Article

Novel *N,N'*-Disubstituted Acylselenoureas as Potential Antioxidant and Cytotoxic Agents

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- 4. NMR spectra (¹H, ¹³C and ⁷⁷Se) of final products (**Figures S28-S168**)

Table S1. Cytotoxic a	activity of all acylselen	ourea derivative	es synthesized.	The data are	expressed as
percentage of cell gro	wth ± SEM in at least 3	3 independent ex	xperiments perf	ormed in qu	adruplicates.

		MCF-7		HT-29		HTB-54	
Comp.	Dose (µM)	Growth (%)	SEM	Growth (%)	SEM	Growth (%)	SEM
1a	10	70.5	7.0	56.9	2.5	67.8	4.7
	50	6.6	1.5	23.4	2.3	57.1	2.8
1b	10	64.2	5.8	60.4	3.5	75.8	4.5
	50	12.6	2.8	28.0	2.1	61.1	4.9
1c	10	67.8	1.7	74.9	6.6	64.4	6.6
	50	13.9	1.8	31.9	0.2	57.2	1.7
1d	10	73.6	7.7	97.3	8.8	84.9	7.3
	50	21.9	1.1	25.1	1.0	38.7	2.7
1e	10	74.0	3.9	77.9	4.2	82.3	5.1
	50	13.9	3.9	33.8	2.5	57.2	0.9
2a	10	93.6	8.4	79.1	9.4	91.3	6.0
	50	30.5	3.1	37.8	3.6	65.6	3.5
2b	10	60.1	14.0	80.2	8.0	87.9	4.1
	50	24.7	1.1	46.1	2.0	66.6	9.7
2c	10	62.6	10.1	76.3	8.3	84.9	7.5
	50	26.4	1.6	44.8	6.6	66.7	2.0
2d	10	94.2	0.7	87.1	10.9	100.4	0.2
	50	10.4	2.2	51.7	6.4	37.6	2.0
2e	10	118.1	9.2	77.8	5.3	96.7	7.0
	50	16.0	9.2	57.9	3.3	18.6	1.8
3a	10	84.1	6.2	71.1	5.1	88.8	5.5
	50	23.1	6.4	42.7	1.7	49.9	10.1
3b	10	64.2	4.9	64.7	4.0	45.1	13.0
	50	24.5	2.5	42.5	2.0	22.2	3.5
3c	10	73.9	6.5	67.9	2.2	79.0	7.6
	50	23.7	1.5	44.4	1.3	27.6	2.8
3e	10	105.1	5.6	76.6	1.4	79.4	10.7
	50	32.4	5.2	73.0	1.7	35.8	15.4
4a	10	68.8	11.5	99.1	5.5	83.1	6.4
	50	29.3	4.9	34.1	1.1	67.6	6.7
4b	10	77.6	5.1	99.2	2.5	87.0	2.2
	50	32.4	5.5	51.7	2.1	64.8	3.9
4c	10	86.6	7.3	99.1	7.2	88.9	5.0
	50	33.0	2.9	51.6	6.4	68.5	2.5
4d	10	67.1	2.9	103.2	11.8	90.5	0.8
	50	48.9	5.8	62.2	5.2	62.2	5.6
4e	10	90.6	6.7	93.4	8.7	92.1	7.8

				3 of 90
51	67.0	61	63 5	23
1.6	72.5	2.2	76.8	2.0
4.0	20.0	2.2	12.7	4.4 11.6
2.0	39.0	2.7	43.7	2.2
4.4	82.8	7.0	66.8	2.2
2.1	36.8	2.3	66.7	4./
4.1	57.5	4.5	85.0	6.0
2.2	34.6	2.6	60.2	8.5
9.9	60.6	4.7	76.2	1.0
3.4	29.3	2.0	4.3	0.2
2.4	78.1	1.3	73.2	4.2
4.4	37.8	3.6	58.1	2.2
1.5	72.6	3.0	72.8	5.6
0.9	35.5	1.9	0.7	1.3
2.4	87.6	1.1	73.0	8.0
2.0	48.4	1.7	1.6	1.0
4.7	74.5	2.9	74.2	4.2
2.8	35.9	4.3	3.8	1.1
3.7	81.5	8.0	59.4	3.7
0.3	18.7	1.9	4.6	1.9
7.0	75.2	2.6	84.1	2.0
1.6	31.1	3.1	4.0	1.5

5b	10	64.2	4.4	82.8	7.0	66.8	2.2
	50	17.5	2.1	36.8	2.3	66.7	4.7
5c	10	90.7	4.1	57.5	4.5	85.0	6.0
	50	11.8	2.2	34.6	2.6	60.2	8.5
5d	10	46.7	9.9	60.6	4.7	76.2	1.0
	50	23.5	3.4	29.3	2.0	4.3	0.2
5e	10	77.6	2.4	78.1	1.3	73.2	4.2
	50	20.8	4.4	37.8	3.6	58.1	2.2
6a	10	39.9	1.5	72.6	3.0	72.8	5.6
	50	5.0	0.9	35.5	1.9	0.7	1.3
6b	10	64.9	2.4	87.6	1.1	73.0	8.0
	50	5.8	2.0	48.4	1.7	1.6	1.0
6c	10	70.0	4.7	74.5	2.9	74.2	4.2
	50	13.1	2.8	35.9	4.3	3.8	1.1
6d	10	71.7	3.7	81.5	8.0	59.4	3.7
	50	11.9	0.3	18.7	1.9	4.6	1.9
6e	10	62.7	7.0	75.2	2.6	84.1	2.0
	50	11.2	1.6	31.1	3.1	4.0	1.5
7c	10	91.8	5.3	59.6	4.2	98.4	5.1
	50	24.3	8.7	34.0	3.7	48.3	9.5
7d	10	87.9	8.2	49.5	2.8	92.9	5.3
	50	25.3	9.2	29.6	5.8	79.8	6.6
7e	10	83.9	6.4	53.5	2.8	110.7	7.7
	50	39.0	8.2	45.9	2.1	36.4	5.4
8a	10	75.8	7.2	98.6	12.4	65.2	7.3
	50	15.3	2.1	34.2	2.5	49.7	4.9
8b	10	95.5	1.4	95.3	7.3	85.9	7.3
	50	82.3	3.5	76.9	9.4	72.8	2.8
8c	10	70.2	5.8	73.4	3.9	64.1	3.5
	50	5.7	1.0	42.5	6.6	19.3	2.8
8d	10	91.1	11.1	76.0	5.7	90.0	5.6
	50	18.5	3.4	37.3	8.1	41.1	8.4
8e	10	69.6	9.2	85.2	13.3	76.1	4.0
	50	11.8	2.1	40.6	3.2	31.2	4.8
9a	10	64.9	6.8	62.0	4.1	66.9	6.6
	50	43.4	5.2	28.6	2.3	3.3	1.2
9b	10	76.8	18.1	64.3	6.7	79.0	11.8
	50	62.8	6.2	36.2	1.7	19.0	6.1
9c	10	63.0	11.1	47.9	8.2	64.2	1.3
	50	49.2	7.3	37.3	4.1	7.1	1.3

50

10

50

5a

60.2

70.3

27.4

9d	10	91.1	9.2	61.2	8.2	84.5	6.4
	50	70.2	0.4	36.0	6.2	79.3	7.2
9e	10	54.8	7.8	45.4	7.5	32.9	6.7
	50	44.4	11.6	33.5	5.5	9.0	2.4
10a	10	37.8	7.7	57.3	4.2	44.0	7.9
	50	22.4	5.7	49.5	5.1	13.1	4.5
10b	10	63.0	3.3	63.3	9.1	16.4	3.2
	50	7.4	0.5	43.9	3.9	12.0	2.3
10c	10	52.7	5.4	55.7	6.7	78.2	4.2
	50	15.6	3.1	35.5	4.3	5.1	0.7
10d	10	60.6	1.6	66.5	4.5	79.6	5.1
	50	8.4	1.0	13.9	1.4	5.1	0.7
10e	10	55.6	1.9	54.4	4.0	45.5	8.9
	50	16.9	4.5	21.4	2.0	6.5	1.4

2. SUPPLEMENTARY DATA FOR DPPH AND ABTS ASSAYS







Figure S2. DPPH scavenging activity at a concentration of 0.03 mg/mL and after 90 minutes.



Figure S3. DPPH scavenging activity at a concentration of 0.03 mg/mL and after 120 minutes.



Figure S4. DPPH scavenging activity at a concentration of 0.003 mg/mL and after 30 minutes.



Figure S5. DPPH scavenging activity at a concentration of 0.003 mg/mL and after 60 minutes.



Figure S6. DPPH scavenging activity at a concentration of 0.003 mg/mL and after 90 minutes.



Figure S7. DPPH scavenging activity at a concentration of 0.003 mg/mL and after 120 minutes.



Figure S8. DPPH scavenging activity at a concentration of 0.0006 mg/mL and 0 minutes.



Figure S9. DPPH scavenging activity at a concentration of 0.0006 mg/mL and after 30 minutes.



Figure S10. DPPH scavenging activity at a concentration of 0.0006 mg/mL and after 60 minutes.



Figure S11. DPPH scavenging activity at a concentration of 0.0006 mg/mL and after 90 minutes.



Figure S12. DPPH scavenging activity at a concentration of 0.0006 mg/mL and after 120 minutes.



Figure S13. DPPH scavenging activity at a concentration of 0.0003 mg/mL and 0 minutes.



Figure S14. DPPH scavenging activity at a concentration of 0.0003 mg/mL and after 30 minutes.



Figure S15. DPPH scavenging activity at a concentration of 0.0003 mg/mL and after 60 minutes.





Figure S16. DPPH scavenging activity at a concentration of 0.0003 mg/mL and after 90 minutes.



Figure S17. DPPH scavenging activity at a concentration of 0.0003 mg/mL and after 120 minutes.



Figure S18. ABTS scavenging activity at a concentration of 0.03 mg/mL and after 30 minutes.



Figure S19. ABTS scavenging activity at a concentration of 0.03 mg/mL and after 60 minutes.



Figure S20. ABTS scavenging activity at a concentration of 0.03 mg/mL and after 90 minutes.



Figure S21. ABTS scavenging activity at a concentration of 0.03 mg/mL and after 120 minutes.



Figure S22. ABTS scavenging activity at a concentration of 0.003 mg/mL and after 6 minutes of incubation.



Figure S23. ABTS scavenging activity at a concentration of 0.003 mg/mL and after 30 minutes.



Figure S24. ABTS scavenging activity at a concentration of 0.003 mg/mL and after 60 minutes.



Figure S25. ABTS scavenging activity at a concentration of 0.003 mg/mL and after 90 minutes.



Figure S26. ABTS scavenging activity at a concentration of 0.003 mg/mL and after 120 minutes.

3. CHARACTERIZATION



Figure S27. General structure of the new acylselenoureas.

N-(*phenylcarbamoselenoyl*)*benzamide* **(1a)**. Brown solid; yield: 45%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.98 (1H, s, CONH), 11.80 (1H, s, Ph-NH), 7.99 (2H, d, *J* = 7.6 Hz, R-H), 7.68 (2H, d, *J* = 7.7 Hz, R'-H), 7.67-7.65 (1H, m, R-H), 7.55 (2H, t, *J* = 7.6 Hz, R-H), 7.45 (2H, t, *J* = 7.7 Hz, R'-H), 7.33 (1H, t, *J* = 7.7 Hz, R'-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.0, 168.6, 139.4 133.7, 132.4, 129.2, 129.2, 128.9, 127.4, 125.6. ⁷⁷Se-NMR (75 MHz, CDCl₃) δ: 416.

N-*[*(4-*methylphenyl*)*carbamoselenoyl*]*benzamide* (**1b**). Brown solid; yield: 55%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.94 (1H, s, CONH), 11.76 (1H, s, Ph-NH), 7.98 (2H, d, *J* = 7.3 Hz, R-H), 7.68 (1H, t, *J* = 7.3 Hz, R-H), 7.56-7.52 (4H, m, R'-H+R-H), 7.24 (2H, d, *J* = 8.1 Hz, R'-H), 2.33 (3H, s, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.8, 168.6, 136.9, 136.8, 133.7, 132.4, 129.6, 129.2, 128.9, 125.4, 21.1. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 412.

N-*[*(4-*methoxyphenyl*)*carbamoselenoyl*]*benzamide* (1c). Brown solid; yield: 66%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.85 (1H, s, CONH), 11.75 (1H, s, Ph-NH), 7.98 (2H, d, *J* = 7.3 Hz, R-H), 7.68 (1H, t, *J* = 7.3 Hz, R-H), 7.56 (2H, d, *J* = 8.9 Hz, R'-H), 7.55-7.53 (2H, m, R-H), 6.99 (2H, d, *J* = 8.9 Hz, R'-H), 3.79 (3H, s, OCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.9, 168.6, 158.3, 133.7, 132.4, 132.3, 129.2, 128.9, 127.1, 114.3, 55.8. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 405.

N-*[*(4-*trifluoromethylphenyl*)*carbamoselenoyl]benzamide* (1d). Brown solid; yield: 90%. ¹H-NMR (400 MHz, CDCl₃) δ: 13.06 (1H, s, CONH), 11.98 (1H, s, Ph-NH), 7.99 (2H, d, *J* = 7.4 Hz, R-H), 7.95 (2H, d, *J* = 8.3 Hz, R'-H), 7.81 (2H, d, *J* = 8.3 Hz, R'-H), 7.69 (1H, t, *J* = 7.4Hz, R-H), 7.56 (2H, t, *J* = 7.4 Hz, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.6, 168.4, 143.2, 133.8, 132.3, 129.3, 128.9, 126.3. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 436.

N-[(4-chlorophenyl)carbamoselenoyl]benzamide **(1e)**. Yellow solid; yield: 95%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.92 (1H, s, CONH), 11.87 (1H, s, Ph-NH), 7.98 (2H, d, *J* = 7.5 Hz, R-H), 7.71 (2H, d, *J* = 8.5 Hz, R'-H), 7.69-7.65 (2H, m, R-H), 7.55 (1H, t, *J* = 7.5 Hz, R-H), 7.50 (2H, d, *J* = 8.5 Hz, R'-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.4, 168.5, 138.5, 133.7, 132.4, 131.5, 129.3, 129.1, 128.9, 127.7. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 423.

2-*chloro-N-(phenylcarbamoselenoyl)benzamide* **(2a)**. Orange solid; yield: 11%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.76 (1H, s, CONH), 12.31 (1H, s, Ph-NH), 7.70 (2H, d, *J* = 7.7 Hz, R'-H), 7.65 (1H, d, *J* = 7.5 Hz, R-H), 7.58-7.53 (2H, m, R'-H), 7.49-7.43 (3H, m, R-H), 7.34 (1H, t, *J* = 7.7 Hz, R'-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.6, 168.0, 139.3, 134.6, 132.6, 130.5, 130.0, 129.8, 129.2, 127.6, 127.5, 125.6. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 423.

2-*chloro-N-[*(4-*methylphenyl*)*carbamoselenoyl]benzamide* (**2b**). Orange solid; yield: 36%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.71 (1H, s, CONH), 12.27 (1H, s, Ph-NH), 7.64 (1H, d, *J* = 7.6 Hz, R-H), 7.57 (2H, d, *J* = 3.2 Hz, R-H), 7.56-7.53 (2H, m, R'-H), 7.46 (1H, t, *J* = 7.6 Hz, R-H), 7.25 (2H, d, *J* = 8.1 Hz, R'-H), 2.33 (3H, s, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.4, 168.0, 136.9, 136.8, 134.6, 132.6, 130.5, 130.0, 129.8, 129.6, 127.5, 125.4, 21.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 419.

2-*chloro-N-[(4-methoxyphenyl)carbamoselenoyl]benzamide* (**2c**). Orange solid; yield: 15%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.63 (1H, s, CONH), 12.25 (1H, s, Ph-NH), 7.64 (1H, d, *J* = 7.5 Hz, R-H), 7.57 (2H, d, *J* = 7.5 Hz, R-H), 7.57-7.53 (2H, m, R'-H), 7.45 (1H, t, *J* = 7.5 Hz, R-H), 6.99 (2H, d, *J* = 8.9 Hz, R'-H), 3.80 (3H, s, OCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.6, 168.0, 158.4, 134.6, 132.6, 132.2, 130.5, 130.0, 129.8, 127.5, 127.1, 114.3, 55.8. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 411.

2-*chloro-N-[(4-trifluoromethylphenyl)carbamoselenoyl]benzamide* **(2d)**. Orange solid; yield: 18%. ¹H-NMR (400 MHz, CDCl₃) δ: 13.02 (1H, s, CONH), 9.69 (1H, s, Ph-NH), 7.96 (2H, d, *J* = 8.5 Hz, R'-H), 7.80 (1H, dd, *J* = 7.8, 1.6 Hz, R-H), 7.71 (2H, d, *J* = 8.5 Hz, R'-H), 7.56-7.51 (2H, m, R-H), 7.49-7.43 (1H, m, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.8, 166.0, 133.8, 131.4, 131.3, 131.2, 130.8, 127.7, 126.3, 126.2, 124.4. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 460.

2-*chloro-N-[(4-chlorophenyl)carbamoselenoyl]benzamide* **(2e)**. Pink solid; yield: 26%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.69 (1H, s, CONH), 12.37 (1H, s, Ph-NH), 7.71 (2H, d, *J* = 8.3 Hz, R'-H), 7.64 (1H, d, *J* = 7.2 Hz, R-H), 7.59-7.53 (2H, m, R-H), 7.50 (2H, d, *J* = 8.3 Hz, R'-H), 7.50-7.45 (1H, m, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.0, 167.8, 138.4, 134.5, 132.7, 131.5, 130.5, 130.0, 129.8, 129.1, 127.7, 127.6. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 430.

2-*chloro-5-methylthio-N-(phenylcarbamoselenoyl)benzamide* **(3a)**. Yellow solid; yield: 12%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.74 (1H, s, CONH), 12.32 (1H, s, Ph-NH), 7.69 (2H, d, *J* = 7.8 Hz, R'-H), 7.53 (1H, d, *J* = 2.1 Hz, R-H), 7.46 (2H, d, *J* = 7.8 Hz, R'-H), 7.44-7.40 (2H, m, R-H), 7.34 (1H, t, *J* = 7.8 Hz, R'-H), 2,54 (3H, s, SCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.6, 167.5, 139.3, 138.2, 134.8, 130.3, 129.6, 129.2, 127.5, 126.6, 126.6, 125.6, 15.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 425.

2-*chloro-5-methylthio*-*N*-[(4-*methylphenyl*)*carbamoselenoyl*]*benzamide* (**3b**). Grey solid; yield: 12%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.69 (1H, s, CONH), 12.28 (1H, s, Ph-NH), 7.56 (2H, d, *J* = 8.3 Hz, R'-H), 7.52 (1H, d, *J* = 2.3 Hz, R-H), 7.48 (1H, d, *J* = 8.5 Hz, R-H), 7.41 (1H, dd, *J* = 8.5, 2.3 Hz, R-H), 7.25 (2H, d, *J* = 8.3 Hz, R'-H), 2.54 (3H, s, SCH₃), 2.33 (3H, s, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.4, 167.5, 138.2, 136.9, 136.7, 134.8, 130.3, 129.7, 129.6, 126.6, 126.5, 125.4, 21.2, 15.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 421.

2-*chloro-5-methylthio*-*N*-[(4-*methoxyphenyl*)*carbamoselenoyl*]*benzamide* **(3c)**. Grey solid; yield: 11%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.61 (1H, s, CONH), 12.26 (1H, s, Ph-NH), 7.56 (2H, d, *J* = 8.9 Hz, R'-H), 7.52 (1H, d, *J* = 2.3 Hz, R-H), 7.48 (1H, d, *J* = 8.5 Hz, R-H), 7.41 (1H, dd, *J* = 8.5, 2.3 Hz, R-H), 7.00 (2H, d, *J* = 8.9 Hz, R'-H), 3.80 (3H, s, OCH₃), 2,54 (3H, s, SCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.6, 167.5, 158.4, 138.2, 134.9, 130.3, 129.5, 127.1, 126.5, 114.3, 55.8, 15.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 413.

2-*chloro-5-methylthio*-*N*-[(4-*chlorophenyl*)*carbamoselenoyl*]*benzamide* (**3e**). Grey solid; yield: 24%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.67 (1H, s, CONH), 12.37 (1H, s, Ph-NH), 7.70 (2H, d, *J* = 8.6 Hz, R'-H), 7.52-7.51 (2H, m, R-H), 7.50-7.47 (2H, m, R'-H), 7.42 (1H, dd, *J* = 8.5, 2.3 Hz, R-H), 2,54 (3H, s, SCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.1, 167.3, 138.4, 138.2, 134.8, 131.6, 130.3, 129.6, 129.1, 127.7, 126.6, 126.5, 15.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 431.

2-*chloro-N*-(*phenylcarbamoselenoyl*)*nicotinamide* **(4a)**. Orange solid; yield: 28%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.61 (1H, s, CONH), 9.79 (1H, s, Ph-NH), 8.55 (1H, dd, *J* = 4.7, 1.8 Hz, R-H), 8.12 (1H, dd, *J* = 7.7, 1.8 Hz, R-H), 7.66 (2H, d, *J* = 7.8 Hz, R'-H), 7.42-7.40 (1H, m, R-H), 7.38 (2H, d, *J* = 7.8 Hz, R'-H), 7.30 (1H, t, *J* = 7.8 Hz, R'-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 178.3, 163.2, 151.9, 146.3, 139.1, 137.2, 128.1, 127.4, 126.8, 123.6, 122.0. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 443.

2-*chloro-N-[(4-methylphenyl)carbamoselenoyl]nicotinamide* **(4b)**. Yellow solid; yield: 43%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.51 (1H, s, CONH), 9.75 (1H, s, Ph-NH), 8.55 (1H, dd, *J* = 4.8, 1.8 Hz, R-H), 8.12 (1H, dd, *J* = 7.7, 1.8 Hz, R-H), 7.51 (2H, d, *J* = 7.3 Hz, R'-H), 7.40 (1H, dd, *J* = 7.7, 4.8 Hz, R-H), 7.18

(2H, d, *J* = 7.3 Hz, R'-H), 2.32 (3H, s, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 178.2, 163.1, 151.8, 139.0, 136.9, 134.6, 128.7, 127.4, 123.5, 122.0, 20.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 576.

2-*chloro-N-[(4-methoxyphenyl)carbamoselenoyl]nicotinamide* (4c). Yellow solid; yield: 40%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.46 (1H, s, CONH), 9.84 (1H, s, Ph-NH), 8.54 (1H, d, *J* = 4.8 Hz, R-H), 8.10 (1H, d, *J* = 7.6 Hz, R-H), 7.52 (2H, d, *J* = 8.8 Hz, R'-H), 7.39 (1H, dd, *J* = 7.6, 4.8 Hz, R-H), 6.90 (2H, d, *J* = 8.8 Hz, R'-H), 3.78 (3H, s, OCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.5, 164.3, 158.9, 152.8, 147.4, 140.0, 131.1, 128.6, 126.2, 123.0, 114.3, 55.51. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 424.

2-*chloro-N-[(4-trifluoromethylphenyl)carbamoselenoyl]nicotinamide* (4d). Orange solid; yield: 51%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.82 (1H, s, CONH), 9.87 (1H, s, Ph-NH), 8.56 (1H, dd, *J* = 4.8, 2.0 Hz, R-H), 8.14 (1H, dd, *J* = 7.7, 2.0 Hz, R-H), 7.88 (2H, d, *J* = 8.5 Hz, R'-H), 7.64 (2H, d, *J* = 8.5 Hz, R'-H), 7.41 (1H, dd, *J* = 7.7, 4.8 Hz, RH). ¹³C-NMR (100 MHz, CDCl₃) δ: 178.6, 163.4, 152.1, 140.1, 139.1, 127.2, 125.3, 123.4, 122.1, 120.1, 118.8. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 478.

2-*chloro-N-[(4-chlorophenyl)carbamoselenoyl]nicotinamide* **(4e)**. Orange solid; yield: 53%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.62 (1H, s, CONH), 9.86 (1H, s, Ph-NH), 8.56 (1H, dd, *J* = 4.8, 1.6 Hz, R-H), 8.12 (1H, dd, *J* = 7.7, 1.6 Hz, R-H), 7.63 (2H, d, *J* = 8.7 Hz, R'-H), 7.41 (1H, dd, *J* = 7.7, 4.8 Hz, R-H), 7.35 (2H, d, *J* = 8.7 Hz, R'-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.6, 164.4, 153.0, 140.1, 136.7, 133.2, 129.3, 128.4, 128.3, 125.9, 123.1. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 455.

N-(phenylcarbamoselenoyl)-2-thiophencarboxamide **(5a)**. Yellow crystals; yield: 35%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.73 (1H, s, CONH), 9.24 (1H, s, Ph-NH), 7.68 (2H, dd, *J* = 4.6, 3.5 Hz, R-H), 7.62 (2H, d, *J* = 7.8 Hz, R'-H), 7.36 (2H, t, *J* = 7.8 Hz, R'-H), 7.26 (1H, t, *J* = 7.8 Hz, R'-H), 7.13 (1H, dd, *J* = 4.6, 3.5 Hz, R-H).¹³C-NMR (100 MHz, CDCl₃) δ: 179.7, 161.1, 138.4, 135.6, 134.7, 131.1, 129.0, 128.7, 127.6, 124.7. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 408.

N-[(4-methylphenyl)carbamoselenoyl]-2-thiophencarboxamide **(5b)**. Yellow solid; yield: 50%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.63 (1H, s, CONH), 9.26 (1H, s, Ph-NH), 7.68 (1H, d, *J* = 4.5 Hz, R-H), 7.67 (1H, d, *J* = 4.5 Hz, R-H), 7.46 (2H, d, *J* = 8.3 Hz, R'-H), 7.15 (2H, d, *J* = 8.3 Hz, R'-H), 7.12 (1H, t, *J* = 4.5 Hz, R-H), 2.29 (3H, s, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 178.7, 160.1, 136.6, 134.9, 134.6, 133.6, 130.0, 128.6, 127.6, 123.6, 20.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 400.

N-[(4-methoxyphenyl)carbamoselenoyl]-2-thiophencarboxamide **(5c)**. Yellow solid; yield: 46%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.56 (1H, s, CONH), 9.25 (1H, s, Ph-NH), 7.67 (2H, t, *J* = 4.0 Hz, R-H), 7.48 (2H, d, *J* = 8.9 Hz, R'-H), 7.12 (1H, dd, *J* = 5.0, 4.0 Hz, R-H), 6.87 (2H, d, *J* = 8.9 Hz, R'-H), 3.75 (3H, s, OCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 178.8, 160.1, 157.7, 134.6, 133.6, 130.4, 127.6, 125.2, 113.2, 54.5. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 393.

N-*[*(4-*trifluoromethylphenyl*)*carbamoselenoyl*]-2-*thiophencarboxamide* **(5d)**. Yellow crystals; yield: 32%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.95 (1H, s, CONH), 9.29 (1H, s, Ph-NH), 7.83 (2H, d, *J* = 7.3 Hz, R-H), 7.72-7.68 (2H, m, R'-H), 7.61 (2H, d, *J* = 7.0 Hz, R'-H), 7.16-7.11 (1H, m, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.0, 160.2, 140.3, 134.3, 134.0, 130.2, 127.7, 125.2, 123.4, 118.9. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 438.

N-[(4-chlorophenyl)carbamoselenoyl]-2-thiophencarboxamide **(5e)**. Yellow solid; yield: 53%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.74 (1H, s, CONH), 9.27 (1H, s, Ph-NH), 7.71-7.67 (2H, m, R'H), 7.58 (2H, d, *J* = 8.9 Hz, R'-H), 7.31 (2H, d, *J* = 8.9 Hz, R'-H), 7.12 (1H, dd, *J* = 4.8, 4.0 Hz, R'H). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.0, 160.2, 135.9, 134.4, 133.9, 132.0, 130.2, 128.1, 127.7, 124.9. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 419.

N-(*phenylcarbamoselenoyl*)-2-*furancarboxamide* **(6a)**. White solid; yield: 39%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.73 (1H, s, CONH), 11.43 (1H, s, Ph-NH), 8.10 (1H, d, *J* = 1.3 Hz, R-H), 7.90 (1H, d,

J = 3.6 Hz, R-H), 7.65 (2H, d, *J* = 7.8 Hz, R'-H), 7.44 (2H, t, *J* = 7.8 Hz, R'-H), 7.33 (1H, t, *J* = 7.8 Hz, R'-H), 6.78 (1H, dd, *J* = 3.6, 1.3 Hz, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.4, 157.7, 149.1, 144.9, 139.4, 129.2, 127.4, 125.7, 119.5, 113.3. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 417.

N-*[*(4-*methylphenyl*)*carbamoselenoyl*]-2-*furancarboxamide* (6b). Yellow solid; yield: 66%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.67 (1H, s, CONH), 11.38 (1H, s, Ph-NH), 8.09 (1H, d, *J* = 1.4 Hz, R-H), 7.88 (1H, d, *J* = 3.6 Hz, R-H), 7.51 (2H, d, *J* = 8.3 Hz, R'-H), 7.23 (2H, d, *J* = 8.3 Hz, R'-H), 6.78 (1H, dd, *J* = 3.6, 1.4 Hz, R-H), 2.32 (3H, s, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.2, 157.7, 149.1, 144.9, 136.9, 129.6, 125.5, 119.5, 113.3, 21.1. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 413.

N-((4-*methoxyphenyl*)*carbamoselenoyl*)-2-*furancarboxamide* (6c). Yellow solid; yield: 39%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.59 (1H, s, CONH), 11.37 (1H, s, Ph-NH), 8.09 (1H, s, R-H), 7.88 (1H, d, *J* = 3.6 Hz, R-H), 7.52 (2H, d, *J* = 8.9 Hz, R'-H), 6.98 (2H, d, *J* = 8.9 Hz, R'-H), 6.78 (1H, dd, *J* = 3.6, 1.6 Hz, R-H), 3.79 (3H, s, OCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.4, 158.4, 157.7, 149.0, 145.0, 132.3, 127.1, 119.4, 114.3, 113.3, 55.8. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 406.

N-*[*(4-*trifluoromethylphenyl*)*carbamoselenoyl*]-2-*furancarboxamide* (6d). White solid; yield: 42%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.81 (1H, s, CONH), 11.61 (1H, s, Ph-NH), 8.11 (1H, d, *J* = 1.4 Hz, R-H), 7.92 (1H, m, R-H), 7.91 (2H, d, *J* = 8.5 Hz, R'-H), 7.80 (2H, d, *J* = 8.5 Hz, R'-H), 6.79 (1H, dd, *J* = 3.6, 1.4 Hz, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.1, 156.9, 149.2, 147.5, 146.6, 144.9, 143.1, 142.7, 126.4, 120.6, 119.7, 116.0, 113.3, 112.8. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 437.

N-[(4-*chlorophenyl*)*carbamoselenoyl*]-2-*furancarboxamide* (6e). White solid; yield: 39%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.67 (1H, s, CONH), 11.52 (1H, s, Ph-NH), 8.10 (1H, s, R-H), 7.89 (1H, d, *J* = 3.5 Hz, R-H), 7.67 (2H, d, *J* = 8.6 Hz, R'-H), 7.49 (2H, d, *J* = 8.6 Hz, R'-H), 6.78 (1H, dd, *J* = 3.5, 1.6 Hz, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.9, 157.6, 149.1, 144.9, 138.5, 131.5, 129.1, 127.7, 119.6, 113.3. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 424.

(1*S*,3*s*)-*N*-[(4-methoxyphenyl)carbamoselenoyl]adamantane-1-carboxamide (7c). Pink solid; yield: 28%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.83 (1H, s, CONH), 10.65 (1H, s, Ph-NH), 7.48 (2H, d, *J* = 8.9 Hz, R'-H), 6.96 (2H, d, *J* = 8.9 Hz, R'-H), 3.78 (3H, s, OCH₃), 2.05-1.99 (3H, m, R-H), 1.98-1.93 (6H, m, R-H), 1.79-1.64 (6H, m, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.0, 179.9, 158.3, 132.3, 127.1, 114.2, 55.8, 42.1, 37.3, 36.0, 27.9. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 381.

(1*S*,3*s*)-*N*-[(4-trifluoromethylphenyl)carbamoselenoyl]adamantane-1-carboxamide (7d). Pink solid; yield: 31%. ¹H-NMR (400 MHz, CDCl₃) δ: 13.08 (1H, s, CONH), 10.91 (1H, s, Ph-NH), 7.87 (2H, d, *J* = 8.4 Hz, R'-H), 7.77 (2H, d, *J* = 8.4 Hz, R'-H), 2.05-1.99 (3H, m, R-H), 1.99-1.95 (6H, m, R-H), 1.76-1.65 (6H, m, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.7, 179.9, 143.1, 127.5, 127.2, 126.4, 126.2, 125.9, 123.2, 42.1, 37.2, 36.0, 27.9. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 410.

(1*S*,3*s*)-*N*-((4-chlorophenyl)carbamoselenoyl)adamantane-1-carboxamide (7e). Yellow solid; yield: 37%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.91 (1H, s, CONH), 10.82 (1H, s, Ph-NH), 7.62 (2H, d, *J* = 8.7 Hz, R'-H), 7.46 (2H, d, *J* = 8.7 Hz, R'-H), 2.05-1.99 (3H, m, R-H), 1.98-1.94 (6H, m, R-H), 1.79-1.65 (6H, m, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.5, 179.9, 138.4, 131.4, 129.0, 127.8, 42.1, 37.2, 36.0, 27.9. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 397.

N-(*phenylcarbamoselenoyl*)*cinnamamide* **(8a)**. Yellow solid; yield: 45%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.97 (1H, s, CONH), 9.39 (1H, s, Ph-NH), 7.78 (1H, d, *J* = 15.5 Hz, C=C-H), 7.61 (2H, d, *J* = 7.7 Hz, R'-H), 7.49 (2H, d, *J* = 7.7 Hz, R'-H), 7.41-7.32 (5H, m, R-H), 7.26 (1H, t, *J* = 7.7 Hz, R'-H), 6.51 (1H, d, *J* = 15.5 Hz, C=C-H).¹³C-NMR (100 MHz, CDCl₃) δ: 179.0, 164.8, 146.2, 137.4, 132.6, 130.3, 128.1, 128.0, 127.6, 126.5, 123.8, 117.0. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 392.

N-[(4-methylphenyl)carbamoselenoyl]cinnamamide (8b). Brown solid; yield: 42%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.84 (1H, s, CONH), 9.24 (1H, s, Ph-NH), 7.78 (1H, d, *J* = 15.5 Hz, C=C-H), 7.51-7.48 (2H,

m, R-H), 7.47 (2H, d, *J* = 8.3 Hz, R'-H), 7.40-7.32 (3H, m, R-H), 7.15 (2H, d, *J* = 8.3 Hz, R'-H), 6.46 (1H, d, *J* = 15.5 Hz, C=C-H), 2.30 (3H, s, CH₃).¹³C-NMR (100 MHz, CDCl₃) δ: 178.9, 164.6, 146.1, 136.5, 134.9, 132.6, 130.3, 128.6, 128.1, 127.6, 123.7, 117.0, 20.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 386.

N-*[*(4-*methoxyphenyl*)*carbamoselenoyl*]*cinnamamide* (8c). Yellow solid; yield: 48%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.80 (1H, s, CONH), 9.47 (1H, s, Ph-NH), 7.77 (1H, d, *J* = 15.5 Hz, C=C-H), 7.50-7.47 (2H, m, R-H), 7.47 (2H, d, *J* = 8.5 Hz, R'-H), 7.39-7.31 (3H, m, R-H), 6.86 (2H, d, *J* = 8.5 Hz, R'-H), 6.52 (1H, d, *J* = 15.5 Hz, C=C-H), 3.76 (3H, s, OCH₃).¹³C-NMR (100 MHz, CDCl₃) δ: 179.1, 164.8, 157.7, 146.0, 132.6, 130.4, 130.3, 128.1, 127.6, 125.3, 117.0, 113.1, 54.4. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 376.

N-*[*(4-*trifluoromethylphenyl*)*carbamoselenoyl]cinnamamide* **(8d)**. Yellow solid; yield: 49%. ¹H-NMR (400 MHz, CDCl₃) δ: 13.20 (1H, s, CONH), 9.37 (1H, s, Ph-NH), 7.83 (2H, d, *J* = 8.3 Hz, R'-H), 7.79 (1H, m, C=C-H), 7.60 (2H, d, *J* = 8.3 Hz, R'-H), 7.50 (2H, d, *J* = 6.8 Hz, R-H), 7.41-7.31 (3H, m, R-H), 6.48 (1H, d, *J* = 15.5 Hz, C=C-H).¹³C-NMR (100 MHz, CDCl₃) δ: 179.3, 164.9, 146.7, 140.3, 132.5, 130.5, 128.2, 127.6, 125.1, 123.5, 116.6. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 421.

N-((*4*-*chlorophenyl*)*carbamoselenoyl*)*cinnamamide* (8e). Yellow solid; yield: 46%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.95 (1H, s, CONH), 9.10 (1H, s, Ph-NH), 7.79 (1H, d, *J* = 15.5 Hz, C=C-H), 7.59 (2H, d, *J* = 8.7 Hz, R'-H), 7.52-7.48 (2H, m, R-H), 7.42-7.35 (3H, m, R-H), 7.32 (2H, d, *J* = 8.7 Hz, R'-H), 6.41 (1H, d, *J* = 15.5 Hz, C=C-H).¹³C-NMR (100 MHz, CDCl₃) δ: 180.3, 165.6, 147.5, 136.9, 133.5, 132.9, 131.5, 129.2, 128.6, 125.9, 117.7. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 408.

N-(*phenylcarbamoselenoyl*)*benzo*[*b*]*thiophene-2-carboxamide* (9a). Yellow solid; yield: 44%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.72 (1H, s, CONH), 9.40 (1H, s, Ph-NH), 7.97 (1H, s, CH), 7.85 (2H, t, *J* = 8.7 Hz, R-H), 7.63 (2H, d, *J* = 7.8 Hz, R'-H), 7.46 (1H, t, *J* = 7.8 Hz, R'-H), 7.41-7.27 (4H, m, R-H+R'-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.5, 161.8, 142.4, 138.7, 138.4, 135.1, 129.1, 128.4, 128.0, 127.7, 126.1, 125.7, 124.7, 122.9. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 415.

N-[(4-*methylphenyl*)*carbamoselenoyl*]*benzo*[*b*]*thiophene-2-carboxamide* (9b). Yellow solid; yield: 62%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.72 (1H, s, CONH), 9.40 (1H, s, Ph-NH), 7.96 (1H, s, CH), 7.84 (2H, t, *J* = 8.4 Hz, R-H), 7.48 (2H, d, *J* = 7.7 Hz, R'-H), 7.46-7.43 (1H, m, R-H), 7.39 (1H, t, *J* = 7.4 Hz, R-H), 7.16 (2H, d, *J* = 7.7 Hz, R'-H), 2.30 (3H, s, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.5, 161.7, 142.4, 138.7, 137.7, 135.9, 135.2, 129.7, 128.3, 127.9, 126.0, 125.6, 124.6, 122.9, 21.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 408.

N-[(4-*methoxyphenyl*)*carbamoselenoyl*]*benzo*[*b*]*thiophene-2-carboxamide* (9c). Yellow solid; yield: 37%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.56 (1H, s, CONH), 9.44 (1H, s, Ph-NH), 7.95 (1H, s, CH), 7.83 (2H, t, *J* = 7.8 Hz, R-H), 7.48 (2H, d, *J* = 8.4 Hz, R'-H), 7.45-7.36 (2H, m, R-H), 6.86 (2H, d, *J* = 8.4 Hz, R'-H), 3.75 (3H, s, OCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.6, 161.8, 158.8, 142.4, 138.7, 135.2, 131.4, 128.4, 127.9, 126.2, 126.0, 125.6, 122.9, 114.2, 55.5. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 401.

N-[(4-trifluoromethylphenyl)carbamoselenoyl]benzo[b]thiophene-2-carboxamide (9d). Yellow solid; yield: 51%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.95 (1H, s, CONH), 9.45 (1H, s, Ph-NH), 7.98 (1H, s, CH), 7.86-7.83 (4H, m, R-H+R'-H), 7.61 (2H, d, *J* = 8.5 Hz, R'-H), 7.50-7.37 (2H, m, R-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.8, 161.9, 142.5, 141.3, 138.6, 134.7, 128.6, 128.1, 126.3, 126.2, 126.1, 125.7, 124.4, 122.9. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 448.

N-((*4-chlorophenyl*)*carbamoselenoyl*)*benzo*[*b*]*thiophene-2-carboxamide* (9e). Yellow solid; yield: 43%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.73 (1H, s, CONH), 9.40 (1H, s, Ph-NH), 7.97 (1H, s, CH), 7.90-7.82 (2H, m, R-H), 7.61 (2H, d, *J* = 8.7 Hz, R'-H), 7.47 (1H, t, *J*= 7.0 Hz, R-H), 7.41 (1H, t, *J*= 7.0 Hz, R-H), 7.33 (2H, d, *J* = 8.7 Hz, R'-H). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.8, 161.8, 142.5, 138.7, 136.9, 134.9, 133.1, 129.2, 128.5, 128.1, 126.1, 125.9, 125.7, 122.9. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 427. *N*-(*phenylcarbamoselenoyl*)*benzo*[*d*][1,3]*dioxole-5-carboxamide* (10a). Orange solid; yield: 66%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.95 (1H, s, CONH), 9.38 (1H, s, Ph-NH), 7.62 (2H, d, *J* = 7.7 Hz, R'-H), 7.41 (1H, dd, *J* = 8.2, 1.9 Hz, R-H), 7.37 (2H, t, *J* = 7.7Hz, R'-H), 7.31 (1H, d, *J* = 1.9 Hz, R-H), 7.27 (1H, t, *J* = 7.7 Hz, R'-H), 6.85 (1H, d, *J* = 8.2 Hz, R-H), 6.03 (2H, s, CH₂). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.1, 165.1, 151.6, 147.7, 137.4, 128.0, 124.1, 123.7, 122.3, 107.6, 106.9, 101.4. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 394.

N-[(4-*methylphenyl*)*carbamoselenoyl*]*benzo*[*d*][1,3]*dioxole-5-carboxamide* (**10b**). Orange solid; yield: 68%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.82 (1H, s, CONH), 9.29 (1H, s, Ph-NH), 7.47 (2H, d, *J* = 8.3 Hz, R'-H), 7.38 (1H, dd, *J* = 8.2, 1.8 Hz, R-H), 7.28 (1H, d, *J* = 1.8 Hz, R-H), 7.15 (2H, d, *J* = 8.3 Hz, R'-H), 6.83 (1H, d, *J* = 8.2 Hz, R-H), 6.01 (2H, s, CH₂), 2.29 (3H, s, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.0, 166.1, 152.6, 148.7, 137.6, 136.0, 129.6, 125.2, 124.7, 123.2, 108.6, 107.9, 102.4, 21.2. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 390.

N-[(4-*methoxyphenyl*)*carbamoselenoyl*]*benzo*[*d*][1,3]*dioxole-5-carboxamide* (10c). Orange solid; yield: 62%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.76 (1H, s, CONH), 9.31 (1H, s, Ph-NH), 7.48 (2H, d, *J* = 8.9 Hz, R'-H), 7.38 (1H, dd, *J* = 8.2, 1.6 Hz, R-H), 7.29 (1H, d, *J* = 1.6 Hz, R-H), 6.87 (2H, d, *J* = 8.9 Hz, R'-H), 6.84 (1H, d, *J* = 8.2 Hz, R-H), 6.03 (2H, s, CH₂), 3.76 (3H, s, OCH₃). ¹³C-NMR (100 MHz, CDCl₃) δ: 180.2, 166.1, 158.7, 152.6, 148.7, 131.5, 126.3, 125.2, 123.2, 114.2, 108.6, 107.9, 102.4, 55.5. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 383.

N-*[*(4-*trifluoromethylphenyl*)*carbamoselenoyl*]*benzo*[*d*][1,3]*dioxole-5-carboxamide* (10d). Orange solid; yield: 56%. ¹H-NMR (400 MHz, CDCl₃) δ: 13.08 (1H, s, CONH), 11.72 (1H, s, Ph-NH), 7.93 (2H, d, *J* = 8.4 Hz, R'-H), 7.79 (2H, d, *J* = 8.4 Hz, R'-H), 7.66 (1H, dd, *J* = 8.2, 1.5 Hz, R-H), 7.55 (1H, d, *J* = 1.5 Hz, R-H), 7.07 (1H, d, *J* = 8.2 Hz, R-H), 6.17 (2H, s, CH₂). ¹³C-NMR (100 MHz, CDCl₃) δ: 181.5, 152.2, 147.9, 143.2, 126.2, 125.7, 125.6, 120.5, 109.0, 108.5, 102.7, 102.4. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 432.

N-((4-*chlorophenyl*)*carbamoselenoyl*)*benzo*[*d*][1,3]*dioxole-5-carboxamide* (10e). Orange solid; yield: 67%. ¹H-NMR (400 MHz, CDCl₃) δ: 12.95 (1H, s, CONH), 9.33 (1H, s, Ph-NH), 7.59 (2H, d, *J* = 8.4 Hz, R'-H), 7.38 (1H, dd, *J* = 8.2, 1.9 Hz, R-H), 7.31 (2H, d, *J* = 8.4 Hz, R'-H), 7.28 (1H, d, *J* = 1.9 Hz, R-H), 6.84 (1H, d, *J* = 8.2 Hz, R-H), 6.03 (2H, s, CH₂). ¹³C-NMR (100 MHz, CDCl₃) δ: 179.3, 165.1, 151.7, 147.7, 135.9, 131.9, 128.1, 124.9, 123.9, 122.2, 107.6, 106.8, 101.4. ⁷⁷Se-NMR (76 MHz, CDCl₃) δ: 408.

4. NMR SPECTRA (1H, 13C AND 77Se) OF FINAL PRODUCTS









Figure S31. ¹H-NMR of compound 1b.







Figure S33. ⁷⁷Se-NMR of compound 1b.







Figure S37. ¹H-NMR of compound 1d.



Figure S39. ⁷⁷Se-NMR of compound 1d.



Figure S41. ¹³C-NMR of compound 1e.









Figure S45. ⁷⁷Se-NMR of compound 2a.











Figure S51. ⁷⁷Se-NMR of compound 2c.











Figure S57. ⁷⁷Se-NMR of compound 2e.







-425.06






Figure S63. ⁷⁷Se-NMR of compound 3b.







Figure S67. ¹H-NMR of compound 3e.



Figure S69. ⁷⁷Se-NMR of compound 3e.











10.5

1.00-

12.5

11.5

13.5

1.12-1

8.5

0.93-

9.5

1.02-1

1.22 Å

7.5 7.0 6.5 f1 (ppm)

5.5

4.5

3.5

2.87-

1.5

0.5

2.5

590

-443.31

















Figure S79. ¹H-NMR of compound 4d.

-424.14



Figure S81. 77Se-NMR of compound 4d.











Figure S87. ⁷⁷Se-NMR of compound 5a.





Figure S89. ¹³C-NMR of compound 5b.



Figure S91. ¹H-NMR of compound 5c.





Figure S93. ⁷⁷Se-NMR of compound 5c.













Figure S99. ⁷⁷Se-NMR of compound 5e.









Figure S103. ¹H-NMR of compound 6b.





Figure S105. ⁷⁷Se-NMR of compound 6b.











Figure S111. ⁷⁷Se-NMR of compound 6d.













Figure S117. ⁷⁷Se-NMR of compound 7c.







Figure S121. ¹H-NMR of compound 7e.



Figure S123. ⁷⁷Se-NMR of compound 7e.



Figure S124. ¹H-NMR of compound 8a.

6	26	975513413
20	40	16.226.228.332.16
-	Ĩ	







Figure S127. ¹H-NMR of compound 8b.



Figure S129. ⁷⁷Se-NMR of compound 8b.










Figure S135. ⁷⁷Se-NMR of compound 8d.



Figure S137. ¹³C-NMR of compound 8e.







Figure S141. ⁷⁷Se-NMR of compound 9a.





Figure S143. ¹³C-NMR of compound 9b.







Figure S147. ⁷⁷Se-NMR of compound 9c.



Figure S149. ¹³C-NMR of compound 9d.



Figure S151. ¹H-NMR of compound 9e.



Figure S153. 77Se-NMR of compound 9e.



Figure S155. ¹³C-NMR of compound 10a.



Figure S157. ¹H-NMR of compound 10b.



Figure S159. ⁷⁷Se-NMR of compound 10b.











Figure S165. ⁷⁷Se-NMR of compound 10d.



Figure S166. ¹H-NMR of compound 10e.







Figure S168. ⁷⁷Se-NMR of compound 10e.