Supporting Information

Discovery of Novel Dual-Target Inhibitor of Bromodomain-Containing Protein 4/Casein Kinase 2 Inducing Apoptosis and Autophagy-Associated Cell Death for Triple-Negative Breast Cancer Therapy

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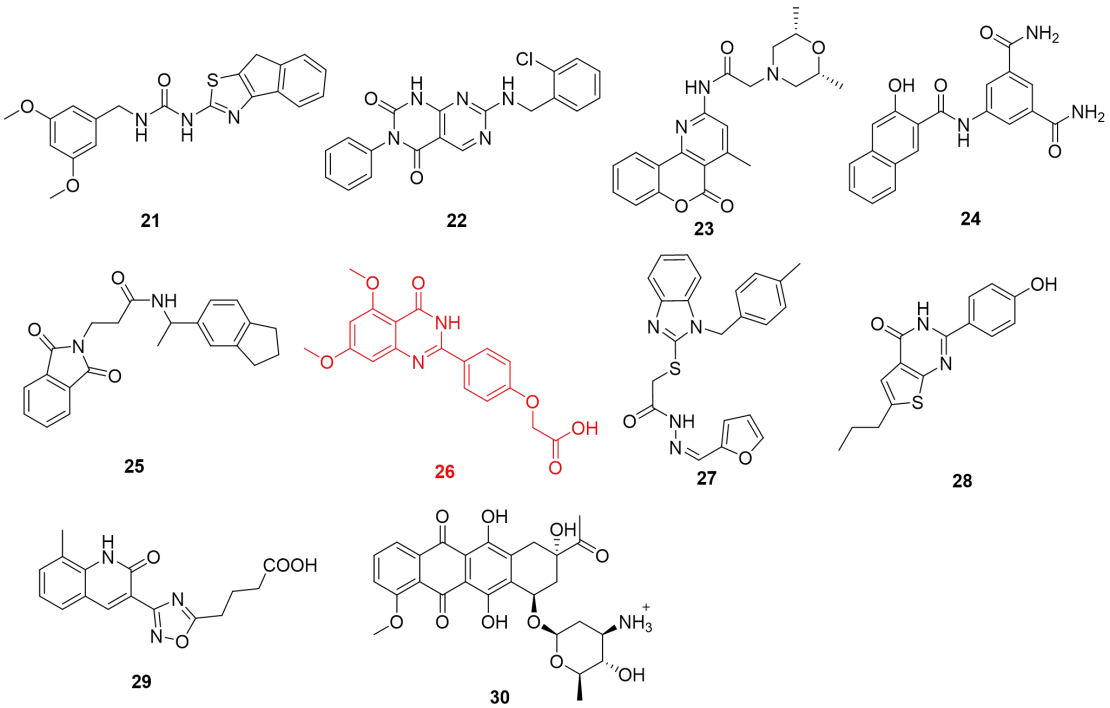


Figure S1. The top 10 candidate dual-target inhibitors of BRD4 and CK2 were selected.

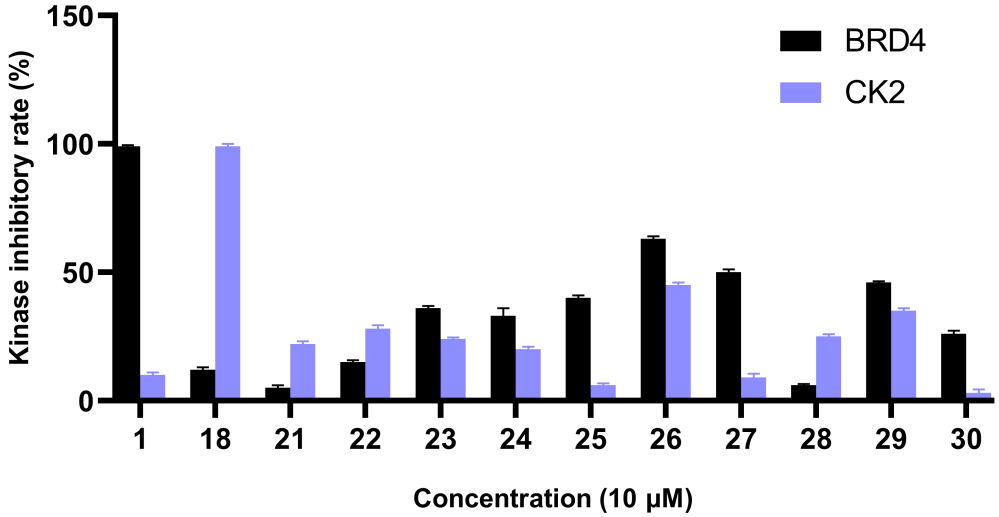


Figure S2. BRD4 and CK2 inhibition rates of top 10 candidate compounds. The inhibitory activity of BRD4 and CK2 for top 10 candidate compounds (**21**-**30**) were detected at 10 μM. JQ1 (**1**) and CX-4945 (**18**) were used as referenced BRD4 inhibitor and CK2 inhibitor, respectively.

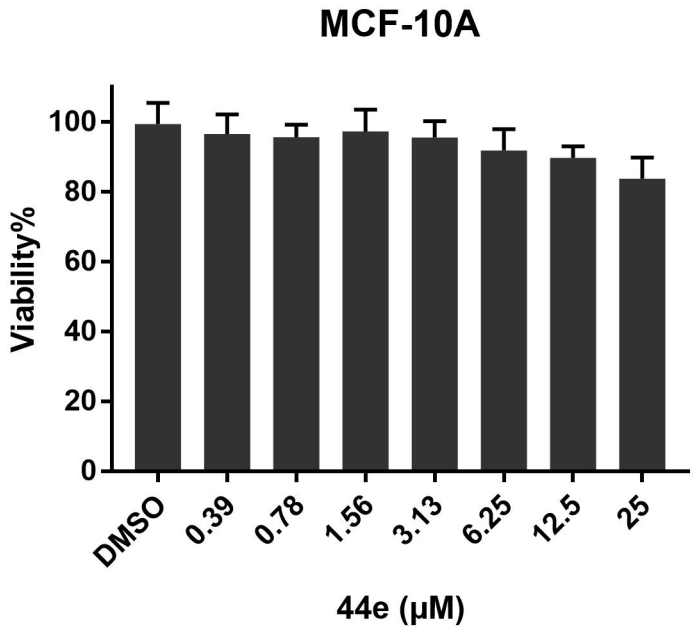


Figure S3. Toxicity of candidate compound **44e** to MCF-10A cell.

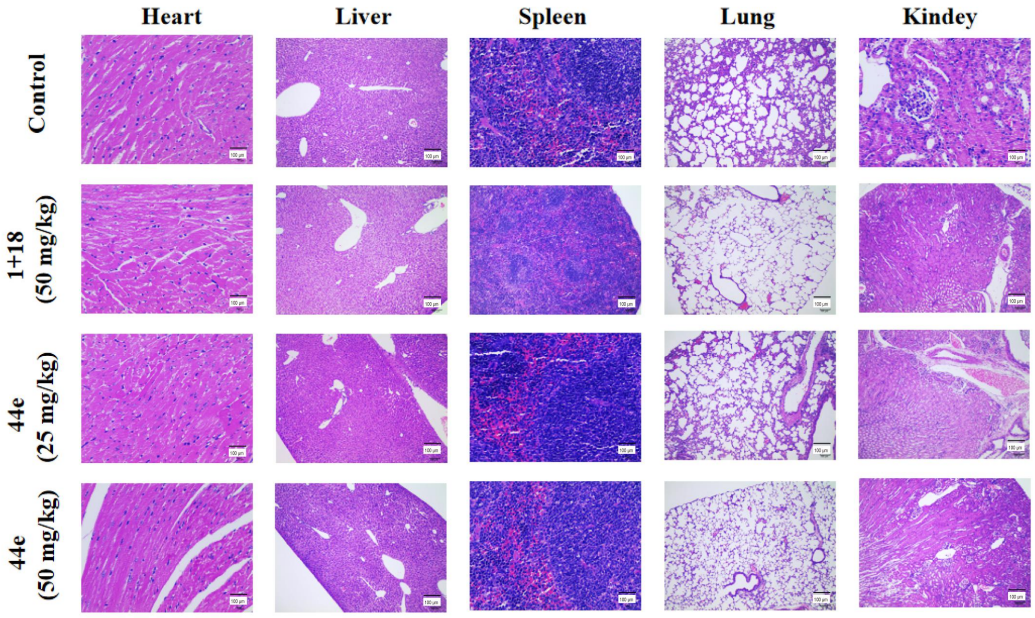


Figure S4. Representative images of main organ tissues after staining with hematoxylin-eosin (H&E) in MDA-MB-231 tumor xenograft model. Scale bar, 100 μm.

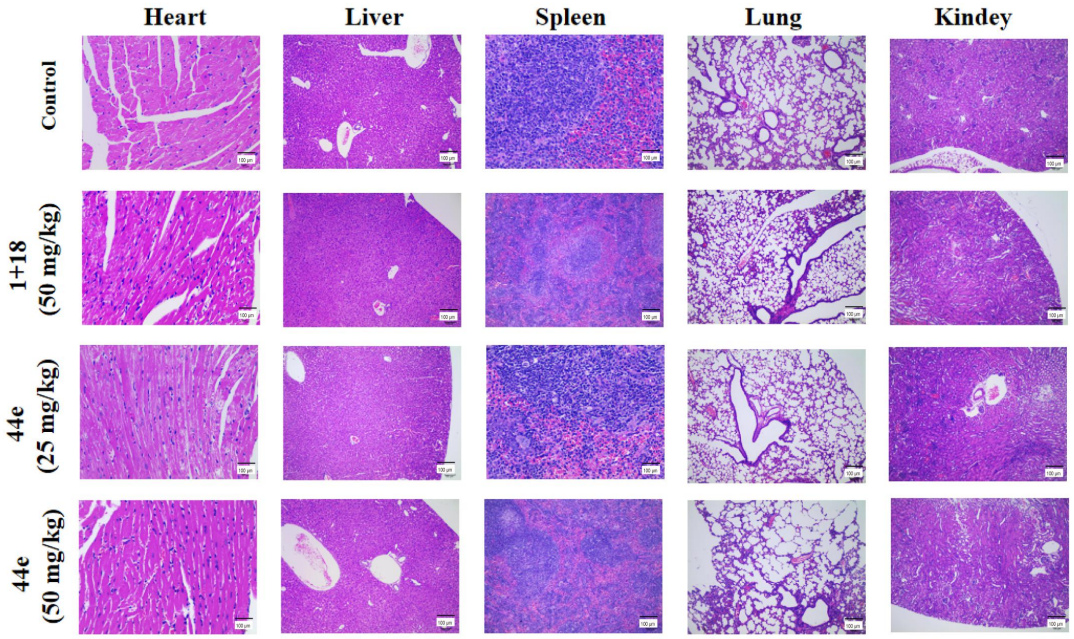
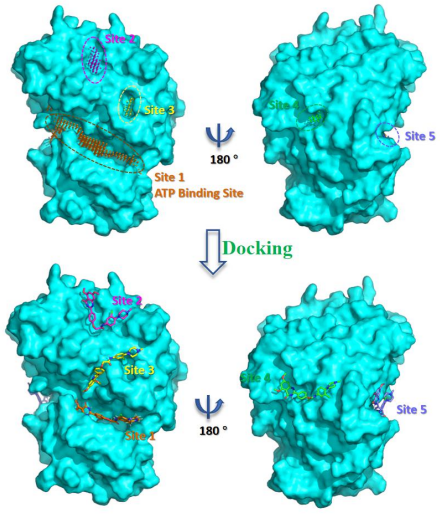


Figure S5. Representative images of main organ tissues after staining with hematoxylin-eosin (H&E) in MDA-MB-468 tumor xenograft model. Scale bar, 100 μm.



	Volume （Å）	Docking score （kcal/mol）
Site 1(ATP)	**373**	**-9.6**
Site 2	57	-6.8
Site 3	26	-6.3
Site 4	22	-7.2
Site 5	21	-7.3

Protein Active Site Prediction Web：
http://altair.sci.hokudai.ac.jp/g6/Research/POCASA_e.html
Docking software： Autodock vina 1.1.2

Figure S6. 44e was docked and scored with the 5 potential active sites of CK2.

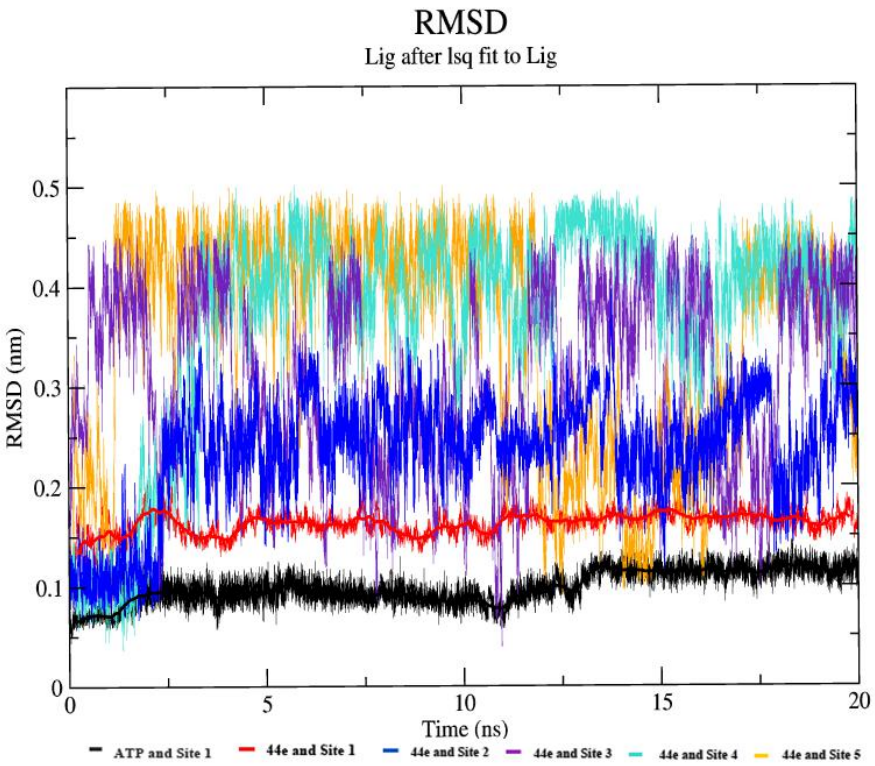


Figure S7. Root mean square deviation (RMSD) of ATP and compound **44e** on 5 potential active sites of CK2.

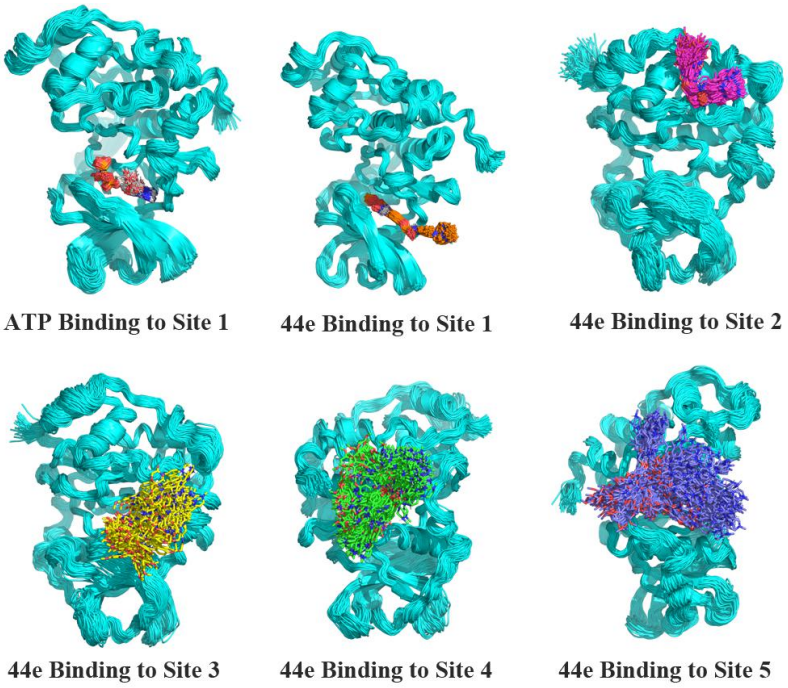


Figure S8. Molecular dynamics conformation superposition of ATP and compound **44e** (200 frames) on 5 potential active sites of CK2.

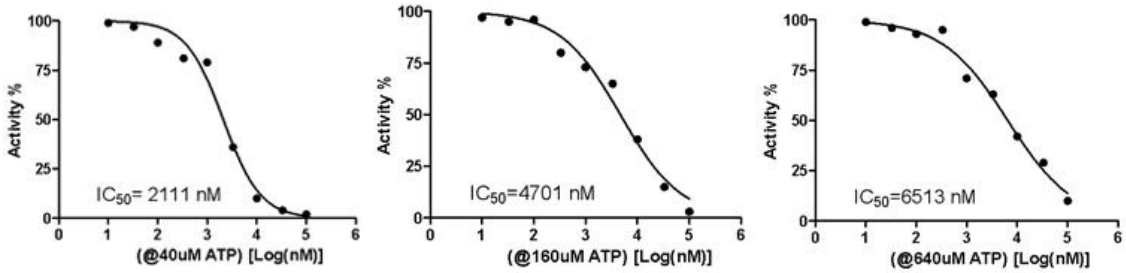


Figure S9. ATP competitive binding test. The inhibition rate of compound **44e** on CK2 was tested at ATP concentrations of 40 μM, 160 μM and 640 μM.

Table S1. Selectivity profiling of compound **44e** at 1000 nM against 412 kinases.

Kinase	Activity%	Kinase	Activity%
AAK1(h)	87	MARK3(h)	62
Abl (H396P) (h)	90	MARK4(h)	70
Abl (M351T)(h)	74	MEK1(h)	95
Abl (Q252H) (h)	79	MEK2(h)	98
Abl(h)	96	MEKK2(h)	84
Abl(T315I)(h)	112	MEKK3(h)	76
Abl(Y253F)(h)	134	MELK(h)	104
ACK1(h)	98	Mer(h)	72
ACTR2(h)	78	Met(D1246H)(h)	85
ALK(h)	83	Met(D1246N)(h)	93
ALK1(h)	107	Met(h)	77
ALK2(h)	86	Met(M1268T)(h)	82
ALK4(h)	90	Met(Y1248C)(h)	105
ALK6(h)	95	Met(Y1248D)(h)	79
AMPKα1(h)	93	Met(Y1248H)(h)	87
AMPKα2(h)	107	MINK(h)	70
A-Raf(h)	88	MKK3(h)	58
Arg(h)	85	MKK6(h)	80
ARK5(h)	94	MLCK(h)	73
ASK1(h)	78	MLK1(h)	81
ATM(h)	90	MLK2(h)	75
ATR/ATRIP(h)	81	MLK3(h)	94
Aurora-A(h)	85	MLK4(h)	76
Aurora-B(h)	96	Mnk2(h)	72
Aurora-C(h)	87	MOK(h)	36
Axl(h)	92	MRCKα(h)	80

BIKe(h)	83	MRCKβ(h)	120
Blk(h)	76	MRCKγ(h)	105
BMPR2(h)	81	MSK1(h)	87
Bmx(h)	107	MSK2(h)	92
B-Raf(h)	93	MSSK1(h)	94
B-Raf(V599E)(h)	77	MST1(h)	76
BRK(h)	103	MST2(h)	88
BrSK1(h)	85	MST3(h)	93
BrSK2(h)	88	MST4(h)	75
BTK(h)	79	mTOR(h)	79
BTK(R28H)(h)	82	mTOR/FKBP12(h)	80
CaMKI(h)	58	MuSK(h)	106
CaMKIIα(h)	72	MYLK2(h)	82
CaMKIIβ(h)	90	MYO3B(h)	93
CaMKIIγ(h)	85	NDR1(h)	70
CaMKIIδ(h)	93	NDR2(h)	65
CaMKIß(h)	91	NEK1(h)	90
CaMKIV(h)	84	NEK11(h)	92
CaMKIγ(h)	73	NEK2(h)	102
CaMKIδ(h)	75	NEK3(h)	96
CaMKK1(h)	82	NEK4(h)	88
CaMKK2(h)	70	NEK6(h)	79
Cdc7/cyclinB1(h)	82	NEK7(h)	68
CDK1/cyclinB(h)	47	NEK9(h)	91
CDK12/cyclinK(h)	80	NIM1(h)	90
CDK13/cyclinK(h)	72	NLK(h)	93
CDK14/cyclinY(h)	95	NUAK2(h)	72
CDK16/cyclinY(h)	95	OSR1(h)	37

CDK17/cyclinY(h)	79	p70S6K(h)	68
CDK18/cyclinY(h)	82	PAK1(h)	91
CDK2/cyclinA(h)	90	PAK2(h)	87
CDK2/cyclinE(h)	123	PAK3(h)	75
CDK3/cyclinE(h)	86	PAK4(h)	95
CDK4/cyclinD3(h)	97	PAK5(h)	103
CDK5/p25(h)	70	PAK6(h)	89
CDK5/p35(h)	73	PAR-1Bα(h)	90
CDK6/cyclinD3(h)	98	PASK(h)	79
CDK7/cyclinH/MAT1(h)	102	PDGFRα(D842V)(h)	67
CDK9/cyclin T1(h)	117	PDGFRα(h)	75
CDKL1(h)	60	PDGFRα(V561D)(h)	78
CDKL2(h)	82	PDGFRβ(h)	92
CDKL3(h)	79	PDHK2(h)	83
CDKL4(h)	83	PDHK4(h)	75
ChaK1(h)	92	PDK1(h)	86
CHK1(h)	95	PEK(h)	105
CHK2(h)	80	PhKγ1(h)	66
CHK2(I157T)(h)	77	PhKγ2(h)	78
CHK2(R145W)(h)	75	PI3 Kinase (p110a(E542K)/p85a)(h)	72
CK1α(h)	95	PI3 Kinase (p110a(E545K)/p85a)(h)	84
CK1γ1(h)	98	PI3 Kinase (p110a(H1047R)/p85a)(h)	96

CK1γ2(h)	110	PI3 Kinase (p110a/p65a)(h)	114
CK1γ3(h)	94	PI3 Kinase (p110a/p85a)(h)	89
CK1δ(h)	96	PI3 Kinase (p110b/p85a)(h)	73
CK1ε(h)	107	PI3 Kinase (p110d/p85a)(h)	86
CK2(h)	0	PI3 Kinase (p120g)(h)	93
CK2α1(h)	20	PI3KC2a(h)	75
CK2α2(h)	34	PI3KC2g(h)	69
cKit(D816H)(h)	80	Pim-1(h)	55
cKit(D816V)(h)	97	Pim-2(h)	62
cKit(h)	106	Pim-3(h)	68
cKit(V560G)(h)	98	PIP4K2a(h)	75
cKit(V654A)(h)	101	PIP5K1a(h)	81
CLIK1(h)	85	PIP5K1g(h)	90
CLK1(h)	70	PKA(h)	77
CLK2(h)	45	PKAcβ(h)	69
CLK3(h)	59	PKBα(h)	78
CLK4(h)	84	PKBβ(h)	92
c-RAF(h)	90	PKBγ(h)	95
CRIK(h)	105	PKCα(h)	84
CSK(h)	83	PKCβI(h)	79
cSRC(h)	60	PKCβII(h)	80
DAPK1(h)	88	PKCγ(h)	115
DAPK2(h)	108	PKCδ(h)	90
DCAMKL1(h)	81	PKCε(h)	65

DCAMKL2(h)	75	PKCζ(h)	70
DCAMKL3(h)	120	PKCη(h)	73
DDR1(h)	93	PKCθ(h)	78
DDR2(h)	80	PKCι(h)	80
DMPK(h)	77	PKCμ(h)	84
DNA-PK(h)	75	PKD2(h)	102
DRAK1(h)	89	PKD3(h)	96
DRAK2(h)	94	PKG1α(h)	71
DYRK1A(h)	48	PKG1β(h)	80
DYRK1B(h)	45	PKR(h)	64
DYRK2(h)	55	Plk1(h)	73
DYRK3(h)	40	Plk3(h)	90
eEF-2K(h)	79	Plk4(h)	102
EGFR(h)	78	PRAK(h)	59
EGFR(L858R)(h)	93	PRK1(h)	72
EGFR(L861Q)(h)	86	PRK2(h)	68
EGFR(T790M)(h)	76	PRKG2(h)	91
EGFR(T790M,L858R)(h)	90	PrKX(h)	60
EphA1(h)	115	PRP4(h)	71
EphA2(h)	98	PTK5(h)	83
EphA3(h)	102	Pyk2(h)	48
EphA4(h)	84	Ret (V804L)(h)	70
EphA5(h)	85	Ret(h)	80
EphA7(h)	96	Ret(V804M)(h)	75
EphA8(h)	74	RIPK1(h)	92
EphB1(h)	110	RIPK2(h)	84
EphB2(h)	105	ROCK-I(h)	84

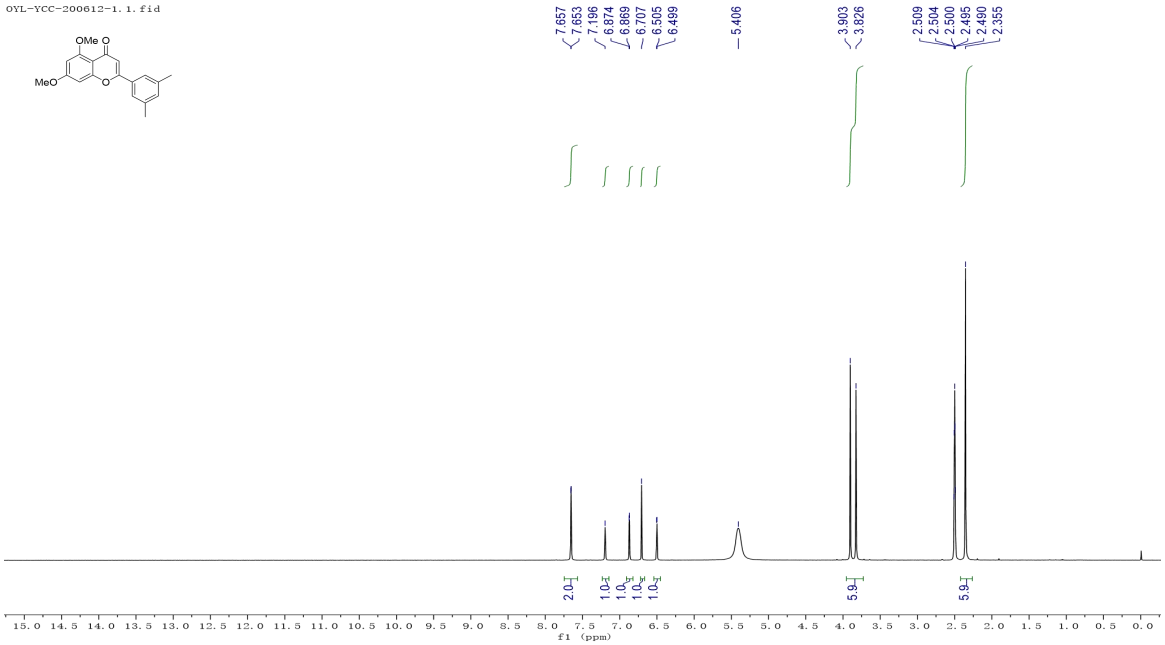
EphB3(h)	88	ROCK-II(h)	79
EphB4(h)	96	Ron(h)	74
ErbB2(h)	79	Ros(h)	67
ErbB4(h)	92	Rse(h)	69
FAK(h)	80	Rsk1(h)	80
Fer(h)	99	Rsk2(h)	99
Fes(h)	68	Rsk3(h)	65
FGFR1(h)	50	Rsk4(h)	105
FGFR1(V561M)(h)	90	SAPK2a(h)	70
FGFR2(h)	83	SAPK2a(T106M)(h)	95
FGFR2(N549H)(h)	82	SAPK2b(h)	88
FGFR3(h)	70	SAPK3(h)	81
FGFR4(h)	103	SAPK4(h)	70
Fgr(h)	91	SBK1(h)	25
Flt1(h)	94	SGK(h)	106
Flt3(D835Y)(h)	110	SGK2(h)	92
Flt3(h)	69	SGK3(h)	80
Flt4(h)	95	SIK(h)	110
Fms(h)	98	SIK2(h)	94
Fms(Y969C)(h)	87	SIK3(h)	85
Fyn(h)	105	SLK(h)	79
GCK(h)	42	Snk(h)	28
GCN2(h)	80	SNRK(h)	97
GRK1(h)	87	Src(1-530)(h)	83
GRK2(h)	65	Src(T341M)(h)	88
GRK3(h)	70	SRMS(h)	90
GRK5(h)	86	SRPK1(h)	93
GRK6(h)	95	SRPK2(h)	82

GRK7(h)	78	STK16(h)	79
GSK3α(h)	105	STK25(h)	81
GSK3β(h)	97	STK32A(h)	96
Haspin(h)	78	STK32B(h)	85
Hck(h)	92	STK32C(h)	70
Hck(h) activated	95	STK33(h)	114
HIPK1(h)	83	STK39(h)	84
HIPK2(h)	73	Syk(h)	40
HIPK3(h)	90	TAF1L(h)	65
HIPK4(h)	110	TAK1(h)	93
HPK1(h)	77	TAO1(h)	85
HRI(h)	85	TAO2(h)	78
ICK(h)	75	TAO3(h)	60
IGF-1R(h)	104	TBK1(h)	128
IGF-1R(h), activated	99	Tec(h) activated	79
IKKα(h)	107	TGFBR1(h)	81
IKKβ(h)	84	TGFBR2(h)	88
IKKε(h)	89	Tie2 (h)	119
IR(h)	96	Tie2(R849W)(h)	83
IR(h), activated	115	Tie2(Y897S)(h)	80
IRAK1(h)	112	TLK1(h)	49
IRAK4(h)	99	TLK2(h)	34
IRE1(h)	72	TNIK(h)	87
IRR(h)	45	TRB2(h)	91
Itk(h)	116	TrkA(h)	79
JAK1(h)	80	TrkB(h)	82
JAK2(h)	75	TrkC(h)	90
JAK3(h)	91	TSSK1(h)	118

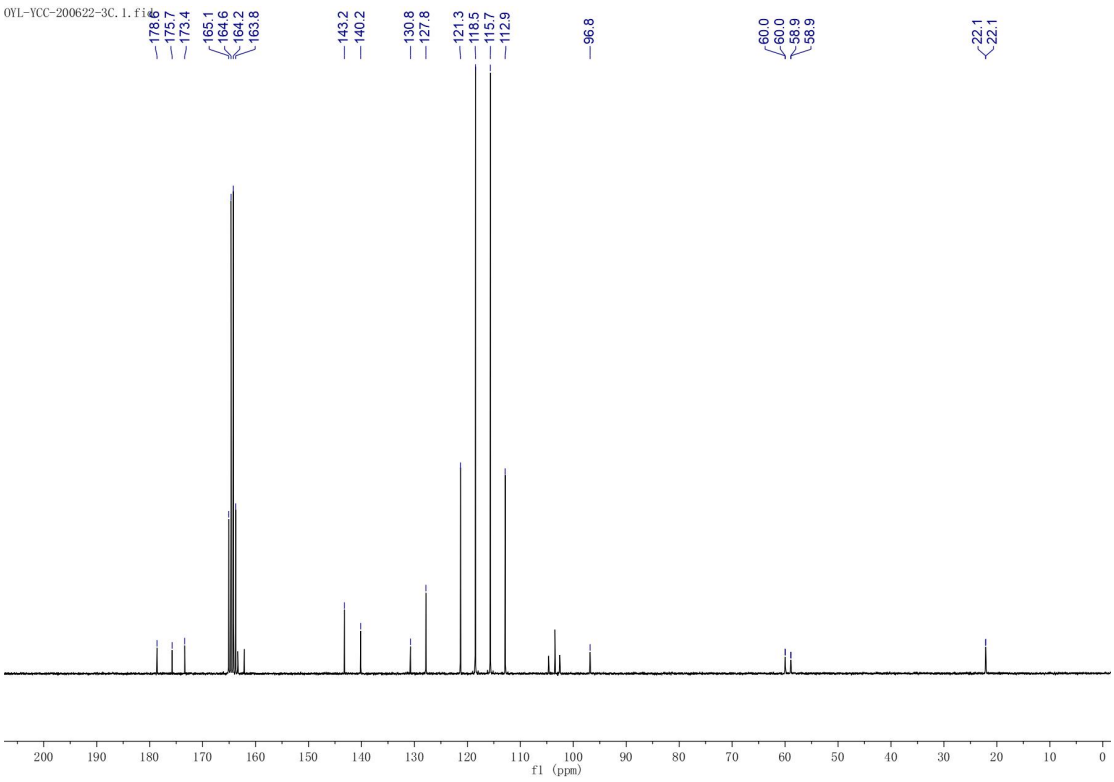
JNK1α1(h)	89	TSSK2(h)	99
JNK2α2(h)	75	TSSK3(h)	74
JNK3(h)	82	TSSK4(h)	84
KDR(h)	93	TTBK1(h)	80
LATS1(h)	92	TTBK2(h)	96
LATS2(h)	104	TTK(h)	102
Lck(h) activated	90	Txk(h)	70
LIMK1(h)	85	TYK2(h)	89
LIMK2(h)	94	ULK1(h)	92
LKB1(h)	110	ULK2(h)	126
LOK(h)	97	ULK3(h)	88
LRRK2(h)	75	VRK1(h)	84
LTK(h)	60	VRK2(h)	67
Lyn(h)	73	Wee1(h)	80
MAK(h)	87	Wee1B(h)	92
MAP4K3(h)	90	WNK1(h)	74
MAP4K4(h)	76	WNK2(h)	103
MAP4K5(h)	85	WNK3(h)	82
MAPK1(h)	93	WNK4(h)	110
MAPK2(h)	98	Yes(h)	61
MAPKAP-K2(h)	106	ZAK(h)	89
MAPKAP-K3(h)	120	ZAP-70(h)	93
MARK1(h)	88	ZIPK(h)	72

2. NMR Spectra Data

33a

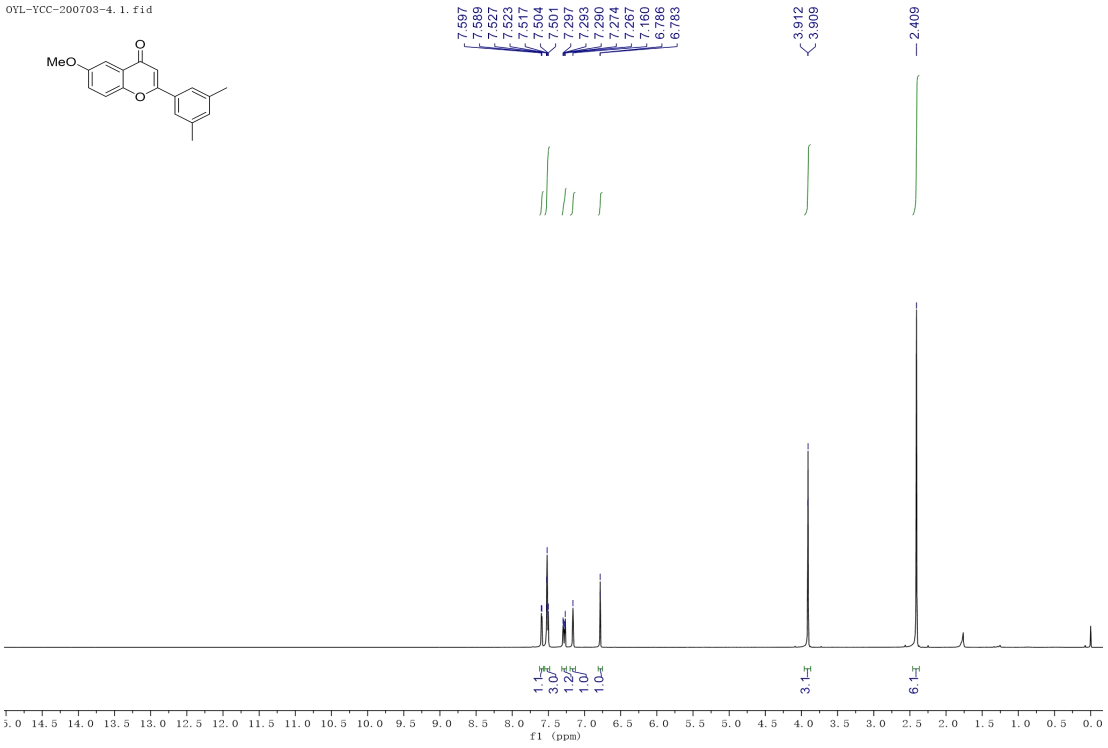


^{1}H NMR Spectrum of Compound **33a**

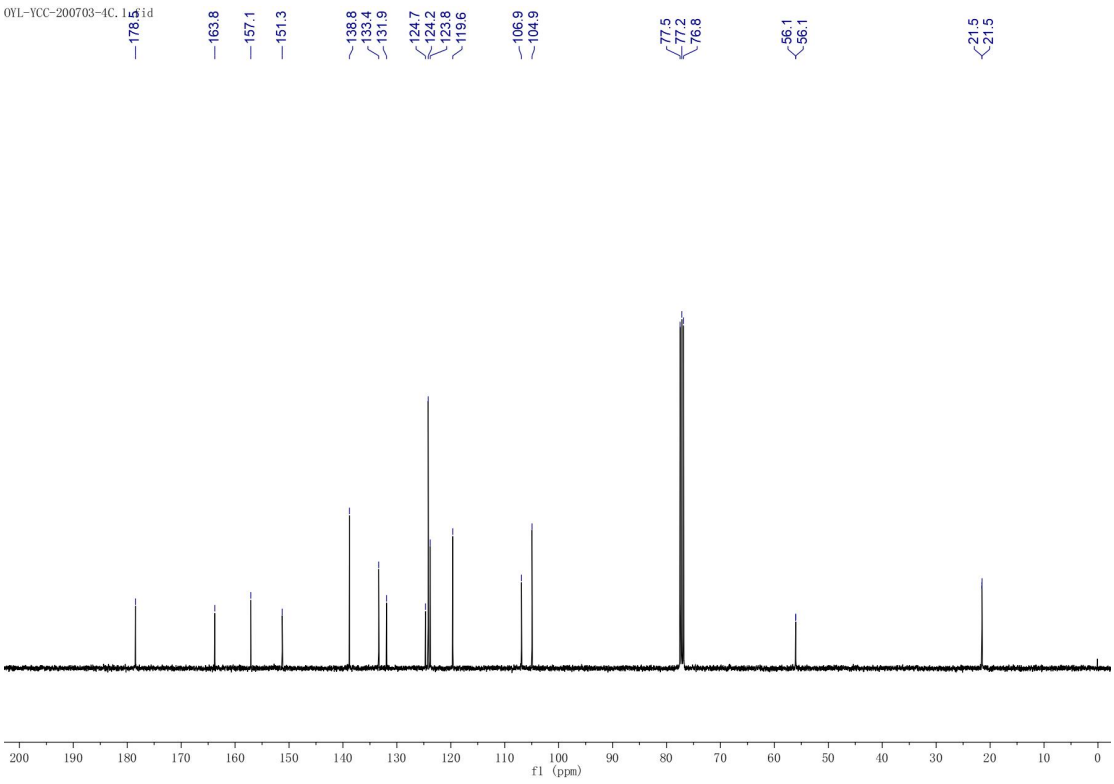


^{13}C NMR Spectrum of Compound **33a**

33b

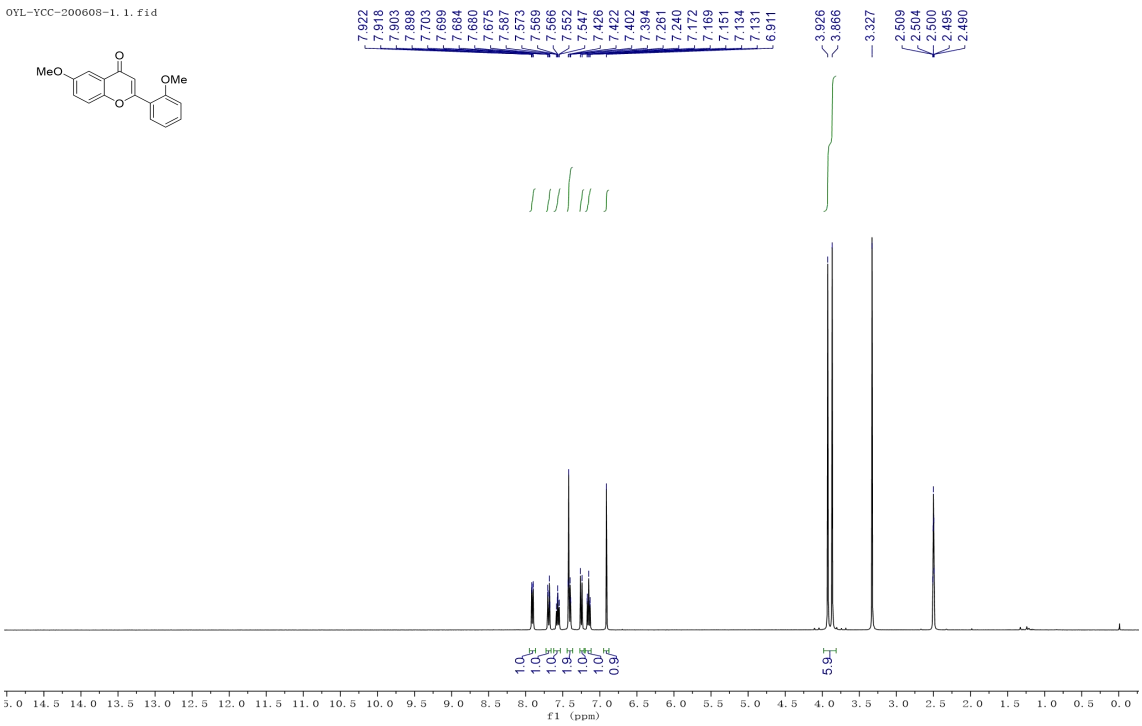


^{1}H NMR Spectrum of Compound **33b**

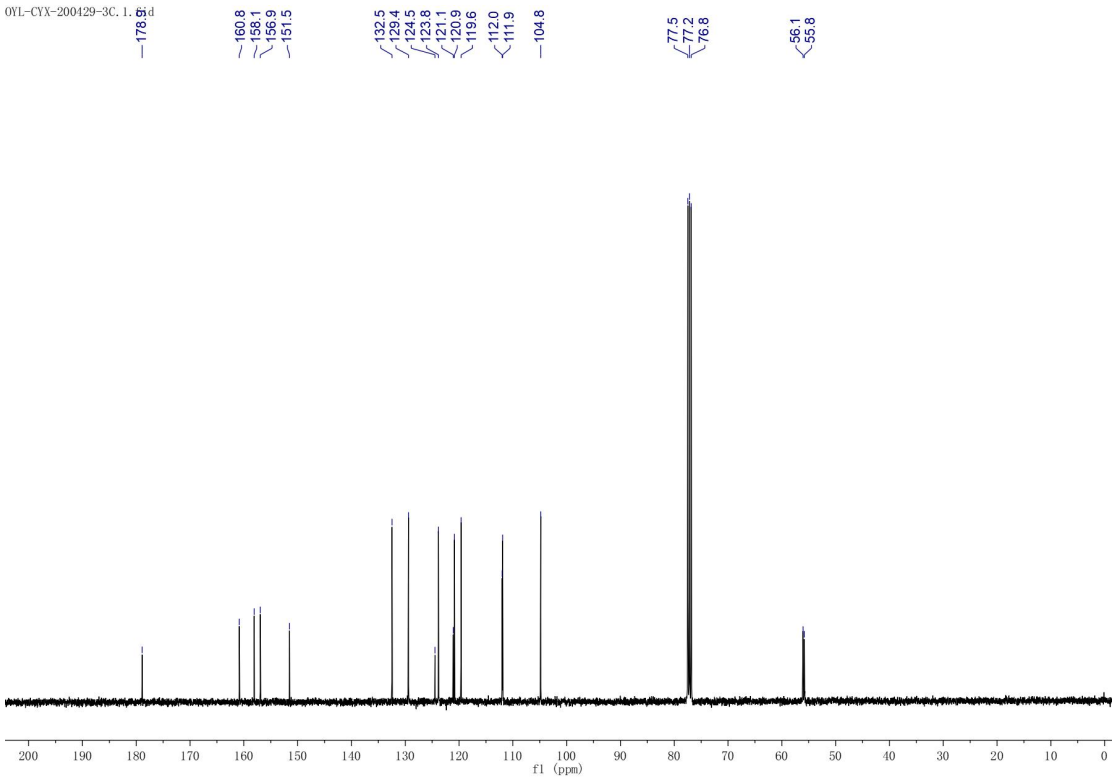


^{13}C NMR Spectrum of Compound **33b**

33c

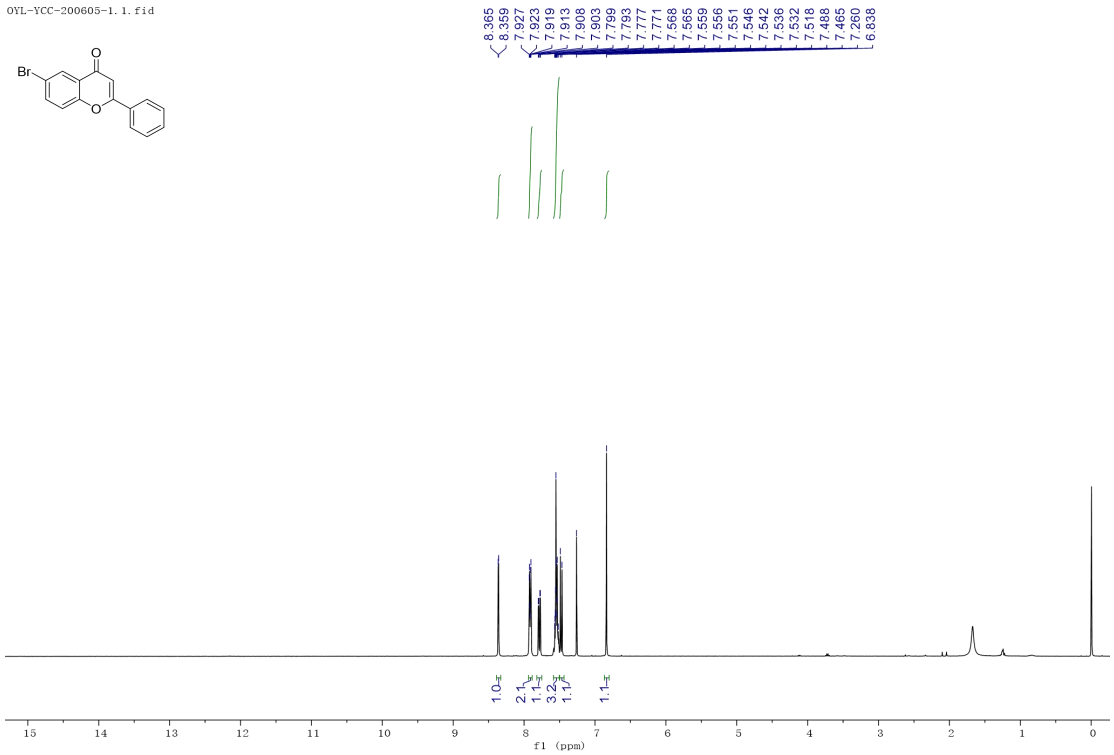


^{1}H NMR Spectrum of Compound **33c**

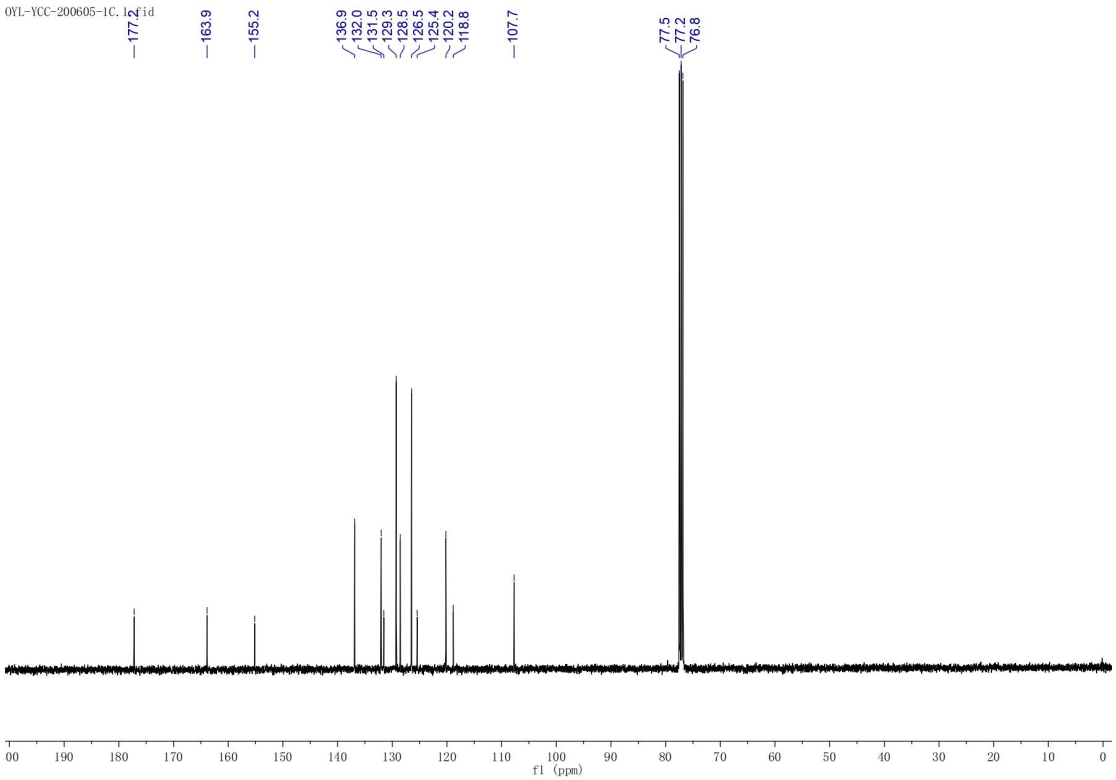


^{13}C NMR Spectrum of Compound **33c**

33d

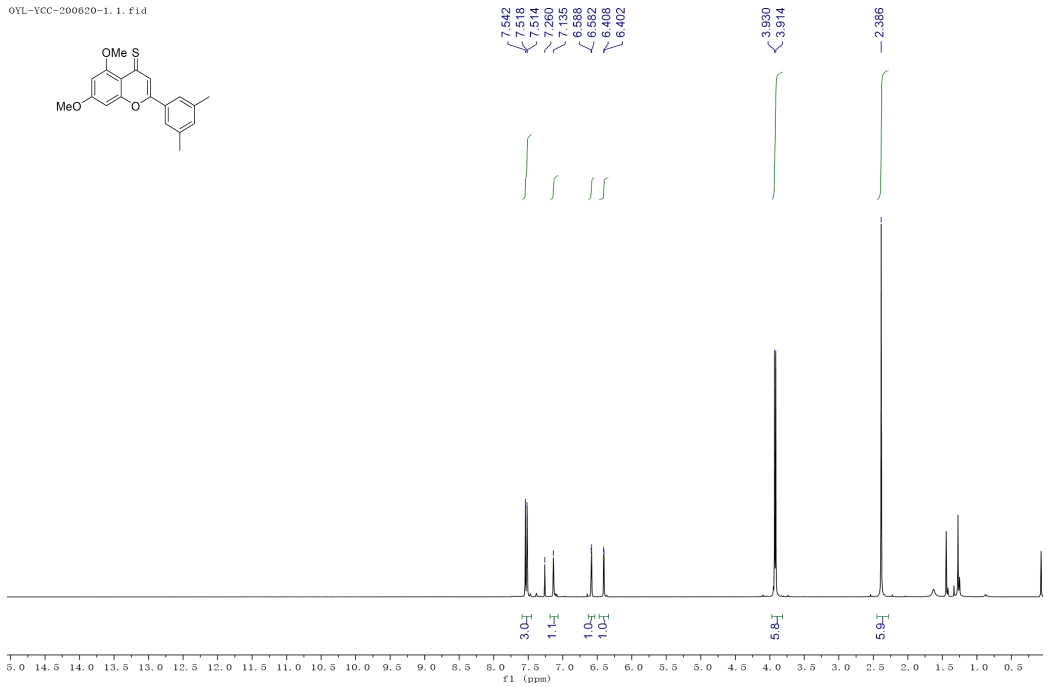


^{1}H NMR Spectrum of Compound **33d**

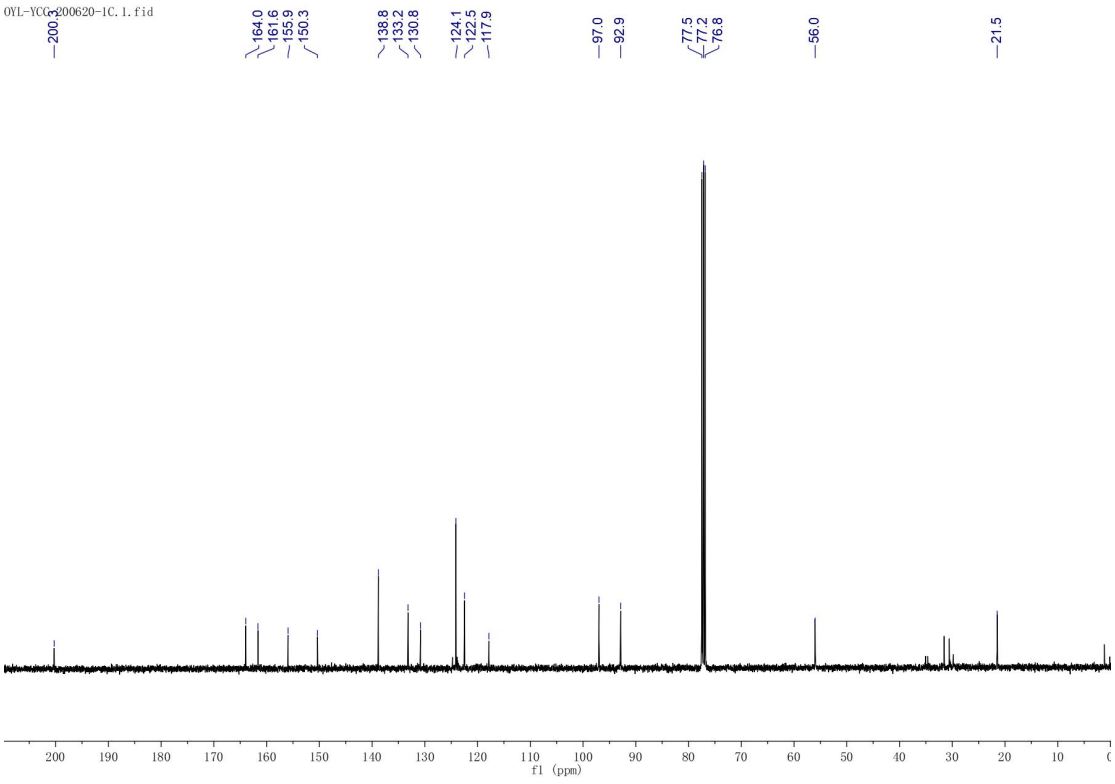


^{13}C NMR Spectrum of Compound **33d**

34a

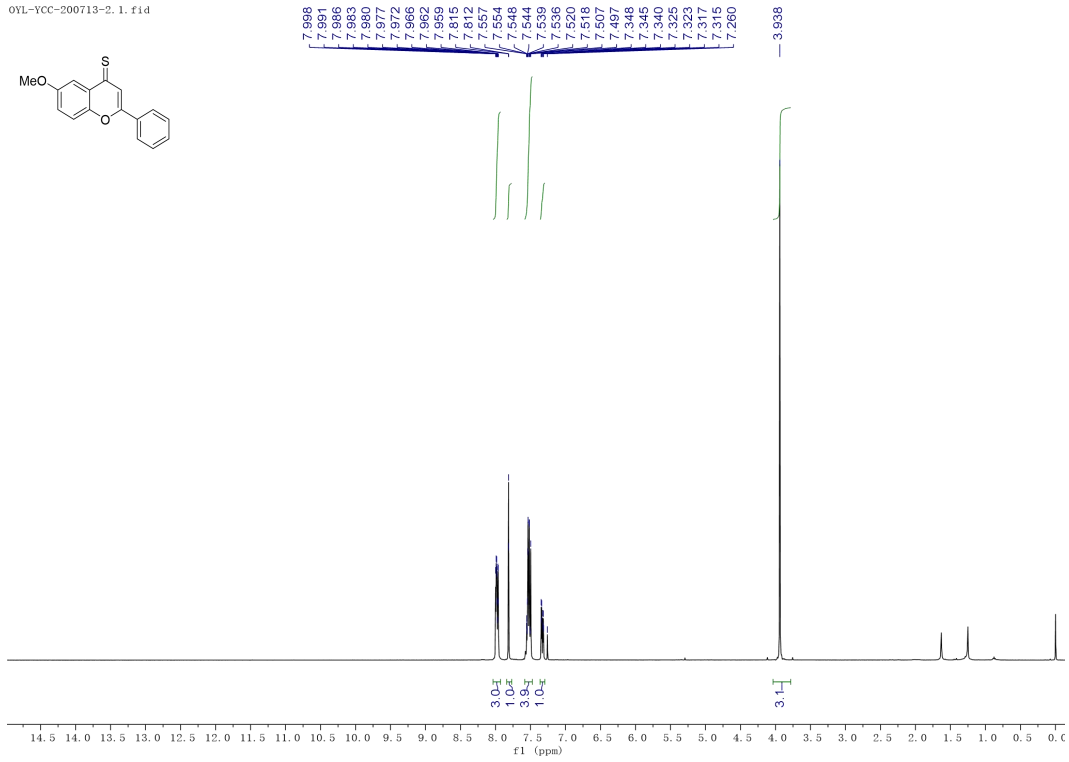


^{1}H NMR Spectrum of Compound **34a**

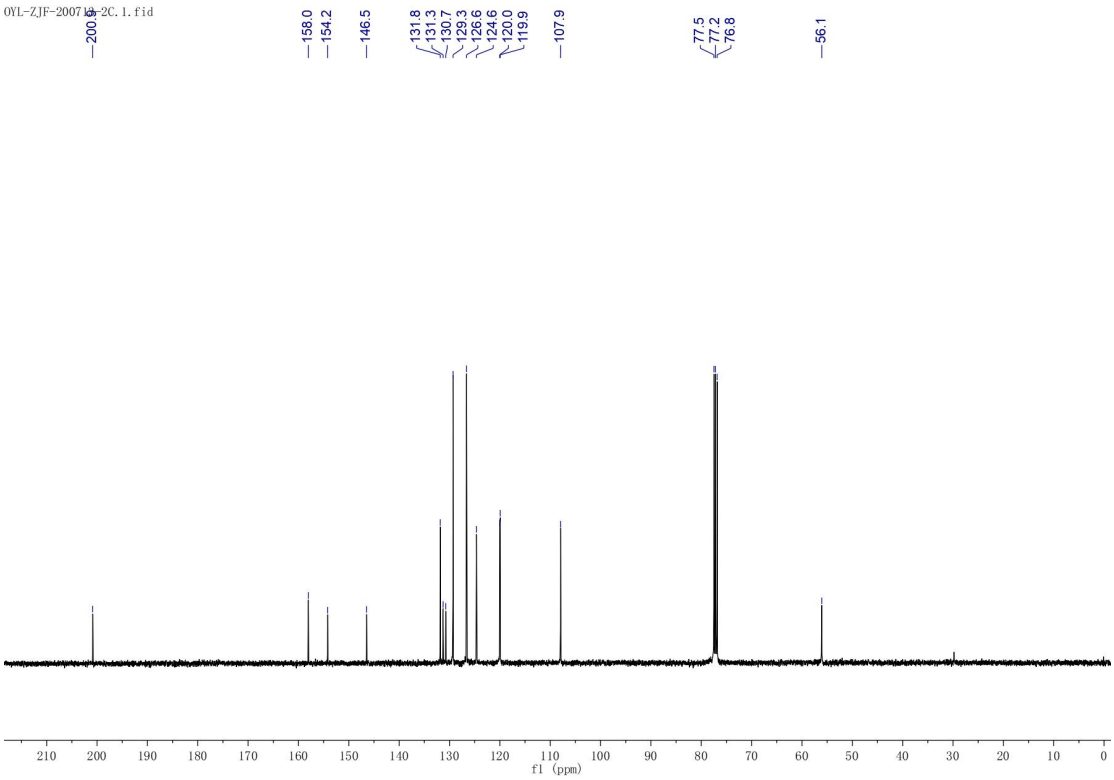


^{13}C NMR Spectrum of Compound **34a**

34b

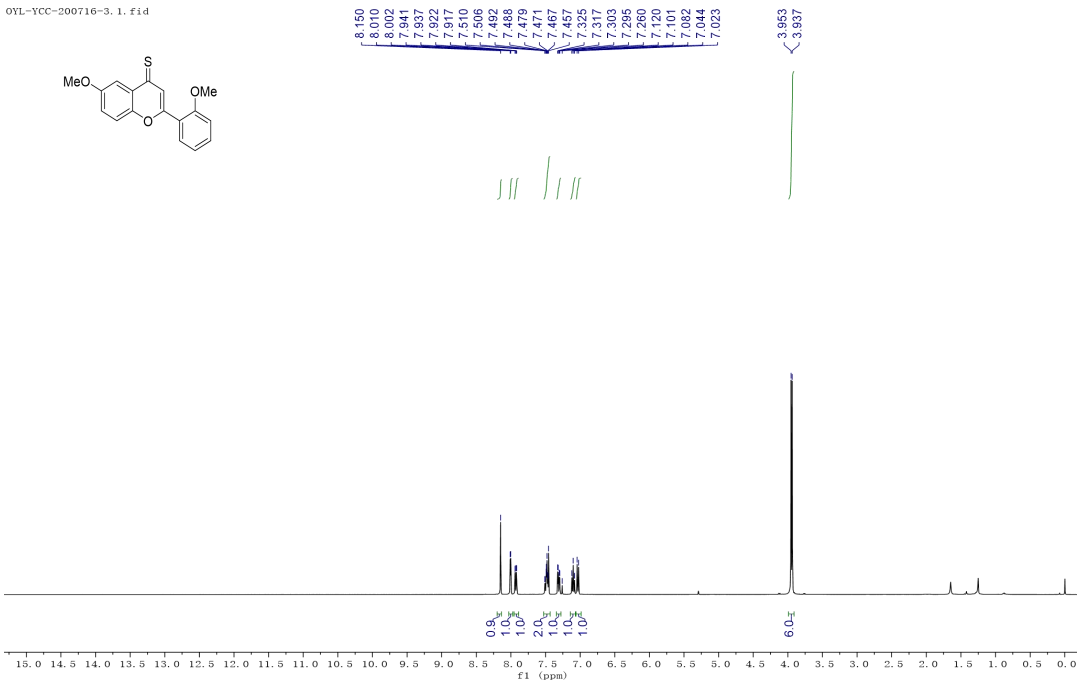


^{1}H NMR Spectrum of Compound **34b**

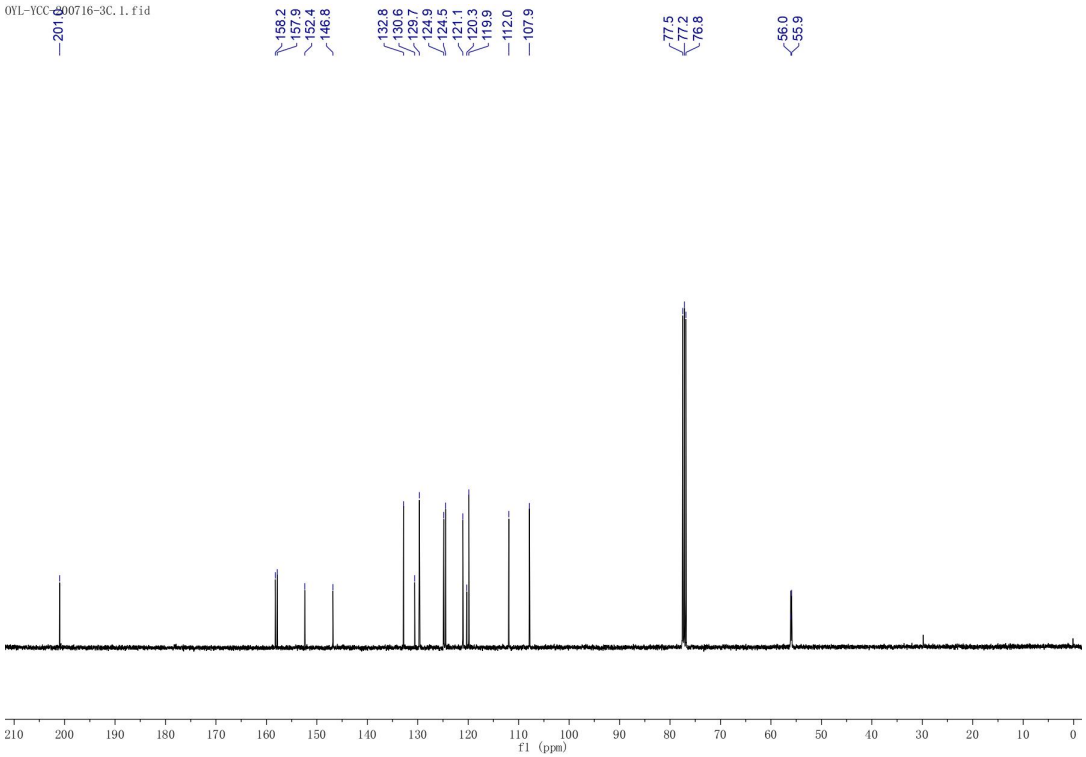


^{13}C NMR Spectrum of Compound **34b**

34c

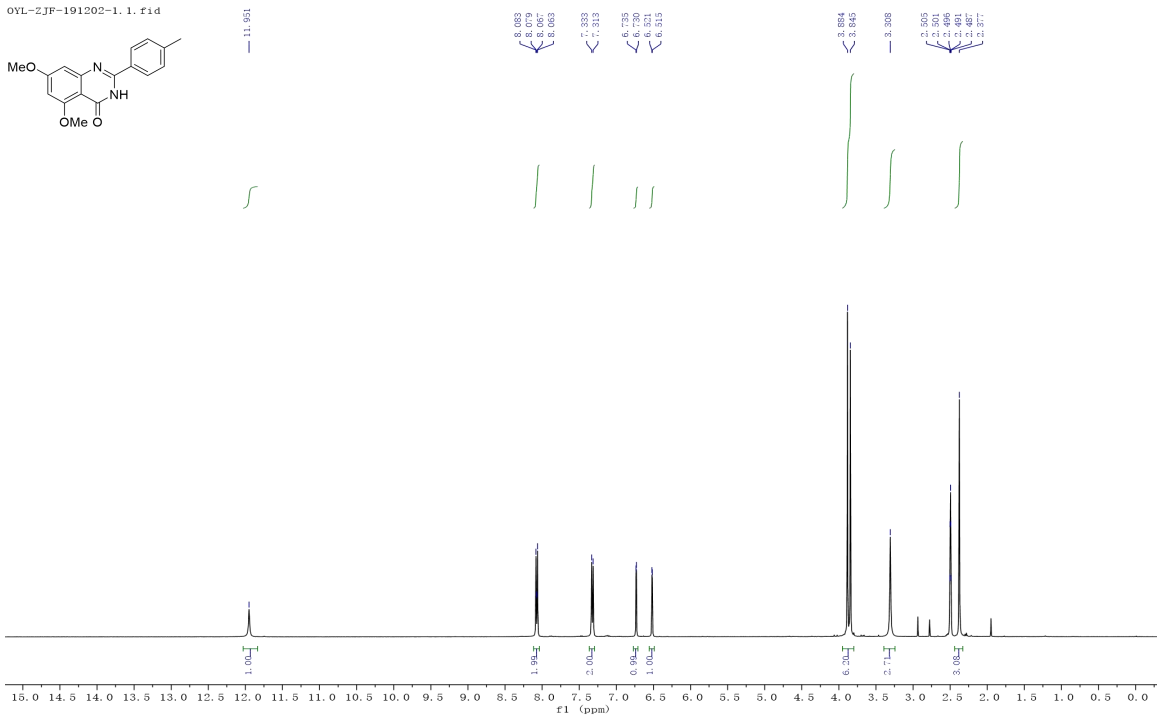


^{1}H NMR Spectrum of Compound **34c**

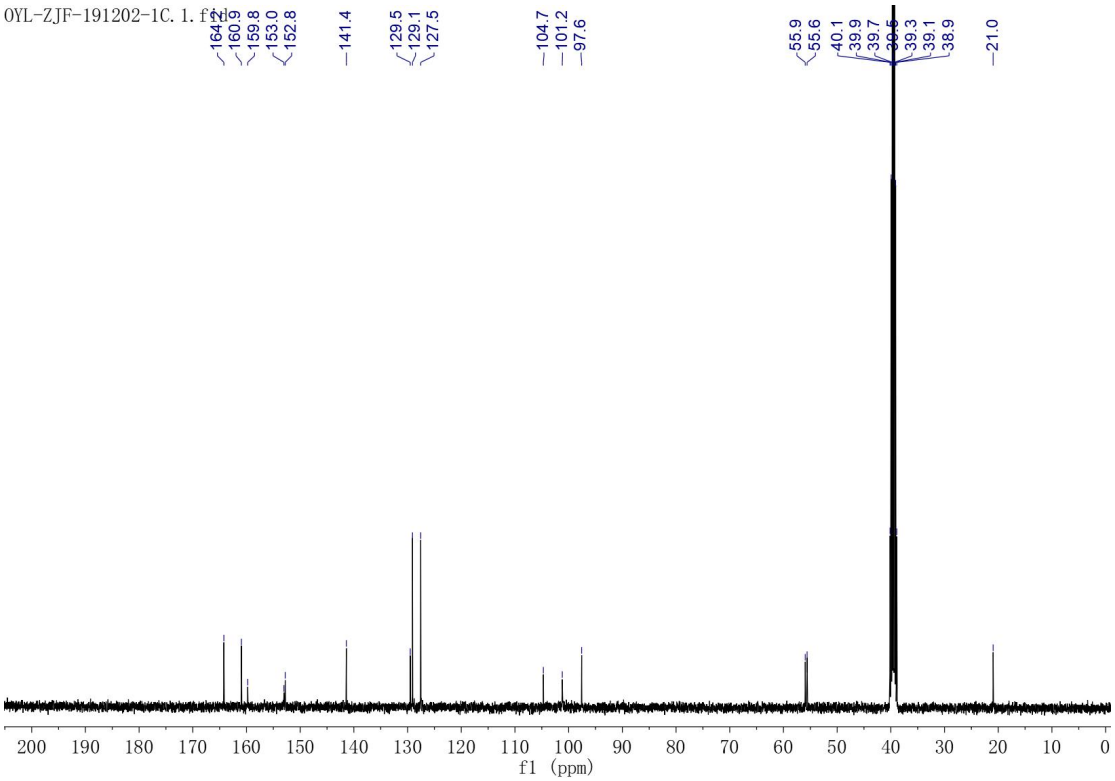


^{13}C NMR Spectrum of Compound **34c**

38a

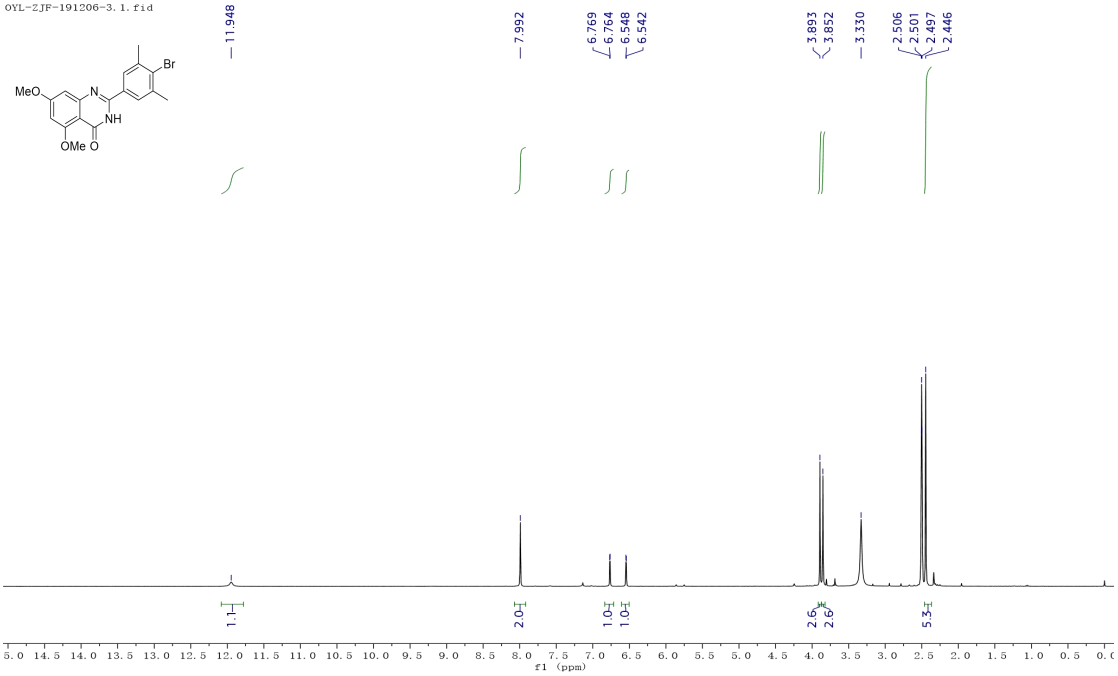


^{1}H NMR Spectrum of Compound **38a**

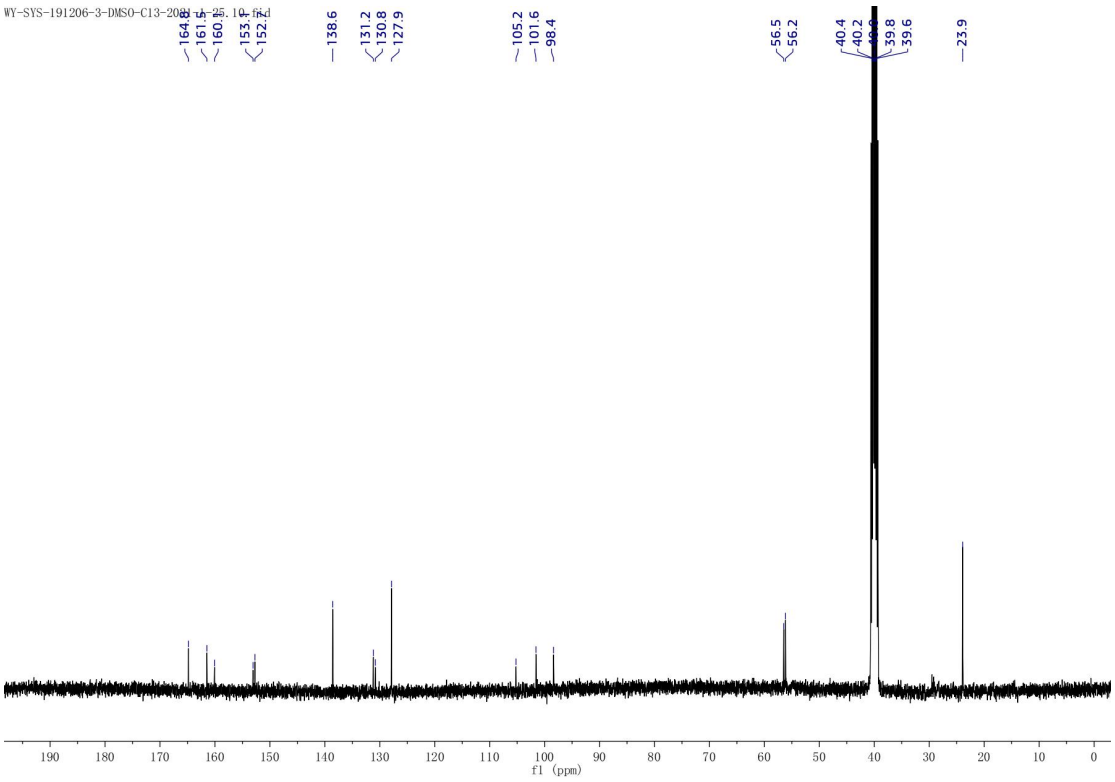


^{13}C NMR Spectrum of Compound **38a**

38b

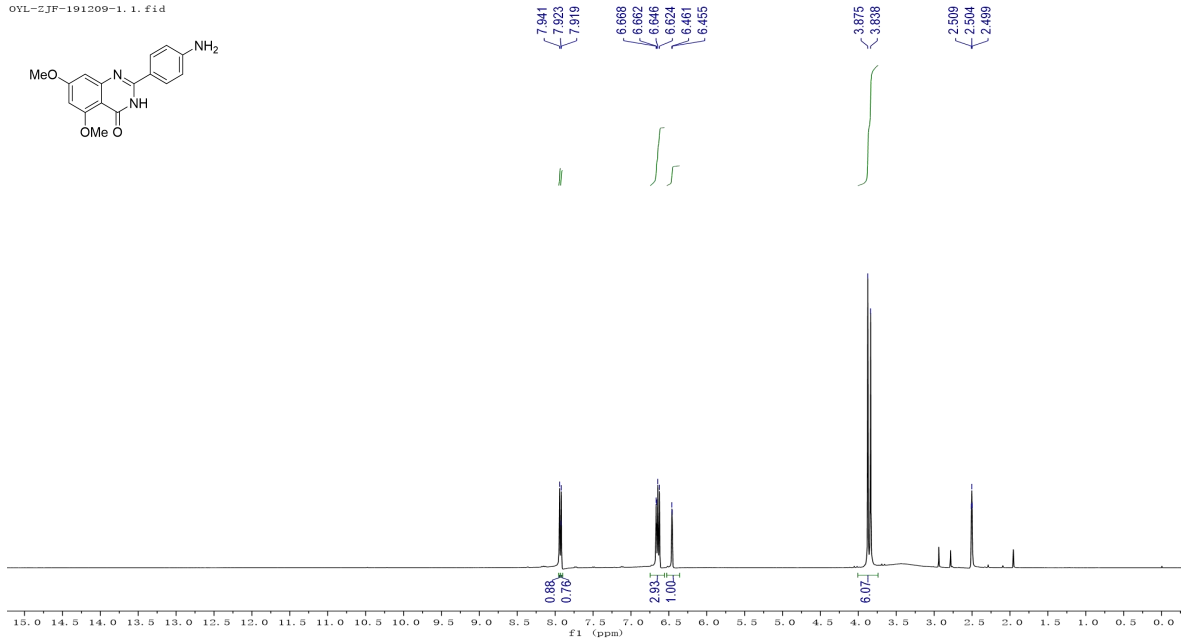


^{1}H NMR Spectrum of Compound **38b**

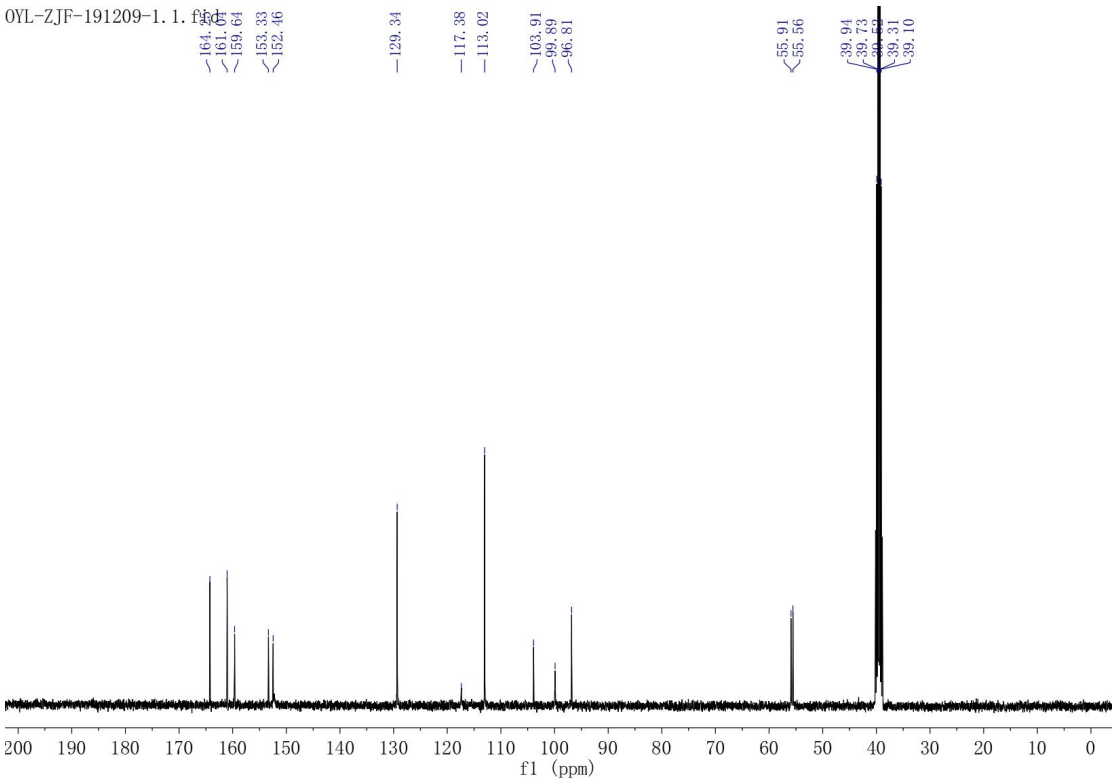


^{13}C NMR Spectrum of Compound **38b**

38c

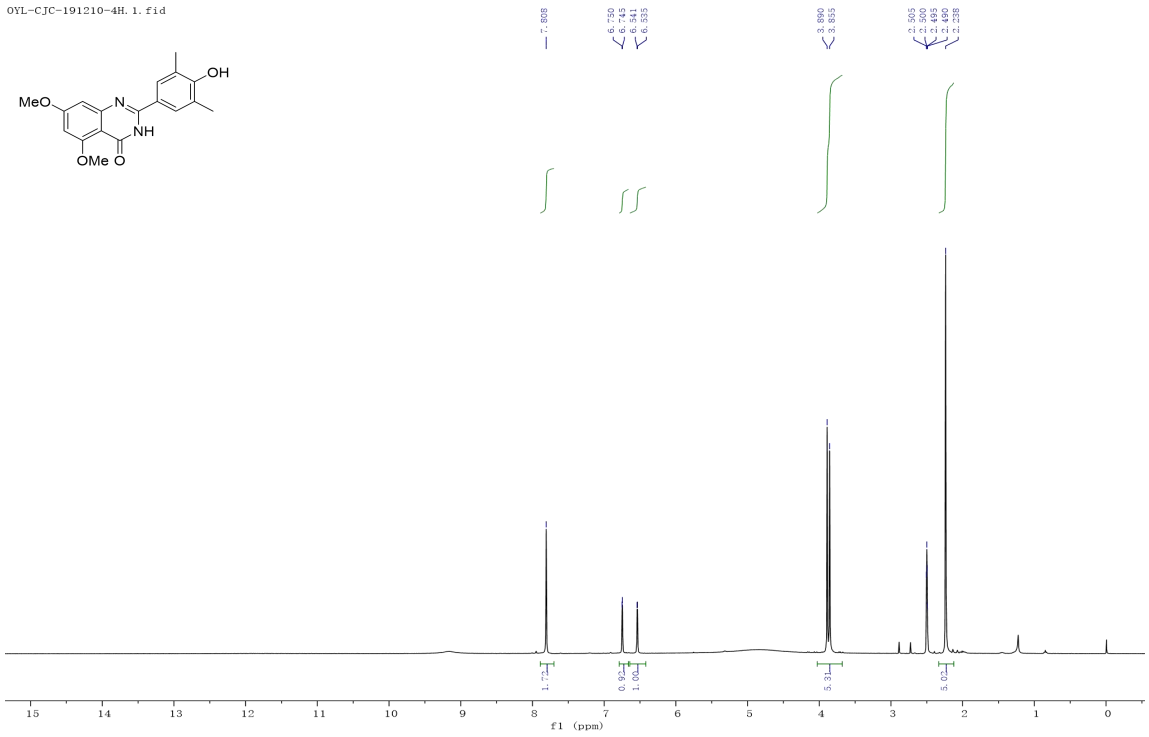


^{1}H NMR Spectrum of Compound **38c**

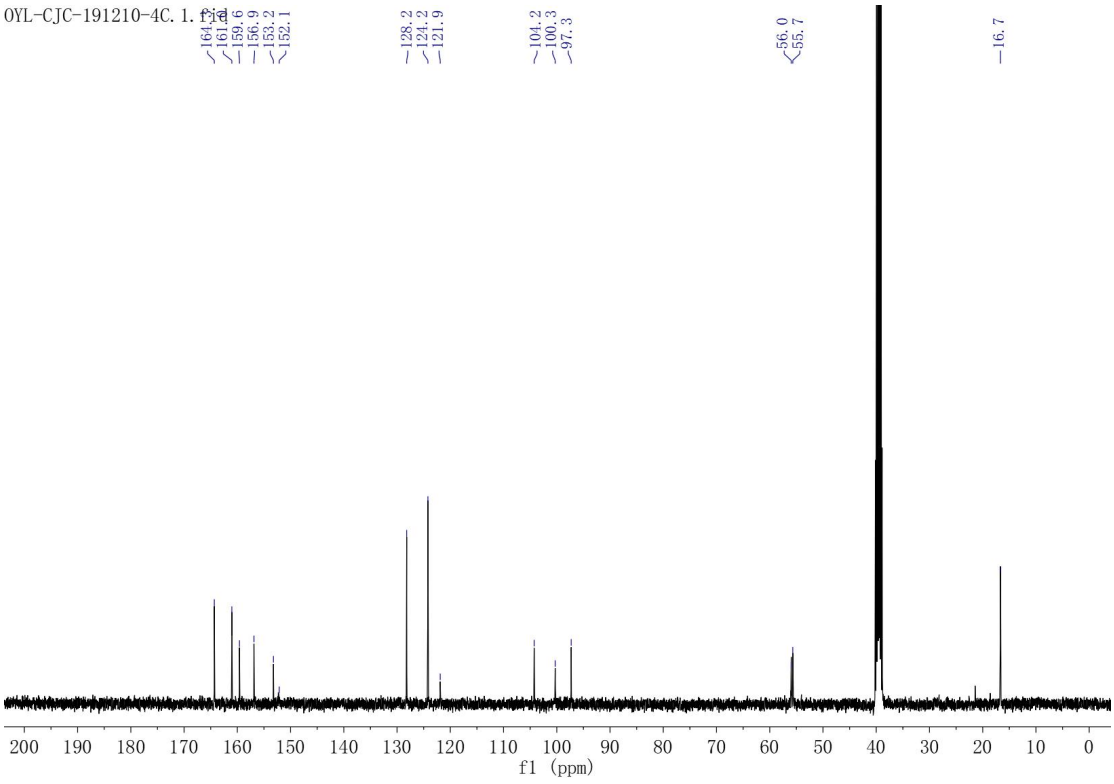


^{13}C NMR Spectrum of Compound **38c**

38d

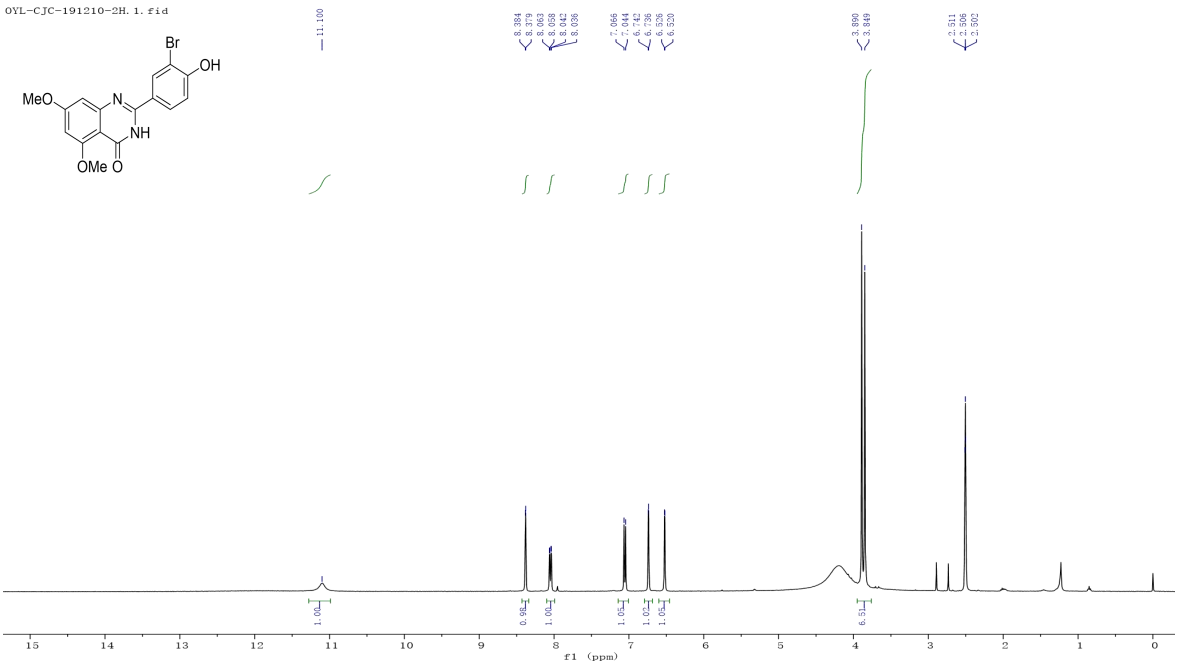


^{1}H NMR Spectrum of Compound **38d**

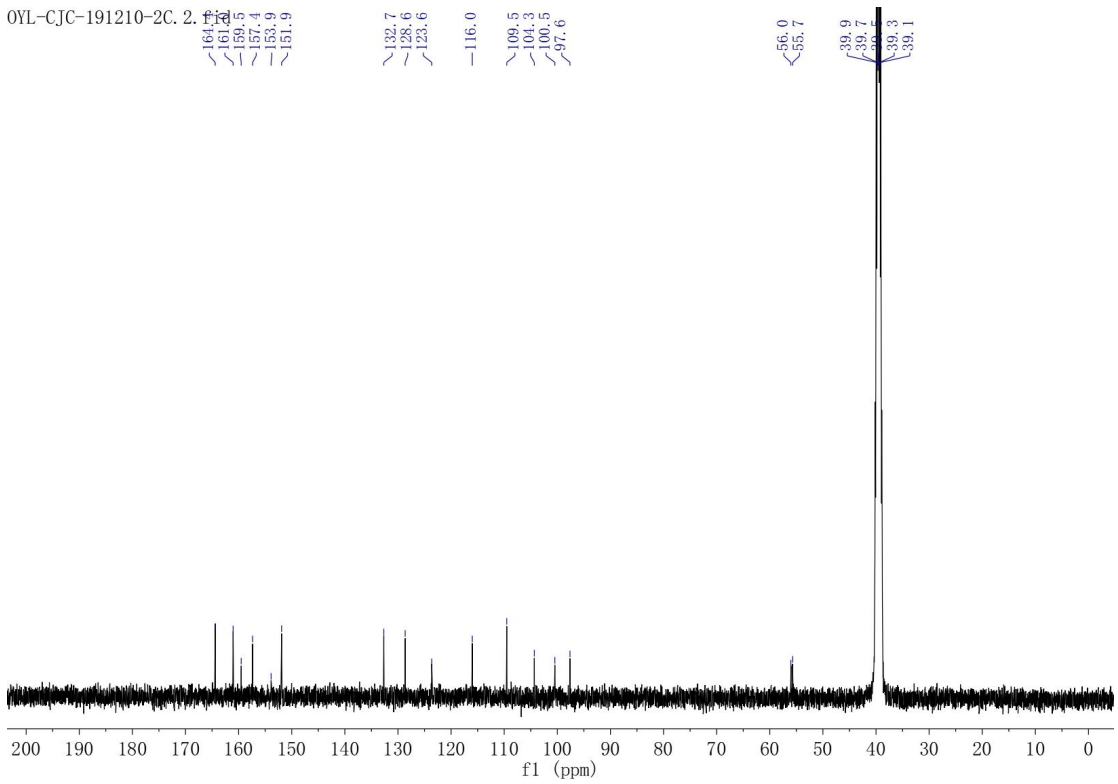


^{13}C NMR Spectrum of Compound **38d**

38e

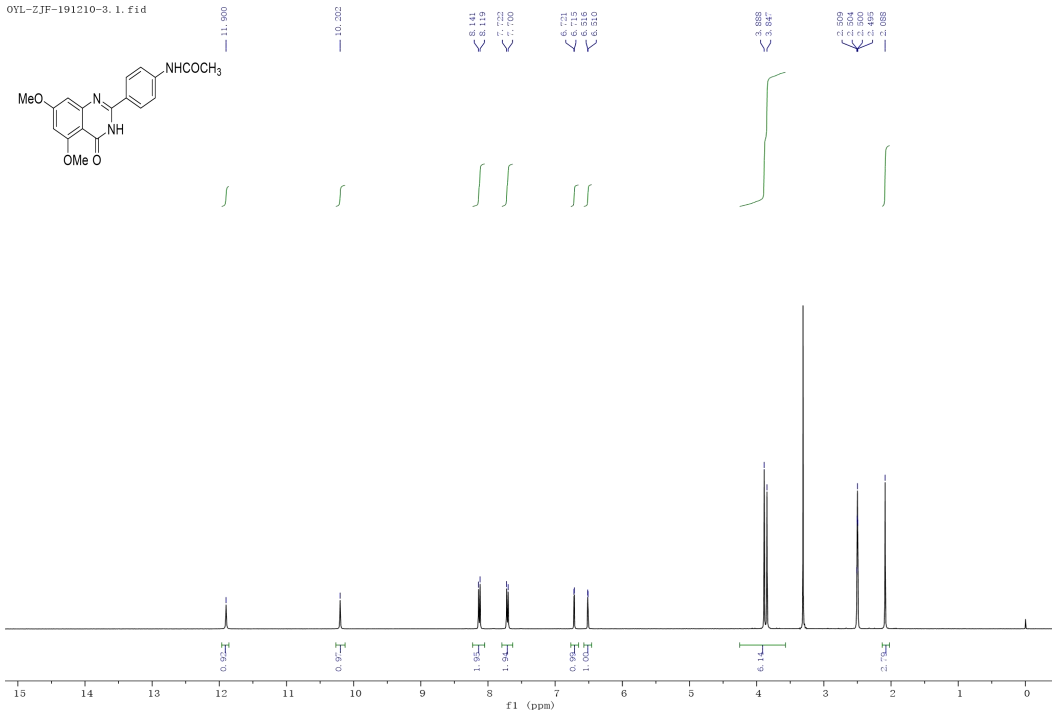


^{1}H NMR Spectrum of Compound **38e**

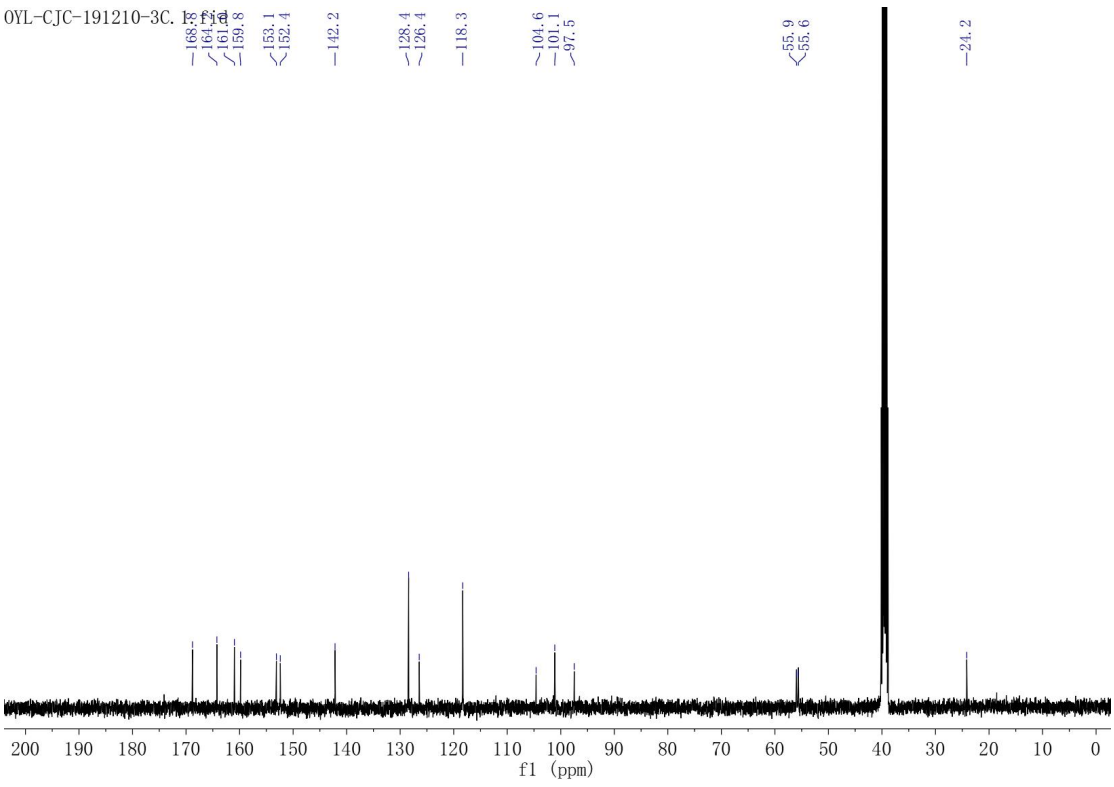


^{13}C NMR Spectrum of Compound **38e**

38f

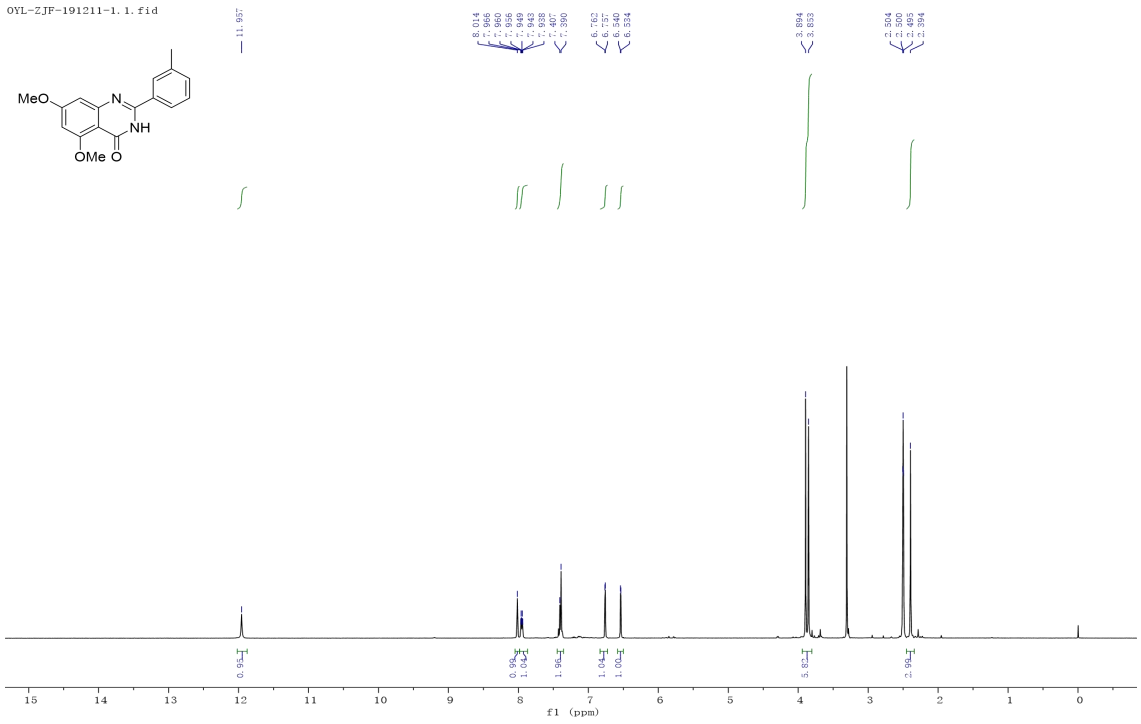


^{1}H NMR Spectrum of Compound **38f**

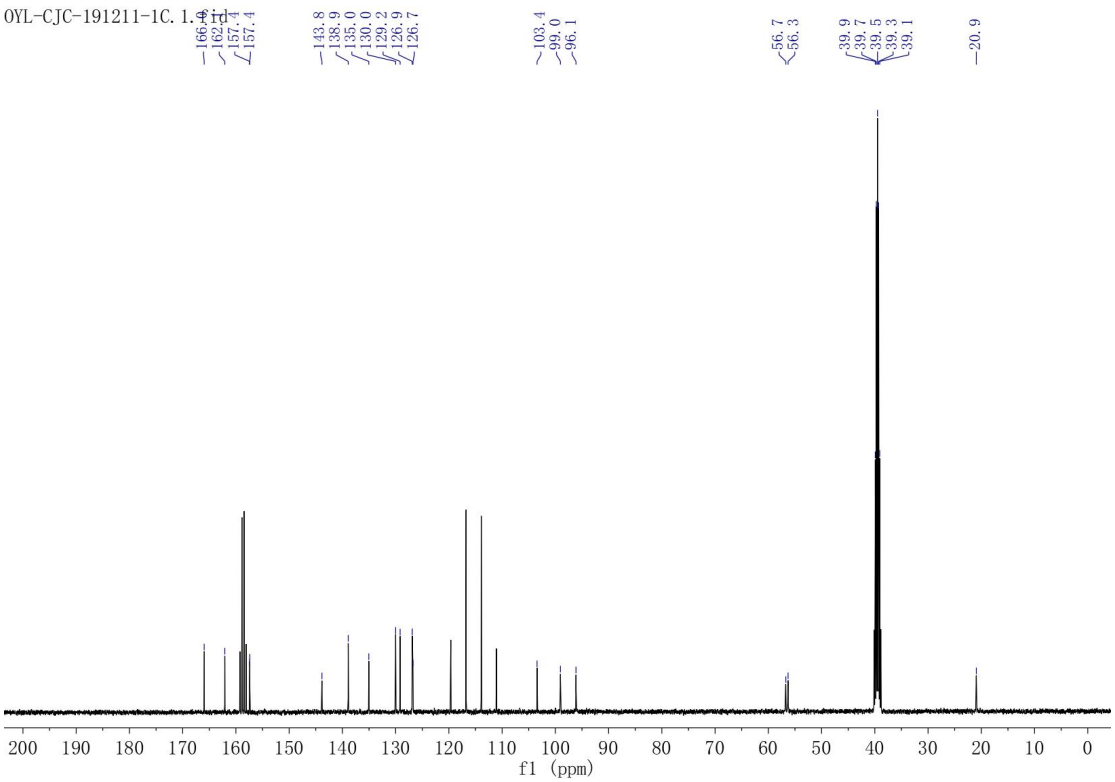


^{13}C NMR Spectrum of Compound **38f**

38g

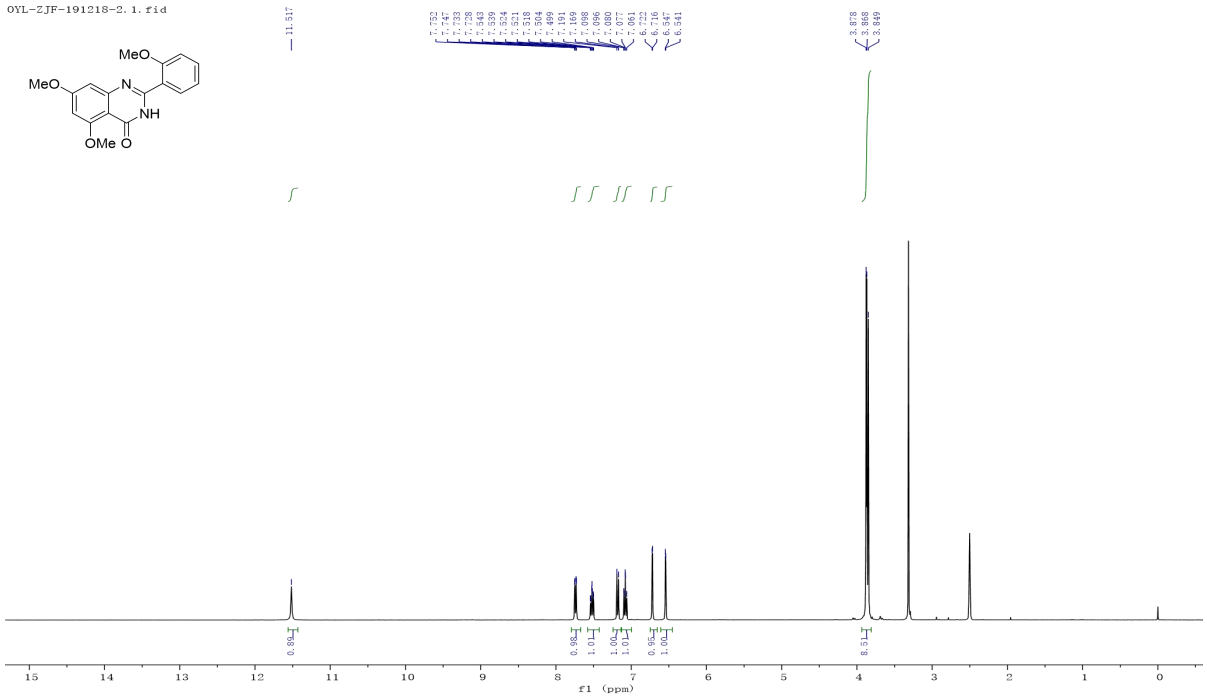


^{1}H NMR Spectrum of Compound **38g**

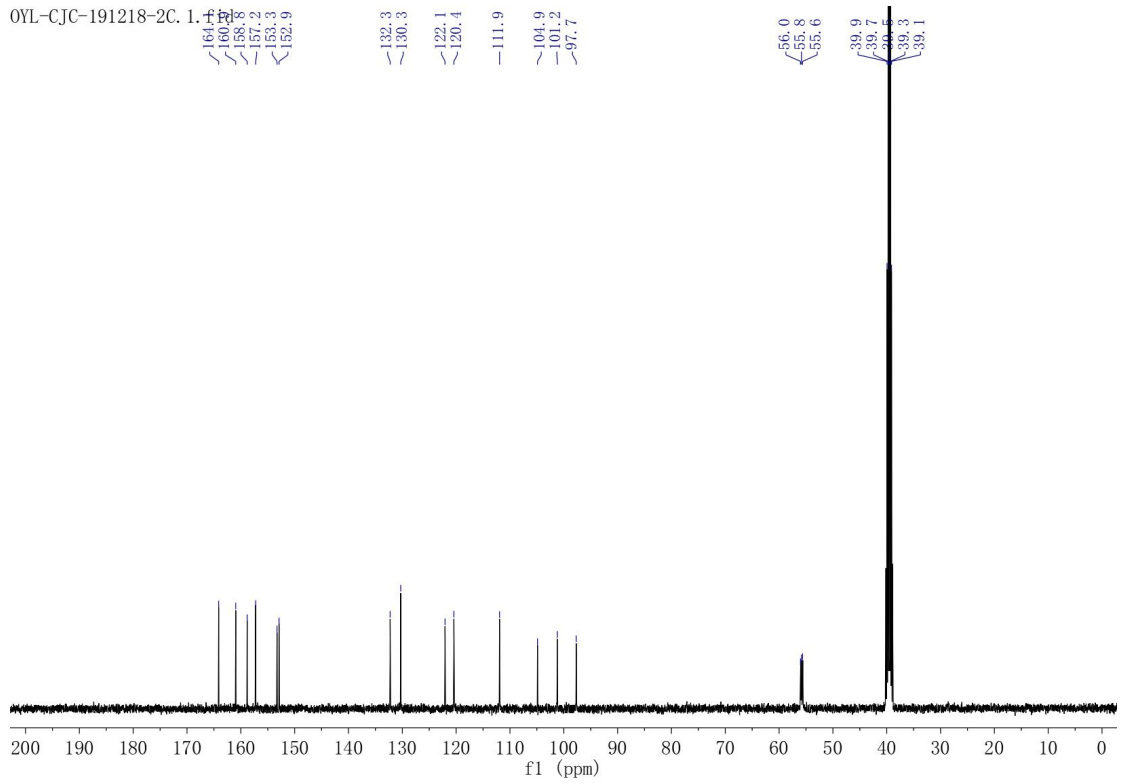


^{13}C NMR Spectrum of Compound **38g**

38h

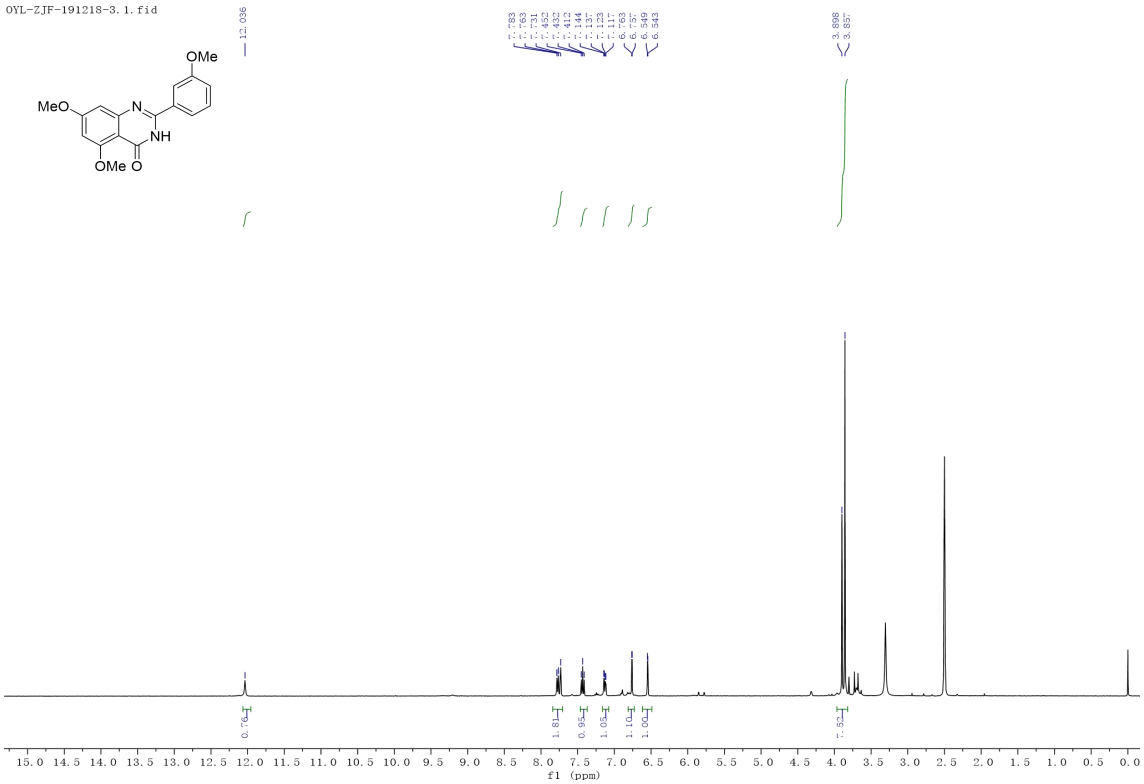


^{1}H NMR Spectrum of Compound **38h**

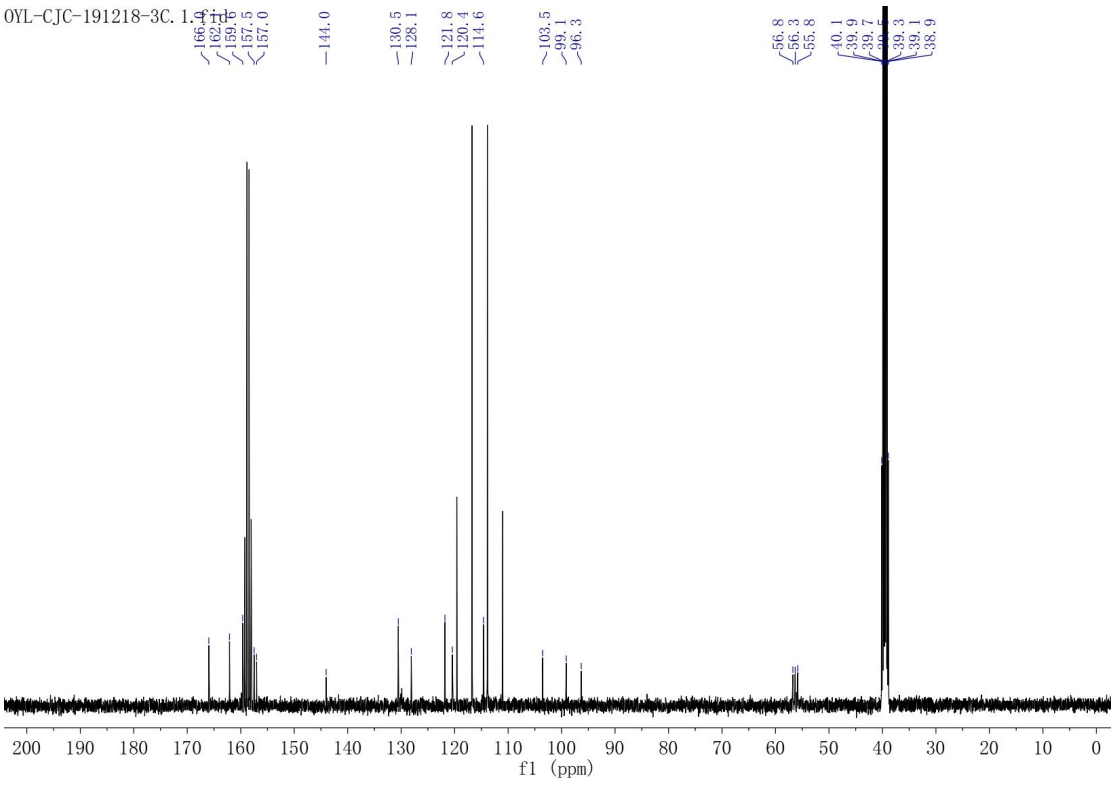


^{13}C NMR Spectrum of Compound **38h**

38i

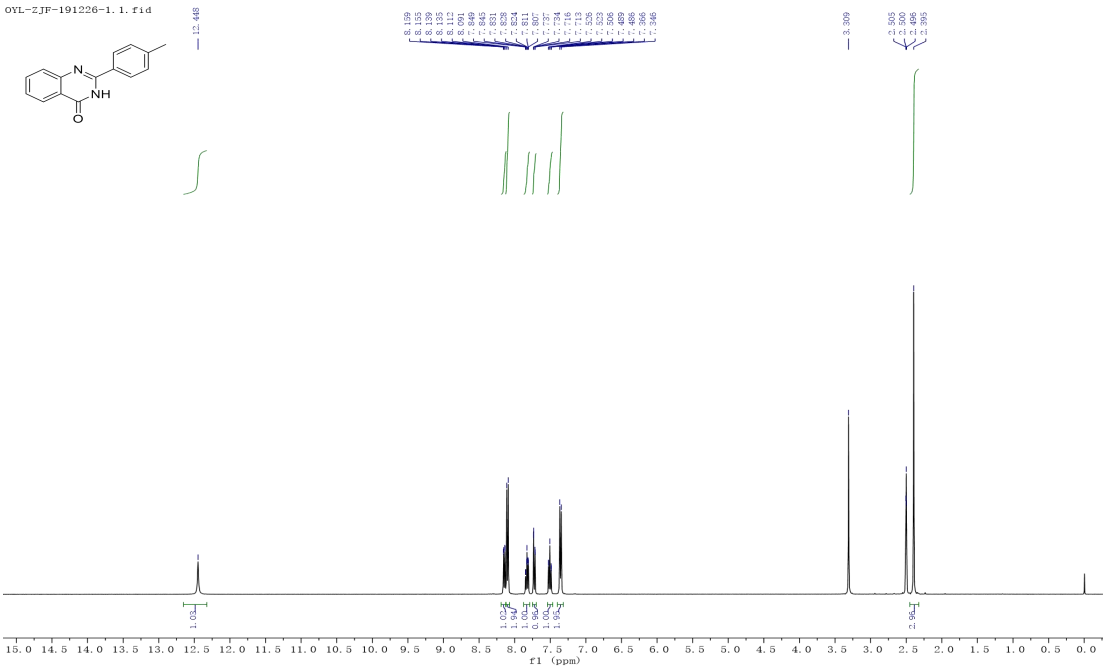


^{1}H NMR Spectrum of Compound **38i**

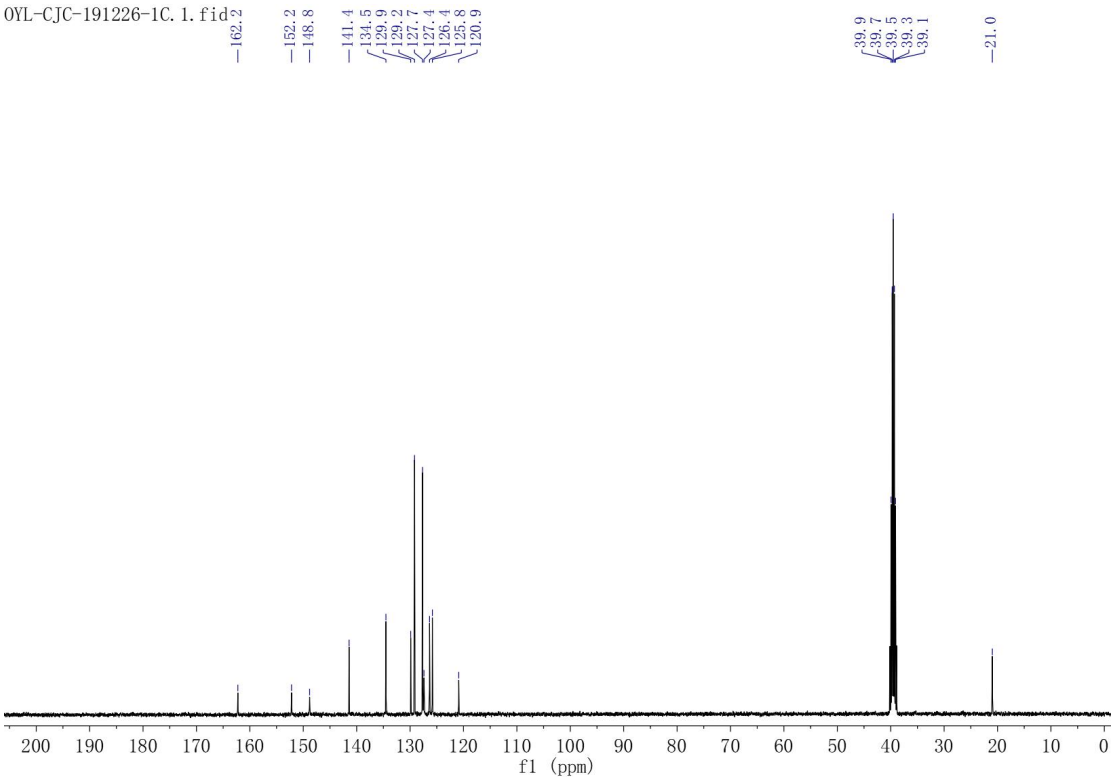


^{13}C NMR Spectrum of Compound **38i**

38j

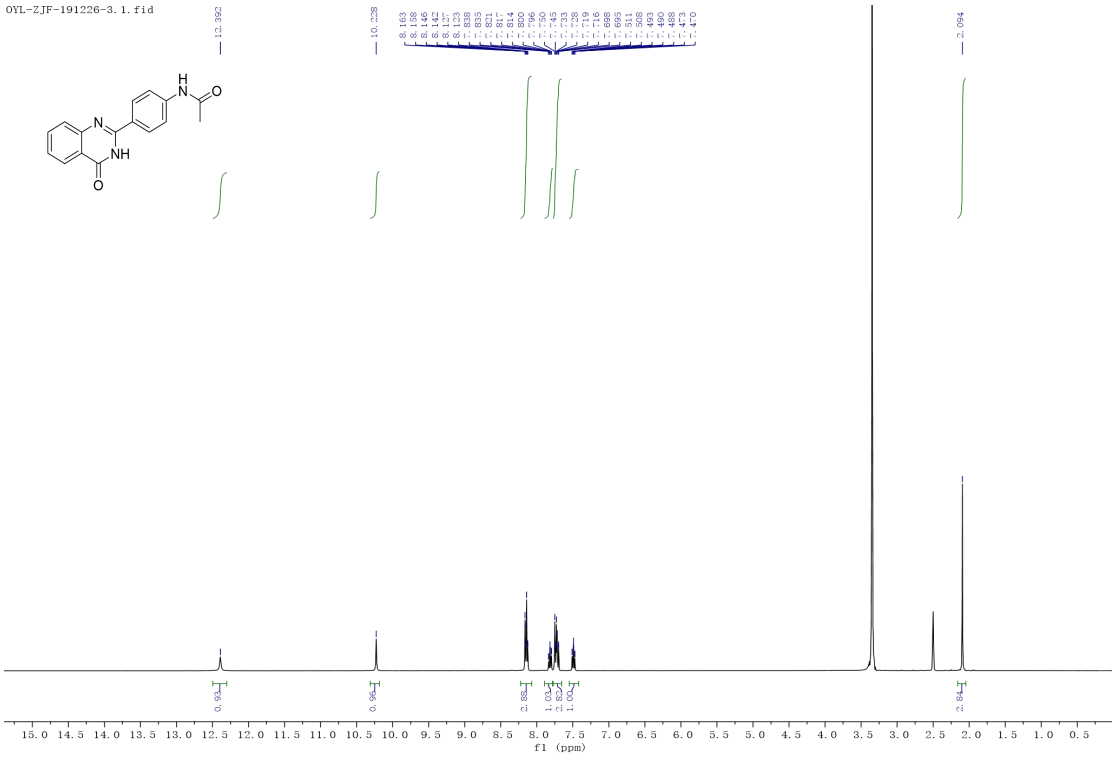


^{1}H NMR Spectrum of Compound **38j**

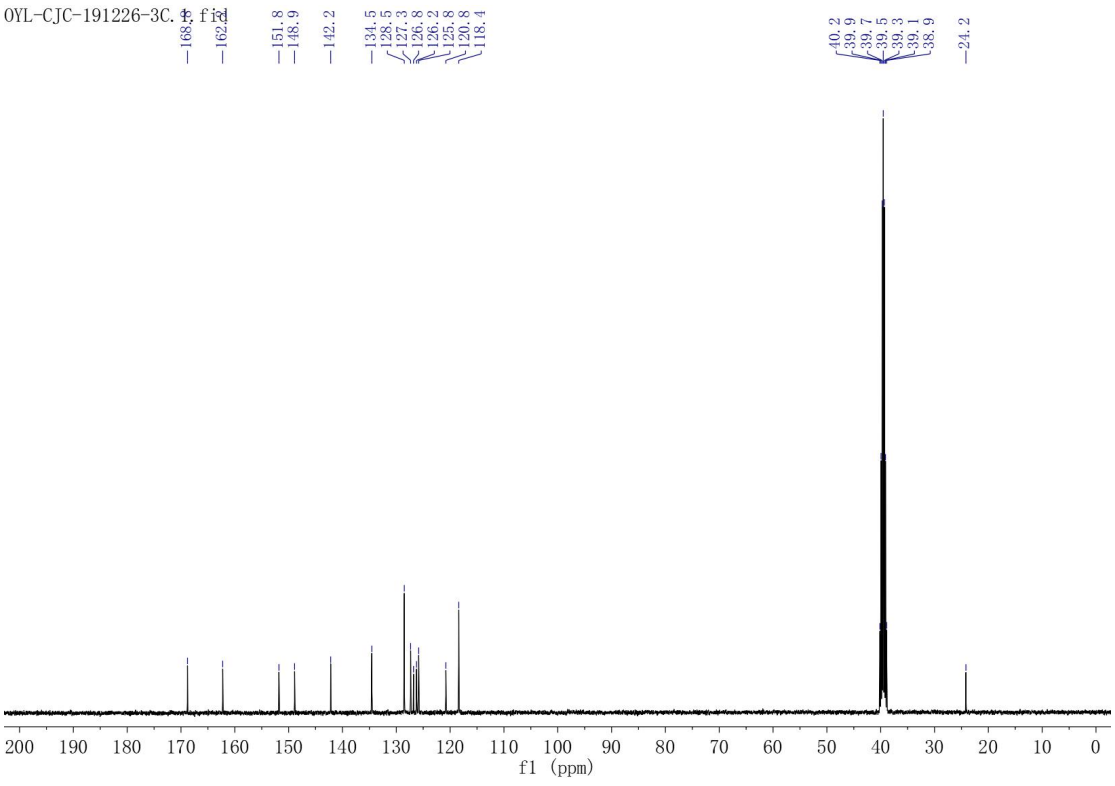


^{13}C NMR Spectrum of Compound **38j**

38k

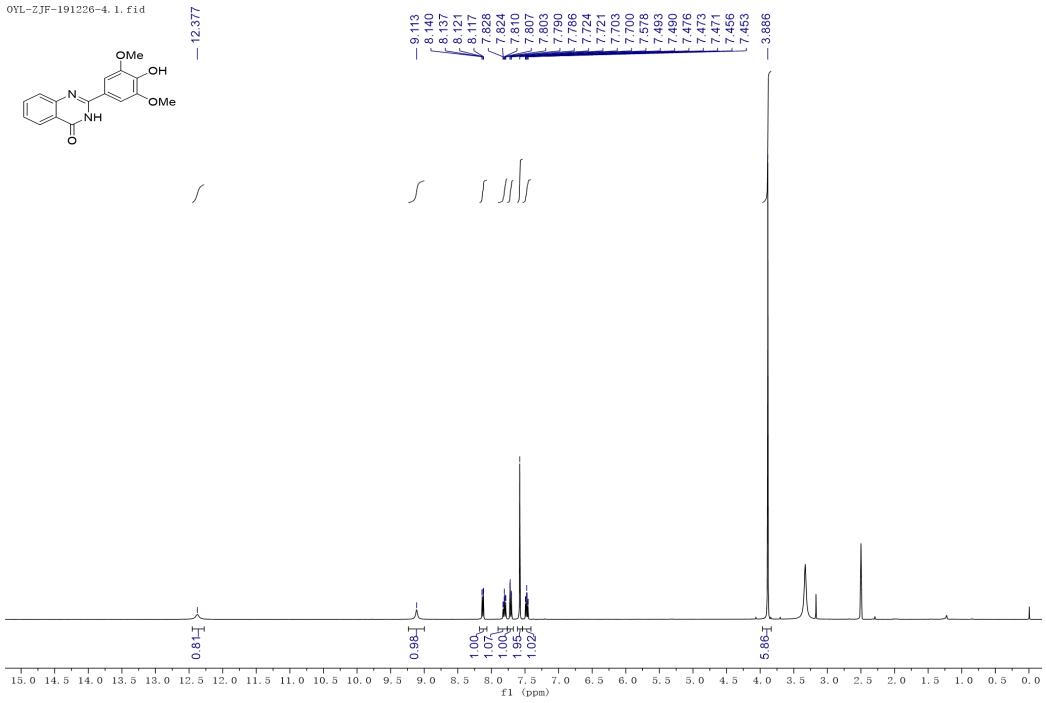


^{1}H NMR Spectrum of Compound **38k**

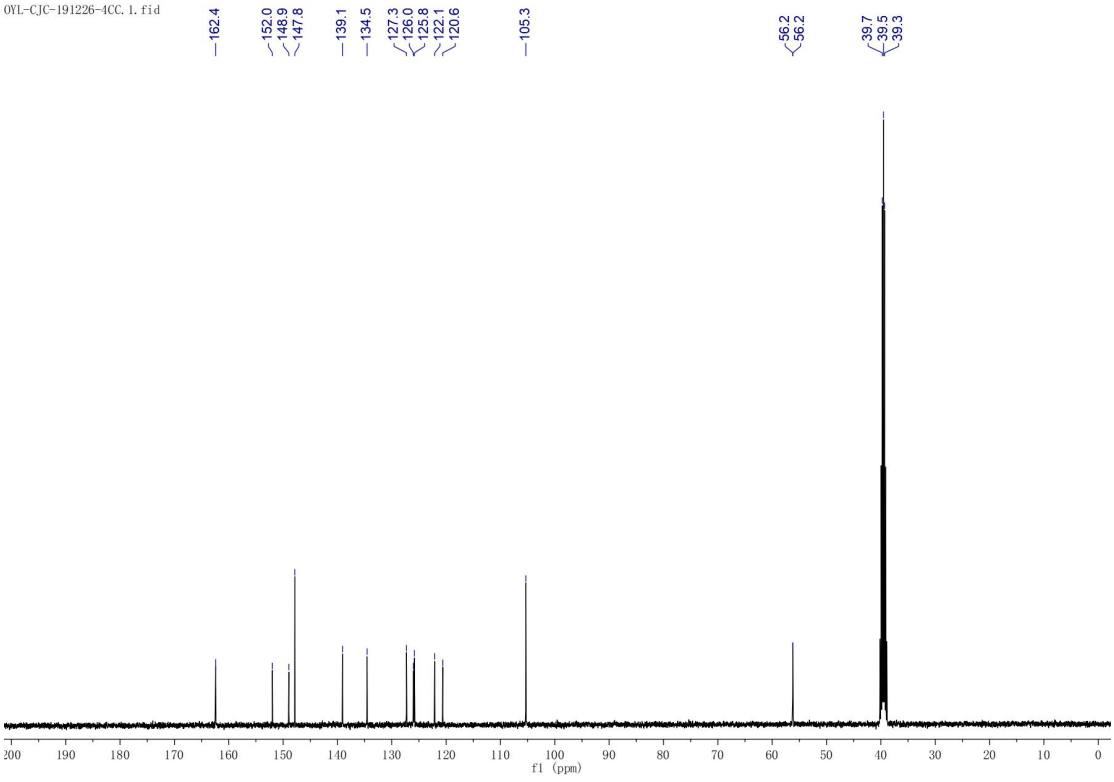


^{13}C NMR Spectrum of Compound **38k**

38l

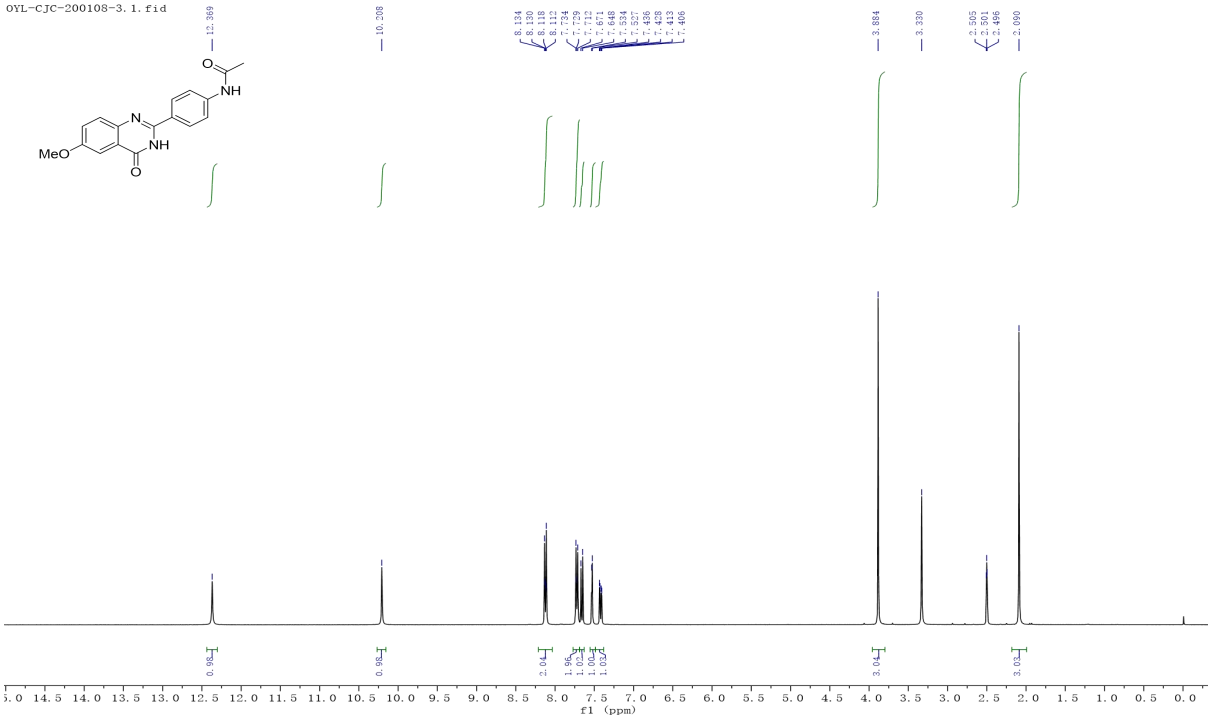


^{1}H NMR Spectrum of Compound **38l**

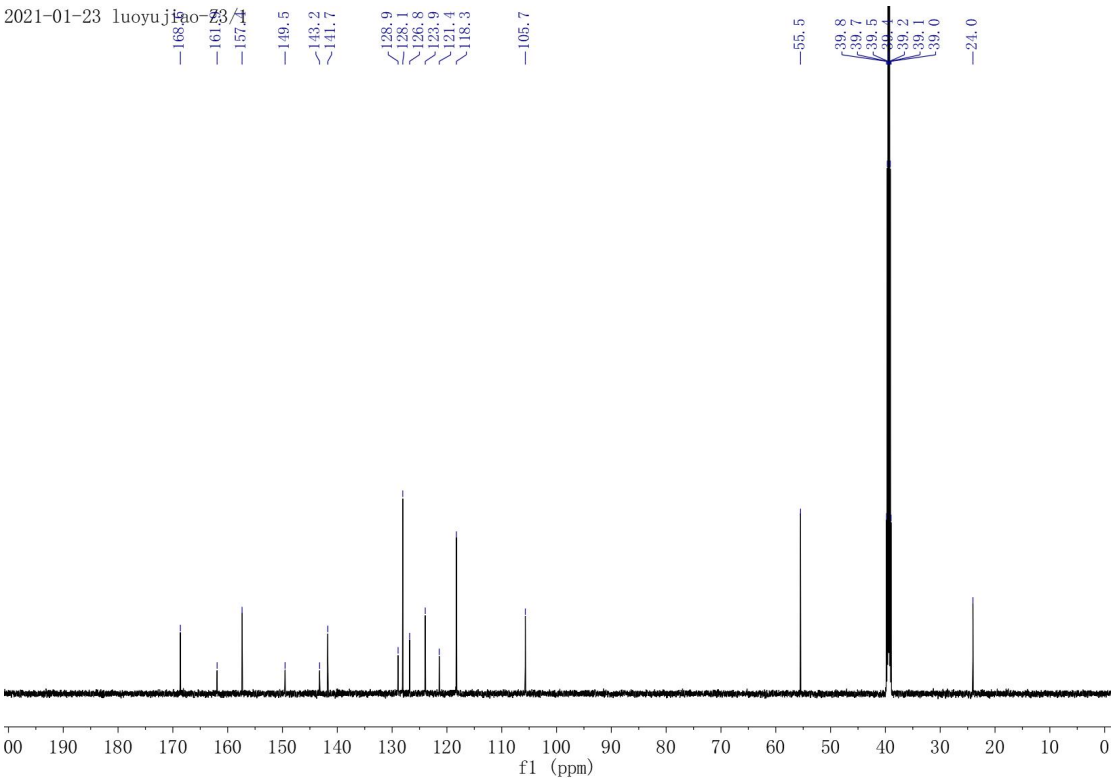


^{13}C NMR Spectrum of Compound **38l**

38m

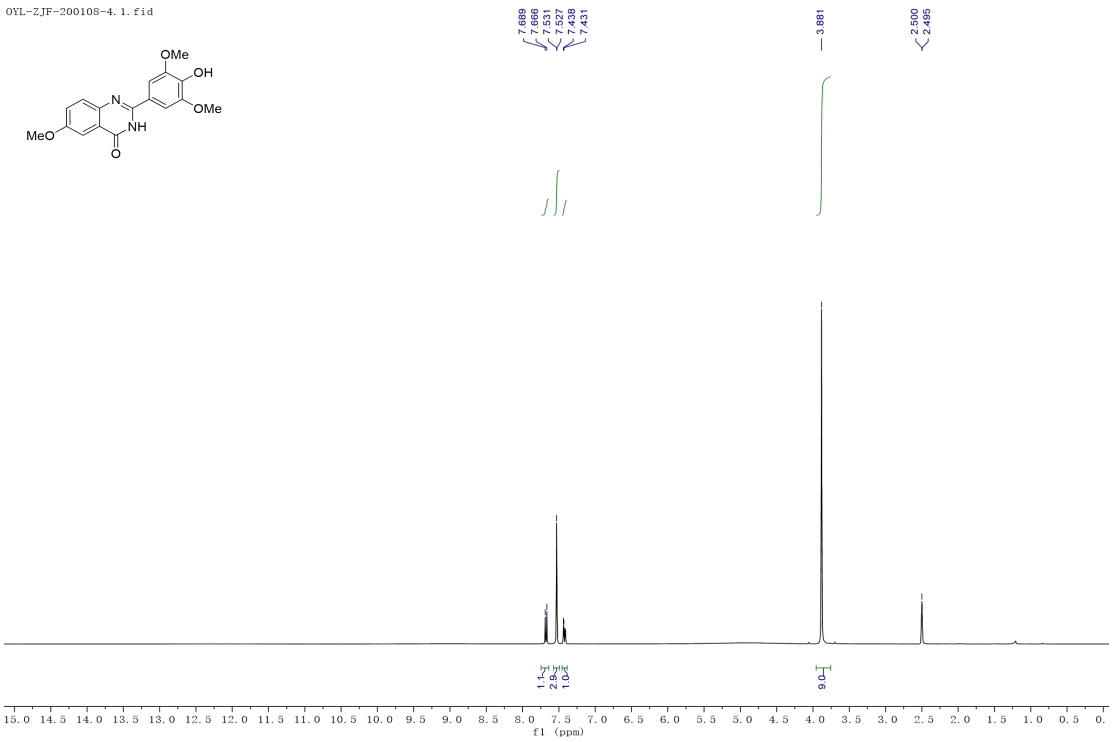


^{1}H NMR Spectrum of Compound **38m**

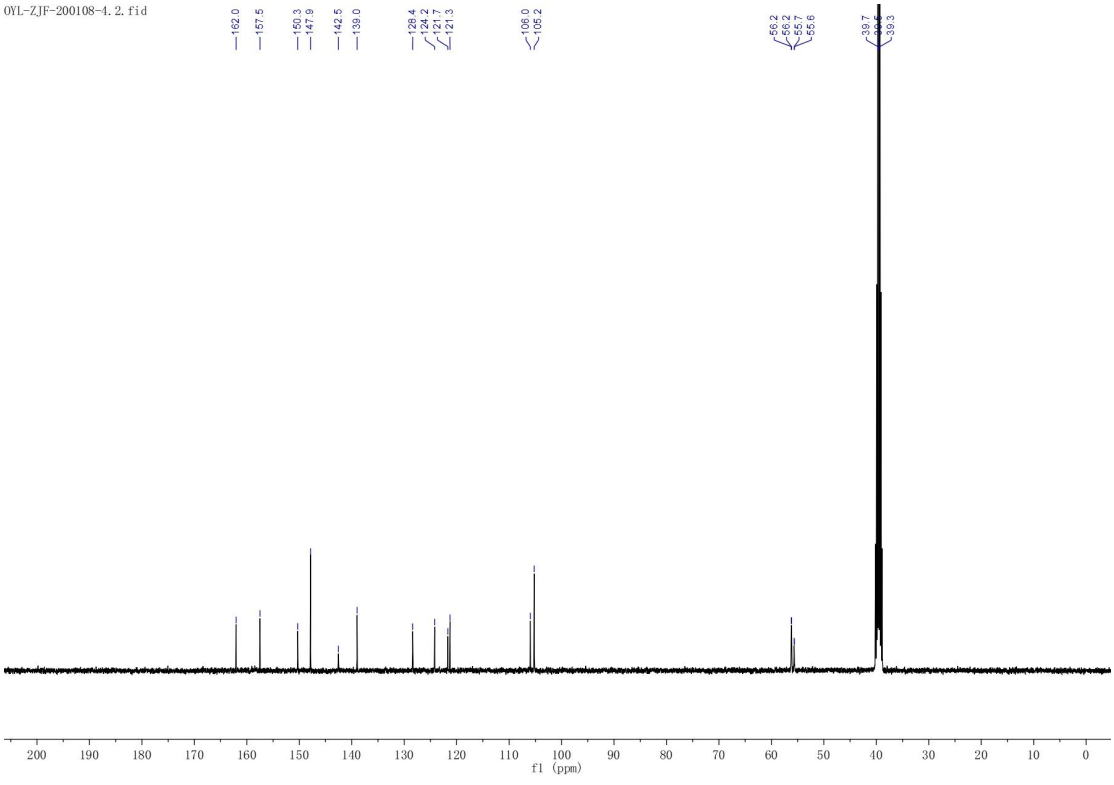


^{13}C NMR Spectrum of Compound **38m**

38n

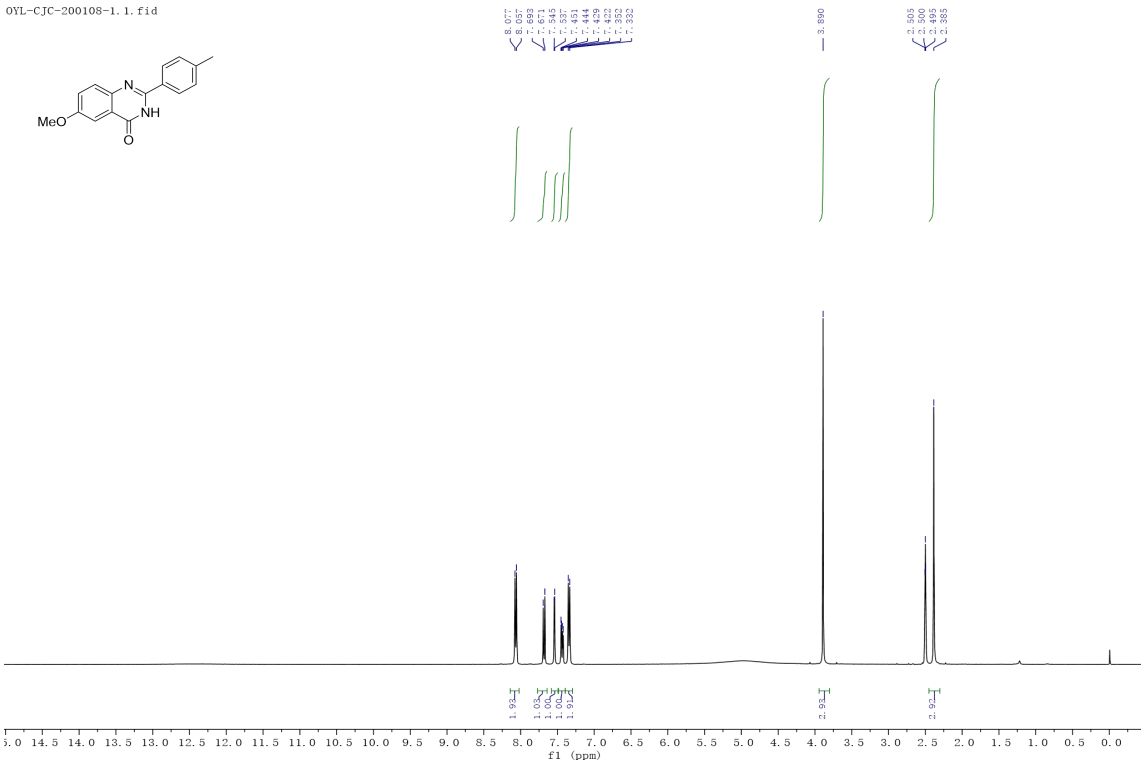


^{1}H NMR Spectrum of Compound **38n**

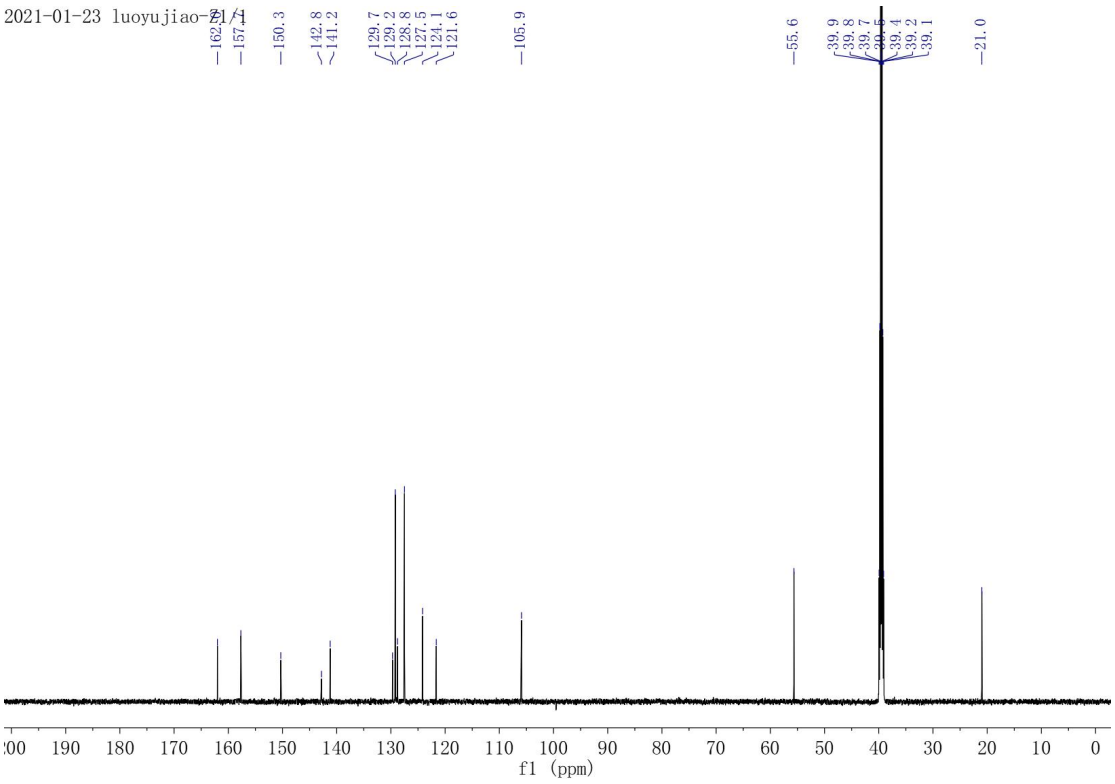


^{13}C NMR Spectrum of Compound **38n**

38o

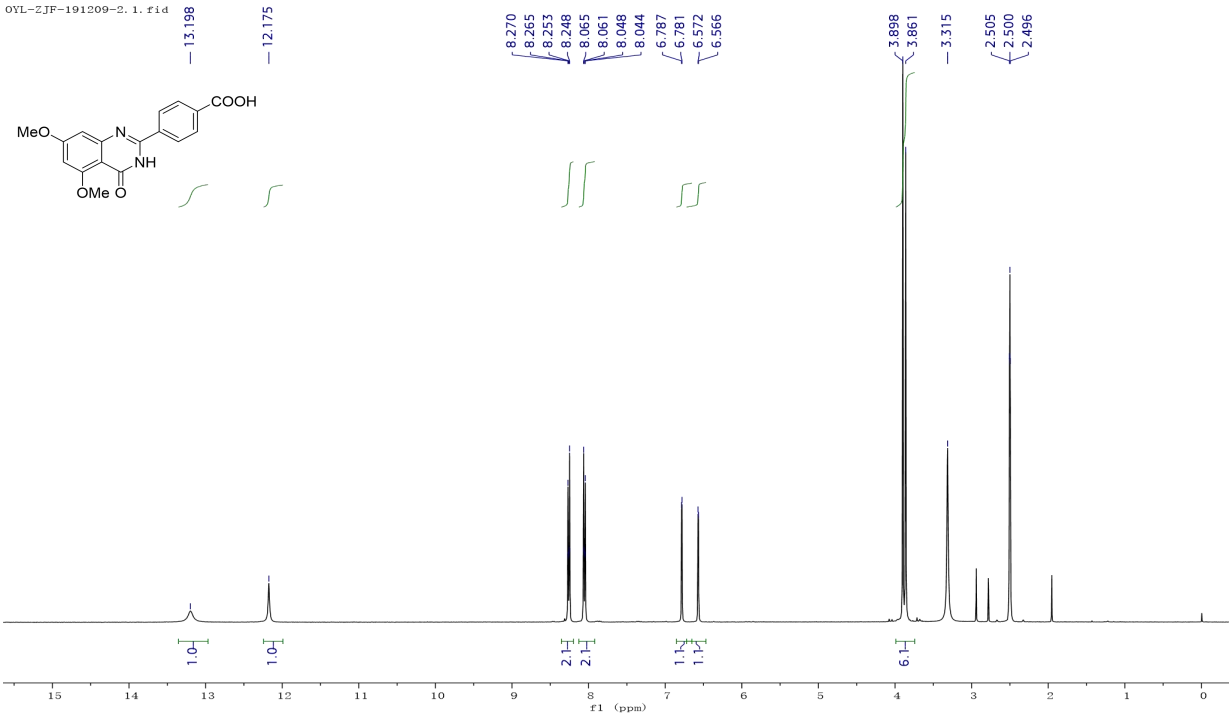


^{1}H NMR Spectrum of Compound **38o**

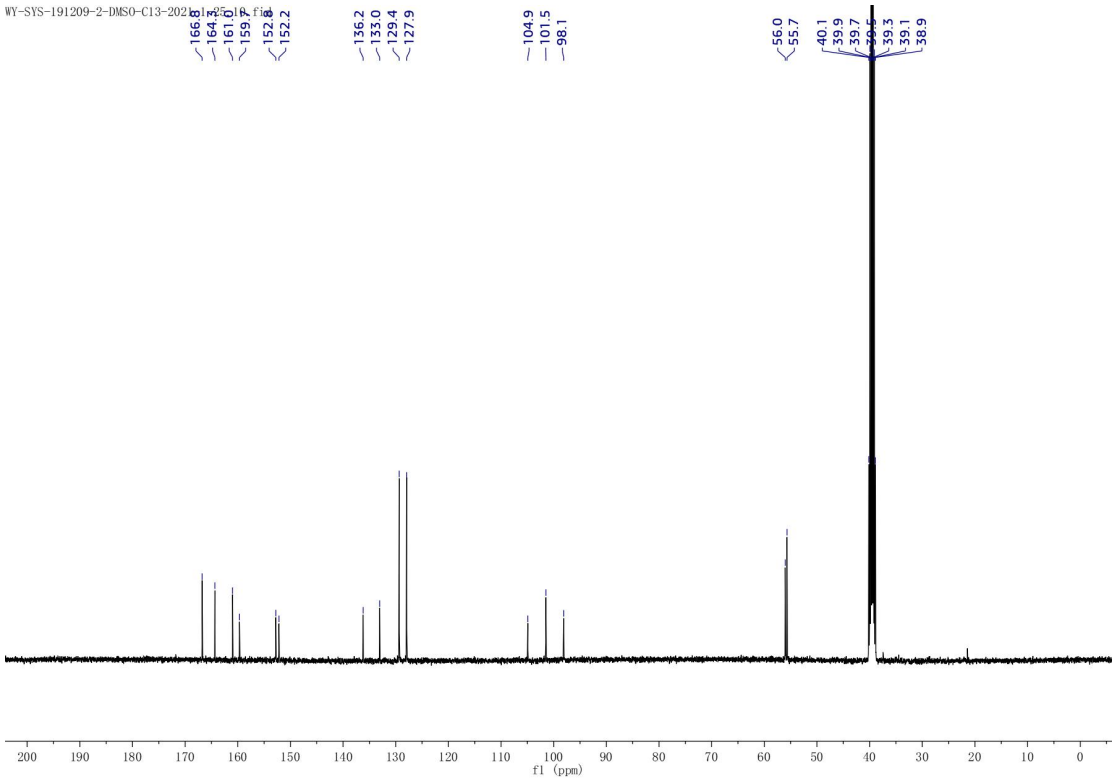


^{13}C NMR Spectrum of Compound **38o**

38p

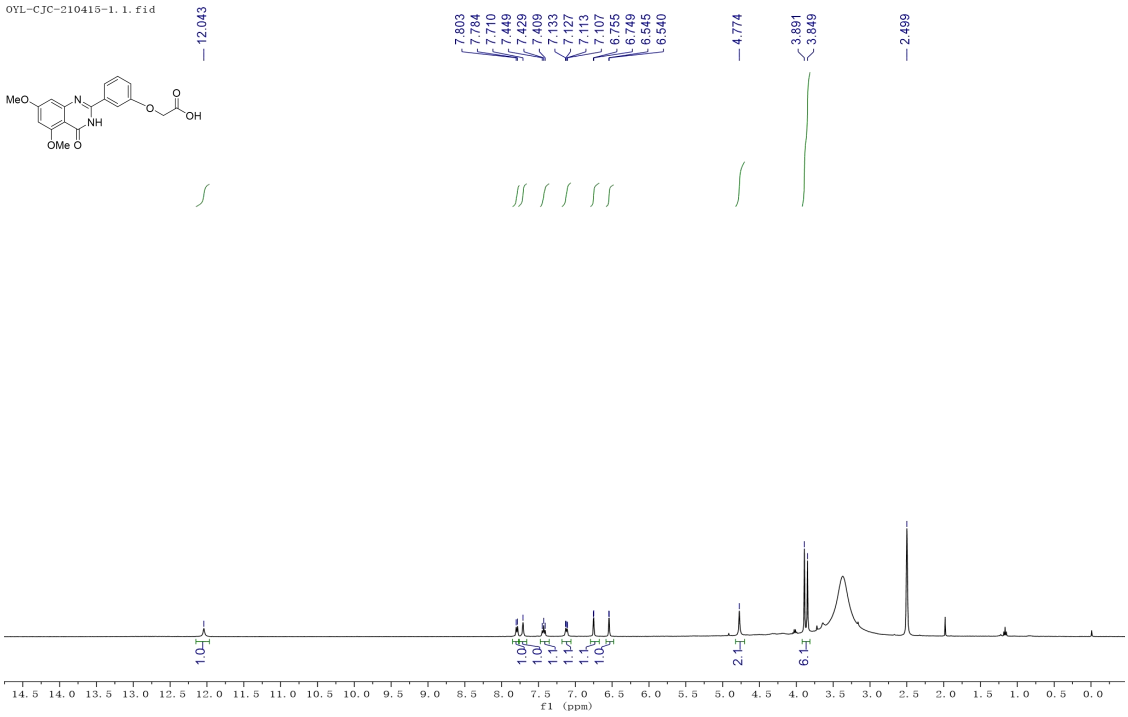


^{1}H NMR Spectrum of Compound **38p**

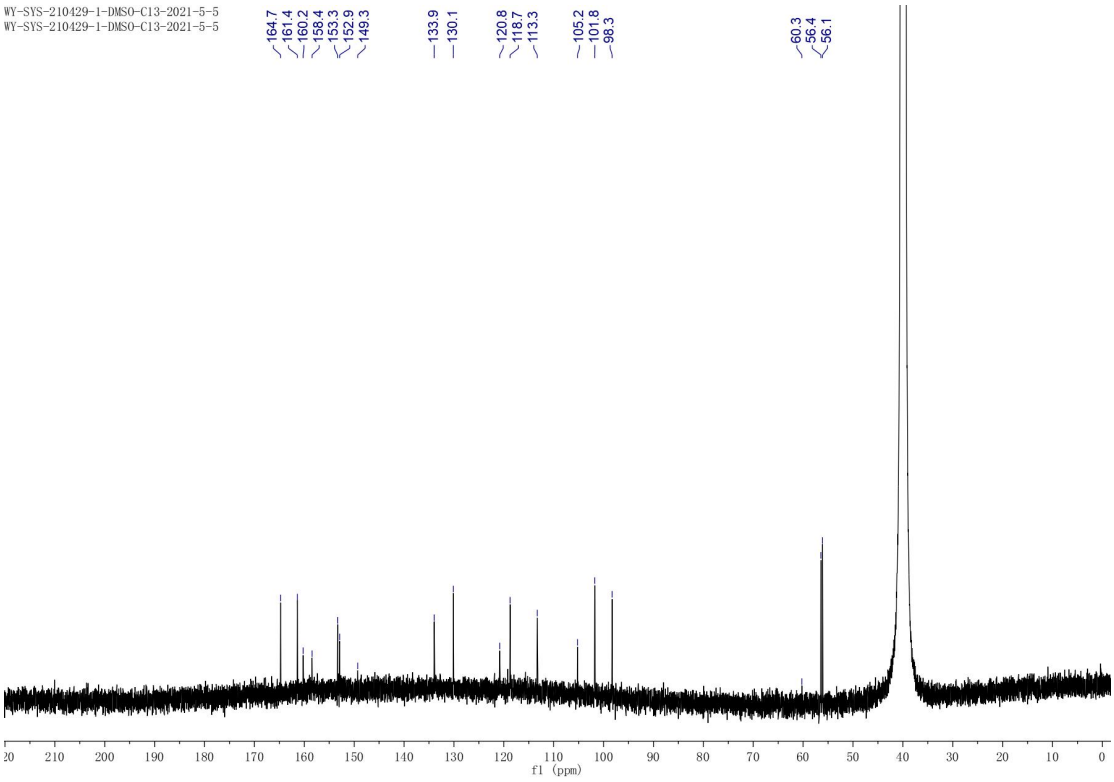


^{13}C NMR Spectrum of Compound **38p**

38q

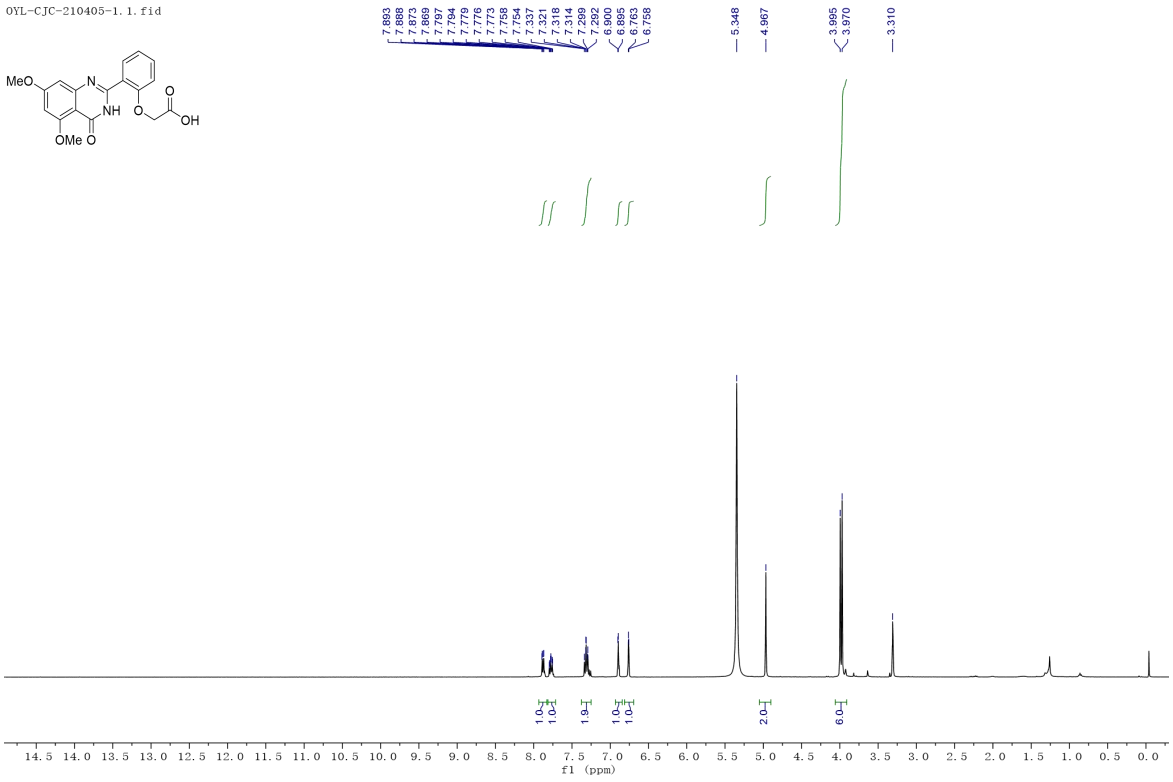


^{1}H NMR Spectrum of Compound **38q**

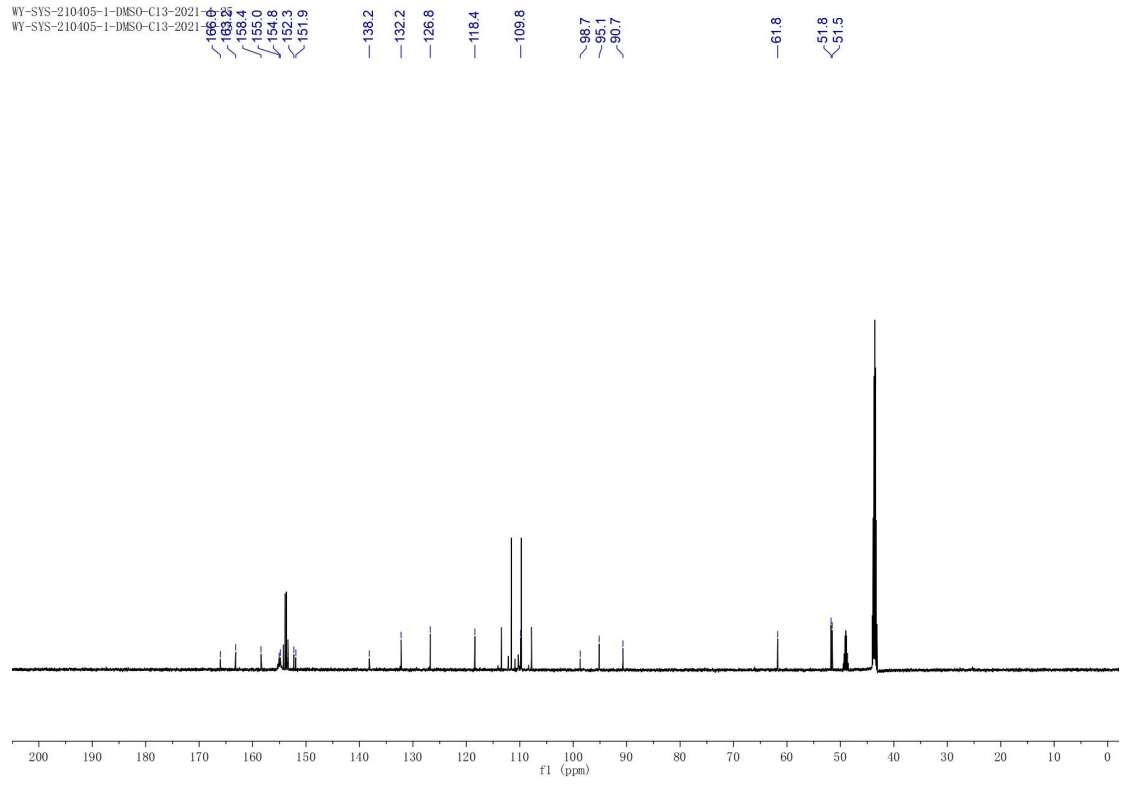


^{13}C NMR Spectrum of Compound **38q**

38r

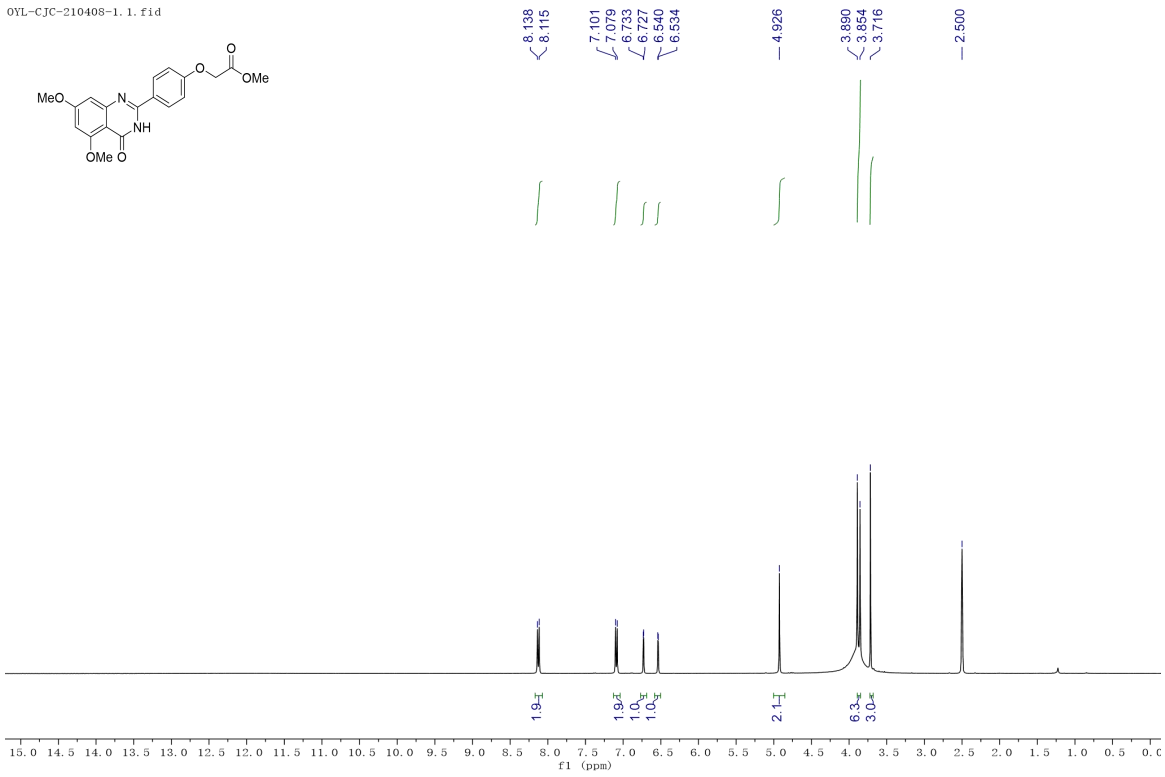


^{1}H NMR Spectrum of Compound **38r**

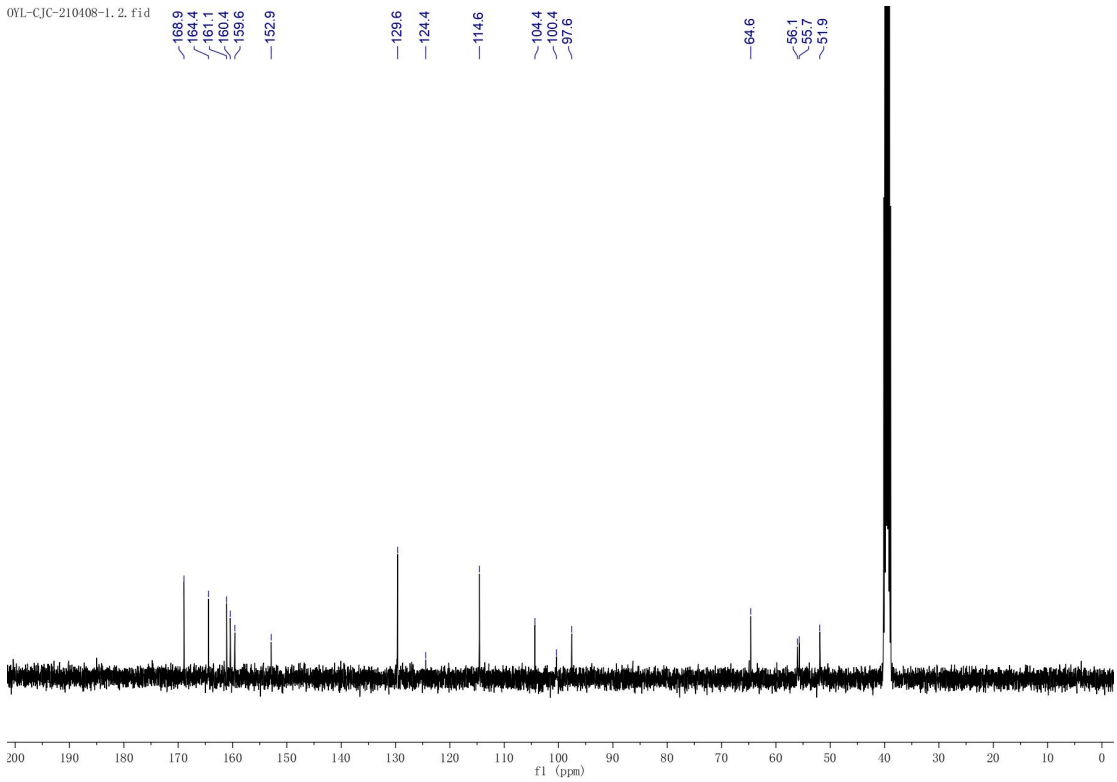


^{13}C NMR Spectrum of Compound **38r**

38s

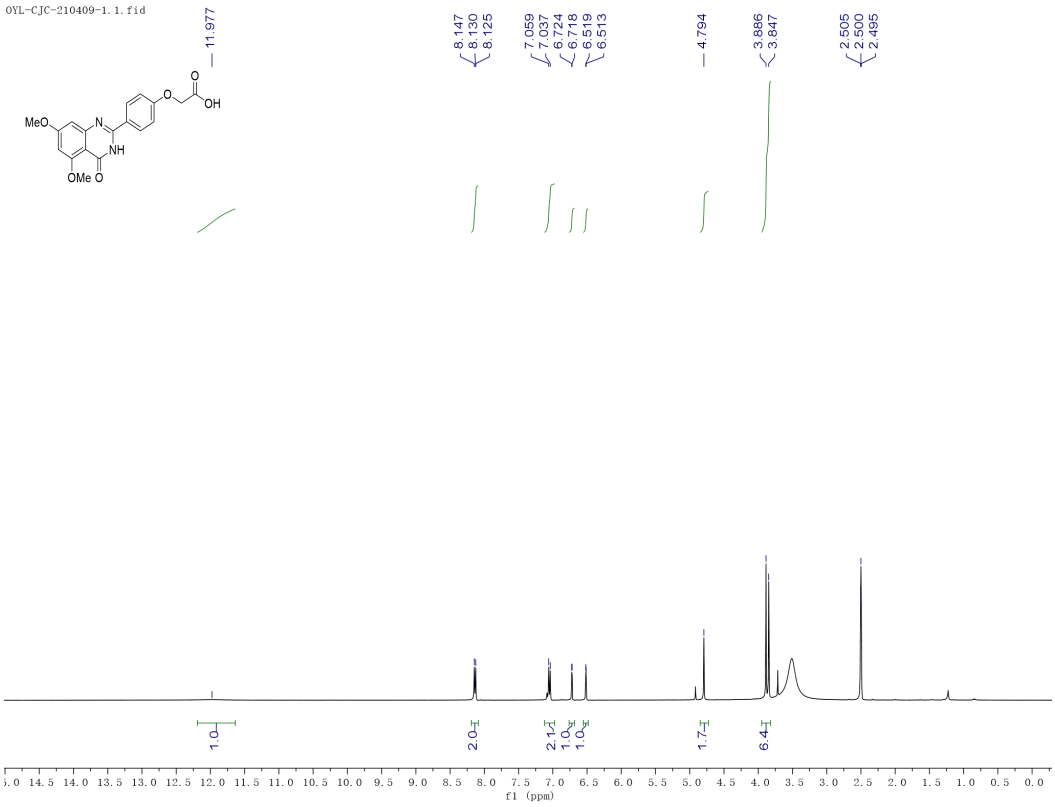


^{1}H NMR Spectrum of Compound **38s**

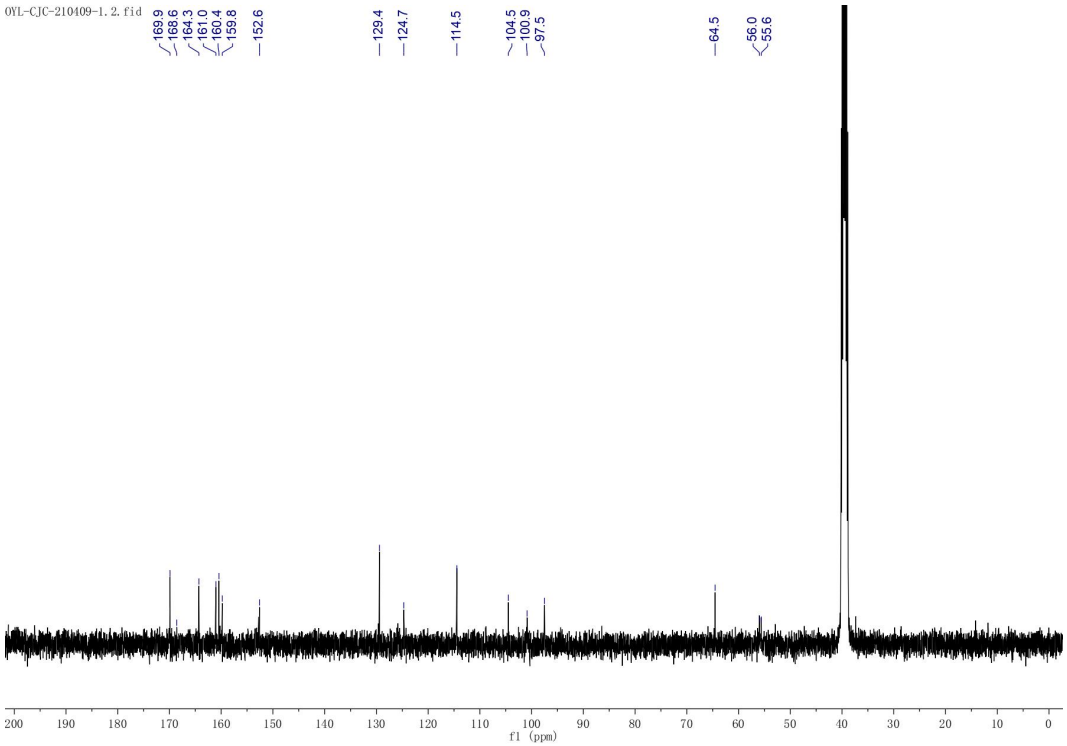


^{13}C NMR Spectrum of Compound **38s**

26

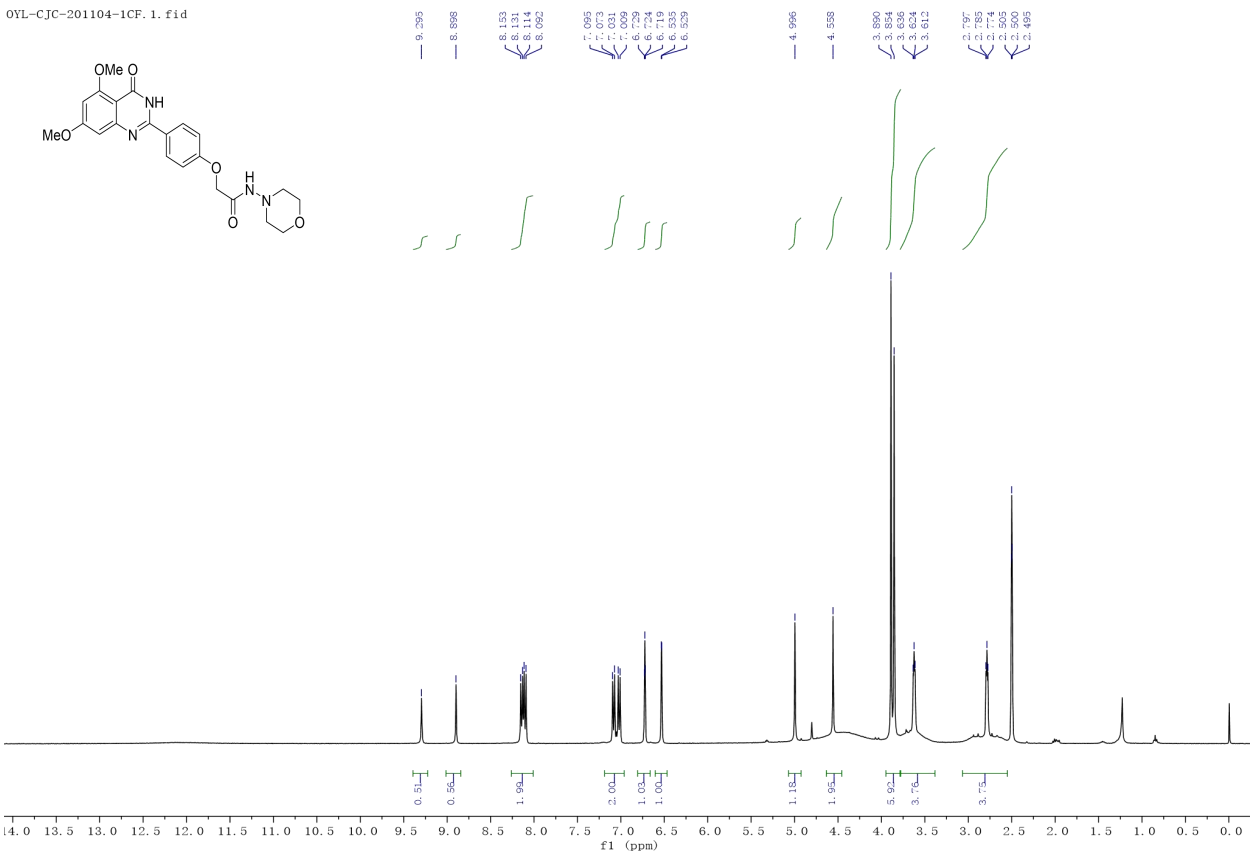


^{1}H NMR Spectrum of Compound **26**

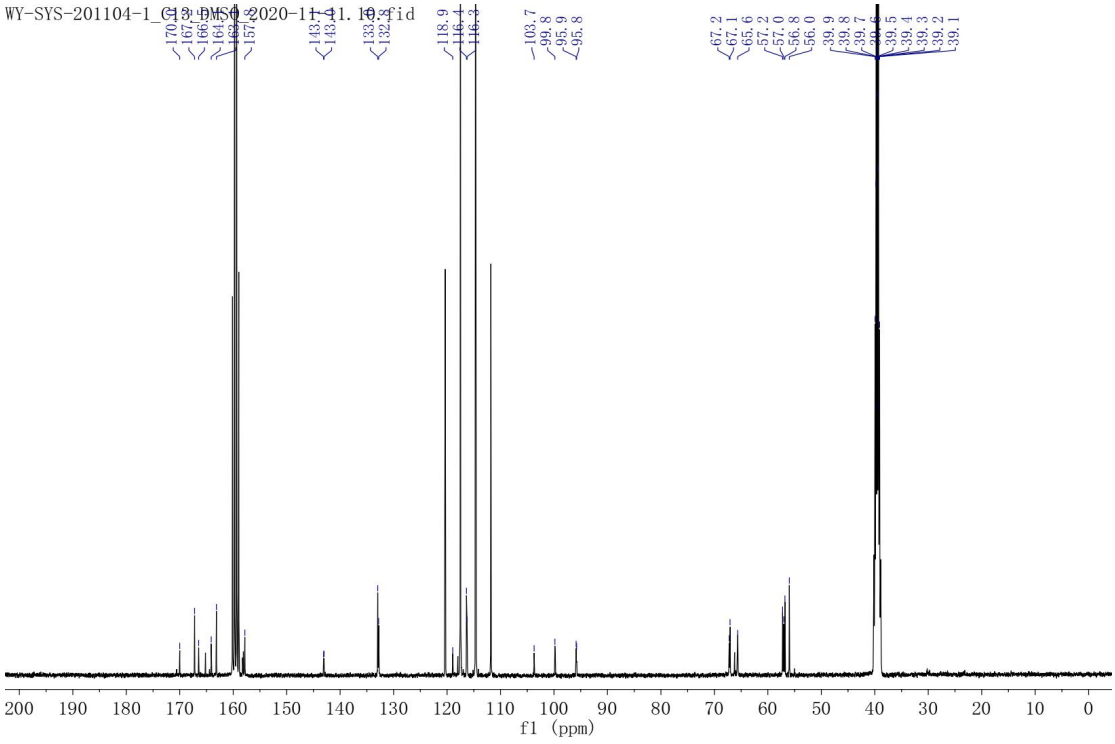


^{13}C NMR Spectrum of Compound 2**6**

42a

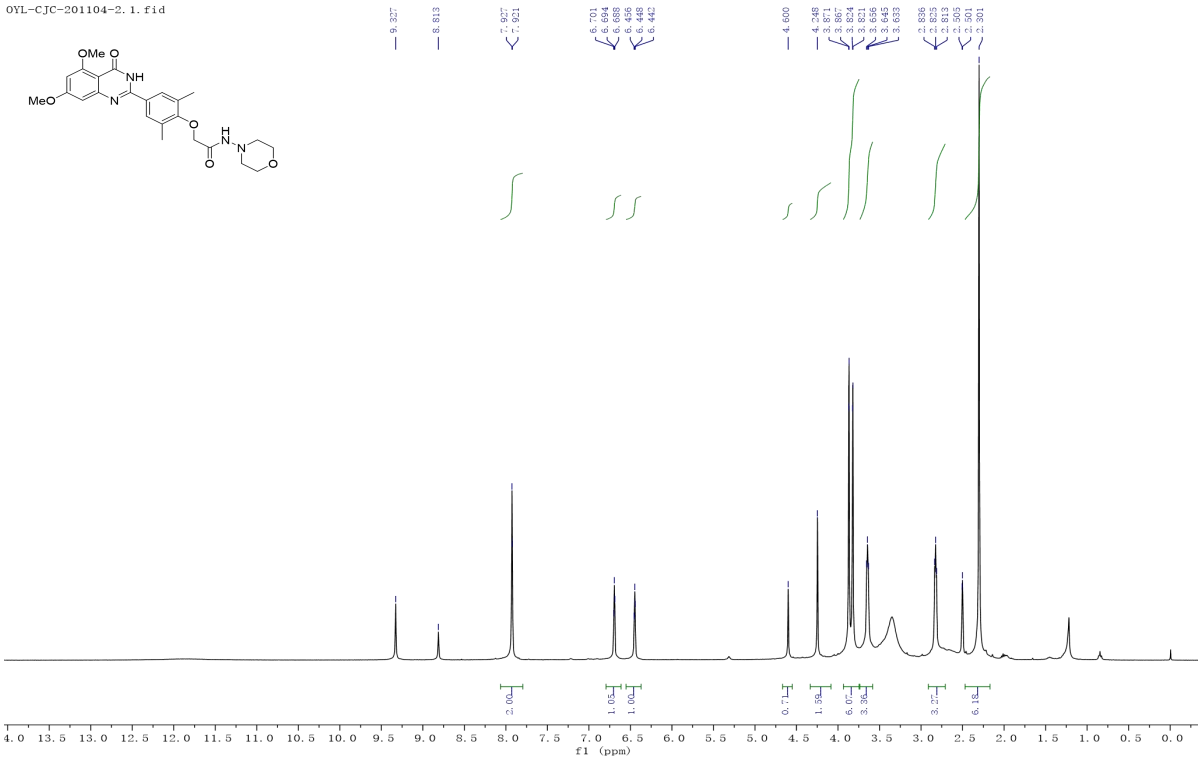


^{1}H NMR Spectrum of Compound **42a**

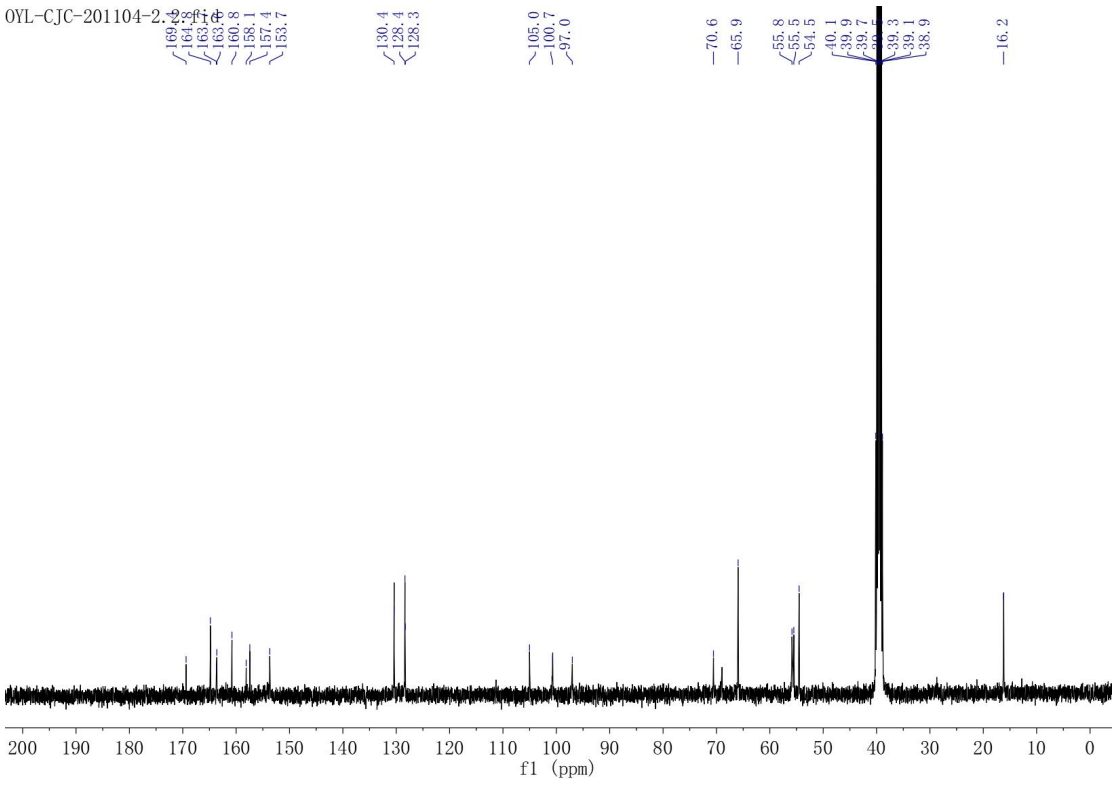


^{13}C NMR Spectrum of Compound **42a**

42b

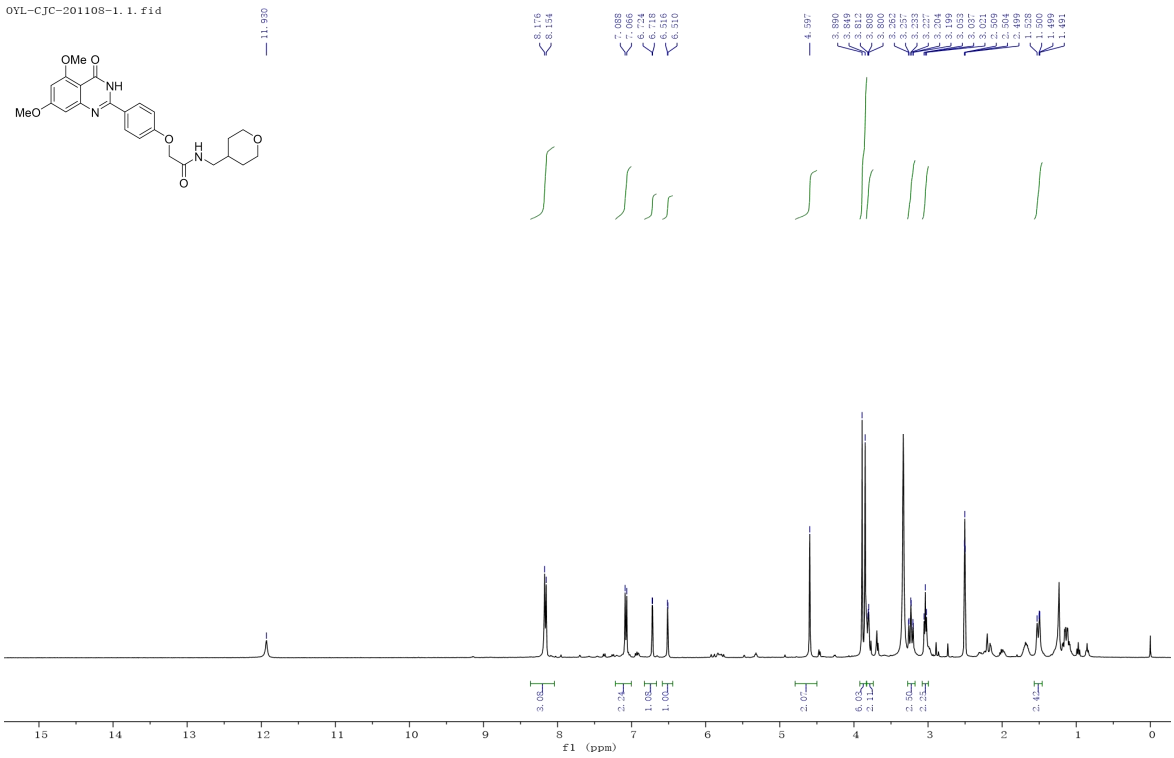


^{1}H NMR Spectrum of Compound **42b**

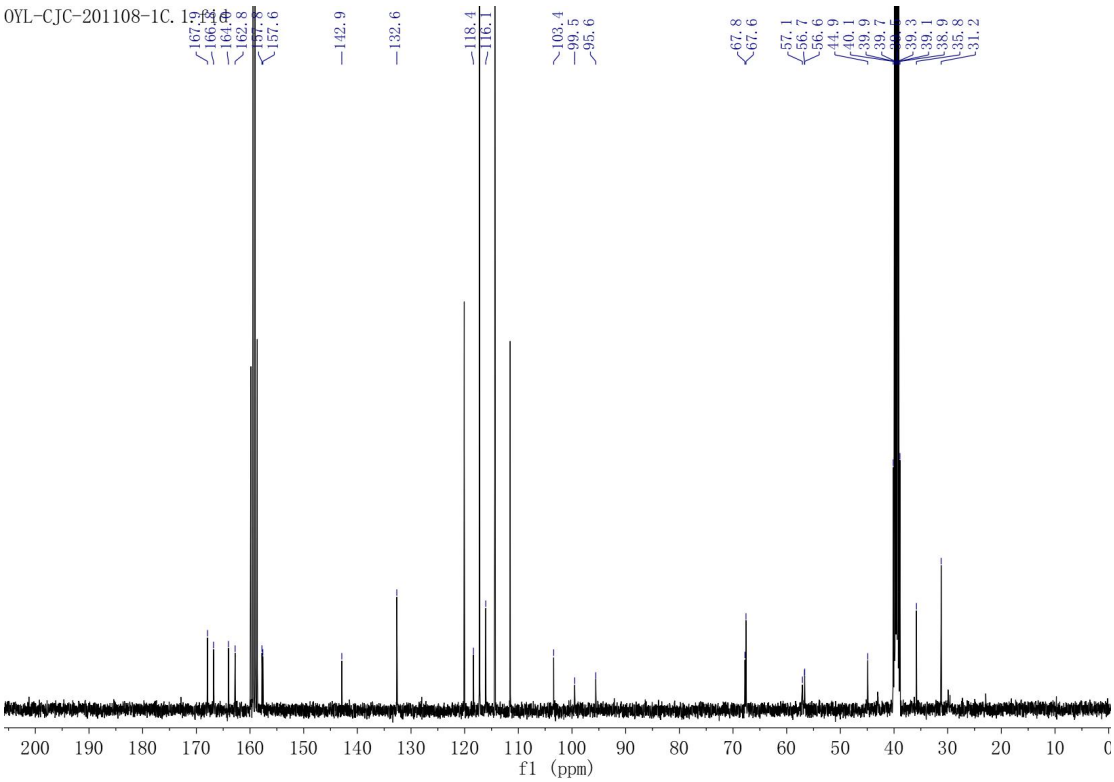


^{13}C NMR Spectrum of Compound **42b**

42c

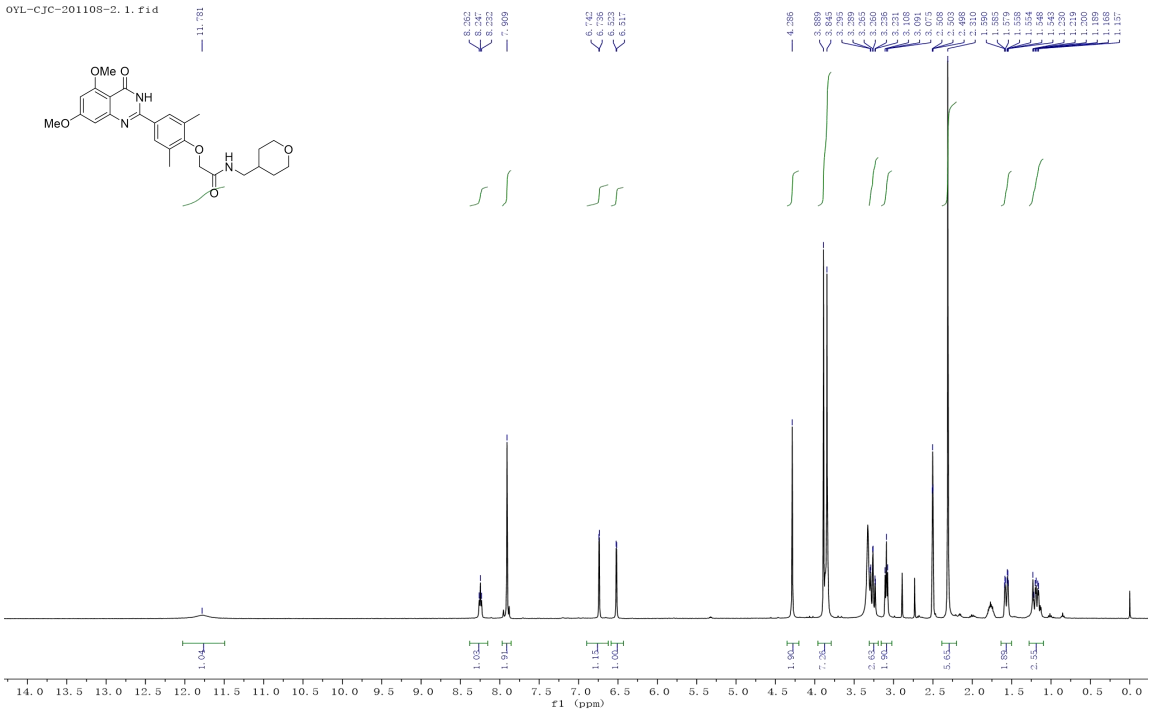


^{1}H NMR Spectrum of Compound **42c**

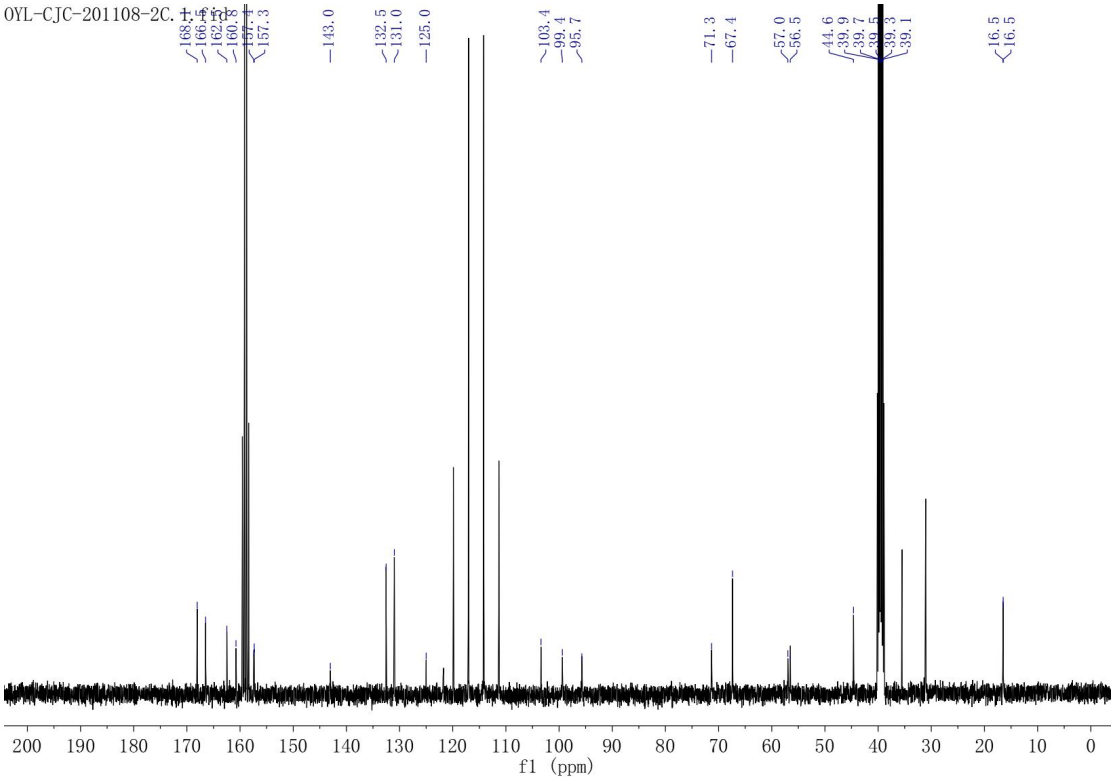


^{13}C NMR Spectrum of Compound **42c**

42d

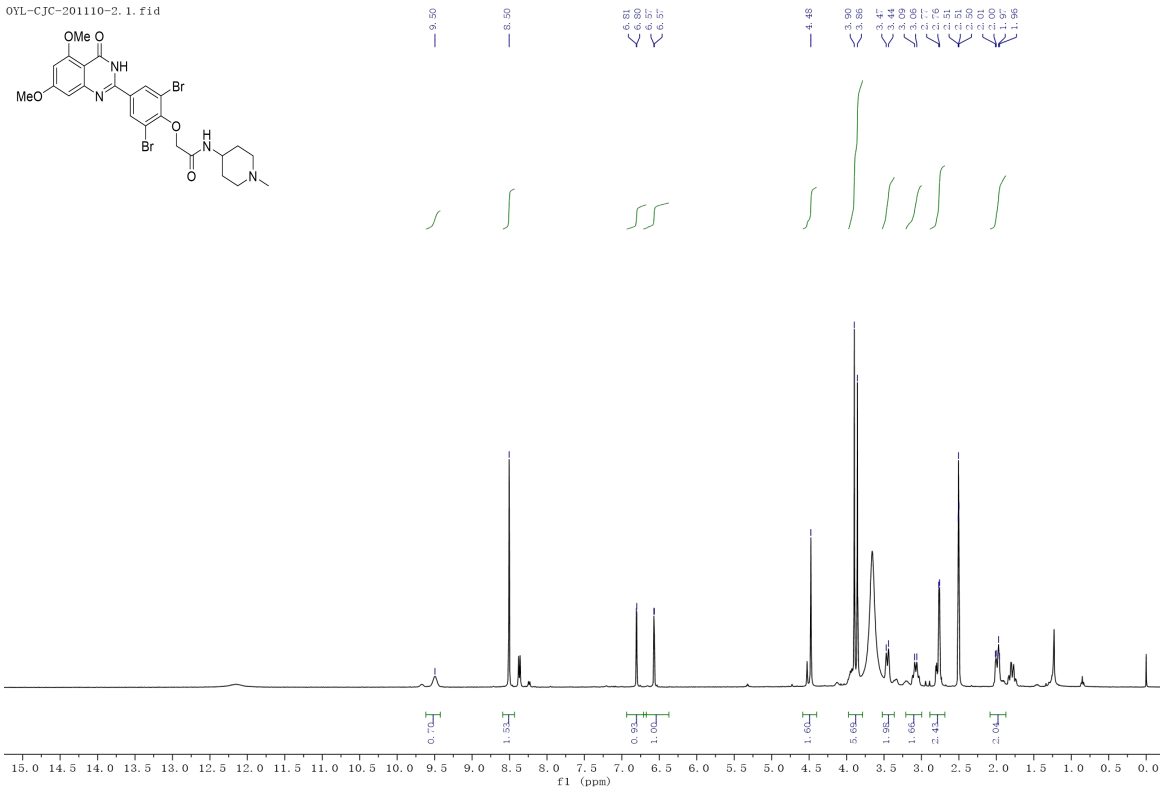


^{1}H NMR Spectrum of Compound **42d**

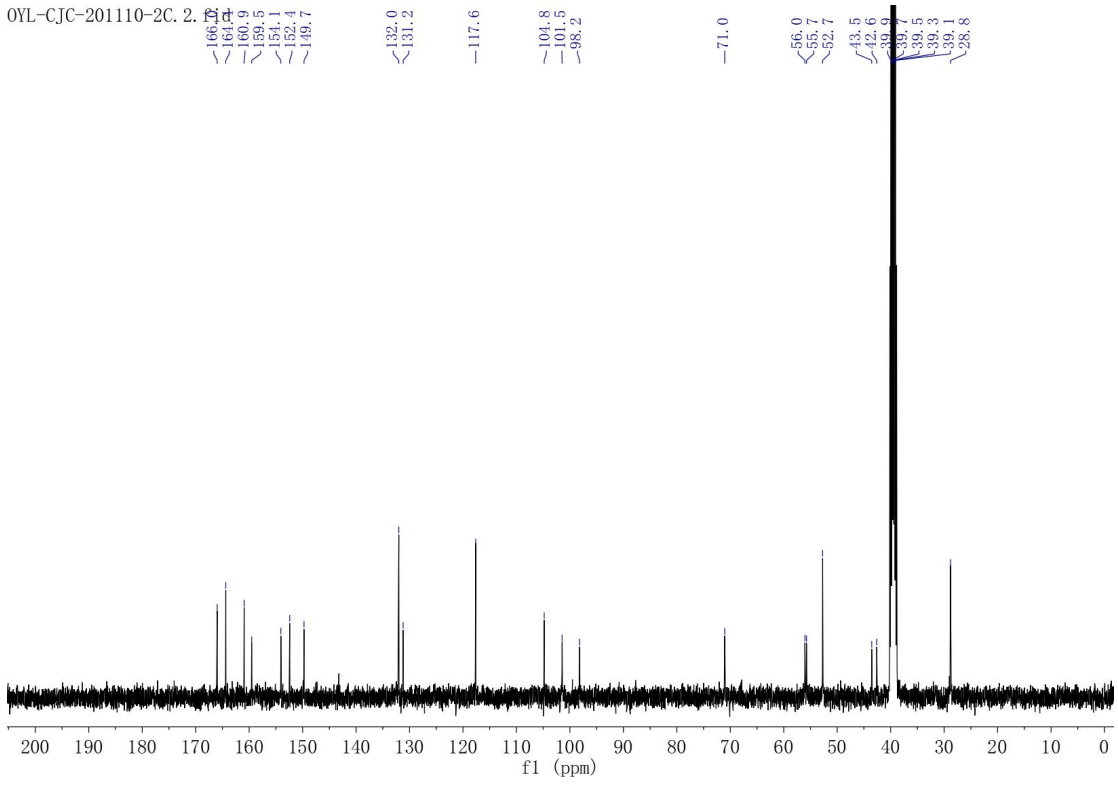


^{13}C NMR Spectrum of Compound **42d**

42e

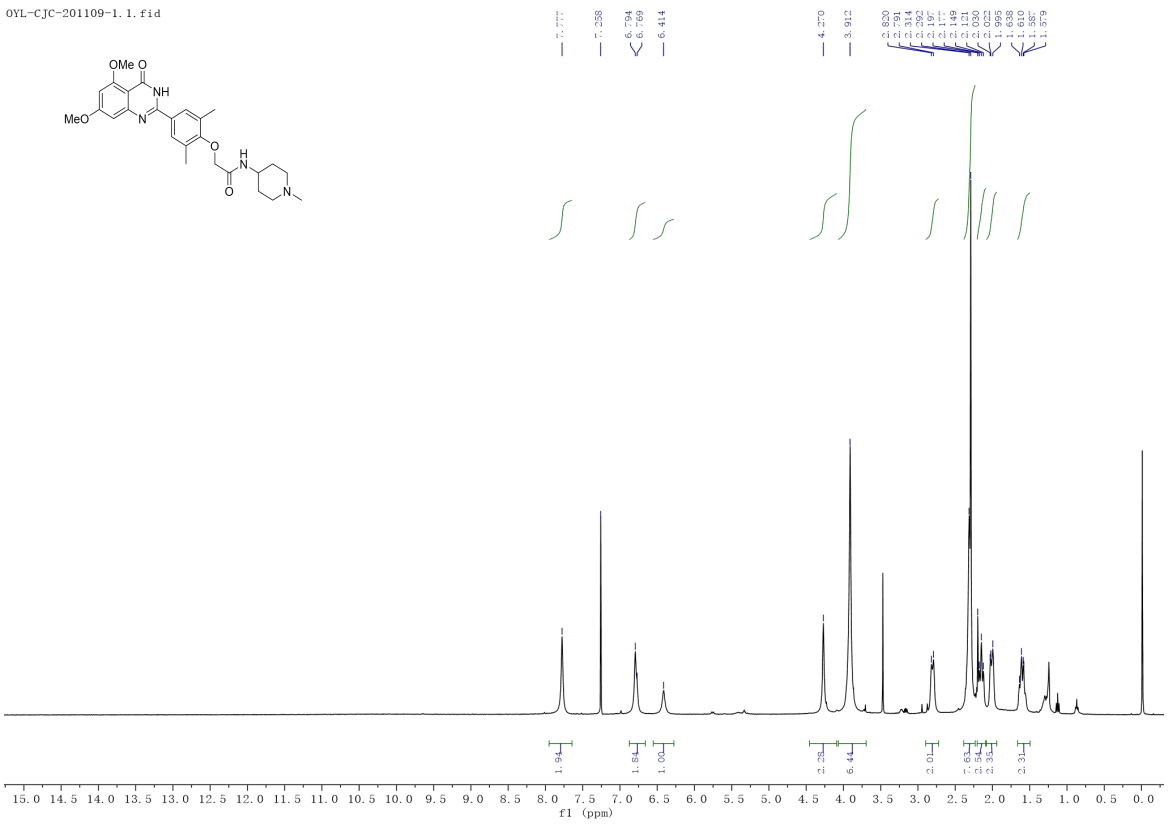


^{1}H NMR Spectrum of Compound **42e**

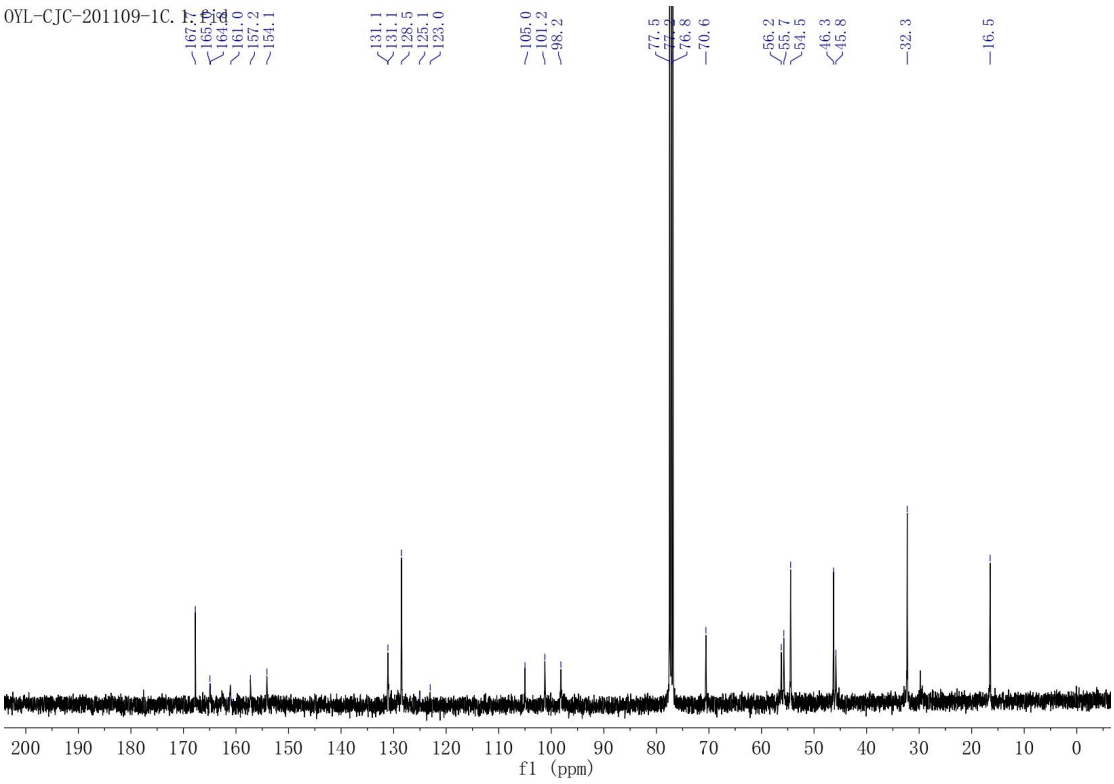


^{13}C NMR Spectrum of Compound **42e**

42f

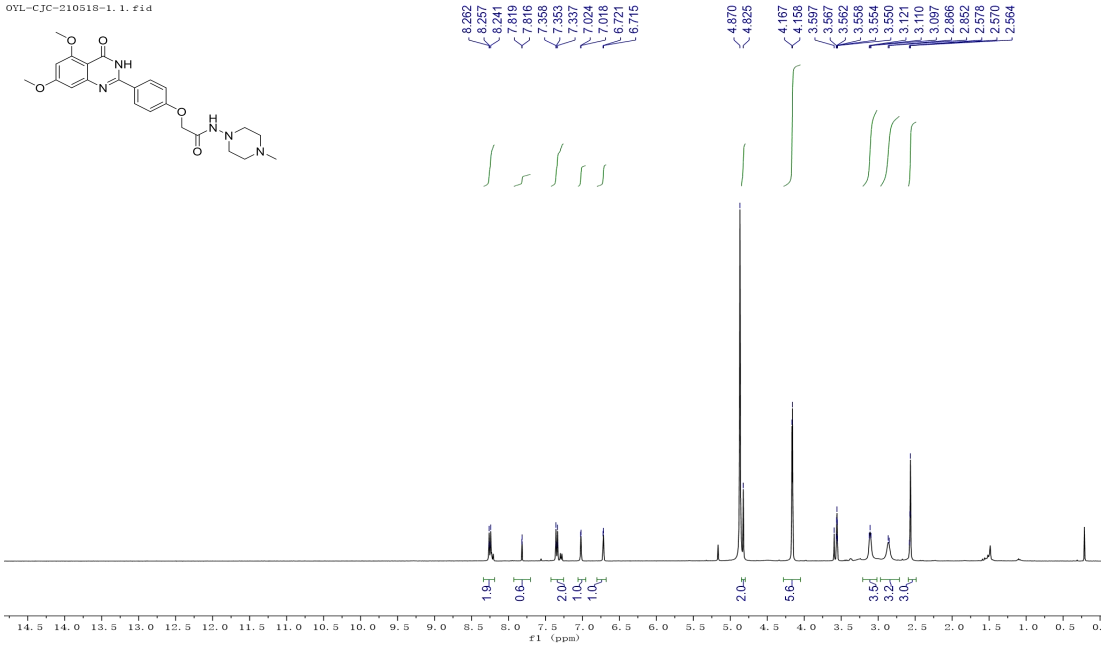


^{1}H NMR Spectrum of Compound **42f**

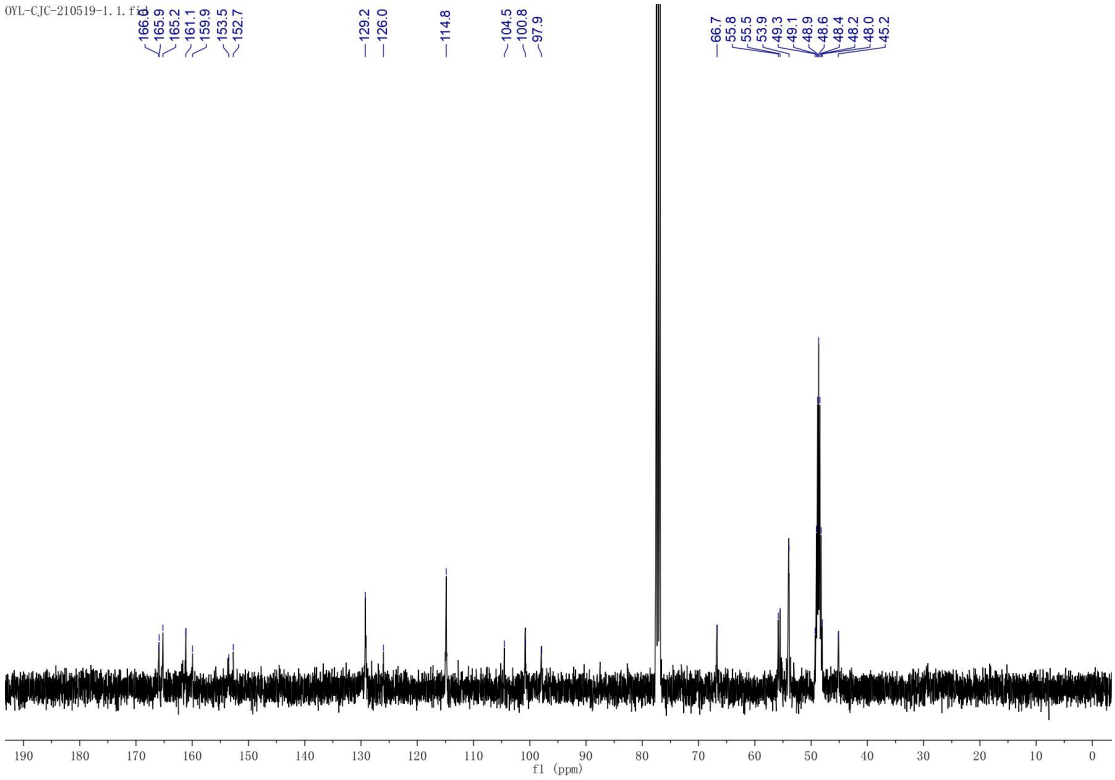


^{13}C NMR Spectrum of Compound **42f**

42g

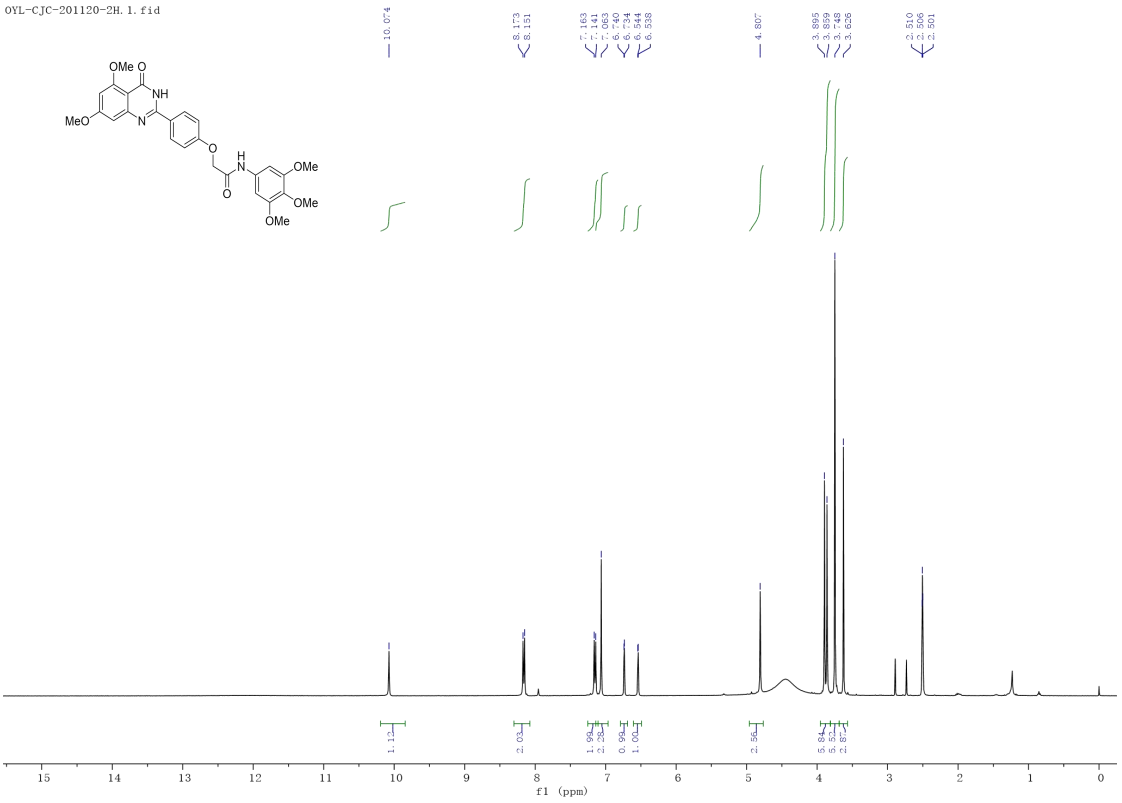


^{1}H NMR Spectrum of Compound **42g**

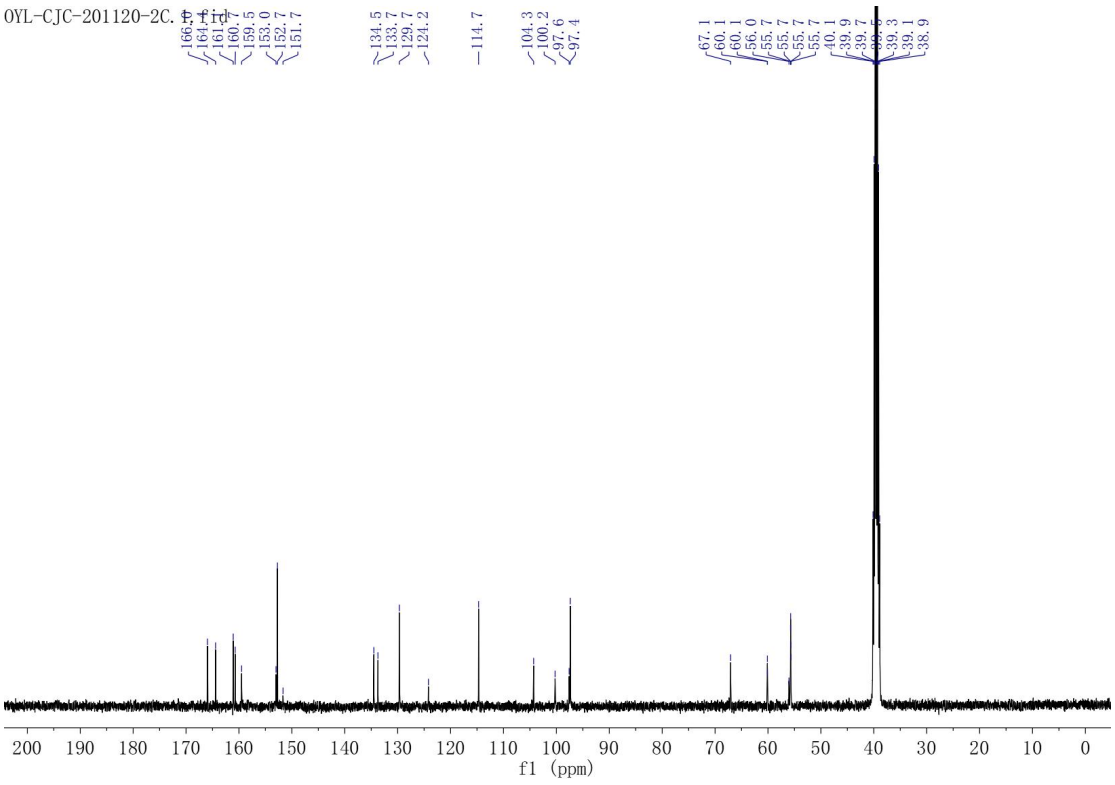


^{13}C NMR Spectrum of Compound **42g**

42h

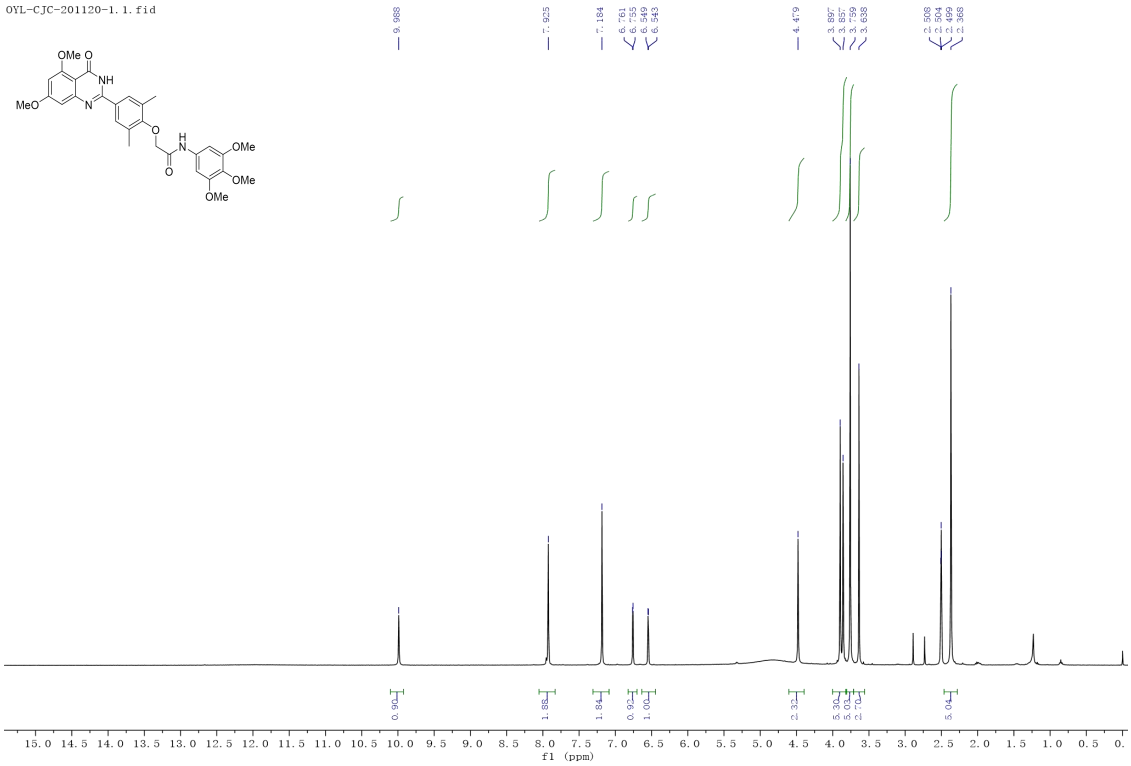


^{1}H NMR Spectrum of Compound **42h**

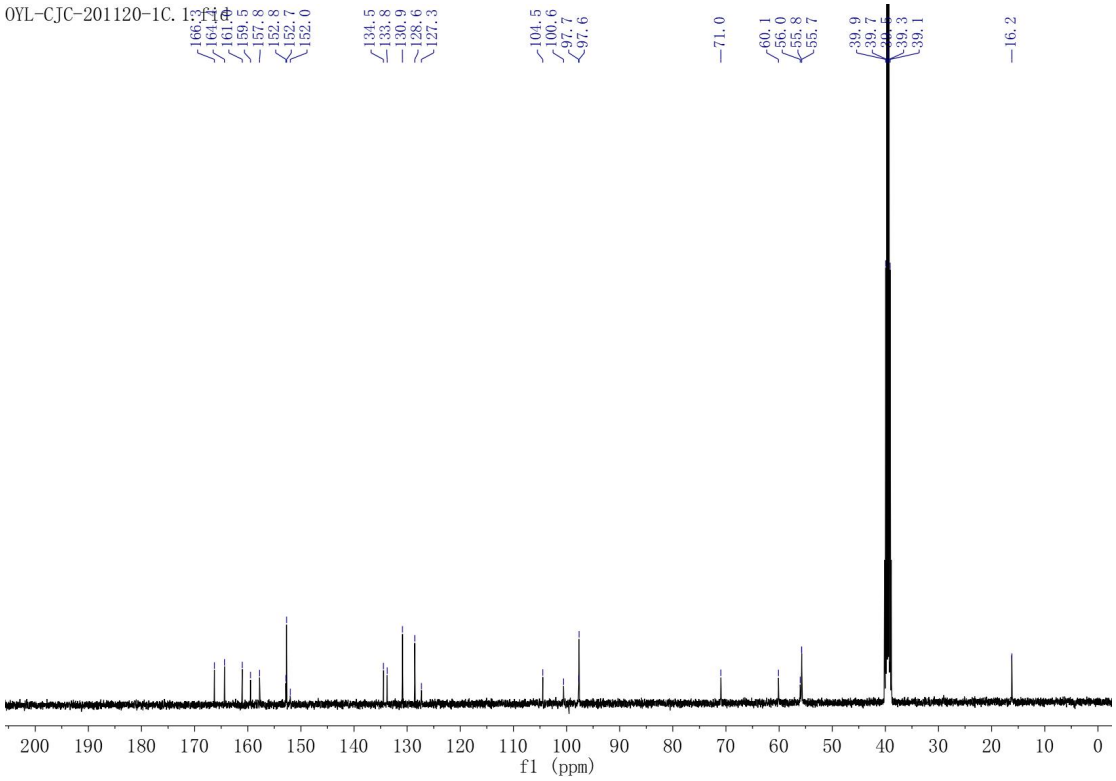


^{13}C NMR Spectrum of Compound **42h**

42i

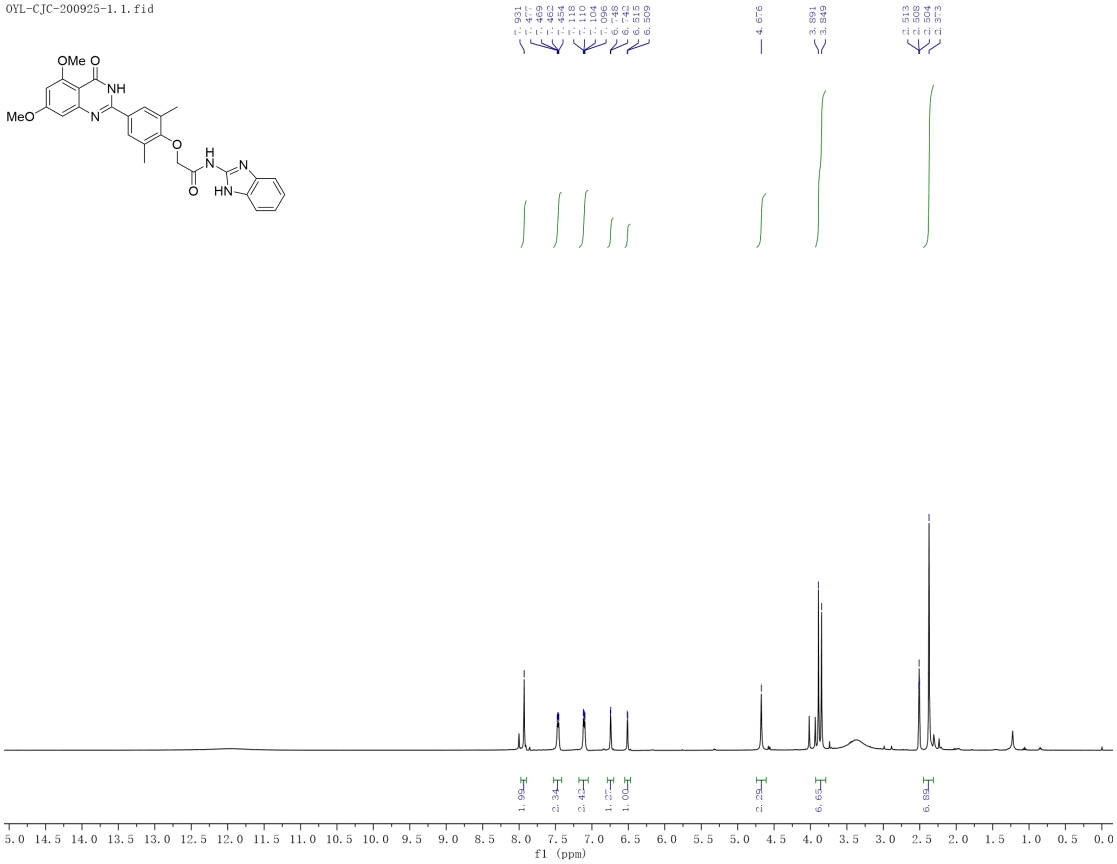


^{1}H NMR Spectrum of Compound **42i**

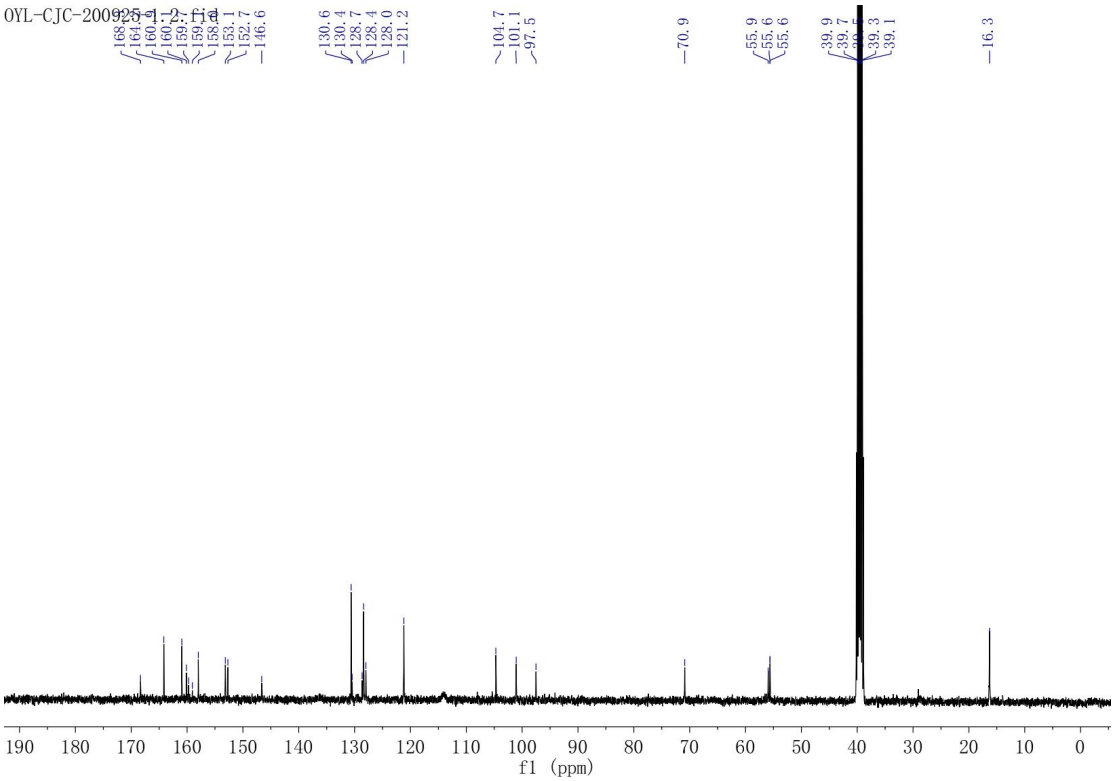


^{13}C NMR Spectrum of Compound **42i**

42j

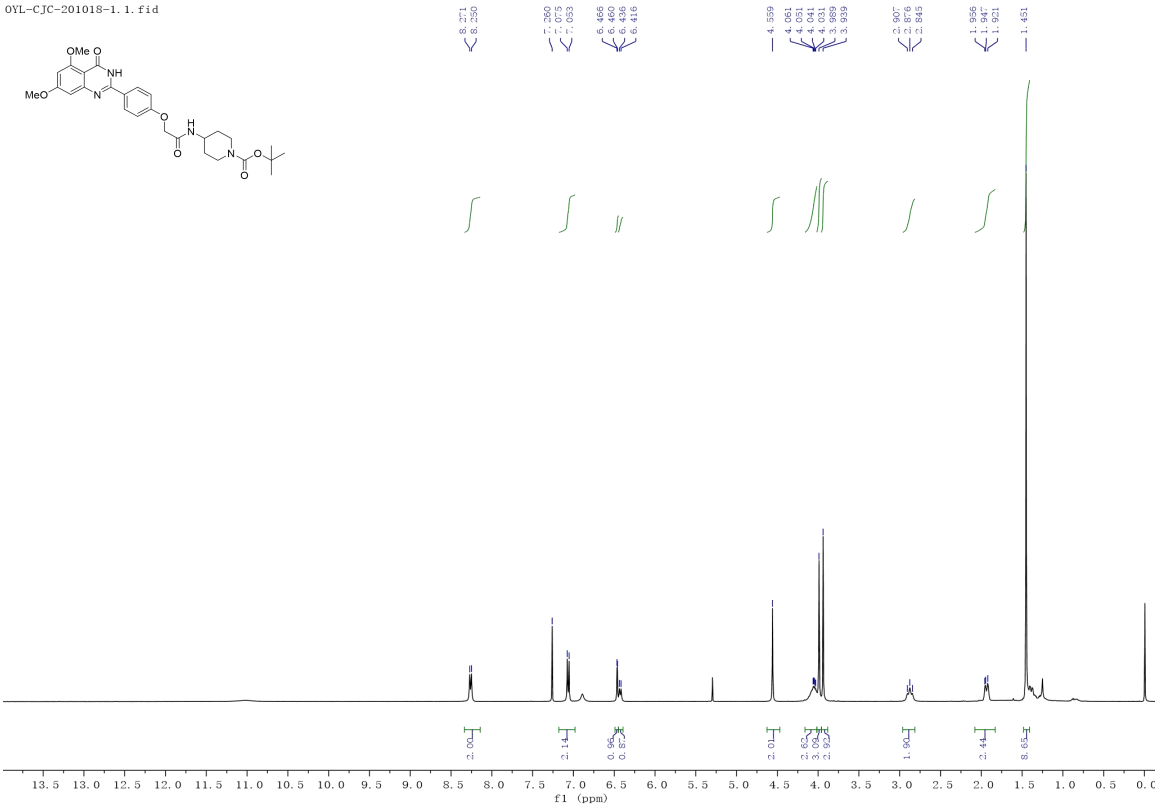


^{1}H NMR Spectrum of Compound **42j**

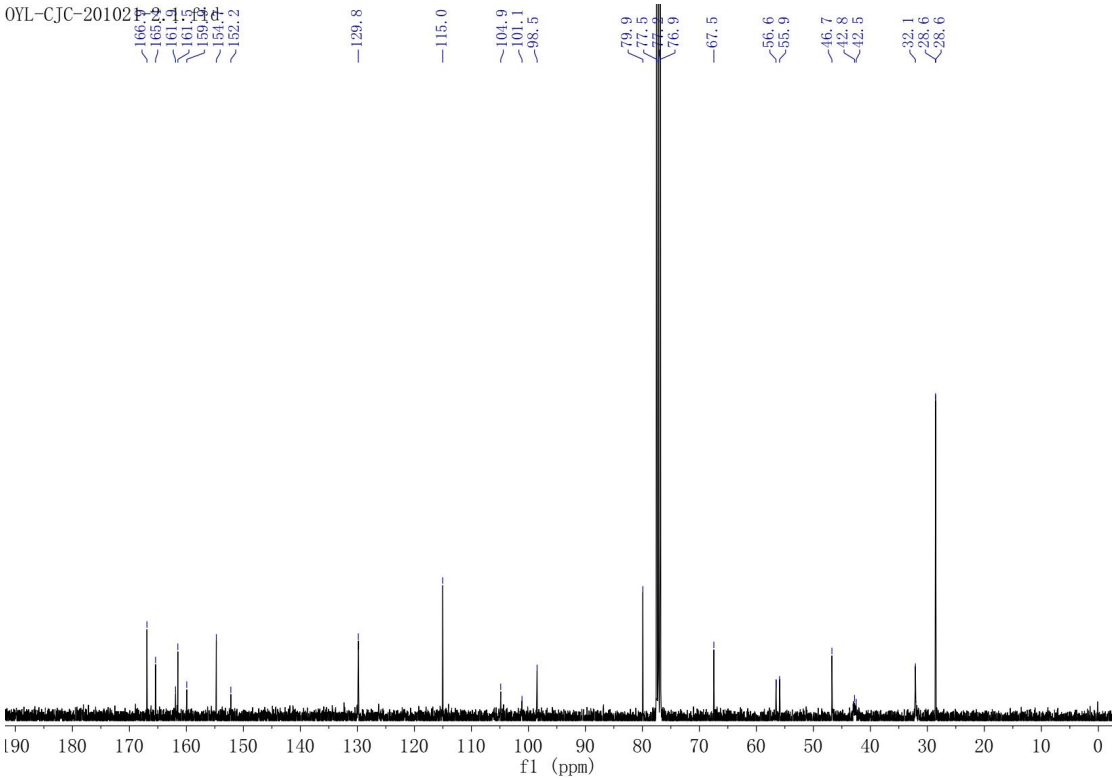


^{13}C NMR Spectrum of Compound **42j**

43a

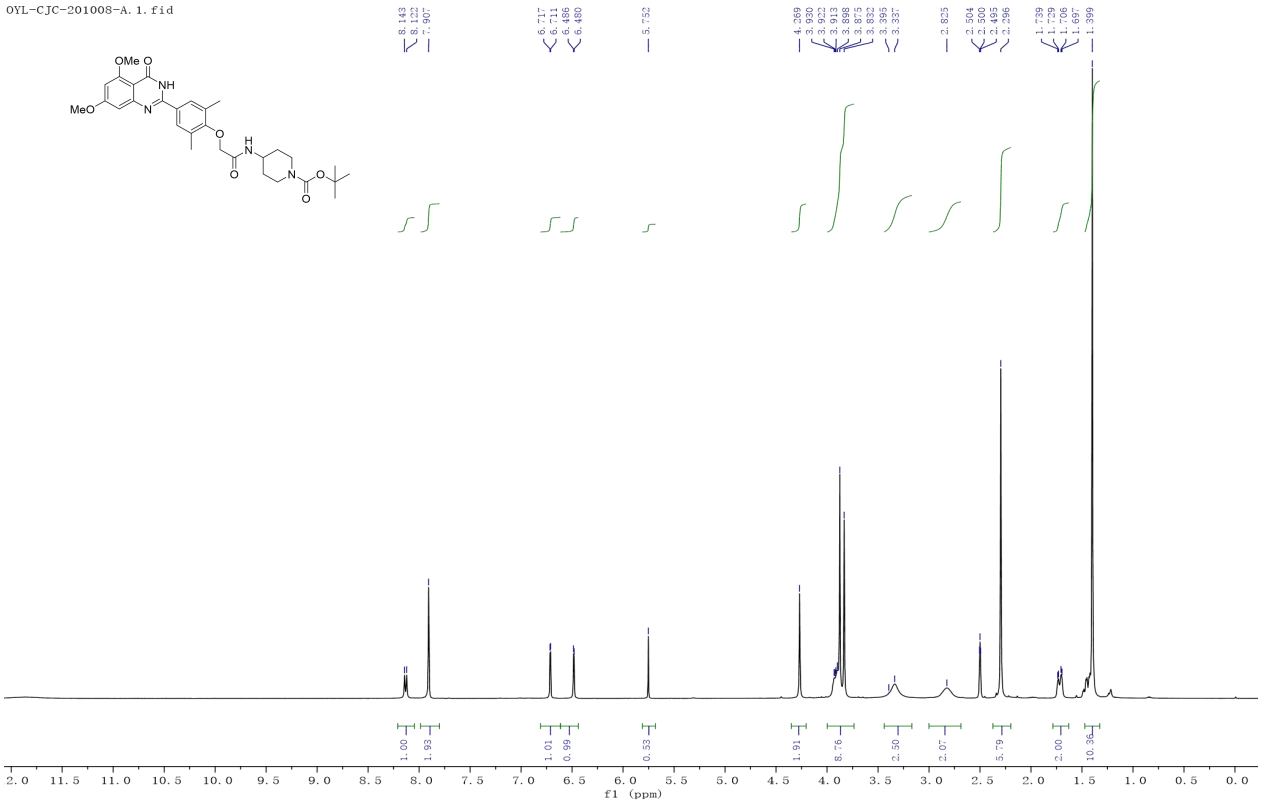


^{1}H NMR Spectrum of Compound **43a**

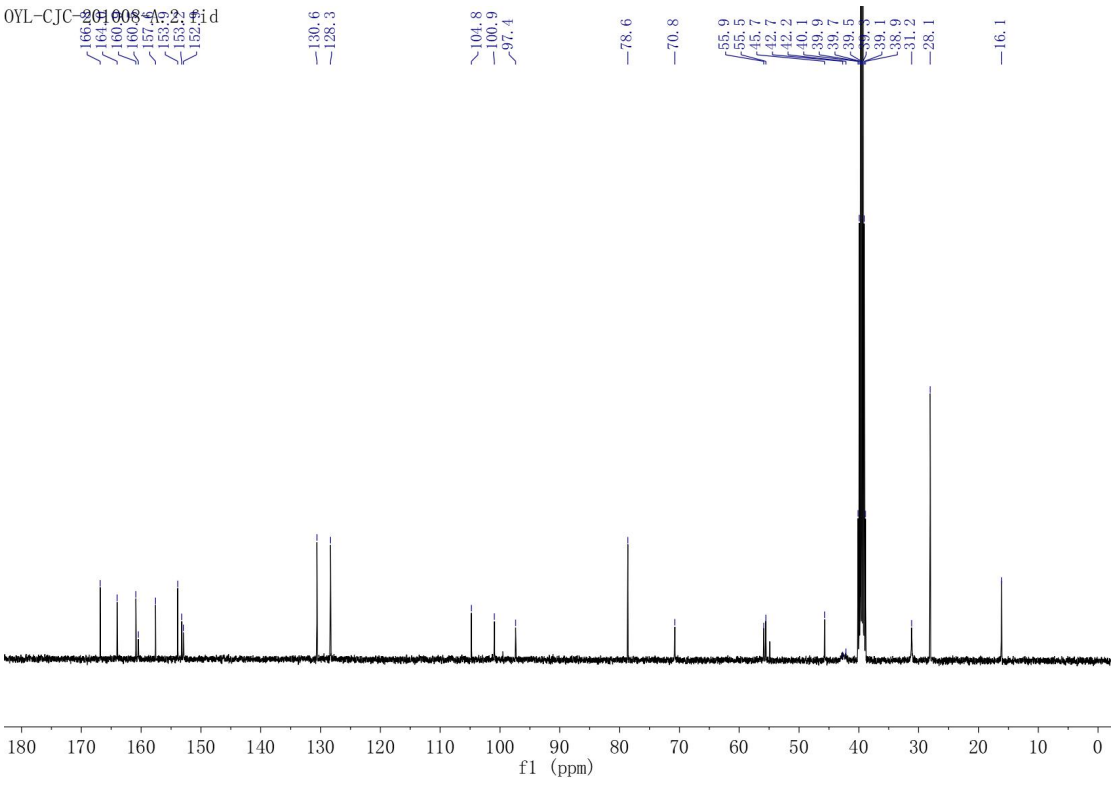


^{13}C NMR Spectrum of Compound **43a**

43b

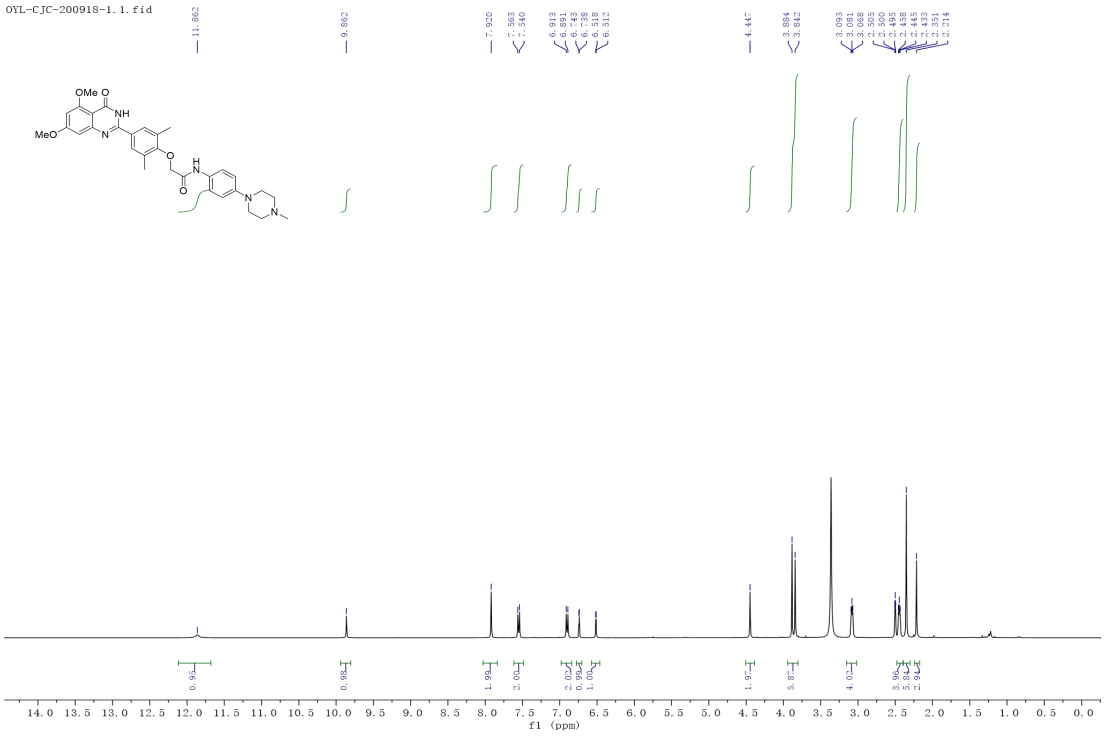


^{1}H NMR Spectrum of Compound **43b**

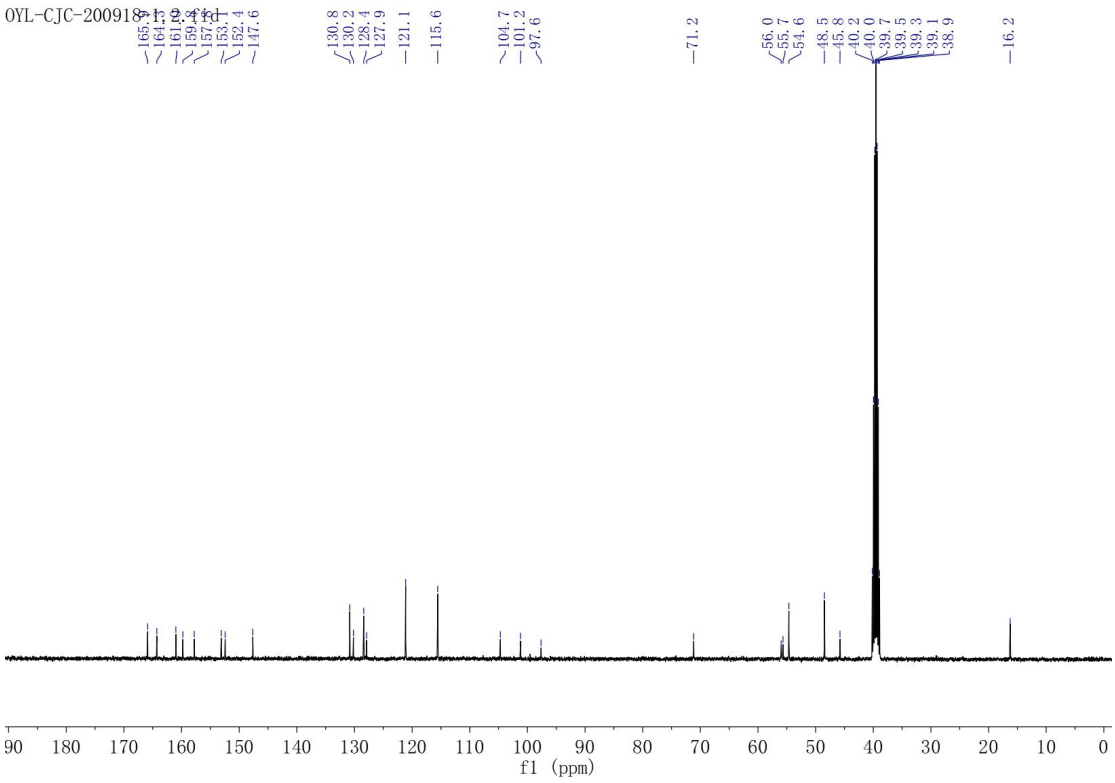


^{13}C NMR Spectrum of Compound **43b**

43c

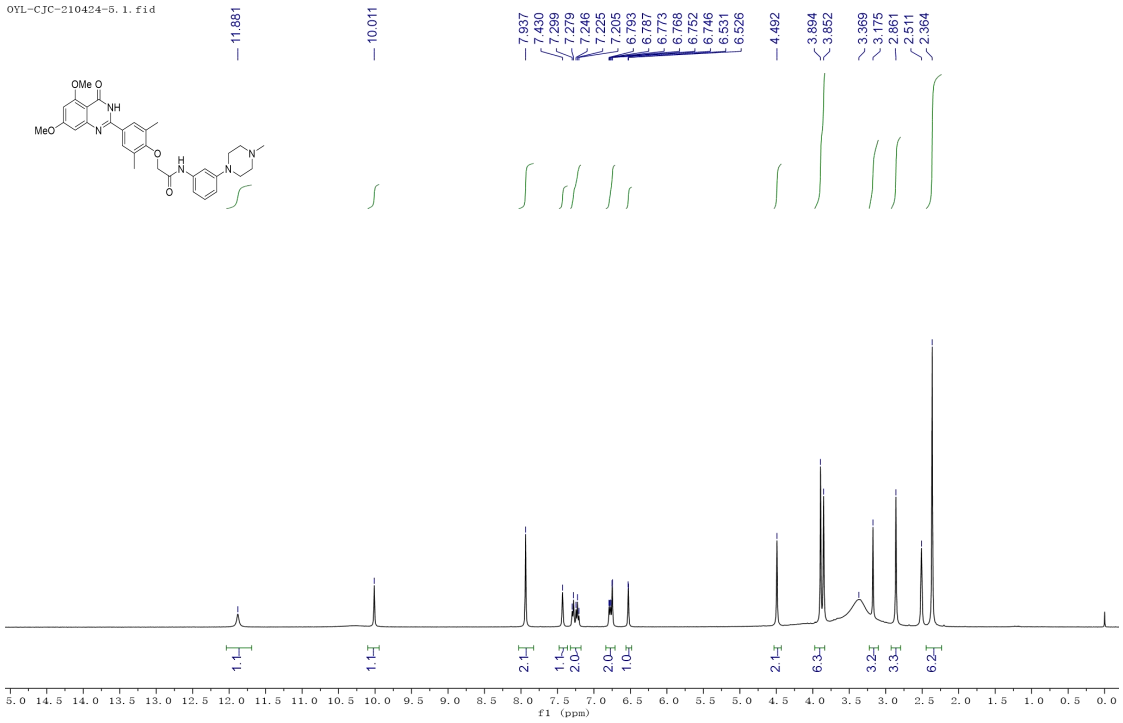


^{1}H NMR Spectrum of Compound **43c**

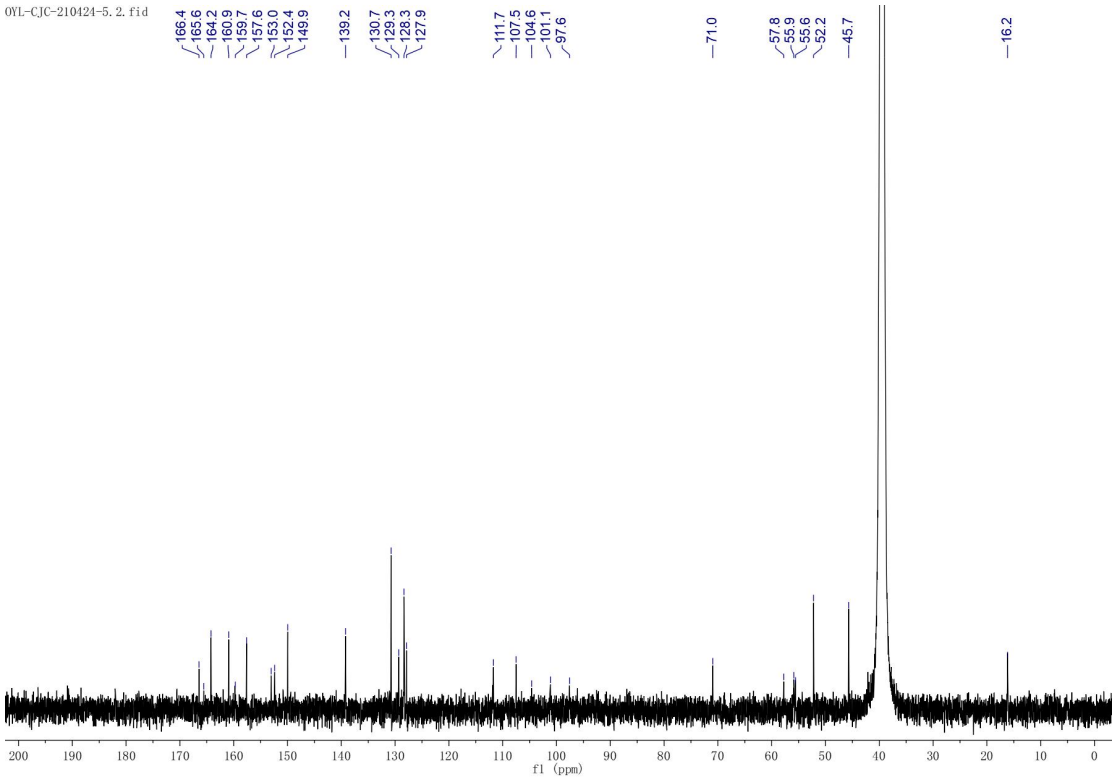


^{13}C NMR Spectrum of Compound **43c**

43d

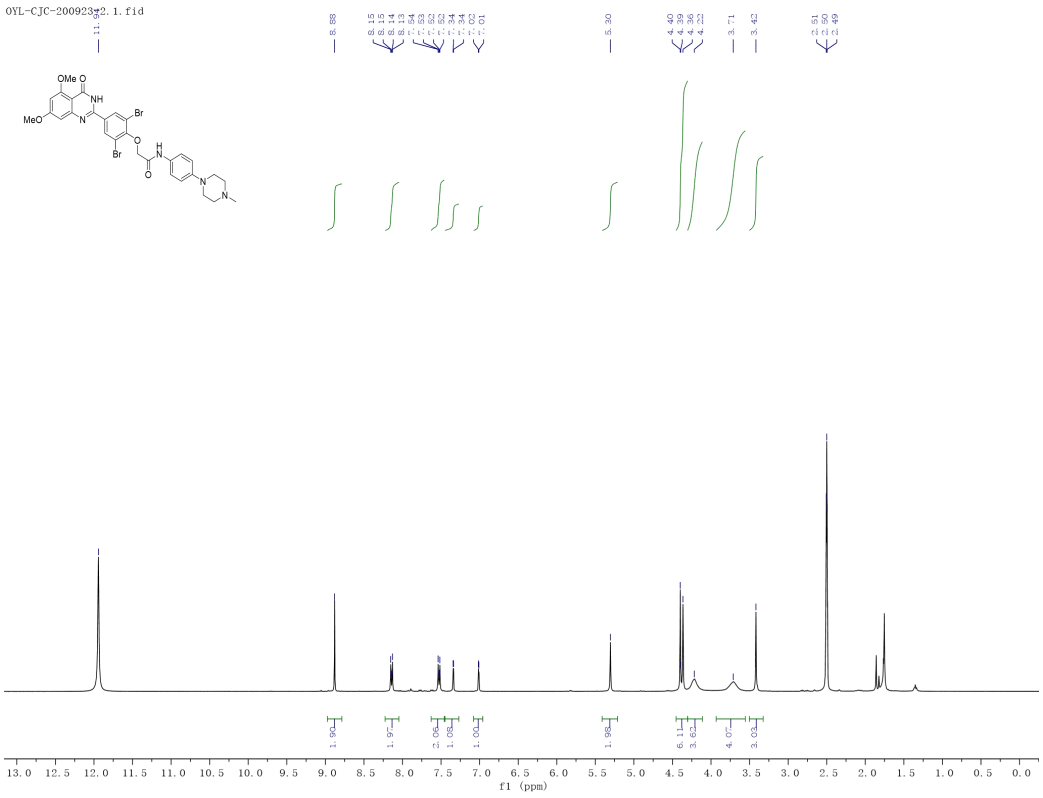


^{1}H NMR Spectrum of Compound **43d**

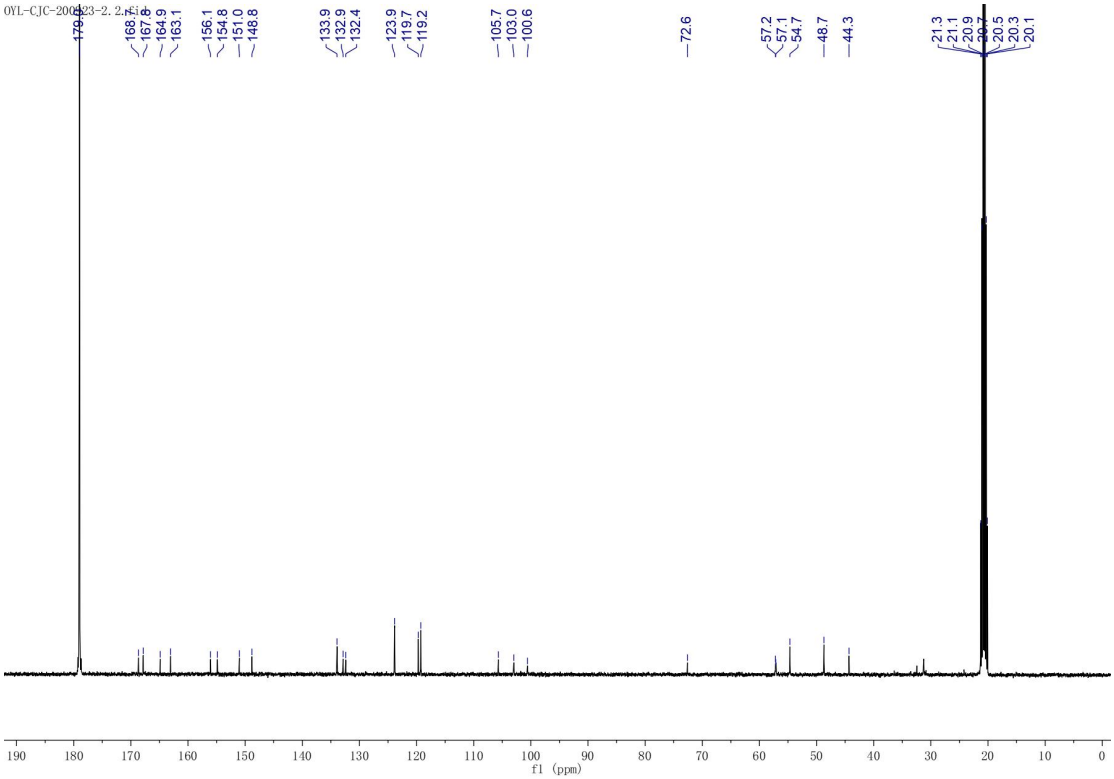


^{13}C NMR Spectrum of Compound **43d**

43e

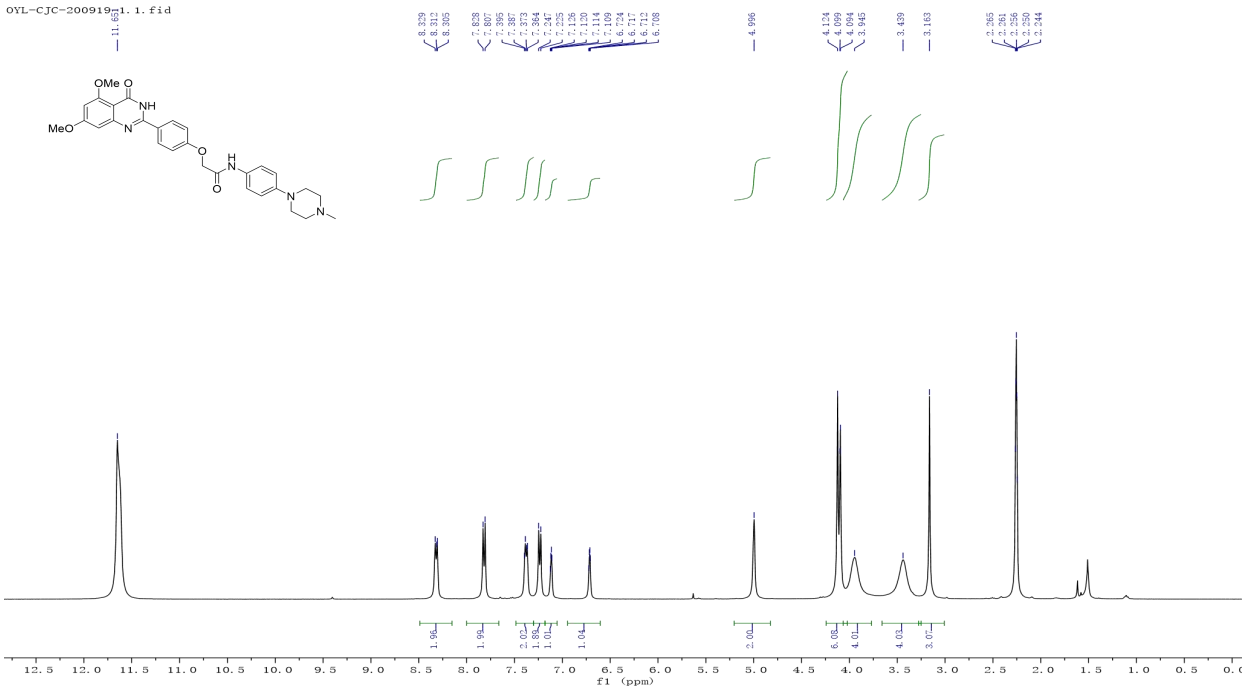


^{1}H NMR Spectrum of Compound **43e**

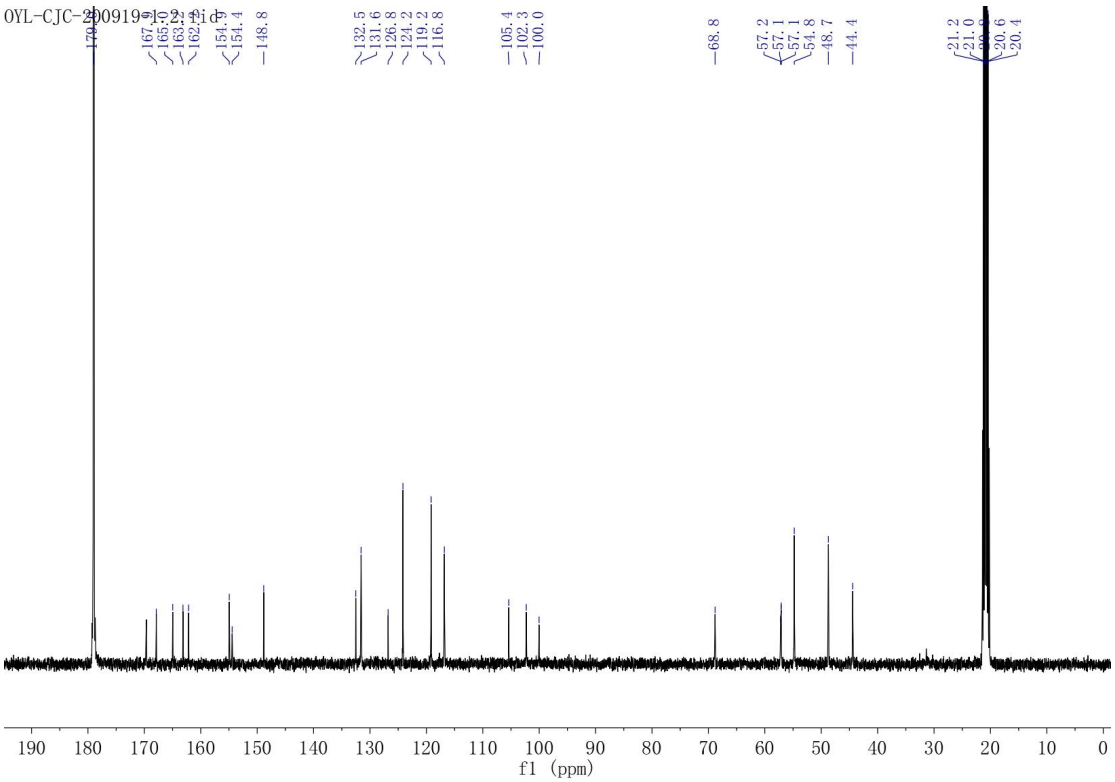


^{13}C NMR Spectrum of Compound **43e**

43f

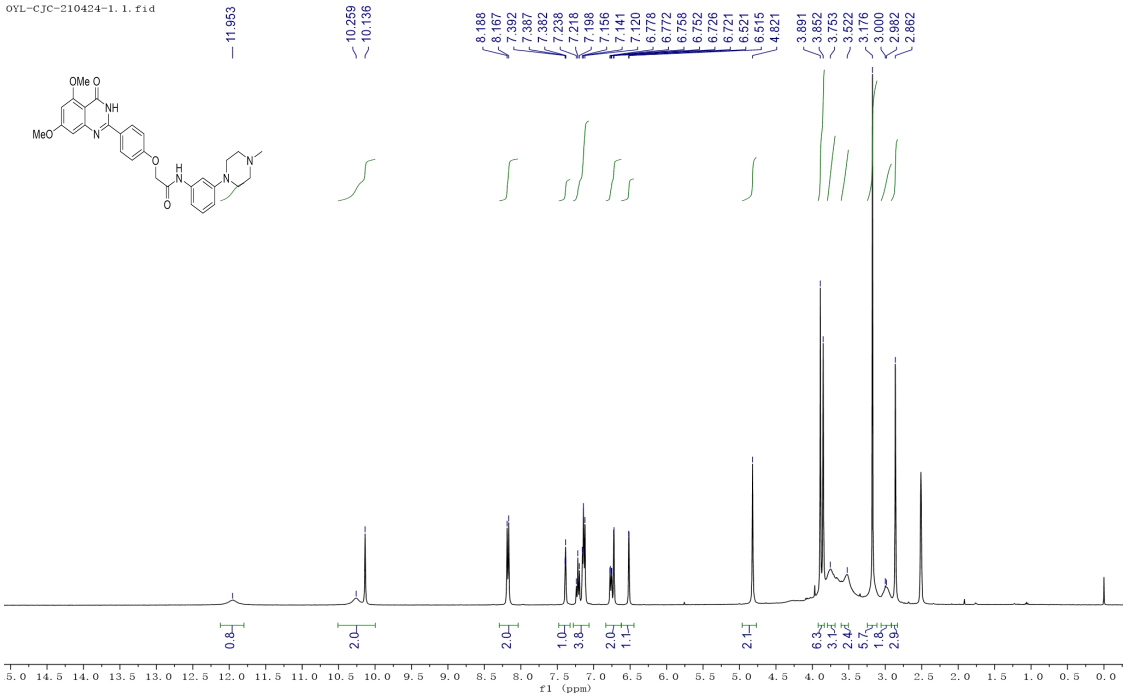


^{1}H NMR Spectrum of Compound **43f**

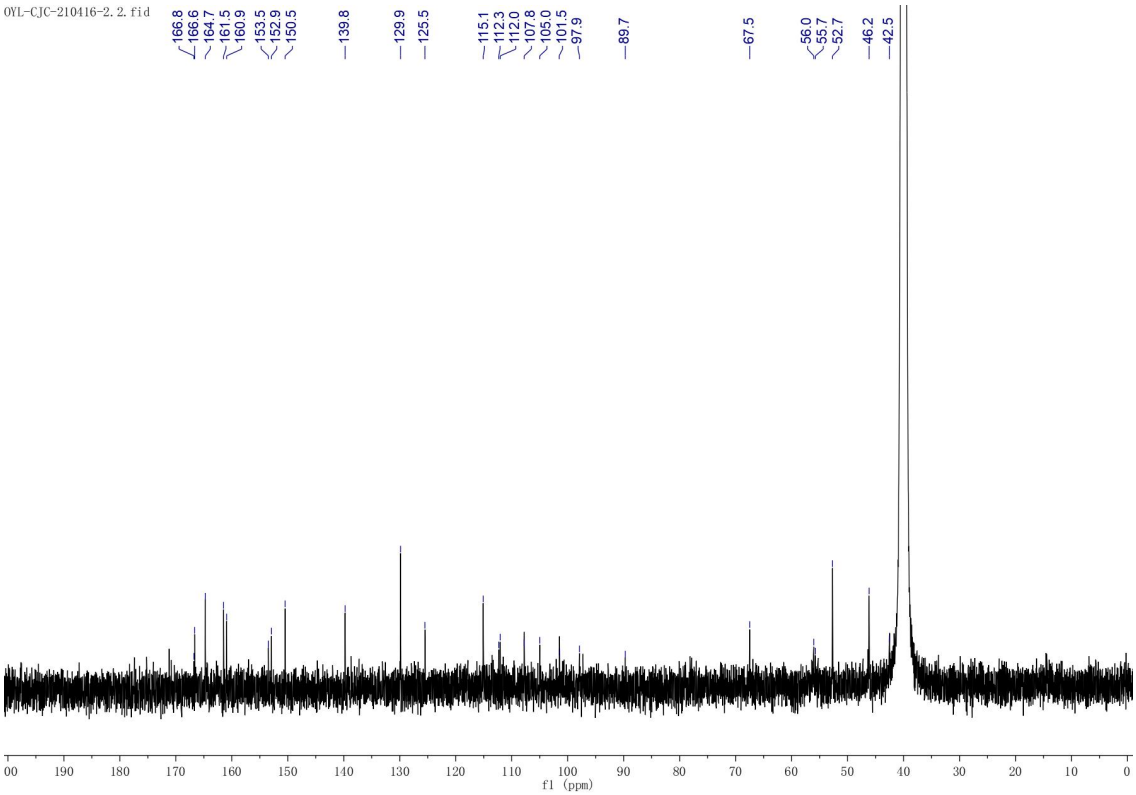


^{13}C NMR Spectrum of Compound **43f**

43g

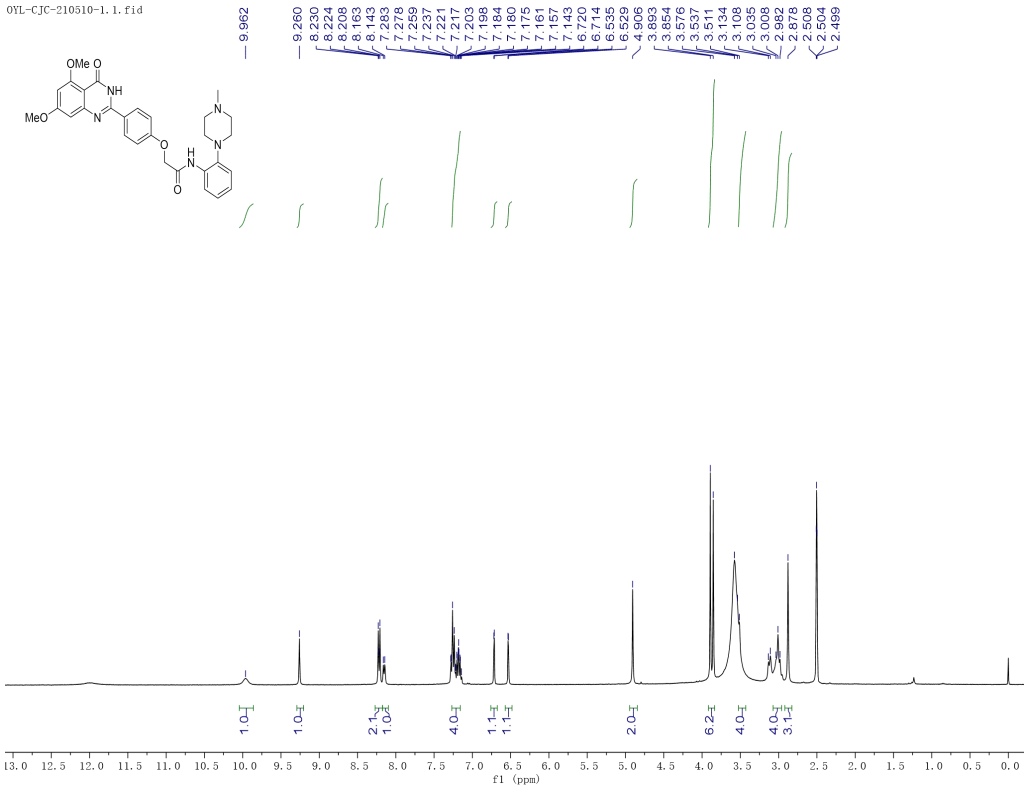


^{1}H NMR Spectrum of Compound **43g**

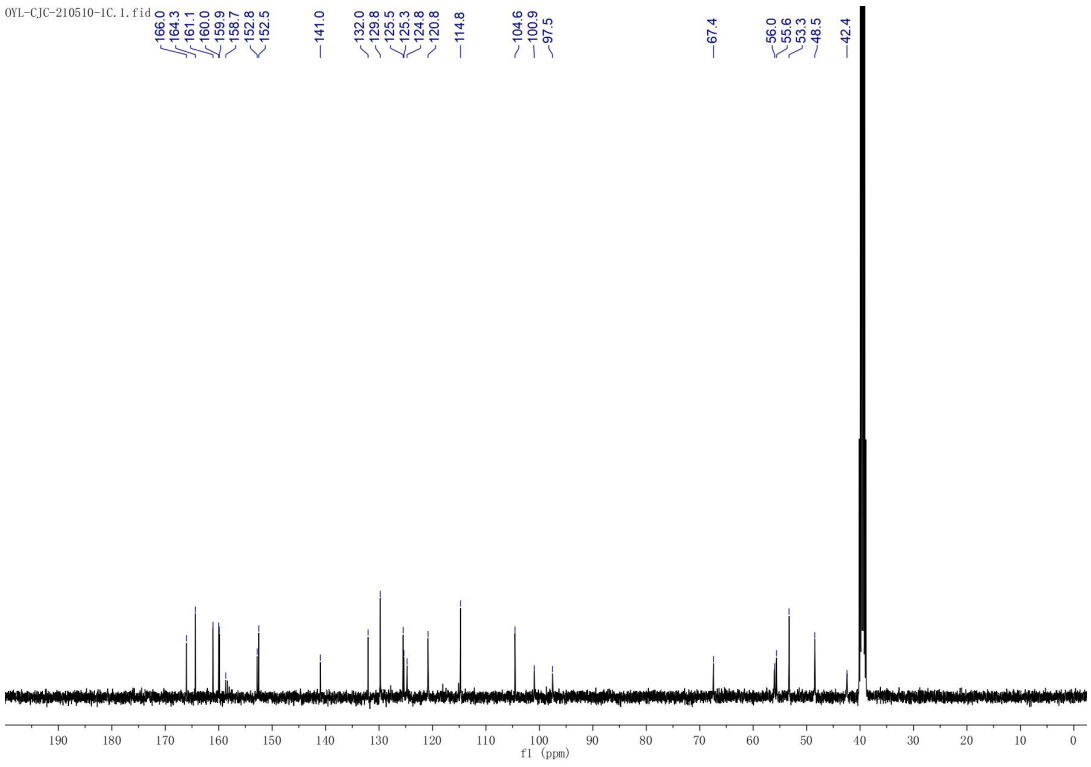


^{13}C NMR Spectrum of Compound **43g**

43h

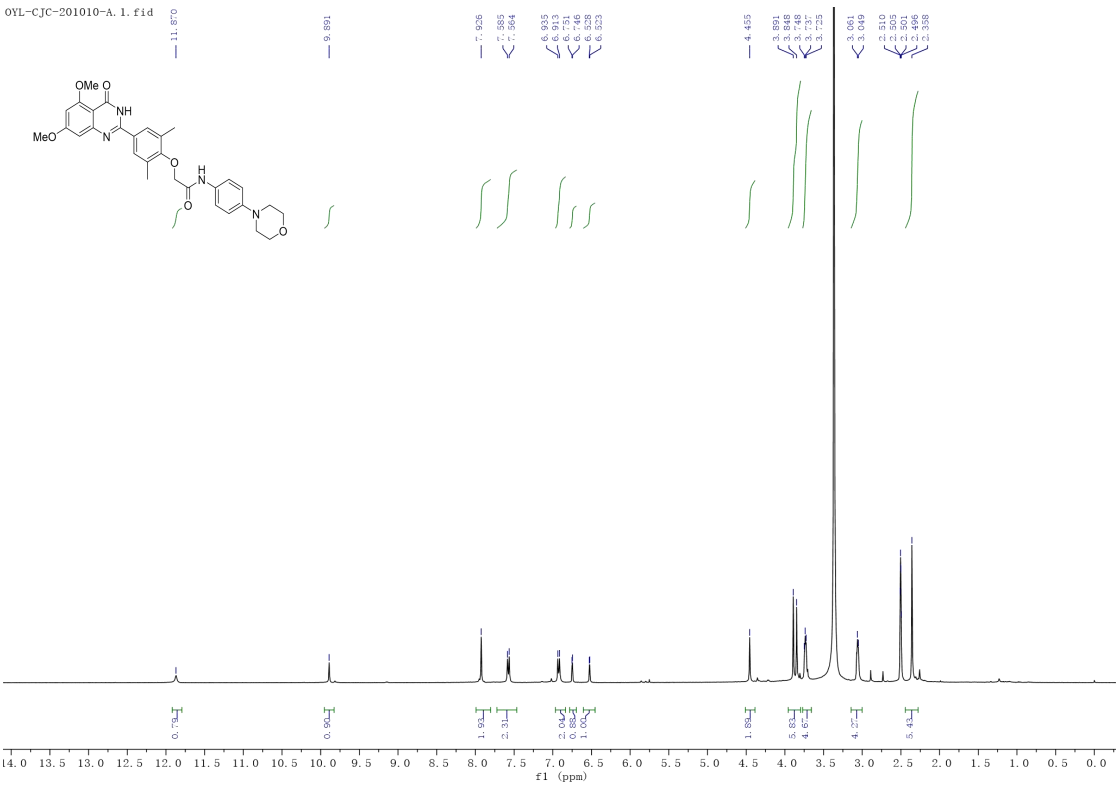


^{1}H NMR Spectrum of Compound **43h**

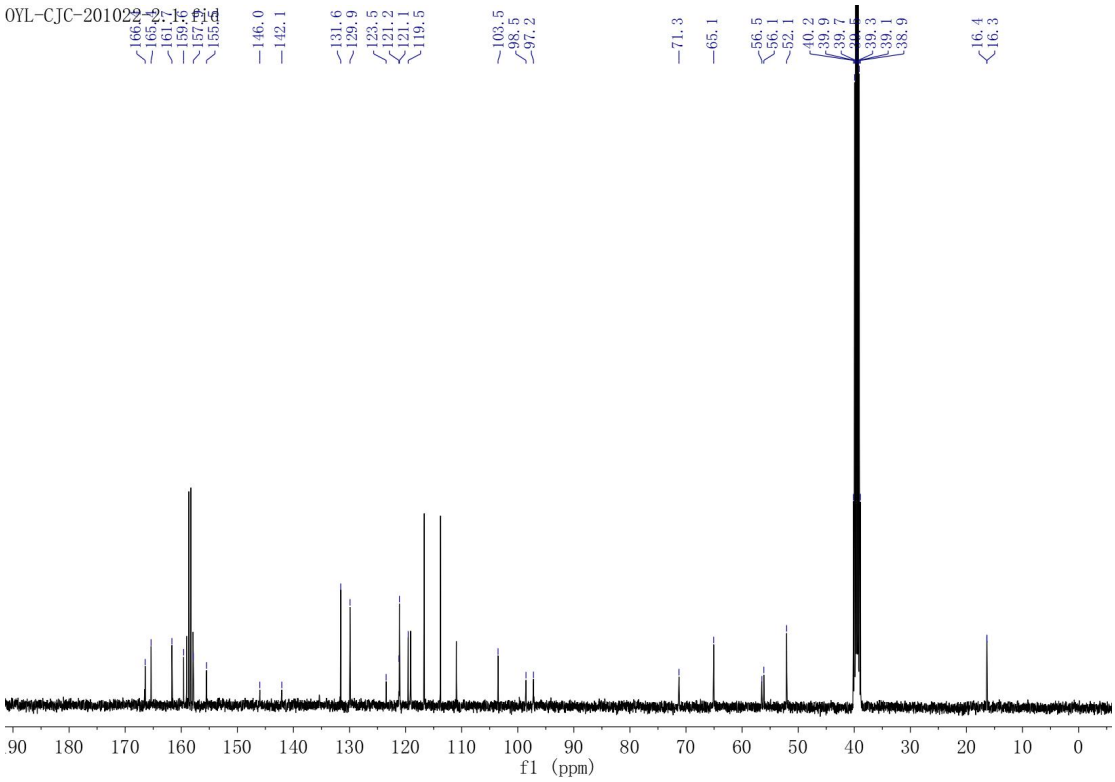


^{13}C NMR Spectrum of Compound **43h**

43i

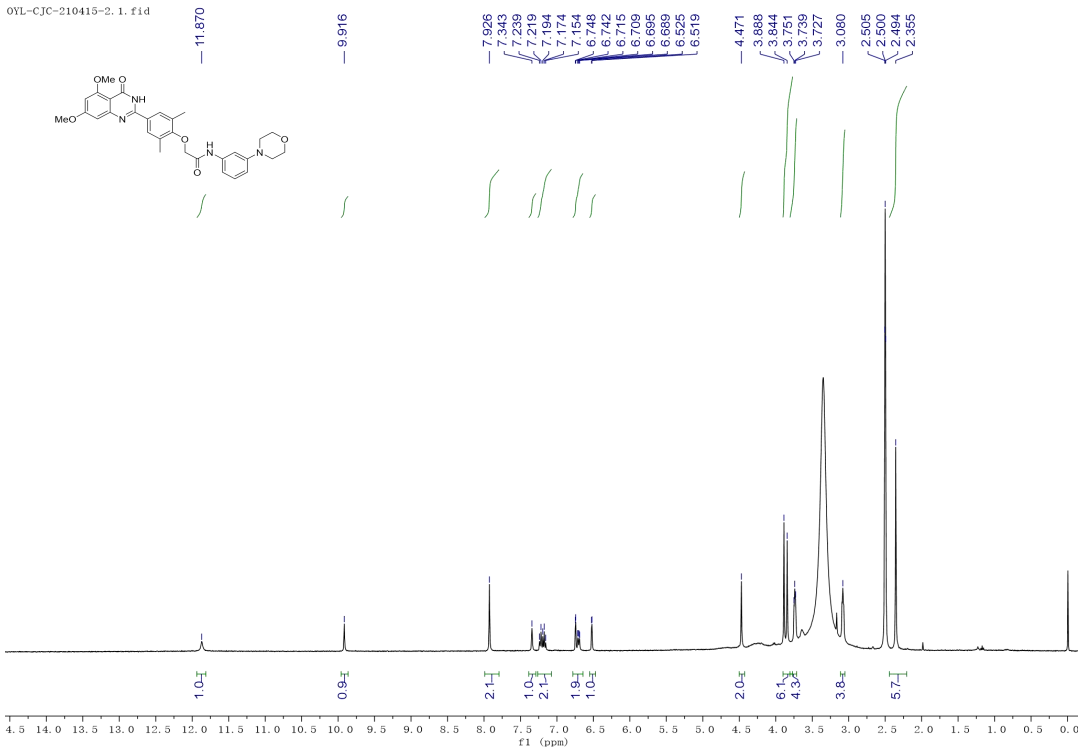


^{1}H NMR Spectrum of Compound **43i**

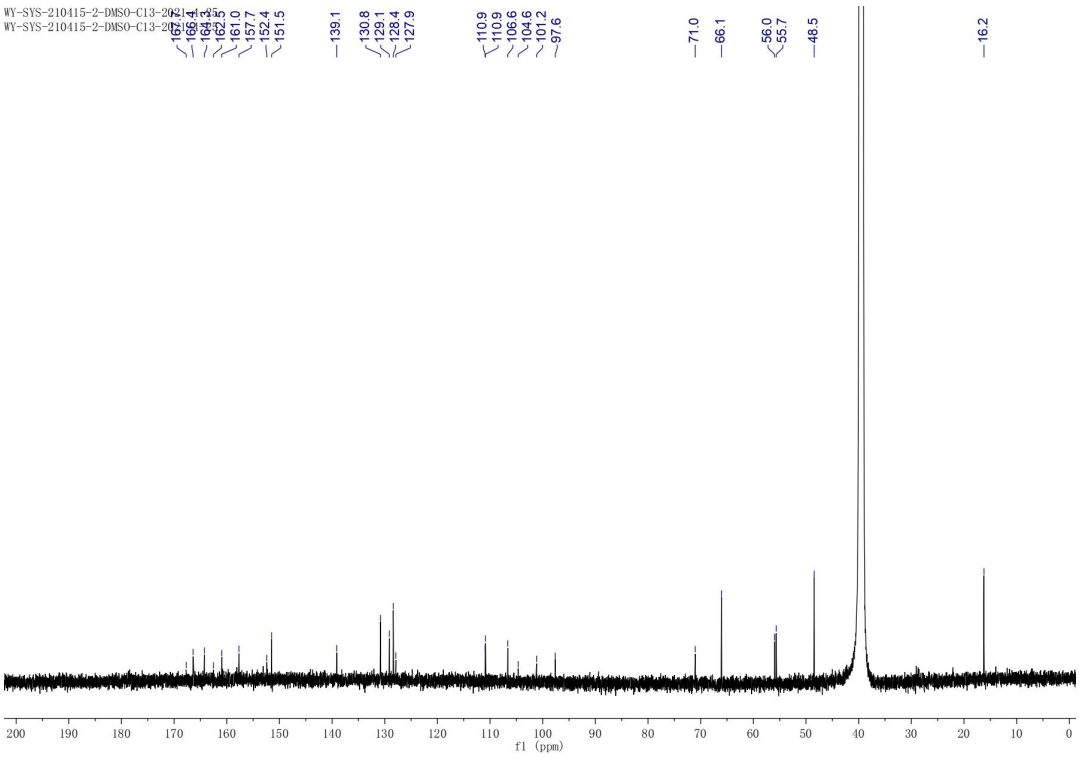


^{13}C NMR Spectrum of Compound **43i**

43j

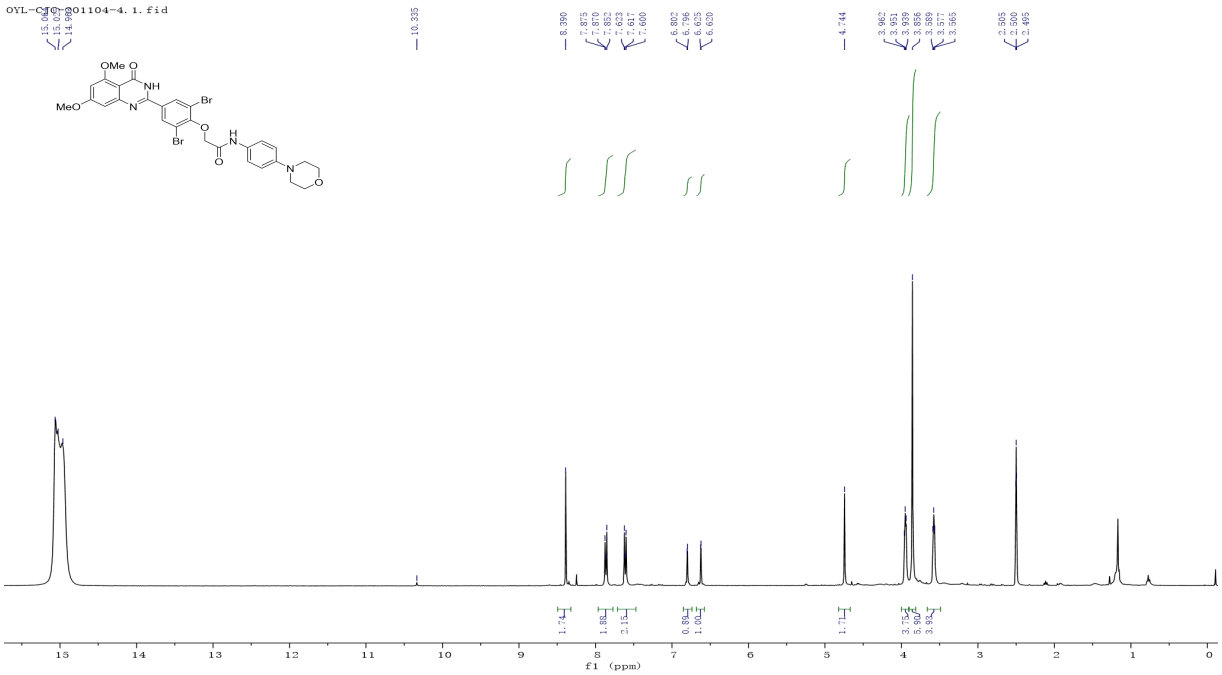


^{1}H NMR Spectrum of Compound **43j**

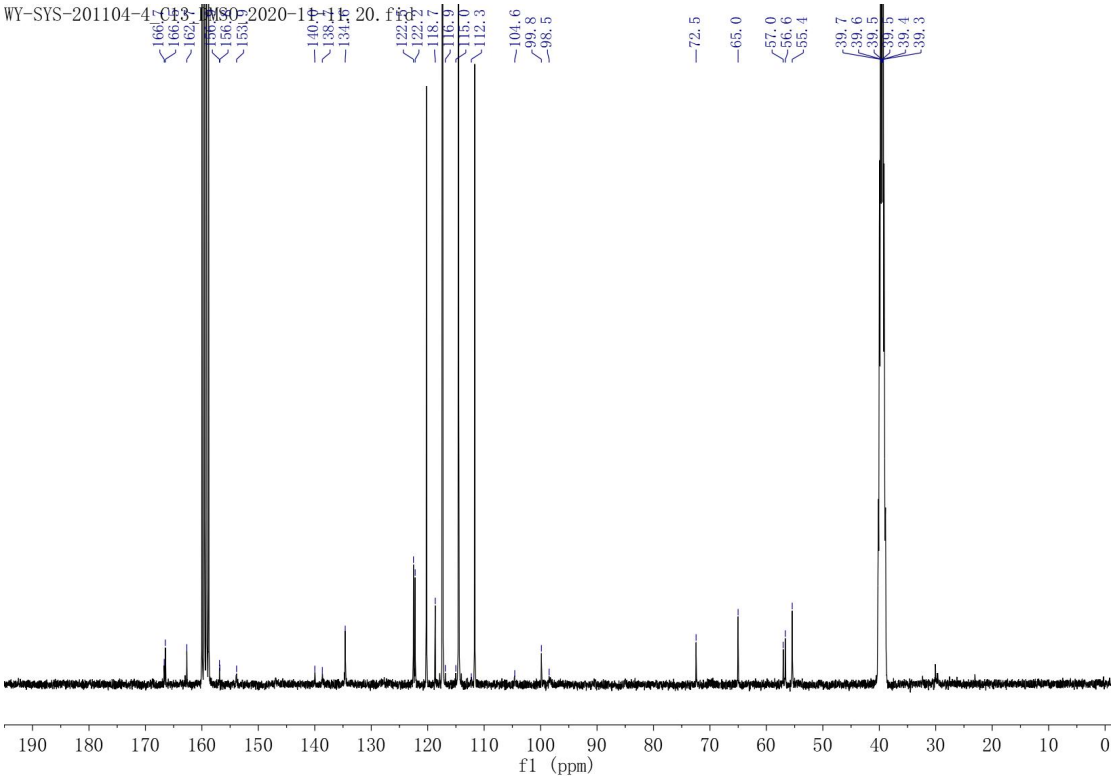


^{13}C NMR Spectrum of Compound **43j**

43k

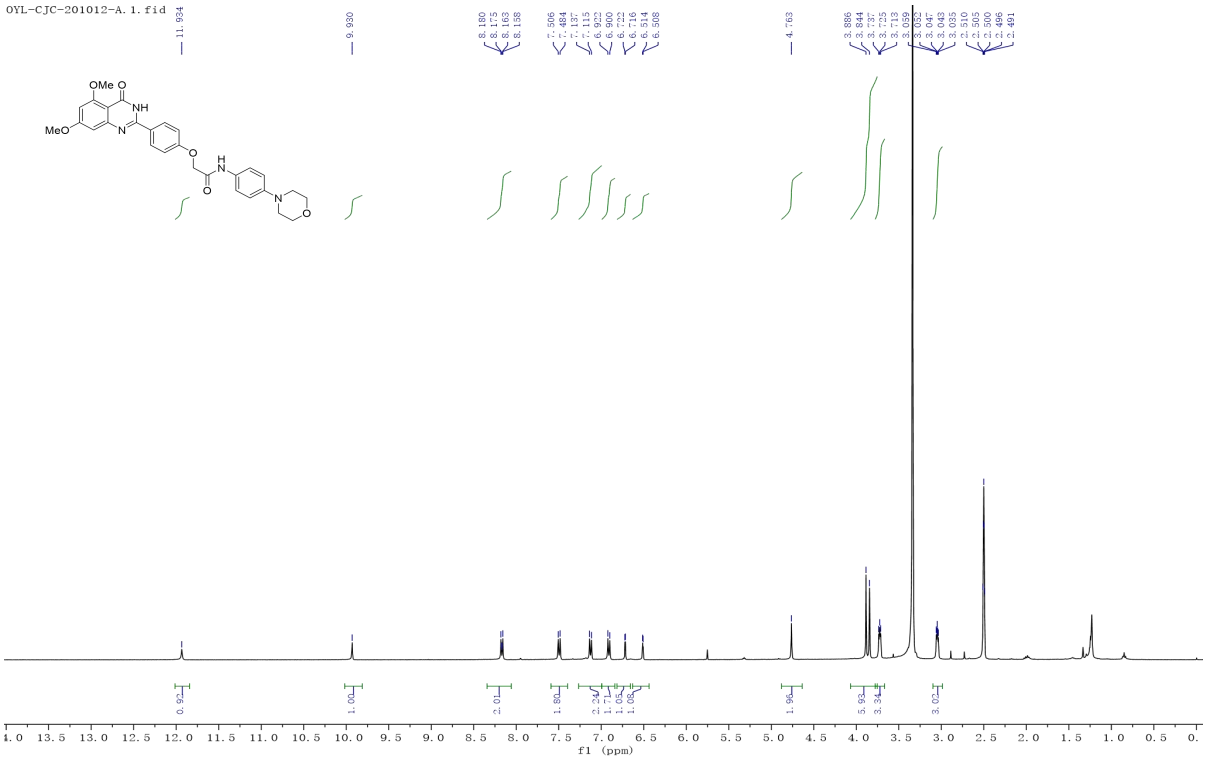


^{1}H NMR Spectrum of Compound **43k**

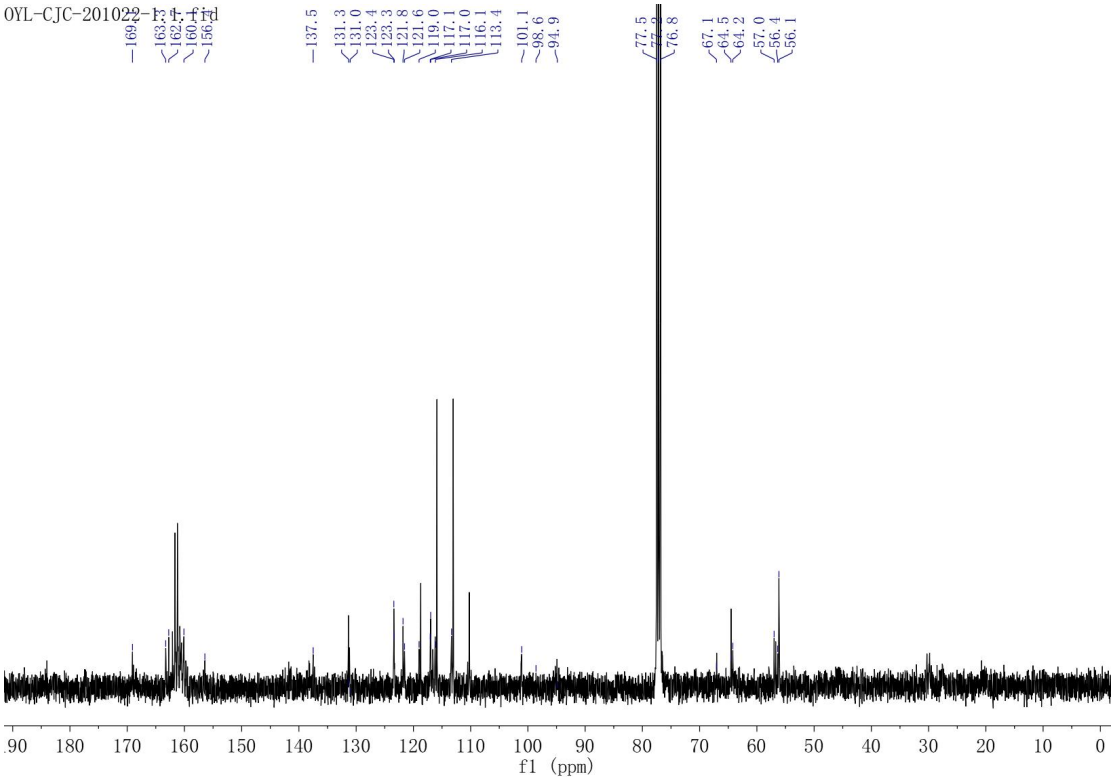


^{13}C NMR Spectrum of Compound **43k**

43l

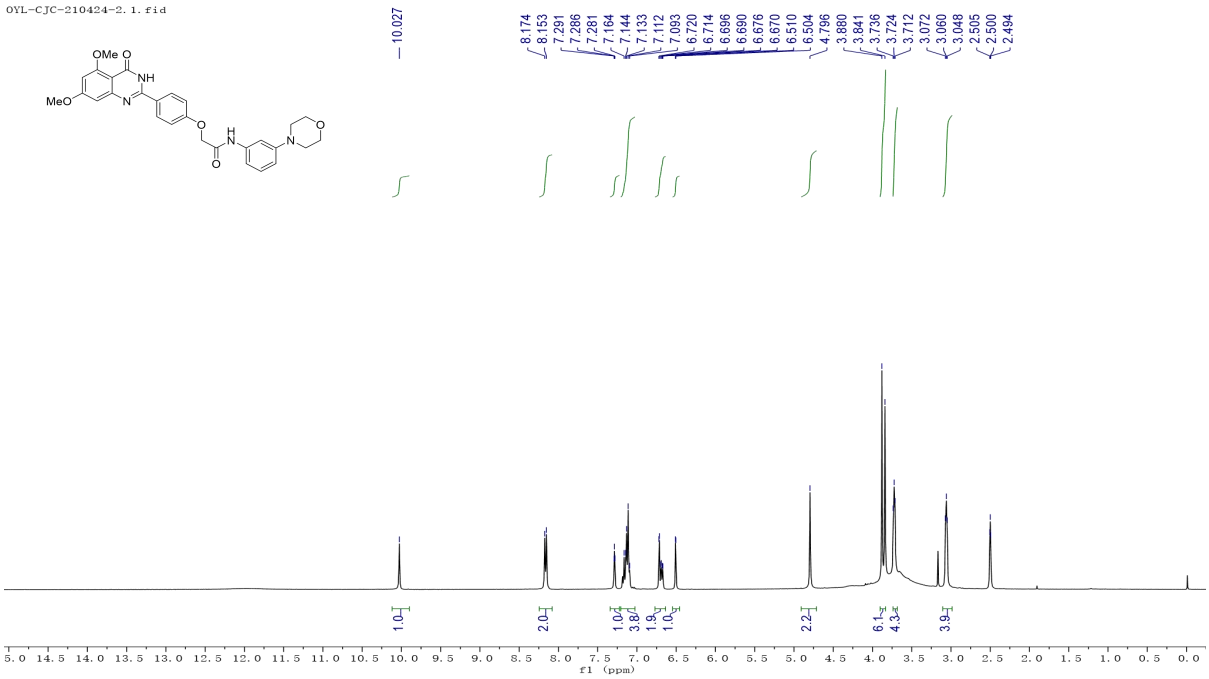


^{1}H NMR Spectrum of Compound **43l**

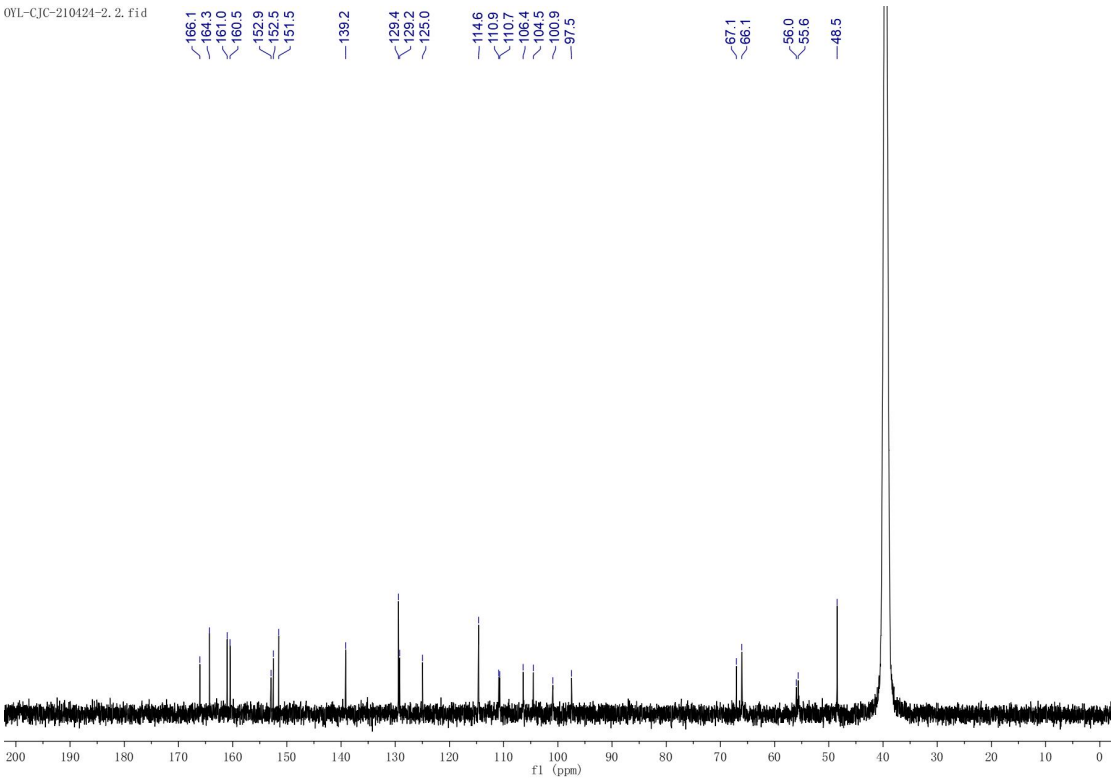


^{13}C NMR Spectrum of Compound **43l**

43m

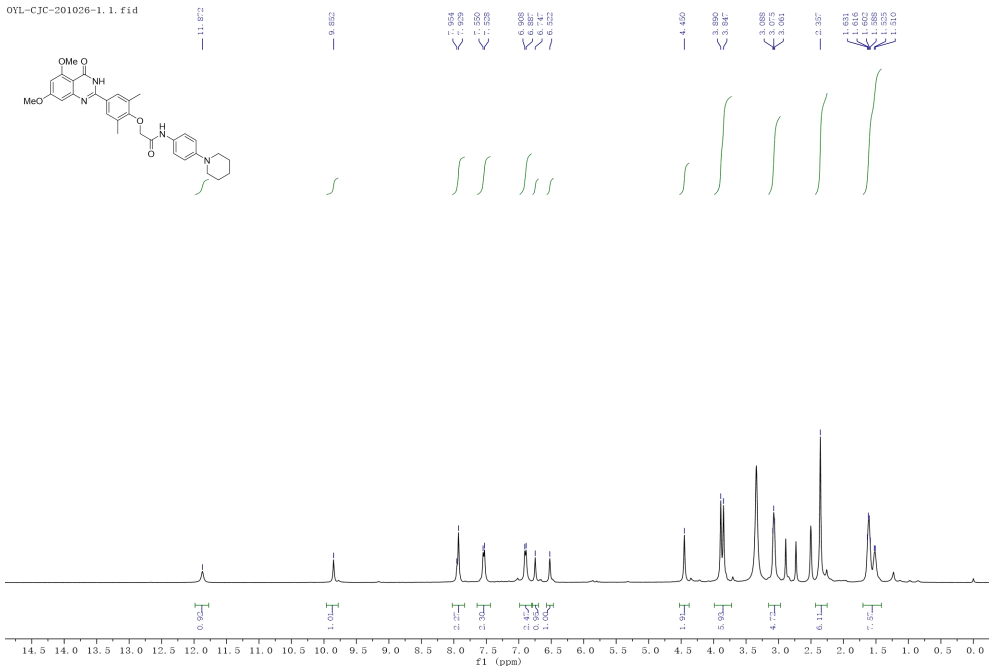


^{1}H NMR Spectrum of Compound **43m**

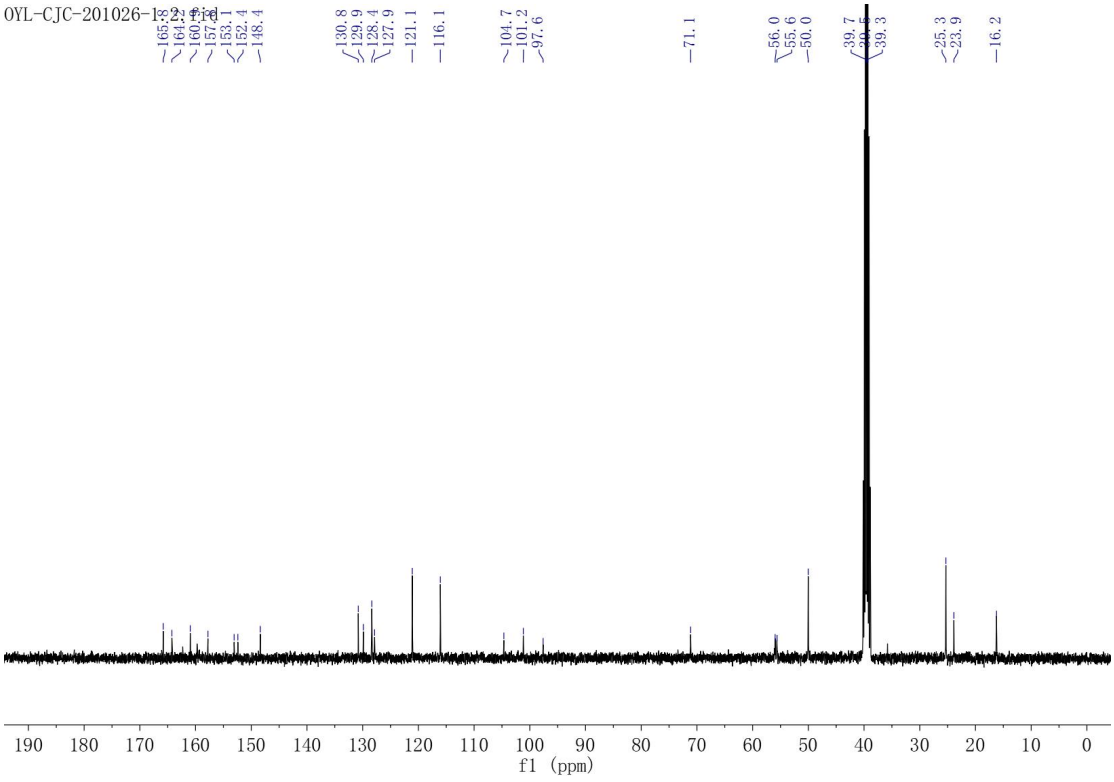


^{13}C NMR Spectrum of Compound **43m**

43n

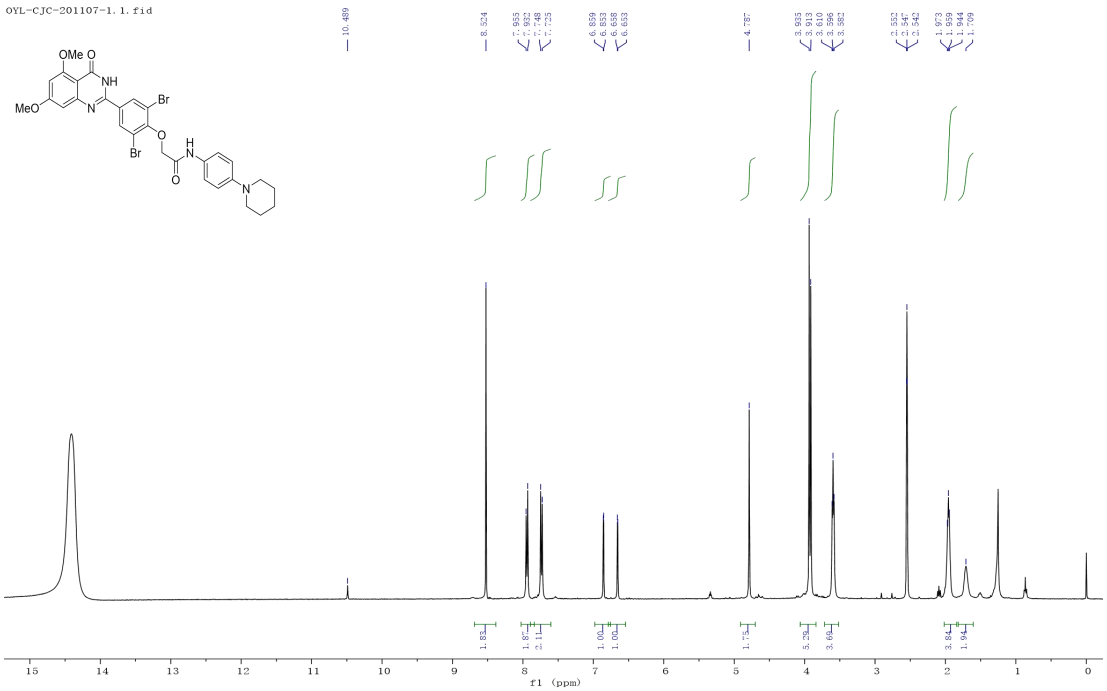


^{1}H NMR Spectrum of Compound **43n**

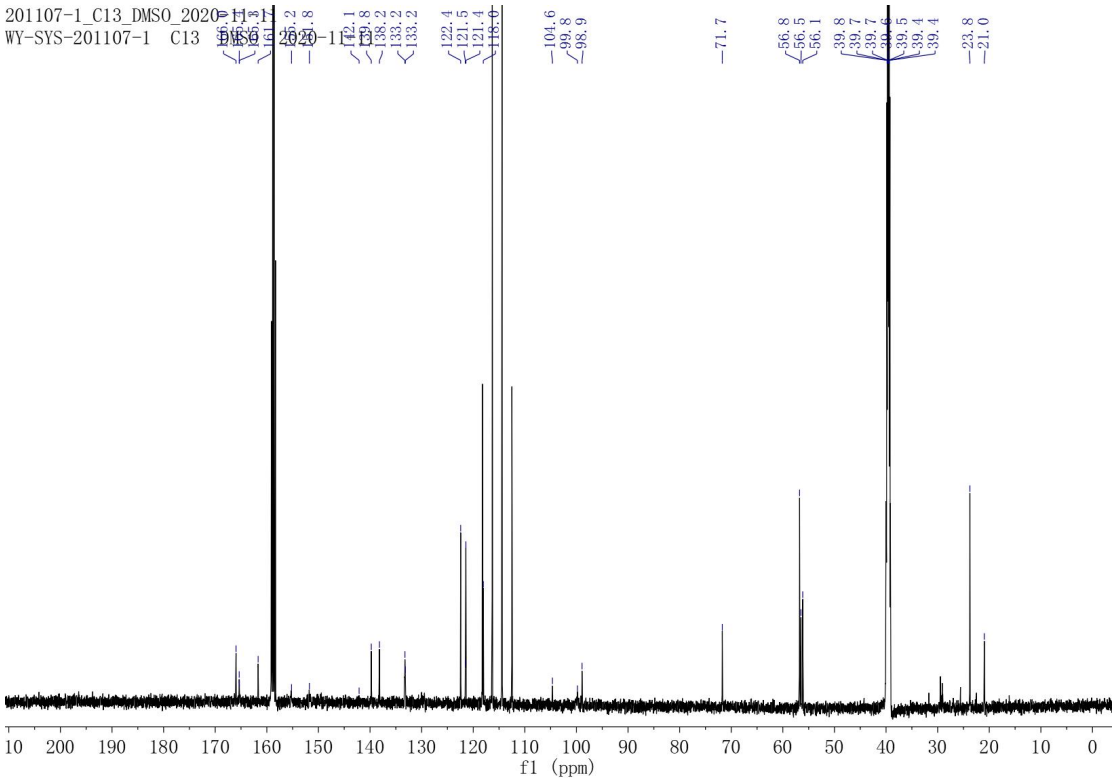


^{13}C NMR Spectrum of Compound **43n**

43o

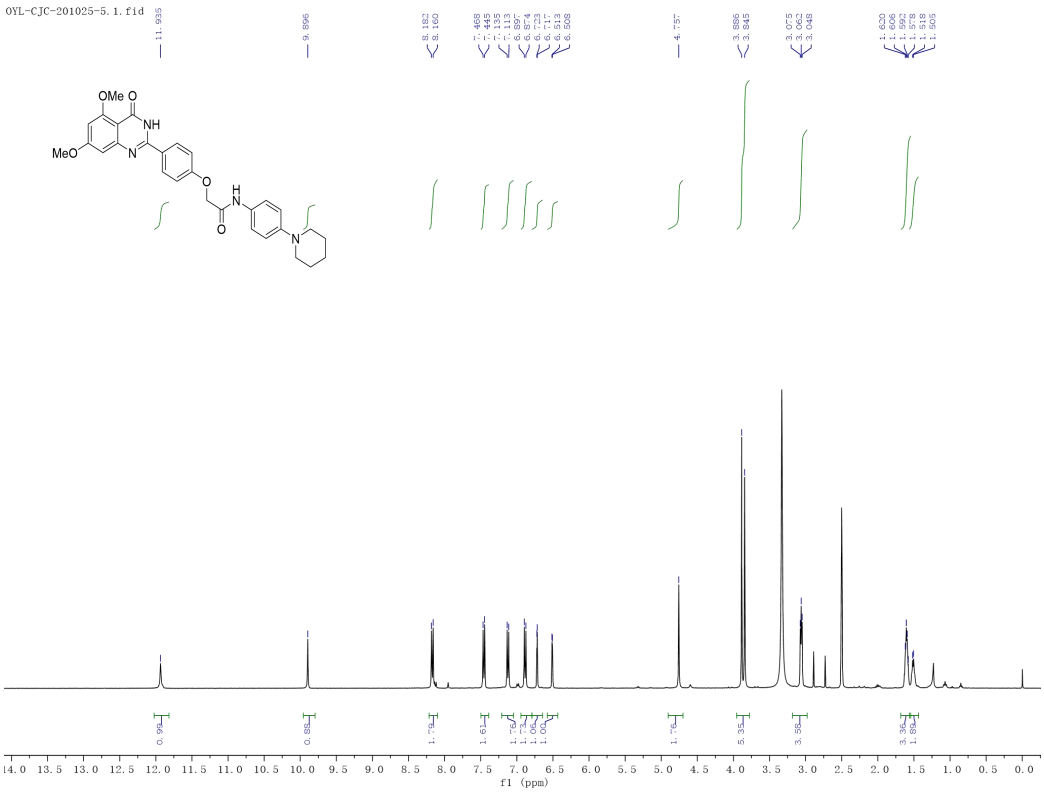


^{1}H NMR Spectrum of Compound **43o**

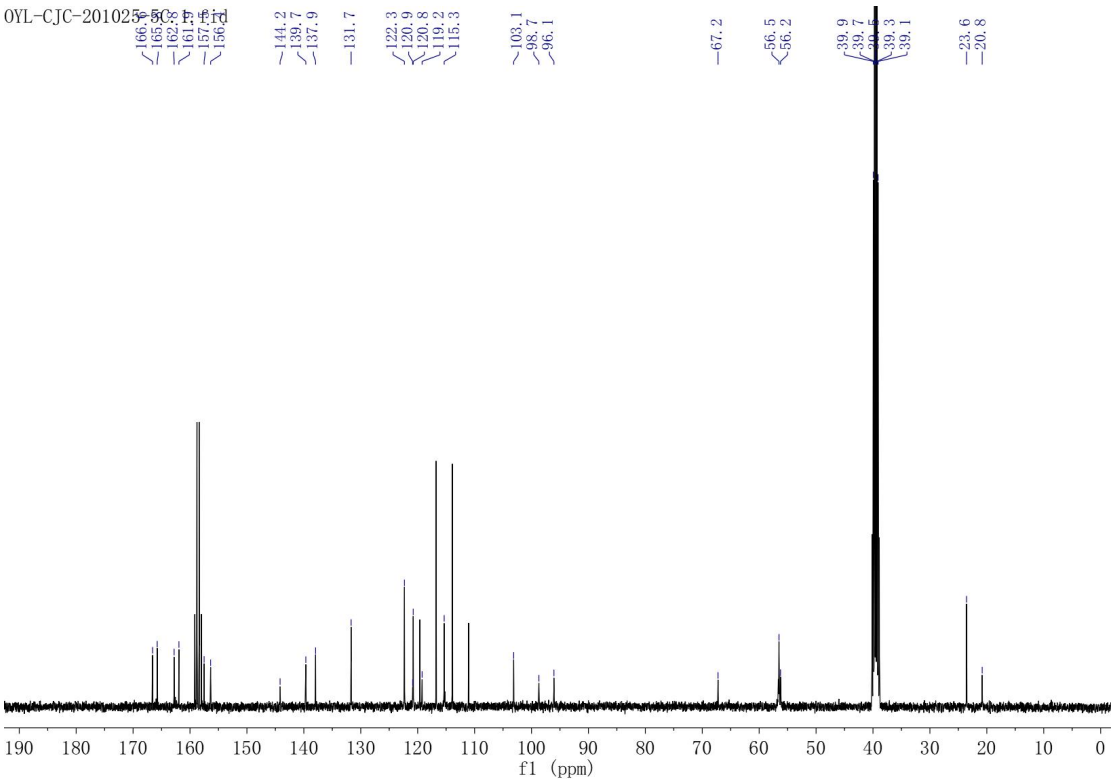


^{13}C NMR Spectrum of Compound **43o**

43p

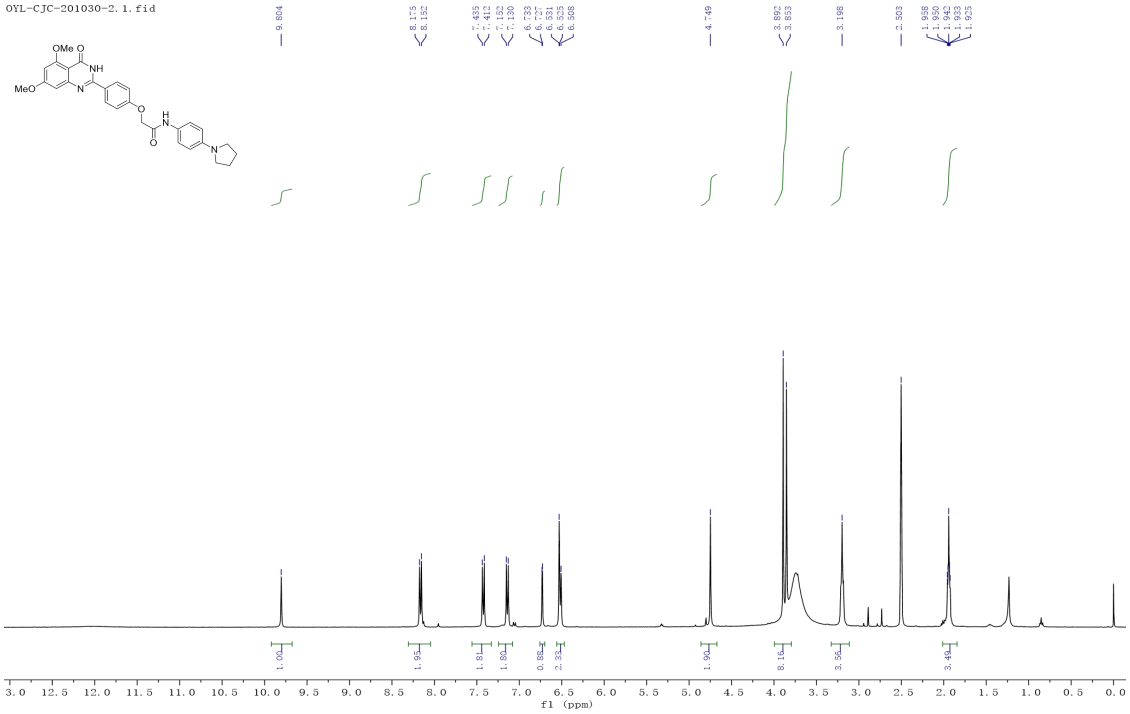


^{1}H NMR Spectrum of Compound **43p**

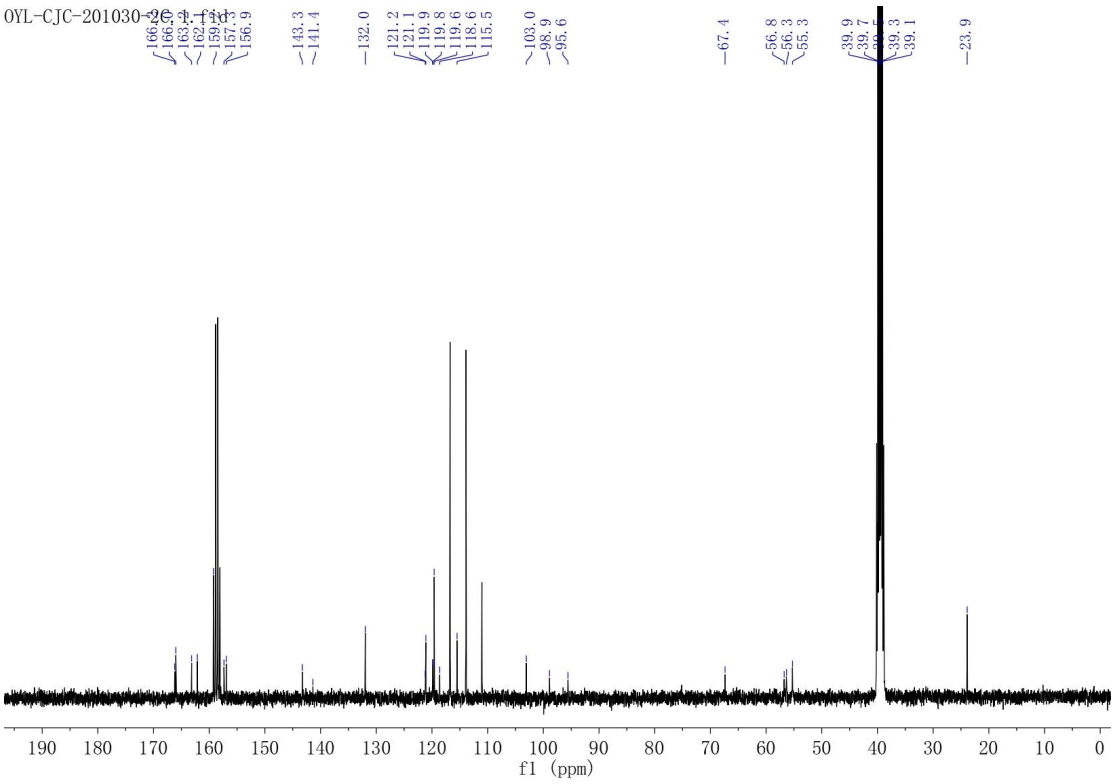


^{13}C NMR Spectrum of Compound **43p**

43q

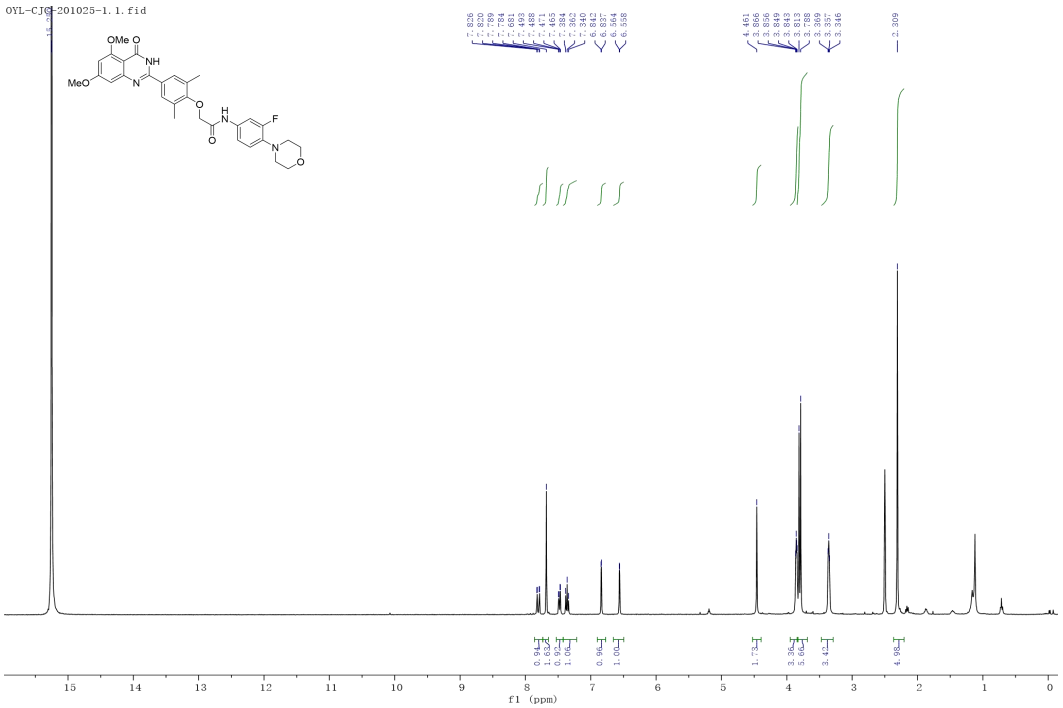


^{1}H NMR Spectrum of Compound **43q**

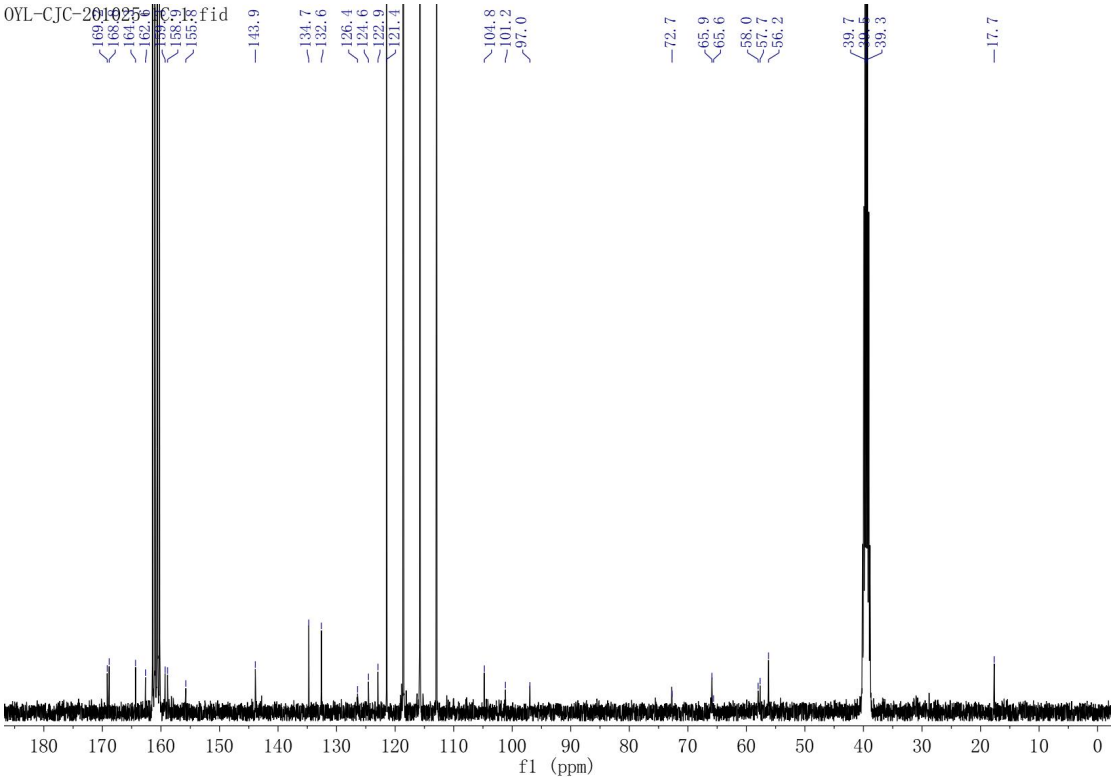


^{13}C NMR Spectrum of Compound **43q**

44a

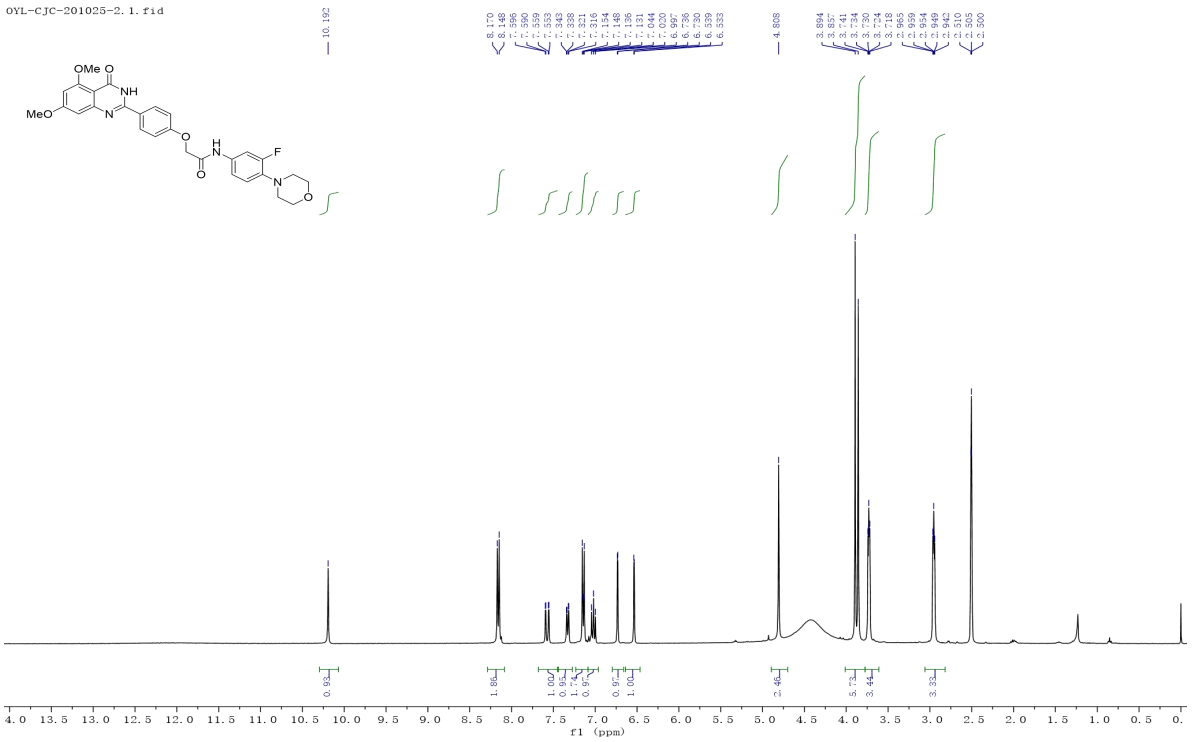


^{1}H NMR Spectrum of Compound **44a**

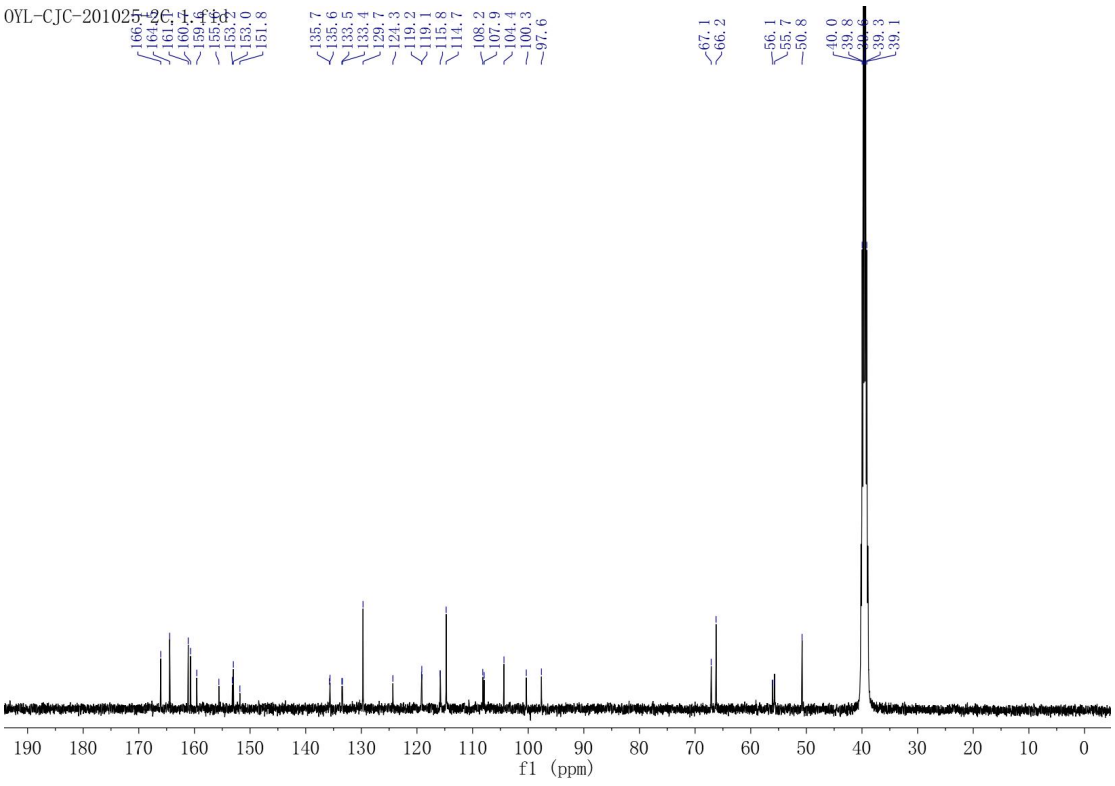


^{13}C NMR Spectrum of Compound **44a**

44b

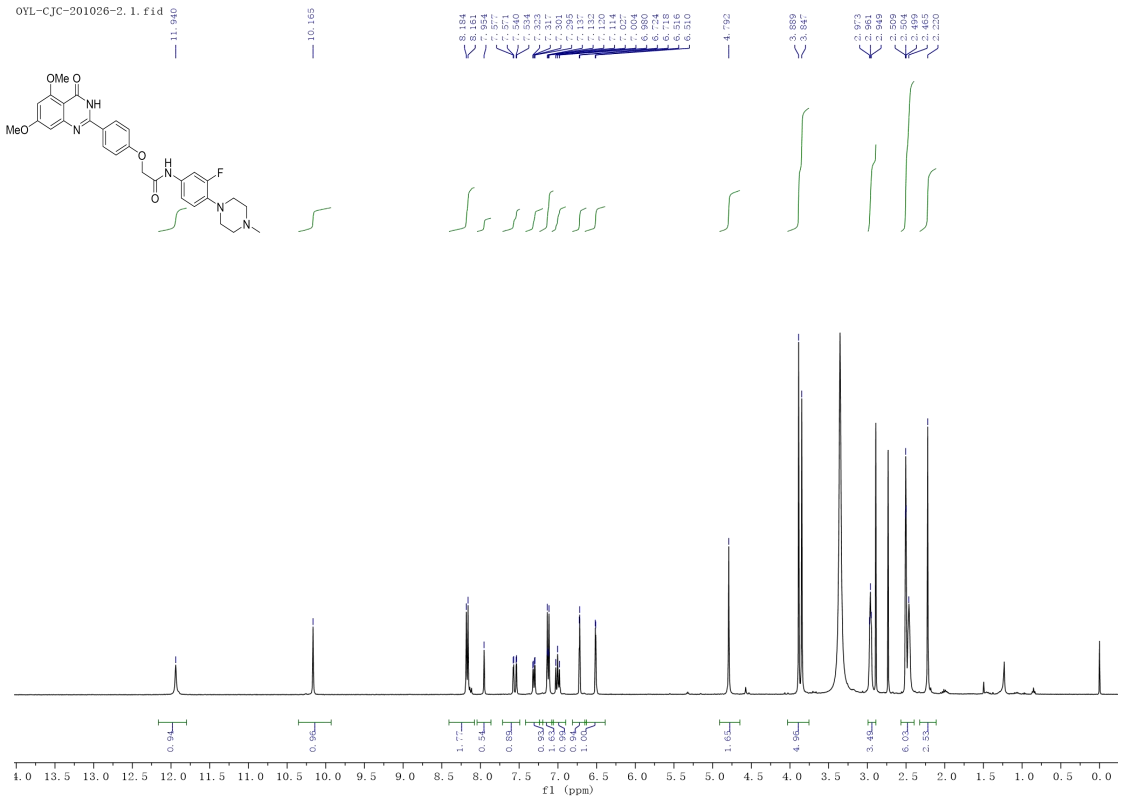


^{1}H NMR Spectrum of Compound **44b**

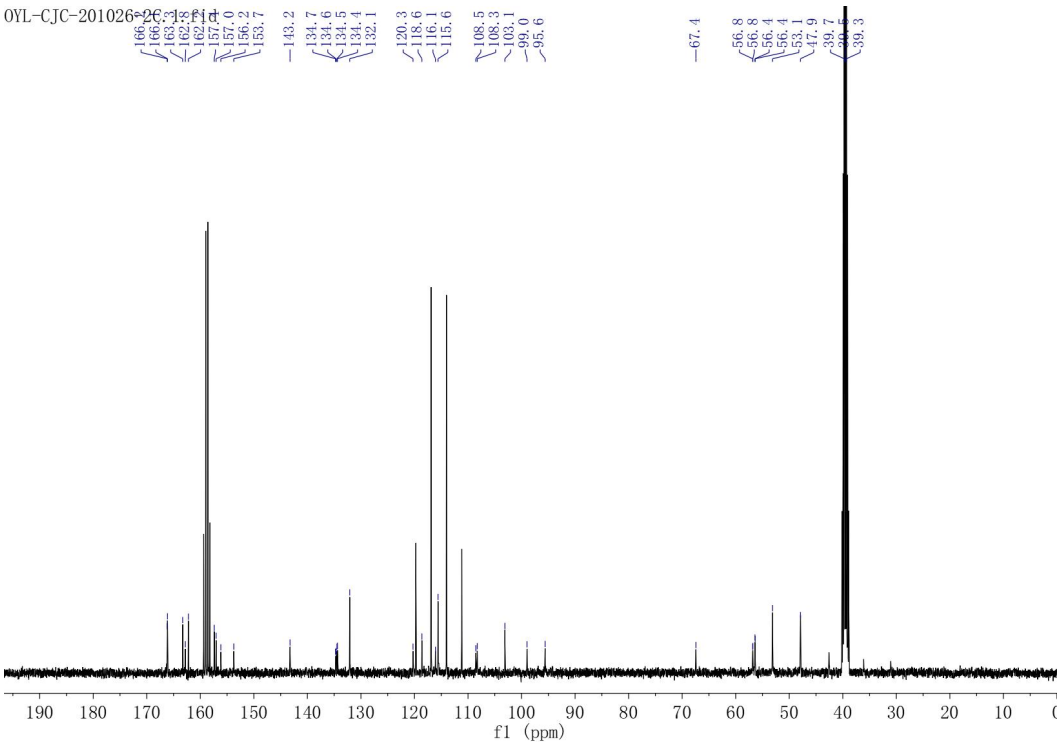


^{13}C NMR Spectrum of Compound **44b**

44c

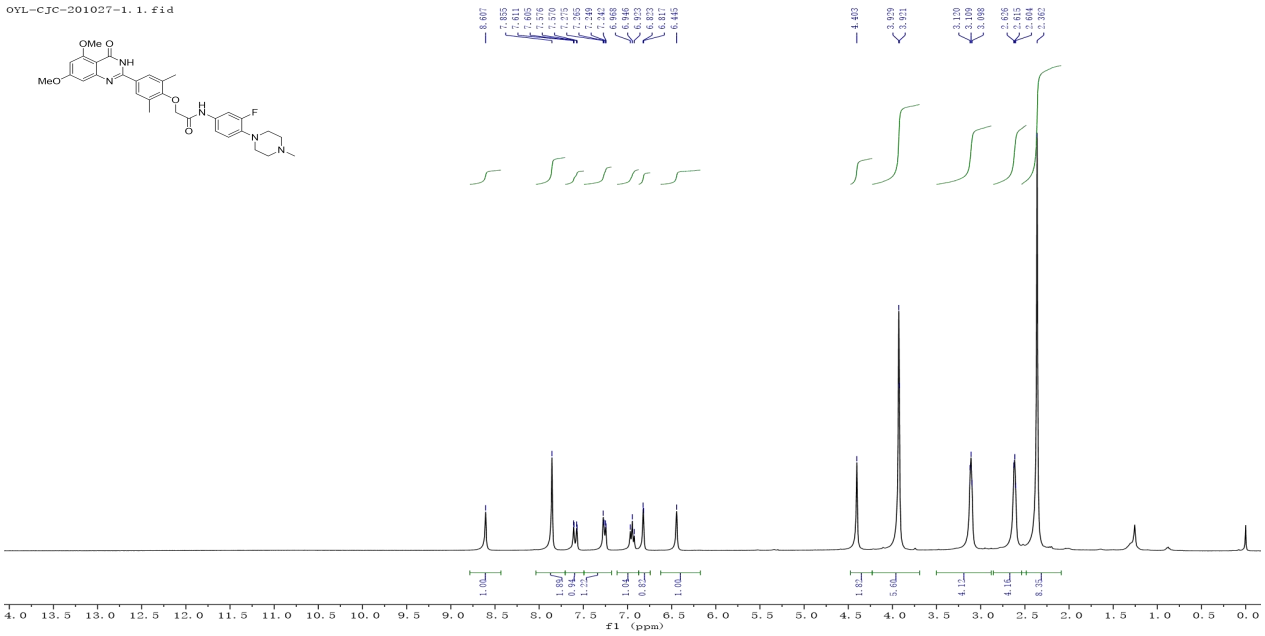


^{1}H NMR Spectrum of Compound **44c**

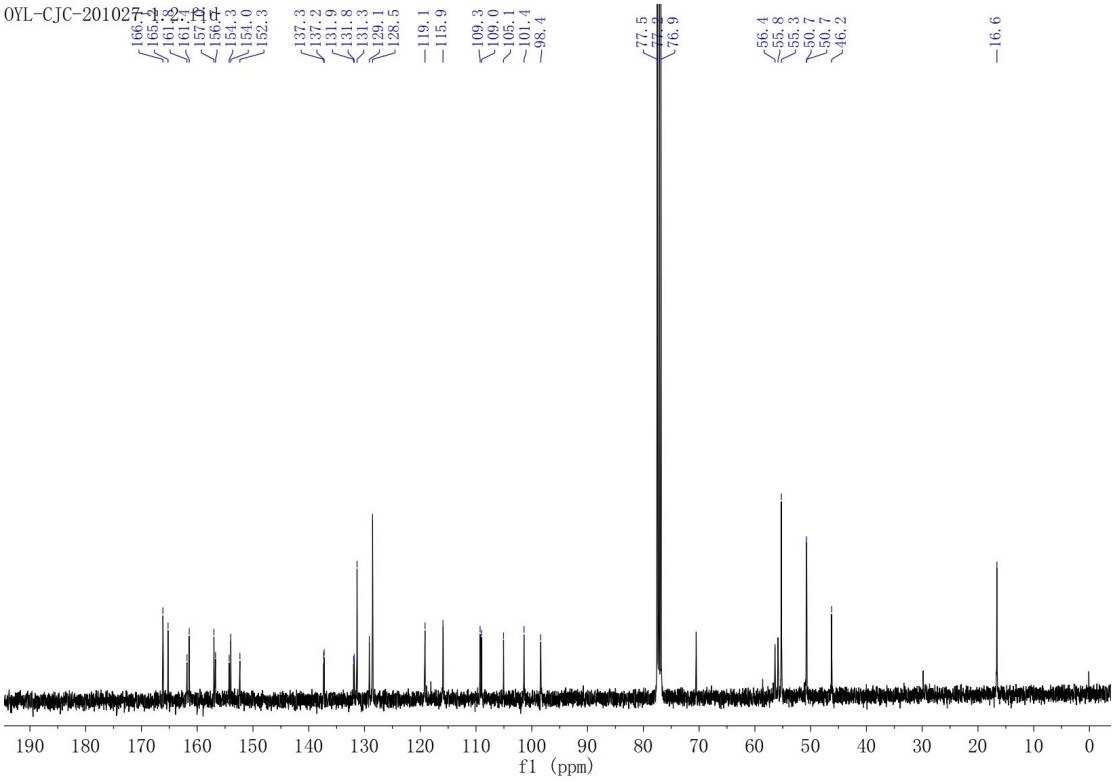


^{13}C NMR Spectrum of Compound **44c**

44d

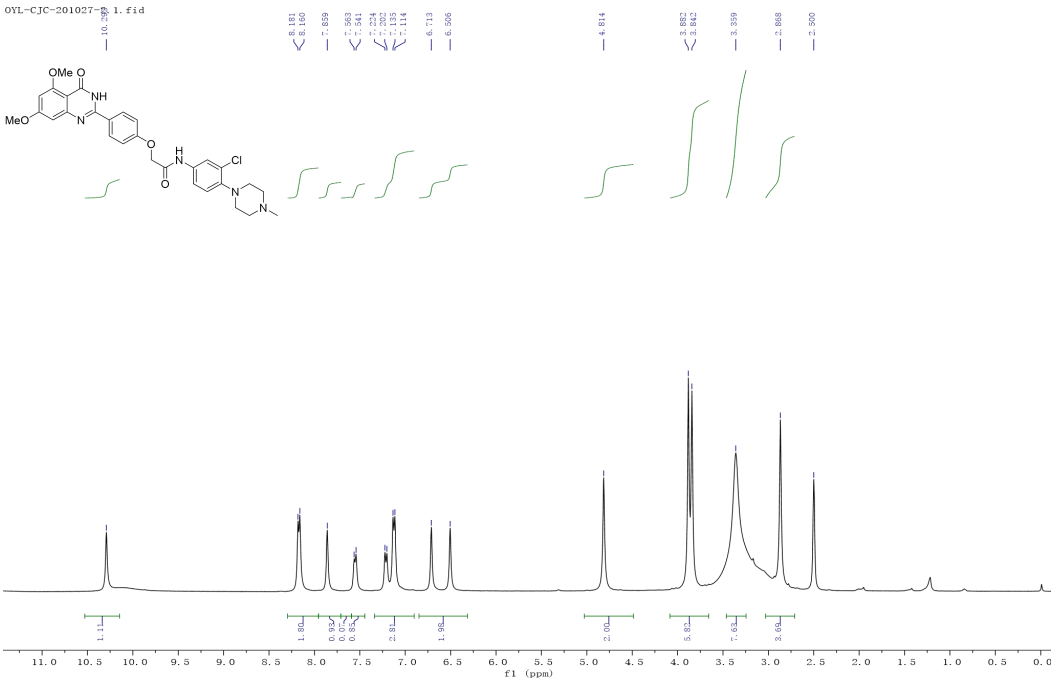


^{1}H NMR Spectrum of Compound **44d**

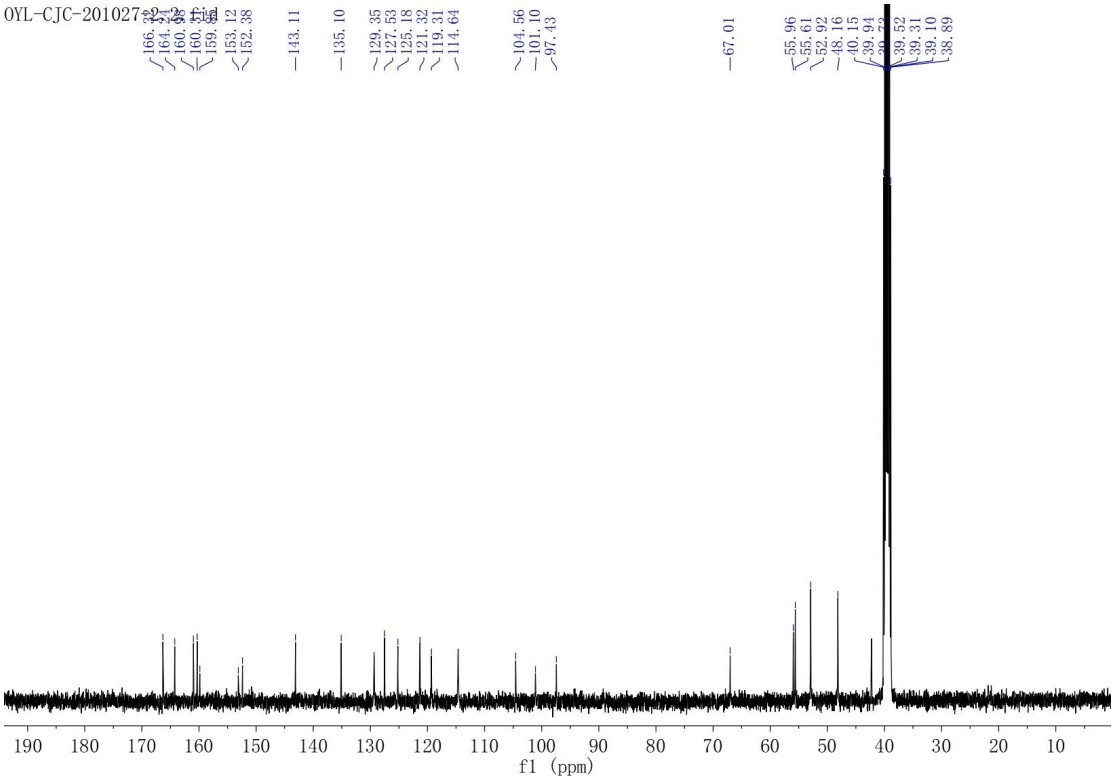


^{13}C NMR Spectrum of Compound **44d**

44e

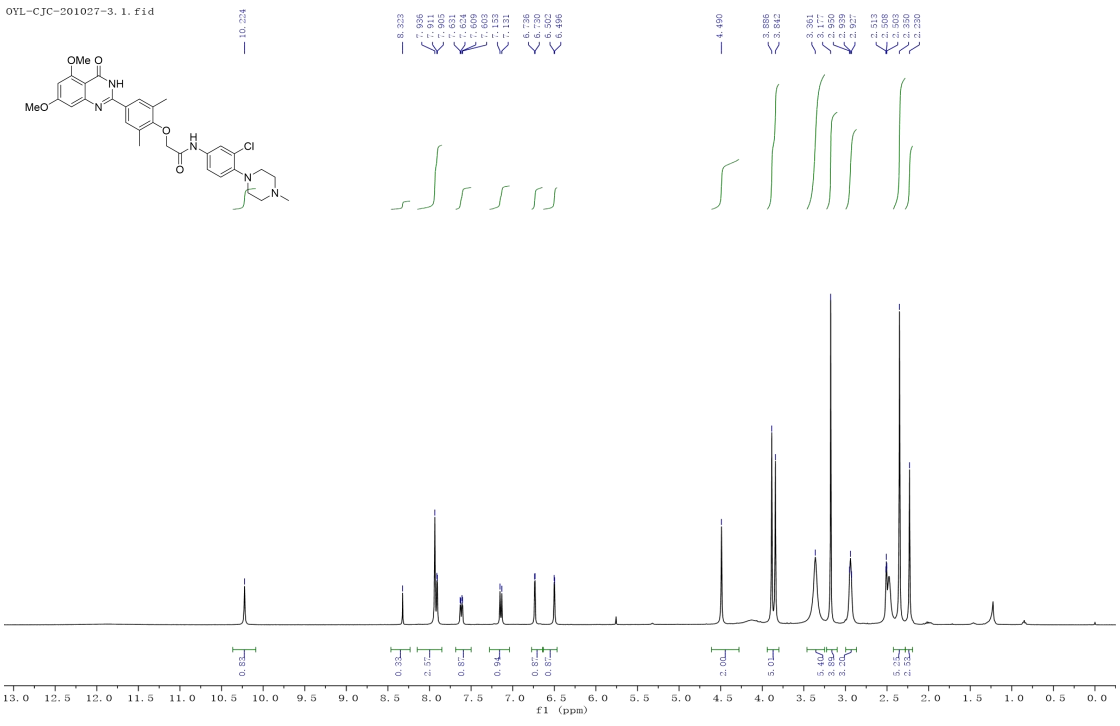


^{1}H NMR Spectrum of Compound **44e**

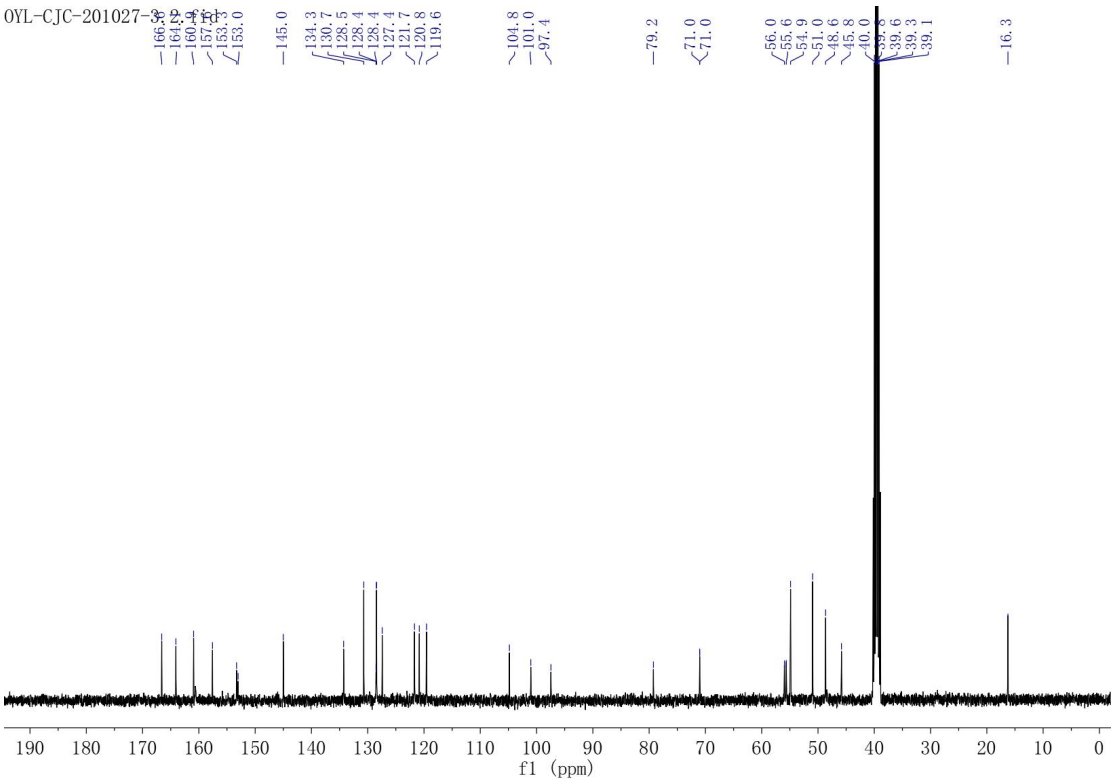


^{13}C NMR Spectrum of Compound **44e**

44f

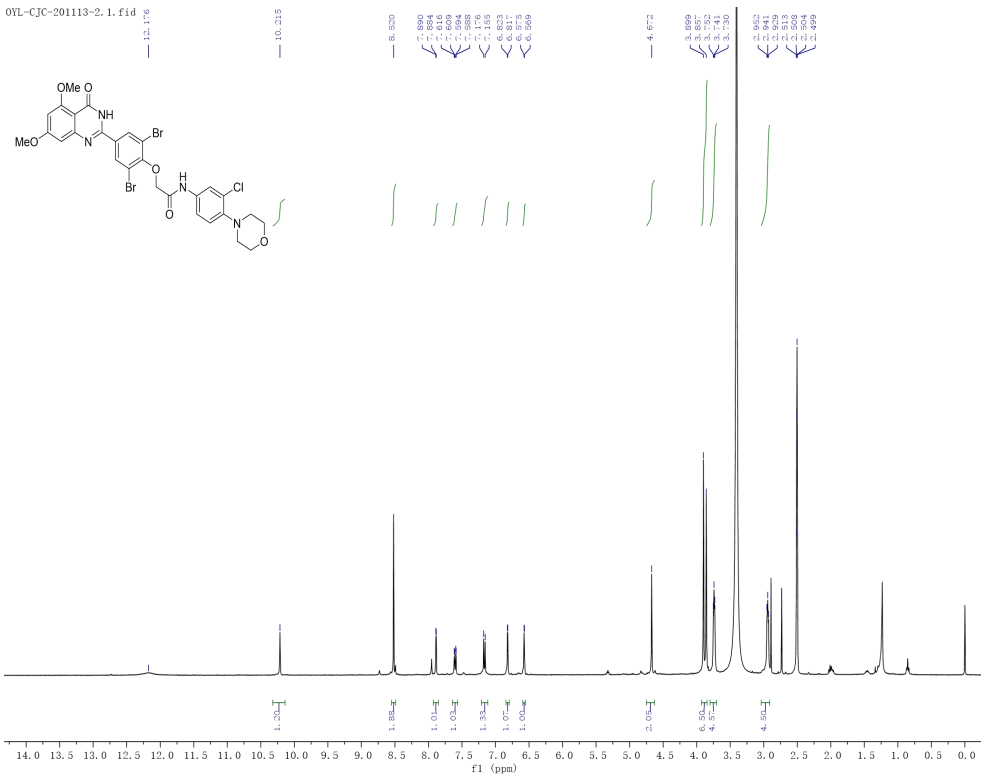


^{1}H NMR Spectrum of Compound **44f**

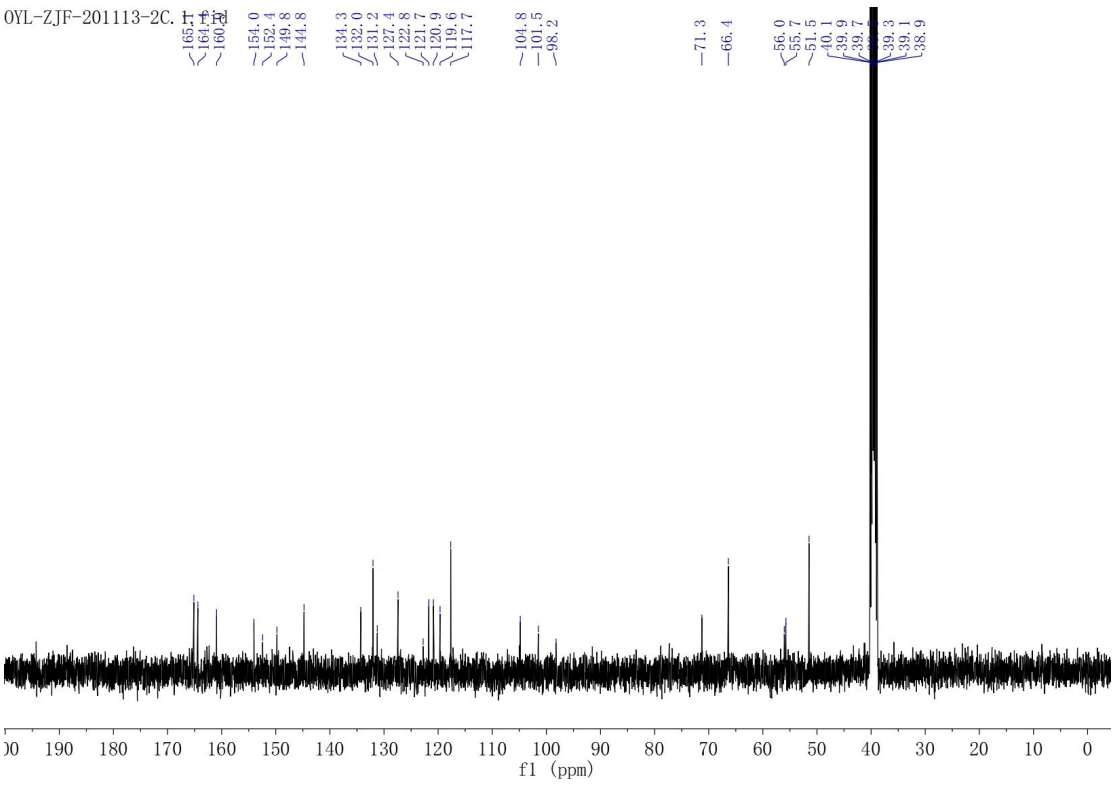


^{13}C NMR Spectrum of Compound **44f**

44g

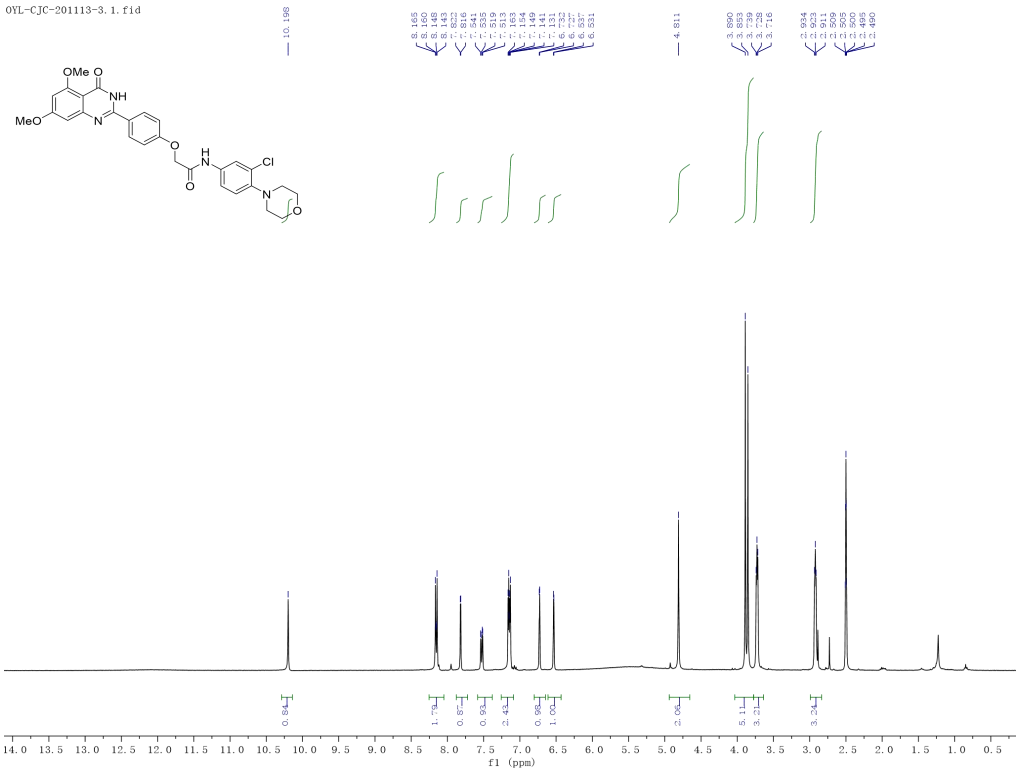


^{1}H NMR Spectrum of Compound **44g**

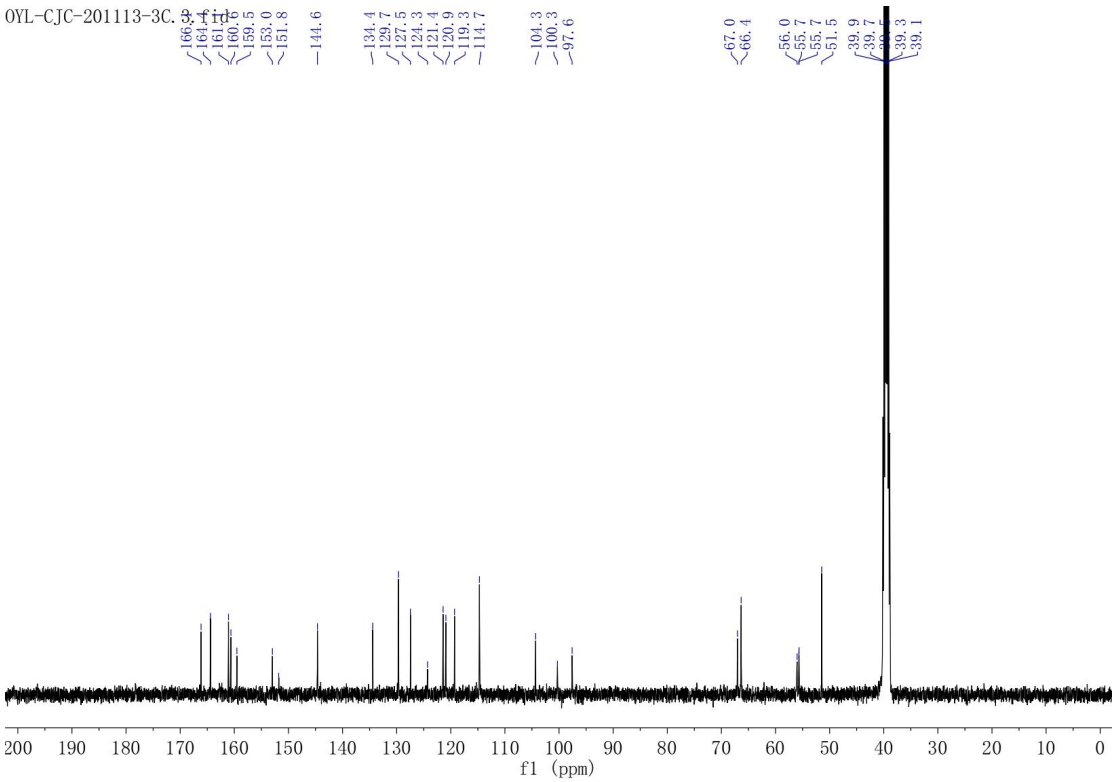


^{13}C NMR Spectrum of Compound **44g**

44h

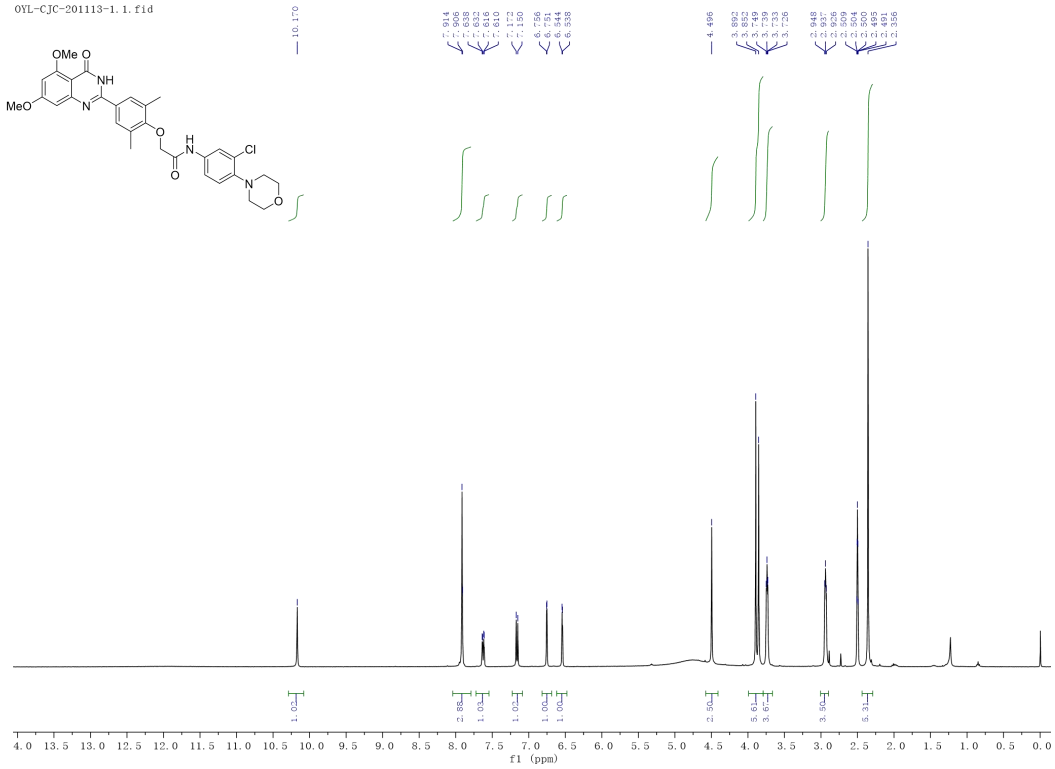


^{1}H NMR Spectrum of Compound **44h**

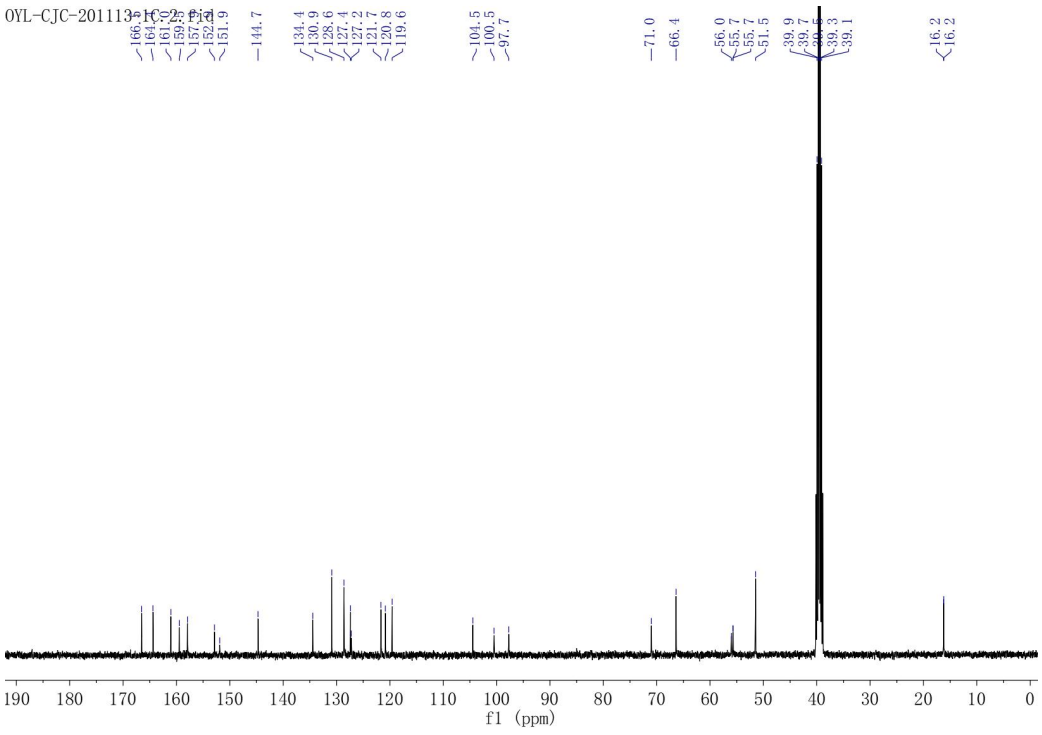


^{13}C NMR Spectrum of Compound **44h**

44i

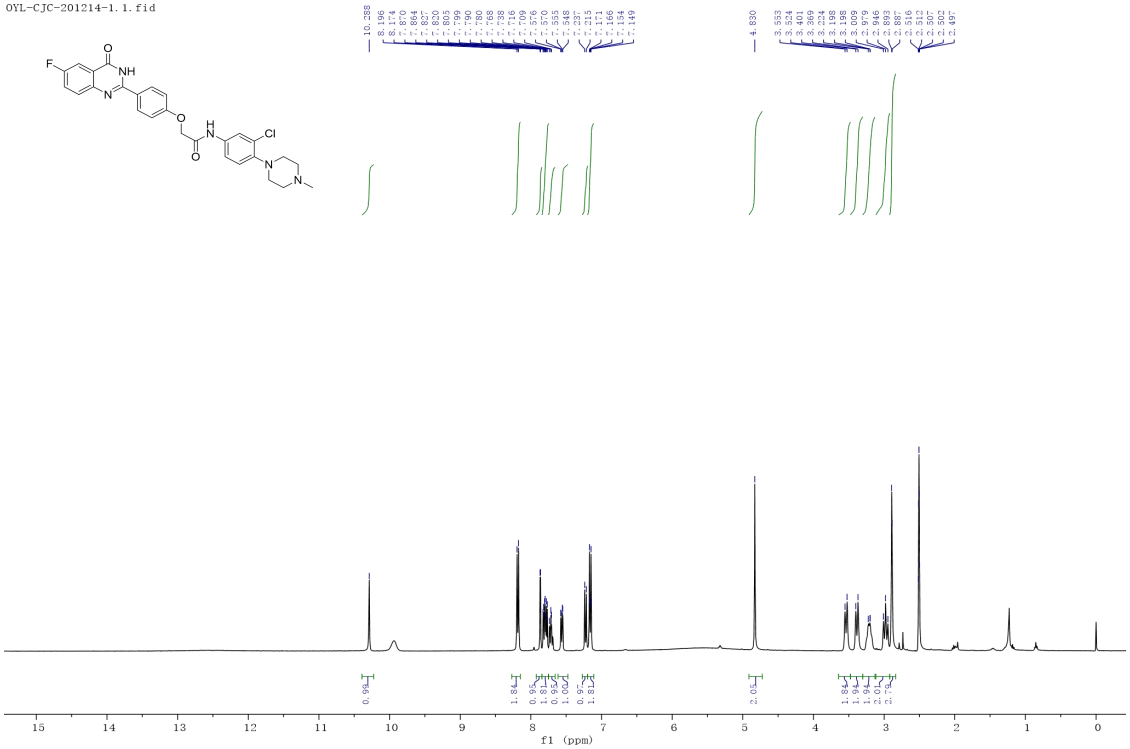


^{1}H NMR Spectrum of Compound **44i**

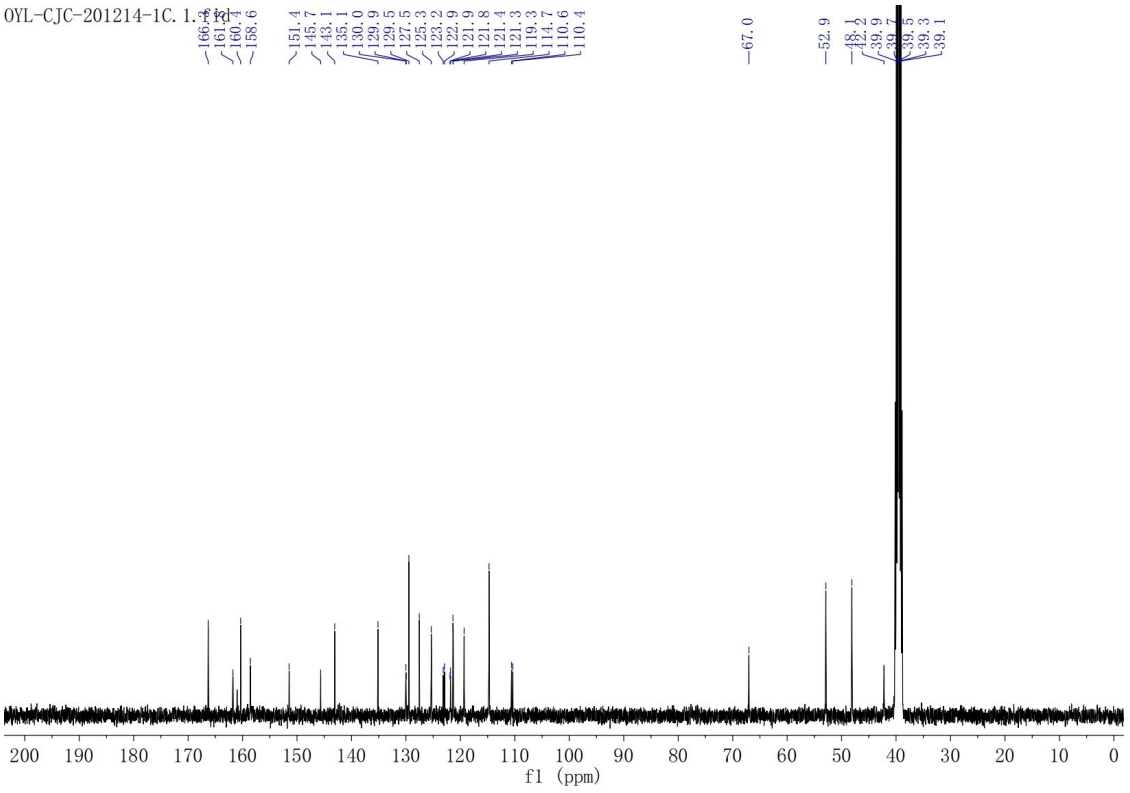


^{13}C NMR Spectrum of Compound **44i**

44j

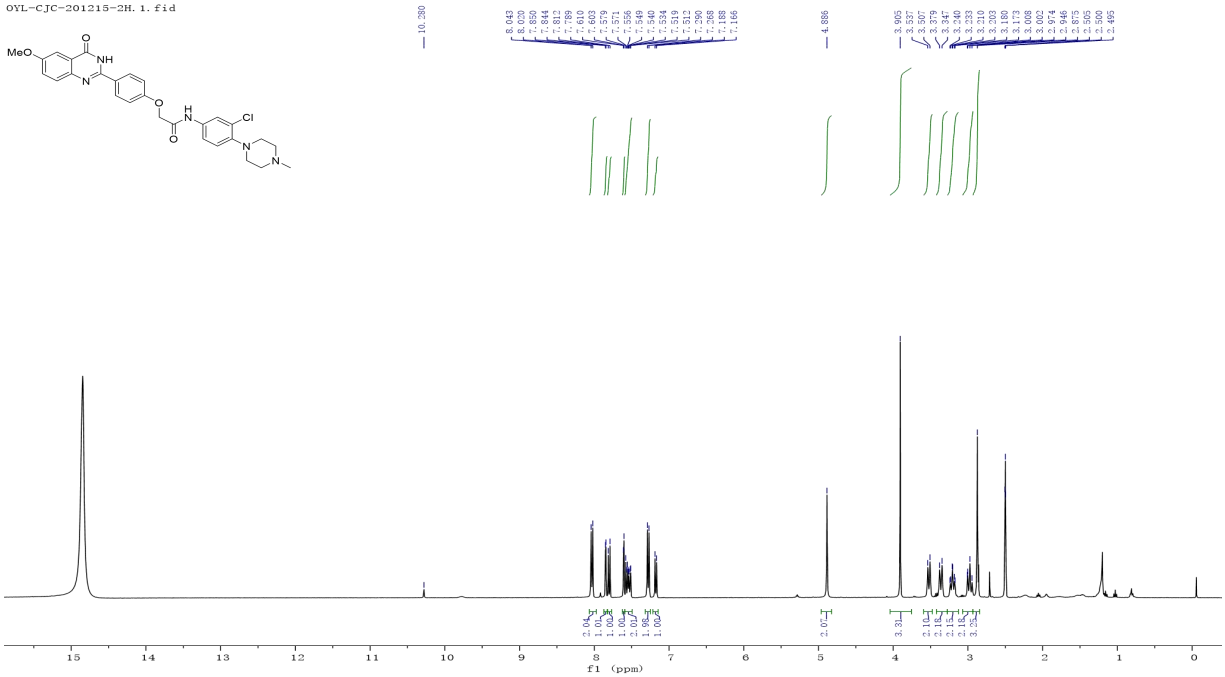


^{1}H NMR Spectrum of Compound **44j**

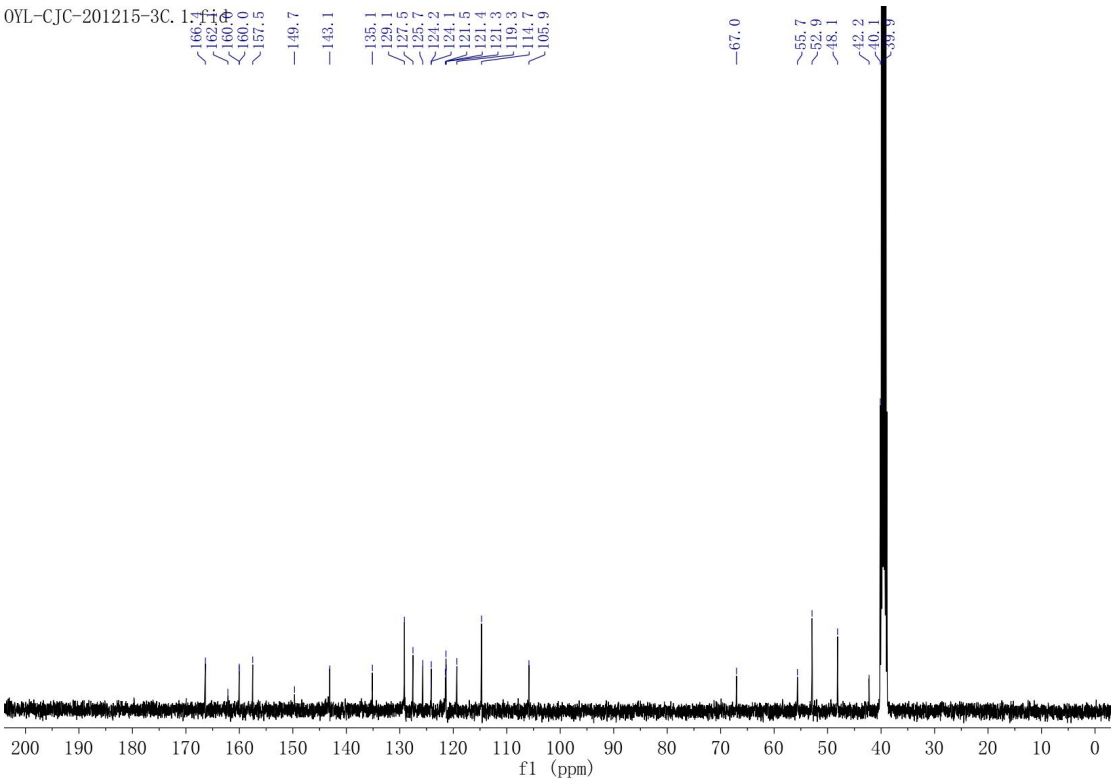


^{13}C NMR Spectrum of Compound **44j**

44k

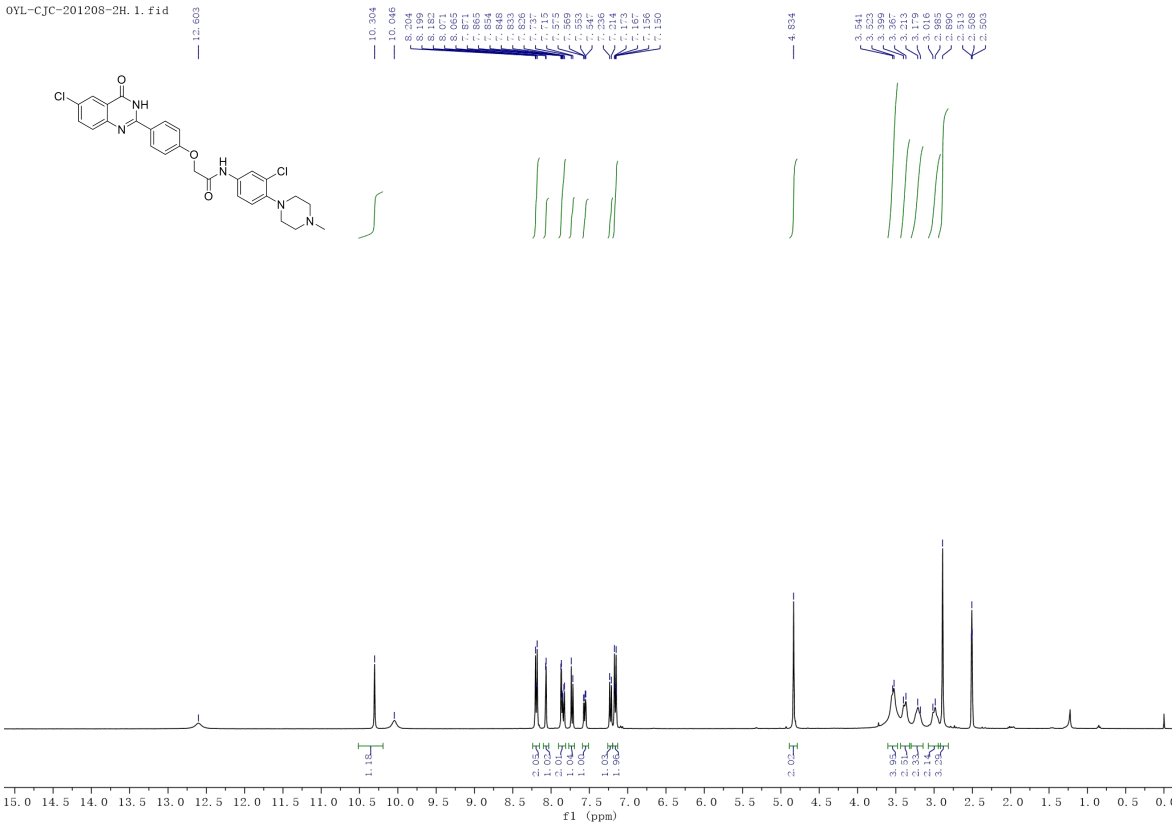


^{1}H NMR Spectrum of Compound **44k**

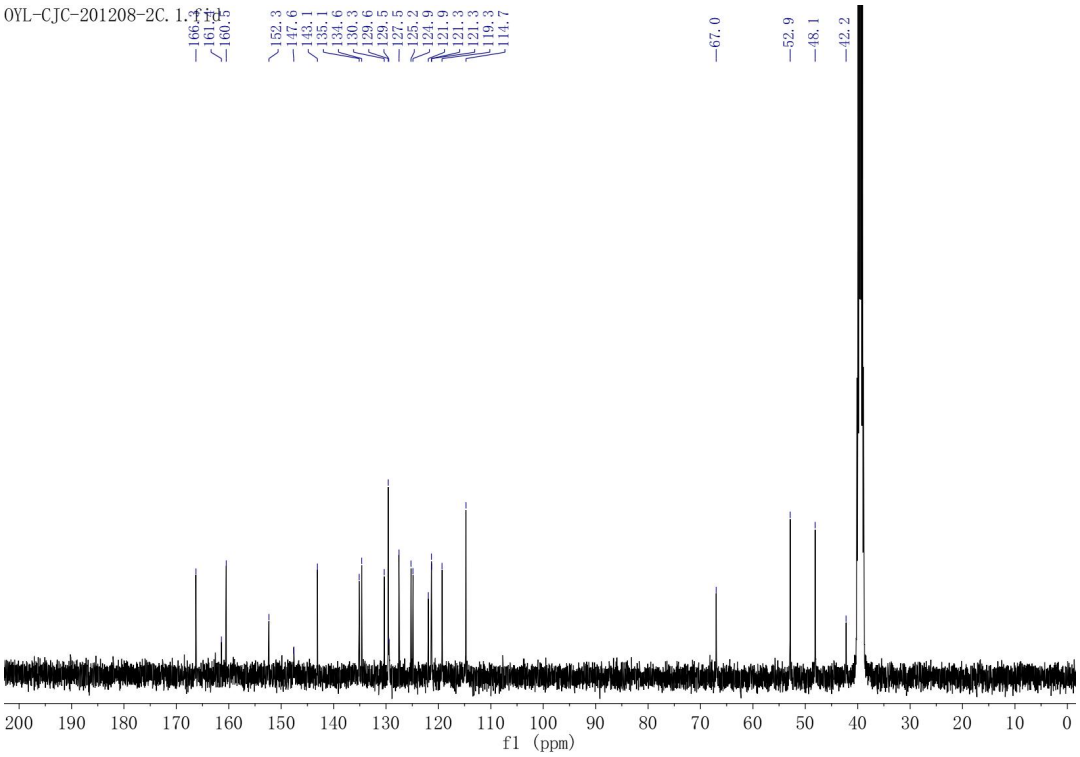


^{13}C NMR Spectrum of Compound **44k**

44l

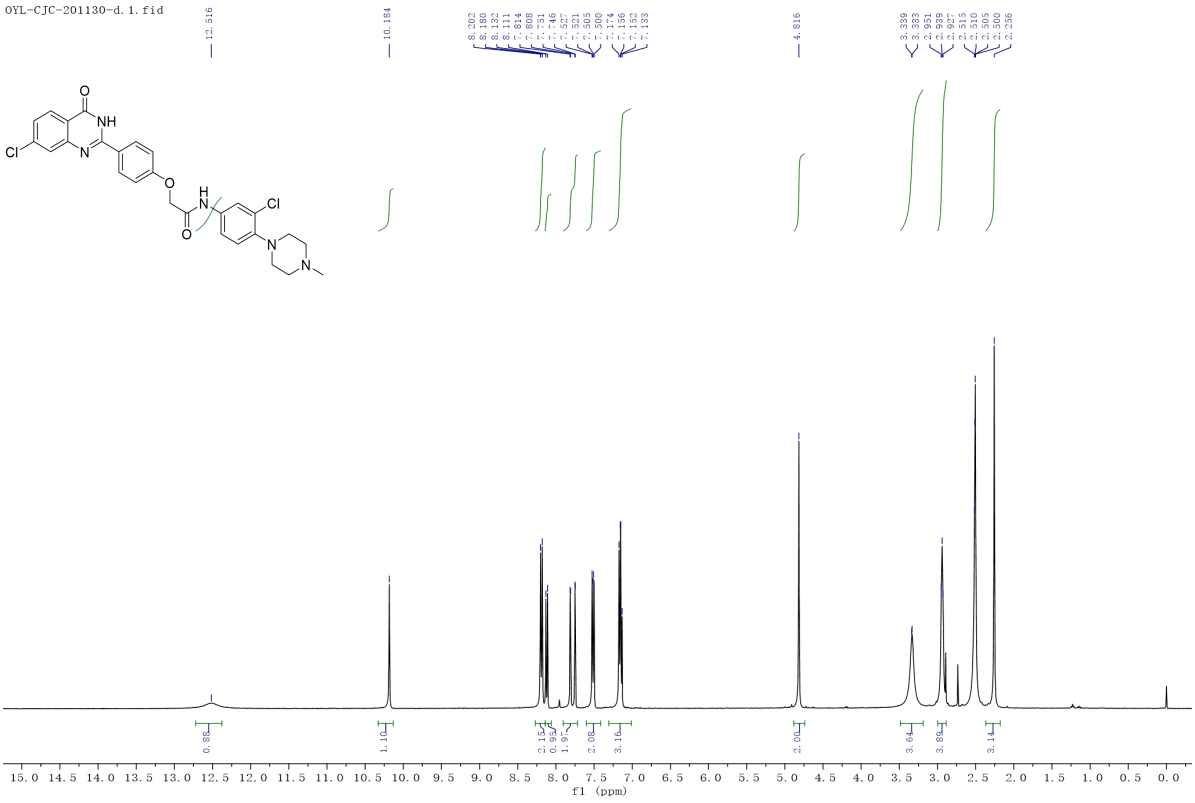


^{1}H NMR Spectrum of Compound **44l**

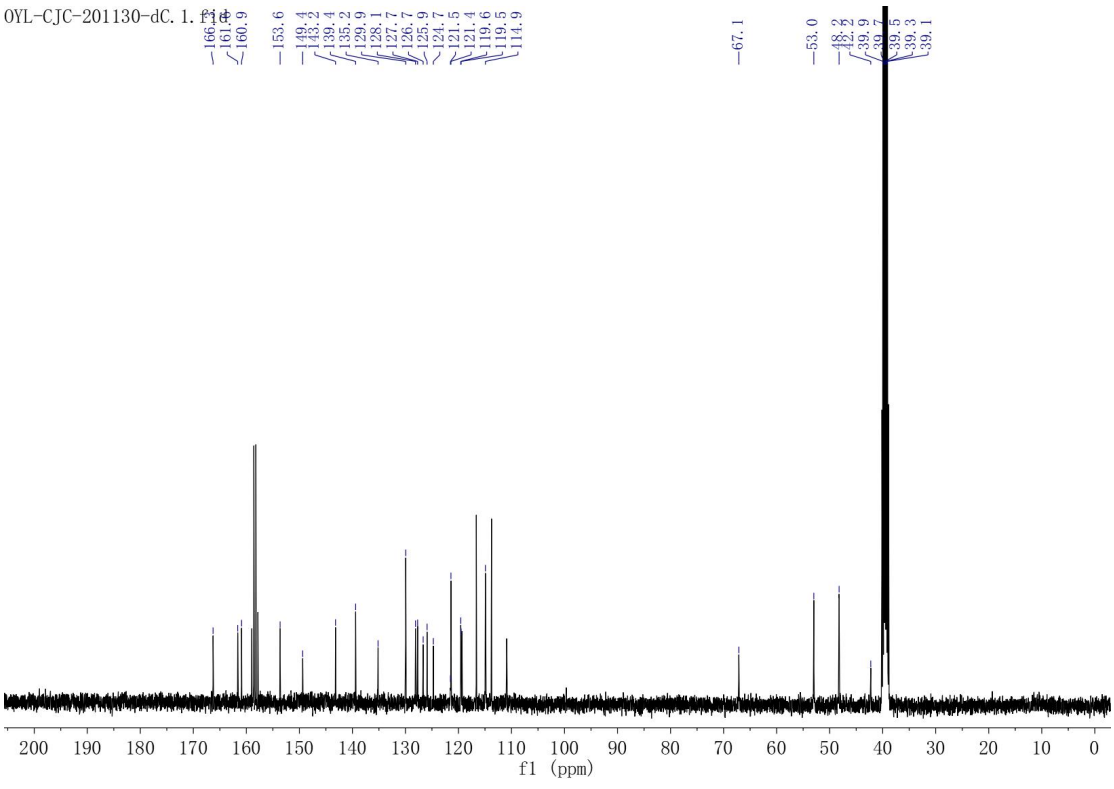


^{13}C NMR Spectrum of Compound **44l**

44m

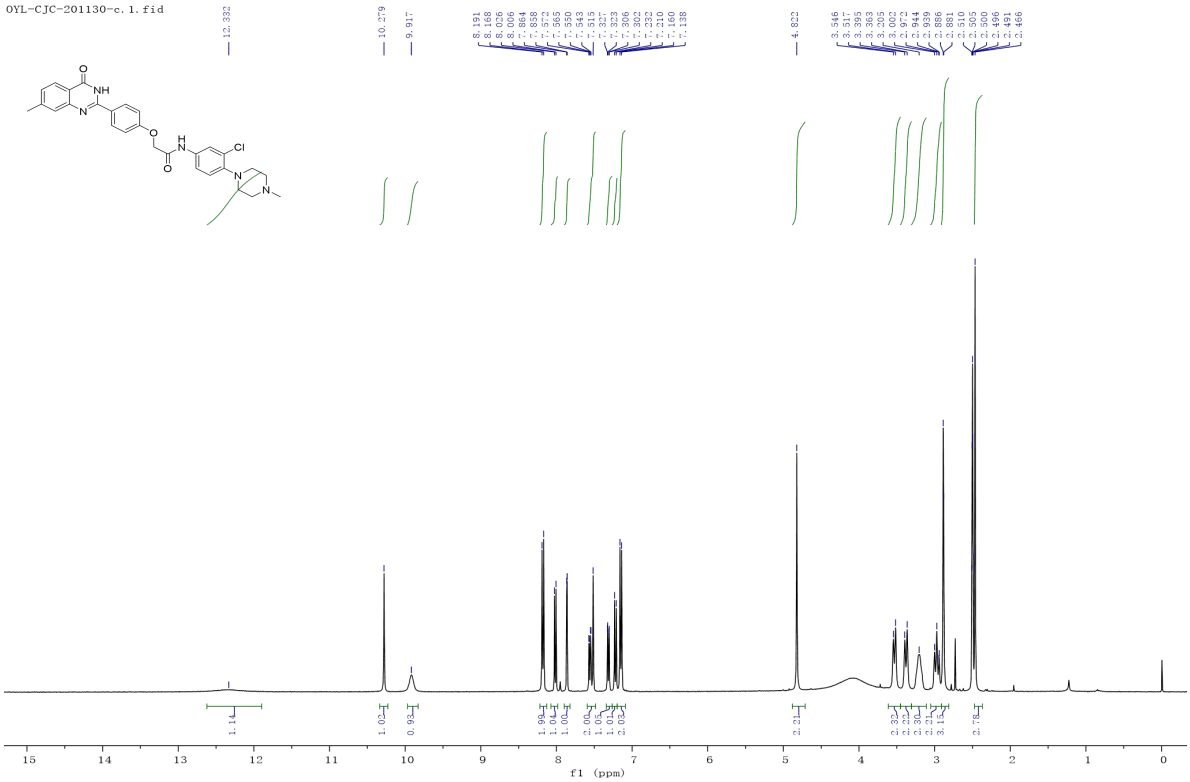


^{1}H NMR Spectrum of Compound **44m**

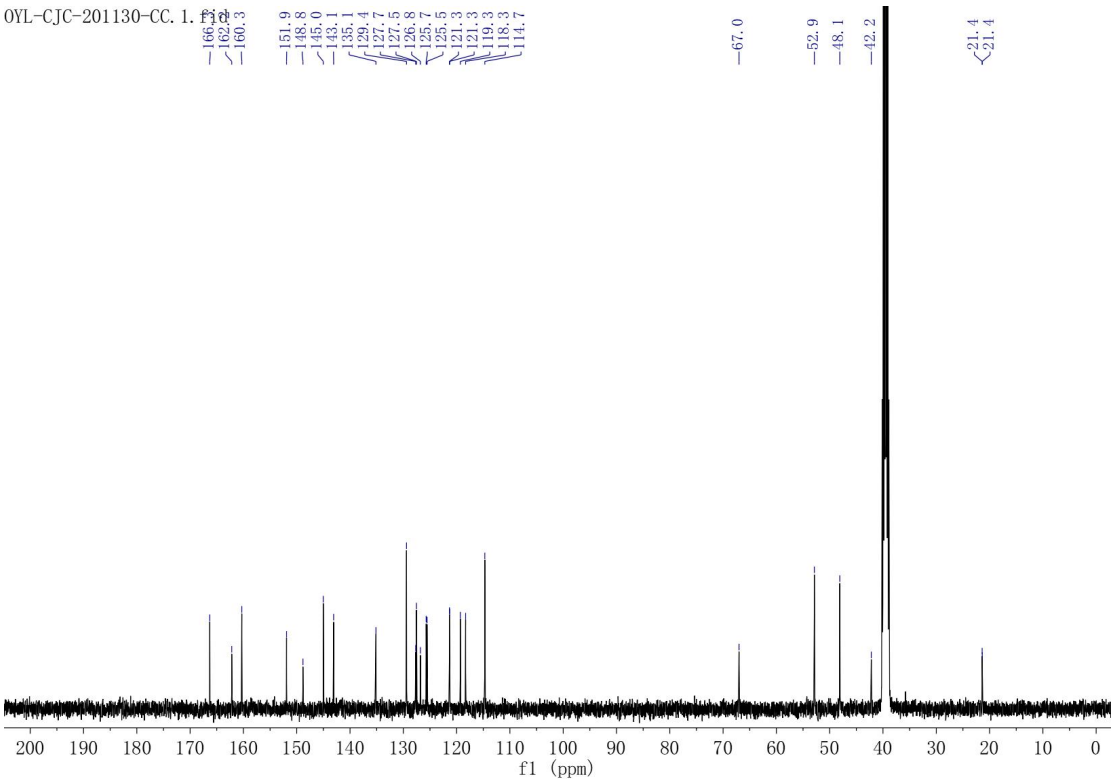


^{13}C NMR Spectrum of Compound **44m**

44n



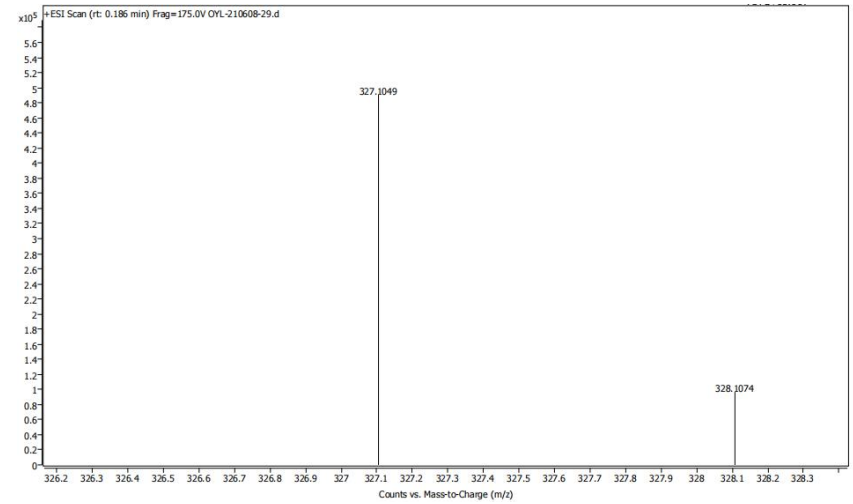
^{1}H NMR Spectrum of Compound **44n**



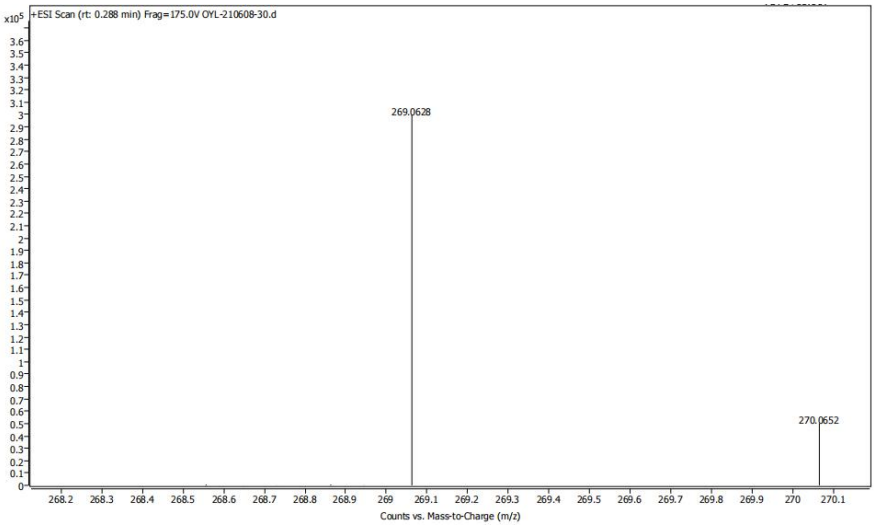
^{13}C NMR Spectrum of Compound **44n**

3. MS data

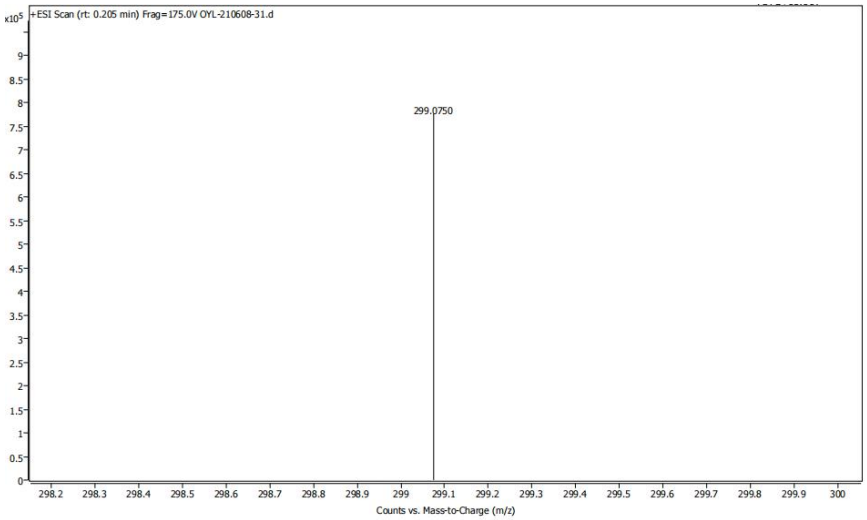
34a



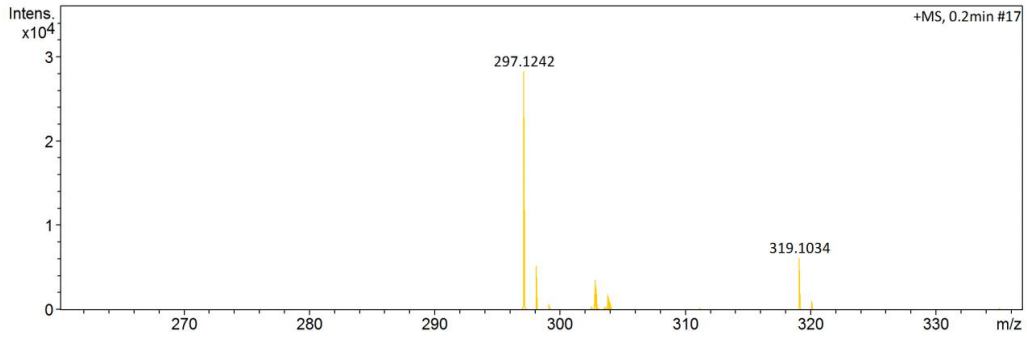
34b



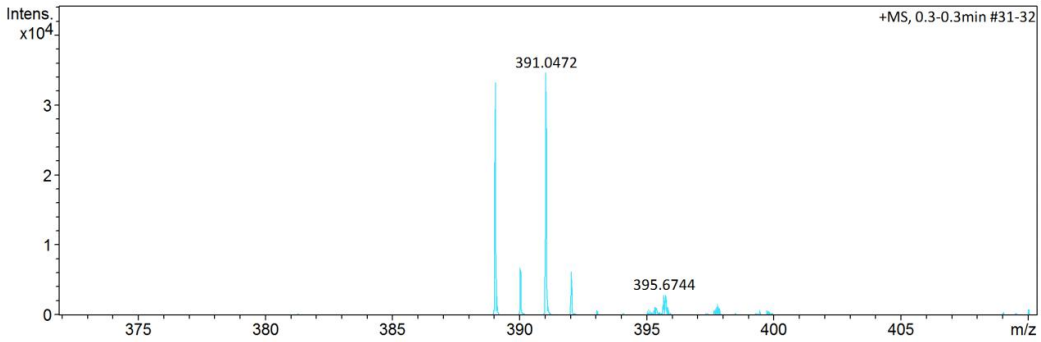
34c



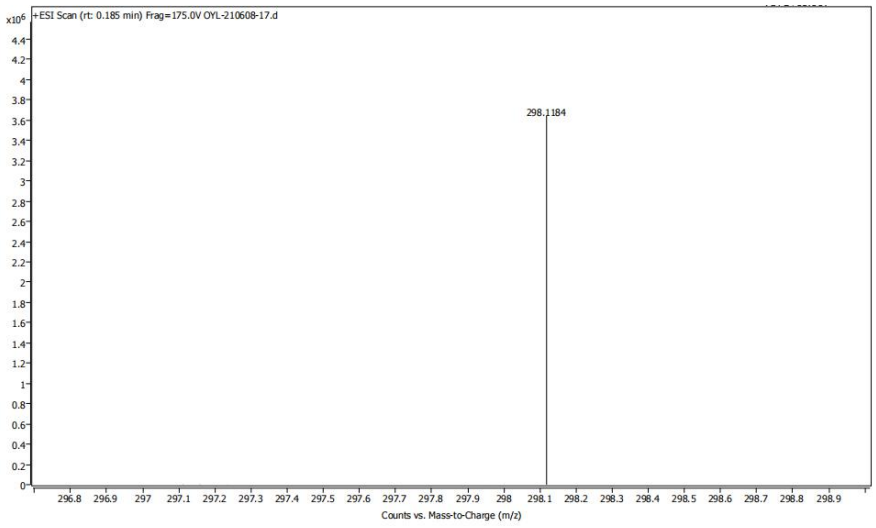
38a



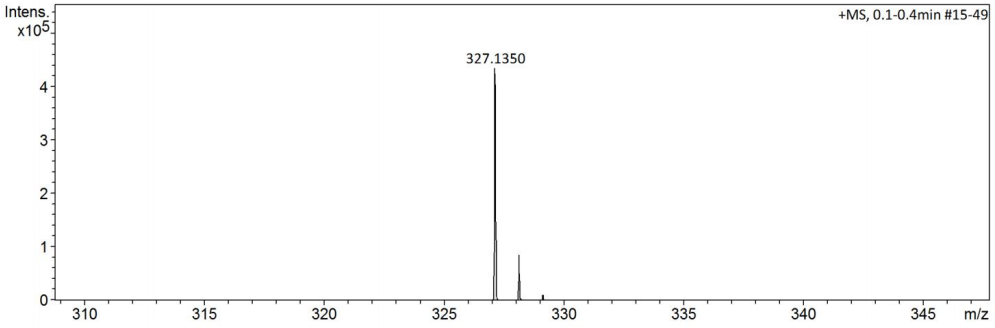
38b



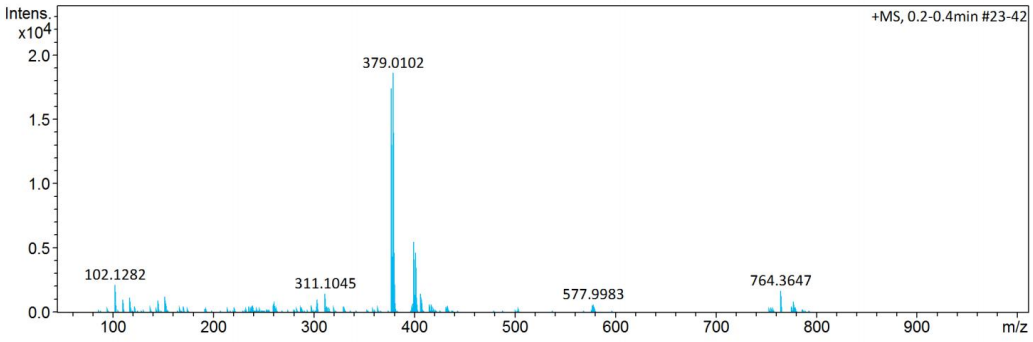
38c



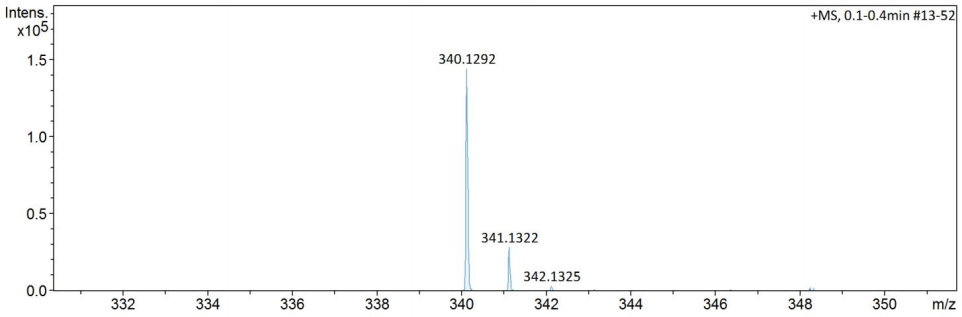
38d



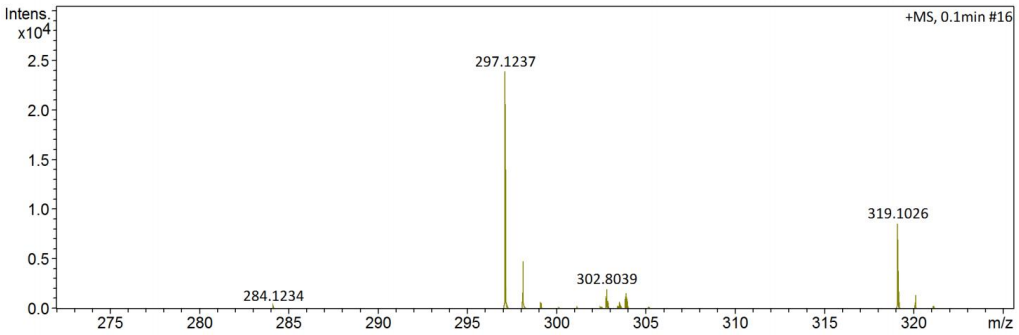
38e



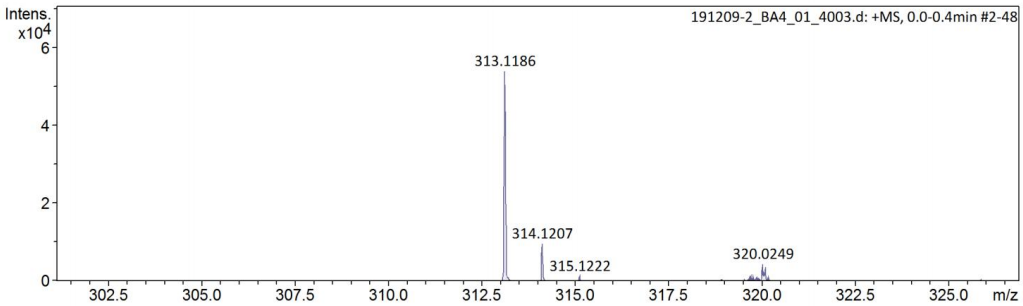
38f



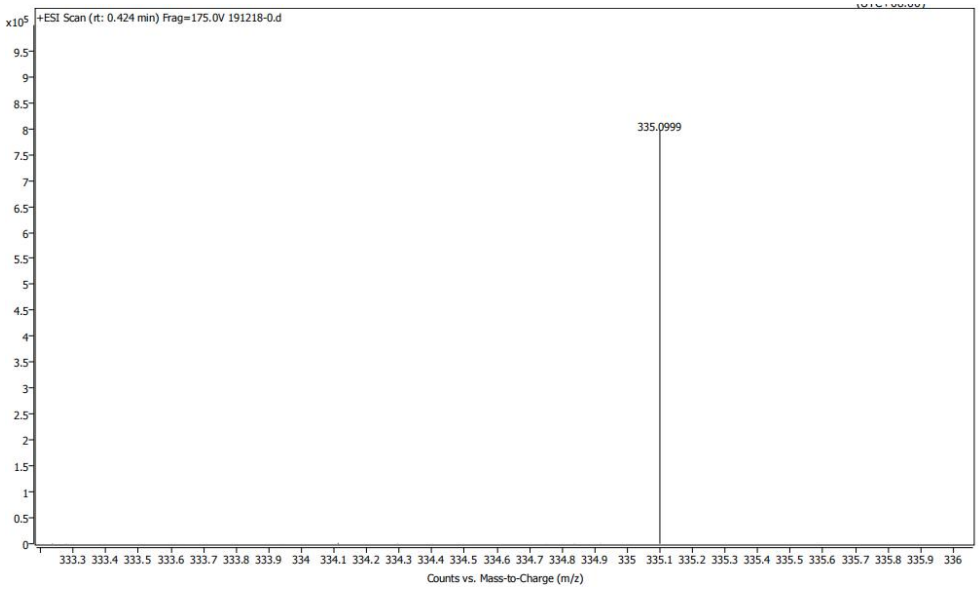
38g



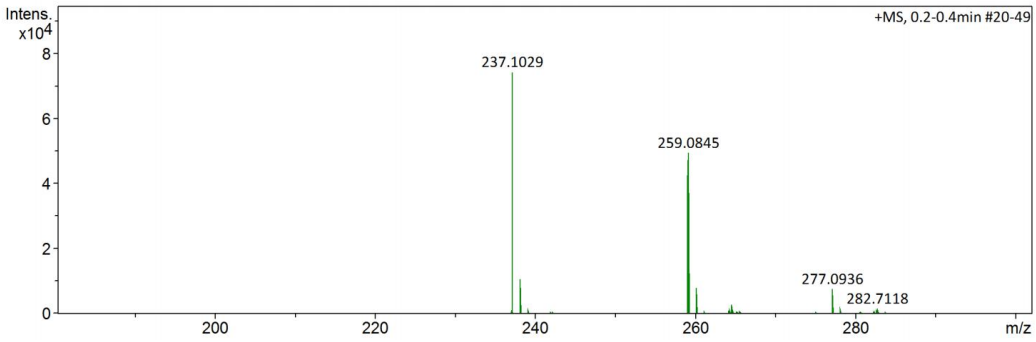
38h



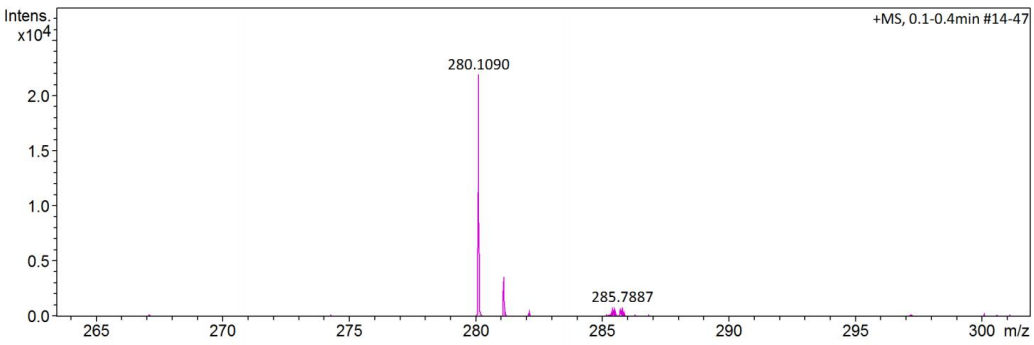
38i



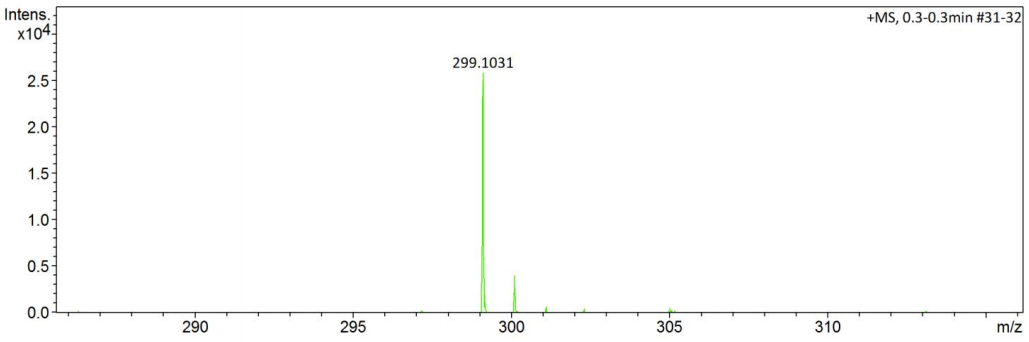
38j



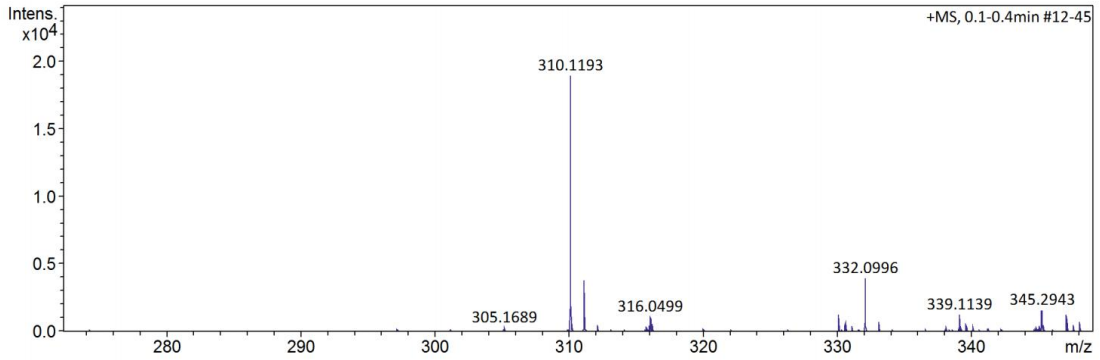
38k



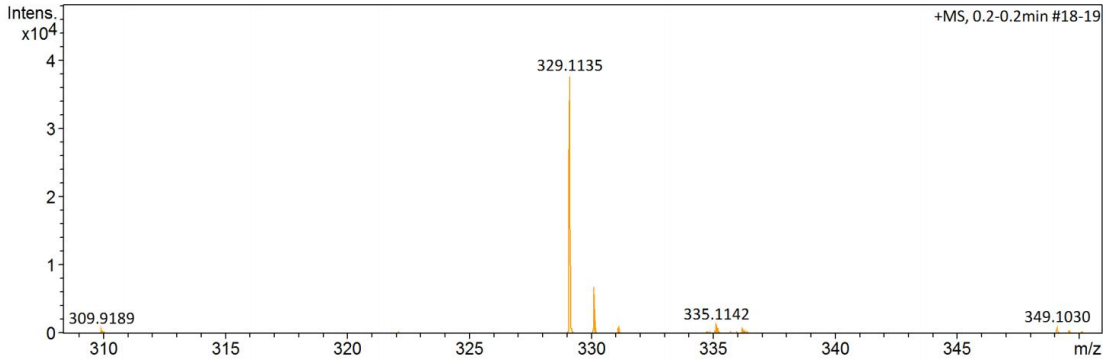
38l



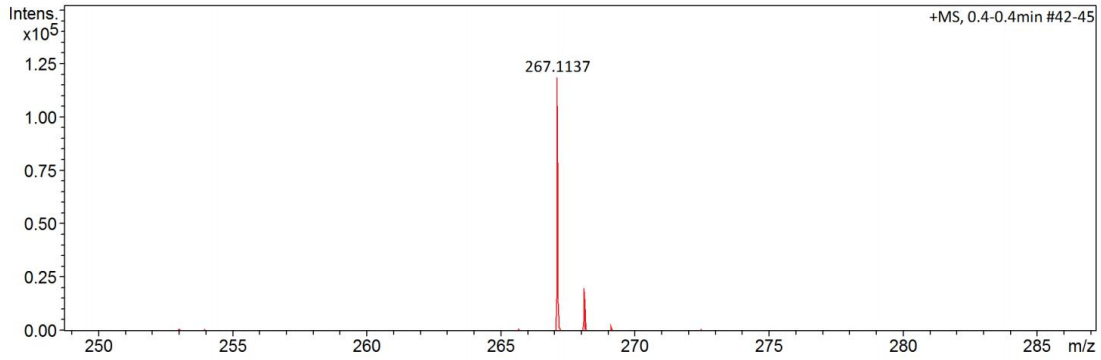
38m



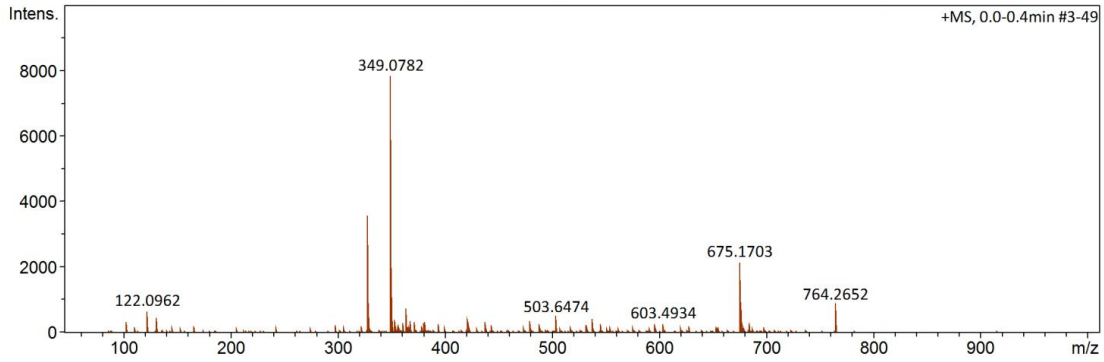
38n



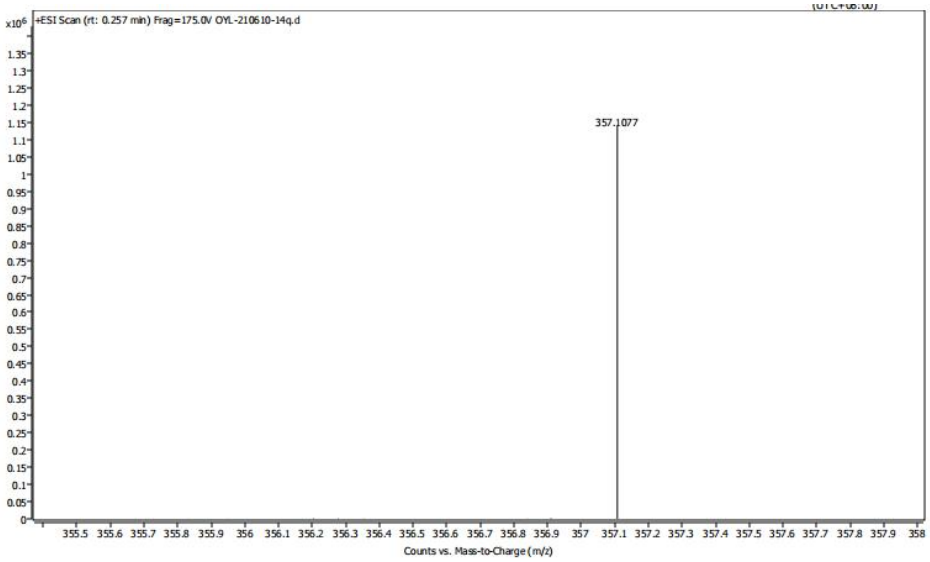
38o



38p



38q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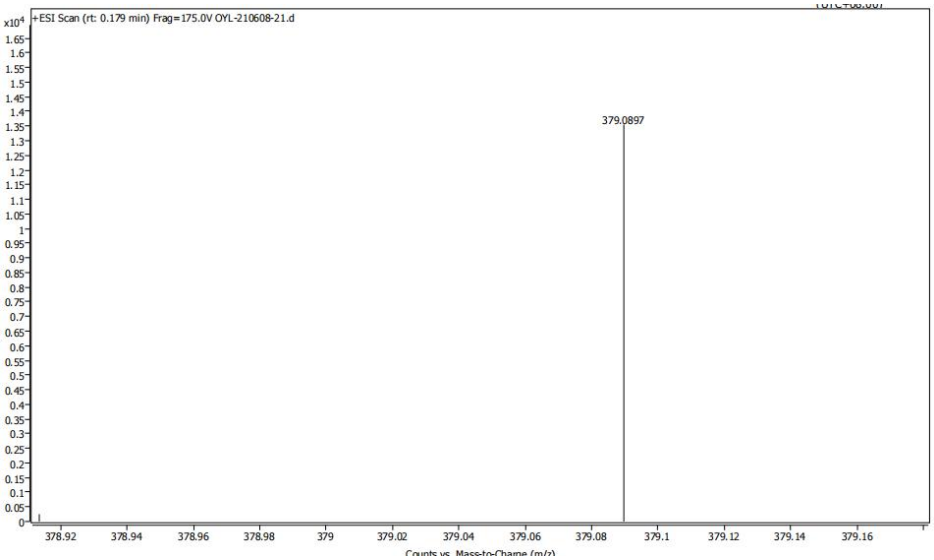
357.1077
Counts vs. Mass-to-Charge (m/z)

38r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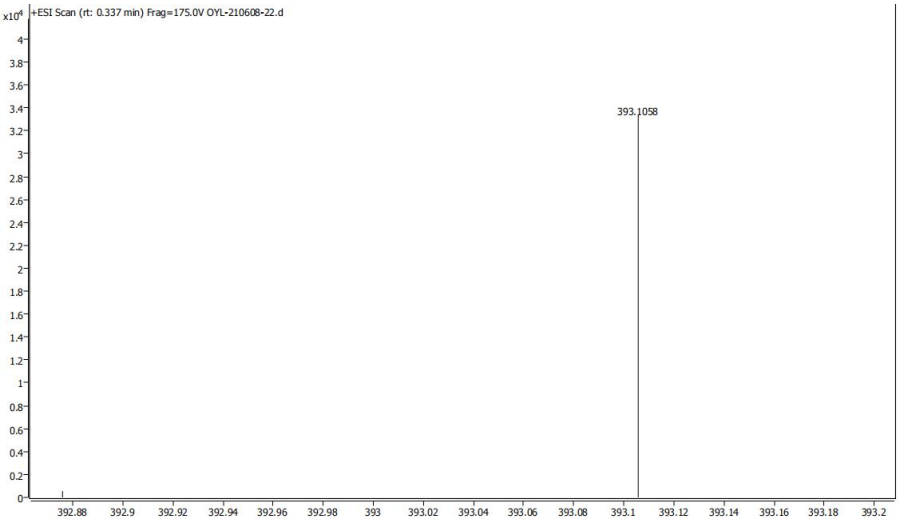
379.0897

38s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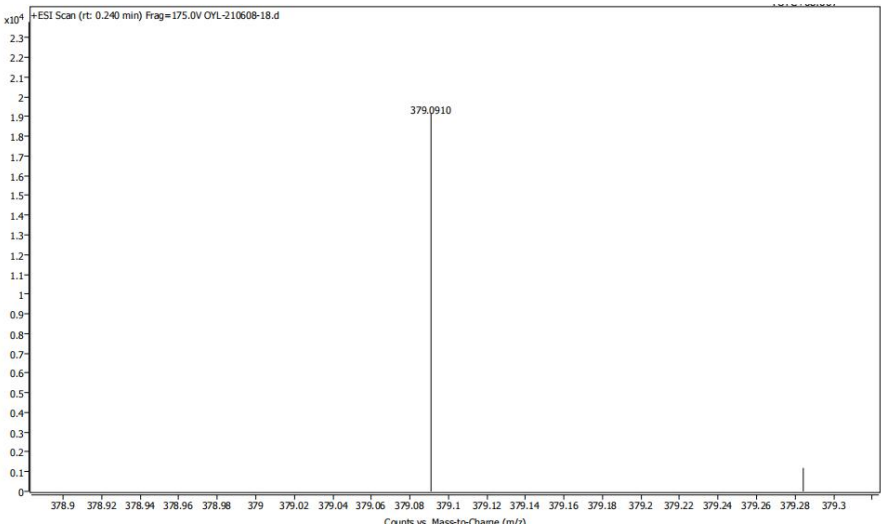
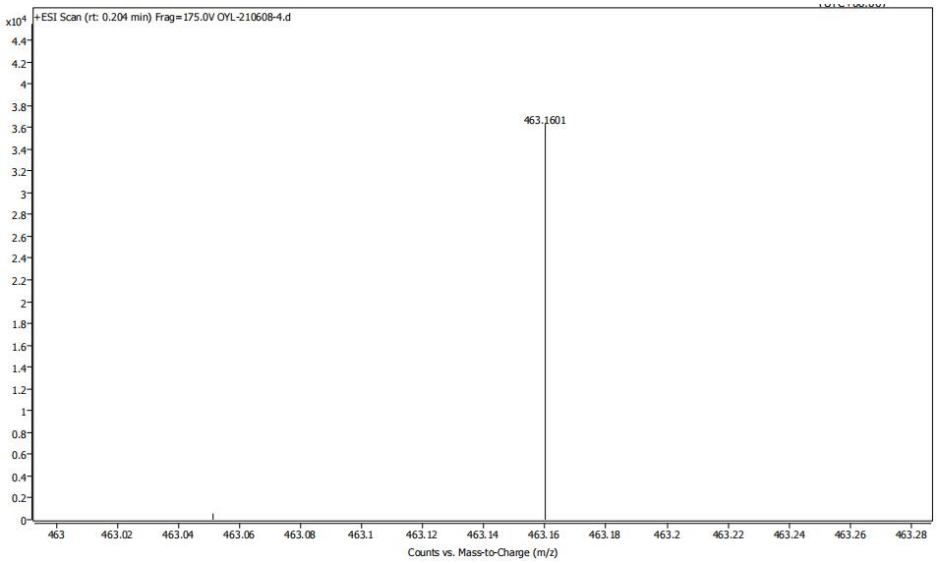
393.1058

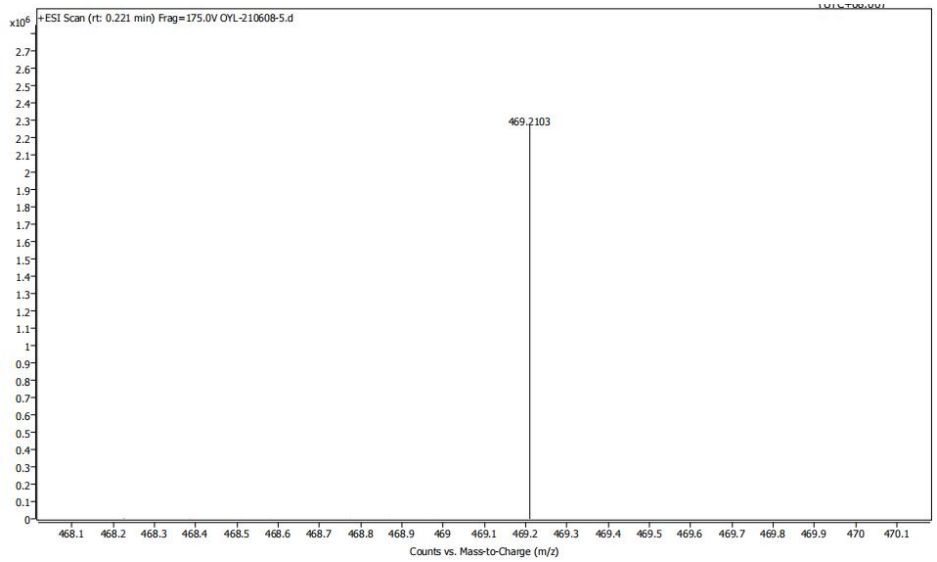
26


+ESI Scan (rt: 0.240 min) Frag=175.0V OYL-210608-18.d
x10^4
379.0910
Counts vs. Mass-to-Charge (m/z)

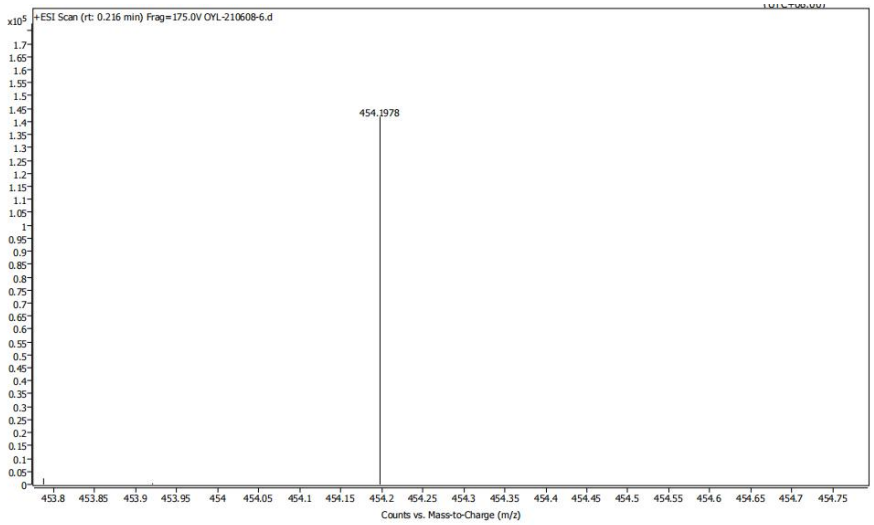
42a


+ESI Scan (rt: 0.204 min) Frag=175.0V OYL-210608-4.d
x10^4
463.1601
Counts vs. Mass-to-Charge (m/z)

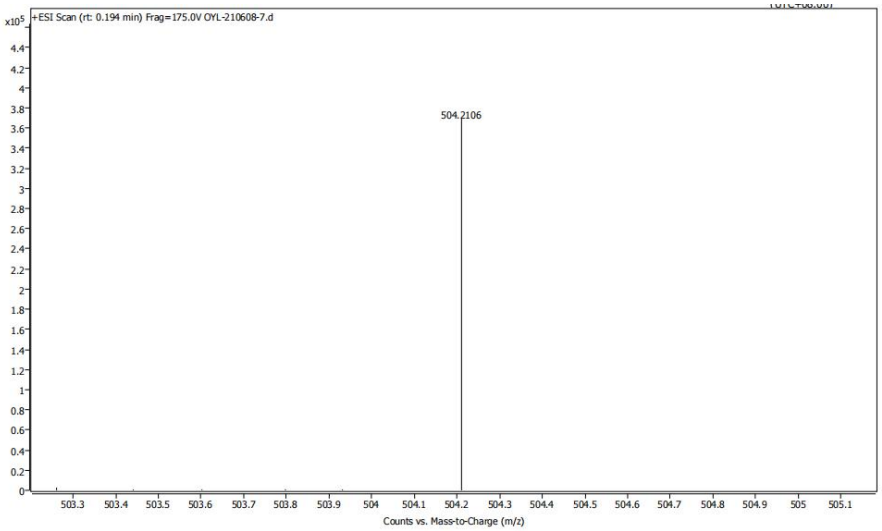
42b


+ESI Scan (rt: 0.221 min) Frag=175.0V OYL-210608-5.d
x10^6
469.2103
Counts vs. Mass-to-Charge (m/z)

42c


+ESI Scan (rt: 0.216 min) Frag=175.0V OYL-210608-6.d
x10^5
454.1978
Counts vs. Mass-to-Charge (m/z)

42d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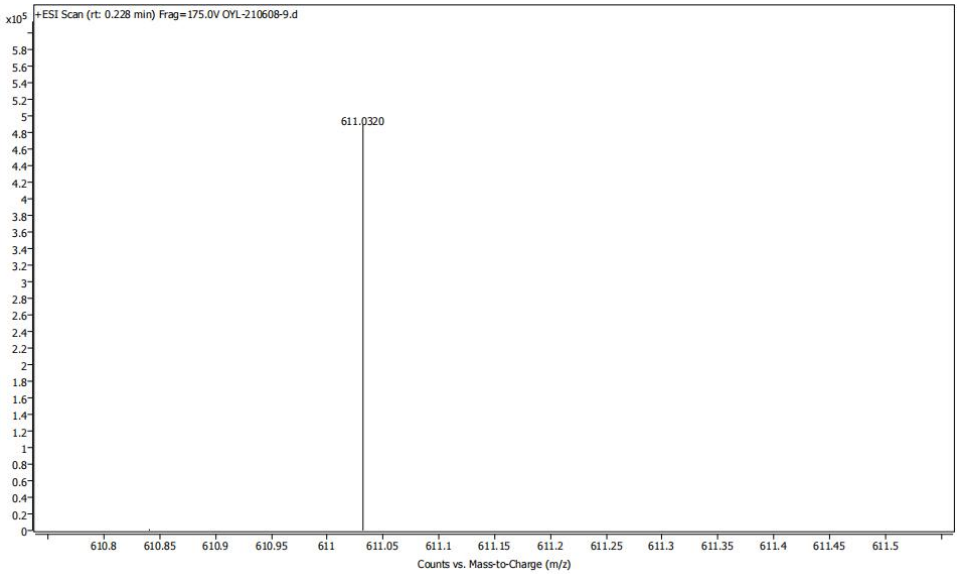
x10^5
504.2106
Counts vs. Mass-to-Charge (m/z)

42e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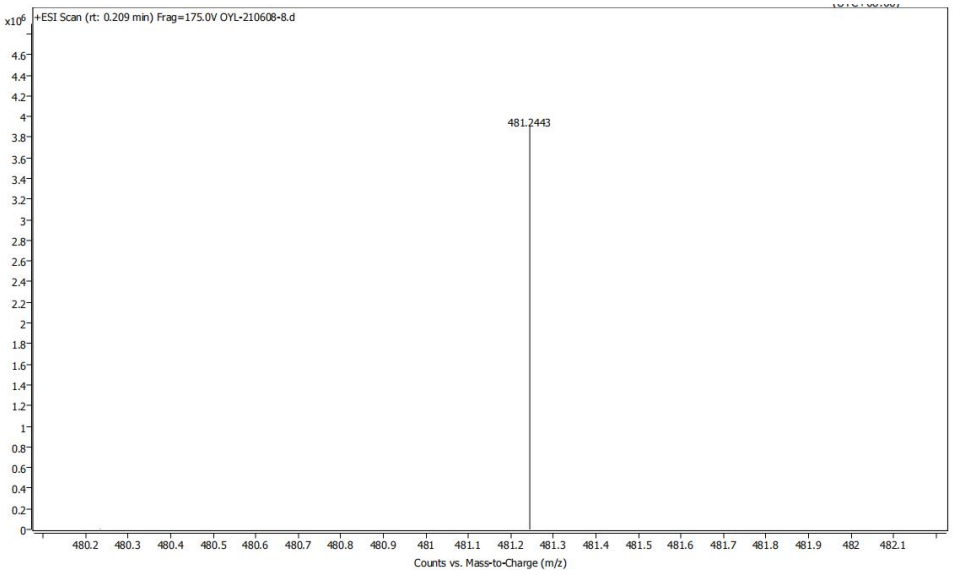
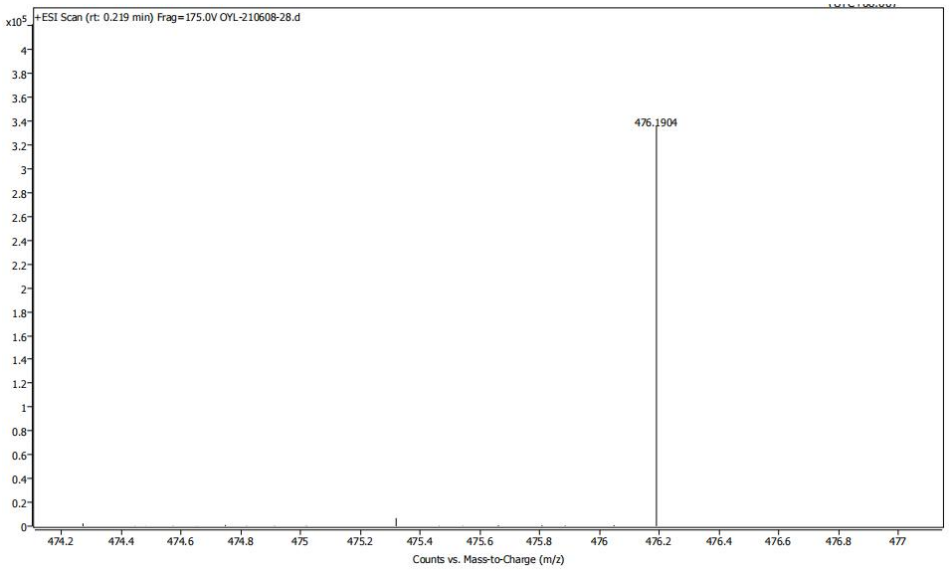
x10^5
611.0320
Counts vs. Mass-to-Charge (m/z)

42f


x10^6
+ESI Scan (rt: 0.209 min) Frag=175.0V OYL-210608-8.d
481.2443
Counts vs. Mass-to-Charge (m/z)

42g


x10^5
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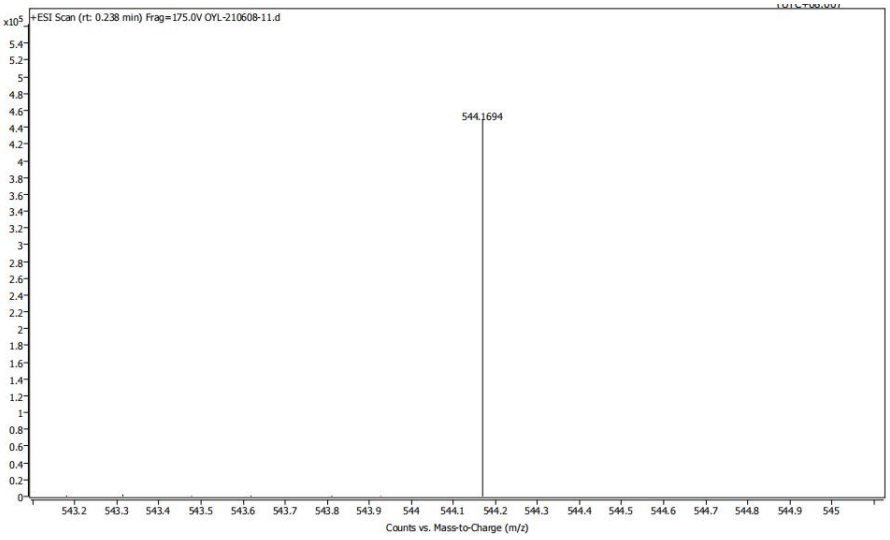
476.1904
Counts vs. Mass-to-Charge (m/z)

42h


x10^5
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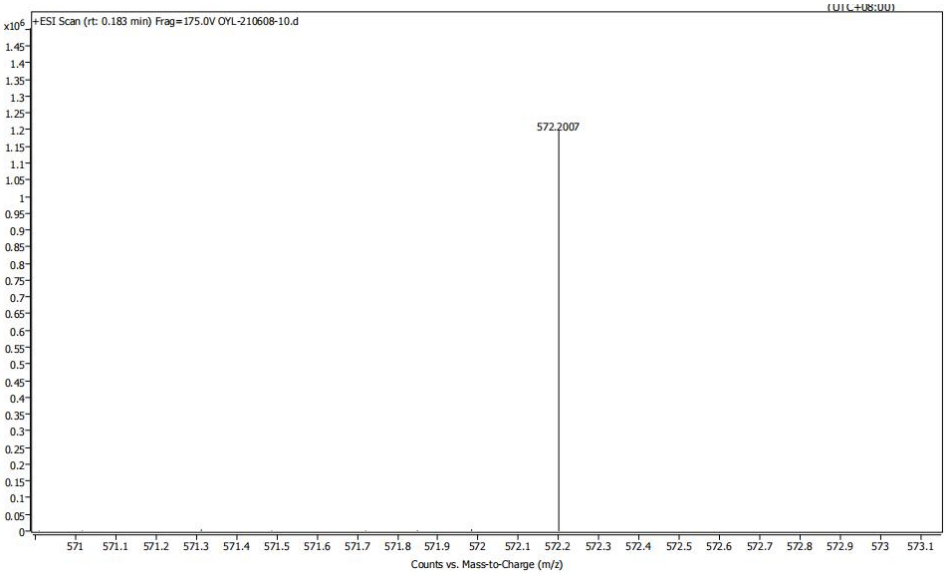
544.1694
Counts vs. Mass-to-Charge (m/z)

42i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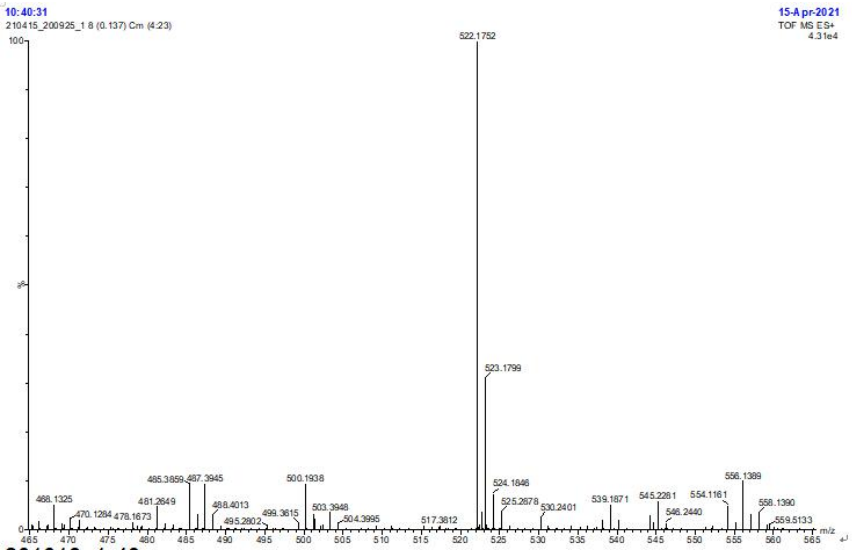
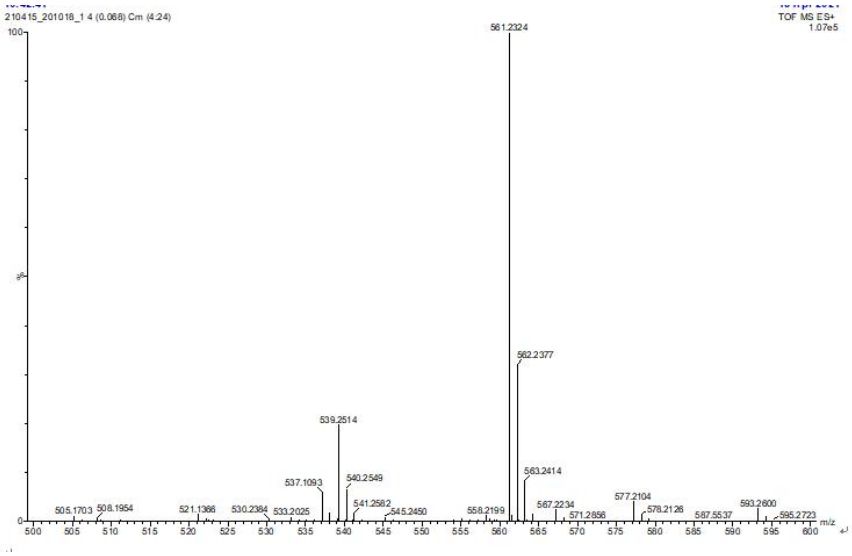
572.2007
Counts vs. Mass-to-Charge (m/z)

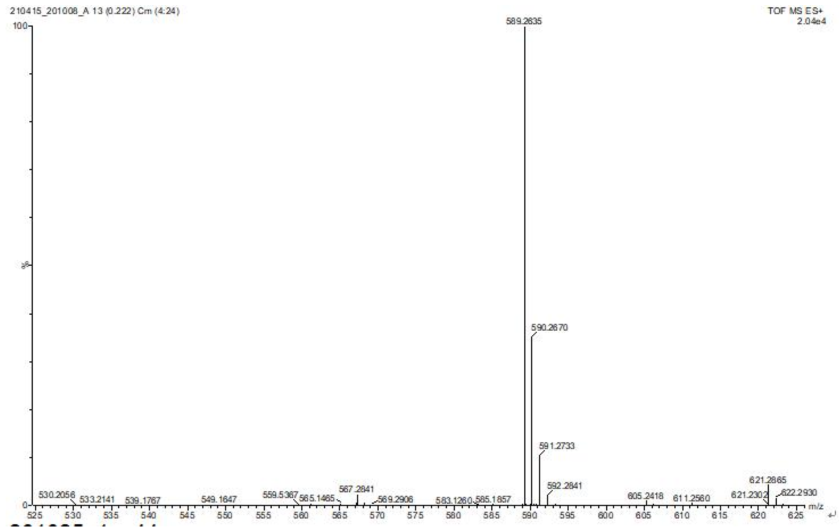
42j


10:40:31
210415_200925_1 8 (0.137) Cm (4:23)
15-Apr-2021
TOF MS ES+
4.31e4
522.1752
523.1799
m/z

43a

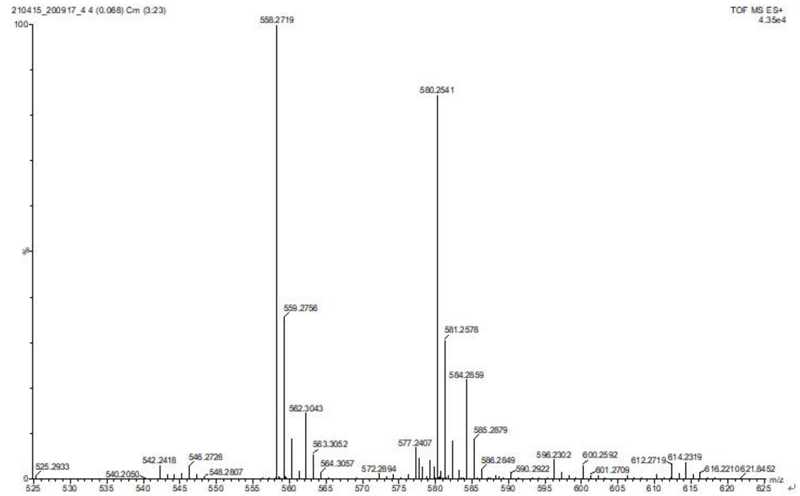

210415_201018_1 4 (0.068) Cm (4:24)
TOF MS ES+
1.07e5
561.2324
562.2377
539.2514
563.2414
m/z

43b



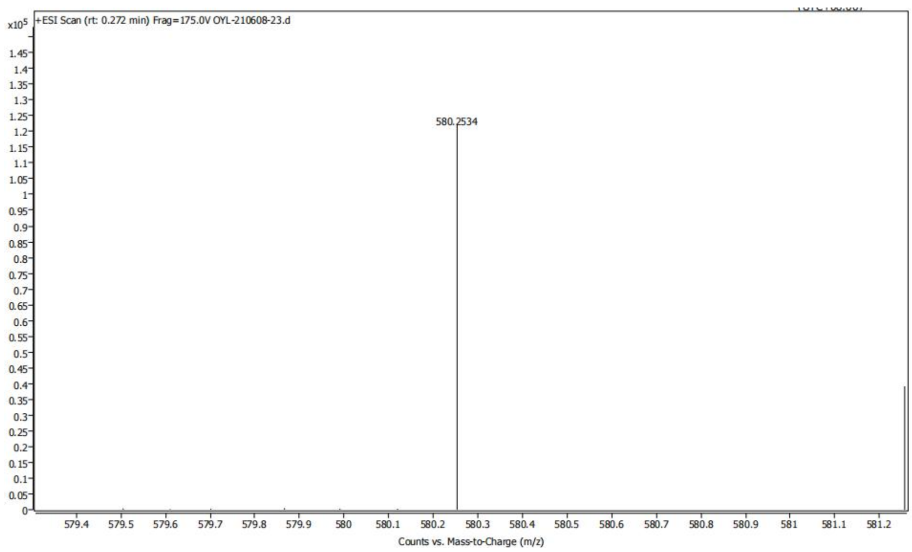
210415_201008_A 13 (0.222) Cm (4:24)
TOF MS ES+
2.04e4
589.2635
590.2670
591.2733
592.2841
m/z

43c



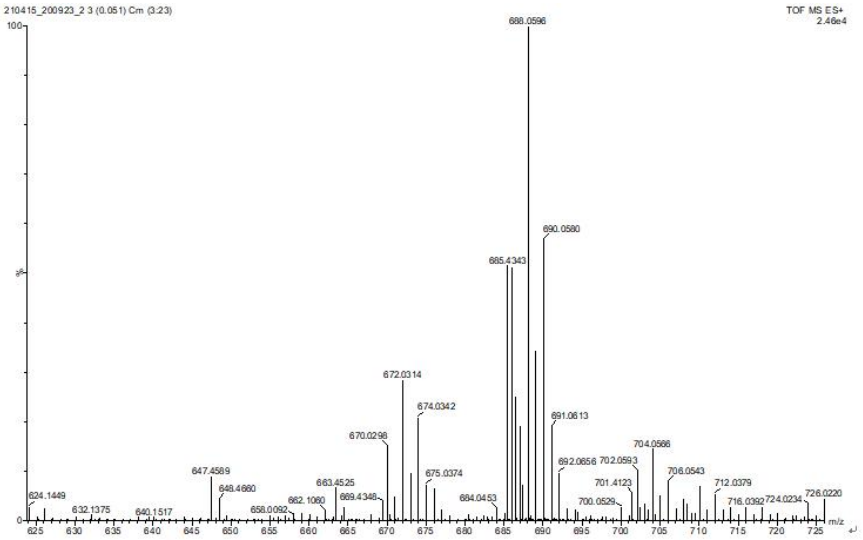
210415_200917_4 4 (0.068) Cm (3:23)
TOF MS ES+
4.35e4
558.2719
580.2541
559.2756
581.2578
584.2859
562.3043
585.2879
m/z

43d

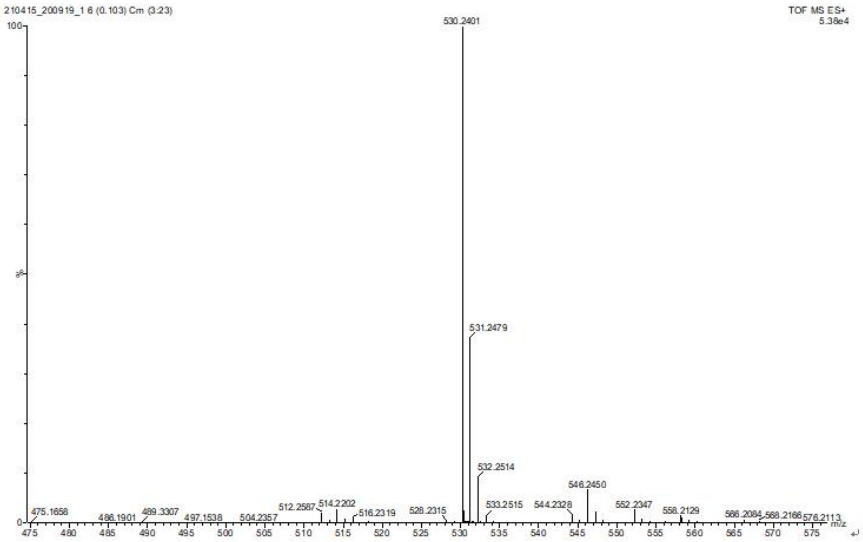


+ESI Scan (rt: 0.272 min) Frag=175.0V OYL-210608-23.d
580.2534
Counts vs. Mass-to-Charge (m/z)

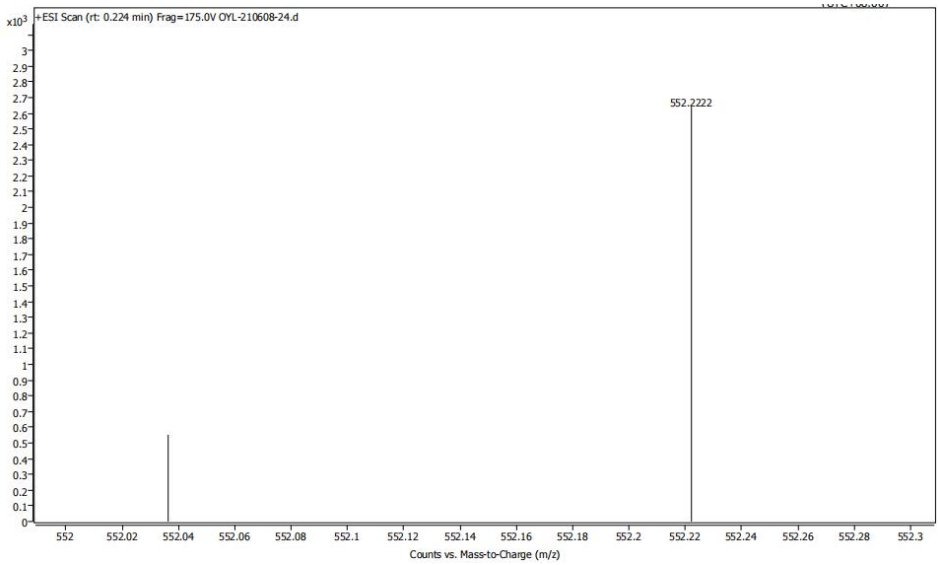
43e


210415_200923_2 3 (0.051) Cm (3:23)
TOF MS ES+
2.46e4
688.0596
690.0580
685.4343
672.0314
674.0342
691.0613
670.0298
704.0566
692.0656
702.0593
706.0543
647.4589
675.0374
701.4123
712.0379
648.4660
663.4525
669.4348
662.1060
684.0453
624.1449
632.1375
640.1517
658.0992
700.0529
716.0392
724.0234
726.0220
m/z

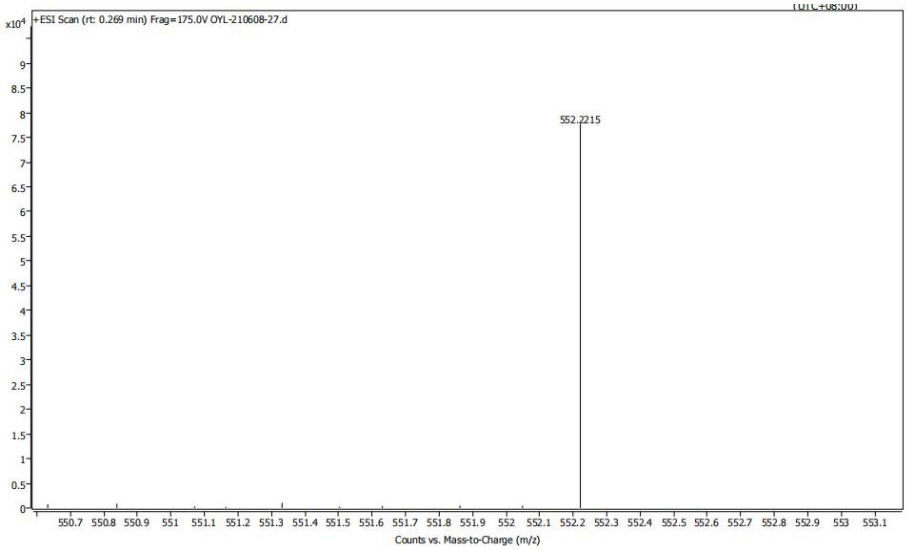
43f


210415_200919_1 6 (0.103) Cm (3:23)
TOF MS ES+
5.38e4
530.2401
531.2479
532.2514
546.2450
475.1658
486.1901
489.3307
497.1538
504.2357
512.2567
514.2202
516.2319
526.2315
533.2515
544.2328
552.2347
558.2129
566.2094
568.2166
576.2113
m/z

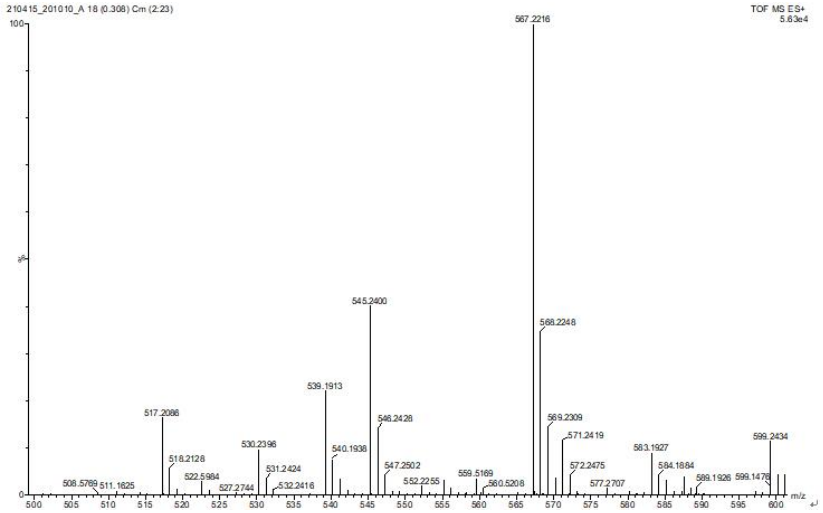
43g


+ESI Scan (rt: 0.224 min) Frag=175.0V OYL-210608-24.d
x10^3
552.2222
Counts vs. Mass-to-Charge (m/z)

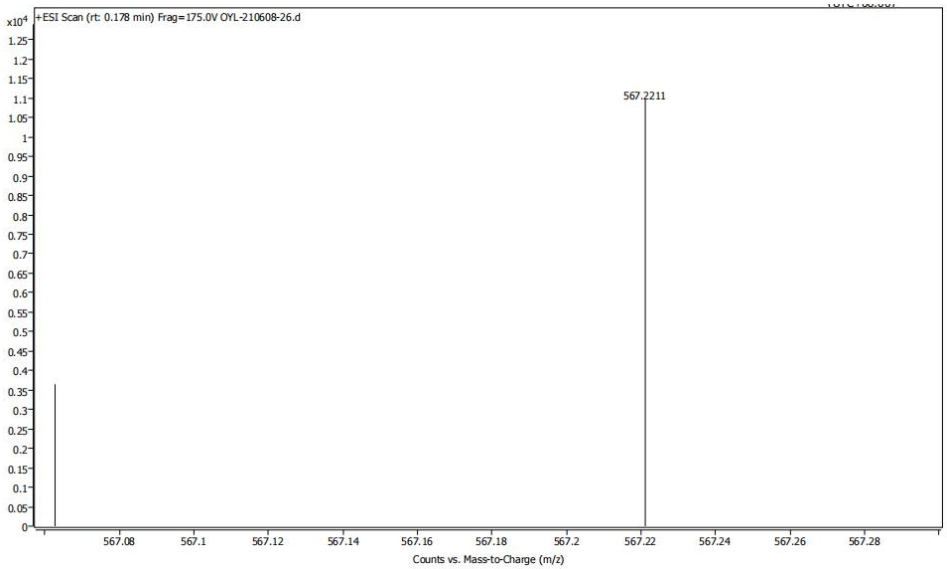
43h


+ESI Scan (rt: 0.269 min) Frag=175.0V OYL-210608-27.d
552.2215
Counts vs. Mass-to-Charge (m/z)

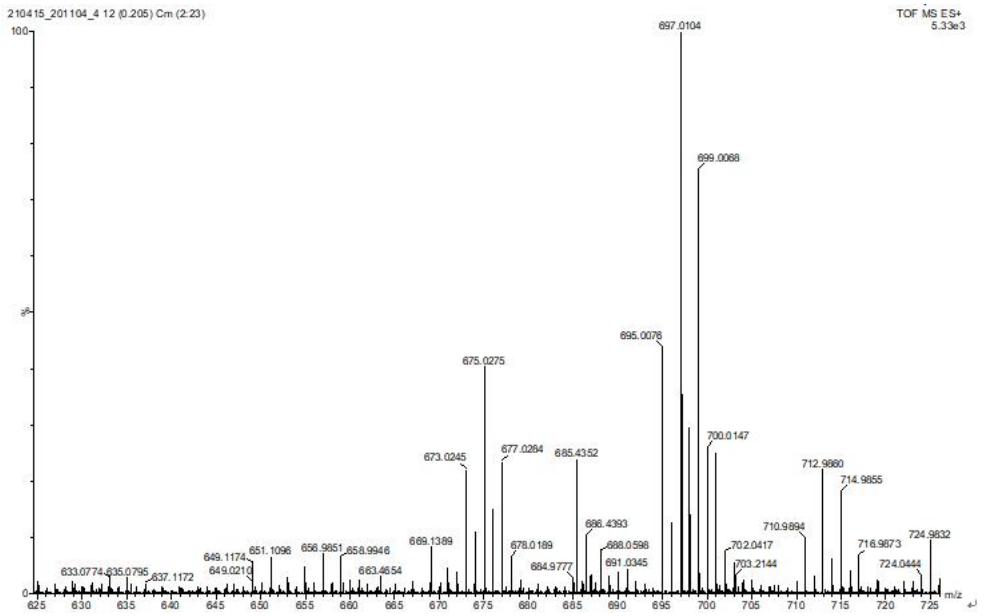
43i


210415_201010_A 18 (0.308) Cm (2:23)
TOF MS ES+
5.63e4
567.2216
545.2400
568.2248
539.1913
517.2098
546.2428
569.2309
571.2419
530.2396
518.2128
540.1938
583.1927
599.2434
531.2424
547.2502
572.2475
584.1884
522.5984
552.2255
559.5169
589.1926
599.1478
508.5789
511.1825
527.2744
532.2416
560.5208
577.2707
m/z

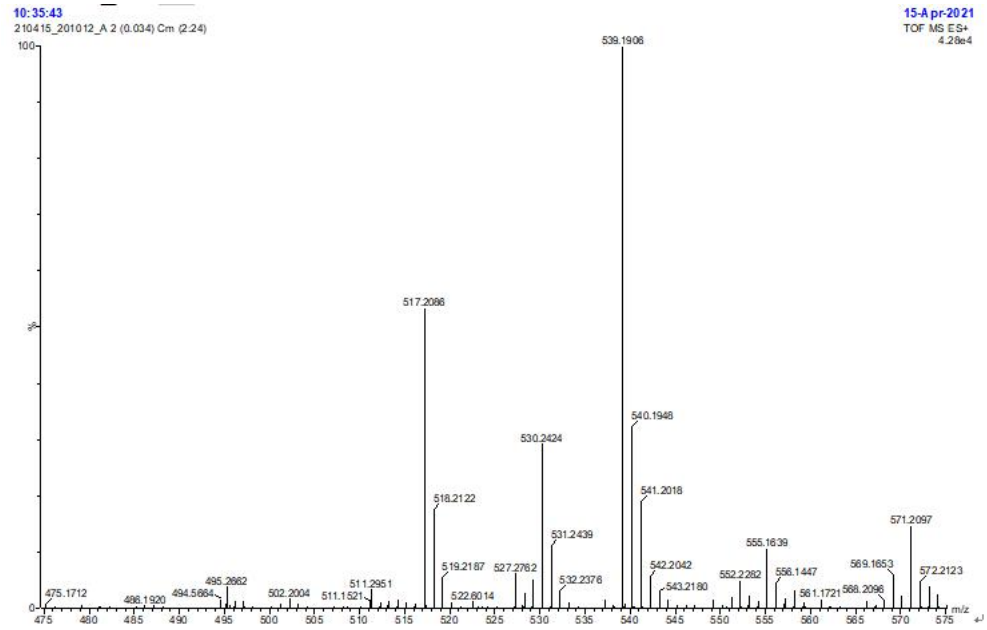
43j


+ESI Scan (rt: 0.178 min) Frag=175.0V OYL-210608-26.d
567.2211
Counts vs. Mass-to-Charge (m/z)

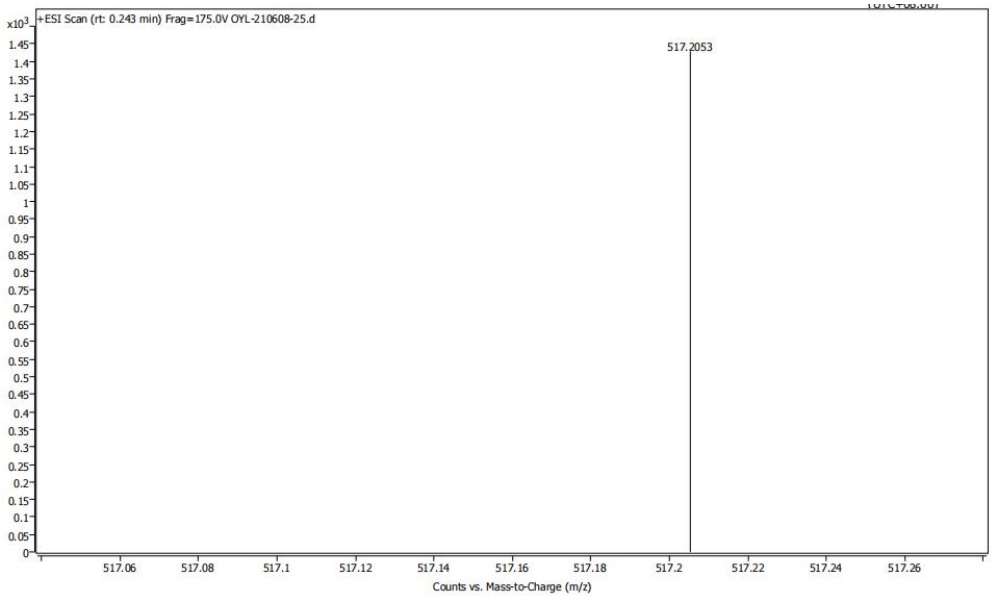
43k


210415_201104_4 12 (0.205) Cm (2:23)
TOF MS ES+
5.33e3
100
%
0
697.0104
699.0068
695.0078
675.0275
700.0147
673.0245
677.0284
685.4352
712.9860
714.9855
686.4393
710.9894
669.1389
678.0189
724.9832
688.0598
716.9873
702.0417
649.1174
651.1096
656.9851
658.9946
691.0345
703.2144
724.0444
649.0210
684.9777
633.0774
635.0795
637.1172
663.4654
625
630
635
640
645
650
655
660
665
670
675
680
685
690
695
700
705
710
715
720
725
m/z

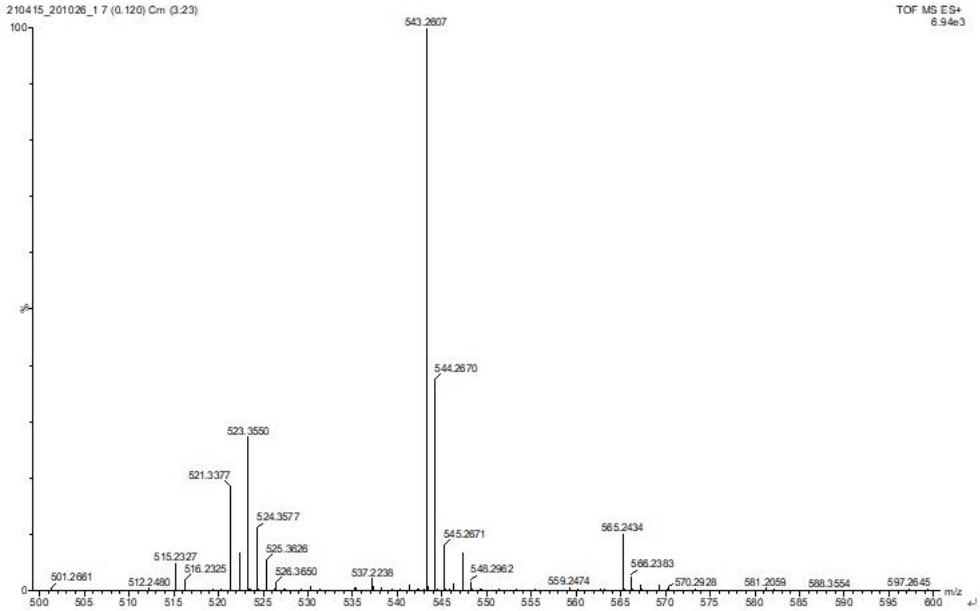
43l


10:35:43
15-Apr-2021
210415_201012_A 2 (0.034) Cm (2:24)
TOF MS ES+
4.26e4
100
%
0
539.1906
517.2086
540.1948
530.2424
518.2122
541.2018
571.2097
531.2439
555.1639
519.2187
527.2762
542.2042
569.1653
572.2123
552.2282
556.1447
532.2376
543.2180
495.2662
511.2951
475.1712
496.1920
494.5664
502.2004
511.1521
522.6014
561.1721
568.2096
475
480
485
490
495
500
505
510
515
520
525
530
535
540
545
550
555
560
565
570
575
m/z

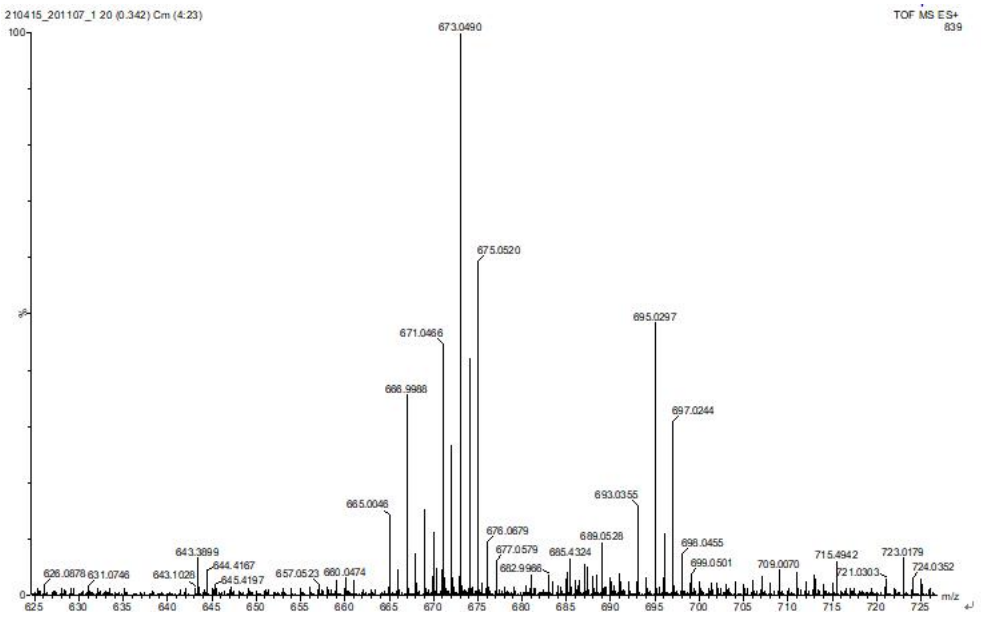
43m


+ESI Scan (rt: 0.243 min) Frag=175.0V OYL-210608-25.d
x10^3
517.2053
Counts vs. Mass-to-Charge (m/z)

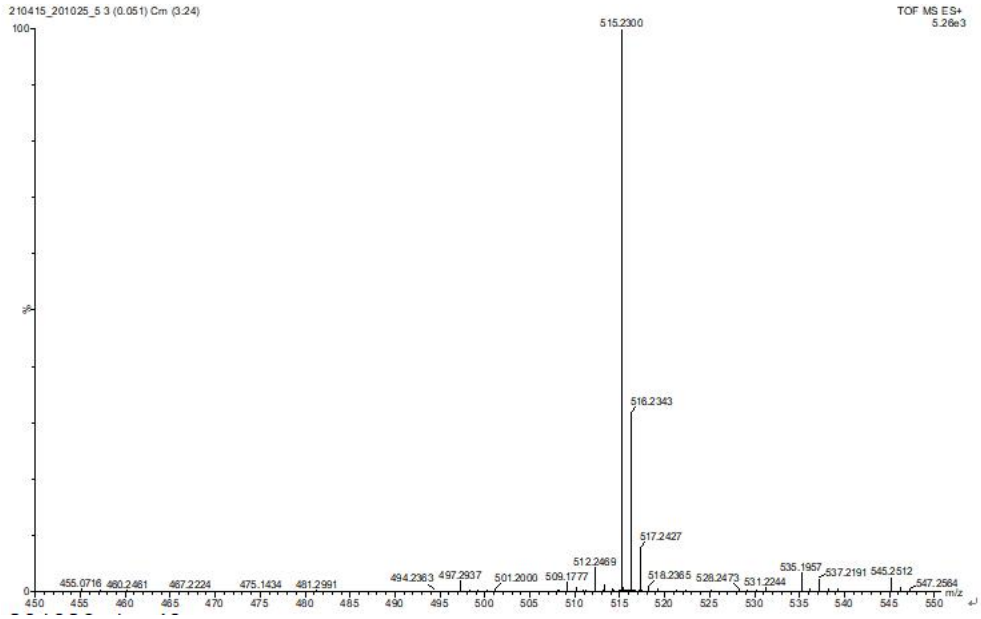
43n


210415_201026_1 7 (0.120) Cm (3:23)
TOF MS ES+
6.94e3
543.2607
544.2670
523.3550
521.3377
524.3577
525.3626
515.2327
516.2325
526.3650
545.2671
548.2962
565.2434
566.2383
501.2681
512.2490
537.2238
559.2474
570.2928
581.2059
588.3554
597.2645
m/z

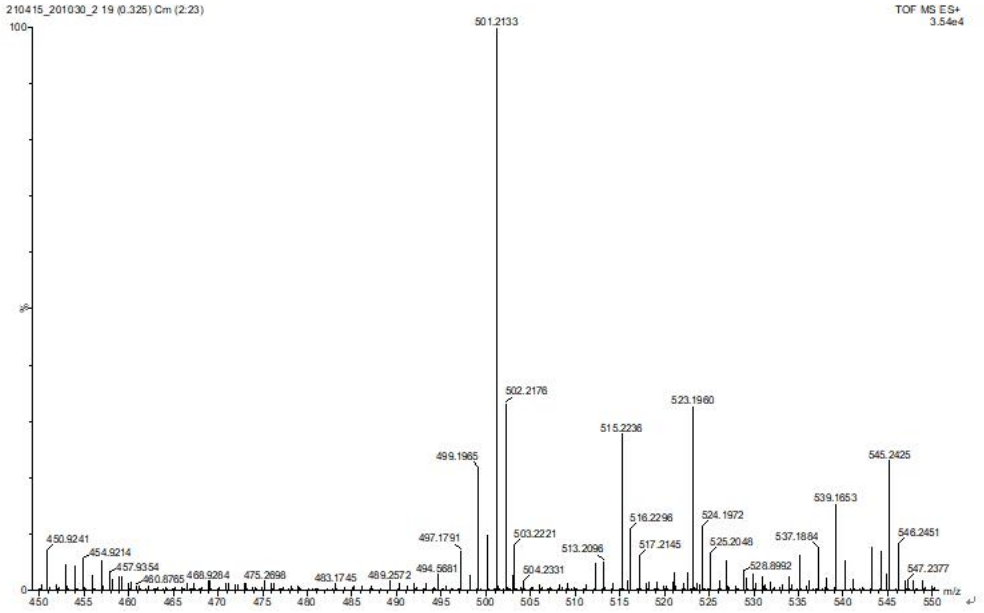
43o


210415_201107_1 20 (0.342) Cm (4:23)
TOF MS ES+
839
673.0490
675.0520
671.0466
695.0297
666.9988
697.0244
693.0355
665.0046
676.0679
689.0528
698.0455
643.3899
644.4167
645.4197
626.0878
631.0746
643.1028
657.0523
660.0474
677.0579
682.9966
685.4324
699.0501
709.0070
715.4942
721.0303
723.0179
724.0352
m/z

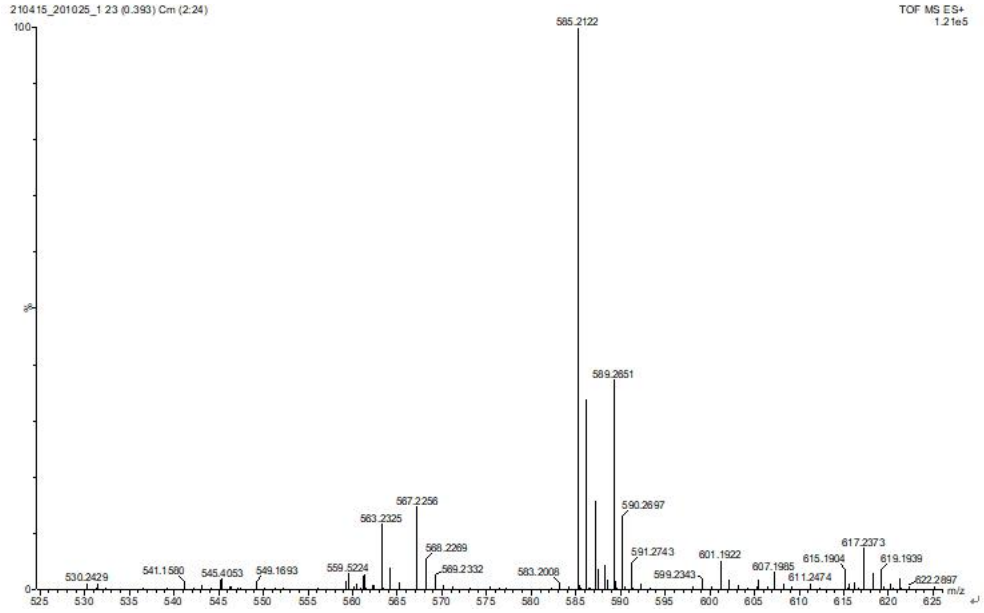
43p


210415_201025_5 3 (0.051) Cm (3:24)
TOF MS ES+
5.26e3
515.2300
516.2343
517.2427
512.2469
455.0716
460.2461
467.2224
475.1434
481.2991
494.2363
497.2937
501.2000
509.1777
518.2365
528.2473
531.2244
535.1957
537.2191
545.2512
547.2564
m/z

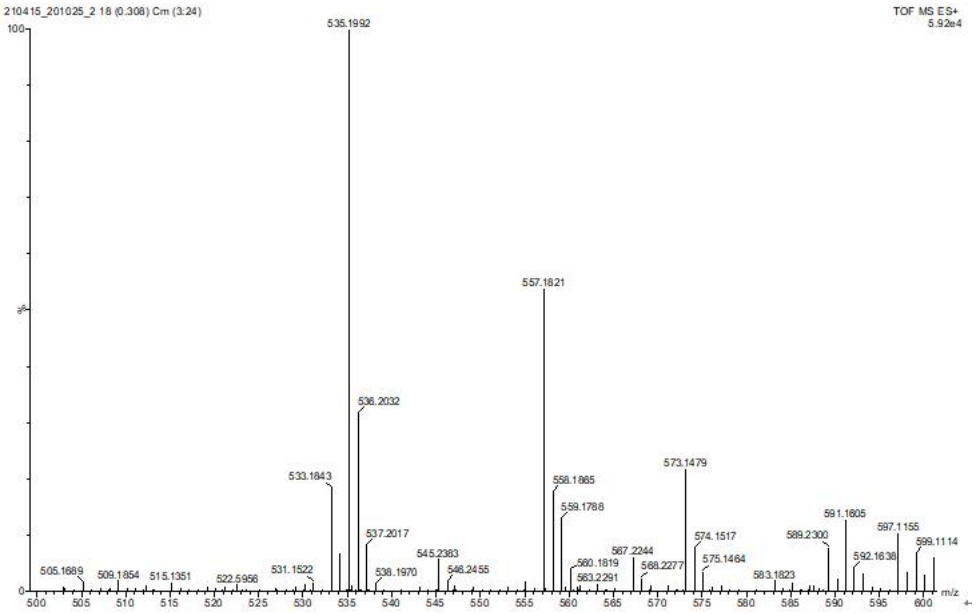
43q


210415_201030_2 19 (0.325) Cm (2:23)
TOF MS ES+
3.54e4
501.2133
502.2178
523.1960
515.2236
499.1965
545.2425
539.1653
516.2296
524.1972
546.2451
503.2221
497.1791
513.2096
517.2145
525.2048
537.1884
450.9241
454.9214
457.9354
460.8765
468.9264
475.2698
483.1745
489.2572
494.5681
504.2331
528.8992
547.2377
m/z

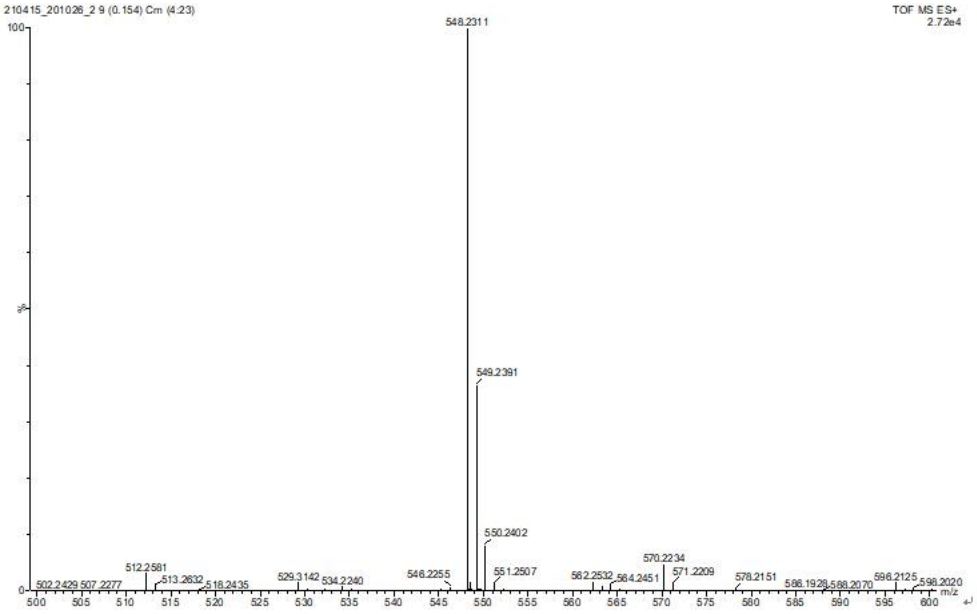
44a


210415_201025_1 23 (0.393) Cm (2:24)
TOF MS ES+
1.21e5
585.2122
589.2651
567.2256
590.2697
563.2325
568.2269
591.2743
617.2373
601.1922
615.1904
619.1939
607.1985
569.2332
583.2008
599.2343
611.2474
622.2897
530.2429
541.1580
545.4053
549.1693
559.5224
m/z

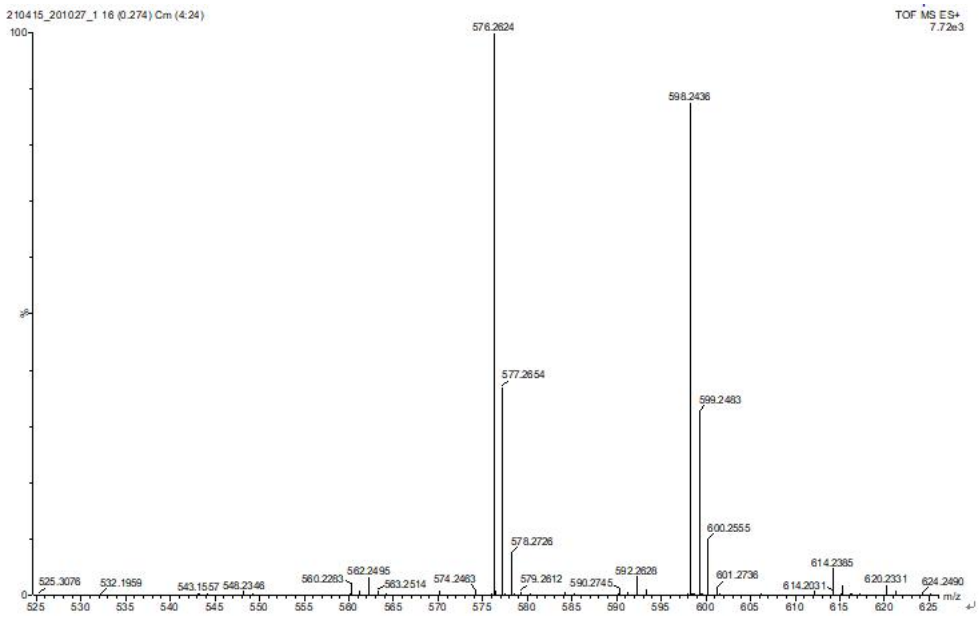
44b


210415_201025_2 18 (0.308) Cm (3:24)
TOF MS ES+
5.92e4
100
%
0
535.1992
557.1821
536.2032
533.1843
573.1479
558.1885
559.1788
591.1605
597.1155
574.1517
589.2300
599.1114
537.2017
545.2383
567.2244
592.1638
575.1464
505.1689
509.1854
515.1351
522.5956
531.1522
538.1970
548.2455
560.1819
563.2291
568.2277
583.1823
500 505 510 515 520 525 530 535 540 545 550 555 560 565 570 575 580 585 590 595 600
m/z

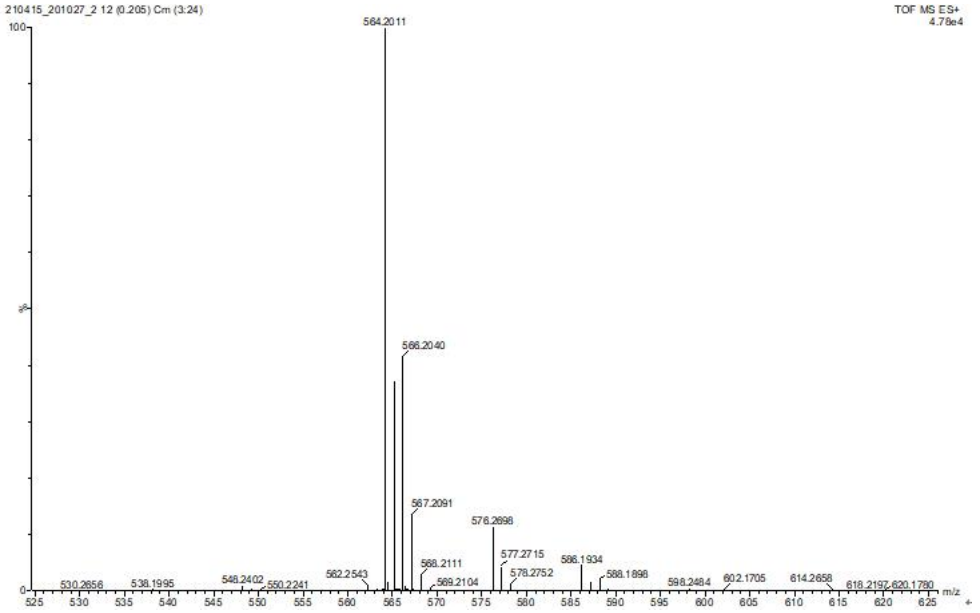
44c


210415_201026_2 9 (0.154) Cm (4:23)
TOF MS ES+
2.72e4
100
%
0
548.2311
549.2391
550.2402
570.2234
512.2581
571.2209
502.2429
507.2277
513.2632
518.2435
529.3142
534.2240
546.2255
551.2507
562.2532
564.2451
578.2151
586.1928
588.2070
596.2125
598.2020
500 505 510 515 520 525 530 535 540 545 550 555 560 565 570 575 580 585 590 595 600
m/z

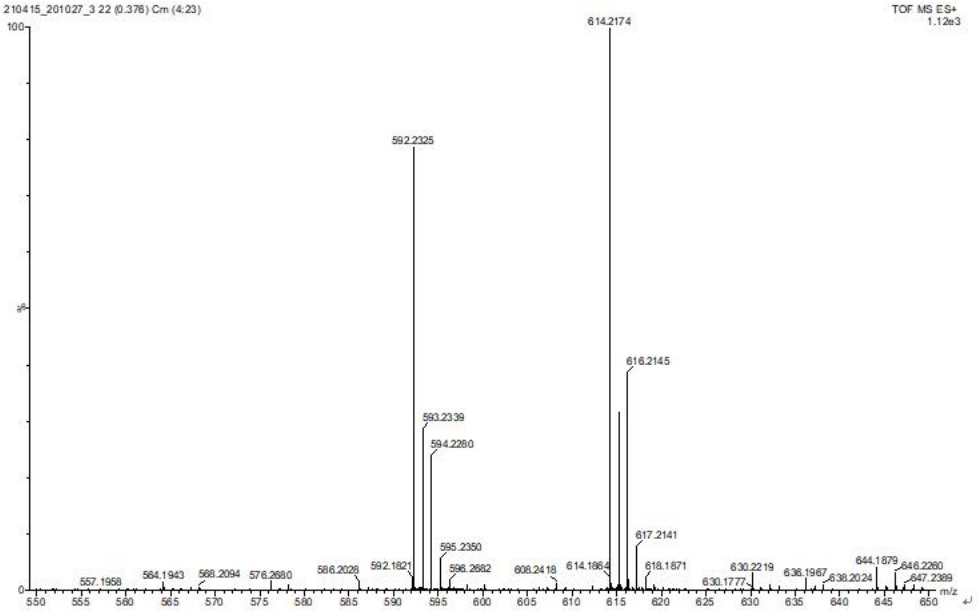
44d


210415_201027_1 16 (0.274) Cm (4:24)
TOF MS ES+
7.72e3
100
%
0
576.2624
598.2436
577.2654
599.2483
578.2726
600.2555
614.2385
525.3076
532.1959
543.1557
548.2346
560.2283
562.2495
563.2514
574.2463
579.2612
590.2745
592.2626
601.2736
614.2031
620.2331
624.2490
525
530
535
540
545
550
555
560
565
570
575
580
585
590
595
600
605
610
615
620
625
m/z

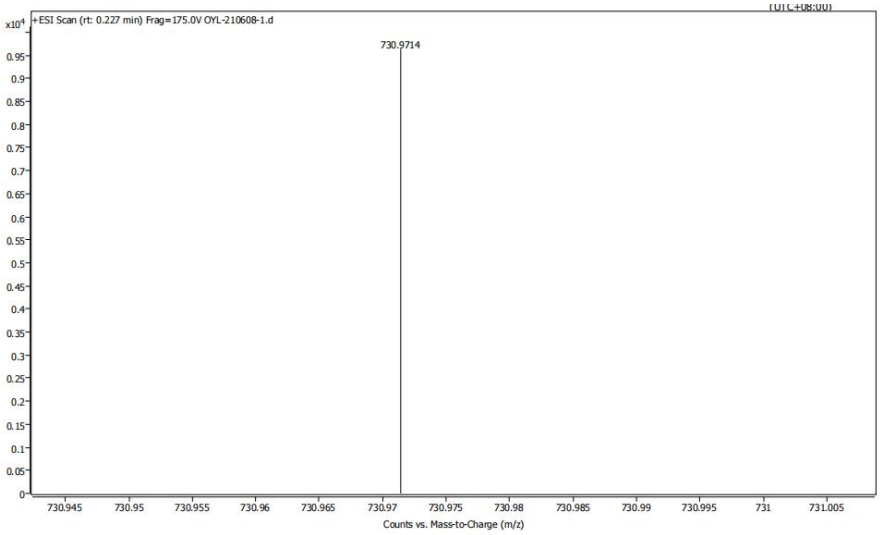
44e


210415_201027_2 12 (0.205) Cm (3:24)
TOF MS ES+
4.78e4
100
%
0
564.2011
566.2040
567.2091
576.2698
577.2715
568.2111
578.2752
586.1934
588.1898
569.2104
530.2656
538.1995
546.2402
550.2241
562.2543
598.2484
602.1705
614.2658
618.2197
620.1780
525
530
535
540
545
550
555
560
565
570
575
580
585
590
595
600
605
610
615
620
625
m/z

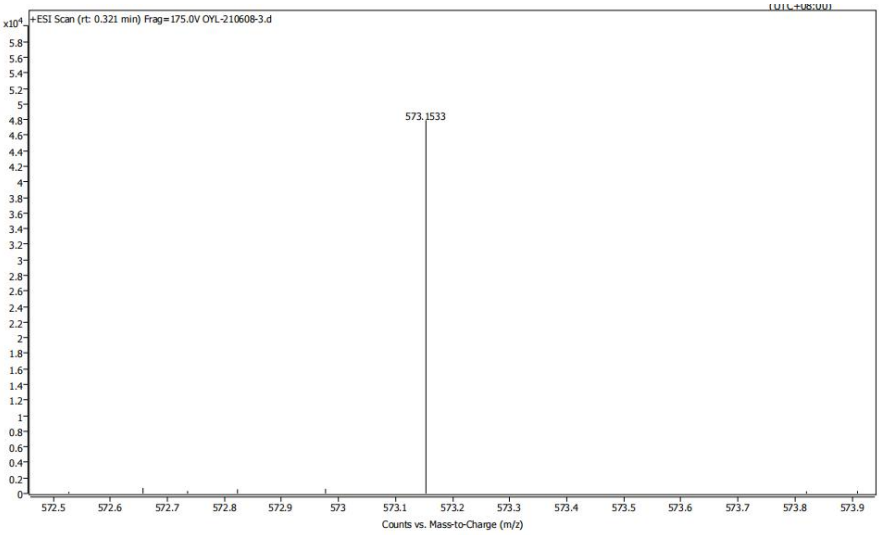
44f


210415_201027_3 22 (0.378) Cm (4:23)
TOF MS ES+
1.12e3
100
%
0
614.2174
592.2325
616.2145
593.2339
594.2280
617.2141
595.2350
557.1958
564.1943
568.2094
576.2680
586.2028
592.1821
596.2682
608.2418
614.1884
618.1871
630.2219
630.1777
636.1967
638.2024
644.1879
646.2260
647.2389
m/z
550
555
560
565
570
575
580
585
590
595
600
605
610
615
620
625
630
635
640
645
650

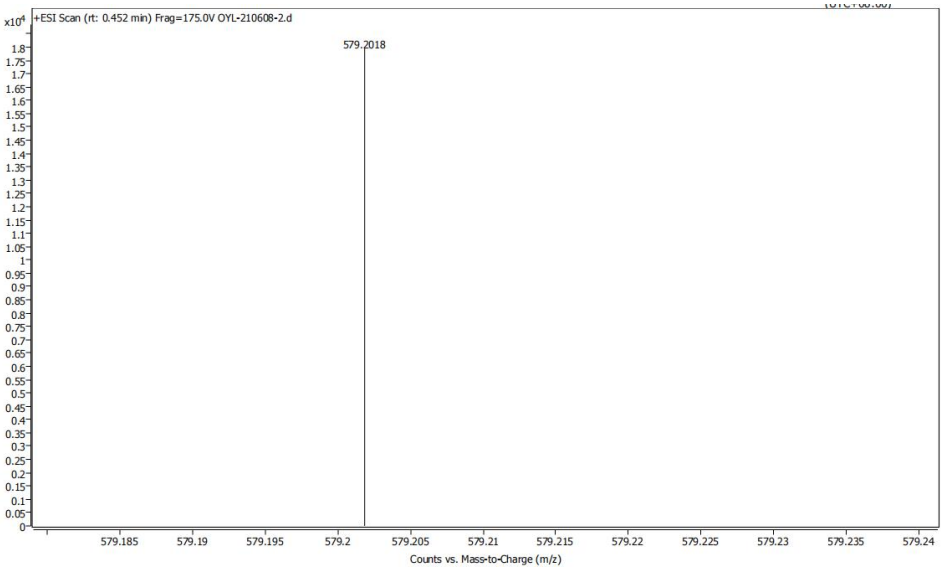
44g


+ESI Scan (rt: 0.227 min) Frag=175.0V OYL-210608-1.d
x10^4
730.9714
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
730.945
730.95
730.955
730.96
730.965
730.97
730.975
730.98
730.985
730.99
730.995
731
731.005
Counts vs. Mass-to-Charge (m/z)

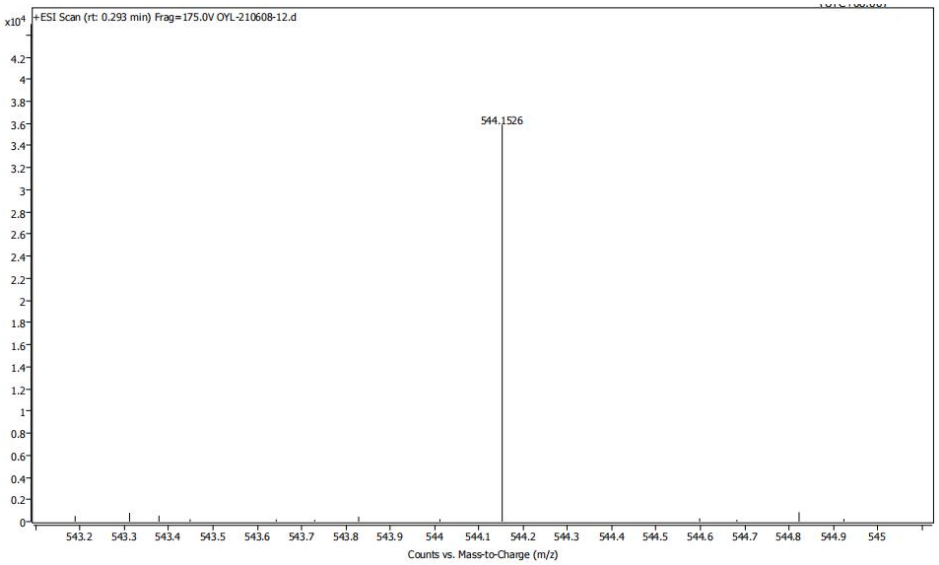
44h


+ESI Scan (rt: 0.321 min) Frag=175.0V OYL-210608-3.d
x10^4
573.1533
Counts vs. Mass-to-Charge (m/z)

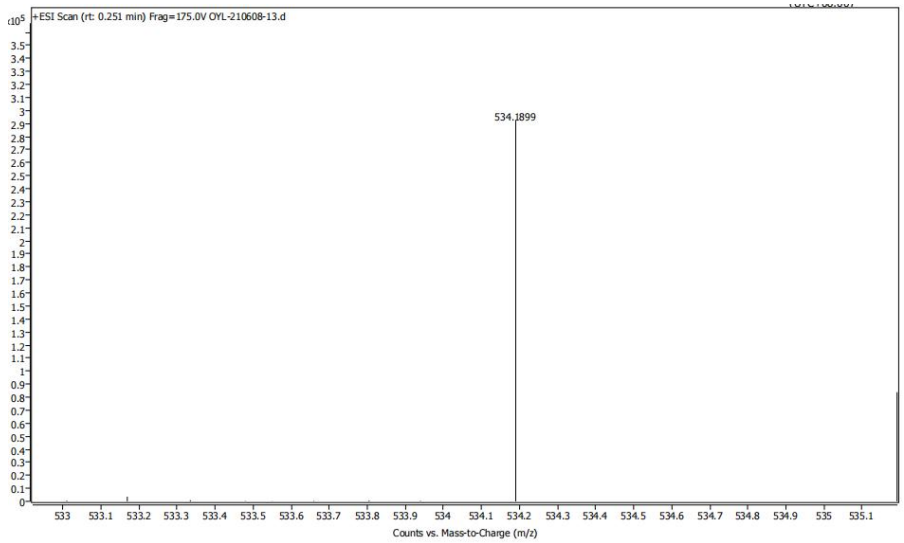
44i


+ESI Scan (rt: 0.452 min) Frag=175.0V OYL-210608-2.d
x10^4
579.2018
Counts vs. Mass-to-Charge (m/z)

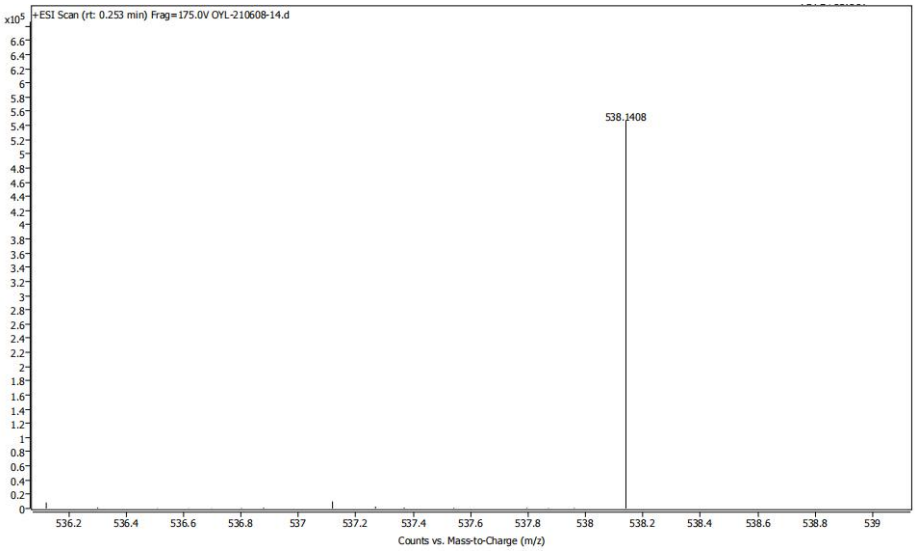
44j


+ESI Scan (rt: 0.293 min) Frag=175.0V OYL-210608-12.d
x10^4
544.1526
Counts vs. Mass-to-Charge (m/z)

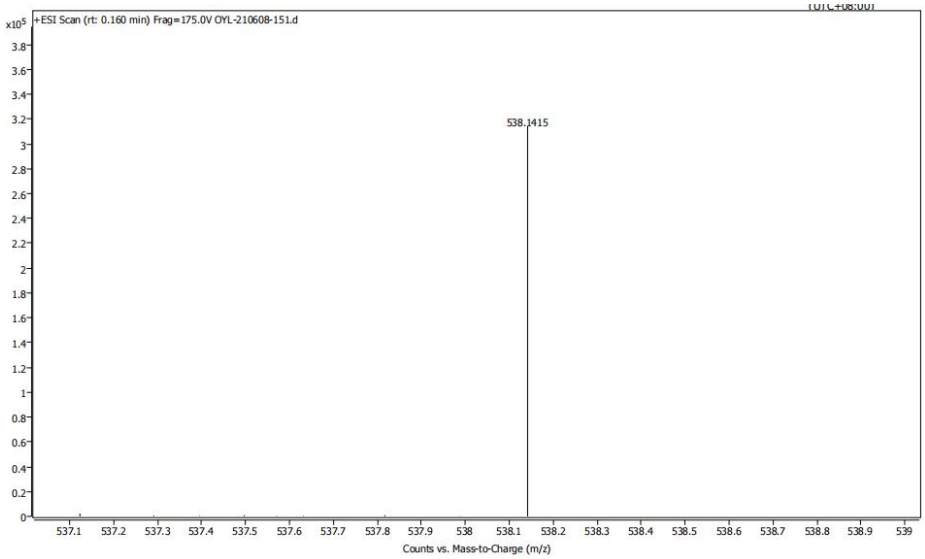
44k


+ESI Scan (rt: 0.251 min) Frag=175.0V OYL-210608-13.d
x10^5
534.1899
Counts vs. Mass-to-Charge (m/z)

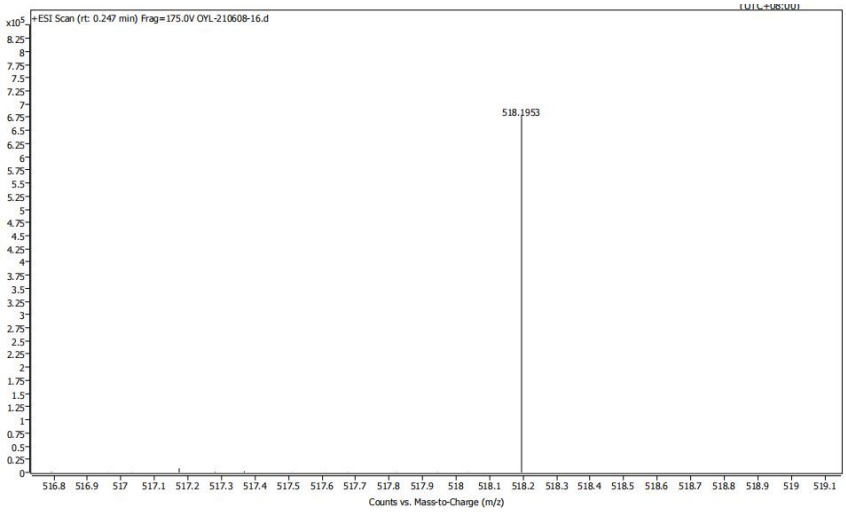
44l


+ESI Scan (rt: 0.253 min) Frag=175.0V OYL-210608-14.d
x10^5
538.1408
Counts vs. Mass-to-Charge (m/z)

44m

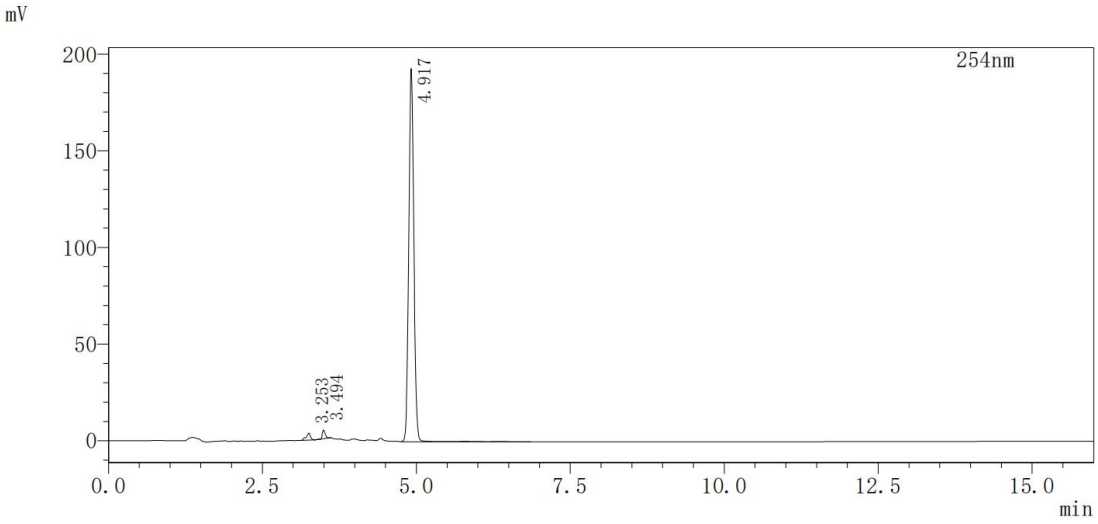

+ESI Scan (rt: 0.160 min) Frag=175.0V OYL-210608-151.d
x10^5
538.1415
Counts vs. Mass-to-Charge (m/z)

44n



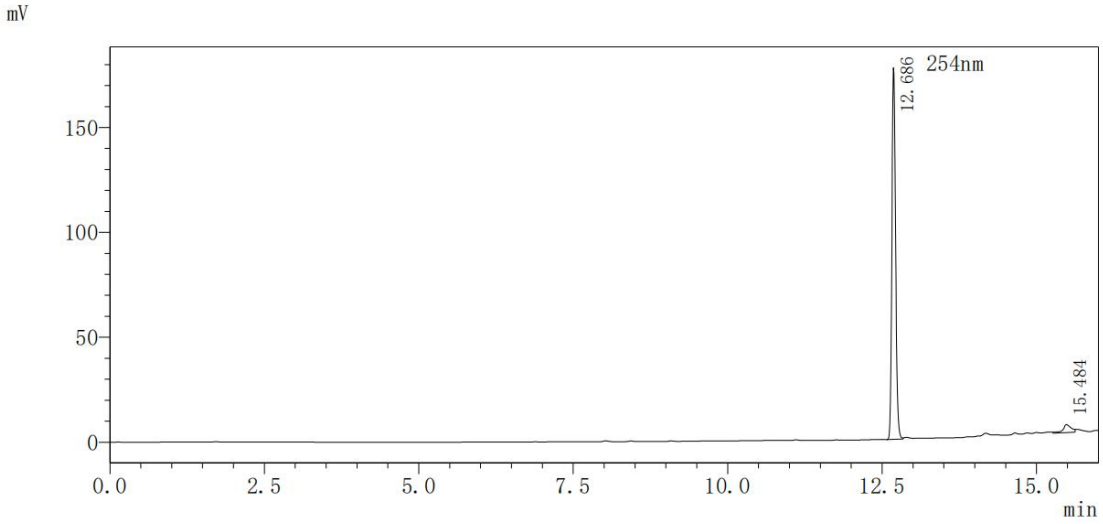
4. HPLC data

33a



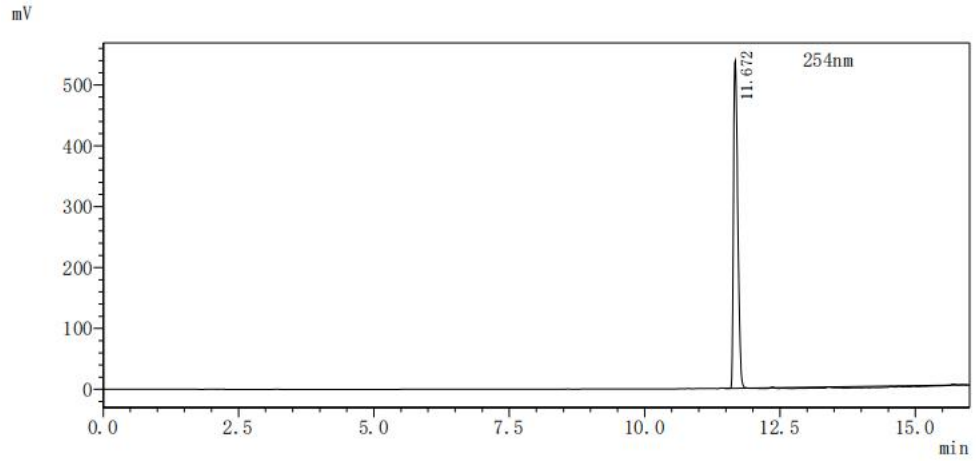
Peak	Retention time	Area	Height	Concentration	Height%
1	3.253	17843	3620	1.554	1.798
2	3.494	15440	4557	1.344	2.264
3	4.917	1115241	193095	97.102	95.937
Total		1148525	201273		100.000

33b



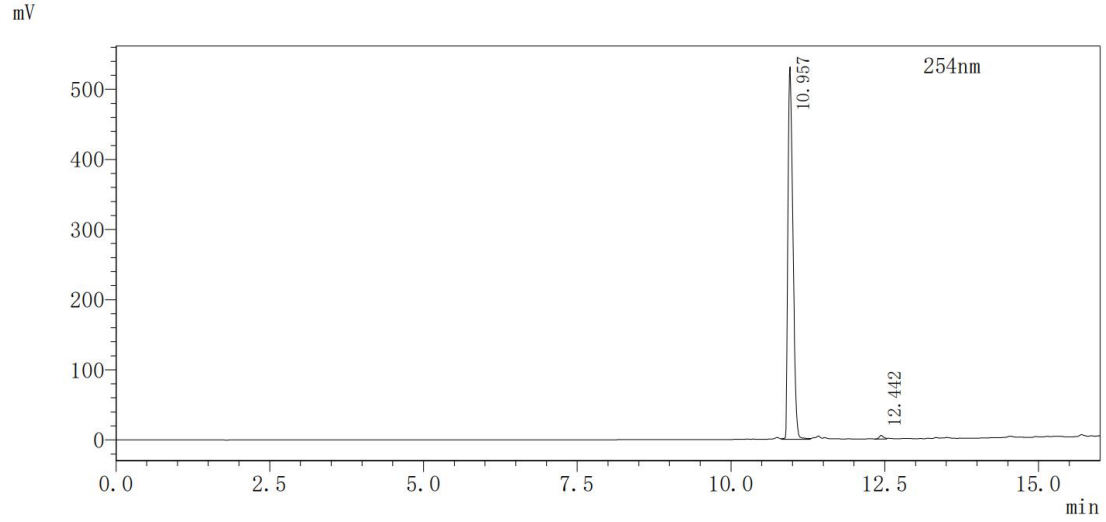
Peak	Retention time	Area	Height	Concentration	Height%
1	12.686	733923	177088	95.213	97.862
2	15.484	36900	3868	4.787	2.138
Total		770823	180956		100.000

33c



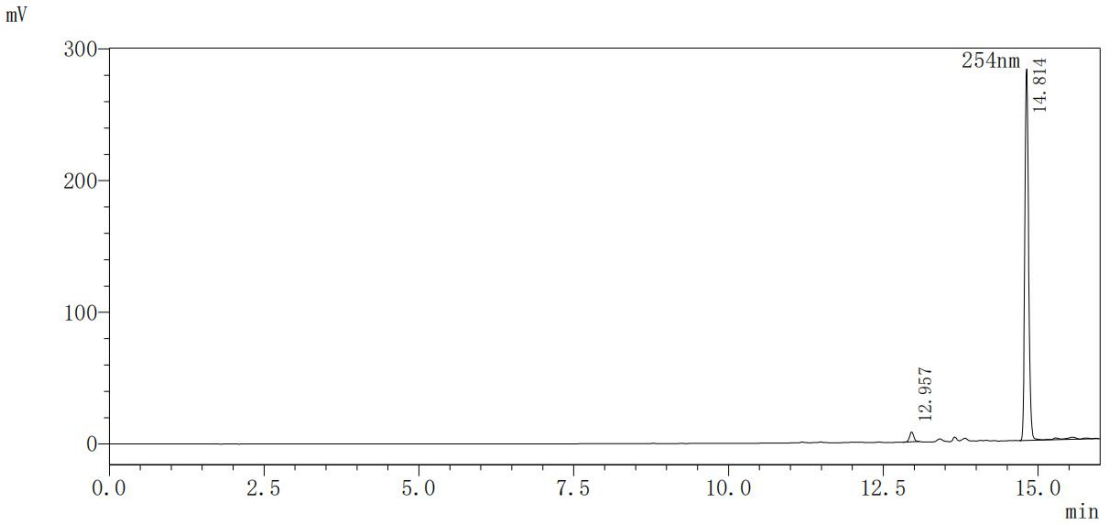
Peak	Retention time	Area	Height	Concentration	Height%
1	11.672	2721146	537371	100.000	100.000
Total		2721146	537371		100.000

33d



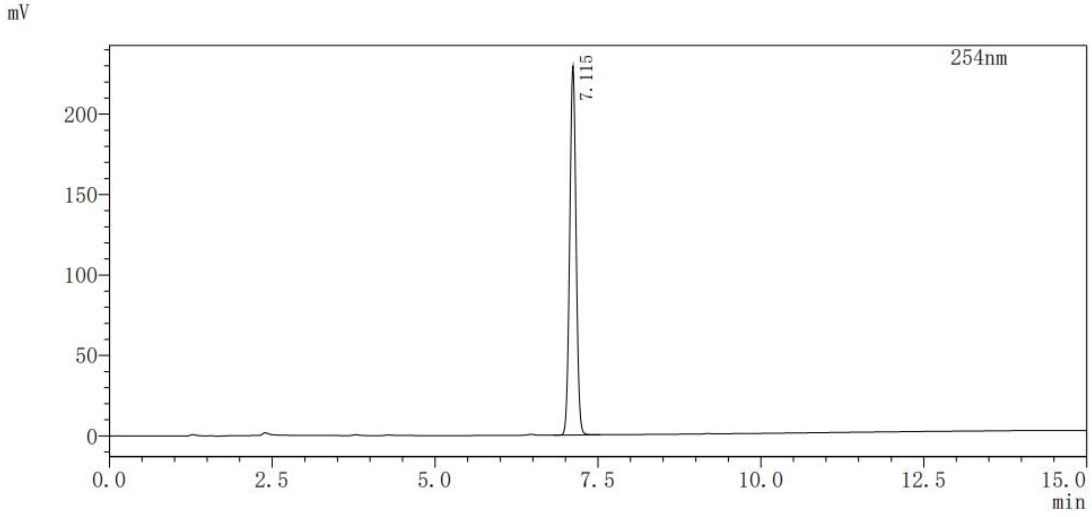
Peak	Retention time	Area	Height	Concentration	Height%
1	10.957	3022064	531122	99.206	99.076
2	12.442	24185	4954	0.794	0.924
Total		3046250	536076		100.000

34a



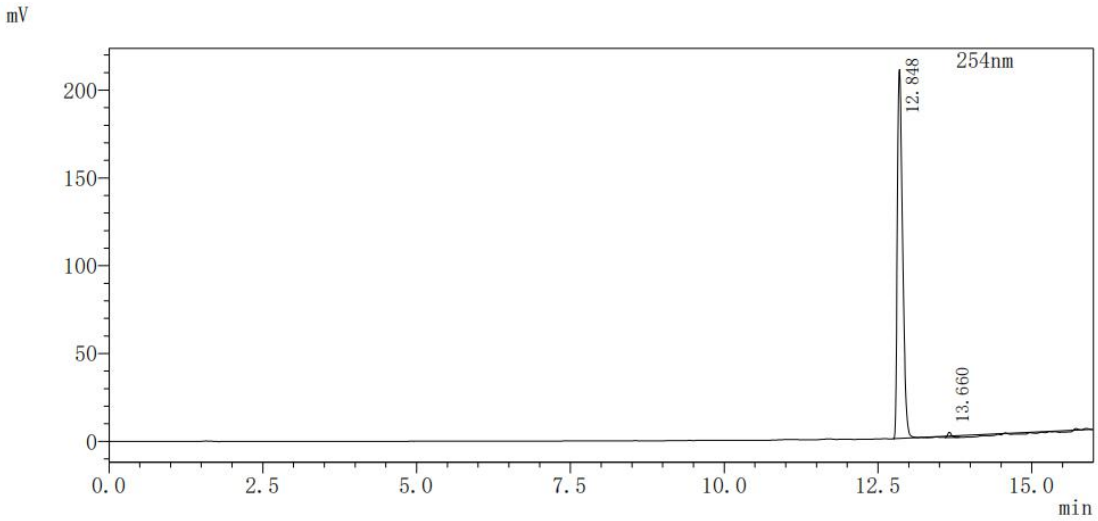
Peak	Retention time	Area	Height	Concentration	Height%
1	12.957	34527	7449	2.796	2.573
2	14.814	1200497	282077	97.204	97.427
Total		1235024	289526		100.000

34b



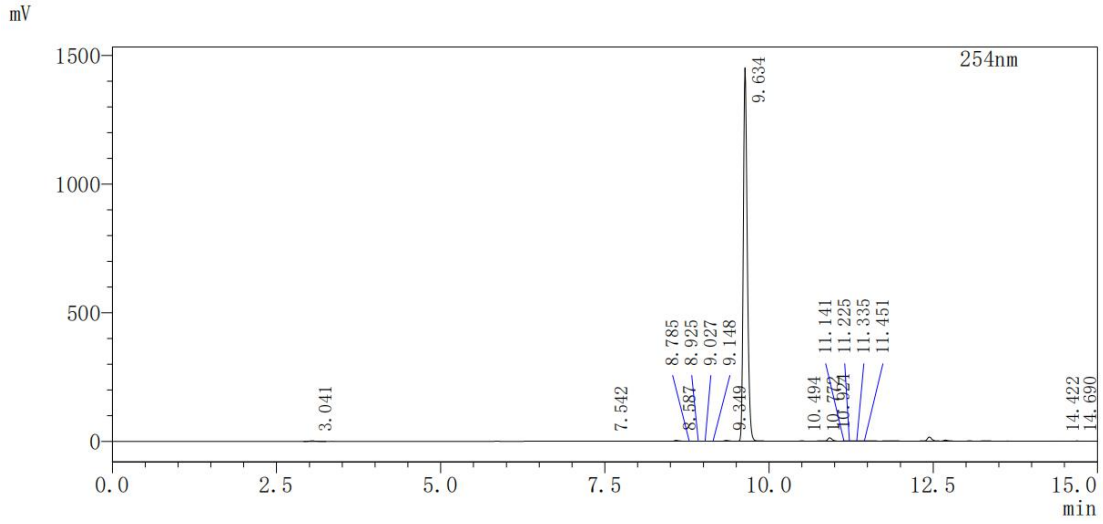
Peak	Retention time	Area	Height	Concentration	Height%
1	7.115	1561783	229312	100.000	100.000
Total		1561783	229312		100.000

34c



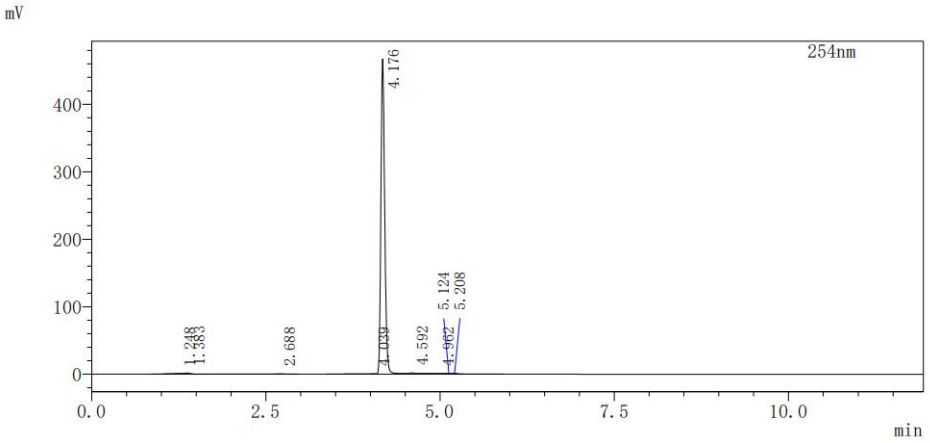
Peak	Retention time	Area	Height	Concentration	Height%
1	12.848	1175126	210333	99.005	98.598
2	13.660	11812	2992	0.995	1.402
Total		1186938	213325		100.000

38a



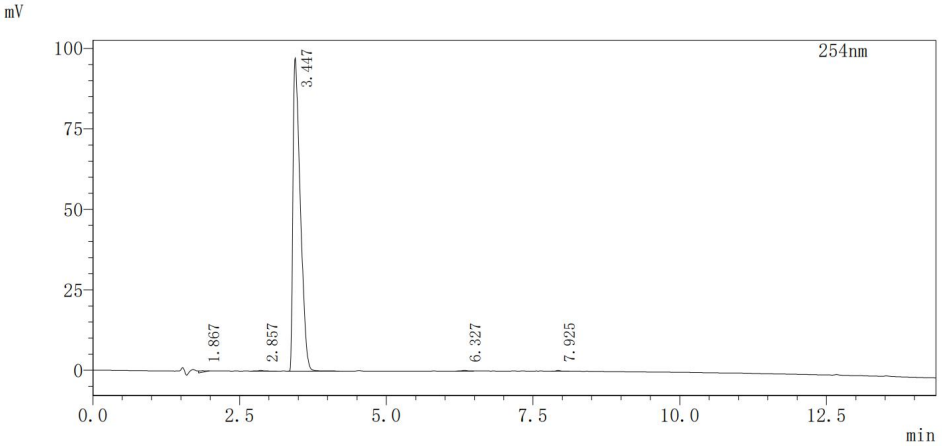
Peak	Retention time	Area	Height	Area%	Height%
1	3.041	9755	1897	0.152	0.128
2	7.542	1555	152	0.024	0.010
3	8.587	17885	3192	0.279	0.216
4	8.785	3179	526	0.050	0.036
5	8.925	2191	459	0.034	0.031
6	9.027	3782	554	0.059	0.037
7	9.148	2834	509	0.044	0.034
8	9.349	18942	2994	0.295	0.202
9	9.634	6266908	1451080	97.606	98.057
10	10.494	3364	569	0.052	0.038
11	10.772	4492	644	0.070	0.044
12	10.924	60670	13133	0.945	0.887
13	11.141	2581	563	0.040	0.038
14	11.225	3998	925	0.062	0.063
15	11.335	8174	1221	0.127	0.083
16	11.451	7287	958	0.113	0.065
17	14.422	1558	204	0.024	0.014
18	14.690	1437	253	0.022	0.017
Total		6420593	1479834	100.000	100.000

38b



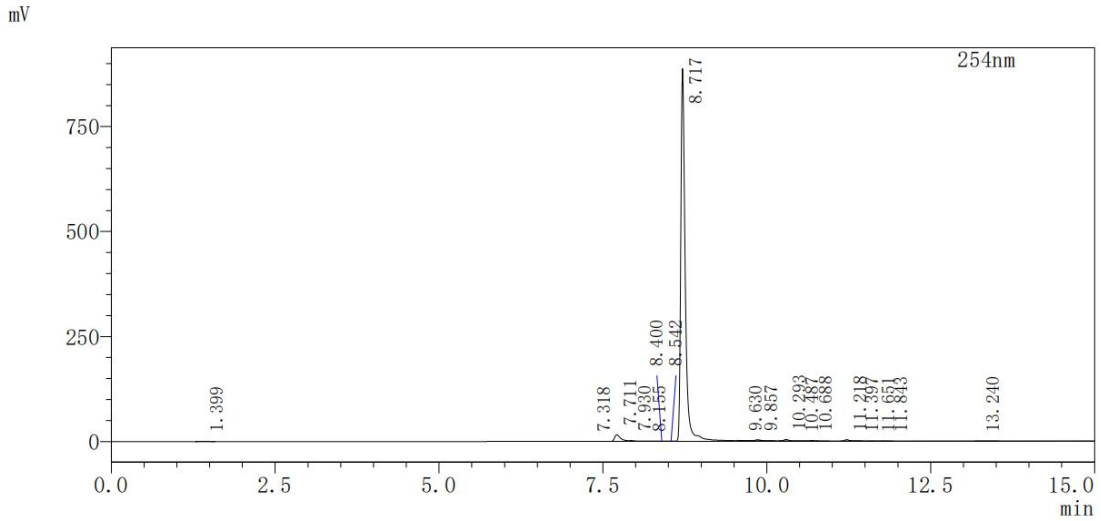
Peak	Retention time	Area	Height	Area%	Height%
1	1.248	15007	1196	0.794	0.250
2	1.383	12522	1790	0.663	0.374
3	2.688	4608	513	0.244	0.107
4	4.039	15134	767	0.801	0.161
5	4.176	1780515	467450	94.210	97.821
6	4.592	22302	2026	1.180	0.424
7	4.962	22474	1312	1.189	0.275
8	5.124	6151	1252	0.325	0.262
9	5.208	11232	1558	0.594	0.326
Total		1889945	477864	100.000	100.000

38c



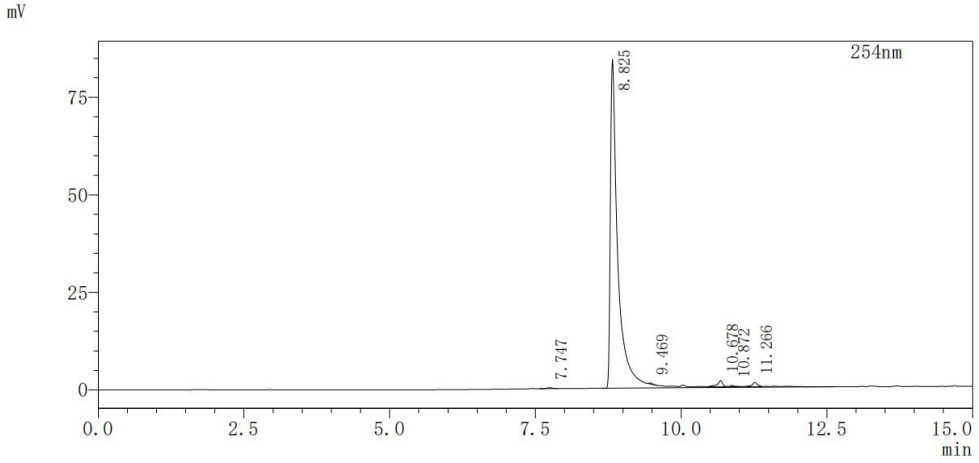
Peak	Retention time	Area	Height	Concentration	Height%
1	1.867	3396	440	0.395	0.447
2	2.857	1217	197	0.142	0.200
3	3.447	851983	97275	99.193	98.880
4	6.327	1270	212	0.148	0.216
5	7.925	1045	252	0.122	0.256
Total		858911	98377		100.000

38d



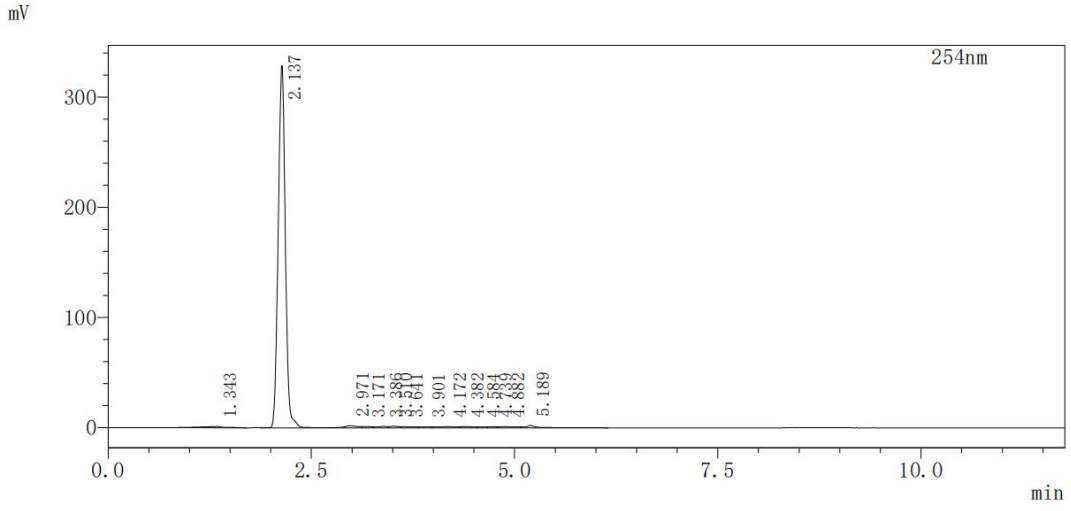
Peak	Retention time	Area	Height	Area%	Height%
1	1.399	2371	291	0.052	0.032
2	7.318	1094	157	0.024	0.017
3	7.711	105740	15788	2.327	1.715
4	7.930	16075	2168	0.354	0.236
5	8.155	7106	689	0.156	0.075
6	8.400	2901	467	0.064	0.051
7	8.542	5237	731	0.115	0.079
8	8.717	4333296	887724	95.349	96.414
9	9.630	2494	547	0.055	0.059
10	9.857	15611	2534	0.344	0.275
11	10.293	17405	3566	0.383	0.387
12	10.487	2874	444	0.063	0.048
13	10.688	6119	1086	0.135	0.118
14	11.218	17509	3348	0.385	0.364
15	11.397	4890	605	0.108	0.066
16	11.651	1071	173	0.024	0.019
17	11.843	1021	155	0.022	0.017
18	13.240	1834	266	0.040	0.029
Total		4544648	920739	100.000	100.000

38e



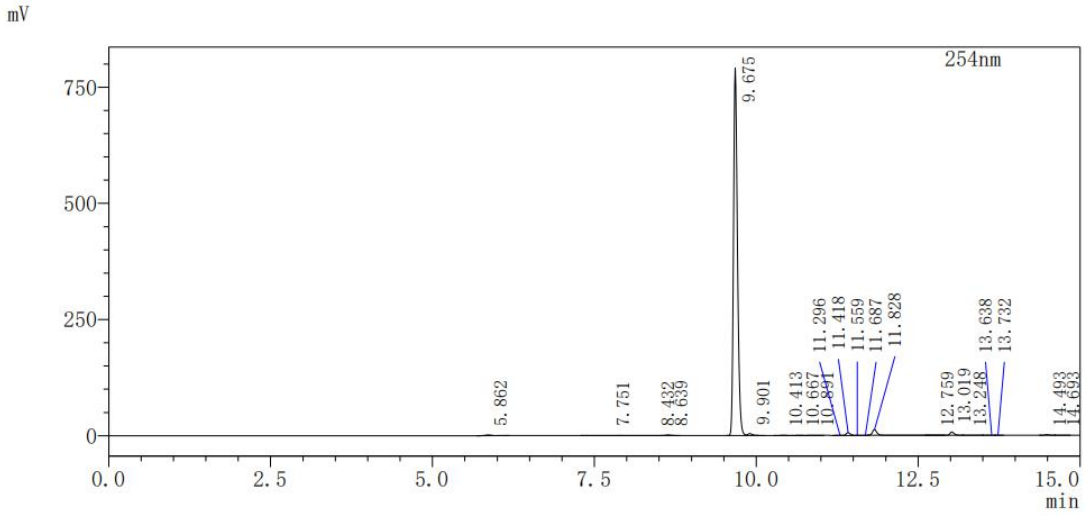
Peak	Retention time	Area	Height	Area%	Height%
1	7.747	1686	243	0.209	0.276
2	8.825	782472	84208	97.077	95.885
3	9.469	1011	270	0.125	0.307
4	10.678	10400	1617	1.290	1.841
5	10.872	2262	369	0.281	0.420
6	11.266	8201	1116	1.017	1.270
Total		806032	87821	100.000	100.000

38f



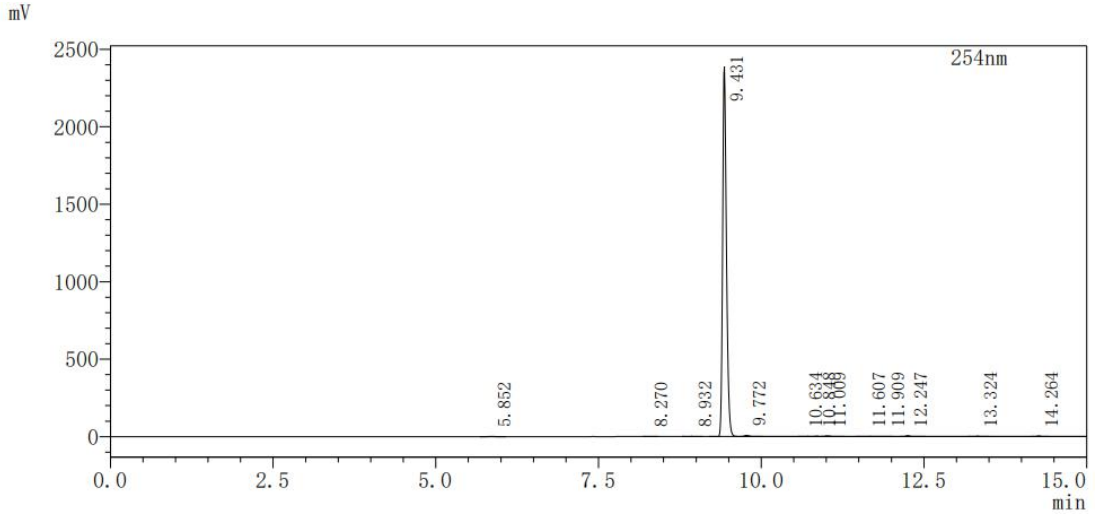
Peak	Retention time	Area	Height	Height%
1	1.343	26596	1237	0.358
2	2.137	1998517	328621	95.153
3	2.971	23611	1941	0.562
4	3.171	8240	1096	0.317
5	3.386	12519	1337	0.387
6	3.510	11152	1606	0.465
7	3.641	12311	1026	0.297
8	3.901	9091	938	0.272
9	4.172	19573	1063	0.308
10	4.382	13118	1197	0.347
11	4.584	6789	936	0.271
12	4.739	7110	1004	0.291
13	4.882	15948	1076	0.312
14	5.189	21652	2280	0.660
Total		2186229	345359	100.000

38g



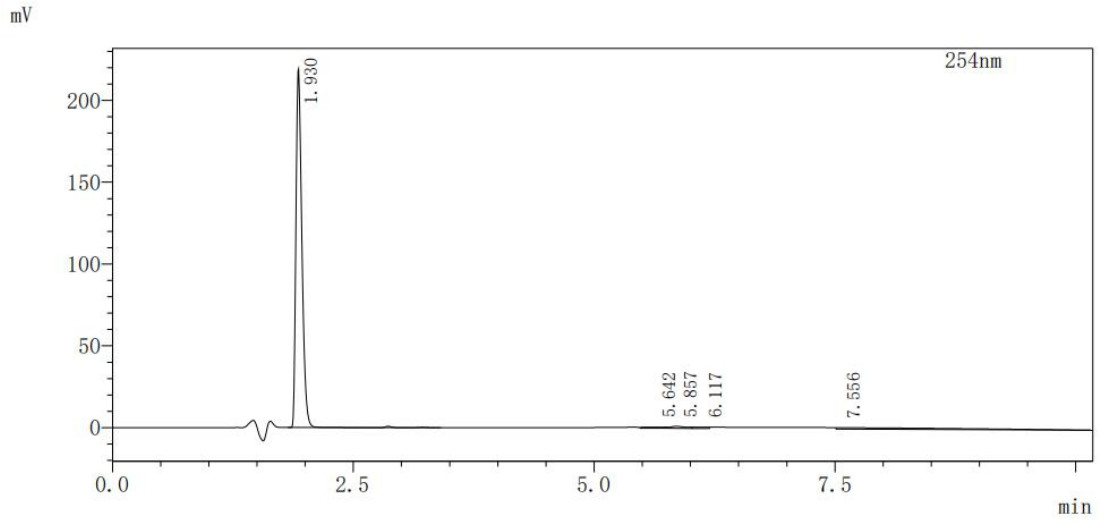
Peak	Retention time	Area	Height	Area%	Height%
1	5.862	11496	1445	0.325	0.174
2	7.751	3362	320	0.095	0.039
3	8.432	5895	259	0.167	0.031
4	8.639	7087	1218	0.201	0.147
5	9.675	3338456	791599	94.465	95.457
6	9.901	19849	3947	0.562	0.476
7	10.413	1625	194	0.046	0.023
8	10.667	1461	208	0.041	0.025
9	10.891	3910	598	0.111	0.072
10	11.296	1157	211	0.033	0.025
11	11.418	26460	5854	0.749	0.706
12	11.559	2884	661	0.082	0.080
13	11.687	1796	413	0.051	0.050
14	11.828	63323	12641	1.792	1.524
15	12.759	1069	127	0.030	0.015
16	13.019	32942	7351	0.932	0.886
17	13.248	2778	416	0.079	0.050
18	13.638	1041	172	0.029	0.021
19	13.732	1187	262	0.034	0.032
20	14.493	5276	1187	0.149	0.143
21	14.693	1031	196	0.029	0.024
Total		3534081	829277	100.000	100.000

38h



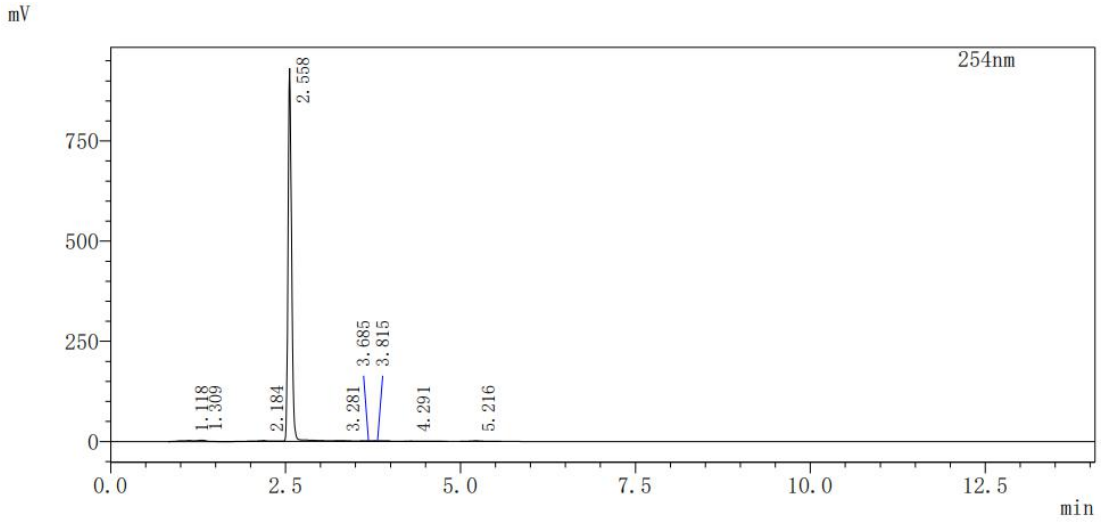
Peak	Retention time	Area	Height	Height%
1	5.852	4751	700	0.048
2	8.270	1550	360	0.016
3	8.932	7358	1615	0.075
4	9.431	9709719	2388428	98.586
5	9.772	33100	6862	0.336
6	10.634	1402	280	0.014
7	10.848	12460	2850	0.127
8	11.009	26548	4700	0.270
9	11.607	1111	123	0.011
10	11.909	3580	244	0.036
11	12.247	24711	5347	0.251
12	13.324	8751	1727	0.089
13	14.264	13960	3379	0.142
Total		9849003	2416617	100.000

38i



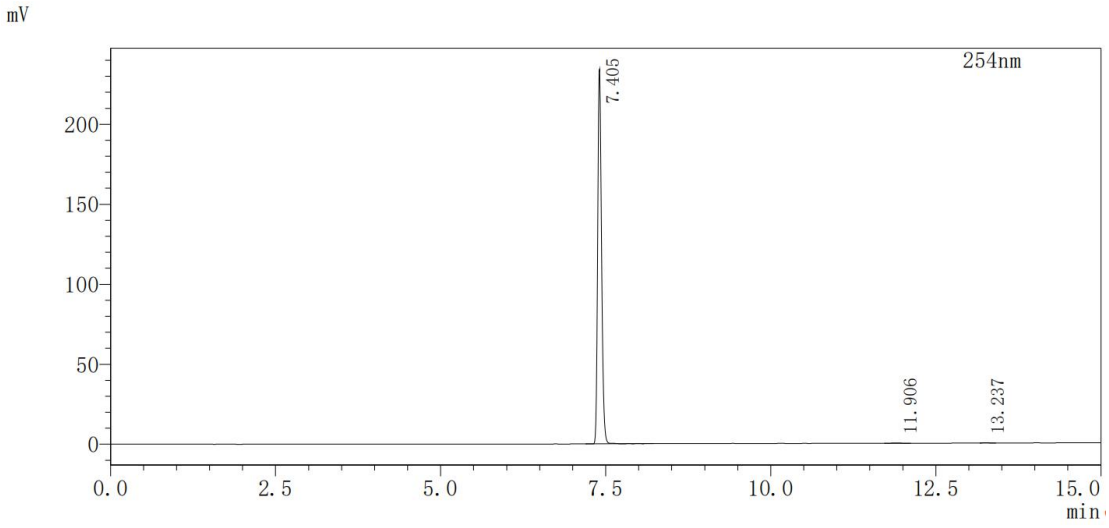
Peak	Retention time	Area	Height	Concentration	Height%
1	1.930	959773	218892	88.939	98.426
2	5.642	9280	599	0.860	0.269
3	5.857	14328	1239	1.328	0.557
4	6.117	8126	748	0.753	0.336
5	7.556	87633	915	8.121	0.412
Total		1079140	222393		100.000

38j



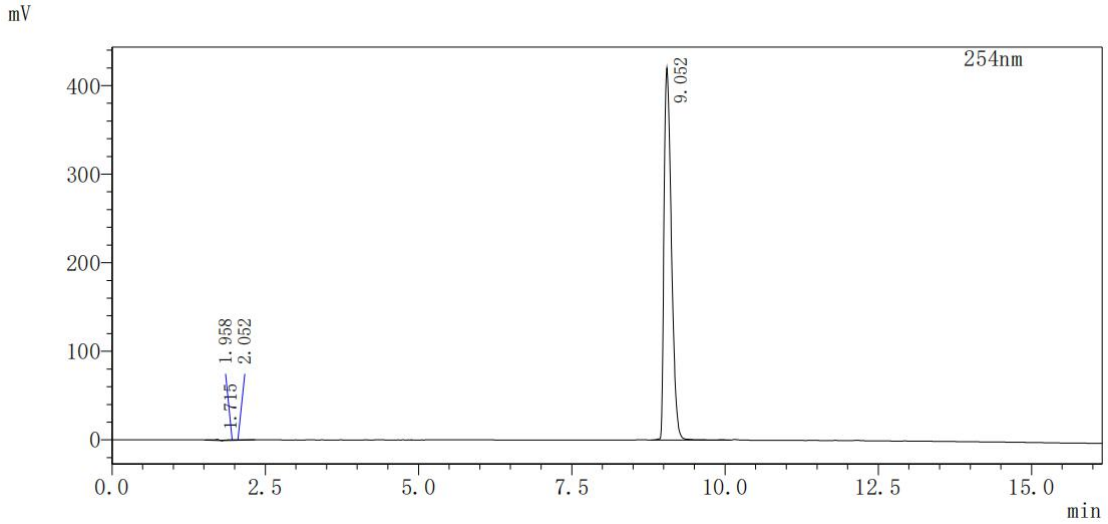
Peak	Retention time	Area	Height	Height%
1	1.118	30956	2615	0.278
2	1.309	30888	3206	0.340
3	2.184	34541	2353	0.250
4	2.558	3390611	931474	98.839
5	3.281	3696	583	0.062
6	3.685	1300	164	0.017
7	3.815	1892	437	0.046
8	4.291	1103	74	0.008
9	5.216	11351	1513	0.161
Total		3506338	942420	100.000

38k



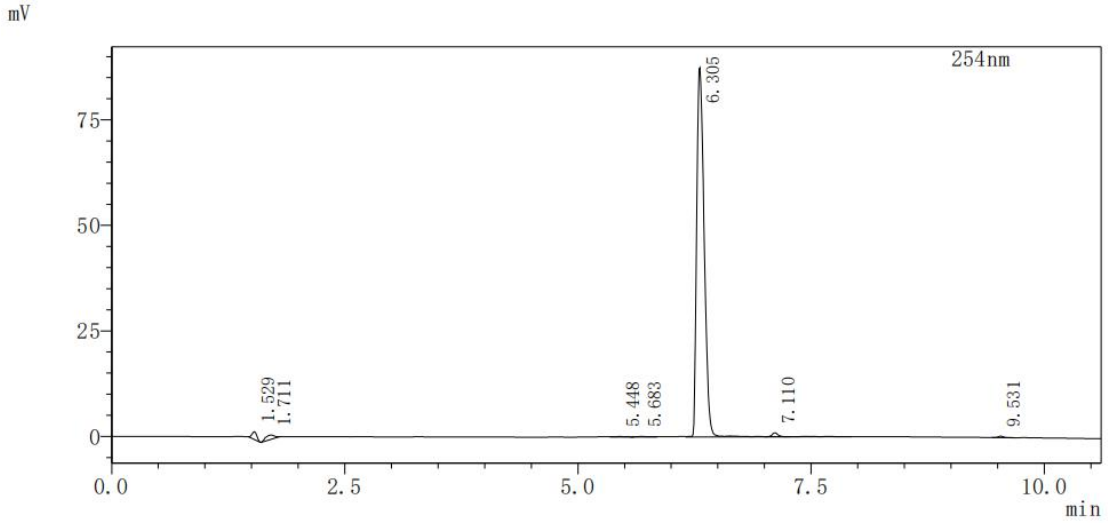
Peak	Retention time	Area	Height	Area%	Height%
1	7.405	951766	234227	99.701	99.834
2	11.906	1524	149	0.160	0.063
3	13.237	1335	240	0.140	0.102
Total		954625	234615	100.000	100.000

38l



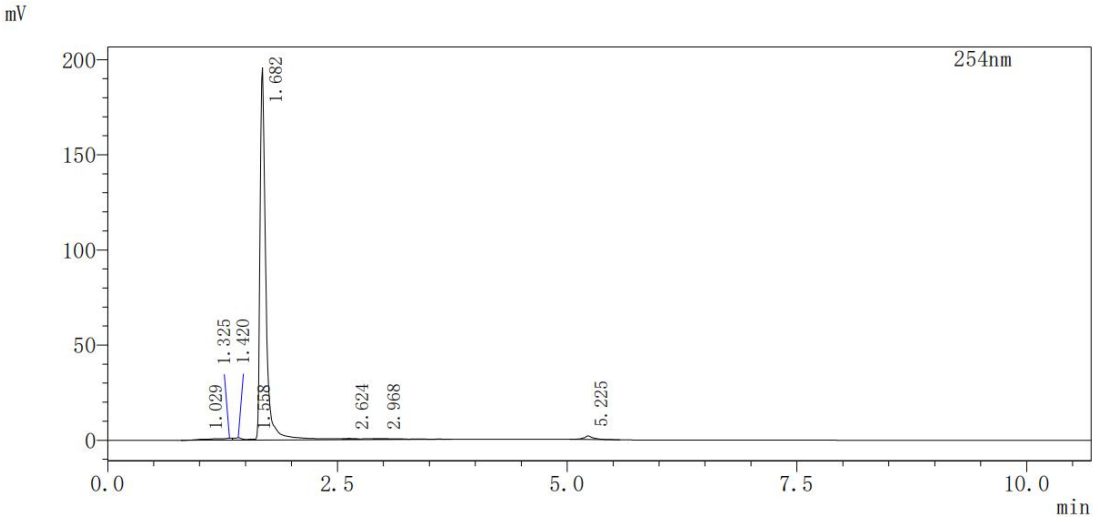
Peak	Retention time	Area	Height	Concentration	Height%
1	1.715	6170	1121	0.175	0.266
2	1.958	6435	687	0.183	0.163
3	2.052	4302	489	0.122	0.116
4	9.052	3504065	419960	99.520	99.456
Total		3520971	422258		100.000

38m



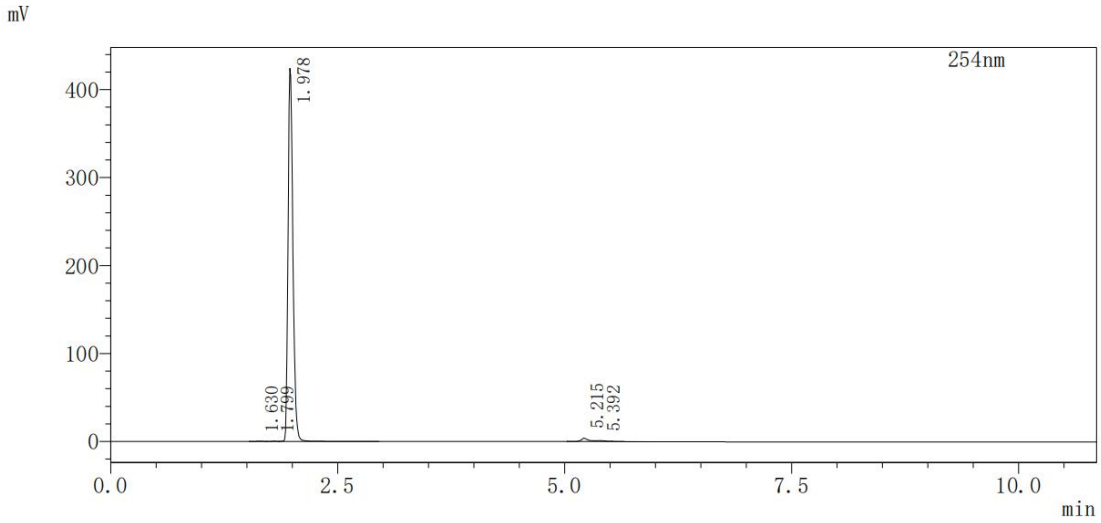
Peak	Retention time	Area	Height	Area%	Height%
1	1.529	6322	1802	1.241	1.963
2	1.711	7451	1002	1.463	1.092
3	5.448	1084	125	0.213	0.136
4	5.683	1154	126	0.227	0.137
5	6.305	488127	87482	95.842	95.296
6	7.110	3780	922	0.742	1.005
7	9.531	1384	342	0.272	0.372
Total		509301	91800	100.000	100.000

38n



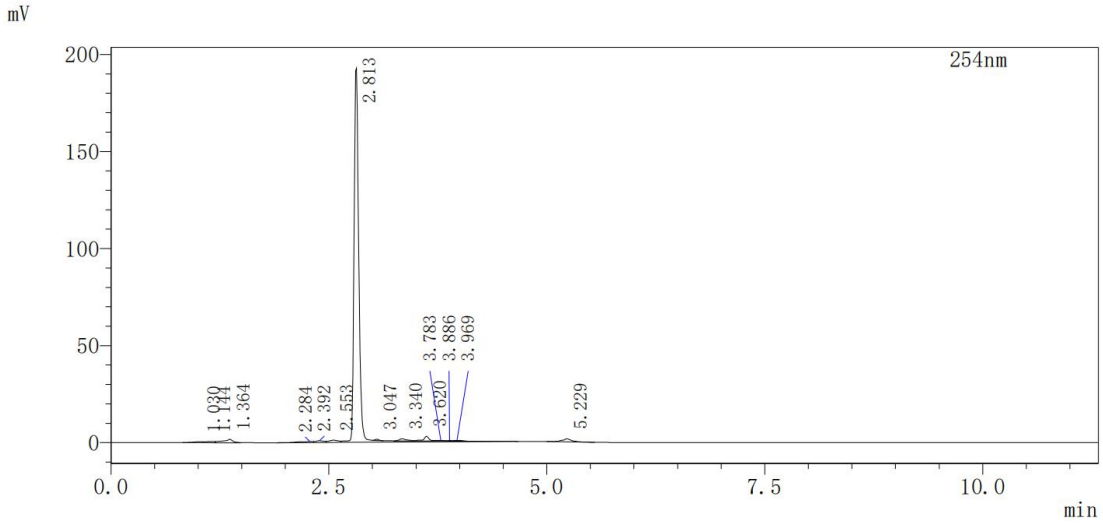
Peak	Retention time	Area	Height	Height%
1	1.029	3578	485	0.241
2	1.325	12788	962	0.479
3	1.420	7081	1229	0.612
4	1.558	1773	389	0.194
5	1.682	873287	195576	97.371
6	2.624	1005	224	0.111
7	2.968	1506	130	0.065
8	5.225	12948	1862	0.927
Total		913966	200856	100.000

38o



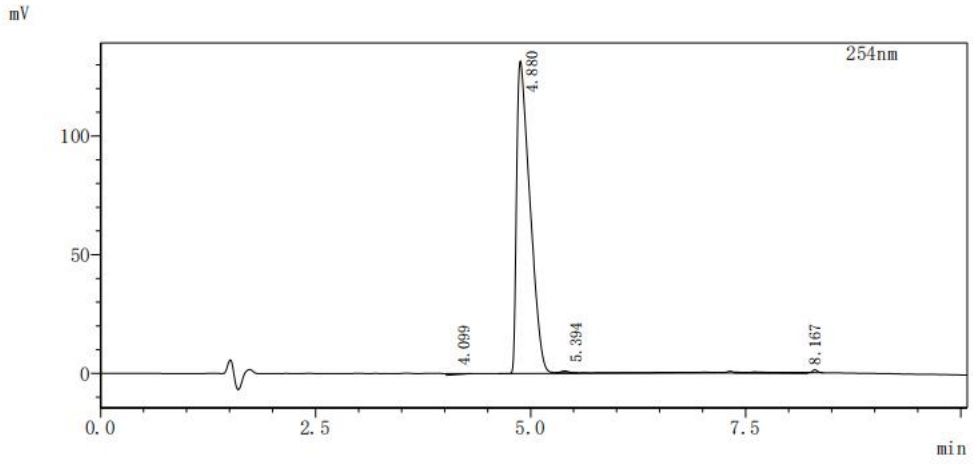
Peak	Retention time	Area	Height	Area%	Height%
1	1.630	1643	372	0.102	0.087
2	1.799	1318	188	0.082	0.044
3	1.978	1575032	424241	97.854	98.729
4	5.215	21187	3882	1.316	0.903
5	5.392	10395	1020	0.646	0.237
Total		1609575	429702	100.000	100.000

38p



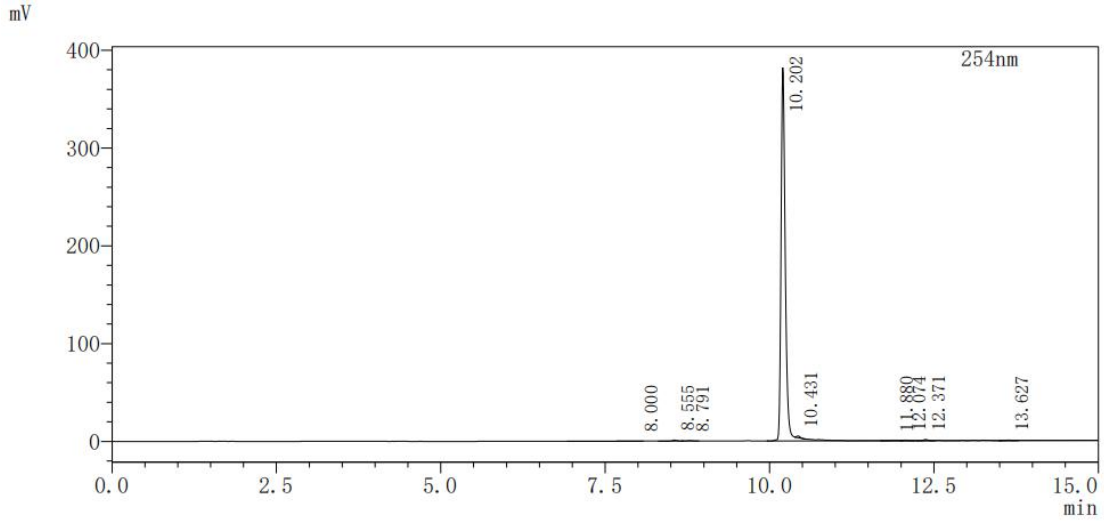
Peak	Retention time	Area	Height	Height%
1	1.030	4226	527	0.257
2	1.144	5120	646	0.315
3	1.364	14115	1761	0.859
4	2.284	7007	584	0.285
5	2.392	6032	910	0.444
6	2.553	9216	1183	0.577
7	2.813	746156	192697	94.001
8	3.047	1746	588	0.287
9	3.340	6622	1098	0.536
10	3.620	10523	2373	1.158
11	3.783	2726	396	0.193
12	3.886	1393	316	0.154
13	3.969	2753	376	0.184
14	5.229	11809	1540	0.751
Total		829443	204995	100.000

38q



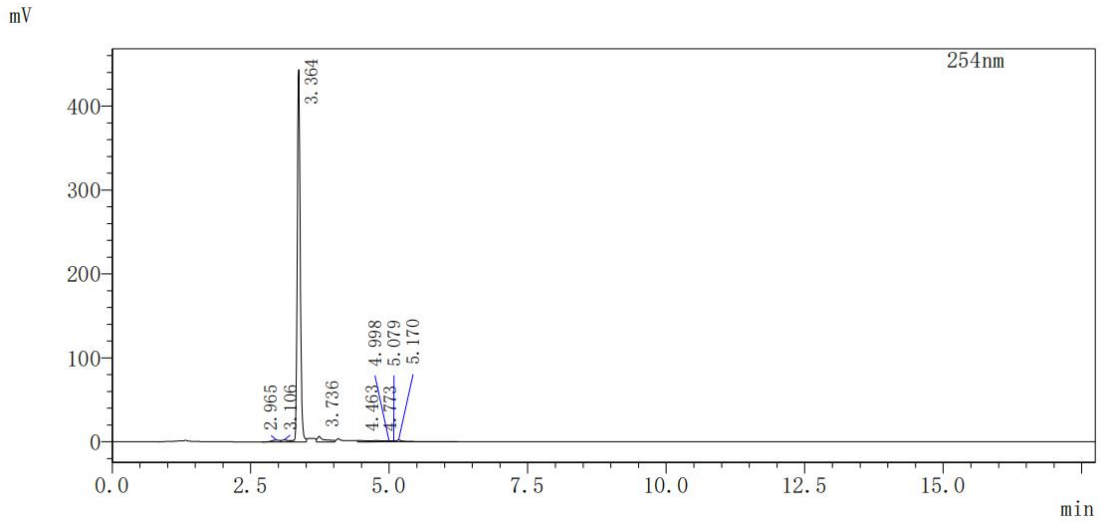
Peak	Retention time	Area	Height	Concentration	Height%
1	4.099	6364	538	0.429	0.404
2	4.880	1456929	131545	98.288	98.840
3	5.394	4332	764	0.292	0.574
4	8.167	14683	242	0.991	0.182
Total			1482307	133089	100.000

38r



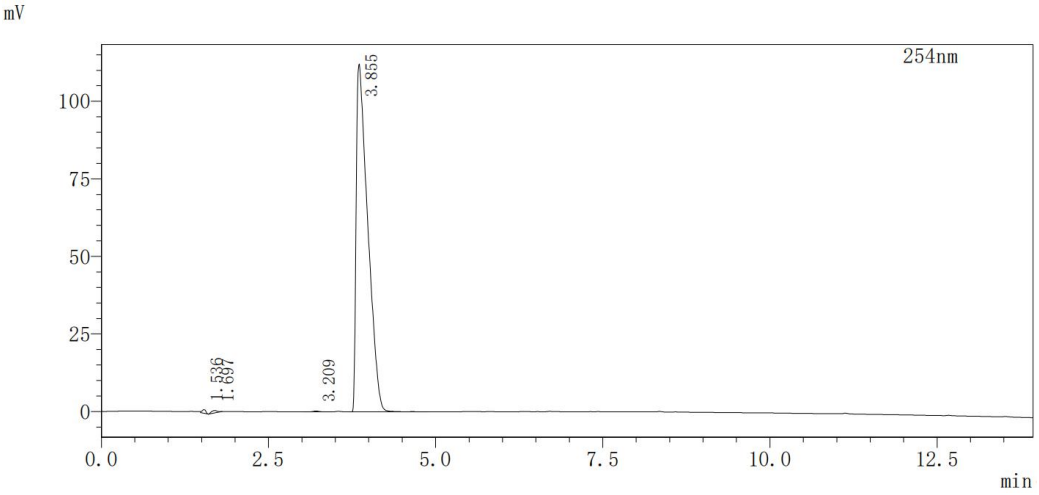
Peak	Retention time	Area	Height	Area%	Height%
1	8.000	4682	98	0.262	0.025
2	8.555	6473	1017	0.362	0.262
3	8.791	3574	483	0.200	0.125
4	10.202	1753587	381815	98.143	98.561
5	10.431	5818	1699	0.326	0.439
6	11.880	2874	258	0.161	0.067
7	12.074	2207	444	0.124	0.115
8	12.371	4978	1112	0.279	0.287
9	13.627	2580	463	0.144	0.120
Total		1786774	387389	100.000	100.000

38s



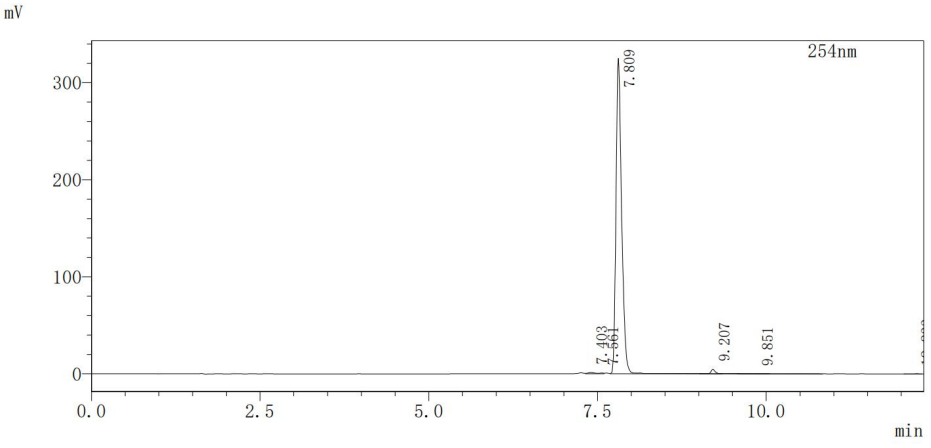
Peak	Retention time	Area	Height	Concentration	Height%
1	2.965	21086	2101	1.141	0.454
2	3.106	19805	2356	1.072	0.510
3	3.364	1672624	443553	90.523	95.922
4	3.736	60397	6545	3.269	1.415
5	4.463	16531	1658	0.895	0.358
6	4.773	20130	1355	1.089	0.293
7	4.998	9676	1230	0.524	0.266
8	5.079	5364	1202	0.290	0.260
9	5.170	22119	2408	1.197	0.521
Total		1847732	462409		100.000

26



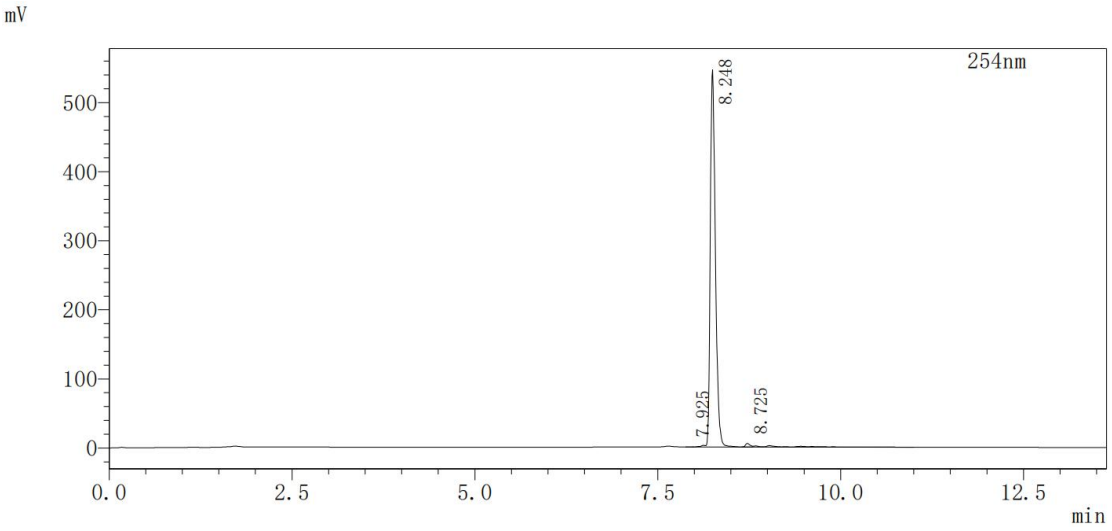
Peak	Retention time	Area	Height	Height%
1	1.536	4277	1166	1.020
2	1.697	5109	778	0.681
3	3.209	1617	285	0.250
4	3.855	1347736	112051	98.049
Total		1358739	114281	100.000

42a



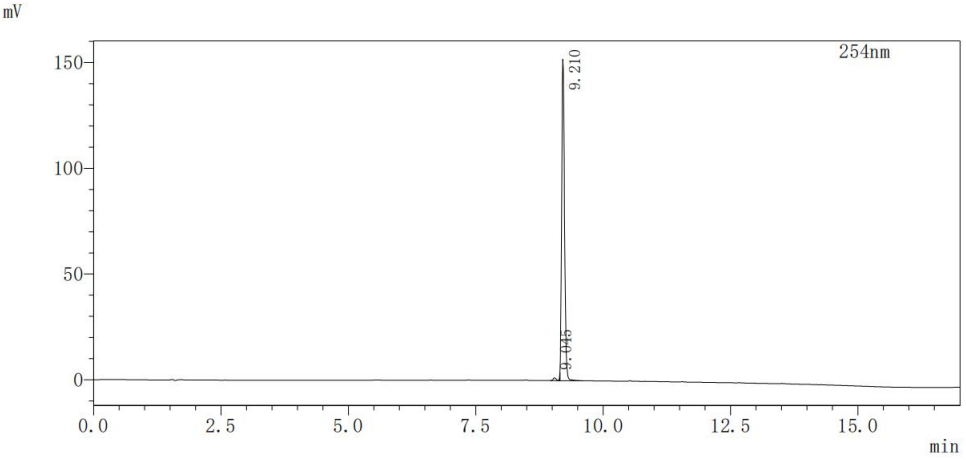
Peak	Retention time	Area	Height	Area%	Height%
1	7.403	10235	1295	0.526	0.390
2	7.561	3604	902	0.185	0.272
3	7.809	1912438	325052	98.215	97.935
4	9.207	18292	4370	0.939	1.317
5	9.851	1381	79	0.071	0.024
6	12.233	1245	209	0.064	0.063
Total		1947195	331907	100.000	100.000

42b



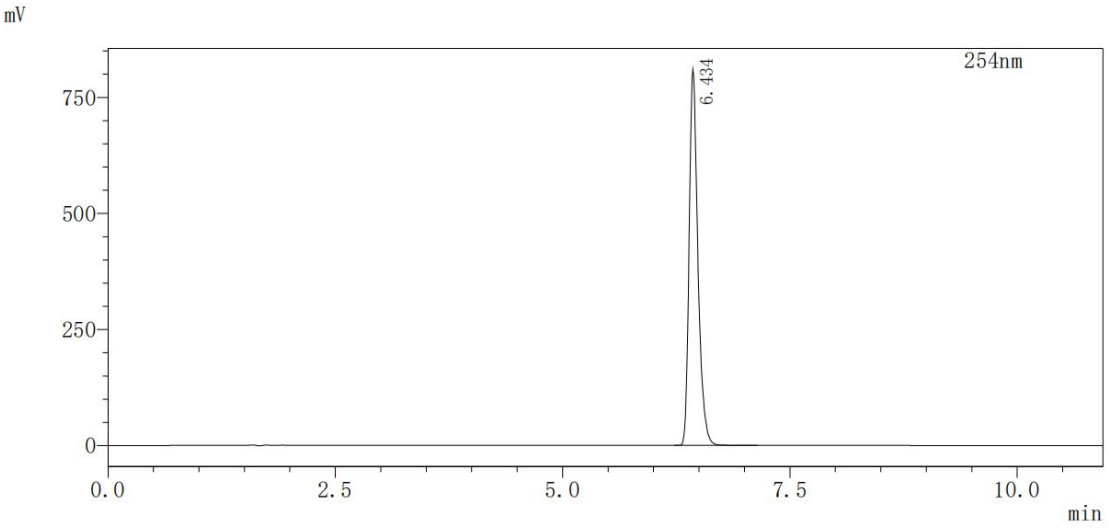
Peak	Retention time	Area	Height	Concentration	Height%
1	7.925	1130	218	2.074	0.039
2	8.248	2741957	546177	2.761	99.053
3	8.725	21013	5002	95.165	0.907
Total		2764100	551397		100.000

42c



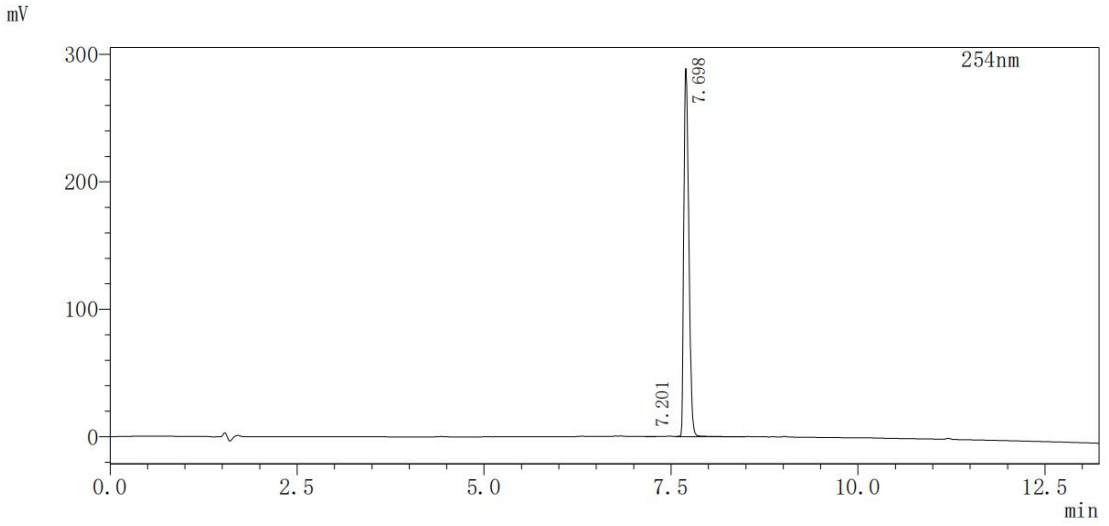
Peak	Retention time	Area	Height	Concentration	Height%
1	9.045	7848	1355	1.310	0.884
2	9.210	591005	151953	98.690	99.116
Total		598852	153309		100.000

42d



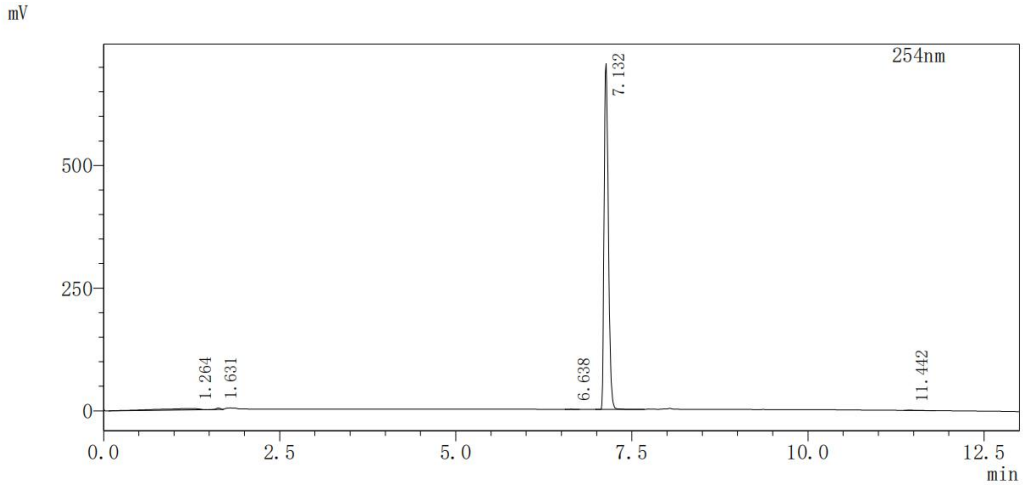
Peak	Retention time	Area	Height	Concentration	Height%
1	6.434	5426904	809601	100.000	
Total		5426904	809601		

42e



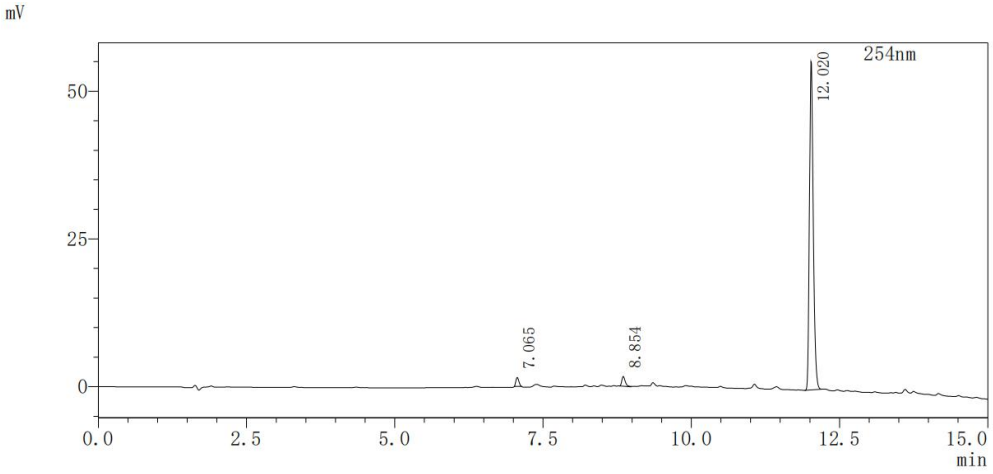
Peak	Retention time	Area	Height	Area%	Height%
1	7.201	1180	158	0.088	0.055
2	7.698	1347150	288999	99.912	99.945
Total		1348330	289156	100.000	100.000

42f



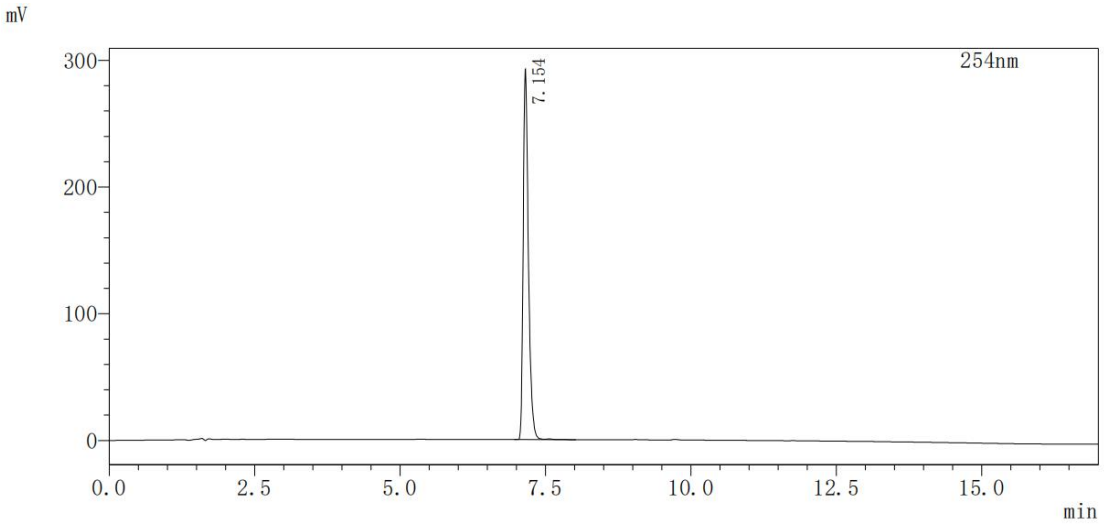
Peak	Retention time	Area	Height	Area%	Height%
1	1.264	122566	2537	3.955	0.357
2	1.631	13764	3046	0.444	0.428
3	6.638	1547	327	0.050	0.046
4	7.132	2958563	704846	95.457	99.086
5	11.442	2921	591	0.094	0.083
Total		3099361	711346	100.000	100.000

42g



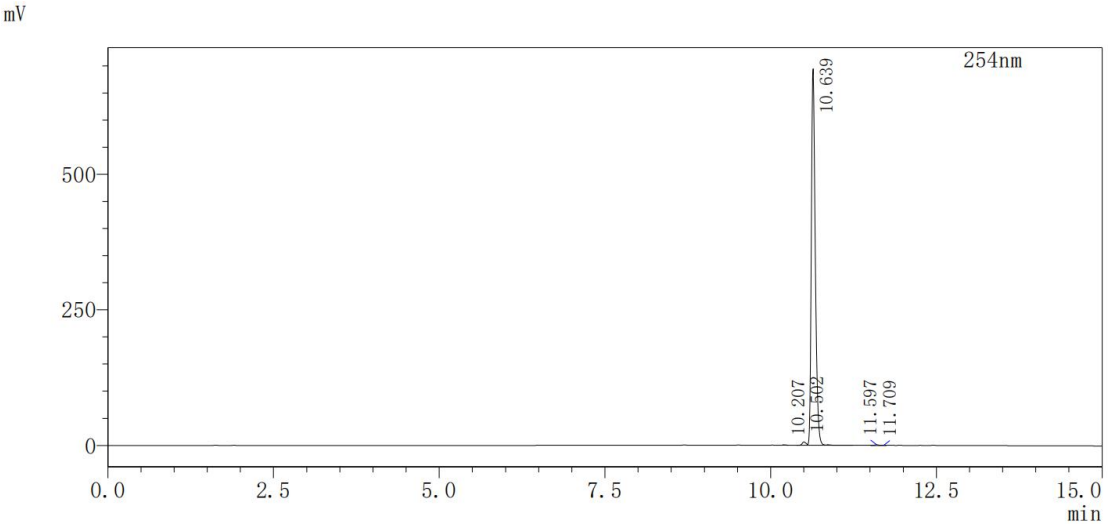
Peak	Retention time	Area	Height	Concentration	Height%
1	7.065	5252	1501	2.074	2.558
2	8.854	6993	1664	2.761	2.834
3	12.020	241010	55532	95.165	94.608
Total		253255	58697		100.000

42h



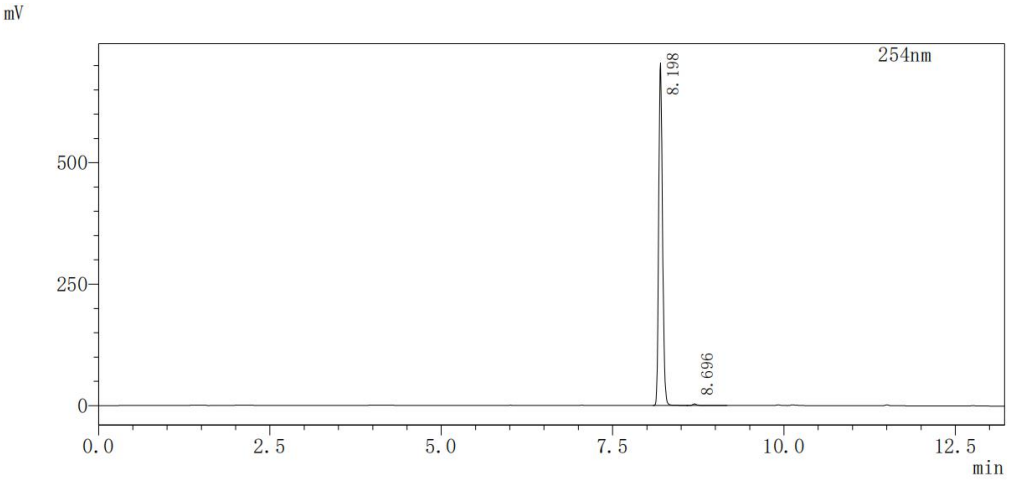
Peak	Retention time	Area	Height	Concentration	Height%
1	7.154	1818715	292284	100.000	100.000
Total		1818715	292284		100.000

42i



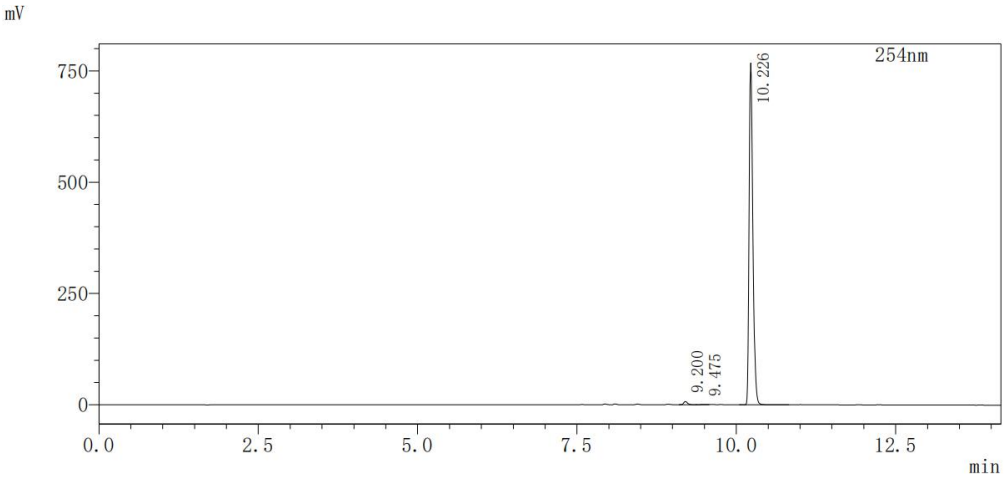
Peak	Retention time	Area	Height	Concentration	Height%
1	10.207	919	411	0.031	0.058
2	10.502	25287	6412	0.866	0.912
3	10.639	2889312	694478	98.896	98.826
4	11.597	5013	1140	0.172	0.162
5	11.709	1027	287	0.035	0.041
Total		2921560	702728		100.000

42j



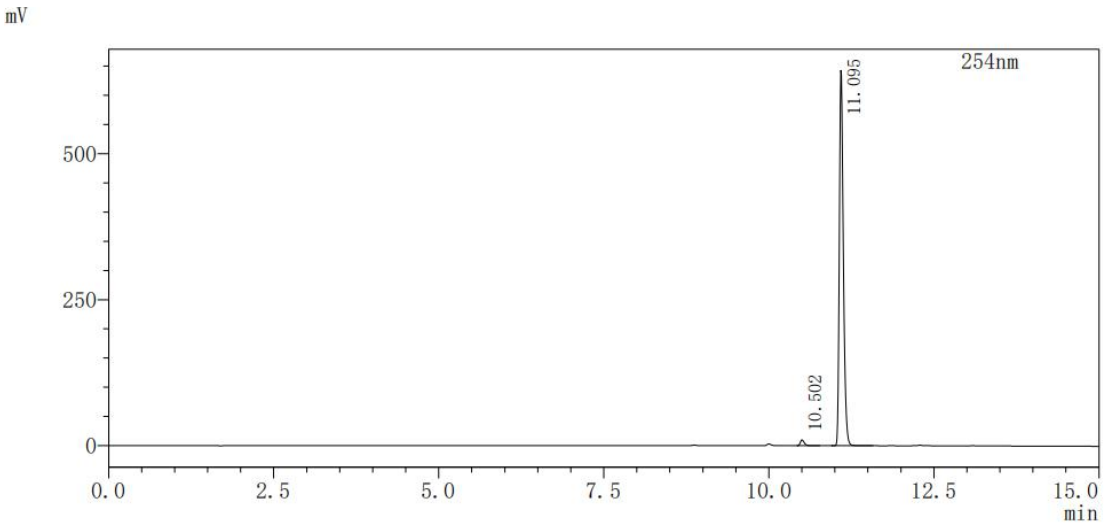
Peak	Retention time	Area	Height	Concentration	Height%
1	8.198	2725956	704990	99.525	99.567
2	8.696	13011	3068	0.475	0.433
Total		2738968	708058		100.000

43a



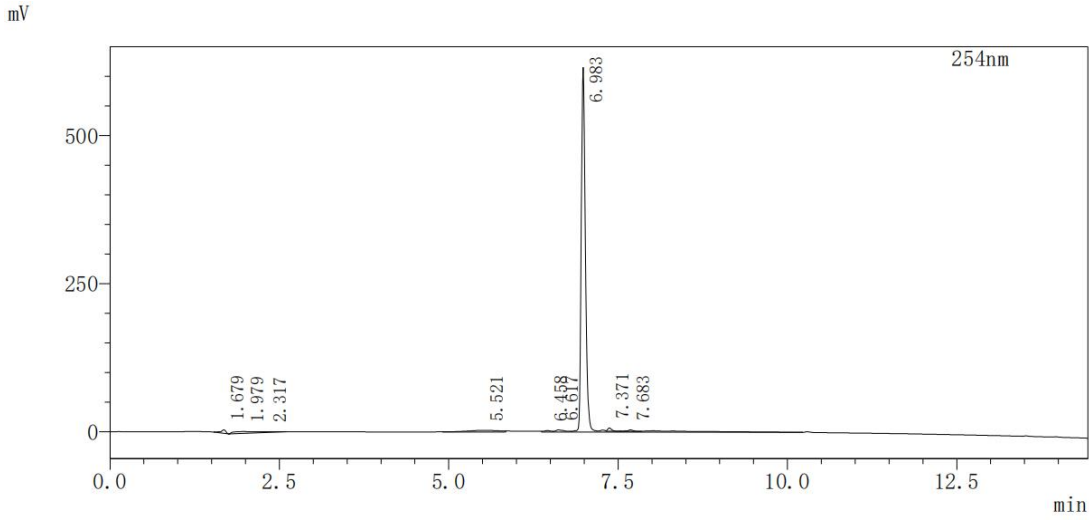
Peak	Retention time	Area	Height	Concentration	Height%
1	9.200	33934	7197	1.067	0.928
2	9.475	6486	829	0.204	0.107
3	10.226	3139682	767917	98.729	98.966
Total		3180103	775943		100.000

43b



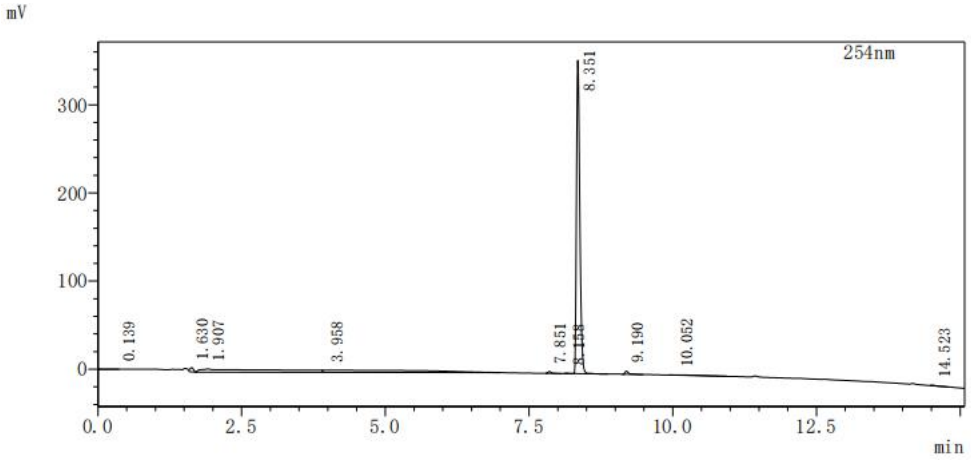
Peak	Retention time	Area	Height	Concentration	Height%
1	10.502	40433	9789	1.465	1.499
2	11.095	2718628	643044	98.535	98.501
Total		2759061	652833		100.000

43c



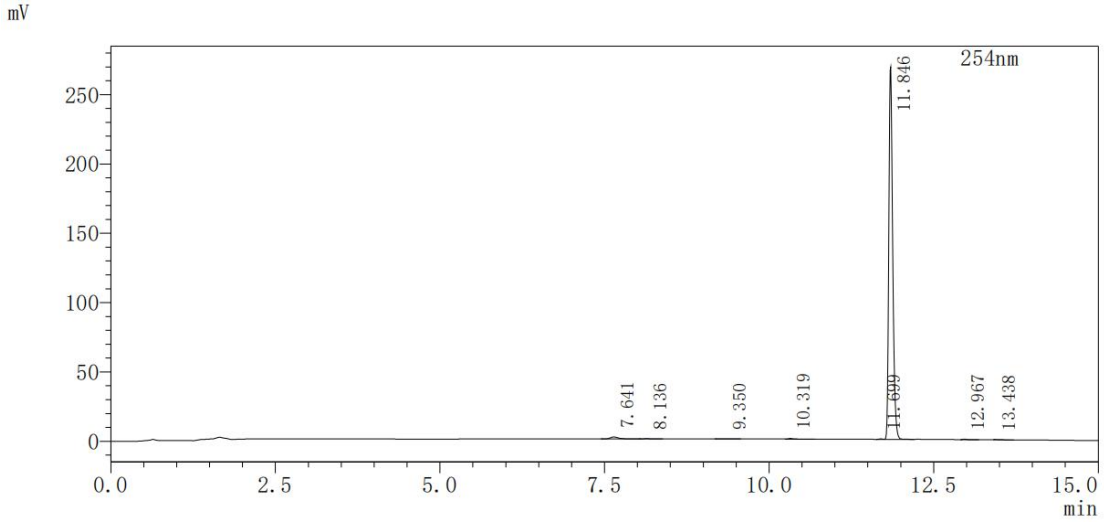
Peak	Retention time	Area	Height	Concentration	Height%
1	1.679	27319	5524	0.876	0.859
2	1.979	72311	3314	2.319	0.516
3	2.317	12677	1167	0.406	0.182
4	5.521	94156	2850	3.019	0.443
5	6.458	20336	2620	0.652	0.408
6	6.617	37421	3825	1.2	0.595
7	6.983	2819817	615929	90.417	95.833
8	7.371	20896	5172	0.67	0.805
9	7.683	13732	2308	0.44	0.359
Total		3118664	642708		100

43d



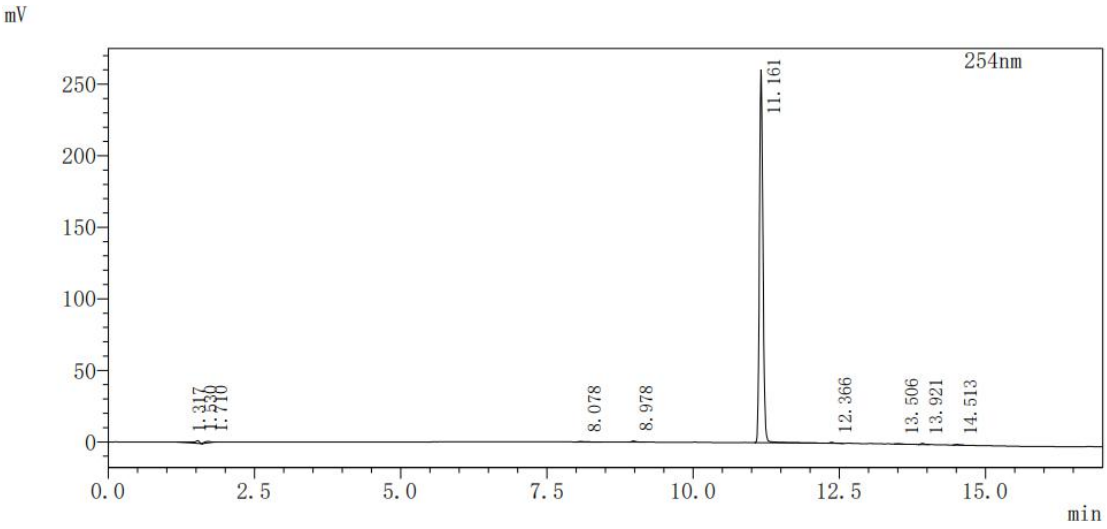
Peak	Retention time	Area	Height	Area%	Height%
1	0.139	2129	139	0.099	0.037
2	1.630	19431	4665	0.905	1.248
3	1.907	347990	3744	16.213	1.002
4	3.958	315752	2392	14.711	0.640
5	7.851	7847	2109	0.366	0.564
6	8.158	1824	510	0.085	0.136
7	8.351	1422967	355652	66.298	95.173
8	9.190	14987	3402	0.698	0.910
9	10.052	10393	264	0.484	0.071
10	14.523	2998	812	0.140	0.217
Total		2146317	373688	100.000	100.000

43e



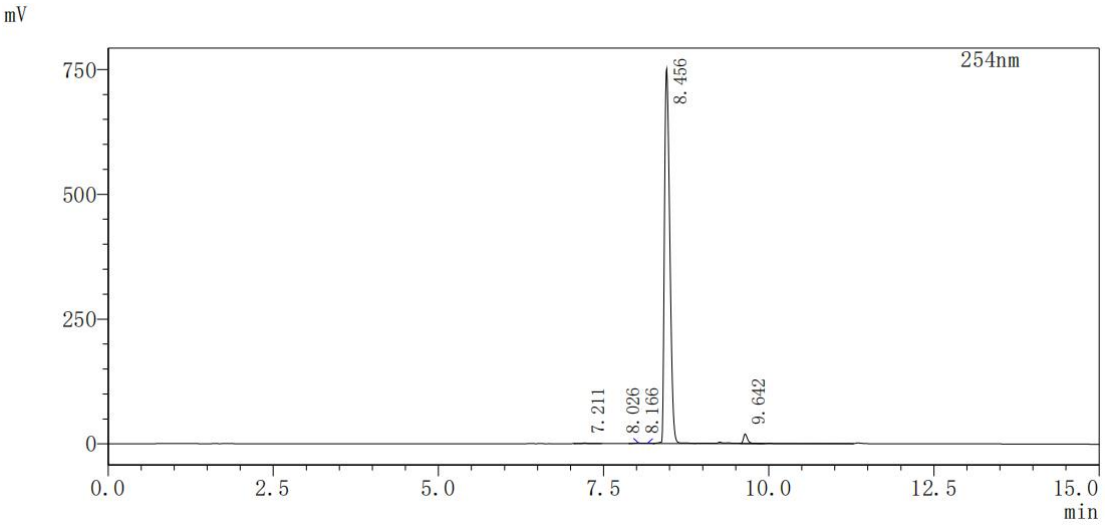
Peak	Retention time	Area	Height	Concentration	Height%
1	7.641	12534	1448	1.117	0.533
2	8.136	1314	219	0.117	0.081
3	9.35	1405	66	0.125	0.024
4	10.319	2293	435	0.204	0.16
5	11.699	1135	312	0.101	0.115
6	11.846	1101078	268491	98.119	98.883
7	12.967	1294	336	0.115	0.124
8	13.438	1139	219	0.101	0.08
Total		1122192	271526		100

43f



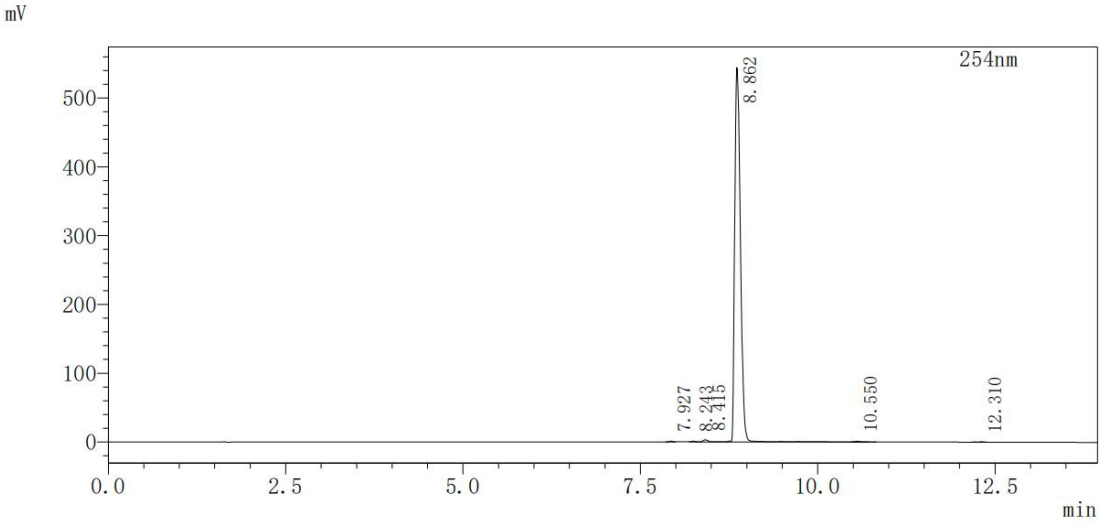
Peak	Retention time	Area	Height	Concentration	Height%
1	1.317	5782	415	0.000	0.155
2	1.530	10019	1945	0.000	0.727
3	1.710	7057	950	0.000	0.355
4	8.078	2145	393	0.000	0.147
5	8.978	3732	721	0.000	0.269
6	11.161	1090799	260792	0.000	97.533
7	12.366	2685	686	0.000	0.257
8	13.506	1103	219	0.000	0.082
9	13.921	2877	752	0.000	0.281
10	14.513	2042	515	0.000	0.192
Total		1128241	267388		100.000

43g



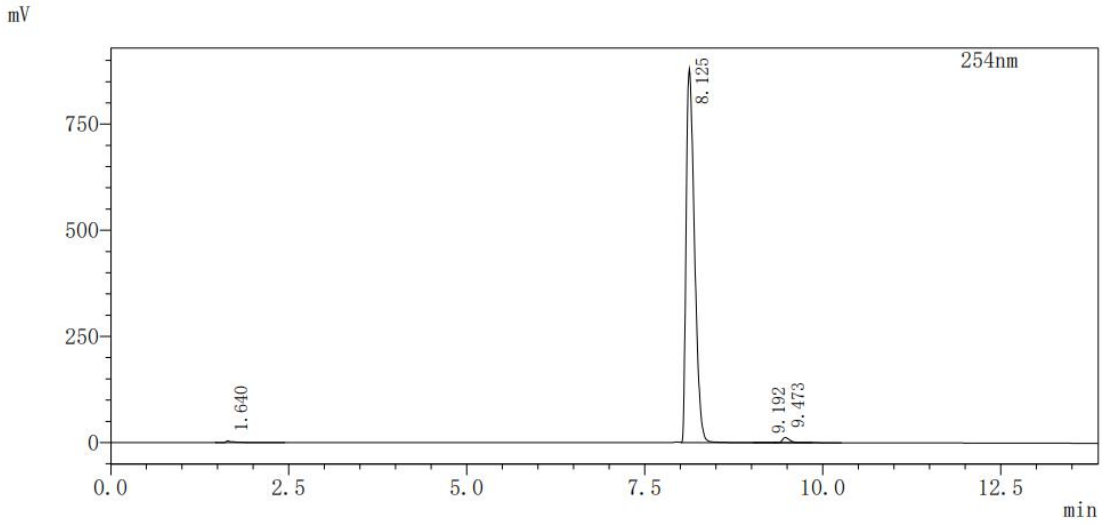
Peak	Retention time	Area	Height	Concentration	Height%
1	7.211	6791	1310	0.154	0.169
2	8.026	10244	1397	0.232	0.181
3	8.166	8073	1040	0.183	0.134
4	8.456	4312323	750334	97.593	97.034
5	9.642	81258	19187	1.839	2.481
Total		4418689	773268		100.000

43h



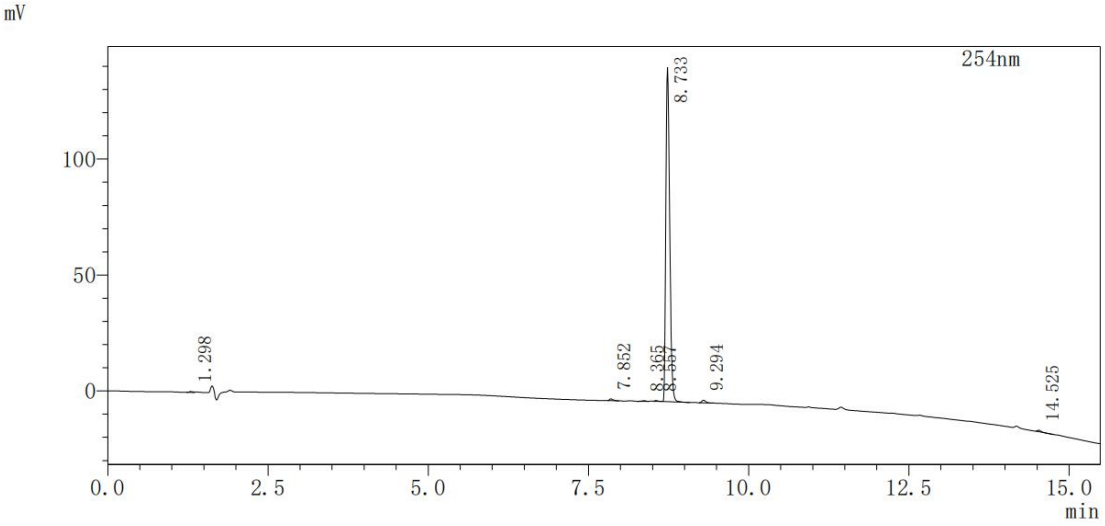
Peak	Retention time	Area	Height	Concentration	Height%
1	7.927	4665	1159	0.151	0.210
2	8.243	5417	1131	0.176	0.205
3	8.415	16425	3027	0.532	0.550
4	8.862	3050487	543752	98.887	98.740
5	10.550	4465	1050	0.145	0.191
6	12.310	3370	574	0.109	0.104
Total		3084829	550693		100.000

43i



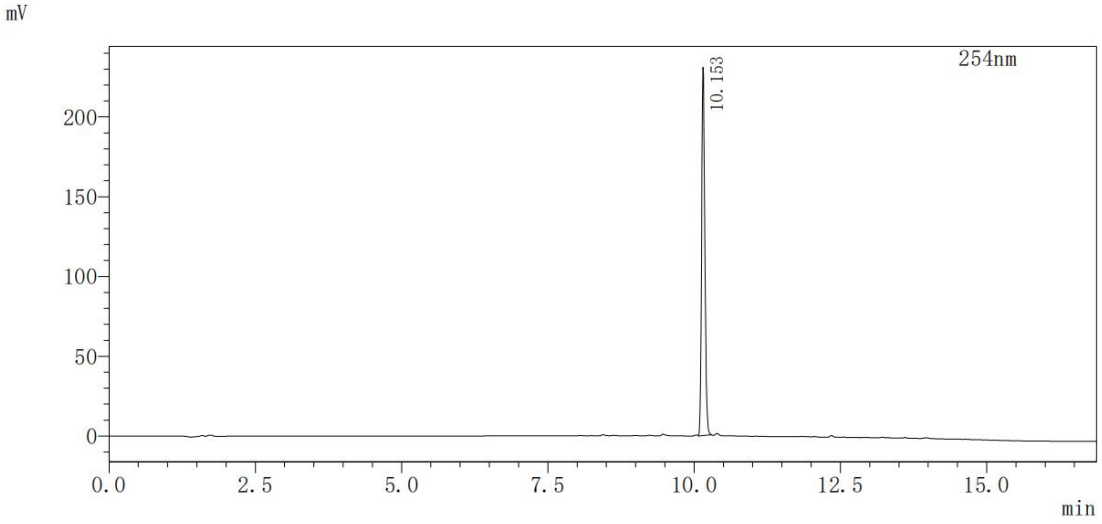
Peak	Retention time	Area	Height	Concentration	Height%
1	1.640	26450	3876	0.362	0.432
2	8.125	7201230	880100	98.470	98.190
3	9.192	1768	250	0.024	0.028
4	9.473	83671	12099	1.144	1.350
Total		7313120	896326		100.000

43j



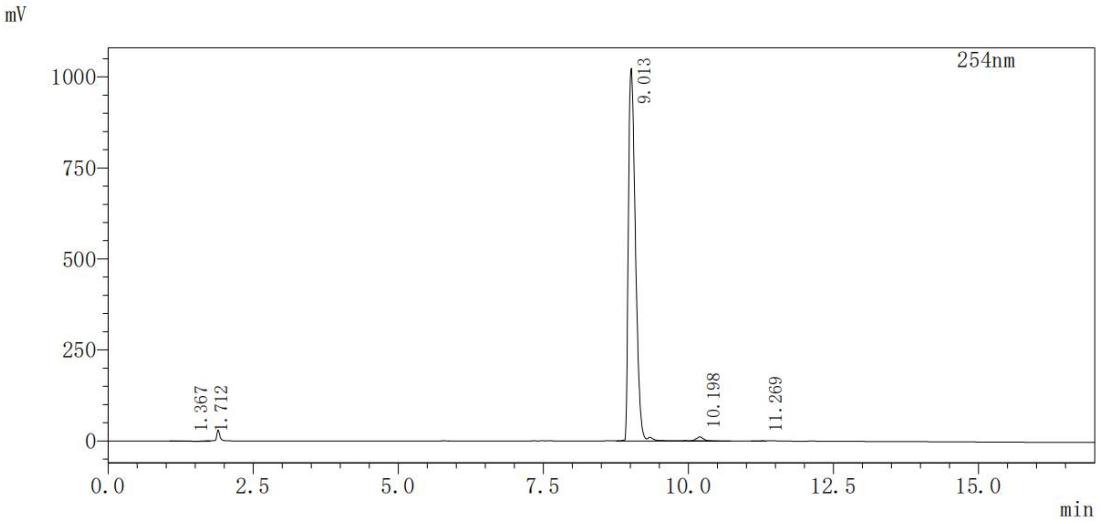
Peak	Retention time	Area	Height	Area%	Height%
1	1.298	1537	357	0.252	0.241
2	7.852	3256	841	0.535	0.569
3	8.365	1213	297	0.199	0.201
4	8.557	1408	383	0.231	0.259
5	8.733	594838	144130	97.660	97.512
6	9.294	4538	1141	0.745	0.772
7	14.525	2301	658	0.378	0.445
Total		609092	147807	100.000	100.000

43k



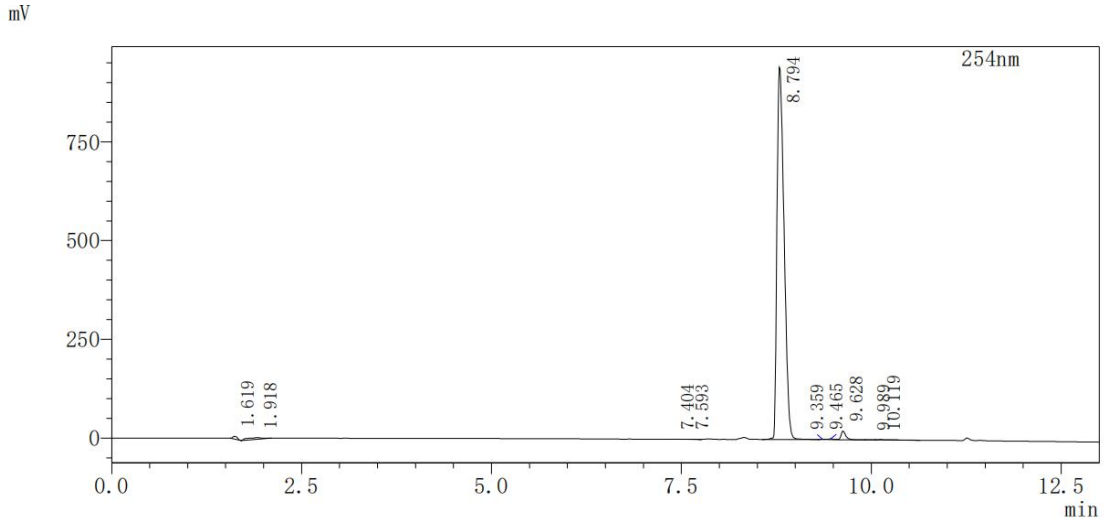
Peak	Retention time	Area	Height	Area%	Height%
1	10.153	885534	230782	100.000	100.000
Total		885534	230782	100.000	100.000

43l



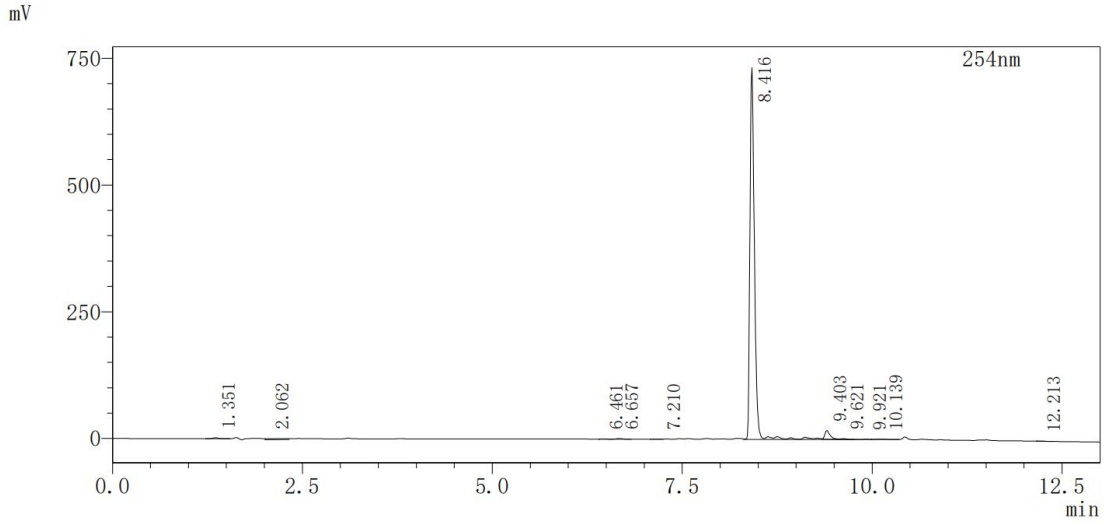
Peak	Retention time	Area	Height	Area%	Height%
1	1.367	8582	666	0.098	0.064
2	1.712	10975	1466	0.125	0.141
3	9.013	8685523	1022423	98.692	98.667
4	10.198	90802	11071	1.032	1.068
5	11.269	4761	605	0.054	0.058
Total		8800643	1036231	100.000	100.000

43m



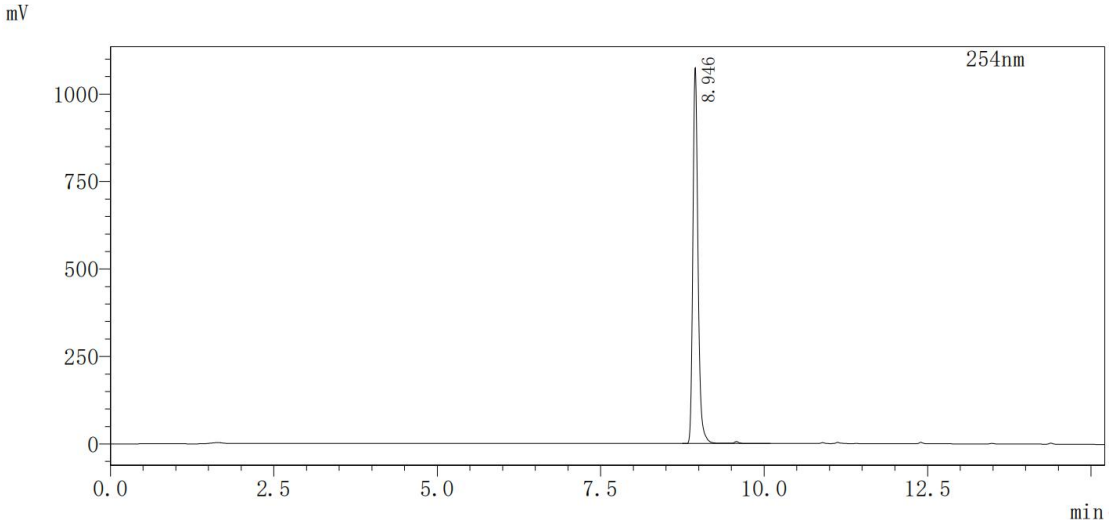
Peak	Retention time	Area	Height	Area%	Height%
1	1.619	29555	7334	0.465	0.748
2	1.918	63620	4327	1.000	0.442
3	7.404	1148	308	0.018	0.031
4	7.593	1232	286	0.019	0.029
5	8.794	6139670	941719	96.550	96.094
6	9.359	4260	1164	0.067	0.119
7	9.465	11023	1802	0.173	0.184
8	9.628	93761	21898	1.474	2.234
9	9.989	1523	267	0.024	0.027
10	10.119	13241	893	0.208	0.091
Total		6359032	979997	100.000	100.000

43n



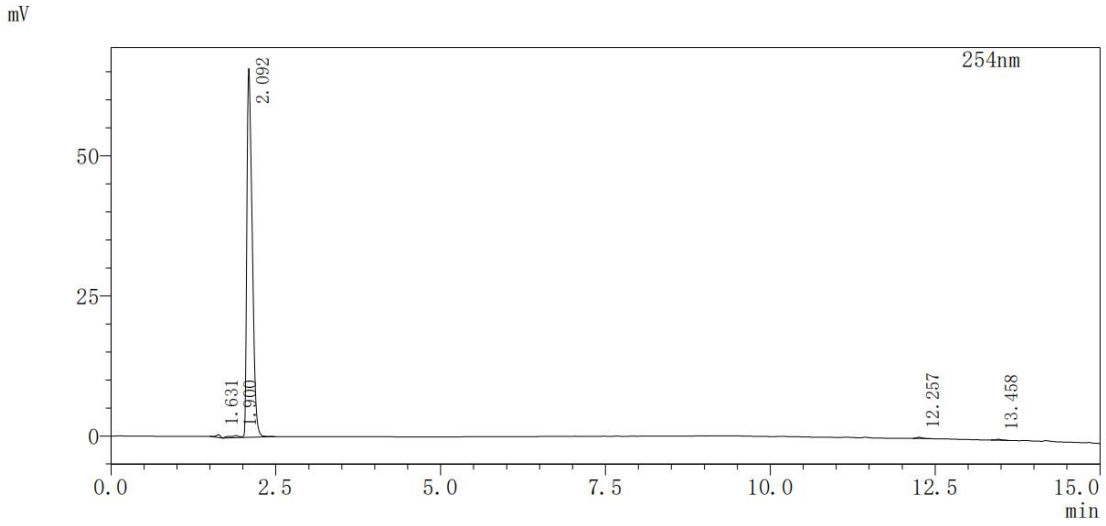
Peak	Retention time	Area	Height	Area%	Height%
1	1.351	10084	2011	0.311	0.265
2	2.062	30782	1917	0.949	0.253
3	6.461	1694	413	0.052	0.054
4	6.657	6380	995	0.197	0.131
5	7.210	2042	290	0.063	0.038
6	8.416	3088261	733080	95.171	96.552
7	9.403	84999	17202	2.619	2.266
8	9.621	7517	1587	0.232	0.209
9	9.921	3220	477	0.099	0.063
10	10.139	8425	946	0.260	0.125
11	12.213	1553	339	0.048	0.045
Total		3244957	759258	100.000	100.000

43o



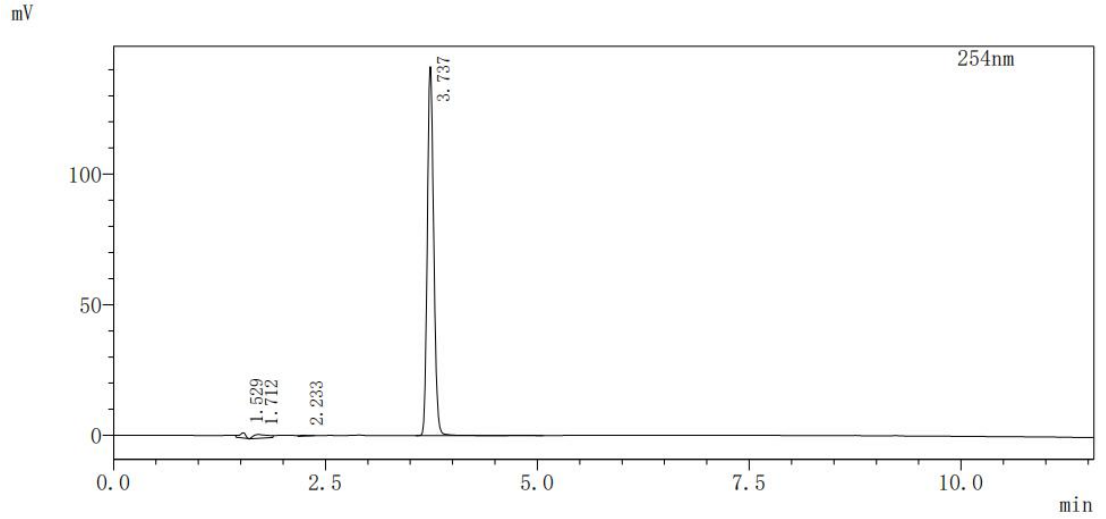
Peak	Retention time	Area	Height	Concentration	Height%
1	8.946	5827062	1073645	100.000	100.000
Total		5827062	1073645		100.000

43p



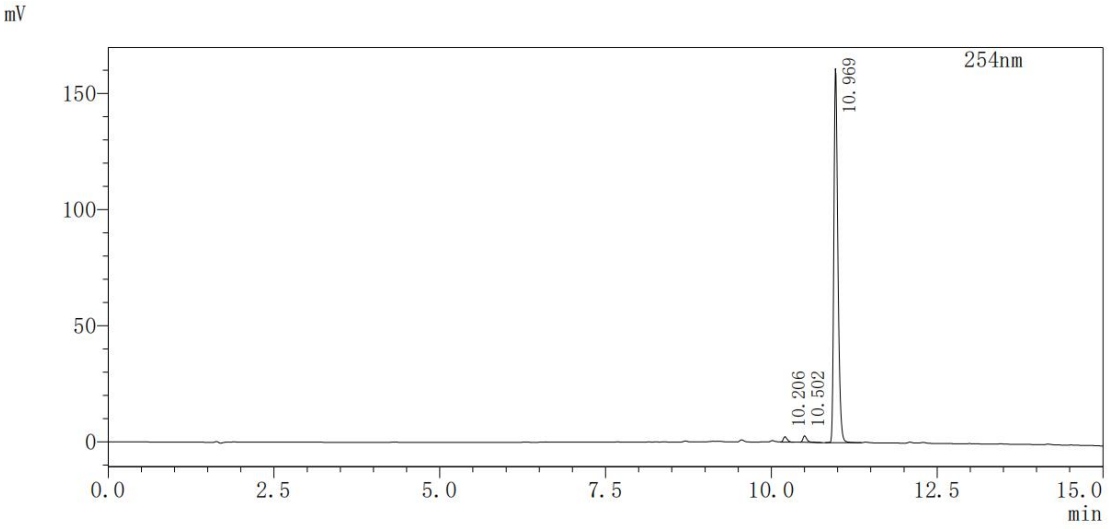
Peak	Retention time	Area	Height	Area%	Height%
1	1.631	2340	516	0.613	0.769
2	1.900	4017	370	1.053	0.551
3	2.092	372928	65797	97.744	98.063
4	12.257	1200	220	0.315	0.328
5	13.458	1051	194	0.275	0.289
Total		381536	67097	100.000	100.000

43q



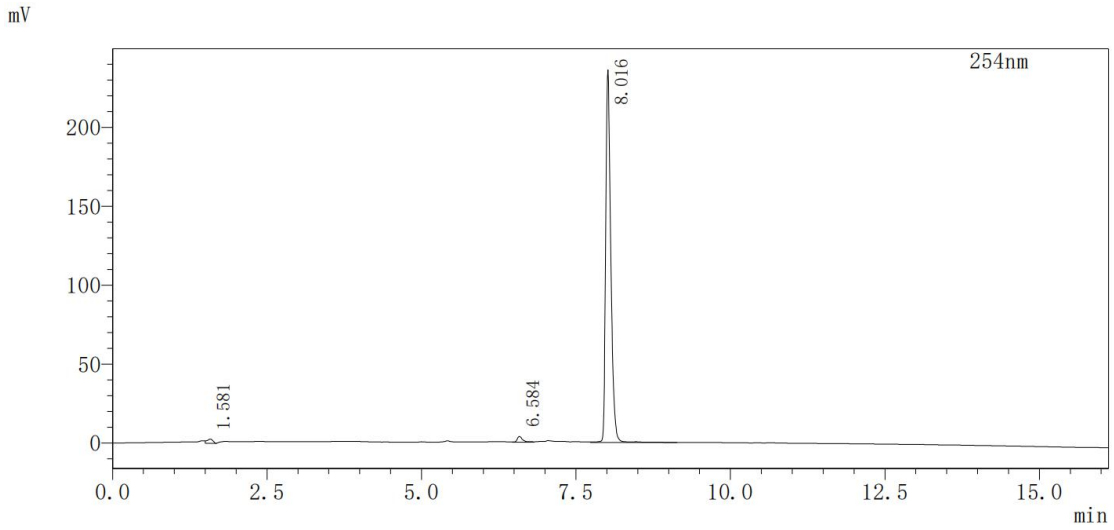
Peak	Retention time	Area	Height	Area%	Height%
1	1.529	9962	2044	1.294	1.411
2	1.712	17574	1493	2.283	1.031
3	2.233	1830	241	0.238	0.167
4	3.737	740333	141036	96.185	97.391
Total		769699	144814	100.000	100.000

44a



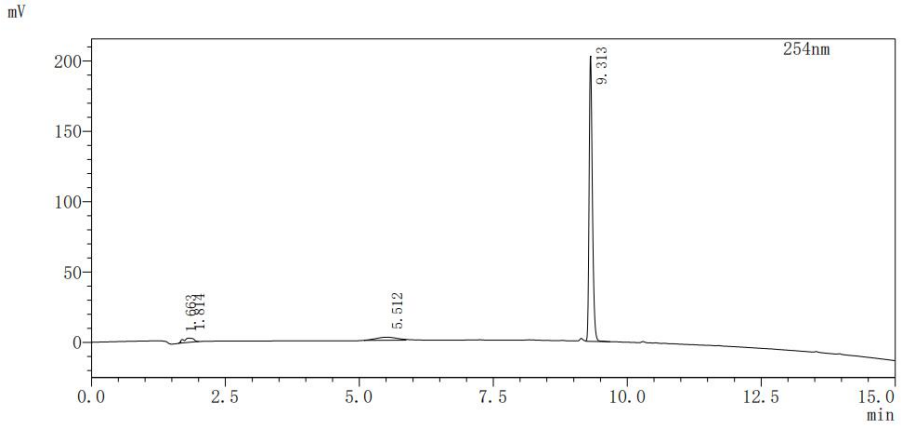
Peak	Retention time	Area	Height	Concentration	Height%
1	10.206	9789	2366	1.398	1.424
2	10.502	11633	2752	1.662	1.657
3	10.969	678698	161002	96.940	96.919
Total		700120	166120		100.000

44b



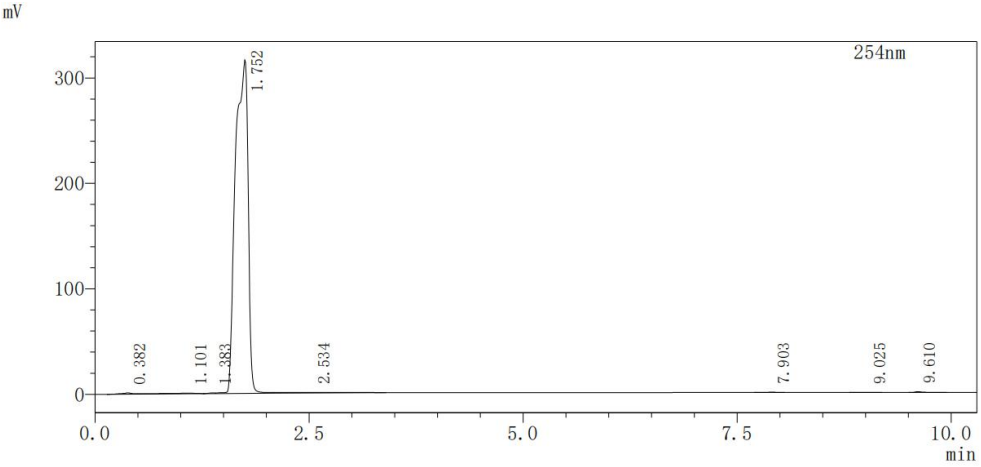
Peak	Retention time	Area	Height	Concentration	Height%
1	1.581	17233	2654	1.239	1.095
2	6.584	24592	3693	1.768	1.524
3	8.016	1349025	236018	96.993	97.381
Total		1390850	242366		100.000

44c



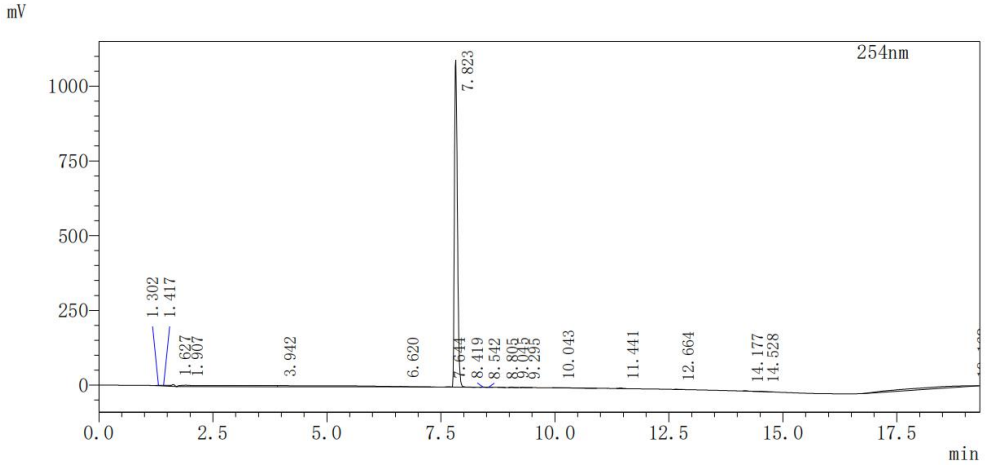
Peak	Retention time	Area	Height	Concentration	Height%
1	1.663	1755	970	0.183	0.464
2	1.814	37864	2982	3.952	1.427
3	5.512	59479	2167	6.209	1.037
4	9.313	858917	202908	89.656	97.072
Total		958014	209028		100.000

44d



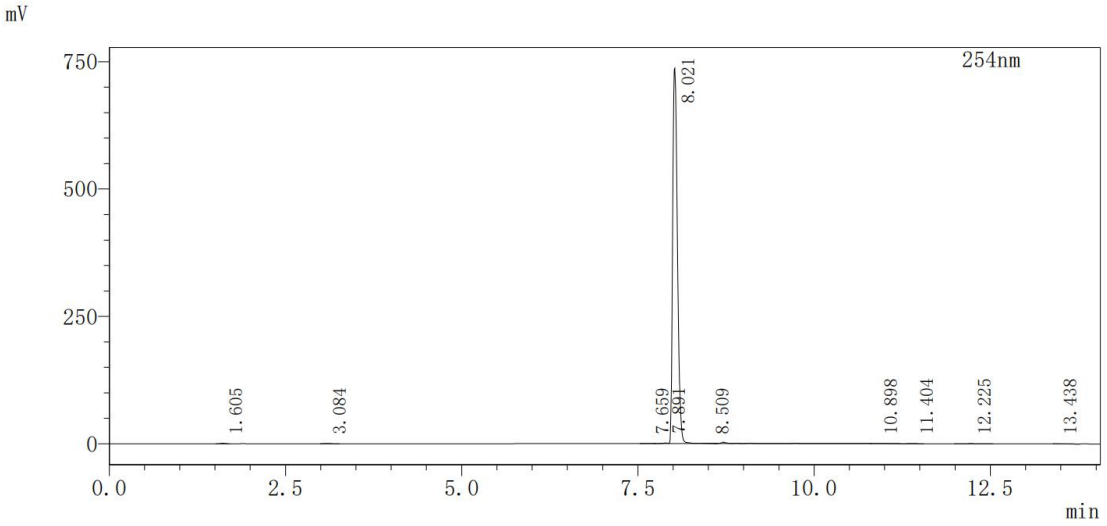
Peak	Retention time	Area	Height	Concentration	Height%
1	0.382	10539	1249	0.000	0.390
2	1.101	19249	537	0.000	0.168
3	1.383	4071	756	0.000	0.236
4	1.752	3236424	315948	0.000	98.628
5	2.534	31550	582	0.000	0.182
6	7.903	1795	319	0.000	0.100
7	9.025	1426	97	0.000	0.030
8	9.610	5395	856	0.000	0.267
Total		3310450	320344		100.000

44e



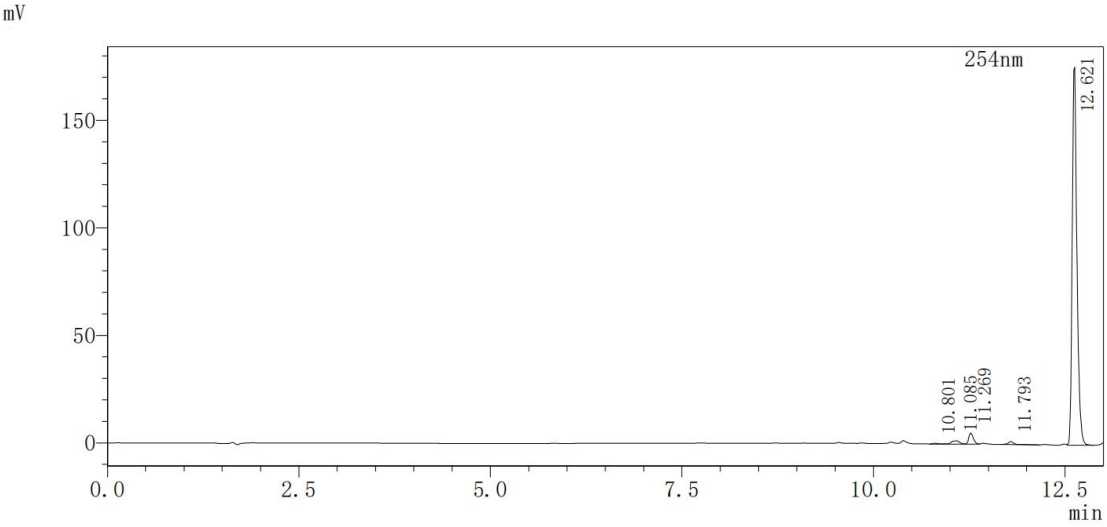
Peak	Retention time	Area	Height	Area%	Height%
1	1.302	4911	997	0.074	0.089
2	1.417	26166	1761	0.394	0.157
3	1.627	28277	6212	0.426	0.553
4	1.907	470641	4705	7.083	0.419
5	3.942	457983	3427	6.892	0.305
6	6.620	25727	1586	0.387	0.141
7	7.644	2989	597	0.045	0.053
8	7.823	4975290	1093825	74.875	97.371
9	8.419	3982	1070	0.060	0.095
10	8.542	1056	324	0.016	0.029
11	8.805	2340	626	0.035	0.056
12	9.045	6327	1517	0.095	0.135
13	9.295	3798	748	0.057	0.067
14	10.043	9220	217	0.139	0.019
15	11.441	9425	1974	0.142	0.176
16	12.664	1494	379	0.022	0.034
17	14.177	4788	1152	0.072	0.103
18	14.528	3876	1010	0.058	0.090
19	19.168	606503	1231	9.127	0.110
Total		6644793	1123358	100.000	100.000

44f



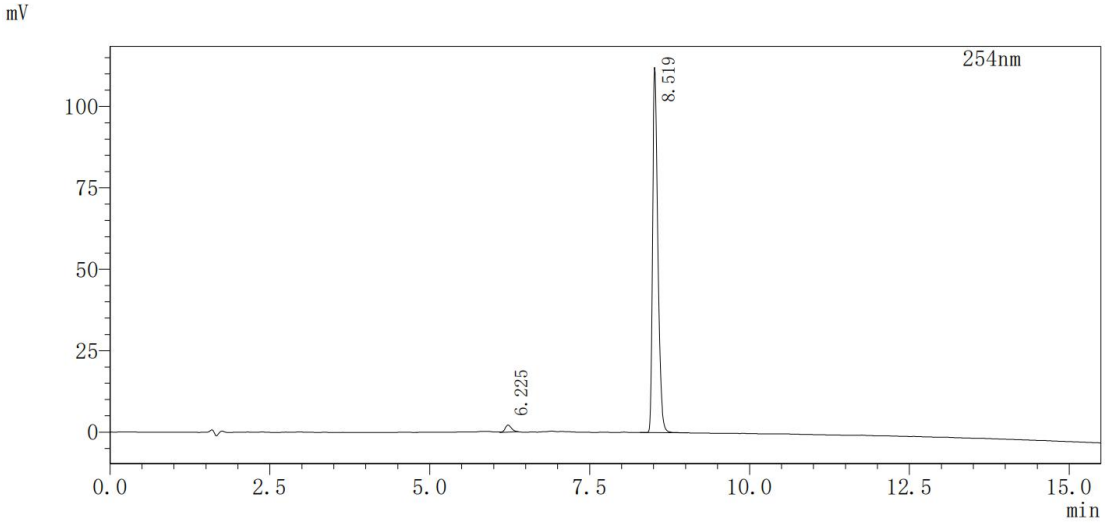
Peak	Retention time	Area	Height	Area%	Height%
1	1.605	4536	1089	0.127	0.147
2	3.084	1646	344	0.046	0.046
3	7.659	2382	296	0.067	0.040
4	7.891	6796	1201	0.191	0.162
5	8.021	3536226	736663	99.334	99.468
6	8.509	1407	293	0.040	0.040
7	10.898	1051	35	0.030	0.005
8	11.404	1235	170	0.035	0.023
9	12.225	2931	267	0.082	0.036
10	13.438	1736	248	0.049	0.033
Total		3559945	740606	100.000	100.000

44g



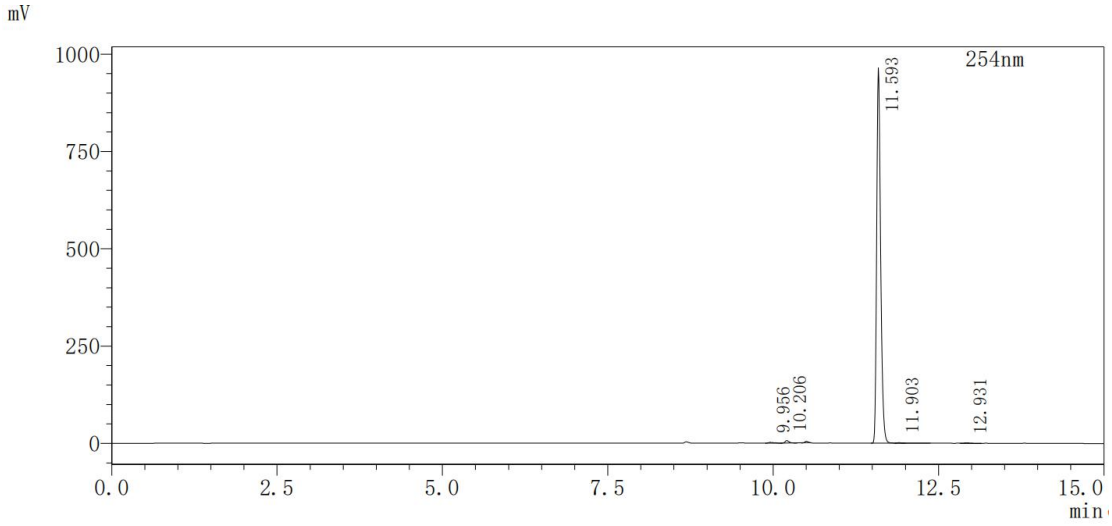
Peak	Retention time	Area	Height	Concentration	Height%
1	10.801	1694	355	0.213	0.193
2	11.085	10976	1541	1.380	0.838
3	11.269	21176	5143	2.662	2.797
4	11.793	8032	1415	1.010	0.769
5	12.621	753610	175448	94.735	95.403
Total		795489	183902		100.000

44h



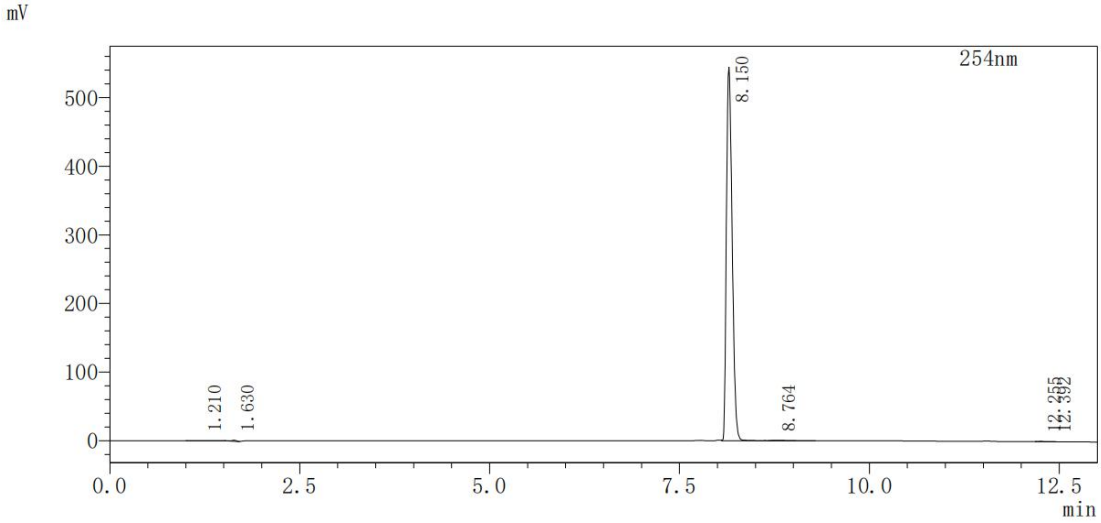
Peak	Retention time	Area	Height	Area%	Height%
1	6.225	14687	2147	2.228	1.878
2	8.519	644630	112187	97.772	98.122
Total		659317	114334	100.000	100.000

44i



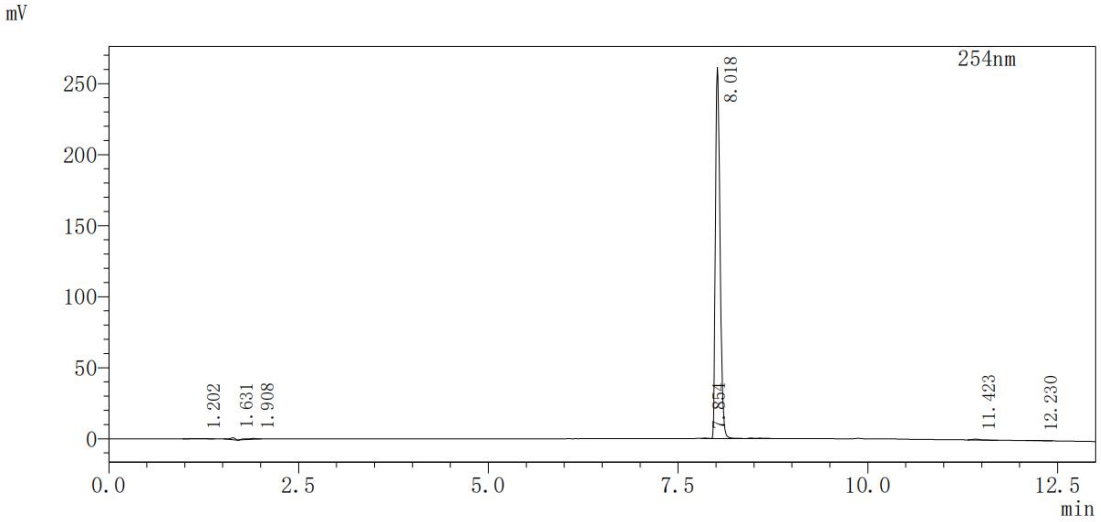
Peak	Retention time	Area	Height	Concentration	Height%
1	9.956	9963	1851	0.244	0.190
2	10.206	32827	6152	0.804	0.631
3	11.593	4028480	964276	98.679	98.947
4	11.903	3319	938	0.081	0.096
5	12.931	7819	1323	0.192	0.136
Total		4082408	974540		100.000

44j



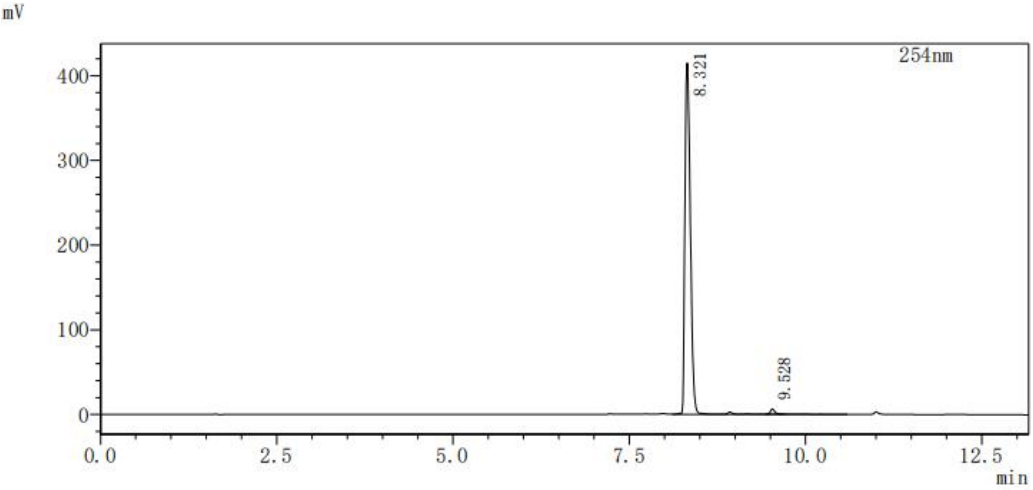
Peak	Retention time	Area	Height	Concentration	Height%
1	1.210	2166	121	0.075	0.022
2	1.630	6625	1398	0.229	0.256
3	8.150	2878132	544167	99.466	99.517
4	8.764	3083	467	0.107	0.085
5	12.255	2471	457	0.085	0.084
6	12.392	1106	196	0.038	0.036
Total		2893582	546806		100.000

44k



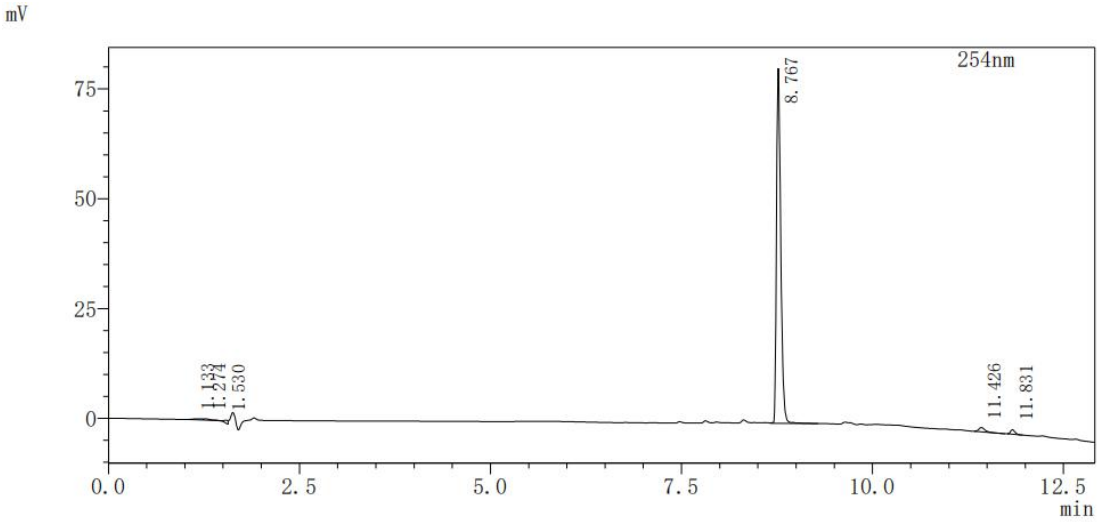
Peak	Retention time	Area	Height	Concentration	Height%
1	1.202	1831	110	0.160	0.042
2	1.631	5775	1263	0.506	0.477
3	1.908	7276	560	0.637	0.212
4	7.854	2178	428	0.191	0.162
5	8.018	1120006	261387	98.052	98.816
6	11.423	3747	589	0.328	0.223
7	12.230	1438	183	0.126	0.069
Total		1142252	264520		100.000

44l



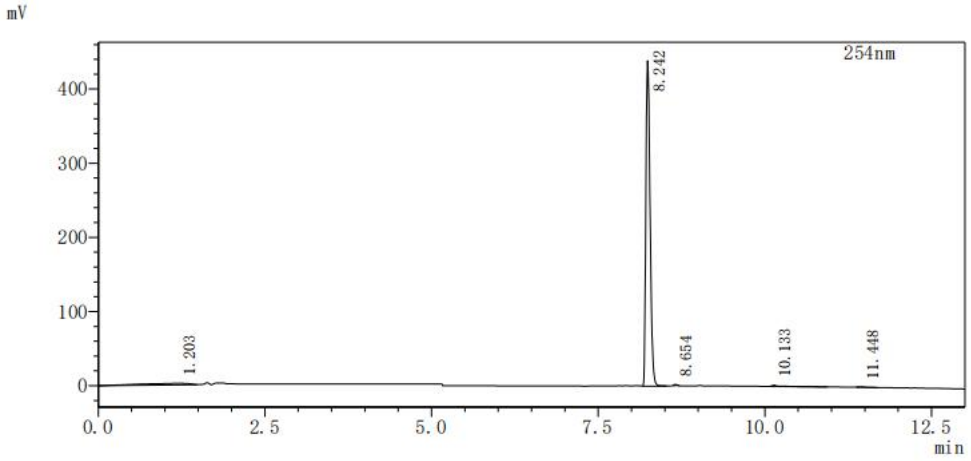
Peak	Retention time	Area	Height	Concentration	Height%
1	8.321	2242783	414489	98.838	98.536
2	9.528	26361	6158	1.162	1.464
Total		2269145	420647		100.000

44m



Peak	Retention time	Area	Height	Area%	Height%
1	1.133	2047	186	0.614	0.222
2	1.274	2081	279	0.624	0.333
3	1.530	2403	571	0.720	0.681
4	8.767	317604	80835	95.201	96.377
5	11.426	5462	980	1.637	1.169
6	11.831	4018	1023	1.204	1.219
Total		333616	83874	100.000	100.000

44n



Peak	Retention time	Area	Height	Concentration	Height%
1	1.203	125723	2181	6.084	0.491
2	8.242	1921399	438886	92.978	98.737
3	8.654	3270	1155	0.158	0.260
4	10.133	13298	1706	0.643	0.384
5	11.448	2830	571	0.137	0.128
Total		2066519	444499		100.000