Electronic Supplementary Information

A general phosphoric acid-catalyzed desymmetrization of *meso*-aziridines with silylated selenium nucleophiles

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Contents

1. General information

All the aziridines desymmetrizations were performed in flame-dried Schlenk tubes, under a dry nitrogen atmosphere and with magnetic stirring. Reactions were monitored by thin layer chromatography (TLC) on Merck silica gel plates (0.25 mm) and visualized by UV light or by phosphomolybdic acid/ethanol spray test. Flash chromatography was performed on Merck silica gel (60, particle size: 0.040–0.063 mm). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker DRX 400 300 spectrometer at room temperature in $CDCl_3$, acetone-d_6 or CD_3OD as solvents. Chemical shifts for protons are reported using residual $CHCl_3$ (δ 7.26) or CHD_2COD_3 (δ 2.04) as internal reference. Carbon spectra are referenced to the shift of the ^{13}C signal of $CDCl_3$ (δ 77.0) or acetone-d_6 (δ 206.7). Optical rotations measurements were performed on a Jasco DIP-1000 digital polarimeter using the Na lamp. ESI-MS was performed using a Bio-Q triple quadrupole mass spectrometer (Micromass, Manchester, UK) equipped with an electrospray ion source. Melting points are uncorrected. Elemental analyses were carried out by using Flash EA 1112 (Thermo Electron Corporation) analyzer. Enantiomeric excesses were measured by HPLC (Jasco PU-2089 quaternary gradient pump equipped with an MD-2010 plus adsorbance detector) using Daicel Chiralcel AD-H and AS-H chiral columns.

All the solvents used in moisture sensitive reactions were distilled over calcium hydride and stored over activated molecular sieves, except for anhydrous 1,2-dichloroethane and acetonitrile which were purchased from Aldrich, and anhydrous chlorobenzene which was purchased from Fluka. Benzeneselenol (**5**) was purchased from Aldrich. (*R*)-VAPOL hydrogen phosphate (**1**)[1], (phenylseleno)-*t*-butyldimethylsilane (**4a**)[2] and (phenylseleno)trimethylsilane (**4b**)[3] were prepared according to literature procedures. All the acylaziridines **2a-h** were synthesized as described in literature, by opening of epoxides with sodium azide, followed by Staudinger rearrangement of azido alcohols and then in situ acylation of unsubstituted aziridines with aroyl chlorides and triethyl amine.[3] The characterization data of aziridines **2a-d,f-h**,[4] and **2e**[5] were identical to those previously

reported.

2. General procedure for the desymmetrization of aziridines 3a-h with (phenylseleno)trimethylsilane/benzeneselenol

To a solution of (phenylseleno)trimethylsilane (**4b**; 0.040-0.080 mmol) in anhydrous toluene (0.8 mL), under nitrogen, (*R*)-VAPOL hydrogen phosphate ((*R*)-**1**; 0.0080-0.016 mmol) was added. The mixture was stirred at room temperature for 10 min, after which the solid dissolved. Benzeneselenol (**5**; 0.040-0.080 mmol) was introduced, and the mixture was brought to 0-20°C. The aziridine **2** (0.080-0.120 mmol) was finally added and the mixture immediately turned red-brown. Precipitation of *N*-dinitrobenzoyl derivatives **3a-h** was observed as the reaction proceeded.

Method A: **4b** (0.040 mmol), **5** (0.080 mmol), (*R*)-**1** (0.0080 mmol), **2** (0.080 mmol), toluene (0.8 mL).

Method B: **4b** (0.080 mmol), **5** (0.160 mmol), (*R*)-**1** (0.016 mmol), **2** (0.080 mmol), toluene (0.8 mL).

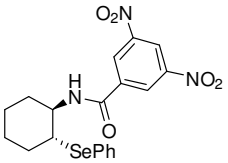
Method C: **4b** (0.040 mmol), **5** (0.040 mmol), (*R*)-**1** (0.0080 mmol), **2** (0.120 mmol), toluene (0.8 mL).

The reaction mixture was diluted with CH_2Cl_2 until dissolution of the precipitate and the solution was passed through a plug of silica gel eluting with CH_2Cl_2 (3 mL) and then ethyl acetate (3 mL). The solvent was removed under reduced pressure and the residue was purified by flash-chromatography.

3. Characterization data for all the the products

(1*R*,2*R*)-1-Phenylseleno-2-[*N*-(3,5-dinitrobenzoyl)amino]cyclohexane (3a).

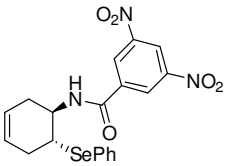
Prepared by following the general procedure (method A, 0°C). Purification by FC (silica gel, $CHCl_3$) gave **3a** as a pale yellow solid (334 mg, 92% yield); mp 176-177°C; $[\alpha]^{21}_D$ −109.3 (*c* 0.6,



3a

CH_2Cl_2, 99% *ee*); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.13 (t, J = 2.1 Hz, 1H), 8.76 (d, J = 2.1 Hz, 2H), 7.52 (m, 2H), 7.21-7.15 (m, 3H), 6.26 (d, J = 7.7 Hz, 1H), 4.06 (m, 1H), 3.22 (m, 1H), 2.35-2.22 (m, 2H), 1.86-1.72 (m, 2H), 1.68-1.52 (m, 2H), 1.51-1.25 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.8, 148.5, 138.0, 134.9, 129.2, 128.2, 127.9, 127.0, 120.9, 55.6, 47.7, 34.1, 33.8, 26.8, 24.7; MS (ESI): *m*/*z* 488 $[M+K]^+$, 292 $[M+H-PhSeH]^+$; elemental analysis calcd. (%) for $C_{19}H_{19}N_3O_5Se$: C 50.90, H 4.27, N 9.37, Se 17.61; found: C 50.82, H 4.18, N 9.44, Se 17.71; HPLC (Chiralcel AD-H, hexane/*i*PrOH 85:15, flow 1.0 mL/min): t_R = 13.5 min (minor), 19.6 min (major).

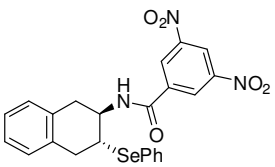
(1*R*,2*R*)-4-Phenylseleno-5-[*N*-(3,5-dinitrobenzoyl)amino]cyclohexene (3b).



3b

Prepared by following the general procedure (method A, 0°C). Purification by FC (silica gel, gradient: $CHCl_3$ to $CHCl_3$/acetone 90:10) afforded **3b** as a pale yellow solid (26.7 mg, 73% yield); mp 169-170°C; $[\alpha]^{28}_D$ −126.0 (*c* 0.6, acetone, 95% *ee*); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.06 (t, J = 2.1 Hz, 1H), 9.00 (d, J = 2.1 Hz, 2H), 8.48 (d, J = 7.8 Hz, 1H), 7.60 (m, 2H), 7.27-7.21 (m, 3H), 5.71-5.59 (m, 2H), 4.42 (m, 1H), 3.79 (m, 1H), 2.72-2.57 (m, 2H), 2.42-2.30 (m, 2H); ^{13}C NMR (100 MHz, acetone-d_6): δ 163.4, 150.1, 139.3, 136.0, 130.5, 130.0, 128.9, 128.8, 127.2, 126.1, 122.1, 51.7, 44.1, 33.8, 32.8; MS (ESI): *m*/*z* 290 $[M+H-PhSeH]^+$; elemental analysis calcd. (%) for $C_{19}H_{17}N_3O_5Se$: C 51.13, H 3.84, N 9.41, Se 17.92; found: C 51.27, H 4.06, N 9.17, Se 17.78; HPLC (Chiralcel AS-H, hexane/*i*PrOH 80:20, flow 1.0 mL/min): t_R = 15.7 min (major), 28.0 min (minor).

(1*R*,2*R*)-2-Phenylseleno-3-[*N*-(3,5-dinitrobenzoyl)amino]tetralin (3c).

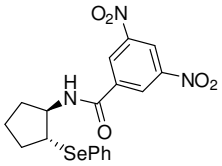


3c

Prepared by following the general procedure (method A, 0°C). Purification by FC (silica gel, $CHCl_3$) afforded **3c** as a pale yellow solid (25.4 mg, 74% yield); mp 244-245°C (dec.); $[\alpha]^{28}_D$ −9.7 (*c* 0.6, acetone, 98% *ee*); ^{1}H NMR (400 MHz, acetone-d_6): δ 9.07-9.02 (m, 3H), 8.69 (d, J = 7.7 Hz, 1H), 7.66 (m, 2H), 7.30-7.25 (m,

3H), 7.17-7.03 (m, 4H), 4.63 (m, 1H), 4.02 (dt, J = 9.1, 5.2 Hz, 1H), 3.48-3.35 (m, 2H), 3.13-3.02 (m, 2H); ^{13}C NMR (100 MHz, acetone-d_6): δ 163.6, 150.1, 139.4, 136.1, 135.9, 135.3, 130.6, 130.3, 130.1, 129.9, 129.0, 128.9, 127.7 (2C), 122.2, 52.1, 44.1, 36.8, 35.8; MS (ESI): m/z 340 $[M+H-PhSeH]^+$; elemental analysis calcd. (%) for $C_{23}H_{19}N_3O_5Se$: C 55.65, H 3.86, N 8.47, Se 15.91; found: C 55.57, H 3.93, N 8.38, Se 16.06; HPLC (Chiralcel AD-H, hexane/*i*PrOH 80:20, flow 1.0 mL/min): t_R = 16.8 min (major), 23.8 min (minor).

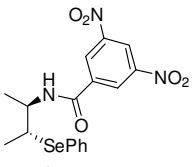
(1*R*,2*R*)-1-Phenylseleno-2-[*N*-(3,5-dinitrobenzoyl)amino]cyclopentane (3d).



3d

Prepared by following the general procedure (method A, 0°C). Purification by FC (silica gel, $CHCl_3$) gave **3d** as a pale yellow solid (31.7 mg, 90% yield); mp 178-180°C; $[\alpha]^{26}_D$ –82.6 (c 0.6, CH_2Cl_2, 96% *ee*); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.12 (t, J = 2.1 Hz, 1H), 8.72 (d, J = 2.1 Hz, 2H), 7.61 (m, 2H), 7.24-7.15 (m, 3H), 6.19 (d, J = 7.0 Hz, 1H), 4.40 (quint, J = 8.0 Hz, 1H), 3.48 (m, 1H), 2.40-2.33 (m, 2H), 1.89-1.72 (m, 3H), 1.58 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.3, 148.5, 137.7, 135.1, 129.2, 128.3, 127.9, 127.0, 120.9, 59.5, 46.3, 31.8, 31.3, 22.1; MS (ESI): m/z 474 $[M+K]^+$, 278 $[M+H-PhSeH]^+$; elemental analysis calcd. (%) for $C_{18}H_{17}N_3O_5Se$: C 49.78, H 3.95, N 9.68, Se 18.18; found: C 49.81, H 4.00, N 9.44, Se 18.08; HPLC (Chiralcel AS-H, hexane/*i*PrOH 80:20, flow 1.0 mL/min): t_R = 21.8 min (major), 40.1 min (minor).

(1*R*,2*R*)-2-Phenylseleno-3-[*N*-(3,5-dinitrobenzoyl)amino]butane (3e).

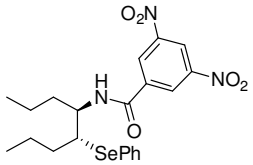


3e

Prepared by following the general procedure (method A, 20°C). Purification by FC (silica gel, $CHCl_3$) gave **3e** as a pale yellow solid (27.9 mg, 72% yield); mp 142-143°C; $[\alpha]^{27}_D$ –49.7 (c 0.6, $CHCl_3$, 92% *ee*); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.15 (t, J =2 .1 Hz, 1H), 8.84 (d, J = 2.1 Hz, 2H), 7.60 (m, 2H), 7.29-7.24 (m, 3H), 6.50 (d, J = 8.2 Hz, 1H), 4.42 (m, 1H), 3.57 (ddd, J = 14.3, 7.1, 5.0 Hz, 1H), 1.50 (d, J = 7.1 Hz, 3H), 1.37 (d, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.1, 148.6, 137.9, 134.8, 12.4, 128.3, 128.0, 127.1,

121.0, 51.7, 44.9, 19.5, 19.4; MS (ESI): *m*/*z* 462 $[M+K]^+$, 266 $[M+H-PhSeH]^+$; elemental analysis calcd. (%) for $C_{17}H_{17}N_3O_5Se$: C 48.35, H 4.06, N 9.95, Se 18.70; found: C 48.20, H 3.92, N 10.14, Se 18.52; HPLC (Chiralcel AS-H, hexane/*i*PrOH 80:20, flow 1.0 mL/min): t_R = 13.6 min (major), 24.1 min (minor).

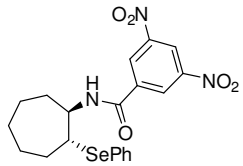
(1*R*,2*R*)-4-Phenylseleno-5-[*N*-(3,5-dinitrobenzoyl)amino]octane (3f).



3f

Prepared by following the general procedure (method A, 20°C). Purification by FC (silica gel, gradient: petroleum ether/ethyl acetate 95:5 to 90:10) gave **3f** as a pale yellow solid (23.6 mg, 66% yield); mp 94-96°C; $[\alpha]^{27}_D$ +30.2 (*c* 0.6, $CHCl_3$, 84% *ee*); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.15 (t, *J* = 2.1 Hz, 1H), 8.83 (d, *J* = 2.1 Hz, 2H), 7.62 (m, 2H), 7.31-7.22 (m, 3H), 6.45 (d, *J* = 9.1 Hz, 1H), 4.45 (m, 1H), 3.39 (m, 1H), 1.77-1.50 (m, 6H), 1.42-1.17 (m, 2H), 0.94 (t, *J* = 7.0 Hz, 3H), 0.85 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.3, 148.6, 138.0, 134.7, 129.4, 129.1, 128.0, 127.0, 121.0, 54.4, 52.1, 36.7, 35.9, 21.3, 19.4, 13.7, 13.7; MS (ESI): *m*/*z* 518 $[M+K]^+$, 322 $[M+H-PhSeH]^+$; elemental analysis calcd. (%) for $C_{21}H_{25}N_3O_5Se$: C 52.72, H 5.27, N 8.78, Se 16.51; found: C 52.68, H 5.36, N 8.66, Se 16.44; HPLC (Chiralcel AD-H, hexane/*i*PrOH 95:5, flow 1.0 mL/min): t_R = 14.3 min (minor), 16.0 min (major).

(1*R*,2*R*)-1-Phenylseleno-2-[*N*-(3,5-dinitrobenzoyl)amino]cycloheptane (3g).

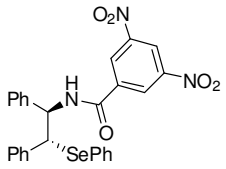


3g

Prepared by following the general procedure (method B, 20°C). Purification by FC (silica gel, $CHCl_3$) gave **3g** as a pale yellow solid (17.2 mg, 46% yield); mp 172-174°C; $[\alpha]^{20}_D$ –61.7 (*c* 0.7, $CHCl_3$, 96% *ee*); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.11 (t, *J* = 2.1 Hz, 1H), 8.78 (d, *J* = 2.1 Hz, 2H), 7.52 (m, 2H), 7.22-7.14 (m, 3H), 6.49 (d, *J* = 7.6 Hz, 1H), 4.29 (m, 1H), 3.42 (ddd, *J* = 9.9, 9.0, 3.4 Hz, 1H), 2.24 (m, 2H), 2.06 (m, 1H), 1.98-1.50 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.6, 148.5, 138.0, 134.5, 129.2 (2C), 127.7, 127.1, 120.9, 58.0, 50.1, 34.0, 33.0, 27.7, 26.5, 23.9; MS (ESI): *m*/*z* 502

[M+K]$^+$, 306 [M+H–PhSeH]$^+$; elemental analysis calcd. (%) for $C_{20}H_{21}N_3O_5Se$: C 51.95, H 4.58, N 9.09, Se 17.08; found: C 52.25, H 4.82, N 8.90, Se 16.90; HPLC (Chiralcel AS-H, hexane/*i*PrOH 80:20, flow 1.0 mL/min): t_R = 18.8 min (major), 35.4 min (minor).

(1*R*,2*R*)-1-Phenylseleno-2-[*N*-(3,5-dinitrobenzoyl)amino]-1,2-diphenylethane (3h).



3h

Prepared by following the general procedure (method C, 0°C). Purification by FC (silica gel, $CHCl_3$) gave **3h** as a pale yellow solid (13.1 mg, 45% yield); mp 88-90°C; $[\alpha]^{19}_D$ –105.9 (*c* 0.7, $CHCl_3$, 84% *ee*); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.10 (t, *J* = 2.1 Hz, 1H), 8.87 (d, *J* = 2.1 Hz, 2H), 7.40-7.27 (m, 3H), 7.20-7.00 (m, 13H), 5.77 (dd, *J* = 10.3, 8.1 Hz, 1H), 4.86 (d, *J* = 10.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.1, 148.5, 139.1, 138.4, 137.5, 134.8, 129.2, 128.9, 128.5, 128.5, 128.3, 128.1, 127.9, 127.7, 127.3, 127.2, 121.2, 59.5, 58.7; MS (ESI): *m*/*z* 570 [M+Na]$^+$, 390 [M+H–PhSeH]$^+$; elemental analysis calcd. (%) for $C_{27}H_{21}N_3O_5Se$: C 59.35, H 3.87, N 7.69, Se 14.45; found: C 59.52, H 3.95, N 7.48, Se 14.20; HPLC (Chiralcel AD-H, hexane/*i*PrOH 80:20, flow 1.0 mL/min): t_R = 10.3 min (major), 12.7 min (minor).

4. Determination of the absolute configuration of 3a through conversion into (1*S*,2*R*)-7

To a suspension of silver trifluoromethanesulfonate (206 mg, 0.801 mmol) in CH_2Cl_2 (8.5 mL), phenylselenyl bromide (196 mg, 0.830 mmol) was added. The red mixture was stirred at room temperature for 20 min, then a solution of (1*S*,2*R*)-**3a** in CH_2Cl_2 (17 mL) was introduced. The orange mixture gradually turned to yellow. After 24 h, the mixture was filtered over basic alumina. The filtrate was purified by FC (silica gel, $CHCl_3$) affording (1*S*,2*R*)-**6** as a white solid (178 mg, 88% yield); mp 124-126°C; $[\alpha]^{20}_D$ +17.7 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.06 (m, 1H), 9.03 (m, 2H), 4.81 (dt, *J* = 8.2, 5.2 Hz, 1H), 4.21 (m, 1H), 2.01-1.82 (m, 3H), 1.64-1.33 (m,

5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.6, 148.6, 132.2, 128.0, 120.6, 80.6, 64.2, 27.4, 26.0, 19.6, 18.8; MS (ESI): *m/z* 292 $[M+H]^+$; elemental analysis calcd. (%) for $C_{13}H_{13}N_3O_5$: C 53.61, H 4.50, N 14.43; found: C 53.65, H 4.54, N 14.33.

The oxazoline (1*S*,2*R*)-**6** (138 mg, 0.474 mmol), was dissolved in 6N HCl and the mixture was refluxed. After 24 h, the suspension was cooled to room temperature and the solid formed was separated by centrifugation and discarded. The acidic aqueous solution was washed with CH_2Cl_2 (5 x 4 mL), and concentrated *in vacuo*, giving the known *cis*-aminoalcohol hydrochloride (1*S*,2*R*)-**7**[6,7] (71.7 mg, quantitative yield) as a white solid, whose absolute configuration was determined by comparison with literature data;[6] $[\alpha]^{22}_D$ +26.1 (*c* 1.0, EtOH); ^{1}H NMR (400 MHz, CD_3OD): δ 4.01 (m, 1H), 3.20 (m, 1H), 1.90-1.53 (m, 6H), 1.52-1.34 (m, 2H).

5. References

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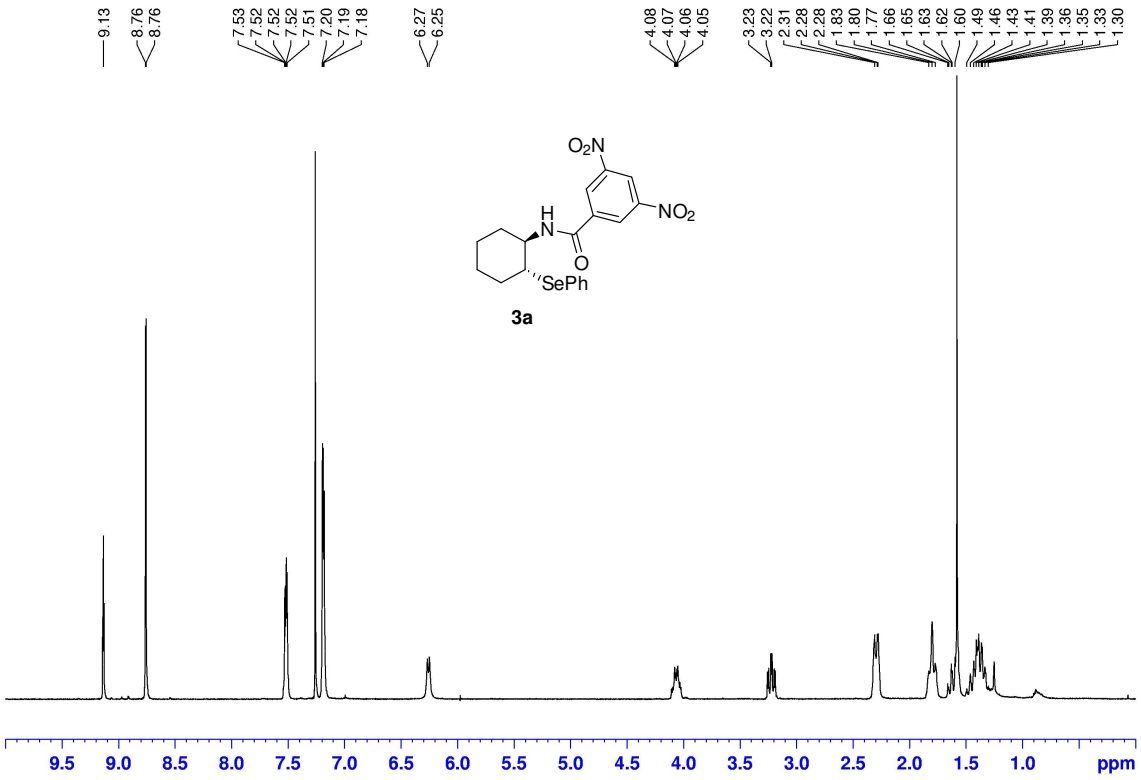
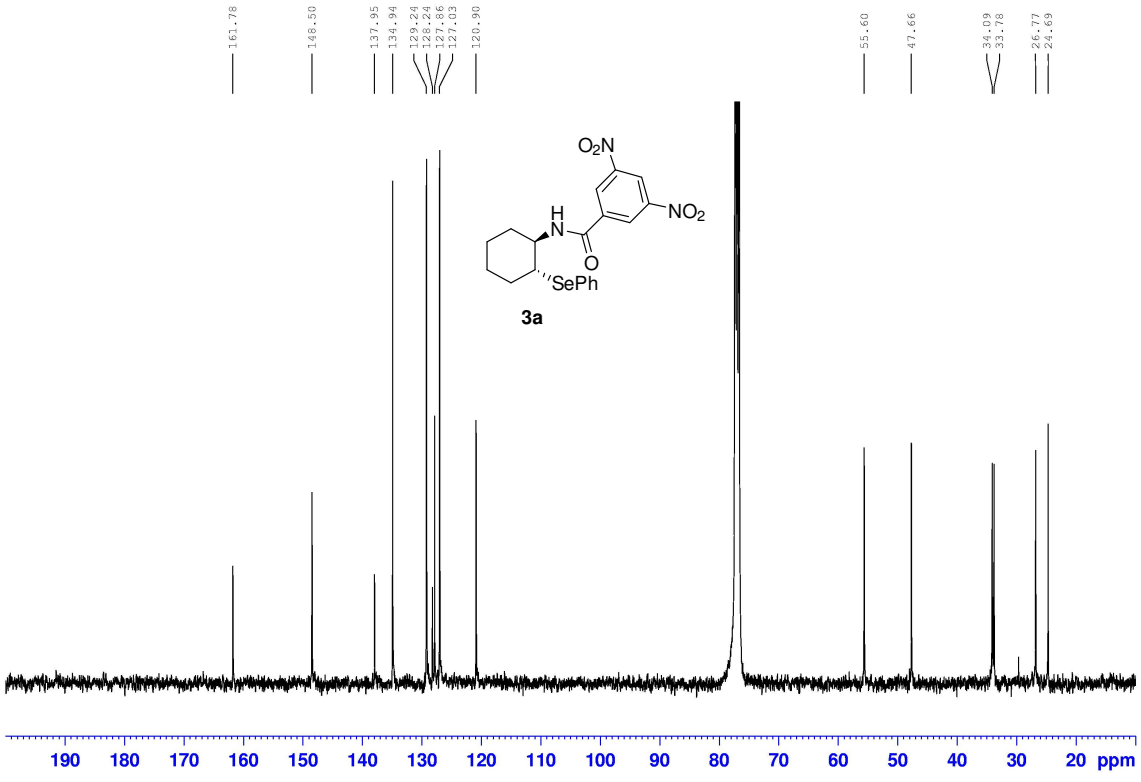
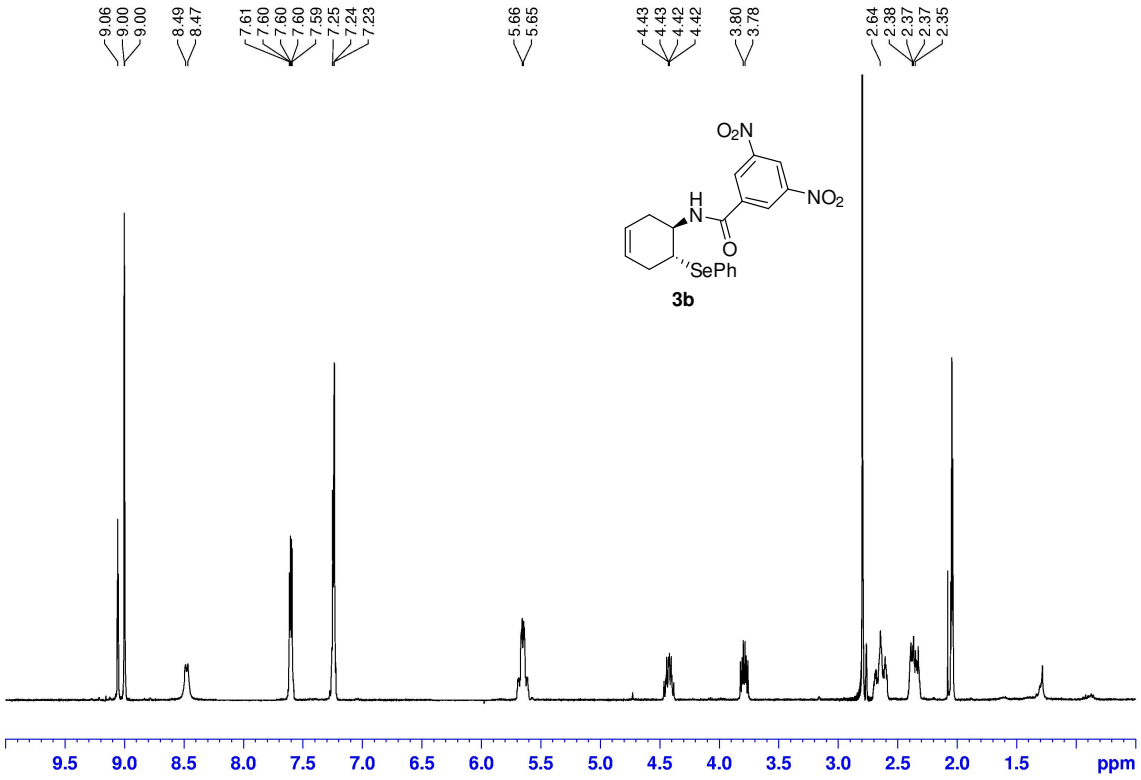
6. Copies of ^{1}H NMR and ^{13}C NMR spectra of unknown compounds



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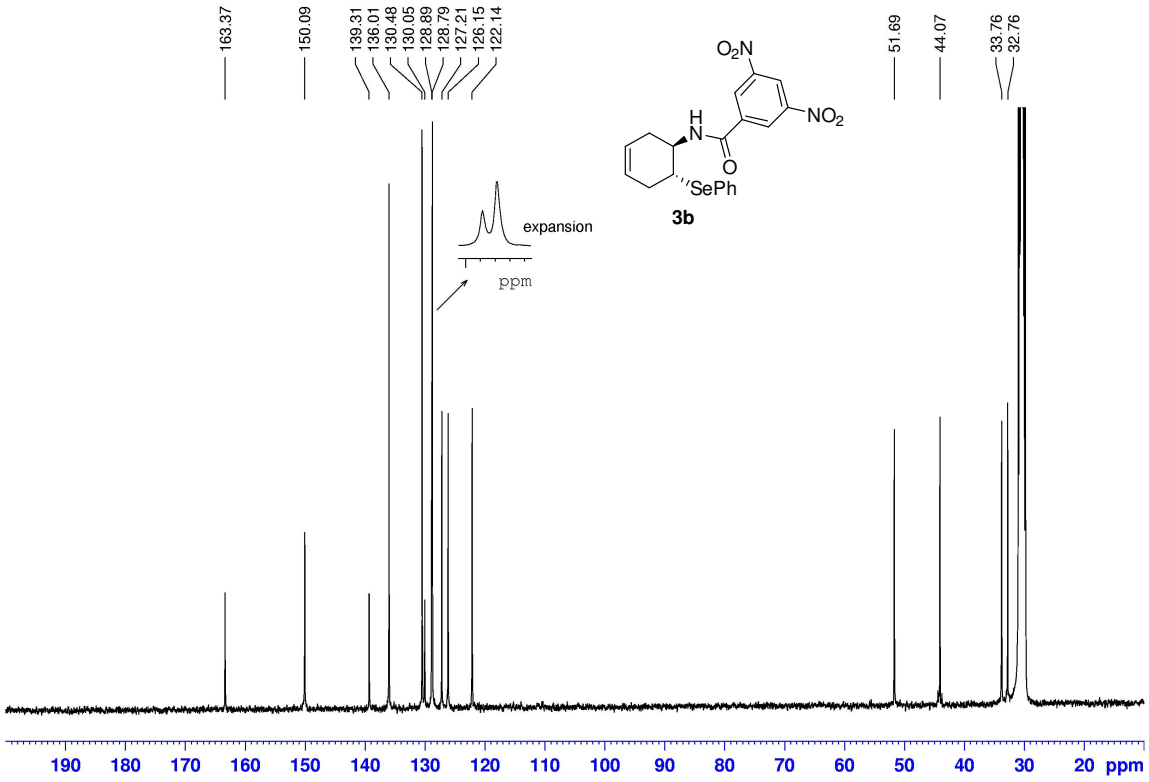
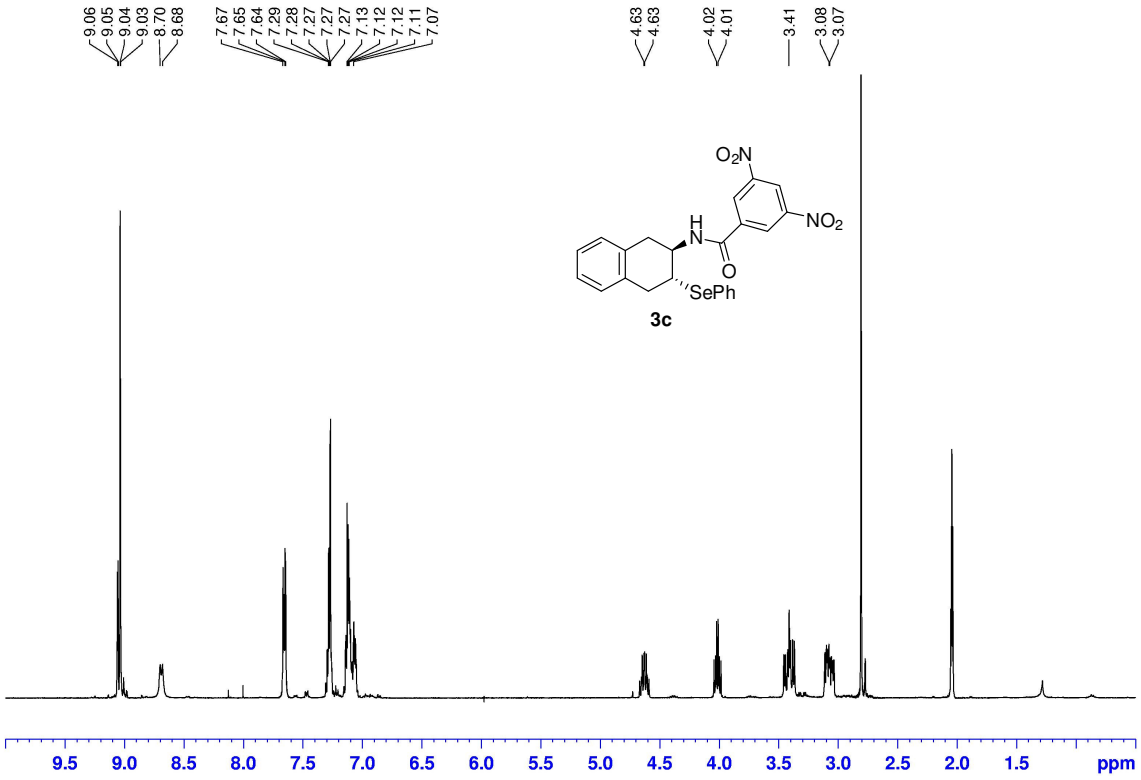
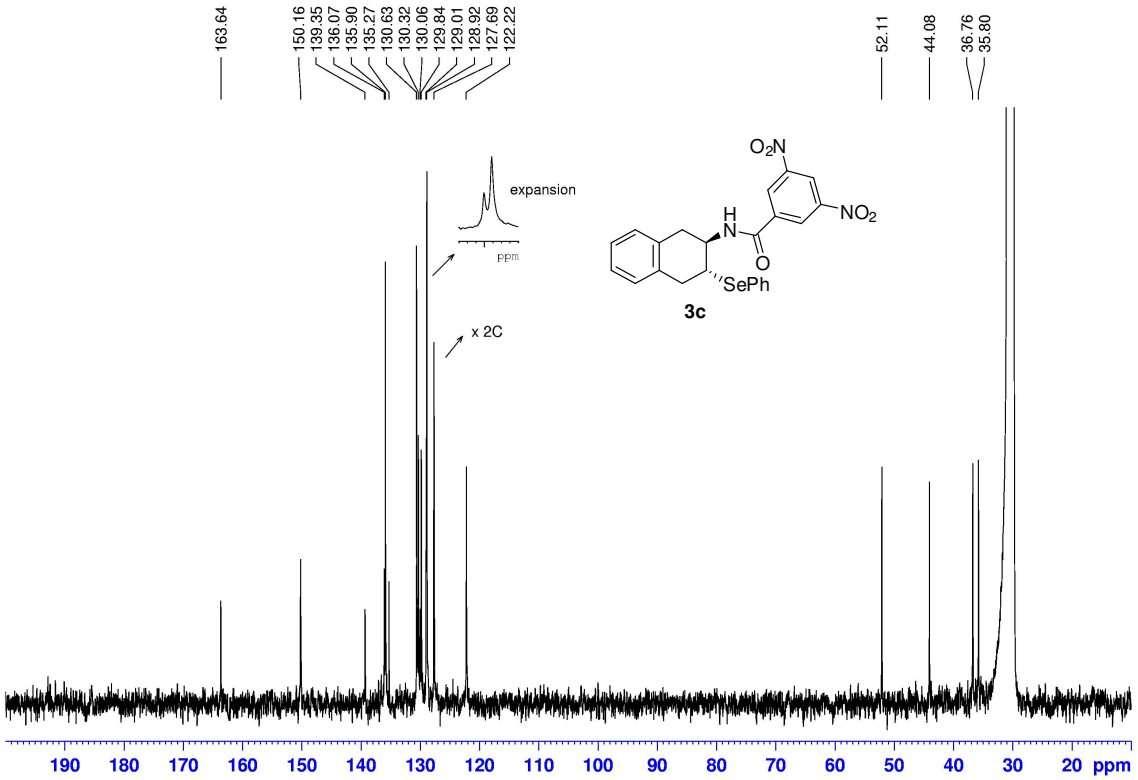
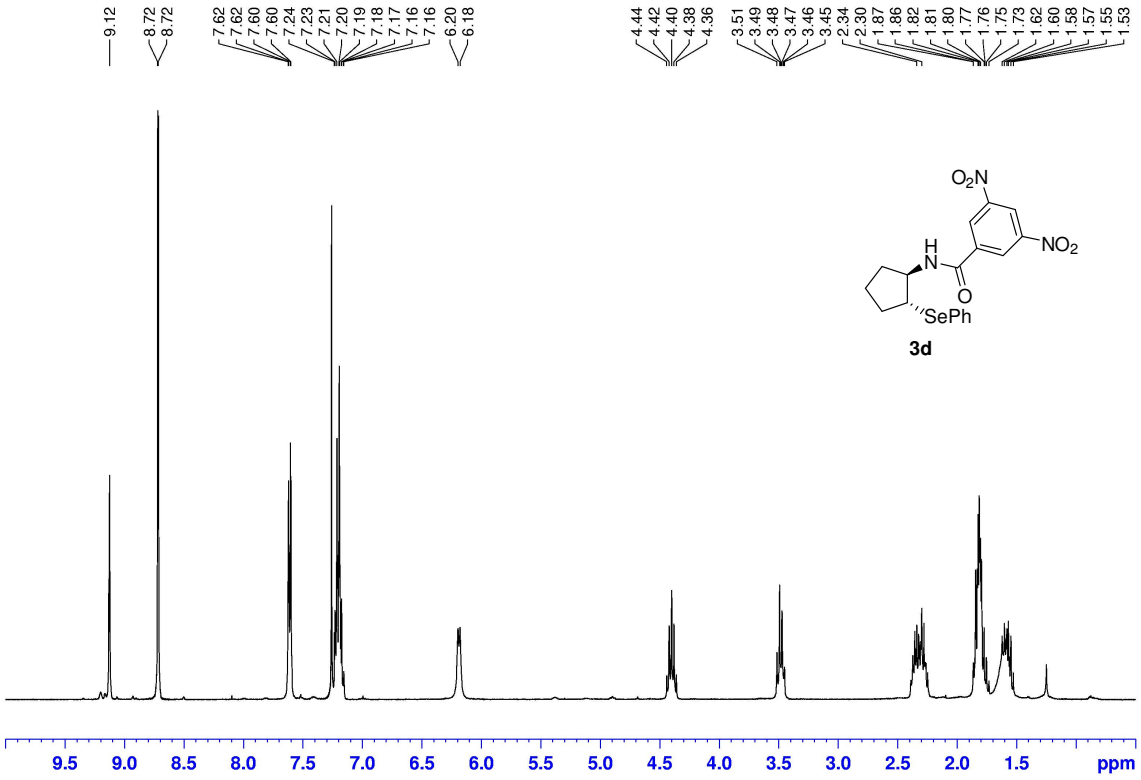
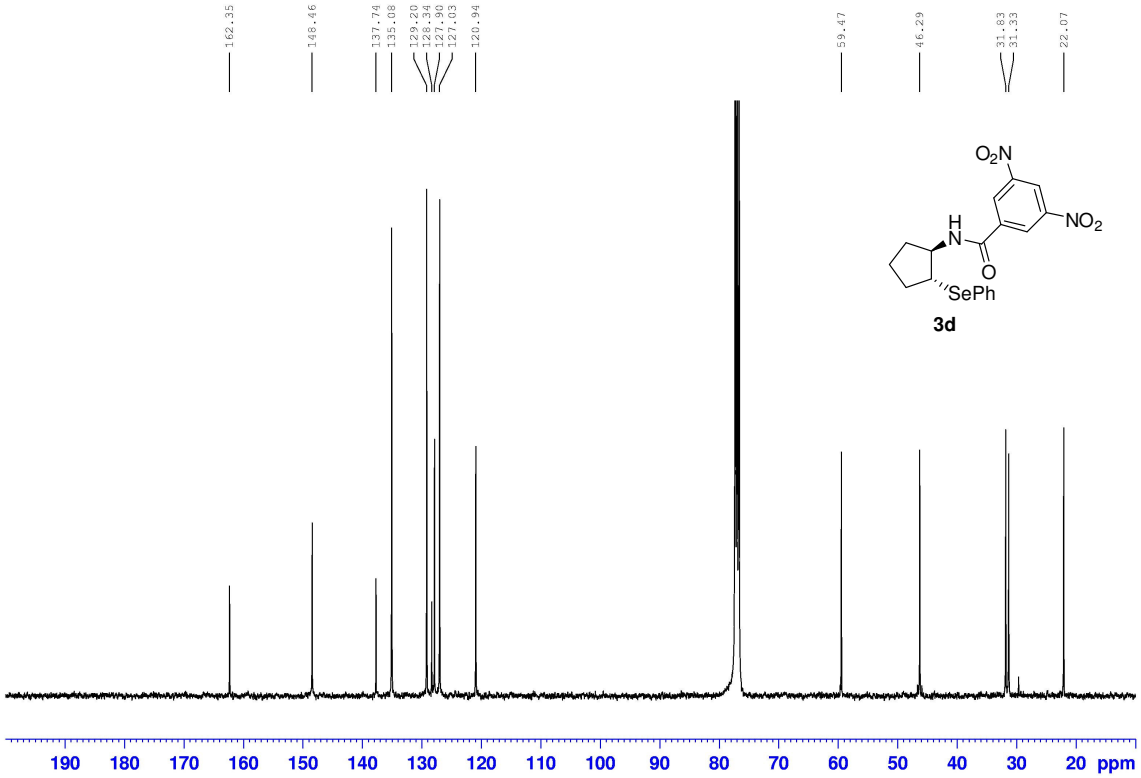
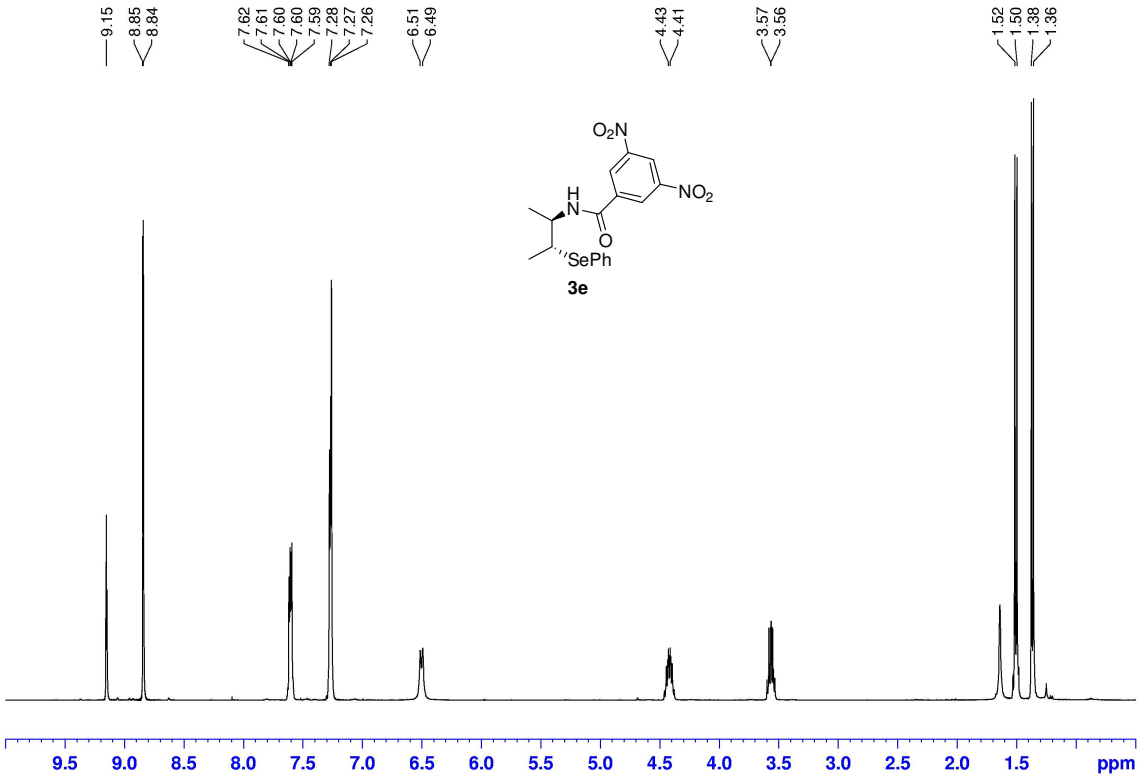

163.37
150.09
139.31
136.01
130.48
130.05
128.89
128.79
127.21
126.15
122.14
51.69
44.07
33.76
32.76
O2N
NO2
H
N
O
SePh
3b
expansion
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

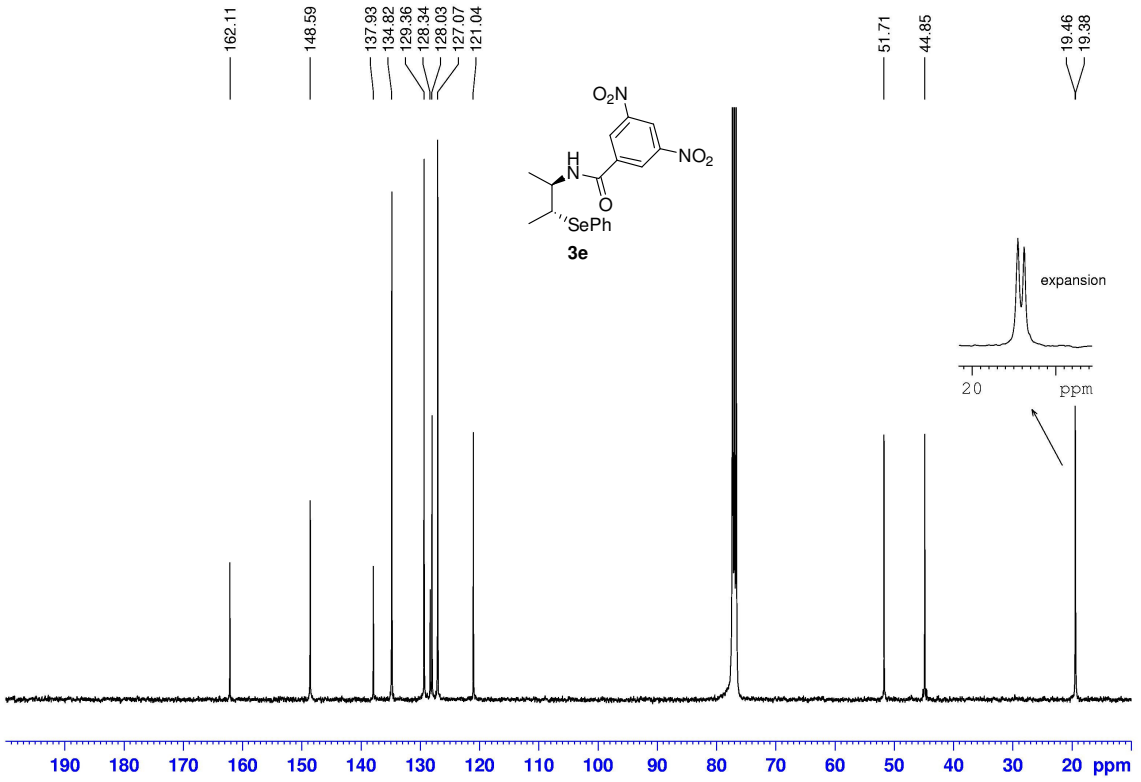


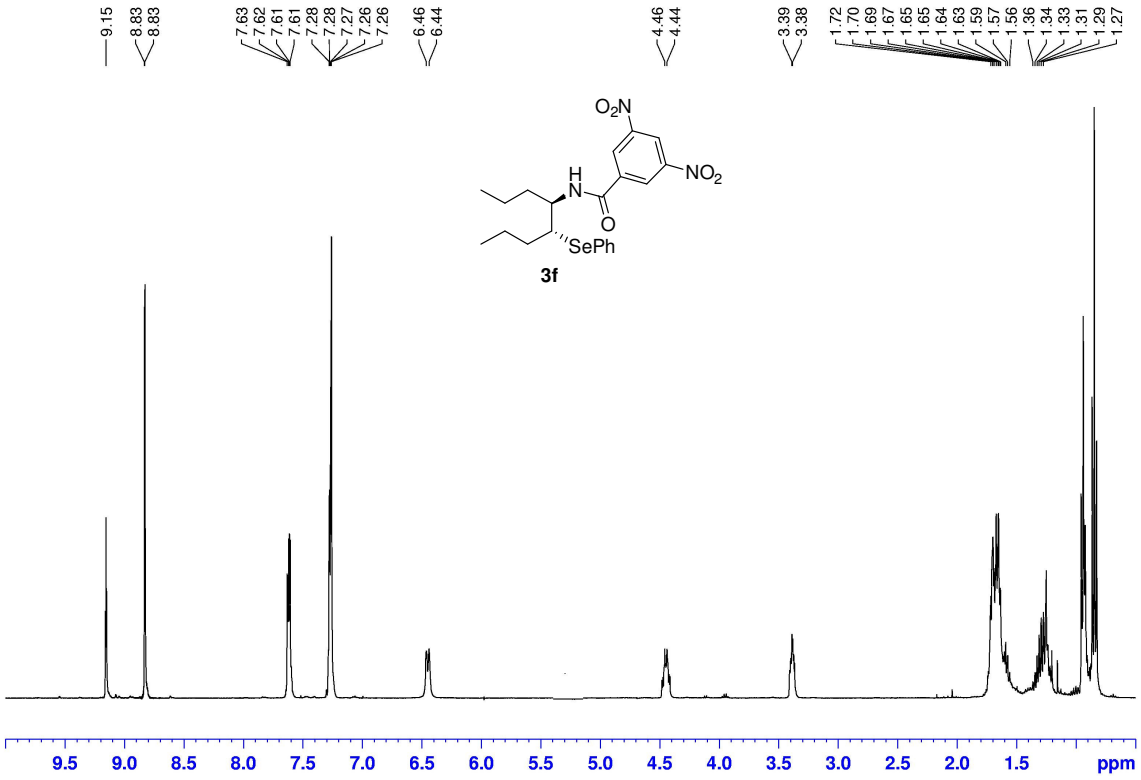


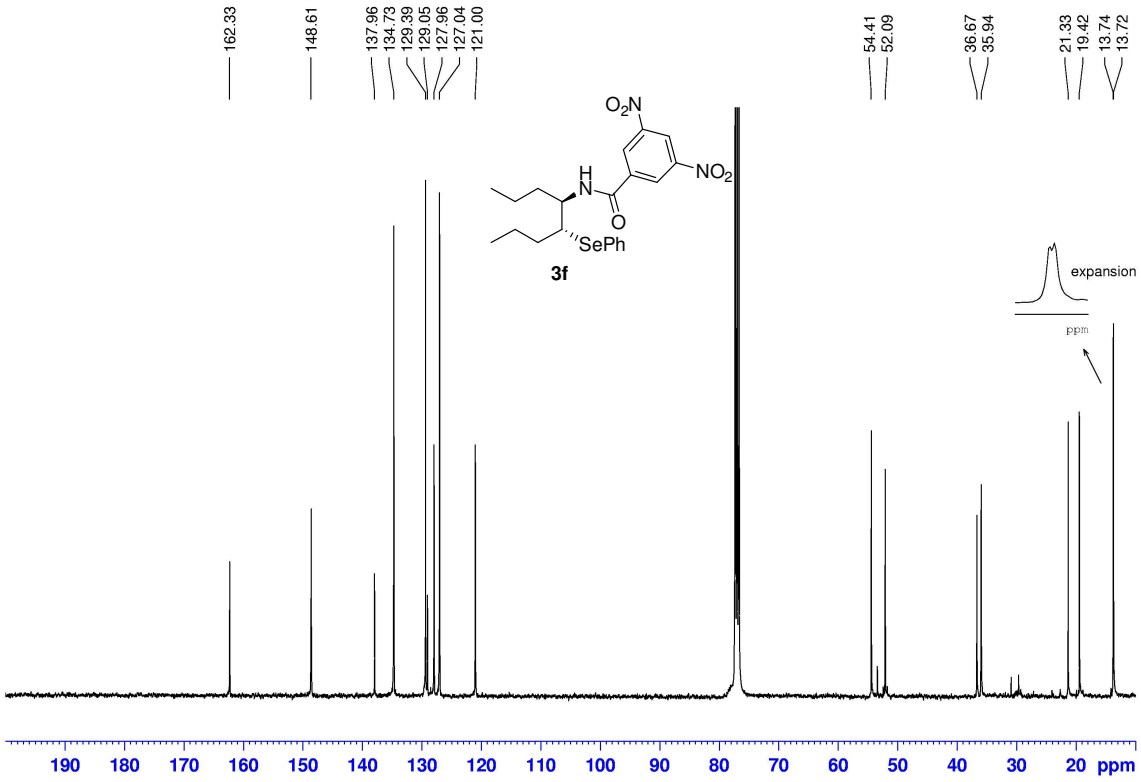

9.12
8.72
8.72
7.62
7.62
7.60
7.60
7.24
7.23
7.21
7.20
7.19
7.18
7.17
7.16
7.16
6.20
6.18
4.44
4.42
4.40
4.38
4.36
3.51
3.49
3.48
3.47
3.46
3.45
2.34
2.30
1.87
1.86
1.82
1.81
1.80
1.77
1.76
1.75
1.73
1.62
1.60
1.58
1.57
1.55
1.53
O2N
NO2
H
N
O
SePh
3d
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm

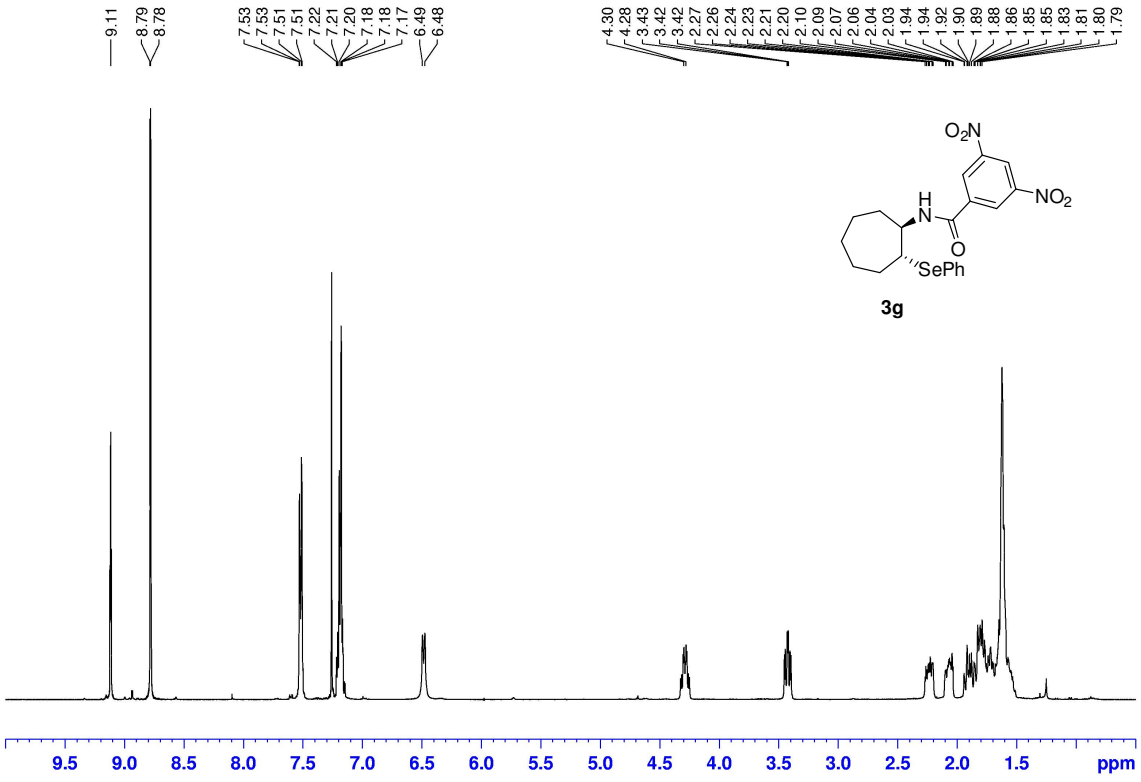

162.35
148.46
137.74
135.08
129.20
128.34
127.90
127.03
120.94
59.47
46.29
31.83
31.33
22.07
O2N
NO2
H
N
O
SePh
3d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

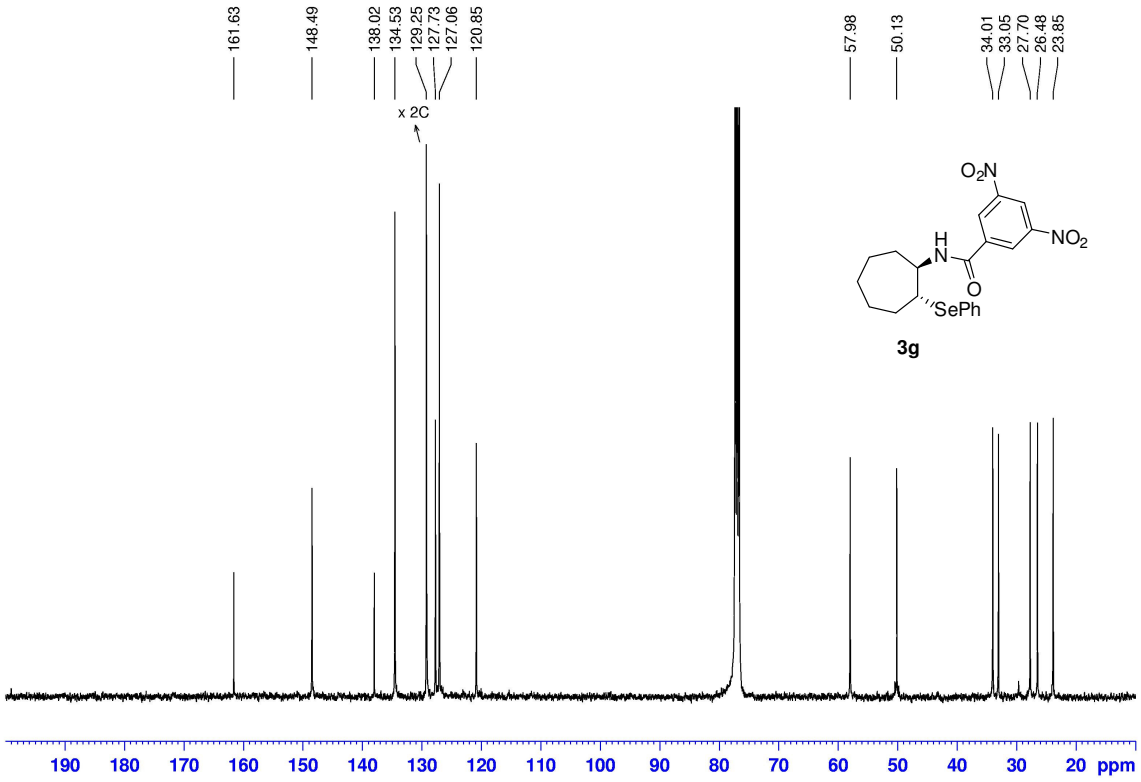


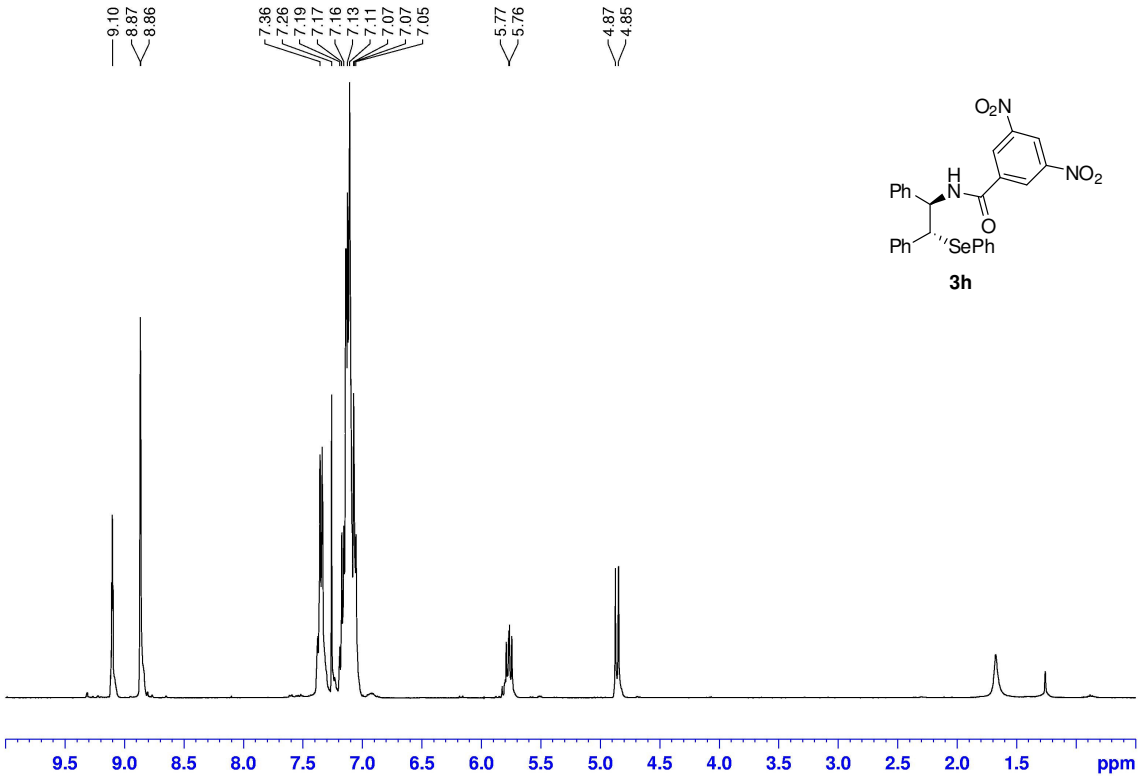


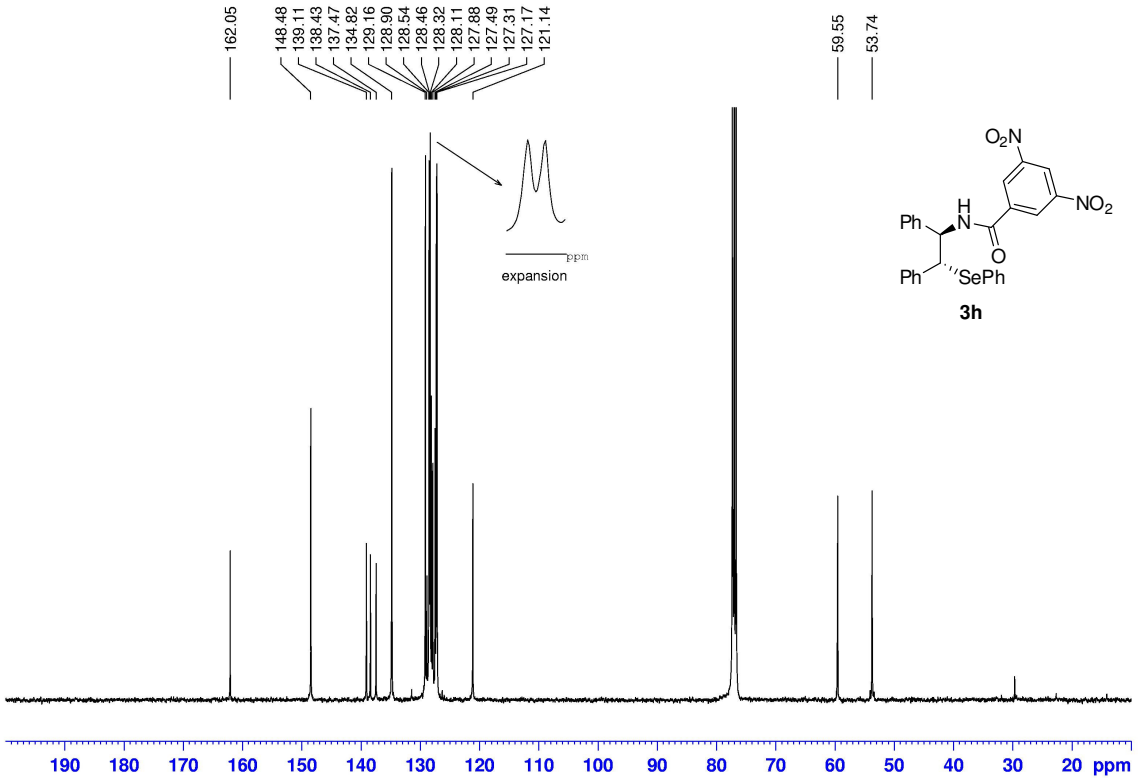









9.10
8.87
8.86
7.36
7.26
7.19
7.17
7.16
7.13
7.11
7.07
7.07
7.05
5.77
5.76
4.87
4.85
O2N
NO2
Ph
H
N
O
Ph
SePh
3h
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm


162.05
148.48
139.11
138.43
137.47
134.82
129.16
128.90
128.54
128.46
128.32
128.11
127.88
127.49
127.31
127.17
121.14
59.55
53.74
expansion
ppm
O2N
NO2
Ph
H
N
O
Ph
SePh
3h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm