Electronic Supplementary Material (ESI) for RSC Advances.

Highly efficient synthesis and antioxidant capacity of N-substituted benzisoselenazol-3(2H)-ones

Agata J. Pacuła, Jacek Ścianowski and Krzysztof B. Aleksandrzak

Department of Organic Chemistry, Faculty of Chemistry, Nicolaus Copernicus University,
7 Gagarin Street, 87-100 Torun, Poland
E-mail: jsch@chem.umk.pl

Supporting Information: procedures, characterization and NMR Spectra

Index of content

I. General

^{1}H NMR spectra were obtained at 400 or 700 MHz and chemical shifts were recorded relative to $SiMe_4$ (δ 0.00) or solvent resonance ($CDCl_3$ δ7.26, CD_3OD δ3.31). Multiplicities were given as: s (singlet), d (doublet), dd (double doublet), ddd (double double doublet), t (triplet), dt (double triplet) and m (multiplet). The number of protons (n) for a given resonance was indicated by *n*H. Coupling constants were reported as a *J* value in Hz. ^{13}C NMR spectra were acquired at 100.6 MHz and chemical shifts were recorded relative to solvent resonance ($CDCl_3$ δ77.25). NMR spectra were carried out using ACD/NMR Processor Academic Edition. Elemental analyses were performed on a Vario MACRO CHN analyzer. Commercially available solvents DMF, DCM and MeOH (Aldrich) and chemicals were used without further purification. Column chromatography was performed using Merck 40-63D 60Å silica gel.

II. **Substrate synthesis**

General procedure for the preparation of N-substituted *o*-iodobenzamides: 2% NaOH (4.4 ml) was added to a solution of an amine (1.0 mmol) in DCM (2 mL). The mixture was cooled to 0°C and *o*-iodobenzoic acid chloride (1.1 mmol) dissolved in DCM (3 ml) was added dropwise. The reaction mixture was stirred in room temperature for 20h and the product was extracted with DCM. Combined organic layers were washed with saturated $NaHCO_3$ and dried over magnesium sulphate. The solvent was removed under reduced pressure and the product was obtained as white solid.

***N*-methyl-*o*-iodobenzamide (9a)**

Yield: 89%; mp 148-150°C (lit.[1] mp 145-147°C); ^{1}H NMR (700 MHz, $CDCl_3$) δ = 3.04 (d, *J*= 4.9 Hz, 3H, CH_3), 5.81 (s, 1H, NH), 7.12 (ddd, *J*=2.1, 6.3, 7.7 Hz, 1H_{ar}), 7.38-7.43 (m, 2H_{ar}), 7.88 (ddd, *J*=0.7, 1.4, 7.7 Hz, 1H, CH_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 26.7 (CH_3), 92.4 (C_{ar}), 128.1 (CH_{ar}), 128.2 (CH_{ar}), 131.0 (CH_{ar}), 139.8 (CH_{ar}), 142.3 (C_{ar}), 170.0 (C=O) ppm; IR 3282, 1626, 1584, 1540, 1404, 1314, 1257, 1780 cm^{-1}.

***N*-butyl-*o*-iodobenzamide (10a)**

Yield: 97%; mp 94-96°C (lit.[2] mp 94-96°C); ^{1}H NMR (700 MHz, $CDCl_3$) δ = 0.98 (t, *J*=7.7 Hz, 3H, CH_3), 1.42-1.49 (m, 2H, CH_2), 1.61-1.66 (m, 2H, CH_2), 3.48 (dt, *J*=5.6, 7.0 Hz, 2H, N-CH_2), 5.74 (s, 1H, NH), 7.09 (ddd, *J*=2.1, 7.0, 7.7 Hz, 1H_{ar}), 7.36-7.41 (m, 2H_{ar}), 7.86 (ddd, *J*=0.7, 1.4, 7.7 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 13.7 (CH_3), 20.2 (CH_2), 31.4 (CH_2), 39.8 (CH_2), 92.4 (C_{ar}), 128.1 (CH_{ar}), 128.2 (CH_{ar}), 131.0 (CH_{ar}), 139.8 (CH_{ar}), 142.5 (C_{ar}), 169.3 (C=O) ppm; IR 3271, 2952, 2928, 2863, 1632, 1584, 1543, 1425, 1313, 1257, 1012 cm^{-1}.

***N*-decyl-*o*-iodobenzamide (11a)**

Yield: 88%; mp 81-83 °C (lit.[3] mp 88 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ = 0.90 (t, *J*=6.8 Hz, 3H, CH_3), 1.25-1.46 (m, 14H, 7 x CH_2), 1.61-1.70 (m, 2H, CH_2), 3.46 (dt, *J*=6.0, 6.8 Hz, 2H, N-CH_2), 5.75 (s, 1H, NH), 7.10 (ddd, *J*=2.8, 6.8, 8.0 Hz, 1H_{ar}), 7.36-7.42 (m, 2H_{ar}), 7.87 (d, *J*=8.0 Hz, 1H, CH_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ =14.1 (CH_3), 22.6 (CH_2), 27.0 (CH_2), 29.2 (CH_2), 29.3

(CH_2), 29.4 (CH_2), 29.5 (2xCH_2), 31.9 (CH_2), 40.1 (CH_2), 92.4 (C_{ar}), 128.1 (CH_{ar}), 128.2 (CH_{ar}), 131.0 (CH_{ar}), 139.8 (CH_{ar}), 142.6 (C_{ar}), 169.3 (C=O) ppm; IR 2853, 1634, 1540, 1377 cm^{-1}.

_N_-(3-methylbutyl)-_o_-iodobenzamide (12a)[4]

Yield: 90%; mp 72-74°C; ^1H NMR (700 MHz, $CDCl_3$) δ = 0.97 (d, *J*=7.0 Hz, 6H, 2 x CH_3), 1.51-1.56 (m, 2H, CH_2), 1.69-1.76 (m, 1H, CH), 3.46-3.51 (m, 2H, N-CH_2), 5.70 (s, 1H, NH), 7.09 (ddd, *J*=2.1, 7.0, 7.7 Hz, 1H_{ar}), 7.39-7.41 (m, 2H_{ar}), 7.86 (ddd, *J*=0.7, 1.4, 7.7 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 22.4 (2 x CH_3), 25.9 (CH), 38.2 (CH_2), 38.4 (CH_2), 92.4 (C_{ar}), 128.1 (CH_{ar}), 128.2 (CH_{ar}), 131.0 (CH_{ar}), 139.8 (CH_{ar}), 142.5 (C_{ar}), 169.3 (C=O) ppm; IR 3253, 3069, 2952, 2863, 1637, 1584, 1542, 1463, 1305, 1013 cm^{-1}.

N-tert-butyl-_o_-iodobenzamide (13a)

Yield: 70%; mp 120-122 °C (lit.[5] mp 124-125°C); ^1H NMR (700 MHz, $CDCl_3$) δ = 1.49 (s, 9H, 3 x CH_3), 5.53 (s, 1H, NH), 7.05-7.10 (m, 1H_{ar}), 7.35-7.40 (m, 2H_{ar}), 7.84 (ddd, *J*=0.7, 1.4, 8.4 Hz, 1H, CH_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 28.7 (3 x CH_3), 52.2 (C), 92.3 (C_{ar}), 128.1 (CH_{ar}), 128.2 (CH_{ar}), 130.7 (CH_{ar}), 139.7 (CH_{ar}), 143.2 (C_{ar}), 168.7 (C=O) ppm; IR 3274, 2970, 1629, 1587, 1541, 1449, 1430, 1361 cm^{-1}.

_N_-cyclohexyl-_o_-iodobenzamide (8a)

Yield: 95%; mp 141-143°C, (lit.[6] mp 140°C); ^1H NMR (700 MHz, $CDCl_3$): *δ* = 1.20-1.35 (m, 3H), 1.42-1.50 (m, 2H), 1.68 (dt, *J*= 3.5, 13.3 Hz, 1H), 1.79 (dt, *J*= 4.2, 14.0 Hz, 2H), 2.07-2.15 (m, 2H), 4.00-4.08 (m, 1H), 5.65 (s, 1H, NH), 7.11 (ddd, *J*=2.1, 7.0, 8.4 Hz, 1H_{ar}), 7.38-7.44 (m, 2H_{ar}), 7.88 (dd, *J*=0.7, 8.4 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$): *δ* = 25.8 (CH_2), 26.5 (2xCH_2), 33.9 (2xCH_2), 49.9 (CH), 93.4 (C), 129.1 (CH_{ar}), 129.2 (CH_{ar}), 131.9 (CH_{ar}), 140.7 (CH_{ar}), 143.6 (C_{ar}), 169.5 (C=O) ppm; IR 3286, 2853, 1730, 1636, 1537, 1168, 1015 cm^{-1}.

_N_-(1-phenylethyl)-_o_-iodobenzamide (14a)

Yield: 87%; mp 120-122°C, (lit.[7] mp 120-121°C); 1H NMR (400 MHz, $CDCl_3$) δ = 1.67 (d, *J*=6.8 Hz, 3H, CH_3), 5.32-5.40 (m 1H, CH), 6.00 (d, *J*=6.8 Hz, 1H, NH), 7.10 (ddd, *J*=2.0, 7.2, 8.0 Hz, $1H_{ar}$), 7.28-7.33 (m, $1H_{ar}$), 7.36-7.46 (m, $6H_{ar}$), 7.86 (dd, *J*=0.8, 8.0 Hz, $1H_{ar}$) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 21.4 (CH_3), 49.5 (CH), 92.3 (C_{ar}), 126.4 (2 x CH_{ar}), 127.6 (CH_{ar}), 128.1 (CH_{ar}), 128.3 (CH_{ar}), 128.7 (2 x CH_{ar}), 131.1 (CH_{ar}), 139.8 (CH_{ar}), 142.1 (C_{ar}), 142.4 (C_{ar}), 168.3 (C=O) ppm; IR 3435, 2853, 1652, 1376, 1256, 1104 cm^{-1}.

_N_-(2-(4-methoxyphenyl)ethyl)-_o_-iodobenzamide (15a)[8]

Yield: 93%; mp 118-120°C; ^1H NMR (700 MHz, $CDCl_3$) δ = 2.94 (t, *J*=7.0 Hz, 2H, CH_2), 3.73 (dt, *J*=6.3, 7.0 Hz, 2H, CH_2), 3.82 (s, 3H, OCH_3), 5.80 (s, 1H, NH), 6.88 (dd, *J*=2.1, 7.0 Hz, $2H_{ar}$), 7.10 (ddd, *J*=2.1, 7.0, 7.7 Hz, $1H_{ar}$), 7.22 (dd, *J*=2.1, 6.3 Hz, $2H_{ar}$), 7.32-7.39 (m, $2H_{ar}$), 7.22 (ddd, *J*=0.7, 1.4, 7.7 Hz, $1H_{ar}$) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 34.5 (CH_2), 41.2 (CH_2), 55.2 (OCH_3), 92.4 (C_{ar}), 114.1 (2 x CH_{ar}), 128.14 (CH_{ar}), 128.17 (CH_{ar}), 129.8 (2 x CH_{ar}), 130.6 (C_{ar}), 131.0 (CH_{ar}), 139.8 (CH_{ar}), 142.3 (C_{ar}), 158.3 (C_{ar}), 169.3 (C=O) ppm; IR 3302, 2936, 1639, 1583, 1531, 1301, 1242, 1030 cm^{-1}.

_N_-phenyl-_o_-iodobenzamide (1a)

Yield: 95%; mp 142-144°C, (lit.[9] mp 143-145°C); ^1H NMR (400 MHz, $CDCl_3$): *δ* = 7.13-7.23 (m, 2H), 7.32-7.50 (m, 4H), 7.55 (dd, *J*= 1.6, 7.6 Hz, 1H), 7.66 (d, *J*= 7.6, 2H), 7.93 (dd, *J*= 0.8, 8.0 Hz, 1H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) *δ* = 92.3 (C_{ar}), 120.0 (2xCH_{ar}), 124. 9 (CH_{ar}), 128.3 (CH_{ar}), 128.5 (CH_{ar}), 129.1 (2xCH_{ar}), 131.5 (CH_{ar}), 137.5 (C_{ar}), 140.0 (CH_{ar}), 142.1 (C_{ar}), 167.1 (C=O) ppm; IR 3310, 2965, 1661, 1596, 1522, 1257, 1013 cm^{-1}.

_N_-(1-naphthyl)-_o_-iodobenzamide (16a)

Yield 85%; mp 234-236°C, (lit.[10] mp 233-234°C); ^{1}H NMR (700 MHz, $CDCl_3$): δ = 7.19-7.23 (m $1H_{ar}$), 7.48-7.59 (m, $4H_{ar}$), 7.64-7.69 (m, $1H_{ar}$), 7.77 (d, J= 8.4 Hz, $1H_{ar}$), 7.8 (s, 1H, NH), 7.91 (d, J= 7.7 Hz, $1H_{ar}$), 7.82-7.95 (m, $2H_{ar}$), 8.17 (d, J= 7.7 Hz, $1H_{ar}$) ppm ;^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 92.3 (C_{ar}), 120.7 (CH_{ar}), 120.9 (CH_{ar}), 125.8 (CH_{ar}), 126.1 (CH_{ar}), 126.3 (CH_{ar}), 126.5 (CH_{ar}), 127.1 (C_{ar}), 128.4 (CH_{ar}), 128.6 (CH_{ar}), 128.8 (CH_{ar}), 131.5 (CH_{ar}), 131.8 (C_{ar}), 134.1 (C_{ar}), 140.1 (CH_{ar}), 142.4 (C_{ar}), 167.8 (C=O) ppm; IR 3250, 3053, 1650, 1524, 1502, 1346, 1294, 1014 cm^{-1}.

_N_-(2-naphthyl)-_o_-iodobenzamide (17a)

Yield: 88%; mp 180-182 °C, (lit.[11] mp 179-180°C); ^{1}H NMR (700 MHz, $CDCl_3$) δ = 7.16-7.20 (m, $1H_{ar}$), 7.43-7.51 (m, $3H_{ar}$), 7.56-7.60 (m, $2H_{ar}$), 7.64 (s, 1H, NH), 7.82 (d, J=7.7 Hz, $1H_{ar}$), 7.86 (d, J=8.4 Hz, $2H_{ar}$), 7.94 (d, J=8.4 Hz, $1H_{ar}$), 8.36 (d, J=1.4 Hz, $1H_{ar}$) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 92.4 (C_{ar}), 117.0 (CH_{ar}), 119.7 (CH_{ar}), 125.3 (CH_{ar}), 126.6 (CH_{ar}), 127.6 (CH_{ar}), 127.8 (CH_{ar}), 128.4 (CH_{ar}), 128.6 (CH_{ar}), 128.9 (CH_{ar}), 130.9 (C_{ar}), 131.6 (CH_{ar}), 133.8 (C_{ar}), 134.9 (C_{ar}), 140.1 (CH_{ar}), 142.0 (C_{ar}), 167.3 (C=O) ppm; IR 3243, 3050, 1653, 1537, 1500, 1430, 1294, 1013 cm^{-1}.

_N_-(2-antryl)-_o_-iodobenzamide (18a)

Yield: 75%; mp 232-234 C; ^{1}H NMR (700 MHz, $CDCl_3$) δ = 7.18-7.25 (m, $1H_{ar}$), 7.45-7.55 (m, $4H_{ar}$), 7.60-7.65 (m, $2H_{ar}$), 7.95-8.06 (m, $4H_{ar}$), 8.43 (d, J=11.6 Hz, $2H_{ar}$), 8.58 (s, 1H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 94.2 (C_{ar}), 115.2 (CH_{ar}), 121.5 (CH_{ar}), 125.5 (CH_{ar}), 125.7 (CH_{ar}), 126.1 (CH_{ar}), 126.3 (CH_{ar}), 128.2 (CH_{ar}), 128.5 (CH_{ar}), 128,6 (2xCH_{ar}), 129.1 (C_{ar}), 129.3 (CH_{ar}), 131.0 (C_{ar}), 131.6 (CH_{ar}), 131.9 (C_{ar}), 132.2 (C_{ar}), 136.5 (C_{ar}), 139.5 (CH_{ar}), 143.5 (C_{ar}), 168.4 (C=O) ppm; IR 3282, 3045, 1655, 1512, 1460, 1429, 1309, 1014 cm^{-1}. Elemental Anal. Calcd for $C_{21}H_{14}NOI$ (423.25): C, 59.59; H, 3.33. Found: C, 59.48; H, 3.32.

***N*-(4-nitrophenyl)-*o*-iodobenzamide (19a)[12]**

Yield: 84%; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.23 (ddd, *J*=1.6, 7.2, 8.0 Hz, 1H_{ar}), 7.50 (dt, *J*=1.2, 7.2, Hz, 1H_{ar}), 7.57 (dd, *J*=1.6, 8.0 Hz, 1H_{ar}), 7.85 (d, *J*=9.2 Hz, 2H_{ar}), 7.93 (s, 1H, NH), 7.95-7.98 (m, 1H_{ar}), 8.28 (dd, *J*=1.6, 6.8 Hz, 2H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 92.1 (C_{ar}), 119.4 (2 x CH_{ar}), 125.1 (2 x CH_{ar}), 128.5 (CH_{ar}), 128.7 (CH_{ar}), 132.1 (CH_{ar}), 140.2 (CH_{ar}), 141.2 (C_{ar}), 143.2 (C_{ar}), 144.0 (C_{ar}), 167.3 (C=O) ppm; IR 3263, 3087, 1666, 1557, 1495, 1307, 1108 cm^{-1}.

***N*-(4-bromophenyl)-*o*-iodobenzamide (20a)**

Yield: 87%; mp 153-155^{o}C, (lit.[13] mp 159-160^{o}C); ^{1}H NMR (700 MHz, $CDCl_3$) δ = 7.18 (ddd, *J*=1.4, 7.7, 7.7 Hz, 1H_{ar}), 7.46 (ddd, *J*=0.7, 7.0, 7.0 Hz, 1H_{ar}), 7.50-7.58 (m, 6H, NH i 5H_{ar}), 7.93 (dd, *J*=1.4, 8.4 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 77.2 (C_{ar}), 92.3 (C_{ar}), 117.6 (C_{ar}), 121.6 (2 x CH_{ar}), 128.4 (CH_{ar}), 128.5 (CH_{ar}), 131.7 (CH_{ar}), 132.5 (2 x CH_{ar}), 140.1 (CH_{ar}), 141.7 (C_{ar}), 167.2 (C=O) ppm; IR 3237, 3167, 3097, 3048, 1654, 1594, 1528, 1483, 1390, 1319, 1015 cm^{-1}.

***N*-(4-jodophenyl)-*o*-iodobenzamide (21a)[14]**

Yield: 93%; mp 189-191 ^{o}C; ^{1}H NMR (700 MHz, $CDCl_3$) δ = 7.20 (ddd, *J*=1.4, 7.7, 7.7 Hz, 1H_{ar}), 7.42 (s, 1H, NH), 7.45-7.50 (m, 3H_{ar}), 7.56 (dd, *J*=1.4, 7.7 Hz, 1H_{ar}), 7.72 (dd, *J*=2.1, 7.0 Hz, 2H_{ar}), 7.95 (dd, *J*=0.7, 8.4 Hz, 1H_{ar})ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 89.2 (C_{ar}), 93.2 (C_{ar}), 122.8 (2 x CH_{ar}), 129.4 (CH_{ar}), 129.6 (CH_{ar}), 132.7 (CH_{ar}), 138.2 (C_{ar}), 139.1 (2 x CH_{ar}), 141.1 (CH_{ar}), 142.7 (C_{ar}), 168.1 (C=O) ppm; IR 3240, 1652, 1583, 1514, 1467, 1430, 1302, 1014 cm^{-1}.

***N*-(4-methoxyphenyl)-*o*-iodobenzamide (22a)**

Yield: 82%; mp 167-169^{o}C, (lit.[15] mp 167-169^{o}C); ^{1}H NMR (700 MHz, $CDCl_3$) δ =3.81 (s, 3H, -OCH_3), 6.91 (dd, *J*=2.1, 7.0 Hz, 2H_{ar}), 7.12 (ddd, *J*=1.4, 7.7, 7.7 Hz, 1H_{ar}), 7.40 (ddd, *J*= 1.4, 7.7, 7.7 Hz, 1H_{ar}), 7.45 (s, 1H, NH), 7.49 (dd, *J*= 1.4, 7.7 Hz, 1H_{ar}), 7.53 (dd, *J*= 2.1, 7.0 Hz, 2H_{ar}), 7.88 (dd, *J*= 0.7, 7.7 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 55.5 (-OCH_3), 92.4 (C_{ar}), 114.3

(2xCH_{ar}), 122.0 (2xCH_{ar}), 128.3 (CH_{ar}), 128.5 (CH_{ar}), 130.6 (C_{ar}), 131.3 (CH_{ar}), 140.0 (CH_{ar}), 142.2 (C_{ar}), 156.9 (C_{ar}), 167.1 (C=O) ppm; IR 3305, 1649, 1512, 1412, 1316, 1234, 1026 cm^{-1}.

II. **Benzizoselenazol-3(2H)-one synthesis**

General procedure: Hydrazine hydride (8.0 mmol) was added dropwise to the mixture of selenium powder (1.2 mmol) and lithium hydroxide (3.6 mmol) in DMF (3 ml). Reaction was heated to 120°C and stirred for 15 minutes under argon atmosphere. After cooling to room temperature the amide (1.0 mmol) in DMF (2 mL) was added. The reaction mixture was heated to 120°C and stirred for 20h under argon atmosphere. The solution was cooled, 25 mL of brine was added and the mixture was stirred for additional 20h. Precipitate was filtered under vacume, washed with water and dried in air. The crude product was purified by column chromatography (silica gel, DCM:MeOH 99.2 : 0.8).

***N*-methyl-1,2-benzisoselenazol-3(2*H*)-one (9)**

Yield: 59%; mp 155-157°C, (lit.[16] mp 156-158°C); ^{1}H NMR (700 MHz, $CDCl_3$) δ = 3.44 (s, 3H, CH_3), 7.44 (ddd, *J*=1.4, 7.0, 7.7 Hz, 1H_{ar}), 7.59-7.63 (m, 1H, CH_{ar}), 7.66 (dt, *J*=1.4, 8.4 Hz, 1H_{ar}), 8.06 (ddd, *J*=0.7, 1.4, 7.7 Hz, 1H, CH_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 31.5 (CH_3), 124.0 (CH_{ar}), 126.2 (CH_{ar}), 127.0 (C_{ar}), 128.7 (CH_{ar}), 131.9 (CH_{ar}), 137.5 (C_{ar}), 167.5 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 915.44 ppm; IR 2966, 2927, 1589, 1558, 1441, 1355, 1023 cm^{-1}.

***N*-butyl-1,2-benzisoselenazol-3(2*H*)-one (10)**

Yield: 82%; mp 86-88°C, (lit.[17] mp 90-91°C); ^{1}H NMR (400 MHz, $CDCl_3$) δ = 0.98 (t, *J*=7.6 Hz, 3H, CH_3), 1.39-1.50 (m, 2H, CH_2), 1.68-1.77 (m, 2H, CH_2), 3.88 (t, *J*=7.2 Hz, 2H, N-CH_2), 7.44 (ddd, *J*=1.2, 6.8, 8.0 Hz, 1H_{ar}), 7.56-7.67 (m, 2H_{ar}), 8.06 (ddd, *J*=0.8, 1.2, 7.6 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 13.7 (CH_3), 19.8 (CH_2), 32.6 (CH_2), 44.5 (CH_2), 123.9 (CH_{ar}), 126.1

(CH_{ar}), 127.6 (C_{ar}), 128.8 (CH_{ar}), 131.8 (CH_{ar}), 137.6 (C_{ar}), 167.1 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 884.15 ppm; IR 3270, 2956, 2925, 2865, 1634, 1601, 1585, 1257 cm^{-1}

_N_-decyl-1,2-benzisoselenazol-3(2_H_)-one (11)[18]

Yield: 70%; mp 70-72°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 0.89 (t, *J*=6.8 Hz, 3H, CH_3), 1.24-1.43 (m, 14H, 7 x CH_2), 1.70-1.79 (m, 2H, CH_2), 3.87 (t, *J*=7.2 Hz, 2H, CH_2), 7.40-7.46 (m, 1H_{ar}), 7.56-7.62 (m, 1H_{ar}), 7.64 (d, *J*=7.6 Hz, 1H, CH_{ar}), 8.05 (d, *J*=7.6 Hz, 1H, CH_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 14.1 (CH_3), 22.6 (CH_2), 26.6 (CH_2), 29.2 (CH_2), 29.4 (2xCH_2), 29.5 (CH_2), 30.5 (CH_2), 31.8 (CH_2), 44.9 (CH_2), 123.9 (CH_{ar}), 126.1 (CH_{ar}), 127.7 (C_{ar}), 128.8 (CH_{ar}), 131.8 (CH_{ar}), 137.6 (C_{ar}), 167.1 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 884.12 ppm; IR 3303, 2921, 2851, 1626, 1615, 1584, 1534, 1467, 1317 cm^{-1}.

_N_-(3-methylbutyl)-1,2-benzisoselenazol-3(2_H_)-one (12)

Yield: 98%; mp 139-141°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 0.99 (d, *J*=6.4 Hz, 6H, 2 x CH_3), 1.60-1.65 (m, 2H, CH_2), 1.67-1.76 (m, 1H, CH), 3.90 (t, *J*=7.2 Hz, 2H, N-CH_2), 7.44 (ddd, *J*=1.2, 6.8, 8.0 Hz, 1H_{ar}), 7.57-7.62 (m, 1H_{ar}), 7.65 (ddd, *J*= 0.8, 1.2, 8.8 Hz, 1H_{ar}) 8.06 (ddd, *J*=0.8, 1.2, 7.6 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 22.4 (2 x CH_3), 25.7 (CH), 39.4 (CH_2), 43.2 (CH_2), 123.9 (CH_{ar}), 126.1 (CH_{ar}), 127.7 (C_{ar}), 128.7 (CH_{ar}), 131.8 (CH_{ar}), 137.6 (C_{ar}), 167.1 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 882.23 ppm; IR 2945, 2912, 2863, 1588, 1558, 1439, 1376, 1348, 1306, 1021 cm^{-1}, Elemental Anal. Calcd for $C_{12}H_{15}NOSe$ (268.21): C, 53.74; H, 5.64. Found: C, 54.34; H, 5.73.

N-tert-butyl-1,2-benzisoselenazol-3(2_H_)-one (13)

Yield: 92%; mp 113-115°C, (lit.[19] mp 137-138°C); ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.70 (s, 9H, 3 x CH_3), 7.41 (ddd, *J*=2.4, 6.0, 8.0 Hz, 1H_{ar}), 7.54-7.61 (m, 2H_{ar}), 7.98 (ddd, *J*=0.8, 1.2, 8.0 Hz, 1H, CH_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 29.1 (3xCH_3), 58.8

(C), 123.2 (CH_{ar}), 125.9 (CH_{ar}), 128.3 (CH_{ar}), 130.0 (C_{ar}), 131.5 (CH_{ar}), 136.8 (CH_{ar}), 166.9 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 856.54 ppm; IR 2966, 2925, 2870, 1587, 1557, 1443, 1304, 1022 cm^{-1}.

_N_-cyclohexyl-1,2-benzisoselenazol-3(2_H_)-one (8)

Yield: 88%; mp 158-160°C, (lit.[20] mp 158-160°C); ^{1}H NMR (700 MHz, $CDCl_3$): *δ* = 1.19-1.26 (m, 1H), 1.42 (ddd, *J*= 3.50, 11.90, 23.8 Hz, 2H), 1.48-1.55 (m, 2H), 1.73-1.78 (m, 1H), 1.84-1.91 (m, 2H), 2.11-2.16 (m, 2H), 4.48-4.54 (m, 1H), 7.44 (ddd, *J*= 0.7, 7.0, 7.7 Hz, 1H), 7.59 (ddd, *J*= 1.4, 7.0, 8.4 Hz, 1H), 7.66 (dt, *J*= 0.7, 7.7 Hz, 1H), 8.07 (ddd, *J*= 0.7, 1.4, 7.7 Hz, 1H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$): *δ* = 25.3 (CH_2), 25.5 (2 x CH_2), 34.2 (2 x CH_2), 53.7 (CH), 123.9 (CH), 126.0 (CH), 128.5 (2 x CH), 131.5 (CH), 137.9 (C), 166.5 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 837.33 ppm; IR 3285, 2925, 1636, 1583, 1551, 1244 cm^{-1}.

_N_-(1-phenylethyl)-1,2-benzisoselenazol-3(2_H_)-one (14)

Yield: 65%; mp 126-128°C(lit.[21] mp 116-117.5°C); 1H NMR (400 MHz, $CDCl_3$) δ = 1.76 (d, *J*=6.8 Hz, 3H, CH_3), 5.94 (q, *J*=6.8 Hz, 1H, CH), 7.34-7.48 (m, 6H_{ar}), 7.55-7.58 (m, 2H), 8.08 (dt, *J*=1.2, 8.0 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 19.7 (CH_3), 52.8 (CH), 123.8 (CH_{ar}), 126.1 (CH_{ar}), 127.3 (2 x CH_{ar}), 128.21 (C_{ar}), 128.28 (CH_{ar}), 128.73 (2 x CH_{ar}), 128.78 (CH_{ar}), 131.7 (CH_{ar}), 138.1 (C_{ar}), 141.3 (C_{ar}), 166.6 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 843.03 ppm; IR 2971, 2904, 1585, 1532, 1443, 1340, 1263, 1088, 1022 cm^{-1}.

_N_-(2-(4-metoxyphenyl)ethyl)-1,2-benzisoselenazol-3(2_H_)-one (15)

Yield: 85%; mp 120-122°C; ^{1}H NMR (700 MHz, $CDCl_3$) δ = 2.98 (t, *J*=7.7 Hz, 2H, CH_2), 3.79 (s, 3H, OCH_3), 4.08 (t, *J*=7.7 Hz, 2H, CH_2), 6.85 (dd, *J*=2.1, 6.3 Hz, 2H_{ar}), 7.18 (dd, *J*=2.1, 6.3 Hz, 2H_{ar}), 7.41 (ddd, *J*=1.4, 4.9, 7.7 Hz, 1H_{ar}), 7.56-7.58 (m, 2H_{ar}), 8.04 (dt, *J*=1.4, 8.4 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 35.5 (CH_2), 46.3 (CH_2), 56.2 (OCH_3), 77.2 (C_{ar}), 114.0 (2 x CH_{ar}), 123.8 (CH_{ar}), 126.1 (CH_{ar}), 127.2 (C_{ar}), 128.7 (CH_{ar}), 129.9 (2 x CH_{ar}), 131.9 (CH_{ar}), 138.0 (C_{ar}), 158.5 (C_{ar}), 167.2 (C=O) ppm; ^{77}Se (76.3

MHz, $CDCl_3$), δ = 901.43 ppm; IR 2969, 2899, 1591, 1508, 1373, 1244, 1042 cm^{-1}, Elemental Anal. Calcd for $C_{16}H_{15}NOSe$ (332.26): C, 57.84; H, 4.55. Found: C, 57.87; H, 4.46.

_N_-phenyl-1,2-benzisoselenazol-3(2_H_)-one (1)

Yiedl: 92%; mp 184-186°C, (lit.[22] mp 182-183°C); ^1H NMR (400 MHz, $CDCl_3$): δ = 7.28-7.34 (m, 1H), 7.44-7.54 (m, 3H), 7.64-7.70 (m, 4H), 8.14 (dt, *J*= 1.20, 8.00 Hz, 1H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 123.7 (CH_{ar}), 125.4 (2xCH_{ar}), 126.5 (CH_{ar}), 126.7 (CH_{ar}), 127.5 (C_{ar}), 129.3 (2xCH_{ar}), 129.4 (CH_{ar}), 132.5 (CH_{ar}), 137.6 (C_{ar}), 139.1 (C_{ar}), 165.7 (C=O) ppm;;^{77}Se (76.3 MHz, $CDCl_3$), δ = 962.24 ppm; IR 1585, 1576, 1559, 1343, 1027 cm^{-1}.

_N_-(1-naphthyl)-1,2-benzisoselenazol-3(2_H_)-one (16)

Yield: 85%; mp 225-227 °C; ^1H NMR (400 MHz, $CDCl_3$): δ = 7.50-7.58 (m, 4H_{ar}), 7.62 (dd, *J*=1.2, 7.2 Hz, 1H_{ar}), 7.69-7.77 (m, 2H_{ar}), 7.78-7.83 (m, 1H_{ar}), 7.92-7.97 (m, 2H_{ar}), 8.21 (ddd, *J*=0.8, 1.2, 7.6 Hz, 1H_{ar}) ppm ;^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 123.2 (CH_{ar}), 124.0 (CH_{ar}), 125.4 (CH_{ar}), 126.2 (C_{ar}), 126.5 (CH_{ar}), 126.6 (CH_{ar}), 127.0 (CH_{ar}), 127.4 (CH_{ar}), 128.4 (CH_{ar}), 129.4 (CH_{ar}), 129.6 (CH_{ar}), 130.8 (C_{ar}), 132.5 (CH_{ar}), 134.5 (C_{ar}), 134.6 (C_{ar}), 139.2 (C_{ar}), 167.0 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 994.30 ppm; IR 1572, 1598, 1340, 1019 cm^{-1}, Elemental Anal. Calcd for $C_{17}H_{11}NOSe$ (324.24): C, 62.97; H, 3.42, Found: C, 62.76; H, 3.41.

_N_-(2-naphthyl)-1,2-benzisoselenazol-3(2_H_)-one (17)

Yield: 87%; mp 189-191°C; ^1H NMR (700 MHz, $CDCl_3$) δ = 7.52-7.56 (m, 3H_{ar}), 7.69-7.74 (m, 2H_{ar}), 7.84 (dd, *J*=2.1, 9.1 Hz, 1H_{ar}), 7.87-7.91 (m, 2H_{ar}), 7.93 (d, *J*=8.4 Hz, 1H_{ar}), 8.09 (d, *J*=2.1 Hz, 1H_{ar}), 8.18 (ddd, *J*=0.7, 1.4, 7.7 Hz, 1H_{ar}) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 123.5 (CH_{ar}), 123.7 (CH_{ar}), 123.8 (CH_{ar}), 126.2 (CH_{ar}), 126.6 (CH_{ar}), 126.7 (CH_{ar}), 127.6 (C_{ar}), 127.7 (CH_{ar}), 127.8 (CH_{ar}), 129.1 (CH_{ar}), 129.4 (CH_{ar}), 131.9 (C_{ar}), 132.6 (CH_{ar}), 133.5 (C_{ar}), 136.7 (C_{ar}), 137.7 (C_{ar}), 165.8 (C=O) ppm;

^{77}Se (76.3 MHz, $CDCl_3$), δ = 965.42 ppm; IR 1588, 1499, 1318, 1304, 1262, 1021 cm^{-1}, Elemental Anal. Calcd for $C_{17}H_{11}NOSe$ (324.24): C, 62.97; H, 3.42, Found: C, 62.95; H, 3.34.

_N_-(2-antryl)-1,2-benzisoselenazol-3(2_H_)-one (18)

Yield: 89%; mp 250-252°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.49-7.56 (m, $3H_{ar}$), 7.68-7.74 (m, $2H_{ar}$), 7.86 (dd, *J*=2.4, 9.2 Hz, $1H_{ar}$), 8.0-8.05 (m, $2H_{ar}$), 8.08 (d, *J*=8.8 Hz, $1H_{ar}$), 8.17-8.19 (m, $2H_{ar}$), 8.45 (s, $2H_{ar}$) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 121.9 (CH_{ar}), 124.4 (CH_{ar}), 126.0 (CH_{ar}), 126.3 (CH_{ar}), 126.41 (CH_{ar}), 126.44 (CH_{ar}), 126.5 (CH_{ar}), 126.8 (CH_{ar}), 128.3 (CH_{ar}), 128.4 (CH_{ar}), 128.6 (CH_{ar}), 129.0 (C_{ar}), 129.5 (CH_{ar}), 129.7 (C_{ar}), 131.5 (C_{ar}), 131.6 (C_{ar}), 132.1 (C_{ar}), 132.8 (CH_{ar}), 137.6 (C_{ar}), 139.6 (C_{ar}), 165.7 (C=O) ppm ; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 965.08 ppm; IR 1607, 1444, 1257, 1080 cm^{-1}. Elemental Anal. Calcd for $C_{21}H_{13}NOSe$ (374.29): C, 67.39; H, 3.50, Found: C, 67.48; H, 3.48.

_N_-(4-nitrophenyl)-1,2-benzisoselenazol-3(2_H_)-one (19)[23]

Yield: 60%; mp 280-282 °C; ^{1}H NMR (700 MHz, $CDCl_3$) δ = 7.52 (ddd, *J*=0.7, 7.0, 7.7 Hz, $1H_{ar}$), 7.68-7.74 (m, $2H_{ar}$), 7.93 (dd, *J*=2.1, 7.0 Hz, $2H_{ar}$), 8.14 (ddd, *J*=0.7, 1.4, 7.7 Hz, $1H_{ar}$), 8.31 (dd, *J*=2.8, 7.0 Hz, $2H_{ar}$) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 124.9 (2 x CH_{ar}), 126.3 (2 x CH_{ar}), 127.4 (CH_{ar}), 128.0 (CH_{ar}), 129.7 (CH_{ar}), 129.9 (C_{ar}), 134.5 (CH_{ar}), 140.0 (C_{ar}), 144.9 (C_{ar}), 147.8 (C_{ar}), 167.2 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 922.92 ppm; IR 1602, 1582, 1504, 1493, 1326, 1317, 1301, 1265, 1138, 1112 cm^{-1}

_N_-(4-bromophenyl)-1,2-benzisoselenazol-3(2_H_)-one (20)

Yield: 72%; mp 196-198 °C, (lit.[24] mp 194-196°C); ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.50 (ddd, *J*=3.6, 4.8, 8.0 Hz, $1H_{ar}$), 7.53-7.59 (m, $4H_{ar}$), 7.67-7.70 (m, $2H_{ar}$), 8.13 (dt, *J*=1.2, 8.0 Hz, $1H_{ar}$) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 119.9 (C_{ar}), 123.7 (CH_{ar}), 126.74 (CH_{ar}), 126.76 (2 x CH_{ar}), 127.2 (C_{ar}), 129.4 (CH_{ar}), 132.3 (2 x CH_{ar}), 132.8 (CH_{ar}), 137.3 (C_{ar}), 138.2 (C_{ar}), 165.6 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 967.11 ppm; IR 1589, 1486, 1442, 1326, 1024 cm^{-1}.

_N_-(4-iodophenyl)-1,2-benzisoselenazol-3(2_H_)-one (21)

Yield: 82%; mp 198-200°C, (lit.[25] mp 201-202°C); ^{1}H NMR (700 MHz, $CDCl_3$) δ = 7.44-7.46 (m, $2H_{ar}$), 7.51 (ddd, *J*=2.1, 5.6, 7.7 Hz, $1H_{ar}$), 7.67-7.72 (m, $2H_{ar}$), 7.76-7.79 (m, $2H_{ar}$), 8.14 (ddd, *J*=0.7, 1.4, 7.7 Hz, $1H_{ar}$) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 90.9 (C_{ar}), 123.7 (CH_{ar}), 126.7 (CH_{ar}), 126.9 (2 x CH_{ar}), 127.3 (C_{ar}), 129.5 (CH_{ar}), 132.8 (CH_{ar}), 137.2 (C_{ar}), 138.3 (2 x CH_{ar}), 139.0 (C_{ar}), 165.6 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 965.95 ppm; IR 1617, 1585, 1536, 1481, 1444, 1316, 1260 cm^{-1}.

_N_-(4-metoxyphenyl)-1,2-benzisoselenazol-3(2_H_)-one (22)

Yield: 86%; mp 155-157 °C, (lit.[26] mp 178-179°C); ^{1}H NMR (400 MHz, $CDCl_3$) δ = 3.85 (s, $-OCH_3$), 6.97 (dd, *J*= 1.6, 6.8 Hz, $2H_{ar}$), 7.46-7.55 (m, $3H_{ar}$), 7.65-7.69 (m, $2H_{ar}$), 8.13 (ddd, *J*= 0.8, 1.2, 7.6 Hz, $1H_{ar}$) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 55.5 ($-OCH_3$), 114.5 (2xCH_{ar}), 123.7 (CH_{ar}), 126.4 (CH_{ar}), 126.9 (CH_{ar}), 127.38 (CH_{ar}), 128.7 (C_{ar}), 129.3 (CH_{ar}), 131.6 (C_{ar}), 132.3 (CH_{ar}), 137.8 (C_{ar}), 158.4 (C_{ar}), 165.9 (C=O) ppm; ^{77}Se (76.3 MHz, $CDCl_3$), δ = 964.71 ppm; IR 2957, 2926, 1611, 1506, 1442, 1334, 1245, 1022 cm^{-1}.

IV. Benzisoselenazolone synthesis from corresponding diselenide

IV.I Reaction with potassium iodate

Potassium iodate (0.14 mmol) was added to the dicyclohexyl diselenide (0.14 mmol) dissolved in DMF (3 ml). The reaction mixture was heated to 120°C for 20h under argon atmosphere. Brine was added and the mixture was stirred for additional 20h. Hydrochloric acid was added and the precipitated solid was filtered under reduce pressure, washed with water and dried on air. Yield: 50%.

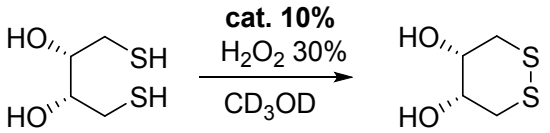
IV.II Reaction with sodium iodide and lithium hydroxide

Lithium hydroxide (0.28 mmol) and sodium iodide (0.28 mmol) was added to dicyclohexyl diselenide (0.14 mmol) dissolved in DMF (3 ml). The reaction mixture was heated to 120°C for 20h under argon atmosphere. Brine was added and the mixture was

stirred for additional 20h. Hydrochloric acid was added and the precipitated solid was filtered under reduce pressure, washed with water and dried on air. Yield: 57%.

V. Evaluation of antioxidant activity.

30% H_2O_2 (0.15 mmol) was added to the reaction mixture of benzisoselenazol-3(2H)-one **1, 8-22** (0.015 mmol) and dithiothreitole DTT^{red} (0.15 mmol) in CD_3OD (1.1 ml). ^1H NMR spectra were measuared in specific time intervals. The concentarion of the substrate was determined from the ^1H NMR spectra.



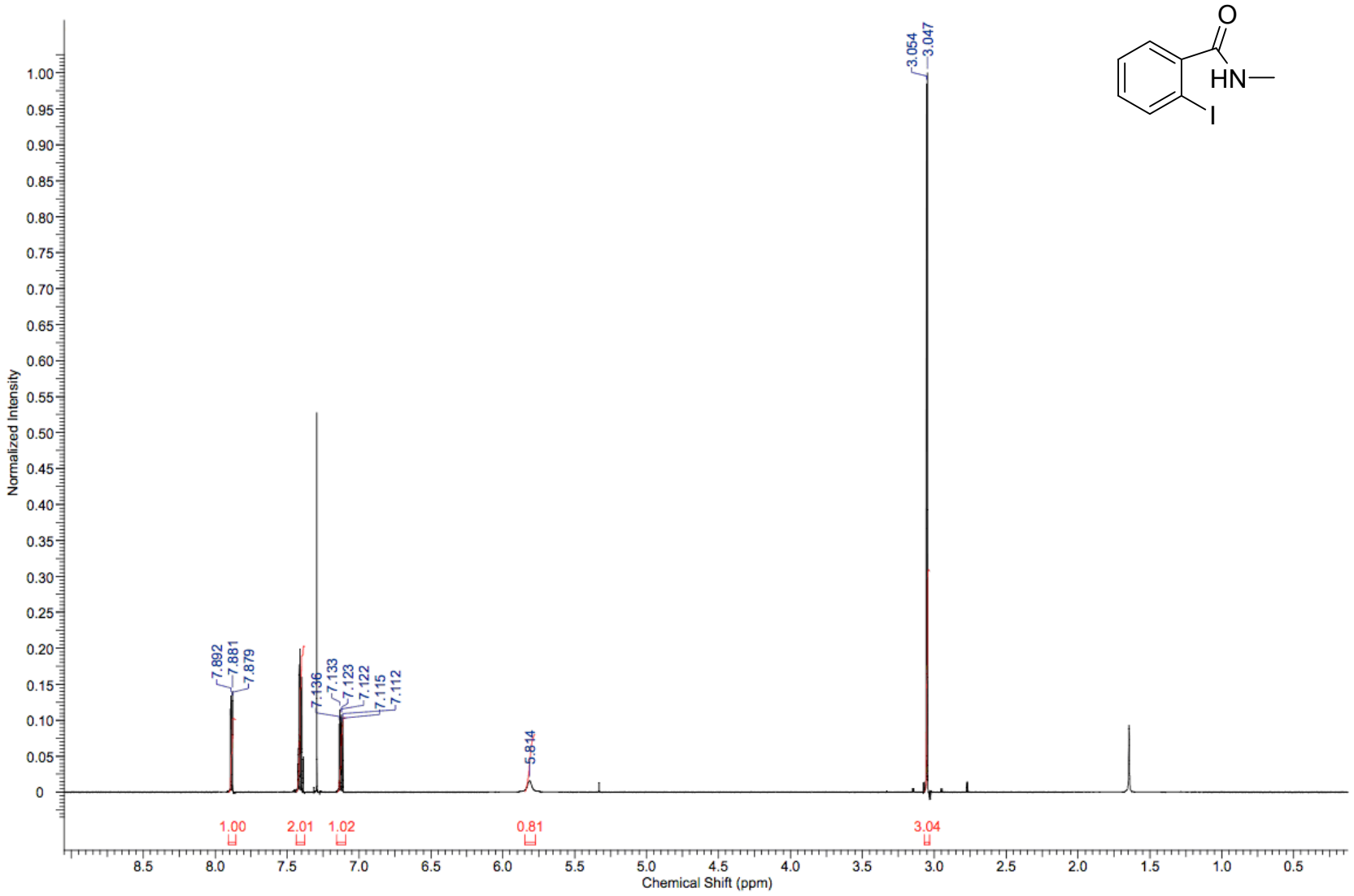
DTT^{red} [1eq.] DTT^{ox}

	DTT^{red} concentration [%]				
Catalyst [10%]	**3 min**	**5 min**	**15 min**	**30 min**	**60 min**
1 (Ebselen)	84	75	64	58	52
9	78	65	35	11	0
10	81	59	41	32	29
11	98	97	94	91	85
12	77	58	42	28	13
13	97	96	94	93	91
8	75	69	62	55	44
14	85	74	55	35	11
15	0	0	0	0	0
16	99	98	97	96	95
17	87	83	78	71	62
18	96	94	91	89	88
19	25	7	5	0	0
20	86	83	79	75	71
21	42	0	0	0	0
22	64	41	5	0	0

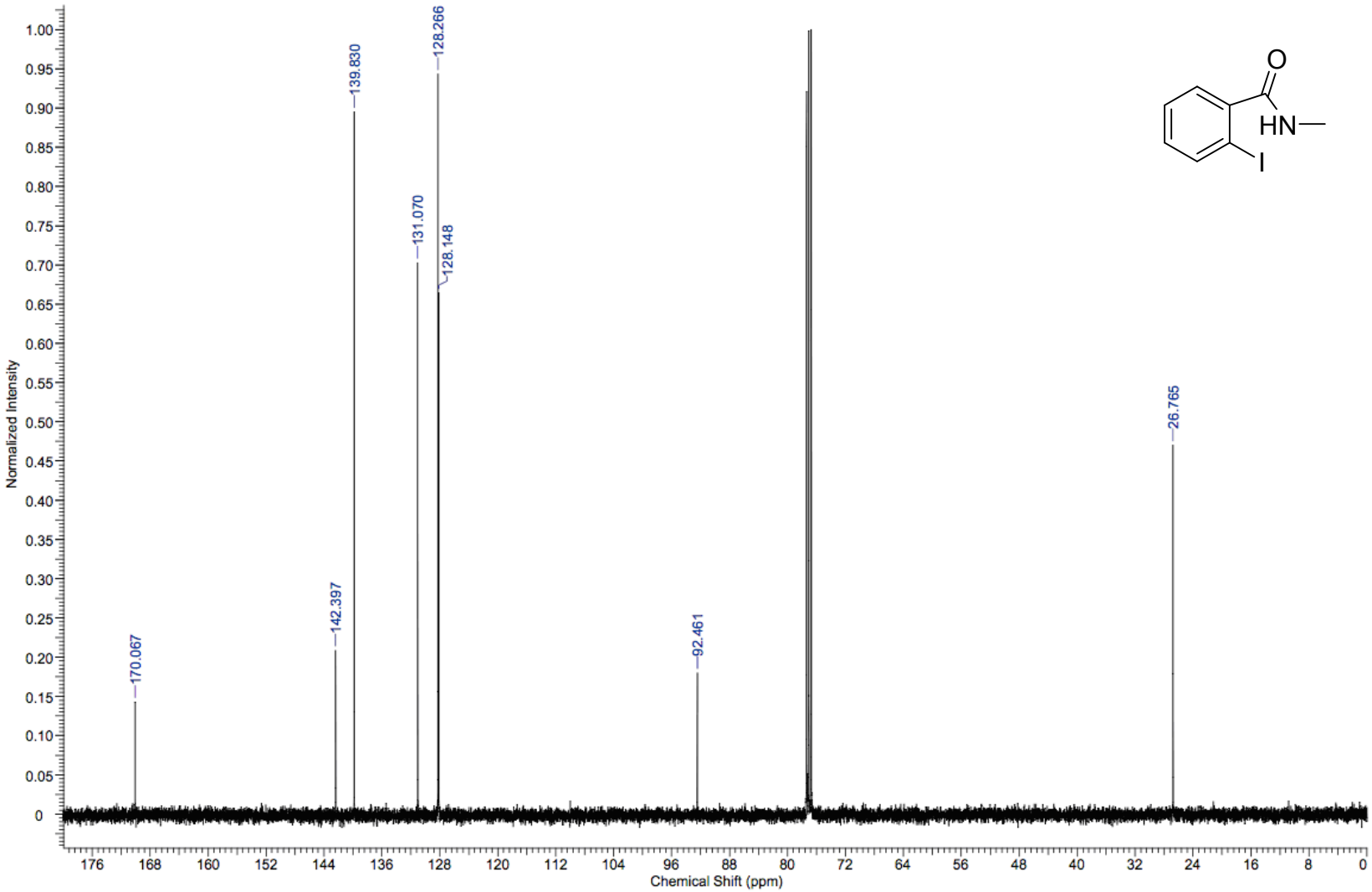
Table 1. Reactivity of the tested „ebselen-like“ catalysts

VI. NMR spectra

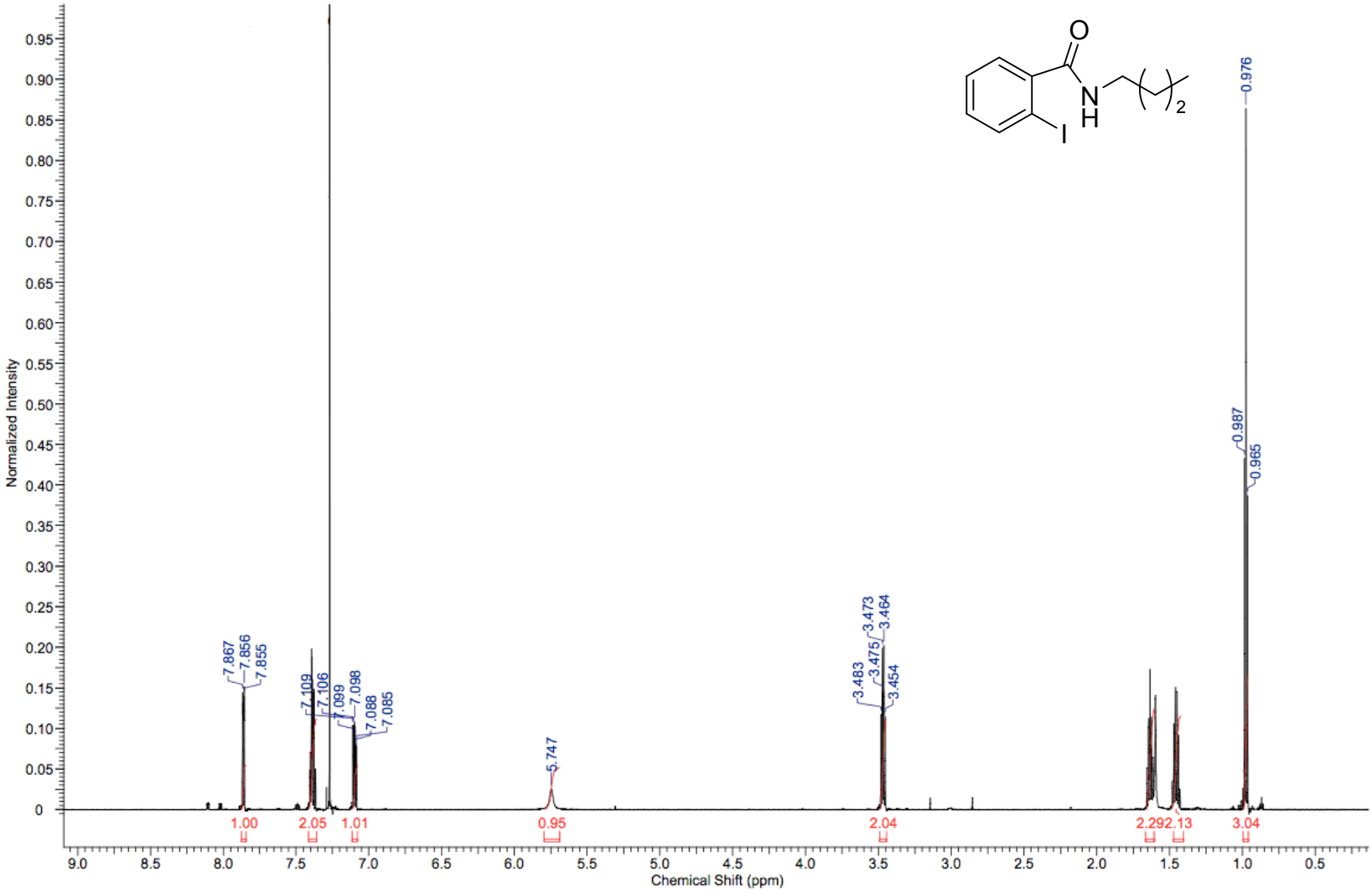
N-methyl-*o*-iodobenzamide (9a)



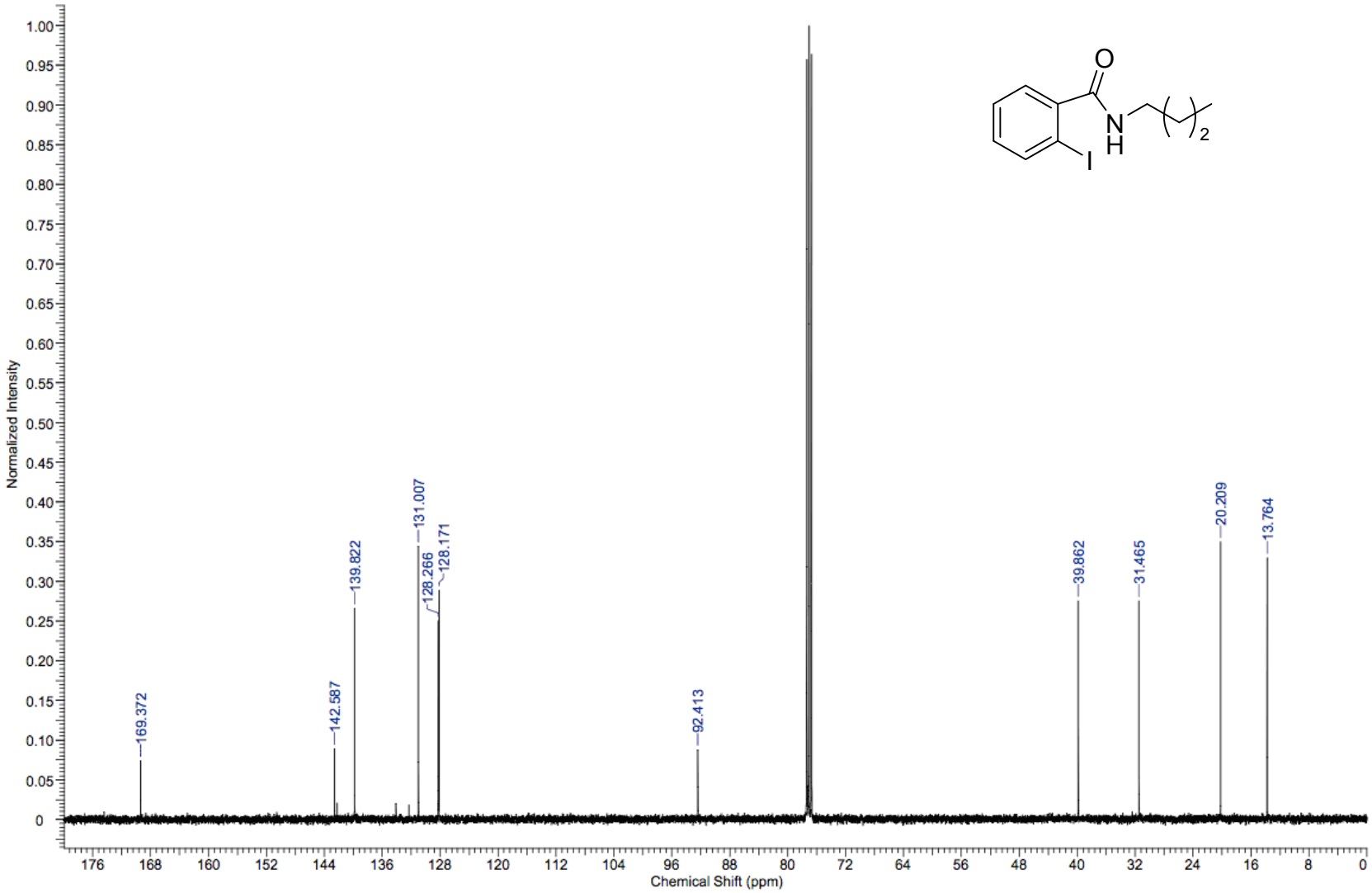
_N_-methyl-_o_-iodobenzamide (9a)



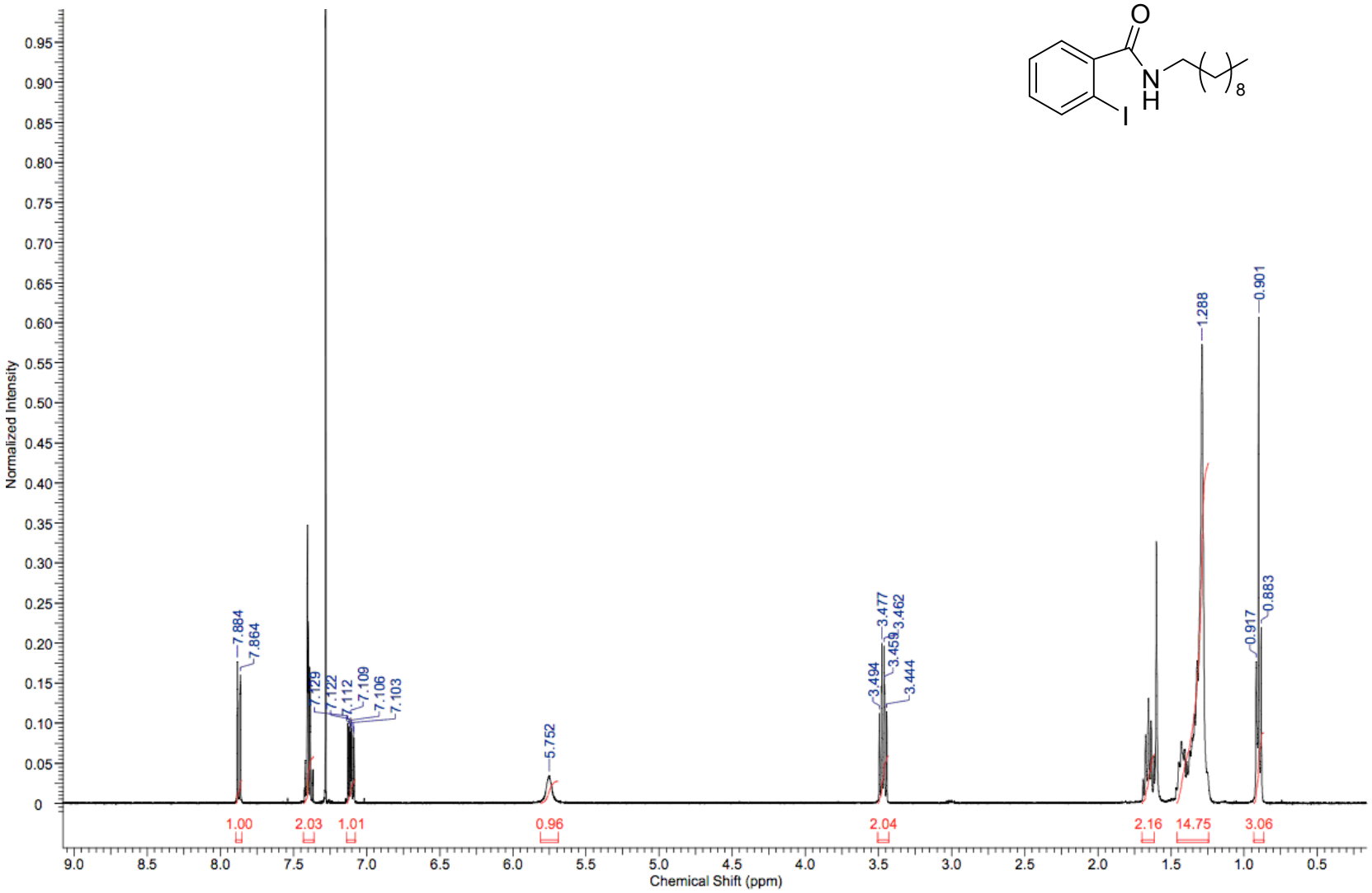
_N_-butyl-_o_-iodobenzamide (10a)



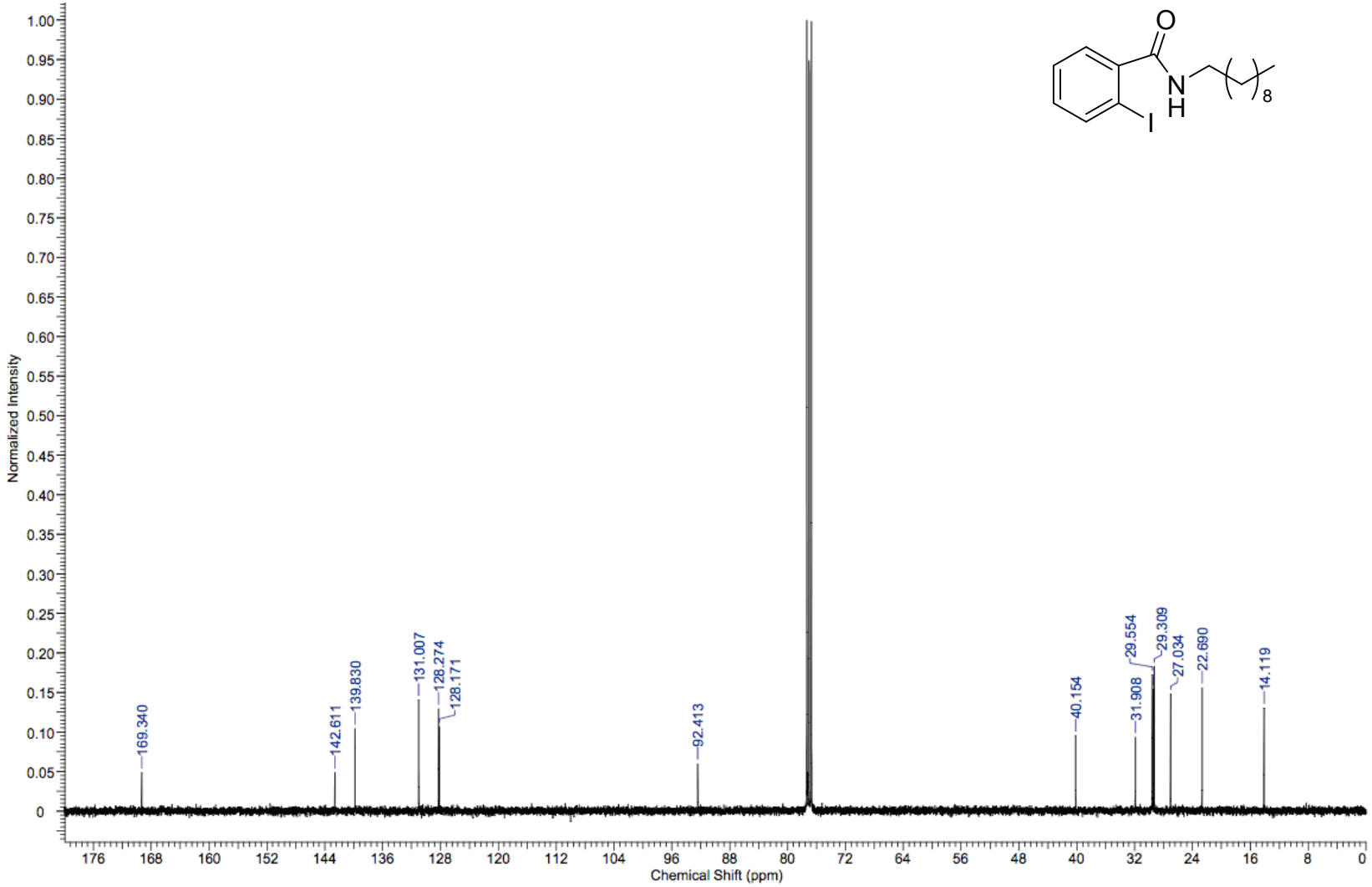
_N_-butyl-_o_-iodobenzamide (10a)



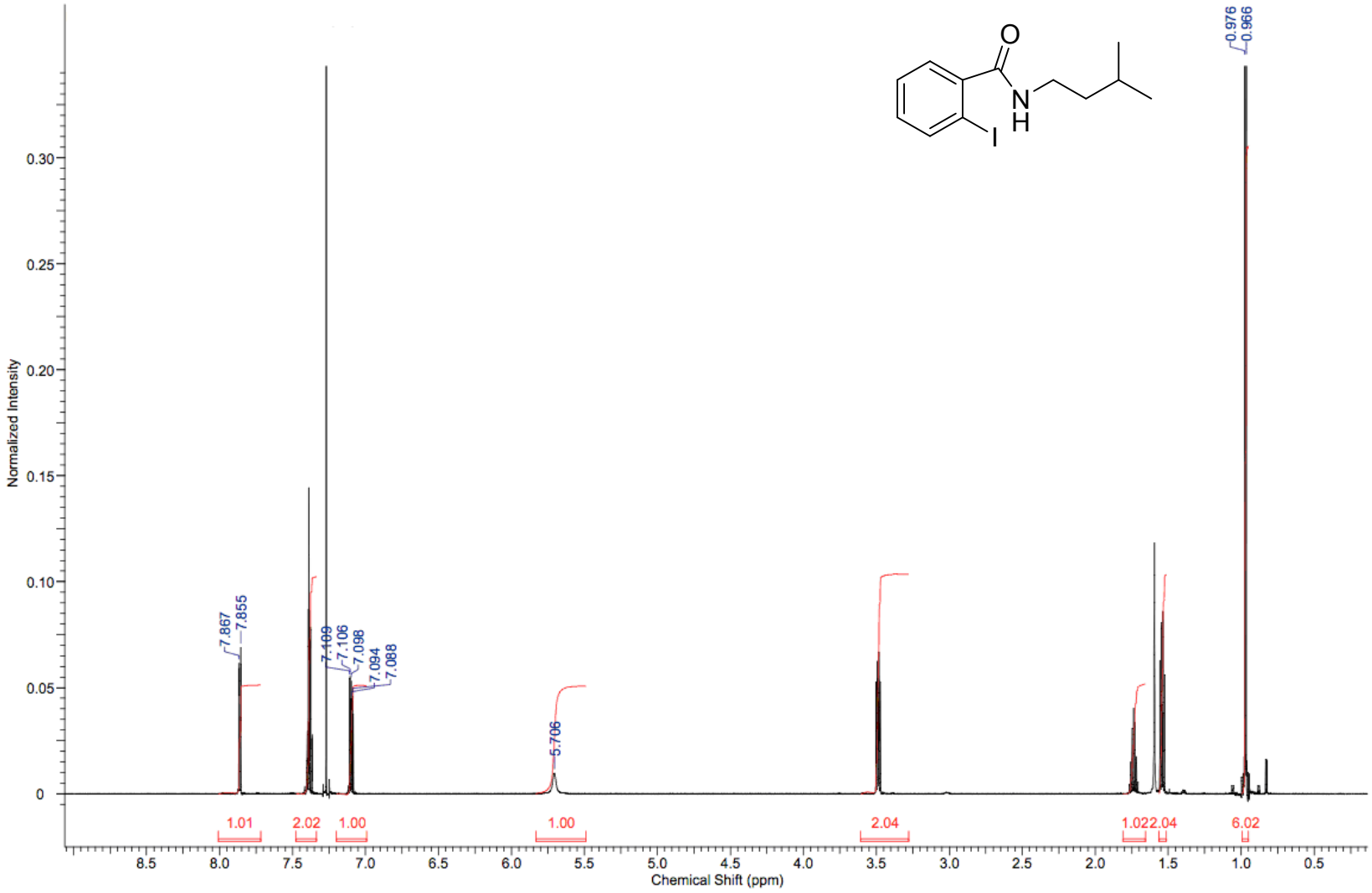
_N_-decyl-_o_-iodobenzamide (11a)



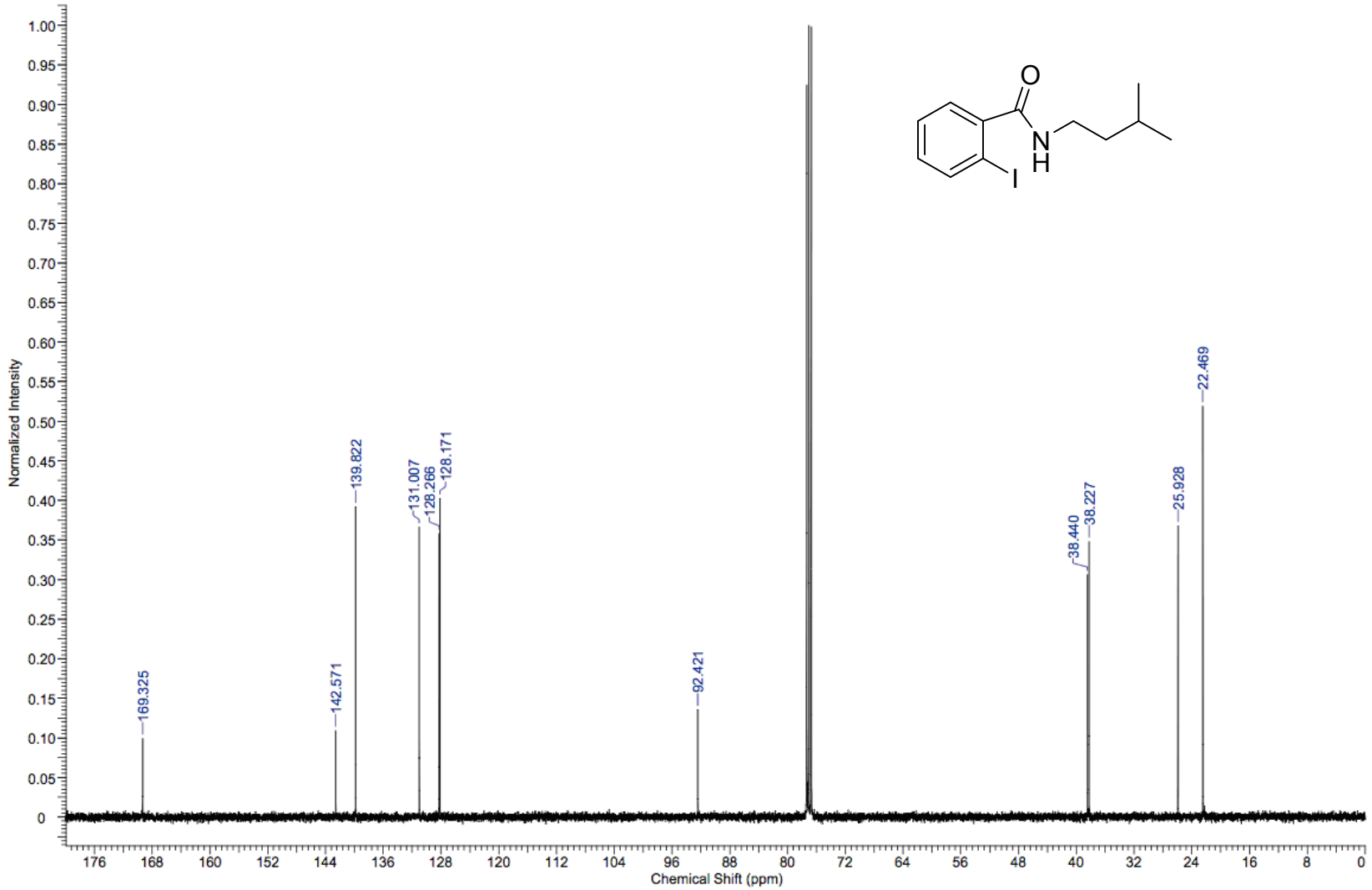
_N_-decyl-_o_-iodobenzamide (11a)



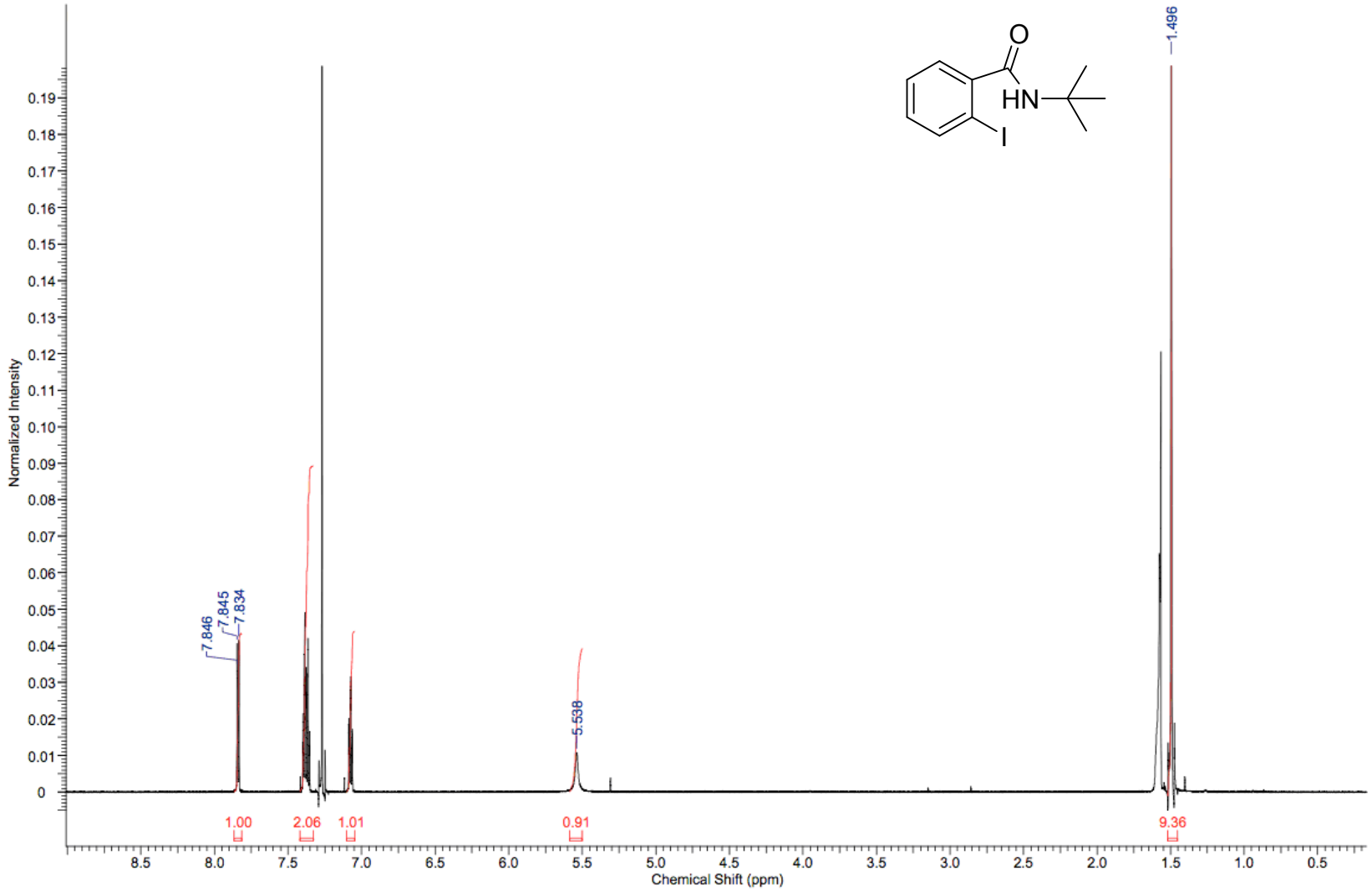
***N*-(3-methylbutyl)-*o*-iodobenzamide (12a)**



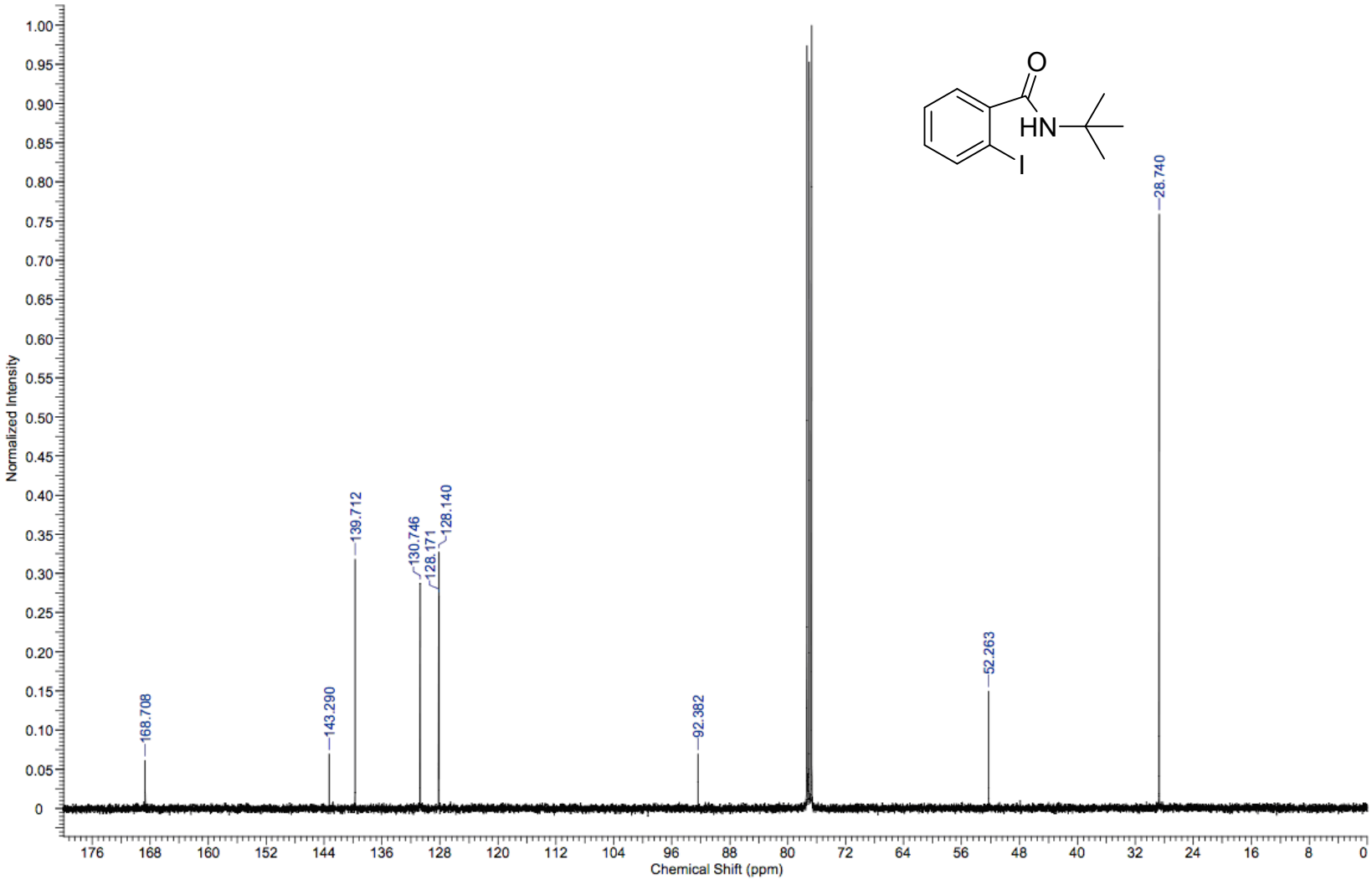
***N*-(3-methylbutyl)-*o*-iodobenzamide (12a)**



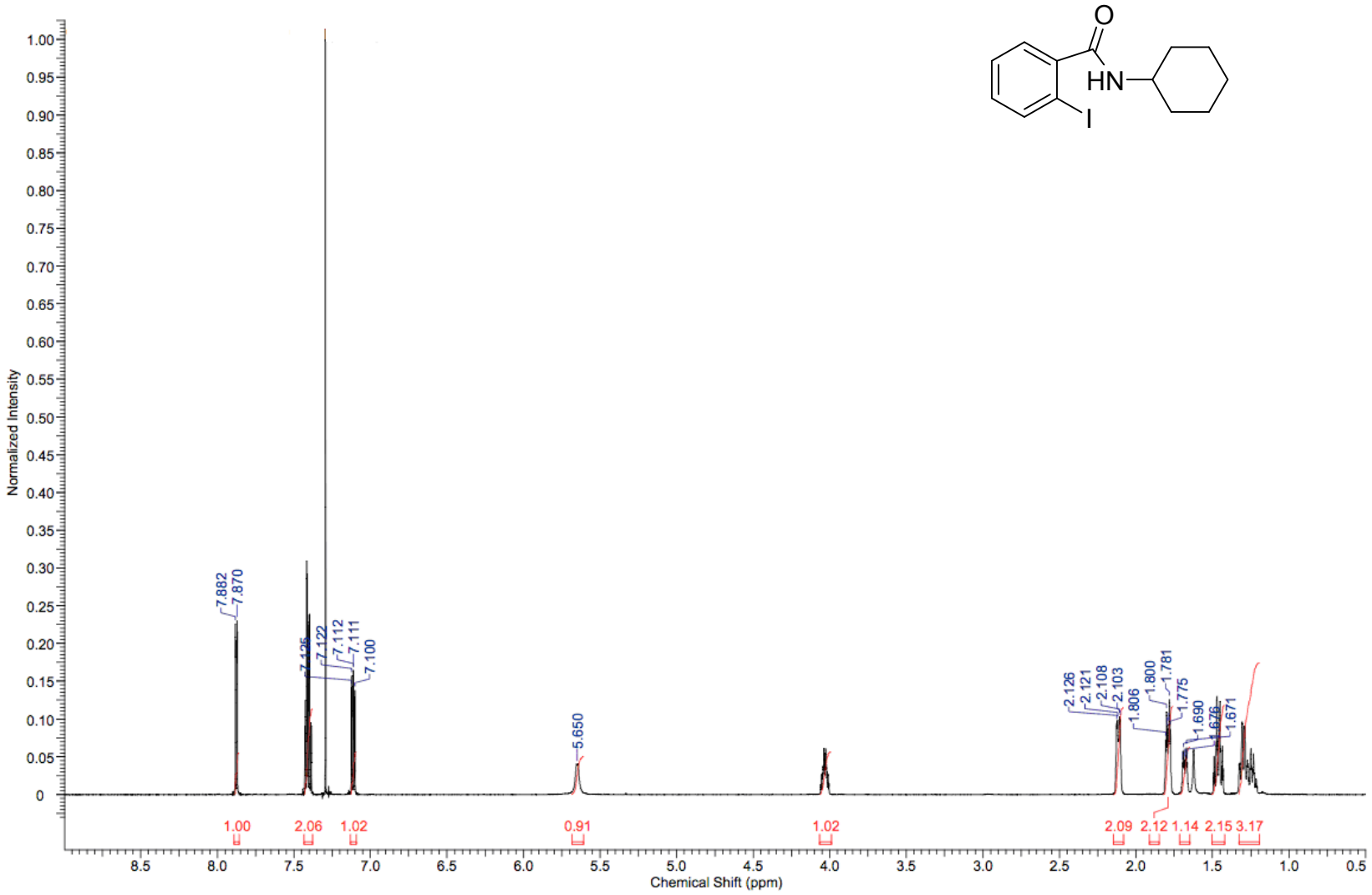
***N*-*tert*-butyl-*o*-iodobenzamide (13a)**



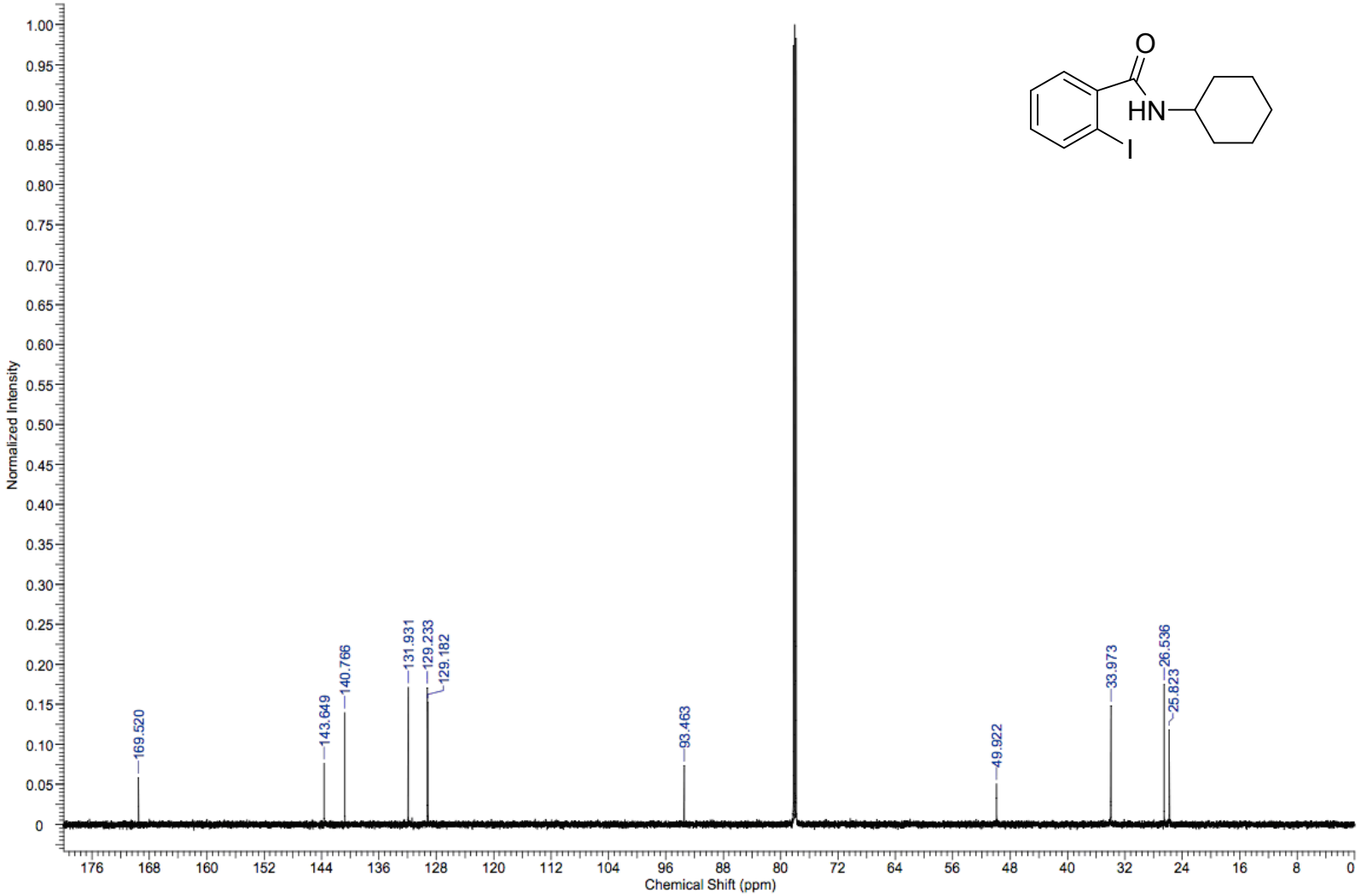
***N*-*tert*-butyl-*o*-iodobenzamide (13a)**



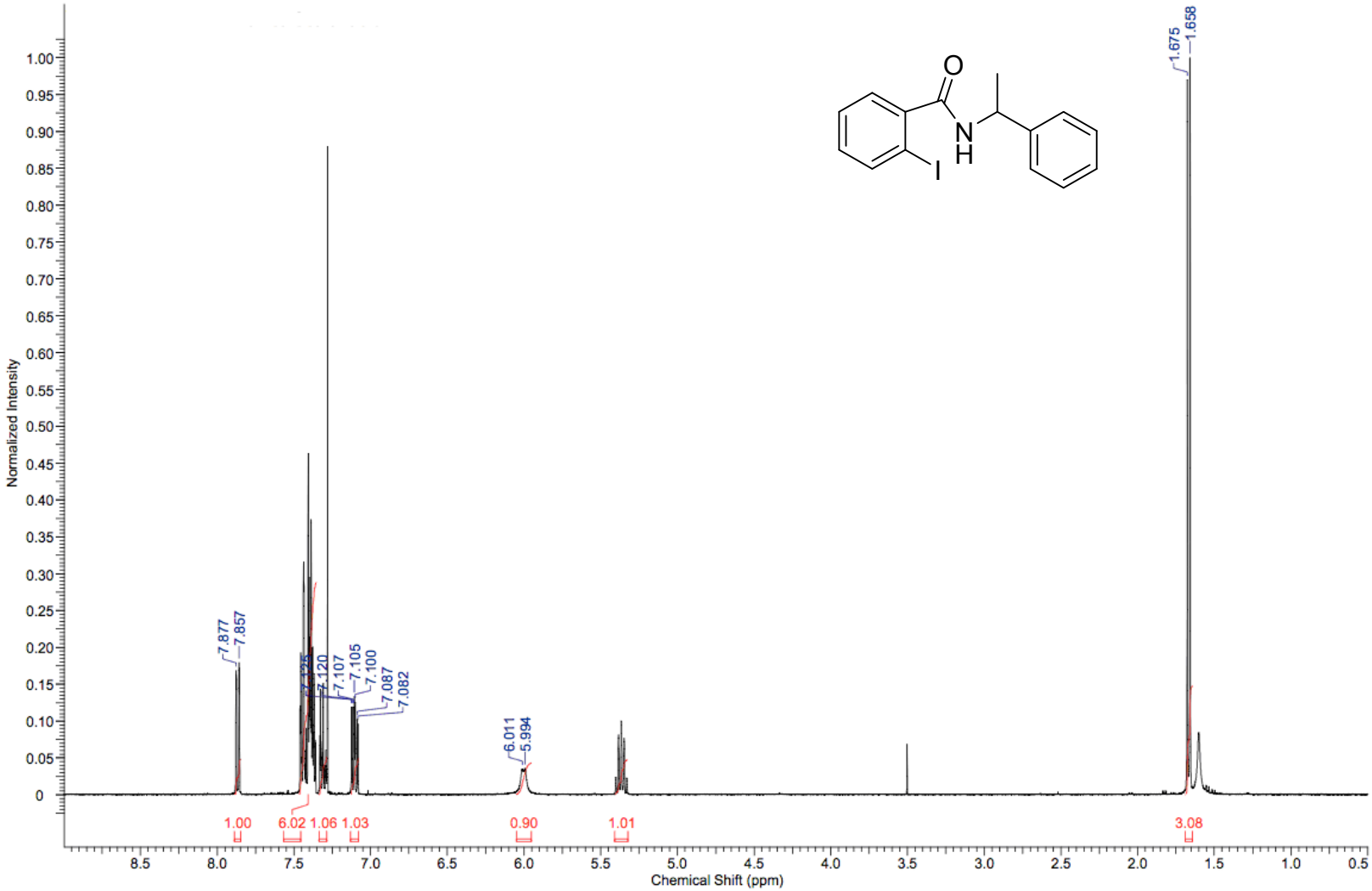
***N*-cyclohexyl-*o*-iodobenzamide (8a)**



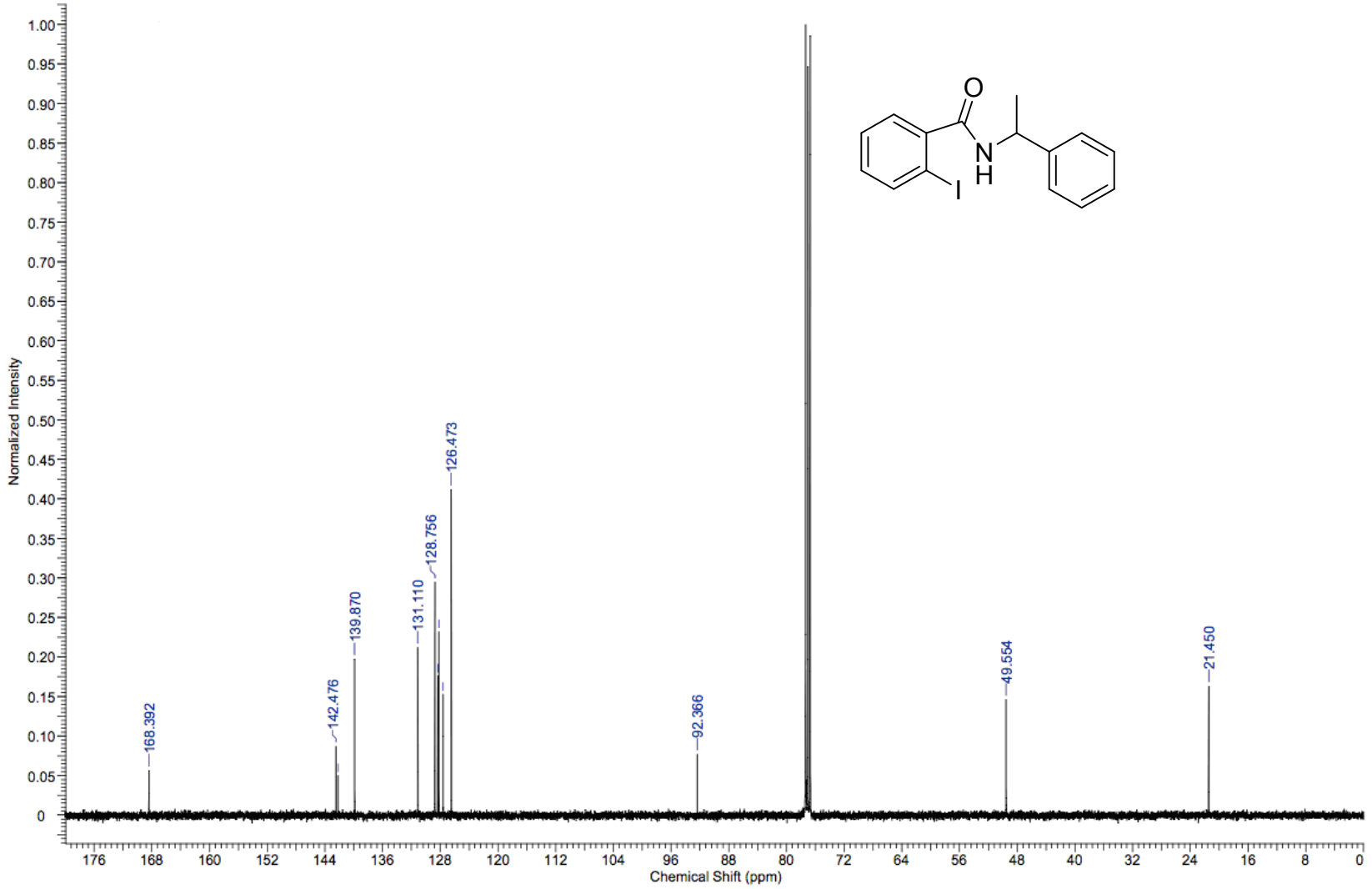
_N_-cyclohexyl-_o_-iodobenzamide (8a)



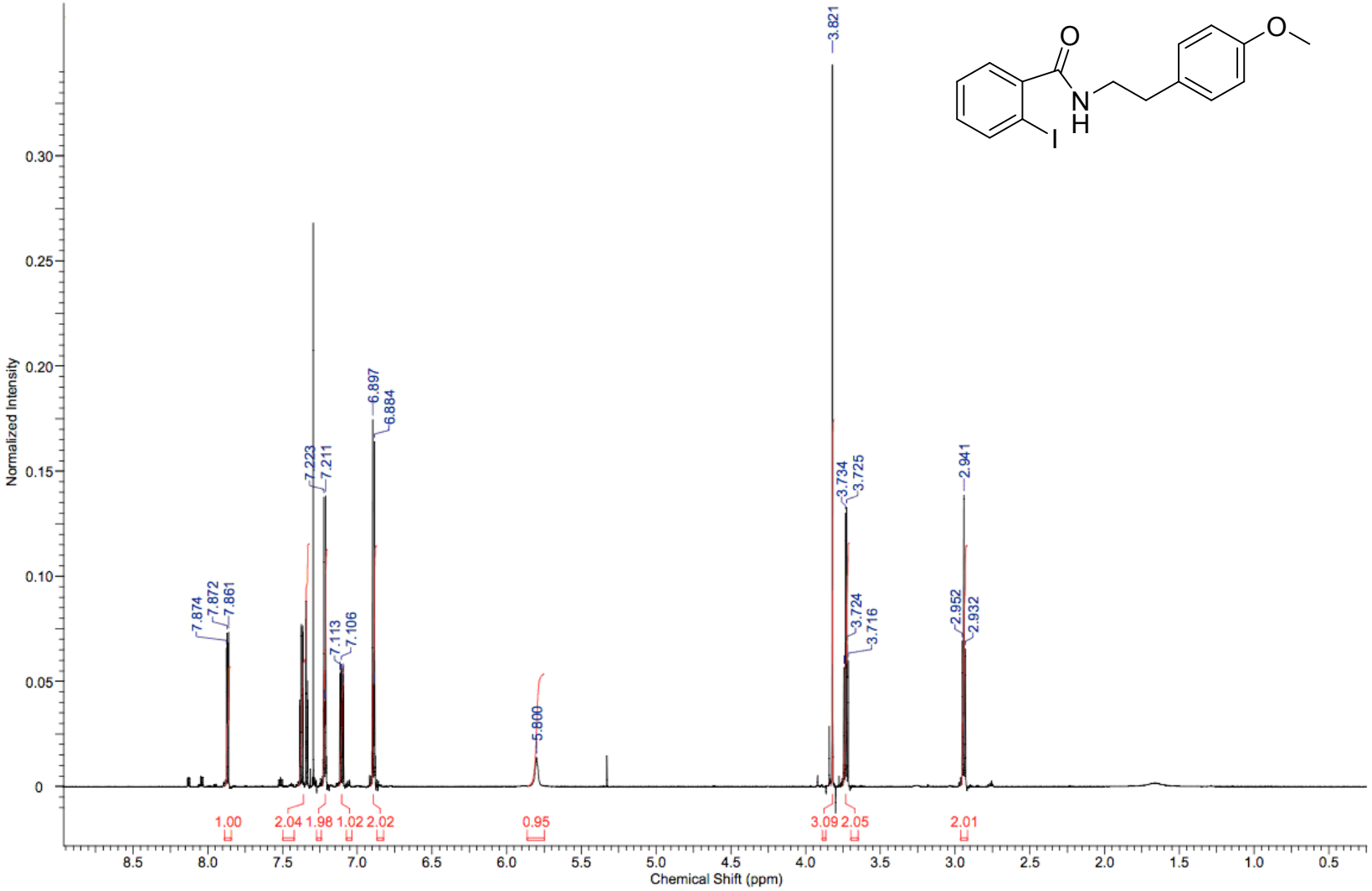
***N*-(1-phenylethyl)-*o*-iodobenzamide (14a)**



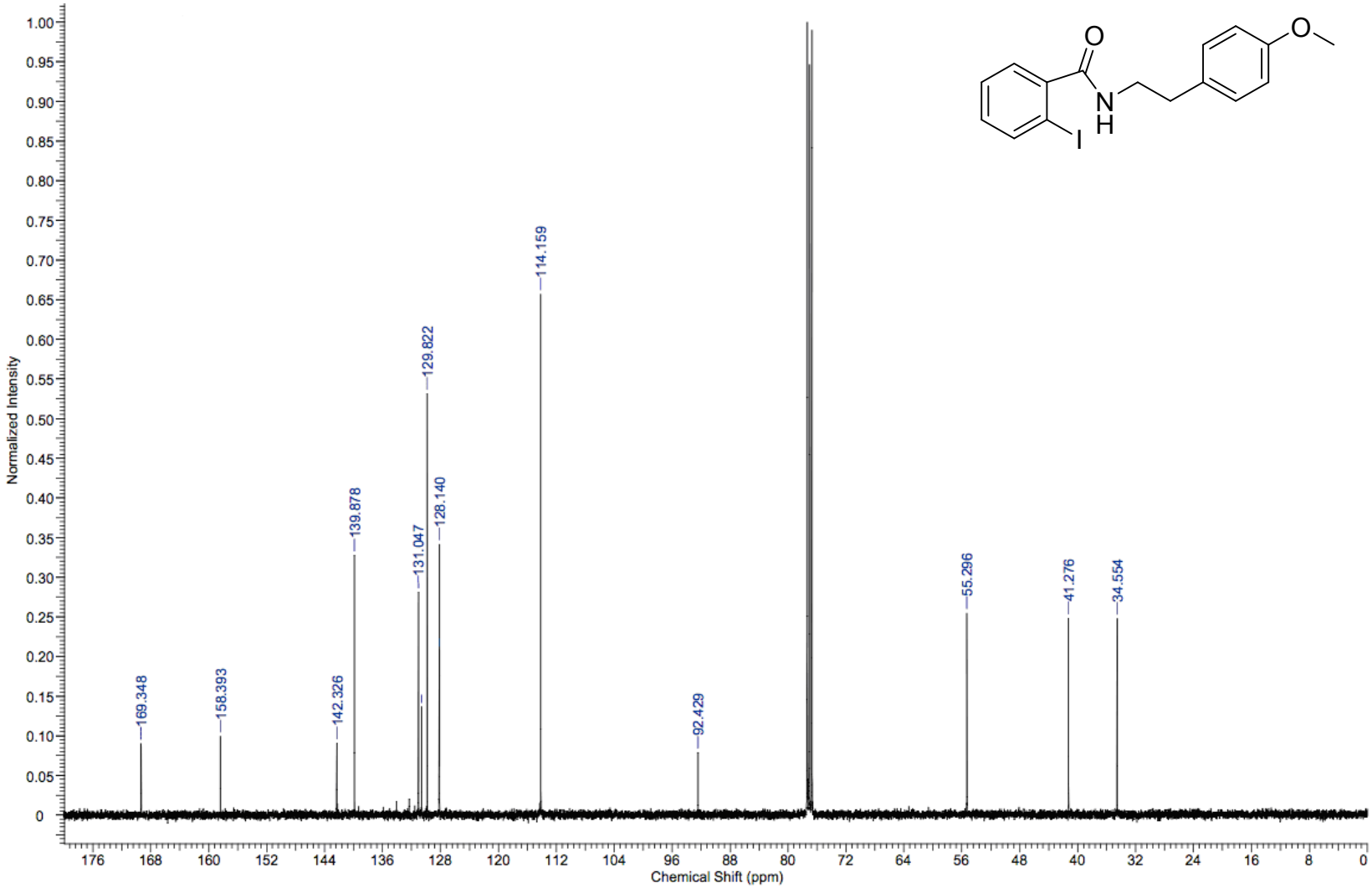
***N*-(1-phenylethyl)-*o*-iodobenzamide (14a)**



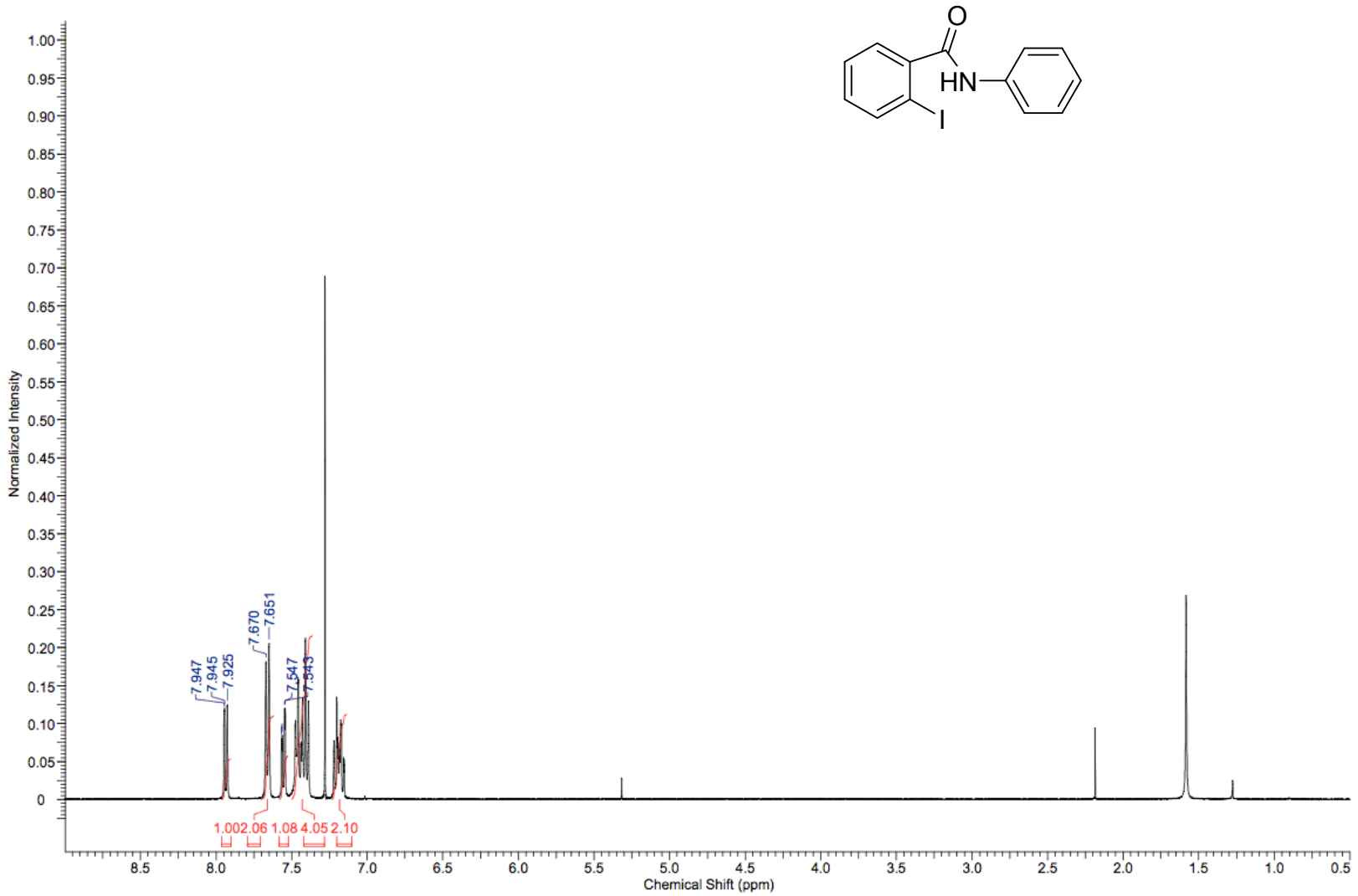
***N*-(2-(4-methoxyphenyl)ethyl)-*o*-iodobenzamide (15a)**



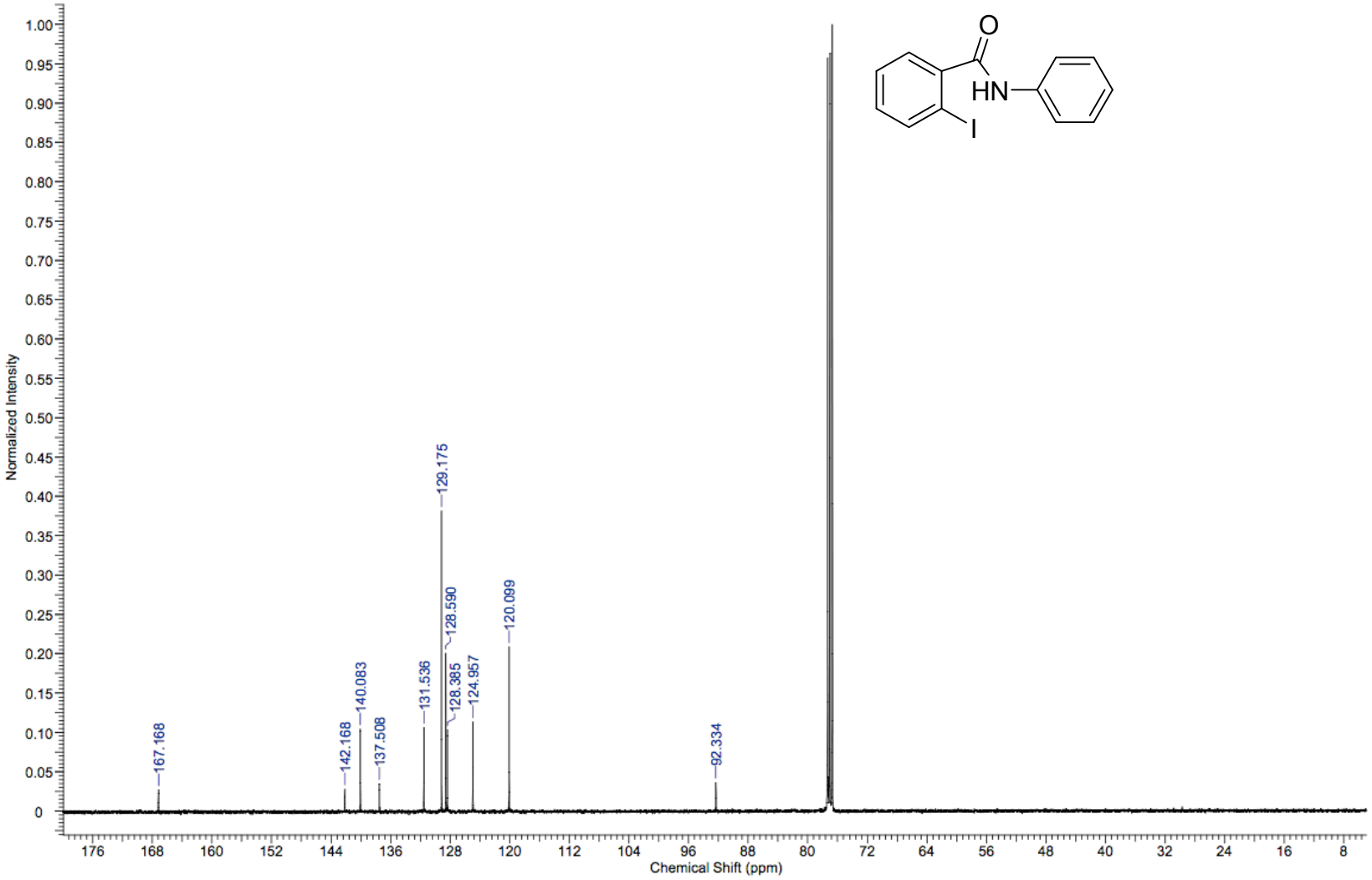
***N*-(2-(4-methoxyphenyl)ethyl)-*o*-iodobenzamide (15a)**



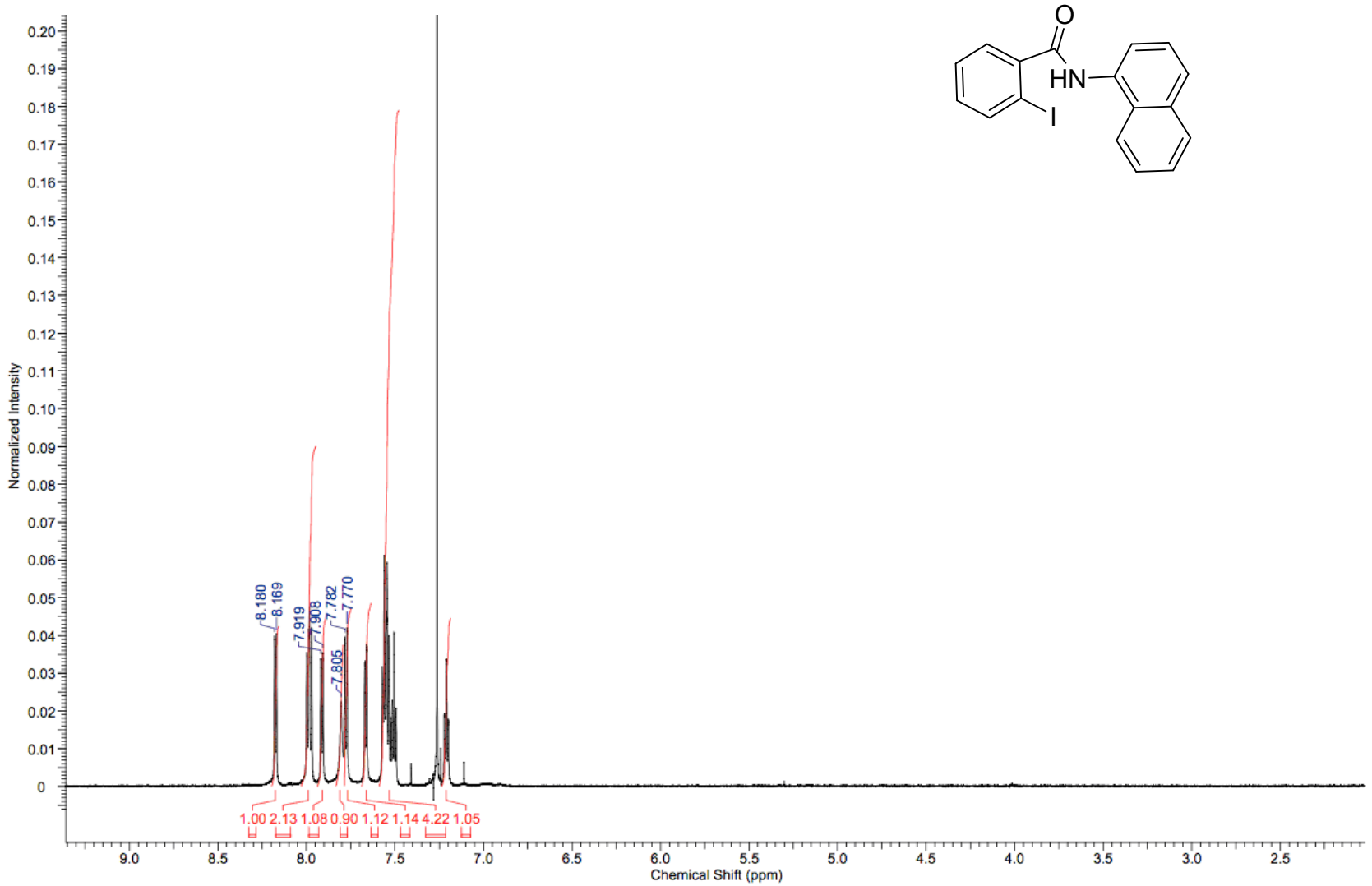
_N_-phenyl-_o_-iodobenzamide (1a)



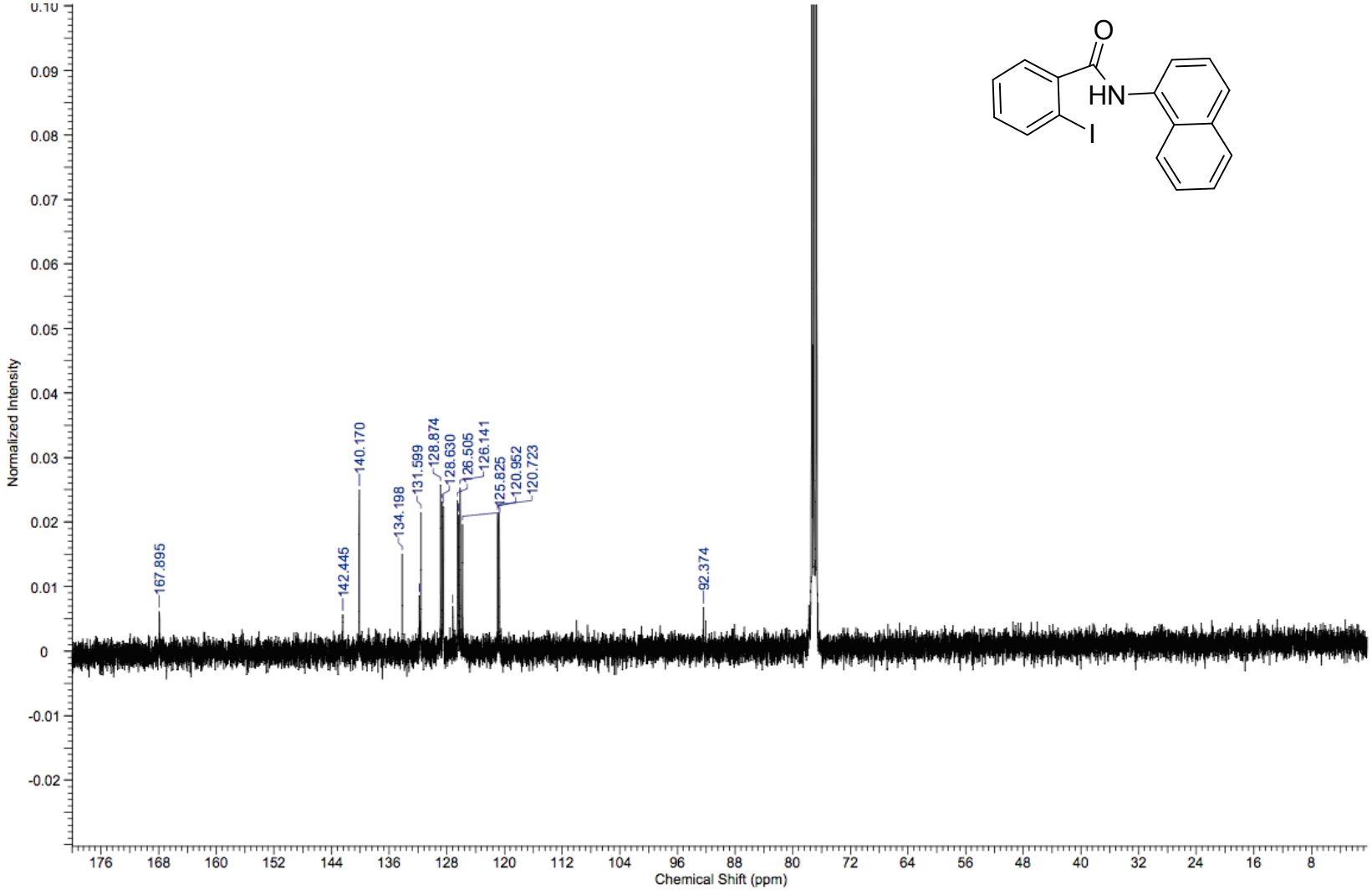
_N_-phenyl-_o_-iodobenzamide (1a)



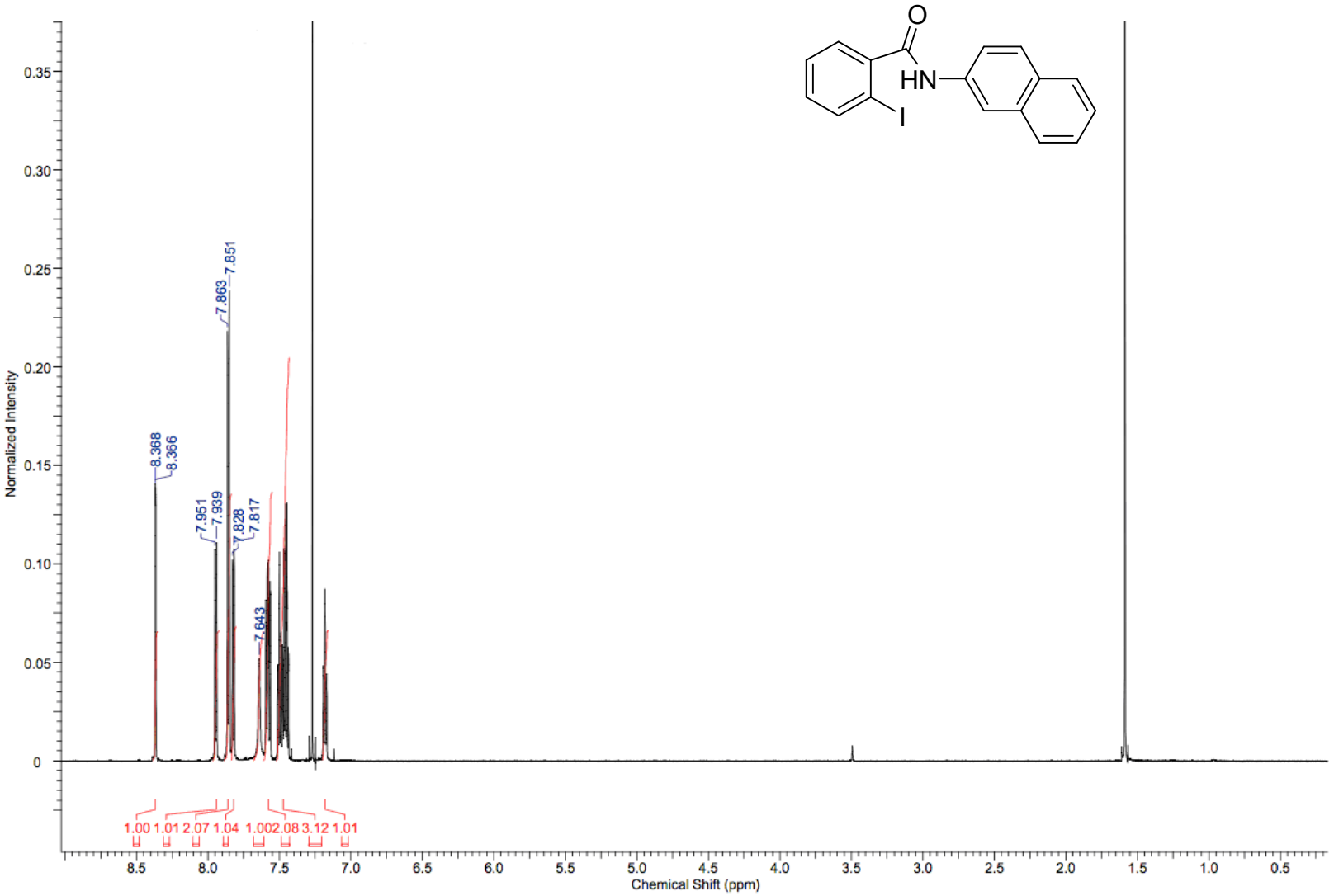
***N*-(1-naphthyl)-*o*-iodobenzamide (16a)**



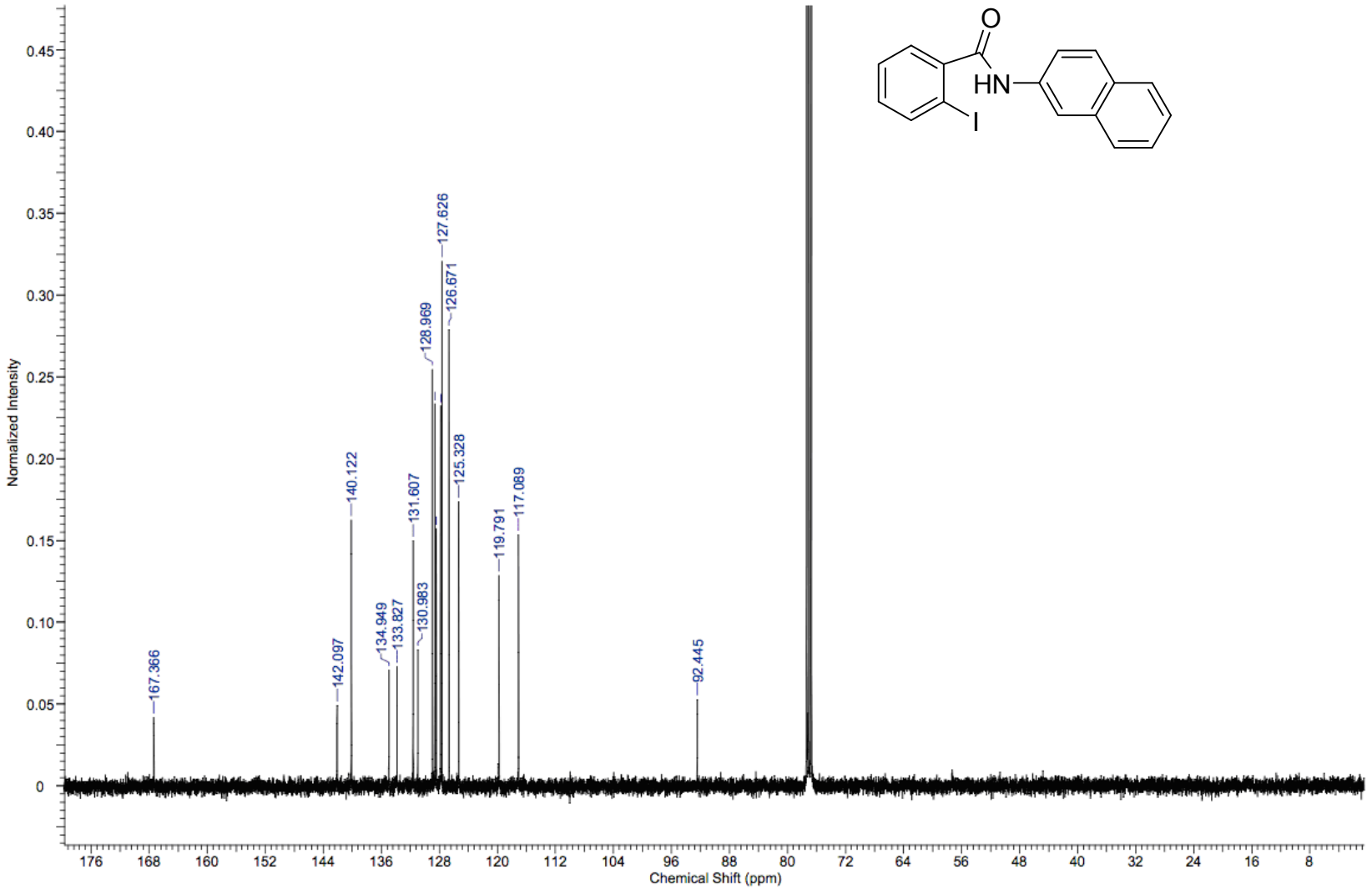
***N*-(1-naphthyl)-*o*-iodobenzamide (16a)**



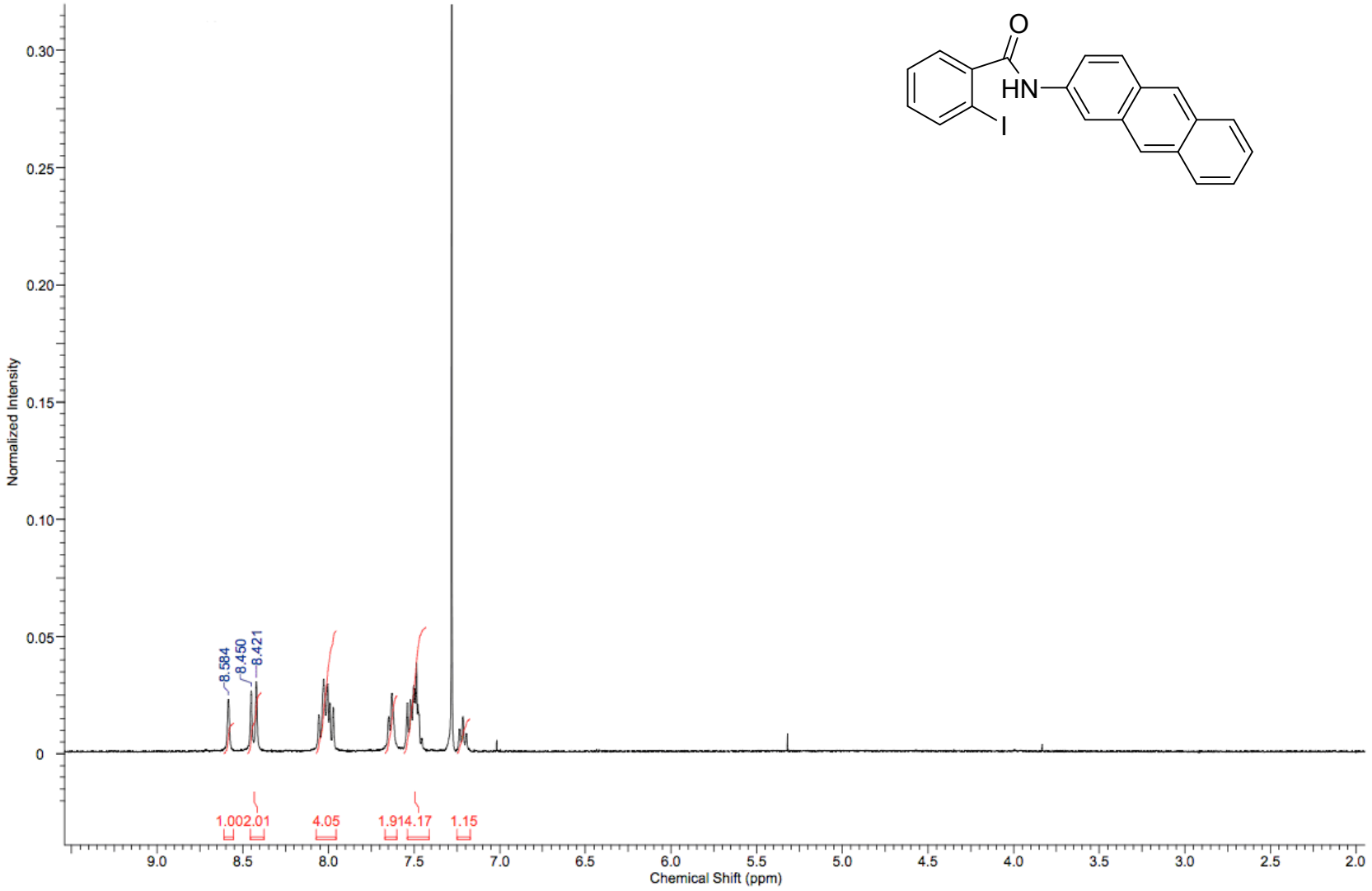
***N*-(2-naphthyl)-*o*-iodobenzamide (17a)**



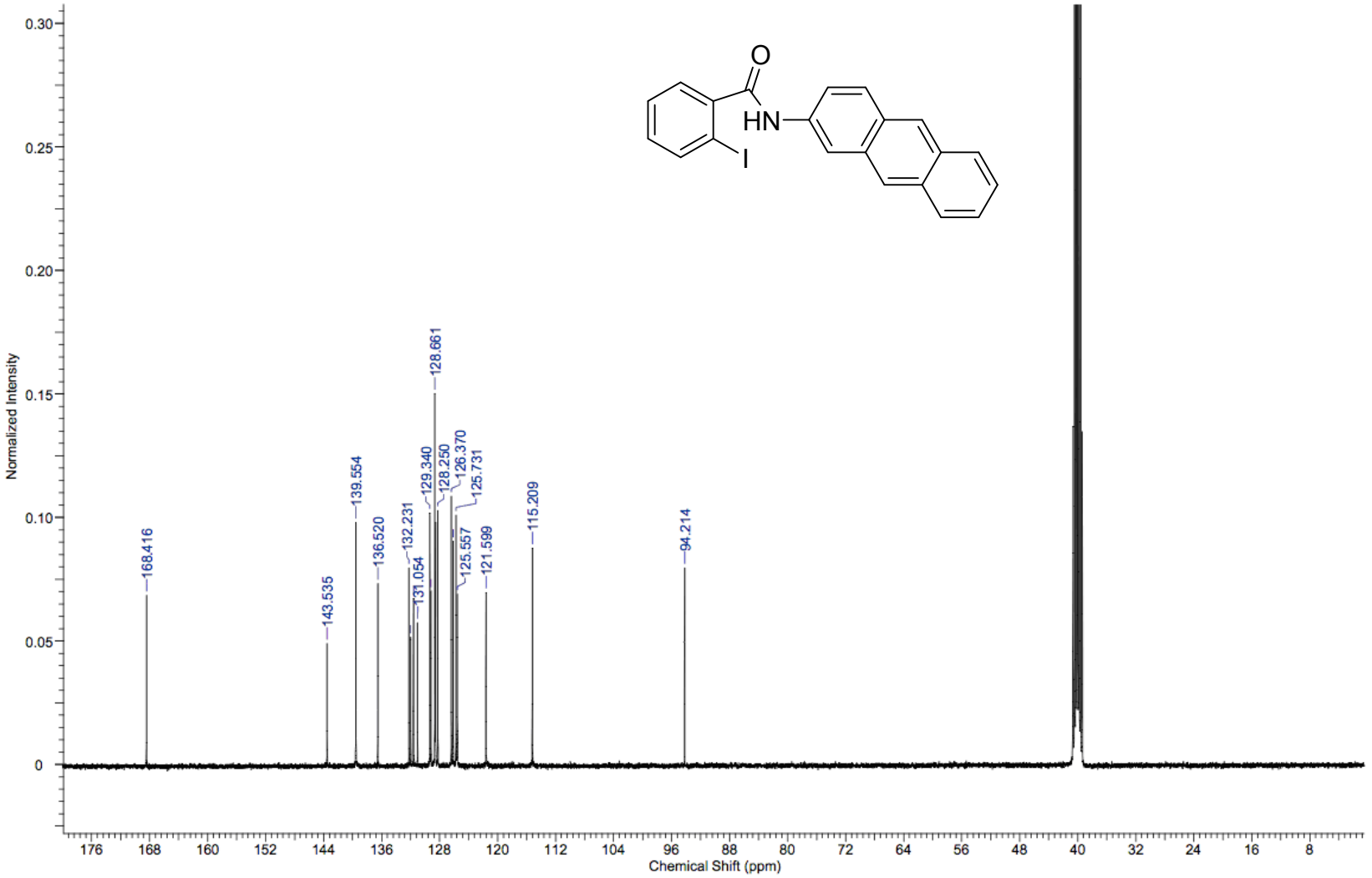
***N*-(2-naphthyl)-*o*-iodobenzamide (17a)**



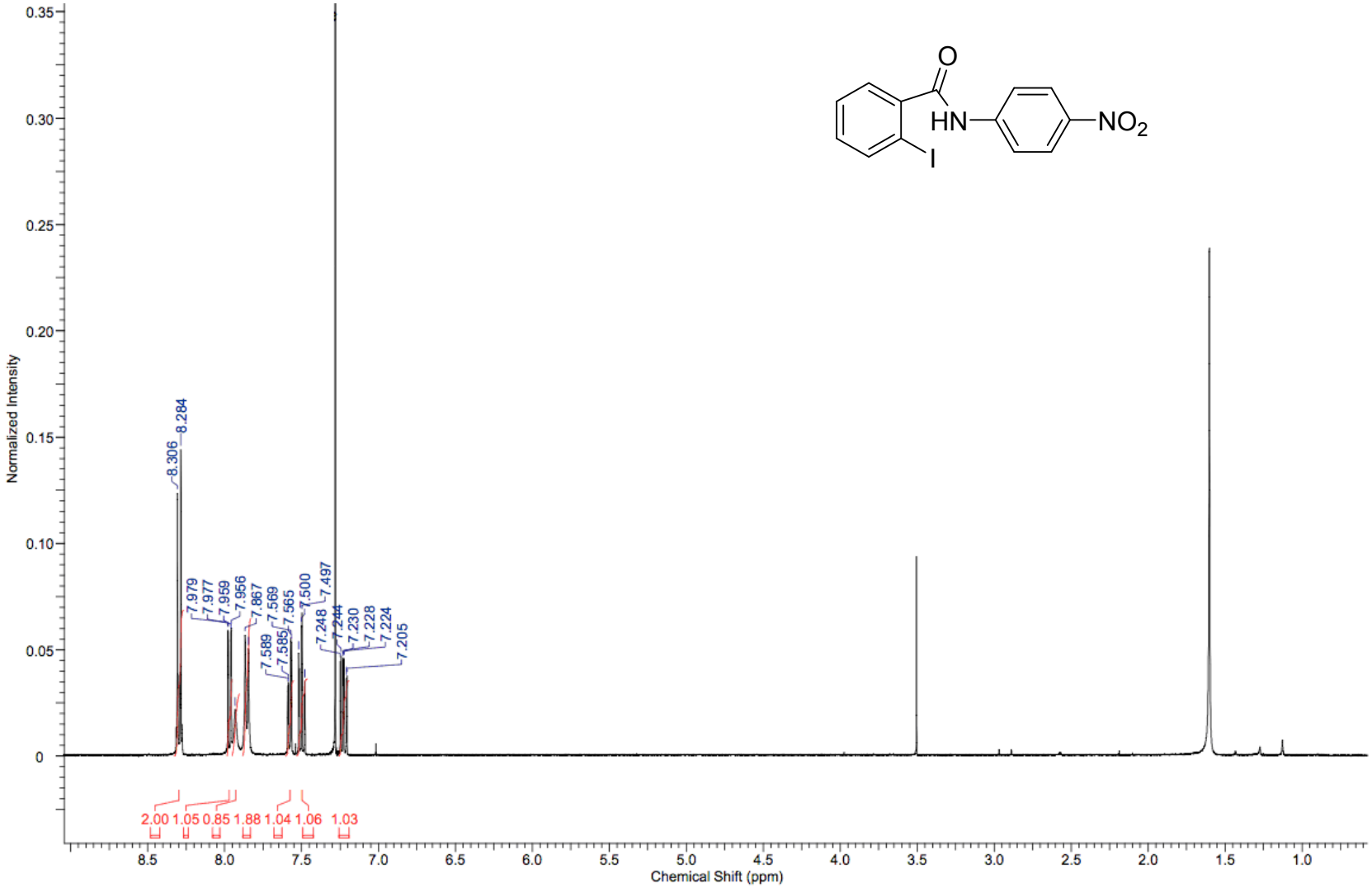
_N_-(2-antryl)-_o_-iodobenzamide (18a)



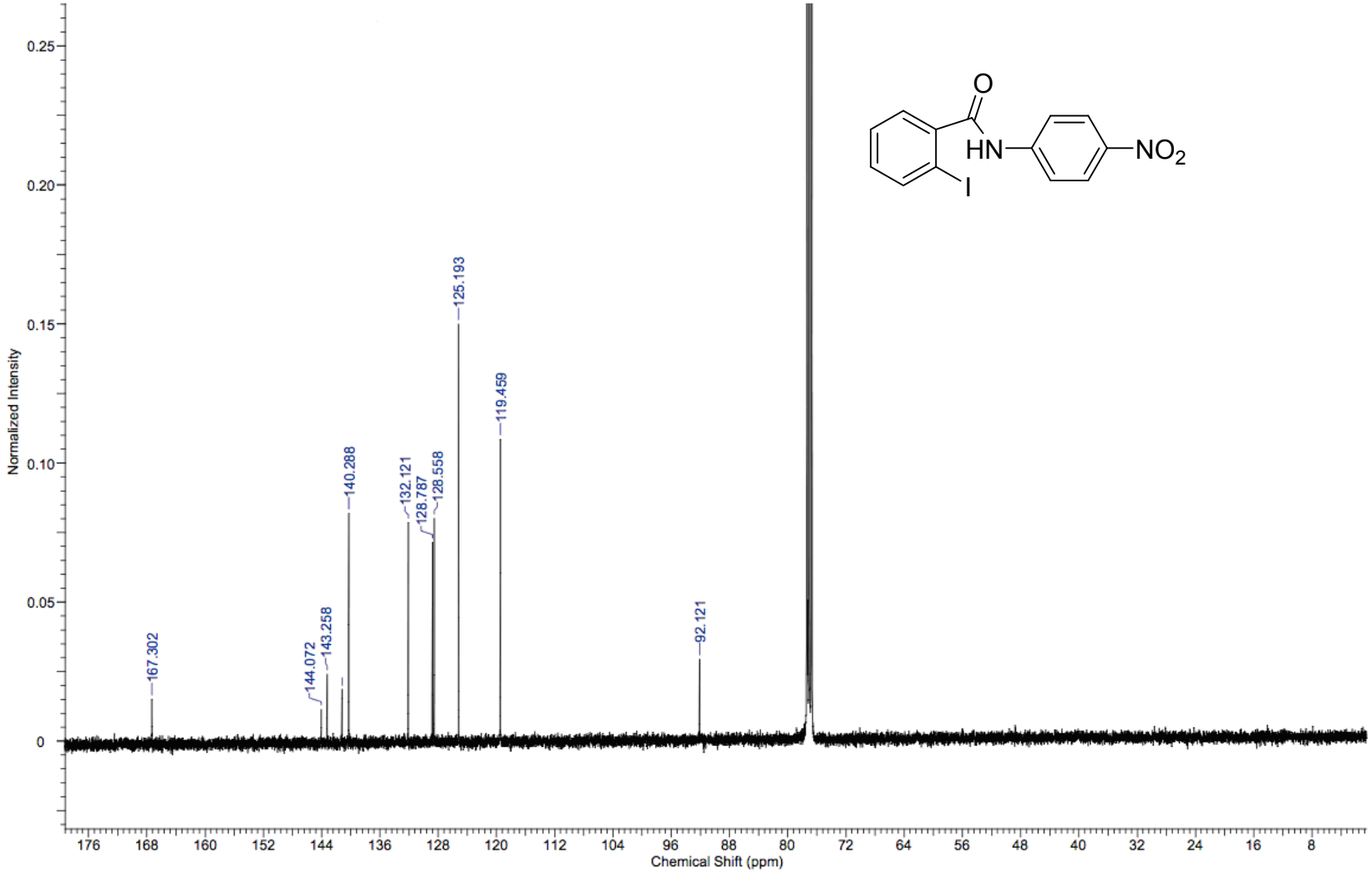
***N*-(2-antryl)-*o*-iodobenzamide (18a)**



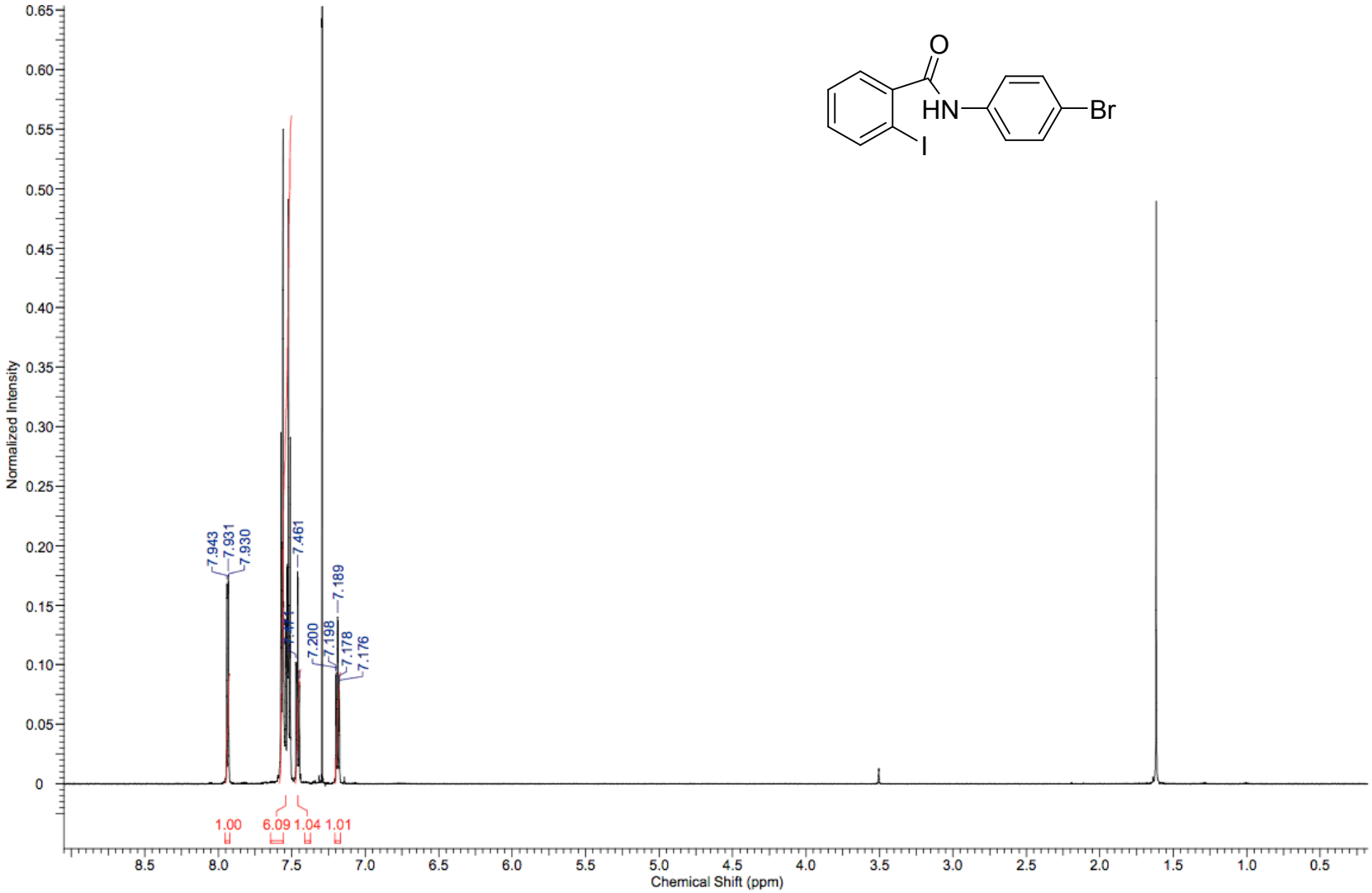
***N*-(4-nitrophenyl)-*o*-iodobenzamide (19a)**



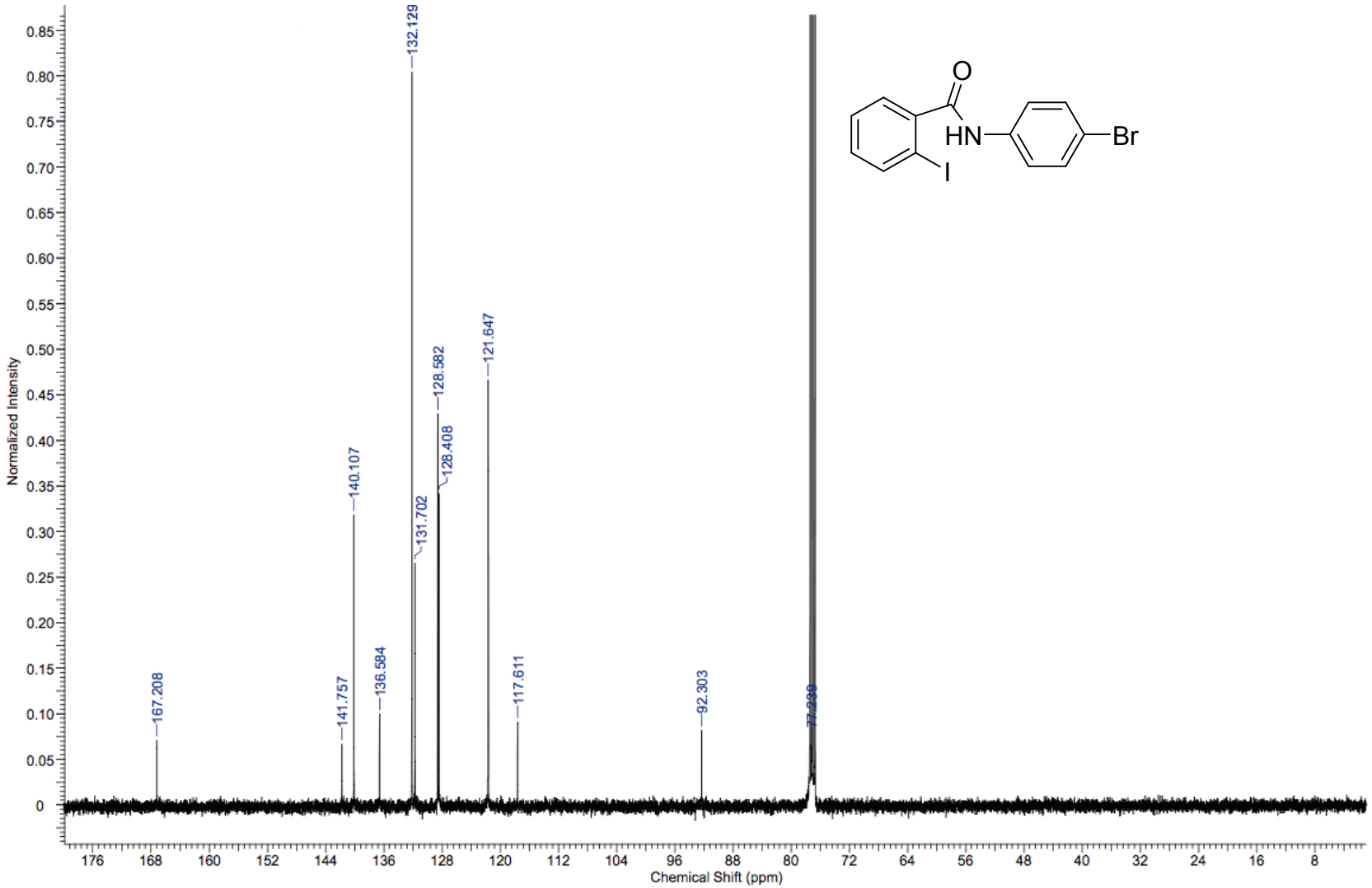
***N*-(4-nitrophenyl)-*o*-iodobenzamide (19a)**



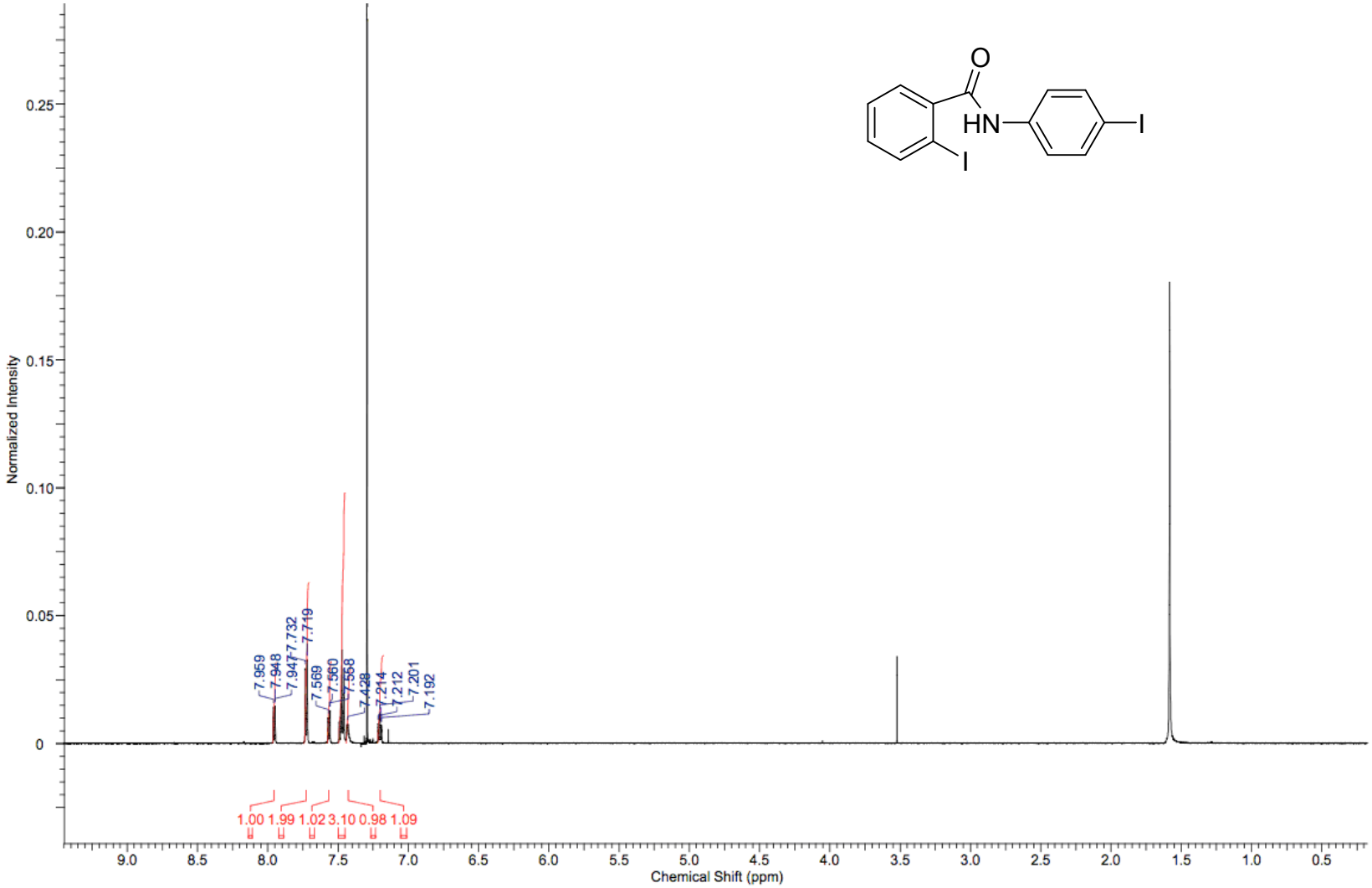
***N*-(4-bromophenyl)-*o*-iodobenzamide (20a)**



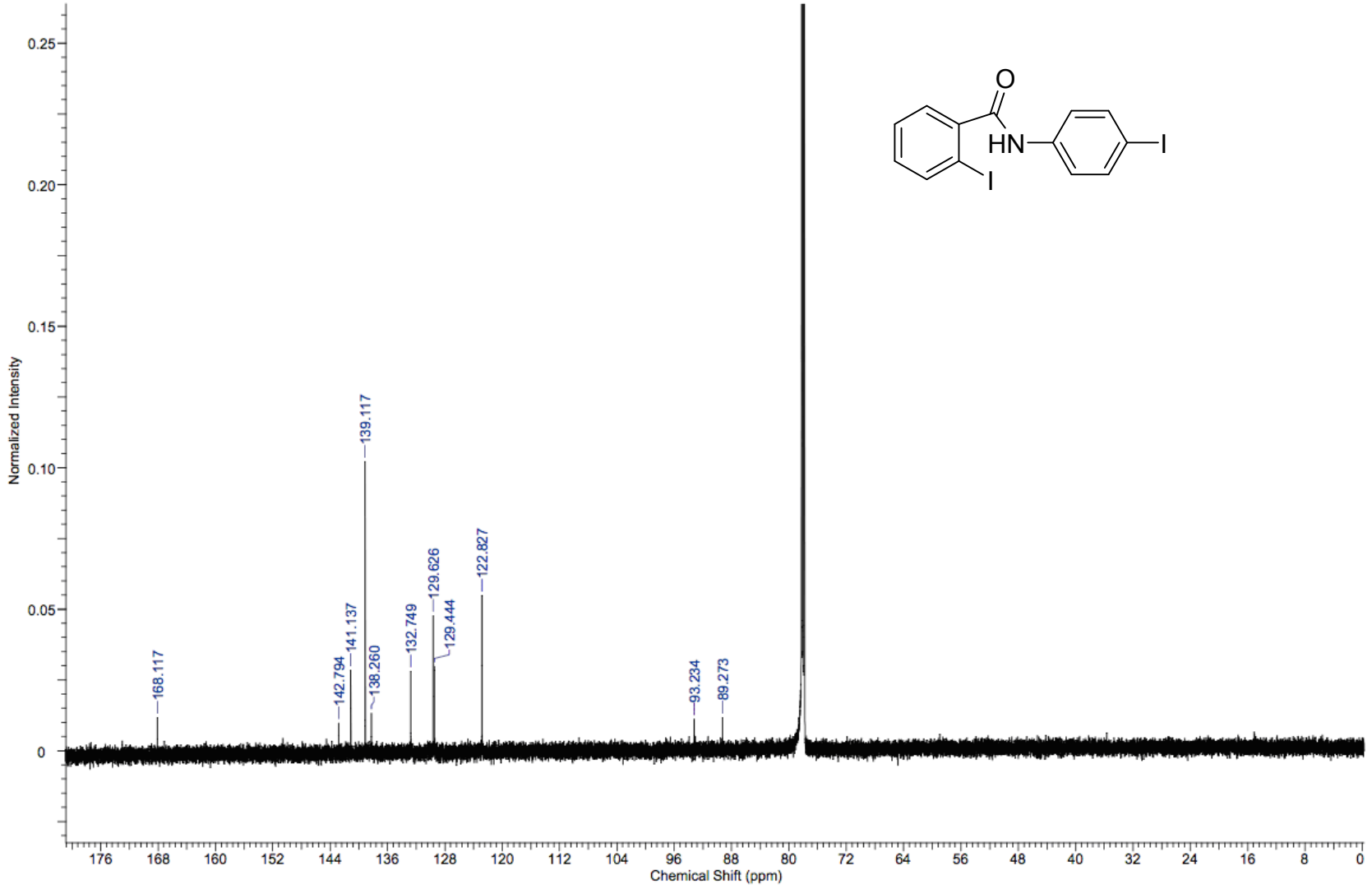
***N*-(4-bromophenyl)-*o*-iodobenzamide (20a)**



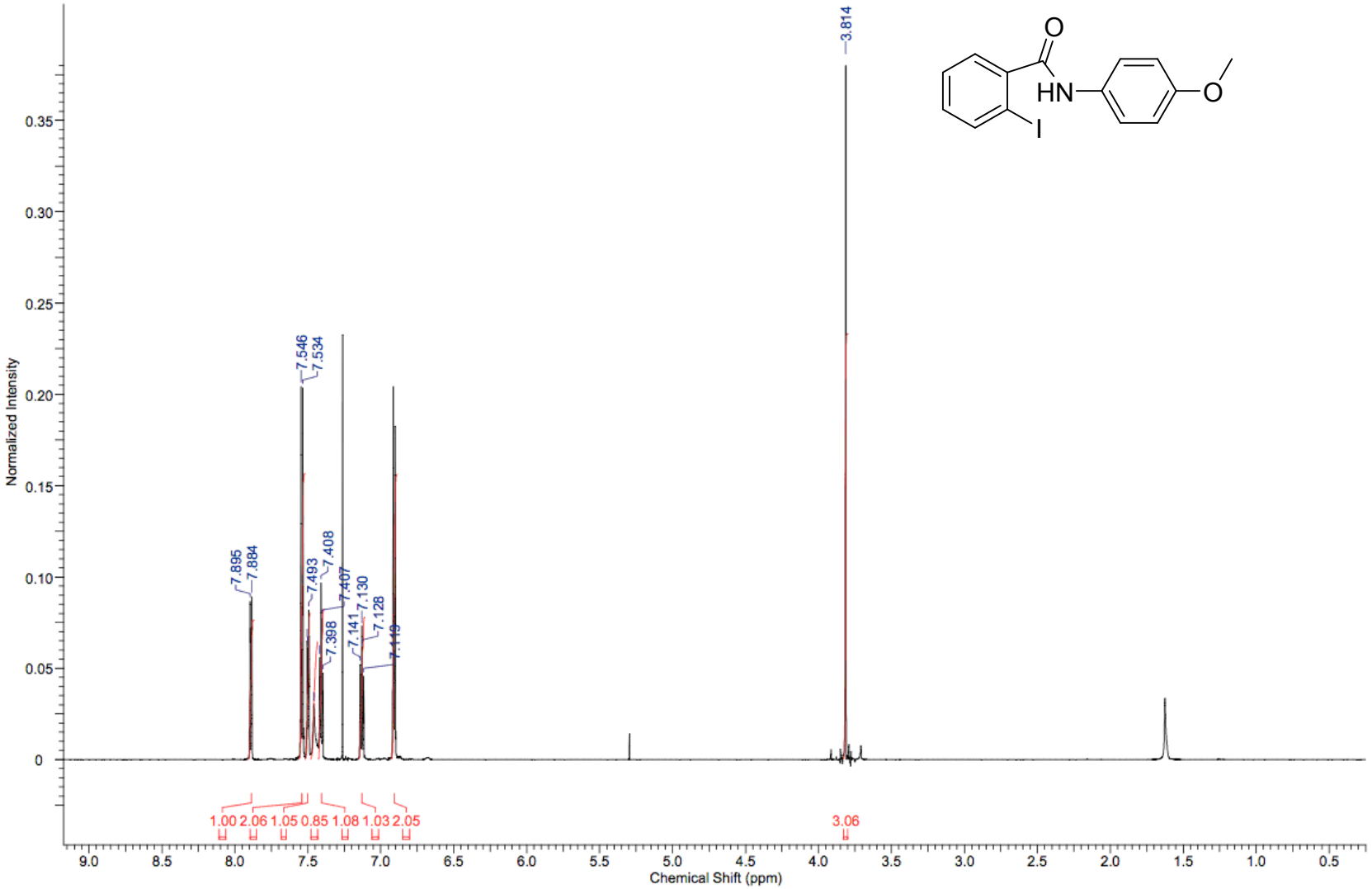
***N*-(4-jodophenyl)-*o*-iodobenzamide (21a)**



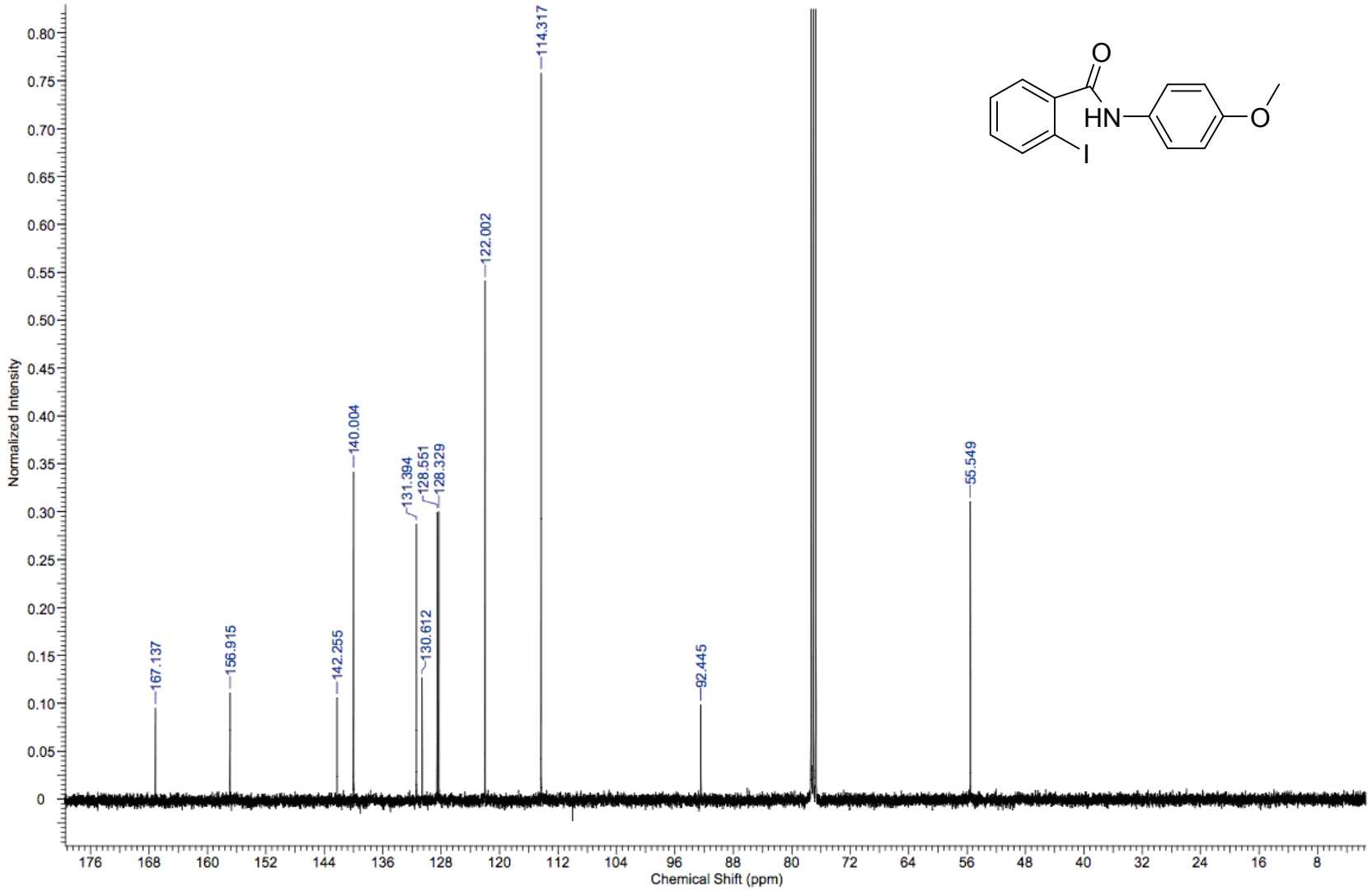
***N*-(4-jodophenyl)-*o*-iodobenzamide (21a)**



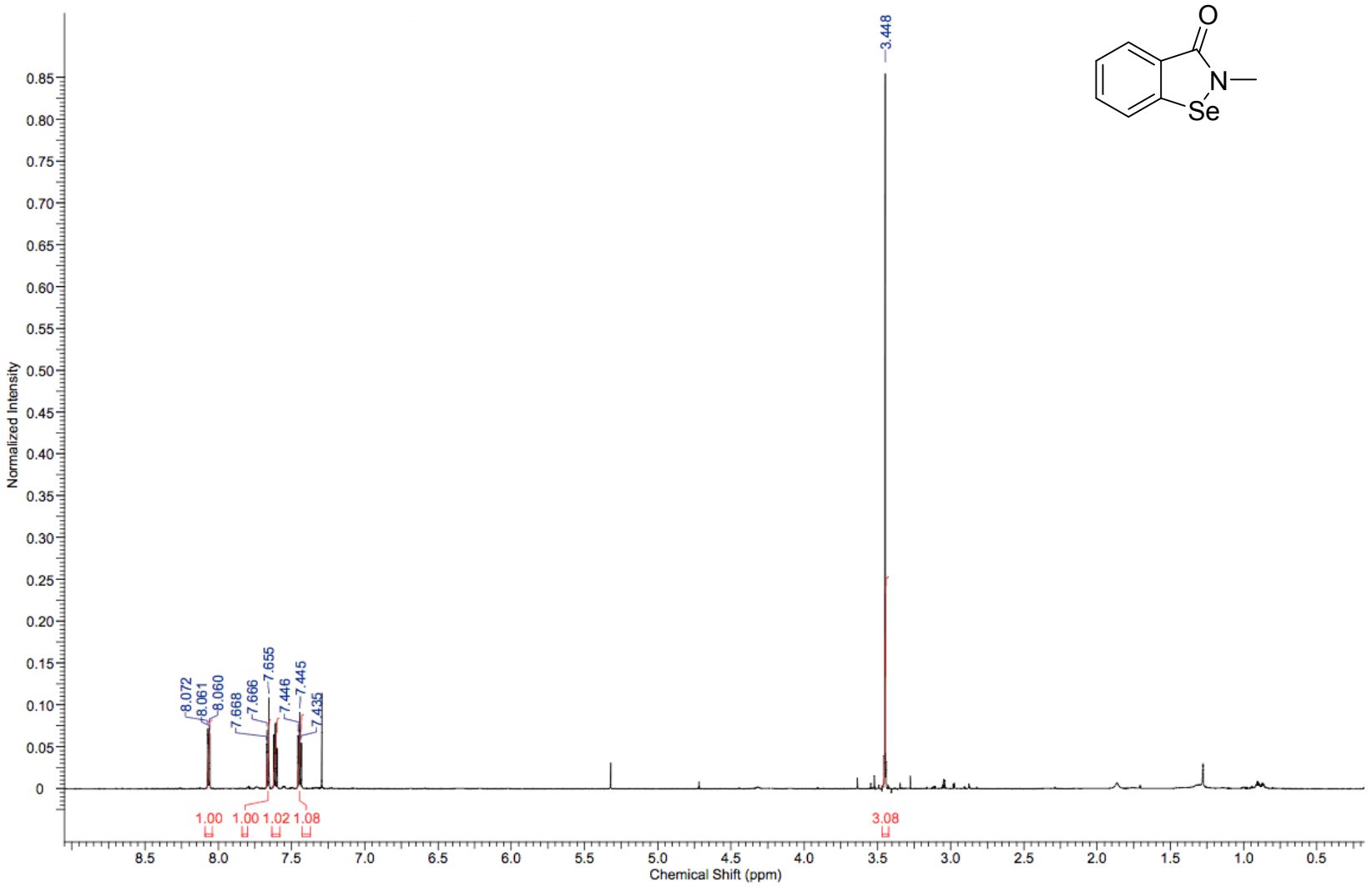
***N*-(4-methoxyphenyl)-*o*-iodobenzamide (22a)**



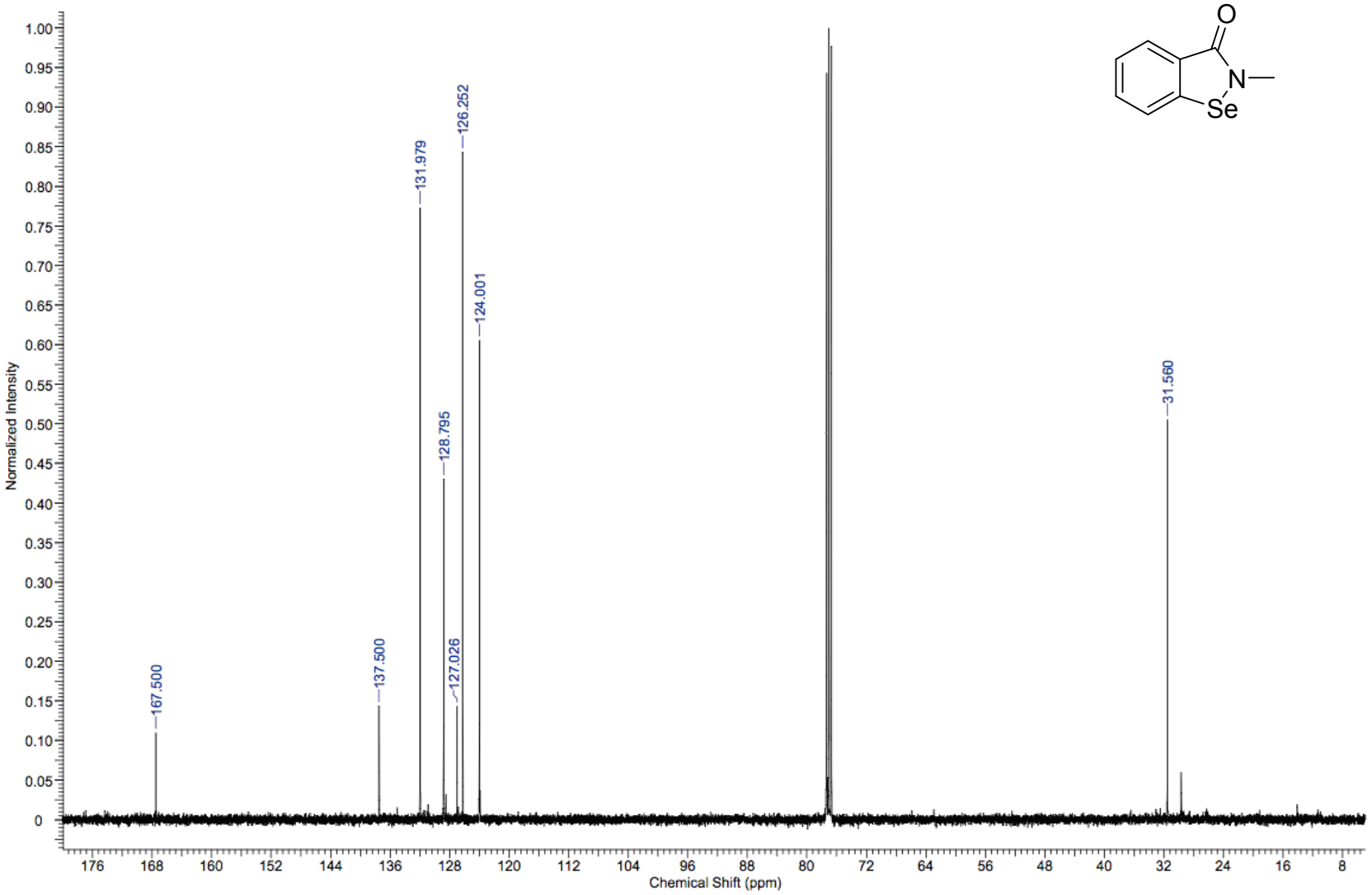
***N*-(4-methoxyphenyl)-*o*-iodobenzamide (22a)**



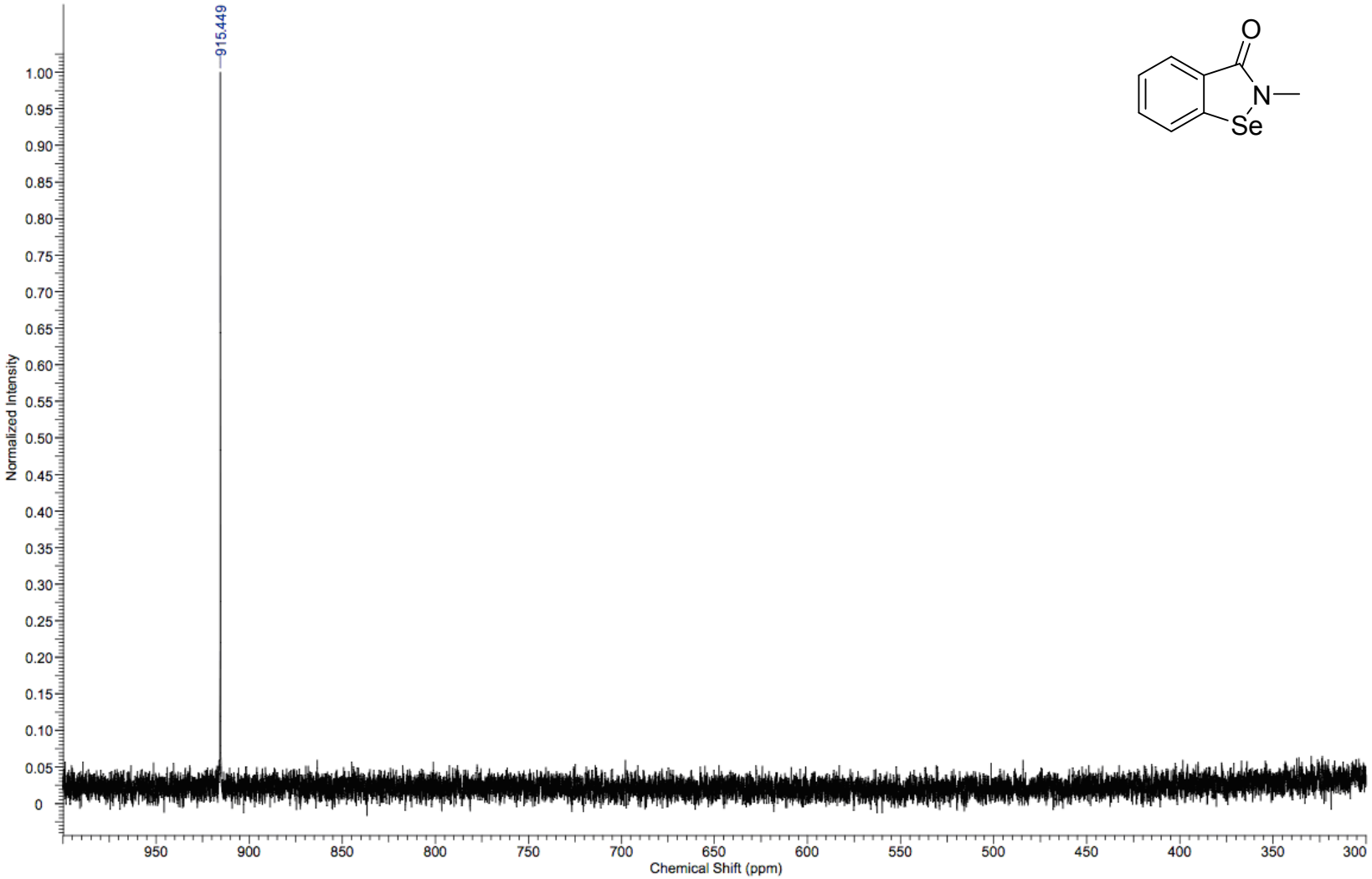
_N_-methyl-1,2-benzisoselenazol-3(2_H_)-one (9)



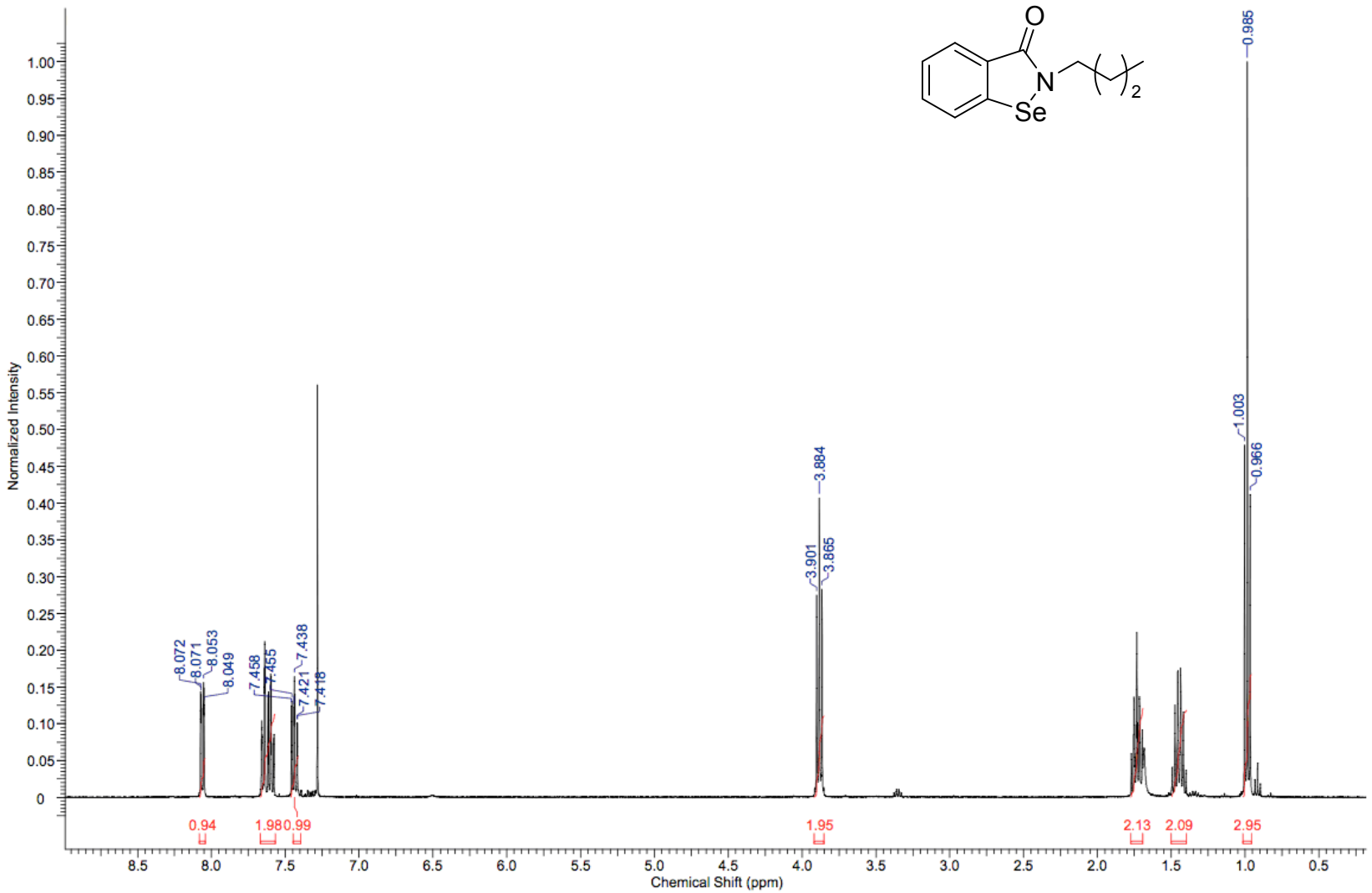
***N*-methyl-1,2-benzisoselenazol-3(2*H*)-one (9)**



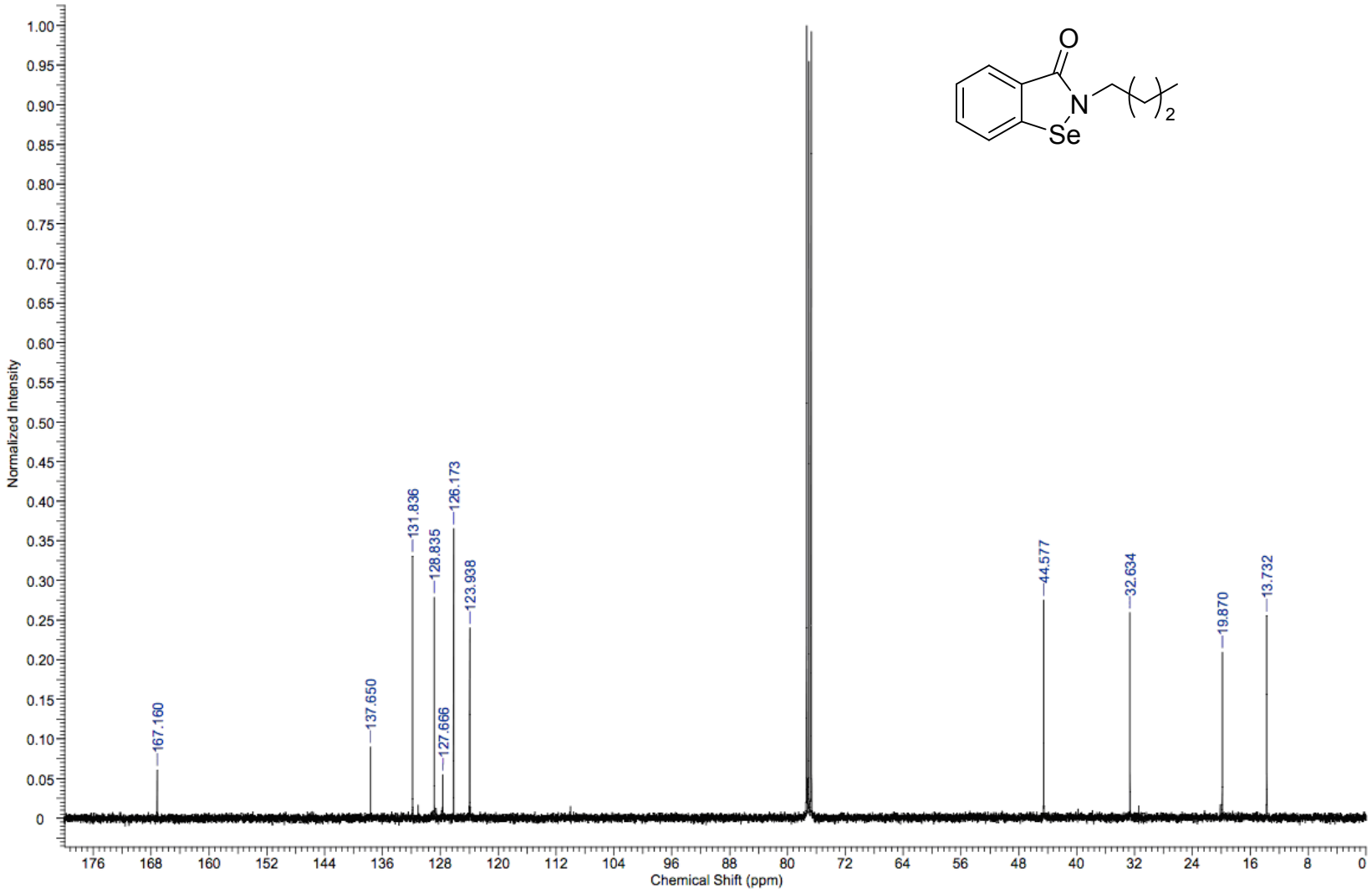
***N*-methyl-1,2-benzisoselenazol-3(2*H*)-one (9)**



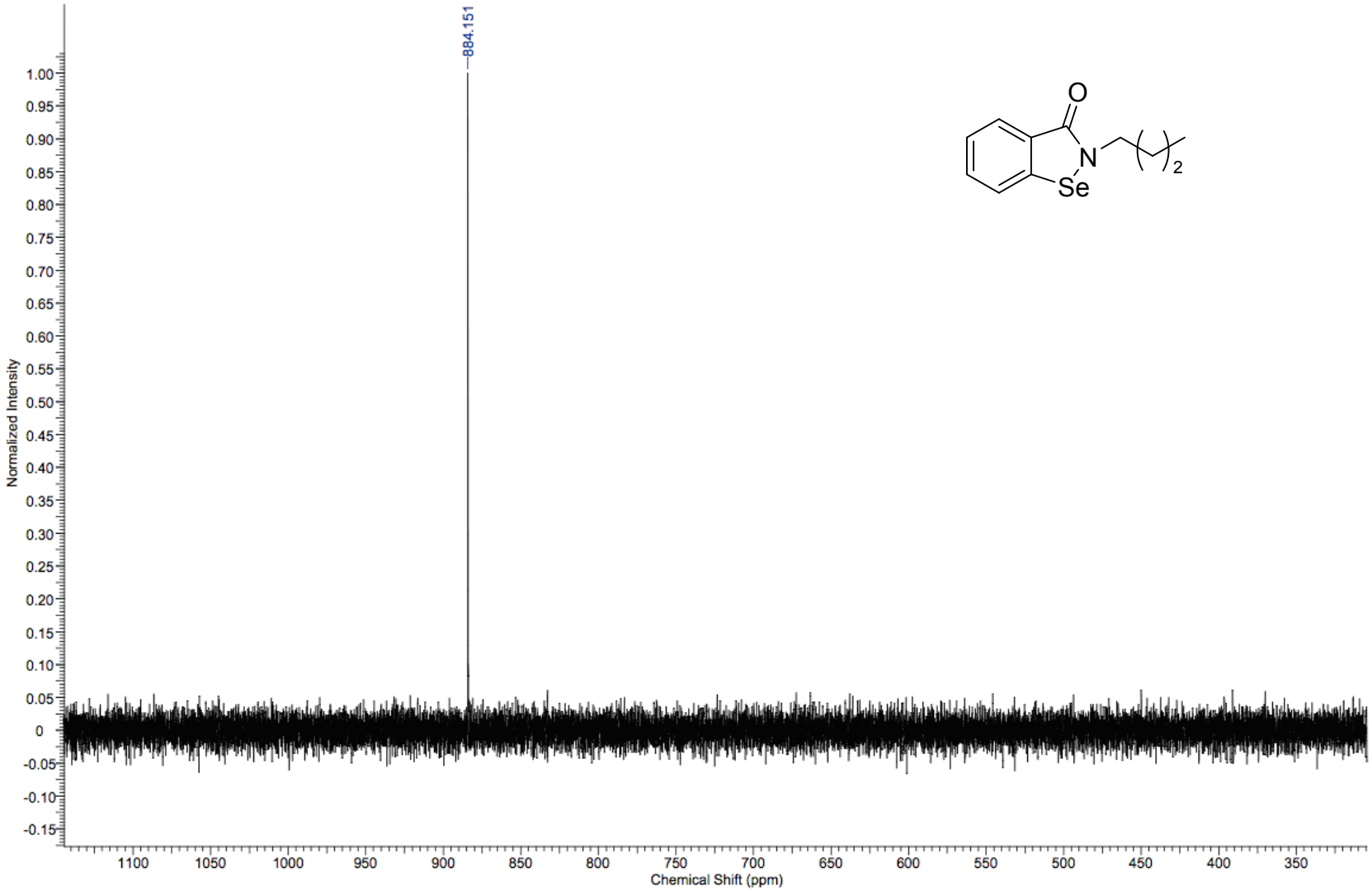
***N*-butyl-1,2-benzisoselenazol-3(2*H*)-one (10)**



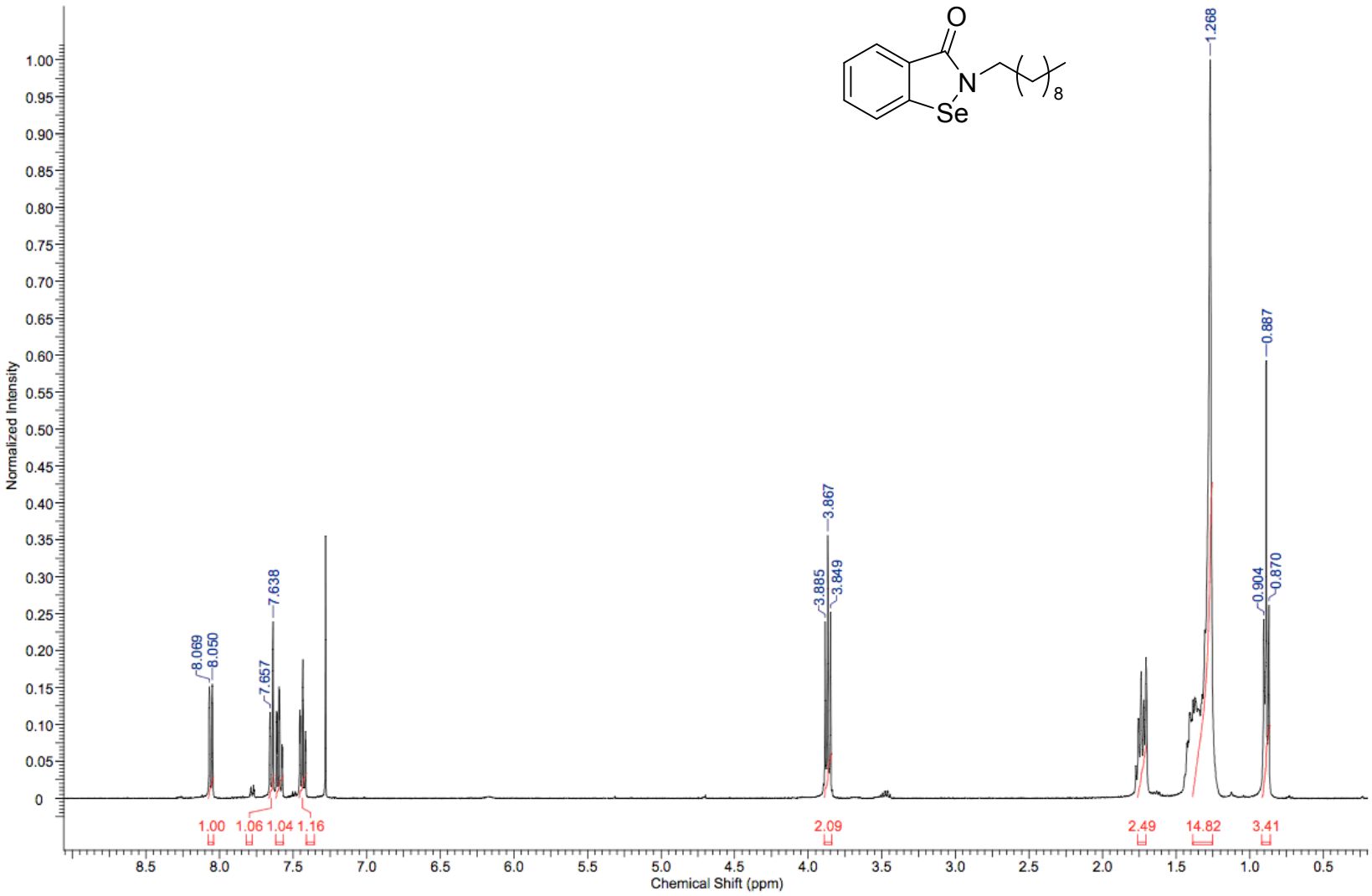
***N*-butyl-1,2-benzisoselenazol-3(2*H*)-one (10)**



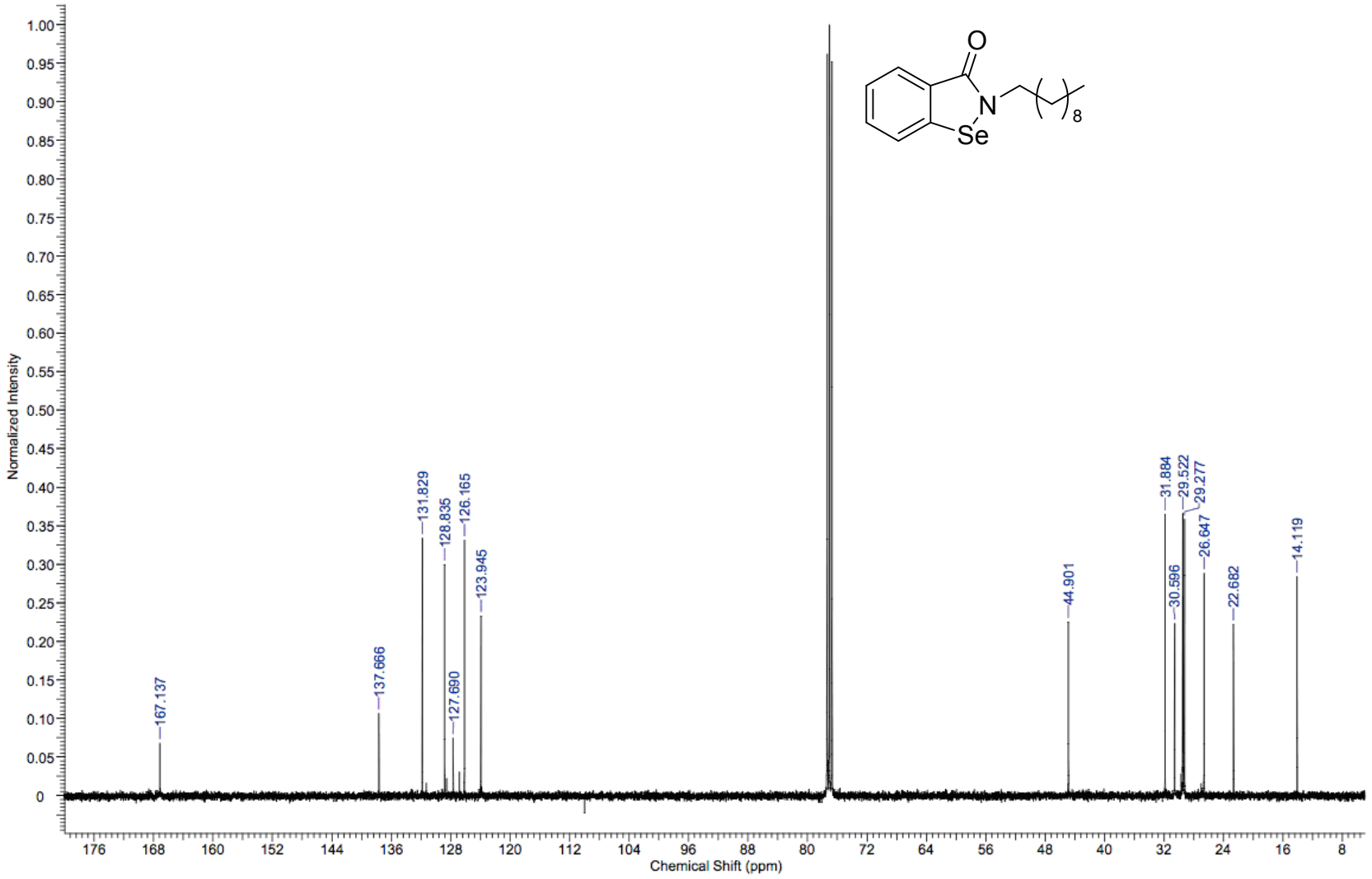
***N*-butyl-1,2-benzisoselenazol-3(2*H*)-one (10)**



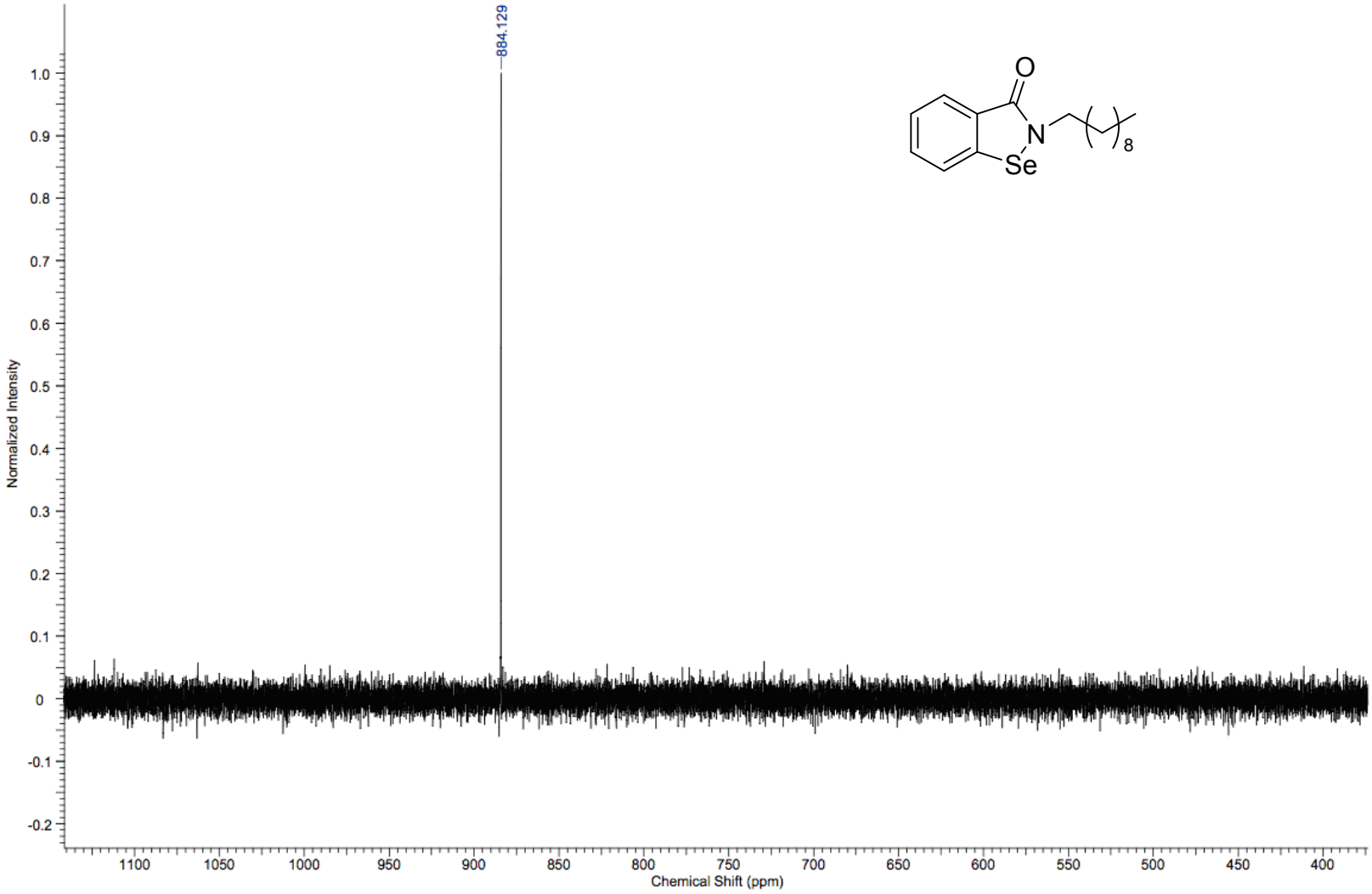
***N*-decyl-1,2-benzisoselenazol-3(2*H*)-one (11)**



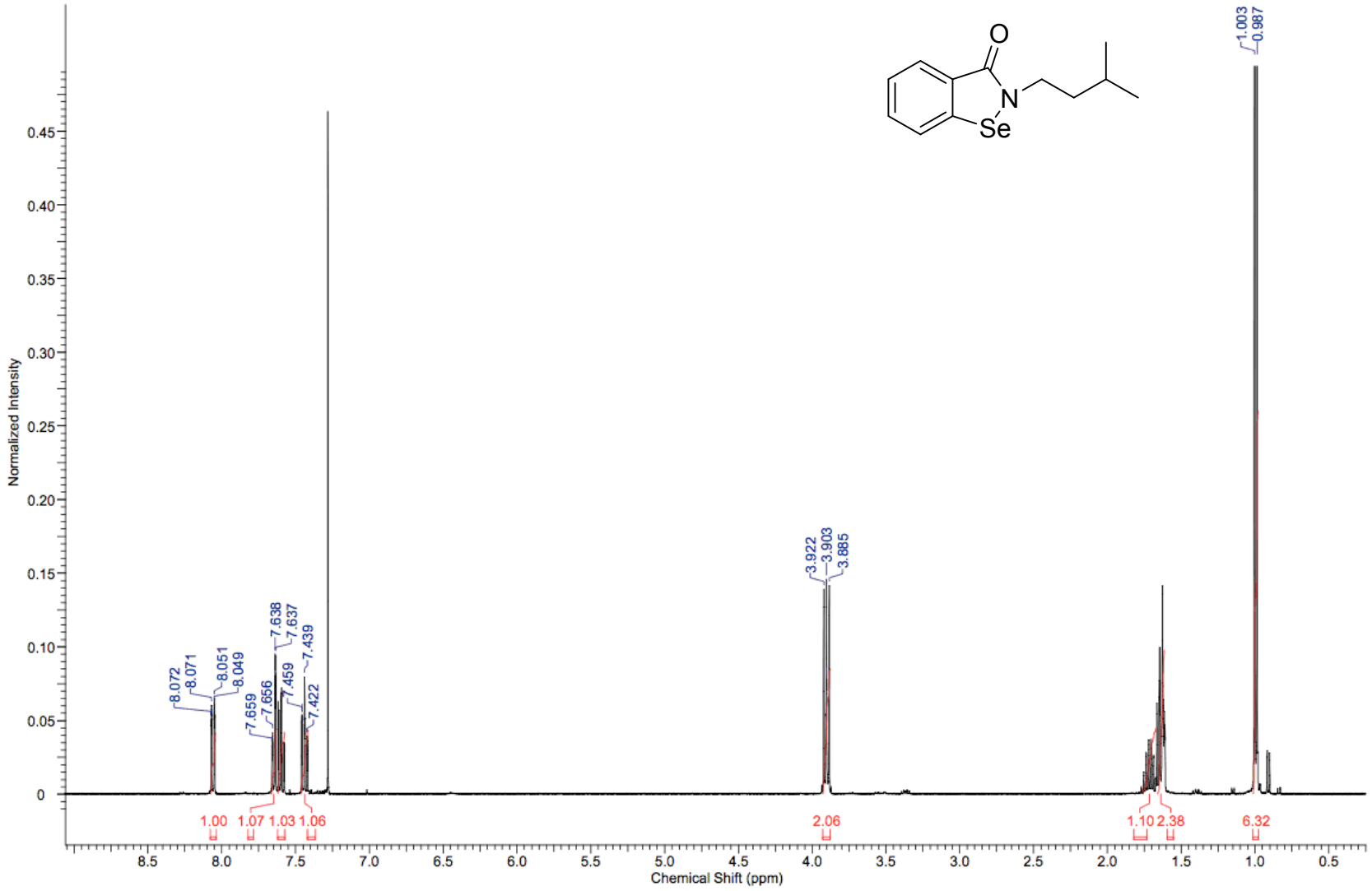
***N*-decyl-1,2-benzisoselenazol-3(2*H*)-one (11)**



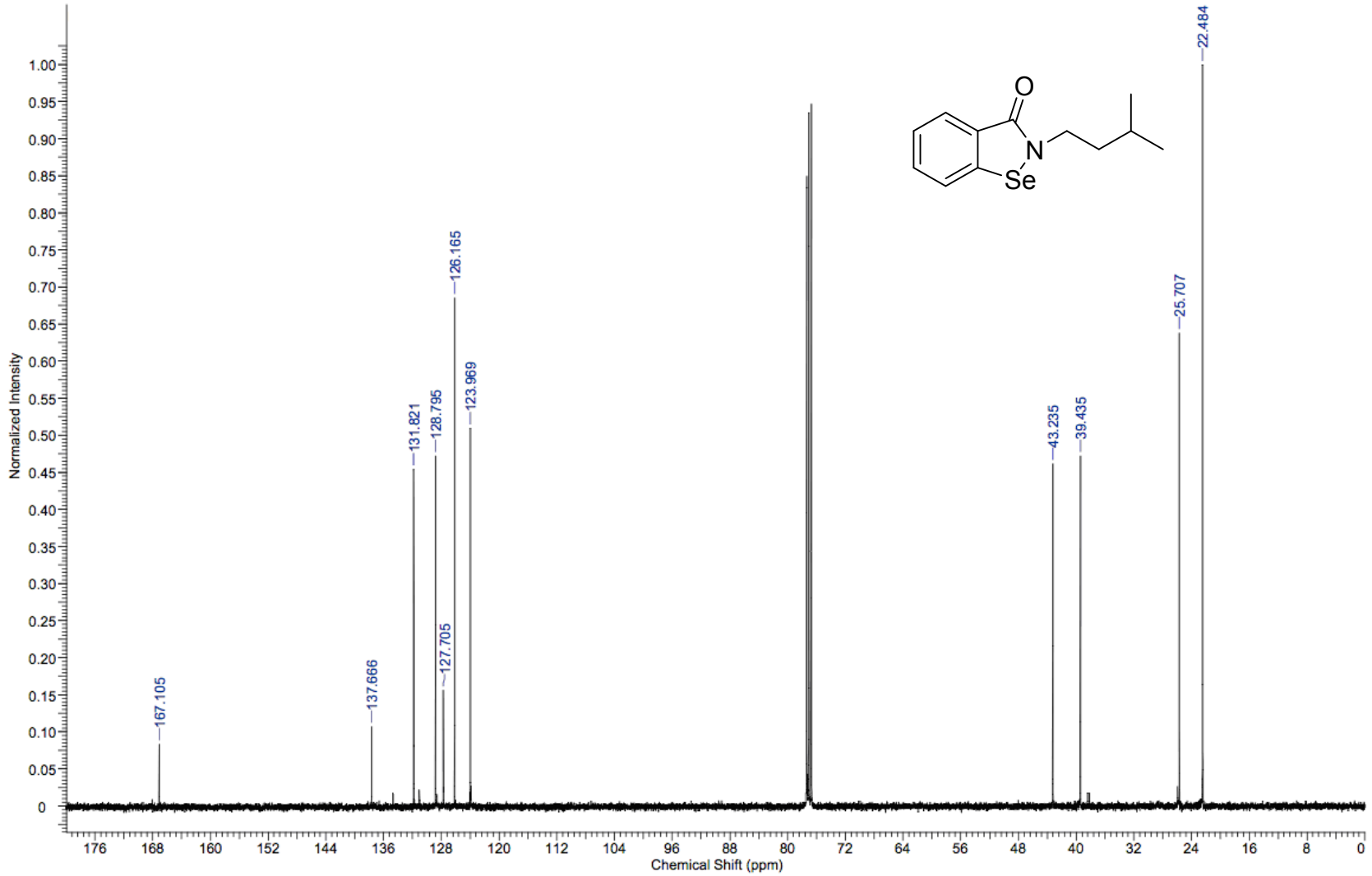
_N_-decyl-1,2-benzisoselenazol-3(2_H_)-one (11)



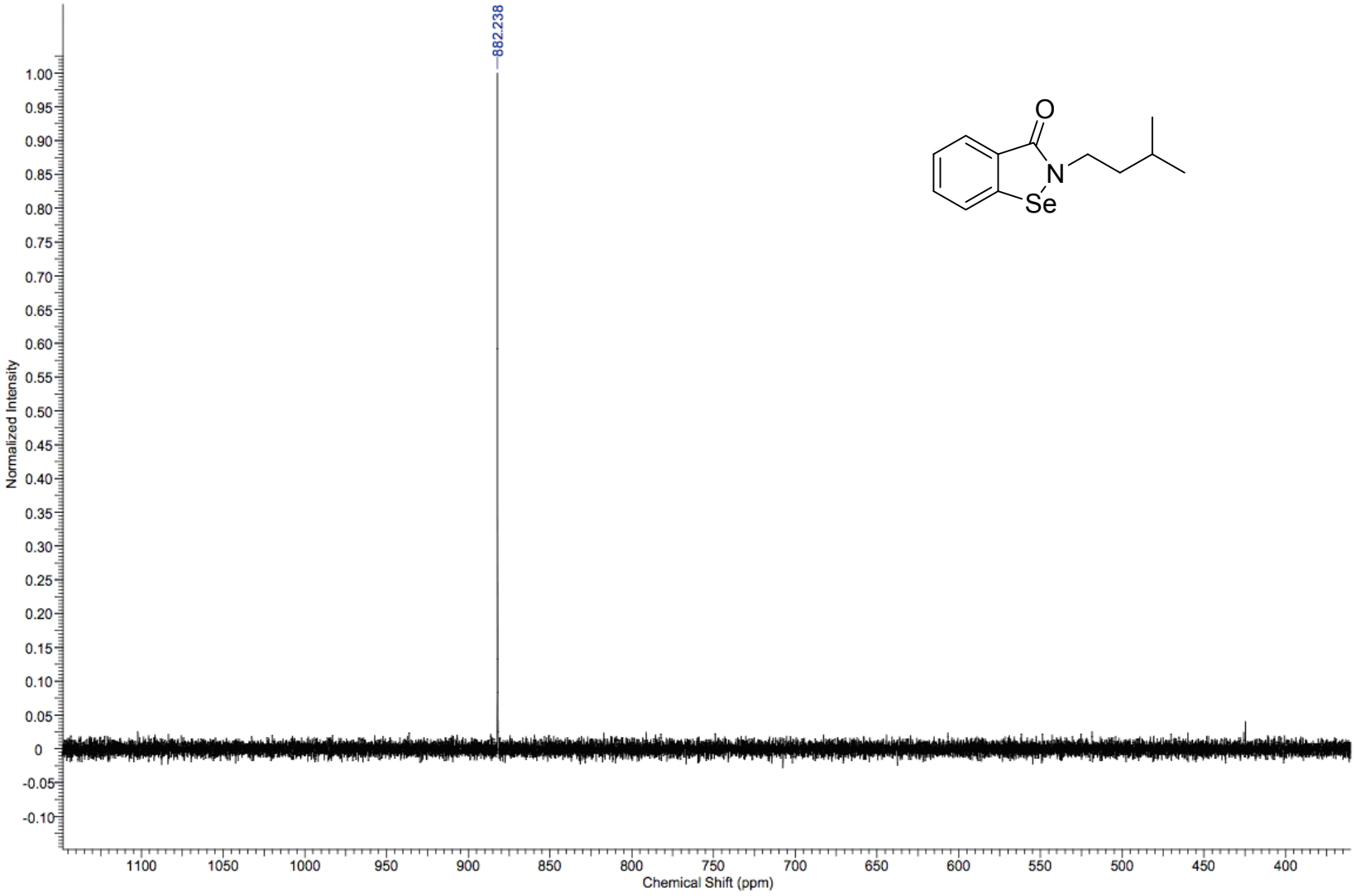
***N*-(3-methylbutyl)-1,2-benzisoselenazol-3(2*H*)-one (12)**



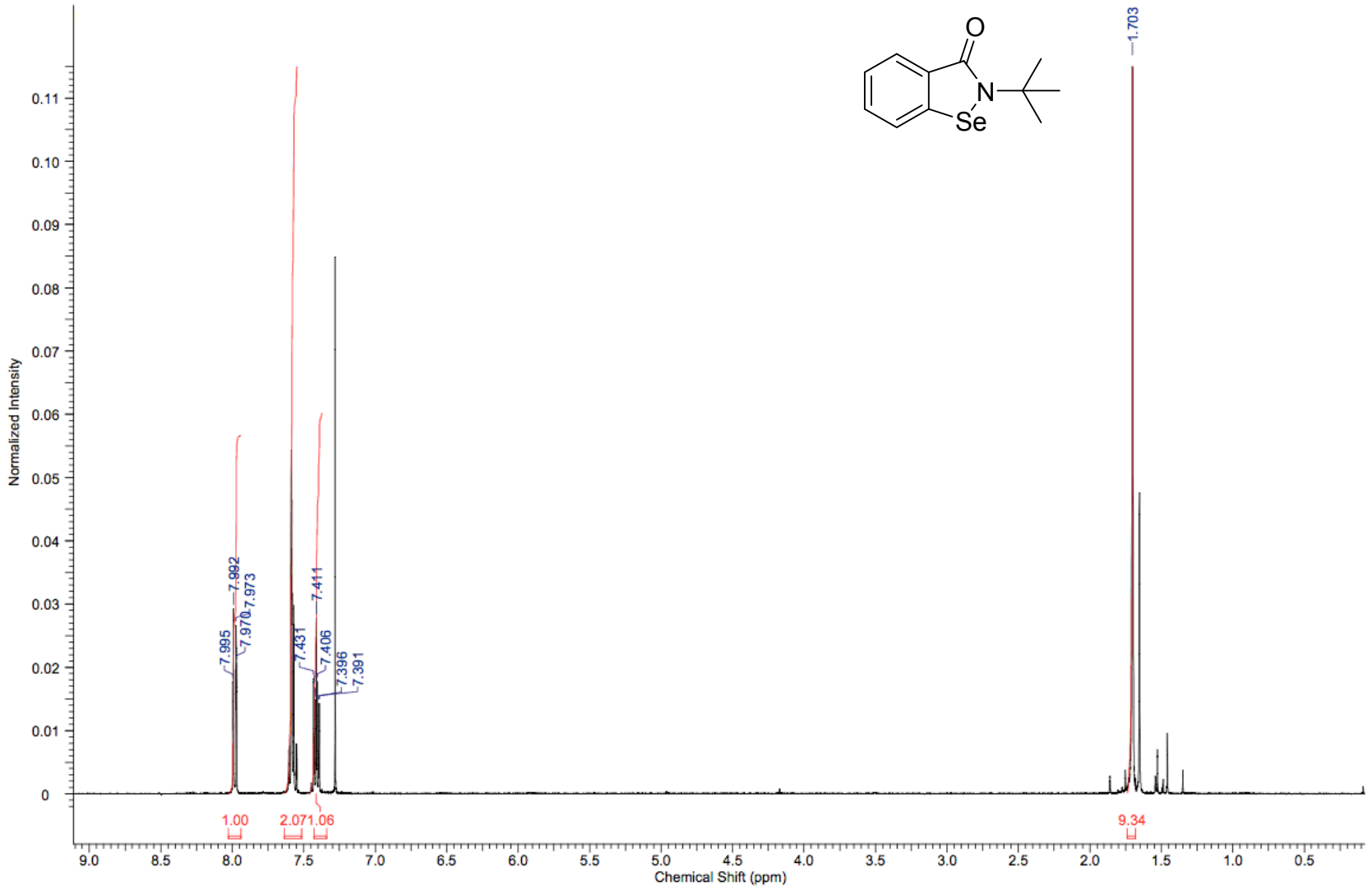
***N*-(3-methylbutyl)-1,2-benzisoselenazol-3(2*H*)-one (12)**



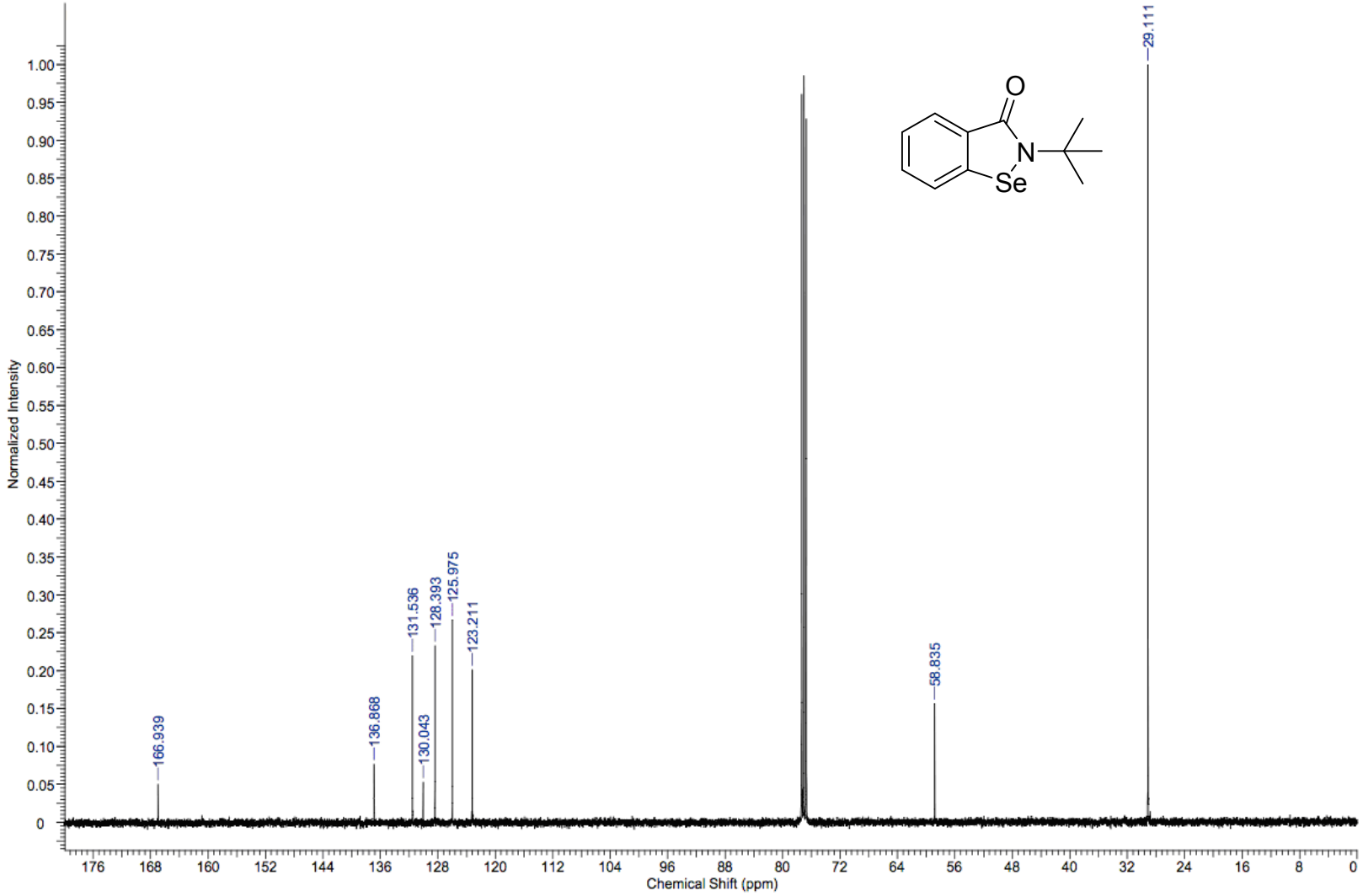
_N_-(3-methylbutyl)-1,2-benzisoselenazol-3(2_H_)-one (12)



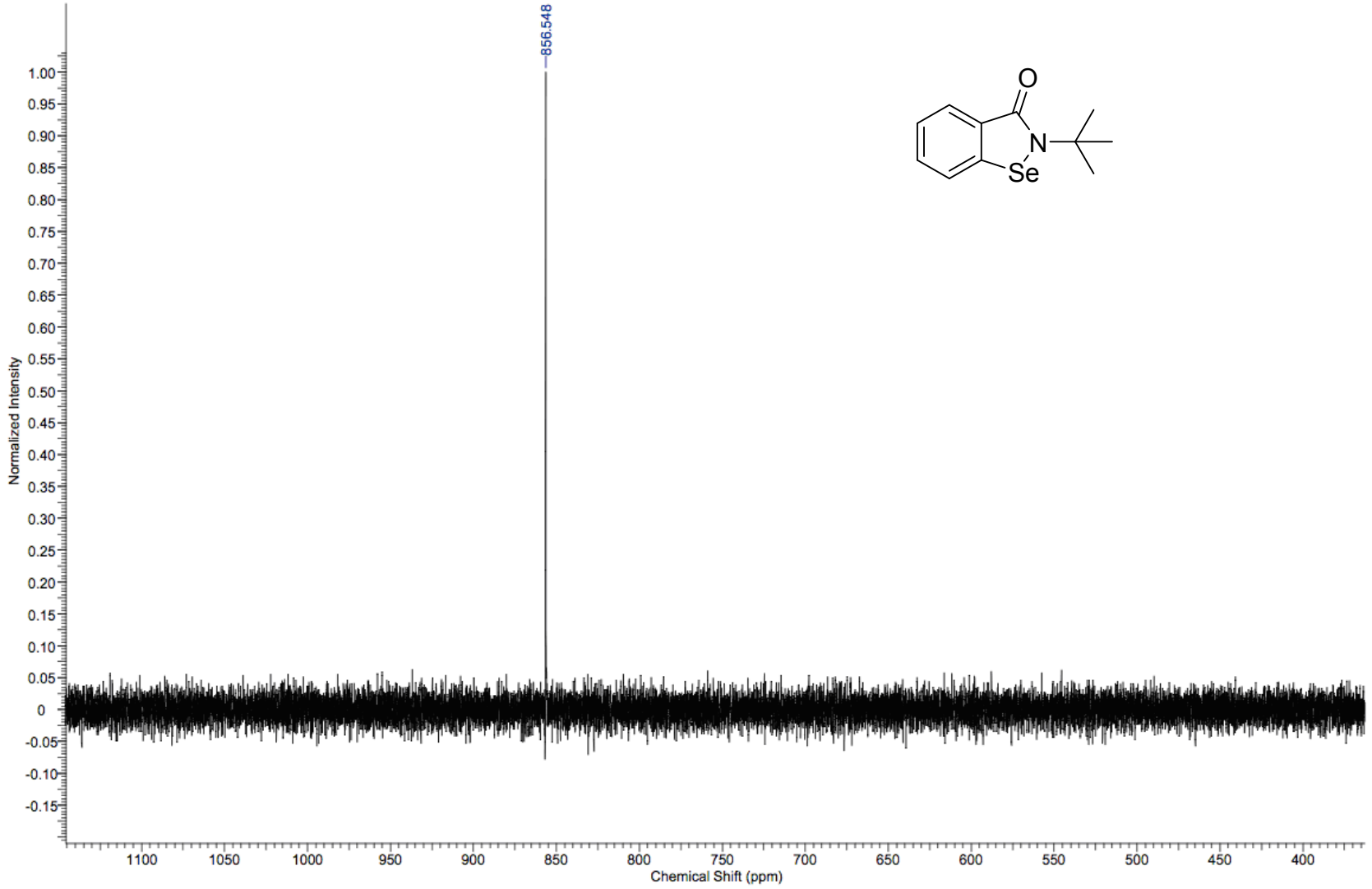
***N*-*tert*-butyl-1,2-benzisoselenazol-3(2*H*)-one (13)**



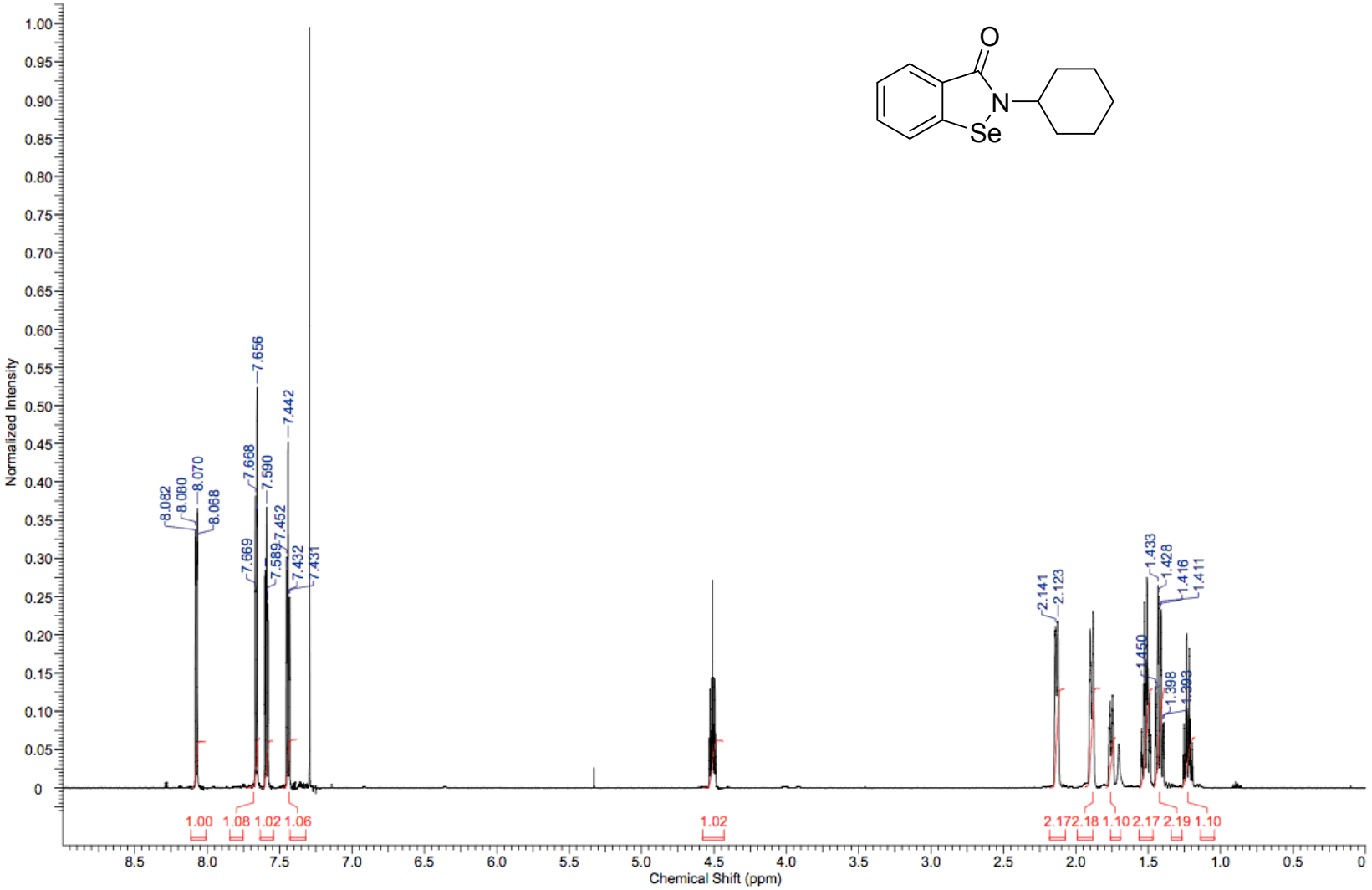
***N*-*tert*-butyl-1,2-benzisoselenazol-3(2*H*)-one (13)**



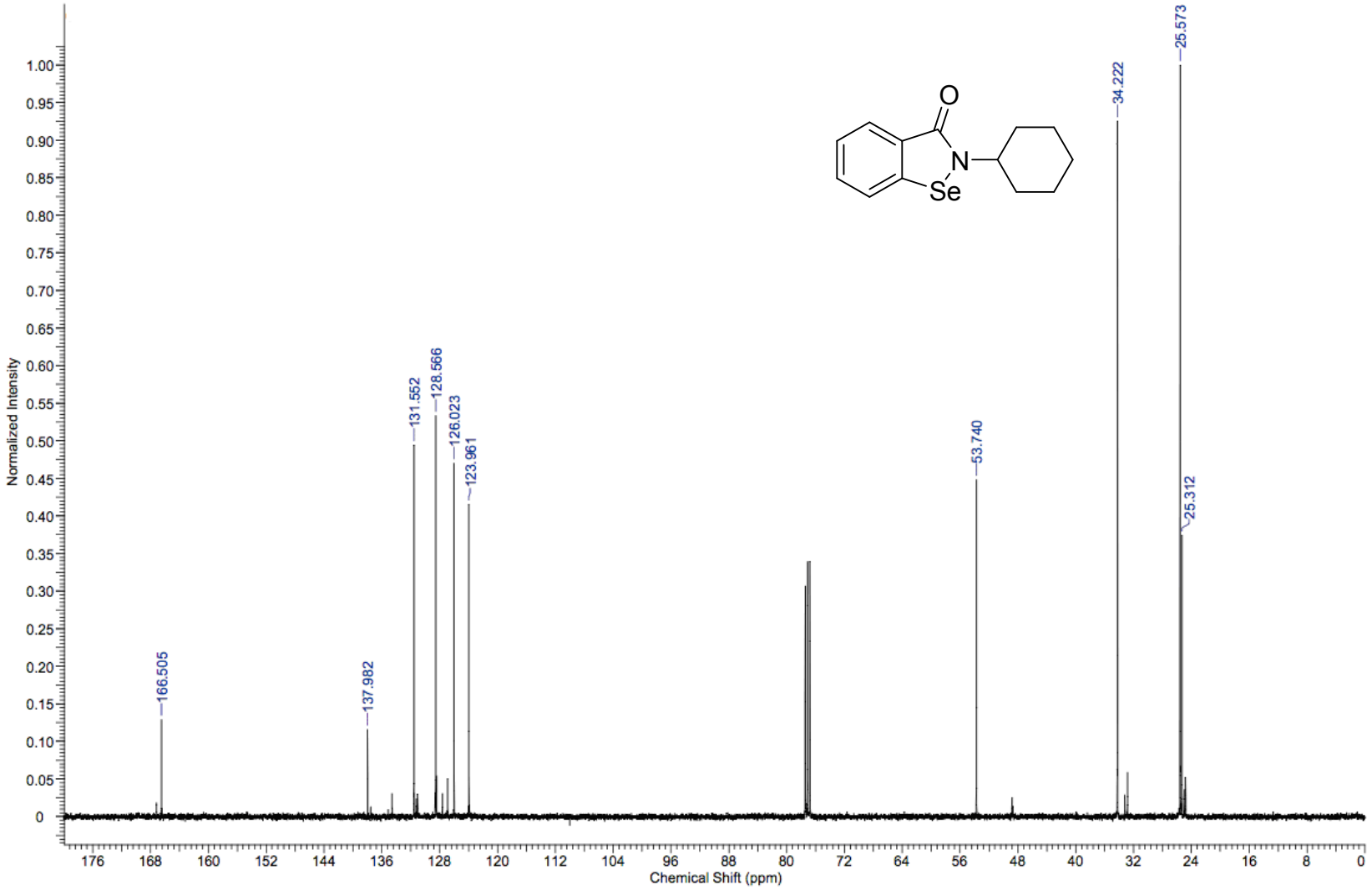
***N*-*tert*-butyl-1,2-benzisoselenazol-3(2*H*)-one (13)**



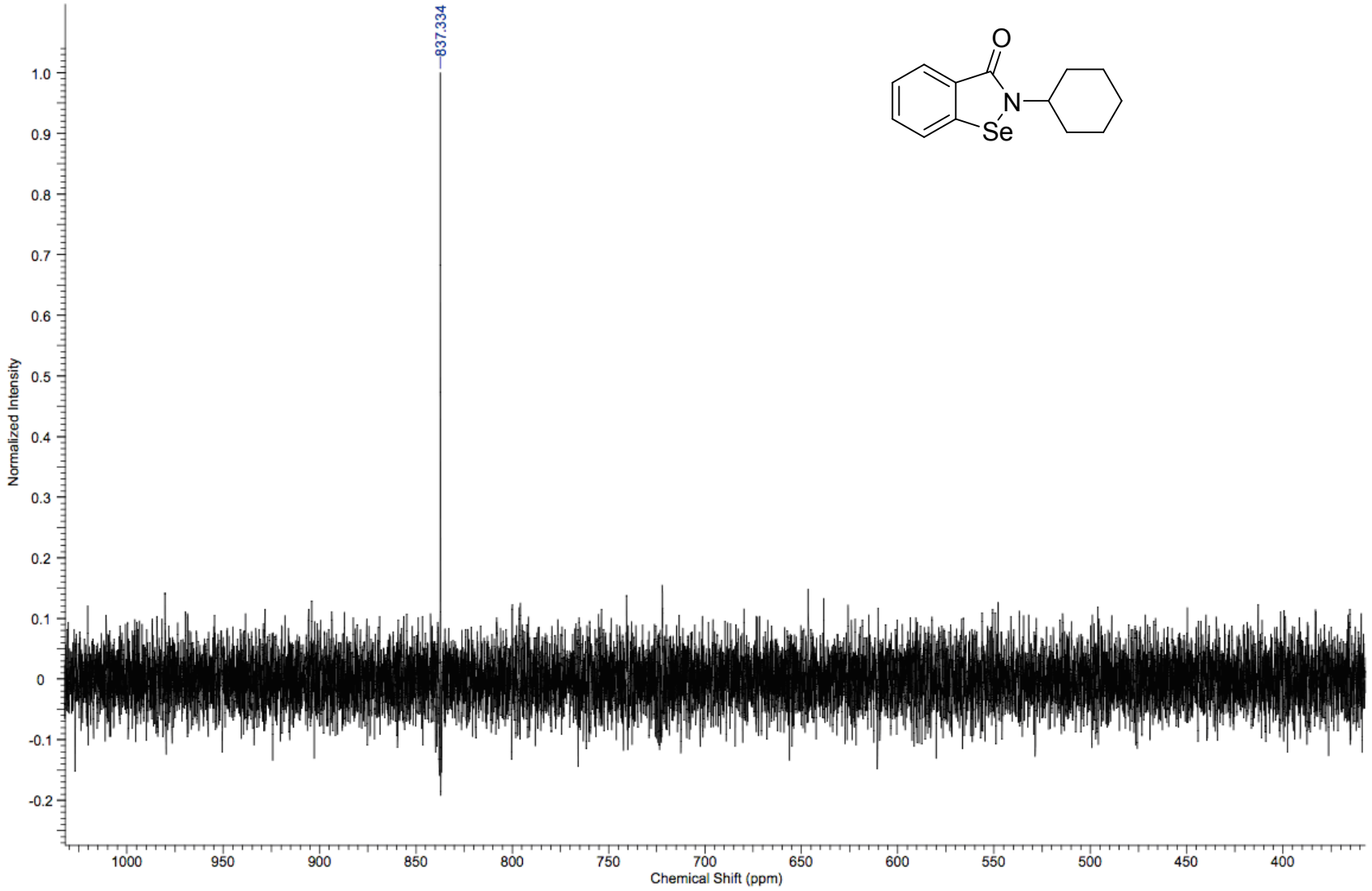
***N*-cyclohexyl-1,2-benzisoselenazol-3(2*H*)-one (8)**



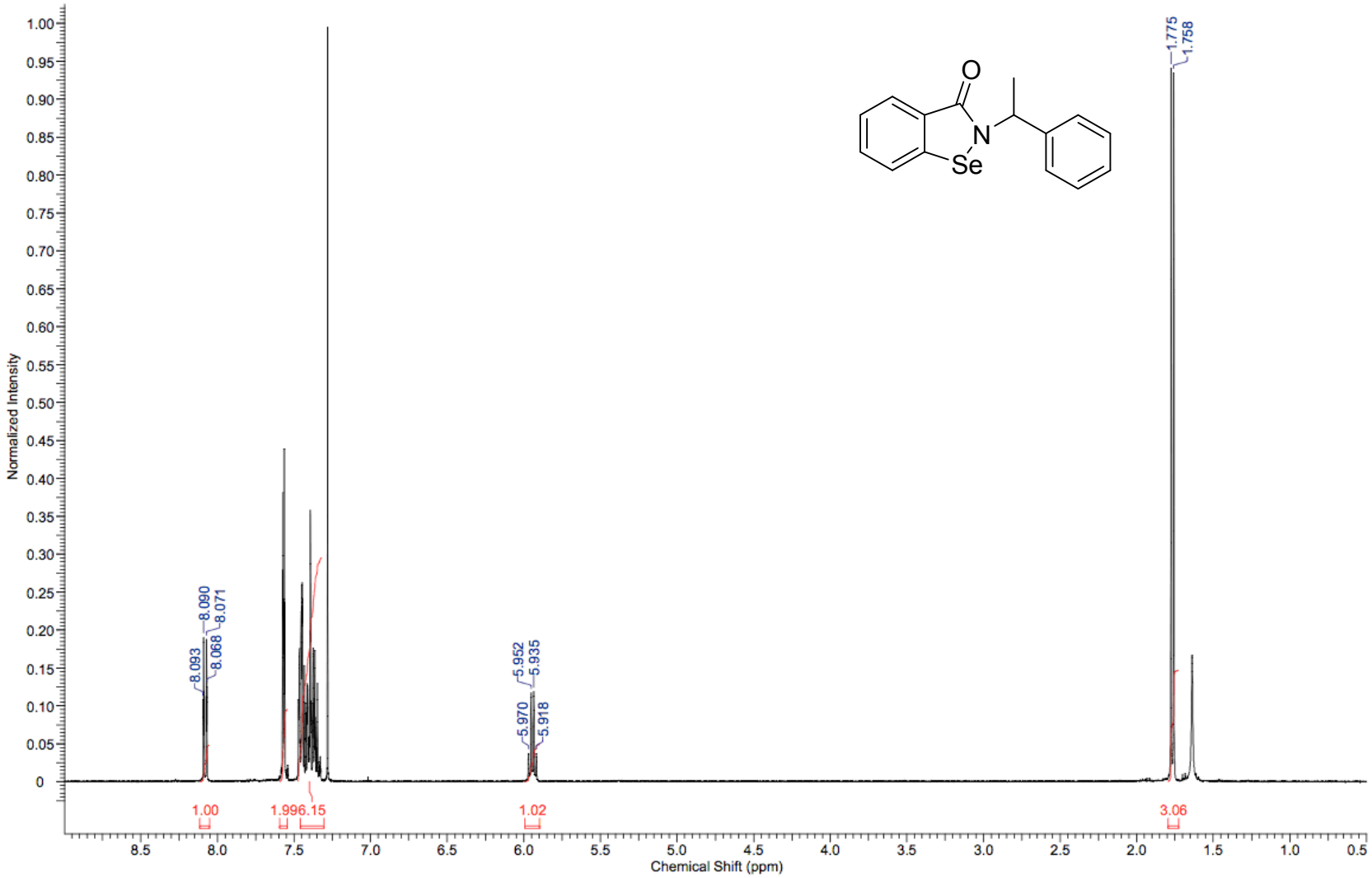
***N*-cyclohexyl-1,2-benzisoselenazol-3(2*H*)-one (8)**



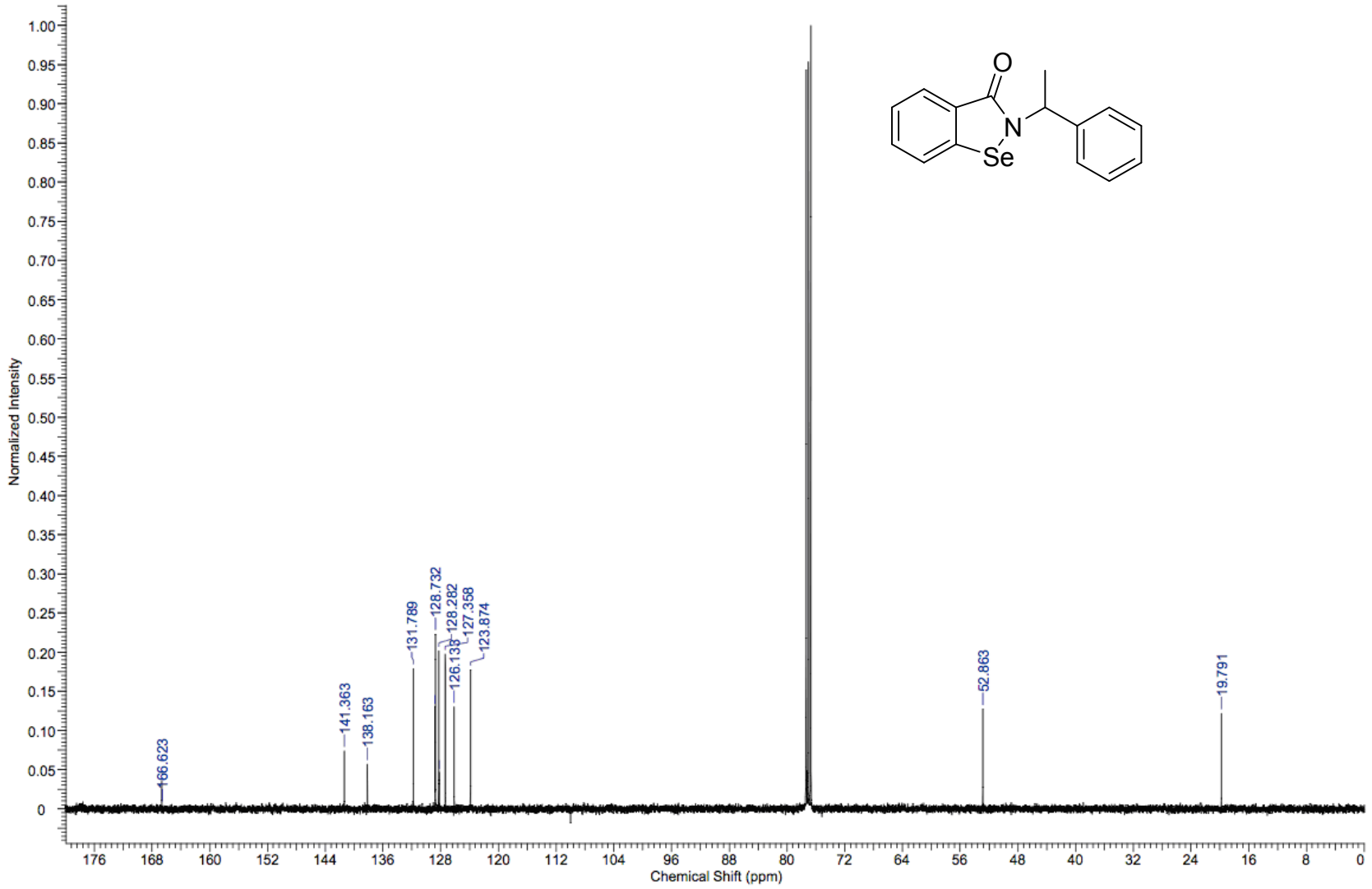
***N*-cyclohexyl-1,2-benzisoselenazol-3(2*H*)-one (8)**



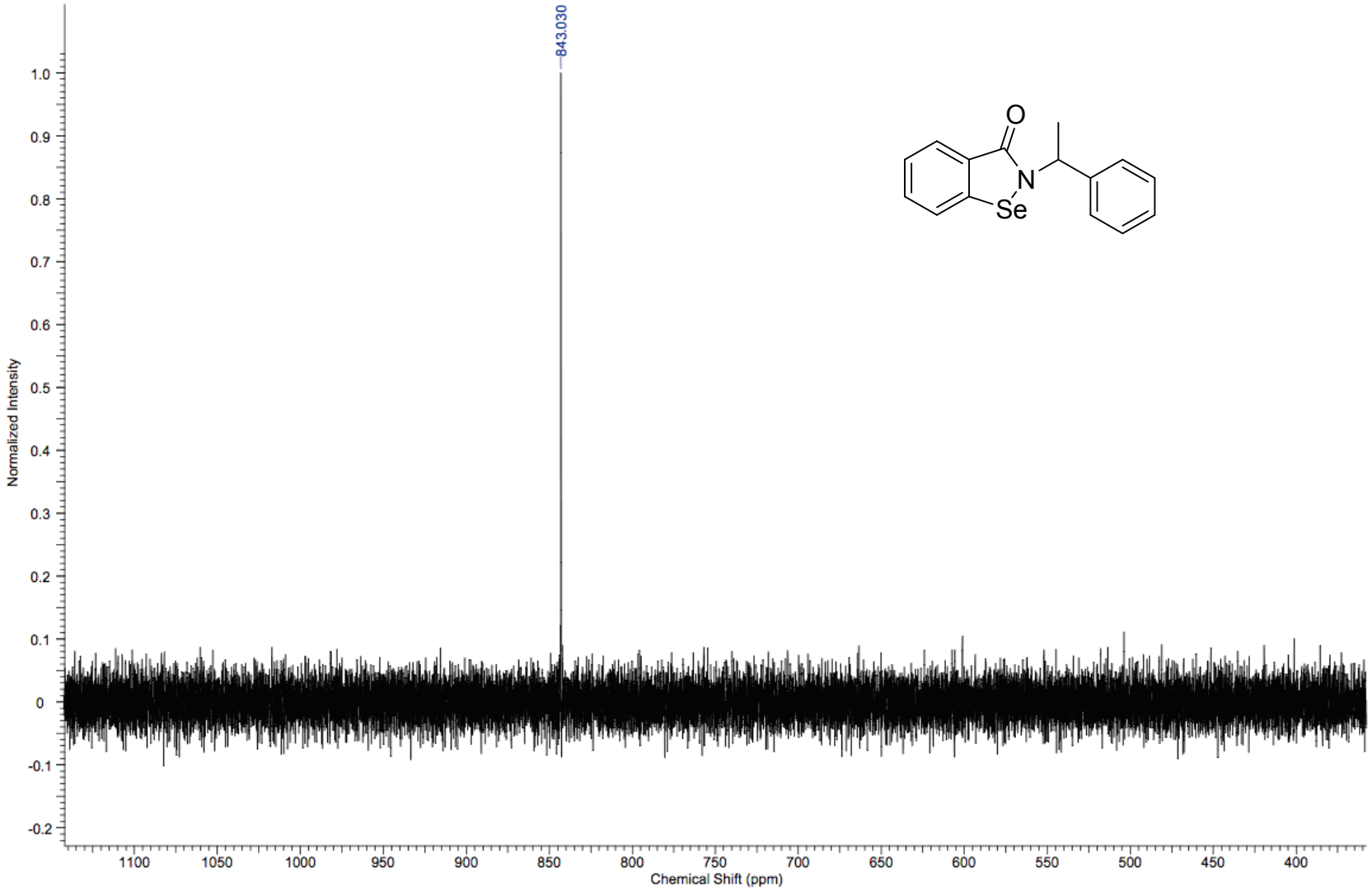
***N*-(1-phenylethyl)-1,2-benzisoselenazol-3(2*H*)-one (14)**



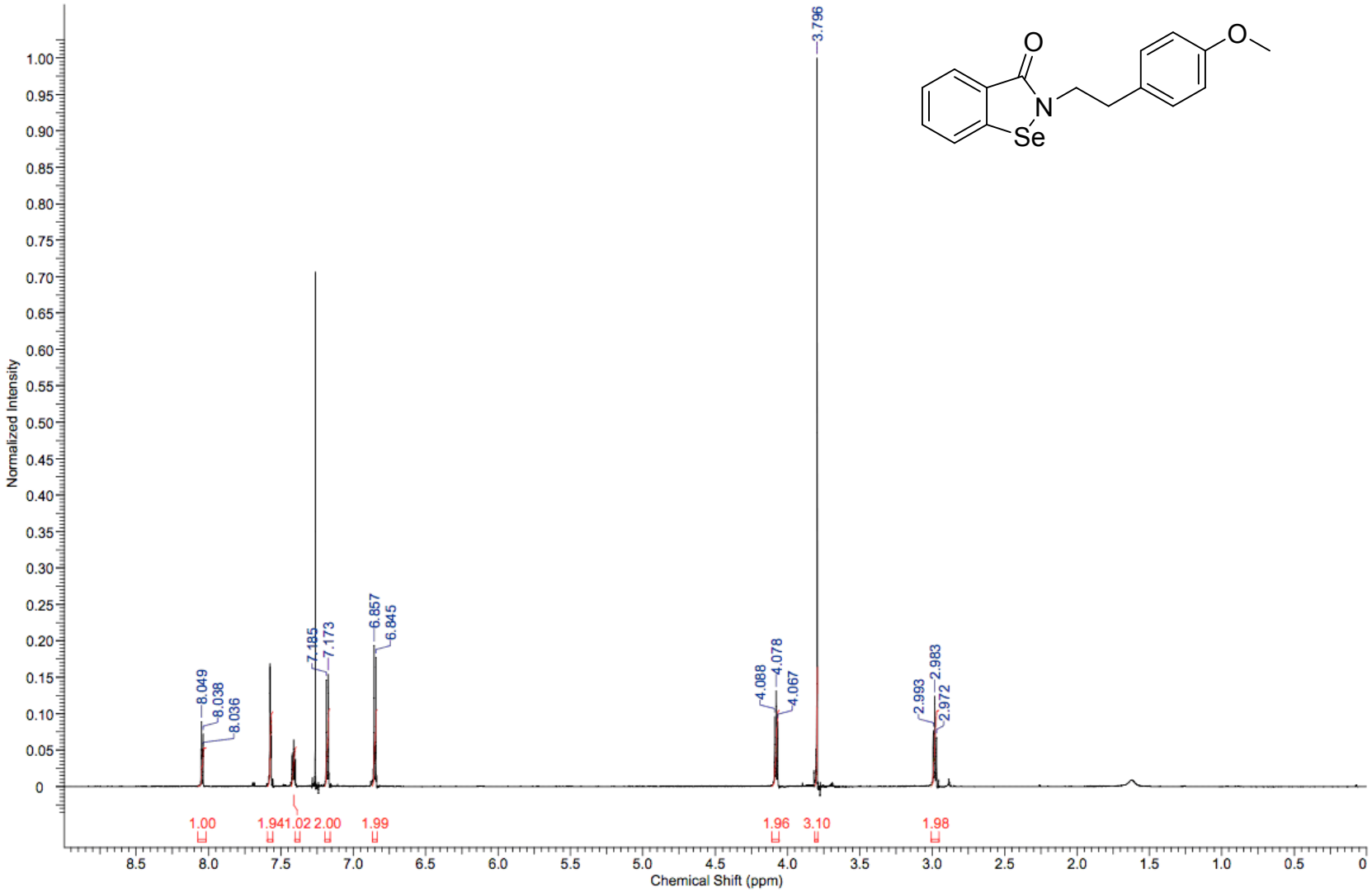
***N*-(1-phenylethyl)-1,2-benzisoselenazol-3(2*H*)-one (14)**



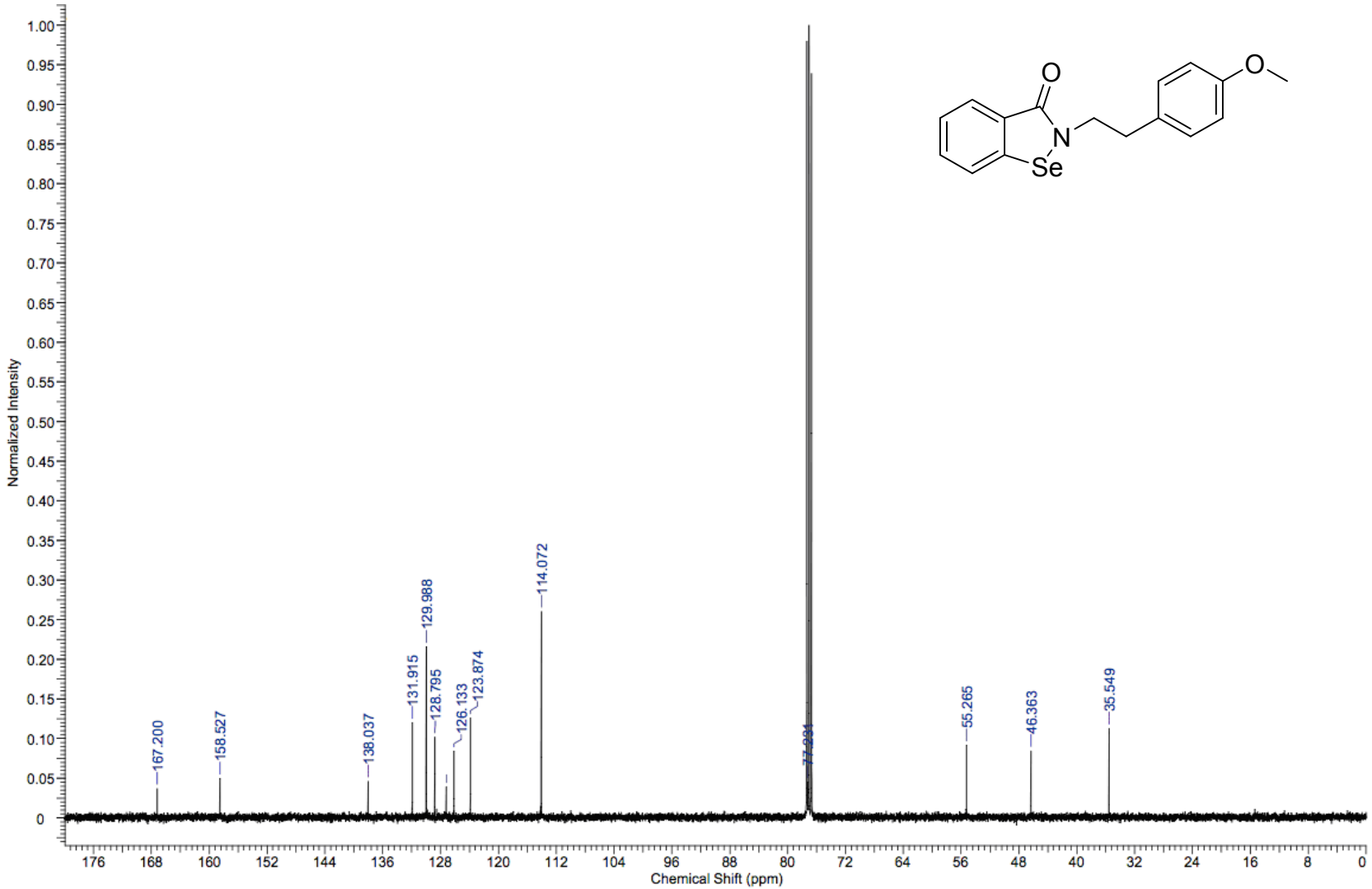
***N*-(1-phenylethyl)-1,2-benzisoselenazol-3(2*H*)-one (14)**



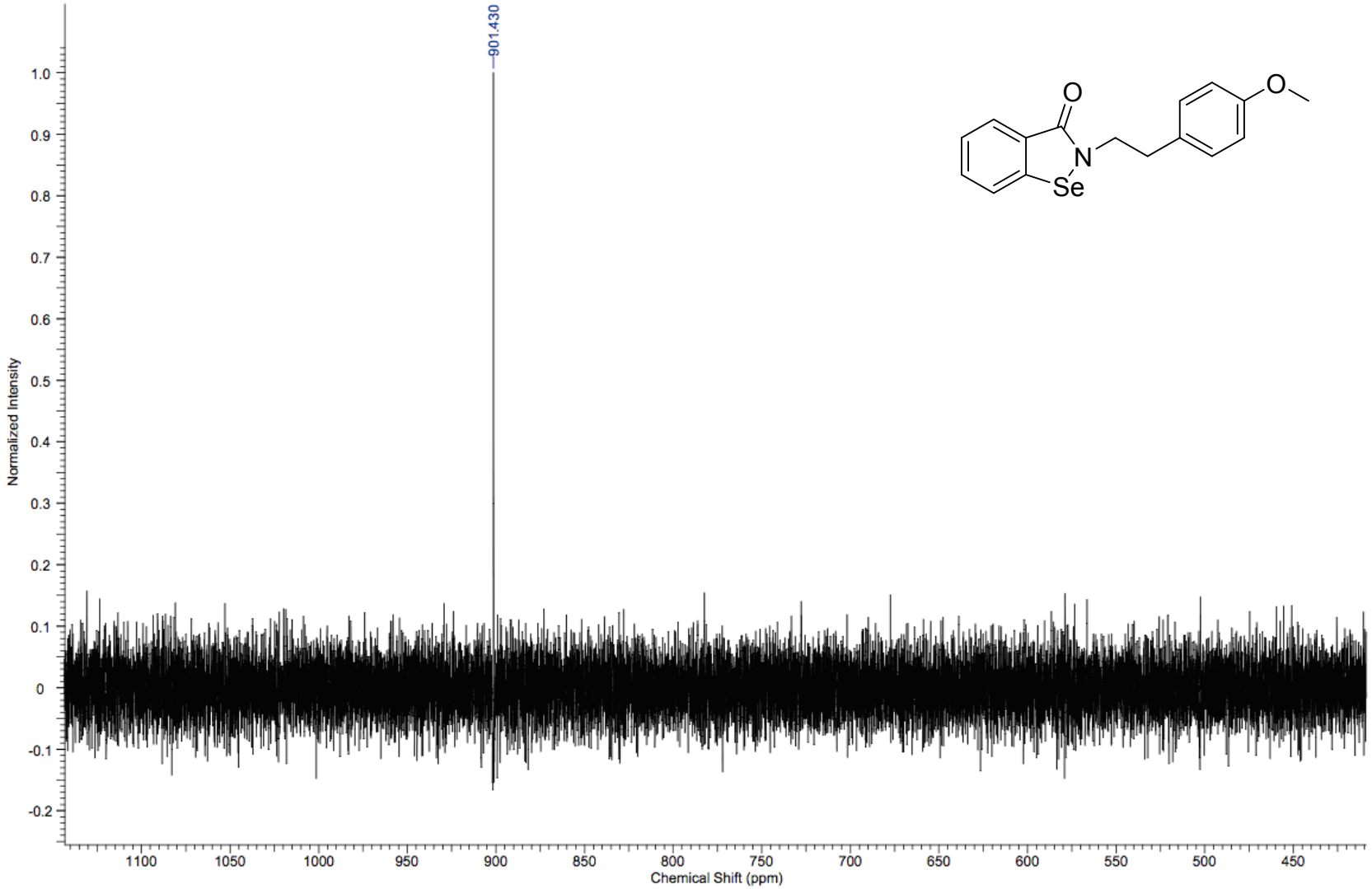
***N*-(2-(4-methoxyphenyl)ethyl)-1,2-benzisoselenazol-3(2*H*)-one (15)**



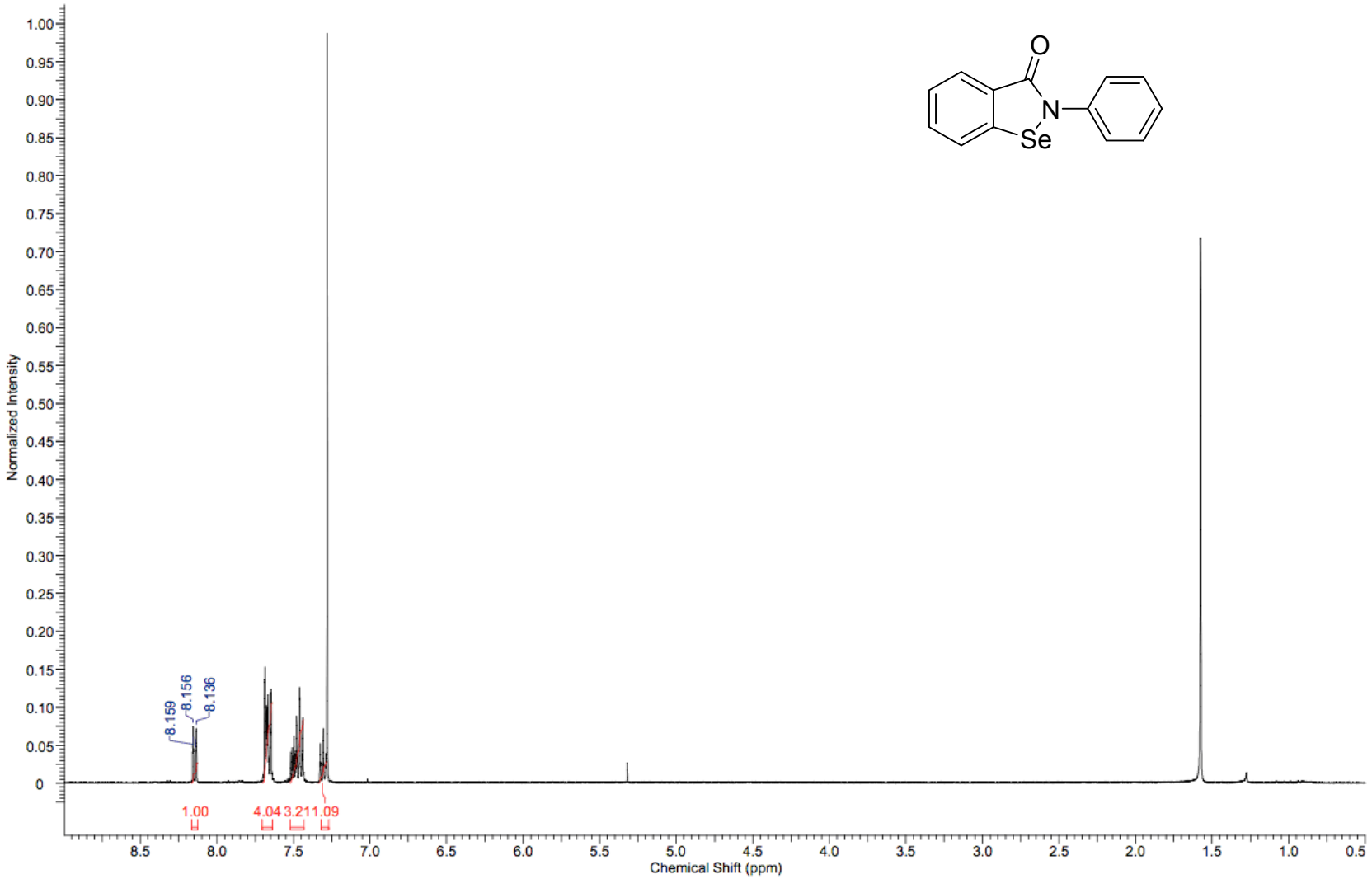
***N*-(2-(4-methoxyphenyl)ethyl)-1,2-benzisoselenazol-3(2*H*)-one (15)**



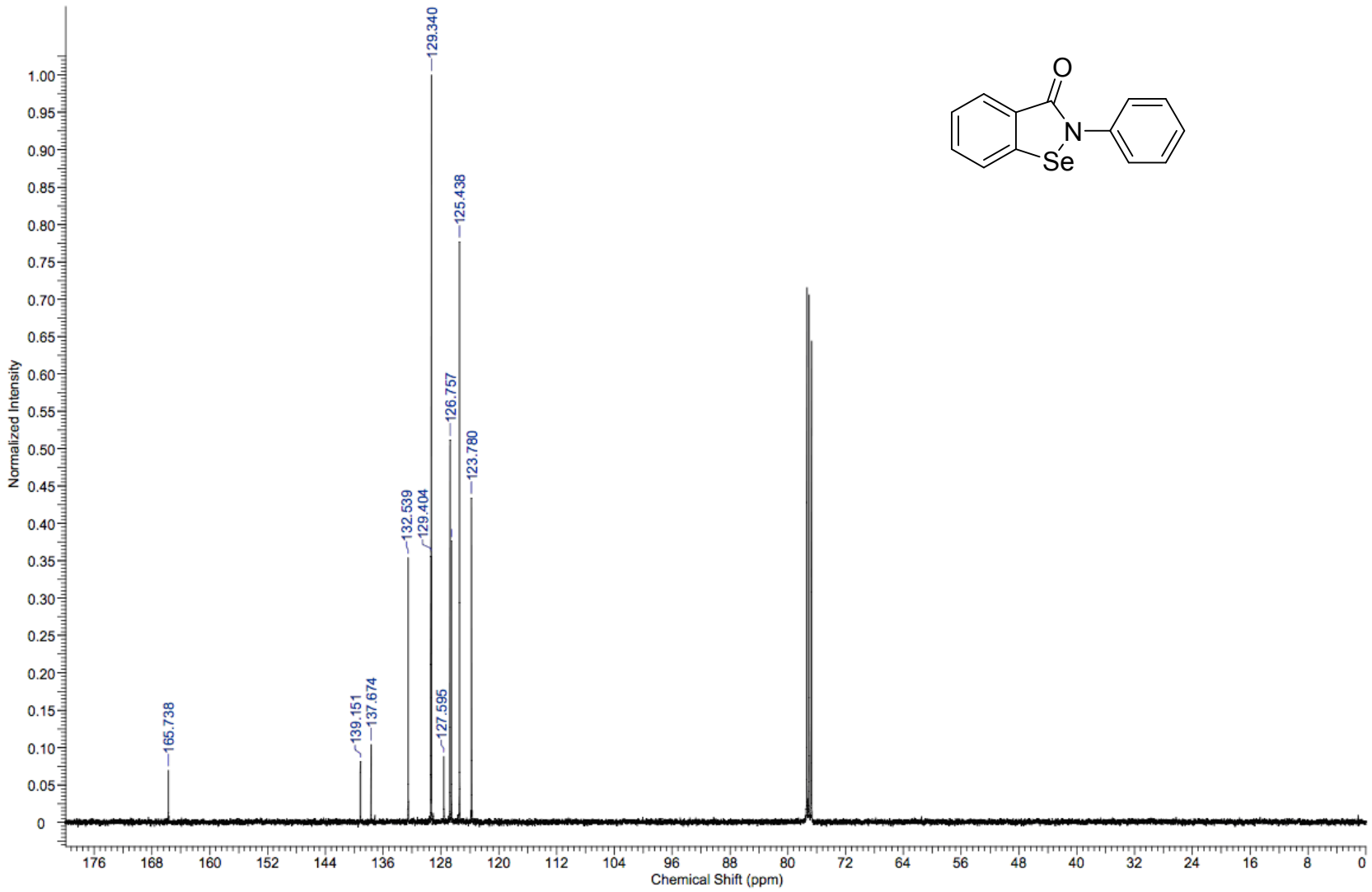
***N*-(2-(4-methoxyphenyl)ethyl)-1,2-benzisoselenazol-3(2*H*)-one (15)**



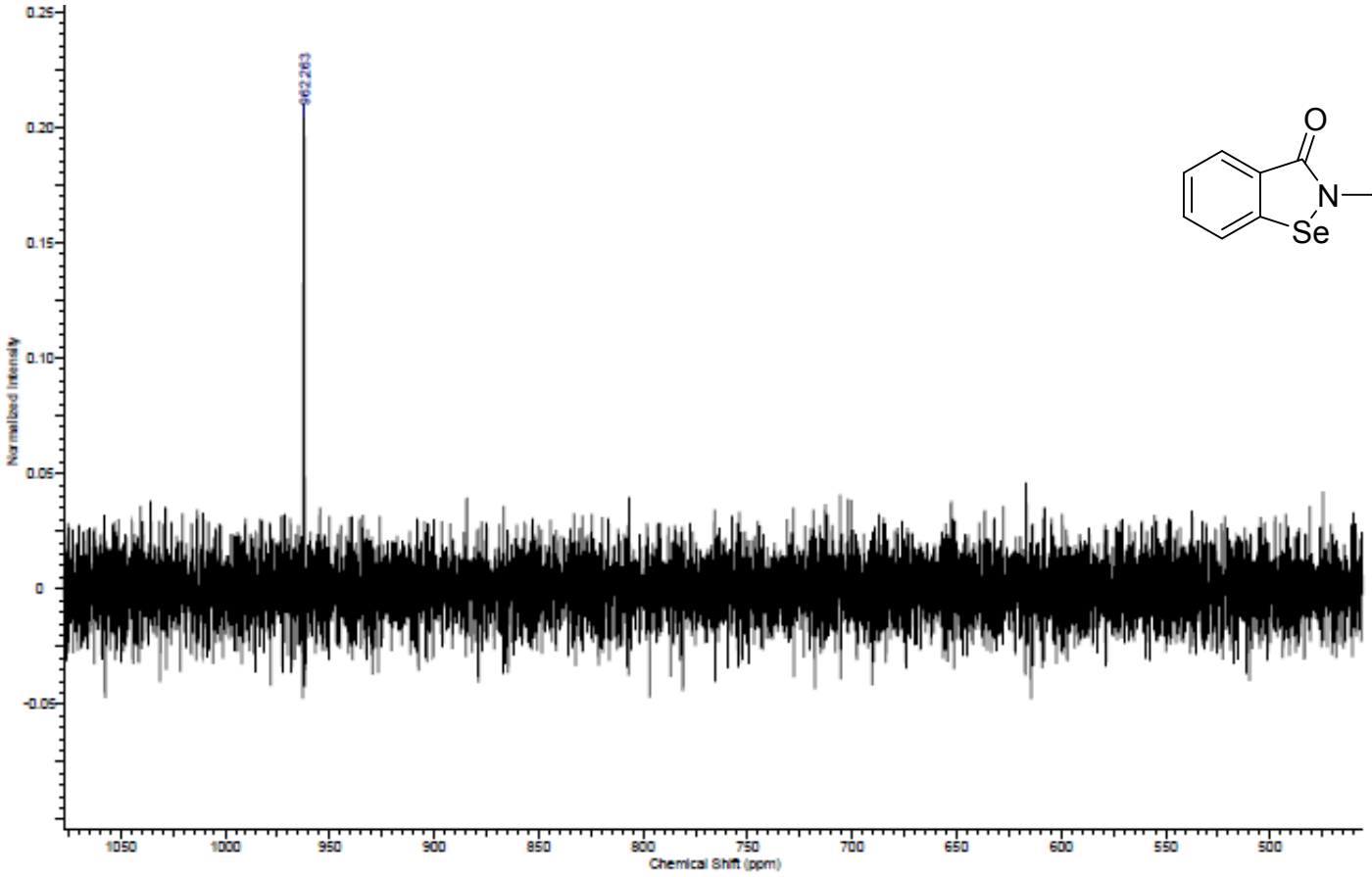
***N*-phenyl-1,2-benzisoselenazol-3(2*H*)-one (1)**



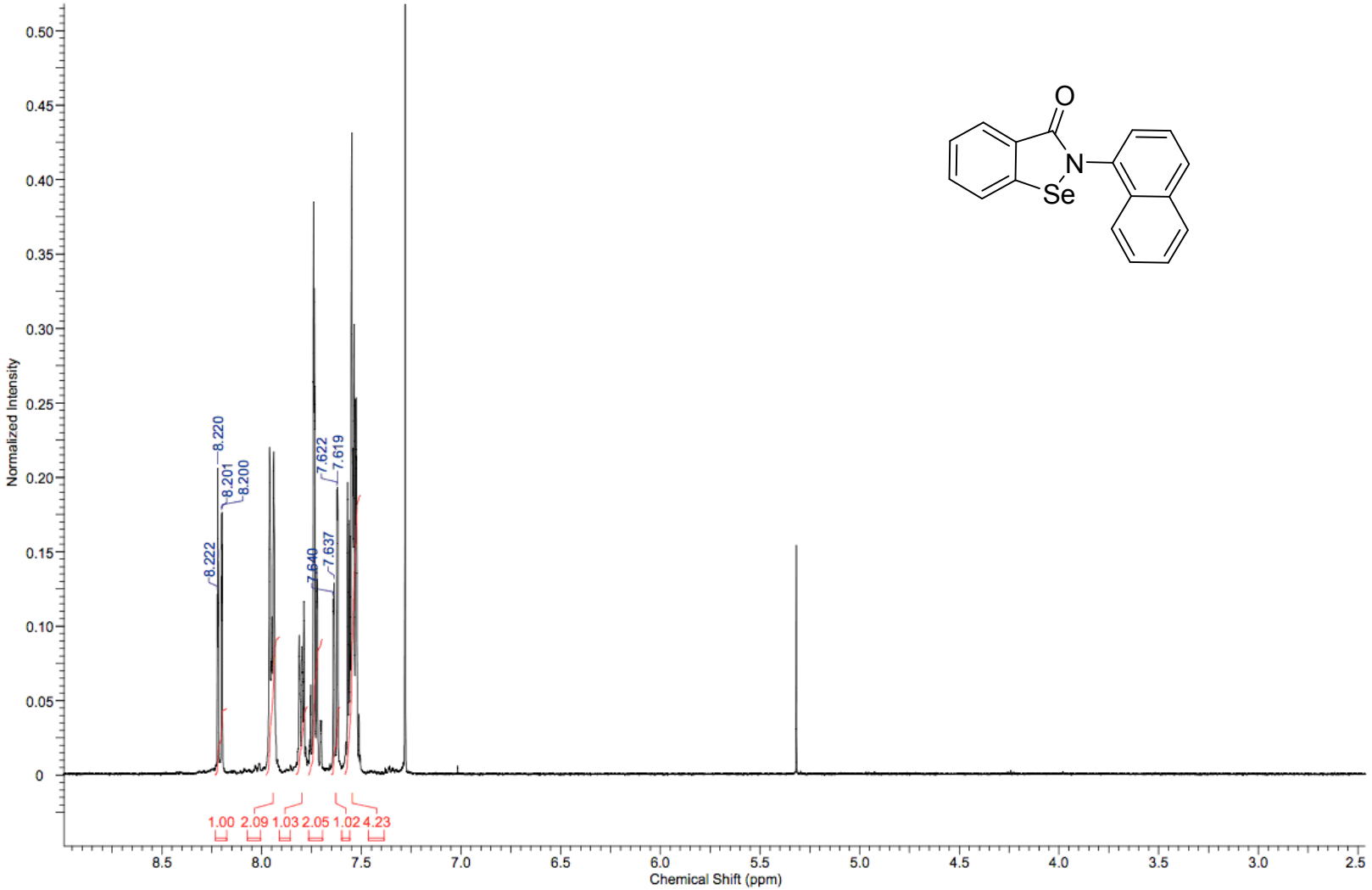
***N*-phenyl-1,2-benzisoselenazol-3(2*H*)-one (1)**



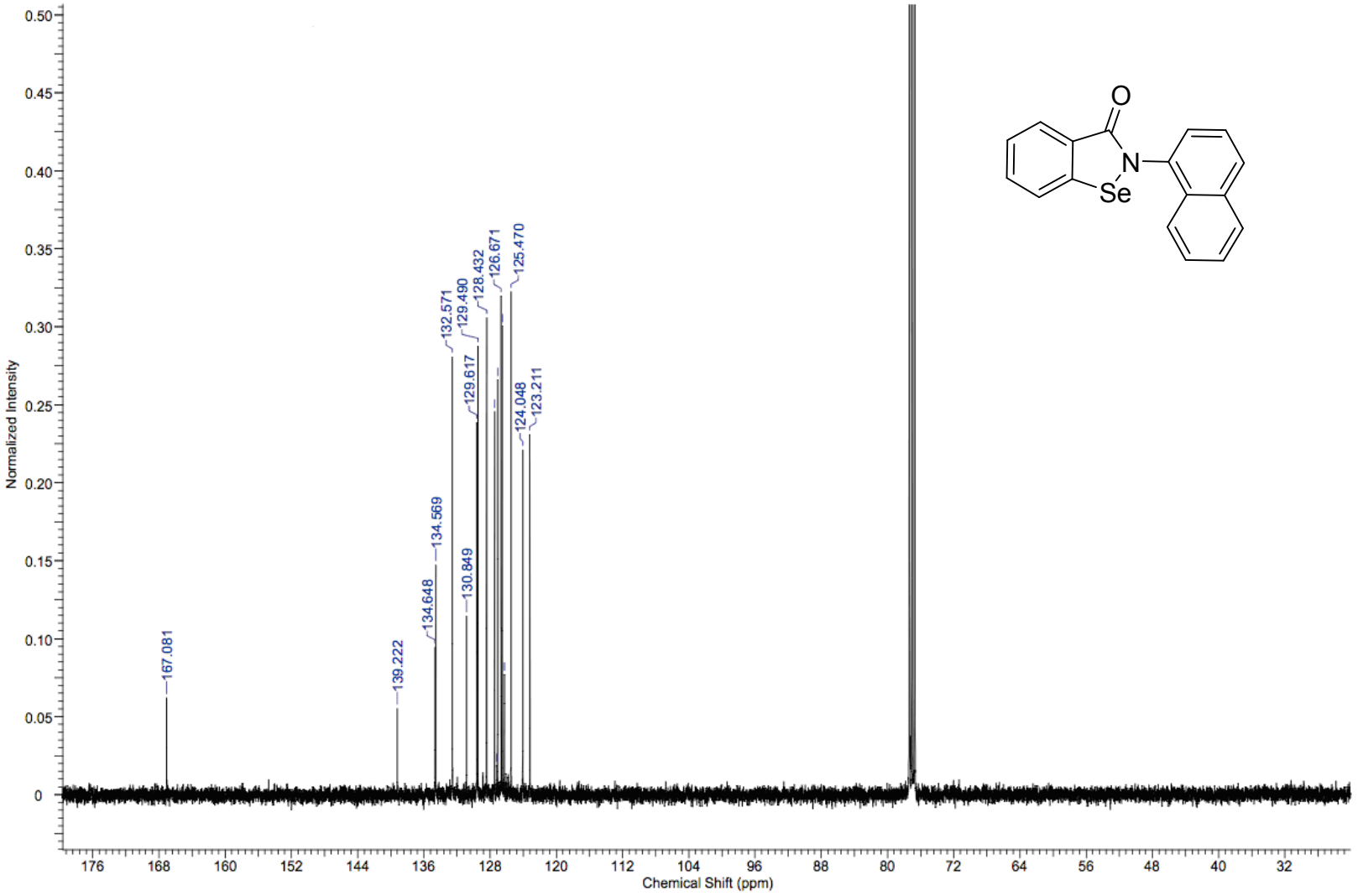
***N*-phenyl-1,2-benzisoselenazol-3(2*H*)-one (1)**



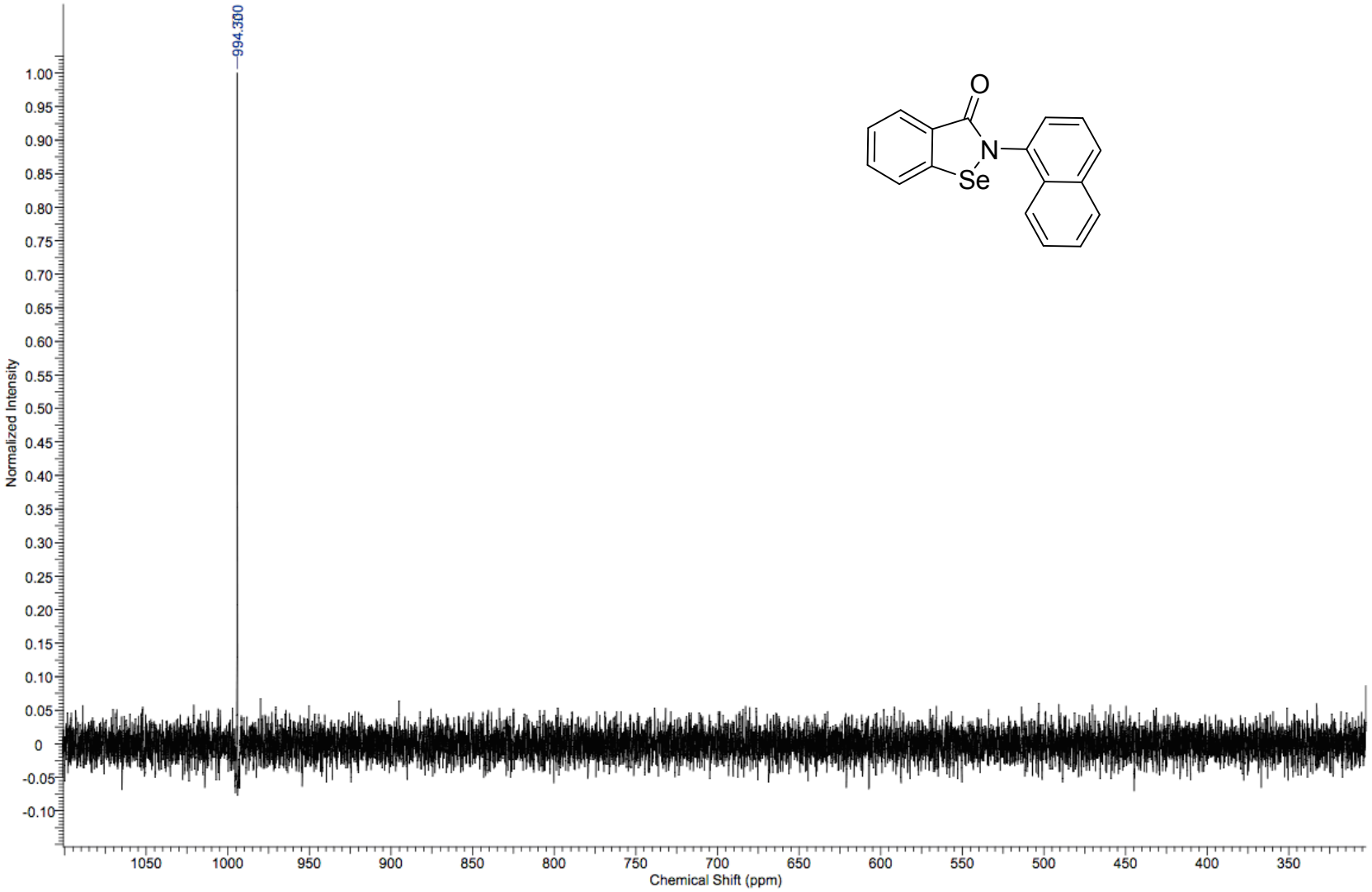
***N*-(1-naphthyl)-1,2-benzisoselenazol-3(2*H*)-one (16)**



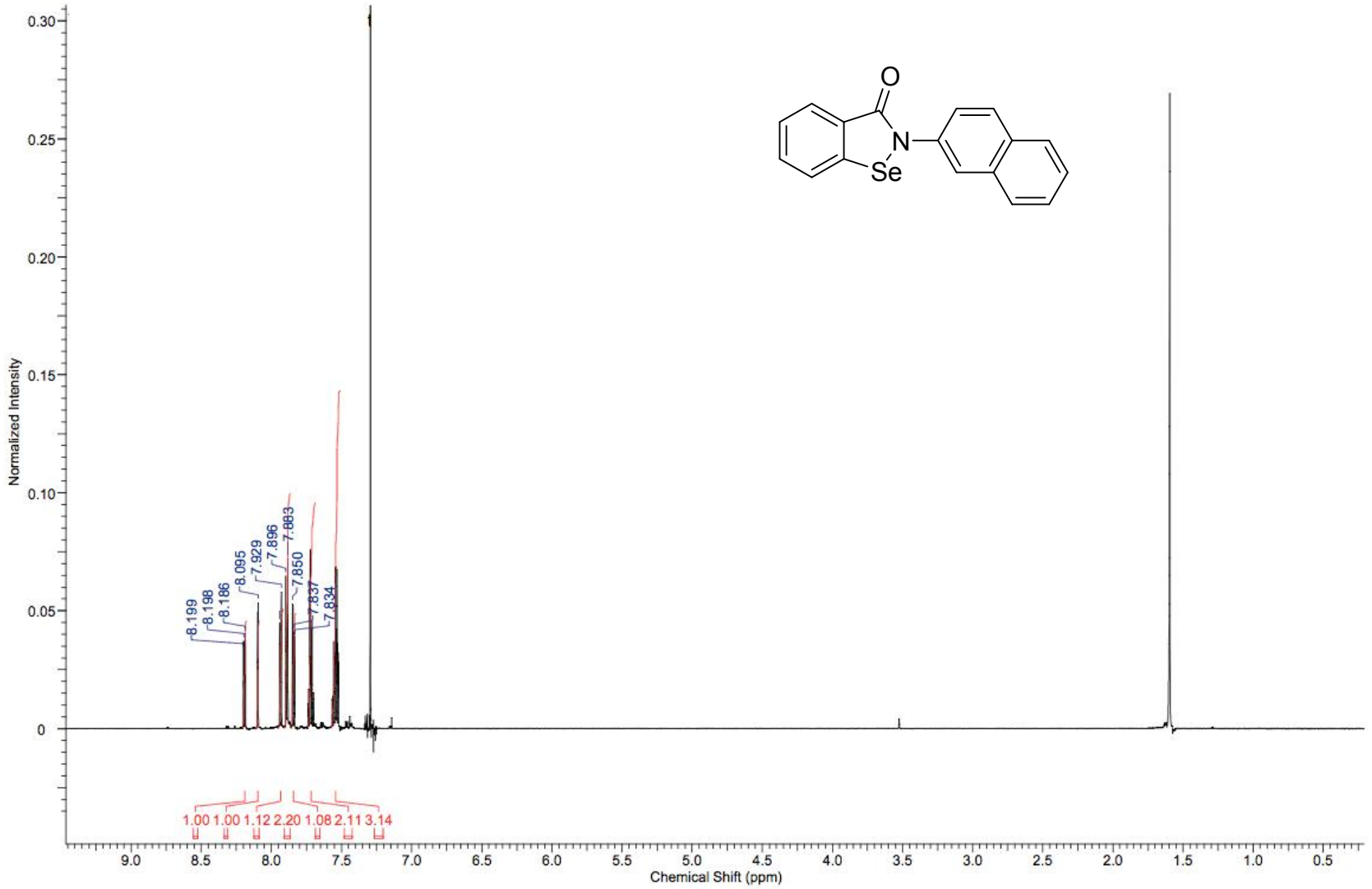
***N*-(1-naphthyl)-1,2-benzisoselenazol-3(2*H*)-one (16)**



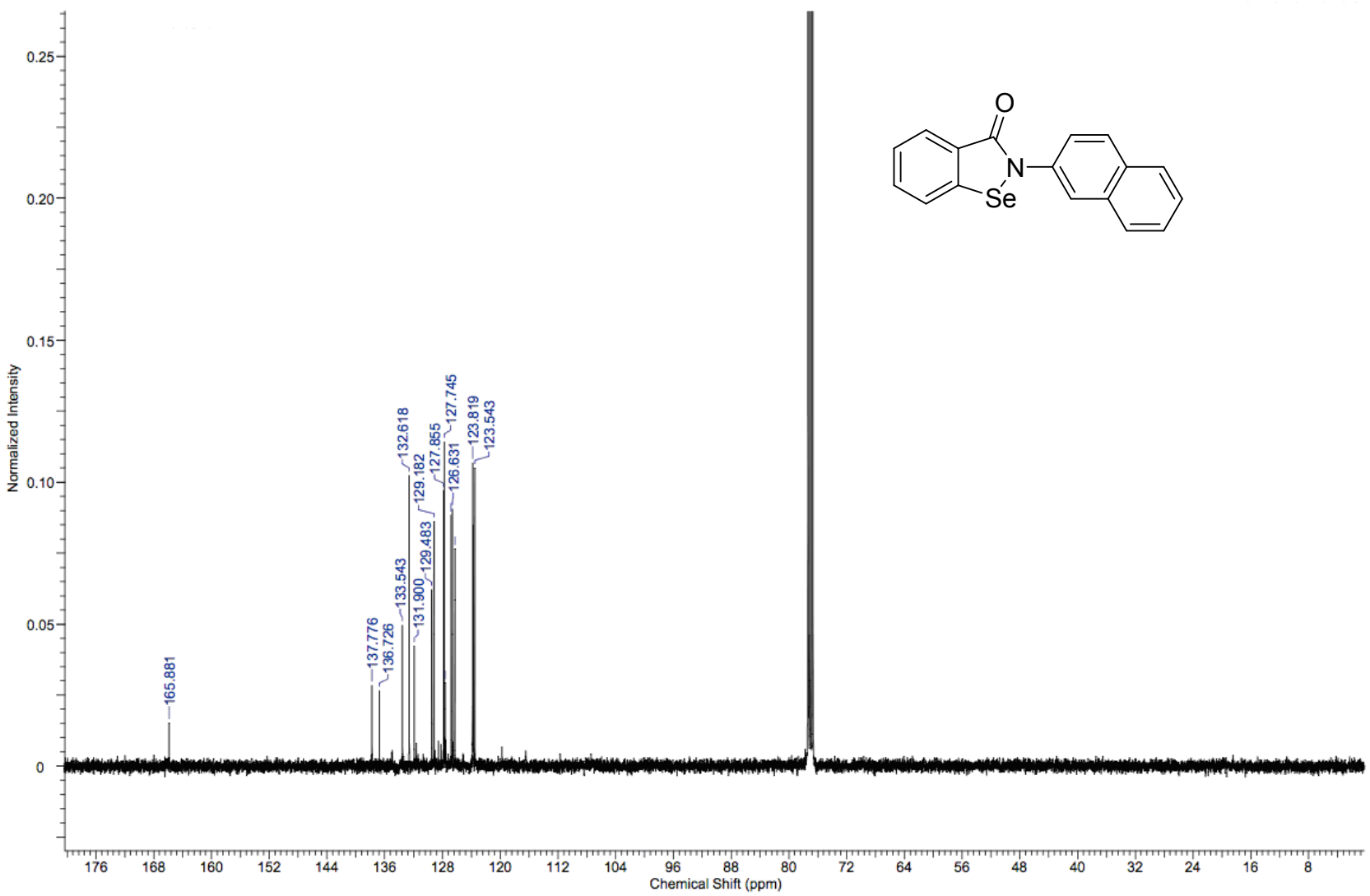
***N*-(1-naphthyl)-1,2-benzisoselenazol-3(2*H*)-one (16)**



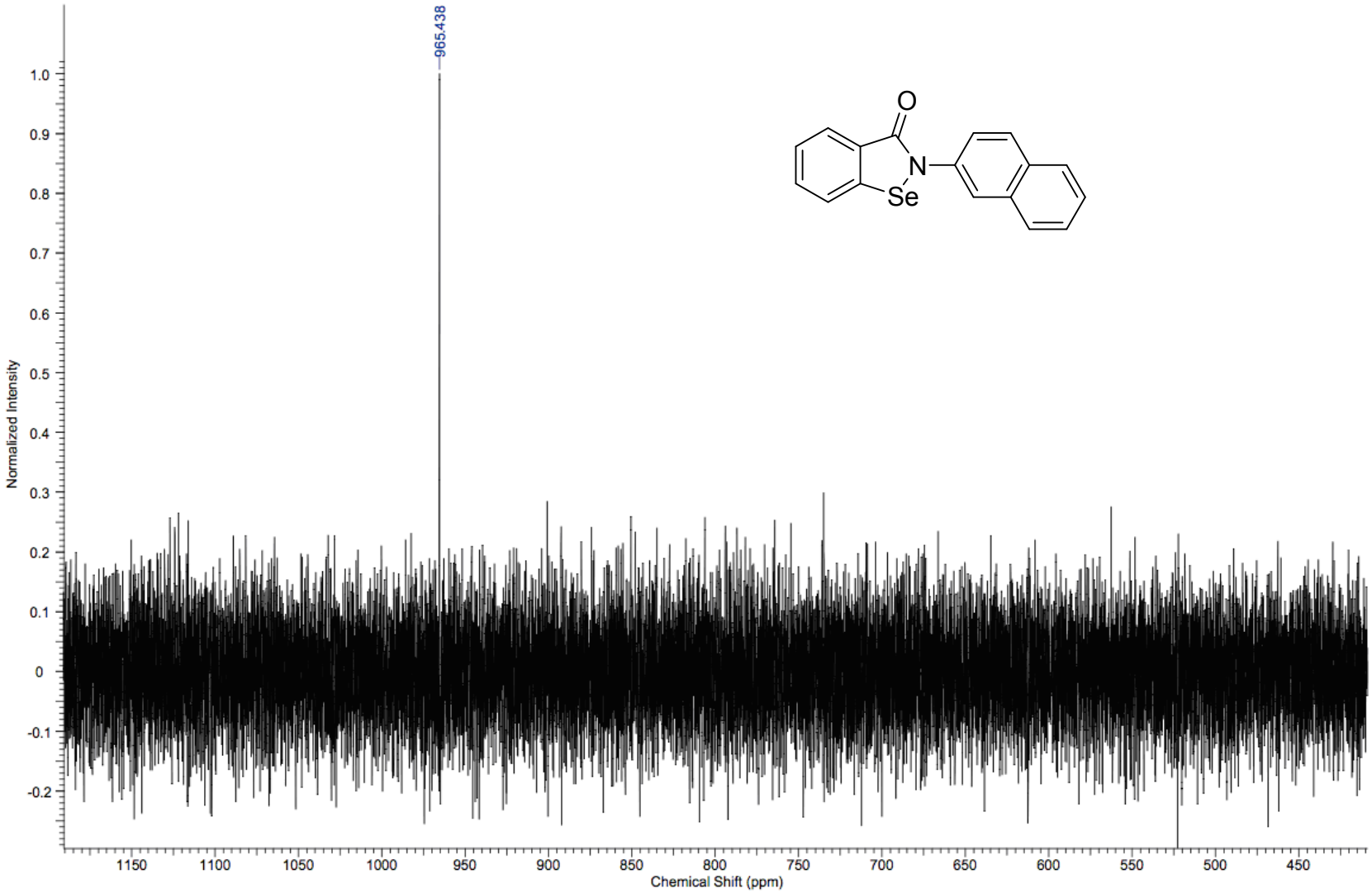
_N_-(2-naphthyl)-1,2-benzisoselenazol-3(2_H_)-one (17)



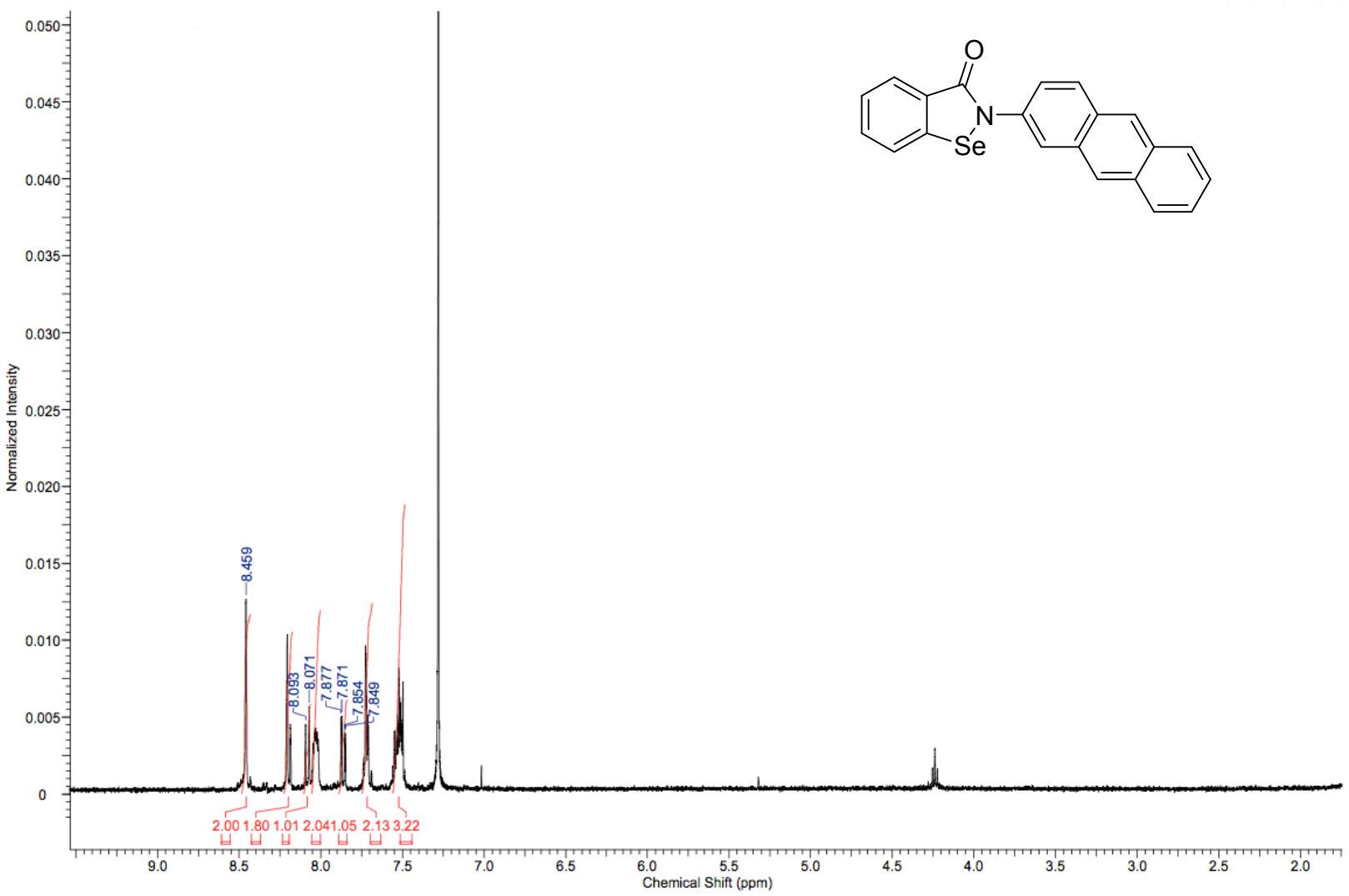
***N*-(2-naphthyl)-1,2-benzisoselenazol-3(2*H*)-one (17)**



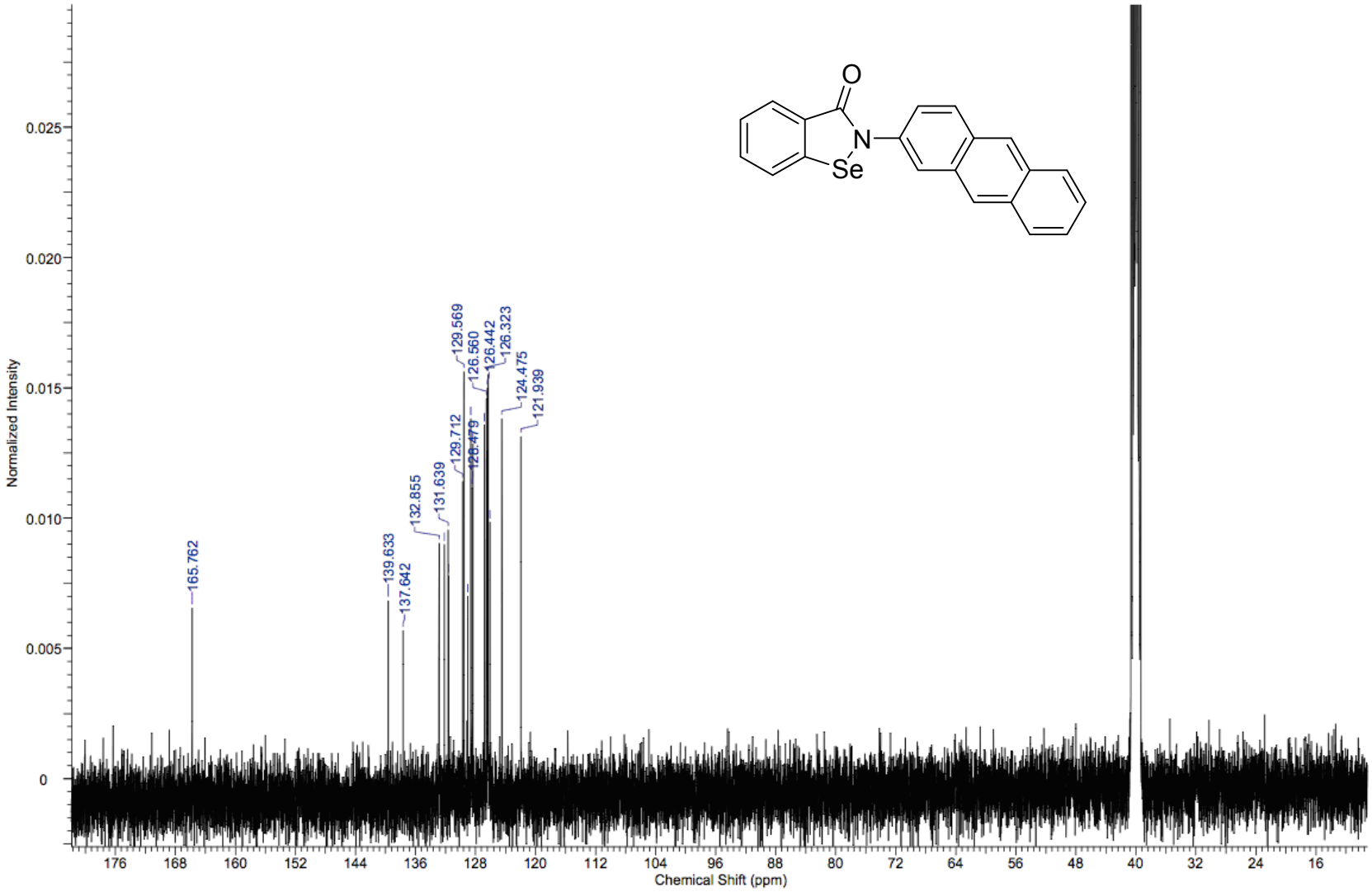
***N*-(2-naphthyl)-1,2-benzisoselenazol-3(2*H*)-one (17)**



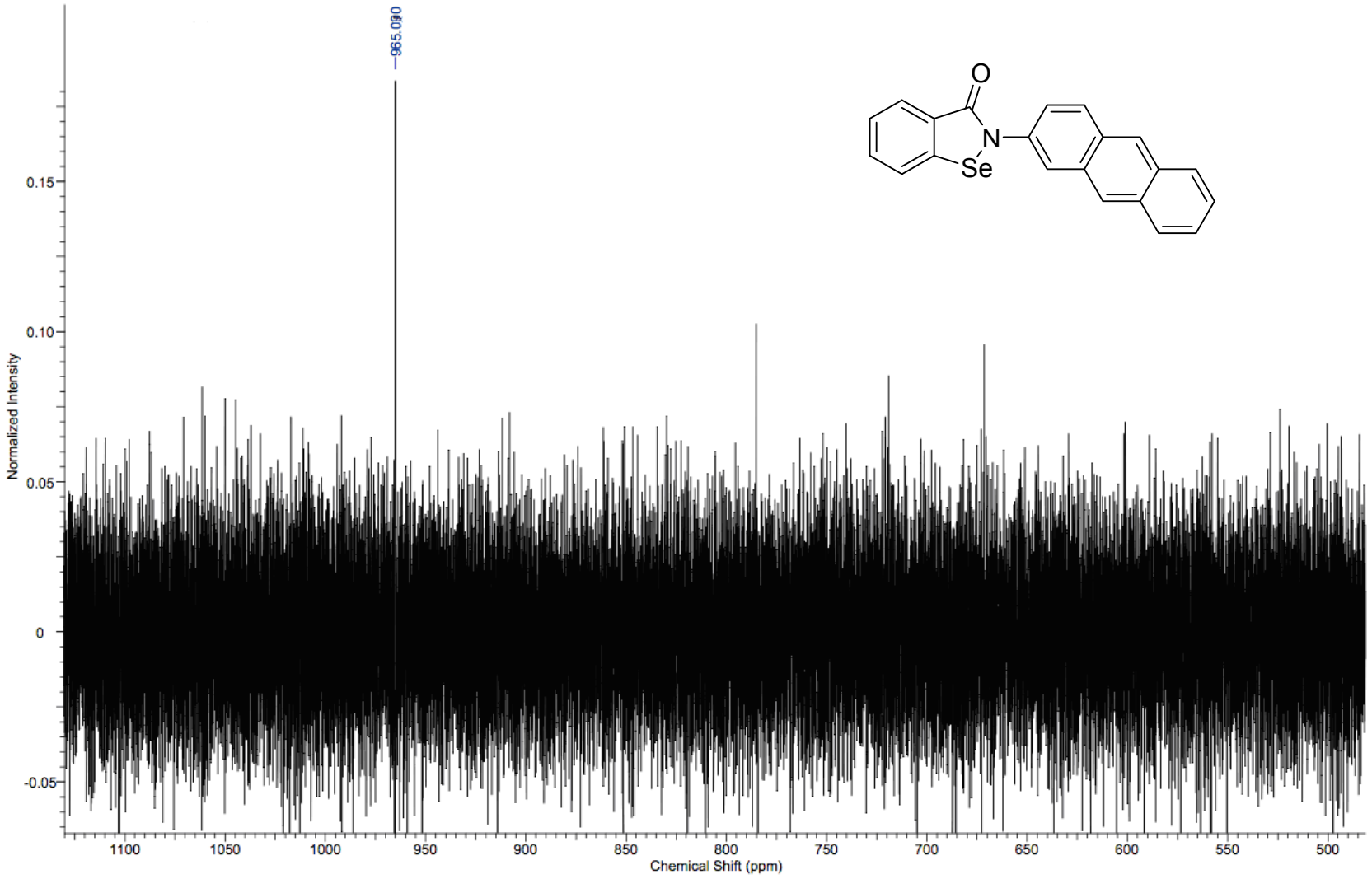
***N*-(2-antryl)-1,2-benzisoselenazol-3(2*H*)-one (18)**



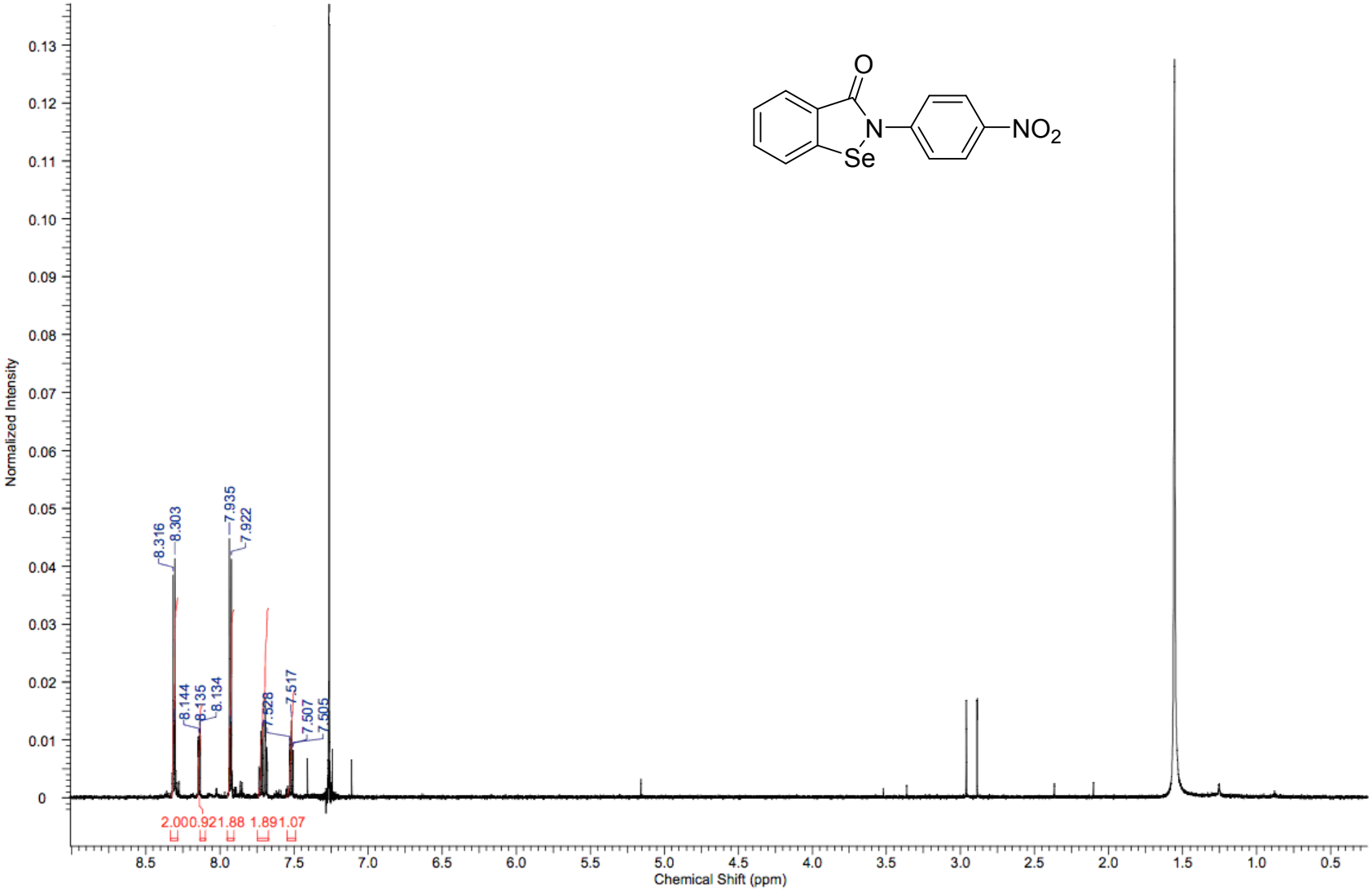
***N*-(2-antryl)-1,2-benzisoselenazol-3(2*H*)-one (18)**



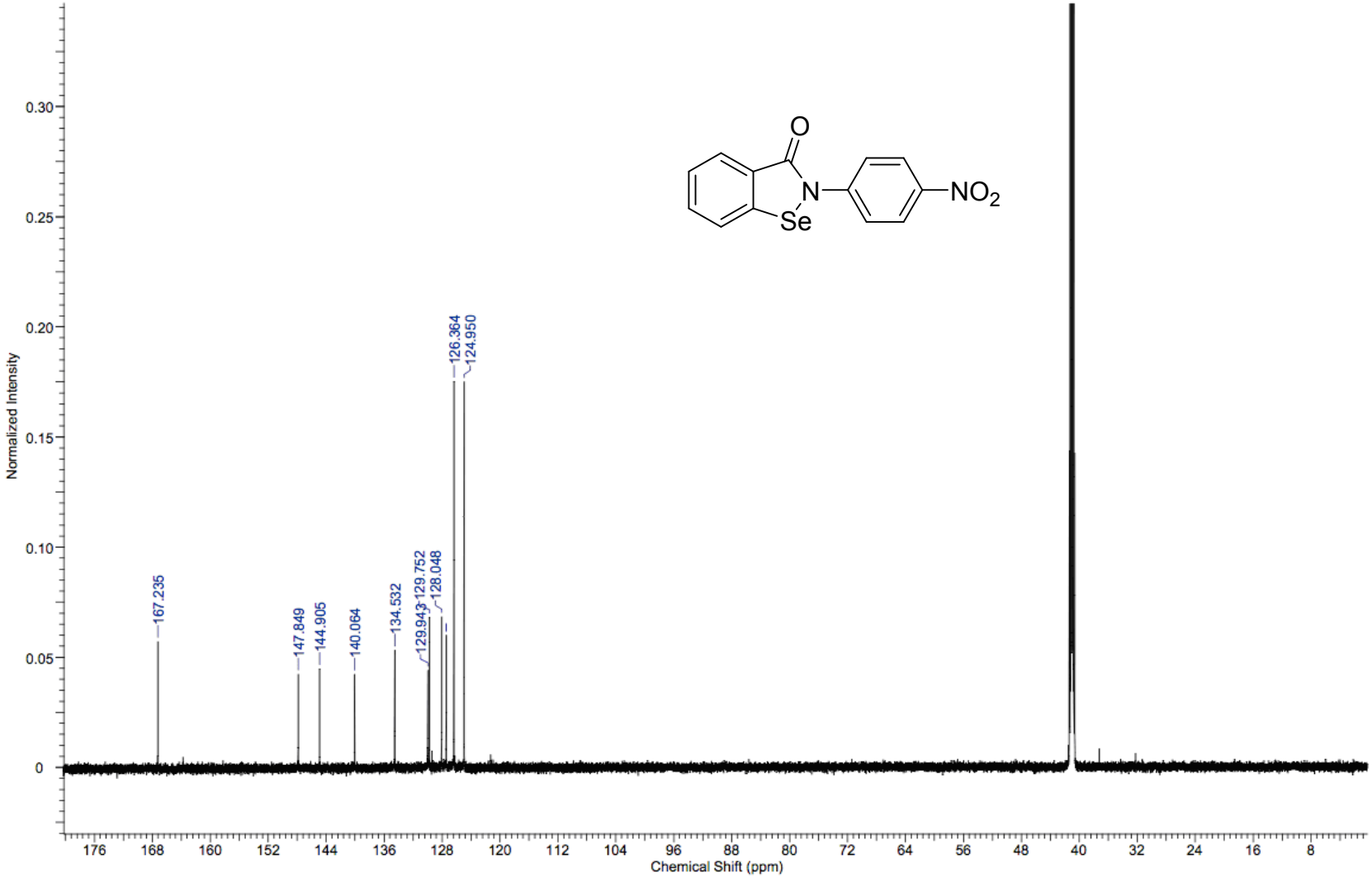
***N*-(2-antryl)-1,2-benzisoselenazol-3(2*H*)-one (18)**



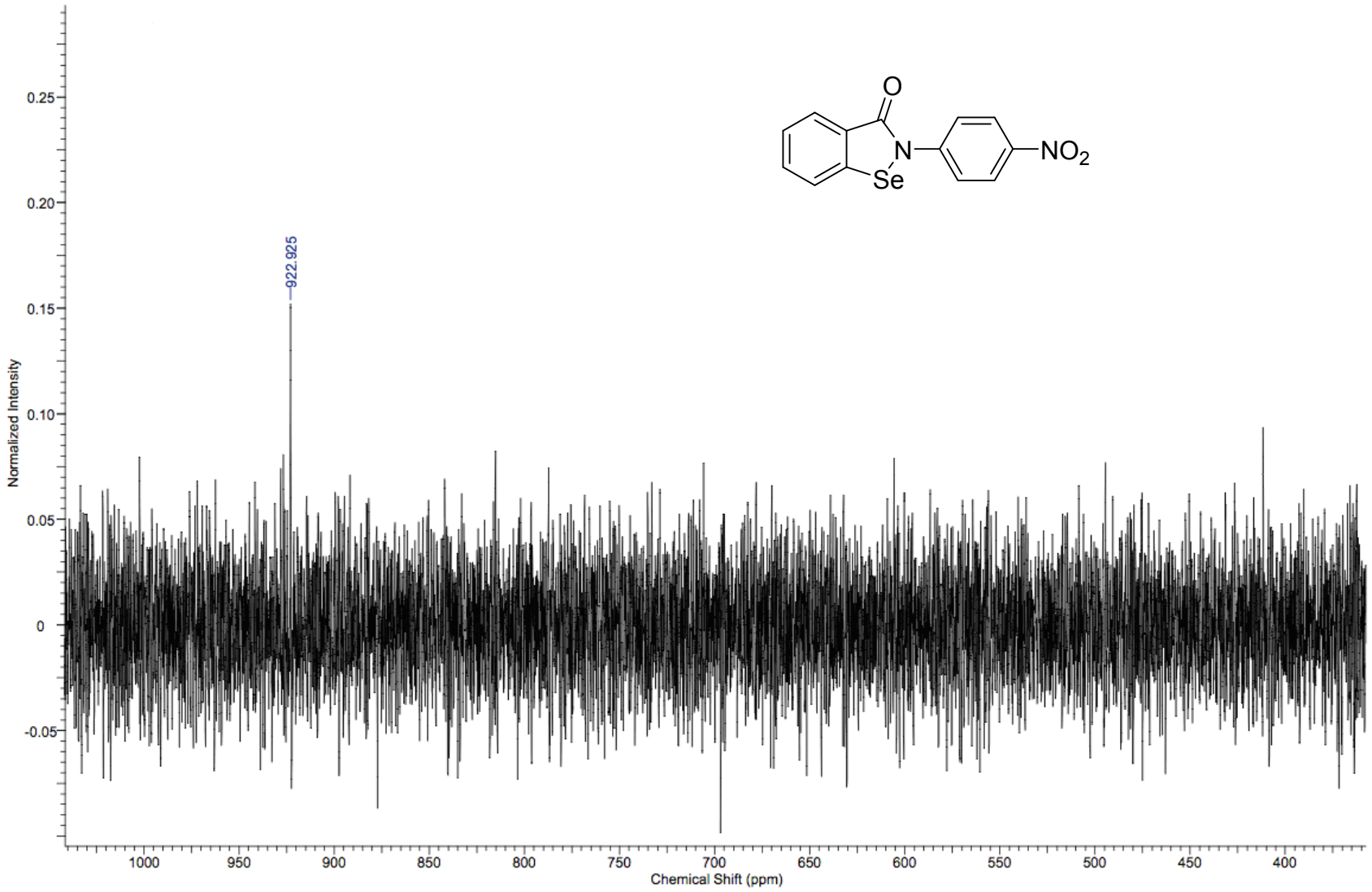
***N*-(4-nitrophenyl)-1,2-benzisoselenazol-3(2*H*)-one (19)**



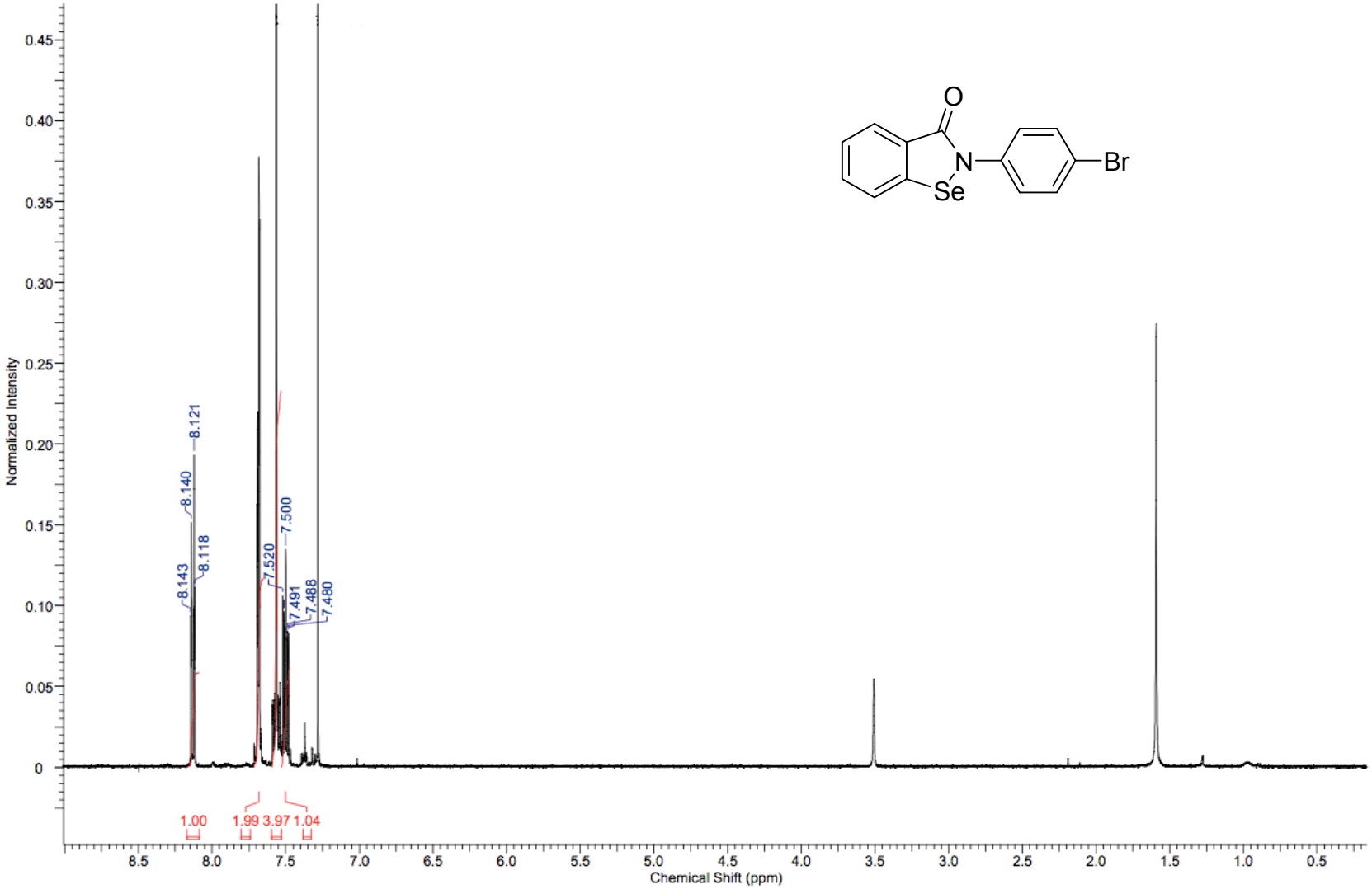
***N*-(4-nitrophenyl)-1,2-benzisoselenazol-3(2*H*)-one (19)**



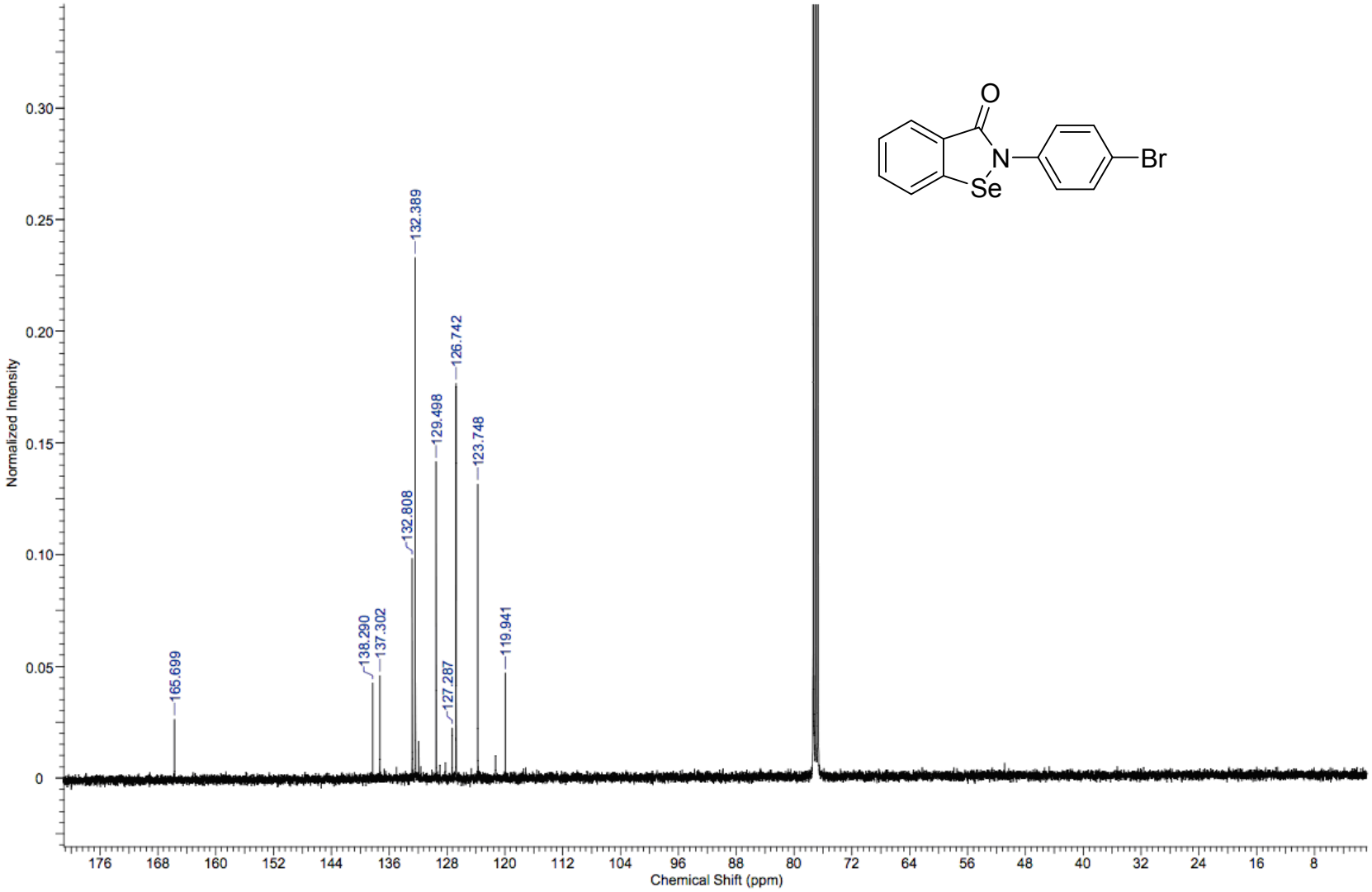
***N*-(4-nitrophenyl)-1,2-benzisoselenazol-3(2*H*)-one (19)**



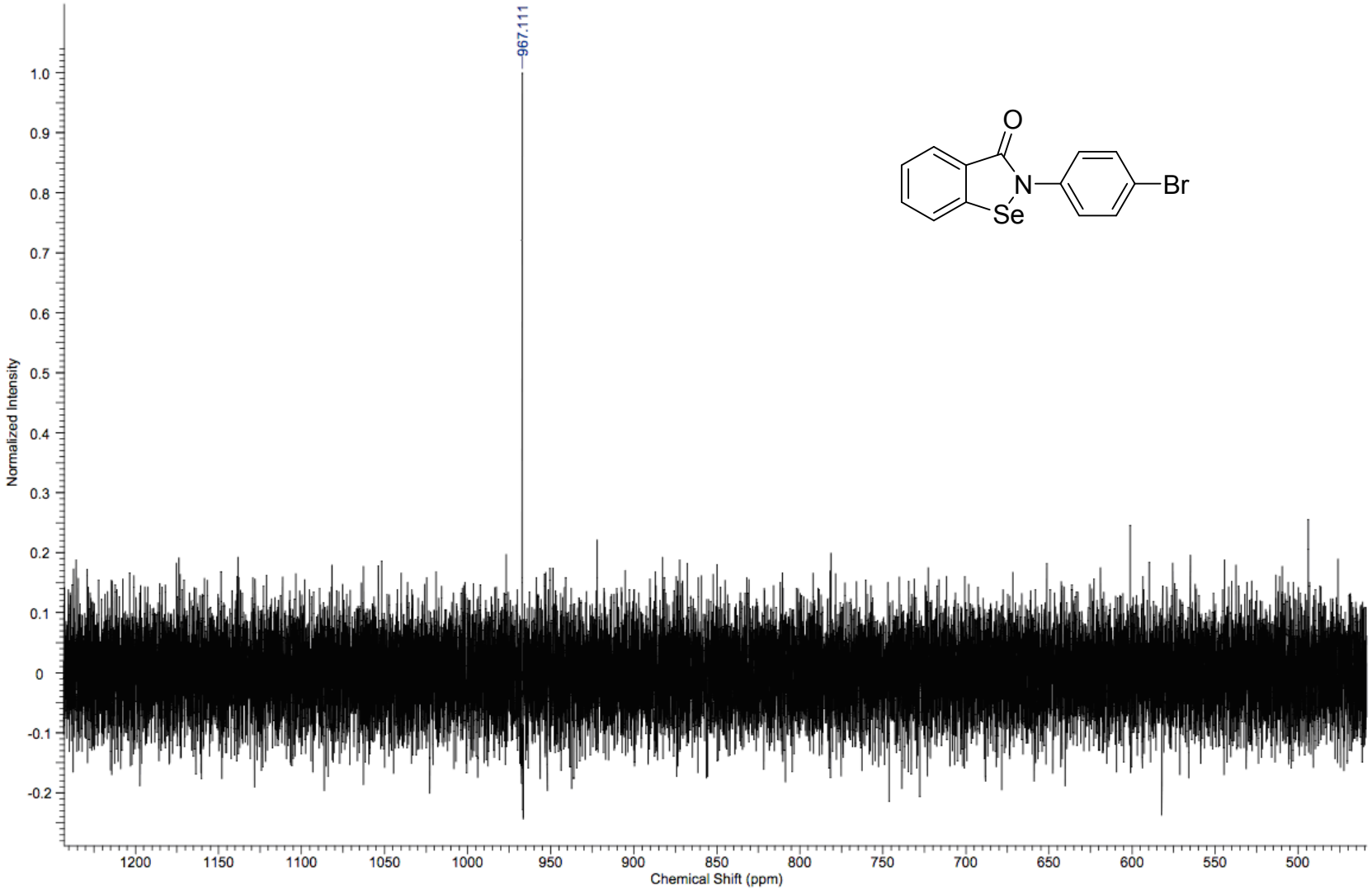
***N*-(4-bromophenyl)-1,2-benzisoselenazol-3(2*H*)-one (20)**



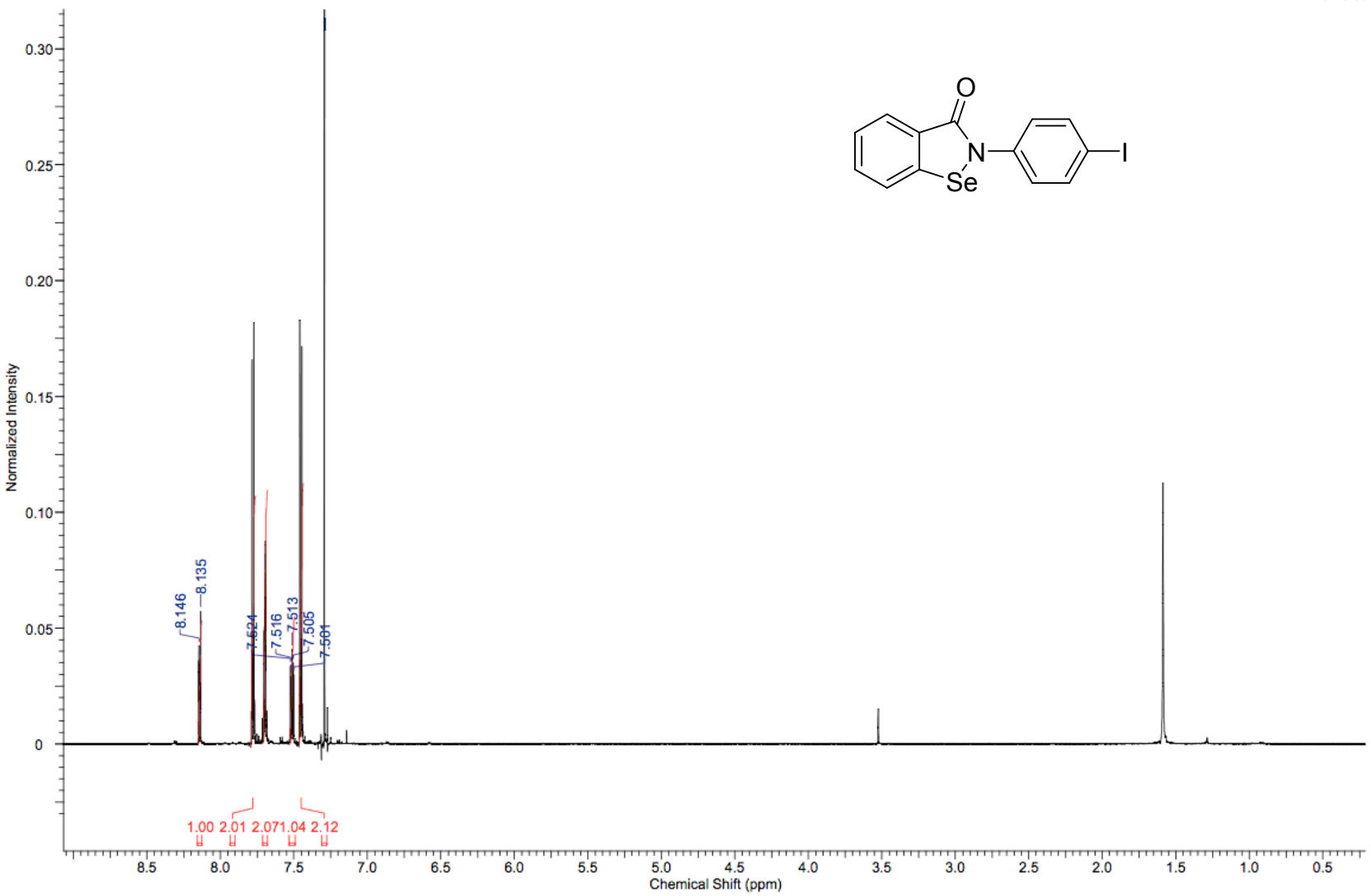
***N*-(4-bromophenyl)-1,2-benzisoselenazol-3(2*H*)-one (20)**



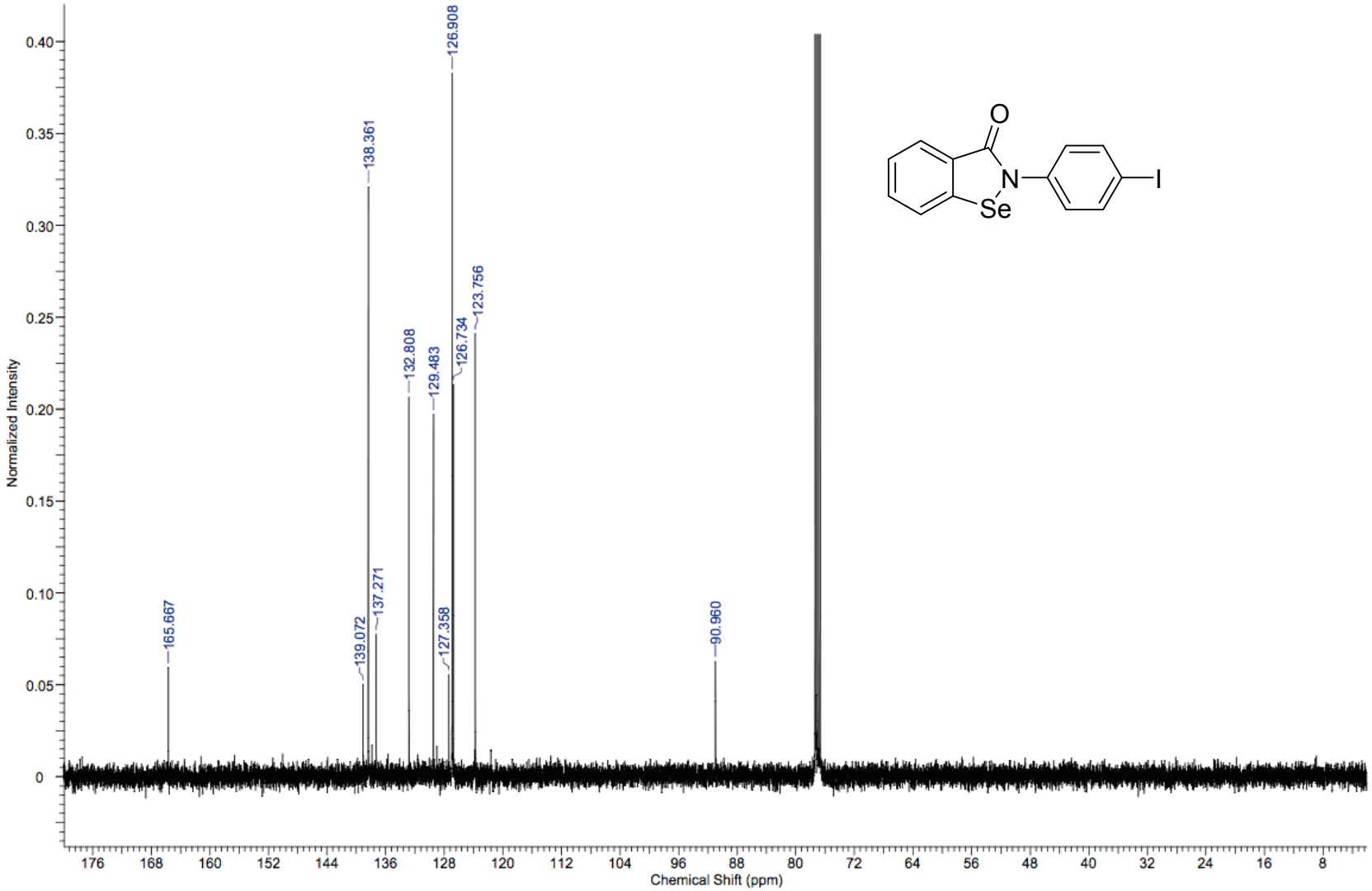
***N*-(4-bromophenyl)-1,2-benzisoselenazol-3(2*H*)-one (20)**



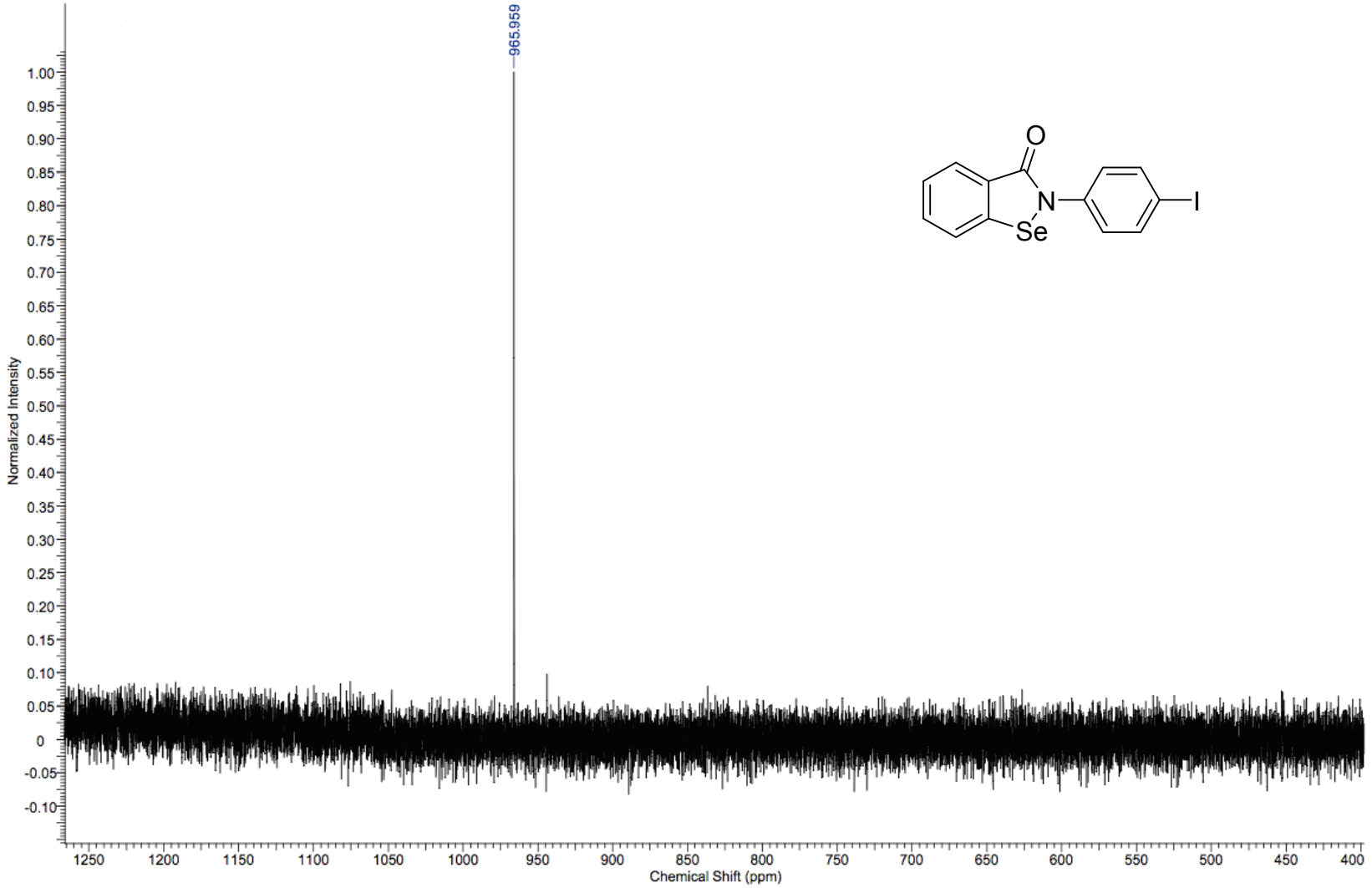
***N*-(4-iodophenyl)-1,2-benzisoselenazol-3(2*H*)-one (21)**



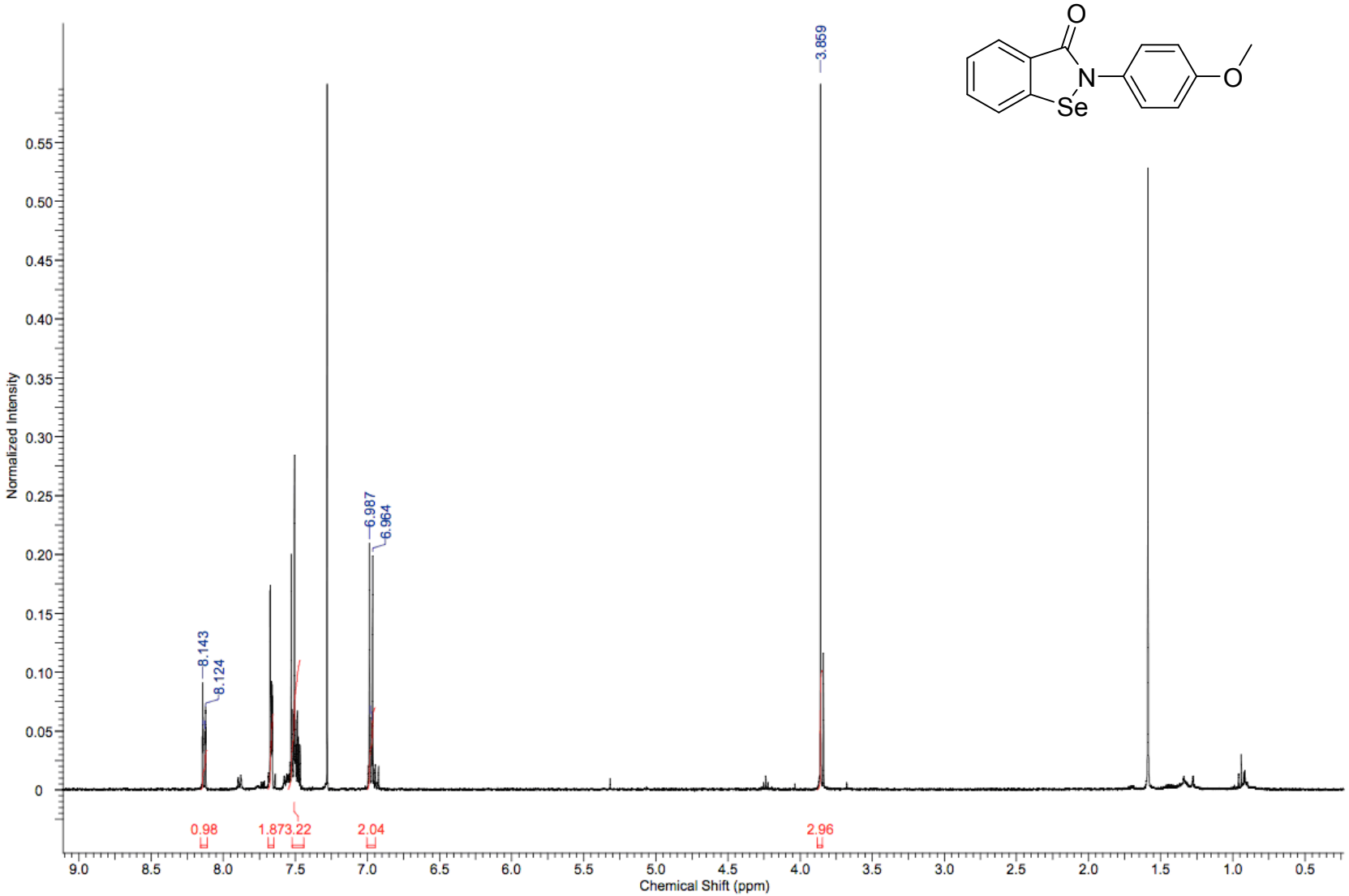
***N*-(4-iodophenyl)-1,2-benzisoselenazol-3(2*H*)-one (21)**



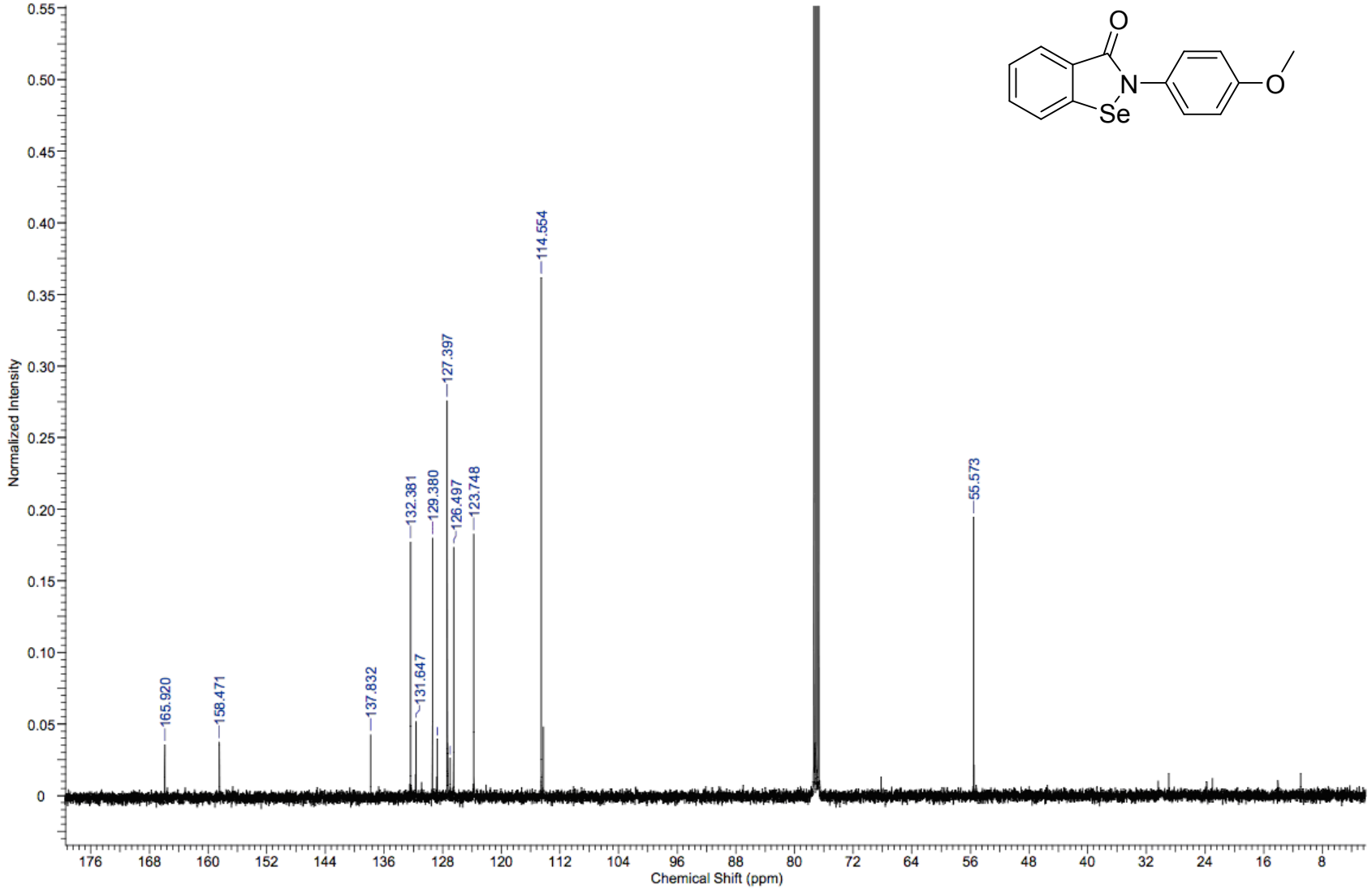
***N*-(4-iodophenyl)-1,2-benzisoselenazol-3(2*H*)-one (21)**



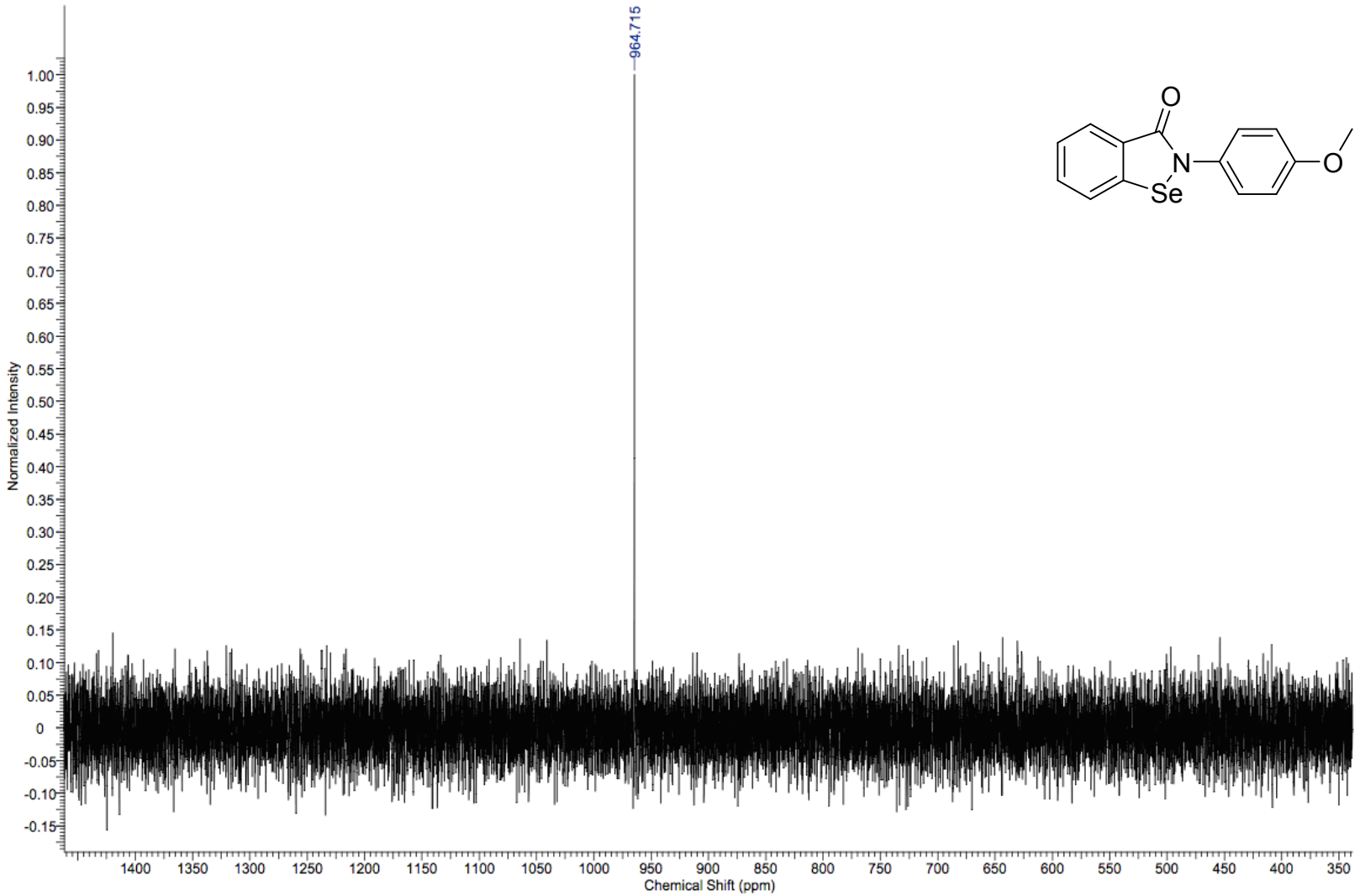
***N*-(4-methoxyphenyl)-1,2-benzisoselenazol-3(2*H*)-one (22)**



***N*-(4-methoxyphenyl)-1,2-benzisoselenazol-3(2*H*)-one (22)**



***N*-(4-methoxyphenyl)-1,2-benzisoselenazol-3(2*H*)-one (22)**



VII. References

1. N. G. Kundu and W. M. Khan, *Tetrahedron*, 2000, **56**, 4777-4792.
2. A. Varela-Fernandez, J. A. Varela and C. Saa, *Synthesis (Germany)*, 2012, **44**, 3285-3295.
3. L. Syper and J. Młochowski, *Tetrahedron*, 1988, **44**, 6119-6130.
4. PubChem CID 835976
5. E. Bellamy, O. Bayh, Ch. Hoarau, F. Trecourt, G. Queguiner and F. Marsais, *Chem. Comm.*, 2010, **46**, 7043-7045.
6. A. Soliman, *Pharmazie*, 1981, **36**, 535-537.
7. B. Yao, Q. Wang and J. Zhu, *Angew. Chem.*, 2013, **125**, 12992-12996.
8. F. Liu, X. Ding, L. Zhang, Y. Zhou, L. Zhao, H. Iiang and H. Liu, *J. Org. Chem.*, 2010, **75**, 5810-5820.
9. B. S. Bhakuni, K. Shrimali, A. Kumar and S. Kumar, *Organic Syntheses*, 2013, **90**, 164-173.
10. J. Grimshaw and R. J. Haslett, *Org. & Bio-Org. Chem.*, 1980, 657-660.
11. J. Grimshaw and R. J. Haslett, *Org. & Bio-Org. Chem.*, 1980, 657-660.
12. Grescher et al., *Org. & Bio-Org. Chem.*, 1977, 103, 105, 106.
13. G. F. Dregval, *Sov. Prog. Chem.*, 1977, **43**, 384-387, 44-46.
14. PubChem CID 3118704
15. Hey et al. *Org. & Bio-Org. Chem.*, 1972, 1162-1167.
16. M. Piętka-Ottlik, H. Wojtowicz-Młochowska, K. Kołodziejczyk, E. Piasecki and J. Młochowski, *Chem. & Pharm. Bull.*, 2008, **56**, 1423-1427.
17. M. Piętka-Ottlik, H. Wojtowicz-Młochowska, K. Kołodziejczyk, E. Piasecki and J. Młochowski, *Chem. & Pharm. Bull.*, 2008, **56**, 1423-1427.
18. Patent: US4774252A1, 1988.
19. Y. Nakashima, T. Shimizu, K. Hirabayashi and N. Kamigata, *J. Org. Chem.*, 2005, **70**, 868-873.
20. Sh. J. Balkrishna, B. S. Bhakuni, D. Chopra and S. Kumar, *Org. Lett.*, 2010, **12**, 5394-5397.
21. J. Młochowski, R. J. Gryglewski, A. D. Inglot, A. Jakubowski, L. Juchniewicz and K. Kloc, *Lieb. Ann.*, 1996, **11**, 1751-1755.
22. Sh. J. Balkrishna, B. S. Bhakuni, D. Chopra and S. Kumar, *Org. Lett.*, 2010, **12**, 5394-5397.
23. Patent: US 4618669A1, 1986.
24. K. P. Bhabak and G. Mugesh, *Chem. – Eur. J.* 2007, **13**, 4594-4601.
25. J. Młochowski, K. Kloc, L. Syper, A. D. Inglot and E. Piasecki, *Lieb. Ann. Chem.*, 1993, **12**, 1239-1244.
26. N. Kamigata, H. Iizuka, A. Izuoka and M. Kobayashi, *Bull. Chem. Soc. Jap.*, 1986, **59**, 2179-2184.