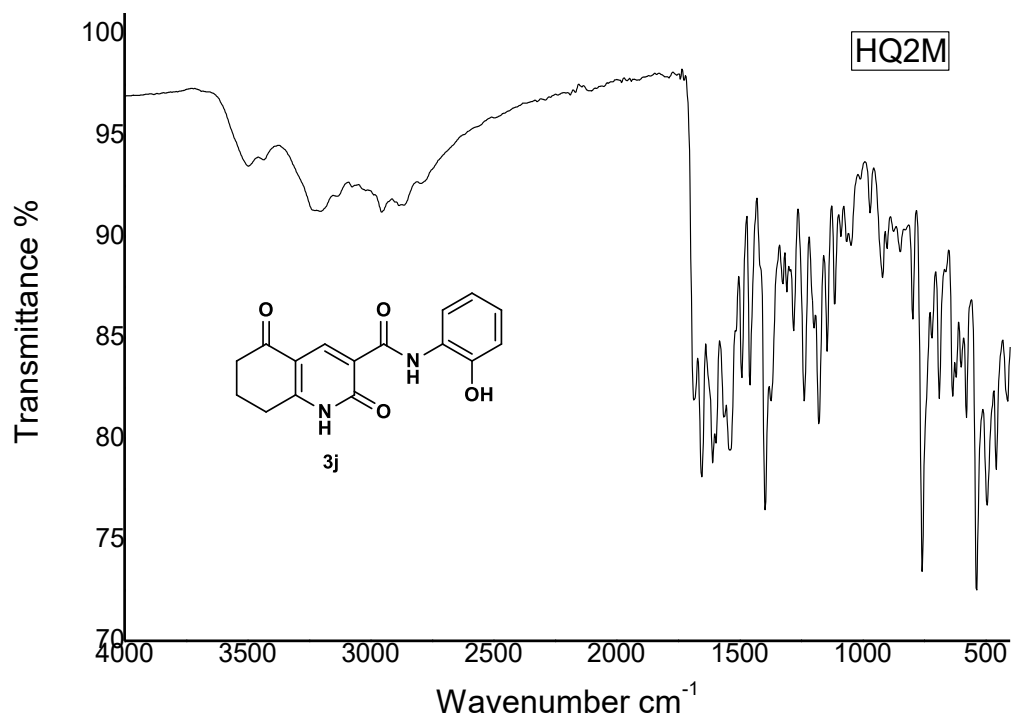
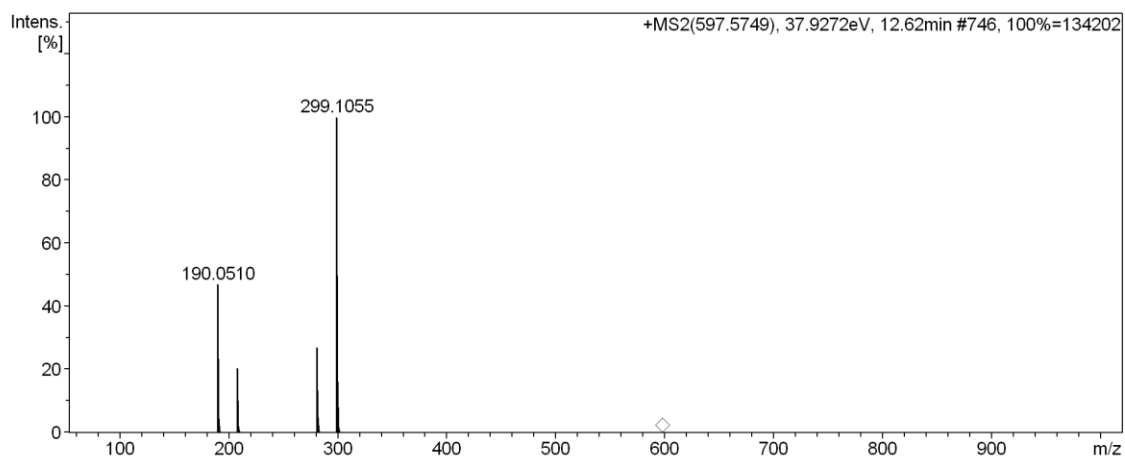
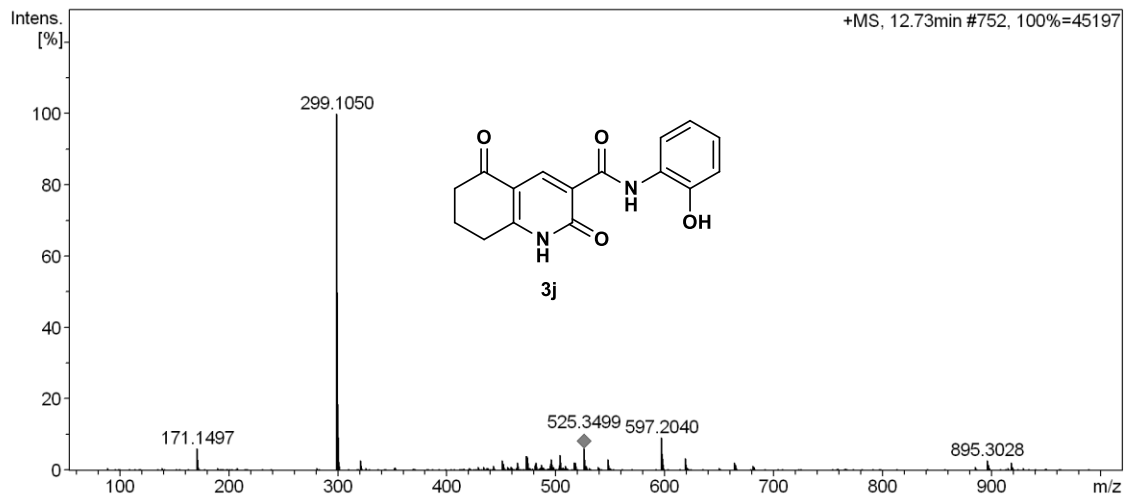


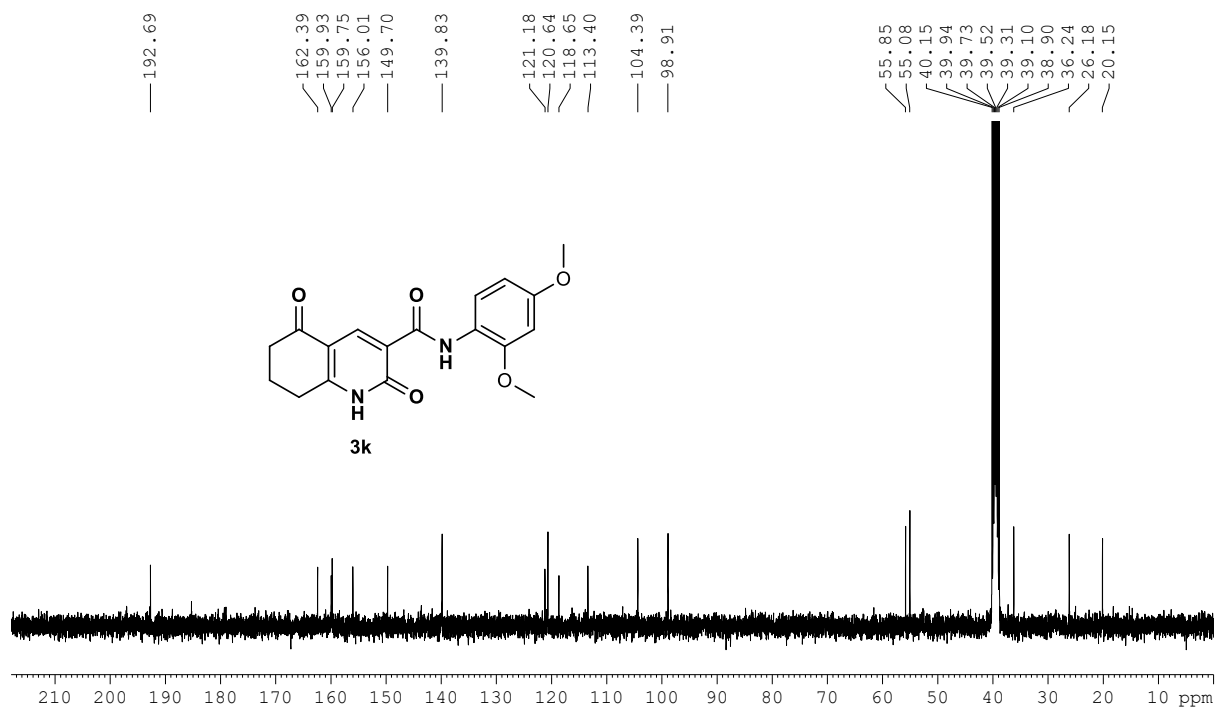
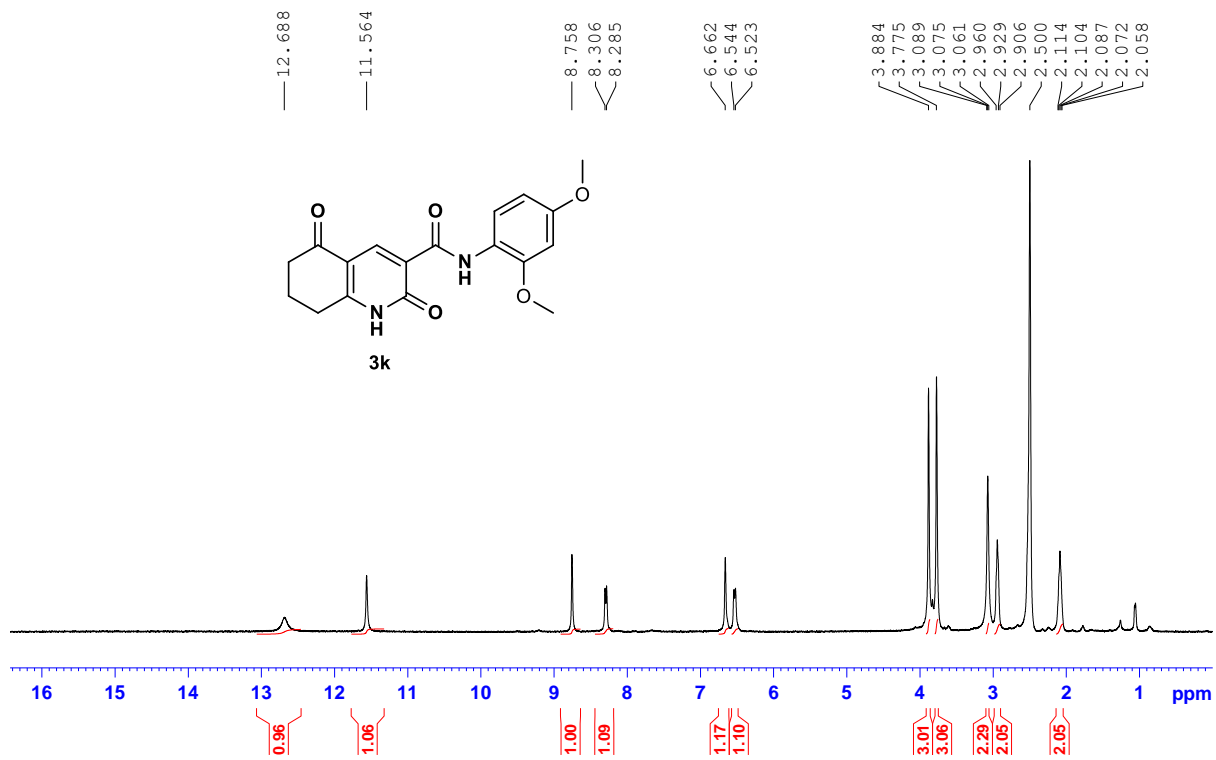


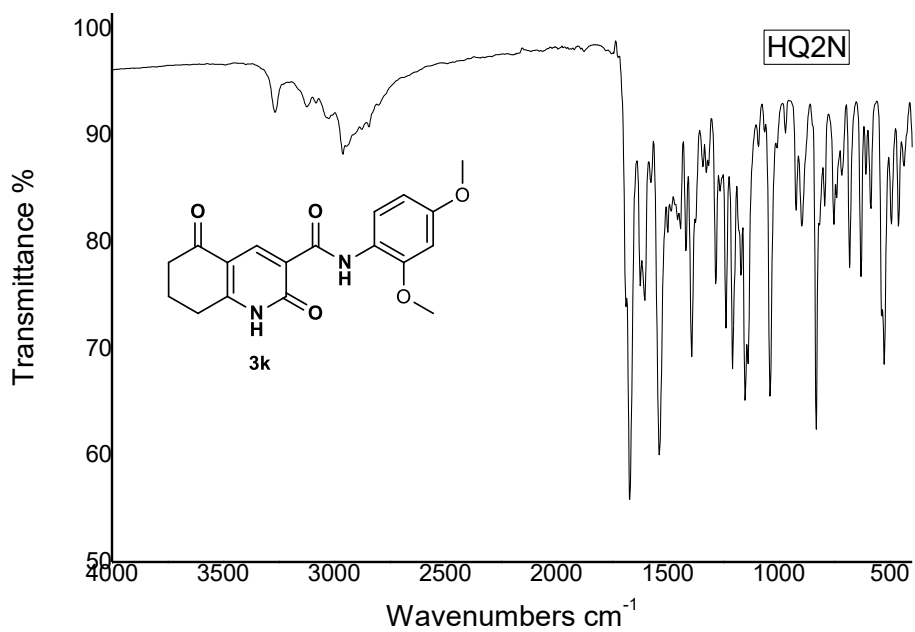
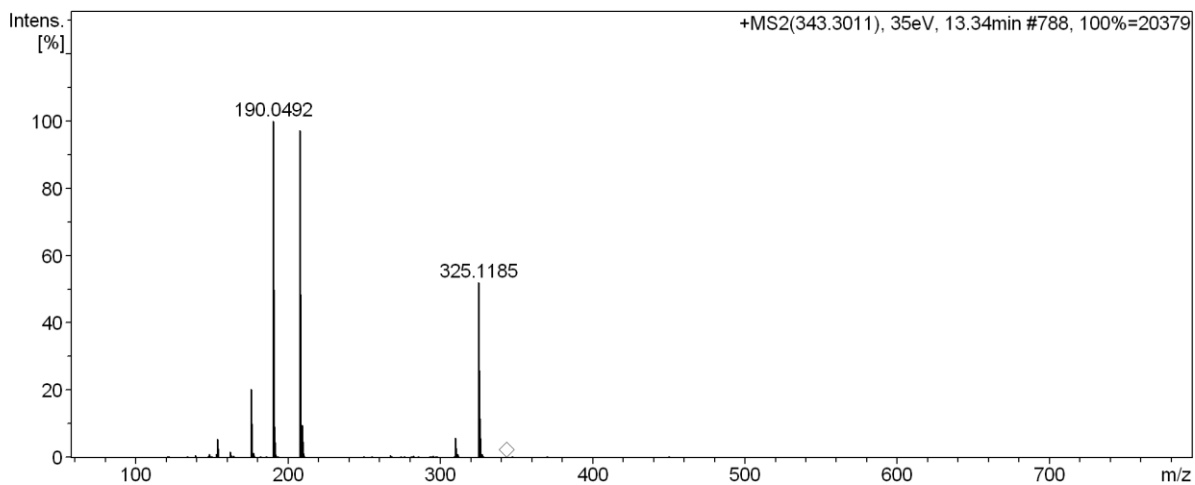
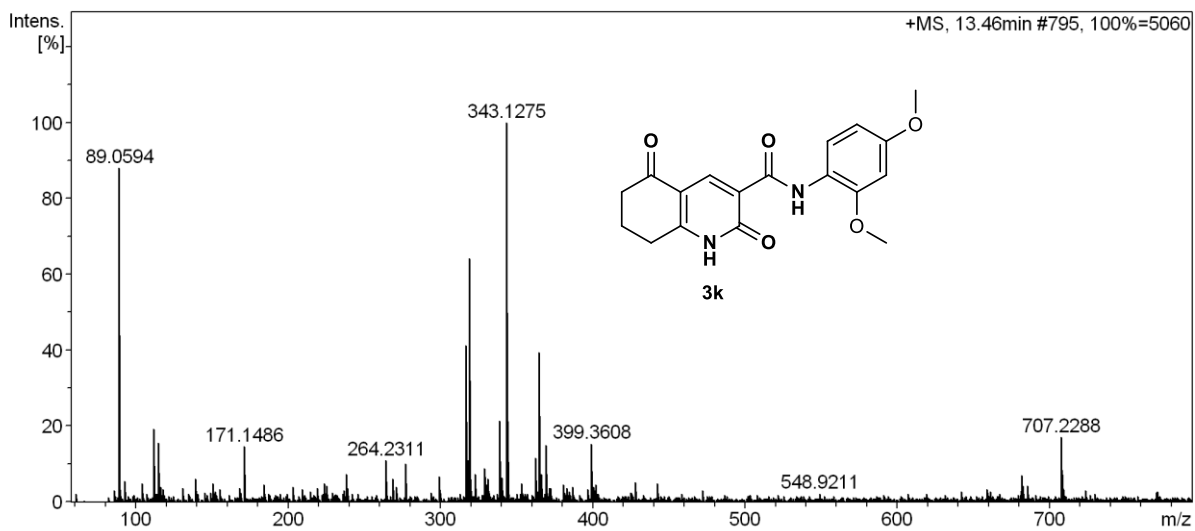


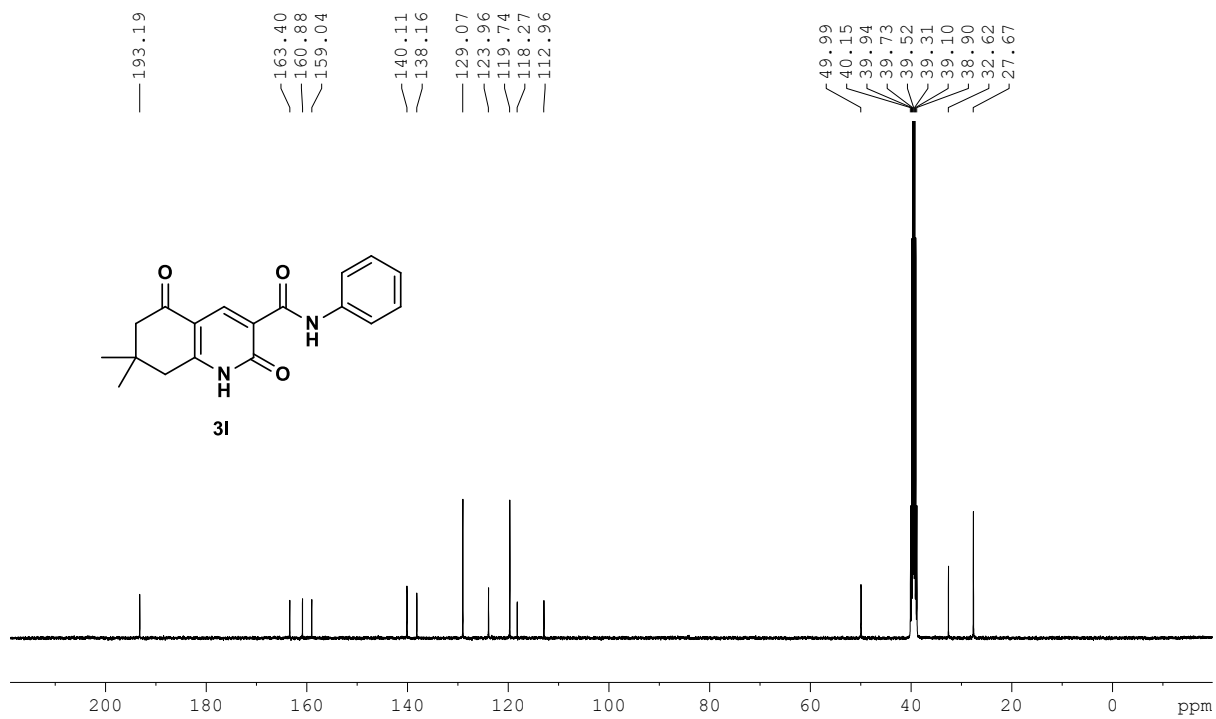
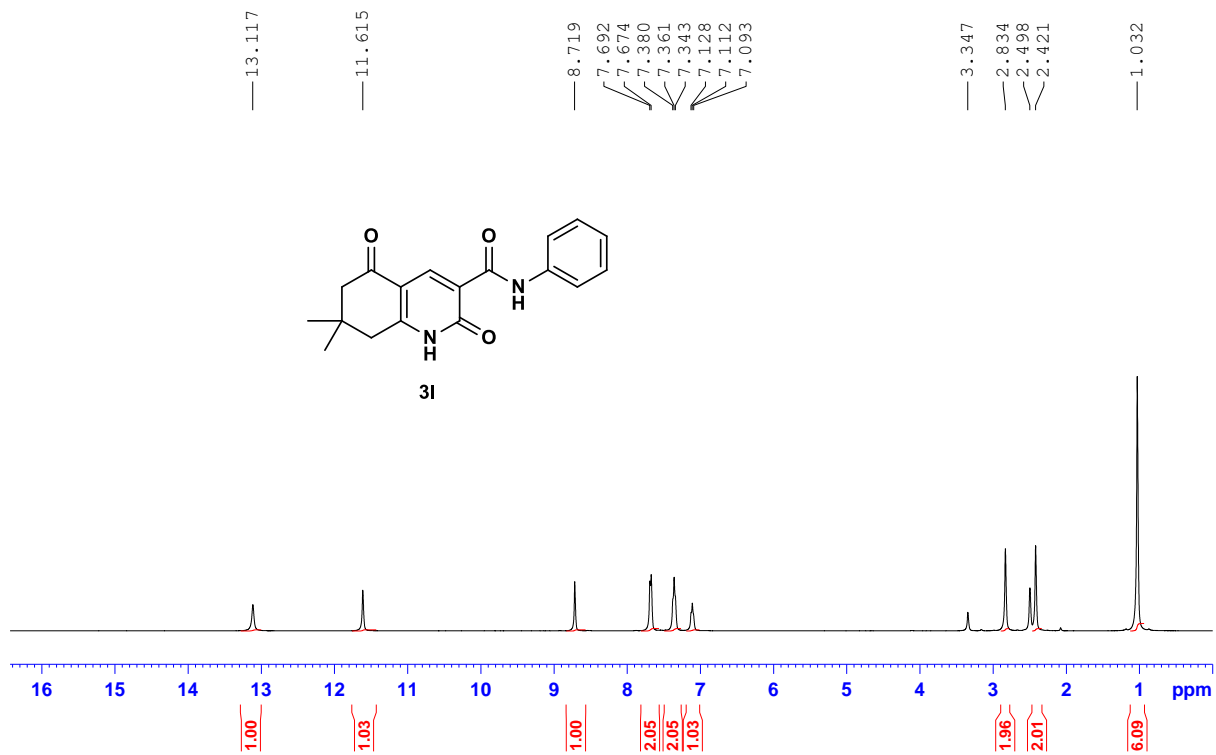


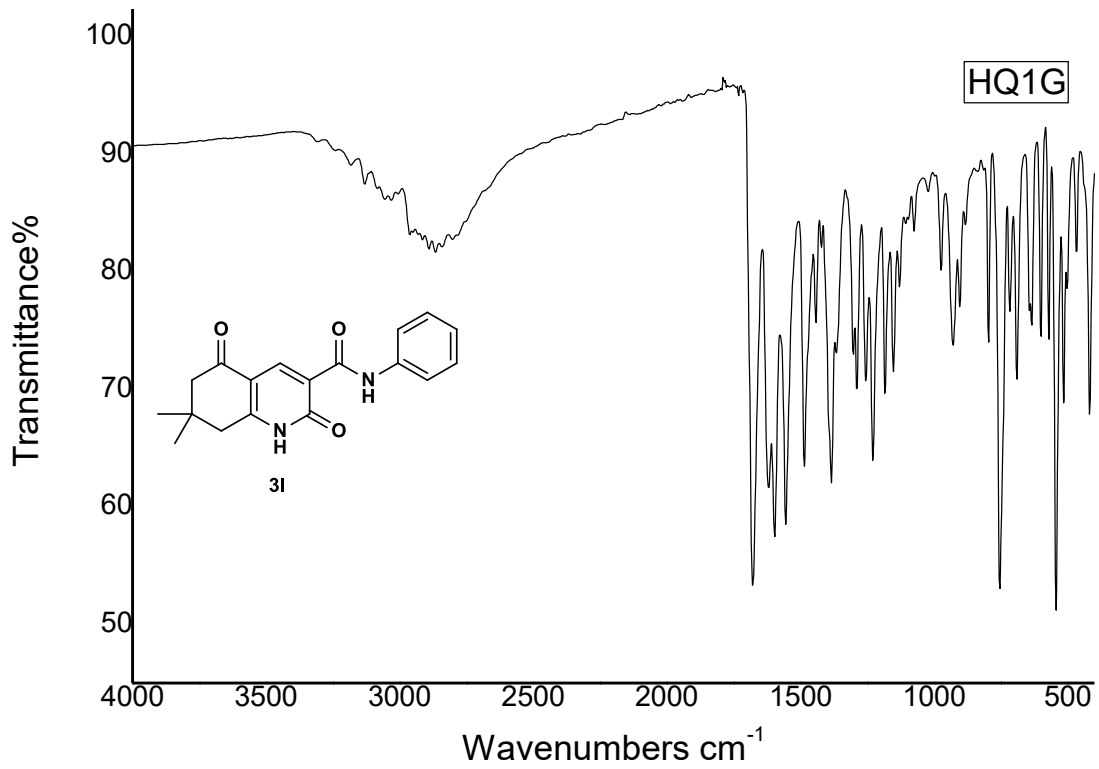
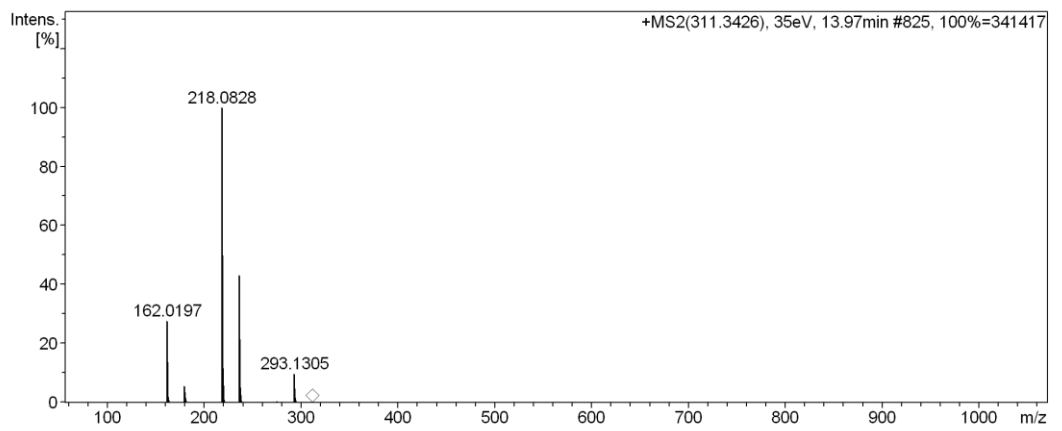
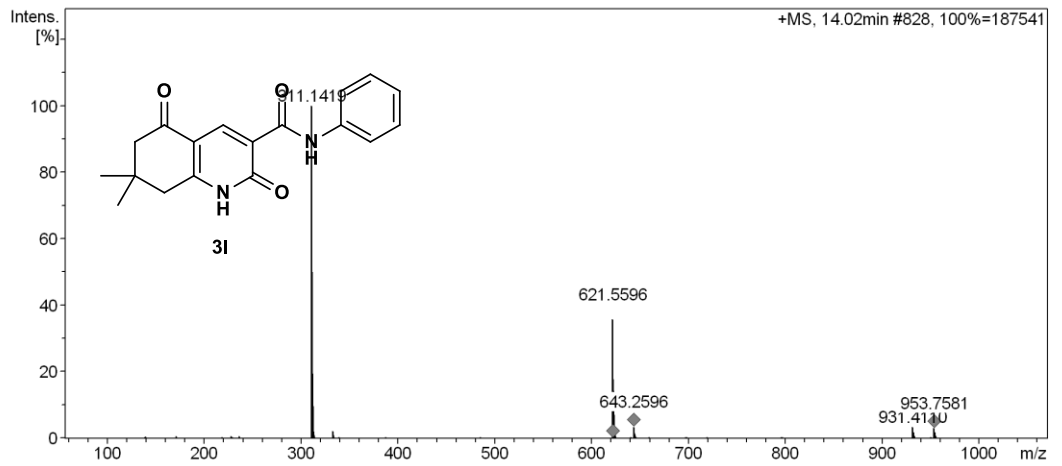


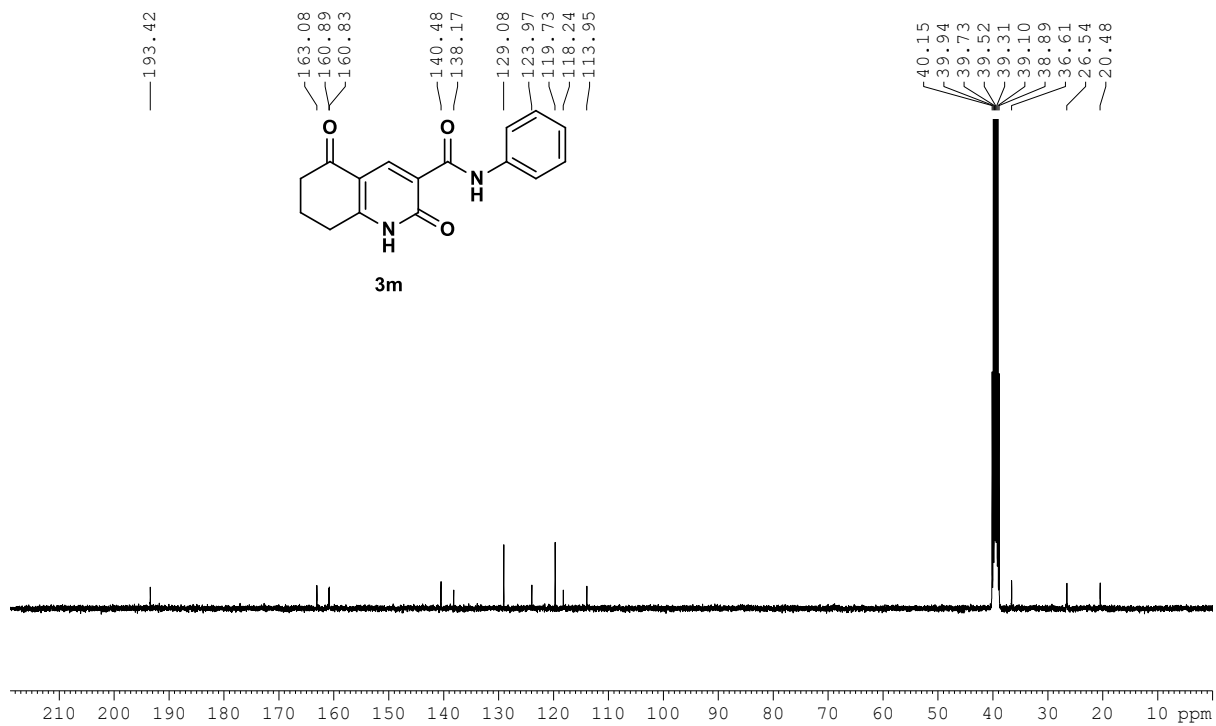
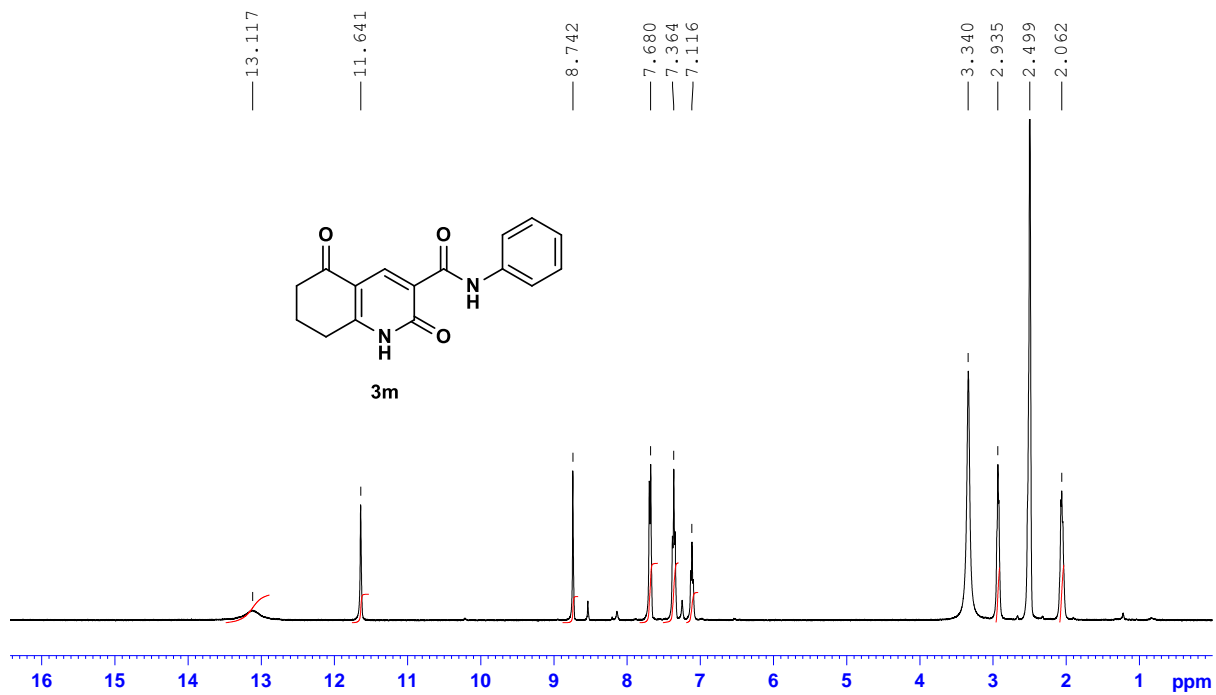


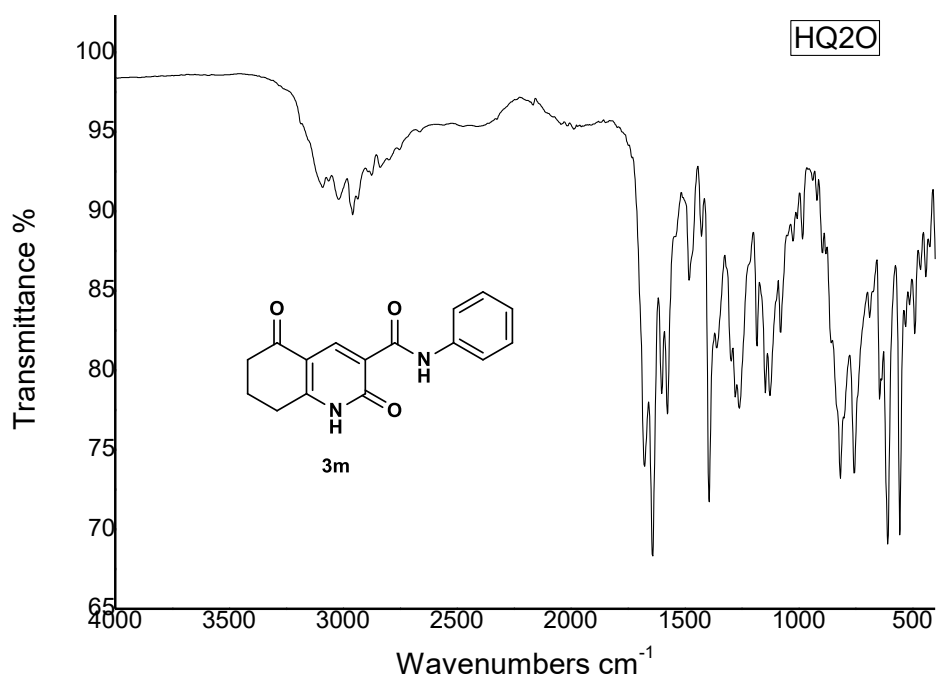
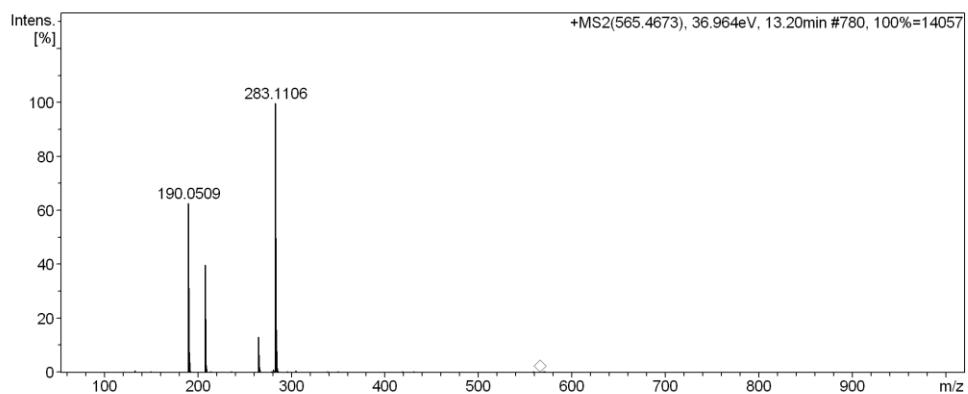
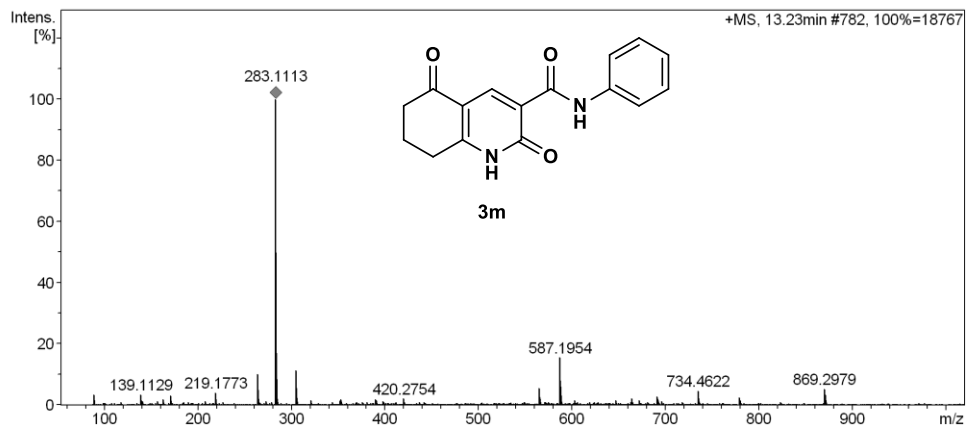


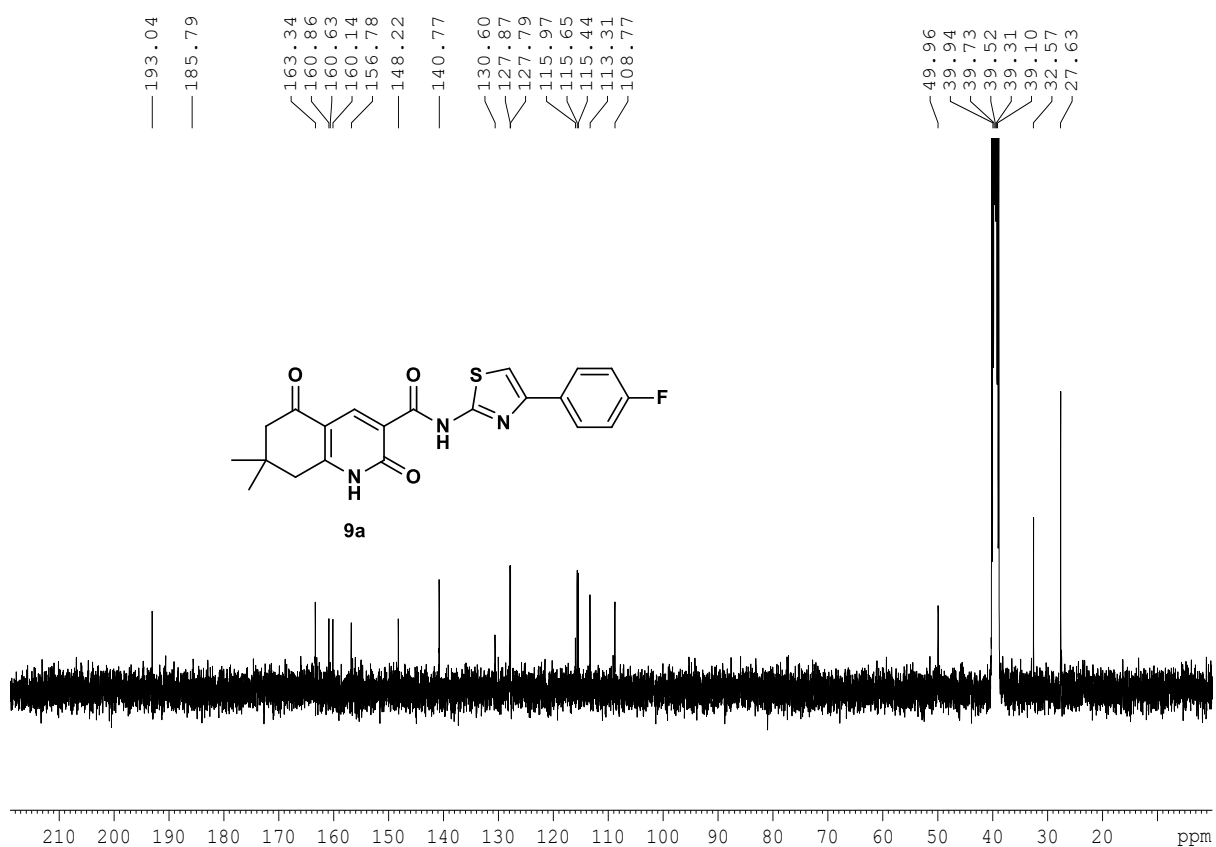
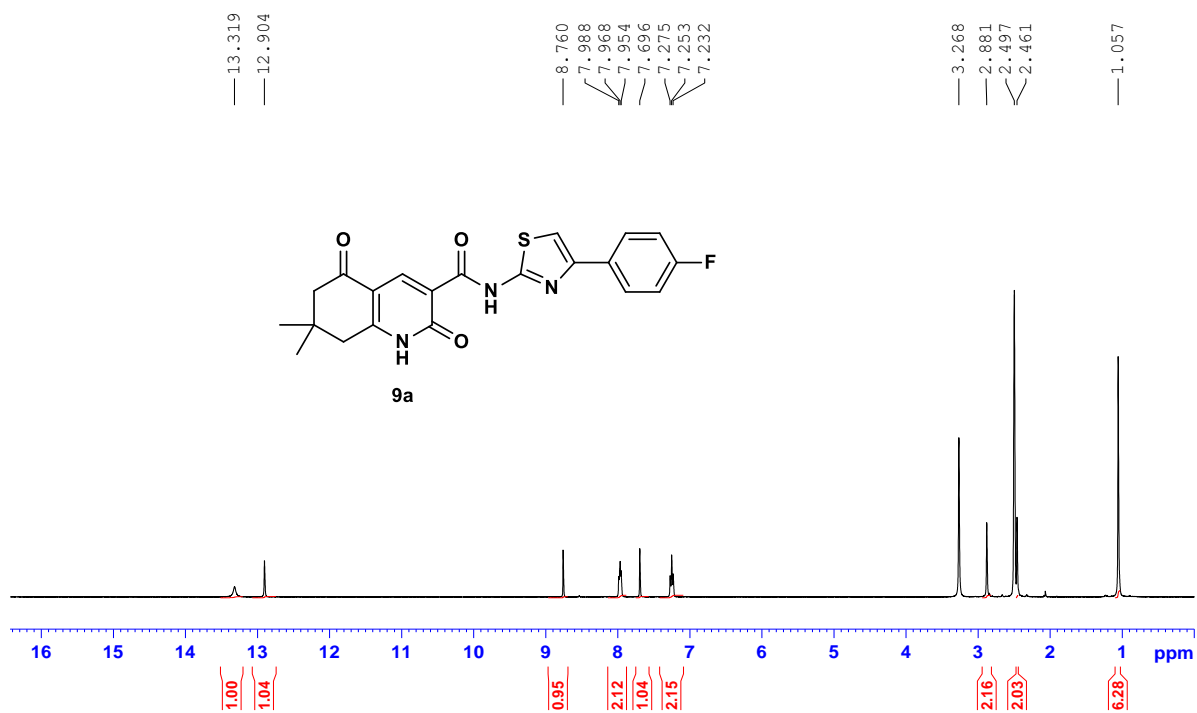


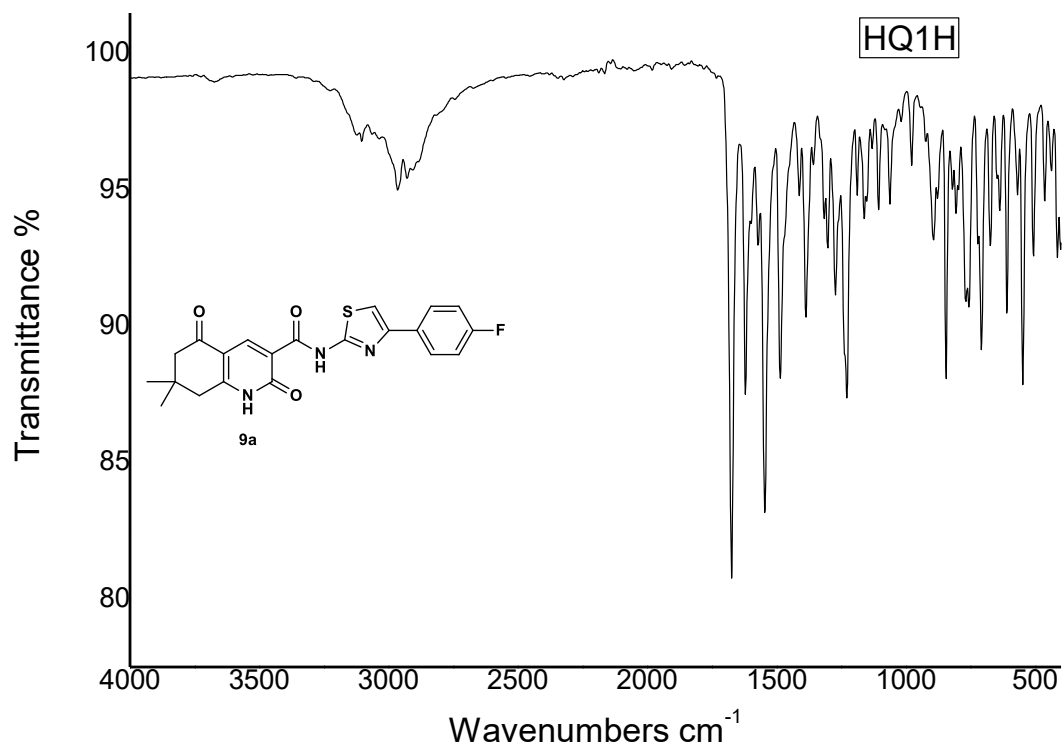
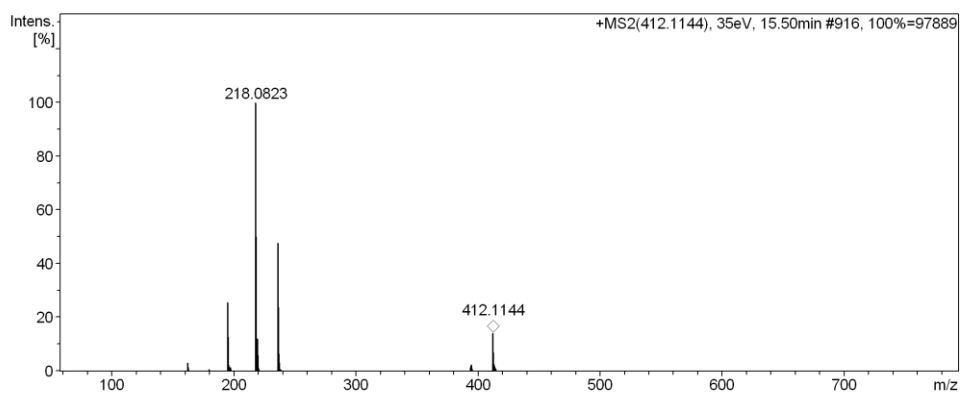
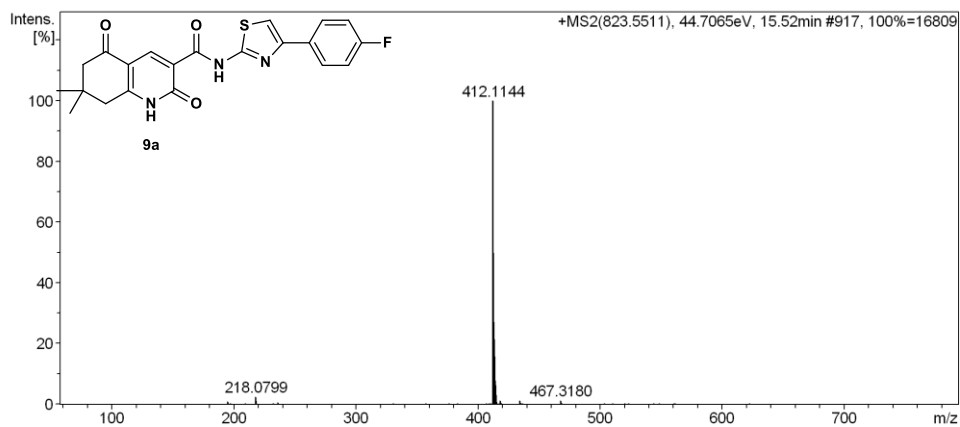


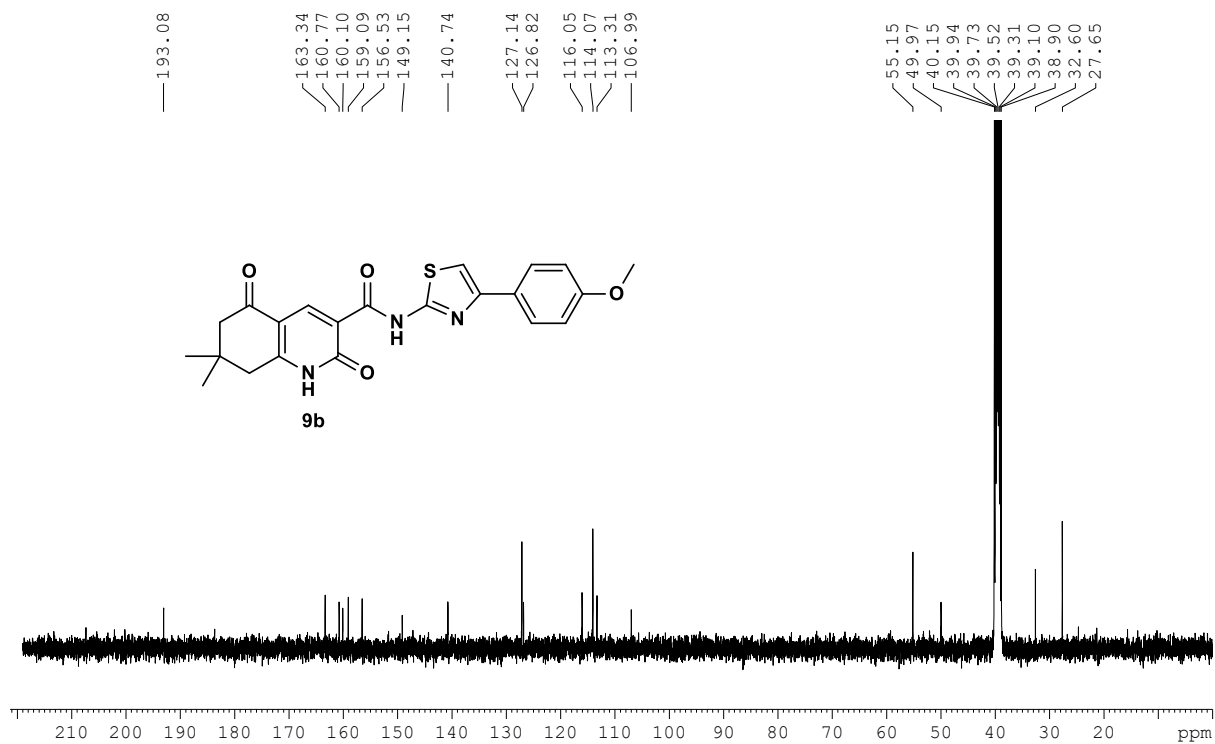
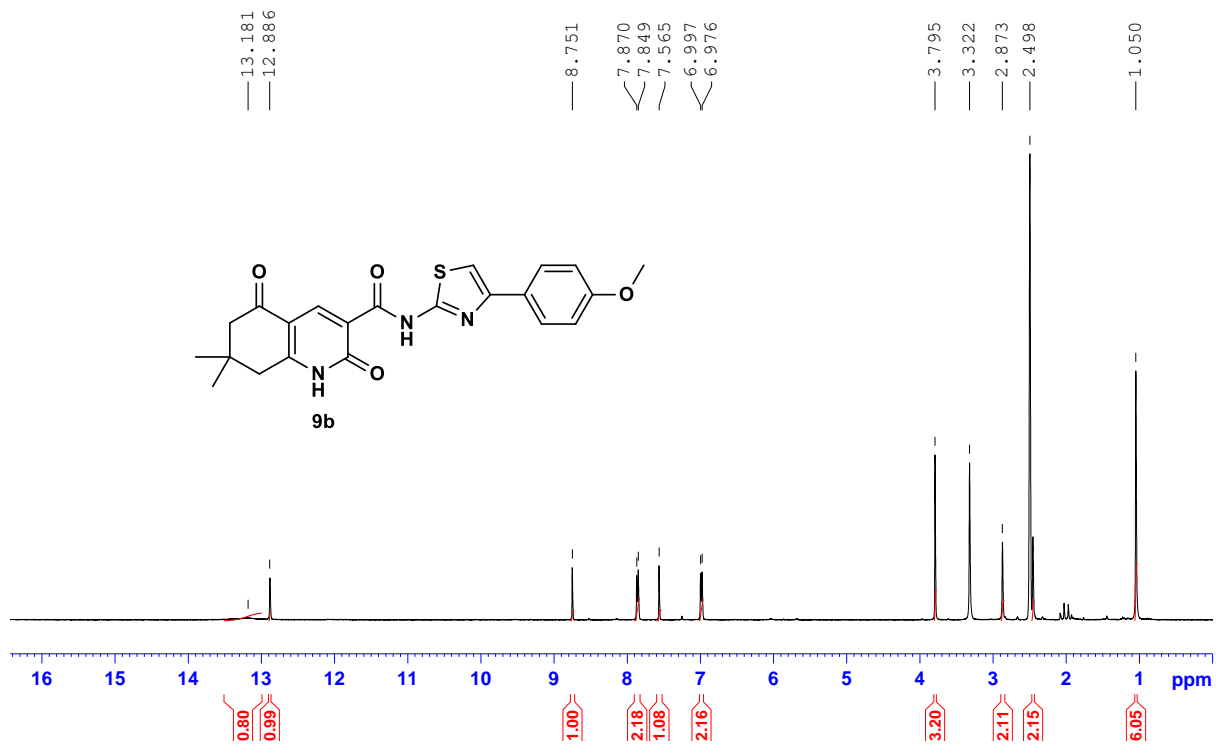


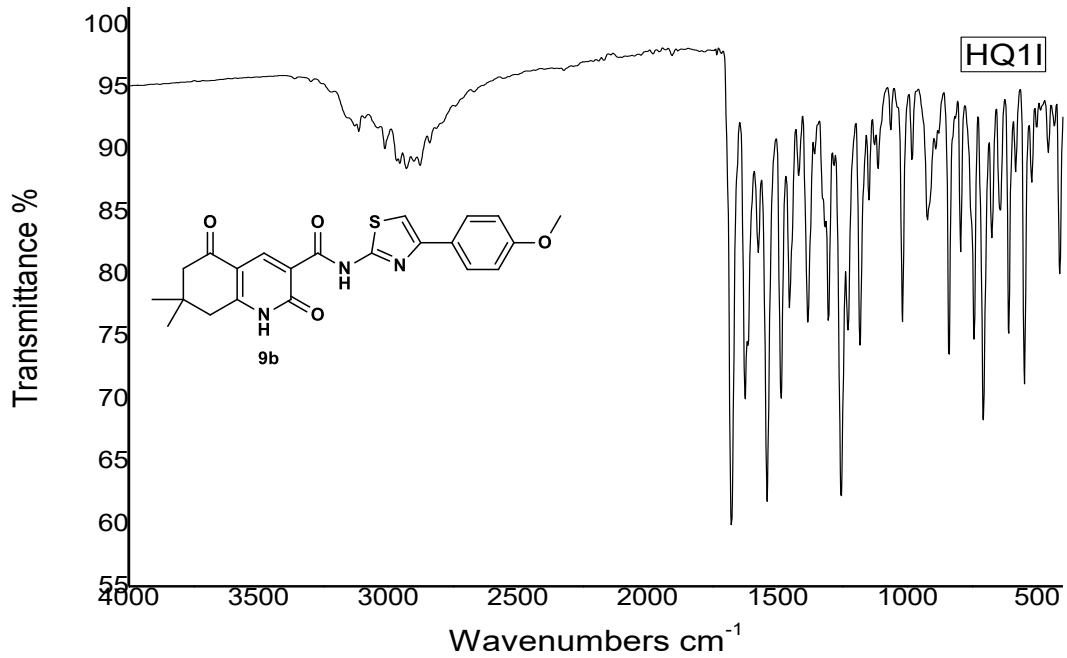
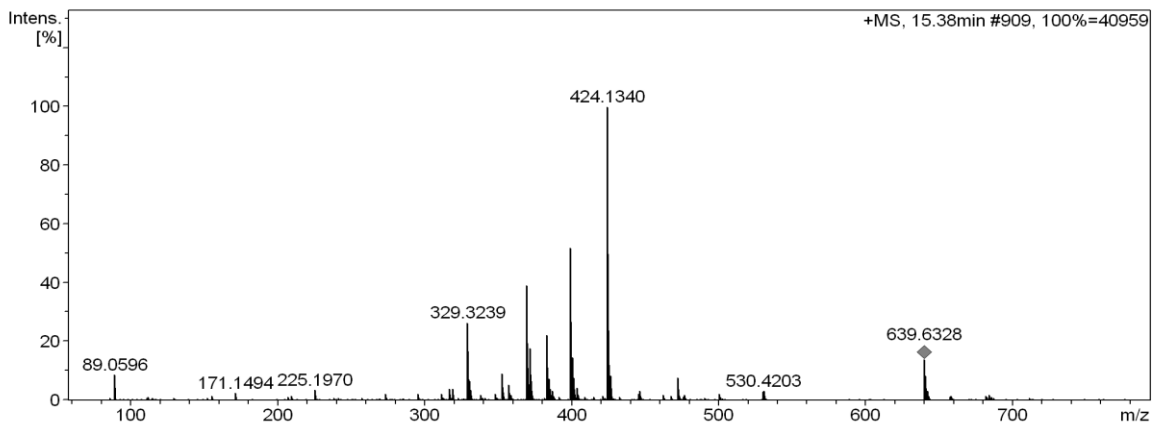
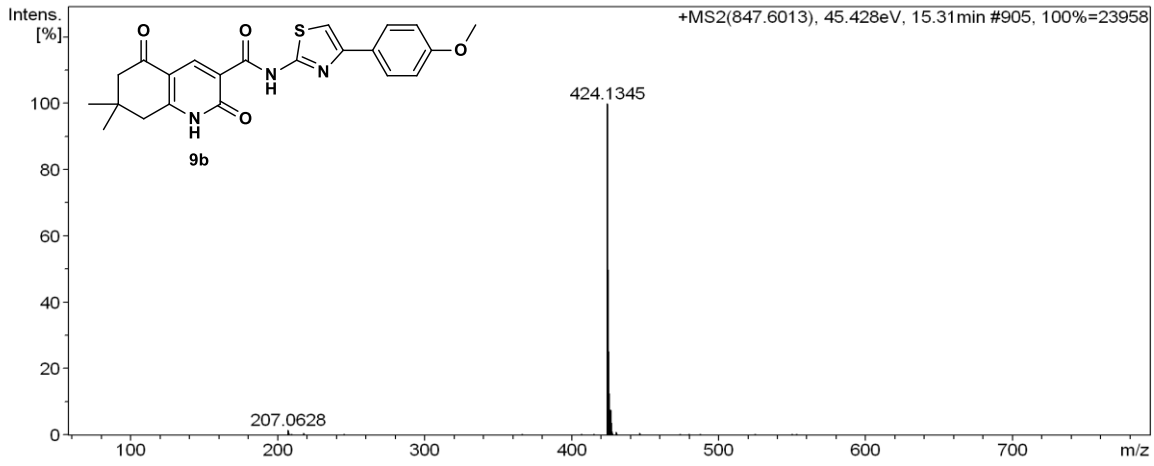


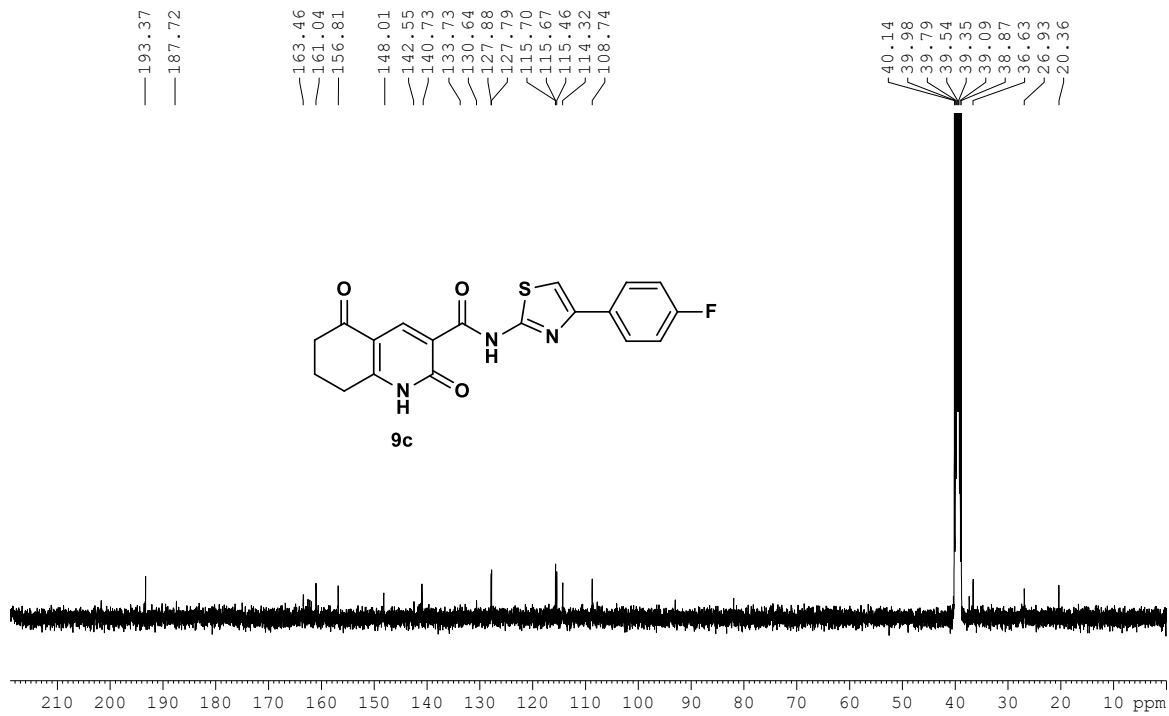
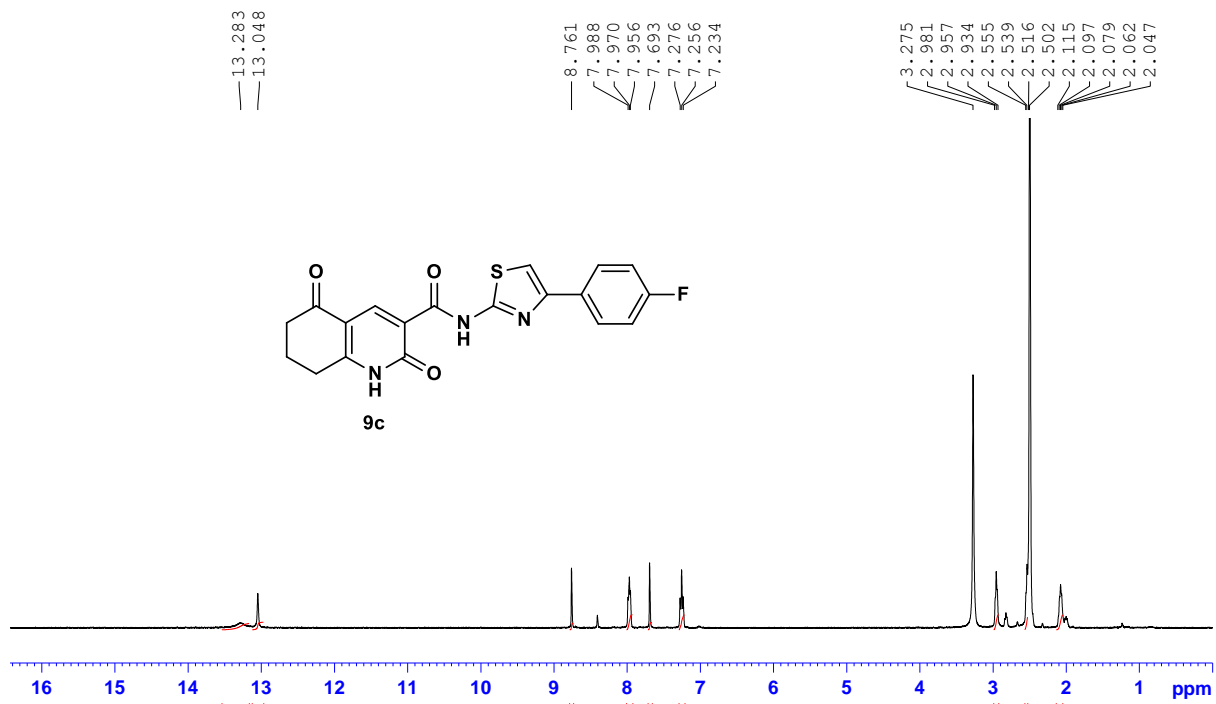


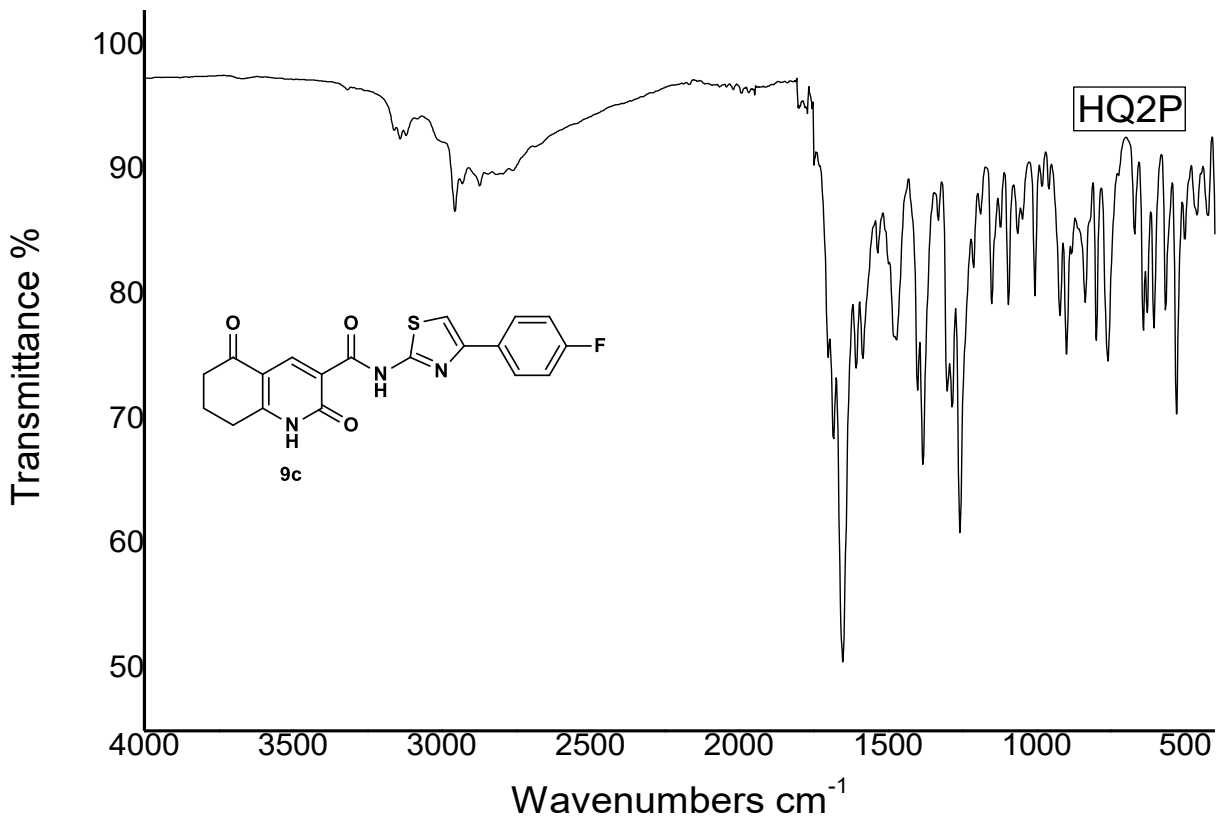
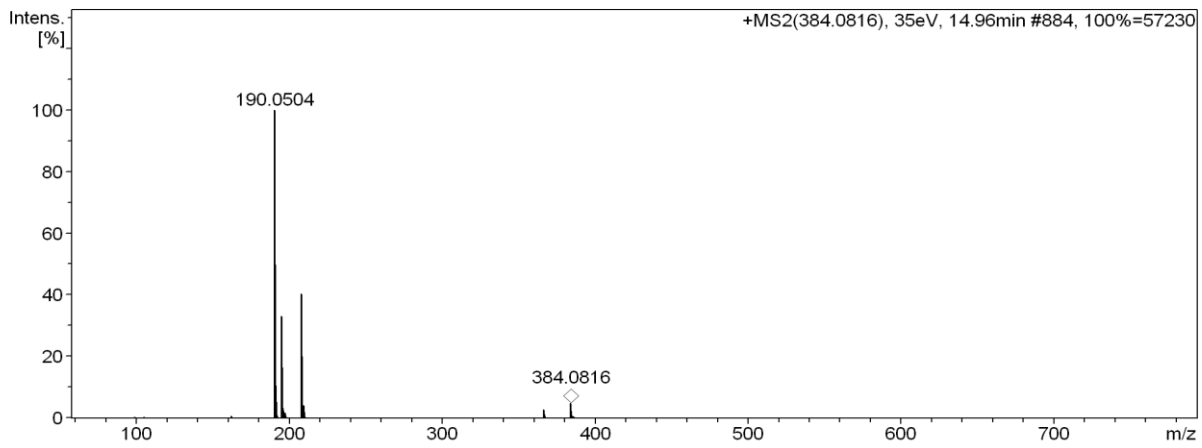
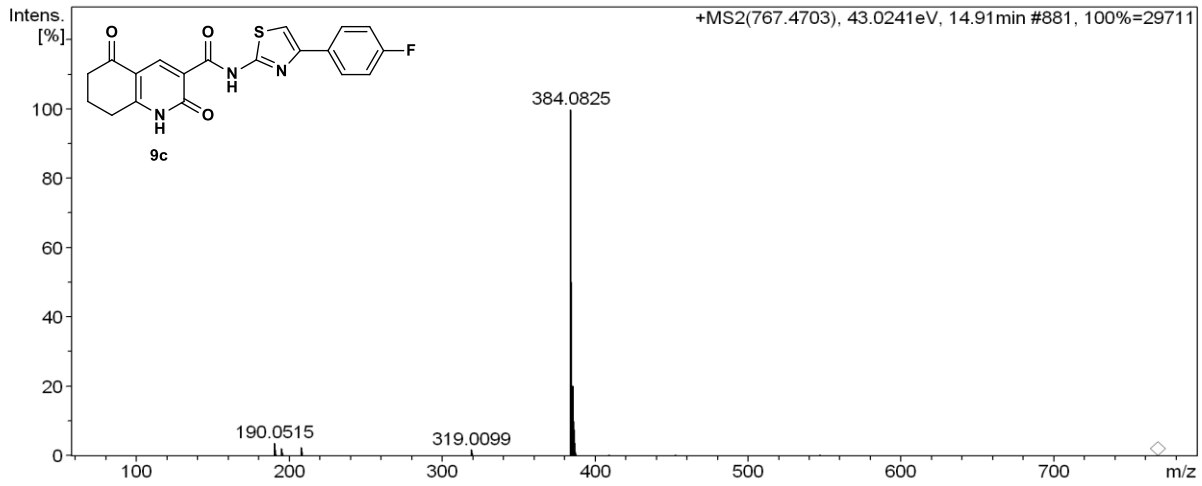


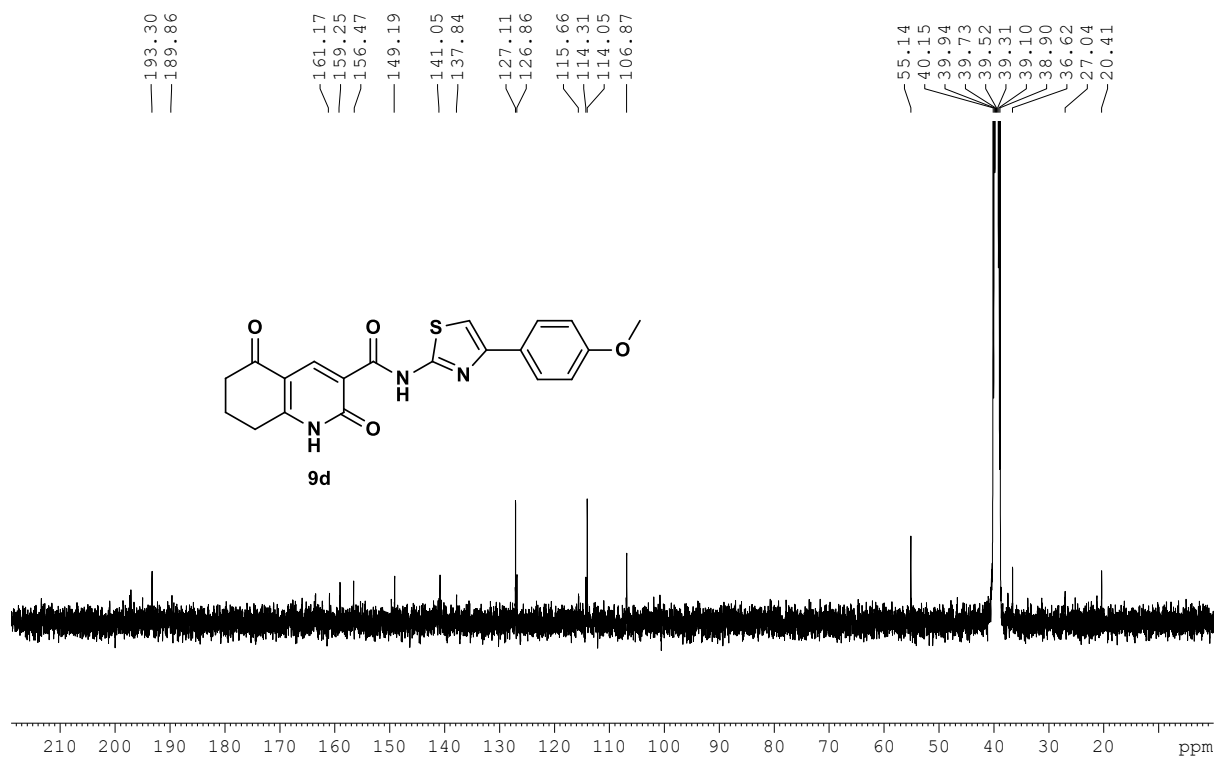
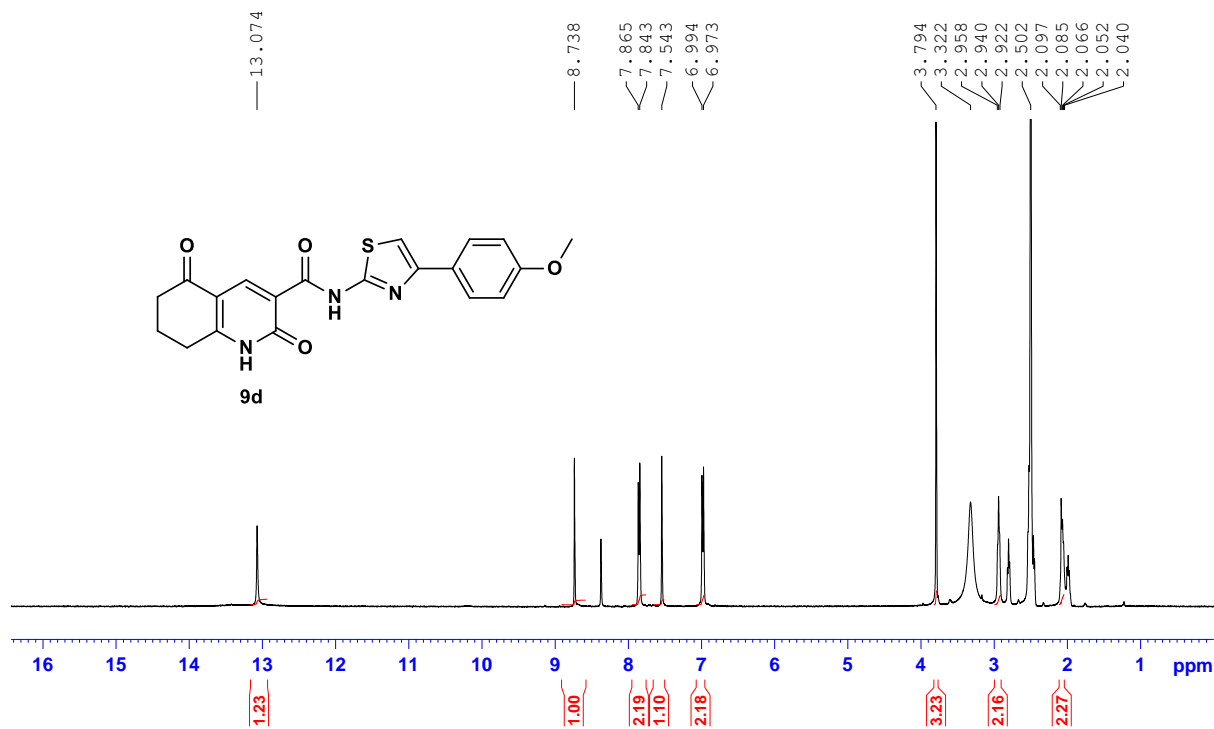


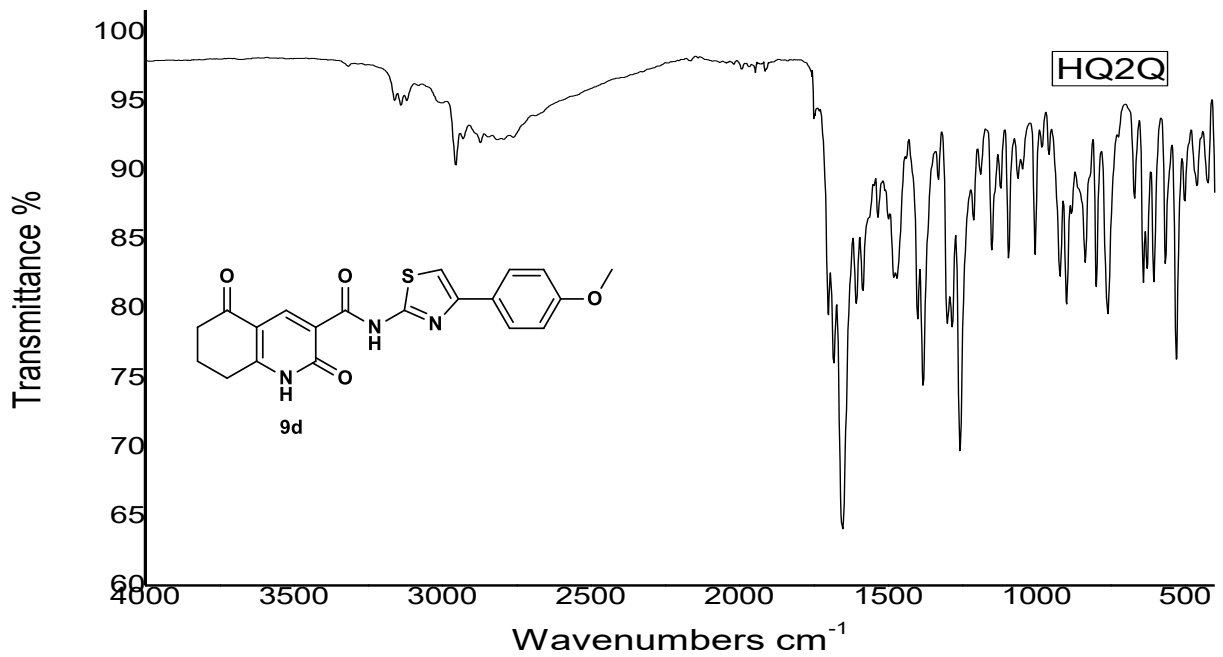
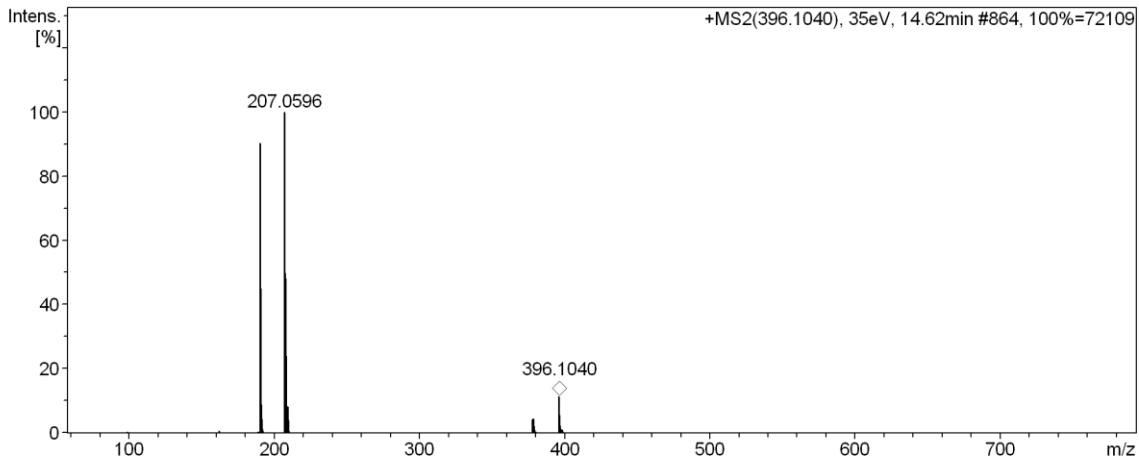
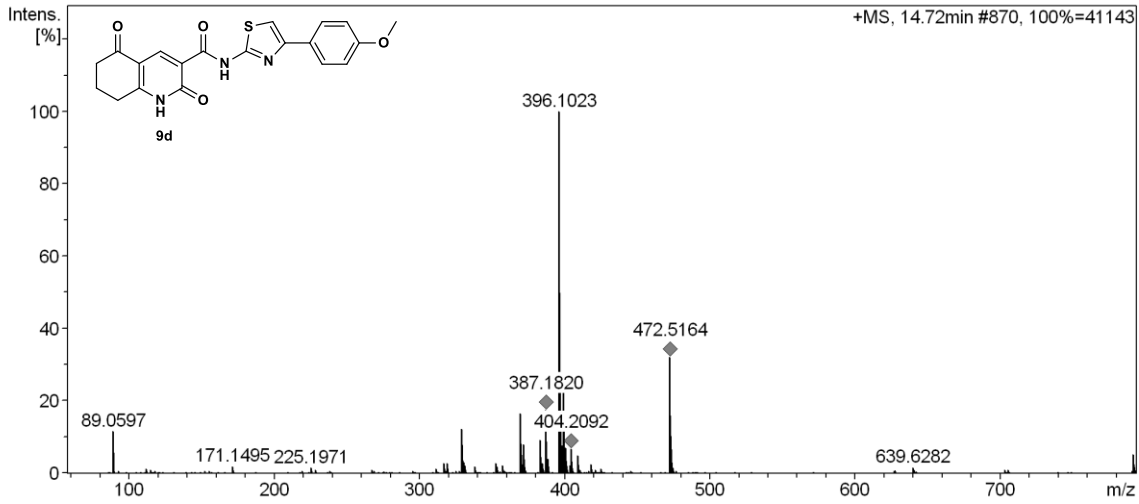


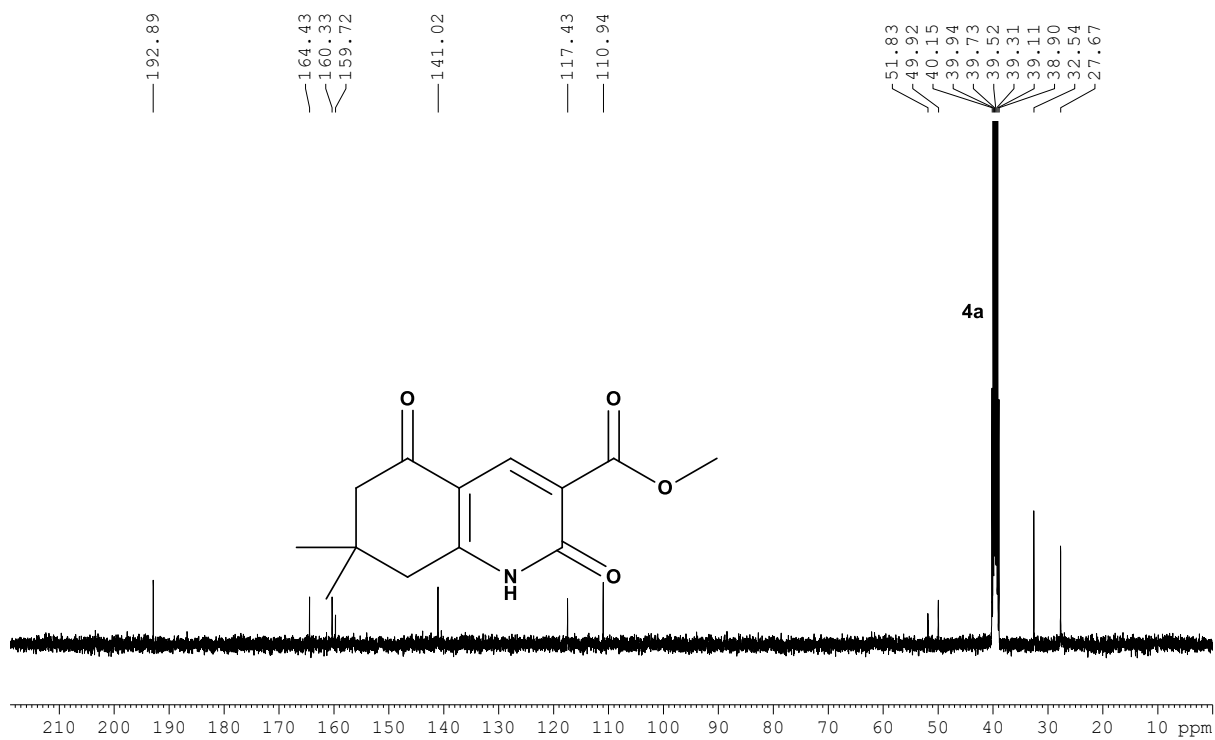
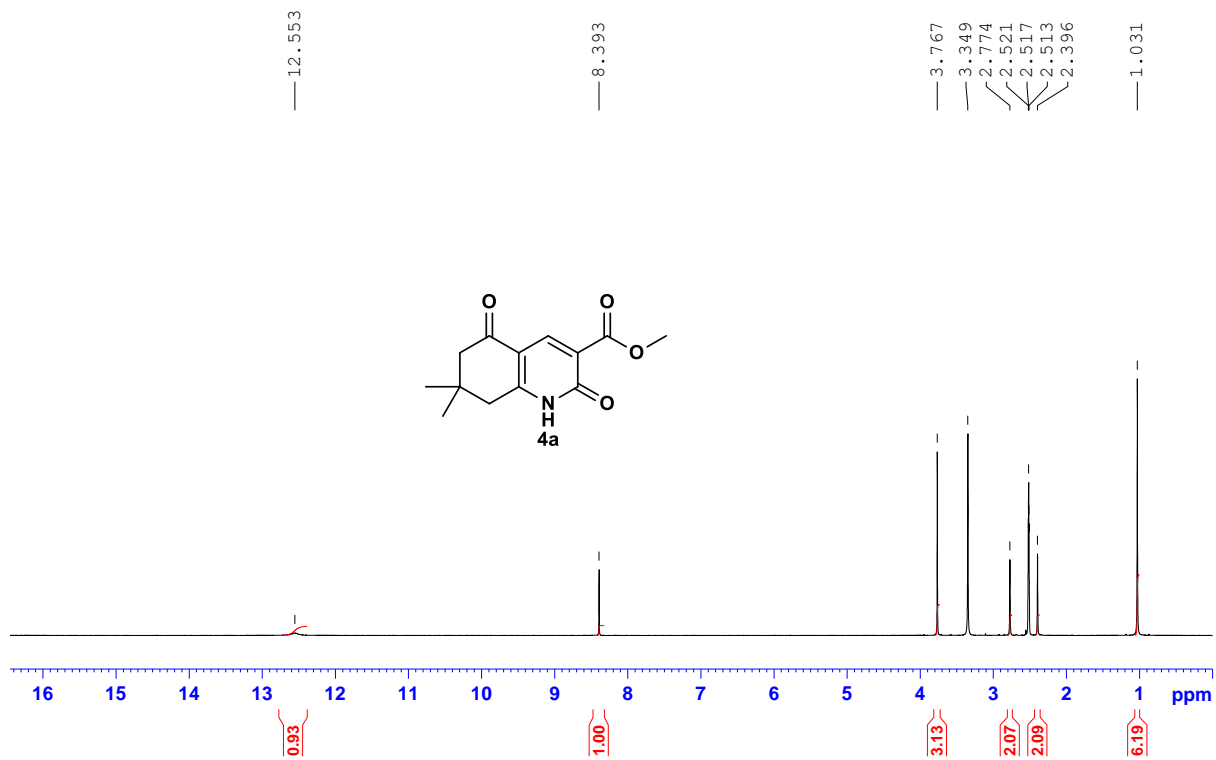


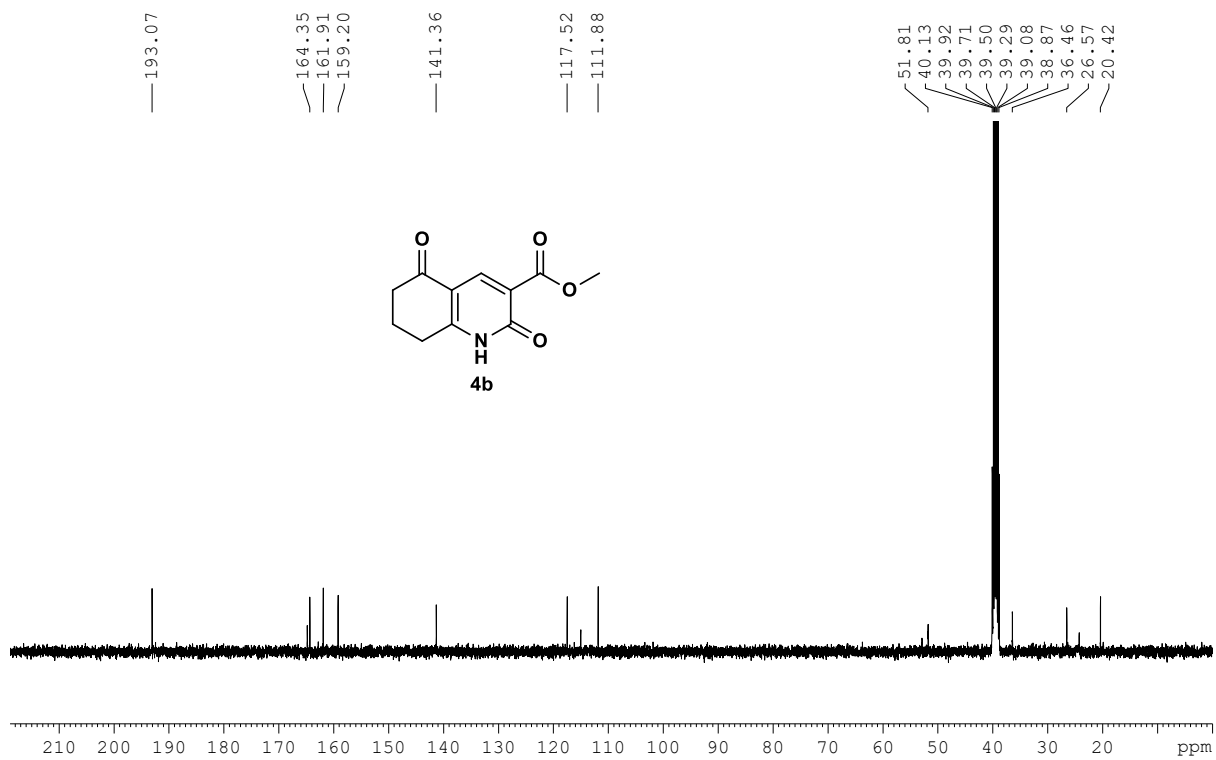
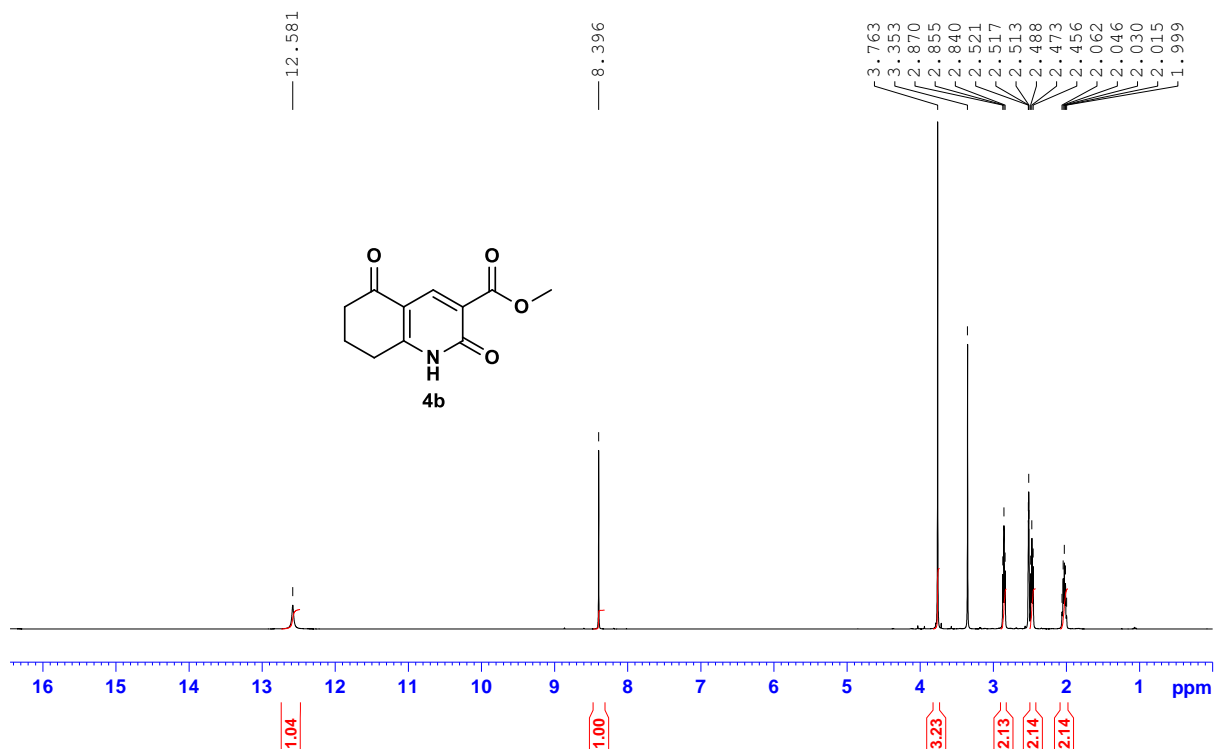


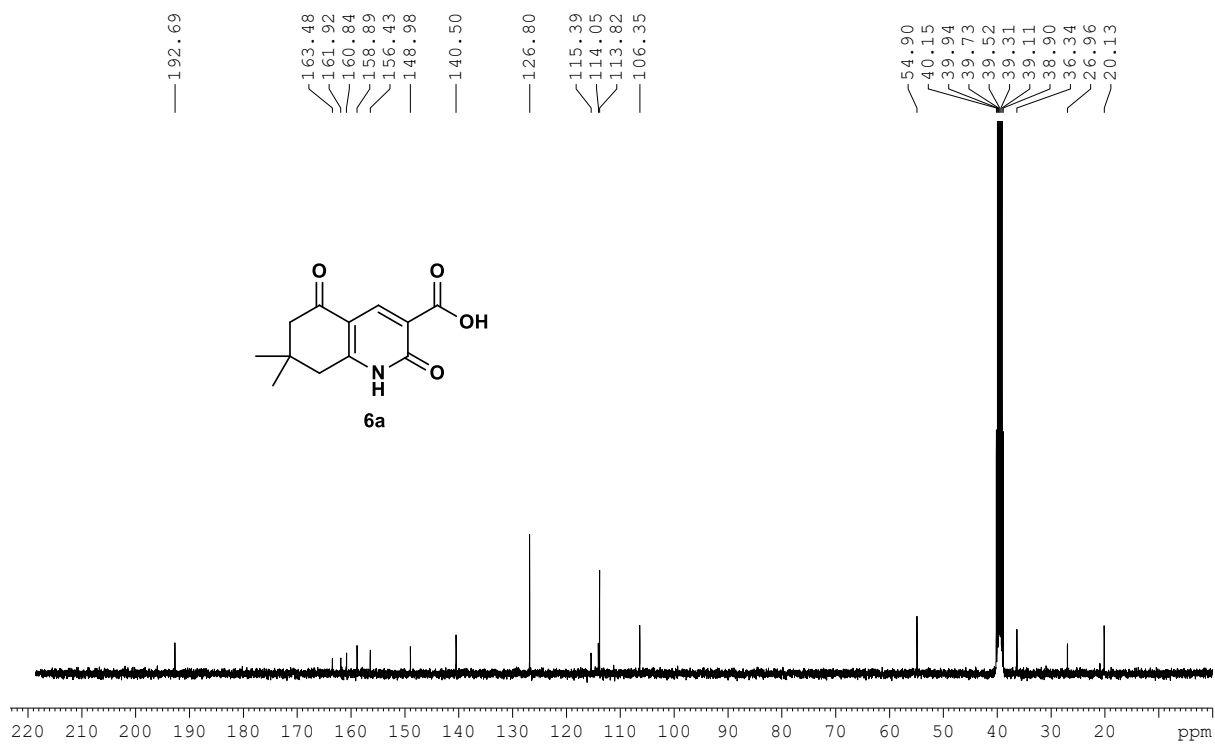
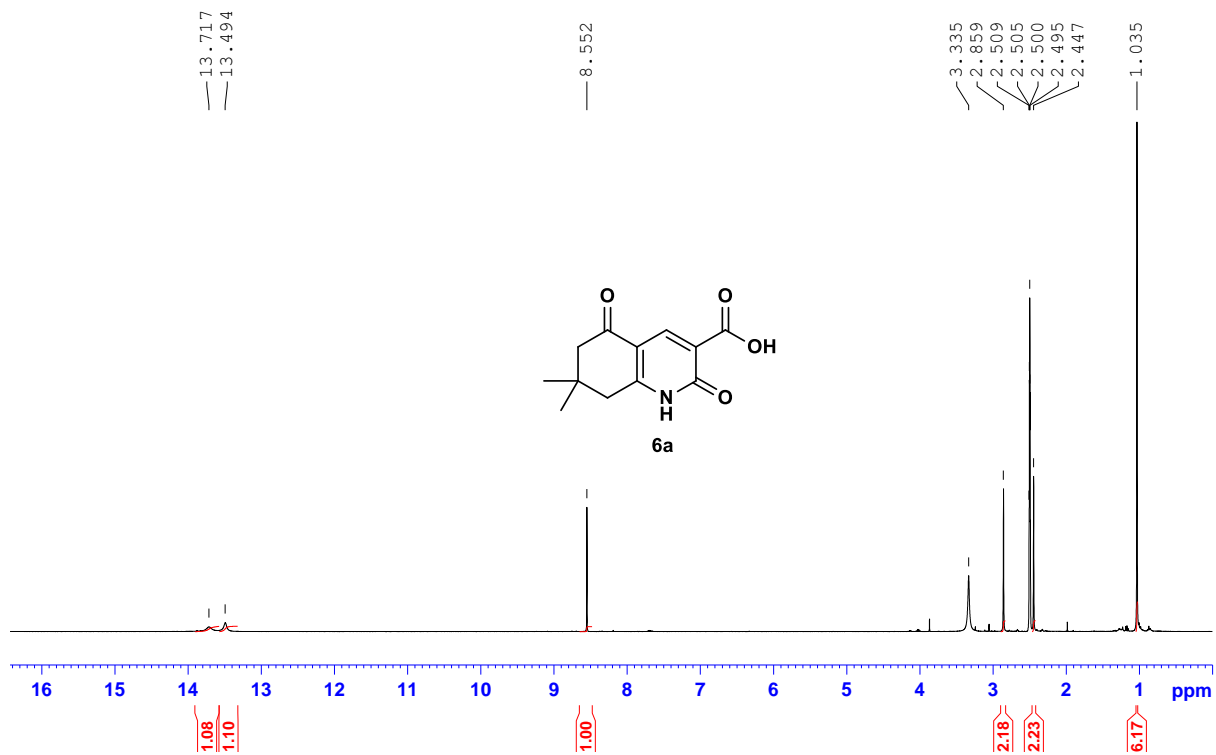


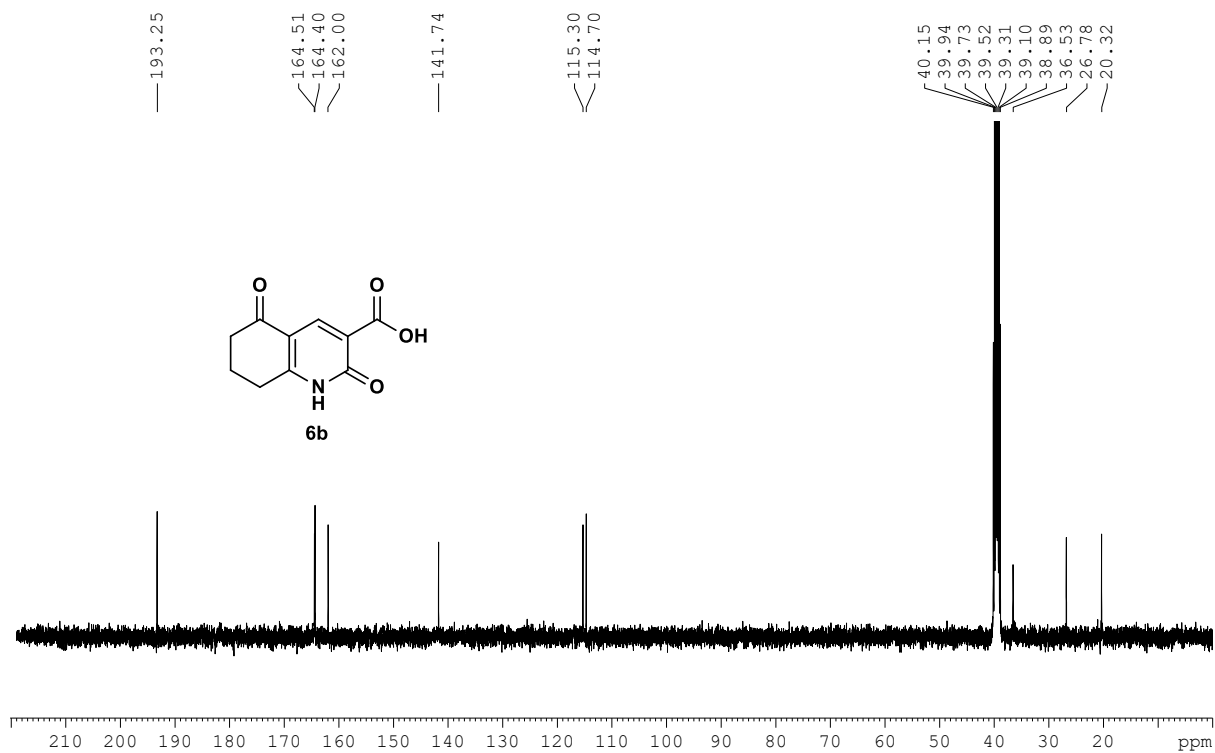
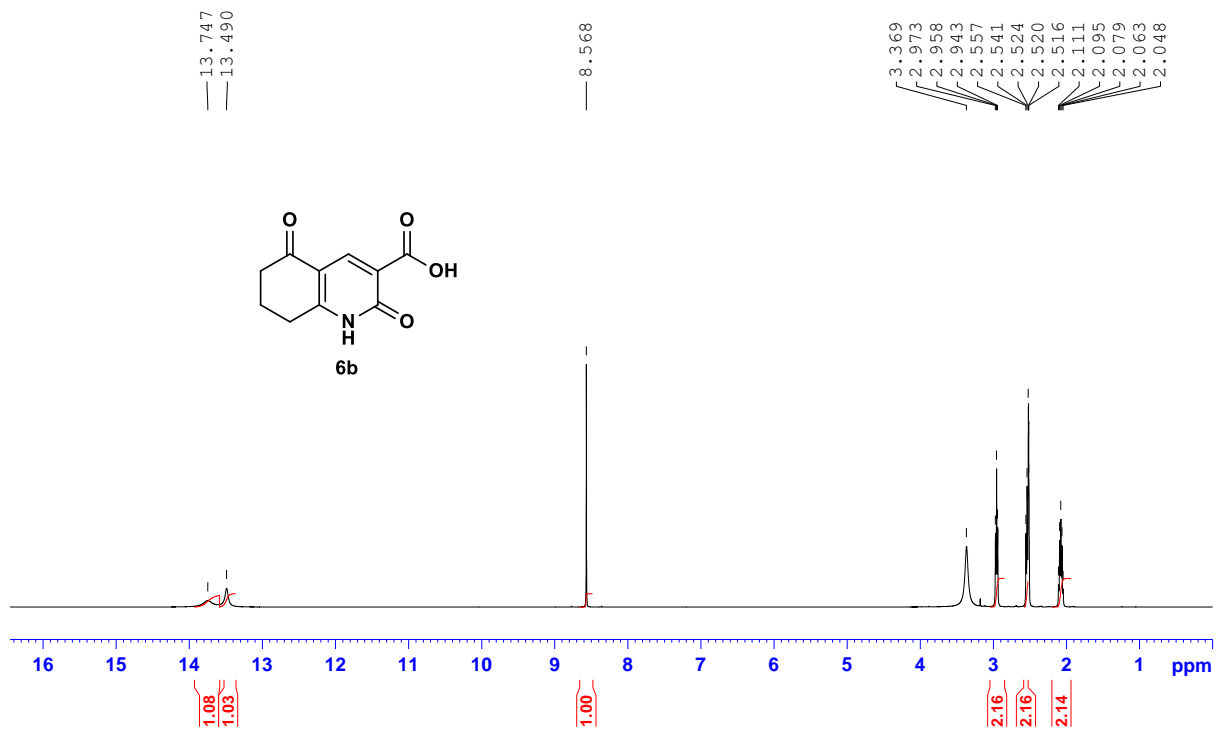


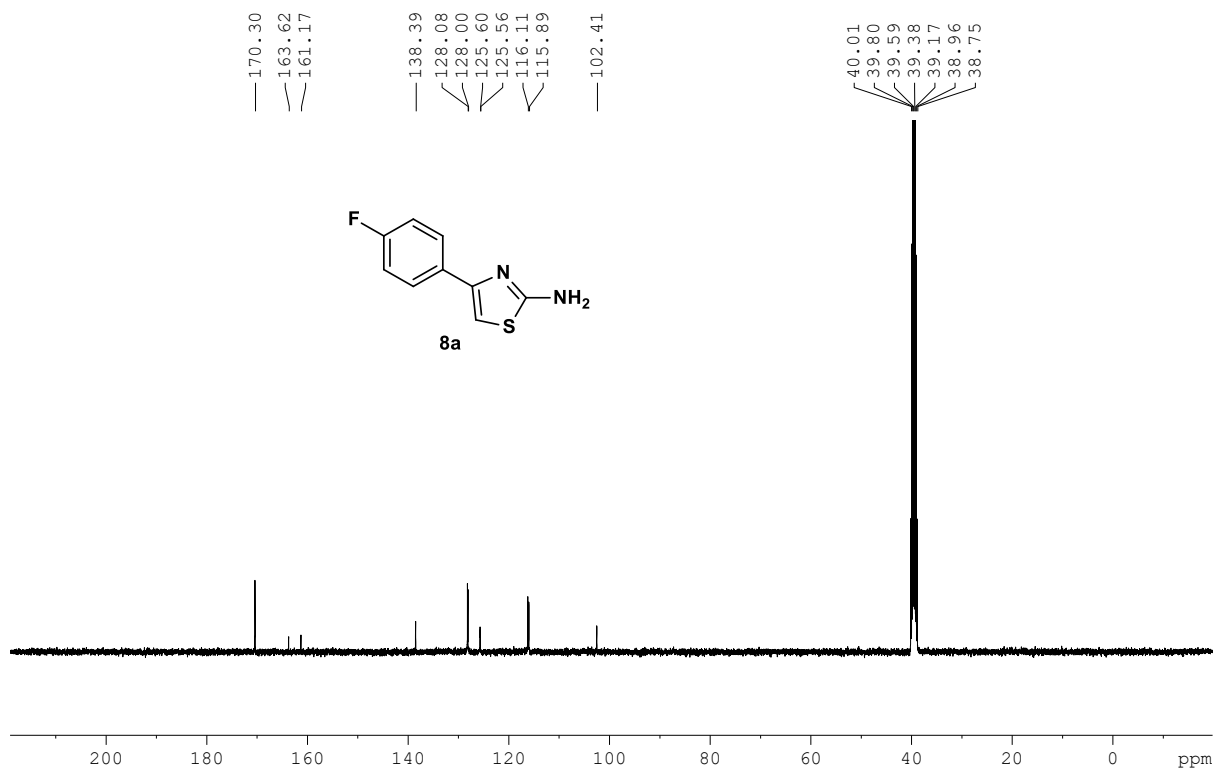
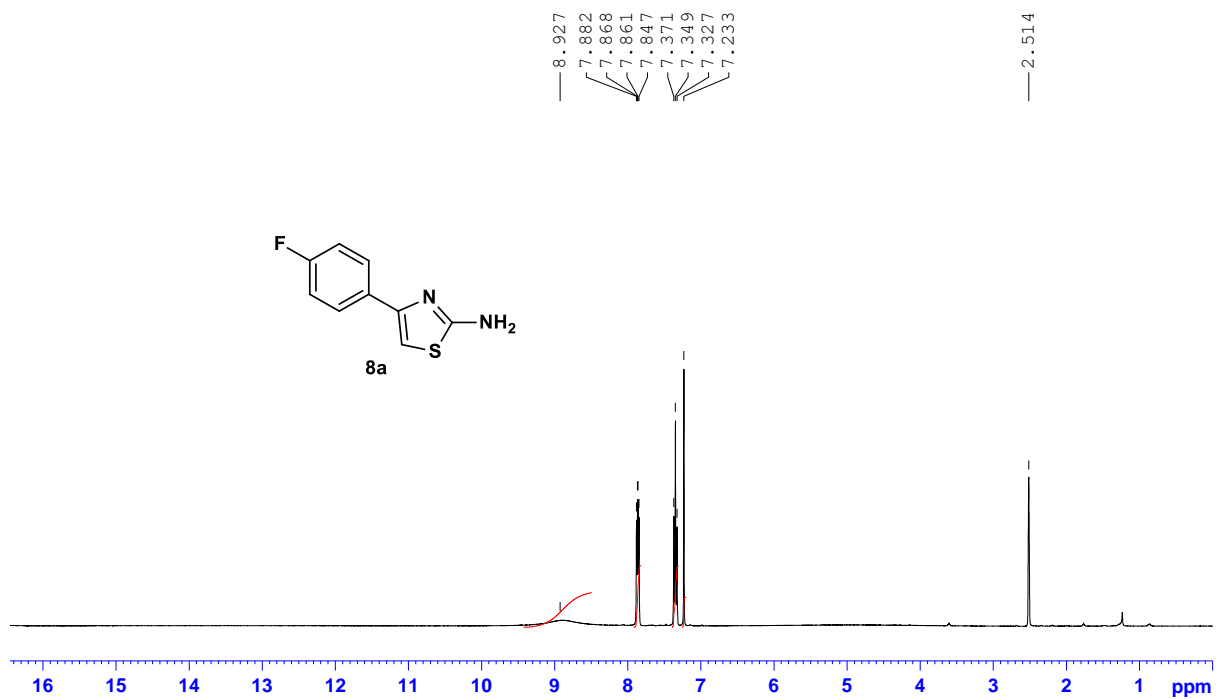


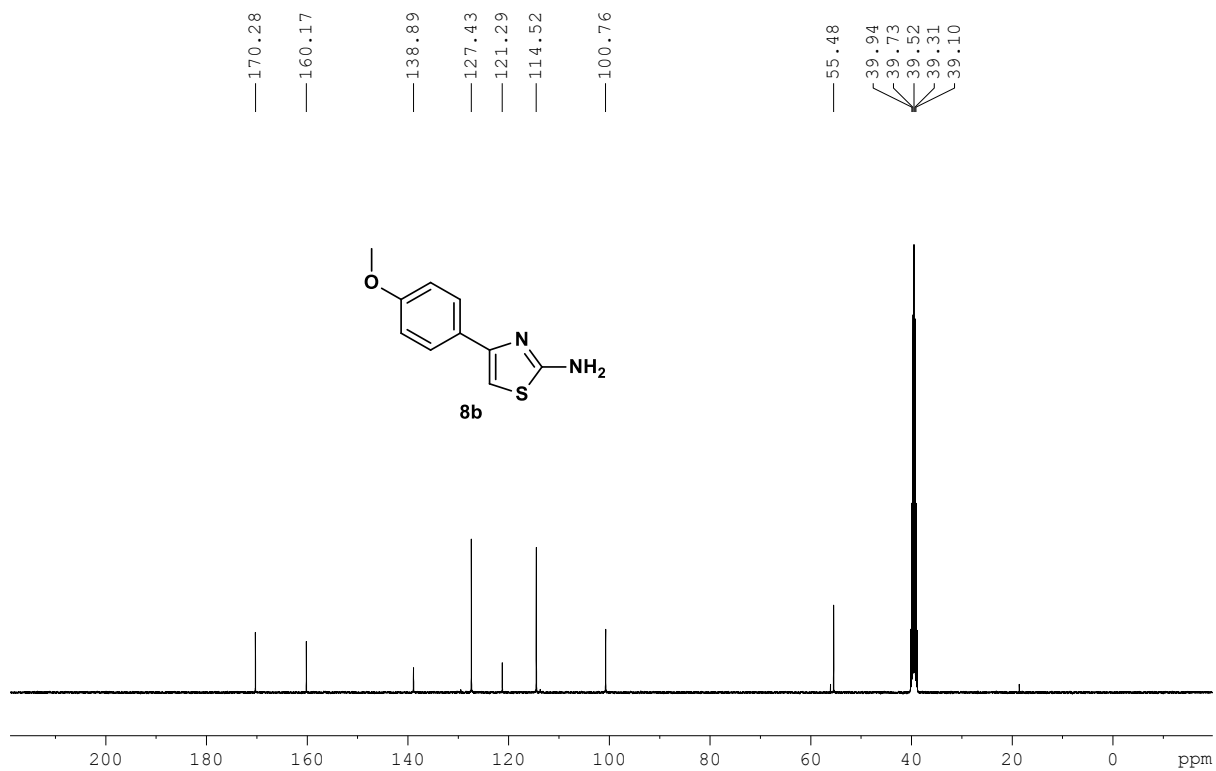
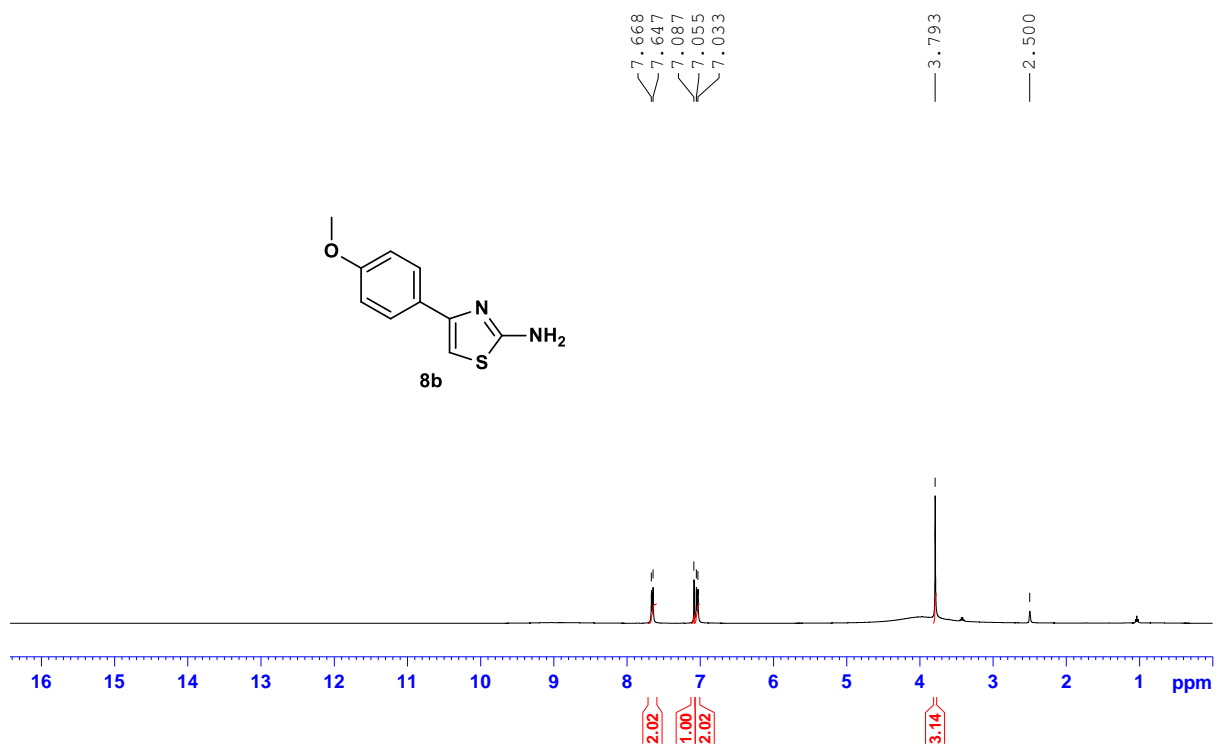












Virtual screening

The ChemBridge Library is a commercial library of chemically diverse compounds for the purpose of performing screening against diverse targets. This library was purchased in July 2010 and consisted in 20,000 pre-plated compounds. The Cambridge library is continuously expanding (now it is 150,000 diverse compounds) and can be purchased in sets of 5,000 or 10,000.

[ChemBridge](#) | [Screening Libraries](#) | [Diversity Libraries](#) | [DIVERSet](#)

From this website: **DIVERSet™ Diverse Screening Libraries**

Structurally diverse libraries with extensive pharmacophore coverage: For hit finding across different targets, against novel targets, or for the discovery of new chemical series against existing targets, ChemBridge offers up to 150,000 DIVERSet Library compounds in economical, pre-plated format. Researchers can purchase all available DIVERSet Library compounds or partial sets of as few as 5,000 or 10,000 compounds.

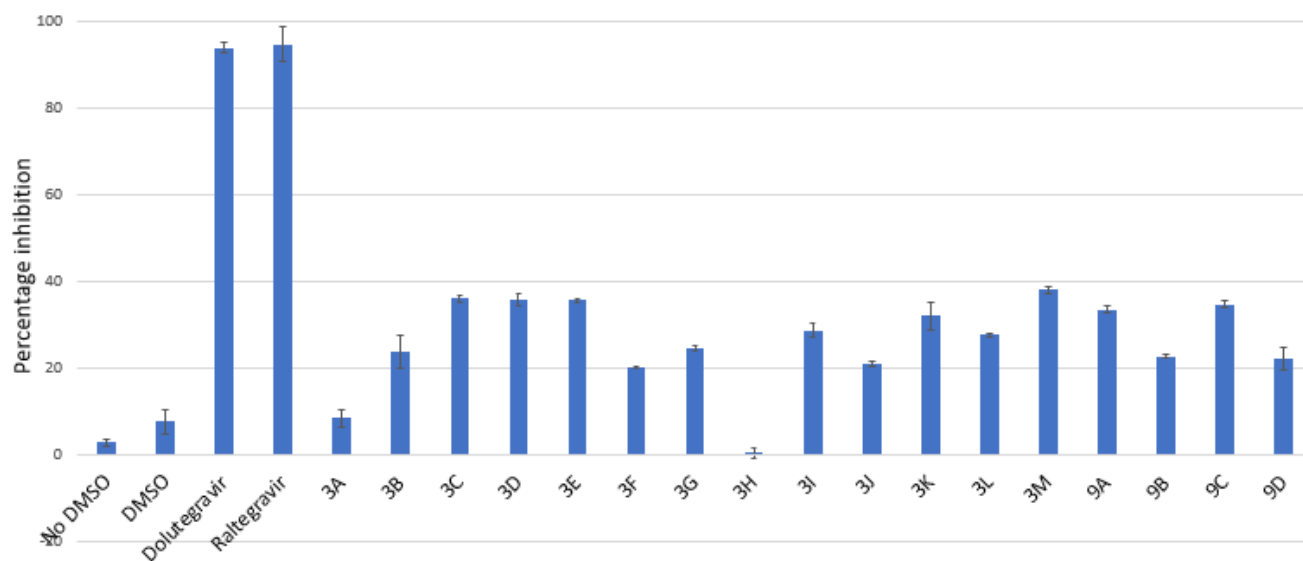
Table 1: Molecular docking results of synthesised hexahydroquinoline compounds and reference compounds CX05168 and Mut101.

ENTRY	Docking score (Kcal/mol)	Gscore (Kcal/mol)	XP G score	Glide emodel (Kcal/mol)	MMGBSA (Kcal/mol)
3a	-4.333	-4.333	-4.333	-58.112	-52.529
3b	-4.417	-4.417	-4.417	-56.382	-43.968
3c	-4.646	-4.646	-4.646	-46.220	-43.406
3d	-5.205	-4.490	-4.490	-50.818	-56.104
3e	-5.264	-5.264	-5.264	-52.124	-42.325
3f	-4.443	-4.443	-4.443	-55.581	-39.724
3g	-4.701	-4.701	-4.701	-55.075	-44.082
3h	-4.302	-4.302	-4.302	-54.890	-45.209
3i	-5.055	-5.055	-5.055	-53.178	-45.952
3j	-4.368	-4.368	-4.368	-45.403	-32.703
3k	-5.096	-5.096	-5.096	-47.228	-34.155
3l	-4.602	-4.602	-4.602	-49.346	-40.224
3m	-4.441	-4.441	-4.441	-45.085	-34.6000
9a	-3.396	-3.396	-3.396	-55.500	-46.722
9b	-3.969	-3.990	-3.990	-56.051	-50.378
9c	-3.073	-3.095	-3.095	-55.383	-47.773
9d	-2.028	-3.984	-3.984	-57.395	-40.528
CX05168	-5.329	-5.339	-5.339	-52.558	-51.171
Mut101	-6.176	-6.621	-6.621	-63.191	-59.389

Table 2: ADME-drug-likeness parameters of synthesised hexahydroquinoline compounds and reference compounds CX05168 and Mut101, using QikProp protocol.

ENTRY	MW (g/mol) (<500)	HBD (≤5)	HBA (≤10)	QPlogBB (-3.0 to1.2)	QPlog_{o/w} (-2 to 6.5)	QPlog HERG (>-5)
3a	344.797	0	5.0	-0.997	3.139	-5.366
3b	389.248	0	5.0	-0.992	3.217	-5.397
3c	324.379	0	5.0	-1.184	2.959	-5.369
3d	338.405	0	5.0	-1.117	3.255	-5.069
3e	326.351	1	5.6	-1.625	2.199	-5.274
3f	370.404	0	6.5	-1.317	2.827	-5.247
3g	310.352	0	5.0	-1.137	2.637	-5.442
3h	316.743	0	5.0	-1.007	2.472	-5.268
3i	361.194	0	5.0	-1.002	2.551	-5.299
3j	296.325	0	5.0	-1.194	2.293	-5.273
3k	298.298	1	5.8	-1.625	1.563	-5.164
3l	342.351	0	6.5	-1.324	2.161	-5.142
3m	282.298	0	5.0	-1.147	1.967	-5.342
9a	411.450	0	6.5	-1.171	3.643	-6.154
9b	423.486	0	7.3	-1.373	3.472	-6.160
9c	383.396	0	6.5	-1.162	2.945	-6.014
9d	395.432	0	7.3	-1.389	2.805	-6.102
CX05168	305.376	1	3.0	-0.386	4.494	-3.034
Mut 101	409.524	1	4.5	-0.271	5.558	-1.975

Antiviral activities



Antiviral activity testing of **3a-m** and **9a-d** in a cell-based assay at a single dose of 100 μ M.