Supporting Information for

Stimuli-Triggered Modulation of Solid-State Excimer Emission in Push-Pull Cyanovinylene Dyes

Dongho Keum,‡[a] Siyoung Cho,‡[b] Jean Bouffard,[c] and Youngmi Kim*,[b]

[a]*Department of Chemistry, Dankook University, 152 Jukjeon-ro, Suji-gu, Yongin-si, Gyeonggi-do, 448-701, Korea*

[b]*Department of Chemistry and Research Institute of Basic Sciences, Kyung Hee University, 26 Kyungheedae-ro, Dongdaemun-gu, Seoul 02447, Korea*

[c]*Department of Chemistry and Nanoscience, Ewha Womans University, 52 Ewhayeodae-gil, Seodaemun-gu, Seoul, 03760, Korea*

youngmi.kim@khu.ac.kr

Tel: +82 2-961-9537; Fax: +82 2-961-0443

Table of Contents:

Experimental

Materials

All chemicals were purchased commercially and used as received without further purification. All solvents were spectral grade unless otherwise noted. Anhydrous *N,N*-dimethylformamide (DMF) was obtained as a sure-seal bottle from Sigma-Aldrich Co. Inc. (Saint Louis, MO). Flash column chromatography was performed using silica-gel (40 μm) was obtained from Merck Inc.

General methods, instrumentation and measurements

Synthetic manipulations that required an inert atmosphere (where noted) were carried out under argon using standard Schlenk techniques. NMR (^{1}H and ^{13}C) spectra were recorded on JEOL 400 MHz spectrometer. The ^{1}H and ^{13}C chemical shifts (δ) were reported in parts per million (ppm), referenced to the residual solvent resonances. Splitting patterns are denoted as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and br (broad). Melting point determinations for compounds were performed using open capillaries and are reported without additional corrections. High-resolution electrospray ionization (ESI) mass spectra were obtained at the Korean National Center for Inter-University Research. UV/Vis absorption spectra were obtained on a SCINCO UV S-3100 spectrophotometer. Fluorescence measurements were recorded on a Hitachi F-7000 fluorescence spectrophotometer using quartz cuvettes with a path length of 1 cm. Solution fluorescence quantum yields were determined using rhodamine 6G (Φ_{FL} = 0.95 in ethanol) as a standard. Fluorescence quantum yields in the solid state were determined by the integrating sphere method on an absolute PL (photoluminescence) quantum yield measurement system (Hamamatsu C11347-11, Hamamatsu, Japan). Lifetime measurements were conducted at the Korea Basic Science Institute (KBSI), Daegu Center, South Korea.

1. Notes on the use of the "excimer" (borrowed and adapted from the Supporting Information document of *Angew. Chem. Int. Ed.* 2015, *54*, 3912)

One commonly encountered definition of an excimer is that originally introduced by B. Stevens and E. Hutton (*Nature* **1960**, 186, 1045–1046) to distinguish dimers that are stable in the ground state from those that are not. This, as paraphrased by J. B. Birks (*Rep. Prog. Phys.* **1975**, *38*, 903–945), defined the excimer as: *"a dimer which is associated in an electronic excited state and dissociated in its ground electronic state."* The IUPAC Gold Book (http://goldbook.iupac.org/E02242.html) offers a similar definition: *"An electronically excited dimer, 'non-bonding' in the ground state."*

These definitions are valid for intermolecular excimers in fluid media (e.g. solutions), but exclude excimers in rigid media (e.g. aggregates, crystal lattice) and intramolecular excimers. Nevertheless, the excimeric nature of luminescent emission of aromatic molecules like pyrene in the crystal, where intermolecular interactions such as van der Waals forces and π-π stacking are significant, has long being recognized as excimeric in nature as well. For instance, Th. Förster wrote in his seminal review in *Angew. Chem.* (**1969**, *81*, 364–374; *Angew. Chem. Int. Ed.* **1969**, *8*, 333–343):

> *"The fluorescence of crystalline pyrene is blue and structureless, and its maximum (4600 Å) hardly differs from that of the long-wave component in solution (4760–4780 Å).* ***This fluorescence is also due to excimers.*** *(...) Excimer fluorescence occurs only in crystals of B type, in whose lattices adjacent molecules have an arrangement similar to that in the excimer. Nevertheless, this arrangement is by no means the same, as is shown by the absorption spectra of type B crystals, which (apart from a slight Davydov splitting) are very similar to the solution spectra. Thus here too the excimer configuration is only achieved after light absorption, with further approach of two molecules that were already adjacent.(...) Excimer formation appears from these observations to concern parallel pairs of adjacent molecules within the crystal rather than the crystal as such."* [emphasis ours]

The acceptance of the term 'excimer emission' for other crystalline dimers is broadly shared, as exemplified by J. B. Birks, in his own seminal review of excimers (*Rep. Prog. Phys.* **1975**, *38*, 903–945):

> *"The pyrene crystal is dimeric in structure, with the molecules arranged in (M || M) sandwich pairs which form the elementary lattice units. The molecules of the unexcited dimer have their planes and axes parallel at an interplanar distance of r_0 = 3.53 Å. (...) because r_0 is less than the range of the attractive excimer interaction, an excimer $^1D^*$ is rapidly formed by $^1M^*$ and its unexcited neighbor ^1M, so that the crystal fluorescence spectrum consists entirely of excimer emission."*

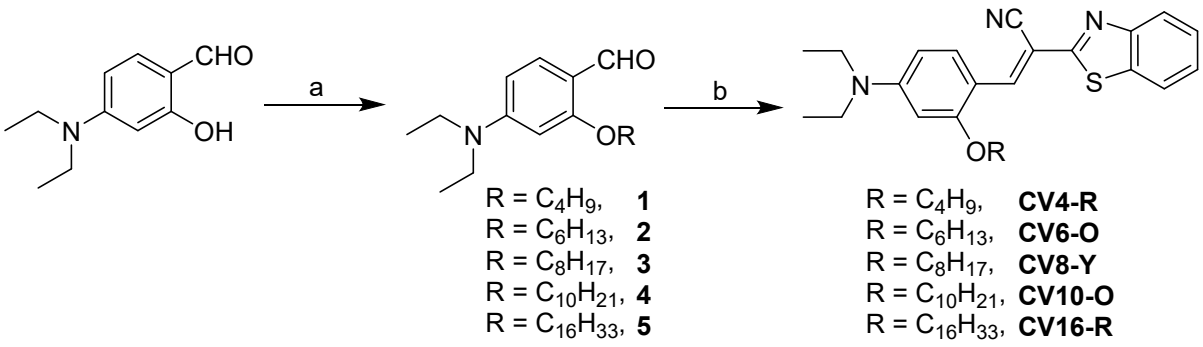
Consequently, Birks and others have promoted a revised definition of an excimer as *"a dimer which is associated in an excited electronic state and which is* dissociative *(i.e. would dissociate in the absence of restraints) in its ground electronic state."* to include crystal dimers, intramolecular excimers and sandwich dimers in rigid solutions, all of which were excluded by the original definition [emphasis in the original text, *Rep. Prog. Phys.* **1975**, *38*, 903–945]. As discussed, additional terminology has been developed to distinguish situations in which interactions are present in the ground state (but where dissociation would occur in the absence of restraints, such as those found in condensed non-fluid phases, and thus remain 'dissociative') and those where no interactions are present. For instance, F. Winnik in her review of pyrene excimers in organized media (*Chem. Rev.* **1993**, *93*, 587-614) discusses dynamic vs. static excimers, and introduces the distinction of (pre)associated excimers.

On the basis of these definitions, the conclusion that the emission of **CV** dyes, composed of an electron acceptor (benzothiazole), a π-conjugated bridge (cyanovinyl), an electron donor (*N*,*N*-dialkylaniline), is excimer emission remains valid. The experimental evidence is consistent with the assertion that the photophysical properties of the dyes are entirely analogous to that of pyrene, the reference excimer-forming aromatic molecule:

- In both the case of pyrene and that of the **CV** dyes, the crystals are dimeric in structure, forming face-to-face sandwich pairs (type B crystals) by a combination of van der Waals forces and π-π stacking interactions. These interactions are sufficient to slightly affect the absorption spectra and result in a splitting of the absorption bands, but not strong enough to maintain the stability of the dimer in solution. In other words, while interactions exist in the ground state, they do not amount to bonding, which is consistent with the IUPAC Gold Book definition of an excimer.

- In both the case of pyrene and that of the **CV** dyes, these ground state interactions are nevertheless not significant enough to be responsible for the new emission, and are not the same as that of the excimer. By maintaining a short distance and a proper respective orientation of the molecules, they merely facilitate the formation of a *dissociative* emissive excimer upon irradiation. Comparable ground state interactions are also present in the aggregates of the **CV** dyes, as evidenced by the small change in their absorption and excitation spectra.

2. Synthesis of Compounds



Scheme S1. Synthetic scheme for compounds, reagents, and conditions. (a) RBr, K_2CO_3, DMF, 80 °C, 12 h; (b) 2-benzothiazole- acetonitrile, piperidine, ethanol, room temperature, 12 h.

(a) Synthesis of compounds 1-5

2-Butoxy-4-(diethylamino)benzaldehyde (1). To a stirred mixture of 4-(diethylamino)salicylaldehyde (300 mg, 1.55 mmol) and K_2CO_3 (540 mg, 3.88 mmol) in dry DMF (5 mL) under an argon atmosphere was added 1-bromobutane (210 µL, 1.86 mmol) at room temperature. After the resulting mixture was stirred at 80 °C for 12 hours, the reaction solution was evaporated under reduced pressure, diluted with CH_2Cl_2, and washed with water (3 × 100 mL). The combined organic layer was dried over $MgSO_4$, filtered, and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using progressively more polar 100:1 to 80:1 hexanes:ethyl acetate as the mobile phase to afford **1** as a brown liquid (390 mg, 99%). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 10.18 (s, 1H), 7.71 (d, J = 9.2 Hz, 1H), 6.26 (d, J = 8.8 Hz, 1H), 6.01 (s, 1H), 4.03 (t, J = 6.4 Hz, 2H), 3.41 (q, J = 6.8 Hz, 4H), 1.81 (m, 2H), 1.52 (m, 2H), 1.21 (m, 6H), 0.98 (t, J = 7.2 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 187.3, 164.0, 153.9, 130.2, 114.3, 104.3, 93.1, 67.8, 44.9, 31.3, 19.4, 14.0, 12.7. HR-MS (ESI): calcd. for $C_{15}H_{23}NO_2$ $[M]^+$ 249.1729, found 249.1730.

4-(Diethylamino)-2-(hexyloxy)benzaldehyde (2). To a stirred mixture of 4-(diethylamino)salicylaldehyde (400 mg, 2.07 mmol) and K_2CO_3 (720 mg, 5.18 mmol) in dry DMF (5 mL) under an argon atmosphere was added 1-bromohexane (270 µL, 2.48 mmol) at room temperature. After the resulting mixture was stirred at 80 °C for 12 hours, the reaction solution was evaporated under reduced pressure, diluted with CH_2Cl_2, and washed with water (3 × 100 mL). The combined organic layer was dried over $MgSO_4$, filtered, and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using progressively more polar 100:1 to 80:1 hexanes:ethyl acetate as the mobile phase to afford **2** as a brown liquid (545 mg, 95%). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 10.18 (s, 1H), 7.71 (d, J = 9.2 Hz, 1H), 6.27 (d, J = 9.2 Hz, 1H), 6.02 (s, 1H), 4.02 (t, J = 6.4 Hz, 2H), 3.42 (q, J = 7.2 Hz, 4H), 1.83 (m, 2H), 1.49 (m, 2H), 1.35 (m, 4H), 1.21 (m, 6H), 0.91 (t, J = 6.8 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 187.3, 164.0, 153.9, 130.2, 114.5, 104.3, 93.3, 68.2, 44.8, 31.6, 29.2, 25.9, 22.7, 14.1, 12.7. HR-MS (ESI): calcd. for $C_{17}H_{27}NO_2$ $[M]^+$ 277.2042, found 277.2042.

4-(Diethylamino)-2-(octyloxy)benzaldehyde (3). To a stirred mixture of 4-(diethylamino)salicylaldehyde (400 mg, 2.07 mmol) and K_2CO_3 (720 mg, 5.18 mmol) in dry DMF (5 mL) under an argon atmosphere was added 1-bromooctane (430 µL, 2.48 mmol) at room temperature. After the resulting mixture was stirred at 80 °C for 12 hours, the reaction solution was evaporated under reduced pressure, diluted with CH_2Cl_2, and washed with water (3 × 100 mL). The combined organic layer was dried over $MgSO_4$, filtered, and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using progressively more polar 100:1 to 80:1 hexanes:ethyl acetate as the mobile phase to afford **3** as a brown liquid (650 mg, 99%). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 10.18 (s, 1H), 7.71 (d, J = 9.2 Hz, 1H), 6.27 (d, J =

8.8 Hz, 1H), 6.02 (s, 1H), 4.02 (t, J = 6.4 Hz, 2H), 3.42 (q, J = 7.2 Hz, 4H), 1.83 (m, 2H), 1.49 (m, 2H), 1.26 (m, 14H), 0.89 (t, J = 7.2 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 187.3, 164.0, 153.9, 130.2, 114.5, 104.3, 93.3, 68.2, 44.8, 31.9, 29.4, 29.3, 29.3, 26.2, 22.7, 14.2, 12.7. HR-MS (ESI): calcd. for $C_{19}H_{31}NO_2$ $[M]^+$ 305.2355, found 305.2357.

2-(Decyloxy)-4-(diethylamino)benzaldehyde (4). To a stirred mixture of 4-(diethylamino)salicylaldehyde (200 mg, 1.03 mmol) and K_2CO_3 (360 mg, 2.58 mmol) in dry DMF (5 mL) under an argon atmosphere was added 1-bromodecane (270 µL, 1.24 mmol) at room temperature. After the resulting mixture was stirred at 80 °C for 12 hours, the reaction solution was evaporated under reduced pressure, diluted with CH_2Cl_2, and washed with water (3 × 100 mL). The combined organic layer was dried over $MgSO_4$, filtered, and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using progressively more polar 100:1 to 80:1 hexanes:ethyl acetate as the mobile phase to afford **4** as a brown liquid (310 mg, 89%). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 10.18 (s, 1H), 7.71 (d, J = 8.8 Hz, 1H), 6.27 (d, J = 8.4 Hz, 1H), 6.02 (s, 1H), 4.02 (t, J = 6.4 Hz, 2H), 3.42 (q, J = 7.2 Hz, 4H), 1.83 (m, 2H), 1.48 (m, 2H), 1.29 (m, 18H), 0.88 (t, J = 6.4 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 187.3, 164.0, 153.9, 130.2, 114.5, 104.3, 93.3, 68.2, 44.8, 32.0, 29.7, 29.5, 29.4, 29.3, 26.2, 22.8, 14.2, 12.7. HR-MS (ESI): calcd. for $C_{21}H_{35}NO_2$ $[M]^+$ 333.2668, found 333.2669.

4-(Diethylamino)-2-(hexadecyloxy)benzaldehyde (5). To a stirred mixture of 4-(diethylamino) salicylaldehyde (200 mg, 1.03 mmol) and K_2CO_3 (360 mg, 2.58 mmol) in dry DMF (5 mL) under an argon atmosphere was added 1-bromohexadecane (380 µL, 1.24 mmol) at room temperature. After the resulting mixture was stirred at 80 °C for 12 hours, the reaction solution was evaporated under reduced pressure, diluted with CH_2Cl_2, and washed with water (3 × 100 mL). The combined organic layer was dried over $MgSO_4$, filtered and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using progressively more polar 100:1 to 80:1 hexanes:ethyl acetate as the mobile phase to afford **5** as a white solid (390 mg, 90%). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 10.18 (s, 1H), 7.71 (d, J = 8.8 Hz, 1H), 6.27 (d, J = 8.4 Hz, 1H), 6.02 (s, 1H), 4.02 (t, J = 6.4 Hz, 2H), 3.42 (q, J = 7.2 Hz, 4H), 1.83 (m, 2H), 1.48 (m, 2H), 1.26 (m, 30H), 0.88 (t, J = 7.2 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 187.3, 164.0, 153.9, 130.2, 114.5, 104.3, 93.3, 68.2, 44.8, 32.0, 29.8, 29.7, 29.5, 29.4, 29.3, 26.2, 22.8, 14.2, 12.7. HR-MS (ESI): calcd. for $C_{27}H_{48}NO_2$ $[M+H]^+$ 418.3680, found 418.3685.

(b) Synthesis of CV*n*-X dyes

(*E*)-2-(Benzo[*d*]thiazol-2-yl)-3-(2-butoxy-4-(diethylamino)phenyl)acrylonitrile (CV4-R). To a stirred solution of 2-butoxy-4-(diethylamino)benzaldehyde **1** (380 mg, 1.52 mmol) and 2-benzothiazoleacetonitrile (265 mg, 1.52 mmol) in ethanol (10 mL) at room temperature was added piperidine (190 µL, 1.82 mmol). The resulting solution was stirred at room temperature for 12 hours. The precipitate formed was collected by filtration, washed with ethanol, and dried under vacuum to afford **CV4-R** as an orange solid (453 mg, 73%). m.p. 122-123 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.53 (s, 1H), 8.44 (d, J = 9.2 Hz, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.83 (d, J = 8.8 Hz, 1H), 7.45 (t, J = 6.4 Hz, 1H), 7.33 (t, J = 8.4 Hz, 1H), 6.36 (d, J = 9.2 Hz, 1H), 6.07 (s, 1H), 4.05 (t, J = 6.4 Hz, 2H), 3.44 (q, J = 7.2 Hz, 4H), 1.90 (m, 2H), 1.61 (m, 2H), 1.24 (t, J = 7.2 Hz, 6H), 1.05 (t, J = 7.2 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 166.2, 161.1, 154.1, 152.7, 141.5, 134.4, 130.5, 126.4, 124.9, 123.0, 121.3, 118.7, 110.0, 105.1, 96.3, 93.8, 68.2, 44.9, 31.3, 19.5, 14.0, 12.8. HR-MS (ESI): calcd. for $C_{24}H_{27}N_3OS$ $[M]^+$ 405.1875, found 405.1875.

(*E*)-2-(Benzo[*d*]thiazol-2-yl)-3-(4-(diethylamino)-2-(hexyloxy)phenyl)acrylonitrile (CV6-O). To a stirred solution of 4-(diethylamino)-2-(hexyloxy)benzaldehyde **2** (545 mg, 1.96 mmol) and 2-benzothiazoleacetonitrile (340 mg, 1.96 mmol) in ethanol (15 mL) at room temperature was added piperidine (240 µL, 2.35 mmol). The resulting solution was stirred at room temperature for 12 hours. The precipitate formed was collected by filtration, washed with ethanol, and dried under vacuum to afford **CV6-O** as an orange solid (680 mg, 80%). m.p. 120-122 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.53 (s, 1H), 8.44 (d, J = 9.2

Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.45 (t, *J* = 8.4 Hz, 1H), 7.33 (t, *J* = 6.8 Hz, 1H), 6.36 (d, *J* = 9.6 Hz, 1H), 6.06 (s, 1H), 4.04 (t, *J* = 6.4 Hz, 2H), 3.44 (q, *J* = 7.2 Hz, 4H), 1.90 (m, 2H), 1.57 (m, 2H), 1.39 (m, 4H), 1.23 (t, *J* = 7.2 Hz, 6H), 0.94 (t, *J* = 6.8 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 166.2, 161.1, 154.1, 152.7, 141.5, 134.4, 130.5, 126.4, 124.9, 123.0, 121.3, 118.7, 110.0, 105.1, 96.3, 93.8, 68.5, 44.9, 31.7, 29.2, 26.0, 22.7, 14.2, 12.8. HR-MS (ESI): calcd. for $C_{26}H_{31}N_3OS$ $[M]^+$ 433.2188, found 433.2189.

(*E*)-2-(Benzo[*d*]thiazol-2-yl)-3-(4-(diethylamino)-2-(octyloxy)phenyl)acrylonitrile (CV8-Y). To a stirred solution of 4-(diethylamino)-2-(octyloxy)benzaldehyde **3** (650 mg, 2.13 mmol) and 2-benzothiazoleacetonitrile (370 mg, 2.13 mmol) in ethanol (15 mL) at room temperature was added piperidine (260 µL, 2.56 mmol). The resulting solution was stirred at room temperature for 12 hours. The precipitate formed was collected by filtration, washed with ethanol, and dried under vacuum to afford **CV8-Y** as an orange solid (865 mg, 88%). m.p. 96-98 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.52 (s, 1H), 8.44 (d, *J* = 9.2 Hz, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 1H), 7.33 (t, *J* = 6.8 Hz, 1H), 6.35 (d, *J* = 9.2 Hz 1H), 6.06 (s, 1H), 4.04 (t, *J* = 6.4 Hz. 2H), 3.44 (q, *J* = 6.8 Hz, 4H), 1.90 (m, 2H), 1.56 (m, 2H), 1.45-1.21 (m, 14H), 0.87 (t, *J* = 7.2 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 166.2, 161.1, 154.1, 152.7, 141.5, 134.4, 130.5, 126.4, 124.9, 123.0 ,121.3, 118.7, 110.0, 105.1, 96.2, 93.7, 68.5, 44.9, 31.9, 29.5, 29.4, 26.3, 22.8, 14.2, 12.8. HR-MS (ESI): calcd. for $C_{28}H_{35}N_3OS$ $[M]^+$ 461.2501, found 461.2500.

(*E*)-2-(Benzo[*d*]thiazol-2-yl)-3-(2-(decyloxy)-4-(diethylamino)phenyl)acrylonitrile (CV10-O). To a stirred solution of 2-(decyloxy)-4-(diethylamino)benzaldehyde **4** (310 mg, 0.93 mmol) and 2-benzothiazoleacetonitrile (162 mg, 0.93 mmol) in ethanol (10 mL) at room temperature was added piperidine (120 µL, 1.12 mmol). The resulting solution was stirred at room temperature for 12 hours. The precipitate was collected by filtration, washed with ethanol, and dried under vacuum to afford **CV10-O** as an orange solid (300 mg, 79%). m.p. 110-112 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.53 (s, 1H), 8.44 (d, *J* = 9.2 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.45 (t, *J* = 8.4 Hz, 1H), 7.33 (t, *J* = 8.0 Hz, 1H), 6.36 (d, *J* = 9.2 Hz, 1H), 6.07 (s, 1H), 4.04 (t, *J* = 6.4 Hz, 2H), 3.44 (q, *J* = 7.2 Hz, 4H), 1.90 (m, 2H), 1.57 (m, 2H), 1.42 -1.22 (m, 18H), 0.86 (t, *J* = 6.2 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 166.1, 161.1, 154.1, 152.7, 141.5, 134.4, 130.5, 126.3, 124.9, 123.0, 121.3, 118.7, 110.1, 105.1, 96.3, 93.8, 68.5, 44.9, 32.0, 29.8, 29.7, 29.5, 29.5, 26.3, 22.8, 14.2, 12.8. HR-MS (ESI): calcd. for $C_{30}H_{39}N_3OS$ $[M]^+$ 489.2814, found 489.2815.

(*E*)-2-(Benzo[*d*]thiazol-2-yl)-3-(4-(diethylamino)-2-(hexadecyloxy)phenyl)acrylonitrile (CV16-R). To a stirred solution of 4-(diethylamino)-2-(hexadecyloxy)benzaldehyde **5** (200 mg, 0.48 mmol) and 2-benzothiazoleacetonitrile (85 mg, 0.48 mmol) in ethanol (5 mL) at room temperature was added piperidine (60 µL, 0.57 mmol). The resulting solution was stirred at room temperature for 12 hours. The precipitate was collected by filtration, washed with ethanol, and dried under vacuum to afford **CV16-R** as an orange solid (230 mg, 83%). m.p. 92 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.54 (s, 1H), 8.44 (d, *J* = 9.2 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.33 (t, *J* = 8.0 Hz, 1H), 6.37 (d, *J* = 9.2 Hz, 1H), 6.07 (s, 1H), 4.04 (t, *J* = 6.4 Hz, 2H), 3.45 (q, *J* = 6.8 Hz, 4H), 1.90 (m, 2H), 1.56 (m, 2H), 1.42 - 1.22 (m, 30H), 0.88 (t, *J* = 6.6 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 166.2, 161.2, 154.2, 152.8, 141.6, 134.5, 130.6, 126.4, 125.0, 123.1 ,121.3, 118.7, 110.2, 105.2, 96.4, 93.9, 68.6, 45.0, 32.1, 29.9, 29.8, 29.6, 29.5, 29.3, 26.4, 22.8, 14.3, 12.9. HR-MS (ESI): calcd. for $C_{36}H_{52}N_3OS$ $[M+H]^+$ 574.3821, found 574.3831.

3. Photophysical Property Studies

Table S1. Photophysical properties of compounds at 25 °C.

Compounds	Solution						Powdered Solid		
	Solvents	$\lambda_{abs,max}$ (nm)	ε^a ($M^{-1}cm^{-1}$)	$\lambda_{em,max}{}^b$ (nm)	$\Phi_{FL}{}^c$	τ^e (ns)	$\lambda_{em,max}{}^b$ (nm)	$\Phi_{FL}{}^d$	τ^e (ns)
CV4-R	CH_2Cl_2	464	74100	526	0.004	N.D.	632	0.16	6.59
	THF	461	74700	524	0.005	N.D.			
	CH_3CN	467	68100	531	0.001	0.064			
CV6-O	CH_2Cl_2	465	79000	526	0.003	N.D.	594	0.18	4.60
	THF	460	67300	521	0.002	N.D.			
	CH_3CN	470	71100	530	0.001	0.065			
CV8-Y	CH_2Cl_2	464	64900	527	0.003	N.D.	576	0.40	1.59
	THF	460	69400	520	0.001	N.D.			
	CH_3CN	465	66800	532	0.001	0.063			
CV10-O	CH_2Cl_2	463	83400	526	0.003	N.D.	589	0.20	2.00
	THF	460	65200	522	0.004	N.D.			
	CH_3CN	465	68000	532	0.001	0.064			
CV16-R	CH_2Cl_2	463	62200	525	0.002	N.D.	671	0.07	5.45
	THF	461	70600	525	0.001	N.D.			
	CH_3CN	466	59400	528	0.001	0.067			

[a]Measured at each absorption maximum. [b]Excited at 440 nm [c]Quantum yields vs. rhodamine 6G in ethanol (Φ_{FL} = 0.95). [d]Absolute fluorescence quantum yield in the solid state evaluated using an integrating sphere. [e]The average weighted lifetimes. τ_{avg} = average fluorescence lifetime calculated by $\langle\tau\rangle_{amp} = \{\Sigma (f_i*\tau_i)\}/\{\Sigma(f_i)\}$. N.D.= not determined.

(a) Absorption and emission spectra of CV*n* dyes in organic solvents

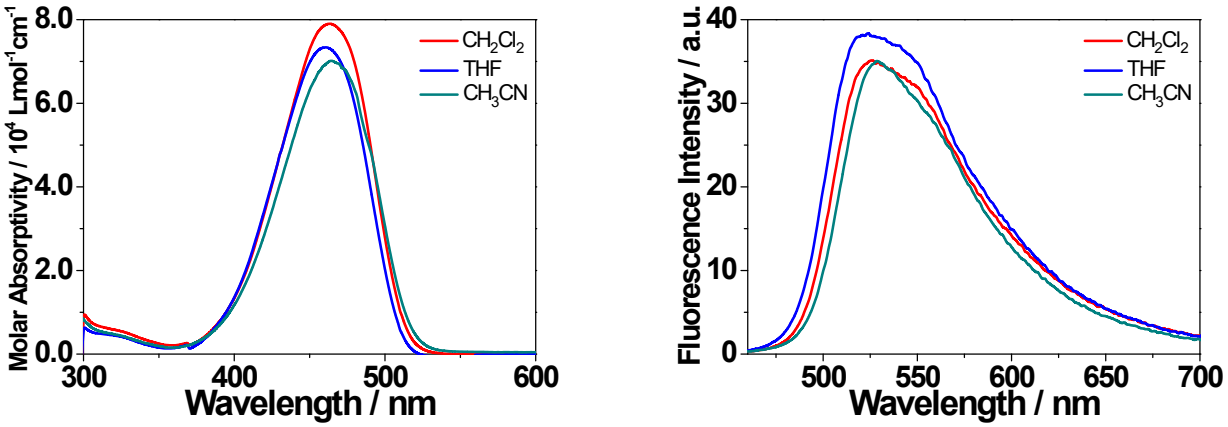


Figure S1. Absorption (left) and emission (right) spectra of **CV4-R** (20 μM) in various organic solvents at 25 °C. Excited at 440 nm.

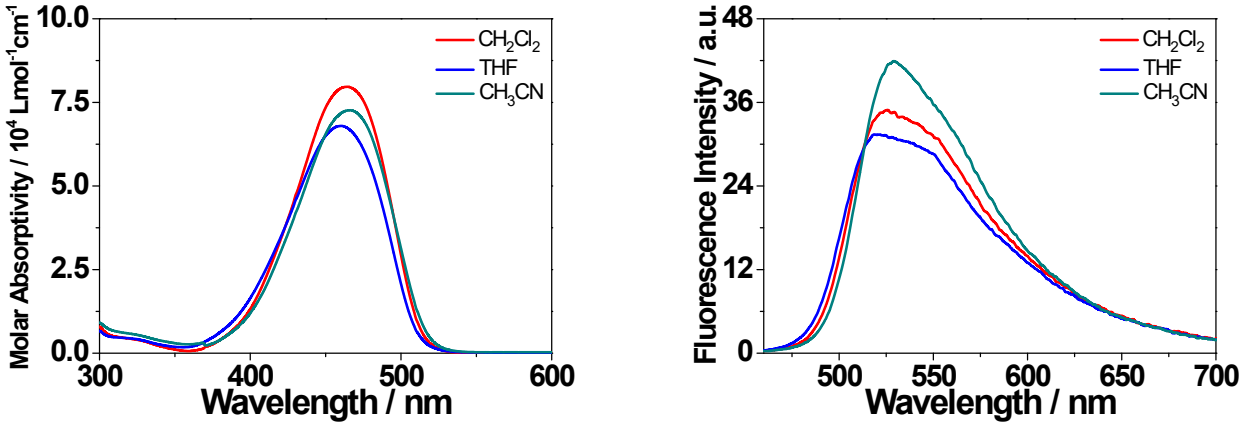


Figure S2. Absorption (left) and emission (right) spectra of **CV6-O** (20 μM) in various organic solvents at 25 °C. Excited at 440 nm.

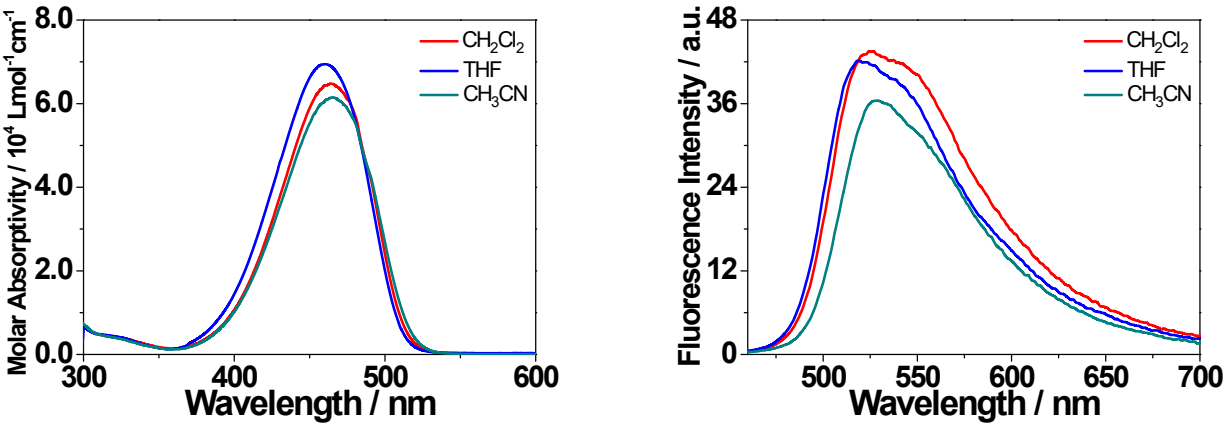


Figure S3. Absorption (left) and emission (right) spectra of **CV8-Y** (20 μM) in various organic solvents at 25 °C. Excited at 440 nm.

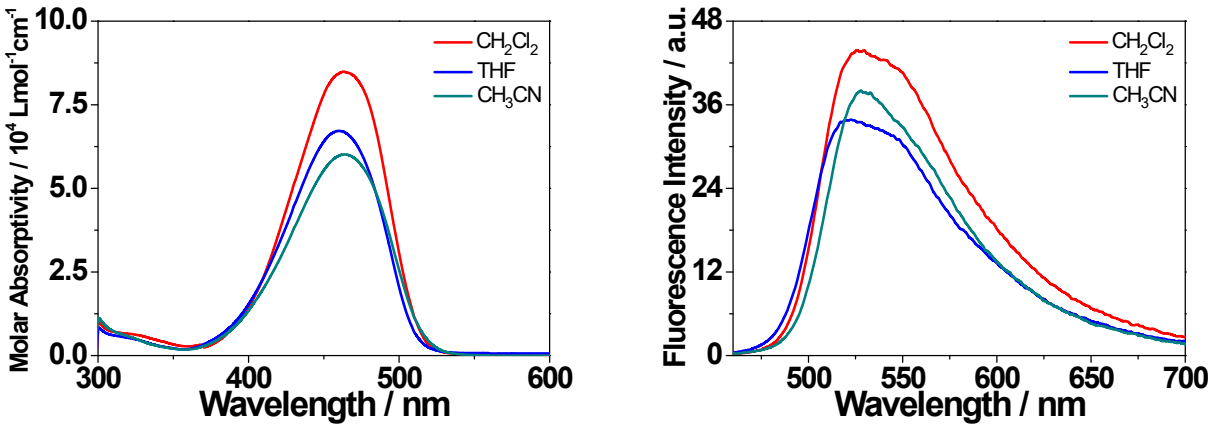


Figure S4. Absorption (left) and emission (right) spectra of **CV10-O** (20 μM) in various organic solvents at 25 °C. Excited at 440 nm.

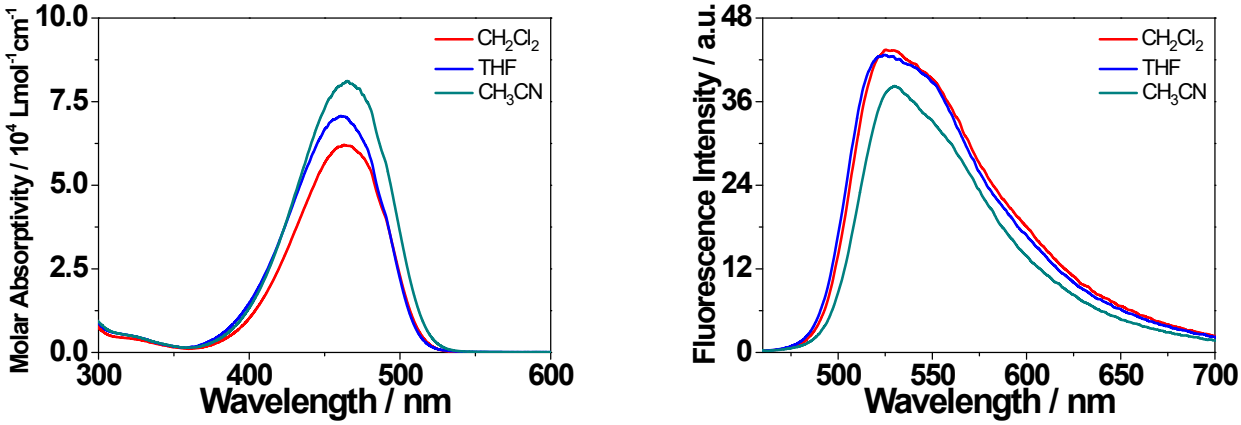


Figure S5. Absorption (left) and emission (right) spectra of **CV16-R** (20 μM) in various organic solvents at 25 °C. Excited at 440 nm.

(b) Comparision of absorption and emission spectra of CV*n* dyes in CH_3CN

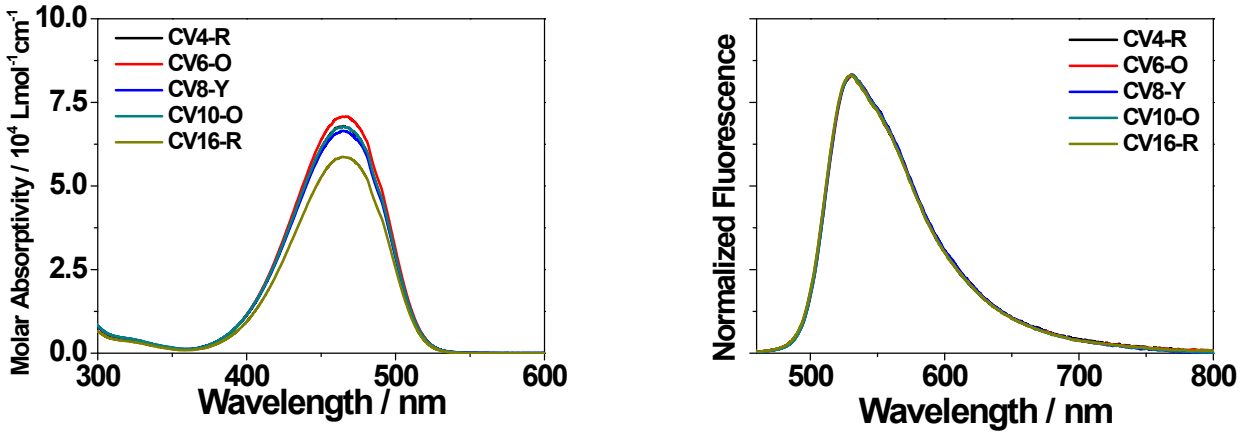


Figure S6. Absorption (left) and normalized emission (right) spectra of compounds in CH_3CN at 25 °C. Excited at 440 nm.

(c) Comparison of emission spectra of CV8-Y in Different States

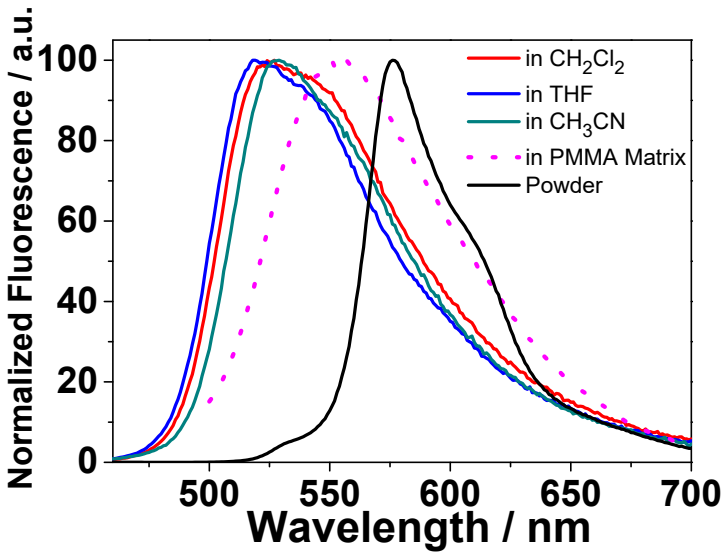


Figure S7. Emission spectra of **CV8-Y** in various organic solvents (red: CH_2Cl_2, blue: THF, dark green: CH_3CN), in a PMMA film with 10 wt % of **CV8-Y** (dotted pink), and in a powder (black). Excited at 440 nm.

4. Aggregation Behaviors of CV*n* Dyes in Aqueous Solutions

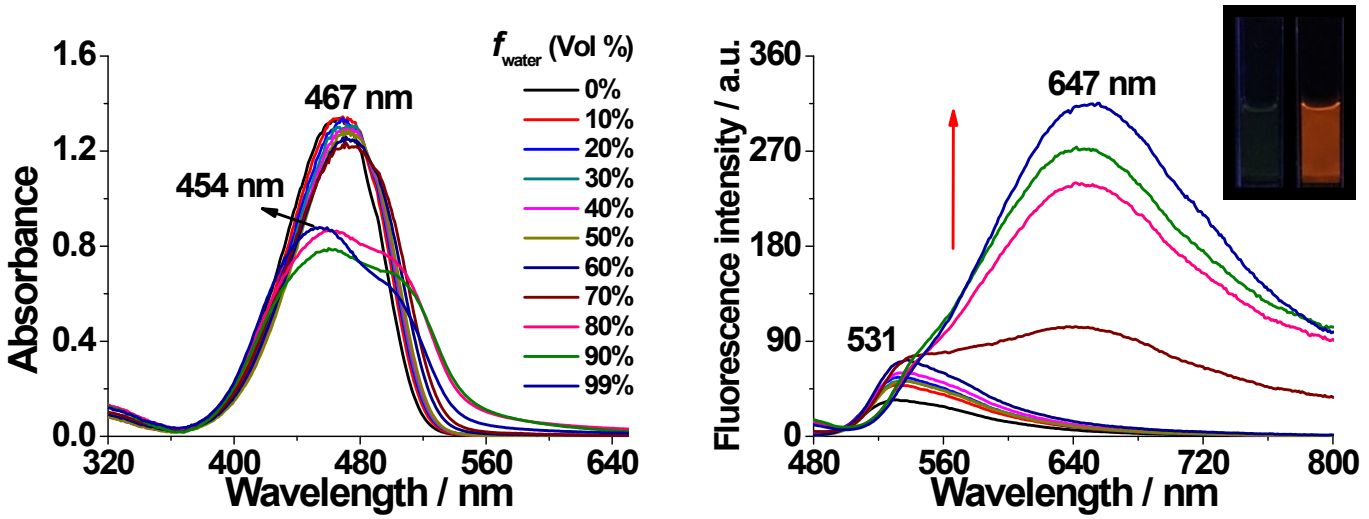


Figure S8. Absorption (left) and emission (right) spectra of **CV4-R** (20 μM) in CH_3CN–water mixtures with different water fraction (f_{water}(vol%): 0–99%) at 25 °C. Excited at 440 nm. Inset shows photographs of each solution (left: CH_3CN, right: CH_3CN/H_2O = 1:9 (v/v)) under irradiation at 365 nm.

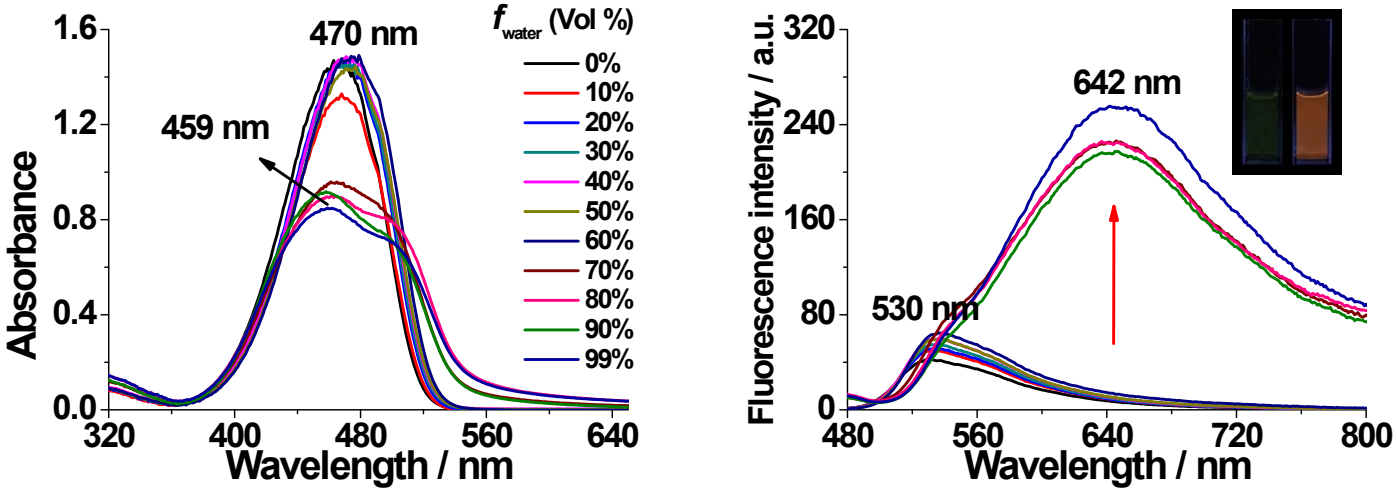


Figure S9. Absorption (left) and emission (right) spectra of **CV6-O** (20 μM) in CH_3CN–water mixtures with different water fraction (f_{water}(vol%): 0–99%) at 25 °C. Excited at 440 nm. Inset shows photographs of each solution (left: CH_3CN, right: CH_3CN/H_2O = 1:9 (v/v)) under irradiation at 365 nm.

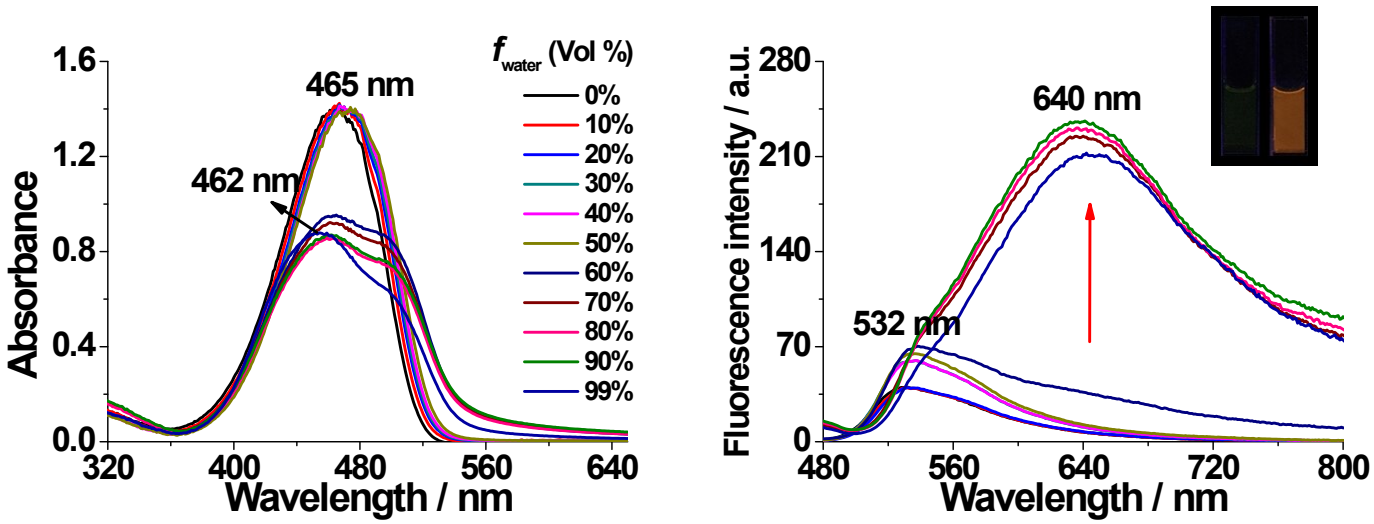


Figure S10. Absorption (left) and emission (right) spectra of **CV8-Y** (20 μM) in CH_3CN–water mixtures with different water fraction (f_{water}(vol%): 0–99%) at 25 °C. Excited at 440 nm. Inset shows photographs of each solution (left: CH_3CN, right: CH_3CN/H_2O = 1:9 (v/v)) under irradiation at 365 nm.

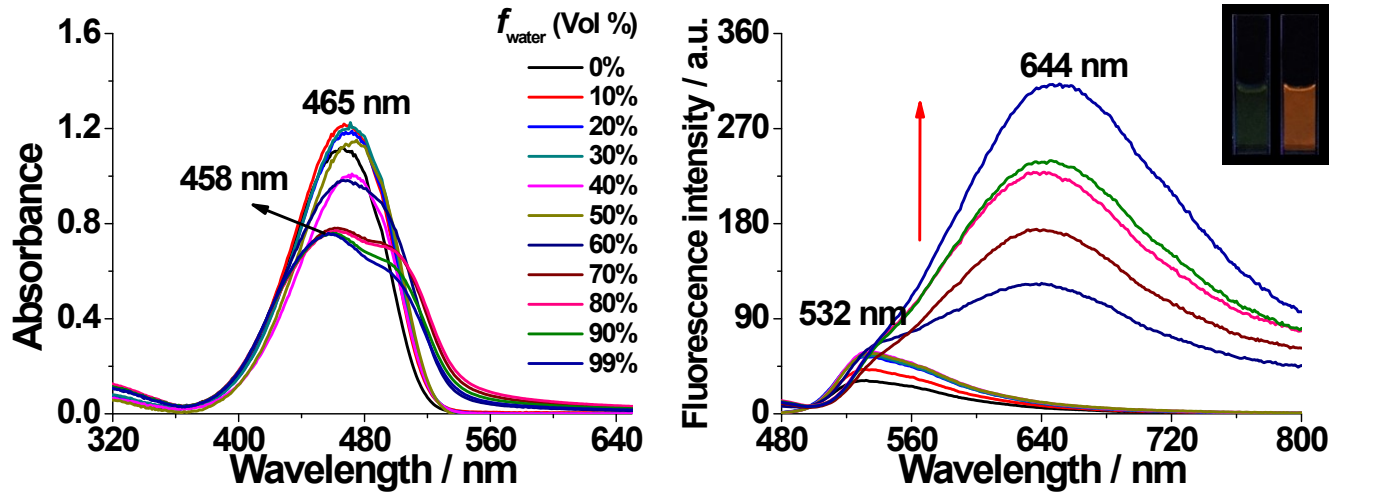


Figure S11. Absorption (left) and emission (right) spectra of **CV10-O** (20 μM) in CH_3CN–water mixtures with different water fraction (f_{water}(vol%): 0–99%) at 25 °C. Excited at 440 nm. Inset shows photographs of each solution (left: CH_3CN, right: CH_3CN/H_2O = 1:9 (v/v)) under irradiation at 365 nm.

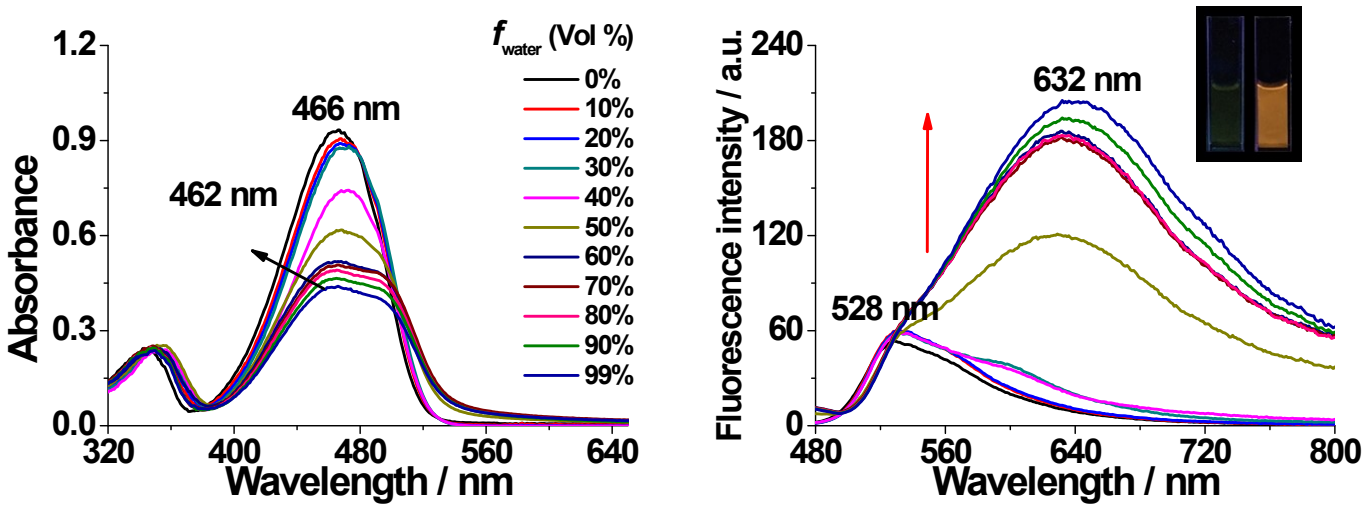


Figure S12. Absorption (left) and emission (right) spectra of **CV16-R** (20 μM) in CH_3CN–water mixtures with different water fraction (f_{water}(vol%): 0–99%) at 25 °C. Excited at 440 nm. Inset shows photographs of each solution (left: CH_3CN, right: CH_3CN/H_2O = 1:9 (v/v)) under irradiation at 365 nm.

5. Time-Resolved Photoluminescence Decay Dynamics

(a) Time-resolved photoluminescence decay dynamics of CV*n* dyes in CH_3CN

Time-resolved fluorescence decay study was carried out using a confocal microscope (MicroTime-200, Picoquant, Germany) with a 10 × (air) objective. A single-mode pulsed diode laser (470 nm with a pulse width of ~30 ps and an average power of 1~4 μW operating in 40 MHz repetition rate) was used as an excitation source. A dichroic mirror (490 DCXR, AHF), a long-pass filter (HQ500lp, AHF), a bandpass filter (500-550 nm, Thorlabs) and a single photon avalanche diode (PDM series, MPD) were used to collect emission from the samples. A time-correlated single-photon counting system (PicoHarp-300, PicoQuant GmbH, Germany) was used to count emission photons. Exponential function fitting for the obtained fluorescence decays was performed using Symphotime-64 software (Ver. 2.2).

Table S2. Fluorescence decays of compounds in CH_3CN

Compounds	λ_{em} [nm]	τ_1 (f_1)[a] [ns]	τ_2 (f_2)[a] [ns]	τ_3 (f_3)[a] [ns]	τ_{avg}[b] [ns]
CV4-R	530	0.032 (0.81)	0.198 (0.19)	1.50 (0.0005)	0.064
CV6-O	530	0.033 (0.81)	0.205 (0.19)		0.065
CV8-Y	530	0.031 (0.81)	0.198 (0.19)	2.30 (0.0005)	0.063
CV10-O	530	0.032 (0.81)	0.204 (0.19)		0.064
CV16-R	530	0.034 (0.81)	0.205 (0.19)		0.067

[a]Lifetime (τ) and fraction (f) of shorter (1) or longer (2 and 3) lived species. [b]Average weighted lifetimes (τ_{avg}) calculated by $\langle\tau\rangle_{amp} = \{\Sigma (f_i*\tau_i)\}/\{\Sigma(f_i)\}$. [**CV*n*-X**] = 20 μM.

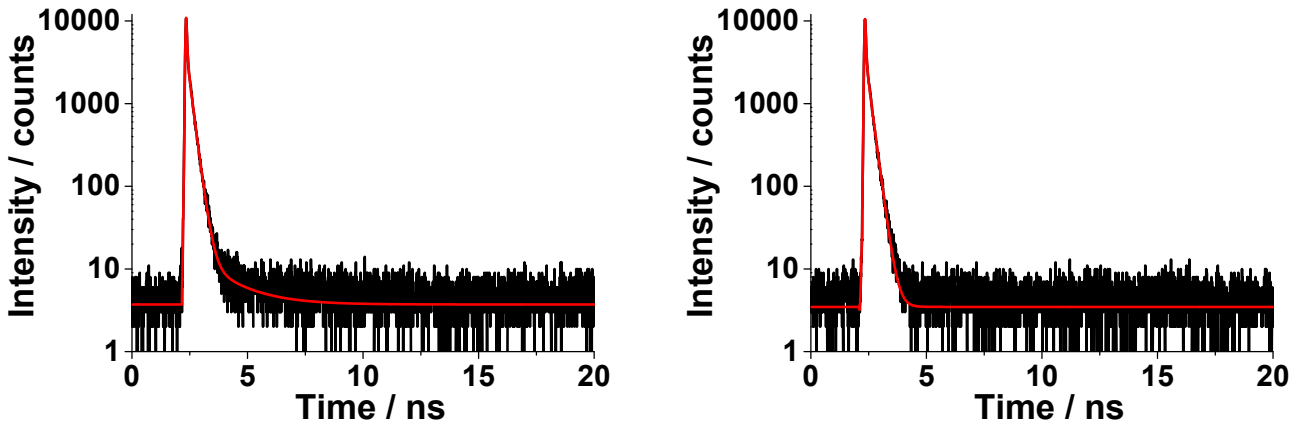


Figure S13. (left) Time-resolved fluorescence decays of **CV4-R** (Ex/Em = 470 nm/530 nm) in CH_3CN at 25 °C. **CV4-R** tri-exponential decays gave lifetimes of 0.032 ns (81%), 0.198 ns (19%) and 1.50 ns (0.05%). Average time is 0.064 ns. (right) Time-resolved fluorescence decays of **CV6-O** (Ex/Em = 470 nm/530 nm) in CH_3CN at 25 °C. **CV6-O** bi-exponential decays gave lifetimes of 0.033 ns (81%) and 0.205 ns (19%). Average time is 0.065 ns.

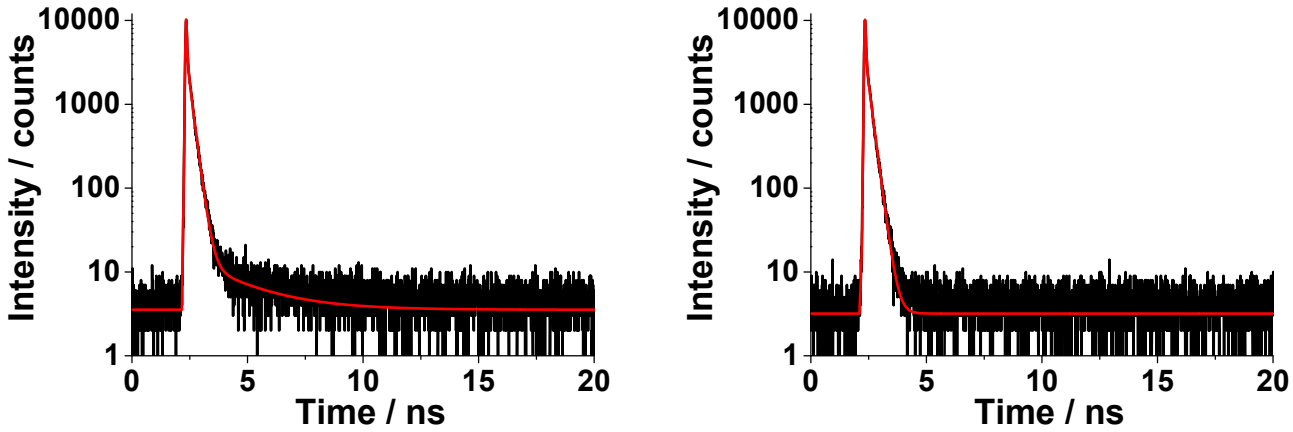


Figure S14. (left) Time-resolved fluorescence decays of **CV8-Y** (Ex/Em = 470 nm/530 nm) in CH_3CN at 25 °C. **CV8-Y** tri-exponential decays gave lifetimes of 0.031 ns (81%), 0.198 ns (19%) and 2.30 ns (0.05%). Average time is 0.063 ns. (right) Time-resolved fluorescence decays of **CV10-O** (Ex/Em = 470 nm/530 nm) in CH_3CN at 25 °C. **CV10-O** bi-exponential decays gave lifetimes of 0.032 ns (81%) and 0.204 ns (19%). Average time is 0.064 ns.

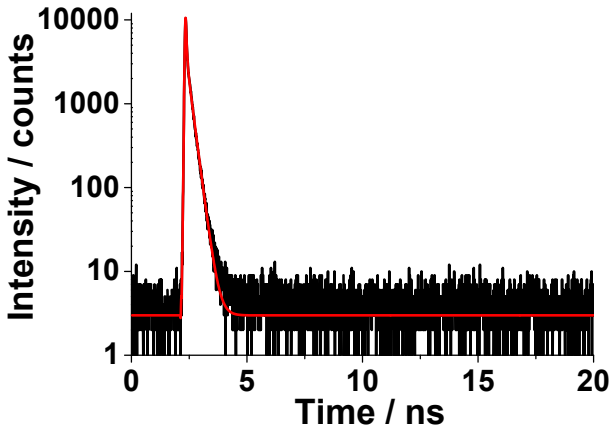


Figure S15. Time-resolved fluorescence decays of **CV16-R** (Ex/Em = 470 nm/530 nm) in CH_3CN at 25 °C. **CV16-R** bi-exponential decays gave lifetimes of 0.034 ns (81%) and 0.205 ns (19%). Average time is 0.067 ns.

(b) Time-resolved photoluminescence decay dynamics of CV*n* dyes in solid powder

Fluorescence lifetime decays for **CV6-O**, **CV8-Y**, **CV10-O** and **CV16-R** were measured using an inverted-type scanning confocal microscope (MicroTime-200, Picoquant, Germany) with a 20 × objective. A 470 nm single-mode pulsed diode laser (~100 ps pulse width) was used as an excitation source. A dichroic mirror (490 DCXR, AHF), a long-pass filter (HQ500lp, AHF), a 50 μm pinhole, and a single photon avalanche diode (PDM series, MPD) were used to collect emissions from the samples. Time-correlated single-photon counting technique was used to obtain fluorescence decay curves as a function of time with a resolution of 16 ps. Exponential fittings for the obtained fluorescence decays were performed by the iterative least-squares deconvolution fitting using the Symphotime software (version 5.3). Fluorescence lifetime decays for **CV4-R** was conducted using an inverted-type scanning confocal microscope (SP8 FALCON, Leica Microsystems, Germany) with a 40 × (air) objective lens. A 470 nm picosecond laser line (10 MHz, PicoQuant, Germany) was used as an excitation source. A hybrid photon detector was used to collect emissions at 630±20 and 650±30 nm from the samples. The confocal and PL lifetime images of 512×512 pixels were simultaneously recorded using a galvo-stage and time-correlated single-photon counting technique. Exponential fittings for the recorded PL decay profiles were performed using the suited Leica software (LAS X Ver.3.5.5).

Table S3. Fluorescence decays of **CV*n*** dyes in solid powder

Compounds	λ_{em} [nm]	τ_1 (f_1)[a] [ns]	τ_2 (f_2)[a] [ns]	τ_{avg}[b] [ns]
CV4-R	630	3.57 (0.35)	8.23 (0.65)	6.59
CV6-O	590	6.39 (0.50)	2.80 (0.50)	4.60
CV8-Y	580	2.29 (0.27)	1.33 (0.73)	1.59
CV10-O	590	2.52 (0.74)	0.53 (0.26)	2.00
CV16-R	670	5.45 (1.00)		5.45

[a]Lifetime (τ) and fraction (f) of shorter (1) or longer (2) lived species. [b]Average weighted lifetimes (τ_{avg}) calculated by $\langle\tau\rangle_{amp} = \{\Sigma (f_i*\tau_i)\}/\{\Sigma(f_i)\}$.

Table S4. Fluorescence decays of **CV*n*** dyes (powered solids) upon external stimuli (heat, pressure, vapor)

Compd	Treatment Conditions	λ_{em}^{max} [nm] (τ_{avg}[a] [ns])		
		A	**B**	**C**
CV4-R	Initial (**A**) → Annealing (**B**) → Fuming (**C**)	632 nm (6.59 ns)	640 nm (4.54 ns)	634 nm (7.53 ns)
	Initial (**A**) → Grinding (**B**) → Fuming(**C**)	632 nm (6.59 ns)	642 nm (4.31 ns)	629 nm (4.15 ns)
CV8-Y	Initial (**A**) → Annealing (**B**) → Fuming (**C**)	576 nm (1.59 ns)	654 nm (4.50 ns)	570 nm (1.18 ns)
	Initial (**A**) → Grinding (**B**) → Fuming (**C**)	576 nm (1.59 ns)	662 nm (3.92 ns)	566 nm (1.00 ns)
CV16-R	Initial (**A**) → Annealing (**B**) → Fuming (**C**)	671 nm (5.45 ns)	663 nm (4.80 ns)	671 nm (4.86 ns)
	Initial (**A**) → Grinding (**B**) → Fuming(**C**)	671 nm (5.45 ns)	595 nm (3.51 ns)	670 nm (4.61 ns)

[a]Average weighted lifetimes (τ_{avg}) calculated by $\langle\tau\rangle_{amp} = \{\Sigma (f_i*\tau_i)\}/\{\Sigma(f_i)\}$.

Table S5. Fluorescence quantum yields (Φ_{FL}) of **CV*n*** dyes (powered solids) upon external stimuli (heat, pressure, vapor)

Compd	Treatment Conditions	Φ_{FL}		
		A	**B**	**C**
CV4-R	Initial (**A**) → Annealing (**B**) → Fuming (**C**)	0.162±0.008	0.088±0.006	0.146±0.008
	Initial (**A**) → Grinding (**B**) → Fuming(**C**)	0.162±0.008	0.058±0.005	0.135±0.004
CV6-O	Initial (**A**) → Annealing (**B**) → Fuming (**C**)	0.175±0.003	0.049±0.006	0.124±0.003
	Initial (**A**) → Grinding (**B**) → Fuming(**C**)	0.175±0.003	0.065±0.002	0.212±0.007
CV8-Y	Initial (**A**) → Annealing (**B**) → Fuming (**C**)	0.402±0.012	0.062±0.003	0.324±0.009
	Initial (**A**) → Grinding (**B**) → Fuming (**C**)	0.402±0.012	0.067±0.003	0.302±0.005
CV10-O	Initial (**A**) → Annealing (**B**) → Fuming (**C**)	0.198±0.014	0.051±0.003	0.151±0.006
	Initial (**A**) → Grinding (**B**) → Fuming(**C**)	0.198±0.014	0.063±0.003	0.233±0.012
CV16-R	Initial (**A**) → Annealing (**B**) → Fuming (**C**)	0.070±0.007	0.061±0.002	0.065±0.007
	Initial (**A**) → Grinding (**B**) → Fuming(**C**)	0.070±0.007	0.167±0.006	0.062±0.001

[a]Absolute fluorescence quantum yield in the solid state evaluated using an integrating sphere.

(c) Fluorescence decays of solid powder CV4-R upon external stimuli (heating-fuming process and grinding-fuming process)

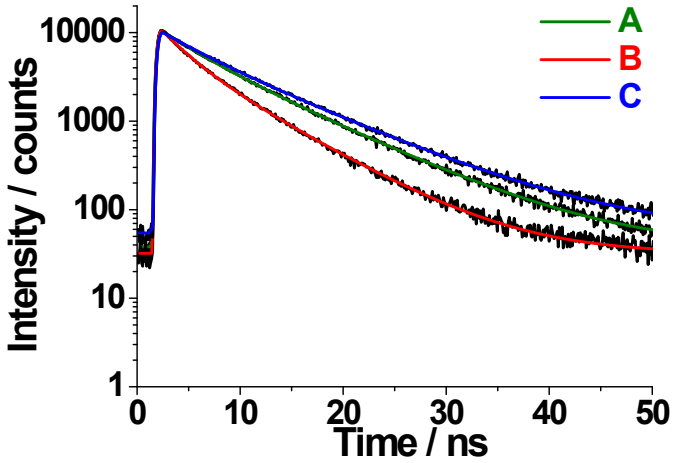


Figure S16. Time-resolved emission decays of solid powder **CV4-R** in different conditions. (A) Initial, as-prepared solid power, **CV4-R** bi-exponential decays gave lifetimes of 3.57 ns (35%) and 8.23 ns (65%). Average time is 6.59 ns. (B) Heating at 124 °C for 1 min and cooling to RT, **CV4-R** bi-exponential decays gave lifetimes of 2.52 ns (51%) and 6.61 ns (49%). Average time is 4.54 ns. (C) Subsequent fuming with CH_2Cl_2 vapor at RT, **CV4-R** bi-exponential decays gave lifetimes of 4.31 ns (33%) and 9.13 ns (49%). Average time is 7.53 ns.

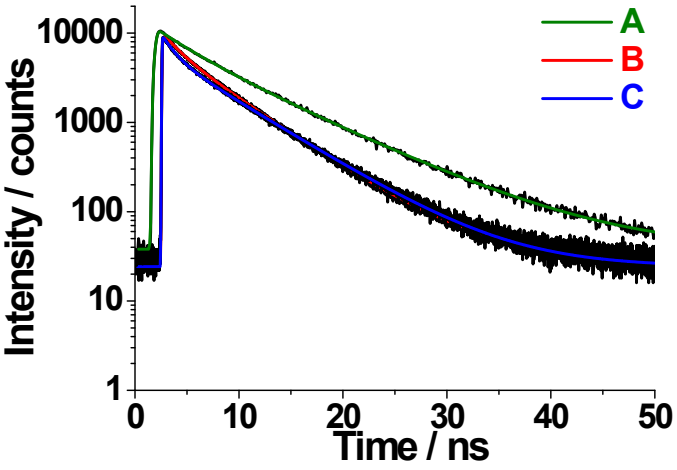


Figure S17. Time-resolved emission decays of solid powder **CV4-R** in different conditions. (A) Initial, as-prepared solid power, **CV4-R** bi-exponential decays gave lifetimes of 3.57 ns (35%) and 8.23 ns (65%). Average time is 6.59 ns. (B) Grinding at RT, **CV4-R** bi-exponential decays gave lifetimes of 5.56 ns (68%) and 1.66 ns (32%). Average time is 4.31 ns. (C) Subsequent fuming with CH_2Cl_2 vapor at RT, **CV4-R** bi-exponential decays gave lifetimes of 6.06 ns (60%) and 1.24 ns (40%). Average time is 4.15 ns.

(d) Fluorescence decays of solid powder CV8-Y upon external stimuli (heating-fuming process and grinding-fuming process)

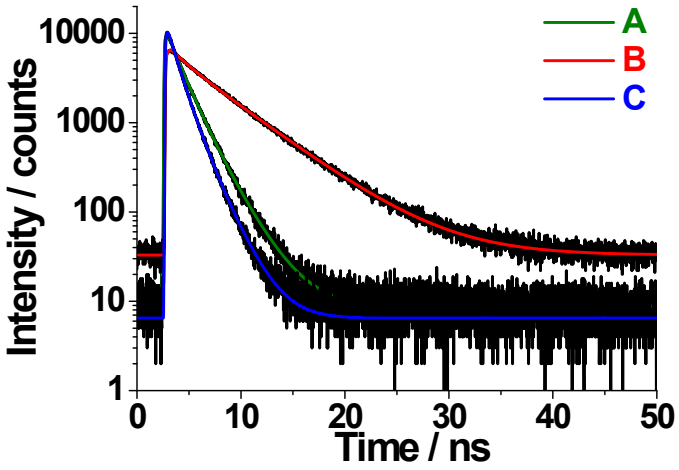


Figure S18. Time-resolved emission decays of solid powder **CV8-Y** in different conditions. (A) Initial, as-prepared solid power, **CV8-Y** bi-exponential decays gave lifetimes of 2.29 ns (27%) and 1.33 ns (73%). Average lifetime of 1.59 ns. (B) Heating at 98 °C for 1 min and cooling to RT, **CV8-Y** bi-exponential decays gave lifetimes of 5.12 ns (82%) and 1.62 ns (18%). Average lifetime of 4.50 ns. (C) Subsequent fuming with CH_2Cl_2 vapor at RT, **CV8-Y** bi-exponential decays gave lifetimes of 1.83 ns (22%) and 1.00 ns (78%). Average lifetime of 1.18 ns.

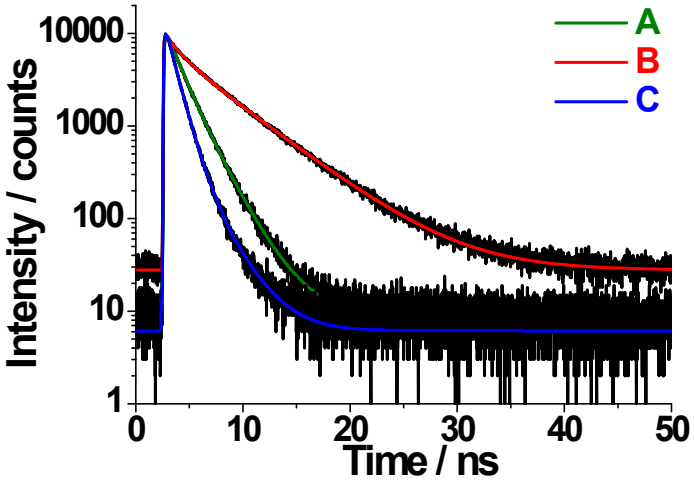


Figure S19. Time-resolved emission decays of solid powder **CV8-Y** in different conditions. (A) Initial, as-prepared solid power, **CV8-Y** bi-exponential decays gave lifetimes of 2.29 ns (27%) and 1.33 ns (73%). Average lifetime of 1.59 ns. (B) Grinding at RT, **CV8-Y** bi-exponential decays gave lifetimes of 5.01 ns (69%) and 1.47 ns (31%). Average lifetime of 3.92 ns. (C) Subsequent fuming with CH_2Cl_2 vapor at RT, **CV8-Y** bi-exponential decays gave lifetimes of 2.29 ns (6%) and 0.91 ns (97%). Average lifetime of 1.00 ns.

(e) Fluorescence decays of solid powder CV16-R upon external stimuli (heating-fuming process and grinding-fuming process)

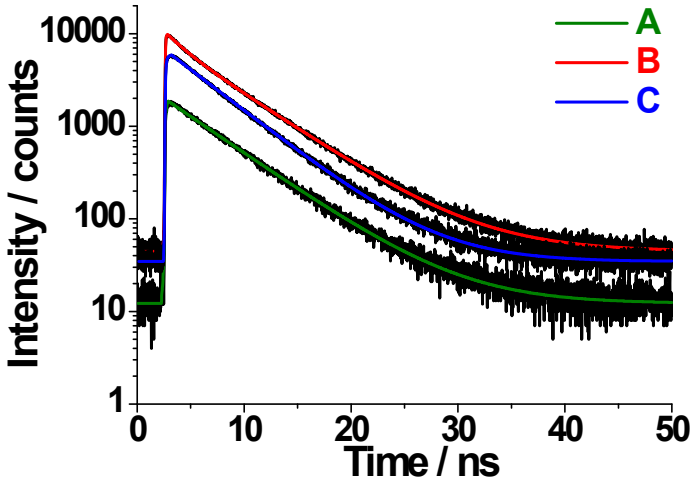


Figure S20. Time-resolved emission decays of solid powder **CV16-R** in different conditions. (A) Initial, as-prepared solid power, **CV16-R** mono-exponential decays gave lifetime of 5.45 ns (100%). (B) Heating at 92 °C for 1 min and cooling to RT, **CV16-R** bi-exponential decays gave lifetimes of 5.66 ns (78%) and 1.72 ns (22%). Average lifetime of 4.80 ns. (C) Subsequent fuming with CH_2Cl_2 vapor at RT, **CV16-R** mono-exponential decays gave lifetime of 4.86 ns (100%).

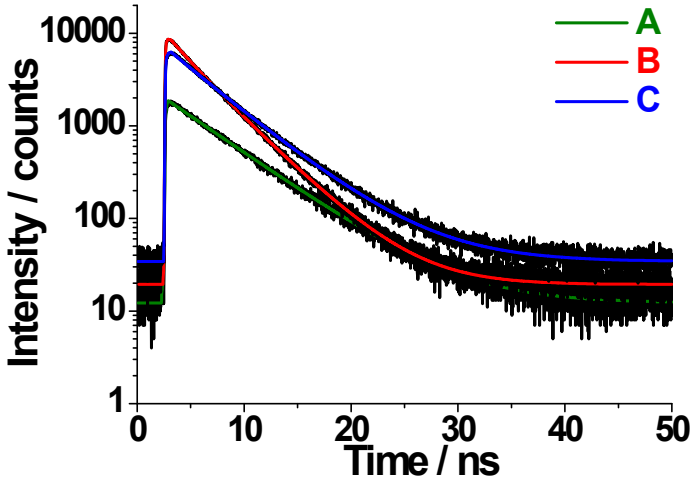


Figure S21. Time-resolved emission decays of solid powder **CV16-R** in different conditions. (A) Initial, as-prepared solid power, **CV16-R** mono-exponential decays gave lifetime of 5.45 ns (100%). (B) Grinding at RT, **CV16-R** bi-exponential decays gave lifetimes of 4.05 ns (67%) and 2.39 ns (33%). Average lifetime of 3.51 ns. (C) Subsequent fuming with CH_2Cl_2 vapor at RT, **CV16-R** bi-exponential decays gave lifetimes of 5.47 ns (47%) and 3.86 ns (53%). Average lifetime of 4.61 ns.

(f) Fluorescence decays of solid powder CV6-O

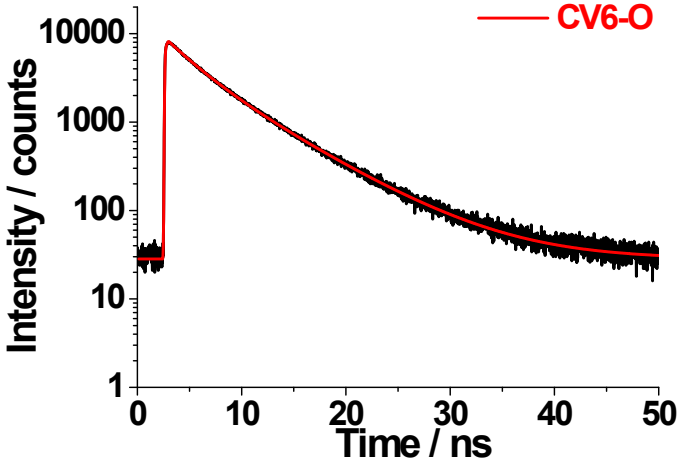


Figure S22. Time-resolved emission decays of as-prepared solid power **CV6-O**. **CV6-O** bi-exponential decays gave lifetimes of 6.39 ns (50%) and 2.80 ns (50%). Average lifetime of 4.60 ns.

(g) Fluorescence decays of solid powder CV10-O

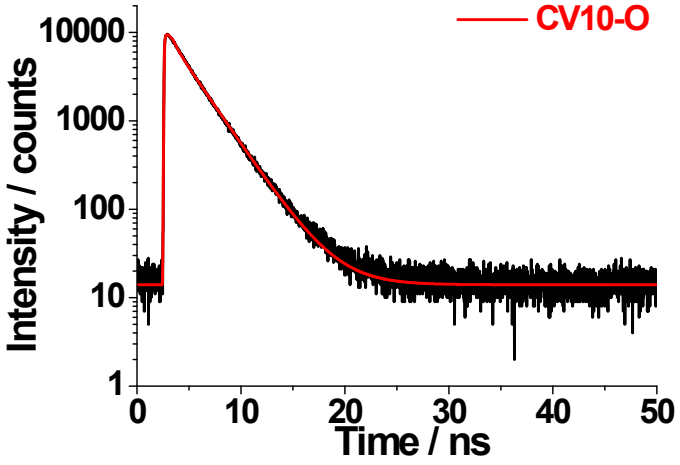


Figure S23. Time-resolved emission decays of as-prepared solid power **CV10-O**. **CV10-O** bi-exponential decays gave lifetimes of 2.52 ns (74%) and 0.53 ns (26%). Average lifetime of 2.00 ns.

6. Thermochromic and Mechanochromic Effects

(a) Mechanochromic effect of solid powder CV4-R

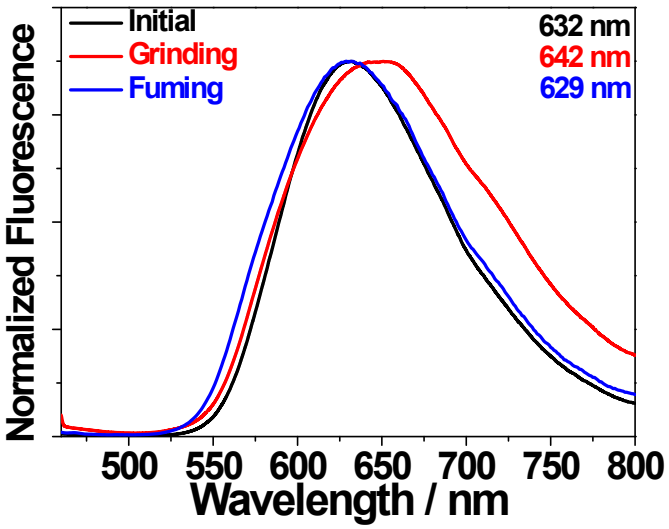


Figure S24. Normalized fluorescence emission spectra of **CV4-R** (black) as-prepared solid powder, (red) ground with spatula, and (blue) the same sample subsequently fumed with CH_2Cl_2 for 20 min. Excited at 440 nm.

(b) Thermochromic and mechanochromic effect of solid powder CV6-O

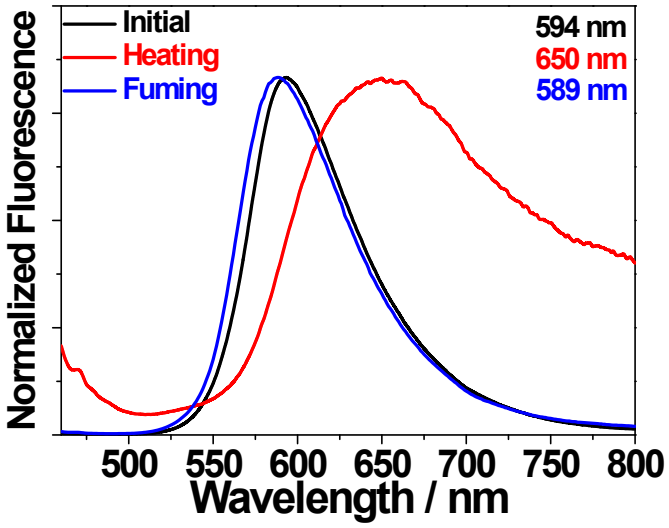


Figure S25. Normalized fluorescence emission spectra of **CV6-O** (black) as-prepared solid powder, (red) heated at 122 °C for 1 min and followed by cooling to RT, and (blue) the same sample subsequently fumed with CH_2Cl_2 for 20 min. Excited at 440 nm.

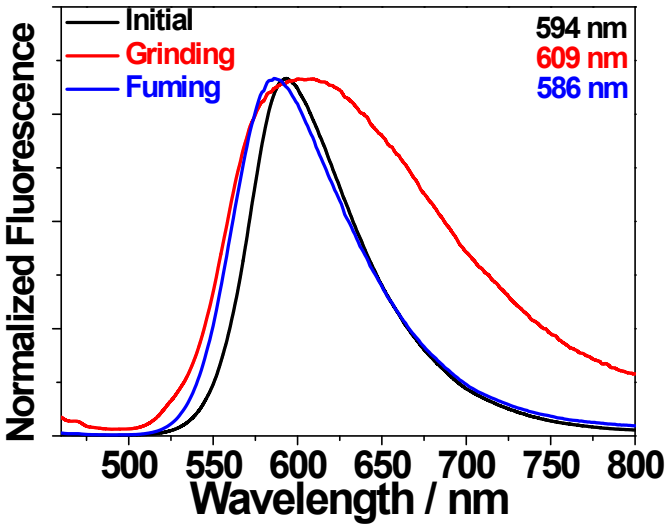


Figure S26. Normalized fluorescence emission spectra of **CV6-O** (black) as-prepared solid powder, (red) ground with spatula, and (blue) the same sample subsequently fumed with CH_2Cl_2 for 20 min. Excited at 440 nm.

(c) Thermochromic and mechanochromic effect of solid powder CV10-O

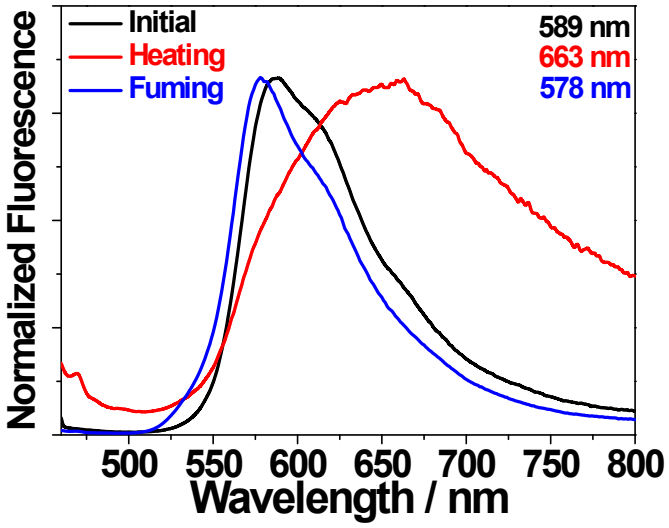


Figure S27. Normalized fluorescence emission spectra of **CV10-O** (a) as-prepared powder (black solid-line), (b) heated at 112 °C for 1 min and followed by cooling to RT (red solid-line), and (c) the same sample subsequently fumed with CH_2Cl_2 for 20 min (red dotted-line). Excited at 440 nm.

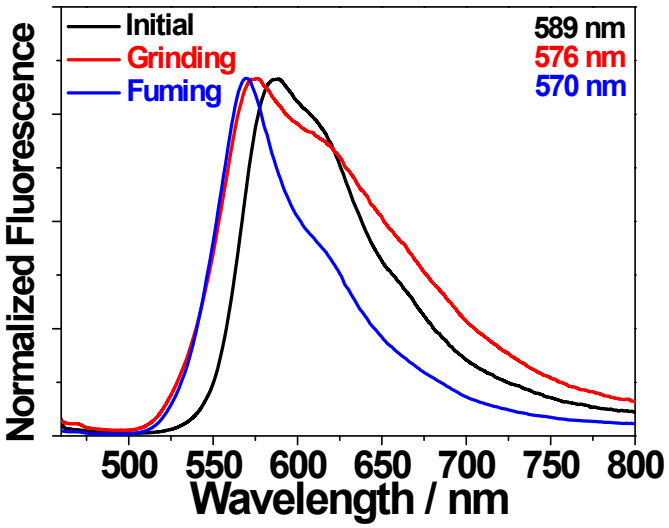


Figure S28. Normalized fluorescence emission spectra of **CV10-O** (a) as-prepared powder (black solid-line), (b) ground with spatula (blue solid-line), and (c) the same sample subsequently fumed with CH_2Cl_2 for 20 min (blue dotted-line). Excited at 440 nm.

(d) Thermochromic and mechanochromic effect of solid powder CV16-R

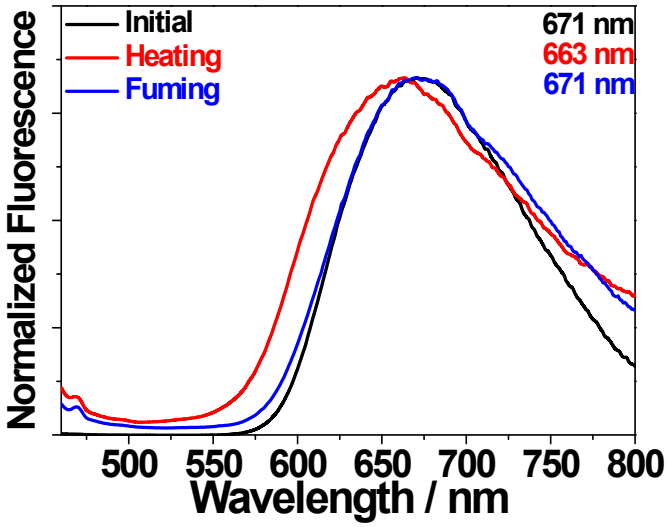


Figure S29. Normalized fluorescence emission spectra of **CV16-R** (a) as-prepared powder (black solid-line), (b) heated at 92 °C for 1 min and followed by cooling to RT (red solid-line), and (c) the same sample subsequently fumed with CH_2Cl_2 for 20 min (red dotted-line). Excited at 440 nm.

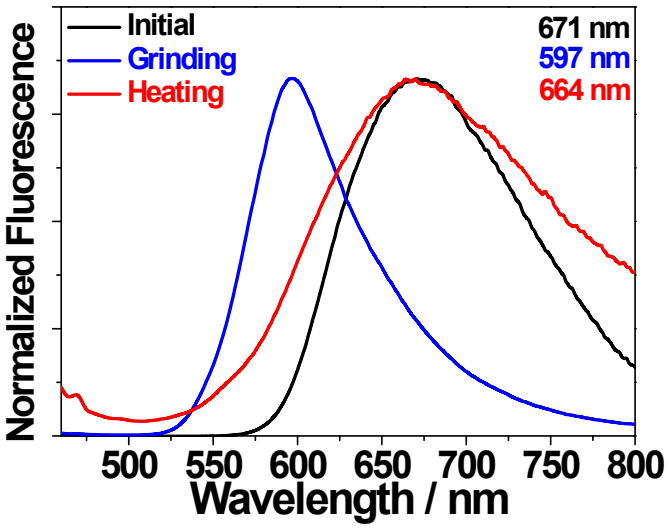


Figure S30. Normalized fluorescence emission spectra of **CV16-R** (a) as-prepared powder (black), (b) ground with spatula (blue), (c) the same sample subsequently heated at 92 °C for 1 min and followed by cooling to RT (red). Excited at 440 nm.

(e) Emission spectrum of red-emitting CV6-R single crystal

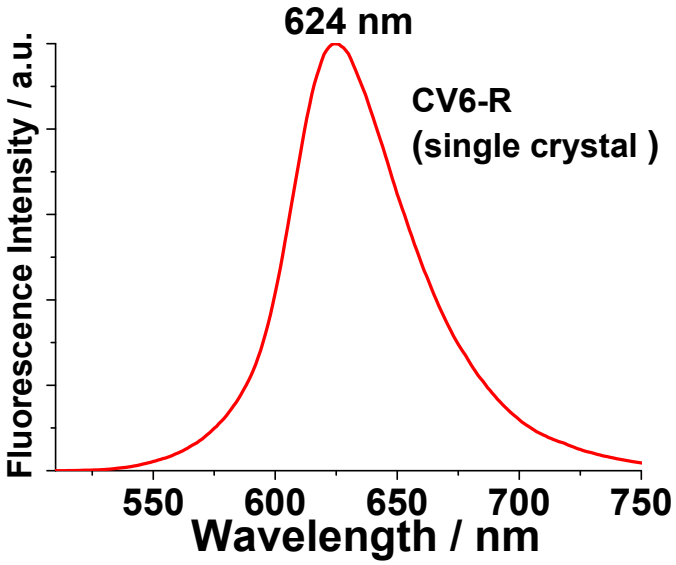


Figure S31. Fluorescence emission spectra of red-emitting **CV6-R** single crystal. Excited at 440 nm.

7. Differential Scanning Calorimetry (DSC) Measurements

(a) DSC analysis of CV4-R and CV8-Y solid powders

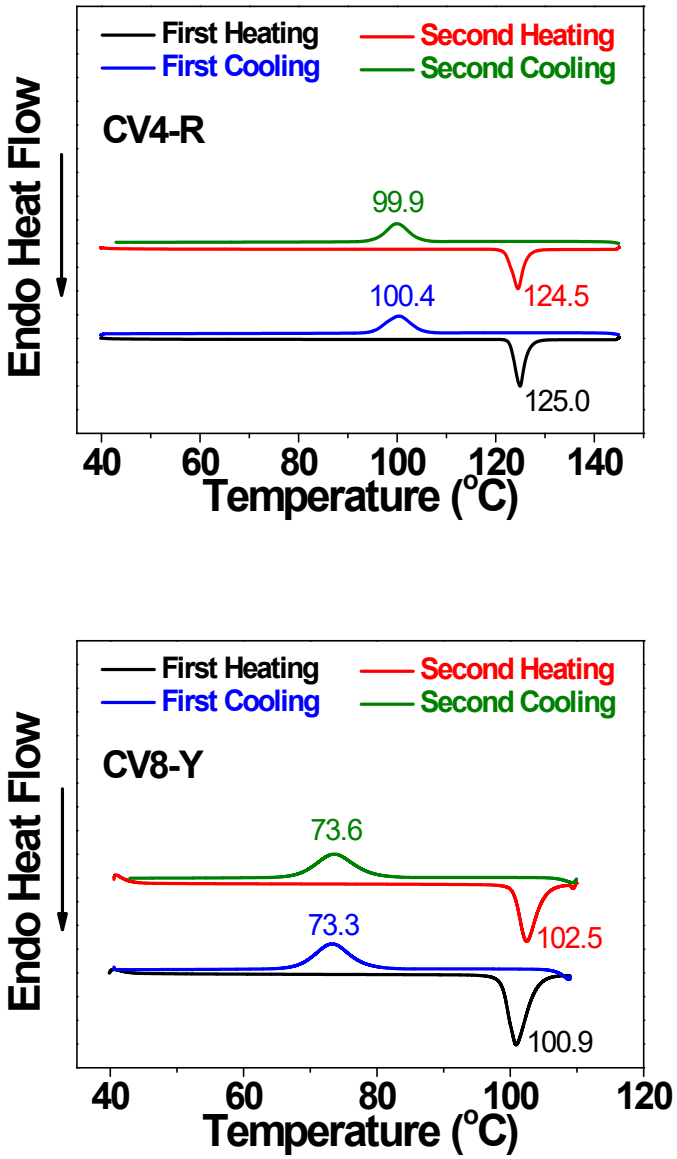


Figure S32. Differential scanning calorimetry curves of **CV4-R** (top) and **CV8-Y** (bottom) under the heating rate of 10 °C/min: 1st heating–cooling cycle (black and blue, respectively) and 2nd heating–cooling cycle (red and green, respectively) of as-prepared solid powders **CV4-R** (top) and **CV8-Y** (bottom).

(b) DSC analysis of solid powder CV8-Y in different states

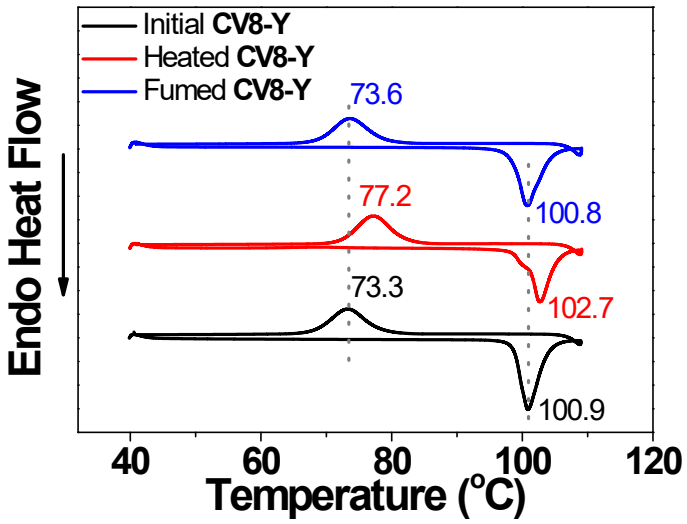


Figure S33. DSC thermograms of solid powder **CV8-Y** under the heating rate of 10 °C/min: As-prepared solid powder (black), heating at 98 °C for 1 min and cooling to RT (red), and the same sample subsequently fumed with CH_2Cl_2 at RT for 20 min (blue).

8. Powder X-ray Diffraction (PXRD) Analysis

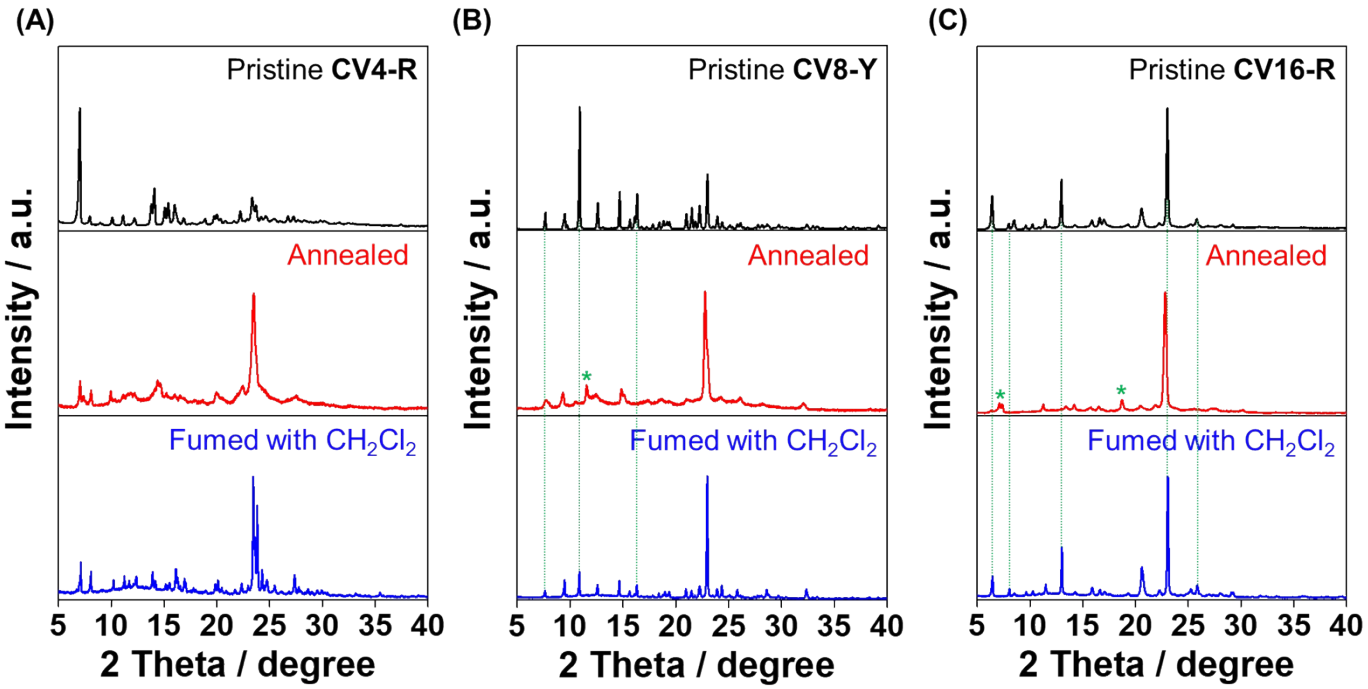


Figure S34. Powder X-ray diffraction patterns of **CV4-R** (A), **CV8-Y** (B) and **CV16-R** (C) in different states. As-prepared solid powder (black), after heating at melting temperature for 1 min and cooling to RT (red), and the same sample subsequently exposed to CH_2Cl_2 for 20 min (blue). Green dot line indicates changes in diffraction peaks. Green * indicates new peaks appeared.

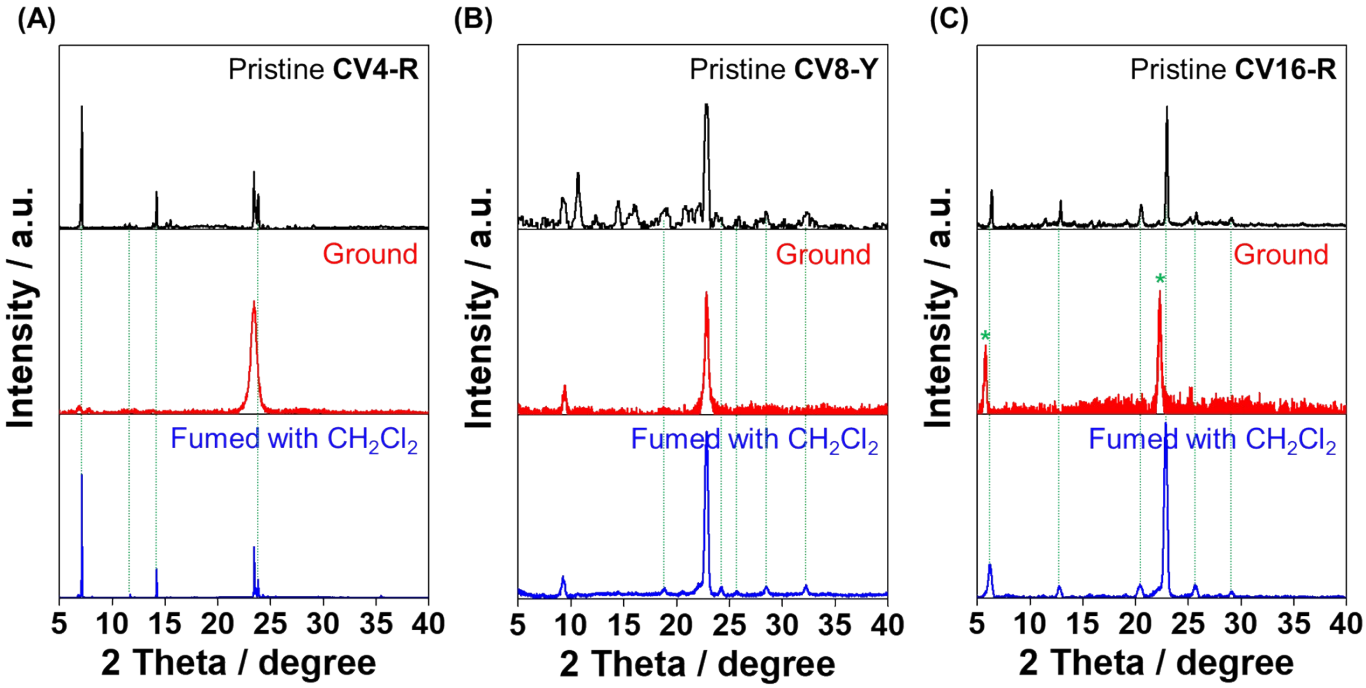


Figure S35. Powder X-ray diffraction patterns of **CV4-R** (A), **CV8-Y** (B) and **CV16-R** (C) in different states. As-prepared solid powder (black), after grinding with a spatula (red), and the same sample subsequently exposed to CH_2Cl_2 for 20 min (blue). Green dot line indicates changes in diffraction peaks. Green * indicates new peaks appeared.

9. X-ray Crystallographic Data for CV*n* Dyes

Single crystals suitable for X-ray structure analysis were obtained by slow evaporation from 1,2-dichloroethane/hexane mixture solution for **CV4-R** and **CV8-Y**, dichloroethane/cyclohexane/ether mixture solution for **CV6-R**, and dichloromethane/methanol mixture solution for **CV10-O** and **CV16-R**.

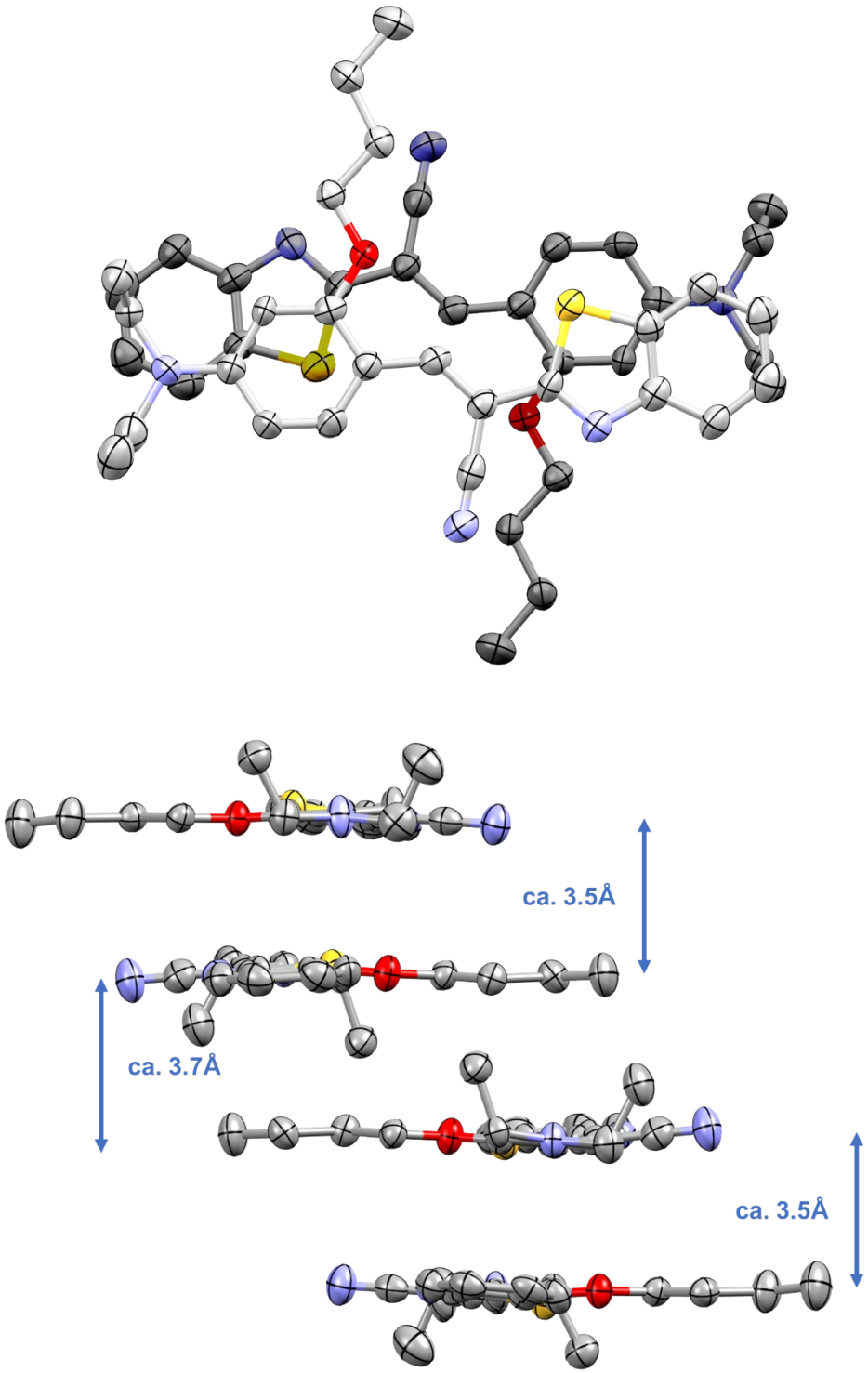


Figure S36. π-Stacking observed in the X-ray crystal structure of **CV4-R** (top view: (top); side view (bottom)) drawn with thermal ellipsoids set at 50% probability and with hydrogen atoms omitted for clarity.

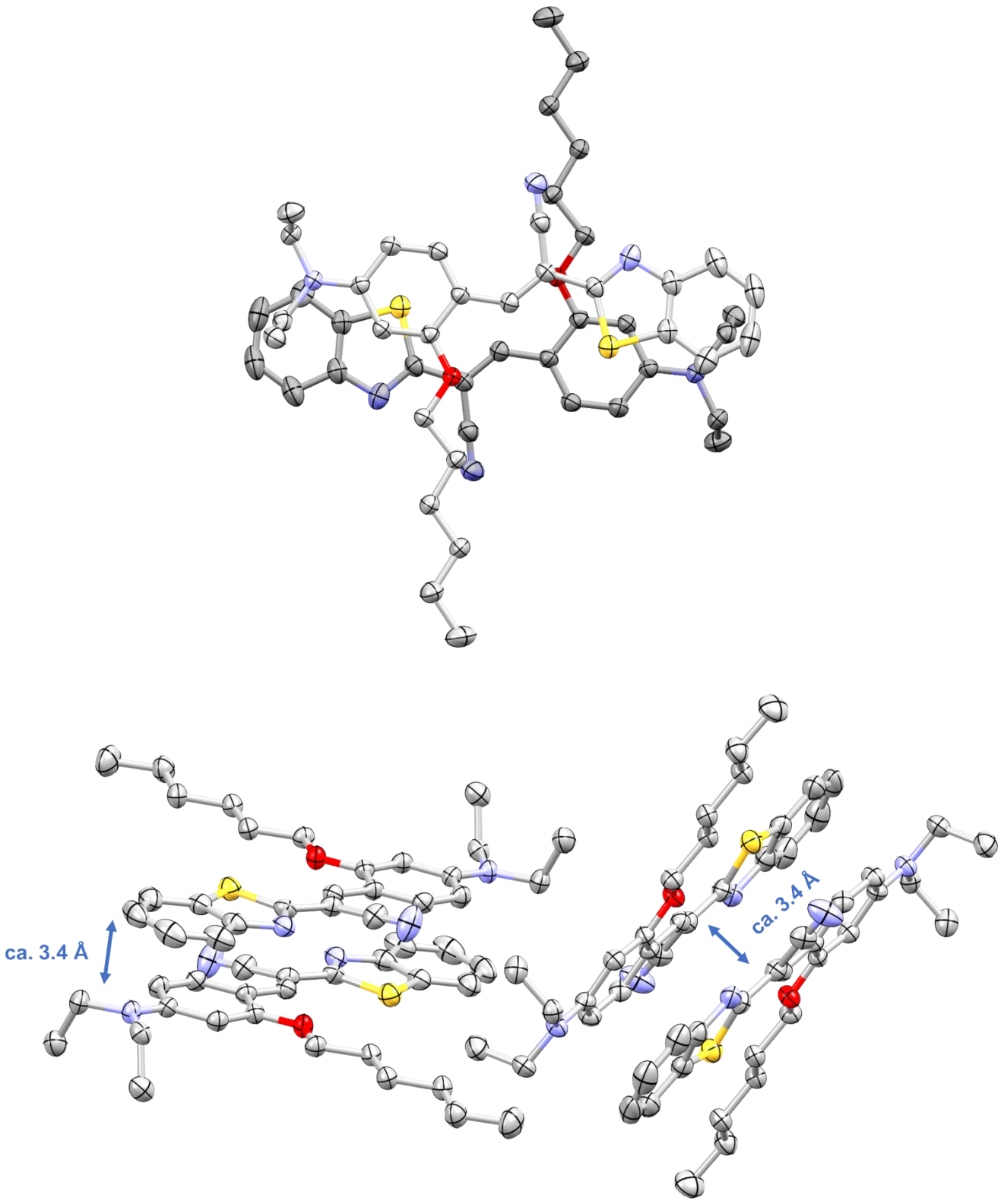


Figure S37. π-Stacking observed in the X-ray crystal structure of **CV6-R** (top view: (top); side view (bottom)) drawn with thermal ellipsoids set at 50% probability and with hydrogen atoms omitted for clarity.

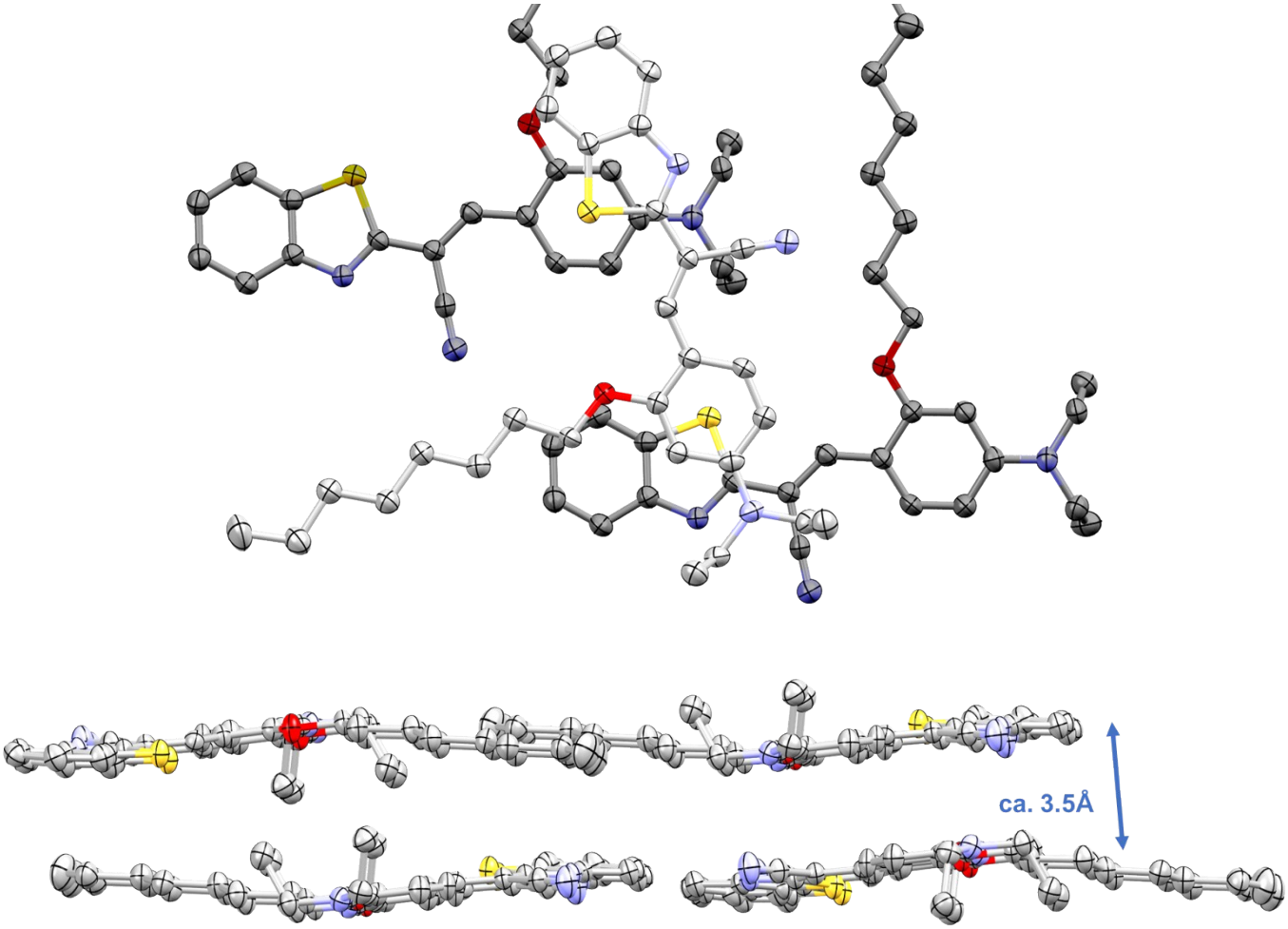


Figure S38. π-Stacking observed in the X-ray crystal structure of **CV8-Y** (top view: (top); side view (bottom)) drawn with thermal ellipsoids set at 50% probability. The alkoxy side chains were truncated and hydrogen atoms were omitted for clarity.

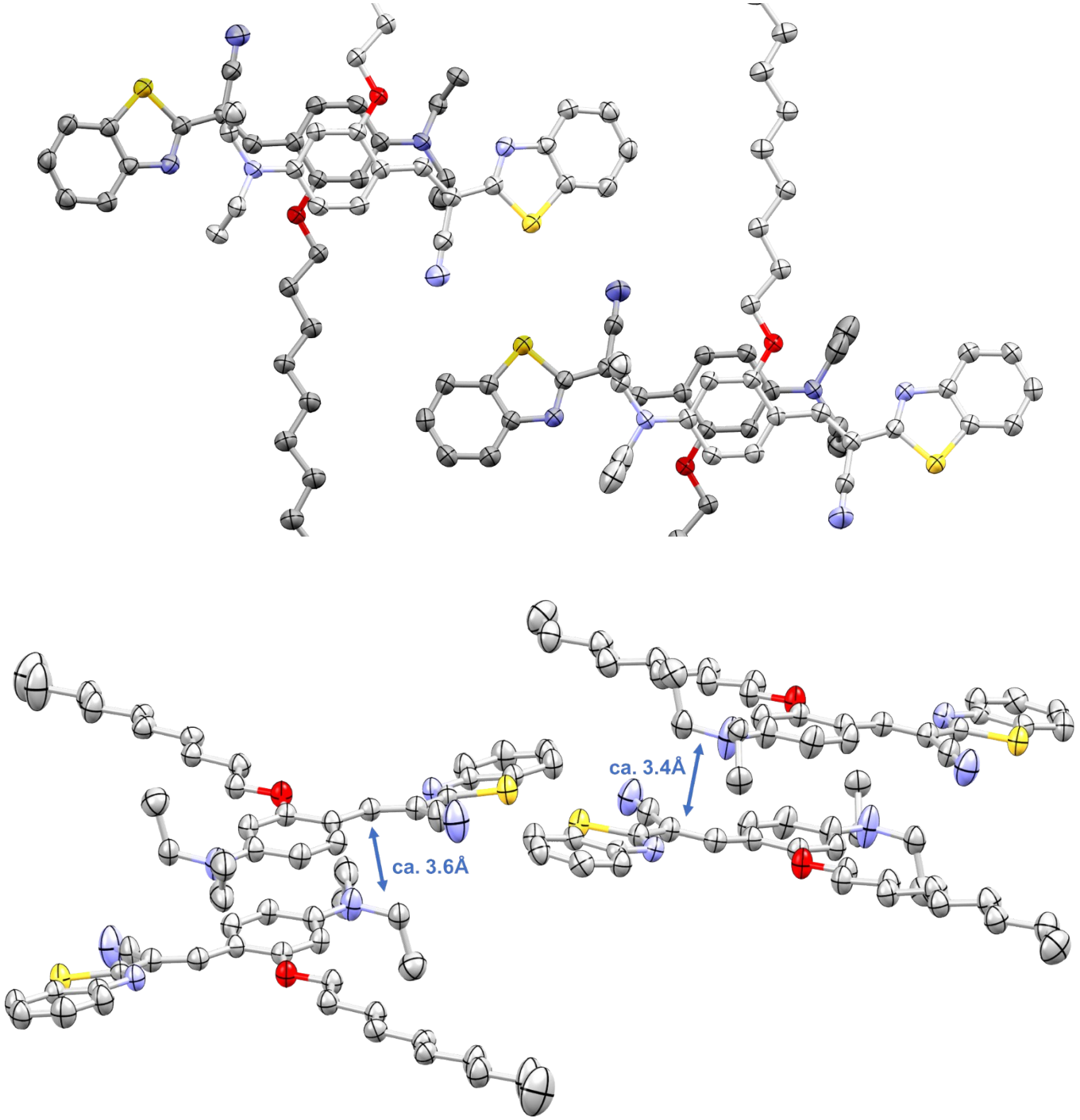


Figure S39. π-Stacking observed in the X-ray crystal structure of **CV10-O** (top view: (top); side view (bottom)) drawn with thermal ellipsoids set at 50% probability. The alkoxy side chains were truncated and hydrogen atoms were omitted for clarity.

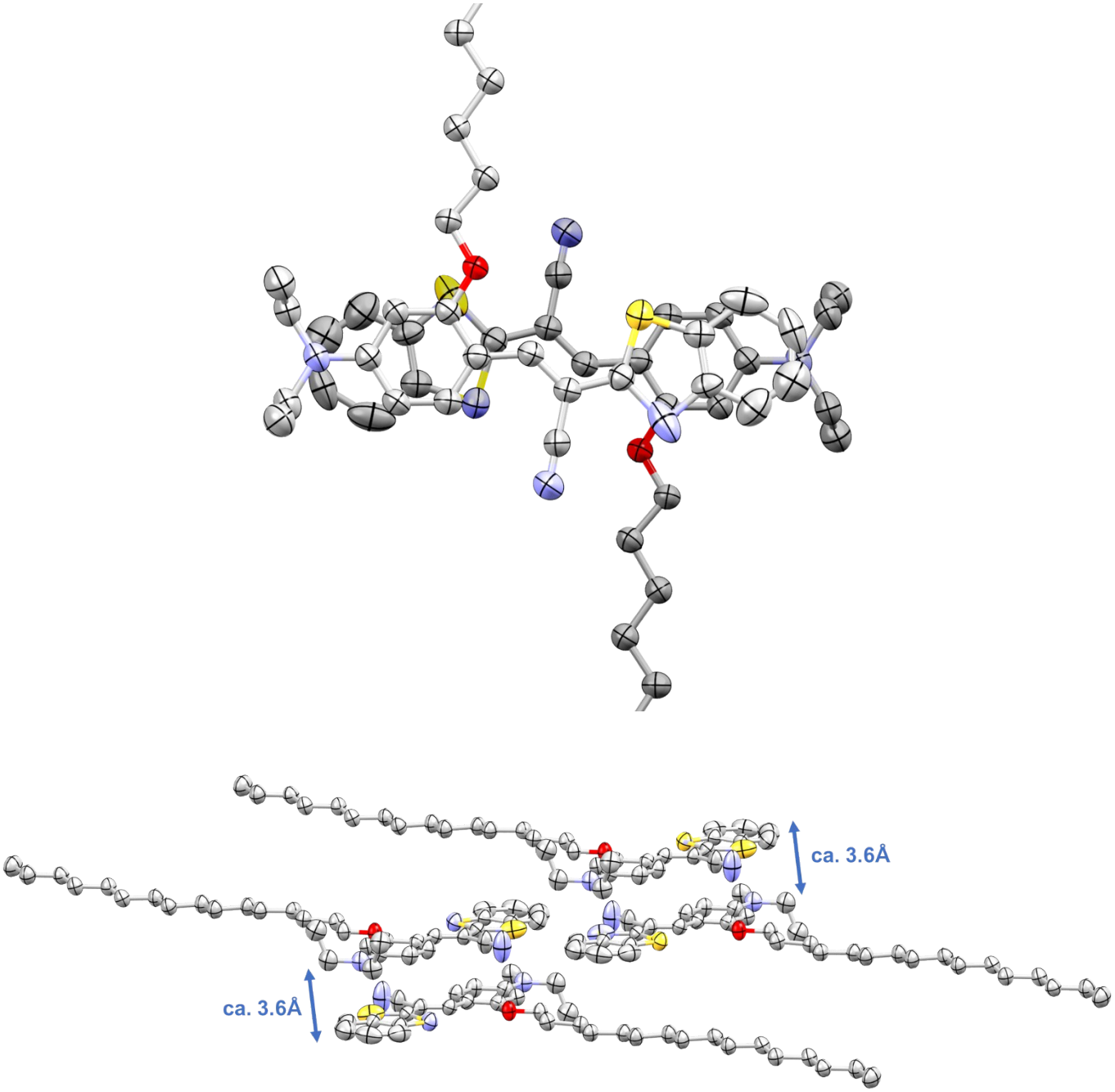


Figure S40. π-Stacking observed in the X-ray crystal structure of **CV16-R** (top view: (top); side view (bottom)) drawn with thermal ellipsoids set at 50% probability. The alkoxy side chains were truncated and hydrogen atoms were omitted for clarity.

Table S6. Crystal data and structure refinement for **CV4-R**.

Identification code	**CV4-R**
Empirical formula	$C_{96}\ H_{108}\ N_{12}\ O_4\ S_4$
Formula weight	1622.18
Temperature	186(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.6543(8) Å b = 15.9640(12) Å c = 25.0748(18) Å
Volume	4347.9(5) $Å^3$
Z	2
Density (calculated)	1.239 Mg/m^3
Absorption coefficient	0.169 mm^{-1}
F(000)	1728
Crystal size	0.24 x 0.12 x 0.10 mm^3
Theta range for data collection	0.82 to 26.03°.
Index ranges	-11<=h<=14, -19<=k<=19, -23<=l<=30
Reflections collected	27138
Independent reflections	16980 [R(int) = 0.0444]
Completeness to theta = 26.03°	99.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16980 / 0 / 1057
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0797, wR2 = 0.2099
R indices (all data)	R1 = 0.1585, wR2 = 0.2665
Largest diff. peak and hole	0.554 and -0.448 $e.Å^{-3}$

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **CV4-R**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2911(4)	1163(3)	9821(2)	41(1)
C(2)	2049(4)	1085(3)	9505(2)	45(1)
C(3)	802(5)	1353(3)	9695(2)	49(1)
C(4)	473(5)	1667(4)	10233(2)	51(1)
C(5)	1349(5)	1700(3)	10554(2)	51(1)
C(6)	2597(5)	1451(3)	10365(2)	46(1)
C(7)	3548(5)	1526(3)	10666(2)	43(1)
C(8)	3568(5)	1661(3)	11203(2)	46(1)
N(1)	4750(4)	1780(3)	11941(2)	46(1)
S(1)	5840(1)	1860(1)	10994(1)	64(1)
C(9)	4634(5)	1750(3)	11422(2)	45(1)
C(10)	5865(5)	1876(3)	12012(2)	47(1)
C(11)	6591(5)	1924(4)	11542(2)	52(1)
C(12)	7739(5)	2000(4)	11566(2)	68(2)
C(13)	8140(5)	2035(4)	12067(2)	63(2)
C(14)	7420(5)	2001(4)	12527(2)	58(2)
C(15)	6290(5)	1920(3)	12510(2)	58(1)
O(1)	4116(3)	957(2)	9638(1)	49(1)
C(16)	4469(4)	836(3)	9072(2)	44(1)
C(17)	5734(4)	873(3)	8971(2)	46(1)
C(18)	6147(4)	810(4)	8375(2)	54(1)
C(19)	7402(5)	846(5)	8247(3)	96(2)
N(2)	-55(4)	1313(3)	9379(2)	67(1)
C(20)	-1376(5)	1587(4)	9570(2)	59(2)
C(21)	-1701(5)	868(4)	9857(2)	69(2)
C(22)	282(7)	1172(6)	8657(5)	160(6)

C(23)	570(8)	350(8)	8769(4)	155(5)
C(24)	2577(5)	1676(4)	11593(2)	56(1)
N(3)	1769(5)	1682(4)	11895(2)	76(2)
C(25)	6991(4)	1084(3)	5946(2)	43(1)
C(26)	7893(4)	1048(3)	6277(2)	41(1)
C(27)	8988(4)	1160(3)	6068(2)	48(1)
C(28)	9150(5)	1263(4)	5513(2)	59(2)
C(29)	8267(5)	1283(4)	5193(2)	53(1)
C(30)	7131(4)	1213(3)	5386(2)	42(1)
C(31)	6145(4)	1256(3)	5075(2)	43(1)
C(32)	5968(4)	1431(3)	4551(2)	42(1)
C(33)	4861(4)	1404(3)	4323(2)	42(1)
N(4)	4627(4)	1619(3)	3831(2)	44(1)
S(2)	3786(1)	1086(1)	4718(1)	51(1)
C(34)	3496(5)	1544(3)	3742(2)	45(1)
C(35)	2893(4)	1272(3)	4188(2)	46(1)
C(36)	1758(5)	1195(4)	4157(2)	53(1)
C(37)	1212(5)	1393(4)	3690(2)	56(1)
C(38)	1812(5)	1641(3)	3250(2)	55(1)
C(39)	2961(5)	1720(3)	3263(2)	51(1)
O(2)	5900(3)	1001(2)	6134(1)	46(1)
C(40)	5700(4)	819(3)	6689(2)	43(1)
C(41)	4481(4)	698(3)	6778(2)	45(1)
C(42)	4190(5)	524(4)	7366(2)	64(2)
C(43)	2935(5)	486(5)	7493(3)	85(2)
N(5)	9851(4)	1172(3)	6402(2)	59(1)
C(44)	10962(5)	1395(4)	6194(2)	69(2)
C(45)	11950(6)	605(5)	5975(2)	84(2)

C(46)	9706(5)	1008(4)	6971(2)	50(1)
C(47)	10003(5)	48(4)	7106(2)	58(1)
C(48)	6825(5)	1667(3)	4181(2)	48(1)
N(6)	7518(4)	1854(3)	3896(2)	64(1)
C(49)	6870(4)	6424(3)	5190(2)	44(1)
C(50)	7777(4)	6367(3)	5512(2)	40(1)
C(51)	8846(4)	6544(3)	5315(2)	45(1)
C(52)	8927(5)	6774(4)	4773(2)	50(1)
C(53)	8028(5)	6820(3)	4456(2)	50(1)
C(54)	6958(4)	6643(3)	4638(2)	44(1)
C(55)	5988(4)	6669(3)	4328(2)	44(1)
C(56)	5857(4)	6756(3)	3789(2)	44(1)
C(57)	4752(4)	6734(3)	3567(2)	41(1)
N(7)	4601(3)	6808(3)	3038(2)	47(1)
S(3)	3559(1)	6588(1)	3988(1)	54(1)
C(58)	3462(5)	6736(3)	2970(2)	46(1)
C(59)	2776(5)	6614(3)	3437(2)	45(1)
C(60)	1622(5)	6534(3)	3416(2)	54(1)
C(61)	1180(5)	6575(4)	2922(2)	63(2)
C(62)	1864(6)	6700(4)	2462(2)	62(2)
C(63)	2999(5)	6777(4)	2477(2)	55(1)
O(3)	5839(3)	6243(2)	5362(1)	50(1)
C(64)	5655(4)	6038(3)	5912(2)	45(1)
C(65)	4459(4)	5875(3)	5998(2)	44(1)
C(66)	4163(4)	5724(4)	6585(2)	48(1)
C(67)	2928(5)	5627(4)	6706(2)	72(2)
N(8)	9747(4)	6494(3)	5641(2)	47(1)
C(68)	10845(5)	6697(4)	5442(2)	57(1)

C(69)	11826(5)	5904(4)	5159(2)	74(2)
C(70)	9672(4)	6204(3)	6190(2)	41(1)
C(71)	10067(5)	5201(4)	6242(2)	60(2)
C(72)	6806(5)	6831(4)	3404(2)	53(1)
N(9)	7565(4)	6896(4)	3104(2)	70(1)
C(73)	3244(4)	5750(3)	9052(2)	39(1)
C(74)	2440(4)	5568(3)	8740(2)	41(1)
C(75)	1314(4)	5530(3)	8971(2)	43(1)
C(76)	1035(4)	5702(3)	9526(2)	47(1)
C(77)	1828(4)	5894(3)	9831(2)	44(1)
C(78)	2968(4)	5928(3)	9611(2)	41(1)
C(79)	3856(4)	6109(3)	9908(2)	40(1)
C(80)	3871(4)	6287(3)	10441(2)	40(1)
C(81)	4886(4)	6473(3)	10645(2)	38(1)
N(10)	4952(4)	6604(3)	11158(2)	46(1)
S(4)	6102(1)	6542(1)	10205(1)	50(1)
C(82)	6044(5)	6748(3)	11226(2)	45(1)
C(83)	6788(4)	6725(3)	10755(2)	45(1)
C(84)	7930(5)	6835(3)	10760(2)	52(1)
C(85)	8288(5)	6974(3)	11258(2)	57(1)
C(86)	7534(5)	6996(3)	11723(2)	58(2)
C(87)	6408(5)	6891(3)	11717(2)	53(1)
O(4)	4360(3)	5761(2)	8846(1)	46(1)
C(88)	4696(4)	5636(3)	8279(2)	43(1)
C(89)	5923(4)	5752(3)	8166(2)	42(1)
C(90)	6284(4)	5768(3)	7571(2)	46(1)
C(91)	7495(5)	5909(4)	7453(2)	65(2)
N(11)	538(4)	5318(3)	8662(2)	48(1)

C(92)	-568(4)	5183(3)	8902(2)	51(1)
C(93)	-1679(5)	6042(4)	8992(2)	64(2)
C(94)	762(5)	5237(4)	8077(2)	53(1)
C(95)	433(5)	6121(4)	7811(2)	67(2)
C(96)	2886(5)	6305(3)	10835(2)	47(1)
N(12)	2082(4)	6338(3)	11148(2)	63(1)

Table S8. Bond lengths [Å] and angles [°] for **CV4-R**.

C(1)-O(1)	1.359(5)
C(1)-C(2)	1.374(6)
C(1)-C(6)	1.414(6)
C(2)-C(3)	1.400(6)
C(2)-H(2)	0.9500
C(3)-N(2)	1.350(6)
C(3)-C(4)	1.412(6)
C(4)-C(5)	1.372(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.403(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.436(6)
C(7)-C(8)	1.369(6)
C(7)-H(7)	0.9500
C(8)-C(24)	1.437(7)
C(8)-C(9)	1.456(6)
N(1)-C(9)	1.323(6)
N(1)-C(10)	1.389(6)
S(1)-C(11)	1.720(5)
S(1)-C(9)	1.746(5)
C(10)-C(15)	1.397(7)
C(10)-C(11)	1.403(7)
C(11)-C(12)	1.391(7)
C(12)-C(13)	1.389(7)
C(12)-H(12)	0.9500
C(13)-C(14)	1.374(7)
C(13)-H(13)	0.9500
C(14)-C(15)	1.372(7)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
O(1)-C(16)	1.435(5)
C(16)-C(17)	1.494(6)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900

C(17)-C(18)	1.521(6)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.489(7)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
N(2)-C(20)	1.478(6)
N(2)-C(22)	1.814(13)
C(20)-C(21)	1.492(7)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.271(11)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-N(3)	1.149(6)
C(25)-O(2)	1.366(5)
C(25)-C(26)	1.384(6)
C(25)-C(30)	1.421(6)
C(26)-C(27)	1.402(6)
C(26)-H(26)	0.9500
C(27)-N(5)	1.372(6)
C(27)-C(28)	1.404(7)
C(28)-C(29)	1.356(6)
C(28)-H(28)	0.9500
C(29)-C(30)	1.409(6)
C(29)-H(29)	0.9500
C(30)-C(31)	1.430(6)

C(31)-C(32)	1.362(6)
C(31)-H(31)	0.9500
C(32)-C(48)	1.445(7)
C(32)-C(33)	1.473(6)
C(33)-N(4)	1.306(6)
C(33)-S(2)	1.739(5)
N(4)-C(34)	1.402(6)
S(2)-C(35)	1.725(5)
C(34)-C(39)	1.387(6)
C(34)-C(35)	1.413(7)
C(35)-C(36)	1.380(6)
C(36)-C(37)	1.367(7)
C(36)-H(36)	0.9500
C(37)-C(38)	1.381(7)
C(37)-H(37)	0.9500
C(38)-C(39)	1.392(7)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
O(2)-C(40)	1.433(5)
C(40)-C(41)	1.496(6)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-C(42)	1.527(7)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-C(43)	1.490(7)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
N(5)-C(46)	1.454(6)
N(5)-C(44)	1.507(6)
C(44)-C(45)	1.446(8)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900

C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-C(47)	1.492(7)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-N(6)	1.145(6)
C(49)-O(3)	1.363(5)
C(49)-C(50)	1.367(6)
C(49)-C(54)	1.430(6)
C(50)-C(51)	1.417(6)
C(50)-H(50)	0.9500
C(51)-N(8)	1.370(6)
C(51)-C(52)	1.410(6)
C(52)-C(53)	1.355(6)
C(52)-H(52)	0.9500
C(53)-C(54)	1.408(6)
C(53)-H(53)	0.9500
C(54)-C(55)	1.420(6)
C(55)-C(56)	1.374(6)
C(55)-H(55)	0.9500
C(56)-C(72)	1.436(7)
C(56)-C(57)	1.462(6)
C(57)-N(7)	1.353(6)
C(57)-S(3)	1.747(5)
N(7)-C(58)	1.399(6)
S(3)-C(59)	1.719(5)
C(58)-C(63)	1.385(7)
C(58)-C(59)	1.407(6)
C(59)-C(60)	1.399(6)
C(60)-C(61)	1.378(7)
C(60)-H(60)	0.9500
C(61)-C(62)	1.394(7)

C(61)-H(61)	0.9500
C(62)-C(63)	1.376(7)
C(62)-H(62)	0.9500
C(63)-H(63)	0.9500
O(3)-C(64)	1.431(5)
C(64)-C(65)	1.501(6)
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900
C(65)-C(66)	1.518(6)
C(65)-H(65A)	0.9900
C(65)-H(65B)	0.9900
C(66)-C(67)	1.504(6)
C(66)-H(66A)	0.9900
C(66)-H(66B)	0.9900
C(67)-H(67A)	0.9800
C(67)-H(67B)	0.9800
C(67)-H(67C)	0.9800
N(8)-C(70)	1.453(6)
N(8)-C(68)	1.471(6)
C(68)-C(69)	1.502(7)
C(68)-H(68A)	0.9900
C(68)-H(68B)	0.9900
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-C(71)	1.512(7)
C(70)-H(70A)	0.9900
C(70)-H(70B)	0.9900
C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800
C(71)-H(71C)	0.9800
C(72)-N(9)	1.140(6)
C(73)-O(4)	1.360(5)
C(73)-C(74)	1.381(6)
C(73)-C(78)	1.417(6)
C(74)-C(75)	1.405(6)

C(74)-H(74)	0.9500
C(75)-N(11)	1.372(5)
C(75)-C(76)	1.406(6)
C(76)-C(77)	1.365(6)
C(76)-H(76)	0.9500
C(77)-C(78)	1.409(6)
C(77)-H(77)	0.9500
C(78)-C(79)	1.437(6)
C(79)-C(80)	1.371(6)
C(79)-H(79)	0.9500
C(80)-C(96)	1.434(6)
C(80)-C(81)	1.452(6)
C(81)-N(10)	1.318(5)
C(81)-S(4)	1.748(4)
N(10)-C(82)	1.395(6)
S(4)-C(83)	1.731(5)
C(82)-C(87)	1.385(6)
C(82)-C(83)	1.391(6)
C(83)-C(84)	1.404(6)
C(84)-C(85)	1.393(7)
C(84)-H(84)	0.9500
C(85)-C(86)	1.386(7)
C(85)-H(85)	0.9500
C(86)-C(87)	1.382(7)
C(86)-H(86)	0.9500
C(87)-H(87)	0.9500
O(4)-C(88)	1.435(5)
C(88)-C(89)	1.506(6)
C(88)-H(88A)	0.9900
C(88)-H(88B)	0.9900
C(89)-C(90)	1.513(6)
C(89)-H(89A)	0.9900
C(89)-H(89B)	0.9900
C(90)-C(91)	1.508(6)
C(90)-H(90A)	0.9900
C(90)-H(90B)	0.9900

C(91)-H(91A)	0.9800
C(91)-H(91B)	0.9800
C(91)-H(91C)	0.9800
N(11)-C(92)	1.455(5)
N(11)-C(94)	1.463(6)
C(92)-C(93)	1.521(7)
C(92)-H(92A)	0.9900
C(92)-H(92B)	0.9900
C(93)-H(93A)	0.9800
C(93)-H(93B)	0.9800
C(93)-H(93C)	0.9800
C(94)-C(95)	1.497(7)
C(94)-H(94A)	0.9900
C(94)-H(94B)	0.9900
C(95)-H(95A)	0.9800
C(95)-H(95B)	0.9800
C(95)-H(95C)	0.9800
C(96)-N(12)	1.151(6)

O(1)-C(1)-C(2)	122.7(4)
O(1)-C(1)-C(6)	115.6(4)
C(2)-C(1)-C(6)	121.7(4)
C(1)-C(2)-C(3)	121.4(4)
C(1)-C(2)-H(2)	119.3
C(3)-C(2)-H(2)	119.3
N(2)-C(3)-C(2)	121.7(4)
N(2)-C(3)-C(4)	121.0(5)
C(2)-C(3)-C(4)	117.3(4)
C(5)-C(4)-C(3)	120.9(5)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	122.3(5)
C(4)-C(5)-H(5)	118.8
C(6)-C(5)-H(5)	118.8
C(5)-C(6)-C(1)	116.3(4)
C(5)-C(6)-C(7)	125.4(4)

C(1)-C(6)-C(7)	118.2(4)
C(8)-C(7)-C(6)	131.2(5)
C(8)-C(7)-H(7)	114.4
C(6)-C(7)-H(7)	114.4
C(7)-C(8)-C(24)	122.9(5)
C(7)-C(8)-C(9)	121.9(5)
C(24)-C(8)-C(9)	115.1(4)
C(9)-N(1)-C(10)	109.2(4)
C(11)-S(1)-C(9)	89.4(2)
N(1)-C(9)-C(8)	123.9(4)
N(1)-C(9)-S(1)	115.9(4)
C(8)-C(9)-S(1)	120.1(4)
N(1)-C(10)-C(15)	124.5(5)
N(1)-C(10)-C(11)	115.9(4)
C(15)-C(10)-C(11)	119.6(5)
C(12)-C(11)-C(10)	120.8(5)
C(12)-C(11)-S(1)	129.6(4)
C(10)-C(11)-S(1)	109.5(4)
C(13)-C(12)-C(11)	118.2(5)
C(13)-C(12)-H(12)	120.9
C(11)-C(12)-H(12)	120.9
C(14)-C(13)-C(12)	120.9(5)
C(14)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
C(15)-C(14)-C(13)	121.6(5)
C(15)-C(14)-H(14)	119.2
C(13)-C(14)-H(14)	119.2
C(14)-C(15)-C(10)	118.9(5)
C(14)-C(15)-H(15)	120.6
C(10)-C(15)-H(15)	120.6
C(1)-O(1)-C(16)	119.1(3)
O(1)-C(16)-C(17)	107.9(4)
O(1)-C(16)-H(16A)	110.1
C(17)-C(16)-H(16A)	110.1
O(1)-C(16)-H(16B)	110.1
C(17)-C(16)-H(16B)	110.1

H(16A)-C(16)-H(16B)	108.4
C(16)-C(17)-C(18)	111.2(4)
C(16)-C(17)-H(17A)	109.4
C(18)-C(17)-H(17A)	109.4
C(16)-C(17)-H(17B)	109.4
C(18)-C(17)-H(17B)	109.4
H(17A)-C(17)-H(17B)	108.0
C(19)-C(18)-C(17)	113.8(4)
C(19)-C(18)-H(18A)	108.8
C(17)-C(18)-H(18A)	108.8
C(19)-C(18)-H(18B)	108.8
C(17)-C(18)-H(18B)	108.8
H(18A)-C(18)-H(18B)	107.7
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(3)-N(2)-C(20)	122.8(4)
C(3)-N(2)-C(22)	121.1(4)
C(20)-N(2)-C(22)	114.6(4)
N(2)-C(20)-C(21)	113.1(5)
N(2)-C(20)-H(20A)	109.0
C(21)-C(20)-H(20A)	109.0
N(2)-C(20)-H(20B)	109.0
C(21)-C(20)-H(20B)	109.0
H(20A)-C(20)-H(20B)	107.8
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-N(2)	81.9(10)
C(23)-C(22)-H(22A)	115.0

N(2)-C(22)-H(22A)	115.0
C(23)-C(22)-H(22B)	115.0
N(2)-C(22)-H(22B)	115.0
H(22A)-C(22)-H(22B)	112.0
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(3)-C(24)-C(8)	178.2(6)
O(2)-C(25)-C(26)	122.5(4)
O(2)-C(25)-C(30)	115.0(4)
C(26)-C(25)-C(30)	122.5(4)
C(25)-C(26)-C(27)	120.6(4)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
N(5)-C(27)-C(26)	120.4(4)
N(5)-C(27)-C(28)	122.2(4)
C(26)-C(27)-C(28)	117.4(4)
C(29)-C(28)-C(27)	121.3(5)
C(29)-C(28)-H(28)	119.3
C(27)-C(28)-H(28)	119.3
C(28)-C(29)-C(30)	123.3(5)
C(28)-C(29)-H(29)	118.3
C(30)-C(29)-H(29)	118.3
C(29)-C(30)-C(25)	114.8(4)
C(29)-C(30)-C(31)	126.3(4)
C(25)-C(30)-C(31)	118.9(4)
C(32)-C(31)-C(30)	132.6(5)
C(32)-C(31)-H(31)	113.7
C(30)-C(31)-H(31)	113.7
C(31)-C(32)-C(48)	123.3(4)
C(31)-C(32)-C(33)	121.6(4)
C(48)-C(32)-C(33)	115.1(4)
N(4)-C(33)-C(32)	123.2(4)

N(4)-C(33)-S(2)	117.1(4)
C(32)-C(33)-S(2)	119.7(3)
C(33)-N(4)-C(34)	109.3(4)
C(35)-S(2)-C(33)	89.1(2)
C(39)-C(34)-N(4)	124.9(5)
C(39)-C(34)-C(35)	120.1(5)
N(4)-C(34)-C(35)	115.0(4)
C(36)-C(35)-C(34)	120.7(5)
C(36)-C(35)-S(2)	129.7(4)
C(34)-C(35)-S(2)	109.6(3)
C(37)-C(36)-C(35)	119.3(5)
C(37)-C(36)-H(36)	120.3
C(35)-C(36)-H(36)	120.3
C(36)-C(37)-C(38)	120.0(5)
C(36)-C(37)-H(37)	120.0
C(38)-C(37)-H(37)	120.0
C(37)-C(38)-C(39)	122.5(5)
C(37)-C(38)-H(38)	118.8
C(39)-C(38)-H(38)	118.8
C(34)-C(39)-C(38)	117.3(5)
C(34)-C(39)-H(39)	121.3
C(38)-C(39)-H(39)	121.3
C(25)-O(2)-C(40)	119.2(3)
O(2)-C(40)-C(41)	108.1(4)
O(2)-C(40)-H(40A)	110.1
C(41)-C(40)-H(40A)	110.1
O(2)-C(40)-H(40B)	110.1
C(41)-C(40)-H(40B)	110.1
H(40A)-C(40)-H(40B)	108.4
C(40)-C(41)-C(42)	111.1(4)
C(40)-C(41)-H(41A)	109.4
C(42)-C(41)-H(41A)	109.4
C(40)-C(41)-H(41B)	109.4
C(42)-C(41)-H(41B)	109.4
H(41A)-C(41)-H(41B)	108.0
C(43)-C(42)-C(41)	113.9(5)

C(43)-C(42)-H(42A)	108.8
C(41)-C(42)-H(42A)	108.8
C(43)-C(42)-H(42B)	108.8
C(41)-C(42)-H(42B)	108.8
H(42A)-C(42)-H(42B)	107.7
C(42)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(27)-N(5)-C(46)	121.5(4)
C(27)-N(5)-C(44)	120.9(4)
C(46)-N(5)-C(44)	117.5(4)
C(45)-C(44)-N(5)	110.9(5)
C(45)-C(44)-H(44A)	109.5
N(5)-C(44)-H(44A)	109.5
C(45)-C(44)-H(44B)	109.5
N(5)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	108.1
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
N(5)-C(46)-C(47)	114.9(4)
N(5)-C(46)-H(46A)	108.5
C(47)-C(46)-H(46A)	108.5
N(5)-C(46)-H(46B)	108.5
C(47)-C(46)-H(46B)	108.5
H(46A)-C(46)-H(46B)	107.5
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5

H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
N(6)-C(48)-C(32)	178.7(5)
O(3)-C(49)-C(50)	123.0(4)
O(3)-C(49)-C(54)	114.8(4)
C(50)-C(49)-C(54)	122.2(4)
C(49)-C(50)-C(51)	121.3(4)
C(49)-C(50)-H(50)	119.4
C(51)-C(50)-H(50)	119.4
N(8)-C(51)-C(52)	122.3(4)
N(8)-C(51)-C(50)	121.0(4)
C(52)-C(51)-C(50)	116.7(5)
C(53)-C(52)-C(51)	121.6(4)
C(53)-C(52)-H(52)	119.2
C(51)-C(52)-H(52)	119.2
C(52)-C(53)-C(54)	123.1(5)
C(52)-C(53)-H(53)	118.4
C(54)-C(53)-H(53)	118.4
C(53)-C(54)-C(55)	126.2(4)
C(53)-C(54)-C(49)	115.1(4)
C(55)-C(54)-C(49)	118.7(4)
C(56)-C(55)-C(54)	132.7(5)
C(56)-C(55)-H(55)	113.6
C(54)-C(55)-H(55)	113.6
C(55)-C(56)-C(72)	122.9(4)
C(55)-C(56)-C(57)	121.6(4)
C(72)-C(56)-C(57)	115.4(4)
N(7)-C(57)-C(56)	123.0(4)
N(7)-C(57)-S(3)	116.9(3)
C(56)-C(57)-S(3)	120.0(3)
C(57)-N(7)-C(58)	107.4(4)
C(59)-S(3)-C(57)	89.0(2)
C(63)-C(58)-N(7)	123.7(5)
C(63)-C(58)-C(59)	120.0(5)
N(7)-C(58)-C(59)	116.3(4)
C(60)-C(59)-C(58)	121.3(5)

C(60)-C(59)-S(3)	128.4(4)
C(58)-C(59)-S(3)	110.3(4)
C(61)-C(60)-C(59)	117.8(5)
C(61)-C(60)-H(60)	121.1
C(59)-C(60)-H(60)	121.1
C(60)-C(61)-C(62)	120.5(5)
C(60)-C(61)-H(61)	119.7
C(62)-C(61)-H(61)	119.7
C(63)-C(62)-C(61)	122.1(5)
C(63)-C(62)-H(62)	118.9
C(61)-C(62)-H(62)	118.9
C(62)-C(63)-C(58)	118.2(5)
C(62)-C(63)-H(63)	120.9
C(58)-C(63)-H(63)	120.9
C(49)-O(3)-C(64)	118.9(4)
O(3)-C(64)-C(65)	108.4(4)
O(3)-C(64)-H(64A)	110.0
C(65)-C(64)-H(64A)	110.0
O(3)-C(64)-H(64B)	110.0
C(65)-C(64)-H(64B)	110.0
H(64A)-C(64)-H(64B)	108.4
C(64)-C(65)-C(66)	110.8(4)
C(64)-C(65)-H(65A)	109.5
C(66)-C(65)-H(65A)	109.5
C(64)-C(65)-H(65B)	109.5
C(66)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	108.1
C(67)-C(66)-C(65)	113.6(4)
C(67)-C(66)-H(66A)	108.9
C(65)-C(66)-H(66A)	108.9
C(67)-C(66)-H(66B)	108.9
C(65)-C(66)-H(66B)	108.9
H(66A)-C(66)-H(66B)	107.7
C(66)-C(67)-H(67A)	109.5
C(66)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5

C(66)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(51)-N(8)-C(70)	121.0(4)
C(51)-N(8)-C(68)	121.2(4)
C(70)-N(8)-C(68)	117.7(4)
N(8)-C(68)-C(69)	112.1(4)
N(8)-C(68)-H(68A)	109.2
C(69)-C(68)-H(68A)	109.2
N(8)-C(68)-H(68B)	109.2
C(69)-C(68)-H(68B)	109.2
H(68A)-C(68)-H(68B)	107.9
C(68)-C(69)-H(69A)	109.5
C(68)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(68)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
N(8)-C(70)-C(71)	114.2(4)
N(8)-C(70)-H(70A)	108.7
C(71)-C(70)-H(70A)	108.7
N(8)-C(70)-H(70B)	108.7
C(71)-C(70)-H(70B)	108.7
H(70A)-C(70)-H(70B)	107.6
C(70)-C(71)-H(71A)	109.5
C(70)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(70)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
N(9)-C(72)-C(56)	179.0(6)
O(4)-C(73)-C(74)	122.5(4)
O(4)-C(73)-C(78)	115.3(4)
C(74)-C(73)-C(78)	122.2(4)
C(73)-C(74)-C(75)	120.7(4)
C(73)-C(74)-H(74)	119.7

C(75)-C(74)-H(74)	119.7
N(11)-C(75)-C(74)	120.4(4)
N(11)-C(75)-C(76)	122.1(4)
C(74)-C(75)-C(76)	117.5(4)
C(77)-C(76)-C(75)	121.5(4)
C(77)-C(76)-H(76)	119.3
C(75)-C(76)-H(76)	119.3
C(76)-C(77)-C(78)	122.4(4)
C(76)-C(77)-H(77)	118.8
C(78)-C(77)-H(77)	118.8
C(77)-C(78)-C(73)	115.8(4)
C(77)-C(78)-C(79)	125.4(4)
C(73)-C(78)-C(79)	118.8(4)
C(80)-C(79)-C(78)	132.6(4)
C(80)-C(79)-H(79)	113.7
C(78)-C(79)-H(79)	113.7
C(79)-C(80)-C(96)	122.4(4)
C(79)-C(80)-C(81)	122.1(4)
C(96)-C(80)-C(81)	115.5(4)
N(10)-C(81)-C(80)	123.4(4)
N(10)-C(81)-S(4)	116.2(3)
C(80)-C(81)-S(4)	120.4(3)
C(81)-N(10)-C(82)	109.7(4)
C(83)-S(4)-C(81)	88.5(2)
C(87)-C(82)-C(83)	120.6(5)
C(87)-C(82)-N(10)	124.4(5)
C(83)-C(82)-N(10)	115.0(4)
C(82)-C(83)-C(84)	121.5(5)
C(82)-C(83)-S(4)	110.5(4)
C(84)-C(83)-S(4)	128.0(4)
C(85)-C(84)-C(83)	117.3(5)
C(85)-C(84)-H(84)	121.4
C(83)-C(84)-H(84)	121.4
C(86)-C(85)-C(84)	120.5(5)
C(86)-C(85)-H(85)	119.8
C(84)-C(85)-H(85)	119.8

C(87)-C(86)-C(85)	122.3(5)
C(87)-C(86)-H(86)	118.9
C(85)-C(86)-H(86)	118.9
C(86)-C(87)-C(82)	117.9(5)
C(86)-C(87)-H(87)	121.0
C(82)-C(87)-H(87)	121.0
C(73)-O(4)-C(88)	119.4(3)
O(4)-C(88)-C(89)	107.5(3)
O(4)-C(88)-H(88A)	110.2
C(89)-C(88)-H(88A)	110.2
O(4)-C(88)-H(88B)	110.2
C(89)-C(88)-H(88B)	110.2
H(88A)-C(88)-H(88B)	108.5
C(88)-C(89)-C(90)	112.1(4)
C(88)-C(89)-H(89A)	109.2
C(90)-C(89)-H(89A)	109.2
C(88)-C(89)-H(89B)	109.2
C(90)-C(89)-H(89B)	109.2
H(89A)-C(89)-H(89B)	107.9
C(91)-C(90)-C(89)	112.6(4)
C(91)-C(90)-H(90A)	109.1
C(89)-C(90)-H(90A)	109.1
C(91)-C(90)-H(90B)	109.1
C(89)-C(90)-H(90B)	109.1
H(90A)-C(90)-H(90B)	107.8
C(90)-C(91)-H(91A)	109.5
C(90)-C(91)-H(91B)	109.5
H(91A)-C(91)-H(91B)	109.5
C(90)-C(91)-H(91C)	109.5
H(91A)-C(91)-H(91C)	109.5
H(91B)-C(91)-H(91C)	109.5
C(75)-N(11)-C(92)	121.2(4)
C(75)-N(11)-C(94)	121.9(4)
C(92)-N(11)-C(94)	116.9(4)
N(11)-C(92)-C(93)	113.7(4)
N(11)-C(92)-H(92A)	108.8

C(93)-C(92)-H(92A)	108.8
N(11)-C(92)-H(92B)	108.8
C(93)-C(92)-H(92B)	108.8
H(92A)-C(92)-H(92B)	107.7
C(92)-C(93)-H(93A)	109.5
C(92)-C(93)-H(93B)	109.5
H(93A)-C(93)-H(93B)	109.5
C(92)-C(93)-H(93C)	109.5
H(93A)-C(93)-H(93C)	109.5
H(93B)-C(93)-H(93C)	109.5
N(11)-C(94)-C(95)	113.4(5)
N(11)-C(94)-H(94A)	108.9
C(95)-C(94)-H(94A)	108.9
N(11)-C(94)-H(94B)	108.9
C(95)-C(94)-H(94B)	108.9
H(94A)-C(94)-H(94B)	107.7
C(94)-C(95)-H(95A)	109.5
C(94)-C(95)-H(95B)	109.5
H(95A)-C(95)-H(95B)	109.5
C(94)-C(95)-H(95C)	109.5
H(95A)-C(95)-H(95C)	109.5
H(95B)-C(95)-H(95C)	109.5
N(12)-C(96)-C(80)	178.6(6)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **CV4-R**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	42(3)	42(3)	40(3)	3(2)	-1(2)	-18(2)
C(2)	45(3)	61(4)	35(3)	-2(2)	-6(2)	-24(3)
C(3)	53(3)	56(4)	42(3)	-3(2)	-8(3)	-23(3)
C(4)	49(3)	66(4)	39(3)	-5(3)	0(2)	-23(3)
C(5)	59(3)	53(4)	36(3)	-7(2)	-1(3)	-15(3)
C(6)	52(3)	43(3)	42(3)	2(2)	-7(2)	-16(3)
C(7)	54(3)	38(3)	38(3)	4(2)	-12(2)	-14(2)
C(8)	54(3)	43(3)	39(3)	2(2)	-7(2)	-13(3)
N(1)	46(2)	45(3)	45(3)	-2(2)	-5(2)	-11(2)
S(1)	70(1)	89(1)	39(1)	-4(1)	-3(1)	-36(1)
C(9)	56(3)	44(3)	33(3)	-2(2)	-6(2)	-14(3)
C(10)	49(3)	44(3)	41(3)	-4(2)	-13(3)	-5(2)
C(11)	55(3)	55(4)	44(3)	2(2)	-6(3)	-18(3)
C(12)	63(4)	88(5)	57(4)	-1(3)	0(3)	-33(4)
C(13)	64(4)	59(4)	74(4)	-1(3)	-19(3)	-27(3)
C(14)	64(4)	53(4)	54(4)	-2(3)	-12(3)	-14(3)
C(15)	66(4)	52(4)	51(3)	4(3)	-14(3)	-14(3)
O(1)	47(2)	65(3)	35(2)	1(2)	-8(2)	-19(2)
C(16)	49(3)	51(3)	32(3)	-1(2)	-1(2)	-18(3)
C(17)	44(3)	47(3)	51(3)	6(2)	-16(2)	-18(2)
C(18)	43(3)	72(4)	48(3)	2(3)	-10(2)	-19(3)
C(19)	67(4)	157(8)	74(5)	9(5)	4(4)	-54(5)
N(2)	46(3)	105(4)	52(3)	-23(3)	-2(2)	-28(3)
C(20)	52(3)	71(4)	53(3)	4(3)	-13(3)	-17(3)
C(21)	65(4)	78(5)	68(4)	2(3)	-7(3)	-29(3)
C(22)	52(5)	87(7)	344(17)	-82(9)	-30(7)	-23(5)

C(23)	130(8)	286(15)	116(7)	112(9)	-70(6)	-143(10)
C(24)	62(4)	63(4)	42(3)	2(3)	-15(3)	-18(3)
N(3)	68(3)	115(5)	45(3)	0(3)	-2(3)	-32(3)
C(25)	48(3)	42(3)	39(3)	3(2)	-1(2)	-15(2)
C(26)	41(3)	53(3)	31(3)	6(2)	-13(2)	-17(2)
C(27)	43(3)	61(4)	40(3)	4(2)	-7(2)	-18(3)
C(28)	38(3)	99(5)	44(3)	16(3)	-5(3)	-28(3)
C(29)	46(3)	77(4)	35(3)	2(3)	-4(2)	-19(3)
C(30)	42(3)	44(3)	37(3)	4(2)	-6(2)	-11(2)
C(31)	49(3)	44(3)	36(3)	2(2)	-2(2)	-17(2)
C(32)	43(3)	41(3)	39(3)	3(2)	-5(2)	-9(2)
C(33)	48(3)	47(3)	30(3)	1(2)	-11(2)	-13(2)
N(4)	49(3)	44(3)	37(2)	2(2)	-7(2)	-14(2)
S(2)	58(1)	62(1)	37(1)	3(1)	-9(1)	-24(1)
C(34)	50(3)	35(3)	41(3)	-3(2)	-7(2)	-5(2)
C(35)	46(3)	47(3)	43(3)	-9(2)	-5(2)	-14(2)
C(36)	55(3)	65(4)	43(3)	-5(3)	-2(3)	-27(3)
C(37)	54(3)	57(4)	54(3)	-18(3)	-8(3)	-16(3)
C(38)	59(4)	51(4)	49(3)	-7(3)	-13(3)	-9(3)
C(39)	58(3)	54(4)	36(3)	0(2)	-8(3)	-13(3)
O(2)	44(2)	61(2)	37(2)	7(2)	-7(2)	-24(2)
C(40)	47(3)	46(3)	41(3)	2(2)	-6(2)	-21(2)
C(41)	43(3)	45(3)	49(3)	1(2)	-6(2)	-17(2)
C(42)	53(3)	91(5)	58(4)	15(3)	-9(3)	-37(3)
C(43)	61(4)	121(6)	79(5)	21(4)	1(3)	-43(4)
N(5)	39(2)	93(4)	48(3)	16(2)	-7(2)	-28(3)
C(44)	70(4)	79(5)	63(4)	4(3)	-22(3)	-29(4)
C(45)	75(4)	99(6)	62(4)	-9(4)	-13(3)	-10(4)

C(46)	44(3)	67(4)	44(3)	9(3)	-12(2)	-26(3)
C(47)	64(4)	61(4)	51(3)	6(3)	-15(3)	-22(3)
C(48)	54(3)	43(3)	41(3)	-3(2)	-17(3)	-8(3)
N(6)	72(3)	84(4)	45(3)	14(2)	-10(2)	-38(3)
C(49)	45(3)	45(3)	40(3)	-1(2)	3(2)	-17(2)
C(50)	41(3)	51(3)	33(3)	4(2)	-13(2)	-20(2)
C(51)	43(3)	48(3)	43(3)	3(2)	-3(2)	-17(2)
C(52)	49(3)	66(4)	38(3)	2(2)	4(2)	-27(3)
C(53)	55(3)	56(4)	37(3)	6(2)	-5(3)	-18(3)
C(54)	46(3)	47(3)	36(3)	5(2)	-5(2)	-14(2)
C(55)	44(3)	44(3)	41(3)	2(2)	-2(2)	-13(2)
C(56)	48(3)	46(3)	37(3)	7(2)	-6(2)	-16(2)
C(57)	48(3)	44(3)	30(3)	2(2)	-7(2)	-13(2)
N(7)	41(2)	42(3)	60(3)	6(2)	-10(2)	-16(2)
S(3)	62(1)	59(1)	42(1)	3(1)	-5(1)	-22(1)
C(58)	56(3)	44(3)	36(3)	4(2)	-2(2)	-14(3)
C(59)	51(3)	46(3)	38(3)	1(2)	-4(2)	-17(3)
C(60)	64(4)	57(4)	44(3)	0(3)	4(3)	-26(3)
C(61)	60(4)	63(4)	67(4)	-9(3)	-8(3)	-23(3)
C(62)	76(4)	61(4)	44(3)	-5(3)	-13(3)	-15(3)
C(63)	62(4)	58(4)	44(3)	8(3)	-10(3)	-20(3)
O(3)	51(2)	65(3)	41(2)	11(2)	-7(2)	-29(2)
C(64)	51(3)	45(3)	41(3)	7(2)	-5(2)	-18(3)
C(65)	43(3)	52(3)	42(3)	6(2)	-12(2)	-20(2)
C(66)	41(3)	58(4)	44(3)	-4(2)	-5(2)	-16(3)
C(67)	57(4)	99(5)	65(4)	8(3)	7(3)	-35(4)
N(8)	42(2)	62(3)	40(2)	8(2)	-6(2)	-23(2)
C(68)	49(3)	76(4)	50(3)	5(3)	-8(3)	-28(3)

C(69)	56(4)	99(5)	64(4)	2(4)	4(3)	-28(4)
C(70)	40(3)	51(3)	34(3)	1(2)	-5(2)	-17(2)
C(71)	59(4)	57(4)	62(4)	9(3)	-4(3)	-19(3)
C(72)	57(4)	57(4)	48(3)	9(3)	-20(3)	-19(3)
N(9)	63(3)	103(4)	44(3)	9(3)	0(2)	-31(3)
C(73)	38(3)	44(3)	36(3)	4(2)	1(2)	-17(2)
C(74)	40(3)	49(3)	37(3)	0(2)	-2(2)	-19(2)
C(75)	49(3)	47(3)	37(3)	2(2)	-5(2)	-24(3)
C(76)	42(3)	59(4)	42(3)	5(2)	1(2)	-22(3)
C(77)	45(3)	53(3)	35(3)	-1(2)	-1(2)	-18(3)
C(78)	42(3)	44(3)	38(3)	0(2)	1(2)	-19(2)
C(79)	45(3)	37(3)	36(3)	6(2)	2(2)	-13(2)
C(80)	39(3)	46(3)	34(3)	1(2)	-2(2)	-13(2)
C(81)	44(3)	41(3)	31(3)	3(2)	-6(2)	-17(2)
N(10)	44(2)	47(3)	48(3)	4(2)	-6(2)	-15(2)
S(4)	53(1)	59(1)	40(1)	-1(1)	1(1)	-25(1)
C(82)	48(3)	46(3)	40(3)	2(2)	-5(2)	-15(3)
C(83)	48(3)	43(3)	43(3)	4(2)	-7(2)	-16(2)
C(84)	50(3)	45(3)	60(4)	3(3)	1(3)	-15(3)
C(85)	58(4)	49(4)	67(4)	1(3)	-19(3)	-22(3)
C(86)	72(4)	47(4)	59(4)	4(3)	-17(3)	-22(3)
C(87)	64(4)	55(4)	41(3)	3(2)	-11(3)	-22(3)
O(4)	41(2)	68(2)	36(2)	-3(2)	2(2)	-29(2)
C(88)	45(3)	60(3)	26(3)	-1(2)	5(2)	-21(3)
C(89)	36(3)	51(3)	38(3)	2(2)	-3(2)	-15(2)
C(90)	37(3)	54(3)	44(3)	2(2)	0(2)	-14(2)
C(91)	53(3)	86(5)	59(4)	2(3)	9(3)	-31(3)
N(11)	45(2)	64(3)	42(2)	2(2)	0(2)	-28(2)

C(92)	46(3)	59(4)	55(3)	4(3)	-4(3)	-27(3)
C(93)	50(3)	80(5)	63(4)	-11(3)	0(3)	-25(3)
C(94)	45(3)	73(4)	51(3)	6(3)	-11(3)	-31(3)
C(95)	62(4)	80(5)	64(4)	7(3)	-10(3)	-30(3)
C(96)	60(3)	55(4)	34(3)	5(2)	-6(3)	-30(3)
N(12)	71(3)	90(4)	37(3)	1(2)	-2(2)	-42(3)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **CV4-R**.

	x	y	z	U(eq)
H(2)	2306	845	9149	55
H(4)	-366	1859	10375	61
H(5)	1100	1898	10917	61
H(7)	4294	1472	10456	52
H(12)	8235	2027	11248	81
H(13)	8923	2083	12092	76
H(14)	7712	2034	12865	70
H(15)	5805	1895	12832	69
H(16A)	3884	1314	8877	53
H(16B)	4465	251	8946	53
H(17A)	6319	374	9153	55
H(17B)	5743	1441	9124	55
H(18A)	6130	242	8225	65
H(18B)	5551	1307	8196	65
H(19A)	7425	1410	8390	144
H(19B)	7602	811	7857	144
H(19C)	8004	342	8409	144
H(20A)	-1866	1762	9259	71
H(20B)	-1603	2118	9813	71
H(21A)	-1564	364	9608	103
H(21B)	-2569	1103	10001	103
H(21C)	-1184	664	10153	103
H(22A)	-442	1411	8451	192
H(22B)	978	1349	8508	192
H(23A)	1262	180	8991	233
H(23B)	809	-16	8437	233

H(23C)	-138	254	8966	233
H(26)	7770	947	6648	49
H(28)	9895	1320	5359	71
H(29)	8422	1348	4819	64
H(31)	5484	1139	5273	52
H(36)	1359	1007	4457	63
H(37)	419	1360	3668	67
H(38)	1426	1761	2927	66
H(39)	3362	1888	2956	61
H(40A)	5703	1323	6917	52
H(40B)	6364	270	6784	52
H(41A)	4492	188	6552	54
H(41B)	3828	1242	6670	54
H(42A)	4805	-49	7461	77
H(42B)	4272	1004	7591	77
H(43A)	2316	1070	7432	127
H(43B)	2831	332	7869	127
H(43C)	2832	29	7262	127
H(44A)	10734	1845	5913	83
H(44B)	11246	1658	6490	83
H(45A)	12171	157	6252	126
H(45B)	12668	763	5850	126
H(45C)	11680	358	5673	126
H(46A)	8844	1346	7112	60
H(46B)	10243	1248	7157	60
H(47A)	9408	-177	6963	87
H(47B)	9959	-7	7496	87
H(47C)	10835	-301	6947	87

H(50)	7688	6206	5875	48
H(52)	9629	6899	4627	60
H(53)	8124	6979	4093	60
H(55)	5290	6617	4534	53
H(60)	1159	6455	3732	65
H(61)	403	6518	2894	75
H(62)	1534	6733	2126	75
H(63)	3455	6856	2159	66
H(64A)	5629	6542	6147	54
H(64B)	6341	5498	6002	54
H(65A)	4513	5344	5781	53
H(65B)	3789	6397	5878	53
H(66A)	4809	5178	6695	57
H(66B)	4183	6235	6802	57
H(67A)	2275	6194	6644	108
H(67B)	2831	5467	7081	108
H(67C)	2873	5155	6472	108
H(68A)	11181	6893	5747	68
H(68B)	10606	7198	5192	68
H(69A)	12104	5421	5412	110
H(69B)	12523	6076	5019	110
H(69C)	11491	5699	4863	110
H(70A)	8812	6481	6352	50
H(70B)	10196	6426	6397	50
H(71A)	9582	4969	6024	90
H(71B)	9932	5060	6618	90
H(71C)	10942	4923	6117	90
H(74)	2649	5468	8364	50

H(76)	278	5685	9693	57
H(77)	1603	6009	10205	53
H(79)	4574	6104	9693	48
H(84)	8439	6816	10438	63
H(85)	9053	7053	11278	68
H(86)	7802	7086	12057	70
H(87)	5900	6916	12040	64
H(88A)	4067	6082	8084	52
H(88B)	4756	5030	8161	52
H(89A)	6562	5254	8324	50
H(89B)	5886	6318	8339	50
H(90A)	6343	5194	7400	55
H(90B)	5632	6254	7411	55
H(91A)	7423	6496	7598	97
H(91B)	7708	5883	7064	97
H(91C)	8140	5441	7619	97
H(92A)	-395	4894	9251	61
H(92B)	-770	4769	8667	61
H(93A)	-1479	6465	9215	96
H(93B)	-2374	5908	9173	96
H(93C)	-1901	6307	8646	96
H(94A)	278	4898	7942	64
H(94B)	1644	4890	7977	64
H(95A)	-425	6483	7925	101
H(95B)	537	6023	7421	101
H(95C)	973	6433	7912	101

Table S11. Torsion angles [°] for **CV4-R**.

O(1)-C(1)-C(2)-C(3)	-176.1(5)
C(6)-C(1)-C(2)-C(3)	4.8(7)
C(1)-C(2)-C(3)-N(2)	177.2(5)
C(1)-C(2)-C(3)-C(4)	-2.8(7)
N(2)-C(3)-C(4)-C(5)	179.5(5)
C(2)-C(3)-C(4)-C(5)	-0.5(8)
C(3)-C(4)-C(5)-C(6)	1.9(8)
C(4)-C(5)-C(6)-C(1)	0.0(7)
C(4)-C(5)-C(6)-C(7)	175.5(5)
O(1)-C(1)-C(6)-C(5)	177.6(4)
C(2)-C(1)-C(6)-C(5)	-3.3(7)
O(1)-C(1)-C(6)-C(7)	1.7(6)
C(2)-C(1)-C(6)-C(7)	-179.2(4)
C(5)-C(6)-C(7)-C(8)	15.0(9)
C(1)-C(6)-C(7)-C(8)	-169.6(5)
C(6)-C(7)-C(8)-C(24)	6.0(9)
C(6)-C(7)-C(8)-C(9)	-177.5(5)
C(10)-N(1)-C(9)-C(8)	-179.5(4)
C(10)-N(1)-C(9)-S(1)	-1.3(5)
C(7)-C(8)-C(9)-N(1)	-172.0(5)
C(24)-C(8)-C(9)-N(1)	4.7(7)
C(7)-C(8)-C(9)-S(1)	9.9(7)
C(24)-C(8)-C(9)-S(1)	-173.3(4)
C(11)-S(1)-C(9)-N(1)	1.5(4)
C(11)-S(1)-C(9)-C(8)	179.7(4)
C(9)-N(1)-C(10)-C(15)	-179.3(5)
C(9)-N(1)-C(10)-C(11)	0.4(6)
N(1)-C(10)-C(11)-C(12)	-178.5(5)
C(15)-C(10)-C(11)-C(12)	1.2(8)
N(1)-C(10)-C(11)-S(1)	0.7(6)
C(15)-C(10)-C(11)-S(1)	-179.6(4)
C(9)-S(1)-C(11)-C(12)	177.9(6)
C(9)-S(1)-C(11)-C(10)	-1.1(4)
C(10)-C(11)-C(12)-C(13)	-0.7(8)

S(1)-C(11)-C(12)-C(13)	-179.6(5)
C(11)-C(12)-C(13)-C(14)	-0.3(9)
C(12)-C(13)-C(14)-C(15)	0.8(9)
C(13)-C(14)-C(15)-C(10)	-0.3(8)
N(1)-C(10)-C(15)-C(14)	178.9(5)
C(11)-C(10)-C(15)-C(14)	-0.7(8)
C(2)-C(1)-O(1)-C(16)	13.5(6)
C(6)-C(1)-O(1)-C(16)	-167.4(4)
C(1)-O(1)-C(16)-C(17)	164.5(4)
O(1)-C(16)-C(17)-C(18)	-176.4(4)
C(16)-C(17)-C(18)-C(19)	179.8(5)
C(2)-C(3)-N(2)-C(20)	179.7(5)
C(4)-C(3)-N(2)-C(20)	-0.2(8)
C(2)-C(3)-N(2)-C(22)	-15.0(8)
C(4)-C(3)-N(2)-C(22)	165.0(5)
C(3)-N(2)-C(20)-C(21)	-83.6(6)
C(22)-N(2)-C(20)-C(21)	110.2(6)
C(3)-N(2)-C(22)-C(23)	92.2(7)
C(20)-N(2)-C(22)-C(23)	-101.4(7)
C(7)-C(8)-C(24)-N(3)	5(22)
C(9)-C(8)-C(24)-N(3)	-172(100)
O(2)-C(25)-C(26)-C(27)	-178.3(4)
C(30)-C(25)-C(26)-C(27)	1.5(7)
C(25)-C(26)-C(27)-N(5)	176.5(5)
C(25)-C(26)-C(27)-C(28)	-3.1(7)
N(5)-C(27)-C(28)-C(29)	-177.5(5)
C(26)-C(27)-C(28)-C(29)	2.1(8)
C(27)-C(28)-C(29)-C(30)	0.6(9)
C(28)-C(29)-C(30)-C(25)	-2.2(8)
C(28)-C(29)-C(30)-C(31)	178.0(5)
O(2)-C(25)-C(30)-C(29)	-179.0(4)
C(26)-C(25)-C(30)-C(29)	1.2(7)
O(2)-C(25)-C(30)-C(31)	0.8(6)
C(26)-C(25)-C(30)-C(31)	-179.0(4)
C(29)-C(30)-C(31)-C(32)	-5.5(9)
C(25)-C(30)-C(31)-C(32)	174.7(5)

C(30)-C(31)-C(32)-C(48)	-3.0(9)
C(30)-C(31)-C(32)-C(33)	178.0(5)
C(31)-C(32)-C(33)-N(4)	175.9(5)
C(48)-C(32)-C(33)-N(4)	-3.2(7)
C(31)-C(32)-C(33)-S(2)	-3.4(6)
C(48)-C(32)-C(33)-S(2)	177.5(3)
C(32)-C(33)-N(4)-C(34)	-178.6(4)
S(2)-C(33)-N(4)-C(34)	0.7(5)
N(4)-C(33)-S(2)-C(35)	-1.3(4)
C(32)-C(33)-S(2)-C(35)	178.1(4)
C(33)-N(4)-C(34)-C(39)	-180.0(5)
C(33)-N(4)-C(34)-C(35)	0.4(6)
C(39)-C(34)-C(35)-C(36)	-1.3(7)
N(4)-C(34)-C(35)-C(36)	178.3(4)
C(39)-C(34)-C(35)-S(2)	179.0(4)
N(4)-C(34)-C(35)-S(2)	-1.3(5)
C(33)-S(2)-C(35)-C(36)	-178.2(5)
C(33)-S(2)-C(35)-C(34)	1.4(4)
C(34)-C(35)-C(36)-C(37)	-0.5(7)
S(2)-C(35)-C(36)-C(37)	179.0(4)
C(35)-C(36)-C(37)-C(38)	1.9(8)
C(36)-C(37)-C(38)-C(39)	-1.5(8)
N(4)-C(34)-C(39)-C(38)	-177.9(4)
C(35)-C(34)-C(39)-C(38)	1.7(7)
C(37)-C(38)-C(39)-C(34)	-0.3(7)
C(26)-C(25)-O(2)-C(40)	-3.6(6)
C(30)-C(25)-O(2)-C(40)	176.6(4)
C(25)-O(2)-C(40)-C(41)	-176.1(4)
O(2)-C(40)-C(41)-C(42)	-178.6(4)
C(40)-C(41)-C(42)-C(43)	174.4(5)
C(26)-C(27)-N(5)-C(46)	4.3(8)
C(28)-C(27)-N(5)-C(46)	-176.1(5)
C(26)-C(27)-N(5)-C(44)	-173.0(5)
C(28)-C(27)-N(5)-C(44)	6.6(8)
C(27)-N(5)-C(44)-C(45)	-86.6(6)
C(46)-N(5)-C(44)-C(45)	95.9(6)

C(27)-N(5)-C(46)-C(47)	77.8(6)
C(44)-N(5)-C(46)-C(47)	-104.8(5)
C(31)-C(32)-C(48)-N(6)	-3(26)
C(33)-C(32)-C(48)-N(6)	176(100)
O(3)-C(49)-C(50)-C(51)	178.8(4)
C(54)-C(49)-C(50)-C(51)	1.4(7)
C(49)-C(50)-C(51)-N(8)	179.4(4)
C(49)-C(50)-C(51)-C(52)	-0.4(7)
N(8)-C(51)-C(52)-C(53)	180.0(5)
C(50)-C(51)-C(52)-C(53)	-0.3(7)
C(51)-C(52)-C(53)-C(54)	-0.1(8)
C(52)-C(53)-C(54)-C(55)	-179.3(5)
C(52)-C(53)-C(54)-C(49)	1.0(7)
O(3)-C(49)-C(54)-C(53)	-179.2(4)
C(50)-C(49)-C(54)-C(53)	-1.7(7)
O(3)-C(49)-C(54)-C(55)	1.0(7)
C(50)-C(49)-C(54)-C(55)	178.6(4)
C(53)-C(54)-C(55)-C(56)	8.7(9)
C(49)-C(54)-C(55)-C(56)	-171.6(5)
C(54)-C(55)-C(56)-C(72)	1.0(9)
C(54)-C(55)-C(56)-C(57)	178.0(5)
C(55)-C(56)-C(57)-N(7)	-179.4(5)
C(72)-C(56)-C(57)-N(7)	-2.1(7)
C(55)-C(56)-C(57)-S(3)	-0.5(7)
C(72)-C(56)-C(57)-S(3)	176.8(4)
C(56)-C(57)-N(7)-C(58)	178.5(4)
S(3)-C(57)-N(7)-C(58)	-0.5(5)
N(7)-C(57)-S(3)-C(59)	0.5(4)
C(56)-C(57)-S(3)-C(59)	-178.5(4)
C(57)-N(7)-C(58)-C(63)	-179.7(5)
C(57)-N(7)-C(58)-C(59)	0.2(6)
C(63)-C(58)-C(59)-C(60)	-0.2(8)
N(7)-C(58)-C(59)-C(60)	179.9(4)
C(63)-C(58)-C(59)-S(3)	-180.0(4)
N(7)-C(58)-C(59)-S(3)	0.1(6)
C(57)-S(3)-C(59)-C(60)	179.9(5)

C(57)-S(3)-C(59)-C(58)	-0.3(4)
C(58)-C(59)-C(60)-C(61)	0.4(8)
S(3)-C(59)-C(60)-C(61)	-179.9(4)
C(59)-C(60)-C(61)-C(62)	-0.6(8)
C(60)-C(61)-C(62)-C(63)	0.7(9)
C(61)-C(62)-C(63)-C(58)	-0.6(8)
N(7)-C(58)-C(63)-C(62)	-179.8(5)
C(59)-C(58)-C(63)-C(62)	0.3(8)
C(50)-C(49)-O(3)-C(64)	4.0(7)
C(54)-C(49)-O(3)-C(64)	-178.5(4)
C(49)-O(3)-C(64)-C(65)	179.5(4)
O(3)-C(64)-C(65)-C(66)	-175.6(4)
C(64)-C(65)-C(66)-C(67)	175.6(4)
C(52)-C(51)-N(8)-C(70)	-176.4(5)
C(50)-C(51)-N(8)-C(70)	3.9(7)
C(52)-C(51)-N(8)-C(68)	1.3(7)
C(50)-C(51)-N(8)-C(68)	-178.5(4)
C(51)-N(8)-C(68)-C(69)	-84.2(6)
C(70)-N(8)-C(68)-C(69)	93.5(5)
C(51)-N(8)-C(70)-C(71)	80.0(5)
C(68)-N(8)-C(70)-C(71)	-97.7(5)
C(55)-C(56)-C(72)-N(9)	-30(43)
C(57)-C(56)-C(72)-N(9)	153(42)
O(4)-C(73)-C(74)-C(75)	177.6(4)
C(78)-C(73)-C(74)-C(75)	-1.7(7)
C(73)-C(74)-C(75)-N(11)	-177.7(4)
C(73)-C(74)-C(75)-C(76)	1.4(7)
N(11)-C(75)-C(76)-C(77)	178.7(5)
C(74)-C(75)-C(76)-C(77)	-0.4(7)
C(75)-C(76)-C(77)-C(78)	-0.3(8)
C(76)-C(77)-C(78)-C(73)	0.0(7)
C(76)-C(77)-C(78)-C(79)	-178.8(5)
O(4)-C(73)-C(78)-C(77)	-178.4(4)
C(74)-C(73)-C(78)-C(77)	1.0(7)
O(4)-C(73)-C(78)-C(79)	0.4(6)
C(74)-C(73)-C(78)-C(79)	179.8(4)

C(77)-C(78)-C(79)-C(80)	-0.1(8)
C(73)-C(78)-C(79)-C(80)	-178.8(5)
C(78)-C(79)-C(80)-C(96)	1.4(8)
C(78)-C(79)-C(80)-C(81)	-178.4(5)
C(79)-C(80)-C(81)-N(10)	-176.7(5)
C(96)-C(80)-C(81)-N(10)	3.5(7)
C(79)-C(80)-C(81)-S(4)	3.8(6)
C(96)-C(80)-C(81)-S(4)	-176.0(4)
C(80)-C(81)-N(10)-C(82)	178.8(4)
S(4)-C(81)-N(10)-C(82)	-1.6(5)
N(10)-C(81)-S(4)-C(83)	2.1(4)
C(80)-C(81)-S(4)-C(83)	-178.4(4)
C(81)-N(10)-C(82)-C(87)	-178.7(5)
C(81)-N(10)-C(82)-C(83)	0.2(6)
C(87)-C(82)-C(83)-C(84)	0.6(8)
N(10)-C(82)-C(83)-C(84)	-178.3(4)
C(87)-C(82)-C(83)-S(4)	-179.7(4)
N(10)-C(82)-C(83)-S(4)	1.3(6)
C(81)-S(4)-C(83)-C(82)	-1.8(4)
C(81)-S(4)-C(83)-C(84)	177.8(5)
C(82)-C(83)-C(84)-C(85)	-0.3(7)
S(4)-C(83)-C(84)-C(85)	-179.9(4)
C(83)-C(84)-C(85)-C(86)	0.2(8)
C(84)-C(85)-C(86)-C(87)	-0.5(8)
C(85)-C(86)-C(87)-C(82)	0.8(8)
C(83)-C(82)-C(87)-C(86)	-0.9(7)
N(10)-C(82)-C(87)-C(86)	178.0(5)
C(74)-C(73)-O(4)-C(88)	4.0(7)
C(78)-C(73)-O(4)-C(88)	-176.6(4)
C(73)-O(4)-C(88)-C(89)	175.8(4)
O(4)-C(88)-C(89)-C(90)	-171.7(4)
C(88)-C(89)-C(90)-C(91)	178.4(4)
C(74)-C(75)-N(11)-C(92)	173.5(4)
C(76)-C(75)-N(11)-C(92)	-5.6(7)
C(74)-C(75)-N(11)-C(94)	-7.9(7)
C(76)-C(75)-N(11)-C(94)	173.0(5)

C(75)-N(11)-C(92)-C(93)	86.0(6)
C(94)-N(11)-C(92)-C(93)	-92.7(5)
C(75)-N(11)-C(94)-C(95)	-76.8(6)
C(92)-N(11)-C(94)-C(95)	101.9(5)
C(79)-C(80)-C(96)-N(12)	-82(22)
C(81)-C(80)-C(96)-N(12)	97(22)

Symmetry transformations used to generate equivalent atoms:

Table S12. Crystal data and structure refinement for **CV6-R**.

Identification code	**CV6-R**
Empirical formula	C_{26} H_{31} N_3 O S
Formula weight	433.60
Temperature	177(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 13.0387(9) Å b = 8.5716(6) Å c = 21.3730(14) Å
Volume	2369.3(3) $Å^3$
Z	4
Density (calculated)	1.216 Mg/m^3
Absorption coefficient	0.159 mm^{-1}
F(000)	928
Crystal size	0.26 x 0.20 x 0.18 mm^3
Theta range for data collection	1.92 to 28.29°.
Index ranges	-9<=h<=17, -11<=k<=11, -28<=l<=28
Reflections collected	16941
Independent reflections	5881 [R(int) = 0.0433]
Completeness to theta = 28.29°	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5881 / 0 / 283
Goodness-of-fit on F^2	1.145
Final R indices [I>2sigma(I)]	R1 = 0.0638, wR2 = 0.1456
R indices (all data)	R1 = 0.1126, wR2 = 0.2172
Largest diff. peak and hole	0.693 and -0.835 $e.Å^{-3}$

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **CV6-R**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5770(2)	8605(3)	9016(1)	33(1)
C(2)	6347(2)	8894(3)	8536(1)	33(1)
C(3)	5965(2)	9825(3)	8009(1)	31(1)
C(4)	4941(2)	10410(4)	8001(1)	37(1)
C(5)	4375(2)	10094(3)	8477(1)	36(1)
C(6)	4742(2)	9178(3)	9008(1)	33(1)
C(7)	4171(2)	8784(3)	9511(1)	34(1)
C(8)	3159(2)	8996(3)	9588(1)	35(1)
C(9)	2729(2)	8497(4)	10155(1)	36(1)
N(1)	1773(2)	8878(3)	10257(1)	45(1)
S(1)	3446(1)	7339(1)	10722(1)	42(1)
C(10)	2393(3)	7335(4)	11145(2)	40(1)
C(11)	2303(3)	6603(4)	11720(2)	52(1)
C(12)	1367(4)	6773(5)	11961(2)	63(1)
C(13)	567(3)	7644(5)	11645(2)	63(1)
C(14)	655(3)	8361(5)	11084(2)	55(1)
C(15)	1586(3)	8211(4)	10828(2)	43(1)
O(1)	6120(2)	7728(2)	9535(1)	36(1)
C(16)	7146(2)	7104(3)	9587(1)	34(1)
C(17)	7350(2)	6235(4)	10205(1)	36(1)
C(18)	8411(2)	5487(4)	10283(1)	36(1)
C(19)	8677(2)	4593(4)	10895(1)	38(1)
C(20)	9714(3)	3771(4)	10930(2)	48(1)
C(21)	10024(3)	2920(5)	11551(2)	64(1)
N(2)	6548(2)	10169(3)	7550(1)	35(1)
C(22)	6119(2)	11009(4)	6979(1)	40(1)

C(23)	5447(3)	9999(4)	6509(2)	53(1)
C(24)	7600(2)	9559(4)	7559(1)	38(1)
C(25)	7636(3)	7909(4)	7316(2)	46(1)
C(26)	2412(2)	9714(4)	9118(2)	43(1)
N(3)	1814(2)	10252(4)	8747(2)	63(1)

Table S14. Bond lengths [Å] and angles [°] for **CV6-R**.

C(1)-O(1)	1.370(3)
C(1)-C(2)	1.370(4)
C(1)-C(6)	1.425(4)
C(2)-C(3)	1.417(4)
C(2)-H(2)	0.9500
C(3)-N(2)	1.349(4)
C(3)-C(4)	1.424(4)
C(4)-C(5)	1.358(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.412(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.424(4)
C(7)-C(8)	1.363(4)
C(7)-H(7)	0.9500
C(8)-C(26)	1.444(4)
C(8)-C(9)	1.463(4)
C(9)-N(1)	1.333(4)
C(9)-S(1)	1.743(3)
N(1)-C(15)	1.396(4)
S(1)-C(10)	1.738(3)
C(10)-C(11)	1.397(5)
C(10)-C(15)	1.397(5)
C(11)-C(12)	1.391(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.386(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.366(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.399(5)
C(14)-H(14)	0.9500
O(1)-C(16)	1.432(3)
C(16)-C(17)	1.510(4)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900

C(17)-C(18)	1.514(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.518(4)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.518(4)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.523(5)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
N(2)-C(22)	1.465(4)
N(2)-C(24)	1.466(4)
C(22)-C(23)	1.518(5)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.510(5)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-N(3)	1.136(4)

O(1)-C(1)-C(2)	123.2(3)
O(1)-C(1)-C(6)	114.5(2)
C(2)-C(1)-C(6)	122.3(3)
C(1)-C(2)-C(3)	121.7(3)
C(1)-C(2)-H(2)	119.2

C(3)-C(2)-H(2)	119.2
N(2)-C(3)-C(2)	121.8(3)
N(2)-C(3)-C(4)	121.9(3)
C(2)-C(3)-C(4)	116.3(3)
C(5)-C(4)-C(3)	121.2(3)
C(5)-C(4)-H(4)	119.4
C(3)-C(4)-H(4)	119.4
C(4)-C(5)-C(6)	123.5(3)
C(4)-C(5)-H(5)	118.3
C(6)-C(5)-H(5)	118.3
C(5)-C(6)-C(7)	125.6(3)
C(5)-C(6)-C(1)	115.1(3)
C(7)-C(6)-C(1)	119.4(3)
C(8)-C(7)-C(6)	131.9(3)
C(8)-C(7)-H(7)	114.1
C(6)-C(7)-H(7)	114.1
C(7)-C(8)-C(26)	123.4(3)
C(7)-C(8)-C(9)	122.7(3)
C(26)-C(8)-C(9)	113.9(3)
N(1)-C(9)-C(8)	121.9(3)
N(1)-C(9)-S(1)	117.1(2)
C(8)-C(9)-S(1)	121.0(2)
C(9)-N(1)-C(15)	108.3(3)
C(10)-S(1)-C(9)	88.54(15)
C(11)-C(10)-C(15)	121.8(3)
C(11)-C(10)-S(1)	128.3(3)
C(15)-C(10)-S(1)	110.0(2)
C(12)-C(11)-C(10)	117.0(4)
C(12)-C(11)-H(11)	121.5
C(10)-C(11)-H(11)	121.5
C(13)-C(12)-C(11)	121.2(4)
C(13)-C(12)-H(12)	119.4
C(11)-C(12)-H(12)	119.4
C(14)-C(13)-C(12)	121.8(4)
C(14)-C(13)-H(13)	119.1
C(12)-C(13)-H(13)	119.1

C(13)-C(14)-C(15)	118.5(4)
C(13)-C(14)-H(14)	120.8
C(15)-C(14)-H(14)	120.8
N(1)-C(15)-C(10)	116.1(3)
N(1)-C(15)-C(14)	124.1(3)
C(10)-C(15)-C(14)	119.8(3)
C(1)-O(1)-C(16)	118.6(2)
O(1)-C(16)-C(17)	108.1(2)
O(1)-C(16)-H(16A)	110.1
C(17)-C(16)-H(16A)	110.1
O(1)-C(16)-H(16B)	110.1
C(17)-C(16)-H(16B)	110.1
H(16A)-C(16)-H(16B)	108.4
C(16)-C(17)-C(18)	111.2(2)
C(16)-C(17)-H(17A)	109.4
C(18)-C(17)-H(17A)	109.4
C(16)-C(17)-H(17B)	109.4
C(18)-C(17)-H(17B)	109.4
H(17A)-C(17)-H(17B)	108.0
C(17)-C(18)-C(19)	114.4(3)
C(17)-C(18)-H(18A)	108.6
C(19)-C(18)-H(18A)	108.6
C(17)-C(18)-H(18B)	108.6
C(19)-C(18)-H(18B)	108.6
H(18A)-C(18)-H(18B)	107.6
C(20)-C(19)-C(18)	112.4(3)
C(20)-C(19)-H(19A)	109.1
C(18)-C(19)-H(19A)	109.1
C(20)-C(19)-H(19B)	109.1
C(18)-C(19)-H(19B)	109.1
H(19A)-C(19)-H(19B)	107.9
C(19)-C(20)-C(21)	113.7(3)
C(19)-C(20)-H(20A)	108.8
C(21)-C(20)-H(20A)	108.8
C(19)-C(20)-H(20B)	108.8
C(21)-C(20)-H(20B)	108.8

H(20A)-C(20)-H(20B)	107.7
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(3)-N(2)-C(22)	121.6(2)
C(3)-N(2)-C(24)	121.6(2)
C(22)-N(2)-C(24)	116.4(2)
N(2)-C(22)-C(23)	113.4(3)
N(2)-C(22)-H(22A)	108.9
C(23)-C(22)-H(22A)	108.9
N(2)-C(22)-H(22B)	108.9
C(23)-C(22)-H(22B)	108.9
H(22A)-C(22)-H(22B)	107.7
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(2)-C(24)-C(25)	113.5(3)
N(2)-C(24)-H(24A)	108.9
C(25)-C(24)-H(24A)	108.9
N(2)-C(24)-H(24B)	108.9
C(25)-C(24)-H(24B)	108.9
H(24A)-C(24)-H(24B)	107.7
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
N(3)-C(26)-C(8)	178.6(4)

Symmetry transformations used to generate equivalent atoms:

Table S15. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **CV6-R**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	36(2)	33(2)	29(1)	0(1)	4(1)	2(1)
C(2)	30(1)	34(2)	35(1)	0(1)	5(1)	4(1)
C(3)	33(1)	30(1)	31(1)	2(1)	3(1)	2(1)
C(4)	37(2)	39(2)	37(2)	4(1)	7(1)	6(1)
C(5)	32(2)	37(2)	37(2)	0(1)	3(1)	5(1)
C(6)	34(2)	32(2)	33(1)	1(1)	6(1)	4(1)
C(7)	36(2)	33(2)	32(1)	-3(1)	4(1)	2(1)
C(8)	30(2)	35(2)	38(2)	-3(1)	5(1)	2(1)
C(9)	37(2)	36(2)	36(2)	-7(1)	9(1)	4(1)
N(1)	58(2)	39(2)	38(1)	-5(1)	11(1)	-8(1)
S(1)	43(1)	44(1)	41(1)	-1(1)	10(1)	0(1)
C(10)	41(2)	40(2)	40(2)	-6(1)	12(1)	-7(1)
C(11)	64(2)	49(2)	42(2)	-3(2)	7(2)	-13(2)
C(12)	87(3)	64(2)	44(2)	-11(2)	29(2)	-31(2)
C(13)	51(2)	78(3)	64(2)	-23(2)	29(2)	-23(2)
C(14)	40(2)	65(2)	62(2)	-21(2)	17(2)	-10(2)
C(15)	41(2)	45(2)	44(2)	-8(1)	12(1)	-6(1)
O(1)	33(1)	43(1)	32(1)	6(1)	6(1)	6(1)
C(16)	31(2)	36(2)	36(2)	1(1)	5(1)	5(1)
C(17)	40(2)	39(2)	29(1)	1(1)	4(1)	0(1)
C(18)	36(2)	41(2)	31(1)	1(1)	5(1)	1(1)
C(19)	38(2)	44(2)	31(1)	5(1)	5(1)	1(1)
C(20)	48(2)	55(2)	39(2)	3(2)	0(2)	6(2)
C(21)	61(3)	67(3)	60(2)	15(2)	-12(2)	8(2)
N(2)	35(1)	41(1)	31(1)	4(1)	7(1)	3(1)
C(22)	43(2)	42(2)	35(2)	9(1)	6(1)	1(1)

C(23)	62(2)	53(2)	41(2)	0(2)	-4(2)	8(2)
C(24)	36(2)	46(2)	33(2)	-3(1)	6(1)	-3(1)
C(25)	39(2)	56(2)	44(2)	-8(2)	2(1)	5(2)
C(26)	33(2)	44(2)	51(2)	6(2)	6(1)	-2(1)
N(3)	35(2)	80(2)	73(2)	33(2)	5(2)	2(2)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **CV6-R**.

	x	y	z	U(eq)
H(2)	7021	8460	8556	40
H(4)	4649	11034	7656	45
H(5)	3696	10510	8452	43
H(7)	4568	8280	9856	40
H(11)	2856	6016	11936	62
H(12)	1274	6284	12348	76
H(13)	-60	7745	11824	75
H(14)	98	8948	10872	66
H(16A)	7654	7958	9575	41
H(16B)	7211	6387	9231	41
H(17A)	6817	5418	10220	43
H(17B)	7300	6968	10558	43
H(18A)	8936	6313	10260	43
H(18B)	8454	4765	9926	43
H(19A)	8691	5325	11254	45
H(19B)	8130	3810	10935	45
H(20A)	10253	4550	10869	57
H(20B)	9687	3009	10580	57
H(21A)	10081	3672	11899	97
H(21B)	10693	2406	11540	97
H(21C)	9500	2137	11613	97
H(22A)	6696	11438	6772	48
H(22B)	5703	11899	7100	48
H(23A)	5859	9130	6377	79
H(23B)	5185	10626	6139	79
H(23C)	4865	9588	6706	79

H(24A)	7952	9594	7998	45
H(24B)	7987	10246	7300	45
H(25A)	7251	7221	7569	70
H(25B)	8357	7561	7347	70
H(25C)	7324	7874	6874	70

Table S17. Torsion angles [°] for **CV6-R**.

O(1)-C(1)-C(2)-C(3)	-179.2(3)
C(6)-C(1)-C(2)-C(3)	1.9(5)
C(1)-C(2)-C(3)-N(2)	177.0(3)
C(1)-C(2)-C(3)-C(4)	-1.3(4)
N(2)-C(3)-C(4)-C(5)	-177.9(3)
C(2)-C(3)-C(4)-C(5)	0.4(4)
C(3)-C(4)-C(5)-C(6)	-0.1(5)
C(4)-C(5)-C(6)-C(7)	-178.4(3)
C(4)-C(5)-C(6)-C(1)	0.5(4)
O(1)-C(1)-C(6)-C(5)	179.6(2)
C(2)-C(1)-C(6)-C(5)	-1.5(4)
O(1)-C(1)-C(6)-C(7)	-1.4(4)
C(2)-C(1)-C(6)-C(7)	177.6(3)
C(5)-C(6)-C(7)-C(8)	8.1(5)
C(1)-C(6)-C(7)-C(8)	-170.8(3)
C(6)-C(7)-C(8)-C(26)	1.0(5)
C(6)-C(7)-C(8)-C(9)	-179.7(3)
C(7)-C(8)-C(9)-N(1)	171.8(3)
C(26)-C(8)-C(9)-N(1)	-8.8(4)
C(7)-C(8)-C(9)-S(1)	-9.5(4)
C(26)-C(8)-C(9)-S(1)	169.9(2)
C(8)-C(9)-N(1)-C(15)	178.9(3)
S(1)-C(9)-N(1)-C(15)	0.2(3)
N(1)-C(9)-S(1)-C(10)	0.0(3)
C(8)-C(9)-S(1)-C(10)	-178.8(3)
C(9)-S(1)-C(10)-C(11)	180.0(3)
C(9)-S(1)-C(10)-C(15)	-0.2(2)
C(15)-C(10)-C(11)-C(12)	0.5(5)
S(1)-C(10)-C(11)-C(12)	-179.6(3)
C(10)-C(11)-C(12)-C(13)	-0.6(5)
C(11)-C(12)-C(13)-C(14)	0.6(6)
C(12)-C(13)-C(14)-C(15)	-0.4(6)
C(9)-N(1)-C(15)-C(10)	-0.3(4)
C(9)-N(1)-C(15)-C(14)	-179.7(3)

C(11)-C(10)-C(15)-N(1)	-179.8(3)
S(1)-C(10)-C(15)-N(1)	0.3(4)
C(11)-C(10)-C(15)-C(14)	-0.4(5)
S(1)-C(10)-C(15)-C(14)	179.7(3)
C(13)-C(14)-C(15)-N(1)	179.7(3)
C(13)-C(14)-C(15)-C(10)	0.3(5)
C(2)-C(1)-O(1)-C(16)	1.2(4)
C(6)-C(1)-O(1)-C(16)	-179.8(2)
C(1)-O(1)-C(16)-C(17)	178.3(2)
O(1)-C(16)-C(17)-C(18)	177.9(2)
C(16)-C(17)-C(18)-C(19)	179.8(3)
C(17)-C(18)-C(19)-C(20)	175.9(3)
C(18)-C(19)-C(20)-C(21)	177.5(3)
C(2)-C(3)-N(2)-C(22)	174.3(3)
C(4)-C(3)-N(2)-C(22)	-7.4(4)
C(2)-C(3)-N(2)-C(24)	2.0(4)
C(4)-C(3)-N(2)-C(24)	-179.8(3)
C(3)-N(2)-C(22)-C(23)	-76.5(4)
C(24)-N(2)-C(22)-C(23)	96.3(3)
C(3)-N(2)-C(24)-C(25)	81.2(3)
C(22)-N(2)-C(24)-C(25)	-91.5(3)
C(7)-C(8)-C(26)-N(3)	111(16)
C(9)-C(8)-C(26)-N(3)	-69(16)

Symmetry transformations used to generate equivalent atoms:

Table S18. Crystal data and structure refinement for **CV8-Y**.

Identification code	**CV8-Y**
Empirical formula	C_{28} H_{35} N_3 O S
Formula weight	461.65
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 12.5302(15) Å b = 10.9923(14) Å c = 19.127(2) Å
Volume	2547.0(5) $Å^3$
Z	4
Density (calculated)	1.204 Mg/m^3
Absorption coefficient	0.152 mm^{-1}
F(000)	992
Crystal size	0.44 x 0.38 x 0.34 mm^3
Theta range for data collection	2.16 to 28.35°.
Index ranges	-12<=h<=16, -14<=k<=14, -23<=l<=25
Reflections collected	18372
Independent reflections	6361 [R(int) = 0.0634]
Completeness to theta = 28.35°	99.7 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6361 / 0 / 301
Goodness-of-fit on F^2	1.221
Final R indices [I>2sigma(I)]	R1 = 0.0559, wR2 = 0.1502
R indices (all data)	R1 = 0.1068, wR2 = 0.2172
Largest diff. peak and hole	0.438 and -0.561 $e.Å^{-3}$

Table S19. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **CV8-Y**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6108(2)	2294(2)	1445(1)	36(1)
C(2)	5477(2)	1253(2)	1378(1)	37(1)
C(3)	5961(2)	94(2)	1457(1)	38(1)
C(4)	7121(2)	40(2)	1617(2)	45(1)
C(5)	7740(2)	1085(2)	1684(2)	42(1)
C(6)	7277(2)	2258(2)	1598(1)	36(1)
O(1)	5644(1)	3434(2)	1355(1)	44(1)
C(7)	4466(2)	3517(2)	1188(1)	39(1)
C(8)	4124(2)	4822(2)	1020(2)	45(1)
C(9)	2880(2)	4911(2)	743(2)	46(1)
C(10)	2437(2)	6168(2)	506(2)	44(1)
C(11)	1188(2)	6194(2)	205(2)	44(1)
C(12)	687(2)	7451(2)	7(2)	47(1)
C(13)	-555(2)	7407(3)	-279(2)	54(1)
C(14)	-1099(3)	8633(3)	-447(2)	81(1)
N(1)	5328(2)	-938(2)	1386(1)	40(1)
C(15)	5820(2)	-2150(2)	1392(2)	43(1)
C(16)	6025(2)	-2528(3)	679(2)	54(1)
C(17)	4131(2)	-872(2)	1189(2)	43(1)
C(18)	3610(2)	-664(3)	392(2)	53(1)
C(19)	7887(2)	3378(2)	1643(1)	37(1)
C(20)	8992(2)	3606(2)	1818(1)	35(1)
C(21)	9813(2)	2670(2)	2022(1)	39(1)
N(2)	10458(2)	1914(2)	2191(1)	54(1)
C(22)	9474(2)	4821(2)	1853(1)	34(1)
N(3)	10523(2)	5029(2)	2072(1)	35(1)

S(1)	8640(1)	6124(1)	1601(1)	44(1)
C(23)	10748(2)	6261(2)	2066(1)	36(1)
C(24)	9815(2)	7014(2)	1822(1)	38(1)
C(25)	9935(2)	8272(2)	1788(2)	49(1)
C(26)	10975(2)	8772(2)	2008(2)	47(1)
C(27)	11897(2)	8035(2)	2258(2)	45(1)
C(28)	11793(2)	6794(2)	2288(2)	42(1)

Table S20. Bond lengths [Å] and angles [°] for **CV8-Y**.

C(1)-O(1)	1.374(3)
C(1)-C(2)	1.378(3)
C(1)-C(6)	1.419(3)
C(2)-C(3)	1.403(3)
C(2)-H(2)	0.9500
C(3)-N(1)	1.371(3)
C(3)-C(4)	1.408(4)
C(4)-C(5)	1.374(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.406(3)
C(5)-H(5)	0.9500
C(6)-C(19)	1.441(3)
O(1)-C(7)	1.431(3)
C(7)-C(8)	1.509(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.516(3)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.515(3)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.524(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.525(4)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.512(4)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.507(4)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900

C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
N(1)-C(17)	1.452(3)
N(1)-C(15)	1.467(3)
C(15)-C(16)	1.509(4)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.514(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.362(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.437(3)
C(20)-C(22)	1.461(3)
C(21)-N(2)	1.147(3)
C(22)-N(3)	1.293(3)
C(22)-S(1)	1.765(2)
N(3)-C(23)	1.385(3)
S(1)-C(24)	1.728(3)
C(23)-C(28)	1.397(3)
C(23)-C(24)	1.411(3)
C(24)-C(25)	1.394(4)
C(25)-C(26)	1.377(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.392(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.373(4)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500

O(1)-C(1)-C(2)	122.1(2)
O(1)-C(1)-C(6)	115.6(2)
C(2)-C(1)-C(6)	122.2(2)
C(1)-C(2)-C(3)	121.5(2)
C(1)-C(2)-H(2)	119.3
C(3)-C(2)-H(2)	119.3
N(1)-C(3)-C(2)	121.1(2)
N(1)-C(3)-C(4)	121.8(2)
C(2)-C(3)-C(4)	117.1(2)
C(5)-C(4)-C(3)	120.8(2)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	123.3(2)
C(4)-C(5)-H(5)	118.4
C(6)-C(5)-H(5)	118.4
C(5)-C(6)-C(1)	115.1(2)
C(5)-C(6)-C(19)	125.4(2)
C(1)-C(6)-C(19)	119.5(2)
C(1)-O(1)-C(7)	117.73(19)
O(1)-C(7)-C(8)	109.2(2)
O(1)-C(7)-H(7A)	109.8
C(8)-C(7)-H(7A)	109.8
O(1)-C(7)-H(7B)	109.8
C(8)-C(7)-H(7B)	109.8
H(7A)-C(7)-H(7B)	108.3
C(7)-C(8)-C(9)	110.3(2)
C(7)-C(8)-H(8A)	109.6
C(9)-C(8)-H(8A)	109.6
C(7)-C(8)-H(8B)	109.6
C(9)-C(8)-H(8B)	109.6
H(8A)-C(8)-H(8B)	108.1
C(10)-C(9)-C(8)	115.3(2)
C(10)-C(9)-H(9A)	108.4
C(8)-C(9)-H(9A)	108.4
C(10)-C(9)-H(9B)	108.4

C(8)-C(9)-H(9B)	108.4
H(9A)-C(9)-H(9B)	107.5
C(9)-C(10)-C(11)	113.1(2)
C(9)-C(10)-H(10A)	109.0
C(11)-C(10)-H(10A)	109.0
C(9)-C(10)-H(10B)	109.0
C(11)-C(10)-H(10B)	109.0
H(10A)-C(10)-H(10B)	107.8
C(10)-C(11)-C(12)	115.4(2)
C(10)-C(11)-H(11A)	108.4
C(12)-C(11)-H(11A)	108.4
C(10)-C(11)-H(11B)	108.4
C(12)-C(11)-H(11B)	108.4
H(11A)-C(11)-H(11B)	107.5
C(13)-C(12)-C(11)	112.4(2)
C(13)-C(12)-H(12A)	109.1
C(11)-C(12)-H(12A)	109.1
C(13)-C(12)-H(12B)	109.1
C(11)-C(12)-H(12B)	109.1
H(12A)-C(12)-H(12B)	107.9
C(14)-C(13)-C(12)	114.6(3)
C(14)-C(13)-H(13A)	108.6
C(12)-C(13)-H(13A)	108.6
C(14)-C(13)-H(13B)	108.6
C(12)-C(13)-H(13B)	108.6
H(13A)-C(13)-H(13B)	107.6
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(3)-N(1)-C(17)	121.2(2)
C(3)-N(1)-C(15)	121.2(2)
C(17)-N(1)-C(15)	116.9(2)
N(1)-C(15)-C(16)	114.3(2)

N(1)-C(15)-H(15A)	108.7
C(16)-C(15)-H(15A)	108.7
N(1)-C(15)-H(15B)	108.7
C(16)-C(15)-H(15B)	108.7
H(15A)-C(15)-H(15B)	107.6
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
N(1)-C(17)-C(18)	114.8(2)
N(1)-C(17)-H(17A)	108.6
C(18)-C(17)-H(17A)	108.6
N(1)-C(17)-H(17B)	108.6
C(18)-C(17)-H(17B)	108.6
H(17A)-C(17)-H(17B)	107.5
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(20)-C(19)-C(6)	131.5(2)
C(20)-C(19)-H(19)	114.2
C(6)-C(19)-H(19)	114.2
C(19)-C(20)-C(21)	123.2(2)
C(19)-C(20)-C(22)	124.2(2)
C(21)-C(20)-C(22)	112.5(2)
N(2)-C(21)-C(20)	178.9(3)
N(3)-C(22)-C(20)	123.4(2)
N(3)-C(22)-S(1)	115.28(18)
C(20)-C(22)-S(1)	121.33(17)
C(22)-N(3)-C(23)	111.2(2)
C(24)-S(1)-C(22)	89.13(11)
N(3)-C(23)-C(28)	125.8(2)

N(3)-C(23)-C(24)	115.0(2)
C(28)-C(23)-C(24)	119.2(2)
C(25)-C(24)-C(23)	120.5(2)
C(25)-C(24)-S(1)	130.2(2)
C(23)-C(24)-S(1)	109.32(18)
C(26)-C(25)-C(24)	119.1(2)
C(26)-C(25)-H(25)	120.4
C(24)-C(25)-H(25)	120.4
C(25)-C(26)-C(27)	120.7(2)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
C(28)-C(27)-C(26)	120.9(2)
C(28)-C(27)-H(27)	119.6
C(26)-C(27)-H(27)	119.6
C(27)-C(28)-C(23)	119.7(2)
C(27)-C(28)-H(28)	120.2
C(23)-C(28)-H(28)	120.2

Symmetry transformations used to generate equivalent atoms:

Table S21. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **CV8-Y**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	35(1)	32(1)	42(1)	-2(1)	8(1)	1(1)
C(2)	32(1)	39(1)	40(1)	-2(1)	9(1)	-2(1)
C(3)	38(1)	39(1)	35(1)	-4(1)	8(1)	-7(1)
C(4)	36(1)	36(1)	61(2)	-2(1)	8(1)	0(1)
C(5)	24(1)	41(1)	59(2)	0(1)	4(1)	-2(1)
C(6)	29(1)	38(1)	43(1)	-3(1)	9(1)	-3(1)
O(1)	30(1)	34(1)	67(1)	-3(1)	8(1)	1(1)
C(7)	25(1)	40(1)	51(2)	-5(1)	8(1)	-2(1)
C(8)	37(2)	39(1)	59(2)	-2(1)	10(1)	0(1)
C(9)	38(2)	39(1)	59(2)	-4(1)	10(1)	-1(1)
C(10)	38(2)	39(1)	55(2)	-1(1)	9(1)	0(1)
C(11)	40(2)	42(2)	48(2)	-3(1)	7(1)	1(1)
C(12)	42(2)	44(2)	54(2)	-1(1)	9(1)	0(1)
C(13)	43(2)	60(2)	57(2)	7(2)	9(1)	6(1)
C(14)	64(2)	71(2)	98(3)	6(2)	3(2)	27(2)
N(1)	40(1)	35(1)	46(1)	-1(1)	9(1)	-7(1)
C(15)	46(2)	36(1)	48(2)	2(1)	12(1)	-3(1)
C(16)	55(2)	56(2)	50(2)	-4(1)	7(1)	12(1)
C(17)	37(1)	38(1)	53(2)	-3(1)	11(1)	-9(1)
C(18)	44(2)	53(2)	56(2)	-3(1)	3(1)	0(1)
C(19)	32(1)	40(1)	37(1)	-2(1)	6(1)	-1(1)
C(20)	30(1)	35(1)	39(1)	-2(1)	8(1)	0(1)
C(21)	36(1)	34(1)	47(2)	-2(1)	9(1)	-8(1)
N(2)	40(1)	39(1)	81(2)	1(1)	13(1)	1(1)
C(22)	26(1)	40(1)	37(1)	-2(1)	8(1)	-1(1)
N(3)	32(1)	31(1)	43(1)	1(1)	9(1)	-1(1)

S(1)	32(1)	38(1)	58(1)	4(1)	5(1)	2(1)
C(23)	34(1)	35(1)	40(1)	0(1)	11(1)	-1(1)
C(24)	33(1)	36(1)	46(2)	3(1)	10(1)	4(1)
C(25)	47(2)	39(1)	61(2)	4(1)	14(1)	6(1)
C(26)	45(2)	36(1)	62(2)	0(1)	17(1)	-4(1)
C(27)	44(2)	41(1)	52(2)	-6(1)	17(1)	-9(1)
C(28)	31(1)	42(1)	56(2)	1(1)	14(1)	-1(1)

Table S22. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **CV8-Y**.

	x	y	z	U(eq)
H(2)	4696	1321	1277	44
H(4)	7480	-728	1679	54
H(5)	8521	1012	1795	51
H(7A)	4201	3230	1604	47
H(7B)	4134	2996	766	47
H(8A)	4477	5143	650	54
H(8B)	4374	5322	1462	54
H(9A)	2638	4348	328	55
H(9B)	2542	4628	1129	55
H(10A)	2789	6468	130	53
H(10B)	2644	6728	924	53
H(11A)	845	5829	568	53
H(11B)	992	5675	-232	53
H(12A)	877	7979	441	56
H(12B)	1013	7818	-363	56
H(13A)	-737	6909	-725	64
H(13B)	-870	6993	82	64
H(14A)	-981	9109	0	121
H(14B)	-1893	8522	-655	121
H(14C)	-778	9063	-793	121
H(15A)	5325	-2754	1530	52
H(15B)	6530	-2166	1767	52
H(16A)	5334	-2479	298	82
H(16B)	6301	-3365	715	82
H(16C)	6573	-1984	560	82
H(17A)	3902	-204	1466	51

H(17B)	3837	-1640	1336	51
H(18A)	3906	85	237	79
H(18B)	2808	-589	311	79
H(18C)	3779	-1353	114	79
H(19)	7438	4084	1532	44
H(25)	9308	8777	1615	58
H(26)	11063	9629	1990	57
H(27)	12608	8396	2410	54
H(28)	12428	6299	2458	51

Table S23. Torsion angles [°] for **CV8-Y**.

O(1)-C(1)-C(2)-C(3)	178.6(2)
C(6)-C(1)-C(2)-C(3)	-0.2(4)
C(1)-C(2)-C(3)-N(1)	-179.6(2)
C(1)-C(2)-C(3)-C(4)	0.9(4)
N(1)-C(3)-C(4)-C(5)	179.9(2)
C(2)-C(3)-C(4)-C(5)	-0.7(4)
C(3)-C(4)-C(5)-C(6)	-0.3(4)
C(4)-C(5)-C(6)-C(1)	1.0(4)
C(4)-C(5)-C(6)-C(19)	-178.2(3)
O(1)-C(1)-C(6)-C(5)	-179.6(2)
C(2)-C(1)-C(6)-C(5)	-0.7(4)
O(1)-C(1)-C(6)-C(19)	-0.3(3)
C(2)-C(1)-C(6)-C(19)	178.5(2)
C(2)-C(1)-O(1)-C(7)	0.1(3)
C(6)-C(1)-O(1)-C(7)	179.0(2)
C(1)-O(1)-C(7)-C(8)	-173.0(2)
O(1)-C(7)-C(8)-C(9)	172.3(2)
C(7)-C(8)-C(9)-C(10)	-176.0(2)
C(8)-C(9)-C(10)-C(11)	177.7(2)
C(9)-C(10)-C(11)-C(12)	175.8(2)
C(10)-C(11)-C(12)-C(13)	-179.4(2)
C(11)-C(12)-C(13)-C(14)	176.9(3)
C(2)-C(3)-N(1)-C(17)	3.4(4)
C(4)-C(3)-N(1)-C(17)	-177.2(2)
C(2)-C(3)-N(1)-C(15)	173.5(2)
C(4)-C(3)-N(1)-C(15)	-7.1(4)
C(3)-N(1)-C(15)-C(16)	-80.8(3)
C(17)-N(1)-C(15)-C(16)	89.7(3)
C(3)-N(1)-C(17)-C(18)	78.6(3)
C(15)-N(1)-C(17)-C(18)	-91.9(3)
C(5)-C(6)-C(19)-C(20)	-4.9(5)
C(1)-C(6)-C(19)-C(20)	175.9(2)
C(6)-C(19)-C(20)-C(21)	-1.6(4)
C(6)-C(19)-C(20)-C(22)	-178.6(2)

C(19)-C(20)-C(21)-N(2)	-42(17)
C(22)-C(20)-C(21)-N(2)	135(17)
C(19)-C(20)-C(22)-N(3)	174.5(2)
C(21)-C(20)-C(22)-N(3)	-2.7(3)
C(19)-C(20)-C(22)-S(1)	-4.8(3)
C(21)-C(20)-C(22)-S(1)	177.97(17)
C(20)-C(22)-N(3)-C(23)	-178.6(2)
S(1)-C(22)-N(3)-C(23)	0.8(3)
N(3)-C(22)-S(1)-C(24)	-0.6(2)
C(20)-C(22)-S(1)-C(24)	178.8(2)
C(22)-N(3)-C(23)-C(28)	178.4(2)
C(22)-N(3)-C(23)-C(24)	-0.6(3)
N(3)-C(23)-C(24)-C(25)	-179.7(2)
C(28)-C(23)-C(24)-C(25)	1.3(4)
N(3)-C(23)-C(24)-S(1)	0.1(3)
C(28)-C(23)-C(24)-S(1)	-178.9(2)
C(22)-S(1)-C(24)-C(25)	-180.0(3)
C(22)-S(1)-C(24)-C(23)	0.25(19)
C(23)-C(24)-C(25)-C(26)	-1.2(4)
S(1)-C(24)-C(25)-C(26)	179.0(2)
C(24)-C(25)-C(26)-C(27)	0.5(4)
C(25)-C(26)-C(27)-C(28)	0.2(4)
C(26)-C(27)-C(28)-C(23)	-0.2(4)
N(3)-C(23)-C(28)-C(27)	-179.5(2)
C(24)-C(23)-C(28)-C(27)	-0.6(4)
O(1)-C(1)-C(2)-C(3)	178.6(2)
C(6)-C(1)-C(2)-C(3)	-0.2(4)
C(1)-C(2)-C(3)-N(1)	-179.6(2)
C(1)-C(2)-C(3)-C(4)	0.9(4)
N(1)-C(3)-C(4)-C(5)	179.9(2)
C(2)-C(3)-C(4)-C(5)	-0.7(4)
C(3)-C(4)-C(5)-C(6)	-0.3(4)
C(4)-C(5)-C(6)-C(1)	1.0(4)
C(4)-C(5)-C(6)-C(19)	-178.2(3)
O(1)-C(1)-C(6)-C(5)	-179.6(2)
C(2)-C(1)-C(6)-C(5)	-0.7(4)

O(1)-C(1)-C(6)-C(19)	-0.3(3)
C(2)-C(1)-C(6)-C(19)	178.5(2)
C(2)-C(1)-O(1)-C(7)	0.1(3)
C(6)-C(1)-O(1)-C(7)	179.0(2)
C(1)-O(1)-C(7)-C(8)	-173.0(2)
O(1)-C(7)-C(8)-C(9)	172.3(2)
C(7)-C(8)-C(9)-C(10)	-176.0(2)
C(8)-C(9)-C(10)-C(11)	177.7(2)
C(9)-C(10)-C(11)-C(12)	175.8(2)
C(10)-C(11)-C(12)-C(13)	-179.4(2)
C(11)-C(12)-C(13)-C(14)	176.9(3)
C(2)-C(3)-N(1)-C(17)	3.4(4)
C(4)-C(3)-N(1)-C(17)	-177.2(2)
C(2)-C(3)-N(1)-C(15)	173.5(2)
C(4)-C(3)-N(1)-C(15)	-7.1(4)
C(3)-N(1)-C(15)-C(16)	-80.8(3)
C(17)-N(1)-C(15)-C(16)	89.7(3)
C(3)-N(1)-C(17)-C(18)	78.6(3)
C(15)-N(1)-C(17)-C(18)	-91.9(3)
C(5)-C(6)-C(19)-C(20)	-4.9(5)
C(1)-C(6)-C(19)-C(20)	175.9(2)
C(6)-C(19)-C(20)-C(21)	-1.6(4)
C(6)-C(19)-C(20)-C(22)	-178.6(2)
C(19)-C(20)-C(21)-N(2)	-42(17)
C(22)-C(20)-C(21)-N(2)	135(17)
C(19)-C(20)-C(22)-N(3)	174.5(2)
C(21)-C(20)-C(22)-N(3)	-2.7(3)
C(19)-C(20)-C(22)-S(1)	-4.8(3)
C(21)-C(20)-C(22)-S(1)	177.97(17)
C(20)-C(22)-N(3)-C(23)	-178.6(2)
S(1)-C(22)-N(3)-C(23)	0.8(3)
N(3)-C(22)-S(1)-C(24)	-0.6(2)
C(20)-C(22)-S(1)-C(24)	178.8(2)
C(22)-N(3)-C(23)-C(28)	178.4(2)
C(22)-N(3)-C(23)-C(24)	-0.6(3)
N(3)-C(23)-C(24)-C(25)	-179.7(2)

C(28)-C(23)-C(24)-C(25)	1.3(4)
N(3)-C(23)-C(24)-S(1)	0.1(3)
C(28)-C(23)-C(24)-S(1)	-178.9(2)
C(22)-S(1)-C(24)-C(25)	-180.0(3)
C(22)-S(1)-C(24)-C(23)	0.25(19)
C(23)-C(24)-C(25)-C(26)	-1.2(4)
S(1)-C(24)-C(25)-C(26)	179.0(2)
C(24)-C(25)-C(26)-C(27)	0.5(4)
C(25)-C(26)-C(27)-C(28)	0.2(4)
C(26)-C(27)-C(28)-C(23)	-0.2(4)
N(3)-C(23)-C(28)-C(27)	-179.5(2)
C(24)-C(23)-C(28)-C(27)	-0.6(4)

Symmetry transformations used to generate equivalent atoms:

Table S24. Crystal data and structure refinement for **CV10-O**.

Identification code	**CV10-O**
Empirical formula	$C_{30}\ H_{39}\ N_3\ O\ S$
Formula weight	489.70
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 8.1239(12) Å b = 16.449(3) Å c = 21.785(4) Å
Volume	2768.3(8) $Å^3$
Z	4
Density (calculated)	1.175 Mg/m^3
Absorption coefficient	0.143 mm^{-1}
F(000)	1056
Crystal size	0.322 x 0.109 x 0.070 mm^3
Theta range for data collection	1.953 to 28.288°.
Index ranges	-10<=h<=10, -21<=k<=21, -29<=l<=28
Reflections collected	130915
Independent reflections	13700 [R(int) = 0.1501]
Completeness to theta = 26.03°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13700 / 0 / 656
Goodness-of-fit on F^2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0666, wR2 = 0.1407
R indices (all data)	R1 = 0.1849, wR2 = 0.1858
Largest diff. peak and hole	0.516 and -0.344 $e.Å^{-3}$

Table S25. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **CV10-O**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6428(1)	1457(1)	2264(1)	54(1)
S(2)	5458(1)	3832(1)	2719(1)	53(1)
O(1)	7843(2)	-633(1)	4422(1)	49(1)
O(2)	2453(3)	5659(1)	557(1)	53(1)
N(1)	6608(3)	-14(2)	2496(1)	48(1)
N(2)	6388(5)	2682(2)	3869(1)	91(1)
N(3)	6753(3)	840(2)	6488(1)	61(1)
N(4)	4331(3)	5156(2)	2469(1)	47(1)
N(5)	5320(4)	2592(2)	1112(1)	80(1)
N(6)	2317(4)	3949(2)	-1585(1)	84(1)
C(1)	6493(3)	602(2)	1624(1)	44(1)
C(2)	6474(4)	573(2)	976(1)	58(1)
C(3)	6578(4)	-187(2)	563(2)	60(1)
C(4)	6666(4)	-916(2)	772(2)	64(1)
C(5)	6668(4)	-893(2)	1410(2)	60(1)
C(6)	6586(3)	-125(2)	1842(1)	43(1)
C(7)	6565(3)	777(2)	2772(1)	43(1)
C(8)	6630(3)	1099(2)	3469(1)	44(1)
C(9)	6478(4)	1974(2)	3700(1)	58(1)
C(10)	6868(3)	570(2)	3856(1)	44(1)
C(11)	6892(3)	688(2)	4534(1)	40(1)
C(12)	6418(3)	1391(2)	4947(1)	45(1)
C(13)	6374(3)	1459(2)	5581(1)	46(1)
C(14)	6842(4)	810(2)	5861(1)	46(1)
C(15)	7371(3)	112(2)	5465(1)	44(1)
C(16)	7373(3)	45(2)	4821(1)	40(1)

C(17)	5877(5)	1516(2)	6902(2)	79(1)
C(18)	7186(5)	2207(3)	7224(2)	90(1)
C(19)	7421(4)	230(2)	6803(1)	52(1)
C(20)	9328(4)	349(2)	6956(2)	71(1)
C(21)	8341(4)	-1307(2)	4683(1)	45(1)
C(22)	8711(4)	-1998(2)	4147(1)	48(1)
C(23)	9321(4)	-2714(2)	4399(1)	46(1)
C(24)	9577(4)	-3482(2)	3887(1)	49(1)
C(25)	10188(4)	-4179(2)	4161(1)	51(1)
C(26)	10279(4)	-4992(2)	3663(1)	50(1)
C(27)	10800(4)	-5684(2)	3962(2)	65(1)
C(28)	10898(5)	-6507(2)	3496(2)	70(1)
C(29)	11490(7)	-7166(3)	3834(2)	116(2)
C(30)	11585(7)	-7978(3)	3424(3)	141(2)
C(31)	5364(3)	4681(2)	3359(1)	44(1)
C(32)	5836(4)	4779(2)	4019(1)	56(1)
C(33)	5650(4)	5530(2)	4433(1)	55(1)
C(34)	5003(4)	6166(2)	4212(1)	52(1)
C(35)	4545(4)	6075(2)	3564(1)	50(1)
C(36)	4729(3)	5328(2)	3130(1)	41(1)
C(37)	4657(3)	4406(2)	2196(1)	44(1)
C(38)	4380(3)	4050(2)	1498(1)	45(1)
C(39)	4883(4)	3237(2)	1276(1)	54(1)
C(40)	3700(3)	4494(2)	1102(1)	45(1)
C(41)	3283(3)	4308(2)	418(1)	44(1)
C(42)	3463(4)	3551(2)	-13(1)	54(1)
C(43)	3127(4)	3417(2)	-664(1)	63(1)
C(44)	2563(4)	4053(2)	-940(1)	58(1)

C(45)	2300(3)	4800(2)	-520(1)	47(1)
C(46)	2663(3)	4930(2)	136(1)	42(1)
C(49)	1595(4)	4546(2)	-1892(1)	54(1)
C(50)	-284(4)	4469(2)	-1952(2)	70(1)
C(51)	1974(4)	6347(2)	312(1)	49(1)
C(52)	2031(4)	7105(2)	877(1)	52(1)
C(53)	1730(4)	7885(2)	651(1)	55(1)
C(54)	1737(4)	8682(2)	1180(1)	51(1)
C(55)	1628(4)	9451(2)	919(2)	58(1)
C(56)	1467(4)	10262(2)	1397(1)	55(1)
C(57)	1271(4)	10990(2)	1085(2)	61(1)
C(58)	927(4)	11796(2)	1518(2)	59(1)
C(59)	345(5)	12422(2)	1153(2)	72(1)
C(60)	-61(5)	13225(2)	1573(2)	90(1)
C(47A)	1771(12)	2995(8)	-2017(5)	48(3)
C(48A)	3422(13)	2810(9)	-2237(5)	58(4)
C(47B)	3213(9)	3316(6)	-2011(3)	50(2)
C(48B)	1886(10)	2543(6)	-2290(5)	62(2)

Table S26. Bond lengths [Å] and angles [°] for **CV10-O**.

S(1)-C(1)	1.735(3)
S(1)-C(7)	1.756(3)
S(2)-C(31)	1.734(3)
S(2)-C(37)	1.756(3)
O(1)-C(16)	1.364(3)
O(1)-C(21)	1.439(3)
O(2)-C(46)	1.364(3)
O(2)-C(51)	1.435(3)
N(1)-C(7)	1.300(3)
N(1)-C(6)	1.389(3)
N(2)-C(9)	1.147(4)
N(3)-C(14)	1.365(3)
N(3)-C(19)	1.462(3)
N(3)-C(17)	1.555(4)
N(4)-C(37)	1.306(3)
N(4)-C(36)	1.386(3)
N(5)-C(39)	1.147(4)
N(6)-C(44)	1.360(4)
N(6)-C(49)	1.451(4)
N(6)-C(47B)	1.535(10)
N(6)-C(47A)	1.601(14)
C(1)-C(6)	1.396(4)
C(1)-C(2)	1.399(4)
C(2)-C(3)	1.370(4)
C(2)-H(2)	0.9400
C(3)-C(4)	1.390(4)
C(3)-H(3)	0.9400
C(4)-C(5)	1.379(4)
C(4)-H(4)	0.9400
C(5)-C(6)	1.396(4)
C(5)-H(5)	0.9400
C(7)-C(8)	1.474(4)
C(8)-C(10)	1.363(4)
C(8)-C(9)	1.431(4)

C(10)-C(11)	1.439(4)
C(10)-H(10)	0.9400
C(11)-C(12)	1.407(4)
C(11)-C(16)	1.421(4)
C(12)-C(13)	1.365(4)
C(12)-H(12)	0.9400
C(13)-C(14)	1.417(4)
C(13)-H(13)	0.9400
C(14)-C(15)	1.407(4)
C(15)-C(16)	1.379(4)
C(15)-H(15)	0.9400
C(17)-C(18)	1.435(5)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(18)-H(18C)	0.9700
C(19)-C(20)	1.521(4)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(20)-H(20C)	0.9700
C(21)-C(22)	1.507(4)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(22)-C(23)	1.522(4)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(23)-C(24)	1.523(4)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(24)-C(25)	1.520(4)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(25)-C(26)	1.520(4)

C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(26)-C(27)	1.518(4)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(27)-C(28)	1.500(4)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(28)-C(29)	1.539(5)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(29)-C(30)	1.431(5)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(30)-H(30A)	0.9700
C(30)-H(30B)	0.9700
C(30)-H(30C)	0.9700
C(31)-C(32)	1.403(4)
C(31)-C(36)	1.404(4)
C(32)-C(33)	1.378(4)
C(32)-H(32)	0.9400
C(33)-C(34)	1.380(4)
C(33)-H(33)	0.9400
C(34)-C(35)	1.380(4)
C(34)-H(34)	0.9400
C(35)-C(36)	1.394(4)
C(35)-H(35)	0.9400
C(37)-C(38)	1.469(4)
C(38)-C(40)	1.364(4)
C(38)-C(39)	1.433(4)
C(40)-C(41)	1.433(4)
C(40)-H(40)	0.9400
C(41)-C(42)	1.402(4)
C(41)-C(46)	1.422(4)
C(42)-C(43)	1.368(4)
C(42)-H(42)	0.9400

C(43)-C(44)	1.418(4)
C(43)-H(43)	0.9400
C(44)-C(45)	1.399(4)
C(45)-C(46)	1.381(4)
C(45)-H(45)	0.9400
C(49)-C(50)	1.503(4)
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(50)-H(50A)	0.9700
C(50)-H(50B)	0.9700
C(50)-H(50C)	0.9700
C(51)-C(52)	1.516(4)
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(52)-C(53)	1.515(4)
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(53)-C(54)	1.520(4)
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(54)-C(55)	1.515(4)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(55)-C(56)	1.511(4)
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(56)-C(57)	1.528(4)
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(57)-C(58)	1.507(4)
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(58)-C(59)	1.527(4)
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(59)-C(60)	1.511(4)

C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(60)-H(60A)	0.9700
C(60)-H(60B)	0.9700
C(60)-H(60C)	0.9700
C(47A)-C(48A)	1.52(2)
C(47A)-H(47A)	0.9800
C(47A)-H(47B)	0.9800
C(48A)-H(48A)	0.9700
C(48A)-H(48B)	0.9700
C(48A)-H(48C)	0.9700
C(47B)-C(48B)	1.514(14)
C(47B)-H(47C)	0.9800
C(47B)-H(47D)	0.9800
C(48B)-H(48D)	0.9700
C(48B)-H(48E)	0.9700
C(48B)-H(48F)	0.9700

C(1)-S(1)-C(7)	88.69(14)
C(31)-S(2)-C(37)	88.87(14)
C(16)-O(1)-C(21)	118.4(2)
C(46)-O(2)-C(51)	118.9(2)
C(7)-N(1)-C(6)	110.0(2)
C(14)-N(3)-C(19)	122.5(2)
C(14)-N(3)-C(17)	121.3(2)
C(19)-N(3)-C(17)	116.2(2)
C(37)-N(4)-C(36)	110.4(2)
C(44)-N(6)-C(49)	123.4(3)
C(44)-N(6)-C(47B)	119.9(3)
C(49)-N(6)-C(47B)	114.9(3)
C(44)-N(6)-C(47A)	116.0(4)
C(49)-N(6)-C(47A)	111.4(4)
C(6)-C(1)-C(2)	121.1(3)

C(6)-C(1)-S(1)	109.4(2)
C(2)-C(1)-S(1)	129.5(2)
C(3)-C(2)-C(1)	118.1(3)
C(3)-C(2)-H(2)	121.0
C(1)-C(2)-H(2)	121.0
C(2)-C(3)-C(4)	121.6(3)
C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(5)-C(4)-C(3)	120.6(3)
C(5)-C(4)-H(4)	119.7
C(3)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	119.0(3)
C(4)-C(5)-H(5)	120.5
C(6)-C(5)-H(5)	120.5
N(1)-C(6)-C(5)	124.6(3)
N(1)-C(6)-C(1)	115.7(3)
C(5)-C(6)-C(1)	119.7(3)
N(1)-C(7)-C(8)	122.8(2)
N(1)-C(7)-S(1)	116.1(2)
C(8)-C(7)-S(1)	121.1(2)
C(10)-C(8)-C(9)	123.9(3)
C(10)-C(8)-C(7)	119.6(3)
C(9)-C(8)-C(7)	116.5(2)
N(2)-C(9)-C(8)	177.7(4)
C(8)-C(10)-C(11)	131.9(3)
C(8)-C(10)-H(10)	114.1
C(11)-C(10)-H(10)	114.1
C(12)-C(11)-C(16)	115.7(2)
C(12)-C(11)-C(10)	125.1(3)
C(16)-C(11)-C(10)	119.1(3)
C(13)-C(12)-C(11)	123.3(3)

C(13)-C(12)-H(12)	118.3
C(11)-C(12)-H(12)	118.3
C(12)-C(13)-C(14)	120.4(3)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
N(3)-C(14)-C(15)	120.4(3)
N(3)-C(14)-C(13)	122.1(3)
C(15)-C(14)-C(13)	117.5(3)
C(16)-C(15)-C(14)	121.2(3)
C(16)-C(15)-H(15)	119.4
C(14)-C(15)-H(15)	119.4
O(1)-C(16)-C(15)	122.6(2)
O(1)-C(16)-C(11)	115.6(2)
C(15)-C(16)-C(11)	121.7(3)
C(18)-C(17)-N(3)	105.6(3)
C(18)-C(17)-H(17A)	110.6
N(3)-C(17)-H(17A)	110.6
C(18)-C(17)-H(17B)	110.6
N(3)-C(17)-H(17B)	110.6
H(17A)-C(17)-H(17B)	108.8
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(3)-C(19)-C(20)	114.8(3)
N(3)-C(19)-H(19A)	108.6
C(20)-C(19)-H(19A)	108.6
N(3)-C(19)-H(19B)	108.6
C(20)-C(19)-H(19B)	108.6

H(19A)-C(19)-H(19B)	107.5
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(1)-C(21)-C(22)	108.5(2)
O(1)-C(21)-H(21A)	110.0
C(22)-C(21)-H(21A)	110.0
O(1)-C(21)-H(21B)	110.0
C(22)-C(21)-H(21B)	110.0
H(21A)-C(21)-H(21B)	108.4
C(21)-C(22)-C(23)	111.0(2)
C(21)-C(22)-H(22A)	109.4
C(23)-C(22)-H(22A)	109.4
C(21)-C(22)-H(22B)	109.4
C(23)-C(22)-H(22B)	109.4
H(22A)-C(22)-H(22B)	108.0
C(22)-C(23)-C(24)	115.1(2)
C(22)-C(23)-H(23A)	108.5
C(24)-C(23)-H(23A)	108.5
C(22)-C(23)-H(23B)	108.5
C(24)-C(23)-H(23B)	108.5
H(23A)-C(23)-H(23B)	107.5
C(25)-C(24)-C(23)	113.2(2)
C(25)-C(24)-H(24A)	108.9
C(23)-C(24)-H(24A)	108.9
C(25)-C(24)-H(24B)	108.9
C(23)-C(24)-H(24B)	108.9
H(24A)-C(24)-H(24B)	107.7

C(24)-C(25)-C(26)	114.6(2)
C(24)-C(25)-H(25A)	108.6
C(26)-C(25)-H(25A)	108.6
C(24)-C(25)-H(25B)	108.6
C(26)-C(25)-H(25B)	108.6
H(25A)-C(25)-H(25B)	107.6
C(27)-C(26)-C(25)	112.5(2)
C(27)-C(26)-H(26A)	109.1
C(25)-C(26)-H(26A)	109.1
C(27)-C(26)-H(26B)	109.1
C(25)-C(26)-H(26B)	109.1
H(26A)-C(26)-H(26B)	107.8
C(28)-C(27)-C(26)	115.2(3)
C(28)-C(27)-H(27A)	108.5
C(26)-C(27)-H(27A)	108.5
C(28)-C(27)-H(27B)	108.5
C(26)-C(27)-H(27B)	108.5
H(27A)-C(27)-H(27B)	107.5
C(27)-C(28)-C(29)	112.2(3)
C(27)-C(28)-H(28A)	109.2
C(29)-C(28)-H(28A)	109.2
C(27)-C(28)-H(28B)	109.2
C(29)-C(28)-H(28B)	109.2
H(28A)-C(28)-H(28B)	107.9
C(30)-C(29)-C(28)	115.9(4)
C(30)-C(29)-H(29A)	108.3
C(28)-C(29)-H(29A)	108.3
C(30)-C(29)-H(29B)	108.3
C(28)-C(29)-H(29B)	108.3
H(29A)-C(29)-H(29B)	107.4
C(29)-C(30)-H(30A)	109.5

C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(36)	121.0(3)
C(32)-C(31)-S(2)	129.4(2)
C(36)-C(31)-S(2)	109.6(2)
C(33)-C(32)-C(31)	117.9(3)
C(33)-C(32)-H(32)	121.1
C(31)-C(32)-H(32)	121.1
C(32)-C(33)-C(34)	121.6(3)
C(32)-C(33)-H(33)	119.2
C(34)-C(33)-H(33)	119.2
C(35)-C(34)-C(33)	120.9(3)
C(35)-C(34)-H(34)	119.5
C(33)-C(34)-H(34)	119.5
C(34)-C(35)-C(36)	119.2(3)
C(34)-C(35)-H(35)	120.4
C(36)-C(35)-H(35)	120.4
N(4)-C(36)-C(35)	125.3(3)
N(4)-C(36)-C(31)	115.3(3)
C(35)-C(36)-C(31)	119.4(3)
N(4)-C(37)-C(38)	123.0(3)
N(4)-C(37)-S(2)	115.8(2)
C(38)-C(37)-S(2)	121.2(2)
C(40)-C(38)-C(39)	123.8(3)
C(40)-C(38)-C(37)	120.2(3)
C(39)-C(38)-C(37)	116.0(2)
N(5)-C(39)-C(38)	178.1(3)
C(38)-C(40)-C(41)	132.3(3)

C(38)-C(40)-H(40)	113.8
C(41)-C(40)-H(40)	113.8
C(42)-C(41)-C(46)	115.6(3)
C(42)-C(41)-C(40)	125.0(3)
C(46)-C(41)-C(40)	119.3(3)
C(43)-C(42)-C(41)	123.0(3)
C(43)-C(42)-H(42)	118.5
C(41)-C(42)-H(42)	118.5
C(42)-C(43)-C(44)	120.8(3)
C(42)-C(43)-H(43)	119.6
C(44)-C(43)-H(43)	119.6
N(6)-C(44)-C(45)	121.2(3)
N(6)-C(44)-C(43)	121.5(3)
C(45)-C(44)-C(43)	117.3(3)
C(46)-C(45)-C(44)	121.2(3)
C(46)-C(45)-H(45)	119.4
C(44)-C(45)-H(45)	119.4
O(2)-C(46)-C(45)	122.5(2)
O(2)-C(46)-C(41)	115.5(2)
C(45)-C(46)-C(41)	121.9(3)
N(6)-C(49)-C(50)	114.2(3)
N(6)-C(49)-H(49A)	108.7
C(50)-C(49)-H(49A)	108.7
N(6)-C(49)-H(49B)	108.7
C(50)-C(49)-H(49B)	108.7
H(49A)-C(49)-H(49B)	107.6
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5

H(50B)-C(50)-H(50C)	109.5
O(2)-C(51)-C(52)	108.0(2)
O(2)-C(51)-H(51A)	110.1
C(52)-C(51)-H(51A)	110.1
O(2)-C(51)-H(51B)	110.1
C(52)-C(51)-H(51B)	110.1
H(51A)-C(51)-H(51B)	108.4
C(53)-C(52)-C(51)	110.9(2)
C(53)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52A)	109.5
C(53)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	108.0
C(52)-C(53)-C(54)	115.3(2)
C(52)-C(53)-H(53A)	108.4
C(54)-C(53)-H(53A)	108.4
C(52)-C(53)-H(53B)	108.4
C(54)-C(53)-H(53B)	108.4
H(53A)-C(53)-H(53B)	107.5
C(55)-C(54)-C(53)	111.8(2)
C(55)-C(54)-H(54A)	109.3
C(53)-C(54)-H(54A)	109.3
C(55)-C(54)-H(54B)	109.3
C(53)-C(54)-H(54B)	109.3
H(54A)-C(54)-H(54B)	107.9
C(56)-C(55)-C(54)	116.1(3)
C(56)-C(55)-H(55A)	108.3
C(54)-C(55)-H(55A)	108.3
C(56)-C(55)-H(55B)	108.3
C(54)-C(55)-H(55B)	108.3
H(55A)-C(55)-H(55B)	107.4

C(55)-C(56)-C(57)	112.4(3)
C(55)-C(56)-H(56A)	109.1
C(57)-C(56)-H(56A)	109.1
C(55)-C(56)-H(56B)	109.1
C(57)-C(56)-H(56B)	109.1
H(56A)-C(56)-H(56B)	107.8
C(58)-C(57)-C(56)	115.5(3)
C(58)-C(57)-H(57A)	108.4
C(56)-C(57)-H(57A)	108.4
C(58)-C(57)-H(57B)	108.4
C(56)-C(57)-H(57B)	108.4
H(57A)-C(57)-H(57B)	107.5
C(57)-C(58)-C(59)	113.0(3)
C(57)-C(58)-H(58A)	109.0
C(59)-C(58)-H(58A)	109.0
C(57)-C(58)-H(58B)	109.0
C(59)-C(58)-H(58B)	109.0
H(58A)-C(58)-H(58B)	107.8
C(60)-C(59)-C(58)	114.2(3)
C(60)-C(59)-H(59A)	108.7
C(58)-C(59)-H(59A)	108.7
C(60)-C(59)-H(59B)	108.7
C(58)-C(59)-H(59B)	108.7
H(59A)-C(59)-H(59B)	107.6
C(59)-C(60)-H(60A)	109.5
C(59)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(59)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(48A)-C(47A)-N(6)	100.5(10)

C(48A)-C(47A)-H(47A)	111.7
N(6)-C(47A)-H(47A)	111.7
C(48A)-C(47A)-H(47B)	111.7
N(6)-C(47A)-H(47B)	111.7
H(47A)-C(47A)-H(47B)	109.4
C(47A)-C(48A)-H(48A)	109.5
C(47A)-C(48A)-H(48B)	109.5
H(48A)-C(48A)-H(48B)	109.5
C(47A)-C(48A)-H(48C)	109.5
H(48A)-C(48A)-H(48C)	109.5
H(48B)-C(48A)-H(48C)	109.5
C(48B)-C(47B)-N(6)	104.2(7)
C(48B)-C(47B)-H(47C)	110.9
N(6)-C(47B)-H(47C)	110.9
C(48B)-C(47B)-H(47D)	110.9
N(6)-C(47B)-H(47D)	110.9
H(47C)-C(47B)-H(47D)	108.9
C(47B)-C(48B)-H(48D)	109.5
C(47B)-C(48B)-H(48E)	109.5
H(48D)-C(48B)-H(48E)	109.5
C(47B)-C(48B)-H(48F)	109.5
H(48D)-C(48B)-H(48F)	109.5
H(48E)-C(48B)-H(48F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 27. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **CV10-O**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	79(1)	43(1)	44(1)	17(1)	10(1)	14(1)
S(2)	72(1)	44(1)	43(1)	14(1)	2(1)	16(1)
O(1)	68(1)	45(1)	39(1)	12(1)	14(1)	21(1)
O(2)	85(2)	41(1)	36(1)	8(1)	9(1)	24(1)
N(1)	64(2)	42(2)	42(1)	16(1)	11(1)	13(1)
N(2)	162(3)	51(2)	66(2)	18(2)	19(2)	31(2)
N(3)	98(2)	57(2)	35(1)	9(1)	16(1)	38(2)
N(4)	54(2)	46(2)	42(1)	12(1)	2(1)	11(1)
N(5)	114(3)	67(2)	62(2)	14(2)	4(2)	40(2)
N(6)	161(3)	64(2)	32(2)	4(1)	8(2)	68(2)
C(1)	51(2)	43(2)	41(2)	12(1)	8(1)	9(1)
C(2)	82(2)	54(2)	44(2)	20(2)	13(2)	18(2)
C(3)	81(2)	66(2)	40(2)	16(2)	17(2)	22(2)
C(4)	92(3)	56(2)	45(2)	7(2)	18(2)	23(2)
C(5)	86(2)	50(2)	53(2)	18(2)	17(2)	20(2)
C(6)	51(2)	42(2)	40(2)	14(1)	11(1)	11(1)
C(7)	48(2)	45(2)	40(2)	17(1)	8(1)	10(1)
C(8)	51(2)	42(2)	40(2)	11(1)	7(1)	10(1)
C(9)	91(2)	50(2)	40(2)	19(2)	13(2)	17(2)
C(10)	49(2)	43(2)	42(2)	12(1)	9(1)	10(1)
C(11)	45(2)	39(2)	37(2)	10(1)	6(1)	7(1)
C(12)	53(2)	39(2)	43(2)	10(1)	4(1)	10(1)
C(13)	60(2)	39(2)	40(2)	8(1)	8(1)	15(1)
C(14)	58(2)	44(2)	35(2)	7(1)	8(1)	11(1)
C(15)	56(2)	41(2)	36(2)	12(1)	4(1)	12(1)

C(16)	46(2)	37(2)	37(2)	8(1)	6(1)	8(1)
C(17)	83(3)	91(3)	64(2)	40(2)	-8(2)	-10(2)
C(18)	82(3)	108(3)	84(3)	52(3)	-3(2)	-3(2)
C(19)	68(2)	51(2)	43(2)	18(2)	13(2)	19(2)
C(20)	71(2)	79(3)	60(2)	14(2)	4(2)	13(2)
C(21)	56(2)	42(2)	40(2)	11(1)	8(1)	13(1)
C(22)	58(2)	45(2)	45(2)	13(2)	11(1)	12(1)
C(23)	51(2)	43(2)	45(2)	12(1)	7(1)	10(1)
C(24)	57(2)	45(2)	49(2)	13(2)	16(1)	15(1)
C(25)	52(2)	48(2)	54(2)	14(2)	10(2)	14(1)
C(26)	54(2)	47(2)	52(2)	15(2)	13(1)	15(1)
C(27)	84(2)	55(2)	63(2)	20(2)	8(2)	28(2)
C(28)	88(3)	57(2)	73(2)	25(2)	17(2)	29(2)
C(29)	199(5)	65(3)	93(3)	26(3)	18(3)	58(3)
C(30)	201(6)	75(3)	151(5)	29(3)	9(4)	59(4)
C(31)	51(2)	41(2)	42(2)	12(1)	7(1)	6(1)
C(32)	72(2)	50(2)	46(2)	18(2)	2(2)	9(2)
C(33)	71(2)	54(2)	36(2)	11(2)	1(2)	1(2)
C(34)	62(2)	46(2)	44(2)	4(2)	7(2)	4(2)
C(35)	58(2)	45(2)	48(2)	13(2)	7(2)	12(1)
C(36)	41(2)	40(2)	42(2)	12(1)	3(1)	6(1)
C(37)	48(2)	42(2)	45(2)	14(1)	6(1)	9(1)
C(38)	53(2)	43(2)	41(2)	11(1)	5(1)	10(1)
C(39)	67(2)	52(2)	45(2)	15(2)	1(2)	18(2)
C(40)	52(2)	40(2)	42(2)	8(1)	6(1)	9(1)
C(41)	52(2)	40(2)	38(2)	9(1)	7(1)	9(1)
C(42)	76(2)	43(2)	44(2)	10(2)	2(2)	22(2)
C(43)	96(3)	50(2)	42(2)	2(2)	6(2)	35(2)

C(44)	89(2)	49(2)	36(2)	6(2)	6(2)	29(2)
C(45)	62(2)	41(2)	39(2)	11(1)	7(1)	17(1)
C(46)	53(2)	38(2)	36(2)	8(1)	7(1)	14(1)
C(49)	75(2)	54(2)	37(2)	11(2)	11(2)	22(2)
C(50)	80(3)	64(2)	63(2)	13(2)	12(2)	6(2)
C(51)	69(2)	42(2)	40(2)	14(1)	8(1)	18(2)
C(52)	72(2)	45(2)	39(2)	9(2)	8(2)	16(2)
C(53)	74(2)	45(2)	48(2)	14(2)	10(2)	14(2)
C(54)	68(2)	40(2)	47(2)	10(2)	11(2)	12(2)
C(55)	81(2)	43(2)	53(2)	14(2)	21(2)	14(2)
C(56)	68(2)	46(2)	55(2)	16(2)	12(2)	13(2)
C(57)	81(2)	45(2)	60(2)	16(2)	16(2)	12(2)
C(58)	74(2)	47(2)	60(2)	16(2)	15(2)	14(2)
C(59)	88(3)	52(2)	77(3)	23(2)	7(2)	12(2)
C(60)	104(3)	57(2)	110(3)	19(2)	13(2)	29(2)
C(47A)	55(6)	54(7)	36(5)	12(5)	3(4)	14(5)
C(48A)	77(7)	50(7)	51(6)	7(5)	22(5)	28(5)
C(47B)	66(5)	42(5)	45(4)	11(4)	14(3)	14(3)
C(48B)	68(5)	53(5)	60(5)	7(4)	3(4)	7(4)

Table 28. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **CV10-O**.

	x	y	z	U(eq)
H(2)	6392	1061	828	69
H(3)	6591	-215	127	72
H(4)	6724	-1430	477	77
H(5)	6724	-1387	1550	73
H(10)	7049	27	3640	53
H(12)	6115	1836	4777	54
H(13)	6031	1940	5834	56
H(15)	7730	-318	5641	53
H(17A)	5024	1704	6630	95
H(17B)	5336	1285	7213	95
H(18A)	6713	2653	7492	135
H(18B)	8020	2009	7488	135
H(18C)	7710	2427	6909	135
H(19A)	7022	-343	6525	62
H(19B)	6965	270	7203	62
H(20A)	9795	293	6563	107
H(20B)	9664	-79	7164	107
H(20C)	9739	908	7241	107
H(21A)	7438	-1531	4883	54
H(21B)	9343	-1093	5011	54
H(22A)	9572	-1762	3935	58
H(22B)	7693	-2222	3829	58
H(23A)	8506	-2901	4651	55
H(23B)	10387	-2490	4690	55
H(24A)	8513	-3711	3596	59
H(24B)	10396	-3299	3635	59
H(25A)	9435	-4313	4453	61
H(25B)	11307	-3964	4415	61
H(26A)	9178	-5196	3393	59

H(26B)	11087	-4870	3387	59
H(27A)	11903	-5475	4231	78
H(27B)	9999	-5793	4244	78
H(28A)	11677	-6404	3205	84
H(28B)	9788	-6736	3237	84
H(29A)	12604	-6932	4087	139
H(29B)	10724	-7249	4134	139
H(30A)	10479	-8232	3185	211
H(30B)	11985	-8342	3682	211
H(30C)	12354	-7910	3128	211
H(32)	6266	4347	4173	67
H(33)	5970	5612	4876	66
H(34)	4873	6666	4507	63
H(35)	4113	6512	3418	60
H(40)	3458	5024	1319	54
H(42)	3832	3115	153	65
H(43)	3273	2897	-932	76
H(45)	1870	5222	-688	56
H(49A)	1902	4461	-2321	65
H(49B)	2089	5123	-1645	65
H(50A)	-673	4887	-2159	105
H(50B)	-602	4565	-1529	105
H(50C)	-789	3905	-2207	105
H(51A)	838	6187	64	59
H(51B)	2748	6487	29	59
H(52A)	1172	6979	1132	62
H(52B)	3130	7215	1151	62
H(53A)	644	7758	368	66
H(53B)	2597	8002	397	66
H(54A)	783	8599	1404	62
H(54B)	2769	8783	1492	62

H(55A)	2635	9553	727	69
H(55B)	659	9317	574	69
H(56A)	2467	10424	1729	66
H(56B)	490	10162	1605	66
H(57A)	2301	11120	914	73
H(57B)	350	10797	721	73
H(58A)	1952	12069	1822	71
H(58B)	63	11654	1767	71
H(59A)	1226	12574	914	86
H(59B)	-656	12139	839	86
H(60A)	-438	13584	1307	134
H(60B)	936	13523	1873	134
H(60C)	-941	13082	1808	134
H(47A)	1386	2612	-1765	58
H(47B)	891	2957	-2380	58
H(48A)	3263	2242	-2521	87
H(48B)	4260	2850	-1868	87
H(48C)	3796	3218	-2465	87
H(47C)	3605	3546	-2351	60
H(47D)	4176	3178	-1758	60
H(48D)	1007	2677	-2578	93
H(48E)	1409	2372	-1946	93
H(48F)	2391	2083	-2526	93

Table 29. Crystal data and structure refinement for **CV16-R**.

Identification code	**CV16-R**
Empirical formula	C_{36} H_{51} N_3 O S
Formula weight	573.85
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.183(2) Å b = 11.367(2) Å c = 14.014(3) Å
Volume	1683.8(6) $Å^3$
Z	2
Density (calculated)	1.132 Mg/m^3
Absorption coefficient	0.127 mm^{-1}
F(000)	624
Crystal size	0.200 x 0.105 x 0.072 mm^3
Theta range for data collection	1.851 to 28.324°.
Index ranges	-14<=h<=14, -15<=k<=15, -18<=l<=18
Reflections collected	63050
Independent reflections	8319 [R(int) = 0.0790]
Completeness to theta = 26.03°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8319 / 24 / 374
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0866, wR2 = 0.2330
R indices (all data)	R1 = 0.1672, wR2 = 0.2917
Largest diff. peak and hole	0.859 and -0.540 $e.Å^{-3}$

Table 30. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **CV16-R**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1A)	-1377(1)	1502(1)	8754(1)	68(1)
N(1A)	-3454(2)	162(2)	9472(2)	98(1)
S(1B)	-3454(2)	162(2)	9472(2)	98(1)
N(1B)	-1377(1)	1502(1)	8754(1)	68(1)
O(1)	1490(2)	-465(2)	7985(2)	60(1)
N(2)	-3015(4)	-2786(4)	9535(4)	124(2)
N(3)	2188(3)	-4482(3)	8246(2)	67(1)
C(1)	-2462(3)	2170(3)	9025(3)	61(1)
C(2)	-2502(5)	3446(4)	8943(3)	100(2)
C(3)	-3589(5)	3775(4)	9269(4)	93(1)
C(4)	-4408(5)	2954(6)	9585(4)	107(2)
C(5)	-4343(5)	1905(6)	9645(4)	98(2)
C(6)	-3392(3)	1483(3)	9378(2)	61(1)
C(7)	-2159(3)	190(3)	9089(2)	55(1)
C(8)	-1675(3)	-914(3)	9024(2)	55(1)
C(9)	-2419(4)	-1950(4)	9310(3)	78(1)
C(10)	-608(3)	-933(3)	8696(2)	53(1)
C(11)	35(3)	-1876(3)	8568(2)	53(1)
C(12)	1152(3)	-1616(3)	8211(2)	52(1)
C(13)	1839(3)	-2474(3)	8093(3)	56(1)
C(14)	1474(3)	-3654(3)	8330(2)	56(1)
C(15)	359(3)	-3926(3)	8670(3)	62(1)
C(16)	-313(3)	-3076(3)	8784(3)	62(1)
C(17)	1804(4)	-5719(3)	8468(3)	77(1)
C(18)	845(4)	-6556(4)	7625(3)	86(1)

C(19)	3360(4)	-4185(4)	7892(3)	78(1)
C(20)	3117(5)	-4306(4)	6806(3)	88(1)
C(21)	2620(3)	-146(3)	7643(3)	56(1)
C(22)	2793(3)	1139(3)	7416(3)	57(1)
C(23)	3956(3)	1462(3)	6995(3)	56(1)
C(24)	4284(3)	2775(3)	6785(3)	58(1)
C(25)	5515(3)	3056(3)	6442(3)	60(1)
C(26)	5997(3)	4392(3)	6352(3)	62(1)
C(27)	7274(3)	4651(3)	6101(3)	64(1)
C(28)	7761(3)	5955(3)	5950(3)	63(1)
C(29)	9035(3)	6201(3)	5689(3)	62(1)
C(30)	9452(3)	7451(3)	5418(3)	61(1)
C(31)	10686(3)	7657(3)	5093(3)	59(1)
C(32)	11055(3)	8868(3)	4727(3)	60(1)
C(33)	12261(3)	9035(3)	4360(3)	60(1)
C(34)	12663(3)	10258(3)	4017(3)	61(1)
C(35)	13857(4)	10378(3)	3642(3)	71(1)
C(36)	14330(4)	11611(4)	3354(3)	88(1)

Table 31. Bond lengths [Å] and angles [°] for **CV16-R**.

S(1A)-C(1)	1.650(4)
S(1A)-C(7)	1.723(4)
N(1A)-C(6)	1.508(4)
N(1A)-C(7)	1.644(4)
S(1B)-C(6)	1.508(4)
S(1B)-C(7)	1.644(4)
N(1B)-C(1)	1.650(4)
N(1B)-C(7)	1.723(4)
O(1)-C(12)	1.370(4)
O(1)-C(21)	1.434(4)
N(2)-C(9)	1.152(5)
N(3)-C(14)	1.369(4)
N(3)-C(17)	1.463(4)
N(3)-C(19)	1.483(5)
C(1)-C(6)	1.373(5)
C(1)-C(2)	1.474(6)
C(2)-C(3)	1.492(7)
C(2)-H(2)	0.9400
C(3)-C(4)	1.340(7)
C(3)-H(3)	0.9400
C(4)-C(5)	1.219(7)
C(4)-H(4)	0.9400
C(5)-C(6)	1.362(6)
C(5)-H(5)	0.9400
C(7)-C(8)	1.471(5)
C(8)-C(10)	1.370(4)
C(8)-C(9)	1.434(5)
C(10)-C(11)	1.429(5)
C(10)-H(10)	0.9400
C(11)-C(16)	1.416(4)
C(11)-C(12)	1.428(4)
C(12)-C(13)	1.380(4)
C(13)-C(14)	1.409(4)
C(13)-H(13)	0.9400

C(14)-C(15)	1.413(5)
C(15)-C(16)	1.361(5)
C(15)-H(15)	0.9400
C(16)-H(16)	0.9400
C(17)-C(18)	1.509(6)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(18)-H(18C)	0.9700
C(19)-C(20)	1.476(6)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(20)-H(20C)	0.9700
C(21)-C(22)	1.505(4)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(22)-C(23)	1.531(4)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(23)-C(24)	1.530(4)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(24)-C(25)	1.536(5)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(25)-C(26)	1.528(5)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(26)-C(27)	1.519(5)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(27)-C(28)	1.518(5)
C(27)-H(27A)	0.9800

C(27)-H(27B)	0.9800
C(28)-C(29)	1.522(5)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(29)-C(30)	1.509(5)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(30)-C(31)	1.523(4)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(31)-C(32)	1.519(5)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(32)-C(33)	1.526(5)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(33)-C(34)	1.523(5)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(34)-C(35)	1.522(5)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(35)-C(36)	1.513(5)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700
C(36)-H(36C)	0.9700

C(1)-S(1A)-C(7)	88.36(18)
C(6)-N(1A)-C(7)	92.6(2)
C(6)-S(1B)-C(7)	92.6(2)
C(1)-N(1B)-C(7)	88.36(18)
C(12)-O(1)-C(21)	117.9(2)
C(14)-N(3)-C(17)	121.3(3)
C(14)-N(3)-C(19)	121.7(3)

C(17)-N(3)-C(19)	116.9(3)
C(6)-C(1)-C(2)	117.3(4)
C(6)-C(1)-S(1A)	117.0(3)
C(2)-C(1)-S(1A)	125.7(3)
C(6)-C(1)-N(1B)	117.0(3)
C(2)-C(1)-N(1B)	125.7(3)
C(1)-C(2)-C(3)	112.3(4)
C(1)-C(2)-H(2)	123.8
C(3)-C(2)-H(2)	123.8
C(4)-C(3)-C(2)	121.0(4)
C(4)-C(3)-H(3)	119.5
C(2)-C(3)-H(3)	119.5
C(5)-C(4)-C(3)	124.8(6)
C(5)-C(4)-H(4)	117.6
C(3)-C(4)-H(4)	117.6
C(4)-C(5)-C(6)	120.5(6)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(5)-C(6)-C(1)	124.1(4)
C(5)-C(6)-N(1A)	114.3(4)
C(1)-C(6)-N(1A)	121.6(3)
C(5)-C(6)-S(1B)	114.3(4)
C(1)-C(6)-S(1B)	121.6(3)
C(8)-C(7)-S(1B)	119.8(3)
C(8)-C(7)-N(1A)	119.8(3)
C(8)-C(7)-S(1A)	119.9(2)
N(1A)-C(7)-S(1A)	120.3(2)
C(8)-C(7)-N(1B)	119.9(2)
S(1B)-C(7)-N(1B)	120.3(2)
C(10)-C(8)-C(9)	123.8(3)
C(10)-C(8)-C(7)	121.6(3)
C(9)-C(8)-C(7)	114.6(3)
N(2)-C(9)-C(8)	179.6(5)
C(8)-C(10)-C(11)	131.9(3)
C(8)-C(10)-H(10)	114.1
C(11)-C(10)-H(10)	114.1

C(16)-C(11)-C(12)	114.9(3)
C(16)-C(11)-C(10)	126.1(3)
C(12)-C(11)-C(10)	119.0(3)
O(1)-C(12)-C(13)	122.3(3)
O(1)-C(12)-C(11)	115.5(3)
C(13)-C(12)-C(11)	122.1(3)
C(12)-C(13)-C(14)	121.4(3)
C(12)-C(13)-H(13)	119.3
C(14)-C(13)-H(13)	119.3
N(3)-C(14)-C(13)	120.9(3)
N(3)-C(14)-C(15)	122.2(3)
C(13)-C(14)-C(15)	116.9(3)
C(16)-C(15)-C(14)	121.3(3)
C(16)-C(15)-H(15)	119.3
C(14)-C(15)-H(15)	119.3
C(15)-C(16)-C(11)	123.3(3)
C(15)-C(16)-H(16)	118.3
C(11)-C(16)-H(16)	118.3
N(3)-C(17)-C(18)	113.2(3)
N(3)-C(17)-H(17A)	108.9
C(18)-C(17)-H(17A)	108.9
N(3)-C(17)-H(17B)	108.9
C(18)-C(17)-H(17B)	108.9
H(17A)-C(17)-H(17B)	107.8
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(20)-C(19)-N(3)	112.8(4)
C(20)-C(19)-H(19A)	109
N(3)-C(19)-H(19A)	109
C(20)-C(19)-H(19B)	109
N(3)-C(19)-H(19B)	109
H(19A)-C(19)-H(19B)	107.8

C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(1)-C(21)-C(22)	109.1(3)
O(1)-C(21)-H(21A)	109.9
C(22)-C(21)-H(21A)	109.9
O(1)-C(21)-H(21B)	109.9
C(22)-C(21)-H(21B)	109.9
H(21A)-C(21)-H(21B)	108.3
C(21)-C(22)-C(23)	109.4(3)
C(21)-C(22)-H(22A)	109.8
C(23)-C(22)-H(22A)	109.8
C(21)-C(22)-H(22B)	109.8
C(23)-C(22)-H(22B)	109.8
H(22A)-C(22)-H(22B)	108.2
C(24)-C(23)-C(22)	114.7(3)
C(24)-C(23)-H(23A)	108.6
C(22)-C(23)-H(23A)	108.6
C(24)-C(23)-H(23B)	108.6
C(22)-C(23)-H(23B)	108.6
H(23A)-C(23)-H(23B)	107.6
C(23)-C(24)-C(25)	111.6(3)
C(23)-C(24)-H(24A)	109.3
C(25)-C(24)-H(24A)	109.3
C(23)-C(24)-H(24B)	109.3
C(25)-C(24)-H(24B)	109.3
H(24A)-C(24)-H(24B)	108
C(26)-C(25)-C(24)	114.5(3)
C(26)-C(25)-H(25A)	108.6
C(24)-C(25)-H(25A)	108.6
C(26)-C(25)-H(25B)	108.6
C(24)-C(25)-H(25B)	108.6
H(25A)-C(25)-H(25B)	107.6

C(27)-C(26)-C(25)	112.9(3)
C(27)-C(26)-H(26A)	109
C(25)-C(26)-H(26A)	109
C(27)-C(26)-H(26B)	109
C(25)-C(26)-H(26B)	109
H(26A)-C(26)-H(26B)	107.8
C(28)-C(27)-C(26)	114.8(3)
C(28)-C(27)-H(27A)	108.6
C(26)-C(27)-H(27A)	108.6
C(28)-C(27)-H(27B)	108.6
C(26)-C(27)-H(27B)	108.6
H(27A)-C(27)-H(27B)	107.5
C(27)-C(28)-C(29)	114.4(3)
C(27)-C(28)-H(28A)	108.7
C(29)-C(28)-H(28A)	108.7
C(27)-C(28)-H(28B)	108.7
C(29)-C(28)-H(28B)	108.7
H(28A)-C(28)-H(28B)	107.6
C(30)-C(29)-C(28)	114.7(3)
C(30)-C(29)-H(29A)	108.6
C(28)-C(29)-H(29A)	108.6
C(30)-C(29)-H(29B)	108.6
C(28)-C(29)-H(29B)	108.6
H(29A)-C(29)-H(29B)	107.6
C(29)-C(30)-C(31)	114.1(3)
C(29)-C(30)-H(30A)	108.7
C(31)-C(30)-H(30A)	108.7
C(29)-C(30)-H(30B)	108.7
C(31)-C(30)-H(30B)	108.7
H(30A)-C(30)-H(30B)	107.6
C(32)-C(31)-C(30)	114.7(3)
C(32)-C(31)-H(31A)	108.6
C(30)-C(31)-H(31A)	108.6
C(32)-C(31)-H(31B)	108.6
C(30)-C(31)-H(31B)	108.6
H(31A)-C(31)-H(31B)	107.6

C(31)-C(32)-C(33)	114.0(3)
C(31)-C(32)-H(32A)	108.8
C(33)-C(32)-H(32A)	108.8
C(31)-C(32)-H(32B)	108.8
C(33)-C(32)-H(32B)	108.8
H(32A)-C(32)-H(32B)	107.7
C(34)-C(33)-C(32)	114.6(3)
C(34)-C(33)-H(33A)	108.6
C(32)-C(33)-H(33A)	108.6
C(34)-C(33)-H(33B)	108.6
C(32)-C(33)-H(33B)	108.6
H(33A)-C(33)-H(33B)	107.6
C(35)-C(34)-C(33)	112.9(3)
C(35)-C(34)-H(34A)	109
C(33)-C(34)-H(34A)	109
C(35)-C(34)-H(34B)	109
C(33)-C(34)-H(34B)	109
H(34A)-C(34)-H(34B)	107.8
C(36)-C(35)-C(34)	114.3(3)
C(36)-C(35)-H(35A)	108.7
C(34)-C(35)-H(35A)	108.7
C(36)-C(35)-H(35B)	108.7
C(34)-C(35)-H(35B)	108.7
H(35A)-C(35)-H(35B)	107.6
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 32. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **CV16-R**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1A)	71(1)	66(1)	75(1)	10(1)	25(1)	25(1)
N(1A)	152(2)	61(1)	79(1)	9(1)	8(1)	43(1)
S(1B)	152(2)	61(1)	79(1)	9(1)	8(1)	43(1)
N(1B)	71(1)	66(1)	75(1)	10(1)	25(1)	25(1)
O(1)	55(1)	45(1)	86(2)	18(1)	29(1)	13(1)
N(2)	121(3)	82(3)	219(5)	74(3)	103(4)	48(2)
N(3)	73(2)	50(2)	87(2)	16(2)	26(2)	23(1)
C(1)	60(2)	63(2)	58(2)	11(2)	13(2)	8(2)
C(2)	101(3)	94(3)	74(3)	21(2)	-1(2)	-28(2)
C(3)	122(3)	61(2)	86(3)	-6(2)	-14(2)	47(2)
C(4)	97(3)	127(4)	93(3)	3(3)	15(2)	31(3)
C(5)	87(3)	121(3)	85(3)	-5(3)	26(2)	26(3)
C(6)	61(2)	67(2)	53(2)	4(2)	20(2)	4(2)
C(7)	56(2)	57(2)	52(2)	6(2)	14(2)	14(2)
C(8)	58(2)	51(2)	62(2)	15(2)	21(2)	12(2)
C(9)	77(3)	66(2)	117(3)	36(2)	51(3)	33(2)
C(10)	56(2)	48(2)	56(2)	11(1)	17(2)	11(1)
C(11)	53(2)	50(2)	55(2)	8(1)	15(2)	9(1)
C(12)	55(2)	45(2)	56(2)	9(1)	12(2)	10(1)
C(13)	55(2)	48(2)	66(2)	10(2)	17(2)	14(2)
C(14)	60(2)	49(2)	60(2)	9(2)	15(2)	14(2)
C(15)	68(2)	45(2)	78(2)	16(2)	26(2)	12(2)
C(16)	63(2)	54(2)	73(2)	14(2)	27(2)	10(2)
C(17)	85(3)	56(2)	99(3)	20(2)	26(2)	28(2)
C(18)	94(3)	64(2)	102(3)	5(2)	30(3)	15(2)
C(19)	88(3)	61(2)	99(3)	19(2)	32(2)	34(2)
C(20)	101(3)	73(3)	101(4)	18(2)	31(3)	31(2)
C(21)	53(2)	47(2)	70(2)	12(2)	23(2)	11(1)
C(22)	55(2)	46(2)	71(2)	11(2)	18(2)	11(1)
C(23)	57(2)	51(2)	63(2)	12(2)	19(2)	15(2)
C(24)	58(2)	53(2)	67(2)	14(2)	20(2)	14(2)
C(25)	60(2)	58(2)	66(2)	15(2)	22(2)	12(2)
C(26)	60(2)	60(2)	74(2)	21(2)	24(2)	15(2)
C(27)	60(2)	64(2)	76(2)	19(2)	25(2)	14(2)
C(28)	57(2)	61(2)	74(2)	18(2)	25(2)	11(2)
C(29)	52(2)	63(2)	74(2)	15(2)	17(2)	11(2)
C(30)	54(2)	62(2)	70(2)	16(2)	21(2)	12(2)
C(31)	49(2)	56(2)	71(2)	10(2)	14(2)	12(2)
C(32)	55(2)	58(2)	71(2)	12(2)	20(2)	16(2)
C(33)	52(2)	55(2)	75(2)	11(2)	19(2)	13(2)

C(34)	57(2)	58(2)	69(2)	12(2)	17(2)	16(2)
C(35)	64(2)	71(2)	83(3)	19(2)	26(2)	13(2)
C(36)	89(3)	83(3)	93(3)	24(2)	34(3)	4(2)

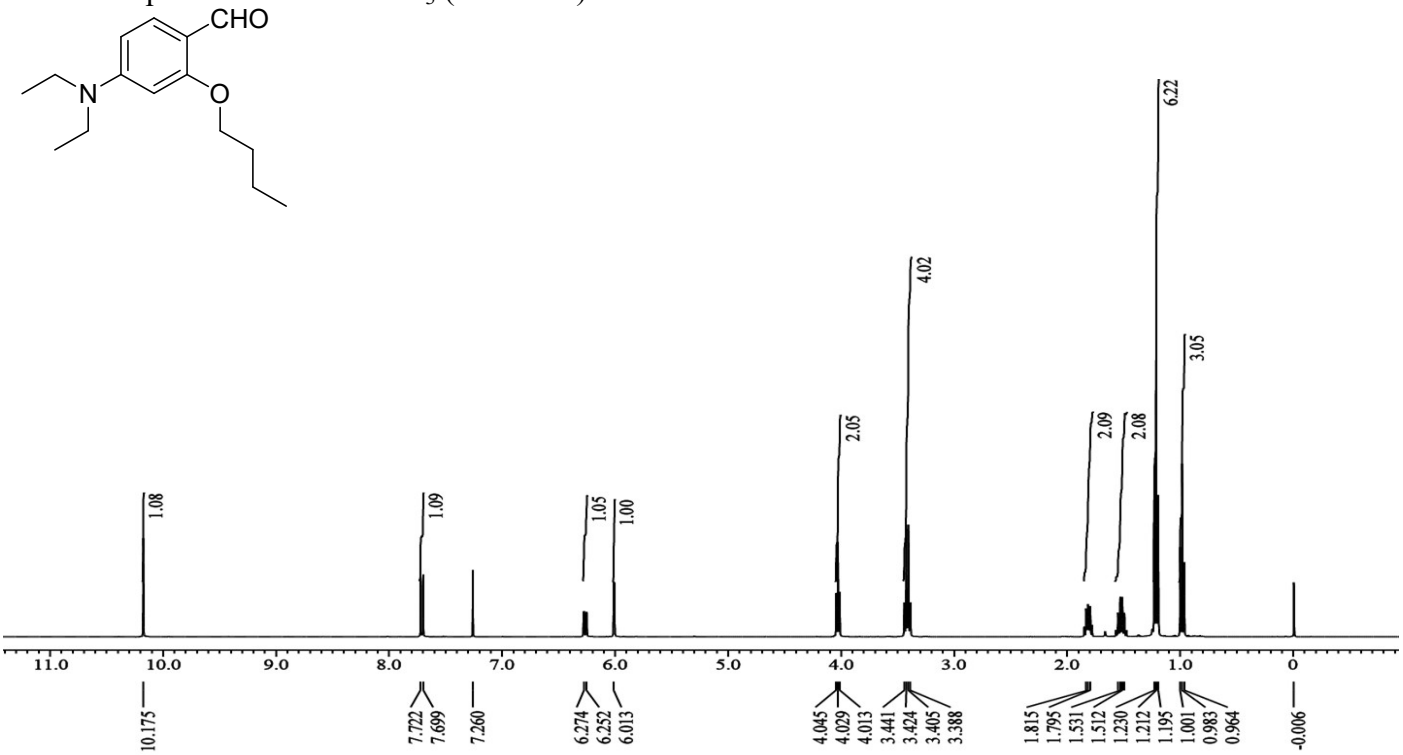
Table 33. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **CV16-R**.

	x	y	z	U(eq)
H(2)	-1909	3990	8711	120
H(3)	-3702	4570	9253	112
H(4)	-5082	3205	9775	128
H(5)	-4953	1384	9878	117
H(10)	-230	-189	8523	63
H(13)	2566	-2266	7851	67
H(15)	76	-4710	8821	75
H(16)	-1045	-3297	9017	74
H(17A)	1449	-5688	9049	93
H(17B)	2550	-6054	8633	93
H(18A)	627	-7359	7813	129
H(18B)	1196	-6607	7051	129
H(18C)	95	-6241	7468	129
H(19A)	3817	-3349	8172	94
H(19B)	3899	-4726	8131	94
H(20A)	3904	-4036	6617	133
H(20B)	2542	-3811	6561	133
H(20C)	2746	-5150	6527	133
H(21A)	2560	-702	7048	67
H(21B)	3345	-215	8151	67
H(22A)	2900	1699	8019	68
H(22B)	2046	1219	6936	68
H(23A)	4680	1316	7461	67
H(23B)	3819	914	6379	67
H(24A)	4369	3331	7386	70
H(24B)	3597	2910	6274	70

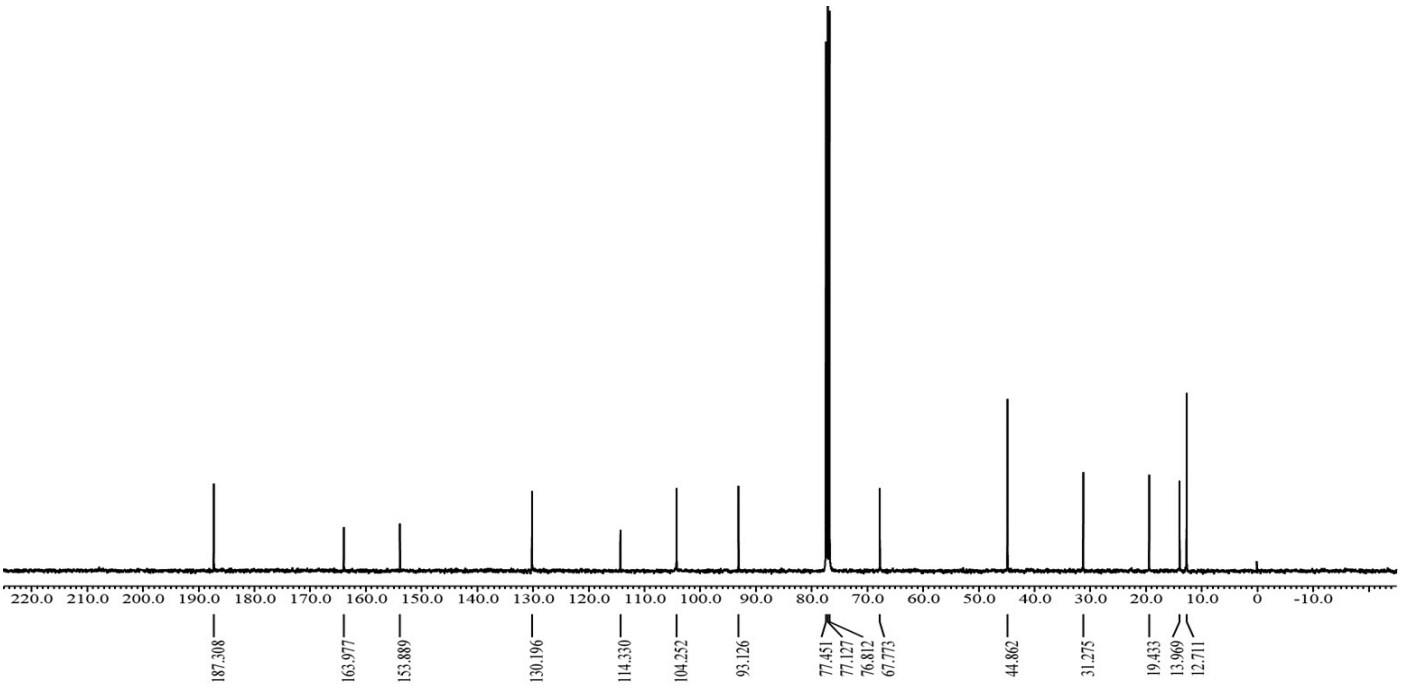
H(25A)	6167	2802	6908	72
H(25B)	5385	2569	5798	72
H(26A)	5386	4630	5838	75
H(26B)	6059	4891	6977	75
H(27A)	7889	4449	6634	77
H(27B)	7219	4113	5498	77
H(28A)	7826	6493	6556	75
H(28B)	7143	6161	5421	75
H(29A)	9671	6092	6253	75
H(29B)	8999	5594	5134	75
H(30A)	9545	8058	5989	73
H(30B)	8790	7582	4883	73
H(31A)	11361	7602	5650	71
H(31B)	10619	7003	4564	71
H(32A)	11164	9525	5266	72
H(32B)	10364	8942	4190	72
H(33A)	12944	8937	4893	72
H(33B)	12142	8389	3811	72
H(34A)	11979	10366	3488	73
H(34B)	12802	10907	4567	73
H(35A)	14521	10212	4157	85
H(35B)	13697	9757	3067	85
H(36A)	15075	11609	3106	132
H(36B)	14539	12229	3928	132
H(36C)	13680	11786	2846	132

10. ^{1}H-NMR and ^{13}C-NMR Spectral Data

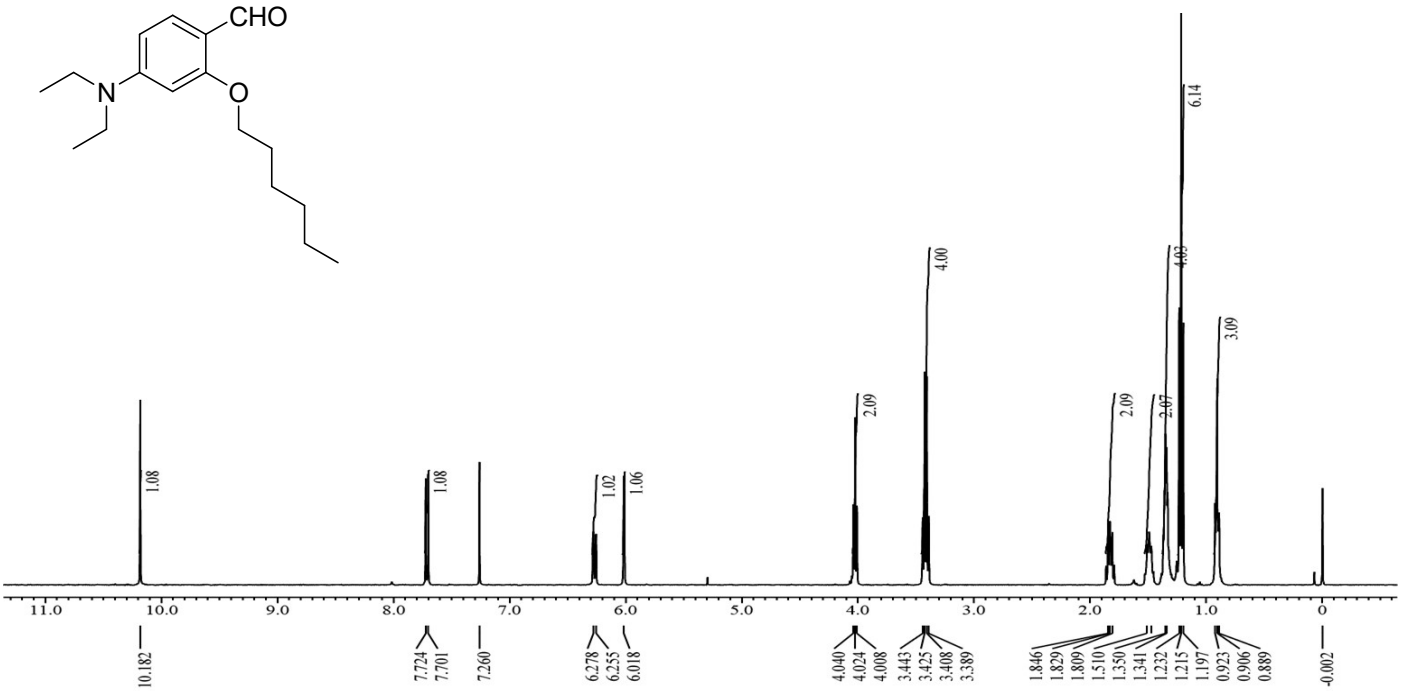
^{1}H-NMR Spectrum of **1** in $CDCl_3$ (400 MHz):



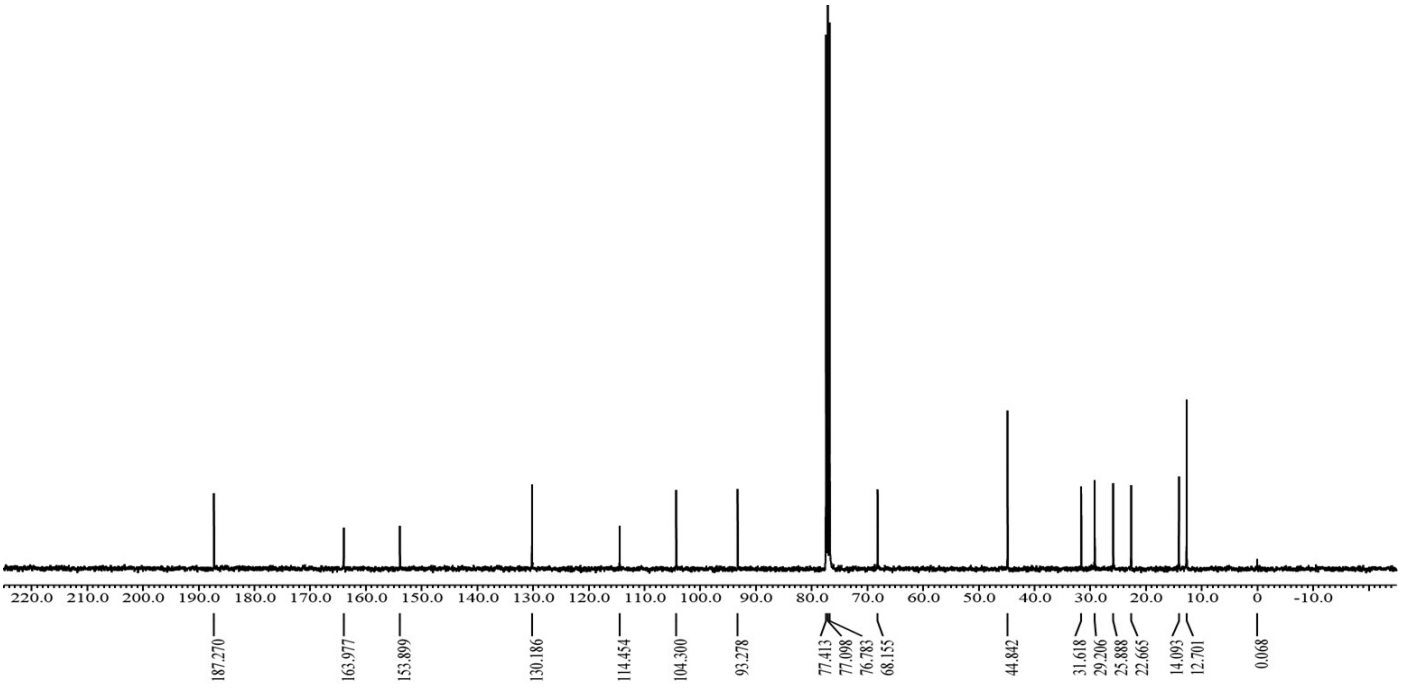
^{13}C-NMR Spectrum of **1** in $CDCl_3$ (100 MHz):



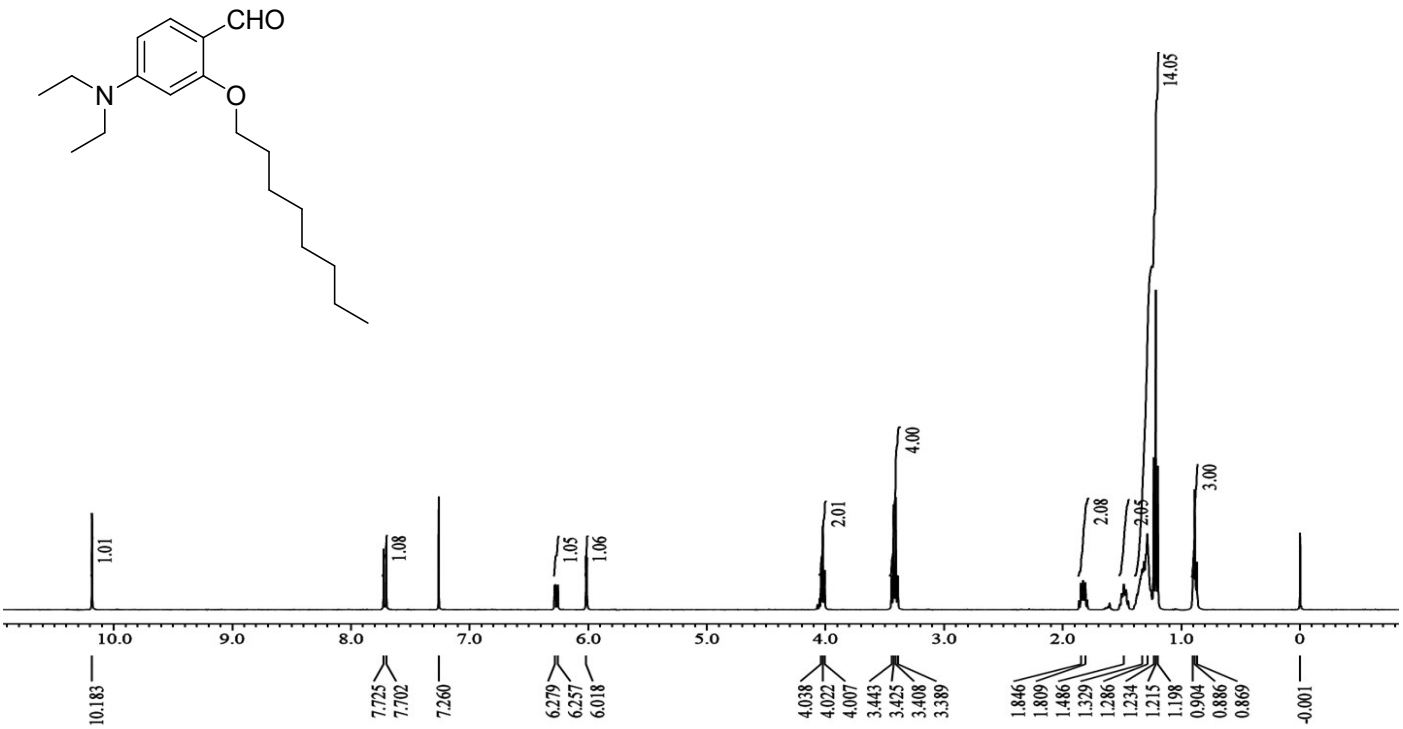
^{1}H-NMR Spectrum of **2** in $CDCl_3$ (400 MHz):



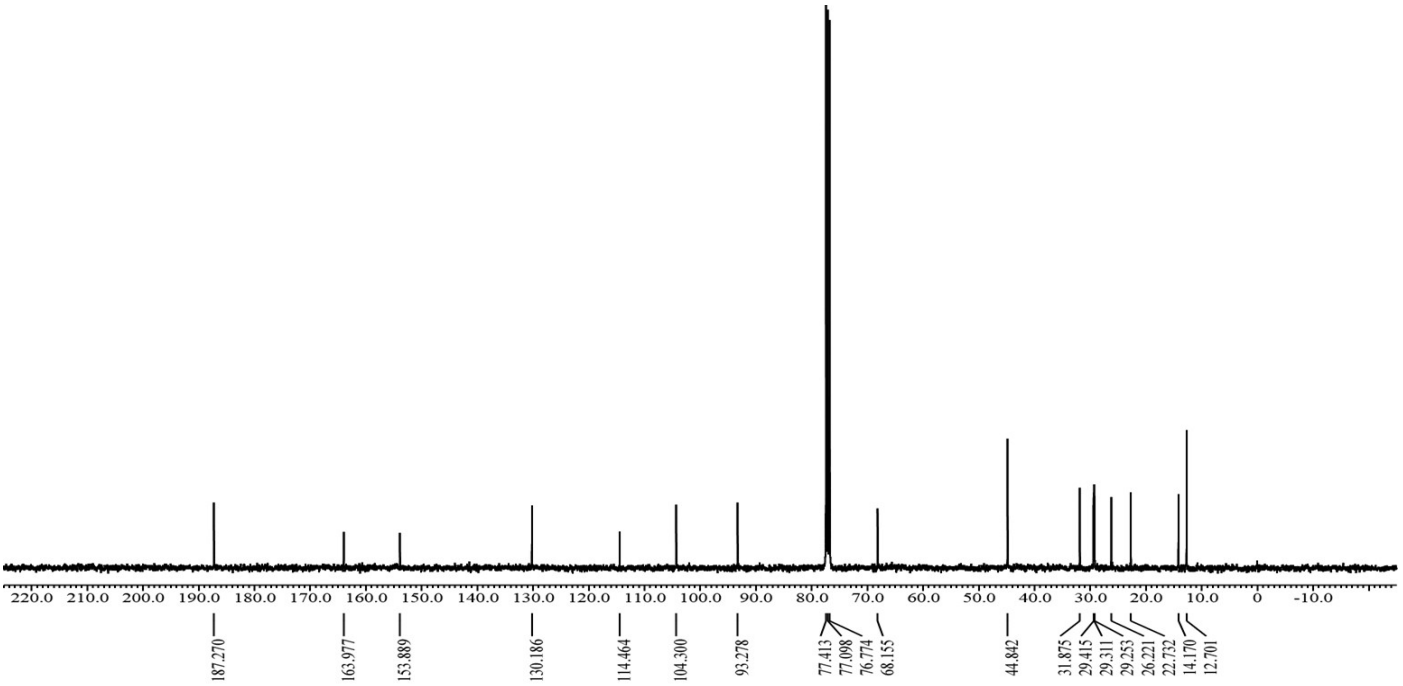
^{13}C-NMR Spectrum of **2** in $CDCl_3$ (100 MHz):



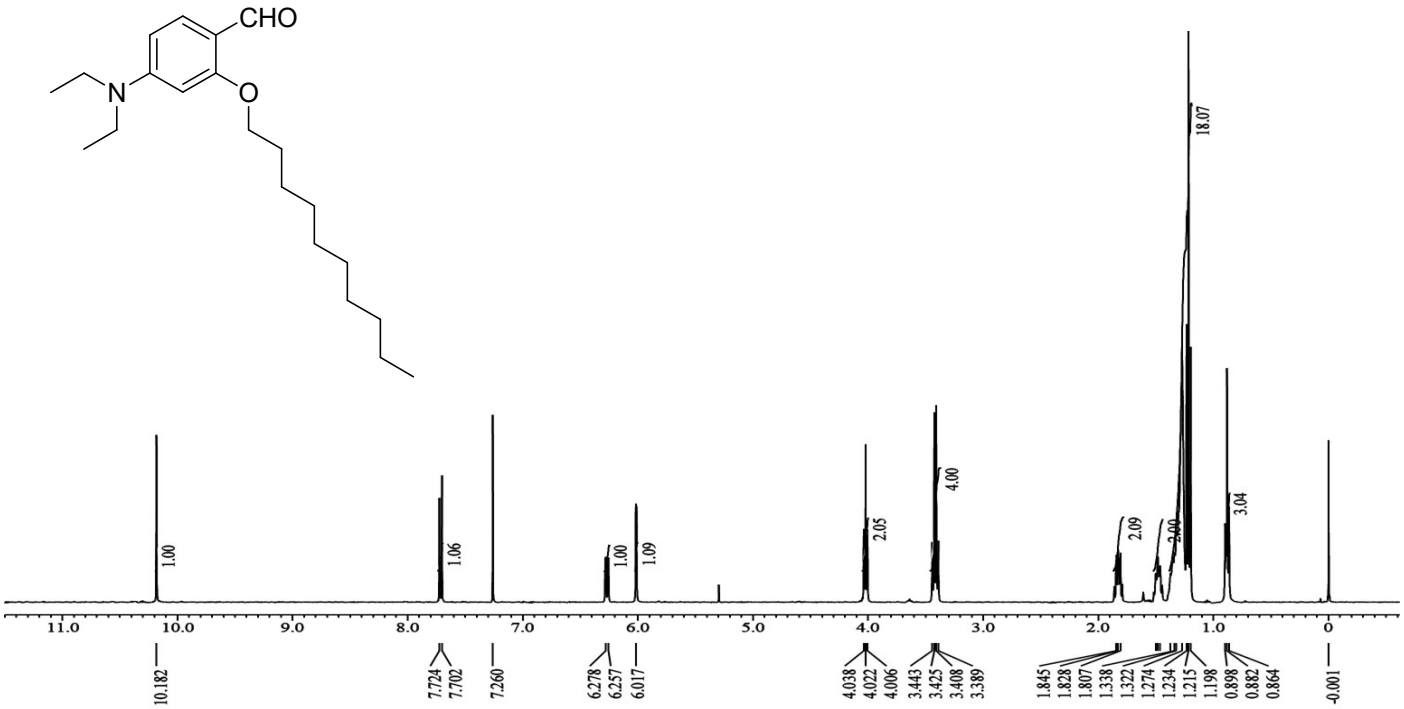
^{1}H-NMR Spectrum of **3** in $CDCl_3$ (400 MHz):



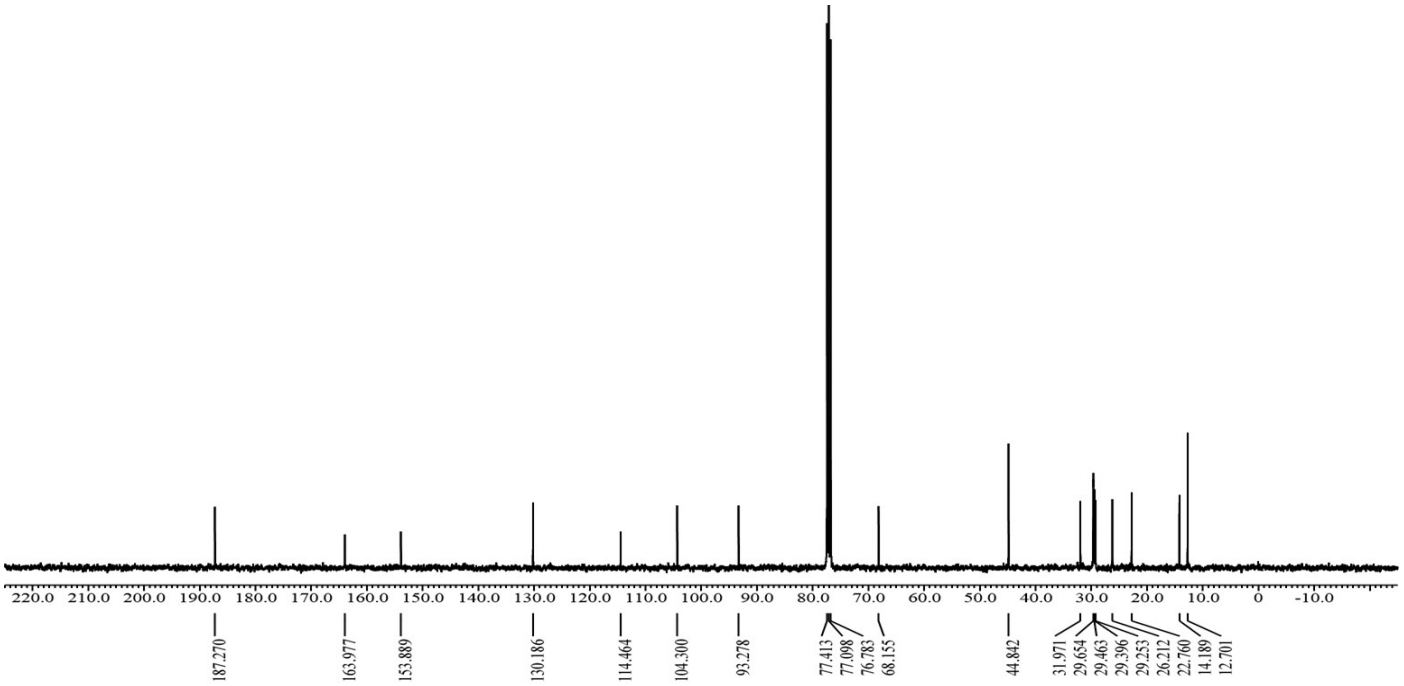
^{13}C-NMR Spectrum of **3** in $CDCl_3$ (100 MHz):



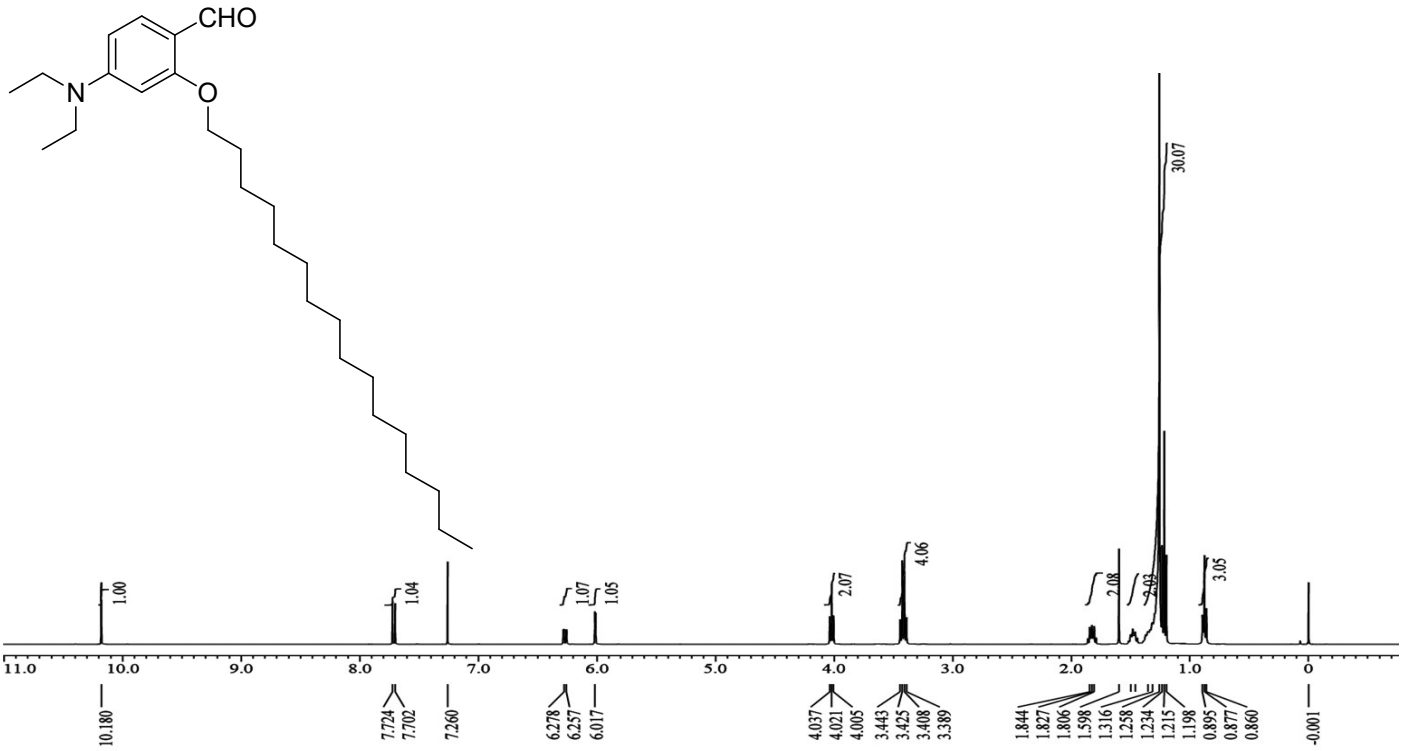
^{1}H-NMR Spectrum of **4** in $CDCl_3$ (400 MHz):



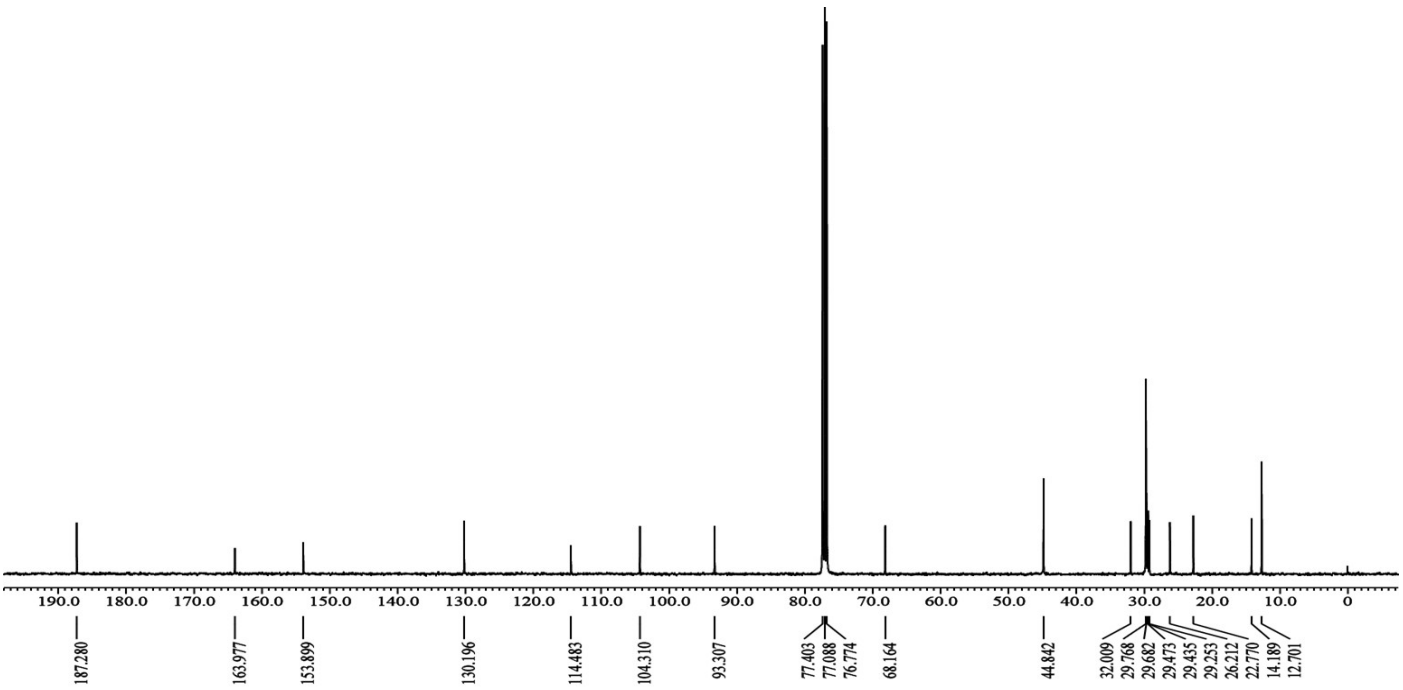
^{13}C-NMR Spectrum of **4** in $CDCl_3$ (100 MHz):



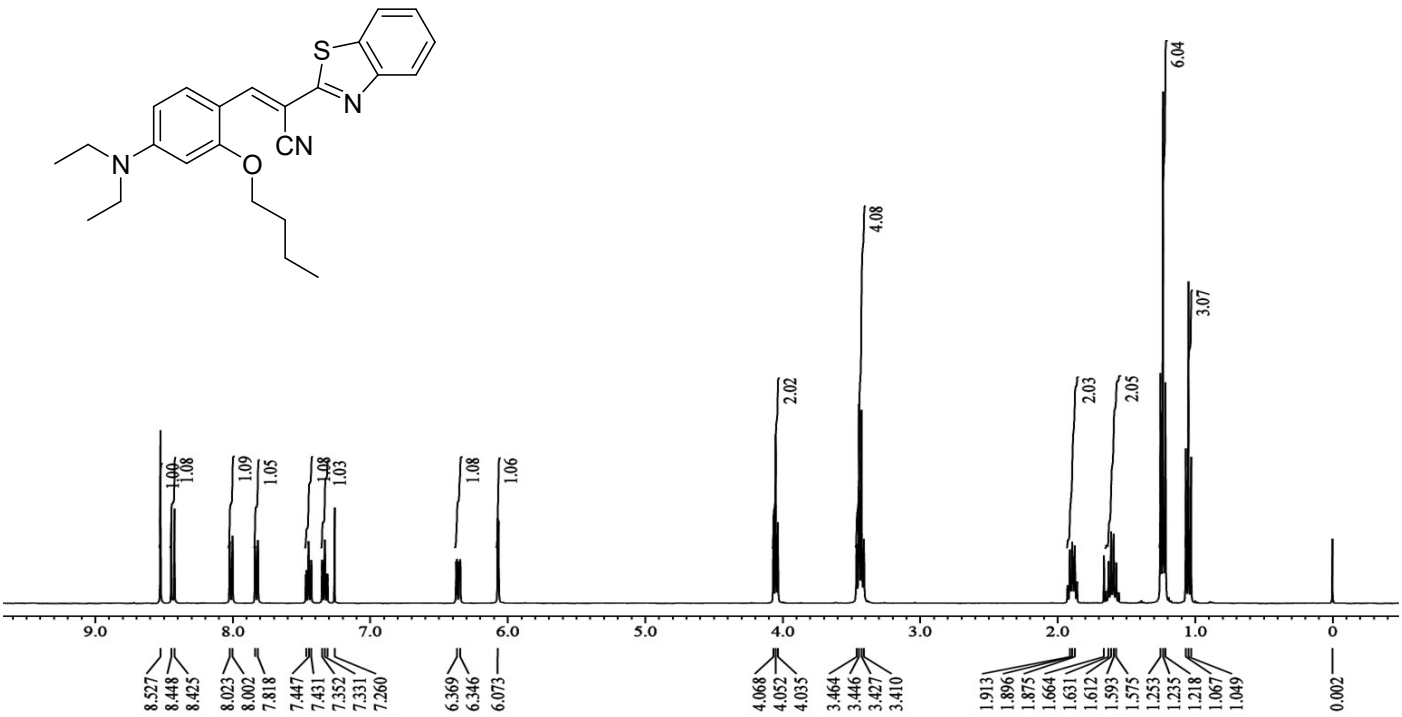
^{1}H-NMR Spectrum of **5** in $CDCl_3$ (400 MHz):



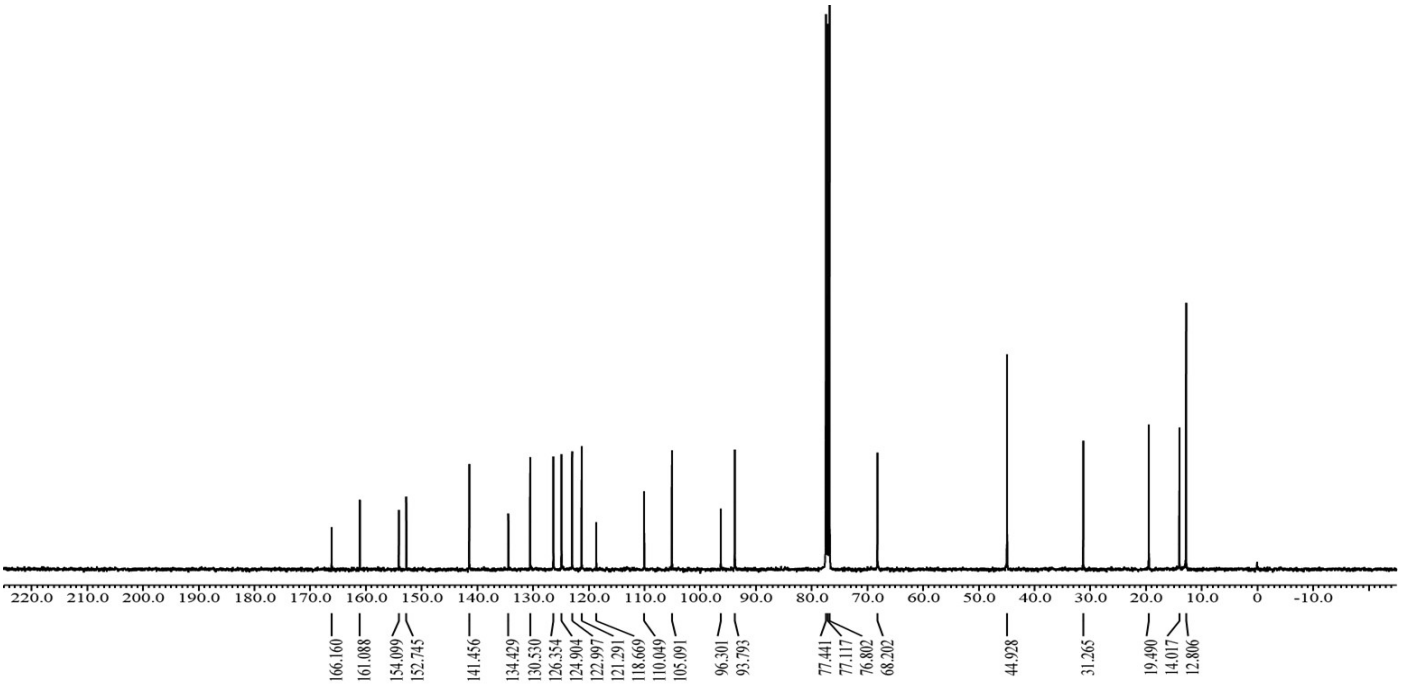
^{13}C-NMR Spectrum of **5** in $CDCl_3$ (100 MHz):



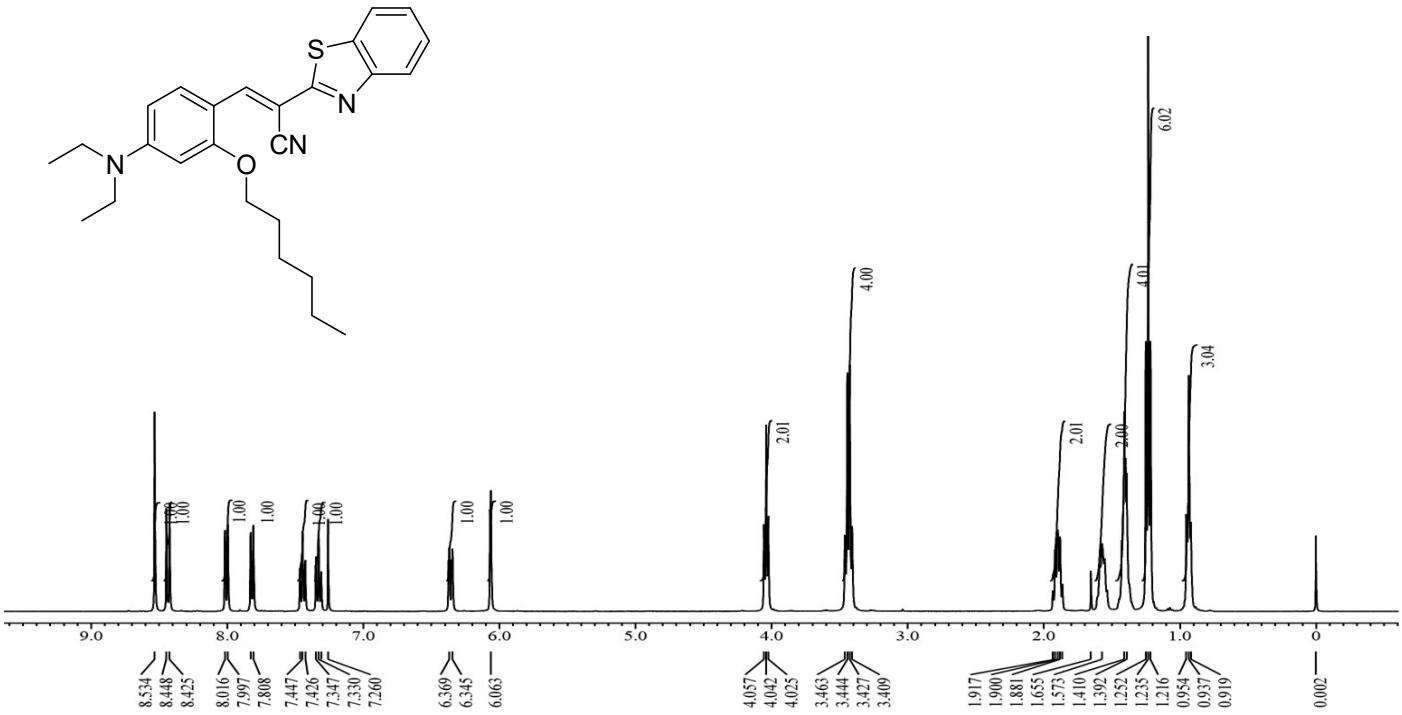
^{1}H-NMR Spectrum of **CV4-R** in $CDCl_3$ (400 MHz):



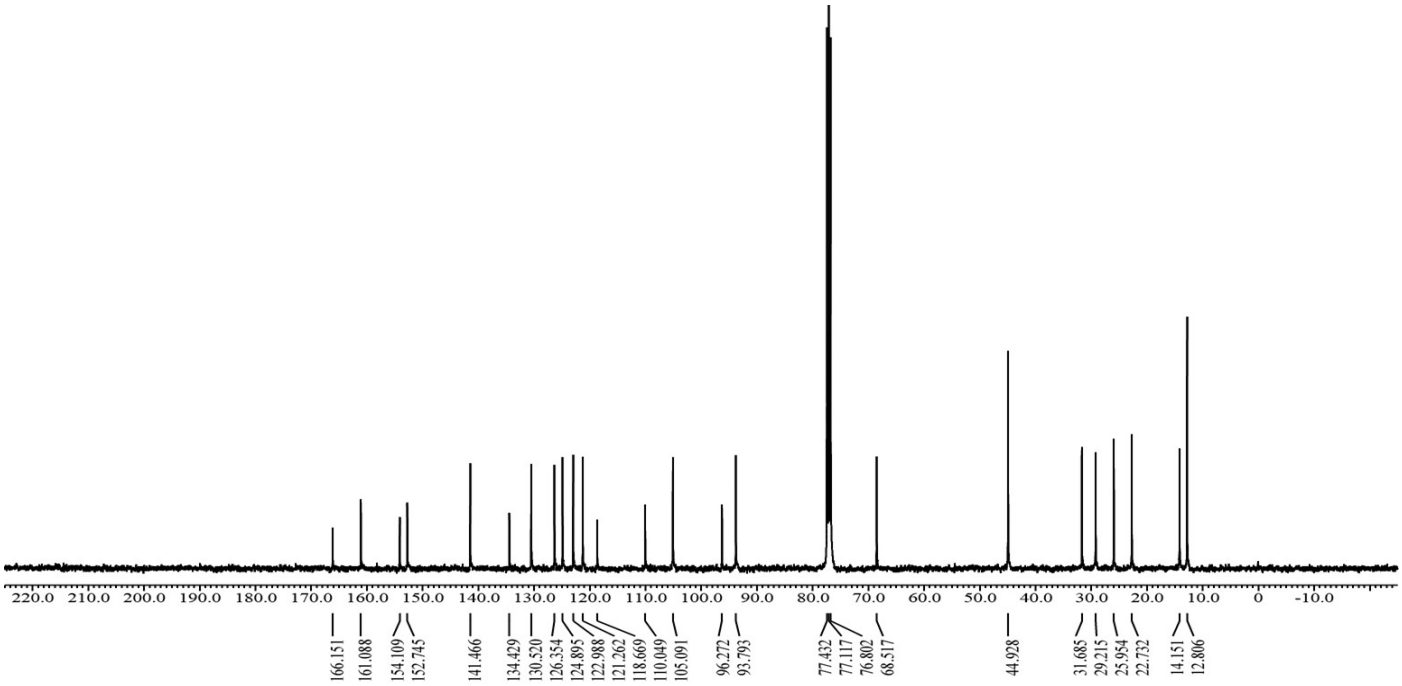
^{13}C-NMR Spectrum of **CV4-R** in $CDCl_3$ (100 MHz):



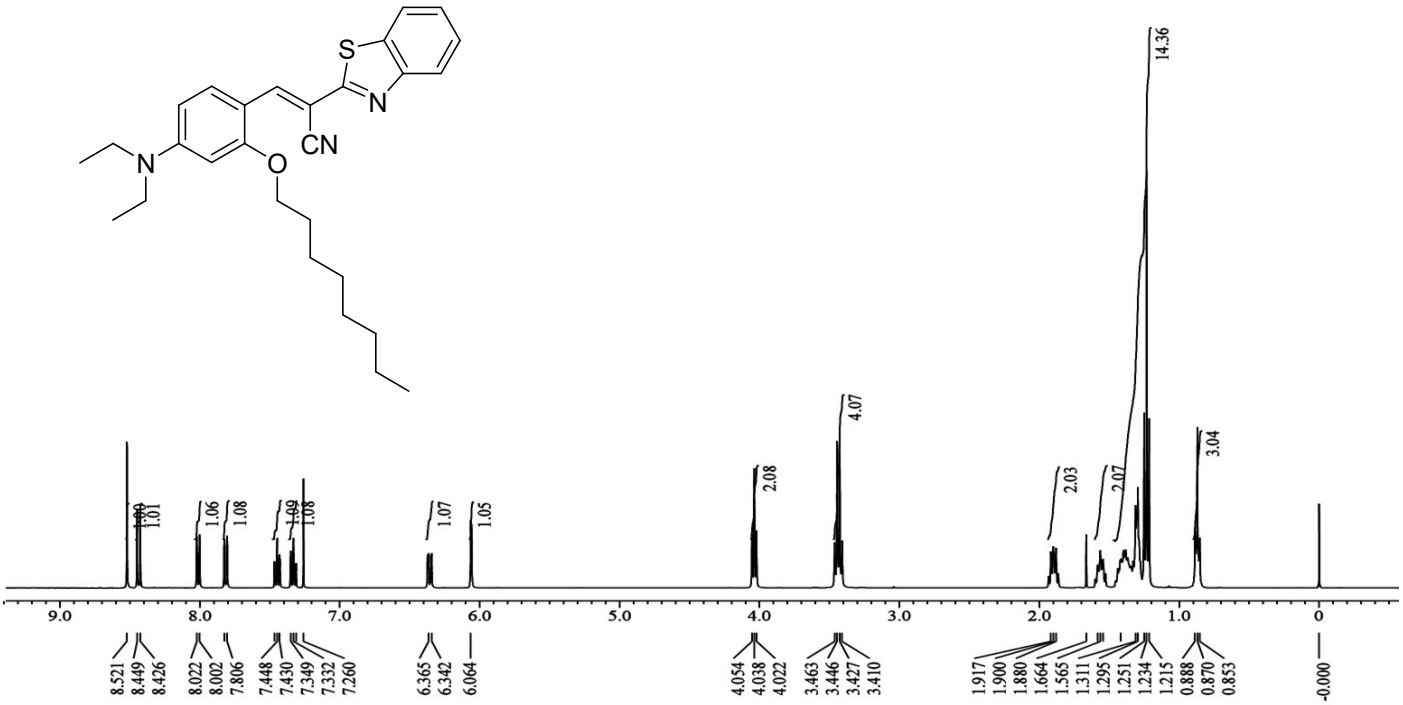
^{1}H-NMR Spectrum of **CV6-O** in $CDCl_3$ (400 MHz):



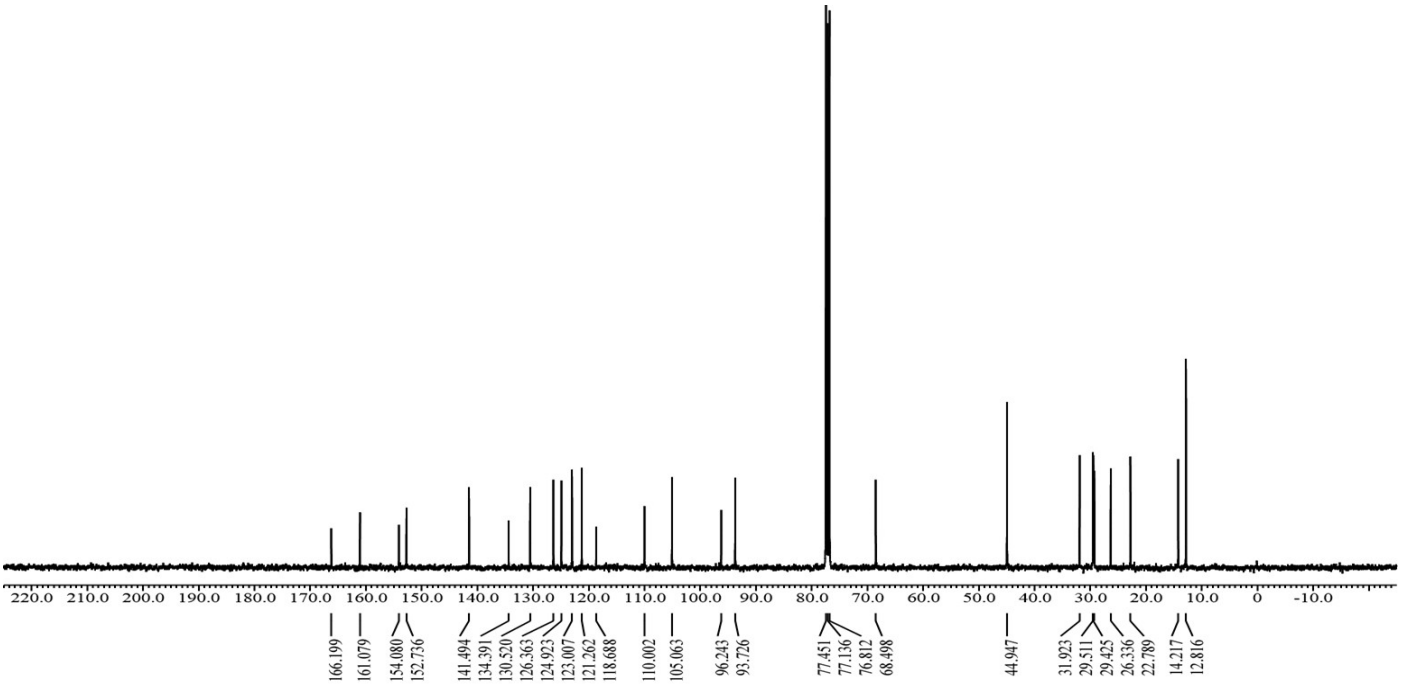
^{13}C-NMR Spectrum of **CV6-O** in $CDCl_3$ (100 MHz):



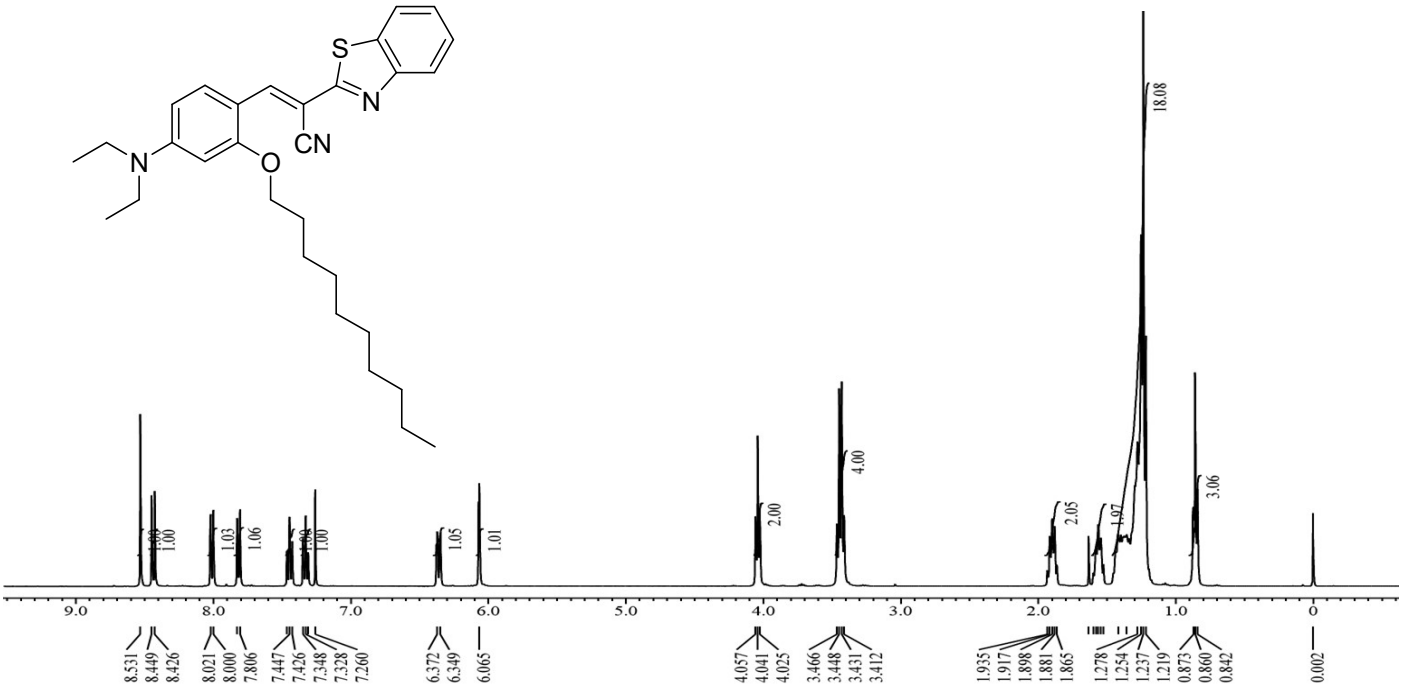
^{1}H-NMR Spectrum of **CV8-Y** in $CDCl_3$ (400 MHz):



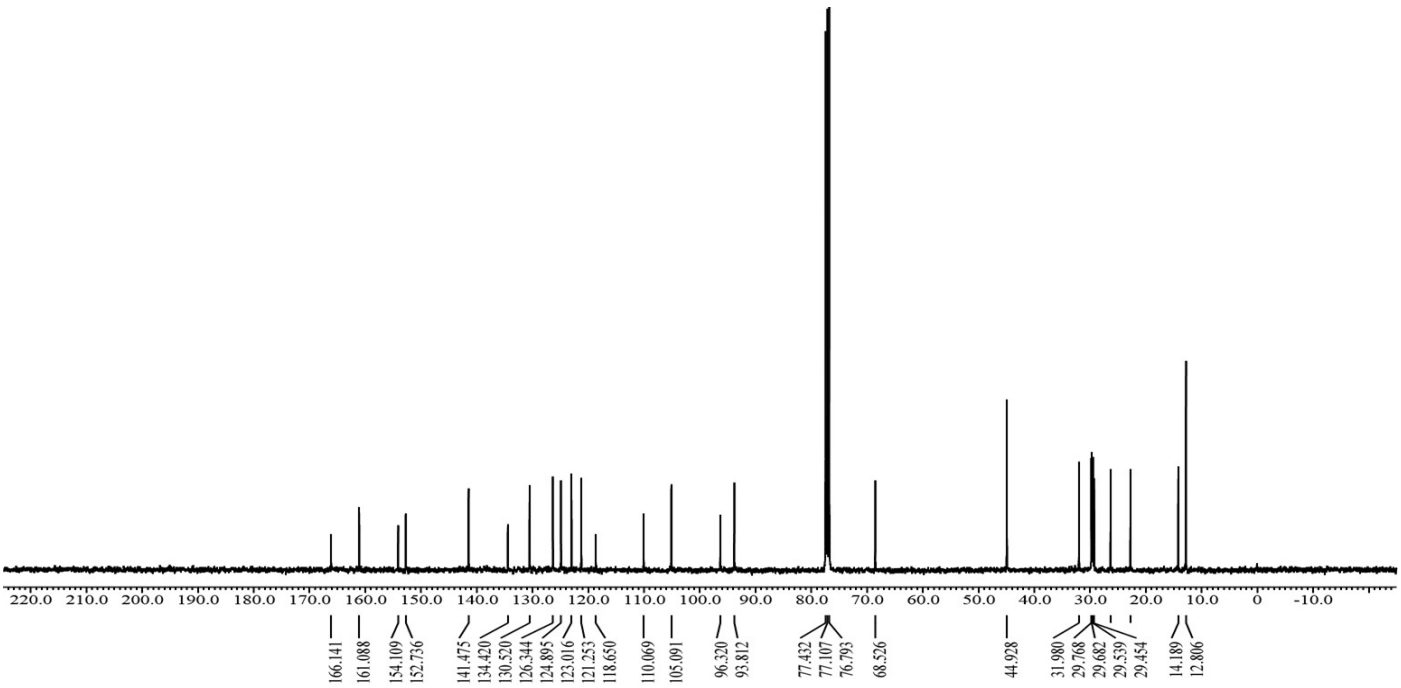
^{13}C-NMR Spectrum of **CV8-Y** in $CDCl_3$ (100 MHz):



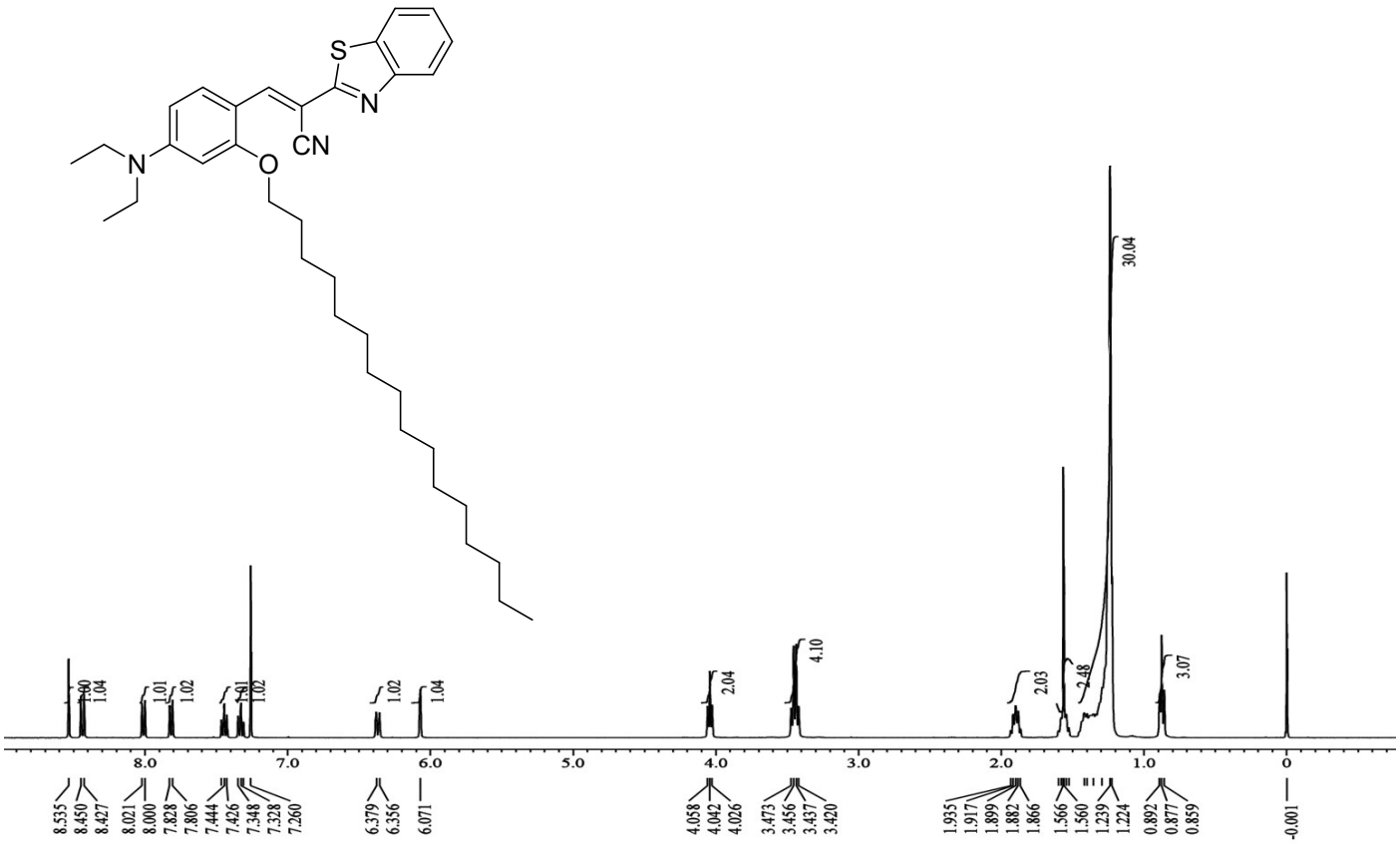
^{1}H-NMR Spectrum of **CV10-O** in $CDCl_3$ (400 MHz):



^{13}C-NMR Spectrum of **CV10-O** in $CDCl_3$ (100 MHz):



^{1}H-NMR Spectrum of **CV16-R** in $CDCl_3$ (400 MHz):



^{13}C-NMR Spectrum of **CV16-R** in $CDCl_3$ (100 MHz):