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Advanced Synthesis & Catalysis

[Bis(trifluoroacetoxy)iodo]benzene Mediated C-3 Selenylation of Pyrido[1,2-*a*]Pyrimidin-4-Ones Under Ambient Conditions

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Abstract: Herein, we report the [Bis(trifluoroacetoxy)iodo]benzene mediated C–H bond arylselenylation of 4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-ones using readily available organodiselenides. This methodology is scalable and permits for the generation of a broad spectrum of functionally and structurally diverse selenoether derivatives in very promising yields (up to 98%). Notably, this protocol proceeds at ambient conditions and in the absence of a metal. The application of this methodology for the facile synthesis of ArSe substituted 5*H*-thiazolo-pyrido[3,2-*a*]pyrimidin-4-ones is also demonstrated.

Keywords: Pyrido[1,2-*a*]Pyrimidin-4-ones; C-3 Selenylation; Metal-free approach; Radical; C–H Functionalization

Introduction

Pyrido[1,2-*a*]pyrimidin-4-one, a *N*-fused heterocycle, is an important scaffold due to its ubiquity and bioactivity as the backbone of many natural and pharmacologic products. Indeed, a variety of derivatives based on this backbone show versatile bioactivities, including MexAB-OprM specific efflux pump inhibitors,[1] acetylcholinesterase inhibitors,[2] antipsychotics,[3] antioxidants,[4] and antiulcer drugs.[5] An example of biologically active products that share the pyrido[1,2-*a*]pyrimidin-4-one moiety are shown in Figure 1.

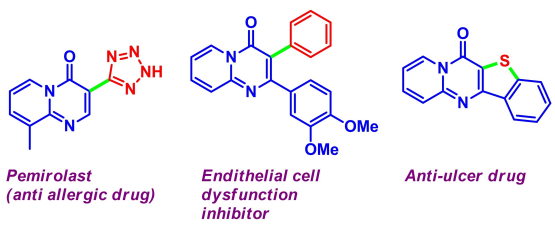


Figure 1. Representative examples of bioactive 4*H*-pyrido[1,2-*a*]pyrimidin-4-ones.

Organochalcogenides have received continuous interest as potential drug candidates due to their ability to serve as molecular scaffolds that accomodate diverse functional groups.[6] They also have broader applications in organic synthesis, agrochemistry, catalysis, and material sciences.[7] For instance, Ebselen, an organoselenium compound first discovered in 1980, is considered a prototypical antioxidant and neuroprotective agent.[8] In addition, a variety of biologically active organoselenides have been identified in recent literature.[9] Consequently, new methodologies leading to the facile creation of C–Se bonds is of high interest and has remained in the bullseye of synthetic chemists. A number of approaches have already been established in the literature during the past few years. However, these methodologies require the use of toxic reagents, metal catalysts, and harsh reaction conditions.[10] Thus, an alternative, efficient, and facile protocol towards the C–Se bond formation is highly desirable. For example, Du and his colleagues established a facile route for the synthesis of α-chalcogenylenamines in the presence of $PhICl_2$ and RXXR (X=S, Se) under ambient conditions.[11a] Very recently, Du and Zhao *et al.* reported a regioselective cyclization of alkynyl aryl ketones mediated by PIFA [Bis(trifluoroacetoxy)iodo]-

benzene in the presence of organochalcogenides, affording several structurally diverse 3-chalcogenyl chromones in reasonable yields.[11b]

A Pd catalyzed direct arylation and alkenylation of 4*H*-pyrido[1,2-*a*]pyrimidin-4-one through C–H bond functionalization has previously been demonstrated by Guchhait[12a] and Wang *et al.*[12b] However, the sustainable development of this approach is hampered by contamination of the final bioactive products with trace amount of the metal catalyst. An alternative metal-free insertion of –SAr groups to 4*H*-pyrido[1,2-*a*] pyrimidin-4-one using a sulfonyl hydrazide/thiol surrogate approach has also recently been reported;[13] however, this approach is slow and only effective at high temperatures. As a continuation of our research interest in C–H functionalization,[14] we herein report the direct selenylation technique of 4*H*-pyrido[1,2-*a*] pyrimidin-4-one *via* a metal-free C–H bond functionalization. Notably, this approach proceeds at ambient conditions, and permits the effective coupling of several organodiselenides with 4*H*-pyrido[1,2-*a*] pyrimidin-4-one in good to high yields (Figure 2). This protocol is equally effective using 5*H*-thiazolo[3,2-*a*] pyrimidin-4-one, a similarly biologically active substrate, indicating its good translatability.

Results and Discussion

The C–Se coupling reaction was first optimized using commercially available diphenyl diselenide (as the aryl selenylating agent) and 2-phenyl-4*H*-pyrido[1,2-*a*] pyrimidin-4-one (**1 a**), as the model coupling partner (Table 1). Our initial attempts to couple these two molecules was unsuccessful when using PIDA [(Diacetoxyiodo)benzene;1 equiv.] as an oxidant, in DCM at room temperature (rt) (Table 1; entry 1). However, we observed a high yield (92%) of the most anticipated

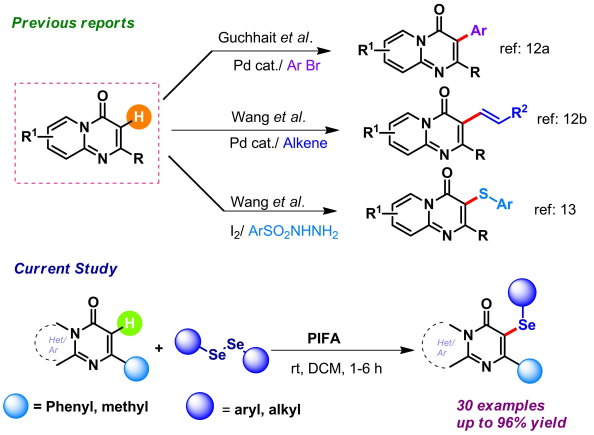
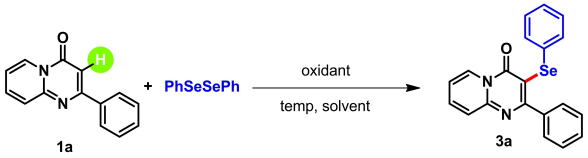


Figure 2. Previously reported and the present C–H bond functionalization approaches of 4*H*-pyrido[1,2-*a*]pyrimidin-4-ones.

Table 1. Optimization of C–H selenylation of 4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-ones: *effect of reaction parameters.*[a]



entry	oxidant (equiv.)	temp (° C)	solvent (ml)	time (h)	yield (%)[b]
1	PIDA (1)	rt	DCM	24	NR
2	**PIFA (1)**	**rt**	**DCM**	**6**	**92**
3	PhIO (1)	rt	DCM	24	47
4	$PhICl_2$(1)	rt	DCM	24	61
5	PIFA(1)	rt	DCE	6	52
6	PIFA (1)	rt	MeCN	12	81
7	PIFA (1)	rt	DMF	24	NR
8	PIFA (1)	rt	DMSO	24	NR
9	PIFA (1)	rt	EtOH	24	NR
10	PIFA (1)	rt	1,4-dioxane	12	47
11	PIFA (1)	rt	toluene	24	41
12	PIFA (1)	rt	THF	24	17
13	PIFA (0.5)	rt	DCM	6	66
14	PIFA (0.6)	rt	DCM	6	68
15	PIFA (0.8)	rt	DCM	6	77
16	PIFA (1)	40	DCM	6	89
17	–	rt	DCM	24	NR

[a] **Reaction conditions**: 2-phenyl-4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-ones (0.125 mmol, 1 equiv.), diphenyl diselenide (0.1875 mmol, 1.5 equiv.), solvent (2 ml), oxidant (0.5–1 equiv.).

[b] Isolated yields are based on the reactant **1 a**. The reaction was run for 6–24 h.

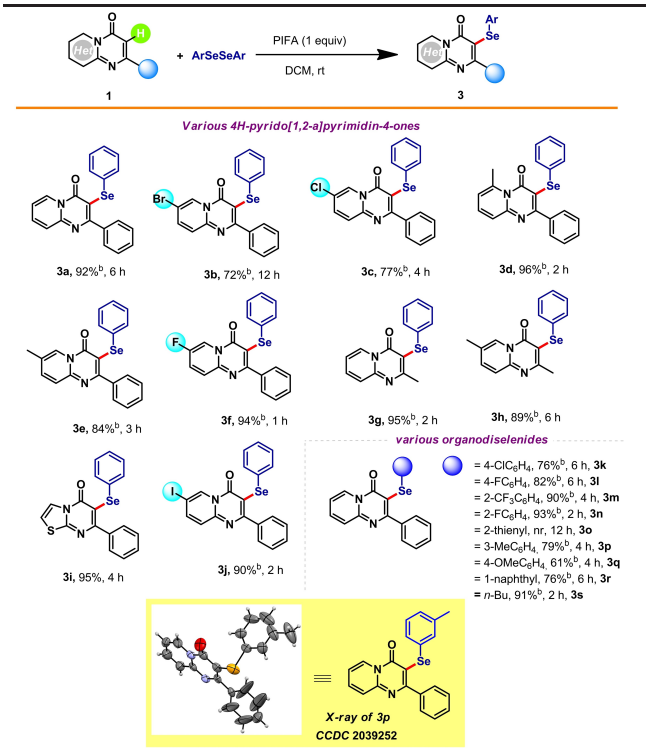
C–H selenylated derivative **3 a** when we instead employed an alternative bench-stable oxidant, PIFA (Table 1; entry 2). Notably, TLC showed a clean reaction with complete consumption of starting material **1 a**, within 6 hours (h) of the reaction's initiation. The use of alternative oxidants to PIFA provided inferior results (entries 3–4). Similarly, conducting the identical reaction in the presence of other polar solvents, including DCE and MeCN, resulted in only 52–81% yield of the coupled product **3 a** (Table 1; entries 5–6). Moreover, the reaction failed to proceed entirely, with the complete recovery of starting material **1 a**, when DMF; DMSO; or EtOH were employed (Table 1; entries 7–9). Screening of other solvents also had detrimental effect on the yield of the coupled product **3 a** (Table 1; entries 10–12). Lowering the amount of PIFA similarly diminished the yield (Table 1; entries 13–15), indicating its stochiometric requirement. We next turned our attention towards the optimization of the reaction temperature, first changing from rt to 40° C. A comparable yield (89%) of the desired selenoether derivative (**3 a**) was obtained (Table 1; entry 14). Control experiments revealed that

the reaction was unproductive in the absence of PIFA, demonstrating an indispensable role for the oxidant (Table 1; entry 15). Thus, from our optimization studies, the combination of PIFA (1 equiv.) as the oxidant, DCM as the solvent, and ambient conditions were found to be optimal for the C–Se coupling of 2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one (**1 a**) and diphenyl diselenide. All three conditions lead to a high yield (92%) of the product **3 a** after 6 h (Table 1; entry 2).

Having optimized the most suitable reaction conditions, we next explored the generalizability and scope of this protocol (Table 2). A variety of substituted 4*H*-pyrido[1,2-*a*]pyrimidin-4-ones were treated with diphenyl diselenide; the corresponding products are compiled in Table 2. The coupling reaction proceeded smoothly and resulted in the desired 3-selenylated scaffolds (**3**) in good to high yields. A marked effect on the product yield was observed due to the influence of substituents present on the arene ring. Noticeably, synthetically modifiable and sensitive halo-functionalities (–Cl, –Br, I) remained unadulterated in the corresponding C–Se coupled products (Table 2; entries **3 b**–**3 c**, **3 f**, **3 j**). Additionally, all were obtained in good yield, although production of 7-bromo-2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-ones required that the reaction proceed for 12 h (entry **3 b**). Interestingly, pyrido[1,2-*a*]pyrimidin-4-ones substituted with a mild electron-releasing group (–Me) at the C-6 and C-7 position furnished the desired C–H selenylated derivative in a faster manner (within 2–3 h; Scheme 1; entries **3 d**–**3 e**). Besides 2-phenyl substituted 4*H*-pyrido[1,2-*a*]pyrimidin-4-ones, 2-alkyl substituted starting materials also showed good reactivity and produced corresponding products in high yields (Table 2; entries **3 g**–**3 h**). 5*H*-thiazolo[3,2-*a*]pyrimidin-5-one also proved to be an effective coupling partner, under the optimal reaction conditions (Table 2, entry **3 i**), indicating this protocols generalizability to other similar heterocyclic substrates.

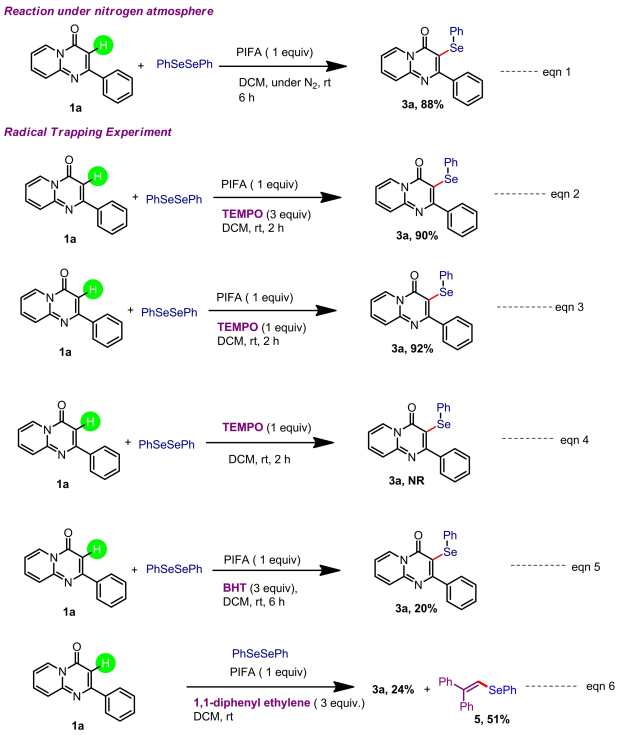
We next investigated the reactivity pattern of various diaryl diselenides. We found that the final product yield varied due to the electronic effects of the group present at different positions of the diaryl diselenides. Remarkably, while halogenated organodiselenides (4-Cl and 4-F) produced good yields (Table 2; entries **3 k**–**3 l**), sterically crowded *ortho* trifluoromethyl and fluoro group containing selenides produced high yield of the desired 3-selenylated derivatives (Table 2; entries **3 m** and **3 n**). Unfortu-

Table 2. Substrate scope of diversely substituted 4*H*-pyrido [1,2-*a*]pyrimidin-4-ones with phenyl diselenides and 2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one with various organodiselenides, using a PIFA-mediated selenylation.[a]



[a] **Reaction conditions**: substituted 4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-ones (0.125 mmol, 1 equiv.), organodiselenide (0.1875 mmol, 1.5 equiv.), DCM (2 ml), PIFA (1 equiv.). For **3 i**, *5H*-thiazolo-[3,2-a]-pyrimidin-4-one (0.125 mmol, 1 equiv.) was used as the substrate.

[b] Isolated yields are based on the reactant **1**. The reaction was run for 2–6 h, except for **3 b** (12 h).



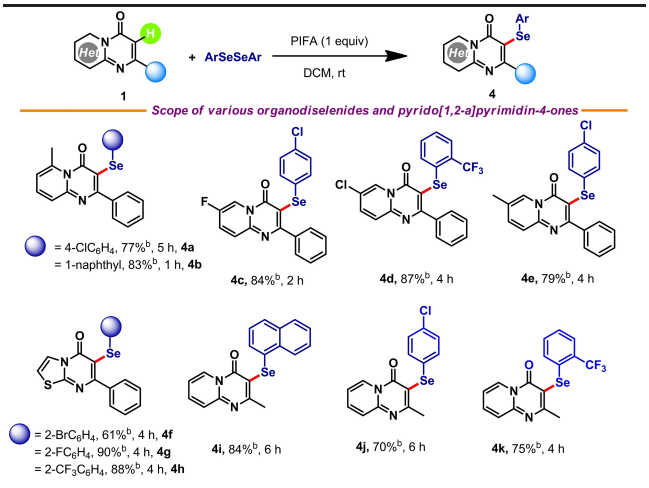
Scheme 1. Mechanistic Studies.

nately, diheteroaryldiselenides like 1,2-di(thiophen-2-yl)diselane (Table 2; entry **3o**), appear to be unreactive using this protocol. We also chose to crystallize the compound **3p**; X-ray analysis unambiguously confirmed the structure of the ArSe substituted product.[15] Interestingly, diaryl diselenides with an electron-donating-group (–OMe) resulted in a more moderate yield of the corresponding coupled product, compared to electron-withdrawing groups. We posit that this might be due to stable dimer formation (see Table 2; entry **3q**). Moreover, selenides bearing bulkier naphthyl groups reacted well with 4*H*-pyrido[1,2-*a*]pyrimidin-4-one **1a**, affording the anticipated product in good yield (76%; Table 2; entry **3r**). Satisfyingly, dibutyl diselenide also actively participated in this transformation to dispense the desired C-3 selenylated derivative (**3s**) in 91% isolated yield.

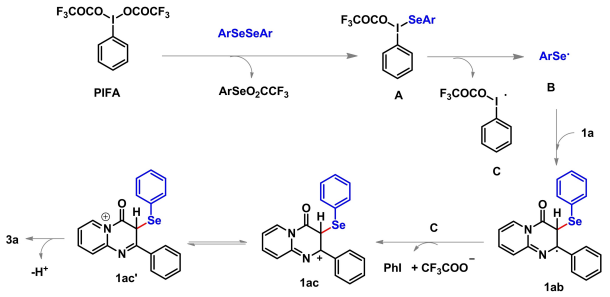
Next, we explored the breadth of substrate compatibility of different 4*H*-pyrido[1,2-*a*]pyrimidin-4-ones with diverse diaryl diselenides, as represented in Table 3. 6-methyl-2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-ones was compatible with organoselenides bearing electron-withdrawing substituents, and afforded the corresponding product in good yields (Table 3; entries **4a**). Furthermore, naphthyl bearing selenides also coupled efficiently with 6-methyl-2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-ones, resulting in 83% of the product (Table 3; entry **4b**). 1,2-Bis(4-chlorophenyl)diselane was employed as a coupling partner with both 7-fluoro and 7-methyl substituted 4*H*-pyrido[1,2-*a*]pyrimidin-4-one and led to the C–Se coupled product in high yields (Scheme 2; entries **4c** and **4e**). The reaction efficiency of 5*H*-thiazolo[3,2-*a*]pyrimidin-4-ones was also investigated, with a broad spectrum of diaryl diselenides. Interestingly, *ortho*-bromo substituted selane resulted in a 61% product yield, when coupled with 5*H*-thiazolo[3,2-*a*]pyrimidin-4-ones, (Table 3; entry **4f**), presumably due to instability of the dimer. Bis(2-trifluoromethyl)diselenide as well as Bis(2-fluoro)-diselane reacted successfully and produced the desired products in 88–90% yield (Table 3; entries **4g**–**4h**). Notably, 2-methyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one also produced the naphthyl selanyl derivative **4i** in decent yield. Gratifyingly, 4-chlorodiphenyl and 2-trifluoromethyl diselenides were capable in coupling with 2-alkyl substituted substrates, although they produced modest yields (**4j** and **4k**, respectively). Collectively, these diverse reactants demonstrate the synthetic utility and wide application of our methodology for drug synthesis.

To gain further insight into a probable mechanism, a series of control experiments were conducted; these are summarized in Scheme 1. When the selenylation reaction was performed under inert conditions (N_2 atm.), the desired 3-selenylated 4*H*-pyrido[1,2-*a*]pyrimidin-4-one was produced in 88% yield, after 6 h (Scheme 1; eqn. 1). This observation indicates that aerial oxygen is unlikely to play a significant role in the transformation reaction. Surprisingly, addition of super stoichiometric amounts of a radical quencher, TEMPO [(2,2,6,6-tetramethylpiperdin-1-yl)oxyl; 3 equiv.], did not inhibit the reaction, but rather reduced the reaction time towards the consumption of the starting material **1a** (Scheme 1; eqn. 2). A similar result was observed upon decreasing the loading of TEMPO to 1 equiv. (Scheme 1; eqn. 3). Conducting the reaction only in presence of TEMPO produced deleterious result, which suggests that the presence of TEMPO accelerated the cleavage of the Se–Se bond of the organo diselenides (Scheme 1; eqn. 4). As a reaction in presence of other radical scavengers, such as BHT (Butylated hydroxytoluene) and 1,1-diphenylene ethylene, significantly inhibited the reactivity, these data indicate the likely involvement of a radical

Table 3. Substrate scope of different substituted pyrido[1,2-*a*]pyrimidin-4-ones and organodiselenides using PIFA-mediated selenylation.[a]



[a] **Reaction conditions**: 2-substituted-4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-ones (0.125 mmol, 1 equiv.), organodiselenides (0.1875 mmol, 1.5 equiv.), DCM (2 ml), PIFA (1 equiv.).
[b] Isolated yields are based on reactant **1**. The reaction was run for 1–6 h.



Scheme 2. Putative mechanism (*Radical Pathway*).

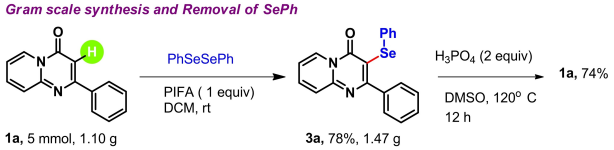
mechanism during the transformation of the final product (Scheme 1; eqn. 5–6).

A probable mechanistic route for the formation of 2-phenyl-3-(phenylselanyl)-4*H*-pyrido[1,2-*a*] pyrimidin-4-one **3 a** is delineated in Scheme 2, on the basis of control experimental results (Scheme 1) and previously literature reports.[16] Our preliminary mechanism is that reaction of PIFA with diphenyl selane furnishes the intermediate **A**, which undergoes homolytic cleavage to produce a phenyl selenide radical **B** and radical **C**. Subsequently, an electrophilic attack from the C-3 position of 2-phenyl-4*H*-pyrido[1,2-*a*] pyrimidin-4-ones moiety **1 a** on phenyl selenide radical **B** results in the generation of another intermediate **1 ab**. Oxidation of **1 ab** by **C** produces an ionic intermediate **1 ac**, which can be resonance stabilized to **1 ac'**. Finally, deprotonation of **1 ac** results in the desired product **3 a**.

Given the optimization of our reaction conditions, its good to high yield, and its ability to accommodate a wide variety of functionalized substituents, we next attempted a small-scale synthesis (5 mmol) of the 3-selenylated derivative (**3 a**) from 2-phenyl-4*H*-pyrido [1,2-*a*]pyrimidin-4-one, on a gram scale level. This amplification experiment resulted in a 78% product (**3 a**) yield (Scheme 3) and was done to demonstrate its potential industrial application. Later, we easily removed the –SePh group using phosphoric acid; this resulted in the recovery of 74% of the starting material (**1 a**).

Conclusion

In summary, we have established a PIFA mediated arylselenylation of various substituted 4*H*-pyrido[1,2-a]pyrimidin-4-one, using readily available diaryldiselenides at room temperature. This protocol offers a green synthetic route that potentiates the generation of a library of 3(arylselanyl)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one scaffolds bearing a diverse variety of functional groups. To our direct knowledge this is the first report of a method employing C-3 arylselenylation of 4*H*-pyrido[1,2-*a*]pyrimidin-4-one at ambient conditions. Moreover, this new experimental protocol is novel due to its operational simplicity, aerobic or anaerobic conditions, metal-free approach, and good scalability. We anticipate that these findings will be of increasing importance towards synthetic organic chemistry and the material sciences, and also offer its use for industrial and pharmaceutical applications.



Scheme 3. Application.

Experimental Section

General Considerations

Unless stated otherwise, all reagents such as various 2-aminopyridines, PIFA and solvents were used as received from commercial suppliers. NMR spectra were recorded on 400 MHz spectrometer at 298 K with calibration done based on solvent residual peaks. Products were purified using column chromatography on silica gel (60–120 mesh). Ethyl acetate and petroleum ether (60–80° C) were used as eluents. Progress of reaction was monitored using silica gel TLC.

Preparation of Various Substituted 4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-Ones

All the starting compounds are prepared by the following literature reports.

[1] a) M. Hussain, J. Liu, *Tetrahedron Lett.*, **2020**, DOI: 10.1016/j.tetlet.2020.152269; b) C. La Motta, S. Sartini, L. Mugnaini, F. Simorini, S. Taliani, S. Salerno, A. M. Marini, F. Da. Settimo, A. Lavecchia, E. Novellino, M. Cantore, P. Failli, M. Ciuff,. *J. Med. Chem.* **2007**, *50*, 4917–4927.

Preparation of Various Seleno Ether Substituted 4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-Ones (3 a–3 s/4 a–4 k)

Initially, various 2-(aryl/alkyl) substituted 4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-ones (0.125 mmol), organodiselenides (0.1875 mmol) and PIFA (1 equiv., 53 mg) were taken in dichloromethane (2 ml) in 25 ml round bottomed flask. Afterwards, the reaction mixture was stirred at room temperature for 1–6 h. Then, it was diluted with sodium thiosulfate solution and the product was extracted with dichloromethane (3 × 20 mL). Organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was then purified by column chromatography using 25–40% ethyl acetate/petroleum ether solution.

Experimental Procedure for Radical Trapping Experiment

Initially, various 2-phenyl substituted 4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-ones (0.125 mmol), diphenyl diselenide (0.1875 mmol), PIFA (1 equiv., 53 mg) and radical scavengers (TEMPO/BHT/1,1-diphenylethylene) were taken in dichloromethane (2 ml) in 25 ml round bottomed flask. Afterwards, the reaction mixture was stirred at room temperature for 2–6 h. Then, it was diluted with sodium thiosulfate solution and the product was extracted with dichloromethane (3 × 20 mL). Organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was then purified by column chromatography using 25–40% ethyl acetate/petroleum ether solution.

Experimental Procedure for Gram-Scale Synthesis (3 a)

Initially, various 2-phenyl substituted 4*H*-Pyrido-[1,2-*a*]-Pyrimidin-4-ones (5 mmol, 1.10 g), diphenyl diselenide (7.5 mmol) and PIFA (5 equiv., 2.14 g) were taken in dichloromethane (8 ml) in 25 ml round bottomed flask. Afterwards, the reaction mixture was stirred at room temperature for 6 h. Then, it was diluted with sodium thiosulfate solution and the product was extracted with dichloromethane (3 × 20 mL). Organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was then purified by column chromatography using 25–40% ethyl acetate/petroleum ether solution and isolated the desired product **3 a** in 78% (1.47 g) yield.

Experimental Procedure for Removal of SePh

Initially, 2-phenyl-3-(phenyl selanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3a, 0.125 mmol, 47.1 mg) and H_3PO_4 (2 equiv.) were mixed in DMSO (2 ml) and heated at 120° C for 12 h. After completion of the reaction, the reaction mixture was poured into 10 ml water and the product was extracted with dichloromethane (3 × 20 mL). Organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was then purified by column chromatography using 25–40% ethyl acetate/petroleum ether solution and isolated the desired product **1 a** (light yellow solid) in 74% yield.

Physical Characteristics and Spectral Data of Compounds

2-Phenyl-3-(phenylselanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3 a): Yellow solid, Yield = (43.3 mg, 92%), melting point: 138–140° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15–7.18 (m, 4H), 7.30 (s, 2H), 7.42 (s, 3H), 7.59 (s, 2H), 7.72–7.79 (m, 2H), 9.08 (d, J = 6.0 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 105.7, 116.1, 126.6, 126.7, 127.9, 128.0, 128.9, 129.0, 129.3, 131.1, 131.8, 136.9, 140.2, 150.2, 157.8, 168.1; HRMS (ESI) m/z: $[M+H]^+$ $C_{20}H_{15}N_2OSe$ calcd 379.0349; found 379.0346.

7-Bromo-2-phenyl-3-(phenylselanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3 b): Yellow solid, Yield = (41.0 mg, 72%), melting point: 136–138° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (s, 3H), 7.30 (s, 2H), 7.43 (s, 3H), 7.59–7.63 (m, 3H), 7.80–7.83 (m, 1H), 9.18 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 107.1, 111.4, 127.0, 127.4, 128.0, 128.9, 129.0, 129.6, 131.2, 131.5, 139.6, 140.2, 148.4, 156.6, 167.2; HRMS (ESI) m/z: $[M+H]^+$ $C_{20}H_{14}BrN_2OSe$ calcd 455.9454; found 455.9447.

7-Chloro-2-phenyl-3-(phenylselanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3 c): Yellow solid, Yield = (39.6 mg, 77%), melting point: 154–156° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (s, 3H), 7.28–7.32 (m, 2H), 7.45 (s, 3H), 7.61 (s, 2H), 7.68–7.71 (m, 2H), 9.09 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 107.0, 124.6, 125.6, 127.0, 127.6, 128.0, 128.9, 129.0, 129.5, 131.3, 131.5, 137.9, 139.8, 148.5, 156.8, 167.5; HRMS (ESI) m/z: $[M+H]^+$ $C_{20}H_{14}ClN_2OSe$ calcd 412.9960; found 412.9954.

6-Methyl-2-phenyl-3-(phenylselanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3 d): Yellow solid, Yield = (46.9 mg, 96%), melting point: 129–131° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.92 (s, 3H), 6.65 (s, 1H), 7.05 (s, 3H), 7.19 (s, 2H), 7.30 (s, 3H), 7.40 (s, 2H), 7.51 (s, 2H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.5, 107.0, 118.8, 125.3, 126.4, 127.8, 128.9, 129.0, 129.3, 130.5, 132.2, 135.9, 139.8, 144.1, 152.7, 161.4, 166.3; HRMS (ESI) m/z: $[M+H]^+$ $C_{21}H_{17}N_2OSe$ calcd 393.0506; found 393.0501.

7-Methyl-2-phenyl-3-(phenyl selanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3 e): Yellow solid, Yield = (41.0 mg, 84%), melting point: 197–199° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.46 (s, 3H), 7.16 (s, 3H), 7.32 (s, 2H), 7.43 (s, 3H), 7.60 (s, 2H), 7.68 (s, 2H), 8.91 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.4, 105.3, 125.4, 126.1, 126.5, 126.6, 127.9, 128.9, 128.9, 129.2, 131.0, 132.0, 139.8, 140.3, 149.2, 157.6, 167.7; HRMS (ESI) m/z: $[M+H]^+$ $C_{21}H_{17}N_2OSe$ calcd 393.0506; found 393.0501.

7-Fluoro-2-phenyl-3-(phenyl selanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3 f): Yellow solid, Yield = (46.4 mg, 94%), melting point: 98–100° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06 (s, 3H), 7.21 (s, 2H), 7.33 (s, 3H), 7.50 (s, 2H), 7.59 (s, 1H), 7.64 (s, 1H), 8.87 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 106.2, 114.0 ($J_{C\text{-}F}$ = 40.8 Hz), 126.9, 128.0, 128.6 ($J_{C\text{-}F}$ = 7.3 Hz), 129.0 ($J_{C\text{-}F}$ = 9.6 Hz), 129.1, 129.3, 129.5, 131.4, 139.9, 148.1, 153.1, 155.6, 157.2, 167.3, ^{19}F NMR (376 MHz, $CDCl_3$) δ −131.5; HRMS (ESI) m/z: $[M+H]^+$ $C_{20}H_{14}FN_2OSe$ calcd 397.0255; found 397.0250.

2-Methyl-3-(phenylselanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3 g): Yellow solid, Yield = (37.4 mg, 95%), melting point: 128–130° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.72 (s, 3H), 7.17–7.19 (m, 4H), 7.38 (s, 2H), 7.60–7.62 (m, 1H), 7.77 (s, 1H), 9.05 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.8, 104.7, 114.7, 124.8, 125.6, 127.2, 128.2, 129.5, 130.4, 136.0, 149.2, 156.2, 168.5; HRMS (ESI) m/z: $[M+H]^+$ $C_{15}H_{13}N_2OSe$ calcd 317.0193; found 317.0179.

2,7-Dimethyl-3-(phenylselanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3 h): Yellow solid, Yield = (36.6 mg, 89%), melting point: 146–148° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.42 (s, 3H), 2.72 (s, 3H), 7.17–7.18 (m, 3H), 7.37 (s, 2H), 7.53–7.55 (m, 1H), 7.63 (s, 1H), 8.86 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.3, 26.7, 105.3, 125.3, 125.6, 126.1, 126.5, 129.1, 130.4, 131.6, 139.9, 149.2, 157.1, 168.9; HRMS (ESI) m/z: $[M+H]^+$ $C_{16}H_{15}N_2OSe$ calcd 331.0349; found 331.0345.

7-Phenyl-6-(phenylselanyl)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one (3 i): Yellow solid, Yield = (45.5 mg, 95%), melting point: 144–146° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.02 (s, 1H), 7.16 (s, 3H), 7.31 (s, 2H), 7.41 (s, 3H), 7.56 (s, 2H), 8.00 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 107.0, 112.3, 122.7, 126.9, 127.9, 128.9, 129.0, 129.5, 131.2, 131.5, 139.5, 158.2, 162.2, 167.0; HRMS (ESI) m/z: $[M+Na]^+$ $C_{18}H_{12}N_2OSSeNa$ calcd 406.9733; found 407.0300.

7-Iodo-2-phenyl-3-(phenylselanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3 j): Yellow solid, Yield = (56.6 mg, 90%), melting point: 174–176° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14–7.17 (m, 3H), 7.29–7.32 (m, 2H), 7.40–7.47 (m, 4H), 7.57–7.60 (m, 2H), 7.89 (dd, J = 9.6 Hz, 2.0 Hz, 1H), 9.28 (d, J = 1.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 79.6, 107.1, 126.9, 127.5, 127.9, 128.9, 129.0, 129.5, 131.4, 131.5, 133.0, 139.9, 144.4, 148.6, 156.5, 167.6; HRMS (ESI) m/z: $[M+H]^+$ $C_{20}H_{14}IN_2OSe$ calcd 504.9316 found 504.9311.

3-((4-Chlorophenyl)selanyl)-2-phenyl-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3k): Yellow solid, Yield = (39.1 mg, 76%), melting point: 178–180 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.01–7.05 (m, 2H), 7.11–7.18 (m, 3H), 7.33–7.37 (m, 3H), 7.48–7.51 (m, 2H), 7.66–7.68 (m, 1H), 7.72–7.76 (m, 1H), 8.99–9.01 (m, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 105.5, 116.2, 126.7, 127.9, 128.8, 129.1, 129.4, 129.9, 132.6, 132.8, 137.0, 140.1, 150.3, 157.6, 168.0; HRMS (ESI) m/z: $[M+H]^+$ $C_{20}H_{14}ClN_2OSe$ calcd 412.9960 found 413.0163.

3-((4-Fluorophenyl)selanyl)-2-phenyl-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3l): Yellow solid, Yield = (40.6 mg, 82%), melting point: 156–158° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.77 (s, 2H), 7.13 (d, J = 5.2 Hz, 1H), 7.19–7.24 (m, 2H), 7.37 (s, 3H), 7.50 (s, 2H), 7.67–7.72 (m, 2H), 9.01 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 106.3, 115.9, 116.1 ($J_{C\text{-}F}$ = 3.5 Hz), 126.0, 126.6, 127.9 ($J_{C\text{-}F}$ = 4.3 Hz), 128.8, 129.4, 134.0 ($J_{C\text{-}F}$ = 7.7 Hz), 136.8, 140.1, 150.1, 157.7, 160.9, 163.4, 167.7, ^{19}F NMR (376 MHz, $CDCl_3$) δ −115.0; HRMS (ESI) m/z: $[M+Na]^+$ $C_{20}H_{13}FN_2OSeNa$ calcd 419.0074; found 419.0079.

2-Phenyl-3-((2-trifluoromethyl)phenyl)selanyl)-4*H*-pyrido [1,2-*a*]-pyrimidin-4-one (3m): Yellow solid, Yield = (50.0 mg, 90%), melting point: 140–142° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (s, 4H), 7.40 (s, 3H), 7.59 (s, 3H), 7.77–7.84 (m, 2H), 9.07 (d, J = 6.0 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 104.1, 116.4, 122.7, 125.4, 126.0, 126.7, 126.9 ($J_{C\text{-}F}$ = 5.2 Hz), 127.9, 128.0, 128.8, 129.1 ($J_{C\text{-}F}$ = 31.2 Hz), 129.6, 131.0, 131.9, 137.4, 139.7, 150.6, 157.7, 168.8, ^{19}F NMR (376 MHz, $CDCl_3$) δ −61.1; HRMS (ESI) m/z: $[M+H]^+$ $C_{21}H_{14}F_3N_2OSe$ calcd 447.0223; found 447.0217.

3-((2-Fluorophenyl)selanyl)-2-phenyl-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3n): Yellow solid, Yield = (45.9 mg, 93%), melting point: 152–154° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.87 (s, 2H), 7.07–7.11 (m, 3H), 7.34 (s, 3H), 7.53 (s, 2H), 7.67–7.74 (m, 2H), 9.01 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 102.7, 114.3 ($J_{C\text{-}F}$ = 22.3 Hz), 115.1, 117.3 ($J_{C\text{-}F}$ = 21.7 Hz), 123.6 ($J_{C\text{-}F}$ = 2.7 Hz), 125.6, 126.9, 127.5 ($J_{C\text{-}F}$ = 7.4 Hz), 127.7, 128.4, 131.3 ($J_{C\text{-}F}$ = 8.6 Hz), 136.0, 138.9, 149.2, 156.5, 158.6, 161.0, 167.0, ^{19}F NMR (376 MHz, $CDCl_3$) δ −104.9; HRMS (ESI) m/z: $[M+H]^+$ $C_{20}H_{14}FN_2OSe$ calcd 397.0255; found 397.0250.

2-Phenyl-3-(m–tolylselanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3p): Yellow solid, Yield = (38.6. mg, 79%), melting point: 152–154° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.22 (s, 3H), 6.93–6.95 (m, 1H), 7.01–7.11 (m, 3H), 7.17 (dt, J = 7.1 Hz, 1.5 Hz, 1H), 7.39–7.43 (m, 3H), 7.58–7.61 (m, 2H), 7.72–7.80 (m, 2H), 9.07–9.09 (m, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 116.0, 126.6, 126.8, 127.6, 127.8, 128.0, 128.2, 128.7, 128.9, 129.2, 131.5, 131.8, 136.7, 138.6, 140.2, 150.2, 157.8, 167.9, HRMS (ESI) m/z: $[M+H]^+$ $C_{21}H_{17}N_2OSe$ calcd 393.0506; found 393.0501.

3-((4-Methoxyphenyl)selanyl)-2-phenyl-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (3q): Yellow solid, Yield = (31.0 mg, 61%), melting point: 151–153 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.75 (s, 3H), 6.71 (d, J = 5.2 Hz, 2H), 7.18 (s, 1H), 7.28–7.32 (m, 2H), 7.46 (s, 3H), 7.60 (s, 2H), 7.71–7.77 (m, 2H), 9.08 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 54.2, 106.1, 113.6, 114.9, 120.5, 125.5, 126.9, 127.9, 128.2, 133.4, 135.5, 139.3, 148.9, 156.7, 158.1, 166.3; HRMS (ESI) m/z: $[M+H]^+$ $C_{21}H_{17}N_2O_2Se$ calcd 409.0455; found 409.0457.

3-(Naphthalen-1-ylselanyl)-2-phenyl-4*H*-pyrido[1,2-*a*] pyrimidin-4-one (3r): Yellow solid, Yield = (40.6 mg, 76%), melting point: 142–144° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07–7.11 (m, 1H), 7.14–7.20 (m, 1H), 7.30–7.38 (m, 5H), 7.46–7.51 (m, 1H), 7.52–7.53 (m, 2H), 7.60–7.70 (m, 4H), 7.97–8.00 (m, 1H), 8.98 (d, J = 6.8 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 105.9, 116.0, 125.7, 125.9, 126.3, 126.6, 127.3, 127.8, 127.9, 128.0, 128.4, 128.9, 129.3, 130.4, 131.1, 133.5, 133.9, 136.7, 140.1, 150.1, 157.7, 168.0; HRMS (ESI) m/z: $[M+H]^+$ $C_{24}H_{17}N_2OSe$ calcd 429.0506; found 429.0501.

3-(Butylselanyl)-2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one (3s): Yellow solid, Yield = (40.6 mg, 91%), melting point: 70–72° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.72 (t, J = 7.3 Hz 3H), 1.18 (q, J = 7.6 Hz, 2H), 1.38–1.42 (m, 2H), 2.79 (t, J = 7.6 Hz, 2H), 7.10 (m, 1H), 7.38–7.43 (m, 3H), 7.54–7.57 (m, 2H), 7.63–7.67 (m, 2H), 9.00–9.01 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 12.5, 21.7, 25.9, 31.1, 104.4, 114.8, 125.5, 126.3, 126.9, 127.9, 128.2, 134.9, 139.4, 148.3, 156.6, 165.5. HRMS (ESI) m/z: $[M+H]^+$ $C_{18}H_{19}N_2OSe$ calcd 359.0662; found 359.0668

3-((4-Chlorophenyl)selanyl)-6-methyl-2-phenyl-4*H*-pyrido [1,2-*a*]-pyrimidin-4-one (4a): Yellow solid, Yield = (41.0 mg, 77%), melting point: 136–138° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.92 (s, 3H), 6.68 (s, 1H), 7.02 (s, 2H), 7.12 (d, J = 2.0 Hz, 2H), 7.32 (s, 3H), 7.42 (s, 2H), 7.49 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.6, 106.7, 119.1, 125.4, 127.9, 128.8, 129.0, 129.4, 130.4, 131.9, 132.5, 136.1, 139.7, 144.2, 152.7, 161.3, 166.9. HRMS (ESI) m/z: $[M+H]^+$ $C_{21}H_{16}ClN_2OSe$ calcd 427.0116; found 427.0109.

6-Methyl-(3-naphthalen-1-yl-selanyl)-2-phenyl-4*H*-pyrido [1,2-*a*]-pyrimidin-4-one (4b): Yellow solid, Yield = (45.8 mg, 83%), melting point: 134–136° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.02 (s, 3H), 6.75 (s, 1H), 7.29–7.28 (m, 1H), 7.33 (s, 3H), 7.45–7.48 (m, 5H), 7.57 (s, 2H), 7.68 (s, 1H), 7.77 (s, 1H), 8.05 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.5, 106.9, 118.8, 125.3, 125.7, 125.9, 126.1, 127.0, 127.5, 127.7, 128.4, 128.7, 129.2, 129.7, 130.8, 133.2, 134.0, 135.8, 139.7, 144.1, 152.6, 161.4, 166.9; HRMS (ESI) m/z: $[M+H]^+$ $C_{25}H_{19}N_2OSe$ calcd 443.0662; found 443.0658.

3-((4-Chlorophenyl)selanyl)-7-fluoro-2-phenyl-4*H*-pyrido [1,2-*a*]-pyrimidin-4-one (4c): Yellow solid, Yield = (45.1 mg, 84%), melting point: 176–178° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12–7.14 (m, 2H), 7.26–7.28 (m, 2H), 7.44–7.47 (m, 3H), 7.57–7.60 (m, 2H), 7.73–7.78 (m, 2H), 8.98–9.00 (m, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 106.0, 114.0 ($J_{C\text{-}F}$ = 41.0 Hz), 128.0, 128.6 ($J_{C\text{-}F}$ = 7.2 Hz), 128.8, 129.1, 129.2, 129.4, 129.6, 133.0, 133.1, 139.7, 148.1, 153.2, 155.6, 157.1, 167.3, ^{19}F NMR (376 MHz, $CDCl_3$) δ −131.3; HRMS (ESI) m/z: $[M+Na]^+$ $C_{20}H_{12}ClFN_2OSeNa$ calcd 452.9684; found 453.0140.

7-Chloro-2-phenyl-3-((2-trifluoromethyl))phenyl selanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (4d): Yellow solid, Yield = (52.2 mg, 87%), melting point: 122–124° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (s, 3H), 7.43 (s, 3H), 7.61 (s, 3H), 7.75 (s, 2H), 9.08 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 105.6, 122.6, 124.9, 125.3, 125.6, 126.3, 126.9 ($J_{C\text{-}F}$ = 5.4 Hz), 127.7, 128.0, 128.8, 129.5 ($J_{C\text{-}F}$ = 30.5 Hz), 129.8, 131.4, 131.5, 131.9,

138.3, 139.3, 148.8, 156.6, 168.1, ^{19}F NMR (376 MHz, $CDCl_3$) δ −61.1; HRMS (ESI) m/z: $[M+H]^+$ $C_{21}H_{13}ClF_3N_2OSe$ calcd 480.9833; found 480.9827.

3-((4-Chlorophenyl)selanyl)-7-methyl-2-phenyl-4*H*-pyrido [1,2-*a*]-pyrimidin-4-one (4e): Yellow solid, Yield = (42.1 mg, 79%), melting point: 202–204° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.45 (s, 3H), 7.11 (s, 2H), 7.21–7.22 (m, 2H), 7.42 (s, 3H), 7.56 (s, 2H), 7.68 (s, 2H), 8.89 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.4, 105.0, 125.4, 126.1, 126.7, 127.9, 128.8, 129.0, 129.4, 130.1, 132.5, 132.7, 140.0, 140.2, 149.2, 157.5, 167.7; HRMS (ESI) m/z: $[M+H]^+$ $C_{21}H_{16}ClN_2OSe$ calcd 427.0116; found 427.0109.

6-(2-Bromophenyl)selanyl)-7-phenyl-5*H*-thiazolo[3,2-*a*] pyrimidin-5-one (4f): Yellow solid, Yield = (35.2 mg, 61%), melting point: 196–198° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (d, J = 6.8 Hz, 2H), 7.11 (s, 2H), 7.42–7.47 (m, 4H), 7.60 (s, 2H), 8.06 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 105.7, 112.5, 122.8, 123.4, 127.3, 127.8, 127.9, 128.8, 129.6, 129.8, 132.8, 134.6, 139.2, 158.0, 162.9, 167.9; HRMS (ESI) m/z: $[M+H]^+$ $C_{18}H_{12}BrN_2OSSe$ calcd 462.9019; found 462.9007.

6-(2-Fluorophenyl)selanyl)-7-phenyl-5*H*-thiazolo[3,2-*a*] pyrimidin-5-one (4g): Yellow solid, Yield = (45.1 mg, 90%), melting point: 139–141° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (s, 2H), 7.07 (s, 1H), 7.17–7.22 (m, 2H), 7.43 (s, 3H), 7.59 (s, 2H), 8.02 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 104.2, 111.3,, 114.4 ($J_{C\text{-}F}$ = 23.0 Hz), 117.0 ($J_{C\text{-}F}$ = 22.0 Hz), 121.6, 123.6, 126.9,, 127.7 ($J_{C\text{-}F}$ = 11.0 Hz), 128.6, 131.5, 138.2, 156.8. 158.7, 161.2 ($J_{C\text{-}F}$ = 21.0 Hz), 165.9, ^{19}F NMR (376 MHz, $CDCl_3$) δ −104.7; HRMS (ESI) m/z: $[M+H]^+$ $C_{18}H_{11}FN_2OSSeNa$ calcd 424.9638; found 425.0061.

7-Phenyl-6-((2-trifluoromethyl)phenyl)selanyl)-5*H*-thiazolo [3,2-*a*]pyrimidin-5-one (4h): Yellow solid, Yield = (49.6 mg, 88%), melting point: 164–166° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (s, 1H), 7.29 (s, 4H), 7.42 (s, 3H), 7.59–7.60 (m, 3H), 8.03 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 105.7, 112.5, 119.9, 122.7, 125.4, 126.9 ($J_{C\text{-}F}$ = 5.5 Hz), 127.9, 128.1, 128.8, 129.3 ($J_{C\text{-}F}$ = 31.0 Hz), 129.8, 131.1, 131.6, 132.0, 139.0, 157.9, 162.8, 167.6, ^{19}F NMR (376 MHz, $CDCl_3$) δ −61.2. HRMS (ESI) m/z: $[M+H]^+$ $C_{19}H_{12}F_3N_2OSSe$ calcd 452.9787; found 452.9786.

2-Methyl-3-(naphthalen-1-yl-selanyl)-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (4i): Yellow solid, Yield = (38.3 mg, 84%), melting point: 112–114° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.73 (s, 3H), 7.16 (d, J = 5.2 Hz, 1H), 7.28 (s, 1H), 7.49–7.64 (m, 4H), 7.72–7.84 (m, 3H), 8.36 (d, J = 4.8 Hz, 1H), 9.08 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.7, 105.4, 115.8, 125.8, 125.9, 126.2, 126.5, 126.6, 127.5, 128.2, 128.6, 129.1, 130.3, 133.3, 134.1, 137.0, 150.2, 157.2, 169.8; HRMS (ESI) m/z: $[M+H]^+$ $C_{19}H_{15}N_2OSe$ calcd 367.0349; found 366.0344.

3-((4-Chlorophenyl)selanyl)-2-methyl-4*H*-pyrido[1,2-*a*]-pyrimidin-4-one (4j): Yellow solid, Yield = (30.6 mg, 70%), melting point: 148–150° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.72 (s, 3H), 7.16 (s, 3H), 7.26–7.31 (m, 2H), 7.62 (s, 1H), 7.78 (d, J = 5.2 Hz, 1H), 9.03 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.8, 105.3, 115.9, 125.9, 128.1, 129.3, 129.6, 132.0, 132.7, 137.2, 150.3, 157.1, 169.4; HRMS (ESI) m/z: $[M+H]^+$ $C_{15}H_{12}ClN_2OSe$ calcd 350.9803; found 350.9795.

2-Methyl-3-((2-trifluoromethyl)phenylselanyl)-4*H*-pyrido [1,2-*a*]-pyrimidin-4-one (4k): Yellow solid, Yield = (35.9 mg, 75%), melting point:130–132° C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.71 (s, 3H), 7.19–7.27 (m, 4H), 7.67 (s, 2H), 7.85 (s, 1H), 9.10 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.6, 104.3, 116.0, 122.8, 125.5, 126.0, 127.0 ($J_{C\text{-}F}$ = 5.5 Hz), 128.3, 129.4 ($J_{C\text{-}F}$ = 30.9 Hz), 130.7, 131.5, 132.0, 137.5, 150.6, 157.3, 170.6, ^{19}F NMR (376 MHz, $CDCl_3$) δ −61.3; HRMS (ESI) m/z: $[M+H]^+$ $C_{16}H_{12}F_3N_2OSe$ calcd 385.0067; found 385.0062.

(2,2-Diphenylvinyl)(phenyl)selane (5):[17] colorless liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06 (s, 1H), 7.18–7.20 (m, 5H), 7.24–7.29 (m, 5H), 7.31–7.33 (m, 1H), 7.35–7.39 (m, 2H), 7.50–7.53 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 122.5, 127.1, 127.2, 127.4, 127.7, 127.9, 128.3, 128.5, 129.3, 131.6, 132.5, 140.3, 141.6, 143.1.

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[15] CCDC-2039252 (compound 3p) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

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