Supporting Information

Copper-Catalyzed Oxidative Multicomponent Reaction: Synthesis of Imidazo Fused Heterocycles with Molecular Oxygen

Xianwei Li,*† Tianzhang Wang,† Yu-Jing Lu,*† Shaomin Ji,† Yanping Huo,† Bifu Liu*‡

†School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou 510006, China.

‡ School of Chemistry and Material Engineering, Huizhou University, Huizhou 516007, China.

Email: xwli@gdut.edu.cn; luyj@gdut.edu.cn; liubf@hzu.edu.cn

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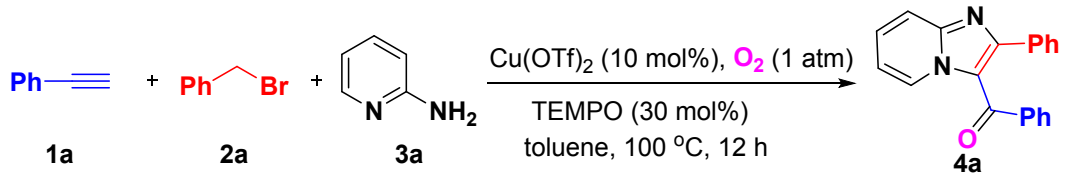
1. General methods

^{1}H NMR, ^{13}C NMR data were obtained on AVANCE III Bruker 400 MHz nuclear resonance spectrometers unless otherwise noted. Chemical shifts (in ppm) were referenced to tetramethylsilane (TMS) (δ = 0.00 ppm) in $CDCl_3$ or dimethyl sulfoxide (δ = 2.50 ppm) in DMSO-d_6 as an internal standard. The data of ^{1}H NMR was reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet and br = broad), coupling constant (*J* values) in Hz and integration. ^{13}C NMR spectra were obtained by the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.16 ppm) or DMSO-d_6 (δ = 39.50 ppm). The data of HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF).

2. Optimization of the reaction conditions

Table SI1. Optimization of the reaction conditions of MCRs to deliver imidazo[1,2‑a]pyridine.



1a **2a** **3a** **4a**

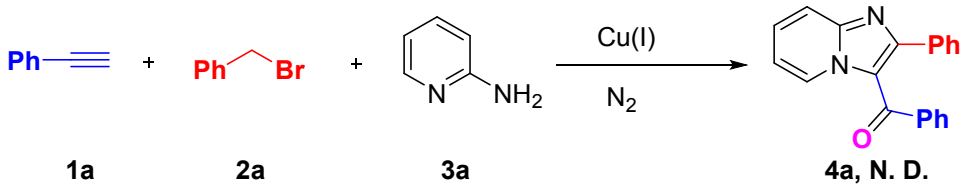
Entry	Variation of optimal conditions	Yield[b] (%)
1	None	92 (90)
2	HOTf instead of $Cu(OTf)_2$	-
3	$NiCl_2$ instead of $Cu(OTf)_2$	trace
4	AgOAc instead of TEMPO	< 10
5	addition of K_2CO_3	42
6	bpy	-
7	1,10-phen	19
8	DABCO	-
9	1,4-dioxane	trace
10	CH_3CN	23
11	DMF	21
12	DMSO	25
13	**1: 2 : 3 = 1.0:1.5:2.0**	72
14	**1: 2 : 3 = 1.0:1.0:1.2**	39

[a] Reaction conditions: catalyst (10 mol%), additive (30 mol%), solvent (1 mL) at the given temperature for 12 h. [b] Yields were determined by GC-MS with *n*-dodecane as the internal standard. Yield in the parentheses is the isolated yield.

3. Mechanistic studies

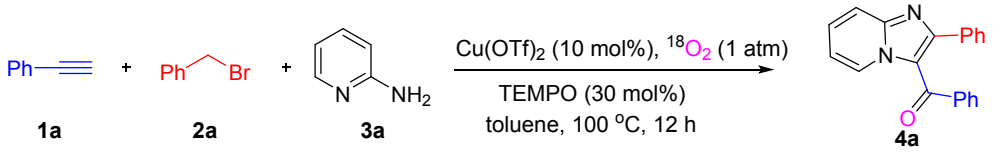
1) Control experiments:

To gain some insight into this transformation, we first conduct control experiment (eq. 1) with the standard condition under N_2 atmosphere, and no desired product **4a** was isolated; while the addition of 2 equivalent of TEMPO also led to no desired product **4a** was detected.



1a **2a** **3a** **4a, N. D.** (eq. 1)

To elucidate the origin of the oxygen atom of the product 4a, we also performed isotopic labeled experiment with $^{18}O_2$, indeed, the ^{18}O labeled product **4a** was confirmed by HRMS.

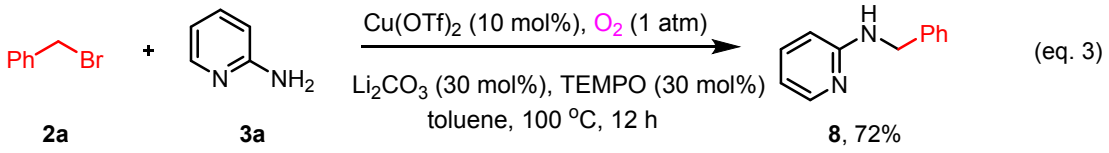


1a **2a** **3a** **4a** (eq. 2)

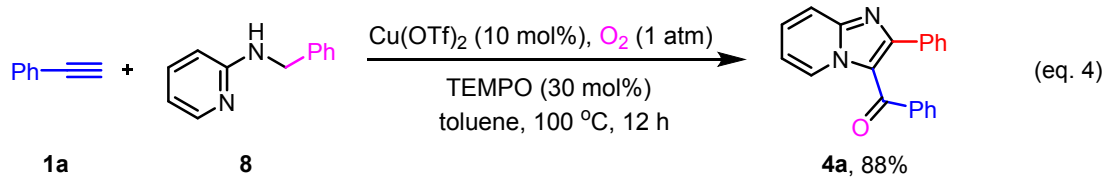
[^{18}O and ^{16}O]-4a

2) Intermediate verification experiments via stepwise reactions

To further investigate the reaction sequence of this multicomponent reaction, we performed two component reactions, and found that benzylic bromide **2a** could react with 2-amino pyridine **3a** to give S_N2 product **8** in 72% yield under standard condition (eq. 3). Moreover, with the obtained S_N2 product **8** and terminal alkyne **1a** under the standard reaction condition, the desired product **4a** was isolated in good yield (eq. 4). These results suggest that this multicomponent reaction might proceed via nucleophilic substitution reaction of **2a** and **3a**, leading to S_N2 product **8** as the intermediate, which would participate the further transformation with terminal alkyne **1a**, and finally led to the desired product **4a**.

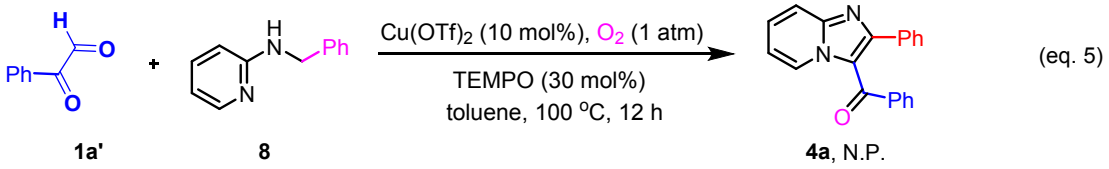


(eq. 3)



(eq. 4)

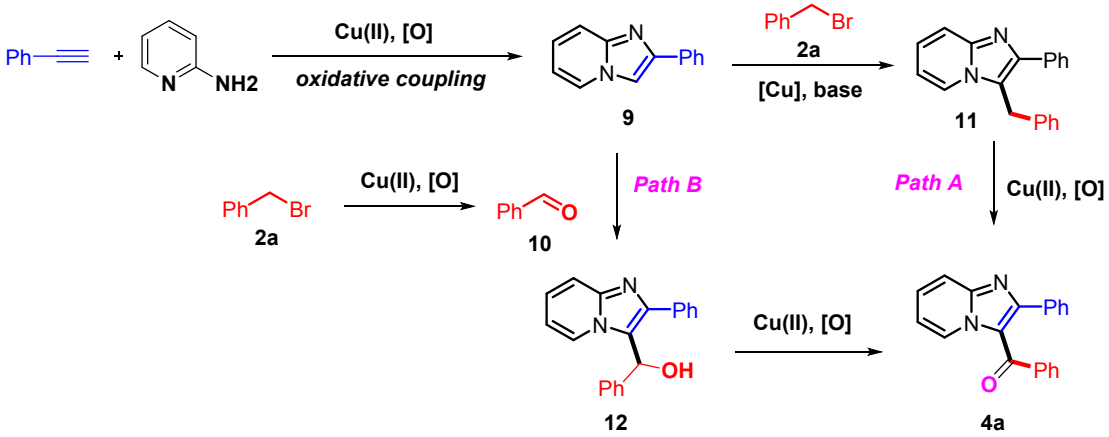
In connection with precedent literature, we proposed that 2-oxo-2-phenylacetaldehyde **1a'** might be generated in situ by selective aerobic oxidation of terminal alkyne **1a**. Control experiment by subjecting 2-oxo-2-phenylacetaldehyde **1a'** and S_N2 product **8** into the standard condition was conducted, and the result was in consistent with the transformation listed in (eq. 5).



(eq. 5)

3) Proposed reaction pathway

Pathway A and B:

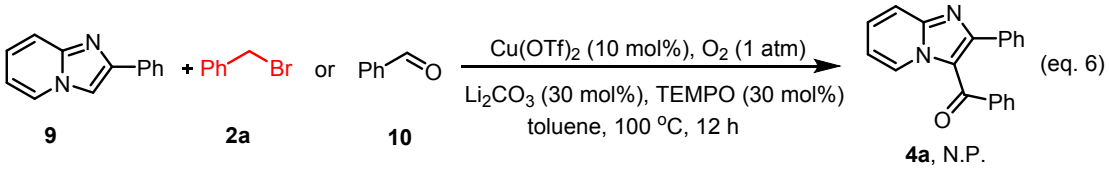


Scheme SI-1. Pathway A and B.

Pathway A and **B** initiated with oxidative coupling of **1a** and **3a** under Cu(II)-catalyzed oxidative condition, delivering **9** as the key intermediate. As for Pathway **A**, further substitution reaction of **9** with benzylic bromide **2a** with the assistance of copper salt and base, affording **11**, which underwent further oxidation of benzylic C-H bond to

generate the desired IP product **4a**.

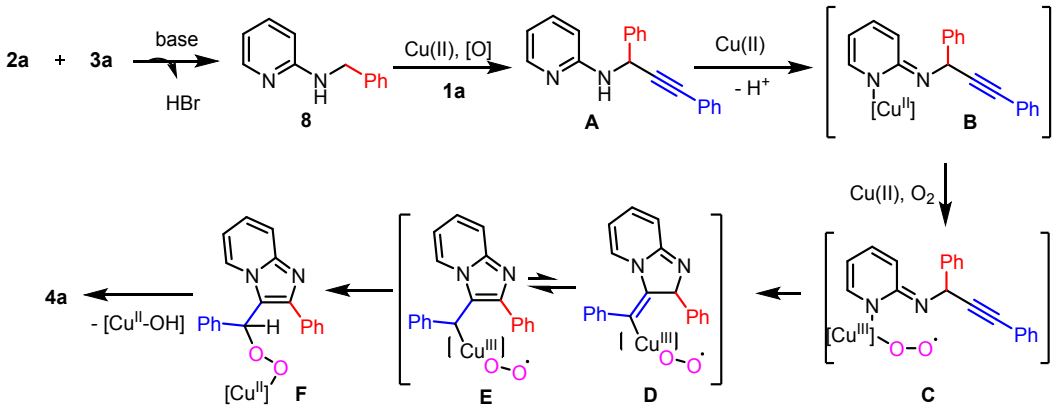
Alternatively, as for **pathway B**, benzylic bromide **2a** was oxidized to the corresponding benzaldehyde **10**, which underwent substitution of key intermediate 9, generating the corresponding alcohol **12**. Further oxidation of **12** took place under copper catalyst and oxidant, delivering **4a** product.



9 **2a** **10** **4a**, N.P.

However, when pre-synthesized intermediate **9** and benzylic bromide **2a** or benzaldehyde **10** were subjected to the standard conditions, respectively, no desired IP product **4a** was obtained. Thus, pathway **A** and pathway **B** were ruled out for this transformation (eq. 6).

Pathway C:

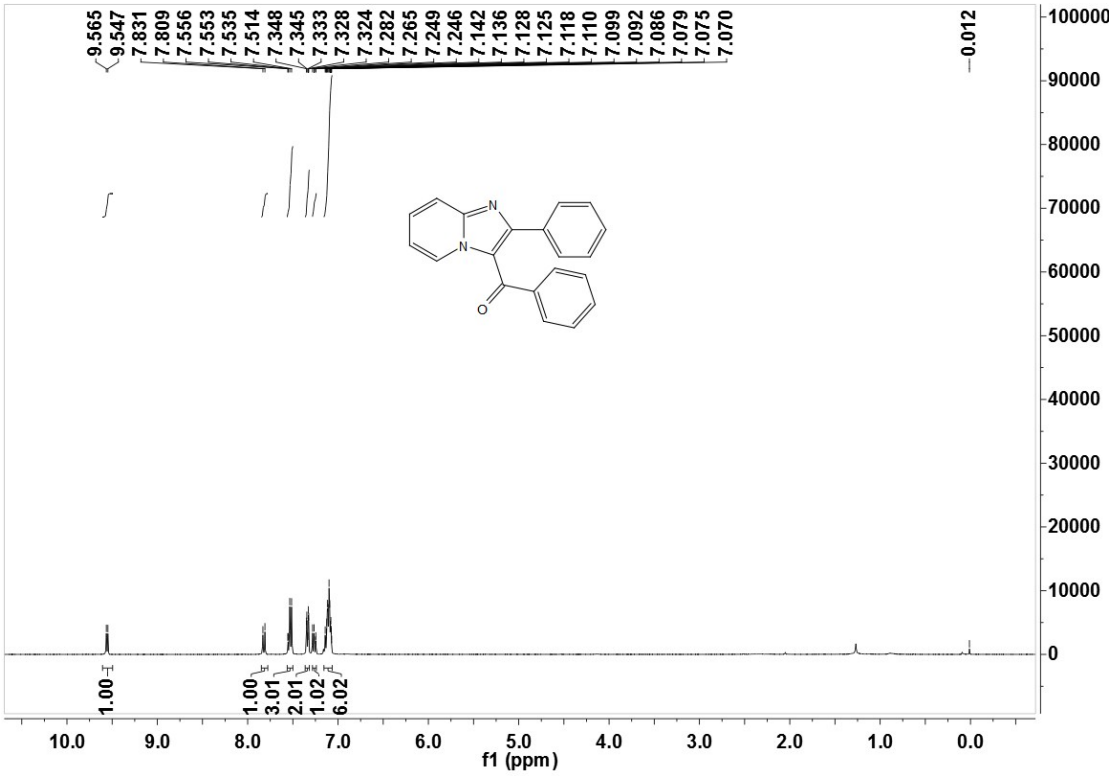


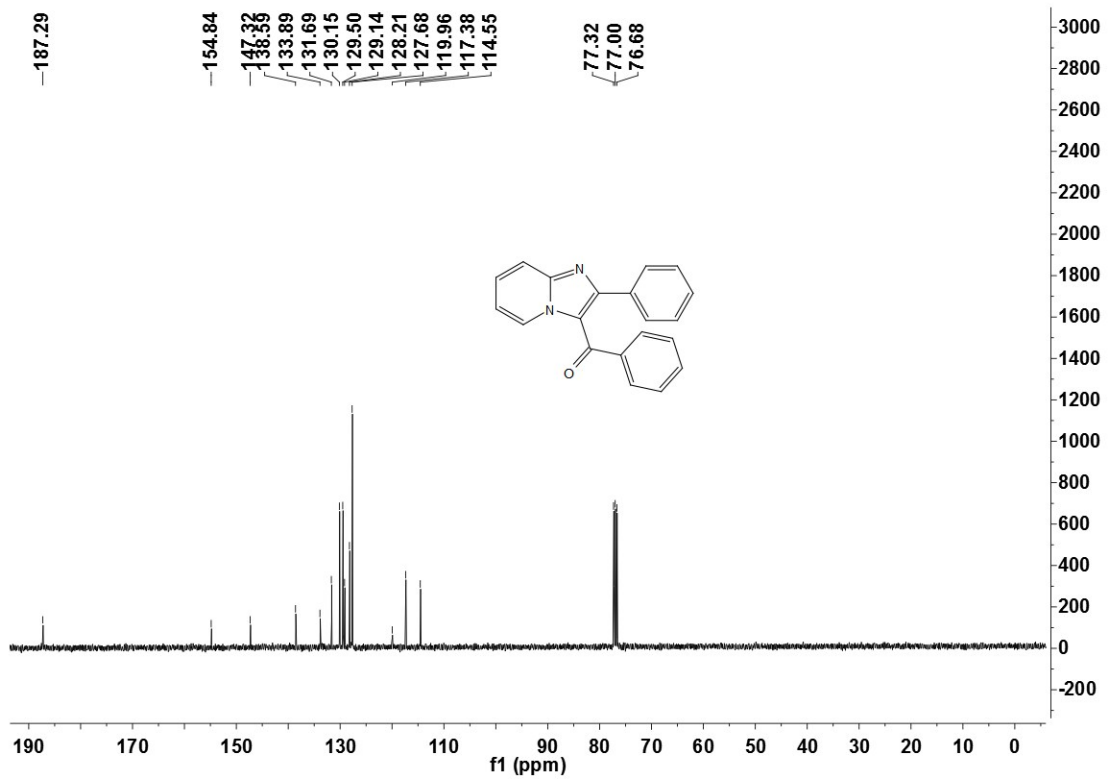
Scheme SI-2. Pathway A and B.

According to the above control experiments, we proposed a possible mechanism as **Pathway C.** Initially, S_N2 reaction of benzylic bromide with 2-amino pyridine **3a** took place, delivering intermediate **8**; further CDC (cross dehydrogenative coupling) reaction of **8** with terminal alkyne **2a** under Cu(II)-catalyzed oxidative conditions led to intermediate **A**. Coordination of **A** with Cu(II) catalyst to form complex **B**. Subsequent SET process occurs with molecular oxygen to deliver peroxy-Cu(III) intermediate **C**, followed by a sequence of intramolecular amino-cuperation of alkynes and oxygenative carbonylation, delivering acylated heterocycle **4a**.

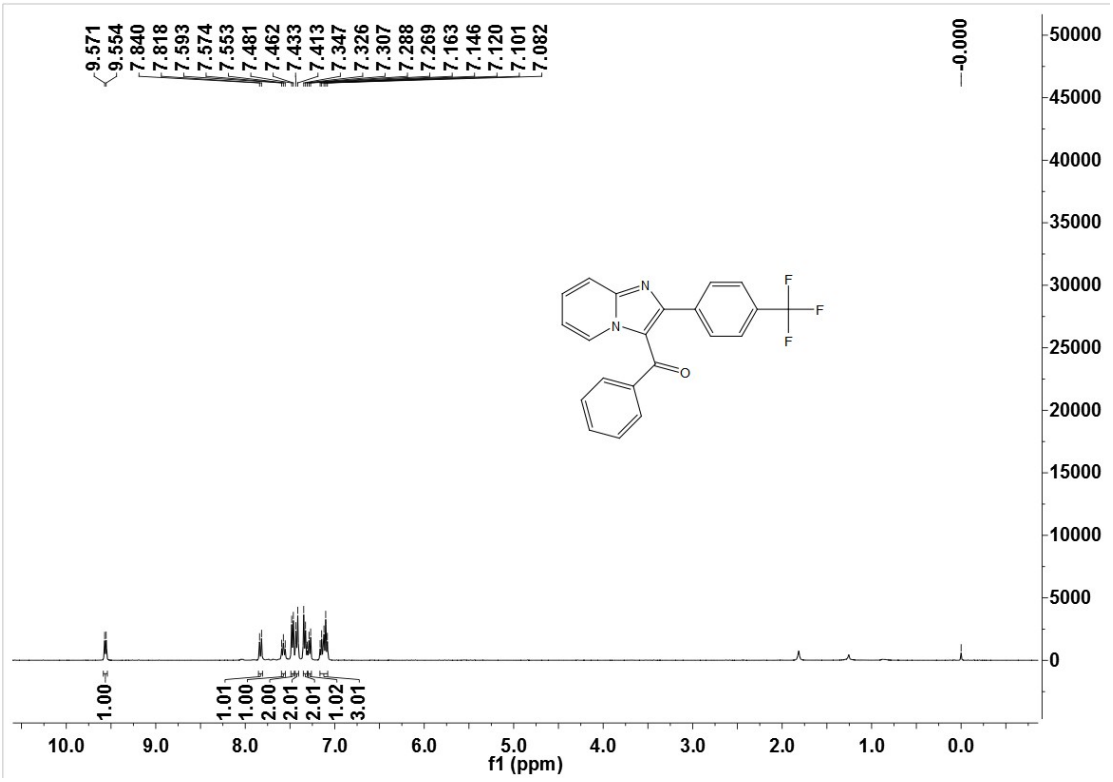
4. NMR Spectrum

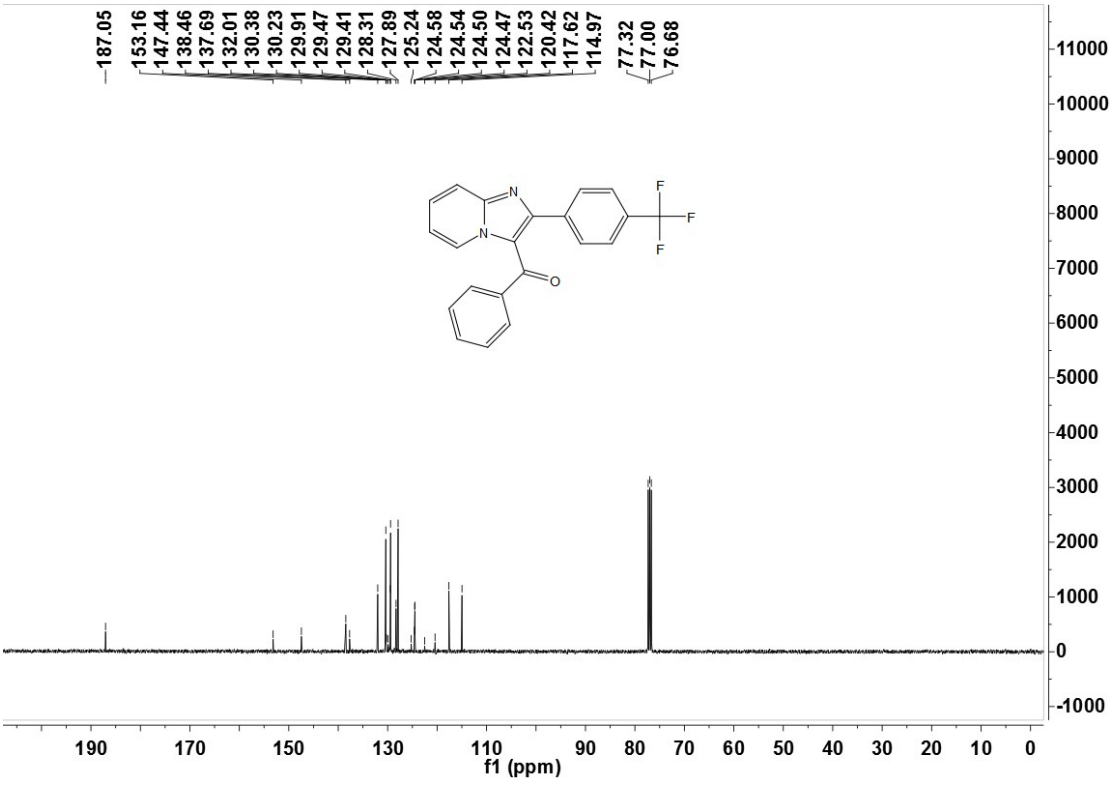
Phenyl(2-phenylimidazo[1,2-a]pyridin-3-yl)methanone (4a)



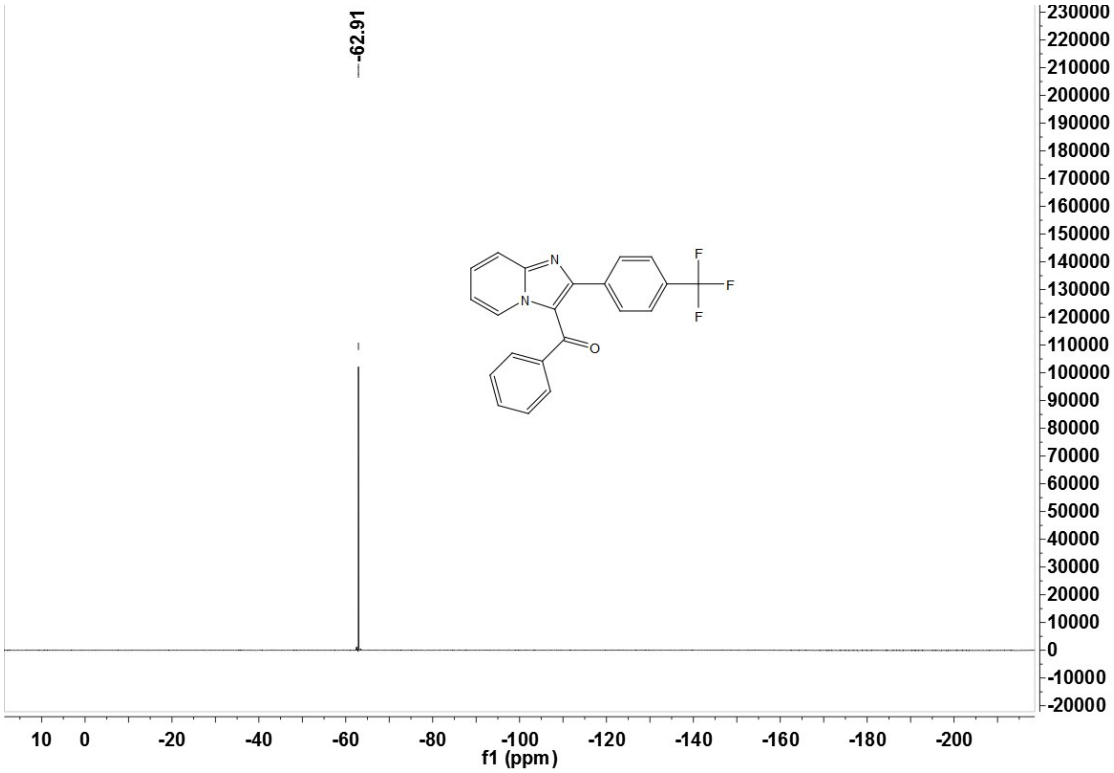


Phenyl(2-(4-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridin-3-yl)methanone (4b)





^{19}F spectrum



HRMS

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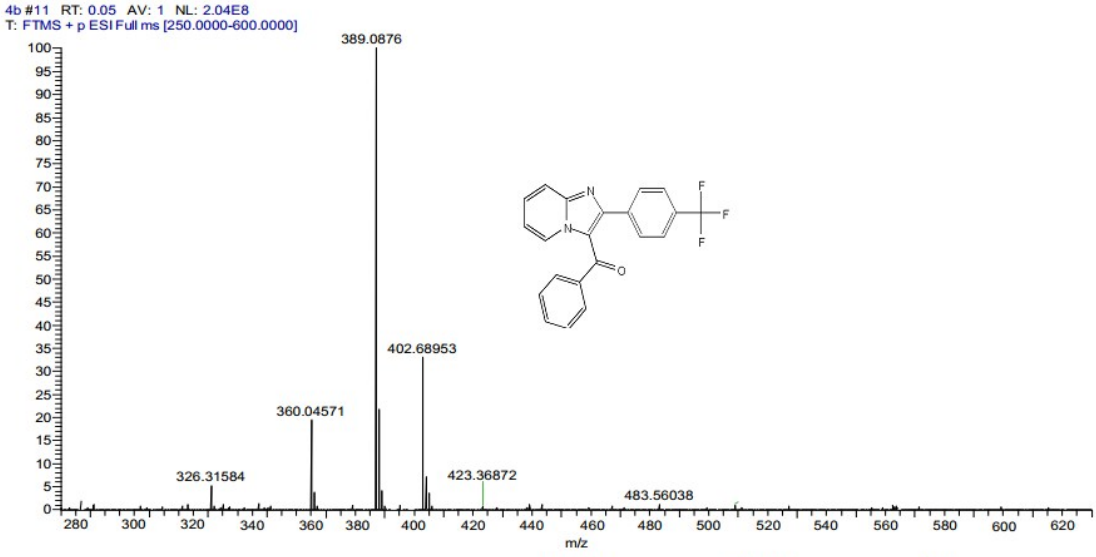

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C21H13F3N2O	+ Na	C21H13F3N2ONa	389.08723	389.08761	0.81

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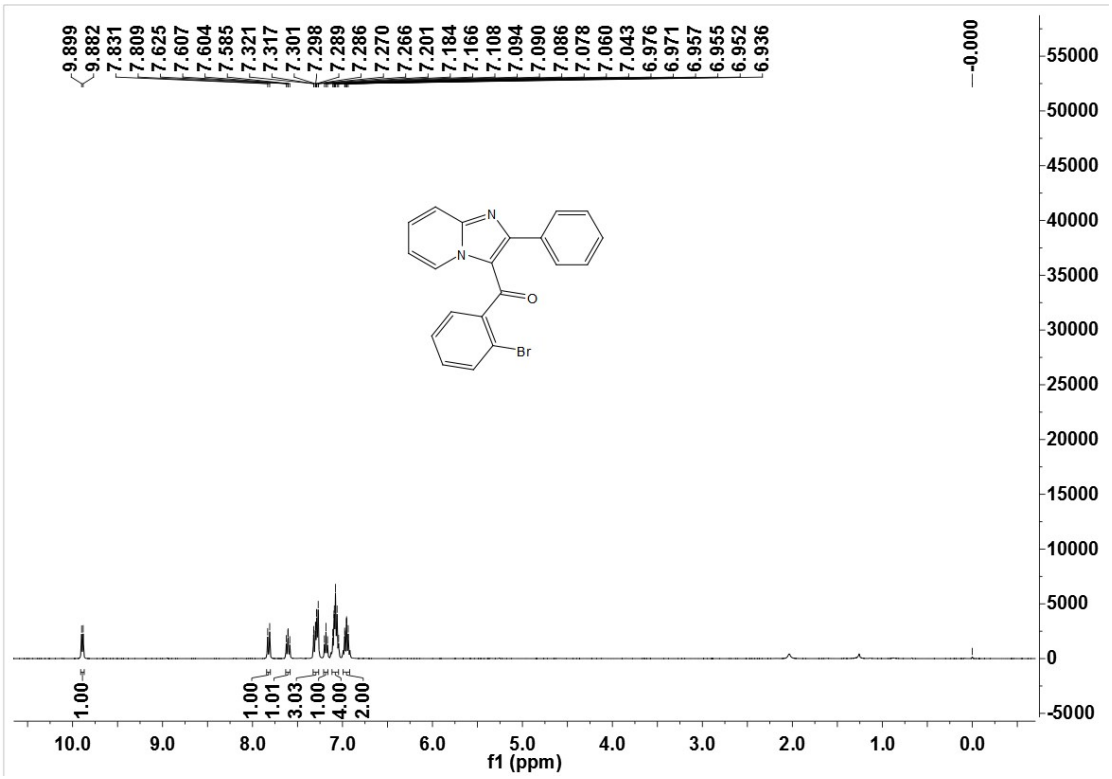

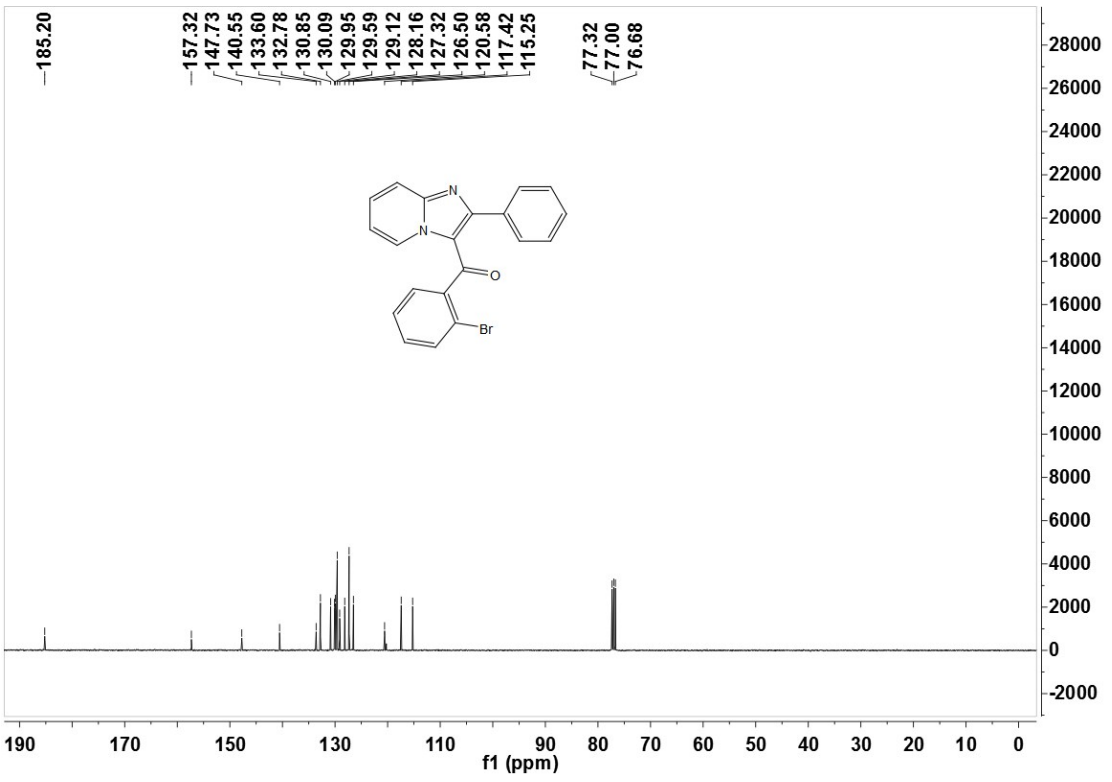

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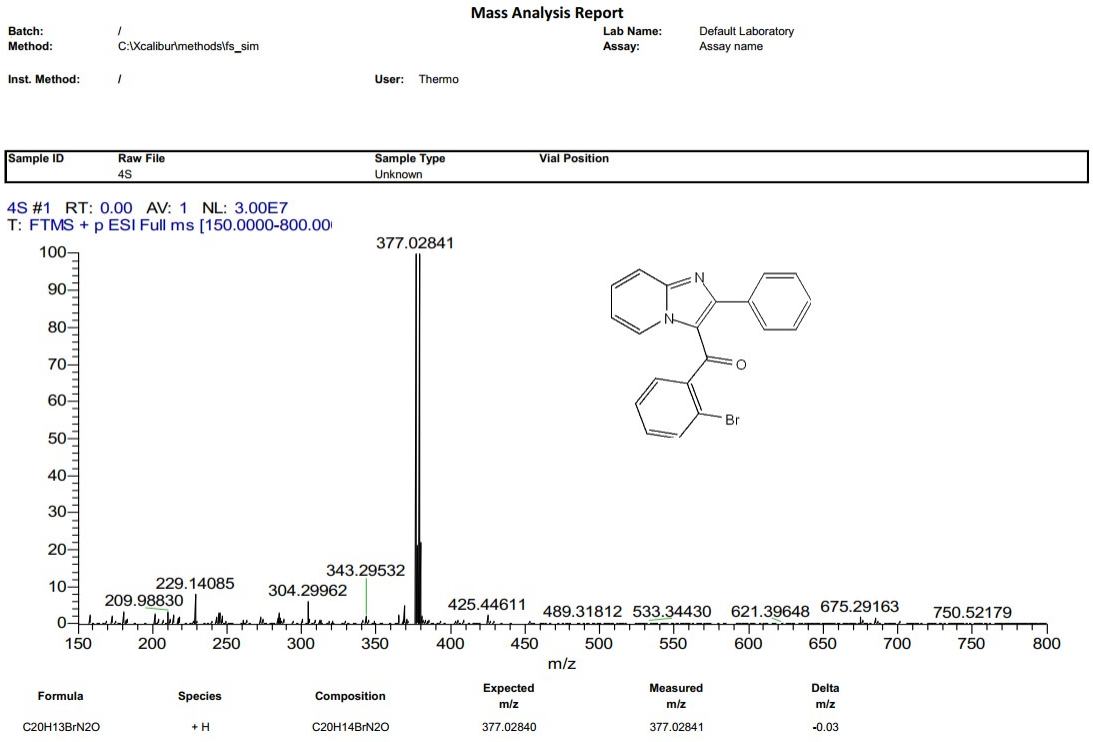

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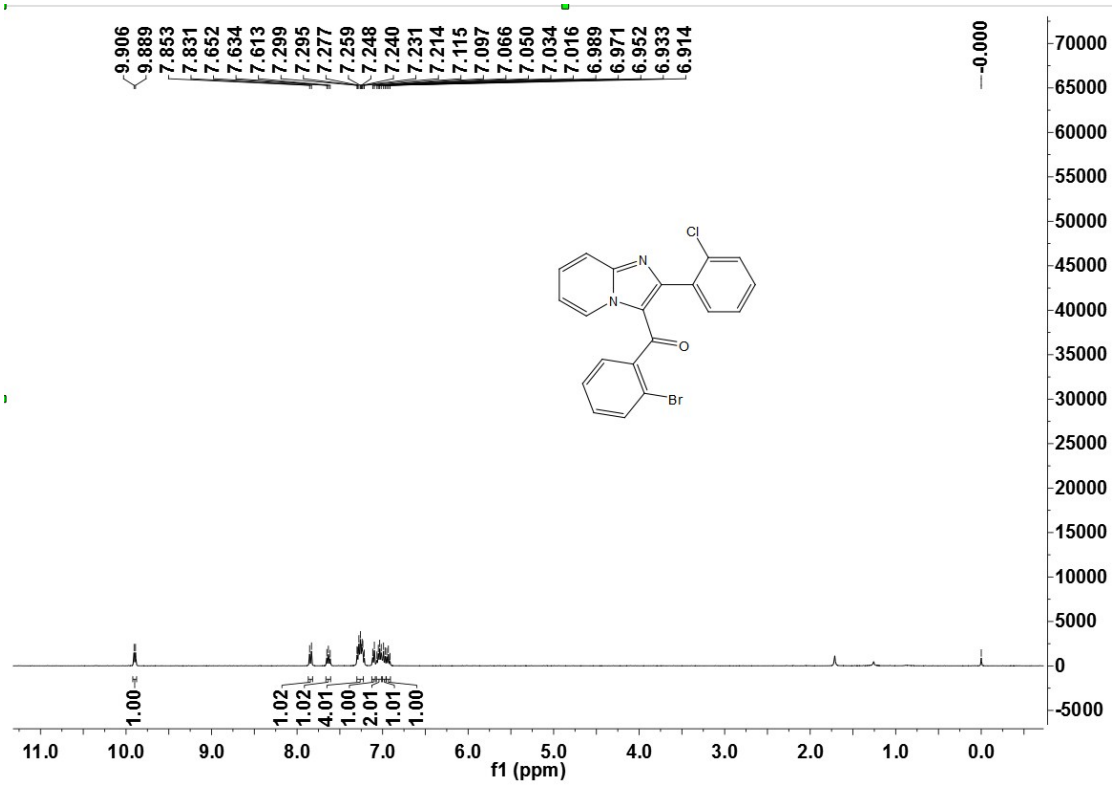

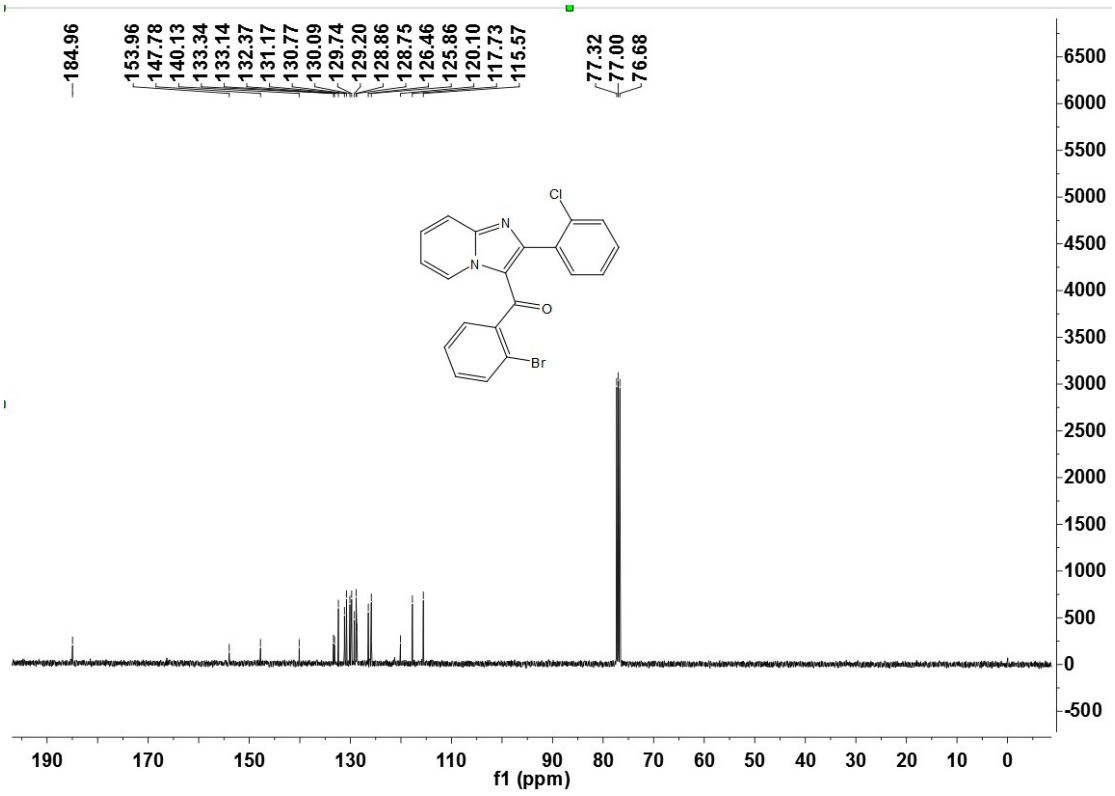

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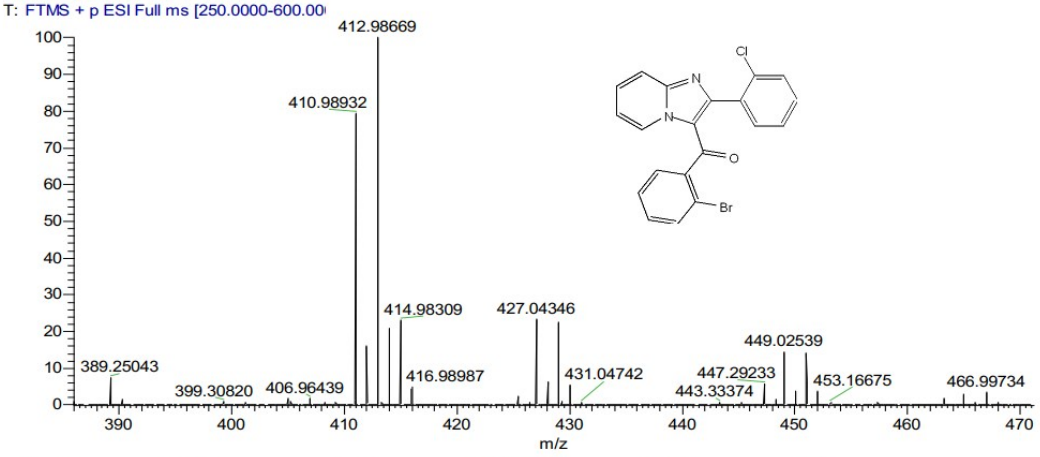
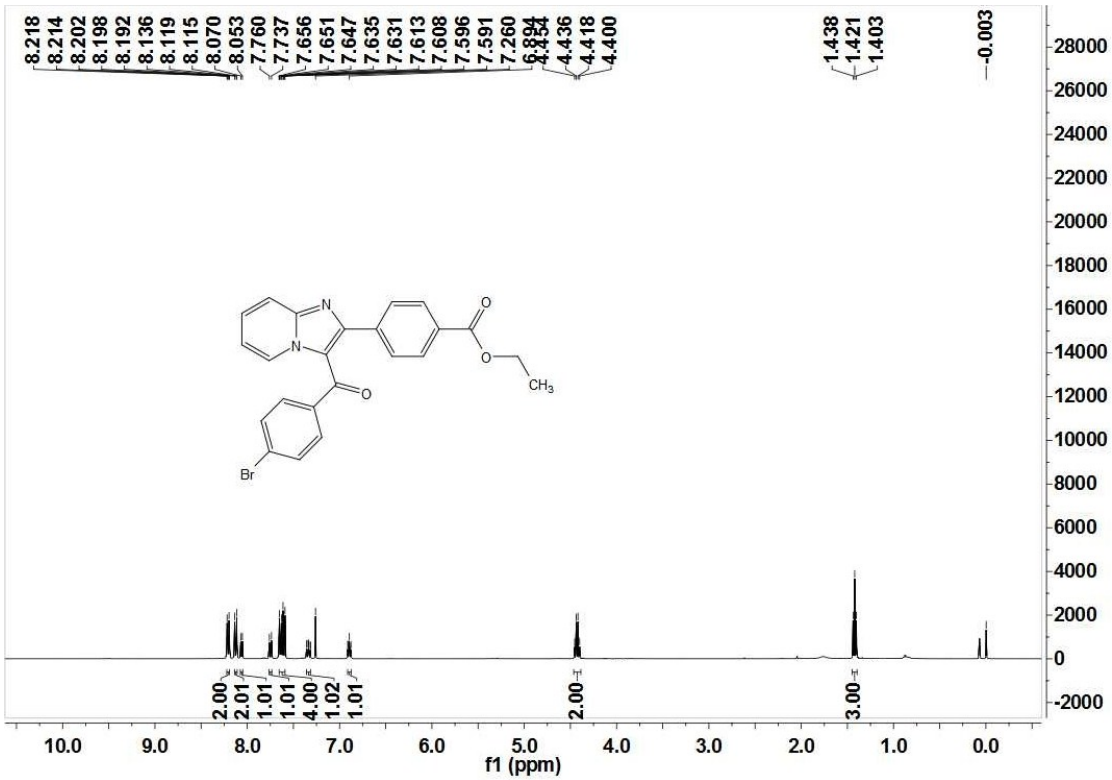
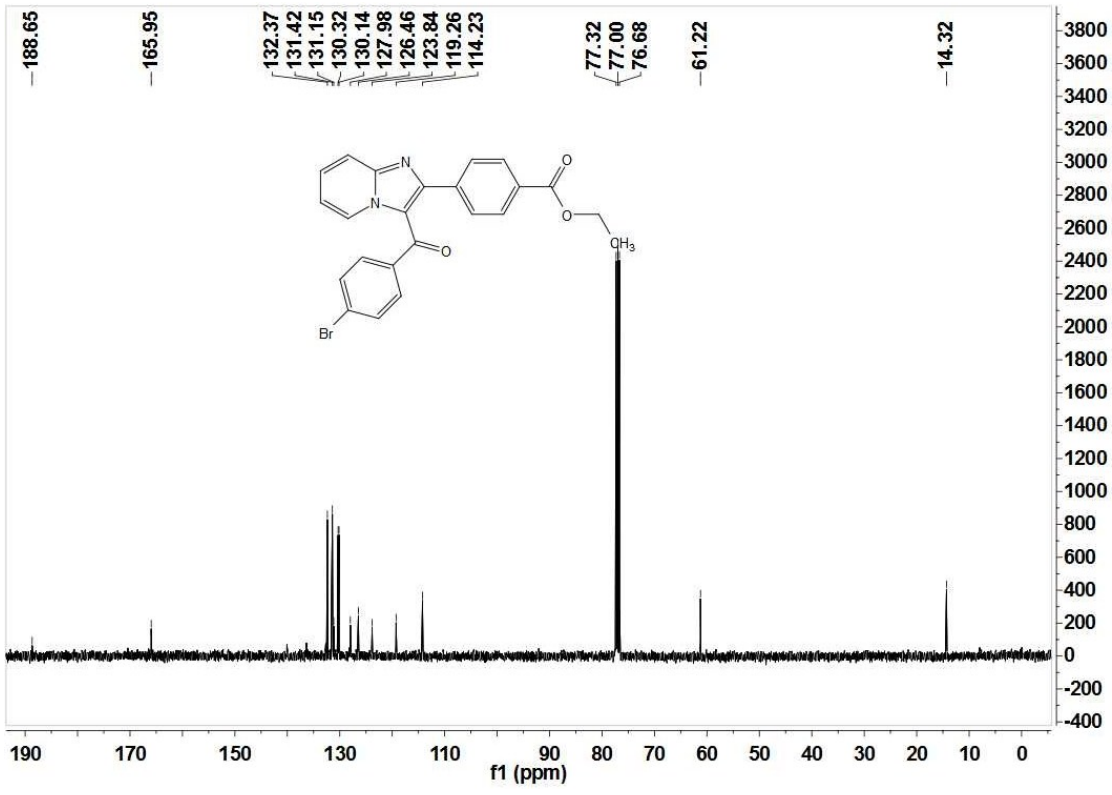


Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C20H12BrClN2O	+ H	C20H13BrClN2O	410.98943	410.98932	0.27

Ethyl 4-(3-(4-bromobenzoyl)imidazo[1,2-a]pyridin-2-yl)benzoate (4e)





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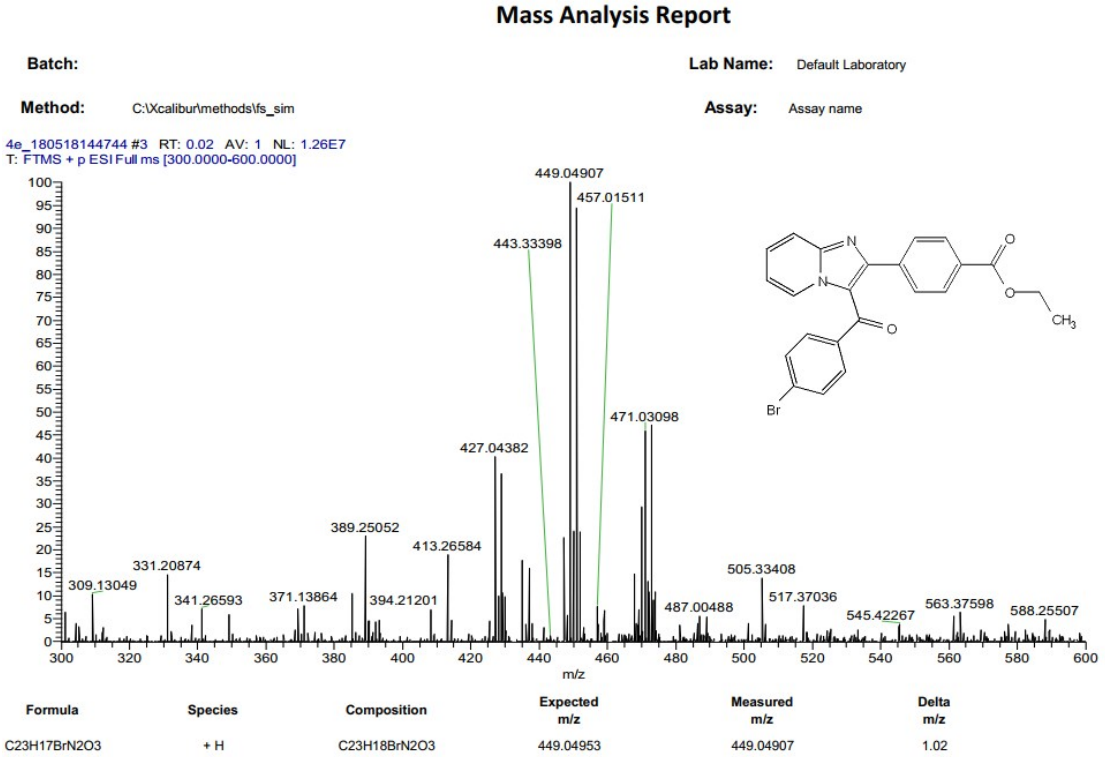

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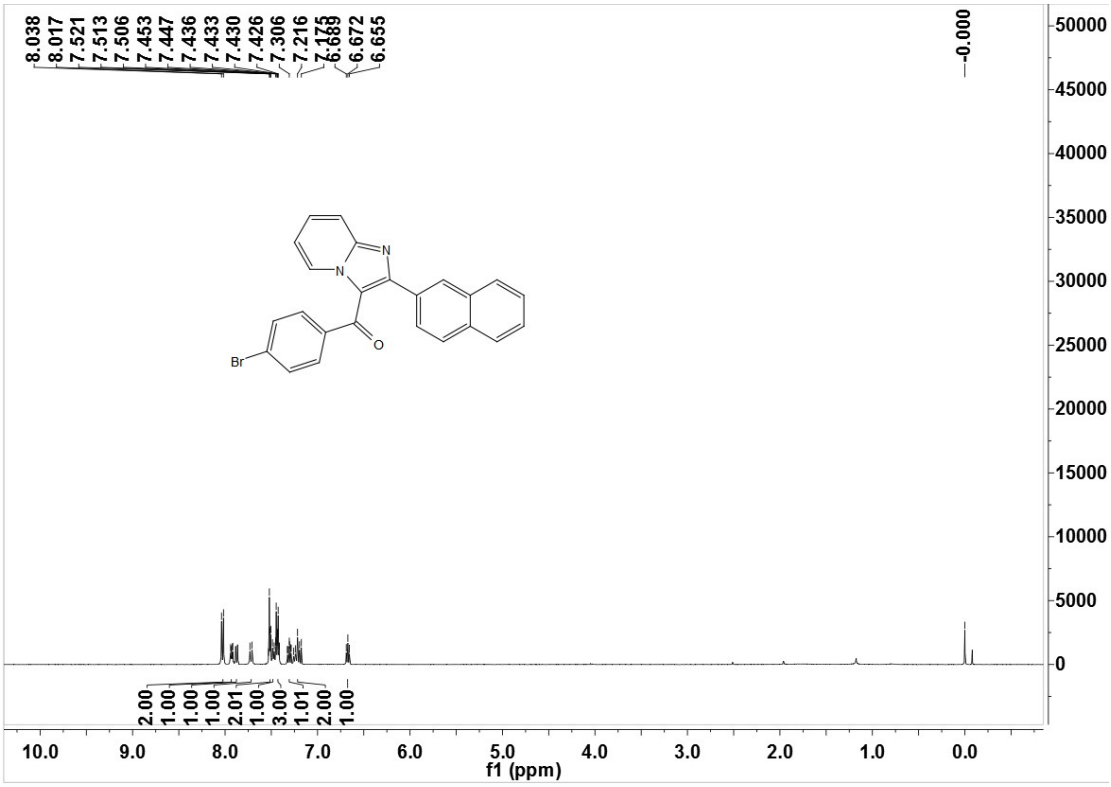

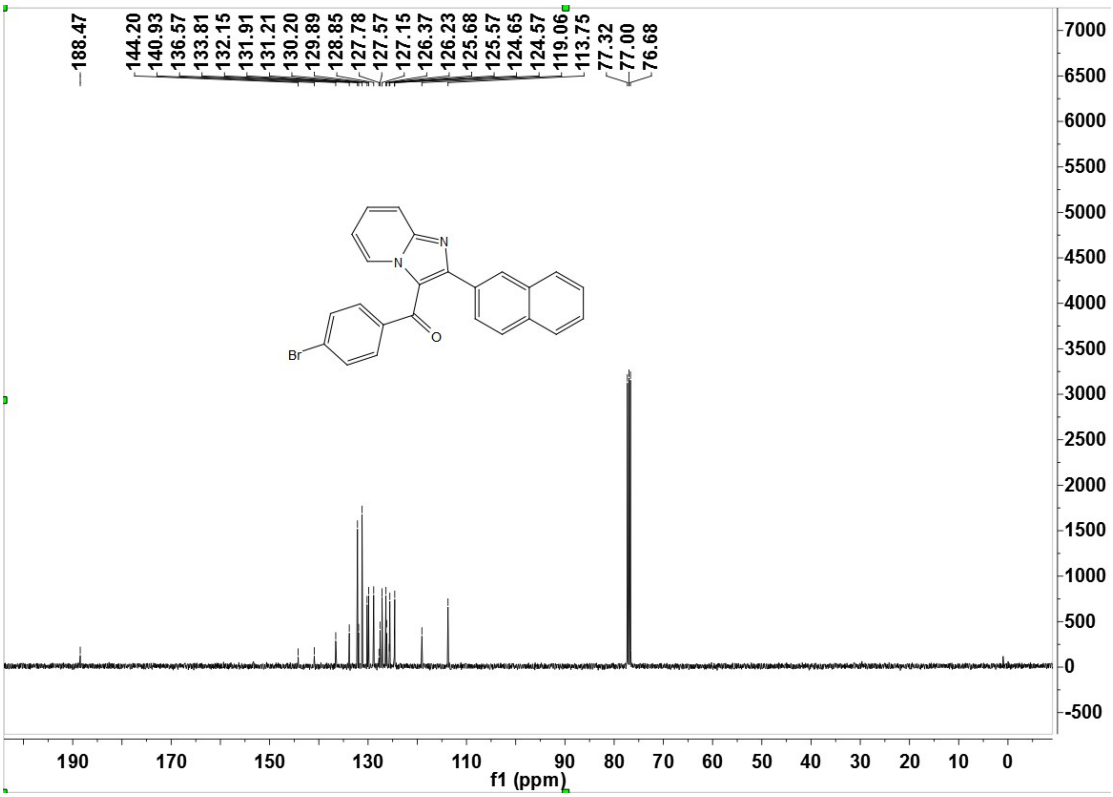

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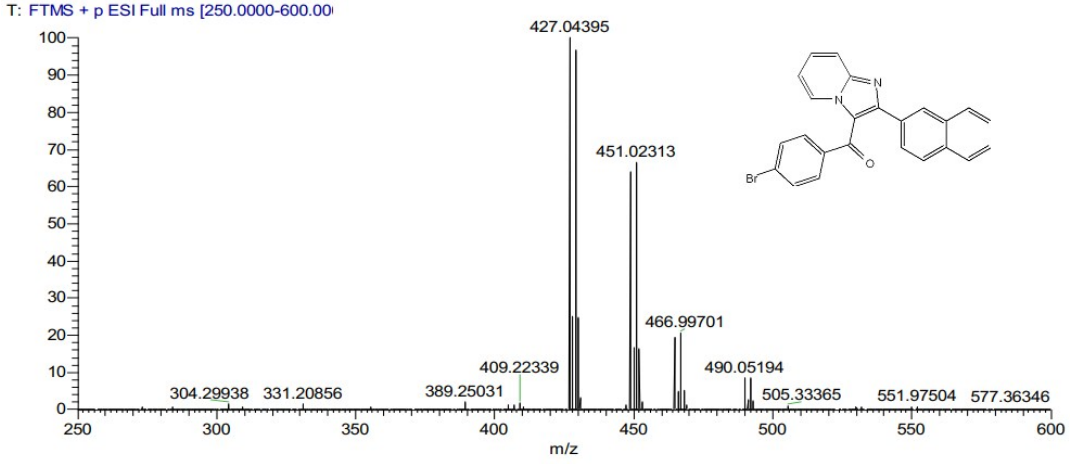
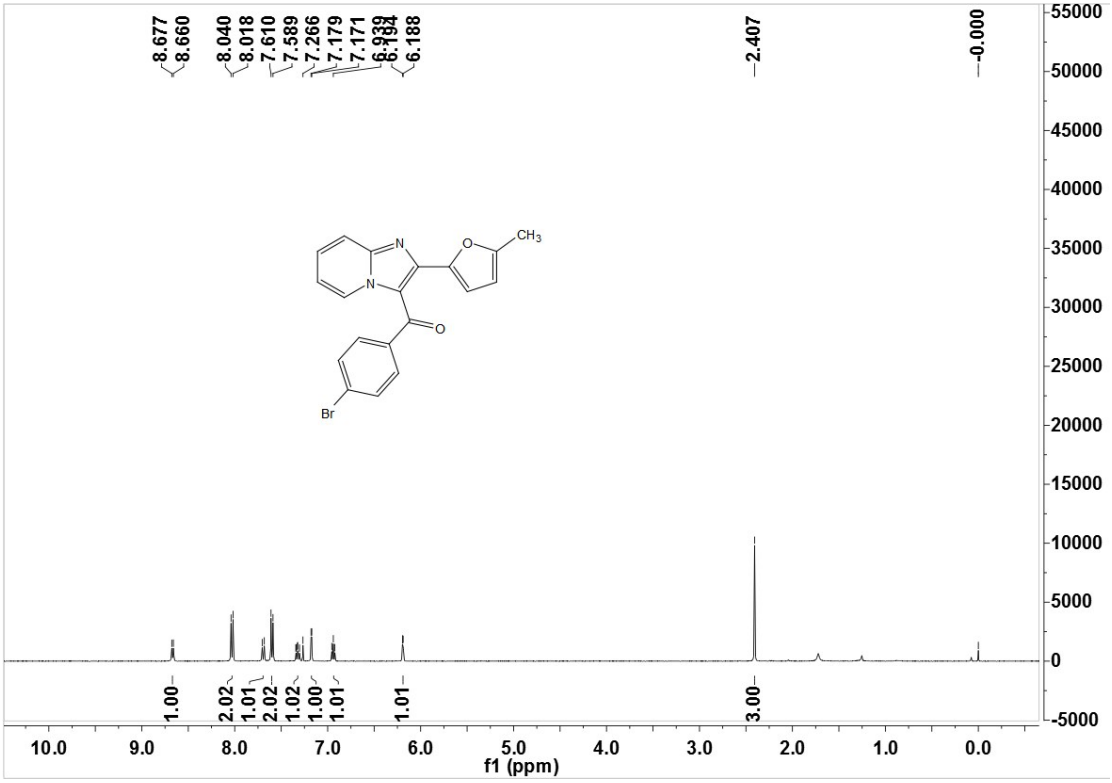
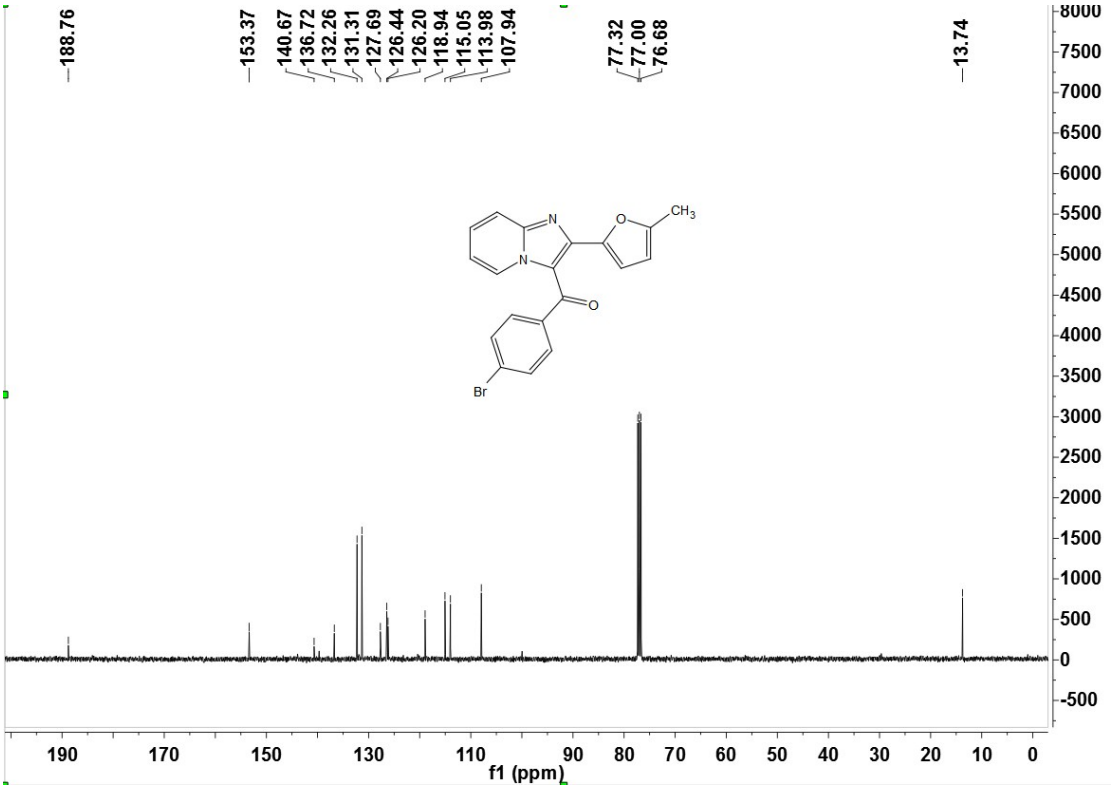


Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C24H15BrN2O	+ H	C24H16BrN2O	427.04405	427.04395	0.23

(4-Bromophenyl)(2-(5-methylfuran-2-yl)imidazo[1,2-a]pyridin-3-yl)methanone

(4g)





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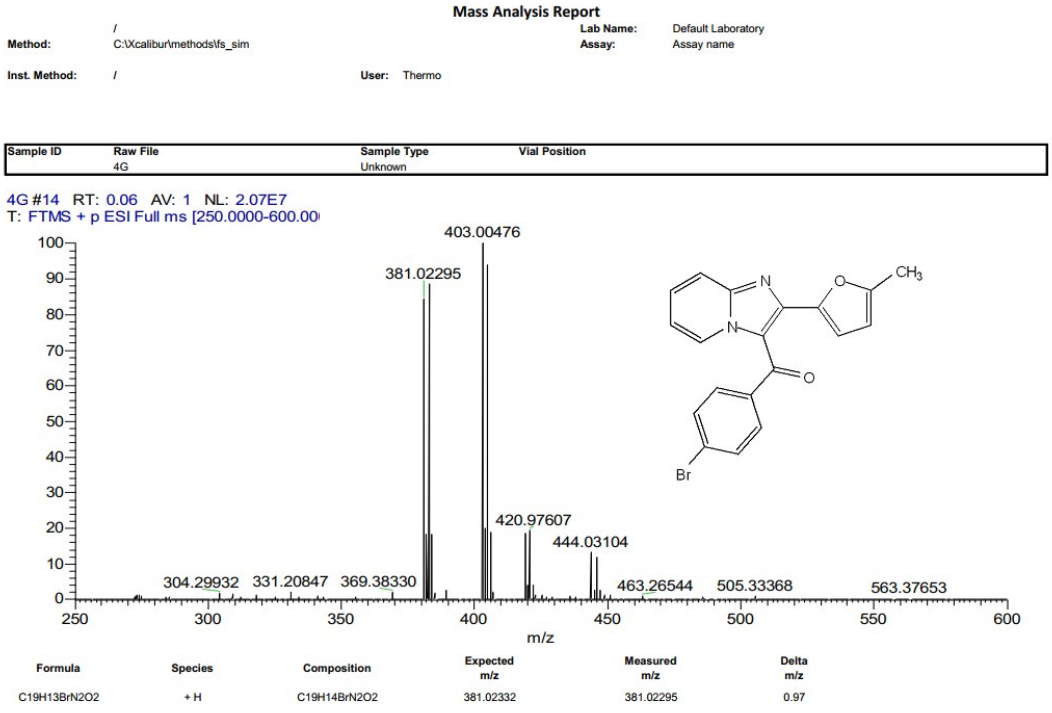

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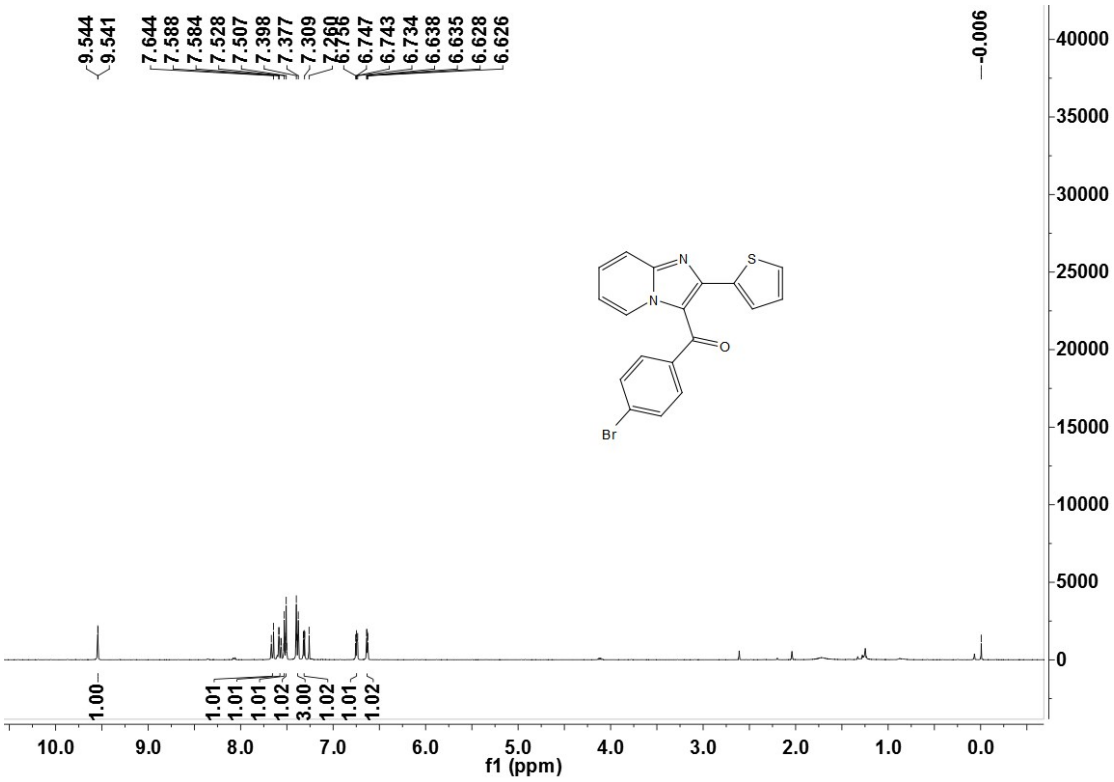

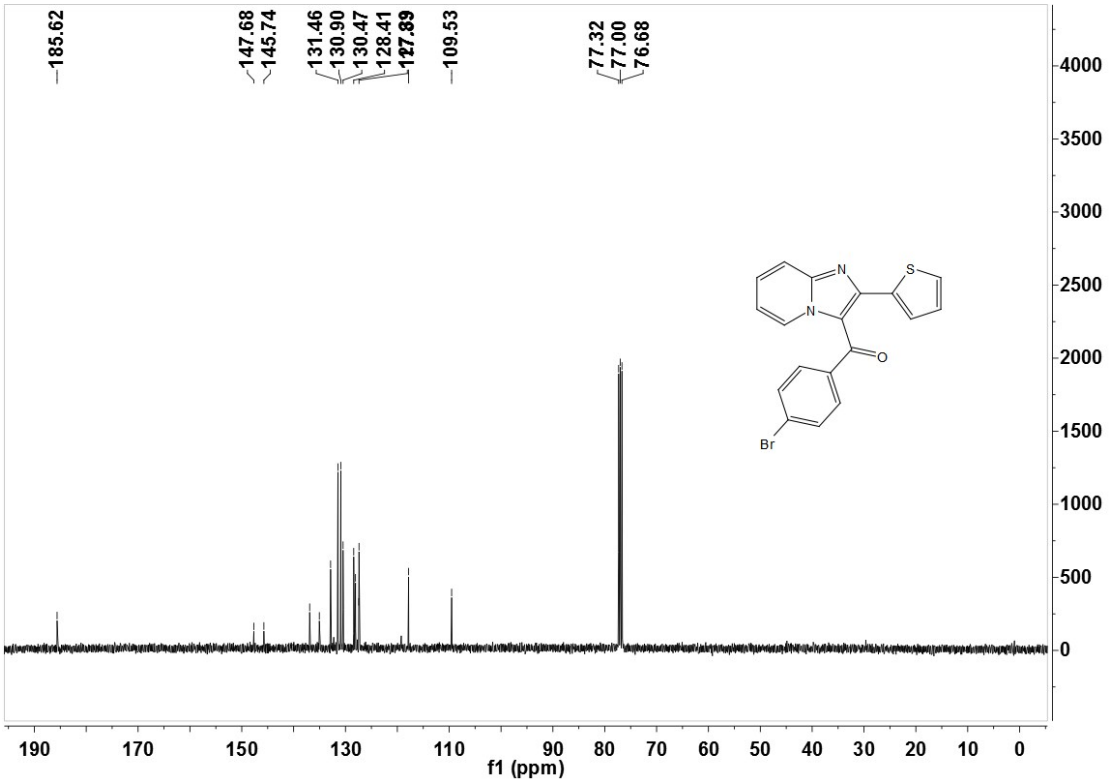
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500
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f1 (ppm)

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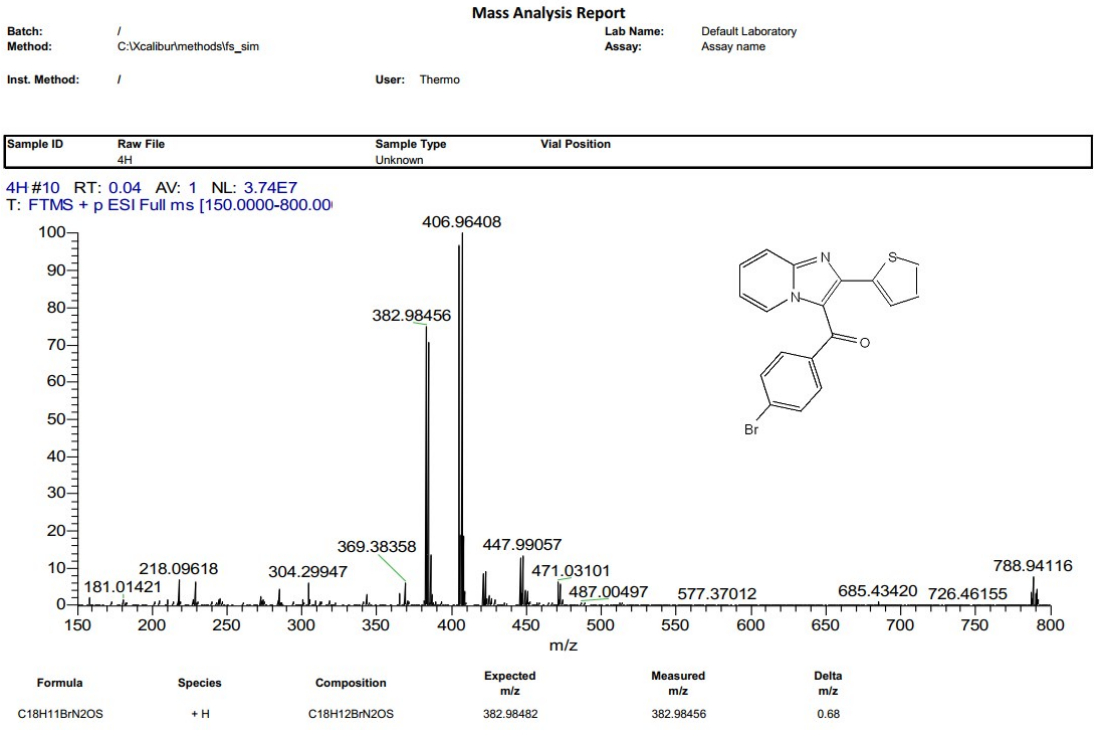
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Species
Composition
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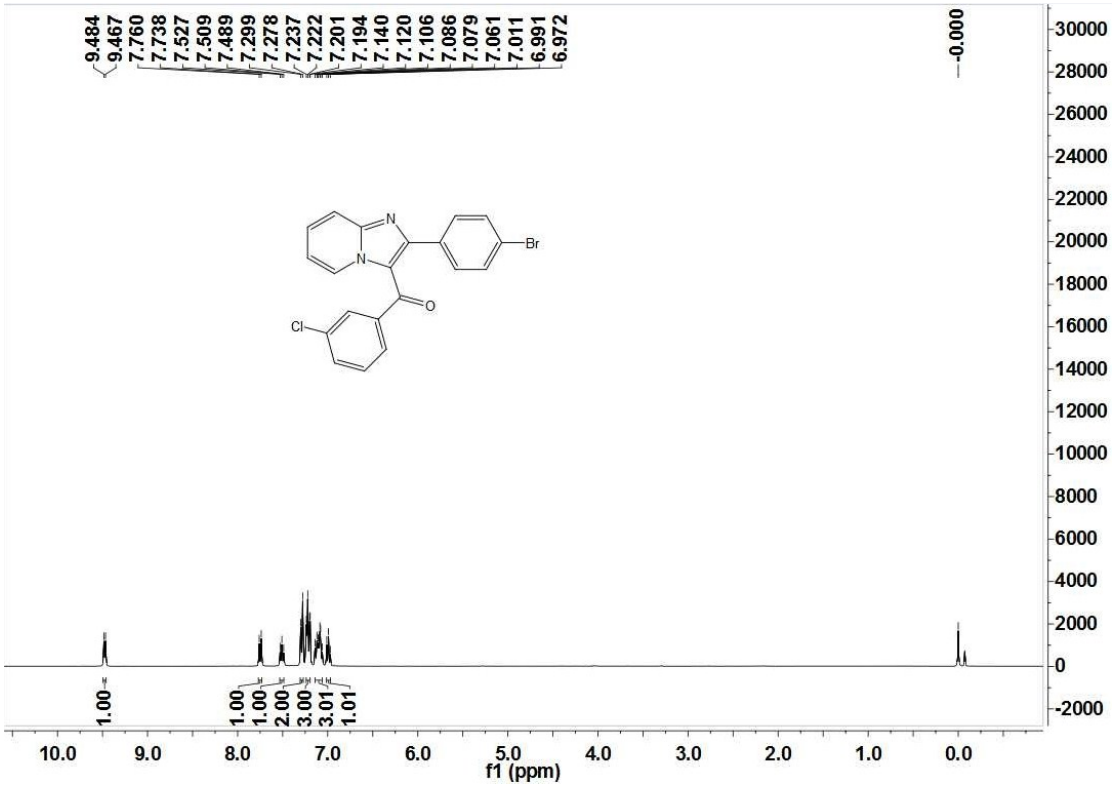

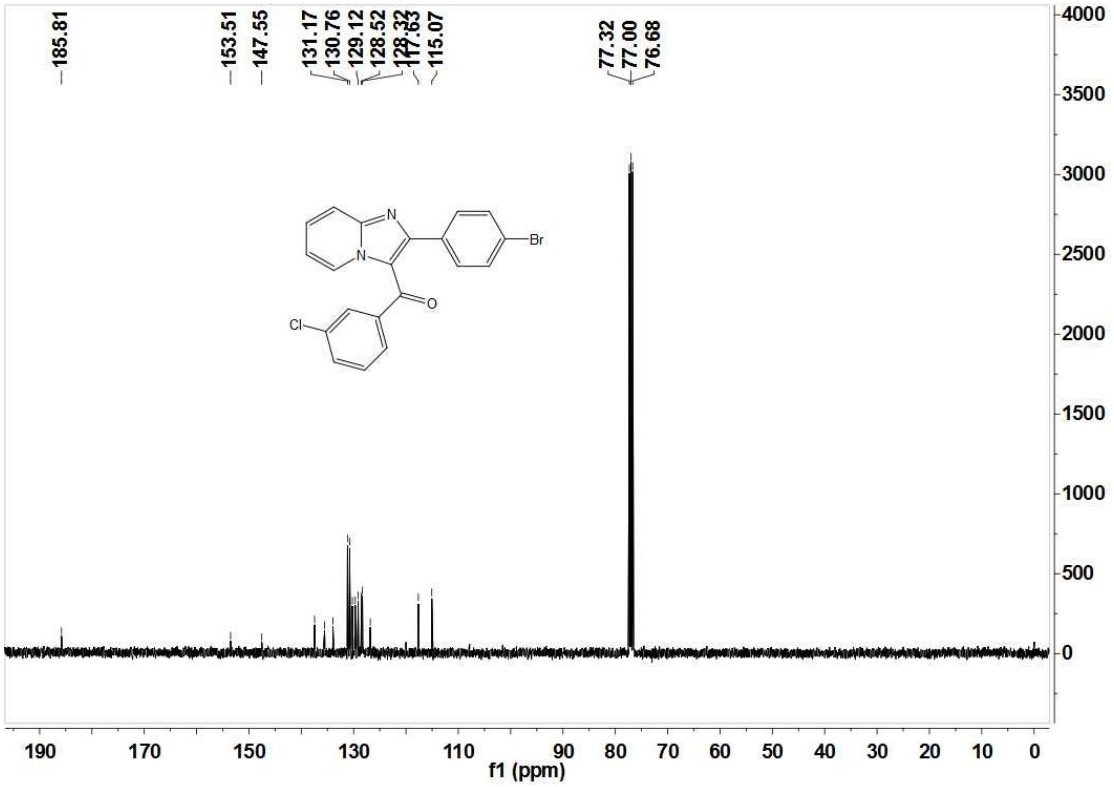

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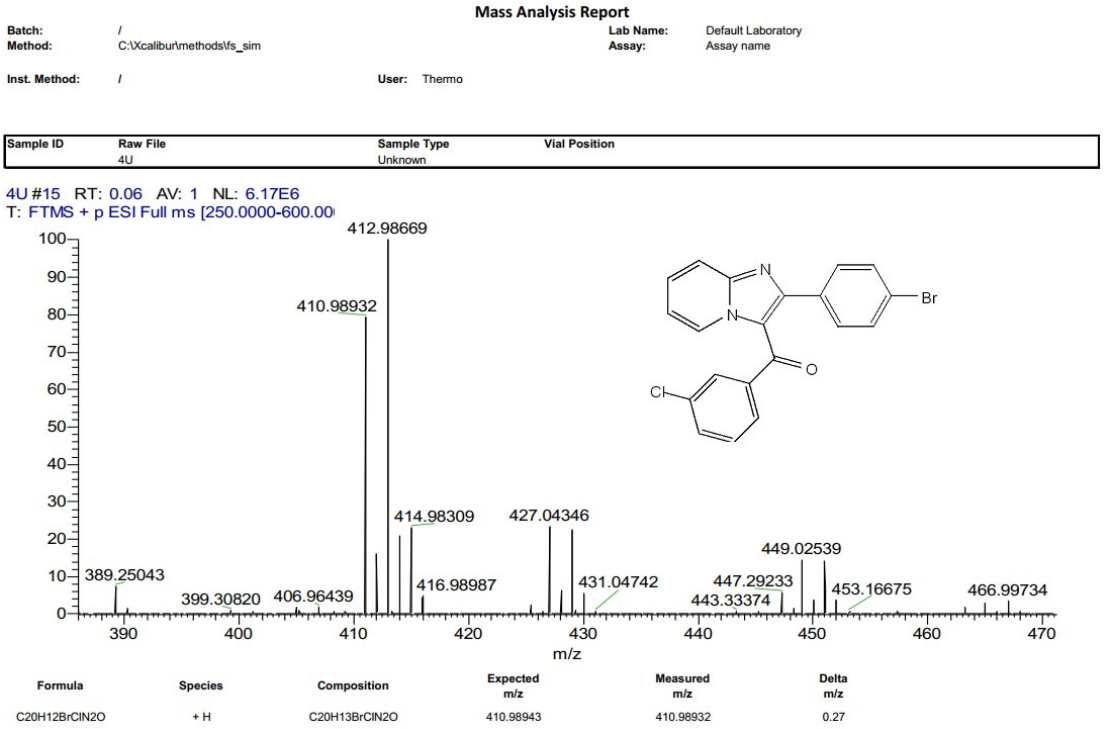
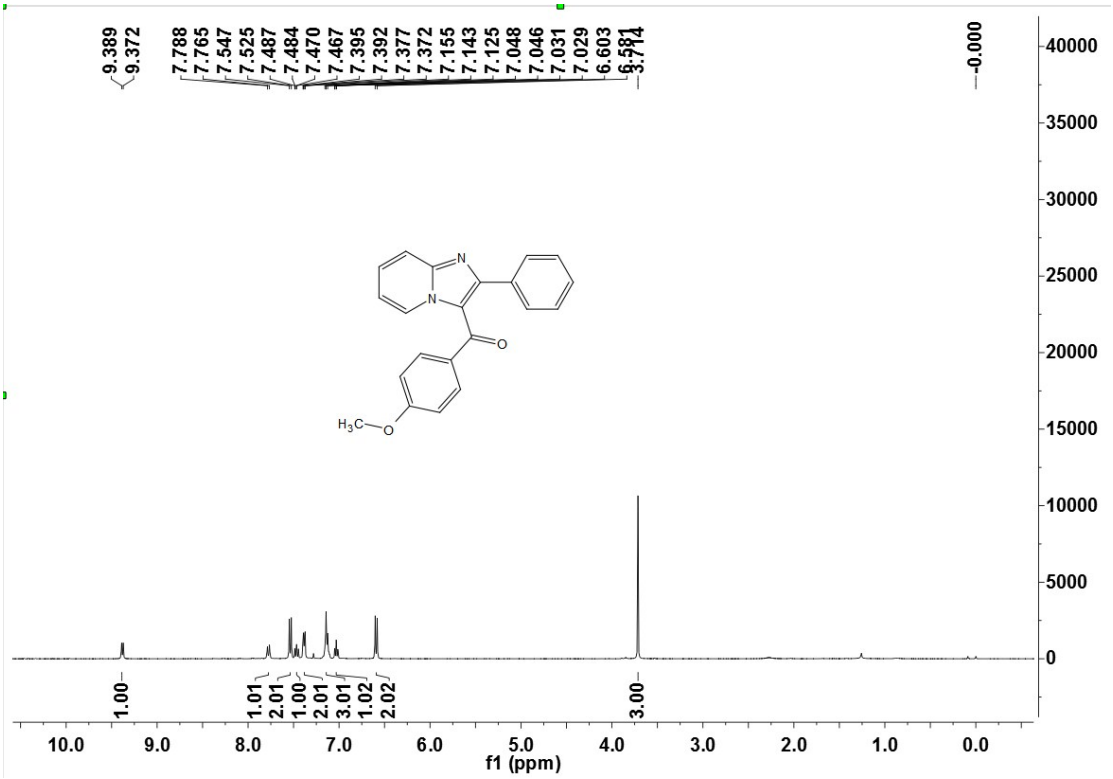
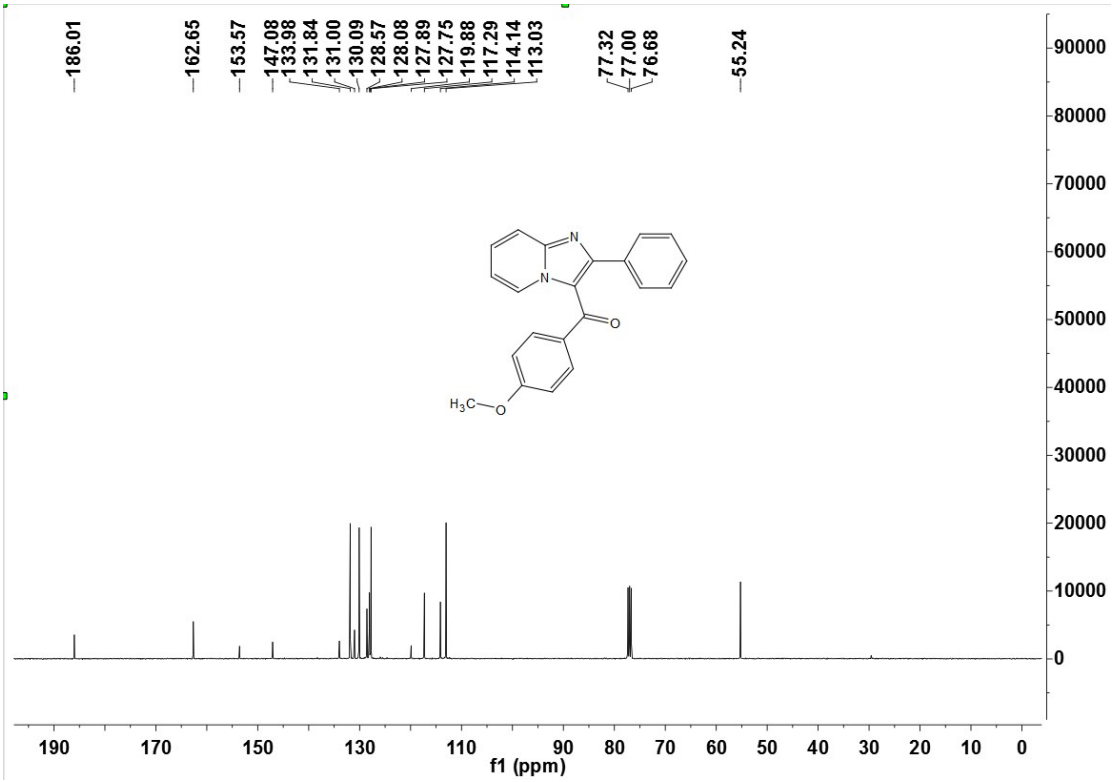
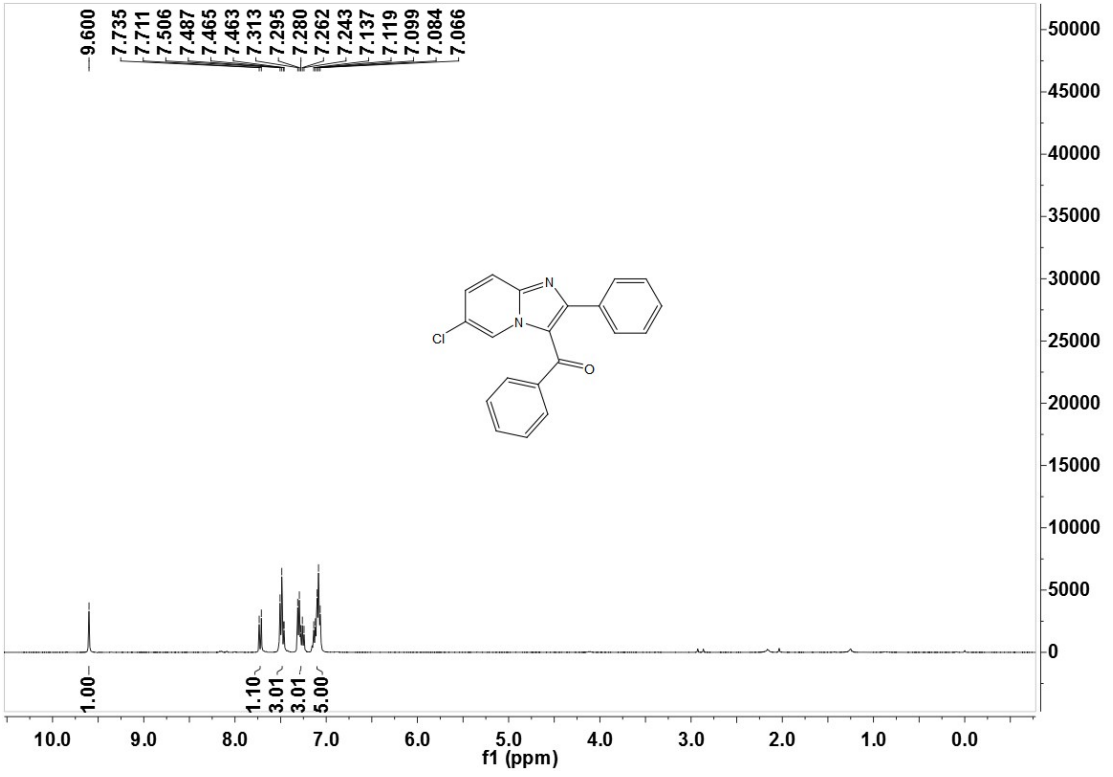


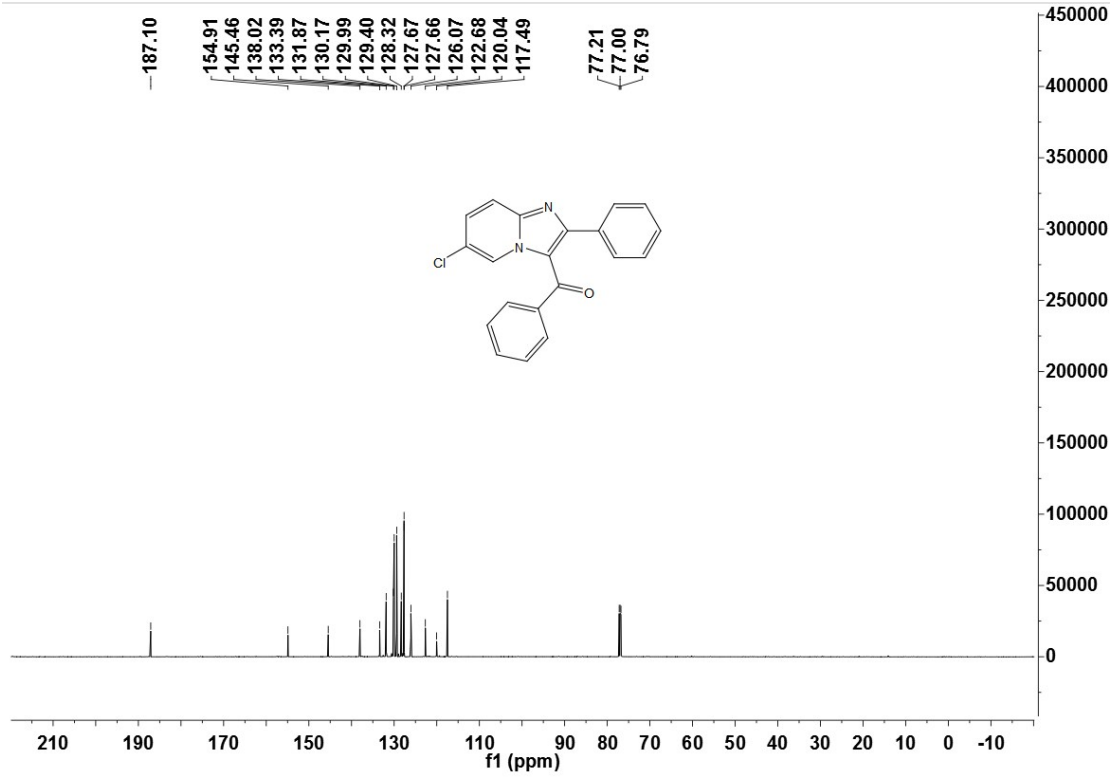
(4-Methoxyphenyl)(2-phenylimidazo[1,2-a]pyridin-3-yl)methanone (4j)



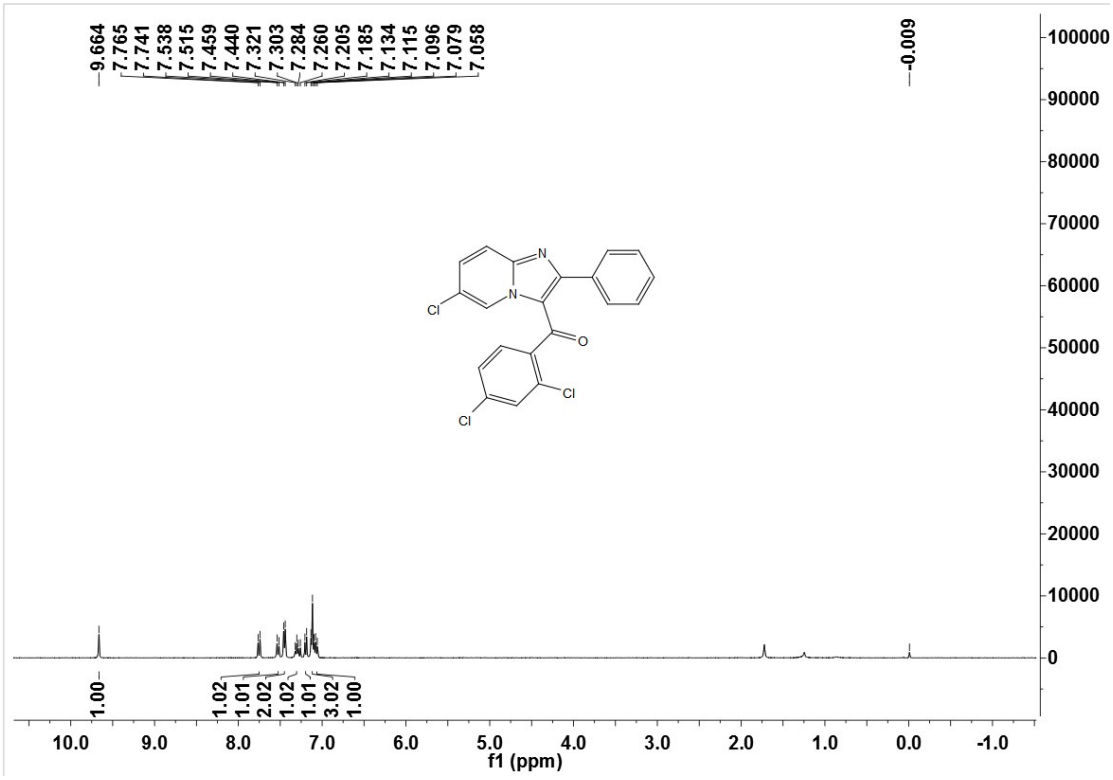


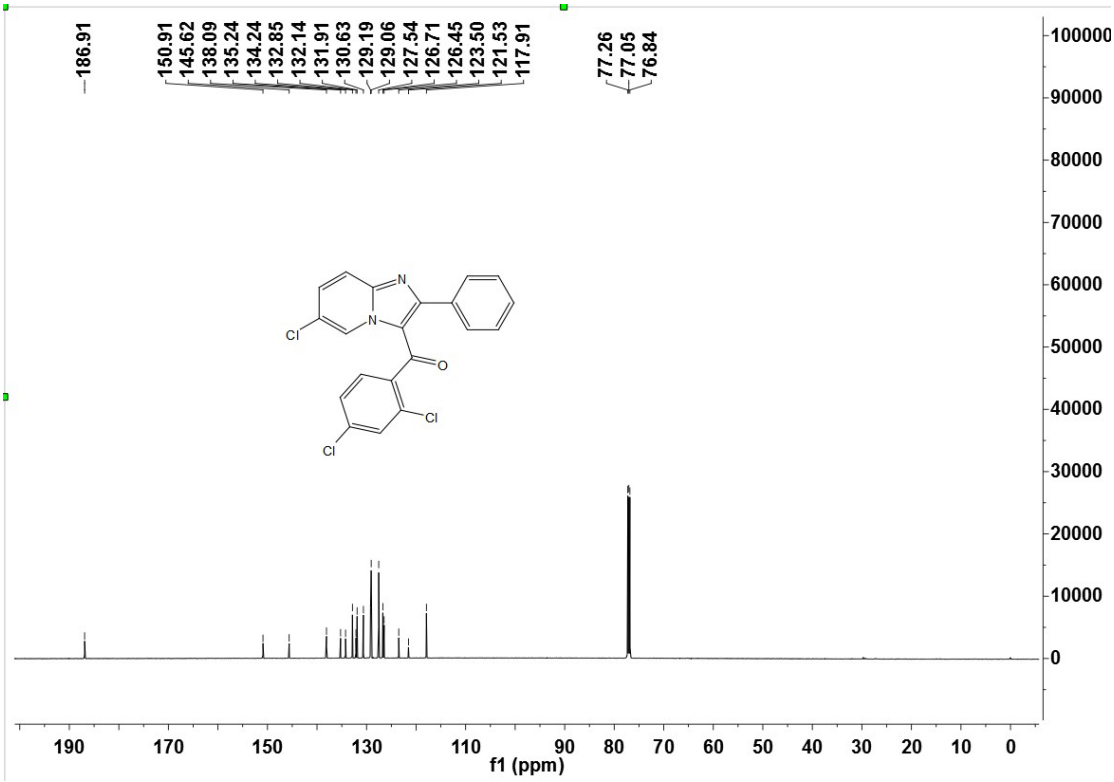
6-Chloro-2-phenylimidazo[1,2-a]pyridin-3-yl)(phenyl)methanone (4k)





(6-Chloro-2-phenylimidazo[1,2-a]pyridin-3-yl)(2,4-dichlorophenyl)methanone (4l)





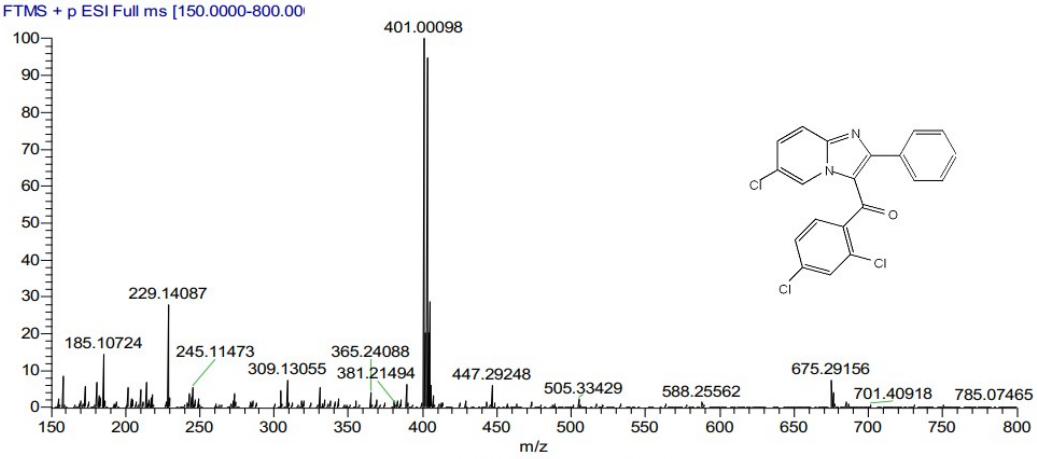
HRMS

Mass Analysis Report

Batch:	/	**Lab Name:**	Default Laboratory
Method:	C:\Xcalibur\methods\fs_sim	**Assay:**	Assay name
Inst. Method:	/	**User:**	Thermo

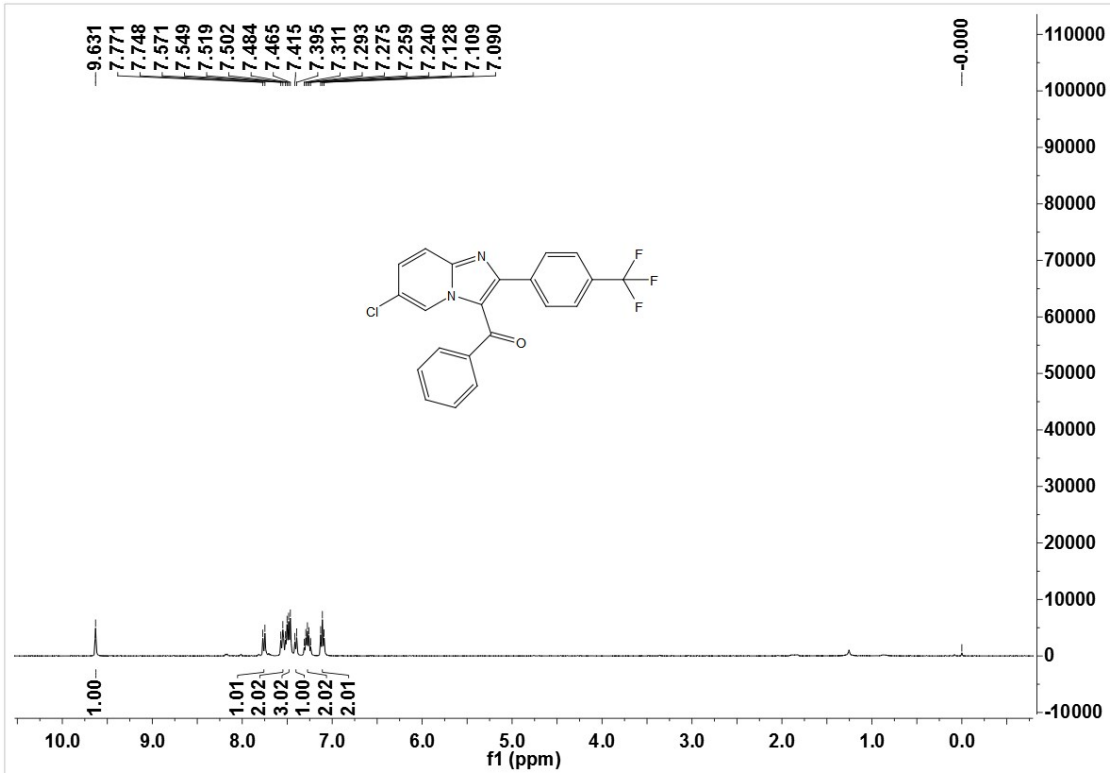
Sample ID	Raw File	Sample Type	Vial Position
	4l	Unknown	

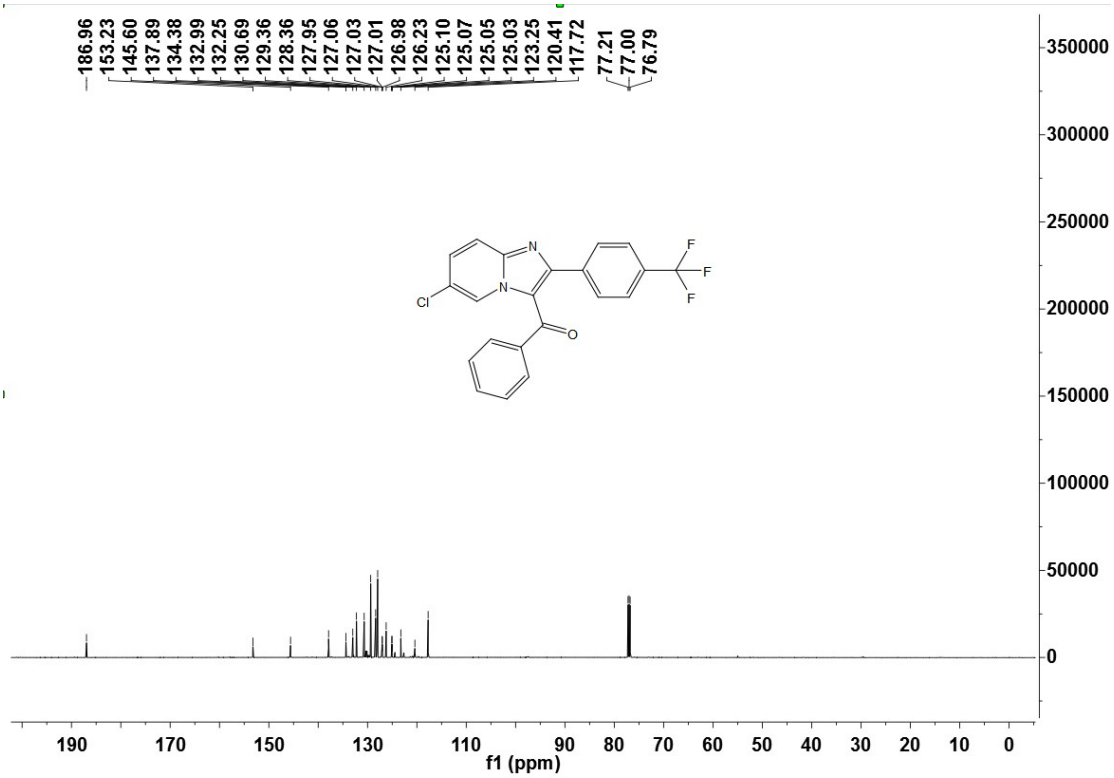
4l #48 RT: 0.21 AV: 1 NL: 9.34E6
T: FTMS + p ESI Full ms [150.0000-800.00



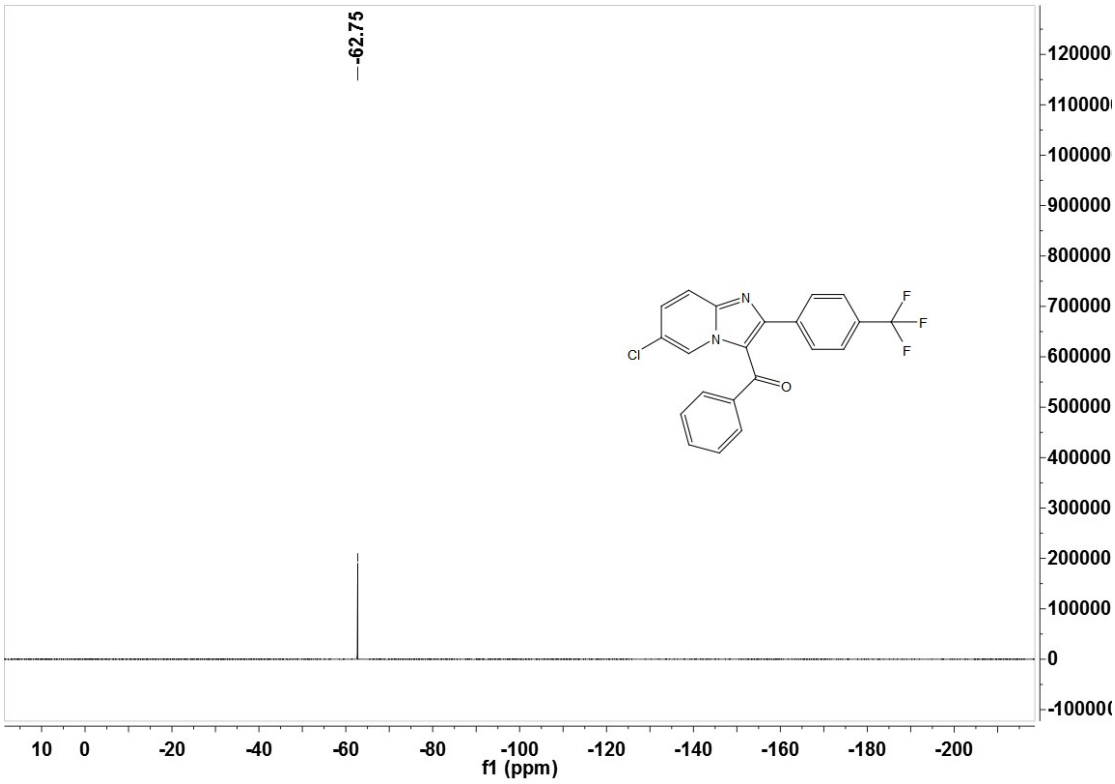
Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C20H11Cl3N2O	+ H	C20H12Cl3N2O	401.00097	401.00098	-0.02

(6-Chloro-2-(4-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridin-3-yl)(phenyl)methanone (4m)





^{19}F spectrum



HRMS

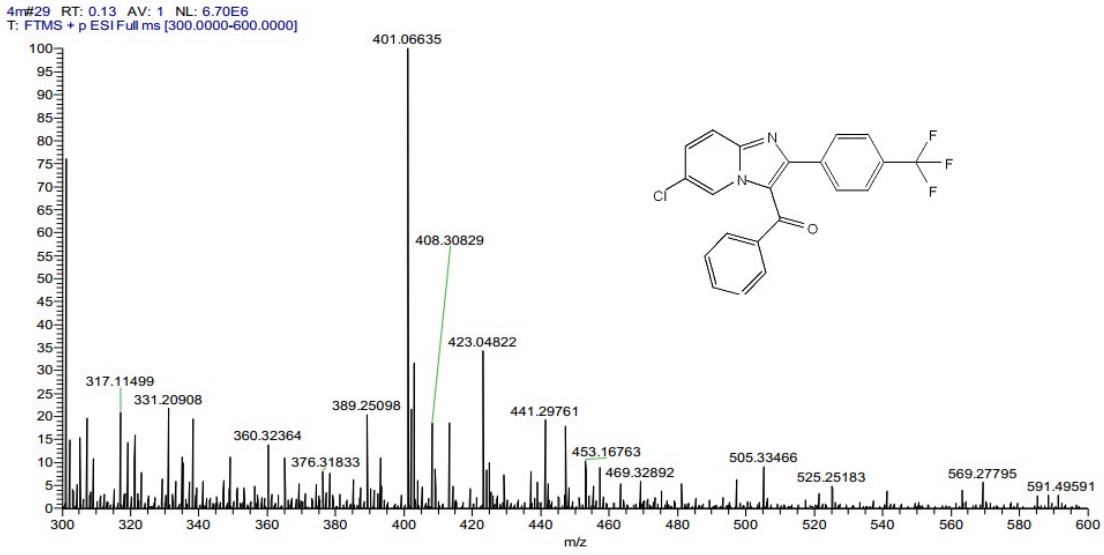
Mass Analysis Report

Batch: /

Lab Name: Default Laboratory

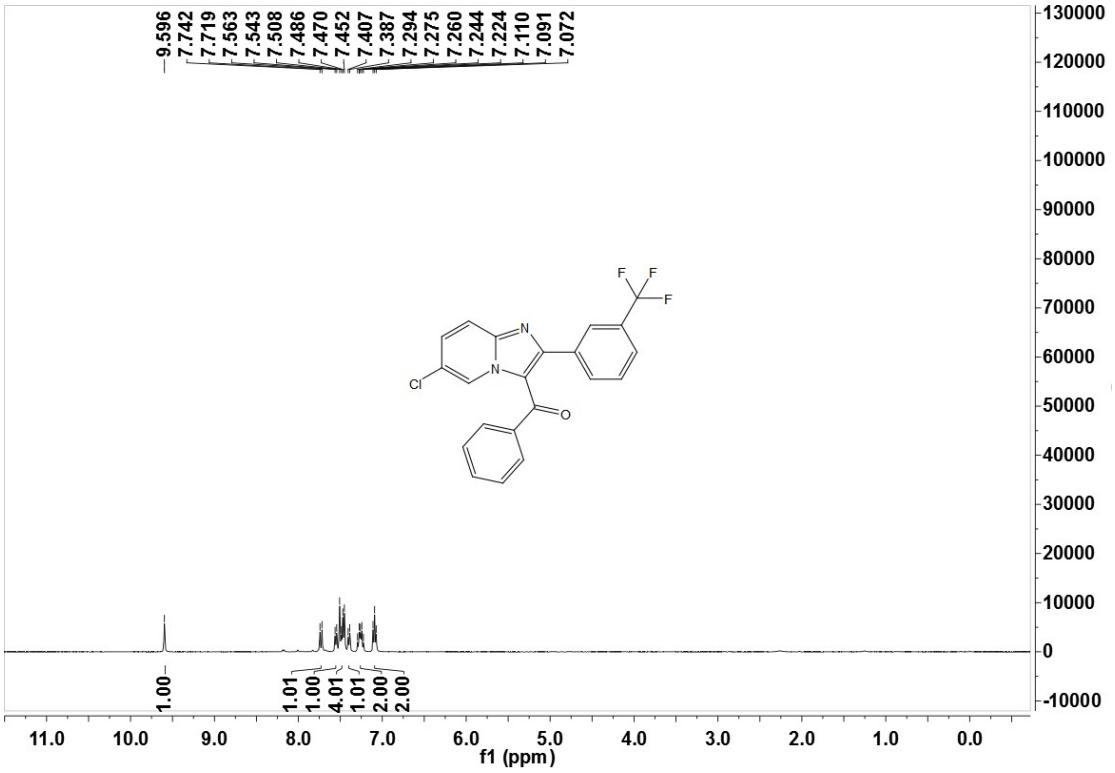
Method: C:\Xcalibur\methods\fs_sim

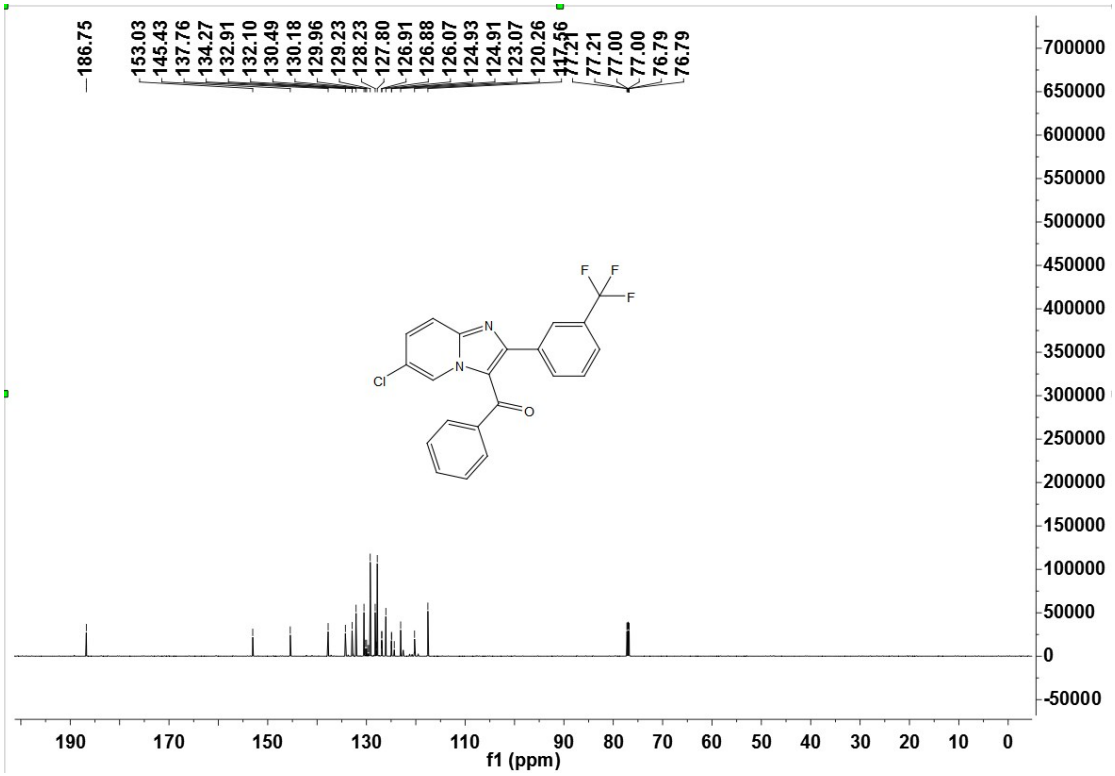
Assay: Assay name



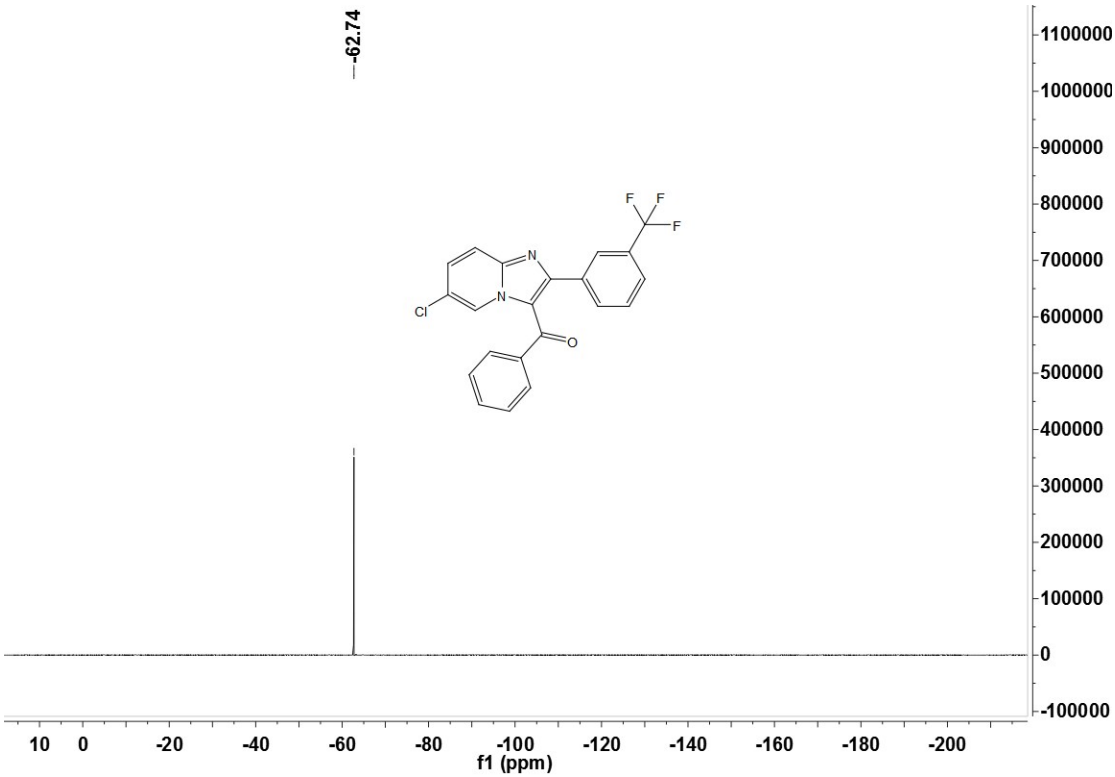
Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C21H12ClF3N2O	+ H	C21H13ClF3N2O	401.0663	401.06635	-0.12

(4-Chloro-2-(3-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridin-3-yl)(phenyl)methanone (4n)





^{19}F spectrum



HRMS

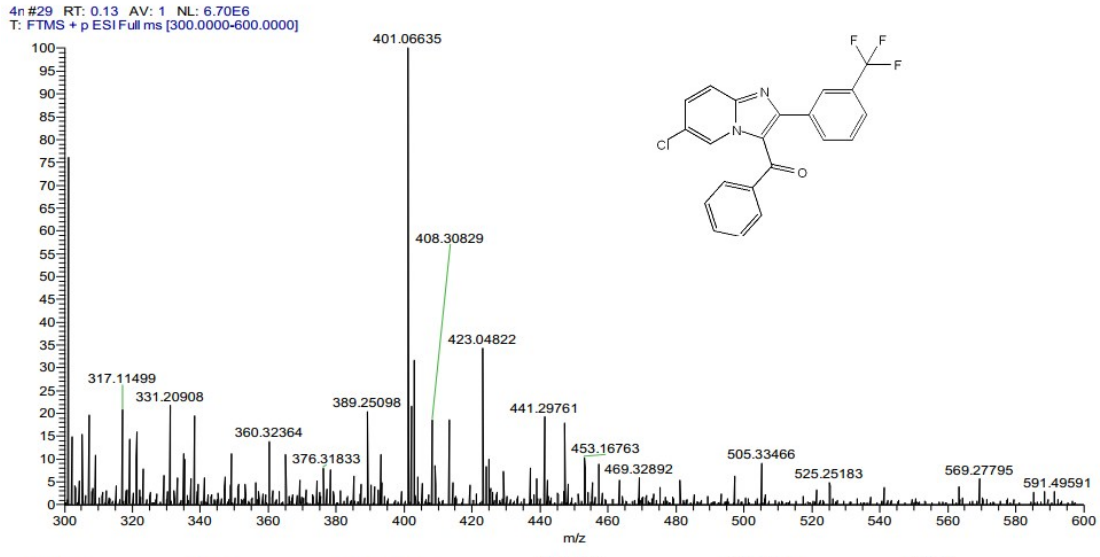
Mass Analysis Report

Batch: /

Lab Name: Default Laboratory

Method: C:\Xcalibur\methods\fs_sim

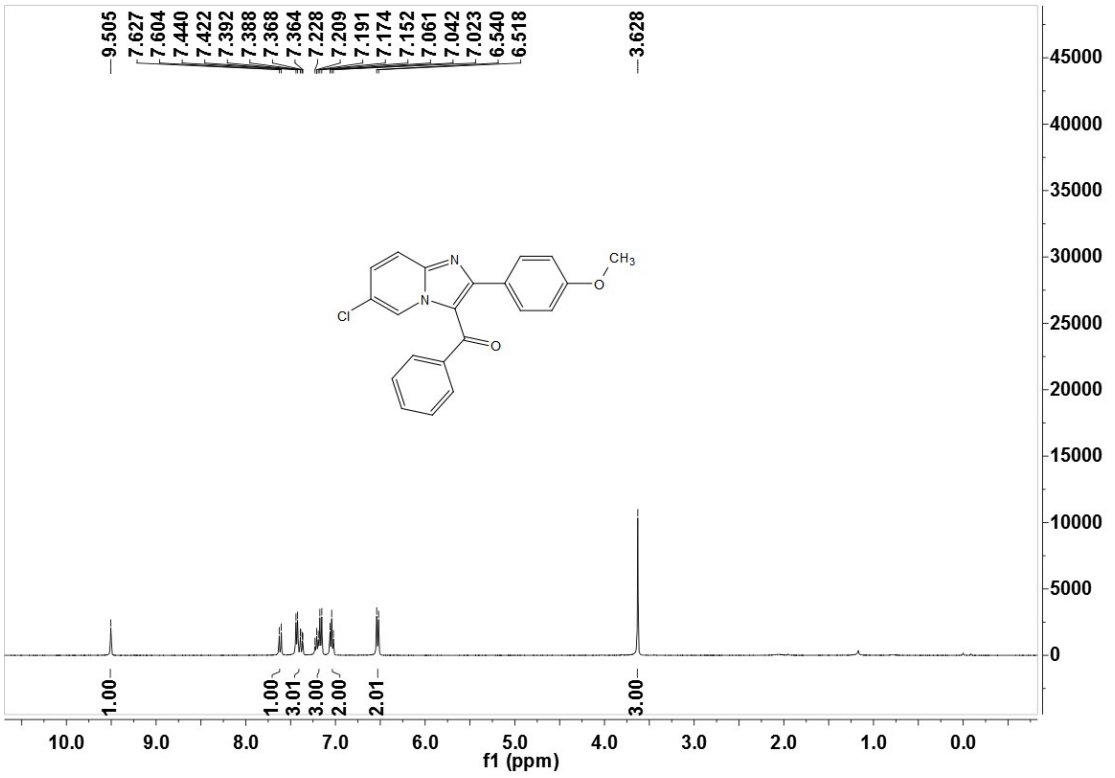
Assay: Assay name

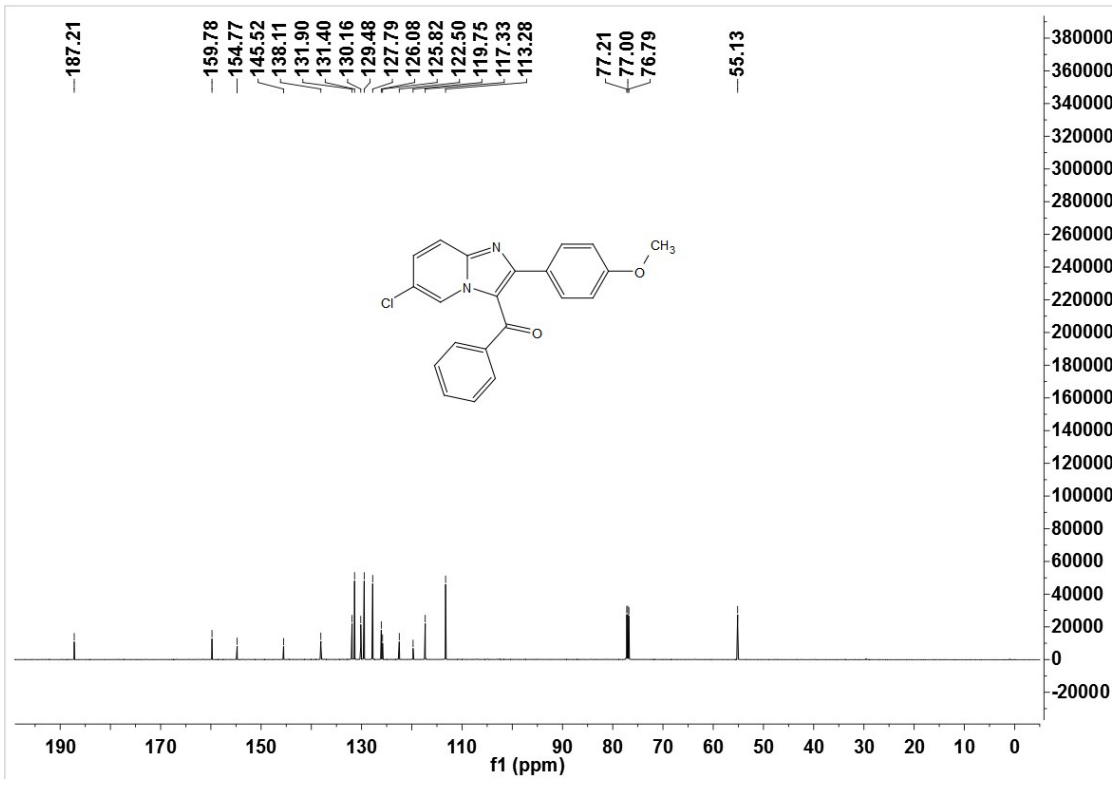


Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C21H12ClF3N2O	+ H	C21H13ClF3N2O	401.0663	401.06635	-0.12

(6-Chloro-2-(4-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)(phenyl)methanone

(4o)





HRMS

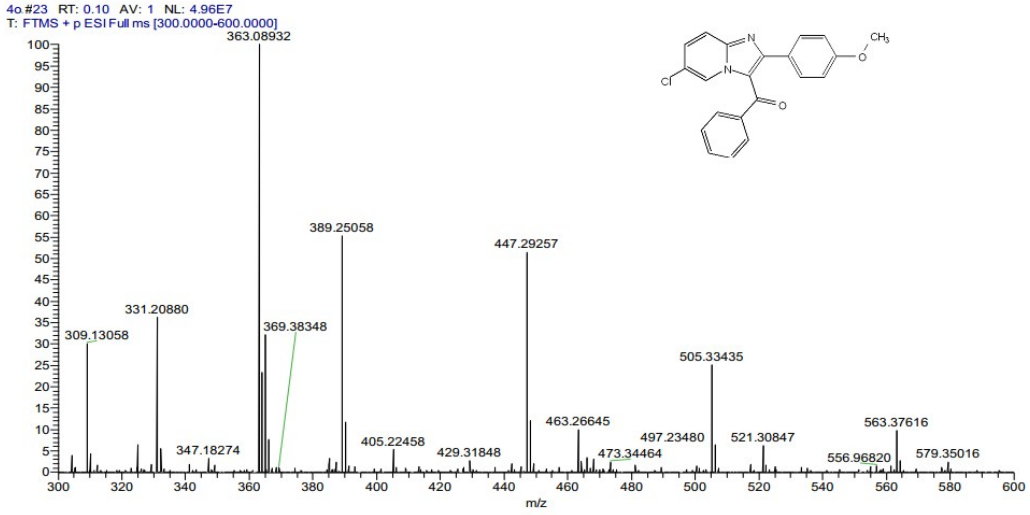
Mass Analysis Report

Batch: /

Lab Name: Default Laboratory

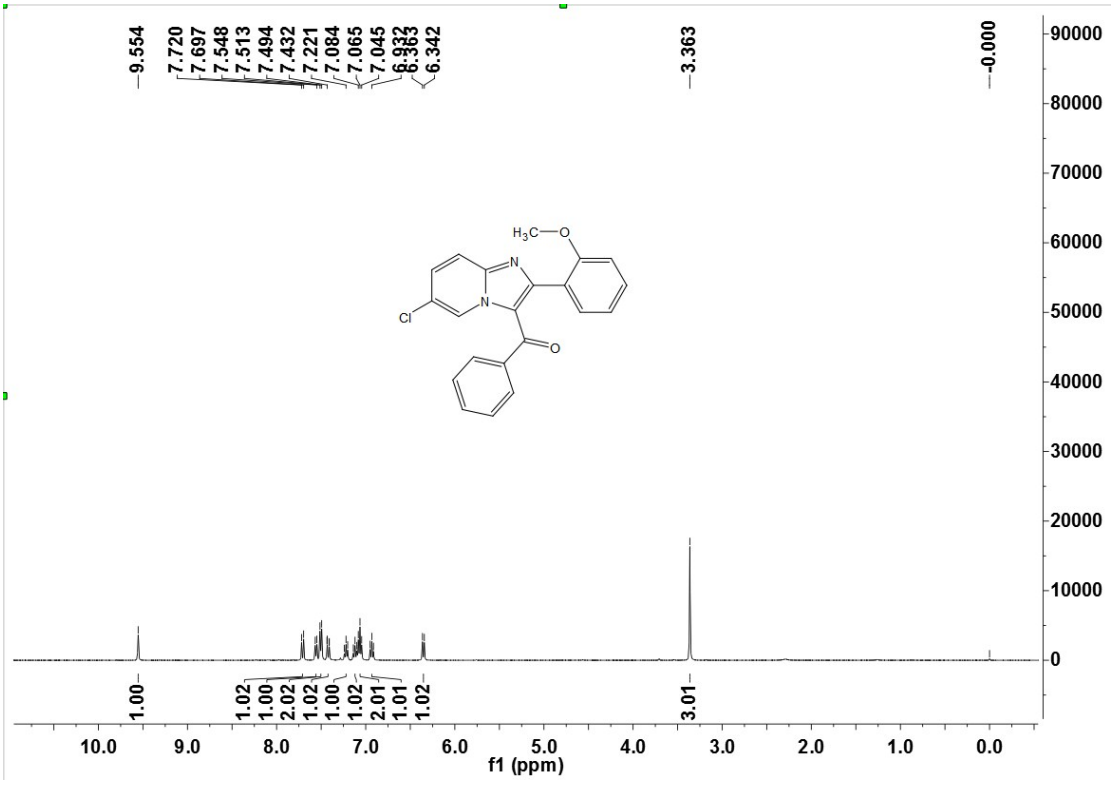
Method: C:\Xcalibur\methods\fs_sim

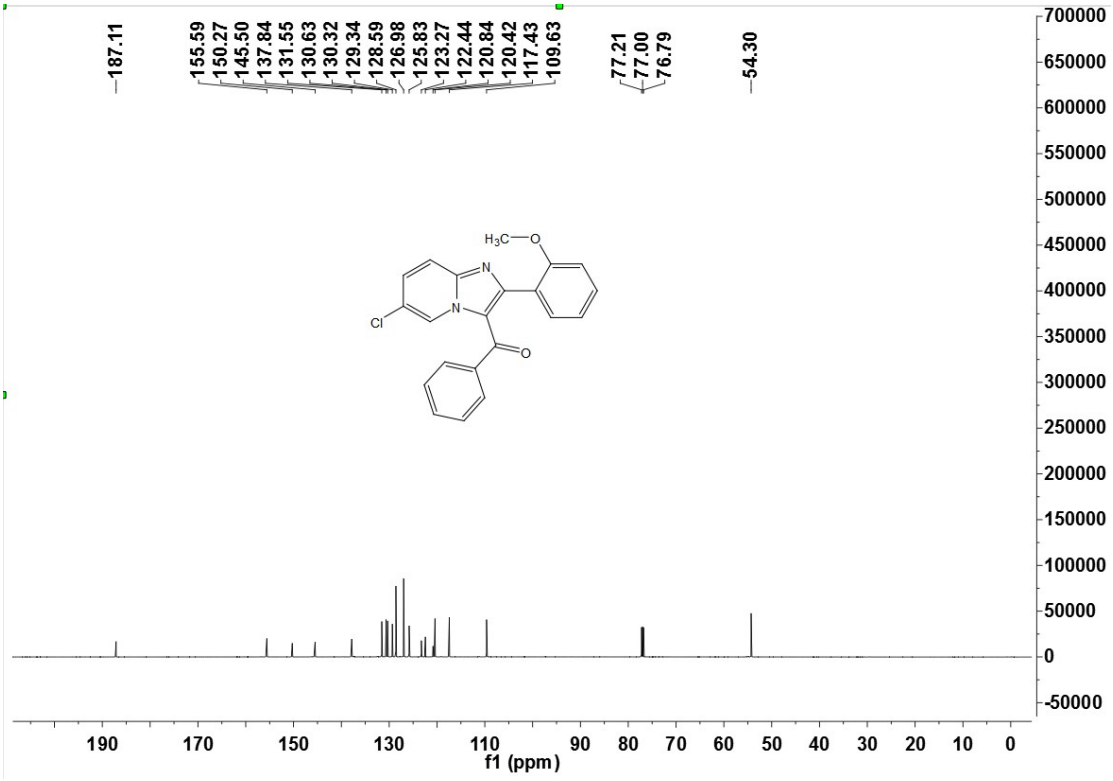
Assay: Assay name



Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C21H15ClN2O2	+ H	C21H16ClN2O2	363.08948	363.08932	0.44

(6-Chloro-2-(2-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)(phenyl)methanone (4p)





HRMS

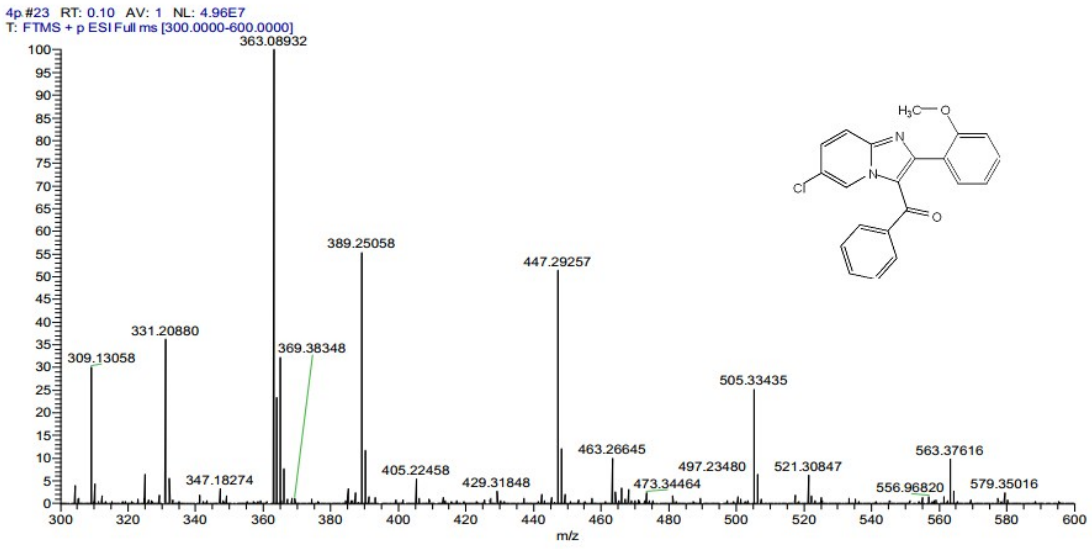
Mass Analysis Report

Batch: /

Lab Name: Default Laboratory

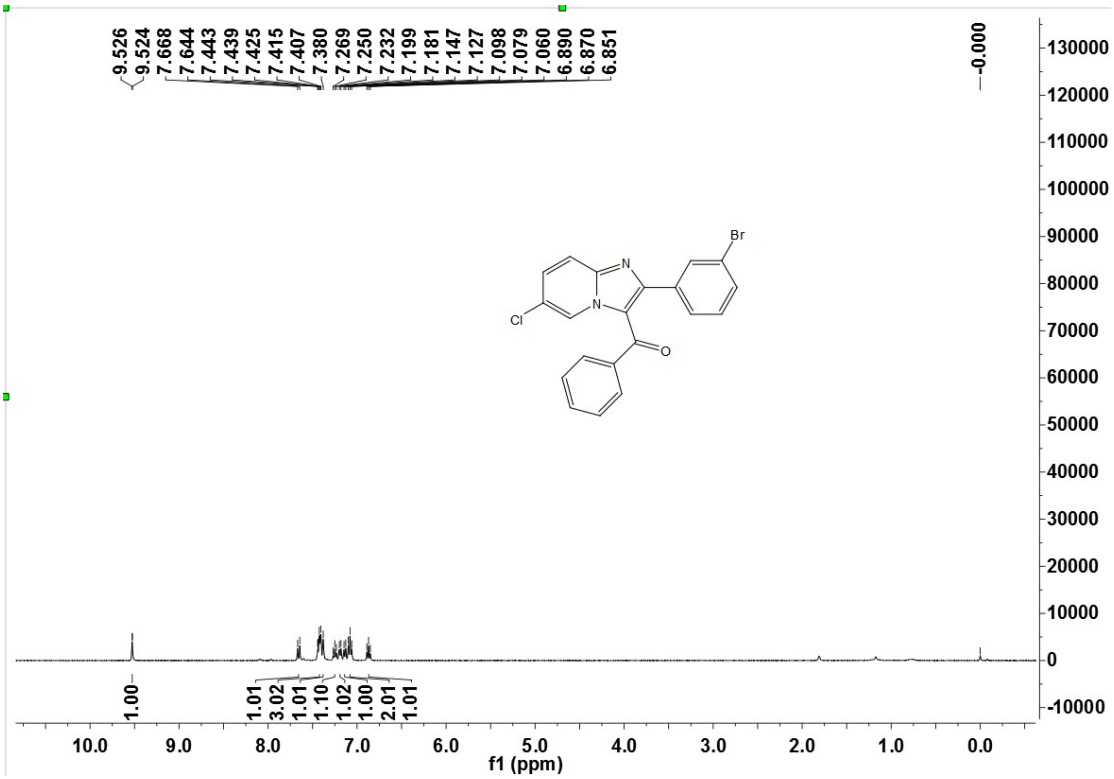
Method: C:\Xcalibur\methods\fs_sim

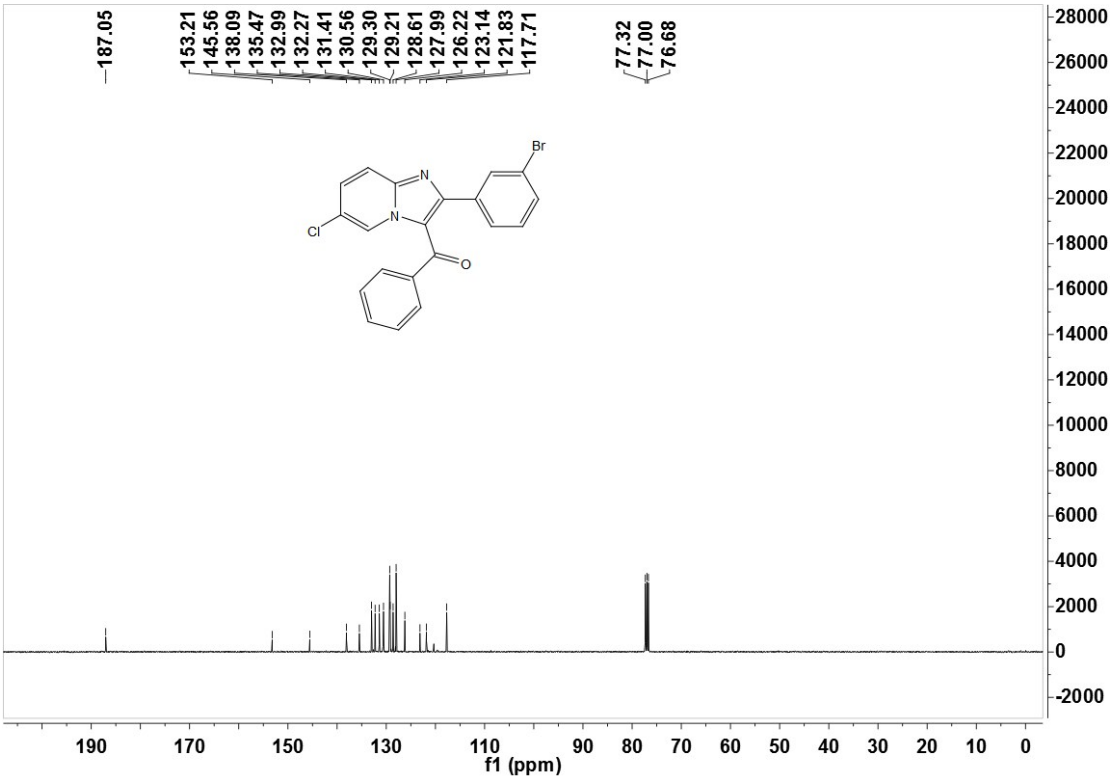
Assay: Assay name



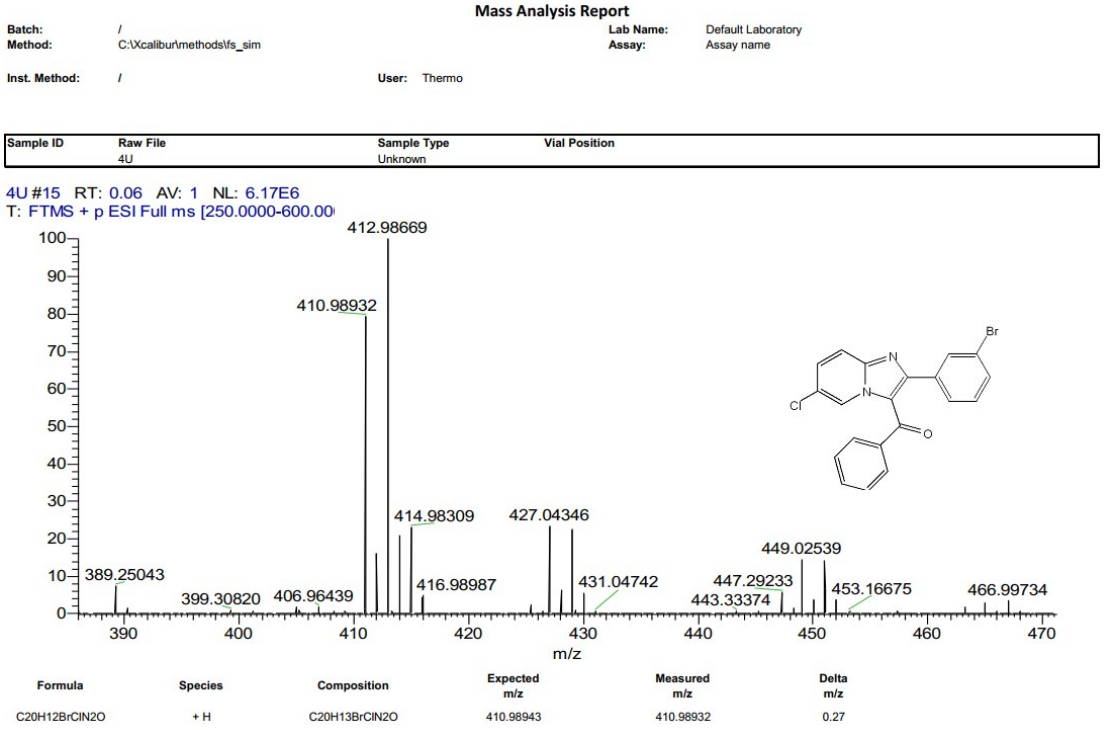
Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C21H15ClN2O2	+ H	C21H16ClN2O2	363.08948	363.08932	0.44

(2-(3-Bromophenyl)-6-chloroimidazo[1,2-a]pyridin-3-yl)(phenyl)methanone (4q)

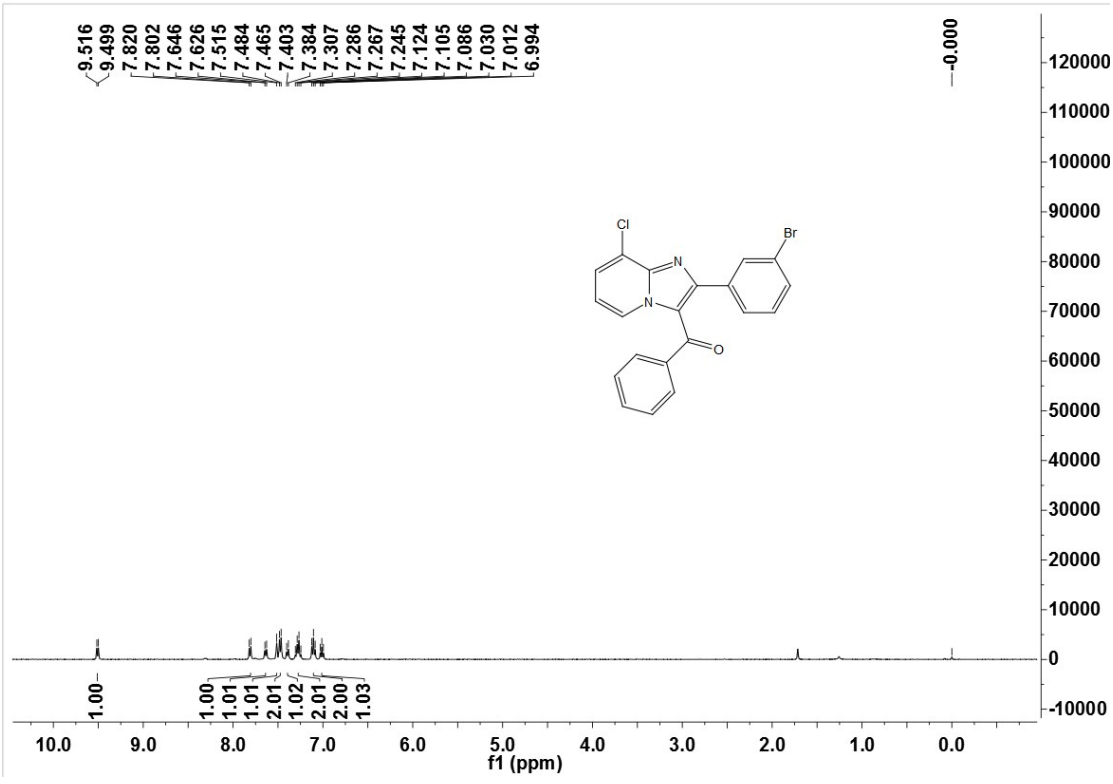


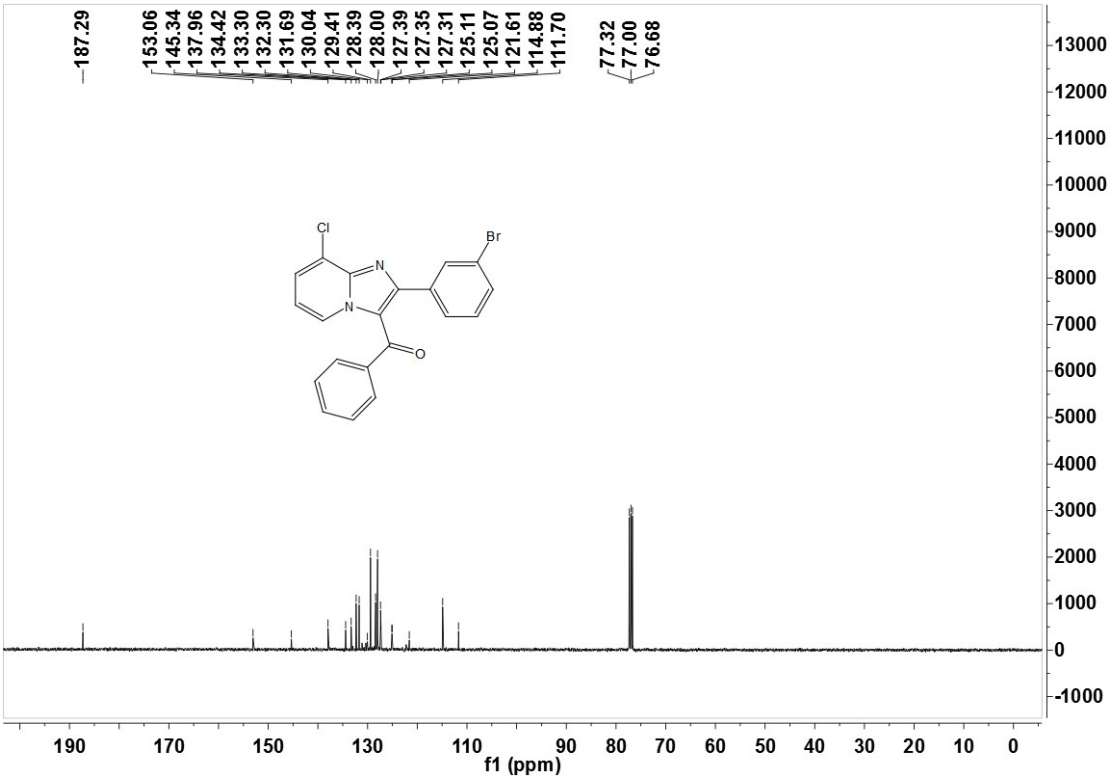


HRMS



(2-(3-Bromophenyl)-8-chloroimidazo[1,2-a]pyridin-3-yl)(phenyl)methanone (4r)





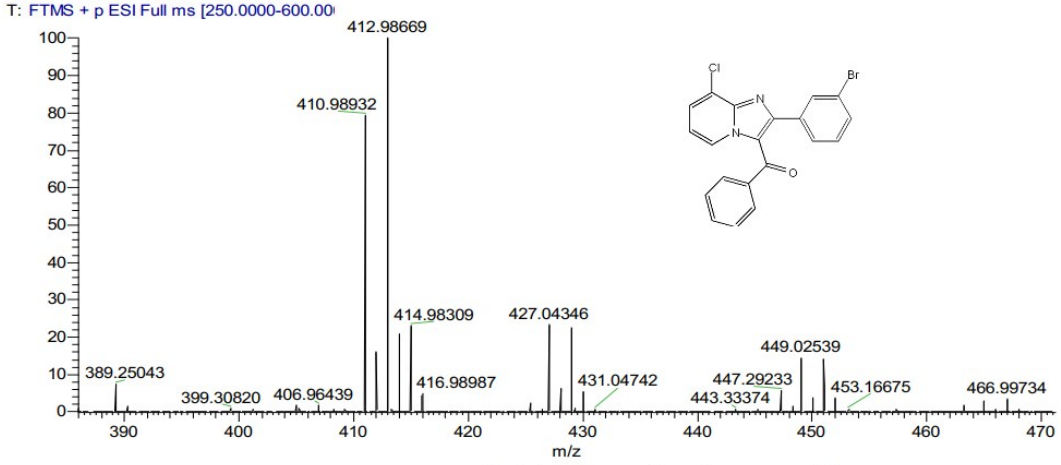
HRMS

Mass Analysis Report

Batch:	/	**Lab Name:**	Default Laboratory
Method:	C:\Xcalibur\methods\fs_sim	**Assay:**	Assay name
Inst. Method:	/	**User:**	Thermo

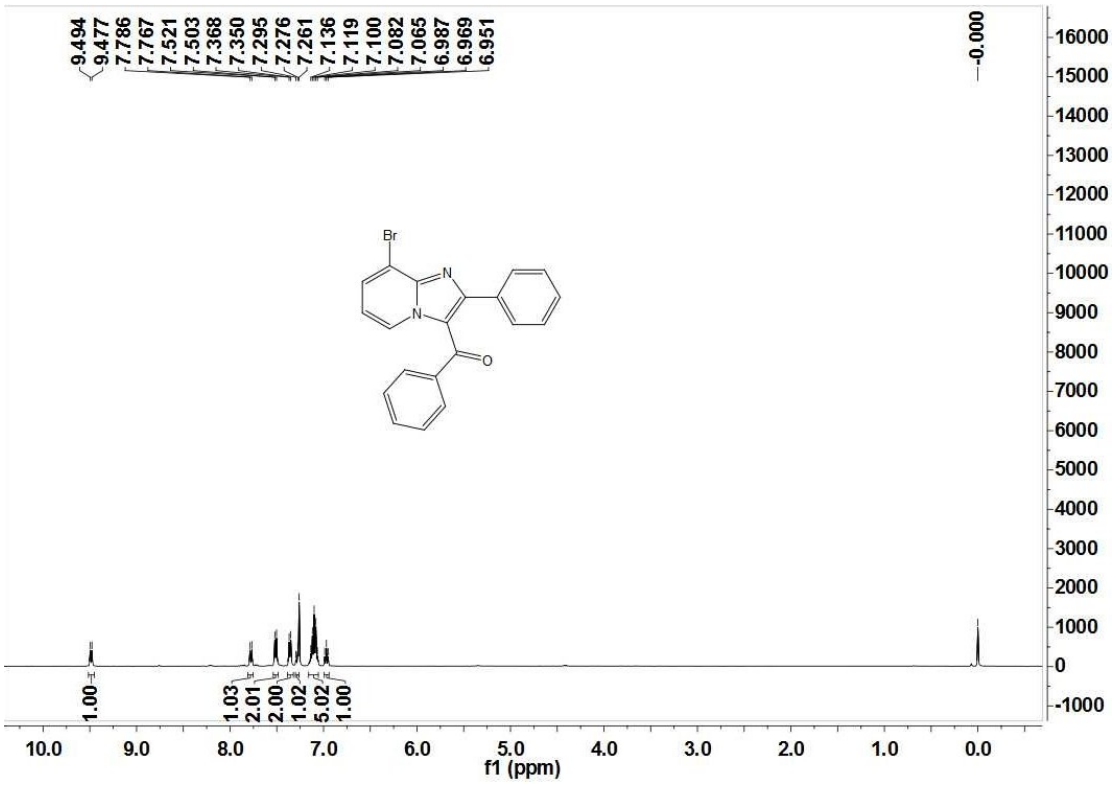
Sample ID	Raw File	Sample Type	Vial Position
	4U	Unknown	

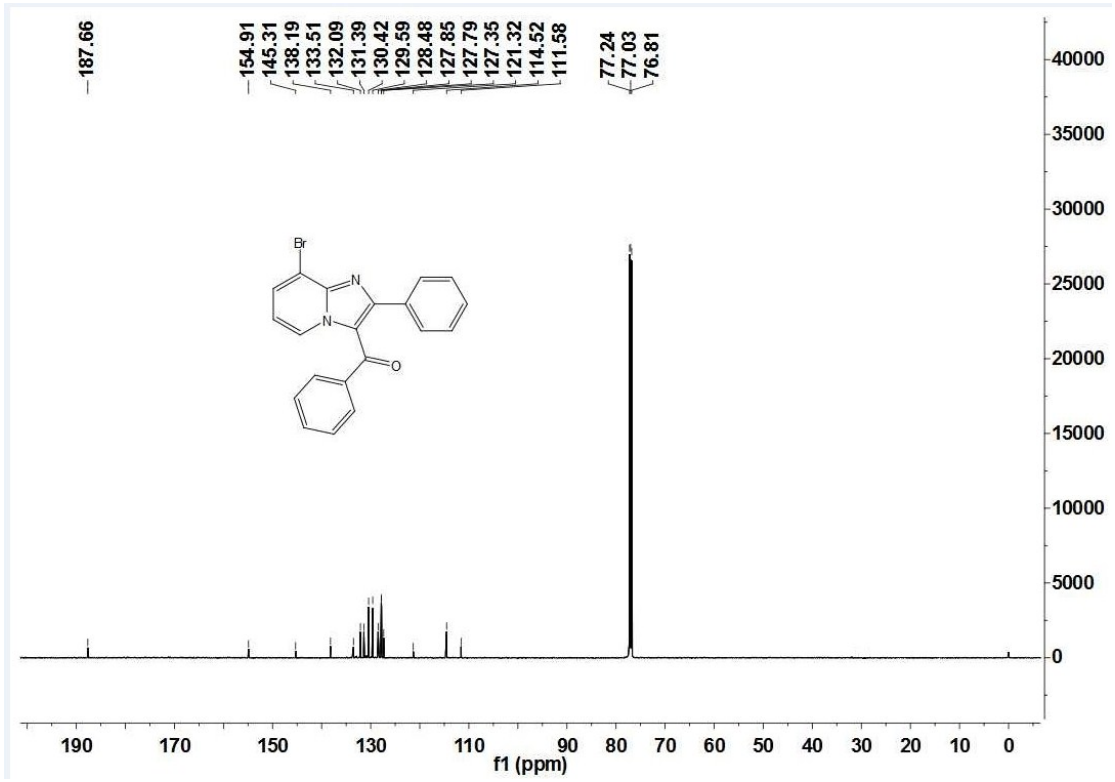
4U #15 RT: 0.06 AV: 1 NL: 6.17E6
T: FTMS + p ESI Full ms [250.0000-600.00



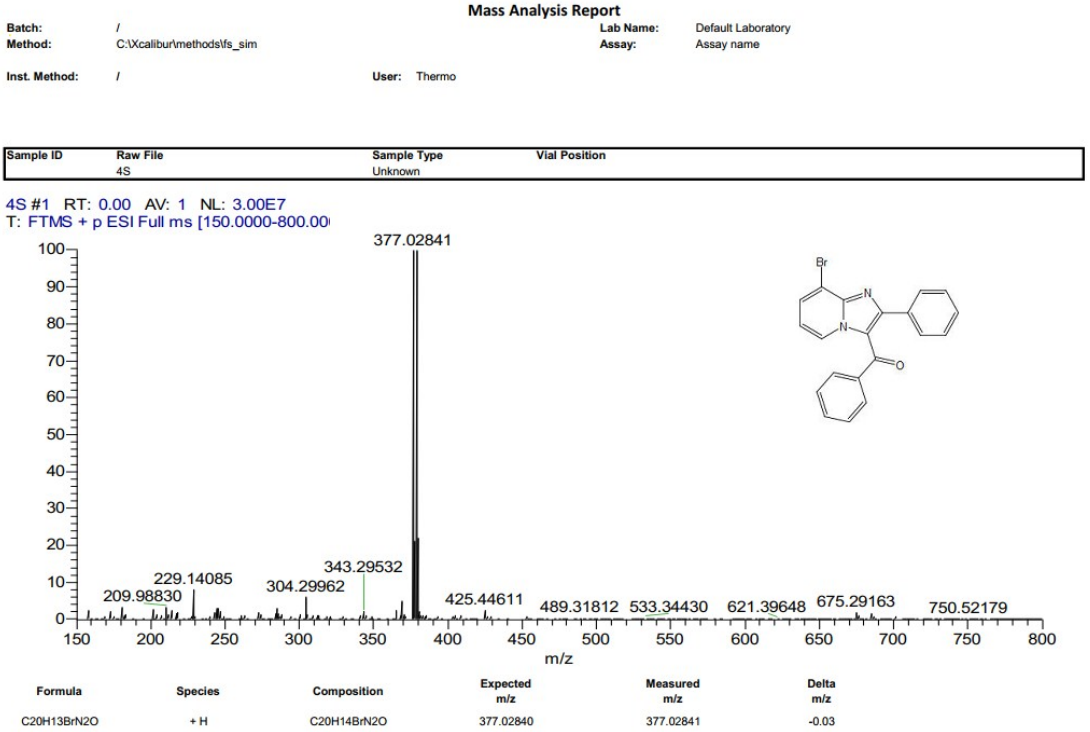
Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C20H12BrClN2O	+ H	C20H13BrClN2O	410.98943	410.98932	0.27

(8-Bromo-2-phenylimidazo[1,2-a]pyridin-3-yl)(phenyl)methanone (4s)

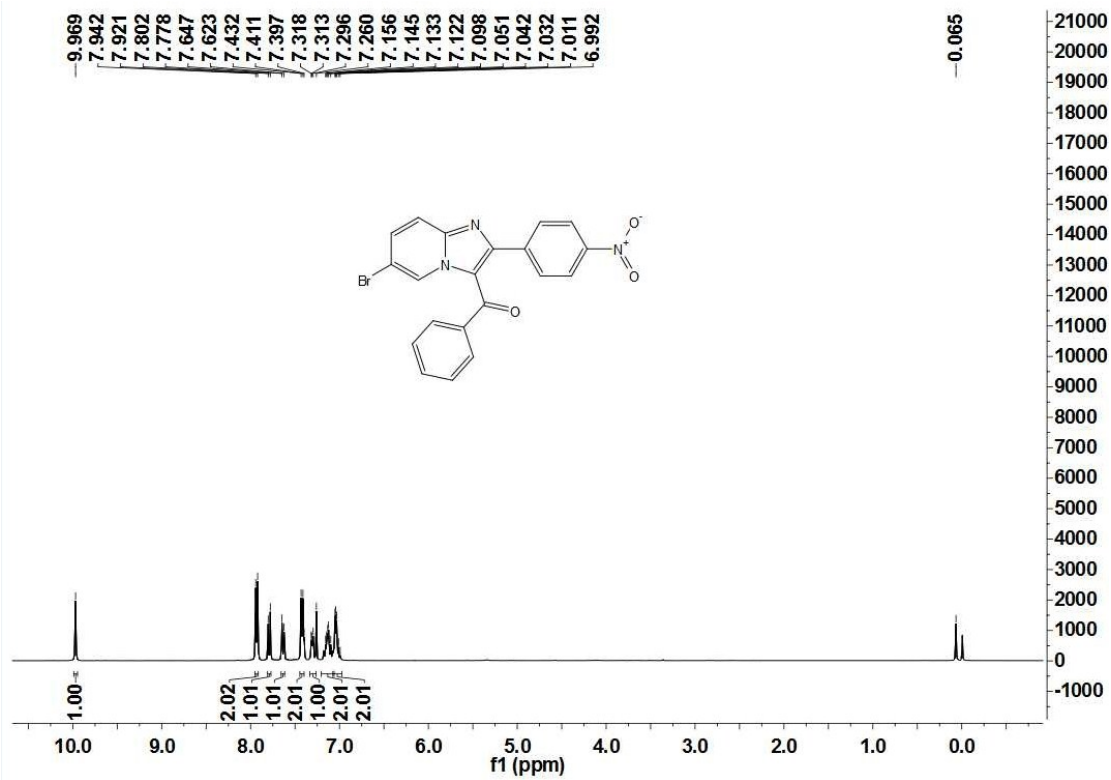


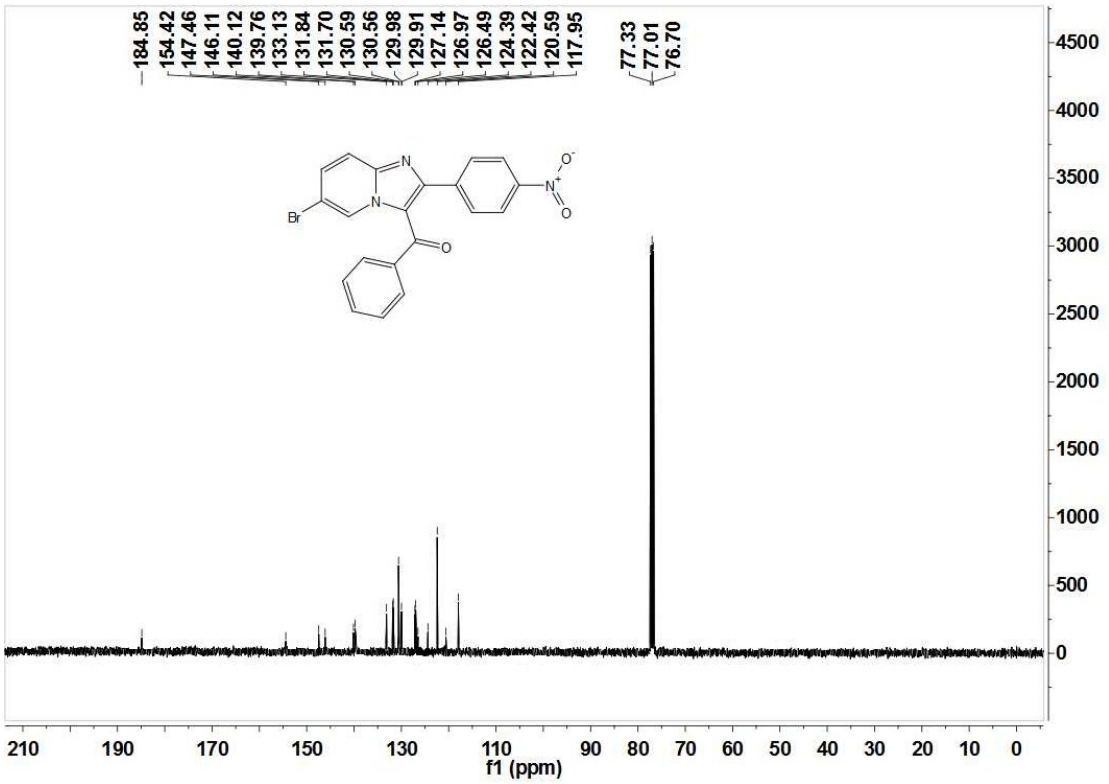


HRMS



(6-Bromo-2-(4-nitrophenyl)imidazo[1,2-a]pyridin-3-yl)(phenyl)methanone (4t)





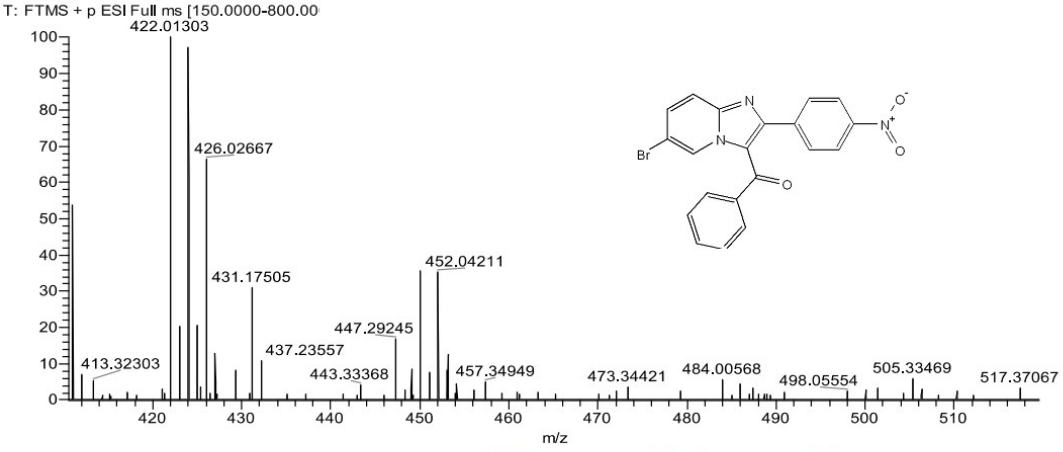
HRMS

Mass Analysis Report

Batch:	/	**Lab Name:**	Default Laboratory
Method:	C:\Xcalibur\methods\fs_sim	**Assay:**	Assay name
Inst. Method:	/	**User:**	Thermo

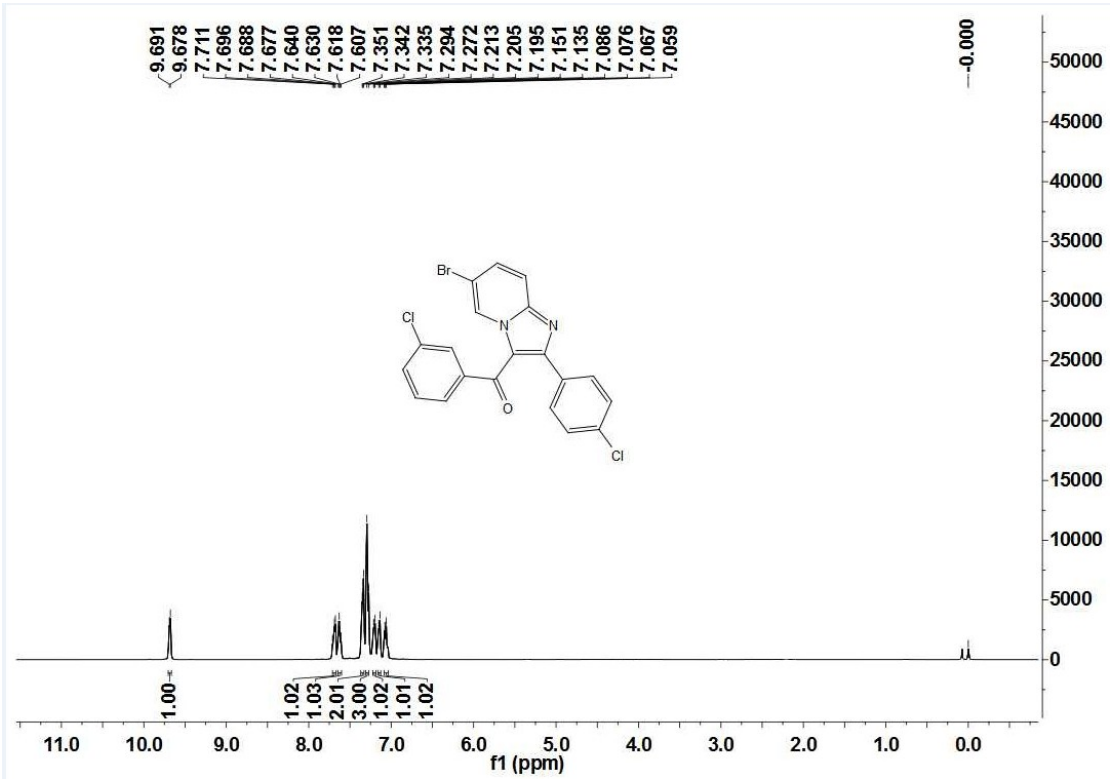
Sample ID	Raw File	Sample Type	Vial Position
	4T	Unknown	

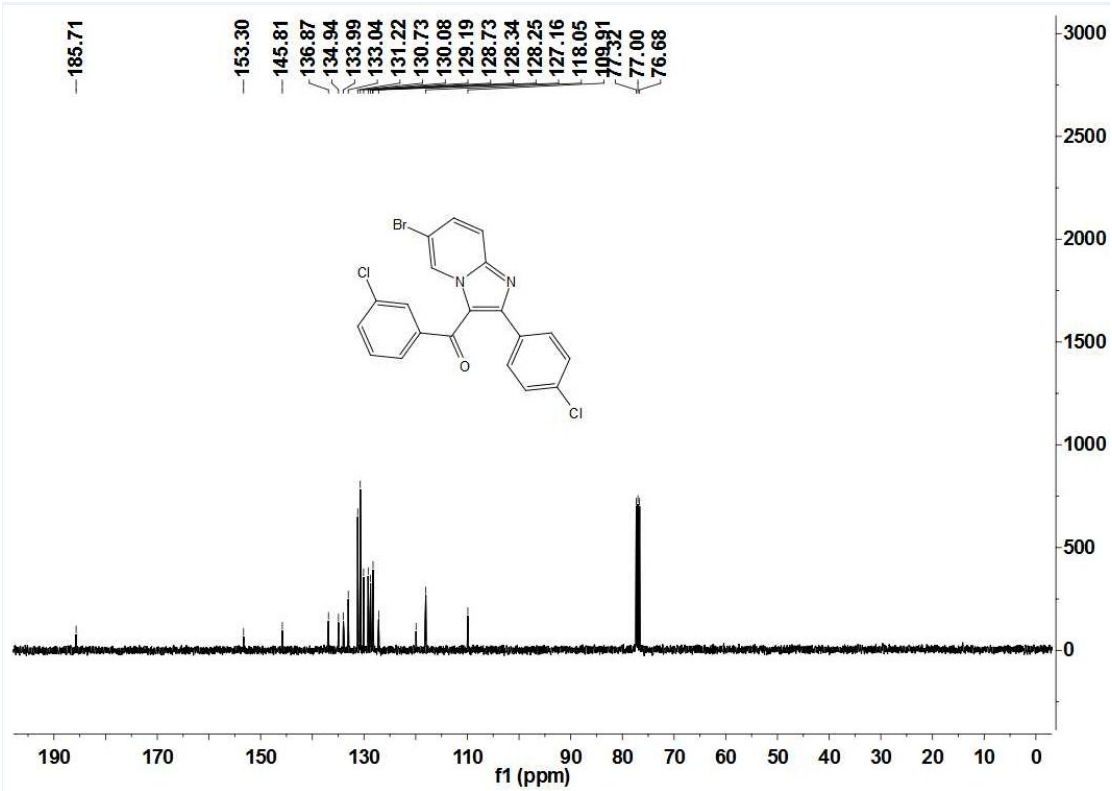
4T #14 RT: 0.06 AV: 1 NL: 3.21E6
T: FTMS + p ESI Full ms [150.0000-800.00



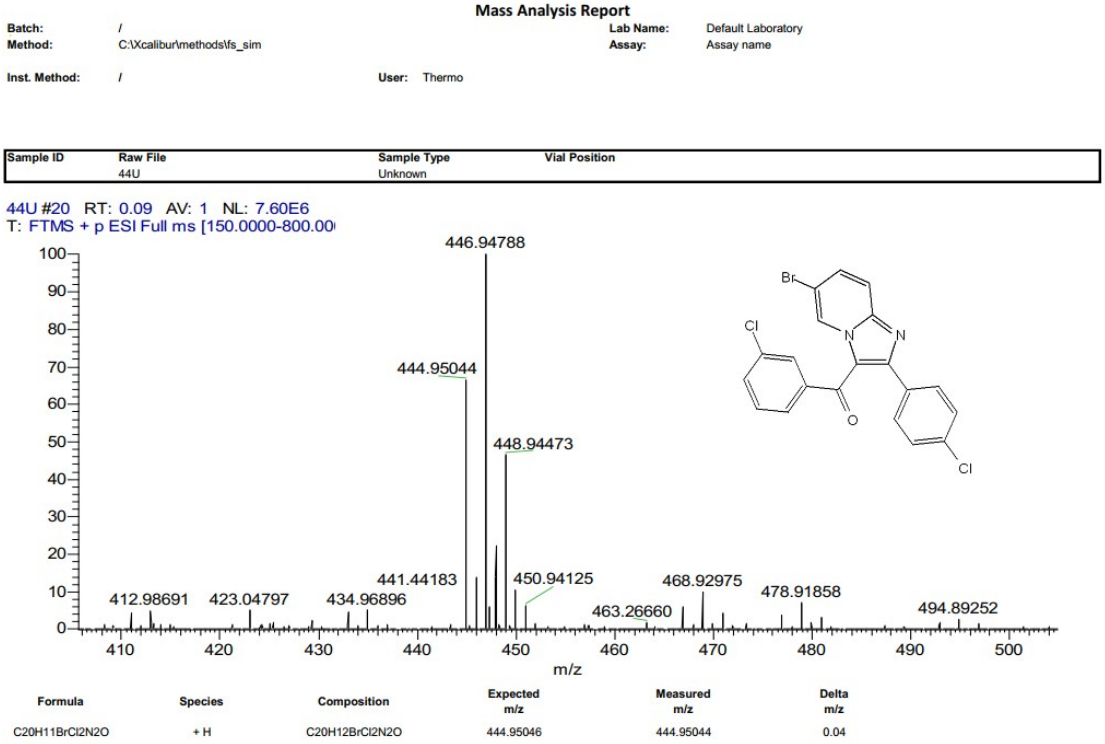
Formula	Species	Composition	Expected m/z	Measured m/z	Delta ppm
C20H12BrN3O3	+ H	C20H13BrN3O3	422.01348	422.01303	1.07

(6-Bromo-2-(4-chlorophenyl)imidazo[1,2-a]pyridin-3-yl)(3-chlorophenyl)methanone (4u)

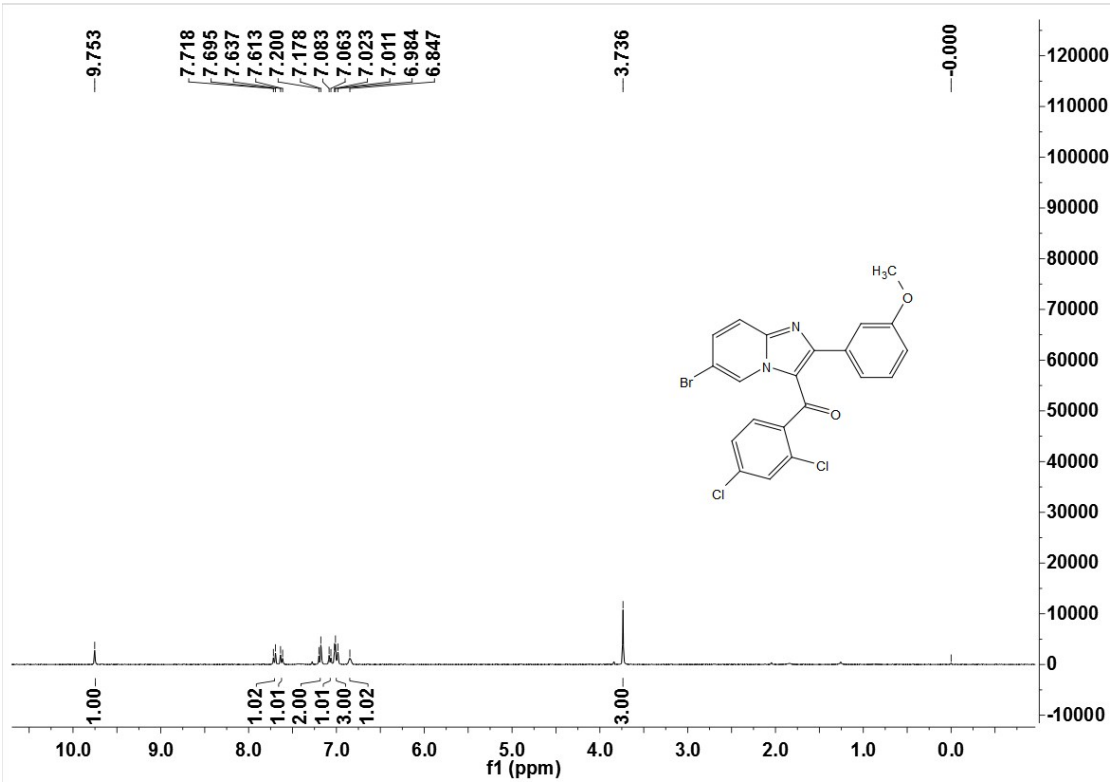


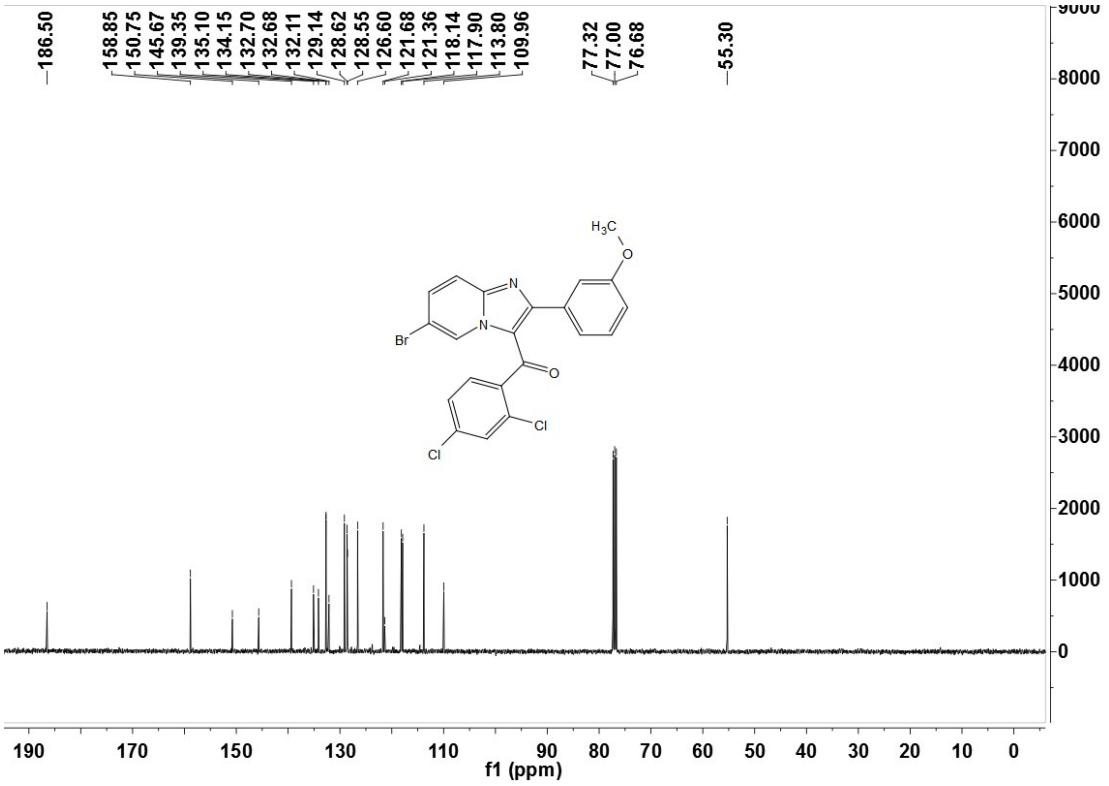


HRMS

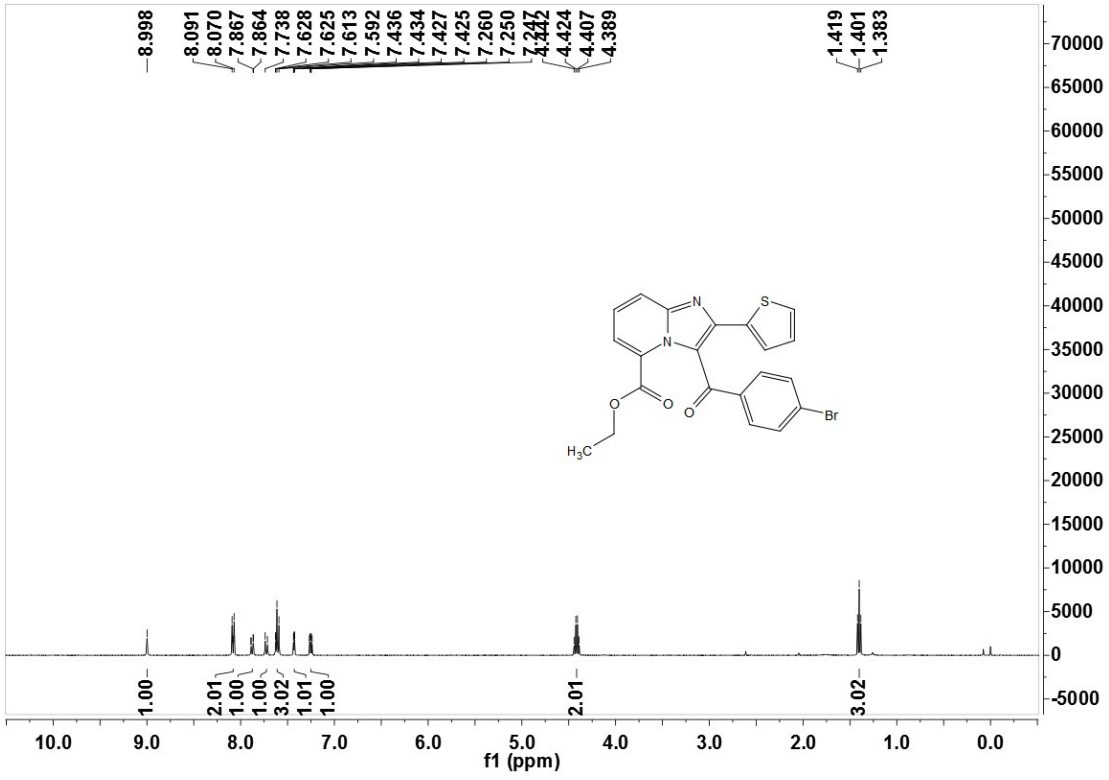


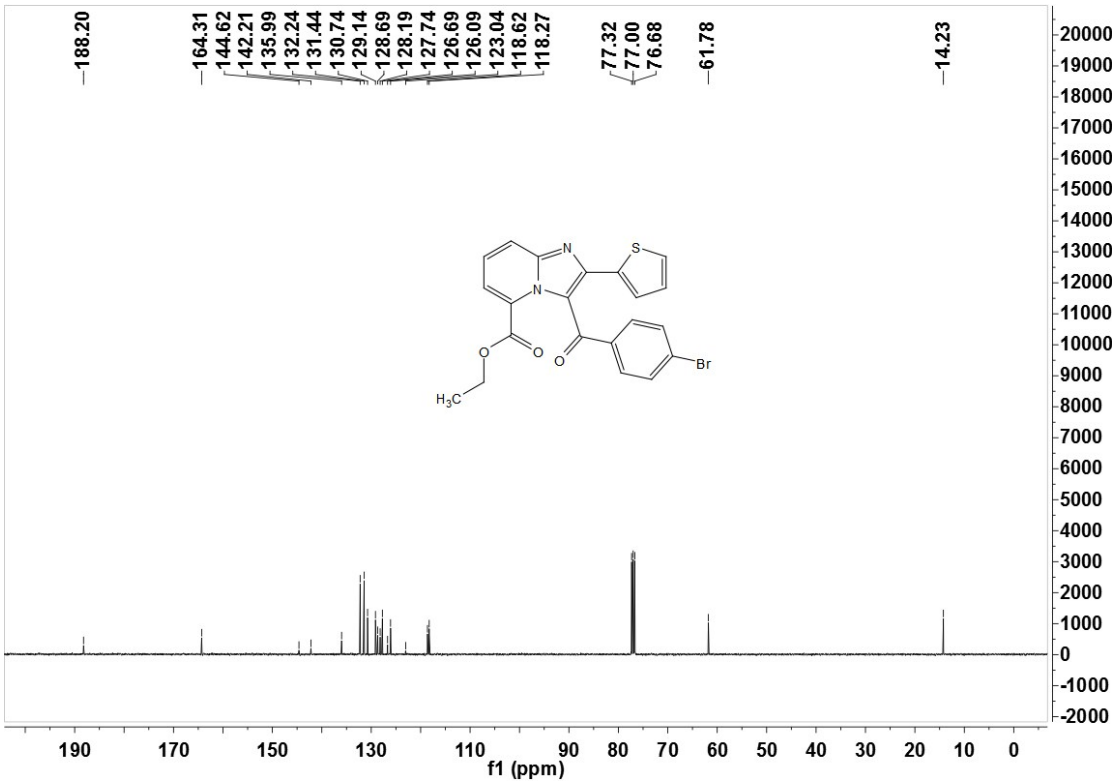
(6-Bromo-2-(3-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)(2,4-dichlorophenyl)methanone (4v)





Ethyl 3-(4-bromobenzoyl)-2-(thiophen-2-yl)imidazo[1,2-a]pyridine-5-carboxylate (4w)





HRMS

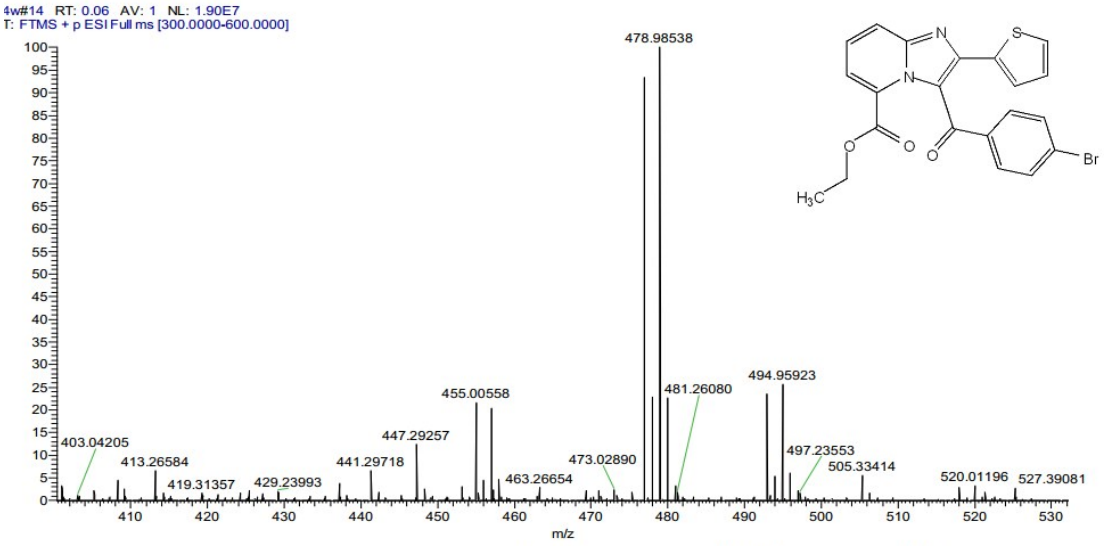
Mass Analysis Report

Batch: /

Lab Name: Default Laboratory

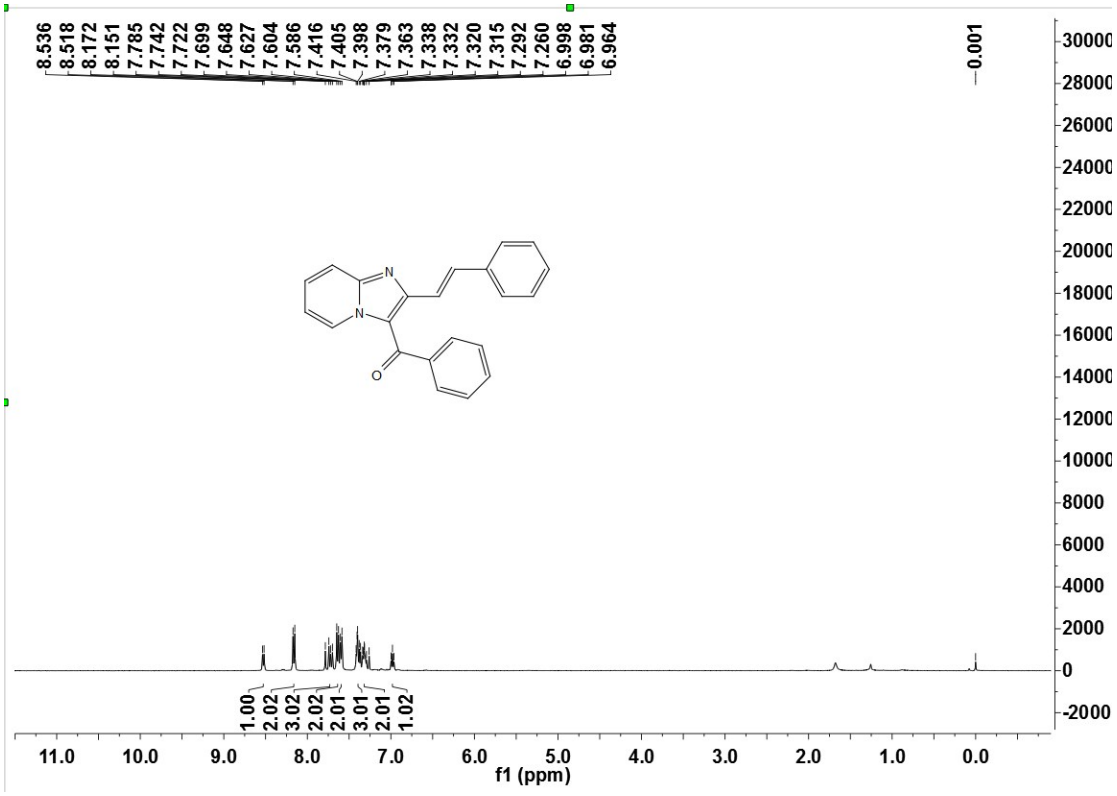
Method: C:\Xcalibur\methods\fs_sim

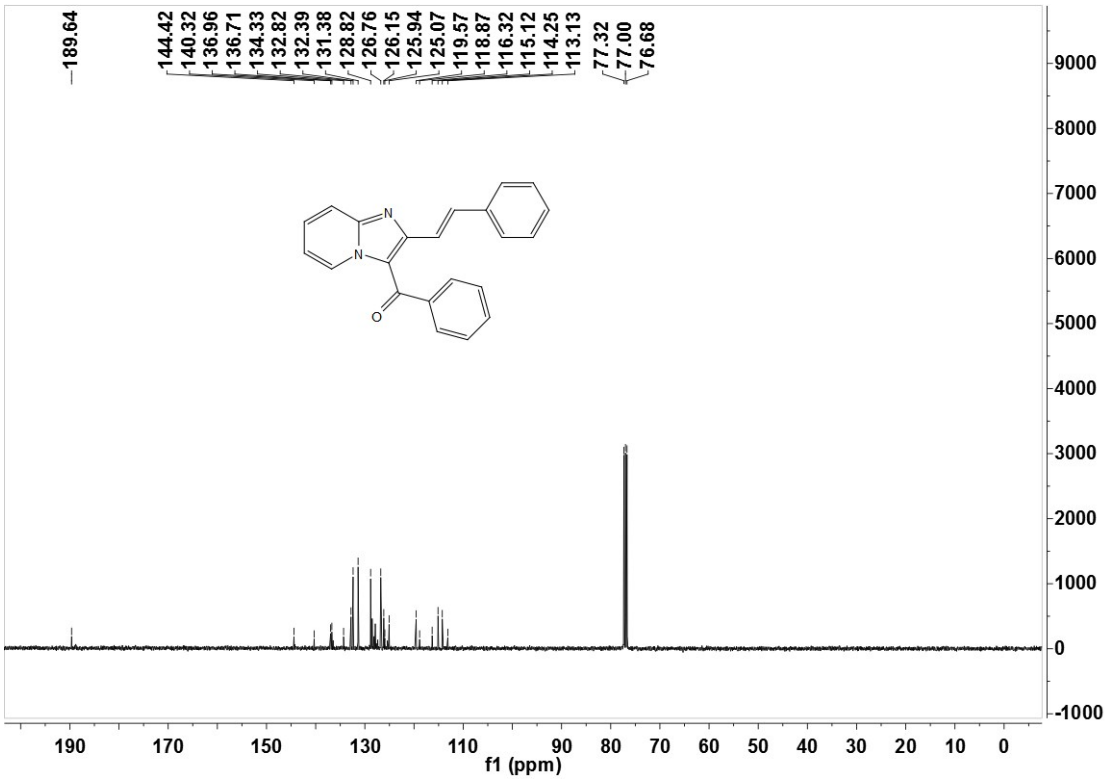
Assay: Assay name



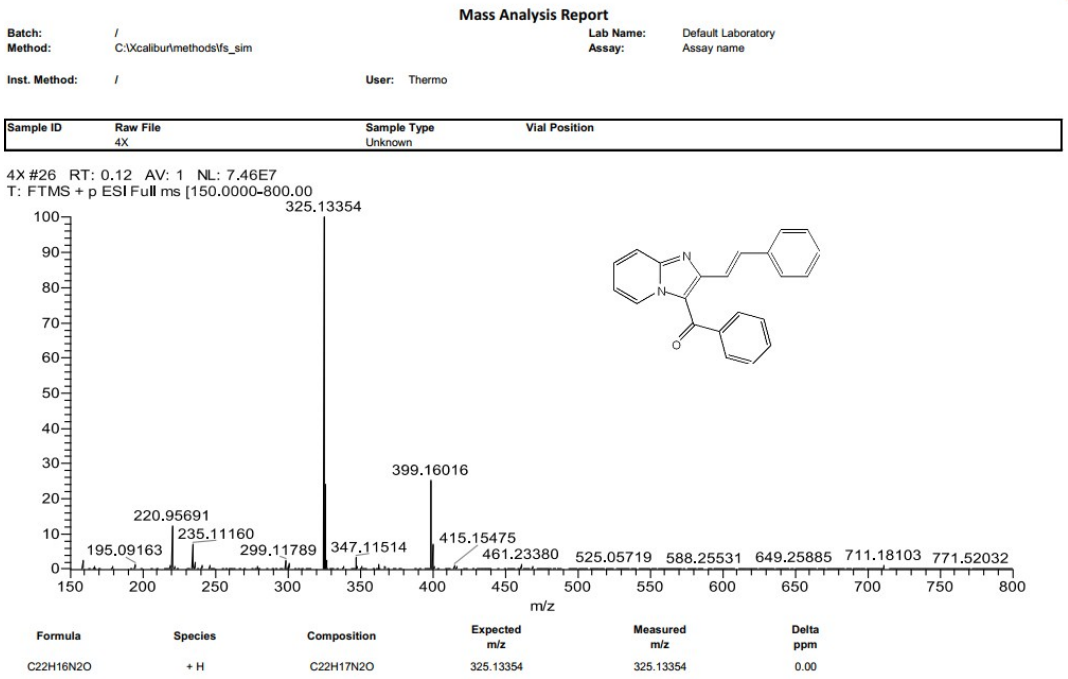
Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
:21H15BrN2O3S	+ Na	C21H15BrN2O3SNa	476.9879	476.98770	0.42

(*E*)-Phenyl(2-styrylimidazo[1,2-a]pyridin-3-yl)methanone (4x)

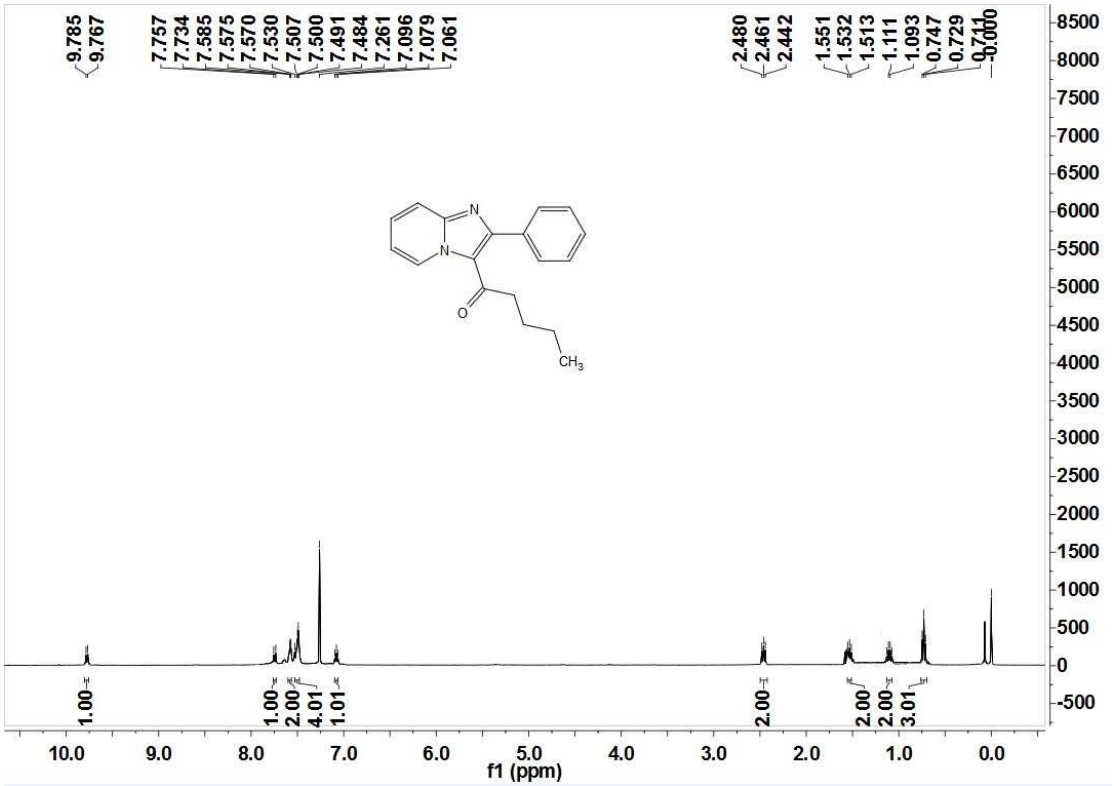


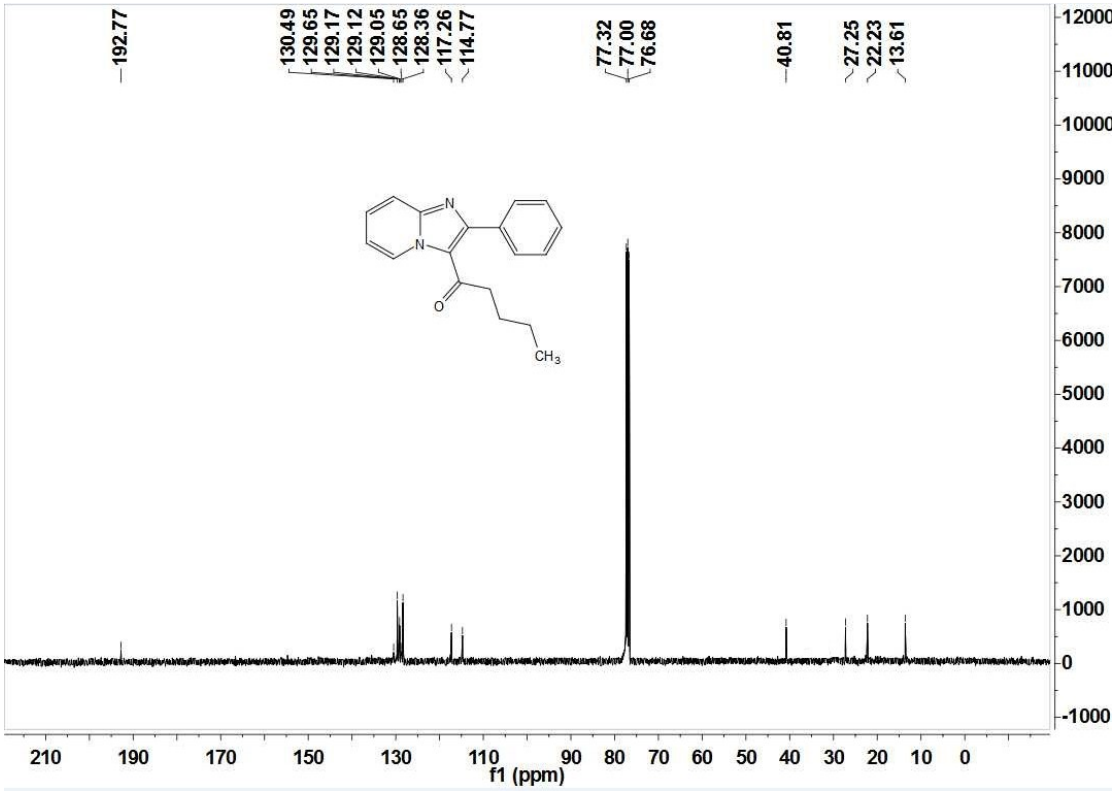


HRMS



1-(2-Phenylimidazo[1,2-a]pyridin-3-yl)pentan-1-one(4y)





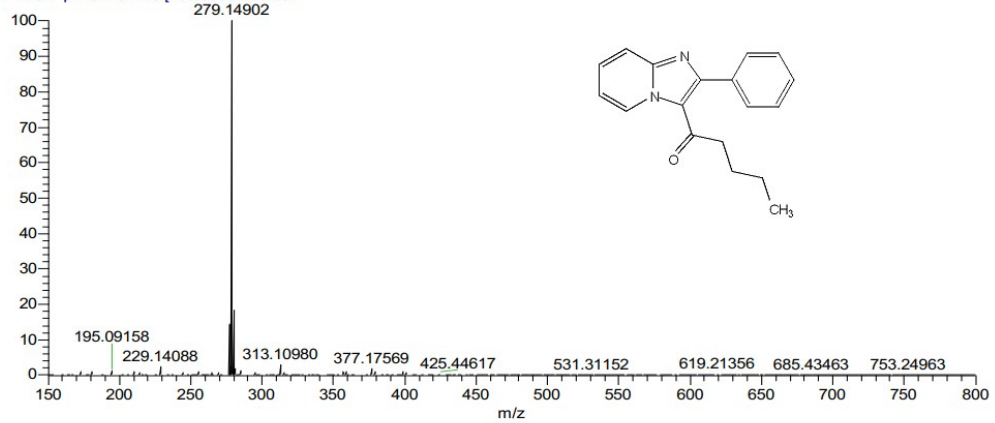
HRMS

Mass Analysis Report

Batch:	/	**Lab Name:**	Default Laboratory
Method:	C:\Xcalibur\methods\fs_sim	**Assay:**	Assay name
Inst. Method:	/	**User:**	Thermo

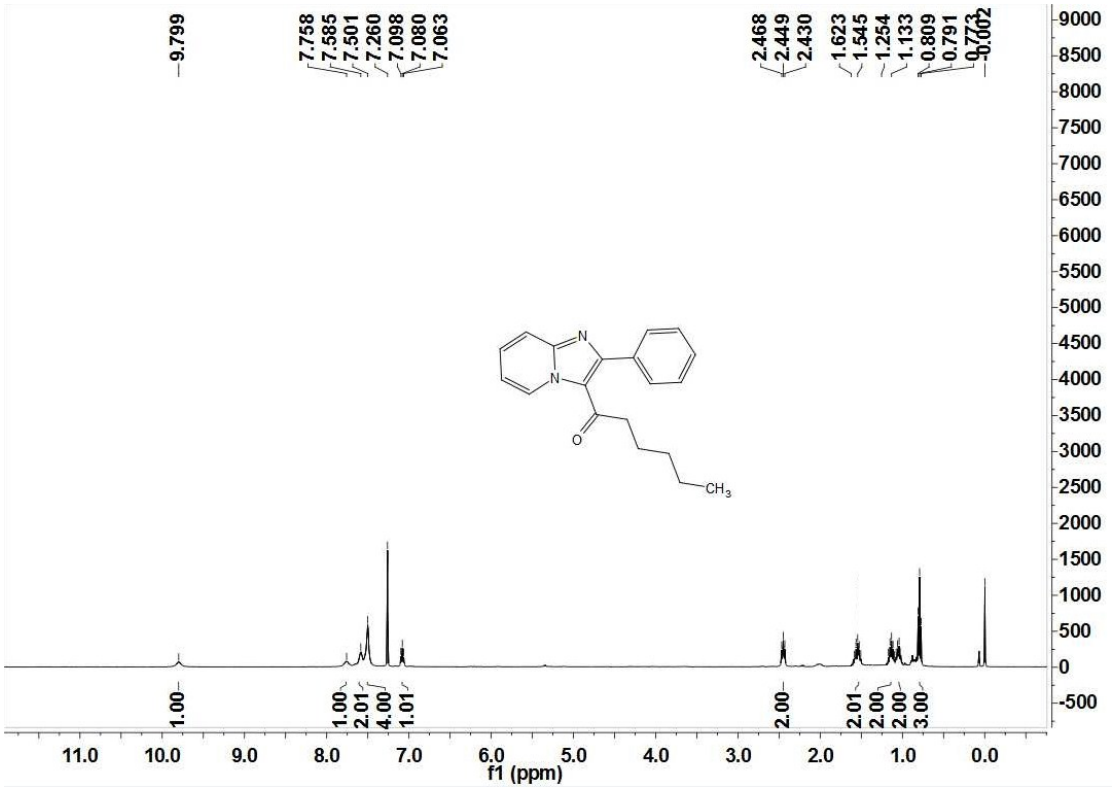
Sample ID	Raw File	Sample Type	Vial Position
	4Y	Unknown	

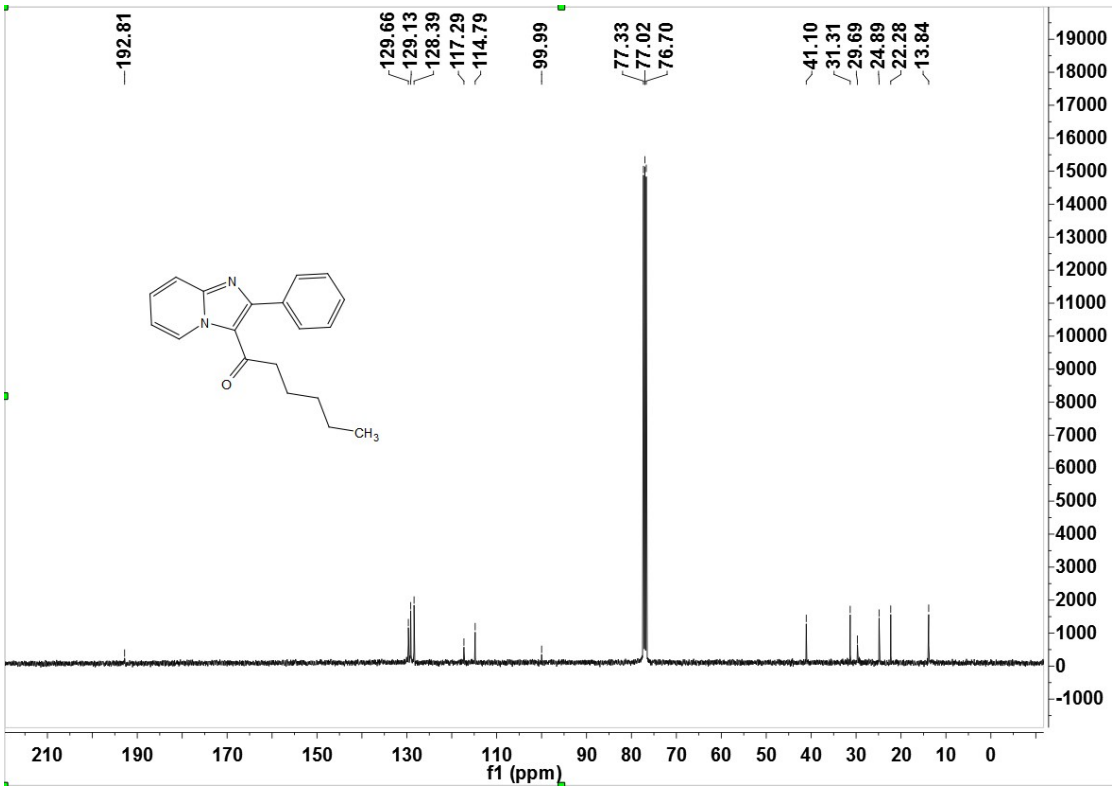
4Y #16 RT: 0.07 AV: 1 NL: 9.61E7
T: FTMS + p ESI Full ms [150.0000-800.00



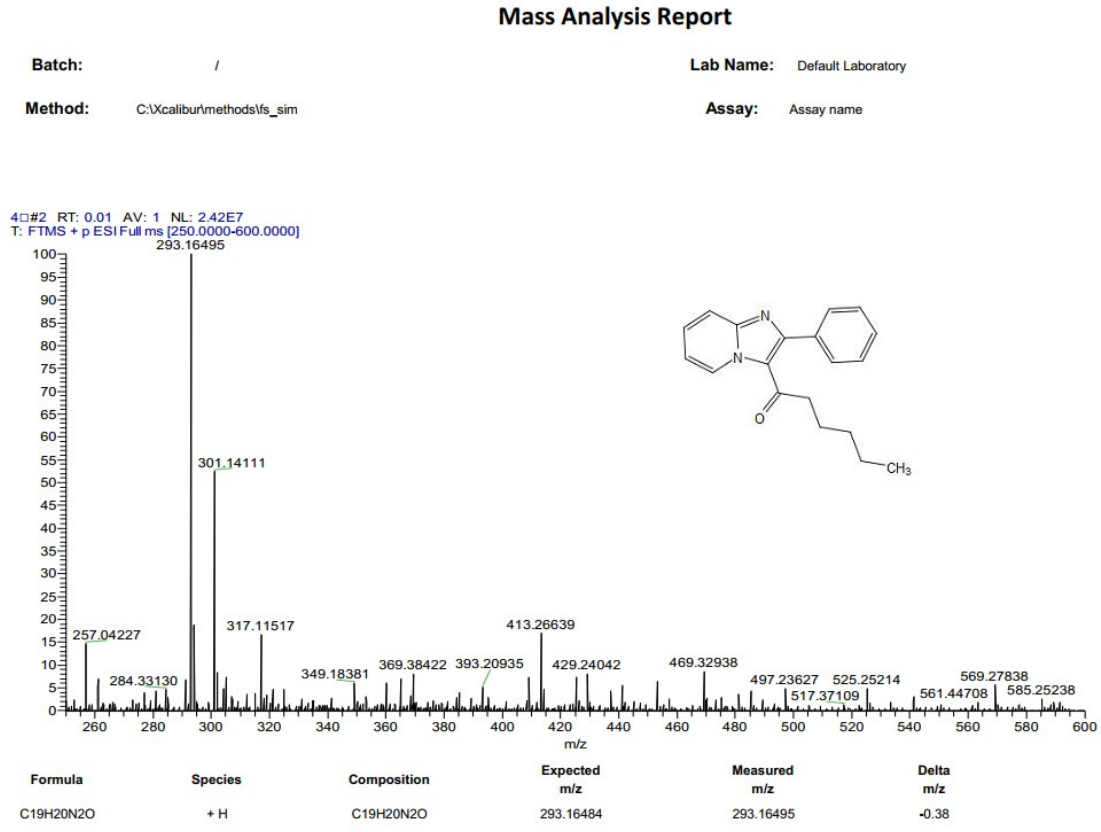
Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C18H18N2O	+ H	C18H19N2O	279.14919	279.14902	0.61

1-(2-Phenylimidazo[1,2-a]pyridin-3-yl)hexan-1-one (4z)

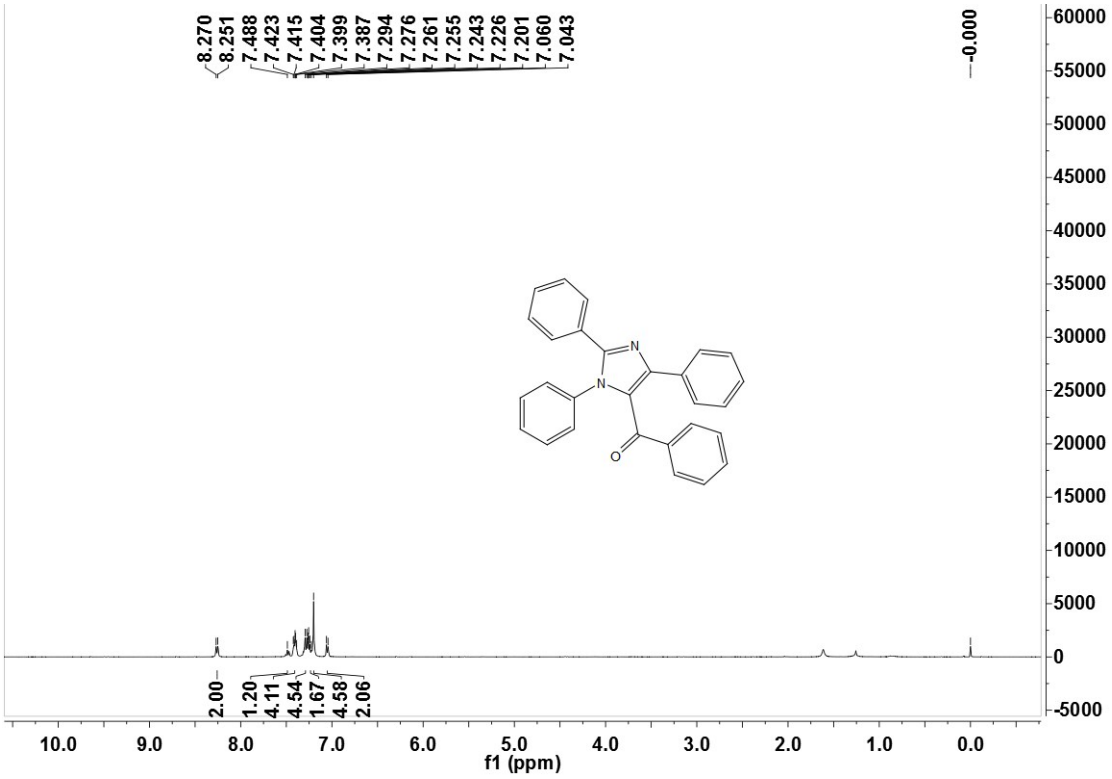


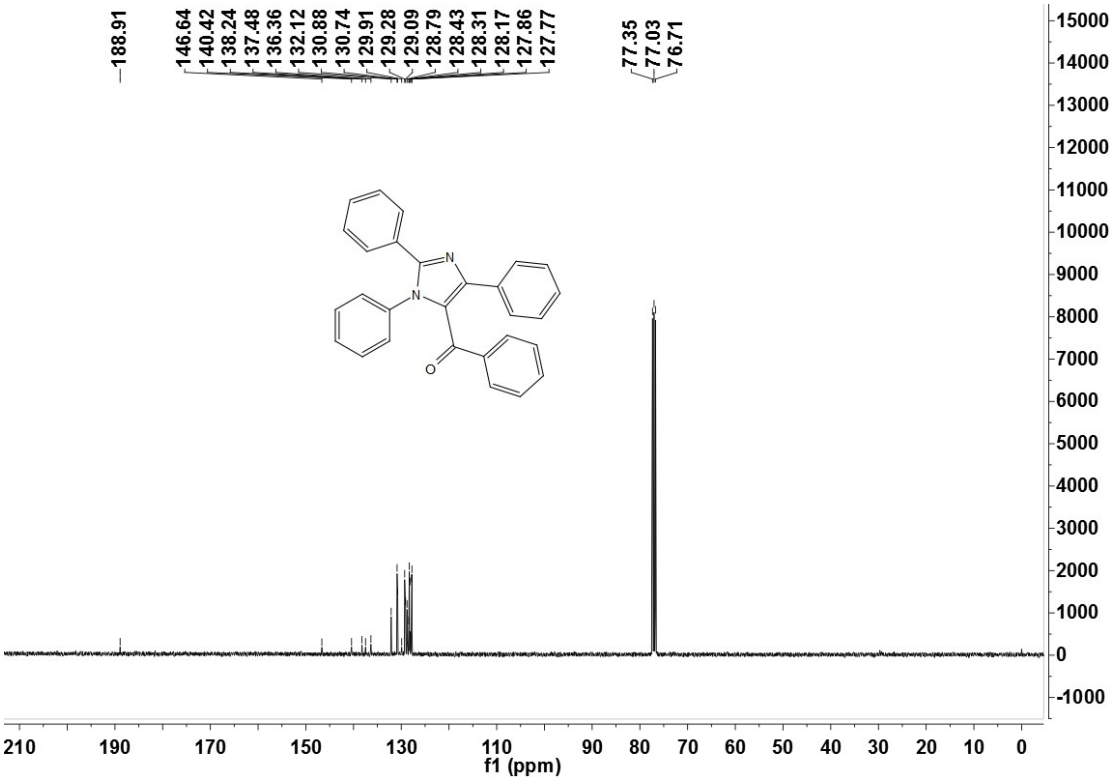


HRMS

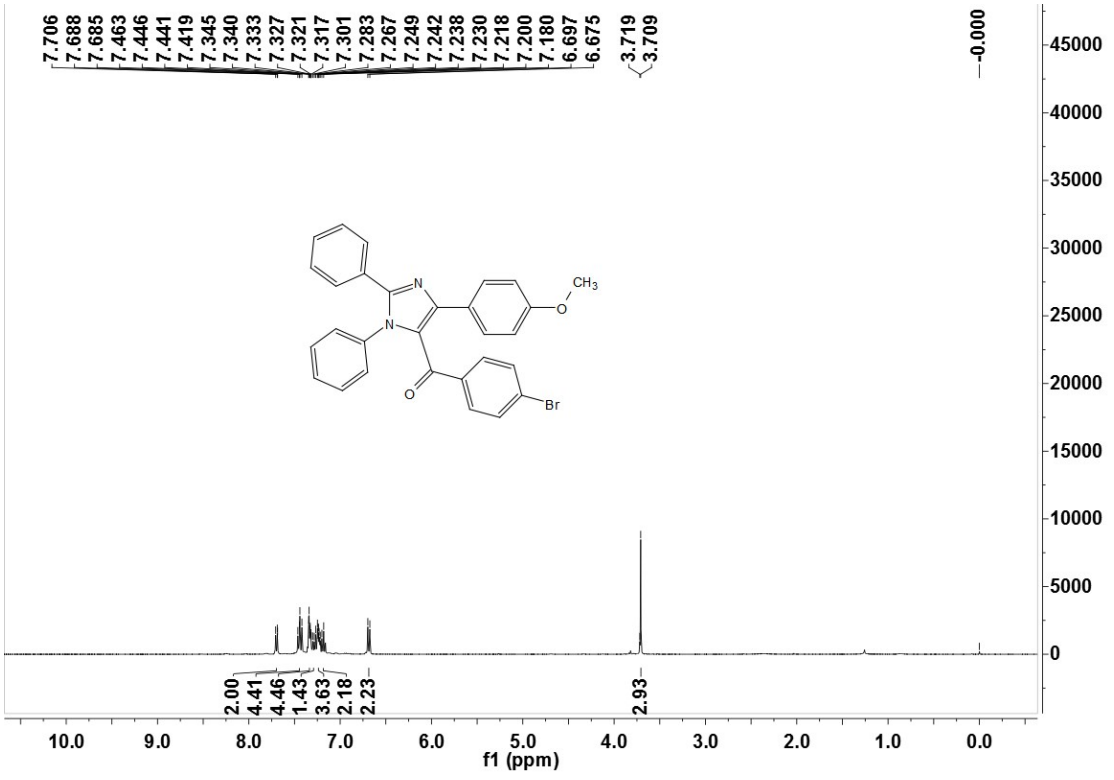


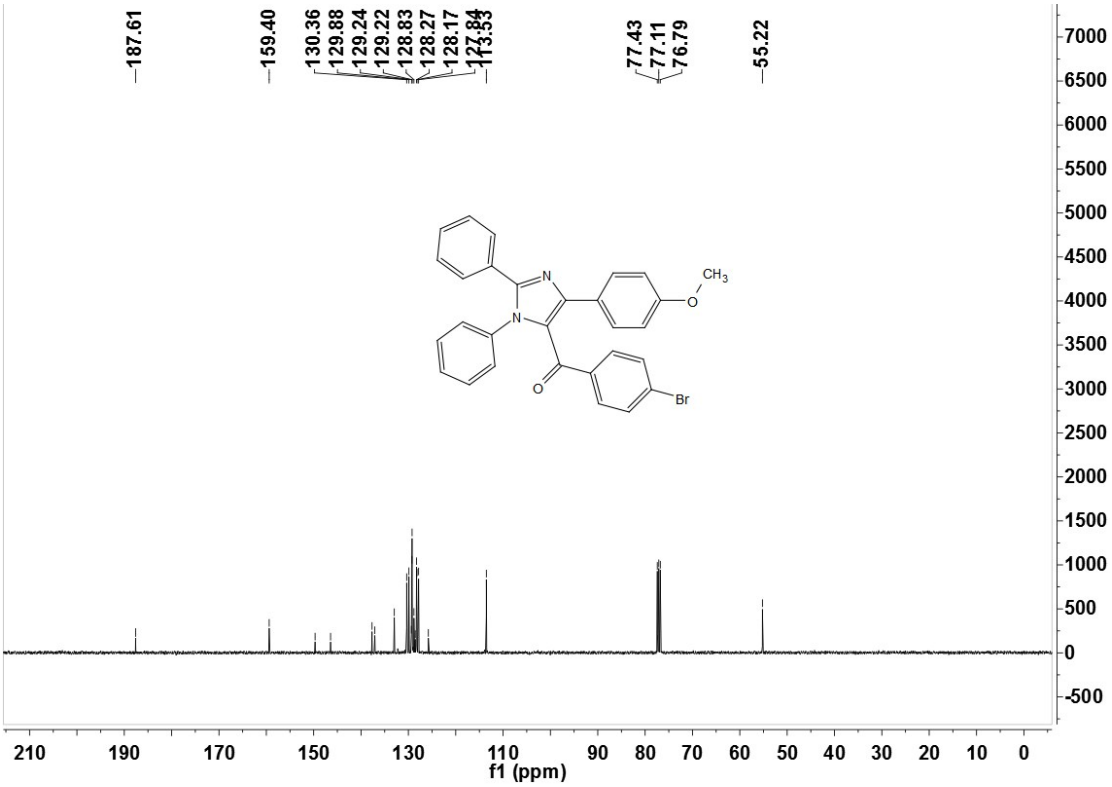
Phenyl (1,2,4-triphenyl-1*H*-imidazol-5-yl)methanone (6a)





(4-(4-Methoxyphenyl)-1,2-diphenyl-1*H*-imidazol-5-yl)(phenyl)methanone (6b)





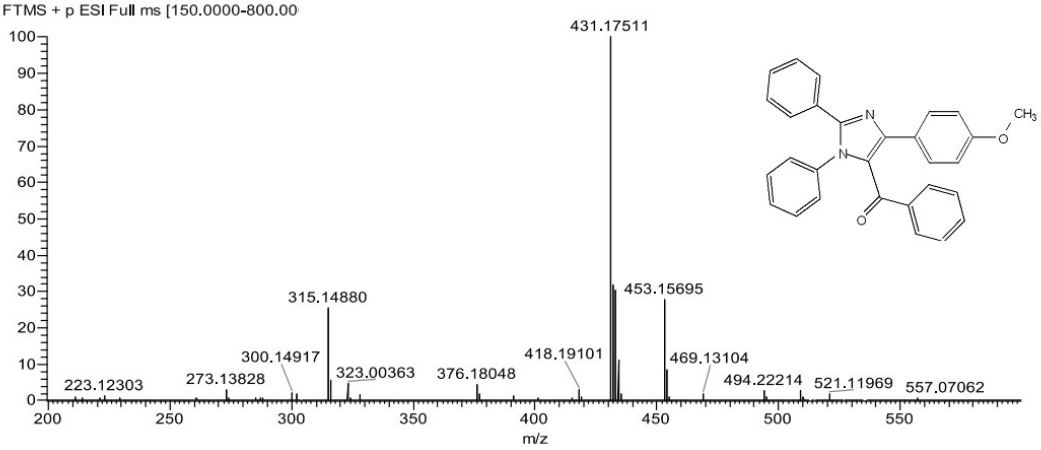
HRMS

Mass Analysis Report

Batch:	/	**Lab Name:**	Default Laboratory
Method:	C:\Xcalibur\methods\fs_sim	**Assay:**	Assay name
Inst. Method:	/	**User:**	Thermo

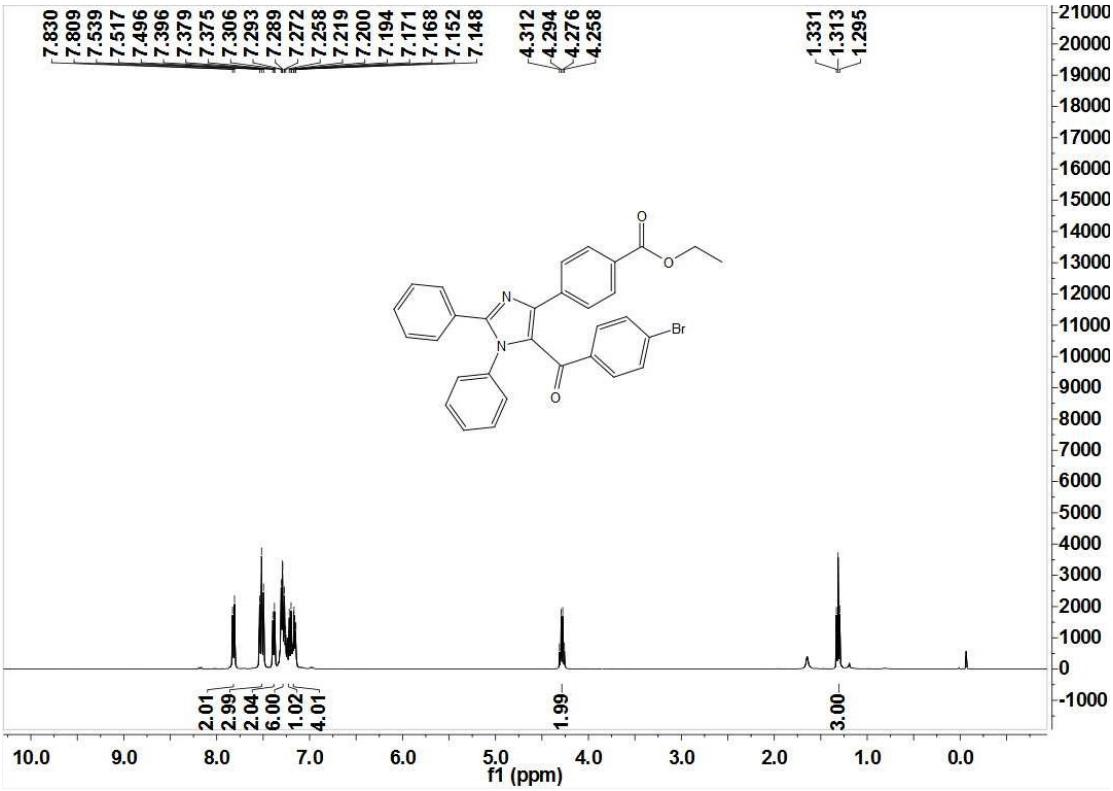
Sample ID	Raw File	Sample Type	Vial Position
	6B	Unknown	

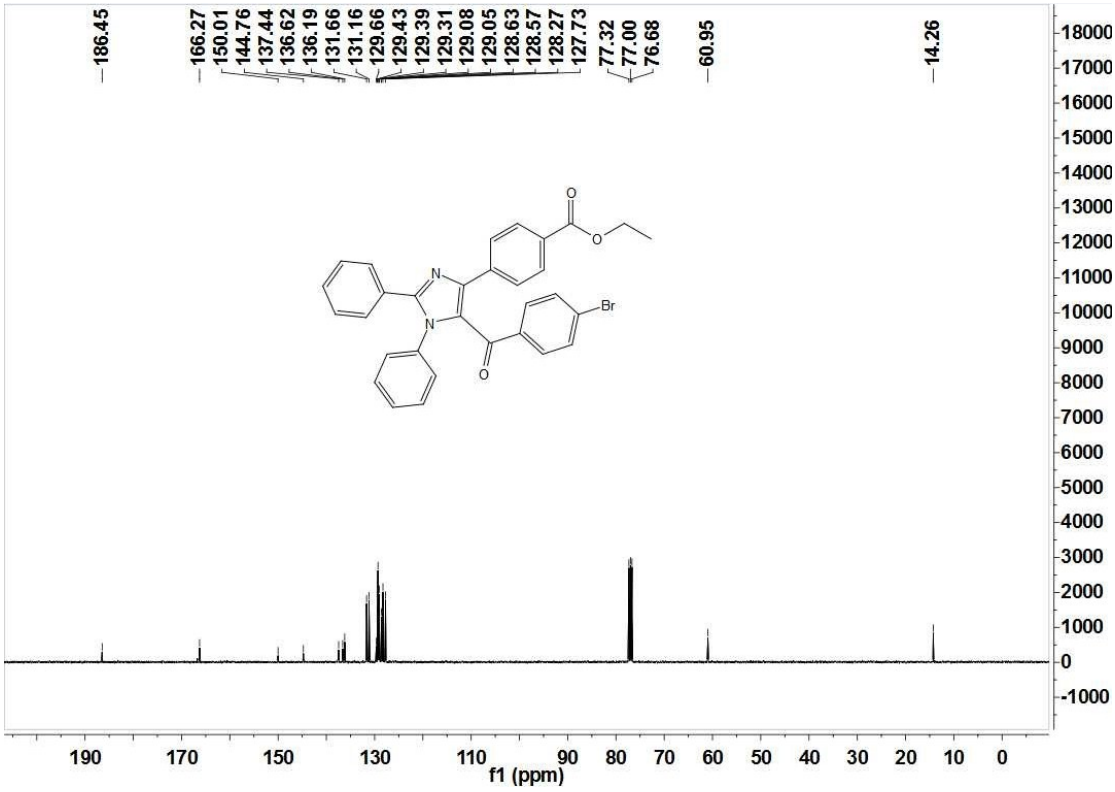
6B #1 RT: 0.00 AV: 1 NL: 2.57E8
T: FTMS + p ESI Full ms [150.0000-800.00



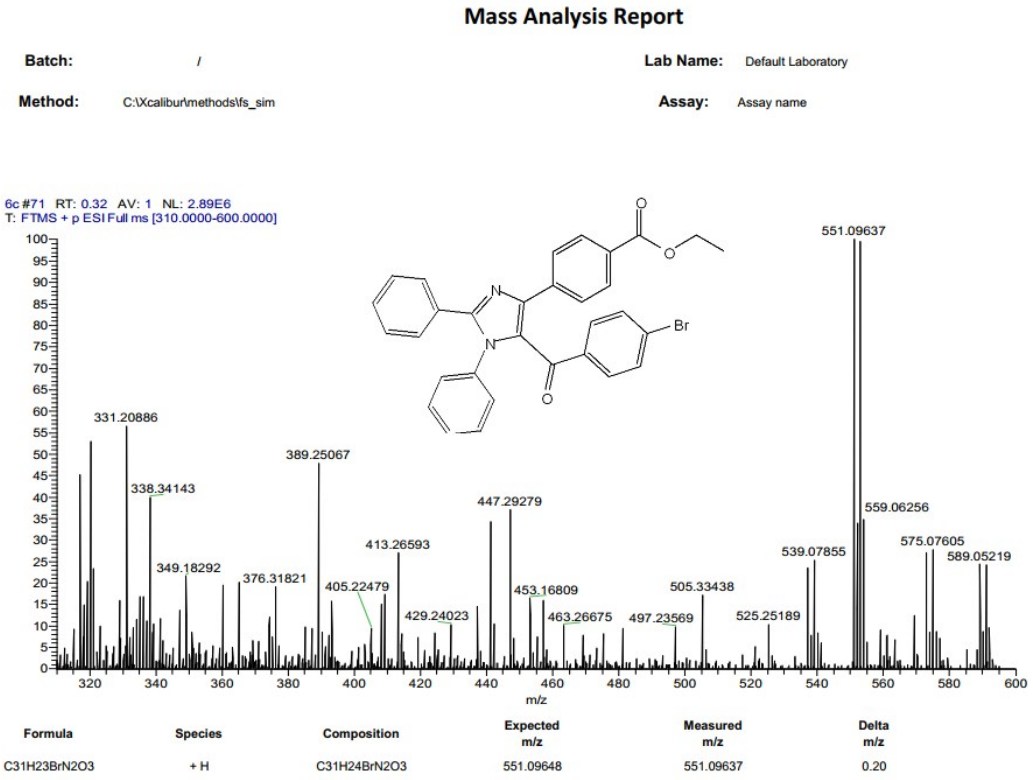
Formula	Species	Composition	Expected m/z	Measured m/z	Delta ppm
C29H22N2O2	+ H	C29H23N2O2	431.17540	431.17511	0.67

Ethyl 4-(5-(4-bromobenzoyl)-1,2-diphenyl-1*H*-imidazol-4-yl)benzoate (6c)



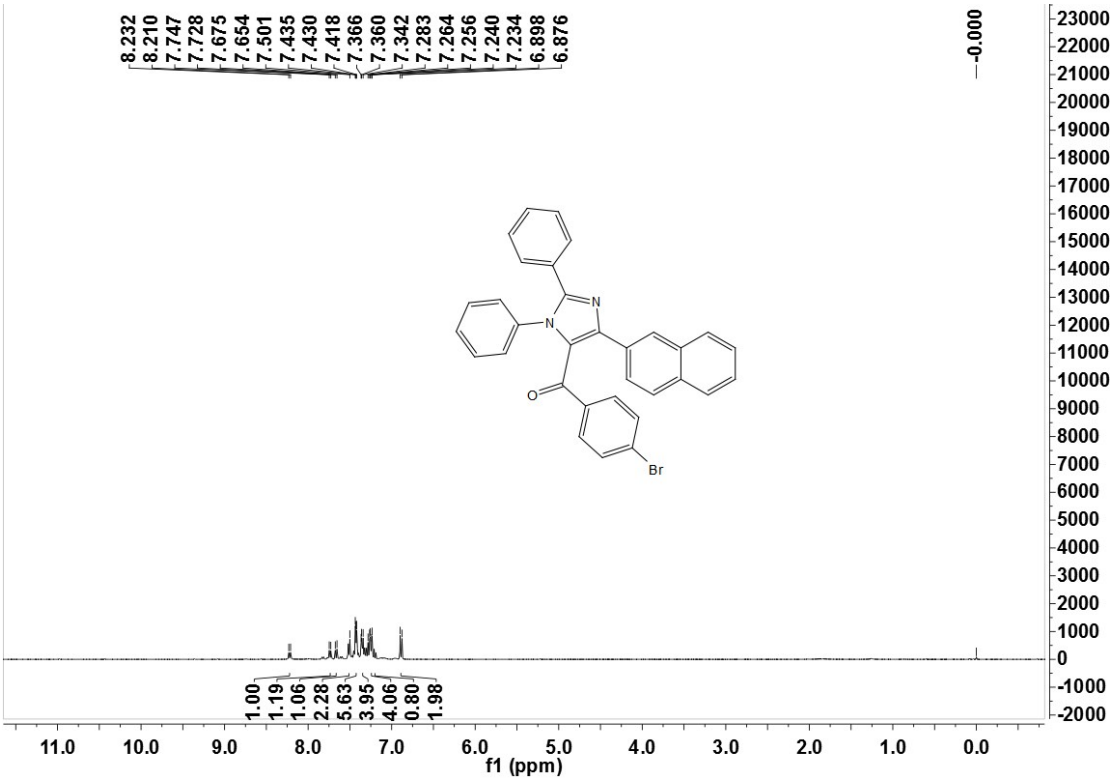


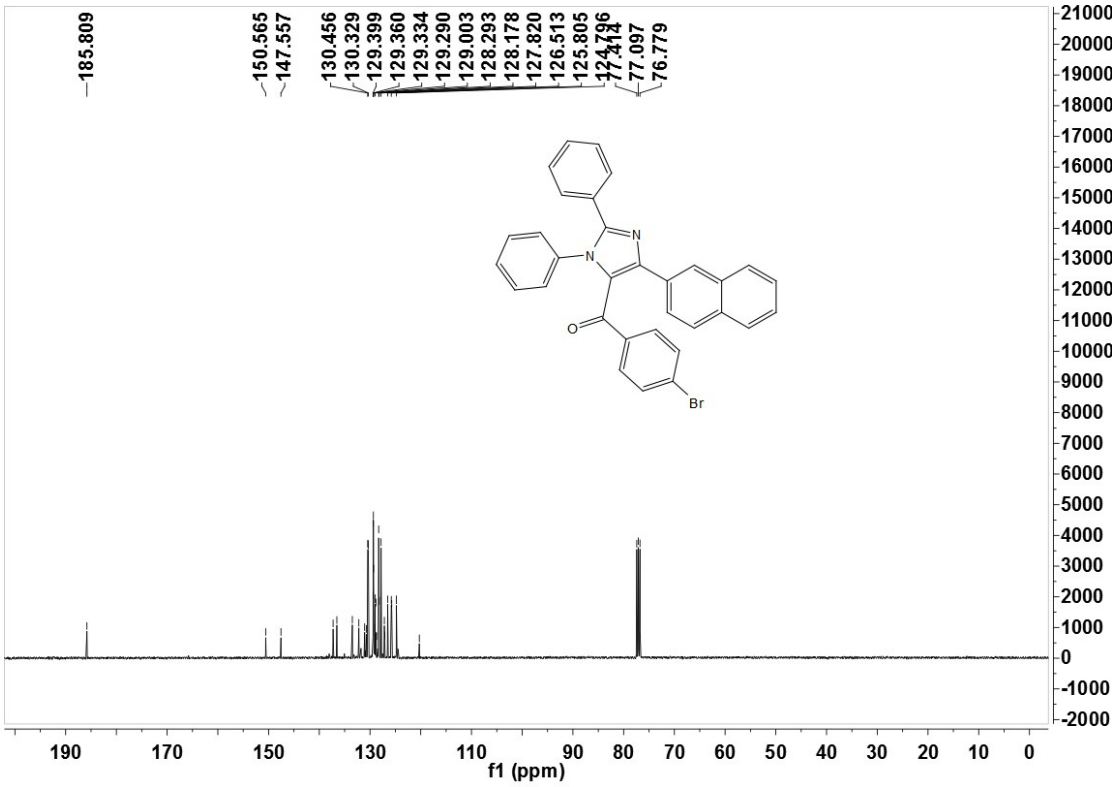
HRMS



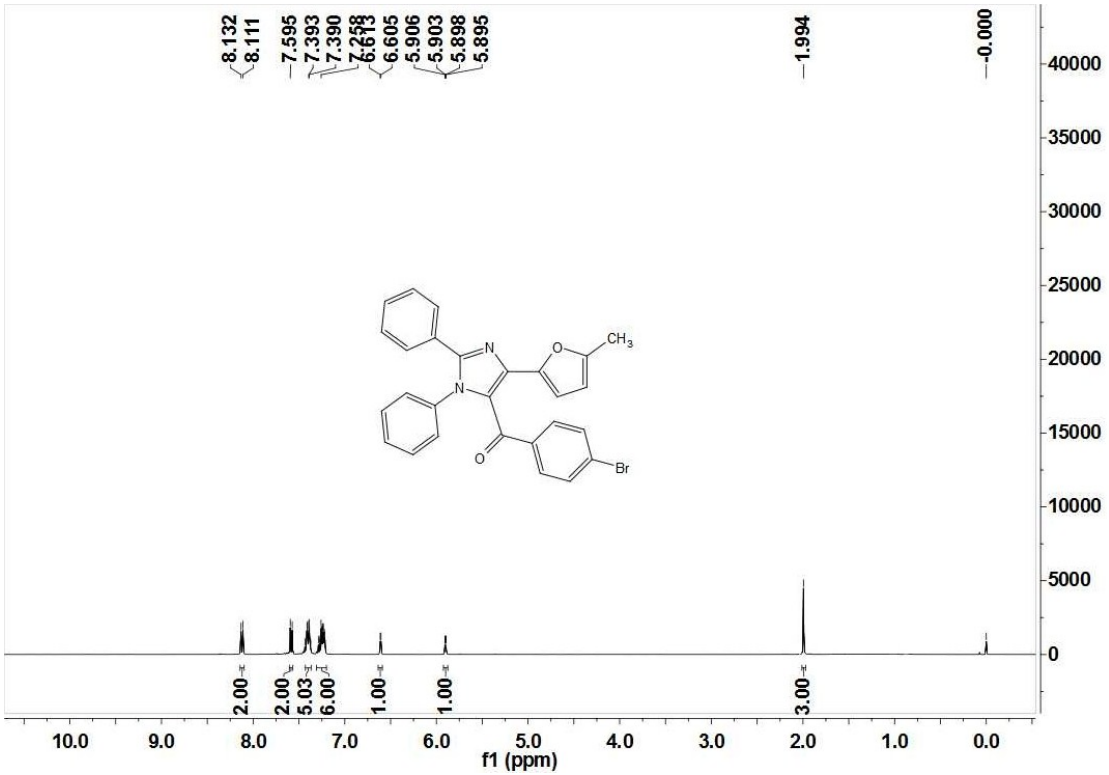
(4-Bromophenyl)(4-(naphthalen-2-yl)-1,2-diphenyl-1*H*-imidazol-5-yl)methanone

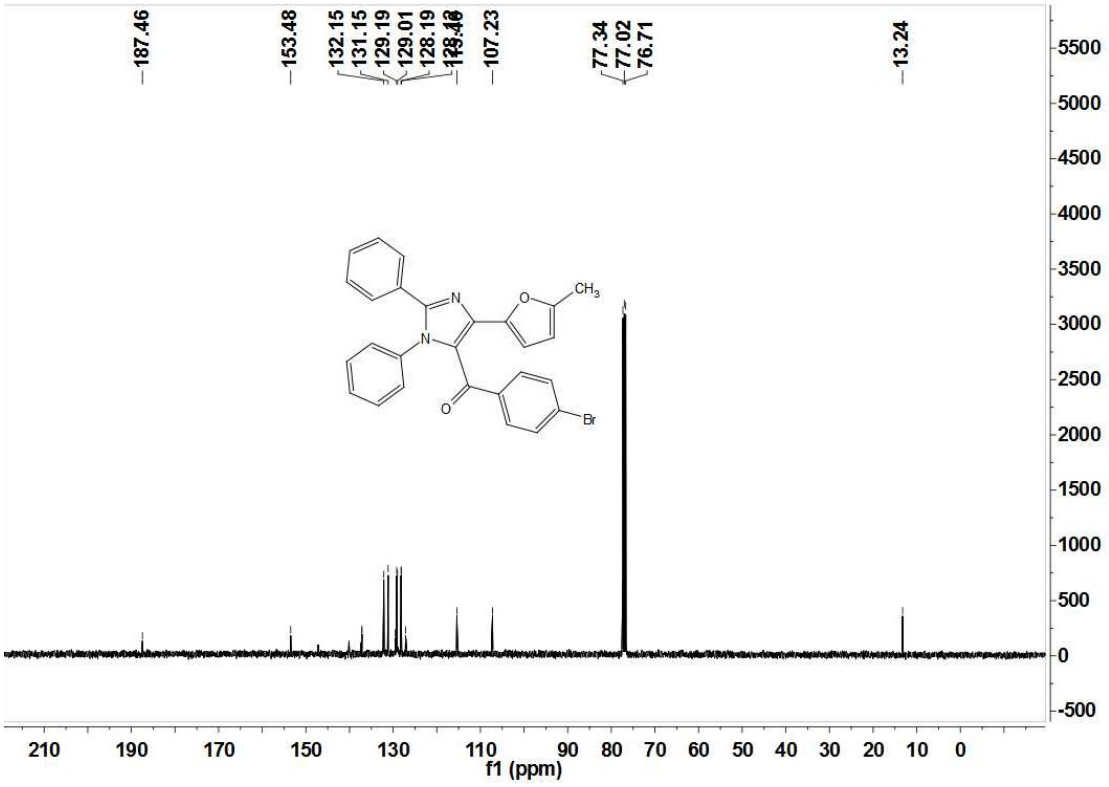
(6d)





(4-Bromophenyl)(4-(5-methylfuran-2-yl)-1,2-diphenyl-1*H*-imidazol-5-yl)methanone (6e)





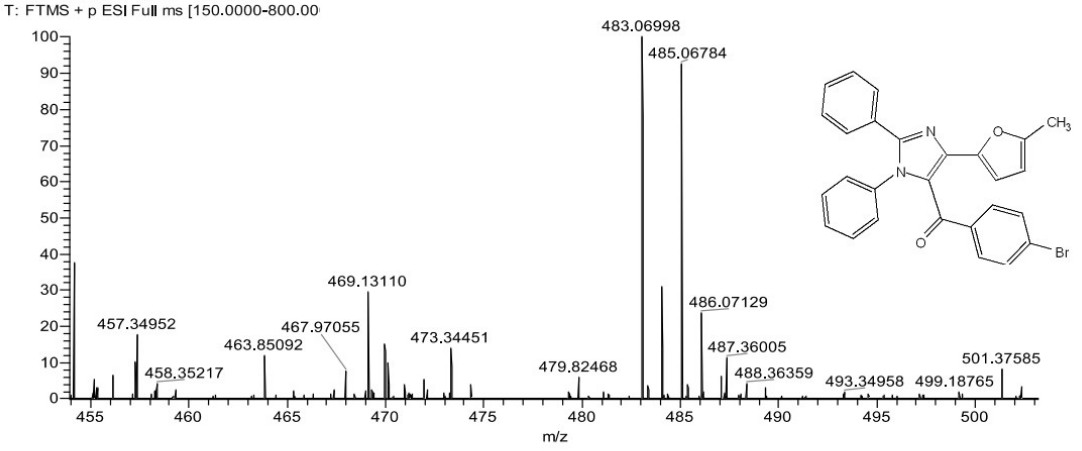
HRMS

Mass Analysis Report

Batch:	/	**Lab Name:**	Default Laboratory
Method:	C:\Xcalibur\methods\fs_sim	**Assay:**	Assay name
Inst. Method:	/	**User:**	Thermo

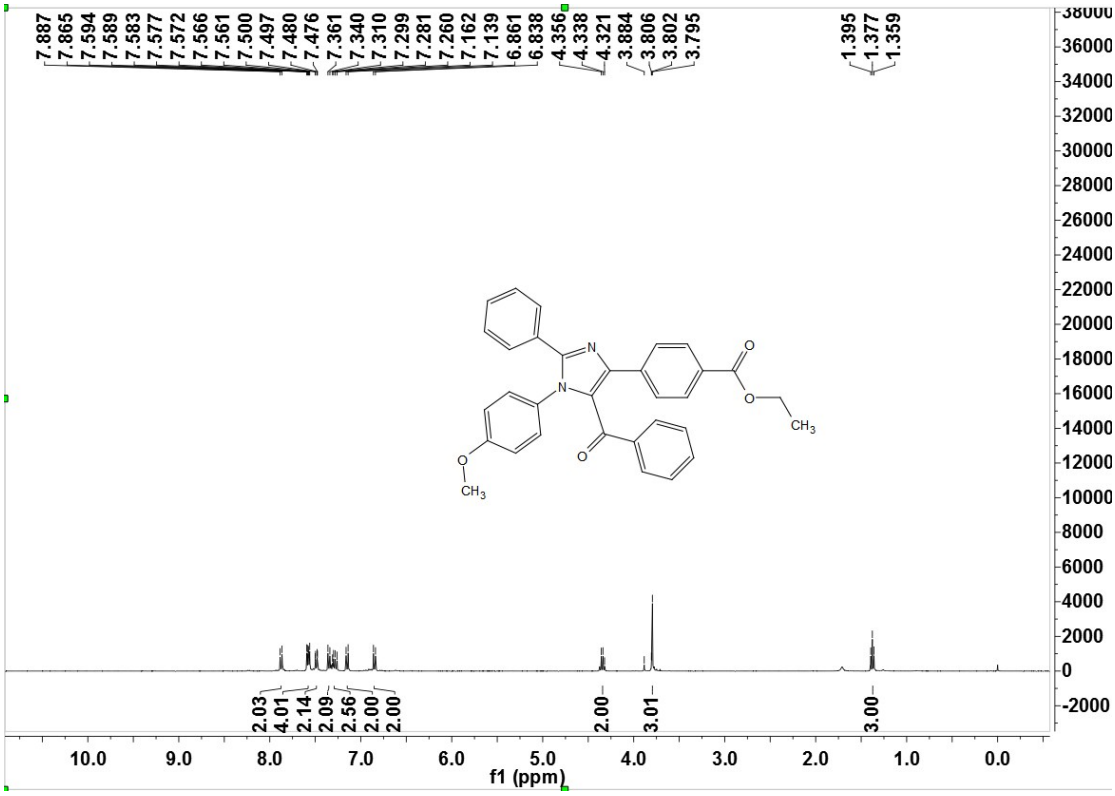
Sample ID	Raw File	Sample Type	Vial Position
	6E	Unknown	

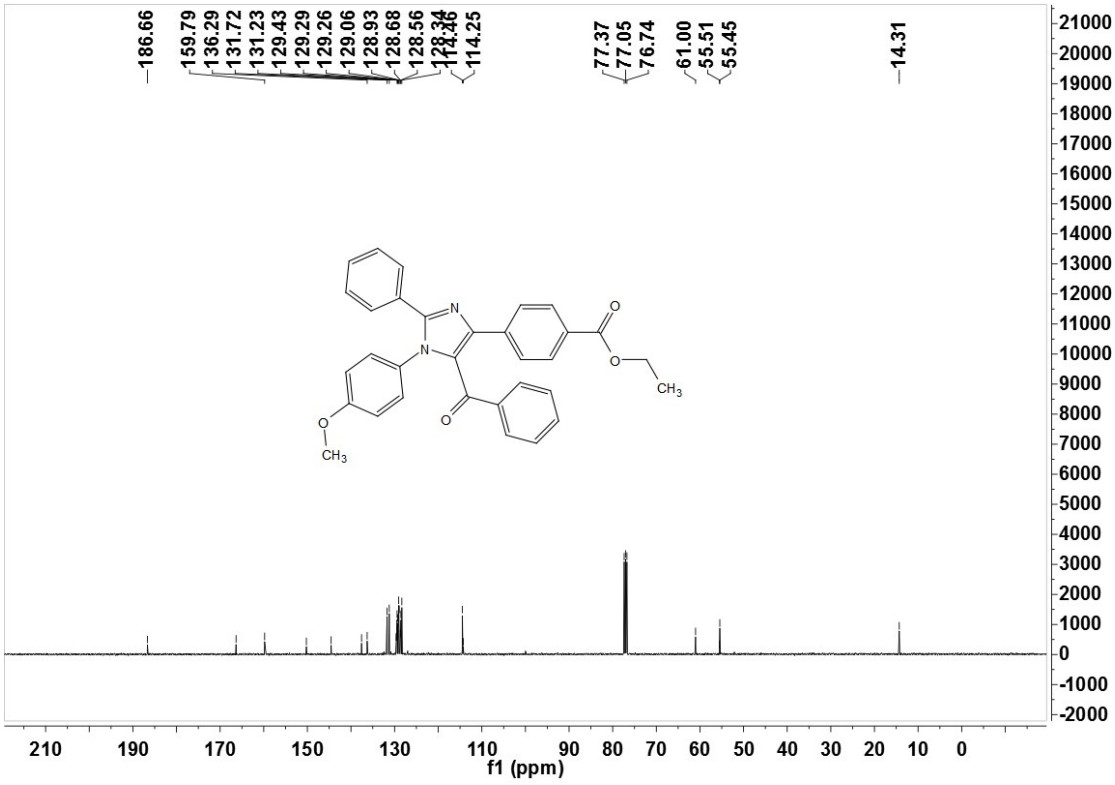
6E #7 RT: 0.03 AV: 1 NL: 4.55E5
T: FTMS + p ESI Full ms [150.0000-800.00



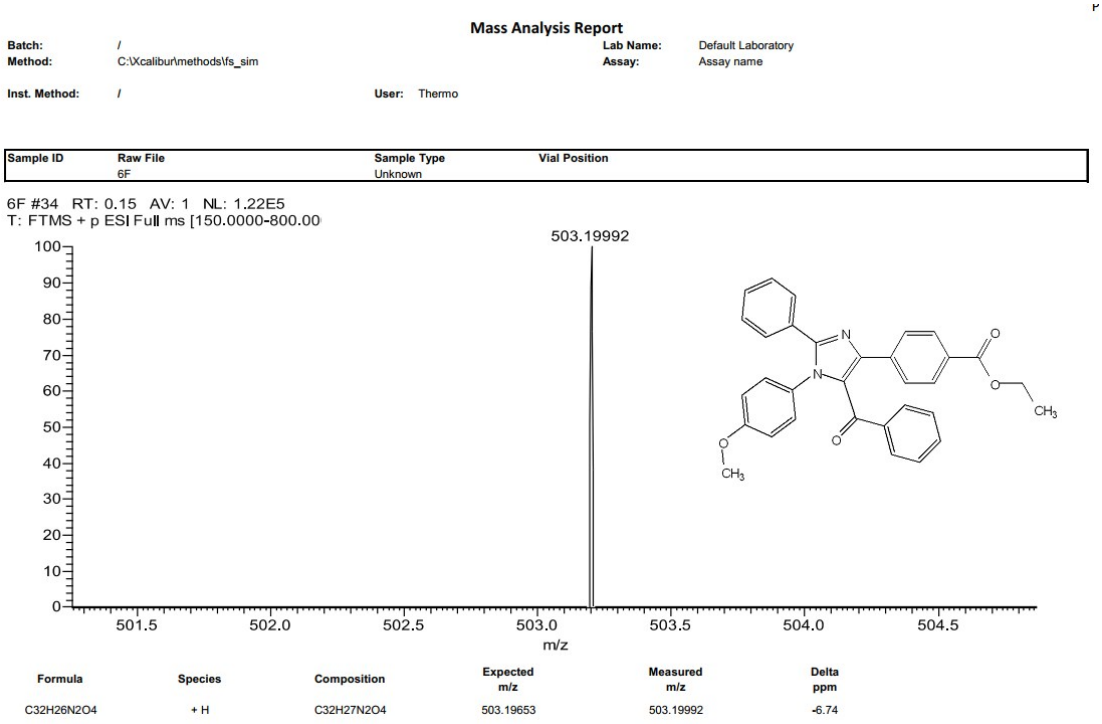
Formula	Species	Composition	Expected m/z	Measured m/z	Delta ppm
C27H19BrN2O2	+ H	C27H20BrN2O2	483.07027	483.06998	0.60

Ethyl 4-(5-benzoyl-1-(4-methoxyphenyl)-2-phenyl-1*H*-imidazol-4-yl) benzoate (6f)

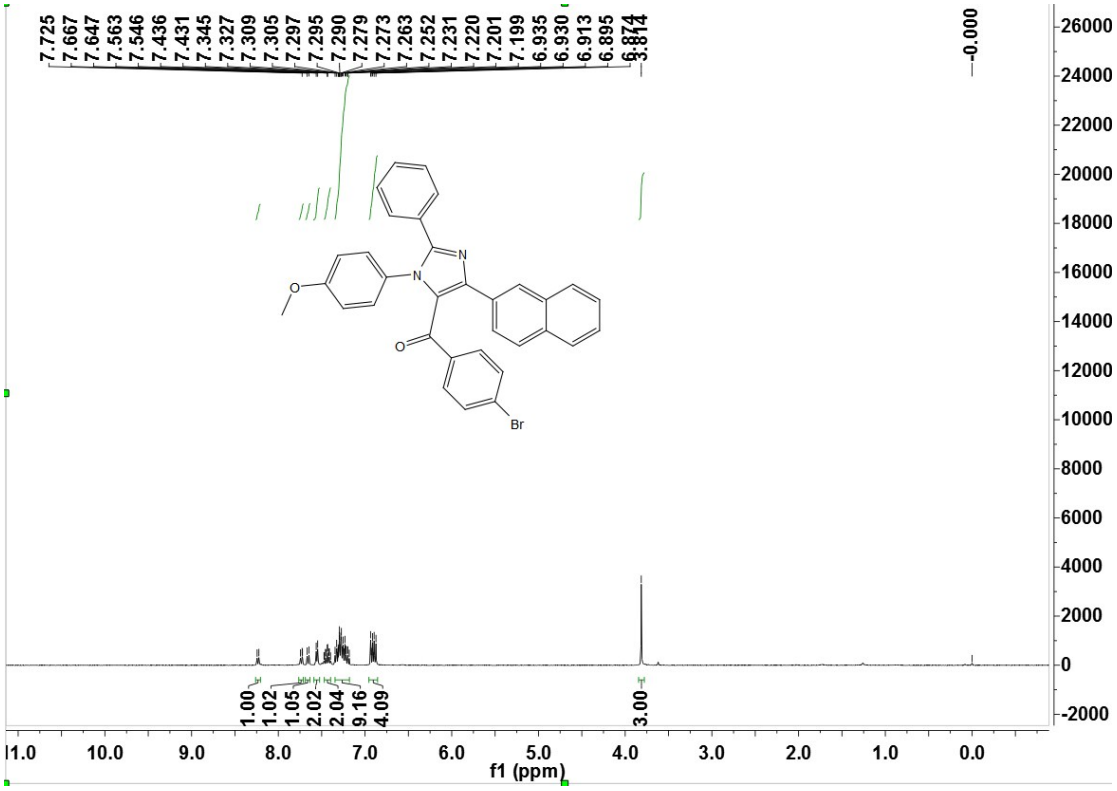


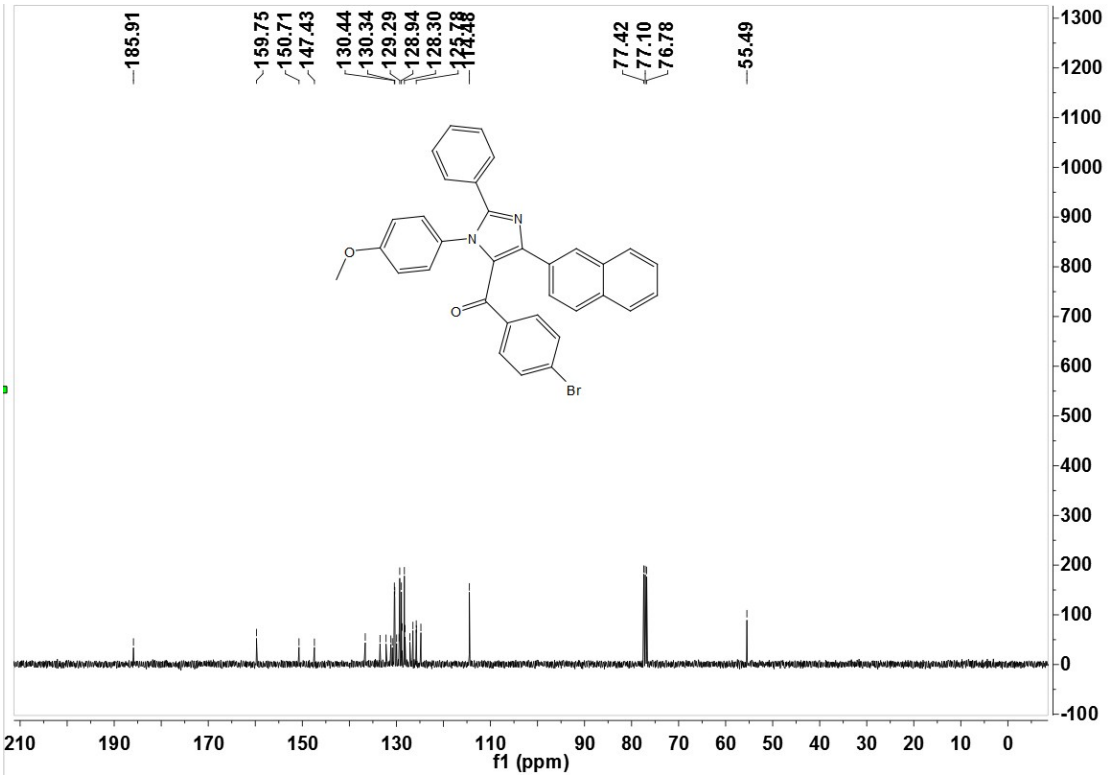


HRMS



(4-Bromophenyl)(1-(4-methoxyphenyl)-4-(naphthalen-2-yl)-2-phenyl-1*H*-imidazol-5-yl)methanone (6g)





HRMS

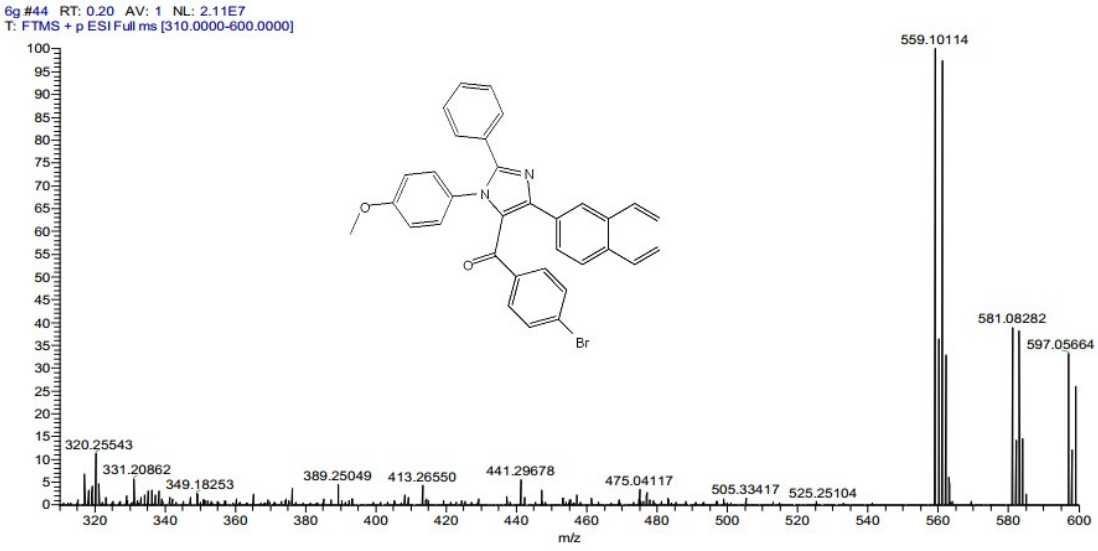
Mass Analysis Report

Batch: /

Lab Name: Default Laboratory

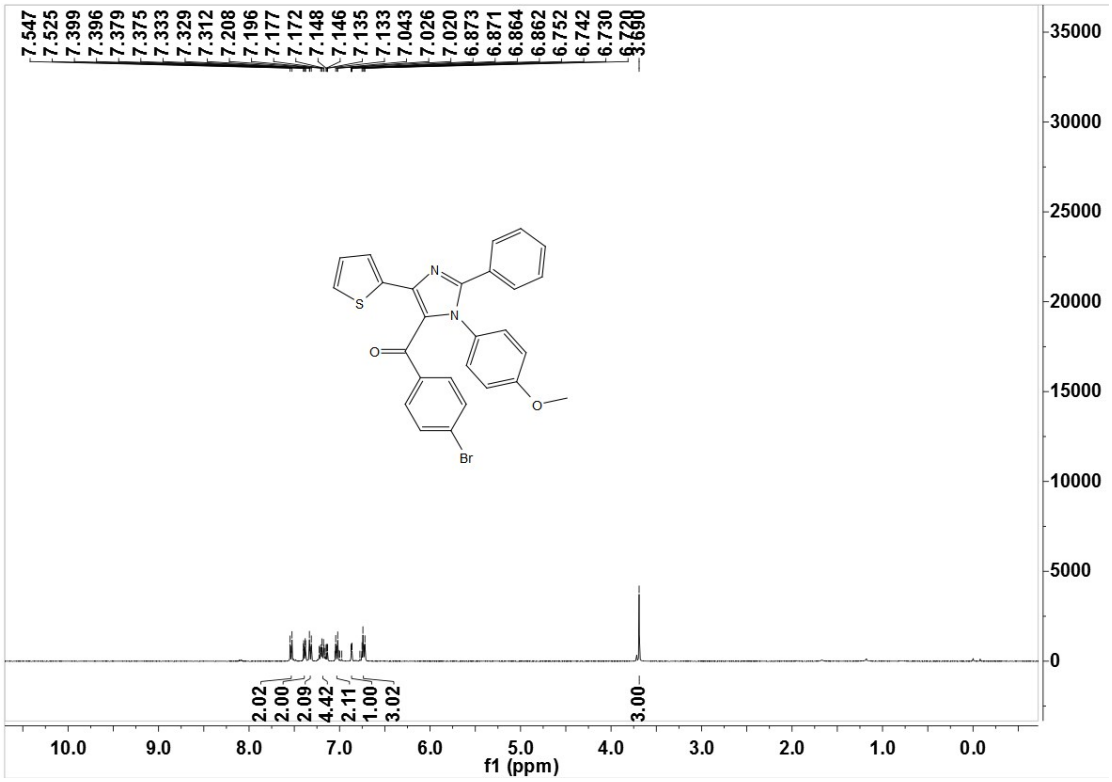
Method: C:\Xcalibur\methods\fs_sim

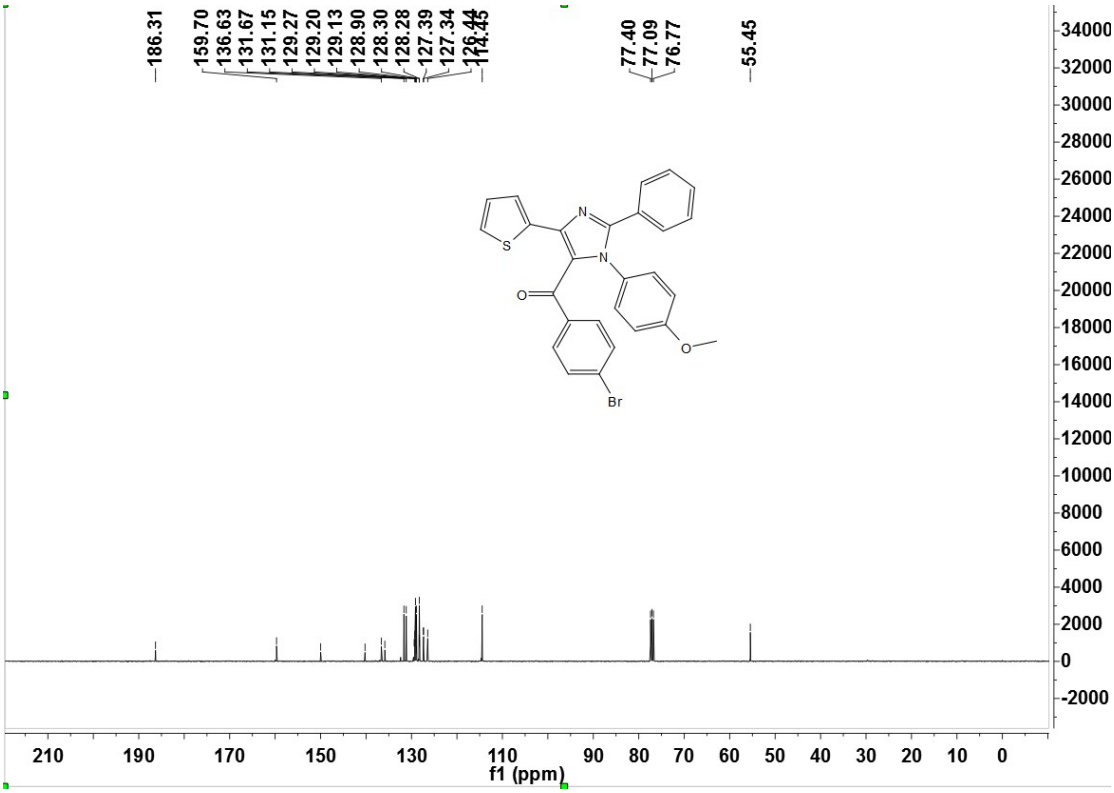
Assay: Assay name



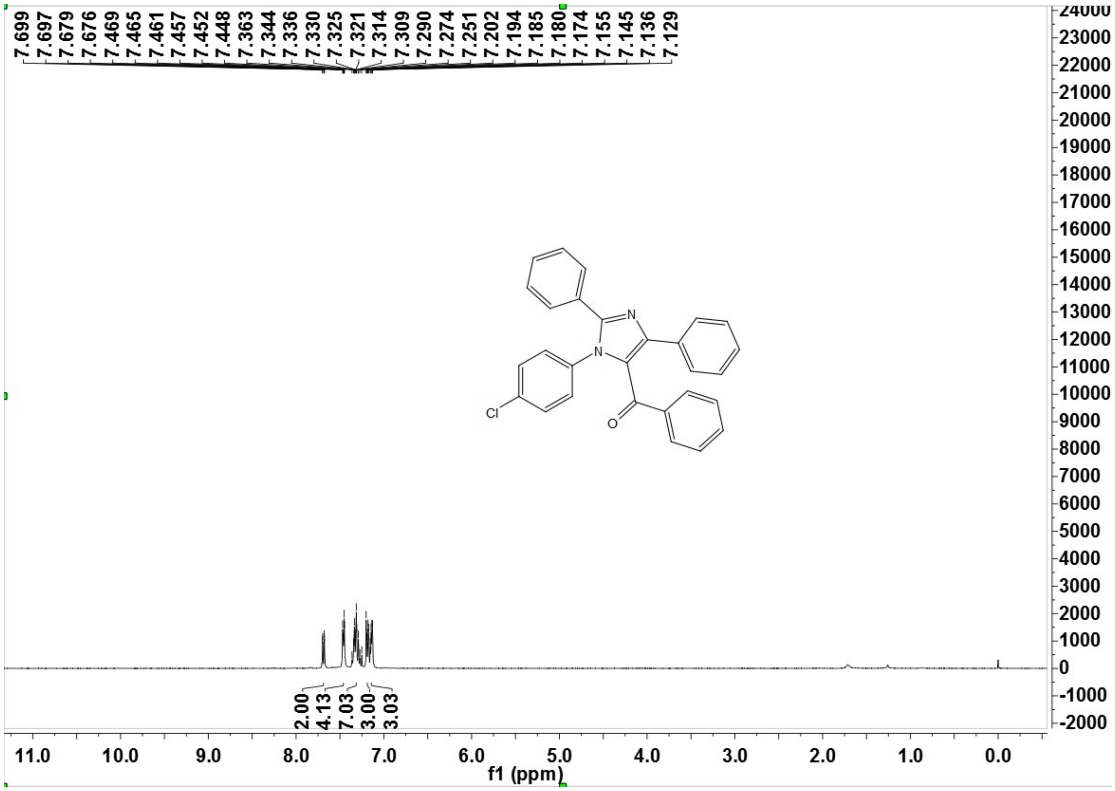
Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C33H23BrN2O2	+ H	C33H23BrN2O2	559.10157	559.10114	0.77

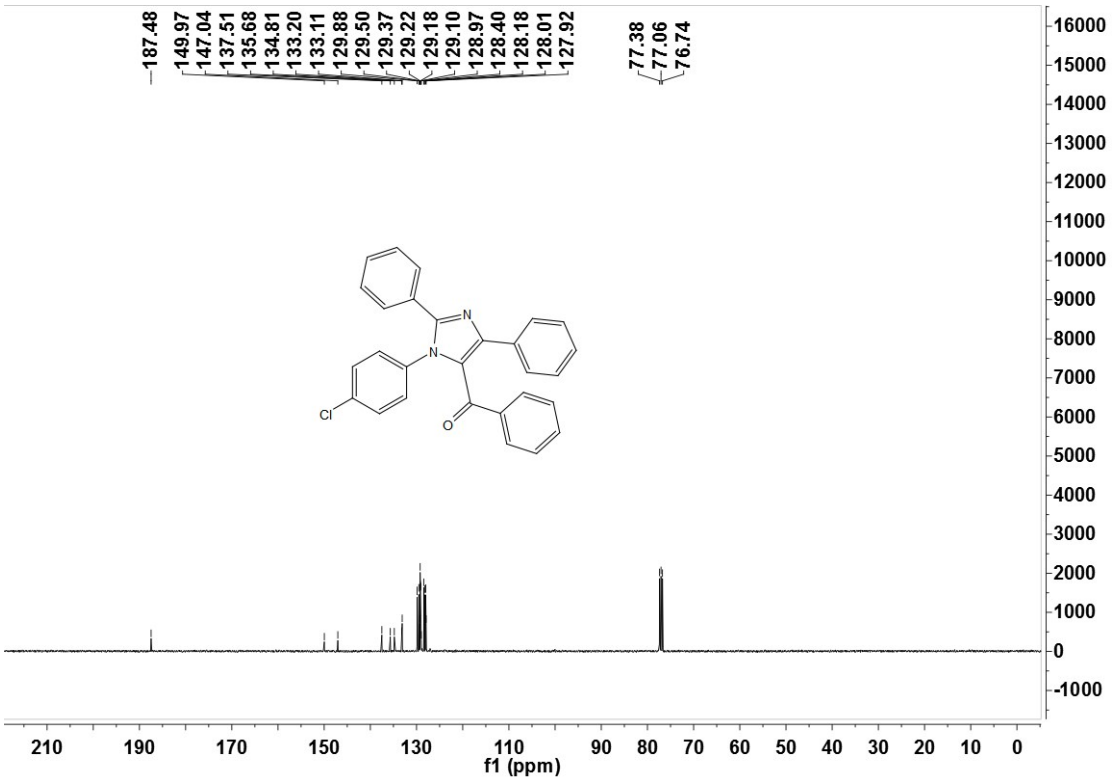
(4-Bromophenyl)(1-(4-methoxyphenyl)-2-phenyl-4-(thiophen-2-yl)-1*H*-imidazol-5-yl)methanone (6h)



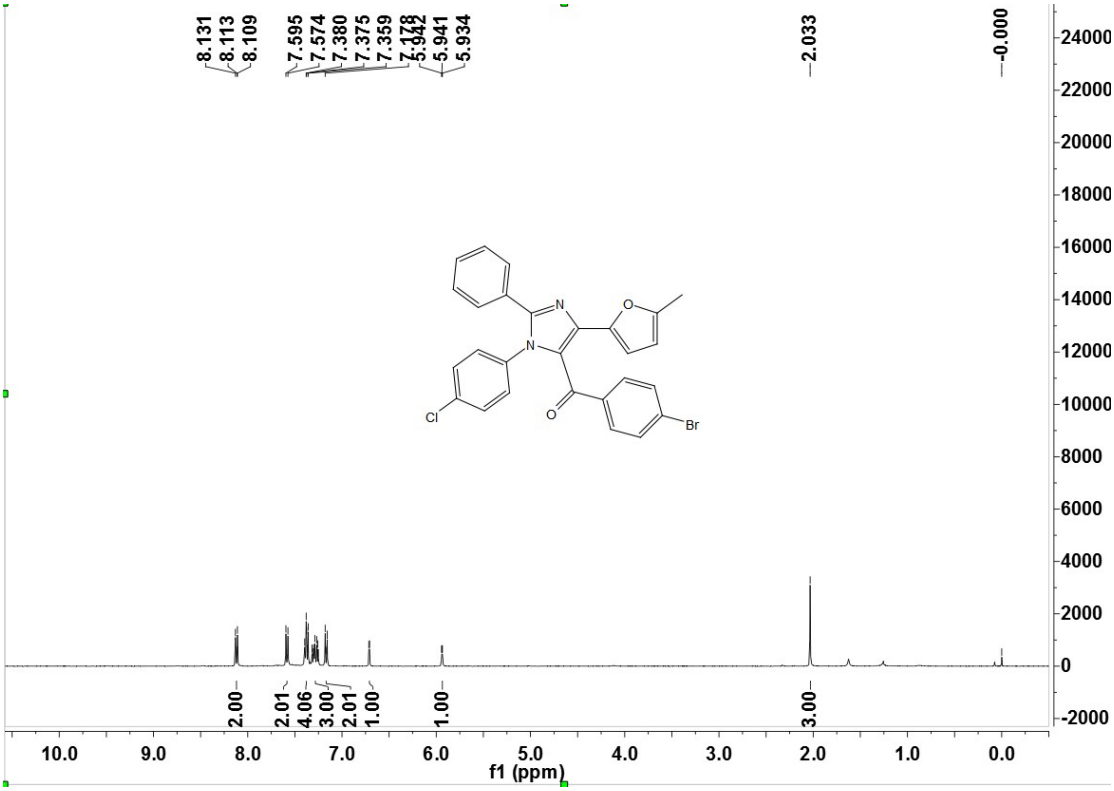


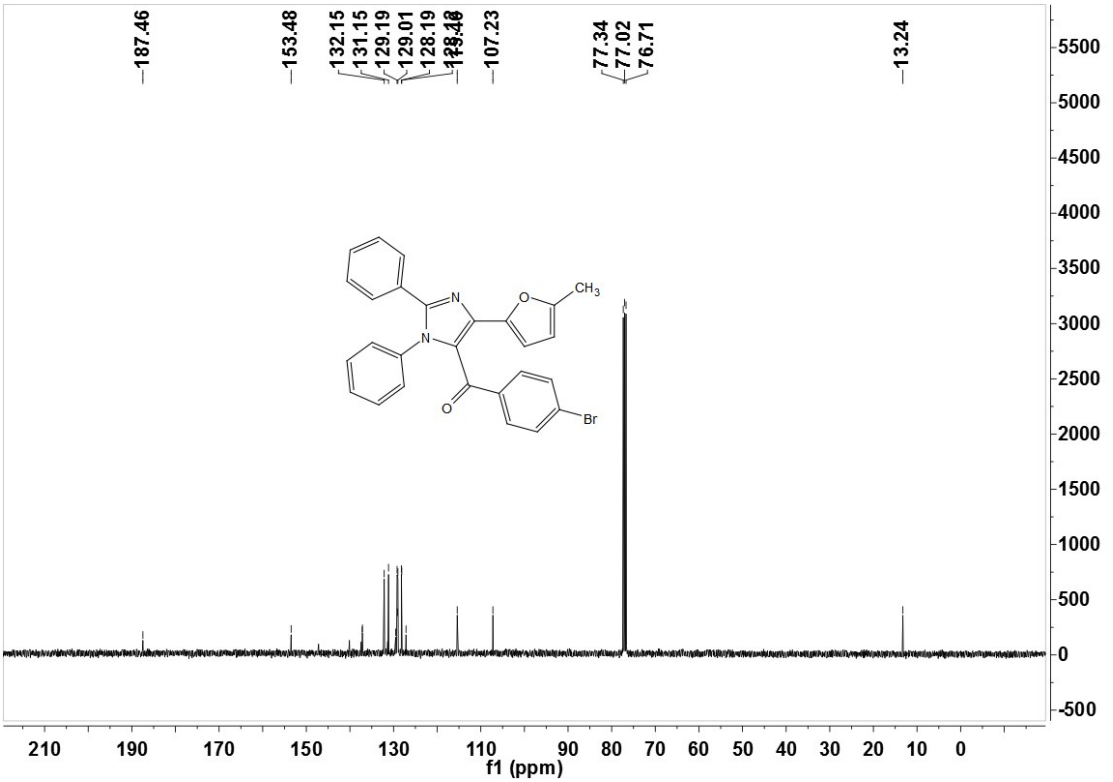
(1-(4-Chlorophenyl)-2,4-diphenyl-1*H*-imidazol-5-yl)(phenyl)methanone (6i)



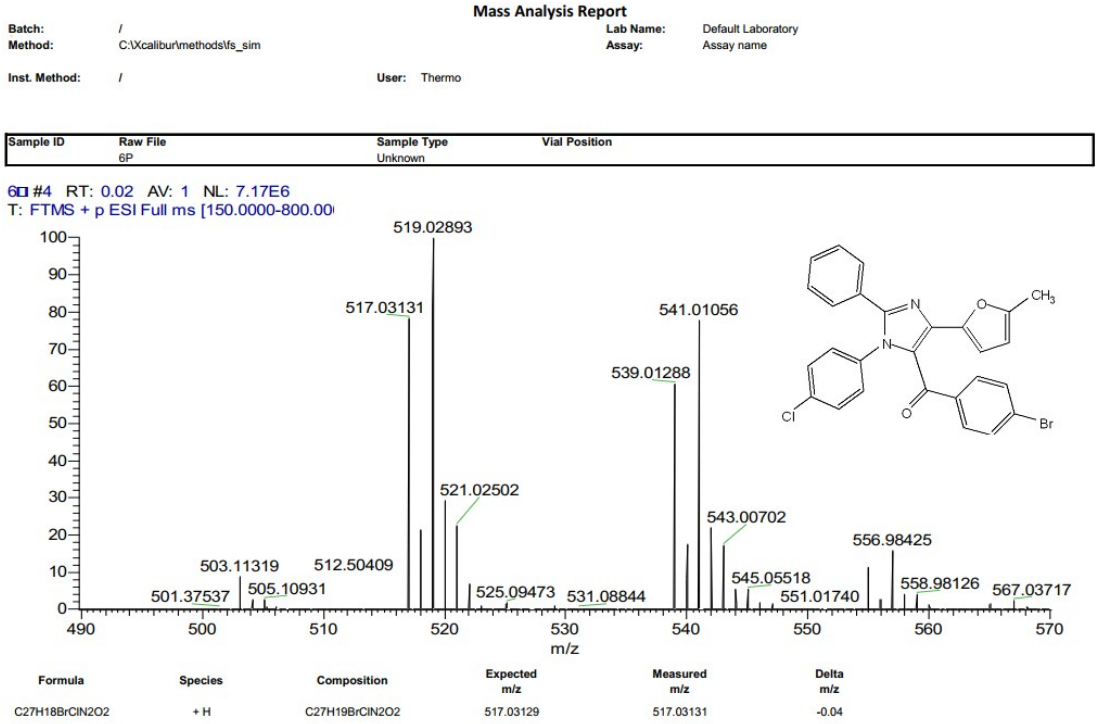


(4-Bromophenyl)(1-(4-chlorophenyl)-4-(5-methylfuran-2-yl)-2-phenyl-1*H*-imidazol-5-yl)methanone (6j)



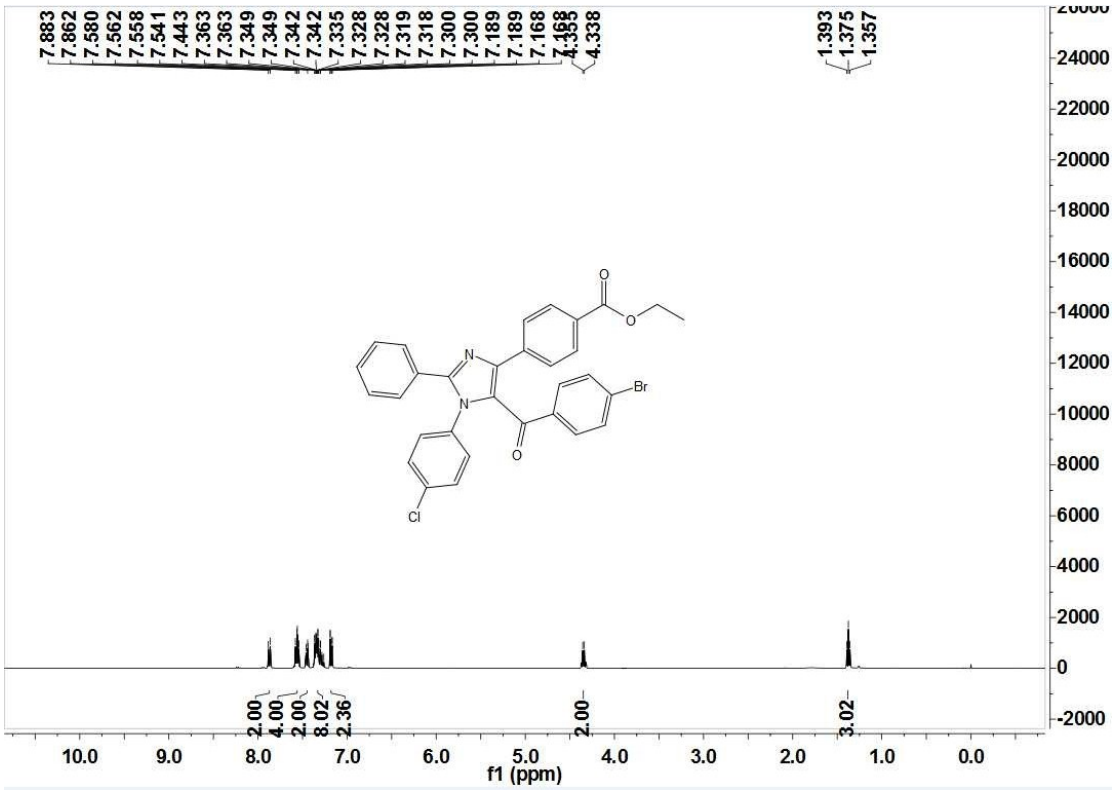


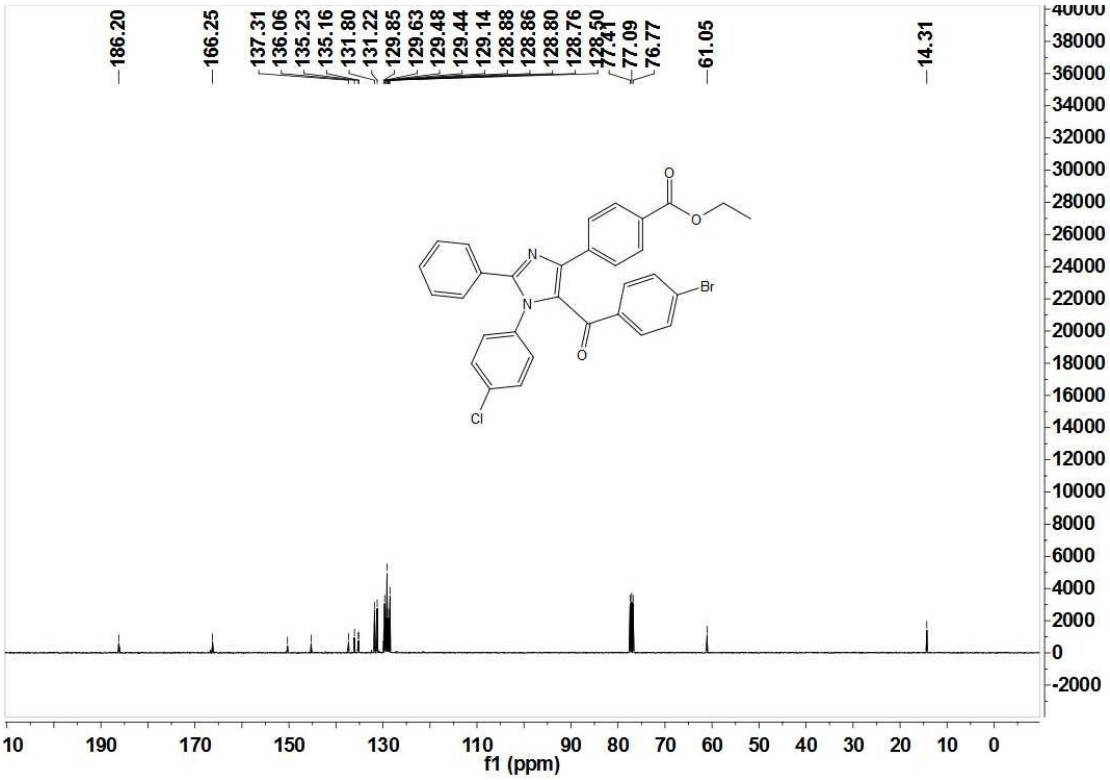
HRMS



Ethyl 4-(5-(4-bromobenzoyl)-1-(4-chlorophenyl)-2-phenyl-1*H*-imidazol-4-yl)benzoate

(6k)





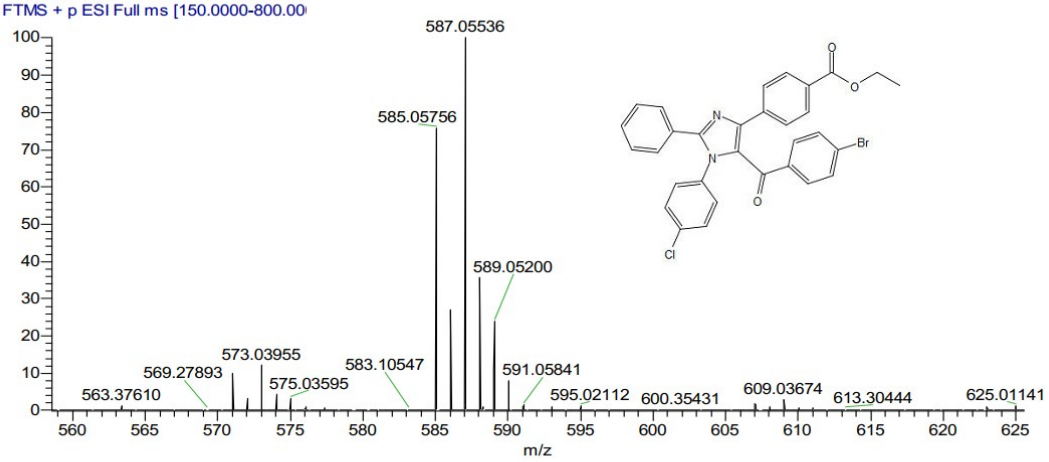
HRMS

Mass Analysis Report

Batch:	/	**Lab Name:**	Default Laboratory
Method:	C:\Xcalibur\methods\fs_sim	**Assay:**	Assay name
Inst. Method:	/	**User:**	Thermo

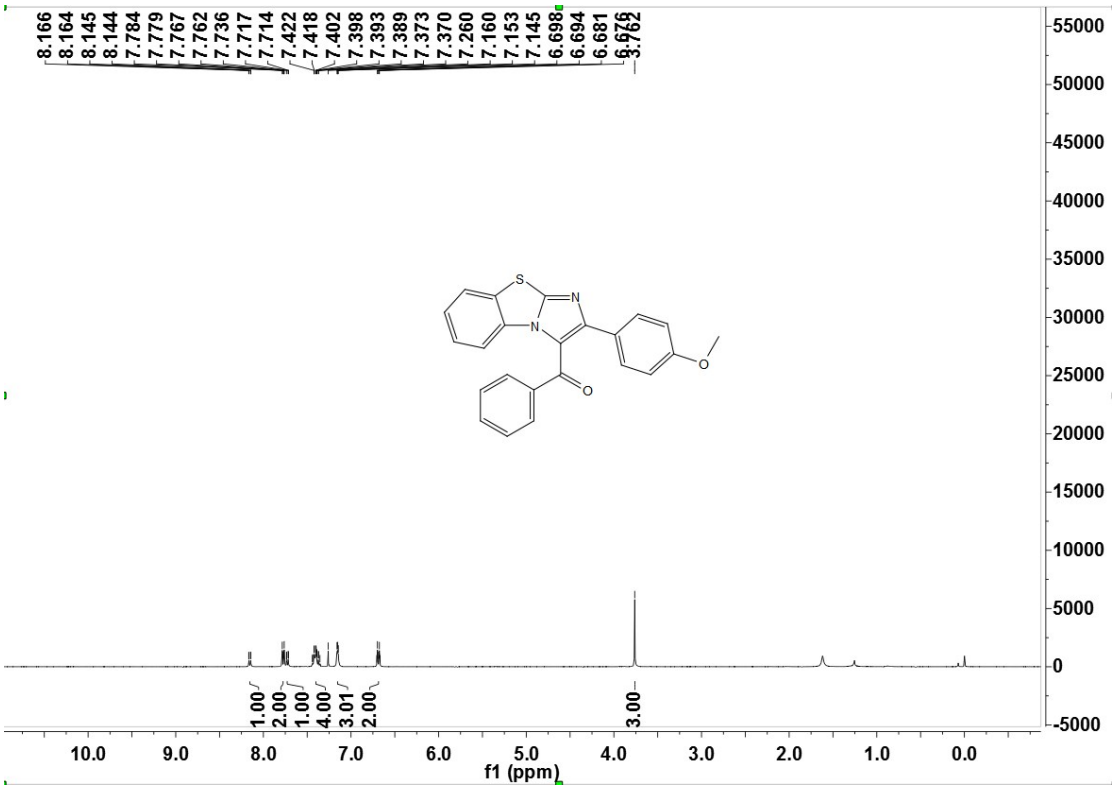
Sample ID	Raw File	Sample Type	Vial Position
	6K	Unknown	

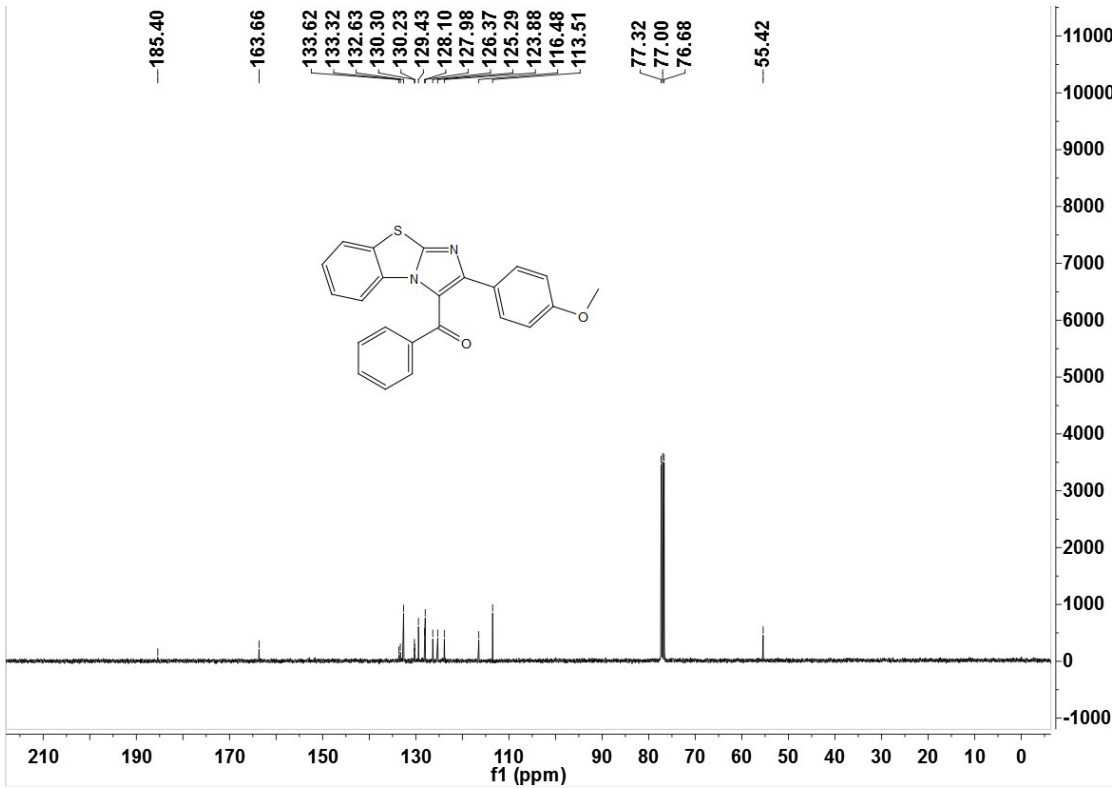
6K #34 RT: 0.15 AV: 1 NL: 4.55E6
T: FTMS + p ESI Full ms [150.0000-800.00



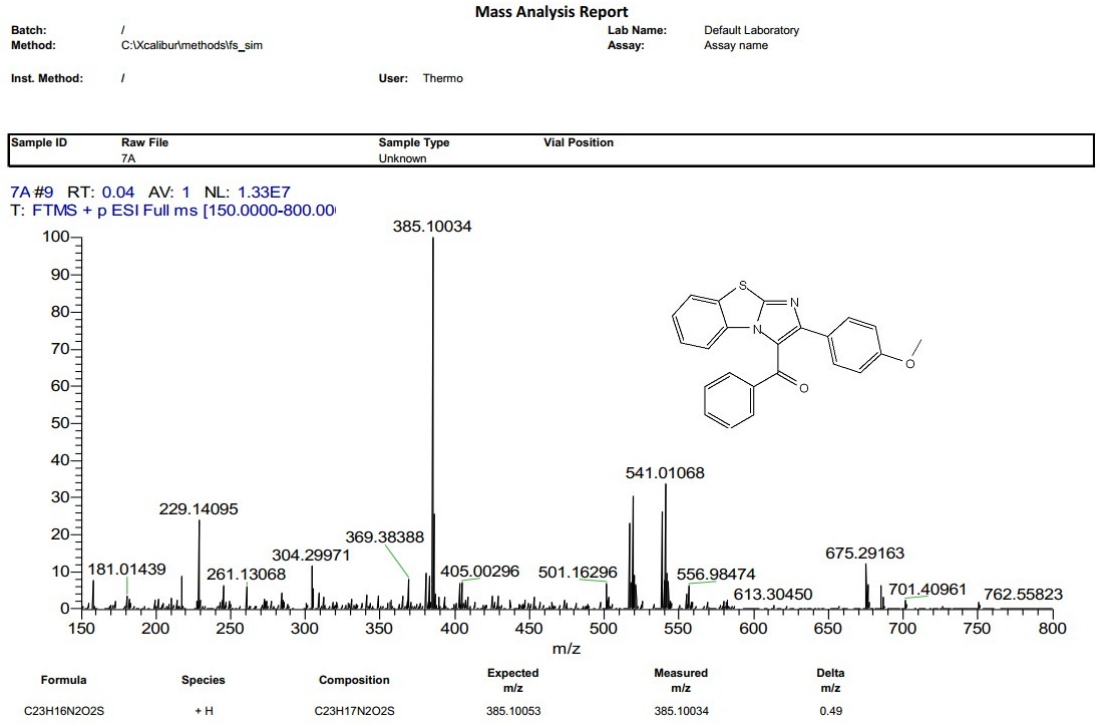
Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C31H22BrClN2O3	+ H	C31H23BrClN2O3	585.05751	585.05756	0.09

(2-(4-methoxyphenyl)benzo[d]imidazo[2,1-b]thiazol-3-yl)(phenyl)methanone (7a)

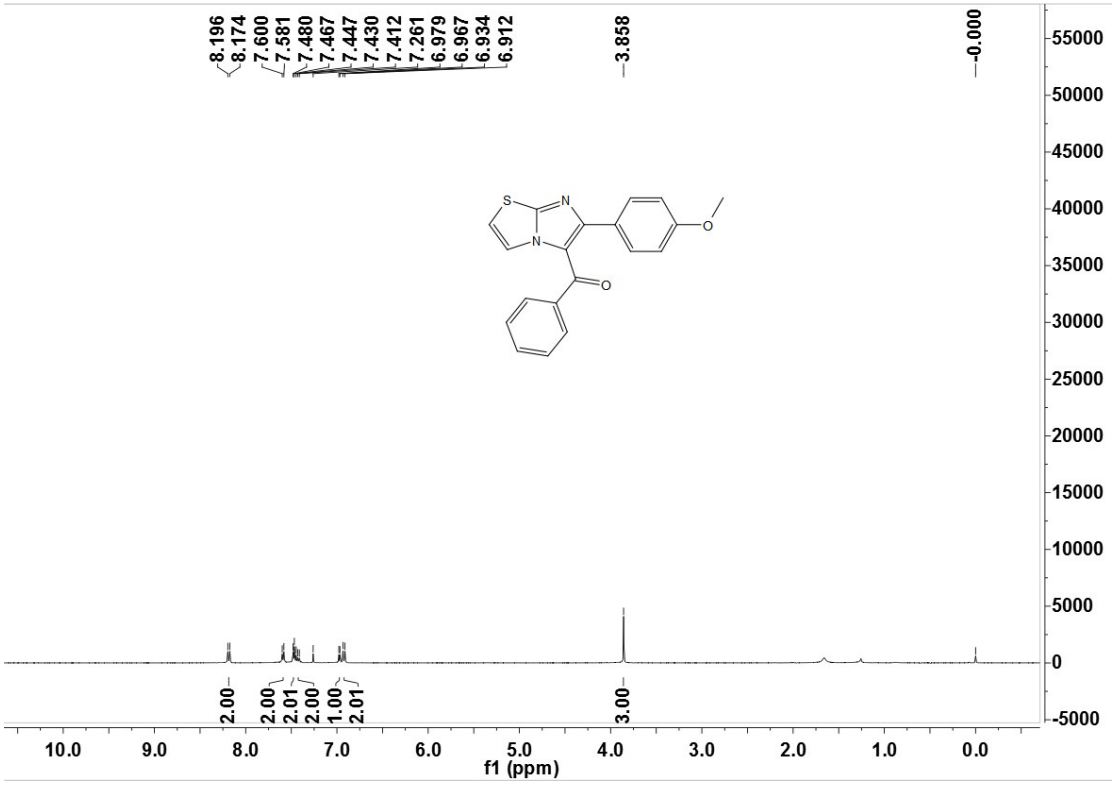


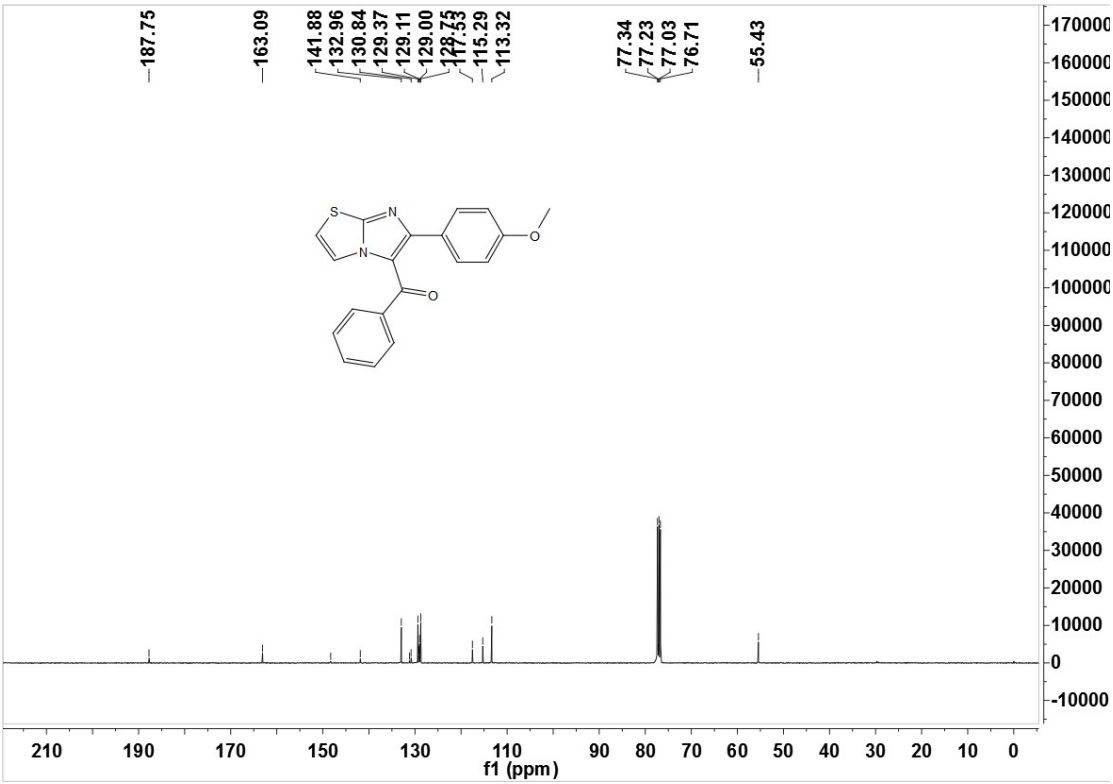


HRMS



(6-(4-Methoxyphenyl)imidazo[2,1-b]thiazol-5-yl)(phenyl)methanone (7b)





HRMS

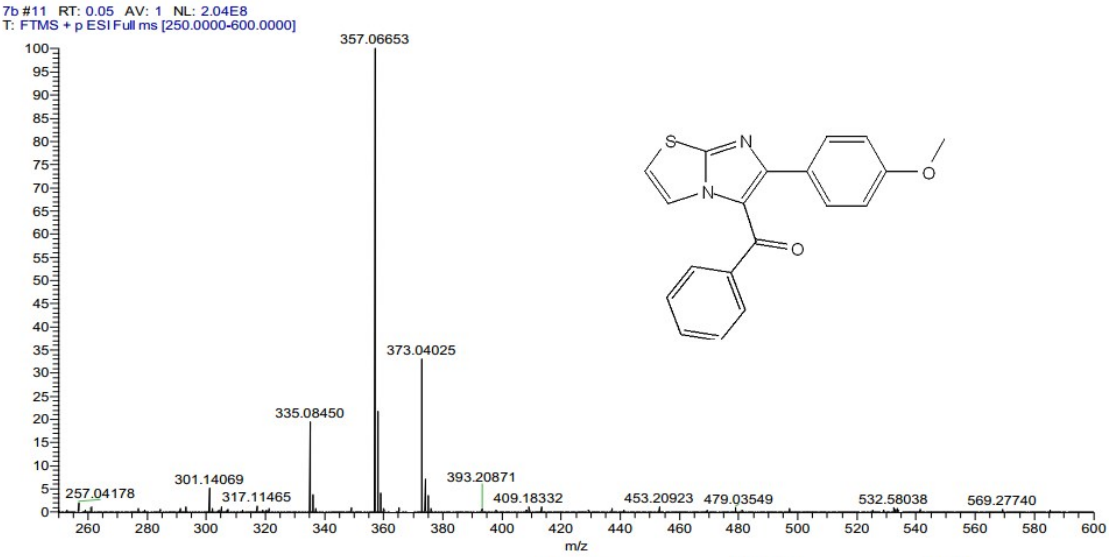
Mass Analysis Report

Batch: /

Lab Name: Default Laboratory

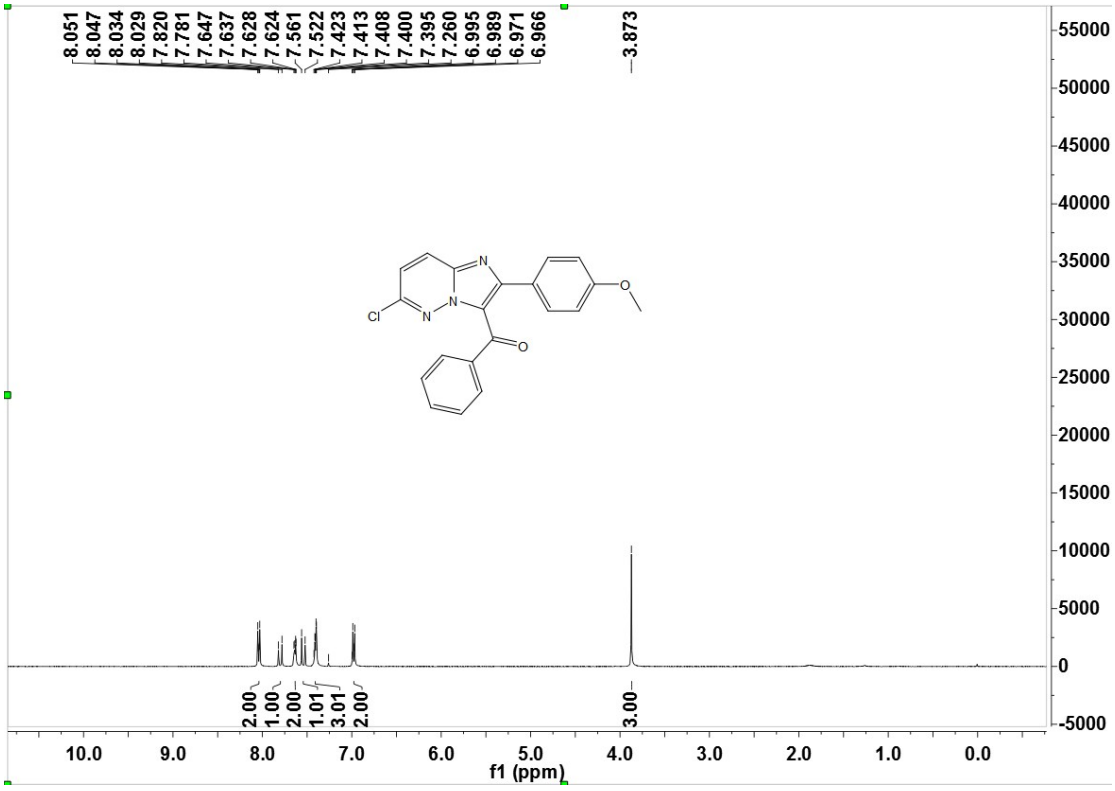
Method: C:\Xcalibur\methods\fs_sim

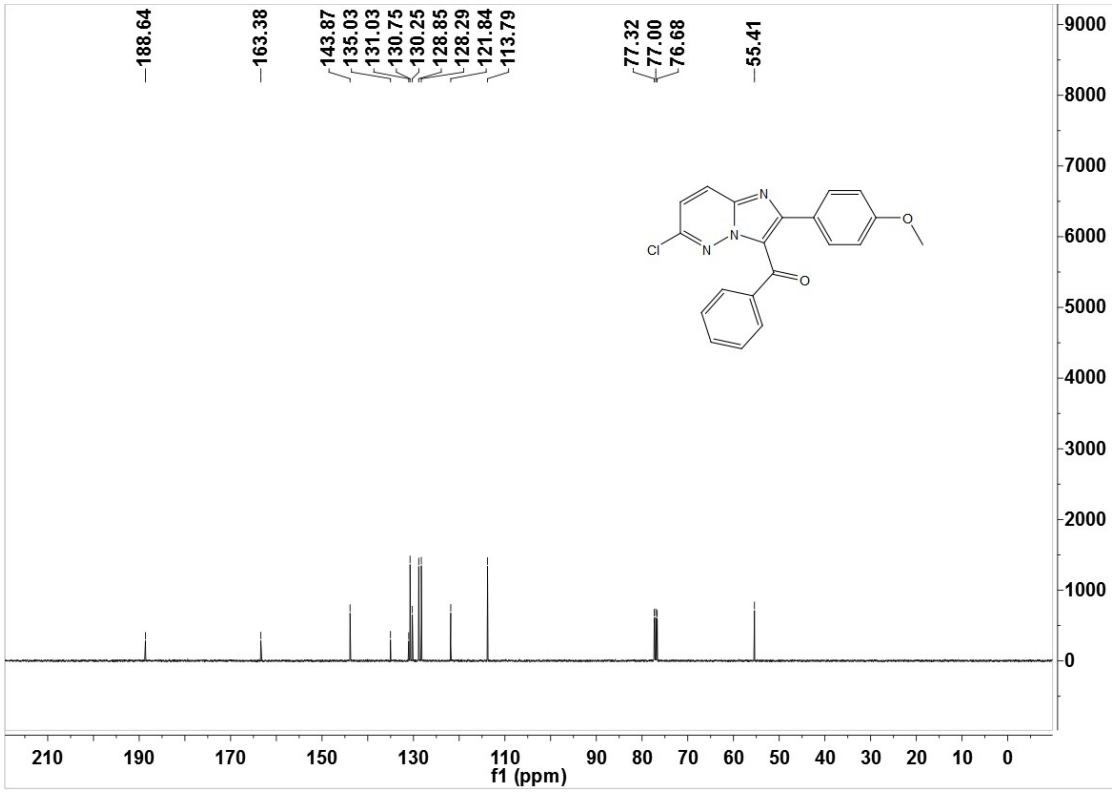
Assay: Assay name



Formula	Species	Composition	Expected m/z	Measured m/z	Delta m/z
C19H14N2O2S	+ Na	C19H14N2O2SNa	357.06682	357.06653	0.81

(6-Chloro-2-(4-methoxyphenyl)imidazo[1,2-b]pyridazin-3-yl)(phenyl)methanone (7c)





HRMS

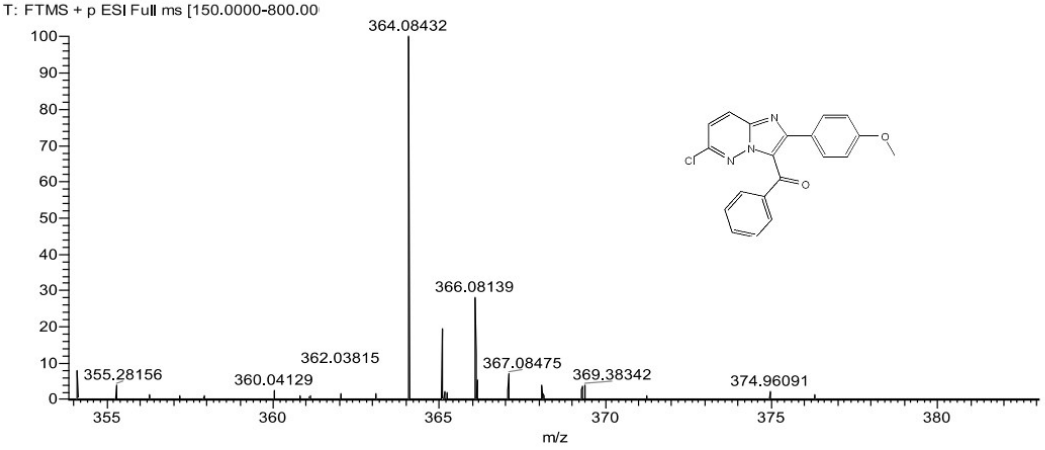
P

Mass Analysis Report

Batch:	/	**Lab Name:**	Default Laboratory
Method:	C:\Xcalibur\methods\fs_sim	**Assay:**	Assay name
Inst. Method:	/	**User:**	Thermo

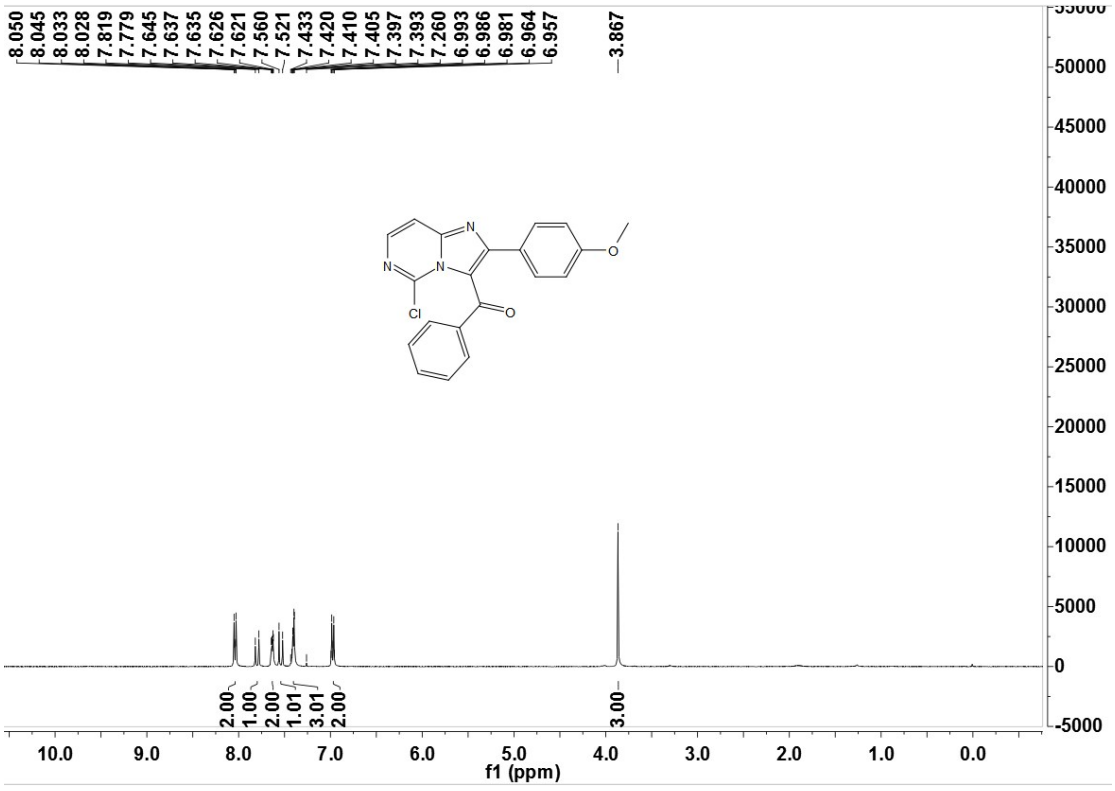
Sample ID	Raw File	Sample Type	Vial Position
	7C	Unknown	

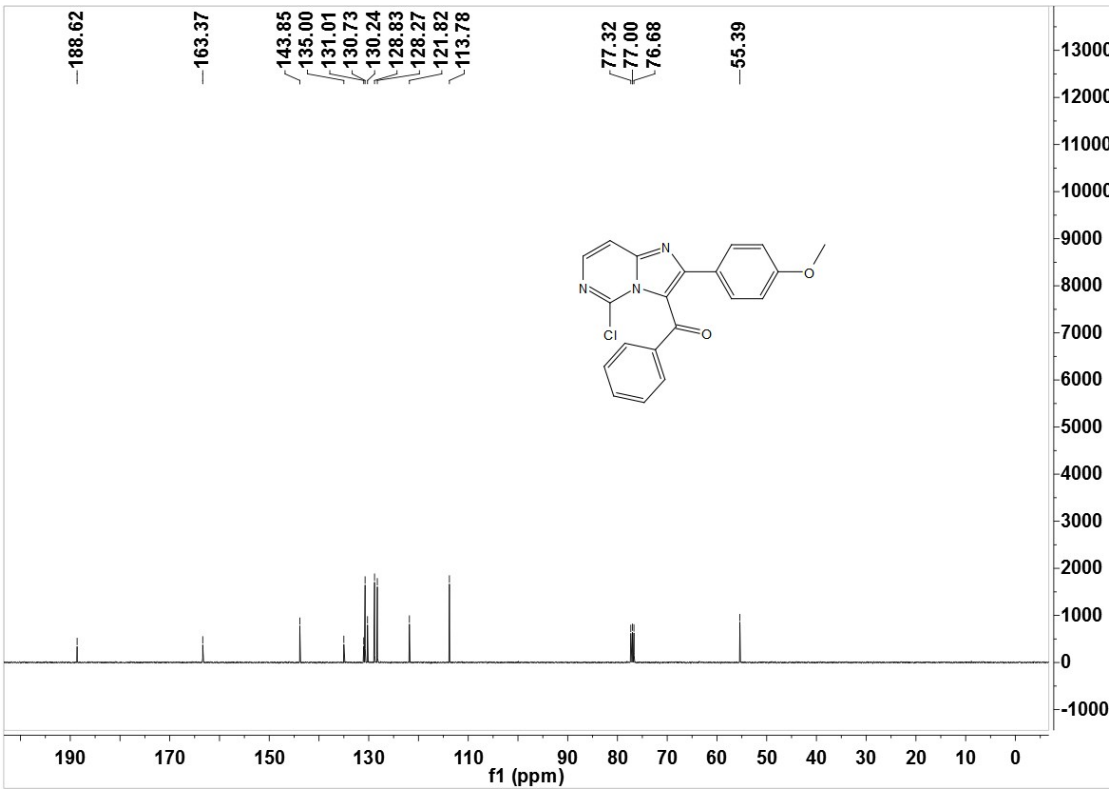
7C #3 RT: 0.01 AV: 1 NL: 3.67E6
T: FTMS + p ESI Full ms [150.0000-800.00



Formula	Species	Composition	Expected m/z	Measured m/z	Delta ppm
C20H14ClN3O2	+ H	C20H15ClN3O2	364.08473	364.08432	1.13

(5-Chloro-2-(4-methoxyphenyl)imidazo[1,2-c]pyrimidin-3-yl)(phenyl)methanone (7d)





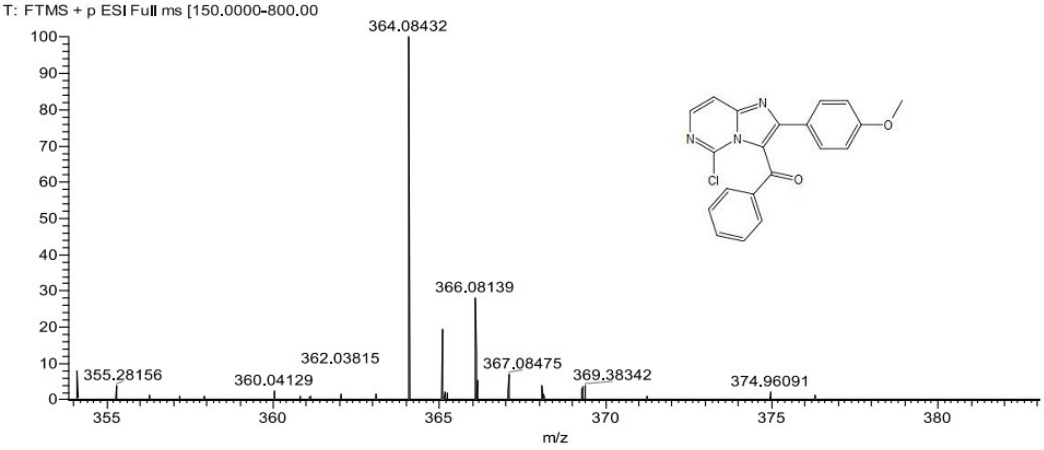
HRMS

Mass Analysis Report

Batch:	/	**Lab Name:**	Default Laboratory
Method:	C:\Xcalibur\methods\fs_sim	**Assay:**	Assay name
Inst. Method:	/	**User:**	Thermo

Sample ID	Raw File	Sample Type	Vial Position
	7C	Unknown	

7C #3 RT: 0.01 AV: 1 NL: 3.67E6
T: FTMS + p ESI Full ms [150.0000-800.00



Formula	Species	Composition	Expected m/z	Measured m/z	Delta ppm
C20H14ClN3O2	+ H	C20H15ClN3O2	364.08473	364.08432	1.13