

New Cyano-Group-Containing 1,3-Oxaselenoles: Nucleophilic Substitution of a Cyano Group with Rearrangement

Andrey V. Kachanov^{*a}

Andrey V. Zamaraev^b

Andrey V. Gerasimenko^c

Konstantin V. Maslov^a

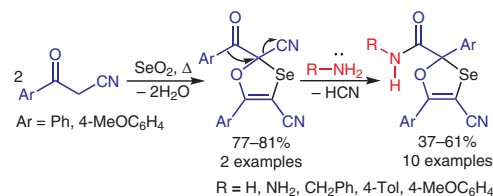
Oleg Yu. Slabko^a

Vladimir A. Kaminskii^a

^a Far Eastern Federal University, School of Natural Sciences, Sukhanov Str., 8, Vladivostok 690950, Russian Federation
kachanov.av@dvfu.ru

^b G. B. Elyakov Pacific Institute of Bioorganic Chemistry, Far East Branch of the Russian Academy of Sciences, prospect 100 let Vladivostoku, 159, Vladivostok 690022, Russian Federation

^c Institute of Chemistry, Far East Branch of the Russian Academy of Sciences, prospect 100 let Vladivostoku, 159, Vladivostok 690022, Russian Federation



Received: 04.06.2018

Accepted after revision: 06.08.2018

Published online: 24.08.2018

DOI: 10.1055/s-0037-1609939; Art ID: st-2018-v0337-I

Abstract New cyano-group-containing 1,3-oxaselenoles were obtained by the treatment of aroylacetonitriles with selenium(IV) oxide. The resulting products were shown to react with ammonia, hydrazine, or primary amines; this reaction was accompanied by aryl rearrangement.

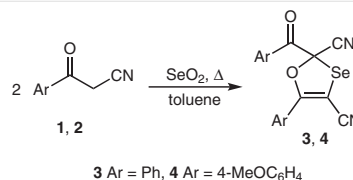
Key words aroylacetonitriles, selenium oxide, oxaselenoles, nucleophilic substitution, rearrangement

1,3-Oxaselenoles are an underinvestigated group of heterocyclic compounds. They are most often prepared by the interaction of selenium(IV) oxide with cyclic 1,3- or 1,2-dicarbonyl compounds or, in some cases, with 1,3,5-tricarbonyl compounds.¹ 1,3-Oxaselenoles are also obtained by the addition of the SeCN[−] anion to certain epoxides,² and they can also be synthesized via α -carbonyl-stabilized sulfur ylides³ or by using α -bromoacetophenones.⁴ 1,3-Oxaselenoles can also be prepared from 2-oxo-1,2-diphenylethyl selenocyanate.⁵

1,3-Selenocyanates are known to react with bromine.^{1a} They can react with diazomethane to form 1,4,7-dioxaselenocines.^{1e,f} A method for converting 1,3-oxaselenole into oxaselenolium perchlorates is also known.⁴ However, the reactions of 1,3-oxaselenoles with N-nucleophiles has not previously been reported.

We previously studied the interaction of malononitrile with selenium(IV) oxide. Depending on the reaction conditions, this proceeds with the formation of various products: pyridinium ylides, tetracyanoethylene, 1,1,2,3,3-pentacyanopropene salts,⁵ or triselenodicyanide.⁶

In this study, we used aroylacetonitriles as active methylene group-containing malononitrile analogues. We found that, on treatment with selenium(IV) oxide, aroylacetonitriles **1** and **2** underwent heterocyclization to give the previously unknown cyano-group-containing 1,3-oxaselenoles **3** and **4** (Scheme 1) in good yields. The starting aroylacetonitriles were obtained from the methyl esters of the corresponding aromatic acids.⁷



Scheme 1 Formation of 1,3-oxaselenoles **3** and **4** from aroylacetonitriles

The formation of oxaselenoles **3** and **4** from the aroylacetonitriles **1** and **2** occurred optimally on reaction for five hours in boiling toluene.⁸ Other solvents, for example, 1,4-dioxane, can also be used as reaction media. However, when 1,4-dioxane was used, the resulting product contained small amounts of insoluble impurities. The proposed mechanism for the formation of oxaselenoles **3** and **4** is similar to that previously proposed for the formation of oxaselenoles from cyclic 1,3-dicarbonyl compounds.^{1d}

The crystalline form of the product **4** was subjected to X-ray analysis, which confirmed its structure to be that of 2-(4-methoxybenzoyl)-5-(4-methoxyphenyl)-1,3-oxaselenole-2,4-dicarbonitrile (Figure 1).⁹

During chromatography of 1,3-oxaselenoles **3** and **4** on Al₂O₃ (eluent: 1,2-dichloroethane), elimination of the aroyl fragment occurred to form the corresponding 2,4-dicyano-5-aryl-1,3-oxazelenoles **5** and **6**, respectively. The weakly

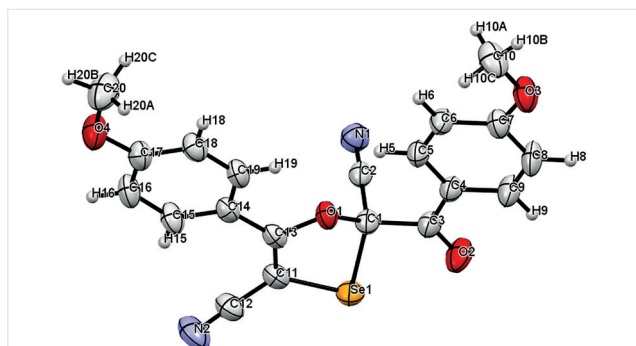
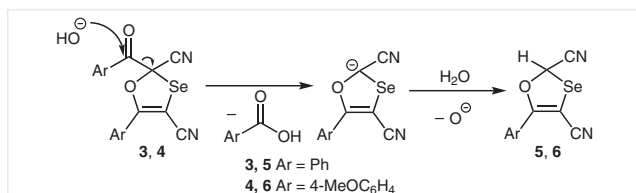


Figure 1 X-Ray structure of compound 4

basic nature of the sorbent contributes to this reaction. Elimination of the aroyl fragment did not occur during chromatography on silica gel. The proposed mechanism for the dearoylation reaction is shown in Scheme 2.¹⁰



Scheme 2 Dearoylation mechanism of oxaselenoles 3 and 4

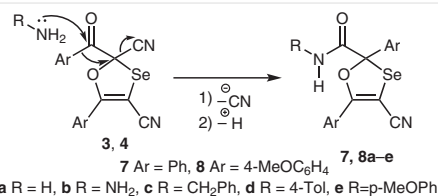
In the IR spectra of products 5 and 6, a broadened absorption band for the CN groups at 2195–2206 cm⁻¹ remained unchanged. There was also an absence of an absorption band in the carbonyl group region compared with the spectra of the starting substances. This showed the absence of the benzoyl-fragment. The ¹H NMR spectra of products 5 and 6 contained proton signals for only one aromatic nucleus, and an additional signal with an intensity corresponding to 1 H appeared at δ = 7.2 ppm. The GC/MS spectra showed isotope splittings for the molecular ions [M⁺], and the *m/z* values coincided with the calculated ones.

Oxaselenoles 3 and 4 and their products are unstable compounds with respect to oxygen, and during prolonged storage they are oxidized with the release of elementary selenium. One product of atmospheric oxidation of oxaselenole 3 is benzoic acid; this was isolated by sublimation from a partially oxidized sample.

Oxidation of oxaselenole 3 with hydrogen peroxide also led to the formation of benzoic acid. The extraction mixture of oxidation products was analyzed by GC/MS. The starting aroylacetonitrile 1 was found in the mixture as a second component, and its presence was confirmed by the detection of an absorption band for the unconjugated cyano group in the IR spectrum of the isolated mixture.

A peculiarity of the 2-cyano-containing oxaselenoles 3 and 4 is their ability to interact selectively with such active N-nucleophiles as ammonia, primary amines, or hydrazine

to give the substituted amides 7a–e and 8a–e. In this reaction, the cyano group at the 2-position is replaced by an aryl fragment that migrates from the carbonyl function. A suggested mechanism of interaction is shown in Scheme 3. The amides 7a–e and 8a–e were prepared from the oxaselenoles 3 and 4 by cooling the reactants in an ethanol or acetonitrile medium.¹¹ The resulting products were amorphous or fine crystalline substances with a gray or pale-yellow color that precipitated spontaneously from of the reaction mixture as the reaction proceeded. The yield of the products purified by crystallization reached 61%.



Scheme 3 Nucleophilic substitution of cyano group with rearrangement in reactions of oxaselenoles 3 and 4 with amines.

The product structures were confirmed by IR and ¹H and ¹³C NMR spectra. The IR spectra for all compounds 7a–e and 8a–e were characterized by the presence of an absorption band for the amide group. The proton signals of the NH₂ group for products 7a and 8a were observed as two separate and equally intense signals. For compounds 7c and 8c, the proton signals of the N–H group underwent splitting and appeared as triplet signals. In this case, the signals of the protons of the benzyl group also underwent splitting, indicating the absence of rotation around the N–CH₂ bond.

A comparison of the X-ray data for oxaselenole 4 (Figure 1) and substitution product 7c (Figure 2)⁹ showed the different positions of the aryl substituent originally at position

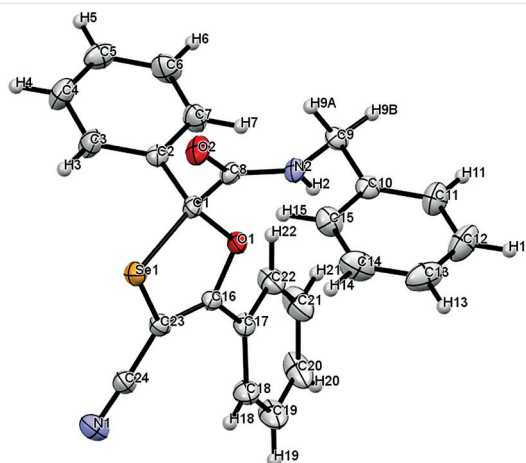


Figure 2 X-Ray structure of compound 7c

2, before and after the reaction. Therefore, the rearrangement process under the conditions of the reaction was confirmed.

In conclusion, it should be noted that the number of known oxaselenoles is small. We have found a method for synthesizing new 2-cyano-1,3-oxaselenoles. These compounds eliminate a cyano group and undergo rearrangement on treatment with an active N-nucleophile. The oxaselenoles were obtained from unsubstituted or electron-donating-group-containing aroylacetonitriles. Unfortunately, attempts to obtain aroylacetonitriles with an electron-acceptor nitro group were unsuccessful.

Supporting Information

Supporting information for this article is available online at <https://doi.org/10.1055/s-0037-1609939>.

References and Notes

- (1) (a) Stamm, H.; Gossrau, K. *Ber. Dtsch. Chem. Ges. A* **1933**, 66, 1558. (b) Borsche, W.; Hartmann, H. *Ber. Dtsch. Chem. Ges. A* **1940**, 73, 839. (c) Laitalainen, T.; Simonen, T.; Kivekäs, R. *Tetrahedron Lett.* **1978**, 19, 3079. (d) Laitalainen, T.; Simonen, T.; Kivekäs, R.; Klinga, M. *J. Chem. Soc., Perkin Trans. 1* **1983**, 333. (e) Matoba, K.; Yamazaki, T. *Chem. Pharm. Bull.* **1987**, 35, 4967. (f) Matoba, K.; Yamazaki, T. *Heterocycles* **1983**, 20, 1959.
- (2) (a) Robert, A.; Le Maréchal, A. M. *J. Chem. Soc., Chem. Commun.* **1978**, 447. (b) Le Maréchal, A. M.; Robert, A.; Leban, I. *J. Chem. Soc., Perkin Trans. 1* **1993**, 351.
- (3) Nakayama, J.; Sugiura, H.; Hoshino, M.; Kobayashi, H. *Tetrahedron Lett.* **1985**, 26, 2201.
- (4) Weber, M.; Hartmann, H. *Z. Chem.* **1987**, 27, 95.
- (5) Gramza, M.; Mitchell, R. B.; Dittmer, D. C. *J. Org. Chem.* **1984**, 49, 2057.
- (6) (a) Kachanov, A. V.; Slabko, O. Yu.; Skronts, M. V.; Kaminskii, V. A. *Russ. J. Org. Chem.* **2006**, 42, 774. (b) Kachanov, A. V.; Slabko, O. Yu.; Kaminskii, V. A. *Russ. J. Org. Chem.* **2017**, 53, 462. (c) Kaminskii, V. A.; Slabko, O. Yu.; Kachanov, A. V.; Buhvetskii, B. V. *Tetrahedron Lett.* **2003**, 44, 139. (d) Kachanov, A. V.; Slabko, O. Yu.; Baranova, O. V.; Shilova, E. V.; Kaminskii, V. A. *Tetrahedron Lett.* **2004**, 45, 4461.
- (7) Baba, A.; Yasuma, T.; Tawada, H.; Yamashita, M. *WO* 2005111046, **2005**.
- (8) **2-Aroyl-1,3-oxaselenole-2,4-dicarbonitriles 3 and 4: General Procedure**
The appropriate aroylacetonitrile **1** or **2** (34 mmol) and SeO₂ (5.66 g, 51 mmol) were added successively, with stirring, to toluene (100 mL), and the mixture was heated to boiling for 5 h until the reaction was complete (TLC). During the reaction, the color of the mixture changed from yellow to dark-red, and a small amount of gray selenium precipitated. The solution was then decanted and the solvent was evaporated to give an oily residue that was dried under reduced pressure. If necessary, the product could be purified chromatographically (silica gel, DCE).
2-Benzoyl-5-phenyl-1,3-oxaselenole-2,4-dicarbonitrile (3)
Red oil; yield: 5.03 g (81%). IR (KBr): 3067, 2206, 1701, 1597 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): δ = 7.57–7.66 (m, 5 H), 7.76 (t, *J* = 7.4 Hz, 1 H), 7.90 (d, *J* = 8.5 Hz, 2 H), 8.13 (d, *J* = 8.5 Hz, 2 H). ¹³C NMR (100 MHz, DMSO-*d*₆): δ = 45.2, 79.6, 114.4, 116.0, 126.6, 127.9, 129.2, 129.3, 129.7, 130.2, 132.5, 135.0, 160.8, 183.8. LC/MS (APCI): *m/z* [M⁺] calcd for C₁₈H₁₀N₂O₂Se: 365.99; found: 365.98.
2-(4-Methoxybenzoyl)-5-(4-methoxyphenyl)-1,3-oxaselenole-2,4-dicarbonitrile (4)
Orange solid; yield: 5.57 g (77%); mp 122–124 °C. IR (KBr): 3076, 2843, 2205, 1655, 1593 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): δ = 3.85 (s, 3 H), 3.88 (s, 3 H), 7.14 (d, *J* = 9.0 Hz, 4 H), 7.87 (d, *J* = 9.0 Hz, 2 H), 8.12 (d, *J* = 9.0 Hz, 2 H). ¹³C NMR (100 MHz, DMSO-*d*₆): δ = 55.7, 55.9, 76.5, 79.20, 114.6, 114.7, 114.9, 116.2, 118.8, 122.5, 130.0, 132.4, 160.8, 162.3, 164.6, 182.4.
(9) CCDC 1824131 and 1824130 contain the supplementary crystallographic data for compounds **4** and **7c**, respectively. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/getstructures.
(10) **1,3-Oxaselenole-2,4-dicarbonitriles 5 and 6; General Method**
The appropriate oxaselenole **3** or **4** (300.0 mg) was applied to a chromatographic plate measuring 250 × 300 mm with an unattached layer of Al₂O₃, and was eluted four times with DCE. During the chromatography, dearoylation occurred and the color of the upper spot changed from yellow to pale yellow. Part of the upper area was collected and extracted with DCE. The solvent was evaporated and the semi-solid residue was dissolved in an Et₂O–hexane mixture. The resulting solution was slowly evaporated at r.t. over a few days. The resulting crystals were separated and dried under reduced pressure.
5-Phenyl-1,3-oxaselenole-2,4-dicarbonitrile (5)
Gray solid; yield: 50.0 mg (24%); mp 78–79 °C. IR (KBr): 2997, 2206, 1595 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): δ = 7.24 (s, 1 H), 7.58 (m, 3 H), 7.78 (m, 2 H). ¹³C NMR (100 MHz, DMSO-*d*₆): δ = 65.4, 77.7, 114.9, 117.5, 127.0, 127.3, 129.4, 132.2, 161.3. GC/MS: *m/z* [M⁺] calcd for C₁₁H₆N₂OSe: 261.97, found: 262.00.
5-(4-Methoxyphenyl)-1,3-oxaselenole-2,4-dicarbonitrile (6)
Gray solid; yield: 70.0 mg (33%); mp 100–101 °C. IR (KBr): 2934, 2839, 2195, 1607 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): δ = 3.83 (s, 3 H), 7.11 (d, *J* = 9.0 Hz, 2 H), 7.20 (s, 1 H), 7.76 (d, *J* = 9.0 Hz, 2 H). ¹³C NMR (100 MHz, DMSO-*d*₆): δ = 55.7, 65.0, 74.6, 114.8, 115.4, 117.6, 119.3, 129.3, 161.3, 162.1. GC/MS: *m/z* [M⁺] calcd for C₁₂H₈N₂O₂Se: 291.98, found: 292.00.
(11) **Replacement Products 7a–e and 8a–e; General Procedure**
A solution of the appropriate oxaselenole **3** or **4** (1.6 mmol) in EtOH or MeCN (3 mL) was cooled and aq. NH₃, N₂H₄·H₂O, or a primary amine was added with stirring. After 2 h, the product spontaneously precipitated as an amorphous precipitate that was collected by filtration, washed once with the cooled solvent, and dried. The resulting product was crystallized from the appropriate solvent.
4-Cyano-2,5-diphenyl-1,3-oxaselenole-2-carboxamide (7a)
White solid; yield: 227.3 mg (40%); mp 207–208 °C (THF–hexane). IR (KBr): 3393, 3312, 3061, 2210, 1674, 1593 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): δ = 7.41–7.47 (m, 3 H), 7.56–7.62 (m, 3 H), 7.64 (d, *J* = 7.7 Hz, 1 H), 7.65 (d, *J* = 8.2 Hz, 1 H), 7.99 (s, 1 H), 8.13 (d, *J* = 8.0 Hz, 1 H), 8.14 (d, *J* = 7.3 Hz, 1 H), 8.21 (s, 1 H). ¹³C NMR (100 MHz, DMSO-*d*₆): δ = 75.2, 97.7, 115.1, 125.1, 127.4, 127.5, 128.6, 129.2, 129.6, 131.9, 139.6, 160.4, 170.1.
4-Cyano-2,5-diphenyl-1,3-oxaselenole-2-carbohydrazide (7b)
White solid; yield: 335.1 mg (57%); mp 184–185 °C (toluene). IR (KBr): 3325, 3275, 3063, 2199, 1663, 1597 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): δ = 4.58 (s, 2 H), 7.40–7.46 (m, 3 H), 7.57–7.61 (m, 3 H), 7.63 (d, *J* = 7.8 Hz, 1 H), 7.64 (d, *J* = 8.3 Hz, 1 H), 8.17 (d, *J* = 8.0 Hz, 1 H), 8.18 (d, *J* = 7.3 Hz, 1 H), 10.06 (s, 1 H). ¹³C NMR

(100 MHz, DMSO- d_6): δ = 75.2, 97.4, 115.1, 125.0, 127.4, 127.5, 128.6, 129.2, 129.7, 131.9, 139.8, 160.4, 166.9.

***N*-Benzyl-4-cyano-2,5-diphenyl-1,3-oxaselenole-2-carboxamide (7c)**

White solid; yield: 299.0 mg (42%); mp 169–170 °C (toluene). IR (KBr): 3312, 3065, 2851, 2205, 1659, 1593 cm^{-1} . ^1H NMR (400 MHz, DMSO- d_6): δ = 4.36 (m, 2 H), 7.15–7.29 (m, 5 H), 7.41–7.48 (m, 3 H), 7.57–7.63 (m, 3 H), 7.66 (d, J = 7.4 Hz, 1 H), 7.67 (d, J = 8.0 Hz, 1 H), 8.12 (d, J = 7.9 Hz, 1 H), 8.13 (d, J = 7.1 Hz, 1 H), 9.31 (t, J = 6.1 Hz, 1 H). ^{13}C NMR (100 MHz, DMSO- d_6): δ = 42.5, 75.4, 97.4, 115.0, 125.1, 127.0, 127.1, 127.4, 128.4, 128.7, 129.2, 129.7, 131.9, 138.7, 139.5, 160.5, 168.2.

4-Cyano-*N*-(4-tolyl)-2,5-diphenyl-1,3-oxaselenole-2-carboxamide (7d)

White solid; yield: 315.7 mg (44%); 145–146 °C (EtOH). IR (KBr): 3331, 3055, 2920, 2201, 1663, 1595 cm^{-1} . ^1H NMR (400 MHz, DMSO- d_6): δ = 2.25 (s, 3 H), 7.15 (d, J = 8.3 Hz, 2 H), 7.45–7.51 (m, 5 H), 7.60–7.64 (m, 3 H), 7.73 (d, J = 8.0 Hz, 1 H), 7.74 (d, J = 8.4 Hz, 1 H), 8.13–8.16 (m, 2 H), 10.31 (s, 1 H). ^{13}C NMR (100 MHz, DMSO- d_6): δ = 20.5, 75.6, 97.8, 115.1, 121.2, 125.7, 127.5, 127.6, 128.8, 129.2, 129.9, 131.9, 134.1, 134.8, 138.9, 160.6, 166.7.

4-Cyano-*N*-(4-methoxyphenyl)-2,5-diphenyl-1,3-oxaselenole-2-carboxamide (7e)

White solid; yield: 274.0 mg (37%); 123–124 °C (EtOH). IR (KBr): 3315, 3061, 2833, 2203, 1657, 1597 cm^{-1} . ^1H NMR (400 MHz, DMSO- d_6): δ = 3.72 (s, 3 H), 6.91 (d, J = 9.1 Hz, 2 H), 7.45–7.51 (m, 5 H), 7.60–7.63 (m, 3 H), 7.73 (d, J = 7.8 Hz, 1 H), 7.74 (d, J = 8.2 Hz, 1 H), 8.14–8.16 (m, 2 H), 10.29 (s, 1 H). ^{13}C NMR (100 MHz, DMSO- d_6): δ = 55.3, 75.6, 97.8, 113.9, 115.1, 122.9, 125.6, 127.5, 127.6, 128.8, 129.2, 129.9, 130.2, 131.9, 139.0, 156.4, 160.6, 166.5.

4-Cyano-2,5-bis(4-methoxyphenyl)-1,3-oxaselenole-2-carboxamide (8a)

Pale-yellow solid; yield: 299.5 mg (45%); 184–185 °C (EtOH). IR (KBr): 3495, 3331, 2935, 2837, 2199, 1691, 1605 cm^{-1} . ^1H NMR (400 MHz, DMSO- d_6): δ = 3.74 (s, 3 H), 3.84 (s, 3 H), 6.98 (d, J = 9.0 Hz, 2 H), 7.12 (d, J = 9.0 Hz, 2 H), 7.55 (d, J = 8.9 Hz, 2 H), 7.91 (s, 1 H), 8.09 (d, J = 9.0 Hz, 2 H), 8.15 (s, 1 H). ^{13}C NMR (100 MHz, DMSO- d_6): δ = 55.4, 55.7, 72.2, 97.7, 113.9, 114.6, 115.7, 120.1, 126.7, 129.4, 131.4, 160.2, 160.6, 161.9, 170.4.

4-Cyano-2,5-bis(4-methoxyphenyl)-1,3-oxaselenole-2-carbohydrazide (8b)

Pale-yellow solid; yield: 344.2 mg (50%); 106–108 °C (toluene). IR (KBr): 3352, 3323, 2935, 2839, 2201, 1670, 1607 cm^{-1} . ^1H NMR (400 MHz, DMSO- d_6): δ = 3.74 (s, 3 H), 3.85 (s, 3 H), 4.55 (s, 2 H), 6.97 (d, J = 8.9 Hz, 2 H), 7.12 (d, J = 8.9 Hz, 2 H), 7.54 (d, J = 8.9 Hz, 2 H), 8.13 (d, J = 8.9 Hz, 2 H), 10.00 (s, 1 H). ^{13}C NMR (100 MHz, DMSO- d_6): δ = 55.4, 55.7, 72.2, 97.4, 113.9, 114.6, 115.7, 120.0, 126.6, 129.5, 131.5, 160.2, 160.6, 161.9, 167.1.

***N*-Benzyl-4-cyano-2,5-bis(4-methoxyphenyl)-1,3-oxaselenole-2-carboxamide (8c)**

Pale-yellow solid; yield: 336.6 mg (42%); 133–134 °C (toluene). IR (KBr): 3319, 2930, 2837, 2197, 1653, 1607 cm^{-1} . ^1H NMR (400 MHz, DMSO- d_6): δ = 3.75 (s, 3 H), 3.84 (s, 3 H), 4.35 (qd, J = 15.3, 6.2 Hz, 2 H), 6.99 (d, J = 9.0 Hz, 2 H), 7.13 (d, J = 9.0 Hz, 2 H), 7.17–7.30 (m, 5 H), 7.57 (d, J = 8.8 Hz, 2 H), 8.08 (d, J = 9.0 Hz, 2 H), 9.25 (t, J = 6.2 Hz, 1 H). ^{13}C NMR (100 MHz, DMSO- d_6): δ = 42.5, 55.4, 55.7, 72.4, 97.4, 114.0, 114.6, 115.7, 120.0, 126.8, 127.0, 128.4, 129.5, 131.2, 138.8, 160.2, 160.6, 161.9, 168.4.

4-Cyano-2,5-bis(4-methoxyphenyl)-*N*-(4-tolyl)-1,3-oxaselenole-2-carboxamide (8d)

White solid; yield: 490.6 mg (61%); 158–161 °C (EtOH). IR (KBr): 3330, 3055, 2201, 1663, 1595 cm^{-1} . ^1H NMR (400 MHz, DMSO- d_6): δ = 2.25 (s, 3 H), 3.75 (s, 3 H), 3.85 (s, 3 H), 7.02 (d, J = 8.9 Hz, 2 H), 7.15 (d, J = 8.9 Hz, 4 H), 7.46 (d, J = 8.5 Hz, 2 H), 7.63 (d, J = 8.9 Hz, 2 H), 8.11 (d, J = 9.0 Hz, 2 H), 10.26 (s, 1 H). ^{13}C NMR (100 MHz, DMSO- d_6): δ = 20.6, 55.5, 55.7, 72.7, 97.8, 113.7, 114.1, 114.6, 115.7, 120.1, 121.2, 127.4, 129.3, 129.7, 130.5, 134.9, 160.4, 160.9, 162.0, 167.0.

4-Cyano-*N*,2,5-tris(4-methoxyphenyl)-1,3-oxaselenole-2-carboxamide (8e)

Yellow solid; yield: 454.1 mg (54%); 212–214 °C (EtOH–1,4-dioxane). IR (KBr): 3306, 2932, 2835, 2199, 1664, 1607 cm^{-1} . ^1H NMR (400 MHz, DMSO- d_6): δ = 3.72 (s, 3 H), 3.75 (s, 3 H), 3.85 (s, 3 H), 6.91 (d, J = 9.0 Hz, 2 H), 7.02 (d, J = 8.9 Hz, 2 H), 7.14 (d, J = 9.0 Hz, 2 H), 7.48 (d, J = 9.1 Hz, 2 H), 7.63 (d, J = 8.9 Hz, 2 H), 8.11 (d, J = 8.9 Hz, 2 H), 10.23 (s, 1 H). ^{13}C NMR (100 MHz, DMSO- d_6): δ = 55.3, 55.5, 55.7, 72.6, 97.8, 113.7, 114.0, 114.1, 114.6, 115.7, 120.1, 122.9, 127.3, 129.7, 130.7, 156.4, 160.4, 160.9, 162.0, 166.8.