Supporting Information

Lewis Acid $InBr_3$-Catalyzed Arylation of Diorgano Diselenides and Ditellurides with Arylboronic Acids

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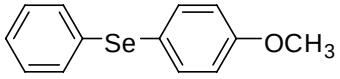
General information. All reactions were carried out under an air atmosphere. All reagents were purchased from commercial suppliers and used after further purification. ^1H NMR, ^{13}C NMR spectra were measured on a Bruker Avance NMR spectrometer (400 MHz or 100MHz, respectively) with $CDCl_3$ as solvent and recorded in ppm relative to internal tetramethylsilane standard. High resolution mass spectroscopy data of the product were collected on a Waters Micromass GCT instrument.

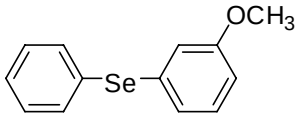
General Procedure for $InBr_3$-Catalyzed Preparation of Monochalcogenides from Dichalcogenides with Arylboronic Acids without any Additive: A 10 mL of reaction tube was charged with dichalcogenide (0.5 mmol), arylboronic acid (1.0 mmol), $InBr_3$ (0.05 mmol), and DMSO (1.0 mL). The reaction vessel was placed in an oil bath at 130 °C. After the reaction was carried out at this temperature for 20 h, it was cooled to room temperature, diluted with H_2O and extracted twice with Et_2O. The organic layers were combined, dried over Na_2SO_4, and concentrated to yield the crude product, which was further purified by flash chromatography on silica gel (eluant: petroleum ether) to give the desired cross-coupling product.

4-Methoxyphenyl phenyl selenide[1]



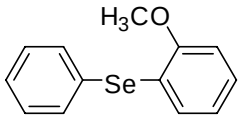
IR (neat): 3058, 2995, 2942, 2840, 1589, 1491, 1476, 1247, 1028, 834, 730 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.50 (d, *J* = 8.8 Hz, 2H), 7.33–7.31 (m, 2H), 7.21–7.16 (m, 3H), 6.84 (d, *J* = 8.4 Hz, 2H), 3.79 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 159.7, 136.5, 133.2, 130.9, 129.1, 126.4, 119.9, 115.1, 55.2. Anal. Calcd for $C_{13}H_{12}OSe$: C, 59.32; H, 4.60. Found: C, 59.57; H, 4.73.

3-Methoxyphenyl phenyl selenide[2]



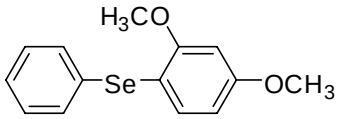
IR (neat): 3057, 2934, 2833, 1587, 1475, 1244, 1039, 737, 688 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.49–7.48 (m, 2H), 7.26–7.25 (m, 3H), 7.18–7.14 (m, 1H), 7.03–7.00 (m, 2H), 6.78 (d, *J* = 8.0 Hz, 1H), 3.72 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 159.9, 133.2, 132.2, 130.7, 130.0, 129.3, 127.4, 124.9, 117.9, 113.0, 55.2. Anal. Calcd for $C_{13}H_{12}OSe$: C, 59.32; H, 4.60. Found: C, 59.53; H, 4.69.

2-Methoxyphenyl phenyl selenide[1]



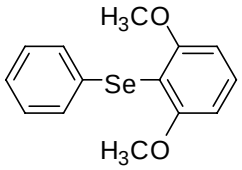
IR (neat): 3056, 2935, 2833, 1587, 1476, 1438, 1284, 1244, 1039, 738, 688 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.58–7.56 (m, 2H), 7.33–7.30 (m, 3H), 7.20–7.15 (m, 1H), 6.94 (q, *J* = 1.6, 6.0 Hz, 1H), 6.84 (q, *J* = 1.2, 7.2 Hz, 1H), 6.80–6.76 (m, 1H), 3.87 (s, 3H). $^1\delta_c$ (100 MHz; $CDCl_3$; Me_4Si) 156.6, 135.5, 130.8, 129.5, 128.3, 128.1, 127.7, 121.9, 121.6, 110.4, 55.9. Anal. Calcd for $C_{13}H_{12}OSe$: C, 59.32; H, 4.60. Found: C, 59.62; H, 4.45.

2,4-Dimethoxyphenyl phenyl selenide[3]



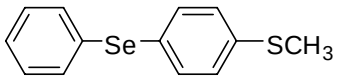
IR (neat): 3056, 2929, 2853, 1578, 1476, 1463, 1437, 1209, 1161, 1023, 737 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.42–7.39 (m, 2H), 7.25–7.22 (m, 4H), 6.50 (d, *J* = 2.4 Hz, 1H), 6.43 (q, *J* = 2.4, 6.0 Hz, 1H), 3.83 (s, 3H), 3.80 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 161.3, 159.2, 135.3, 132.4, 129.1, 126.8, 110.3, 105.7, 99.0, 56.0, 55.5. Anal. Calcd for $C_{14}H_{14}O_2Se$: C, 57.35; H, 4.81. Found: C, 57.51; H, 4.92.

2,6-Dimethoxyphenyl phenyl selenide[4]



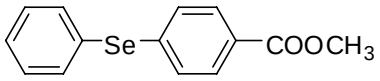
IR (neat): 3056, 2936, 2834, 1575, 1456, 1302, 1160, 1061, 1022, 833, 736, 691 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.41–7.38 (m, 2H), 7.24–7.19 (m, 4H), 6.49 (d, *J* = 2.4 Hz, 1H), 6.41 (q, *J* = 2.4, 6.0 Hz, 1H), 3.81 (s, 3H), 3.78 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 161.2, 159.1, 135.2, 132.3, 131.0, 129.1, 126.8, 110.2, 105.6, 98.9, 55.9, 55.4. Anal. Calcd for $C_{14}H_{14}O_2Se$: C, 57.35; H, 4.81. Found: C, 57.54; H, 4.65.

4-Methylthiophenyl phenyl selenide



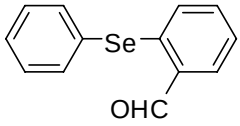
IR (neat): 3056, 2920, 2853, 1577, 1474, 1437, 1386, 1098, 1010, 807, 736, 690 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.39 (d, *J* = 8.4 Hz, 4H), 7.23–7.21 (m, 3H), 7.12 (d, *J* = 8.4 Hz, 2H), 2.43 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 138.4, 134.0, 132.2, 131.6, 129.2, 127.1, 127.0, 126.6, 15.5. HRMS (ESI) ($[M]^+$) Calcd. for $C_{13}H_{12}S^{77}Se$: 276.9859, Found 276.9858.

4-Methoxycarbonylphenyl phenyl selenide[1]



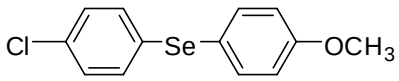
IR (neat): 3056, 2925, 2854, 1708, 1587, 1435, 1397, 1276, 1177, 1010, 759, 748, 694 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.86 (d, J = 8.4 Hz, 2H), 7.58 (q, J = 2.0, 6.0 Hz, 2H), 7.37–7.34 (m, 5H), 3.89 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 166.8, 139.7, 135.0, 1302.3, 130.2, 129.7, 128.7, 128.5, 128.2, 52.1. Anal. Calcd for $C_{14}H_{12}O_2Se$: C, 57.74; H, 4.15. Found: C, 57.89; H, 4.01.

2-Formylphenyl phenyl selenide[5]



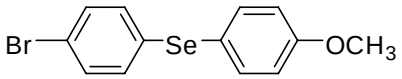
IR (neat): 3056, 2924, 2848, 2738, 1695, 1583, 1557, 1455, 1438, 1202, 1034, 843, 744, 694, 661 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 10.1 (s, 1H), 7.78–7.76 (m, 1H), 7.61–7.59 (m, 2H), 7.41–7.34 (m, 3H), 7.27–7.20 (m, 2H), 6.98 (d, J = 7.2 Hz, 1H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 192.6, 139.6, 136.8, 135.1, 133.9, 133.7, 129.9, 129.1, 128.1, 125.5. Anal. Calcd for $C_{13}H_{10}OSe$: C, 59.78; H, 3.86. Found: C, 59.89; H, 3.95.

4-Chlorophenyl 4′-methoxyphenyl selenide



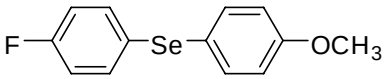
IR (neat): 3056, 2926, 2854, 1708, 1587, 1435, 1276, 1111, 759, 748, 694 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.45 (d, J = 8.8 Hz, 2H), 7.19 (d, J = 8.8 Hz, 2H), 7.12 (d, J = 8.8 Hz, 2H), 6.82 (d, J = 8.8 Hz, 2H), 3.77 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 160.0, 136.7, 132.5, 132.1, 131.6, 129.3, 119.5, 115.3, 55.3. HRMS (ESI) ($[M]^+$) Calcd. for $C_{13}H_{11}ClO^{80}Se$: 297.9664, Found 297.9670; Calcd. for $C_{13}H_{11}ClO^{78}Se$: 295.9671, Found 295.9667.

4-Bromophenyl 4′-methoxyphenyl selenide



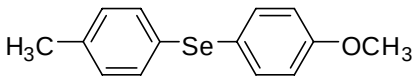
IR (neat): 3056, 2923, 2855, 1630, 1589, 1492, 1465, 1381, 1248, 1079, 1030, 1003, 806 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.49 (d, *J* = 8.8 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 3.81 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 160.0, 136.7, 132.5, 132.1, 131.6, 129.3, 119.5, 115.3, 55.3. (ESI) ($[M]^+$) Calcd. for $C_{13}H_{11}BrO^{80}Se$: 341.9158, Found 341.9157.

4-Flurophenyl 4′-methoxyphenyl selenide[6]



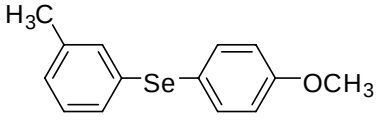
IR (neat): 3056, 2923, 2849, 1587, 1249, 1226, 1024, 835 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.45 (d, *J* = 8.8 Hz, 2H), 7.34 (q, *J* = 5.4, 4.8 Hz, 2H), 6.91 (t, *J* = 8.8 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 163.2, 160.8, 159.7, 135.8, 133.5, 133.4, 127.2, 120.5, 116.3, 116.1, 115.1, 55.2. Anal. Calcd for $C_{13}H_{11}FOSe$: C, 55.53; H, 3.94. Found: C, 55.31; H, 4.17.

4-Methylphenyl 4′-methoxyphenyl selenide



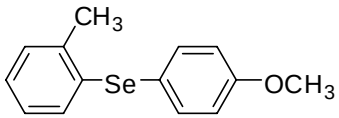
IR (neat): 3057, 3010, 2917, 2849, 1589, 1489, 1287, 1246, 1179, 1031, 804 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.45 (d, *J* = 8.8 Hz, 2H), 7.27 (q, *J* = 8.0 Hz, 2H), 7.03 (t, *J* = 8.0 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 3.77 (s, 3H), 2.28 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 159.5, 136.7, 135.8, 131.8, 130.0, 129.0, 120.9, 115.1, 55.3, 21.1. (ESI) ($[M]^+$) Calcd. for $C_{14}H_{14}O^{80}Se$: 278.0210, Found 278.0211; Calcd. for $C_{14}H_{14}O^{78}Se$: 276.0218, Found 276.0223.

3-Methylphenyl 4′-methoxyphenyl selenide



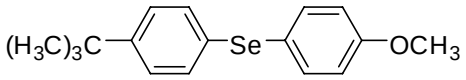
IR (neat): 3051, 3004, 2935, 2835, 1591, 1570, 1490, 1287, 1247, 1173, 1031, 824, 772, 687 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.47 (d, *J* = 8.4 Hz, 2H), 7.16 (s, 1H), 7.11–7.04 (m, 2H), 6.96 (d, *J* = 7.2 Hz, 1H), 6.81 (d, *J* = 8.8 Hz, 2H), 3.75 (s, 3H), 2.24 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 159.6, 138.8, 136.3, 132.7, 131.6, 128.9, 128.1, 127.3, 120.1, 115.0, 55.2, 21.2. (ESI) ($[M]^+$) Calcd. for $C_{14}H_{14}O^{82}Se$: 280.0212, Found 280.0215.

4-Methoxyphenyl 2′-methylphenyl selenide



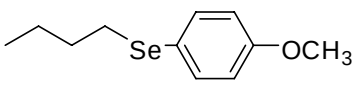
IR (neat): 3059, 3004, 2926, 2836, 1590, 1490, 1464, 1287, 1247, 1173, 1033, 746, 708, 657 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.45 (d, *J* = 8.8 Hz, 2H), 7.15–7.13 (m, 1H), 7.11–7.06 (m, 2H), 7.00–6.96 (m, 1H), 6.85 (d, *J* = 9.2 Hz, 2H), 3.79 (s, 3H), 2.37 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 159.8, 138.0, 136.6, 134.0, 130.8, 130.0, 126.6, 119.3, 115.3, 55.3, 21.9. (ESI) ($[M]^+$) Calcd. for $C_{14}H_{14}O^{78}Se$: 276.0218, Found 276.0219.

4-*t*-Butylphenyl 4′-methoxyphenyl selenide



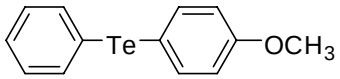
IR (neat): 3073, 2962, 2903, 2866, 1592, 1571, 1489, 1396, 1287, 1246, 1114, 1031, 821, 725 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.48 (d, *J* = 8.8 Hz, 2H), 7.26 (q, *J* = 8.8, 10.0 Hz, 4H), 6.83 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H), 1.28 (s, 9H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 159.6, 149.7, 136.1, 131.0, 129.2, 126.2, 120.4, 115.0, 55.2, 34.4, 31.2. (ESI) ($[M]^+$) Calcd. for $C_{17}H_{20}O^{80}Se$: 320.0679, Found 320.0677; Calcd. for $C_{17}H_{20}O^{78}Se$: 318.0687, Found 318.0680.

***n*-Butyl 4-methoxyphenyl selenide[4]**



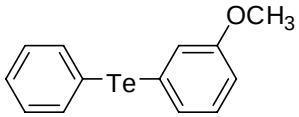
IR (neat): 3063, 2957, 2930, 2871, 1592, 1491, 1284, 1246, 1173, 1031, 823 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.48 (d, *J* = 8.8 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H), 2.83 (t, *J* = 7.6 Hz, 2H), 1.67–1.63 (m, 2H), 1.44–1.39 (m, 2H), 0.91 (t, *J* = 7.6 Hz, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 159.1, 135.5, 120.2, 114.7, 55.3, 32.3, 28.8, 22.9, 13.6. Anal. Calcd for $C_{11}H_{16}OSe$: C, 54.32; H, 6.63. Found: C, 54.16; H, 6.75.

4-Methoxyphenyl phenyl telluride[1]



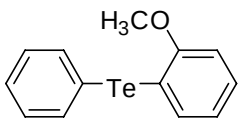
IR (neat): 3055, 2928, 2839, 1714, 1586, 1489, 1362, 1293, 1177, 1026, 824, 738, 690 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.72 (d, *J* = 8.8 Hz, 2H), 7.55 (q, *J* = 2.8, 4.0 Hz, 2H), 7.20–7.13 (m, 3H), 6.78 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 160.0, 141.2, 136.4, 129.4, 127.3, 115.9, 115.6, 103.2, 55.2. Anal. Calcd for $C_{13}H_{12}OTe$: C, 50.07; H, 3.88. Found: C, 49.89; H, 4.01.

3-Methoxyphenyl phenyl telluride



IR (neat): 3058, 2970, 2845, 1735, 1559, 1541, 1474, 1363, 669 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.71 (d, *J* = 9.2 Hz, 2H), 7.31–7.20 (m, 5H), 7.12 (t, *J* = 7.6 Hz, 1H), 6.81 (d, *J* = 8.4 Hz, 1H), 3.74 (s, 3H). δ_c (100 MHz; $CDCl_3$; Me_4Si) 159.9, 138.2, 130.2, 130.1, 129.5, 128.0, 123.0, 113.8, 55.2. (ESI) ($[M]^+$) Calcd. for $C_{13}H_{12}O^{130}Te$: 313.9950, Found 313.9957.

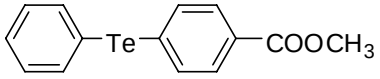
2-Methoxyphenyl phenyl telluride[1]



IR (neat): 3057, 2934, 2833, 1587, 1475, 1284, 1244, 1040, 838, 737, 688 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.88 (d, *J* = 8.0 Hz, 2H), 7.40–7.37 (m, 1H), 7.30–7.26 (m, 2H), 7.18–7.14 (m, 1H), 6.93 (d, *J* =

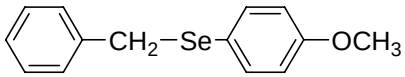
7.6 Hz, 1H), 6.77 (d, J = 8.0 Hz, 1H), 6.72 (t, J = 7.6 Hz, 1H), 3.85 (s, 3H). δ_C (100 MHz; $CDCl_3$; Me_4Si) 157.9, 141.1, 133.4, 129.5, 128.6, 128.0, 122.3, 111.9, 109.5, 107.6, 55.8. Anal. Calcd for $C_{13}H_{12}OTe$: C, 50.07; H, 3.88. Found: C, 50.21; H, 3.75.

4-Methoxycarbonylphenyl phenyl telluride[1]



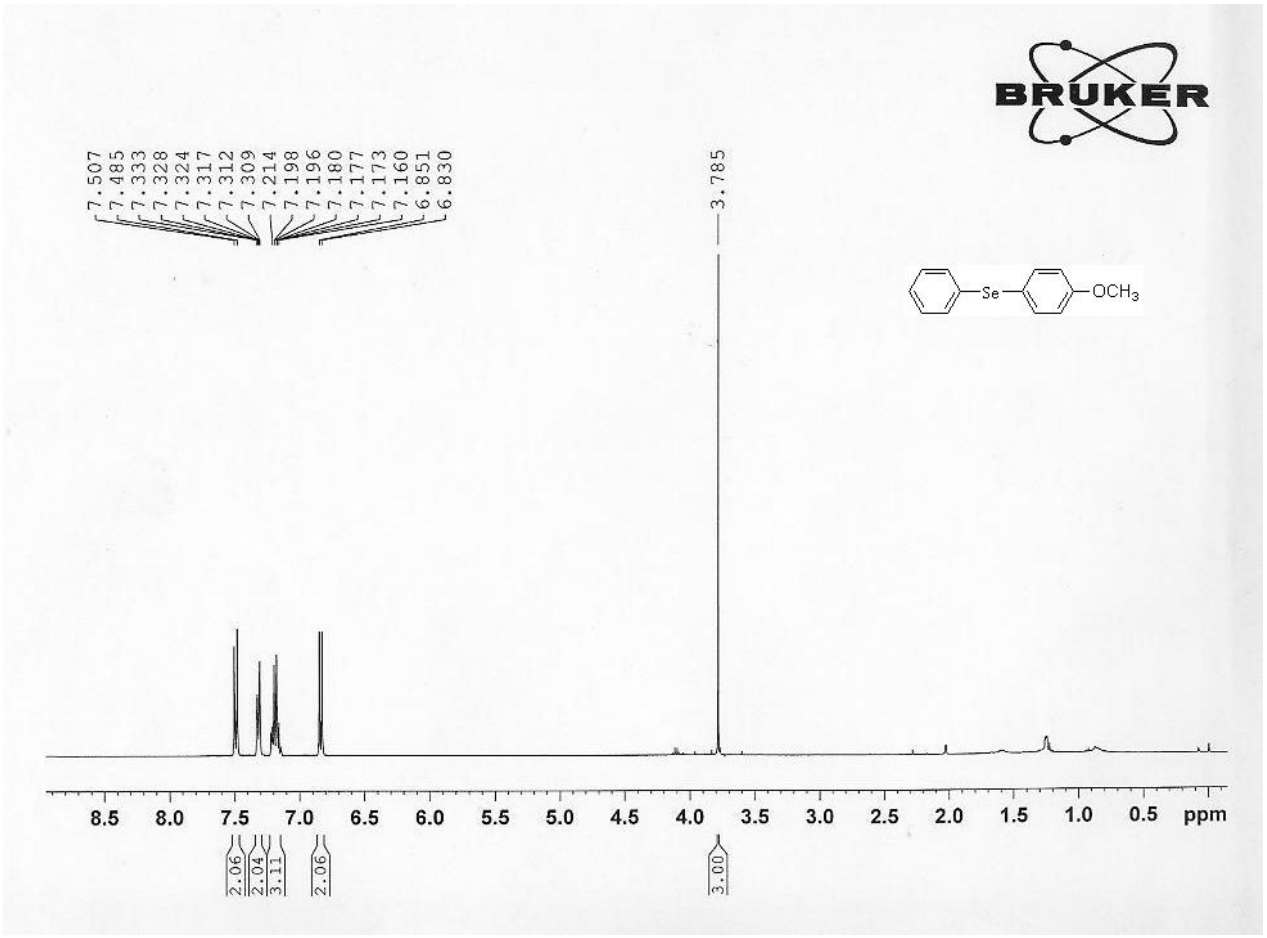
IR (neat): 3055, 2951, 2854, 1717, 1586, 1435, 1390, 1281, 1106, 1012, 823, 755, 688 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.81–7.78 (m, 4H), 7.59 (d, J = 8.4 Hz, 2H), 7.36 (t, J = 6.8 Hz, 1H), 7.26 (t, J = 7.2 Hz, 2H), 3.88 (s, 3H). δ_C (100 MHz; $CDCl_3$; Me_4Si) 166.9, 139.5, 135.9, 130.1, 129.8, 129.0, 128.7, 123.4, 113.4, 52.2. Anal. Calcd for $C_{14}H_{12}O_2Te$: C, 49.48; H, 3.46. Found: C, 49.61; H, 3.52.

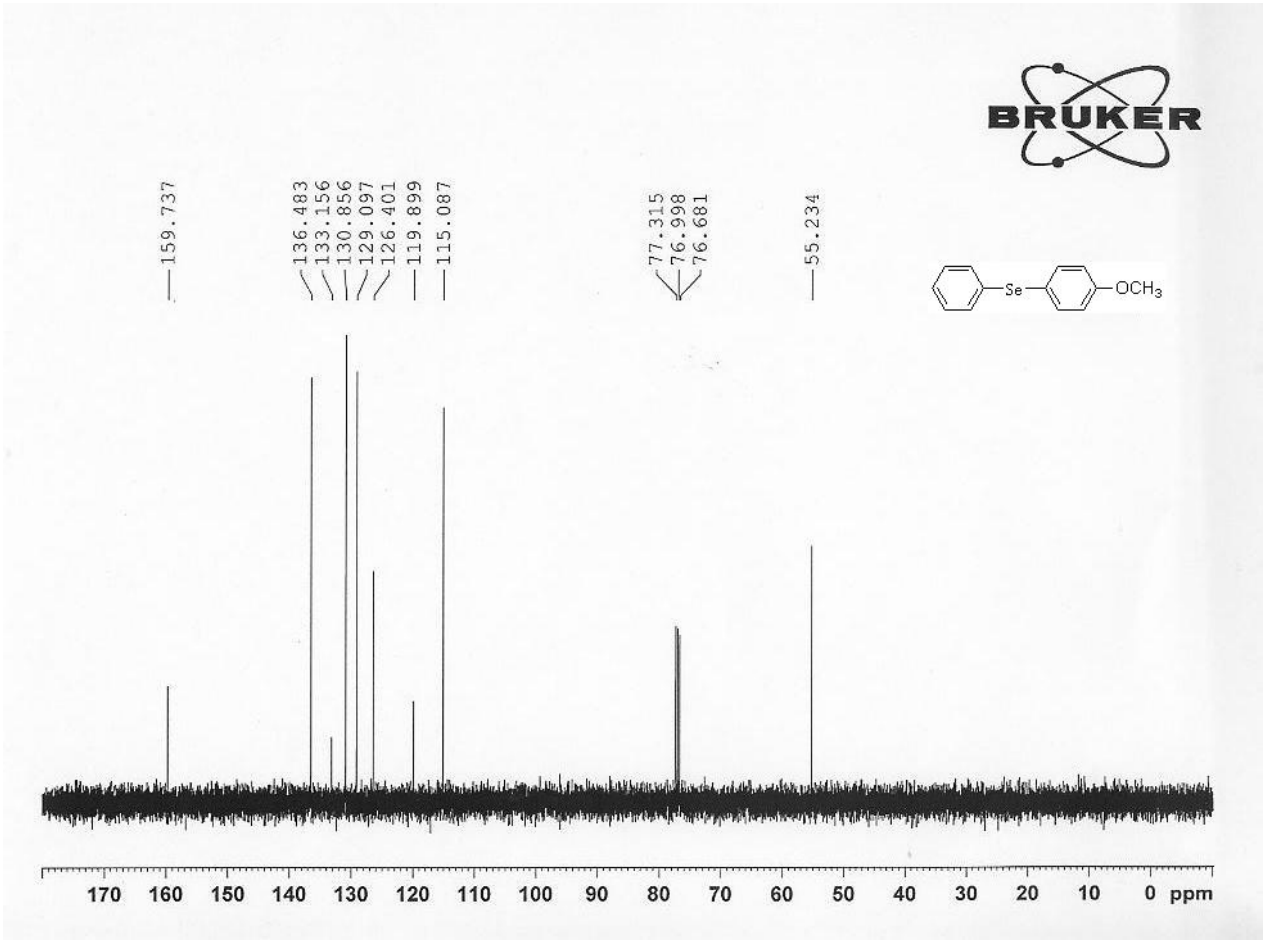
Benzyl 4-methoxyphenyl selenide[7]

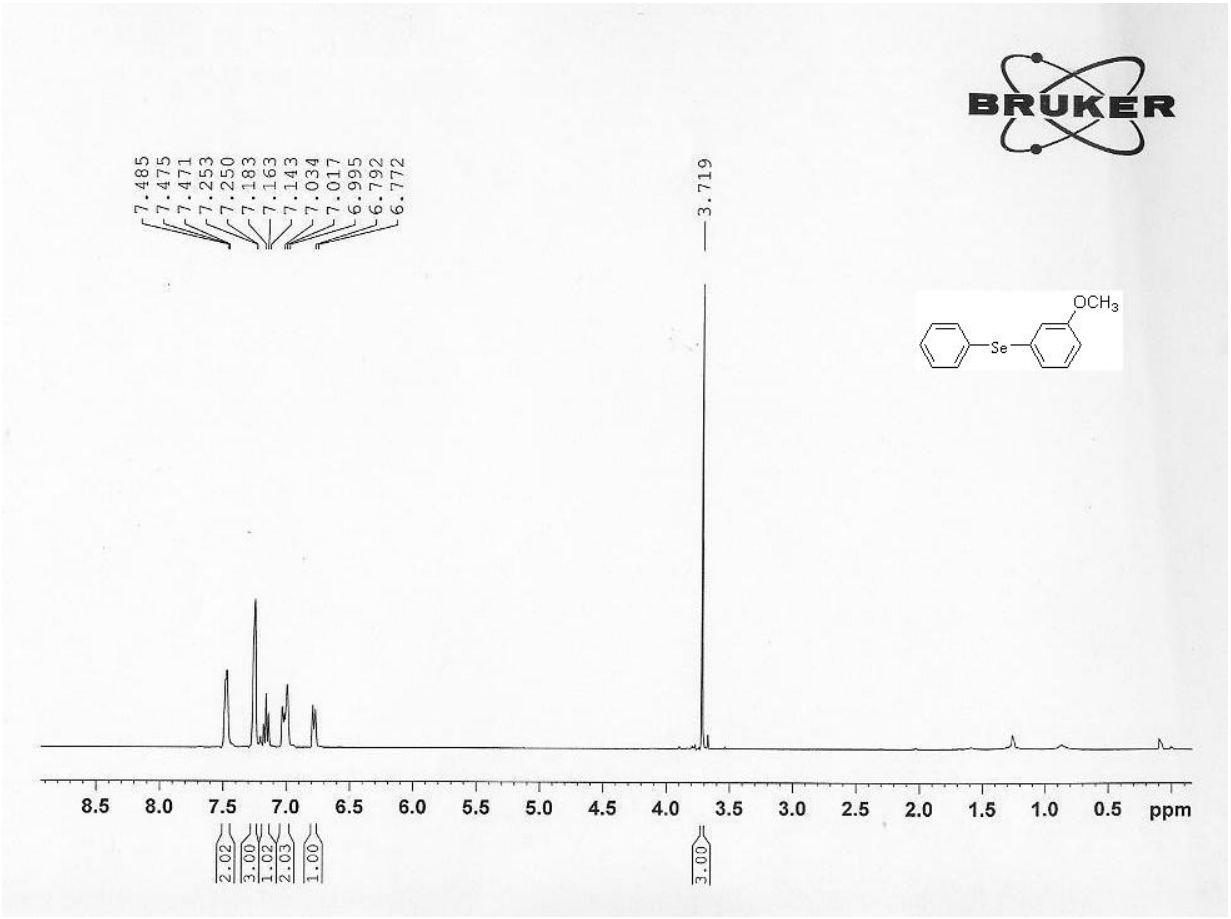


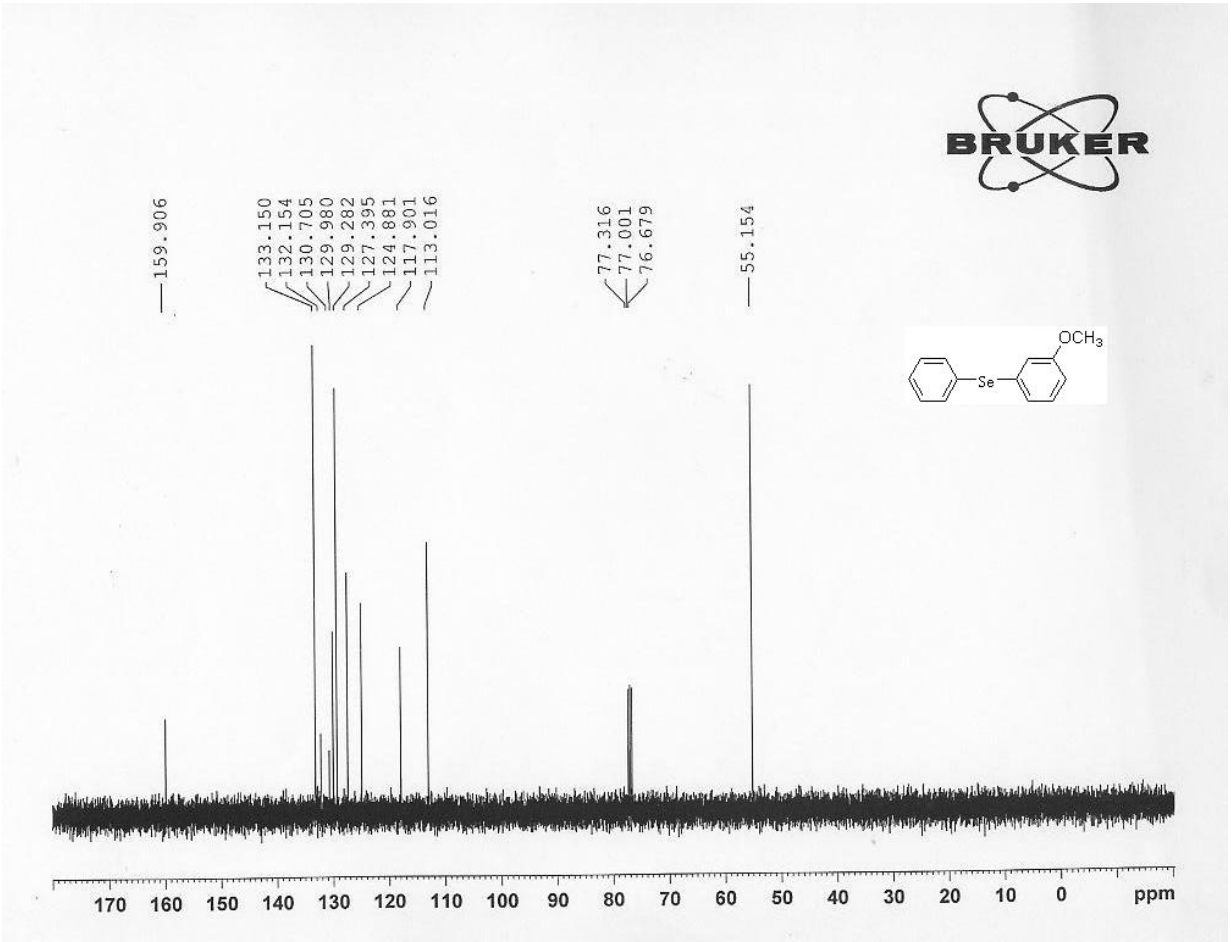
IR (neat): 3055, 2963, 2854, 1717, 1590, 1490, 1260, 1028, 802, 696 cm^{-1}. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.28 (d, J = 8.4 Hz, 2H), 7.16–7.09 (m, 3H), 7.04 (d, J = 6.8 Hz, 2H), 6.69 (d, J = 8.8 Hz, 2H), 3.92 (s, 2H), 3.70 (s, 3H). δ_C (100 MHz; $CDCl_3$; Me_4Si) 159.5, 139.1, 136.5, 128.8, 128.3, 126.6, 120.0, 114.6, 55.2, 33.1. Anal. Calcd for $C_{14}H_{14}OSe$: C, 60.66; H, 5.09. Found: C, 60.79; H, 4.98.

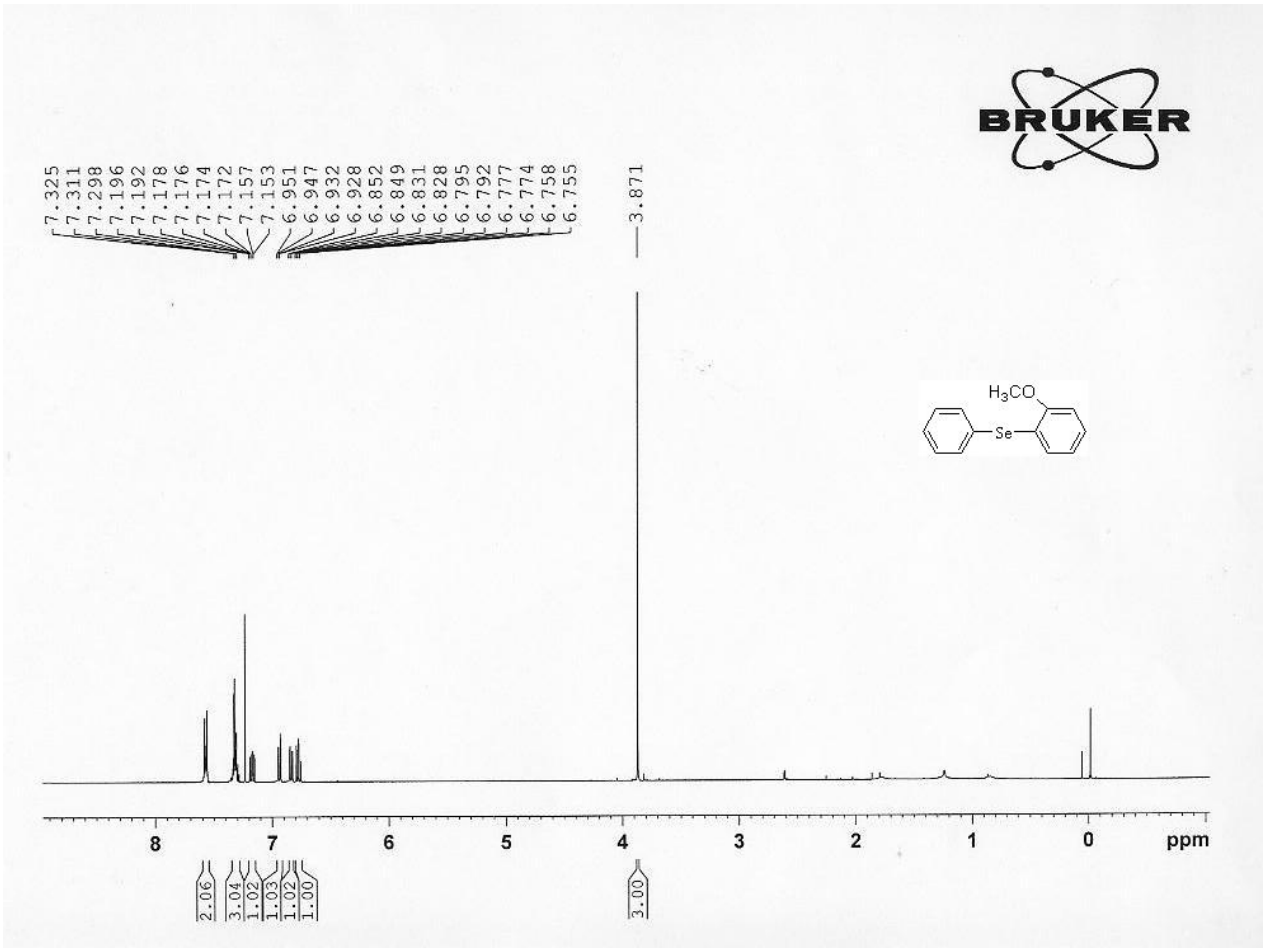
[1] N. Taniguchi, *J. Org. Chem.*, 2007, **72**, 1241–1245.
[2] W. W. Lin, F. Ilgen and P. Knochel, *Tetrahedron Lett.*, 2006, **47**, 1941–1944.
[3] J. Oddershede, L. Henriksen and Larsen, S. *Org. Biomol. Chem.*, 2003, 1, 1053–1060.
[4] L. Wang, M. Wang and F. Huang, *Synlett*, 2005, 2007–2010.
[5] W. W. Lin, I. Sapountzis and Knochel, P. *Angew. Chem. Int. Ed.*, 2005, **44**, 4258–4261.
[6] I. P. Beletskaya, A. S. Sigeev, A. S. Peregudov and P. V. Petrovskii, *Tetrahedron Lett.*, **2003**, **44**, 7039–7041.
[7] A. Krief and F. Lonez, *Tetrehedron Lett.*, 2002, **43**, 6255–6257.

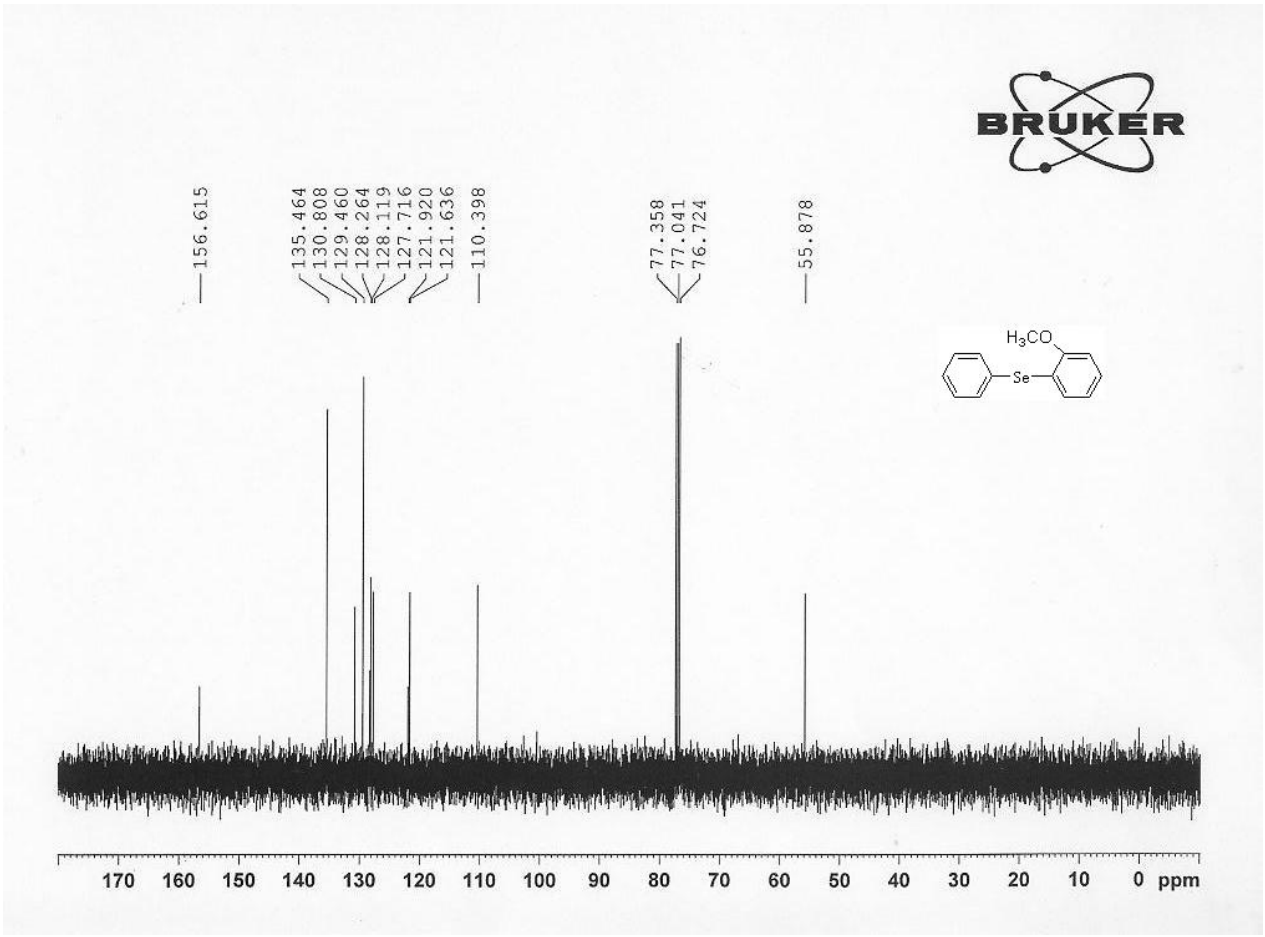

BRUKER
7.507
7.485
7.333
7.328
7.324
7.317
7.312
7.309
7.214
7.198
7.196
7.180
7.177
7.173
7.160
6.851
6.830
3.785
Se
OCH3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.06
2.04
3.11
2.06
3.00

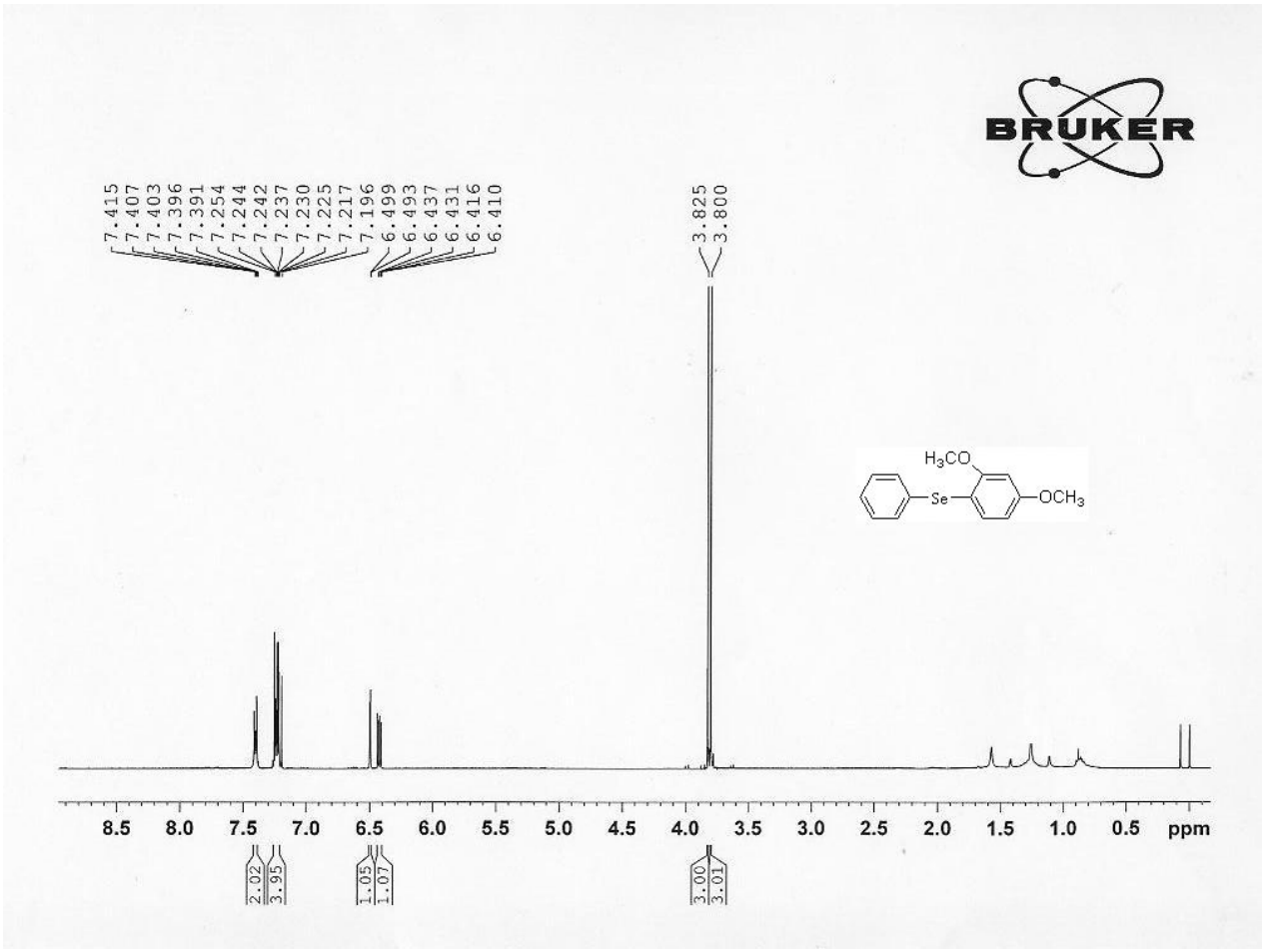

BRUKER
159.737
136.483
133.156
130.856
129.097
126.401
119.899
115.087
77.315
76.998
76.681
55.234
Se
OCH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

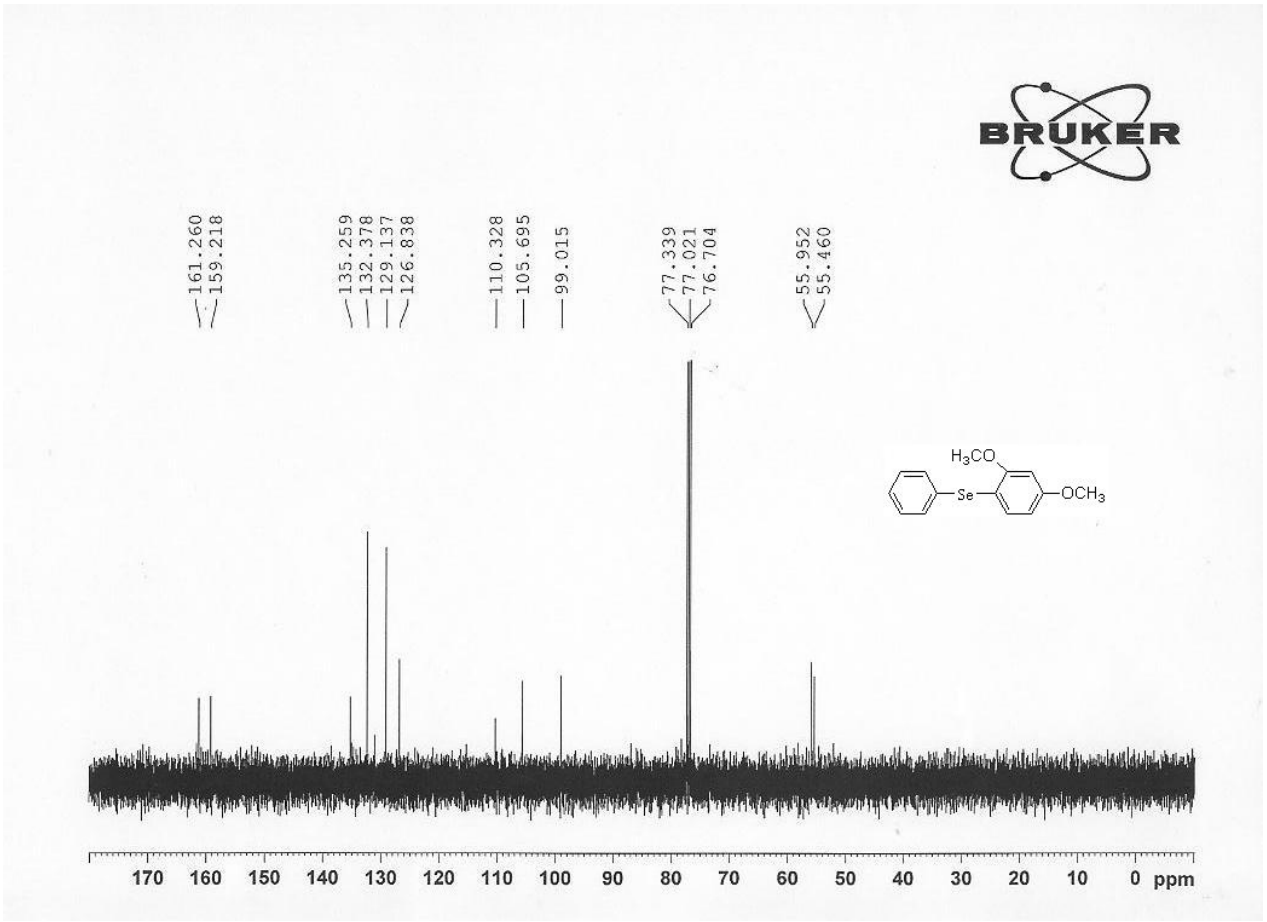

BRUKER
7.485
7.475
7.471
7.253
7.250
7.183
7.163
7.143
7.034
7.017
6.995
6.792
6.772
3.719
OCH3
Se
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.02
3.00
1.02
2.03
1.00
3.00

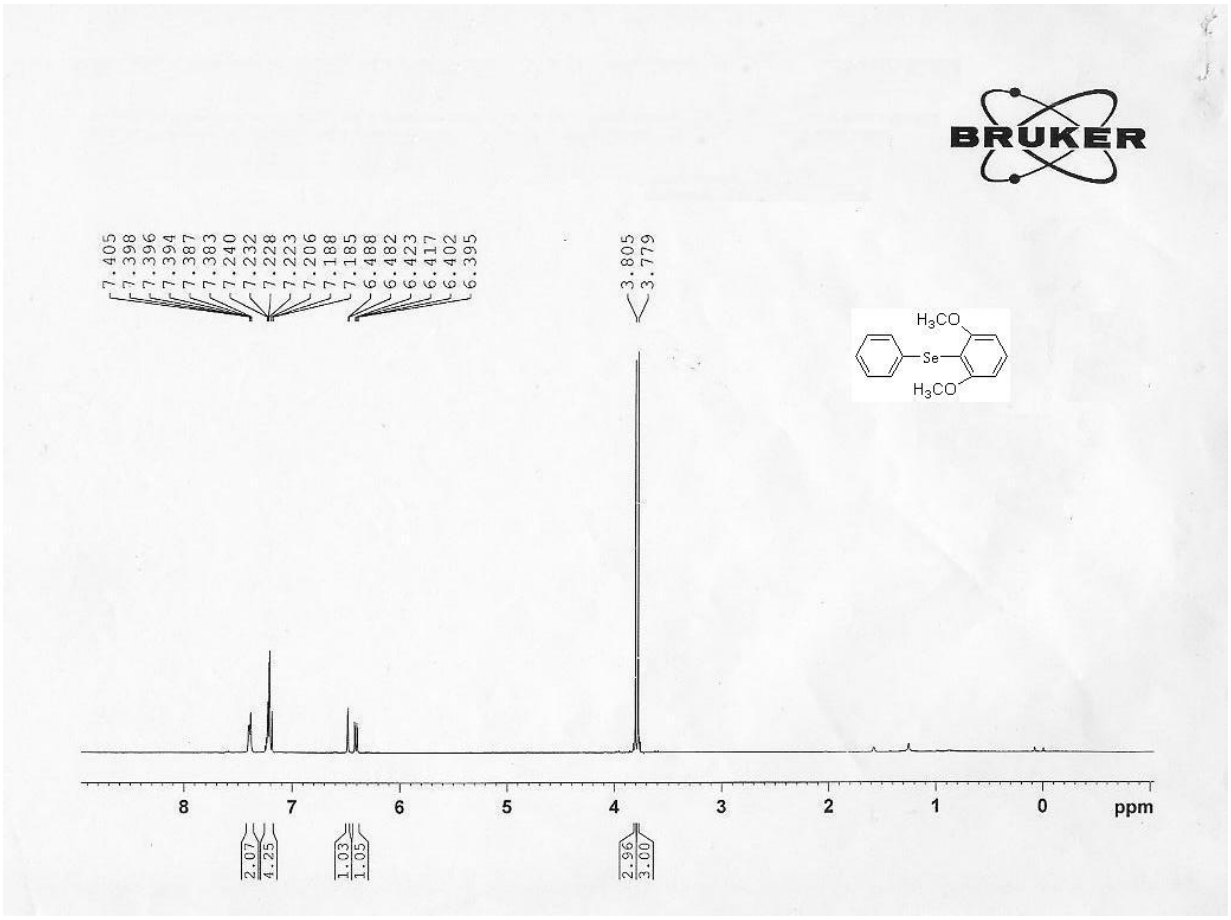

BRUKER
159.906
133.150
132.154
130.705
129.980
129.282
127.395
124.881
117.901
113.016
77.316
77.001
76.679
55.154
OCH3
Se
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

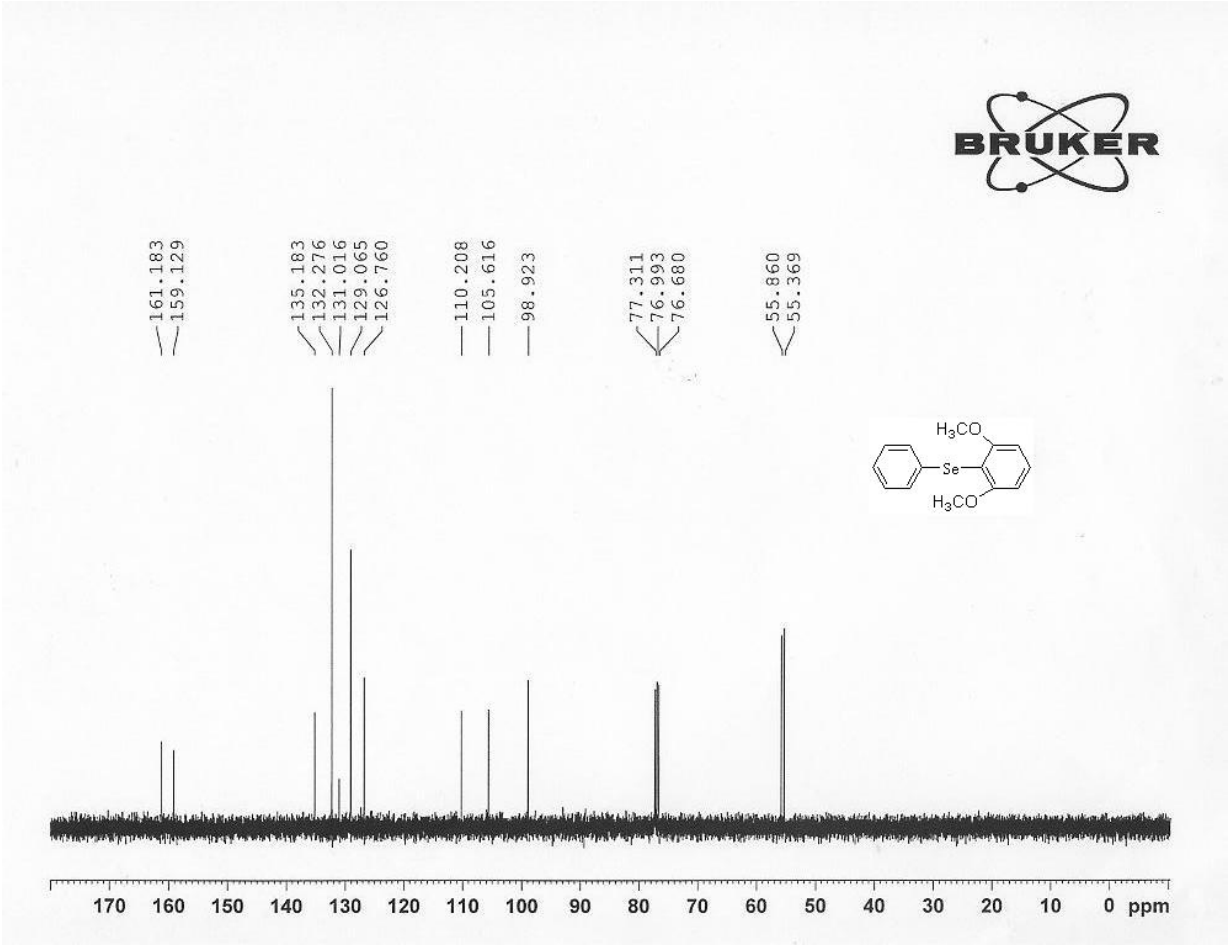

BRUKER
7.325
7.311
7.298
7.196
7.192
7.178
7.176
7.174
7.172
7.157
7.153
6.951
6.947
6.932
6.928
6.852
6.849
6.831
6.828
6.795
6.792
6.777
6.774
6.758
6.755
3.871
H3CO
Se
8
7
6
5
4
3
2
1
0
ppm
2.06
3.04
1.02
1.03
1.02
1.00
3.00

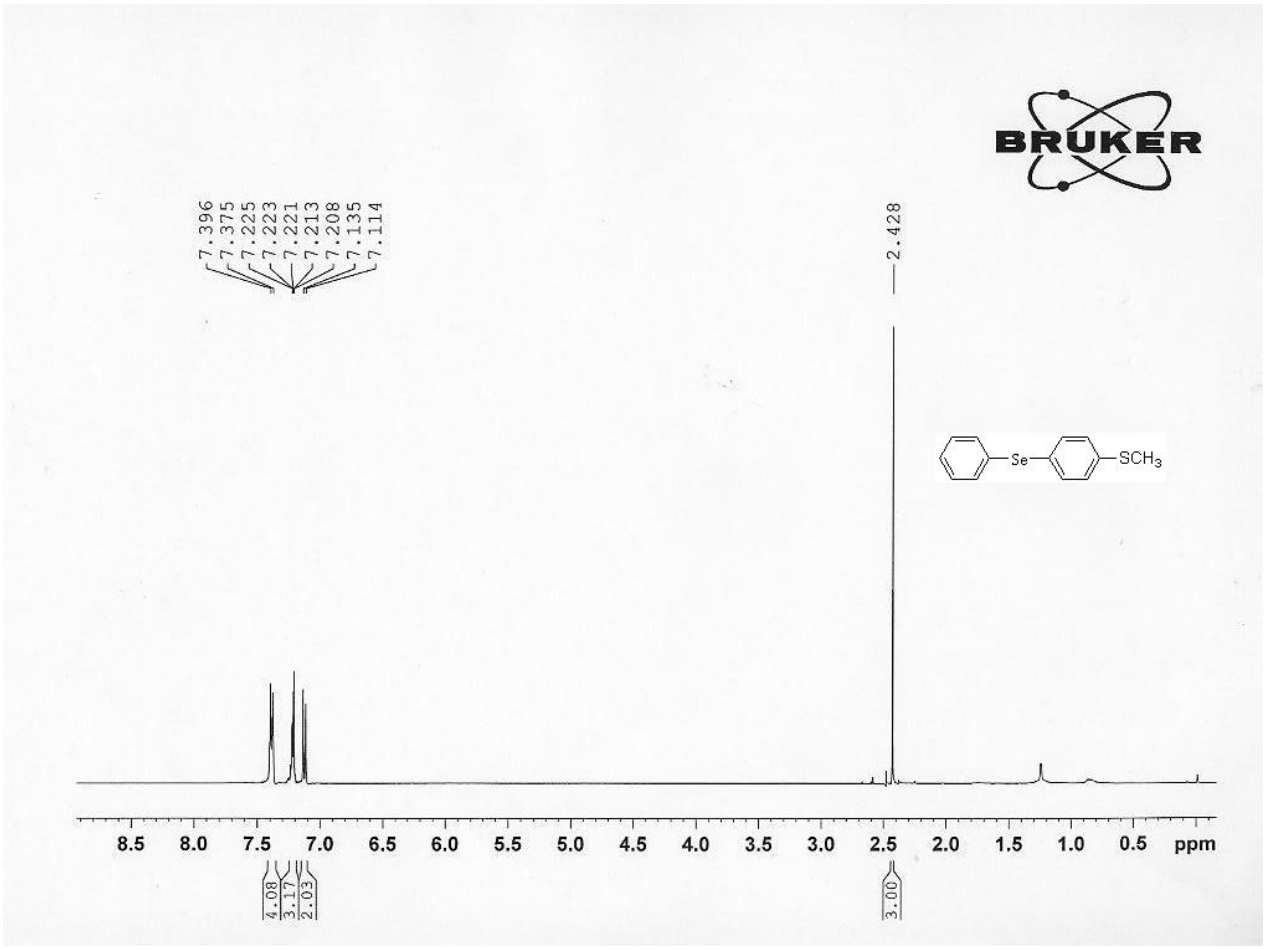

BRUKER
156.615
135.464
130.808
129.460
128.264
128.119
127.716
121.920
121.636
110.398
77.358
77.041
76.724
55.878
H3CO
Se
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

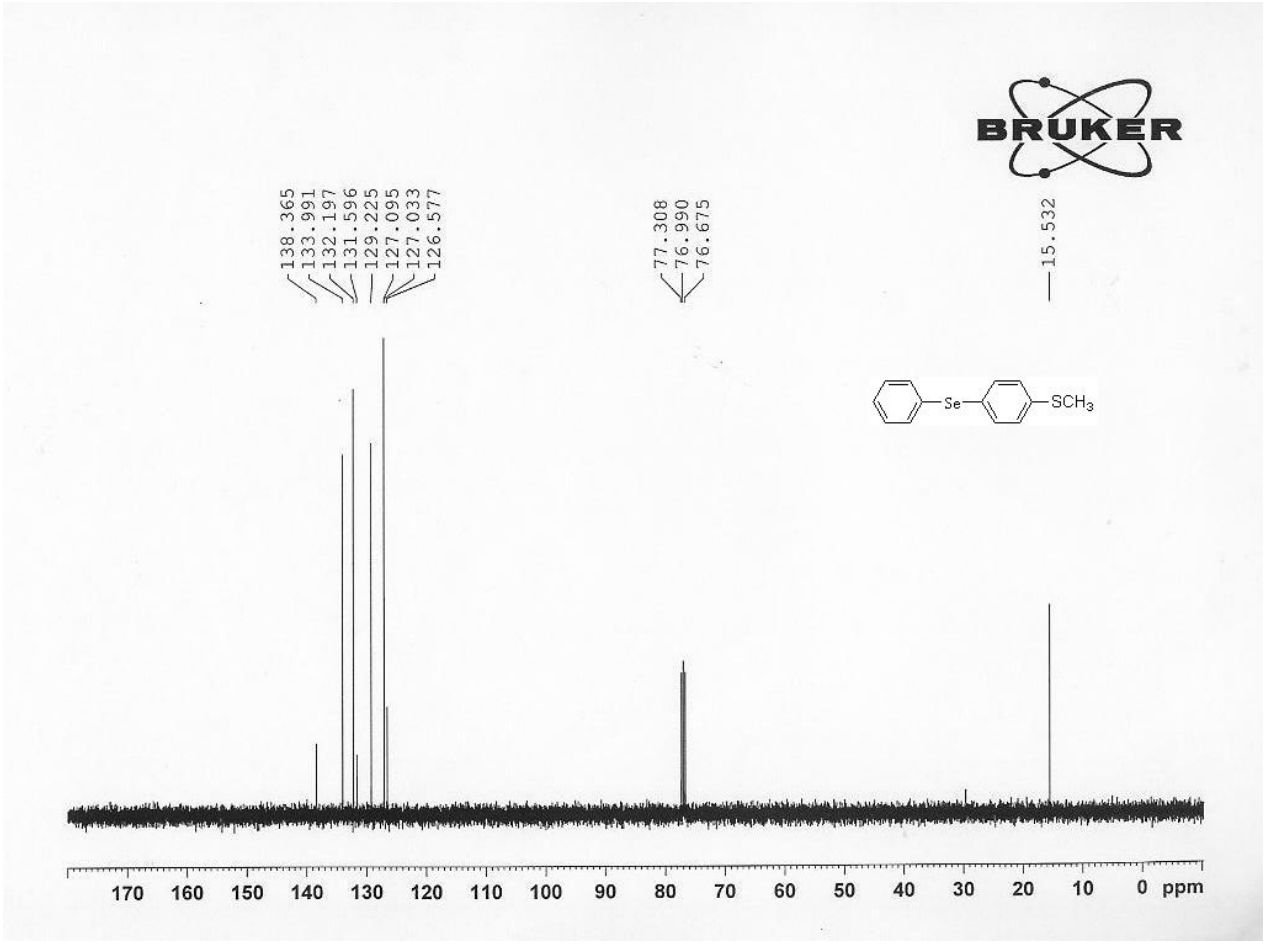

BRUKER
7.415
7.407
7.403
7.396
7.391
7.254
7.244
7.242
7.237
7.230
7.225
7.217
7.196
6.499
6.493
6.437
6.431
6.416
6.410
3.825
3.800
H3CO
Se
OCH3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.02
3.95
1.05
1.07
3.00
3.01

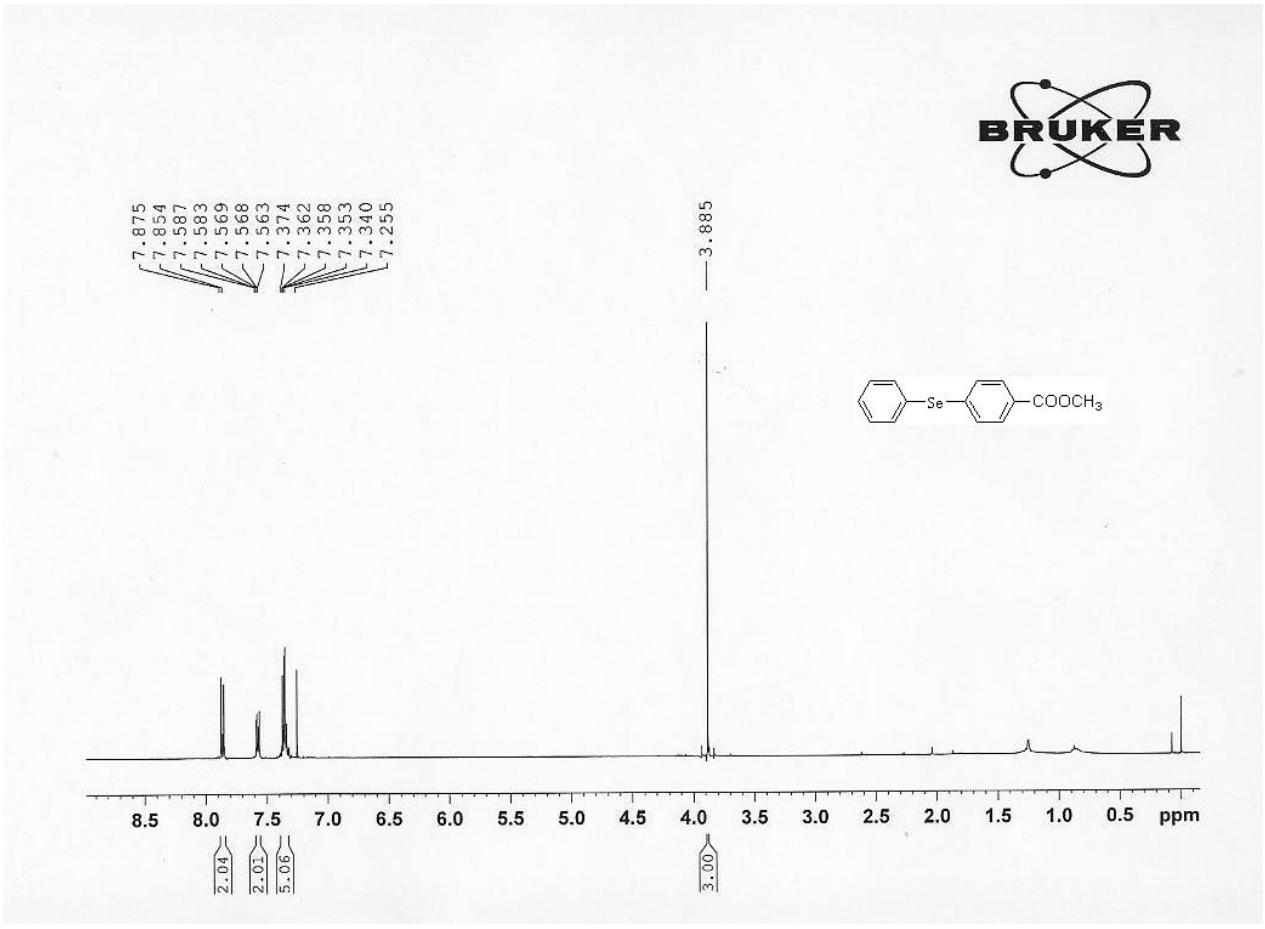

BRUKER
161.260
159.218
135.259
132.378
129.137
126.838
110.328
105.695
99.015
77.339
77.021
76.704
55.952
55.460
H3CO
Se
OCH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

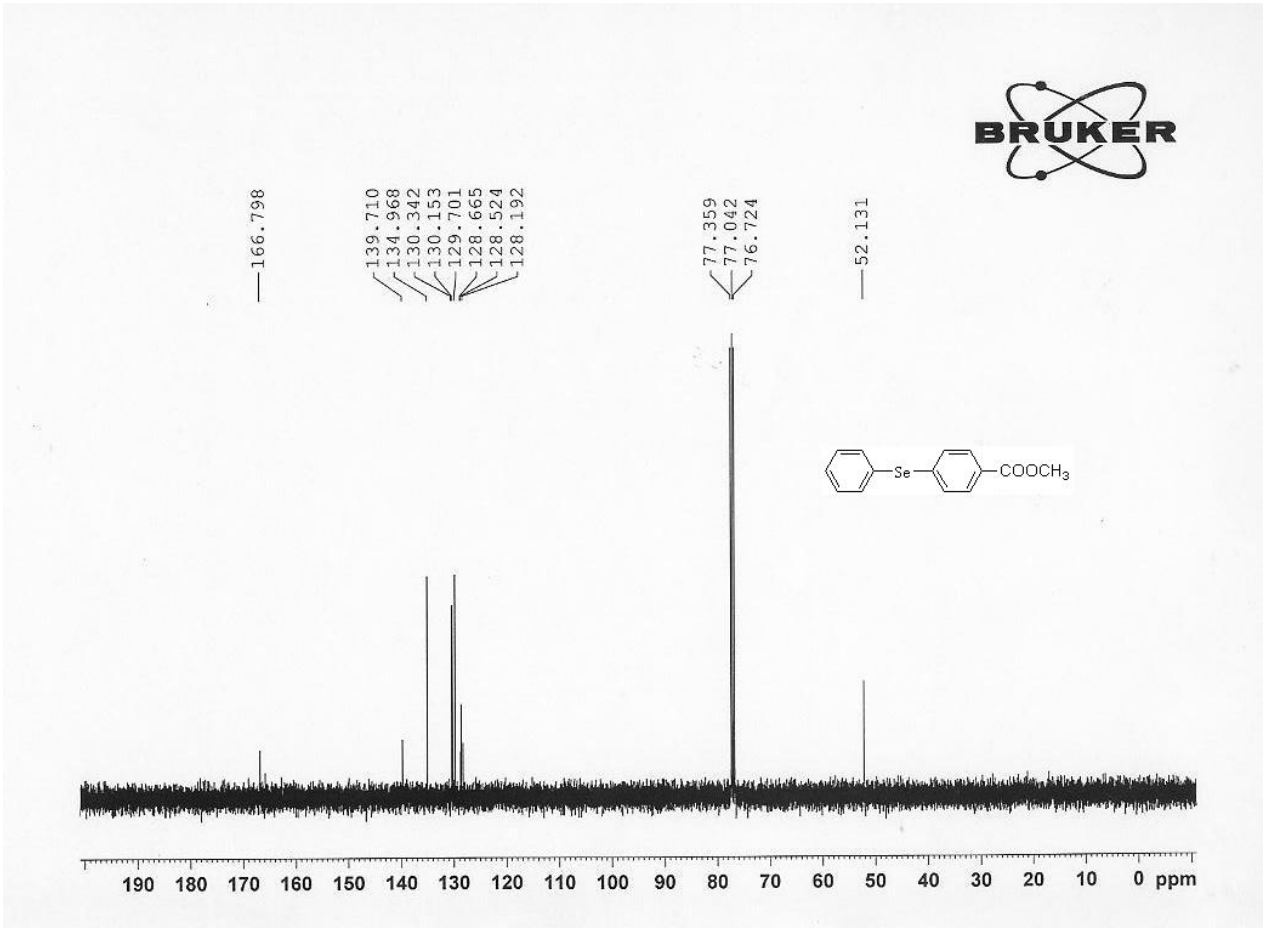

BRUKER
7.405
7.398
7.396
7.394
7.387
7.383
7.240
7.232
7.228
7.223
7.206
7.188
7.185
6.488
6.482
6.423
6.417
6.402
6.395
3.805
3.779
H3CO
Se
H3CO
8
7
6
5
4
3
2
1
0
ppm
2.07
4.25
1.03
1.05
2.96
3.00

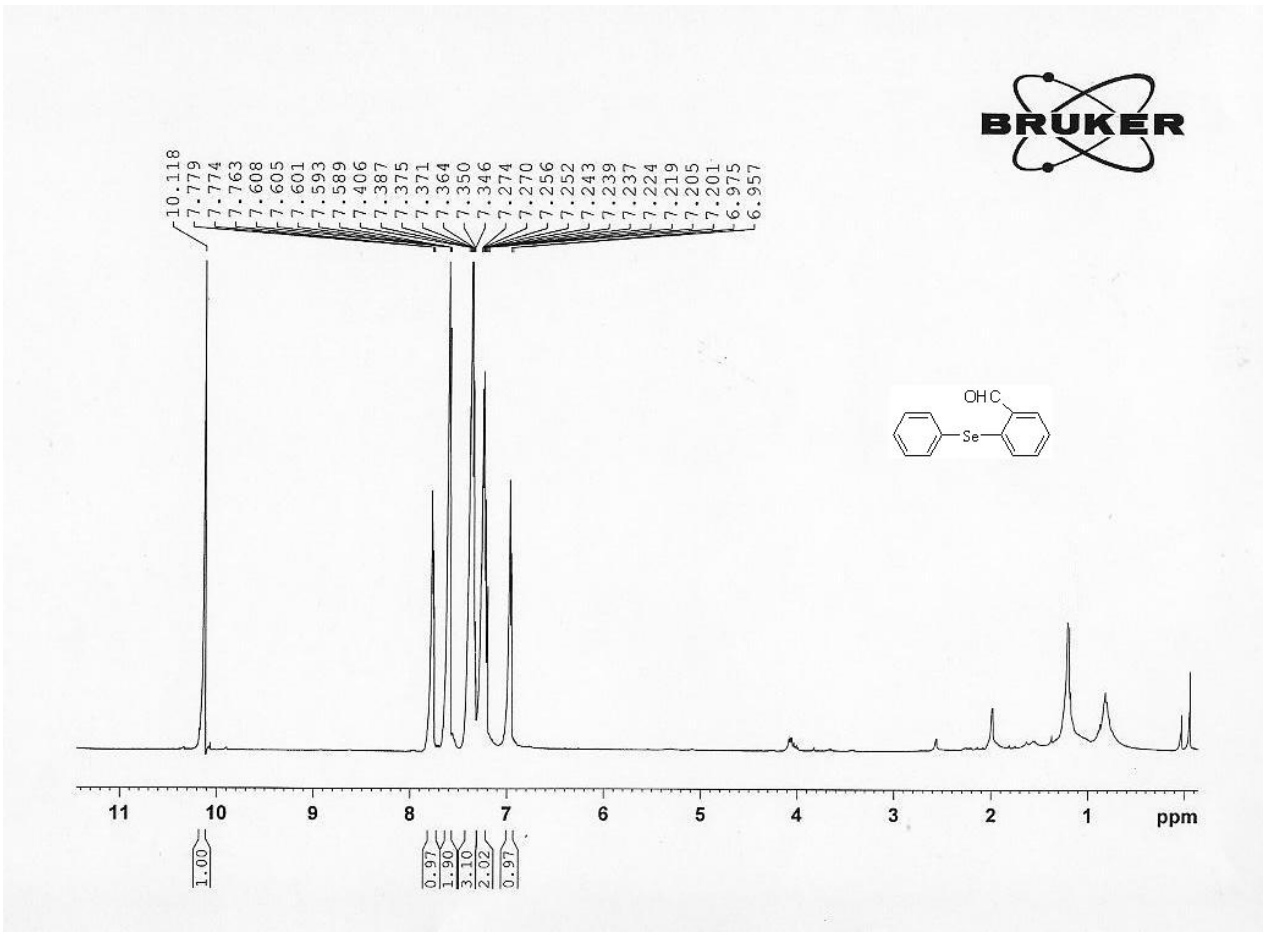

BRUKER
161.183
159.129
135.183
132.276
131.016
129.065
126.760
110.208
105.616
98.923
77.311
76.993
76.680
55.860
55.369
H3CO
Se
H3CO
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

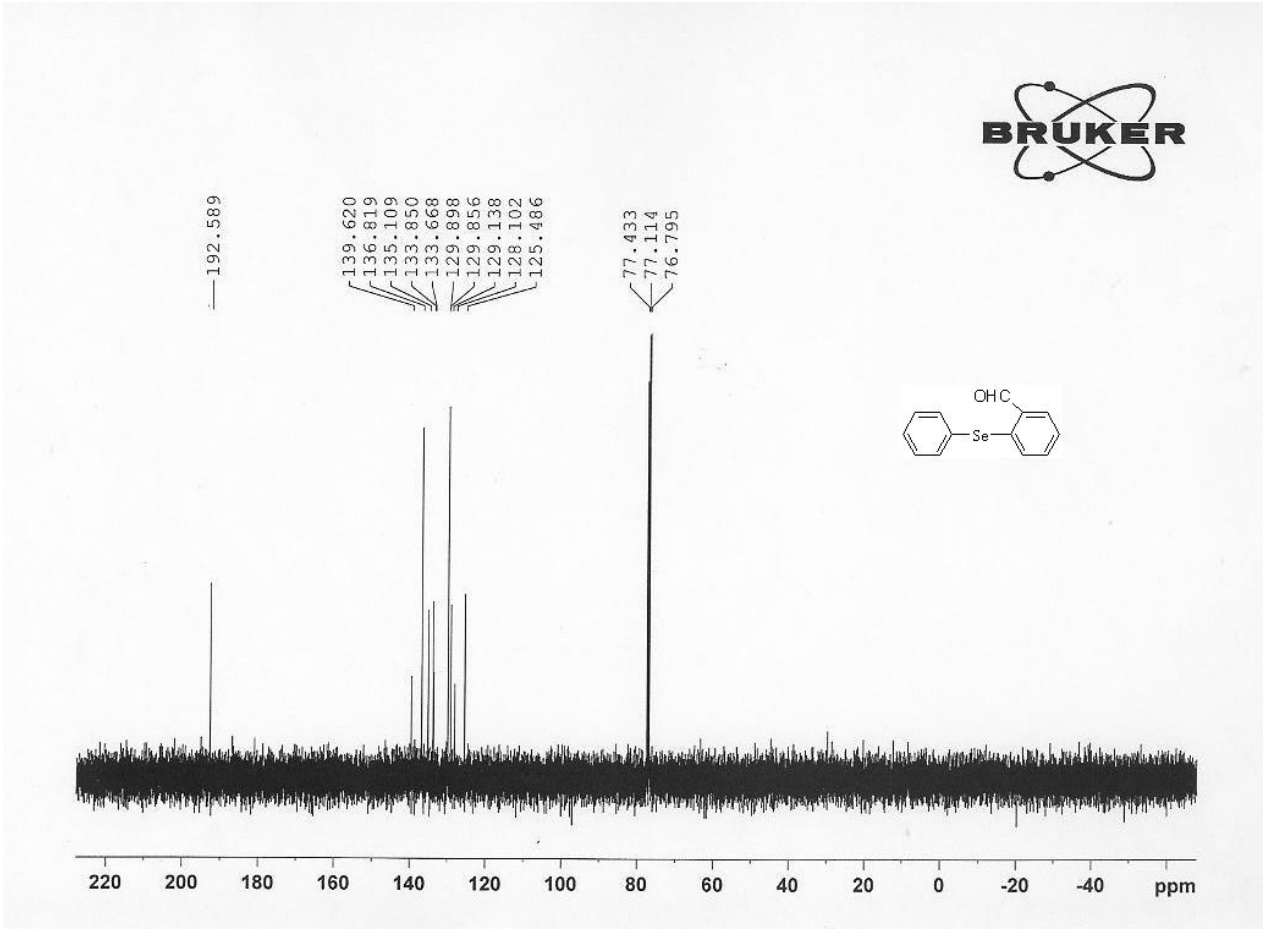

BRUKER
7.396
7.375
7.225
7.223
7.221
7.213
7.208
7.135
7.114
2.428
Se
SCH3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
4.08
3.17
2.03
3.00

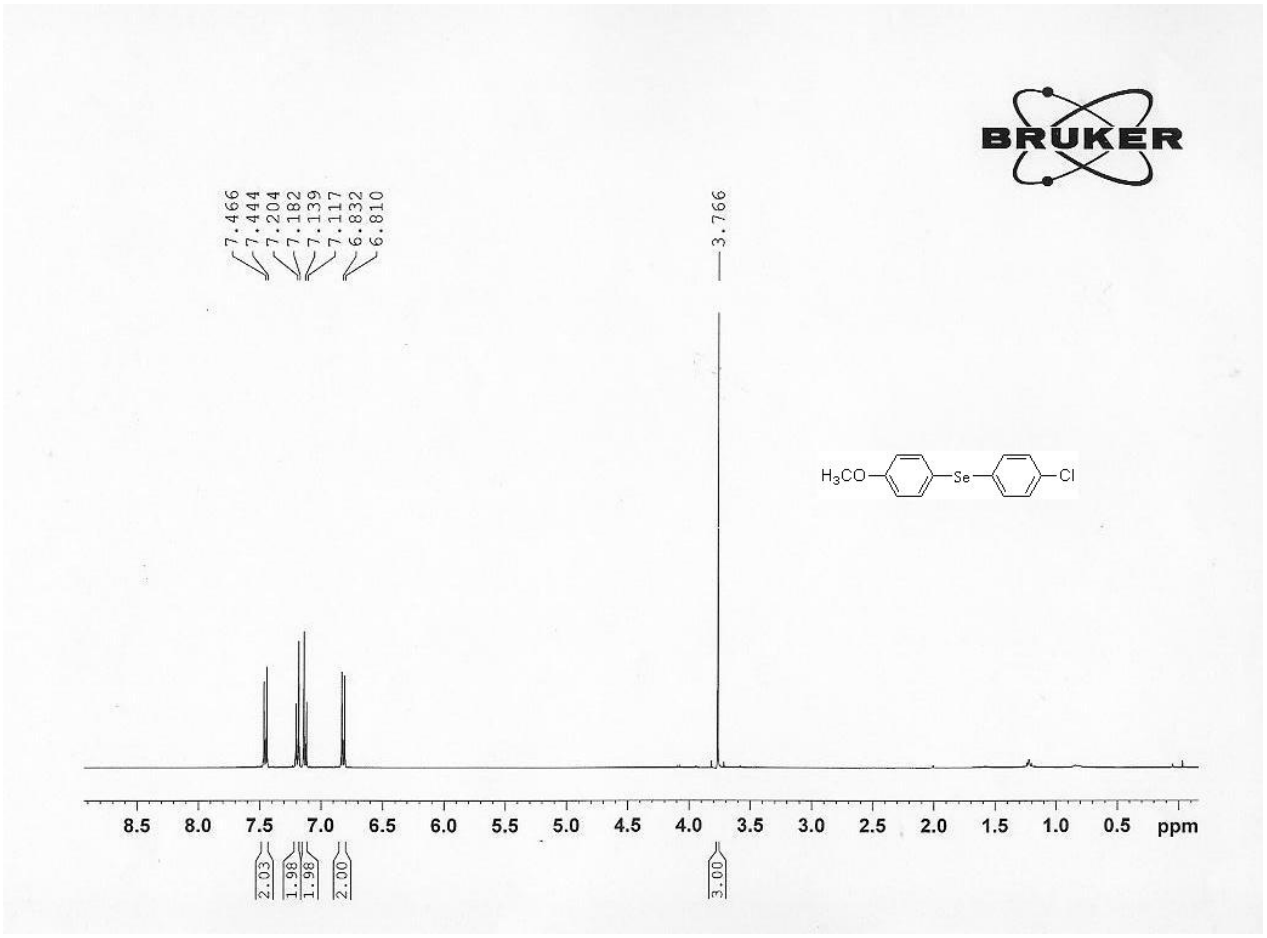

BRUKER
138.365
133.991
132.197
131.596
129.225
127.095
127.033
126.577
77.308
76.990
76.675
15.532
Se
SCH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

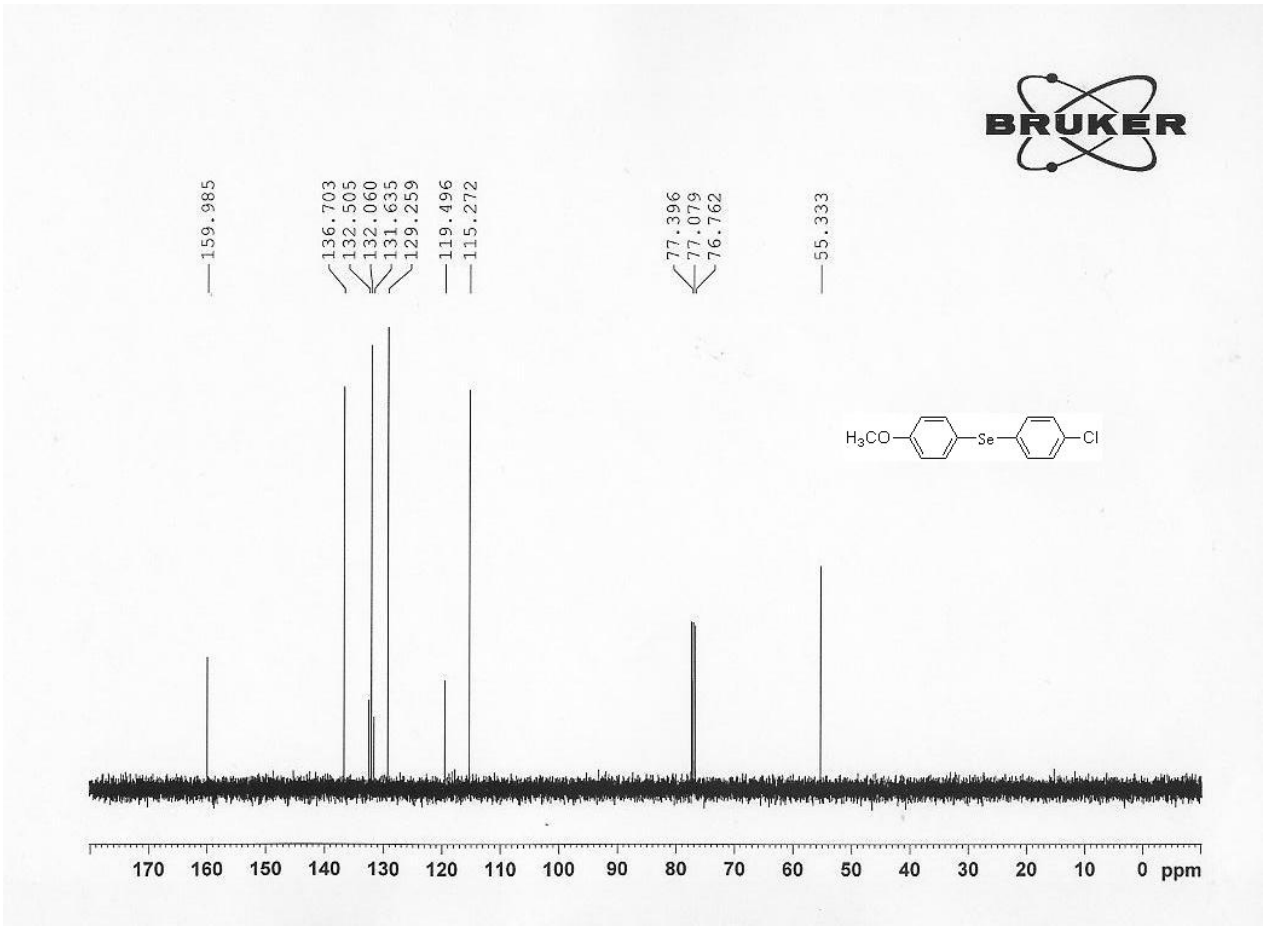

BRUKER
7.875
7.854
7.587
7.583
7.569
7.568
7.563
7.374
7.362
7.358
7.353
7.340
7.255
3.885
Se
COOCH3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.04
2.01
5.06
3.00

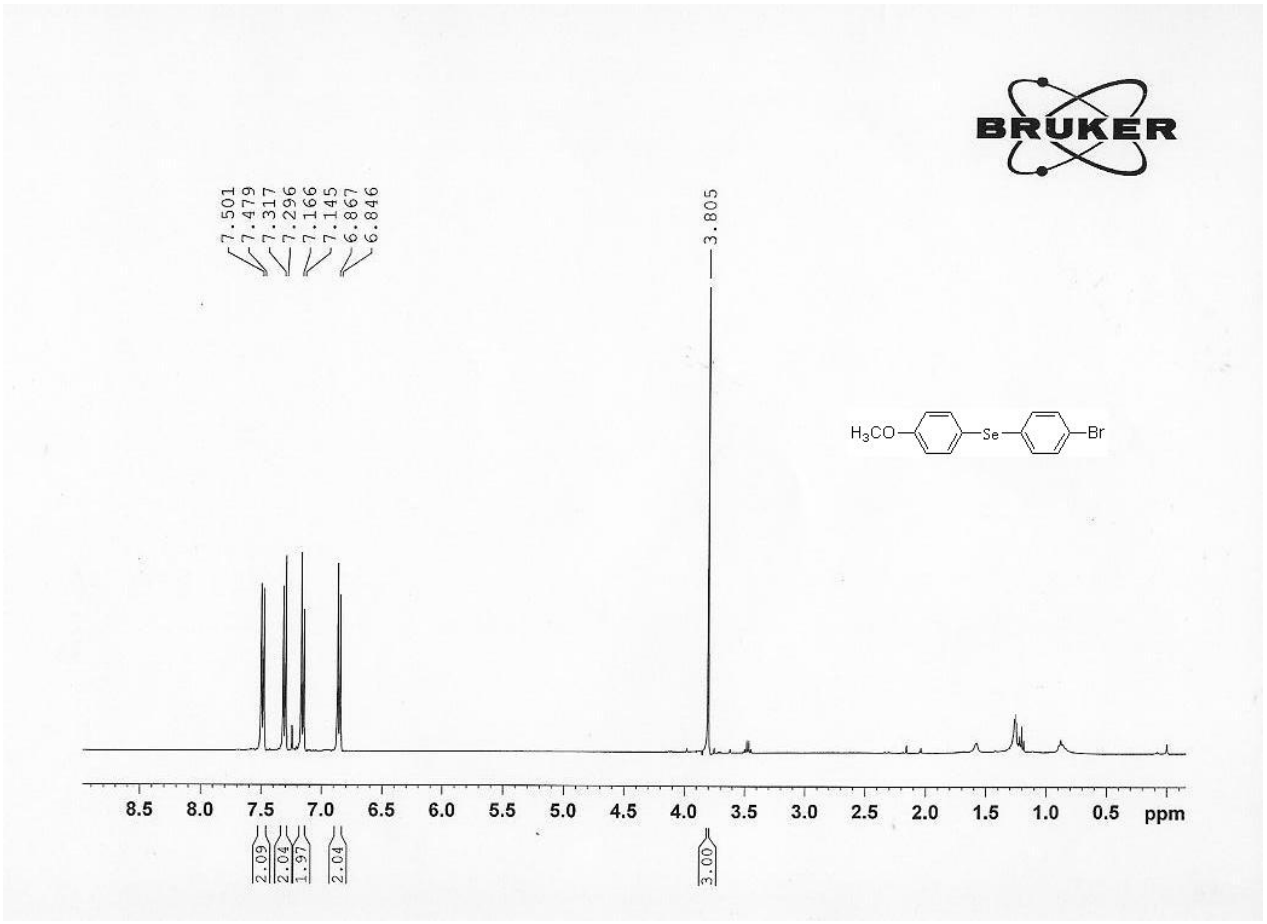

BRUKER
166.798
139.710
134.968
130.342
130.153
129.701
128.665
128.524
128.192
77.359
77.042
76.724
52.131
Se
COOCH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

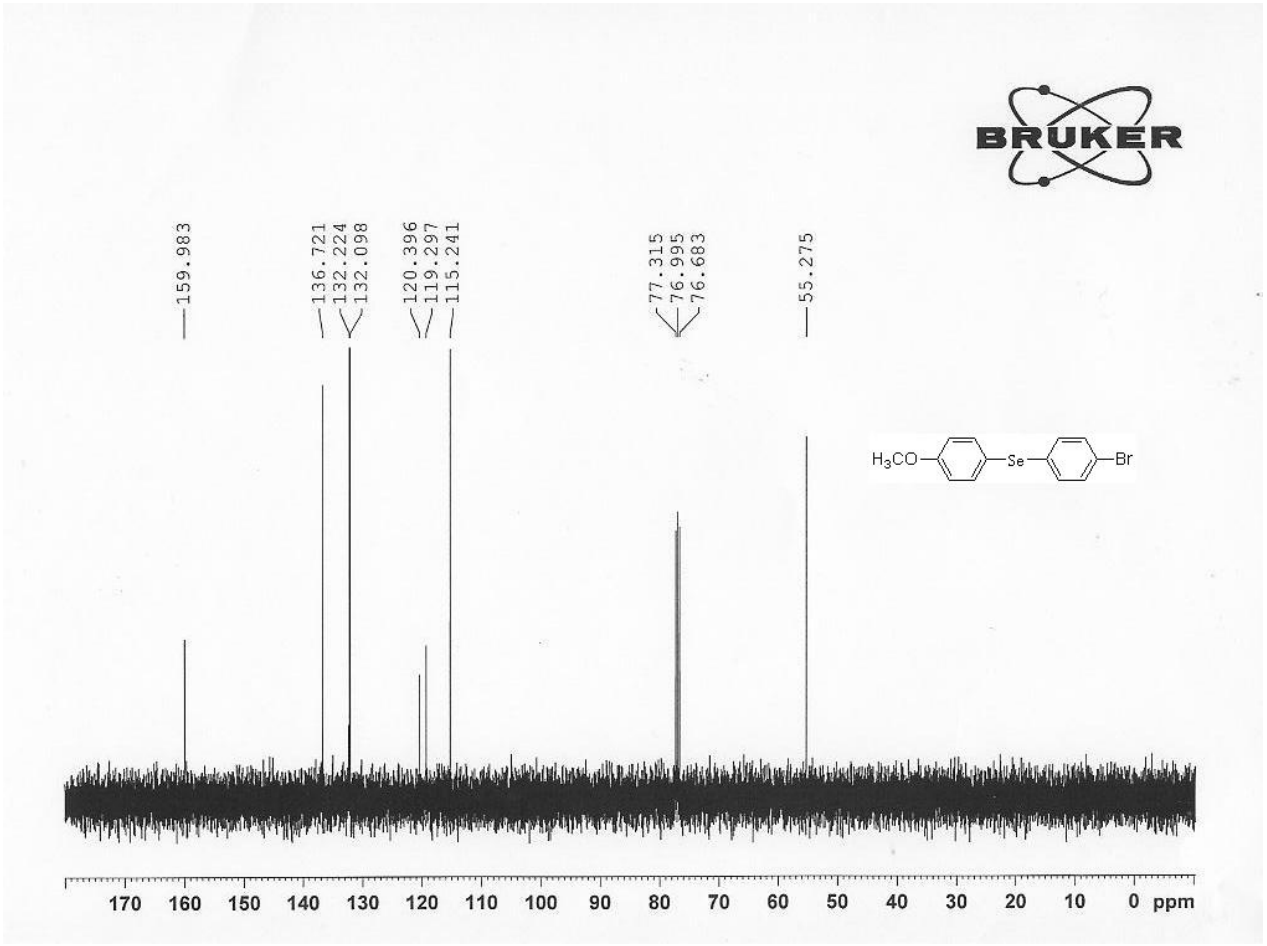

BRUKER
10.118
7.779
7.774
7.763
7.608
7.605
7.601
7.593
7.589
7.406
7.387
7.375
7.371
7.364
7.350
7.346
7.274
7.270
7.256
7.252
7.243
7.239
7.237
7.224
7.219
7.205
7.201
6.975
6.957
OHC
Se
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.97
1.90
3.10
2.02
0.97

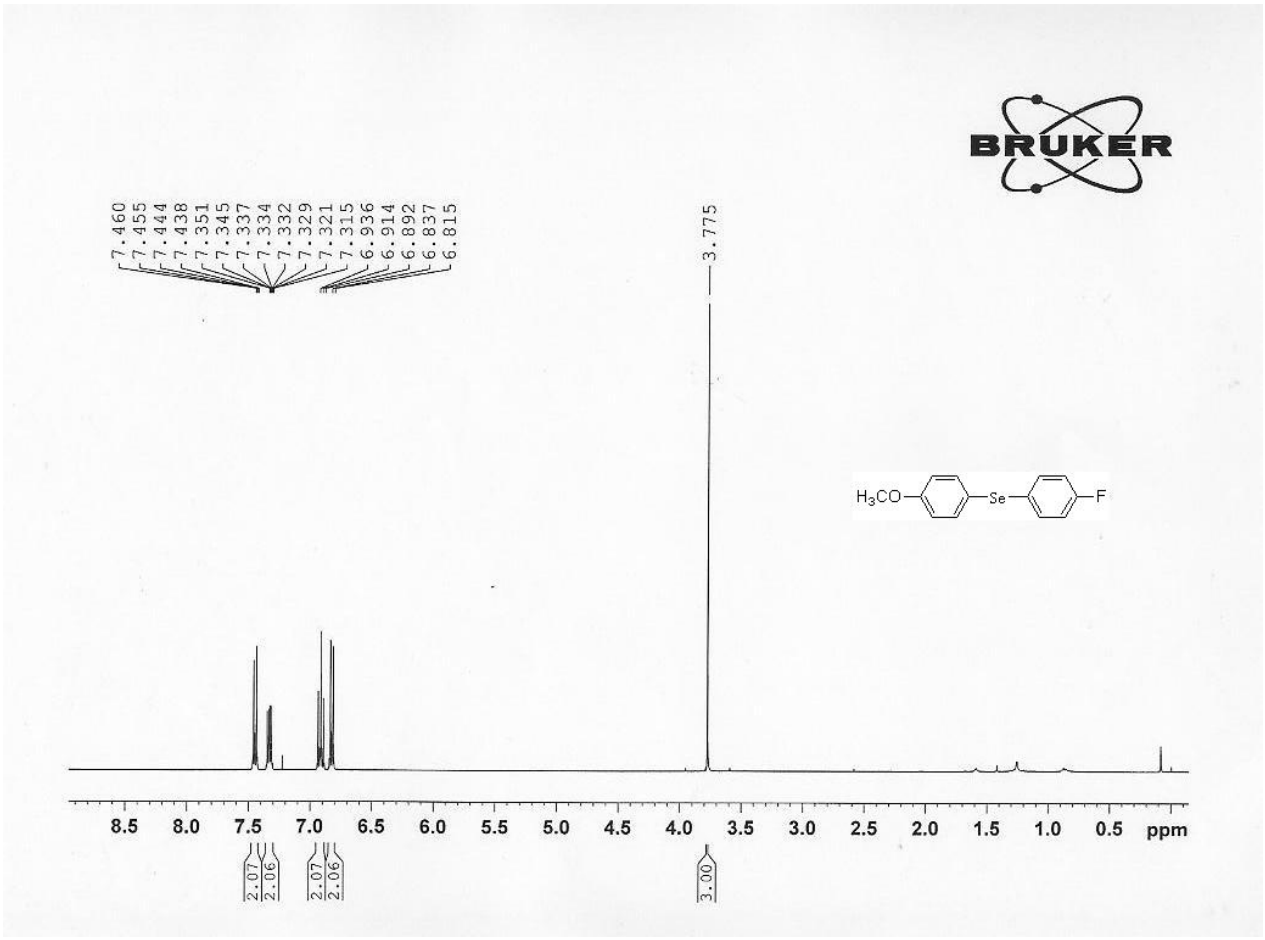

BRUKER
192.589
139.620
136.819
135.109
133.850
133.668
129.898
129.856
129.138
128.102
125.486
77.433
77.114
76.795
OHC
Se
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
ppm

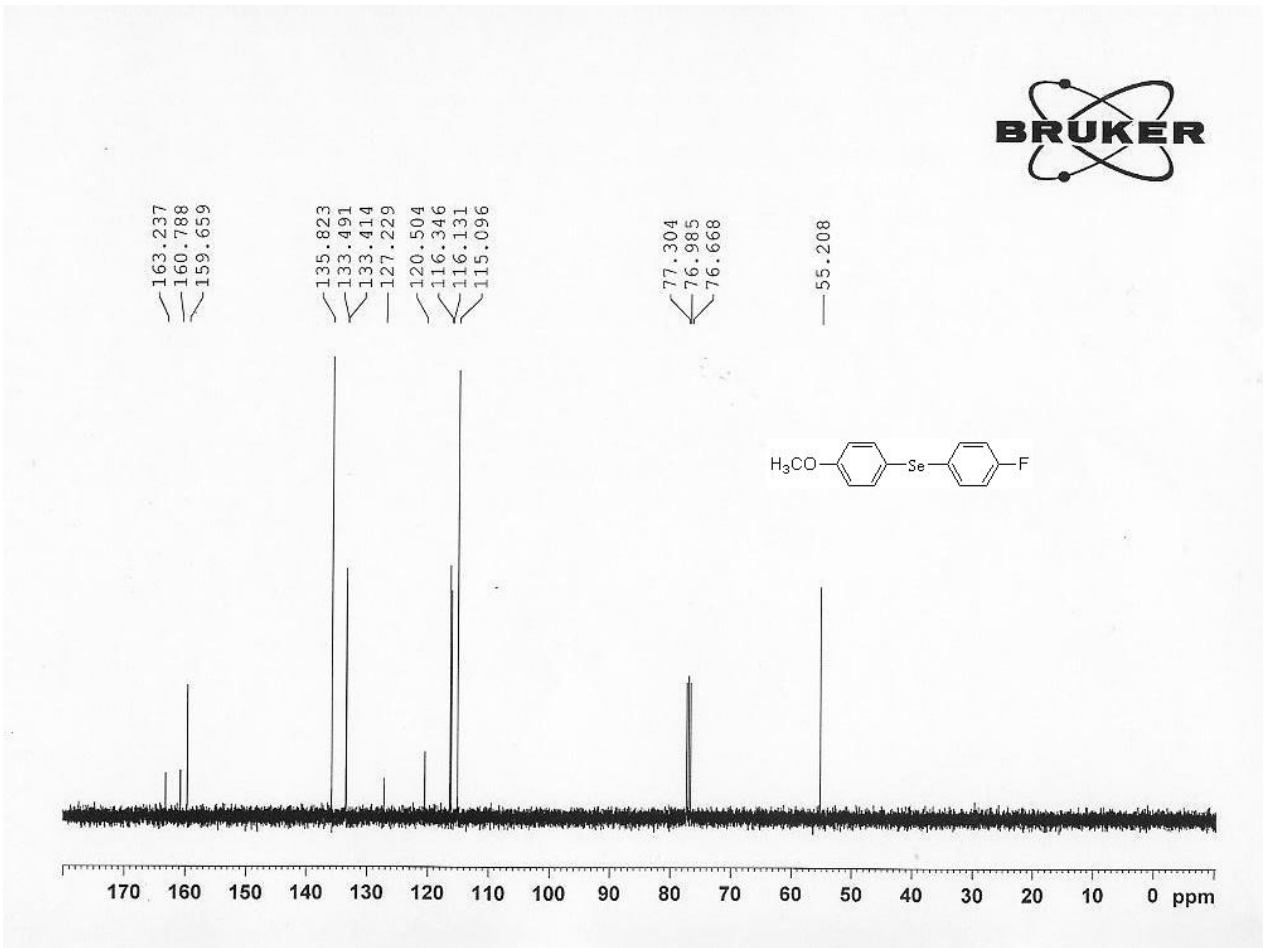

BRUKER
7.466
7.444
7.204
7.182
7.139
7.117
6.832
6.810
3.766
H3CO
Se
Cl
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.03
1.98
1.98
2.00
3.00

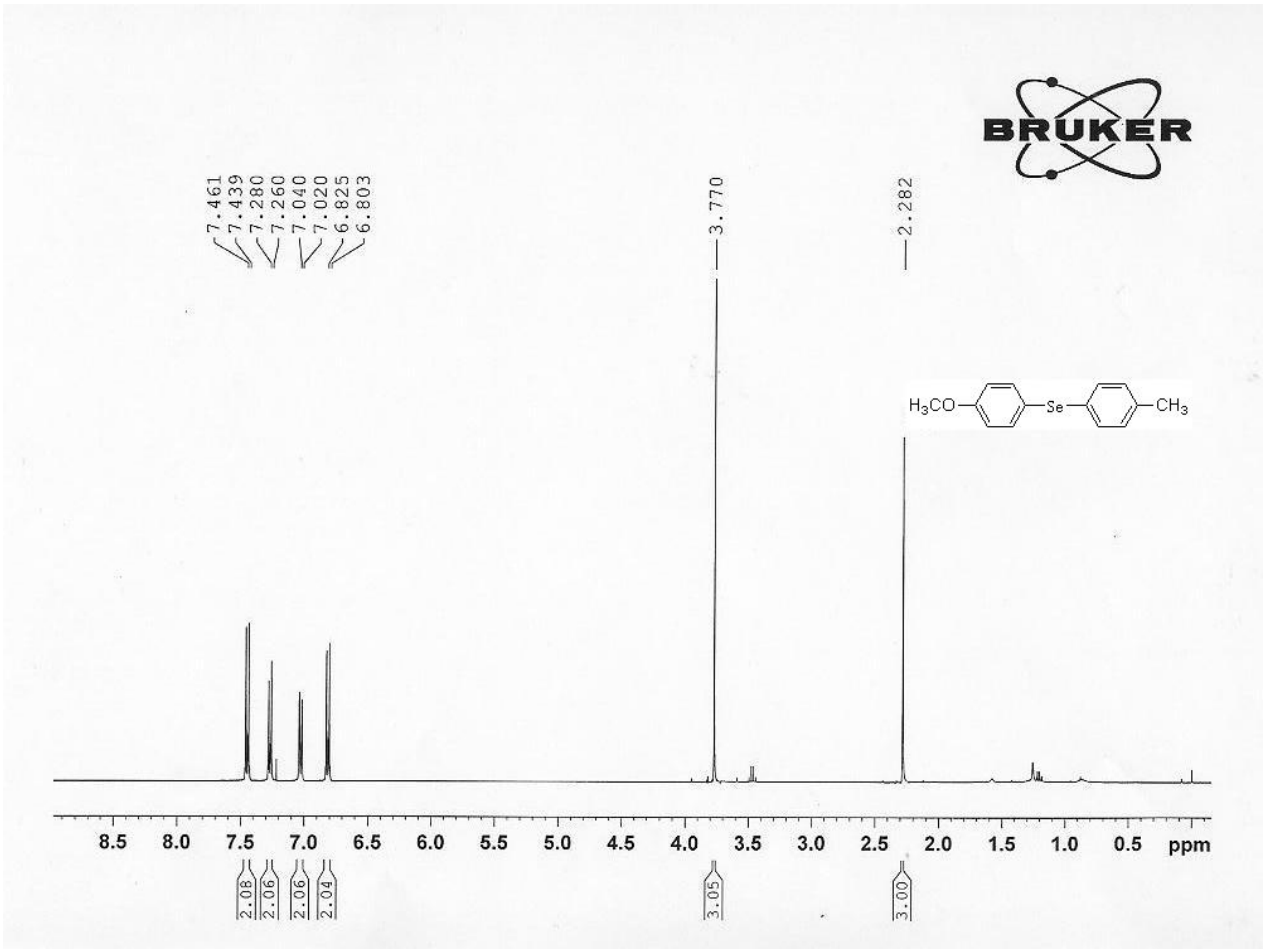

BRUKER
159.985
136.703
132.505
132.060
131.635
129.259
119.496
115.272
77.396
77.079
76.762
55.333
H3CO
Se
Cl
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

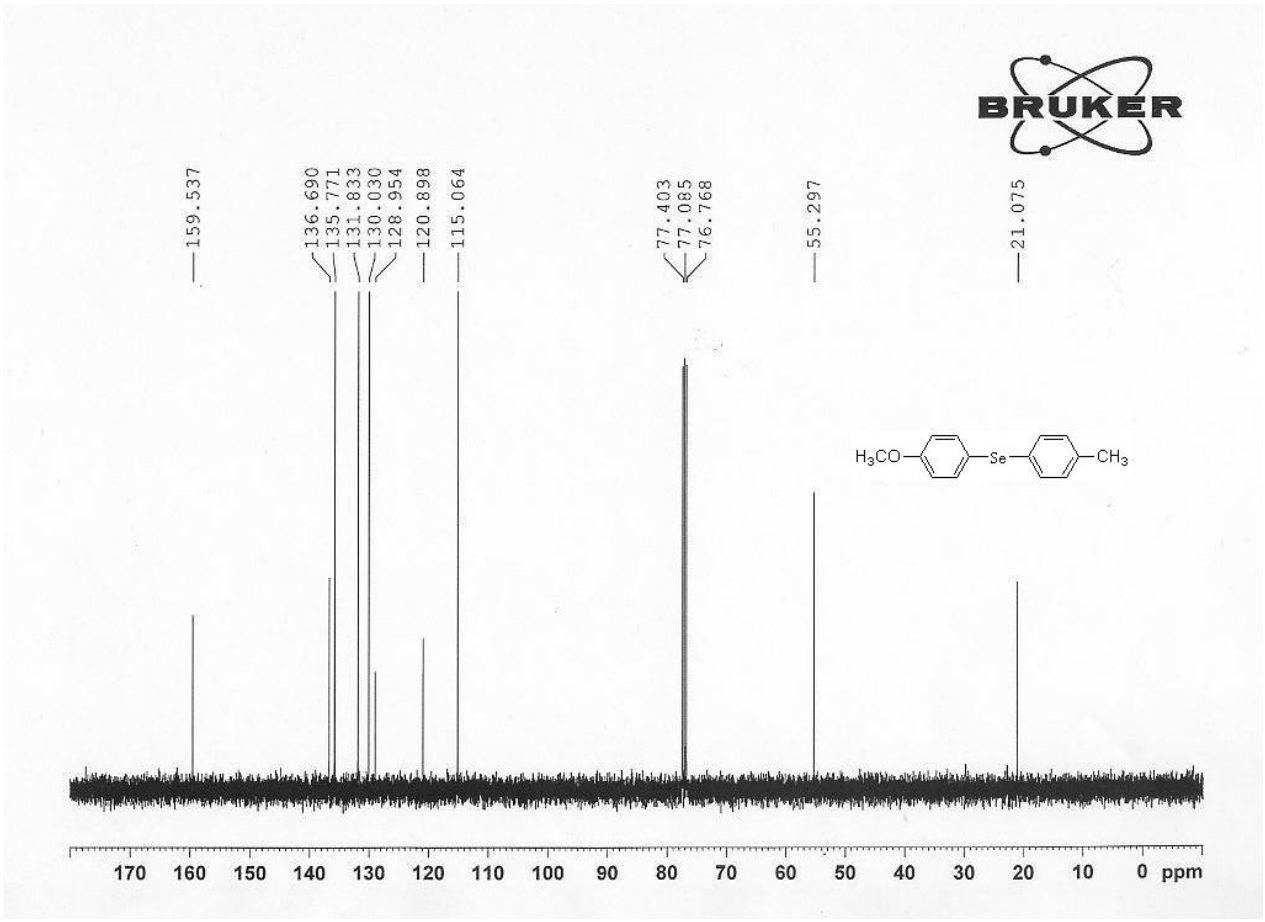

BRUKER
7.501
7.479
7.317
7.296
7.166
7.145
6.867
6.846
3.805
H3CO
Se
Br
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.09
2.04
1.97
2.04
3.00

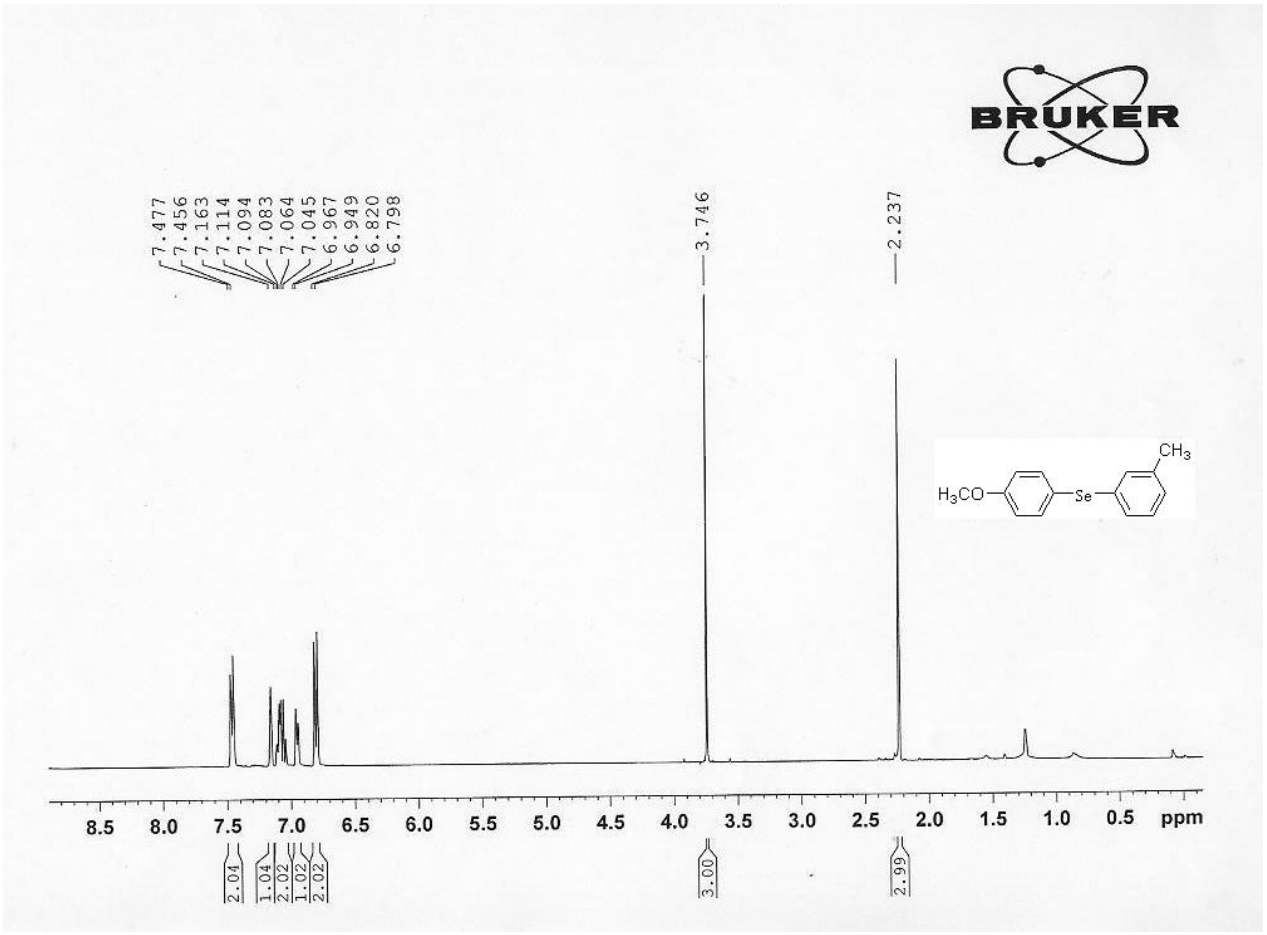

BRUKER
159.983
136.721
132.224
132.098
120.396
119.297
115.241
77.315
76.995
76.683
55.275
H3CO
Se
Br
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

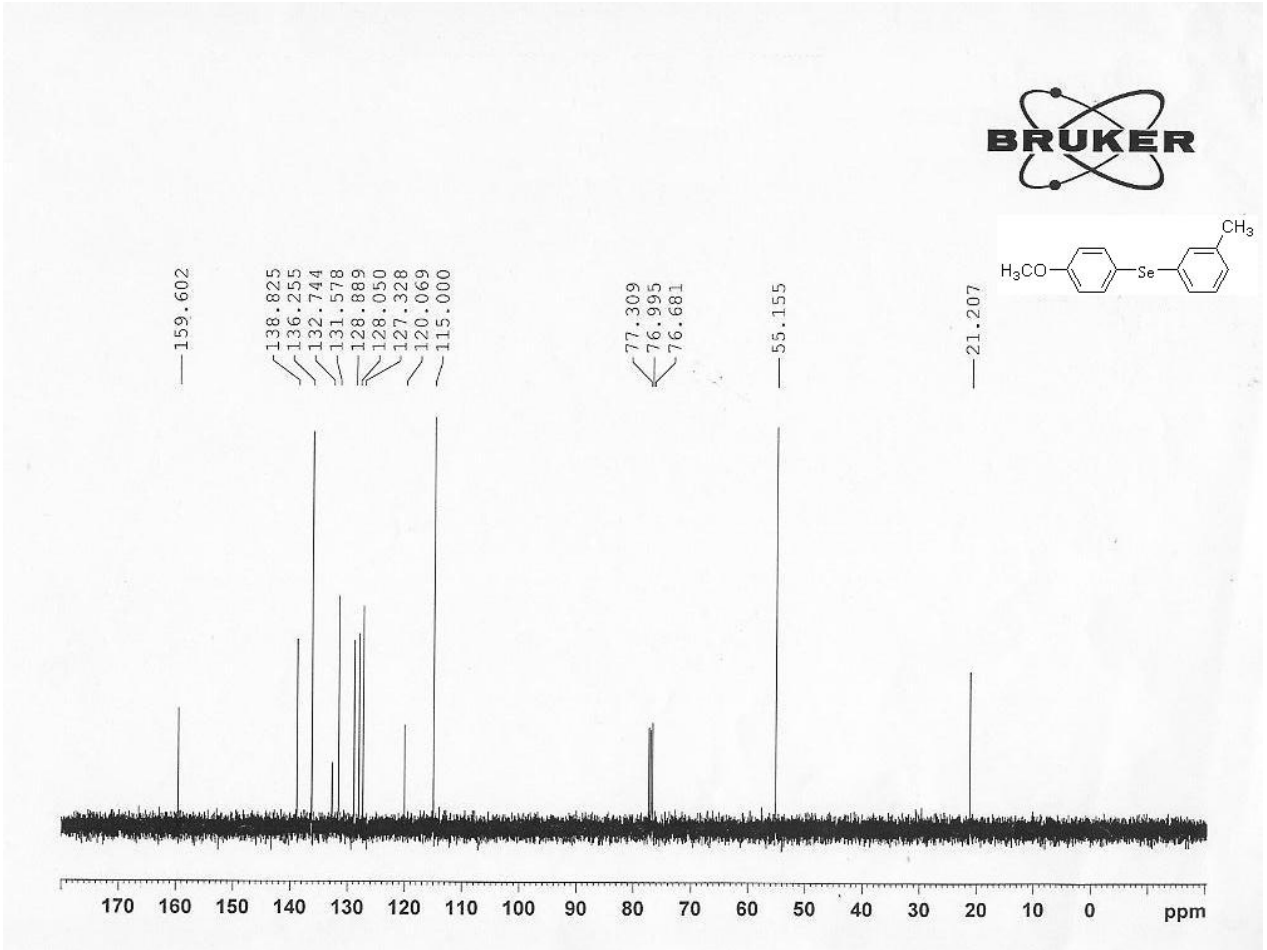

BRUKER
7.460
7.455
7.444
7.438
7.351
7.345
7.337
7.334
7.332
7.329
7.321
7.315
6.936
6.914
6.892
6.837
6.815
3.775
H3CO
Se
F
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.07
2.06
2.07
2.06
3.00

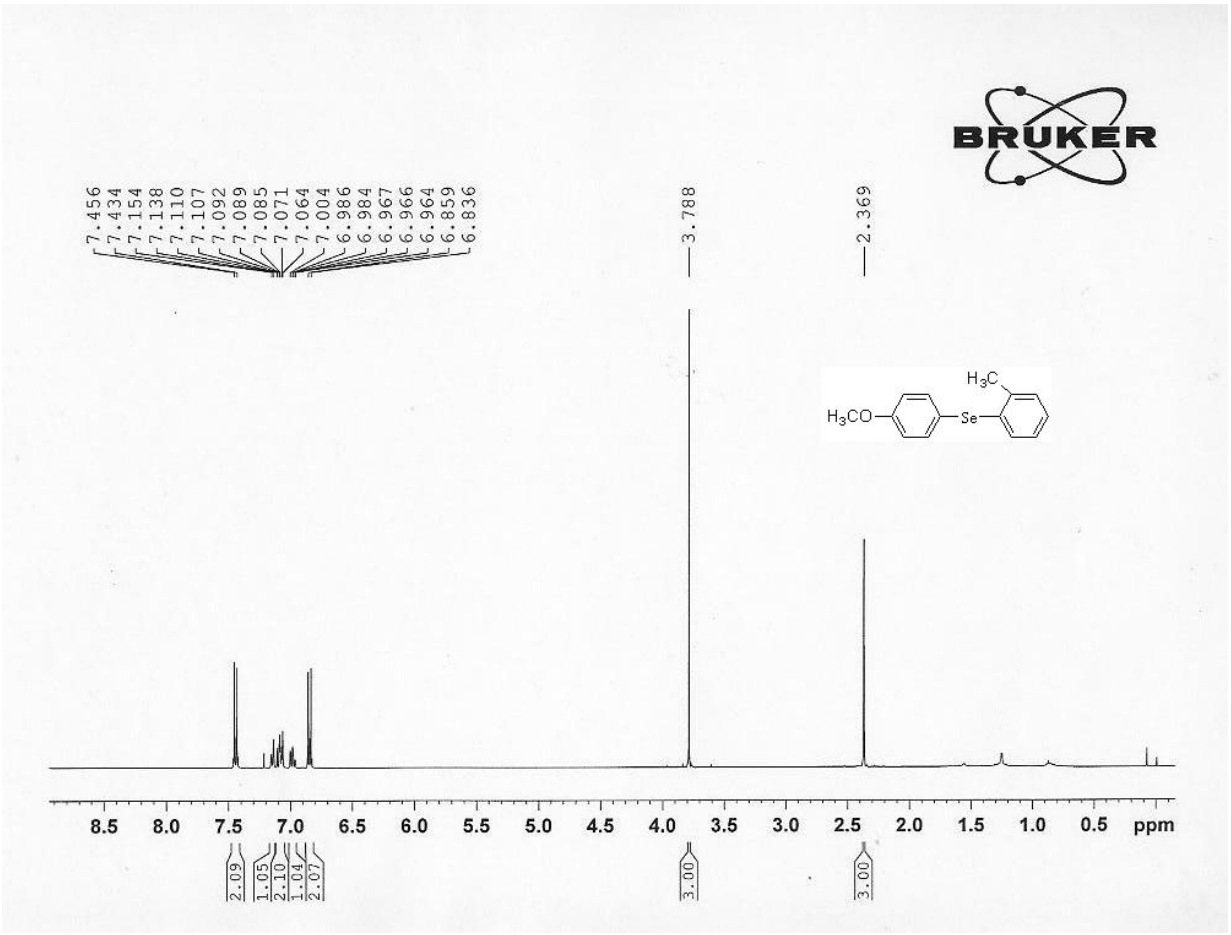

BRUKER
163.237
160.788
159.659
135.823
133.491
133.414
127.229
120.504
116.346
116.131
115.096
77.304
76.985
76.668
55.208
H3CO
Se
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

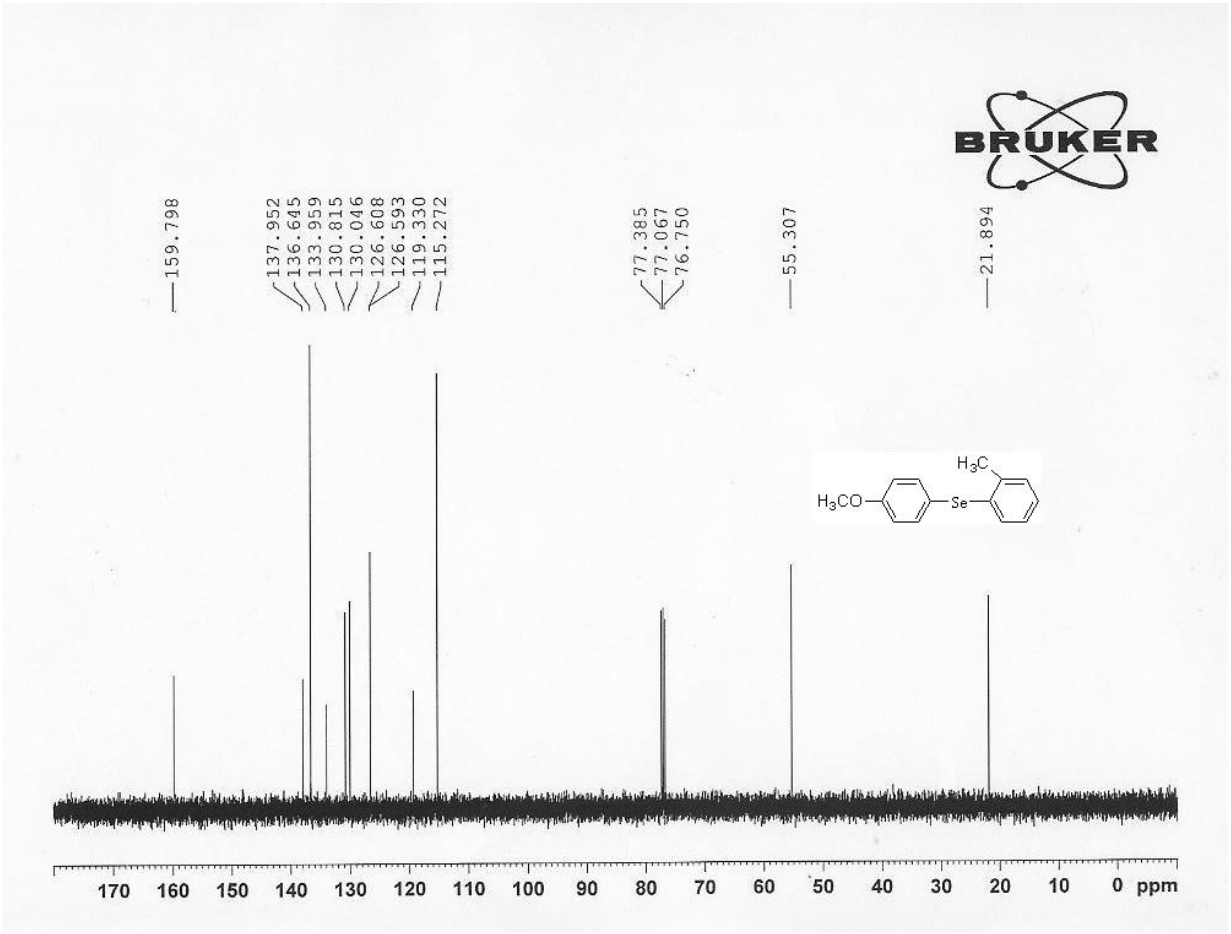

BRUKER
7.461
7.439
7.280
7.260
7.040
7.020
6.825
6.803
3.770
2.282
H3CO
Se
CH3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.08
2.06
2.06
2.04
3.05
3.00

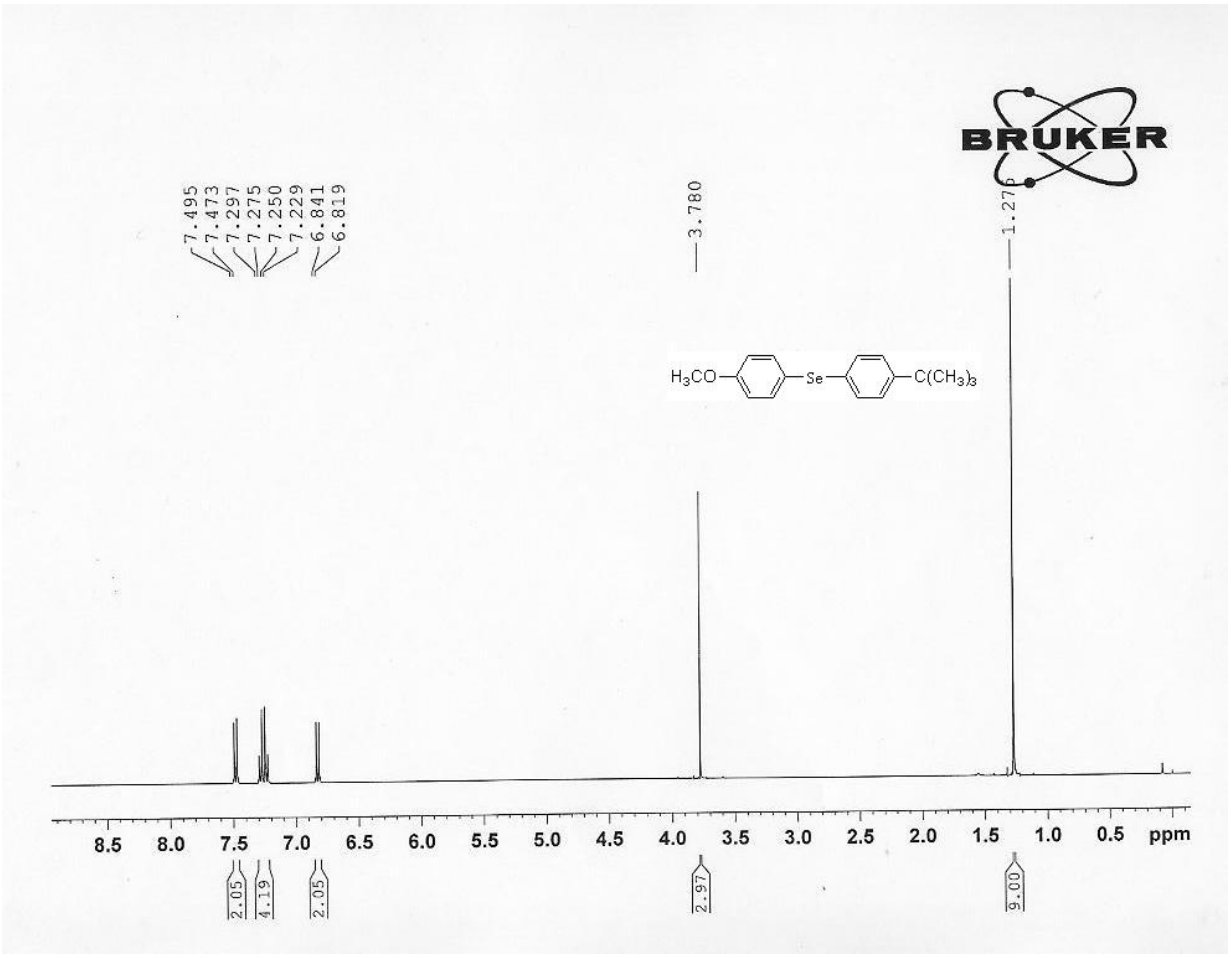

BRUKER
159.537
136.690
135.771
131.833
130.030
128.954
120.898
115.064
77.403
77.085
76.768
55.297
21.075
H3CO
Se
CH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

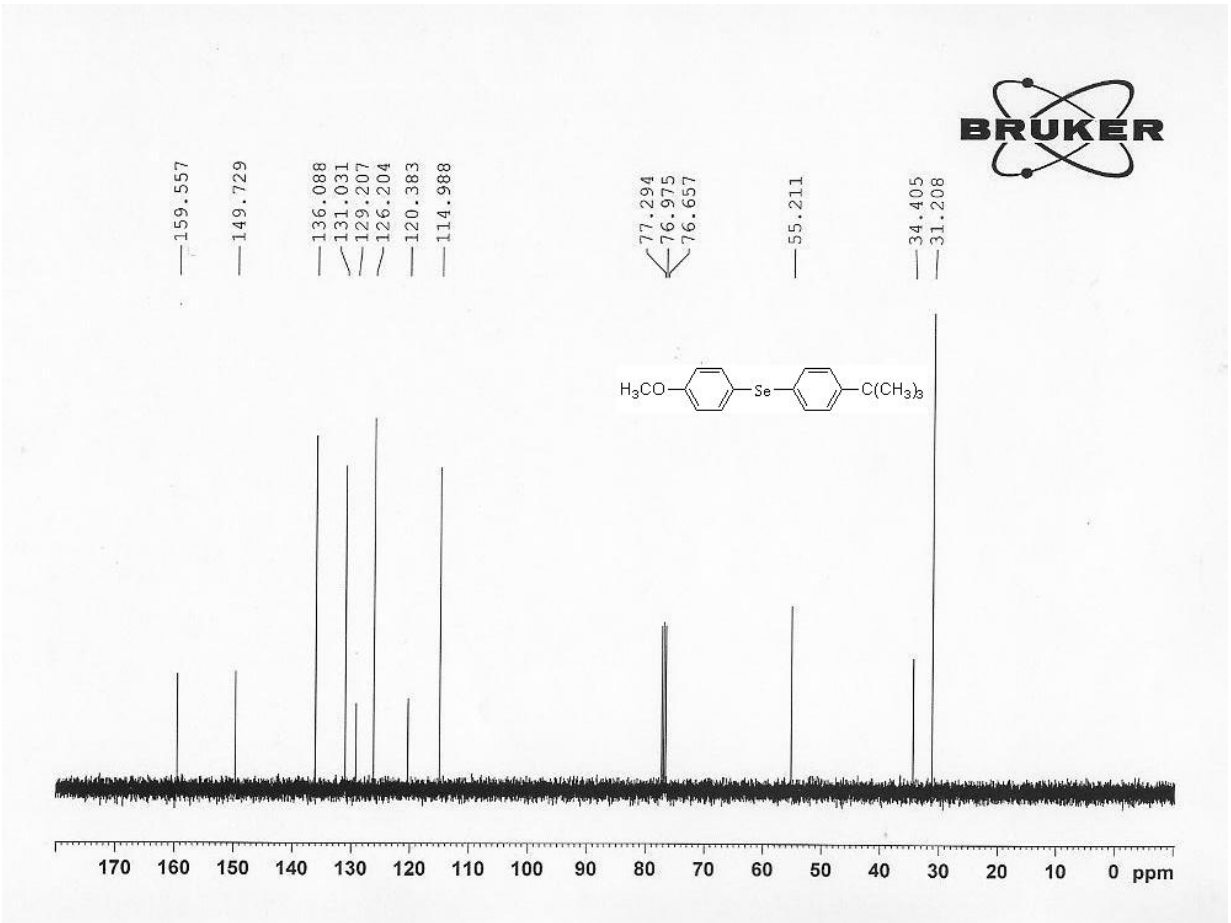

BRUKER
7.477
7.456
7.163
7.114
7.094
7.083
7.064
7.045
6.967
6.949
6.820
6.798
3.746
2.237
H3CO
Se
CH3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.04
1.04
2.02
1.02
2.02
3.00
2.99

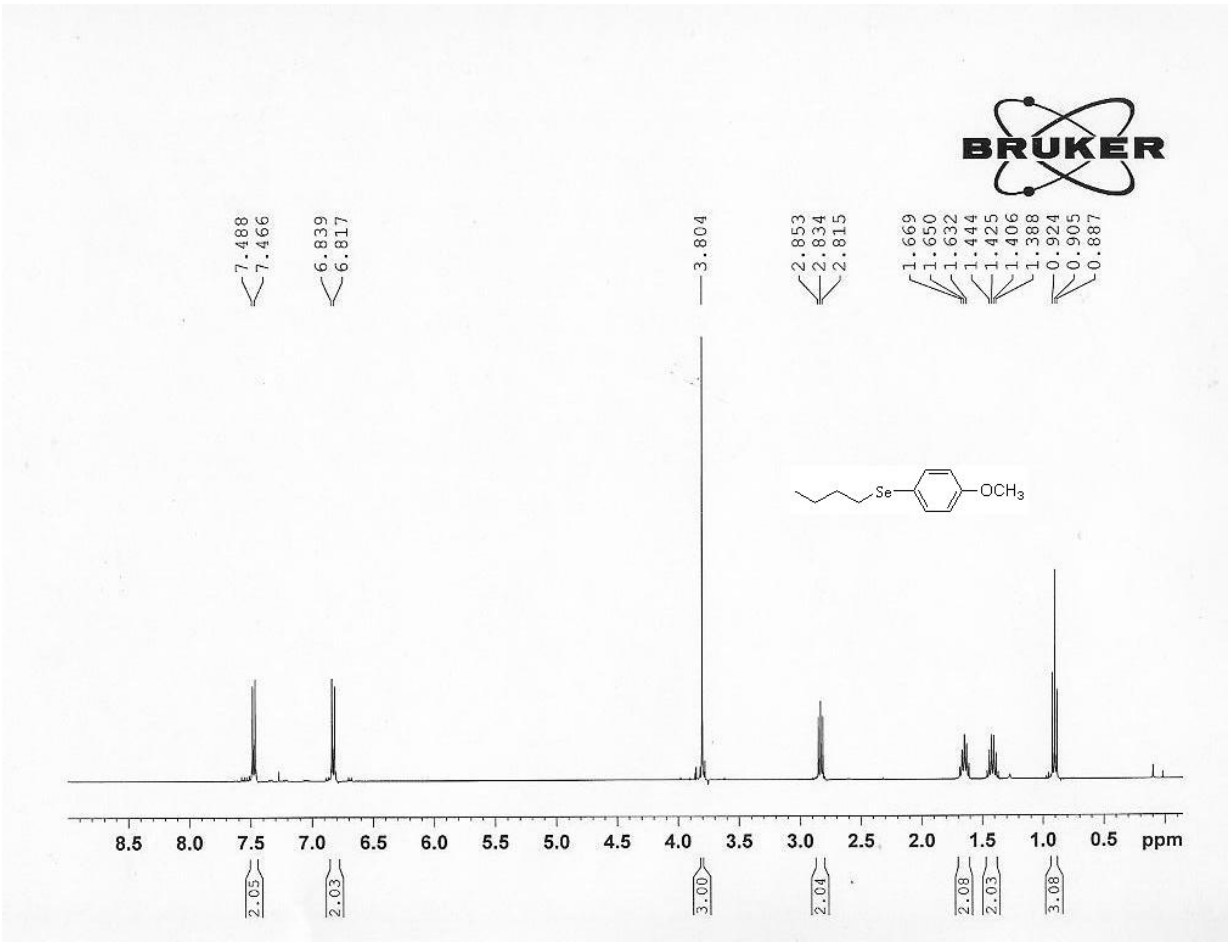

BRUKER
H3CO
Se
CH3
159.602
138.825
136.255
132.744
131.578
128.889
128.050
127.328
120.069
115.000
77.309
76.995
76.681
55.155
21.207
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

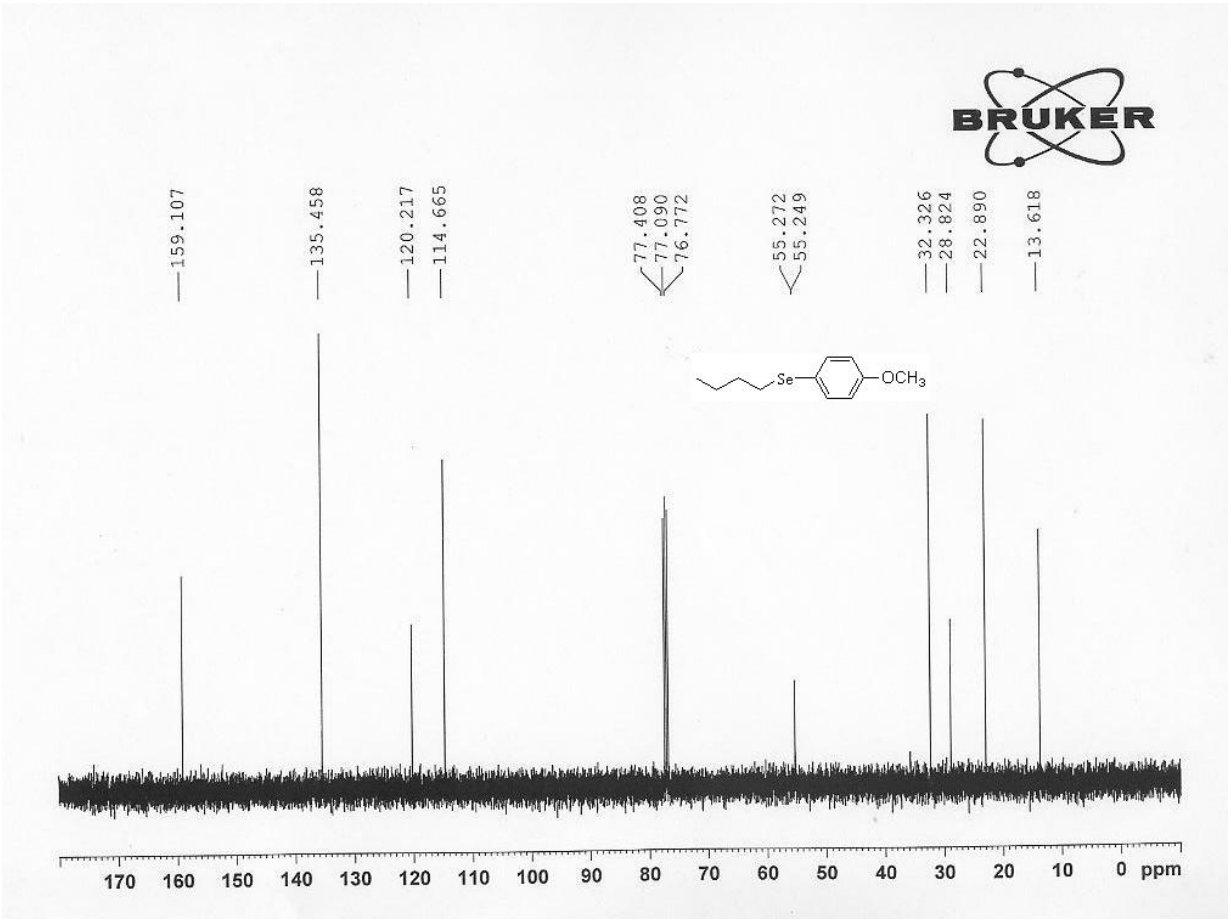

BRUKER
7.456
7.434
7.154
7.138
7.110
7.107
7.092
7.089
7.085
7.071
7.064
7.004
6.986
6.984
6.967
6.966
6.964
6.859
6.836
3.788
2.369
H3C
H3CO
Se
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.09
1.05
2.10
1.04
2.07
3.00
3.00

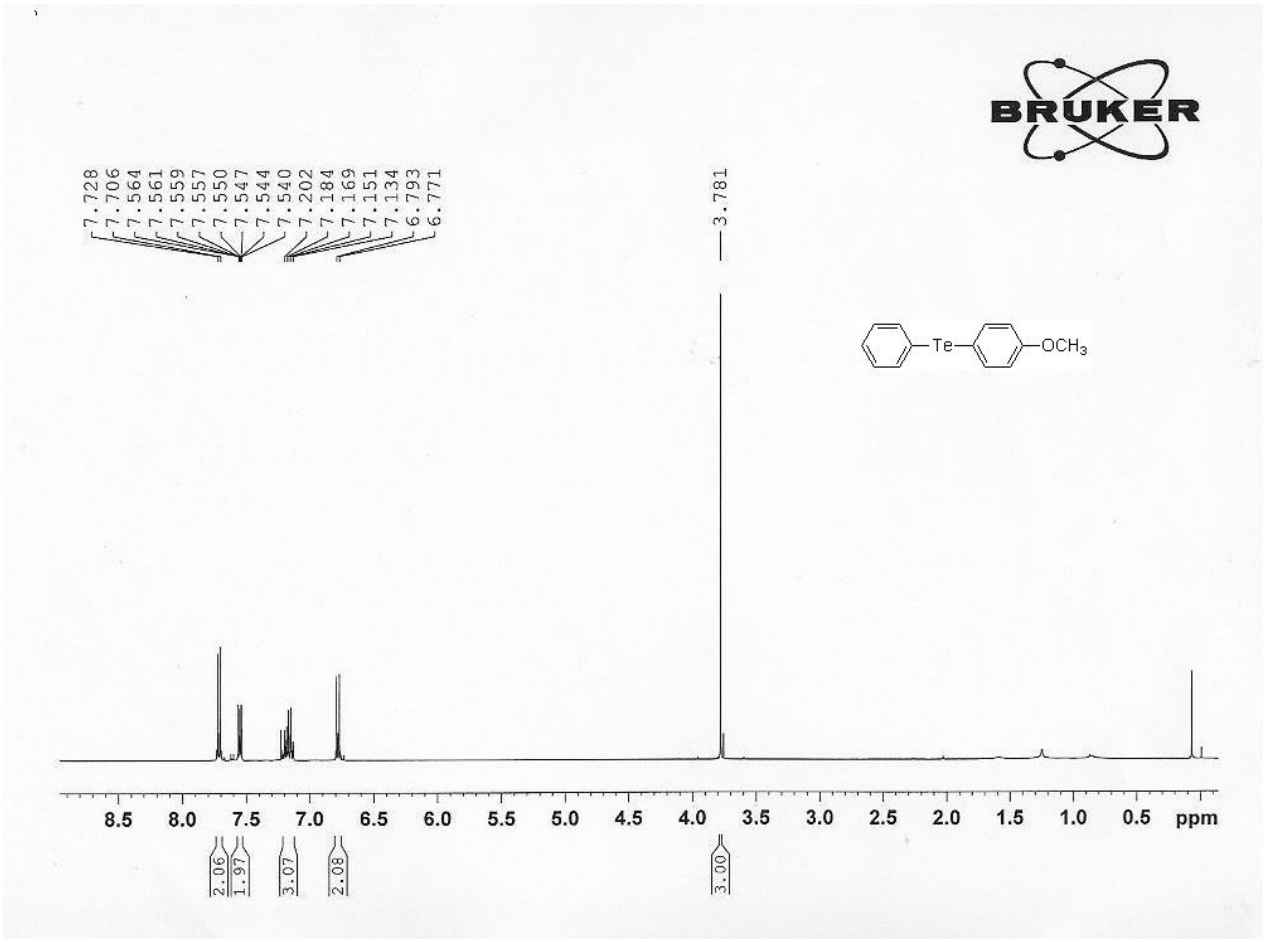

BRUKER
159.798
137.952
136.645
133.959
130.815
130.046
126.608
126.593
119.330
115.272
77.385
77.067
76.750
55.307
21.894
H3C
H3CO
Se
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

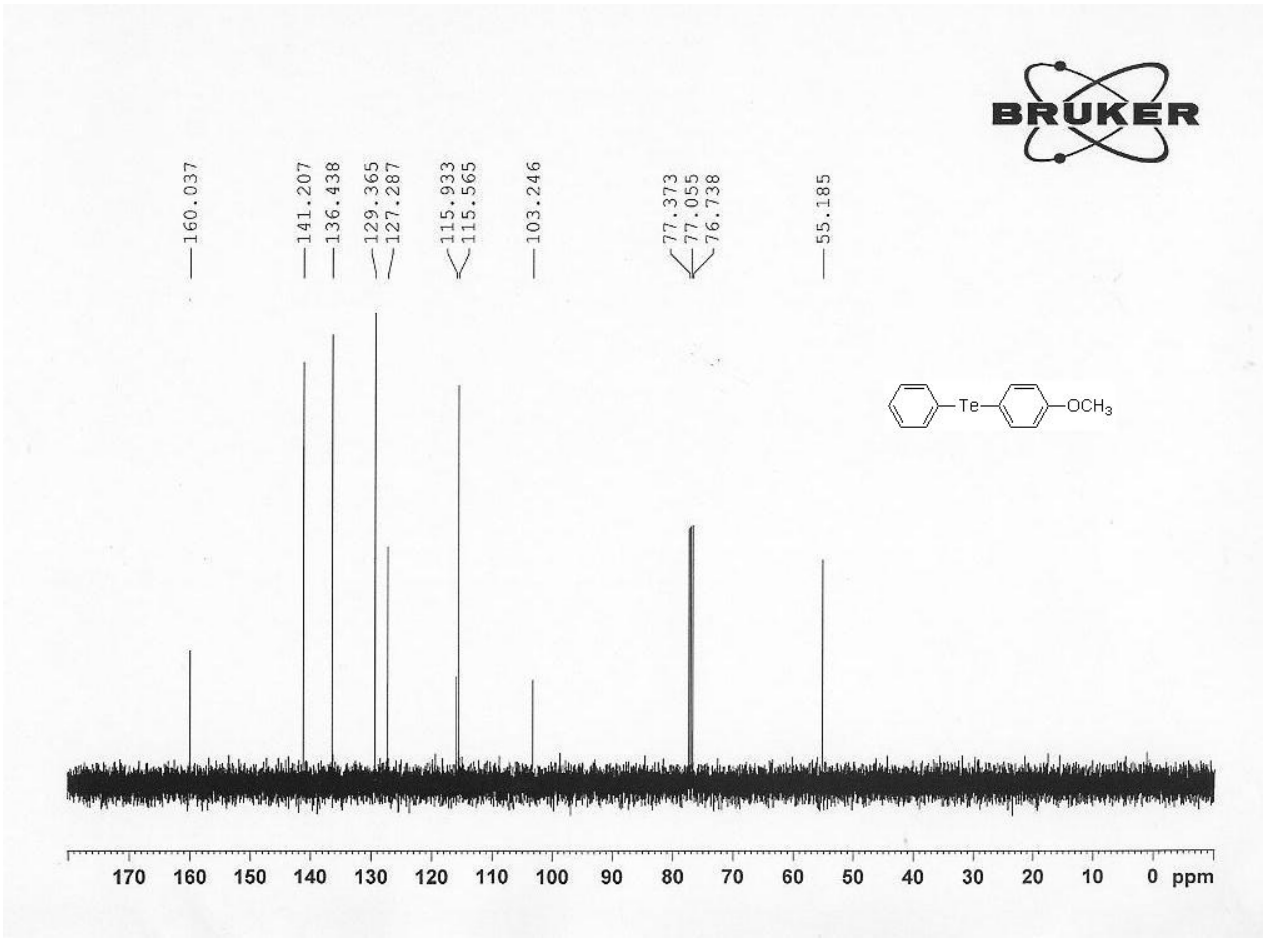

BRUKER
7.495
7.473
7.297
7.275
7.250
7.229
6.841
6.819
3.780
1.27
H3CO
Se
C(CH3)3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.05
4.19
2.05
2.97
9.00

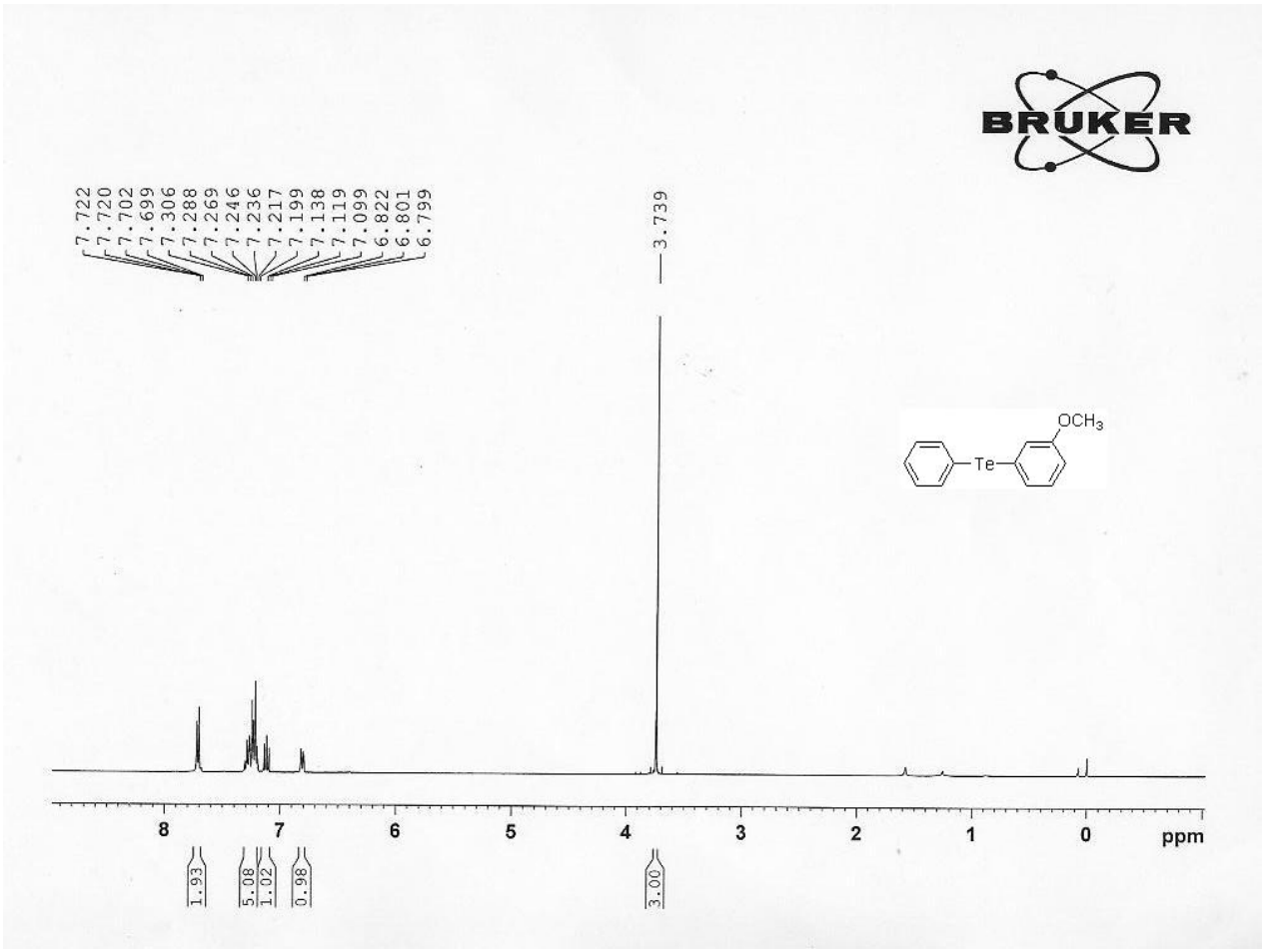

BRUKER
159.557
149.729
136.088
131.031
129.207
126.204
120.383
114.988
77.294
76.975
76.657
55.211
34.405
31.208
H3CO
Se
C(CH3)3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

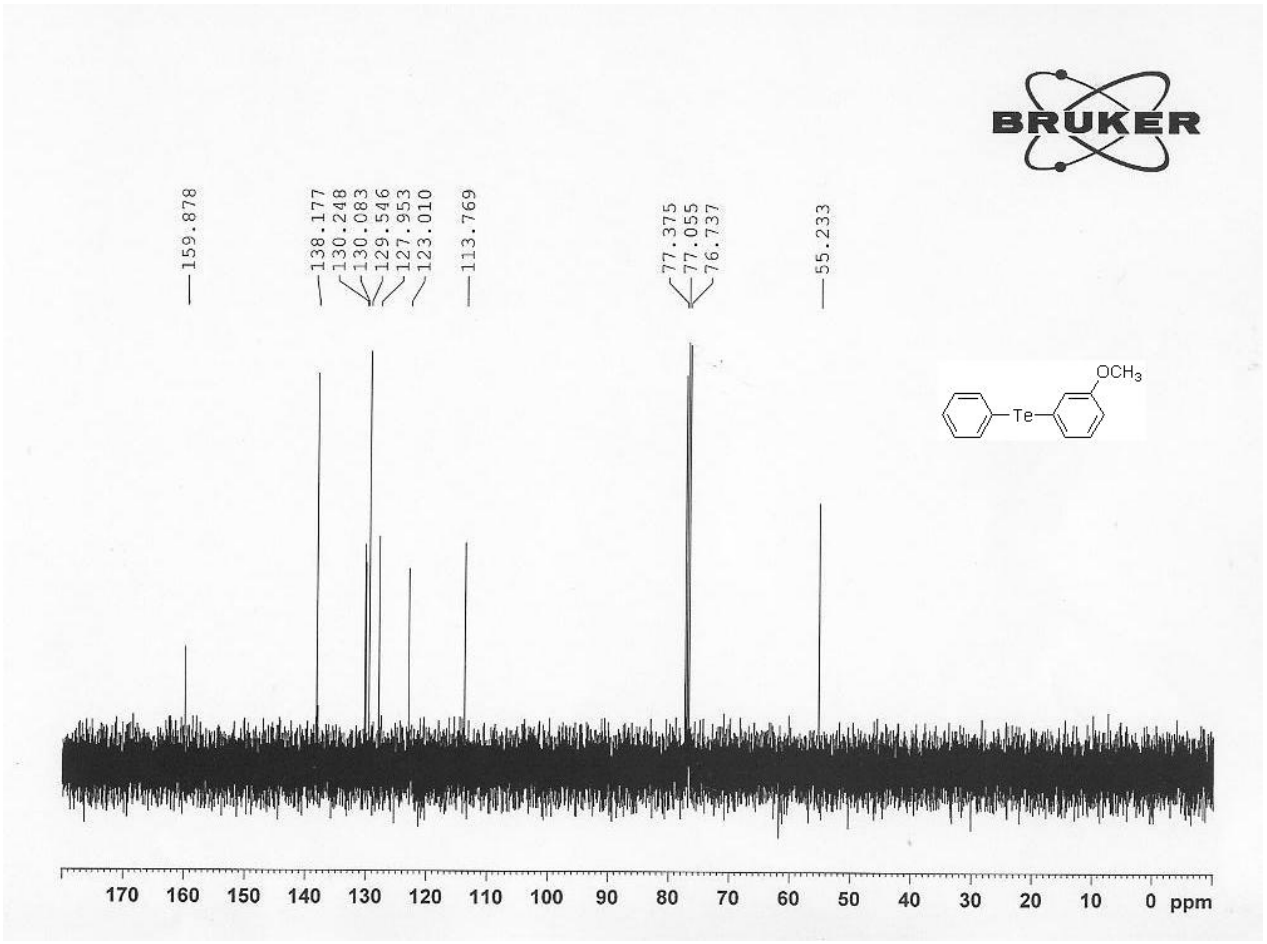

BRUKER
7.488
7.466
6.839
6.817
3.804
2.853
2.834
2.815
1.669
1.650
1.632
1.444
1.425
1.406
1.388
0.924
0.905
0.887
Se
OCH3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.05
2.03
3.00
2.04
2.08
2.03
3.08

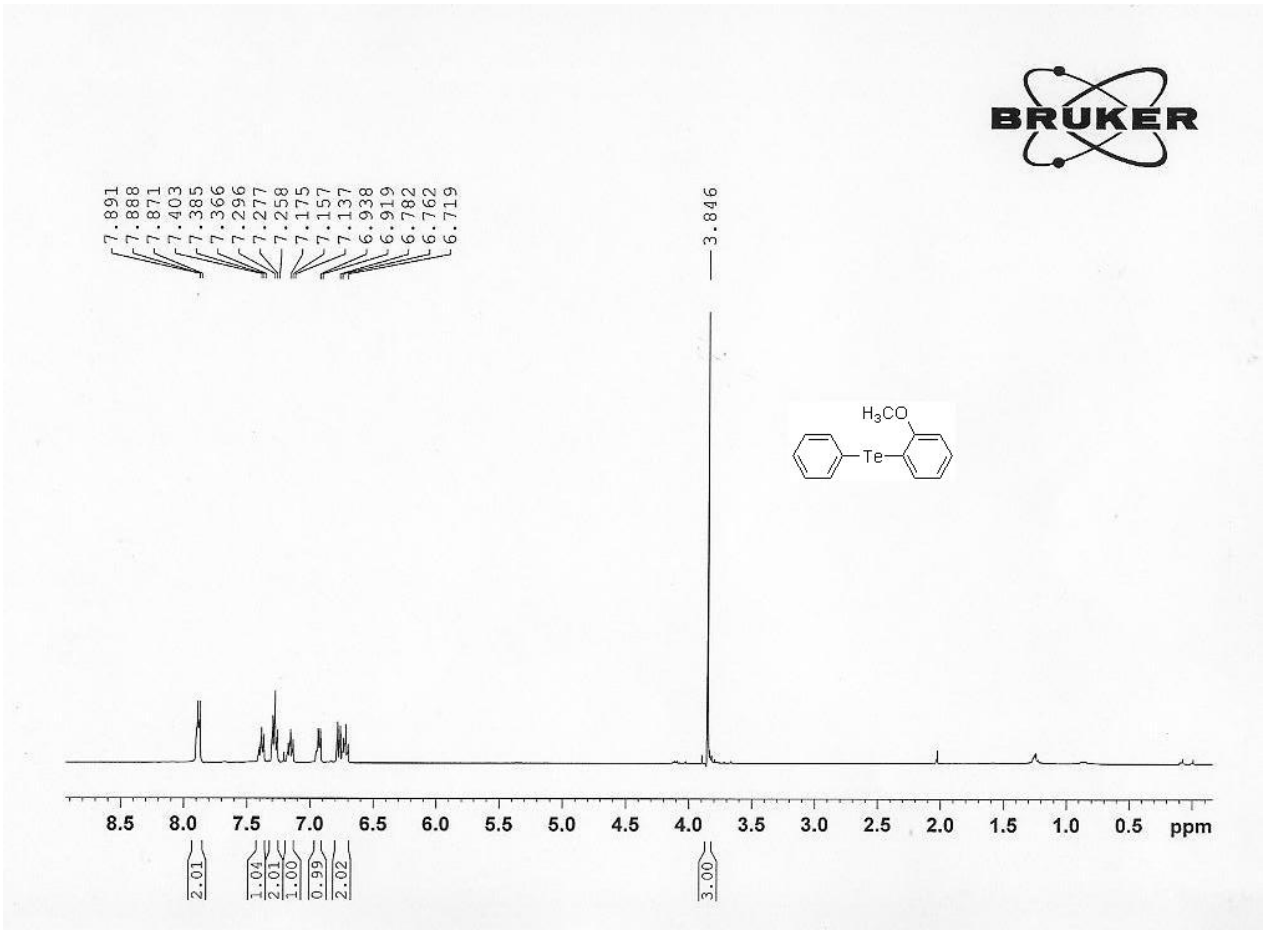

BRUKER
159.107
135.458
120.217
114.665
77.408
77.090
76.772
55.272
55.249
32.326
28.824
22.890
13.618
Se
OCH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

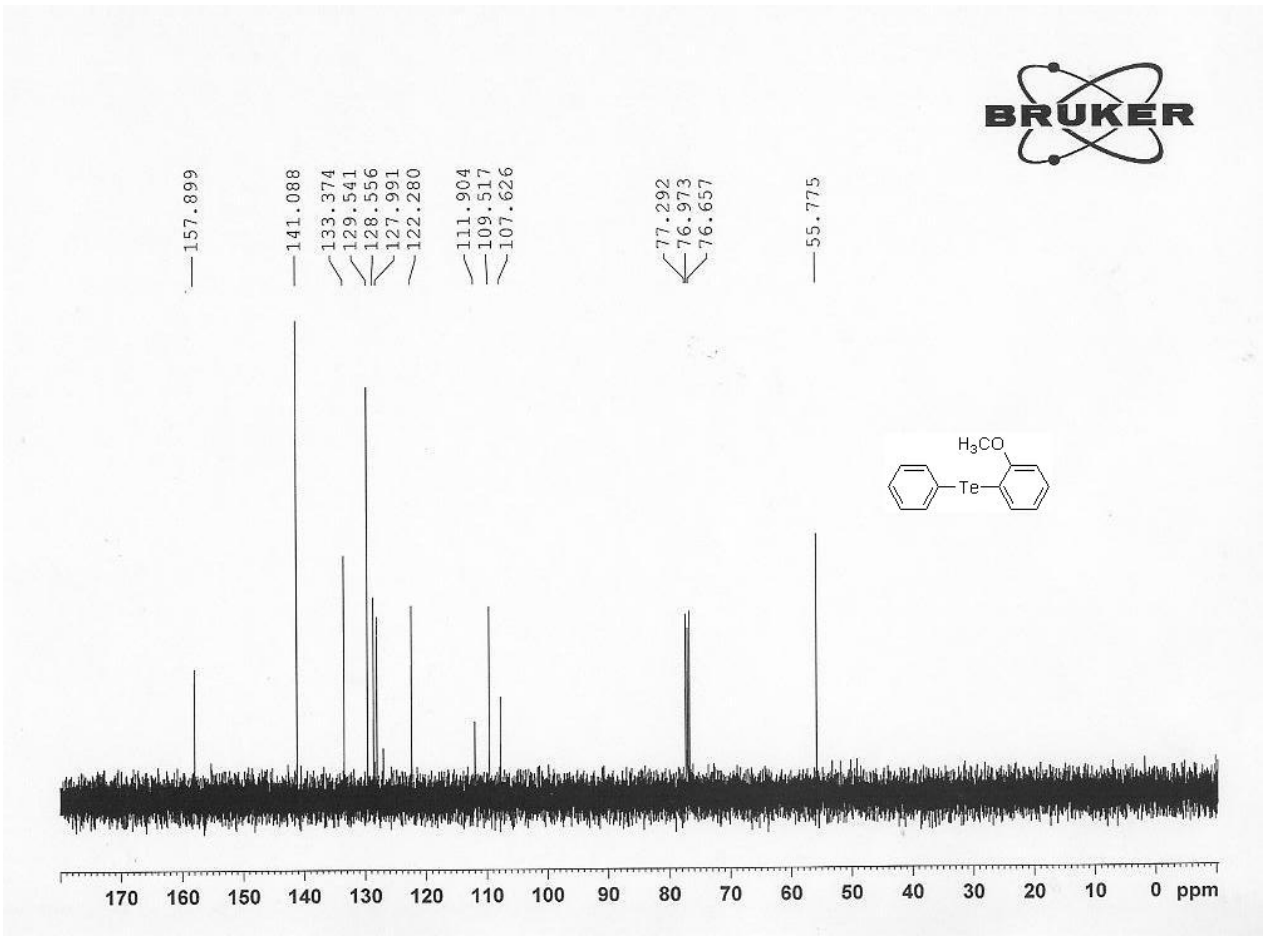

BRUKER
7.728
7.706
7.564
7.561
7.559
7.557
7.550
7.547
7.544
7.540
7.202
7.184
7.169
7.151
7.134
6.793
6.771
3.781
Te
OCH3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.06
1.97
3.07
2.08
3.00

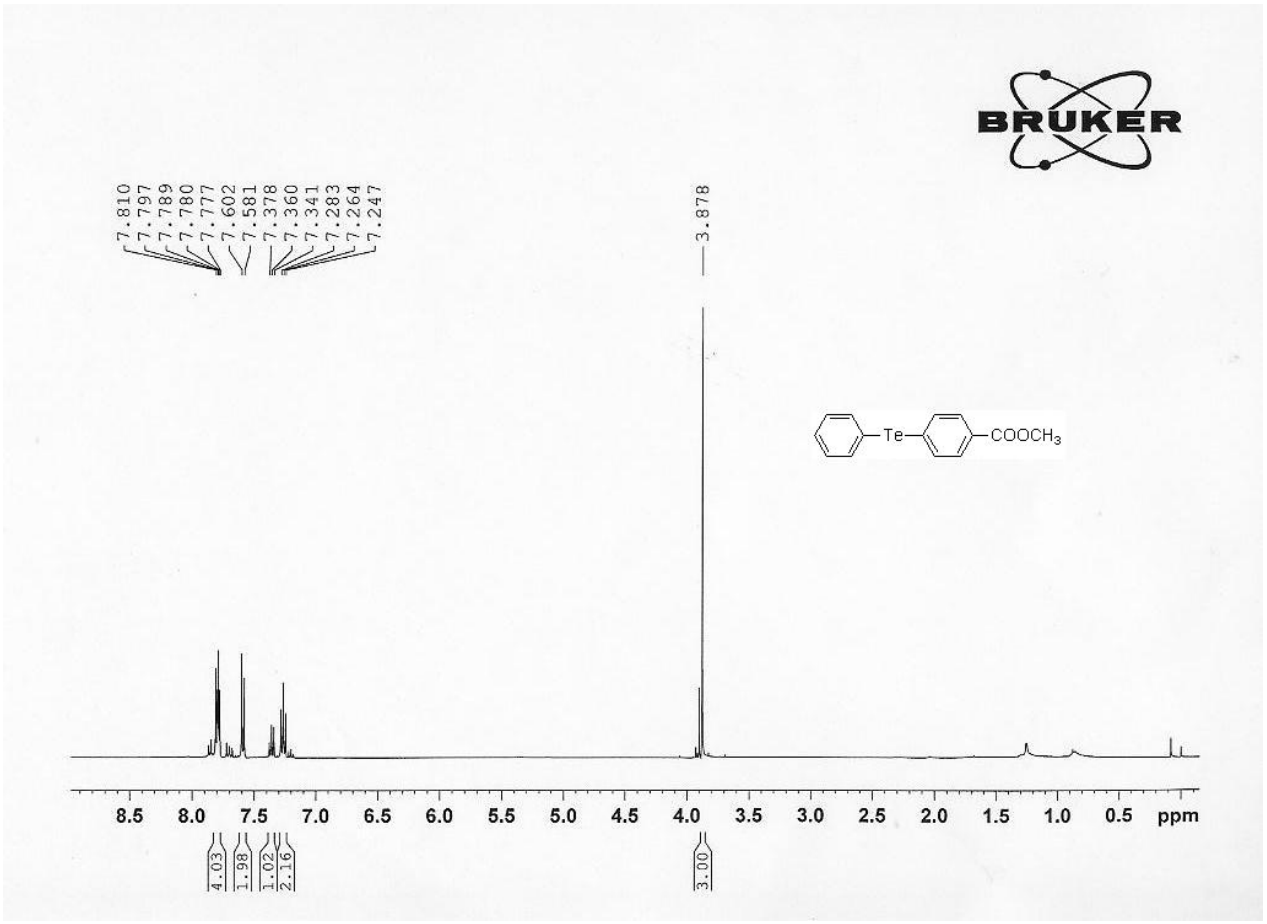

BRUKER
160.037
141.207
136.438
129.365
127.287
115.933
115.565
103.246
77.373
77.055
76.738
55.185
Te
OCH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

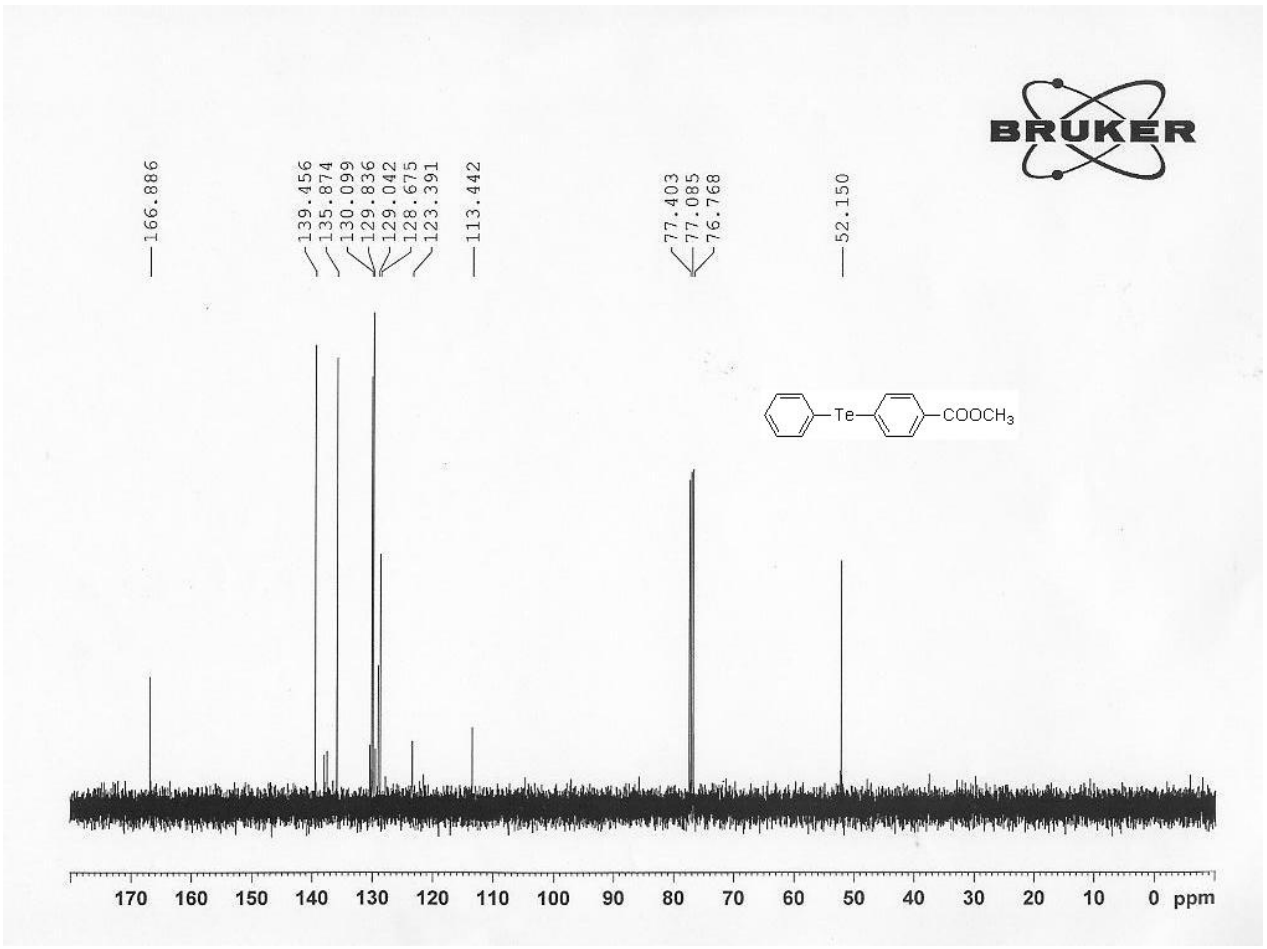

BRUKER
7.722
7.720
7.702
7.699
7.306
7.288
7.269
7.246
7.236
7.217
7.199
7.138
7.119
7.099
6.822
6.801
6.799
3.739
OCH3
Te
8
7
6
5
4
3
2
1
0
ppm
1.93
5.08
1.02
0.98
3.00

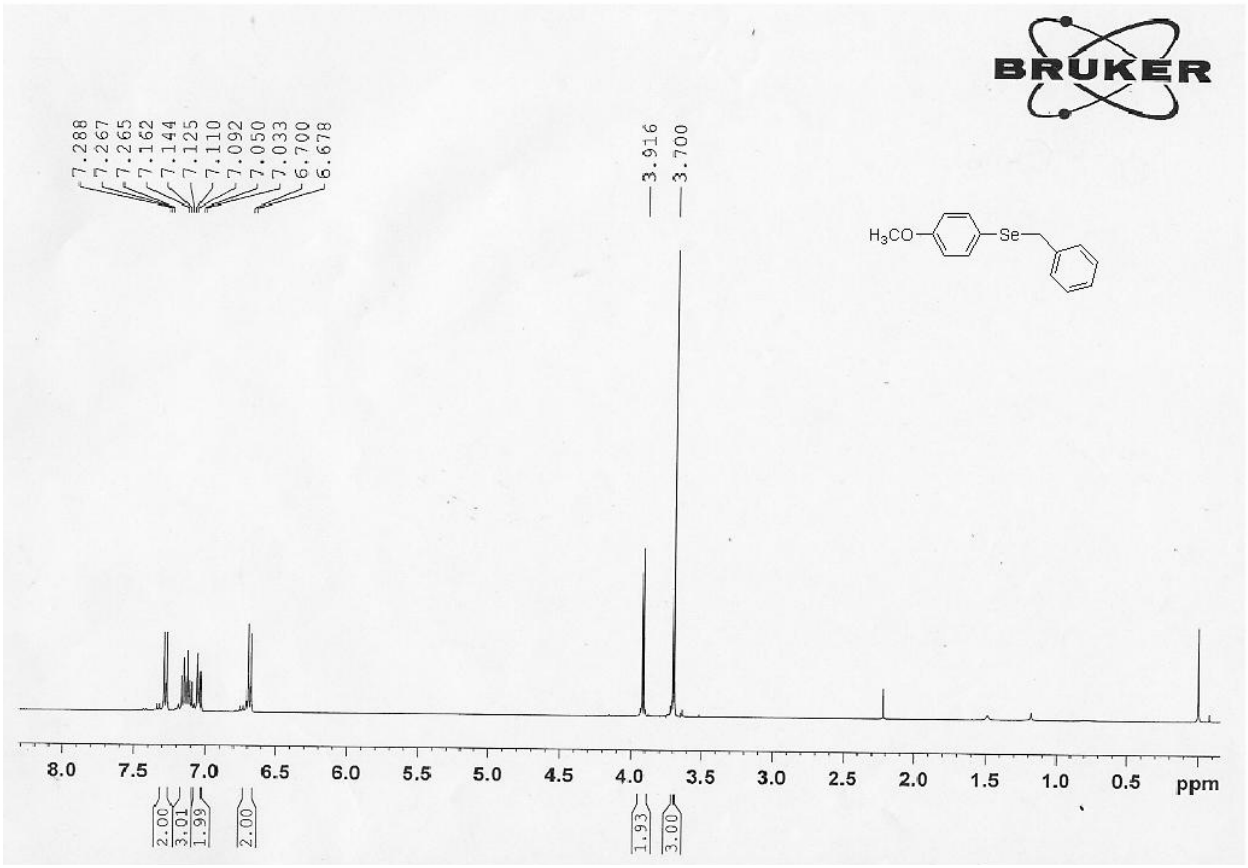

BRUKER
159.878
138.177
130.248
130.083
129.546
127.953
123.010
113.769
77.375
77.055
76.737
55.233
OCH3
Te
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

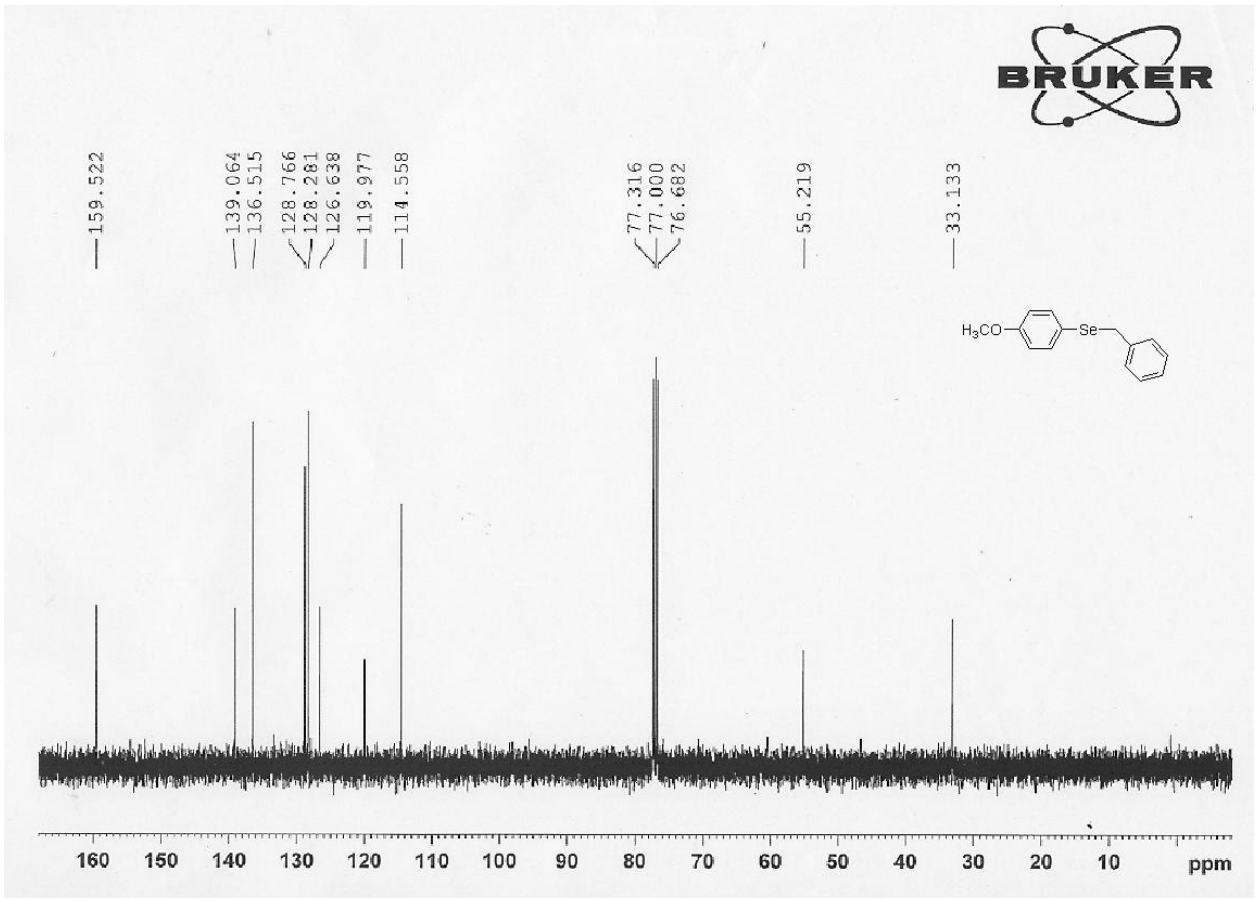

BRUKER
7.891
7.888
7.871
7.403
7.385
7.366
7.296
7.277
7.258
7.175
7.157
7.137
6.938
6.919
6.782
6.762
6.719
3.846
H3CO
Te
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.01
1.04
2.01
1.00
0.99
2.02
3.00


BRUKER
157.899
141.088
133.374
129.541
128.556
127.991
122.280
111.904
109.517
107.626
77.292
76.973
76.657
55.775
H3CO
Te
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


BRUKER
7.810
7.797
7.789
7.780
7.777
7.602
7.581
7.378
7.360
7.341
7.283
7.264
7.247
3.878
Te
COOCH3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
4.03
1.98
1.02
2.16
3.00


BRUKER
166.886
139.456
135.874
130.099
129.836
129.042
128.675
123.391
113.442
77.403
77.085
76.768
52.150
Te
COOCH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


BRUKER
7.288
7.267
7.265
7.162
7.144
7.125
7.110
7.092
7.050
7.033
6.700
6.678
3.916
3.700
H3CO
Se
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
3.01
1.99
2.00
1.93
3.00


BRUKER
159.522
139.064
136.515
128.766
128.281
126.638
119.977
114.558
77.316
77.000
76.682
55.219
33.133
H3CO
Se
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

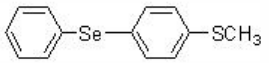
Instrument: Waters Micromass GCT

Card Serial Number: T0803101-2

Sample Serial Number: Ren-15

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
137 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
276.9858	276.9859	-0.1	-0.3	9.0	1	C13 H12 S 77Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

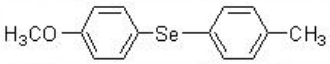
Instrument: Waters Micromass GCT

Card Serial Number: T0803099

Sample Serial Number: Ren-3

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
111 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
278.0211	278.0210	0.1	0.4	9.0	1	C14 H14 O 80Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

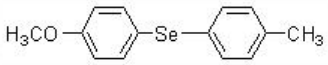
Instrument: Waters Micromass GCT

Card Serial Number: T0803099

Sample Serial Number: Ren-3

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
111 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
276.0223	276.0218	0.5	1.9	9.0	1	C14 H14 O 78Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

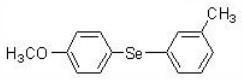
Instrument: Waters Micromass GCT

Card Serial Number: T0803097

Sample Serial Number: Ren-5

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
108 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
280.0215	280.0212	0.3	1.2	9.0	1	C14 H14 O 82Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

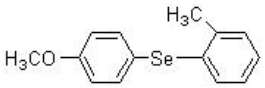
Instrument: Waters Micromass GCT

Card Serial Number: T0803098

Sample Serial Number: Ren-10

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
111 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
276.0219	276.0218	0.1	0.5	9.0	1	C14 H14 O 78Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

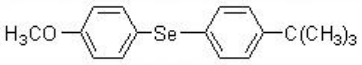
Instrument: Waters Micromass GCT

Card Serial Number: T0803100

Sample Serial Number: Ren-9

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
152 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
318.0680	318.0687	-0.7	-2.3	9.0	1	C17 H20 O 78Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

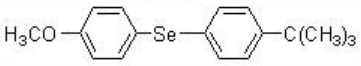
Instrument: Waters Micromass GCT

Card Serial Number: T0803100

Sample Serial Number: Ren-9

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
151 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
320.0677	320.0679	-0.2	-0.7	9.0	1	C17 H20 O 80Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

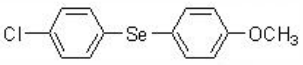
Instrument: Waters Micromass GCT

Card Serial Number: T0803094

Sample Serial Number: Ren-18

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
220 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
297.9670	297.9664	0.6	2.1	9.0	1	C13 H11 O Cl 80Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

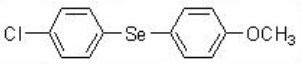
Instrument: Waters Micromass GCT

Card Serial Number: T0803094

Sample Serial Number: Ren-18

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
219 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
295.9667	295.9671	-0.4	-1.5	9.0	1	C13 H11 O Cl 78Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

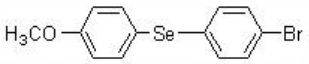
Instrument: Waters Micromass GCT

Card Serial Number: T0803101

Sample Serial Number: Ren-2

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
285 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
341.9157	341.9158	-0.1	-0.4	9.0	1	C13 H11 O Br 80Se
	341.9176	-1.9	-5.6	10.5	2	C13 H11 O 77Se 82Se

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

SIOC

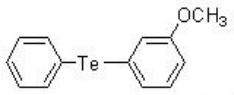
Instrument: Waters Micromass GCT

Card Serial Number: T0803095

Sample Serial Number: Ren-16

Operator: LiGuangping

Date: 2008/12/30



Elemental Composition Report

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
1058 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
313.9957	313.9950	0.7	2.1	8.0	1	C13 H12 O 130Te