Supplementary Information (SI) for RSC Medicinal Chemistry.
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Supporting Information

Design and synthesis of 7-azaindole derivatives as potent CDK8 inhibitors for the treatment of acute myeloid leukemia

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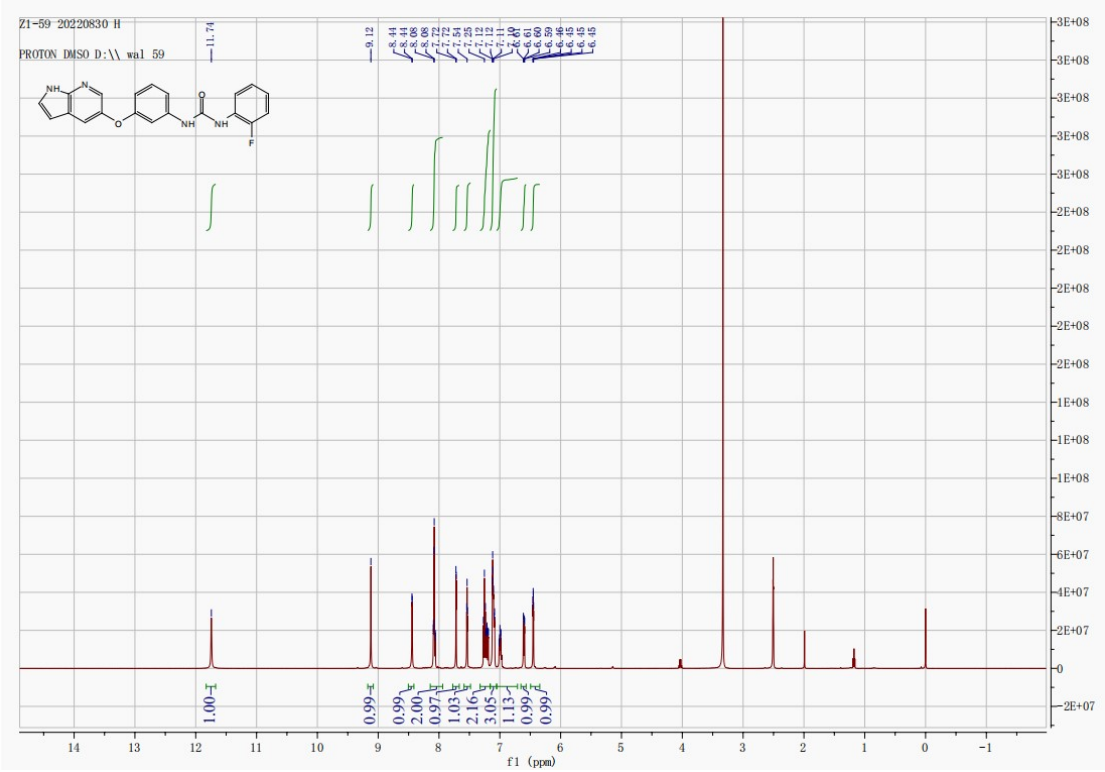
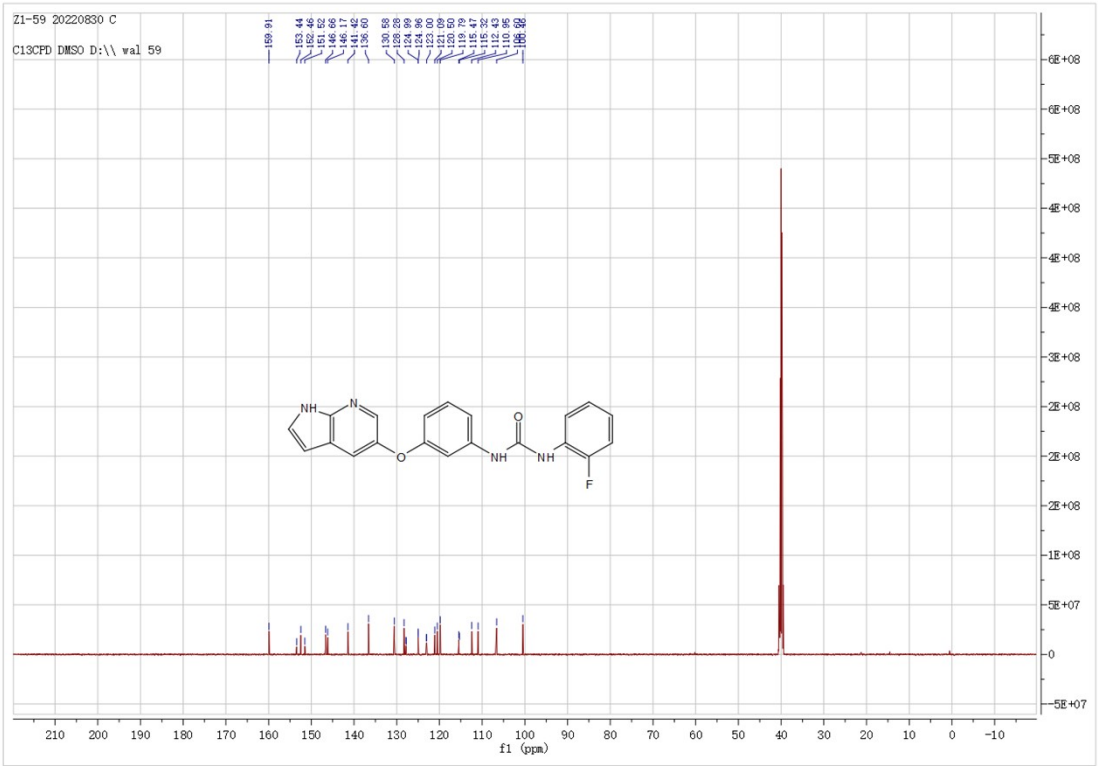
Contents

1. ^{1}H NMR, ^{13}C NMR, HRMS……S2

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(2-fluorophenyl)urea (**1**)



^{1}H NMR spectrum of **1**



^{13}C NMR spectrum of **1**

9

Sample Name	WYM-2022-1129-25	**Position**	Vial 59	**Instrument Name**	Instrument 1	**User Name**	
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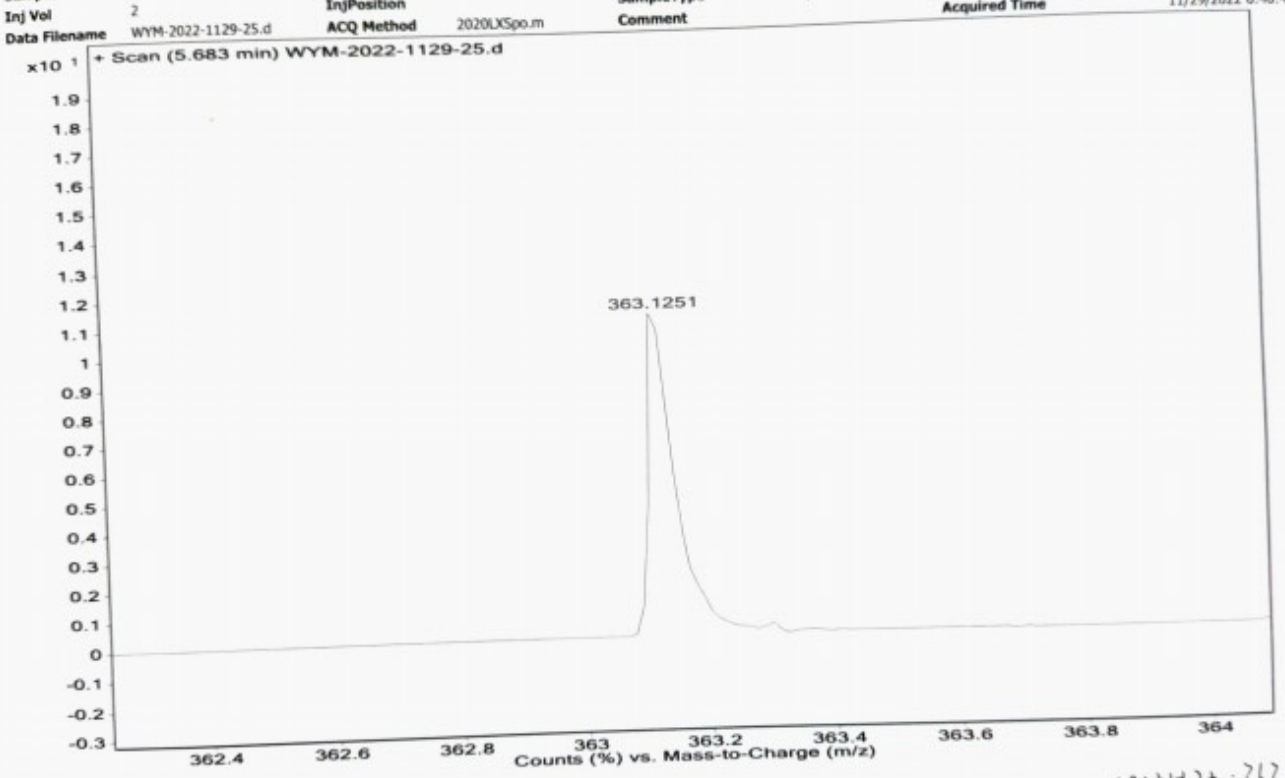


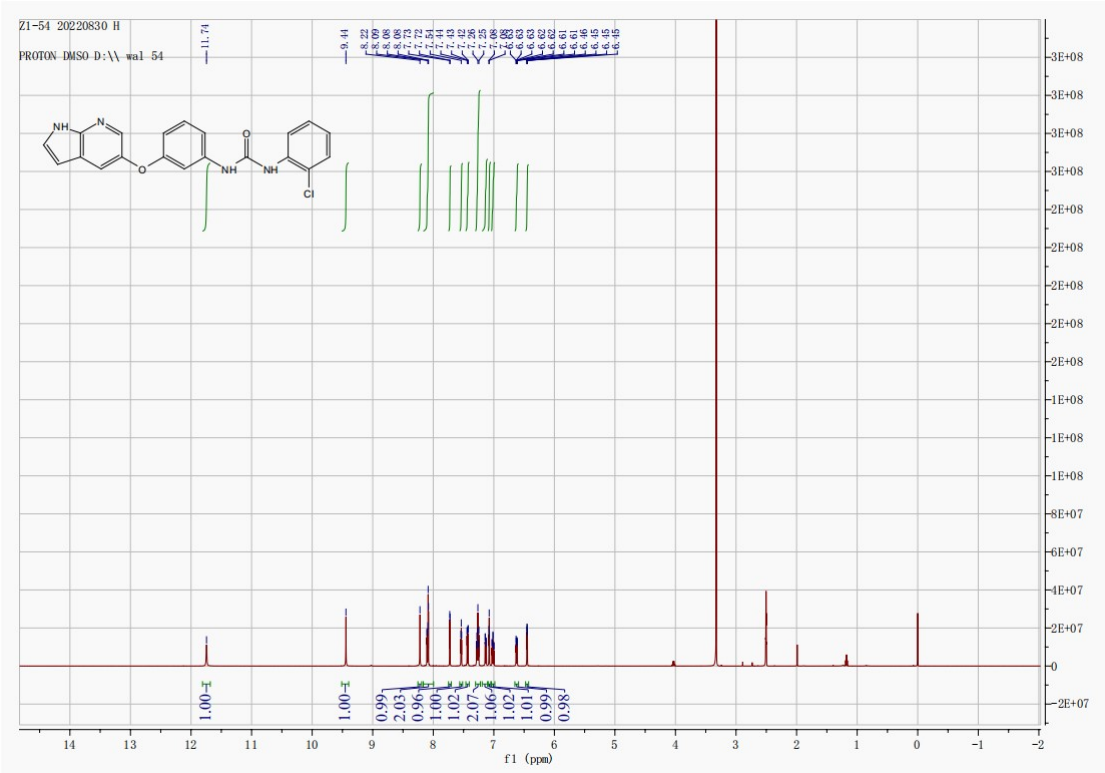
$(M+H)^+$: 363.1252

$C_{20}H_{15}F_4N_4O_2$

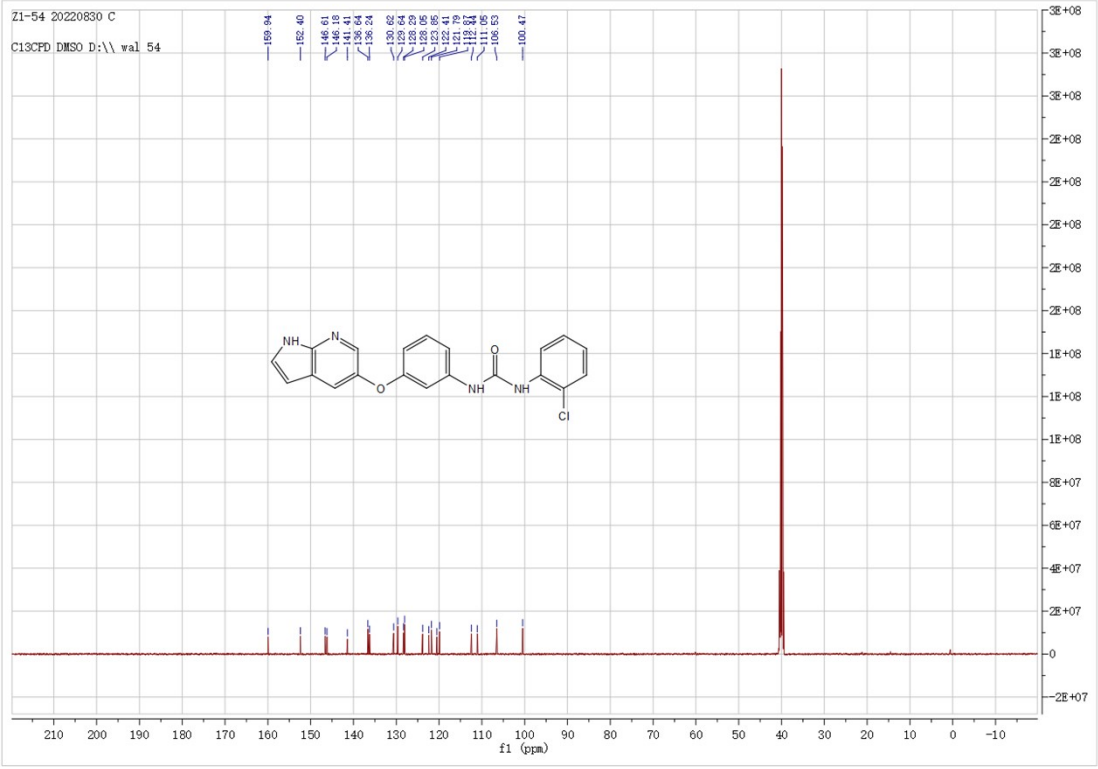
0759-3

HRMS (ESI) spectrum of **1**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(2-chlorophenyl)urea (**2**)



^{1}H NMR spectrum of **2**



^{13}C NMR spectrum of **2**

Sample Name	WQ-1129-14	**Position**	Vial 54	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
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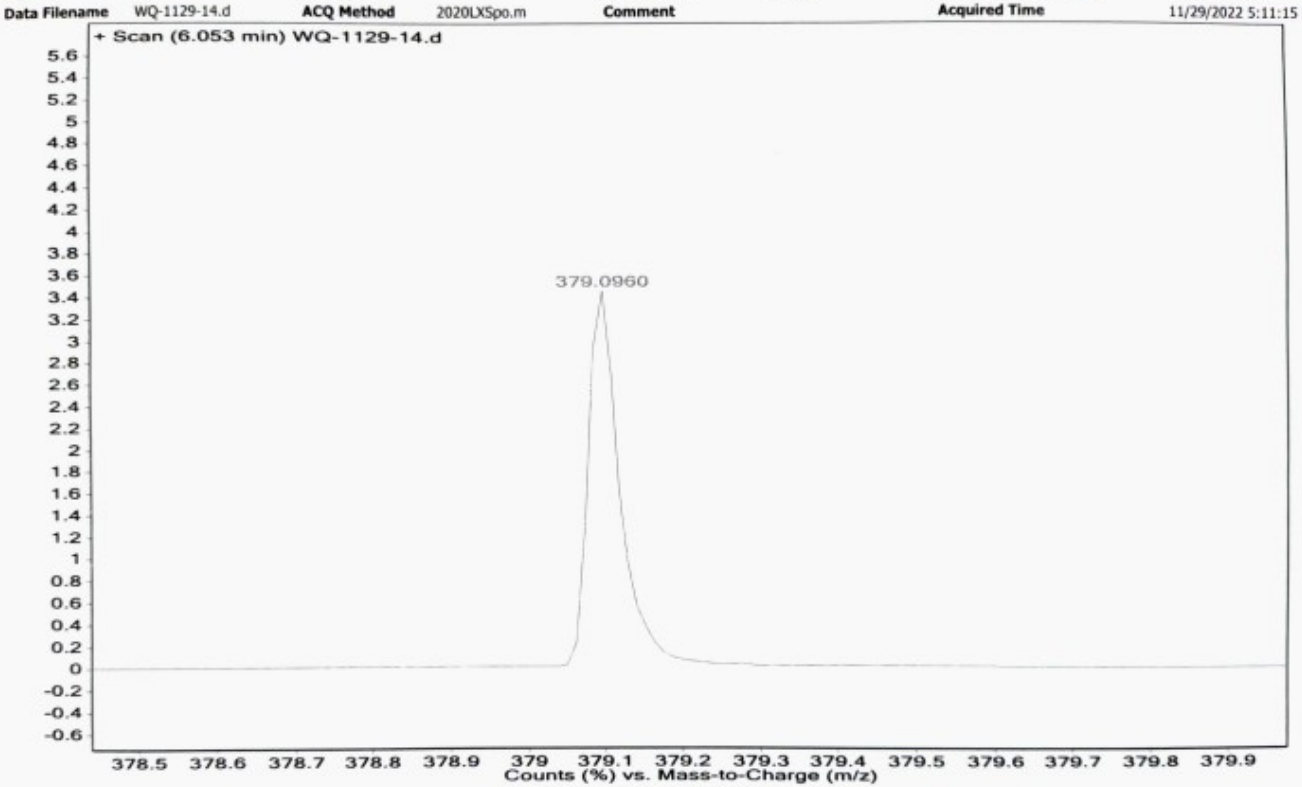
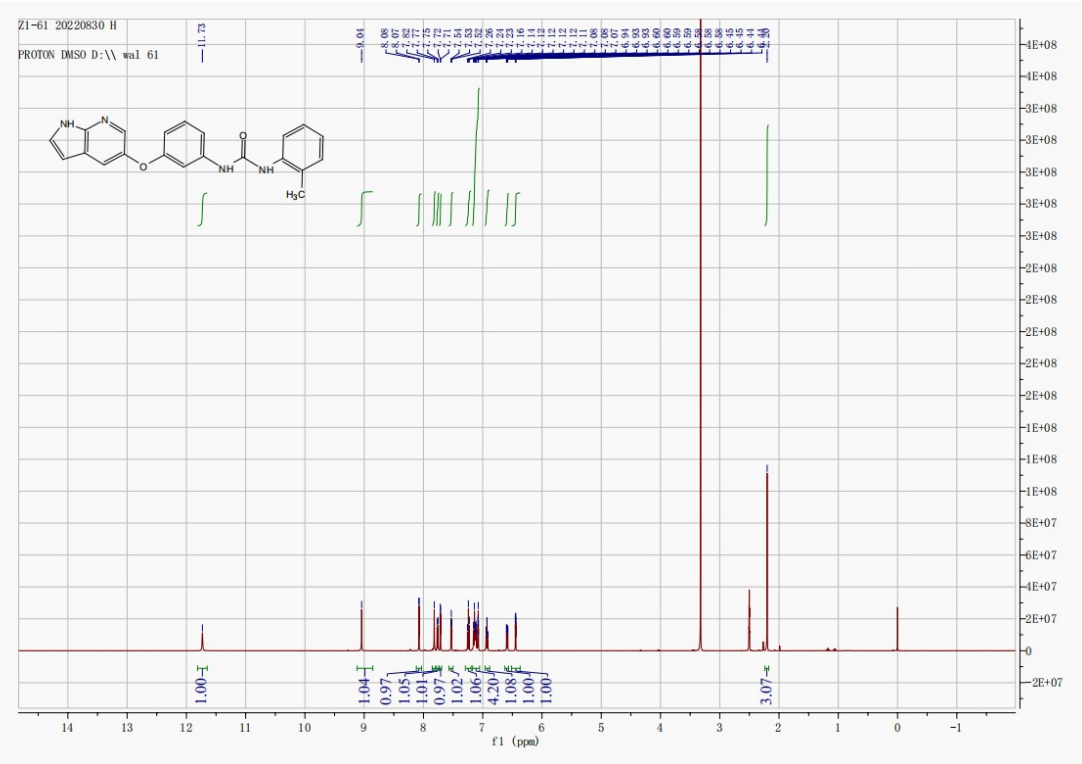


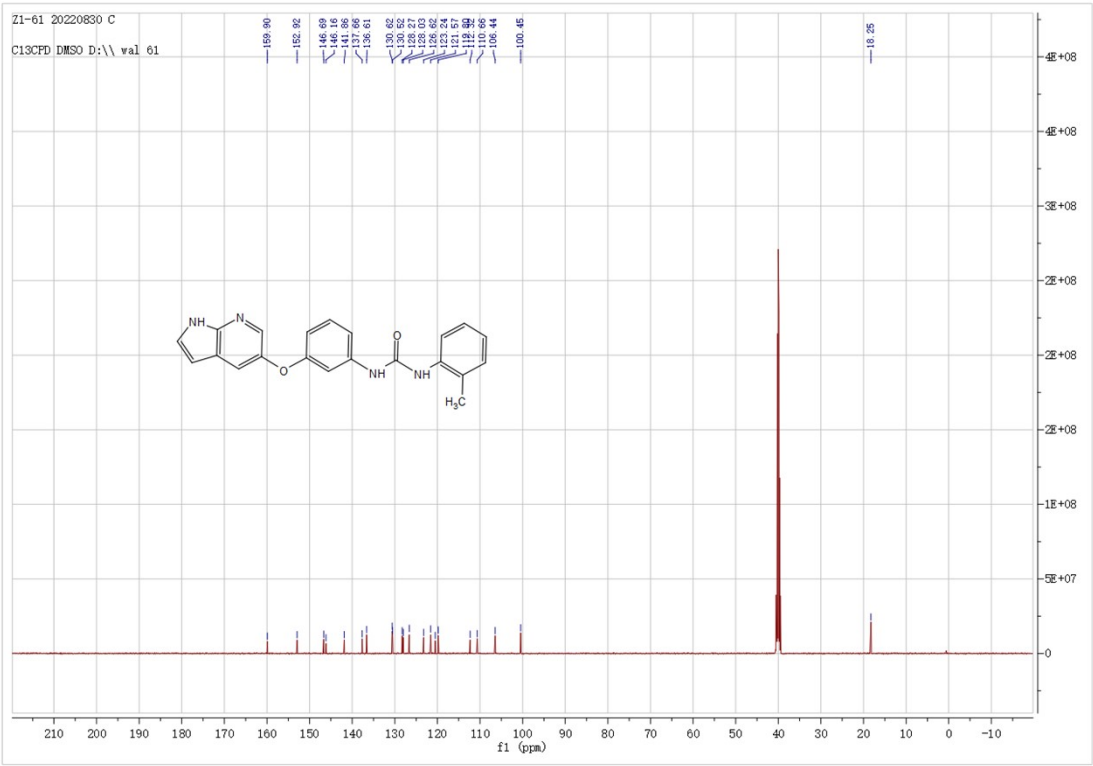
(M+H)+ : 379.0956
0704-4
$C_{20}H_{15}ClN_4O_2$

HRMS (ESI) spectrum of **2**

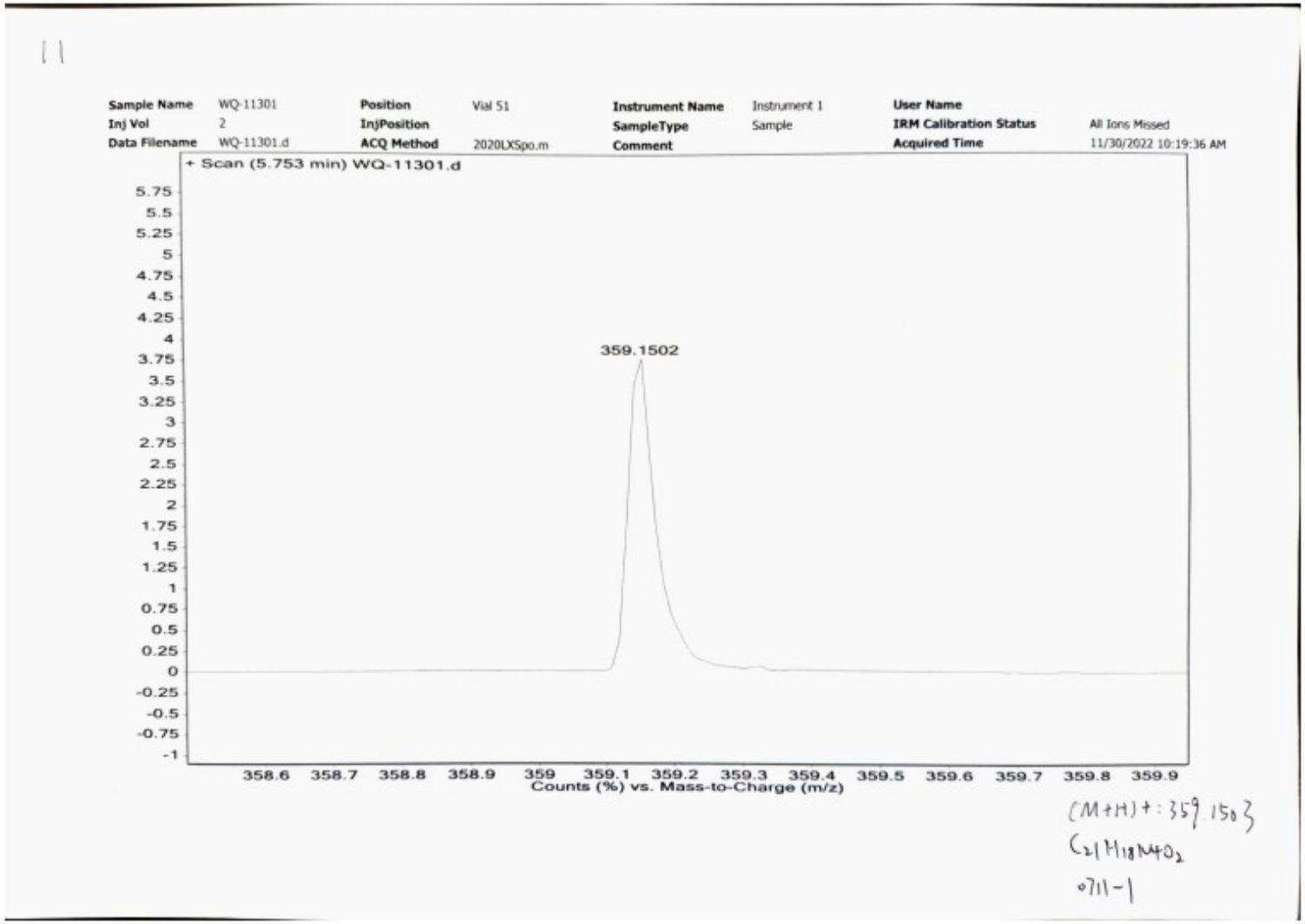
1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(2- methylphenyl)urea (**3**)



^{1}H NMR spectrum of**3**

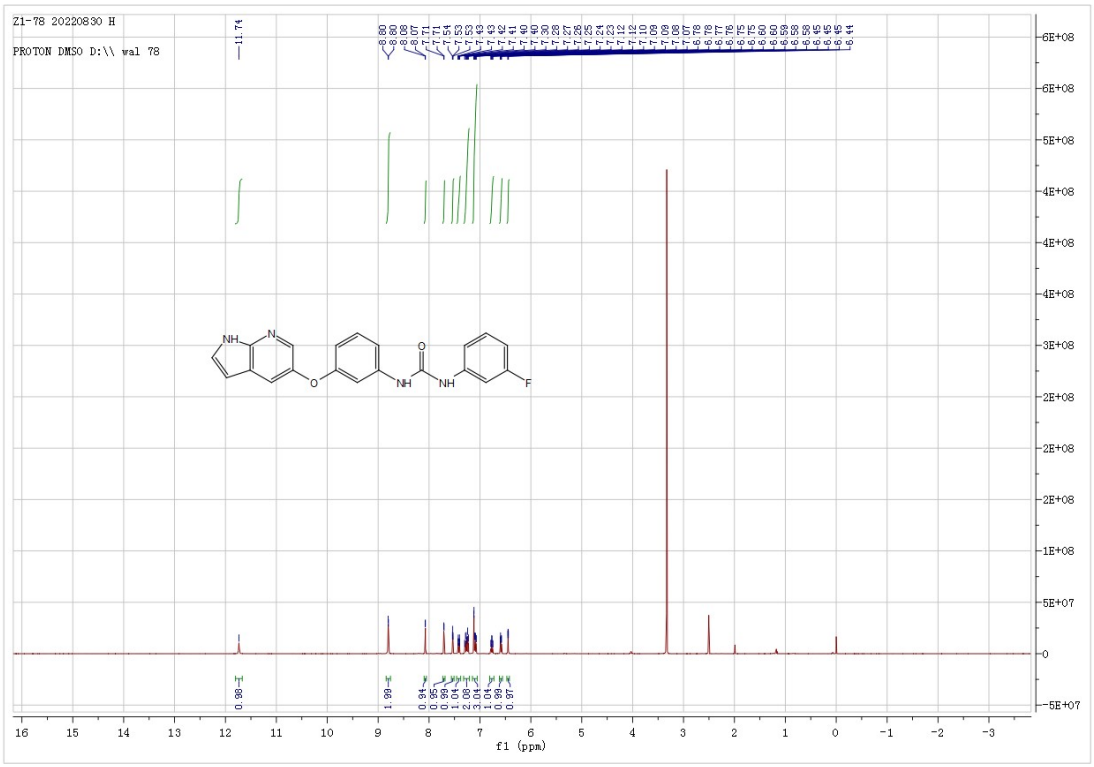


^{13}C NMR spectrum of **3**

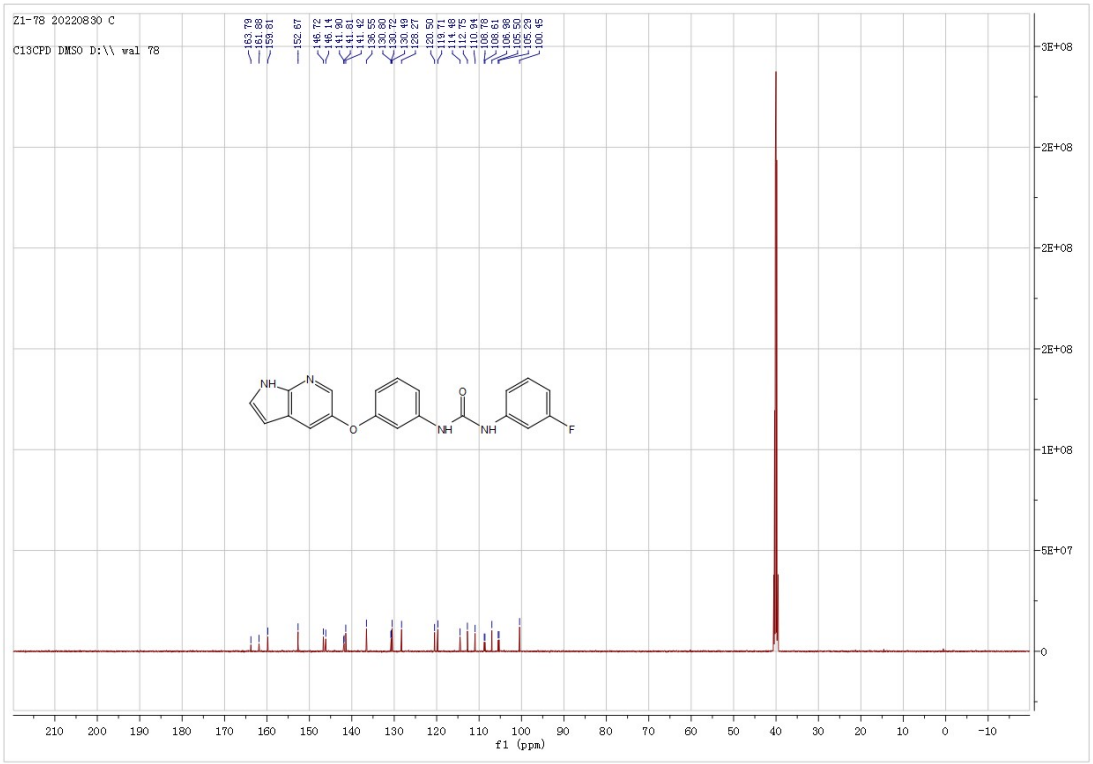


HRMS (ESI) spectrum of **3**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-fluorophenyl)urea (**4**)



^{1}H NMR spectrum of **4**



^{13}C NMR spectrum of **4**

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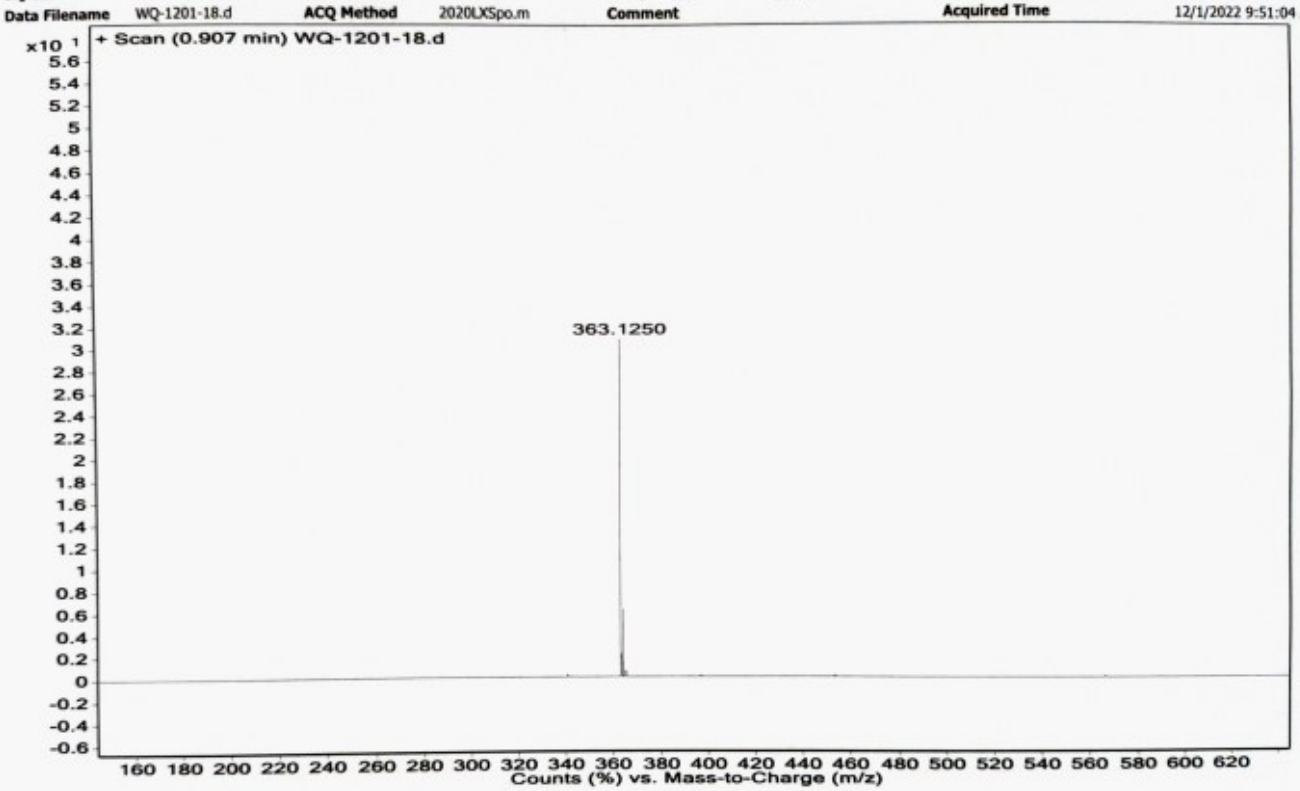


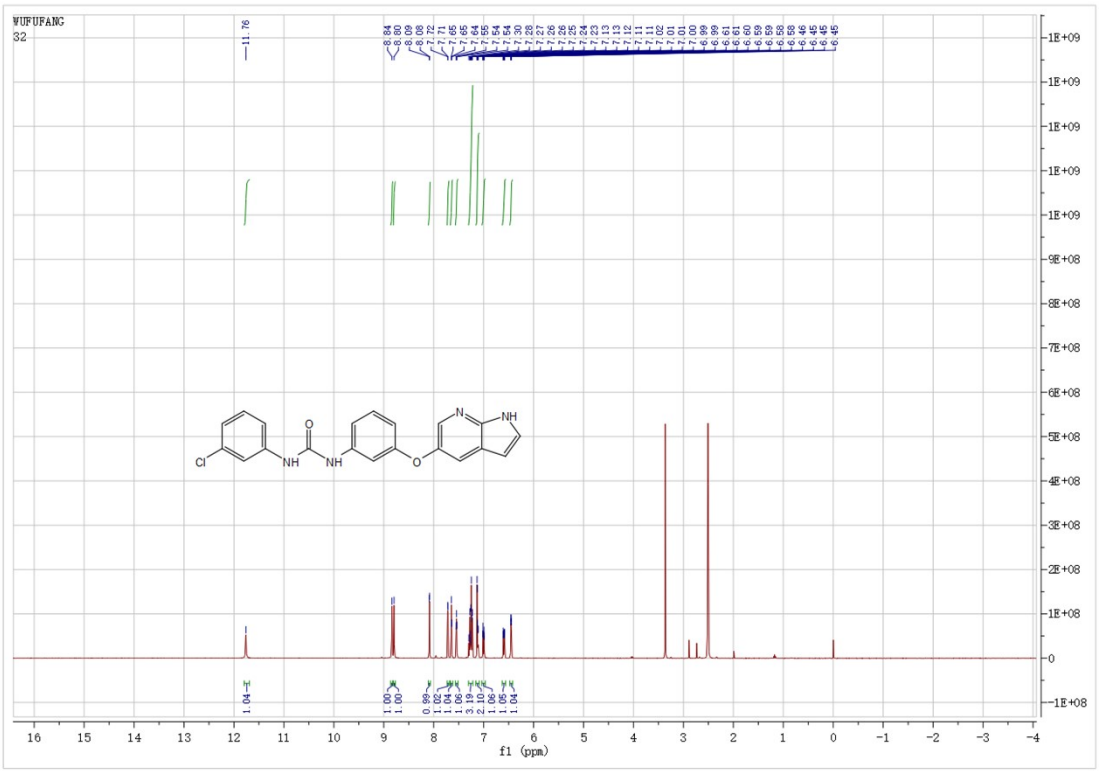
$(M+H)^+$: 363.1252

$C_{20}H_{15}FN_4O_2$

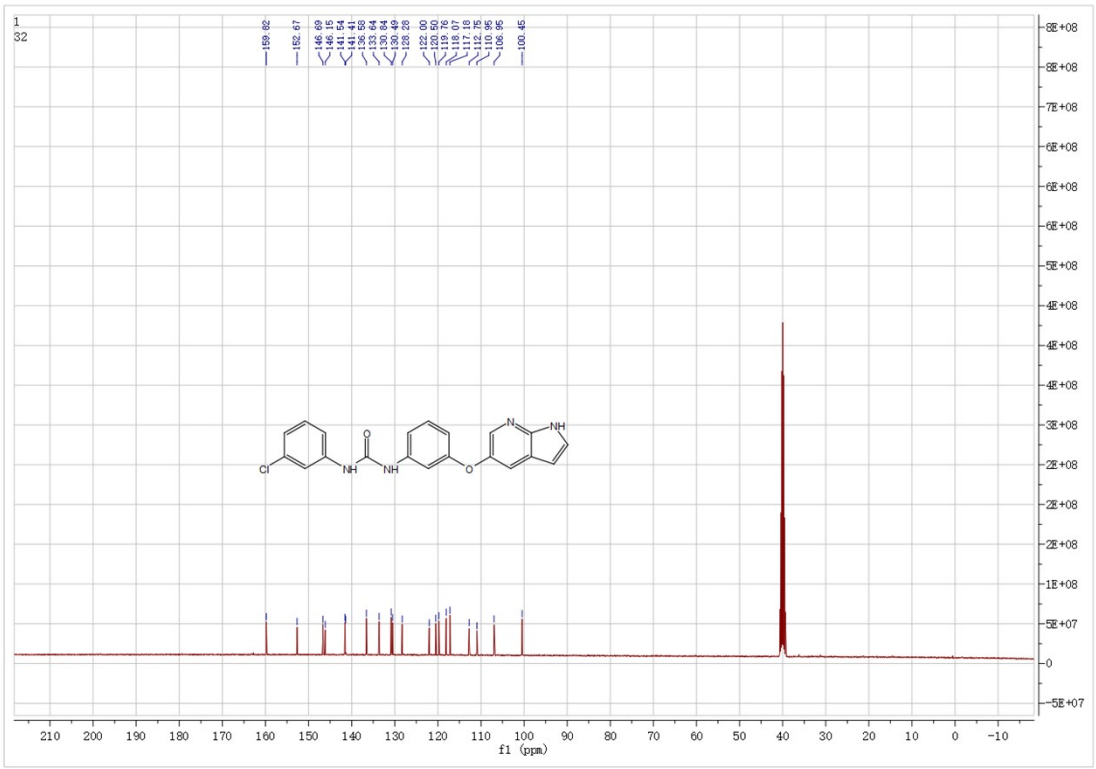
0721-4

HRMS (ESI) spectrum of **4**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-chlorophenyl)urea (**5**)



^{1}H NMR spectrum of **5**



^{13}C NMR spectrum of **5**

HRMS (ESI) spectrum of **5**

Sample Name	ZXX-2022-0321-113	**Position**	Vial 13	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
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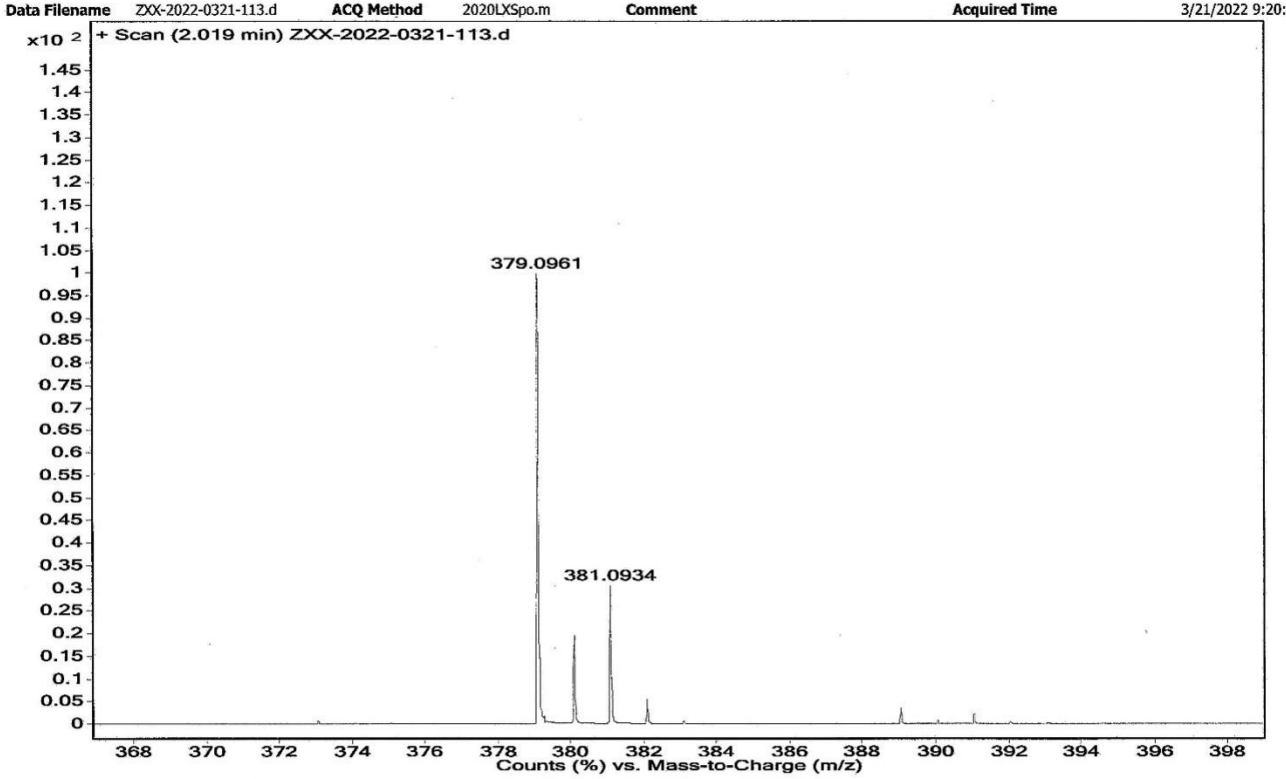
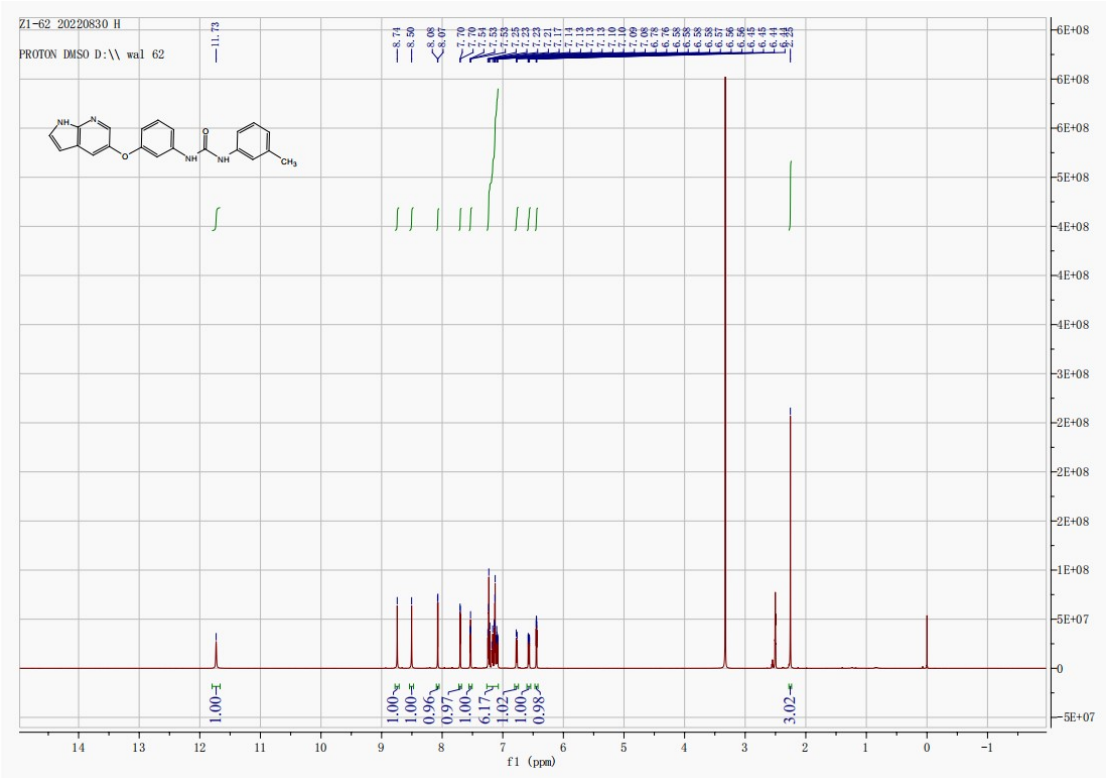
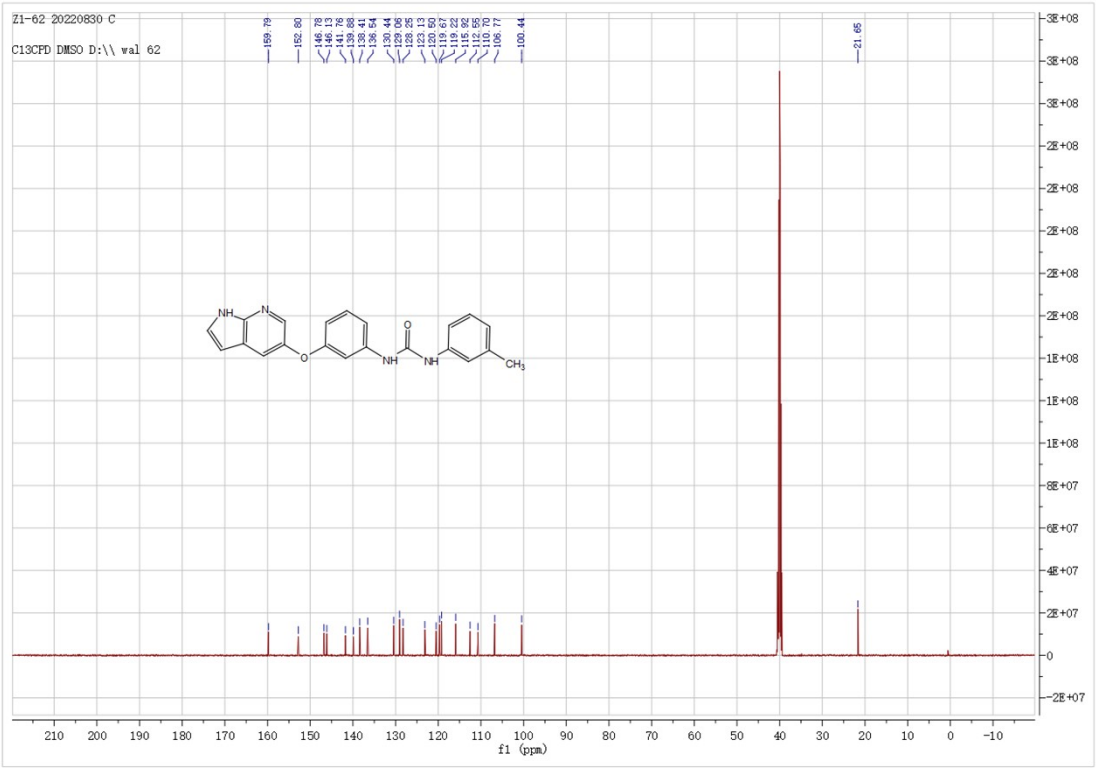


0321-1

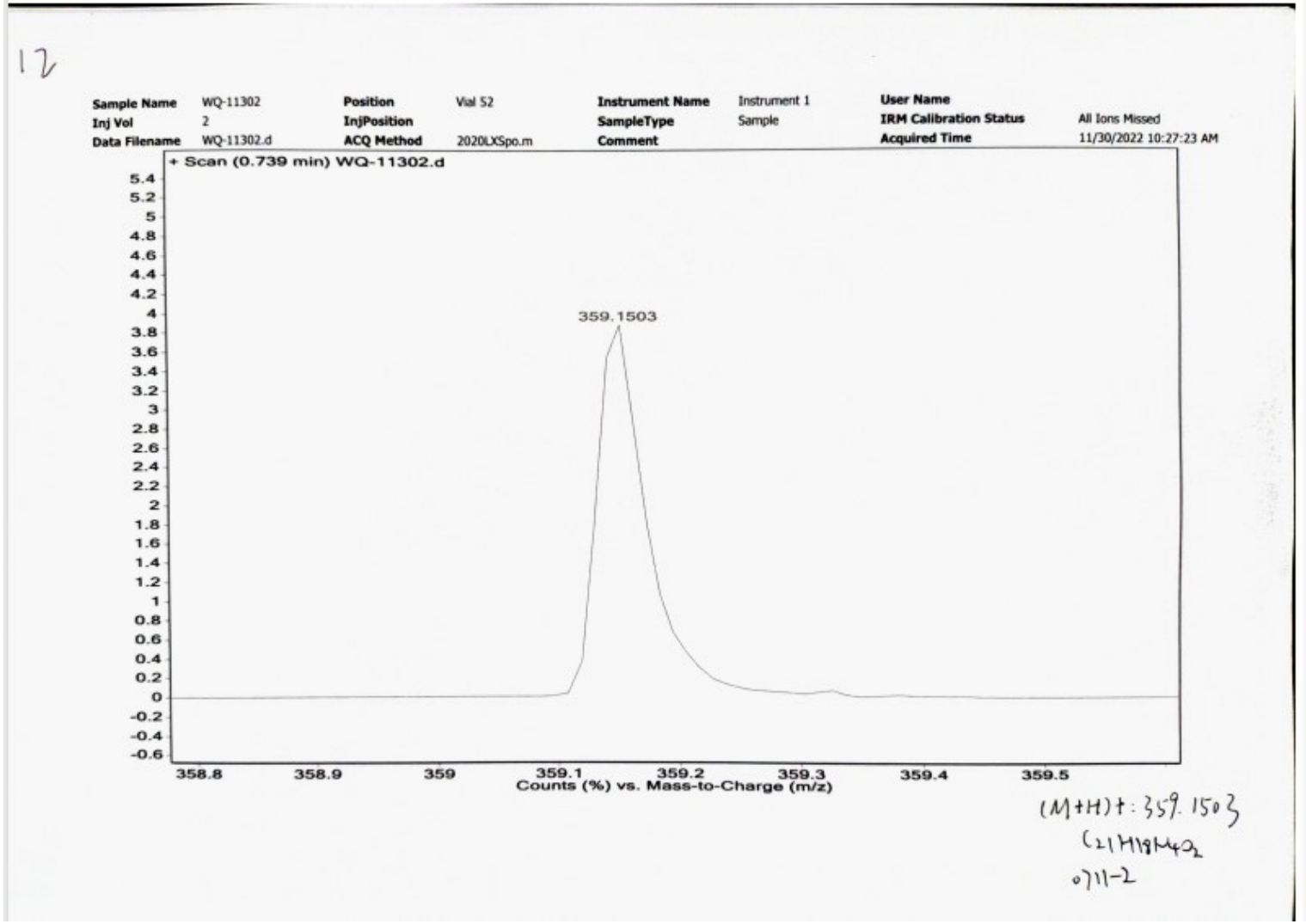
1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-methylphenyl)urea (**6**)



^{1}H NMR spectrum of **6**



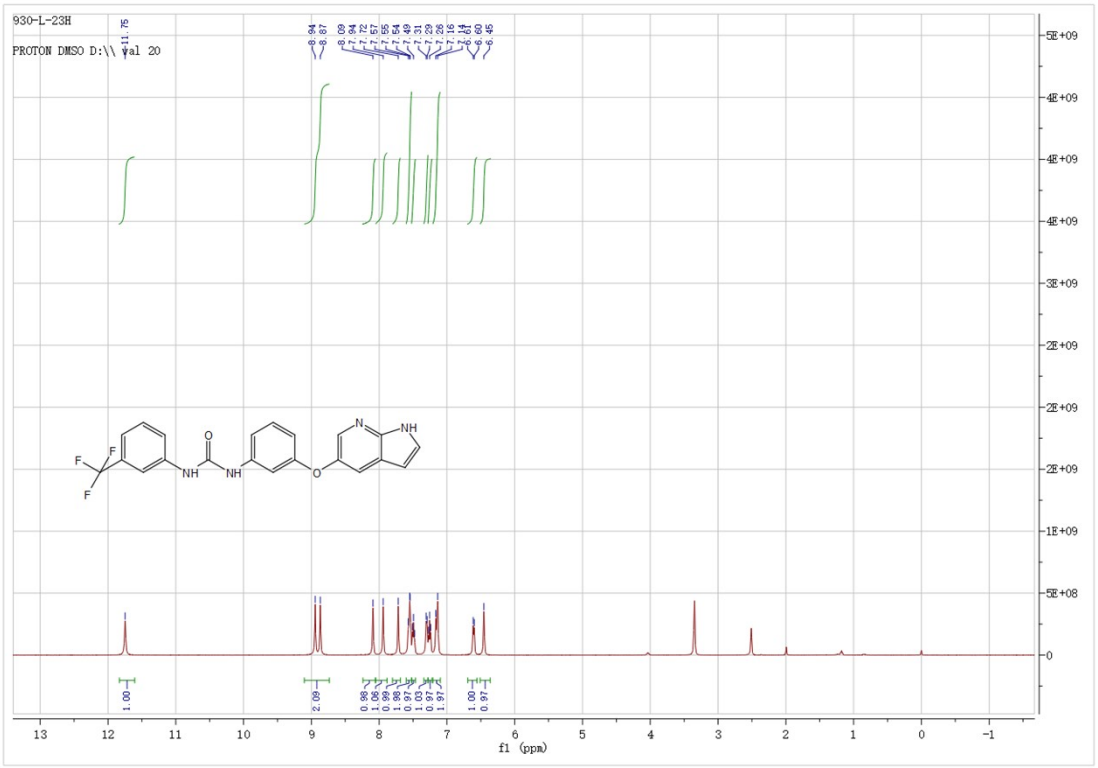
^{13}C NMR spectrum of **6**



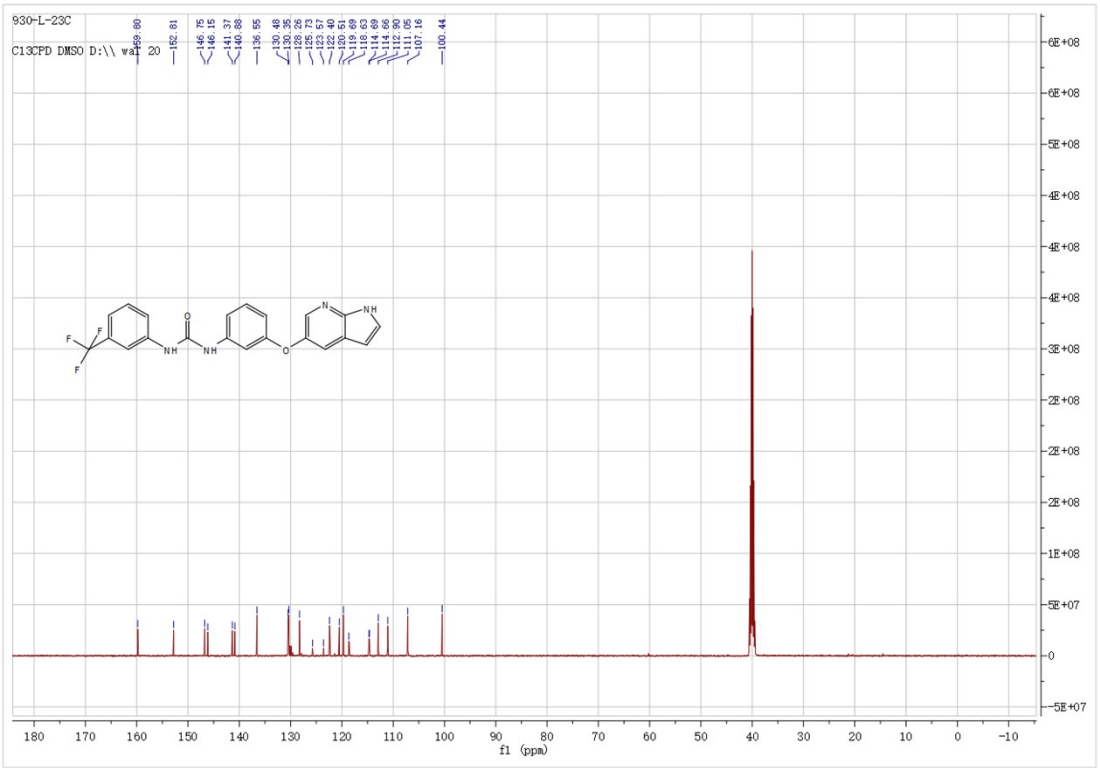
HRMS (ESI) spectrum of **6**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-(trifluoromethyl)phenyl)urea

(**7**)



^{1}H NMR spectrum of **7**



^{13}C NMR spectrum of **7**

HRMS (ESI) spectrum of **7**

Sample Name	zxx-0630-11	Position	Vial 41	Instrument Name	Instrument 1	User Name	
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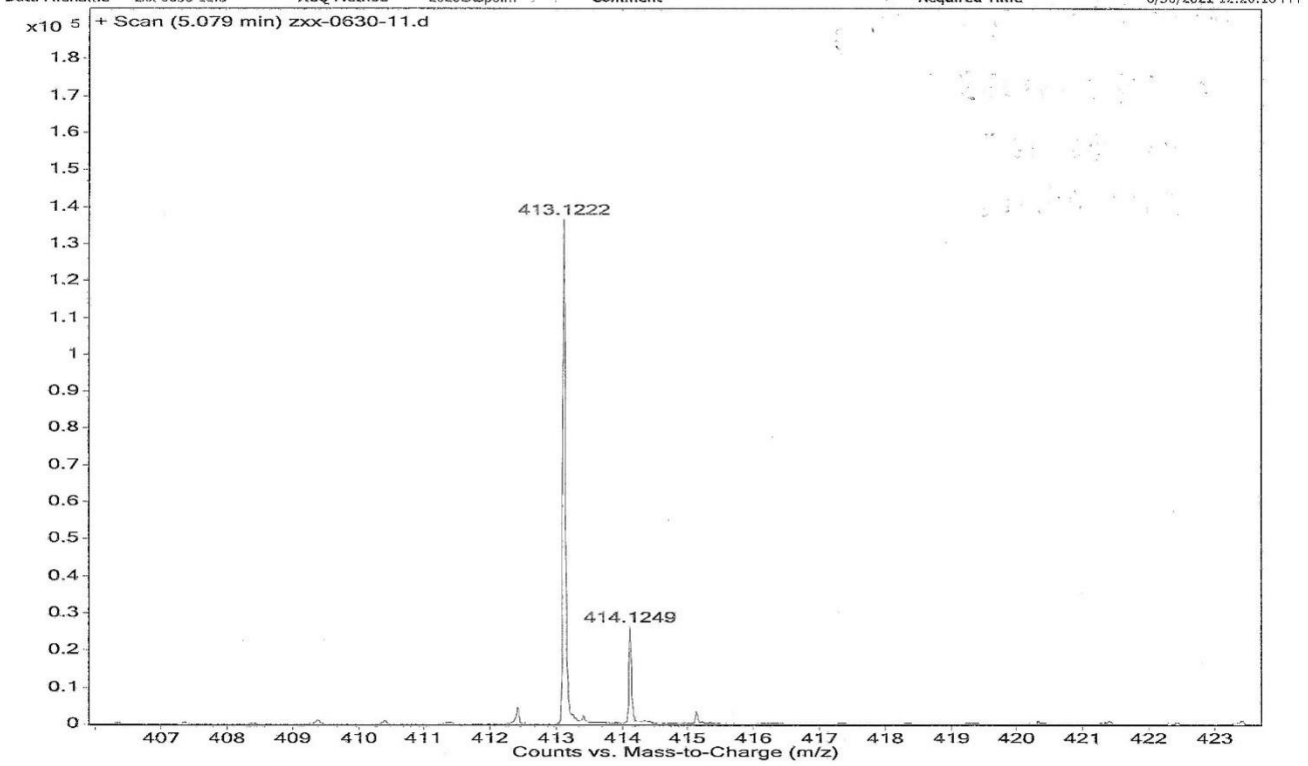
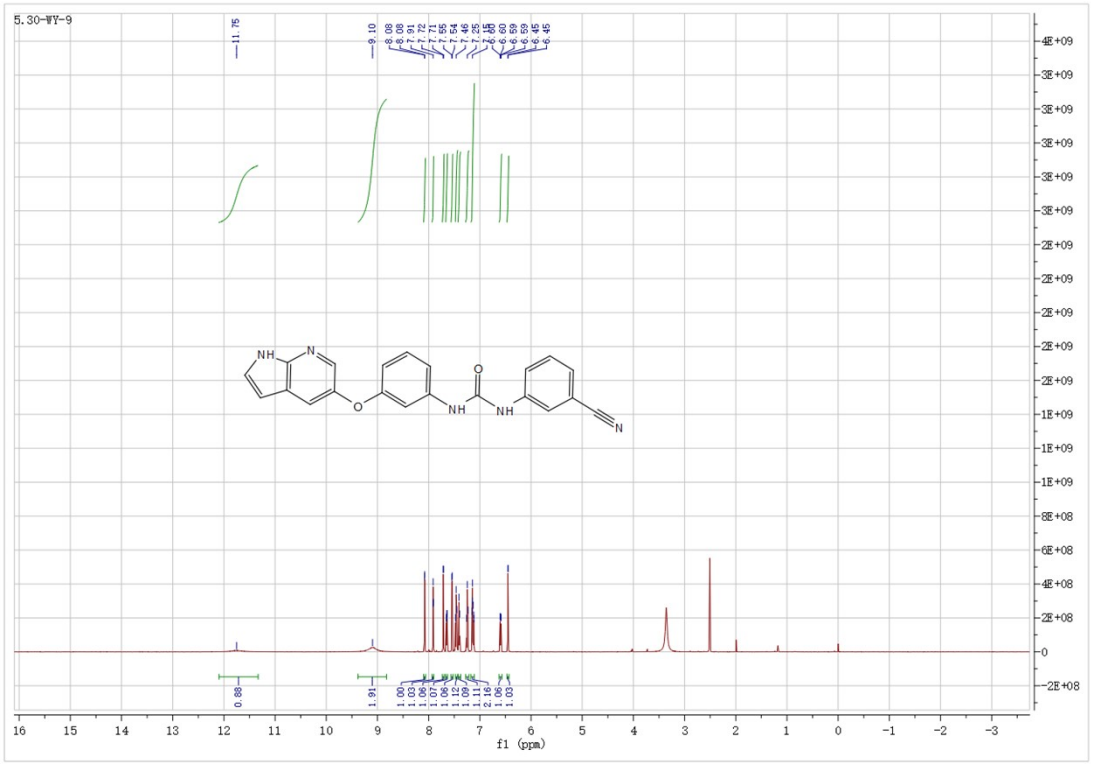
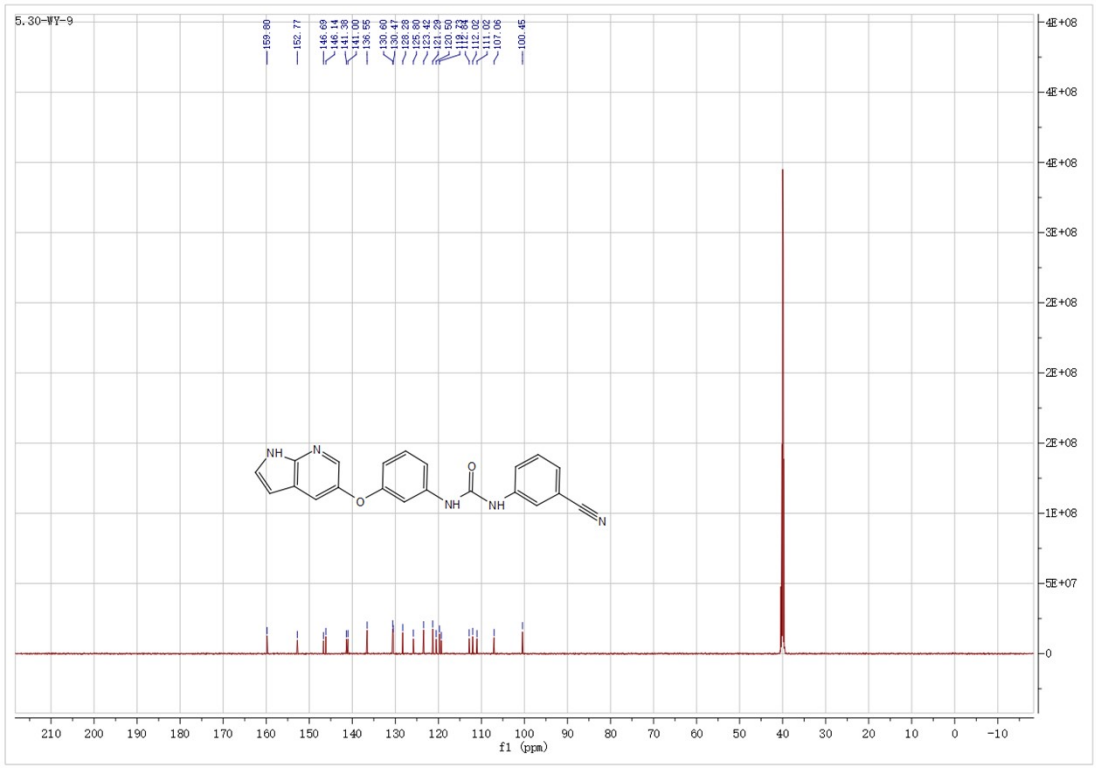


0676-2

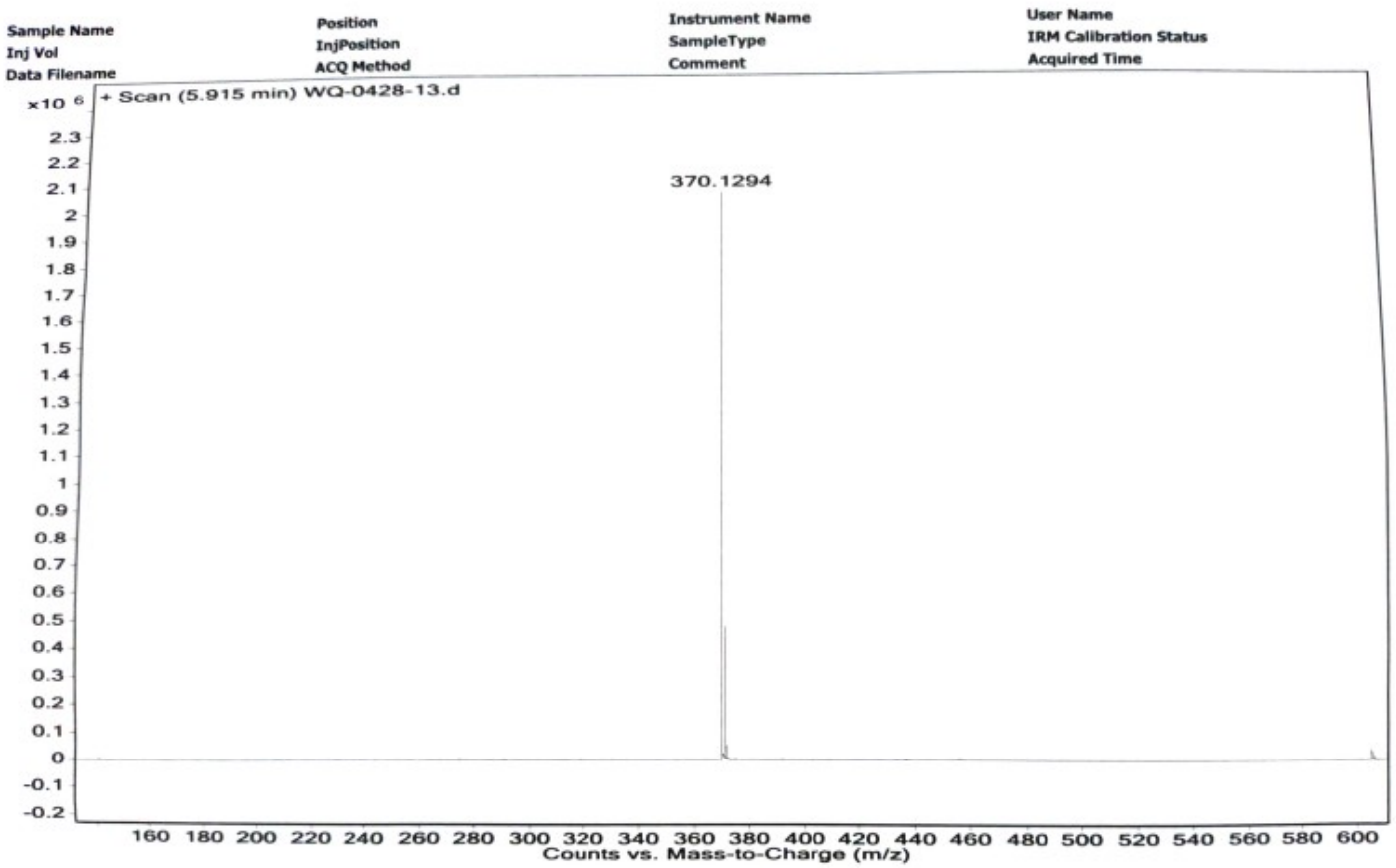
1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-cyanophenyl)urea (**8**)



^{1}H NMR spectrum of **8**



^{13}C NMR spectrum of **8**

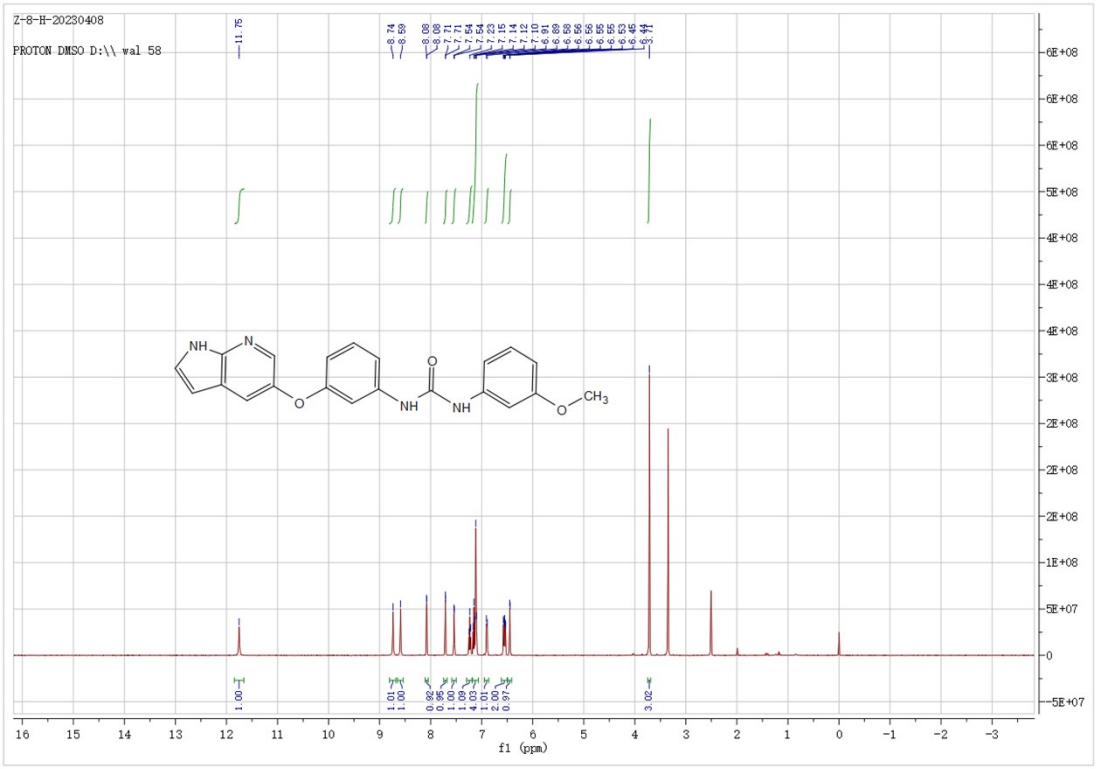


0316-3

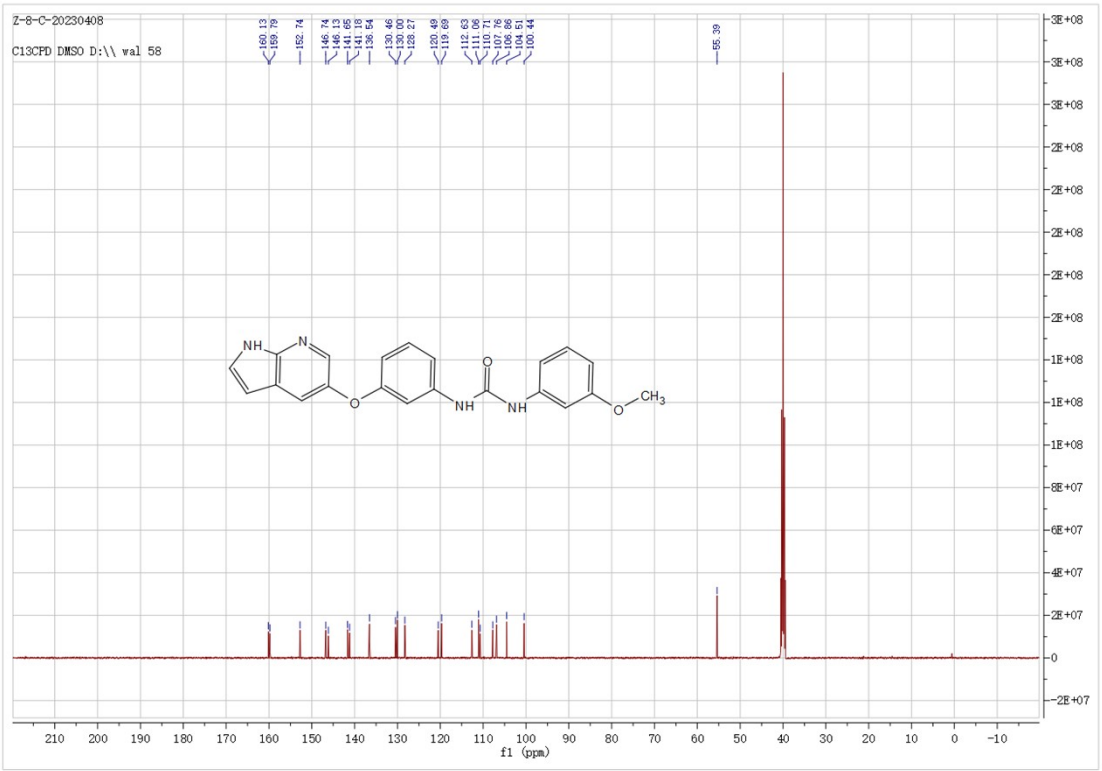
화합식 : $C_{21}H_{15}O_2N_3$

이론분자량 : 370.1299

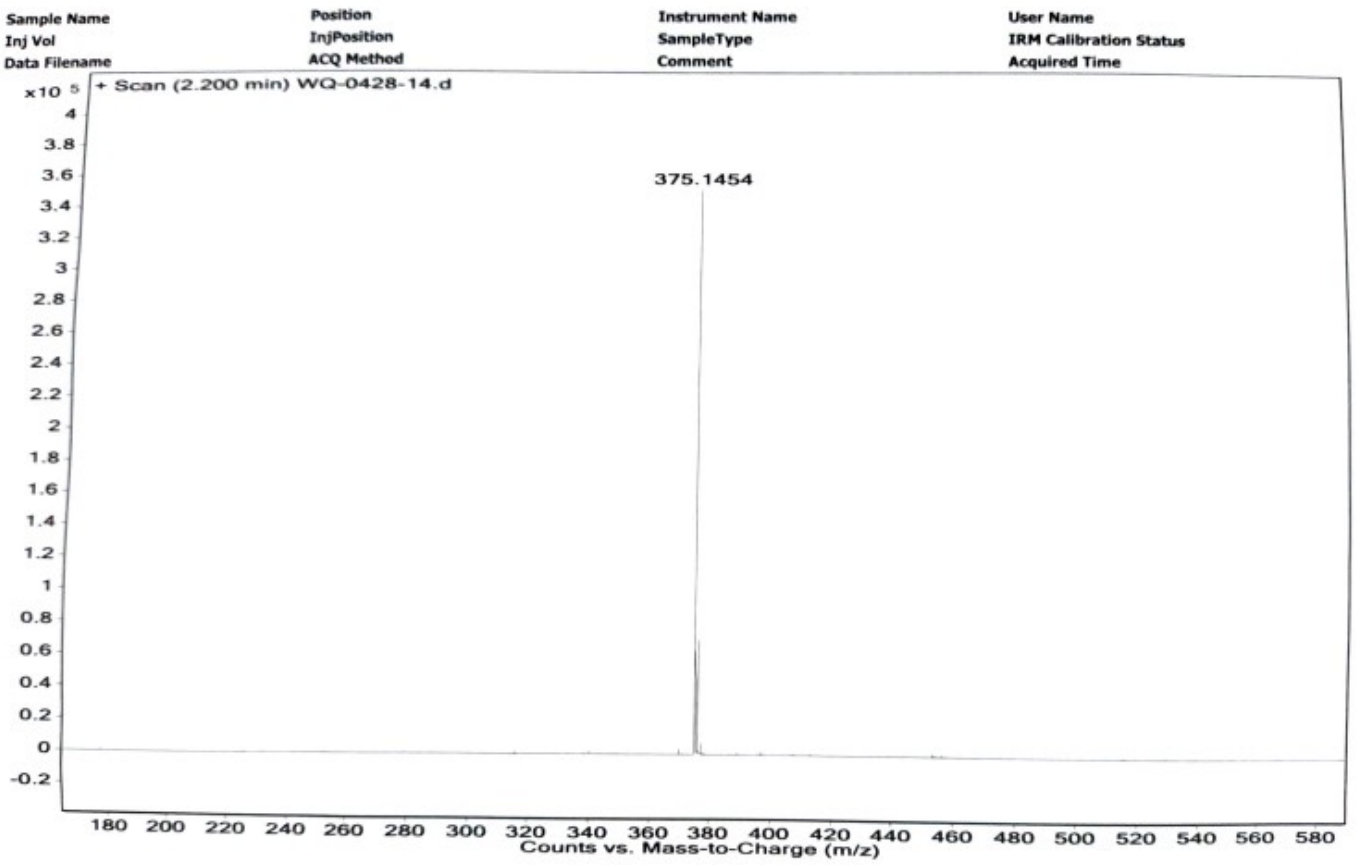
1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-methoxyphenyl)urea (**9**)



^{1}H NMR spectrum of **9**



^{13}C NMR spectrum of **9**



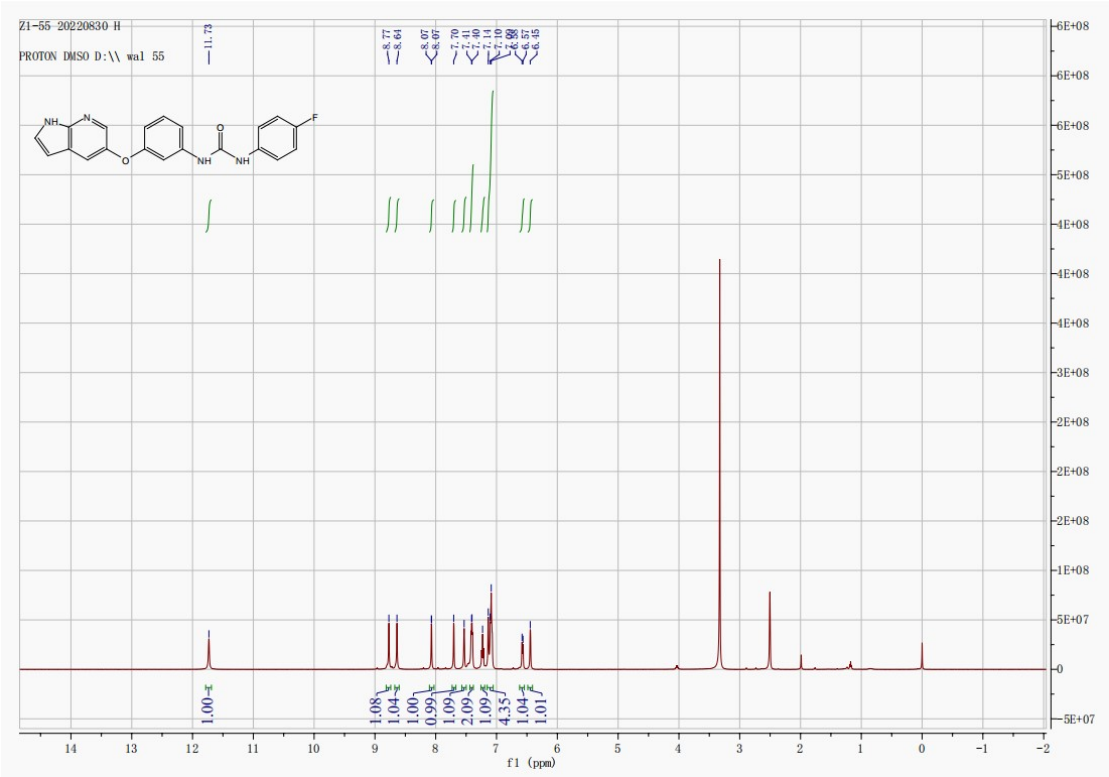
HRMS (ESI) spectrum of **9**

0316-4

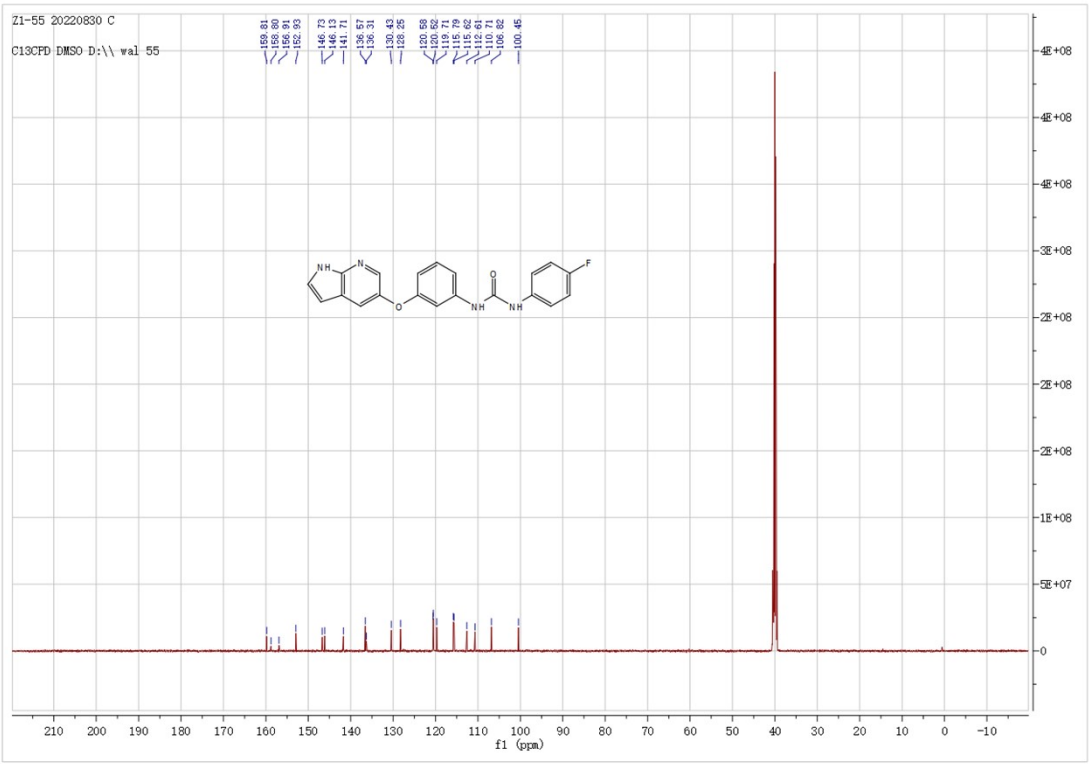
分子式：$C_{21}H_{18}O_3N_4$

分子量：375.1452

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-fluorophenyl)urea (**10**)



^{1}H NMR spectrum of **10**



^{13}C NMR spectrum of **10**

5

Sample Name	WYM-2022-1129-21	**Position**	Vial 55	**Instrument Name**	Instrument 1	**User Name**	
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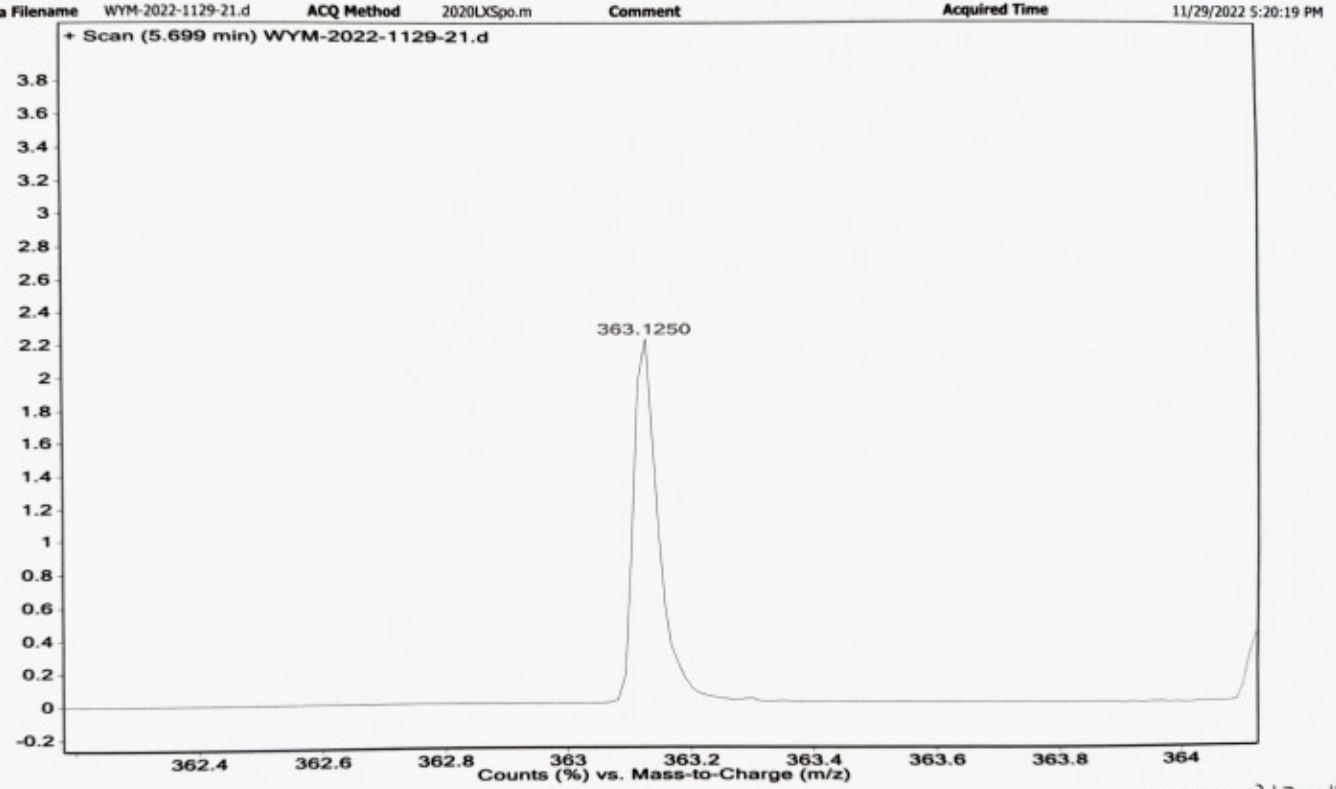


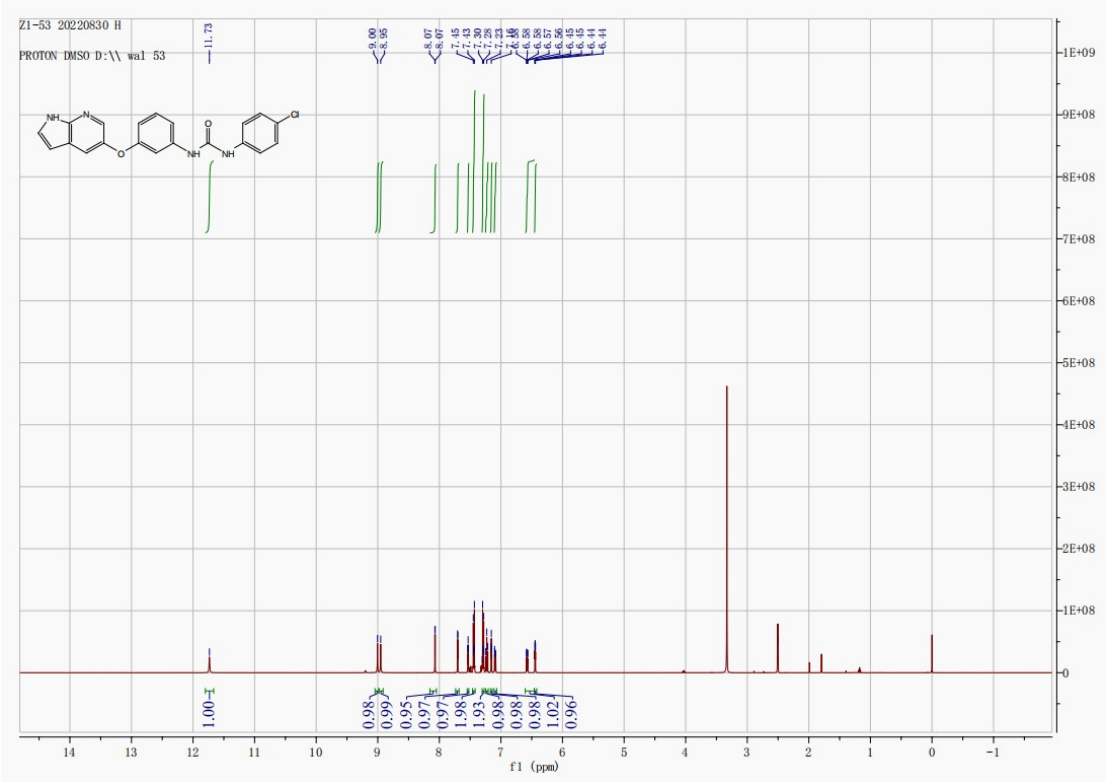
$(M+H)^+$: 363.1252

07084

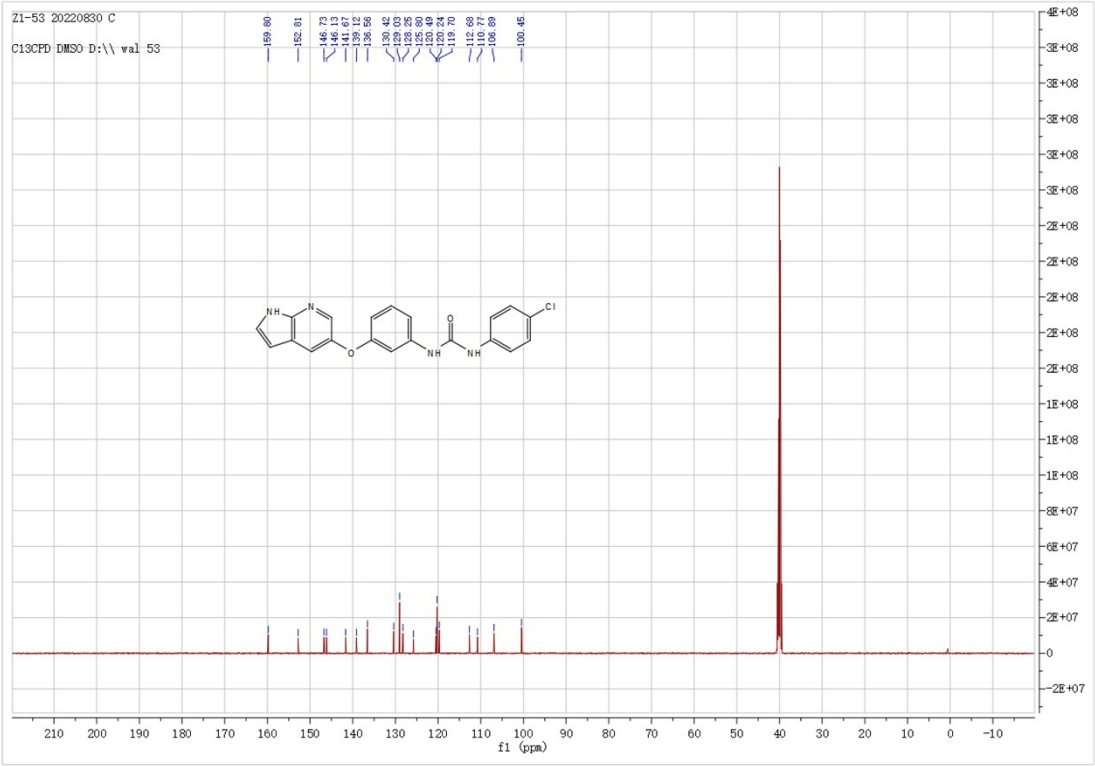
$C_{20}H_{15}FN_4O_2$

HRMS (ESI) spectrum of **10**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-chlorophenyl)urea (**11**)



^{1}H NMR spectrum of **11**



^{13}C NMR spectrum of **11**

3

Sample Name	WQ-1129-13	**Position**	Vial 53	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
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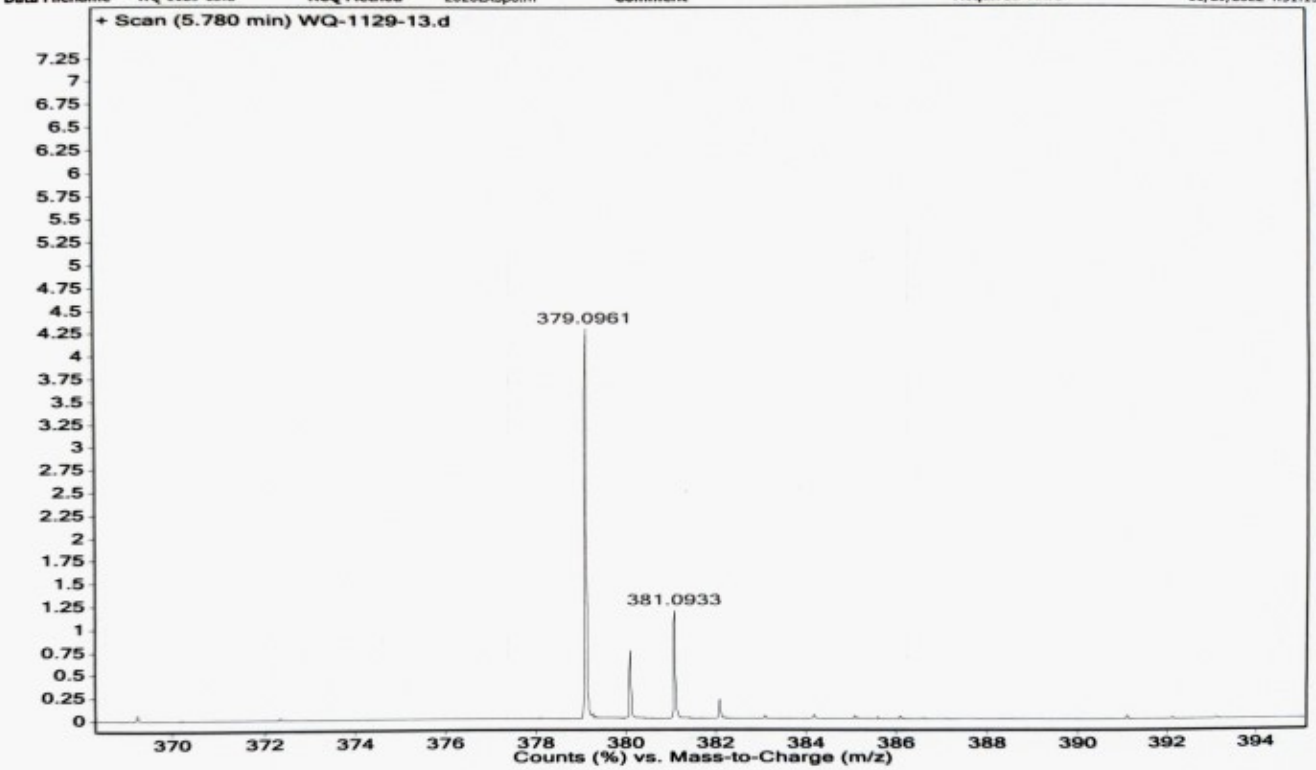
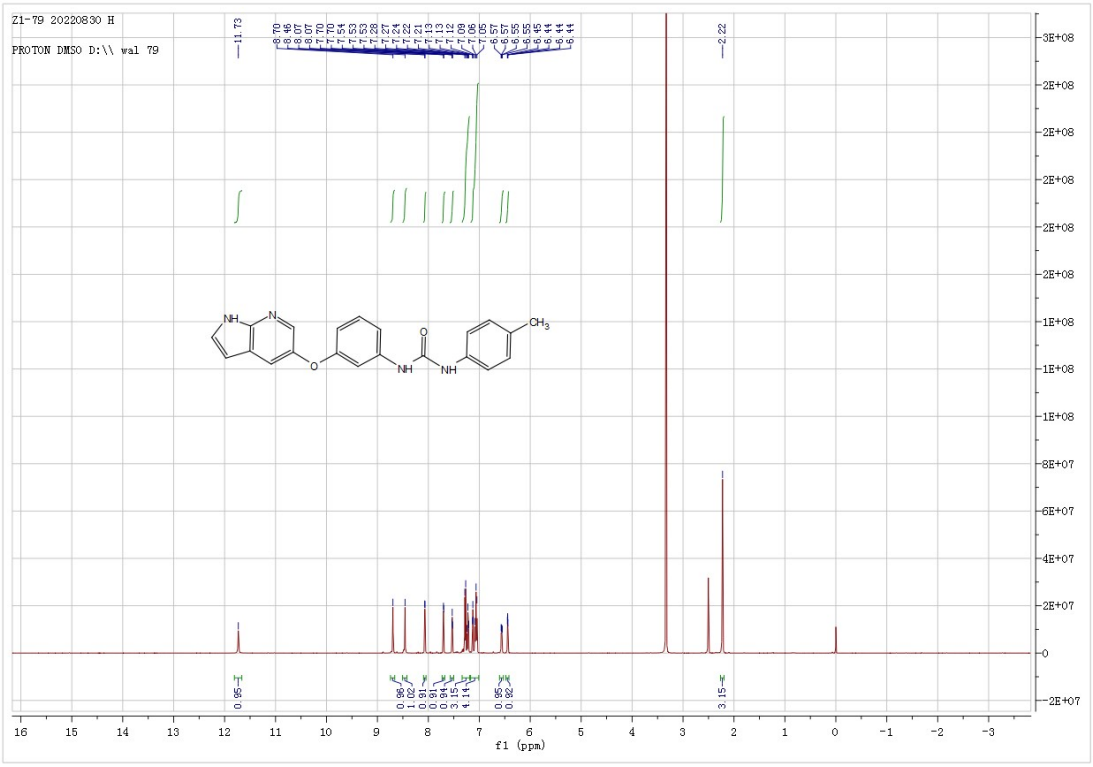


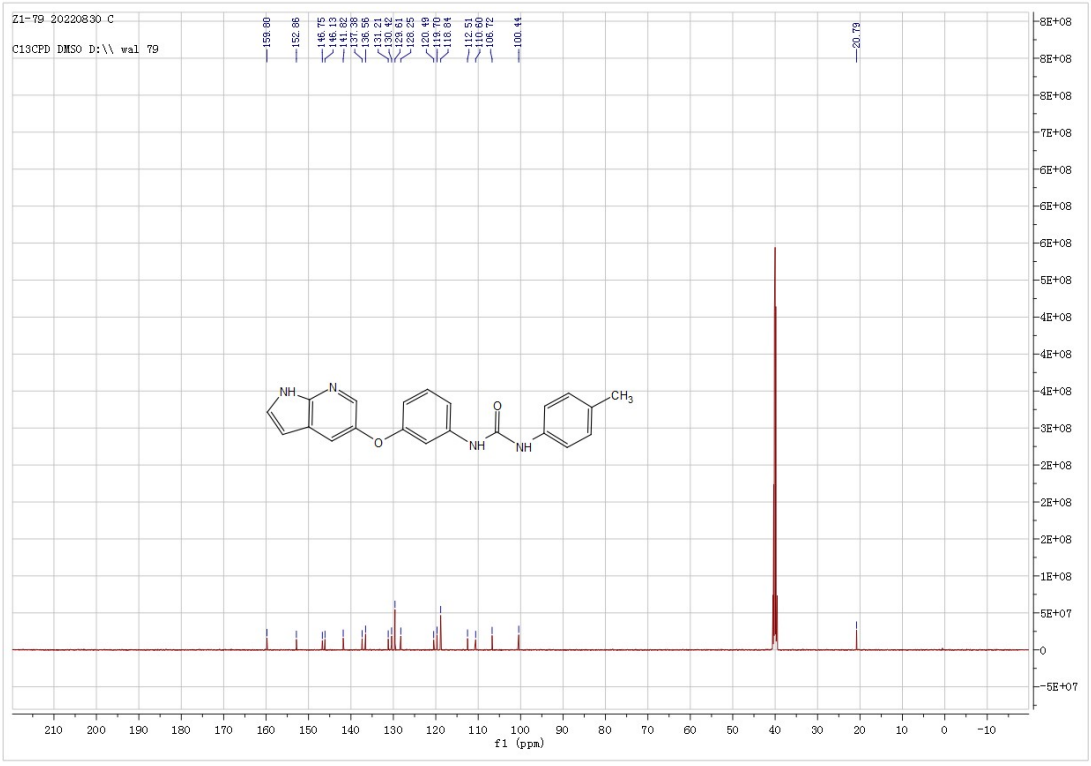
$(C_{20}H_{15}ClNO_2)$
M+H = 379.0956
0704-3

HRMS (ESI) spectrum of **11**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-methylphenyl)urea (**12**)



^{1}H NMR spectrum of **12**



^{13}C NMR spectrum of **12**

Sample Name	WQ-1201-19	**Position**	Vial 59	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
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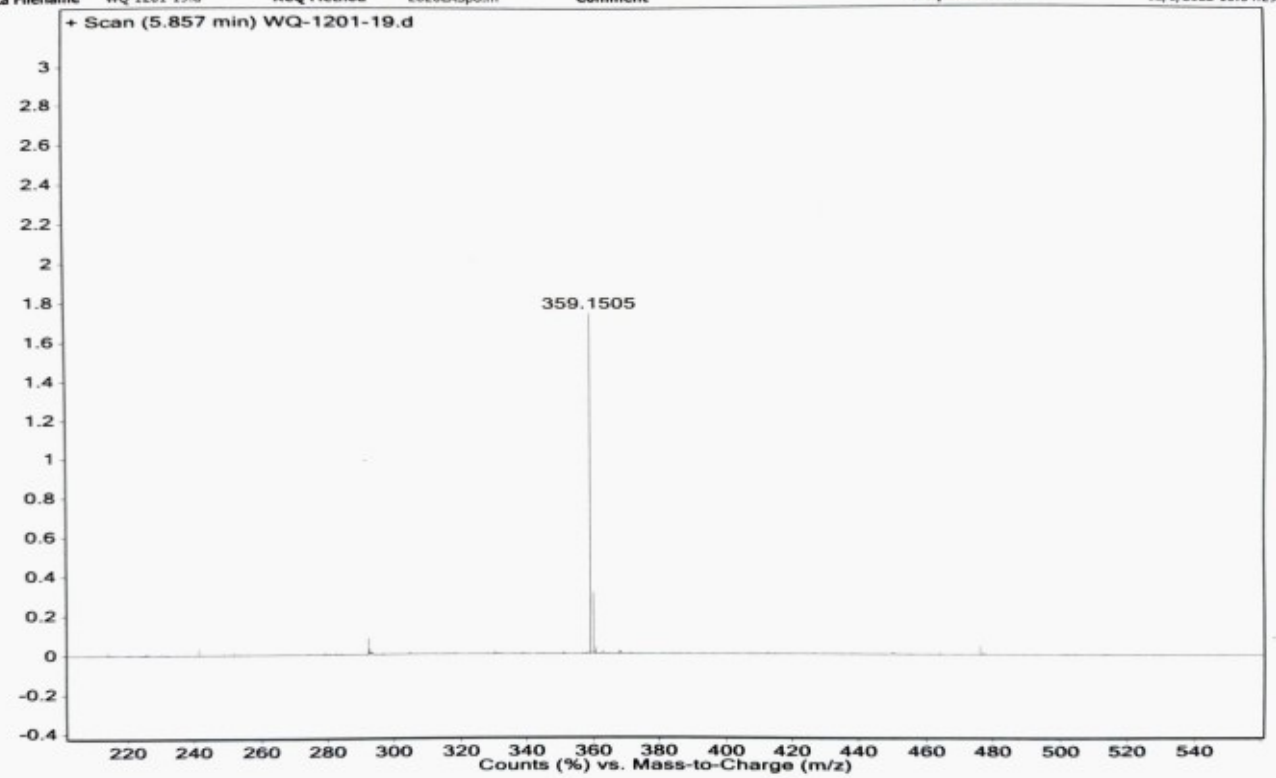
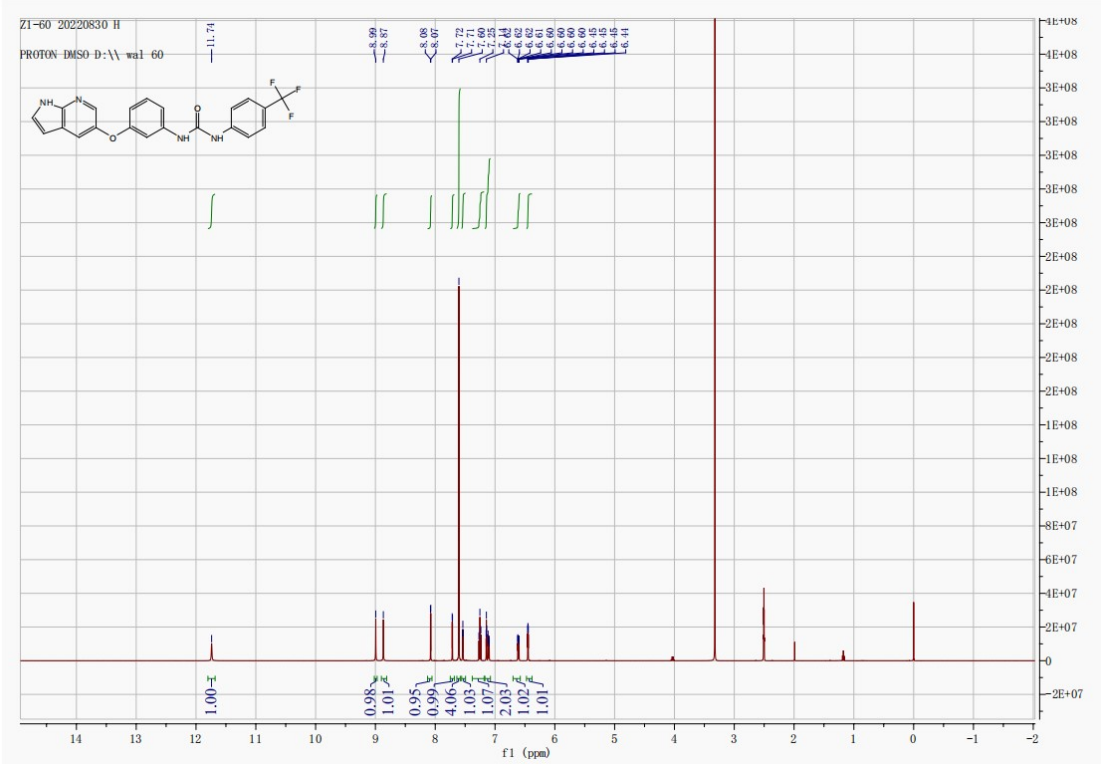


(M+H)+ : 359.1503
$C_{21}H_{18}N_4O_2$
0722-1

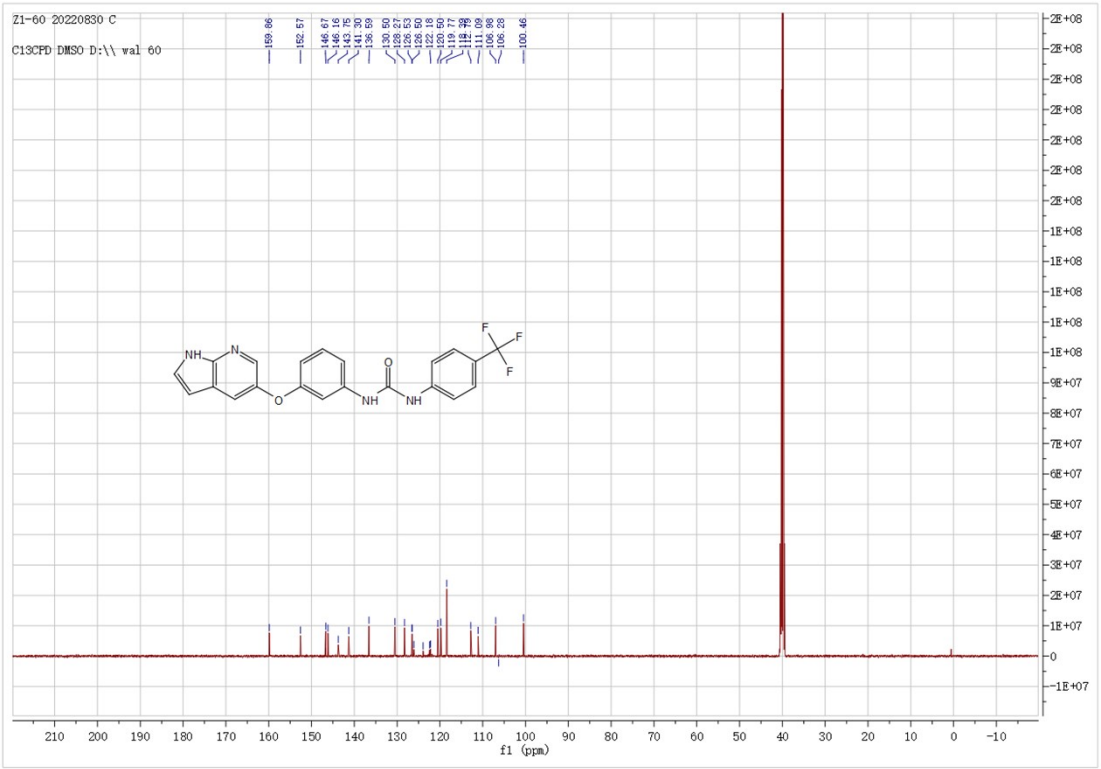
HRMS (ESI) spectrum of **12**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-(trifluoromethyl)phenyl)urea

(13)



^{1}H NMR spectrum of **13**



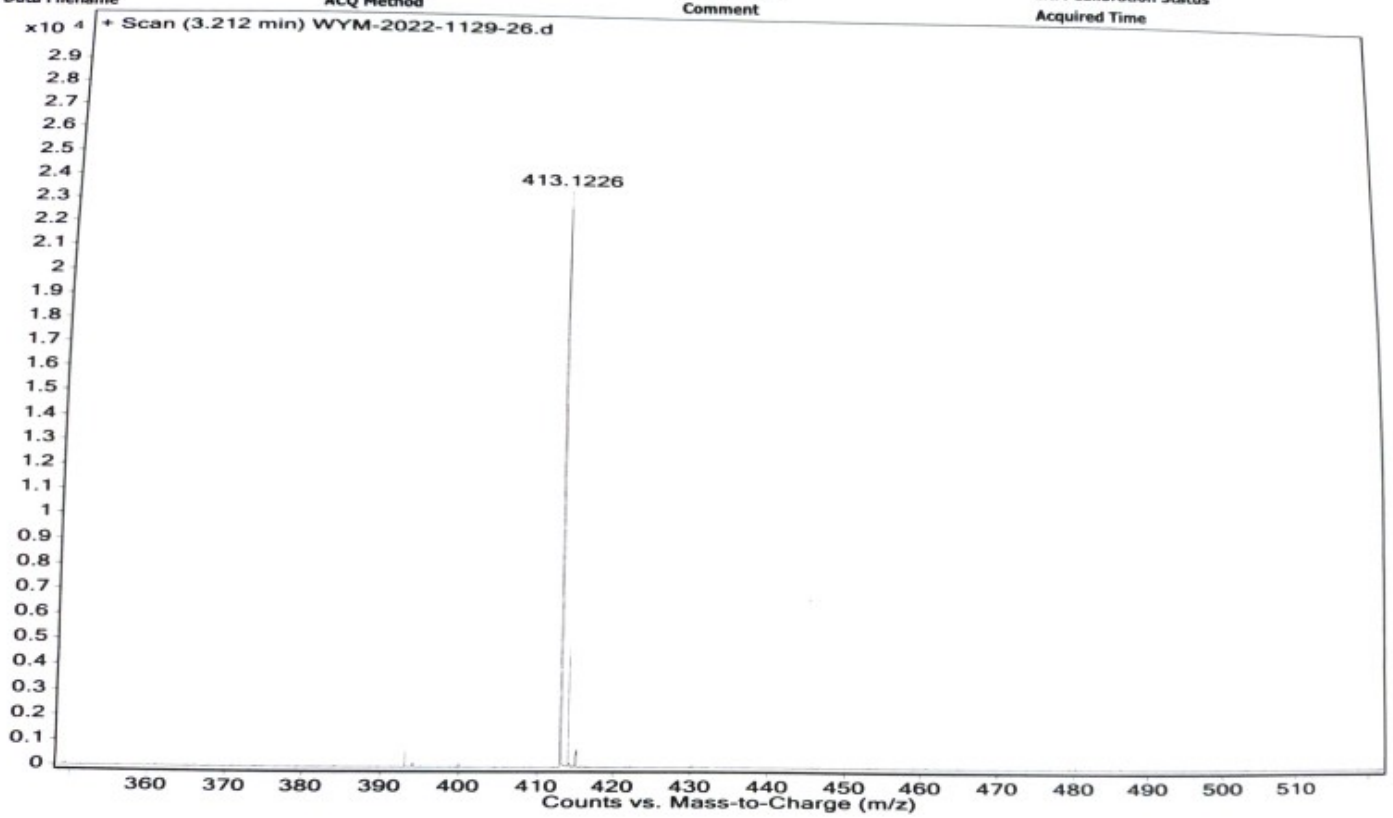
^{13}C NMR spectrum of **13**

Sample Name
Inj Vol
Data Filename

Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

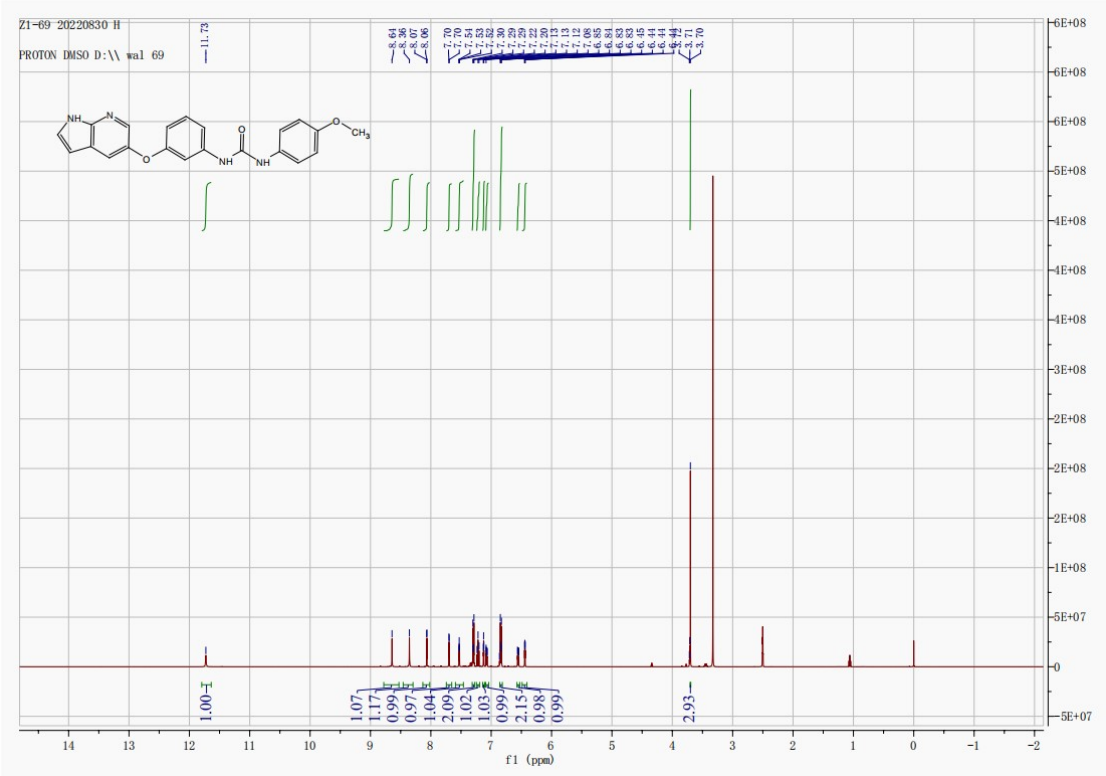
User Name
IRM Calibration Status
Acquired Time



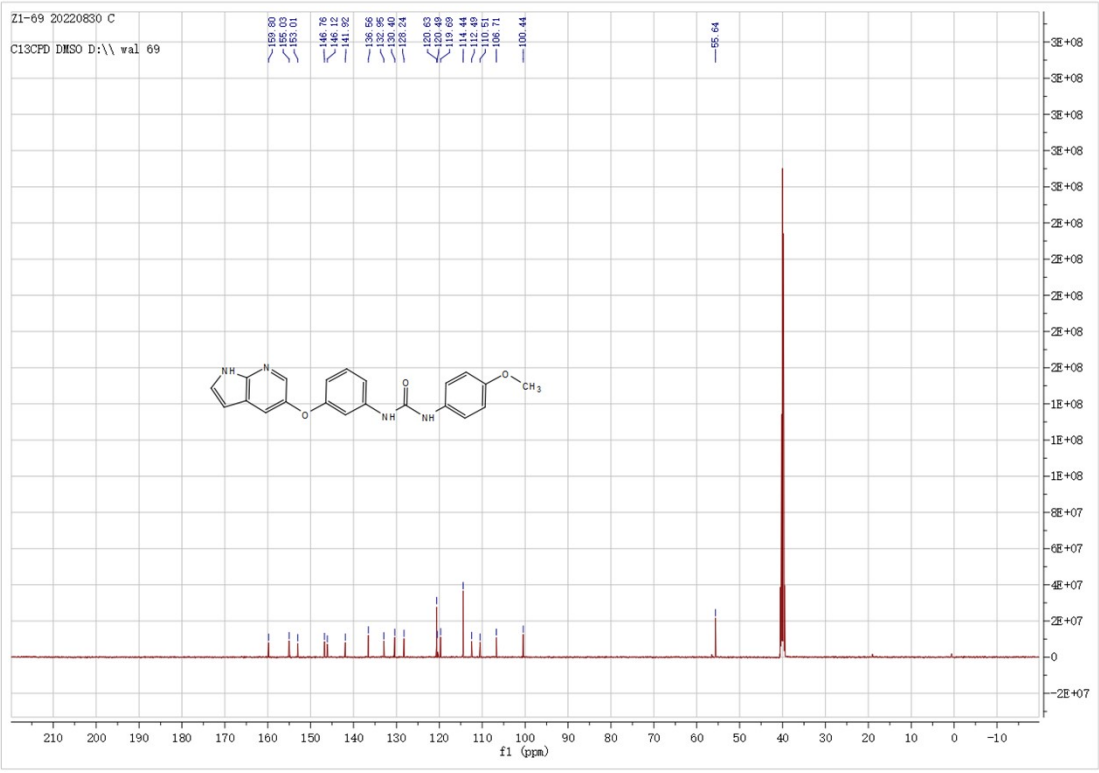
m+H = 413.122
($C_{21}H_{17}F_3N_4O_3$
e709-4

HRMS (ESI) spectrum of **13**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-methoxyphenyl)urea (**14**)



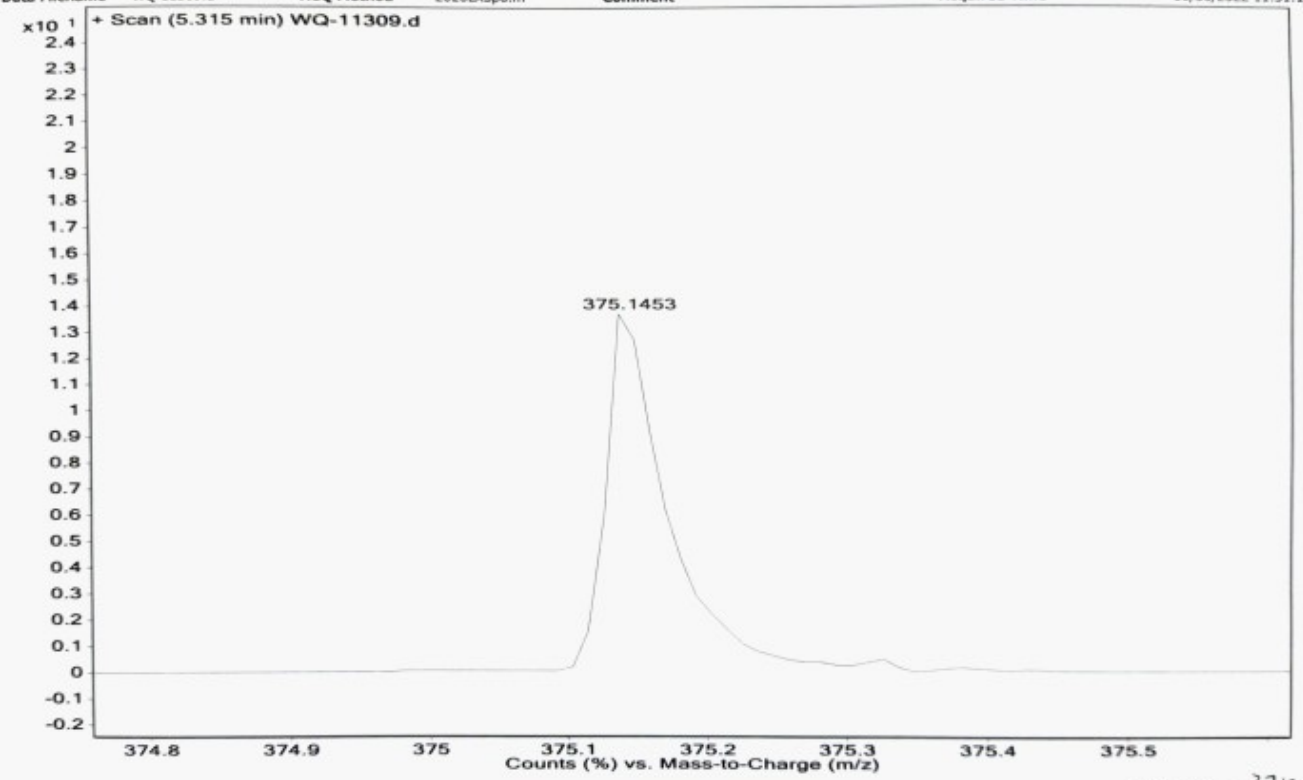
^{1}H NMR spectrum of **14**



^{13}C NMR spectrum of **14**

9.

Sample Name	WQ-11309	**Position**	Vial 59	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-11309.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/30/2022 11:31:11 AM



$(M+H)^+$: 375.1452

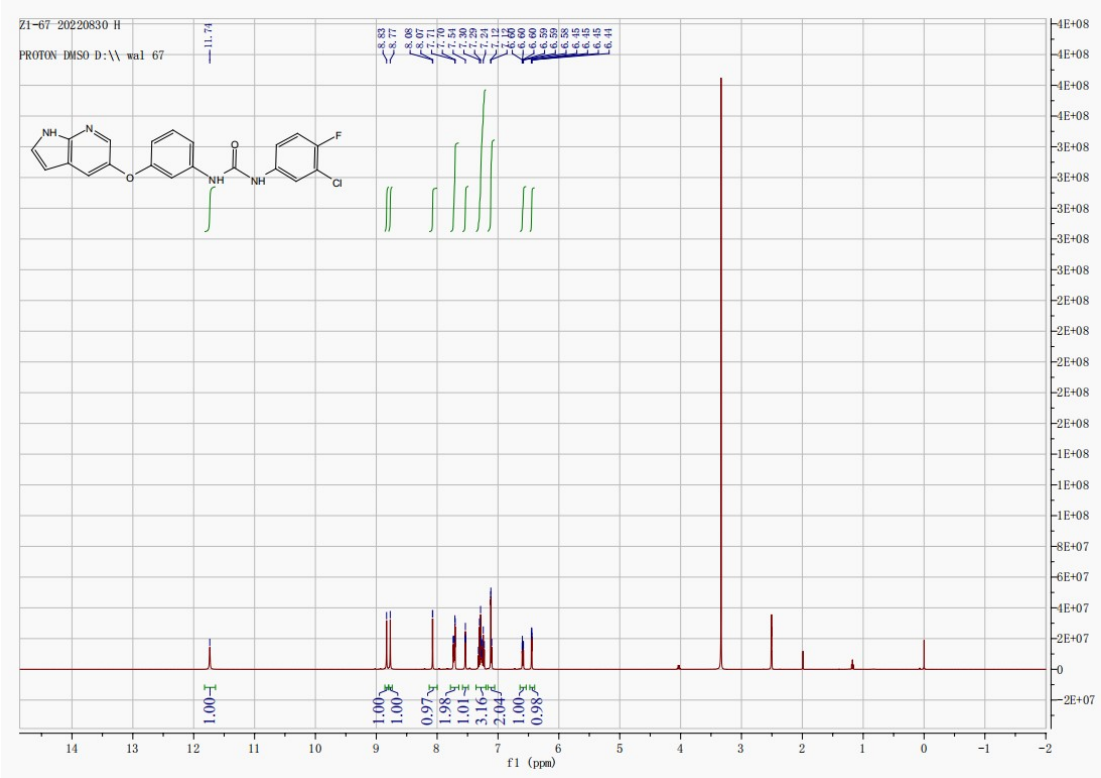
$C_{21}H_{18}N_4O_3$

0718-3

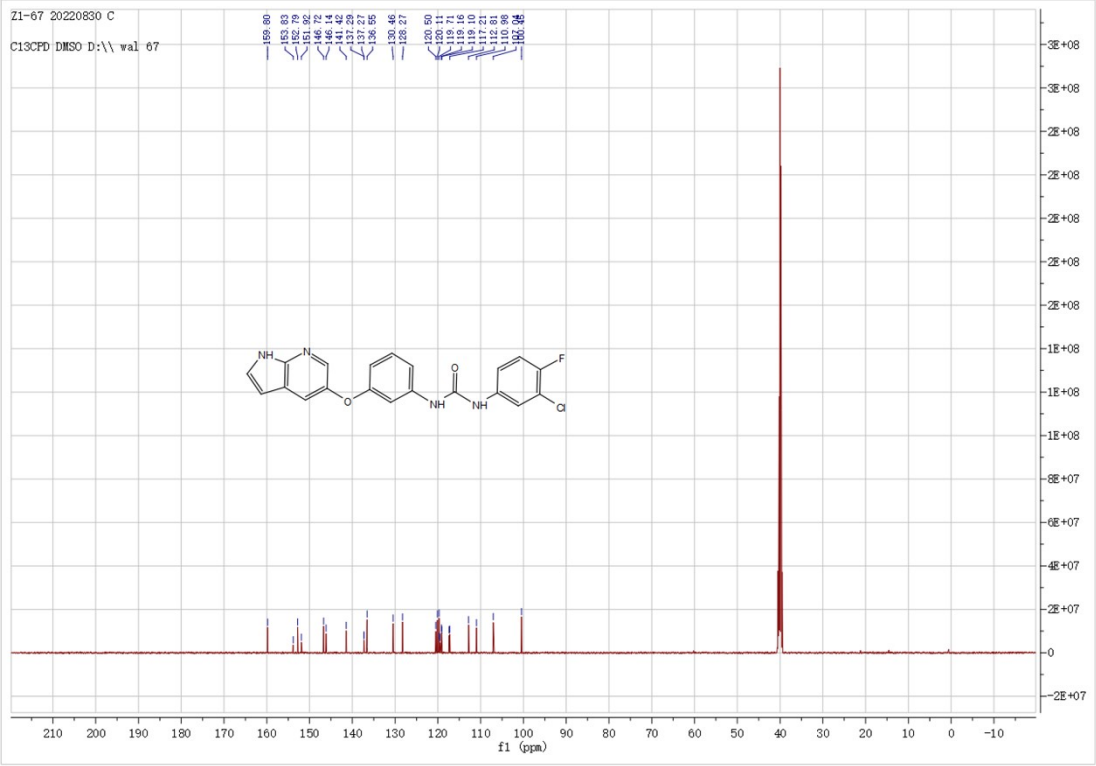
HRMS (ESI) spectrum of **14**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-chloro-4-fluorophenyl)urea

(**15**)



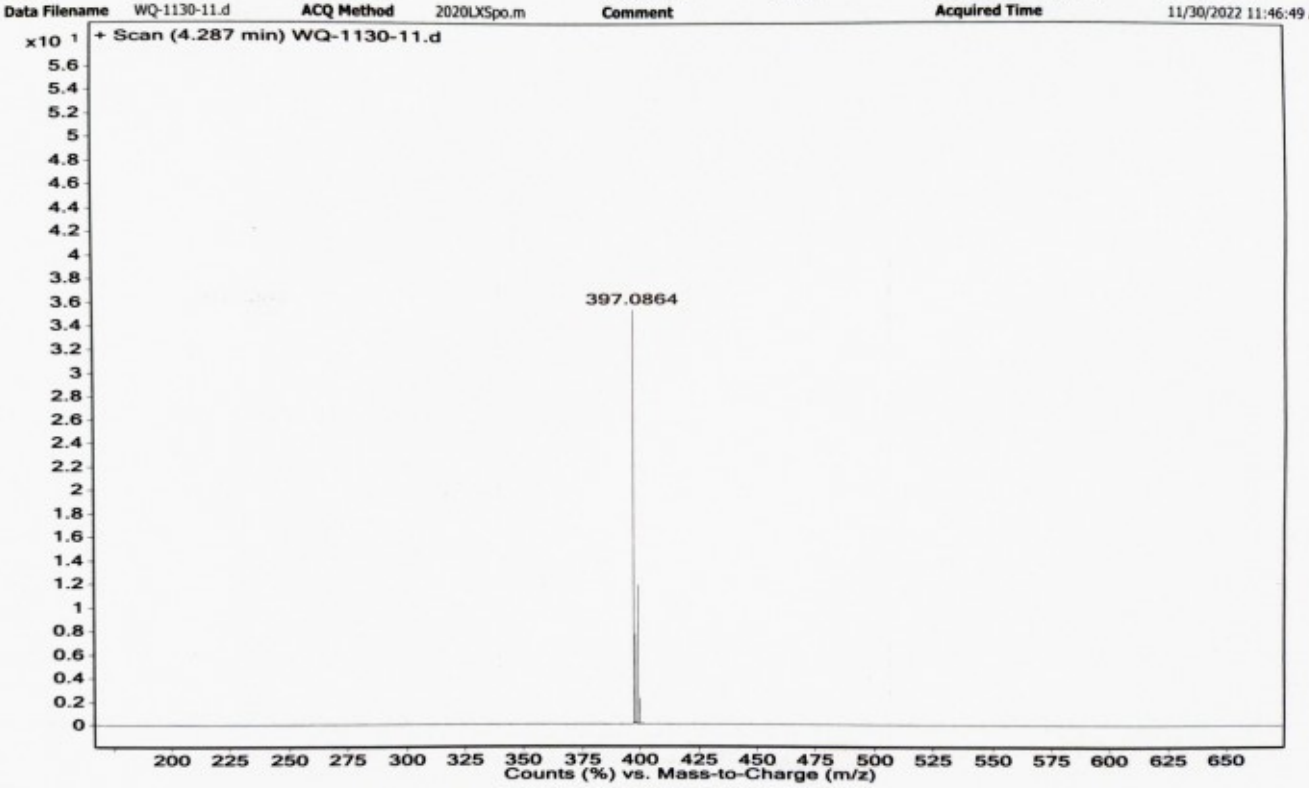
^{1}H NMR spectrum of **15**



^{13}C NMR spectrum of **15**

17

Sample Name	WQ-1130-7	**Position**	Vial 61	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-1130-11.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/30/2022 11:46:49 AM



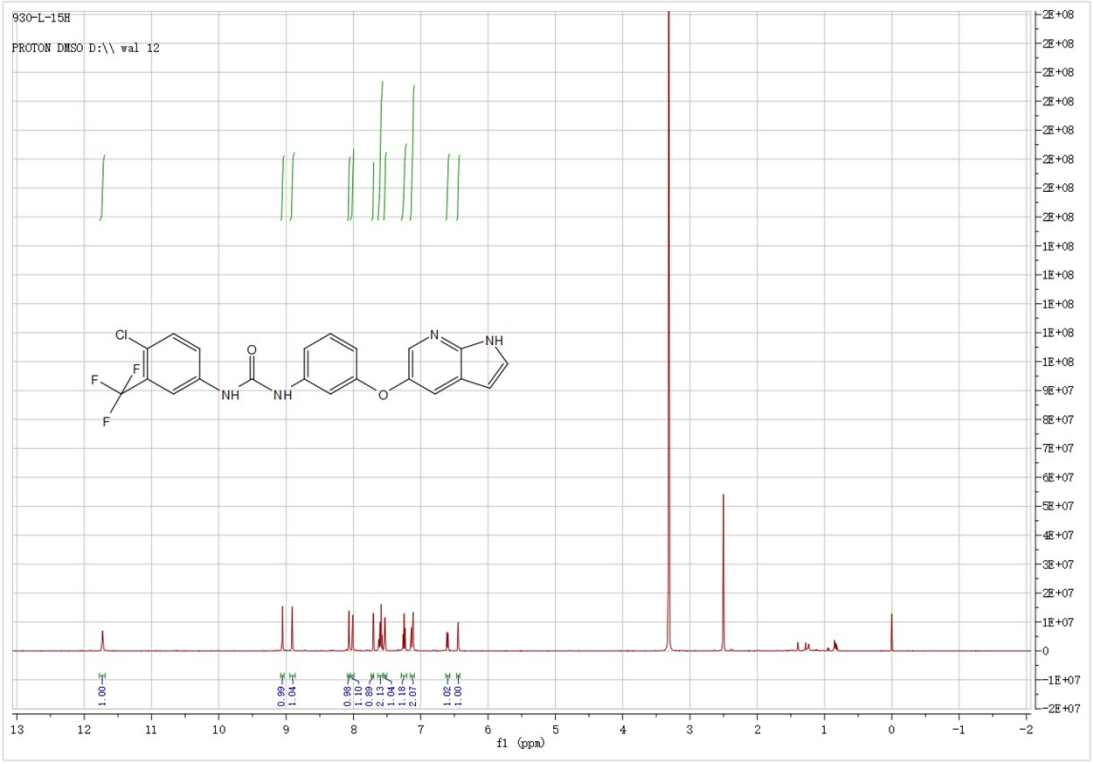
$[M+H]=397.0862$

$C_{20}H_{14}ClF_4N_2$

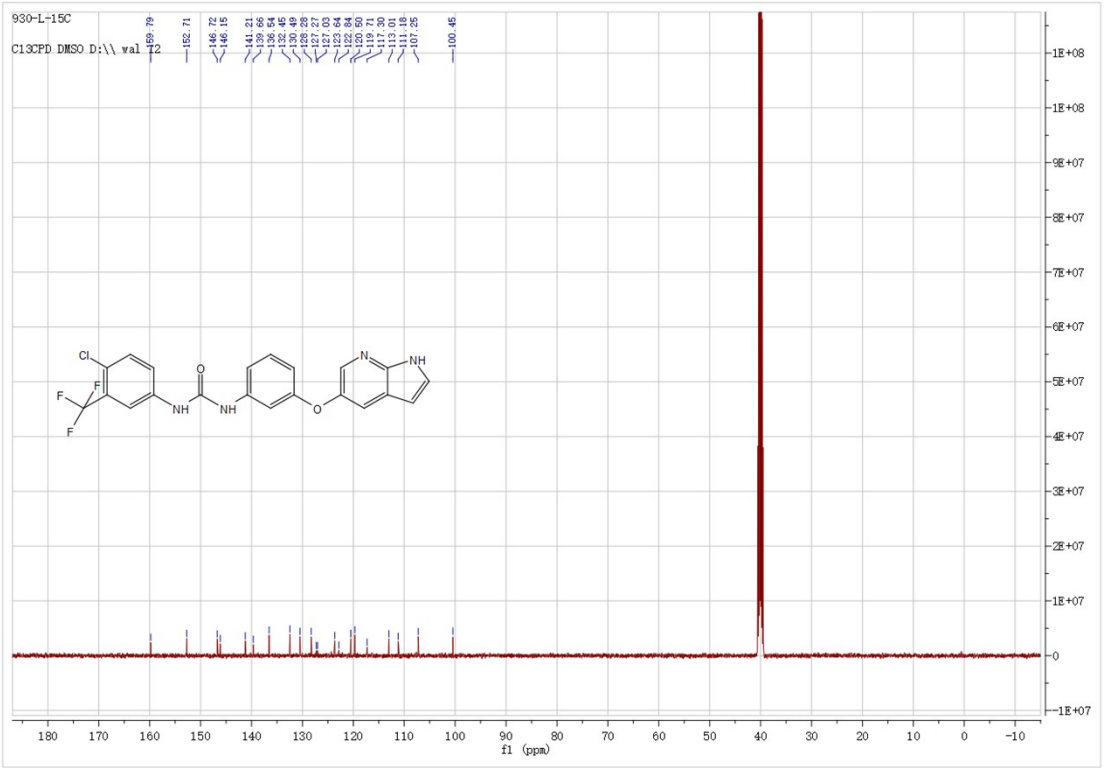
07184

HRMS (ESI) spectrum of **15**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-chloro-3-(trifluoromethyl)phenyl)urea (**16**)



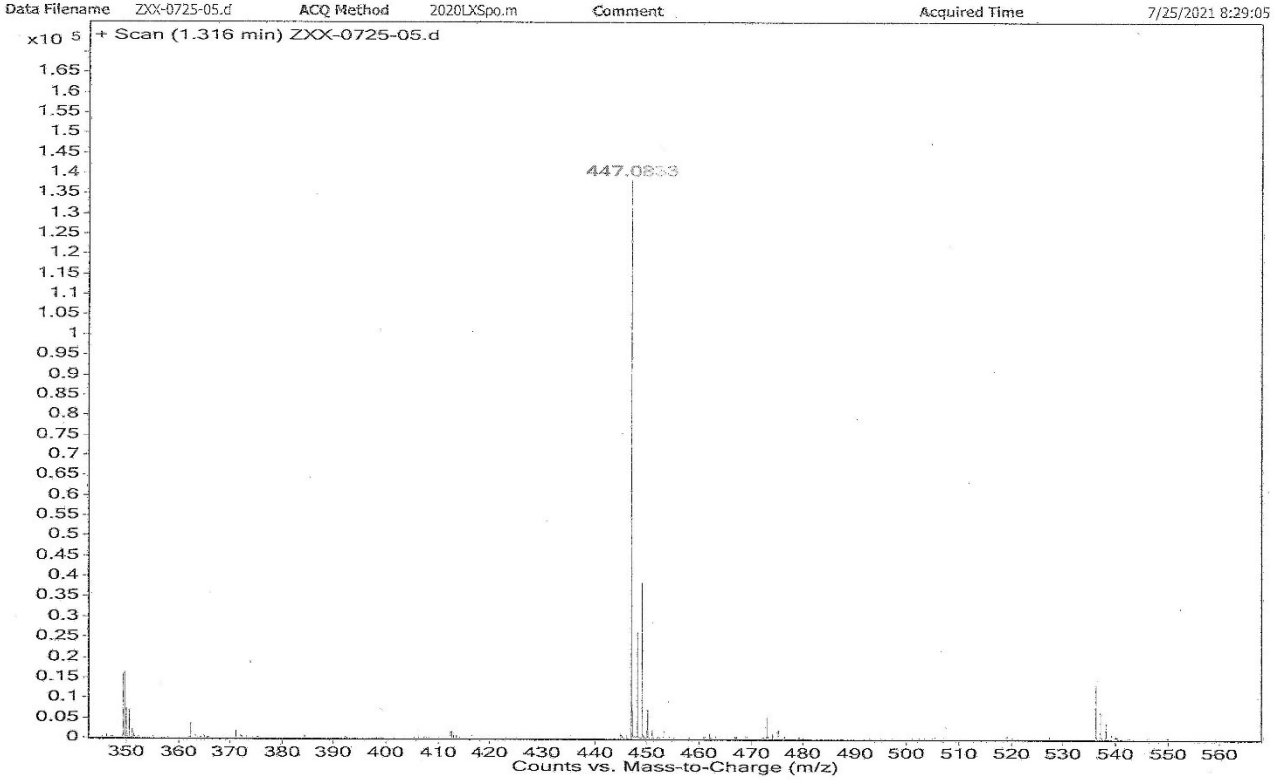
^{1}H NMR spectrum of **16**



^{13}C NMR spectrum of **16**

C31H14N4O2F3Cl
cal[M+] 447.083

Sample Name	ZXX-0725-05	Position	Vial 5	Instrument Name	Instrument 1	User Name	
Inj Vol	2	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	ZXX-0725-05.d	ACQ Method	2020LXSpo.m	Comment		Acquired Time	7/25/2021 8:29:05 AM

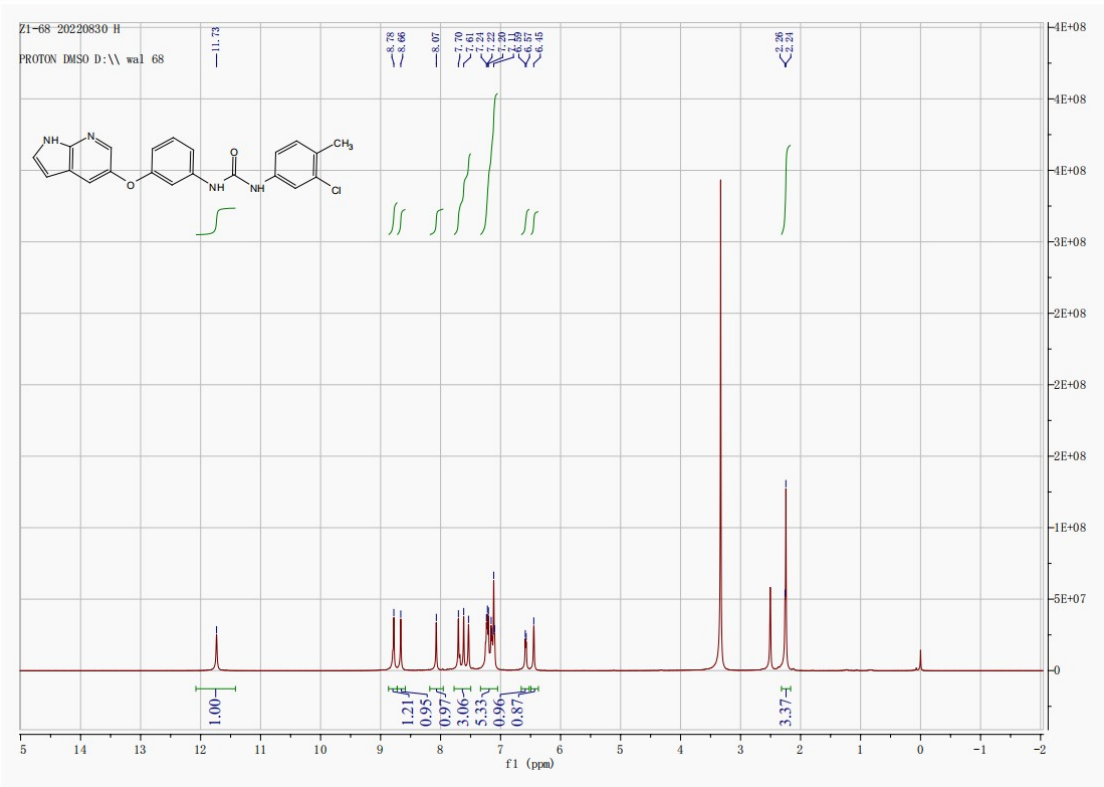


HRMS (ESI) spectrum of **16**

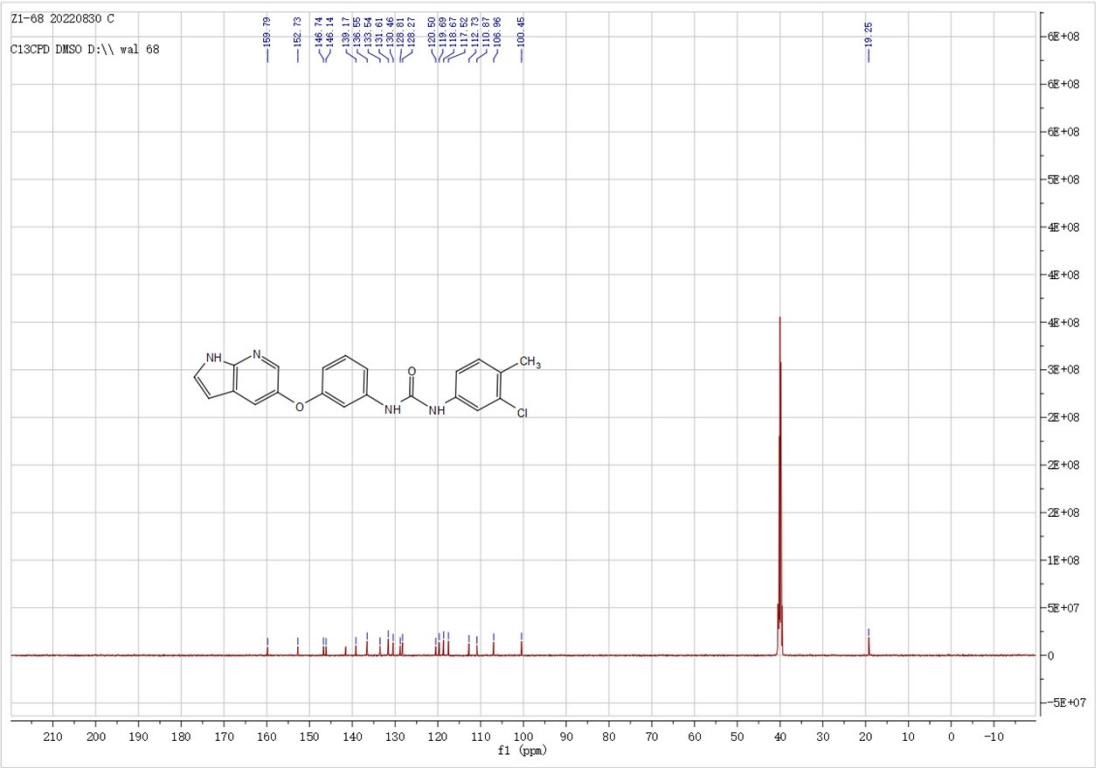
0605-2

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-chloro-4-methylphenyl)urea

(**17**)



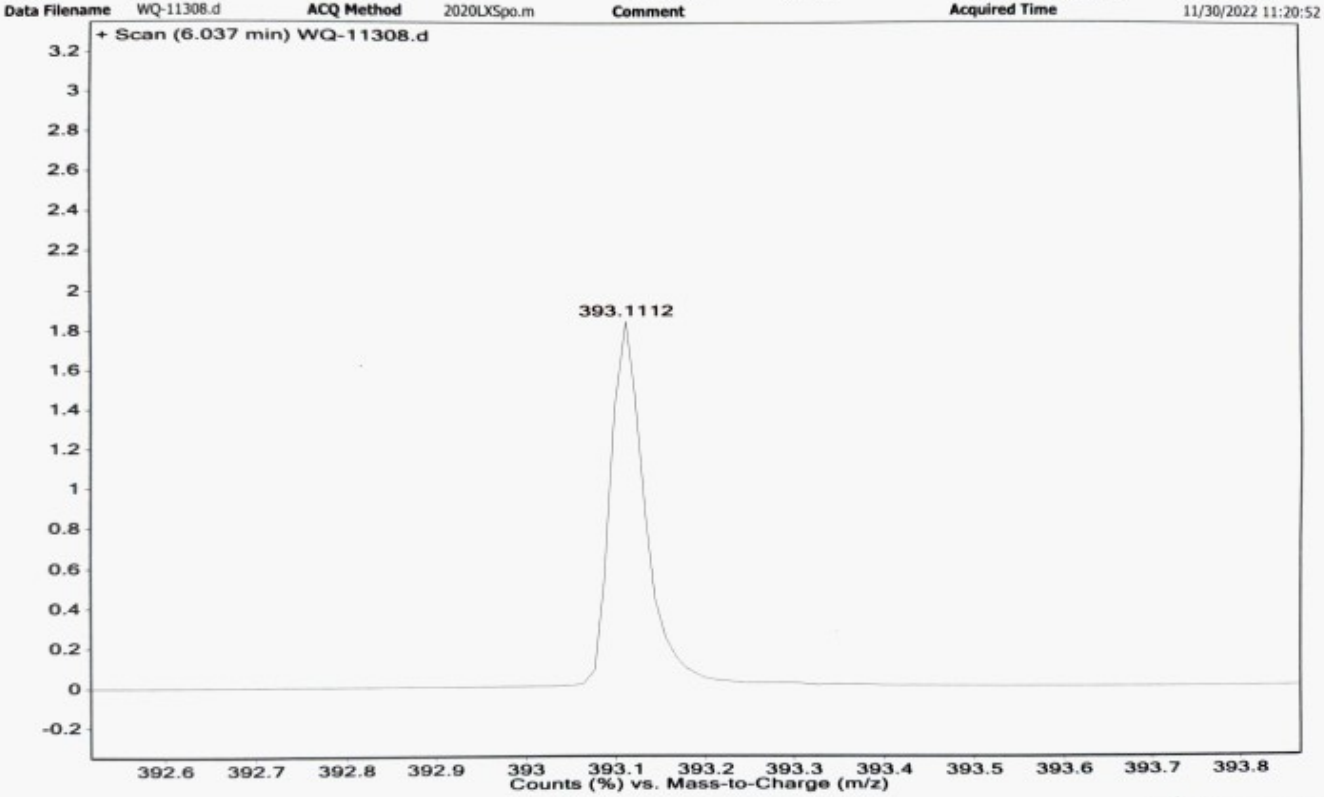
^{1}H NMR spectrum of **17**



^{13}C NMR spectrum of **17**

18

Sample Name	WQ-11308	**Position**	Vial 58	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-11308.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/30/2022 11:20:52 AM



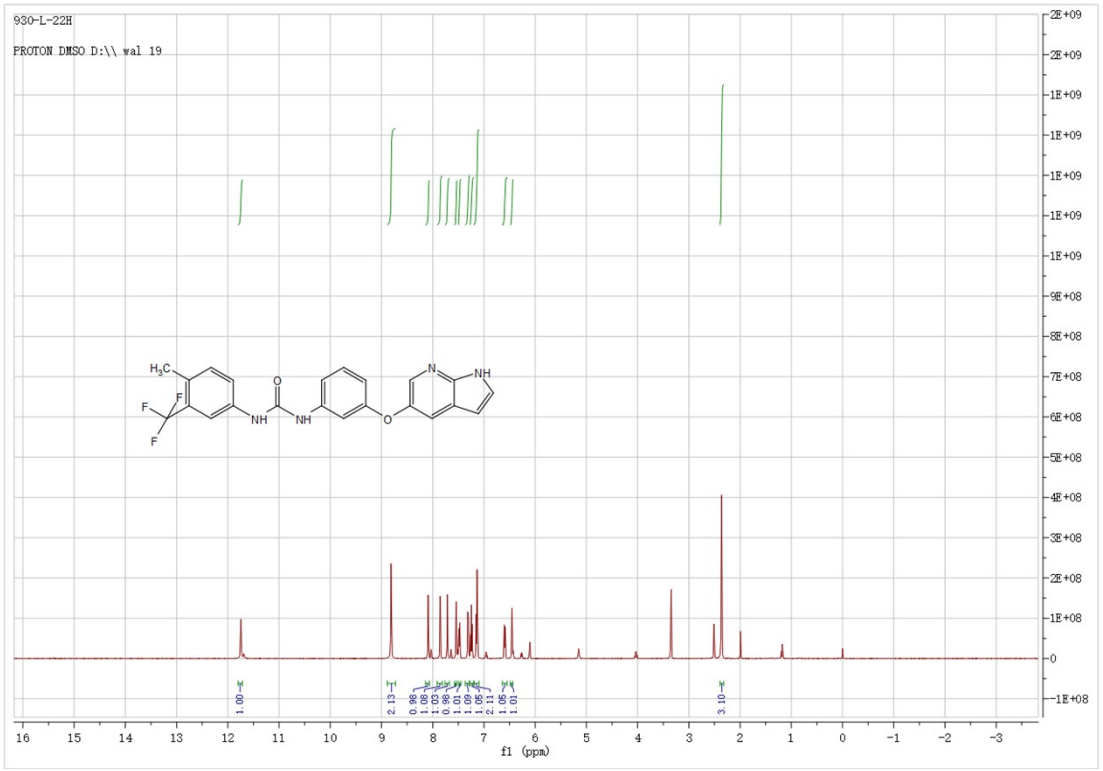
$(M+H)^+$: 393.1113

$C_{21}H_{17}ClN_4O_2$

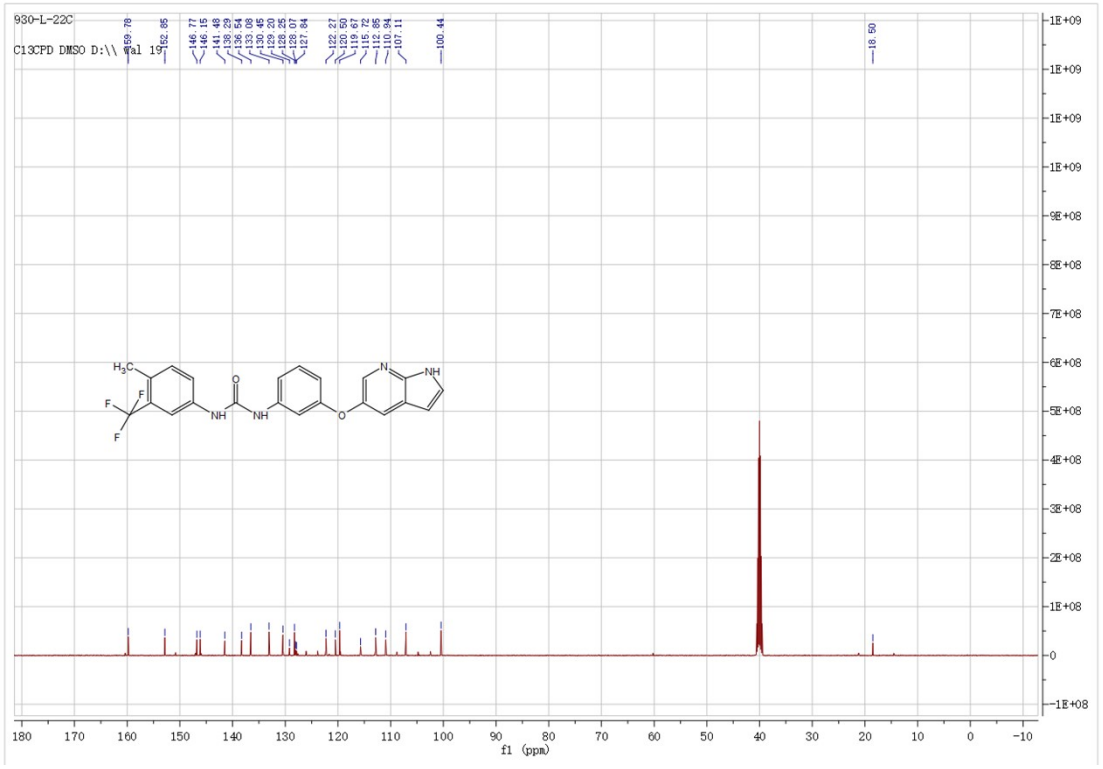
078-2

HRMS (ESI) spectrum of **17**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-methyl-3-(trifluoromethyl)phenyl)urea (**18**)



^{1}H NMR spectrum of **18**

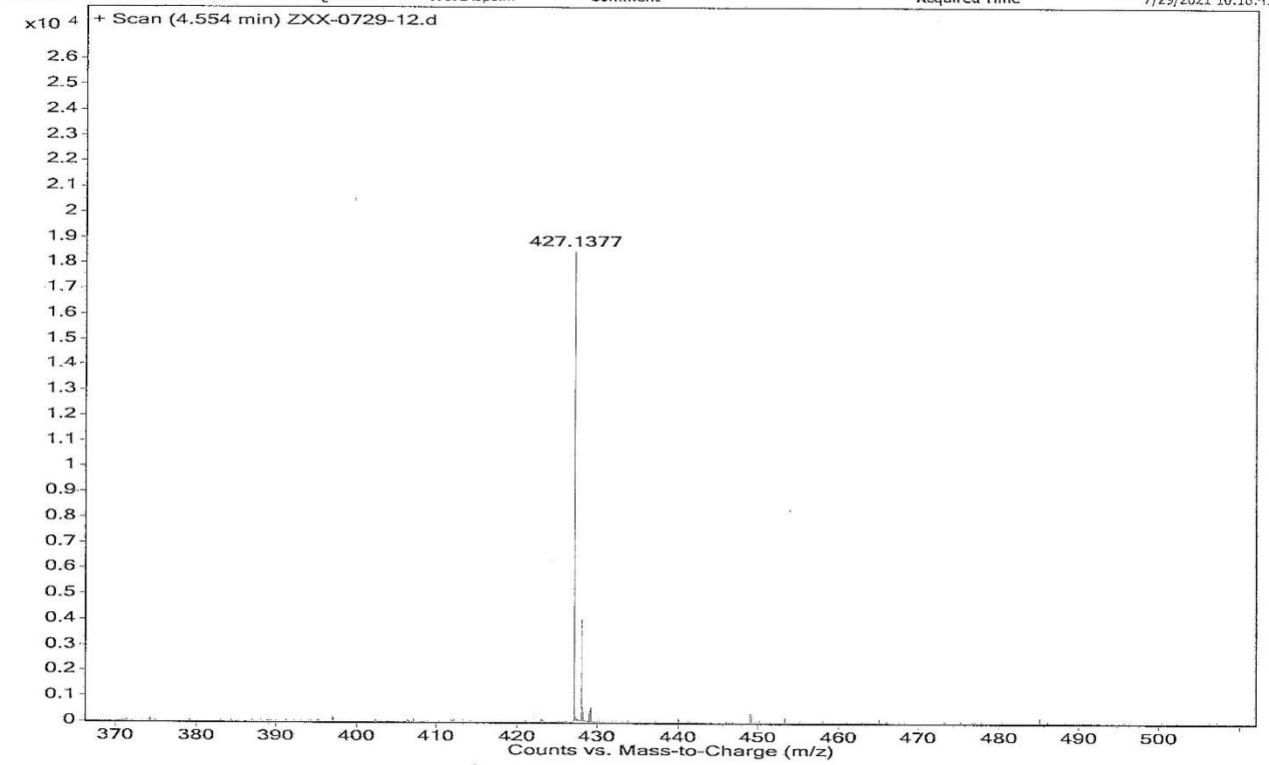


^{13}C NMR spectrum of **18**

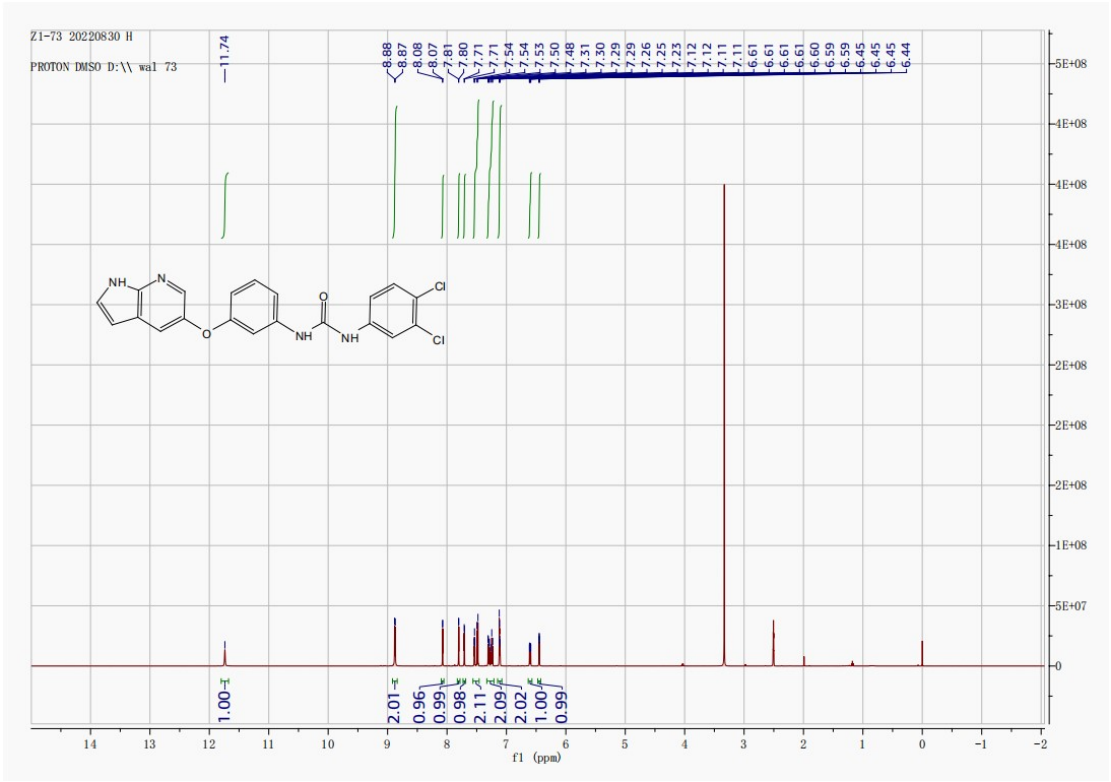
HRMS (ESI) spectrum of **18**

Sample Name	ZXX-0729-12	Position	Vial 42	Instrument Name	Instrument 1	User Name	
Inj Vol	2	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	ZXX-0729-12.d	ACQ Method	2020LXSpo.m	Comment		Acquired Time	7/29/2021 10:18:41 AM

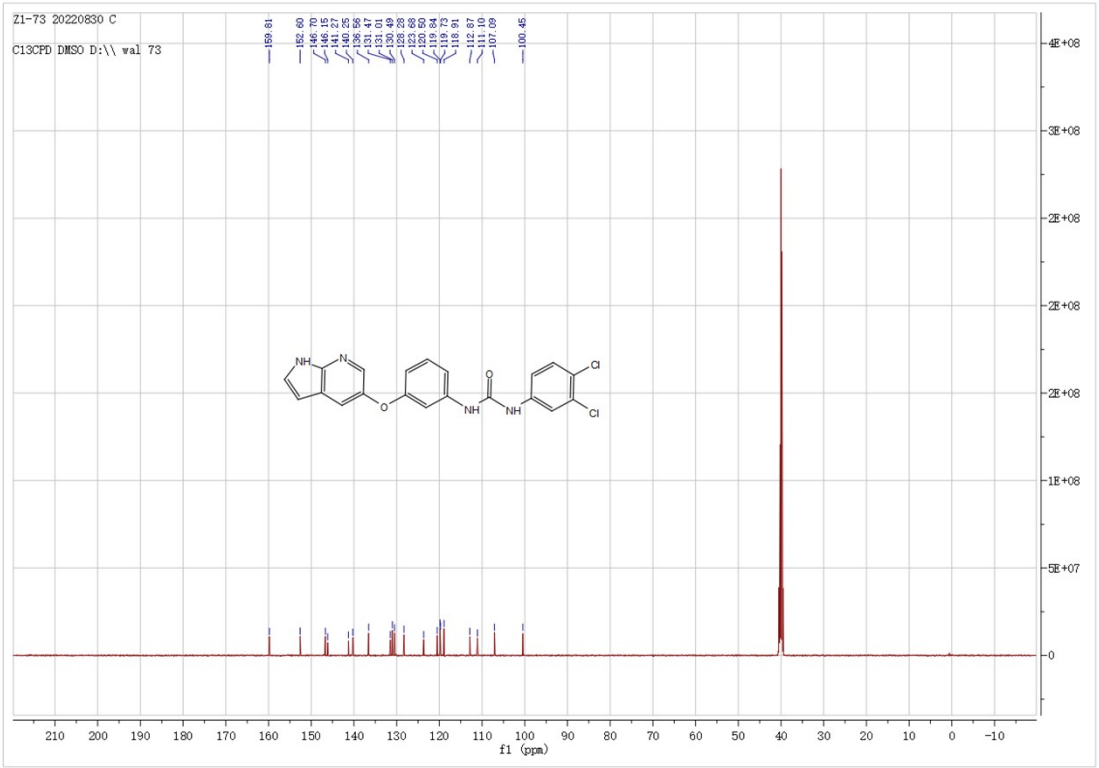
$C_{22}H_{17}N_4O_2F_3$
$[M+H]^+$: 427.1376



1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3,4-dichlorophenyl)urea (**19**)

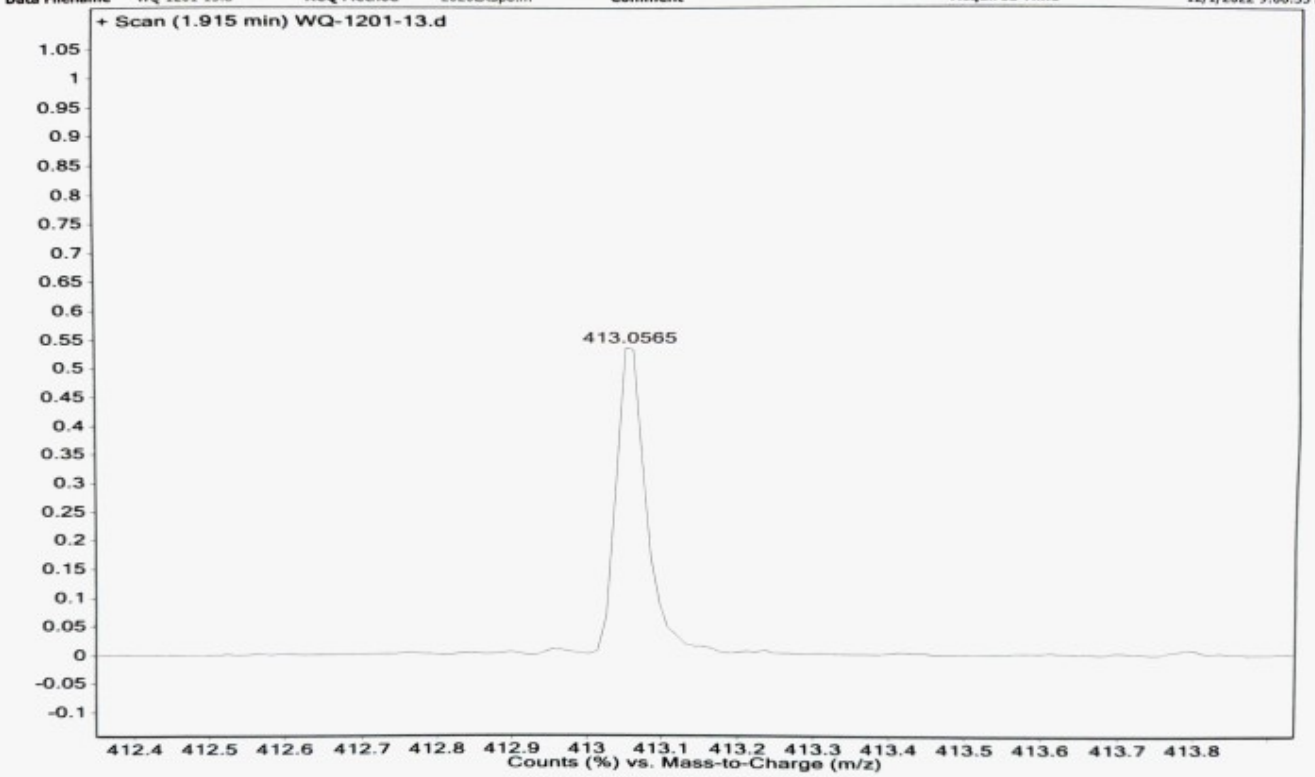


^{1}H NMR spectrum of **19**



^{13}C NMR spectrum of **19**

Sample Name	WQ-1201-13	**Position**	Vial 53	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-1201-13.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	12/1/2022 9:06:33 AM



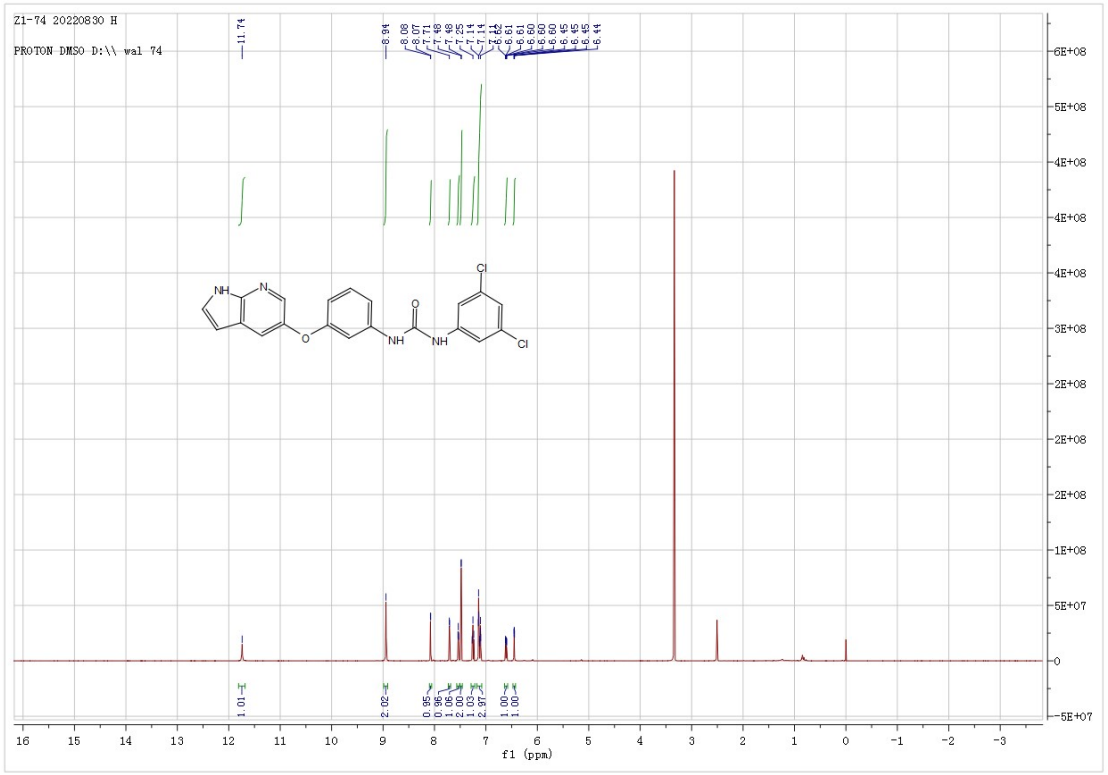
$(M+H)^+$: 413.0567

$C_{20}H_{14}Cl_2N_4O_2$

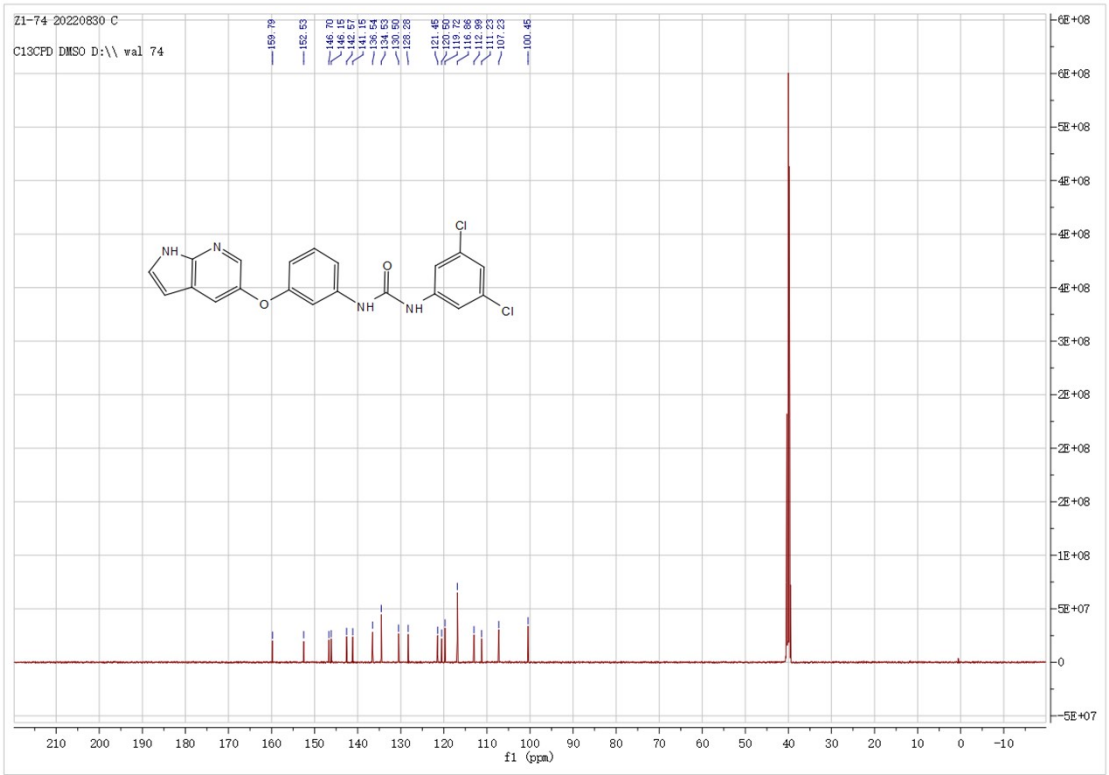
0720-4

HRMS (ESI) spectrum of **19**

1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3,5-dichlorophenyl)urea (**20**)

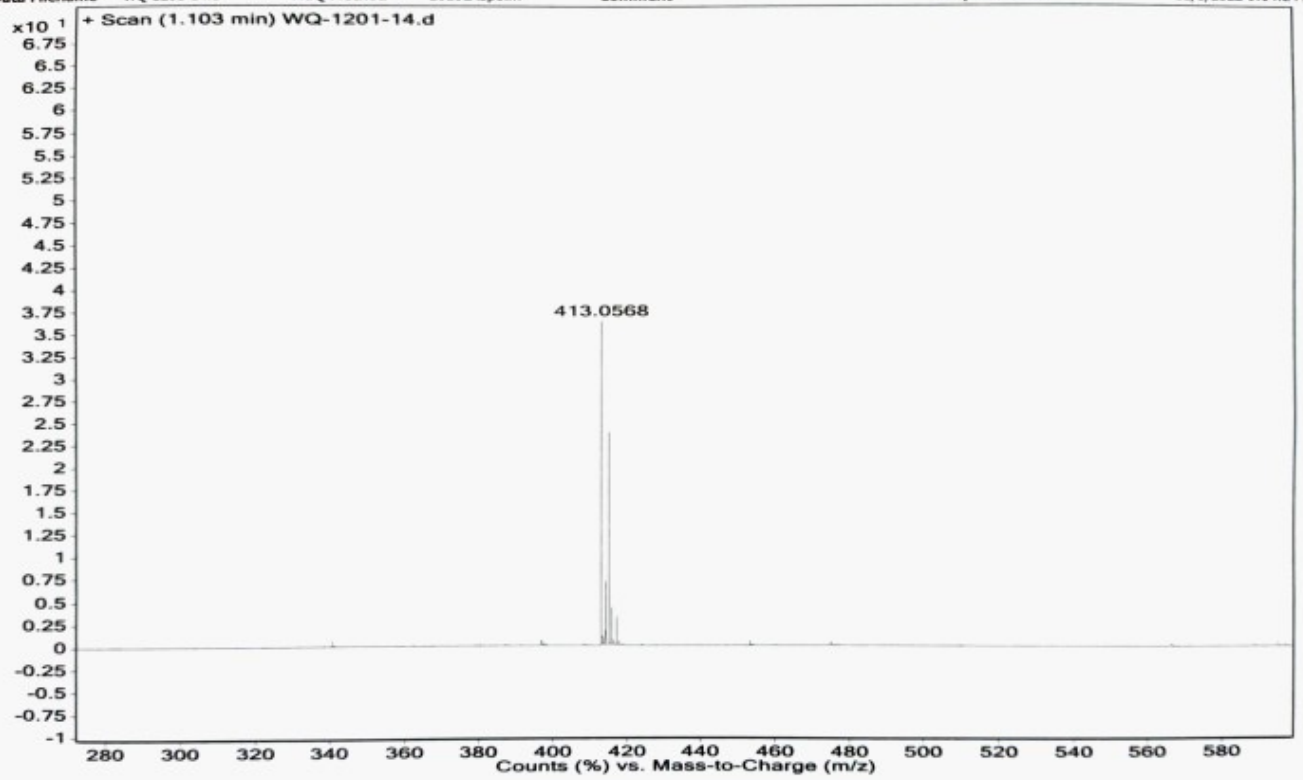


^{1}H NMR spectrum of **20**



^{13}C NMR spectrum of **20**

Sample Name	WQ-1201-14	**Position**	Vial 54	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-1201-14.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	12/1/2022 9:14:24 AM



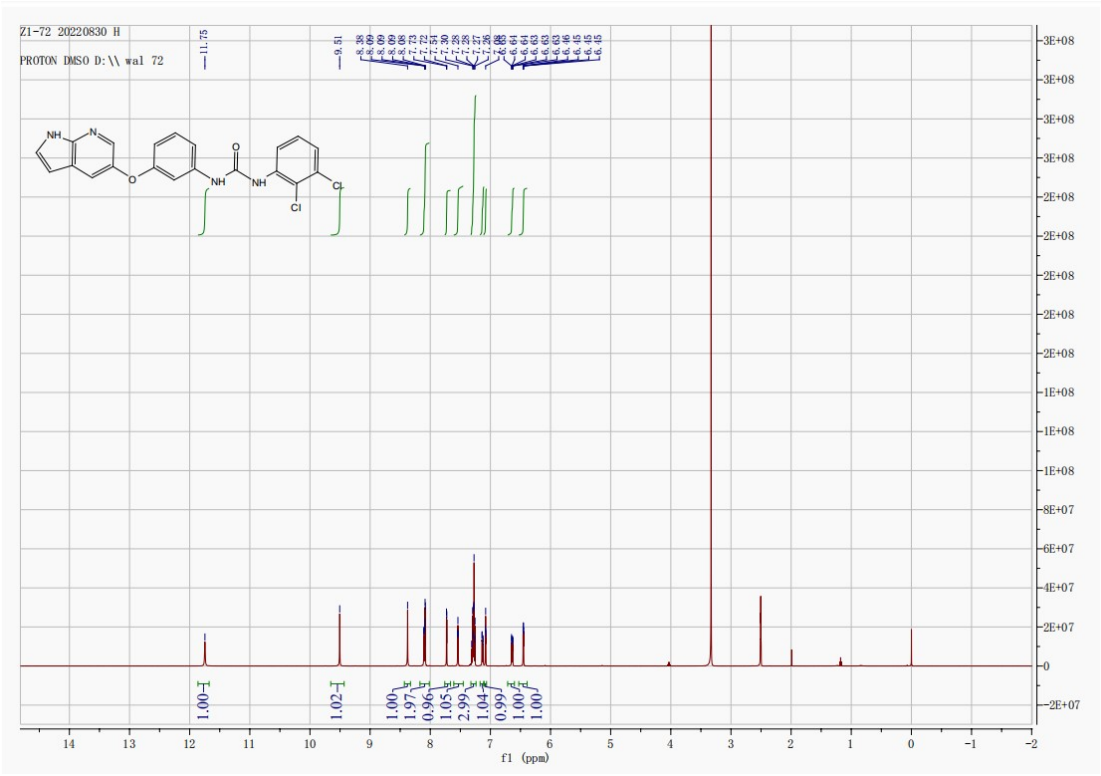
$(M+H)^+$: 413.0567

$C_{20}H_{14}Cl_2N_4O_2$

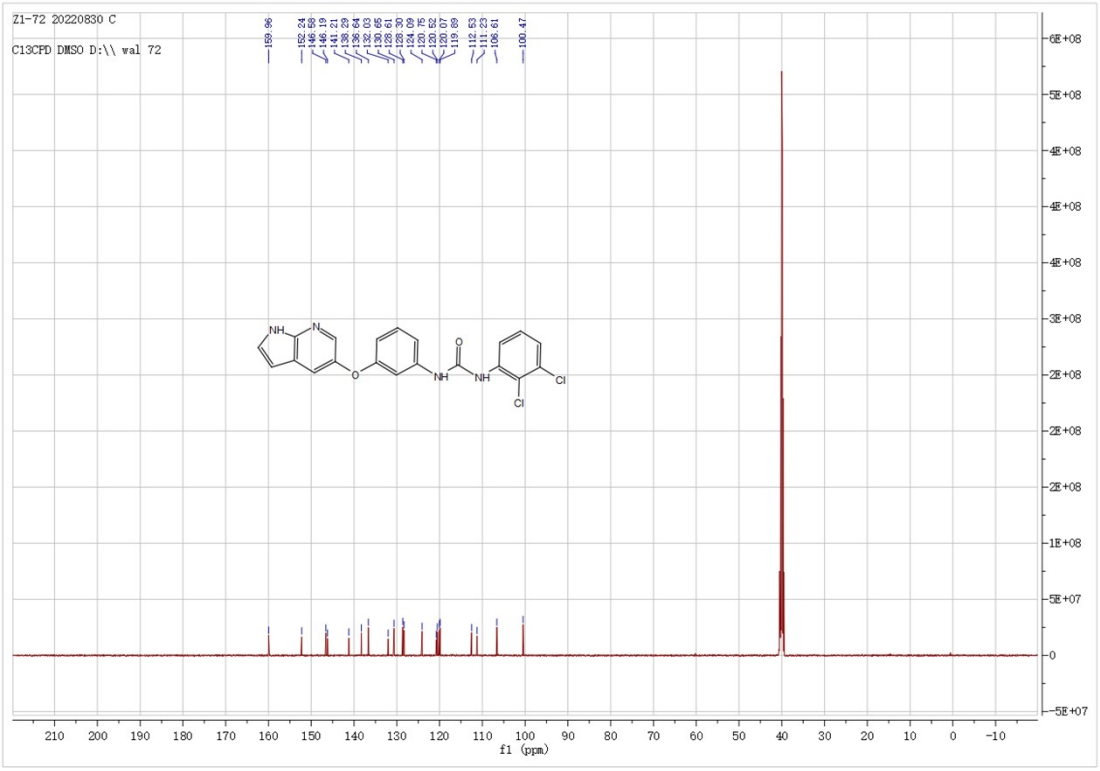
0720-5

HRMS (ESI) spectrum of **20**

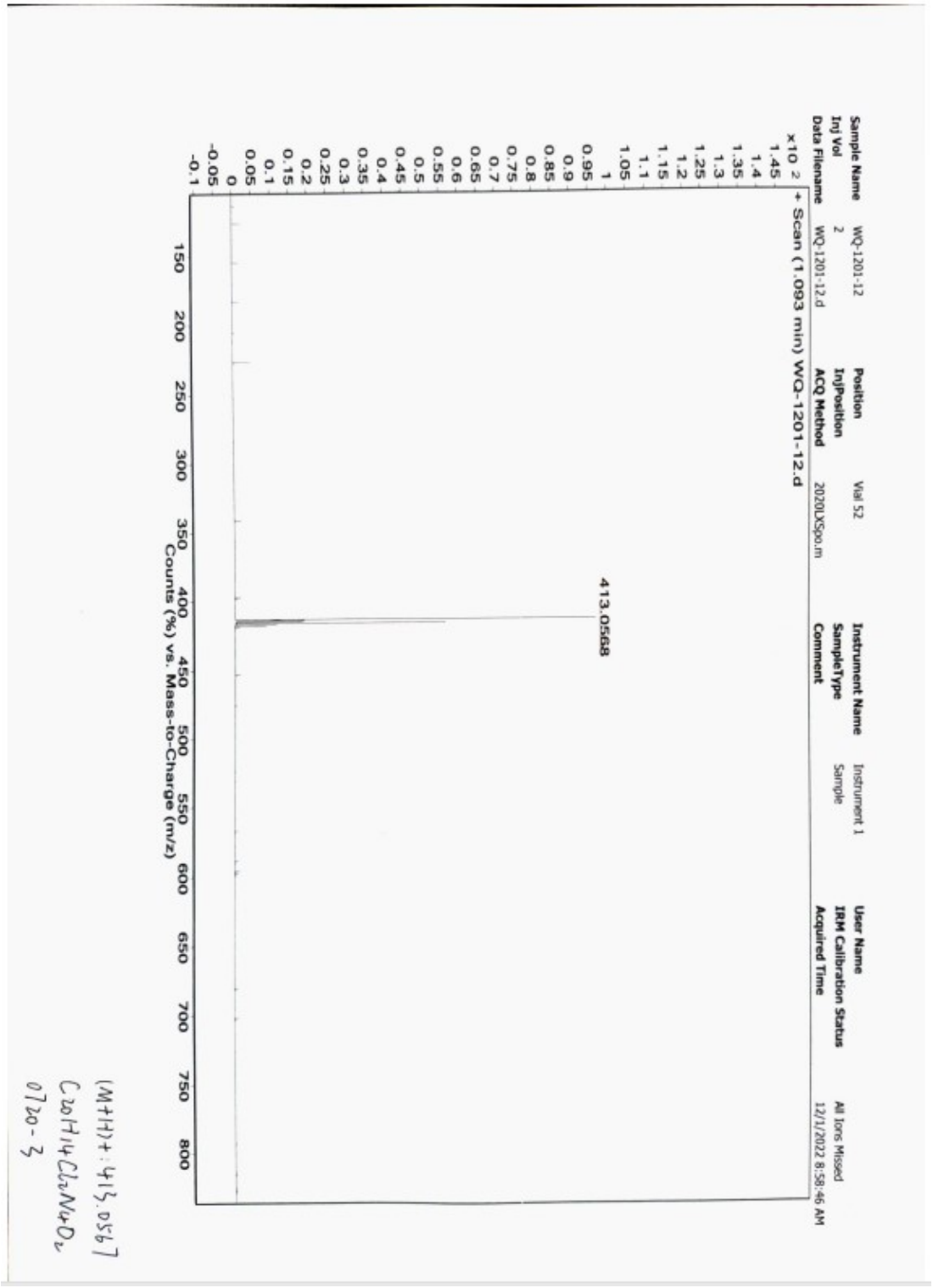
1-(3-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(2,3-dichlorophenyl)urea (**21**)



^{1}H NMR spectrum of **21**

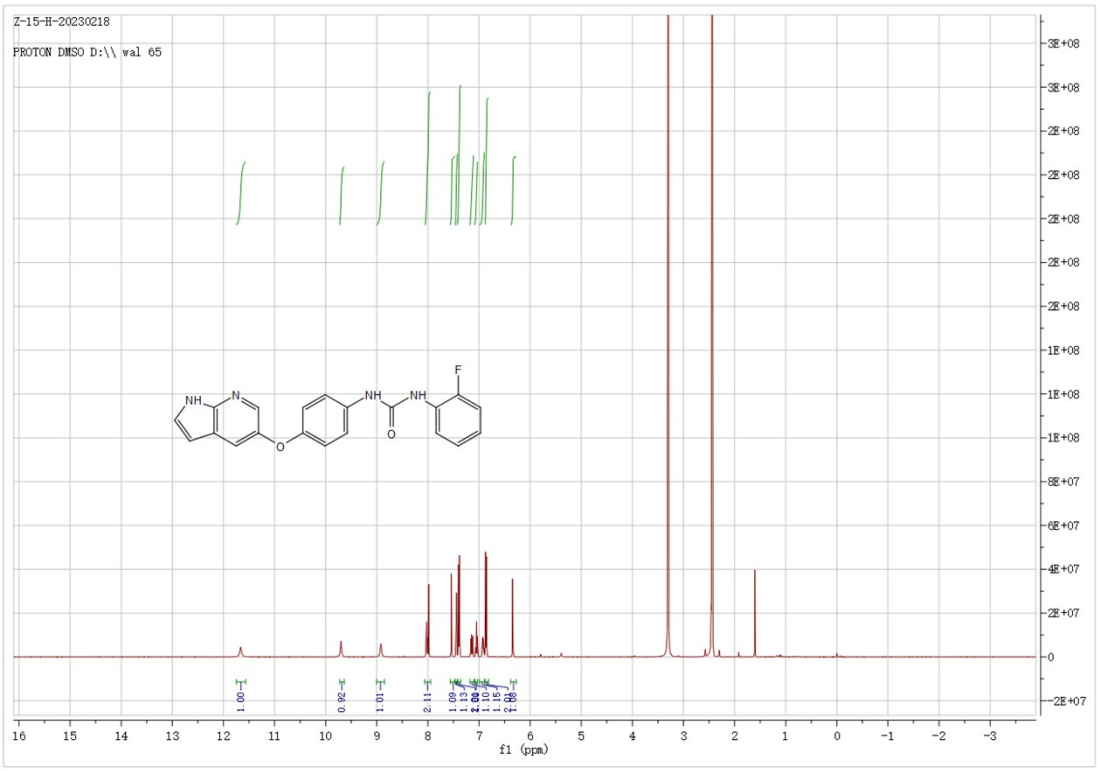


^{13}C NMR spectrum of **21**

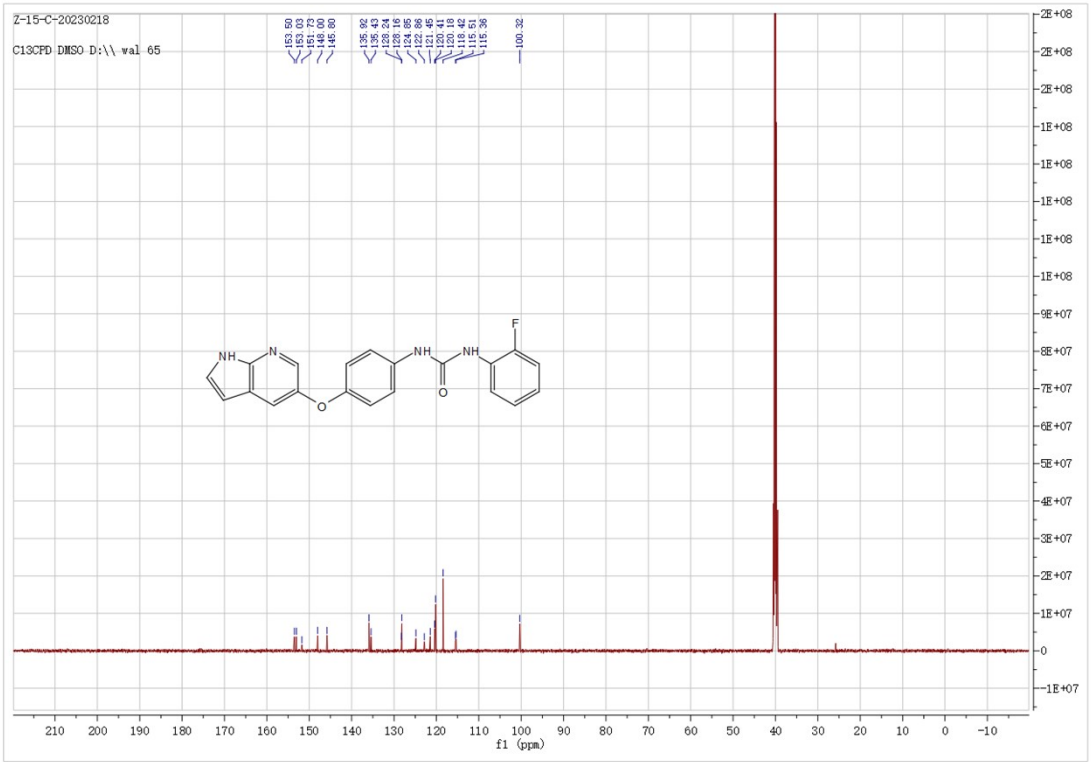


HRMS (ESI) spectrum of **21**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(2-fluorophenyl)urea (**22**)



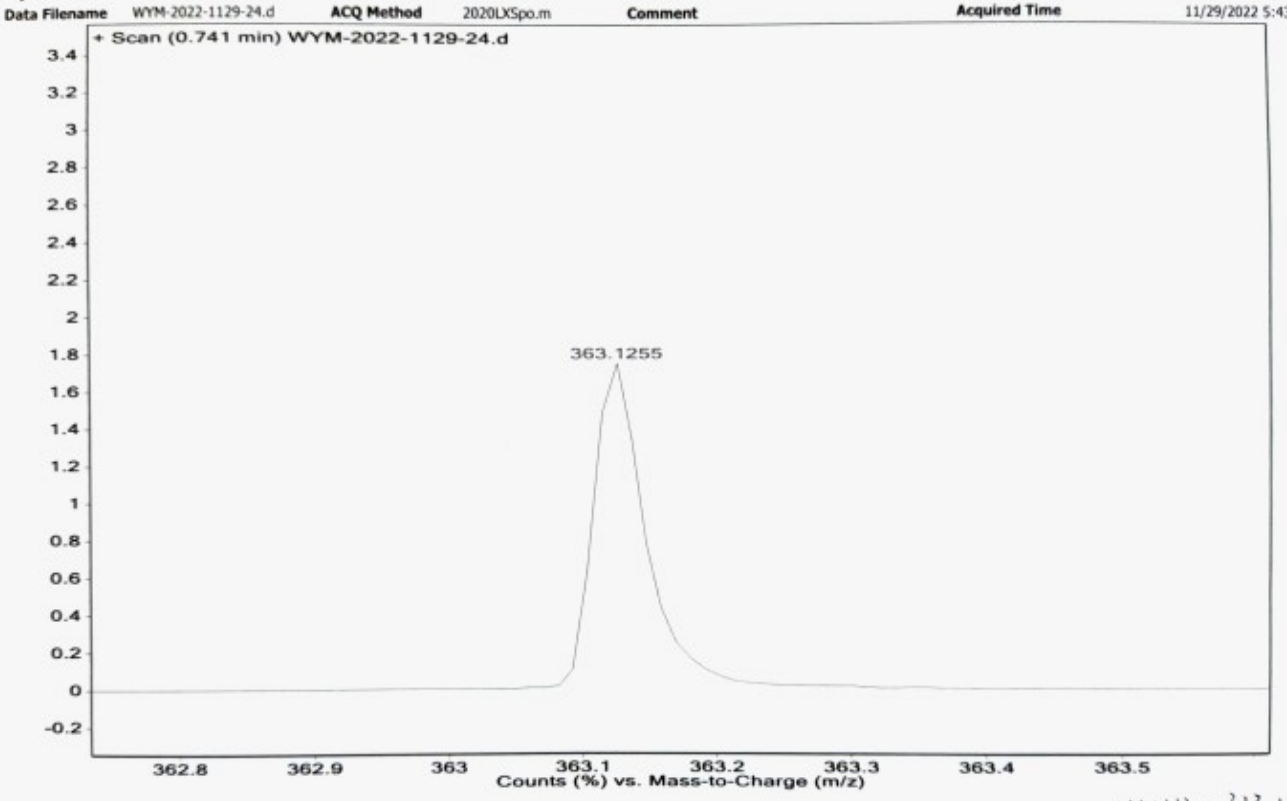
^{1}H NMR spectrum of **22**



^{13}C NMR spectrum of **22**

8

Sample Name	WYM-2022-1129-24	**Position**	Vial 58	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WYM-2022-1129-24.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/29/2022 5:43:46 PM



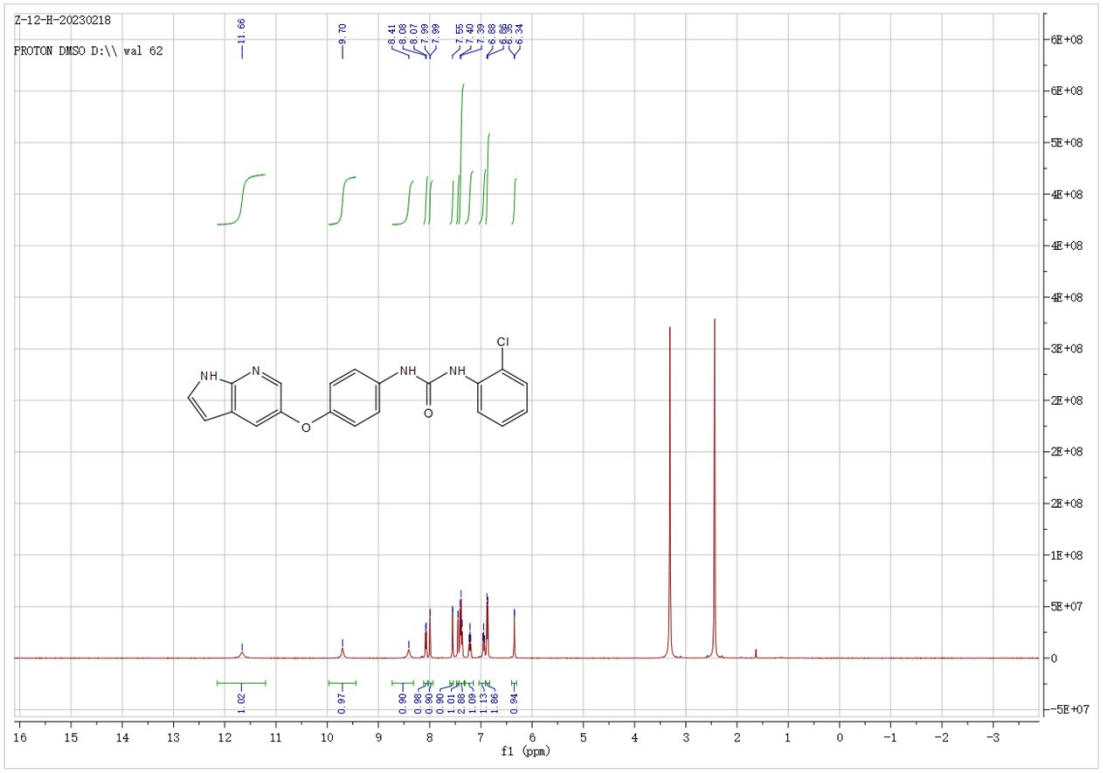
$(M+H)^+$: 363.1252

3709-2

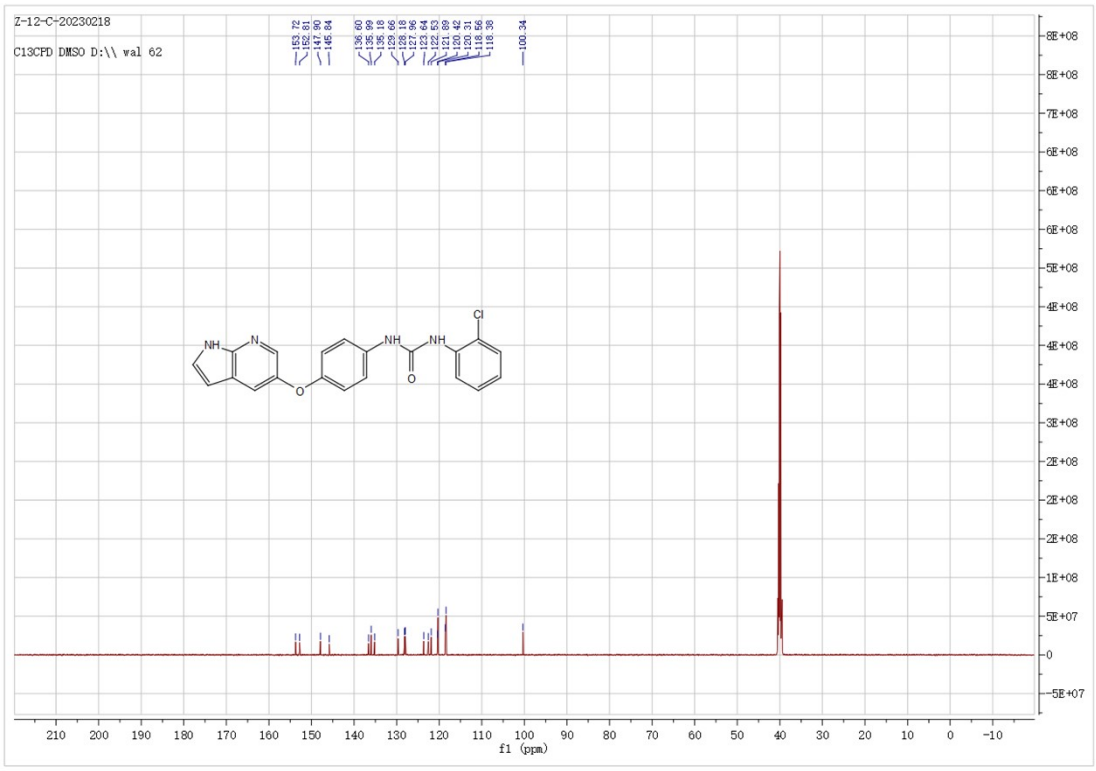
$C_{20}H_{15}FN_4O_2$

HRMS (ESI) spectrum of **22**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(2-chlorophenyl)urea (**23**)



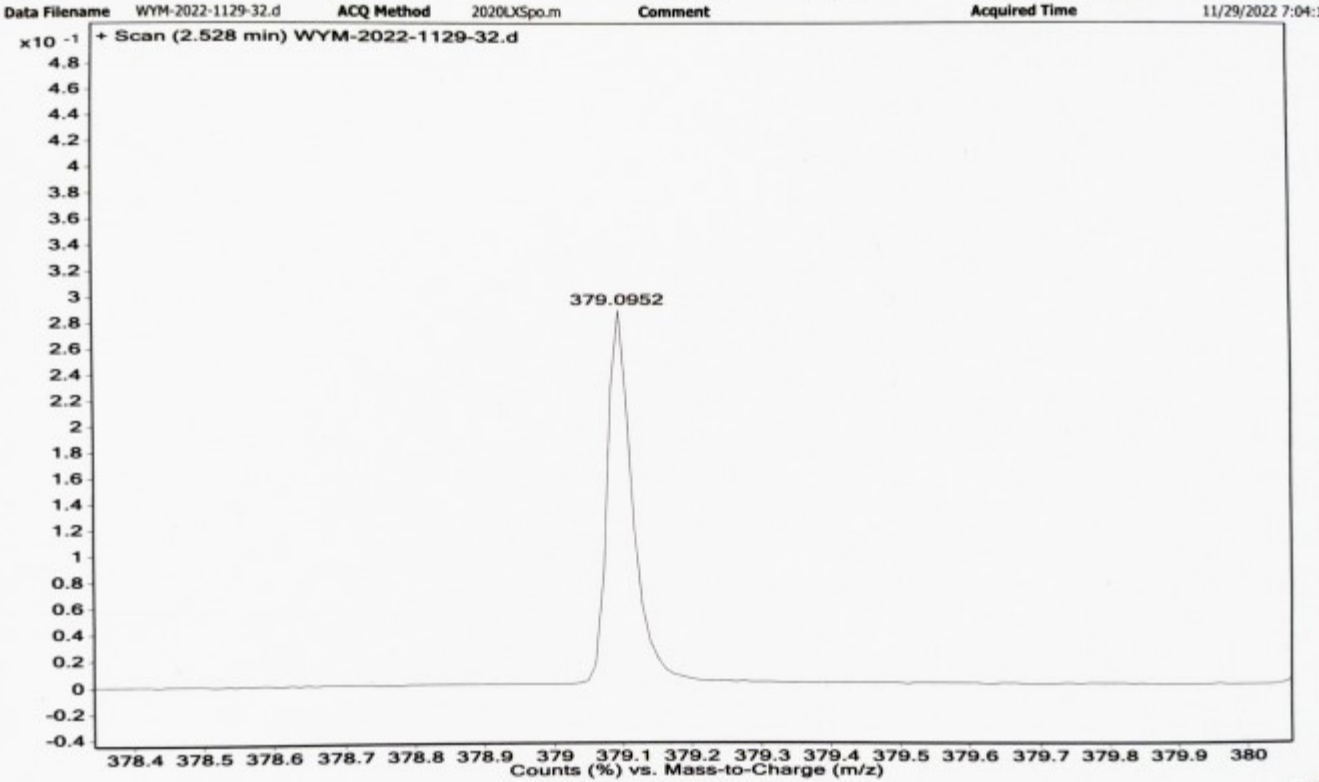
^{1}H NMR spectrum of **23**



^{13}C NMR spectrum of **23**

2

Sample Name	WYM-2022-1129-32	**Position**	Vial 62	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WYM-2022-1129-32.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/29/2022 7:04:13 PM



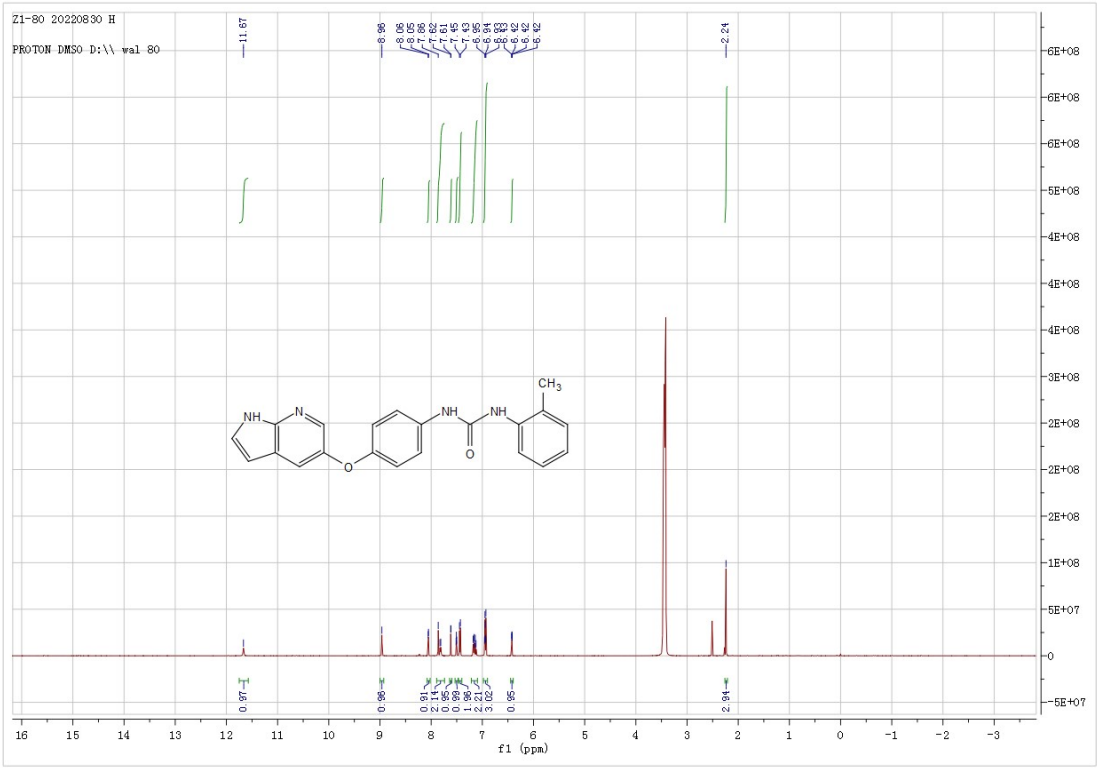
$(M+H)^+$: 379.0956

$C_{20}H_{15}ClN_4O_2$

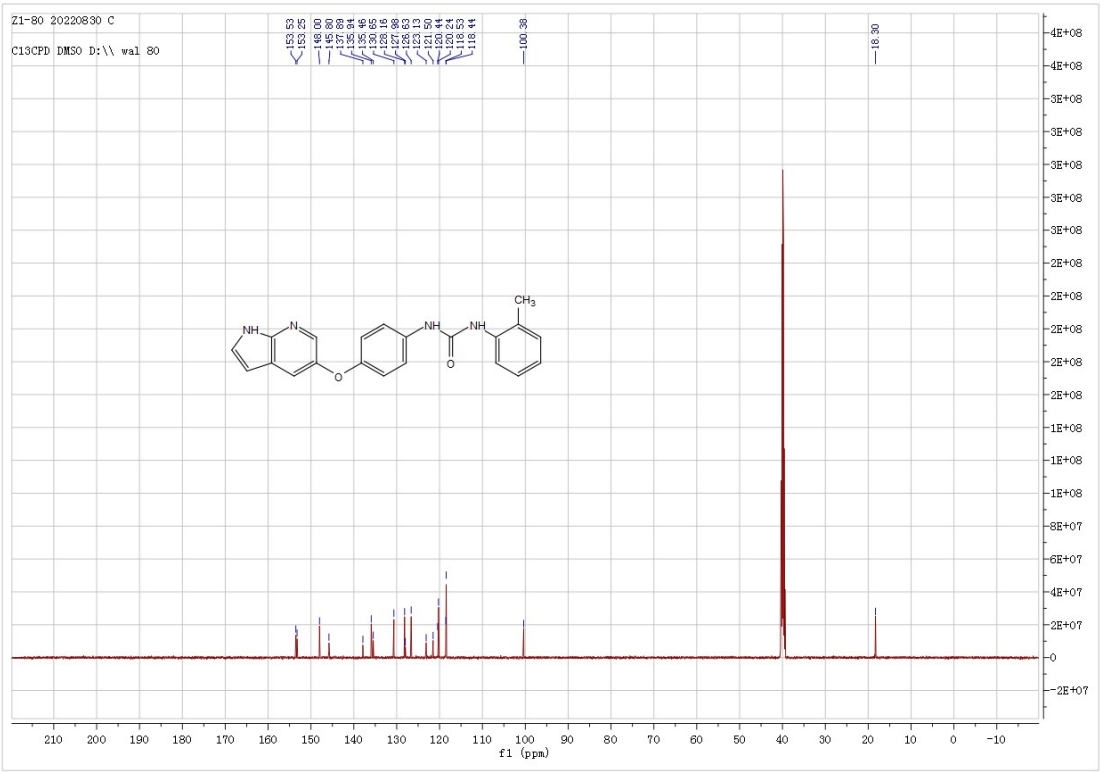
07af-2

HRMS (ESI) spectrum of **23**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(2- methylphenyl)urea (**24**)

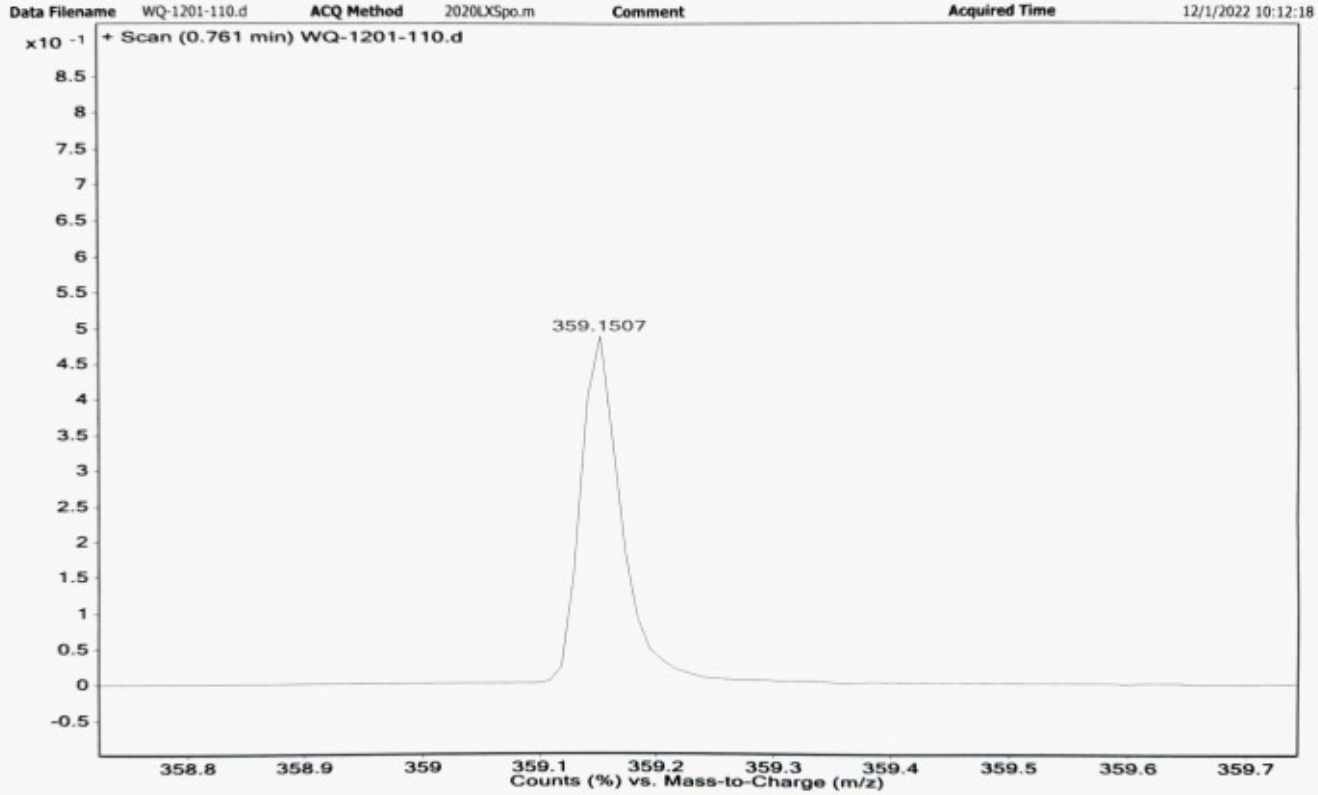


^{1}H NMR spectrum of **24**



^{13}C NMR spectrum of **24**

Sample Name	WQ-1201-110	**Position**	Vial 60	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-1201-110.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	12/1/2022 10:12:18 AM



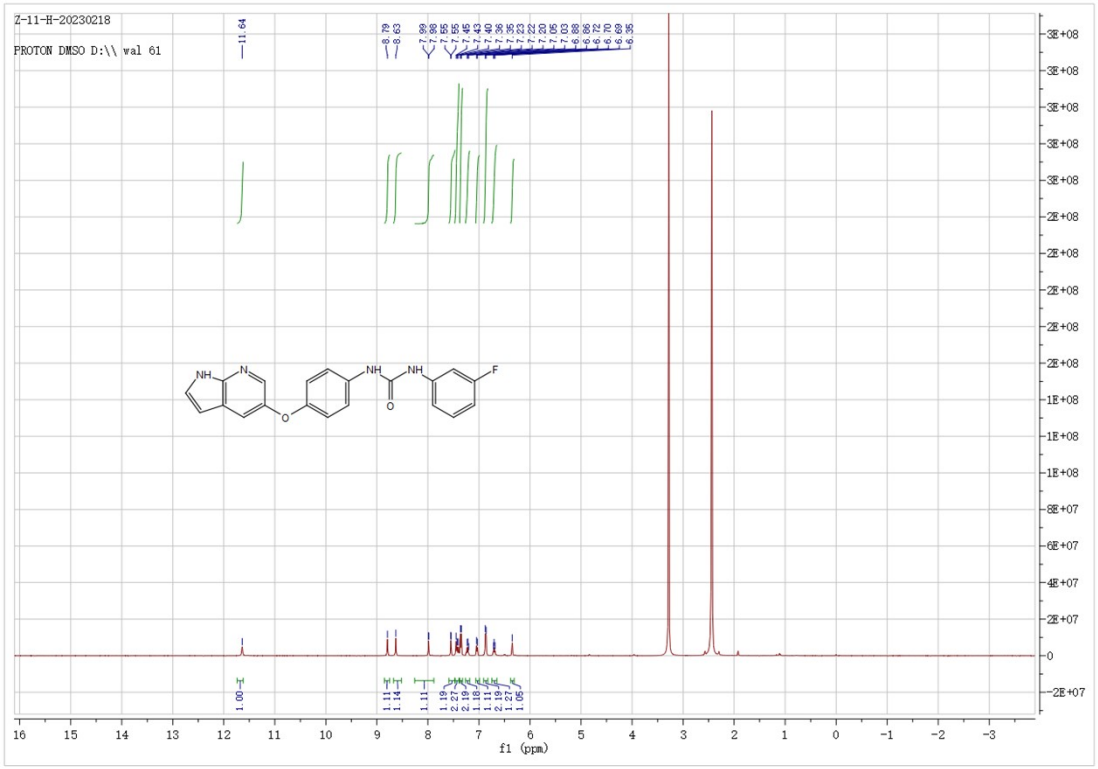
$(M+H)^+$: 359.1503

$C_{21}H_{18}N_4O_2$

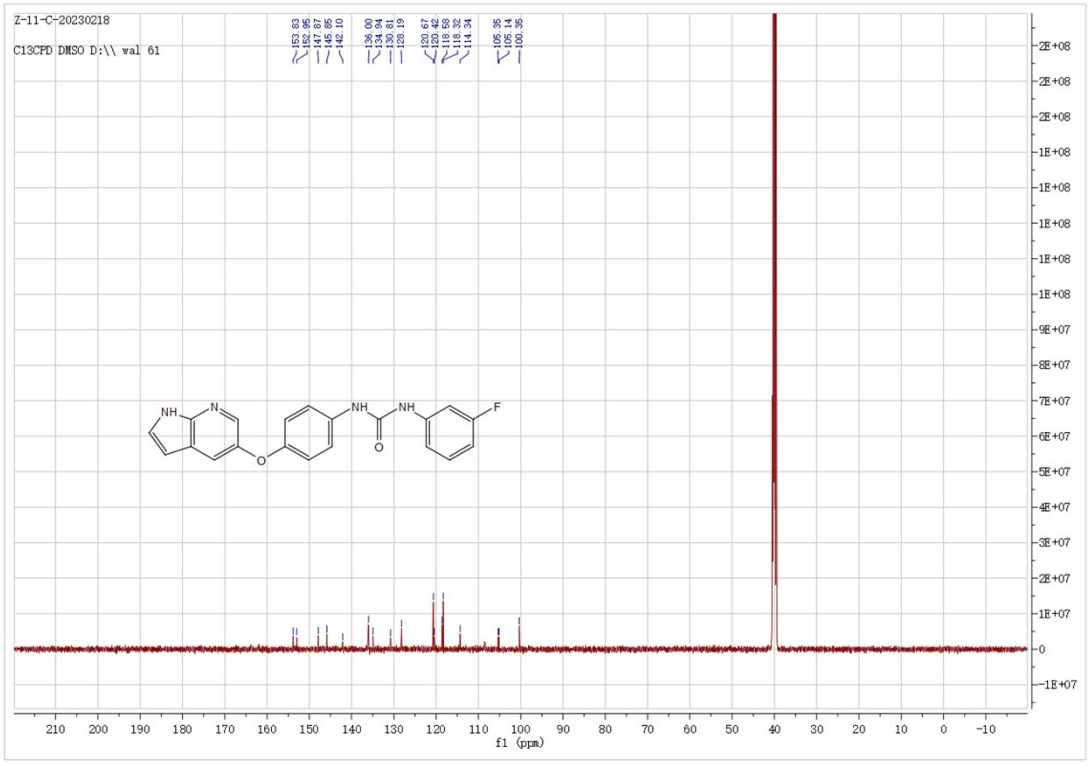
0722-2

HRMS (ESI) spectrum of **24**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-fluorophenyl)urea (**25**)



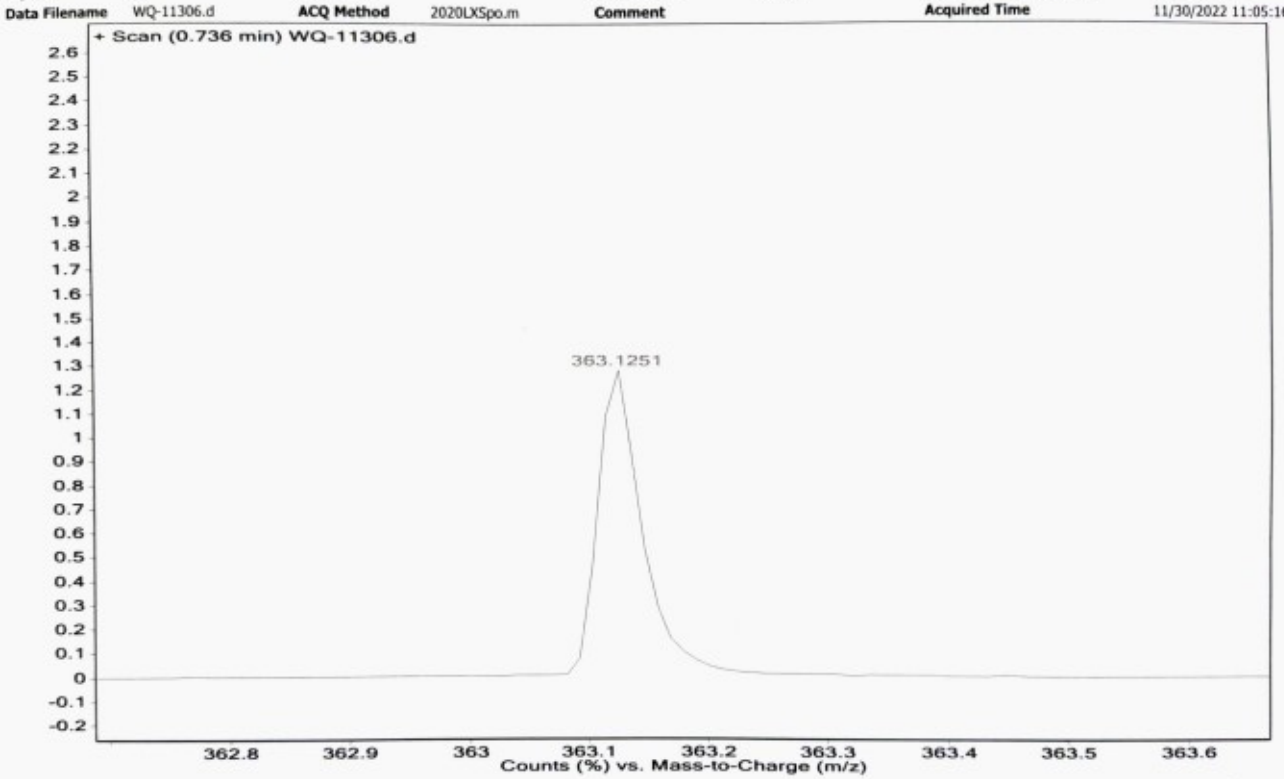
^{1}H NMR spectrum of **25**



^{13}C NMR spectrum of **25**

16

Sample Name	WQ-11306	**Position**	Vial 56	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-11306.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/30/2022 11:05:16 AM



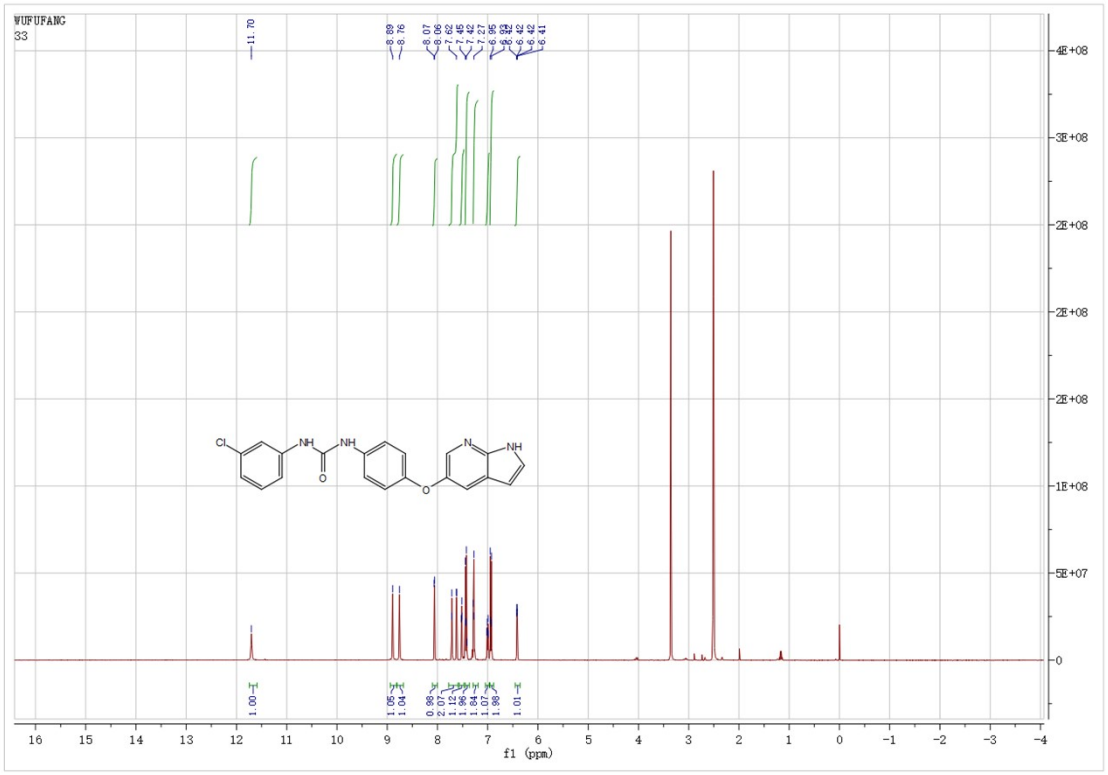
(M+H)+: 363.1252

$C_{20}H_{15}FN_4O_3$

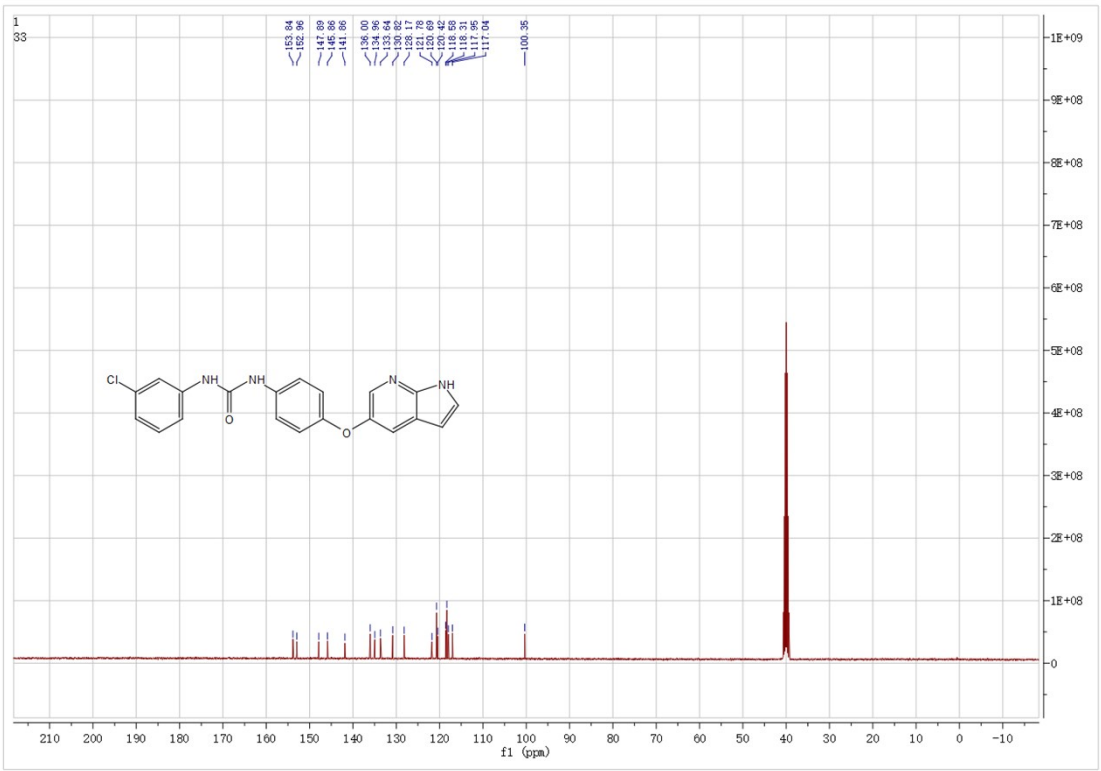
0716-4

HRMS (ESI) spectrum of **25**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-chlorophenyl)urea (**26**)

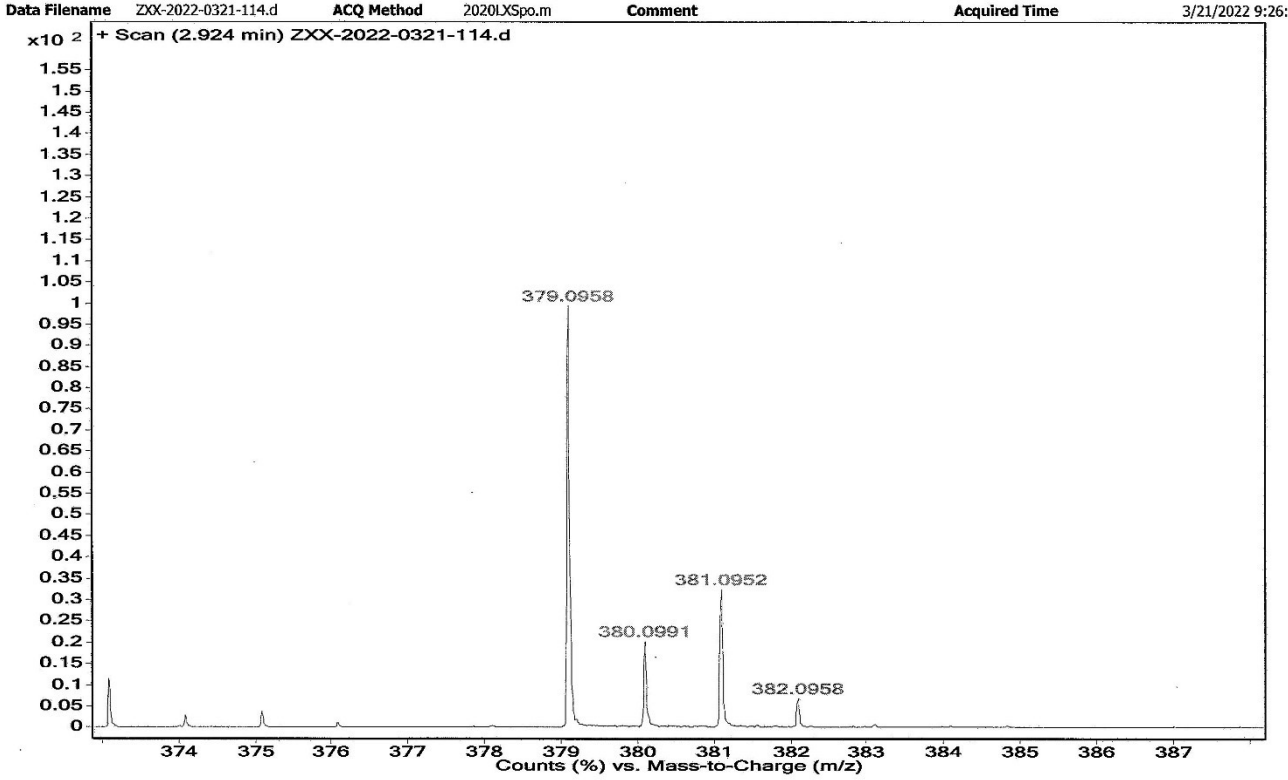


^{1}H NMR spectrum of **26**



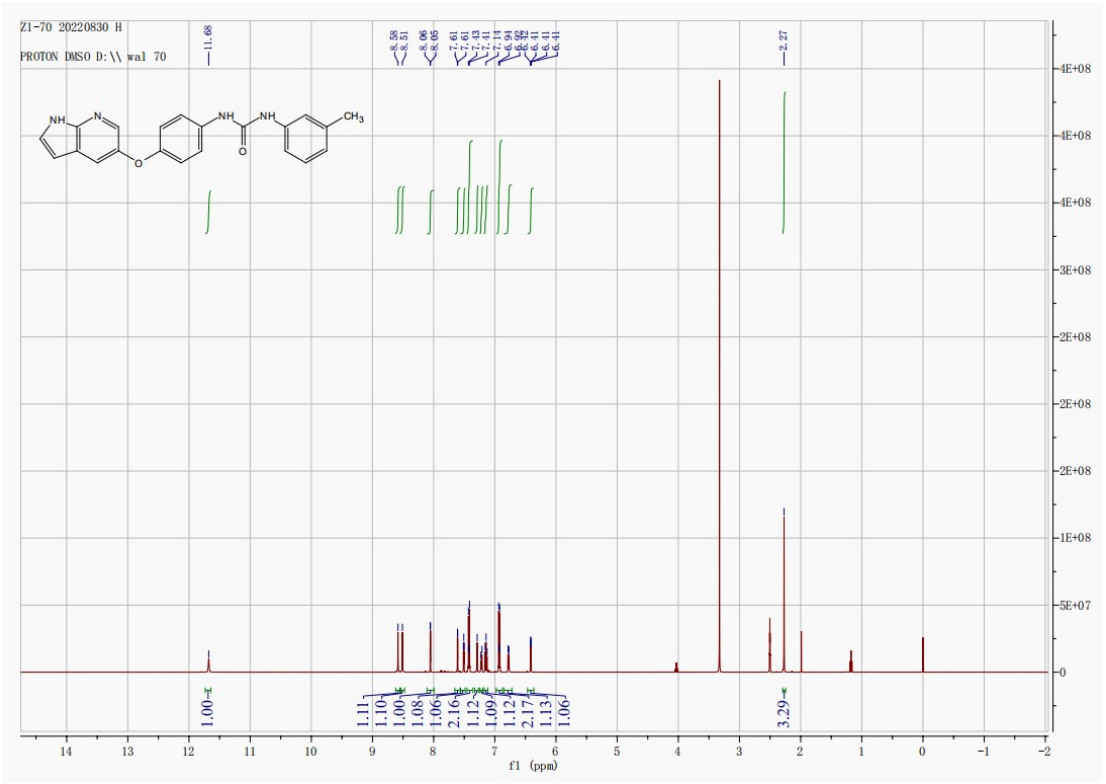
^{13}C NMR spectrum of **26**

Sample Name	ZXX-2022-0321-114	**Position**	Vial 14	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	ZXX-2022-0321-114.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	3/21/2022 9:26:52 PM

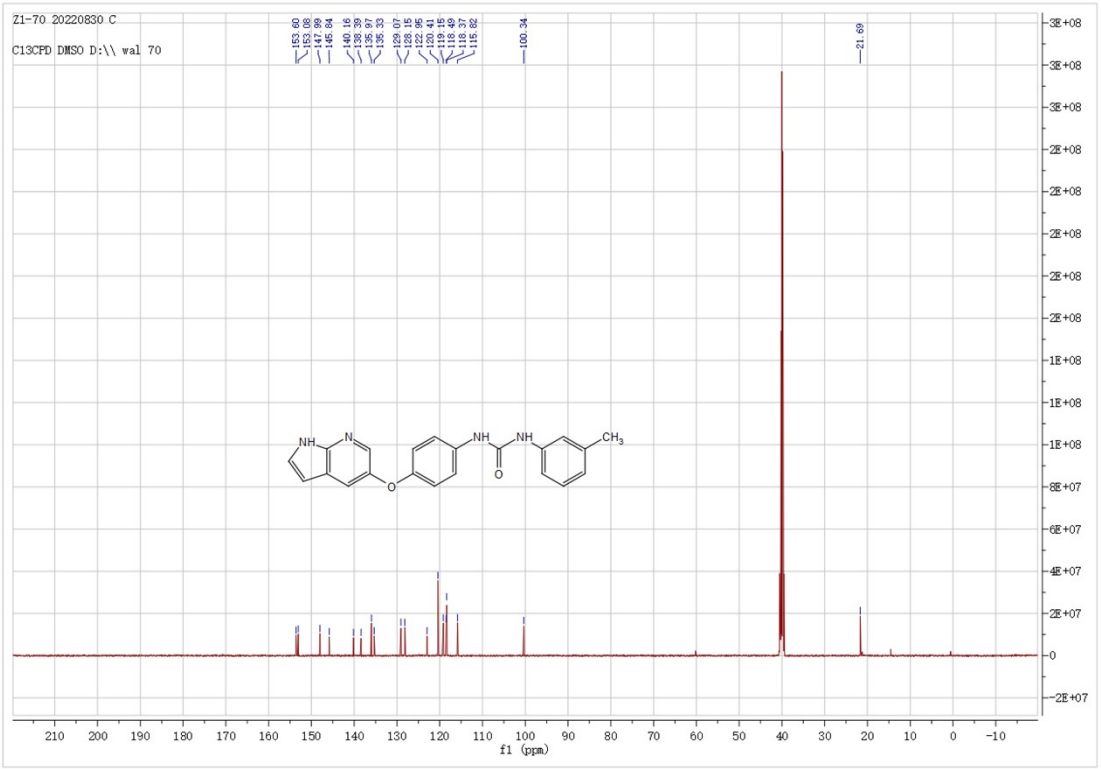


0321-2

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-methylphenyl)urea (**27**)



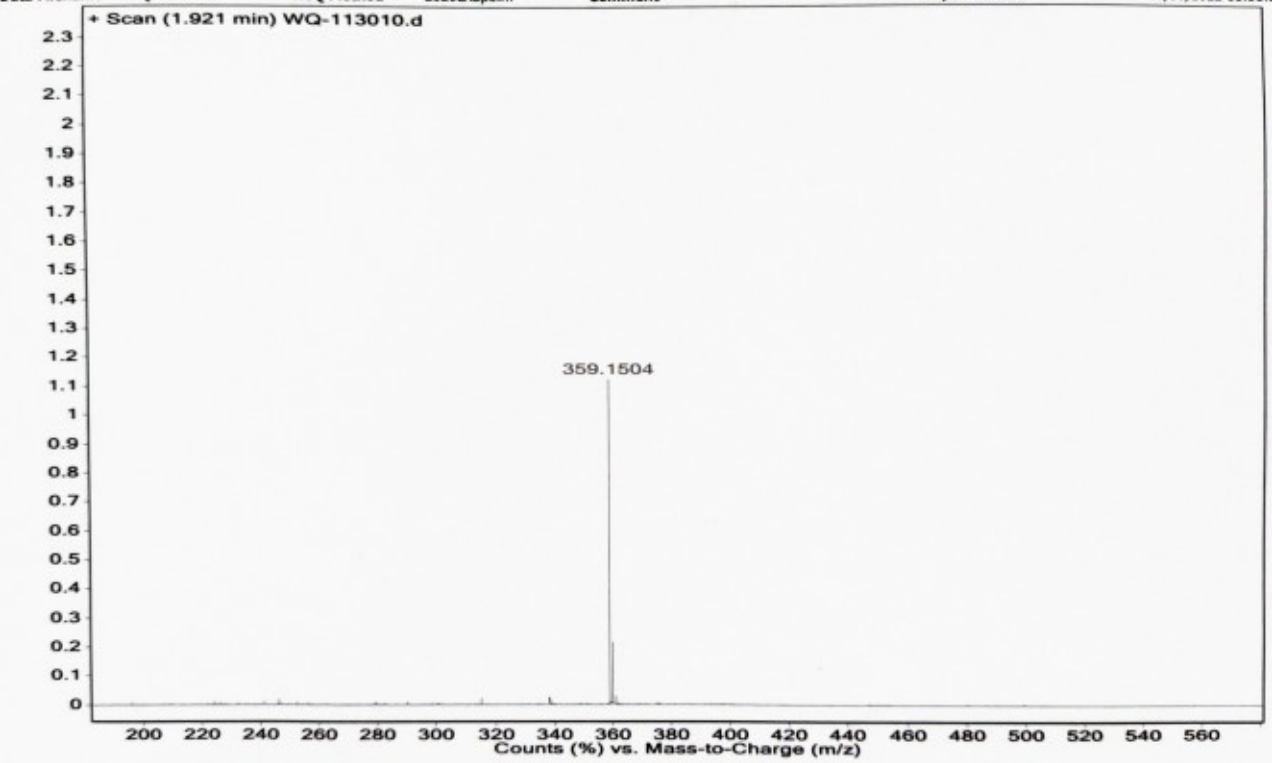
^{1}H NMR spectrum of **27**



^{13}C NMR spectrum of **27**

20

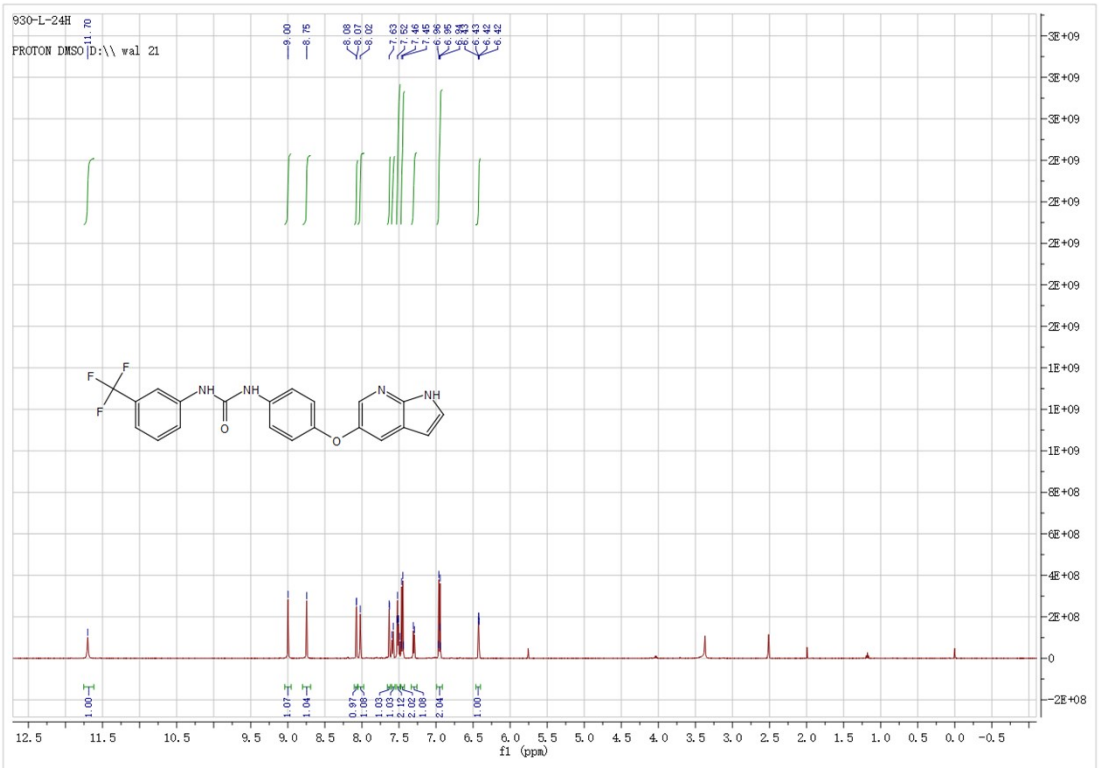
Sample Name	WQ-113010	**Position**	Vial 60	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-113010.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/30/2022 11:38:58 AM



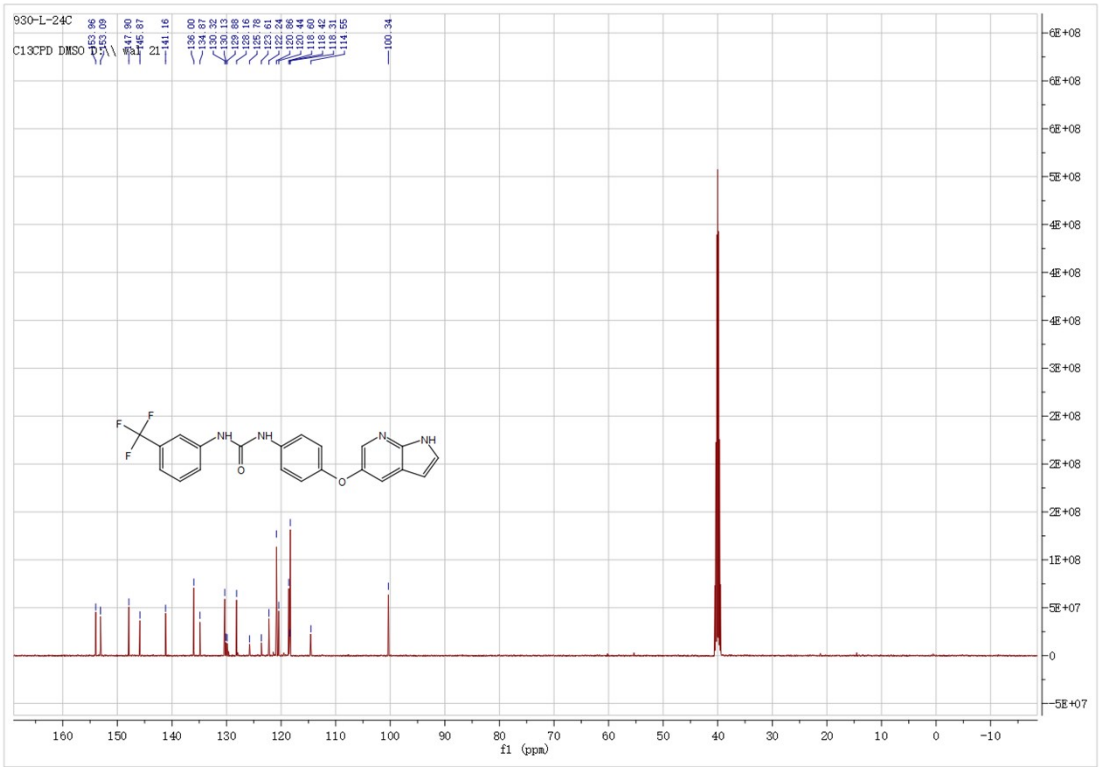
M+H = 359.1503
$C_{21}H_{18}N_4O_2$
0720-1

HRMS (ESI) spectrum of **27**

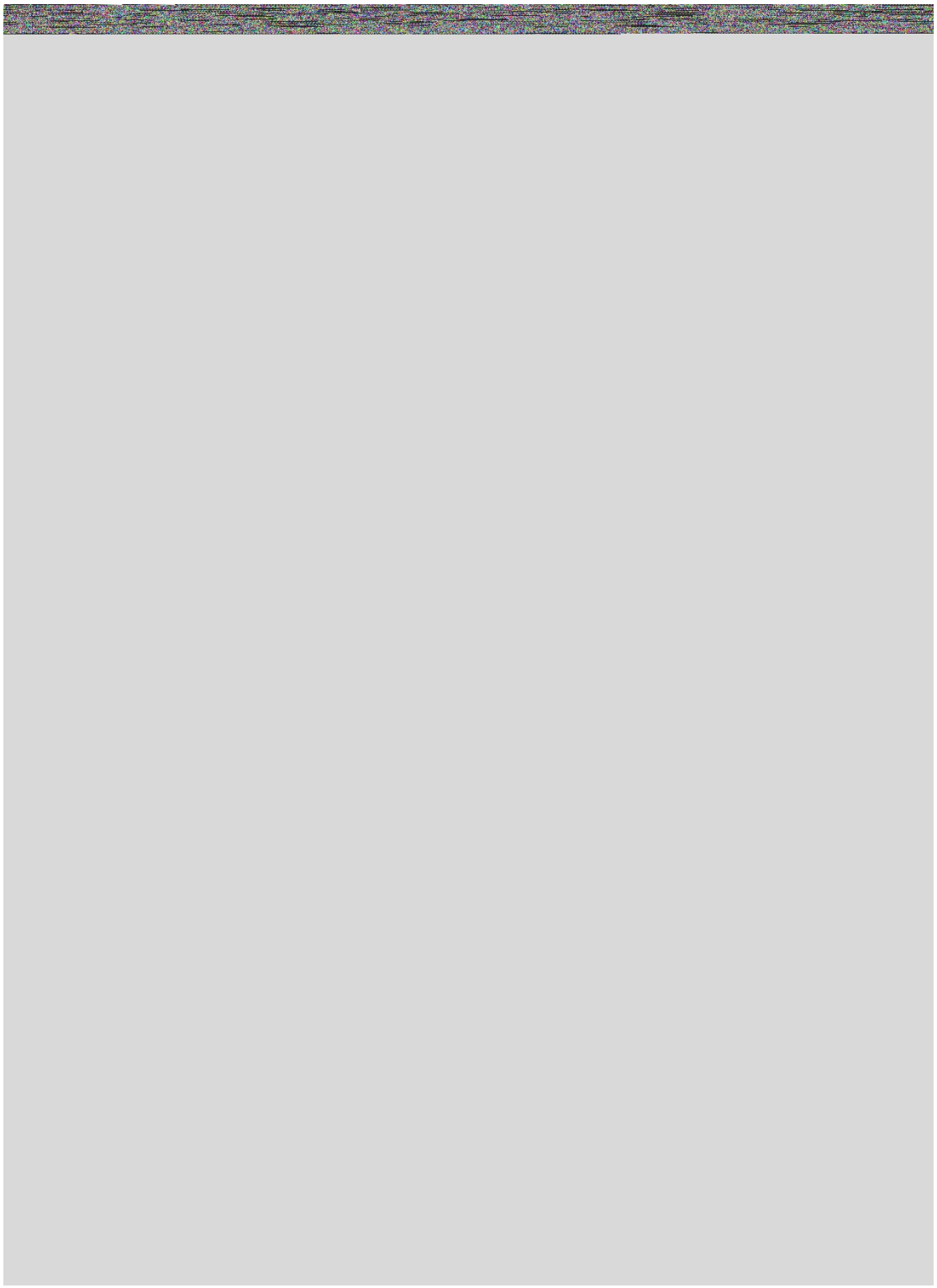
1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-(trifluoromethyl)phenyl)urea (**28**)



^{1}H NMR spectrum of **28**

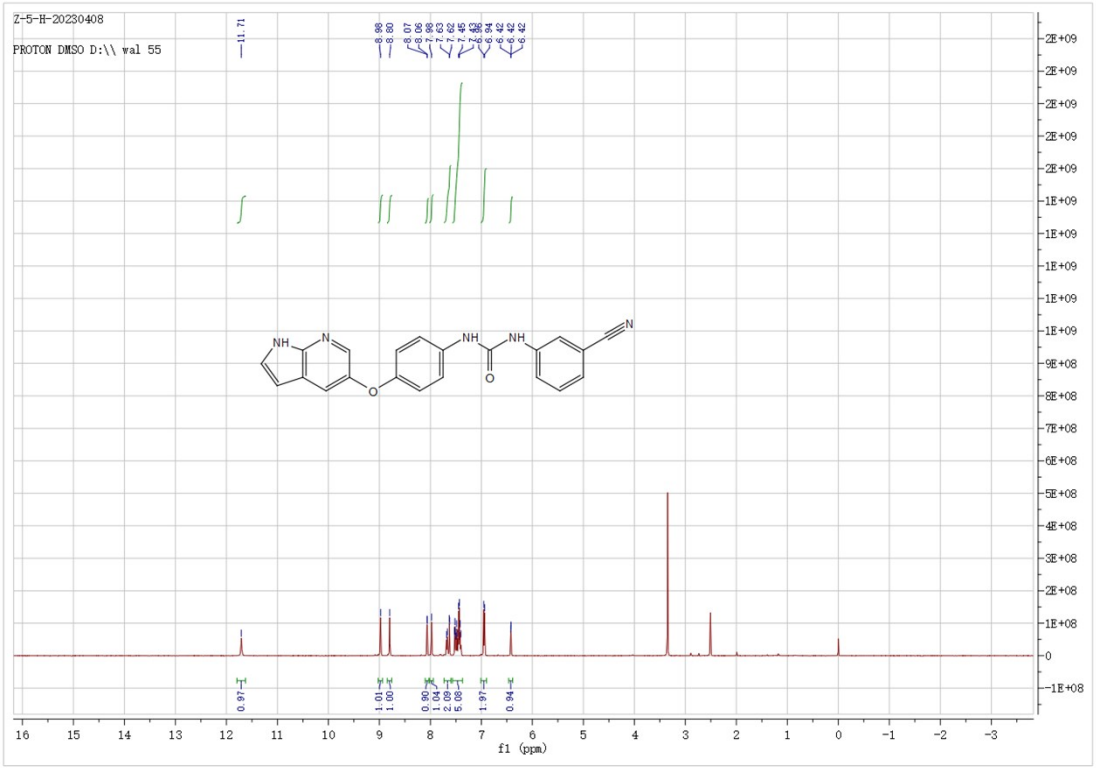


^{13}C NMR spectrum of **28**

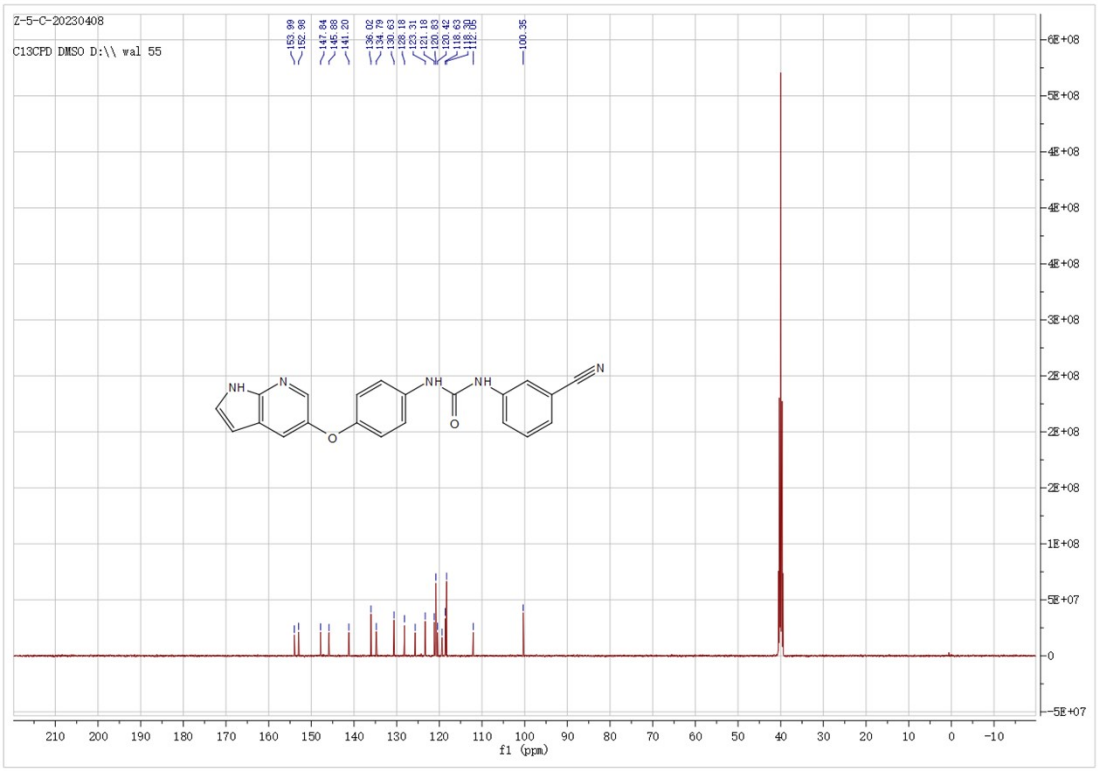


HRMS (ESI) spectrum of **28**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-cyanophenyl)urea (**29**)

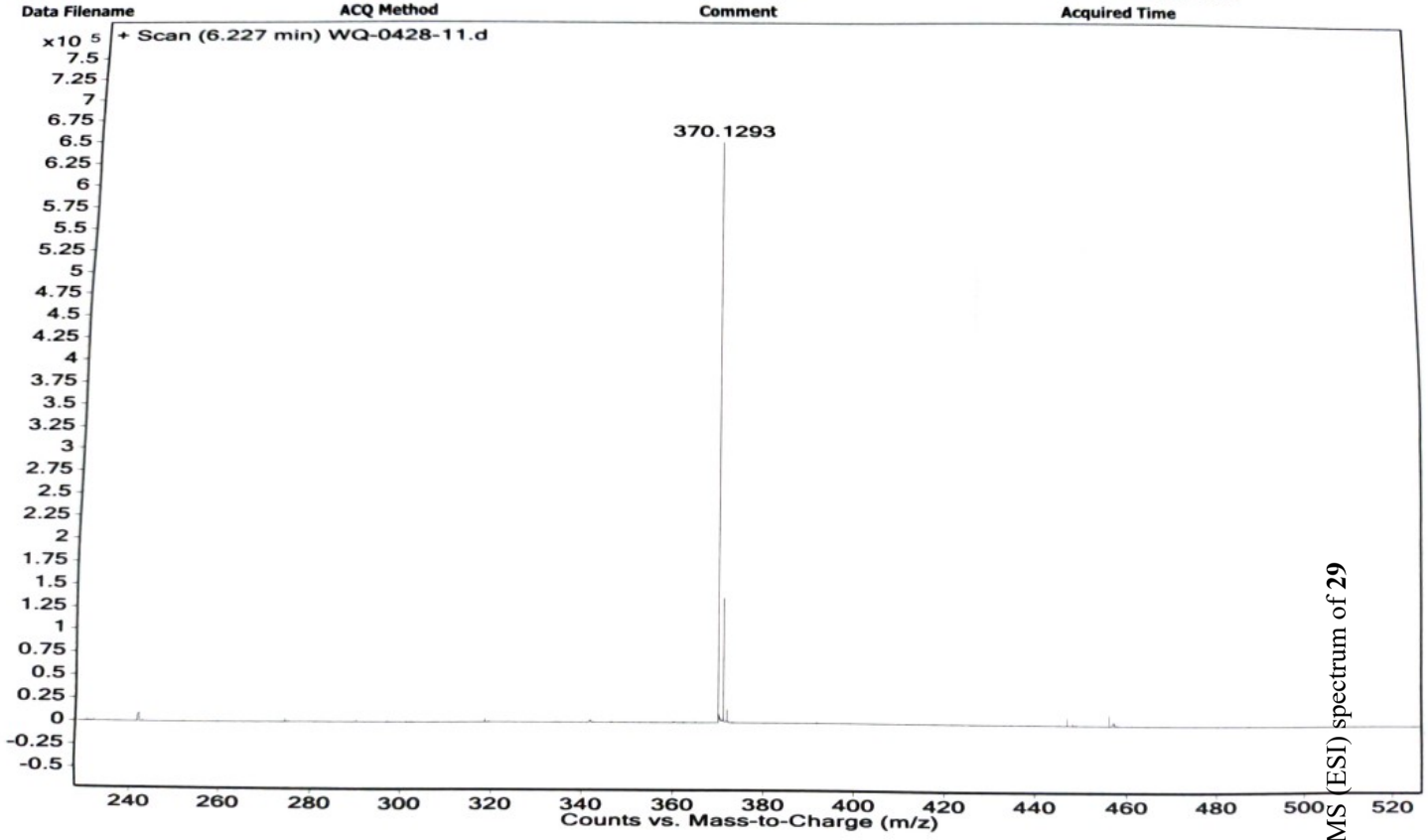


^{1}H NMR spectrum of **29**



^{13}C NMR spectrum of **29**

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



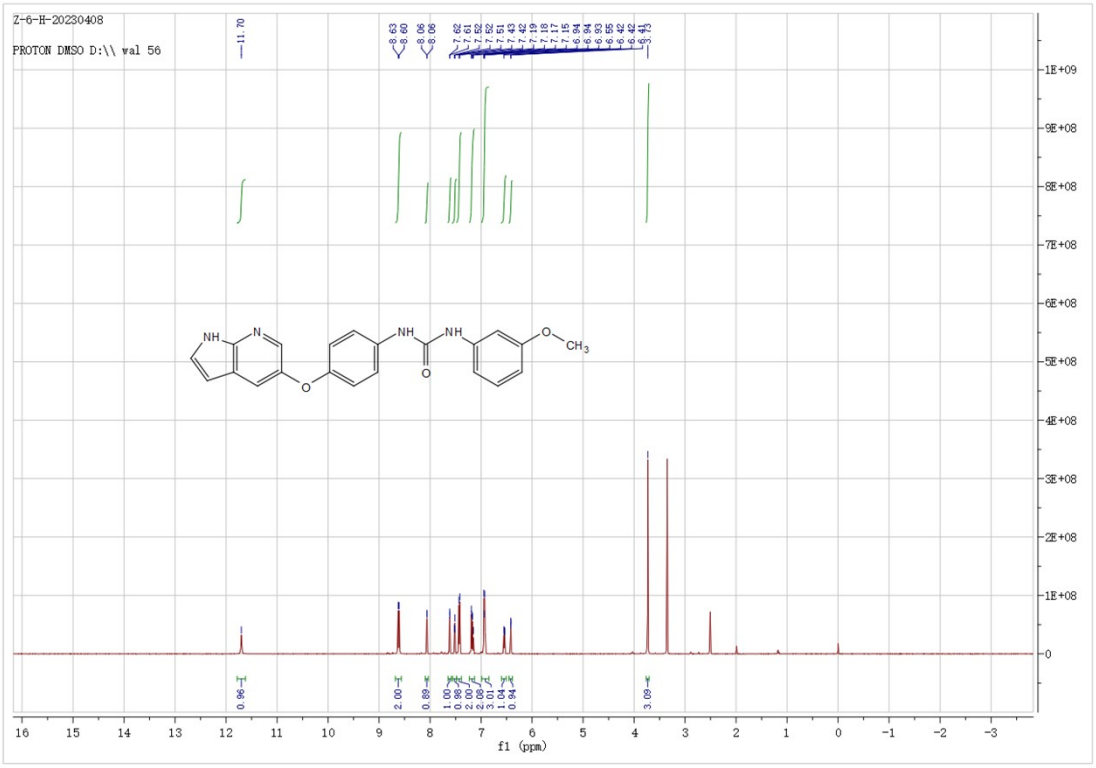
HRMS (ESI) spectrum of **29**

0316-1

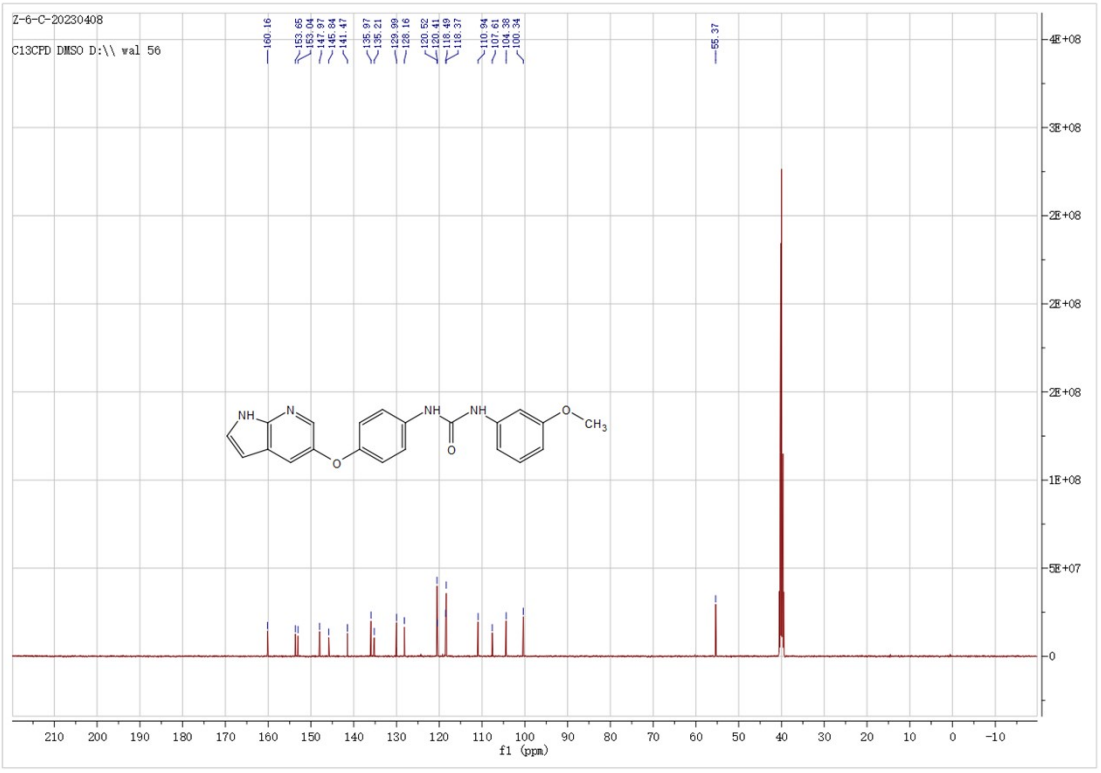
分子式：$C_{14}H_{15}O_2N_5$

分子量：370.1299

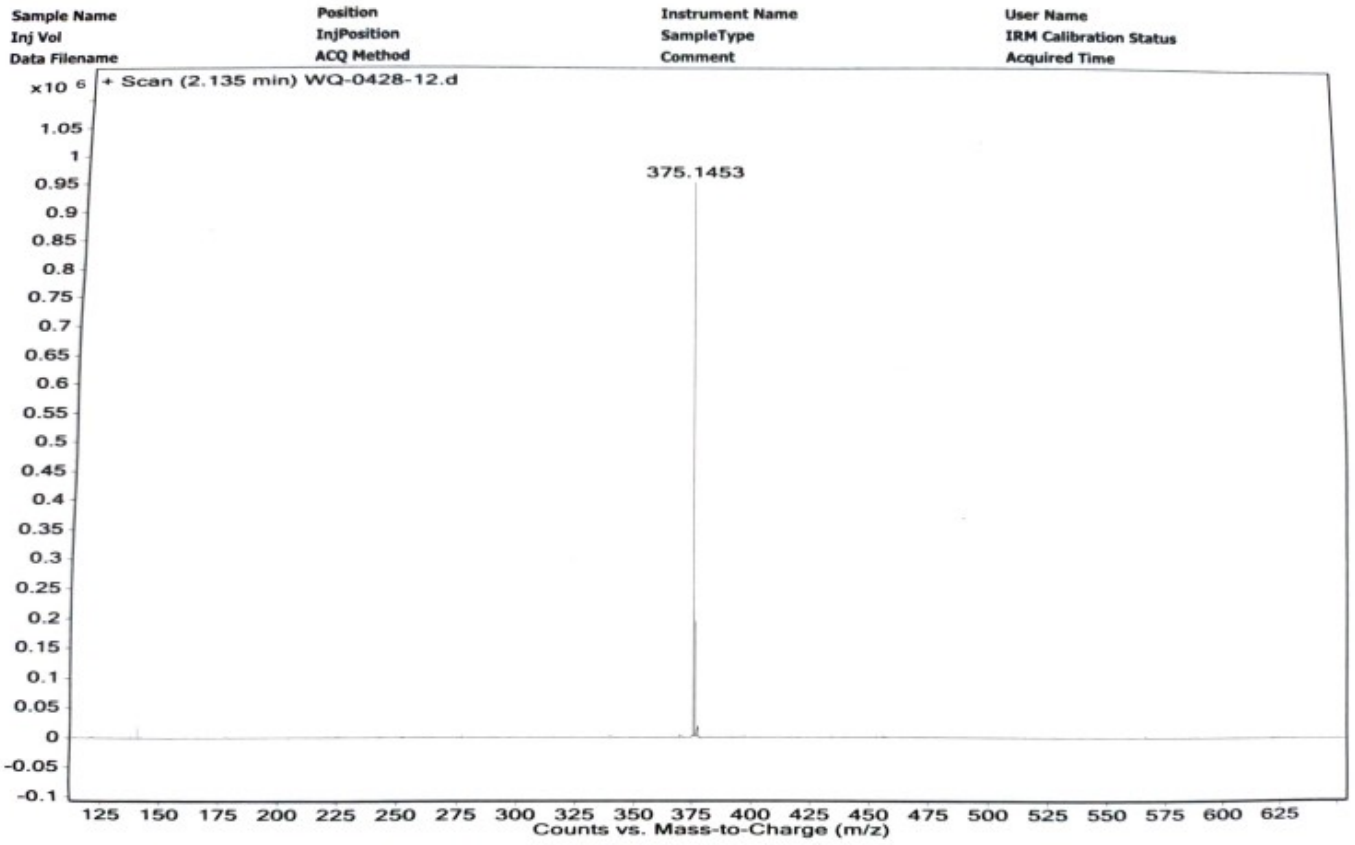
1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-methoxyphenyl)urea (**30**)



^{1}H NMR spectrum of **30**



^{13}C NMR spectrum of **30**

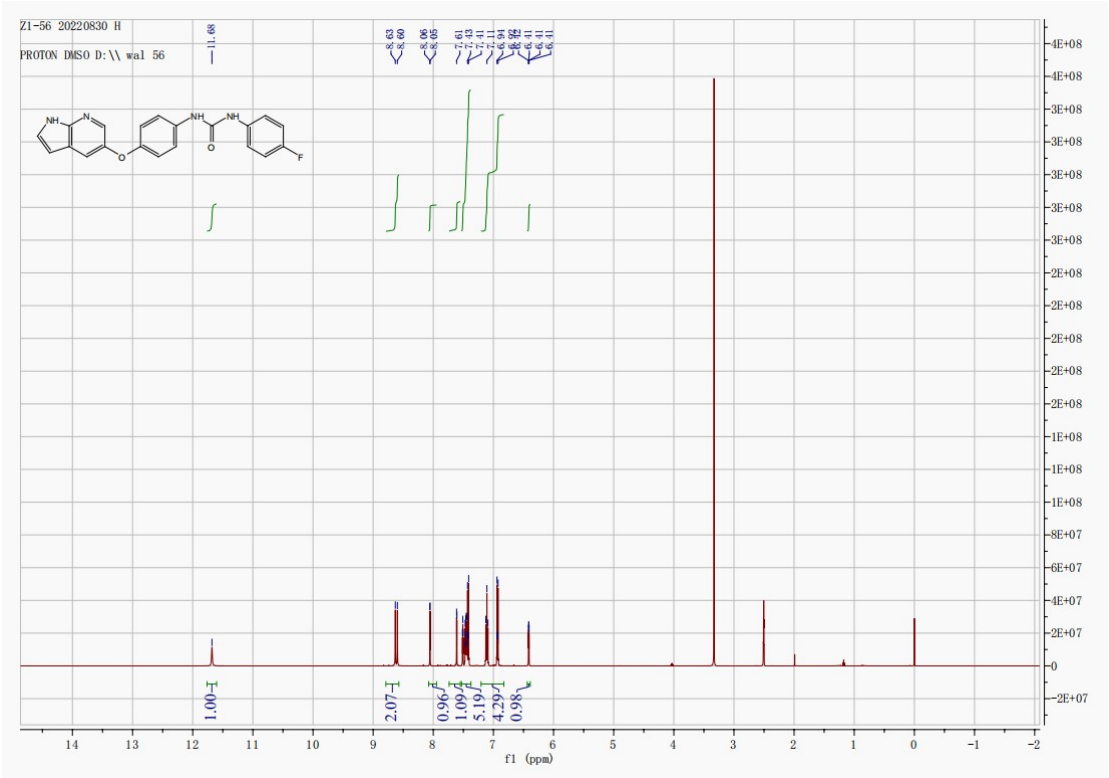


0316-2

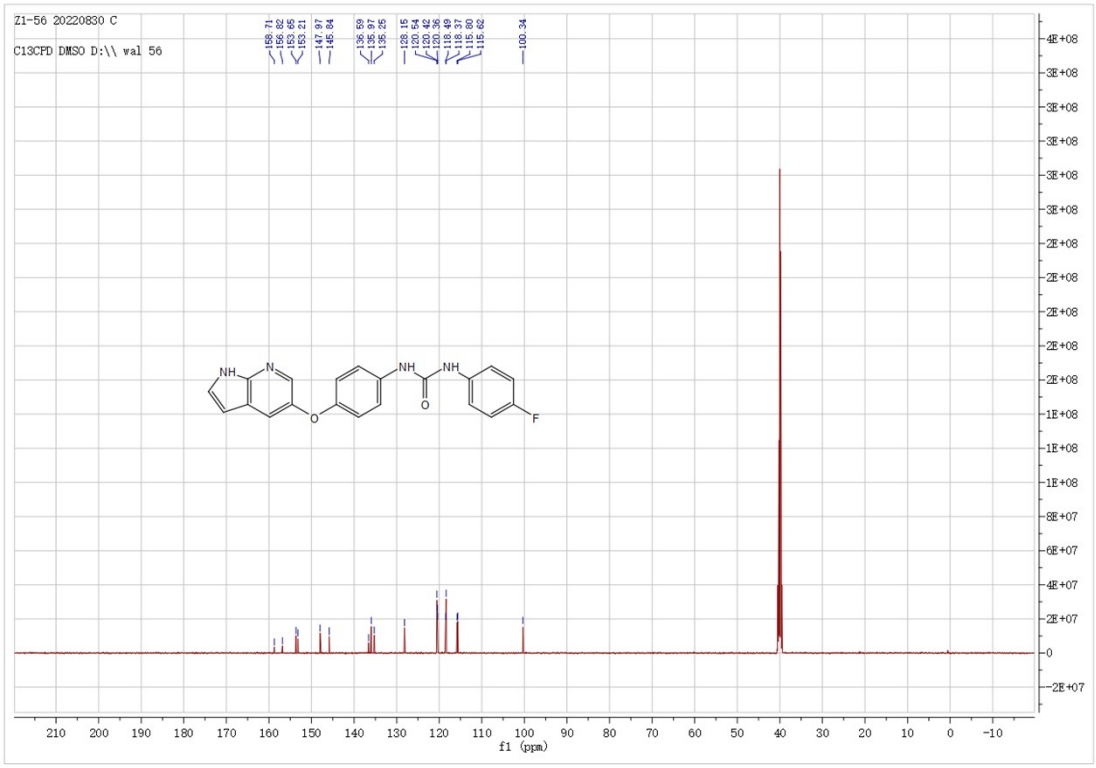
分子式 $C_{21}H_{18}O_3N_4$

分子量：375.1452

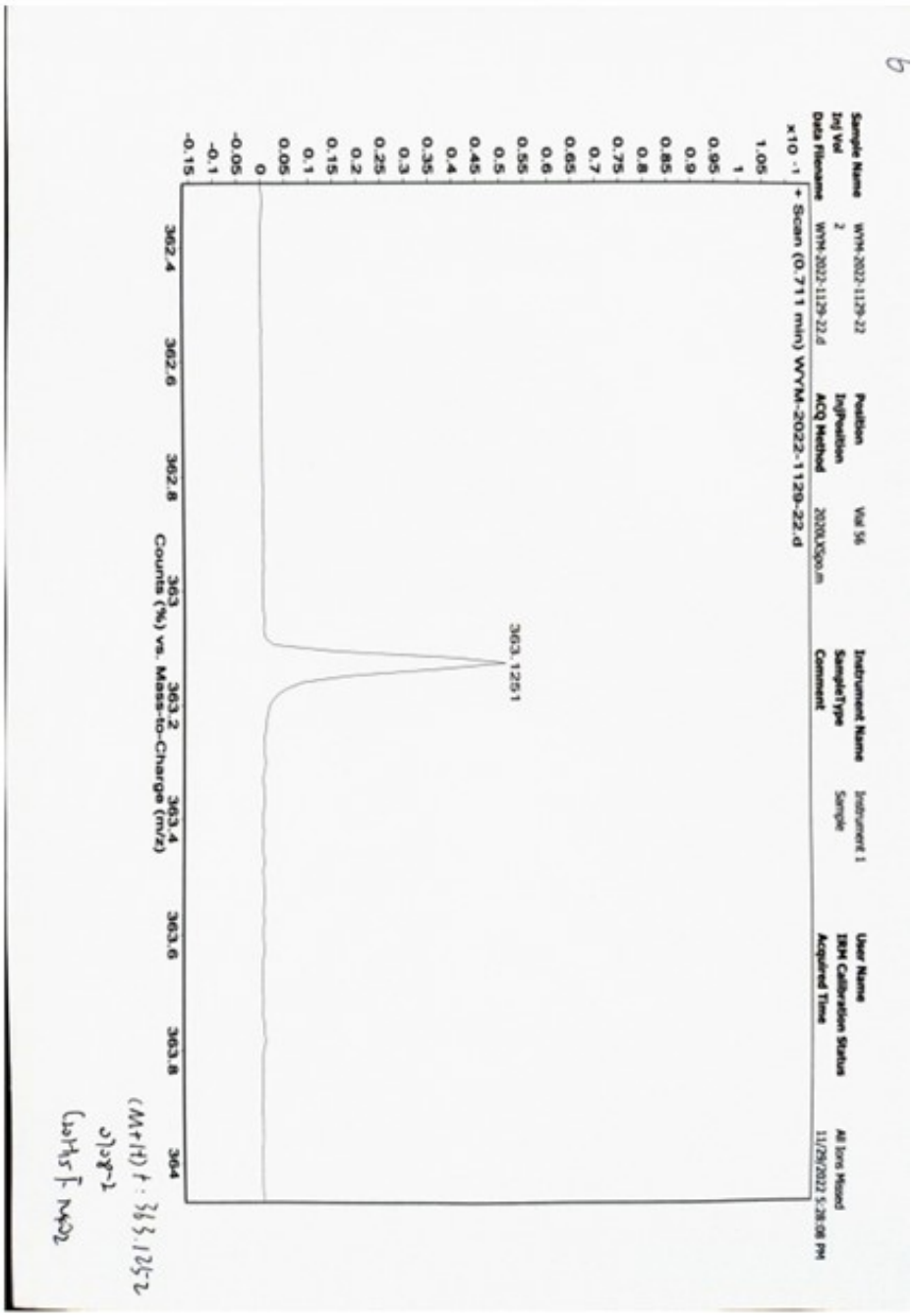
1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-fluorophenyl)urea (**31**)



^{1}H NMR spectrum of **31**

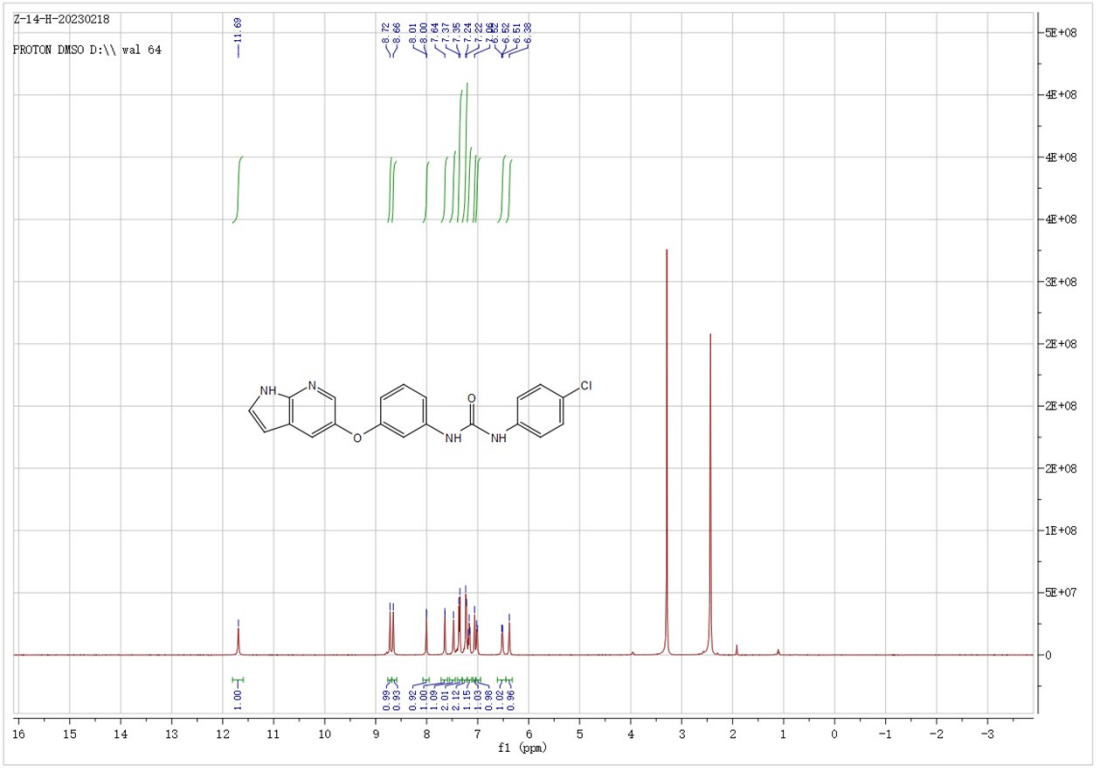


^{13}C NMR spectrum of **31**

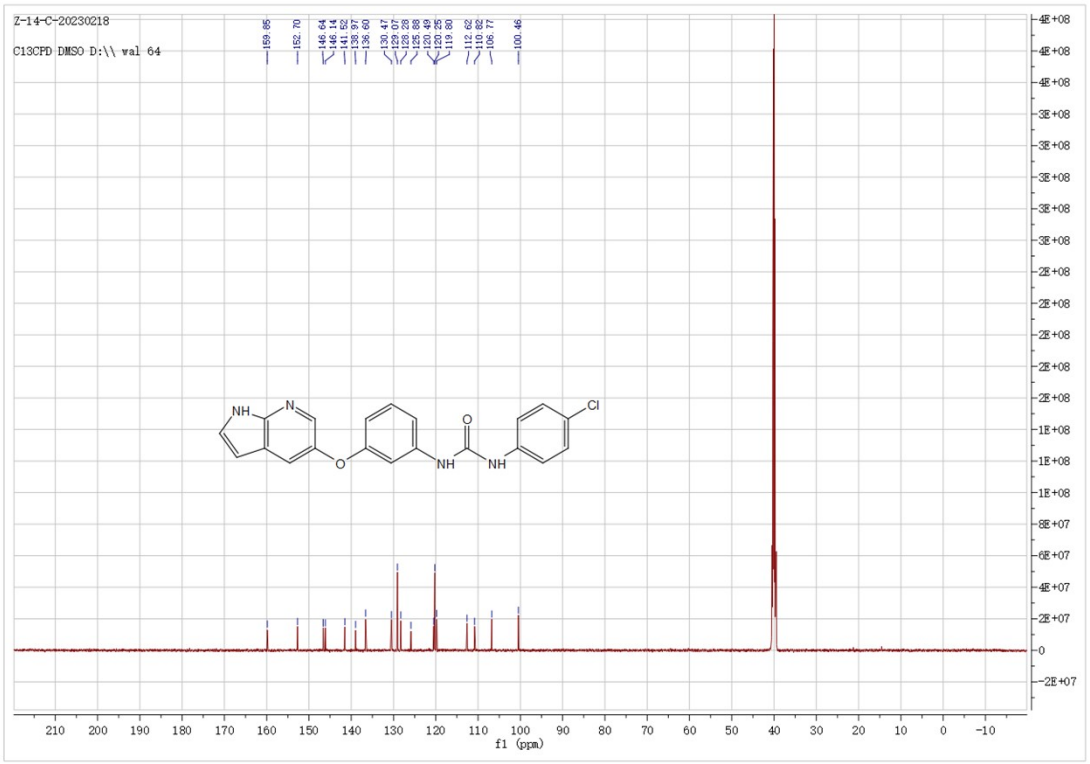


HRMS (ESI) spectrum of **31**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-chlorophenyl)urea (**32**)



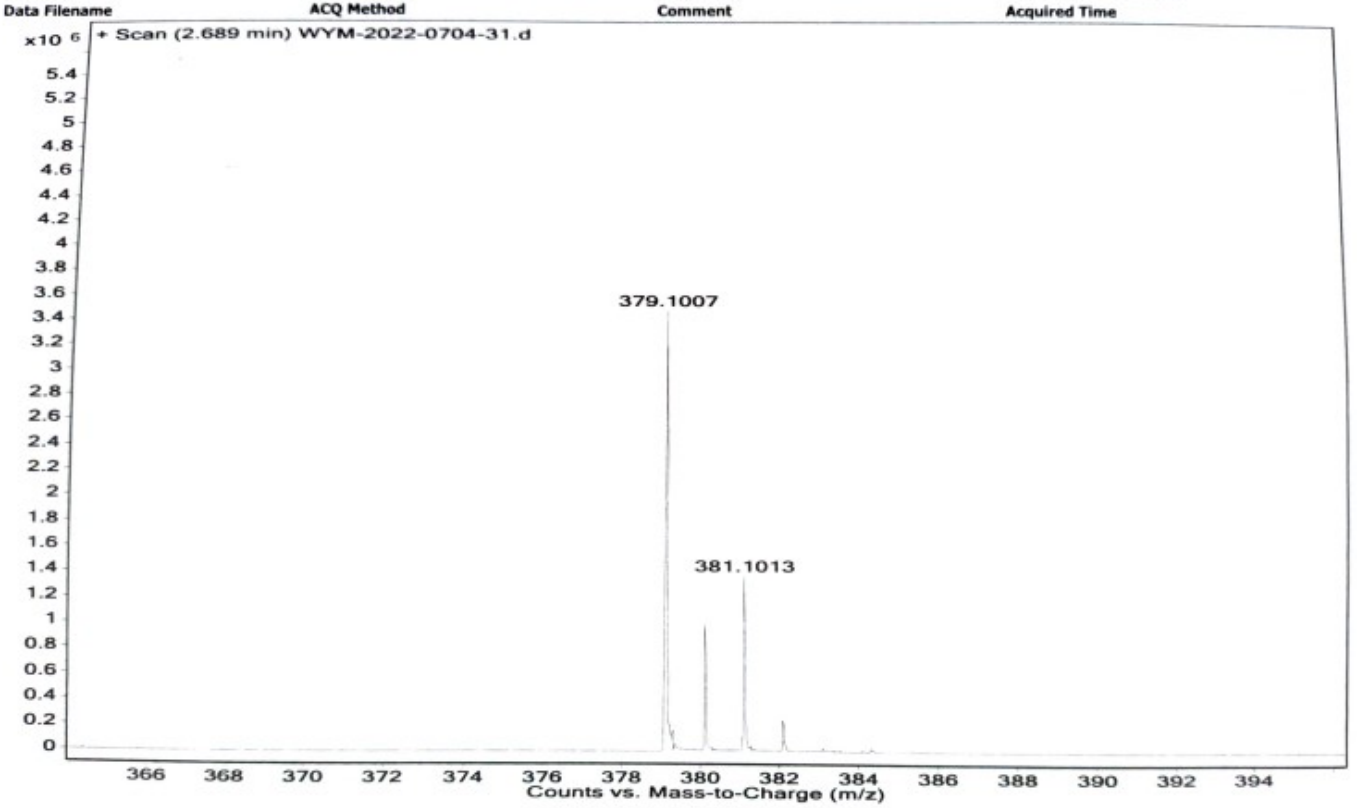
^{1}H NMR spectrum of **32**



^{13}C NMR spectrum of **32**

32

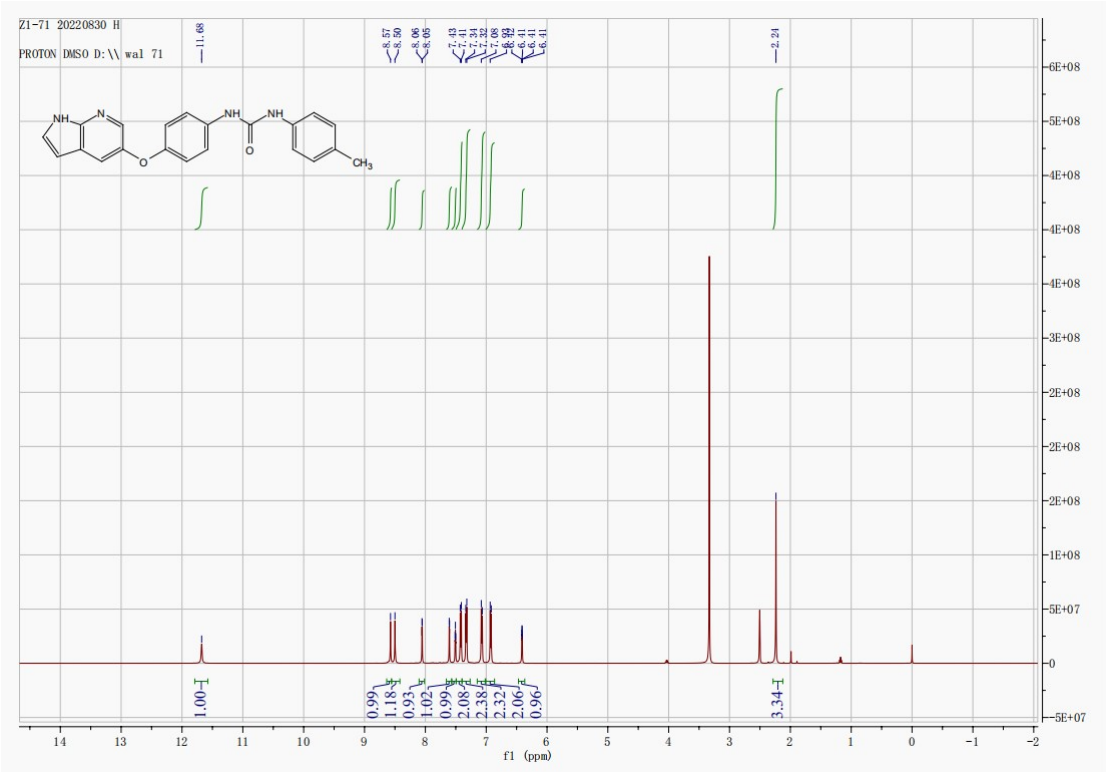
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



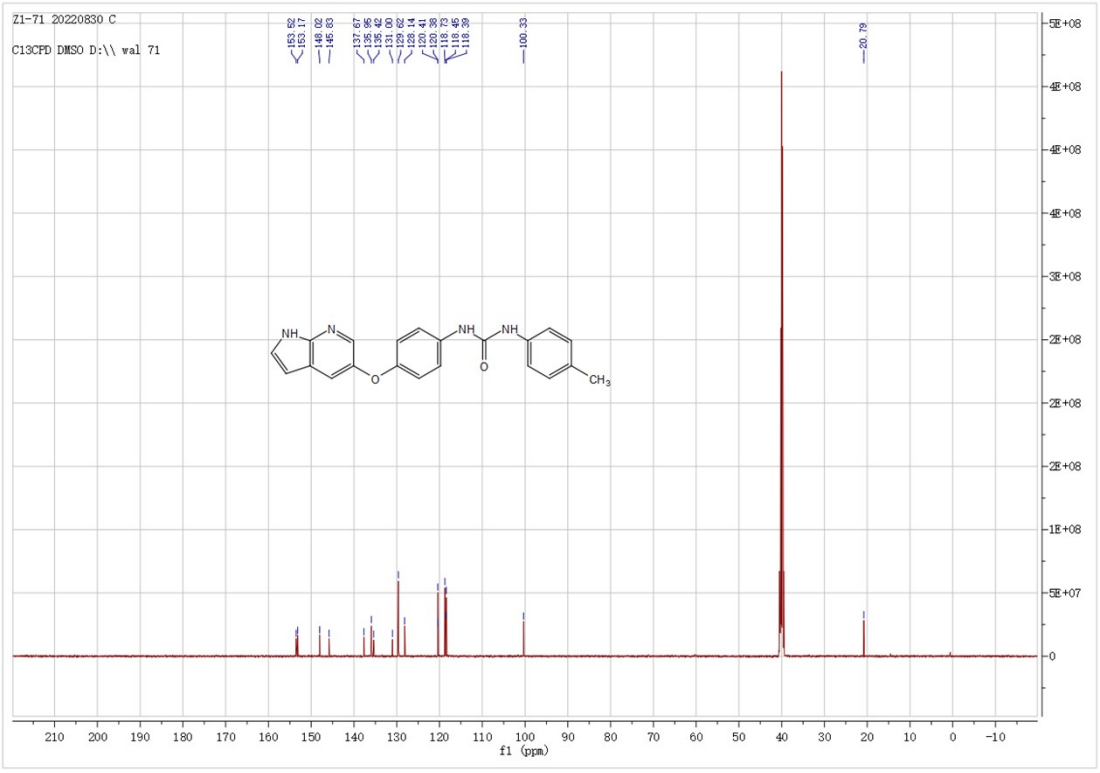
0704-1
M+H+] 379.0956

HRMS (ESI) spectrum of **32**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-methylphenyl)urea (**33**)

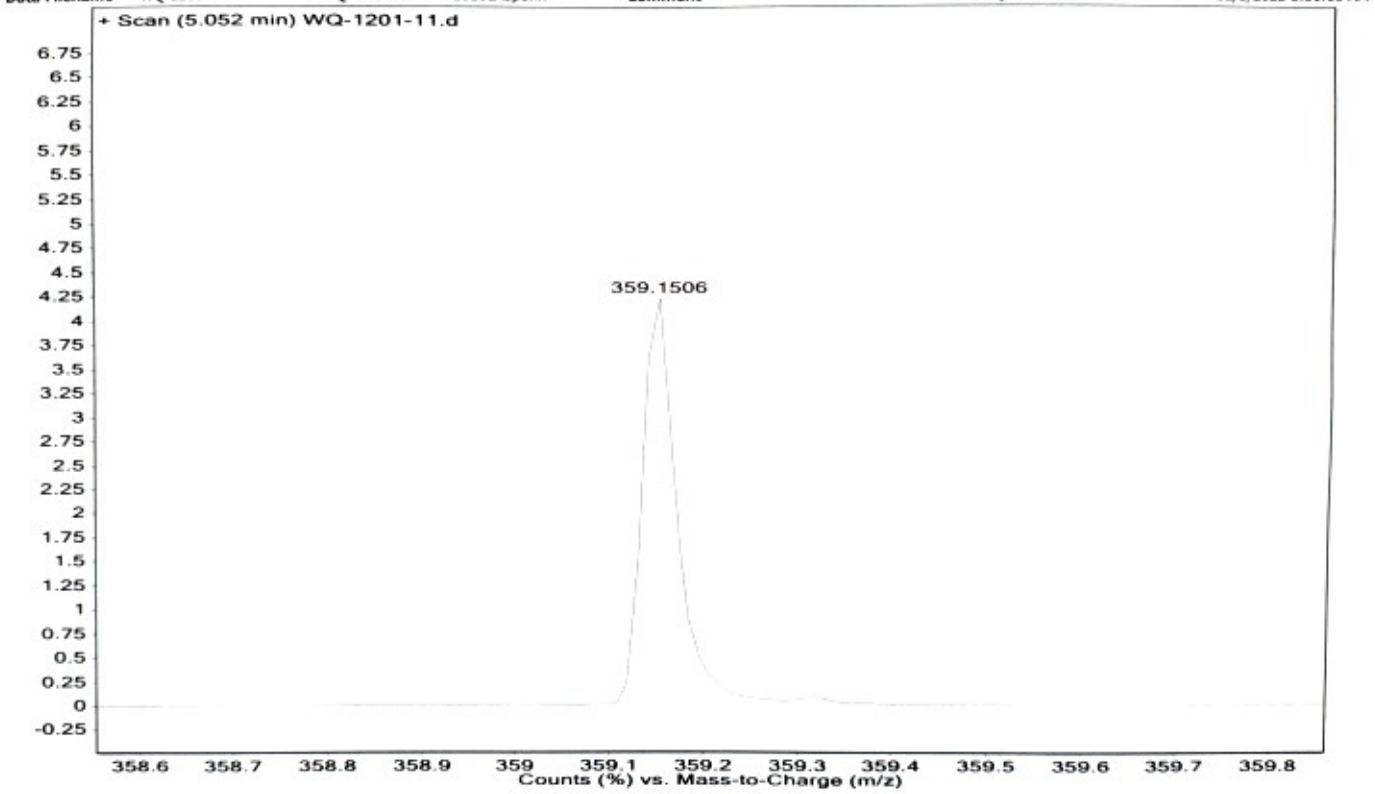


^{1}H NMR spectrum of **33**



^{13}C NMR spectrum of **33**

Sample Name	WQ-1201-11	**Position**	Vial 51	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-1201-11.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	12/1/2022 8:51:00 AM



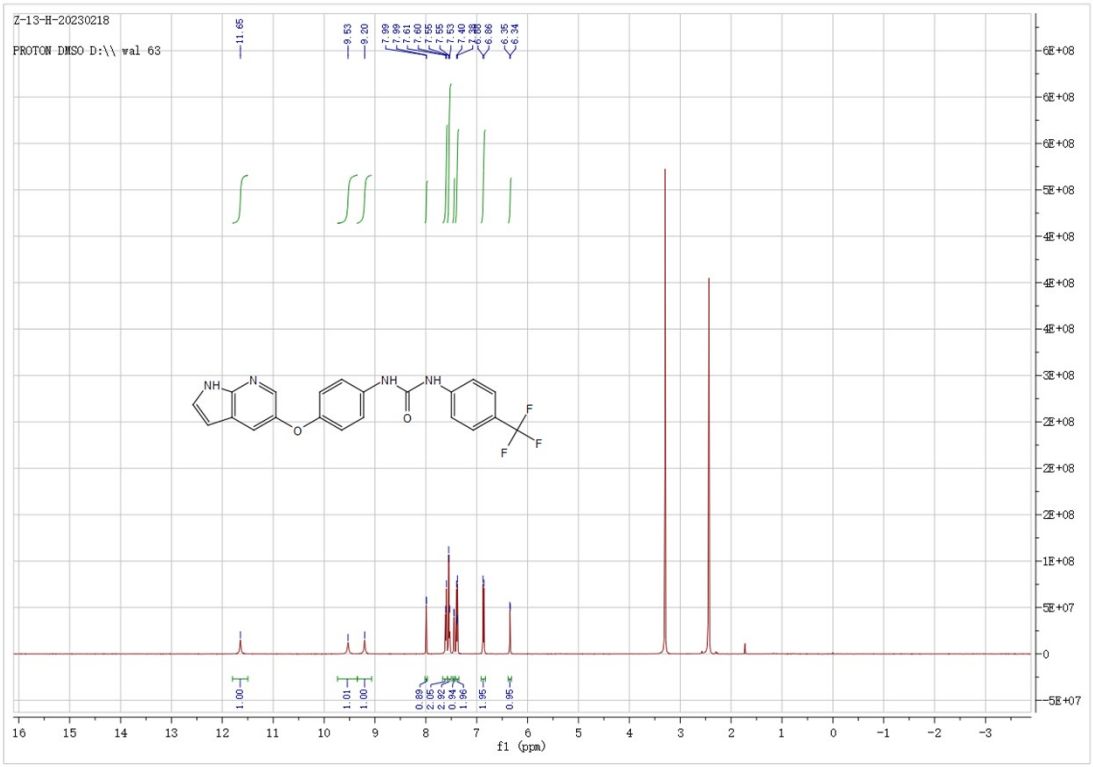
$(M+H)^+$: 359.1503

$C_{21}H_{18}N_4O_2$

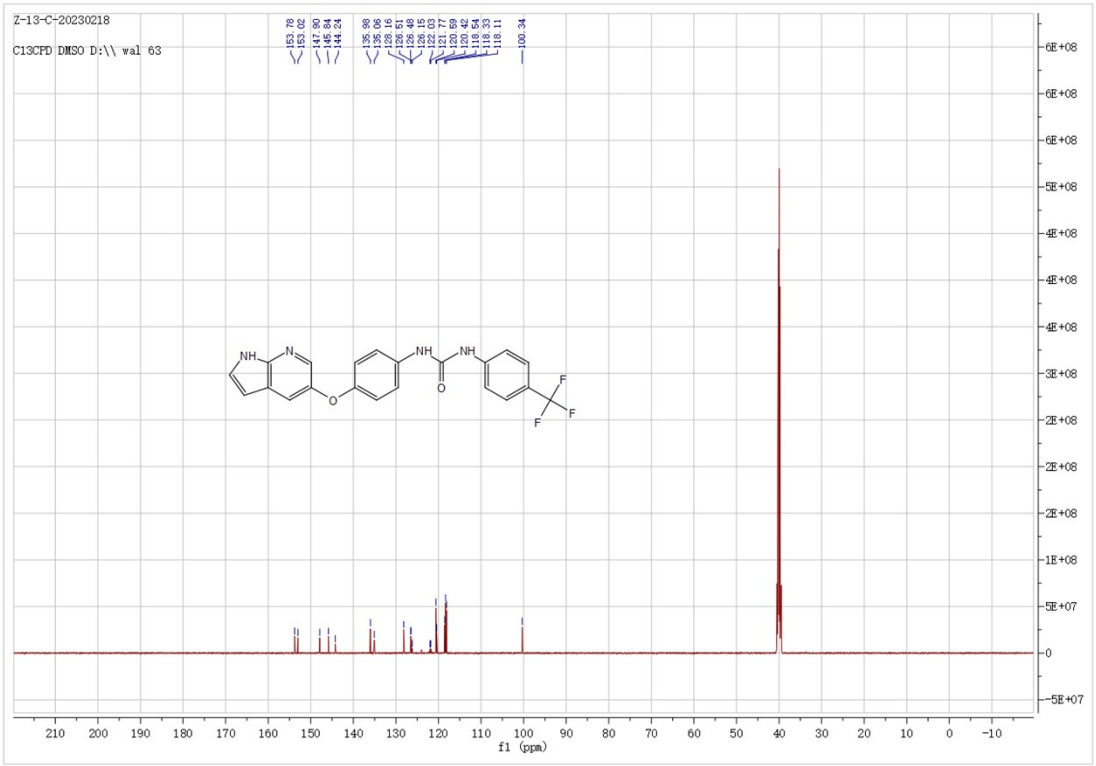
0720-2

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-(trifluoromethyl)phenyl)urea

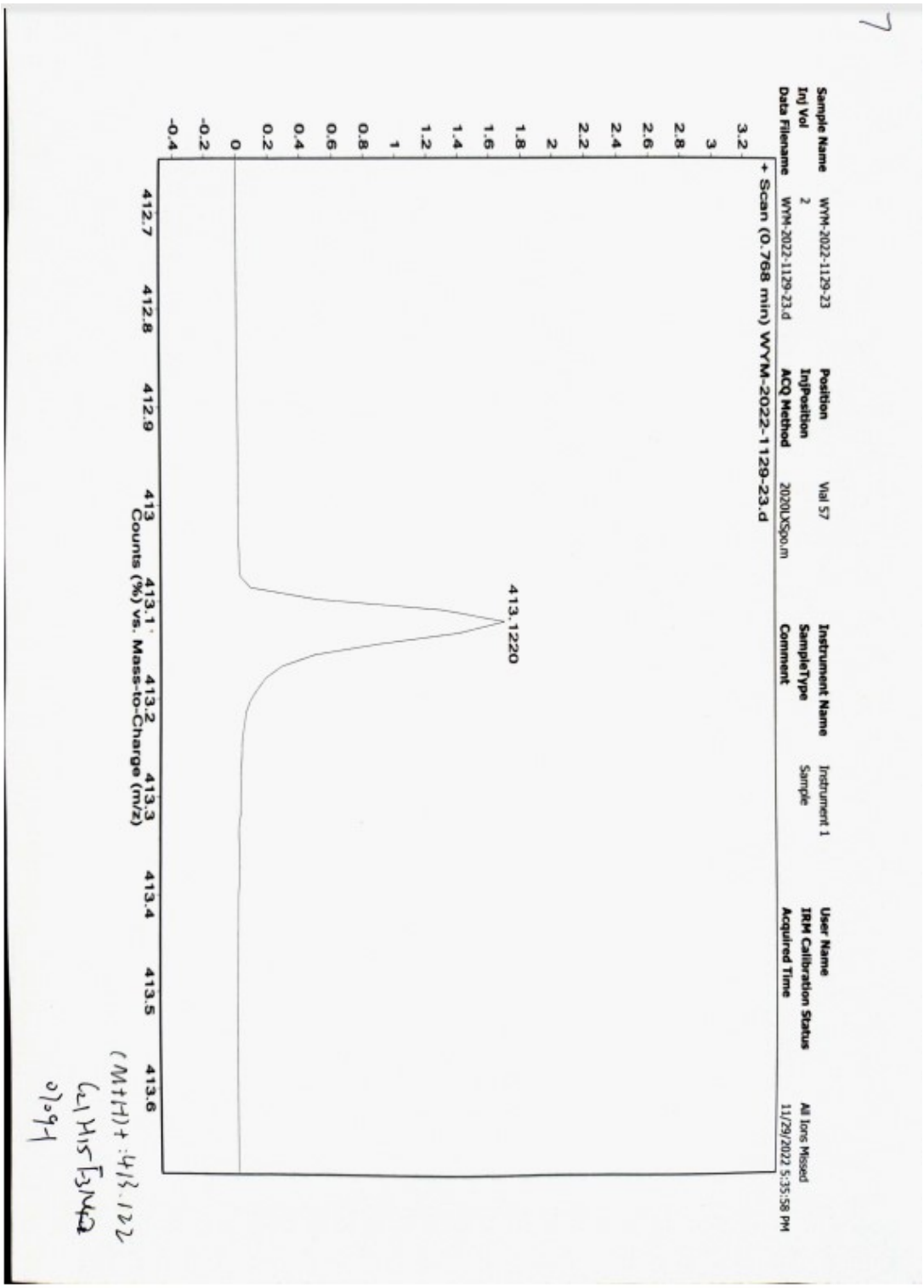
(**34**)



^{1}H NMR spectrum of **34**

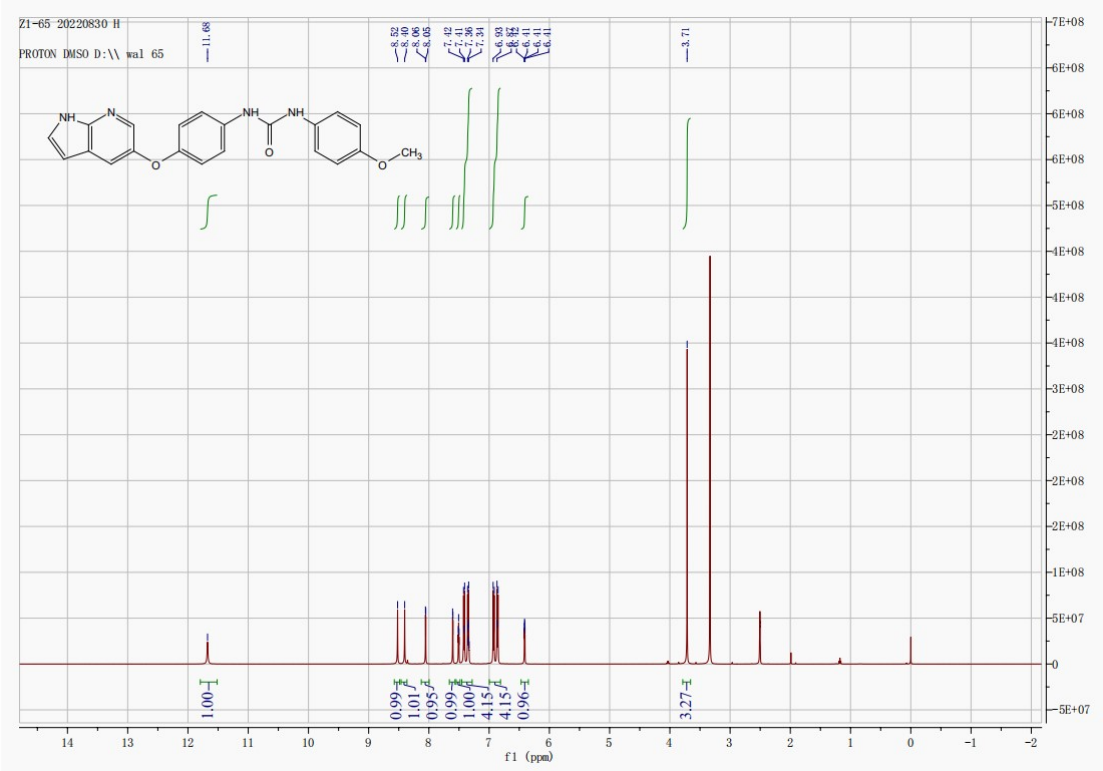


^{13}C NMR spectrum of **34**

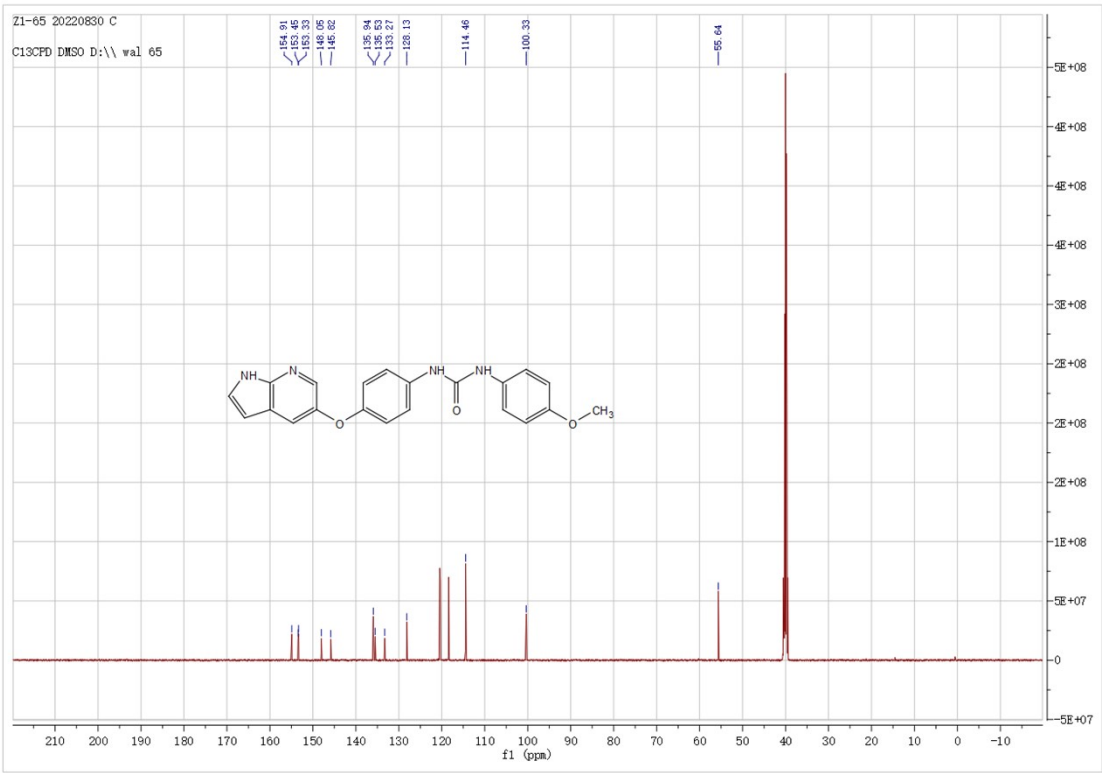


HRMS (ESI) spectrum of **34**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-methoxyphenyl)urea (**35**)



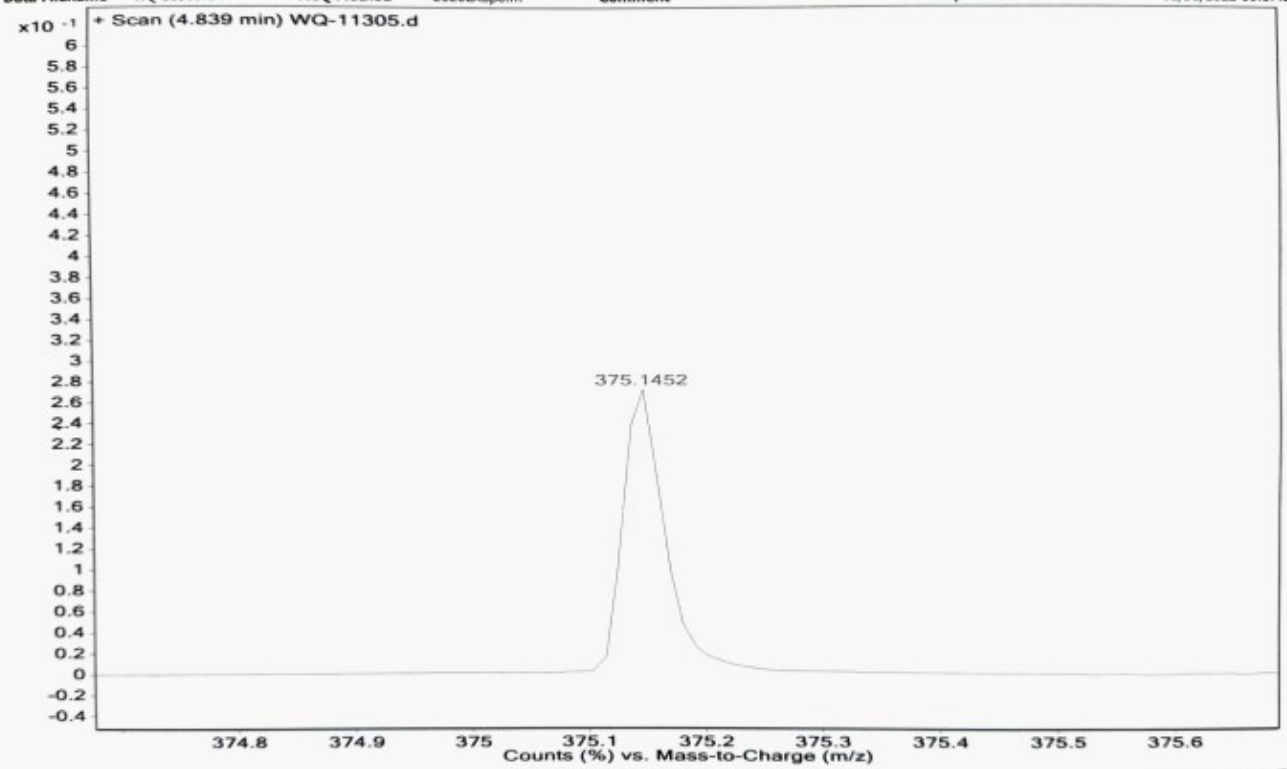
^{1}H NMR spectrum of **35**



^{13}C NMR spectrum of **35**

15

Sample Name	WQ-11305	**Position**	Vial 55	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-11305.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/30/2022 10:57:28 AM



$(M+H)^+$: 375.1452

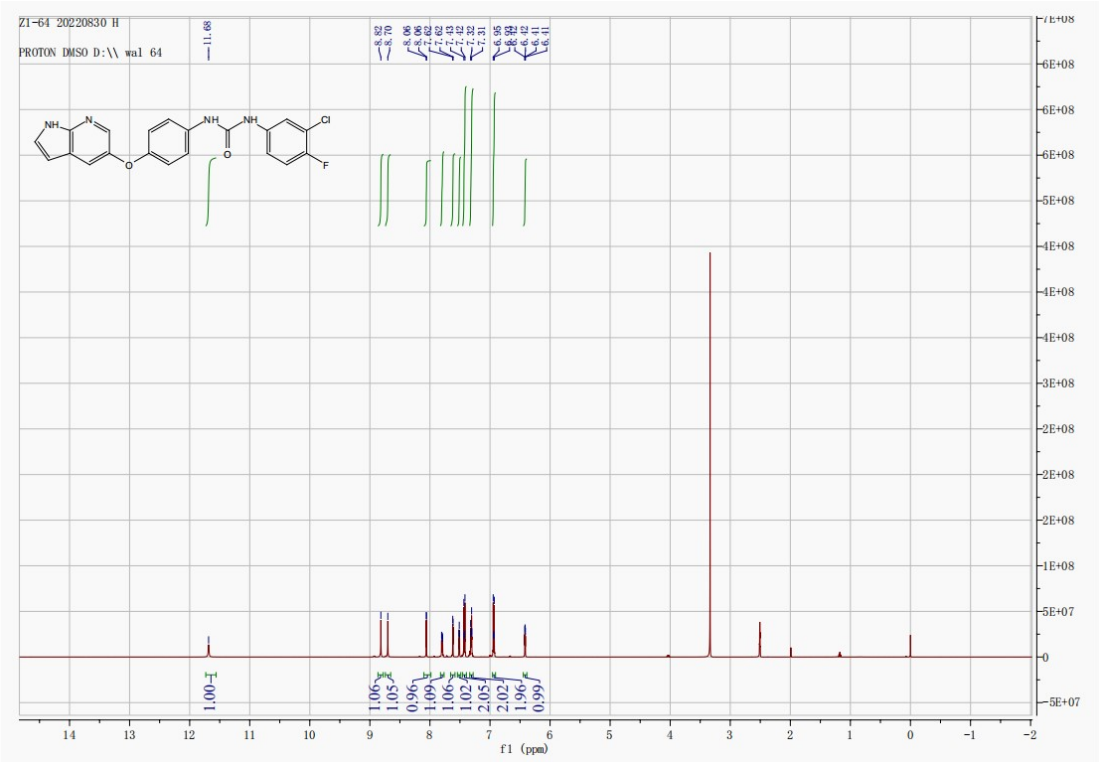
$C_{21}H_{18}N_4O_3$

9716-3

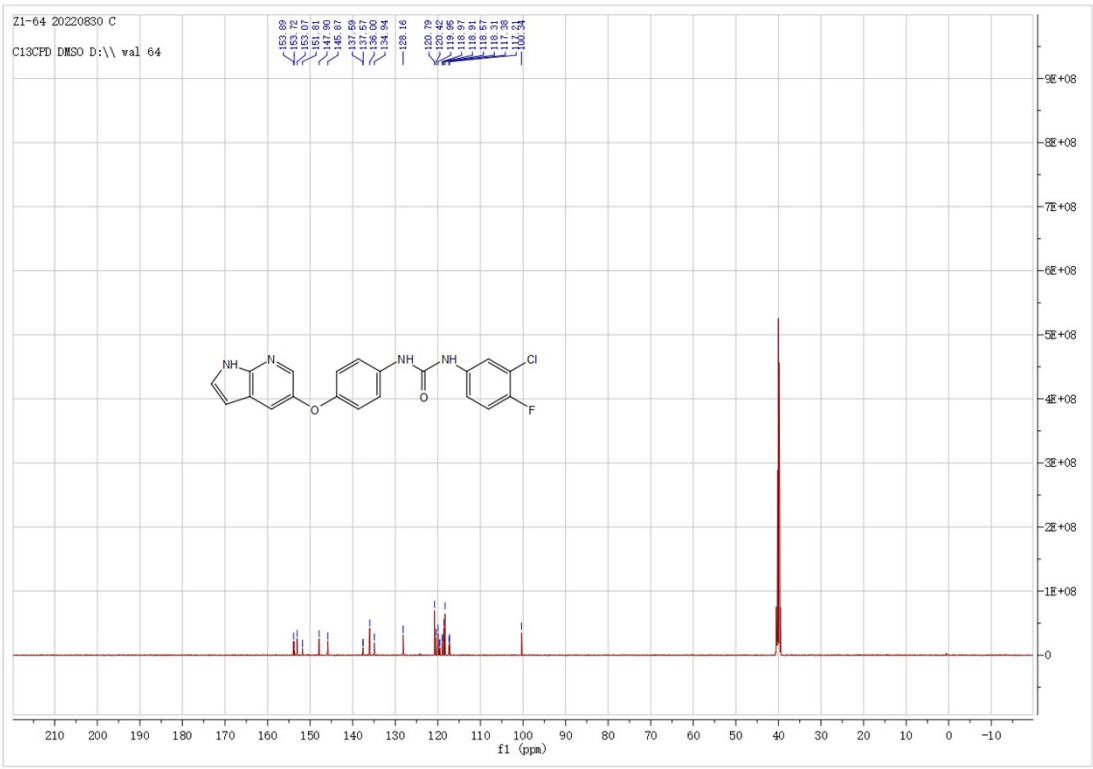
HRMS (ESI) spectrum of **35**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-chloro-4-fluorophenyl)urea

(**36**)



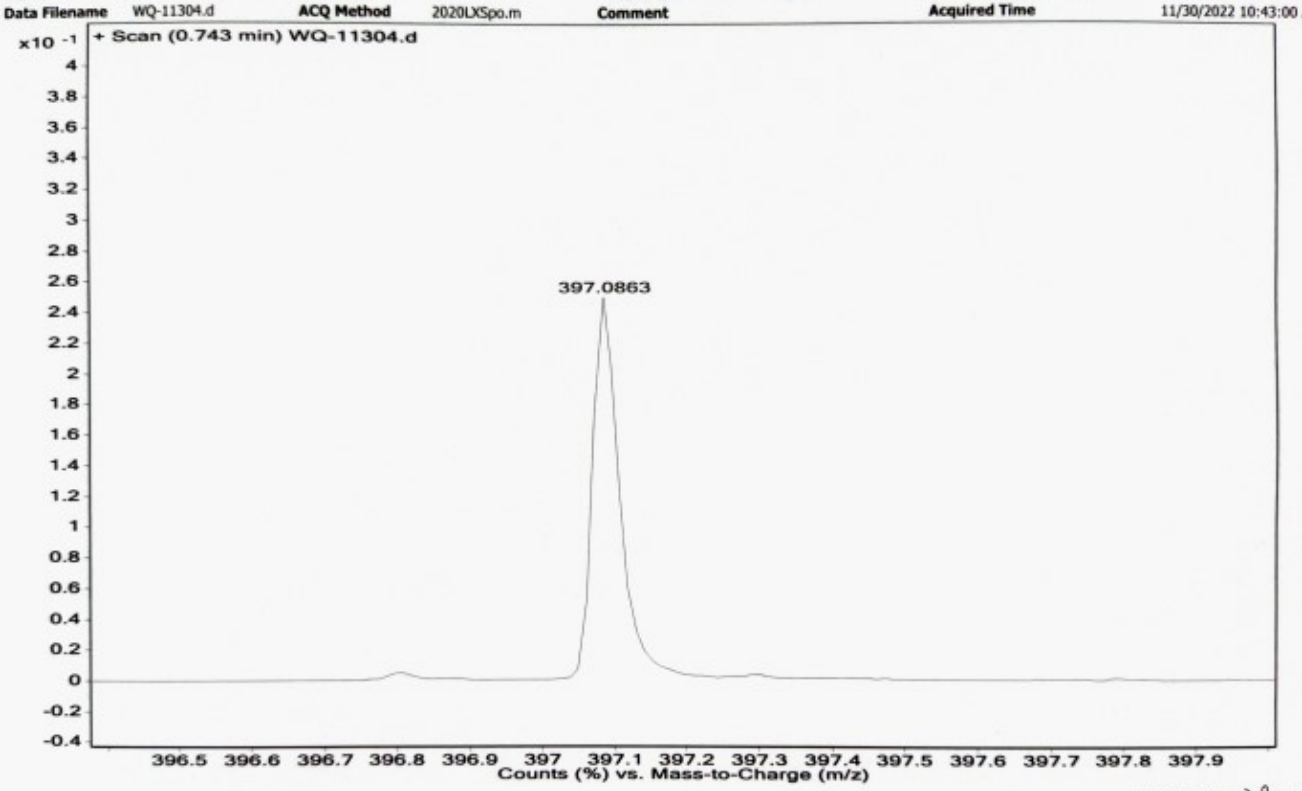
^{1}H NMR spectrum of **36**



^{13}C NMR spectrum of **36**

14

Sample Name	WQ-11304	**Position**	Vial 54	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-11304.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/30/2022 10:43:00 AM



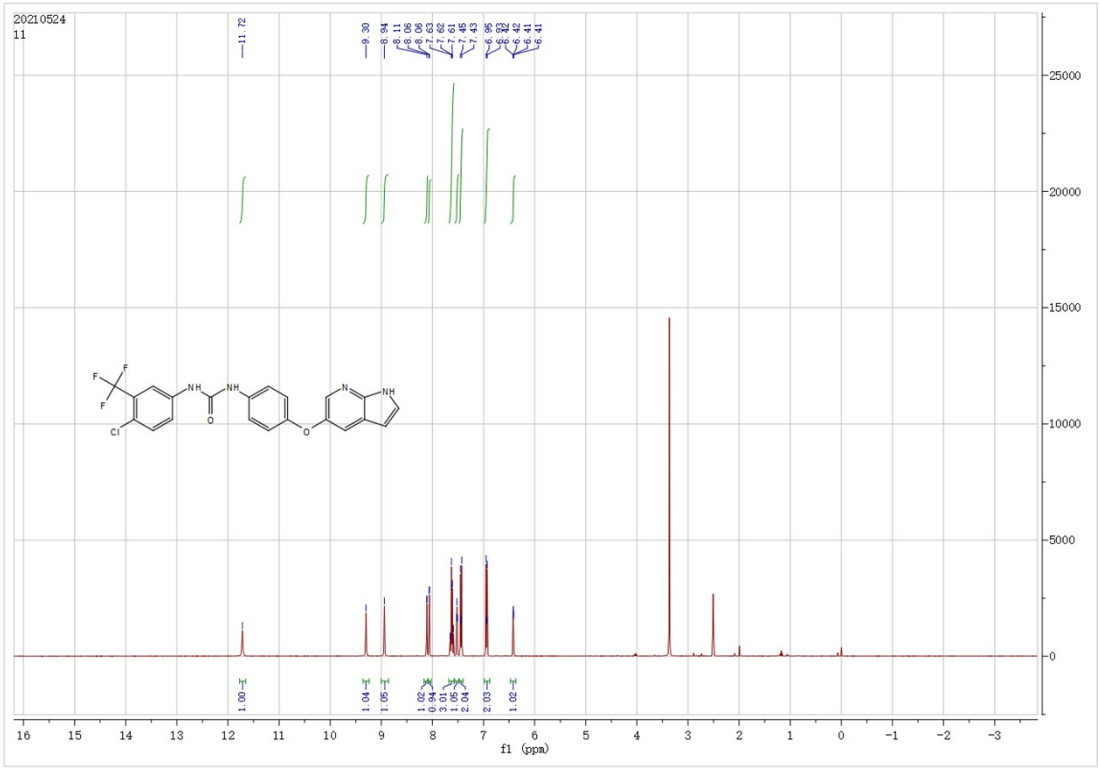
(M+H)+ : 397.0862

$C_{20}H_{14}ClF_4N_4O_2$

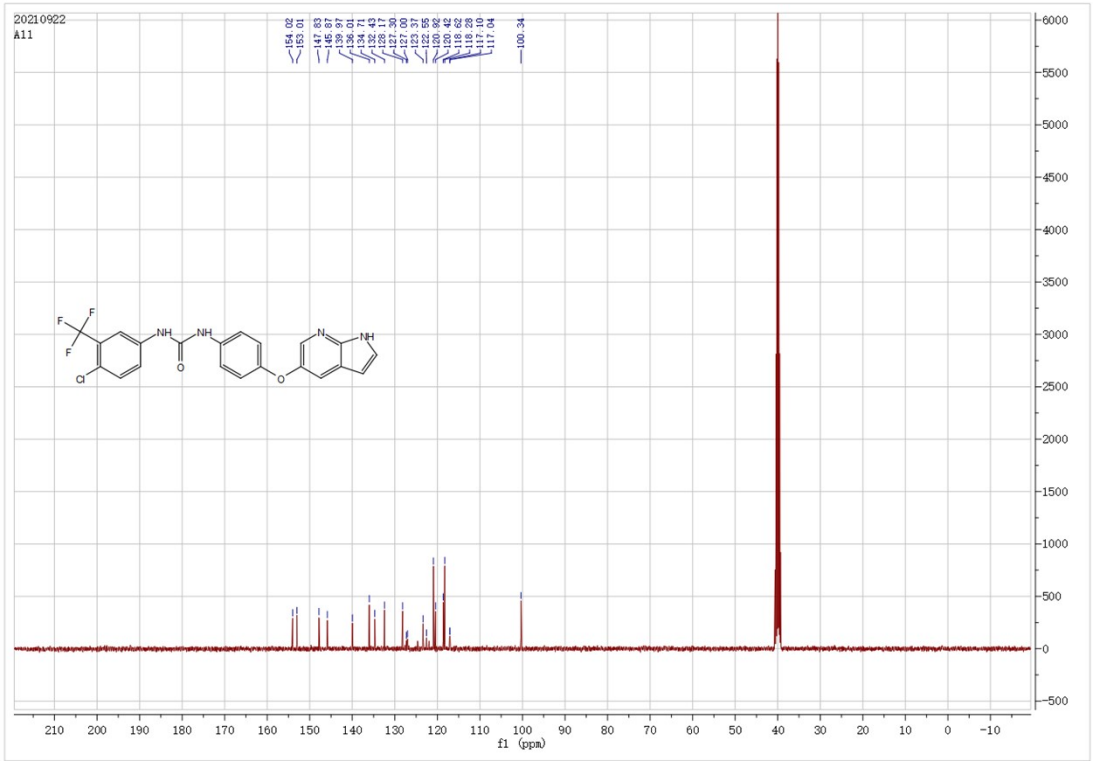
0716-2

HRMS (ESI) spectrum of **36**

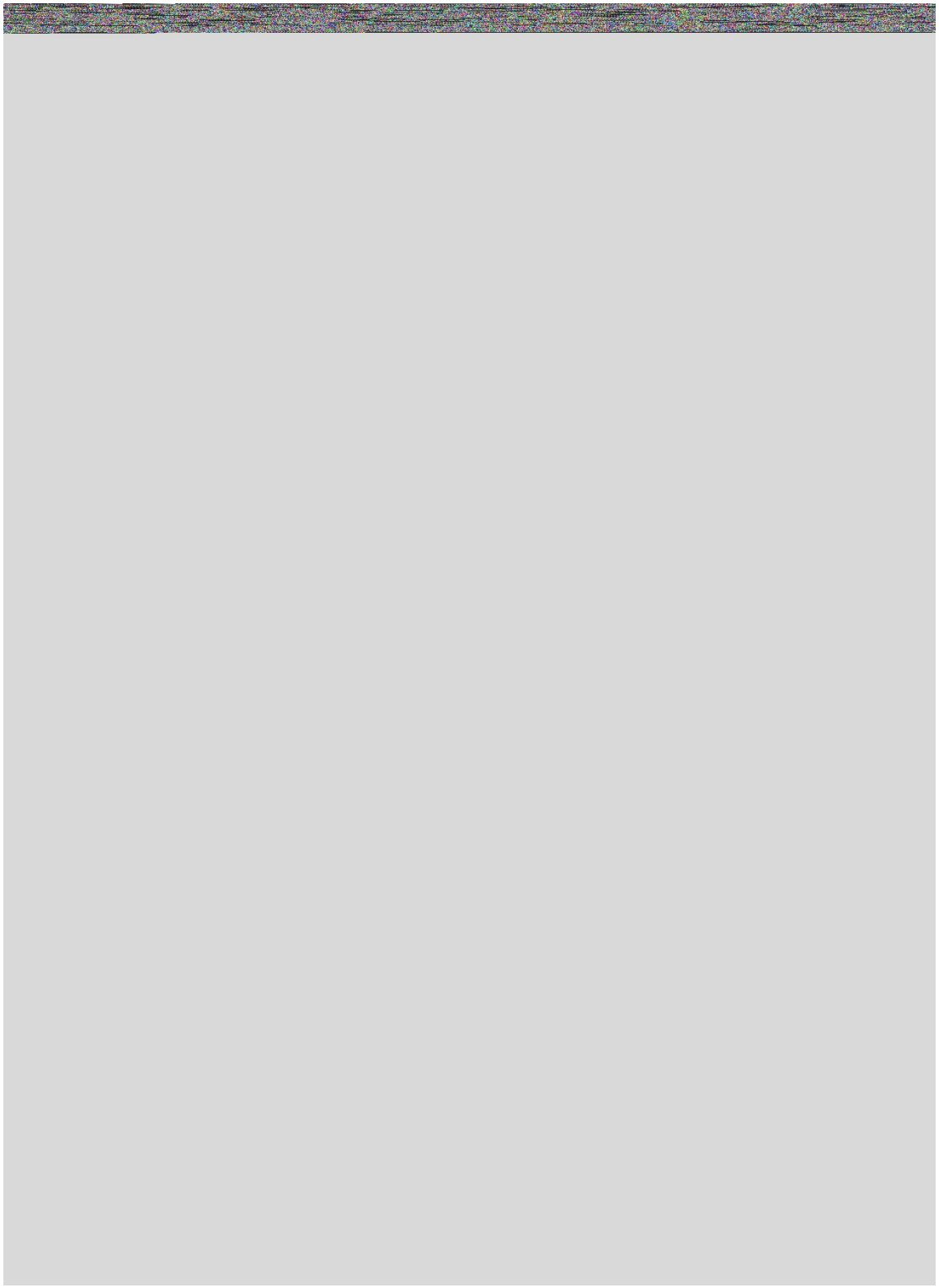
1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-chloro-3-(trifluoromethyl)phenyl)urea (**37**)



^{1}H NMR spectrum of **37**



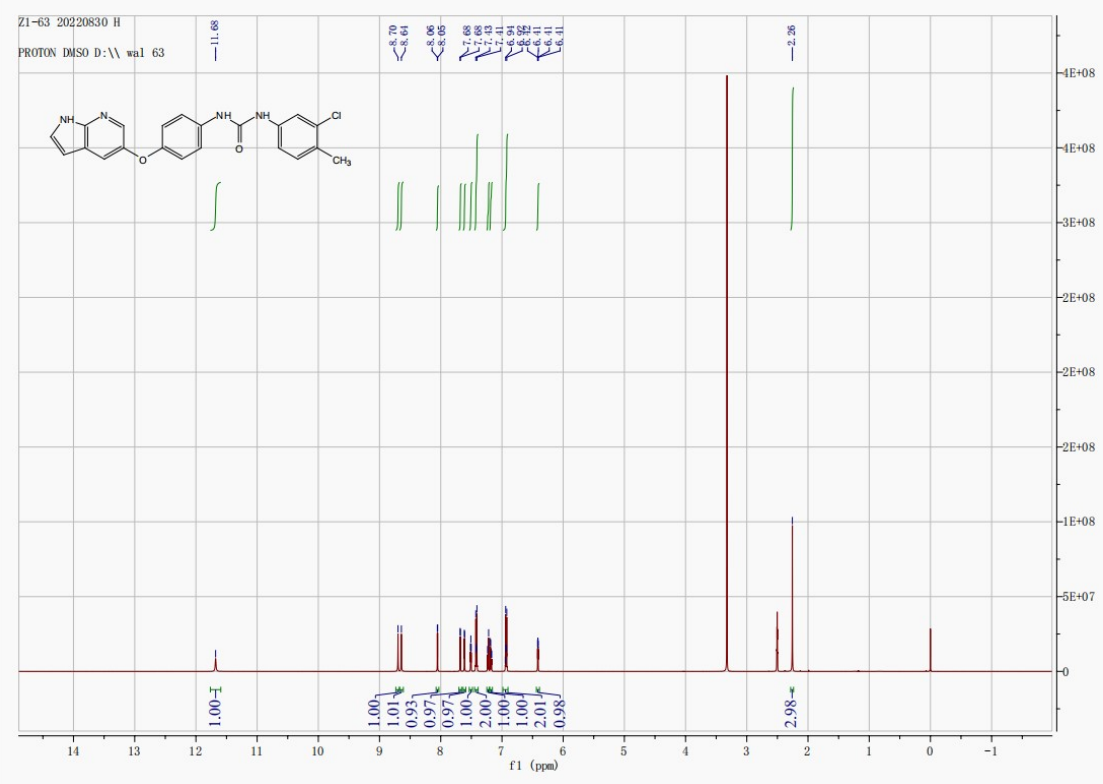
^{13}C NMR spectrum of **37**



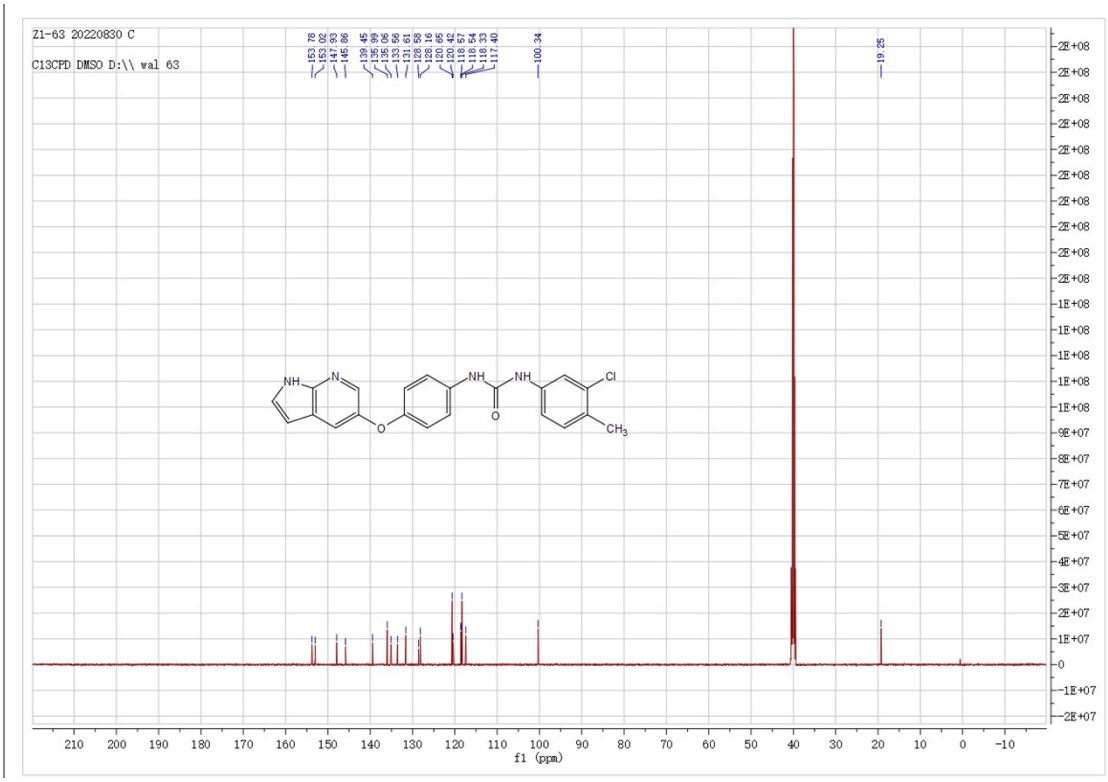
HRMS (ESI) spectrum of **37**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3-chloro-4-methylphenyl)urea

(**38**)



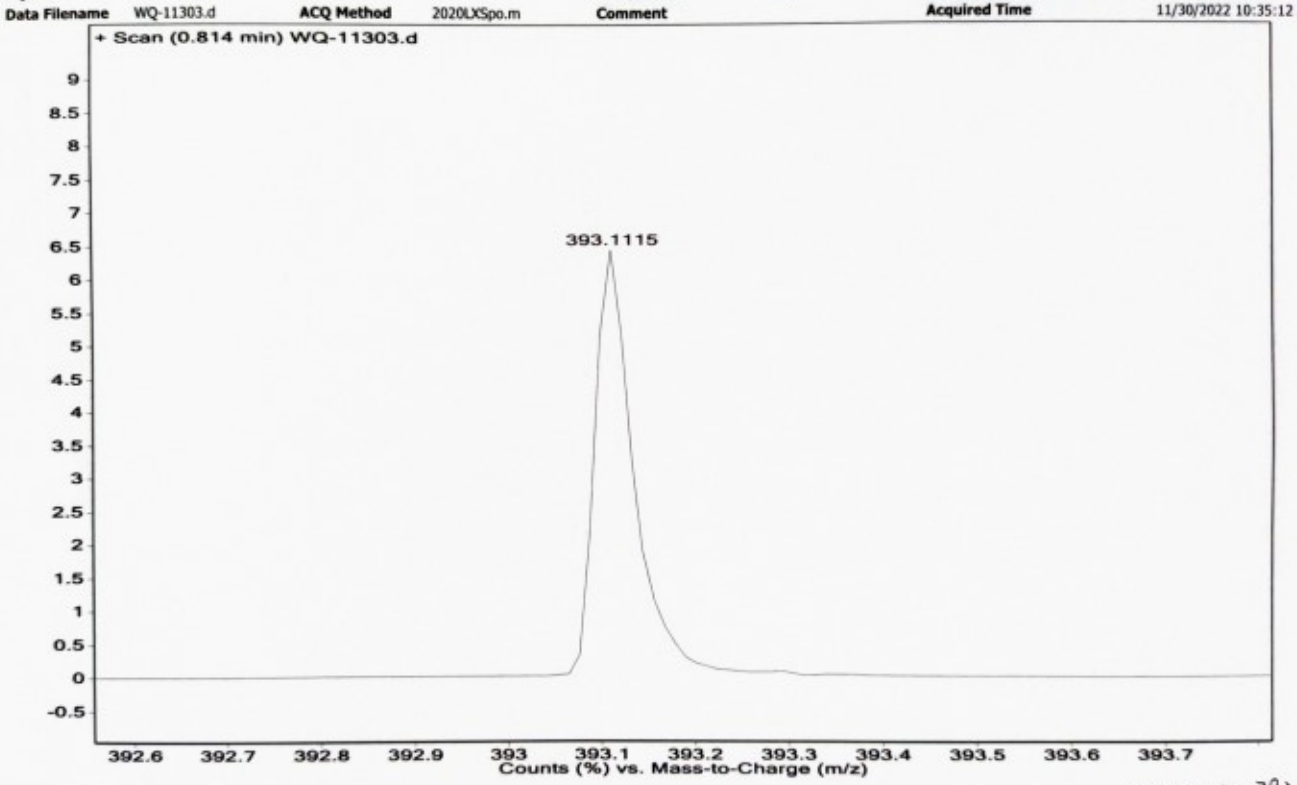
^{1}H NMR spectrum of **38**



^{13}C NMR spectrum of **38**

13

Sample Name	WQ-11303	**Position**	Vial 53	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-11303.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	11/30/2022 10:35:12 AM



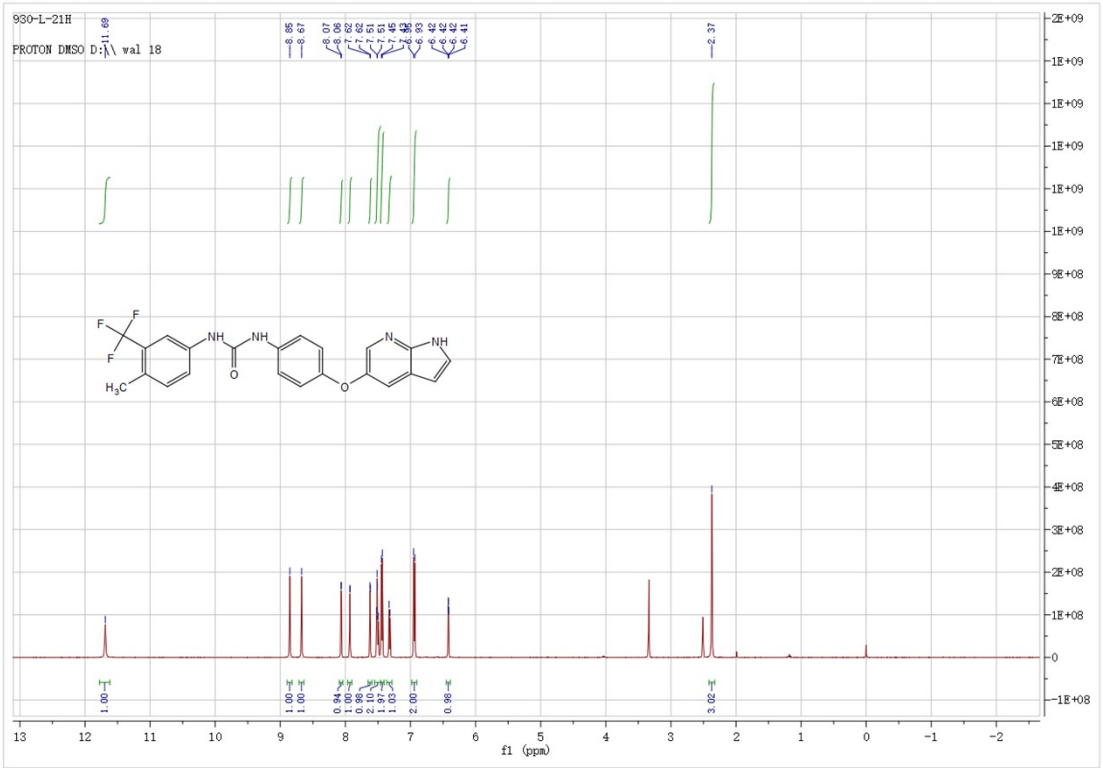
$(M+H)^+$: 393.1113

$C_{21}H_{17}ClN_4O_2$

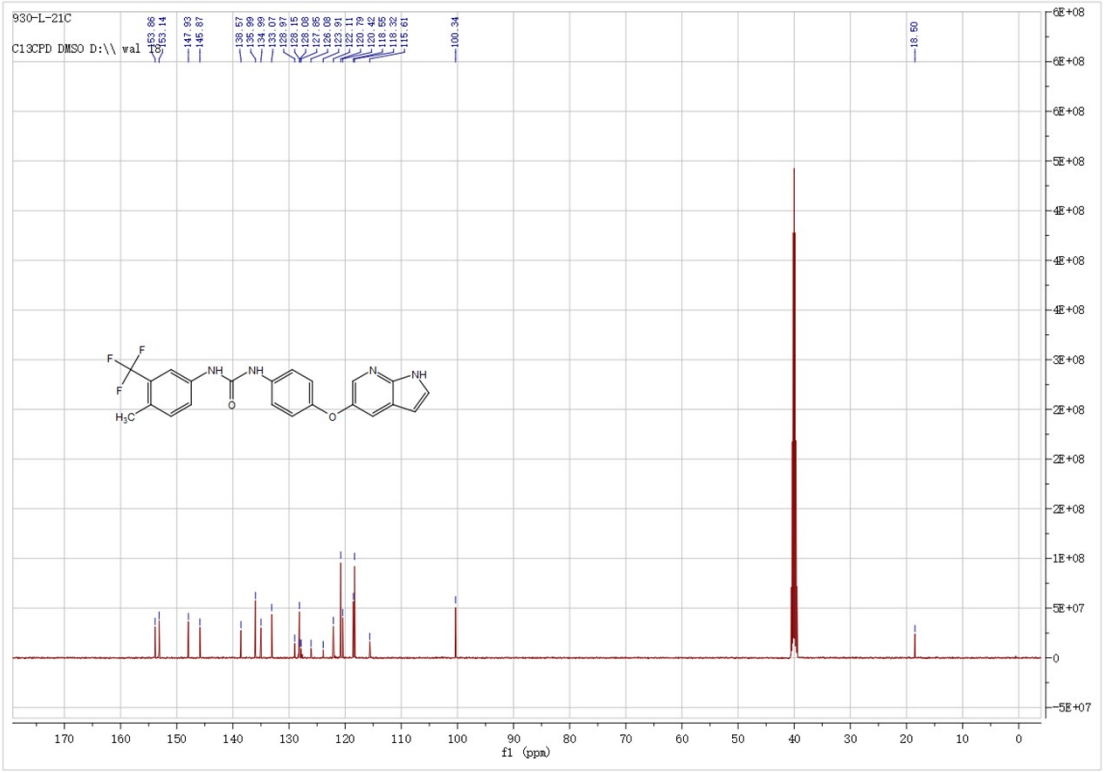
0716-1

HRMS (ESI) spectrum of **38**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(4-methyl-3-(trifluoromethyl)phenyl)urea (**39**)



^{1}H NMR spectrum of **39**

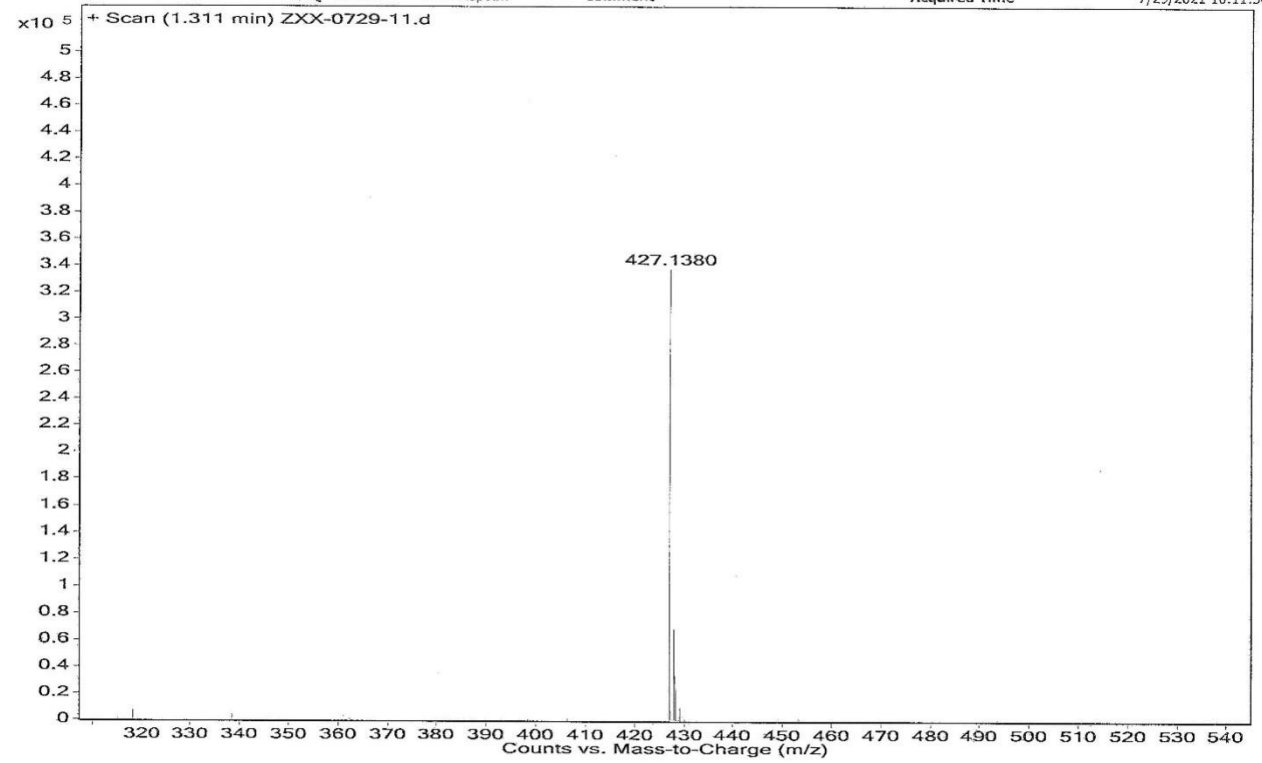


^{13}C NMR spectrum of **39**

HRMS (ESI) spectrum of **39**

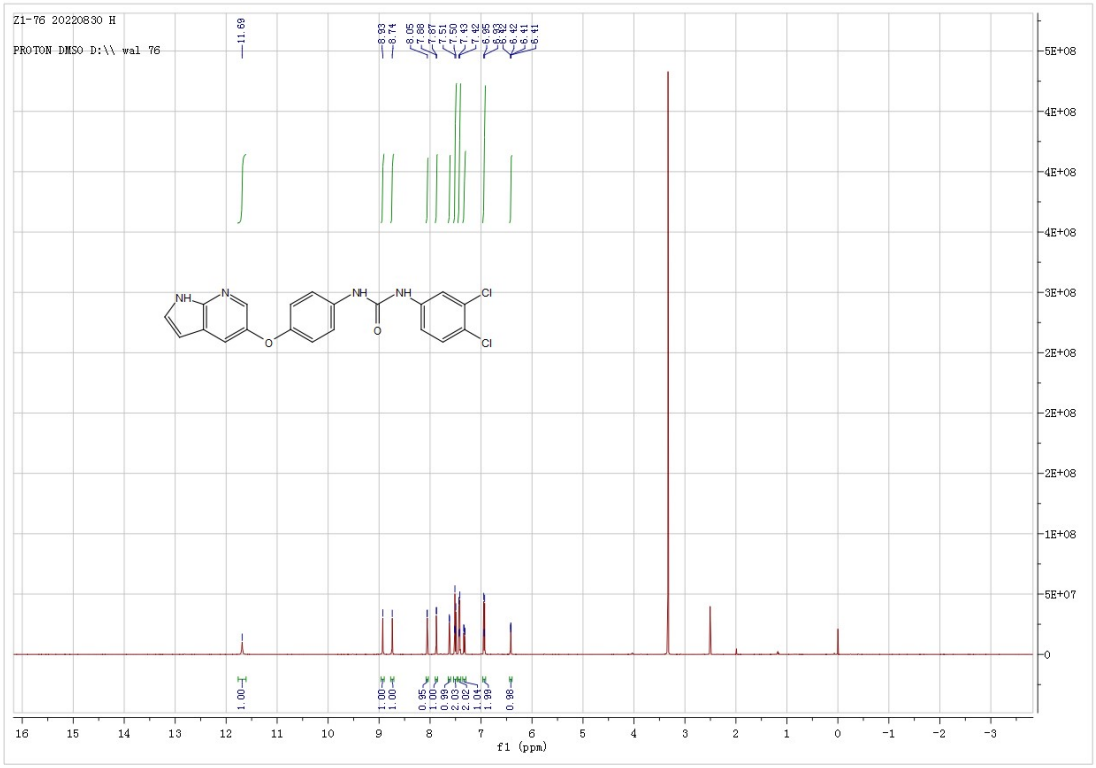
C22H17N4O2F3
Cal'd H+: 427.1376

Sample Name	ZXX-0729-11	Position	Vial 41	Instrument Name	Instrument 1	User Name	
Inj Vol	2	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	ZXX-0729-11.d	ACQ Method	2020LXSpo.m	Comment		Acquired Time	7/29/2021 10:11:56 AM

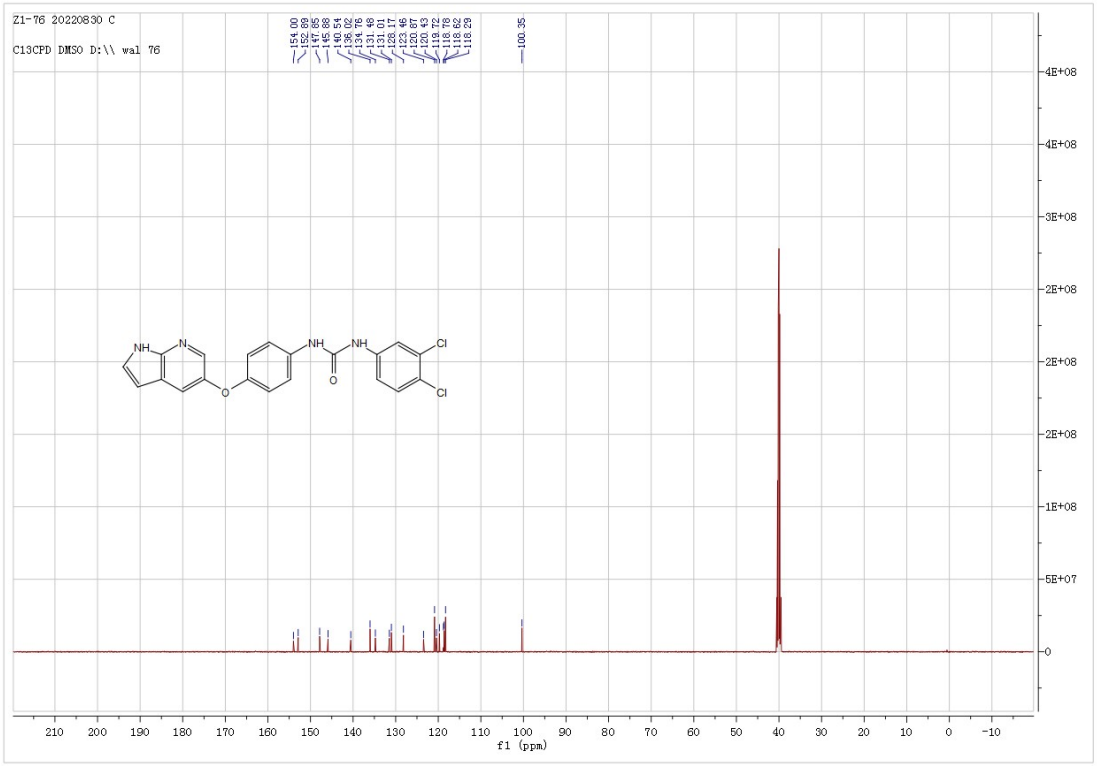


0625-3

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3,4-dichlorophenyl)urea (**40**)

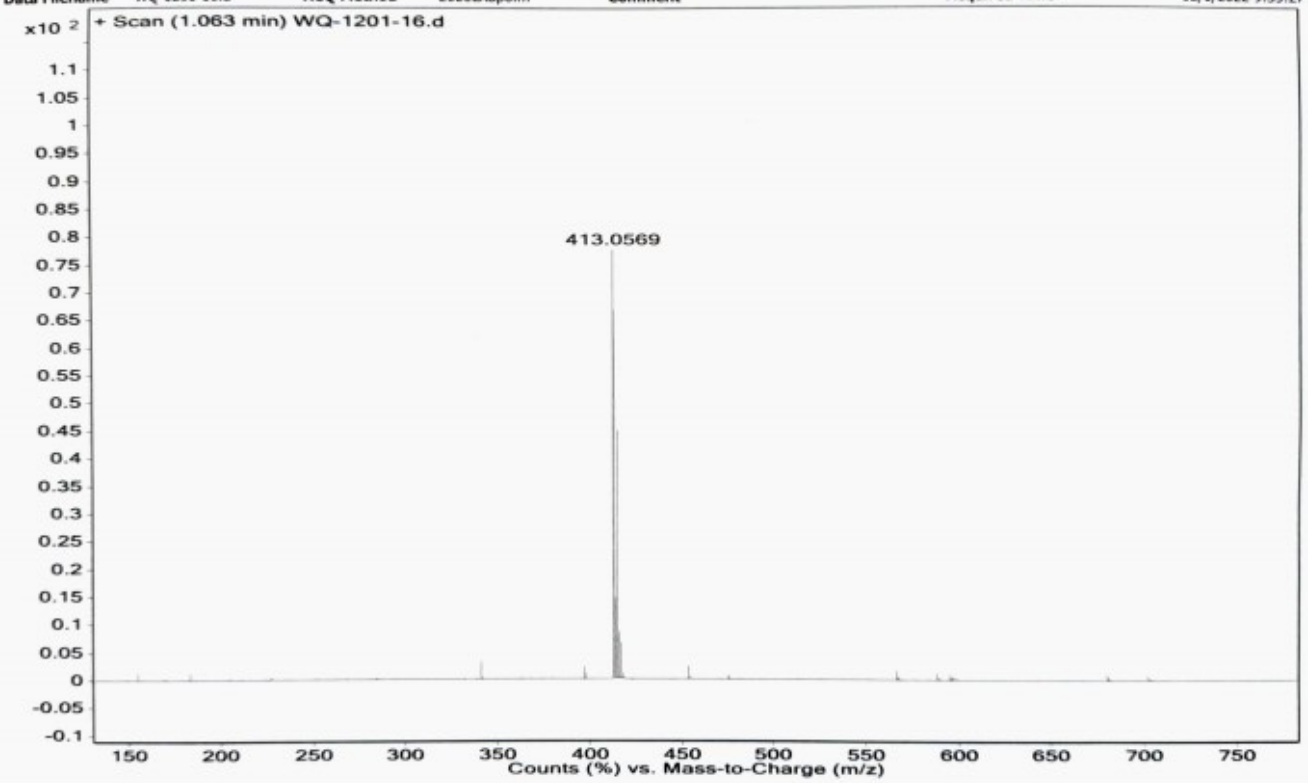


^{1}H NMR spectrum of **40**



^{13}C NMR spectrum of **40**

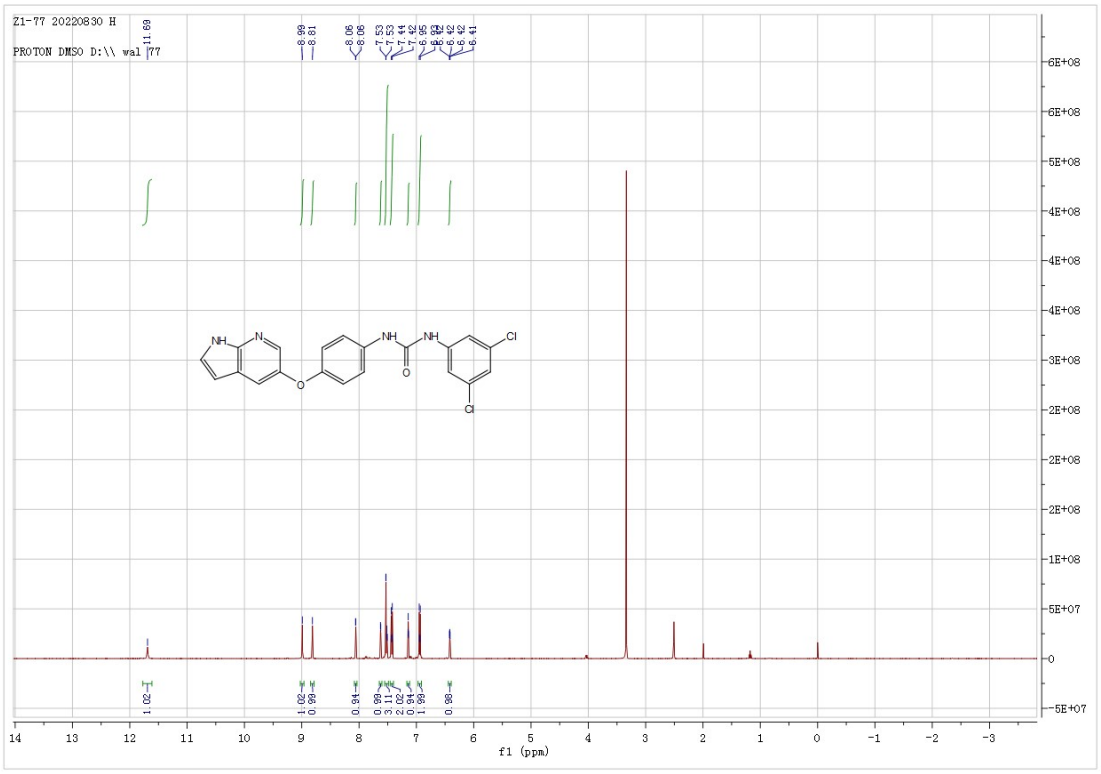
Sample Name	WQ-1201-16	**Position**	Vial 56	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-1201-16.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	12/1/2022 9:35:27 AM



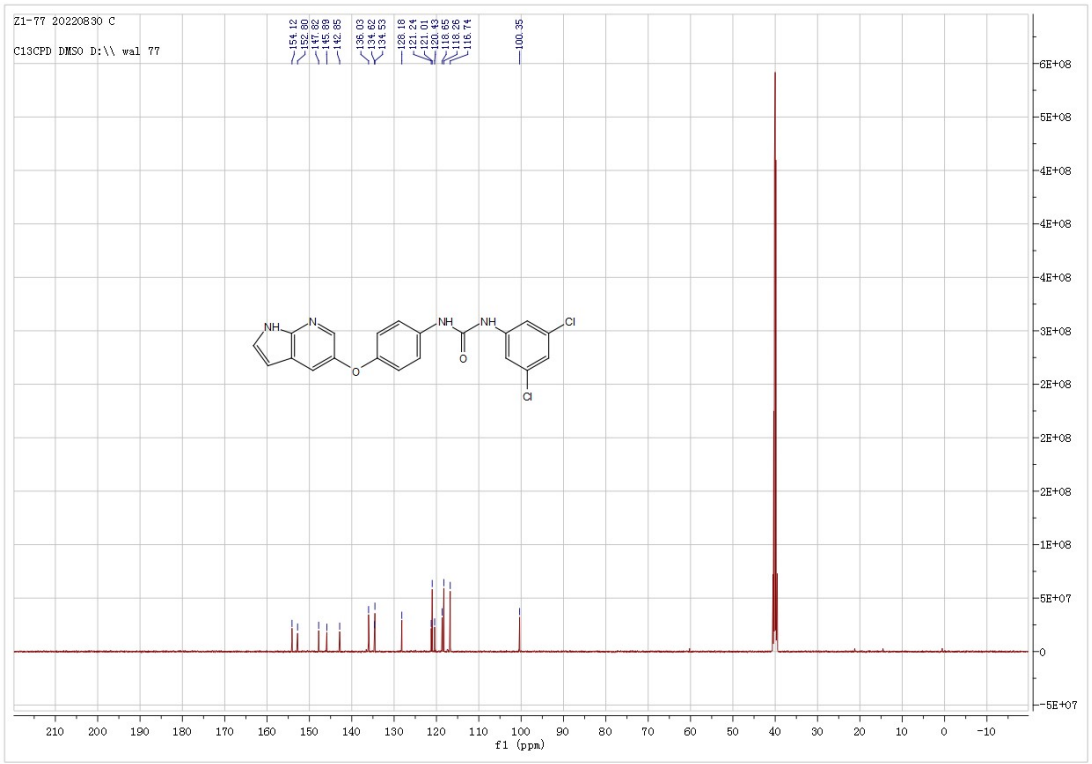
$(M+H)^+$: 413.0567
$C_{20}H_{14}Cl_2N_4O_2$
0721-2

HRMS (ESI) spectrum of **40**

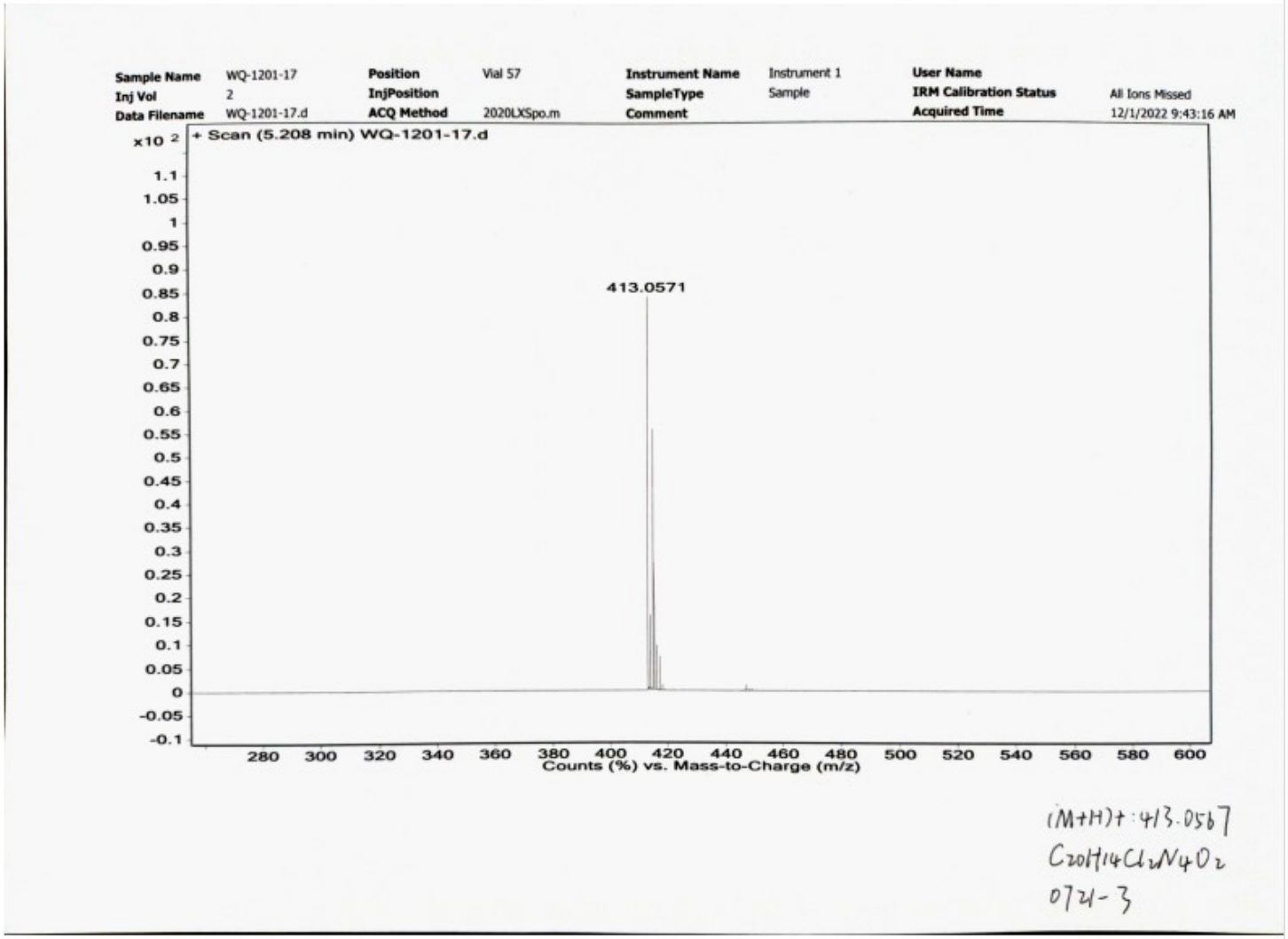
1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(3,5-dichlorophenyl)urea (**41**)



^{1}H NMR spectrum of **41**

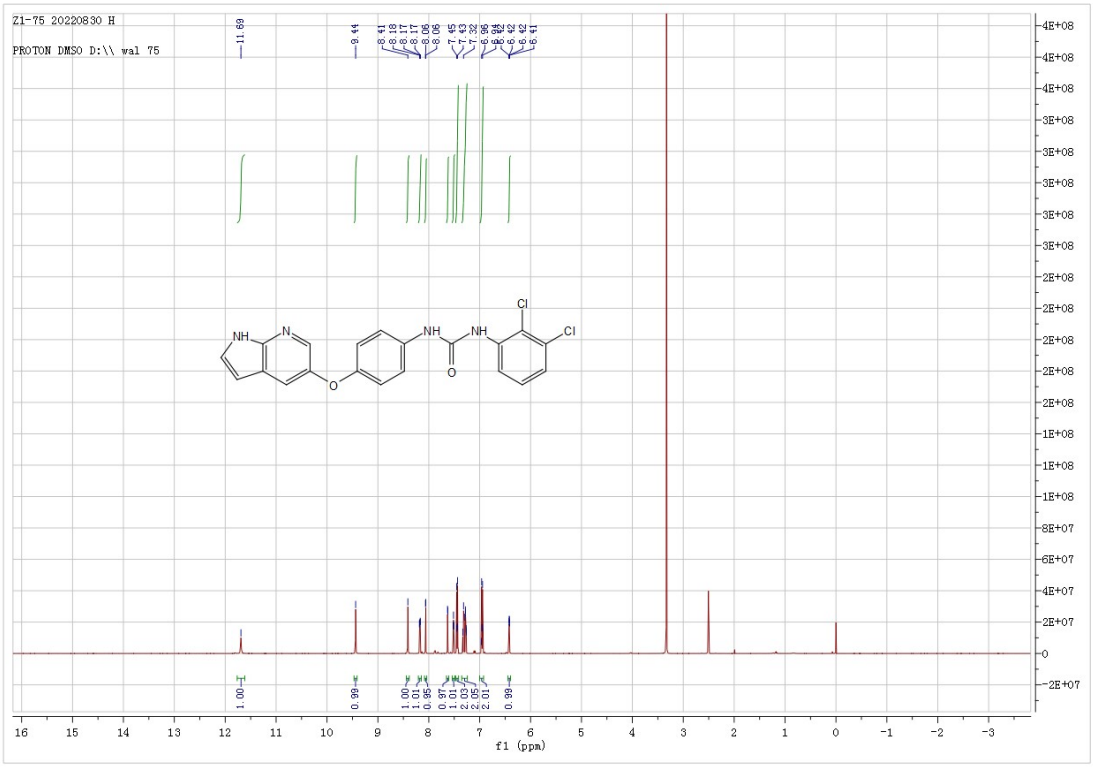


^{13}C NMR spectrum of **41**

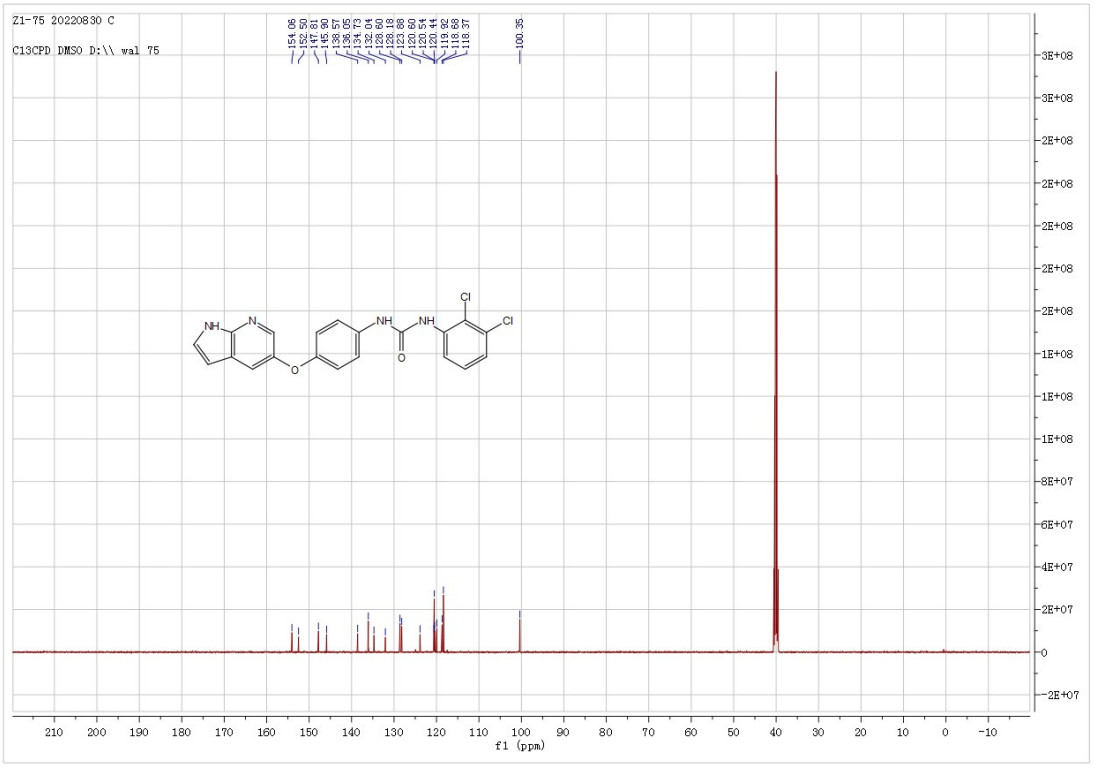


HRMS (ESI) spectrum of **41**

1-(4-((1H-pyrrolo[2,3-b]pyridin-5-yl)oxy)phenyl)-3-(2,3-dichlorophenyl)urea (**42**)

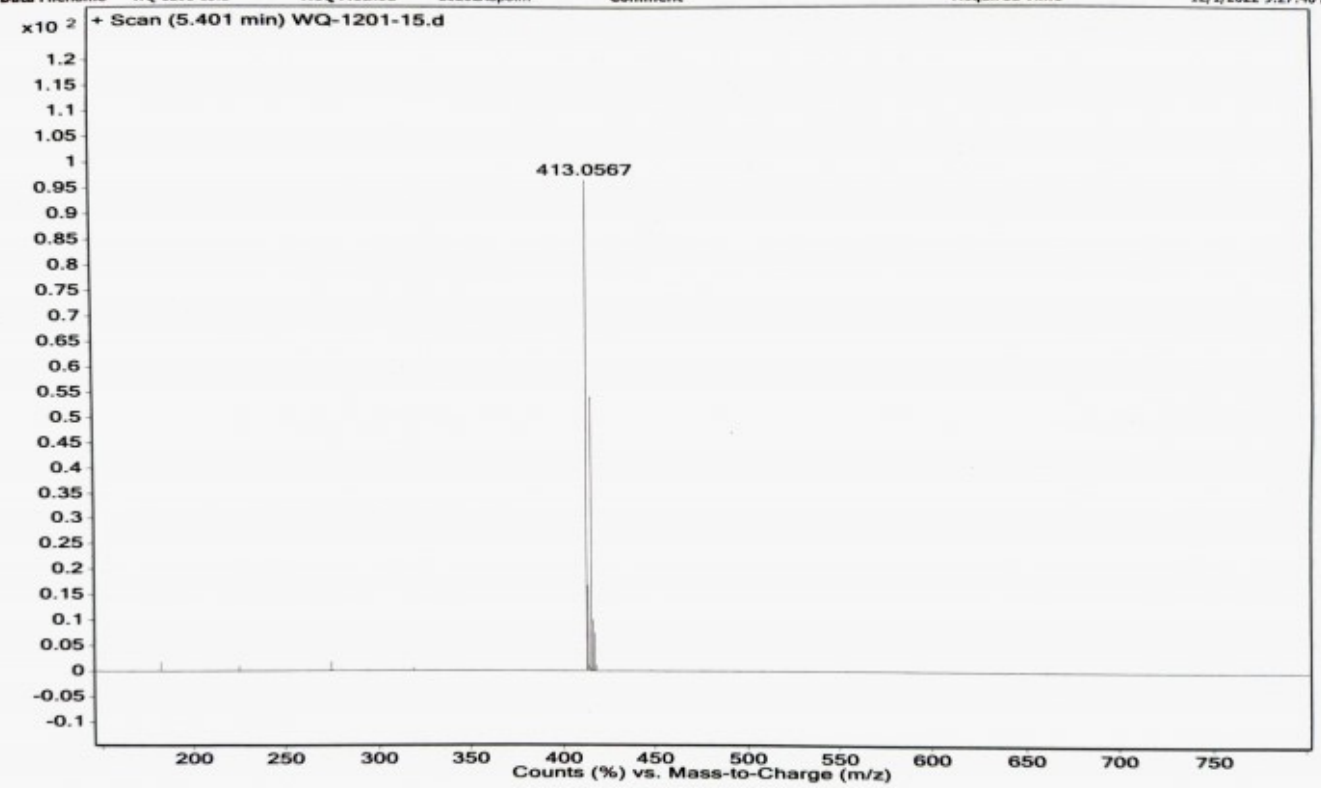


^{1}H NMR spectrum of **42**



^{13}C NMR spectrum of **42**

Sample Name	WQ-1201-15	**Position**	Vial 55	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	WQ-1201-15.d	**ACQ Method**	2020LXSpo.m	**Comment**		**Acquired Time**	12/1/2022 9:27:40 AM



(M+H)+ 413.056]
$C_{20}H_{14}Cl_2N_4O_2$
0721-1