

Synthesis and Antiproliferation Activities Evaluation of Multi-substituted Isatin Derivatives

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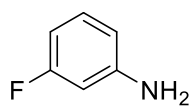
[†] These authors contributed equally to this work.

* Corresponding author.

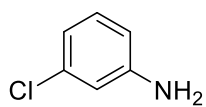
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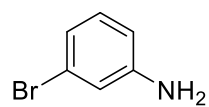
1. Structure of the Intermediates



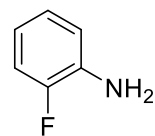
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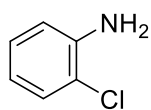
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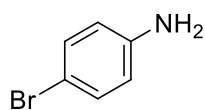
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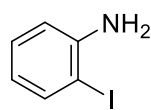
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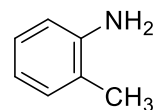
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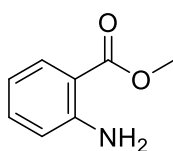
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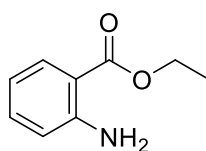
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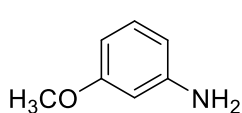
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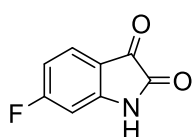
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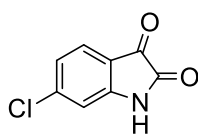
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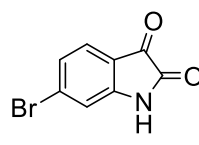
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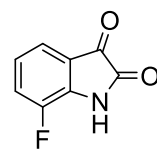
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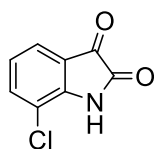
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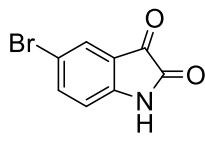
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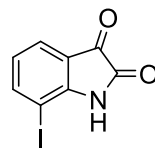
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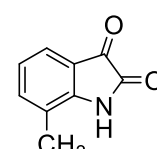
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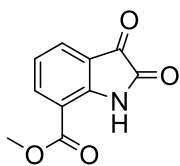
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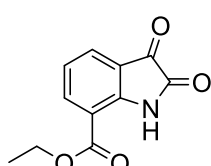
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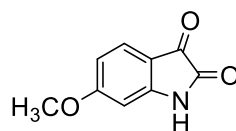
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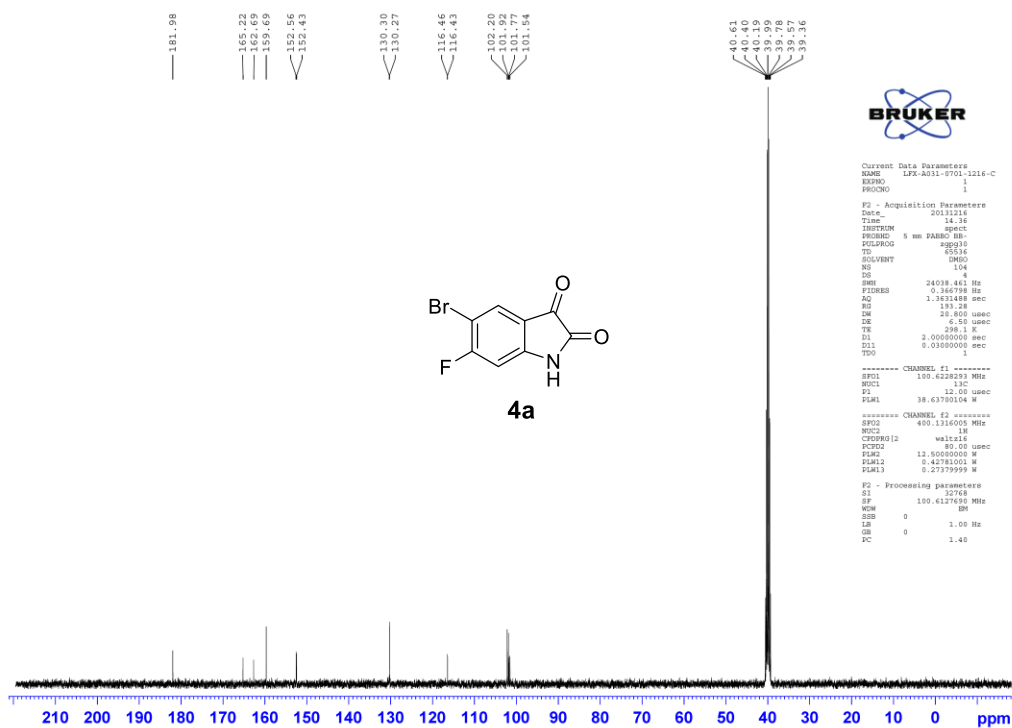
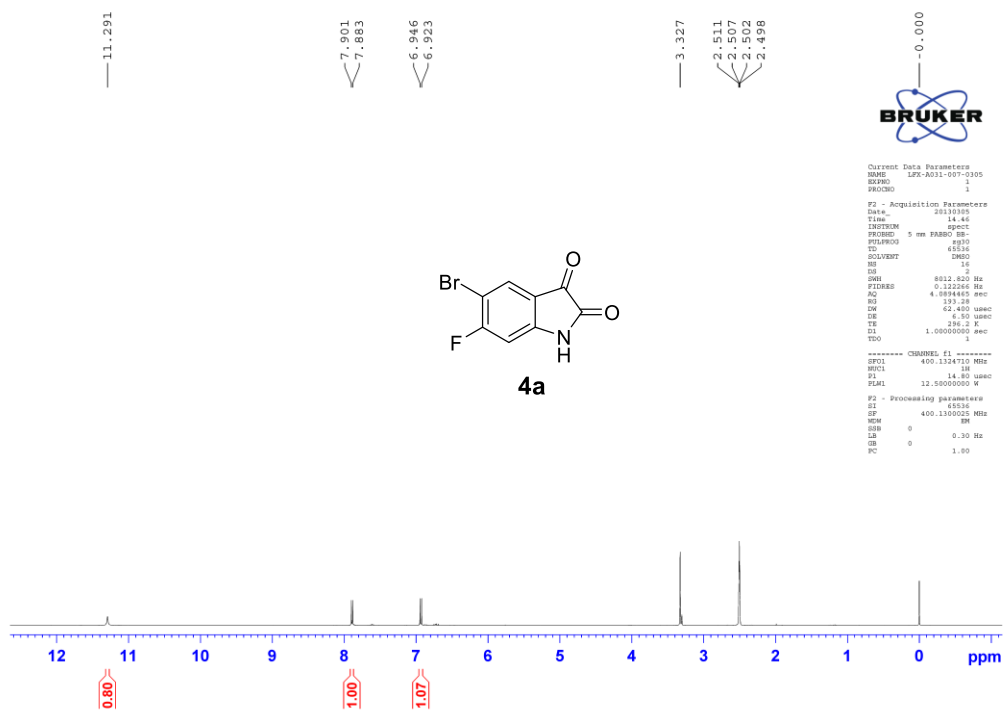
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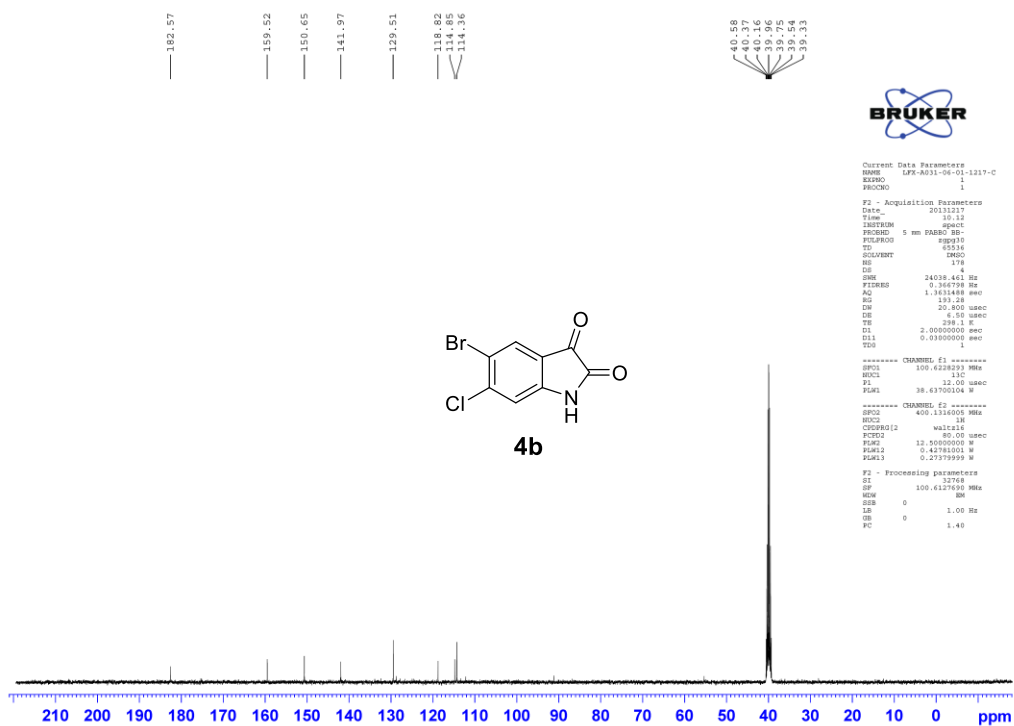
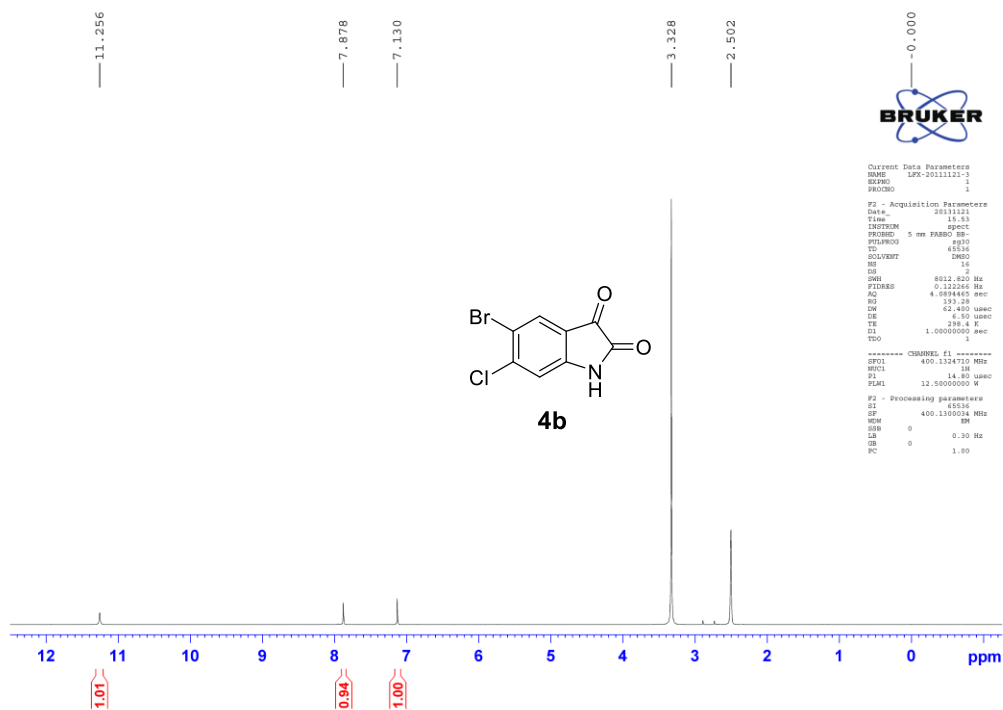


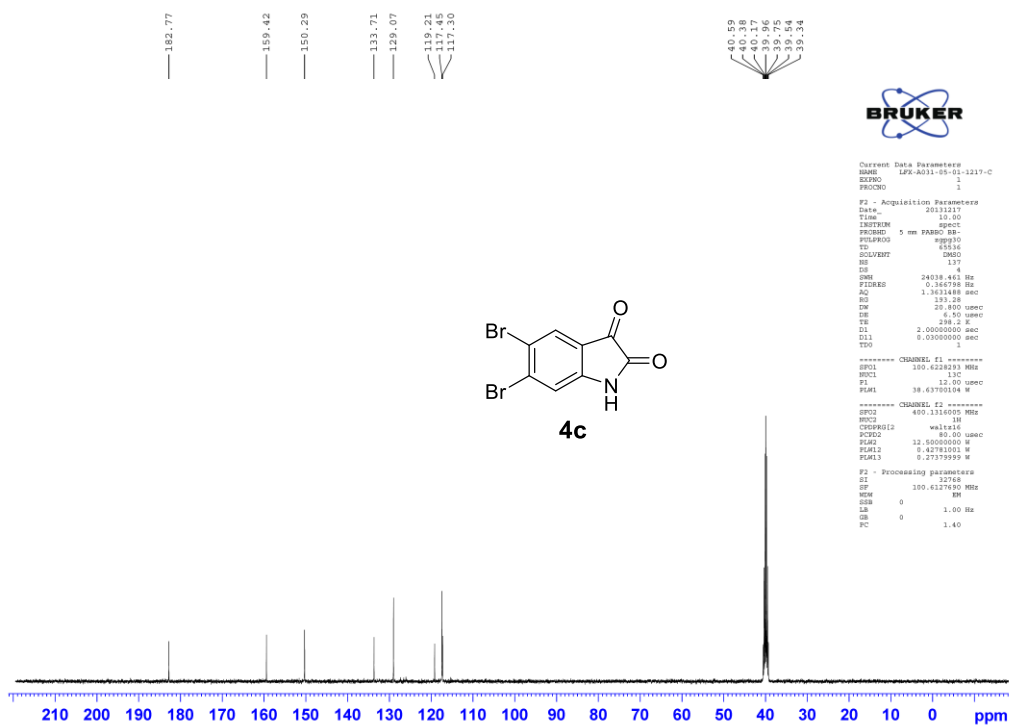
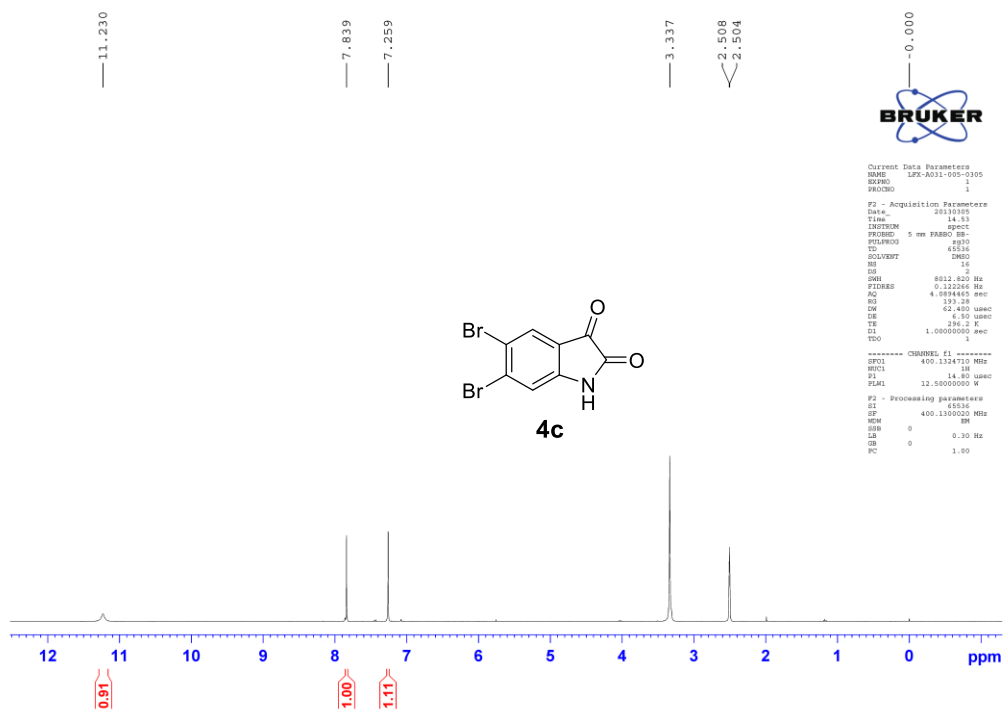
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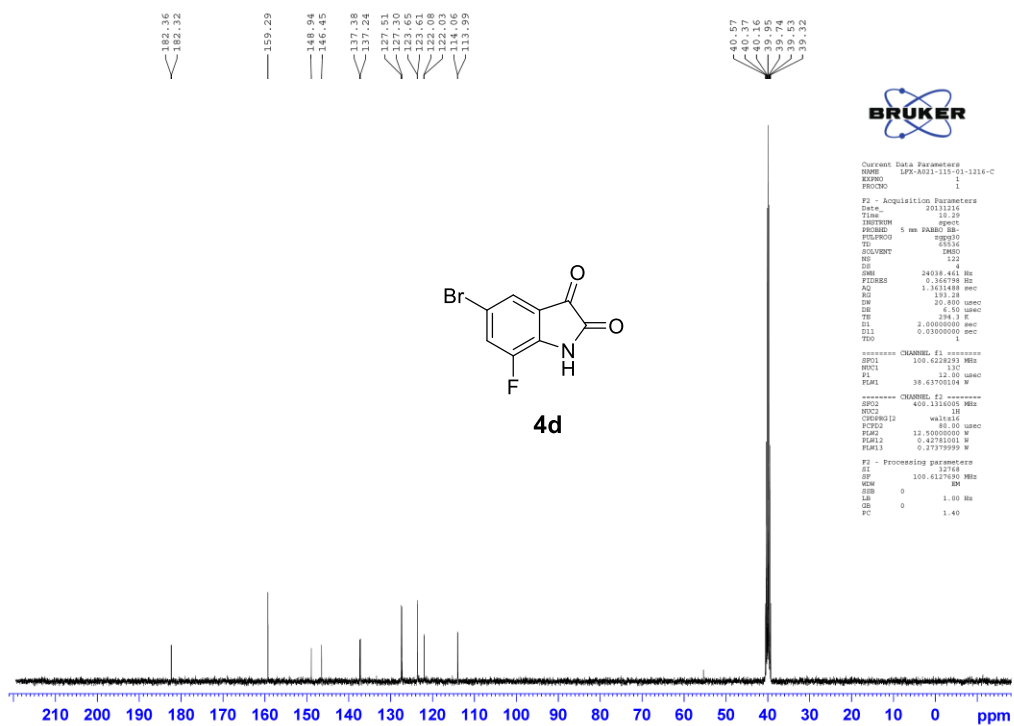
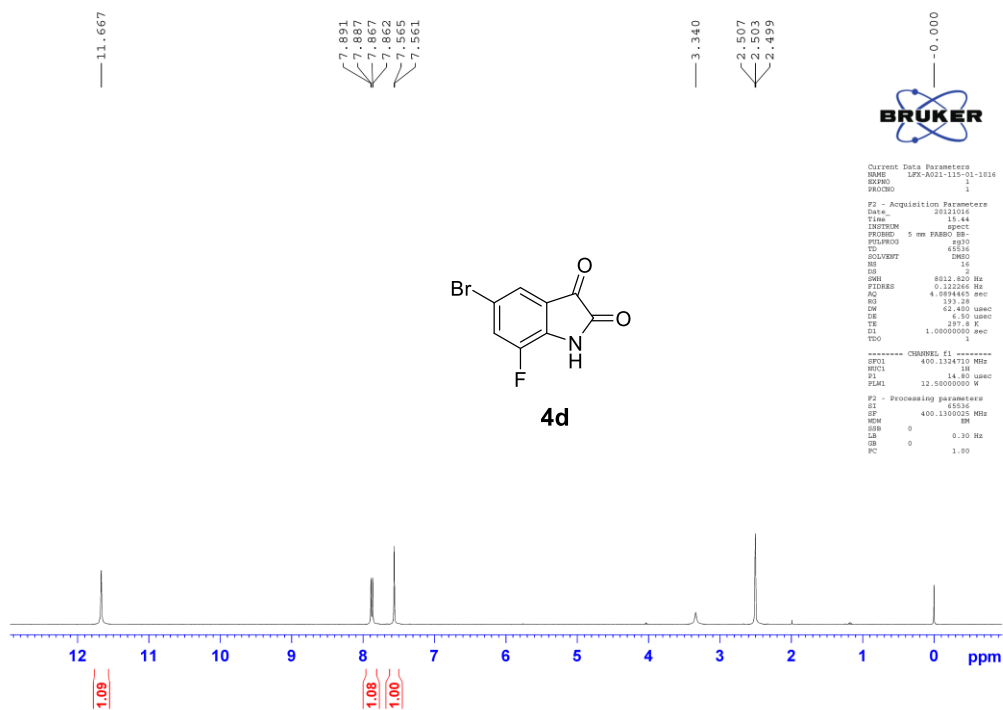
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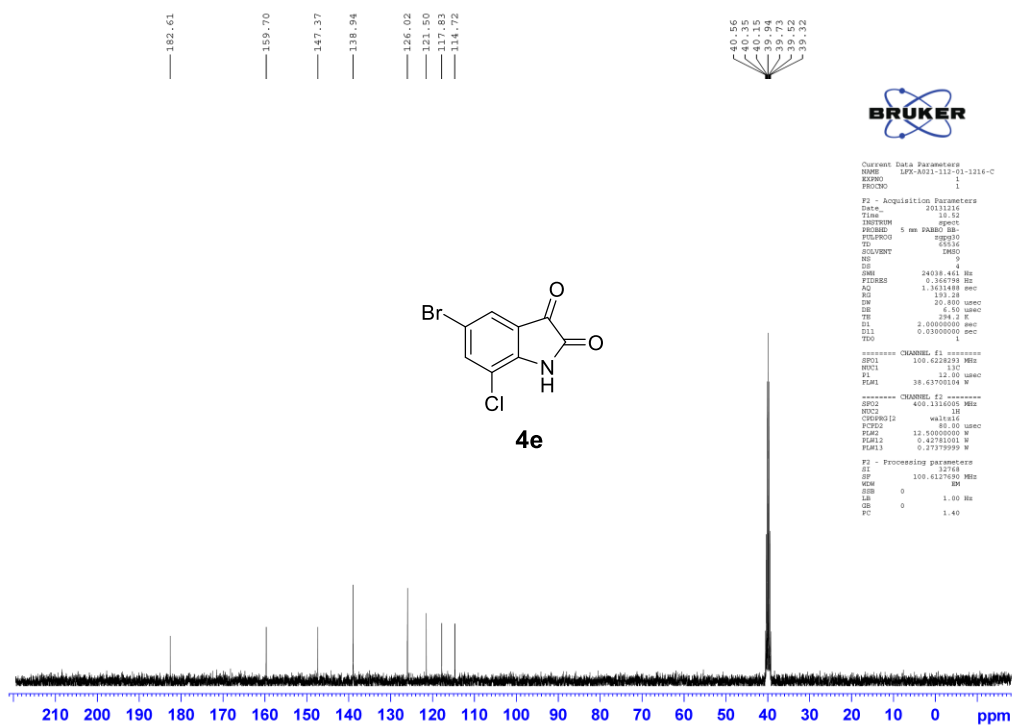
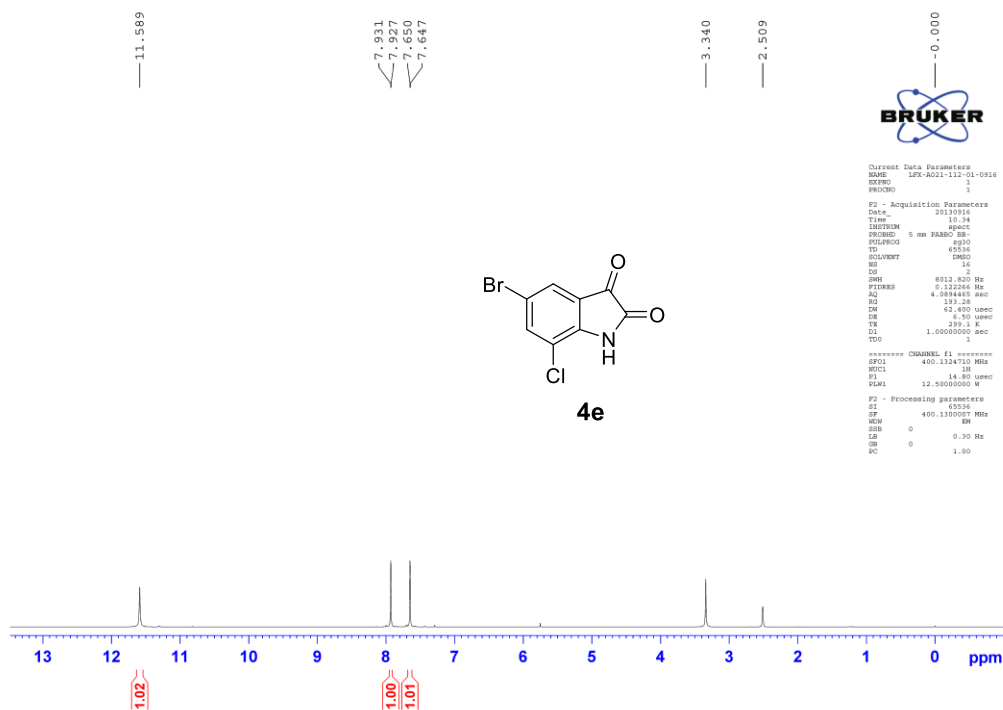
Spectra data are shown from the next page.

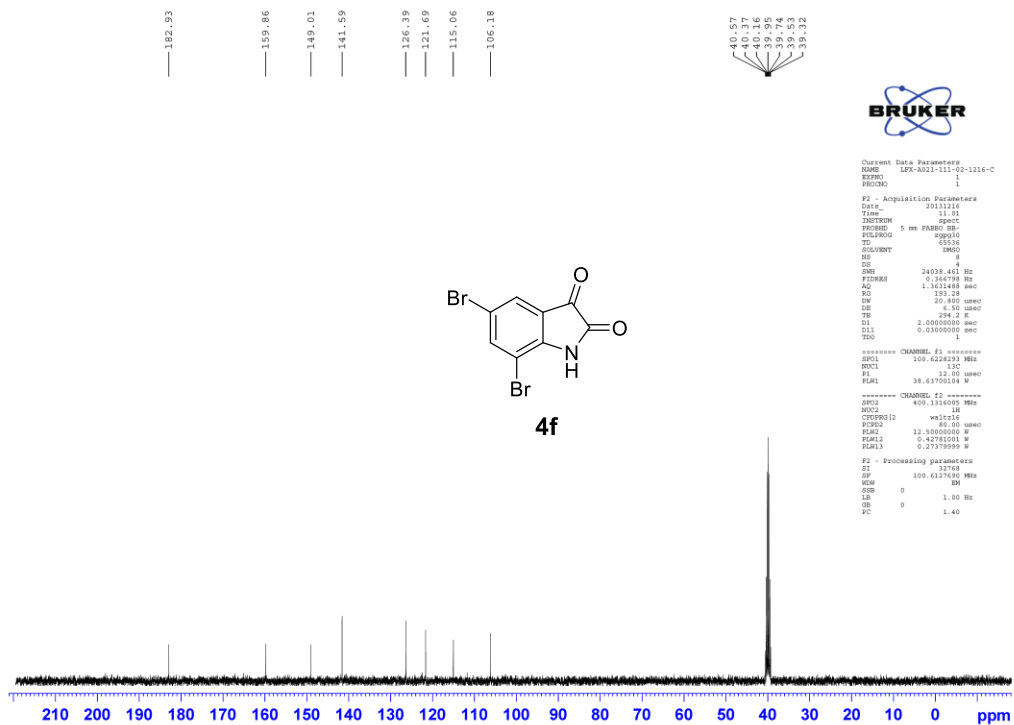
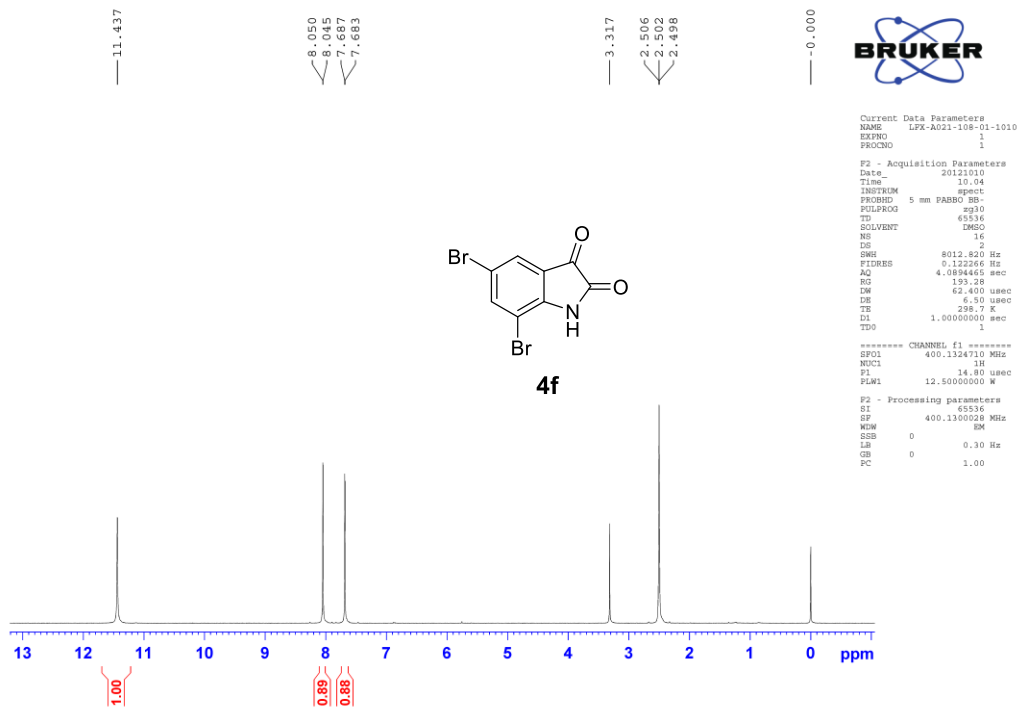


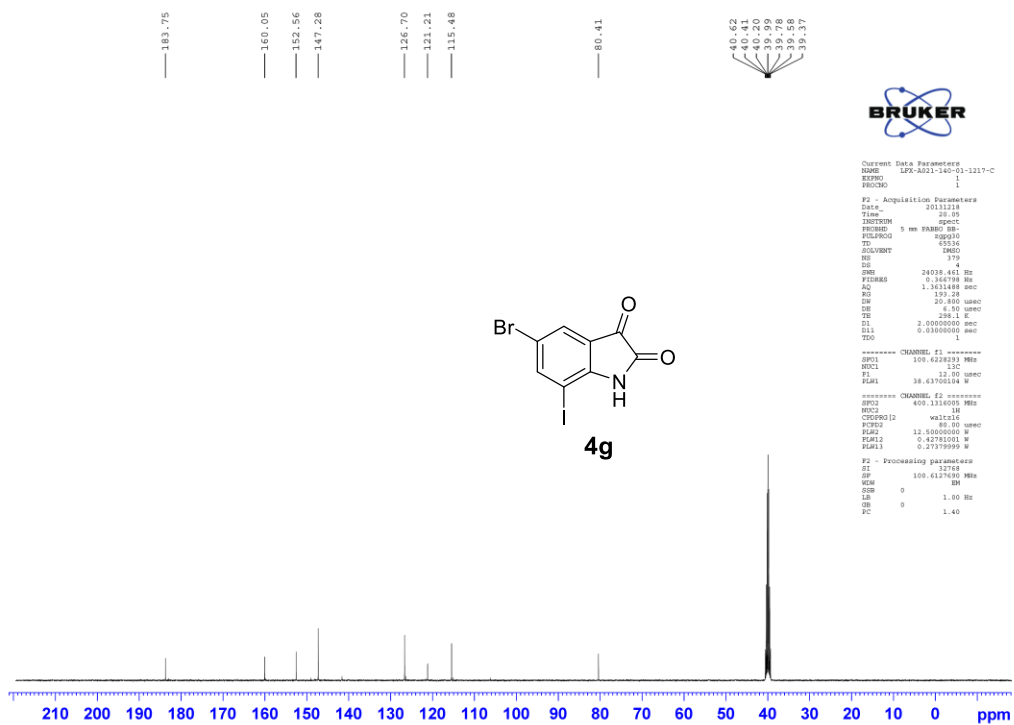
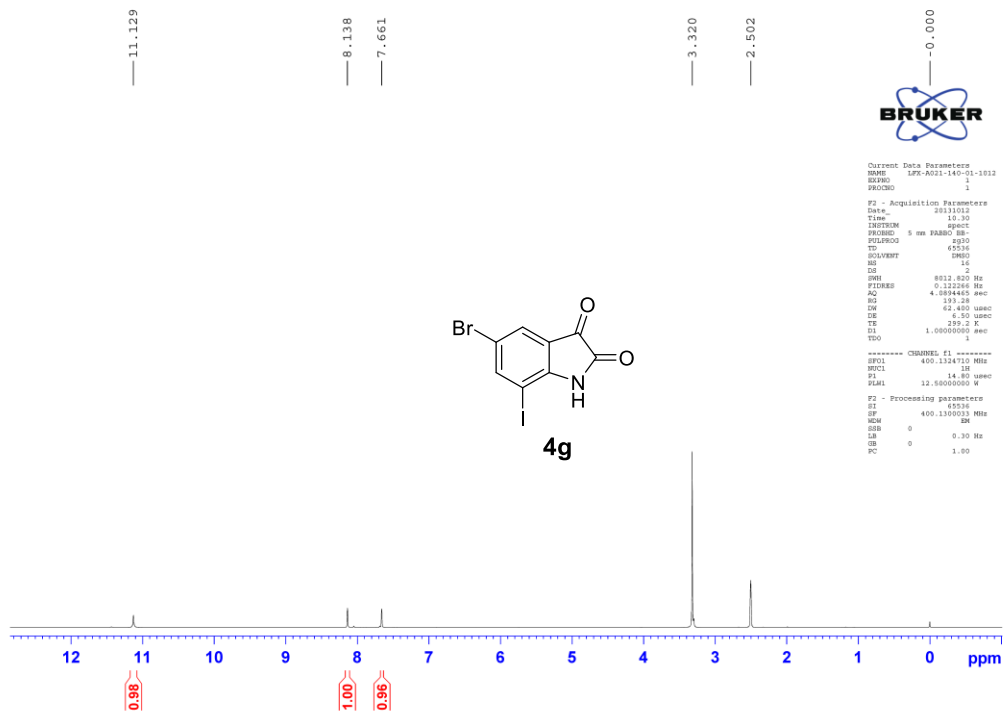


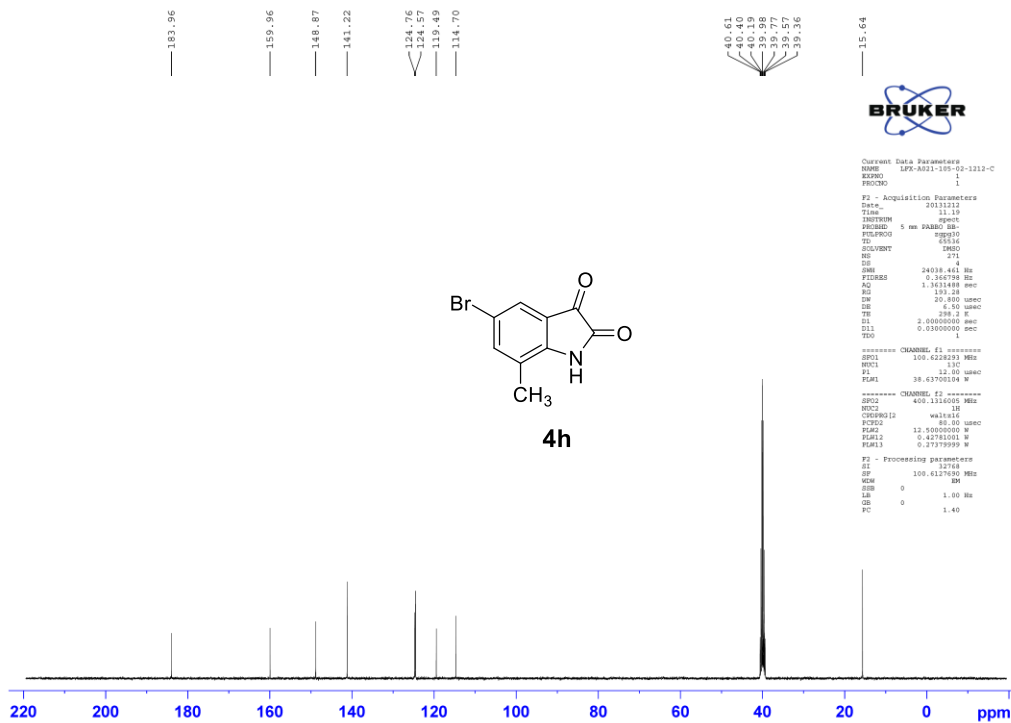
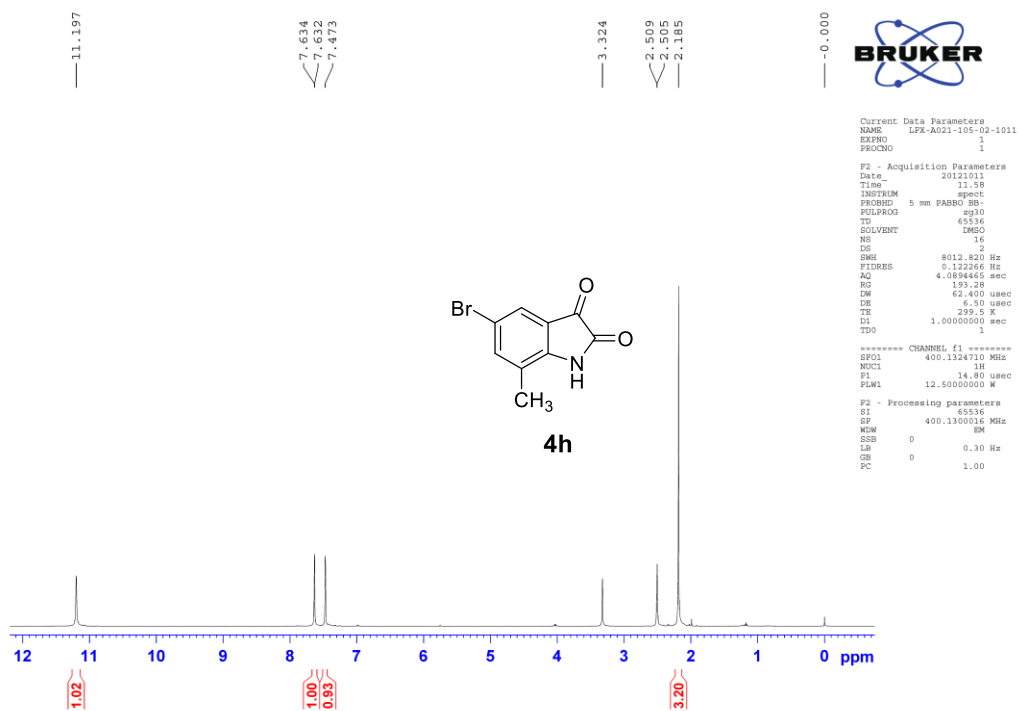


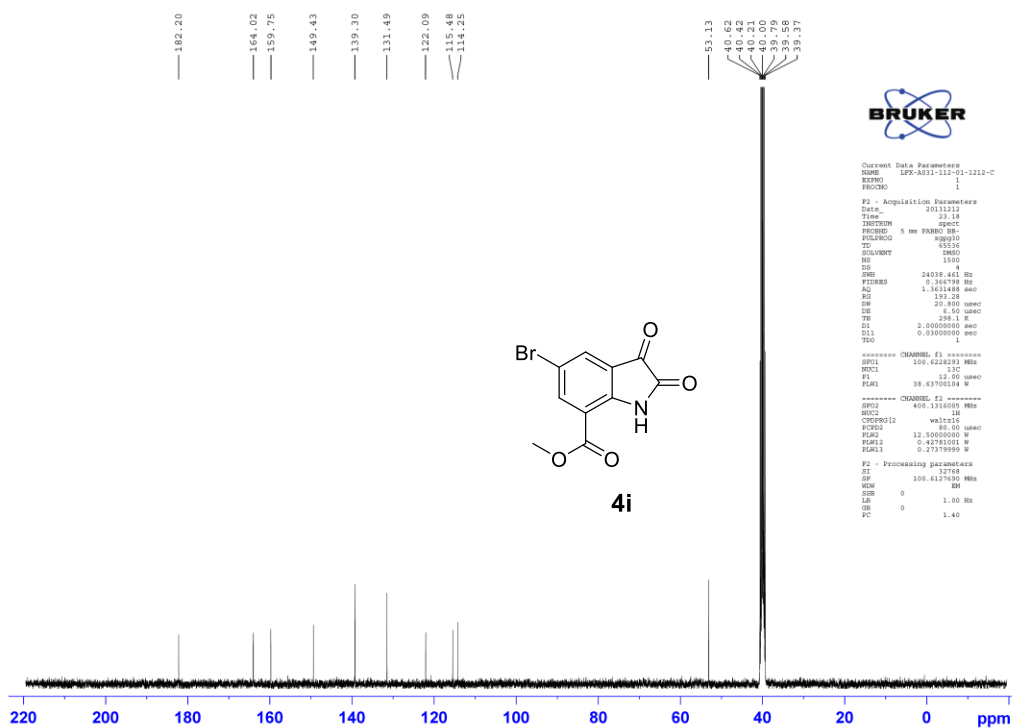
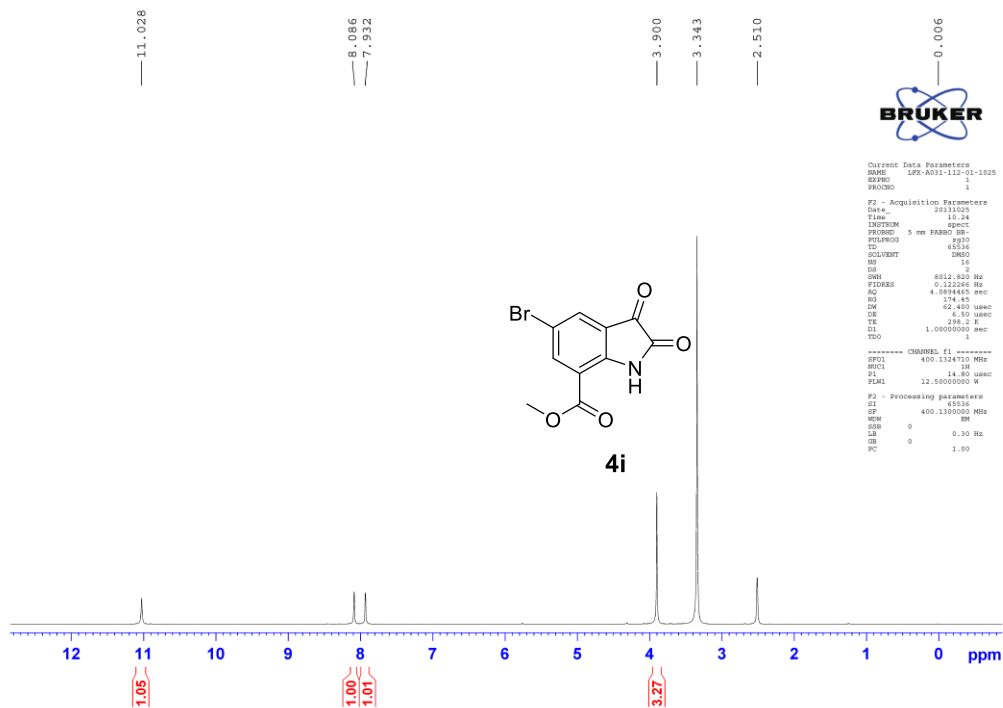


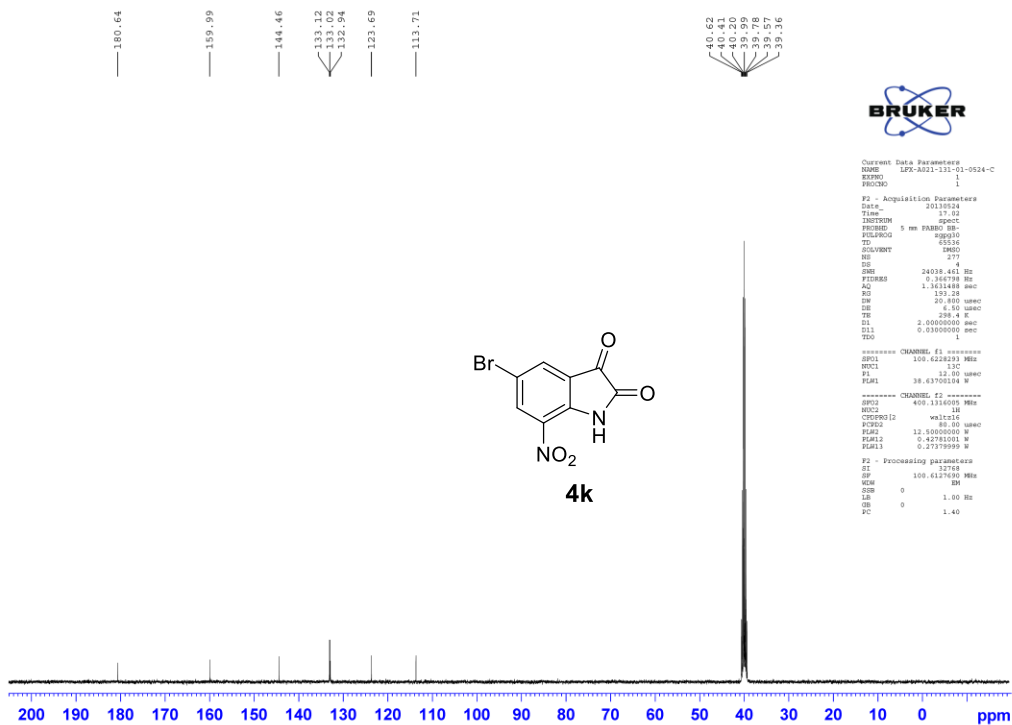
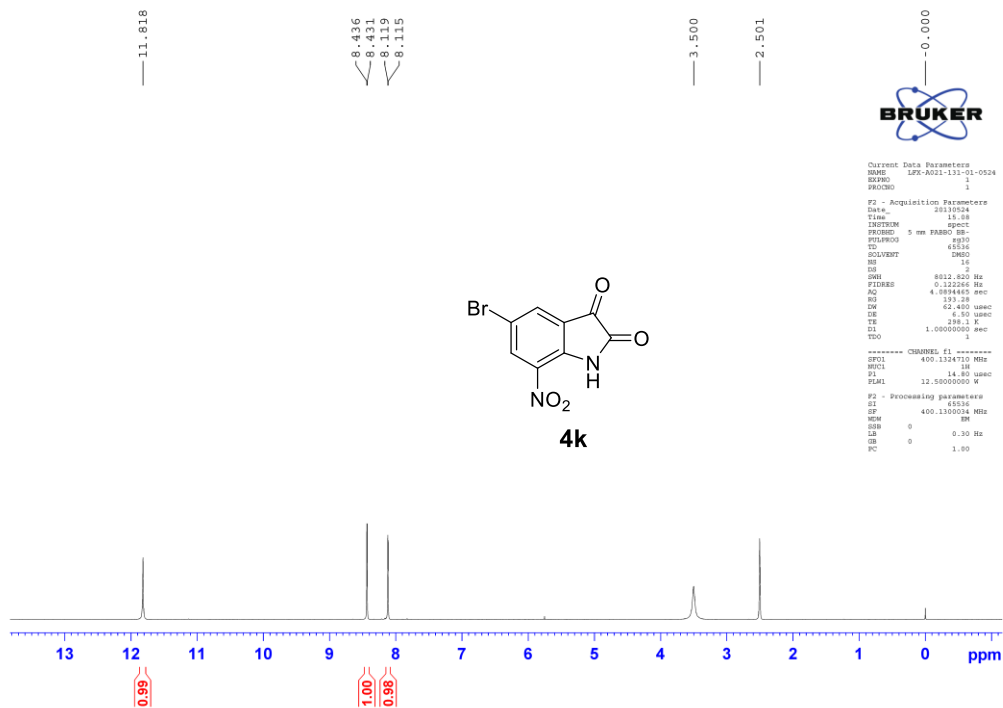


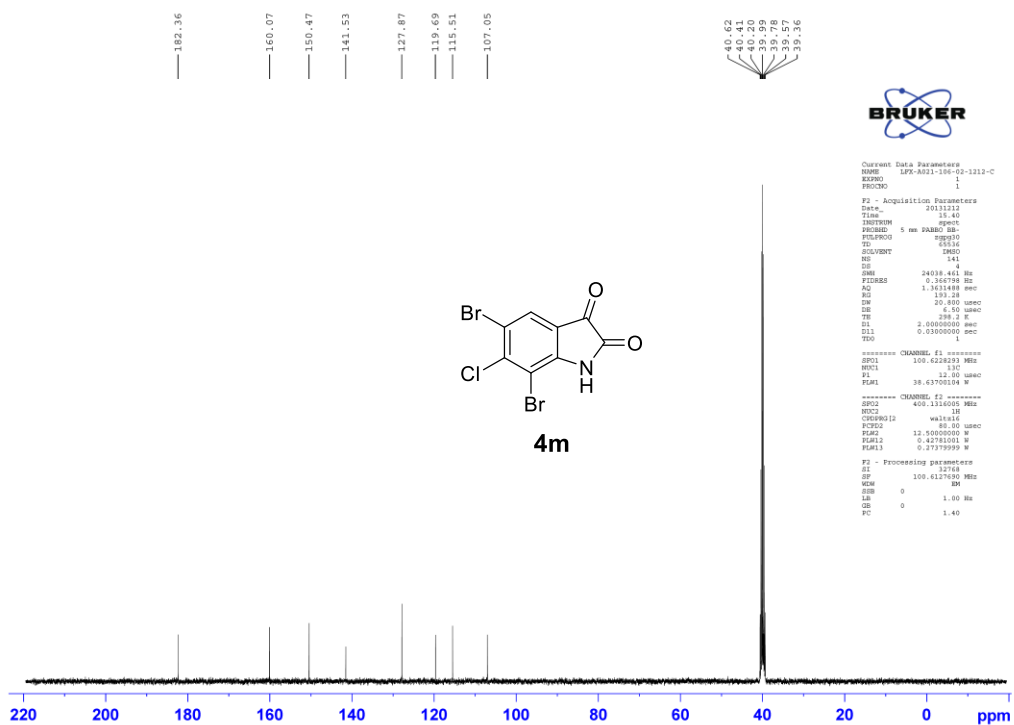
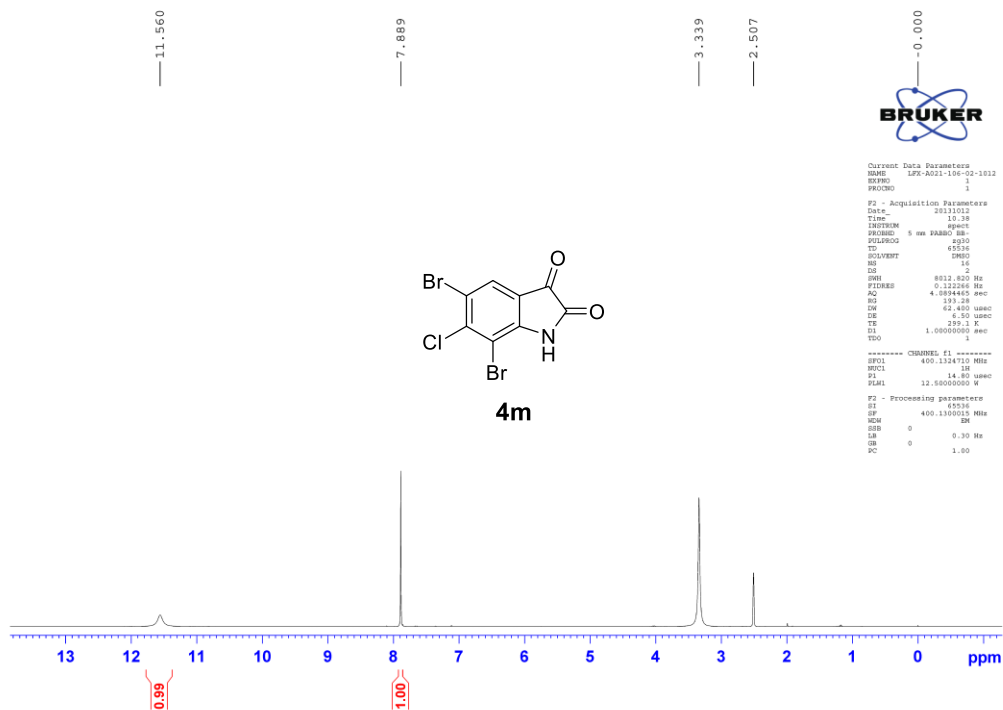


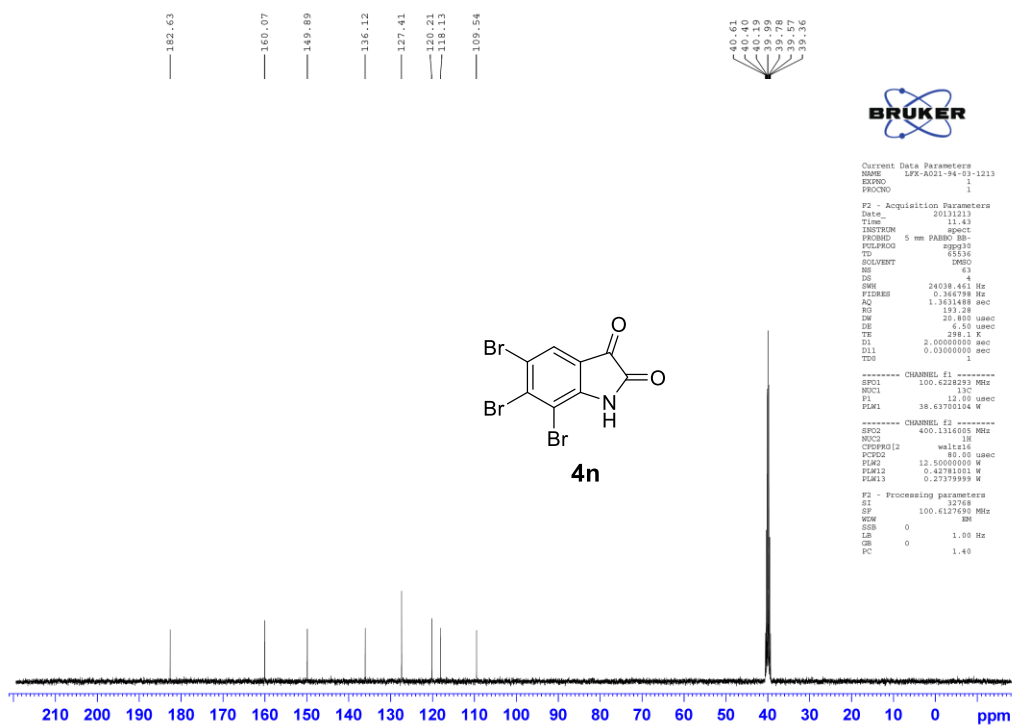
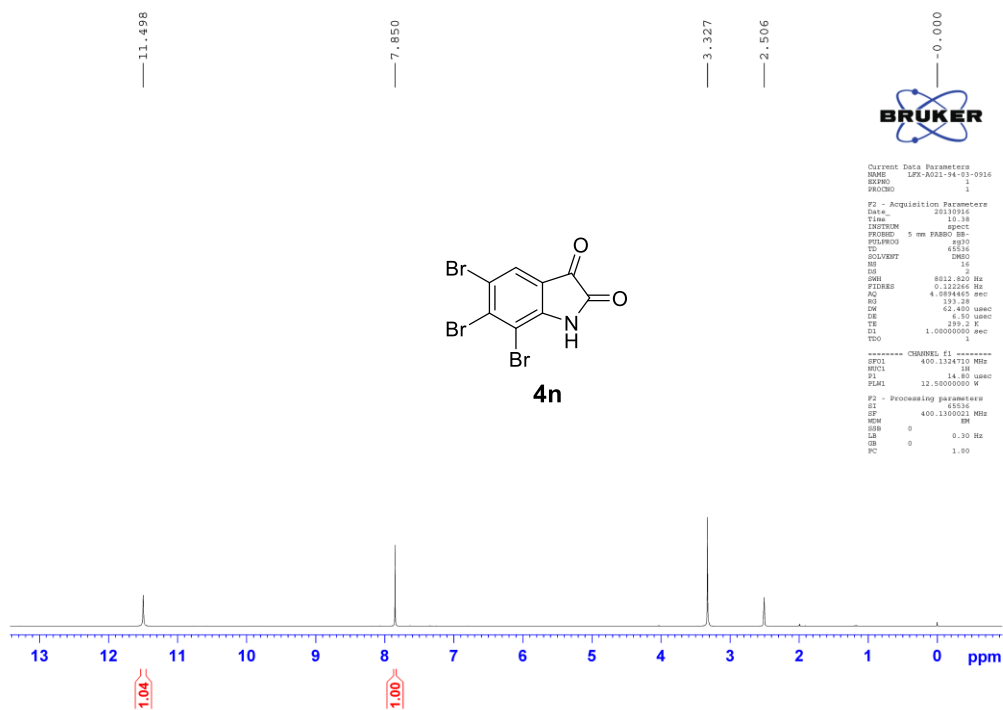


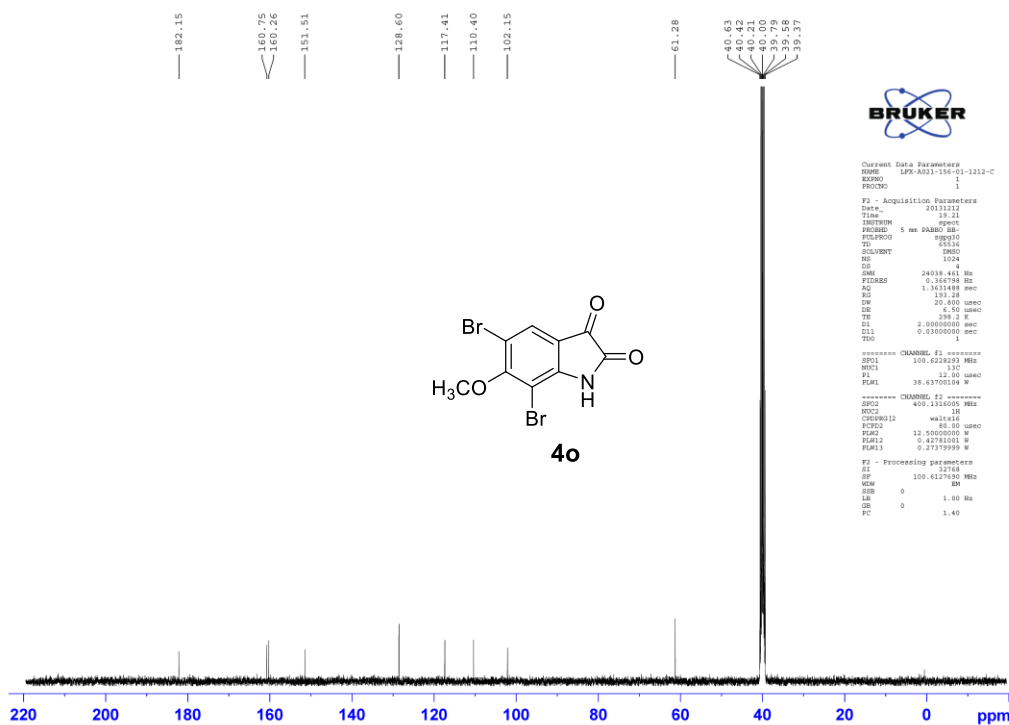
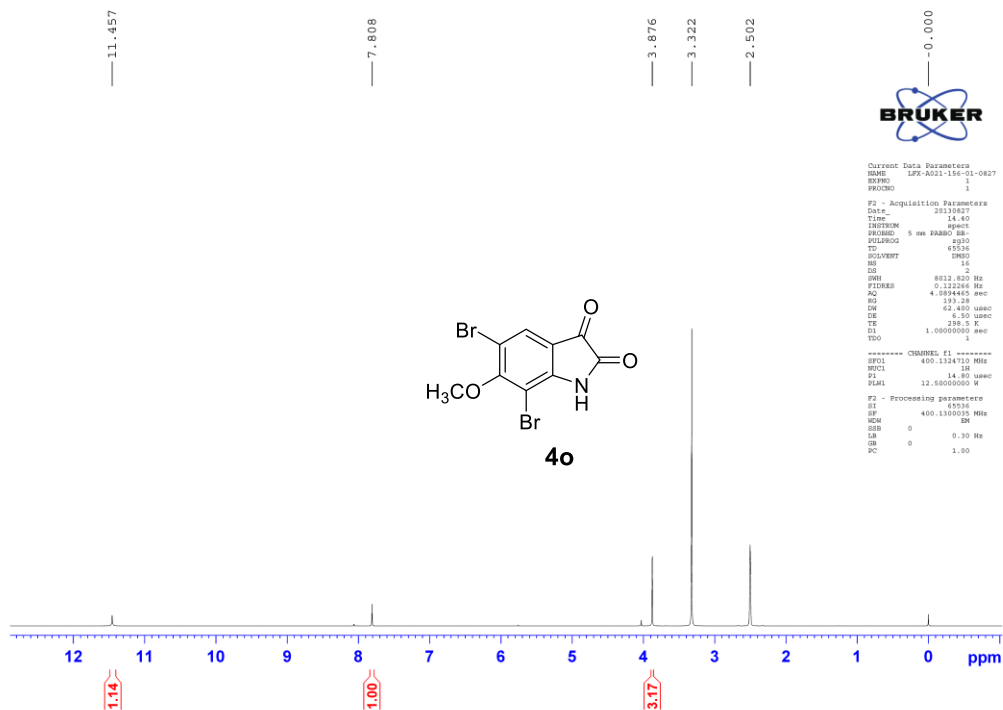












3. HR-MS Spectrum Data of compound 4l,4m,4o.

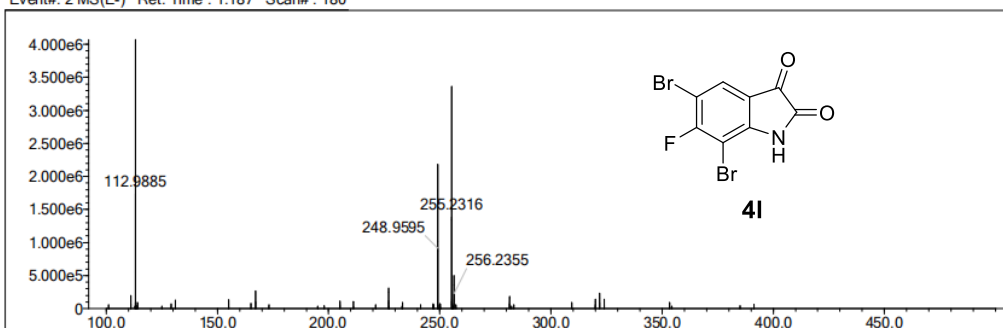
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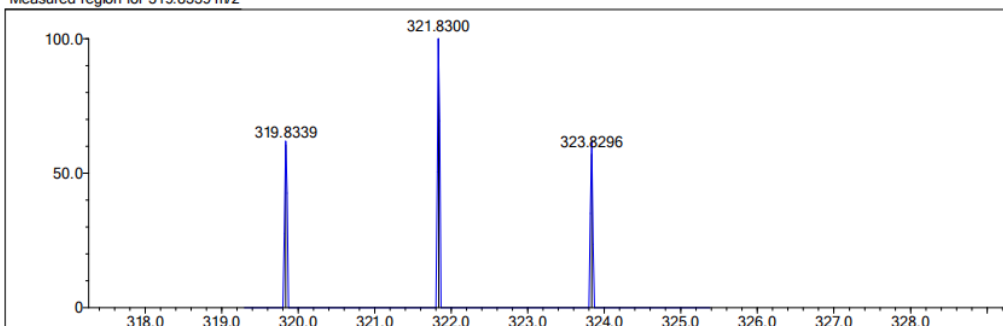
	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
2H	1	0	0	F	1	0	0	H
C	4	0	8	Na	1	0	0	HCOO
N	3	0	1	Si	4	0	0	CH3COO
O	2	0	2	P	3	0	0	Cl

Error Margin (ppm): 9999	DBE Range: 0.0 - 50.0	Electron Ions: both
HC Ratio: unlimited	Apply N Rule: no	Use MSn Info: yes
Max Isotopes: all	Isotope RI (%): 1.00	Isotope Res: 10000
MSn Iso RI (%): 75.00	MSn Logic Mode: AND	Max Results: 100

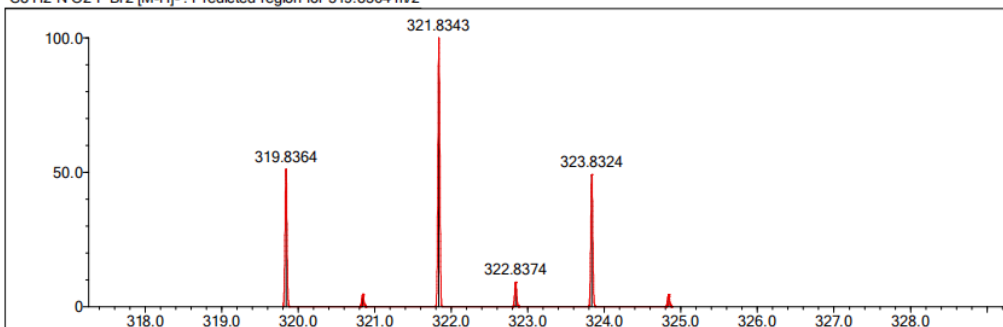
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Measured region for 319.8339 m/z



C8 H2 N O2 F Br2 [M-H]- : Predicted region for 319.8364 m/z



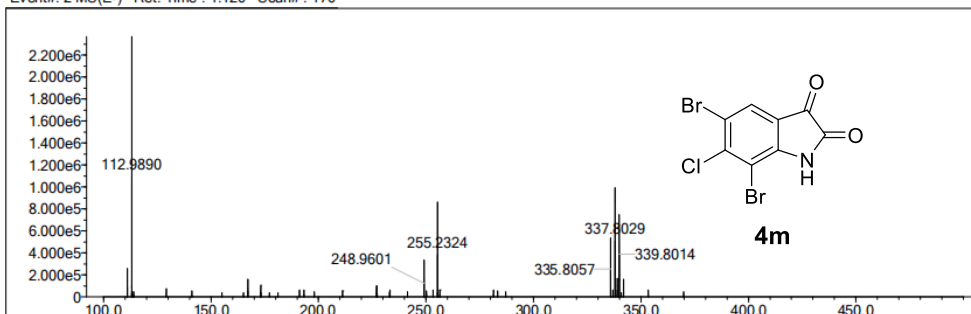
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	28.98	C8 H2 N O2 F Br2	[M-H]-	319.8339	319.8364	-2.5	-7.82	46.89	7.0

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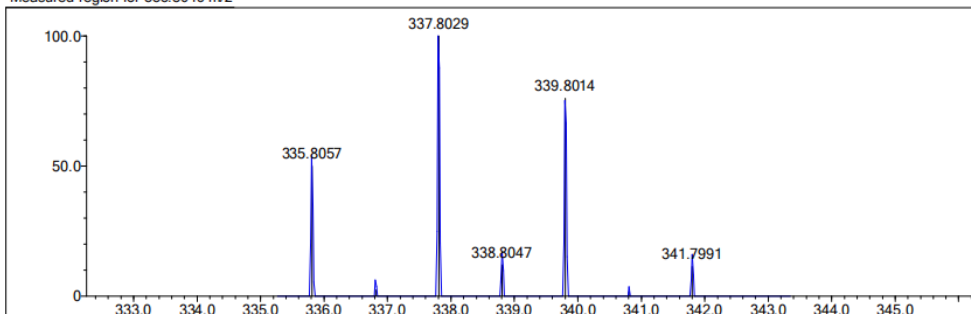
	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
2H	1	0	0	F	1	0	0	H
C	4	0	9	Na	1	0	0	HCOO
N	3	0	1	Si	4	0	0	CH3COO
O	2	0	3	P	3	0	0	Cl
				Cl	1	0	0	
				Se	2	0	0	
				Br	1	0	2	
				I	3	0	0	
				Pt	2	0	0	
				Ni	2	0	0	

Error Margin (ppm): 9999 DBE Range: 0.0 - 50.0
 HC Ratio: unlimited Apply N Rule: no Electron Ions: both
 Max Isotopes: all Isotope RI (%): 1.00 Use MSn Info: yes
 MSn Iso RI (%): 75.00 MSn Logic Mode: AND Isotope Res: 10000
 Max Results: 100

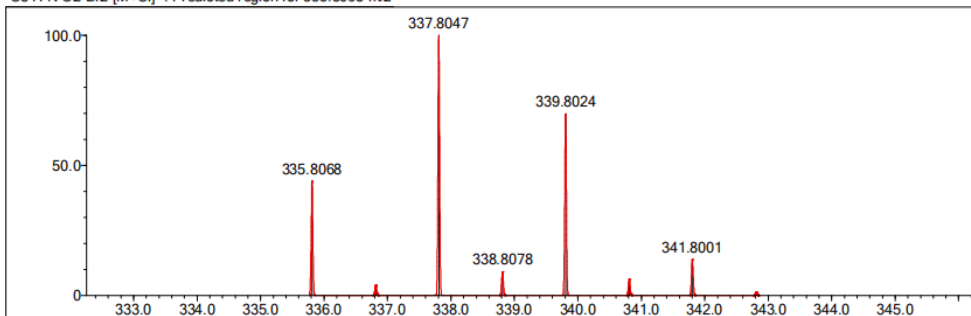
Event#: 2 MS(E-) Ret. Time : 1.120 Scan#: 170



Measured region for 335.8049 m/z



C8 H N O2 Br2 [M+Cl]- : Predicted region for 335.8068 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	70.53	C8 H N O2 Br2	[M+Cl]-	335.8049	335.8068	-1.9	-5.66	84.57	8.0

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	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
2H	1	0	0	F	1	0	0	H
C	4	0	9	Na	1	0	0	HCOO
N	3	0	1	Si	4	0	0	CH3COO
O	2	0	3	P	3	0	0	Cl

Error Margin (ppm): 9999

DBE Range: 0.0 - 50.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: no

Use MSn Info: yes

Max Isotopes: all

Isotope RI (%): 1.00

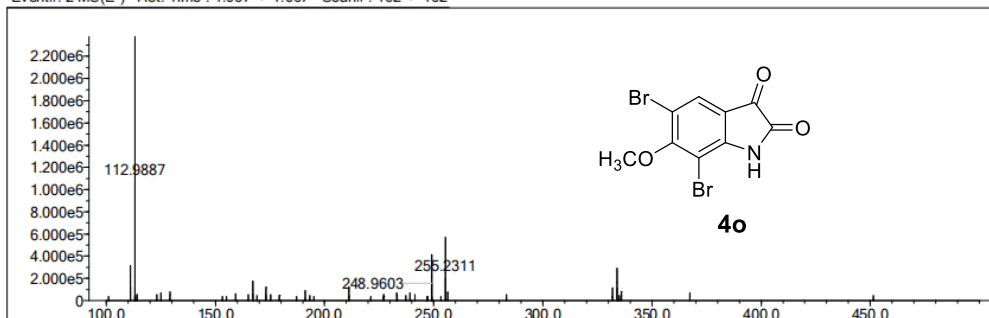
Isotope Res: 10000

MSn Iso RI (%): 75.00

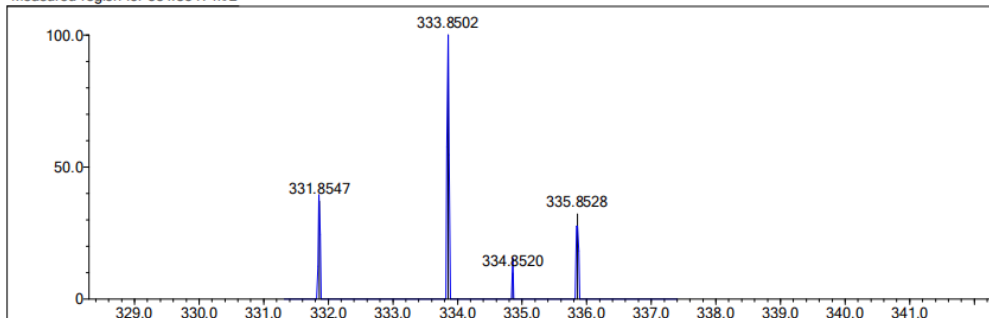
MSn Logic Mode: AND

Max Results: 100

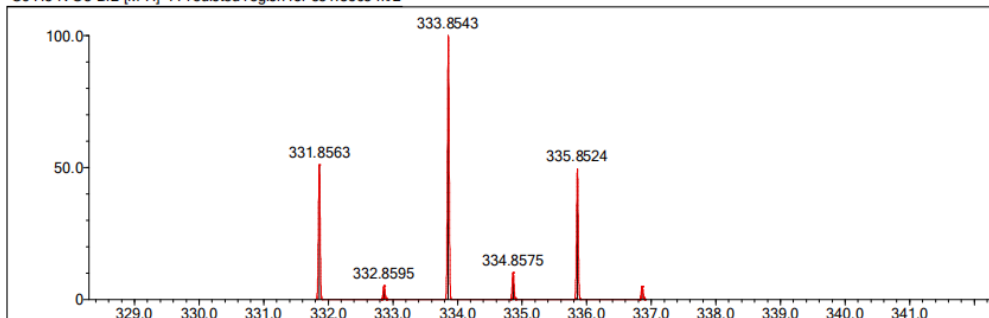
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Measured region for 331.8547 m/z



C9 H5 N O3 Br2 [M-H]- : Predicted region for 331.8563 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	36.64	C9 H5 N O3 Br2	[M-H]-	331.8547	331.8563	-1.6	-4.82	40.51	7.0