Supporting Information

Discovery of a Novel Series of Tricyclic Oxadiazine 4a-Methyl Esters Based on Indoxacarb as Potential Sodium Channel Blocker/ Modulator insecticides

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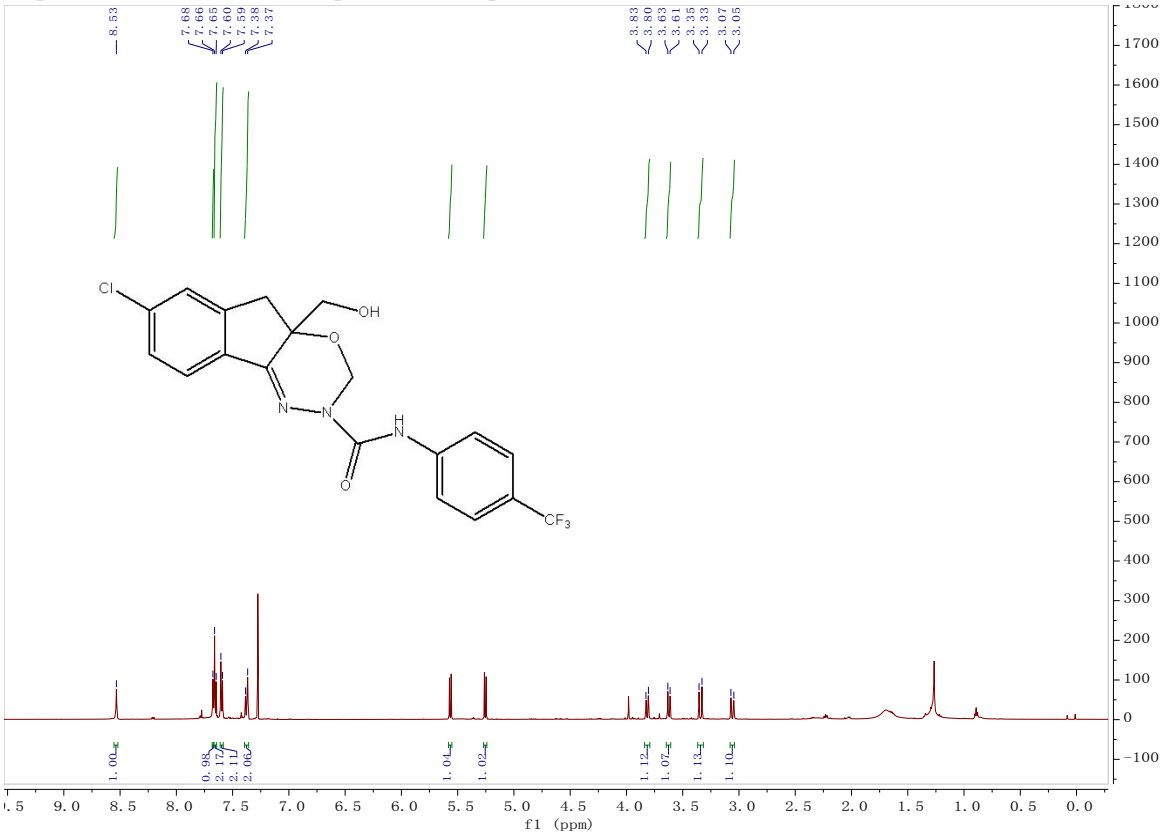
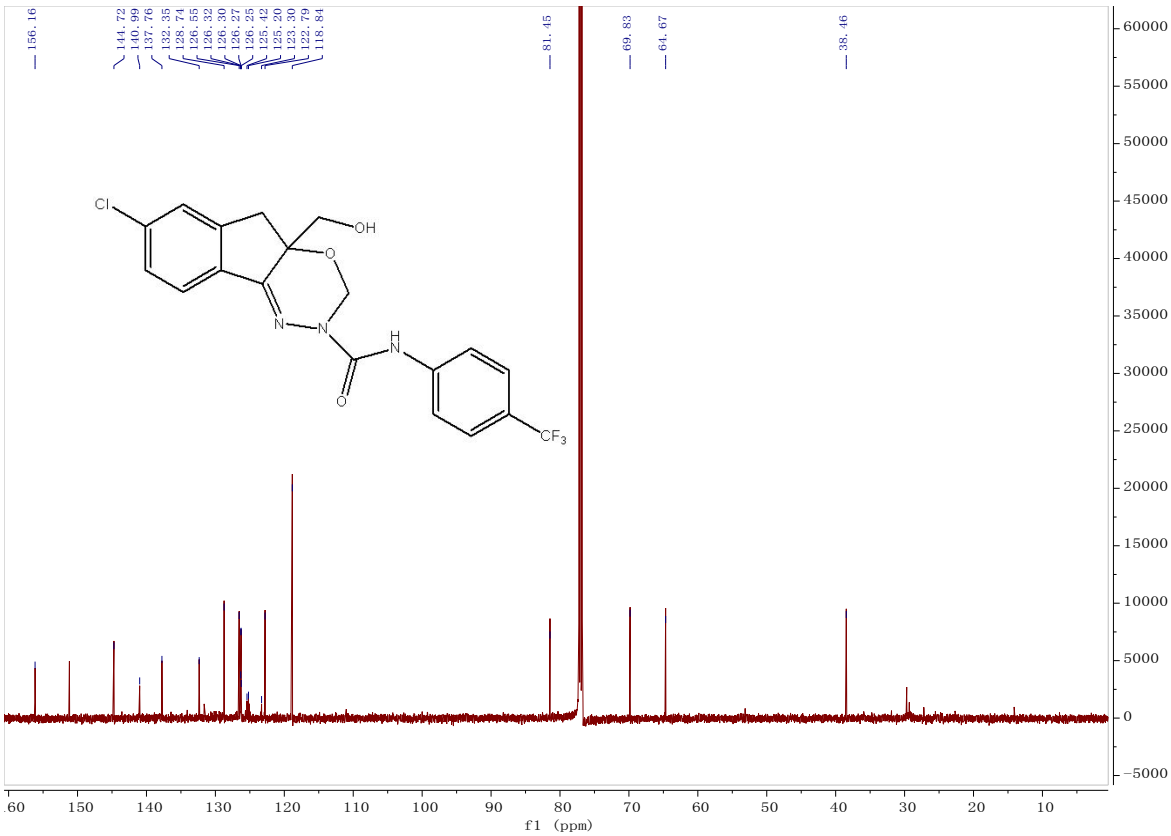
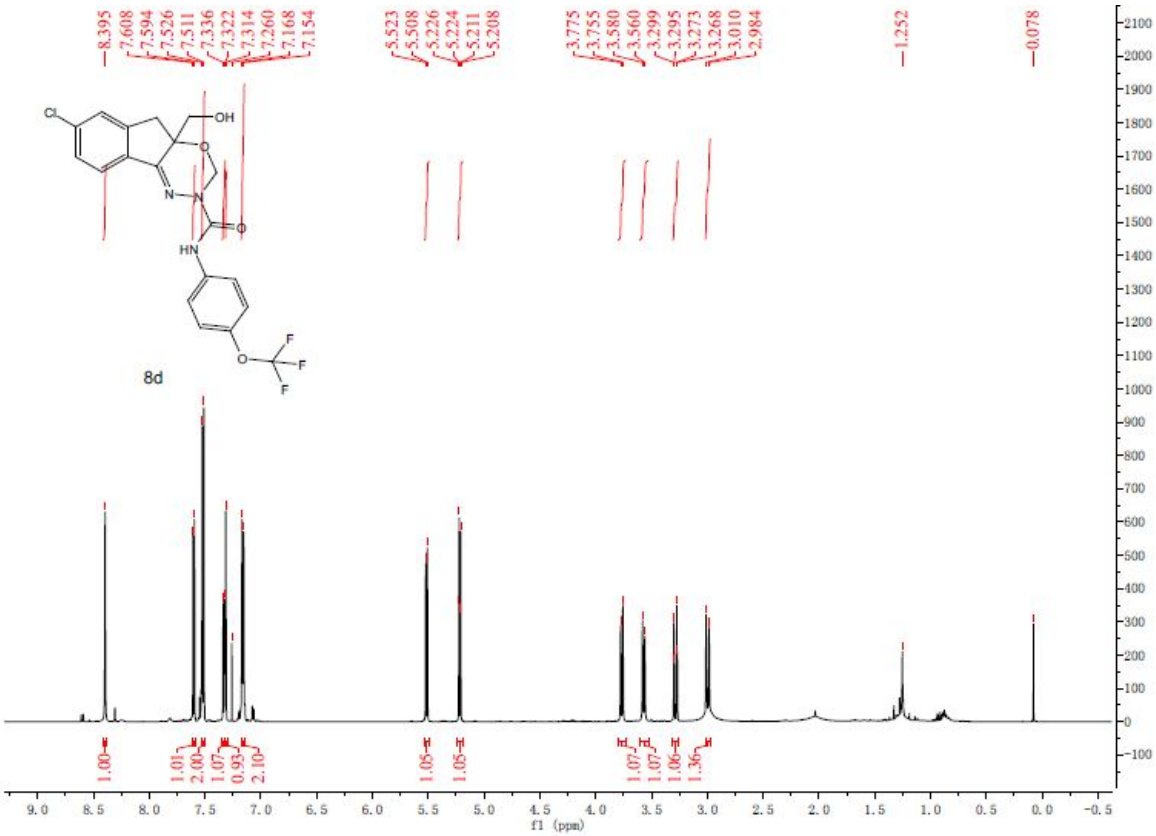
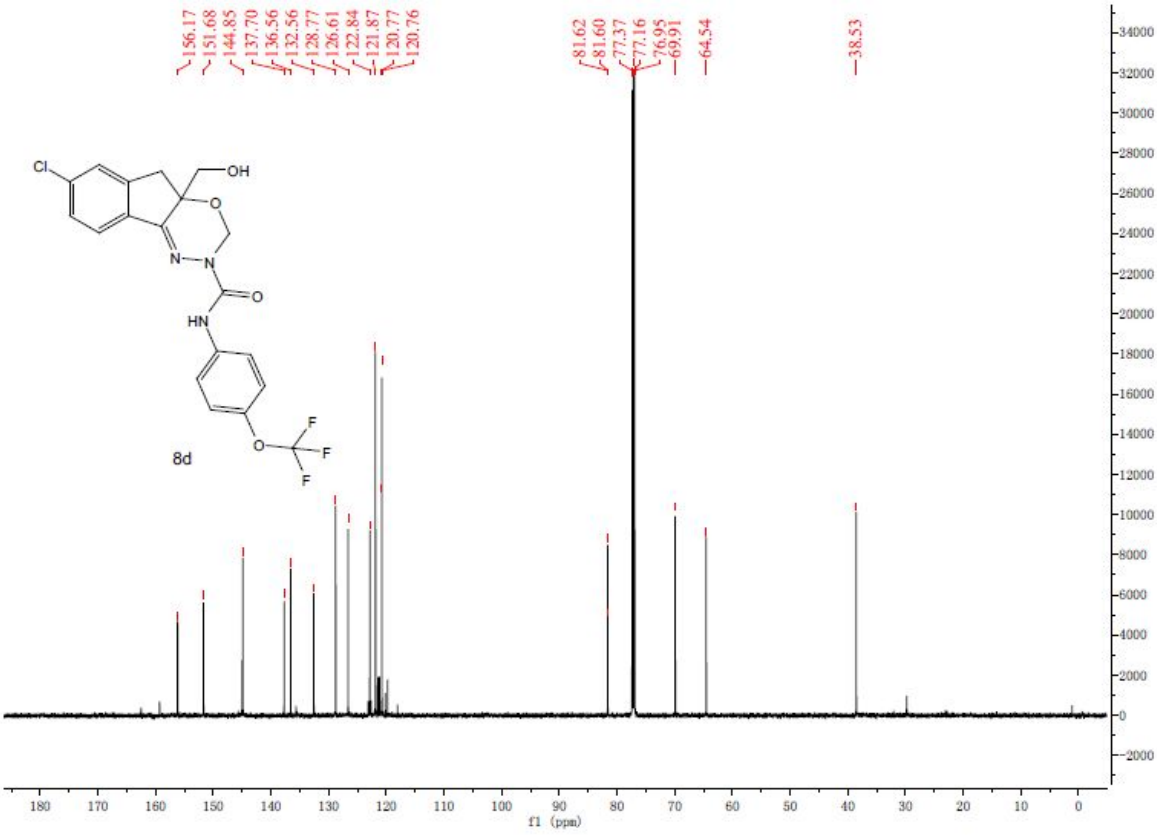
Copies of NMR and HRMS spectra of compounds



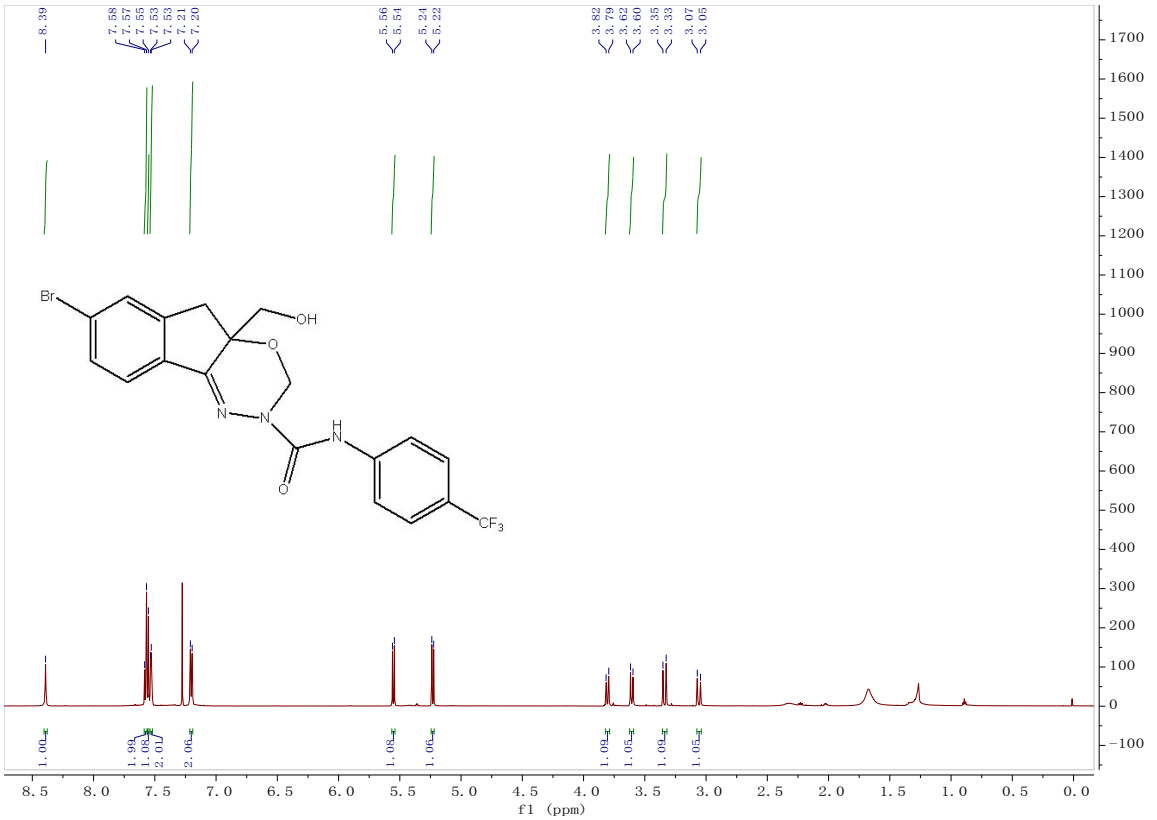


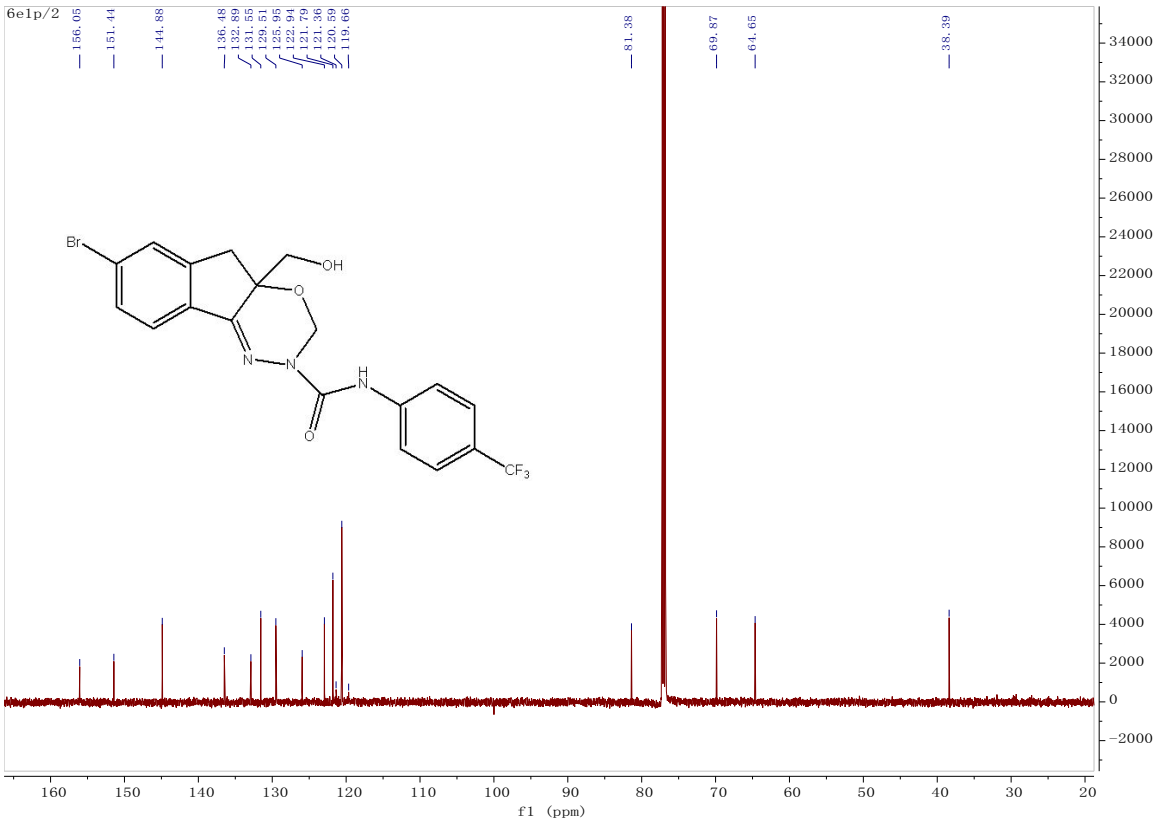
^{1}H NMR and ^{13}C NMR of target compound H1



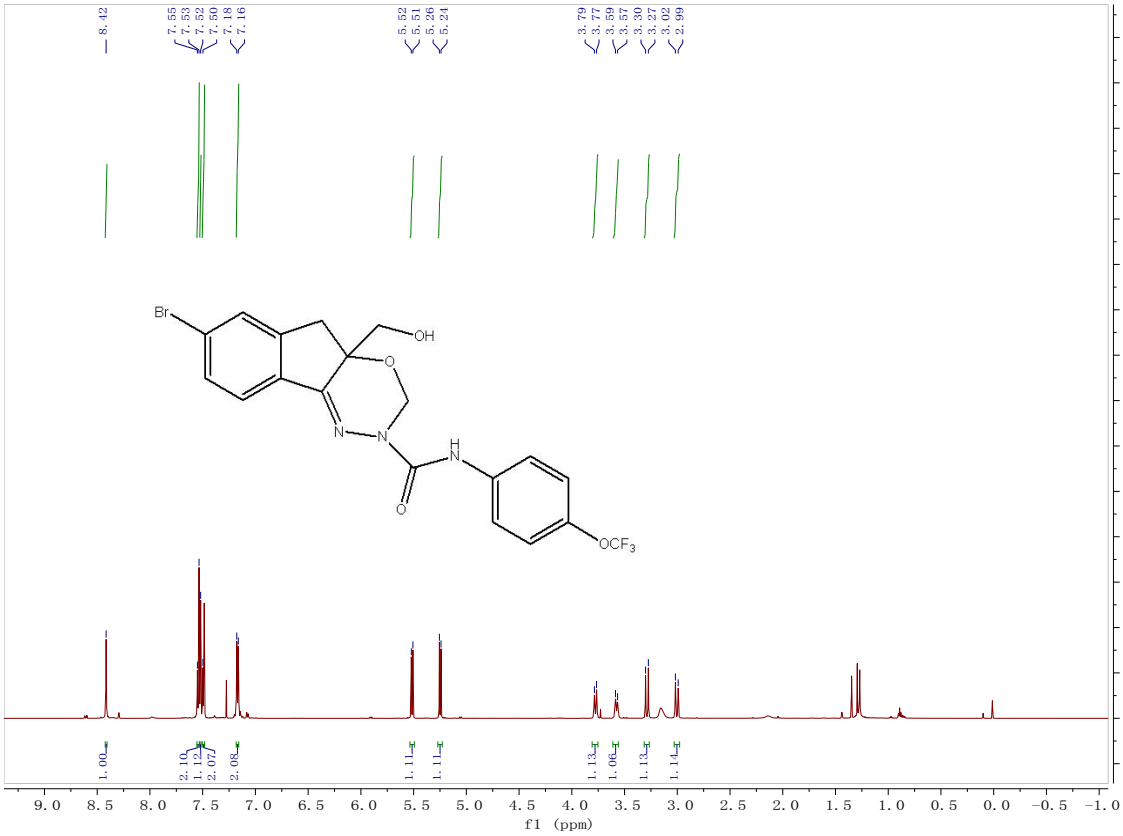


^{1}H NMR and ^{13}C NMR of target compound H2





^{1}H NMR and ^{13}C NMR of target compound H3



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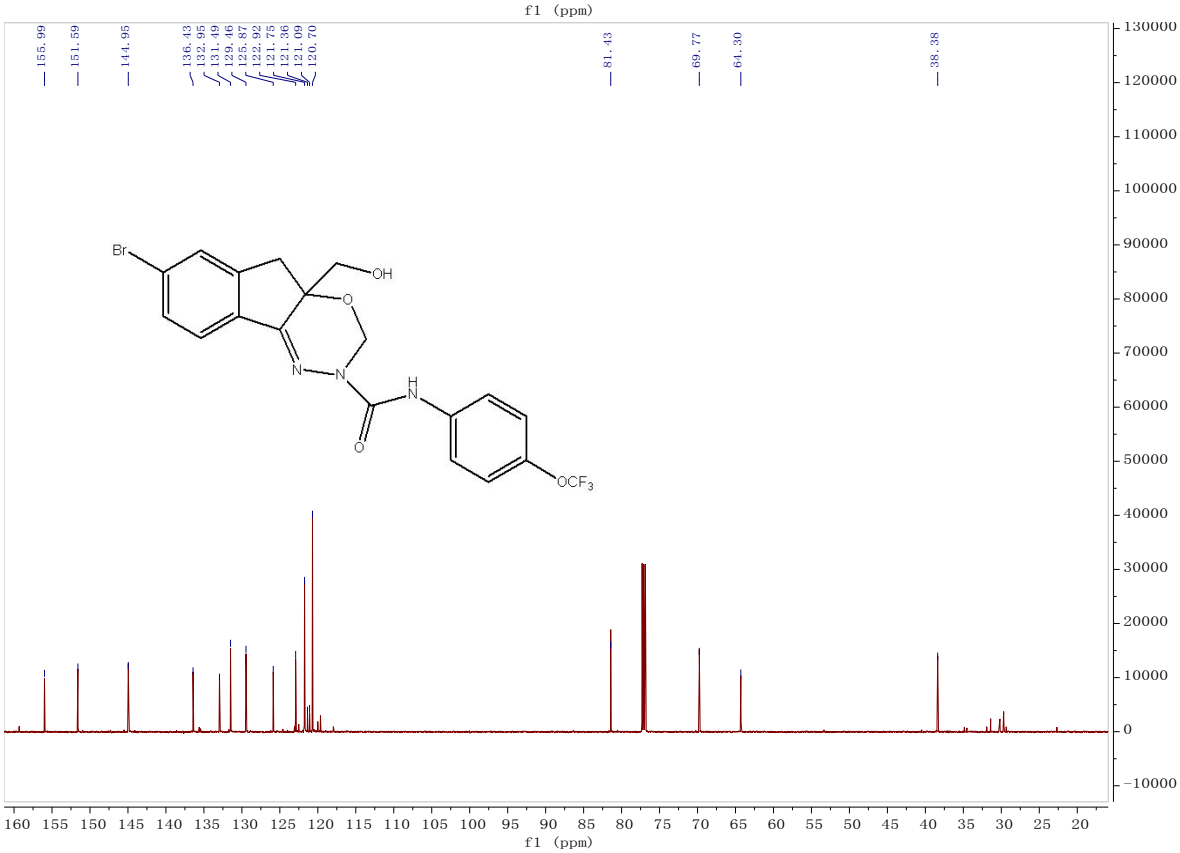

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50 ^{1}H NMR and ^{13}C NMR of target compound H4

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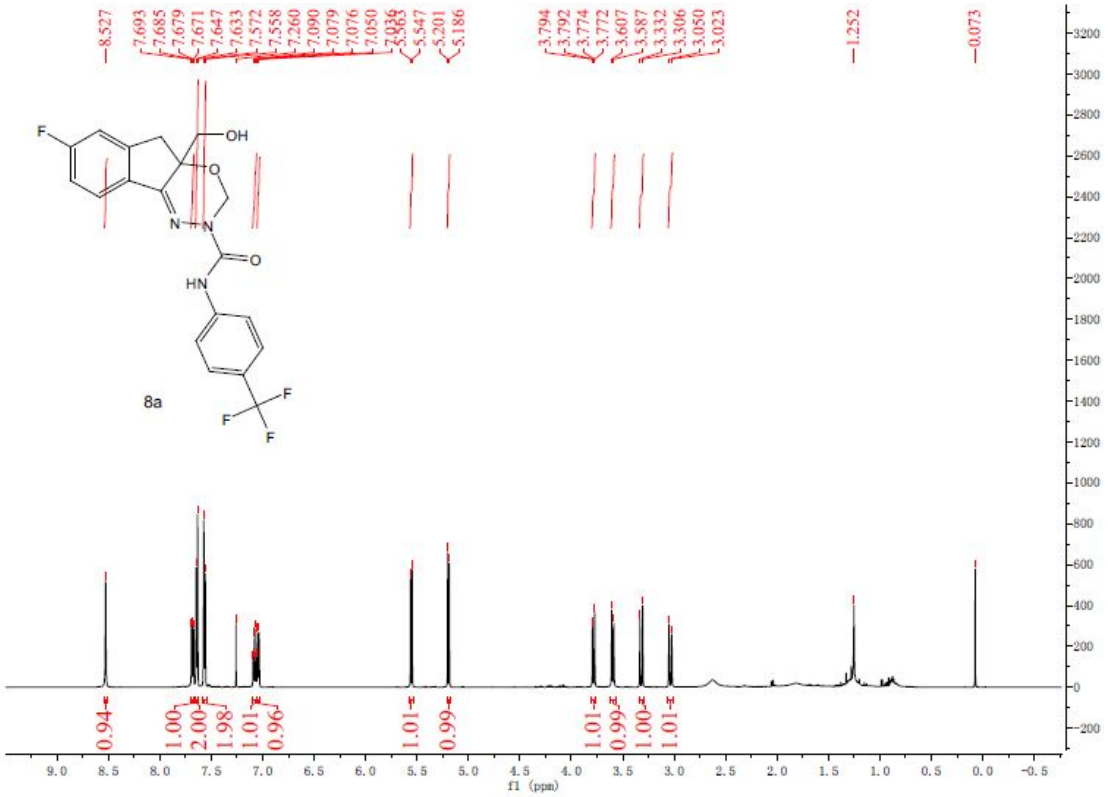

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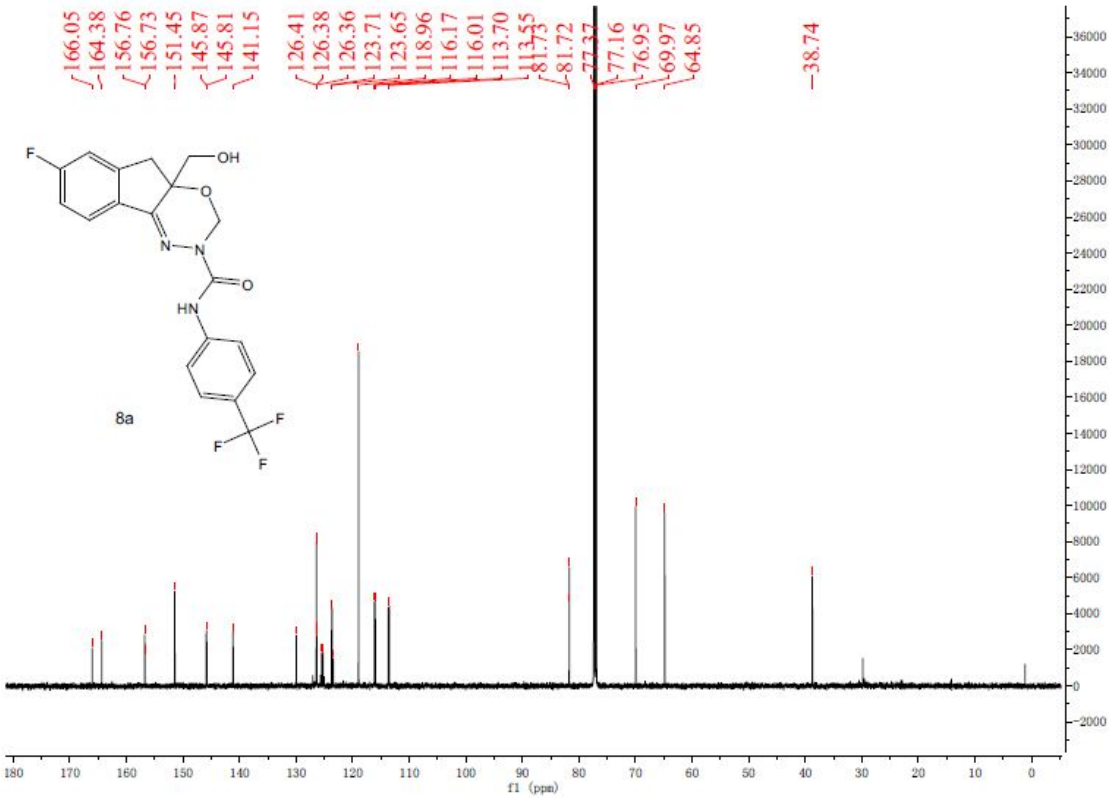

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55 ^{1}H NMR and ^{13}C NMR of target compound H5

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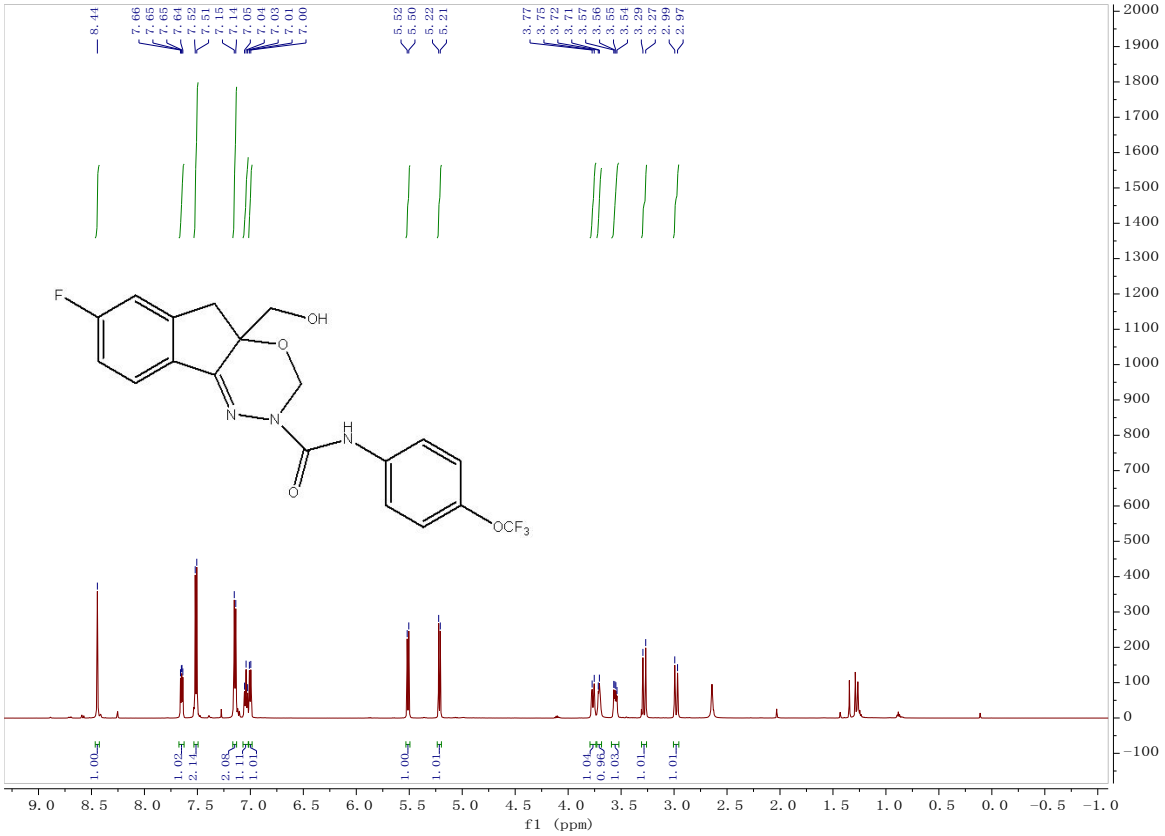

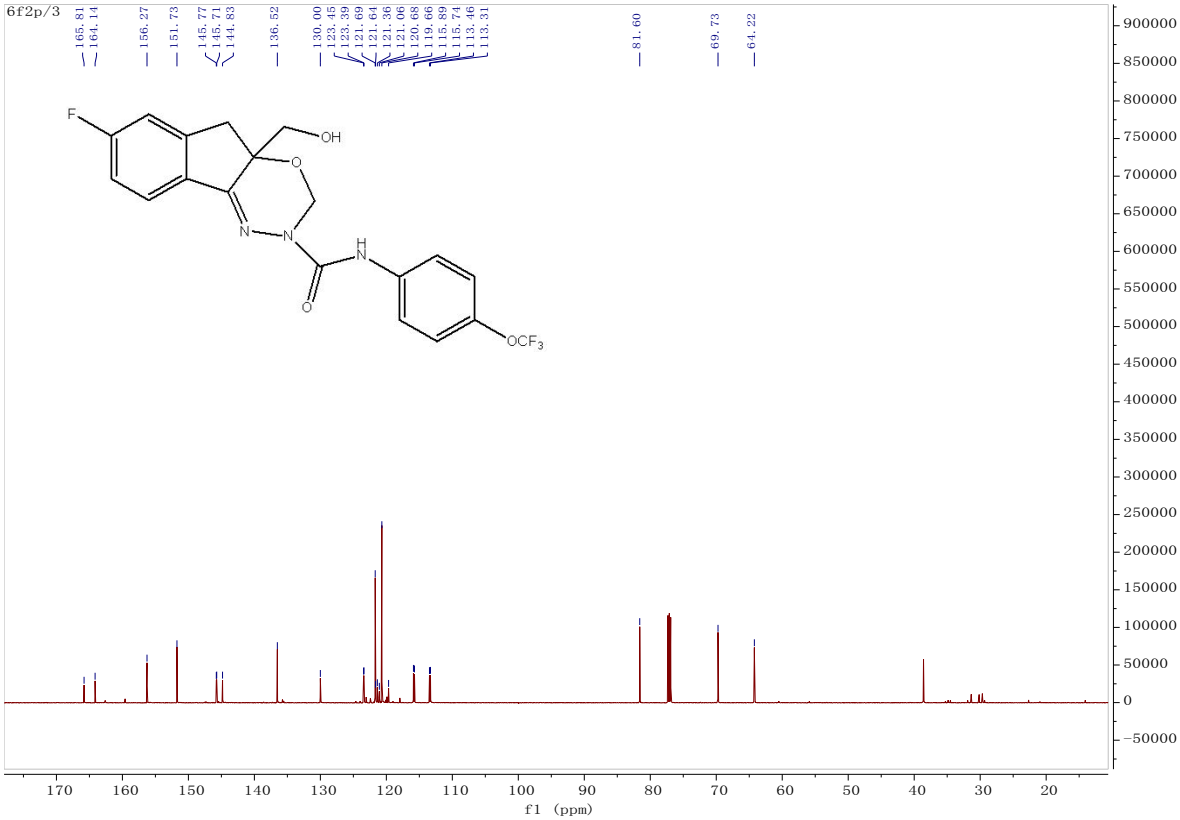

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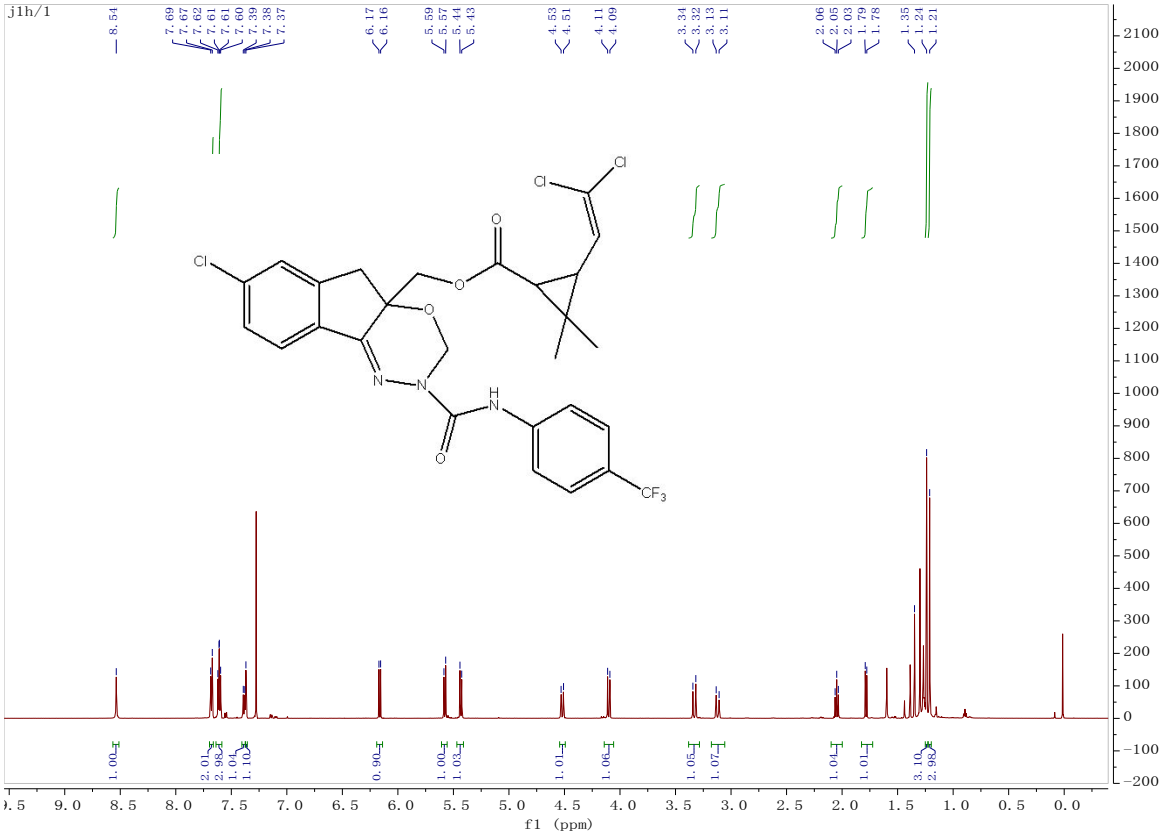
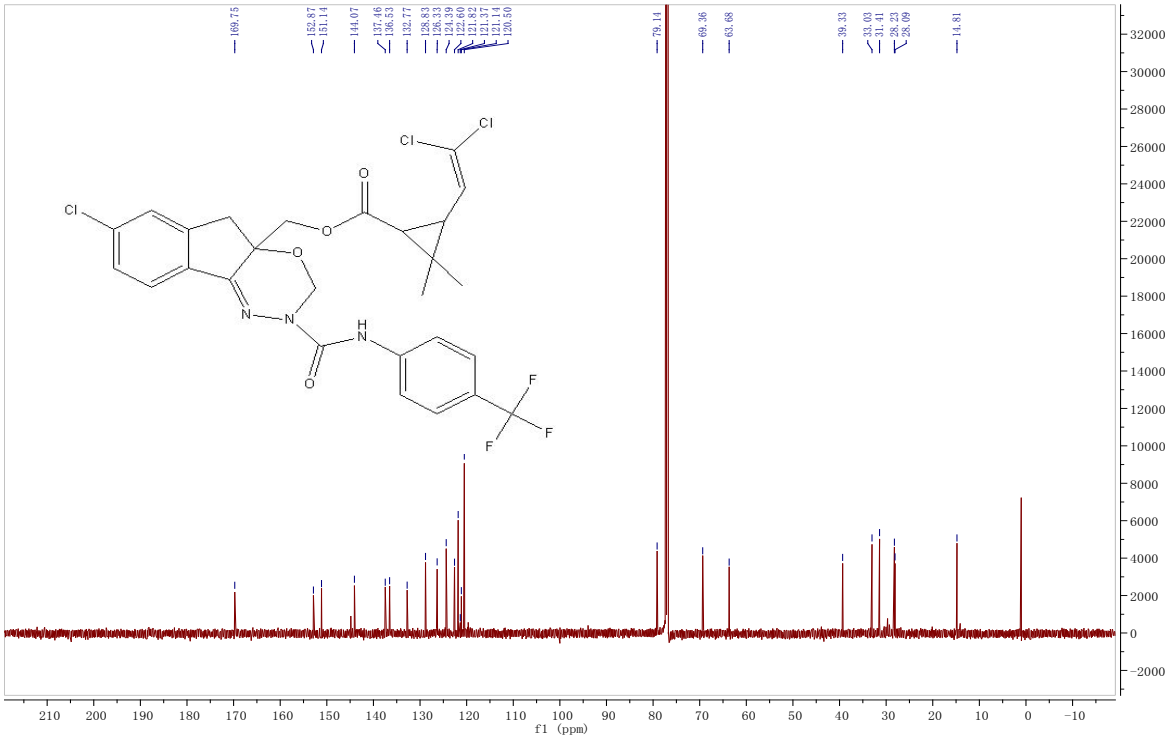
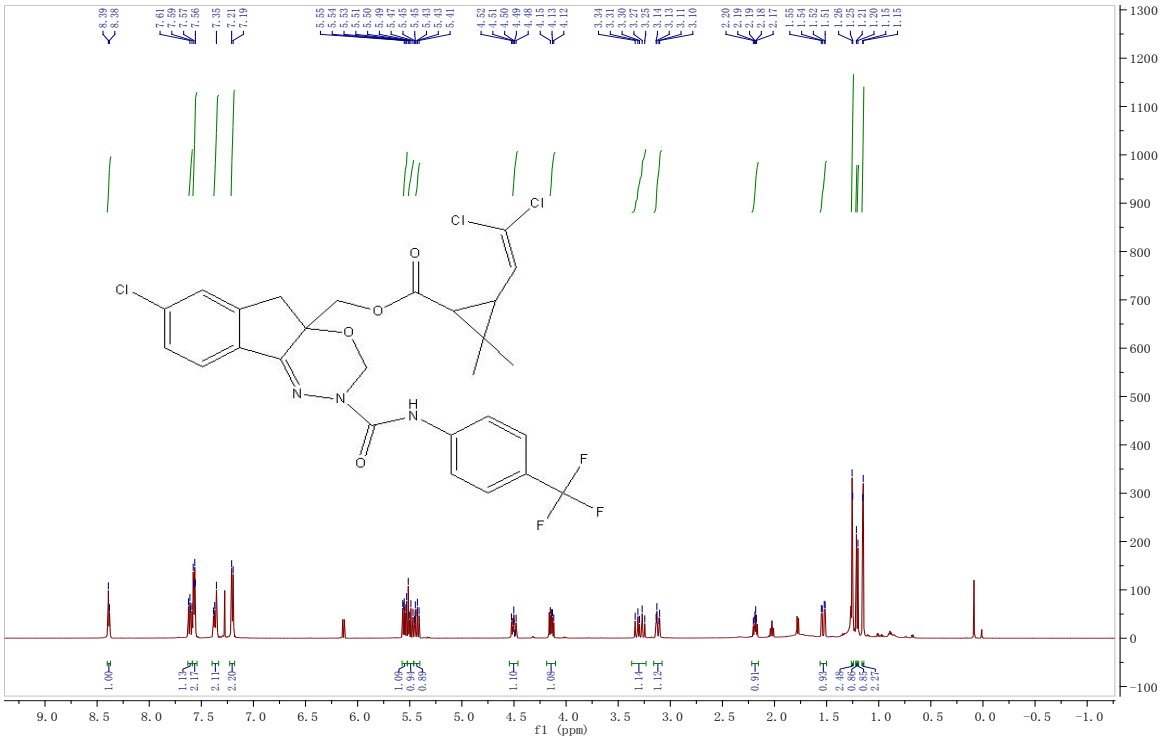
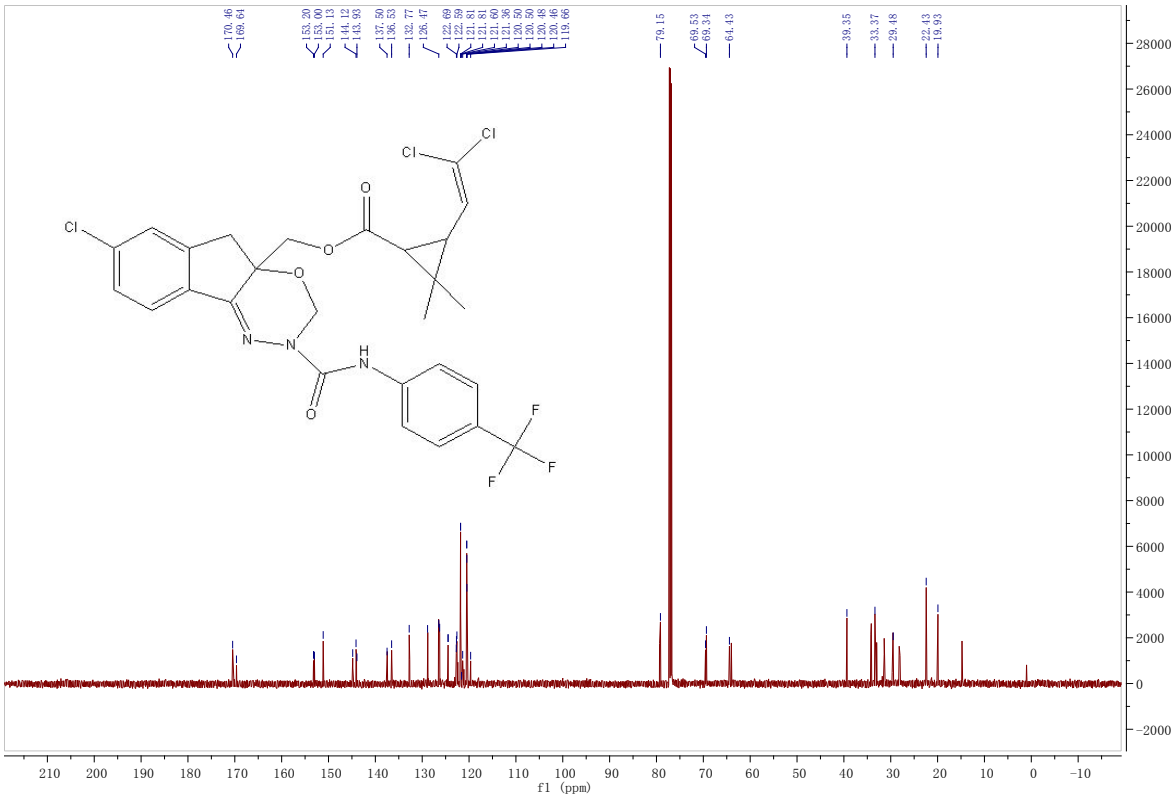


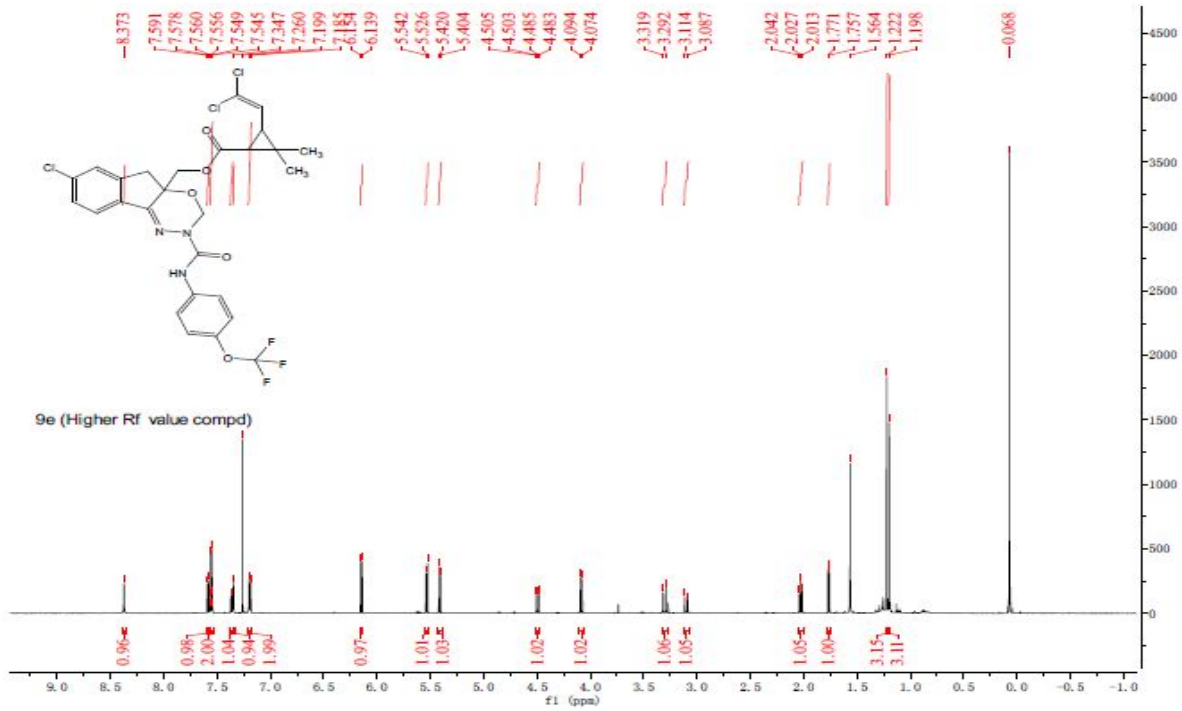


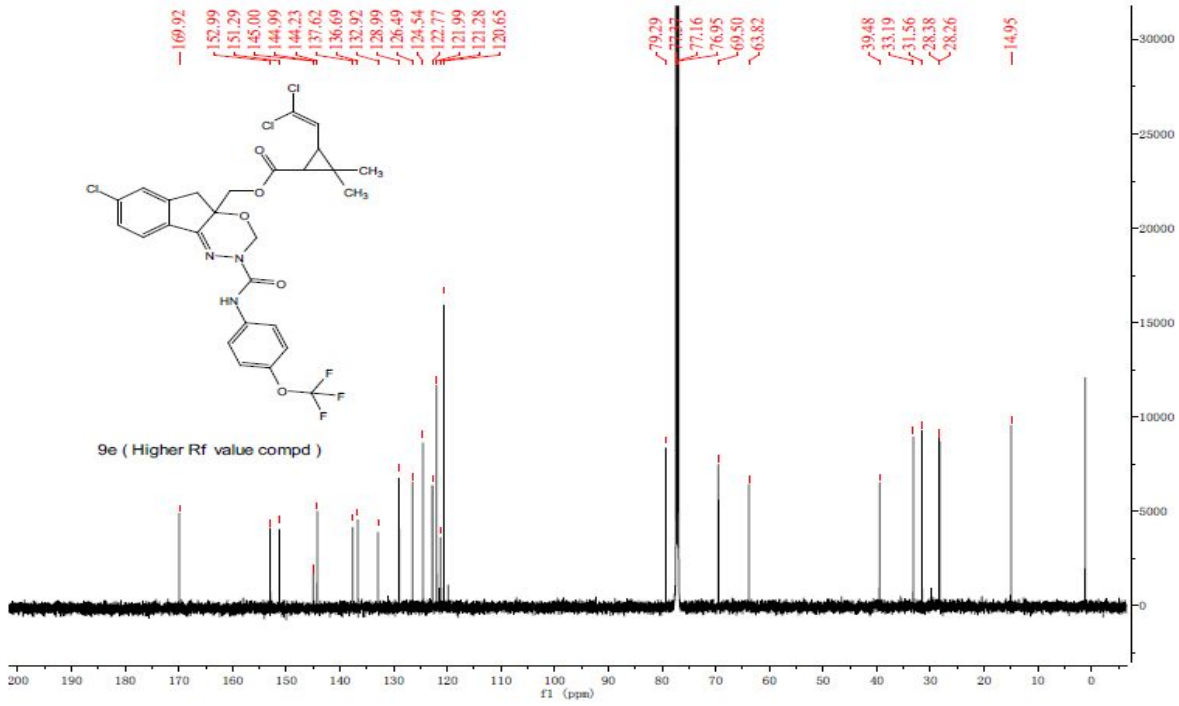
^{1}H NMR and ^{13}C NMR of target compound J1 (Higher Rf value compd)





^{1}H NMR and ^{13}C NMR of target compound J1 (Lower Rf value compd)





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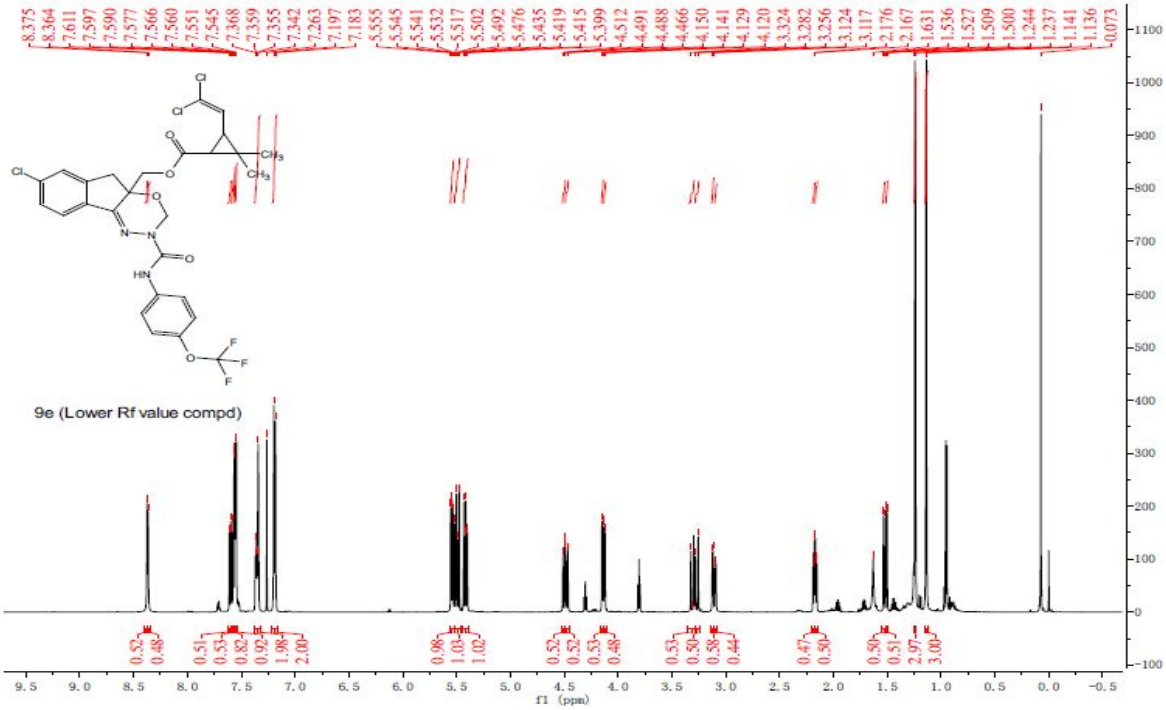

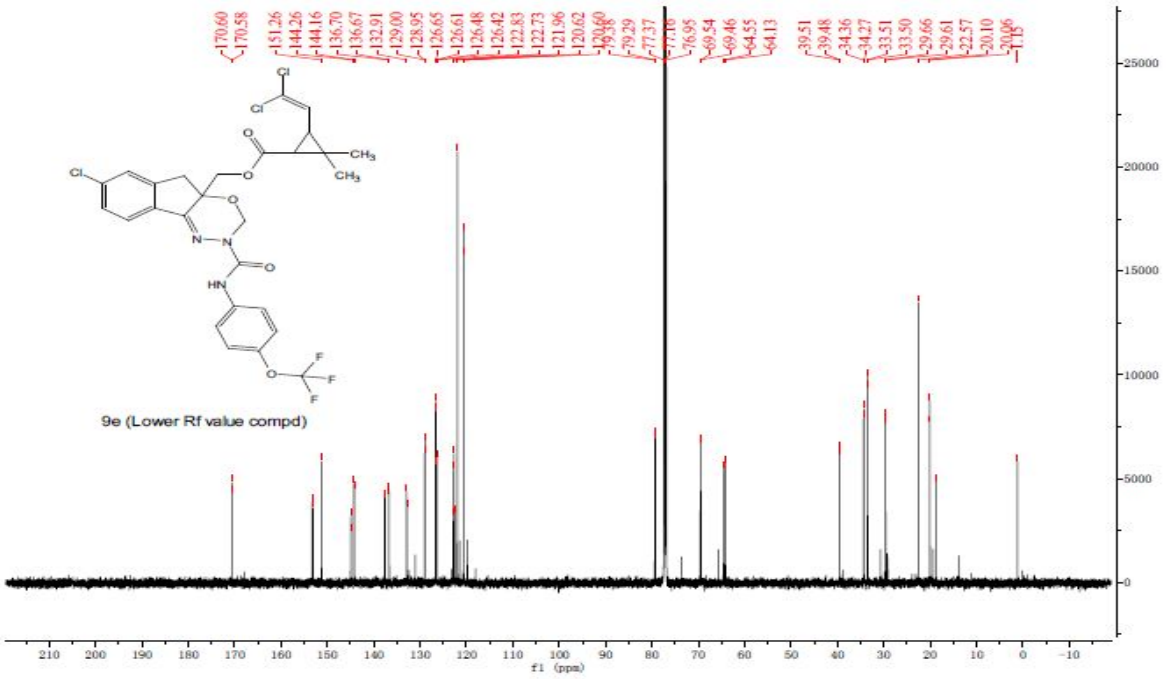

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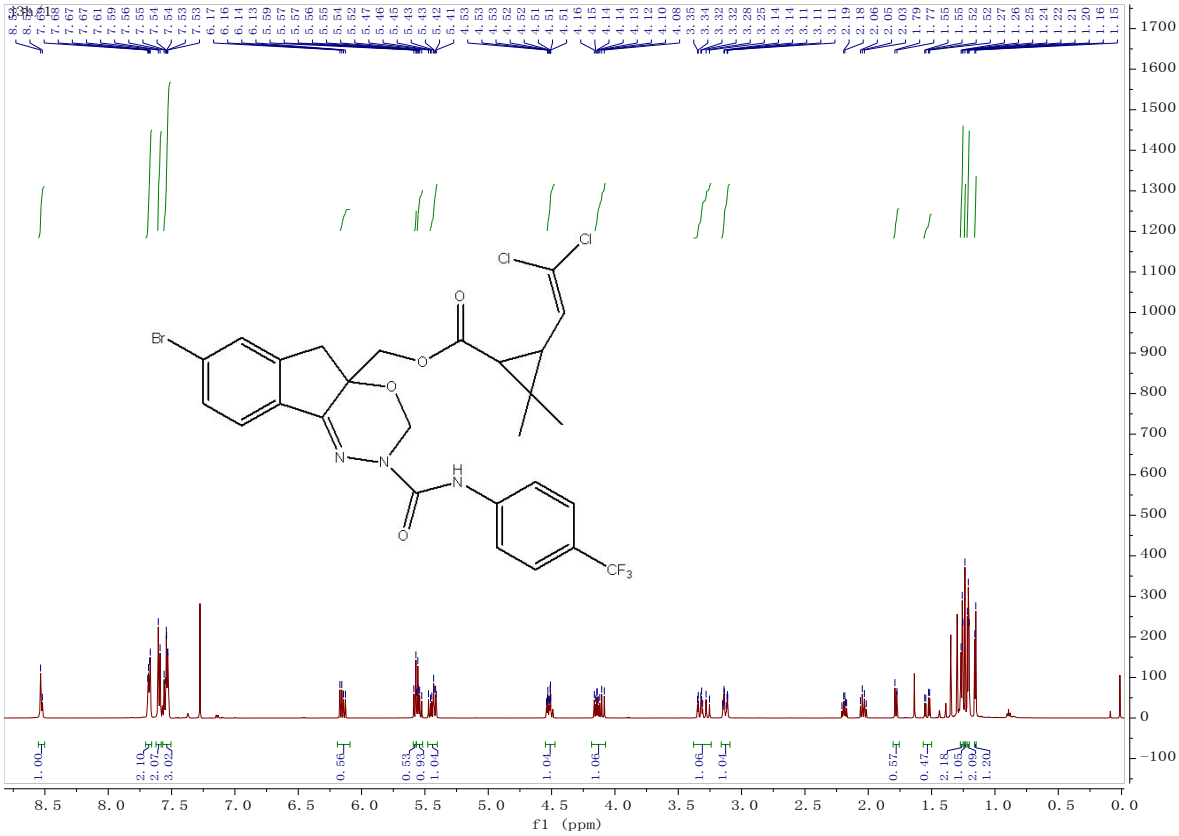
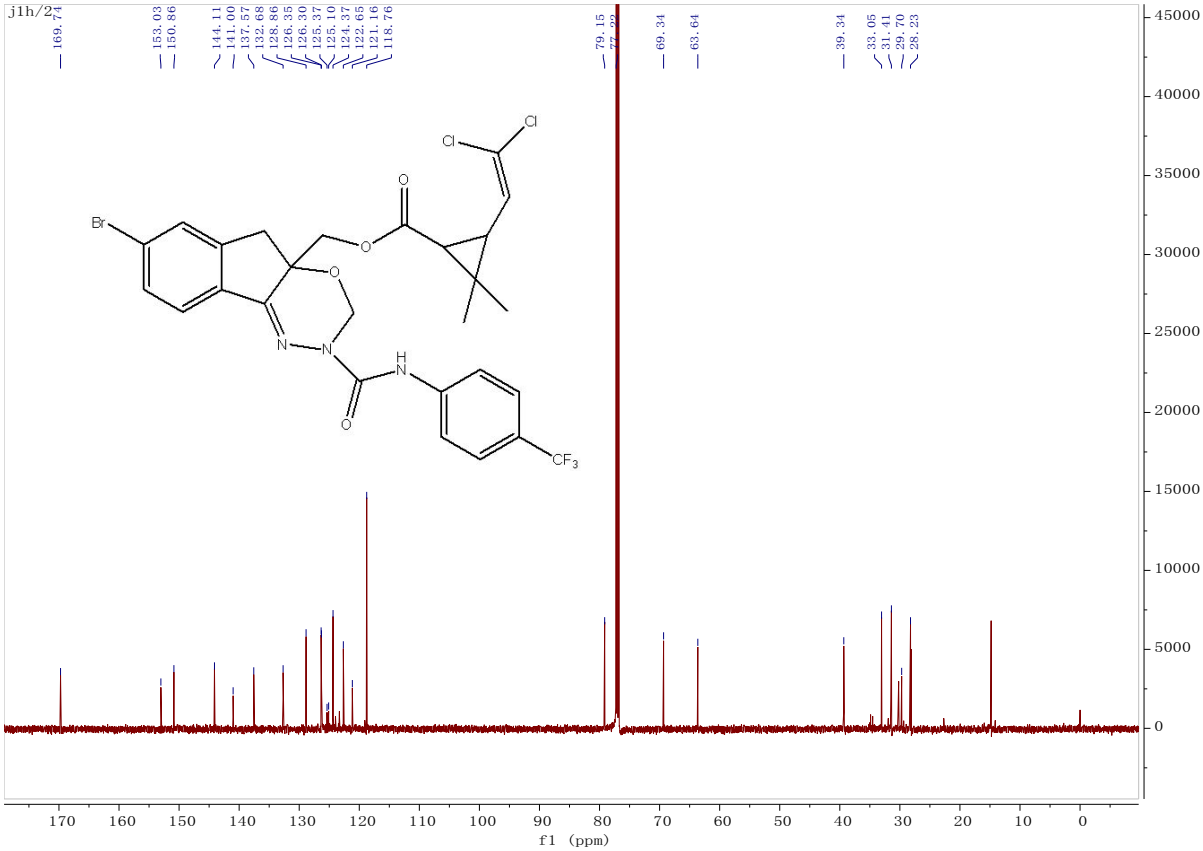
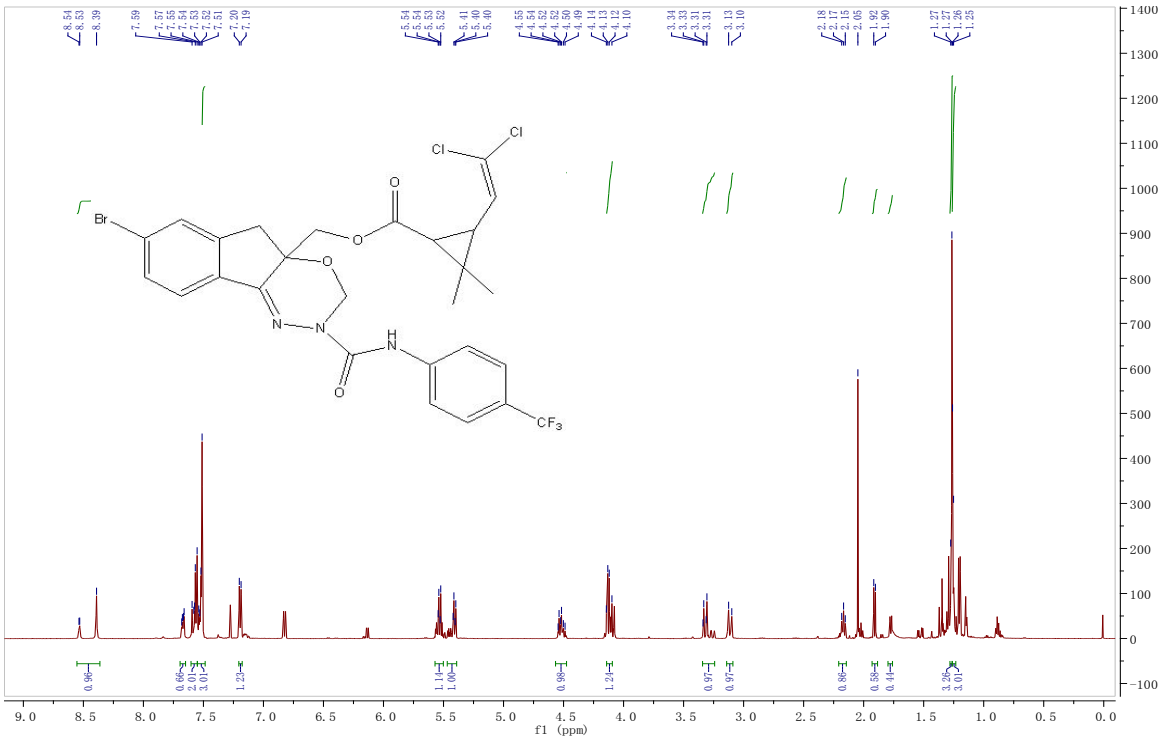
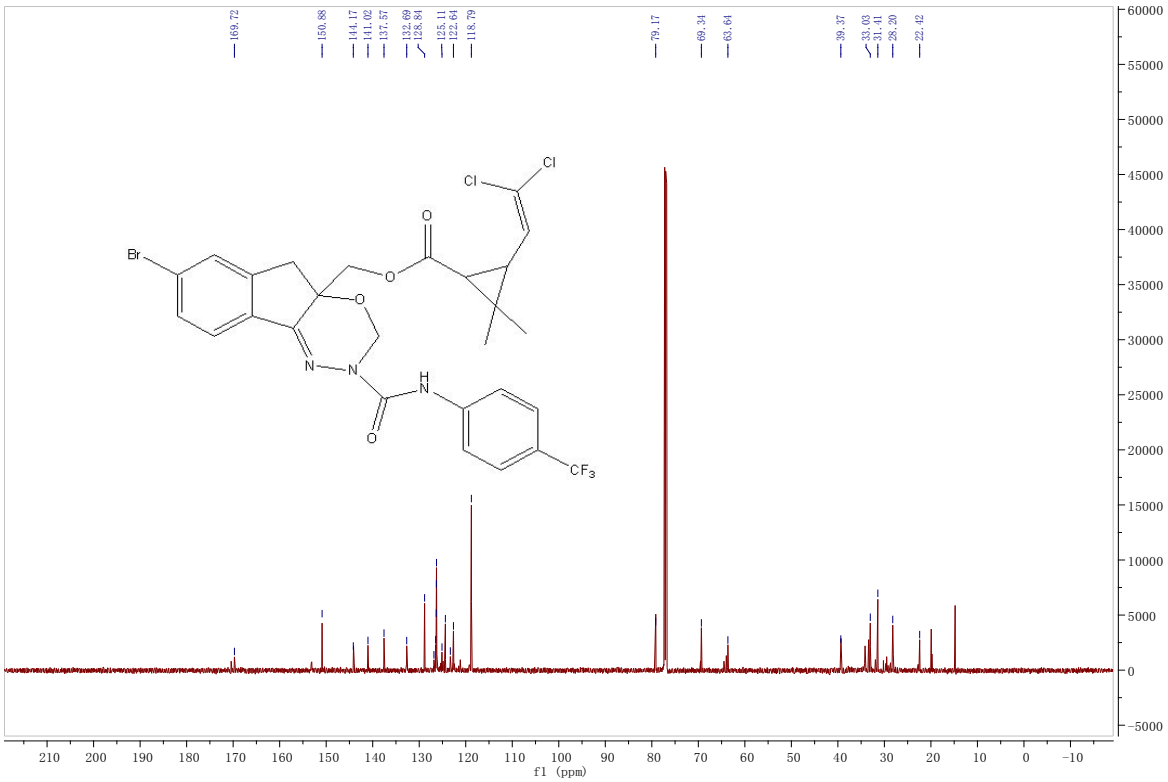


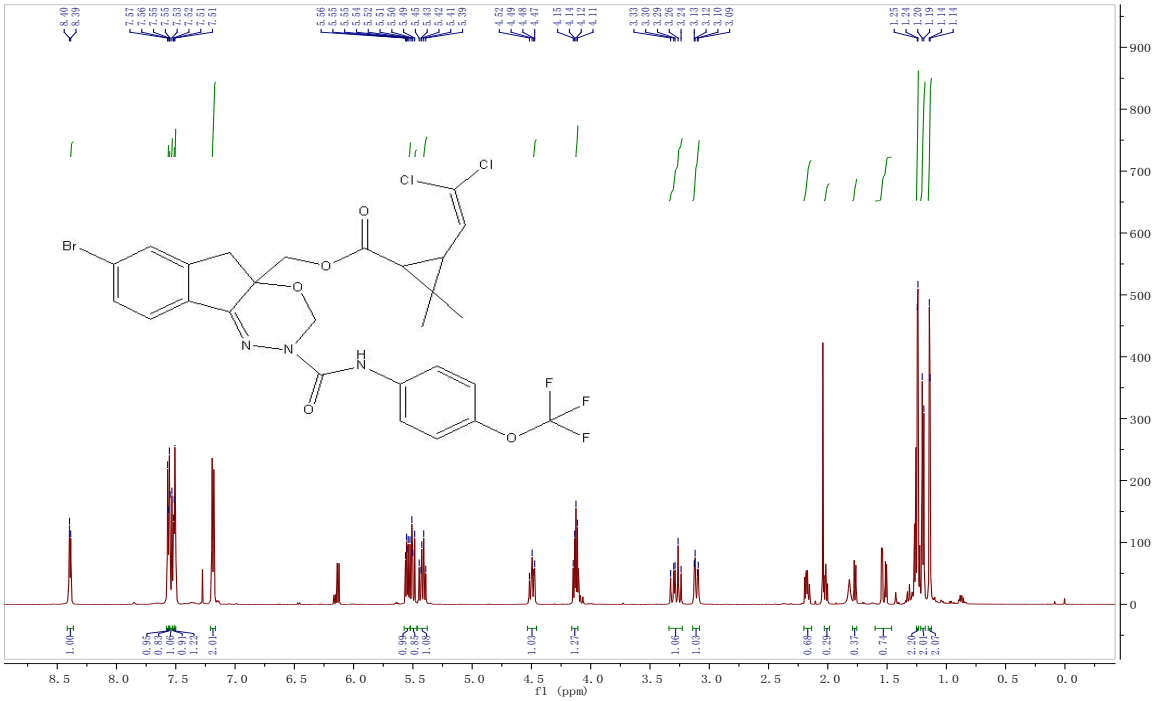


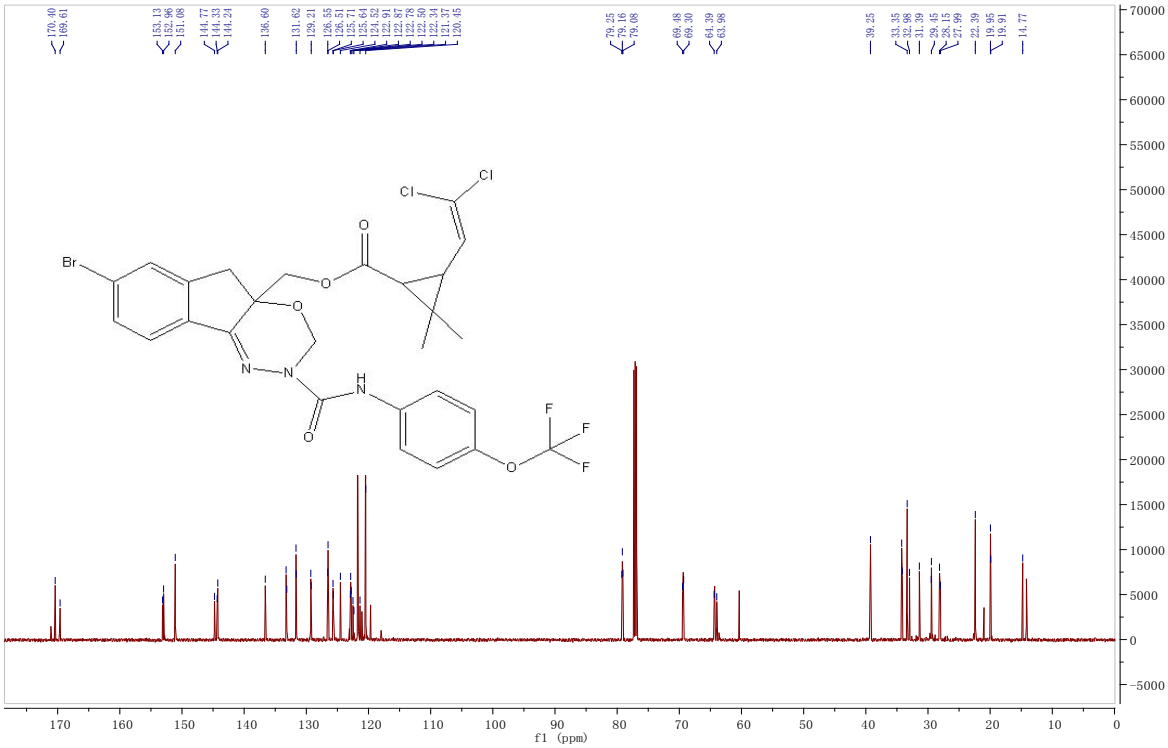
^{1}H NMR and ^{13}C NMR of target compound J3 (Higher Rf value compd)





^{1}H NMR and ^{13}C NMR of target compound J3 (Lower Rf value compd)





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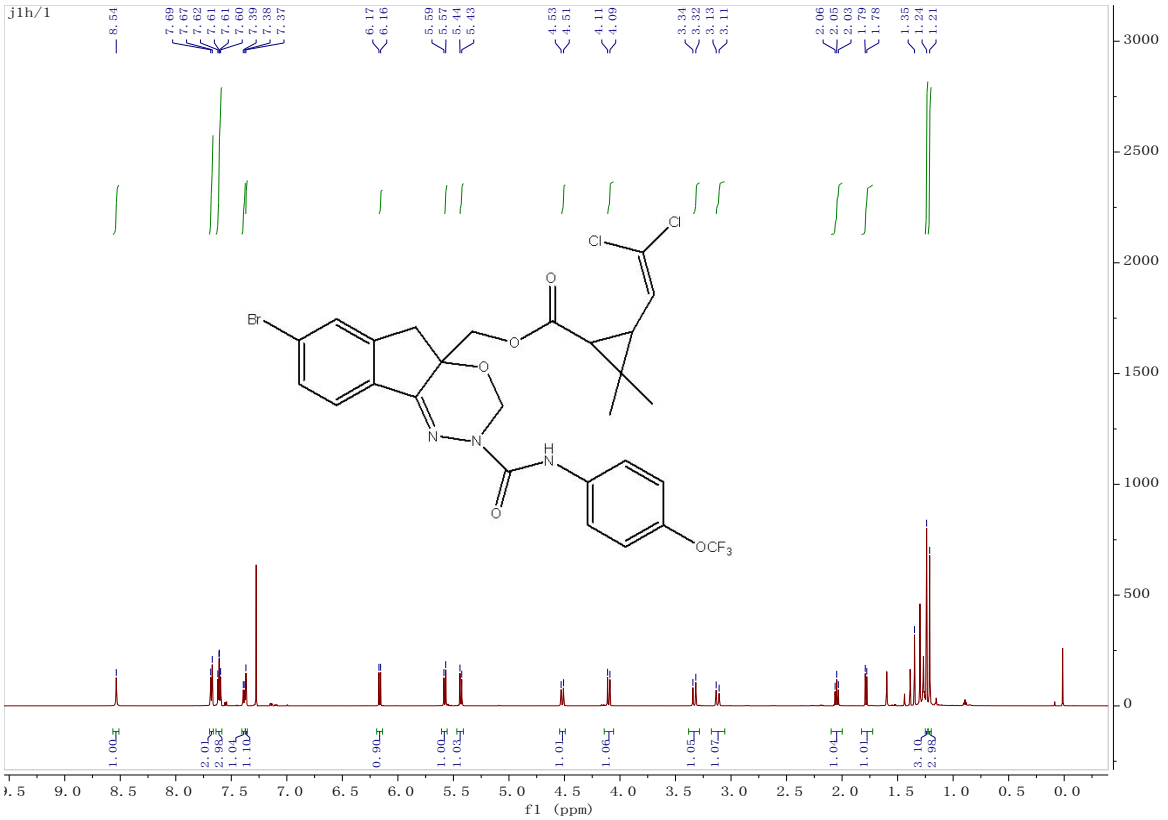
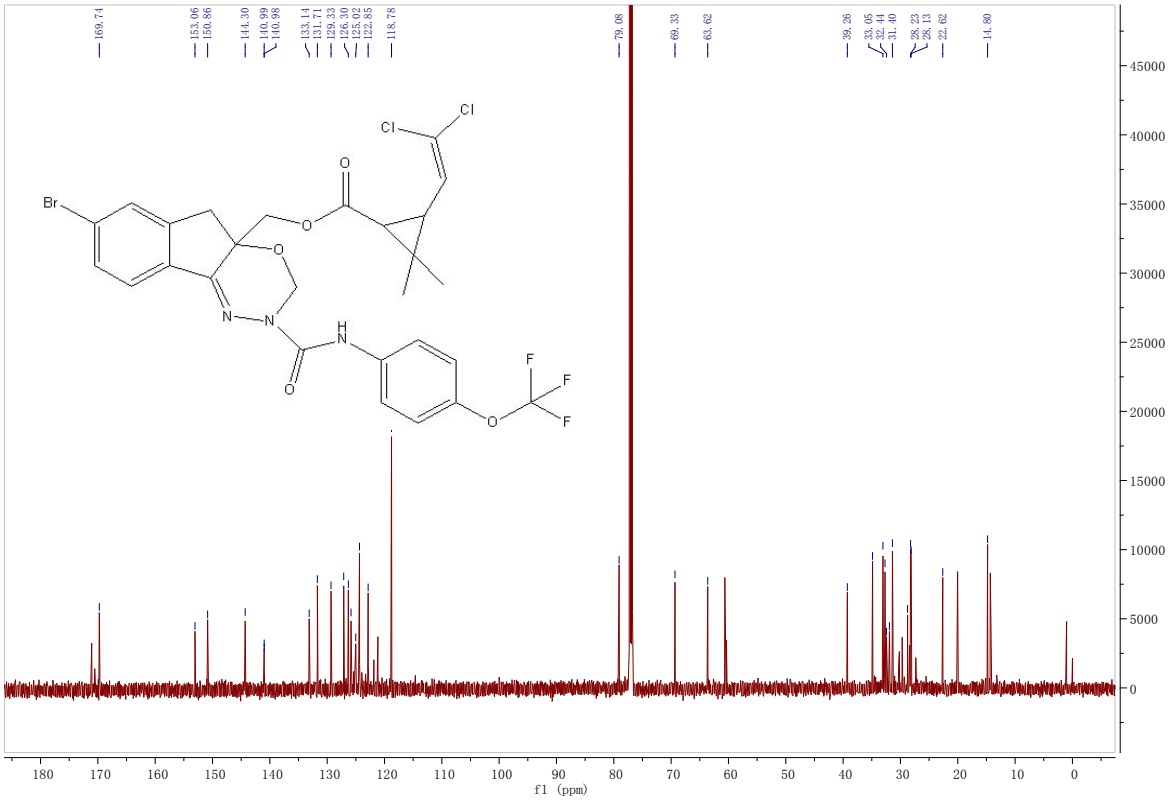
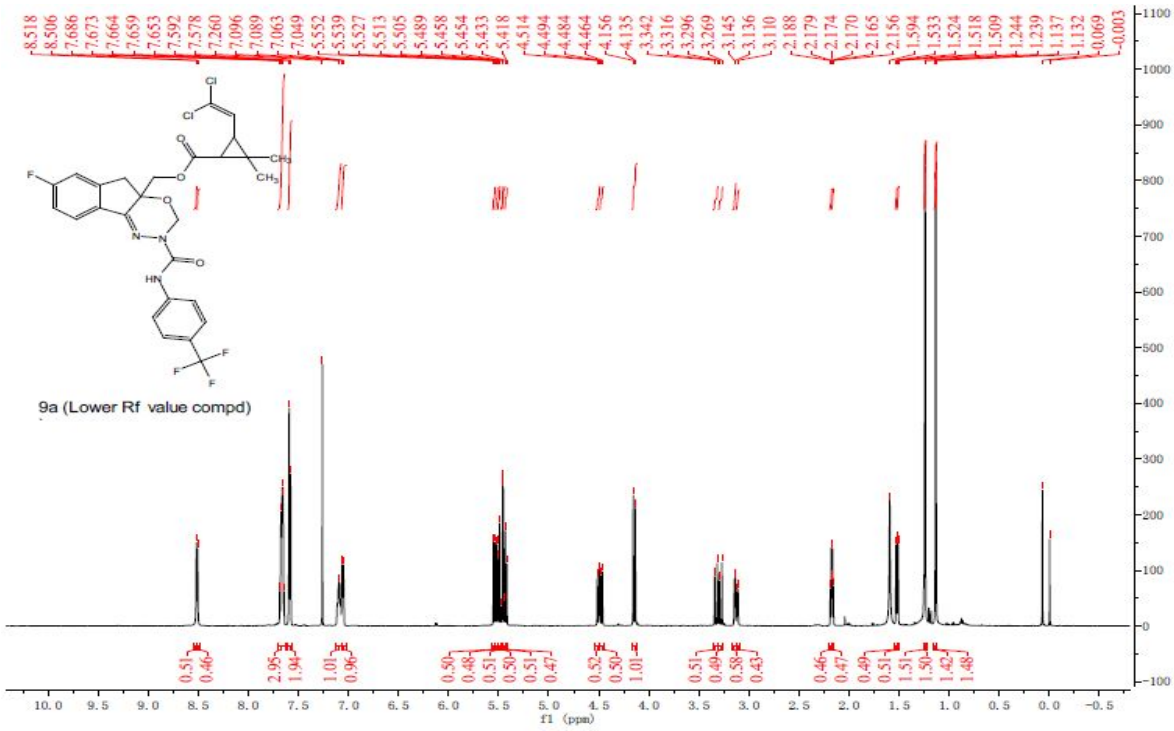
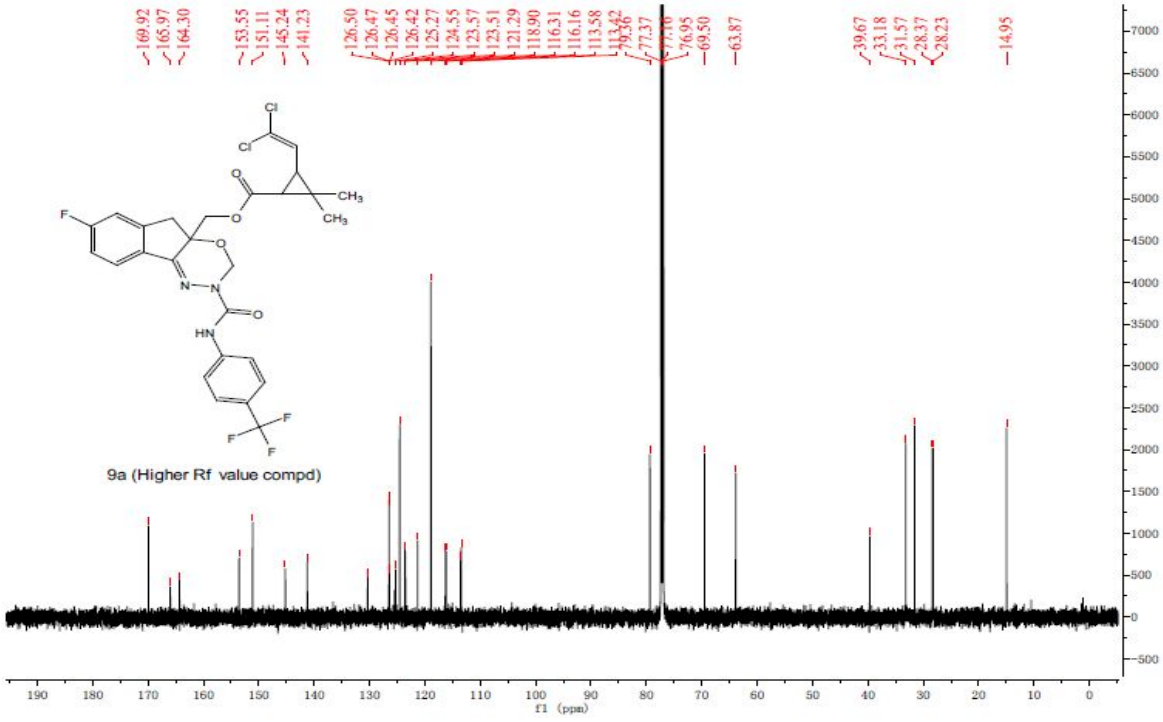


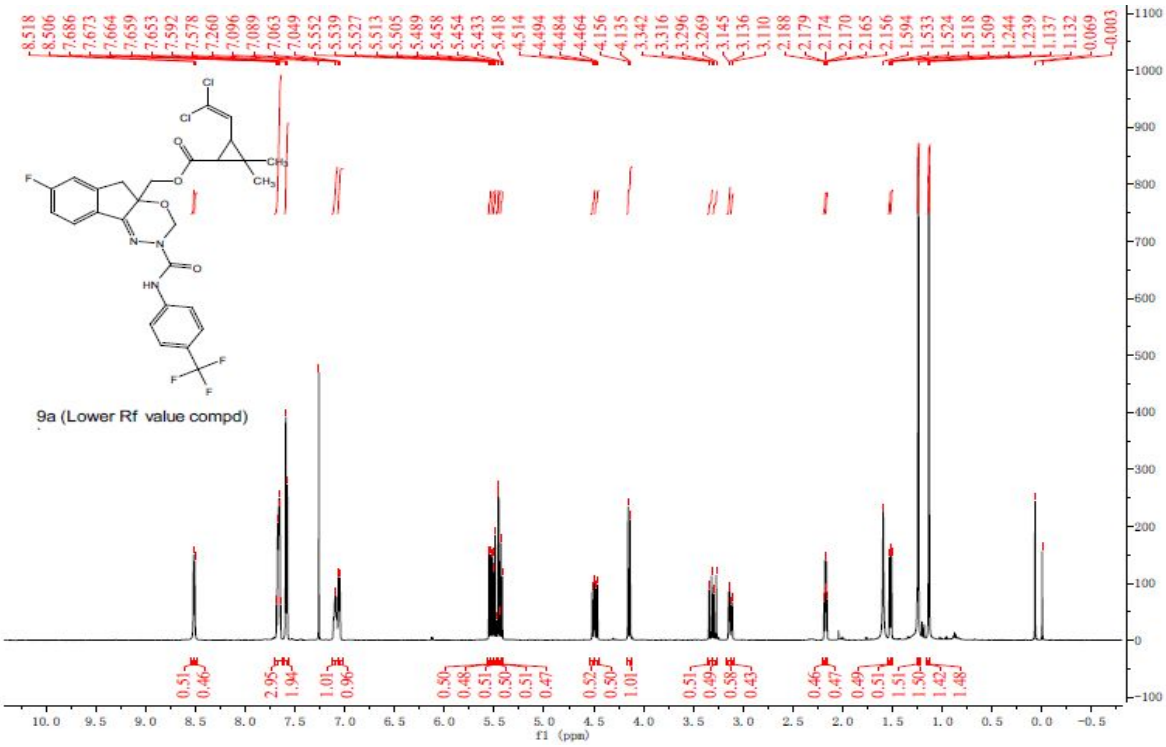


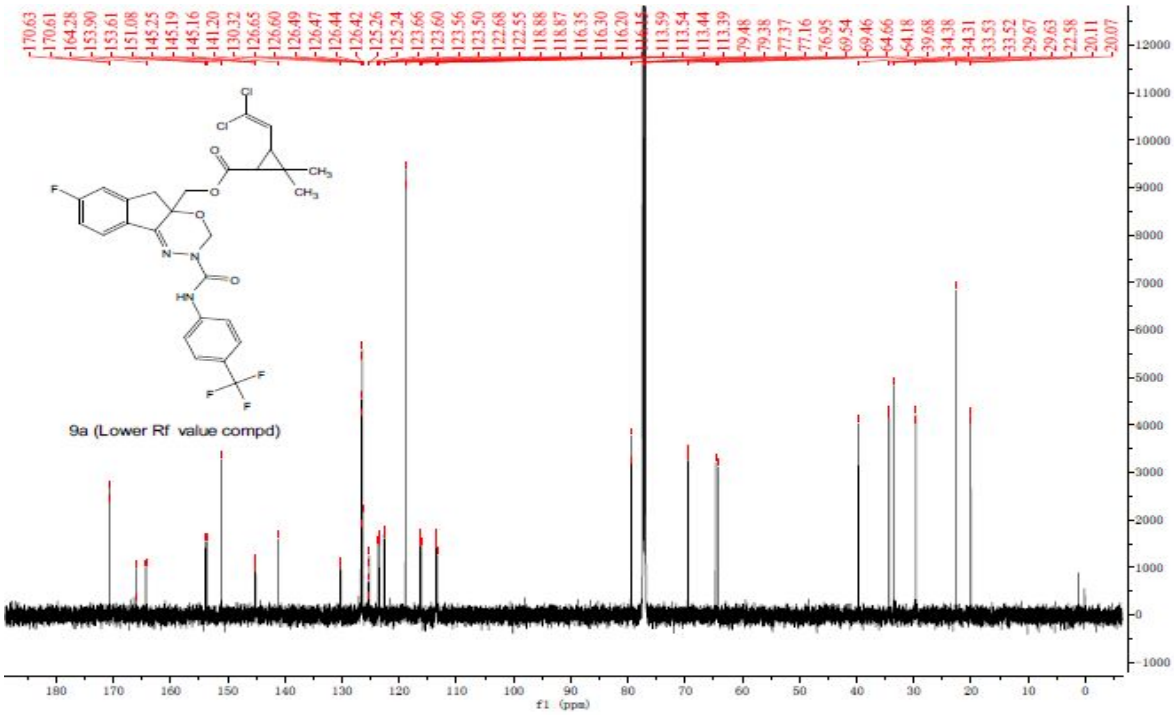
^{1}H NMR and ^{13}C NMR of target compound J4 (Lower Rf value compd)



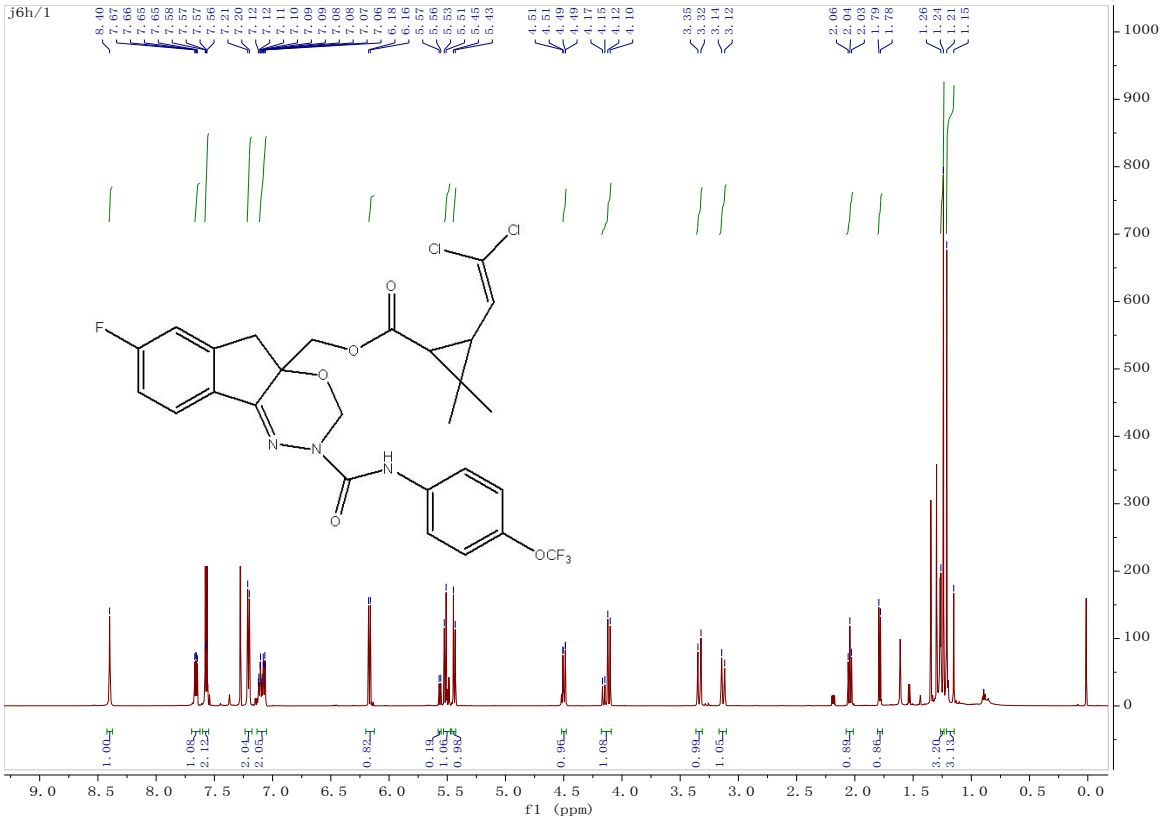


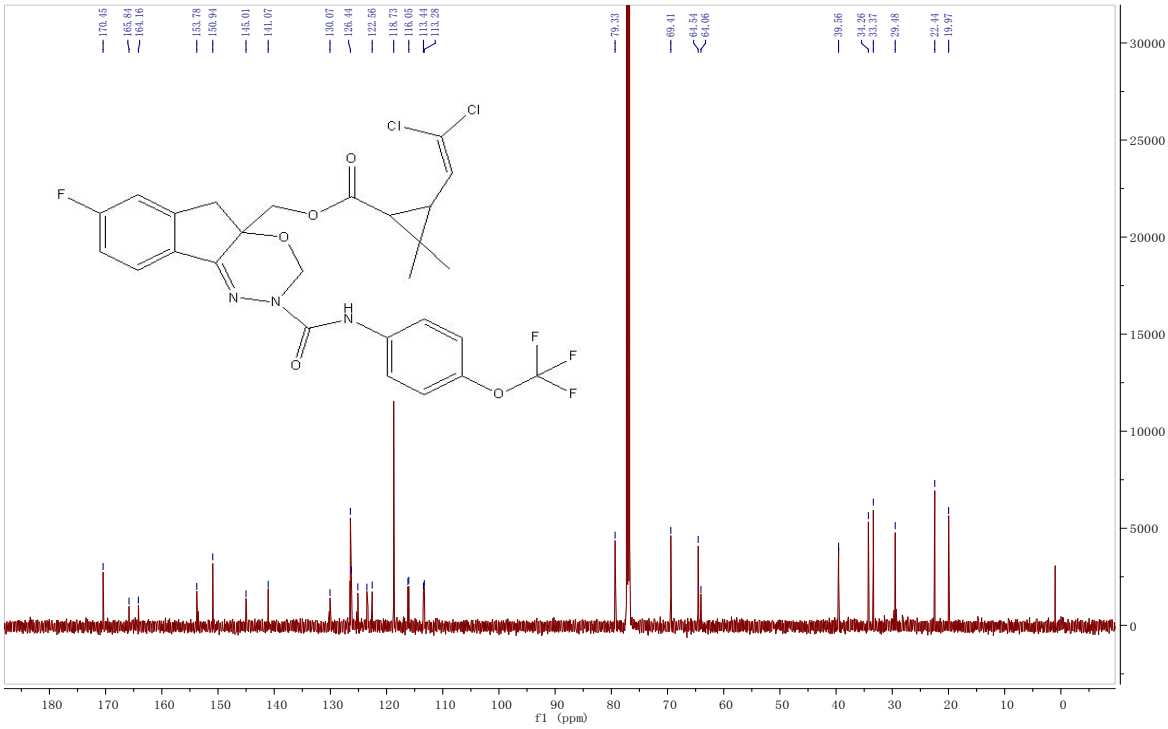
^{1}H NMR and ^{13}C NMR of target compound J5 (Higher Rf value compd)



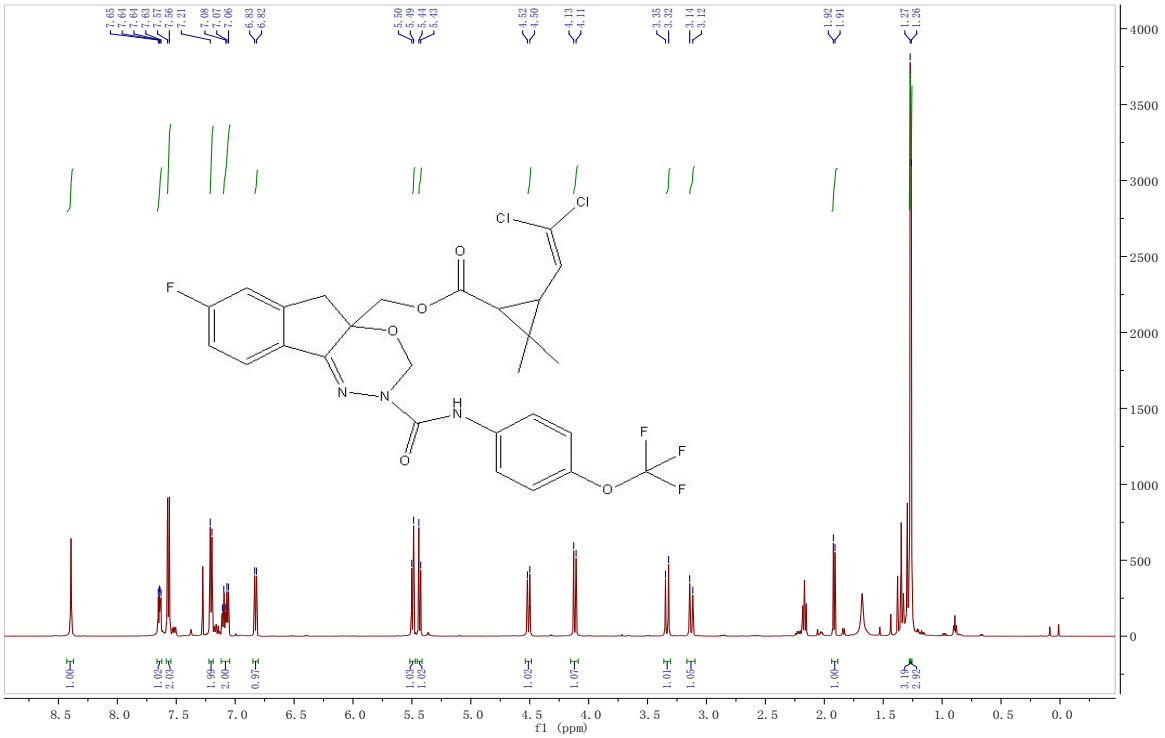


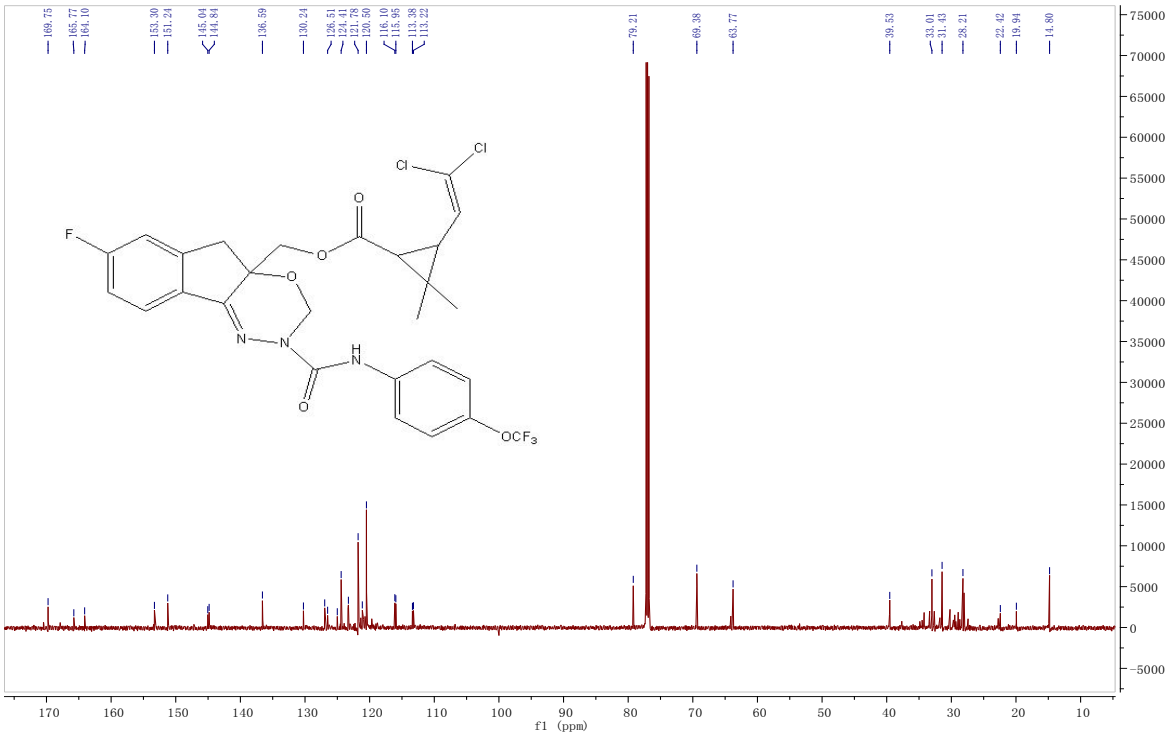
^{1}H NMR and ^{13}C NMR of target compound J5 (Lower Rf value compd)



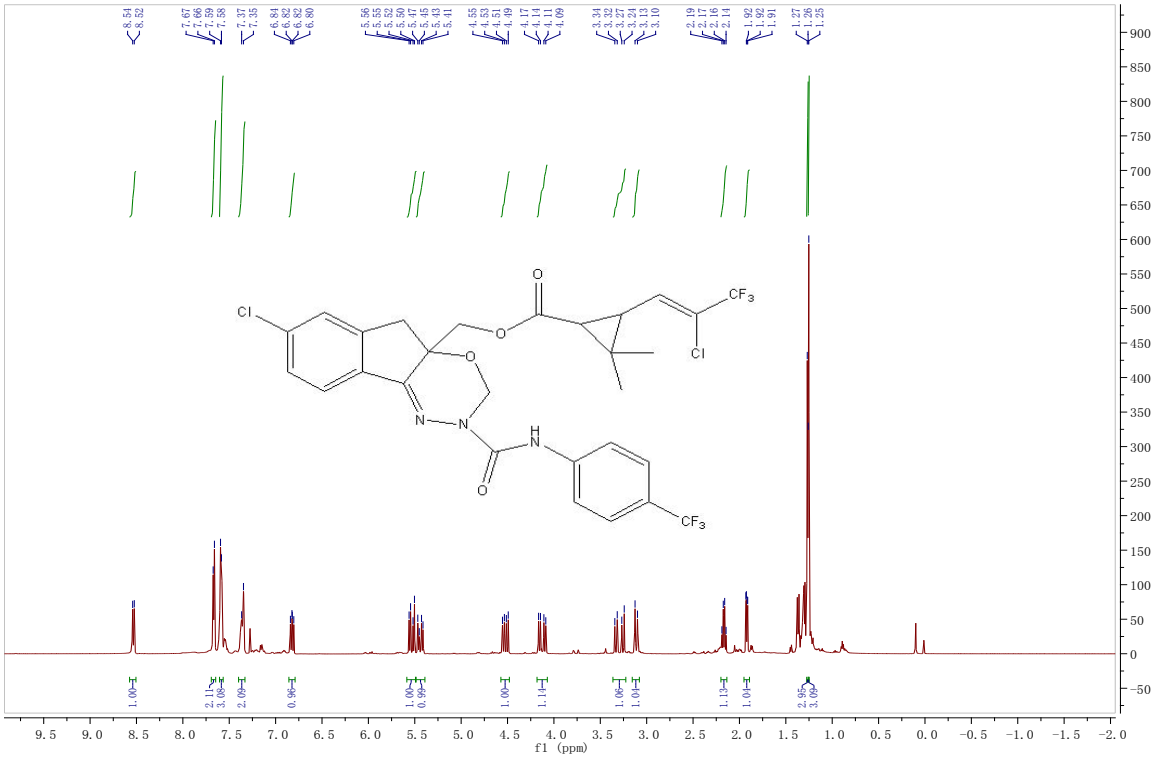


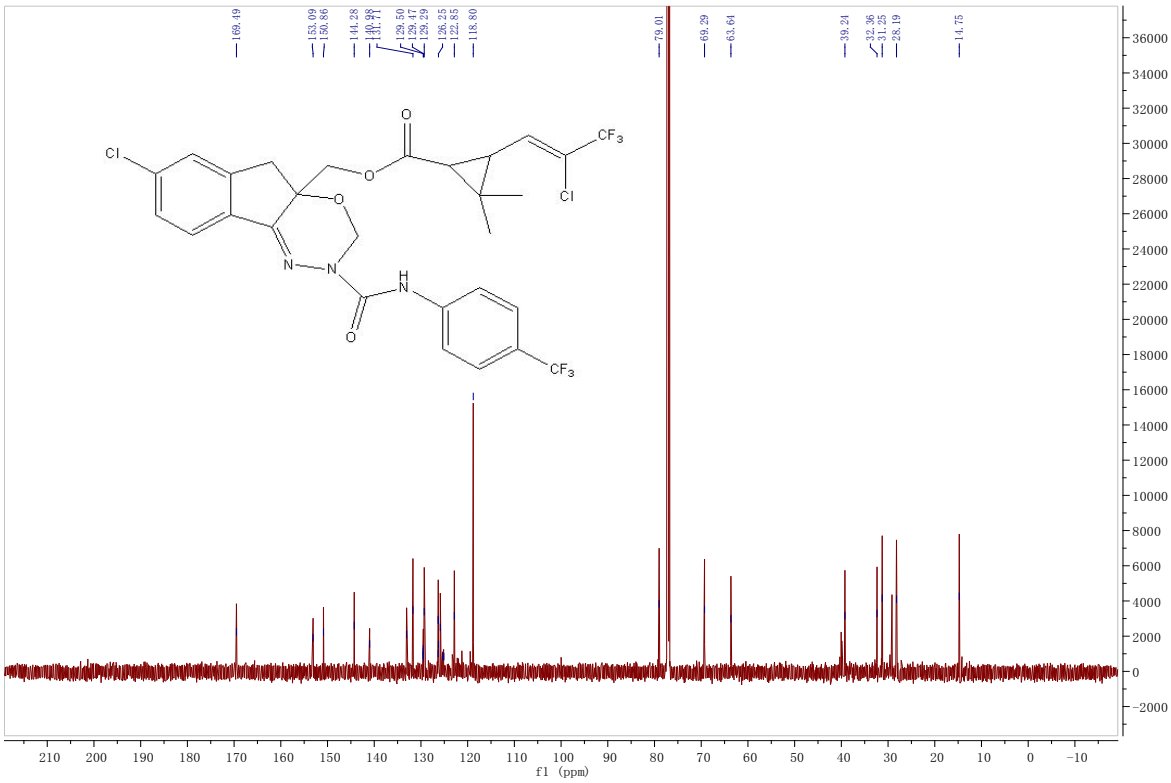
^{1}H NMR and ^{13}C NMR of target compound J6 (Higher Rf value compd)



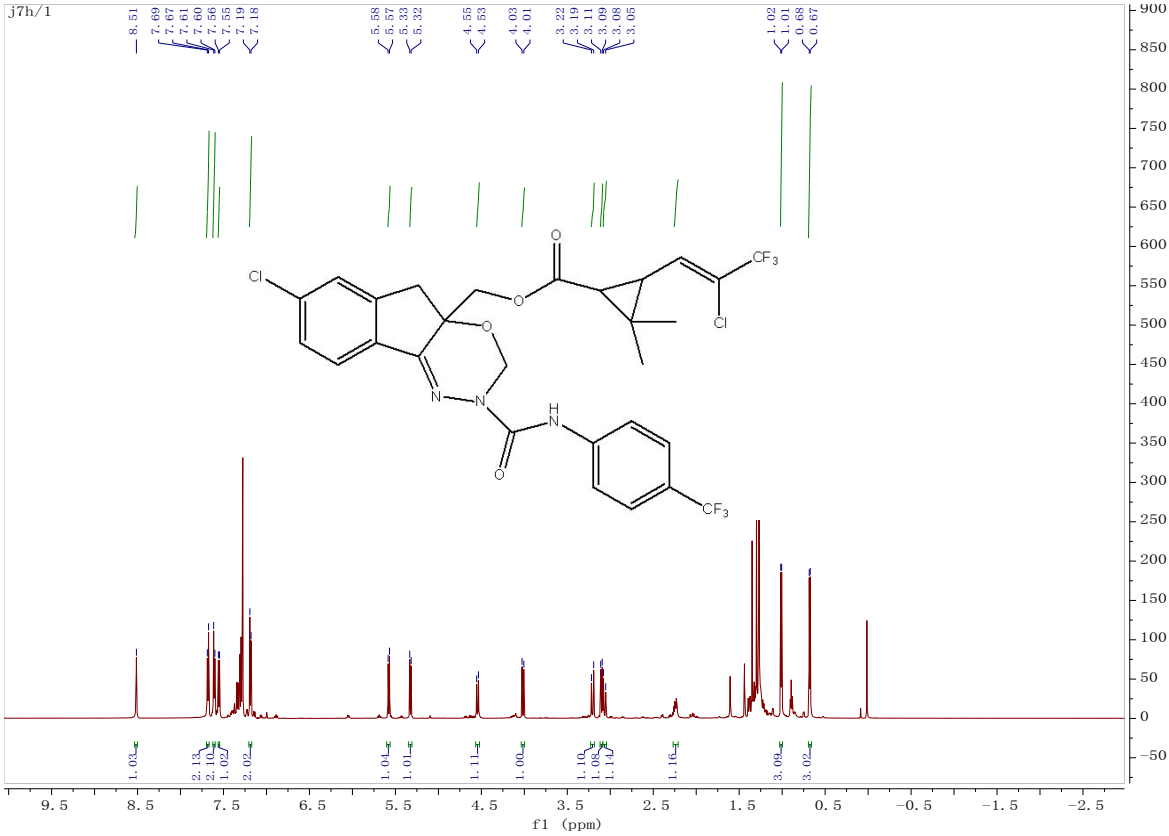


^{1}H NMR and ^{13}C NMR of target compound J6 (Lower Rf value compd)





^{1}H NMR and ^{13}C NMR of target compound J7 (Higher Rf value compd)



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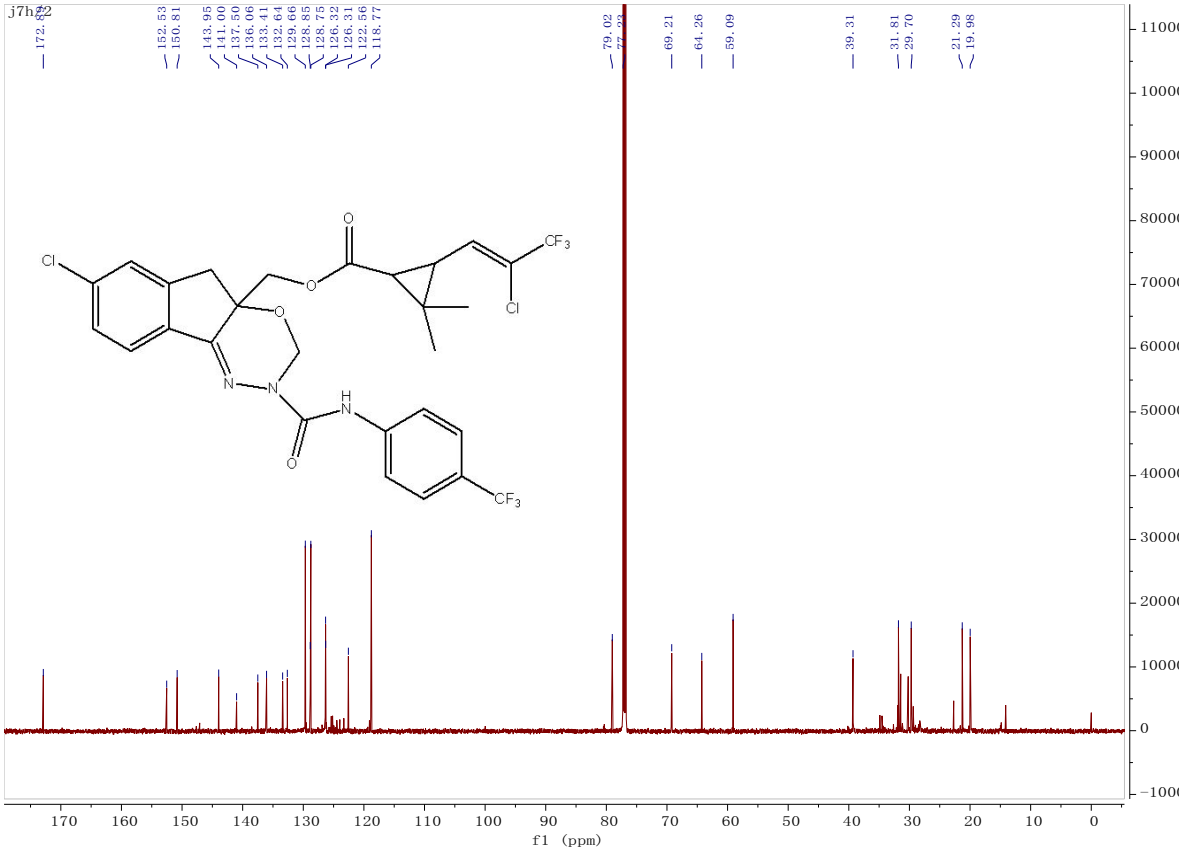

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117 ^{1}H NMR and ^{13}C NMR of target compound J7 (Lower Rf value compd)

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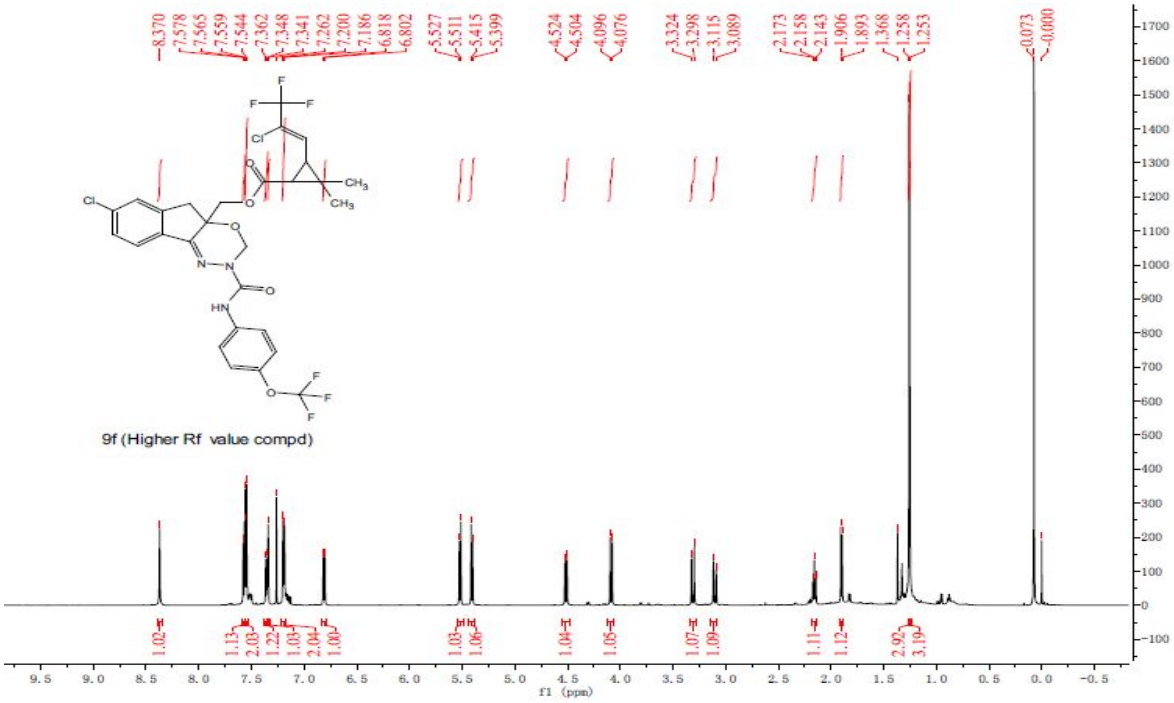

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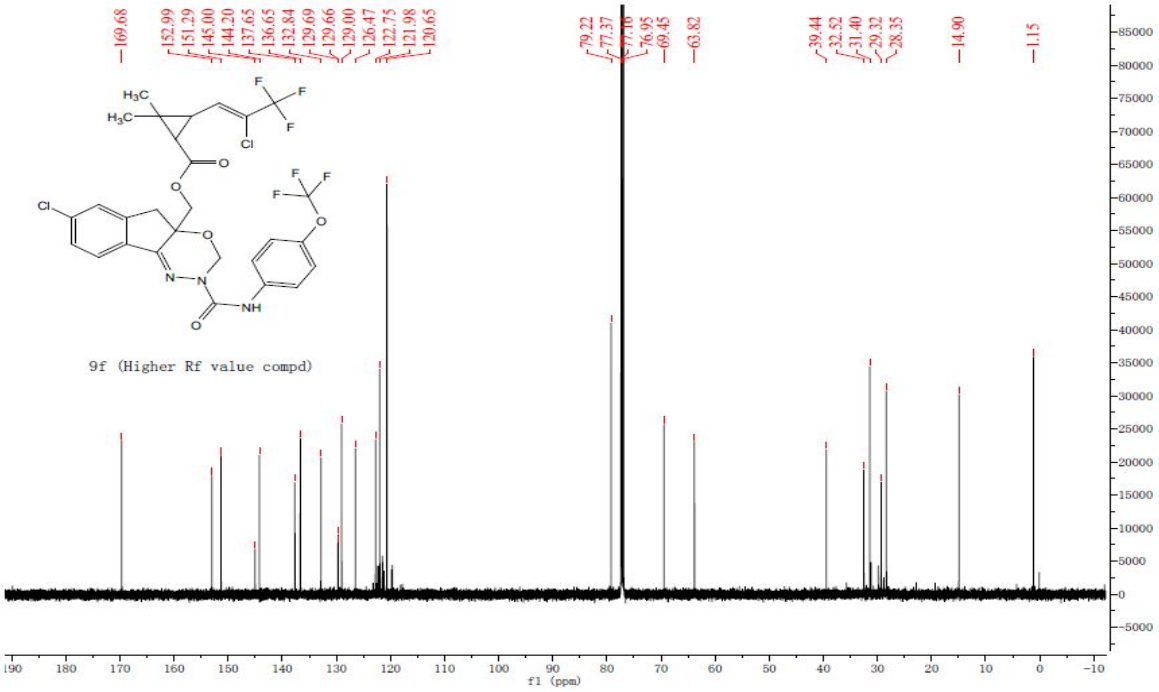

121 ^{1}H NMR and ^{13}C NMR of target compound J8 (Higher Rf value compd)

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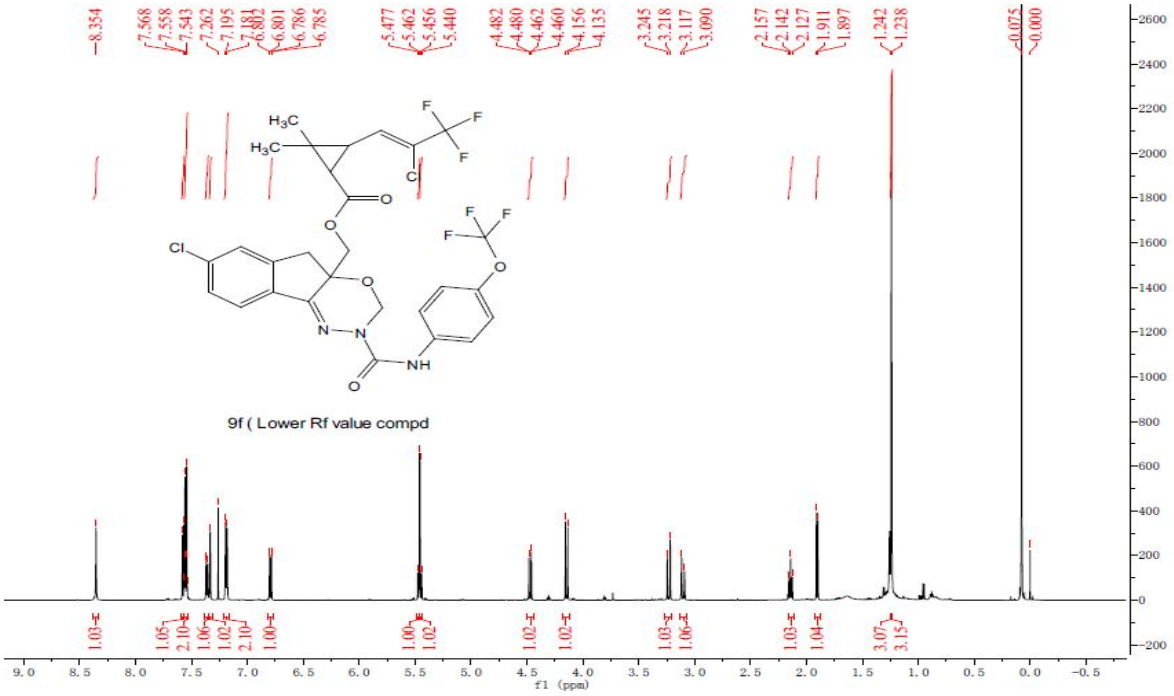
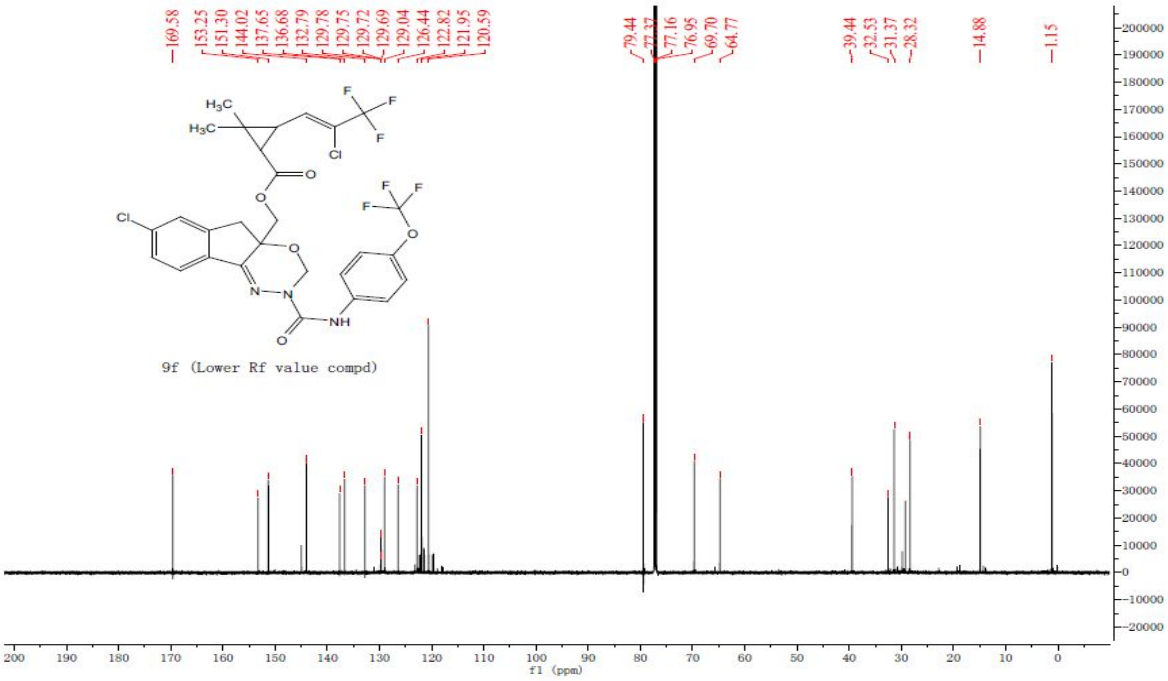
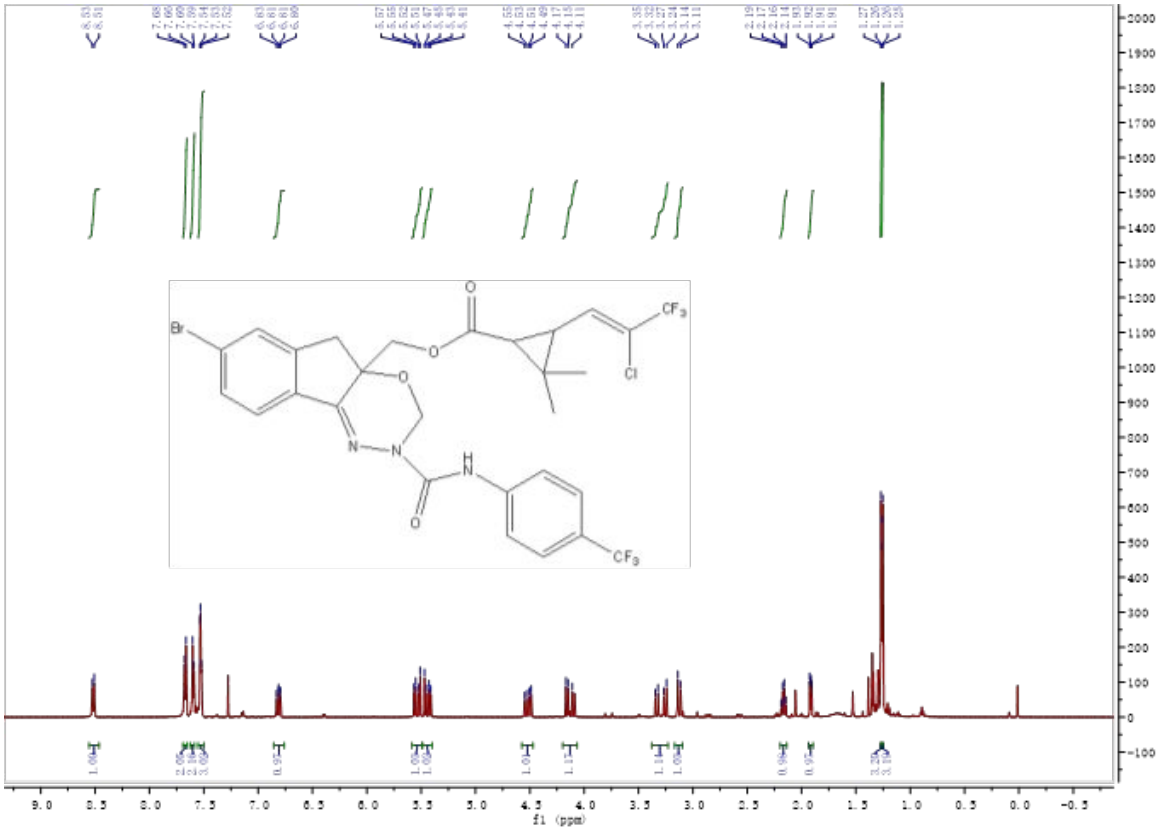
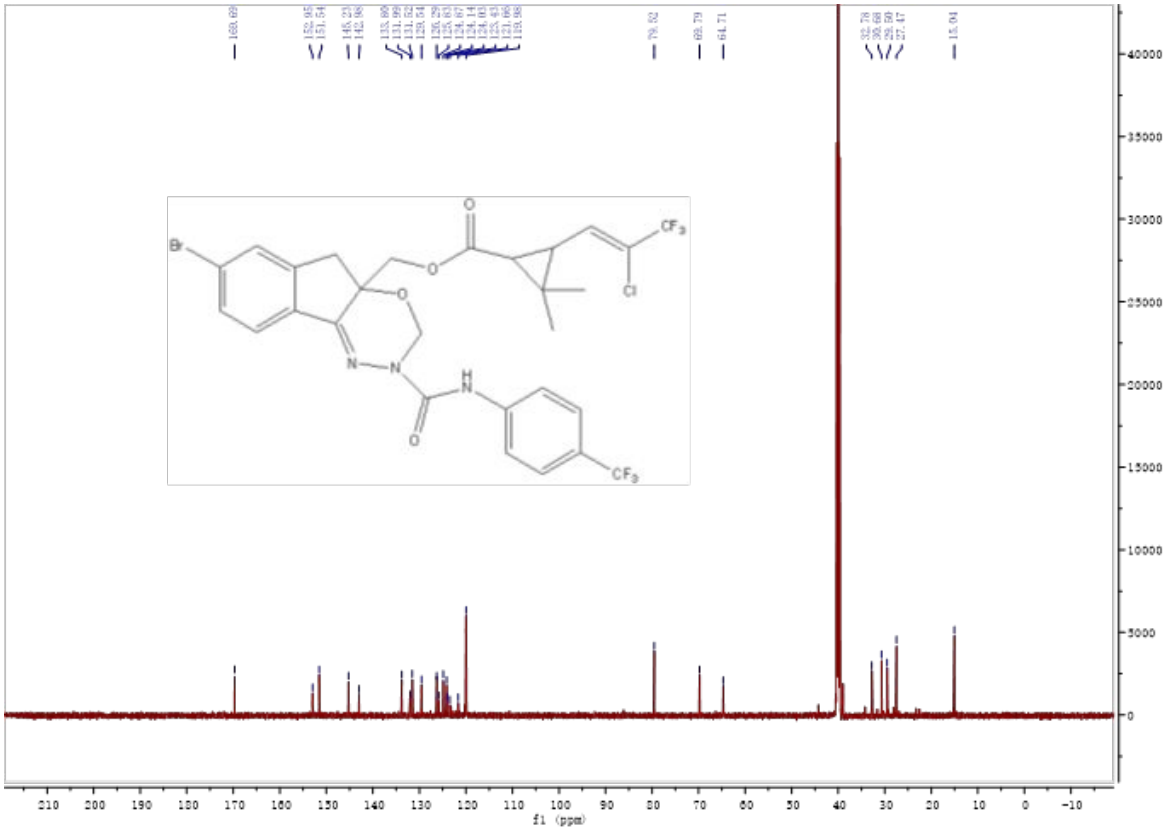


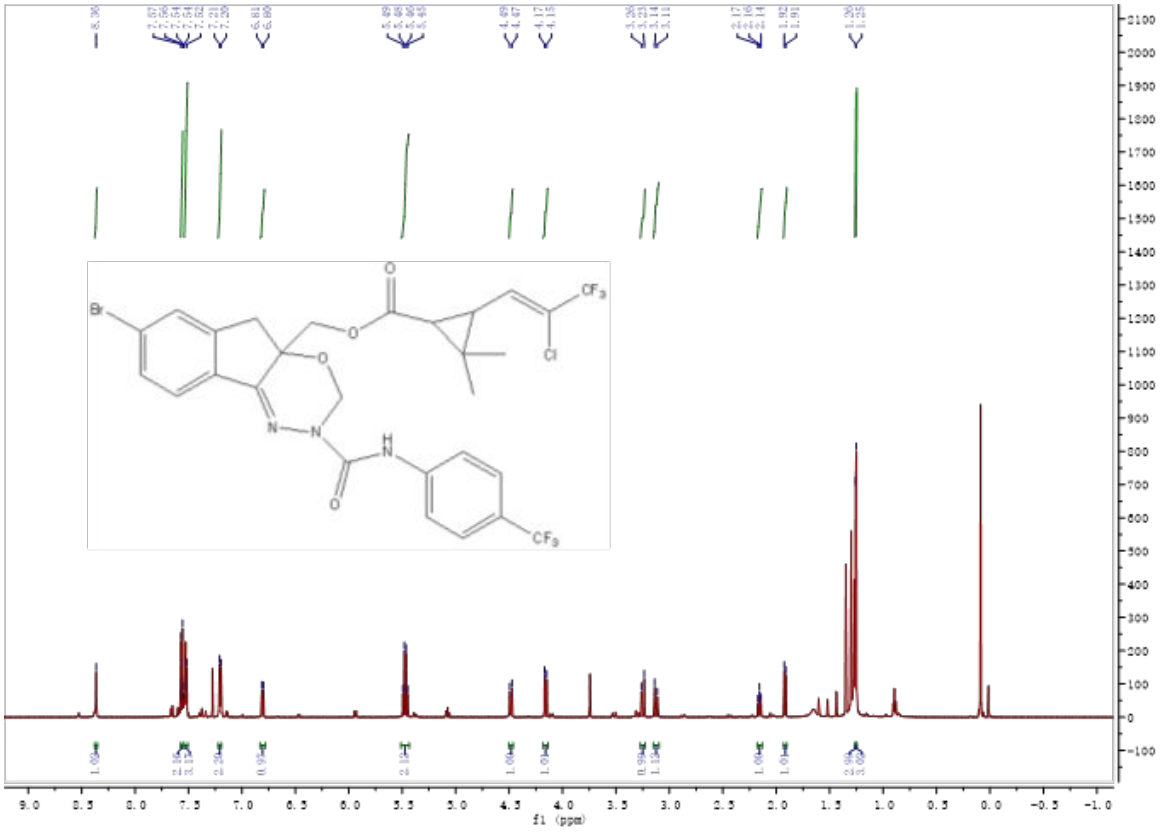


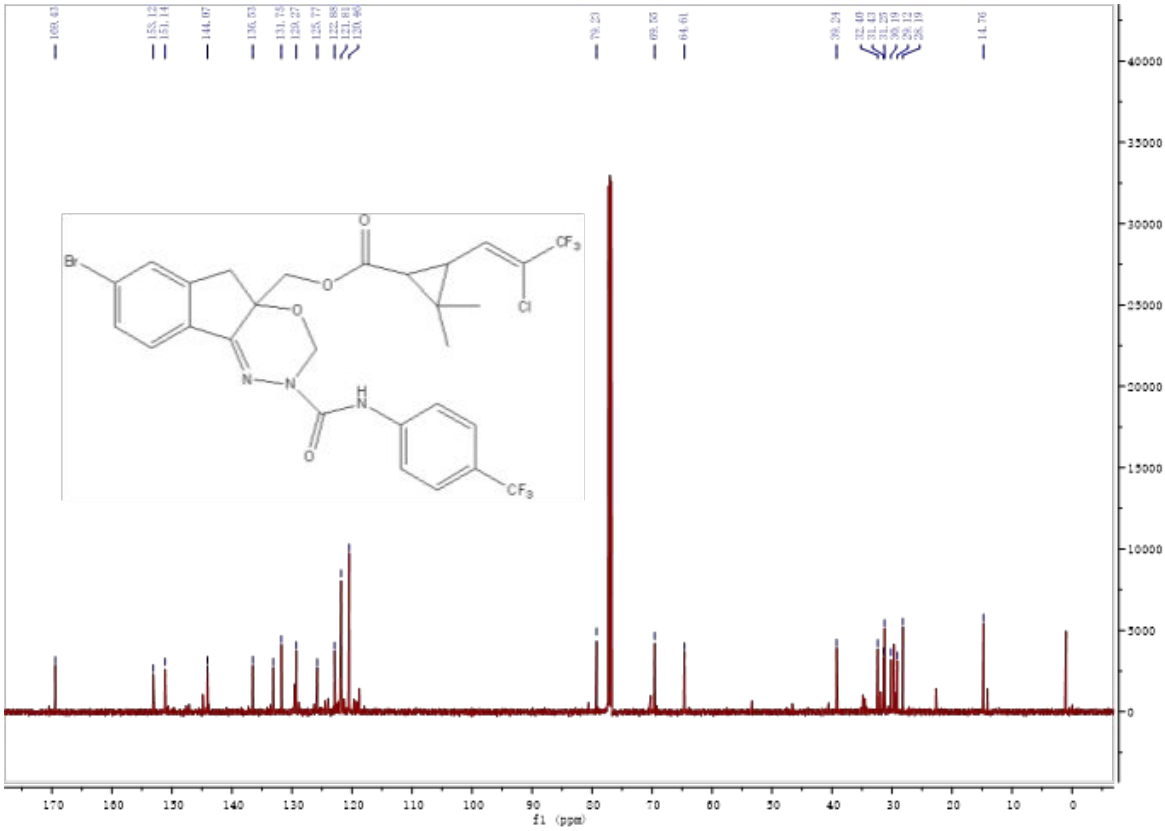
^{1}H NMR and ^{13}C NMR of target compound J8 (Lower Rf value compd)



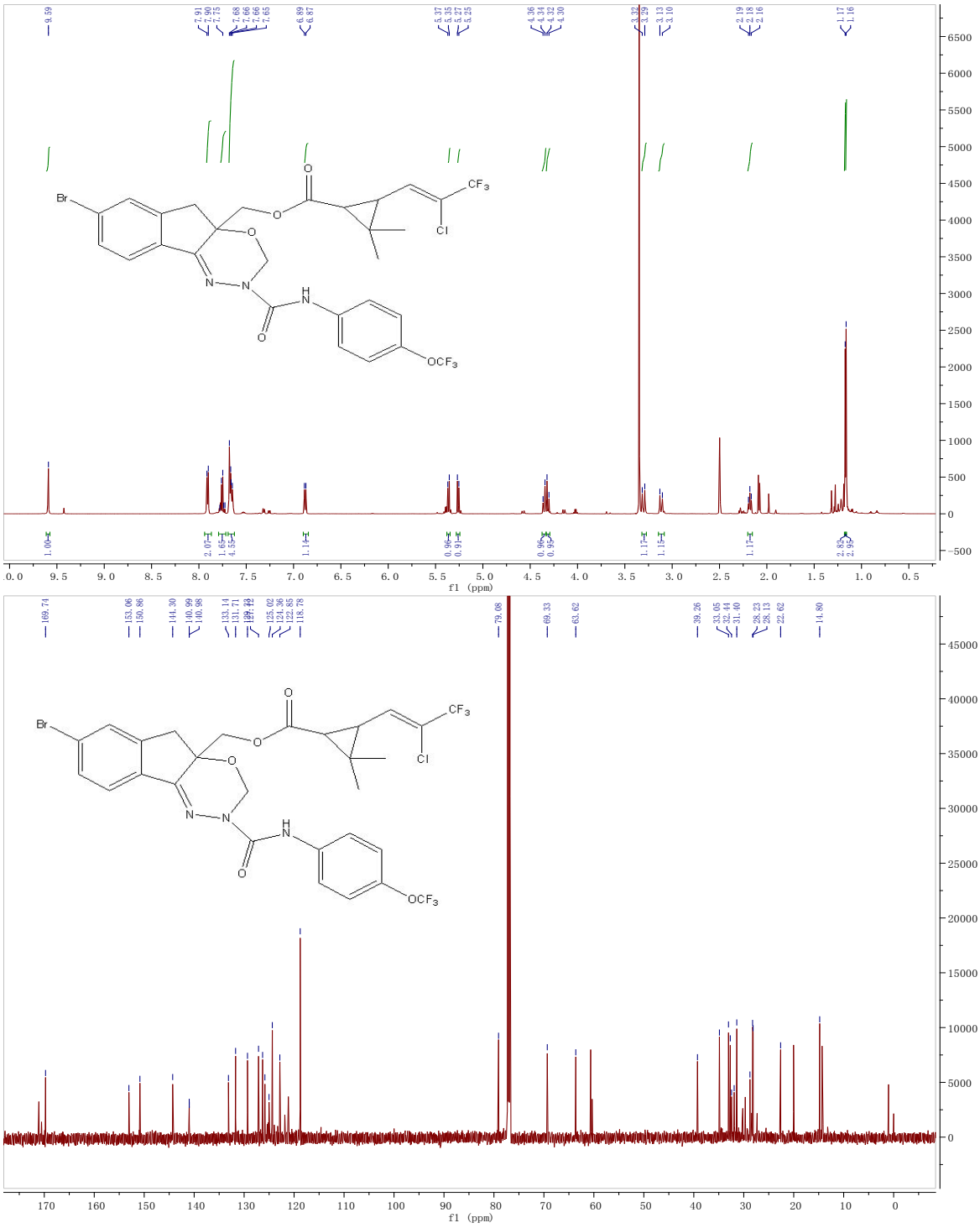


^{1}H NMR and ^{13}C NMR of target compound J9 (Higher Rf value compd)

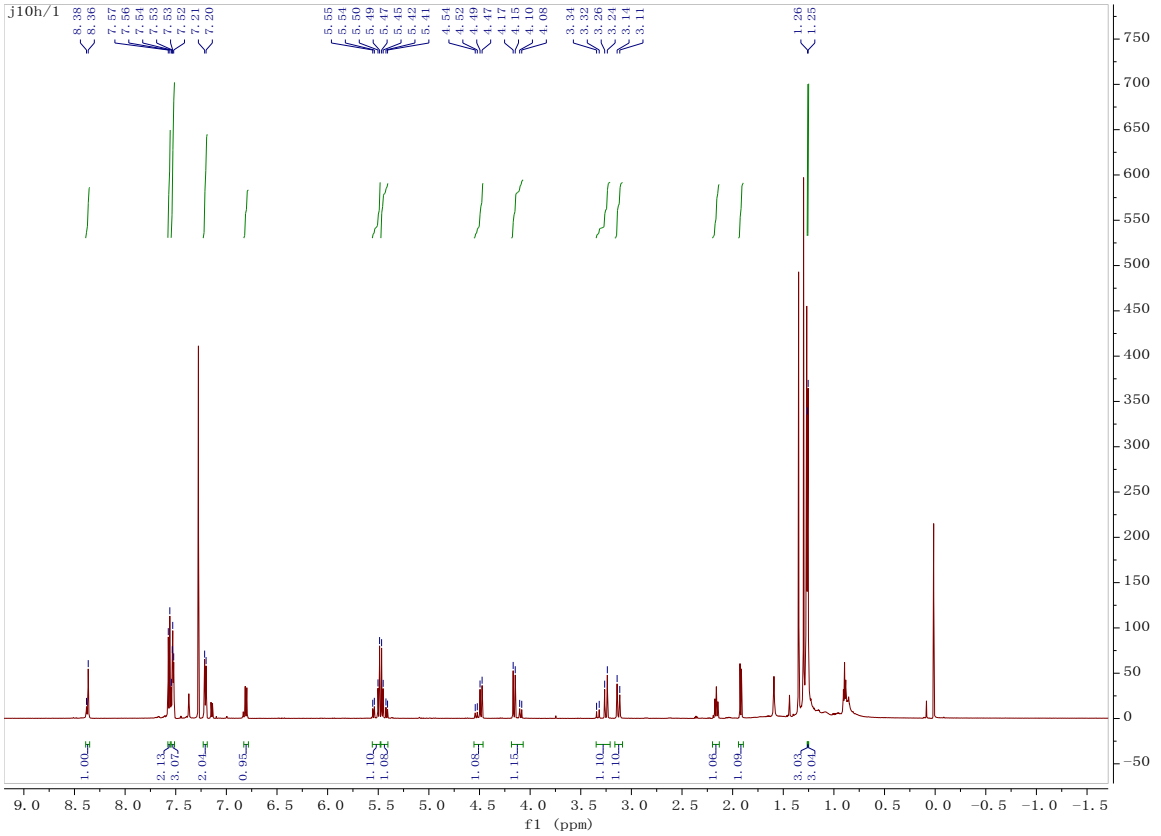


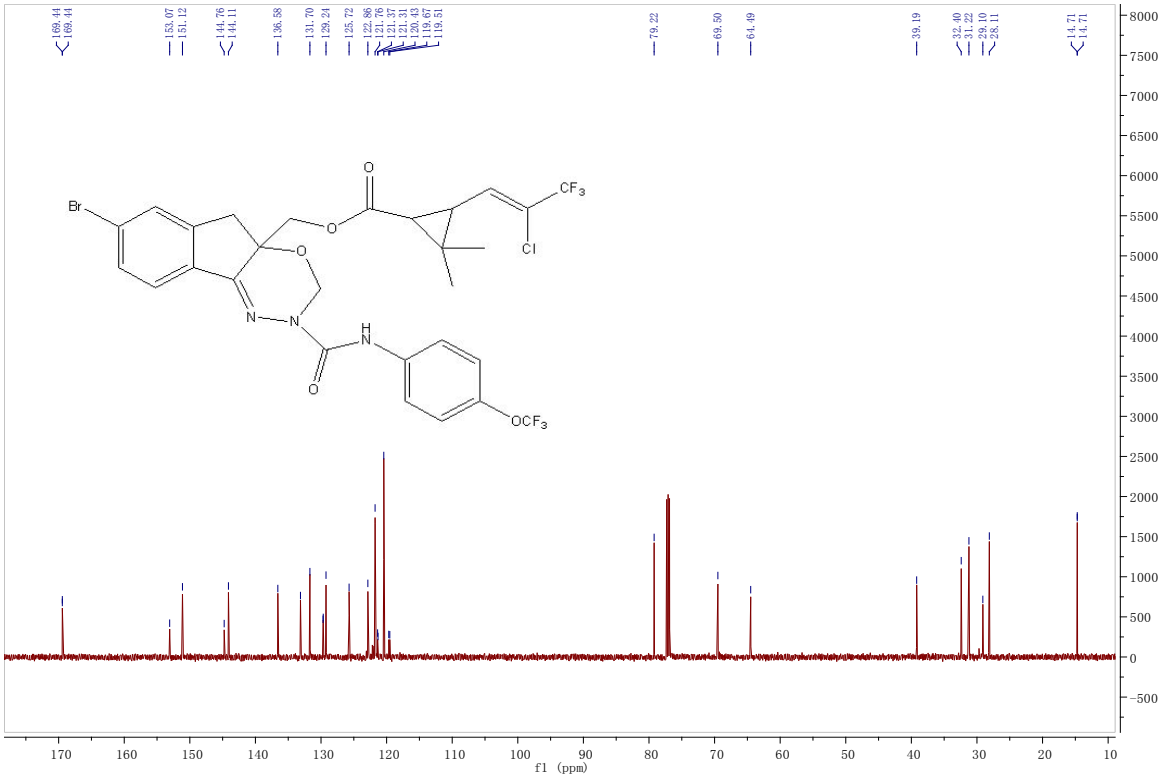


^{1}H NMR and ^{13}C NMR of target compound J9 (Lower Rf value compd)

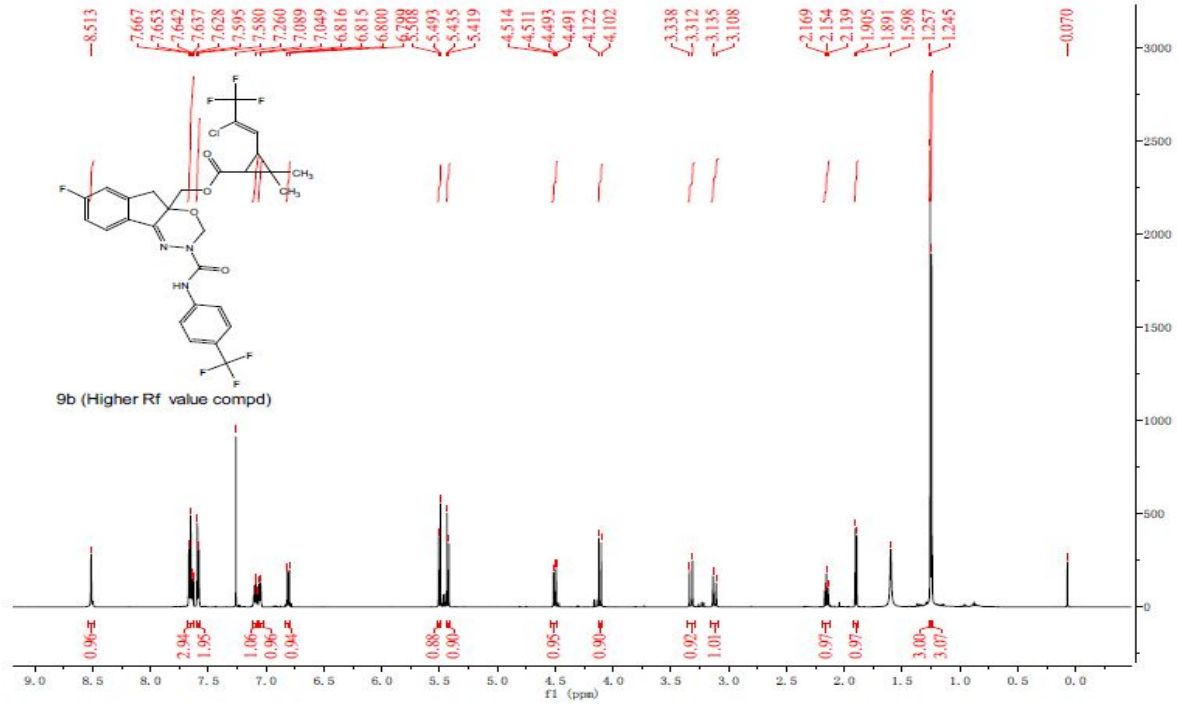


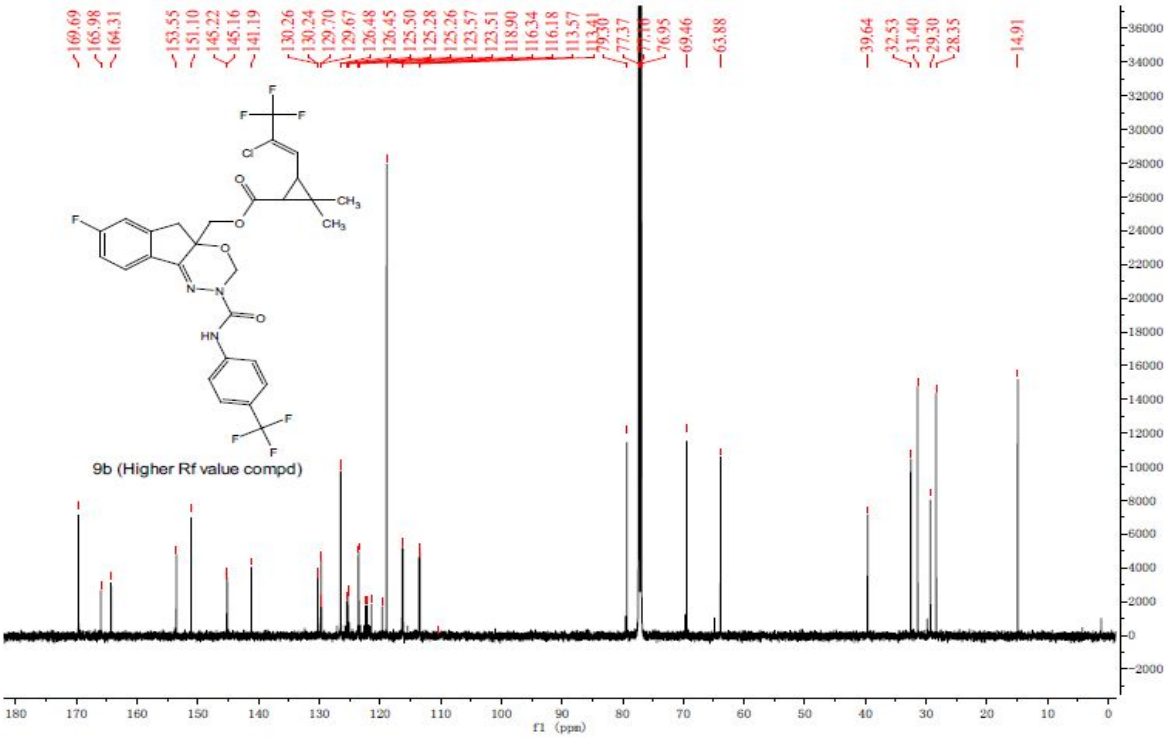
^{1}H NMR and ^{13}C NMR of target compound J10 (Higher Rf value compd)



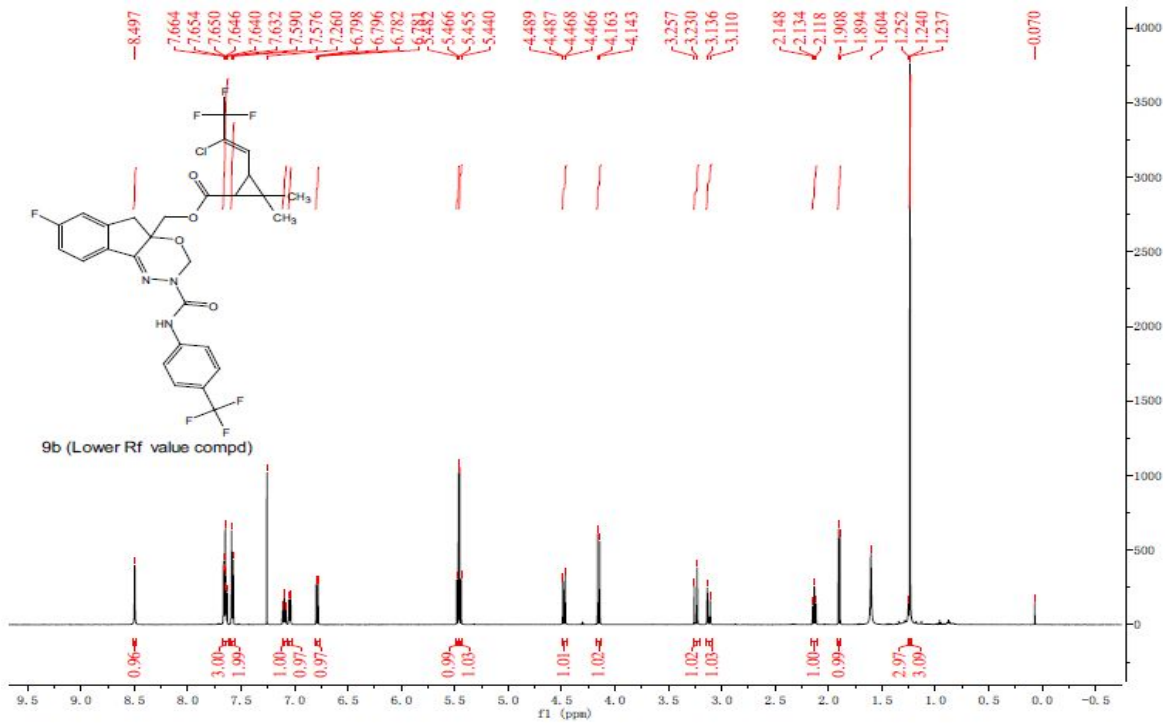


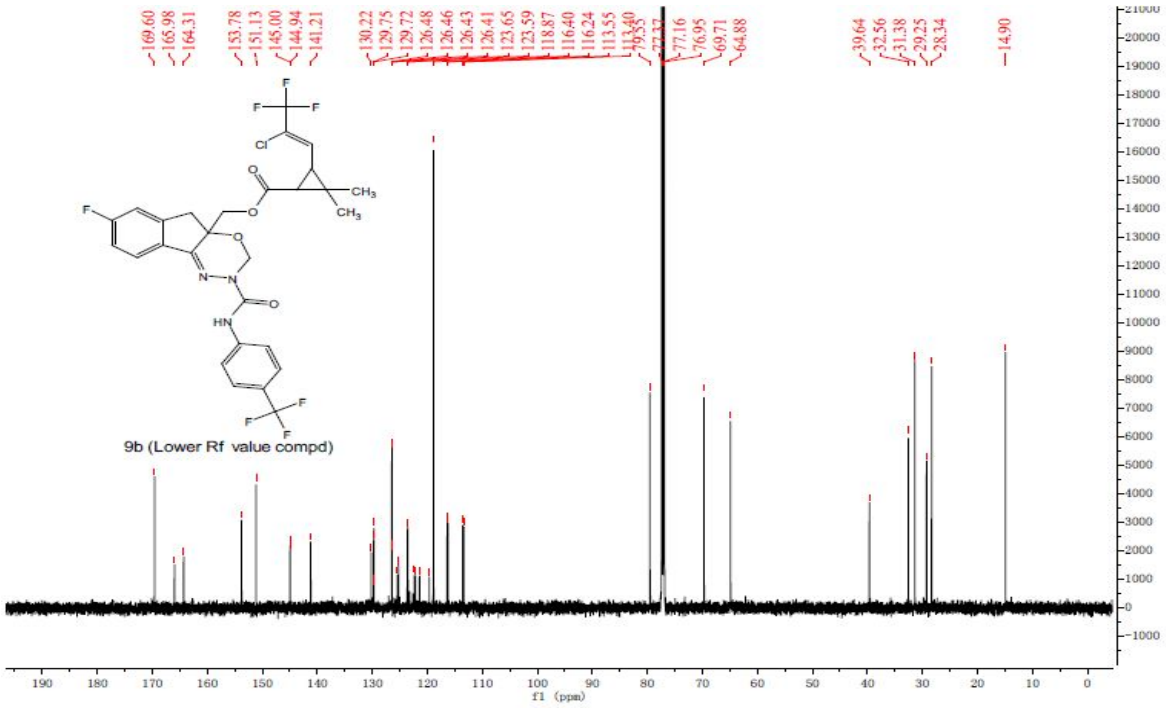
^{1}H NMR and ^{13}C NMR of target compound J10 (Lower Rf value compd)



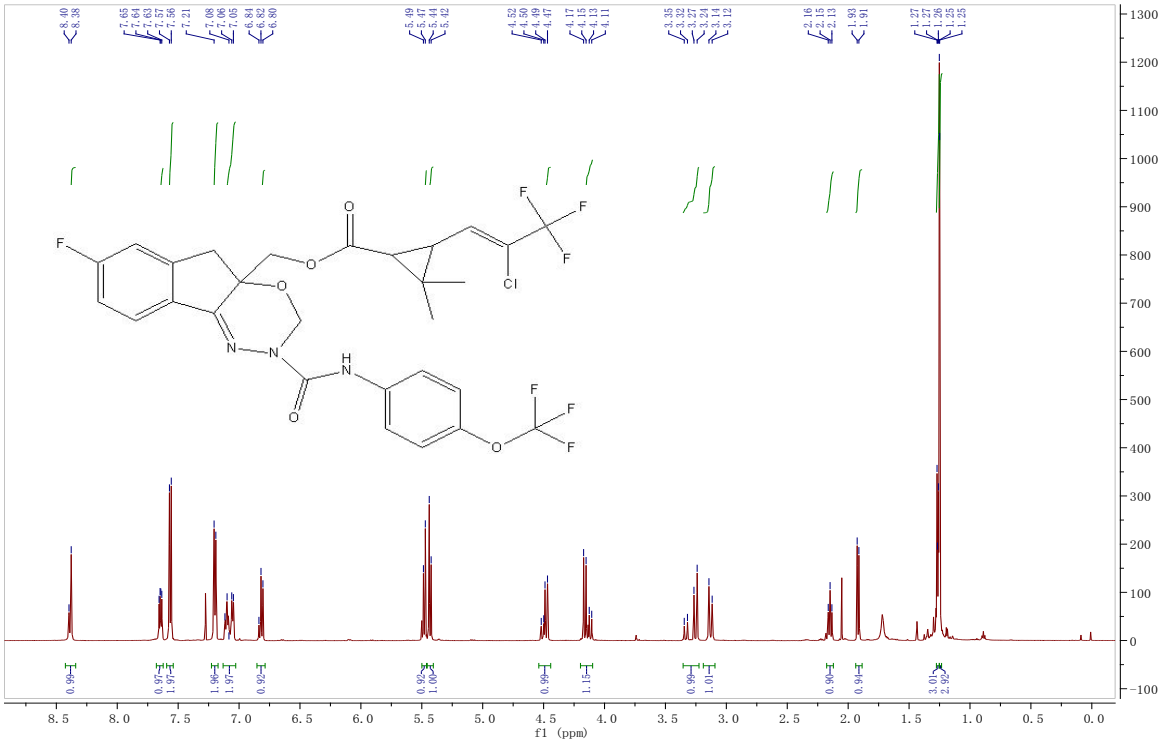


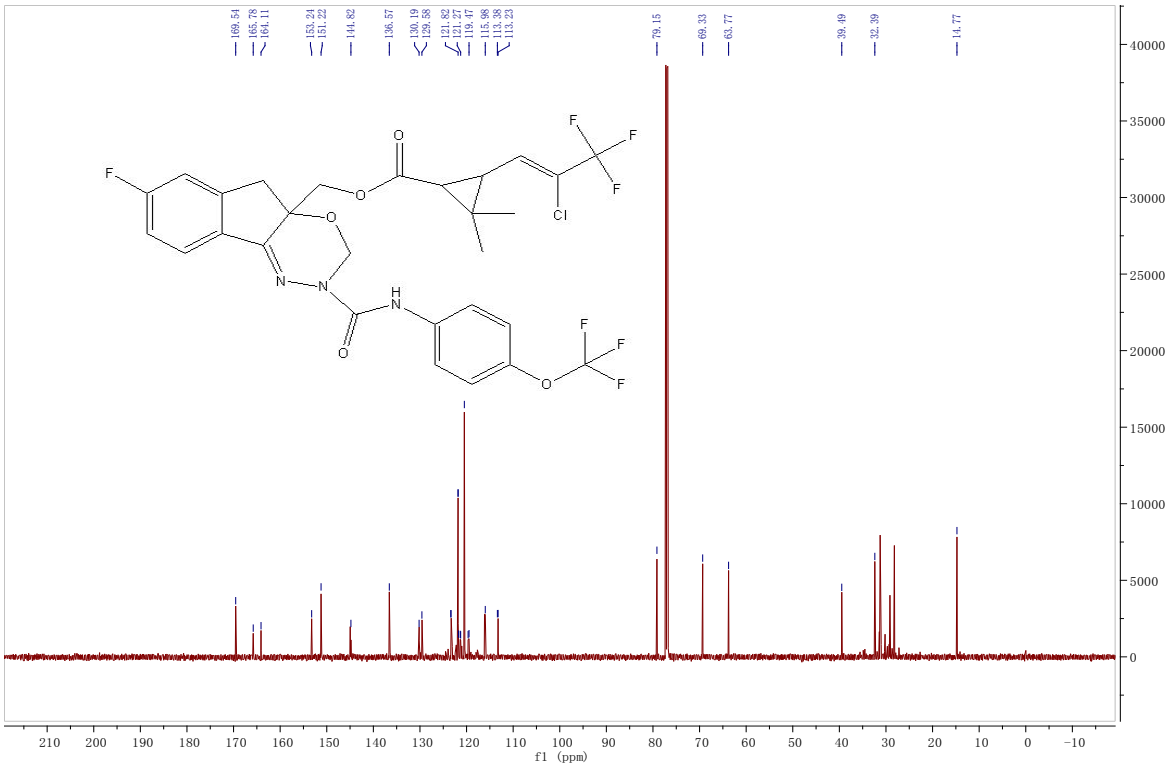
^{1}H NMR and ^{13}C NMR of target compound J11 (Higher Rf value compd)



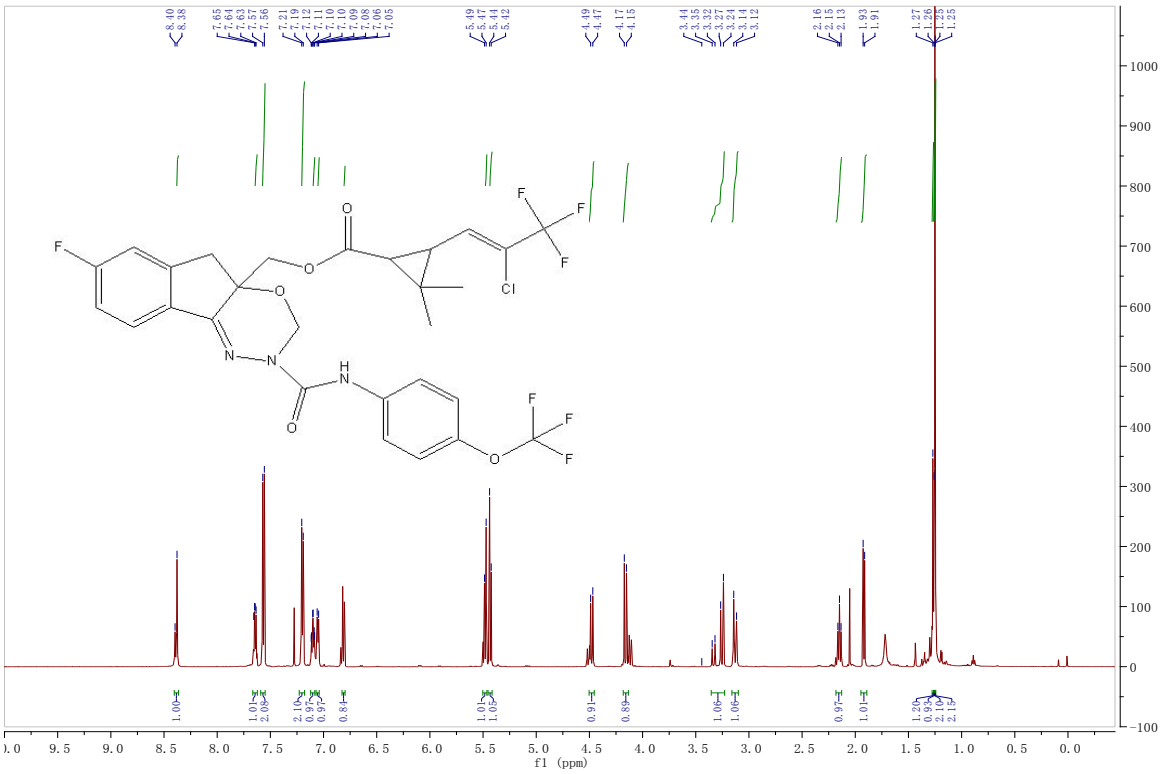


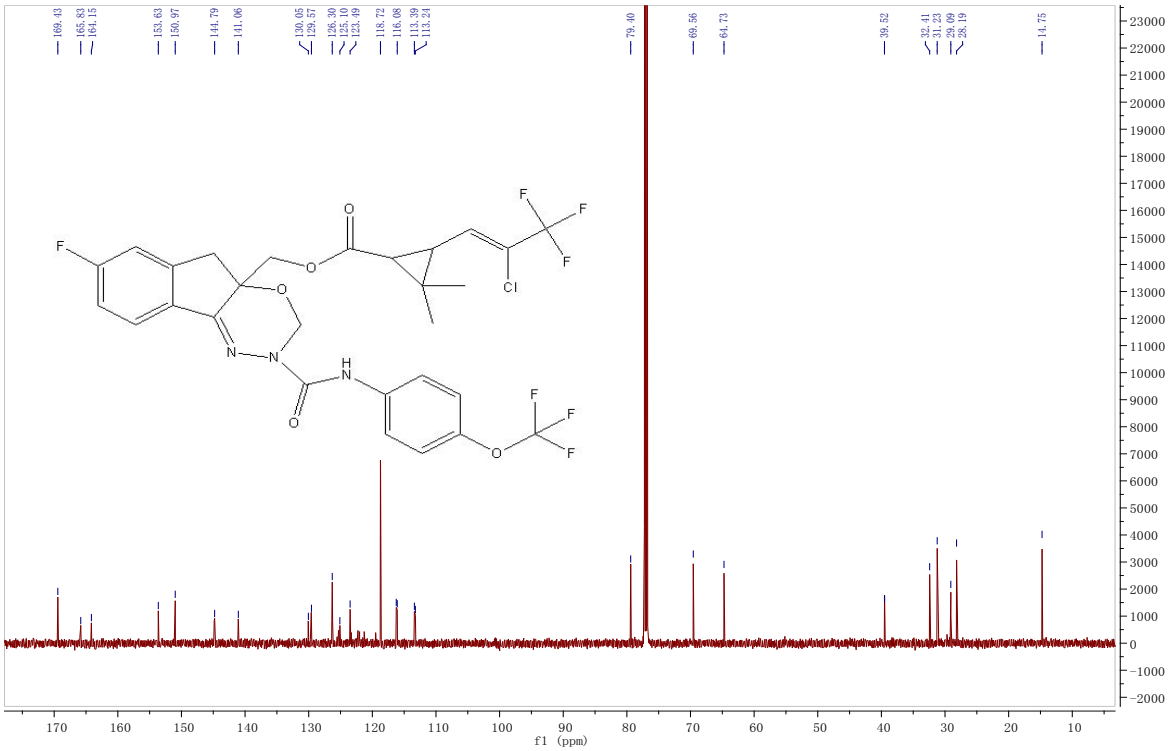
^{1}H NMR and ^{13}C NMR of target compound J11 (Lower Rf value compd)



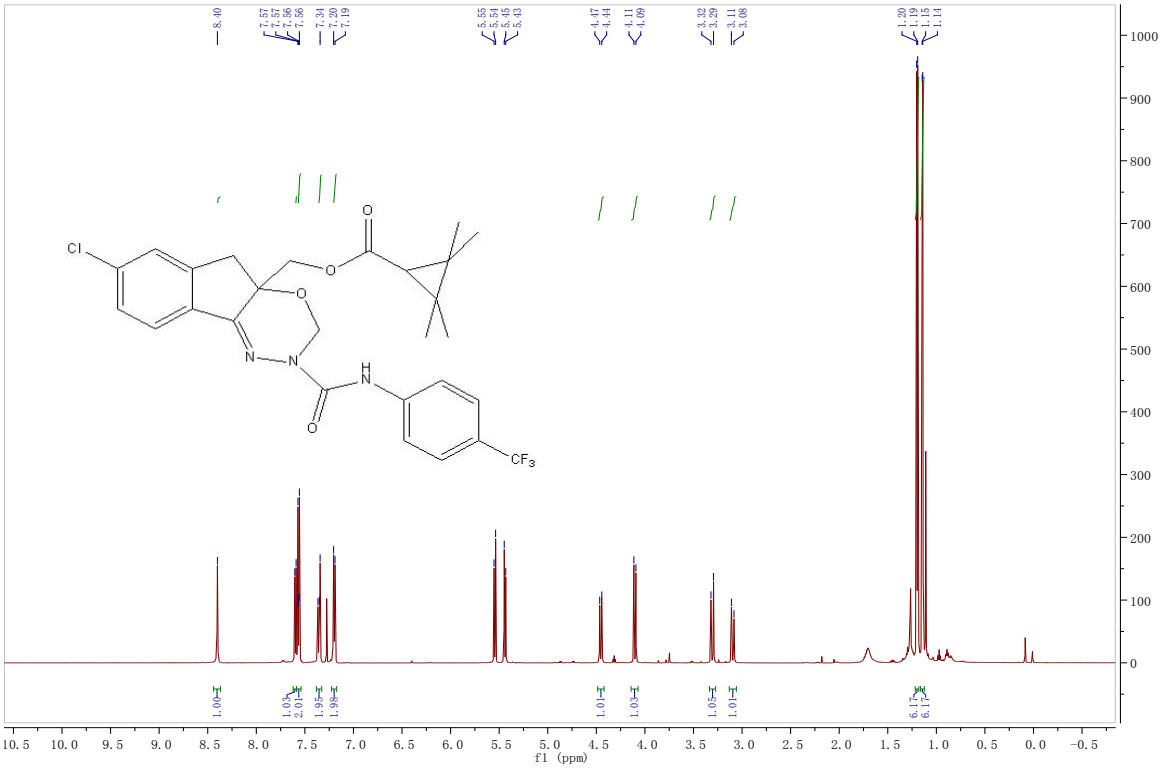


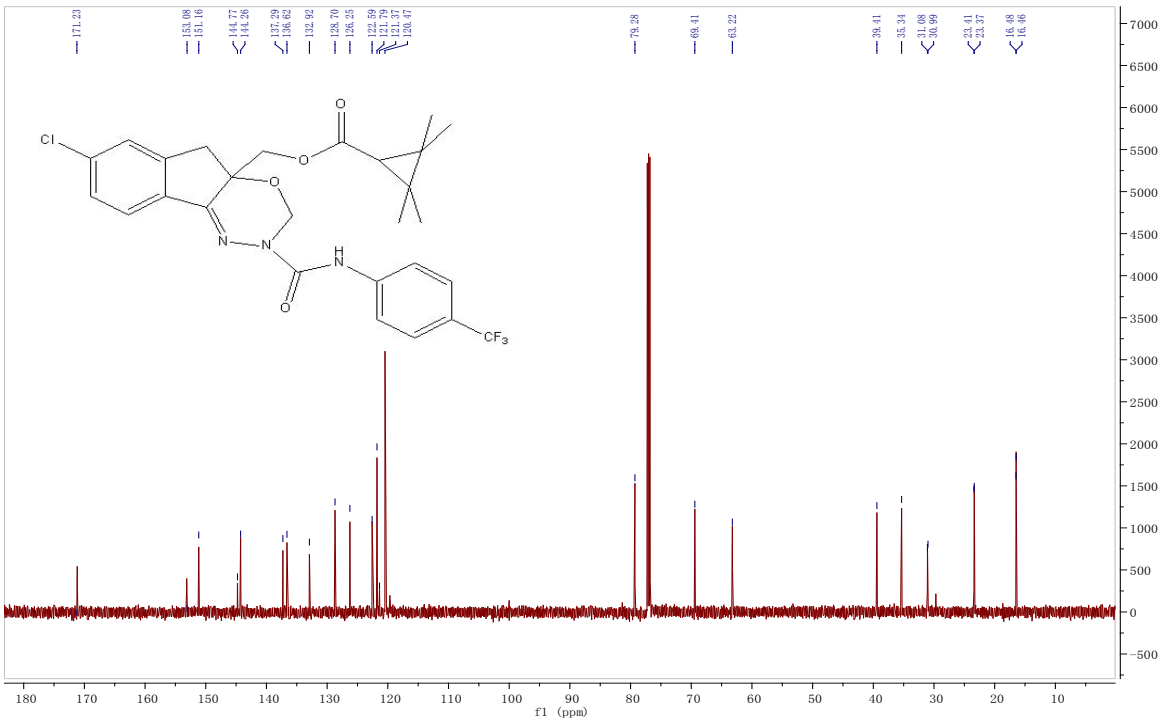
^{1}H NMR and ^{13}C NMR of target compound J12 (Higher Rf value compd)



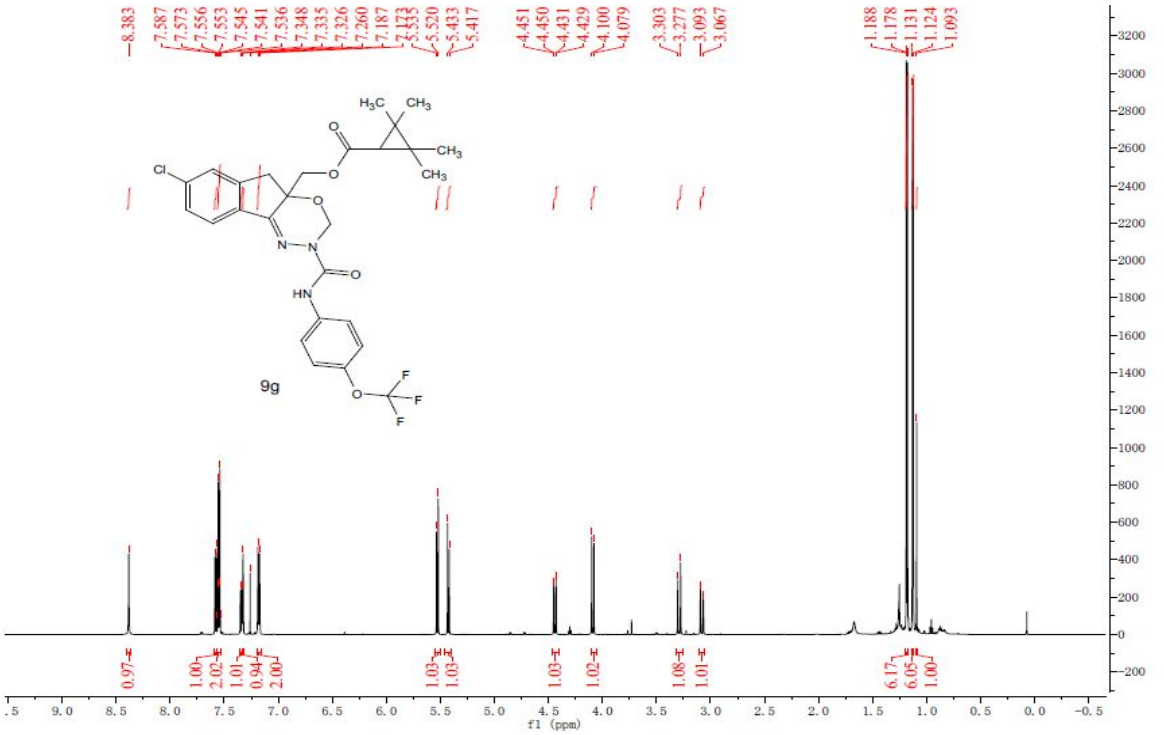


^{1}H NMR and ^{13}C NMR of target compound J12 (Lower Rf value compd)





^{1}H NMR and ^{13}C NMR of target compound J13



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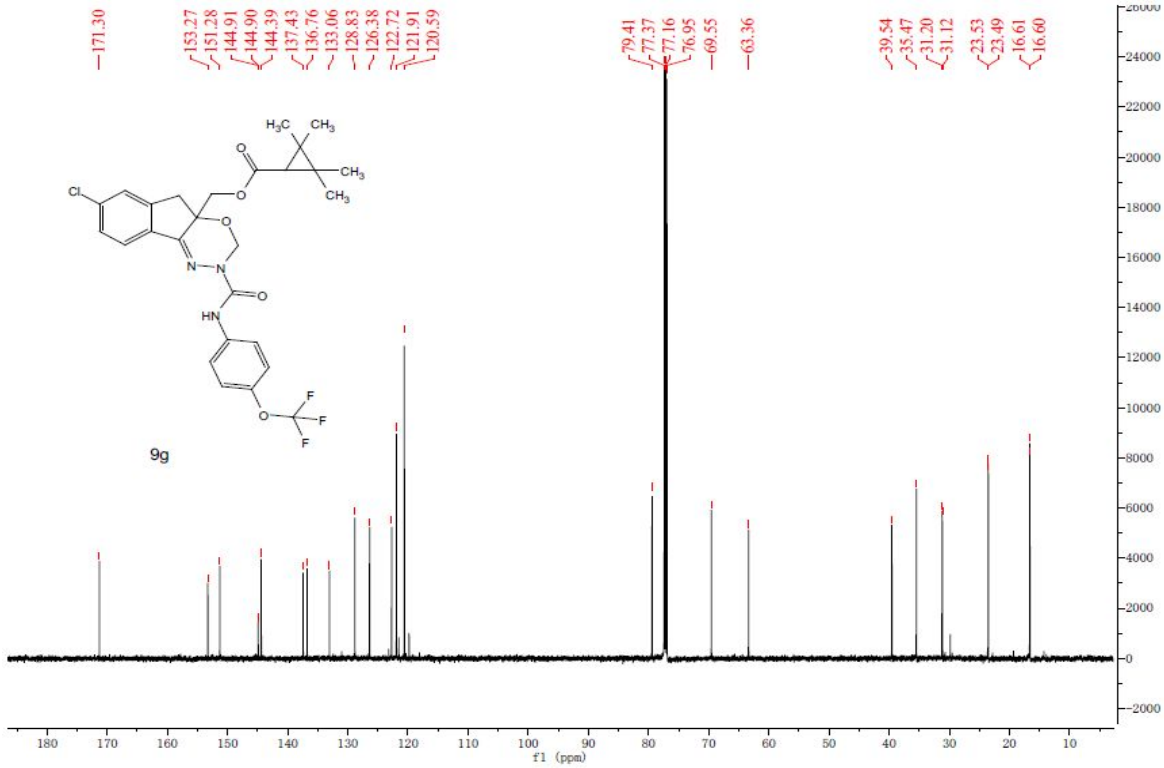

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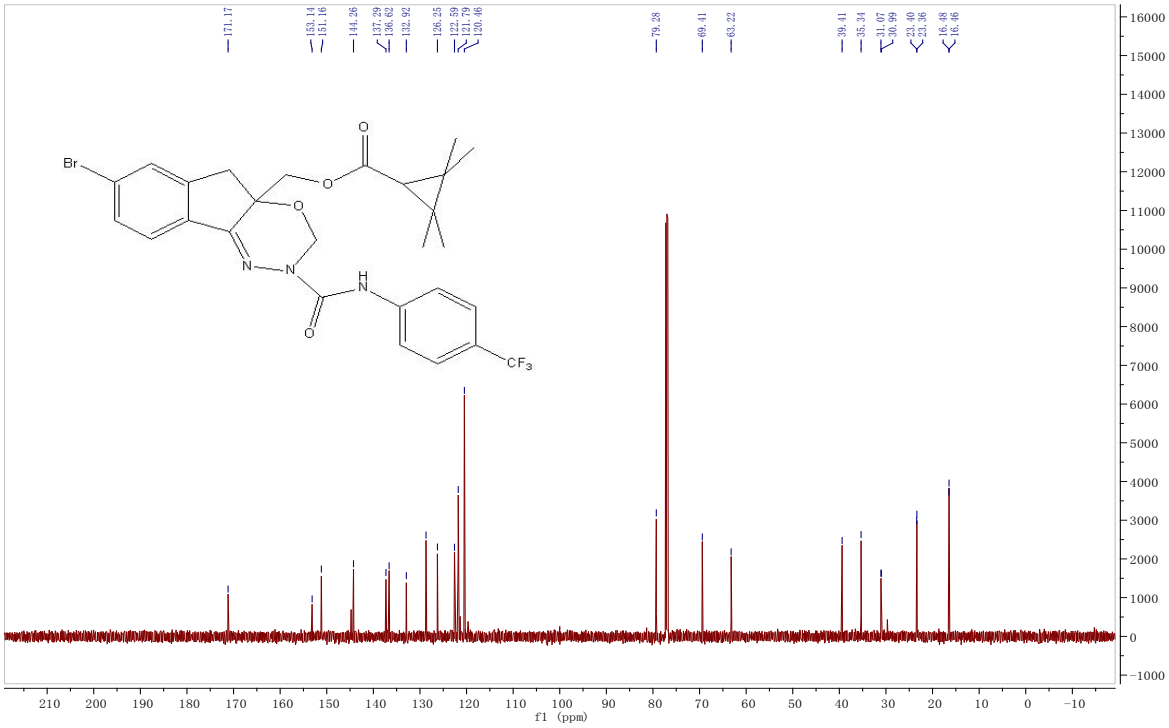
165 ^{1}H NMR and ^{13}C NMR of target compound J14

166



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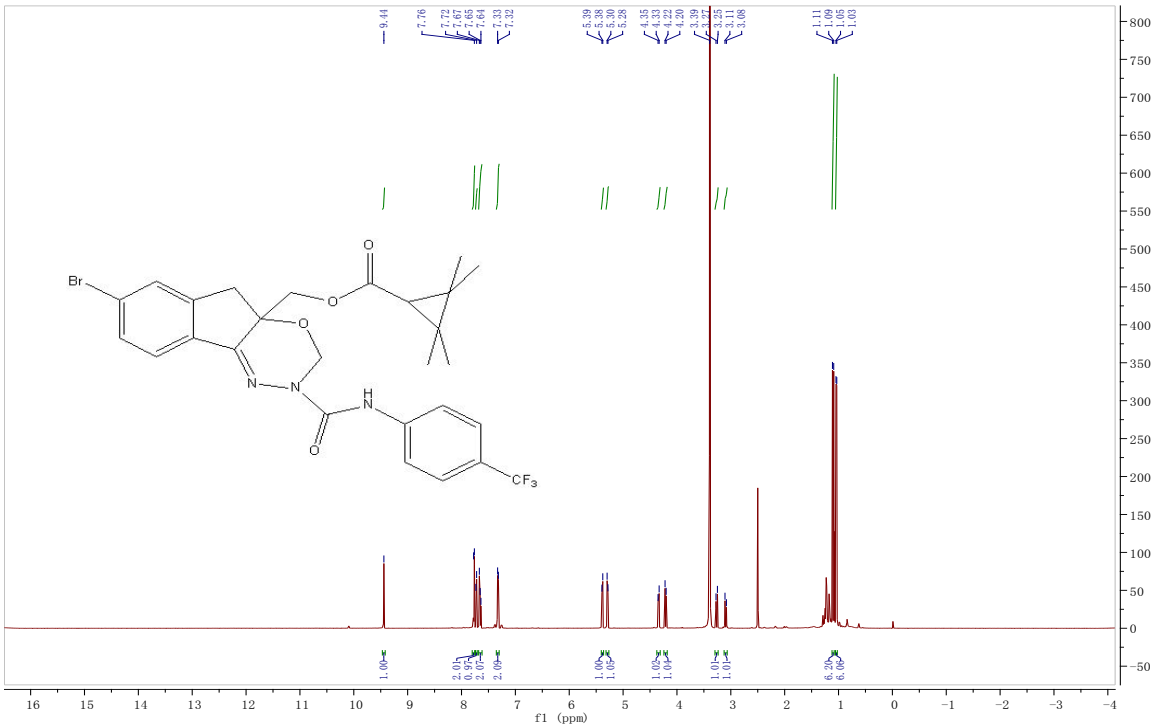

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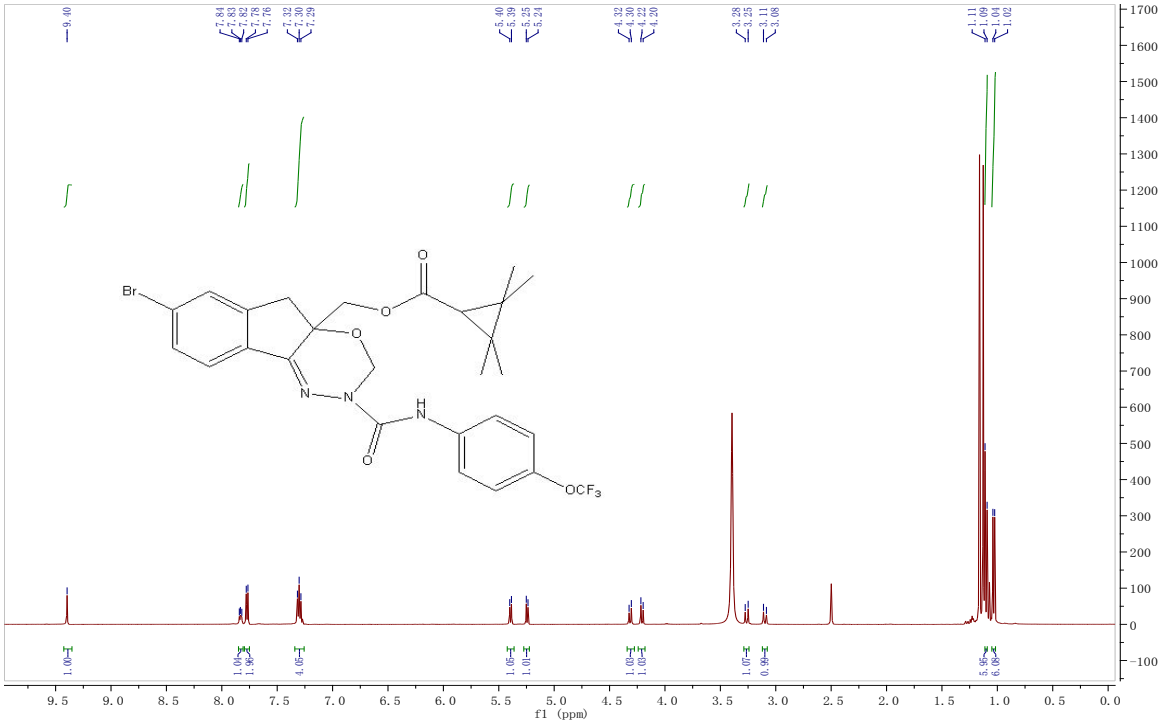
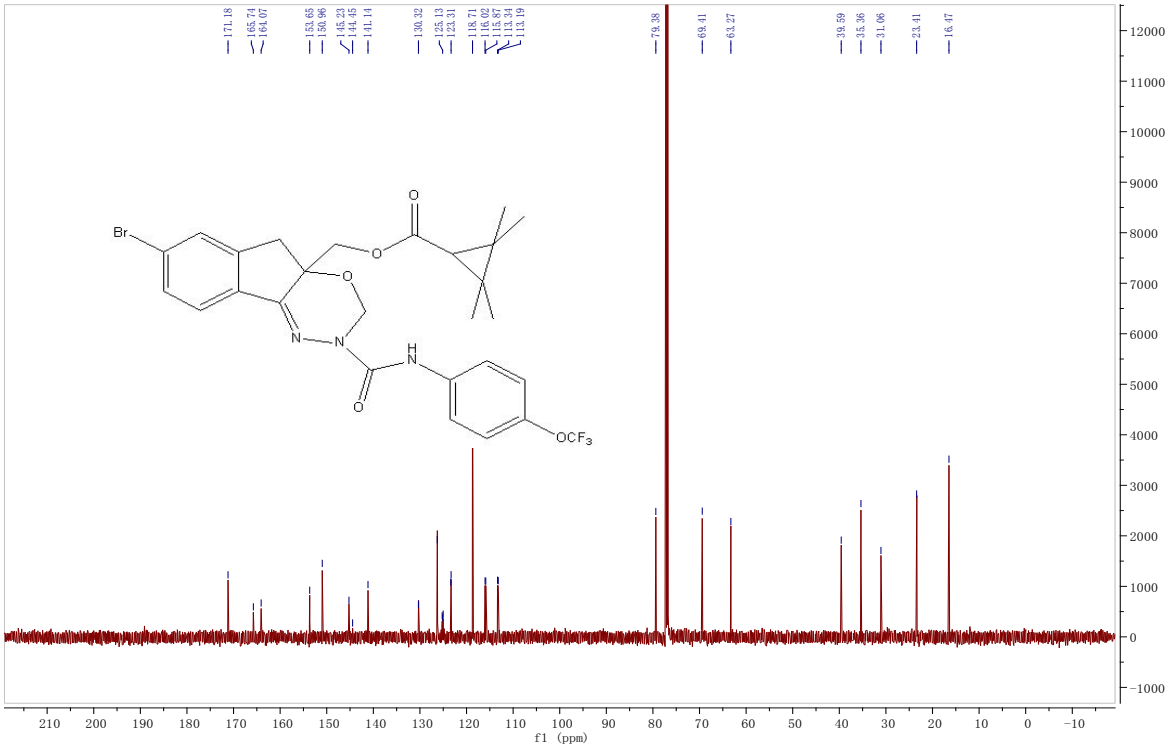
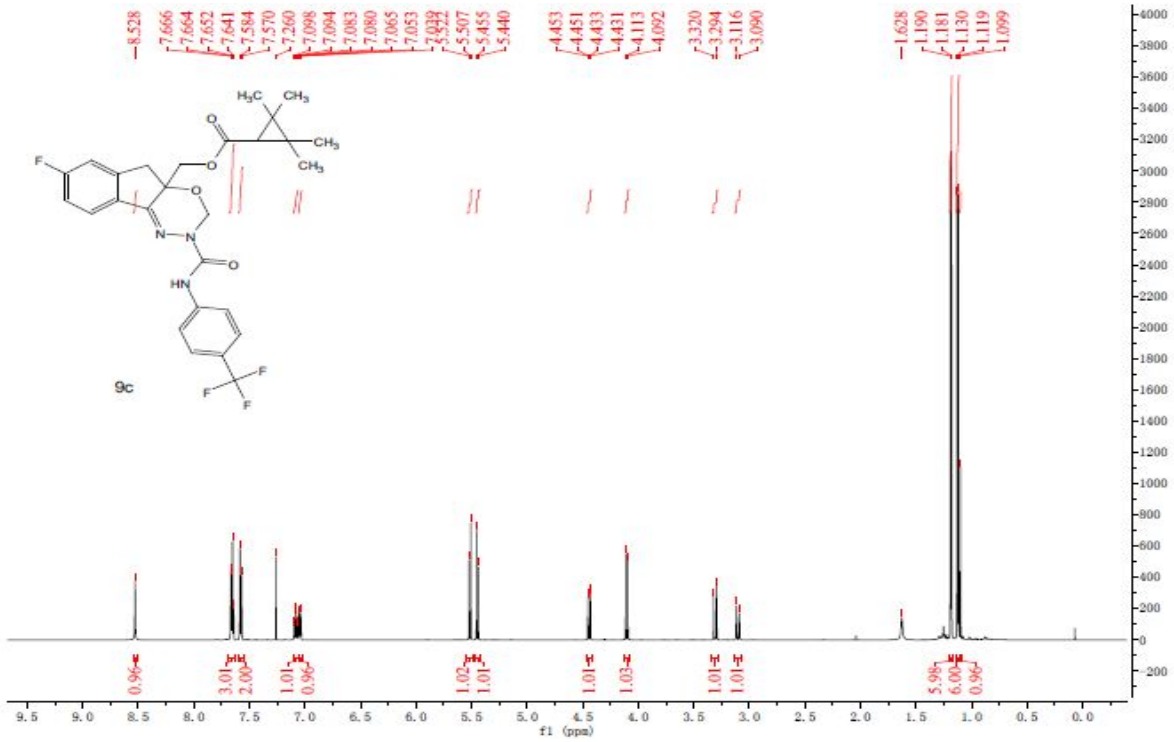
169 ^{1}H NMR and ^{13}C NMR of target compound J15

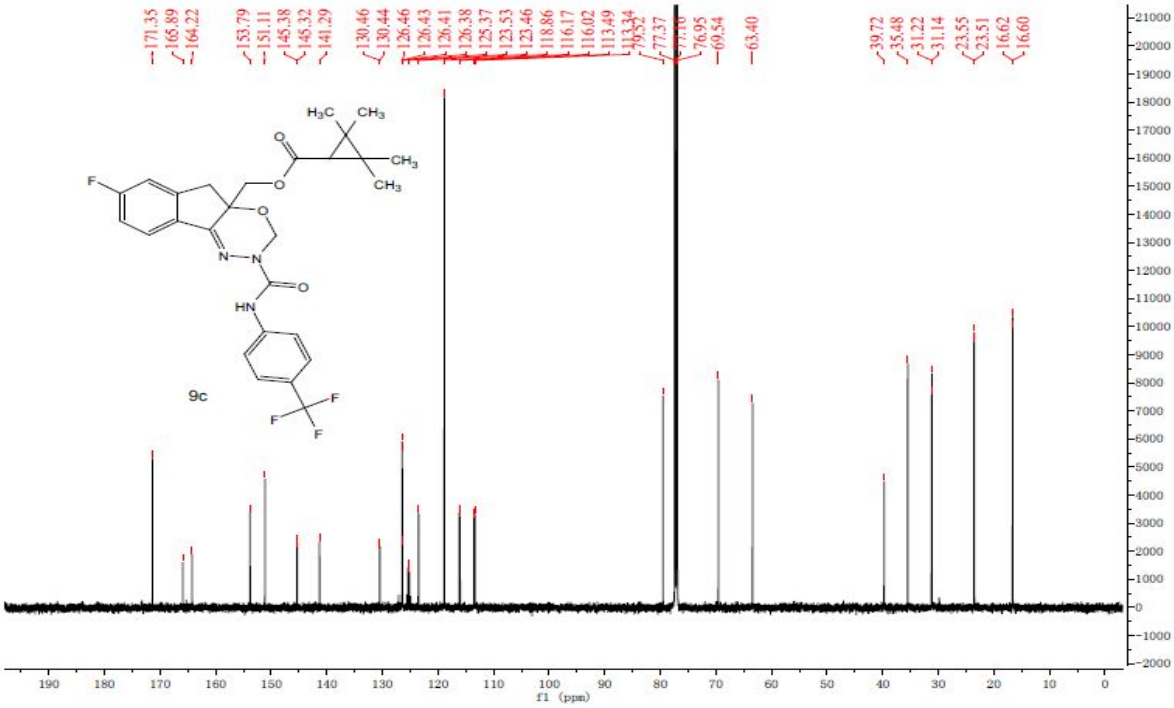
170



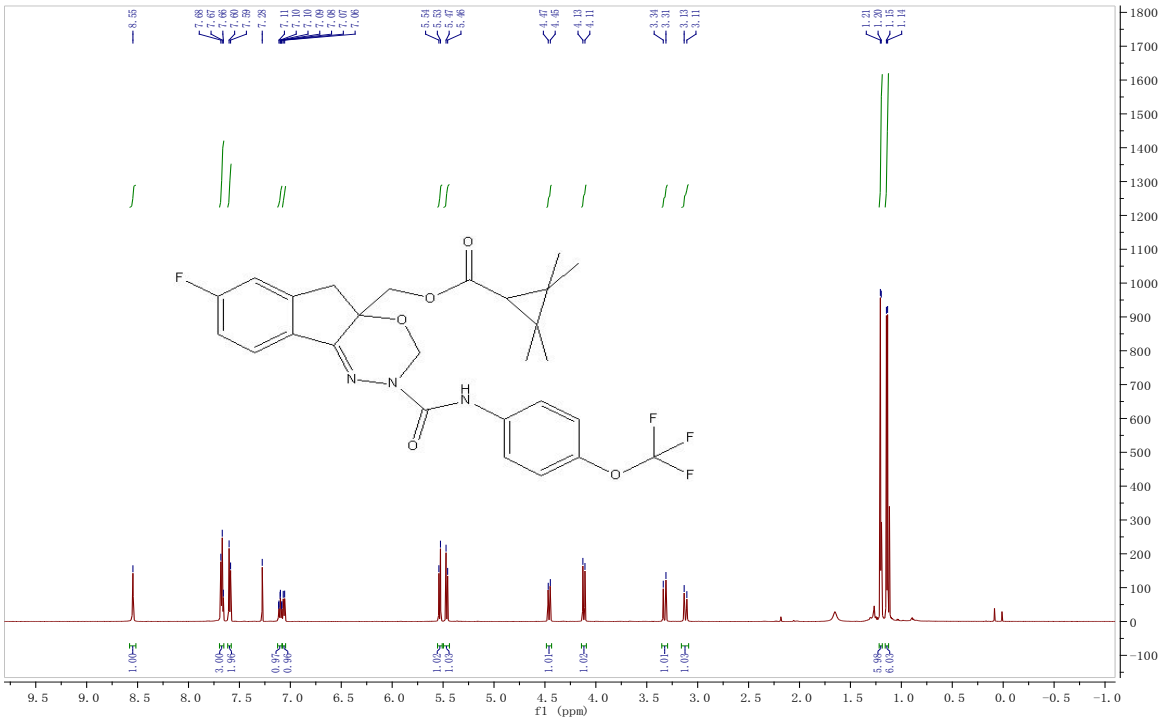


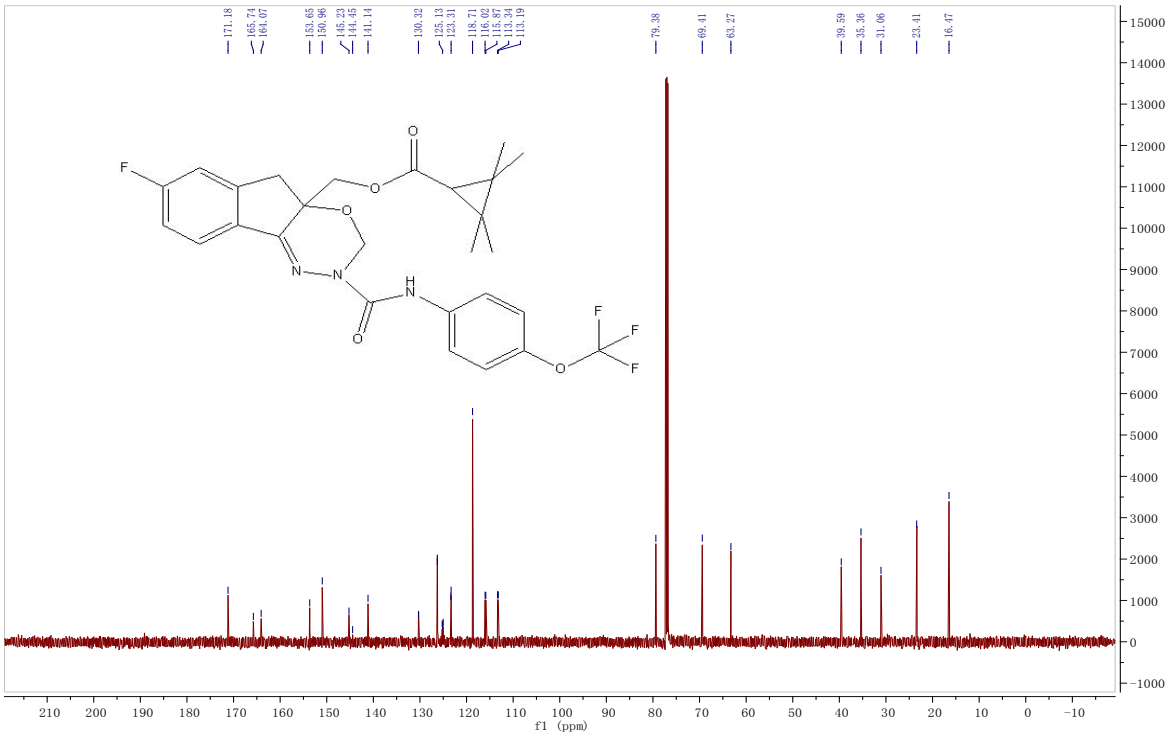
^{1}H NMR and ^{13}C NMR of target compound J16



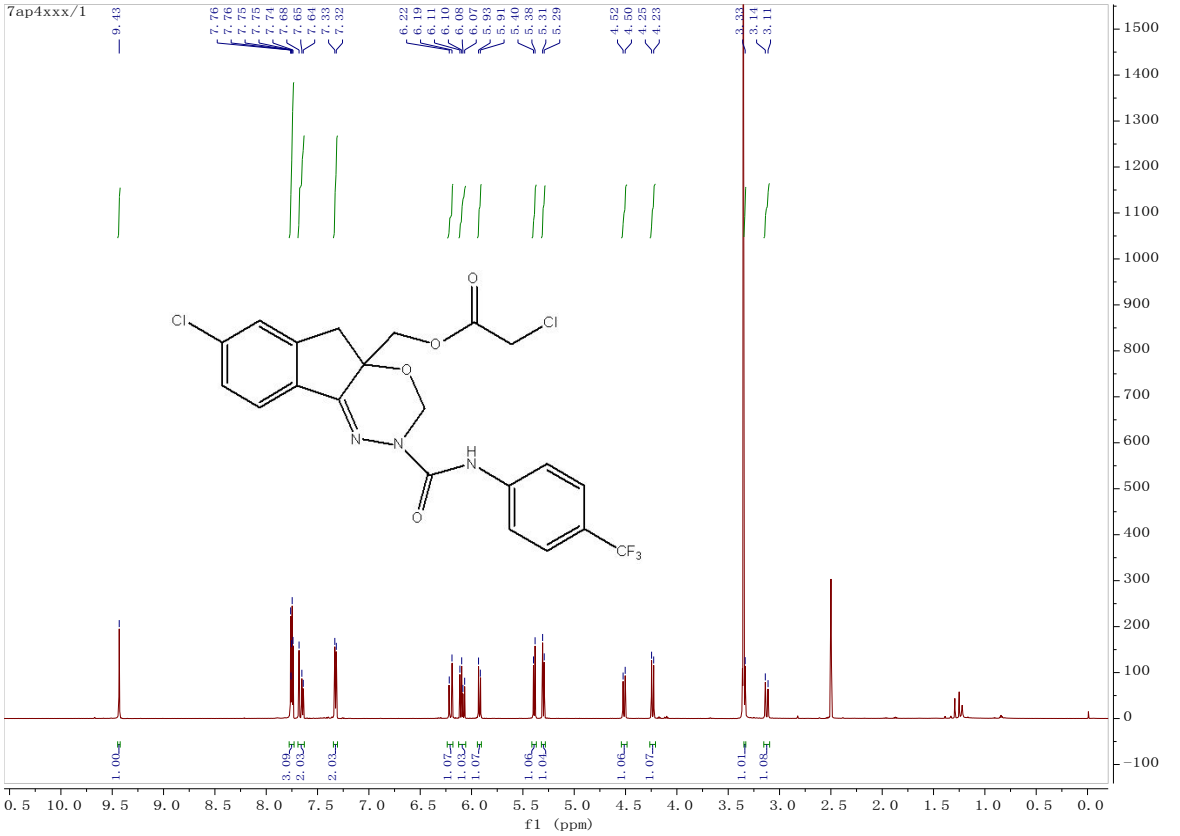


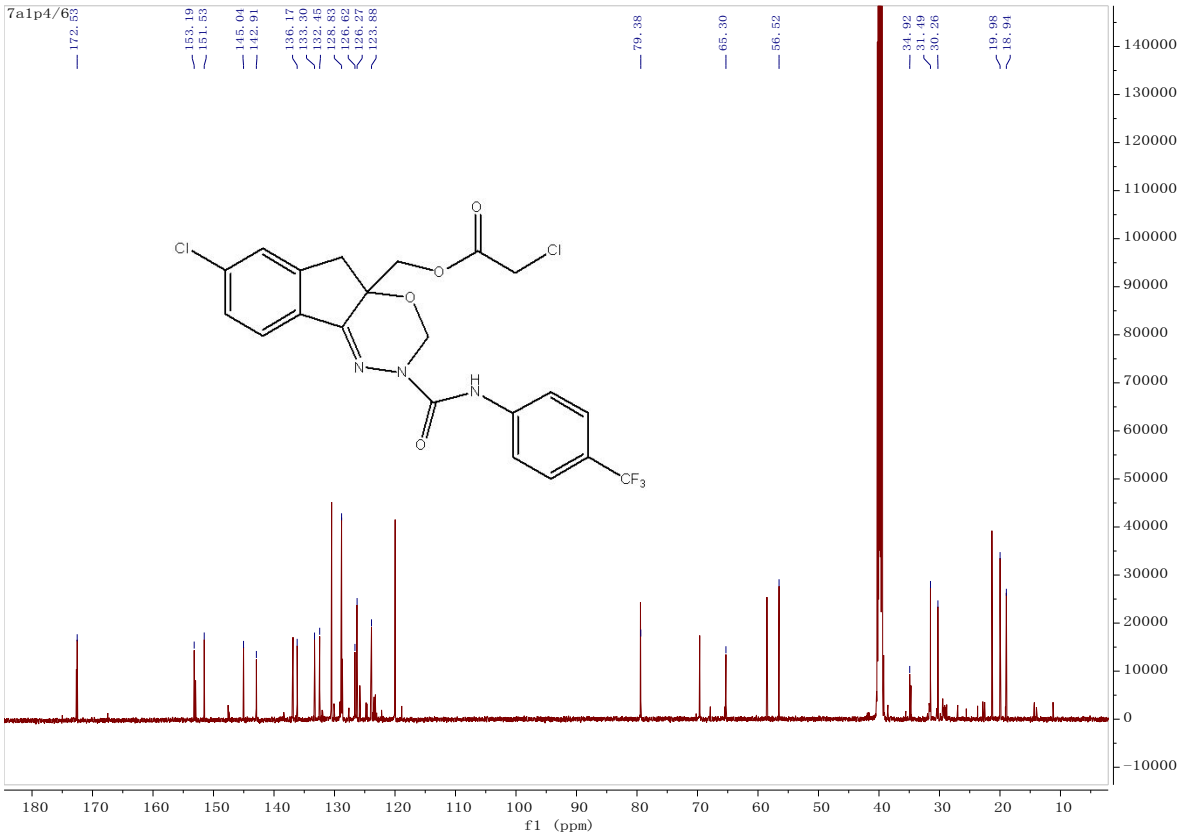
^{1}H NMR and ^{13}C NMR of target compound J17



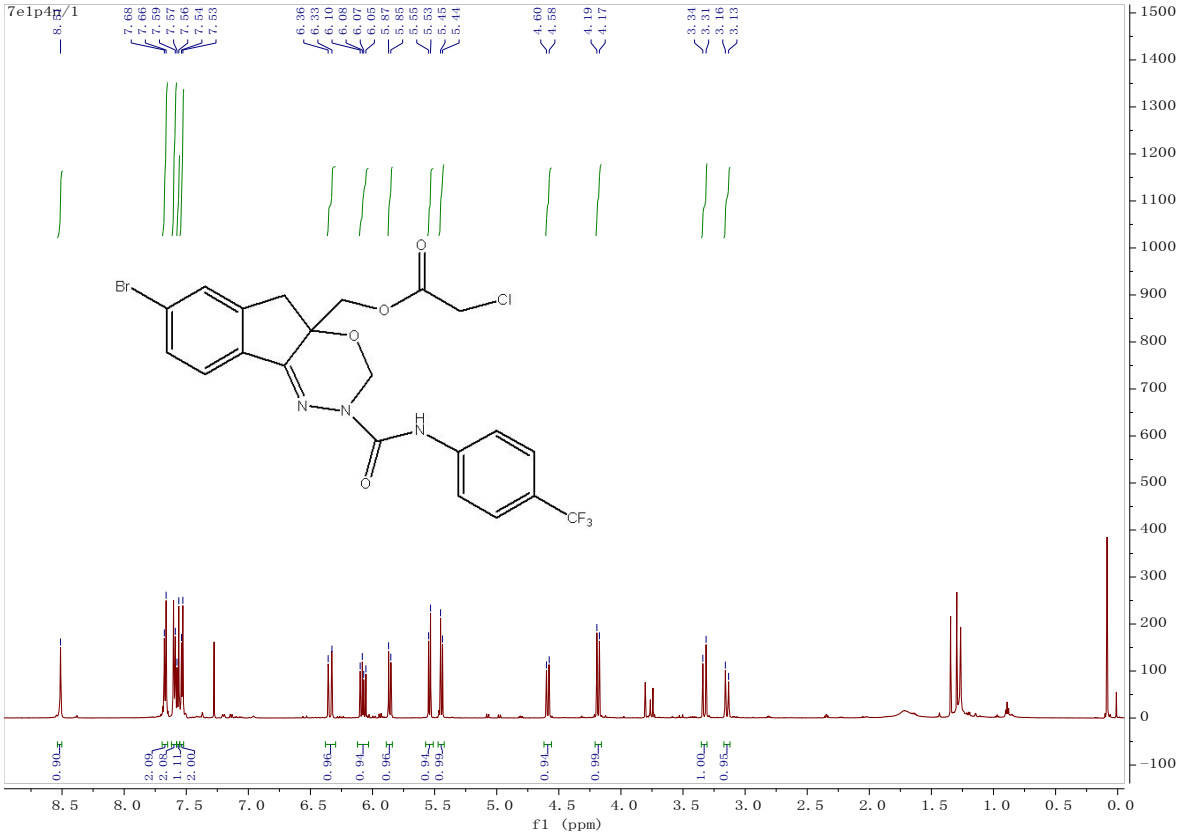


^{1}H NMR and ^{13}C NMR of target compound J18





^{1}H NMR and ^{13}C NMR of target compound J19



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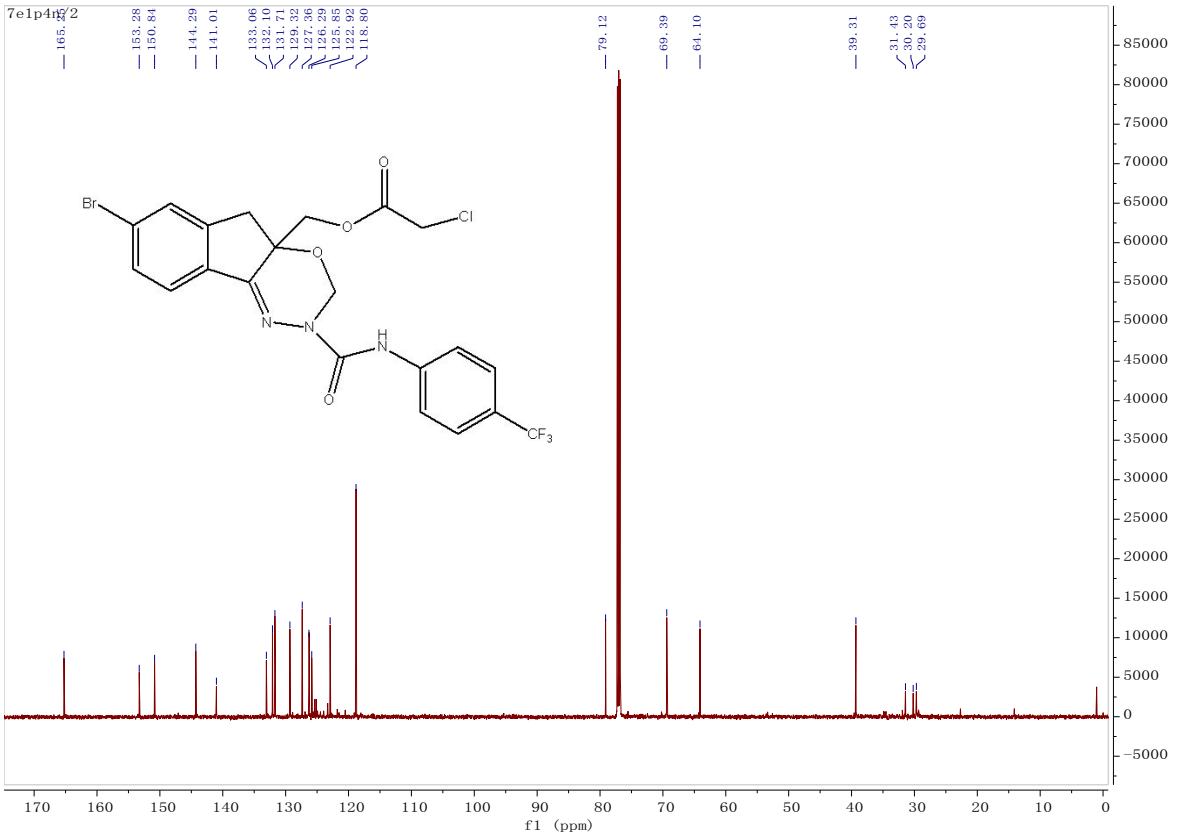
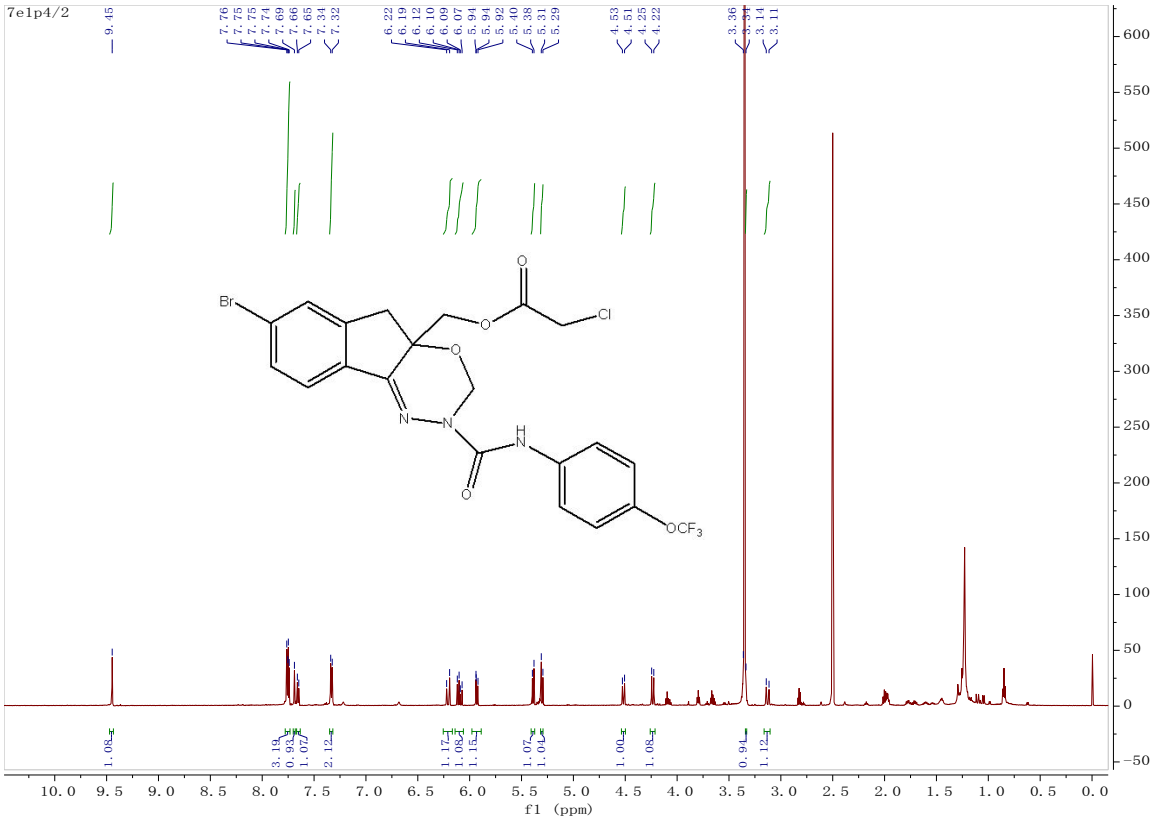
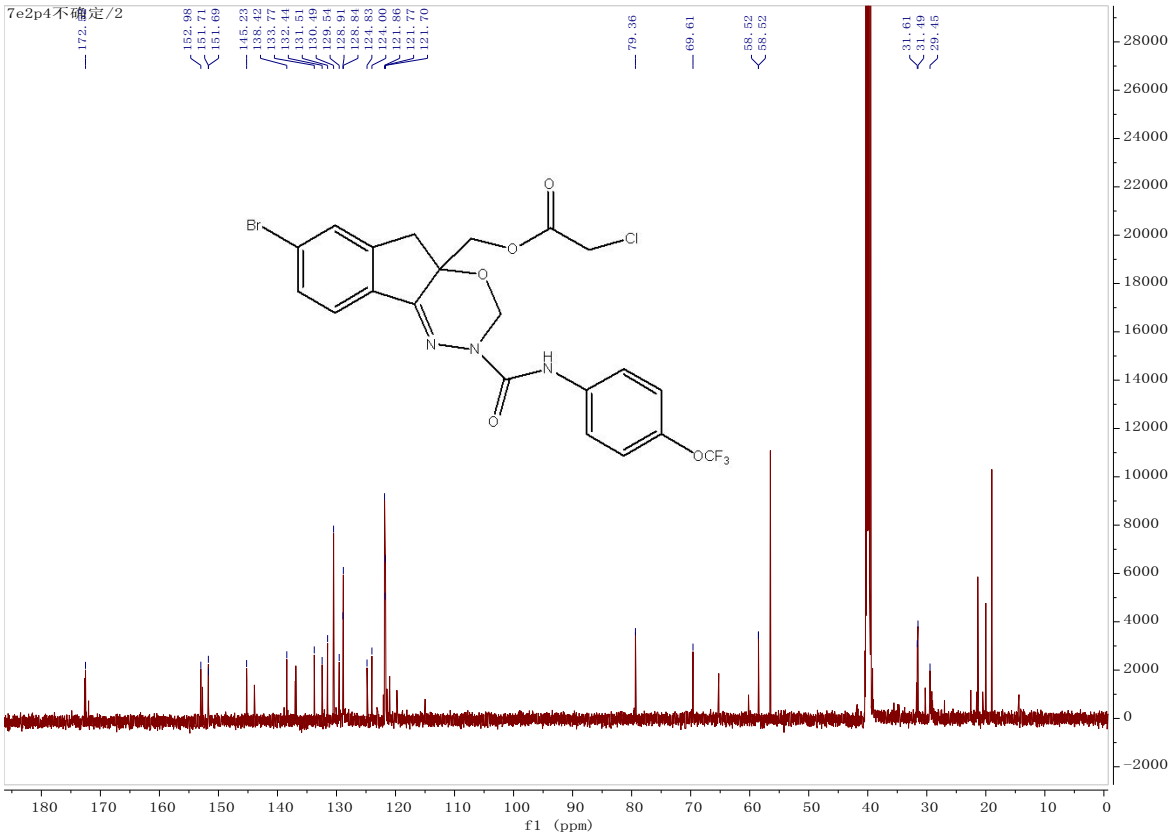


189

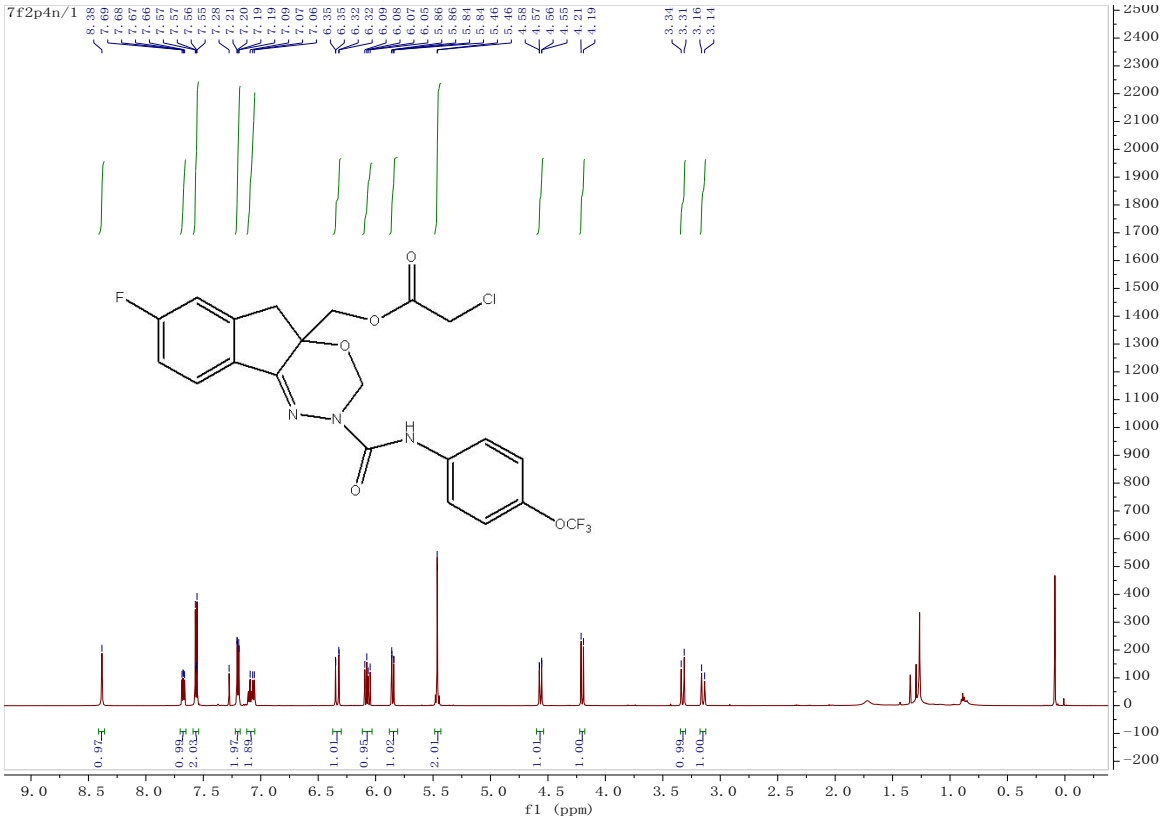
190 ^{1}H NMR and ^{13}C NMR of target compound J20

191





^{1}H NMR and ^{13}C NMR of target compound J21



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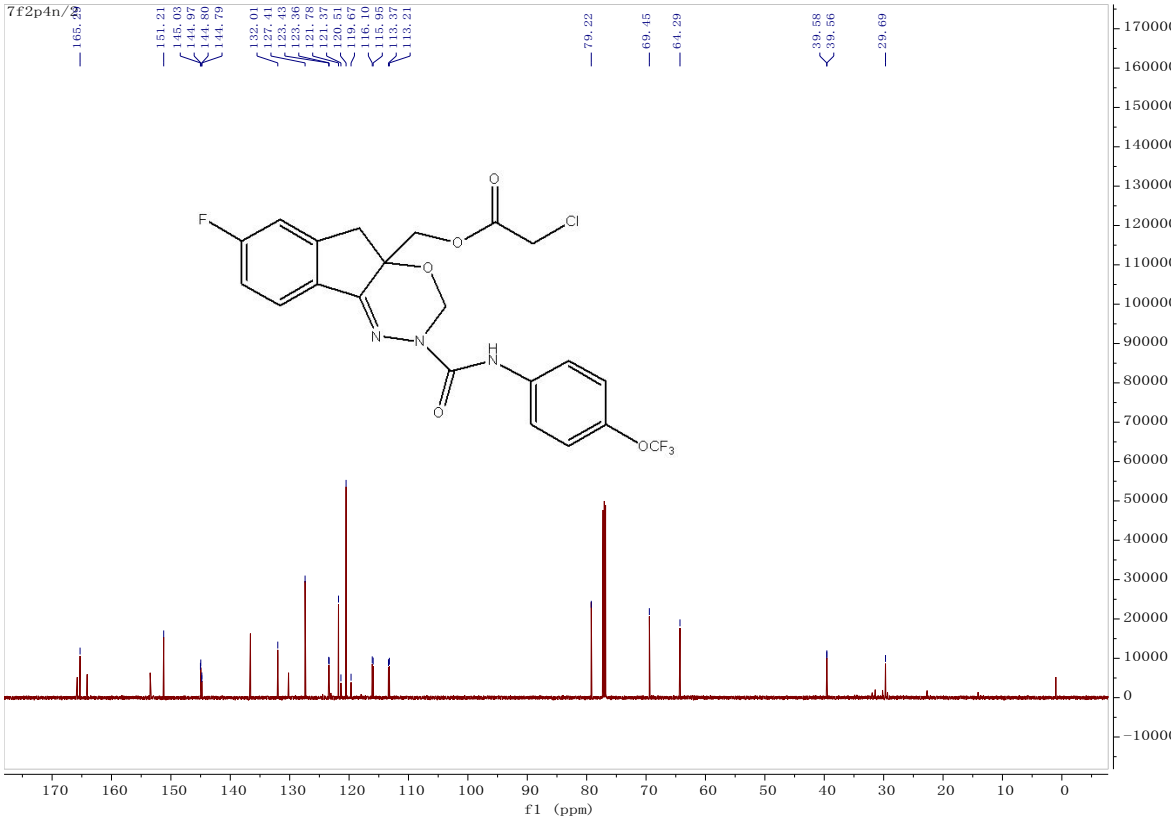

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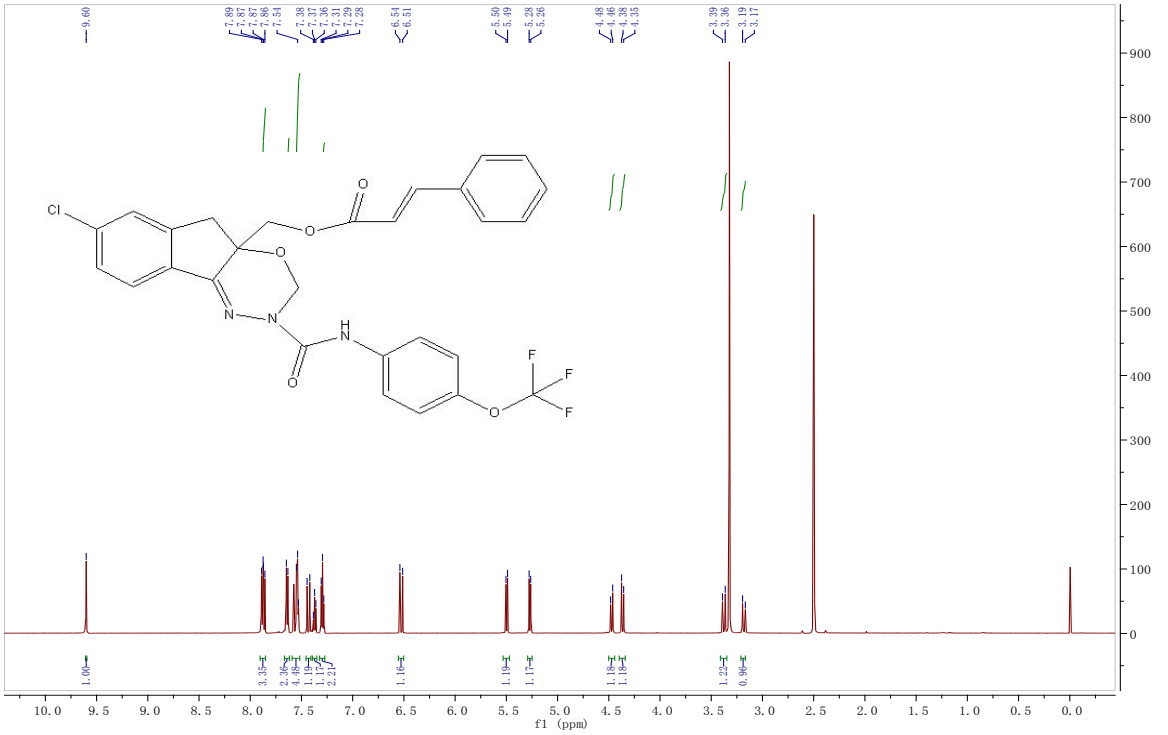
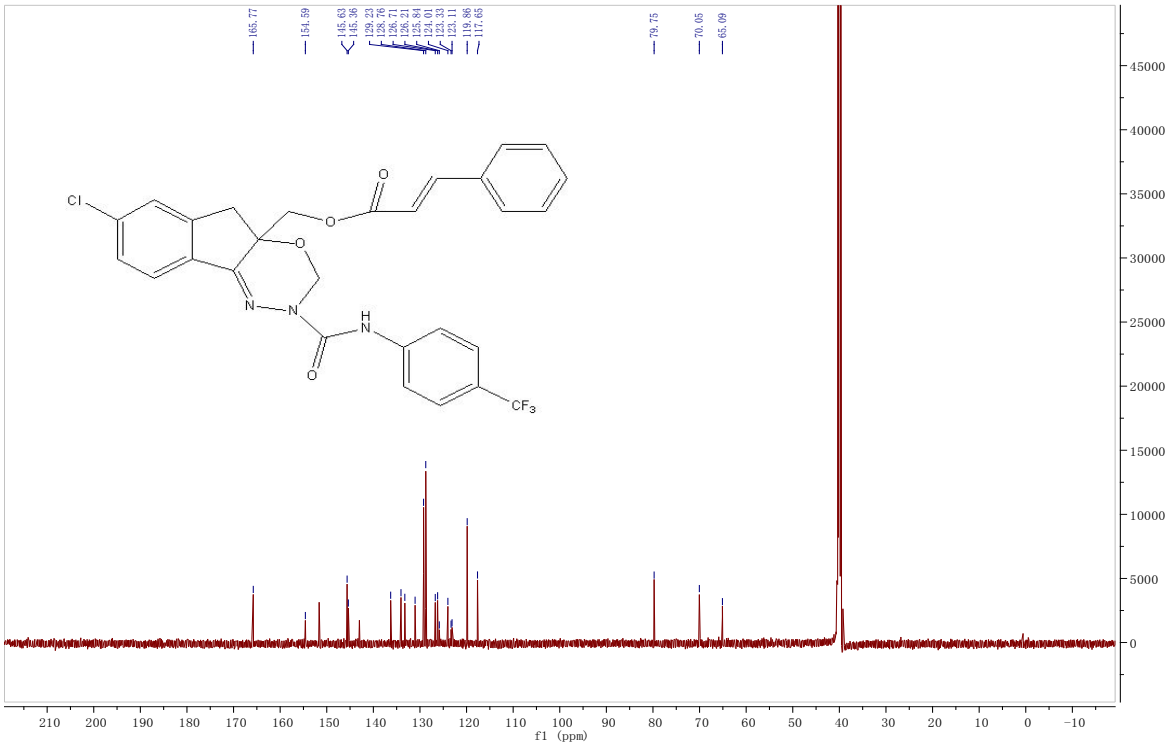
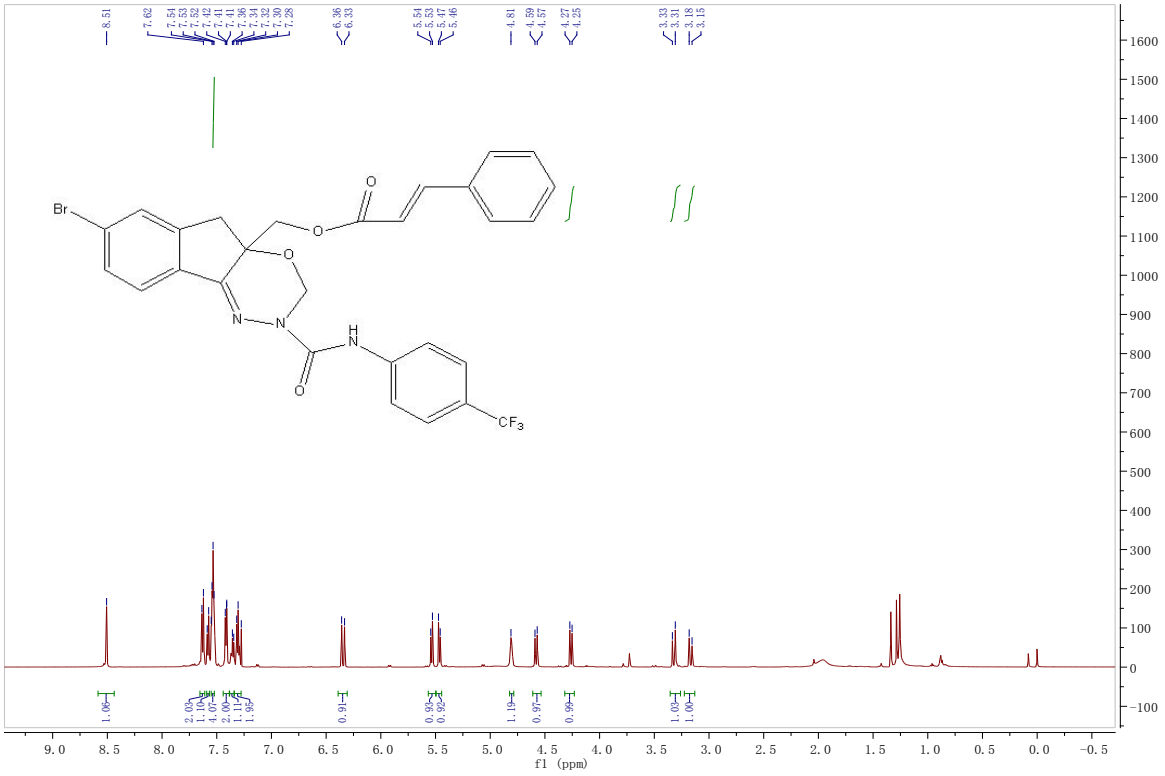
198 ^{1}H NMR and ^{13}C NMR of target compound J22

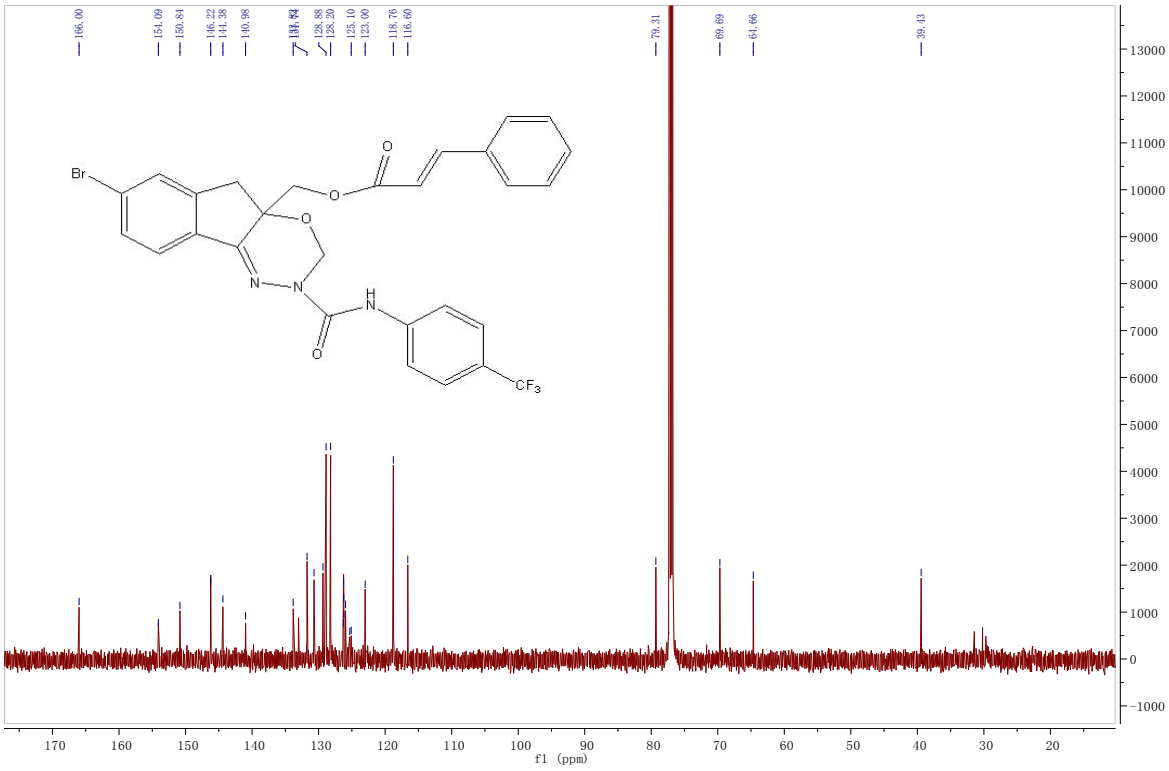
199



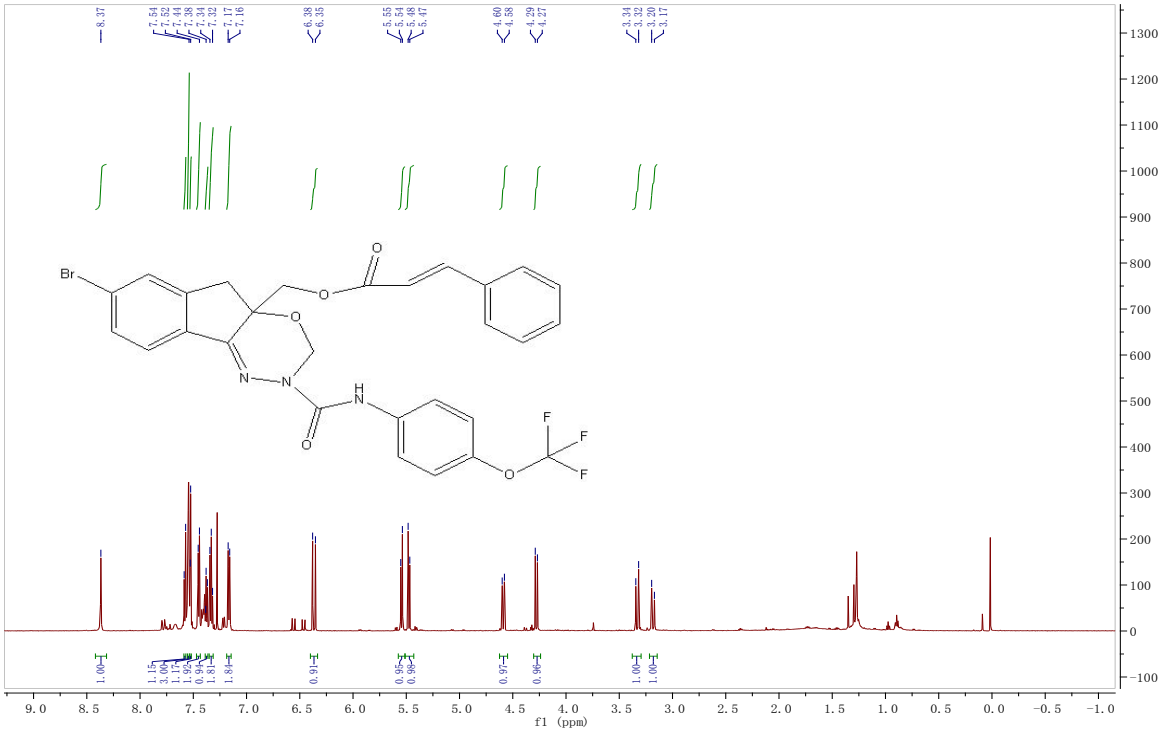


^{1}H NMR and ^{13}C NMR of target compound J23





^{1}H NMR and ^{13}C NMR of target compound J24



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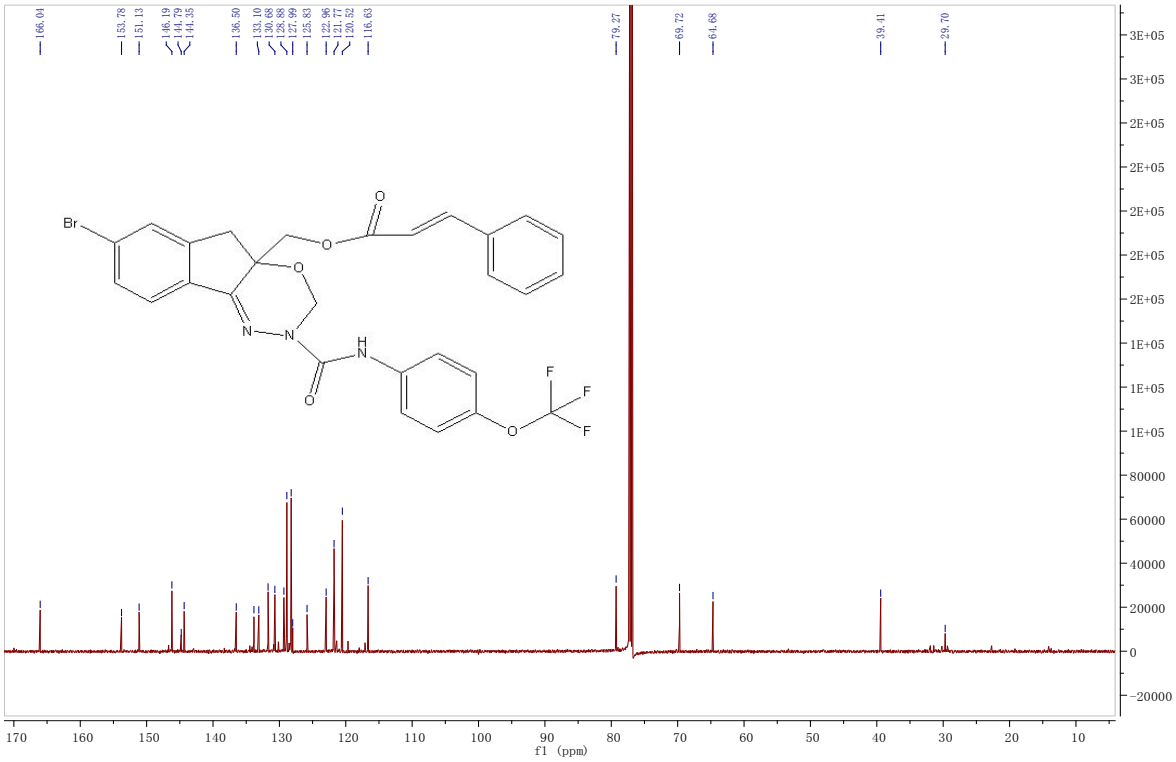
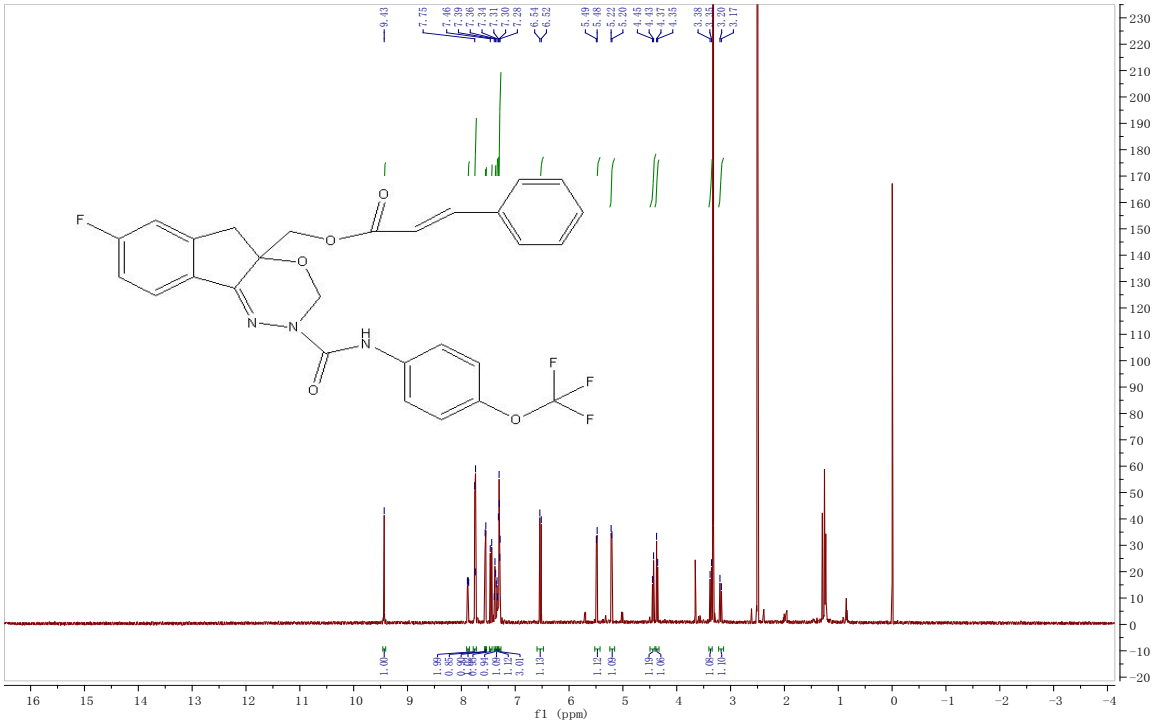
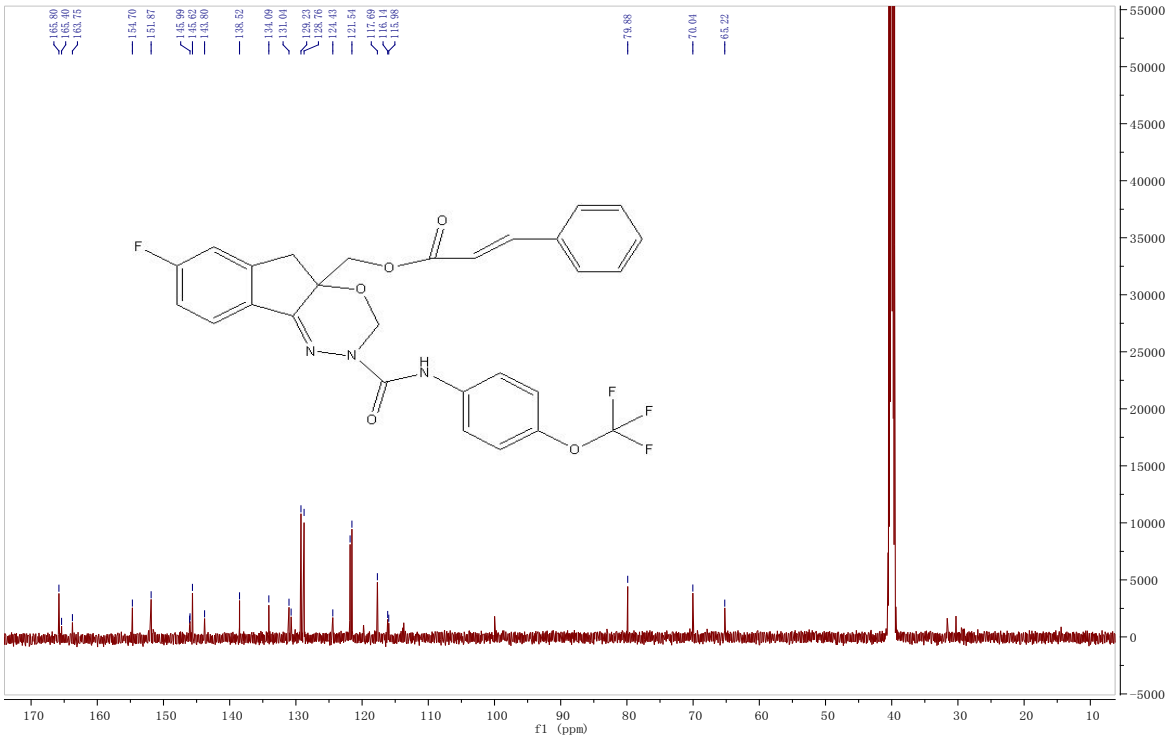


209

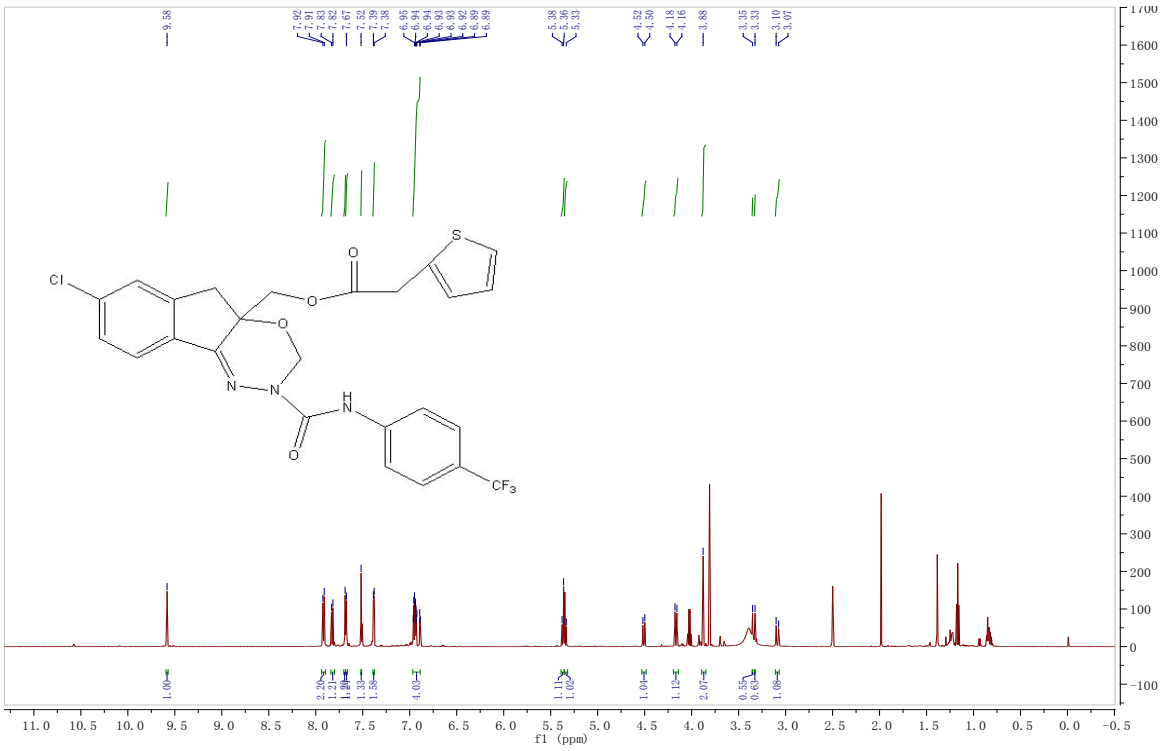
210 ^{1}H NMR and ^{13}C NMR of target compound J25

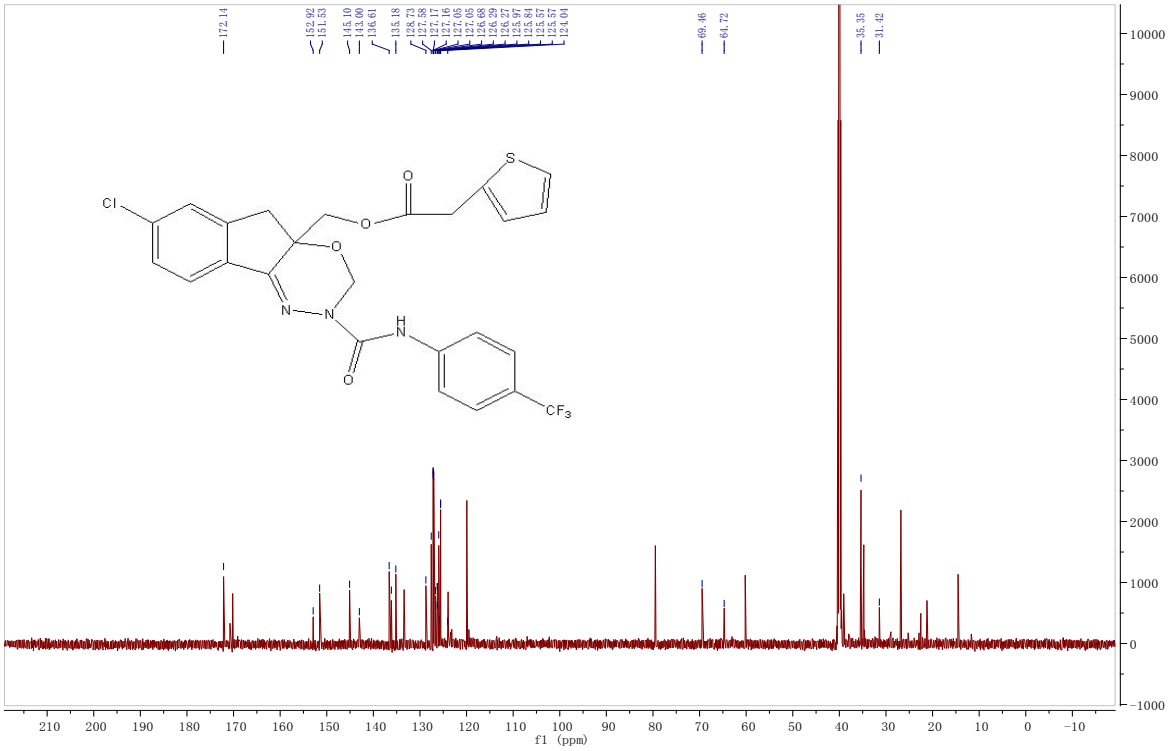
211



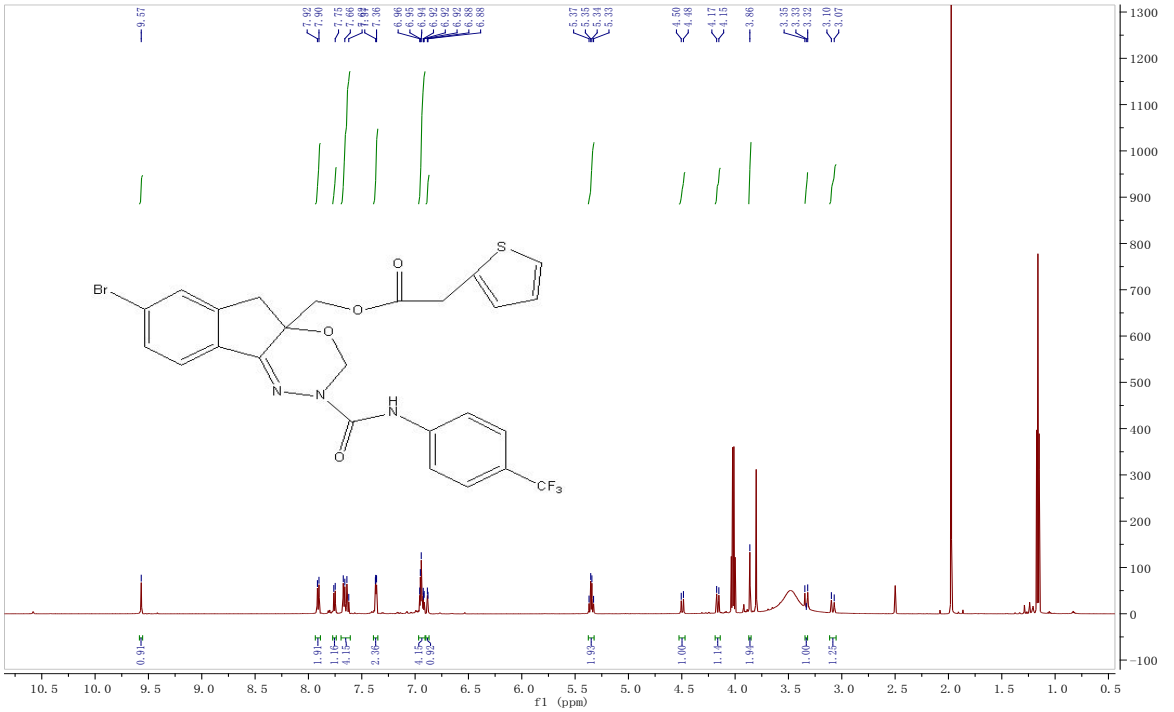


^{1}H NMR and ^{13}C NMR of target compound J26





^{1}H NMR and ^{13}C NMR of target compound J27



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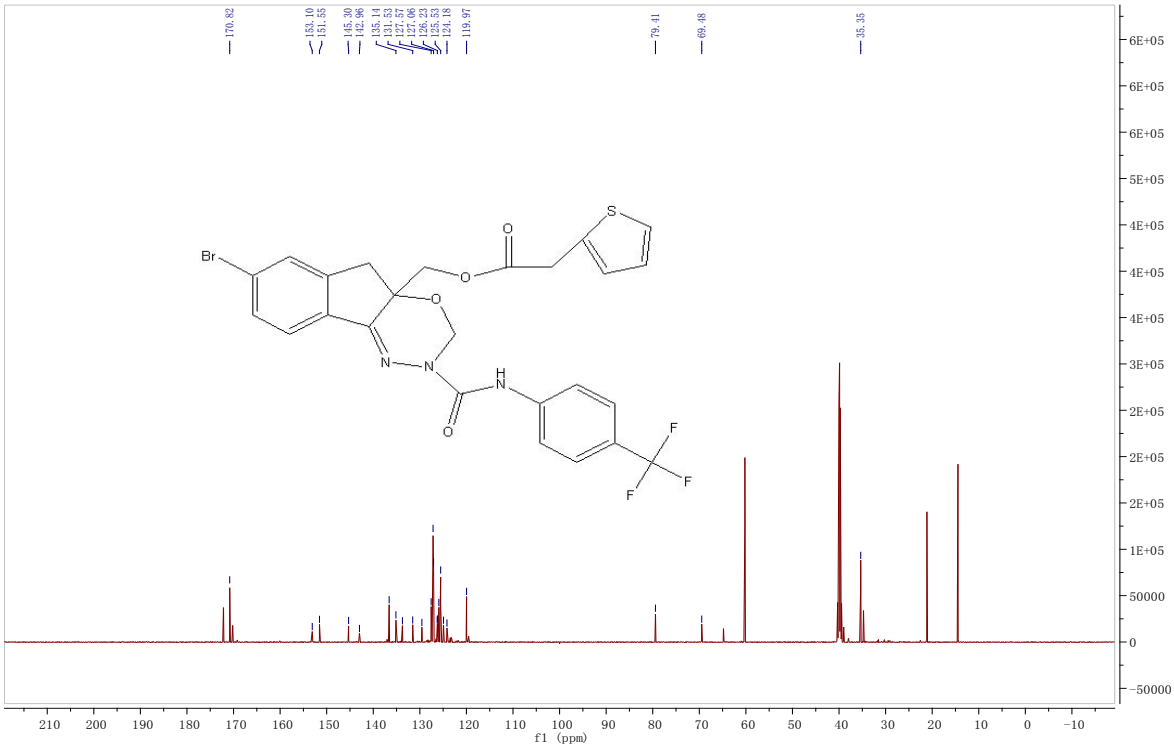
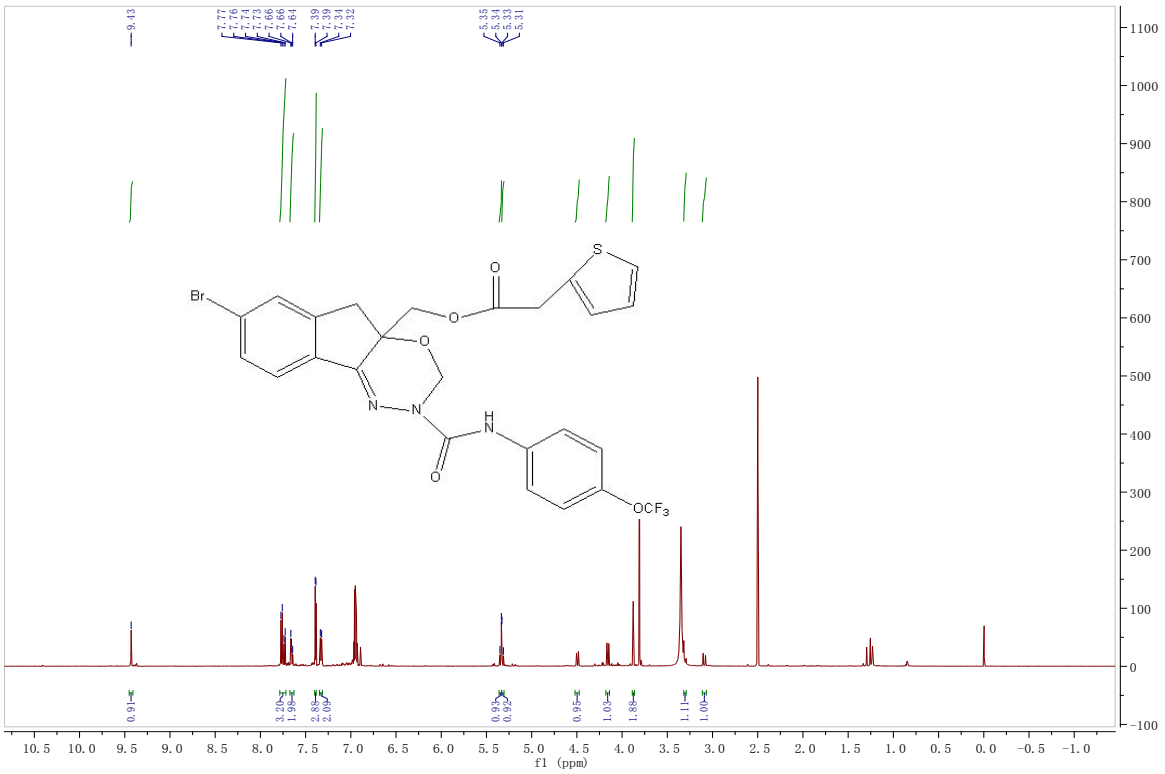
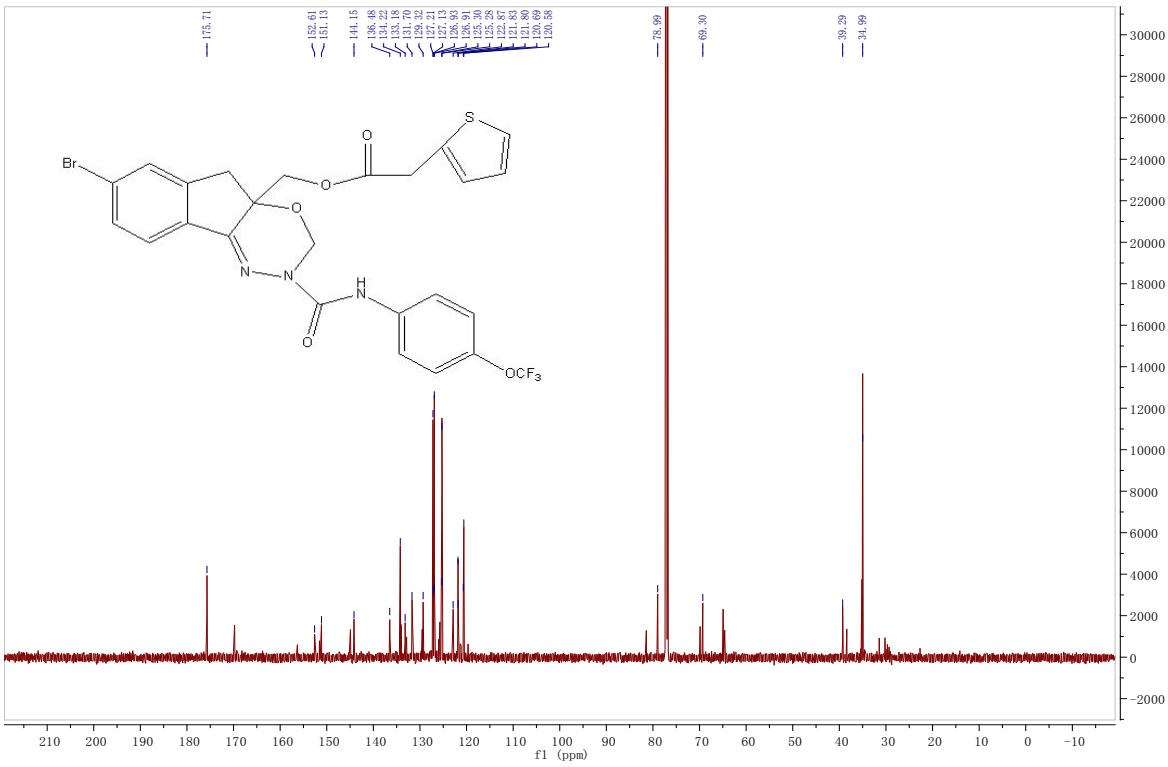


221

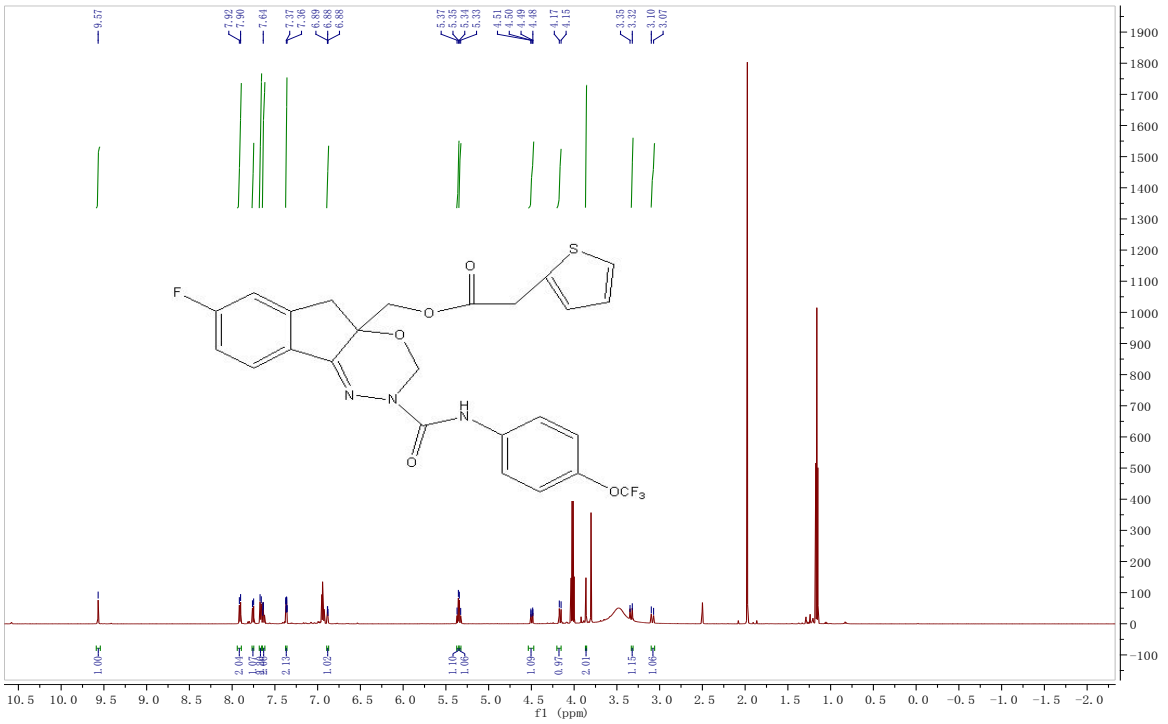
222 ^{1}H NMR and ^{13}C NMR of target compound J28

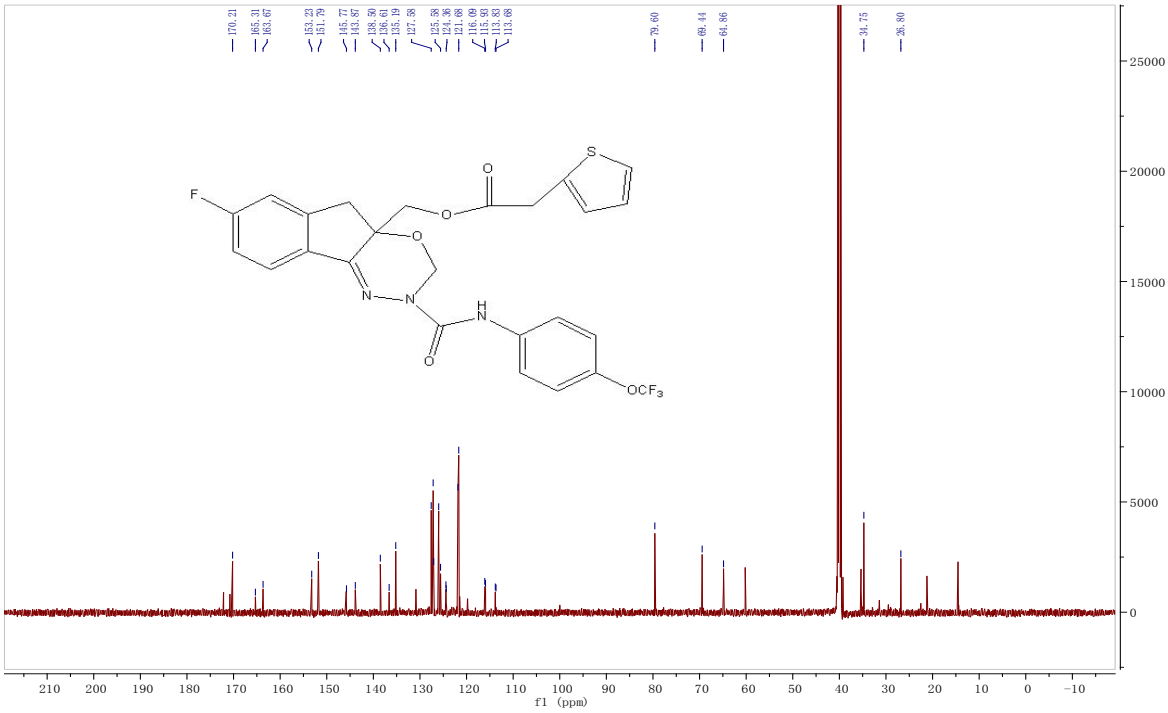
223



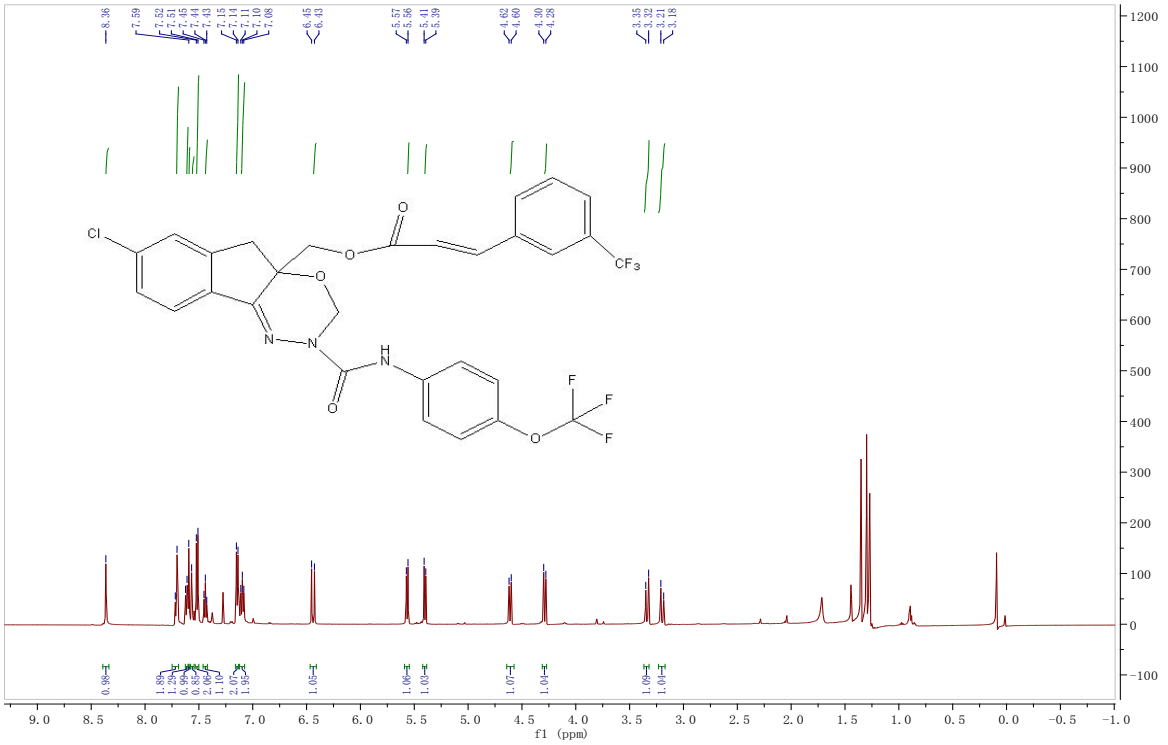


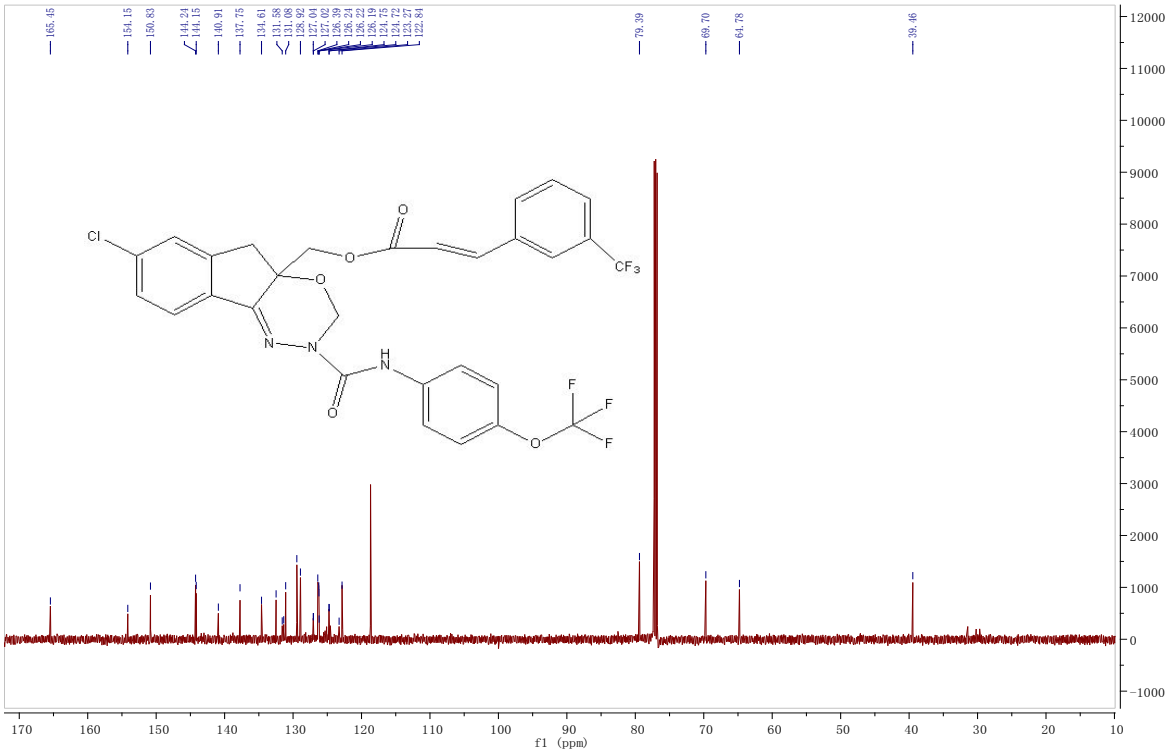
^{1}H NMR and ^{13}C NMR of target compound J29



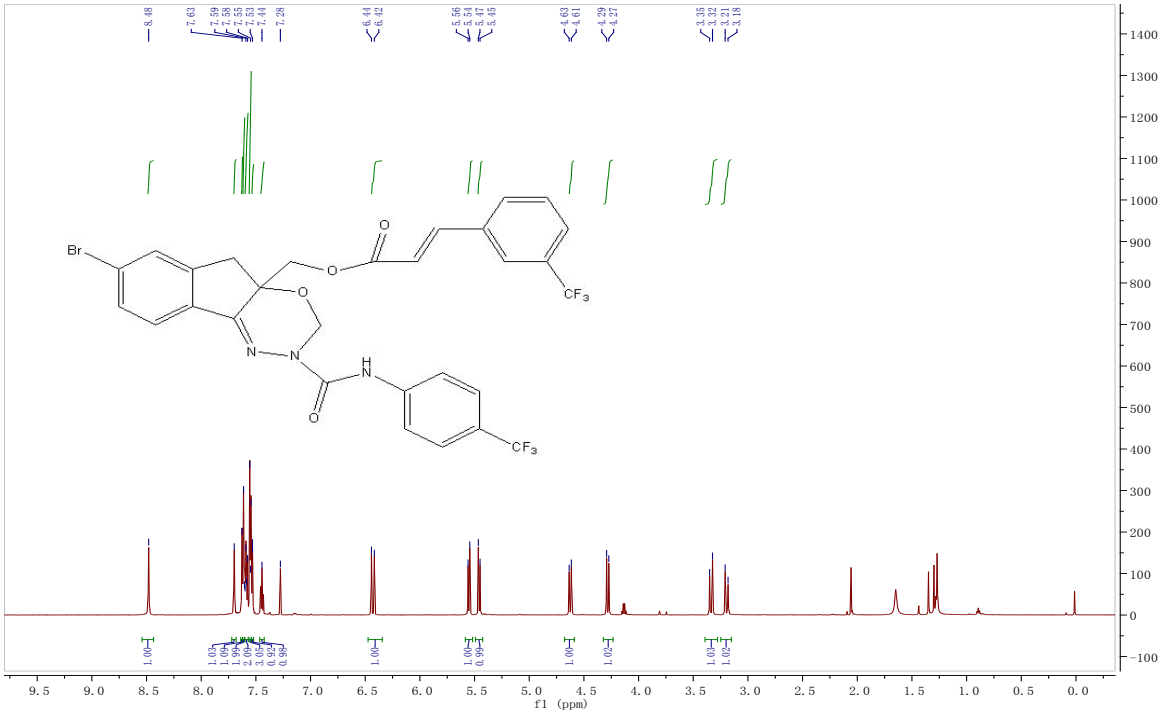


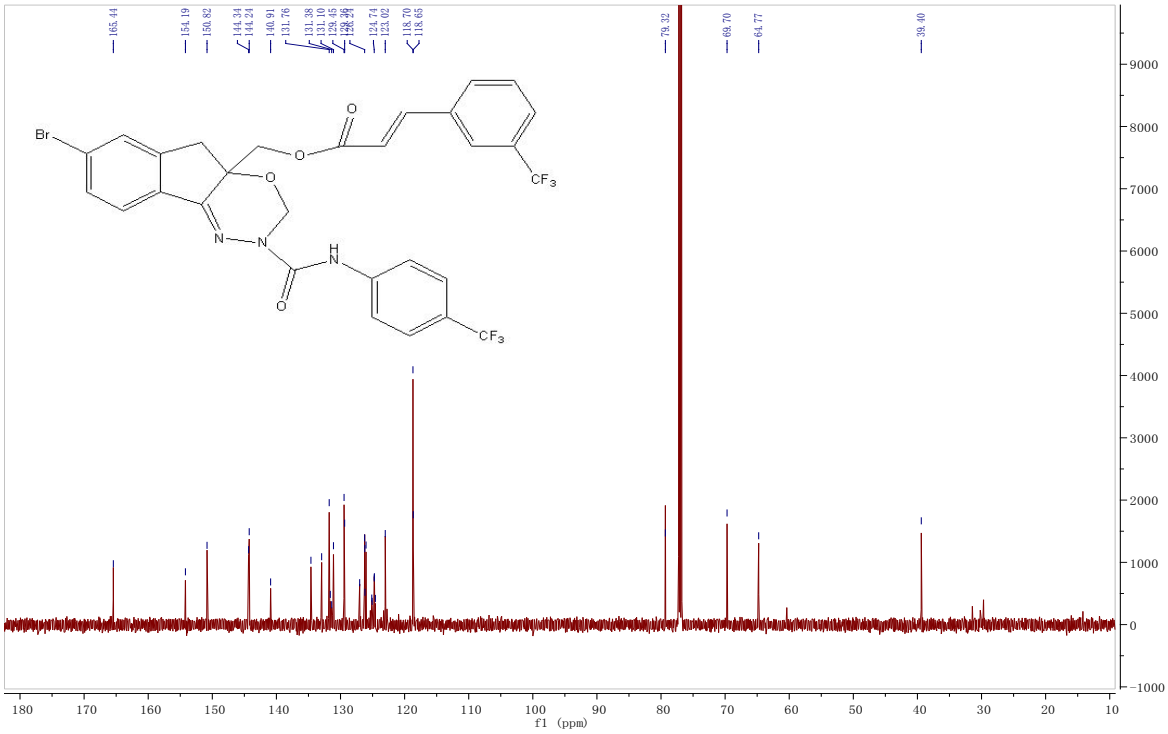
^{1}H NMR and ^{13}C NMR of target compound J30



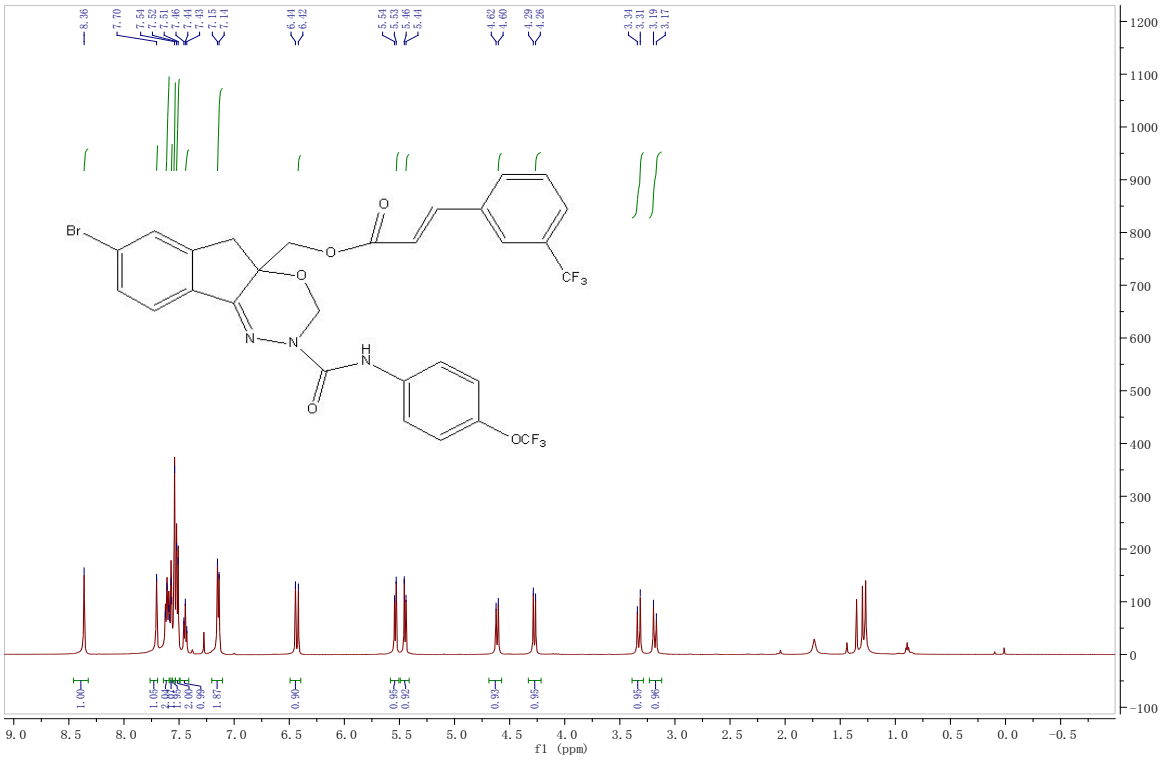


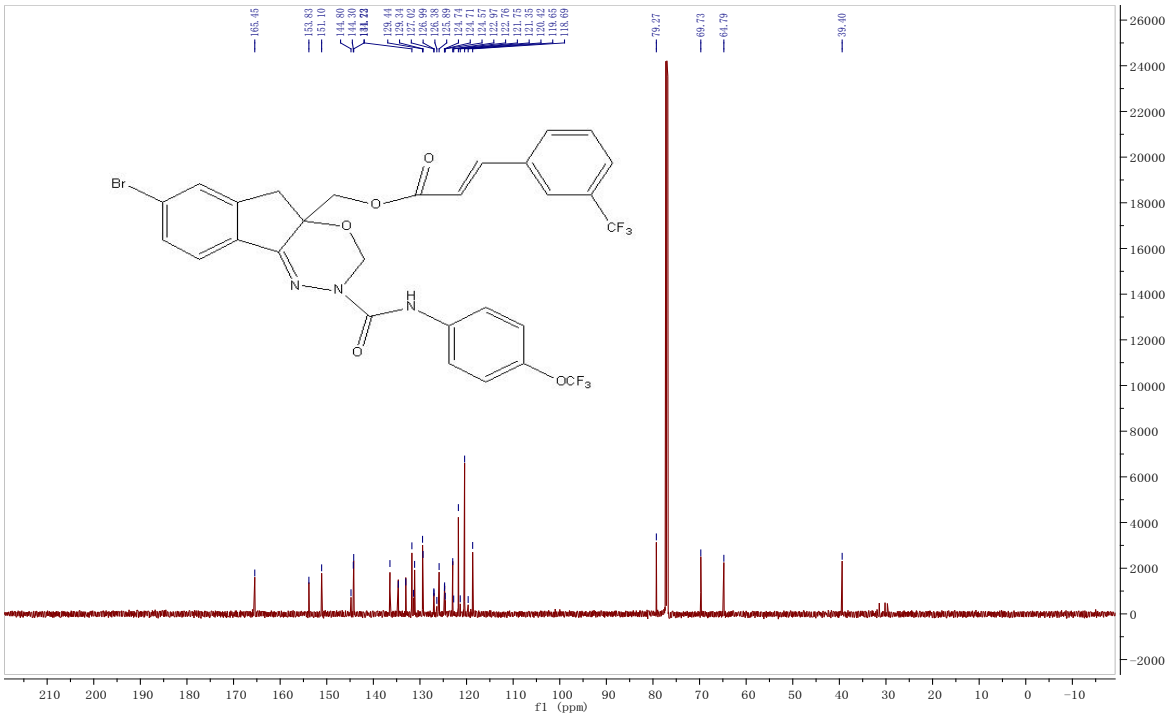
^{1}H NMR and ^{13}C NMR of target compound J31



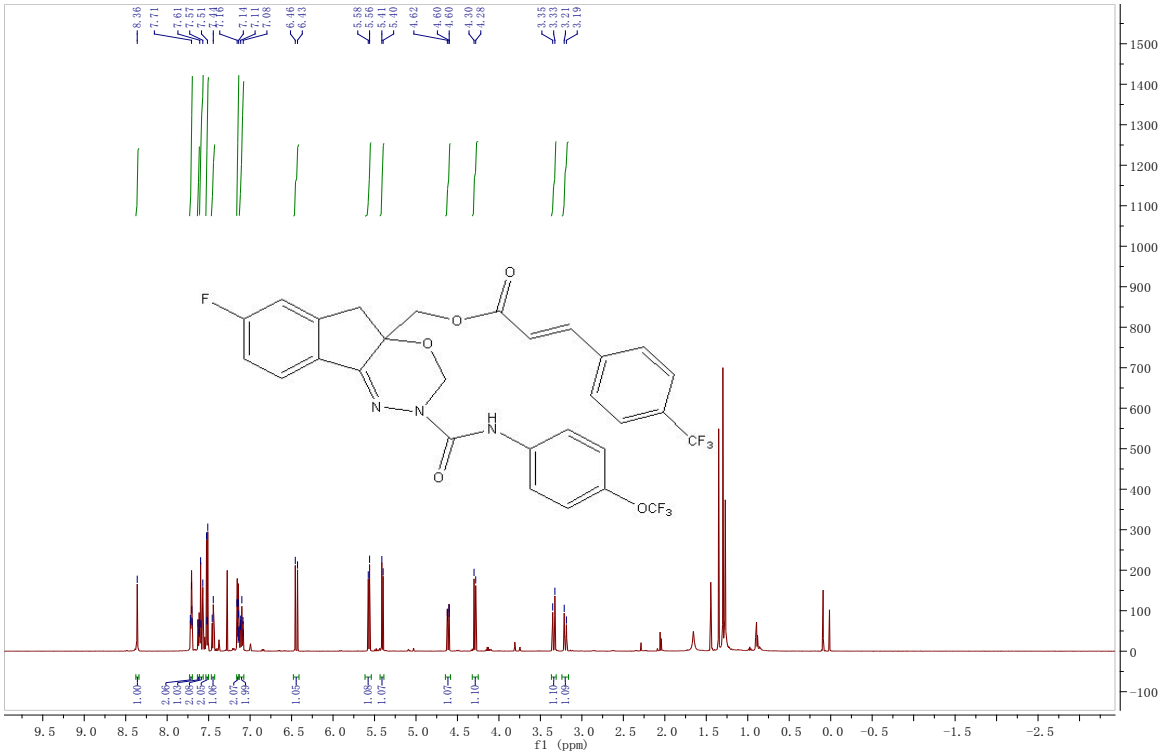


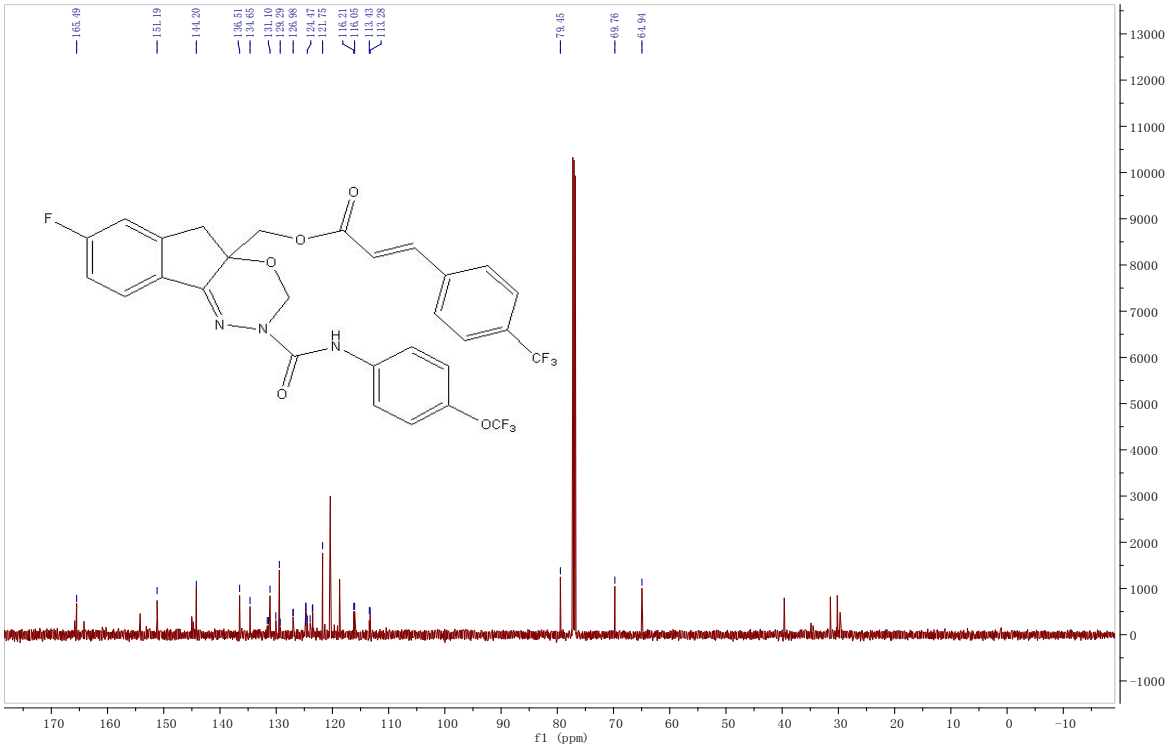
^{1}H NMR and ^{13}C NMR of target compound J32



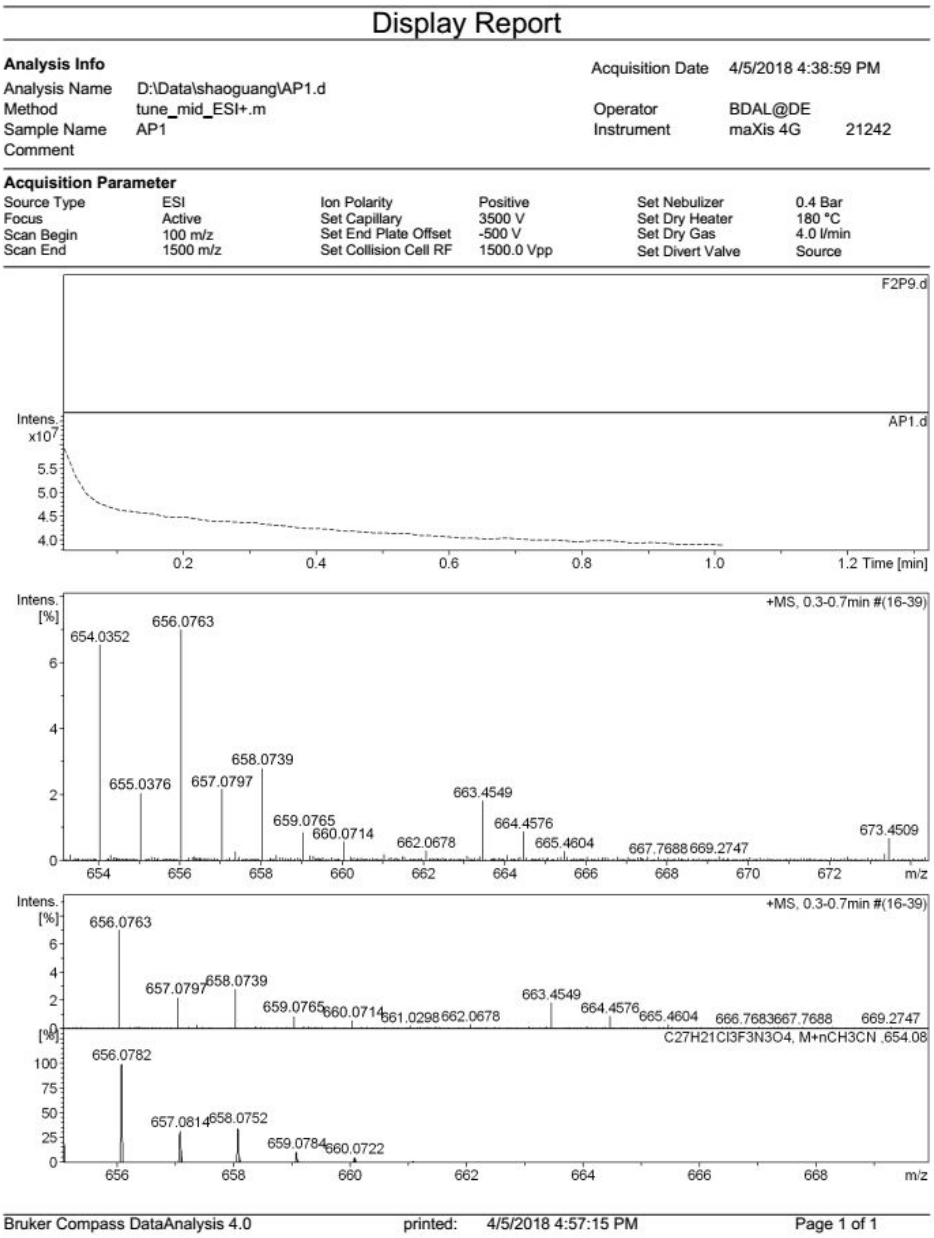


^{1}H NMR and ^{13}C NMR of target compound J33

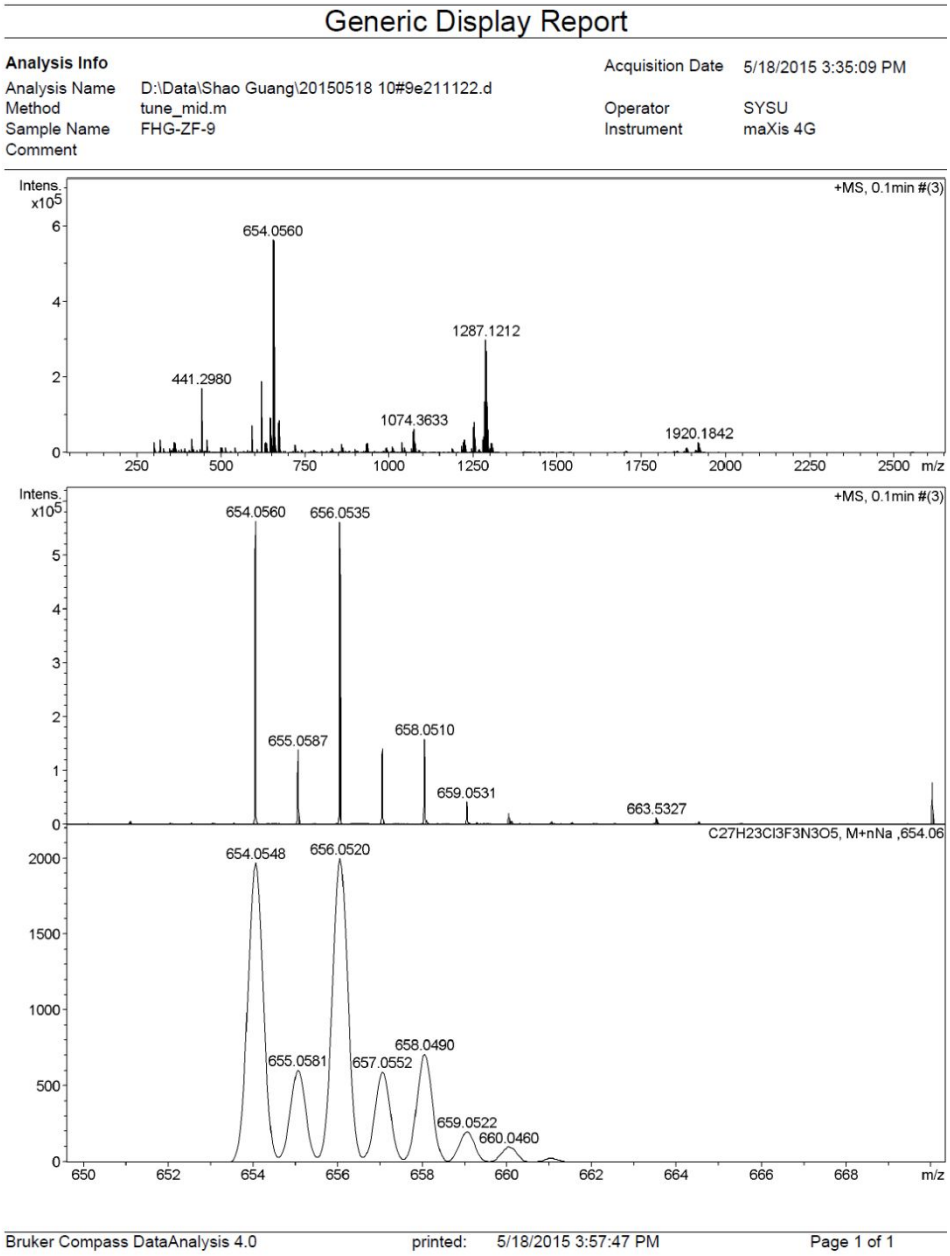




^{1}H NMR and ^{13}C NMR of target compound J34



HRMS of target compound J1



HRMS of target compound J2

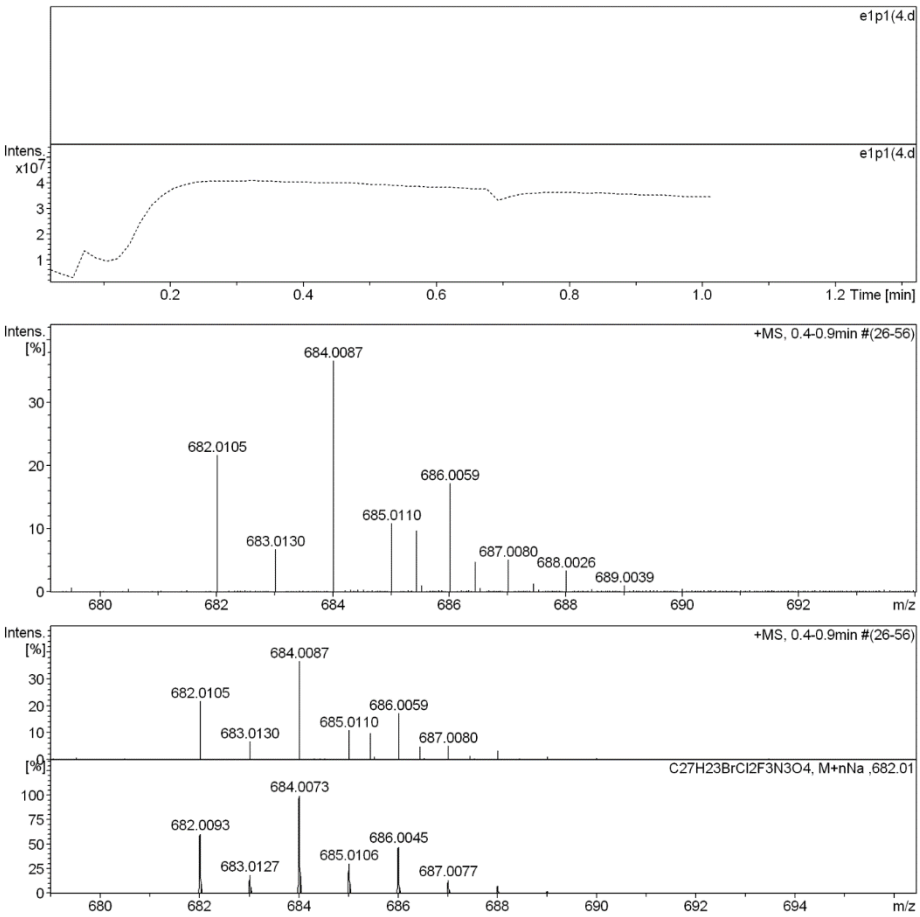
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\e1p1(4.d	Acquisition Date	4/5/2018 5:42:58 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e1p1(4)	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J3

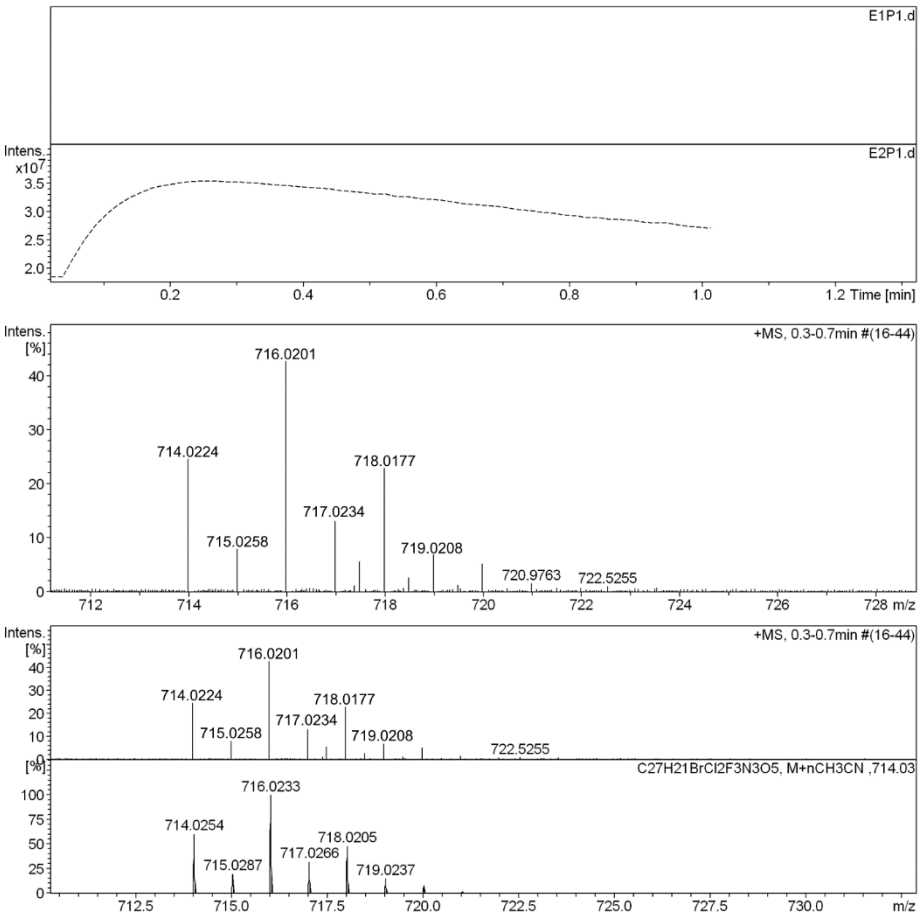
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\E2P1.d	Acquisition Date	4/5/2018 4:34:56 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	E2P1	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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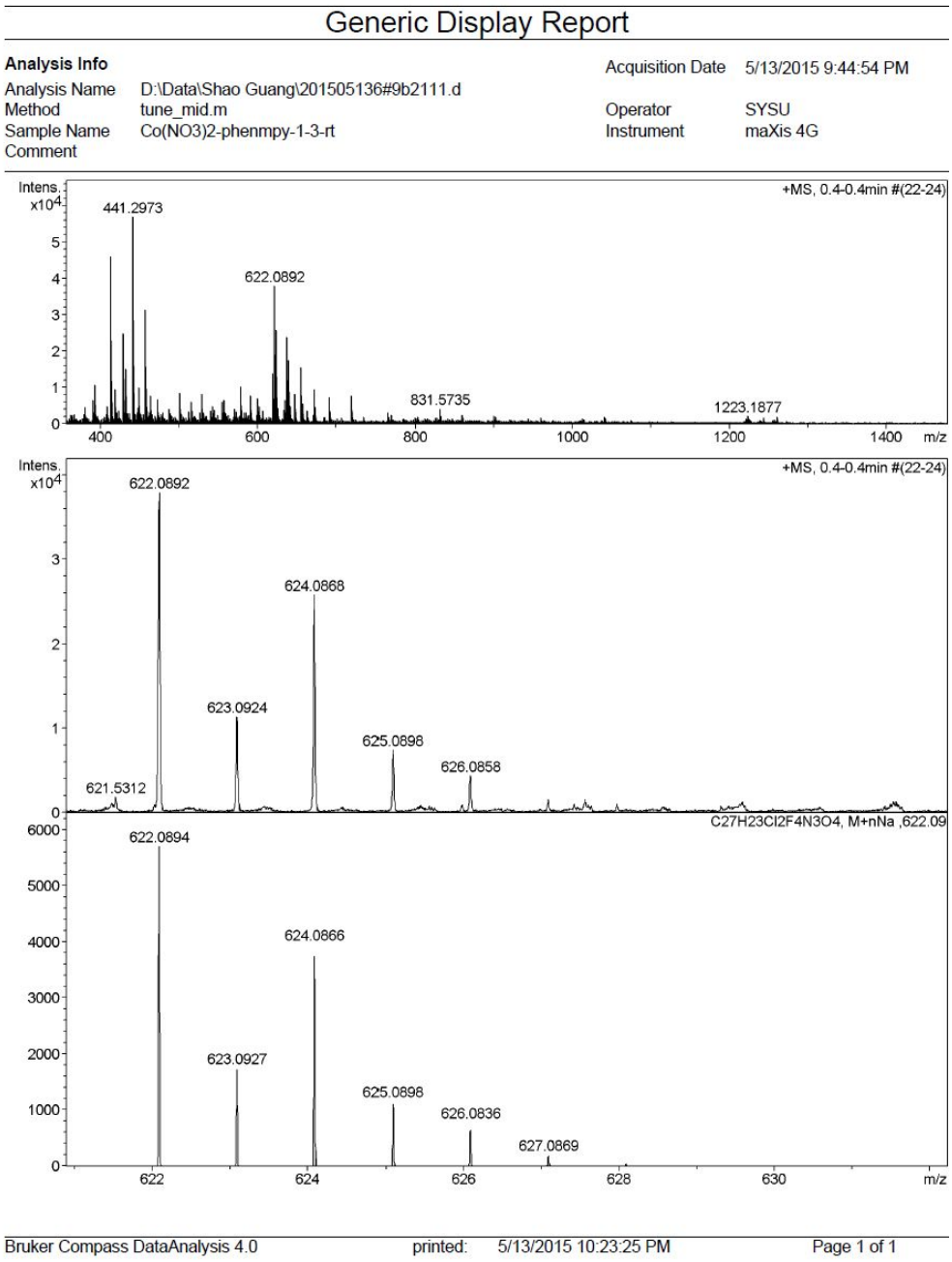
HRMS of target compound J4



HRMS of target compound J5

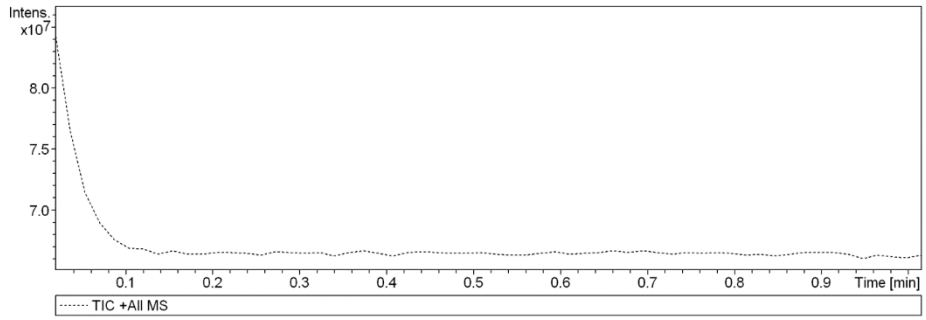
Display Report

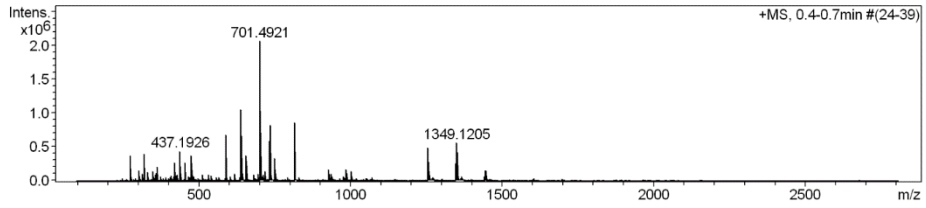
Analysis Info

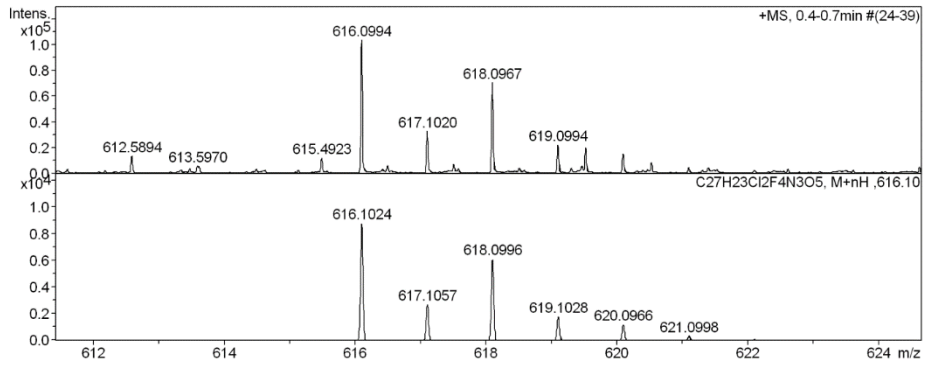
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\e2p31.d	Acquisition Date	8/10/2017 3:41:17 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e2p3	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J6

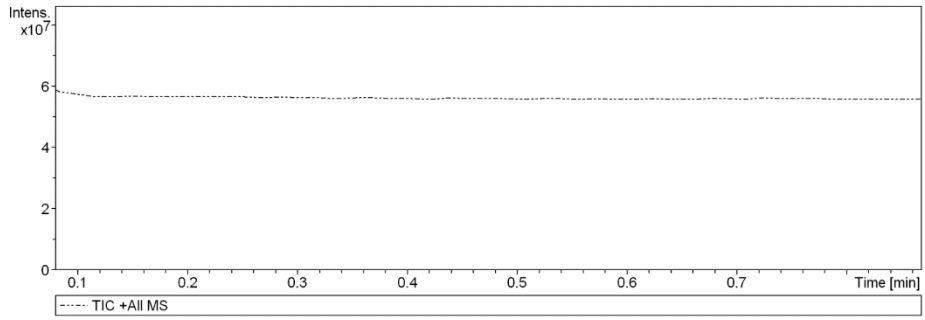
Display Report

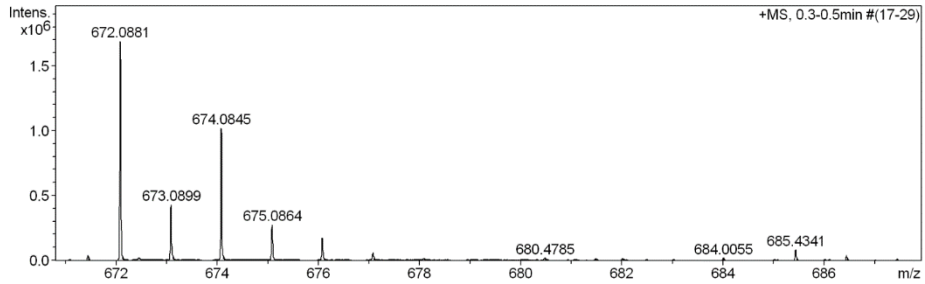
Analysis Info

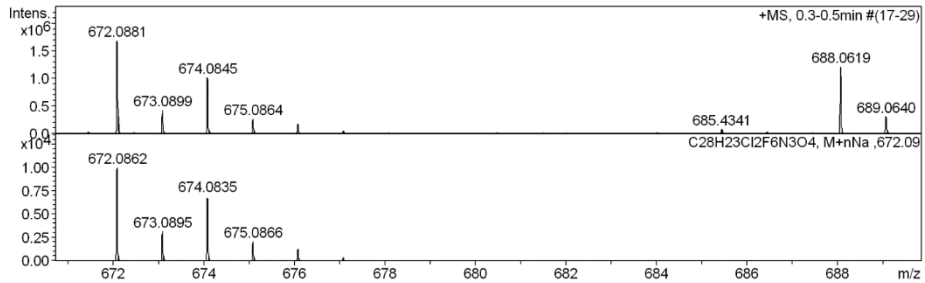
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810L\AP3H.d	Acquisition Date	8/10/2017 8:12:50 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	AP3H	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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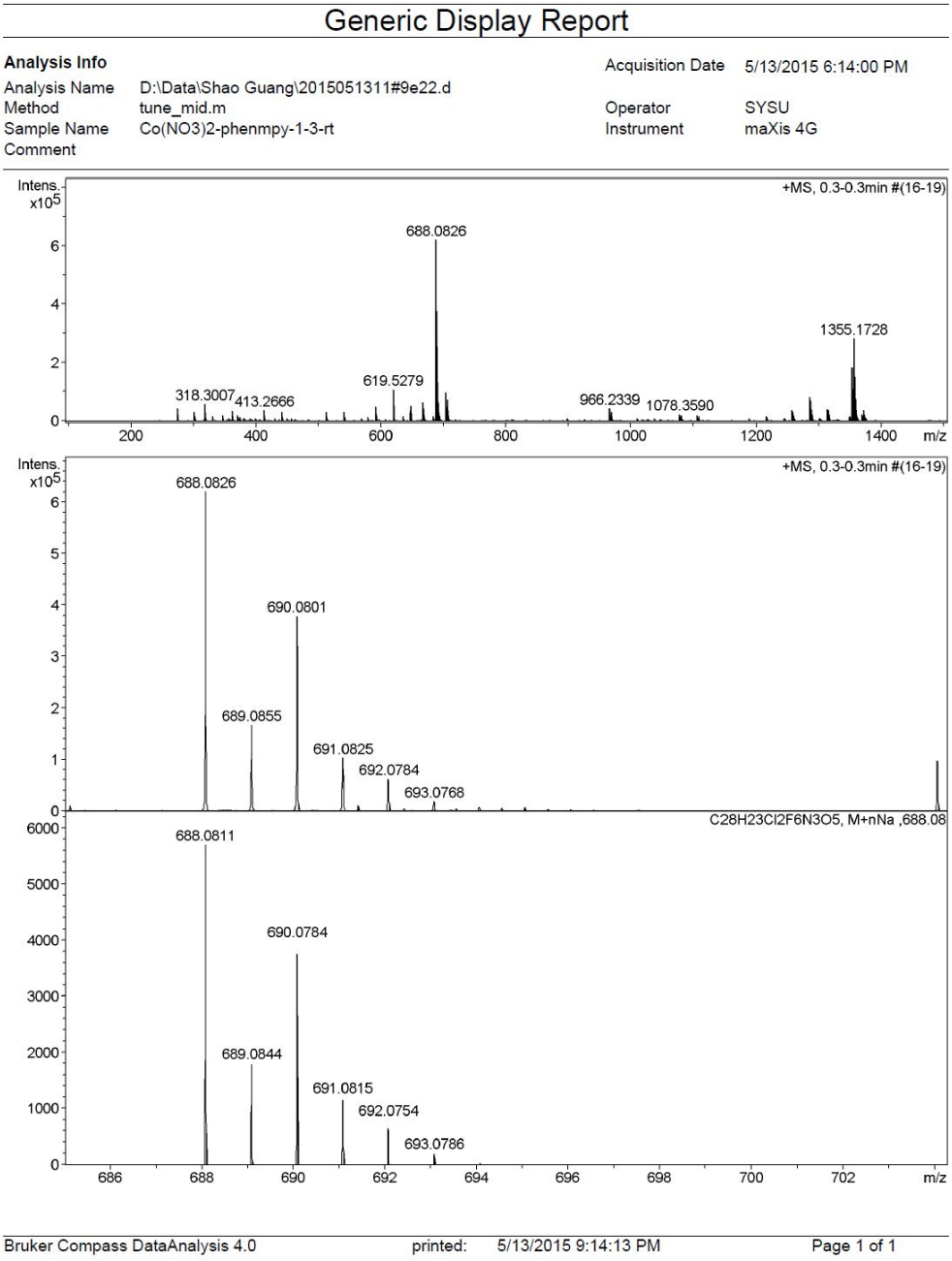
HRMS of target compound J7



HRMS of target compound J8

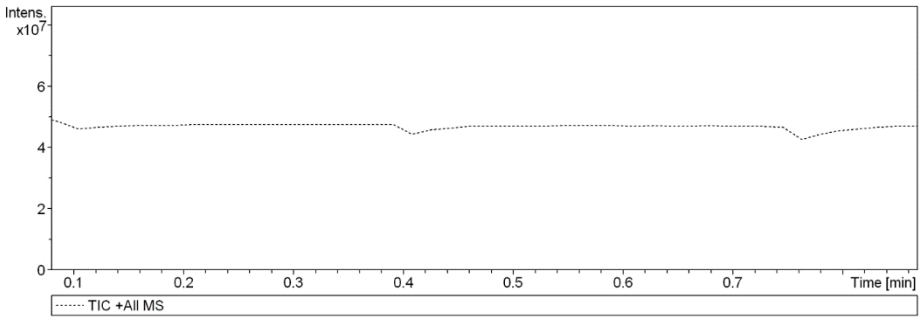
Display Report

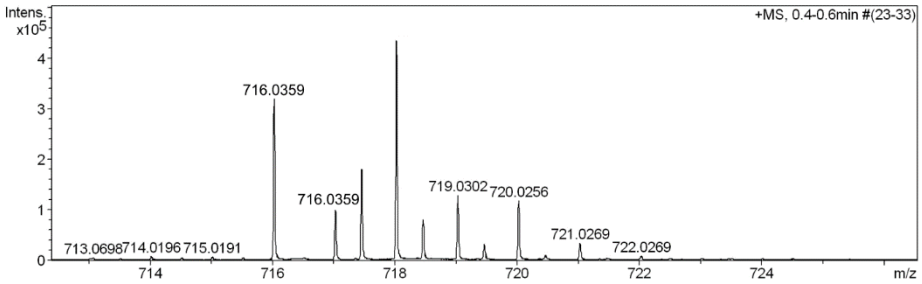
Analysis Info

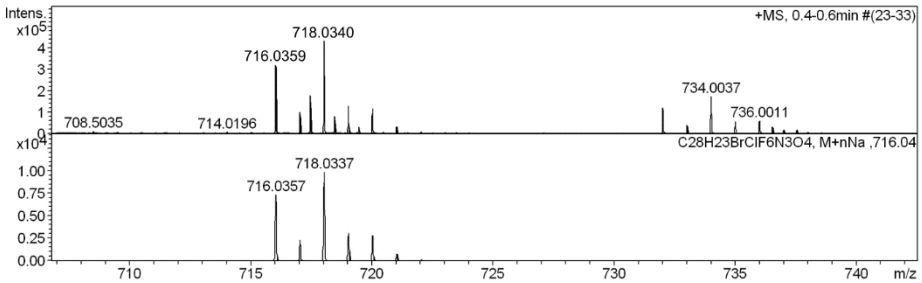
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\e1p3.d	Acquisition Date	8/10/2017 4:30:31 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e2p3	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J9

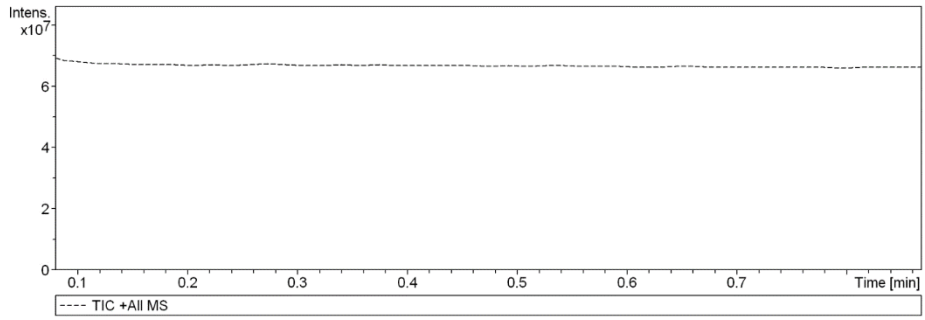
Display Report

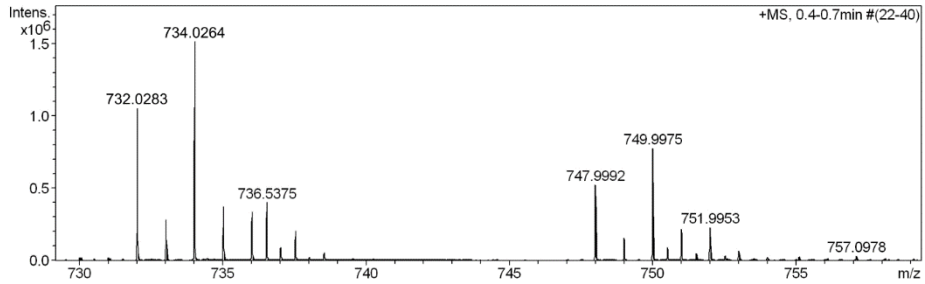
Analysis Info

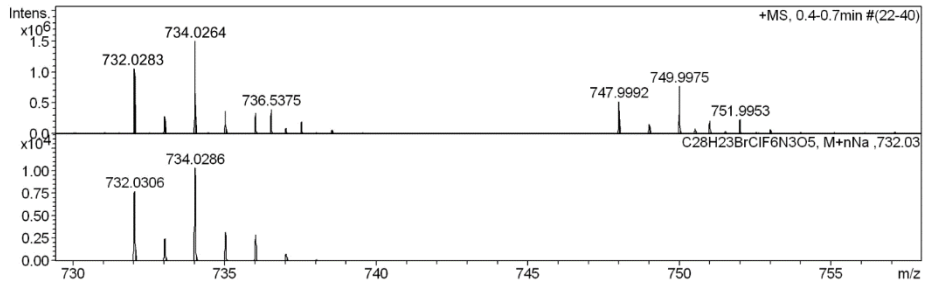
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\e2p3h.d	Acquisition Date	8/10/2017 4:03:49 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e2p3h	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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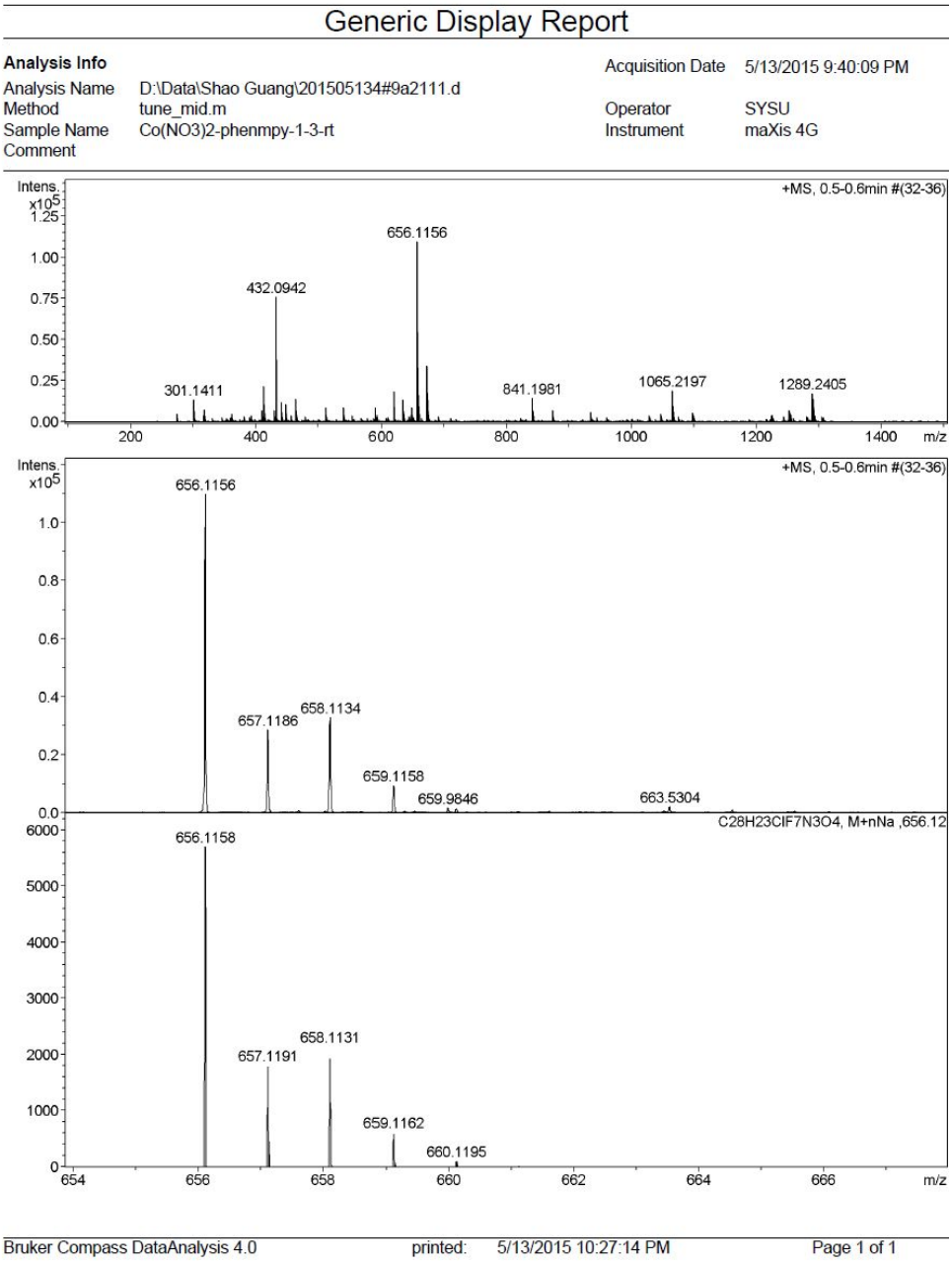
HRMS of target compound J10



HRMS of target compound J11

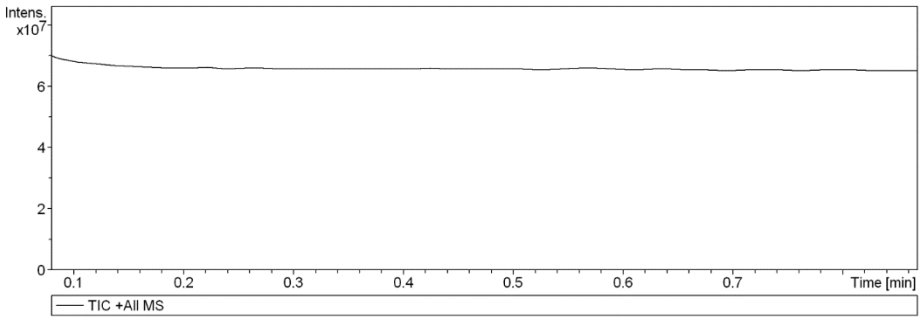
Display Report

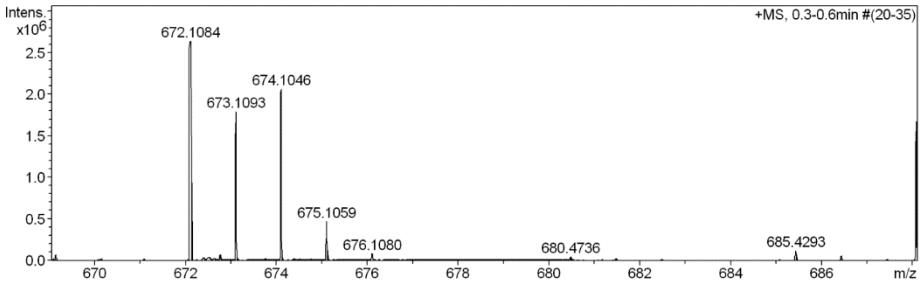
Analysis Info

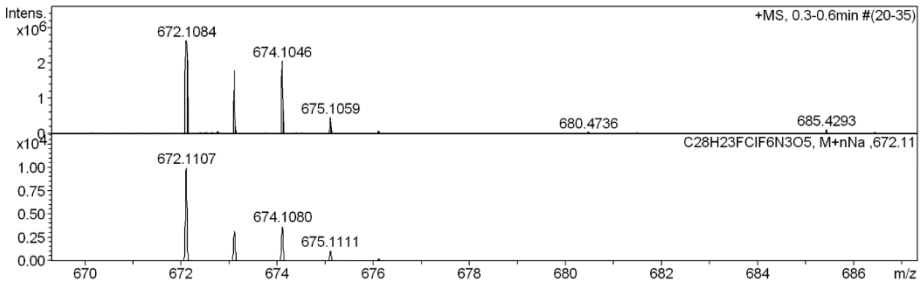
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\f2p3.d	Acquisition Date	8/10/2017 4:19:33 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	huangjianfeng-kongbai	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J12

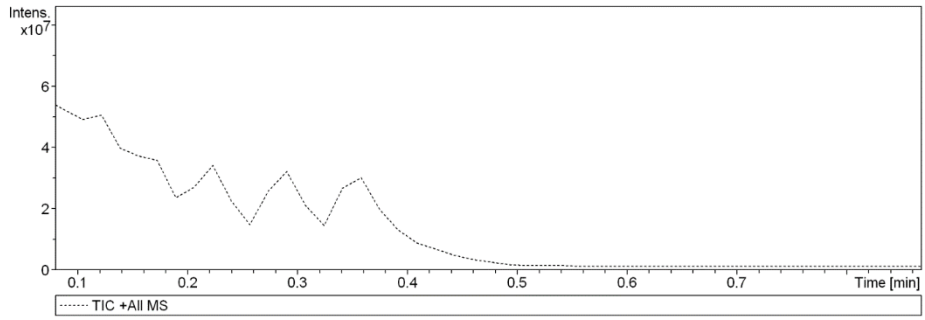
Display Report

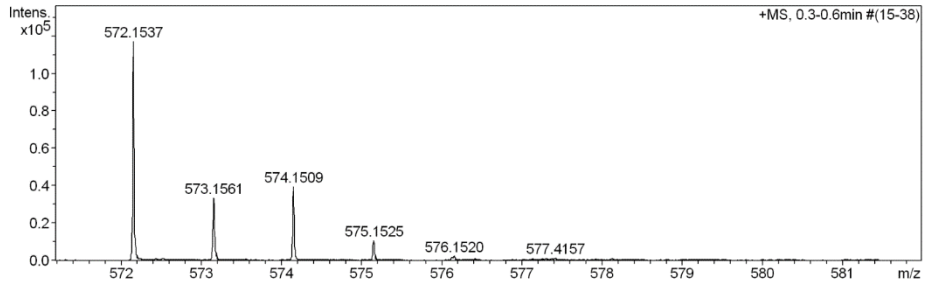
Analysis Info

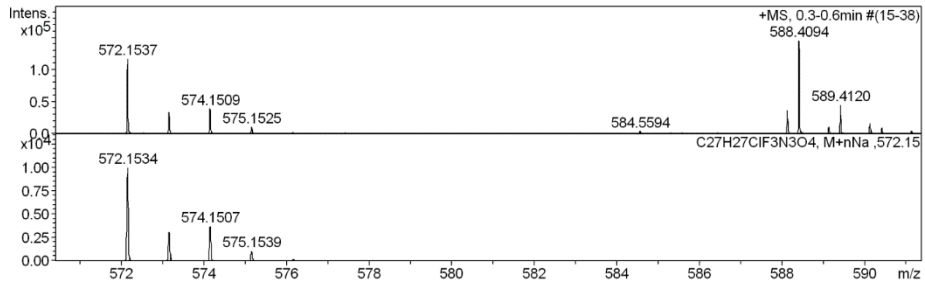
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\7AP6.d	Acquisition Date	8/10/2017 5:41:05 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	7AP6	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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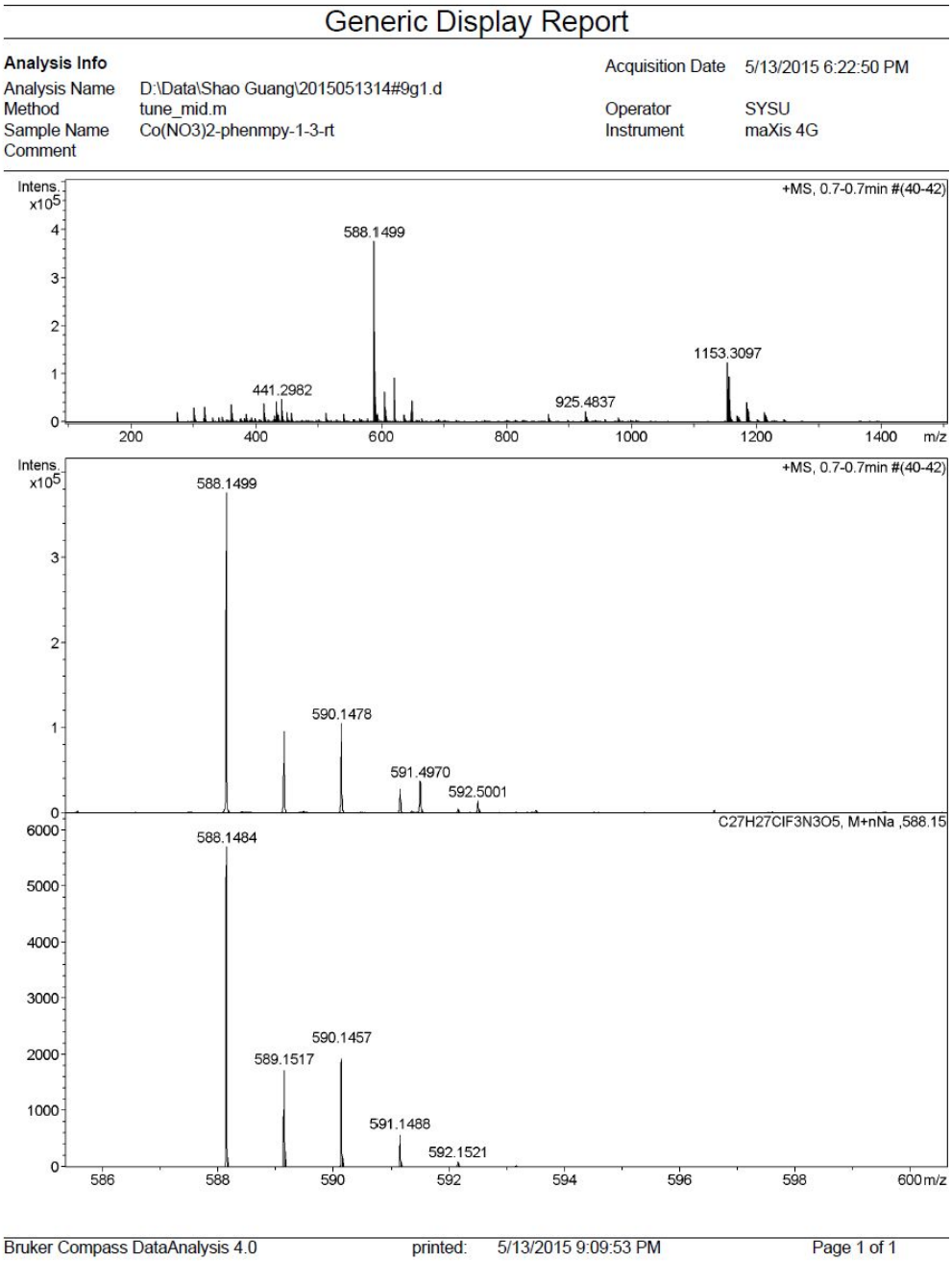
HRMS of target compound J13



HRMS of target compound J14

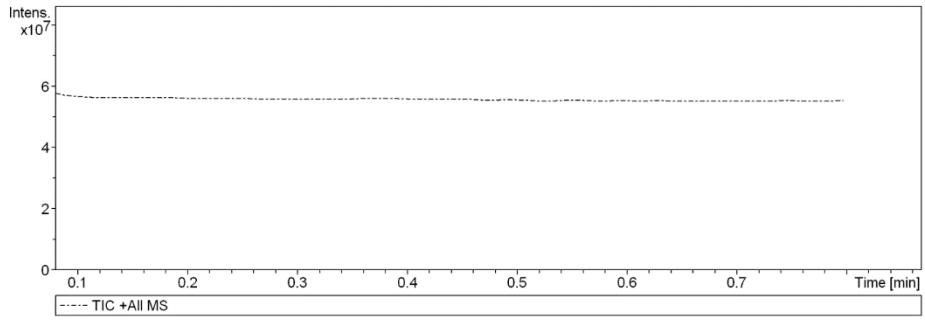
Display Report

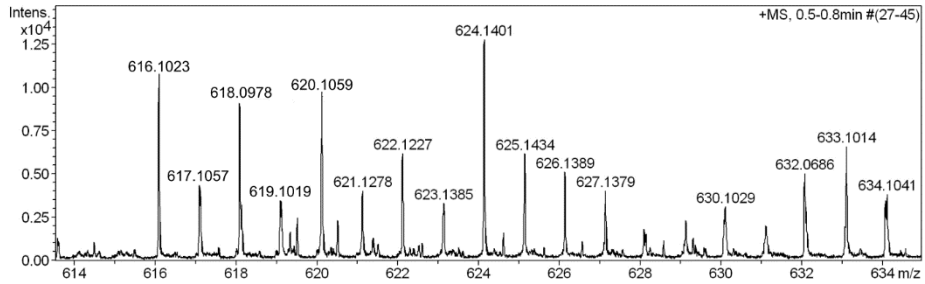
Analysis Info

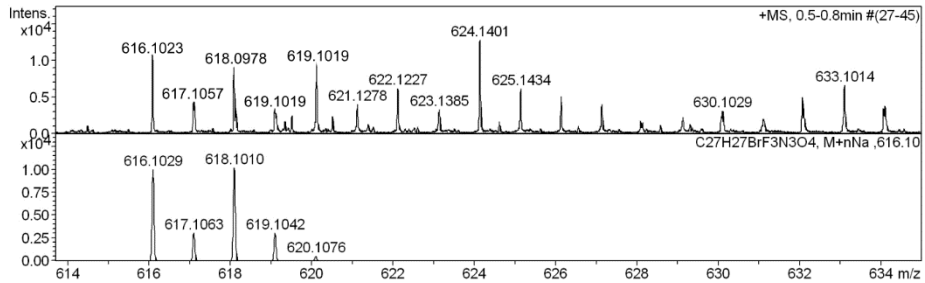
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\e1p6.d	Acquisition Date	8/10/2017 4:44:47 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	huangjianfeng-kongbai	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J15

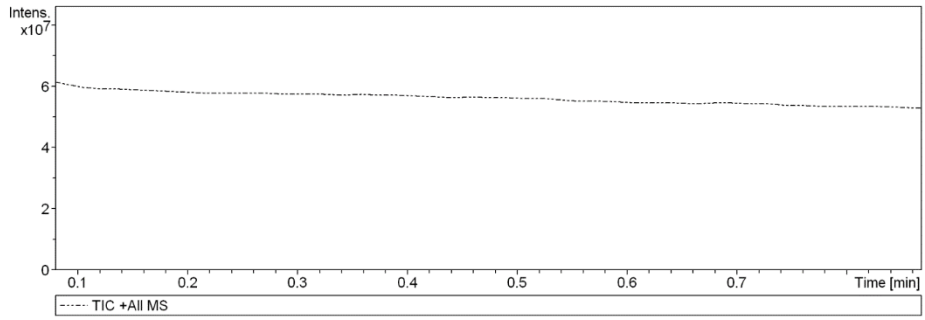
Display Report

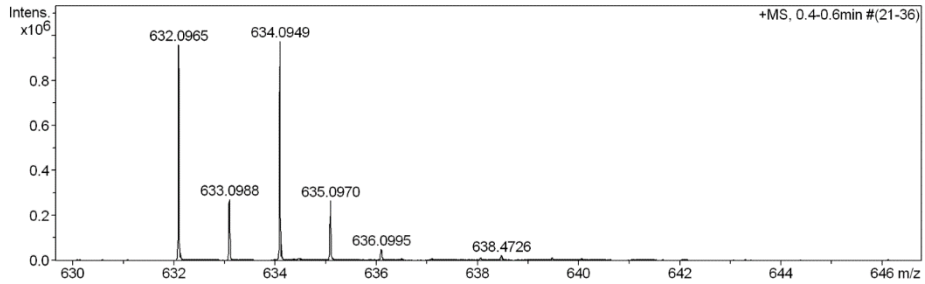
Analysis Info

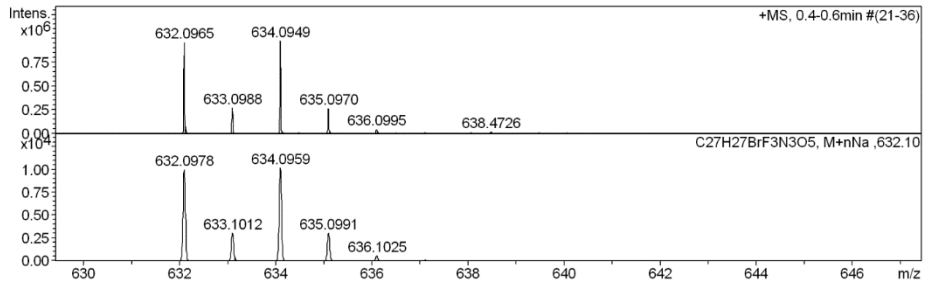
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\e2p6.d	Acquisition Date	8/10/2017 5:04:34 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e2p6	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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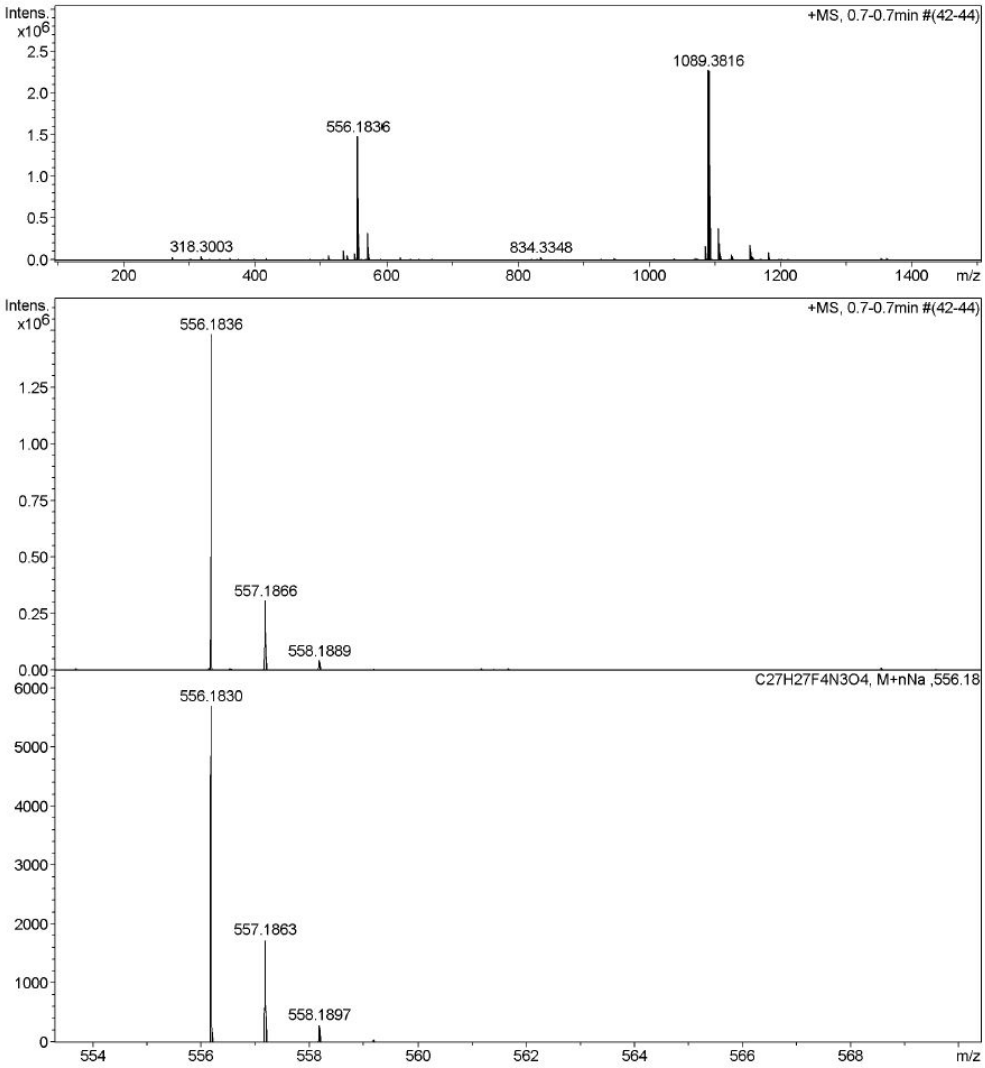
HRMS of target compound J16

Generic Display Report

Analysis Info

Analysis Name	D:\Data\Shao Guang\201505137#9c111.d	Acquisition Date	5/13/2015 9:47:35 PM
Method	tune_mid.m	Operator	SYSU
Sample Name	Co(NO3)2-phenmpy-1-3-rt	Instrument	maXis 4G
Comment			



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HRMS of target compound J17

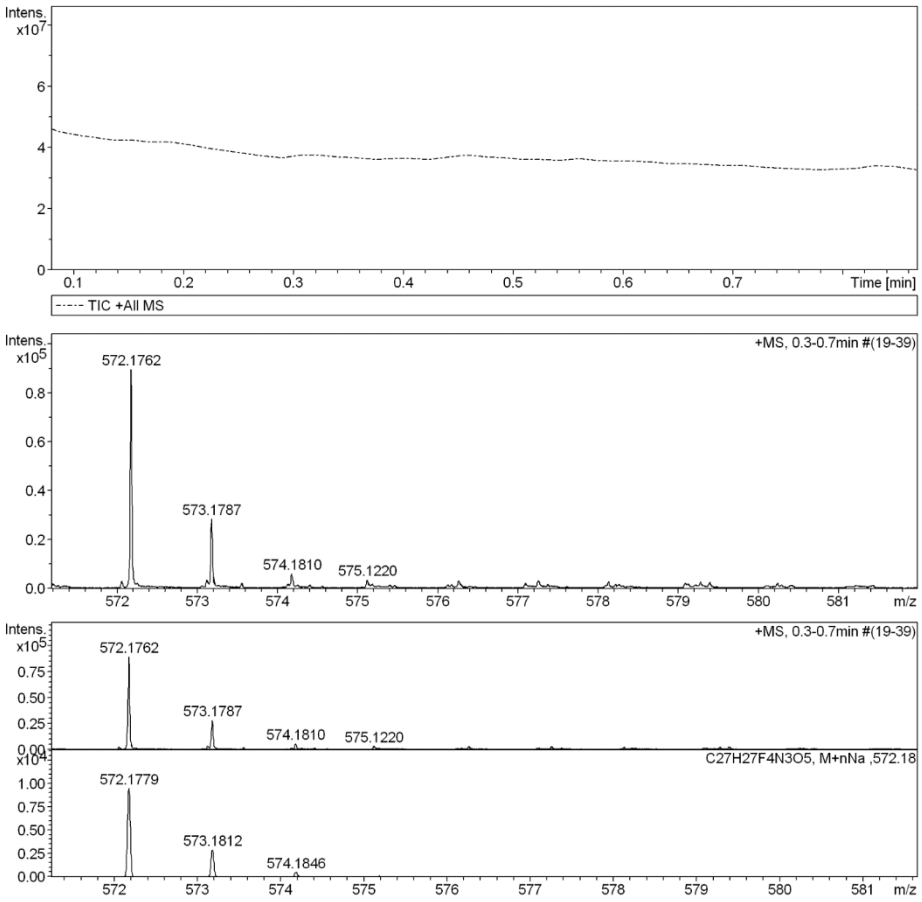
Display Report

Analysis Info

Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\F2P6.d	Acquisition Date	8/10/2017 5:56:32 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	F2P6	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J18

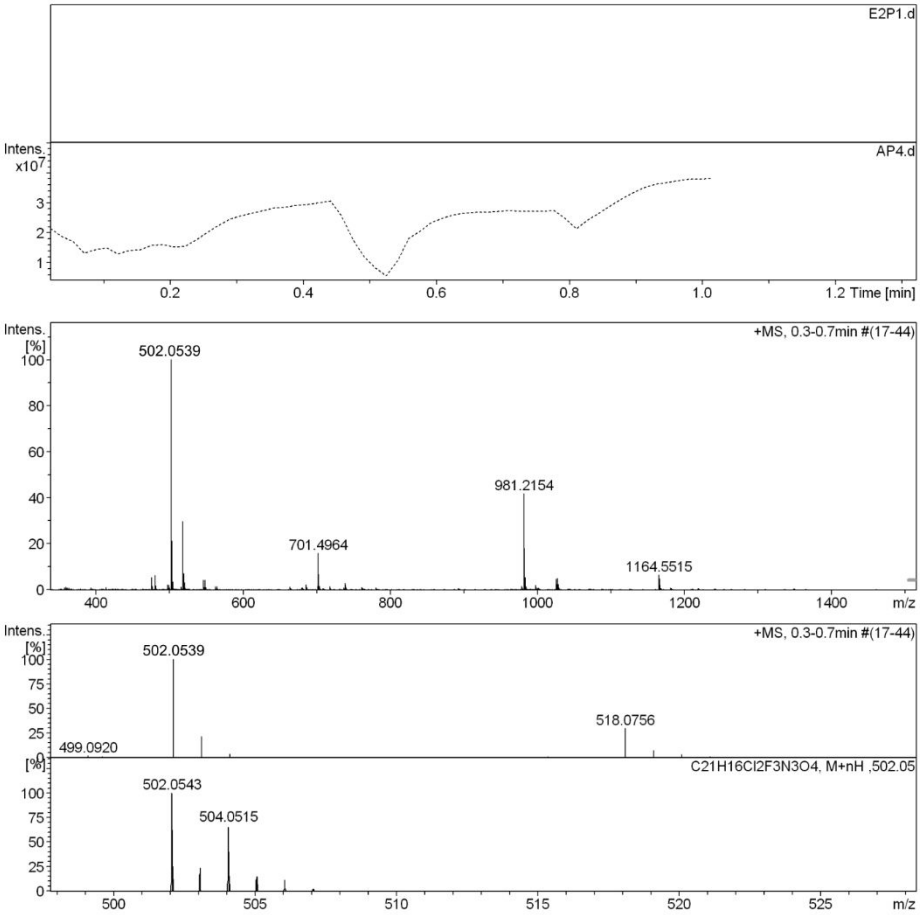
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\AP4.d	Acquisition Date	4/5/2018 4:22:52 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	AP4	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J19

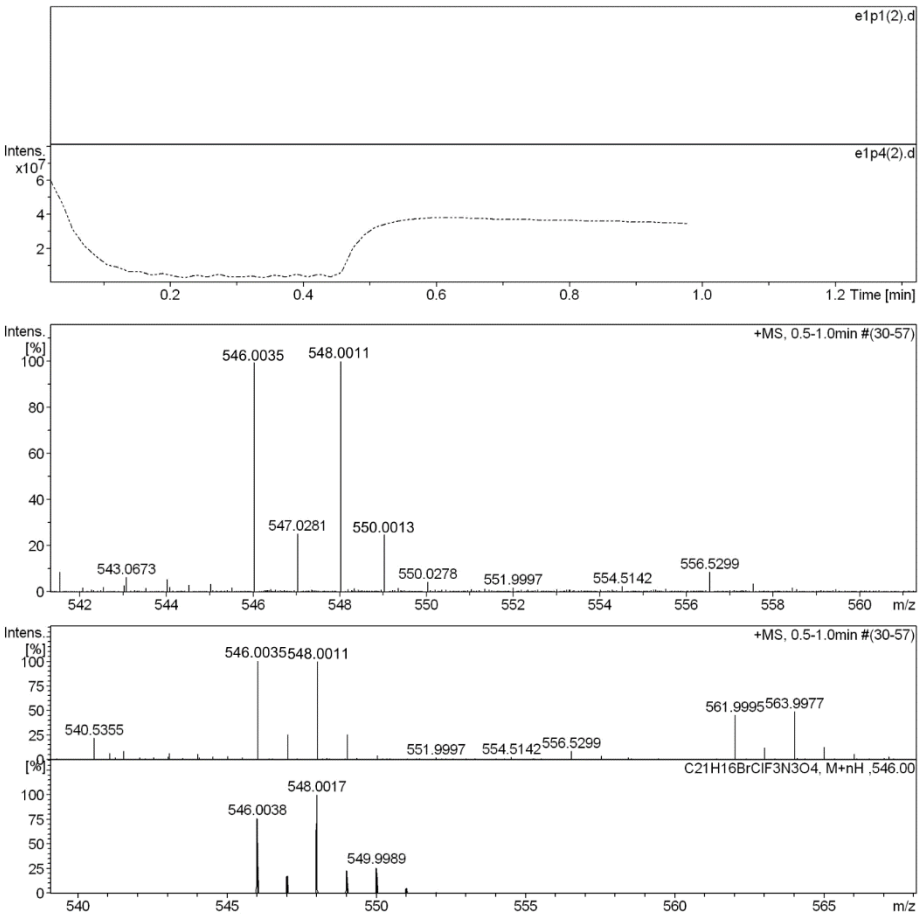
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\e1p4(2).d	Acquisition Date	4/5/2018 5:32:58 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e1p4(2)	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J20

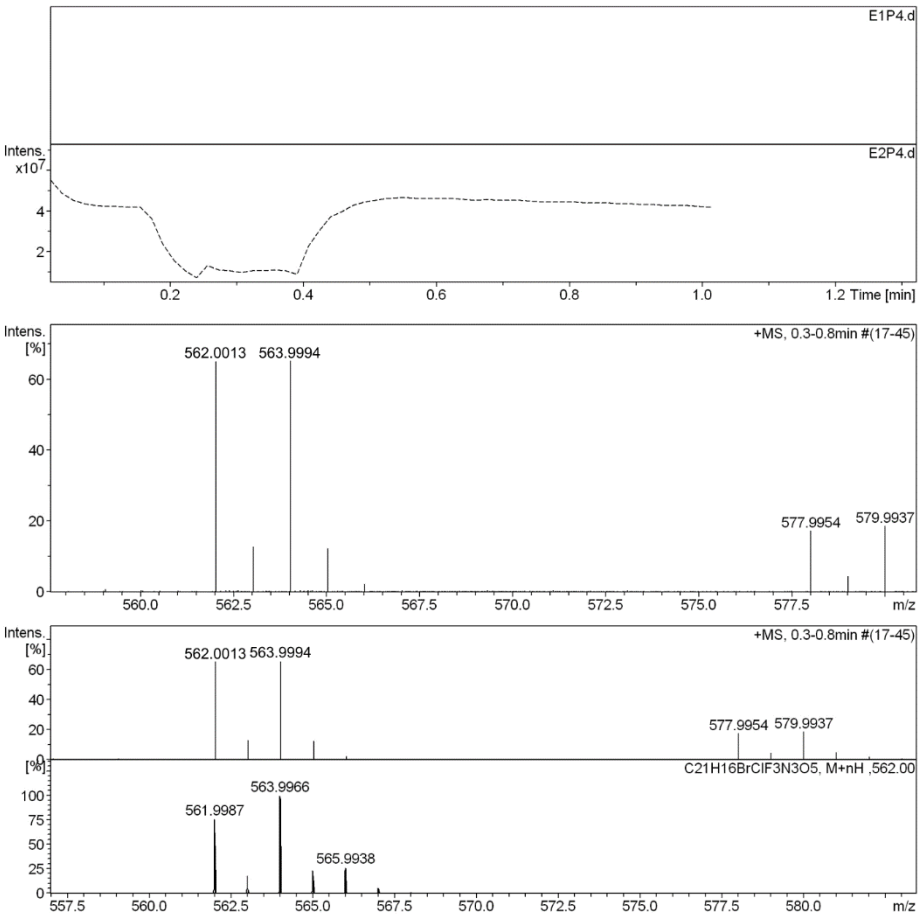
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\E2P4.d	Acquisition Date	4/5/2018 4:26:56 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	E2P4	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J21

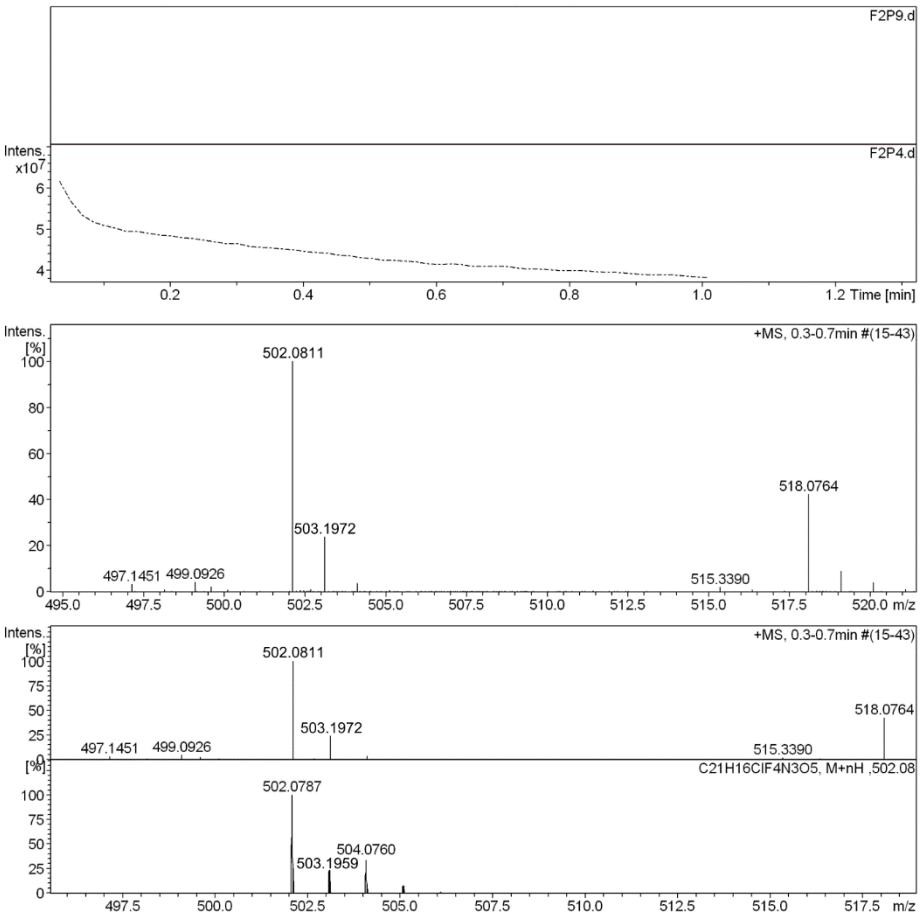
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\F2P4.d	Acquisition Date	4/5/2018 4:19:39 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	F2P4	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J22

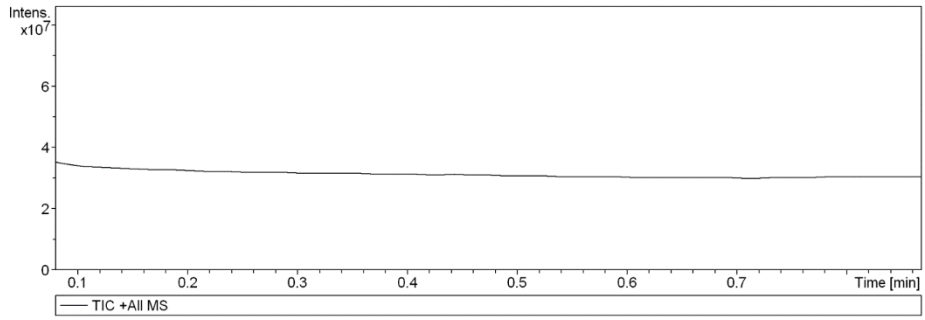
Display Report

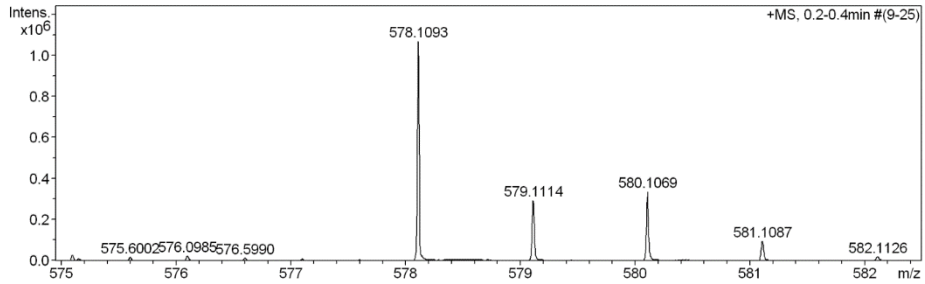
Analysis Info

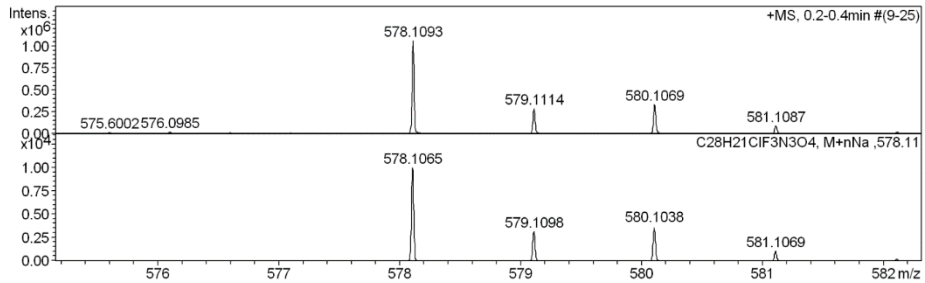
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810L\AP7.d	Acquisition Date	8/10/2017 7:37:08 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	AP7	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J23

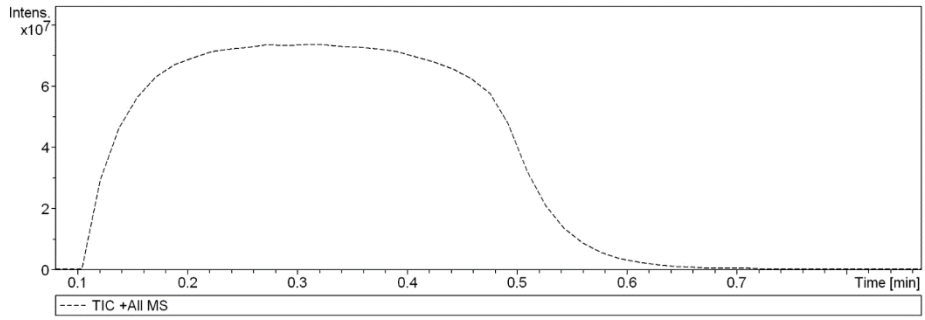
Display Report

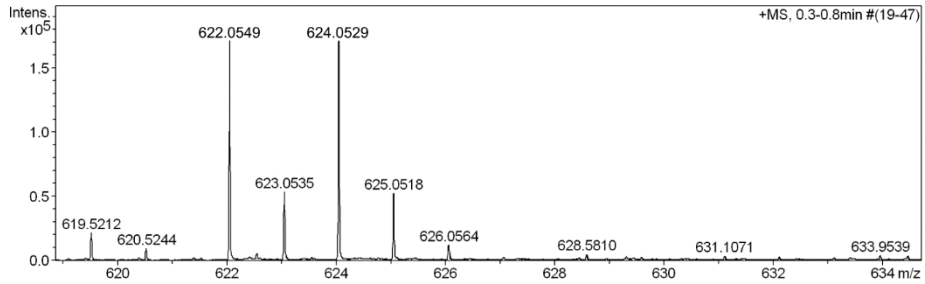
Analysis Info

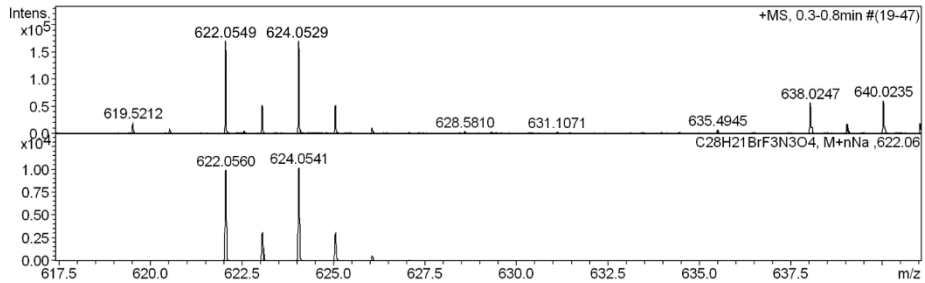
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\e1p7.d	Acquisition Date	8/10/2017 4:10:04 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e1p7	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J24

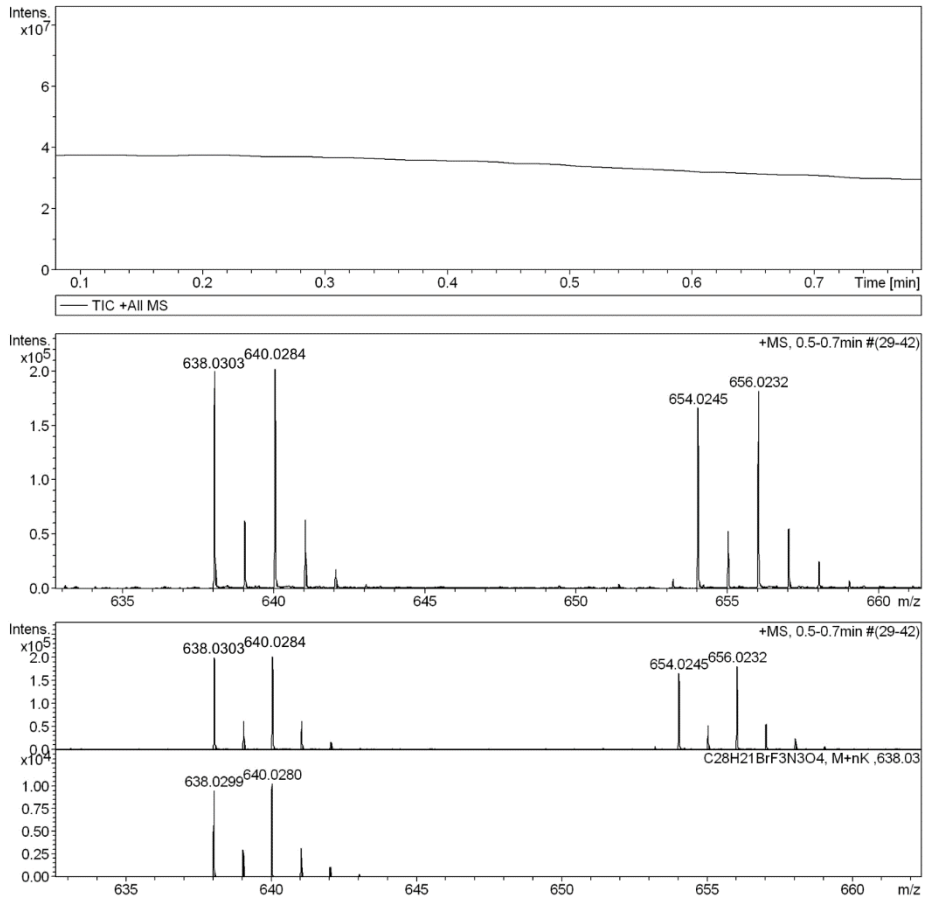
Display Report

Analysis Info

Analysis Name	D:\Data\Shao Guang\SCAU J\20170810M\E2P7.d	Acquisition Date	8/10/2017 9:55:39 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	AP1	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J25

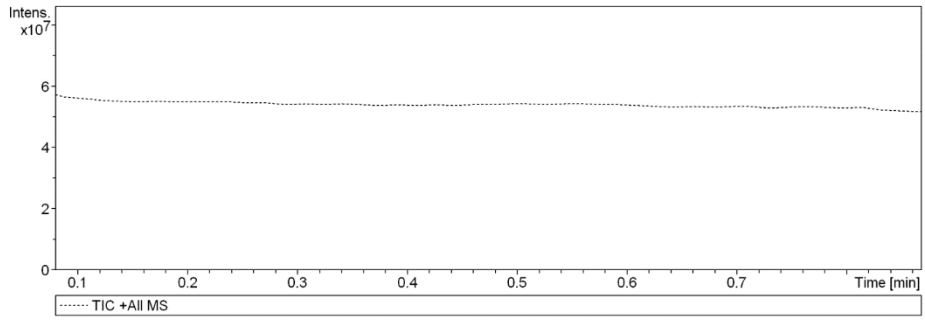
Display Report

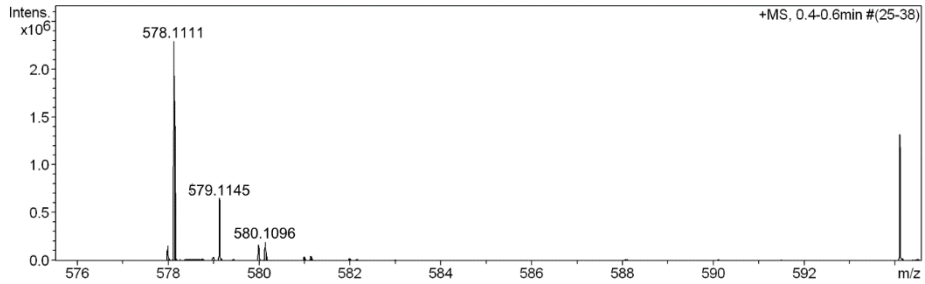
Analysis Info

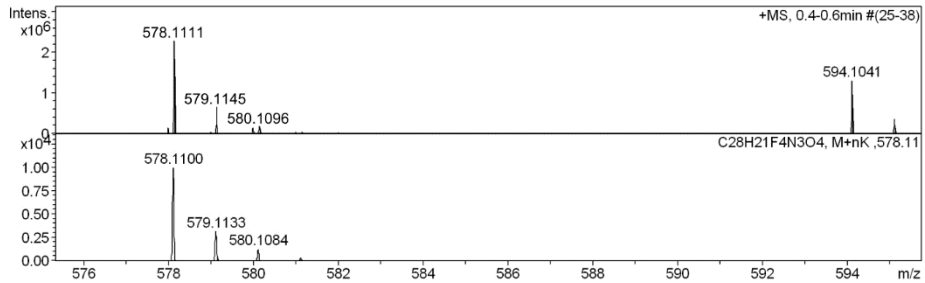
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\F2P7.d	Acquisition Date	8/10/2017 5:36:44 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	F2P7	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J26

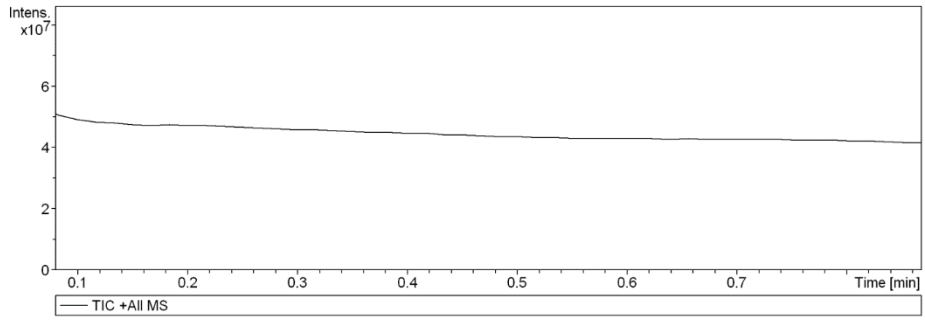
Display Report

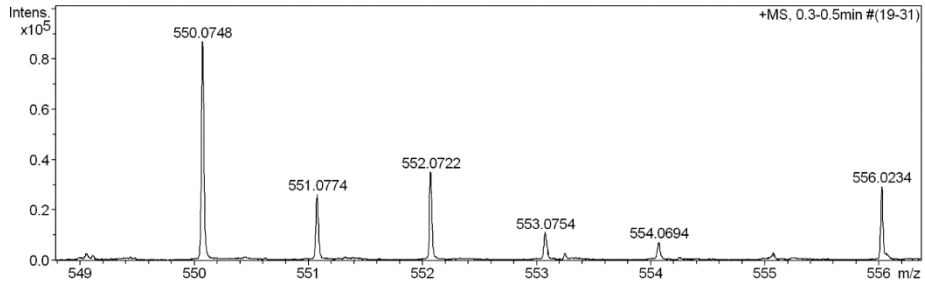
Analysis Info

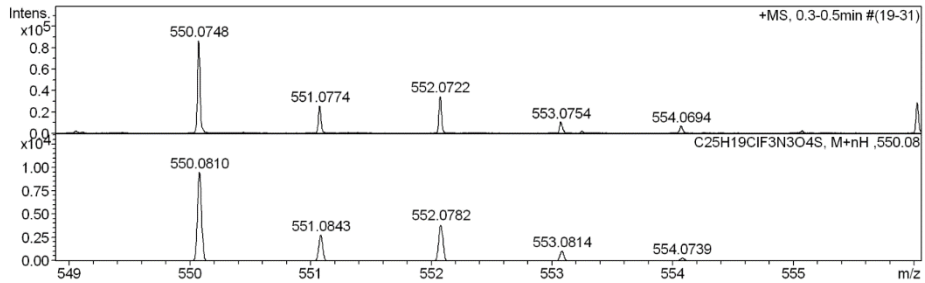
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\ap8.d	Acquisition Date	8/10/2017 4:49:07 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	ap8	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J27

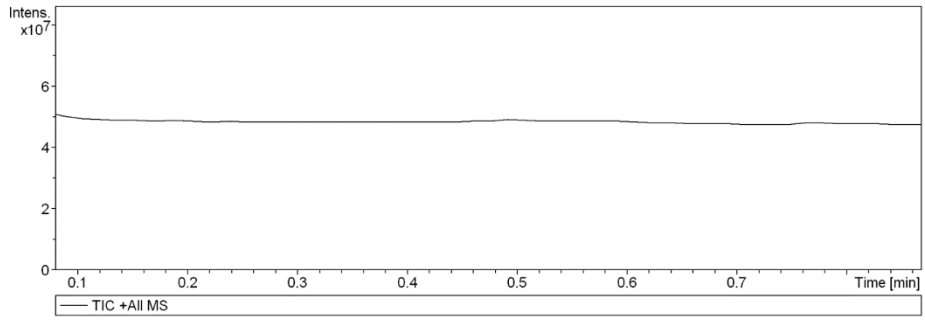
Display Report

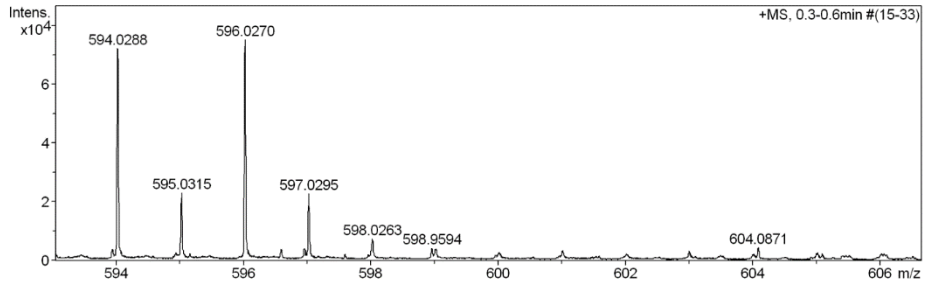
Analysis Info

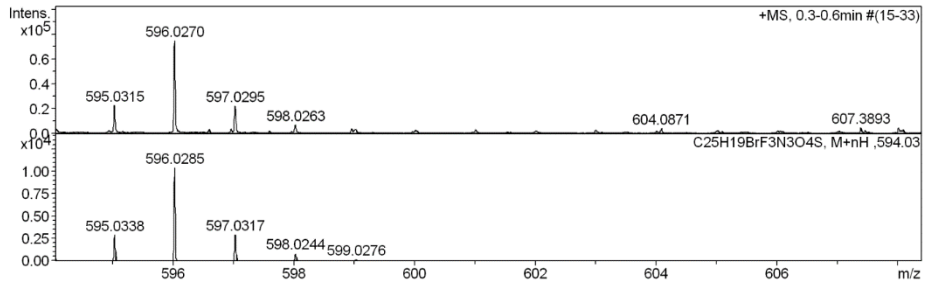
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810L\E1P8.d	Acquisition Date	8/10/2017 8:02:45 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	E1P8	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J28

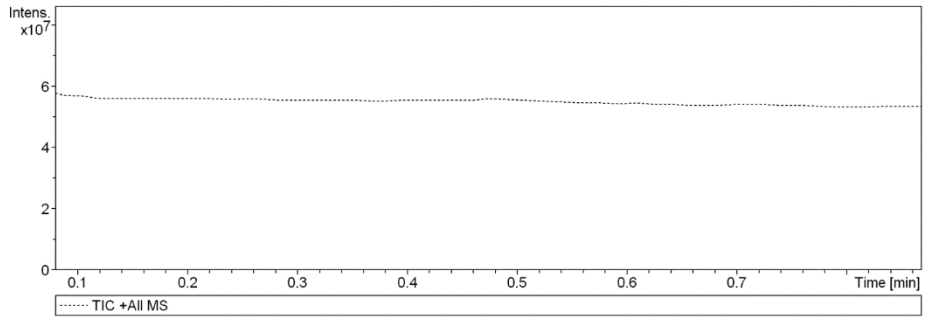
Display Report

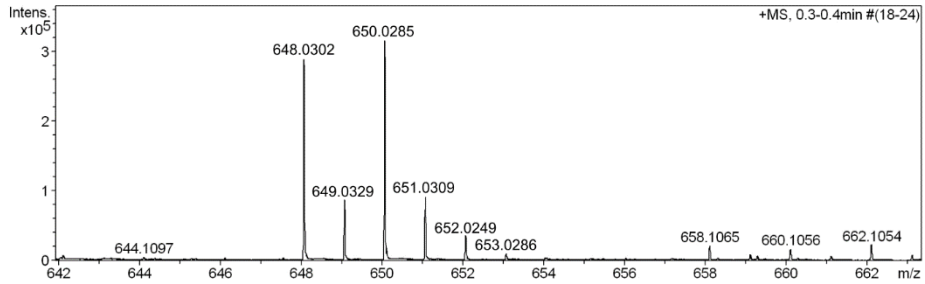
Analysis Info

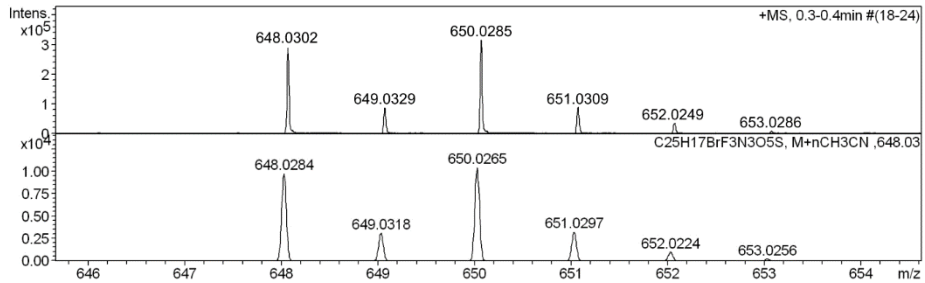
Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\e2p8.d	Acquisition Date	8/10/2017 4:58:53 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e2p8	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source







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HRMS of target compound J29

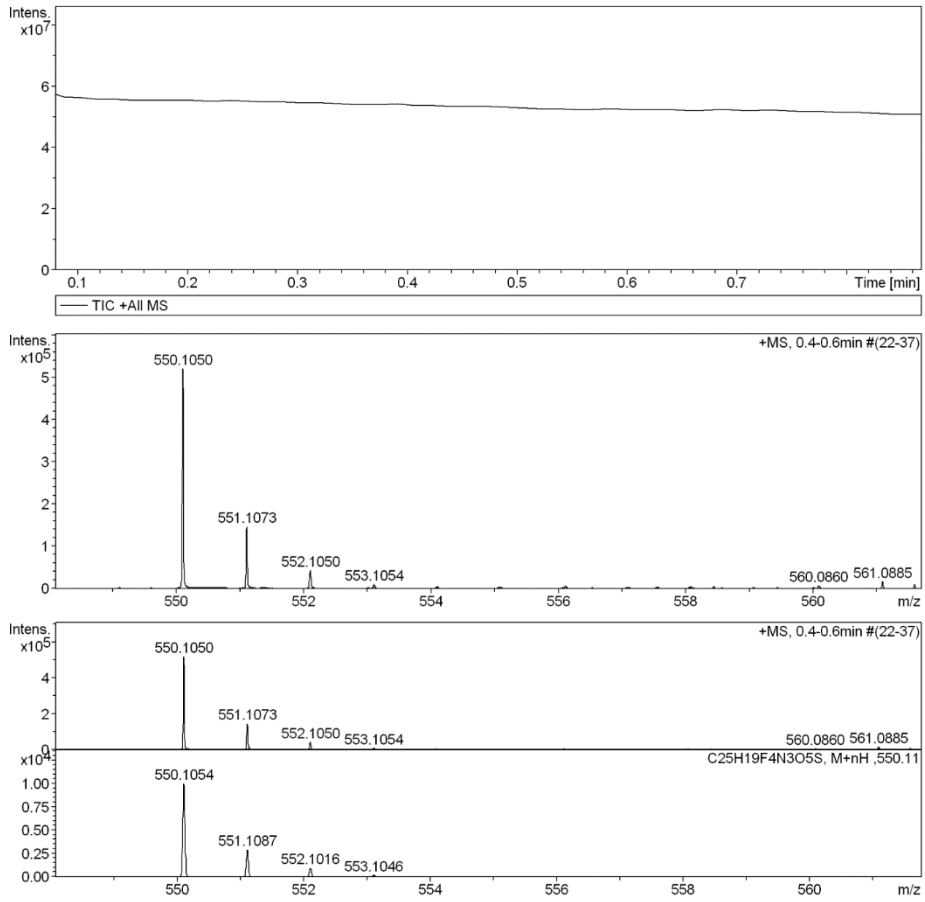
Display Report

Analysis Info

Analysis Name	D:\Data\Shao Guang\SCAU J\20170810\F2P8.d	Acquisition Date	8/10/2017 6:19:03 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	F2P8	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J30

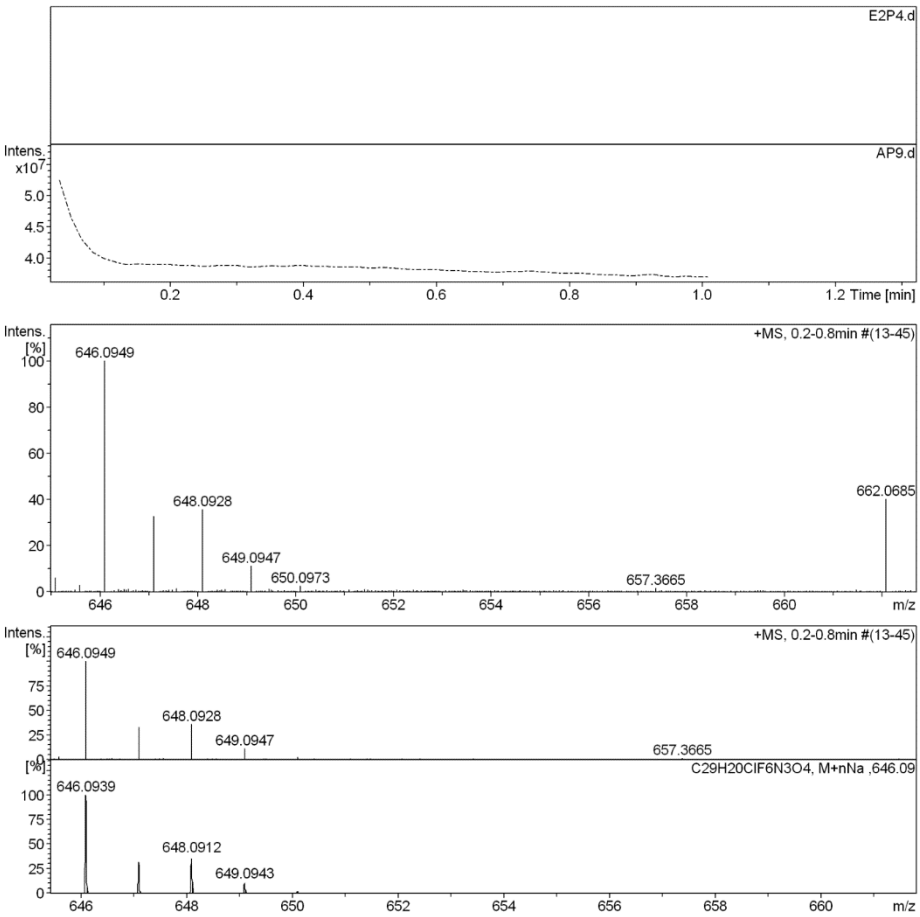
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\AP9.d	Acquisition Date	4/5/2018 4:10:08 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	AP9	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J31

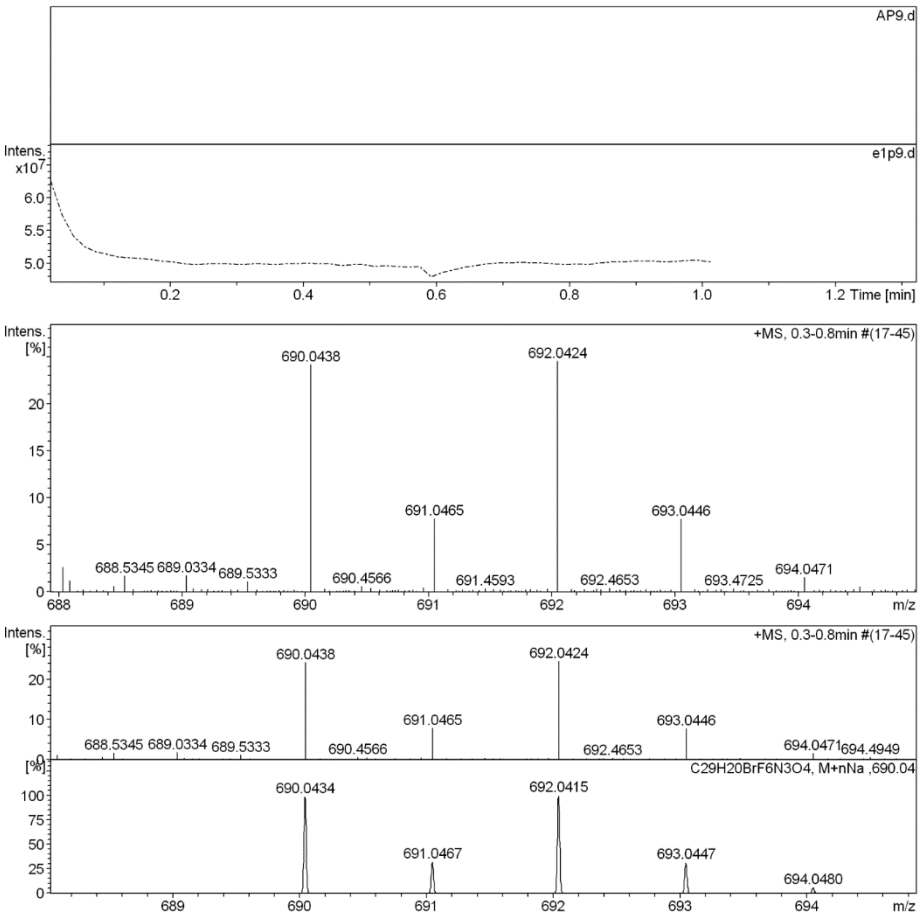
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\e1p9.d	Acquisition Date	4/5/2018 3:33:35 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e1p9	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J32

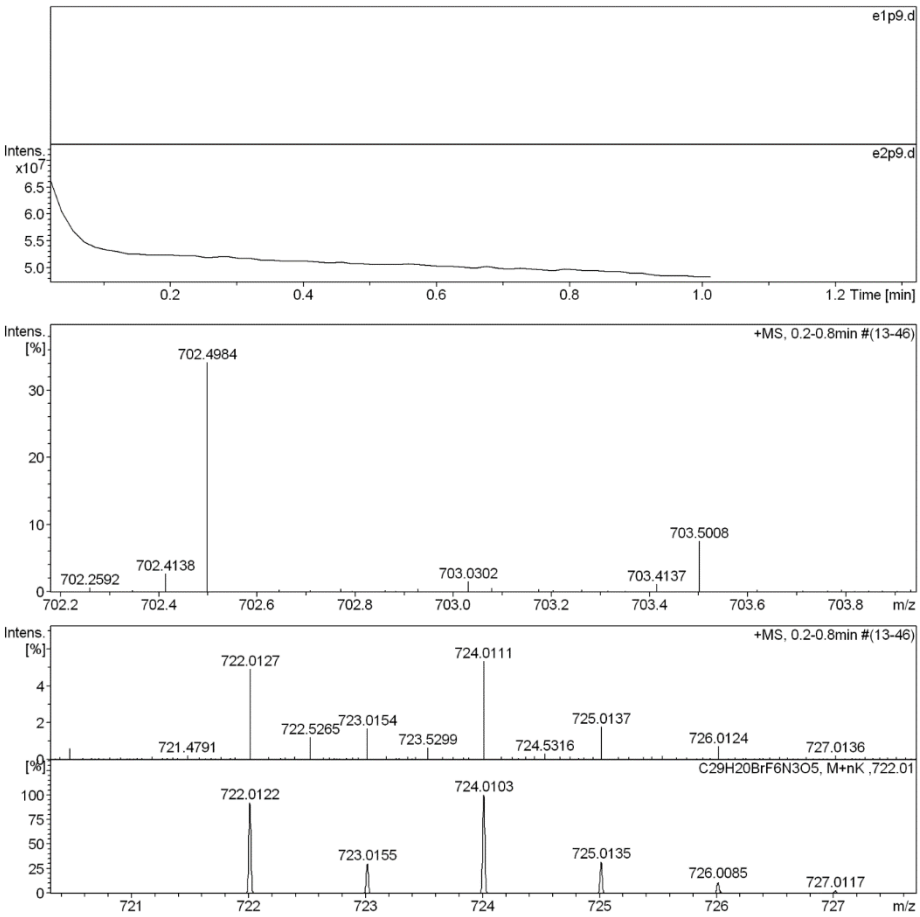
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\e2p9.d	Acquisition Date	4/5/2018 3:56:15 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	e2p9	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J33

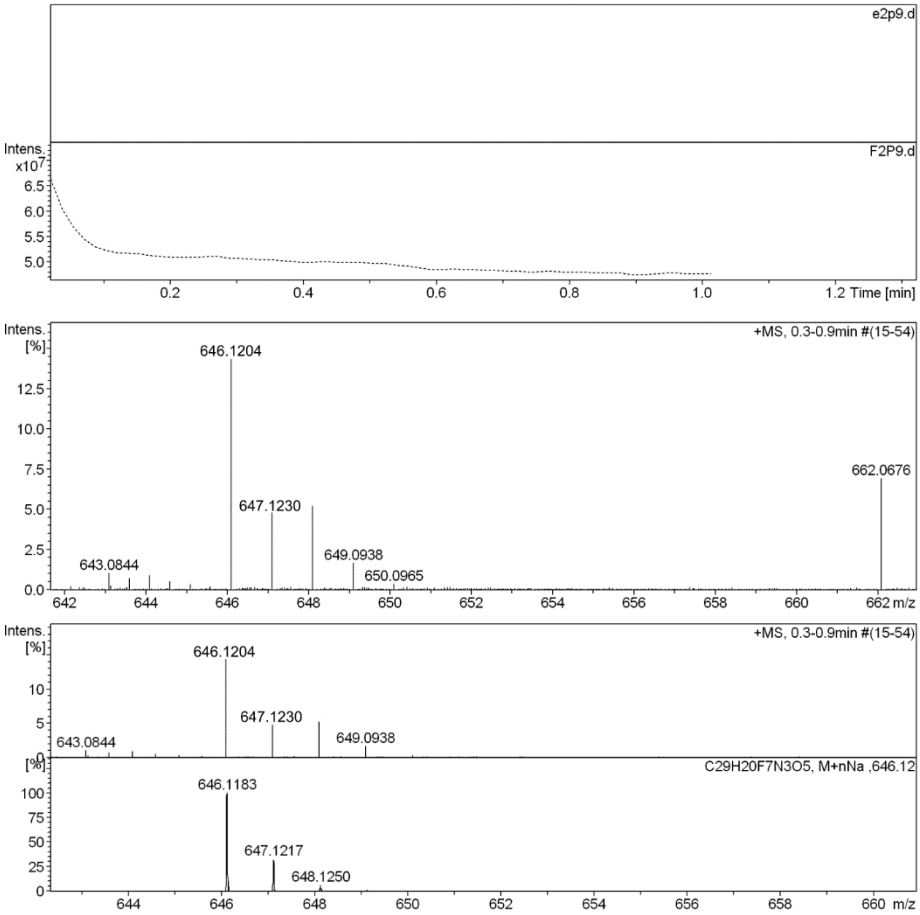
Display Report

Analysis Info

Analysis Name	D:\Data\shaoguang\F2P9.d	Acquisition Date	4/5/2018 4:06:52 PM
Method	tune_mid_ESI+.m	Operator	BDAL@DE
Sample Name	F2P9	Instrument	maXis 4G 21242
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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HRMS of target compound J34