Electrochemical Synthesis of Selenyl-Dihydrofurans via Anodic Selenofunctionalization of Allyl-Naphthol/Phenol Derivatives and their Anti-Alzheimer Activity

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Supplementary Information

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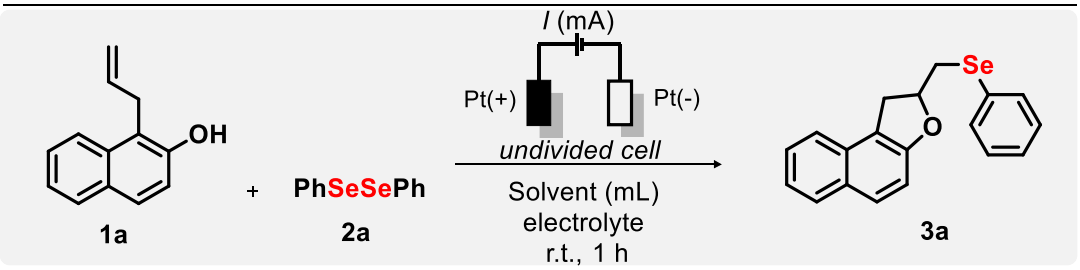
Optimization Table

Table SI: Complete optimization table.



Entry	Solvent (mL)	Electrolyte (equiv.)	Current	PhSeSePh (2a)	Yield%[a]
1	MeCN (10)	$^{n}Bu_4NPF_6$ (0.5)	5 mA	1.0 equiv.	93
2	MeCN (10)	$^{n}Bu_4NPF_6$ (0.5)	10 mA	1.0 equiv.	88
3	MeCN (5)	$^{n}Bu_4NBF_4$ (0.5)	5 mA	1.0 equiv.	74
4	MeCN (5)	KI (0.5)	5 mA	1.0 equiv.	N.R.
5	MeCN (5)	$^{n}Bu_4NClO_4$ (0.5)	5 mA	1.0 equiv.	99
6	MeCN (5)	$^{n}Bu_4NClO_4$ (0.1)	5 mA	1.0 equiv.	86
7	**MeCN (5)**	**$^{n}Bu_4NClO_4$ (0.2)**	**5 mA**	**1.0 equiv.**	**99**
8	MeCN (3)	$^{n}Bu_4NClO_4$ (0.2)	5 mA	1.0 equiv.	80
9	DMC (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA	1.0 equiv.	N.R.
10	DMSO (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA	1.0 equiv.	Trace
11	DCM (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA	1.0 equiv.	17
12	EtOH (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA	1.0 equiv.	28
13	MeCN (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA	0.5 equiv.	73
14	MeCN (5)	$^{n}Bu_4NPF_6$ (0.5)	5 mA	1.0 equiv.	92
15	MeCN/H_2O 1:1 (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA	1.0 equiv.	Trace
16	MeCN/H_2O 4:1 (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA	1.0 equiv	16
17	MeCN (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA (Pt+|C-)	1.0 equiv.	82
18	MeCN (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA (C+|Pt-)	1.0 equiv.	79
19	MeCN (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA (C+|C-)	1.0 equiv.	74
20	MeCN (5)	$^{n}Bu_4NClO_4$ (0.2)	5 mA	0.75 equiv.	83
21	MeCN (5)	$^{n}Bu_4NClO_4$ (0.2)	-	1.0 equiv.	N.R.

General reaction conditions: Pt plate electrode (10 mm × 10 mm × 0.05 mm); graphite rod (Φ 4 mm); (1a) (0.2 mmol), (2a) (0.2 mmol); [a]isolated yields; N.R. = for all cases, starting material was recovered.

General Procedure for Cyclic Voltammetry

Cyclic voltammetry was performed with a conventional three electrode electrochemical cell with a BAS potentiostat–galvanostat (model Epsilon, Bioanalytical Systems, Inc.). The redox properties of each compound, 1-allylnaphthalen-2-ol (**1a**), diphenyl diselenide (**2a**) and 2-((phenylselanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3a)** , was measured in anhydrous acetonitrile (MeCN) containing tetrabutylammonium hexafluorophosphate ($^{n}Bu_4NPF_6$) 0,1 mol L^{-1} as the supporting electrolyte at room temperature, under an argon atmosphere. In the procedure, electrochemical cell employed was of a standard three-electrode configuration: a platinum (working), a platinum wire (counter), and Ag/Ag^{+} (reference). Ferrocene ($E_{1/2}$= 400 mV *vs* NHE) was used as the internal standard.[4] The concentration of sample was 0.01 mol L^{-1}. The potential scan ranged from -0.5 to 2.0 V at a scan rate of 100 mV s^{-1}.

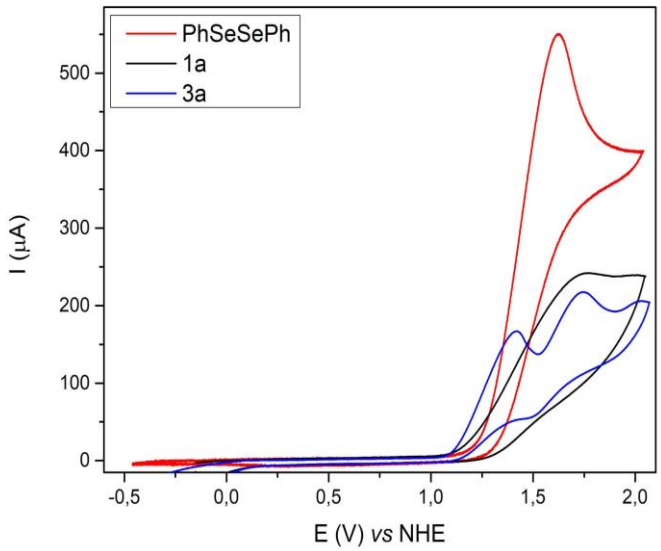


Figure SI: Cyclic voltametry of compounds **1a**, PhSeSePh **2a** and **3a**.

General Remarks

Starting materials obtained from commercial suppliers were used unless otherwise stated. Column chromatography was performed using silica gel 60 (diameter 0.05 - 0.10 mm) Macherey-Nagel. Thin layer chromatography (TLC) was performed using Macherey-Nagel pre-coated TLC sheets ALUGRAM® Xtra SIL with layer of 0.20 mm. Visualization was achieved by UV fluorescence, iodine chamber and acidic vanillin.

General Procedure for Starting Materials

Synthesis of Diselenides

Diselenides were synthesized via Grignard reaction followed by transmetalation with Se powder, or substituted with Na_2Se_2.[1,2]

Synthesis of allyl derivatives

The allyl derivatives were synthesized according reported methods.[3] Silicon carbide (SiC) bath was used for temperatures above 160 °C. The 2-allylphenol and 3-allyl-4-hydroxyacetophenone were obtained from Sigma-Aldrich.

General Procedure for Electrochemical Reactions

General Procedure: An undivided three-necked flask (25 mL) equipped with a stirring bar was charged with allylic derivatives (0.2 mmol), diselenides (0.2 mmol), $^{n}Bu_4NClO_4$ (0.2 equiv.) and MeCN (5 mL). The cell was equipped with platinum electrodes (1.0 × 1.0 x 0.05 mm) as the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA at room temperature and monitored by TLC. Upon completion, the solvent was removed under reduced pressure to afford the crude product, that was purified by flash column chromatography utilizing silica gel as stationary phase and eluate with a mixture of hexane/ethyl acetate afford the desired product.

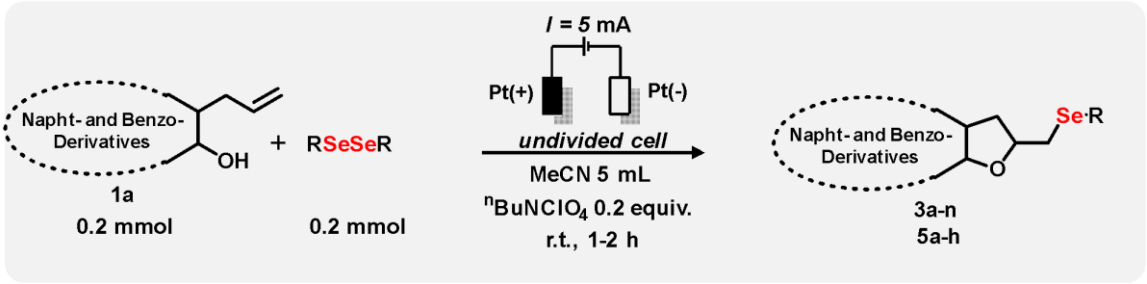


Figure SII: General procedure for electrochemical reactions.

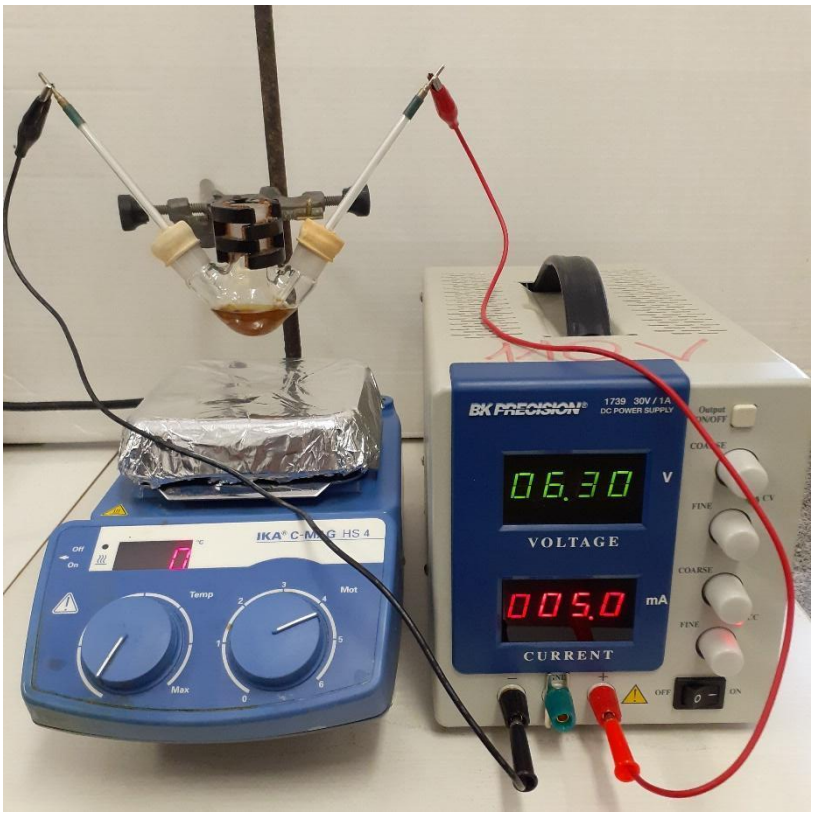


Figure SIII: Electrosynthetic apparatus for the synthesis of compounds **3** and **5**.

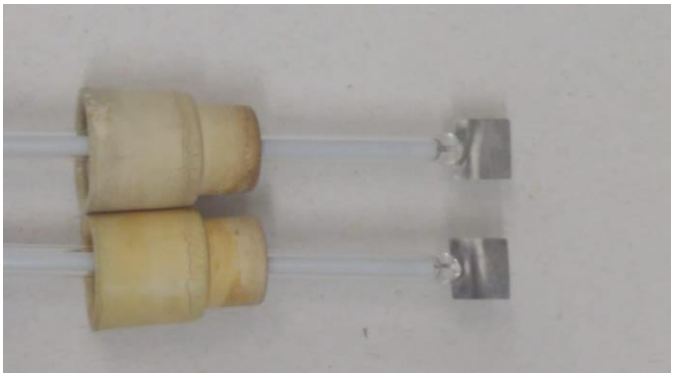


Figure SIV: Platinum work electrodes.

General Procedure for Electrochemical Gram Scale Reaction

An undivided three-necked flask (250 mL) equipped with drying tube containing $CaCl_2$ anhydrous, platinum electrodes (1.0 x 1.0 x 0.05 mm) and stirring bar was charged with 1-allylnaphtalen-2-ol (**1a**, 6 mmol), diphenyl diselenide (**2a**, 6 mmol), $^{n}BuNClO_4$ (1,2 mmol) and 150 mL of MeCN. The reaction was electrolyzed under constant current mode (5 mA) at room temperature. The reaction was monitored with TLC to the complete disappearance of **1a**. Upon completion, the solvent was removed under reduced pressure to afford the crude product, that

was purified by flash column chromatography utilizing silica gel as stationary phase and eluate with a mixture of hexane/ethyl acetate (95:5).

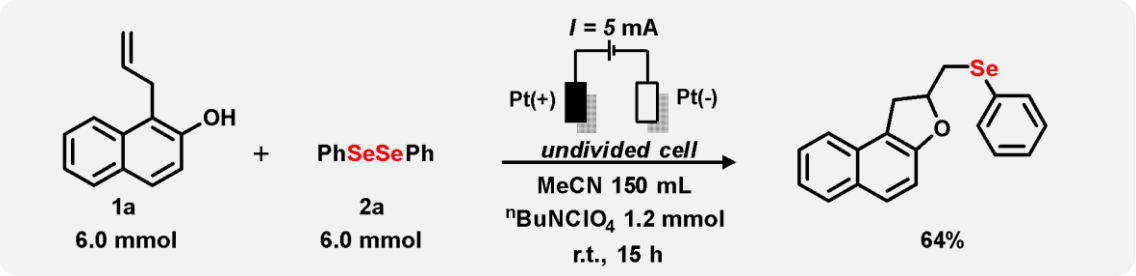


Figure SV: General procedure for Gram-Scale reaction of compound **1a**.

General Procedure for *In Vitro* Protocol of AChE Inhibition Assay

Acetylcholinesterase enzymatic activity was measured by using Ellman et al. (1961) method, with modifications.[6] The assay medium (1 mL) consisted of deionized water, 0.1M phosphate buffer (pH 7.4), 0.01 M DTNB, test compounds at five different concentrations dissolved in MeOH and an AChE (from electric eel) solution containing 0.8 U mL^{-1}. The mixture was incubated at 25 °C for 15 min, and then, 0.01 M acetylthiocholine iodide solution was added immediately. The activity was determined by measuring the absorbance at 412 nm for 10 or 15 minutes on a Cary 50 UV-Vis spectrophotometer. Data from concentration−inhibition experiments with the inhibitors were subjected to linear regression analysis using GraphPad Prism version 5.0 (GraphPad Software Inc.), which gave estimates of the IC50 (concentration of the compound/drug resulting in 50% inhibition of enzyme activity). Galantamine was used as the standard.

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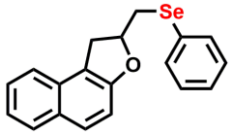
Characterization Data of Products

General considerations: The melting points were taken on a MQAPF-301 melting point apparatus. ^{1}H and ^{13}C NMR spectra were recorded on Varian NMR AS 400 spectrometer, with the samples dissolved in $CDCl_3$. Chemical shifts are informed in ppm downfield from the signal of TMS, used as internal standard, and the coupling constants (*J*) are expressed in Hertz (Hz). High-resolution mass spectral data were obtained on a Bruker microTOF-Q IIT instrument ($APPI^+$ mode). Infrared spectra were recorded on Bruker Alpha using KBr pellets. The instruments for electrochemical studies are BK Precision 1739 V/ 1A DC Power supply with 0.1 mA settable resolution. Anode and cathode platinum plate electrode (1.0 × 1.0 x 0.05 mm).



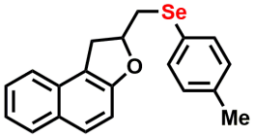
2-((phenylselanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3a).**

Off White solid (67.4 mg, 99% yield):**mp** 69–70 °C. R_f 0.66 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.1, 1H), 7.66 (d, *J* = 8.7, 1H), 7.58 – 7.52 (m, 3H), 7.47 – 7.43 (m, 1H), 7.31 – 7.22 (m, 4H), 7.06 (d, *J* = 8.7, 1H), 5.15 – 5.08 (m, 1H), 3.61 (dd, *J* = 9.4, 15.5, 1H), 3.39 (dd, *J* = 5.4, 12.4, 1H), 3.28 (dd, *J* = 6.6, 15.5, 1H), 3.15 (dd, *J* = 7.7, 12.5, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.6, 133.0, 130.7, 129.2, 129.2, 129.1, 129.0, 128.6, 127.3, 126.6, 122.8, 122.6, 117.7, 112.0, 82.5, 34.3, 32.9. **IR ν_{max}**: 3049,2934, 1631, 1240, 947, 802, 737, 687. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{19}H_{16}OSe$: 340.03616, found: 340,03695.

2-(((4-methoxyphenyl)selanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3b).**

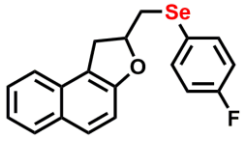
Off White solid (61.3 mg, 83% yield): **mp** 64–65 °C. R_f 0.23 (silica, 5% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.1, 1H), 7.65 (d, *J* = 8.7, 1H), 7.54 – 7.52 (m, 3H), 7.46 – 7.42 (m, 1H), 7.31 – 7.27 (m, 1H), 7.06 (d, *J* = 8.7, 1H), 6.81 (d, *J* = 8.7, 2H), 5.11 – 5.03 (m, 1H), 3.78 (s, 3H), 3.60 (dd, *J* = 9.4, 15.5, 1H), 3.31 – 3.24 (m, 2H), 3.06 (dd, *J* =

7.8, 12.4, 1H). **^{13}C {^{1}H} NMR** (100 MHz, $CDCl_3$) δ 159.5, 156.7, 135.9, 130.7, 129.2, 128.9, 128.6, 126.6, 122.8, 122.6, 118.9, 117.7, 114.8, 112.0, 82.6, 55.2, 34.3, 33.9. **IR ν_{max}**: 2931, 1631, 1490, 1243, 954, 809, 743, 513. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{20}H_{18}O_2Se$: 370.04674, found: 370.04693.



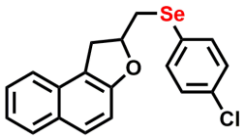
2-((p-tolylselanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3c).**

White solid (69.9 mg, 99% yield): **mp** 70–71 °C. ***R$_f$*** 0.63 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.1, 1H), 7.65 (d, *J* = 8.7, 1H), 7.53 (d, *J* = 8.2, 1H), 7.48 – 7.42 (m, 3H), 7.30 – 7.27 (m, 1H), 7.09 – 7.05 (m, 3H), 5.12 – 5.05 (m, 1H), 3.60 (dd, *J* = 9.4, 15.5, 1H), 3.34 (dd, *J* = 5.4, 12.4, 1H), 3.26 (dd, *J* = 6.7, 15.5, 1H), 3.09 (dd, *J* = 7.8, 12.4, 1H), 2.32 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.6, 137.4, 133.5, 130.7, 129.9, 129.2, 128.9, 128.6, 126.6, 125.3, 122.8, 122.6, 117.7, 112.0, 82.6, 34.3, 33.2, 21.0. **IR ν_{max}**:2918, 1467, 1243, 927, 802, 740, 493. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{20}H_{18}OSe$: 354.05182, found: 354.05147.



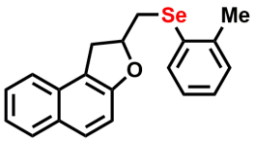
2-(((4-fluorophenyl)selanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3d).**

Yellow solid (56.3 mg, 79% yield): **mp** 51–52 °C. ***R$_f$*** 0.75 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1, 1H), 7.66 (d, *J* = 8.7, 1H), 7.57 – 7.53 (m, 3H), 7.47 – 7.43 (m, 1H), 7.32 – 7.28 (m, 1H), 7.05 (d, *J* = 8.7, 1H), 6.99 – 6.95 (m, 2H), 5.13 – 5.06 (m, 1H), 3.61 (dd, *J* = 9.4, 15.5, 1H), 3.32 (dd, *J* = 5.6, 12.5, 1H), 3.26 (dd, *J* = 6.7, 15.5 , 1H), 3.13 (dd, *J* = 7.3, 12.5, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.5 (d, $J_{C\text{-}F}$ = 247.6), 156.6, 135.7 (d, $J_{C\text{-}F}$ = 7.9), 130.7, 129.2, 129.1, 128.6, 126.7, 123.6 (d, $J_{C\text{-}F}$ = 3.4), 122.9, 122.6, 117.6, 116.3 (d, $J_{C\text{-}F}$ = 21.6), 112.0, 82.4, 34.3, 33.8. **IR ν_{max}**: 3060, 2927, 2851, 1631, 1583, 1487, 960, 746 591, 510. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{19}H_{15}FOSe$: 358.02674, found: 358.02674.



2-(((4-chlorophenyl)selanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3e).**

Yellow oil (27.5 mg, 37% yield). R_f 0.60 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1, 1H), 7.67 (d, *J* = 8.7, 1H), 7.54 (d, *J* = 8.2, 1H), 7.49 – 7.44 (m, 3H), 7.33 – 7.29 (m, 1H), 7.24 – 7.22 (m, 2H), 7.05 (d, *J* = 8.7, 1H), 5.16 – 5.09 (m, 1H), 3.63 (dd, *J* = 9.4, 15.5, 1H), 3.35 (dd, *J* = 5.6, 12.6, 1H), 3.28 (dd, *J* = 6.6, 15.6, 1H), 3.17 (dd, *J* = 7.2, 12.6, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.6, 134.4, 133.6, 130.7, 129.3, 129.2, 129.1, 128.7, 127.5, 126.7, 122.9, 122.6, 117.6, 112.0, 82.3, 34.4, 33.4. **IR ν_{max}**: 3059, 1631, 1474, 1243, 1085, 809, 743, 483. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{19}H_{15}ClOSe$: 379.99693, found: 373.99640.

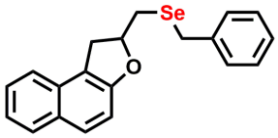


2-((o-tolylselanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3f).**

Yellow oil (62.4 mg, 88% yield). R_f 0.53 (silica, 5% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2, 1H), 7.66 (d, *J* = 8.7, 1H), 7.55 – 7.51 (m, 2H), 7.47 – 7.43 (m, 1H), 7.31 – 7.27 (m, 1H), 7.17 – 7.15 (m, 2H), 7.14 – 7.05 (m, 2H), 5.16 – 5.08 (m, 1H), 3.62 (dd, *J* = 9.3, 15.5, 1H), 3.36 (dd, *J* = 5.4, 12.3, 1H), 3.30 (dd, *J* = 6.6, 15.5, 1H), 3.12 (dd, *J* = 7.9, 12.3, 1H), 2.44 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.6, 139.7, 132.3, 130.7, 130.2, 130.1, 129.2, 129.0, 128.6, 127.2, 126.7, 126.6, 122.8, 122.6, 112.0, 82.5, 34.4, 31.8, 22.4. **IR ν_{max}**: 3059, 1631, 1464, 1240, 954, 743. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{20}H_{18}OSe$: 354.0518, found: 354.0524.

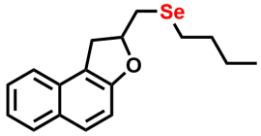
2-(((2-methoxyphenyl)selanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3g).**

Yellow solid (59.1 mg, 80% yield): **mp** 73–75 °C. R_f 0.48 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.2, 1H), 7.65 (d, *J* = 8.7, 1H), 7.53 (d, *J* = 8.2, 1H), 7.46, – 7.42 (m, 2H), 7.30 – 7.21 (m, 2H), 7.06 (d, *J* = 8.7, 1H), 6.91 – 6.87 (m, 1H), 6.83 (d, *J* = 7.6, 1H), 5.17 – 5.10 (m, 1H), 3.86 (s, 3H), 3.61 (dd, *J* = 9.3, 15.6, 1H), 3.41 (dd, *J* = 5.3, 12.3, 1H), 3.31 (dd, *J* = 6.6, 15.6, 1H), 3.10 (dd, *J* = 8.3, 12.3, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.0, 156.6, 132.0, 130.7, 129.1, 128.9, 128.6, 128.3, 126.6, 122.8, 122.6, 121.3, 118.2, 117.7, 112.0, 110.5, 82.6, 55.7, 34.4, 30.1. **IR ν_{max}:** 3049, 1628, 1474, 1237, 954, 747. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{20}H_{18}O_2Se$: 370.04674, found: 370.04680.



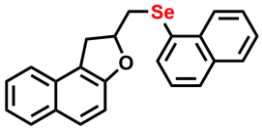
2-((benzylselanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3i).**

Yellow solid (70.5 mg, 99% yield): **mp** 67–68 °C. R_f 0.71 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.1, 1H), 7.65 (d, *J* = 8.7, 1H), 7.52 (d, *J* = 8.1, 1H), 7.46 – 7.42 (m, 1H), 7.30, – 7.26 (m, 5H), 7.22 – 7.18 (m, 1H), 7.08 (d, *J* = 8.7, 1H), 5.09 – 5.02 (m, 1H), 3.87 (s, 2H), 3.54 (dd, *J* = 9.4, 15.5, 1H), 3.18 (dd, *J* = 6.9, 15.5, 1H), 2.91 (dd, *J* = 5.7, 12.7, 1H), 2.81 (dd, *J* = 6.8, 12.7, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.6, 139.0, 130.7, 129.1, 129.0, 128.9, 128.6, 128.5, 126.8, 126.6, 122.8, 122.6, 117.8, 111.9, 83.3, 34.5, 28.8, 27.7. **IR ν_{max}:3056, 3023, 2921** 2921, 1628, 1460, 1243, 937, 812, 697, 460. **HRMS-APPI**: *m/z* $[(M-H)]^+$ calcd. for $C_{20}H_{17}OSe$: 353.04399, found for $C_{20}H_{17}OSe$:353.04774.



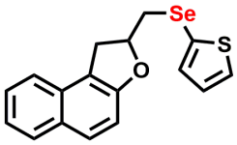
2-((butylselanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3j).**

Yellow oil (44.5 mg, 70% yield). R_f 0.75 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.2, 1H), 7.67 (d, *J* = 8.7, 1H), 7.57 (d, *J* = 8.2, 1H), 7.48, – 7.44 (m, 1H), 7.32 – 7.28 (m, 1H), 7.09 (d, *J* = 8.7, 1H), 5.19 – 5.12 (m, 1H), 3.64 (dd, *J* = 9.3, 15.5, 1H), 3.28 (dd, *J* = 6.8, 15.5, 1H), 3.02 (dd, *J* = 5.6, 12.5, 1H), 2.87 (dd, *J* = 7.4, 12.5, 1H), 2.68 (t, *J* = 7.5, 2H), 1.71 – 1.64 (m, 2H), 1.41 (sextet, *J* = 7.3, 2H), 0.92 (t, *J* = 7.3, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.7, 130.7, 129.1, 129.0, 128.6, 126.6, 122.8, 122.6, 117.8, 111.9, 83.4, 34.5, 32.6, 28.8, 24.6, 22.9, 13.5. **IR ν_{max}:** 3059, 2957, 2924, 1631, 1464, 1243, 957, 812, 743. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{17}H_{20}OSe$: 320.06774, found: 320.06782.



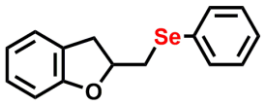
2-((naphthalen-1-ylselanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3l).**

Yellow solid (36.0 mg, 46% yield): **mp** 78–79 °C. R_f 0.68 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.3, 1H), 7.87 (d, *J* = 7.1, 1H), 7.83 – 7.75 (m, 3H), 7.63 (d, *J* = 8.7, 1H), 7.56, – 7.47 (m, 3H), 7.44 – 7.41 (m, 1H), 7.37 – 7.33 (m, 1H), 7.29 – 7.25 (m, 1H), 7.03 (d, *J* = 8.7, 1H), 5.08 – 5.01 (m, 1H), 3.56 (dd, *J* = 9.4, 15.5, 1H), 3.39 (dd, *J* = 5.35, 12.3, 1H), 3.26 (dd, *J* = 6.6, 15.6, 1H), 3.14 (dd, *J* = 7.7, 12.3, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.6, 134.3, 134.0, 133.3, 130.7, 129.2, 129.0, 128.8, 128.7, 128.6, 128.4, 127.6, 126.8, 126.6, 126.2, 125.7, 122.8, 122.6, 117.7, 112.0, 82.6, 34.3, 33.1. **IR ν_{max}:** 3052, 2927, 1628, 1464, 1243, 957, 802, 766. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{23}H_{18}OSe$: 390.05184, found: 390.05157.



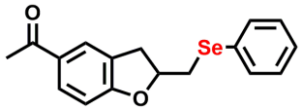
2-((thiophen-2-ylselanyl)methyl)-1,2-dihydronaphtho[2,1-b]furan **(3m).**

Yellow solid (21.3 mg, 31% yield): **mp** 59–61 °C. R_f 0.69 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.1, 1H), 7.6 (d, *J* = 8.7, 1H), 7.56 (d, *J* = 8.2, 1H), 7.48, – 7.40 (m, 1H), 7.40 (d, *J* = 5.2, 1H), 7.32 (d, *J* = 7.9, 1H), 7.29 – 7.25 (m, 1H), 7.09 (d, *J* = 8.7, 1H), 6.99 (dd, *J* = 3.5, 5.1, 1H), 5.17 – 5.10 (m, 1H), 3.66 (dd, *J* = 9.4, 15.5, 1H), 3.32 – 3.26 (m, 2H), 3.06 (dd, *J* = 7.4, 12.4, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.6, 136.1, 131.1, 130.77, 129.2, 129.1, 128.7, 128.1, 126.7, 122.9, 122.7, 122.6, 117.7, 112.0, 82.4, 36.3, 34.2. **IR ν_{max}**: 3062, 1628, 1243, 944, 806, 697. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{17}H_{14}OSSe$: 345.99250, found: 390.99286.



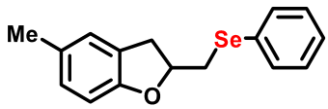
2-((phenylselanyl)methyl)-2,3-dihydrobenzofuran **(5a).**

Off White solid (31.6 mg, 55% yield): **mp** 60–61 °C. R_f 0.66 (silica, 5% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 – 7.54 (m, 2H), 7.28 – 7.24 (m, 3H), 7.14 – 7.08 (m, 2H), 6.85 – 6.82 (m, 1H), 6.75 (d, *J* = 7.9, 1H), 4.97 – 4.89 (m, 1H), 3.39 – 3.30 (m, 2H), 3.09 (dd, *J* = 7.7, 12.5, 1H), 3.02 (dd, *J* = 6.7, 15.7, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.1, 133.0, 129.3, 129.1, 128.0, 127.2, 126.1, 124.9, 120.5, 109.4, 81.8, 35.4, 32.6. **IR ν_{max}:** 2924, 1595, 1483, 1233, 950, 737, 691. **HRMS-APPI**: *m/z* $[(M+OH)]^+$ calcd. for $C_{15}H_{14}OSeOH$: 307.0232, found: 307.0232. Analytical data for compound **5a** was consistent with the literature.[5]



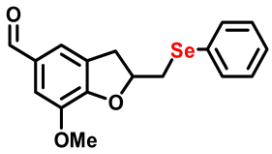
1-(2-((phenylselanyl)methyl)-2,3-dihydrobenzofuran-5-yl)ethan-1-one **(5b).**

White solid (37.6 mg, 57% yield): **mp** 67–69 °C. R_f 0.16 (silica, 5% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 – 7.74 (m, 2H), 7.56 – 7.53 (m, 2H), 7.29 – 7.26 (m, 3H), 6.74 (d, *J* = 8.5, 1H), 5.07 – 5.00 (m, 1H), 3.38 (dd, *J* = 9.1, 15.9, 1H), 3.32 (dd, *J* = 5.3, 12.6, 1H), 3.11 (dd, *J* = 7.5, 12.6, 1H), 3.04 (dd, *J* = 6.7, 15.9, 1H), 2.53 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 196.5, 163.4, 133.2, 130.8, 130.4, 129.2, 129.0, 127.4, 126.9, 125.5, 109.0, 83.2, 34.7, 32.5, 26.3. **IR ν_{max}**: 2924, 1664, 1605, 1243, 825, 733, 463. **HRMS-APPI**: *m/z* $[M+H]^+$ calcd. for $C_{17}H_{17}O_2Se$: 333.0389, found: 333.0384.



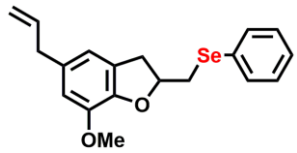
5-methyl-2-((phenylselanyl)methyl)-2,3-dihydrobenzofuran **(5c).**

Off White solid (42.4 mg, 70% yield): **mp** 44-15°C. R_f 0.76 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 – 7.53 (m, 2H), 7.27 – 7.23 (m, 3H), 6.94 (s, 1H), 6.89 (d, *J* = 8.1, 1H), 6.63 (d, *J* = 8.1, 1H), 4.94 – 4.87 (m, 1H), 3.34 – 3.28 (m, 2H), 3.08 (dd, *J* = 7.7, 12.4, 1H), 2.97 (dd, *J* = 6.7, 15.7, 1H), 2.26 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.0, 133.0, 129.8, 129.3, 129.1, 128.3, 127.2, 126.1, 125.5, 108.9, 81.8, 35.5, 32.7, 20.7. **IR ν_{max}**: 2924, 1490, 1240, 1201, 737, 691. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{16}H_{16}OSe$: 304.0361, found: 304.0356



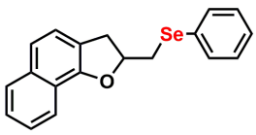
7-methoxy-2-((phenylselanyl)methyl)-2,3-dihydrobenzofuran-5-carbaldehyde **(5d).**

Yellow solid (27.8 mg, 40% yield): **mp** 60-62 °C. R_f 0.2 (silica, 10% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.70 (s, 1H), 7.55 – 7.52 (m, 2H), 7.31 – 7.26 (m, 5H), 5.15 – 5.08 (m, 1H), 3.90 (s, 3H), 3.47 – 3.40 (m, 2H), 3.15 – 3.09 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.4, 153.3, 144.8, 133.0, 131.2, 129.1, 128.6, 127.7, 127.4, 121.4, 111.2, 84.2, 55.9, 34.9, 32.0. **IR ν_{max}:** 2937, 1681, 1592, 1312, 1135, 740. **HRMS-APPI**: *m/z* $[(M+H)]^+$ calcd. for $C_{17}H_{16}O_3Se$: 349.0337, found: 349.0338.



5-allyl-7-methoxy-2-((phenylselanyl)methyl)-2,3-dihydrobenzofuran **(5e).**

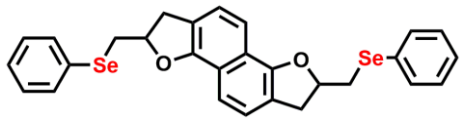
White solid (50.1 mg, 70% yield). **mp** 46-49°C. R_f 0.48 (silica, 5% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 – 7.52 (m, 2H), 7.26 – 7.25 (m, 3H), 6.60 (s, 1H), 6.55 (s, 1H), 5.94 (ddt, *J* = 6.7, 10.0, 16.8, 1H), 5.10 – 5.03 (m, 2H), 4.99 – 4.92 (m, 1H), 3.84 (s, 3H), 3.43 (dd, *J* = 4.3, 12.4, 1H), 3.38 – 3.29 (m, 3H), 3.11 – 3.00 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.9, 144.0, 137.8, 133.2, 132.8, 129.1, 127.7, 127.2, 117.0, 115.4, 111.5, 82.7, 55.8, 40.0, 35.8, 32.2. **IR ν_{max}:** 3075, 2934, 1605, 1500, 1322, 1138, 733, 687. **HRMS-APPI**: *m/z* $[M]^+$ calcd. for $C_{19}H_{20}O_2Se$: 360.0624, found: 360.0620.



2-((phenylselanyl)methyl)-2,3-dihydronaphtho[1,2-b]furan **(5f).**

Brown oil (37.5 mg, 55% yield). R_f 0.46 (silica, 5% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 – 7.87 (m, 1H), 7.79 – 7.77 (m, 1H), 7.58 – 7.56 (m, 2H), 7.42 – 7.35 (m, 3H), 7.29 – 7.24 (m, 4H), 5.20 – 5.13 (m, 1H), 3.53 (dd, *J* = 9.2, 15.4, 1H), 3.43 (dd, *J* =

5.28.2, 12.5, 1H), 3.22 – 3.14 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 133.9, 133.2, 133.1, 129.4, 129.1, 127.7, 127.2, 125.6, 125.2, 122.8, 121.4, 120.4, 120.2, 119.0, 82.7, 36.3, 32.9. **IR ν_{max}**: 3055, 1576, 1376, 1281, 801, 736, 564. **HRMS-APPI**: *m/z* $[(M+H)]^+$ calcd. for $C_{19}H_{16}OSe$: 340.0362, found: 340.0359.



2,7-bis((phenylselanyl)methyl)-1,2,6,7-tetrahydronaphtho[1,2-b:5,6-b']difuran **(5h).**

Brown solid (49.7 mg, 45% yield): **mp** 103–105 °C. ***R$_f$*** 0.28 (silica, 5% EtOAc in Hex). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59 – 7.56 (m, 4H), 7.38 (d, *J* = 8.2, 2H), 7.27 – 7.26 (m, 6H), 7.23 (d, *J* = 8.2, 2H), 3.53 (dd, *J* = 9.3, 15.4, 2H), 3.43 (dd, *J* = 5.2, 12.5, 2H), 3.21 – 3.13 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 154.6, 133.1, 129.4, 129.1, 127.2, 122.3, 120.9, 118.9, 113.9, 82.6, 36.3, 32.9. **IR ν_{max}:** 3070, 1599, 1576, 1399, 969, 738, 469.**HRMS-APPI**: *m/z* $[(M+H)]^+$ calcd. for $C_{28}H_{25}O_2Se_2$: 553.0185, found: 553.0189.

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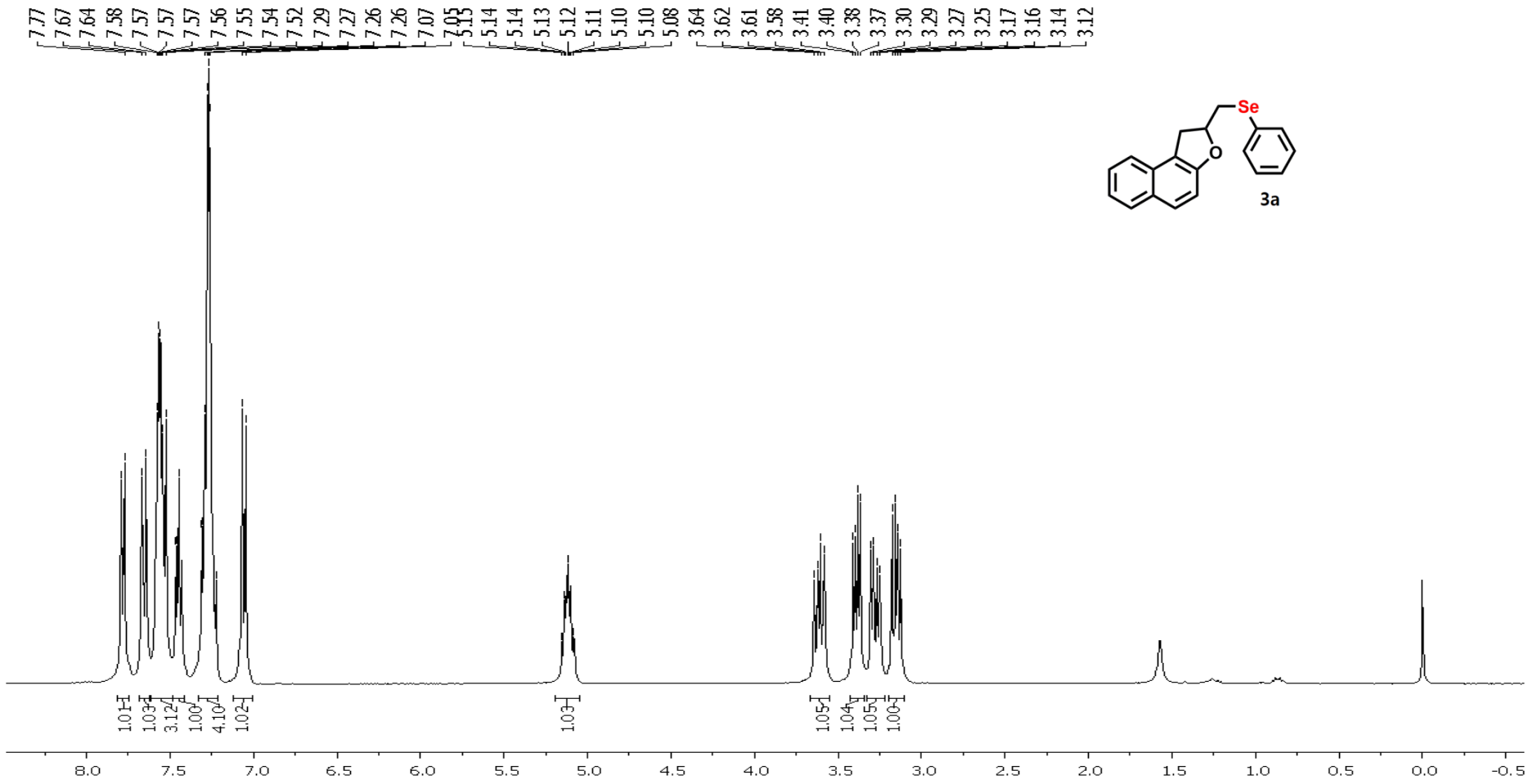
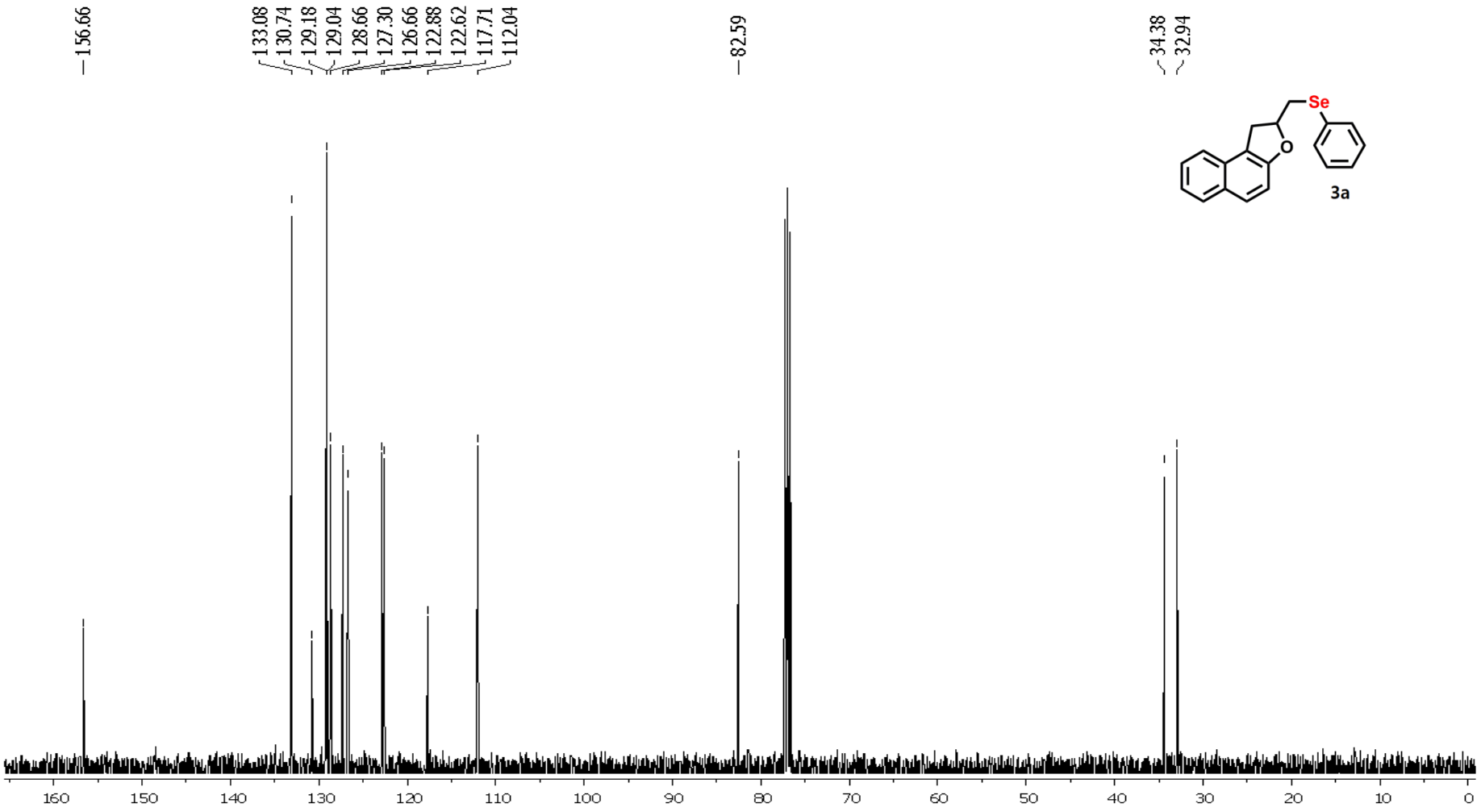


^{1}H NMR $CDCl_3$ spectra of Compound 3a



^{13}C NMR $CDCl_3$ spectra of Compound 3a

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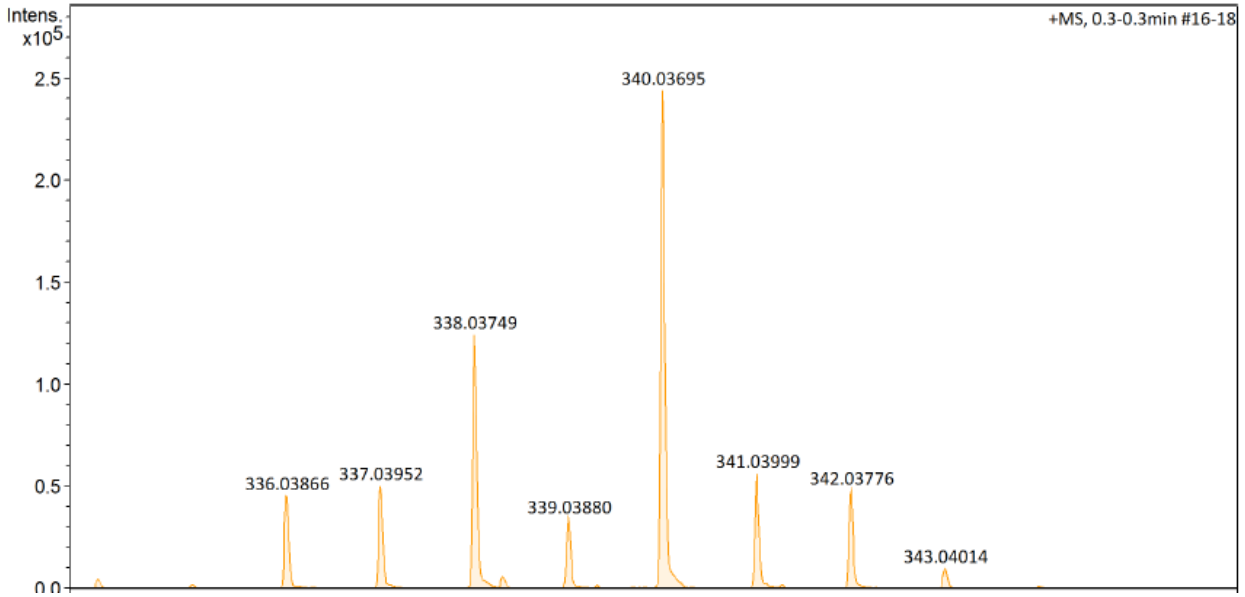

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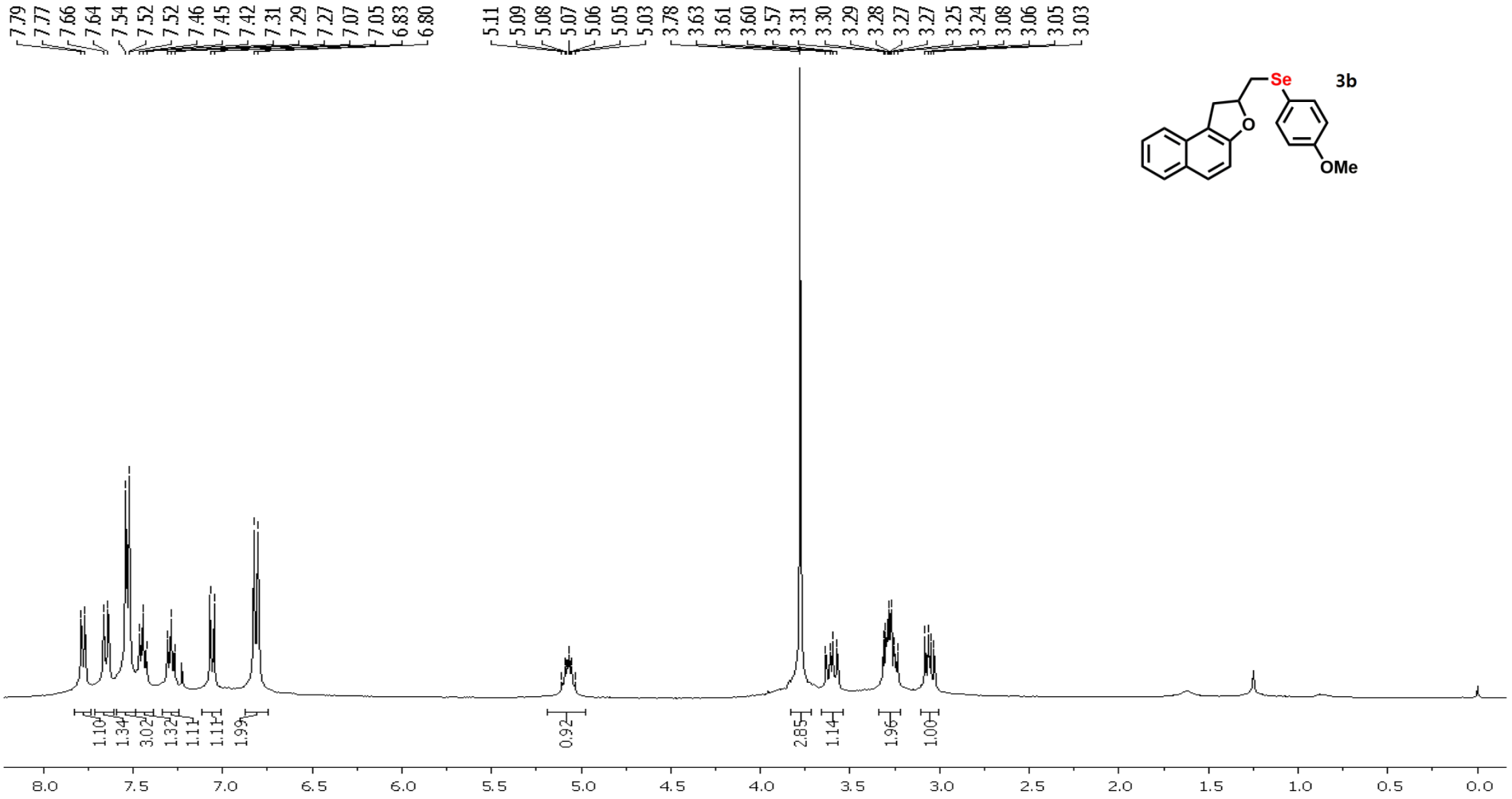

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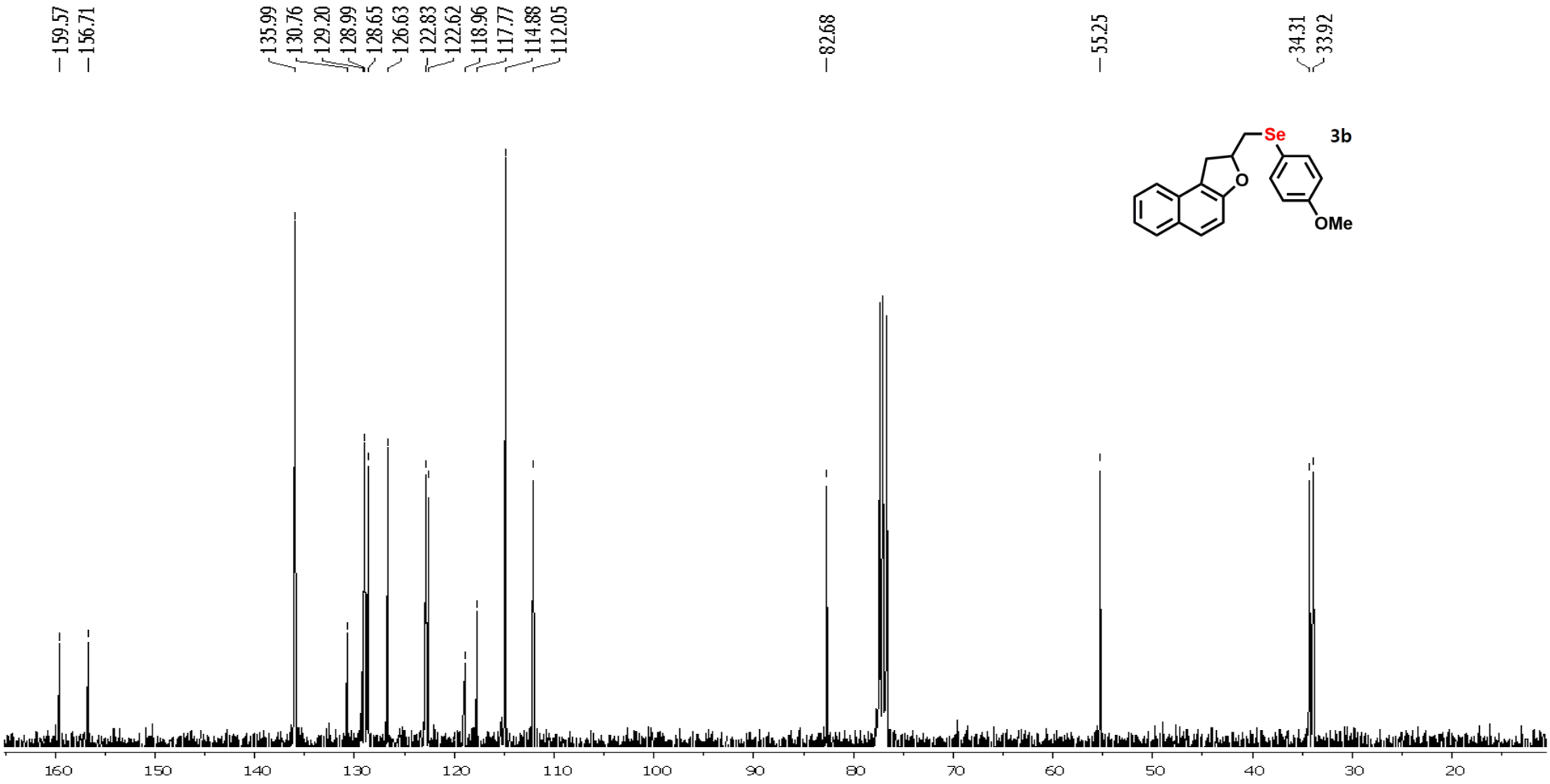

^{13}C NMR $CDCl_3$ spectra of Compound 3b

Display Report

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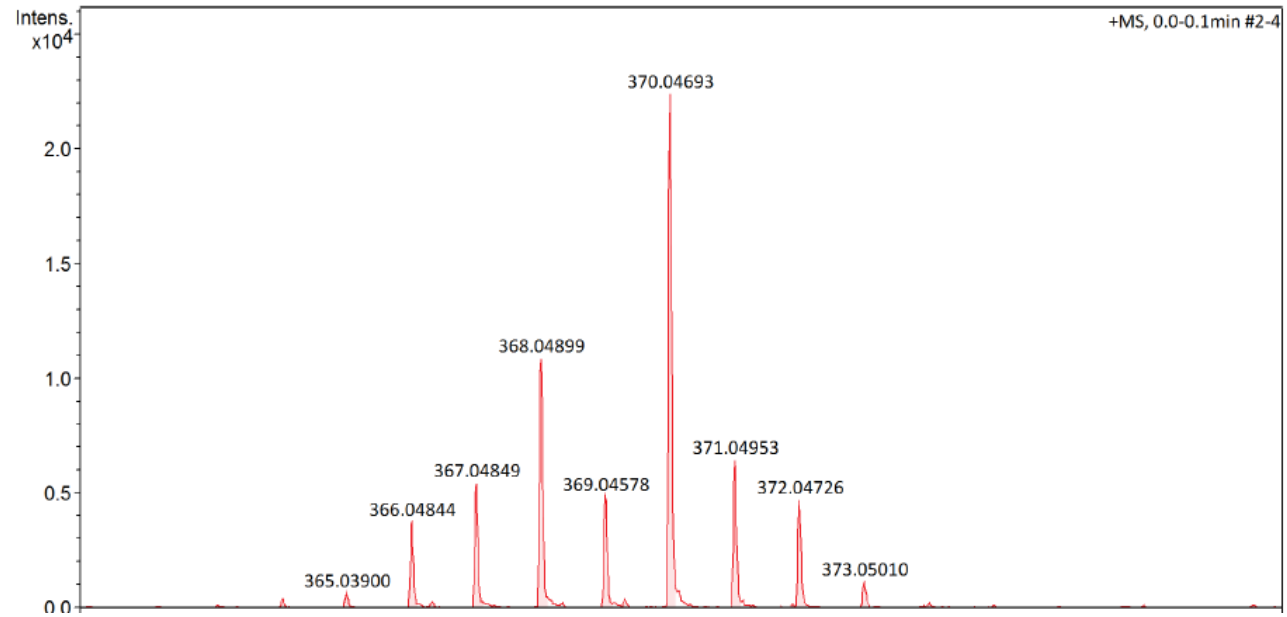
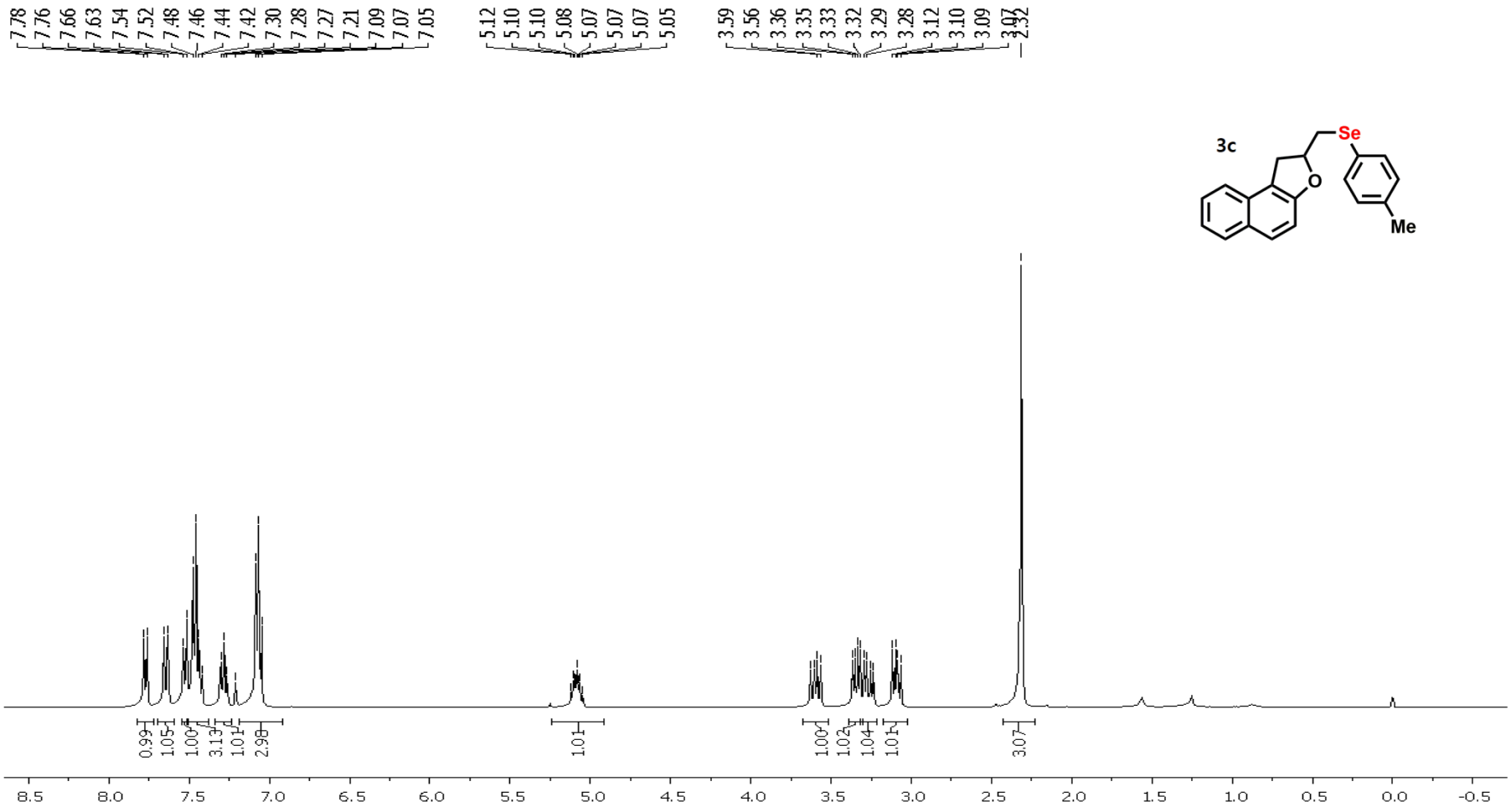
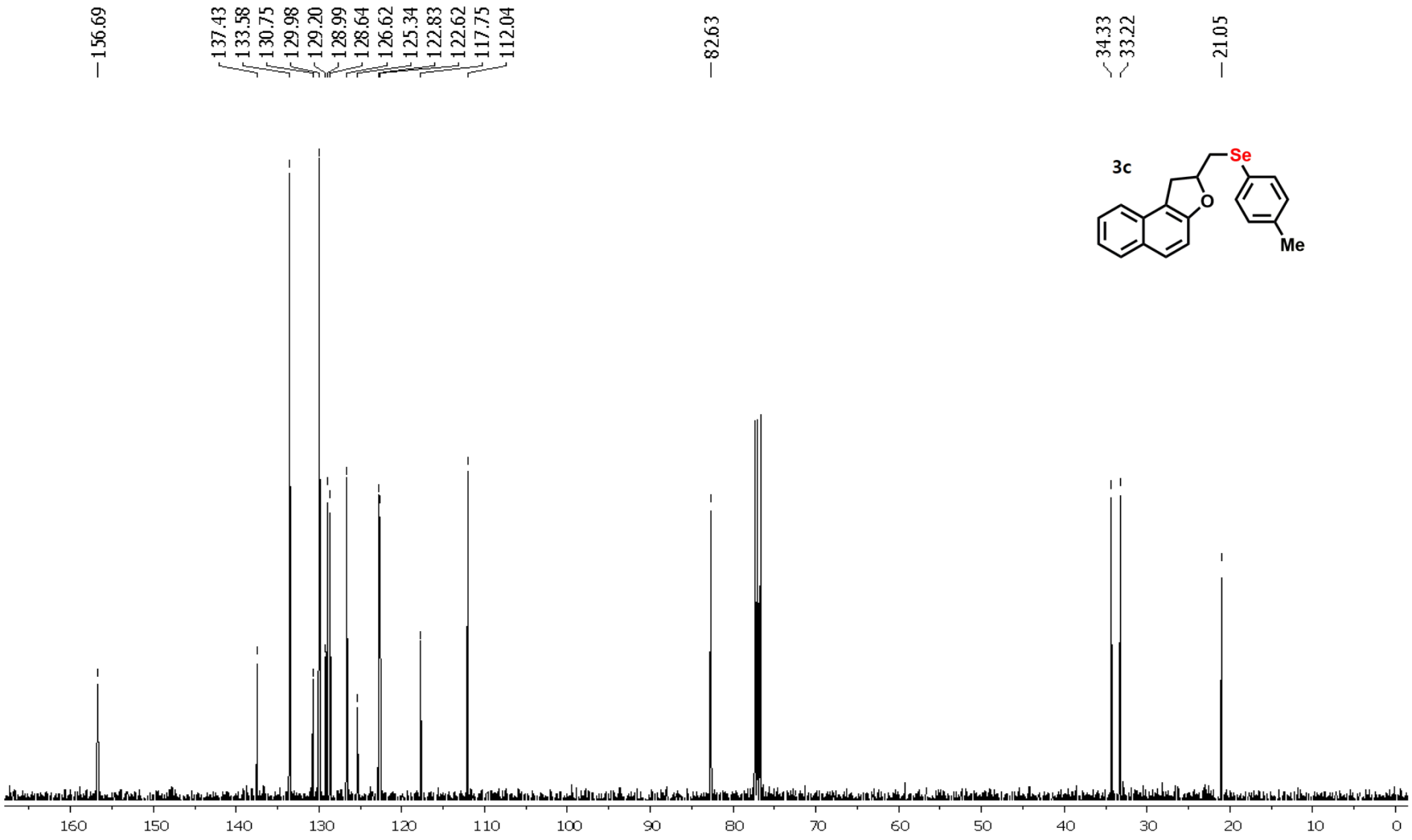


HRMS-APPI Spectrum of Compound 3b



^{1}H NMR $CDCl_3$ spectra of Compound 3c



^{13}C NMR $CDCl_3$ spectra of Compound 3c

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Analysis Info

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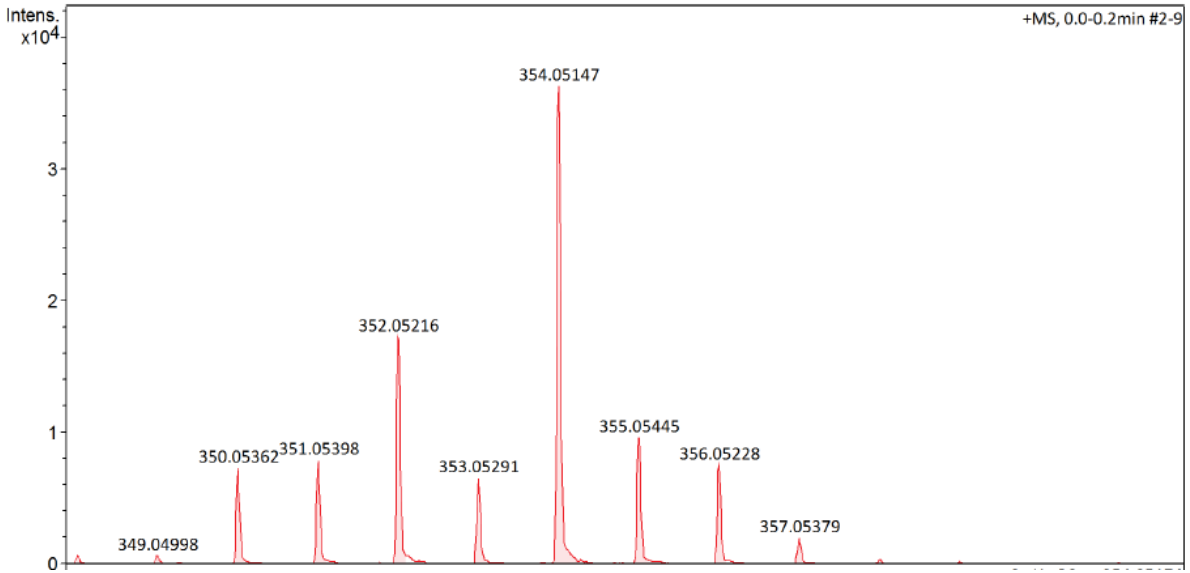
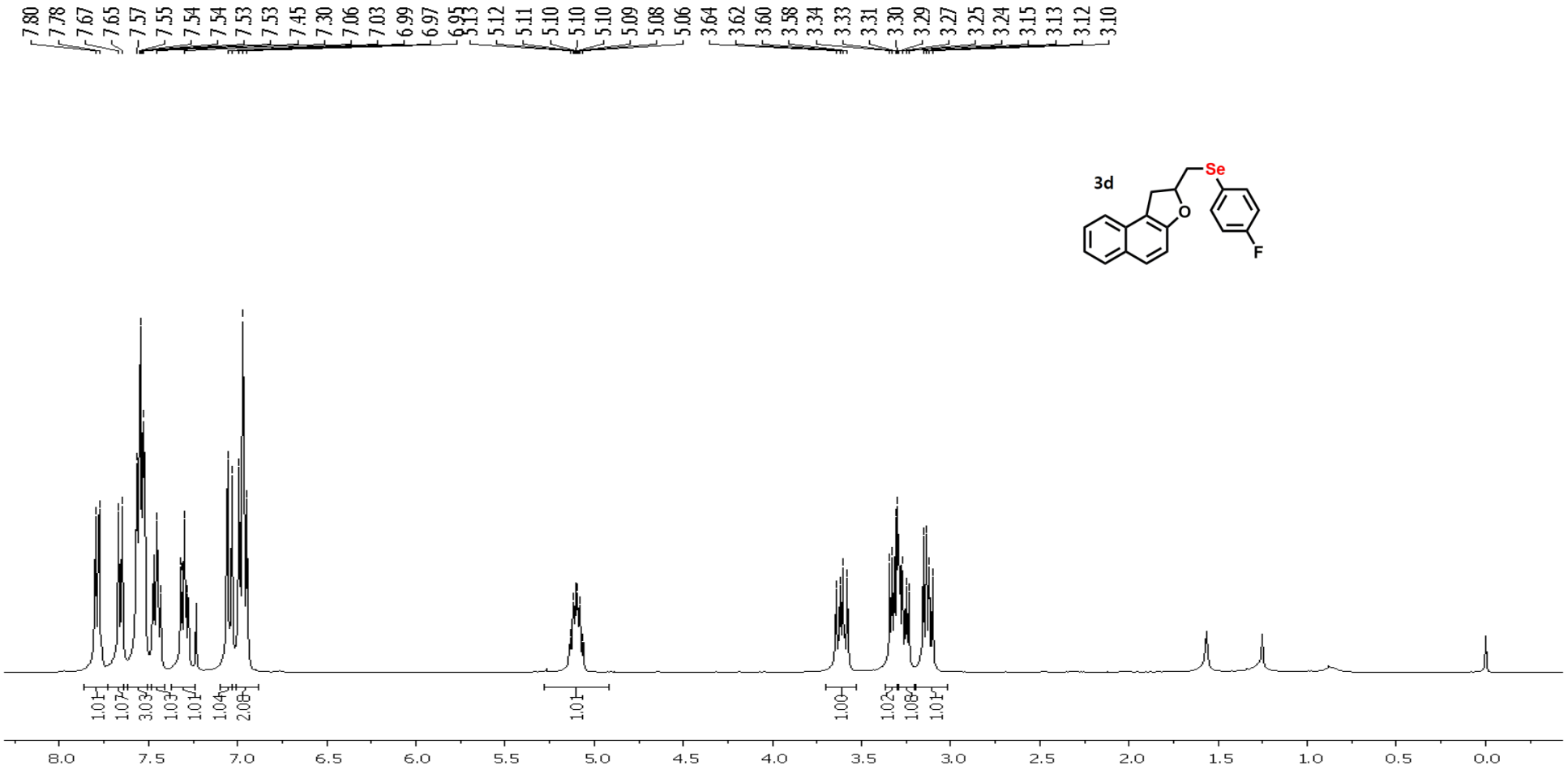
Method	tune low appi 10 06 19 Vanessa.m	Operator	micrOTOF-QII
Sample Name	286b	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

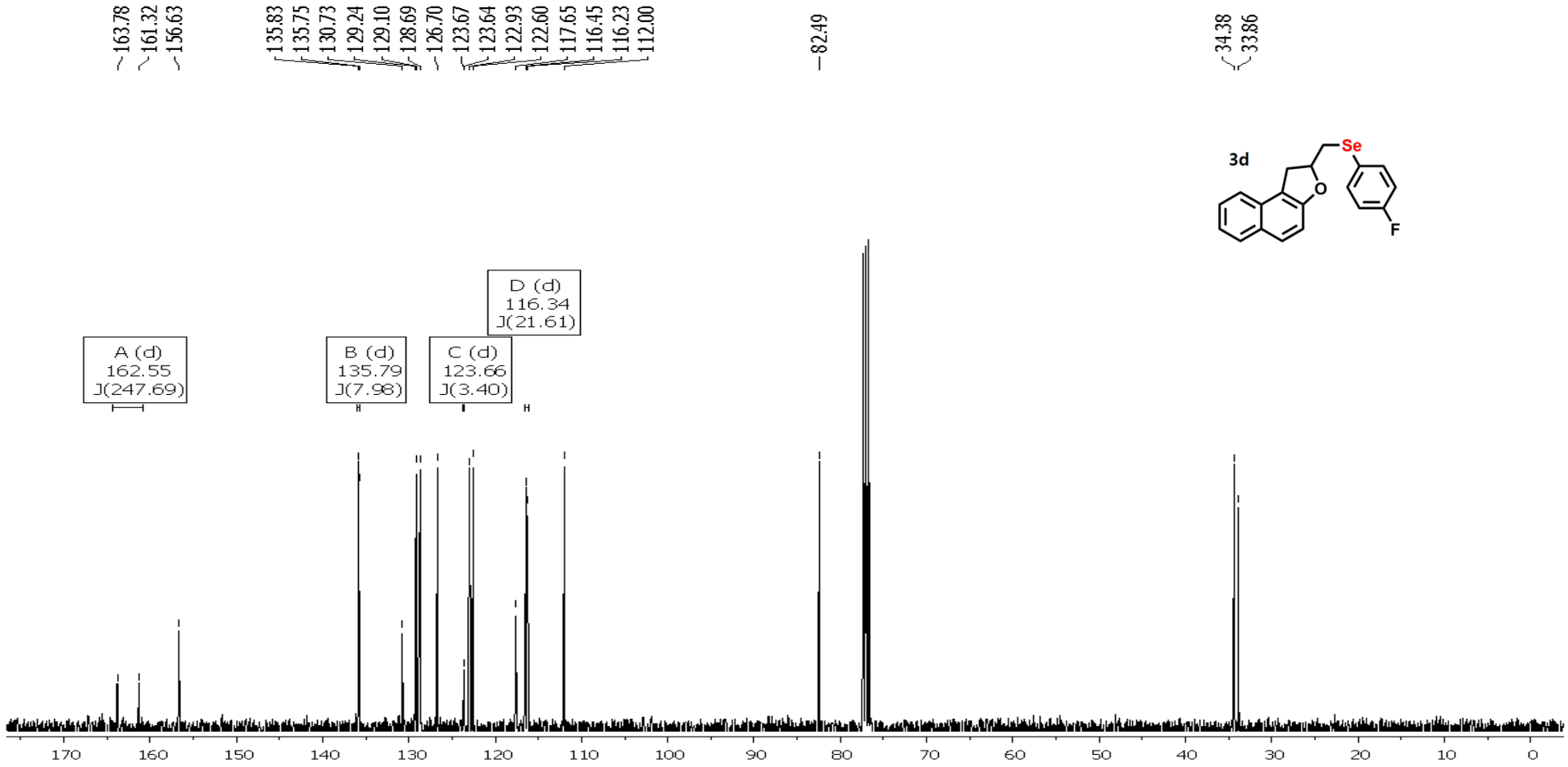
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 3c



^{1}H NMR $CDCl_3$ spectra of Compound 3d



^{13}C NMR $CDCl_3$ spectra of Compound 3d

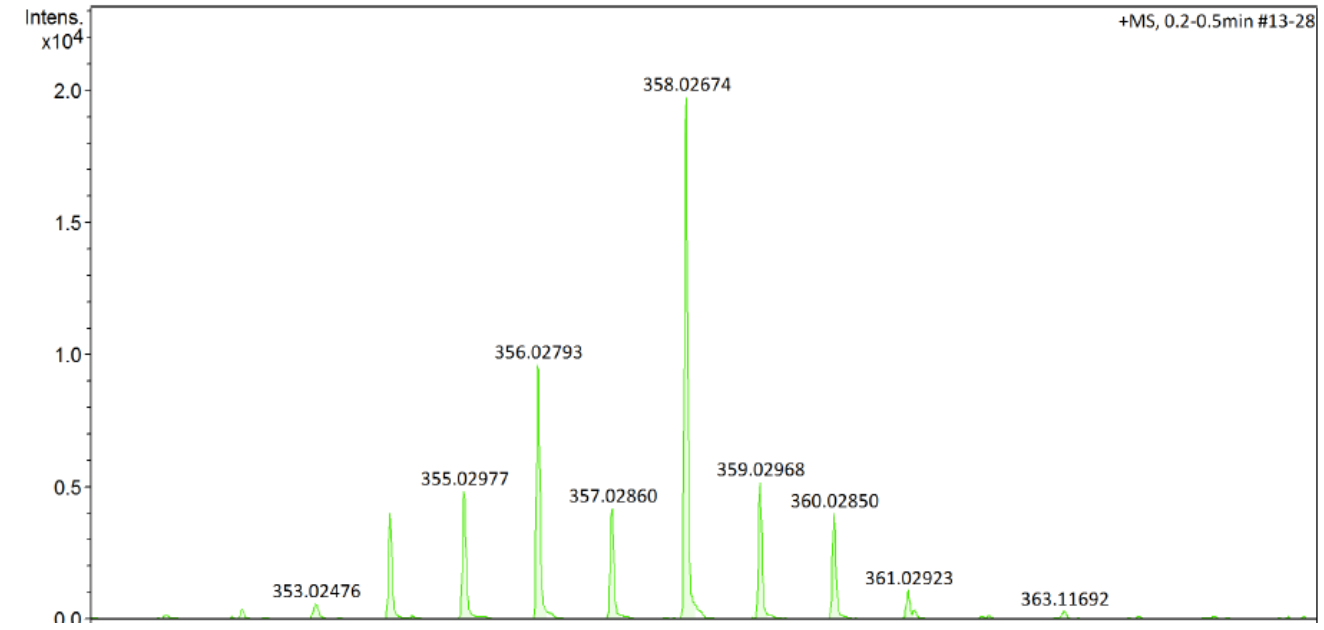
Display Report

Analysis Info

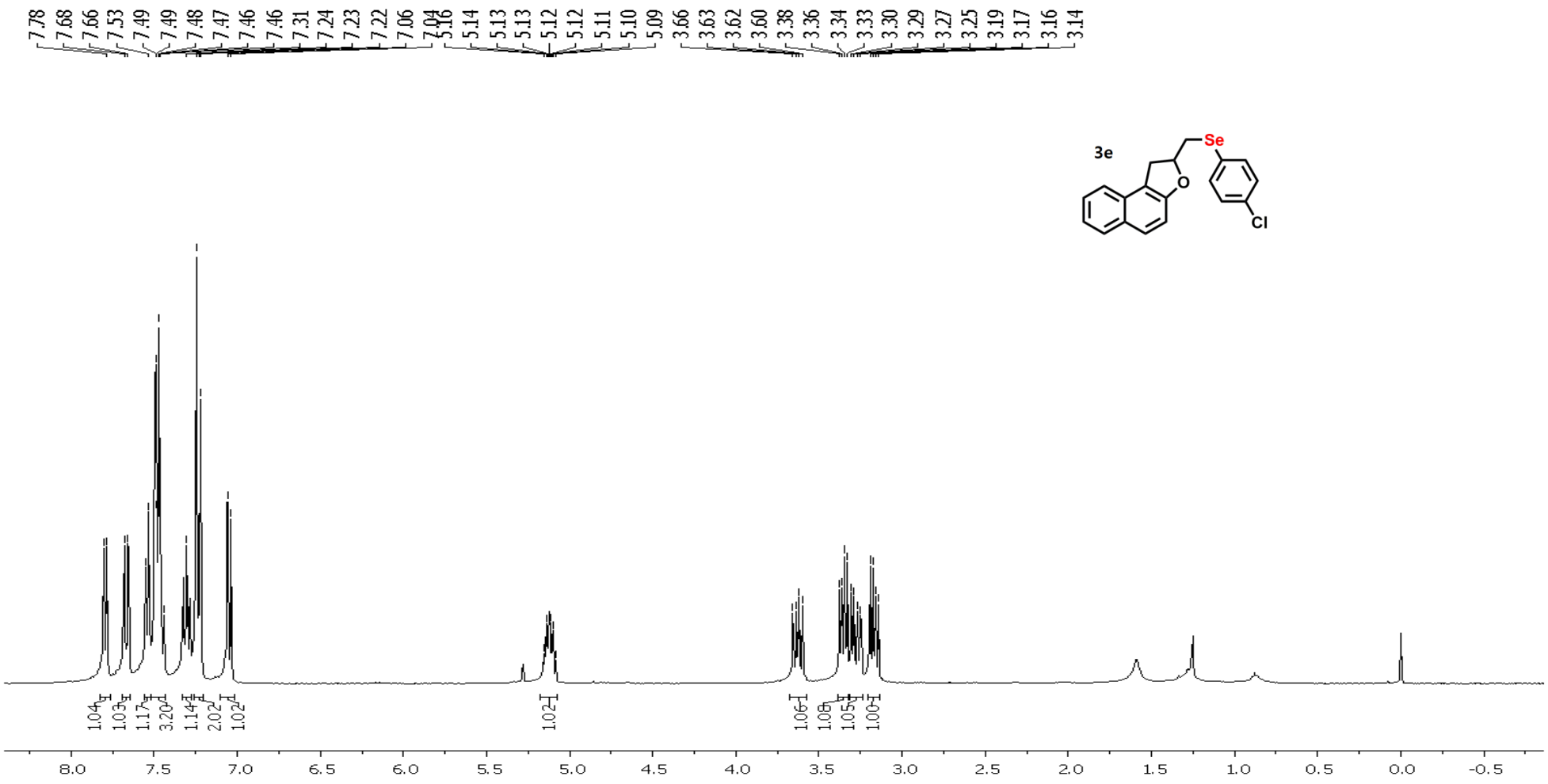
Analysis Name	D:\Data\2019\Q-TOF\UFSC\LabSELEN\ MARCOS LABSELEN QMC-CFM 20-11-2019 - x analises\286e000002.d	Acquisition Date	11/20/2019 5:48:26 PM
Method	tune low appi 10 06 19 Vanessa.m	Operator	micrOTOF-QII
Sample Name	286e	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

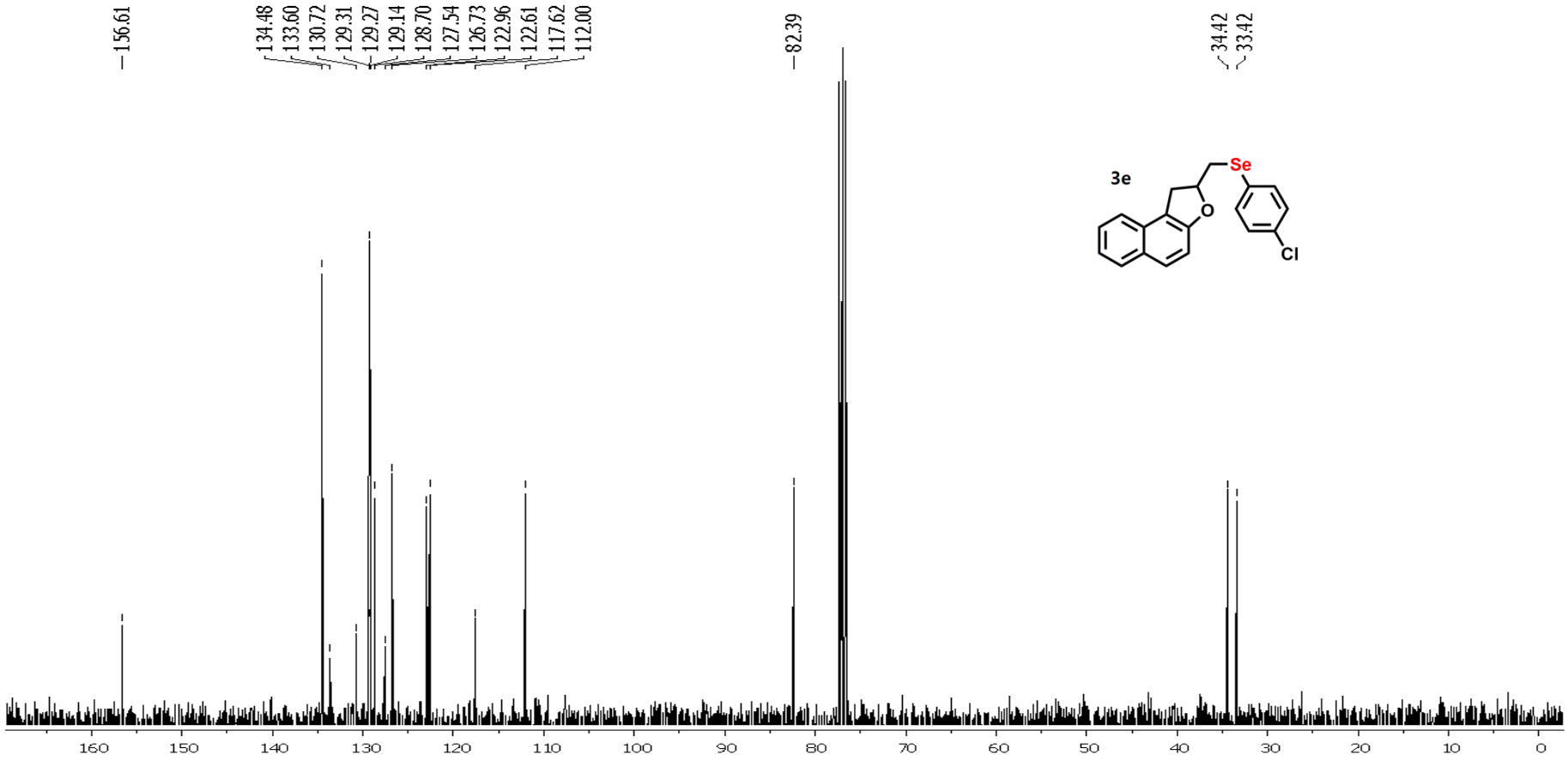
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 3d



^{1}H NMR $CDCl_3$ spectra of Compound 3e



^{13}C NMR $CDCl_3$ spectra of Compound 3e

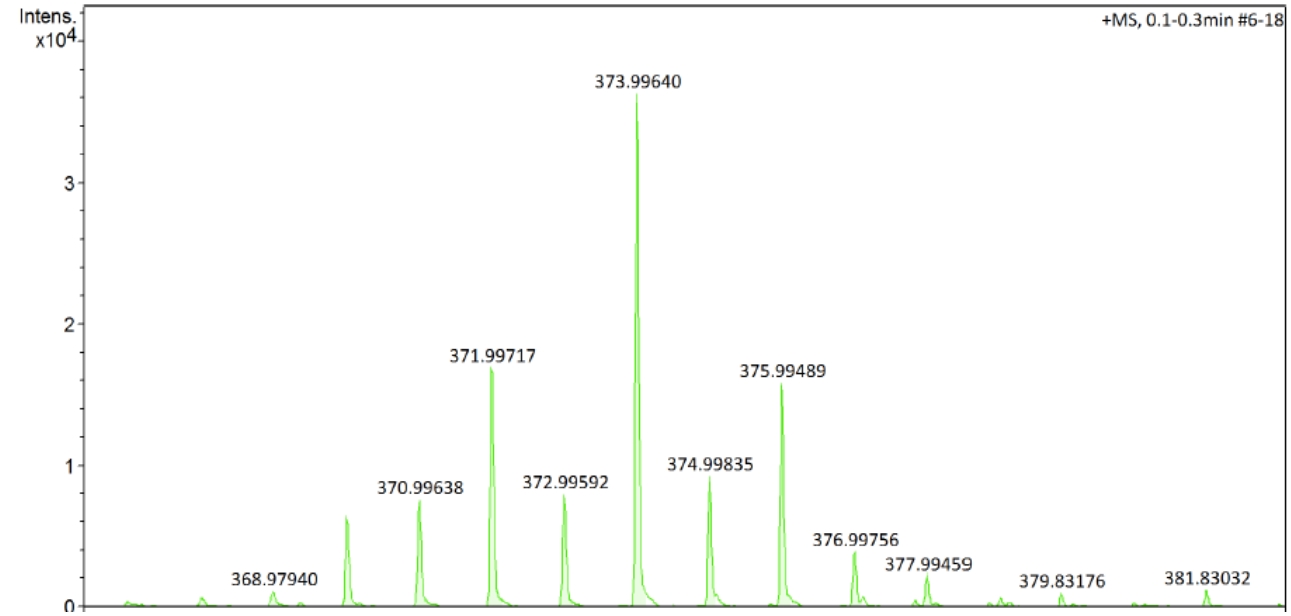
Display Report

Analysis Info

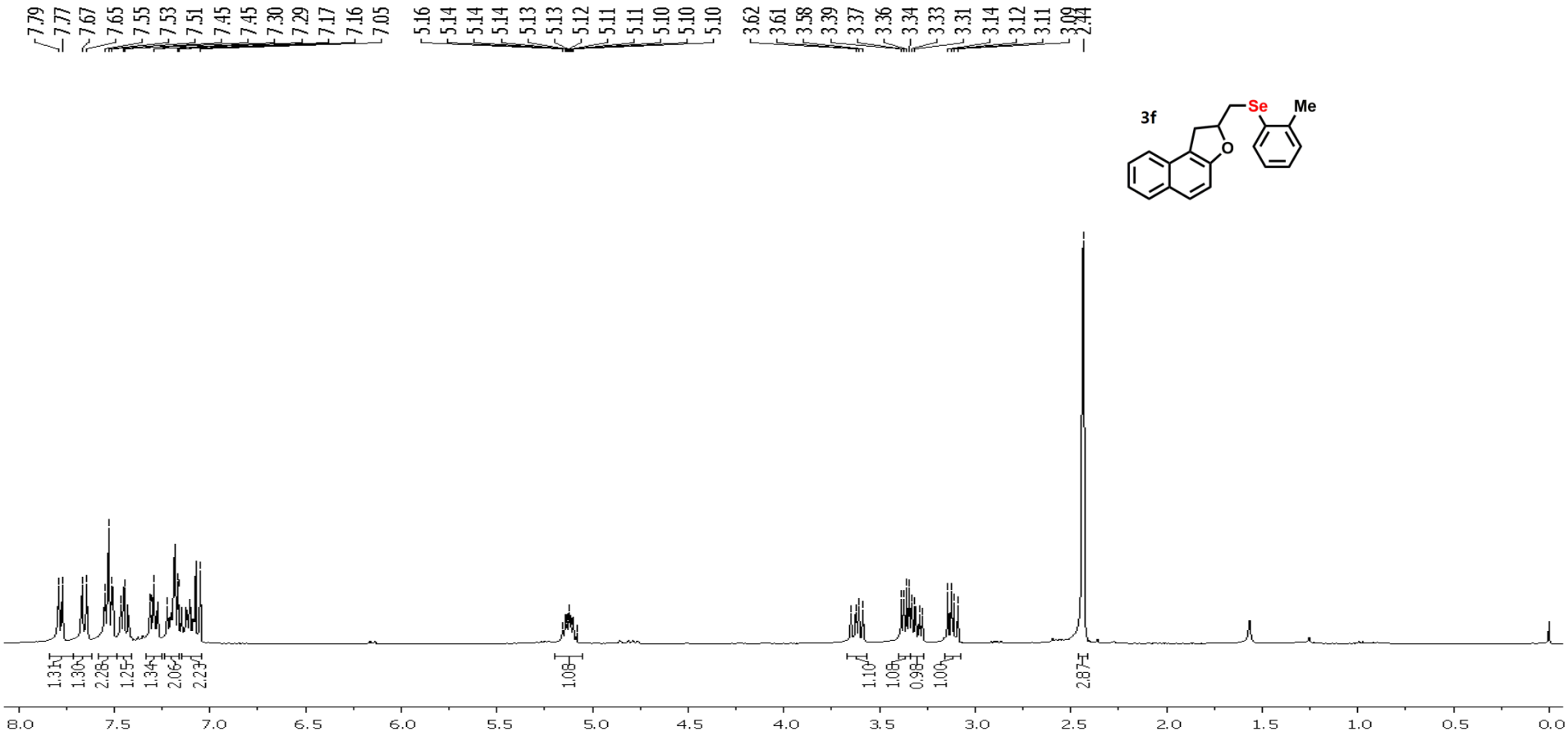
Analysis Name	D:\Data\2019\Q-TOF\UFSC\LabSELEN\ MARCOS LABSELEN QMC-CFM 20-11-2019 - x analises\286a000002.d	Acquisition Date	11/20/2019 6:13:05 PM
Method	tune low appi 10 06 19 Vanessa.m	Operator	micrOTOF-QII
Sample Name	286a	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

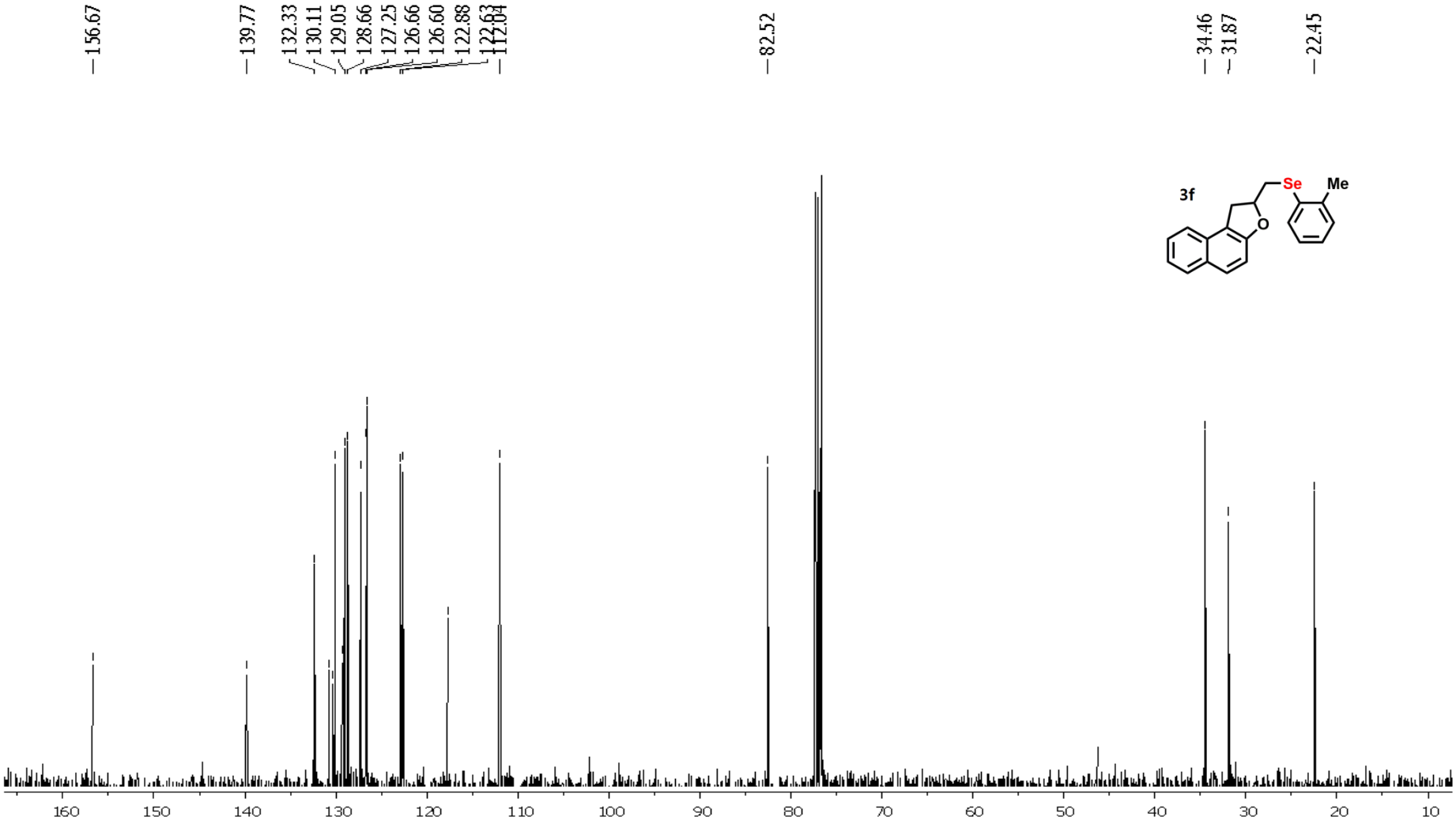
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 3e



^{1}H NMR $CDCl_3$ spectra of Compound 3f



^{13}C NMR $CDCl_3$ spectra of Compound 3f

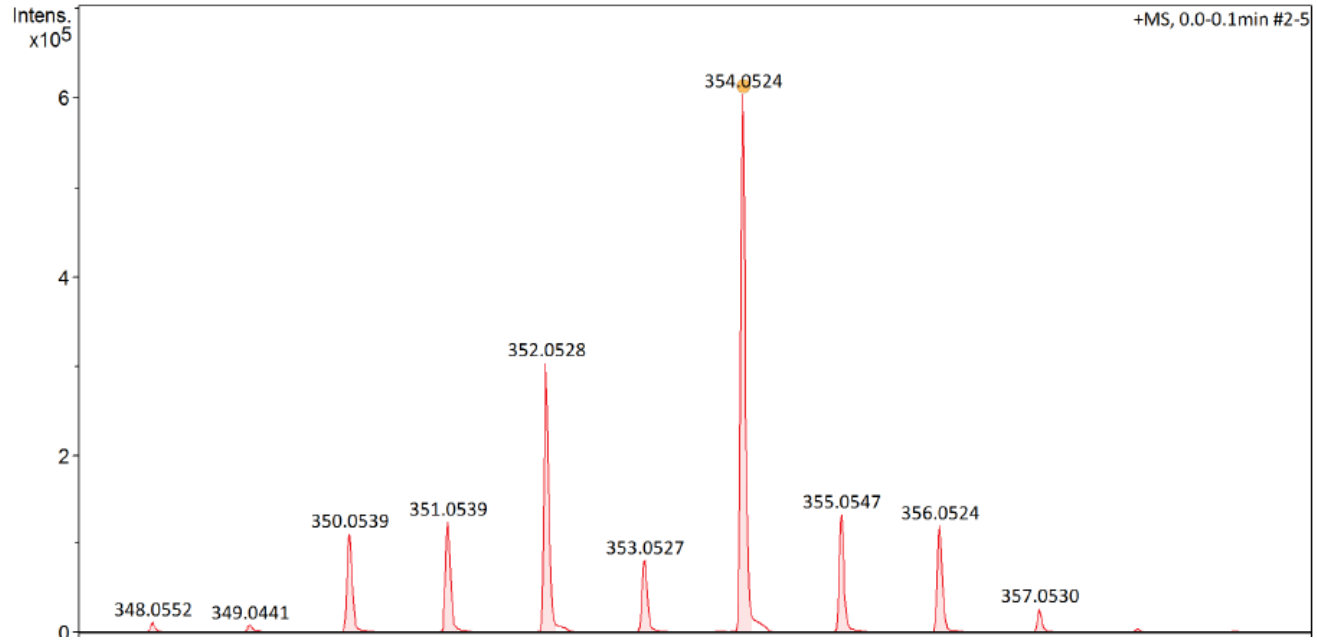
Display Report

Analysis Info

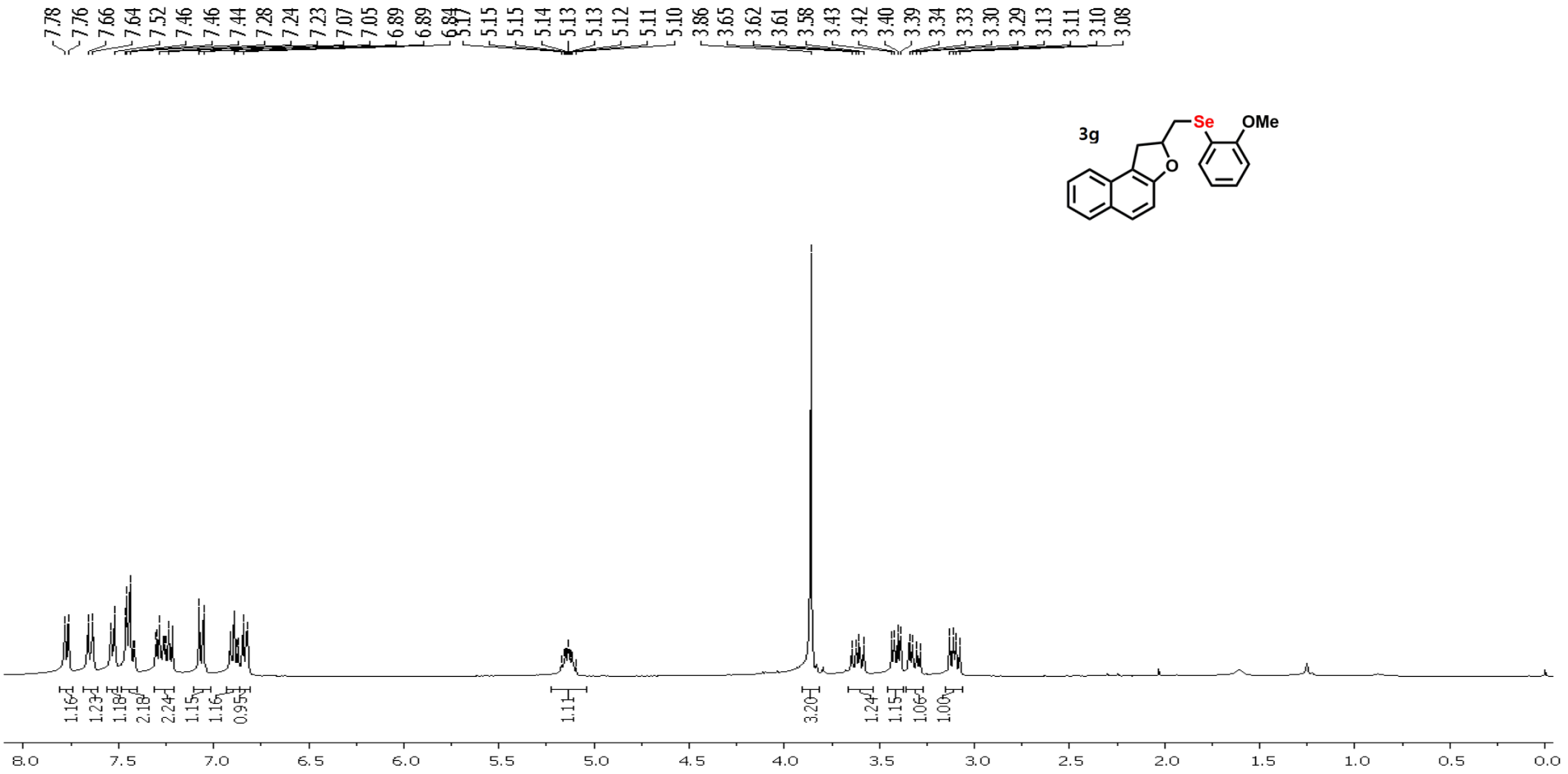
Analysis Name	D:\Data\2020\Q-TOF\UFSC\LabSELEN\LABSELEN QMC-CFM 22-01-2020 - x analises\MR-286m000002.d	Acquisition Date	1/22/2020 12:48:11 PM
Method	appi 22 11 19 VANESSA.m	Operator	micrOTOF-QII
Sample Name	MR-286m	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

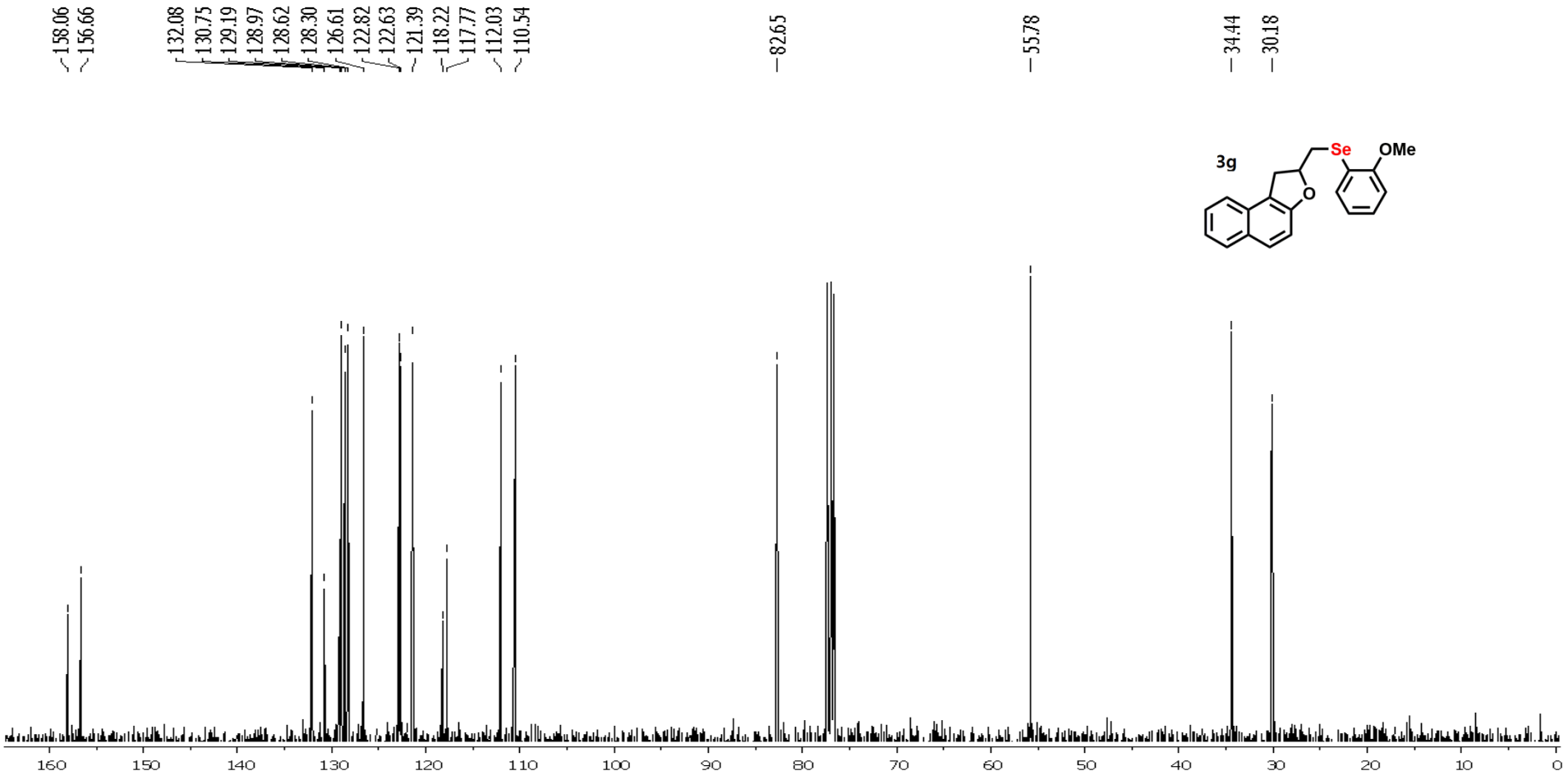
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 3f



^{1}H NMR $CDCl_3$ spectra of Compound 3g



^{13}C NMR $CDCl_3$ spectra of Compound 3g

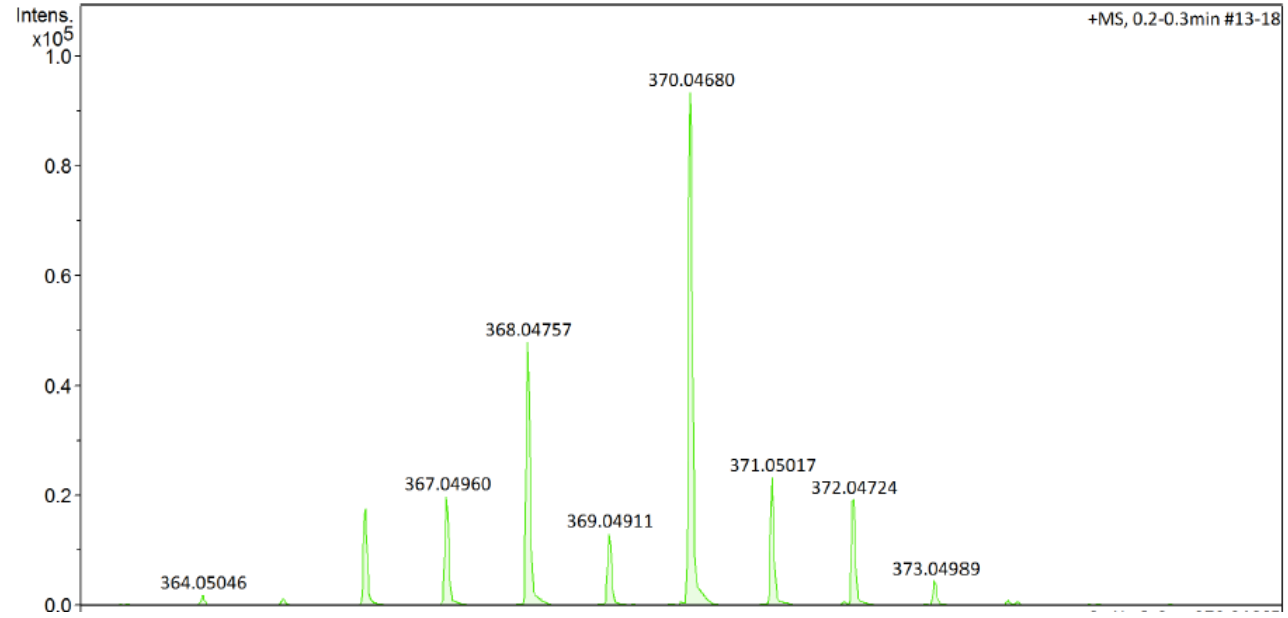
Display Report

Analysis Info

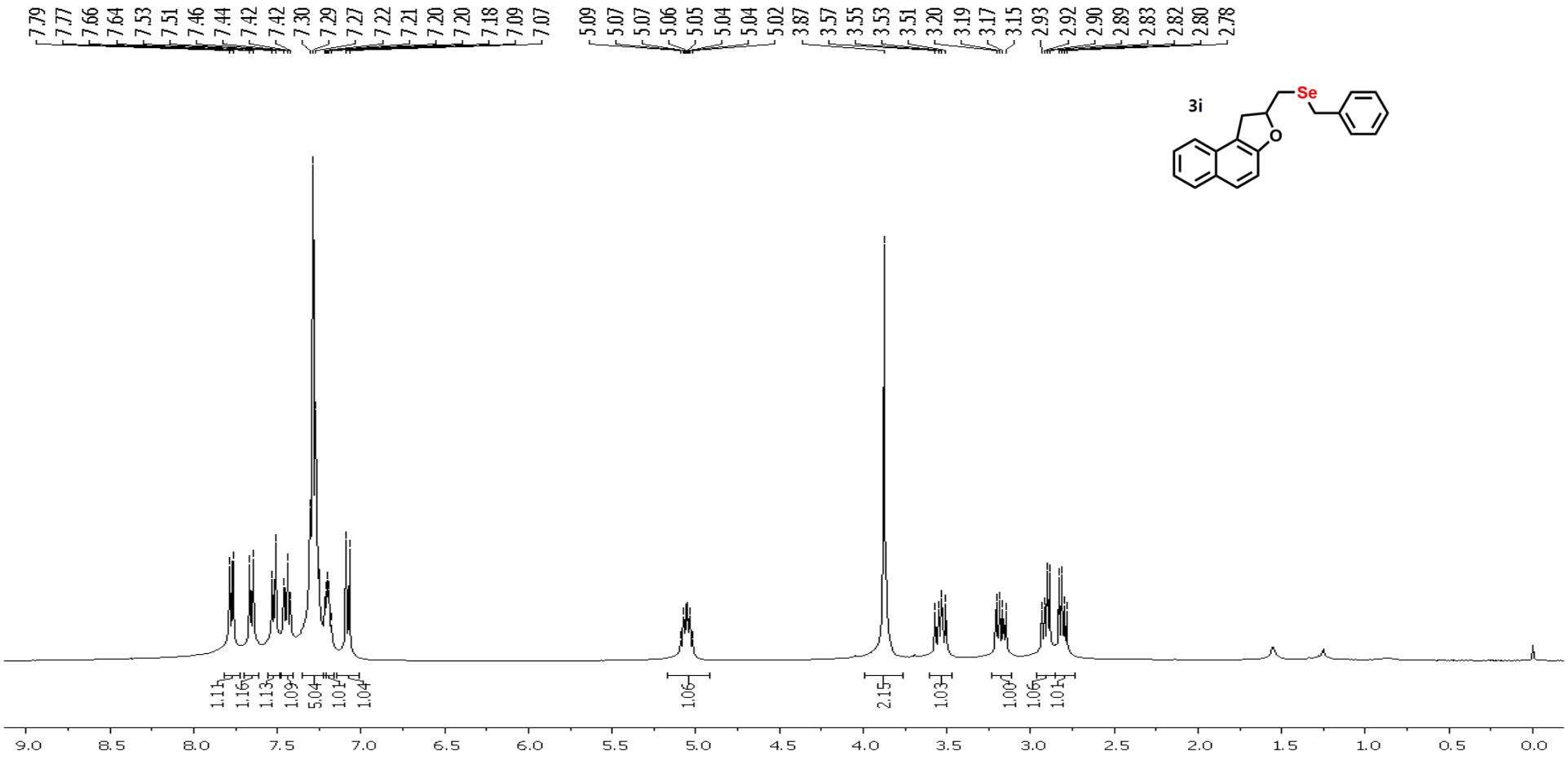
Analysis Name	D:\Data\2019\Q-TOF\UFSC\LabSELEN\ MARCOS LABSELEN QMC-CFM 20-11-2019 - x analises\286k000002.d	Acquisition Date	11/20/2019 6:23:05 PM
Method	tune low appi 10 06 19 Vanessa.m	Operator	micrOTOF-QII
Sample Name	286k	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

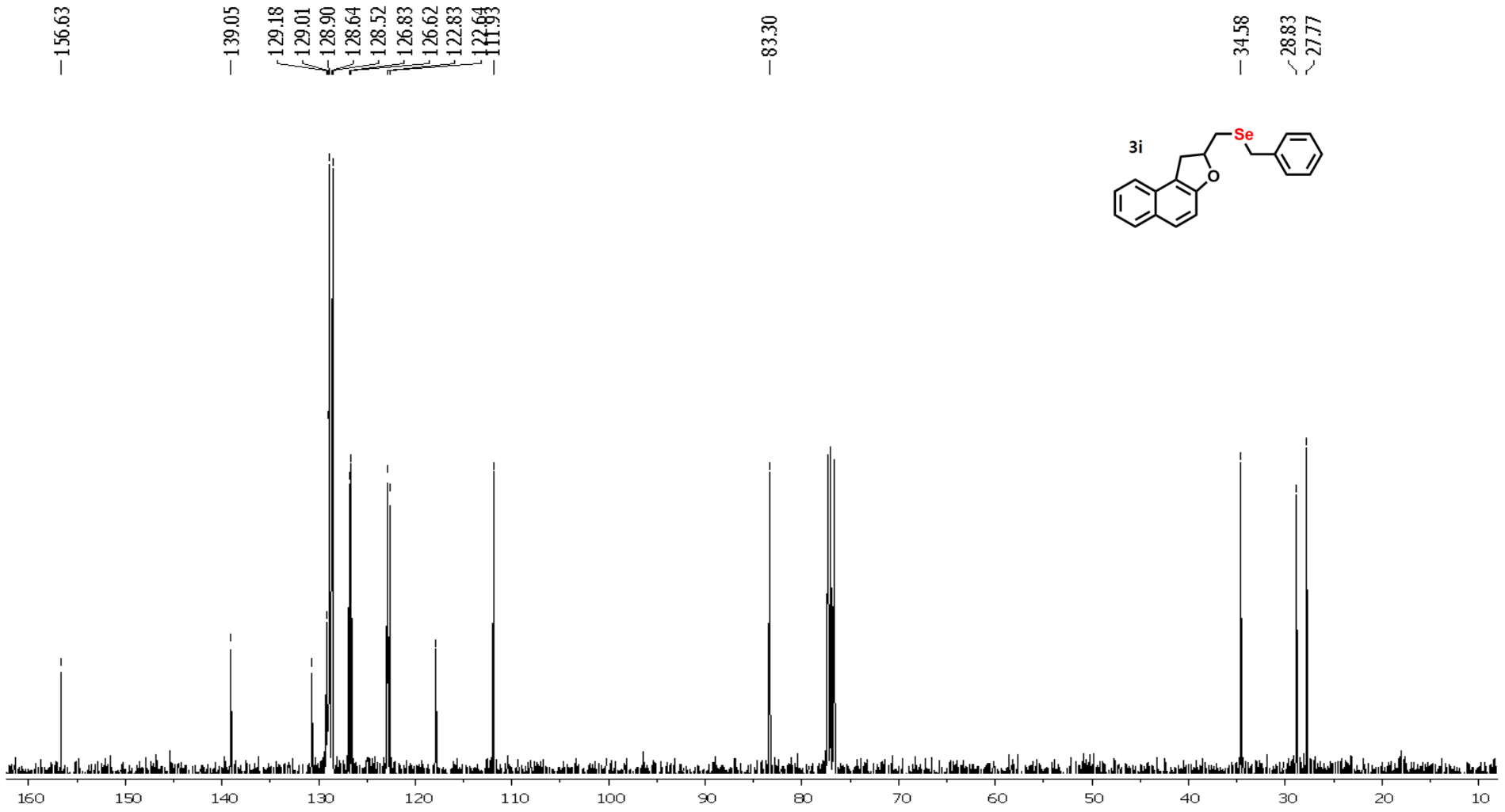
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 3g



^{1}H NMR $CDCl_3$ spectra of Compound 3i



^{13}C NMR $CDCl_3$ spectra of Compound 3i

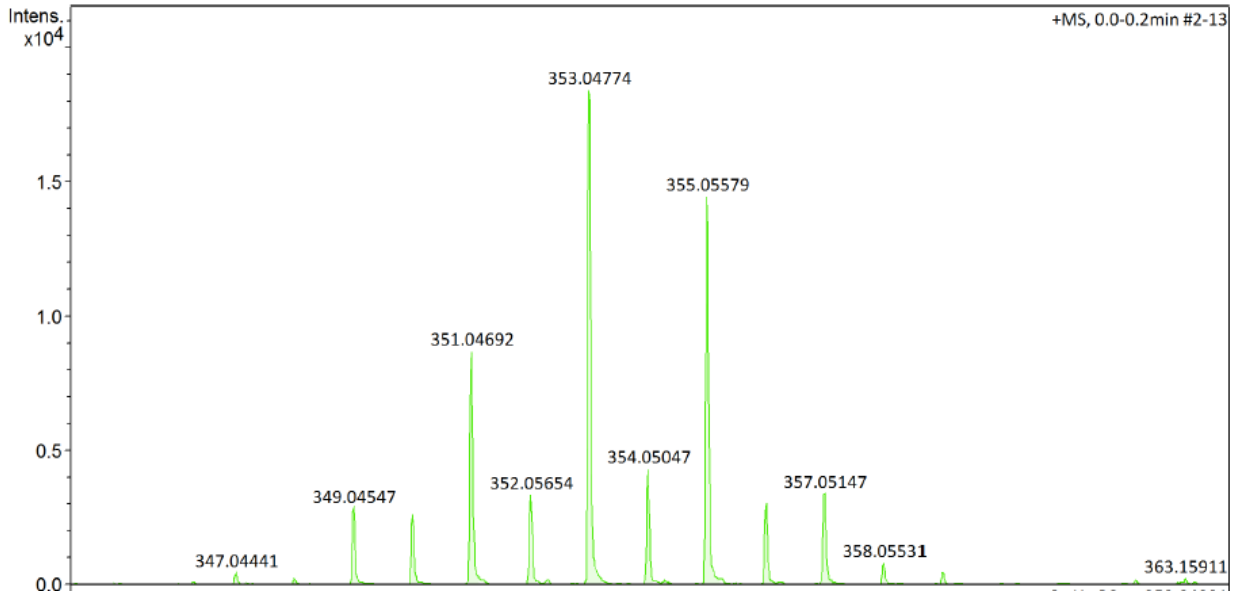
Display Report

Analysis Info

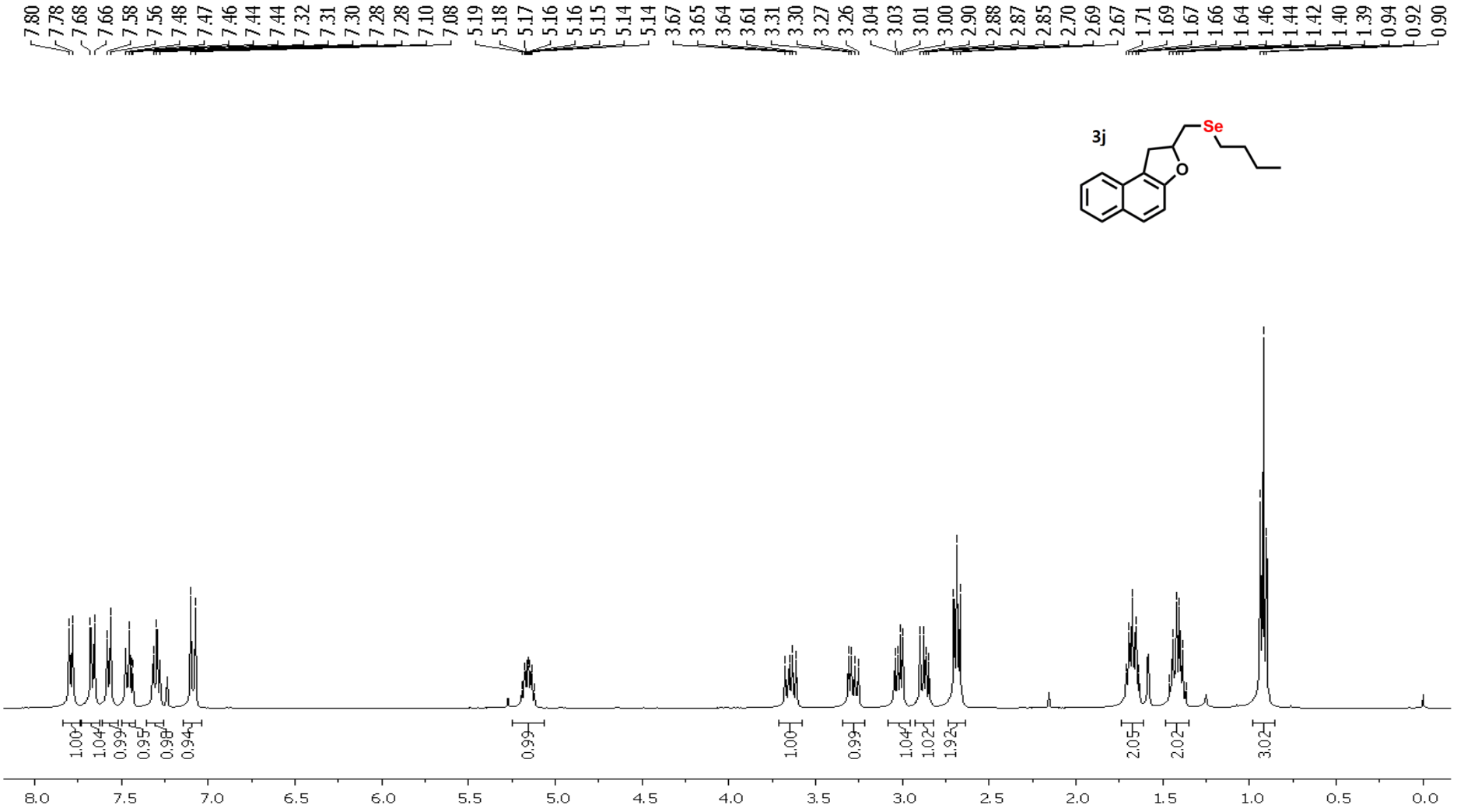
Analysis Name	D:\Data\2019\Q-TOF\UFSC\LabSELEN\ MARCOS LABSELEN QMC-CFM 20-11-2019 - x analises\286c000002.d	Acquisition Date	11/20/2019 5:04:39 PM
Method	tune low appi 10 06 19 Vanessa.m	Operator	micrOTOF-QII
Sample Name	286c	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

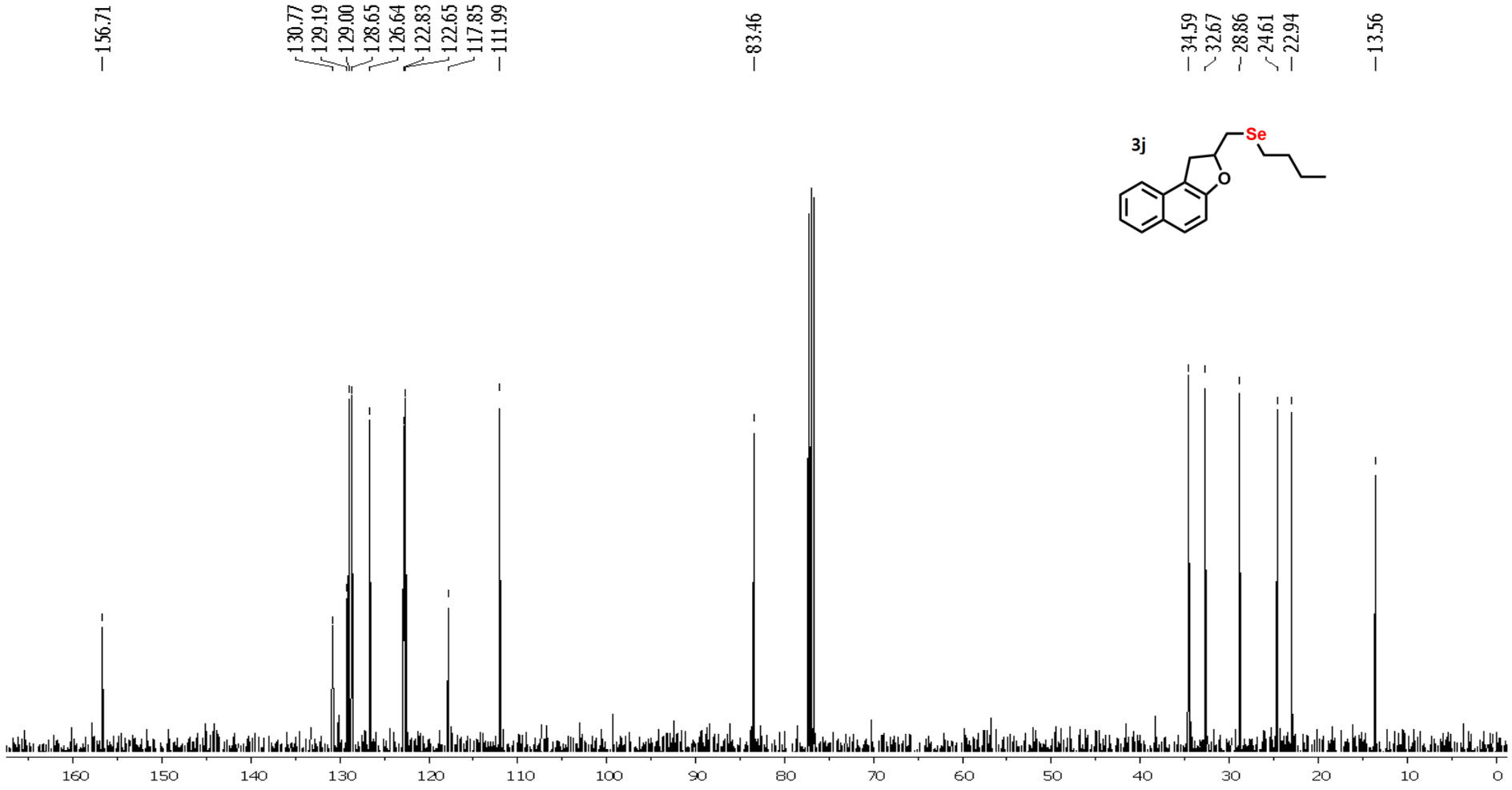
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 3i



^{1}H NMR $CDCl_3$ spectra of Compound 3j



^{13}C NMR $CDCl_3$ spectra of Compound 3j

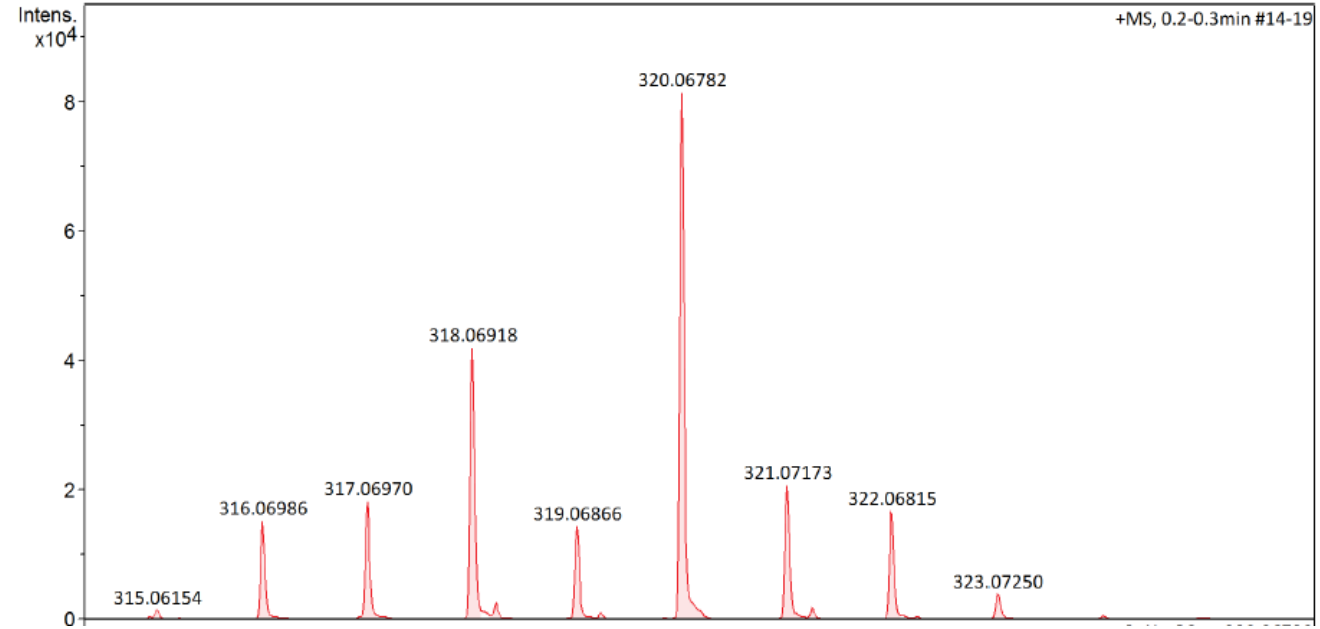
Display Report

Analysis Info

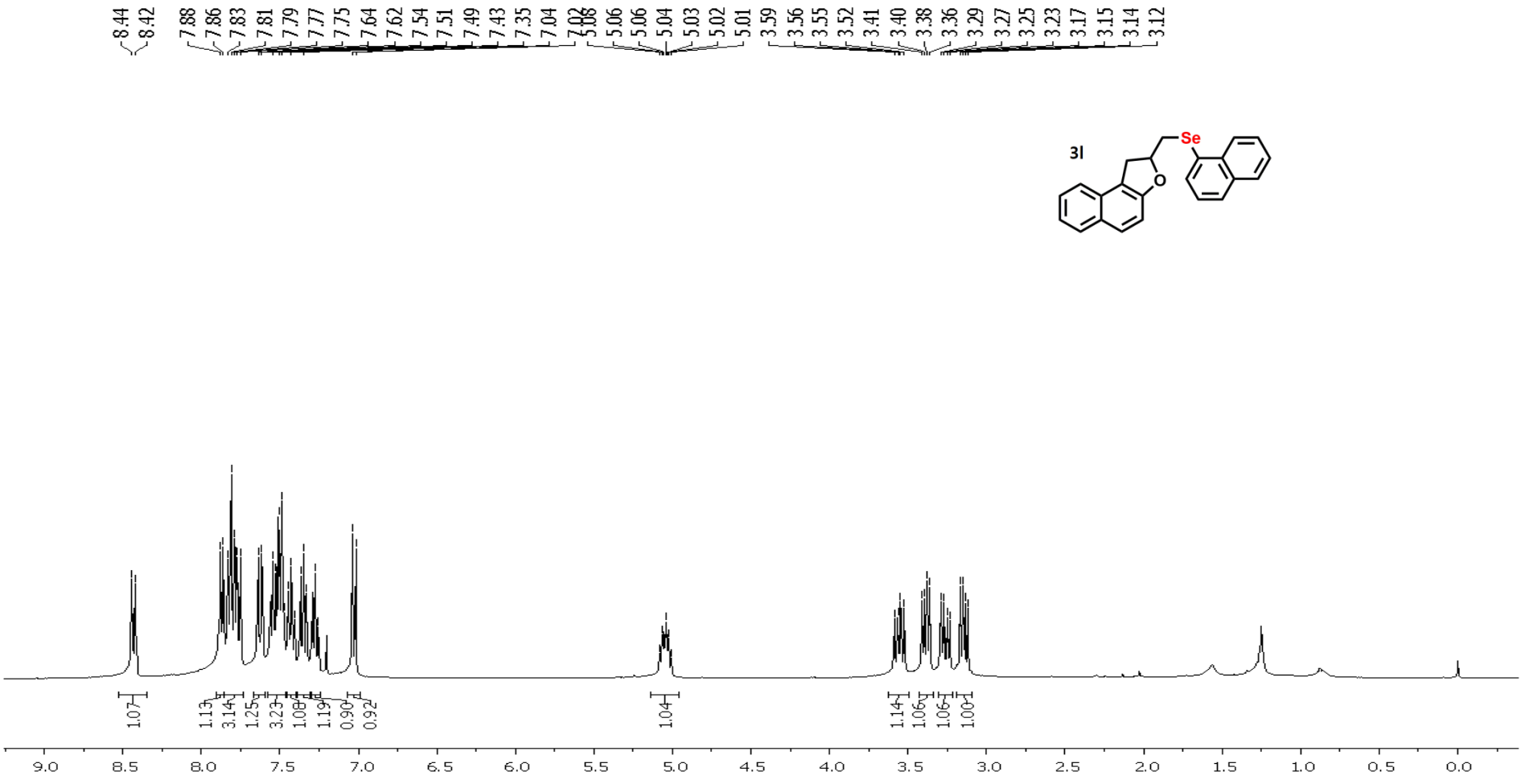
Analysis Name	D:\Data\2019\Q-TOF\UFSC\LabSELEN\ MARCOS LABSELEN QMC-CFM 20-11-2019 - x analises\286i000001.d	Acquisition Date	11/20/2019 6:45:27 PM
Method	tune low appi 10 06 19 Vanessa.m	Operator	micrOTOF-QII
Sample Name	286i	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

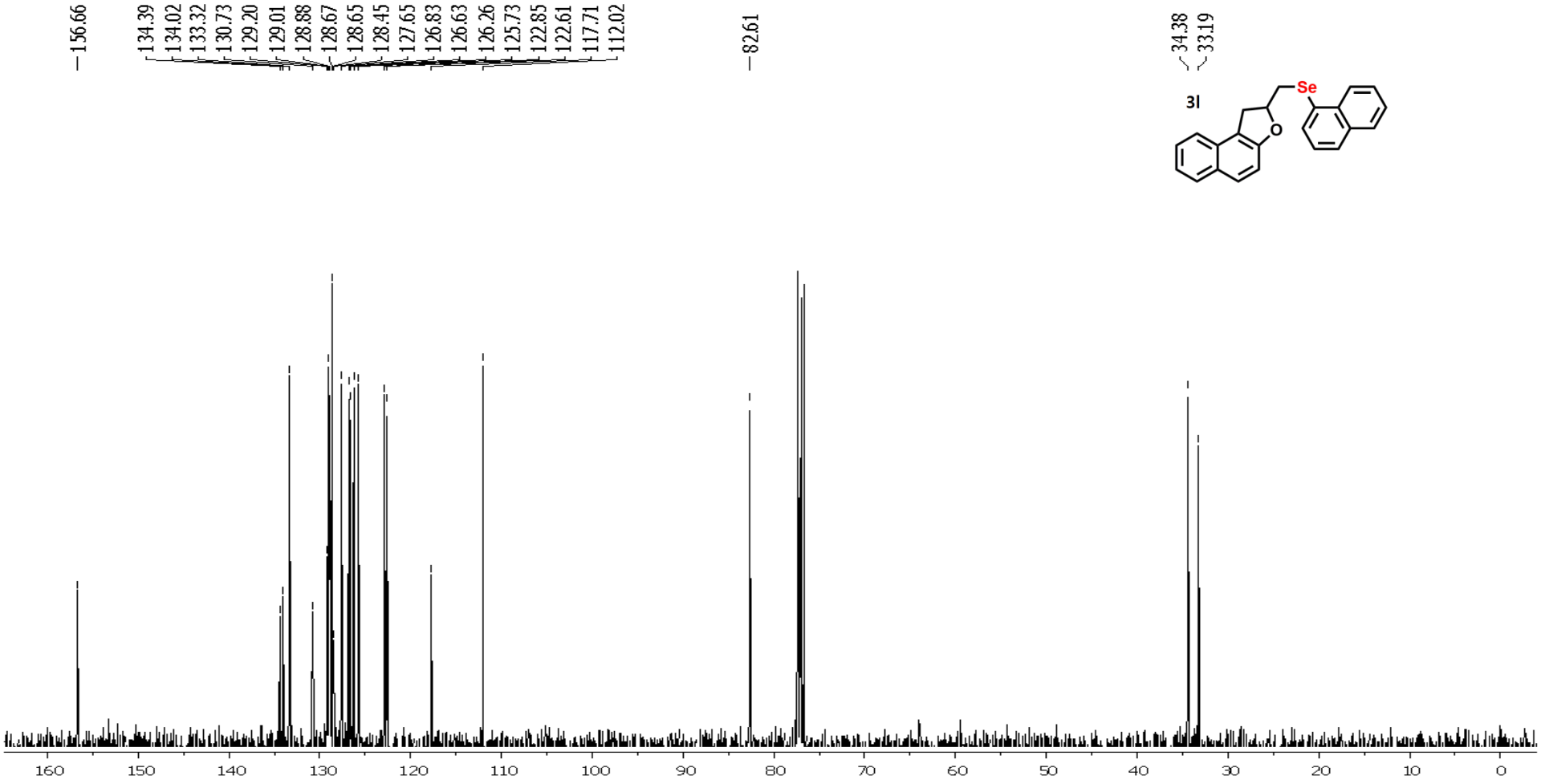
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 3j



^{1}H NMR $CDCl_3$ spectra of Compound 3l



^{13}C NMR $CDCl_3$ spectra of Compound 3l

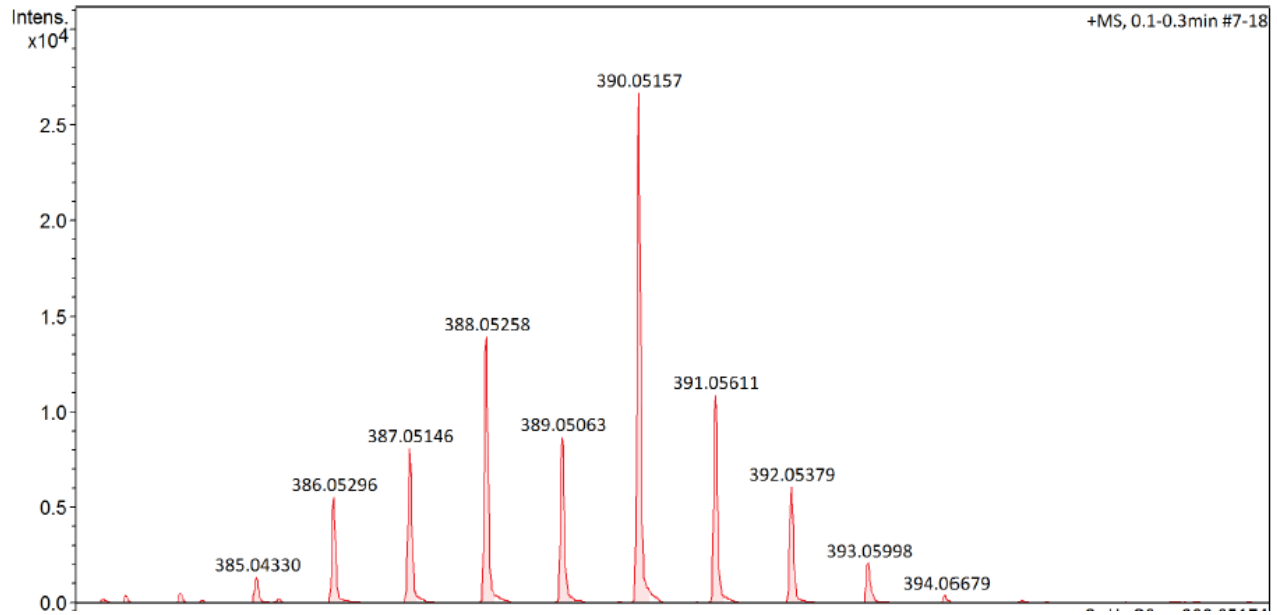
Display Report

Analysis Info

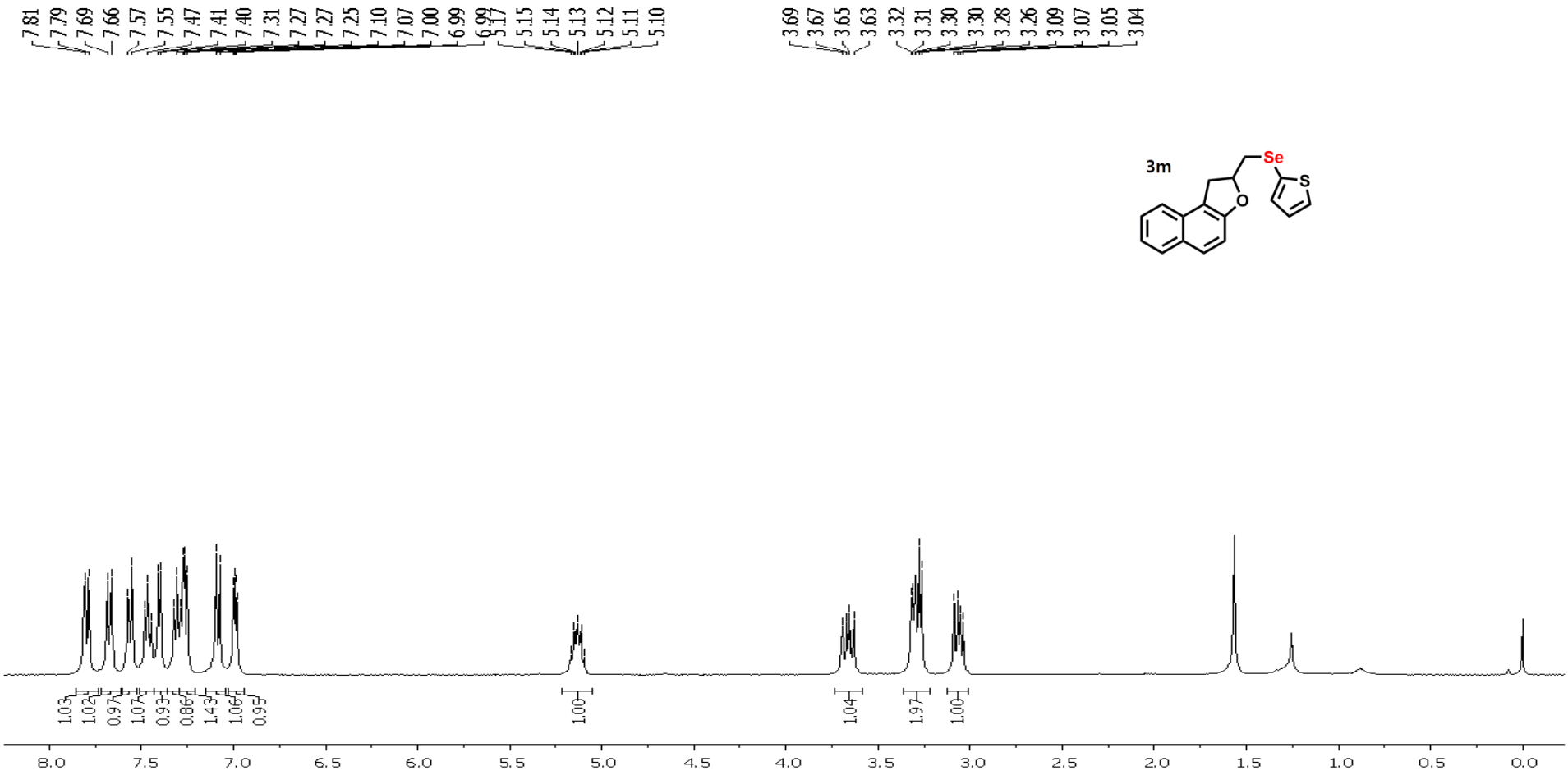
Analysis Name	D:\Data\2019\Q-TOF\UFSC\LabSELEN\ MARCOS LABSELEN QMC-CFM 20-11-2019 - x analises\286d000001.d	Acquisition Date	11/20/2019 4:44:51 PM
Method	tune low appi 10 06 19 Vanessa.m	Operator	micrOTOF-QII
Sample Name	286d	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

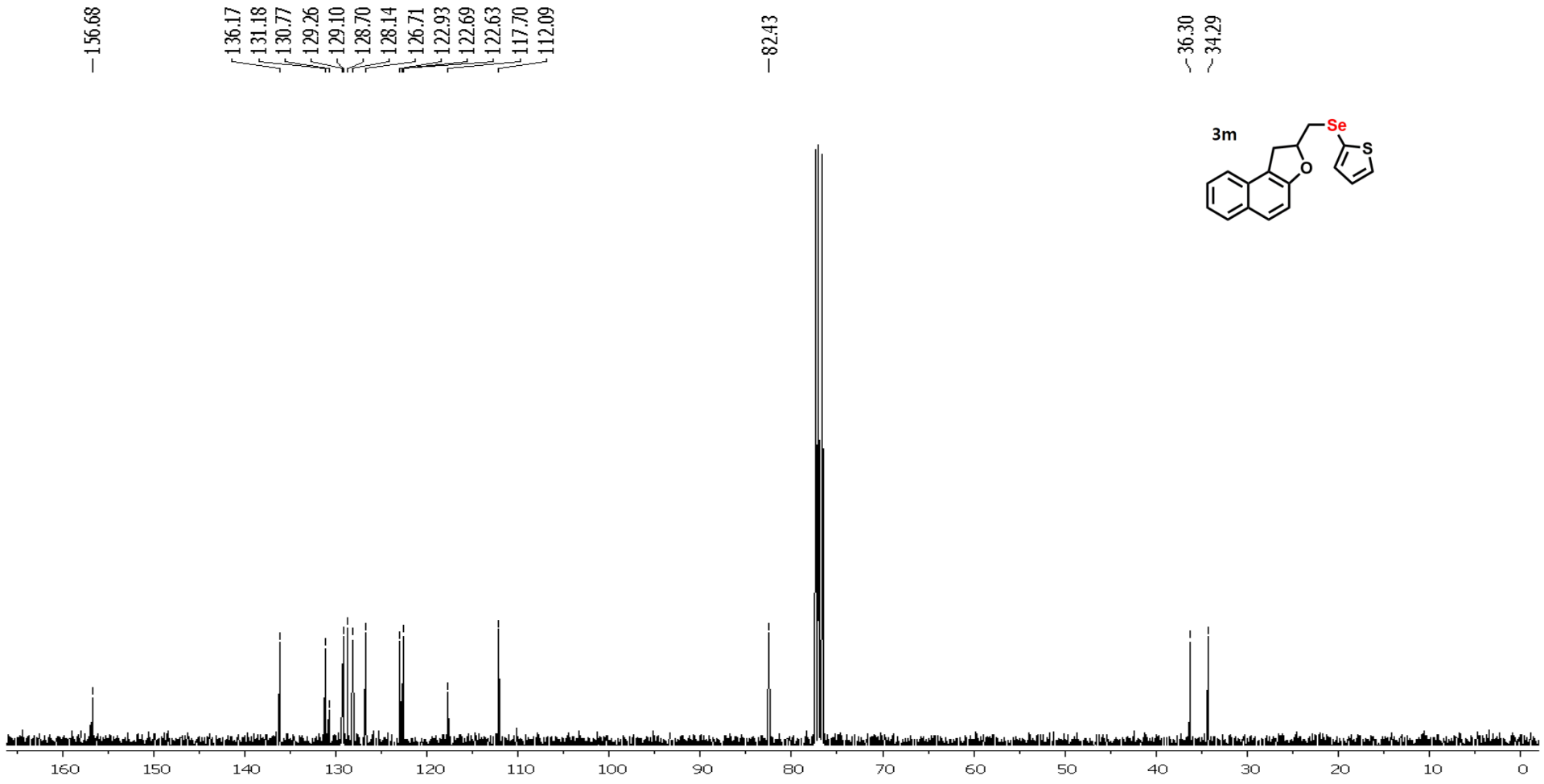
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 3l



^{1}H NMR $CDCl_3$ spectra of Compound 3m



^{13}C NMR $CDCl_3$ spectra of Compound 3m

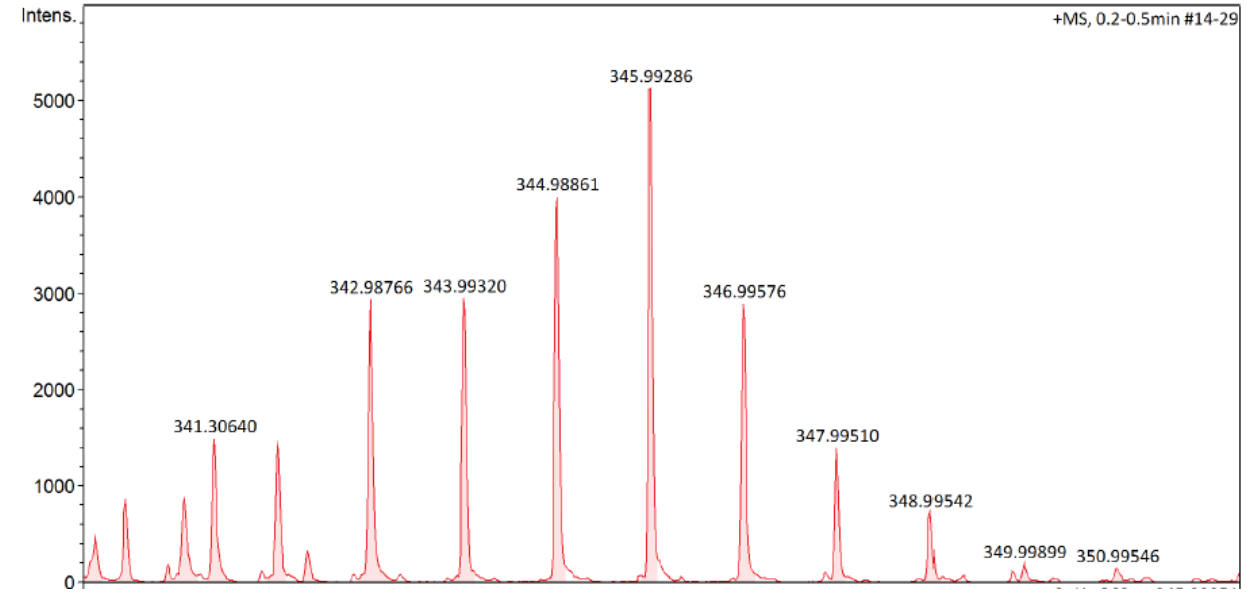
Display Report

Analysis Info

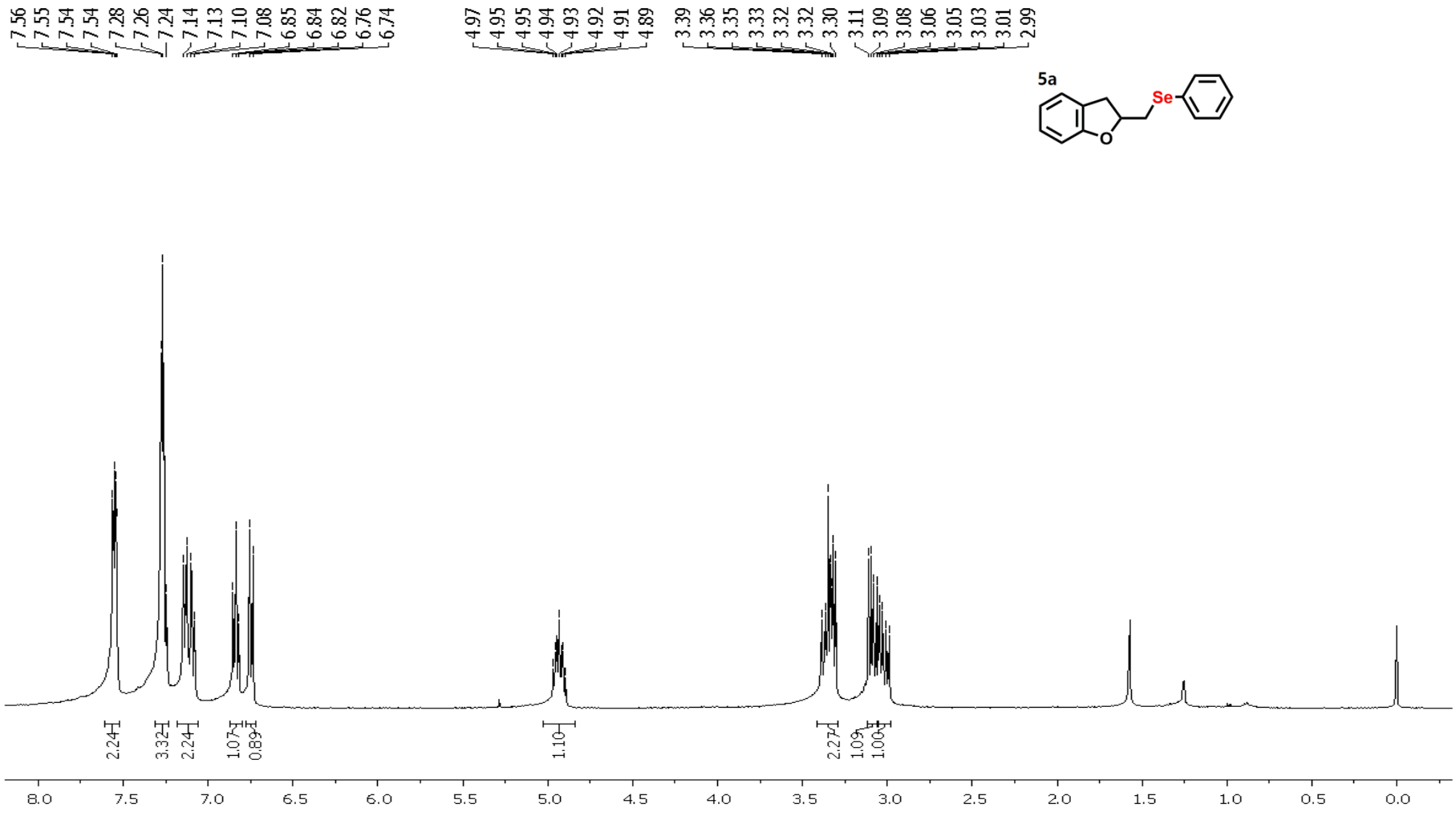
Analysis Name	D:\Data\2019\Q-TOF\UFSC\LabSELEN\ MARCOS LABSELEN QMC-CFM 20-11-2019 - x analises\286h000001.d	Acquisition Date	11/20/2019 6:34:19 PM
Method	tune low appi 10 06 19 Vanessa.m	Operator	micrOTOF-QII
Sample Name	286h	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

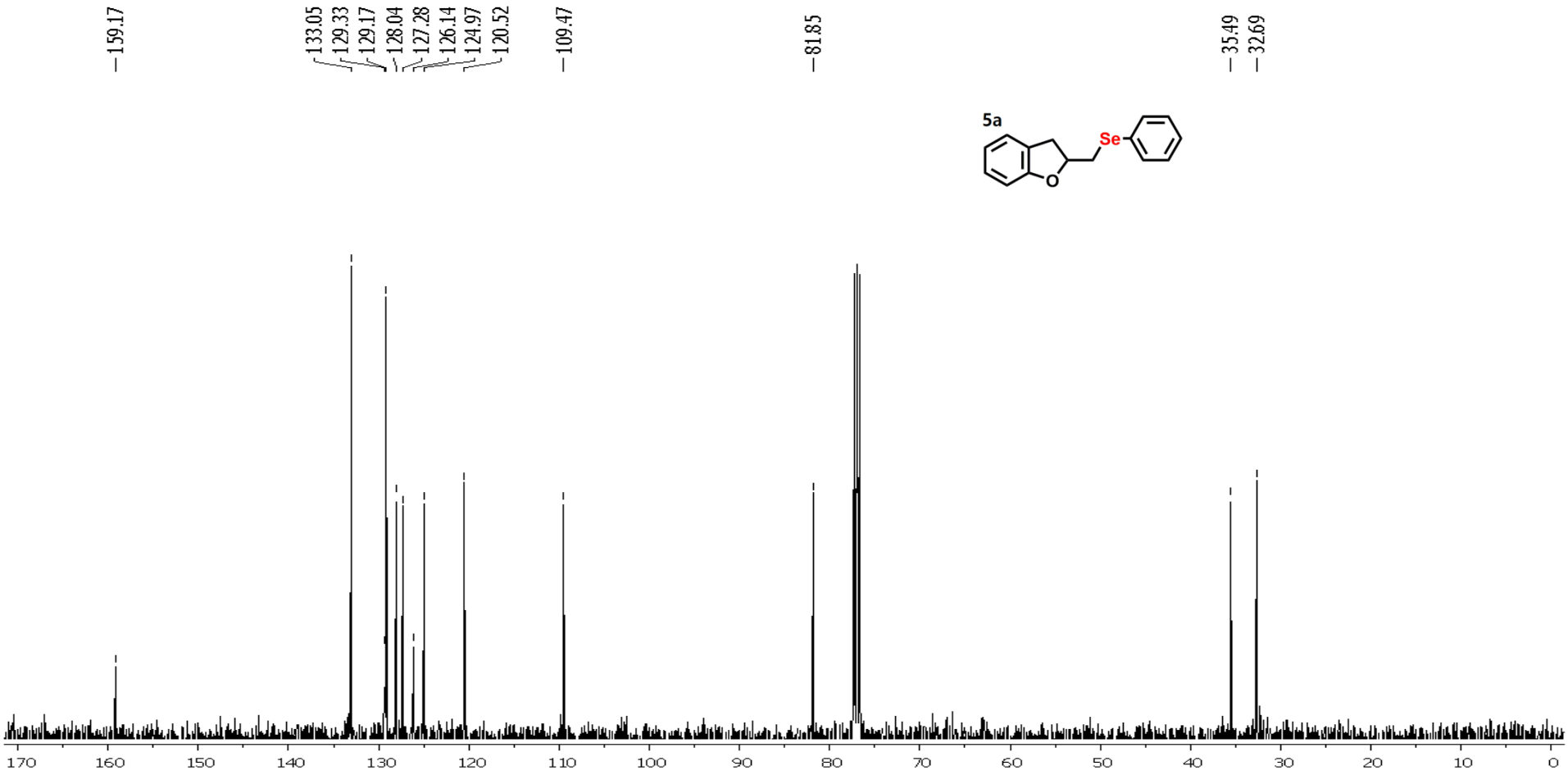
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 3m



^{1}H NMR $CDCl_3$ spectra of Compound 5a



^{13}C NMR $CDCl_3$ spectra of Compound 5a

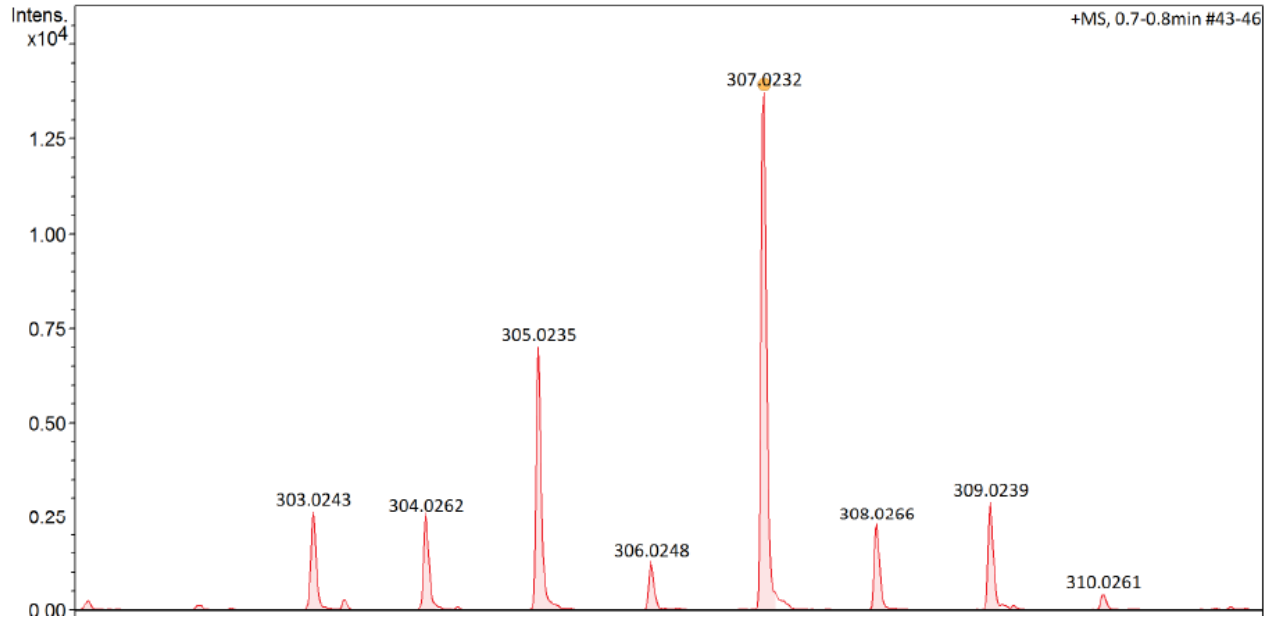
Display Report

Analysis Info

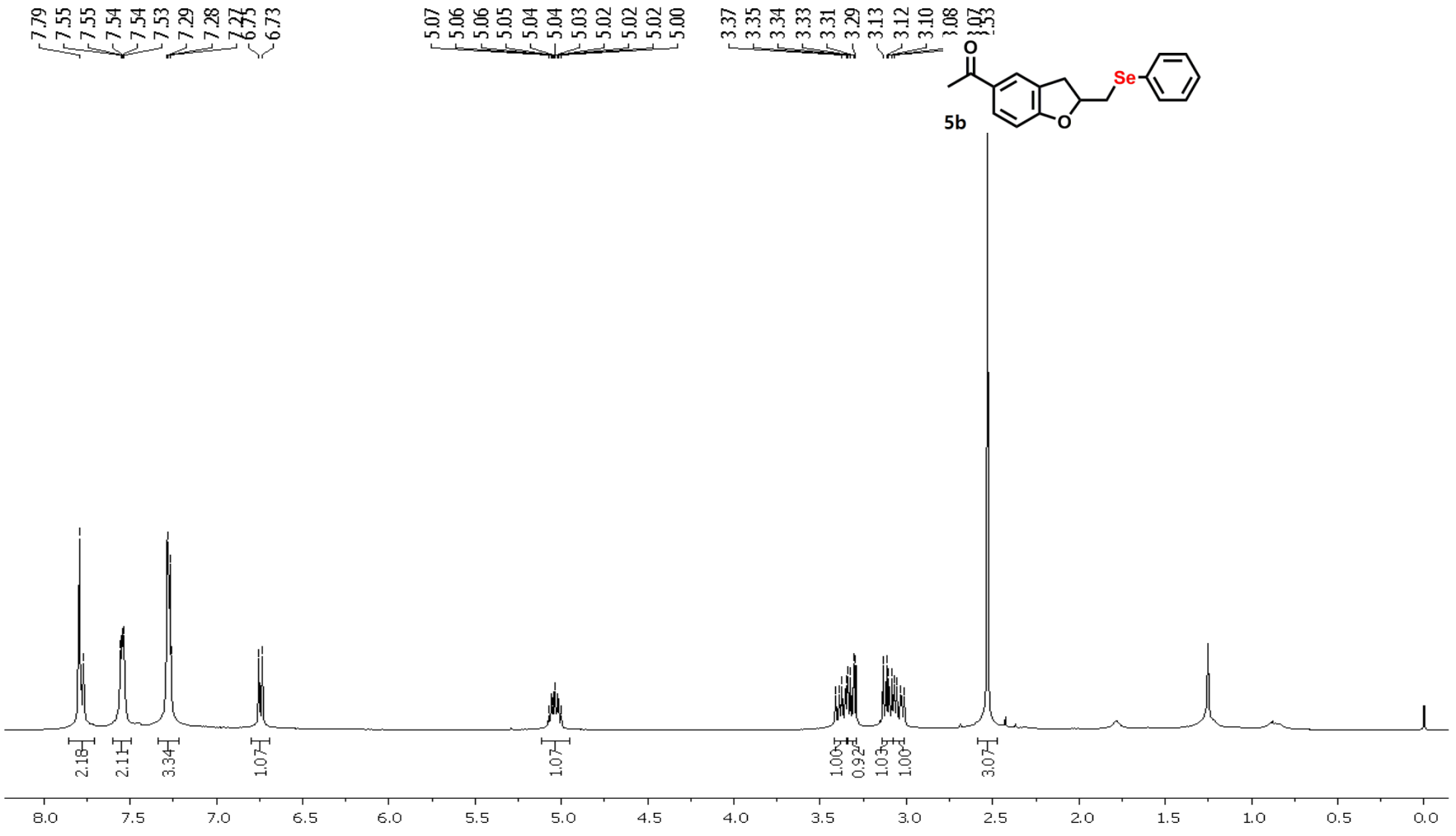
Analysis Name	D:\Data\2020\Q-TOF\UFSC\LabSELEN\LABSELEN QMC-CFM 22-01-2020 - x analises\MR-312000005.d	Acquisition Date	1/24/2020 10:09:33 AM
Method	appi 22 11 19 VANESSA.m	Operator	micrOTOF-QII
Sample Name	MR-312	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

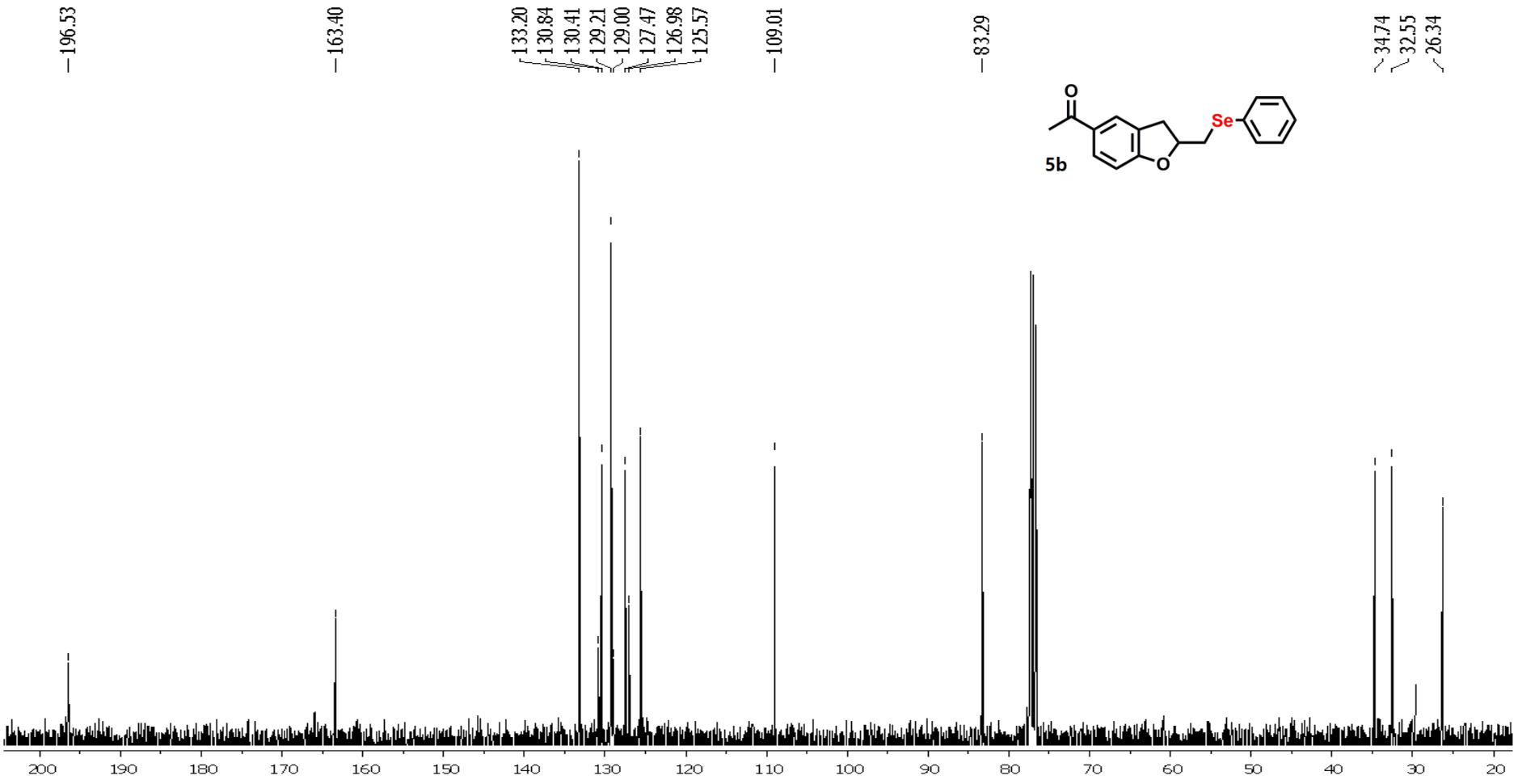
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 5a



^{1}H NMR $CDCl_3$ spectra of Compound 5b



^{13}C NMR $CDCl_3$ spectra of Compound 5b

Display Report

Analysis Info

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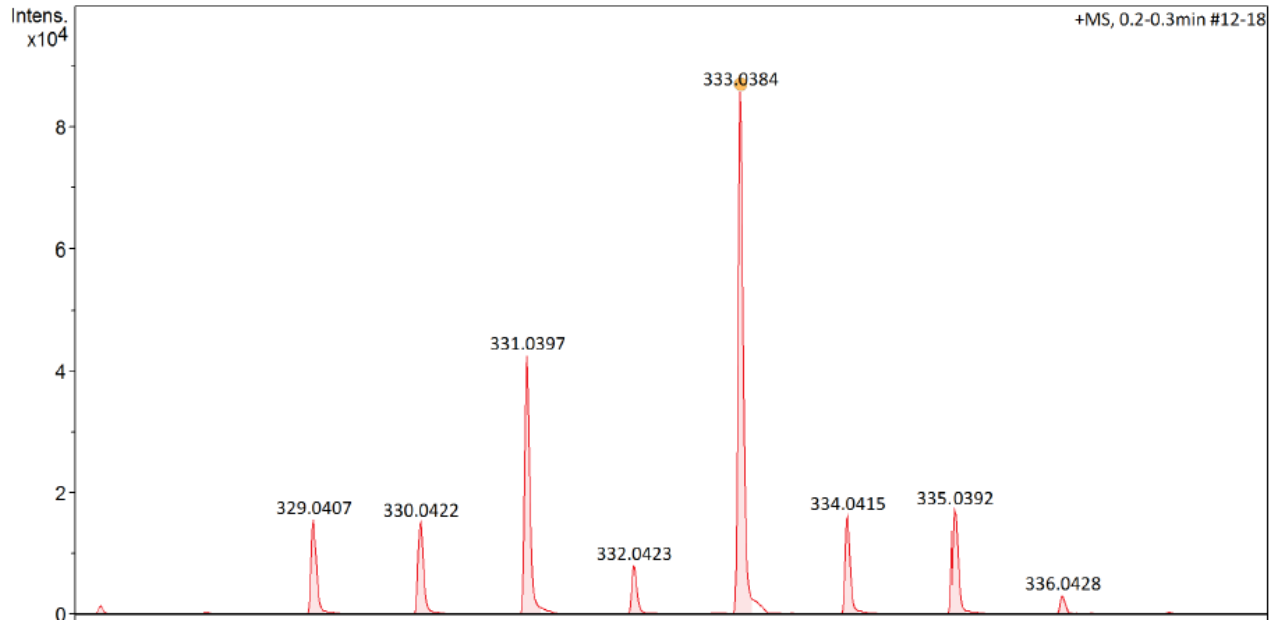
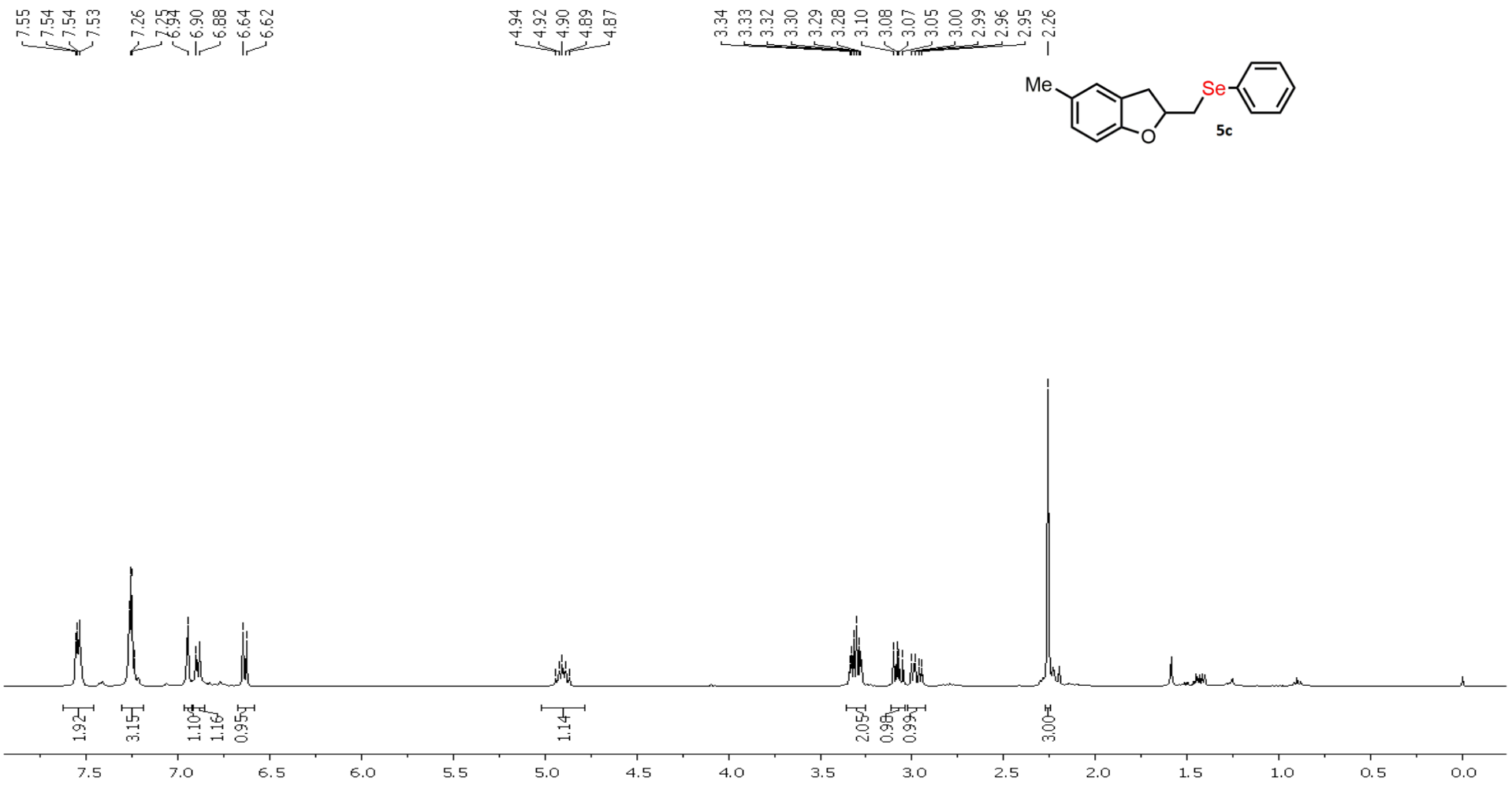
Method	appi 22 11 19 VANESSA.m	Operator	micrOTOF-QII
Sample Name	MR-313	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

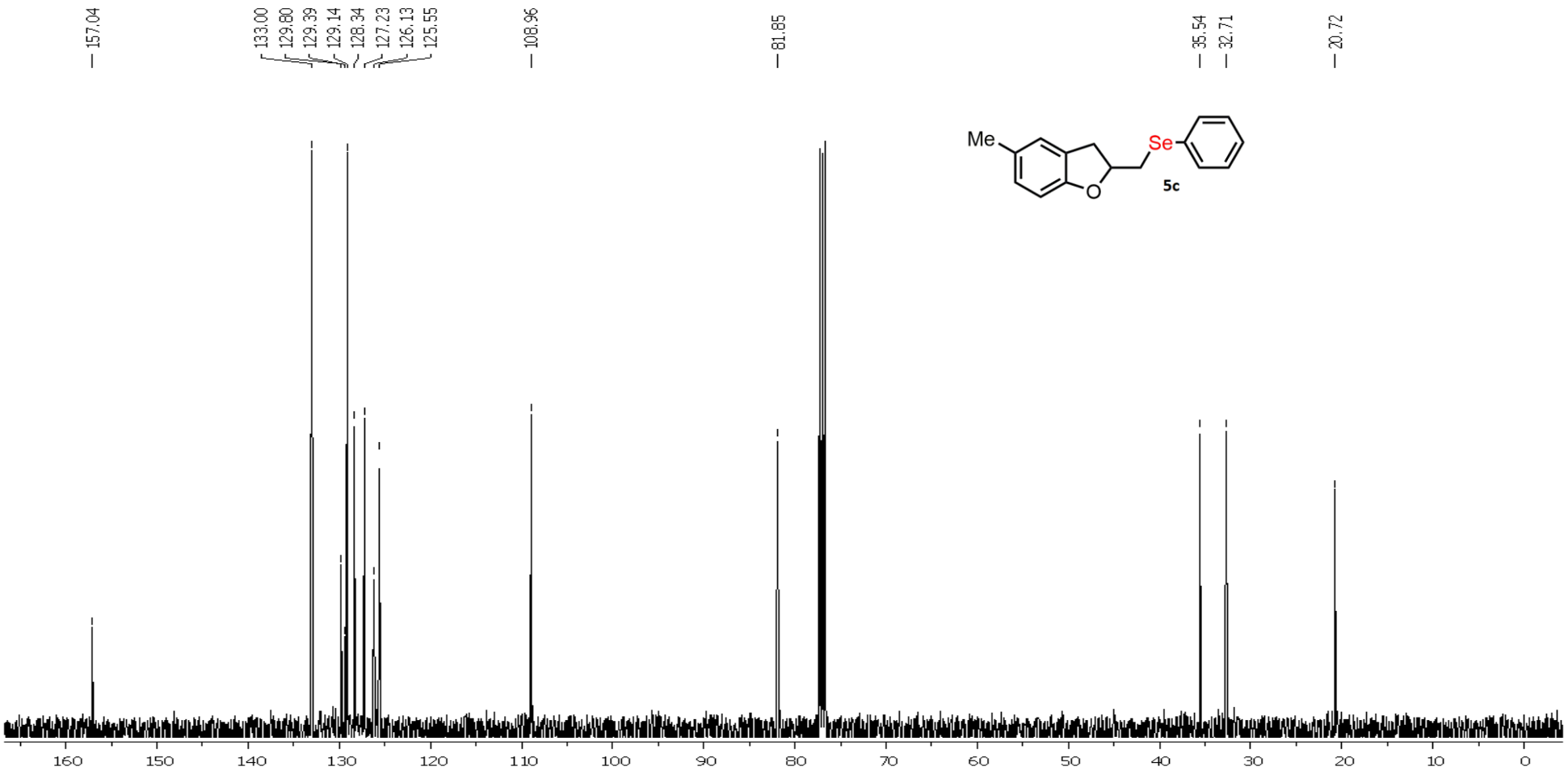
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 5b



^{1}H NMR $CDCl_3$ spectra of Compound 5c



^{13}C NMR $CDCl_3$ spectra of Compound 5c

Display Report

Analysis Info

Analysis Name	D:\Data\2020\Q-TOF\UFSC\LabSELEN\LABSELEN QMC-CFM 22-01-2020 - x analises\AM-296000009.d	Acquisition Date	1/22/2020 12:22:35 PM
Method	appi 22 11 19 VANESSA.m	Operator	micrOTOF-QII
Sample Name	AM-296	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
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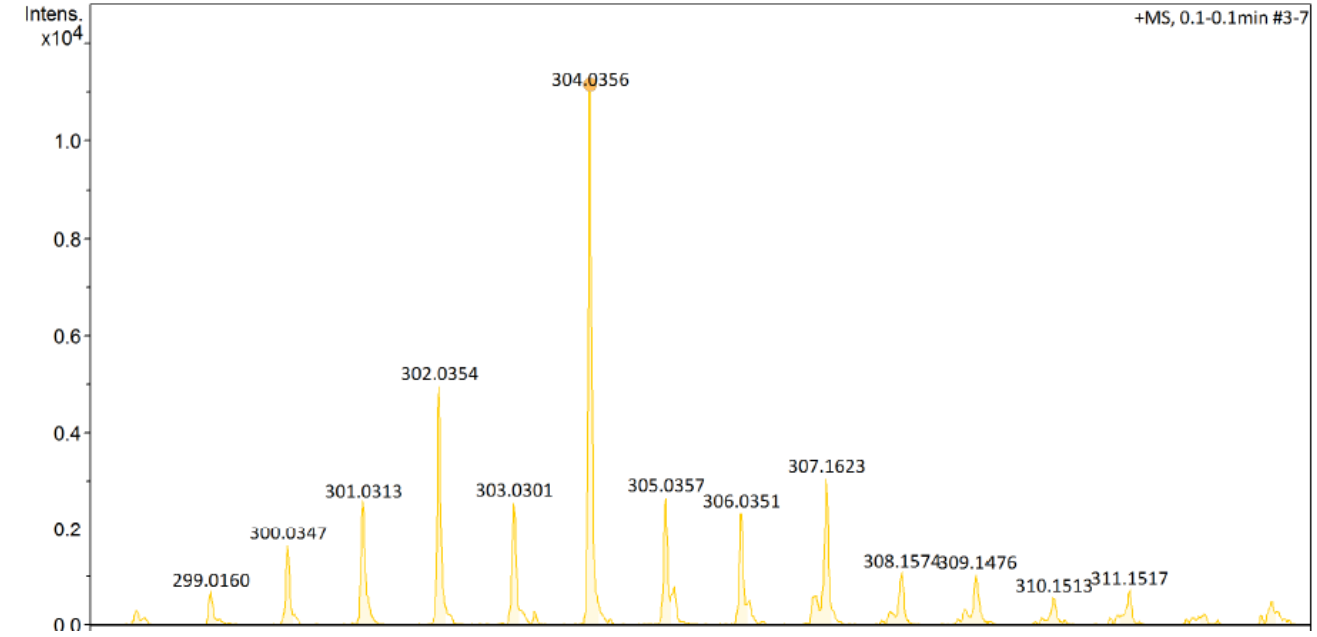
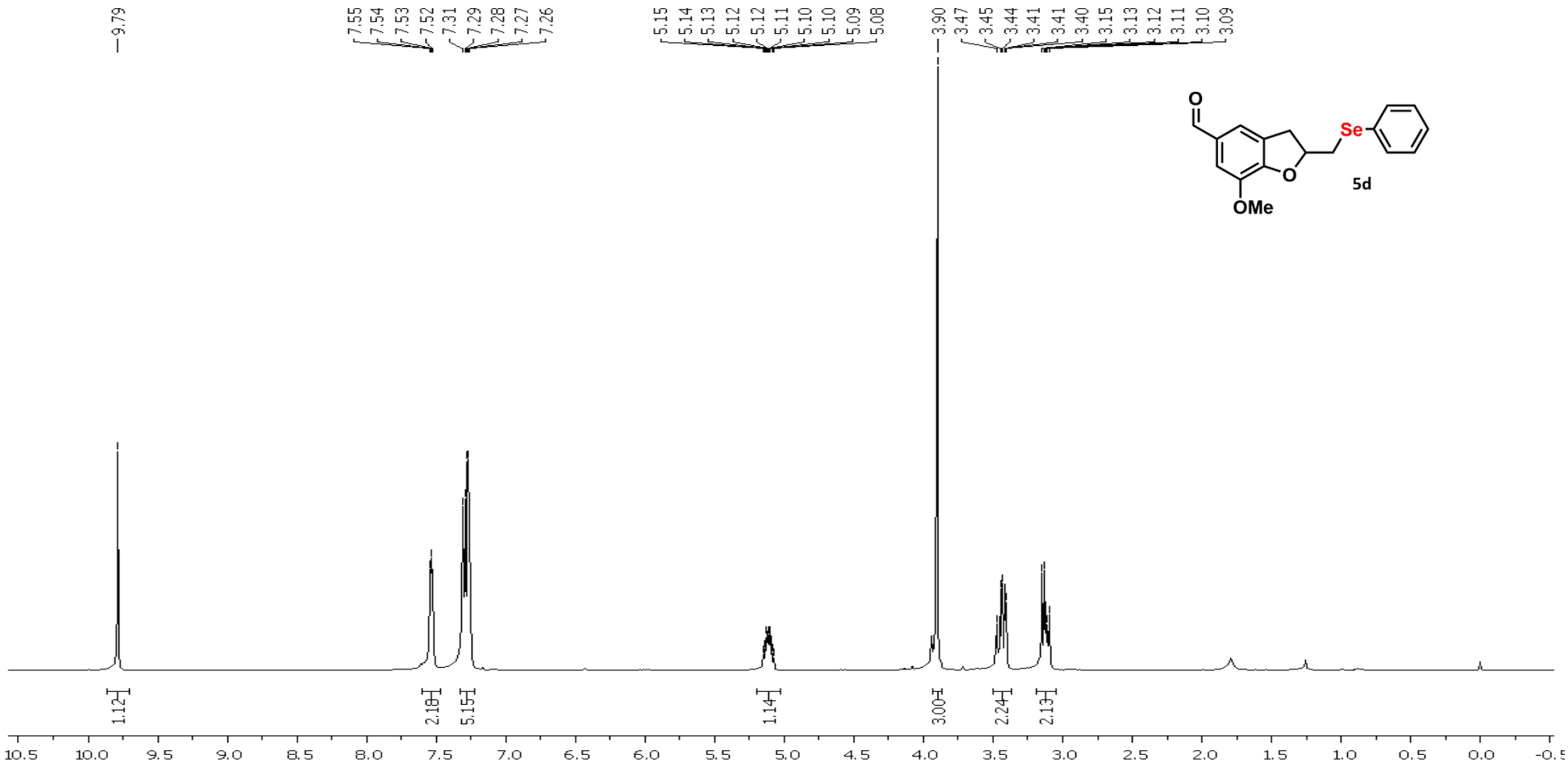
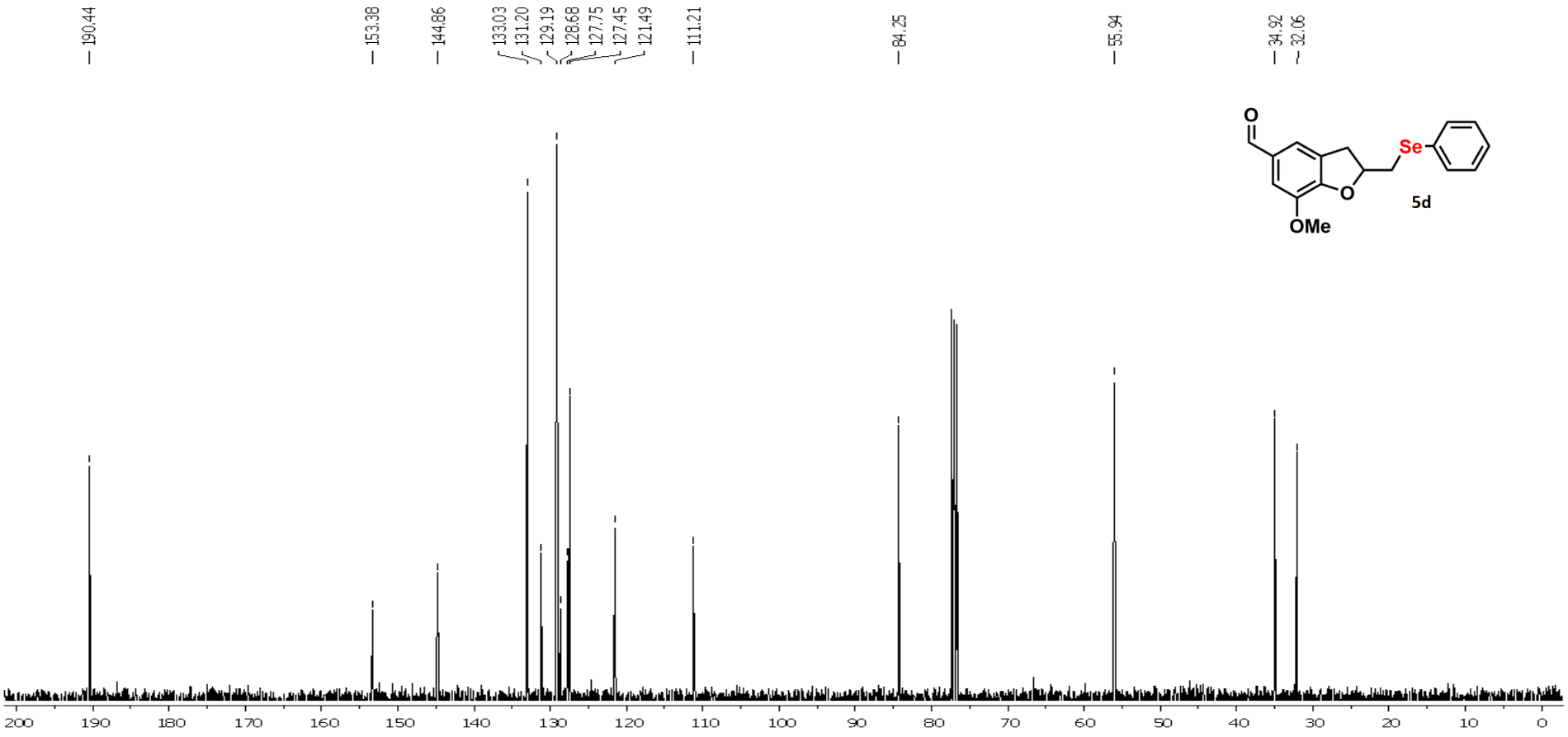
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 5c



^{1}H NMR $CDCl_3$ spectra of Compound 5d



^{13}C NMR $CDCl_3$ spectra of Compound 5d

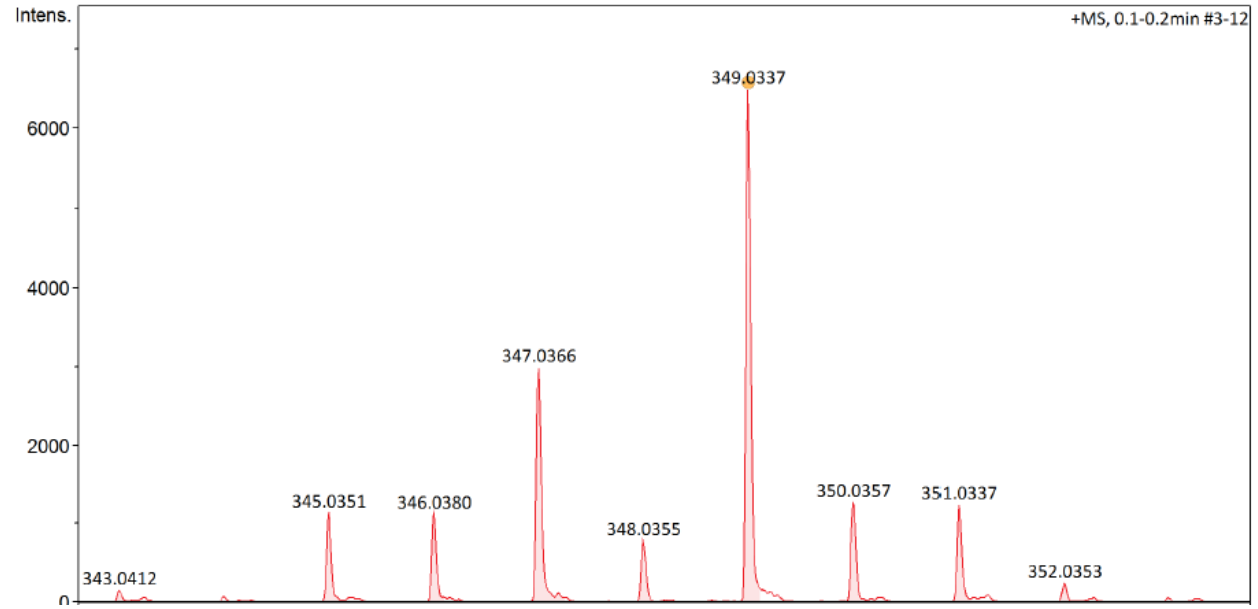
Display Report

Analysis Info

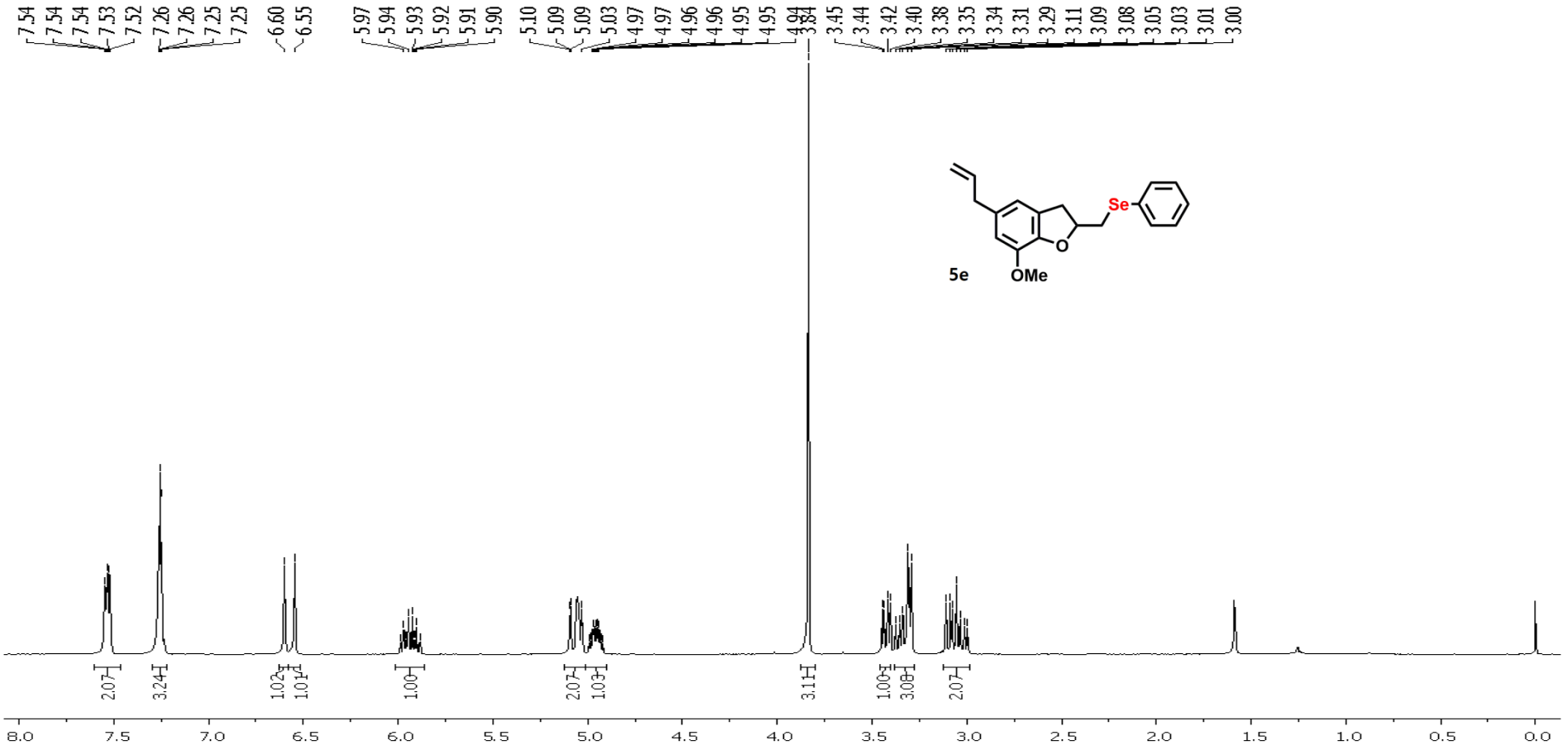
Analysis Name	D:\Data\2020\Q-TOF\UFSC\LabSELEN\LABSELEN QMC-CFM 22-01-2020 - x analises\AM-223000001.d	Acquisition Date	1/22/2020 10:58:43 AM
Method	appi 22 11 19 VANESSA.m	Operator	micrOTOF-QII
Sample Name	AM-223	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

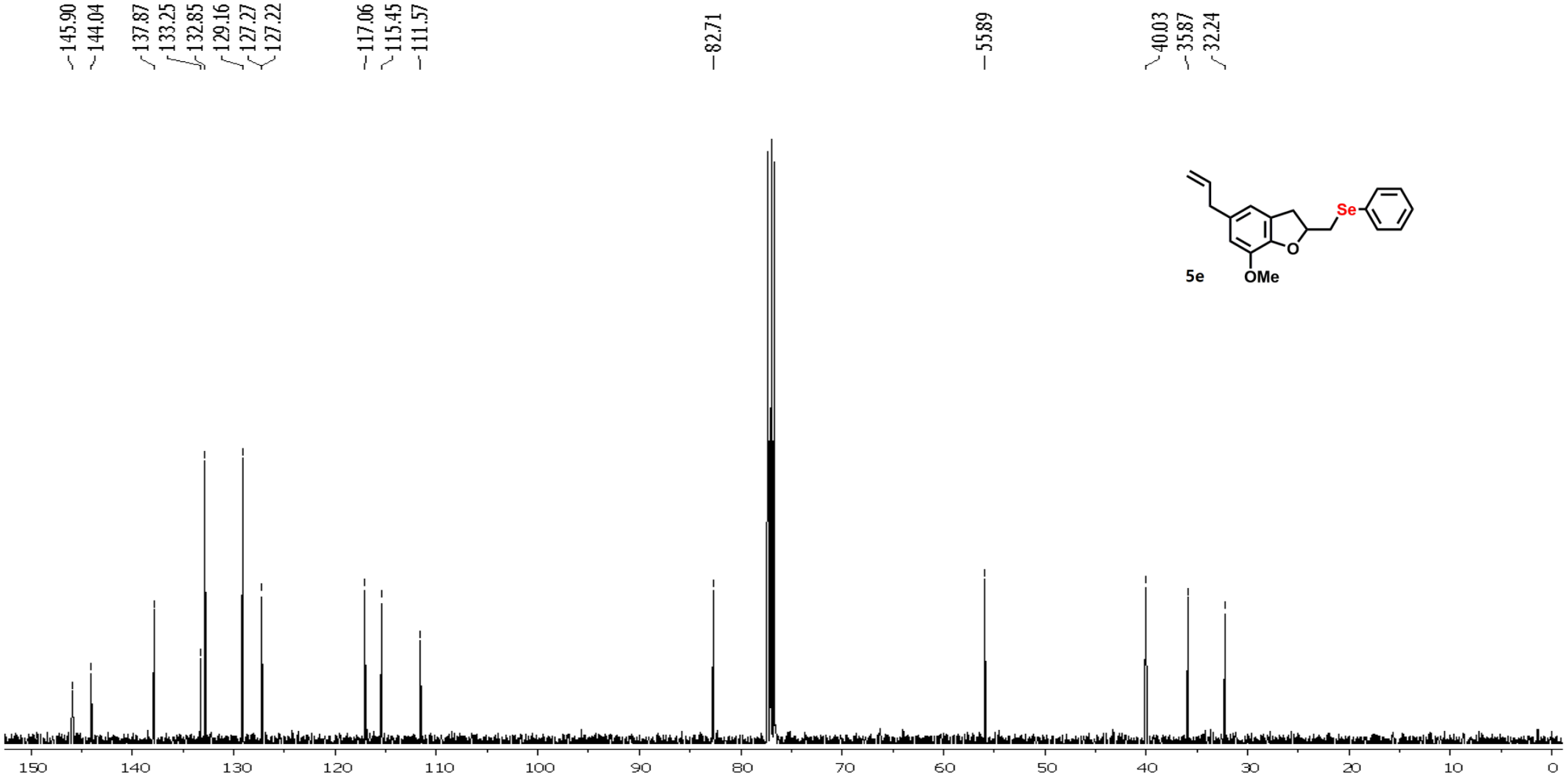
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 5d



^{1}H NMR $CDCl_3$ spectra of Compound 5e



^{13}C NMR $CDCl_3$ spectra of Compound 5e

Display Report

Analysis Info

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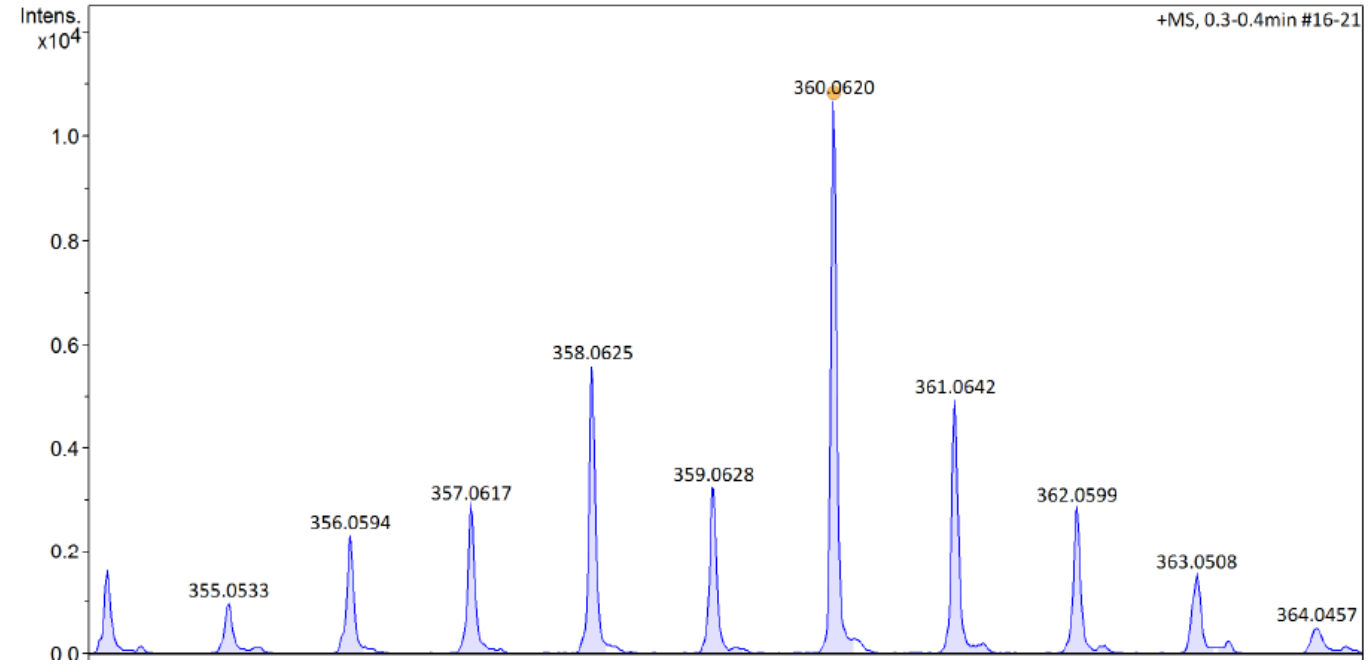
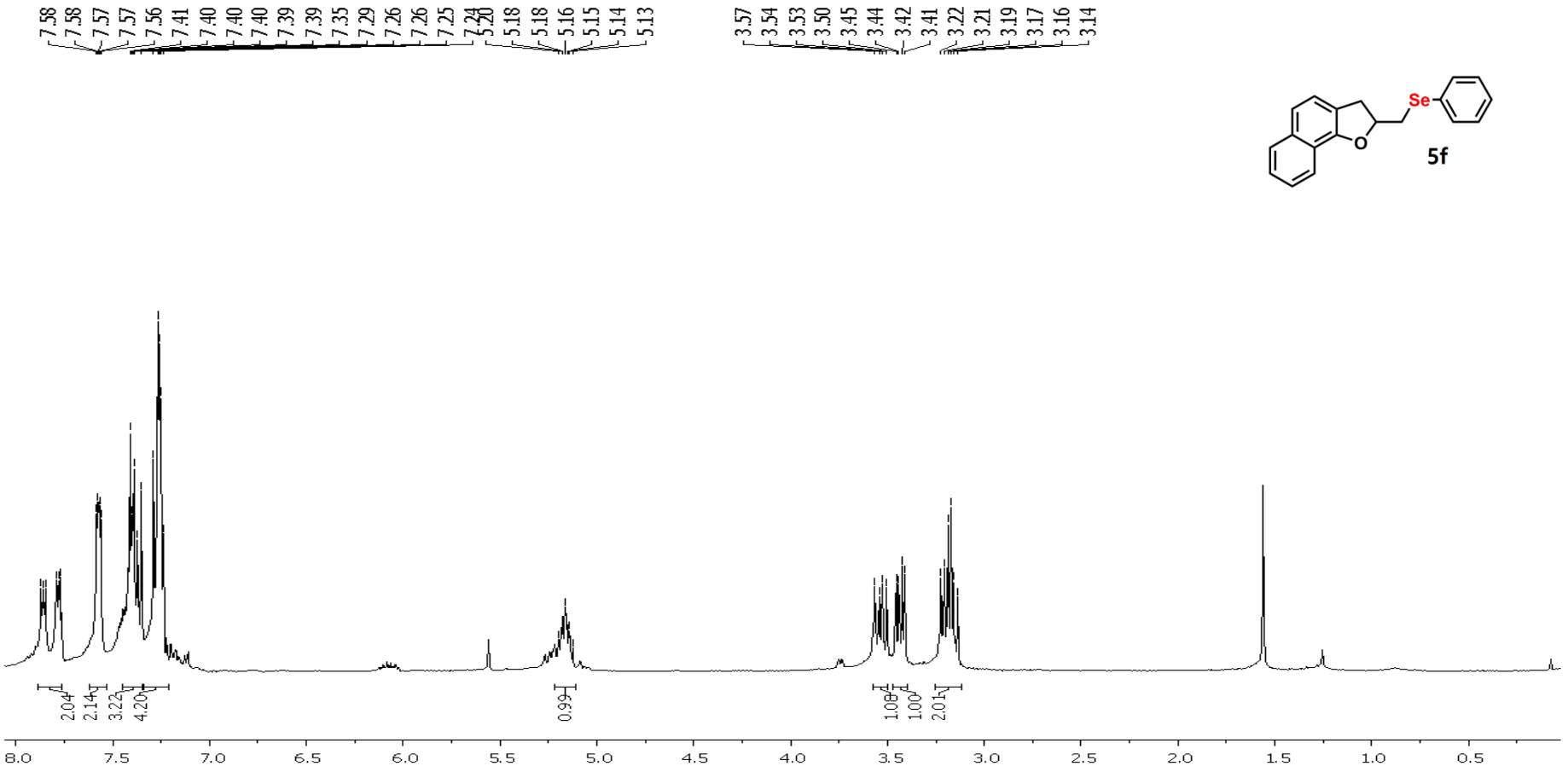
Analysis Name	D:\Data\2020\Q-TOF\UFSC\LabSELEN\LABSELEN QMC-CFM 22-01-2020 - x analises\MR-308000003.d		
Method	appi 22 11 19 VANESSA.m	Operator	micrOTOF-QII
Sample Name	MR-308	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

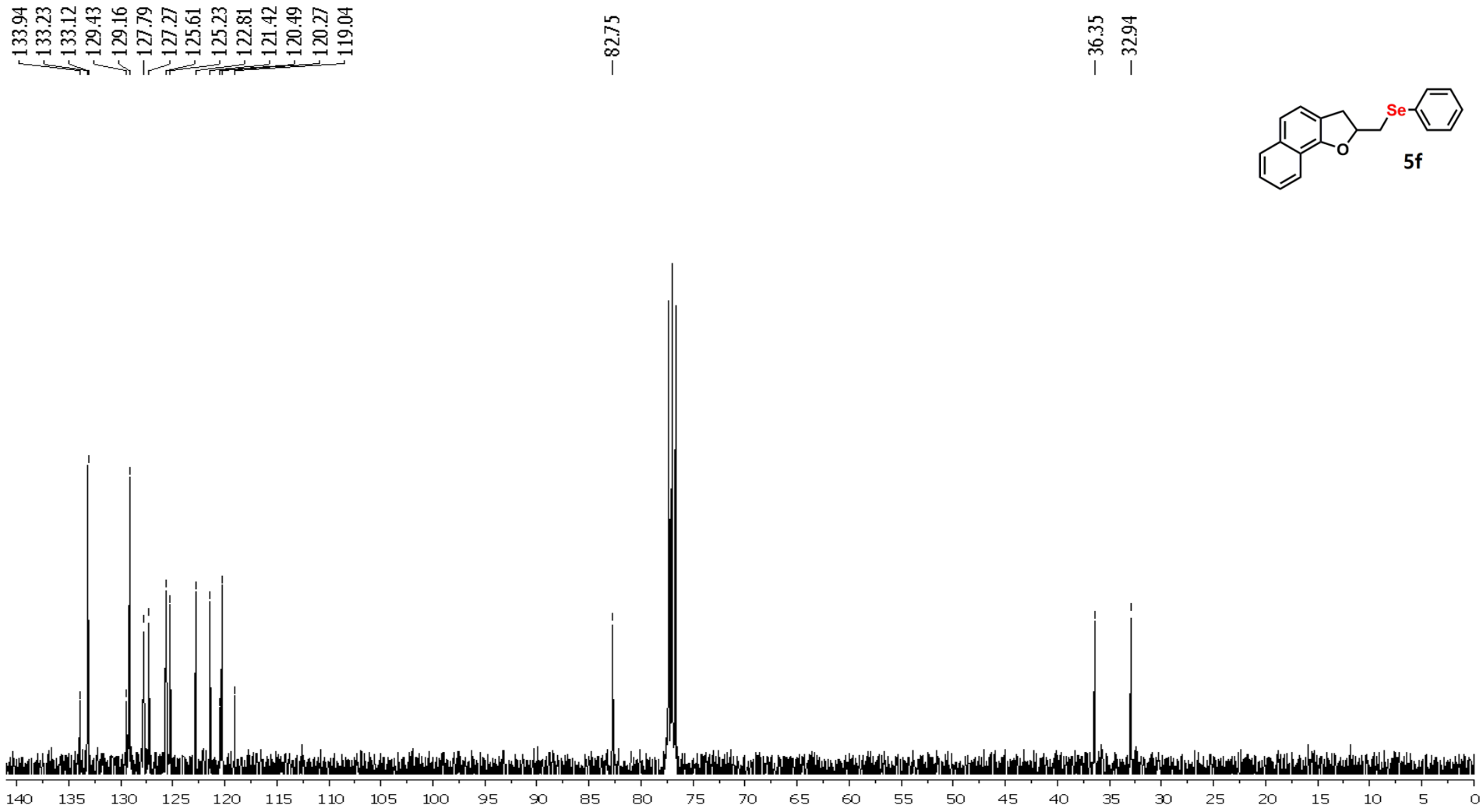
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 5e



^{1}H NMR $CDCl_3$ spectra of Compound 5f



^{13}C NMR $CDCl_3$ spectra of Compound 5f

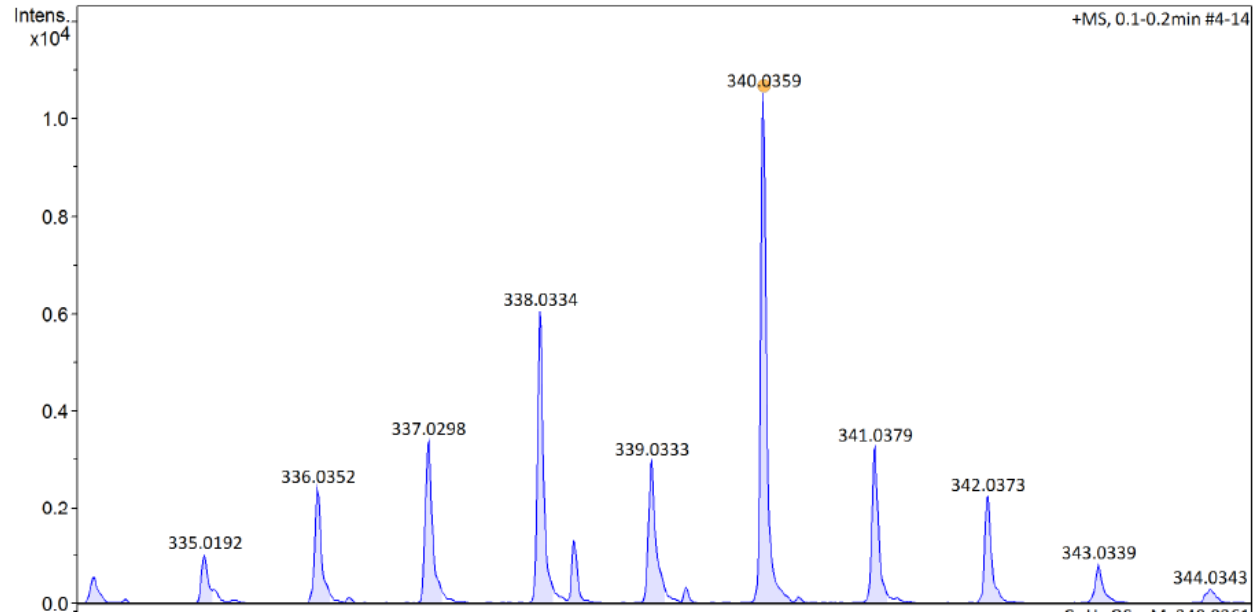
Display Report

Analysis Info

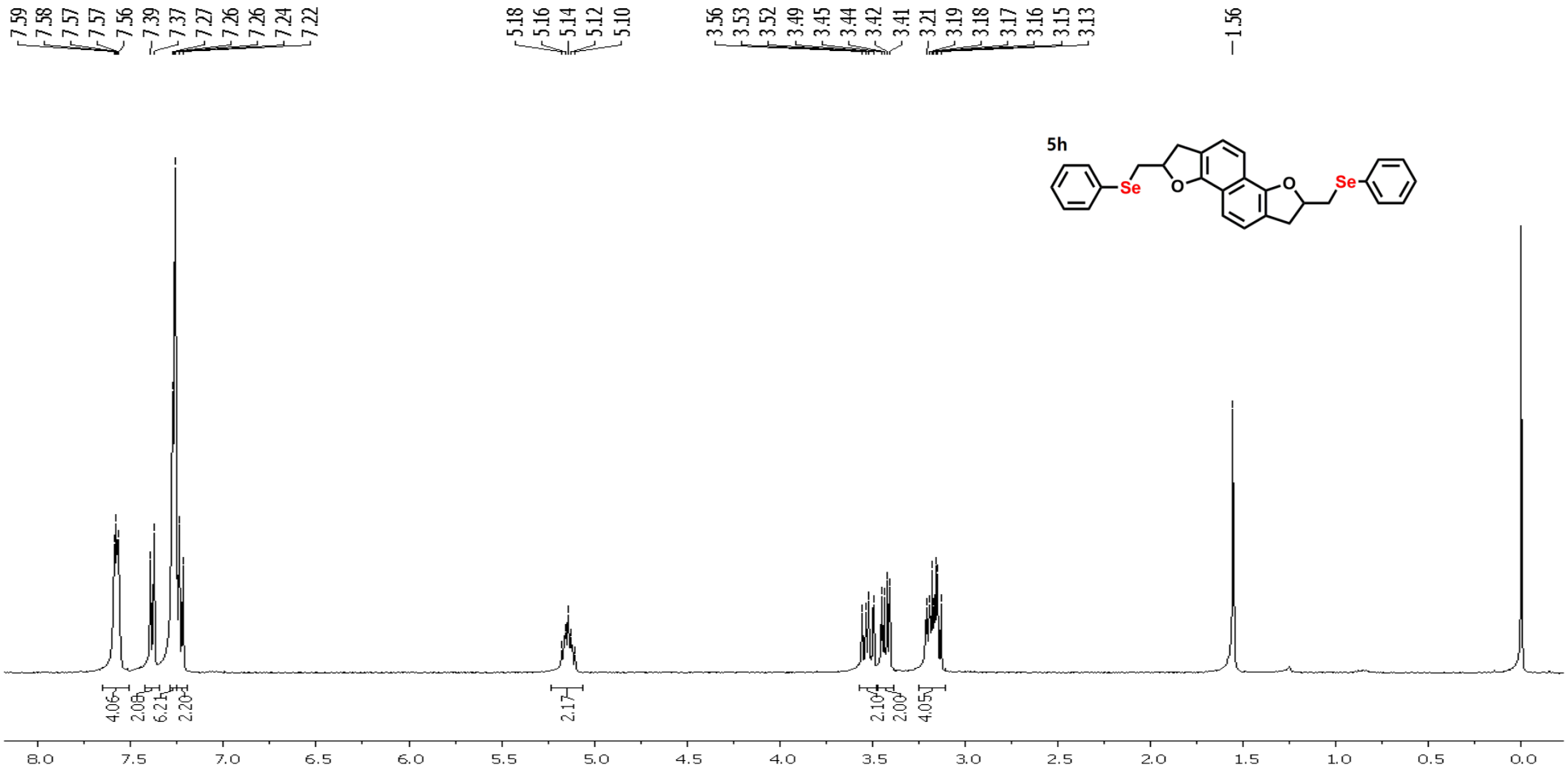
Analysis Name	D:\Data\2020\Q-TOF\UFSC\LabSELEN\LABSELEN QMC-CFM 22-01-2020 - x analises\MR-305000006.d	Acquisition Date	1/22/2020 12:17:30 PM
Method	appi 22 11 19 VANESSA.m	Operator	micrOTOF-QII
Sample Name	MR-305	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

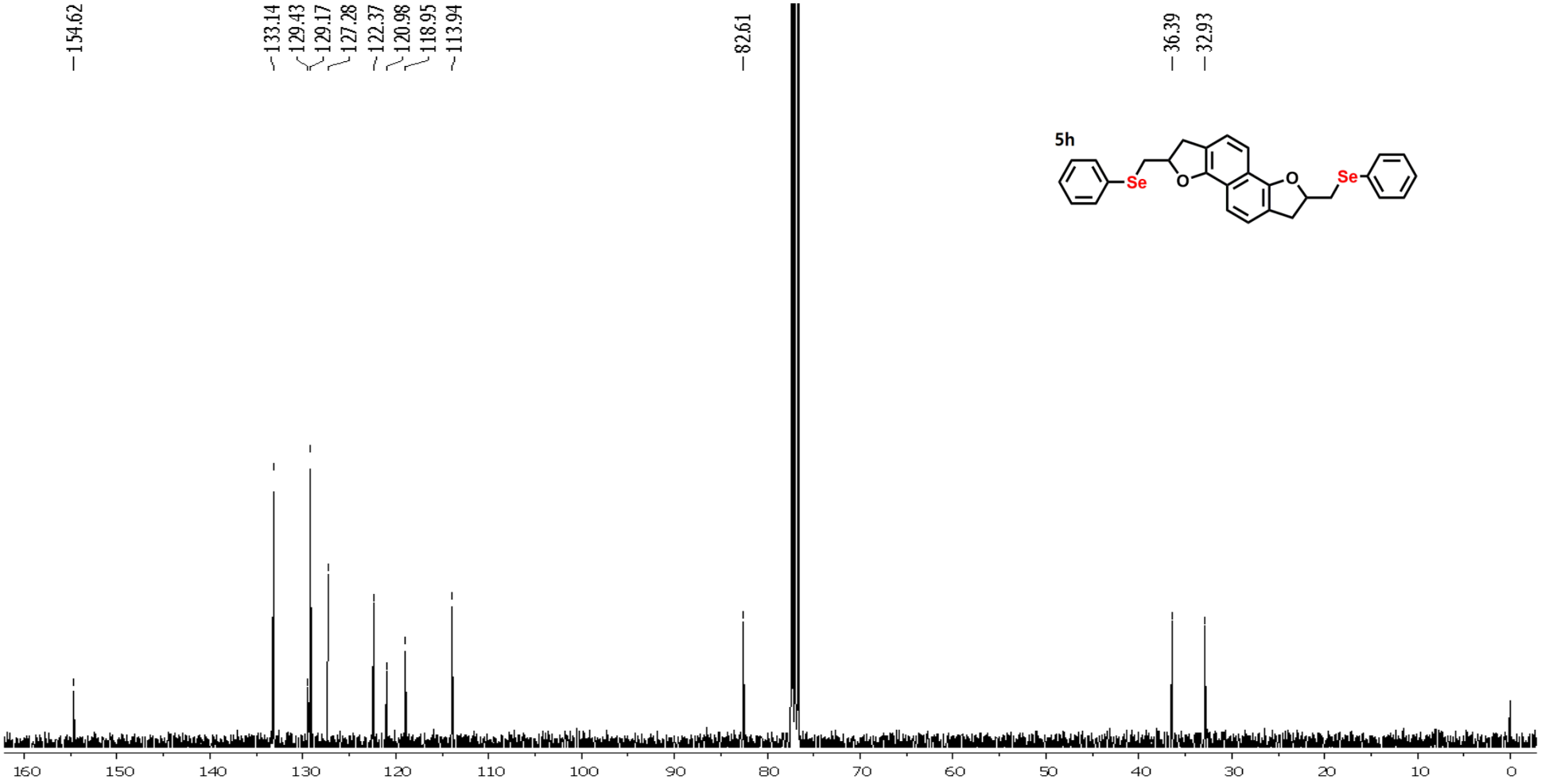
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 5f



^{1}H NMR $CDCl_3$ spectra of Compound 5h



^{13}C NMR $CDCl_3$ spectra of Compound 5h

Display Report

Analysis Info

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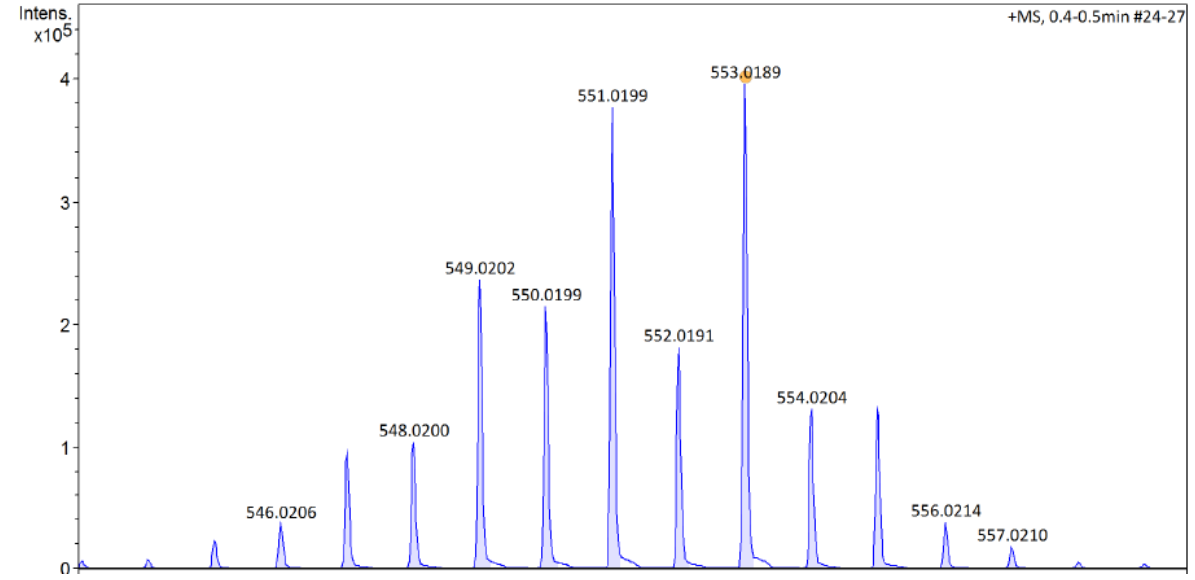
Method	appi 22 11 19 VANESSA.m	Operator	micrOTOF-QII
Sample Name	MR-307	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS-APPI Spectrum of Compound 5h