

Selenium-containing heterocycles: Part 2. Reactions of 3-amino-4,6-dimethylselenolo[2,3-*b*]pyridine-2-carbonitrile and related fused tetracyclic systems

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A novel series of pyrido[3',2':4,5]selenolo[3,2-*d*]pyrimidine, 7,9-dimethylpyrido[3',2':4,5]selenolo[3,2-*d*]pyrimidine-2,4-(1*H*,3*H*)-dithione, 7,9-dimethylpyrido[3',2':4,5]selenolo[2,3-*e*]tetrazolo[1,5-*c*]pyrimidine-6(5*H*)-thione, 9,11-dimethylpyrido[3',2':4,5]selenolo[2,3-*e*][1,2,4]triazolo[1,5-*c*]pyrimidine, 7,9-dimethylpyrido[3',2':4,5]selenolo[2,3-*e*]imidazo[1,2-*c*]pyrimidine and 10,12-dimethylpyrido[3'',2'':4,5']selenolo[3',2':4,5]pyrimido[1,6-*a*]pyrimidine derivatives were prepared from 3-amino-4,6-dimethylselenolo[2,3-*b*]pyridine-2-carbonitrile.

Keywords: *o*-aminonitriles, fused selenophenes, imidazoles, pyridines, pyrimidines, tetrazoles, 1,2,4-triazoles

A literature survey indicates that only few publications are concerned with the incorporation of a selenium atom in the pyridine ring.^{1–5} Consequently, the synthesis of new classes of heterocyclic systems containing the selenolopyridine moiety may be considered to be a virgin research area. Moreover, previous work in our laboratory describes the synthesis of pyrimidoselenolo[2,3-*b*]quinoline⁶ and pyrimidoselenolo[2,3-*c*]pyridazine derivatives,⁷ which indicate that certain compounds bearing the selenophene and quinoline or pyridazine nucleus possess significant anti-inflammatory and analgesic activities with strong fungicidal effects. Therefore, new efficient syntheses are an attractive goal of chemical research. In Part 1⁸ we published the synthesis of selenolo[2,3-*b*]pyridine, pyrido[3',2':4,5]selenolo[3,2-*d*]pyrimidine, 7,8-dihydro-2,4-dimethylpyrrolo[1,2-*a*]pyrido[3',2':4,5]selenolo[3,2-*d*]pyrimidin-10(6*H*)-one and 7,9-dimethylpyrido[3',2':4,5]selenolo[3,2-*d*][1,2,4]triazolo[4,3-*c*]pyrimidine derivatives. The aforementioned properties of selenium organic compounds prompted further efforts in continuation of our work^{6–10} on the quest for novel heterocyclic systems containing selenium exhibiting biological activity, and we report herein new classes of fused selenium-containing derivatives containing the selenolo[2,3-*b*]pyridine system.

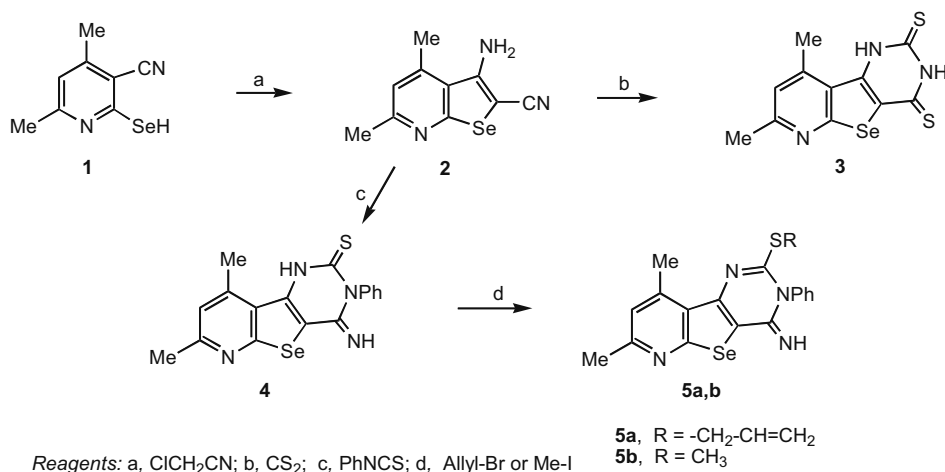
Results and discussion

Our approach to the synthesis of the target compounds started from 3-amino-4,6-dimethylselenolo[2,3-*b*]pyridine-2-carbonitrile (**2**) which was prepared from the selenol **1** as

previously described by Litvinov.² Compound **2** reacted with carbon disulfide and phenyl isothiocyanate to give the 7,9-dimethylpyrido[3',2':4,5]selenolo[3,2-*d*]pyrimidine-2,4-(1*H*,3*H*)-dithione (**3**) and 3,4-dihydro-7,9-dimethyl-3-phenyl-4-iminopyrido[3',2':4,5]selenolo[3,2-*d*]pyrimidine-2(1*H*)-thione (**4**), respectively (Scheme 1). The reactivity of the thione group of compound **4** was tested by alkylation with allyl bromide and methyl iodide which afforded derivatives (**5a,b**) respectively.

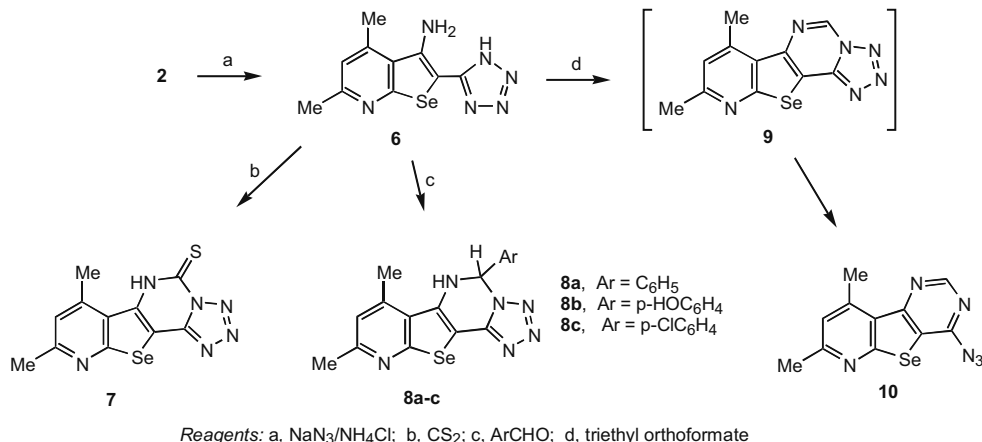
Heating of compound **2** with sodium azide and ammonium chloride in DMF followed by acidification of the reaction mixture led to the formation of the tetrazolyl compound **6**. The IR spectrum of compound **6** showed characteristic bands at 3300, 3400, 3500 cm⁻¹ for NH₂ and NH, and the disappearance of the cyano group of compound **2**. The mass spectrum of **6** showed a molecular ion peak at *m/z* 294 (M⁺, 100) which is in agreement with its molecular formula (C₁₀H₁₀N₆Se). When compound **6** was allowed to react with carbon disulfide and with aromatic aldehydes, the tetrazolopyridoselenolopyrimidine derivatives **7** and **8a–c** respectively were obtained in good yields.

In contrast, the reaction of tetrazolyl derivative **6** with triethyl orthoformate produced the azidopyrimidine derivative (**10**) (Scheme 2). The structure of compounds **7**, **8a–c** and **10** were assigned by elemental and spectral analyses. The IR spectrum of compound **10** showed a characteristic band at 2150 cm⁻¹ for the azido group.



Scheme 1

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Scheme 2

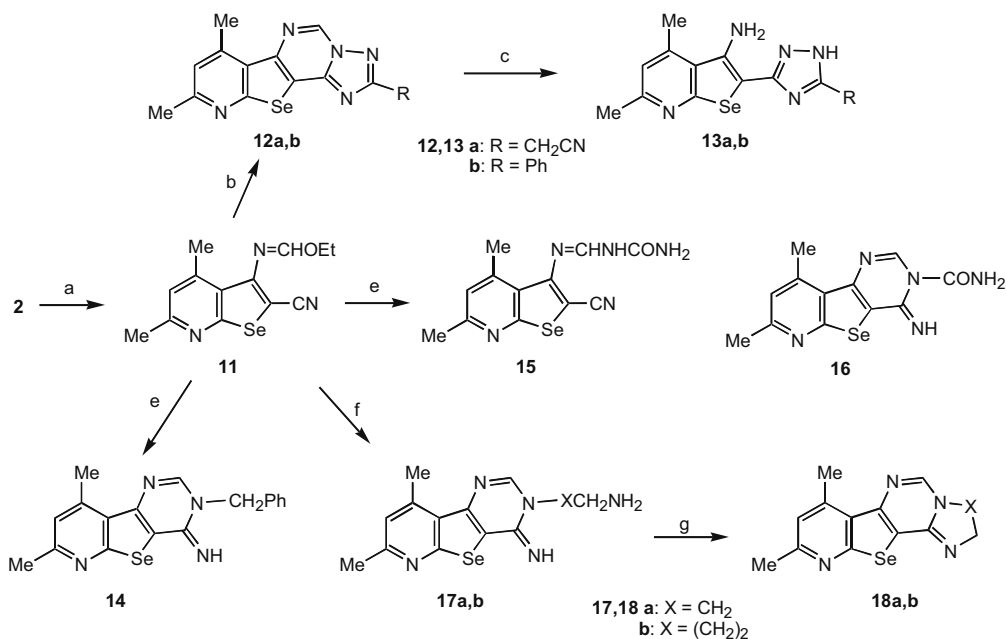
Reaction of compound **2** with triethyl orthoformate afforded the methanimidate derivative **11**, which was prepared as previously described.⁸ Heating of compound **11** with equimolar amounts of cyanoacetic acid or benzoic acid hydrazide furnished the 2-(substituted alkyl/phenyl)-7,9-dimethylpyrido [3',2':4,5]selenolo[2,3-*e*][1,2,4]triazolo[1,5-*c*]pyrimidine derivatives (**12a,b**). Treatment of **12a,b** with hydrochloric acid induced pyrimidine ring opening¹¹ to furnish the amines **13a,b** in excellent yield (Scheme 3).

Finally, stirring of **11** with benzylamine led to amino-deethoxylation accompanied by cyclisation to give 3-benzyl-7,9-dimethylpyrido[3',2':4,5]selenolo[3,2-*d*]pyrimidin-4(3*H*)-imine (**14**), while heating **11** with urea in acetic acid produced *N*'-carboxamido-*N*-(2-cyano-4,6-dimethylselenolo[2,3-*b*]pyridin-3-yl)methanimidate (**15**) rather than the expected fused pyrimidine (**16**) (Scheme 3). The IR spectrum of compound **15** showed characteristic bands at 3200–3400 cm^{-1}

(NH, NH₂) and 2200 cm^{-1} for the CN group. The mass spectrum showed a molecular ion peak at m/z 321 (M^+ , 0.5) in agreement with its molecular formula ($\text{C}_{12}\text{H}_{11}\text{N}_5\text{OSe}$). The ¹H NMR showed a characteristic peak at: δ 8.7 due to the CH=N group. Incorporation of the imidazole and pyrimidine moieties into the selenolopyridine structure was successfully accomplished by reacting **11** with ethylenediamine and propylenediamine to give the intermediate derivatives **17a,b** which were boiled in ethanol to give 2,3-dihydro-7,9-dimethylpyrido[3',2':4,5]selenolo[2,3-*e*]imidazo[1,2-*c*]pyrimidine (**18a**) and 3,4-dihydro-8,10-dimethyl-2*H*-pyrido[3',2':4,5']selenolo[3',2':4,5]pyrimido[1,6-*a*]pyrimidine (**18b**) respectively.

Experimental

Melting points were determined using a Kofler melting point apparatus. IR spectra were recorded on a Pye-Unicam SP3-100 instrument in KBr. The mass spectra (EI, 70 eV, ion source


Scheme 3

temperature 210 °C) were recorded on a JEOL JMS600 instrument. ¹H NMR spectra were obtained on a Varian spectrometer (90 MHz) using tetramethylsilane as internal reference. ¹³C NMR spectra were recorded on a Mercury-300BB NMR300 at Cairo University. Elemental analyses were obtained on an Elementar Vario EL 1150 C analyser. Purity of the compounds was checked by TLC.

Compounds **1**, **2**^{1,2,5} and **11**⁸ were prepared as previously described.

7,9-Dimethylpyrido[3',2':4,5]selenolo[3,2-d]pyrimidine-2,4(1H,3H)-dithione (3): Compound **2** (0.25 g, 1 mmol) and carbon disulfide (5 mL) in pyridine (10 mL) were gently heated on a water bath for 6 h. The solid product that formed while hot was collected and recrystallised from DMF/water mixture, forming yellow crystals (0.21 g, 65%), m.p. >300 °C. IR: ν_{\max} 3100 cm⁻¹ (NH). NMR (TFA): δ_{H} 3.0 (s, 3H, CH₃), 3.2 (s, 3H, CH₃), 7.7 (s, 1H, CH-pyridine). MS: m/z (%) 327 (M⁺, 100). Anal: Calcd for C₁₁H₆N₃S₂Se (326.33): C, 40.48; H, 2.78; N, 12.87; S, 19.65. Found: C, 40.33; H, 2.59; N, 12.58; S, 19.56%.

3,4-Dihydro-7,9-dimethyl-3-phenyl-4-iminopyrido[3',2':4,5]selenolo[3,2-d]pyrimidine 2(1H)-thione (4): Compound **2** (0.250 g, 1 mmol) and phenyl isothiocyanate (0.125 mL, 1 mmol) were gently heated under reflux for 6 h in pyridine (10 mL). The solid product that formed on cooling was collected and recrystallised from acetic acid to give orange crystals of **4** (0.32 g, 85%), m.p. >300 °C. IR: ν_{\max} 3200 cm⁻¹ (NH). NMR (TFA): δ_{H} 3.0 (s, 3H, CH₃), 3.2 (s, 3H, CH₃), 7.5–7.8 (m, 6H, ArH, CH-pyridine). MS: m/z (%) 386 (M⁺, 36). Anal: Calcd for C₁₇H₁₄N₄SSe (385.38): C, 52.97; H, 3.66; N, 14.54; S, 8.32. Found: C, 52.55; H, 3.34; N, 14.24; S, 7.98%.

2-Alkylthio-7,9-dimethyl-3-phenylpyrido[3',2':4,5]selenolo[3,2-d]pyrimidin-4(3H)-imine (5a,b): general procedure

Allyl iodide or methyl iodide (4 mmol) was added to a mixture of **4** (1.54 g, 4 mmol) and sodium acetate trihydrate (1.36 g, 10 mmol) in ethanol (30 mL), and the reaction mixture was heated under reflux for 2 h. After cooling the reaction mixture was poured into ice-water and the precipitate that formed was collected and recrystallised from ethanol to give compounds **5a,b** respectively.

Allylthio compound 5a: Yellow crystals (1.53 g, 90%), m.p. 192–194 °C. IR: ν_{\max} 3200 (NH). NMR (TFA): δ_{H} 3.0 (s, 3H, CH₃), 3.3 (s, 3H, CH₃), 4.2 (d, 2H, SCH₂), 5.2–5.4 (m, 3H, CH=CH₂), 7.3–7.7 (m, 6H, 5H ArH, 1H CH-pyridine). MS: m/z (%) 426 (M⁺, 44). Anal: Calcd for C₂₀H₁₈N₄SSe (425.45): C, 56.45; H, 4.27; N, 13.17; S, 7.53. Found: C, 56.50; H, 4.28; N, 12.98; S, 7.19%.

Methylthio compound 5b: Pale yellow crystals (1.42 g, 89%), m.p. 212–214 °C. IR: ν_{\max} 3200 cm⁻¹ (NH). NMR (DMSO-*d*₆): δ_{H} 2.3 (s, 3H, SCH₃), 2.5 (s, 3H, CH₃), 2.8 (s, 3H, CH₃), 7.4–7.6 (m, 5H, ArH), 7.2 (s, 1H, CH-pyridine), 9.5 (s, 1H, NH); δ_{C} 19.8 (SCH₃), 23.8, 33.0 (2 CH₃-pyridine), 110.55, 117.2, 122.3, 123.8, 125.7, 128.4 (C-Aryl), 134.3, 138.7, 147.5 (C-selenophene), 156.5, 158.8, 159.3, 163.8 (C=N pyrimidine), 165.85 (C=NH pyrimidine). MS: m/z (%) 400 (M⁺, 89). Anal: Calcd for C₁₅H₁₆N₄SSe (399.40): C, 54.12; H, 4.04; N, 14.03; S, 8.02. Found: C, 54.50; H, 4.28; N, 13.98; S, 7.88%.

3-Amino-4,6-dimethyl-2-(tetrazol-5-yl)selenolo[2,3-b]pyridine (6): The aminonitrile **2** (1.25 g, 5 mmol), sodium azide (0.4 g, 6 mmol) and ammonium chloride (0.32 g, 6 mmol) in DMF (15 mL) were heated on a water bath for 5 h. The reaction mixture was cooled and acidified with dilute acetic acid. The solid product that formed was collected and recrystallised from ethanol to give yellow crystals of the tetrazole **6** (1.20 g, 82%), m.p. 273–275 °C. IR: ν_{\max} 3300, 3400, 3500 cm⁻¹ (NH₂, NH). NMR (TFA): δ_{H} 3.1 (s, 3H, CH₃), 3.2 (s, 3H, CH₃), 7.6 (s, 1H, CH-pyridine). MS: m/z (%) 294 (M⁺, 100). Anal: Calcd for C₁₀H₁₀N₆Se (293.22) C, 40.95; H, 3.44; N, 28.66. Found: C, 40.65; H, 3.36; N, 28.45%.

7,9-Dimethylpyrido[3',2':4,5]selenolo[2,3-e]tetrazolo[1,5-c]pyrimidine-5(6H)-thione (7): The tetrazole **6** (0.586 g, 2 mmol) was heated on a water bath with carbon disulfide (5 mL) in pyridine (10 mL) for 6 h. The solid product that formed was collected and recrystallised from DMF-water mixture to give yellow crystals of the thione **7** (0.48 g, 72%), m.p. >300 °C. ¹H NMR (TFA): δ 3.0 (s, 3H, CH₃), 3.3 (s, 3H, CH₃), 7.8 (s, 1H, CH-pyridine). MS: m/z (%) 336 (M⁺, 37). Anal: Calcd for C₁₁H₈N₆Se (335.28): C, 39.40; H, 2.40; N, 25.07; S, 9.56. Found: C, 39.59; H, 2.51; N, 24.98; S, 9.40%.

5-Aryl-5,6-dihydro-7,9-dimethylpyrido[3',2':4,5]selenolo[2,3-e]tetrazolo[1,5-c]pyrimidine (8a–c): general procedure

To a mixture of compound **6** (0.586 g, 2 mmol) and benzaldehyde, *p*-hydroxybenzaldehyde or *p*-chlorobenzaldehyde (2 mmol) in ethanol (15 mL), a few drops of piperidine were added. The reaction mixture was heated under reflux for 2 h. The solid product that

formed on cooling was collected and recrystallised from ethanol to give compounds **8a–c** respectively.

5-Phenyl compound 8a: Formed yellow crystals (0.64 g, 85%), m.p.: 172–174 °C. IR: ν_{\max} 3300 cm⁻¹ (NH). NMR (DMSO-*d*₆): δ_{H} 2.5 (s, 3H, CH₃), 2.8 (s, 3H, CH₃), 7.3–7.5 (m, 7H, ArH, CH-pyridine, pyrimidine). MS: m/z (%) 382 (M⁺, 20). Anal: Calcd for C₁₇H₁₄N₆Se (381.33): C, 53.53; H, 3.70; N, 22.04. Found: C, 53.44; H, 3.56; N, 21.87%.

4-Hydroxyphenyl compound 8b: Yellow crystals (0.68 g, 86%), m.p. 204–206 °C. IR: ν_{\max} 3300 cm⁻¹ (NH). NMR (TFA): δ_{H} 3.2 (s, 3H, CH₃), 3.3 (s, 3H, CH₃), 6.2 (s, 1H, CH pyrimidine), 7.6–7.8 (m, 5H, ArH, CH-pyridine). MS: m/z (%) 398 (M⁺, 16). Anal: Calcd for C₁₇H₁₄N₆OSe (397.20): C, 51.40; H, 3.55; N, 21.16. Found: C, 50.99; H, 3.24; N, 20.97%.

4-Chlorophenyl compound 8c: Pale yellow crystals (0.74 g, 90%) from ethanol, m.p. 152–154 °C. IR: ν_{\max} 3300 cm⁻¹ (NH). NMR (TFA): δ_{H} 3.2 (s, 3H, CH₃), 3.3 (s, 3H, CH₃), 7.5–7.6 (m, 6H, 4H ArH, 1H CH-pyridine, 1H pyrimidine). MS: m/z (%) 417 (M⁺, 17). Anal: Calcd for C₁₇H₁₃ClN₆Se (415.77): C, 49.10; H, 3.15; Cl, 8.52; N, 20.21. Found: C, 48.92; H, 3.11; Cl, 8.32; N, 20.01%.

7,9-Dimethyl-4-azidopyrido[3',2':4,5]selenolo[3,2-d]pyrimidine (10): The tetrazole **6** (0.586 g, 2 mmol) and triethyl orthoformate (10 mL) were heated under reflux for 2 h. The precipitate which formed while hot was collected and recrystallised from ethanol giving yellow crystals of **10** (0.52 g, 87%), m.p. 182–184 °C. IR: ν_{\max} 2150 cm⁻¹ (N₃). NMR (DMSO-*d*₆): δ_{H} 2.6 (s, 3H, CH₃), 2.8 (s, 3H, CH₃), 7.2 (s, 1H, CH-pyridine), 10.2 (s, 1H, CH-pyrimidine). MS: m/z (%) 304 (M⁺, 44). Anal: Calcd for C₁₁H₈N₆Se (303.21): C, 43.57; H, 2.66; N, 27.72. Found: C, 43.26; H, 2.21; N, 27.43%.

2-(Cyanomethylphenyl)-7,9-dimethylpyrido[3',2':4,5]selenolo[2,3-e][1,2,4]triazolo[1,5-c]pyrimidine (12a,b): general procedure

A mixture of the iminoether **11**⁸ (1.53 g, 5 mmol) and cyanoacetic acid or benzoic acid hydrazides (5 mmol) in acetic acid (20 mL) was heated under reflux for 3 h. The precipitate that formed on cooling in the case of **12a** and that formed while hot in case of **12b** were collected and recrystallised from the indicated solvent to give compounds **12a,b**.

Cyanomethyl compound 12a: Yellow crystals (1.45 g, 85%), m.p. >300 °C from acetic acid. IR: ν_{\max} 2200 cm⁻¹ (CN). NMR (TFA): δ_{H} 3.2 (s, 3H, CH₃), 3.6 (s, 3H, CH₃), 4.7 (s, 2H, CH₂), 8.0 (s, 1H, CH-pyridine), 9.8 (s, 1H, CH-pyrimidine). MS: m/z (%) 342 (M⁺, 100). Anal: Calcd for C₁₄H₁₀N₆Se (341.26): C, 49.27; H, 2.95; N, 24.63. Found: C, 49.07; H, 2.53; N, 24.95%.

Phenyl compound 12b: White crystals (1.55 g, 82%) separated from DMF/water, m.p. >300 °C. IR: ν_{\max} 3050 cm⁻¹ (CH-arom). NMR (TFA): δ_{H} 3.1 (s, 3H, CH₃), 3.5 (s, 3H, CH₃), 7.8–8.2 (m, 6H, 5H ArH, 1H CH-pyridine), 9.9 (s, 1H, CH-pyrimidine). MS: m/z (%) 379 (M⁺, 100). Anal: Calcd for C₁₈H₁₃N₆Se (378.32): C, 57.14; H, 3.47; N, 18.51. Found: C, 56.88; H, 3.25; N, 18.22%.

3-Amino-2-[(5-(cyanomethylphenyl)-1,2,4-triazol-3-yl)-4,6-dimethylselenolo[2,3-b]pyridine (13a,b): general procedure

The tetracyclic compound **12a** or **12b** (5 mmol) in 20% aqueous hydrochloric acid (20 mL) was heated under reflux for 3 h. The solid product that formed while hot was collected and recrystallised from dioxan to give compounds **13a,b**.

Cyanomethyl compound 13a: Golden crystals (1.42 g, 86%), m.p. 242–244 °C. IR: ν_{\max} 2200 (CN), 3400–3500 cm⁻¹ (NH, NH₂). NMR (TFA): δ_{H} 2.9 (s, 3H, CH₃), 3.2 (s, 3H, CH₃), 4.7 (s, 2H, CH₂CN), 7.6 (s, 1H, CH-pyridine). MS: m/z (%) 333 (M⁺ + 1, 100). Anal: Calcd for C₁₃H₁₂N₆Se (331.27): C, 47.13; H, 3.65; N, 25.37. Found: C, 46.91; H, 3.25; N, 25.18%.

Phenyl compound 13b separated as yellow crystals (1.47 g, 80%), m.p. >300 °C. IR: ν_{\max} 3400–3500 cm⁻¹ (NH, NH₂). NMR (TFA): δ_{H} 3.2 (s, 3H, CH₃), 3.5 (s, 3H, CH₃), 7.8–8.4 (m, 6H, 5H ArH, 1H CH-pyridine). MS: m/z (%) 369 (M⁺, 100). Anal: Calcd for C₁₇H₁₃N₆Se (368.33): C, 55.43; H, 4.11; N, 19.01. Found: C, 55.15; H, 3.99; N 18.86%.

3-Benzylamino-7,9-dimethylpyrido[3',2':4,5]selenolo[3,2-d]pyrimidin-4(3H)-imine (14)

A mixture of compound **11** (1.53 g, 5 mmol) and benzylamine (0.54 mL, 5 mmol) in dioxan (10 mL) was stirred at room temperature for 4 h. The solid product that formed was collected and recrystallised from ethanol to give compounds **14** as white crystals (1.68 g, 92%), m.p. 173–175 °C. IR: ν_{\max} 3200 (NH), 3050 (CH-arom). ¹H NMR (DMSO-*d*₆): δ 2.6 (s, 3H, CH₃), 2.9 (s, 3H, CH₃), 4.8 (s, 2H, CH₂Ph) 7.1–7.3 (m, 6H, 5H ArH, 1H CH-pyridine), 8.2 (s, 1H, NH), 8.5 (s, 1H, CH-pyrimidine). MS: m/z (%) 368 (M⁺, 100). Anal: Calcd for C₁₈H₁₆N₄Se (367.34) Calcd. C, 58.85; H, 4.39; N, 15.25. Found: C, 58.43; H, 4.57; N, 14.96%.

N'-Carboxamido-*N*-(2-cyano-4,6-dimethylselenolo[2,3-*b*]pyridin-3-yl)methanimidate (**15**).

A mixture of compound **11** (1.53 g, 5 mmol) and urea (0.3 g, 5 mmol) in acetic acid (10 mL) was refluxed for 2 h. The solid product that formed on cooling was collected and recrystallised from acetic acid giving compound **15** as yellow crystals, (1.39 g, 87%), m.p: 242–244°C. IR: ν_{\max} 3200–3400 (NH, NH₂), 2200 cm⁻¹ (CN). NMR (TFA): δ_{H} 3.0 (s, 3H, CH₃), 3.2 (s, 3H, CH₃), 7.8 (s, 1H, CH-pyridine), 8.7 (s, 1H, CH=N). MS: *m/z* (%) 321 (M⁺, 0.5), 277 (M⁺-CONH₂, 15). Anal: Calcd for C₁₂H₁₁N₅OSe (320.24): C, 45.00; H, 3.46, N, 21.87. Found: C, 44.78; H, 3.92; N, 21.55%.

3-(2-Aminoethyl/3-aminopropyl)-3,4-dihydro-4-imino-7,9-dimethylpyrido[3',2':4,5]selenolo[3,2-*d*]pyrimidin-4(3H)-imine (**17a,b**): general procedure

A mixture of compound **11** (1.53 g, 5 mmol) and the appropriate diamine (5 mmol) in dioxan (10 mL) was stirred at room temperature for 4 h. The solid product (**17a,b**) that formed was collected and dried.

Aminoethyl compound 17a: White powder (1.31 g, 82%), m.p undetermined (on heating cyclised to compound **18a**). IR: ν_{\max} 3200–3400 cm⁻¹ (NH, NH₂). NMR (TFA): δ_{H} 3.2 (s, 3H, CH₃), 3.5 (s, 3H, CH₃), 4.1 (m, 2H, CH₂), 5.2 (m, 2H, CH₂), 8.0 (s, 1H, CH-pyridine), 8.9 (s, 1H, CH-pyrimidine). MS (FAB): *m/z* (%) 321 (M⁺, 10), 304 (M⁺-NH₃, 60).

Aminopropyl compound 17b: White powder (1.35 g, 81%), m.p undetermined (on heating cyclised to compound **18b**). IR: ν_{\max} 3200–3400 cm⁻¹ (NH, NH₂). NMR (TFA): δ_{H} 2.4 (m, 2H, CH₂), 3.3 (s, 3H, CH₃), 3.7 (s, 3H, CH₃), 4.1 (m, 2H, CH₂), 4.9 (m, 2H, CH₂), 7.6 (s, 1H, CH-pyridine), 8.9 (s, 1H, CH-pyrimidine). MS (FAB): *m/z* (%) 335 (M⁺, 18), 318 (M⁺-NH₃, 30).

Cyclisation reactions; preparation of 18a,b: general procedure

Compound **17a** (1.6 g, 5 mmol) or **17b** (1.67 g, 5 mmol) was boiled in ethanol for 5 min and the solution left to cool. The crystals that formed on cooling was collected and recrystallised from the proper solvent giving compounds **18a, b**.

7,9-Dimethylpyrido[3',2':4,5]selenolo[2,3-*e*]imidazo[1,2-*c*]pyrimidine (**18a**): Yellow crystals (1.36 g, 90%) from ethanol, m.p. 291–293°C. IR: ν_{\max} 3050 cm⁻¹ (CH-arom). NMR (TFA): δ_{H} 3.2 (s, 3H,

CH₃), 3.5 (s, 3H, CH₃), 4.5 (m, 2H, CH₂-imidazole), 5.2 (m, 2H, CH₂-imidazole), 7.2 (s, 1H, CH-pyridine), 8.1 (s, 1H, CH-pyrimidine). MS: *m/z* (%) 304 (M⁺, 86). Anal: Calcd for C₁₃H₁₂N₄Se (303.25): C, 51.48; H, 3.99; N, 18.47. Found: C, 51.07; H, 3.98; N, 18.47%.

8,10-Dimethylpyrido[3'',2'':4',5']selenolo[3',2':4,5]pyrimido[1,6-*a*]pyrimidine (**18b**): Crystallised from ethanol as yellow crystals (1.42 g, 90%), m.p. 282–284°C. IR: ν_{\max} 3050 cm⁻¹ (CH-arom). NMR (TFA): δ_{H} 2.6 (m, 2H, CH₂-pyrimidine), 3.1 (s, 3H, CH₃), 3.4 (s, 3H, CH₃), 4.0 (m, 2H, CH₂-pyrimidine), 4.6 (m, 2H, CH₂-pyrimidine), 7.8 (s, 1H, CH-pyridine), 8.7 (s, 1H, CH-pyrimidine). MS: *m/z* (%) 318 (M⁺, 100). Anal: Calcd for C₁₄H₁₄N₄Se (317.28): C, 52.99; H, 4.45; N, 17.66. Found: C, 52.50; H, 4.33; N, 17.72%.

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