Supporting Information

for

Molecular iodine-catalyzed one-pot multicomponent synthesis of 5-amino-4-(arylselanyl)-1H-pyrazoles

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General Information: Reactions were monitored by TLC carried out on Merck silica gel (60 F254) by using UV light as visualizing agent and 5% vanillin in 10% H$_2$SO$_4$ and heat as developing agents. Column chromatography was performed by using silica gel. Proton nuclear magnetic resonance spectra ($^1$H NMR) were obtained at 400 MHz with Bruker DPX 400 spectrometer. Spectra were recorded in CDCl$_3$ solutions. Chemical shifts are reported in ppm, referenced to tetramethylsilane (TMS) as the external reference. Hydrogen coupling patterns are described as singlet (s), doublet (d), triplet (t), double doublet (dd) and multiplet (m). Coupling constants (J) are reported in Hertz. Carbon-13 nuclear magnetic resonance spectra ($^{13}$C NMR) were obtained at 100 MHz with Bruker DPX 400 spectrometer. Chemical shifts are reported in ppm, referenced to the solvent peak of CDCl$_3$ (77.0 ppm). Low resolution mass spectra (MS) were obtained with Shimadzu GCMS-QP2010 mass spectrometer 10416. High resolution mass spectra (HRMS) were recorded on a Bruker Micro TOF-QII spectrometer. Melting point (m.p.) values were measured with a Marte PFD III instrument. Infrared spectra were measured using a Shimadzu Prestige-21 IR spectrometer. A Cole Parmer-ultrasonic processor Model CPX 130, with a maximum power of 130 W, operating at amplitude of 60% and a frequency of 20 kHz was used.

General procedure for the synthesis of 5-amino-4-(arylselanyl)pyrazoles (4)

To a 10 mL vial equipped with a reflux condenser containing a mixture of benzoyleacetonitrile 1 (0.5 mmol), arylhydrazine 2 (0.7 mmol) and diaryl diselenide 3 (0.5 mmol) in MeCN (3 mL), molecular iodine (50 mol %) was added. Then the mixture was stirred at reflux temperature for a period of 48 hours. Under these conditions the expected product 4 was obtained and the progress of the reaction was monitored by TLC. The reaction mixture was poured in water (15 mL), extracted with ethyl acetate (3 × 10 mL), dried over MgSO$_4$ and concentrated under vacuum. The residue was purified by column
chromatography by using silica gel and a mixture of hexane/ethyl acetate (95:05) as eluent.

**General procedure for the synthesis of diazo pyrazole derivative (6)**

5-Amino-4-(phenylselanyl)-1H-pyrazol 4a (0.5 mmol) was added to a 10 mL vial containing a mixture of 1,10-phenanthroline (0.15 mmol), tert-butyl peroxide (1.5 mmol) and CuI (0.05 mmol) in dichloromethane (2 mL). Then, the mixture was stirred at room temperature for 2 hours and the expected product 5 was obtained. The progress of the reaction was monitored by TLC. The reaction mixture was received in water (10 mL), extracted with ethyl acetate (3 × 5 mL), dried over MgSO$_4$ and concentrated under vacuum. The residue was purified by column chromatography using silica gel and a mixture of hexane/ethyl acetate (90:10) as eluent.

**1,3-Diphenyl-4-(phenylselanyl)-1H-pyrazol-5-amine (4a):**

Orange oil; Yield: 96%; IR (KBr, cm$^{-1}$): 3450 (s), 3412 (s), 3055 (m), 2922 (w), 1946 (w), 1801 (w), 1600 (s), 1500 (s), 1475 (m), 1371 (m), 1111 (w), 970 (s), 690 (s). $^1$H NMR (CDCl$_3$, 400 MHz): δ=7.93-7.91 (m, 2H), 7.67-7.65 (m, 2H), 7.50-7.46 (m, 2H), 7.37-7.25 (m, 6H), 7.21–7.13 (m, 3H) 4.30 ppm (s, 2H). $^{13}$C NMR (CDCl$_3$, 100 MHz): δ=153.6, 149.5, 138.6, 133.0, 132.9, 129.5, 129.2, 128.1, 127.9 127.8, 127.6, 125.8, 123.6, 82.4 ppm. $^{77}$Se NMR (CDCl$_3$, 76 MHz): δ=193.9 ppm. MS m/z (rel. int.): 391 (43), 389 (23), 311 (100), 293 (3), 208 (15), 155 (8). HRMS calcd. for C$_{21}$H$_{18}$N$_3$Se: [M + H]$^+$ 392.0660. Found: 392.0663.

**1-Phenyl-4-(phenylselanyl)-3-(p-tolyl)-1H-pyrazol-5-amine (4b):**

Reddish oil; Yield: 73%; IR (KBr, cm$^{-1}$): 3433 (s), 3057 (w), 2916 (w), 1598 (s), 1502 (s), 1473 (m), 1367 (w), 1182 (w), 1020 (m), 970 (m), 732 (s), 665 (w). $^1$H NMR (CDCl$_3$, 400 MHz): δ=7.83-7.81 (m, 2H), 7.68–7.66 (m, 2H), 7.51-7.47 (m, 2H), 7.38-7.34 (m, 2H), 7.26-7.12 (m, 6H), 4.30 (s, 2H), 2.33 ppm (s, 3H). $^{13}$C NMR (CDCl$_3$, 100 MHz): δ=153.7, 149.5, 137.9, 133.2, 130.6, 130.2, 129.6, 129.3, 128.9, 128.0 127.8, 127.6, 125.9, 123.7, 82.6, 21.2 ppm. $^{77}$Se NMR (CDCl$_3$, 76 MHz): δ=194.3 ppm. MS m/z (rel. int.): 405 (37), 325 (100), 307 (2), 232 (3), 208 (13), 162 (4), 132 (15), 119 (14), 77 (35). HRMS calcd. for C$_{22}$H$_{20}$N$_3$Se: [M + H]$^+$ 406.0817. Found: 406.0820.
3-(4-methoxyphenyl)-1-phenyl-4-(phenylselanyl)-1H-pyrazol-5-amine (4c): Brownish oil; Yield: 35%; \(^1\)H NMR (CDCl\(_3\), 400 MHz): δ = 7.89-7.85 (m, 2H), 7.66-7.63 (m, 2H), 7.48-7.44 (m, 2H), 7.34-7.30 (m, 1H), 7.26-7.24 (m, 2H), 7.21-7.16 (m, 2H), 7.14-7.10 (m, 1H), 6.87-6.83 (m, 2H), 4.28 (s, 2H), 3.75 ppm (s, 3H). \(^13\)C NMR (CDCl\(_3\), 100 MHz): δ = 159.6, 153.3, 149.4, 138.7, 133.1, 129.5, 129.2, 129.0, 127.8, 127.4, 125.8, 125.6, 123.5, 113.5, 82.1, 55.1 ppm. MS m/z (rel. int.): 421 (1), 408 (1), 345 (4), 280 (61), 265 (51), 146 (47), 131 (23), 119 (47), 104 (49), 77 (100).

3-(4-Bromophenyl)-1-phenyl-4-(phenylselanyl)-1H-pyrazol-5-amine (4d): Brown solid; m.p.: 43-45 °C; Yield: 78%; IR (KBr, cm\(^{-1}\)): 3412 (m), 3055 (w), 2920 (w), 2850 (w), 1598 (s), 1575 (m), 1500 (s), 1498 (s), 1436 (m), 1363 (m), 1008 (m), 912 (w), 829 (s), 665 (w). \(^1\)H NMR (CDCl\(_3\), 400 MHz): δ =7.76-7.74 (m, 2H), 7.56-7.54 (m, 2H), 7.41-7.35 (m, 4H), 7.30-7.28 (m, 1H), 7.16-7.04 (m, 5H), 4.14 ppm (s, 2H). \(^13\)C NMR (CDCl\(_3\), 100 MHz): δ=152.3, 149.7, 138.6, 132.8, 132.0, 131.2, 129.6, 129.3, 127.9, 127.8, 126.0, 123.4, 82.5 ppm. \(^77\)Se NMR (CDCl\(_3\), 76 MHz): δ=192.9 ppm. MS m/z (rel. int.): [M+2] 471 (40) [M+] 469 (51), 389 (99), 309 (7), 267 (5), 233 (4), 208 (33), 155 (13), 127 (15), 119 (28), 77 (100). HRMS calcd. for C\(_{21}\)H\(_{17}\)BrN\(_3\)Se: [M + H]\(^+\) 469.9766. Found: 469.9763.

3-(4-Chlorophenyl)-1-phenyl-4-(phenylselanyl)-1H-pyrazol-5-amine (4e): Brown oil; Yield: 81%; IR (KBr, cm\(^{-1}\)): 3550 (m), 3414 (s), 3057 (m), 2920 (w), 1948 (w), 1884 (w), 1598 (s), 1531 (m), 1500 (s), 1454 (m), 1373 (m), 1087 (s), 759 (s), 659 (w). \(^1\)H NMR (CDCl\(_3\), 400 MHz): δ=7.83-7.81 (m, 2H), 7.58-7.56 (m, 2H), 7.41 (t, J=7.4 Hz, 2H), 7.30-7.26 (m, 1H), 7.22-7.20 (m, 2H), 7.17-7.06 (m, 5H), 4.18 ppm (s, 2H). \(^13\)C NMR (CDCl\(_3\), 100 MHz): δ=152.4, 149.6, 138.6, 134.1, 132.8, 131.6, 129.6, 129.3, 129.1, 128.3, 128.0, 127.8, 126.1, 123.7, 82.5 ppm. MS m/z (rel. int.): [M+2] 427 (10) 425 (31), 421 (6), 347 (35), 345 (100), 309 (4), 267 (3), 233 (2), 208 (16), 180 (2), 162 (9), 153 (3), 177 (35). HRMS calcd. for C\(_{21}\)H\(_{17}\)ClN\(_3\)Se: [M + H]\(^+\) 426.0271. Found: 426.0262.

3-Phenyl-4-(phenylselanyl)-1-(m-tolyl)-1H-pyrazol-5-amine (4g): Brown oil; Yield: 63%; IR (KBr, cm\(^{-1}\)): 3473 (m), 3408 (s),...
3331 (m), 3097 (w), 2852 (w), 1606 (s), 1575 (s), 1496 (m), 1346 (s), 1109 (w), 966 (m), 742 (s), 657 (w). $^1$H NMR (CDCl$_3$, 400 MHz): δ=7.92-7.90 (m, 2H), 7.48-7.12 (m, 12H), 4.28 (s, 2H), 2.39 ppm (s, 3H). $^{13}$C NMR (CDCl$_3$, 100 MHz): δ=153.4, 149.4, 139.8, 138.4, 133.1, 132.9, 129.2, 128.4, 128.1, 127.8, 127.7, 125.8, 124.8, 120.4, 82.1, 21.3 ppm. MS m/z (rel. int.): 405 (31), 391 (3), 325 (100), 283 (17), 248 (3), 222 (15), 146 (17). HRMS calcd. for C$_{22}$H$_{20}$N$_3$Se: [M + H]$^+$ 406.0817. Found: 406.0818.

1-(2,5-Dimethylphenyl)-3-phenyl-4-(phenylselanyl)-1H-pyrazol-5-amine (4h): Orange oil; Yield: 52%; IR (KBr, cm$^{-1}$): 3550 (s), 3415 (s), 3055 (w), 2920 (w), 2854 (w), 1616 (s), 1508 (w), 1143 (w), 968 (m), 742 (s), 657 (w). $^1$H NMR (CDCl$_3$, 400 MHz): δ=7.84 (d, J=8.1 Hz, 2H), 7.24-7.16 (m, 6H), 7.12-7.01 (m, 5H), 3.90 (s, 2H), 2.28 (s, 3H), 2.09 ppm (s, 3H). $^{13}$C NMR (CDCl$_3$, 100 MHz): δ=153.1, 150.3, 139.7, 136.2, 134.2, 133.5, 133.3, 132.9, 128.0, 127.9, 127.8, 127.7, 127.6, 125.7, 125.6, 121.1, 17.4 ppm. MS m/z (rel. int.): 419 (85), 417 (45), 339 (100), 323 (16), 297 (5), 2.62 (12), 235 (38), 184 (6), 159 (15). HRMS calcd. for C$_{23}$H$_{22}$N$_3$Se: [M + H]$^+$ 420.0973. Found: 420.0982.

1-(2,4-Dichlorophenyl)-3-phenyl-4-(phenylselanyl)-1H-pyrazol-5-amine (4i): Brown oil; Yield: 80%; IR (KBr, cm$^{-1}$): 3550 (m), 3473 (s), 3412 (s), 3230 (w), 3051 (w), 2920 (w), 1616 (s), 1508 (s), 1469 (s), 1413 (m), 1296 (m), 1099 (m), 775 (m), 657 (m). $^1$H NMR (CDCl$_3$, 400 MHz): δ=7.80-7.87 (m, 2H), 7.49-7.42 (m, 2H), 7.32-7.05 (m, 9H), 4.02 ppm (s, 2H). $^{13}$C NMR (CDCl$_3$, 100 MHz): δ=154.5, 150.9, 136.2, 134.6, 133.0, 132.9, 132.8, 130.8, 129.3, 128.4, 128.3, 128.1, 127.9, 127.8, 125.9, 82.0 ppm. MS m/z (rel. int.): [M+2] 461 (37), [M+] 459 (35), 424 (100), 381 (50), 321 (8), 276 (17), 218 (11), 199 (14), 128 (41), 77 (60). HRMS calcd. for C$_{21}$H$_{16}$Cl$_2$N$_3$Se: [M + H]$^+$ 459.9881. Found: 459.9882.

1-(2,4-Difluorophenyl)-3-phenyl-4-(phenylselanyl)-1H-pyrazol-5-amine (4j): Brown solid; m.p.: 102-103 °C; Yield: 76%; IR (KBr, cm$^{-1}$): 3550 (m), 3473 (s), 3412 (s), 3230 (w), 3051 (w), 2920 (w), 1616 (m), 1597 (s), 1531 (m), 1363 (w), 831 (m), 723 (m), 620 (w). $^1$H NMR (CDCl$_3$, 400 MHz): δ=7.90-7.87 (m, 2H), 7.68-7.62 (m, 1H), 7.37-7.30 (m, 3H), 7.27-7.20 (m, 4H), 7.18-7.15 (m, 1H), 7.08-7.01 (m, 2H), 4.22 ppm (s, 2H). $^{13}$C NMR (CDCl$_3$, 100 MHz): δ=162.5 (dd, J=241.2 e 11.1 Hz), 156.7 (dd, J=241.2 e 11.1 Hz), 154.7, 151.0, 147.9, 143.4, 132.9, 132.7, 130.0, 129.9, 129.3, 128.3, 128.1, 127.8,
127.7, 127.1, 125.9, 122.6 (dd, \( J = 12.1, 4.0 \) Hz), 112.5 (dd, \( J = 22.5, 3.7 \) Hz), 105.1 (dd, \( J = 26.5, 23.6 \) Hz), 82.3 ppm. \(^{77}\)Se NMR (CDCl\(_3\), 76 MHz): \( \delta = 195.2 \) ppm. MS \( m/z \) (rel. int.): 427 (48), 425 (25), 383 (2), 347 (100), 305 (2), 244 (23), 218 (6), 155 (19), 128 (18). HRMS calcd. for C\(_{21}\)H\(_{16}\)F\(_2\)N\(_3\)Se: [M + H]\(^+\) 428.0472. Found: 428.0486.

1,3-Diphenyl-4-(\(p\)-tolylselanyl)-1\(H\)-pyrazol-5-amine (4l):
Orange oil; Yield: 54%; IR (KBr, cm\(^{-1}\)): 3550 (m), 3477 (m), 3390 (s), 3250 (s), 3109 (s), 1881 (w), 1811 (w), 1743 (w), 1618 (s), 1575 (m), 1469 (s), 1431 (s), 1294 (m), 1139 (m), 1099 (s), 974 (s), 657 (m). \(^1\)H NMR (CDCl\(_3\), 400 MHz): \( \delta = 7.94 - 7.92 \) (m, 2H), 7.65 - 7.63 (m, 2H), 7.47 (t, \( J = 7.5 \) Hz, 2H), 7.35 - 7.28 (m, 4H), 7.15 (d, \( J = 8.0 \) Hz, 2H), 7.01 (d, \( J = 8.0 \) Hz, 2H), 4.28 (s, 2H), 2.25 ppm (s, 3H). \(^{13}\)C NMR (CDCl\(_3\), 100 MHz): \( \delta = 153.5, 149.4, 138.6, 135.6, 132.9, 130.0, 129.5, 129.1, 128.1, 128.0, 127.9, 127.8, 127.5, 123.5, 82.7, 20.9 \) ppm. MS \( m/z \) (rel. int.): 405 (10), 328 (100), 312 (12), 298 (22), 142 (16), 77 (61). HRMS calcd. for C\(_{22}\)H\(_{20}\)N\(_3\)Se: [M + H]\(^+\) 406.0817. Found: 406.0822.

4-((4-Methoxyphenyl)selanyl)-1,3-diphenyl-1\(H\)-pyrazol-5-amine (4m): Brown solid; m.p.: 38-40 °C; Yield: 63%; IR (KBr, cm\(^{-1}\)): 3552 (w), 3442 (m), 3342 (m), 3053 (w), 2920 (w), 1734 (w), 1602 (s), 1529 (m), 1471 (s), 1452 (m), 1384 (m), 1170 (w), 1008 (s), 688 (s). \(^1\)H NMR (CDCl\(_3\), 400 MHz): \( \delta = 7.86 - 7.84 \) (m, 2H), 7.49-7.48 (m, 2H), 7.29 (t, \( J = 7.3 \) Hz, 2H), 7.22-7.16 (m, 4H), 7.06 (d, \( J = 7.0 \) Hz, 2H), 6.60 (d, \( J = 6.9 \) Hz, 2 H), 4.16 (s, 2H), 3.53 ppm (s, 3H). \(^{13}\)C NMR (CDCl\(_3\), 100 MHz): \( \delta = 158.4, 153.1, 149.3, 138.7, 133.1, 132.8, 130.0, 129.3, 127.9, 127.8, 127.3, 123.4, 122.8, 115.0, 83.7, 55.1 ppm. MS \( m/z \) (rel. int.): 421 (6), 347 (34), 345 (100), 327 (7), 309 (8), 281 (28), 267 (8), 253 (16), 235 (7), 207 (84), 191 (12), 155 (5), 119 (25), 104, 77 (82). HRMS calcd. for C\(_{22}\)H\(_{20}\)N\(_3\)OSe: [M + H]\(^+\) 422.0766. Found: 422.0791.

4-((4-Chlorophenyl)selanyl)-1,3-diphenyl-1\(H\)-pyrazol-5-amine (4n): Reddish solid; m.p.: 41-43 °C; Yield: 80%; IR (KBr, cm\(^{-1}\)): 3435 (s), 3059 (m), 2924 (w), 2850 (w), 2733 (w), 2194 (w), 1948 (w), 1884 (w), 1600 (s), 1531 (m), 1500 (s), 1454 (m), 1373 (m), 1174 (w), 1087 (s), 759 (s), 659 (w). \(^1\)H NMR (CDCl\(_3\), 400 MHz): \( \delta = 7.82 \) (d, \( J = 7.9 \) Hz, 2H), 7.56 (d, \( J = 7.5 \) Hz, 2H), 7.39 (t, \( J = 7.7 \) Hz, 2H), 7.26-7.22 (m, 4H), 7.10-7.04 (m, 4H), 6.84-6.64 (m, 1H), 4.22 ppm (s, 2H). \(^{13}\)C NMR (CDCl\(_3\), 100 MHz) \( \delta = 153.5, 149.5, 138.6, 132.9, 131.9, 131.4, 129.6, 129.3, 129.2, 128.2, 128.1, 127.8, 123.6, 113.8, 82.2 ppm. \(^{77}\)Se NMR (CDCl\(_3\), 76 MHz): \( \delta = 196.8 \)
ppm. MS m/z (rel. int.): [M+2] 427 (19), [M+] 425 (42), 386 (13), 345 (100), 306 (44), 267 (3), 242 (11), 217 (8), 119 (20). HRMS calcd. for C_{21}H_{17}ClN_{3}Se: [M + H]^+ 426.0271. Found: 426.0276.

4-((3-(trifluoromethyl)phenyl)selanyl)-1,3-diphenyl-1H-pyrazol-5-amine (4o): Reddish oil; Yield: 24%; $^1$H NMR (CDCl$_3$, 400 MHz): $\delta$ = 7.09-6.96 (m, 2H), 6.69-6.33 (m, 12H), 3.38 ppm (s, 2H). $^{13}$C NMR (CDCl$_3$, 100 MHz): $\delta$ = 153.3, 149.5, 138.3, 134.5, 132.7, 131.8, 131.3 (d, $J$ = 32 Hz), 130.9 (d, $J$ = 1.5 Hz), 129.5, 128.2, 128.1, 127.7, 124.4 (d, $J$ = 3.9 Hz), 123.6 (d, $J$ = 272 Hz) 123.5, 122.6 (d, $J$ = 3.9 Hz), 81.5 ppm. MS m/z (rel. int.): 459 (44), 457 (22), 379 (100), 358 (3), 341 (4), 281 (12), 253 (5), 207 (35), 180 (3), 132 (24), 119 (22), 77 (57).

(E)-1,2-bis(1,3-diphenyl-4-(phenylselanyl)-1H-pyrazol-5-yl)diazene (6): Reddish solid; m.p.: 190-193 °C; Yield: 50%; $^1$H NMR (CDCl$_3$, 400 MHz): $\delta$ = 7.85-7.83 (m, 4H), 7.57-7.36 (m, 24H), 7.30-7.26 ppm (m, 2H). $^{13}$C NMR (CDCl$_3$, 100 MHz): $\delta$ = 151.1, 138.8, 131.6, 130.9, 129.6, 129.4, 129.3, 129.2, 128.9, 128.7, 128.4, 128.2, 125.9, 125.8, 124.9, 124.5, 103.9. MS m/z (rel. int.): 778 (3), 621 (10), 541 (30), 311 (13), 169 (10), 155 (11), 91 (16), 77 (100).

Reference:

Table S1. Crystallographic data and refinement parameters for 6.

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\[ aR₁ = \frac{\sum|F_o| - |F_c|}{\sum|F_o|} \]
\[ bR₂ = \{\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2}\}^{1/2} \]
SELECTED SPECTRA

Figure S1. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4a.
Figure S2. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4a.
Figure S3. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4b.
Figure S4. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4b.
Figure S5. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4b.
Figure S6. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4c.
Figure S7. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4d.
Figure S8. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4d.
Figure S9. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4e.
Figure S10. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4e.
Figure S11. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4g.
Figure S12. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4g.
Figure S13. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4h.
Figure S14. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4h.
Figure S15. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4i.
Figure S16. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4i.
Figure S17. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4j.
Figure S18. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4j.
Figure S19. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4I.
Figure S20. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4l.
Figure S21. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4m.
Figure S22. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4m.
Figure S23. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4n.
Figure S24. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4n.
Figure S25. $^1$H NMR (400 MHz, CDCl$_3$) of the product 4o
Figure S26. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 4o.
Figure S27. $^1$H NMR (400 MHz, CDCl$_3$) of the product 6.
Figure S28. $^{13}$C NMR (100 MHz, CDCl$_3$) of the product 6.