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Supporting Information for

Reaction of tetracyanoethylene with diselenium dichloride: A route to pyrrolo[2,3-*c*]-[1,2,6]selenodiazines

Cory Laurent, Andreas Kourtellaris and Panayiotis A. Koutentis*

Department of Chemistry, University of Cyprus, P.O. Box 20537, 1678 Nicosia, Cyprus

*e-mail: koutenti@ucy.ac.cy

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S1 Computational Section

S1.1 General methods

The geometry of the singlet ground state of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) was fully optimized and analytical second derivatives were computed using vibrational analysis to confirm each stationary point to be a minimum by yielding zero imaginary frequencies. Close-shell singlet ground states were examined using the spin polarized density functional theory (RDFT). The hybrid B3LYP method,[1] utilizing the 6-311G+(2d,p) basis set was employed for all calculations. HOMO and LUMO energies were taken directly from the optimization calculations. NICS values (in ppm) were measured at the RB3LYP/6-311G+G(2d,p) level of theory in the plane [NICS(0)] above [NICS(1), NICS(2), NICS(3)] and below [NICS(-1), NICS(-2), NICS(-3)] the plane at the center of each ring to estimate the local currents for each individual ring. While NICS(0) are often affected by the σ electrons of neighboring bonds, the most accurate NICS values [NICS(1) and NICS(-1)] are the ones measured 1 Å above and below the molecular plane where π electron density is mainly situated.[2] All the above computations were performed using the Gaussian 09 suite of programs.[3,4]

Table S1. Summary of Computational Energies and Properties.

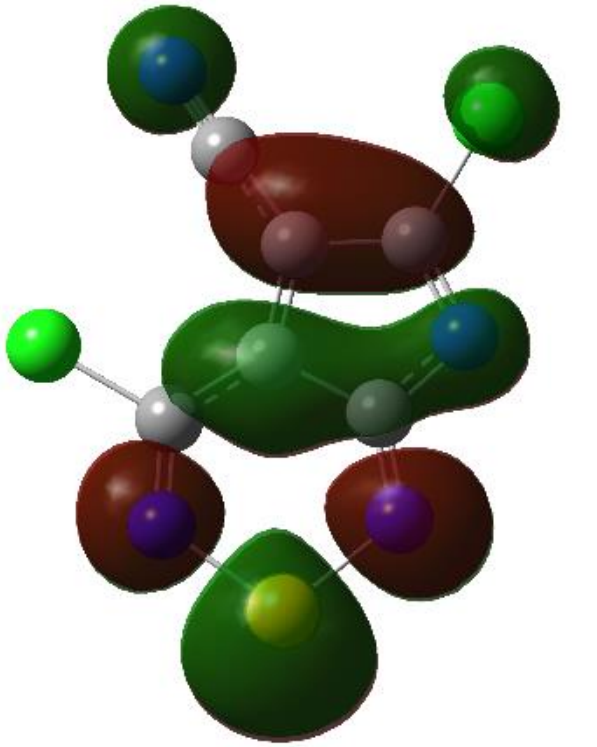
	Dichloro **12**
E_S (eV)	-102578.623542
μ_S (D)	3.9999
LUMO (eV)	-4.2461
HOMO (eV)	-7.5267

Table S2. NICS(0), (1/-1), (2/-2) and (3/-3) for pyrrole and selenadiazine rings of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) calculated at the RB3LYP/6-311G+G(2d,p) level of theory.

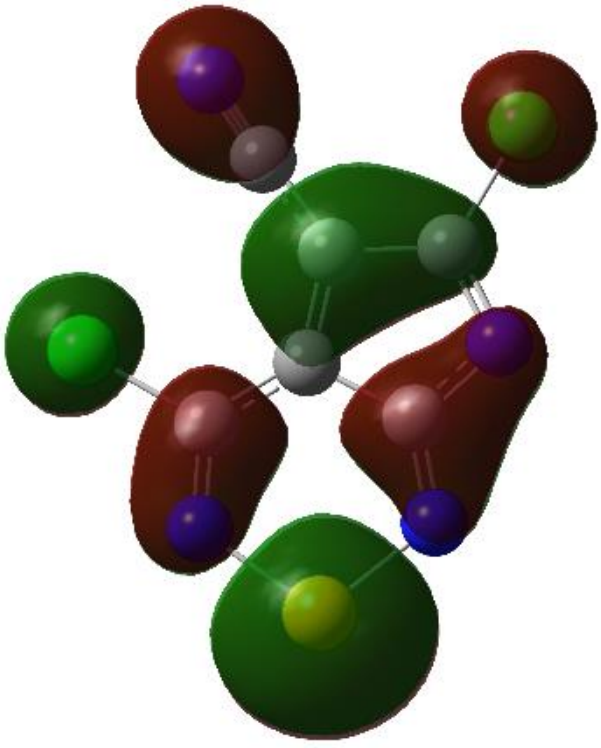
Ring	Pyrrolo	Selenadiazine
NICS(0)	-7.7	-6.0
NICS(1)/(-1)	-9.4	-6.8
NICS(2)/(-2)	-3.8	-3.7
NICS(3)/(-3)	-1.7	-1.8

S1.2 Molecular orbitals

Figure S1. Molecular orbitals of the singlet ground state of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) as calculated at the RB3LYP/6-311G+G(2d,p) level of theory.



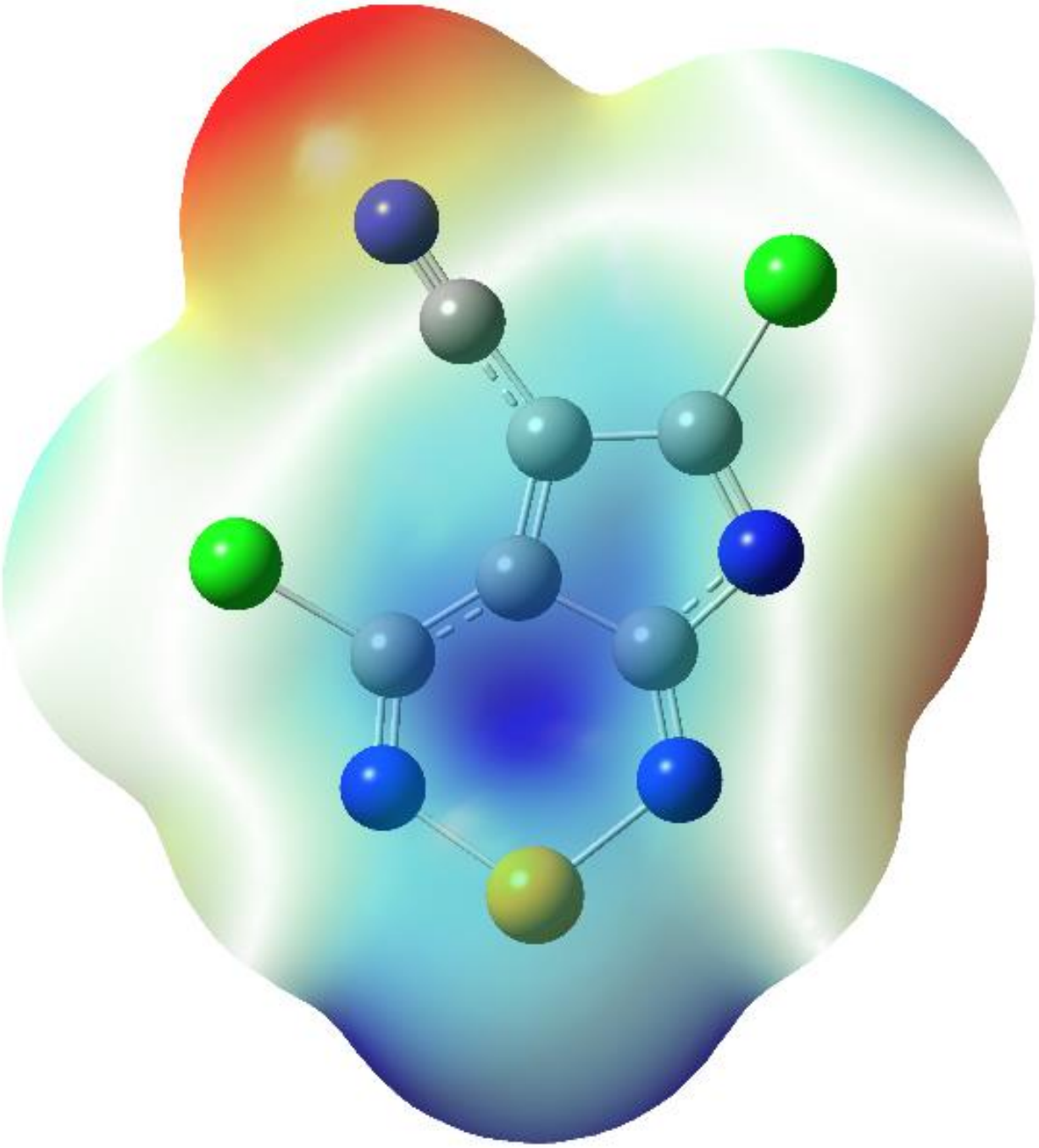
LUMO (E = -4.2461 eV)



HOMO (E = -7.5267 eV)

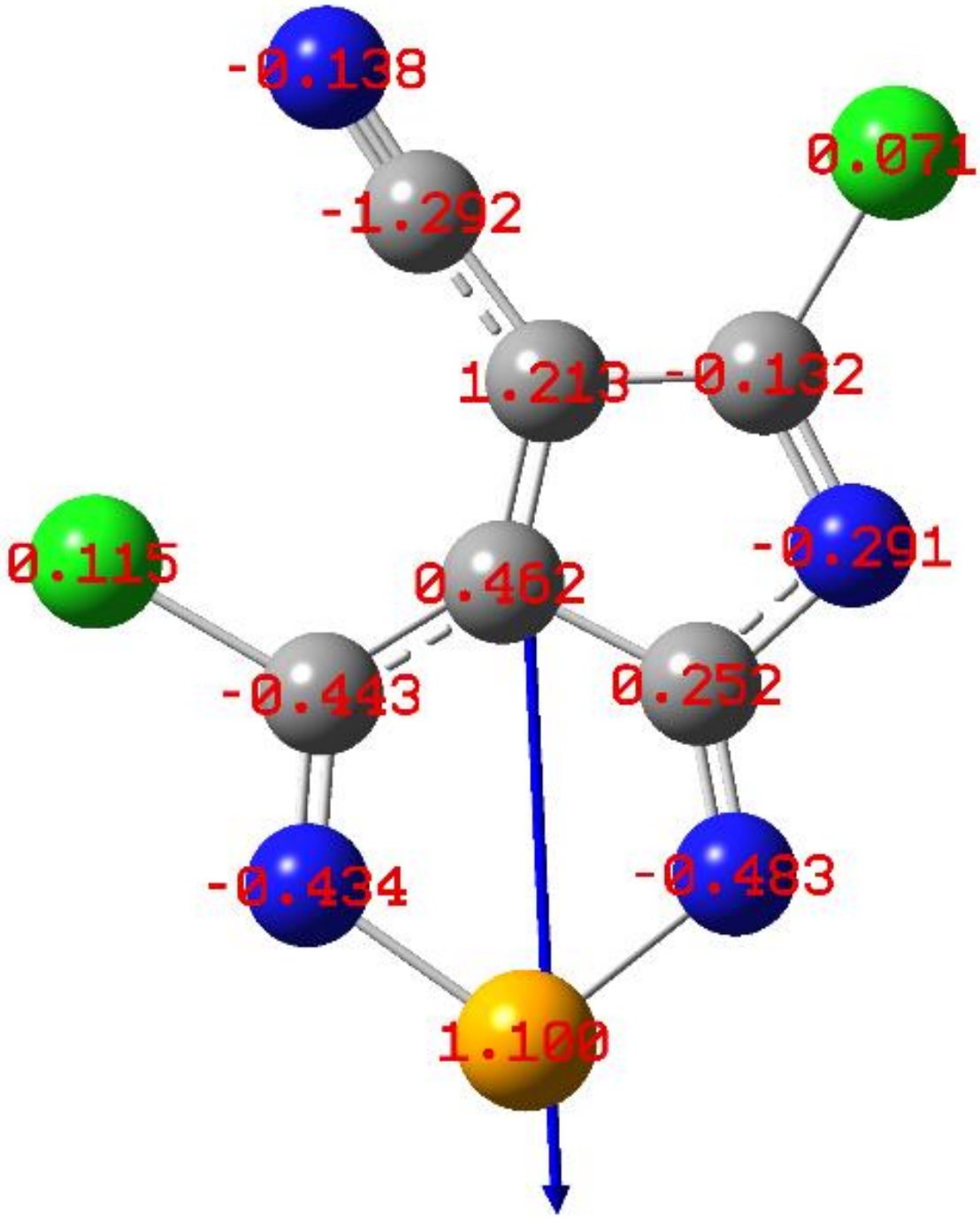
S1.3 Electrostatic potential maps (ESP)

Figure S2. ESP of the singlet ground state of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) as calculated at the RB3LYP/6-311G+G(2d,p) level of theory. Isovalue = 0.004.



S1.4 Mulliken charges and dipole vectors

Figure S3. Mulliken charges and dipole vector of the singlet ground state of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) as calculated at the RB3LYP/6-311G+G(2d,p) level of theory.



μ = 3.999 D

S1.5 Atom coordinates

Table S3. Atom coordinates of the singlet ground state of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) as calculated at the RB3LYP/6-311G+G(2d,p) level of theory.

C(1)	0.1043081	-1.2191611	-0.0001832
C(2)	0.8649930	1.1998391	0.0002398
C(3)	-0.1877140	0.2374940	0.0001238
C(4)	-1.5634551	0.3207779	-0.0000442
C(5)	-2.0174460	-1.0644463	0.0003158
C(6)	-2.4237413	1.4421889	-0.0000732
Cl(7)	0.4332328	2.9003232	0.0002368
N(8)	1.2641893	-1.7966711	-0.0002922
N(9)	2.1247321	0.9372872	0.0000808
N(10)	-3.1755604	2.3169769	0.0000028
Se(11)	2.7186553	-0.7605849	-0.0001752
N(12)	-1.0672759	-1.9490523	-0.0000762
Cl(13)	-3.6755001	-1.5003264	0.0000968

S1.6 Section references

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S2 X-Ray Crystallographic Studies

S2.1 X-Ray crystallographic method

Data for compounds **12**, **13**, and **26** were collected on a Oxford-Diffraction Supernova diffractometer, equipped with a CCD area detector utilizing Cu Kα radiation (λ = 1.5418 Å) for **12** and **26**, and Mo Kα (λ = 0.71073 Å) for **13**. Data for compounds **15**, **33-35** were collected on a XtaLAB Synergy, Single source at home/near, HyPix diffractometer equipped with a CCD area detector utilizing Cu-Kα radiation (λ = 1.5418 Å). Suitable crystals were attached to glass fibers using paratone-*N* oil and transferred to a goniostat where they were cooled for data collection. Unit cell dimensions were determined and refined. Empirical absorption corrections (multi-scan based on symmetry-related measurements) were applied using CrysAlis RED software.[1] The structures **12**, **13**, and **26** were solved by direct method and refined on F^2 using full-matrix least squares using SHELXL97.[2] Software packages used: CrysAlis CCD[1] for data collection, CrysAlis[1] for cell refinement and data reduction, WINGX for geometric calculations,[3] and DIAMOND[4] for molecular graphics. Structures **15**, **33-35** were solved using Olex2,[5] the structure was solved with the olex2.solve[6] structure solution program using Charge Flipping and refined with the SHELXL[7] refinement package using Least Squares minimization. The non-H atoms were treated anisotropically. The hydrogen atoms were placed in calculated, ideal positions and refined as riding on their respective carbon atoms.

Crystallographic data for **12**, **13**, **15**, **26**, **33**, **34** and **35** have been deposited with the Cambridge Crystallographic Data Centre with deposit numbers CCDC-2288302, 2288308, 2288303, 2288307, 2288305, 2288304 and 2288306, respectively. The data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; or e-mail: deposit@ccdc.cam.ac.uk).

S2.1.1 X-Ray crystallographic studies of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (12)

Table S4. Crystal refinement data for 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**)

Empirical formula	$C_6Cl_2N_4Se$
Formula weight	277.96
Temperature	100(2) K
Radiation	Cu Kα (λ = 1.54184 Å)
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 10.7340(13) Å, α = 90° b = 5.6415(3) Å, β = 93.775(9)° c = 13.8208(14) Å, γ = 90°
Volume	835.11(14) $Å^3$
Z	4
Density (calculated)	2.211 g/cm^3
Absorption coefficient	11.597 mm^{-1}
F(000)	528
Crystal size	0.09 × 0.07 × 0.01 mm^3
θ range for data collection	5.059 to 71.778°
Index ranges	-13<=h<=12, -6<=k<=4, -16<=l<=16
Reflections collected	2662
Independent reflections	1589 [R_{int} = 0.0360]
Completeness to θ = 67.684°	99.7%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1589 / 0 / 118
Goodness-of-fit	1.083
Final R indices [I > 2σ(I)]	R_{obs} = 0.0629, wR_{obs} = 0.1810
R indices [all data]	R_{all} = 0.0645, wR_{all} = 0.1858
Extinction coefficient	.
Largest diff. peak and hole	2.437 and -1.409 e·$Å^{-3}$

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/[\sigma^2(Fo^2)+(0.1496P)^2+0.4017P]$ where $P=(Fo^2+2Fc^2)/3$

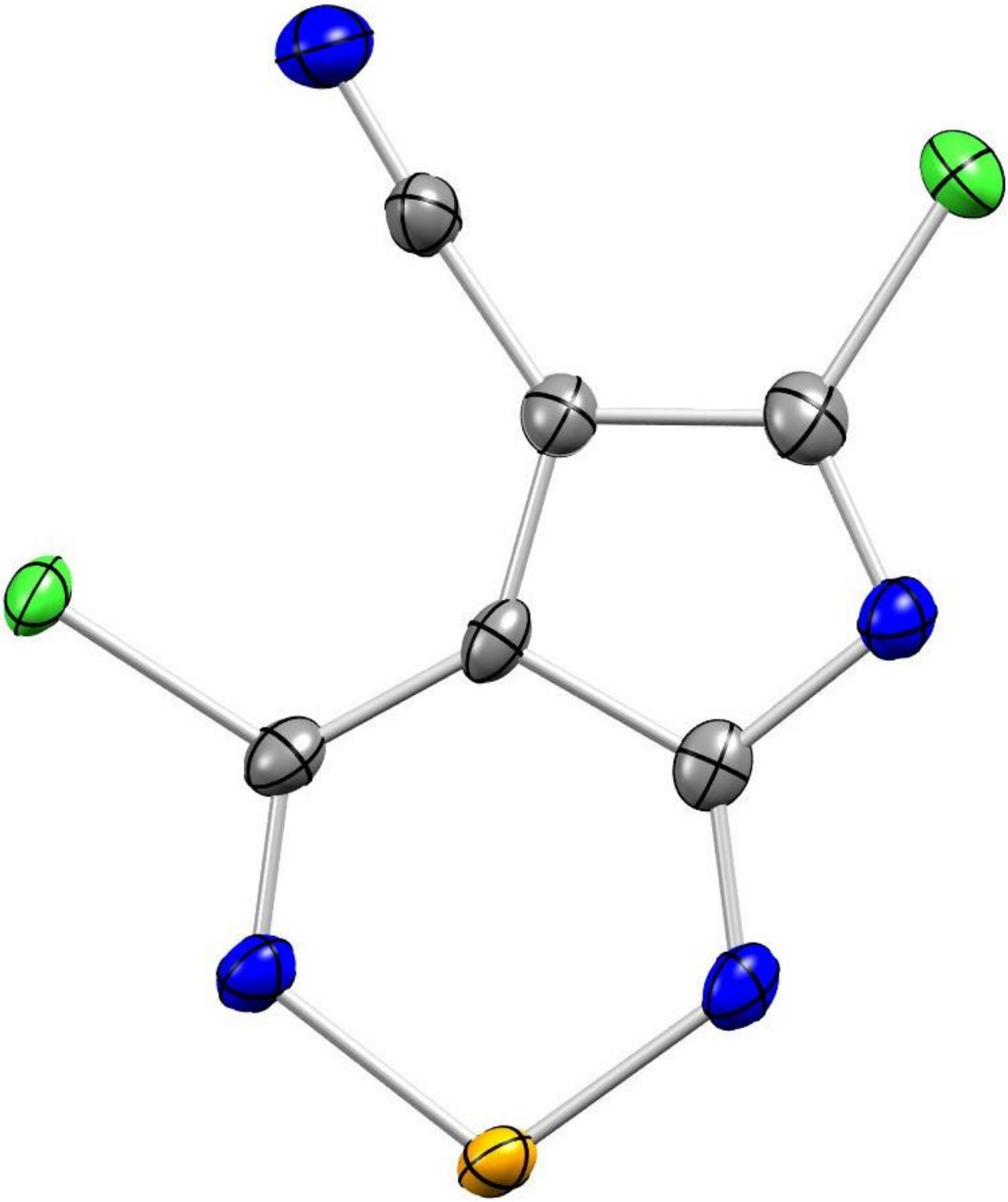

Figure S4. ORTEP view of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**). 50% Probability ellipsoids.

S2.1.2 X-Ray crystallographic studies of 4-chloro-6-oxo-6,7-dihydropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (13)

Table S5. Crystal refinement data for 4-chloro-6-oxo-6,7-dihydropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**13**)

Empirical formula	C_6ClN_4OSe
Formula weight	258.51
Temperature	100(2) K
Radiation	Mo Kα (λ = 0.71073 Å)
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 5.8205(6) Å, α = 66.940(10)° b = 11.1537(12) Å, β = 88.468(8)° c = 13.4660(13) Å, γ = 82.098(9)°
Volume	796.37(15) Å^3
Z	4
Density (calculated)	2.156 g/cm^3
Absorption coefficient	5.007 mm^{-1}
F(000)	492
Crystal size	0.07 × 0.05 × 0.02 mm^3
θ range for data collection	3.290 to 29.646°
Index ranges	-7<=h<=7, -15<=k<=14, -17<=l<=16
Reflections collected	6459
Independent reflections	3745 [R_{int} = 0.0385]
Completeness to θ = 25.242°	99.8%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3745 / 0 / 235
Goodness-of-fit	1.060
Final R indices [I > 2σ(I)]	R_{obs} = 0.0474, wR_{obs} = 0.1002
R indices [all data]	R_{all} = 0.0770, wR_{all} = 0.1175
Extinction coefficient	.
Largest diff. peak and hole	1.249 and -0.973 e·Å^{-3}

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/[\sigma^2(Fo^2)+(0.0439P)^2+0.0423P]$ where $P=(Fo^2+2Fc^2)/3$

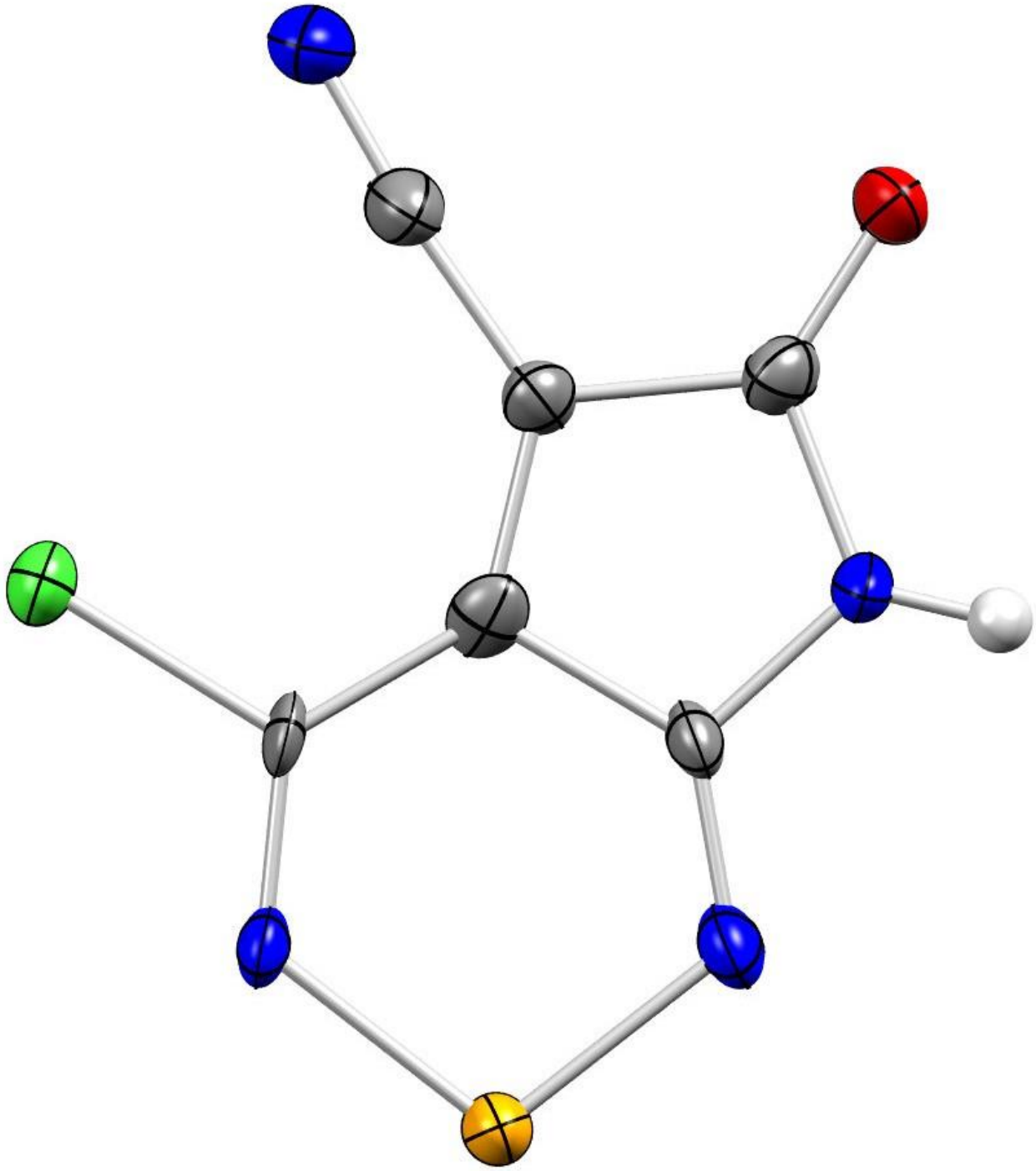

Figure S5. ORTEP view of 4-chloro-6-oxo-6,7-dihydropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**13**). 50% Probability ellipsoids.

S2.1.3 X-Ray crystallographic studies of 4-chloro-6-phenoxypyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (15)

Table S6. Crystal refinement data for 4-chloro-6-phenoxypyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**15**)

Empirical formula	$C_{12}H_5ClN_4OSe$
Formula weight	335.61
Temperature	179.99(10) K
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	5.01700(8)
b/Å	8.67188(13)
c/Å	27.5955(4)
α/°	90
β/°	90.8291(15)
γ/°	90
Volume/Å^3	1200.47(3)
Z	4
ρ_{calc}g/cm^3	1.857
μ/mm^{-1}	6.270
F(000)	656.0
Crystal size/mm^3	0.7 × 0.5 × 0.2
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	6.406 to 153.496
Index ranges	$-6 \leq h \leq 5$, $-10 \leq k \leq 10$, $-34 \leq l \leq 33$
Reflections collected	13273
Independent reflections	2470 [R_{int} = 0.0378, R_{sigma} = 0.0253]
Data/restraints/parameters	2470/0/173
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0214, wR_2 = 0.0521
Final R indexes [all data]	R_1 = 0.0231, wR_2 = 0.0528
Largest diff. peak/hole / e Å^{-3}	0.35/-0.26

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/[\sigma^2(Fo^2)+(0.0439P)^2+0.0423P]$ where $P=(Fo^2+2Fc^2)/3$

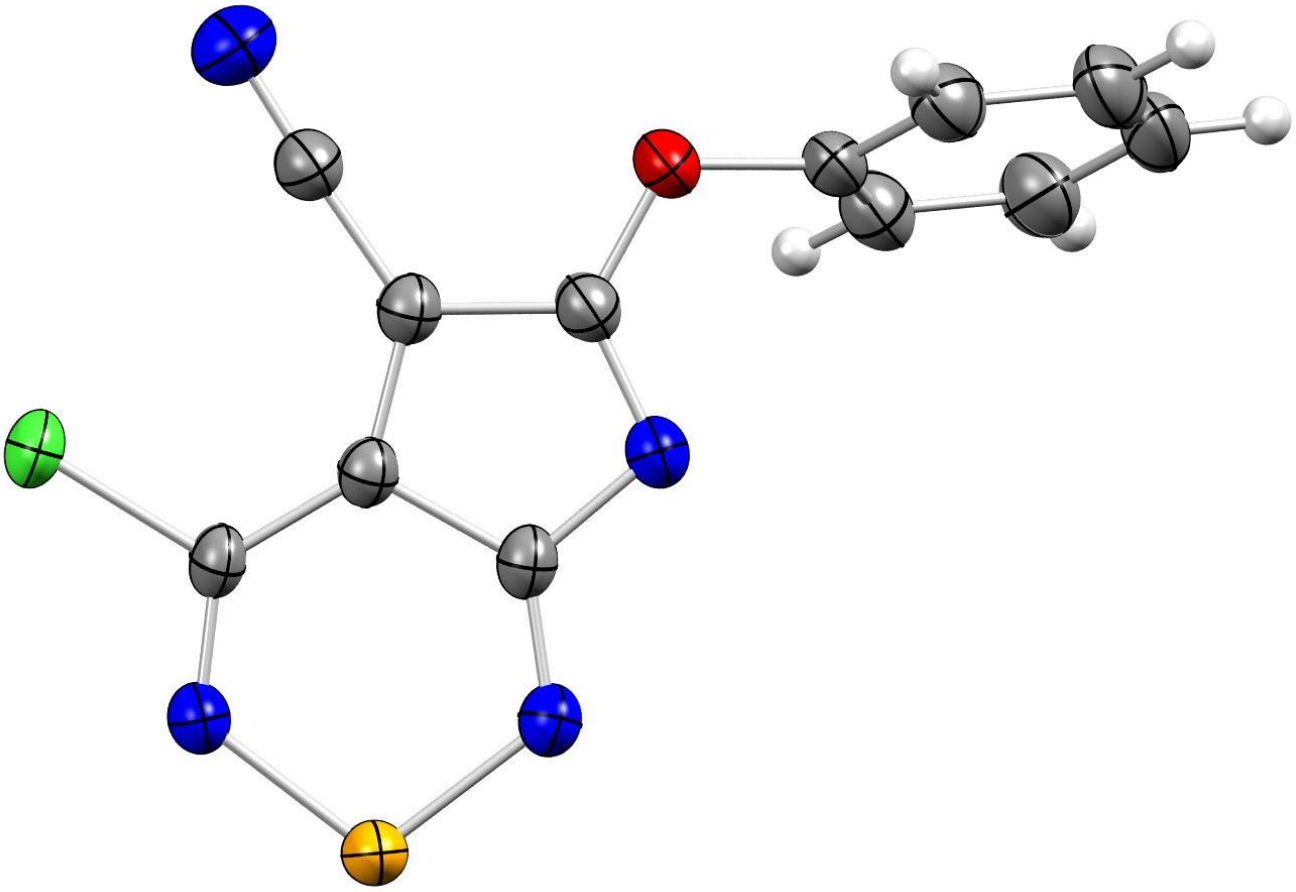

Figure S6. ORTEP view of 4-chloro-6-phenoxypyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**15**). 50% Probability ellipsoids.

S2.1.4 X-Ray crystallographic studies of 4-chloro-6-morpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (26)

Table S7. Crystal data and structure refinement for 4-chloro-6-morpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**26**).

Empirical formula	$C_{10}H_8ClN_5OSe$
Formula weight	328.62
Temperature	100(2) K
Radiation	Cu Kα (λ = 1.54184 Å)
Crystal system	monoclinic
Space group	P2yn
Unit cell dimensions	a = 9.9615(4) Å, α = 90° b = 5.9698(3) Å, β = 92.102(4)° c = 18.9005(8) Å, γ = 90°
Volume	1123.22(9) Å^3
Z	4
Density (calculated)	1.943 g/cm^3
Absorption coefficient	6.700 mm^{-1}
F(000)	648
Crystal size	0.05 × 0.04 × 0.02 mm^3
θ range for data collection	4.682 to 71.663°
Index ranges	-7<=h<=12, -7<=k<=7, -23<=l<=22
Reflections collected	3867
Independent reflections	2138 [R_{int} = 0.0236]
Completeness to θ = 67.684°	100%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2138 / 45 / 163
Goodness-of-fit	1.199
Final R indices [I > 2σ(I)]	R_{obs} = 0.0788, wR_{obs} = 0.1883
R indices [all data]	R_{all} = 0.0830, wR_{all} = 0.1909
Extinction coefficient	.
Largest diff. peak and hole	2.126 and -1.124 e·Å^{-3}

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/[\sigma^2(Fo^2)+(0.0628P)^2+12.8831P]$ where $P=(Fo^2+2Fc^2)/3$

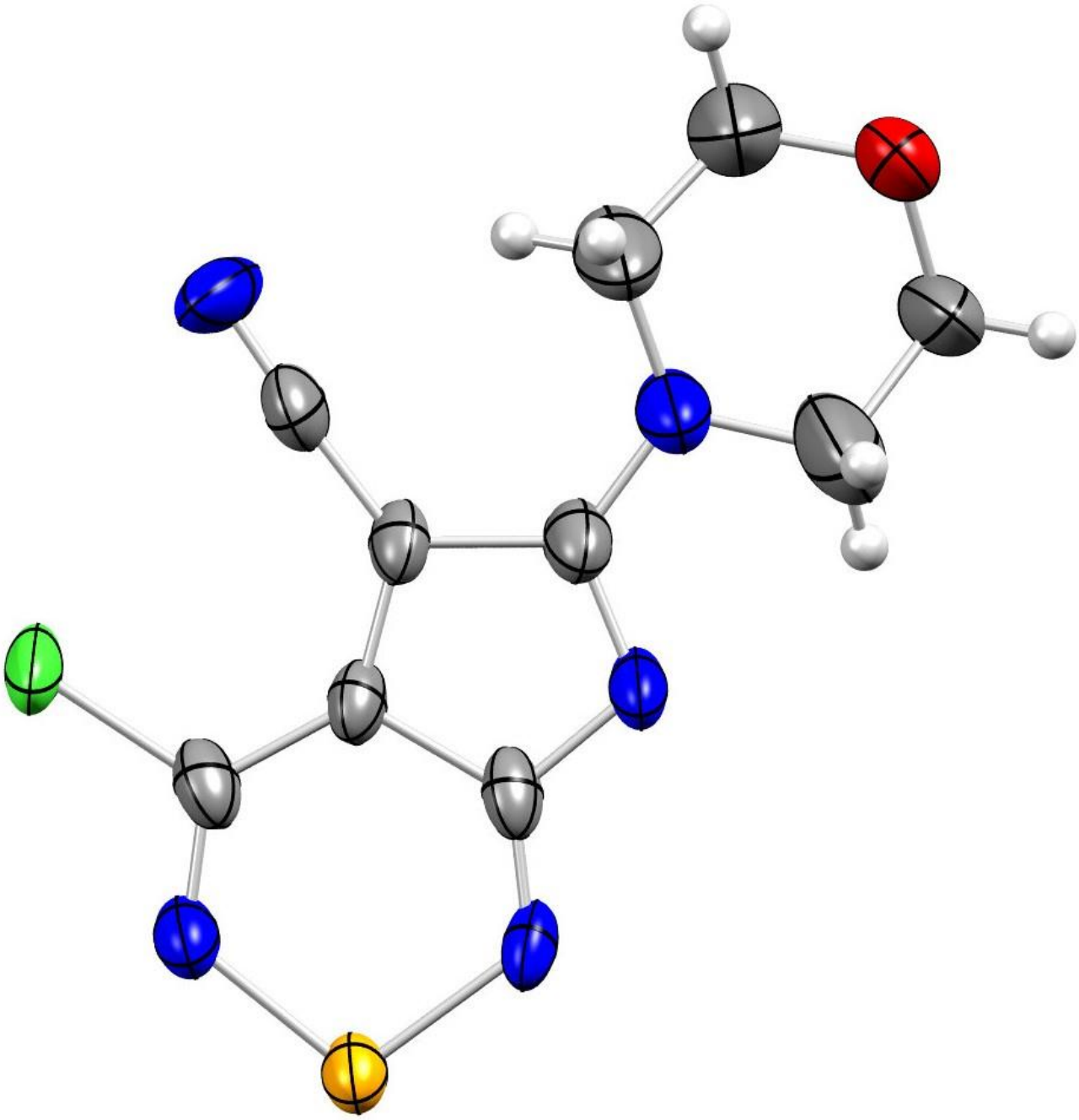

Figure S7. ORTEP view of 4-chloro-6-morpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**26**). 50% Probability ellipsoids.

S2.1.5 X-Ray crystallographic studies of 4,6-dimorpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (33)

Table S8. Crystal data and structure refinement for 4,6-dimorpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**33**).

Empirical formula	$C_{14}H_{16}N_6O_2Se$
Formula weight	379.29
Temperature	200(2) K
Radiation	Cu Kα (λ = 1.54184 Å)
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 5.21970(10) Å, α = 105.672(2)° b = 11.2505(2) Å, β = 95.717(2)° c = 13.0616(2) Å, γ = 94.437(2)°
Volume	730.48(2) Å^3
Z	2
Density (calculated)	1.724 g/cm^3
Absorption coefficient	3.673 mm^{-1}
F(000)	384
Crystal size	0.05 × 0.03 × 0.02 mm^3
θ range for data collection	3.543 to 76.535°
Index ranges	-6<=h<=6, -13<=k<=10, -16<=l<=16
Reflections collected	8143
Independent reflections	2950 [R_{int} = 0.0356]
Completeness to θ = 76.535 °	99.80%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2950 / 0 / 208
Goodness-of-fit	1.060
Final R indices [I > 2σ(I)]	R_{obs} = 0.0297, wR_{obs} = 0.0780
R indices [all data]	R_{all} = 0.0319, wR_{all} = 0.0801
Extinction coefficient	.
Largest diff. peak and hole	0.471 and --0.387 e·Å^{-3}

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/[\sigma^2(Fo^2)+(0.0628P)^2+12.8831P]$ where $P=(Fo^2+2Fc^2)/3$

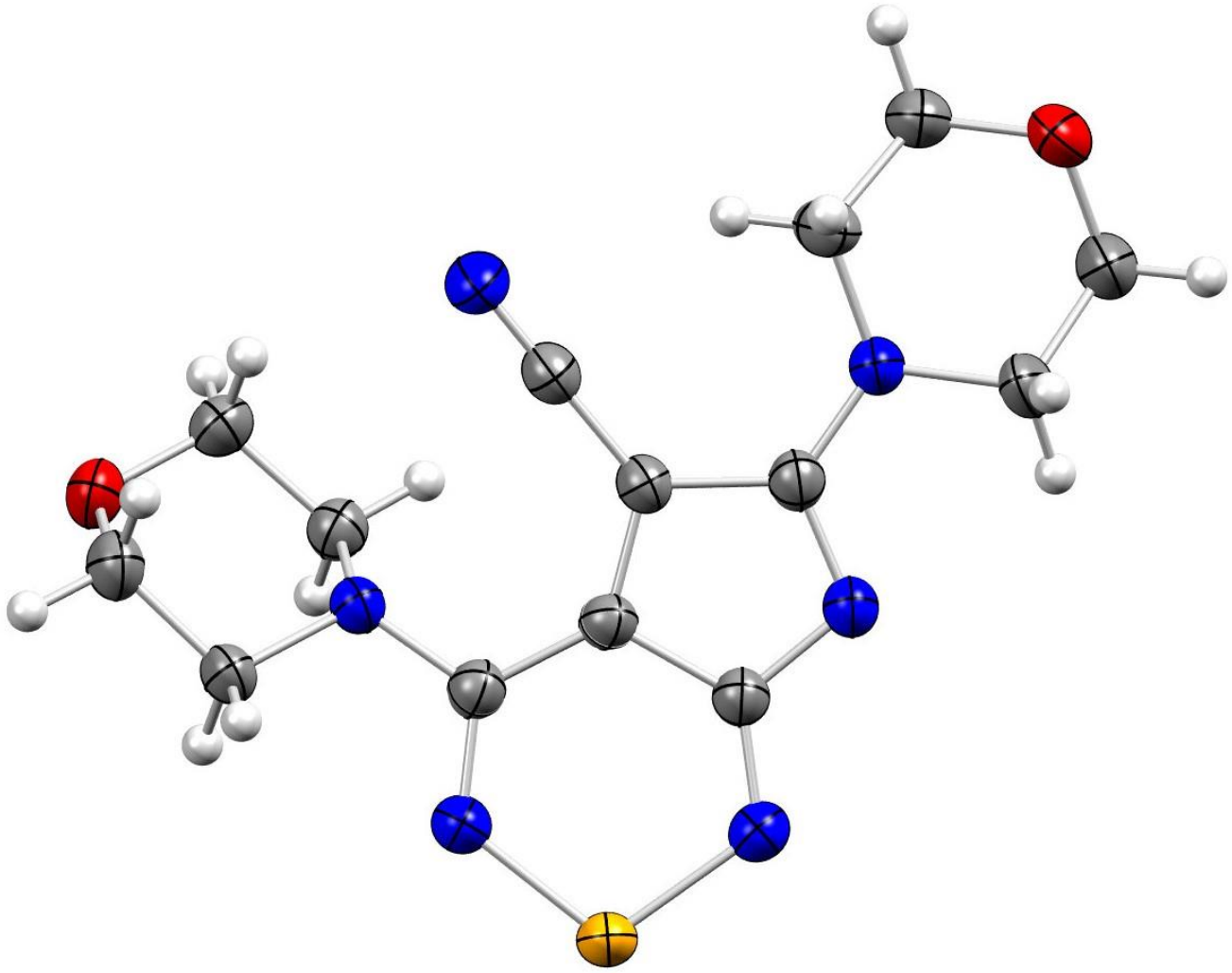

Figure S8. ORTEP view of 4,6-dimorpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**33**). 50% Probability ellipsoids.

S2.1.6 X-Ray crystallographic studies of 2,5-dimorpholino-3-oxo-3*H*-pyrrole-4-carbonitrile (34)

Table S9. Crystal data and structure refinement for 2,5-dimorpholino-3-oxo-3*H*-pyrrole-4-carbonitrile (**34**).

Empirical formula	$C_{13}H_{16}N_4O_3$
Formula weight	276.30
Temperature	177.15 K
Crystal system	Monoclinic
Space group	C2/c
a/Å	22.2254(4)
b/Å	6.7299(2)
c/Å	17.5435(4)
α/°	90
β/°	90.539(2)
γ/°	90
Volume/Å^3	2623.95(11)
Z	8
ρ_{calc}g/cm^3	1.399
μ/mm^{-1}	0.849
F(000)	1168.0
Crystal size/mm^3	0.08 × 0.03 × 0.025
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	7.956 to 155.35
Index ranges	$-28 \leq h \leq 27$, $-5 \leq k \leq 8$, $-22 \leq l \leq 20$
Reflections collected	8413
Independent reflections	2629 [R_{int} = 0.0344, R_{sigma} = 0.0372]
Data/restraints/parameters	2629/0/181
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0381, wR_2 = 0.0980
Final R indexes [all data]	R_1 = 0.0436, wR_2 = 0.1027
Largest diff. peak/hole / e Å^{-3}	0.20/-0.23

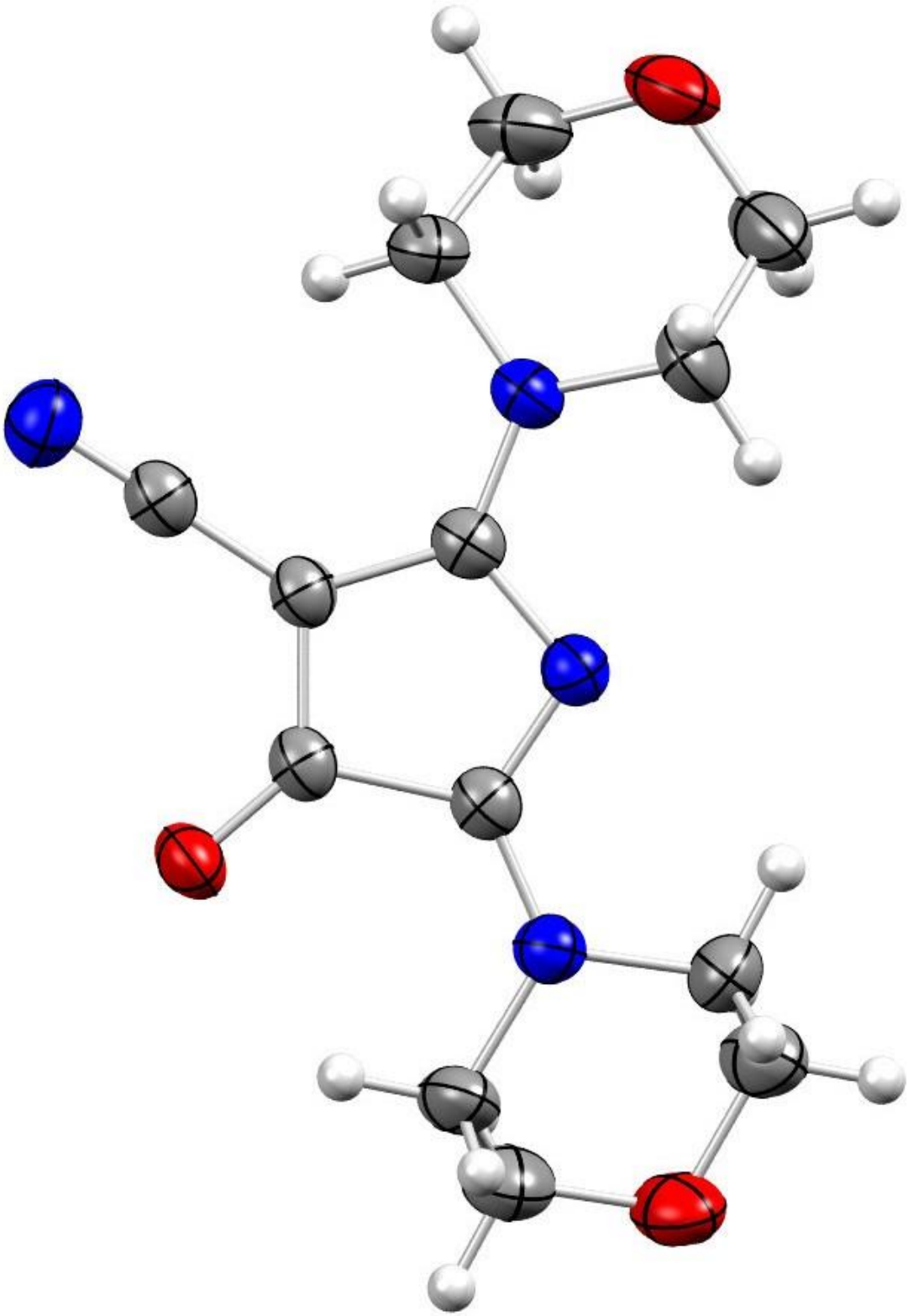

Figure S9. ORTEP view of 2,5-dimorpholino-3-oxo-3*H*-pyrrole-4-carbonitrile (**34**). 50% Probability ellipsoids.

S2.1.7 X-Ray crystallographic studies of 3,5-dimorpholino-2-oxo-2*H*-pyrrole-4-carbonitrile (35)

Table S10. Crystal data and structure refinement for 3,5-dimorpholino-2-oxo-2*H*-pyrrole-4-carbonitrile (**35**).

Empirical formula	$C_{13}H_{16}N_4O_3Se$
Formula weight	275.30
Temperature	114(2) K
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	7.2528(4)
b/Å	9.1018(5)
c/Å	18.9222(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1249.12(12)
Z	4
ρ_{calc}g/cm^3	1.469
μ/mm^{-1}	0.891
F(000)	584.0
Crystal size/mm^3	0.025 × 0.024 × 0.022
Radiation	CuKα (λ = 1.54184 Å)
2Θ range for data collection/°	9.348 to 152.87
Index ranges	$-5 \leq h \leq 8$, $-11 \leq k \leq 9$, $-23 \leq l \leq 22$
Reflections collected	4143
Independent reflections	2007 [R_{int} = 0.0637, R_{sigma} = 0.0845]
Data/restraints/parameters	2007/4/182
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.1325, wR_2 = 0.3368
Final R indexes [all data]	R_1 = 0.1407, wR_2 = 0.3477
Largest diff. peak/hole / e Å^{-3}	0.93/-0.41
Flack parameter	1.3(13)

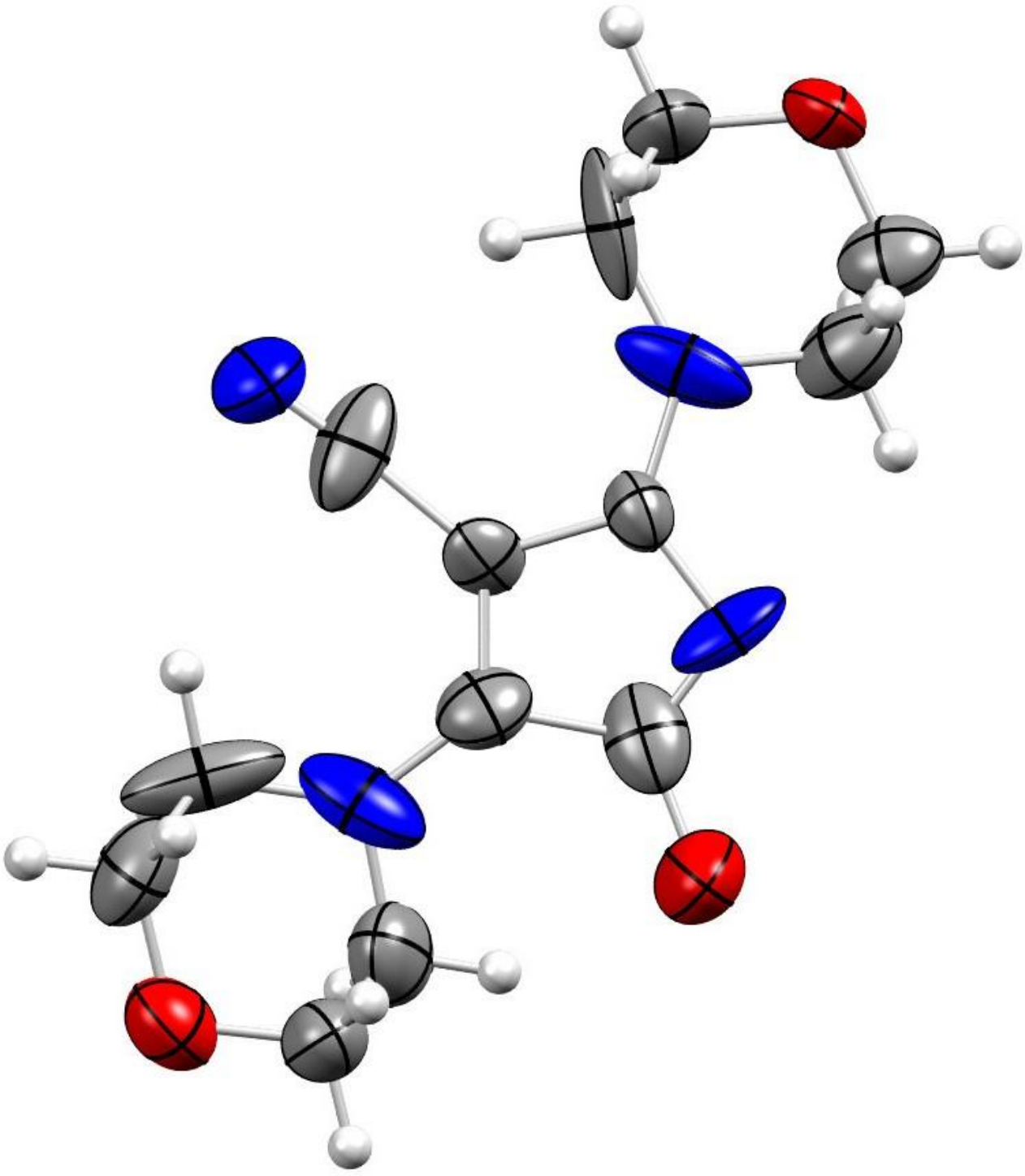

Figure S10. ORTEP view of 3,5-dimorpholino-2-oxo-2*H*-pyrrole-4-carbonitrile (**35**). 50% Probability ellipsoids.

S2.2 Section references

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S3 Experimental Section

S3.1 General methods and materials

All chemicals were commercially available except those whose synthesis is described. Reactions were protected from atmospheric moisture via $CaCl_2$ drying tubes, and monitored by TLC using commercial glass backed thin layer chromatography (TLC) plates (Merck Kieselgel 60 F_{254}). TLC plates were observed under UV light at 254 and 365 nm. The technique of dry flash chromatography was used throughout for all non-TLC scale chromatographic separations using Merck Silica Gel 60 (less than 0.063 mm).[1] Melting points were determined using a PolyTherm-A, Wagner & Munz, Kofler - Hotstage Microscope apparatus or were determined using a TA Instruments DSC Q1000 with samples hermetically sealed in aluminium pans under an argon atmosphere; using heating rates of 5 °C/min (DSC mp listed by onset and peak values). Solvents used for recrystallization are indicated after the melting points. UV-vis spectra were obtained using a Shimadzu UV-1900 spectrophotometer and inflections are identified by the abbreviation "inf". IR spectra were recorded on a Shimadzu FTIR-NIR Prestige-21 spectrometer fitted with a Pike Miracle Ge ATR accessory and strong, medium and weak peaks are represented by s, m and w, respectively. ^{1}H and ^{13}C NMR spectra were recorded, as indicated, on a Bruker Avance 300 machine at 300 and 75 MHz, respectively, or on a Bruker Avance 500 machine at 500 and 125 MHz, respectively. Deuterated solvents were used for homonuclear lock and the signals are referenced to the deuterated solvent peaks. Attached proton test (APT) NMR studies were used for the assignment of the ^{13}C peaks C (quaternary), CH_2, CH_3 and CH_4 as C (s), C (d), C (t) and C (q), respectively. Mass spectrometry was recorded with the Matrix-Assisted Laser Desorption/Ionization-Time of Flight (MALDI-TOF) mass spectrum (+ve mode) on a Bruker Autoflex III Smartbeam instrument or with the Agilent 1260 Infinity II Preparative LC/MSD System. Elemental analysis was performed using a Euro-Vector EA3000 CHN elemental analyzer. Tetracyanoethylene (TCNE)[2] and selenium dichloride ($SeCl_2$)[3] were prepared according to the literature procedures.

S3.2 Experimental procedures

S3.2.1 4,6-Dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (12)

Method A – from Se_2Cl_2 and SO_2Cl_2: To a stirred suspension of tetracyanoethylene (**TCNE**) (100 mg, 0.78 mmol) in DCE (2.5 mL) at *ca.* 20 °C was added first anhydrous benzyltriethylammonium chloride (3.5 mg, 2 mol%), then Se_2Cl_2 (48.0 μL, 0.58 mmol) and finally SO_2Cl_2 (32.0 μL, 0.40 mmol). The reaction mixture was then heated to *ca.* 70 °C for 40 h, allowed to cool to *ca.* 20 °C, adsorbed onto silica, chromatographed (DCM) and recrystallised to give the *title compound* **12** (92 mg, 42%) as yellow prisms,

mp (hot-stage) 210-215 °C (decomp.) (*c*-Hex/DCE), (DSC) mp onset: 204.7 °C, peak: 232.5 °C; 1st decomp. onset: 233.3 °C, peak: 238.3 °C; 2nd decomp. onset: 257.9 °C, peak: 267.8 °C (*c*-Hex/DCE, 80:20); R_f 0.66 (Hex/TBME, 67:33); Anal. Calcd for $C_6Cl_2N_4Se$: C, 25.93; N, 20.16. Found: C, 26.18; N, 20.08%; λ_{max}(DCM)/nm 256 (log ε 4.14), 295 (3.81), 373 inf (3.29), 445 (4.08), 477 inf (3.74); ν_{max}/cm^{-1}(ATR) 2230w (C≡N), 1730w, 1566s, 1547w, 1462w, 1356m, 1339m, 1287s, 1277s, 1165m, 1072m, 957m, 856s, 752s, 708s; δ_C(125 MHz, CD_2Cl_2) 167.7 (s), 162.2 (s), 147.9 (s), 122.4 (s), 112.1 (s), 104.6 (s); *m/z* (MALDI-TOF) 301 ($Se^{80}Cl^{35}$: M^++Na, 18%), 279 (MH^+, 24), 195 (13), 192 (36), 133 (40), 97 (10), 81 (11), 39 (100). Further elution (Hex/TBME, 33:67) gave *4-chloro-6-oxo-6,7-dihydro-pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile* (**13**) (61 mg, 30%) as orange prisms, mp (hot-stage) > 310 °C (decomp.) (DCE), (DSC) 1st decomp. onset: 199.9 °C, peak: 207.5 °C; 2nd decomp. onset: 216.2 °C, peak: 219.6 °C (DCE); R_f 0.56 (Hex/TBME, 67:33); Anal. Calcd for C_6HClN_4OSe: C, 27.77; H, 0.39; N, 21.59. Found: C, 27.41; H, 0.51; N, 21.87%; λ_{max}(DCM)/nm 275 (log ε 3.74), 281 inf (3.72), 429 (4.20), 437 inf (4.19); ν_{max}/cm^{-1}(ATR) 3113w (NH), 2772w, 2230w (C≡N), 1693s (C=O), 1587m, 1566s, 1464w, 1360m, 1337m, 1321m, 1175w, 1123m, 991w, 885m, 808w, 756m, 731m, 716s; δ_H[300 MHz, $(CD_3)_2C$=O] 11.5 (1H, br s, D_2O exchangeable); δ_C[125 MHz, TFA-*d*] 166.9 (s), 149.4 (s), 143.1 (s), 122.8 (s), 109.8 (s), 96.7 (s); *m/z* (MALDI-TOF) 283 ($Se^{80}Cl^{35}$: M^++Na, 39%), 261 (MH^+, 100), 225 (5), 149 (3), 133 (2), 91 (12), 39 (3).

Method B – from in situ prepared $SeCl_2$: To a stirred suspension of elemental selenium (94.8 mg, 1.20 mmol) in anhydrous DCE (2.5 mL) at *ca.* 20 °C was added sulfuryl chloride (97.0 μL, 1.20 mmol) and the mixture was stirred for 24 h at *ca.* 20 °C until no suspension remained. TCNE (100 mg, 0.78 mmol) was then added to the dark red mixture followed by anhydrous $BnEt_3NCl$ (3.5 mg, 2 mol%). The stirred mixture was then heated to *ca.* 70 °C for 40 h and then allowed to cool to *ca.* 20 °C, dissolved in DCM (200 mL), adsorbed onto silica, chromatographed (DCM) and recrystallised to give the title compound **12** (46 mg, 21%), as yellow prisms, mp (hot-stage) 210-215 °C (decomp.) (*c*-Hex/DCE); R_f 0.66 (Hex/TBME, 67:33); ν_{max}/cm^{-1}(ATR) 2230w (C≡N), 1730w, 1566s, 1547w, 1462w, 1356m, 1339m, 1287s, 1277s, 1165m, 1072m, 957m, 856s, 752s, 708s; identical to that described above. Further elution (Hex/TBME, 33:67) gave 4-chloro-6-oxo-6,7-dihydropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**15**) (32 mg, 16%), as orange prisms, mp (hot-stage) > 310 °C (decomp.) (DCE); R_f 0.56 (Hex/TBME, 67:33); ν_{max}/cm^{-1}(ATR) 3113w (NH), 2772w, 2230w (C≡N), 1693s (C=O), 1587m, 1566s, 1464w, 1360m, 1337m, 1321m, 1175w, 1123m, 991w, 885m, 808w, 756m, 731m, 716s; identical to that described above.

Method C – from in situ prepared $SeCl_2$ and chromatography free: To a stirred suspension of selenium powder (593 mg, 7.50 mmol) in anhydrous DCE (15 mL) at *ca.* 20 °C was added sulfuryl chloride (606 μL, 7.50 mmol) and flame dried 4 Å molecular sieves. The mixture was stirred for 24 h at *ca.* 20 °C until no suspension remained. TCNE (640 mg, 5.00 mmol) was then added to the dark red mixture followed by anhydrous $BnEt_3NCl$ (22.5 mg, 2 mol%). The mixture was then heated at reflux for 40 h and then allowed to cool to *ca.* 20 °C. The mixture was dissolved in DCM (300 mL) and filtered to remove insoluble material. The filtrate was then washed (sat. $NaHCO_3$, 4 × 50 mL). The combined aqueous phases were extracted with DCM (2 × 20 mL). The combined organic phases were dried ($MgSO_4$), and passed through a Florisil plug, using DCM as eluent. The volatiles were removed *in vacuo* and the residue recrystallised to give the title compound **12** (977 mg, 70%), as yellow prisms, mp (hot-stage) 210-215 °C (decomp.) (*c*-Hex/DCE); R_f 0.66 (Hex/TBME, 67:33); ν_{max}/cm^{-1}(ATR) 2230w (C≡N), 1730w, 1566s, 1547w, 1462w, 1356m, 1339m, 1287s, 1277s, 1165m, 1072m, 957m, 856s, 752s, 708s; identical to that described above.

S3.2.2 4-Chloro-6-oxo-6,7-dihydropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (13)

A solution of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in 2 mL of 9.2 M H_2SO_4 (H_2O/H_2SO_4, 50:50 v/v) at *ca.* 20 °C was stirred for 2.5 h until no starting material remained (TLC). The mixture was diluted with distilled water (8 mL) and extracted with DCM (3 × 20 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallised to give the *title compound* **13** (16.0 mg, 59%) as orange prisms, mp (hot-stage) > 310 °C (decomp.) (DCE), R_f 0.56 (Hex/TBME, 67:33); ν_{max}/cm^{-1}(ATR) 3113w (NH), 2772w, 2230w (C≡N), 1693s (C=O), 1587m, 1566s, 1464w, 1360m, 1337m, 1321m, 1175w, 1123m, 991w, 885m, 808w, 756m, 731m, 716s; identical to that described above.

S3.2.3 4-Chloro-6-methoxypyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile (14)

Method A – chromatographic isolation: A vigorously stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous methanol (3 mL) was heated to reflux for 10 min until no starting material remained (TLC: Hex/TBME, 50:50). On cooling to *ca.* 20 °C, the mixture was then adsorbed onto silica and chromatographed (Hex/TBME, 67:33) to give the *title compound* **14** (27.0 mg, 99%) as yellow plates, mp (hot-plate) 170-177 °C (DCE) (decomp.); R_f 0.45 (Hex/TBME, 40:60); Anal. Calcd for $C_7H_3ClN_4OSe$: C, 30.74; H, 1.11; N, 20.48. Found: C, 30.99; H, 1.49; N, 20.15%; λ_{max}(DCM)/nm 243 (log ε 4.30), 255 (4.27), 278 (4.13), 407 inf (4.11), 416 inf (4.22), 428 (4.27), 441 inf (4.19), 451 inf (3.97); ν_{max}/cm^{-1}(ATR) 2220w (C≡N), 1701w, 1605m, 1595m,

1572w, 1562w, 1483m, 1449w, 1396m, 1368w, 1352m, 1325s, 1215w, 1180w, 1003w, 949m, 868m, 775w, 725m, 714m; δ_H(500 MHz, $CDCl_3$) 4.36 (3H, s); δ_C(75 MHz, TFA-*d*) 172.5 (s), 151.3 (s), 148.4 (s), 122.3 (s), 108.2 (s), 91.4 (s), 62.6 (q); *m/z* (LCMS) 275 ($Se^{80}Cl^{35}$: MH^+, 82%), 249 (7), 237 (16), 235 (5), 227 (24), 219 (5), 193 (86), 159 (19), 139 (12), 79 (24), 74 (62), 65 (55), 61 (100), 60 (57).

Method B – non-chromatographic work-up: A vigorously stirred suspension of 4,6-dichloro-pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous methanol (3 mL) was heated to reflux for 10 min until no starting material remained (TLC: Hex/TBME, 50:50). On cooling to *ca.* 20 °C, the mixture was diluted with distilled water (40 mL) and extracted with DCM (2 × 40 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallised to give the title compound **14** (27.4 mg, 100%) as yellow plates, mp (hot-plate) 170-177 °C (DCE) (decomp.); R_f 0.45 (Hex/TBME, 40:60); ν_{max}/cm^{-1}(ATR) 2220w (C≡N), 1701w, 1605m, 1595m, 1572w, 1562w, 1483m, 1449w, 1396m, 1368w, 1352m, 1325s, 1215w, 1180w, 1003w, 949m, 868m, 775w, 725m, 714m; identical to that described above.

S3.2.4 4-Chloro-6-phenoxypyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (15)

To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (4 mL) at *ca.* 20 °C was added phenol (47.1 mg, 0.50 mmol) and powdered $NaHCO_3$ (42.0 mg, 0.50 mmol). The reaction mixture was heated at reflux for 72 h until no starting material remained (TLC). On cooling to *ca.* 20 °C, the mixture was diluted with DCM (15 mL) and washed (5% $NaHCO_3$, 2 × 30 mL). The organic phase was then adsorbed onto silica, and chromatographed (Hex/DCM, 20:80) to give the *title compound* **15** (23.0 mg, 65%) as yellow needles, mp (hot-plate) 178-185 °C (*c*-Hex/DCE*)* (decomp.); R_f 0.57 (Hex/TBME, 40:60); Anal. Calcd for $C_{12}H_5ClN_4OSe$: C, 42.94; H, 1.50; N, 16.69. Found: C, 43.27; H, 1.13; N, 16.33%; λ_{max}(DCM)/nm 261 (log ε 4.37), 285 inf (4.21), 411 inf (4.03), 423 inf (4.15), 432 (4.19), 445 inf (4.11), 456 inf (3.93); δ_H(300 MHz, $CDCl_3$) 7.52-7.41 (4H, m), 7.37-7.32 (1H, m); δ_C(125 MHz, $CDCl_3$) one C (s) resonance missing, 175.3 (s), 161.3 (s), 152.9 (s), 145.3 (s), 130.1 (d), 127.1 (d), 123.3 (s), 120.7 (d), 111.8 (s); *m/z* (MALDI-TOF) 336 ($Se^{80}Cl^{35}$: MH^+, 100%), 244 (15).

S3.2.5 6-Amino-4-chloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (16)

A stirred solution of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (55.6 mg, 0.20 mmol) in anhydrous DCM (15 mL) at *ca.* 20 °C was sparged with NH_3 (g) for 30 min, until no starting material remained (TLC). The reaction mixture was then cooled in an ice bath and filtered to collect the formed orange precipitate which was washed with distilled water, MeOH then pentane and recrystallized

to give the *title compound* **16** (30.9 mg, 60%) as yellow prisms, mp (hot-stage) 228-232 °C (decomp.) (THF); R_f 0.39 (DCM/TBME); Anal. Calcd for $C_6H_2ClN_5Se$: C, 27.87; H, 0.78; N, 27.09. Found C, 27.56; H, 1.83; N, 27.37%; λ_{max}(DCM)/nm 251 (log ε 4.30), 267 inf (4.10), 297 (3.79), 453 (4.20); ν_{max}/cm^{-1}(ATR) 3377w & 3323w (NH), 3090w br, 3013w, 2214w (C≡N), 1657s, 1587m, 1566w, 1485m, 1464w, 1373m, 1341s, 1242w, 1136w, 883s, 775w, 754m, 700w; δ_H(500 MHz, CD_3OD) 4.57 (2H, s, D_2O exchangeable); δ_C(125 MHz, TFA-*d*) 160.1 (s), 149.6 (s), 145.9 (s), 122.1 (s), 108.7 (s), 91.8 (s); *m/z* (LCMS) 260 ($Se^{80}Cl^{35}$: MH^+, 100%), 200 (17), 178 (33), 159 (20), 150 (18), 139 (43), 105 (15), 65 (45), 64 (46), 61 (21).

S3.2.6 4-Chloro-6-(methylamino)pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (17)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (4 mL) at *ca.* 20 °C was added a saturated methylamine solution in DCM (100 μL). The mixture was stirred for 10 min until no starting material remained (TLC), adsorbed onto silica and chromatographed (DCM/TBME, 67:33) to give the *title compound* **17** (27.0 mg, 99%) as red prisms, mp (hot-stage) 183.2-189.1 °C (DCE) (decomp.); R_f 0.46 (DCM/TBME; 50:50); Anal. Calcd for $C_7H_4ClN_5Se$: C, 30.85; H, 1.48; N, 25.69. Found: C, 30.47; H, 1.57; N, 25.33%; λ_{max}(EtOH)/nm 254 (log ε 4.38), 305 (3.92), 455 (4.27); ν_{max}/cm^{-1}(ATR) 3273w (NH), 2222w (C≡N), 1612s, 1584w, 1531m, 1468w, 1408m, 1341m, 1306m, 1231m, 1144w, 1053w, 1042w, 970w, 872m, 779w, 721m, 700m; δ_H(500 MHz, DMSO-d_6) 8.81 (1H, br s, D_2O exchangeable), 3.04 (3H, d, *J* 5.0); δ_C(125 MHz, TFA-*d*) 158.7 (s), 149.6 (s), 145.2 (s), 121.9 (s), 108.8 (s), 92.5 (s), 31.0 (q); *m/z* (LCMS) 274 ($Se^{80}Cl^{35}$: MH^+, 100%), 249 (3), 214 (8), 197 (5), 192 (7), 160 (8), 74 (14), 64 (10).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.05 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added a saturated methylamine solution in DCM (50 μL). The mixture was stirred for 10 min until no starting material remained (TLC). The reaction mixture was diluted with DCM (20 mL) and washed with distilled water (2 × 30 mL). The aqueous layer was then extracted with DCM (3 × 20 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, the residue recrystallized to give the title compound **17** (13.5 mg, 99%) as red prisms, mp (hot-stage) 183.2-189.1 °C (DCE) (decomp.); R_f 0.46 (DCM/TBME, 50:50); ν_{max}/cm^{-1}(ATR) 3273w (NH), 2222w (C≡N), 1612s, 1584w, 1531m, 1468w, 1408m, 1341m, 1306m, 1231m, 1144w, 1053w, 1042w, 970w, 872m, 779w, 721m, 700m; identical to that described above.

S3.2.7 6-(Benzylamino)-4-chloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (18)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added benzylamine (24.0 μL, 0.22 mmol). The stirred mixture was heated at reflux for 10 min, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 33:33:34) to give the *title compound* **18** (34.3 mg, 98%) as orange plates, mp (hot-stage) 161-168 °C (decomp.) (*c*-Hex/DCE); R_f 0.59 (Hex/DCM/TBME, 33:33:34); Anal. Calcd for $C_{13}H_8ClN_5Se$: C, 44.78; H, 2.31; N, 20.09. Found C, 44.56; H, 2.62; N, 19.82%; λ_{max}(DCM)/nm 256 (log ε 4.55), 262 inf (4.54), 288 inf (4.47), 302 (4.09), 449 (4.38), 466 (4.38); ν_{max}/cm^{-1}(ATR) 3298m (NH), 2222m (C≡N), 1607s, 1584m, 1533m, 1456w, 1443w, 1433w, 1337m, 1308m, 1296m, 1248w, 1231w, 1221w, 1080w, 1051w, 1038w, 939w, 914w, 874w, 822w, 772w, 754m, 721m, 698s; δ_H(300 MHz, $CDCl_3$) 7.42-7.36 (5H, m), 6.09 (1H, br s, D_2O exchangeable), 4.91 (2H, d, *J* 5.1); δ_C(125 MHz, Pyridine-d_5) 167.3 (s), 164.2 (s), 140.9 (s), 138.5 (s), 128.8 (d), 128.0 (d), 127.6 (d), 125.0 (s), 113.9 (s), 97.2 (s), 47.1 (t); *m/z* (MALDI-TOF) 350 ($Se^{80}Cl^{35}$: MH^+, 99%), 234 (22), 181 (12), 167 (13), 106 (64), 91 (97).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.05 mmol) in anhydrous DCM (1 mL) at *ca.* 20 °C was added benzylamine (12.0 μL, 0.11 mmol). The stirred mixture was heated to reflux for 10 min, until no starting material remained (TLC). The mixture was diluted in DCM (20 mL) and distilled water (60 mL) was added. Layers were separated and the aqueous phase was extracted with DCM (2 × 20 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallised to give the title compound **18** (17.2 mg, 99%) as orange plates, mp (hot-stage) 161-168 °C (decomp.) (*c*-Hex/DCE); R_f 0.59 (Hex/DCM/TBME, 33:33:34); ν_{max}/cm^{-1}(ATR) 3298m NH), 2222m (C≡N), 1607s, 1584m, 1533m, 1456w, 1443w, 1433w, 1337m, 1308m, 1296m, 1248w, 1231w, 1221w, 1080w, 1051w, 1038w, 939w, 914w, 874w, 822w, 772w, 754m, 721m, 698s; identical to that described above.

S3.2.8 4-Chloro-6-(phenylamino)pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (19)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.05 mmol) in anhydrous DCM (1 mL) at *ca.* 20 °C was added aniline (10.0 μL, 0.11 mmol). The mixture was stirred for 45 min, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 10:45:45) to give the *title compound* **19** (16.6 mg, 99%) as red needles, mp (hot stage) 195.8-199.8 °C (decomp.) (DCE); R_f

0.41 (Hex/DCM/TBME, 33:33:33); Anal. Calcd for $C_{12}H_6ClN_5Se$: C, 43.07; H, 1.81; N, 20.93. Found: C, 43.23; H, 2.11; N, 21.16%; λ_{max}(DCM)/nm 248 inf (log ε 4.26), 266 inf (4.40), 271 (4.42), 281 inf (4.30), 318 (4.28), 407 inf (3.80), 477 (4.34); ν_{max}/cm^{-1}(ATR) 3281w, 3210w & 3140w (NH), 3098w & 3057w (aryl C-H), 2239w (C≡N), 1626s, 1605m, 1591s, 1574s, 1555m, 1495m, 1462s, 1445m, 1331m, 1321m, 1302w, 1277m, 1252w, 1240w, 1215w, 1182w, 1159w, 1123w, 1032w, 905w, 889s, 853w, 839w, 764s, 741m, 710s; δ_H[500 MHz, (C*D*$_3$)$_2$C=O)] 9.65 (1H, s, D_2O exchangeable), 8.15 (2H, d, *J* 8.0), 7.45 (2H, t, *J* 8.0), 7.23 (1H, t, *J* 7.5); δ_C[125 MHz, (C*D*$_3$)$_2$C=O] six C (s) resonances missing owing to poor solubility 130.0 (d), 125.9 (d), 122.0 (d), 113.7 (s); *m/z* (MALDI-TOF) 336 ($Se^{80}Cl^{35}$: MH^+, 100%), 246 (1).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added aniline (20.0 μL, 0.22 mmol). The mixture was stirred for 1 h, until no starting material remained (TLC). The reaction mixture was diluted with DCM (60 mL) and distilled water (40 mL) was added. The layers were separated, and the aqueous phase was extracted with DCM (20 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallised to give the title compound **19** (33.4 mg, 100%) as red needles, mp (hot stage) 195.8-199.8 °C (decomp.) (DCE); R_f 0.41 (Hex/DCM/TBME, 33:33:33); ν_{max}/cm^{-1}(ATR) 3281w, 3210w & 3140w (NH), 3098w & 3057w (aryl C-H), 2239w (C≡N), 1626s, 1605m, 1591s, 1574s, 1555m, 1495m, 1462s, 1445m, 1331m, 1321m, 1302w, 1277m, 1252w, 1240w, 1215w, 1182w, 1159w, 1123w, 1032w, 905w, 889s, 853w, 839w, 764s, 741m, 710s; identical to that described above.

S3.2.9 4-Chloro-6-(dimethylamino)pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (20)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added a saturated dimethylamine solution in DCM (200 μL). The mixture was stirred for 10 min until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 20:60:20) to give the *title compound* **20** (28.4 mg, 99%) as red prisms, mp (hot-plate) 163-170 °C (decomp.) (DCE); R_f 0.50 (Hex/DCM/TBME, 20:60:20); Anal. Calcd for $C_8H_6ClN_5Se$: C, 33.53; H, 2.11; N, 24.44. Found: C, 33.26; H, 2.38; N, 24.07%; λ_{max}(DCM) 264 nm (log ε 4.40), 269 (4.40), 276 inf (4.30), 310 (4.09), 320 inf (4.03), 407 inf (3.66), 432 inf (3.82), 480 (4.23), 500 inf (4.15); ν_{max}/cm^{-1}(ATR) 2933w (alkyl C-H), 2212w (C≡N), 1609s, 1557m, 1497s, 1456w, 1423m, 1400m, 1329s, 1285m, 1221w, 1200w, 1111w, 1057w, 988w, 926s, 849m, 818w, 772s, 716s, 704s; δ_H(300 MHz,

$CDCl_3$) 3.64 (3H, br s), 3.45 (3H, br s); δ_C(75 MHz, TFA-*d*) 156.3 (s), 149.4 (s), 145.5 (s), 123.8 (s), 111.2 (s), 91.4 (s), 42.6 (q), 40.8 (q); *m/z* (LCMS) 288 ($Se^{80}Cl^{35}$: MH^+, 100%), 206 (13), 193 (6), 64 (8).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.05 mmol) in anhydrous diethyl ether (2 mL) at *ca.* 20 °C was added a saturated dimethylamine solution in diethyl ether (200 μL). The mixture was stirred for 10 min until no starting material remained (TLC). The reaction mixture was diluted with DCM (30 mL) and washed with distilled water (2 × 30 mL). The aqueous layer was then extracted with DCM (30 mL). The combined organic phases were dried ($MgSO_4$), volatiles removed *in vacuo*, and recrystallized to give the title compound **20** (14.2 mg, 99%) as red prisms, mp (hot-plate) 163-170 °C (decomp.) (DCE); R_f 0.50 (Hex/DCM/TBME, 20:60:20); ν_{max}/cm^{-1}(ATR) 2933w (alkyl C-H), 2212w (C≡N), 1609s, 1557m, 1497s, 1456w, 1423m, 1400m, 1329s, 1285m, 1221w, 1200w, 1111w, 1057w, 988w, 926s, 849m, 818w, 772s, 716s, 704s; identical to that described above.

S2.2.10 4-(Aziridin-1-yl)-6-chloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (21)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (2 mL) was aziridine (11.4 μL, 0.22 mmol). The mixture was stirred for 5 min, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 20:40:40) to give the *title compound* **21** (20.6 mg, 72%), as orange needles, mp (hot-stage) 142-152 °C (decomp.) (DCE); R_f 0.46 (Hex/DCM/TBME, 20:40:40) (DCE); Anal. Calcd for $C_8H_4ClN_5Se$: C, 33.77; H, 1.42; N, 24.61. Found: C, 34.05; H, 1.21; N, 24.72%; λ_{max}(DCM)/nm 260 inf (log ε 4.44), 262 (4.45), 267 inf (4.41), 301 (3.81), 417 inf (4.18), 430 inf (4.31), 440 (4.38), 449 inf (4.34), 463 inf (4.25); ν_{max}/cm^{-1}(ATR) 3148w (alkyl C-H), 2207w (C≡N), 1585m, 1557w, 1452m, 1441m, 1342w, 1321s, 1296w, 1258w, 1150w, 1113w, 1065w, 988w, 907w, 881w, 835w, 810w, 762w, 729w, 712w; δ_H(300 MHz, VT 80 °C, $CDCl_3$) 2.76 (4H, br s); δ_C(125 MHz, VT 80 °C, $CDCl_3$) six C (s) resonances missing owing to poor solubility 28.9 (t); *m/z* (MALDI-TOF) 324 ($Se^{80}Cl^{35}$: M^++K, 11%), 308 (MH^+, 54), 286 (MH^+, 100), 258 (18), 228 (10), 180 (13), 170 (25), 133 (16), 97 (13), 81 (18).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (4 mL) at *ca.* 0 °C was added aziridine (11.4 μL, 0.22 mmol). The mixture was stirred for 10 min, until no starting material remained (TLC), diluted with DCM (50 mL), and washed with distilled water (2 × 50 mL). The combined aqueous layers were extracted with DCM (3 × 30 mL). The combined organic phases were dried

($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallised to give the title compound **21** (28.4 mg, 99%), mp (hot-stage) 142-152 °C (decomp.) (DCE); ν_{max}/cm^{-1}(ATR) 3148w (alkyl C-H), 2207w (C≡N), 1585m, 1557w, 1452m, 1441m, 1342w, 1321s, 1296w, 1258w, 1150w, 1113w, 1065w, 988w, 907w, 881w, 835w, 810w, 762w, 729w, 712w; identical to that described above.

S3.2.11 6-(Azetidin-1-yl)-4-chloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (22)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) (41.7 mg, 0.15 mmol) in anhydrous DCM (4 mL) at *ca.* 20 °C was added azetidine (22.2 μL, 0.33 mmol). The mixture was stirred for 5 min, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 10:20:60) to give the *title compound* **22** (39.0 mg, 87%) as red prisms, mp (hot-stage) 161-166 °C (decomp.) (DCE); R_f 0.36 (Hex/DCM/TBME, 17:33:50); Anal. Calcd for $C_9H_6ClN_5Se$: C, 36.20; H, 2.03; N, 23.45. Found: C, 36.51; H, 1.88; N, 23.63%; λ_{max}(DCM)/nm 263 (log ε 4.44), 269 (4.43), 278 inf (4.24), 302 inf (4.07), 310 (4.10), 320 inf (4.04), 399 inf (3.61), 465 inf (3.22), 477 (4.24), 497 inf (4.17); ν_{max}/cm^{-1}(ATR) 2960w & 2870w (alkyl C-H), 2207m (C≡N), 1626s, 1560m, 1493s, 1462m, 1450m, 1341m, 1325m, 1304m, 1260s, 1229m, 1198w, 1161w, 1123w, 1059w, 1034m, 932w, 918m, 872w, 820w, 768s, 708s; δ_H(300 MHz, $CDCl_3$) 4.79 (2H, t, *J* 7.5), 4.50 (2H, t, *J* 8.1), 2.64 (2H, app. Pentet, *J* 7.9); δ_H(500 MHz, TFA-*d*) 4.99 (2H, br s), 4.64 (2H, br s), 2.76 (2H, br s); δ_C(125 MHz, TFA-*d*) one C (s) resonance missing 156.3 (s), 152.2 (s), 147.4 (s), 125.4 (s), 94.0 (s), 58.4 (t), 58.1 (t), 18.8 (t); *m/z* (MALDI-TOF) 300 ($Se^{80}Cl^{35}$: MH^+, 65%), 272 (20), 217 (100), 189 (20), 133 (19), 56 (7), 39 (33).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (83.4 mg, 0.30 mmol) in anhydrous DCM (6 mL) at *ca.* 20 °C was added azetidine (44.4 μL, 0.66 mmol). The mixture was stirred for 5 min until no starting material remained (TLC). To the reaction mixture was then added distilled water (30 mL) followed by DCM (50 mL). Phases were separated and the aqueous phase was extracted with DCM (4 × 50 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallised to give the title compound **22** (86.6 mg, 97%) as red prisms, mp (hot-stage) 161-166 °C (decomp.) (DCE); R_f 0.36 (Hex/DCM/TBME, 17:33:50); ν_{max}/cm^{-1}(ATR) 2960w & 2870w (alkyl C-H), 2207m (C≡N), 1626s, 1560m, 1493s, 1462m, 1450m, 1341m, 1325m, 1304m, 1260s, 1229m, 1198w, 1161w, 1123w, 1059w, 1034m, 932w, 918m, 872w, 820w, 768s, 708s; identical to that described above.

S3.2.12 4-Chloro-6-(pyrrolidine-1-yl)pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (23)

Method A: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.05 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added pyrrolidine (9.0 μL, 0.11 mmol). The mixture was stirred for 1.5 h, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 20:40:40) to give the *title compound* **23** (12.3 mg, 79%) as red needles, mp (hot-stage) 157-163 °C (decomp.) (*c*-Hex/DCE); R_f 0.52 (Hex/DCM/TBME, 20:40:40); Anal. Calcd for $C_{10}H_8ClN_5Se$: C, 38.42; H, 2.58; N, 22.40. Found: C, 38.80; H, 2.35; N, 22.01%; λ_{max}(DCM)/nm 259 inf (log ε 4.08), 262 (4.12), 268 (4.11), 309 (3.78), 322 inf (3.73), 394 inf (3.27), 477 (3.85), 501 inf (3.76); ν_{max}/cm^{-1}(ATR) 2961w & 2874w (alkyl C-H), 2216w (C≡N), 1609s, 1560m, 1489s, 1454m, 1333s, 1304m, 1294m, 1261s, 1229w, 1184w, 1140w, 1034w, 1003w, 978w, 914s, 858w, 829w, 766s, 716s, 700s; δ_H(300 MHz, $CDCl_3$) 4.12 (2H, t, *J* 6.9), 3.90 (2H, t, *J* 6.8), 2.19 (2H, app. Pentet, *J* 6.7), 2.07 (2H, app. Pentet, *J* 6.6); δ_C(125 MHz, $CDCl_3$) 163.5 (s), 163.1 (s), 142.1 (s), 126.0 (s), 115.5 (s), 96.4 (s), 51.3 (t), 48.7 (t), 26.6 (t), 24.4 (t); *m/z* (MALDI-TOF) 336 ($Se^{80}Cl^{35}$: M^++Na, 6%), 312 (M^+, 100), 277 (25), 200 (51), 133 (17), 110 (17), 70 (39).

S3.2.13 4-Chloro-6-(piperidin-1-yl)pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (24)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) (14.2 mg, 0.05 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added dropwise piperidine (10.9 μL, 0.11 mmol). The mixture was stirred for 5 min, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 20:40:40) to give the *title compound* **24** (16.2 mg, 97%) as red needles, mp (hot-stage) 158-165 °C (decomp.); R_f 0.46 (Hex/TBME, 33:67); Anal. Calcd for $C_{11}H_{10}ClN_5Se$: C, 40.45; H, 3.09; N, 21.44. Found: C, 40.73; H, 2.87; N, 21.04%; λ_{max}(DCM)/nm 256 inf (log ε 4.26), 269 (4.37), 281 inf (4.23), 312 (4.12), 405 inf (3.62), 487 (4.20), 512 inf (4.08); ν_{max}/cm^{-1}(ATR) 2943w & 2862w (alkyl C-H), 2207m (C≡N), 1582s, 1547m, 1493m, 1449m, 1339s, 1325m, 1292s, 1258w, 1217w, 1155w, 1119w, 1022w, 978w, 905s, 845m, 820w, 768s, 708m, 704m; δ_H(300 MHz, $CDCl_3$) 4.13 (4H, br s), 1.80 (6H, br s); δ_C(125 MHz, $CDCl_3$) 164.7 (s), 162.7 (s), 141.9 (s), 126.9 (s), 115.6 (s), 95.4 (s), 49.7 (t), 48.4 (t), 26.9 (t), 25.8 (t), 24.1 (t); *m/z* (MALDI-TOF) 350 ($Se^{80}Cl^{35}$: M^++Na, 19%), 326 (M^+-H, 100), 291 (29), 272 (13), 212 (33), 192 (20), 133 (64), 84 (81).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (28.0 mg, 0.10 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added dropwise piperidine (22.0 μL, 0.22 mmol). The mixture was stirred for 5 min until no starting

material remained (TLC). To the reaction mixture was then added distilled water (30 mL) followed by DCM (30 mL). Phases were separated and the aqueous phase was extracted with DCM (30 mL). The combined organic phases were dried ($MgSO_4$), volatiles removed *in vacuo*, and the residue recrystallized to give the title compound **24** (31.7 mg, 96%) as red needles, mp (hot-stage) 158-165 °C (decomp.); R_f 0.46 (Hex/TBME, 33:67); ν_{max}/cm^{-1}(ATR) 2943w & 2862w (alkyl C-H), 2207m (C≡N), 1582s, 1547m, 1493m, 1460m, 1449m, 1339s, 1325m, 1292s, 1258w, 1217w, 1155w, 1119w, 1022w, 978w, 905s, 845m, 820w, 768s, 708m, 704m; identical to that described above.

S3.2.14 4-Chloro-6-(4-methylpiperazin-1-yl)[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (25)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.50 mmol) in anhydrous DCM (1 mL) at *ca.* 20 °C was added 1-methylpiperazine (12.2 μL, 0.11 mmol). The mixture was stirred for 5 min until no starting material remained (TLC). The reaction mixture was concentrated and chromatography (basic alumina) (Hex/DCM, 10:90) gave the *title compound* **25** (15.9 mg, 93%) as red needles, mp (hot-stage) 158-162 °C (decomp.) (EtOH); R_f 0.36 (Hex/DCM, 10:90, neutral alumina); Anal. Calcd for $C_{11}H_{11}ClN_6Se$: C, 38.67; H, 3.25; N, 24.60. Found: C, 39.03; H, 3.44; N, 24.25%; λ_{max}(DCM)/nm 264 (log ε 4.42), 268 (4.42), 281 inf (4.27), 311 (4.15), 320 inf (4.11), 407 inf (3.74), 481 (4.25), 505 inf (4.15); ν_{max}/cm^{-1}(ATR) 2922w & 2820w (alkyl C-H), 2214w (C≡N), 1587s, 1543m, 1495m, 1445m, 1427w, 1383w, 1341s, 1323m, 1306m, 1283s, 1144m, 1130w, 1072w, 1053w, 1003m, 984w, 907m, 833m, 770m, 706m; δ_H(300 MHz, $CDCl_3$) 4.33 (4H, br s), 2.64 (4H, br s), 2.39 (3H, s); δ_C(75 MHz, $CDCl_3$) 165.2 (s), 162.7 (s), 142.4 (s), 126.9 (s), 115.7 (s), 95.3 (s), 54.9 (br, t), 47.2 (br, t), 46.0 (q); *m/z* (MALDI-TOF) 341 ($Se^{80}Cl^{35}$: M^+-H, 100%), 227 (13), 99 (51), 70 (49).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (83.4 mg, 0.30 mmol) in anhydrous DCM (6 mL) at *ca.* 20 °C was added 1-methylpiperazine (73.1 μL, 0.66 mmol). The mixture was stirred for 5 min until no starting material remained (TLC). To the reaction mixture was then added distilled water (30 mL) followed by DCM (30 mL). Phases were separated and the aqueous phase was extracted with DCM (30 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallized to give the title compound **25** (99.9 mg, 97%) as red needles, mp (hot-stage) 158-162 °C (decomp.) (EtOH); R_f 0.36 (Hex/DCM, 10:90, neutral alumina); ν_{max}/cm^{-1}(ATR) 2922w & 2820w (alkyl C-H), 2214w (C≡N), 1587s, 1543m, 1495m, 1445m, 1427w, 1383w, 1341s, 1323m, 1306m, 1283s,

1144m, 1130w, 1072w, 1053w, 1003m, 984w, 907m, 833m, 770m, 706m; identical to that described above.

S3.2.15 4-Chloro-6-morpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (26)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.05 mmol) in anhydrous DCM (1 mL) at *ca.* 20 °C was added morpholine (9.5 μL, 0.11 mmol). The mixture was heated to reflux for 5 min, until no starting material remained (TLC), allowed to cool to *ca.* 20 °C, adsorbed onto silica and chromatographed (Hex/DCM/TBME, 10:70:20 → 10:50:40) to give the *title compound* **26** (16.3 mg, 99%) as red prisms, mp (hot-stage) 152-158 °C (decomp.) (*c*-Hex/DCE), R_f 0.68 (Hex/DCM/TBME, 20:60:20); Anal. Calcd for $C_{10}H_8ClN_5OSe$: C, 36.55; H, 2.45; N, 21.31. Found: C, 36.37; H, 2.05; N, 21.66%; λ_{max}(DCM)/nm 271 (log ε 4.40), 277 inf (4.35), 310 (4.11), 318 inf (4.06), 412 inf (3.65), 432 inf (3.83), 480 (4.22), 496 inf (4.16); ν_{max}/cm^{-1}(ATR) 2934w br & 2872w (alkyl C-H), 2208w (C≡N), 1573s, 1547m, 1493m, 1441m, 1379w, 1339s, 1327s, 1285s, 1265w, 1144w, 1117s, 1076w, 1043w, 988m, 912s, 858m, 829m, 768s, 710m, 704s; δ_H(300 MHz, $CDCl_3$) 4.19 (4H, br s), 3.90-3.87 (4H, m); δ_C(125 MHz, $CDCl_3$) 165.4 (s), 162.5 (s), 142.7 (s), 126.7 (s), 115.6 (s), 95.1 (s), 66.8 (t, br), 47.7 (t, br); *m/z* (MALDI-TOF) 352 ($Se^{80}Cl^{35}$: M^++Na, 63%), 330 (MH^+, 100), 294 (9), 272 (15), 216 (5), 133 (18), 97 (8), 86 (9).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added morpholine (19.1 μL, 0.22 mmol). The mixture was heated to reflux for 5 min until no starting material remained (TLC) then allowed to cool to *ca.* 20 °C. To the reaction mixture was then added distilled water (60 mL) followed by DCM (30 mL). Phases were separated and the aqueous phase was extracted with DCM (30 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallized to give the title compound **26** (31.9 mg, 97%) as red prisms, mp (hot-stage) 152-158 °C (decomp.) (*c*-Hex/DCE); R_f 0.68 (Hex/DCM/TBME, 20:60:20); ν_{max}/cm^{-1}(ATR) 2934w br & 2872w (alkyl C-H), 2208w (C≡N), 1573s, 1547m, 1493m, 1441m, 1379w, 1339s, 1327s, 1285s, 1265w, 1144w, 1117s, 1076w, 1043w, 988m, 912s, 858m, 829m, 768s, 710m, 704s; identical to that described above.

S3.2.16 4-Chloro-6-thiomorpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (27)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.05 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added thiomorpholine (11.3 μL, 0.11 mmol). The mixture was stirred for 5 min, until no starting material

remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 20:40:40) to give the *title compound* **27** (16.5 mg, 96%) as red needles, mp (hot-stage) 168-175 °C (decomp.) (*c*-Hex/DCE); R_f 0.46 (Hex/TBME, 33:67); Anal. Calcd for $C_{10}H_8ClN_5SSe$: C, 34.85; H, 2.34; N, 20.32. Found: C, 35.11; H, 2.55; N, 20.01%; λ_{max}(DCM)/nm 264 inf (log ε 4.22), 269 (4.23), 283 inf (4.04), 312 (3.95), 320 inf (3.92), 403 inf (3.49), 482 (4.07), 504 inf (3.98); ν_{max}/cm^{-1}(ATR) 2930w (alkyl C-H), 2212w (C≡N), 1790w, 1649w, 1580s, 1547m, 1495s, 1454w, 1439w, 1416w, 1337s, 1314m, 1288w, 1273m, 1238w, 1227w, 1204w, 1165w, 1134w, 1036w, 1026w, 957m, 889s, 829w, 814w, 770m, 712m, 704m; δ_H(300 MHz, $CDCl_3$) 4.45 (4H, br s), 2.88-2.84 (4H, m); δ_C(75 MHz, $CDCl_3$) 165.2 (s), 162.5 (s), 142.7 (s), 126.8 (s), 115.5 (s), 96.2 (s), 50.8 (t, br), 28.0 (t, br); *m/z* (MALDI-TOF) 368 ($Se^{80}Cl^{35}$: M^++Na, 4%), 346 (MH^+, 100), 312 (29), 272 (13), 245 (10), 232 (14), 192 (26), 133 (15), 102 (59).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added thiomorpholine (22.6 μL, 0.22 mmol). The mixture was stirred for 5 min until no starting material remained (TLC). The mixture was then diluted with DCM (30 mL) and distilled water (30 mL) was added. Phases were separated and the aqueous phase was twice extracted with DCM (2 × 30 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallized to give the title compound **27** (33.4 mg, 97%) as red needles, mp (hot-stage) 168-175 °C (decomp.) (*c*-Hex/DCE); R_f 0.46 (Hex/TBME, 33:67); ν_{max}/cm^{-1}(ATR) 2930w (alkyl C-H), 2212w (C≡N), 1790w, 1649w, 1580s, 1547m, 1495s, 1454w, 1439w, 1416w, 1337s, 1314m, 1288w, 1273m, 1238w, 1227w, 1204w, 1165w, 1134w, 1036w, 1026w, 957m, 889s, 829w, 814w, 770m, 712m, 704m; identical to that described above.

S3.2.17 4-Chloro-6-(2-methylpiperidin-1-yl)pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (28)

To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added 2-methylpiperidine (25.8 μL, 0.22 mmol). The mixture was stirred for 5 min, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/TBME, 50:50) to give the *title compound* **28** (24.5 mg, 72%) as red needles, mp (hot-stage) 145-148 °C (decomp.) (*c*-Hex); R_f 0.43 (Hex/TBME, 50:50); Anal. Calcd for $C_{12}H_{12}ClN_5Se$: C, 42.31; H, 3.55; N, 20.56. Found: C, 41.91; H, 3.33; N, 20.21%; λ_{max}(DCM)/nm 264 inf (4.22), 268 (4.24), 272 inf (4.22), 283 inf (4.07), 315 (3.98), 403 inf (3.56), 468 inf (3.95), 487 (4.04), 510 inf (3.95); ν_{max}/cm^{-1}(ATR) 2936w (alkyl C-H), 2208w (C≡N), 1574s, 1537w, 1489m, 1443w, 1337m, 1287m, 1188w, 1142w, 1069w, 1040w, 1007w, 989w, 959w, 941w, 889w, 874w, 800w, 758w; δ_H(500 MHz,

$CDCl_3$) 5.27 (1H, s), 4.87 (1H, d, *J* 13.4), 3.34 (1H, br s), 1.90-1.83 (2H, m), 1.81-1.78 (1H, m), 1.74-1.62 (4H, m), 1.43 (2H, br s); δ_C(125 MHz, $CDCl_3$) 165.0 (s), 162.8 (s), 142.1 (s), 126.9 (s), 115.7 (s), 95.8 (s), 51.1 (d), 42.9 (t), 30.6 (t), 26.0 (t), 18.5 (q), 16.7 (t); *m/z* (MALDI-TOF) 340 ($Se^{80}Cl^{35}$: M^+-H, 100%), 326 (22), 301 (23), 226 (12), 113 (21), 133 (74), 98 (98), 84 (16).

S3.2.18 6-(Azepan-1-yl)-4-chloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (29)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]-selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.05 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added dropwise azepane (12.4 μL, 0.11 mmol). The mixture became deep red and was stirred for 5 min, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/TMBE, 33:67) to give the *title compound* **29** (16.5 mg, 97%) as red needles, mp (hot-stage) 139-143 °C (decomp.) (DCE); R_f 0.43 (Hex/TBME, 33:67); Anal. Calcd for $C_{12}H_{12}ClN_5Se$: C, 42.31; H, 3.55; N, 20.56. Found: C, 42.65; H, 3.17; N, 20.91%; λ_{max}(DCM)/nm 255 inf (log ε 4.31), 269 (4.43), 282 inf (4.28), 312 (4.19), 403 inf (3.76), 463 inf (4.13), 487 (4.25), 512 inf (4.15); ν_{max}/cm^{-1}(ATR) 2928w & 2853w (alkyl C-H), 2207m (C≡N), 1580s, 1547m, 1493w, 1460m, 1454m, 1433w, 1333s, 1287w, 1263w, 1209w, 1165w, 1130w, 1096w, 997w, 966w, 889m, 856w, 825w, 768m, 714m, 706m; δ_H(300 MHz, CD_2Cl_2) 4.10 (2H, t, *J* 6.0), 3.98 (2H, t, *J* 6.0), 1.98-1.88 (4H, br m), 1.67-1.63 (4H, br m); δ_C(125 MHz, TFA-*d*) 157.7 (s), 151.9 (s), 147.8 (s), 126.3 (s), 113.4 (s), 93.6 (s), 56.9 (t), 54.0 (t), 31.0 (t), 28.2 (t), 28.0 (t), 27.5 (t); *m/z* (MALDI-TOF) 342 ($Se^{80}Cl^{35}$: MH^+, 32%), 320 (94), 304 (19), 278 (17), 258 (19), 242 (47), 228 (15), 209 (44), 192 (25), 127 (32), 100 (70), 70 (11).

Method B – non-chromatographic work-up: Upon completion, to the reaction mixture was added distilled water (30 mL) followed by DCM (30 mL). Phases were separated and the aqueous phase was extracted with DCM (30 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallised to give the title compound **29** (16.5 mg, 97%) as red needles, mp (hot-stage) 139-143 °C (decomp.) (DCE); R_f 0.43 (Hex/TBME, 33:67); ν_{max}/cm^{-1}(ATR) 2928w & 2853w (alkyl C-H), 2207m (C≡N), 1580s, 1547m, 1493w, 1460m, 1454m, 1433w, 1333s, 1287w, 1263w, 1209w, 1165w, 1130w, 1096w, 997w, 966w, 889m, 856w, 825w, 768m, 714m, 706m; identical to that described above.

S3.2.19 4-Chloro-6-(dibenzylamino)pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (30)

To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (14.1 mg, 0.05 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added dibenzylamine (27.3 μL, 0.25 mmol). The mixture was stirred for 4 h, until no starting material remained (TLC), adsorbed onto silica and

chromatographed (Hex/TBME, 50:50) to give the *title compound* **30** (18.4 mg, 83%) as red needles, mp (hot-stage) 144-146 °C (decomp.) (*c*-Hex); R_f 0.65 (Hex/TBME, 50:50); Anal. Calcd for $C_{20}H_{14}ClN_5Se$: C, 54.75; H, 3.22; N, 15.96. Found: C, 54.42; H, 2.85; N, 16.23%; λ_{max}(DCM)/nm 265 (log ε 4.38), 269 (4.38), 281 inf (4.23), 310 (4.10), 322 inf (4.02), 407 inf (3.69), 476 (4.21), 500 inf (4.13); ν_{max}/cm^{-1}(ATR) 3063w br (aryl C-H), 2934w (alkyl C-H), 2212w (C≡N), 1574s, 1551w, 1497m, 1445m, 1429w, 1341s, 1300w, 1254w, 1227w, 1200w, 1138w, 1080w, 1030w, 970w, 928w, 899w, 854w, 777w, 750w, 735w, 718w, 698w; δ_H(300 MHz, $CDCl_3$) 7.38-7.31 (10H, br m), 5.12 (4H, br s); δ_C(125 MHz, $CDCl_3$) C (d) resonances overlapping 166.8 (s), 162.8 (s), 142.7 (s), 135.3 (s), 129.2 (d, br), 128.4 (d), 127.1 (s), 115.3 (s), 95.6 (s), 53.8 (t, br), 51.2 (t, br); *m/z* (MALDI-TOF) 438 ($Se^{80}Cl^{35}$: M^+-H, 21%), 348 (45), 194 (16), 181 (14), 133 (36), 97 (14), 91 (100).

S3.2.20 4-Chloro-6-[methyl(phenyl)amino]pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (31)

Method A – chromatographic isolation: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (27.8 mg, 0.10 mmol) in anhydrous DCM (2 mL) at *ca.* 20 °C was added *N*-methylaniline (23.8 μL, 0.22 mmol). The mixture was stirred for 5 min, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 33:33:33) to give the *title compound* **31** (34.2 mg, 98%) as red plates, mp (hot stage) 173.3-178.6 °C (decomp.) (*c*-Hex/DCE); R_f 0.39 (Hex/DCM/TBME, 50:25:25); Anal. Calcd for $C_{13}H_8ClN_5Se$: C, 44.78; H, 2.31; N, 20.09. Found: C, 45.03; H, 2.17; N, 20.27%; λ_{max}(DCM)/nm 264 inf (log ε 4.61), 269 (4.63), 313 (4.28), 469 (452), 487 inf (4.50); ν_{max}/cm^{-1}(ATR) 3067w (aryl C-H), 2928w (alkyl C-H), 2212w (C≡N), 1572s, 1495m, 1485s, 1454w, 1402m, 1331s, 1234m, 1165w, 1119w, 1078w, 1049w, 1026w, 978w, 916w, 878m, 777m, 756m, 712m; δ_H(300 MHz, $CDCl_3$) 7.56-7.53 (3H, m), 7.40-7.37 (2H, m), 3.76 (3H, s); δ_C(125 MHz, $CDCl_3$) 166.4 (s), 163.1 (s), 142.9 (s), 142.5 (s), 130.5 (s), 130.0 (s), 127.5 (s), 126.0 (s), 112.2 (s), 98.0 (s), 42.8 (q); *m/z* (MALDI-TOF) 472 ($Se^{80}Cl^{35}$: M^++Na, 11%), 350 (MH^+, 23), 348 (M^+-H, 26), 313 (4), 234 (30), 199 (5), 133 (5), 106 (6), 97 (10), 81 (9), 39 (100).

Method B – non-chromatographic work-up: To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*]-[1,2,6]selenadiazine-5-carbonitrile (**12**) (13.9 mg, 0.05 mmol) in anhydrous DCM (1 mL) at *ca.* 20 °C was added *N*-methylaniline (11.9 μL, 0.11 mmol). The mixture was stirred for 5 min, until no starting material remained (TLC). The reaction mixture was diluted with DCM (20 mL) and distilled water (40 mL) was added. The layers were separated, and the aqueous phase was extracted with DCM (2 × 20 mL). The combined organic phases were dried ($MgSO_4$), the volatiles removed *in vacuo*, and the residue recrystallised to give the title compound **31** (17.3 mg, 99%) as red plates, mp (hot stage) 173.3-178.6 °C

(decomp.) (*c*-Hex/DCE); R_f 0.39 (Hex/DCM/TBME, 50:25:25); ν_{max}/cm^{-1}(ATR) 3067w (aryl C-H), 2928w (alkyl C-H), 2212w (C≡N), 1572s, 1495m, 1485s, 1454w, 1402m, 1331s, 1234m, 1165w, 1119w, 1078w, 1049w, 1026w, 978w, 916w, 878m, 777m, 756m, 712m; identical to that described above.

S3.2.21 4-Chloro-6-(diphenylamino)pyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (32)

To a stirred suspension of 4,6-dichloropyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**12**) (55.6 mg, 0.20 mmol) in anhydrous DCM (4 mL) at *ca.* 20 °C was added diphenylamine (74.4 mg, 0.44 mmol). The mixture was stirred for 3 h, until no starting material remained (TLC), adsorbed onto silica and chromatographed (Hex/DCM/TBME, 60:20:20) to give the *title compound* **32** (75.5 mg, 93%) as red needles, mp (hot-stage) 122.0-126.5 °C (*c*-Hex/DCE); R_f 0.70 (Hex/DCM/TBME, 33:33:34); Anal. Calcd for $C_{18}H_{10}ClN_5Se$: C, 52.64; H, 2.45; N, 17.05. Found: C, 52.97; H, 2.25; N, 17.00%; λ_{max}(DCM)/nm 261 inf (log ε 4.60), 268 inf (4.66), 271 (4.68), 278 (4.71), 284 inf (4.69), 352 inf (3.86), 487 (3.18); ν_{max}/cm^{-1}(ATR) 2212w (C≡N), 1591w, 1557s, 1493m, 1468m, 1441s, 1337s, 1256w, 1192w, 1173w, 1117w, 1078w, 1026w, 1005w, 922w, 907w, 893w, 826w, 758w, 750m, 712m; δ_H(300 MHz, $CDCl_3$) 7.50-7.26 (10H, m); δ_C(75 MHz, $CDCl_3$) 166.8 (s), 163.1 (s), 143.6 (s), 142.9 (s), 130.1 (d), 128.6 (d), 127.2 (d), 125.4 (s), 112.0 (s), 99.5 (s); *m/z* (MALDI-TOF) 434 ($Se^{80}Cl^{35}$: M^++Na, 28%), 412 (MH^+, 65), 296 (34), 242 (100), 197 (13), 184 (12), 150 (20), 142 (17), 100 (34), 86 (17).

S3.2.22 Displacement of the 4-chloride

Reaction of 4-chloro-6-morpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (26) with morpholine

Method A: To a stirred suspension of 4-chloro-6-morpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**26**) (34.5 mg, 0.10 mmol) in anhydrous DCM (3 mL) at *ca.* 20 °C, was added morpholine (172 μL, 2.00 mmol). The reaction mixture was heated to *ca.* 40 °C for 24 h, until no starting material remained (TLC). The reaction was then allowed to cool to *ca.* 20 °C, diluted with DCM (10 mL) and extracted with distilled water (40 mL). The aqueous phase was then extracted with DCM (2 × 20 mL), and the combined organic phases were dried ($MgSO_4$), filtered, adsorbed onto silica and chromatographed (Hex/DCM/TBME, 20:40:40) to give *4,6-dimorpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile* (**33**) (3.0 mg, 8%) as red prisms, mp (hot-stage) 172-175 °C (*c*-Hex/DCE) (decomp.); R_f 0.40 (DCM/TBME, 50:50); Anal. Calcd for $C_{14}H_{16}N_6O_2Se$: C, 44.33; H, 4.25; N, 22.16. Found: C, 44.21; H, 4.53; N, 22.44%; λ_{max}(DCM)/nm 254 (log ε 4.36), 267 inf (4.22), 313 (4.15), 360 (3.51), 504 (4.18); ν_{max}/cm^{-1}(ATR) 2972w & 2866w (alkyl C-H), 2207w (C≡N), 1557s, 1487w, 1454m, 1445m, 1396w, 1364w, 1323m, 1283s, 1261m, 1192w, 1159w, 1117s, 1065w, 1018w, 974m, 924w,

895w, 862m, 843w, 775w, 760w, 718w; δ_H(300 MHz, $CDCl_3$) 4.11 (4H, t, *J* 4.5), 3.98 (4H, t, *J* 4.5), 3.86 (4H, t, *J* 5.1), 3.34 (4H, t, *J* 4.8); δ_C(75 MHz, $CDCl_3$) 165.3 (s), 165.2 (s), 157.8 (s), 122.8 (s), 116.8 (s), 91.5 (s), 66.8 (t), 66.0 (t), 50.6 (t), 47.6 (t); *m/z* (MALDI-TOF) 382 (Se^{80}: M^++2H, 100%), 380 (M^+, 53), 375 (22), 339 (21), 320 (22), 309 (38), 302 (51), 295 (42), 281 (28), 278 (47), 213 (23), 101 (30). Further elution (Hex/DCM/TBME, 10:45:45) afforded *2,5-dimorpholino-3-oxo-3*H-*pyrrole-4-carbonitrile* (**34**) (3.5 mg, 13%) as orange needles, mp (hot-stage) 247-250 °C (*c*-Hex/DCE); R_f 0.65 (Hex/EtOAc, 10:90); Anal. Calcd for $C_{13}H_{16}N_4O_3$: C, 56.51; H, 5.84; N, 20.28. Found: C, 56.28; H, 6.00; N, 20.51%; λ_{max}(DCM)/nm 311 inf (log ε 4.39), 332 inf (4.15), 427 (3.15); ν_{max}/cm^{-1}(ATR) 2926w & 2866w (alkyl C-H), 2191w (C≡N), 1667w, 1630w, 1557s, 1423m, 1393w, 1366w, 1357w, 1339w, 1306w, 1269m, 1252s, 1213w, 1138w, 1109s, 1067w, 1028w, 974m, 926w, 895m, 858m, 785w, 718m; δ_H(300 MHz, $CDCl_3$) 4.54 (2H, t, *J* 4.8), 4.13 (2H, t, *J* 4.8), 4.03 (2H, t, *J* 4.8), 3.86-3.76 (10H, m); δ_C(125 MHz, $CDCl_3$) 182.4 (s), 174.9 (s), 163.0 (s), 117.0 (s), 68.6 (s), 67.4 (t), 67.0 (t), 66.73 (t), 66.70 (t), 48.3 (t), 47.5 (t), 47.1 (t), 45.1 (t); *m/z* (MALDI-TOF) 315 (M^++K, 29%), 299 (M^++Na, 59), 277 (MH^+, 100), 212 (59), 150 (28), 133 (54), 86 (8), 39 (60). Further elution (Hex/DCM/EtOAc, (Hex/DCM/THF, 20:20:60) gave *3,5-dimorpholino-2-oxo-2*H-*pyrrole-4-carbonitrile* (**35**) (15.5 mg, 55%) as yellow prisms, mp (hot-stage) 225-232 °C (*c*-Hex/DCE); R_f 0.26 (Hex/EtOAc, 5:95); Anal. Calcd for $C_{13}H_{16}N_4O_3$: C, 56.51; H, 5.84; N, 20.28. Found: C, 56.30; H, 5.72; N, 19.88%; λ_{max}(DCM)/nm 303 inf (log ε 3.18), 312 (3.21), 325 inf (3.10), 416 (2.34); ν_{max}/cm^{-1}(ATR) 2924w & 2870w (alkyl C-H), 2185w (C≡N), 1694w, 1614w, 1557s, 1470w, 1441w, 1391w, 1371w, 1327m, 1306w, 1267m, 1231w, 1161w, 1111m, 1063w, 1026m, 976w, 932w, 903w, 858m, 789w, 714w; δ_H(300 MHz, $CDCl_3$) 4.62 (2H, t, *J* 4.2), 4.16 (2H, t, *J* 4.5), 4.06 (4H, t, *J* 4.8), 3.90 (2H, t, *J* 4.5), 3.84-3.78 (6H, m); δ_C(75 MHz, $CDCl_3$) 173.7 (s), 173.3 (s), 159.4 (s), 117.7 (s), 68.4 (s), 67.7 (t), 66.9 (t), 66.84 (t), 66.75 (t), 50.6 (t), 48.8 (t), 48.0 (t), 47.9 (t); *m/z* (MALDI-TOF) 299 (M^++Na, 11%), 277 (MH^+, 100), 251 (10), 234 (7), 219 (4), 150 (10), 86 (5), 39 (9).

Method B – To a stirred solution of 4-chloro-6-morpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**26**) (69.0 mg, 0.20 mmol) in anhydrous toluene (16 mL) at *ca.* 80 °C was added morpholine (37.9 μL, 0.44 mmol). After 24 h, morpholine (37.9 μL, 0.44 mmol) was added and the reaction was left to stir at *ca.* 80 °C until no starting material remained (TLC). After a total of 72 h, volatiles were removed *in vacuo*, dissolved in DCM (25 mL) and filtered through fluted filter paper. The filtrate was then concentrated and chromatographed (Hex/DCM/TBME, 40:30:30) to give 4,6-dimorpholinopyrrolo[2,3-*c*][1,2,6]selenadiazine-5-carbonitrile (**33**) (16.4 mg, 22%) as red prisms, mp (hot-stage) 172-175 °C (*c*-Hex/DCE) (decomp.); R_f 0.40 (DCM/TBME, 50:50); ν_{max}/cm^{-1}(ATR) 2972w & 2866w (alkyl C-H), 2207w (C≡N), 1557s, 1487w, 1454m, 1445m, 1396w, 1364w, 1323m, 1283s, 1261m, 1192w, 1159w,

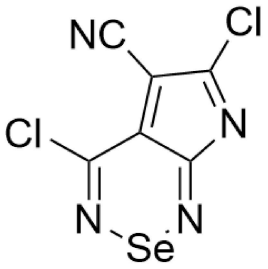
1117s, 1065w, 1018w, 974m, 924w, 895w, 862m, 843w, 775w, 760w, 718w; identical to that described above.

S3.3 Section references

1. Hardwood, L. M. Dry-Column Flash Chromatography. *Aldrichimica Acta* **1985**, *18*, 25-25.
2. Carboni, R. A. TETRACYANOETHYLENE. *Org. Synth.* **1959**, *39*, 64-67.
3. Amosova, S. V.; Penzik, M. V.; Albanov, A. I.; Potapov, V. A. The reaction of selenium dichloride with divinyl sulfide. *J. Organomet. Chem.* **2009**, *694*, 3369–3372.

S4 NMR Spectra

4,6-Dichloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 12

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EXPNO                     151
PROCNO                      1

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PULPROG                zg30
TD                    65536
SOLVENT             CD2Cl2
NS                        16
DS                         2
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FIDRES            0.305176 Hz
AQ                3.2767999 sec
RG                      287
DW                 50.000 usec
DE                 13.55 usec
TE                 298.9 K
D1              1.00000000 sec
TD0                        1
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NUC1                    1H
P0                 4.00 usec
P1                12.00 usec
PLW1           16.34900093 W

F2 - Processing parameters
SI                    65536
SF             500.0330206 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                  1.00
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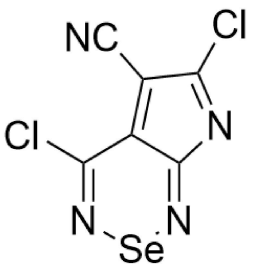
4,6-Dichloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 12

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Current Data Parameters
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EXPNO                     157
PROCNO                      1

F2 - Acquisition Parameters
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Time                  22.54 h
INSTRUM                spect
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PULPROG                 jmod
TD                     65536
SOLVENT             CD2Cl2
NS                     13312
DS                         4
SWH               29761.904 Hz
FIDRES             0.908261 Hz
AQ                1.1010048 sec
RG                      2050
DW                   16.800 usec
DE                    6.50 usec
TE                   299.9 K
CNST2           145.0000000
CNST11            1.0000000
D1                6.00000000 sec
D20               0.00689655 sec
TD0                        1
SFO1            125.7459712 MHz
NUC1                    13C
P1                   10.00 usec
P2                   20.00 usec
PLW1           121.36000061 W
SFO2            500.0350001 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                80.00 usec
PLW2           16.34900093 W
PLW12           0.34647381 W

F2 - Processing parameters
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SF              125.7333492 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                    1.40
```

4-Chloro-6-oxo-6,7-dihydropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 13

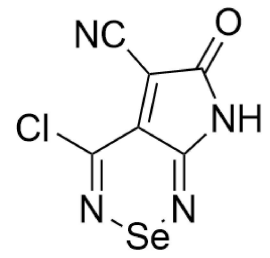
Current Data Parameters
NAME NMR 300
EXPNO 261
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230812
Time 13.52 h
INSTRUM spect
PROBHD Z104275_0375 (
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 64
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 201.81
DW 83.200 usec
DE 13.19 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 7.09999990 W

F2 - Processing parameters
SI 65536
SF 300.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4-Chloro-6-oxo-6,7-dihydropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 13

D2O wash in Acetone-d6



Current Data Parameters

NAME	NMR 300
EXPNO	262
PROCNO	1

F2 - Acquisition Parameters

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INSTRUM	spect
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PULPROG	zg30
TD	65536
SOLVENT	Acetone
NS	64
DS	2
SWH	6009.615 Hz
FIDRES	0.183399 Hz
AQ	5.4525952 sec
RG	201.81
DW	83.200 usec
DE	13.19 usec
TE	297.0 K
D1	1.00000000 sec
TD0	1
SFO1	300.1318533 MHz
NUC1	1H
P0	4.67 usec
P1	14.00 usec
PLW1	7.09999990 W

F2 - Processing parameters

SI	65536
SF	300.1300068 MHz
WDW	EM
SSB	0
LB	0.30 Hz
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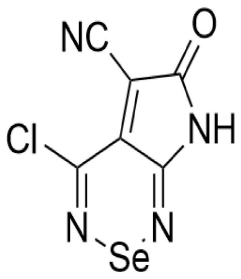
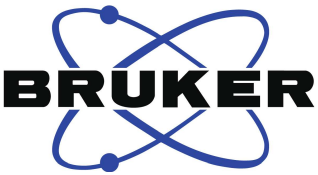
PC	1.00

4-Chloro-6-oxo-6,7-dihydropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile (13)



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Current Data Parameters
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EXPNO                     150
PROCNO                      1

F2 - Acquisition Parameters
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Time                   8.18 h
INSTRUM                spect
PROBHD    Z113652_0078 (
PULPROG                 jmod
TD                     65536
SOLVENT                 TFA2
NS                     11264
DS                         4
SWH               29761.904 Hz
FIDRES             0.908261 Hz
AQ                 1.1010048 sec
RG                      2050
DW                    16.800 usec
DE                     6.50 usec
TE                    301.9 K
CNST2            145.0000000
CNST11             1.0000000
D1                 2.00000000 sec
D20                0.00689655 sec
TD0                        1
SFO1             125.7459712 MHz
NUC1                     13C
P1                    10.00 usec
P2                    20.00 usec
PLW1            121.36000061 W
SFO2             500.0350001 MHz
NUC2                     1H
CPDPRG[2             waltz65
PCPD2                 80.00 usec
PLW2             16.34900093 W
PLW12             0.34647381 W

F2 - Processing parameters
SI                     32768
SF               125.7333979 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                     1.40
```
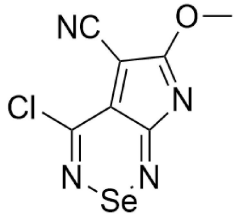

4-Chloro-6-methoxypyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 14

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Current Data Parameters
NAME                  nmr 500
EXPNO                     124
PROCNO                      1

F2 - Acquisition Parameters
Date_              20230731
Time                   9.44 h
INSTRUM               spect
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PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH               10000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                       256
DW                    50.000 usec
DE                    13.55 usec
TE                    299.5 K
D1                1.00000000 sec
TD0                        1
SFO1            500.0360877 MHz
NUC1                      1H
P0                    4.00 usec
P1                   12.00 usec
PLW1           16.34900093 W

F2 - Processing parameters
SI                     65536
SF              500.0330123 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                    1.00
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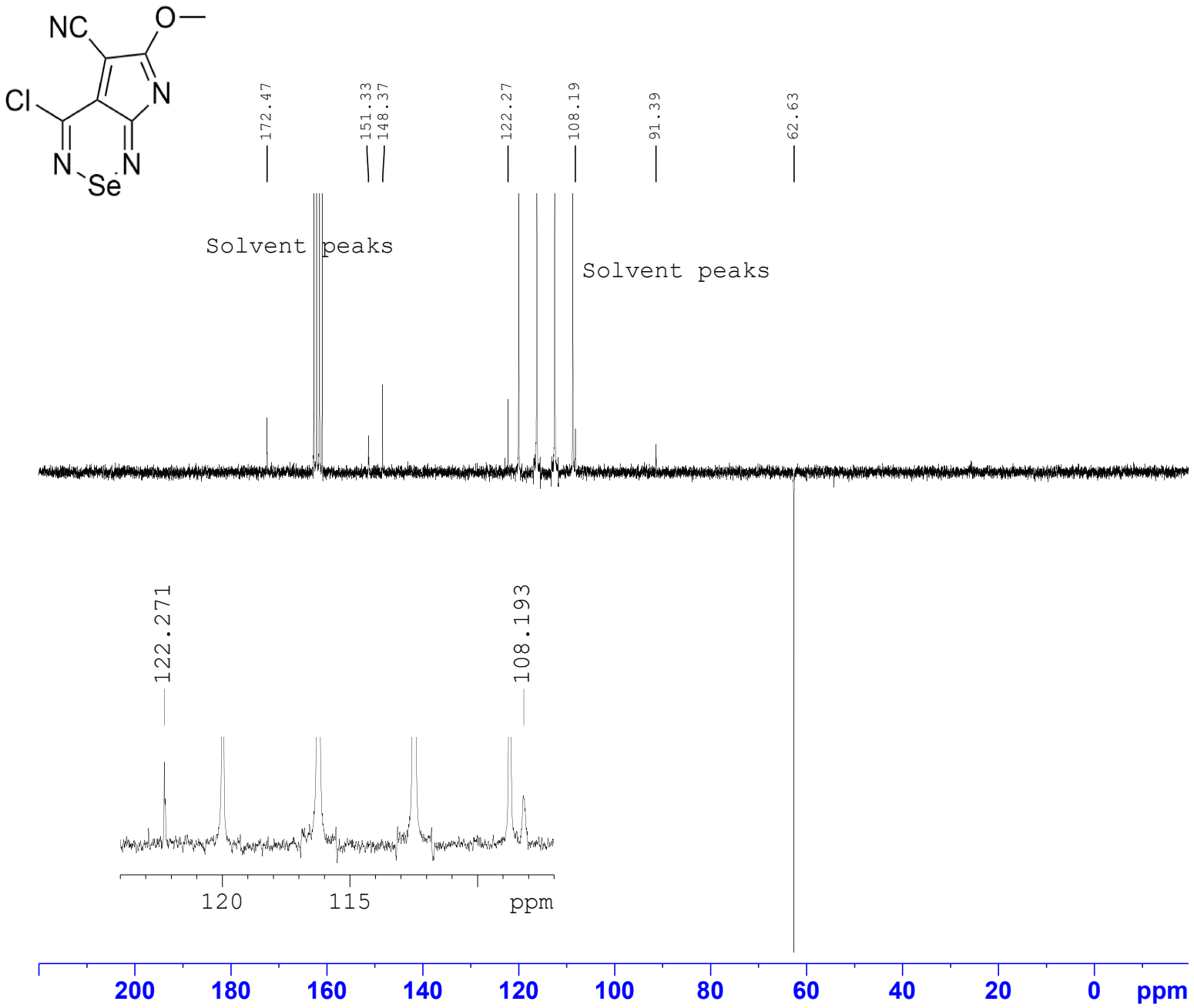
4-Chloro-6-methoxypyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 14



Current Data Parameters

NAME	NMR 300
EXPNO	237
PROCNO	1

F2 - Acquisition Parameters

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Time	9.01 h
INSTRUM	spect
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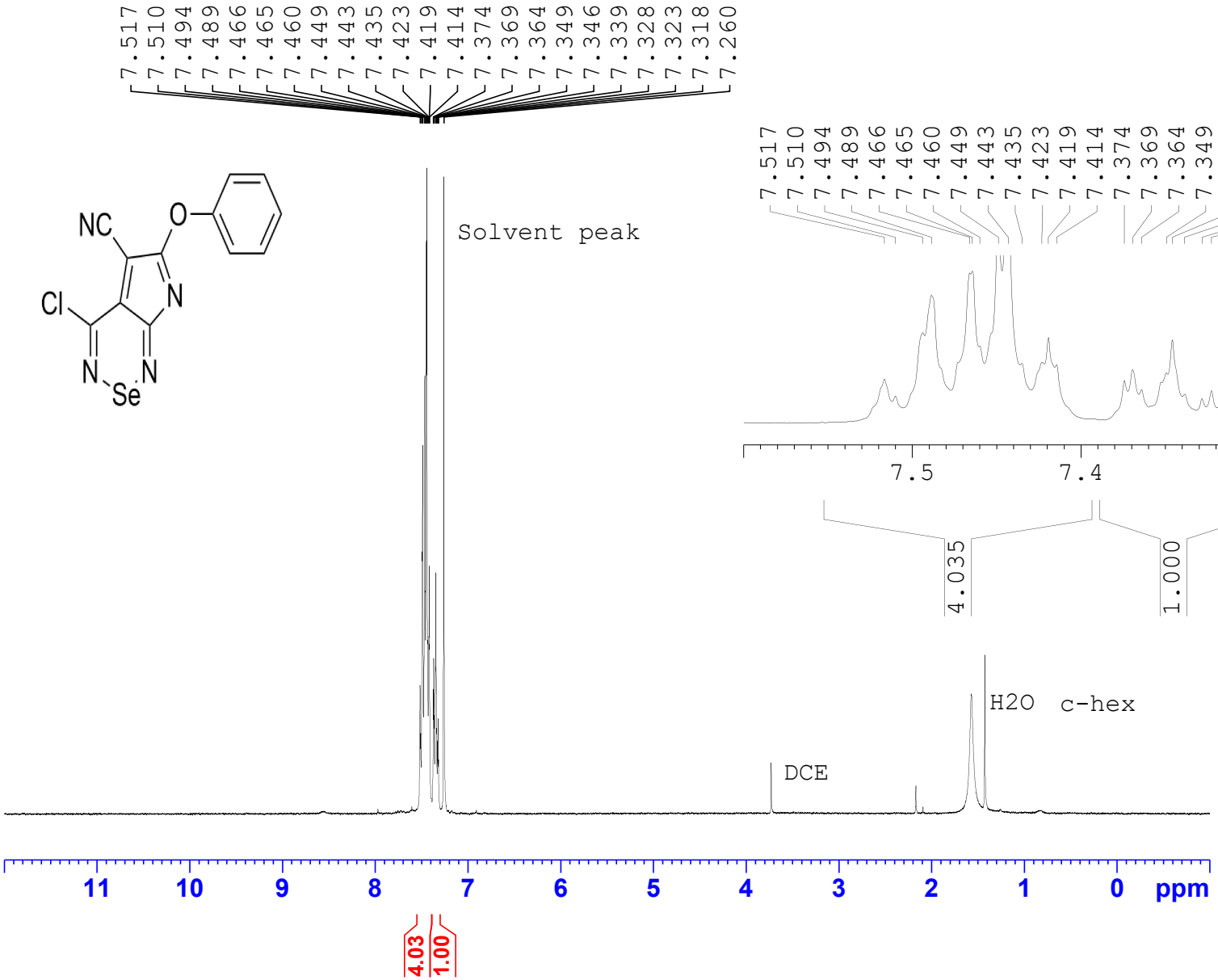
PULPROG	jmod
TD	65536
SOLVENT	TFA-d
NS	10240
DS	4
SWH	18115.941 Hz
FIDRES	0.552855 Hz
AQ	1.8087935 sec
RG	201.81
DW	27.600 usec
DE	6.50 usec
TE	301.4 K
CNST2	145.0000000
CNST11	1.0000000
D1	2.00000000 sec
D20	0.00689655 sec
TD0	1
SFO1	75.4752953 MHz
NUC1	13C
P1	10.00 usec
P2	20.00 usec
PLW1	45.00000000 W
SFO2	300.1312005 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	90.00 usec
PLW2	7.09999990 W
PLW12	0.17180000 W

F2 - Processing parameters

SI	32768
SF	75.4677485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4-Chloro-6-phenoxypyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 15

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Current Data Parameters
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EXPNO                     240
PROCNO                      1

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PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  6009.615 Hz
FIDRES               0.183399 Hz
AQ                   5.4525952 sec
RG                      201.81
DW                      83.200 usec
DE                      13.19 usec
TE                      300.9 K
D1                1.00000000 sec
TD0                         1
SFO1           300.1318533 MHz
NUC1                       1H
P0                      4.67 usec
P1                      14.00 usec
PLW1               7.09999990 W

F2 - Processing parameters
SI                      65536
SF             300.1300073 MHz
WDW                        EM
SSB                         0
LB                   0.30 Hz
GB                          0
PC                       1.00
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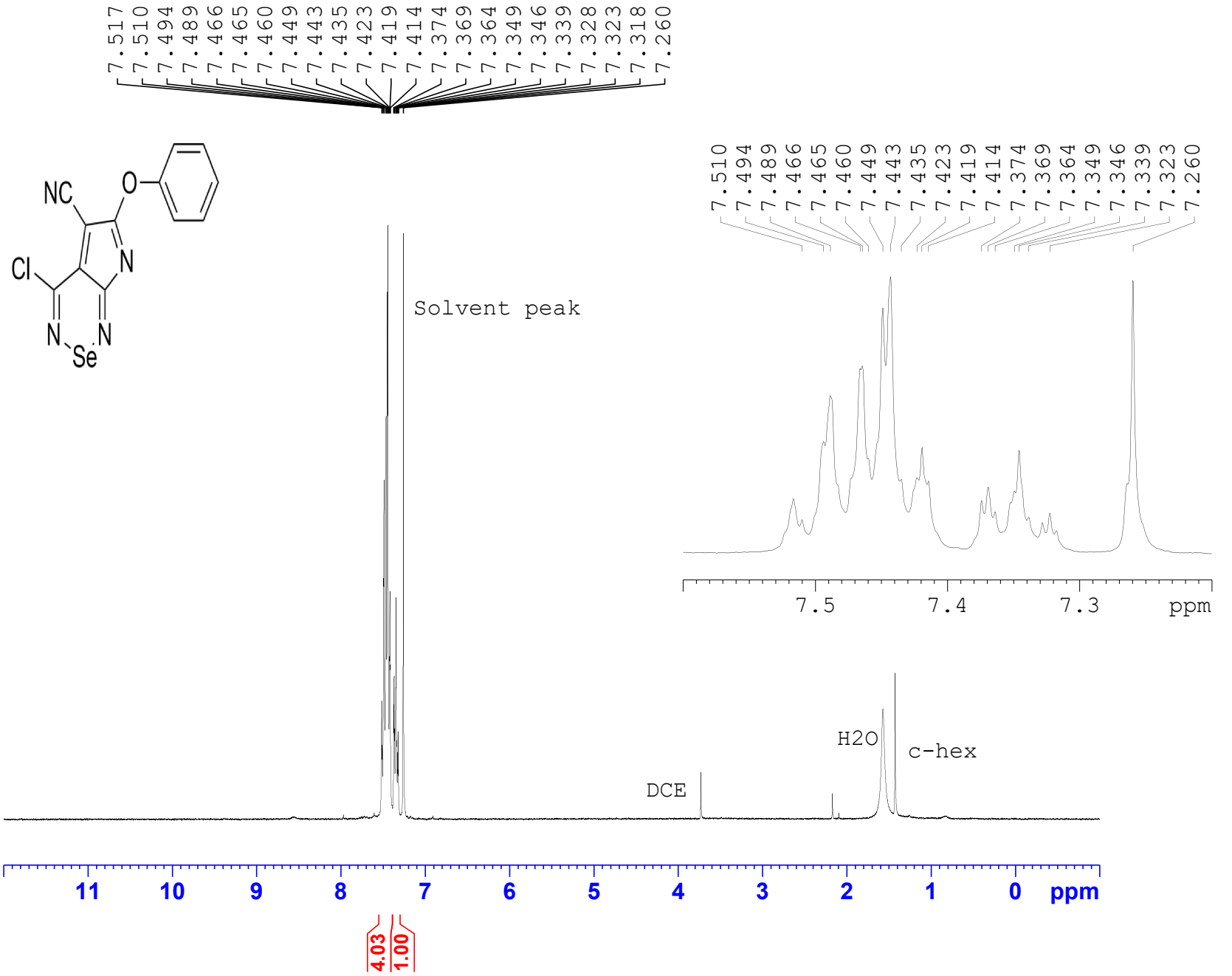
4-Chloro-6-phenoxypyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 15



Current Data Parameters

NAME	NMR 300
EXPNO	240
PROCNO	1

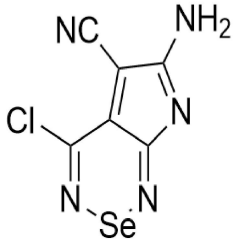
F2 - Acquisition Parameters

Date_	20230725
Time	19.09 h
INSTRUM	spect
PROBHD	Z104275_0375 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6009.615 Hz
FIDRES	0.183399 Hz
AQ	5.4525952 sec
RG	201.81
DW	83.200 usec
DE	13.19 usec
TE	300.9 K
D1	1.00000000 sec
TD0	1
SFO1	300.1318533 MHz
NUC1	1H
P0	4.67 usec
P1	14.00 usec
PLW1	7.09999990 W

F2 - Processing parameters

SI	65536
SF	300.1300073 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

6-Amino-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 16



Current Data Parameters
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EXPNO 108
PROCNO 1

F2 - Acquisition Parameters
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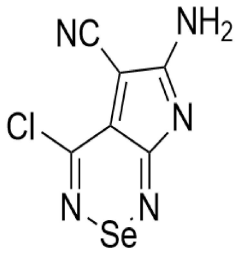
Time 16.05 h
INSTRUM spect
PROBHD Z113652_0078 (
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 13.55 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.0360877 MHz
NUC1 1H
P0 4.00 usec
P1 12.00 usec
PLW1 16.34900093 W

F2 - Processing parameters
SI 65536
SF 500.0330100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

6-Amino-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 16

D2O wash in MeOD

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Current Data Parameters
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EXPNO                     265
PROCNO                      1

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Time                  14.08 h
INSTRUM               spect
PROBHD     Z104275_0375 (
PULPROG                zg30
TD                    65536
SOLVENT                MeOD
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES             0.183399 Hz
AQ                 5.4525952 sec
RG                    113.88
DW                    83.200 usec
DE                    13.19 usec
TE                    296.9 K
D1                1.00000000 sec
TD0                       1
SFO1           300.1318533 MHz
NUC1                    1H
P0                     4.67 usec
P1                    14.00 usec
PLW1           7.09999990 W

F2 - Processing parameters
SI                    65536
SF             300.1300089 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
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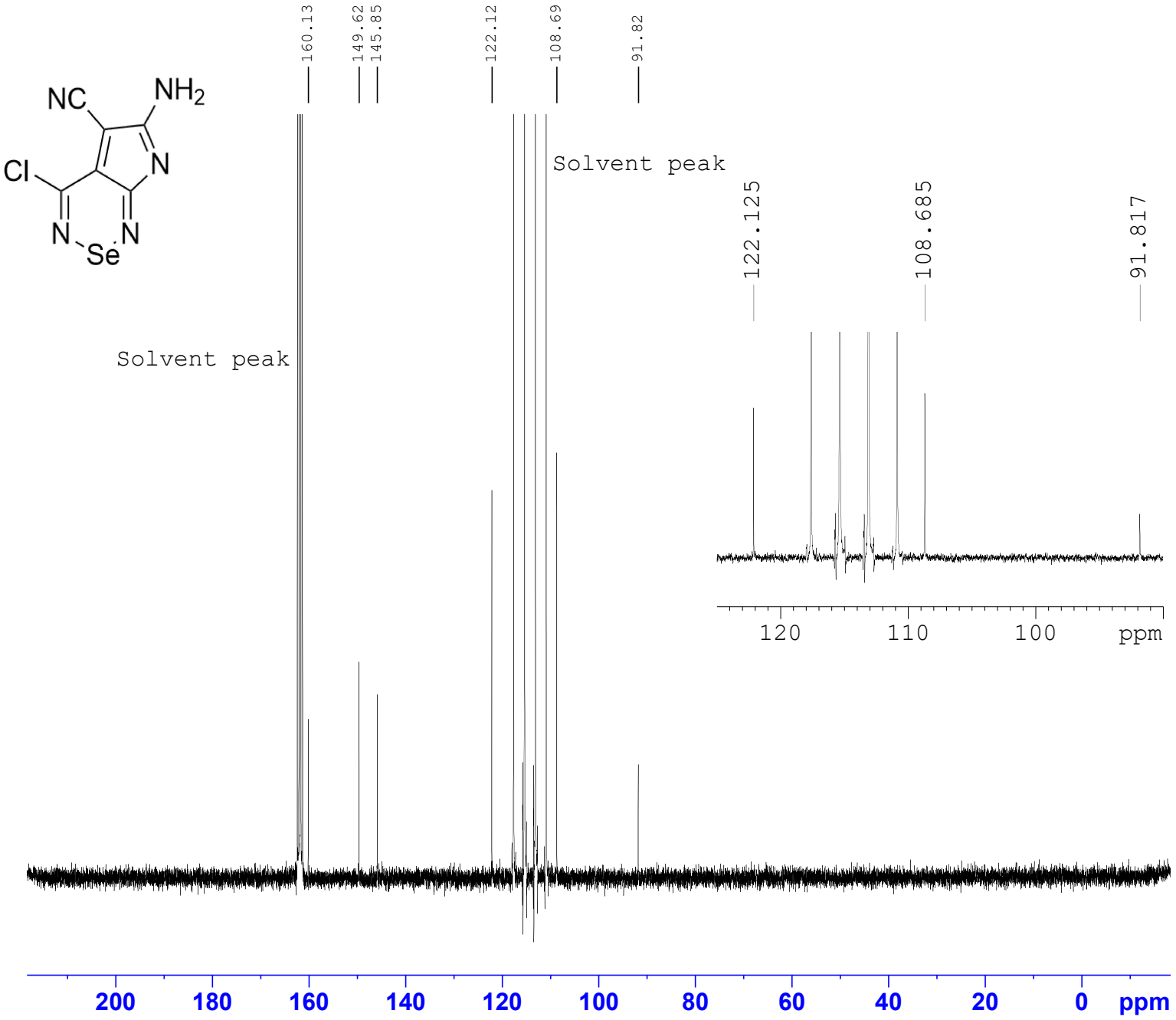
6-Amino-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 16



Current Data Parameters
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EXPNO 90
PROCNO 1

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Time 8.25 h
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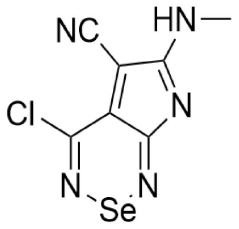
PULPROG jmod
TD 65536
SOLVENT TFA2
NS 13312
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 125.7459712 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 121.36000061 W
SFO2 500.0350001 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 16.34900093 W
PLW12 0.34647381 W

F2 - Processing parameters
SI 32768
SF 125.7333979 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Chloro-6-(methylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 17



Current Data Parameters

NAME	nmr 500
EXPNO	137
PROCNO	1

F2 - Acquisition Parameters

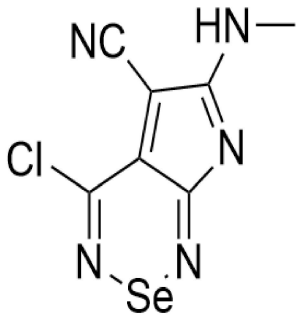
Date_	20230807
Time	14.30 h
INSTRUM	spect
PROBHD	Z113652_0078 (
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.305176 Hz
AQ	3.2767999 sec
RG	203
DW	50.000 usec
DE	13.55 usec
TE	299.2 K
D1	1.00000000 sec
TD0	1
SFO1	500.0360877 MHz
NUC1	1H
P0	4.00 usec
P1	12.00 usec
PLW1	16.34900093 W

F2 - Processing parameters

SI	65536
SF	500.0330043 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4-Chloro-6-(methylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 17

D2O wash in DMSO-d6

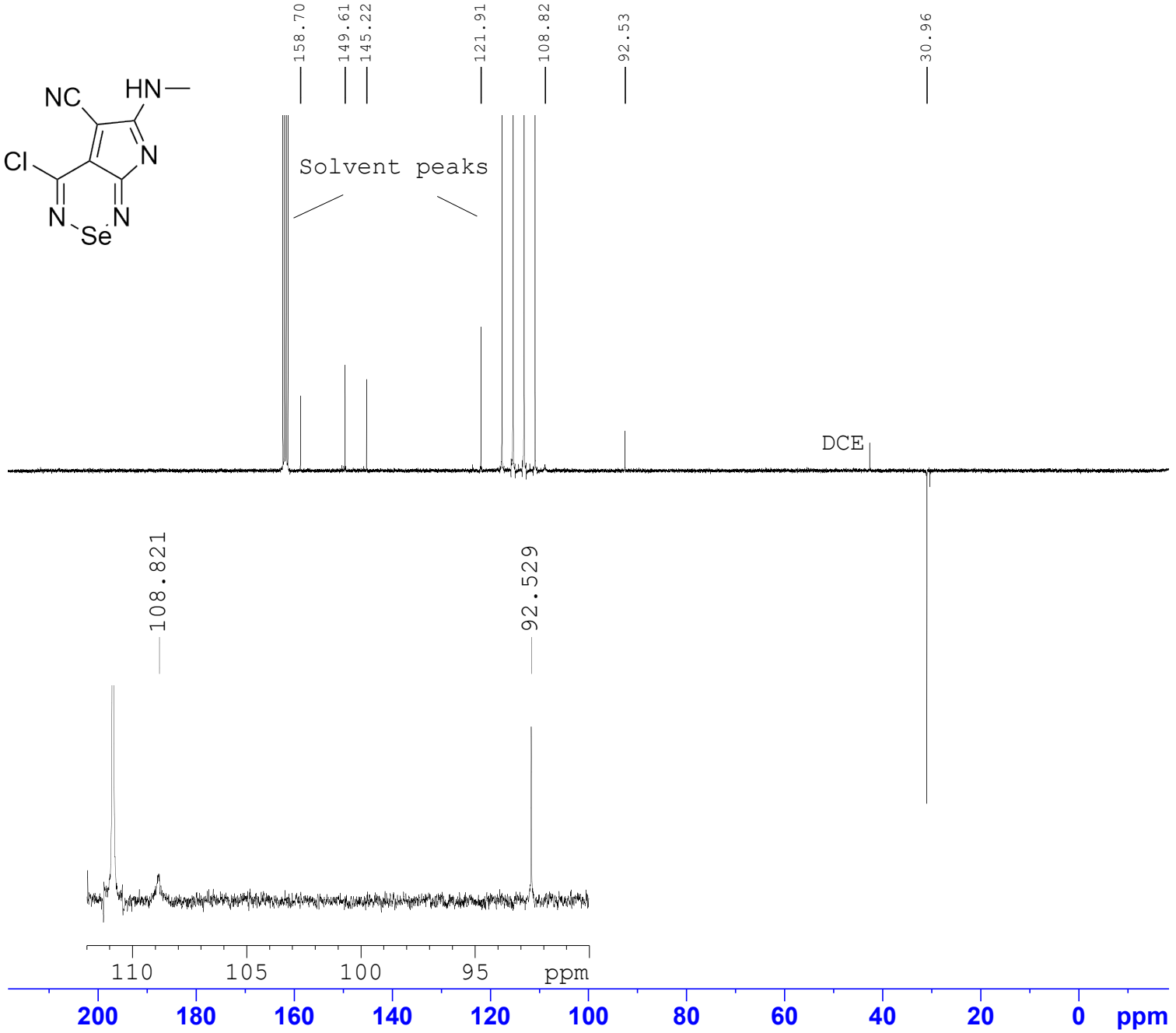


Current Data Parameters
NAME nmr 500
EXPNO 138
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230807
Time 14.43 h
INSTRUM spect
PROBHD Z113652_0078 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 64
DW 50.000 usec
DE 13.55 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.0360877 MHz
NUC1 1H
P0 4.00 usec
P1 12.00 usec
PLW1 16.34900093 W

F2 - Processing parameters
SI 65536
SF 500.0332294 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4-Chloro-6-(methylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 17



Current Data Parameters

NAME	nmr 500
EXPNO	73
PROCNO	1

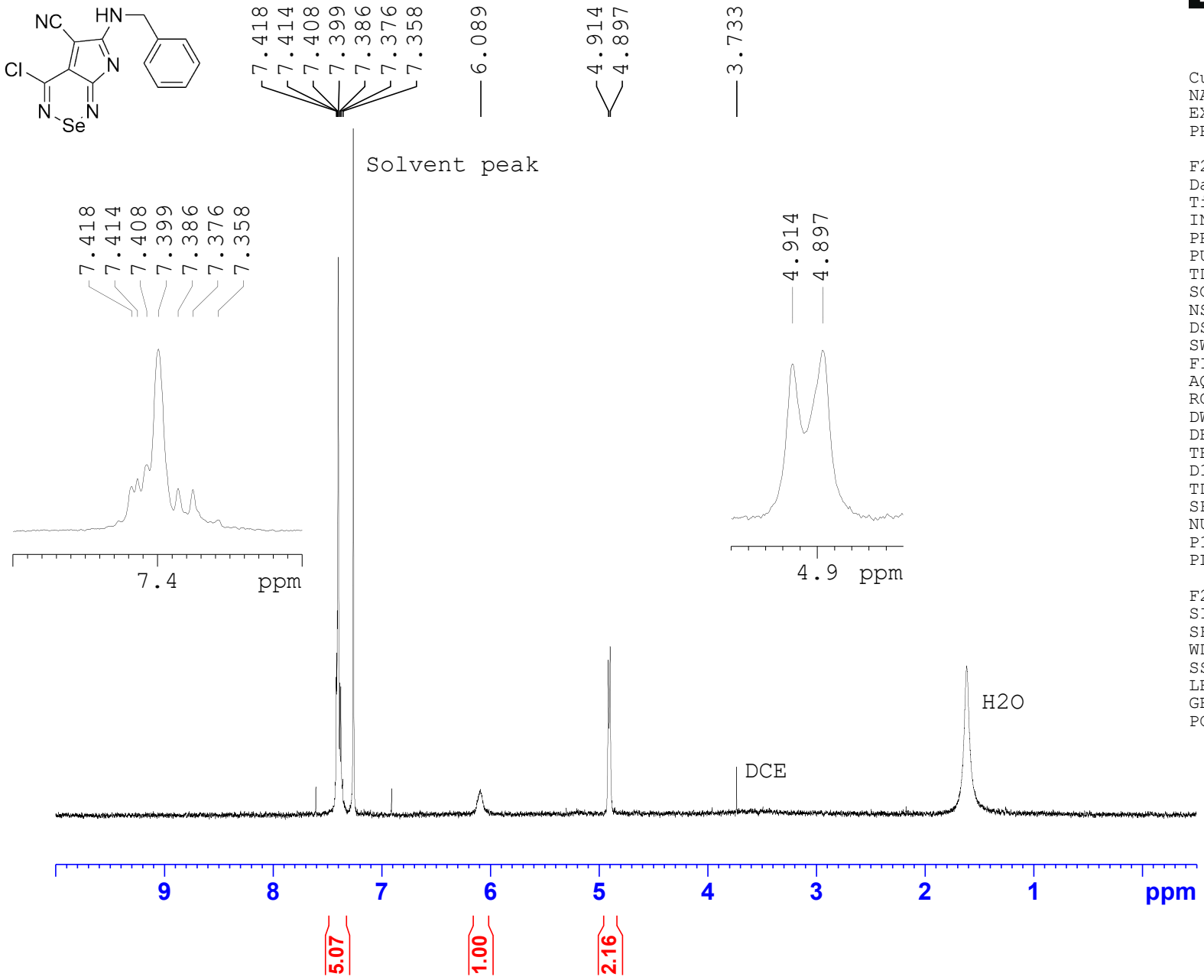
F2 - Acquisition Parameters

Date_	20230517
Time	7.43 h
INSTRUM	spect
PROBHD	Z113652_0078 (
PULPROG	jmod
TD	65536
SOLVENT	TFA2
NS	13312
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	1.1010048 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	299.8 K
CNST2	145.0000000
CNST11	1.0000000
D1	2.00000000 sec
D20	0.00689655 sec
TD0	1
SFO1	125.7459712 MHz
NUC1	13C
P1	10.00 usec
P2	20.00 usec
PLW1	121.36000061 W
SFO2	500.0350001 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	80.00 usec
PLW2	16.34900093 W
PLW12	0.34647381 W

F2 - Processing parameters

SI	32768
SF	125.7333979 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

6-(Benzylamino)-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 18



Current Data Parameters

NAME	NMR 300
EXPNO	170
PROCNO	1

F2 - Acquisition Parameters

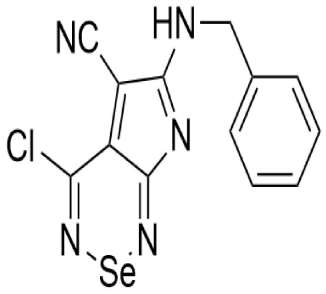
Date_	20230206
Time	17.04 h
INSTRUM	spect
PROBHD	Z104275_0375 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6009.615 Hz
FIDRES	0.183399 Hz
AQ	5.4525952 sec
RG	201.81
DW	83.200 usec
DE	6.50 usec
TE	294.4 K
D1	1.00000000 sec
TD0	1
SFO1	300.1318533 MHz
NUC1	1H
P1	14.00 usec
PLW1	7.85570002 W

F2 - Processing parameters

SI	65536
SF	300.1300074 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

6-(Benzylamino)-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 18

D2O wash in CDCl3

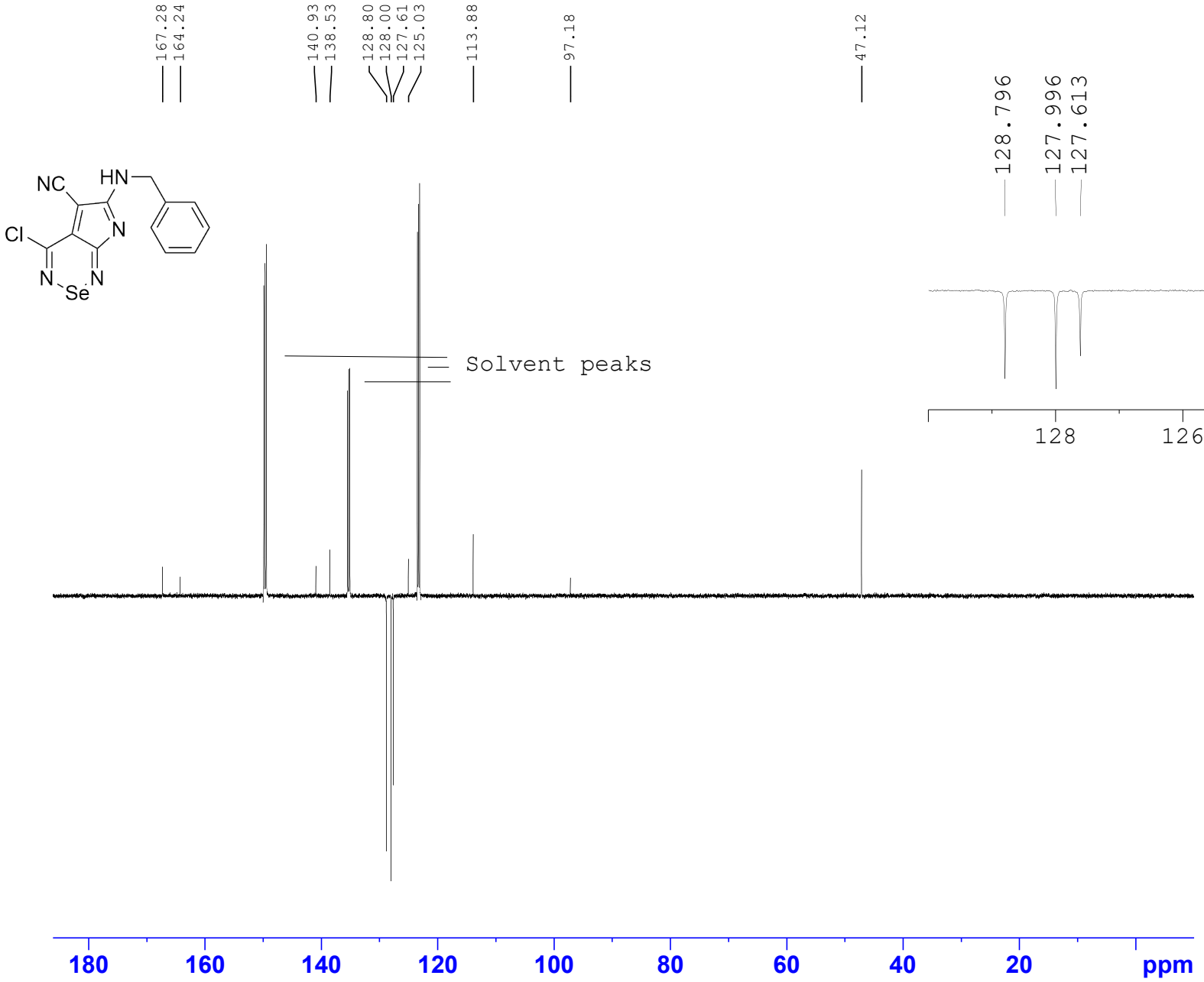



```
Current Data Parameters
NAME                  NMR 300
EXPNO                     267
PROCNO                      1

F2 - Acquisition Parameters
Date_              20230814
Time                  14.47 h
INSTRUM               spect
PROBHD    Z104275_0375 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 6009.615 Hz
FIDRES              0.183399 Hz
AQ                 5.4525952 sec
RG                    201.81
DW                    83.200 usec
DE                    13.19 usec
TE                    296.9 K
D1                1.00000000 sec
TD0                        1
SFO1            300.1318533 MHz
NUC1                      1H
P0                     4.67 usec
P1                    14.00 usec
PLW1               7.09999990 W

F2 - Processing parameters
SI                     65536
SF              300.1300083 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
```

6-(Benzylamino)-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 18



Current Data Parameters

NAME	nmr 500
EXPNO	77
PROCNO	1

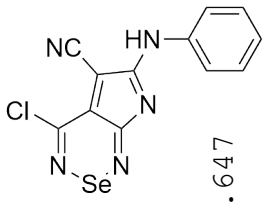
F2 - Acquisition Parameters

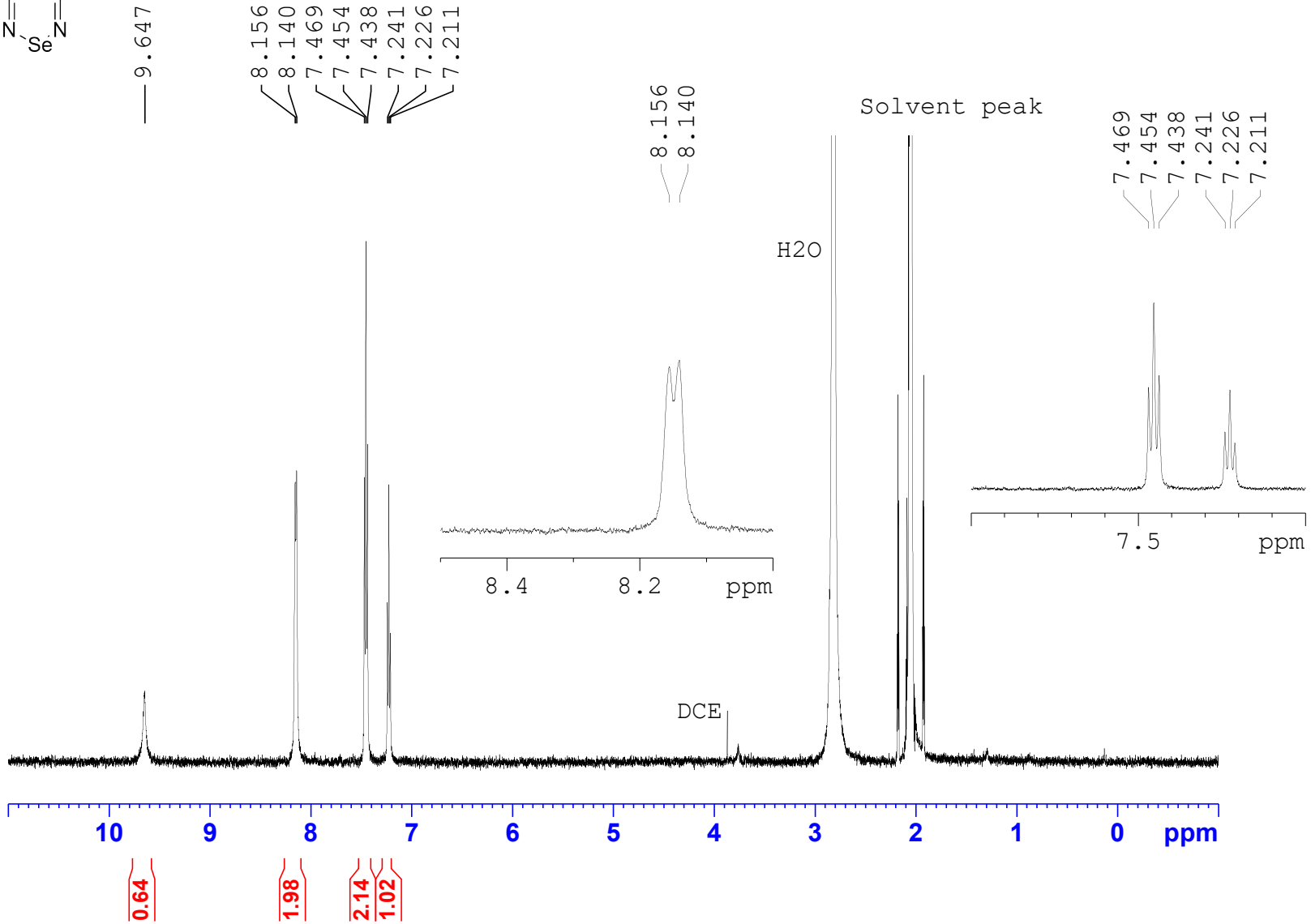
Date_	20230526
Time	15.17 h
INSTRUM	spect
PROBHD	Z113652_0078 (
PULPROG	jmod
TD	65536
SOLVENT	Pyr
NS	655
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	1.1010048 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	297.7 K
CNST2	145.0000000
CNST11	1.0000000
D1	2.00000000 sec
D20	0.00689655 sec
TD0	1
SFO1	125.7459712 MHz
NUC1	13C
P1	10.00 usec
P2	20.00 usec
PLW1	121.36000061 W
SFO2	500.0350001 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	80.00 usec
PLW2	16.34900093 W
PLW12	0.34647381 W

F2 - Processing parameters

SI	32768
SF	125.7333979 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4-Chloro-6-(phenylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 19





Current Data Parameters

NAME	nmr 500
EXPNO	91
PROCNO	1

F2 - Acquisition Parameters

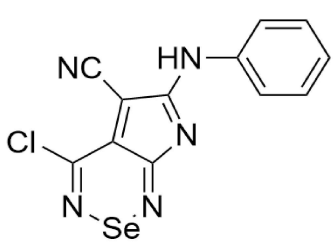
Date_	20230621
Time	14.57 h
INSTRUM	spect
PROBHD	Z113652_0078 (
PULPROG	zg30
TD	65536
SOLVENT	Acetone
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.305176 Hz
AQ	3.2767999 sec
RG	203
DW	50.000 usec
DE	13.55 usec
TE	298.6 K
D1	1.00000000 sec
TD0	1
SFO1	500.0360877 MHz
NUC1	1H
P0	4.00 usec
P1	12.00 usec
PLW1	16.34900093 W

F2 - Processing parameters

SI	65536
SF	500.0330080 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4-Chloro-6-(phenylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 19

D2O wash in Acetone-d6



Current Data Parameters

NAME	nmr 500
EXPNO	92
PROCNO	1

F2 - Acquisition Parameters

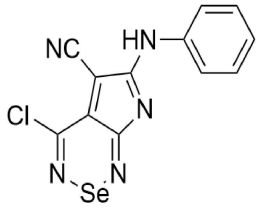
Date_	20230621
Time	15.16 h
INSTRUM	spect
PROBHD	Z113652_0078 (
PULPROG	zg30
TD	65536
SOLVENT	Acetone
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.305176 Hz
AQ	3.2767999 sec
RG	32
DW	50.000 usec
DE	13.55 usec
TE	298.6 K
D1	1.00000000 sec
TD0	1
SFO1	500.0360877 MHz
NUC1	1H
P0	4.00 usec
P1	12.00 usec
PLW1	16.34900093 W

F2 - Processing parameters

SI	65536
SF	500.0330000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4-Chloro-6-(phenylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 19

Very poor solubility, 6 C (s) missing

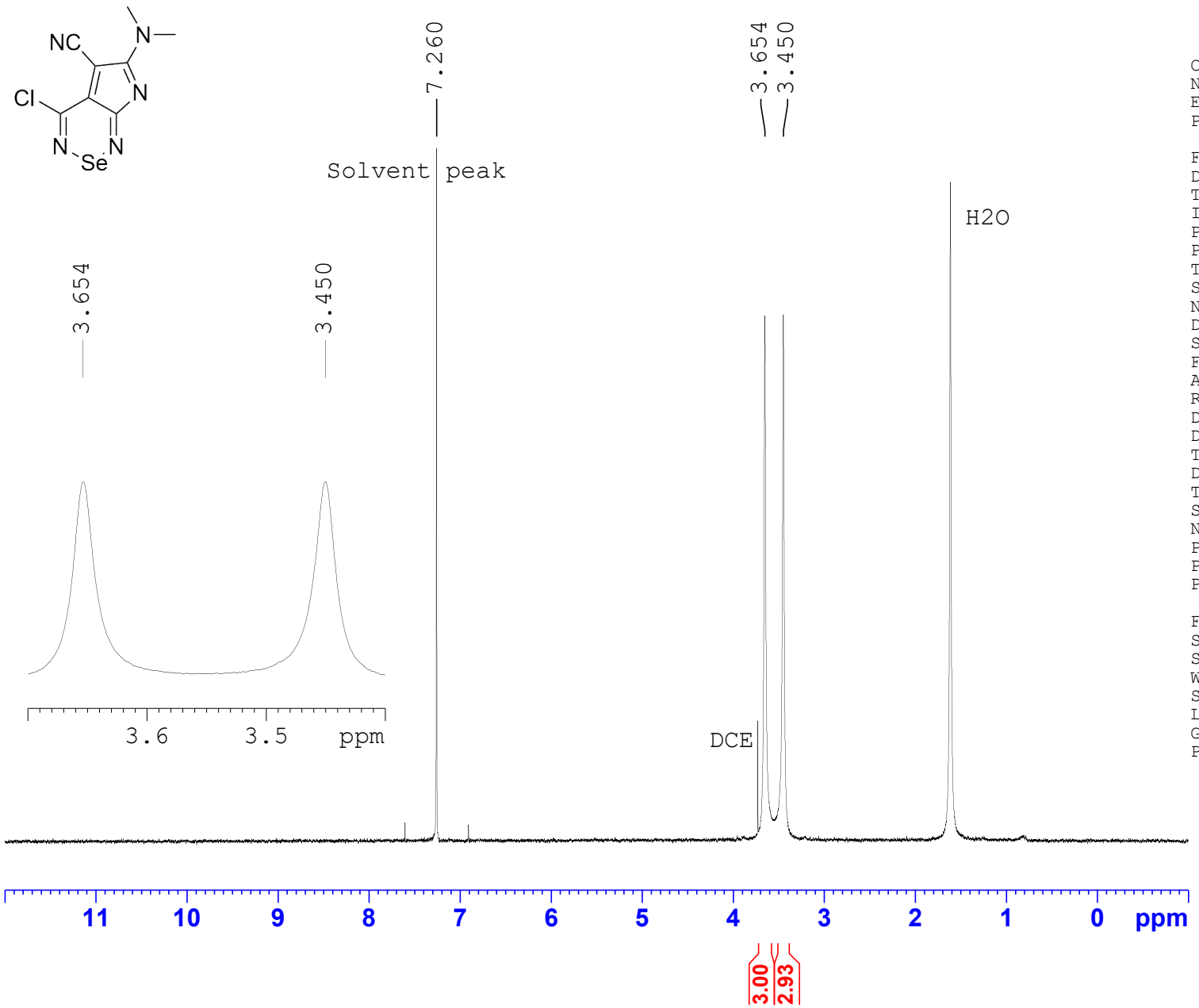



```
Current Data Parameters
NAME                  nmr 500
EXPNO                      96
PROCNO                      1

F2 - Acquisition Parameters
Date_                20230703
Time                     8.45 h
INSTRUM                  spect
PROBHD   Z113652_0078 (
PULPROG                  jmod
TD                      65536
SOLVENT               Acetone
NS                        13312
DS                            4
SWH                  29761.904 Hz
FIDRES                0.908261 Hz
AQ                    1.1010048 sec
RG                         2050
DW                       16.800 usec
DE                        6.50 usec
TE                       301.8 K
CNST2               145.0000000
CNST11                1.0000000
D1                    2.00000000 sec
D20                   0.00689655 sec
TD0                           1
SFO1                125.7459712 MHz
NUC1                       13C
P1                       10.00 usec
P2                       20.00 usec
PLW1               121.36000061 W
SFO2                500.0350001 MHz
NUC2                       1H
CPDPRG[2                waltz65
PCPD2                    80.00 usec
PLW2                16.34900093 W
PLW12                0.34647381 W

F2 - Processing parameters
SI                        32768
SF                  125.7332646 MHz
WDW                          EM
SSB                           0
LB                        1.00 Hz
GB                            0
PC                        1.40
```

4-Chloro-6-(dimethylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 20

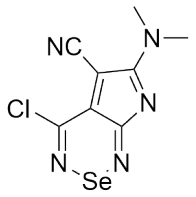



```
Current Data Parameters
NAME                  NMR 300
EXPNO                     193
PROCNO                      1

F2 - Acquisition Parameters
Date_                20230425
Time                    19.12 h
INSTRUM                  spect
PROBHD     Z104275_0375 (
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  6009.615 Hz
FIDRES               0.183399 Hz
AQ                   5.4525952 sec
RG                      201.81
DW                      83.200 usec
DE                      13.19 usec
TE                      -9.5 K
D1                1.00000000 sec
TD0                         1
SFO1              300.1318533 MHz
NUC1                       1H
P0                      4.67 usec
P1                     14.00 usec
PLW1               7.09999990 W

F2 - Processing parameters
SI                      65536
SF                300.1300073 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
PC                      1.00
```

4-Chloro-6-(dimethylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 20

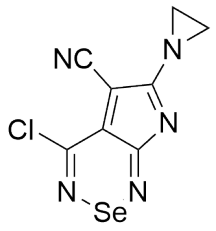



```
Current Data Parameters
NAME                  NMR 300
EXPNO                     203
PROCNO                      1

F2 - Acquisition Parameters
Date_                20230513
Time                   10.46 h
INSTRUM                 spect
PROBHD    Z104275_0375 (
PULPROG                 jmod
TD                     65536
SOLVENT                TFA-d
NS                     13312
DS                         4
SWH                18115.941 Hz
FIDRES              0.552855 Hz
AQ                  1.8087935 sec
RG                     201.81
DW                     27.600 usec
DE                      6.50 usec
TE                     296.1 K
CNST2             145.0000000
CNST11              1.0000000
D1                  2.00000000 sec
D20                 0.00689655 sec
TD0                         1
SFO1               75.4752953 MHz
NUC1                      13C
P1                     10.00 usec
P2                     20.00 usec
PLW1              45.00000000 W
SFO2              300.1312005 MHz
NUC2                      1H
CPDPRG[2              waltz65
PCPD2                  90.00 usec
PLW2               7.09999990 W
PLW12              0.17180000 W

F2 - Processing parameters
SI                      32768
SF                75.4677485 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40
```

4-(Aziridin-1-yl)-6-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 21



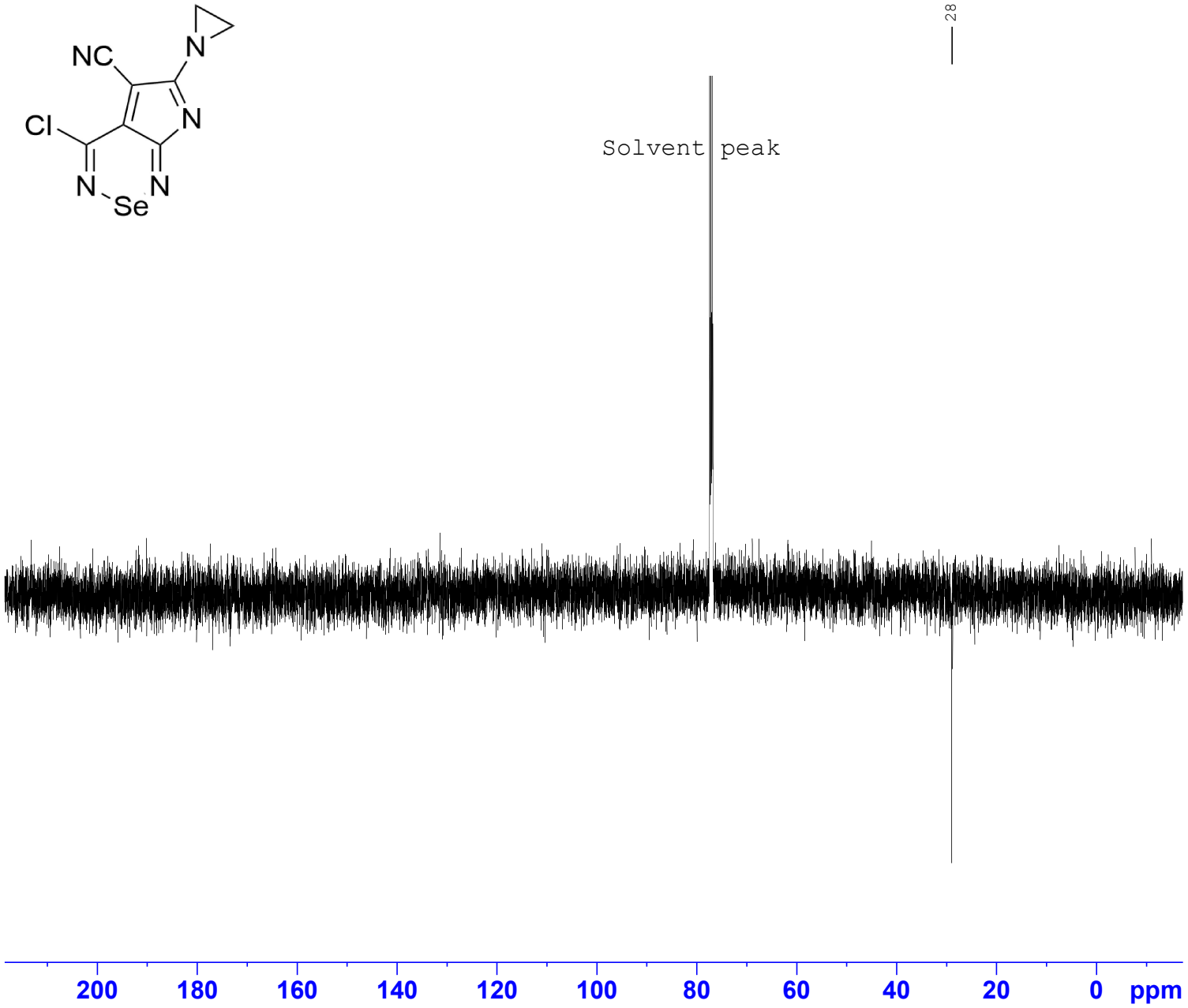
Current Data Parameters
NAME nmr 500
EXPNO 141
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230808
Time 15.13 h
INSTRUM spect
PROBHD Z113652_0078 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 456
DW 50.000 usec
DE 13.55 usec
TE 353.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.0360877 MHz
NUC1 1H
P0 4.00 usec
P1 12.00 usec
PLW1 16.34900093 W

F2 - Processing parameters
SI 65536
SF 500.0330000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4-(Aziridin-1-yl)-6-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 21

Very poor solubility, 6 C (s) missing

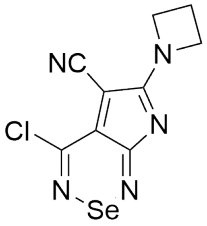



```
Current Data Parameters
NAME                  nmr 500
EXPNO                     143
PROCNO                      1

F2 - Acquisition Parameters
Date_                20230808
Time                    17.31 h
INSTRUM                  spect
PROBHD   Z113652_0078 (
PULPROG                  jmod
TD                      65536
SOLVENT                 CDCl3
NS                       2581
DS                          4
SWH                 29761.904 Hz
FIDRES               0.908261 Hz
AQ                   1.1010048 sec
RG                       2050
DW                     16.800 usec
DE                      6.50 usec
TE                      353.5 K
CNST2               145.0000000
CNST11                1.0000000
D1                    2.00000000 sec
D20                   0.00689655 sec
TD0                         1
SFO1                125.7459712 MHz
NUC1                       13C
P1                     10.00 usec
P2                     20.00 usec
PLW1               121.36000061 W
SFO2                500.0350001 MHz
NUC2                       1H
CPDPRG[2                waltz65
PCPD2                  80.00 usec
PLW2                16.34900093 W
PLW12                0.34647381 W

F2 - Processing parameters
SI                         32768
SF                  125.7333760 MHz
WDW                           EM
SSB                            0
LB                      1.00 Hz
GB                             0
PC                      1.40
```

6-(Azetidin-1-yl)-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 22

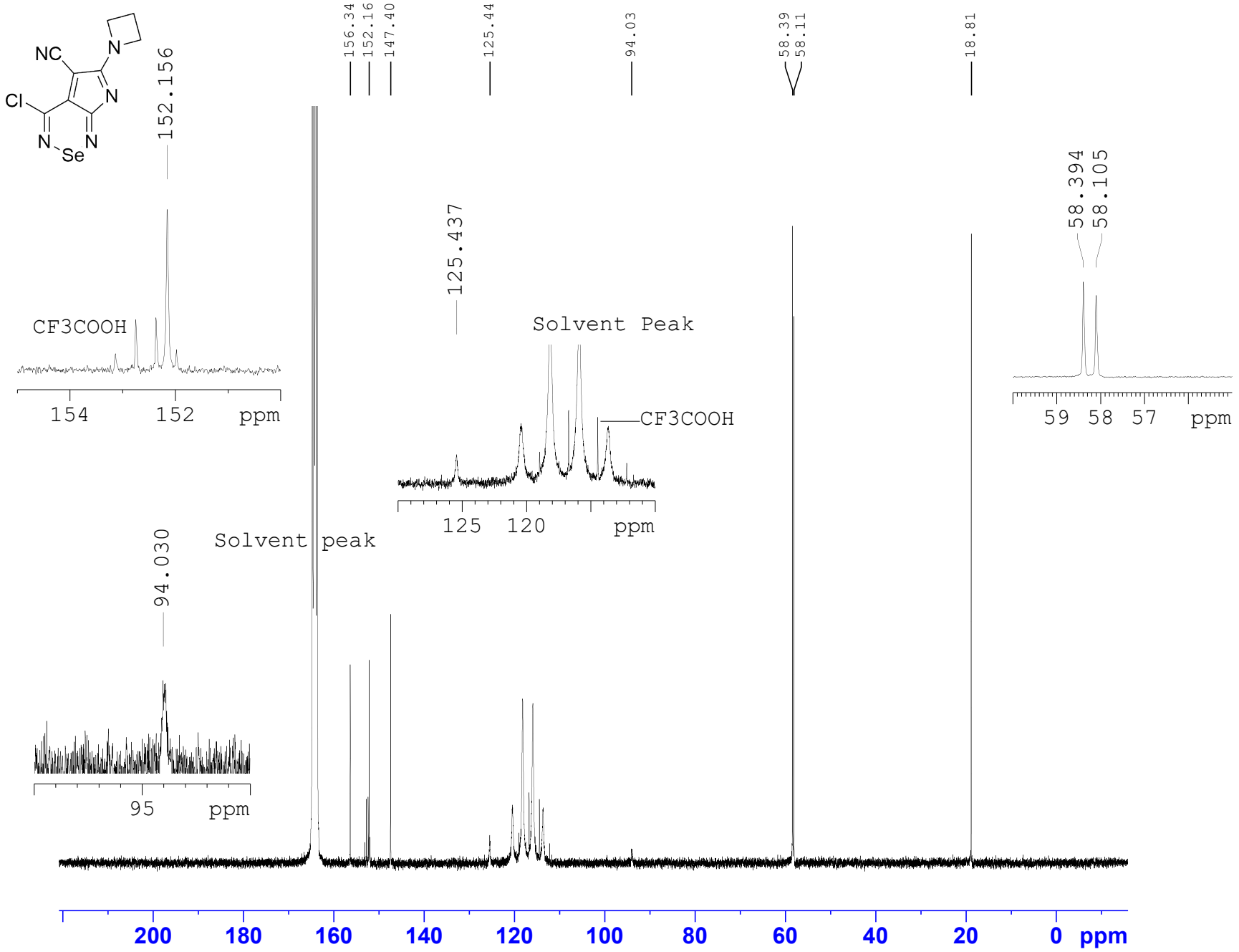


Current Data Parameters
NAME nmr 500
EXPNO 54
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230328
Time 22.52 h
INSTRUM spect
PROBHD Z113652_0078 (
PULPROG zg30
TD 65536
SOLVENT TFA2
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 13.55 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
SFO1 500.0360877 MHz
NUC1 1H
P0 4.00 usec
P1 12.00 usec
PLW1 16.34900093 W

F2 - Processing parameters
SI 65536
SF 500.0330657 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

6-(Azetidin-1-yl)-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 22



Current Data Parameters

NAME	nmr 500
EXPNO	56
PROCNO	1

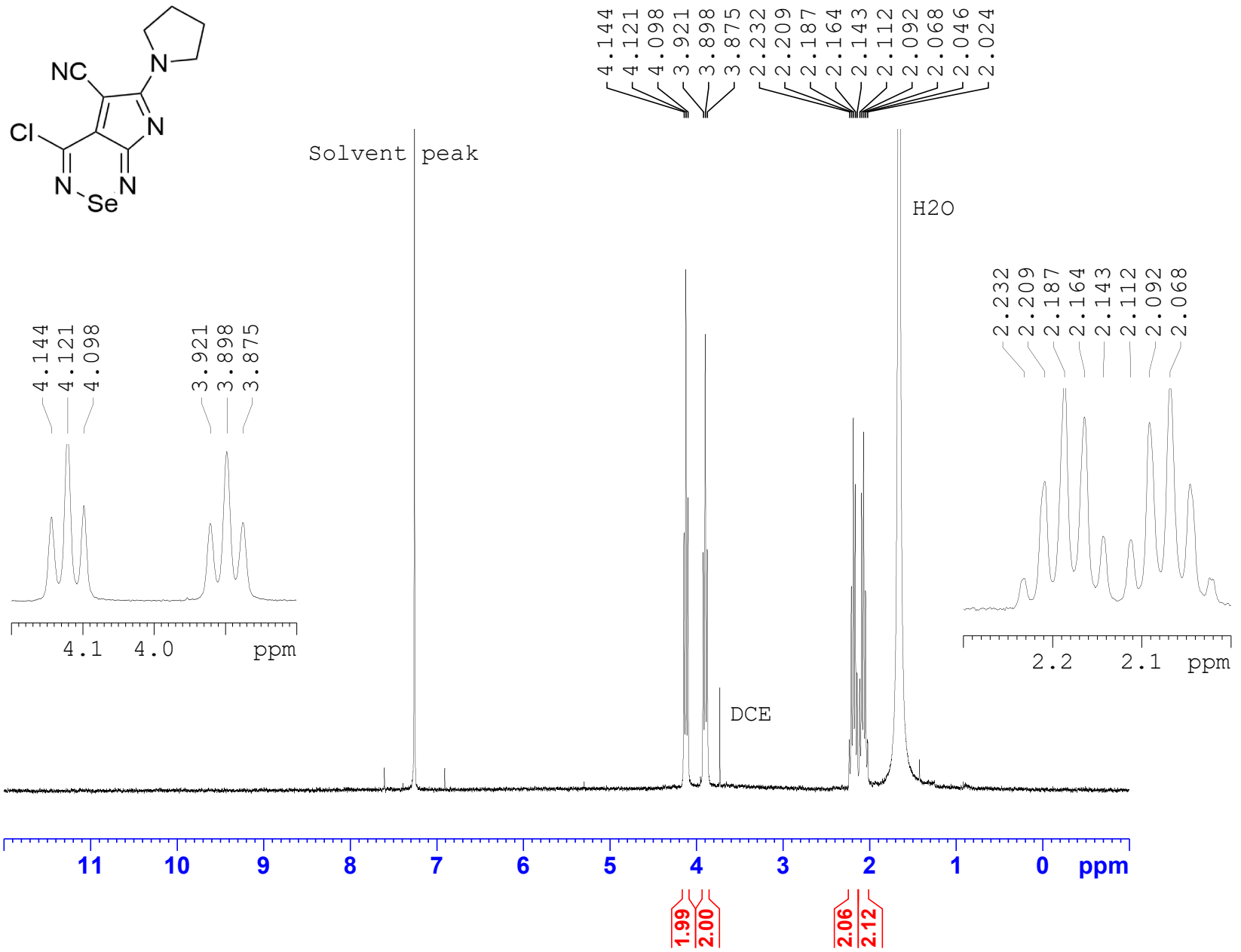
F2 - Acquisition Parameters

Date_	20230329
Time	8.46 h
INSTRUM	spect
PROBHD	Z113652_0078 (
PULPROG	jmod
TD	65536
SOLVENT	TFA2
NS	10240
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	1.1010048 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	299.0 K
CNST2	145.0000000
CNST11	1.0000000
D1	2.00000000 sec
D20	0.00689655 sec
TD0	1
SFO1	125.7459712 MHz
NUC1	13C
P1	10.00 usec
P2	20.00 usec
PLW1	121.36000061 W
SFO2	500.0350001 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	80.00 usec
PLW2	16.34900093 W
PLW12	0.34647381 W

F2 - Processing parameters

SI	32768
SF	125.7330836 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4-Chloro-6-(pyrrolidin-1-yl)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 23

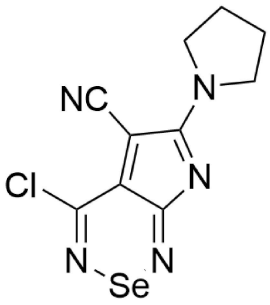



```
Current Data Parameters
NAME                  NMR 300
EXPNO                     123
PROCNO                      1

F2 - Acquisition Parameters
Date_               20221105
Time                  18.40 h
INSTRUM                spect
PROBHD    Z104275_0375 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        64
DS                         2
SWH                6009.615 Hz
FIDRES            0.183399 Hz
AQ                5.4525952 sec
RG                   201.81
DW                   83.200 usec
DE                    6.50 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                        1
SFO1           300.1318533 MHz
NUC1                      1H
P1                   14.00 usec
PLW1            7.85570002 W

F2 - Processing parameters
SI                     65536
SF             300.1300079 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```

4-Chloro-6-(pyrrolidin-1-yl)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 23

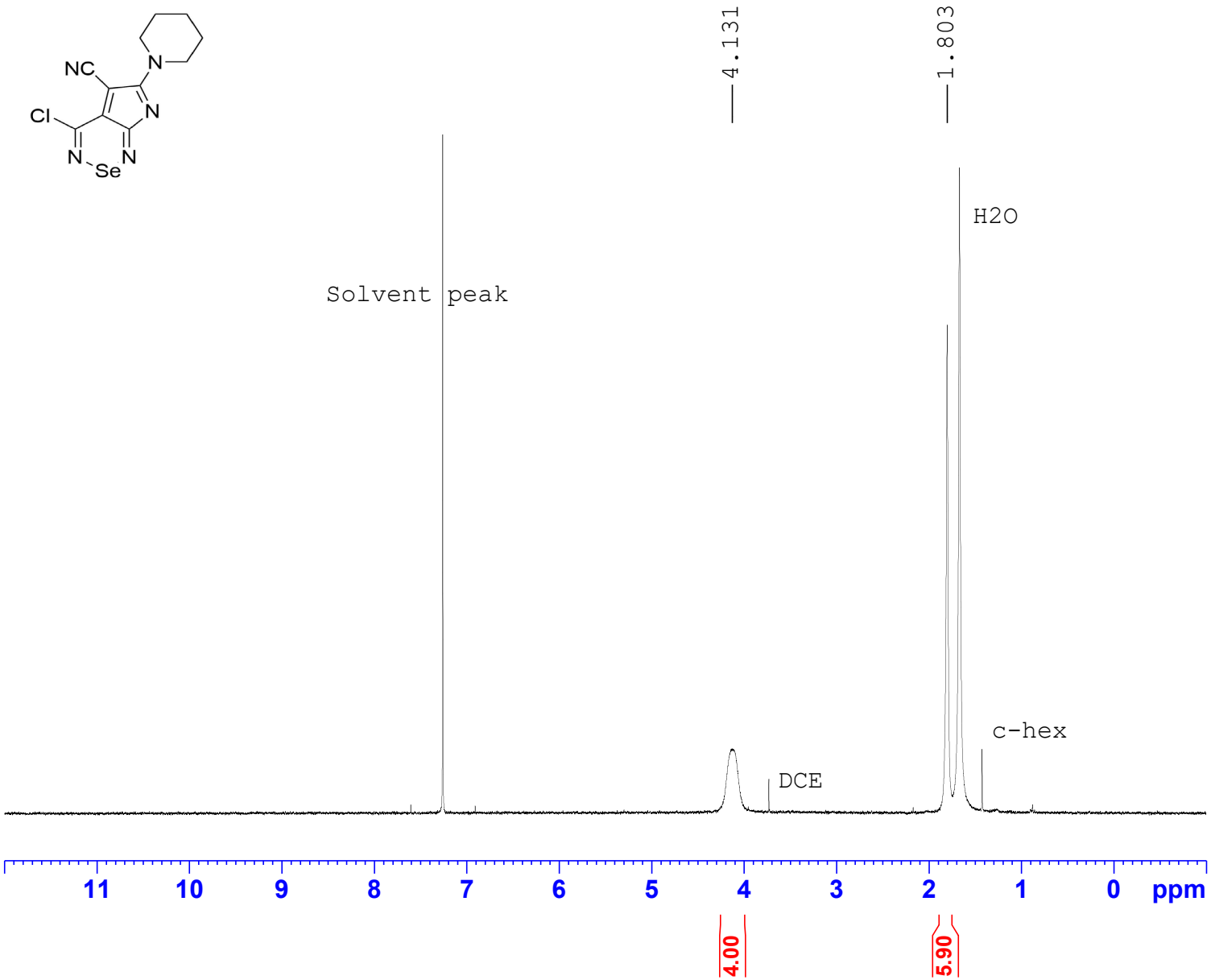


Current Data Parameters
NAME nmr 500
EXPNO 37
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230312
Time 8.38 h
INSTRUM spect
PROBHD Z113652_0078 (
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 14336
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 299.6 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 125.7459712 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 121.36000061 W
SFO2 500.0350001 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 16.34900093 W
PLW12 0.34647381 W

F2 - Processing parameters
SI 32768
SF 125.7333803 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Chloro-6-(piperidin-1-yl)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 24

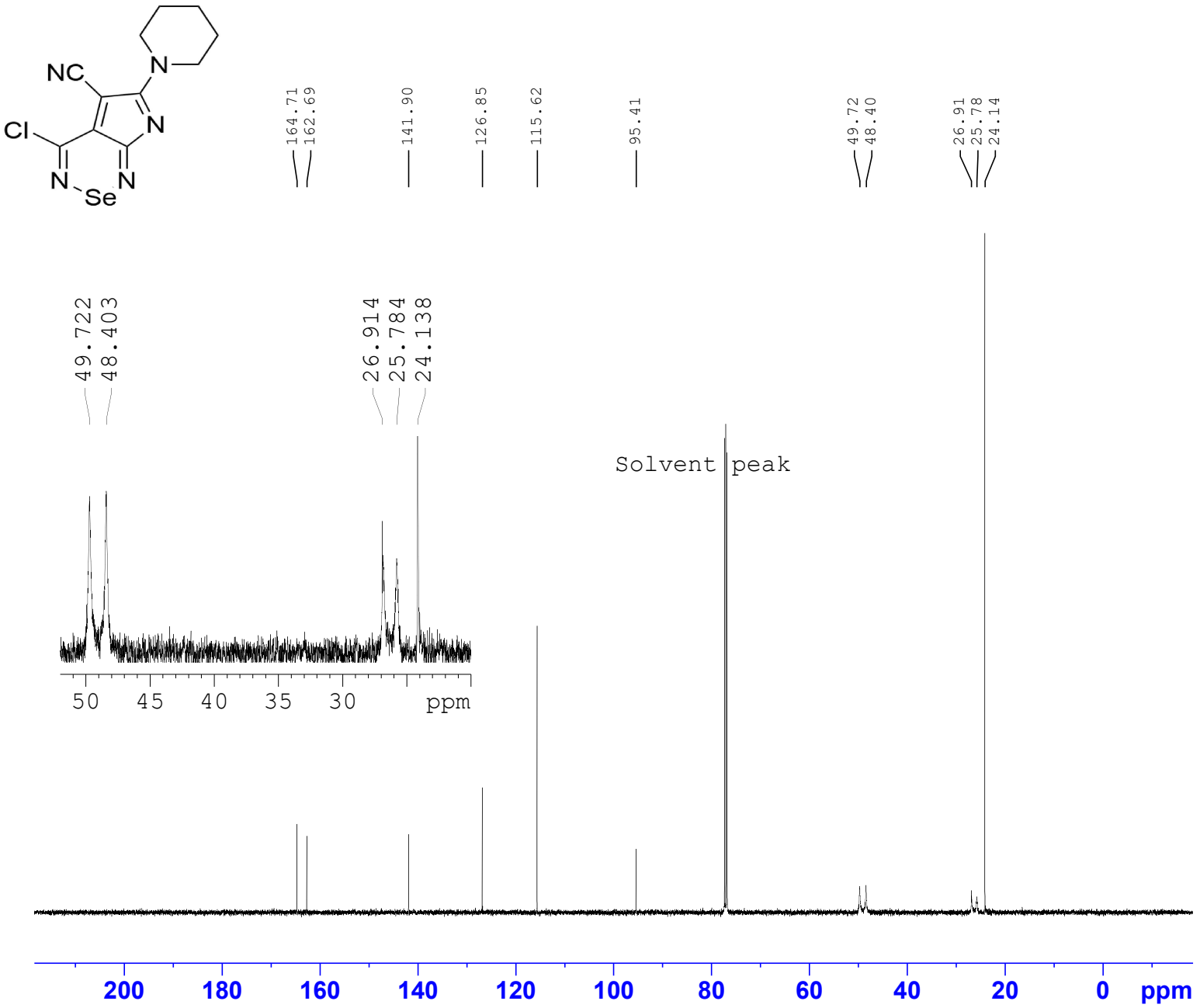


Current Data Parameters
NAME NMR 300
EXPNO 135
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221116
Time 18.58 h
INSTRUM spect
PROBHD Z104275_0375 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 201.81
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 14.00 usec
PLW1 7.85570002 W

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4-Chloro-6-(piperidin-1-yl)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 24

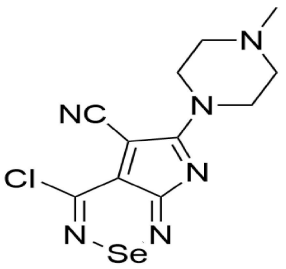



```
Current Data Parameters
NAME                  nmr 500
EXPNO                      35
PROCNO                      1

F2 - Acquisition Parameters
Date_               20230306
Time                  20.00 h
INSTRUM                spect
PROBHD    Z113652_0078 (
PULPROG                 jmod
TD                     65536
SOLVENT                CDCl3
NS                      4352
DS                         4
SWH               29761.904 Hz
FIDRES             0.908261 Hz
AQ                 1.1010048 sec
RG                      2050
DW                   16.800 usec
DE                    6.50 usec
TE                    297.6 K
CNST2           145.0000000
CNST11            1.0000000
D1              2.00000000 sec
D20             0.00689655 sec
TD0                        1
SFO1           125.7459712 MHz
NUC1                    13C
P1                    10.00 usec
P2                    20.00 usec
PLW1          121.36000061 W
SFO2           500.0350001 MHz
NUC2                    1H
CPDPRG[2           waltz65
PCPD2                 80.00 usec
PLW2           16.34900093 W
PLW12           0.34647381 W

F2 - Processing parameters
SI                     32768
SF            125.7333979 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                      1.40
```

4-Chloro-6-(4-methylpiperazin-1-yl)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 25

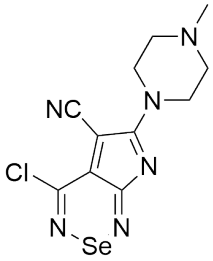


Current Data Parameters
NAME NMR 300
EXPNO 153
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230105
Time 19.34 h
INSTRUM spect
PROBHD Z104275_0375 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 201.81
DW 83.200 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 14.00 usec
PLW1 7.85570002 W

F2 - Processing parameters
SI 65536
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4-Chloro-6-(4-methylpiperazin-1-yl)[2,3-c][1,2,6]selenadiazine-5-carbonitrile 25



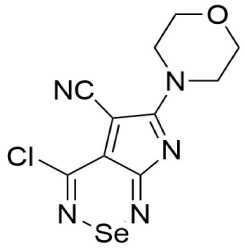
BRUKER

Current Data Parameters
NAME NMR 300
EXPNO 192
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230424
Time 8.57 h
INSTRUM spect
PROBHD Z104275_0375 (
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 10240
DS 4
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 1.8087935 sec
RG 201.81
DW 27.600 usec
DE 6.50 usec
TE -9.5 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 75.4752953 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 45.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 7.09999990 W
PLW12 0.17180000 W

F2 - Processing parameters
SI 32768
SF 75.4677388 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Chloro-6-morpholinopyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 26

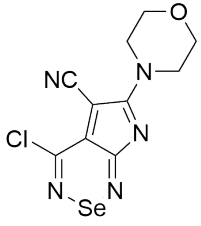



```
Current Data Parameters
NAME                  NMR 300
EXPNO                     119
PROCNO                      1

F2 - Acquisition Parameters
Date_               20221103
Time                   17.35 h
INSTRUM                spect
PROBHD    Z104275_0375 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 6009.615 Hz
FIDRES              0.183399 Hz
AQ                5.4525952 sec
RG                    201.81
DW                   83.200 usec
DE                    6.50 usec
TE                   298.0 K
D1                1.00000000 sec
TD0                        1
SFO1            300.1318533 MHz
NUC1                      1H
P1                   14.00 usec
PLW1              7.85570002 W

F2 - Processing parameters
SI                     65536
SF              300.1300073 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```

4-Chloro-6-morpholinopyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 26

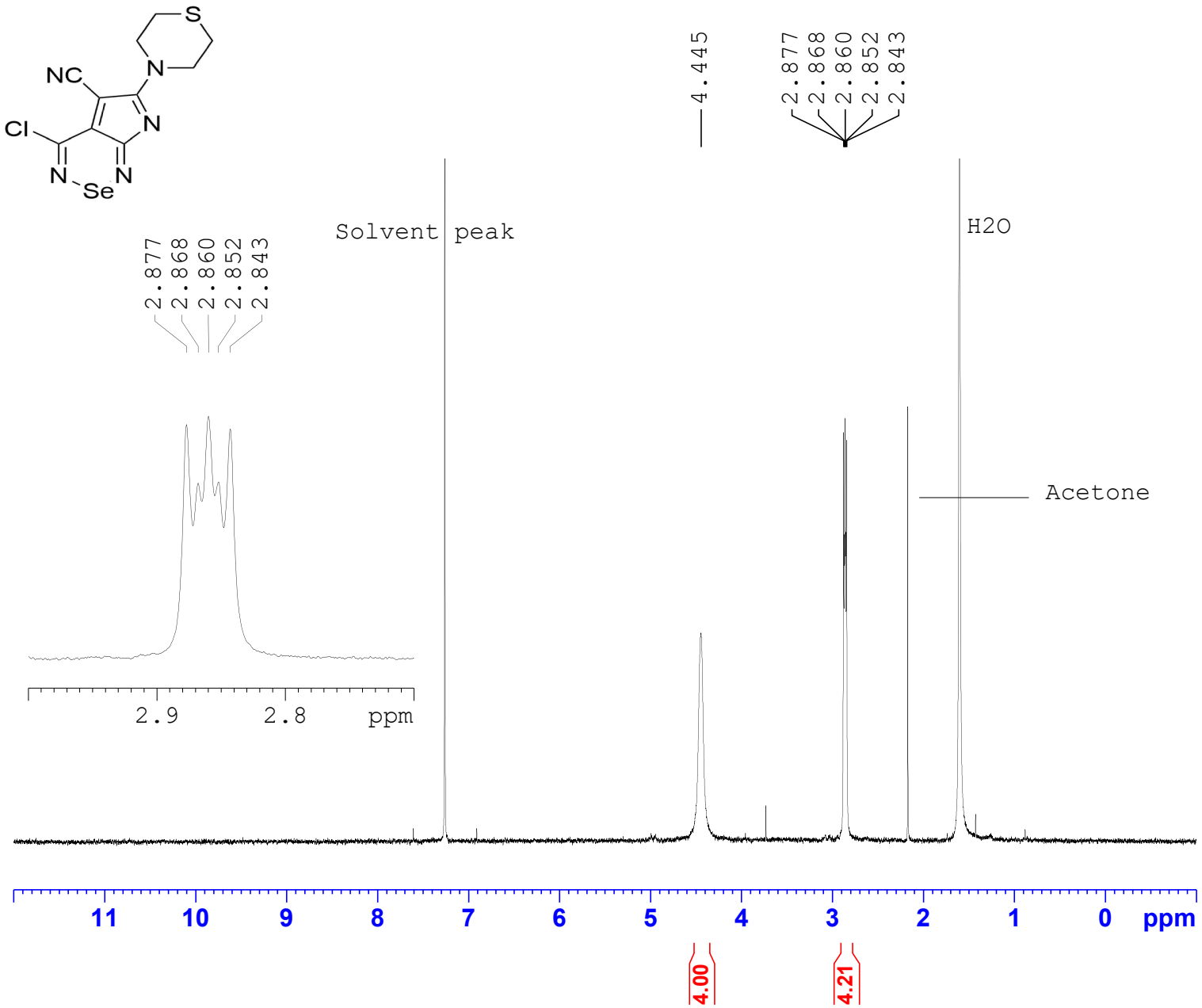



```
Current Data Parameters
NAME                  nmr 500
EXPNO                      43
PROCNO                      1

F2 - Acquisition Parameters
Date_               20230320
Time                    9.04 h
INSTRUM                spect
PROBHD    Z113652_0078 (
PULPROG                 jmod
TD                     65536
SOLVENT                CDCl3
NS                     13312
DS                         4
SWH               29761.904 Hz
FIDRES             0.908261 Hz
AQ                 1.1010048 sec
RG                      2050
DW                    16.800 usec
DE                     6.50 usec
TE                    299.0 K
CNST2           145.0000000
CNST11            1.0000000
D1                2.00000000 sec
D20               0.00689655 sec
TD0                        1
SFO1            125.7459712 MHz
NUC1                    13C
P1                    10.00 usec
P2                    20.00 usec
PLW1           121.36000061 W
SFO2            500.0350001 MHz
NUC2                    1H
CPDPRG[2           waltz65
PCPD2                 80.00 usec
PLW2           16.34900093 W
PLW12           0.34647381 W

F2 - Processing parameters
SI                     32768
SF              125.7333803 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                      1.40
```

4-Chloro-6-thiomorpholinopyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 27

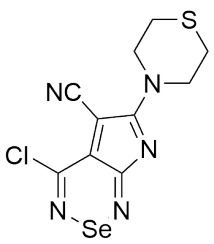



```
Current Data Parameters
NAME                  NMR 300
EXPNO                     139
PROCNO                      1

F2 - Acquisition Parameters
Date_              20221121
Time                  11.37 h
INSTRUM                spect
PROBHD    Z104275_0375 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                6009.615 Hz
FIDRES            0.183399 Hz
AQ                5.4525952 sec
RG                   201.81
DW                   83.200 usec
DE                    6.50 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                        1
SFO1           300.1318533 MHz
NUC1                      1H
P1                    14.00 usec
PLW1            7.85570002 W

F2 - Processing parameters
SI                     65536
SF             300.1300073 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
```

4-Chloro-6-thiomorpholinopyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 27

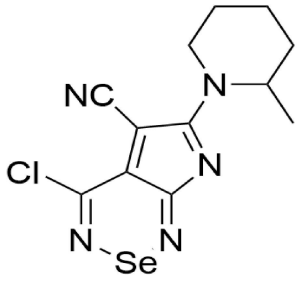



```
Current Data Parameters
NAME                  NMR 300
EXPNO                     185
PROCNO                      1

F2 - Acquisition Parameters
Date_              20230316
Time                    9.29 h
INSTRUM                spect
PROBHD    Z104275_0375 (
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                     12288
DS                         4
SWH               18115.941 Hz
FIDRES             0.552855 Hz
AQ                 1.8087935 sec
RG                     20.09
DW                    27.600 usec
DE                     6.50 usec
TE                    -9.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1              75.4752953 MHz
NUC1                     13C
P0                     3.33 usec
P1                    10.00 usec
PLW1              45.00000000 W
SFO2             300.1312005 MHz
NUC2                     1H
CPDPRG[2             waltz65
PCPD2                  90.00 usec
PLW2               7.09999990 W
PLW12              0.17180000 W
PLW13              0.08641500 W

F2 - Processing parameters
SI                         32768
SF                75.4677393 MHz
WDW                           EM
SSB                            0
LB                      1.00 Hz
GB                             0
PC                      1.40
```

4-Chloro-6-(2-methylpiperidin-1-yl)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 28

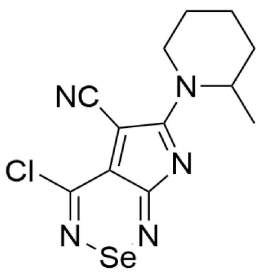



```
Current Data Parameters
NAME                  nmr 500
EXPNO                     122
PROCNO                      1

F2 - Acquisition Parameters
Date_                20230730
Time                   23.28 h
INSTRUM                 spect
PROBHD    Z113652_0078 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                       144
DW                    50.000 usec
DE                    13.55 usec
TE                    299.3 K
D1                 1.00000000 sec
TD0                        1
SFO1            500.0360877 MHz
NUC1                      1H
P0                     4.00 usec
P1                    12.00 usec
PLW1           16.34900093 W

F2 - Processing parameters
SI                     65536
SF              500.0330125 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

4-Chloro-6-(2-methylpiperidin-1-yl)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 28



Current Data Parameters

NAME	nmr 500
EXPNO	123
PROCNO	1

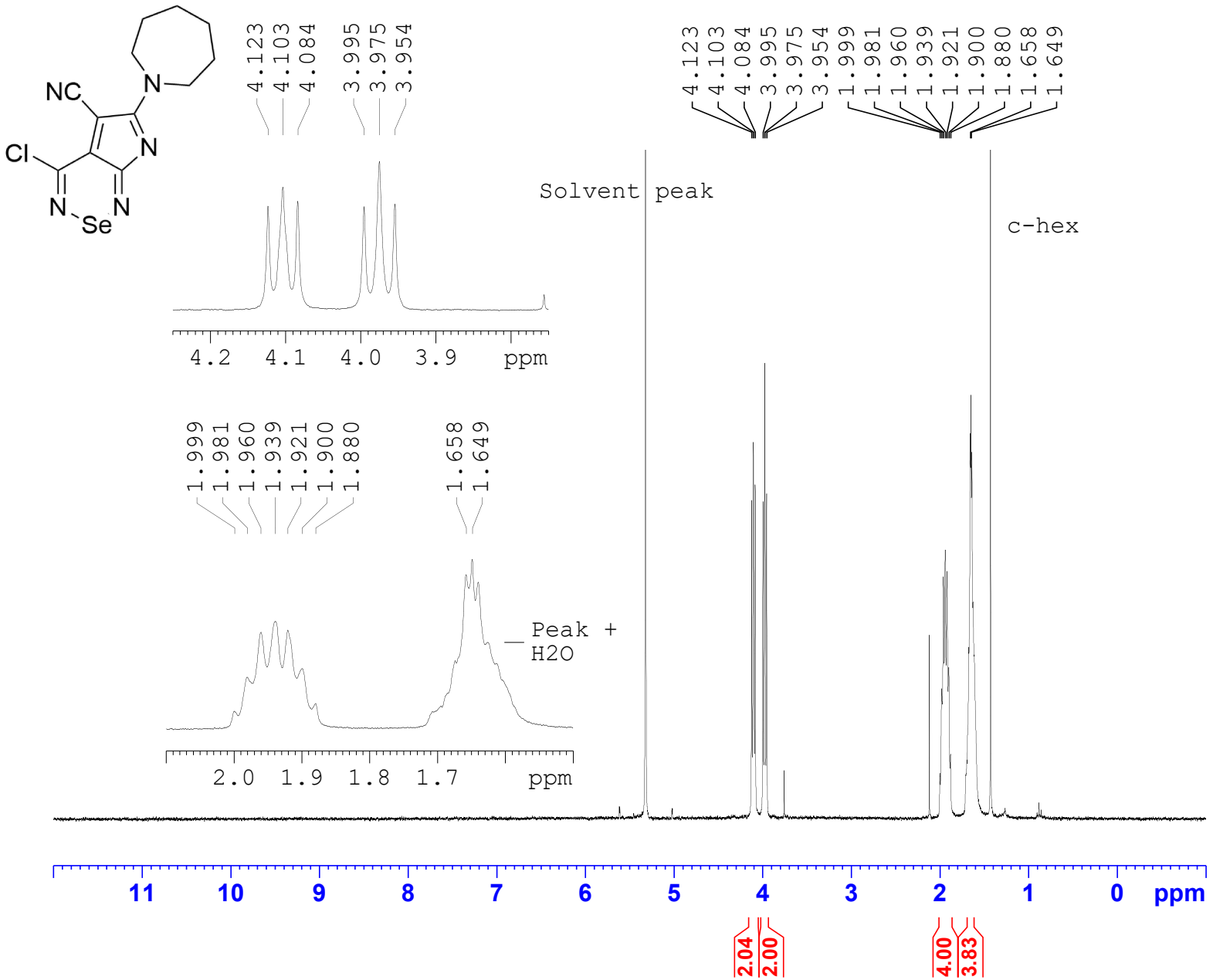
F2 - Acquisition Parameters

Date_	20230731
Time	8.30 h
INSTRUM	spect
PROBHD	Z113652_0078 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10240
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	1.1010048 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	301.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	125.7459712 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
PLW1	121.36000061 W
SFO2	500.0350001 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	80.00 usec
PLW2	16.34900093 W
PLW12	0.34647381 W
PLW13	0.17365260 W

F2 - Processing parameters

SI	32768
SF	125.7333809 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

6-(Azepan-1-yl)-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 29



Current Data Parameters

NAME	NMR 300
EXPNO	137
PROCNO	1

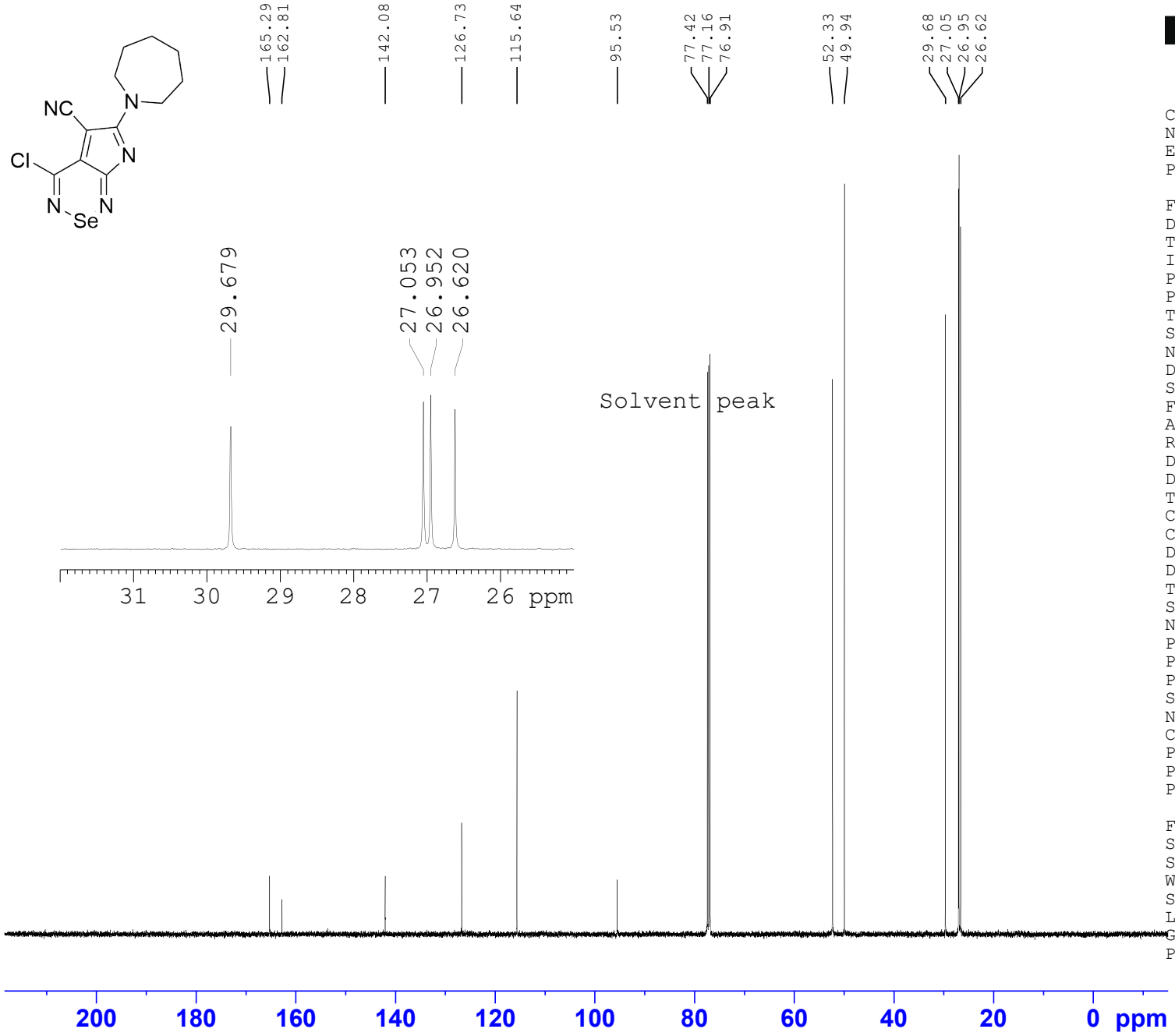
F2 - Acquisition Parameters

Date_	20221117
Time	18.50 h
INSTRUM	spect
PROBHD	Z104275_0375 (
PULPROG	zg30
TD	65536
SOLVENT	CD2Cl2
NS	16
DS	2
SWH	6009.615 Hz
FIDRES	0.183399 Hz
AQ	5.4525952 sec
RG	201.81
DW	83.200 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
SFO1	300.1318533 MHz
NUC1	1H
P1	14.00 usec
PLW1	7.85570002 W

F2 - Processing parameters

SI	65536
SF	300.1300115 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

6-(Azepan-1-yl)-4-chloropyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 29

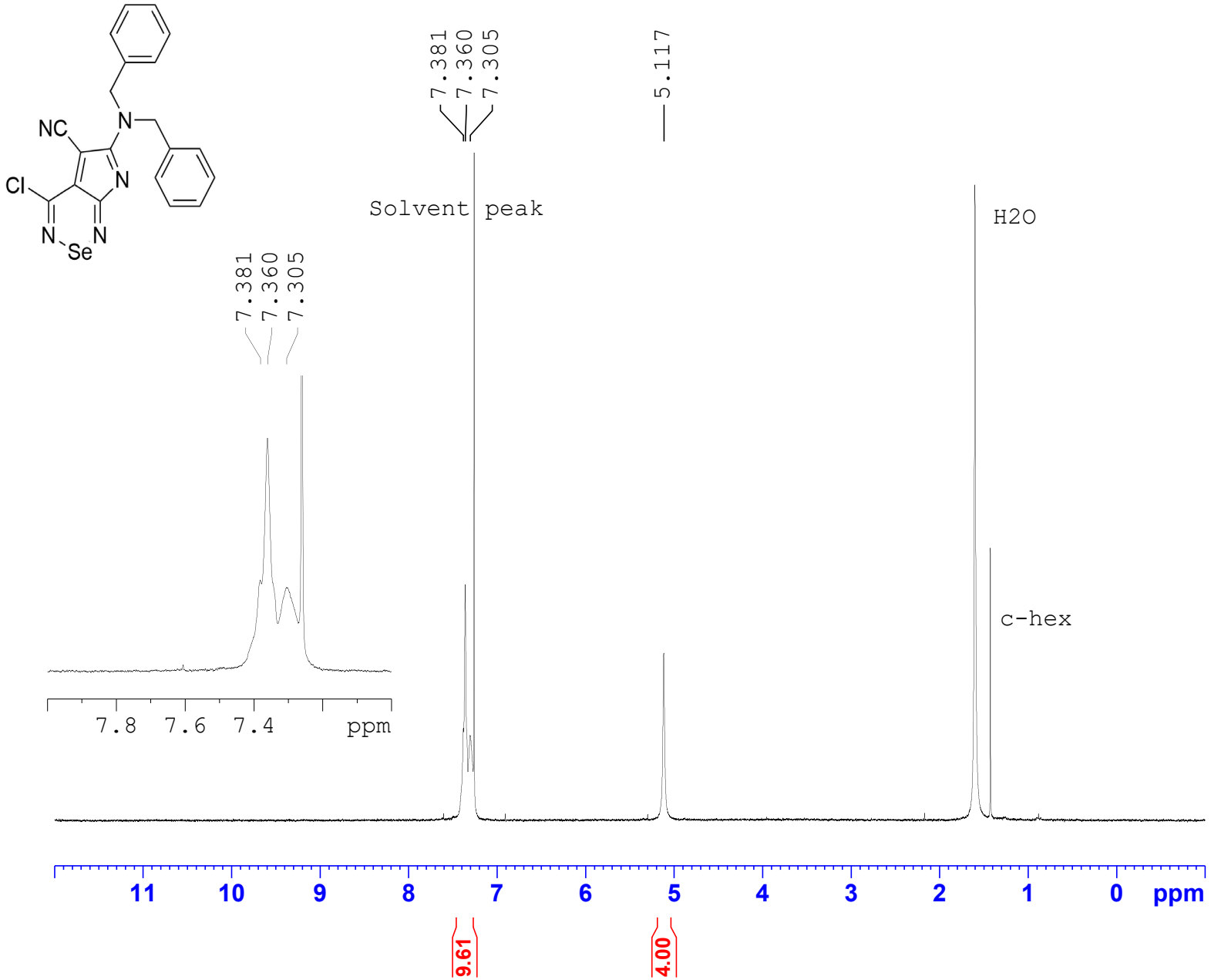


Current Data Parameters
NAME nmr 500
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230319
Time 21.09 h
INSTRUM spect
PROBHD Z113652_0078 (
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 9216
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.7 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 125.7459712 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 121.36000061 W
SFO2 500.0350001 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 16.34900093 W
PLW12 0.34647381 W

F2 - Processing parameters
SI 32768
SF 125.7333831 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Chloro-6-(dibenzylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 30

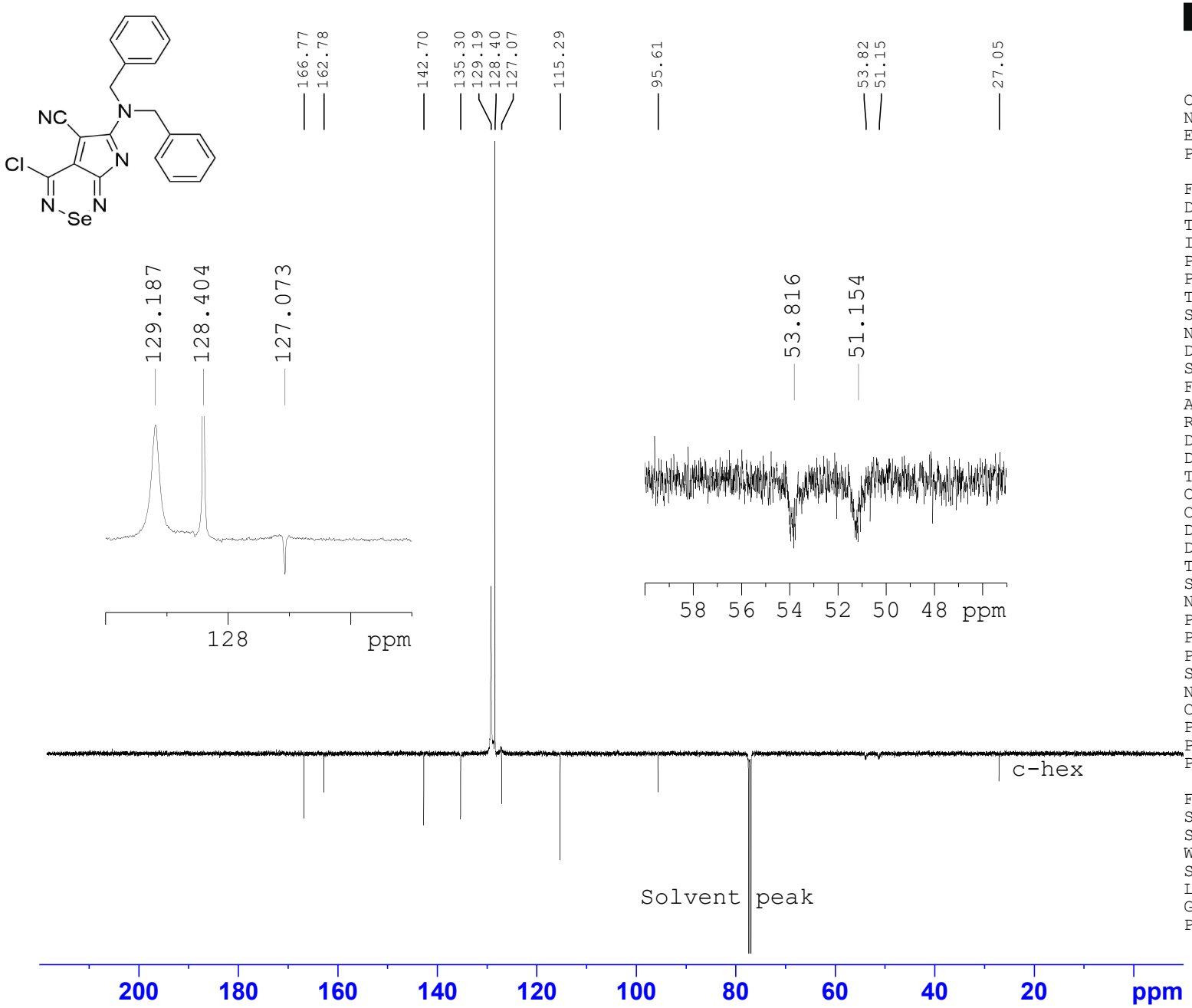



```
Current Data Parameters
NAME                  NMR 300
EXPNO                     103
PROCNO                      1

F2 - Acquisition Parameters
Date_                20221025
Time                   16.50 h
INSTRUM                 spect
PROBHD    Z104275_0375 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 6009.615 Hz
FIDRES              0.183399 Hz
AQ                  5.4525952 sec
RG                     201.81
DW                     83.200 usec
DE                      6.50 usec
TE                     298.0 K
D1                 1.00000000 sec
TD0                         1
SFO1           300.1318533 MHz
NUC1                       1H
P1                     14.00 usec
PLW1            7.85570002 W

F2 - Processing parameters
SI                     65536
SF             300.1300073 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

4-Chloro-6-(dibenzylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 30

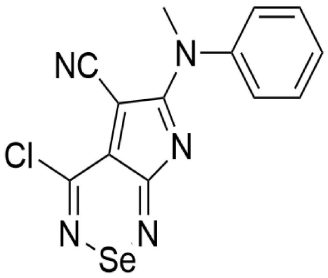


Current Data Parameters
NAME nmr 500
EXPNO 62
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230412
Time 7.02 h
INSTRUM spect
PROBHD Z113652_0078 (
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 12288
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 300.5 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 125.7459712 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 121.36000061 W
SFO2 500.0350001 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 16.34900093 W
PLW12 0.34647381 W

F2 - Processing parameters
SI 32768
SF 125.7333820 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Chloro-6-[methyl(phenyl)amino]pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 31



Current Data Parameters

NAME	NMR 300
EXPNO	159
PROCNO	1

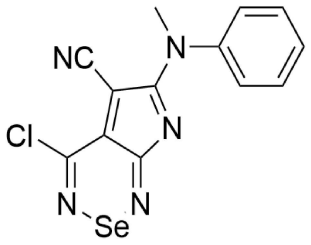
F2 - Acquisition Parameters

Date_	20230124
Time	17.17 h
INSTRUM	spect
PROBHD	Z104275_0375 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6009.615 Hz
FIDRES	0.183399 Hz
AQ	5.4525952 sec
RG	201.81
DW	83.200 usec
DE	6.50 usec
TE	295.7 K
D1	1.00000000 sec
TD0	1
SFO1	300.1318533 MHz
NUC1	1H
P1	14.00 usec
PLW1	7.85570002 W

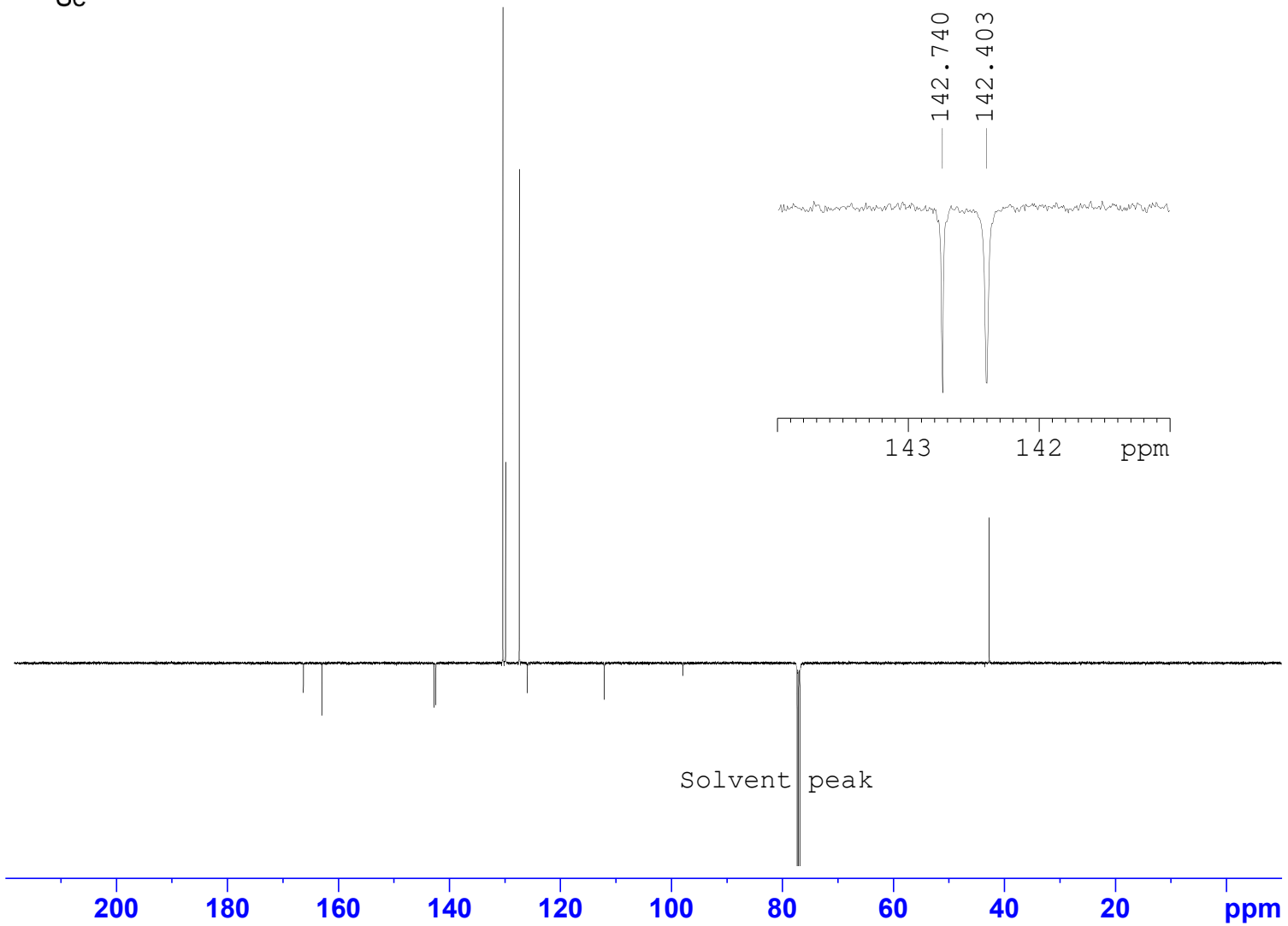
F2 - Processing parameters

SI	65536
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4-Chloro-6-[methyl(phenyl)amino]pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 31



166.26
162.95
142.74
142.40
130.32
129.82
127.36
125.90
112.05
97.87
77.29
77.04
76.78
43.46
42.69



Current Data Parameters

NAME	nmr 500
EXPNO	24
PROCNO	1

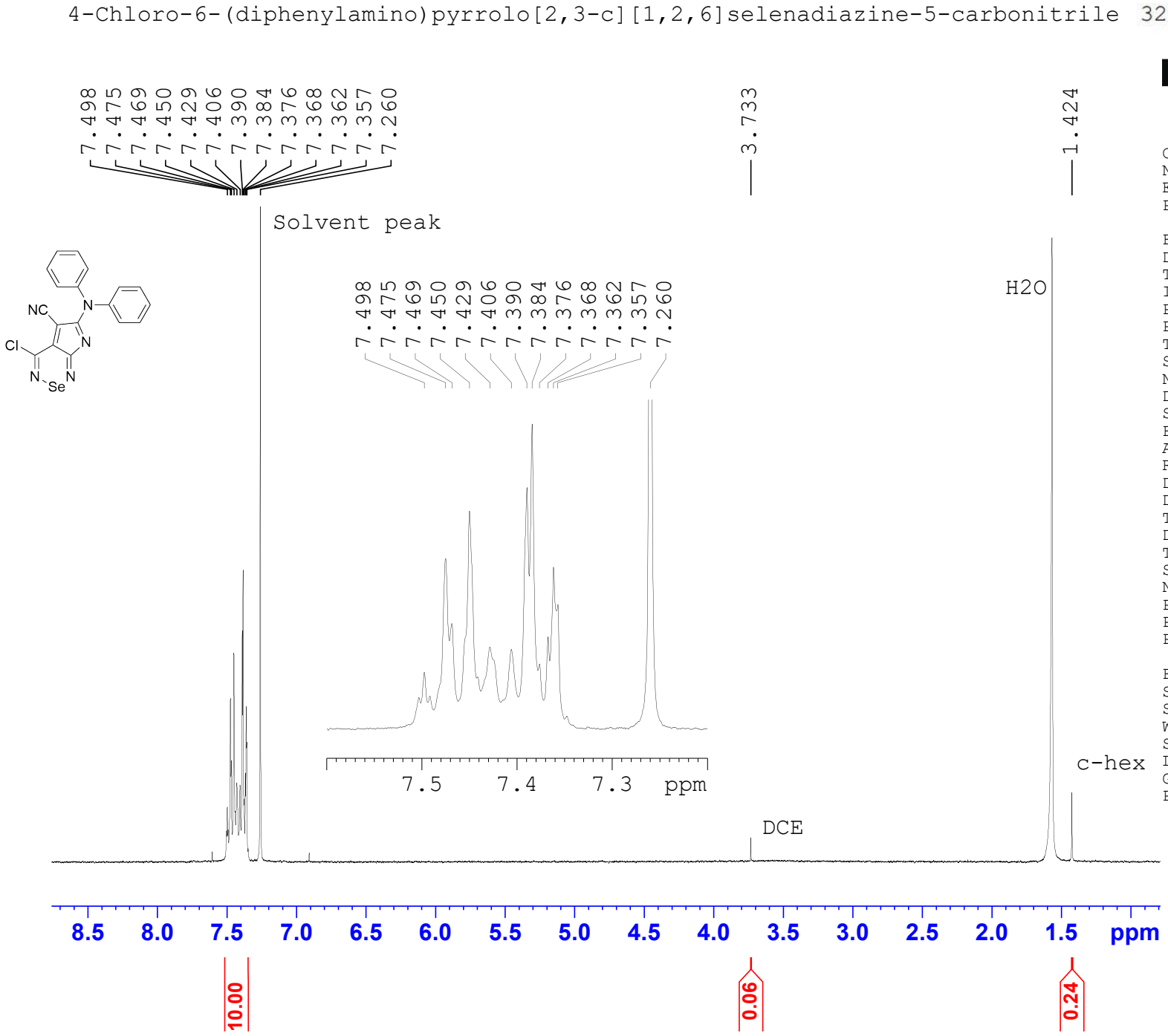
F2 - Acquisition Parameters

Date_	20230201
Time	8.19 h
INSTRUM	spect
PROBHD	Z113652_0078 (
PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	6144
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	1.1010048 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	298.2 K
CNST2	145.0000000
CNST11	1.0000000
D1	6.00000000 sec
D20	0.00689655 sec
TD0	1
SFO1	125.7459712 MHz
NUC1	13C
P1	10.00 usec
P2	20.00 usec
PLW1	121.36000061 W
SFO2	500.0350001 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	80.00 usec
PLW2	16.34900093 W
PLW12	0.34647381 W

F2 - Processing parameters

SI	32768
SF	125.7333979 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4-Chloro-6-(diphenylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 32

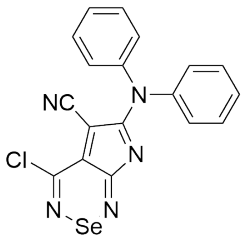



```
Current Data Parameters
NAME                 NMR 300
EXPNO                    174
PROCNO                     1

F2 - Acquisition Parameters
Date_              20230227
Time                 15.31 h
INSTRUM              spect
PROBHD     Z104275_0375 (
PULPROG              zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                5.4525952 sec
RG                   201.81
DW                   83.200 usec
DE                   13.19 usec
TE                   294.3 K
D1              1.00000000 sec
TD0                      1
SFO1           300.1318533 MHz
NUC1                    1H
P0                    4.67 usec
P1                   14.00 usec
PLW1            7.09999990 W

F2 - Processing parameters
SI                   65536
SF             300.1300073 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

4-Chloro-6-(diphenylamino)pyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 32



Current Data Parameters

NAME	NMR 300
EXPNO	175
PROCNO	1

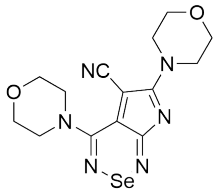
F2 - Acquisition Parameters

Date_	20230228
Time	5.25 h
INSTRUM	spect
PROBHD	Z104275_0375 (
PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	6144
DS	4
SWH	18115.941 Hz
FIDRES	0.552855 Hz
AQ	1.8087935 sec
RG	201.81
DW	27.600 usec
DE	6.50 usec
TE	295.3 K
CNST2	145.0000000
CNST11	1.0000000
D1	6.00000000 sec
D20	0.00689655 sec
TD0	1
SFO1	75.4752953 MHz
NUC1	13C
P1	10.00 usec
P2	20.00 usec
PLW1	45.00000000 W
SFO2	300.1312005 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	90.00 usec
PLW2	7.09999990 W
PLW12	0.17180000 W

F2 - Processing parameters

SI	32768
SF	75.4677396 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4,6-Dimorpholinopyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 33

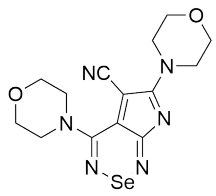


Current Data Parameters
NAME NMR 300
EXPNO 198
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230430
Time 15.31 h
INSTRUM spect
PROBHD Z104275_0375 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 201.81
DW 83.200 usec
DE 13.19 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 7.09999990 W

F2 - Processing parameters
SI 65536
SF 300.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4,6-Dimorpholinopyrrolo[2,3-c][1,2,6]selenadiazine-5-carbonitrile 33

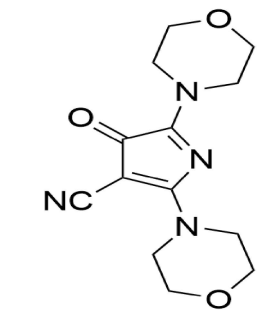


Current Data Parameters
NAME NMR 300
EXPNO 199
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230501
Time 13.02 h
INSTRUM spect
PROBHD Z104275_0375 (
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 20000
DS 4
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 1.8087935 sec
RG 201.81
DW 27.600 usec
DE 6.50 usec
TE 295.5 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 75.4752953 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 45.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 7.09999990 W
PLW12 0.17180000 W

F2 - Processing parameters
SI 32768
SF 75.4677396 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2,5-Dimorpholino-3-oxo-3H-pyrrole-4-carbonitrile 34



Current Data Parameters

NAME	NMR 300
EXPNO	132
PROCNO	1

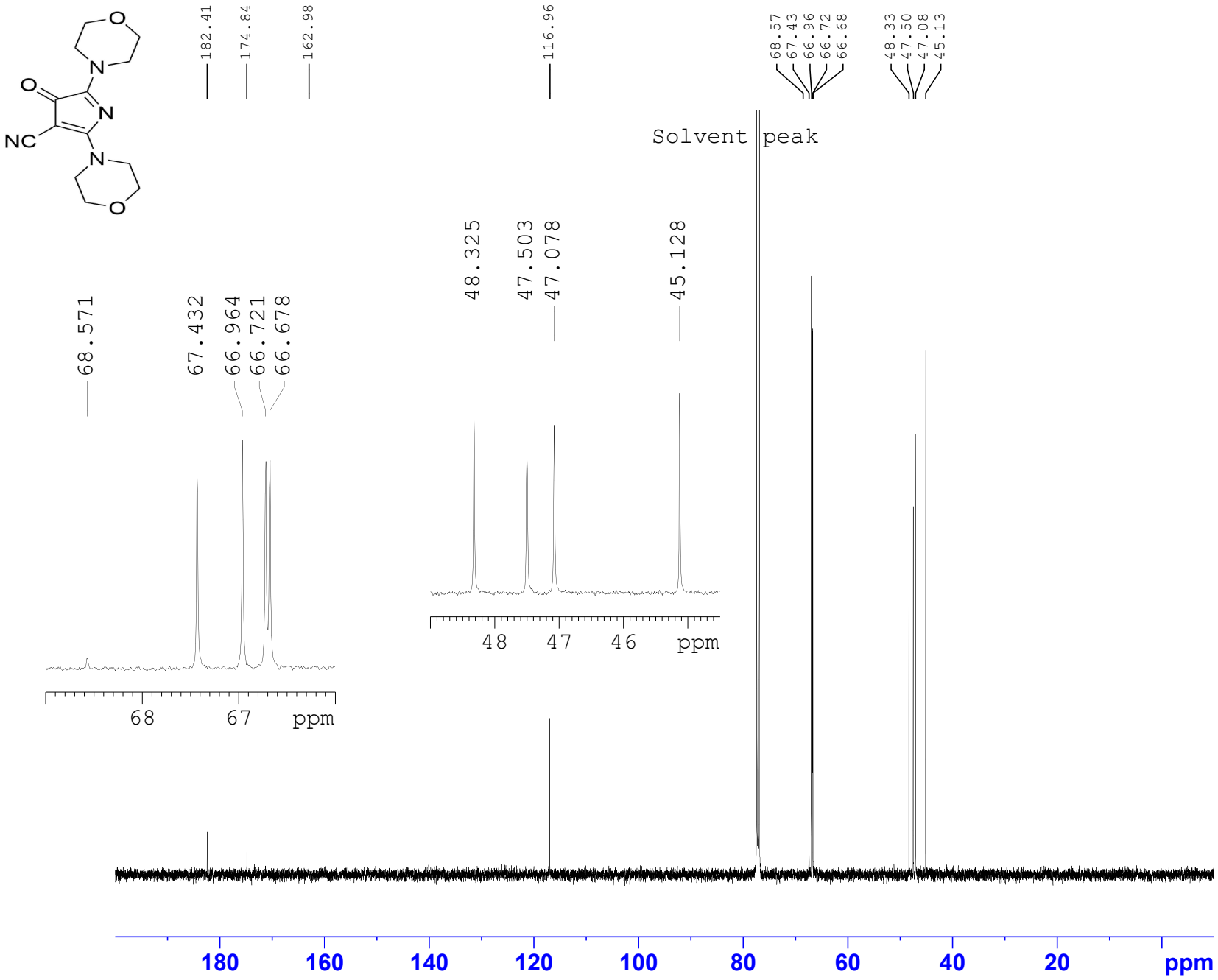
F2 - Acquisition Parameters

Date_	20221113
Time	11.39 h
INSTRUM	spect
PROBHD	Z104275_0375 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6009.615 Hz
FIDRES	0.183399 Hz
AQ	5.4525952 sec
RG	201.81
DW	83.200 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
SFO1	300.1318533 MHz
NUC1	1H
P1	14.00 usec
PLW1	7.85570002 W

F2 - Processing parameters

SI	65536
SF	300.1300073 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

2,5-Dimorpholino-3-oxo-3H-pyrrole-4-carbonitrile 34



Current Data Parameters

NAME	nmr 500
EXPNO	11
PROCNO	1

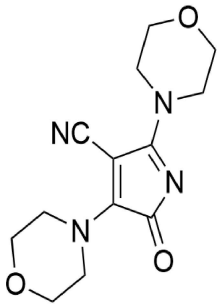
F2 - Acquisition Parameters

Date_	20221114
Time	11.56 h
INSTRUM	spect
PROBHD	Z113652_0078 (
PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	20480
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	1.1010048 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	296.3 K
CNST2	145.0000000
CNST11	1.0000000
D1	2.00000000 sec
D20	0.00689655 sec
TD0	1
SFO1	125.7459712 MHz
NUC1	13C
P1	10.00 usec
P2	20.00 usec
PLW1	121.36000061 W
SFO2	500.0350001 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	80.00 usec
PLW2	16.34900093 W
PLW12	0.34647381 W

F2 - Processing parameters

SI	32768
SF	125.7333812 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3,5-Dimorpholino-2-oxo-2H-pyrrole-4-carbonitrile 35



Current Data Parameters

NAME	NMR 300
EXPNO	141
PROCNO	1

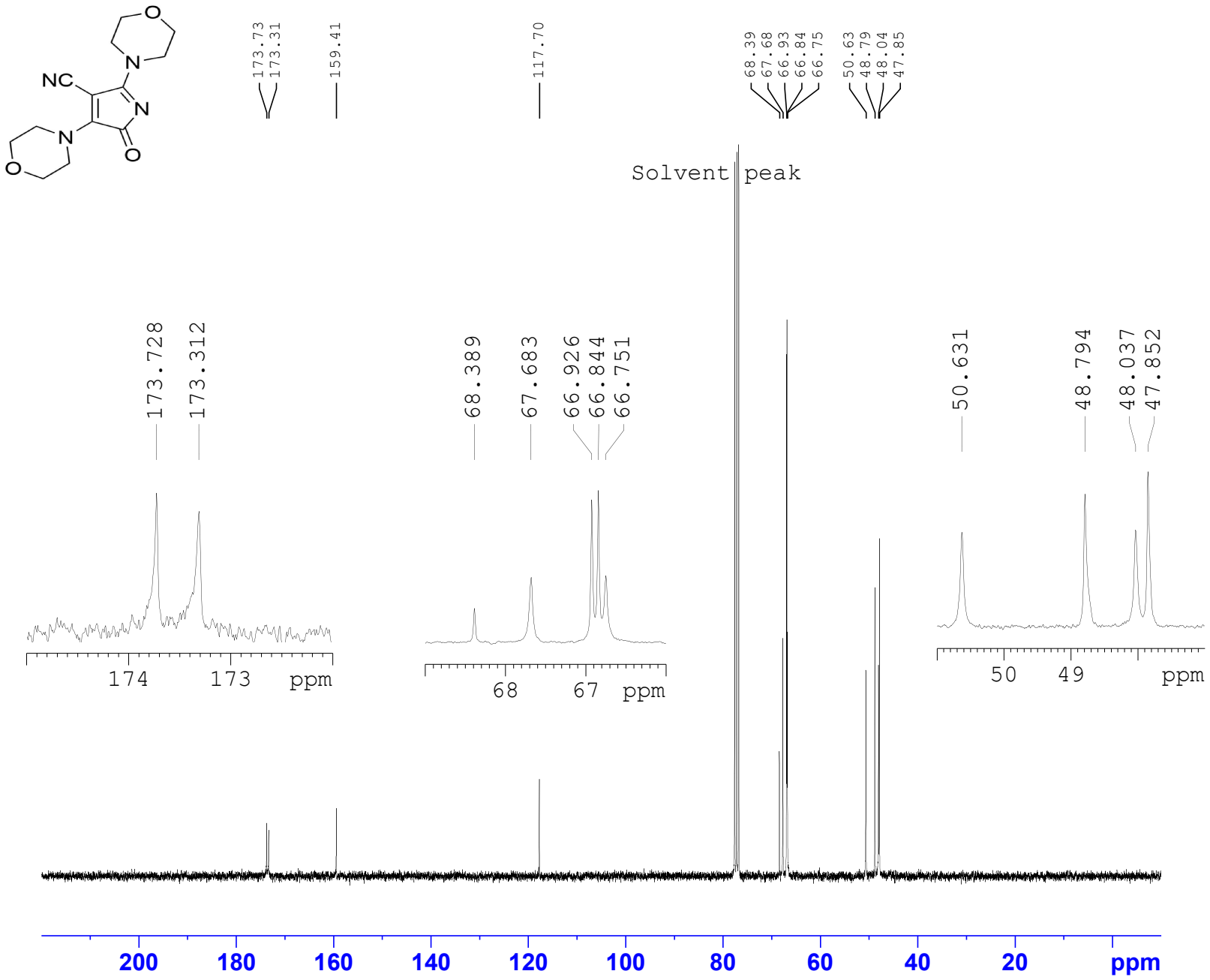
F2 - Acquisition Parameters

Date_	20221122
Time	21.31 h
INSTRUM	spect
PROBHD	Z104275_0375 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6009.615 Hz
FIDRES	0.183399 Hz
AQ	5.4525952 sec
RG	201.81
DW	83.200 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
SFO1	300.1318533 MHz
NUC1	1H
P1	14.00 usec
PLW1	7.85570002 W

F2 - Processing parameters

SI	65536
SF	300.1300073 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

3,5-Dimorpholino-2-oxo-2H-pyrrole-4-carbonitrile 35



Current Data Parameters

NAME	NMR 300
EXPNO	142
PROCNO	1

F2 - Acquisition Parameters

Date_	20221123
Time	8.15 h
INSTRUM	spect
PROBHD	Z104275_0375 (
PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	9890
DS	4
SWH	18115.941 Hz
FIDRES	0.552855 Hz
AQ	1.8087935 sec
RG	201.81
DW	27.600 usec
DE	6.50 usec
TE	298.1 K
CNST2	145.0000000
CNST11	1.0000000
D1	2.00000000 sec
D20	0.00689655 sec
TD0	1
SFO1	75.4752953 MHz
NUC1	13C
P1	10.00 usec
P2	20.00 usec
PLW1	43.01699829 W
SFO2	300.1312005 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	80.00 usec
PLW2	7.85570002 W
PLW12	0.24640390 W

F2 - Processing parameters

SI	32768
SF	75.4677399 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40