Synthesis of Substituted Selenolo[3,2-*d*][1,2,3]triazines and [1,3]Selenazolo[4,5-*d*][1,2,3]triazines

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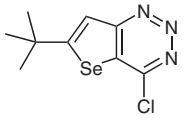
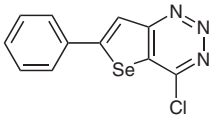
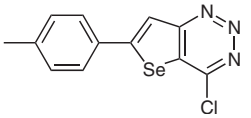
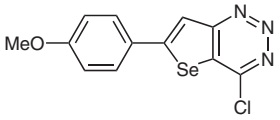
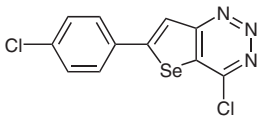
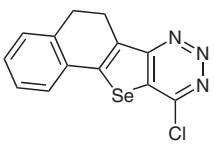
Abstract: 5-Substituted 3-amino-selenophene-2-carbonitriles and 2-substituted 4-amino-1,3-selenazole-5-carbonitriles were reacted with sodium nitrite in hydrochloric acid to give chloroselenolotriazines and chloroselenazolotriazines. These compounds were then subjected to S_NAr reactions with secondary amines under microwave irradiation.

Key words: heterocycles, selenium, microwave, triazines

Polyfunctionally substituted heterocyclic compounds are present as important core structures in many biologically active compounds. For many years, our group has been interested in heterocycles such as thiophenes, selenophenes, thiazoles and, especially, in condensed heterocyclic systems. In previous work, we described access to thienopyridines,[1] selenolopyridines,[2] thiazolopyridines,[3] thienopyrimidinones[4] and selenolopyrimidines.[5] We now report on the formation of selenolo- and selenazolo-triazines.

Indeed, the 1,2,3-triazine ring is also present in compounds with biological activities. For example, pyrazolo[3,4-*d*]-1,2,3-triazin-4-one nucleosides[6] or pyrrolo[2,3-*d*]-1,2,3-triazine[7] were explored for their antiviral/antitumor activity. A few years ago, pyridothienotriazines were also described as anti-histaminic,[8] anti-protozoal[9] and antifungal[10] compounds. In these last publications, the 4-chlorotriazine ring was prepared in one pot, starting from 3-amino-2-cyanothiophenes, using sodium nitrite in concentrated hydrochloric acid; the intermediate obtained by diazotization underwent a spontaneous intramolecular condensation of the diazonium salt with the adjacent nucleophilic function. However, depending on the starting heterocycles, these conditions were sometimes ineffective. Indeed, diazotization of 2-amino-pyrrole-3-carboxamide under these conditions resulted in significant decomposition,[11] whereas Moyano et al.[12] obtained the corresponding pyrazolotriazinones from 5-amino-1*H*-pyrazole-4-carbonitriles instead of the expected chloropyrazolotriazines. We have recently successfully applied this diazotization/chlorination process to 4-amino-1,3-thiazole-5-carbonitriles[3] and we now wanted to extend the approach to selenium-containing heterocycles. To the best of our knowledge, there is only a single report on the synthesis of one selenolotriazine: Abdel–Hafez[13] described the formation of a 4-chloroselenolo[2,3-*d*][1,2,3]triazine by diazotization of a 2-amino-selenophene-3-carbonitrile with sodium nitrite in acetic acid and hydrochloric acid (10:3). The obtained compound was shown to possess relatively high antifungal activity. In our case, the same methodology used on 3-amino-selenophene-2-carbonitriles gave the expected 4-chloroselenolo[3,2-*d*][1,2,3-]triazines **1**–**6** in good yields (Scheme 1 and Table 1).

Table 1 Synthesis of Chloroselenolotriazines **1**–**6**

Product		Yield (%)
1		49
2		85
3		94
4		85
5		95
6		92

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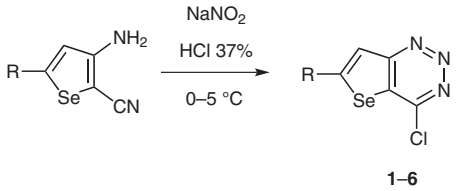
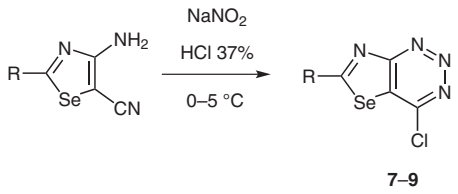


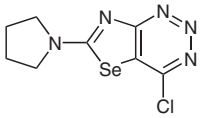
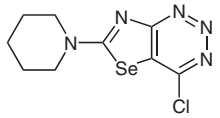
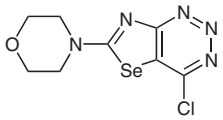
Scheme 1

In 2009, we described the synthesis of 2,4,5-trisubstituted-1,3-selenazoles in a one-pot, four-step procedure,[14] so we had several 4-amino-1,3-selenazole-5-carbonitriles at our disposal. We decided to extend this study to the one-pot diazotization/chlorination of those compounds (Scheme 2 and Table 2). Once again, the expected chloroselenazolotriazines **7–9** were obtained in moderate to good yields.



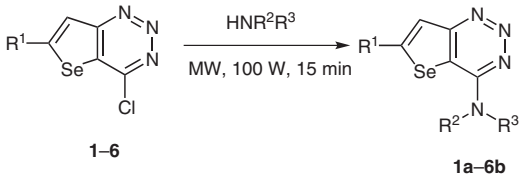
Scheme 2

Table 2 Synthesis of Chloroselenazolotriazines **7–9**

Product		Yield (%)
7		46
8		67
9		29

We then wanted to study whether these chloroselenolo- and chloroselenazolo-triazines would undergo normal halide-displacement by nucleophiles. Compounds **1–6** were reacted with two secondary amines (pyrrolidine and morpholine) under microwave irradiation (Scheme 3 and Table 3). Yields obtained were quite good and reaction times were very short. However, no satisfying results were obtained with compounds **7–9** due to their very low solubility in most organic solvents.

In summary, we have described the synthesis and functionalization of new selenium-containing heterocyclic scaffolds: eighteen seleno[2,3-*d*][1,2,3]triazines and three [1,3]selenazolo[4,5-*d*][1,2,3]triazines were isolated and characterized.



Scheme 3

Table 3 Nucleophilic Substitution on Chloroselenolotriazines

Chloroselenolotriazine	Amine	Product	Yield (%)
1	pyrrolidine	**1a**	88
	morpholine	**1b**	90
2	pyrrolidine	**2a**	98
	morpholine	**2b**	93
3	pyrrolidine	**3a**	96
	morpholine	**3b**	94
4	pyrrolidine	**4a**	93
	morpholine	**4b**	96
5	pyrrolidine	**5a**	91
	morpholine	**5b**	90
6	pyrrolidine	**6a**	94
	morpholine	**6b**	90

Melting points were determined on a Stuart SMP3 apparatus and are uncorrected. ^{1}H and ^{13}C NMR spectra (δ, ppm) were recorded on an AC Bruker 250 MHz spectrometer in DMSO-d_6 or Pyridine-d_5. MS spectra were recorded on an Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry instrument (ESI-FTICR/MS, QFT-9, 4T, Varian-Ion Spec, California) with Omega 9 Software (Varian) used for acquisition and analysis of Fourier transform mass spectra. Exact Mass Calculator, Ion Spec, was used for the calculation of mass, *m*/*z* values and isotope distribution from an elemental formula. A CEM Discover microwave oven was used in open-vessel mode for the microwave-assisted synthesis; the temperature was monitored by an infrared sensor located in the microwave cavity floor.

Synthesis of Chloroselenolotriazines 1–6; General Procedure

A solution of $NaNO_2$ (5.37 mmol) in H_2O (5 mL) was added over 15 min to a suspension of 5-substituted 3-amino-selenophene-2-carbonitrile (3.81 mmol) at 0–5 °C in concd HCl (13 mL). The resulting mixture was stirred at 0 °C for a further 40 min and then allowed to stand at r.t. overnight. The reaction mixture was poured into H_2O (100 mL) and the precipitate was washed with H_2O (2 × 15 mL), dried at r.t., and recrystallized from MeCN (2 mL).

6-*tert*-Butyl-4-chloroselenolo[3,2-*d*][1,2,3]triazine (1)

Yield: 49%; yellow solid; mp 85 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 1.48 (s, 9 H, 3 × CH_3), 8.05 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 31.8, 37.8, 120.9, 133.0, 154.8, 160.4, 179.4.

HRMS (ESI): *m*/*z* calcd for $C_9H_{10}N_3ClSeNa$: 297.9618; found: 297.9633.

4-Chloro-6-phenylselenolo[3,2-*d*][1,2,3]triazine (2)
Yield: 85%; brown solid; mp 135 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 7.57 (m, 3 H, 3 × CH), 8.01 (m, 2 H, 2 × CH), 8.73 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 121.6, 127.6, 129.6, 131.4, 132.9, 133.6, 154.7, 160.9, 161.6.

HRMS (ESI): *m*/*z* calcd for $C_{11}H_7N_3ClSe$: 295.9488; found: 295.9486.

4-Chloro-6-(4-methylphenyl)selenolo[3,2-*d*][1,2,3]triazine (3)
Yield: 94%; orange solid; mp 154 °C.

^{1}H NMR (250 MHz, pyridine-d_5): δ = 2.23 (s, 3 H, CH_3), 7.25 (d, *J* = 7.8 Hz, 2 H, 2 × CH), 7.74 (d, *J* = 7.8 Hz, 2 H, 2 × CH), 8.45 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, pyridine-d_5): δ = 21.7, 121.8, 128.3, 131.0, 131.5, 134.2, 142.6, 155.8, 162.2, 162.7.

HRMS (ESI): *m*/*z* calcd for $C_{12}H_9N_3ClSe$: 309.9645; found: 309.9613.

4-Chloro-6-(4-methoxyphenyl)selenolo[3,2-*d*][1,2,3]triazine (4)
Yield: 85%; brown solid; mp 145 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.85 (s, 3 H, OCH_3), 7.10 (d, *J* = 8.7 Hz, 2 H, 2 × CH), 7.97 (d, *J* = 8.7 Hz, 2 H, 2 × CH), 8.57 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 55.6, 114.9, 119.6, 125.5, 129.4, 132.9, 154.3, 161.3, 161.6, 161.8.

HRMS (ESI): *m*/*z* calcd for $C_{12}H_9ON_3ClSe$: 325.9594; found: 325.9679.

4-Chloro-6-(4-chlorophenyl)selenolo[3,2-*d*][1,2,3]triazine (5)
Yield: 95%; pale-brown solid; mp 164 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 7.63 (d, *J* = 8.6 Hz, 2 H, 2 × CH), 8.04 (d, *J* = 8.6 Hz, 2 H, 2 × CH), 8.74 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 122.4, 129.4, 129.5, 131.8, 133.8, 136.1, 154.7, 159.9, 160.8.

HRMS (ESI): *m*/*z* calcd for $C_{11}H_6N_3Cl_2Se$: 329.9099; found: 329.9099.

10-Chloro-5,6-dihydronaphtho[2′,1′:4,5]selenolo[3,2-*d*][1,2,3]triazine (6)
Yield: 92%; pale-brown solid; mp 149 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.09 (m, 2 H, CH_2), 3.20 (m, 2 H, CH_2), 7.37 (m, 3 H, 3 × CH), 7.66 (m, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 22.0, 26.9, 126.9, 127.6, 128.6, 130.1, 131.2, 132.8, 133.3, 137.3, 152.5, 154.7, 158.4.

HRMS (ESI): *m*/*z* calcd for $C_{13}H_9N_3ClSe$: 321.9645; found: 321.9599.

Synthesis of Aminoselenolotriazine Derivatives 1a–6b; General Procedure

The appropriate chloroselenolotriazine (1 mmol) and corresponding amine (10 mL) were heated under microwave irradiation (*P* = 100 W, *t* = 15 min, T_{max} = 150 °C). The mixture was cooled to r.t. and poured into H_2O (80 mL) under stirring. The precipitate formed was filtered, washed several times with H_2O and dried at r.t. overnight. The products were recrystallized from MeCN (2 mL) to give products **1a–6b**.

6-*tert*-Butyl-4-(1-pyrrolidinyl)selenolo[3,2-*d*][1,2,3]triazine (1a)
Yield: 88%; pale-orange solid; mp 182 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 1.42 (s, 9 H, 3 × CH_3), 1.99 (m, 4 H, 2 × CH_2), 3.81 (m, 4 H, 2 × CH_2), 7.60 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 24.7, 32.1, 36.8, 47.1, 115.0, 120.9, 152.9, 157.5, 172.9.

HRMS (ESI): *m*/*z* calcd for $C_{13}H_{19}N_4Se$: 311.0770; found: 311.0765.

6-Phenyl-4-(1-pyrrolidinyl)selenolo[3,2-*d*][1,2,3]triazine (2a)
Yield: 98%; brown solid; mp 232 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 2.03 (m, 4 H, 2 × CH_2), 3.84 (m, 4 H, 2 × CH_2), 7.49 (m, 3 H, 3 × CH), 7.85 (m, 2 H, 2 × CH), 8.27 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 24.7, 47.2, 115.8, 122.0, 126.8, 129.4, 130.1, 133.5, 152.8, 156.1, 158.0.

HRMS (ESI): *m*/*z* calcd for $C_{15}H_{15}N_4Se$: 331.0457; found: 331.0477.

6-(4-Methylphenyl)-4-(1-pyrrolidinyl)selenolo[3,2-*d*][1,2,3]triazine (3a)
Yield: 96%; dark-red solid; mp 235 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 2.02 (m, 4 H, 2 × CH_2), 2.35 (s, 3 H, CH_3), 3.84 (m, 4 H, 2 × CH_2), 7.31 (d, *J* = 8 Hz, 2 H, 2 × CH), 7.75 (d, *J* = 8 Hz, 2 H, 2 × CH), 8.20 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 20.8, 24.7, 47.2, 115.4, 121.1, 126.7, 130.0, 130.8, 140.1, 152.8, 156.3, 158.1.

HRMS (ESI): *m*/*z* calcd for $C_{16}H_{17}N_4Se$: 345.0613; found: 345.0590.

6-(4-Methoxyphenyl)-4-(1-pyrrolidinyl)selenolo[3,2-*d*][1,2,3]triazine (4a)
Yield: 93%; brown solid; mp 195 °C.

^{1}H NMR (250 MHz, pyridine-d_5): δ = 1.74 (m, 4 H, 2 × CH_2), 3.66 (m, 4 H, 2 × CH_2), 3.71 (s, 3 H, OCH_3), 7.07 (d, *J* = 8.7 Hz, 2 H, 2 × CH), 7.78 (d, *J* = 8.7 Hz, 2 H, 2 × CH), 8.27 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, pyridine-d_5): δ = 25.7, 48.0, 55.9, 115.6, 116.7, 121.8, 127.7, 129.3, 154.0, 157.1, 159.9, 162.1.

HRMS (ESI): *m*/*z* calcd for $C_{16}H_{17}ON_4Se$: 361.0562; found: 361.0568.

6-(4-Chlorophenyl)-4-(1-pyrrolidinyl)selenolo[3,2-*d*][1,2,3]triazine (5a)
Yield: 91%; pale-brown solid; mp 270 °C.

^{1}H NMR (250 MHz, pyridine-d_5): δ = 1.75 (m, 4 H, 2 × CH_2), 3.71 (m, 4 H, 2 × CH_2), 7.49 (d, *J* = 8.7 Hz, 2 H, 2 × CH), 7.74 (d, *J* = 8.7 Hz, 2 H, 2 × CH), 8.36 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, pyridine-d_5): δ = 26.8, 49.2, 118.8, 124.3, 130.4, 130.7, 131.4, 135.0, 155.1, 156.6, 160.6.

HRMS (ESI): *m*/*z* calcd for $C_{15}H_{14}N_4ClSe$: 365.0067; found: 365.0047.

10-(1-Pyrrolidinyl)-5,6-dihydronaphtho[2′,1′:4,5]selenolo[3,2-*d*][1,2,3]triazine (6a)
Yield: 94%; pale-brown solid; mp 299 °C.

^{1}H NMR (250 MHz, pyridine-d_5): δ = 1.74 (m, 4 H, 2 × CH_2), 2.88 (m, 2 H, CH_2), 3.22 (m, 2 H, CH_2), 3.74 (m, 4 H, 2 × CH), 7.23 (m, 3 H, 3 × CH), 7.46 (m, 1 H, CH).

^{13}C NMR (62.9 MHz, pyridine-d_5): δ = 23.3, 25.7, 28.6, 47.9, 116.8, 126.5, 128.2, 129.3, 130.4, 132.3, 134.8, 137.6, 148.1, 154.3, 156.9.

HRMS (ESI): *m*/*z* calcd for $C_{17}H_{17}N_4Se$: 357.0613; found: 357.0626.

6-*tert*-Butyl-4-(4-morpholinyl)selenolo[3,2-*d*][1,2,3]triazine (1b)
Yield: 90%; pale-orange solid; mp 164 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 1.44 (s, 9 H, 3 × CH_3), 3.76 (m, 4 H, 2 × CH_2), 3.88 (m, 4 H, 2 × CH_2), 7.68 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 32.0, 36.8, 45.4, 65.8, 114.5, 121.1, 154.8, 159.1, 173.0.

HRMS (ESI): *m*/*z* calcd for $C_{13}H_{19}ON_4Se$: 327.0719; found: 327.0667.

4-(4-Morpholinyl)-6-phenylselenolo[3,2-*d*][1,2,3]triazine (2b)
Yield: 93%; brown solid; mp 240 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.79 (m, 4 H, 2 × CH_2), 3.94 (m, 4 H, 2 × CH_2), 7.52 (m, 3 H, 3 × CH), 7.89 (m, 2 H, 2 × CH), 8.35 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 45.5, 65.8, 115.2, 122.1, 126.9, 129.5, 130.4, 133.2, 154.8, 156.2, 159.6.

HRMS (ESI): *m*/*z* calcd for $C_{15}H_{15}ON_4Se$: 347.0406; found: 347.0411.

6-(4-Methylphenyl)-4-(4-morpholinyl)selenolo[3,2-*d*][1,2,3]triazine (3b)
Yield: 94%; red solid; mp 275–276 °C.

^{1}H NMR (250 MHz, pyridine-d_5): δ = 2.18 (m, 4 H, 2 × CH_2), 2.24 (s, 3 H, CH_3), 3.81 (m, 2 H, CH_2), 3.94 (m, 2 H, CH_2), 7.24 (d, *J* = 8.1 Hz, 2 H, 2 × CH), 7.71 (d, *J* = 8.1 Hz, 2 H, 2 × CH), 8.36 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, pyridine-d_5): δ = 21.6, 46.6, 67.1, 127.1, 127.4, 127.9, 130.9, 132.0, 141.3, 155.9, 157.4, 161.4.

HRMS (ESI): *m*/*z* calcd for $C_{16}H_{17}ON_4Se$: 361.0562; found: 361.0551.

6-(4-Methoxyphenyl)-4-(4-morpholinyl)selenolo[3,2-*d*][1,2,3]triazine (4b)
Yield: 96%; brown solid; mp 218 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.79 (m, 4 H, 2 × CH_2), 3.82 (s, 3 H, OCH_3), 3.91 (m, 4 H, 2 × CH_2), 7.05 (d, *J* = 8.8 Hz, 2 H, 2 × CH), 7.83 (d, *J* = 8.8 Hz, 2 H, 2 × CH), 8.20 (s, 1 H, CH).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 45.4, 55.4, 65.8, 114.4, 114.8, 120.3, 125.7, 128.5, 154.7, 156.2, 159.9, 161.0.

HRMS (ESI): *m*/*z* calcd for $C_{16}H_{17}O_2N_4Se$: 377.0511; found: 377.0517.

6-(4-Chlorophenyl)-4-(4-morpholinyl)selenolo[3,2-*d*][1,2,3]triazine (5b)
Yield: 90%; brown solid; mp 298–299 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.79 (m, 4 H, 2 × CH_2), 3.93 (m, 4 H, 2 × CH_2), 7.59 (d, *J* = 8.5 Hz, 2 H, 2 × CH), 7.93 (d, *J* = 8.5 Hz, 2 H, 2 × CH), 8.39 (s, 1 H, CH).

Due to its very low solubility, no satisfying ^{13}C NMR spectrum was obtained even with long time accumulation.

HRMS (ESI): *m*/*z* calcd for $C_{15}H_{14}ON_4ClSe$: 381.0016; found: 381.0040.

10-(4-Morpholinyl)-5,6-dihydronaphtho[2′,1′:4,5]selenolo[3,2-*d*][1,2,3]triazine (6b)
Yield: 90%; beige solid; mp 279–280 °C.

^{1}H NMR (250 MHz, pyridine-d_5): δ = 2.90 (m, 2 H, CH_2), 3.22 (m, 2 H, CH_2), 3.82 (m, 4 H, 2 × CH_2), 3.96 (m, 4 H, 2 × CH_2), 7.23 (m, 1 H, CH), 7.29 (m, 2 H, 2 × CH), 7.46 (m, 1 H, CH).

^{13}C NMR (62.9 MHz, pyridine-d_5): δ = 24.8, 30.1, 48.1, 68.6, 117.8, 128.1, 129.7, 130.9, 132.2, 133.4, 136.2, 139.3, 149.7, 157.7, 159.9.

HRMS (ESI): *m*/*z* calcd for $C_{17}H_{17}ON_4Se$: 373.0562; found: 373.0584.

Synthesis of Chloroselenazolotriazines 7–9; General Procedure
A solution of $NaNO_2$ (5.37 mmol) in H_2O (5 mL) was added over 15 min to a suspension of a 2-substituted 4-amino-1,3-selenazole-5-carbonitrile (3.80 mmol) at 0–5 °C in concd HCl (13 mL). The resulting mixture was stirred at 0 °C for a further 40 min and then allowed to stand at r.t. overnight. The reaction mixture was poured into H_2O (100 mL) and, if a precipitated formed, it was washed with H_2O (2 × 15 mL) and dried at r.t. overnight. When no precipitate was formed, the aqueous layer was extracted with EtOAc (2 × 25 mL). The organic layers were washed with 2N HCl (2 × 30 mL) and H_2O (80 mL), dried over $MgSO_4$ and concentrated under reduce pressure. The products were recrystallized from MeCN (2 mL) to give products **7**–**9**.

Recording MS spectra under ESI conditions for compounds **7**–**9** led to spontaneous decomposition of the triazine ring with loss of N_2; *m*/*z* are thus reported for [M – N_2 + Na].

4-Chloro-6-(1-pyrrolidinyl)[1,3]selenazolo[4,5-*d*][1,2,3]triazine (7)
Yield: 46%; brown solid; mp 119–120 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 1.99 (m, 4 H, 2 × CH_2), 3.25 (m, 2 H, CH_2), 3.54 (m, 2 H, CH_2).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 25.2, 49.8, 84.8, 114.7, 147.3, 169.2.

HRMS (ESI): *m*/*z* [M – N_2 + Na] calcd for $C_8H_8N_3ClSeNa$: 283.9462; found: 283.9466.

4-Chloro-6-(1-piperidinyl)[1,3]selenazolo[4,5-*d*][1,2,3]triazine (8)
Yield: 67%; pale-brown solid; mp 236 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 1.63 (m, 6 H, 3 × CH_2), 3.35 (m, 4 H, 2 × CH_2).

^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 23.1, 24.7, 24.5, 85.1, 114.5, 147.4, 172.4.

HRMS (ESI): *m*/*z* [M – N_2 + Na] calcd for $C_9H_{10}N_3ClSeNa$: 297.9618; found: 297.9640.

4-Chloro-6-(4-morpholinyl)[1,3]selenazolo[4,5-*d*][1,2,3]triazine (9)
Yield: 29%; brown solid; mp 148 °C.

^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.48 (m, 4 H, 2 × CH_2), 3.67 (m, 4 H, 2 × CH_2).

Due to its very low solubility, no satisfying ^{13}C NMR spectrum was obtained even with long time accumulation.

HRMS (ESI): *m*/*z* [M – N_2 + Na] calcd for $C_8H_8N_3ClSeNa$: 299.9411; found: 299.9416.

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