

## Supplementary Material

### Unusual reactivity of 2-amino-1H-indole-3-carboxylate esters

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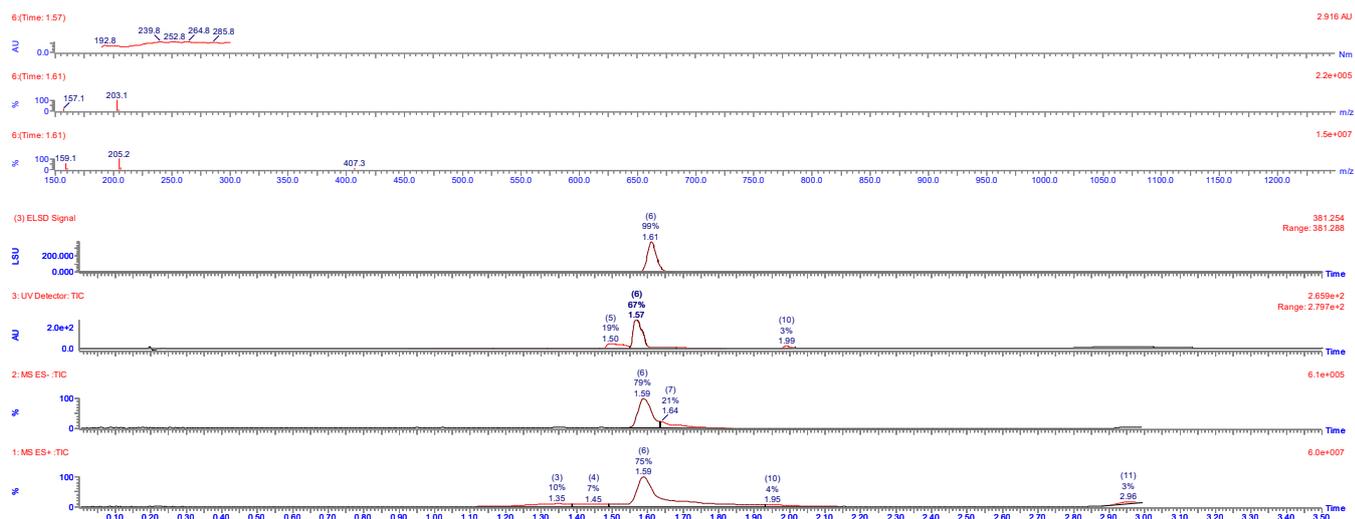
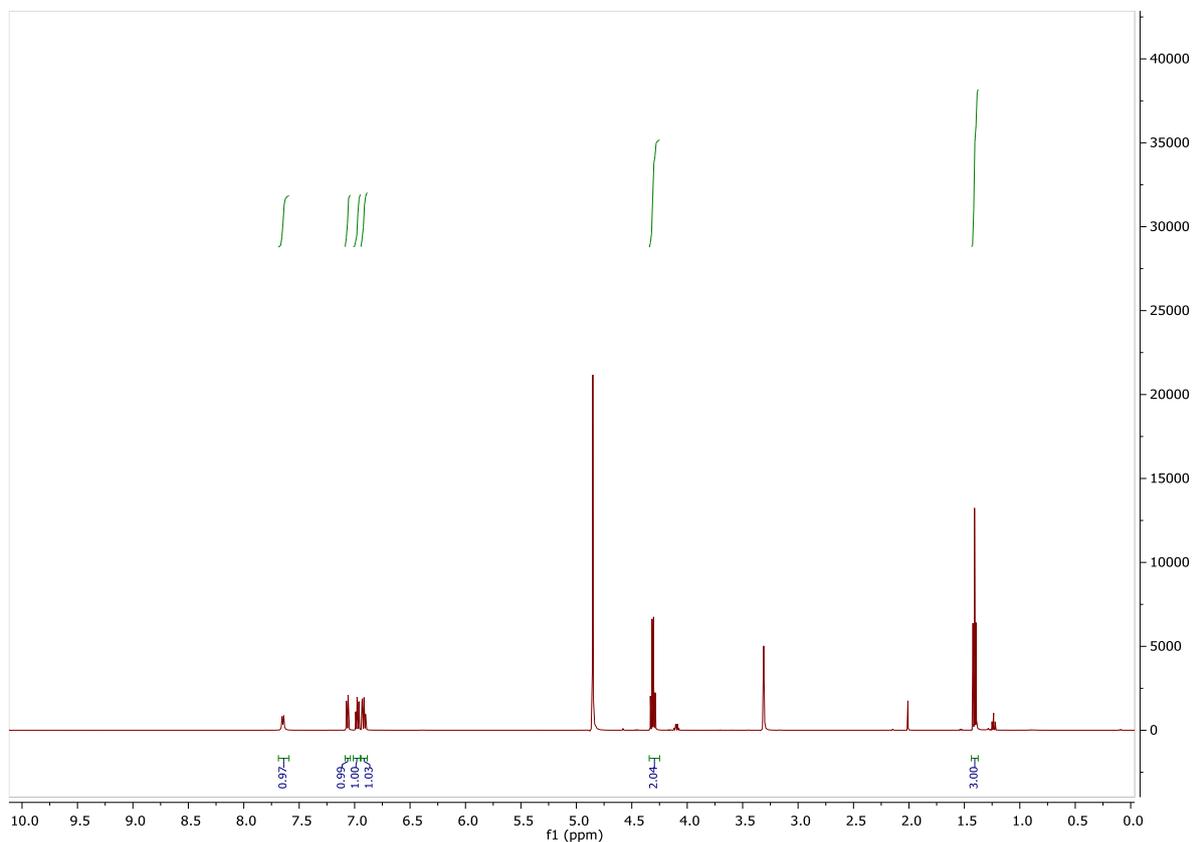
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*Email: [JonesD80@cardiff.ac.uk](mailto:JonesD80@cardiff.ac.uk)*

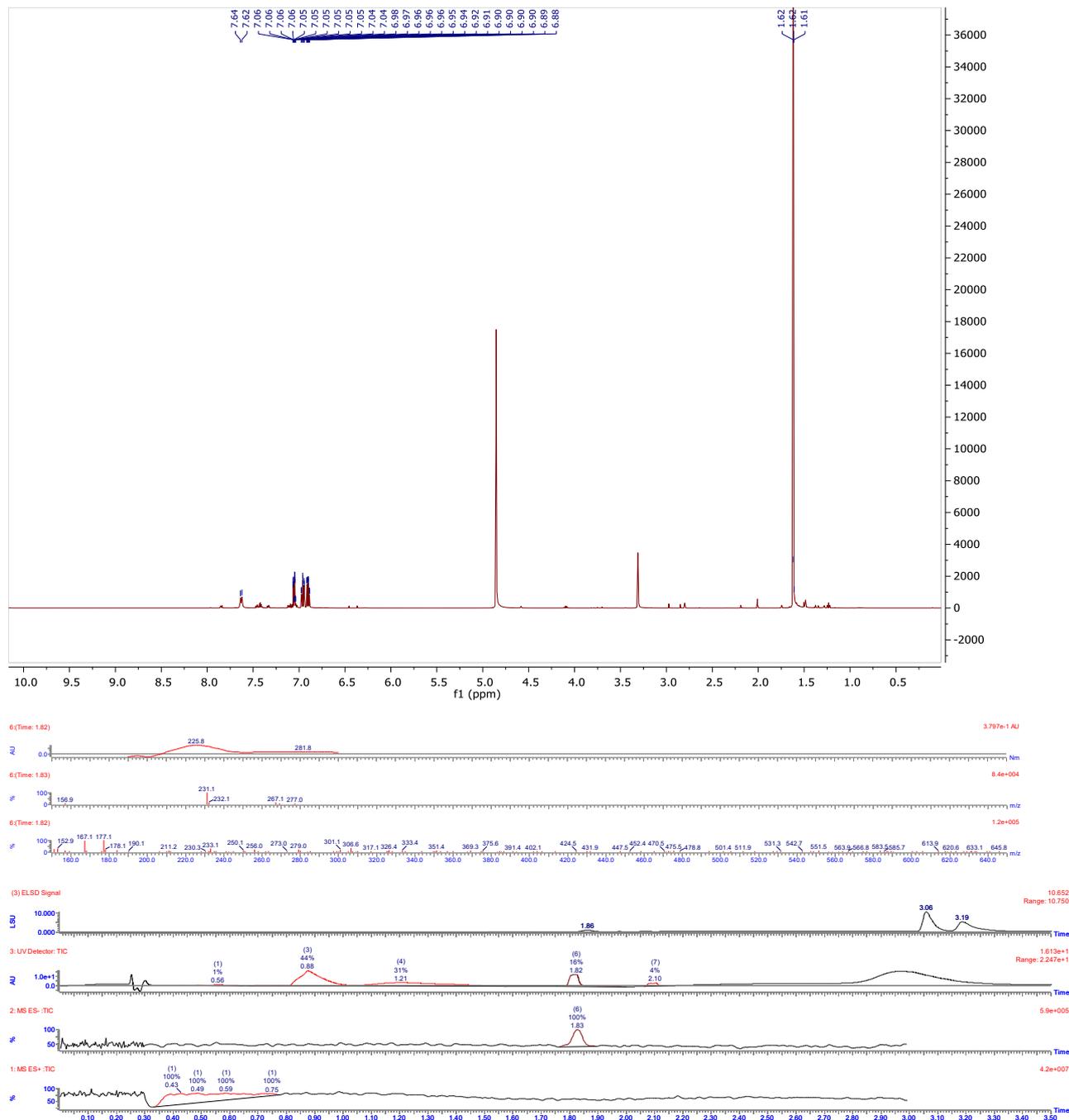
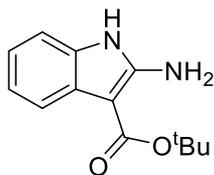
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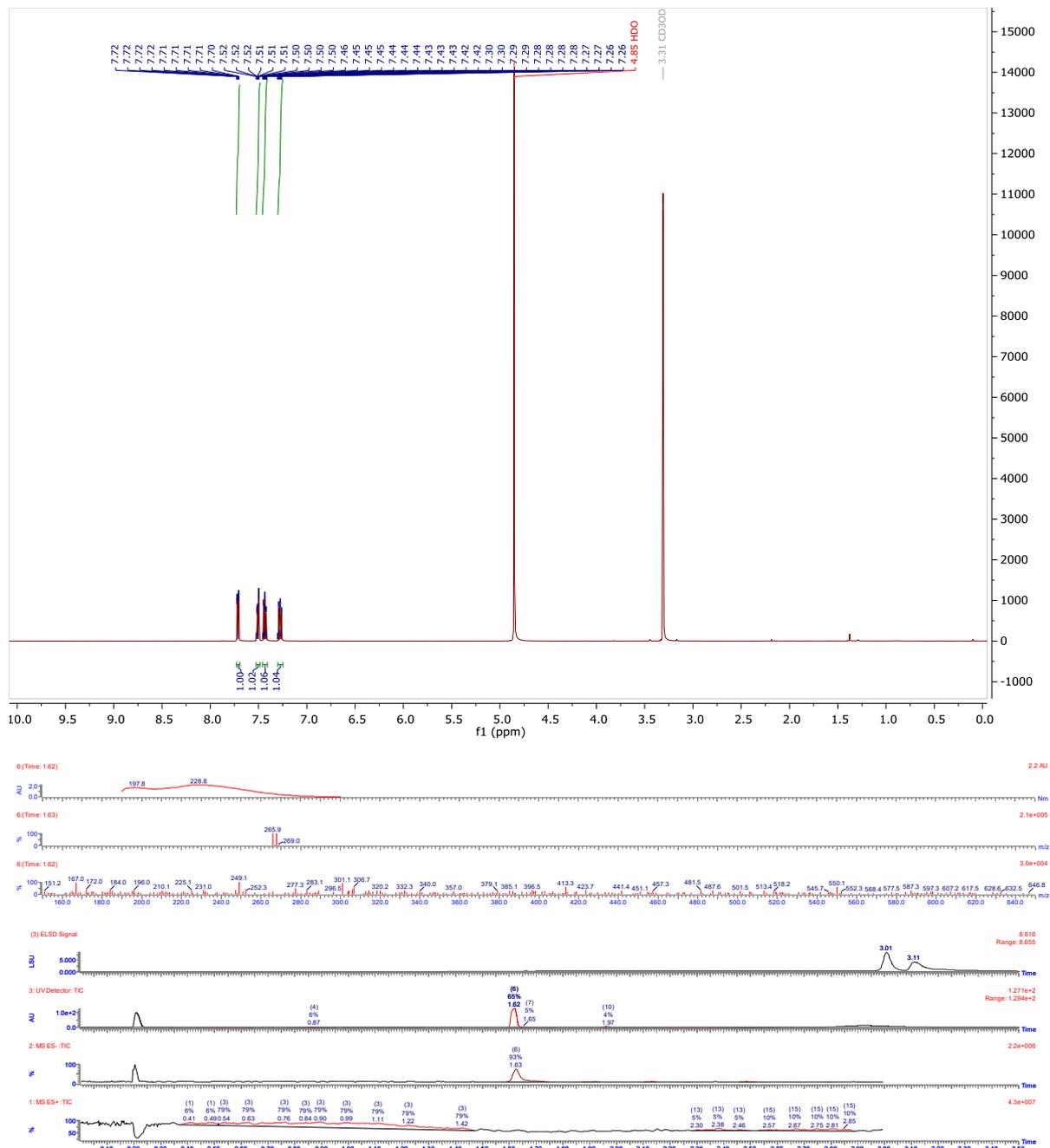
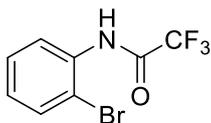
Ethyl 2-amino-1H-indole-3-carboxylate **6**



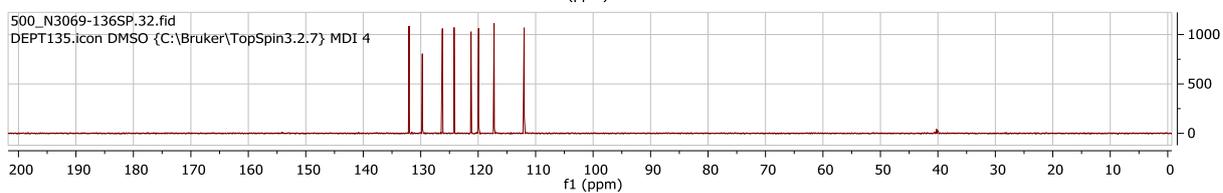
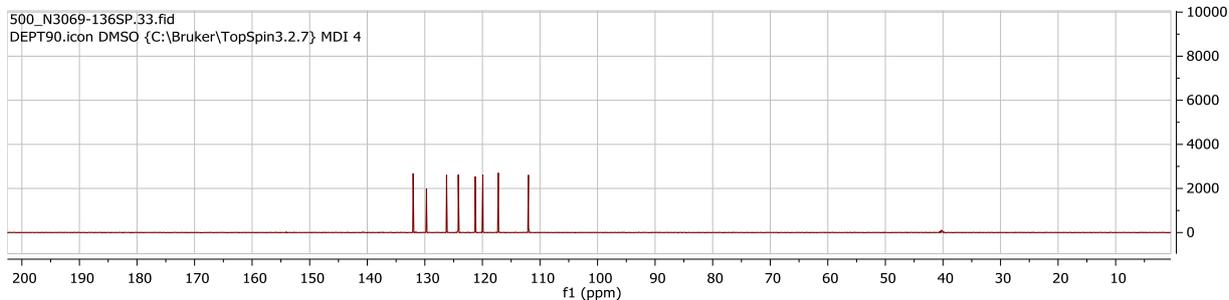
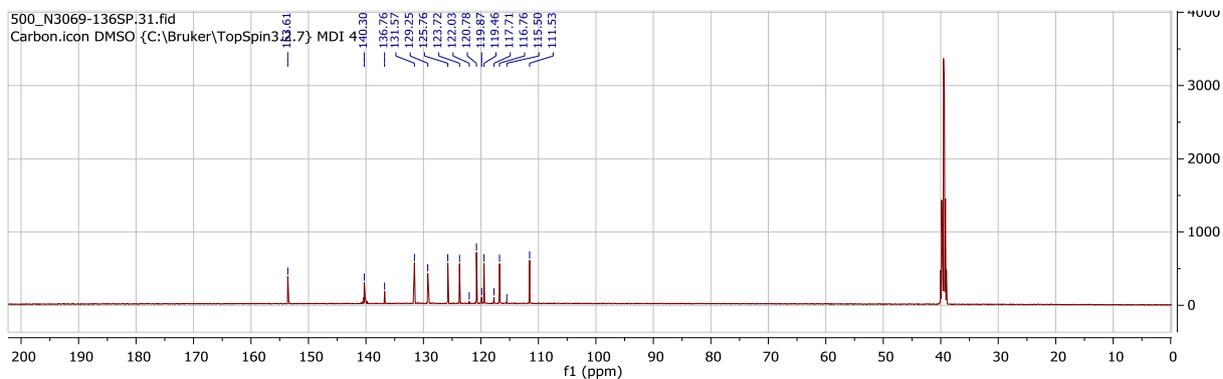
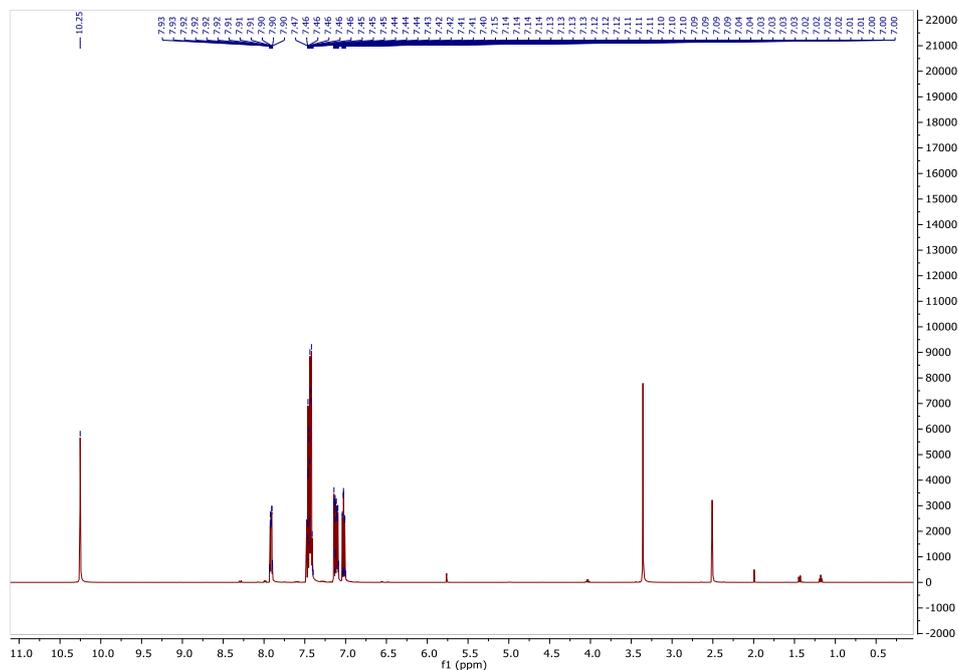
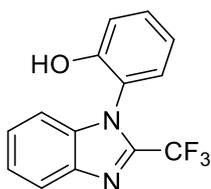
*tert*-Butyl 2-amino-1*H*-indole-3-carboxylate **7**

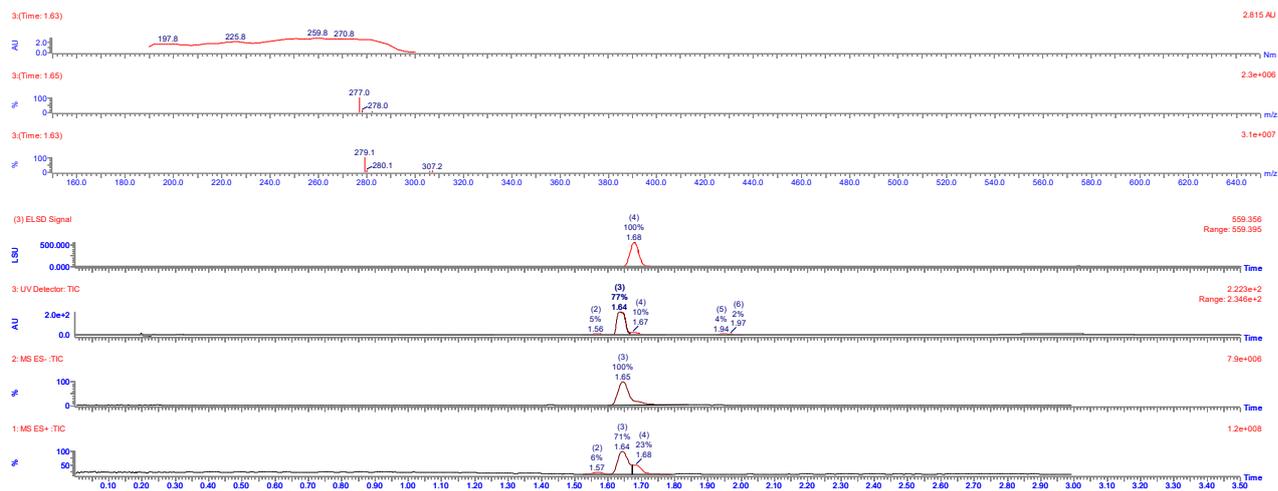
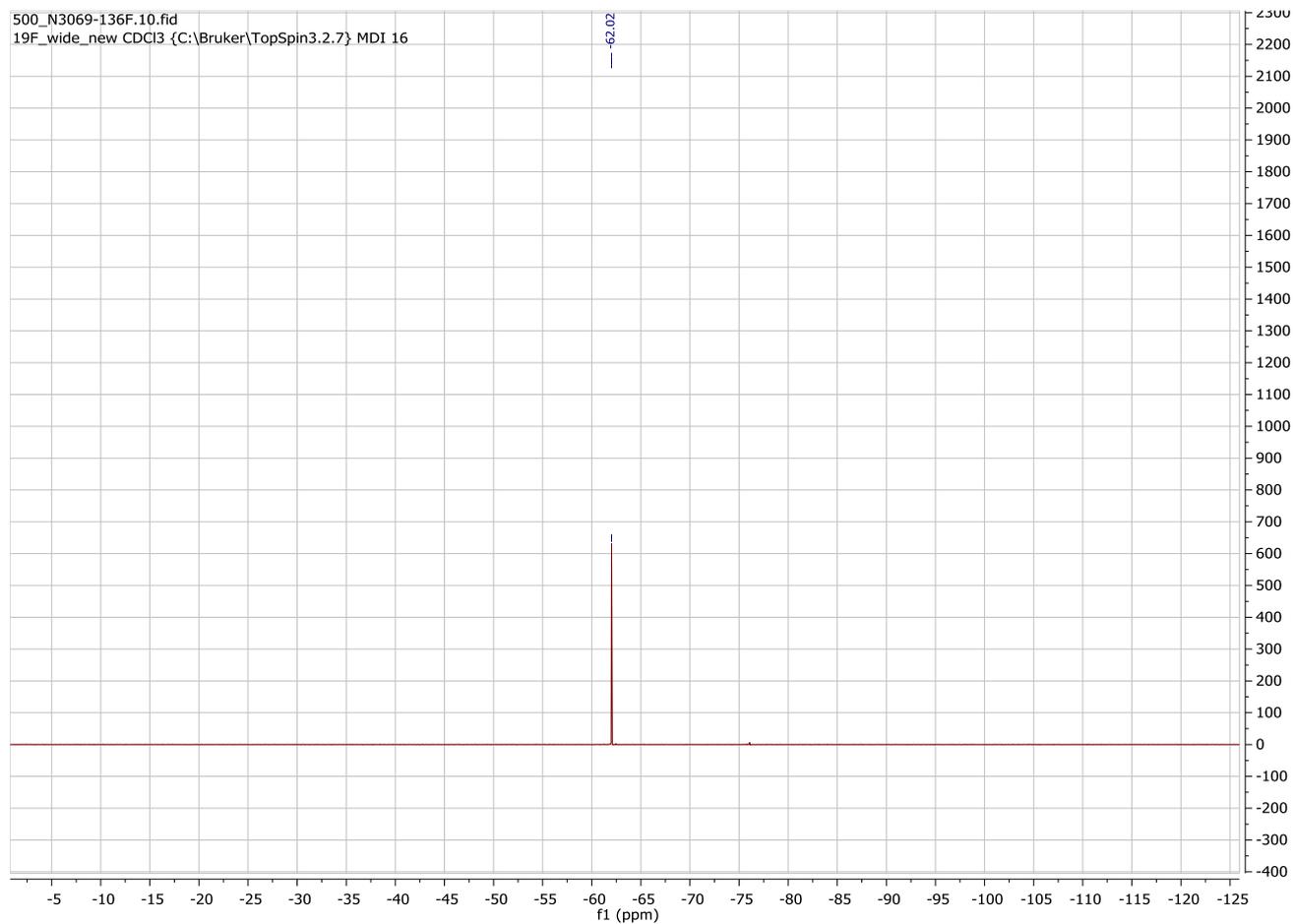


*N*-(2-Bromophenyl)-2,2,2-trifluoroacetamide **8**



2-(2-(Trifluoromethyl)-1H-benzo[d]imidazol-1-yl)phenol **9**







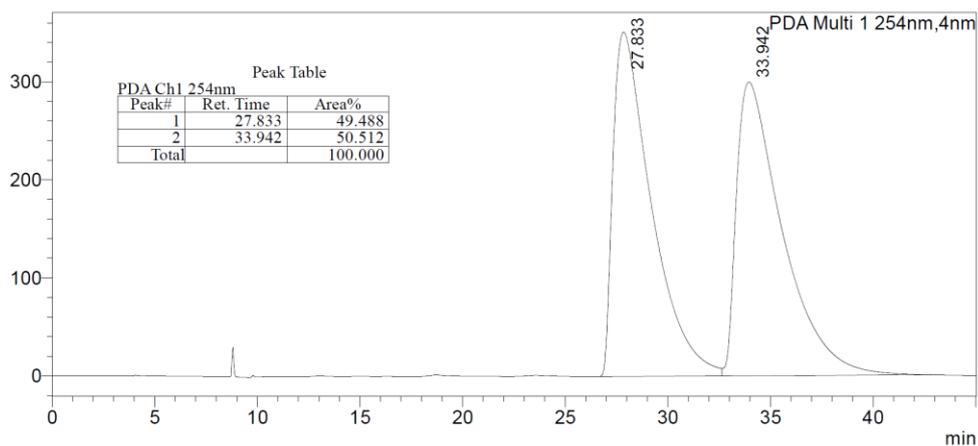
# Analysis Report

## <Sample Information>

Sample Name : N3075-109L\_1%\_OD-H  
 Sample ID : N3075-109L\_1%\_OD-H  
 Data Filename : N3075-109L\_1%\_OD-H.lcd  
 Method Filename : Methodfile.lcm  
 Batch Filename :  
 Vial # : 1-1  
 Injection Volume : 6 uL  
 Date Acquired : 13/12/2022 15:12:29  
 Date Processed : 13/12/2022 15:57:31  
 Sample Type : Unknown  
 Acquired by : System Administrator  
 Processed by : System Administrator

## <Chromatogram>

mAU



### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

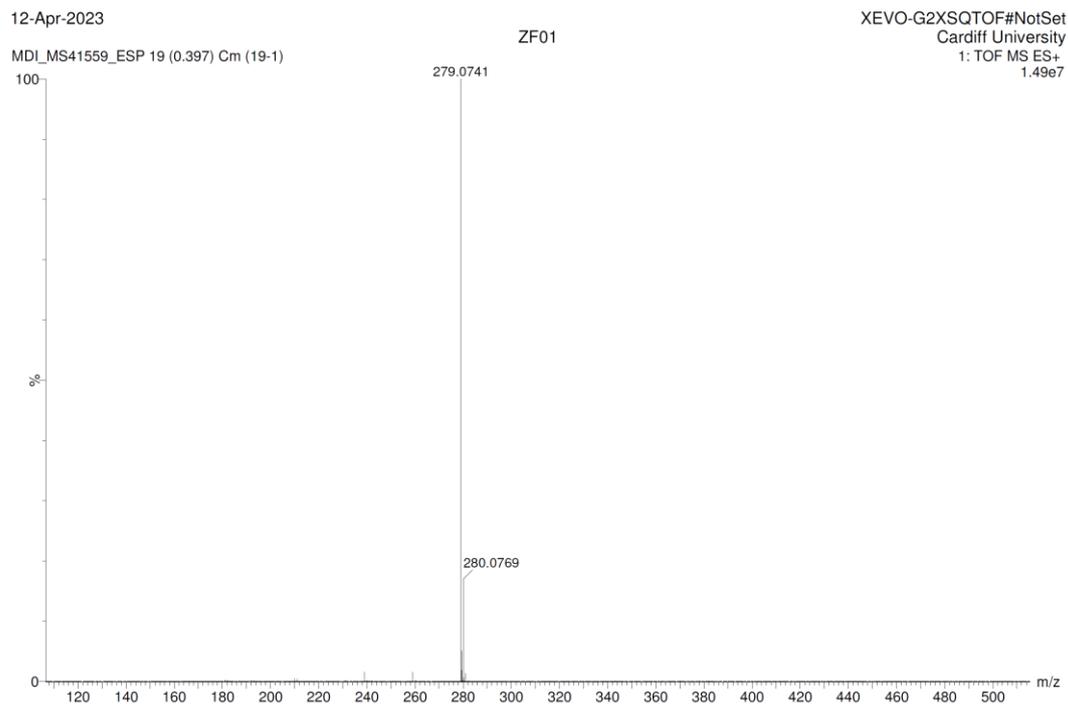
Monoisotopic Mass, Odd and Even Electron Ions

21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

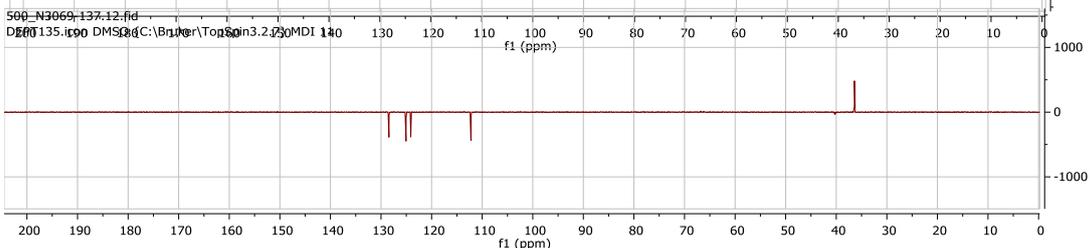
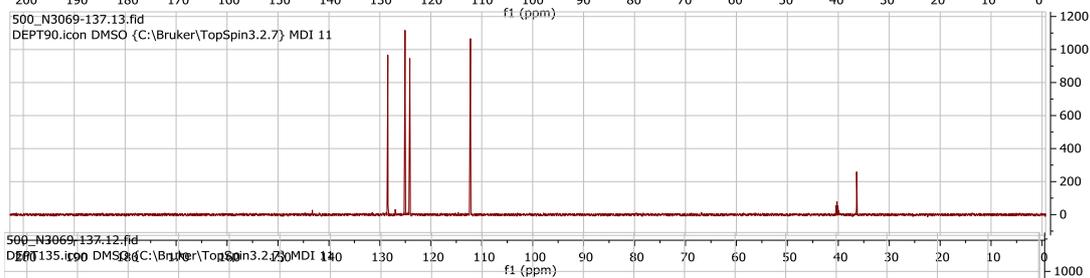
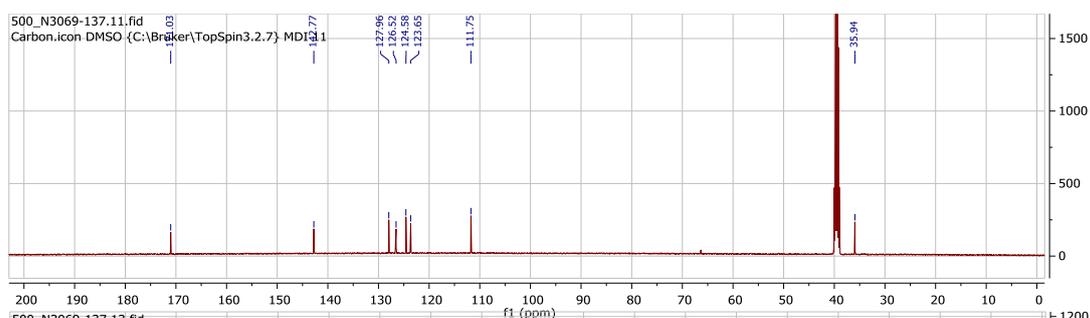
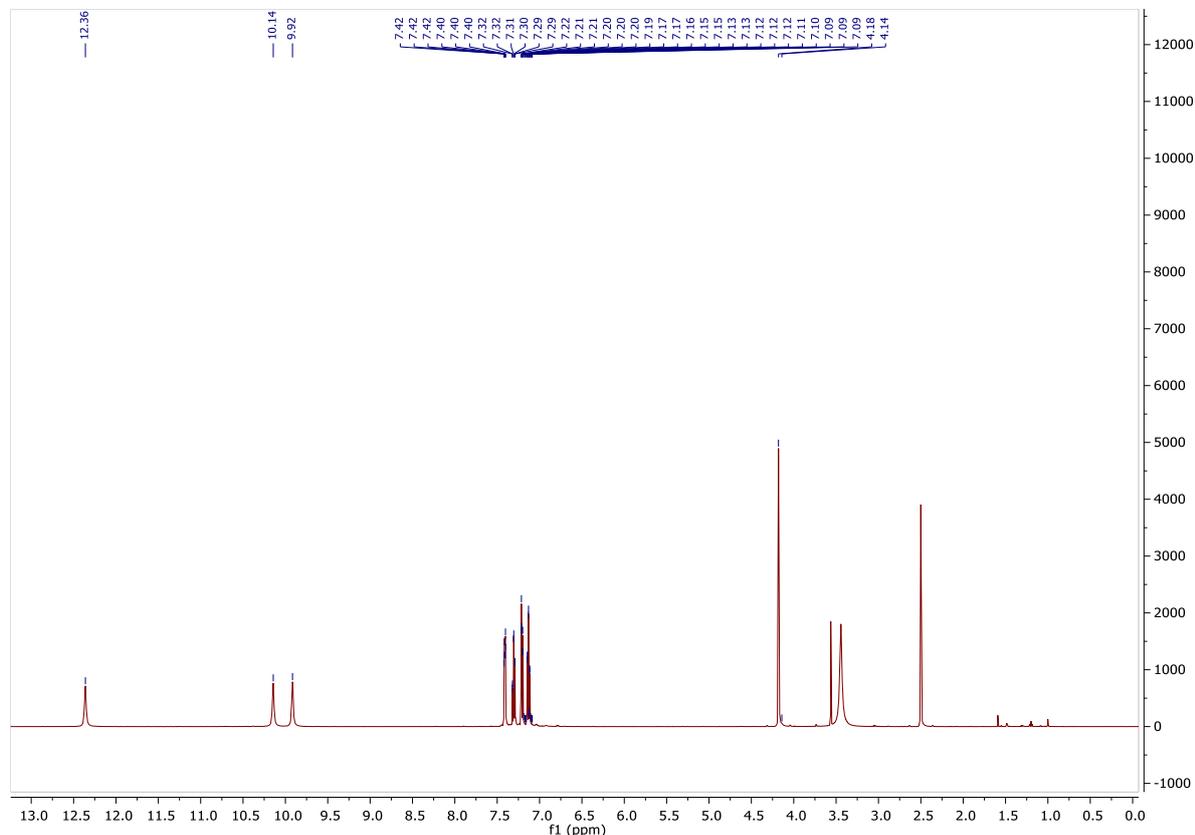
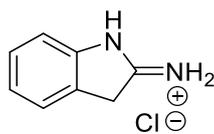
Elements Used:

C: 0-14 H: 0-10 N: 0-2 O: 0-1 F: 0-3

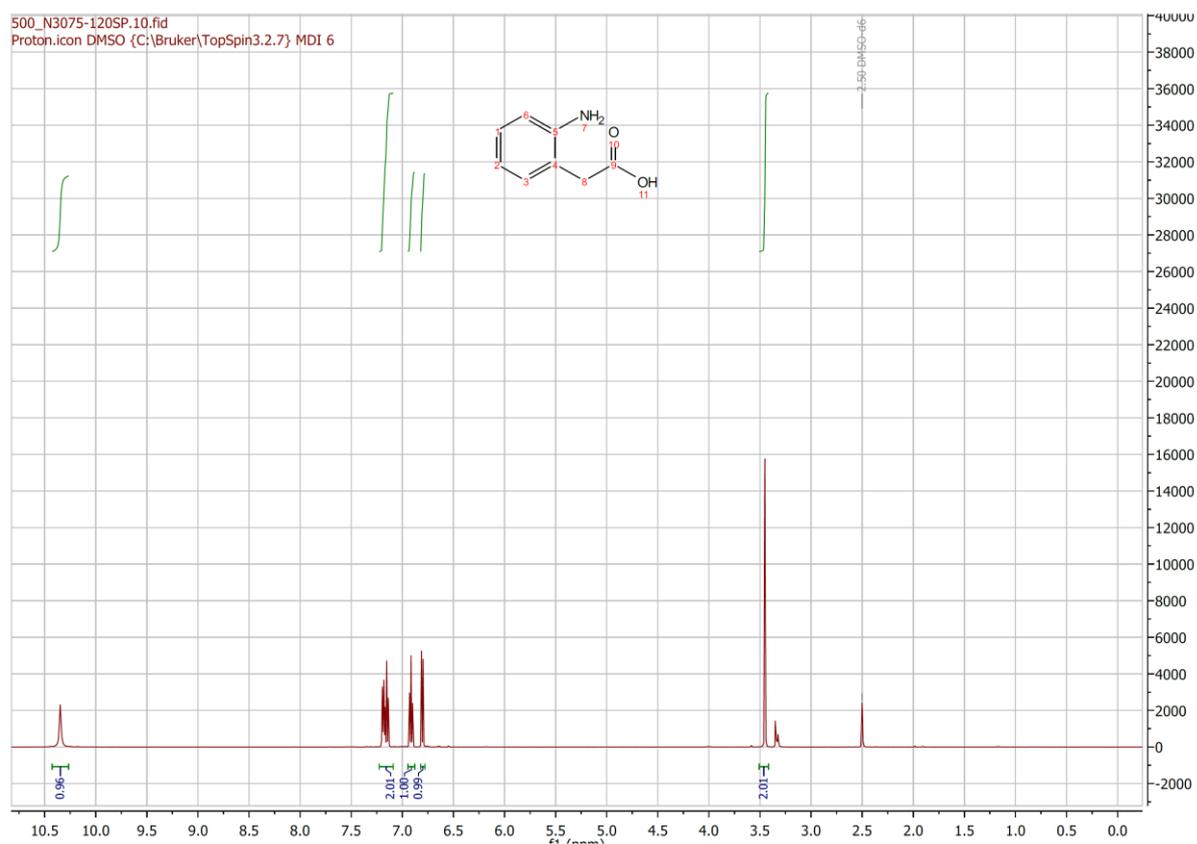
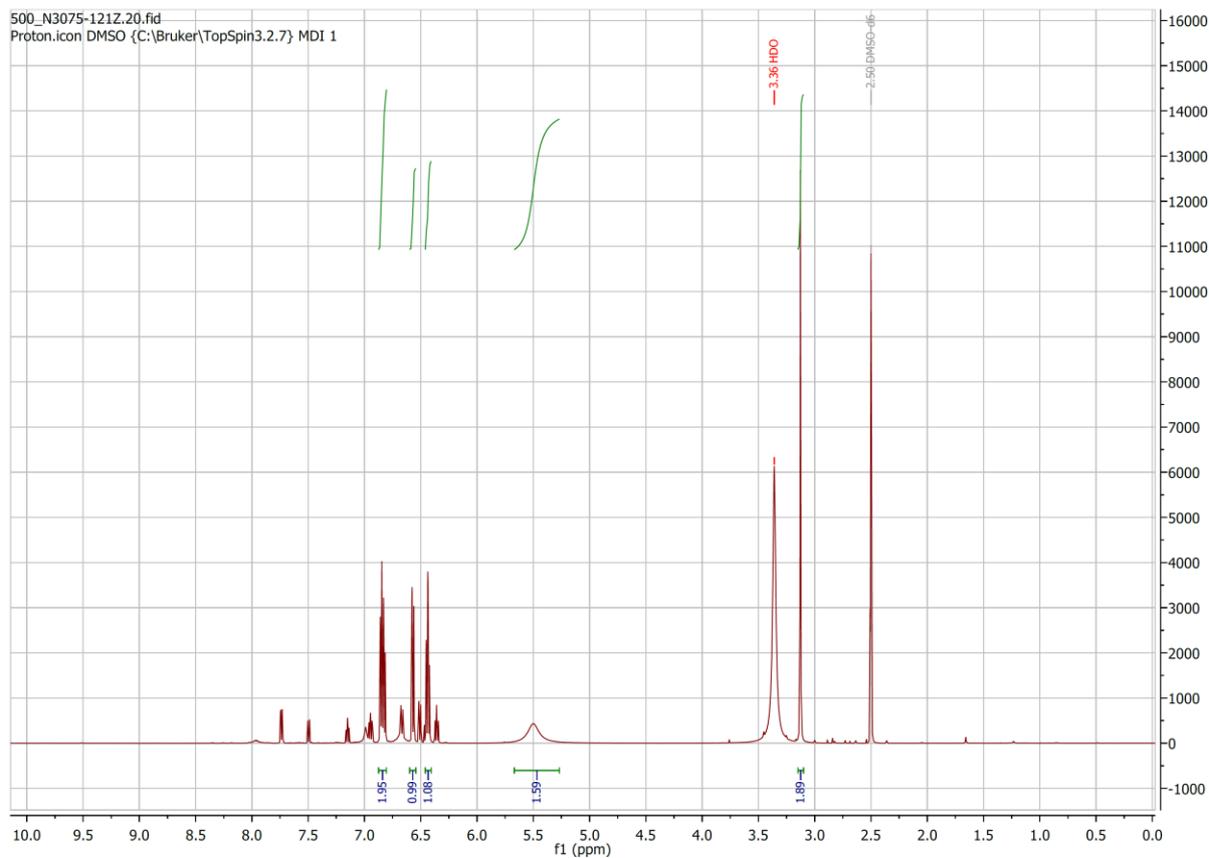
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
279.0741	279.0745	-0.4	-1.4	9.5	1250.8	n/a	n/a	C14 H10 N2 O F3

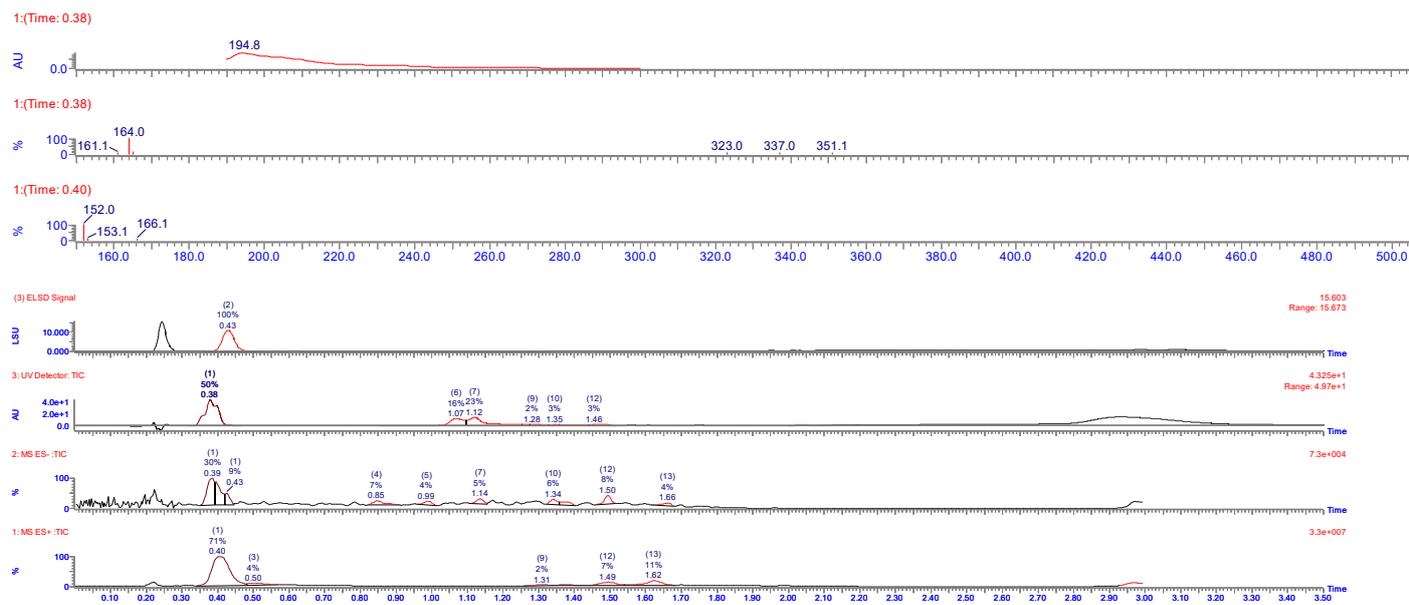


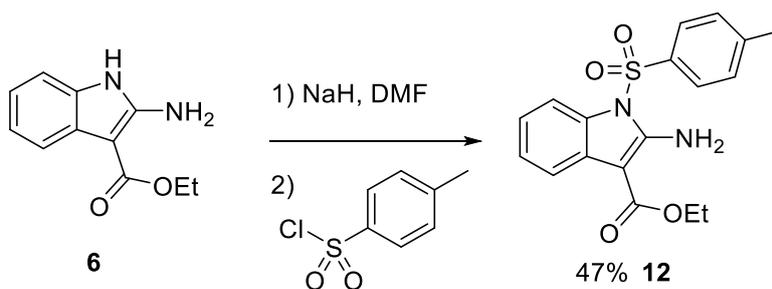
Indolin-2-imine hydrochloride **15**



## Attempted ester hydrolysis of compound 6







Openlynx Report - MDI UPLC MS Report - Aitor

eLN Number:N3122-32-Rx

File:Aitor152-1

Vial:2:28

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Description:

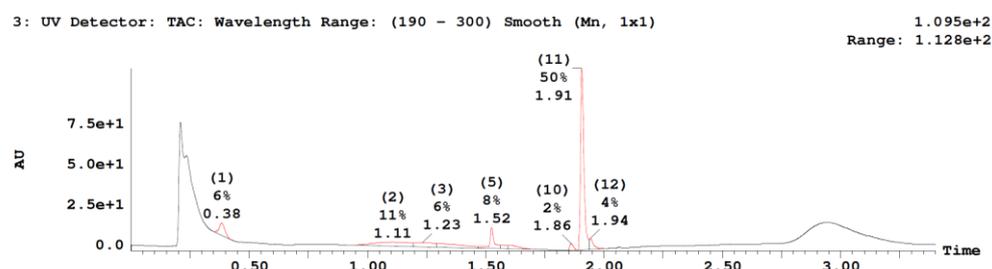
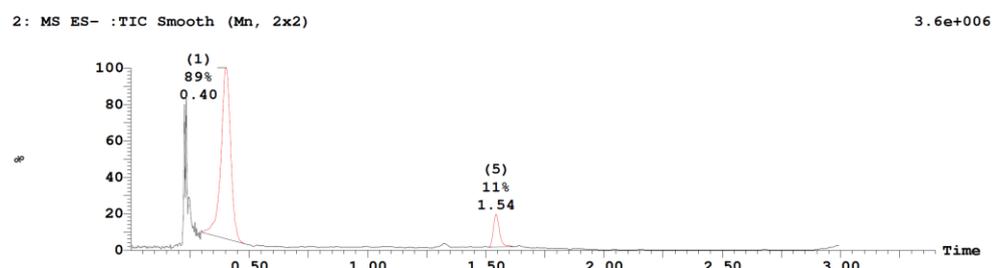
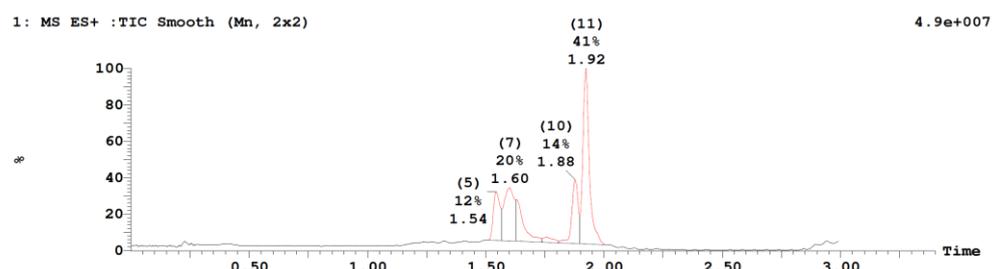
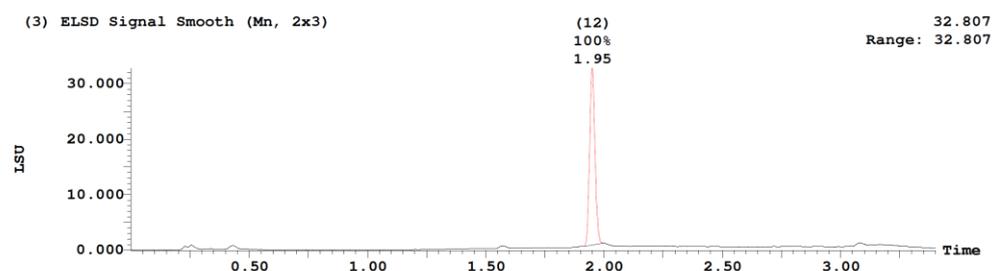
Method:C:\MassLynx\BEH Column (Acidic)

Openlynx Ver 2.0lp

Column Name:ACQUITY UPLC® BEH C18 1.7µm

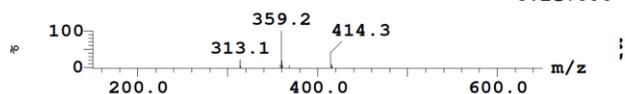
Date:02-Jun-2023

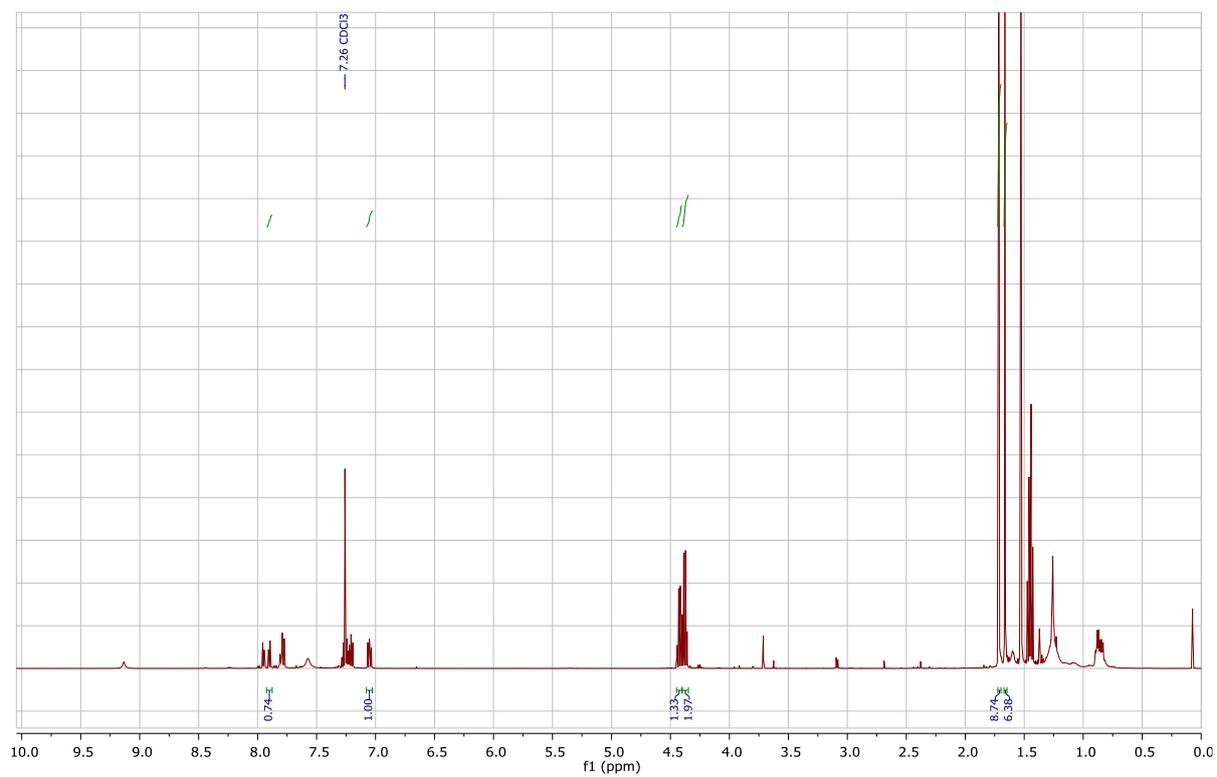
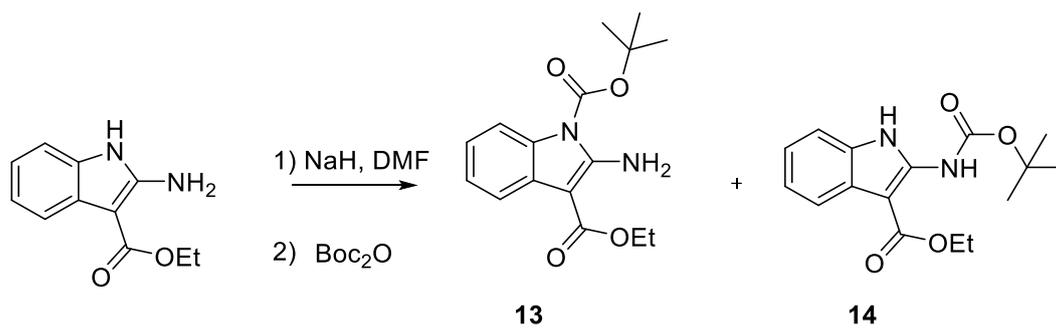
Time:16:31:50



Peak ID	Compound	Time	Mass Found
11		1.92	Not Found

1: MS ES+ 1  
8.2e+006





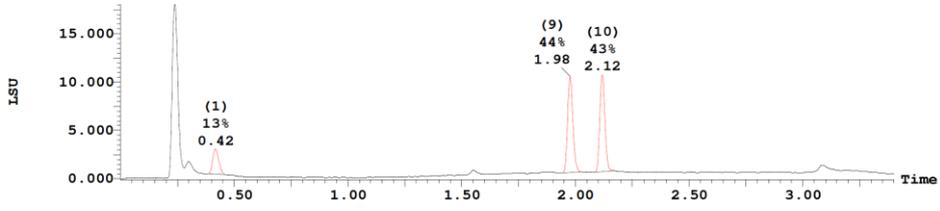
Openlynx Report - MDI UPLC MS Report - Aitor

Page 1

eLN Number:N3122-34-1h File:Aitor155-1 Vial:2:20  
 Description: Method:C:\MassLynx\BEH Column (Acidic) Openlynx Ver 2.0lp  
 Column Name:ACQUITY UPLC® BEH C18 1.7µm Date:06-Jun-2023  
 Time:15:56:34

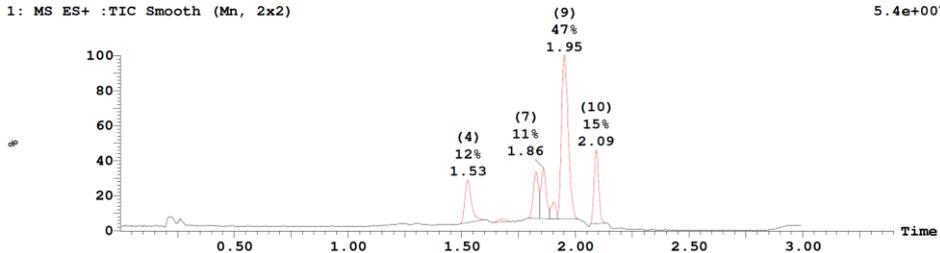
(3) ELSD Signal Smooth (Mn, 2x3)

18.053  
 Range: 18.102



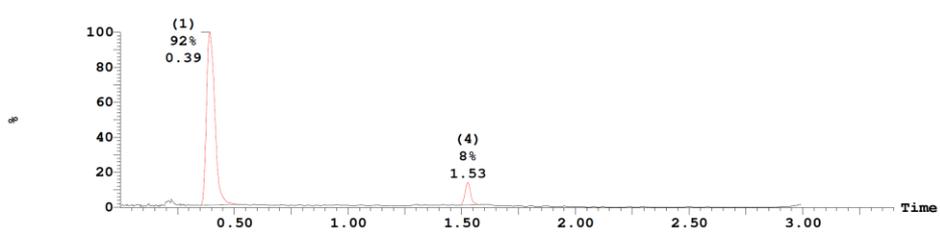
1: MS ES+ :TIC Smooth (Mn, 2x2)

5.4e+007



2: MS ES- :TIC Smooth (Mn, 2x2)

4.8e+006



3: UV Detector: TAC: Wavelength Range: (190 - 300) Smooth (Mn, 1x1)

7.944e+1  
 Range: 8.313e+1

