Supporting Information

Photochemical Synthesis and Ring-Chain-Ring Tautomerism of Benzo[4,5]imidazo[1,2-*a*]cyclopenta[*e*]pyridines

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1. ^{1}H NMR spectra of mixture of compounds **4b** and **5b** at various conditions

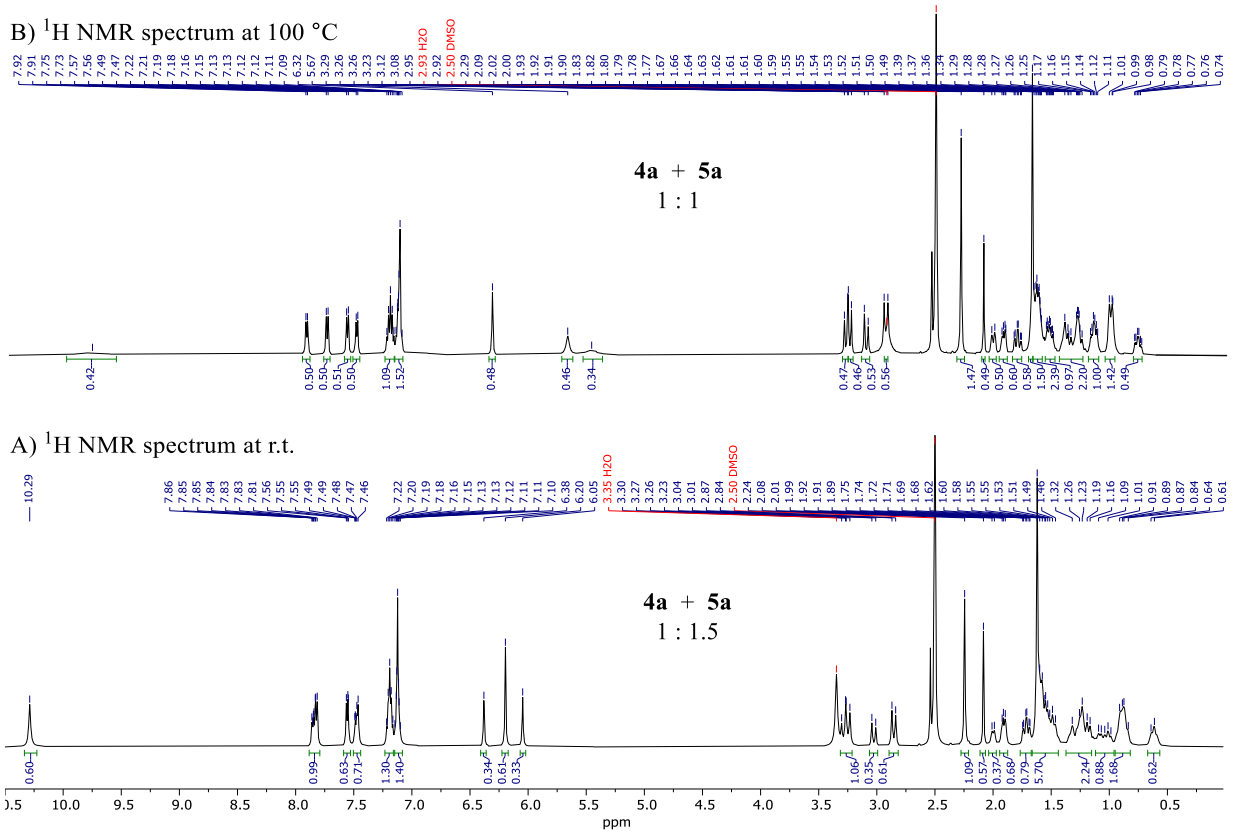


Figure S1. ^{1}H NMR spectra of mixture of compounds **4b** and **5b** at r.t. and 100 °C in DMSO-d_6 solution

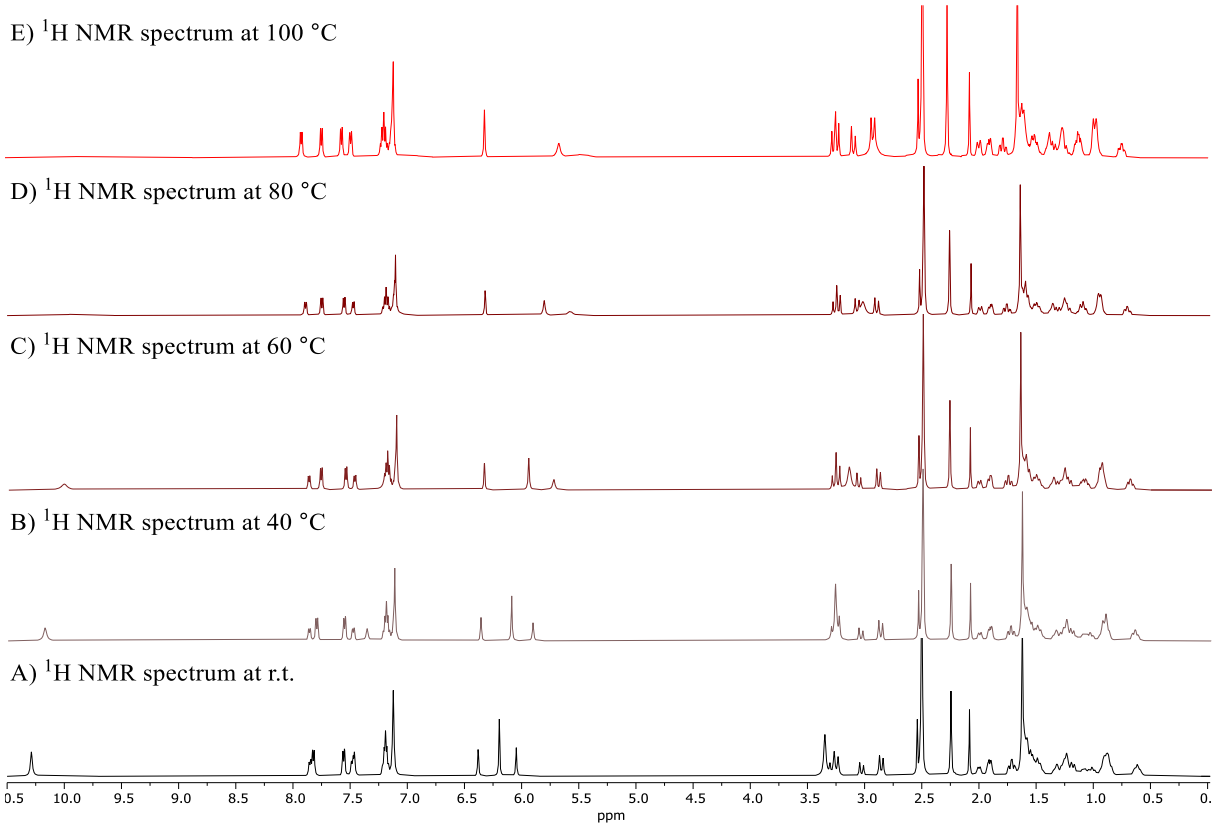


Figure S2. ^{1}H NMR spectra of mixture of compounds **4b** and **5b** at various T °C in DMSO-d_6 solution

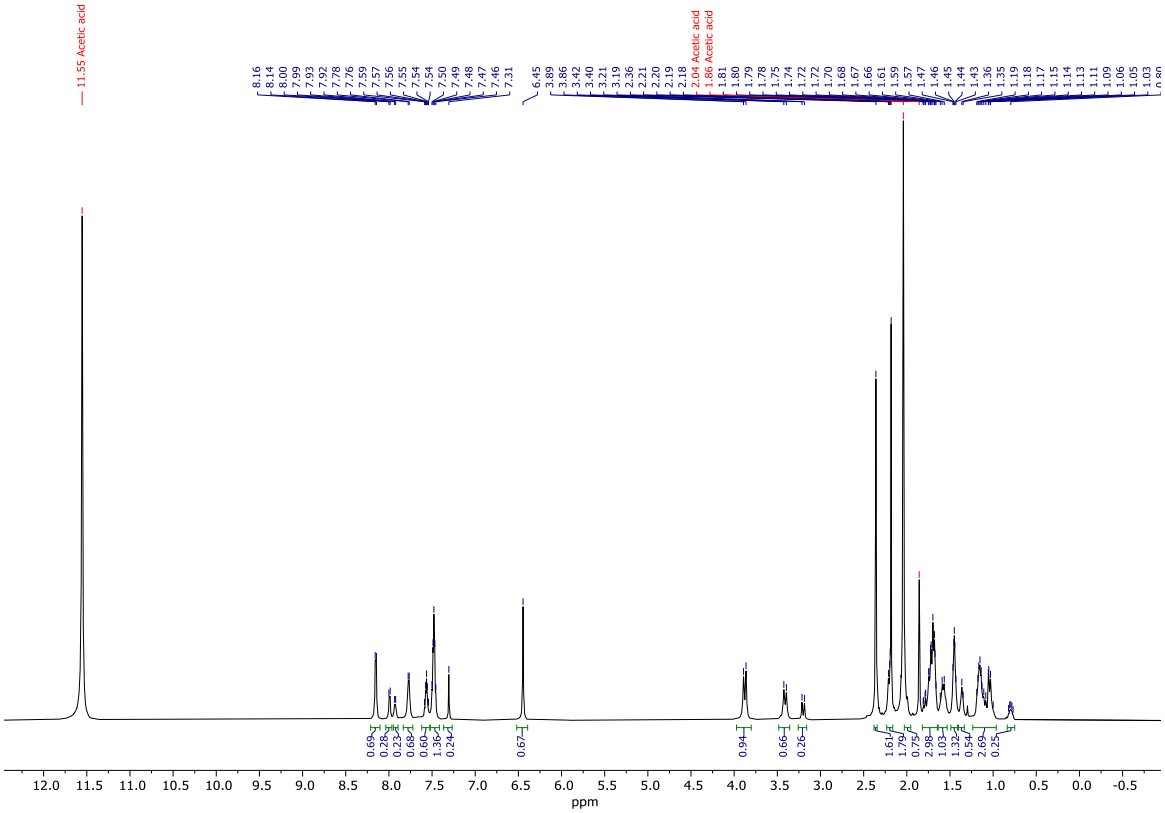


Figure S3. ^{1}H NMR spectra of mixture of compounds **4b** and **5b** at r.t. in Acetic acid-d_4 solution

2. UV-Vis absorption spectrum of compound **3b**

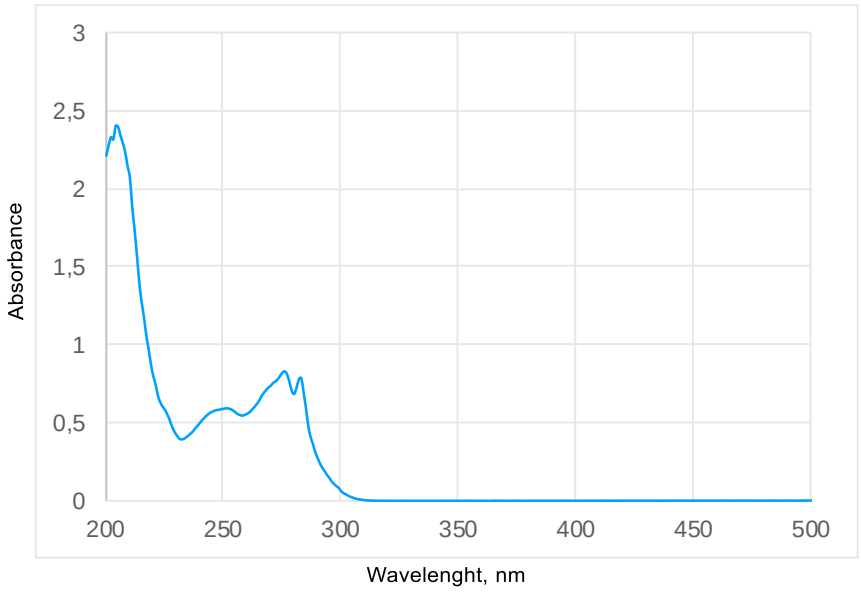


Fig. S4. UV-Vis absorption spectrum of **3b** in acetonitrile (c = 1.1 x 10^{-5})

3. 2D NMR data of mixture of compounds **4a** and **5a**

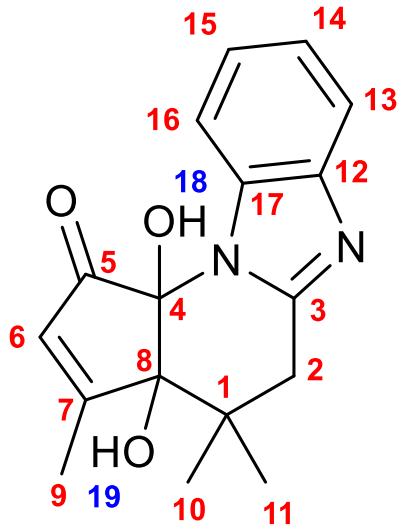


Table S1. Assignment of NMR signals and 2D NMR (HMBC) correlations for compound **4a**

№	^{1}H	^{13}C	HMBC
1	-	38.5	19, 2, 10, 11
2	3.23 (d, *J* = 16.5 Hz, 1H); 2.62 (d, *J* = 16.5 Hz, 1H);	35.0	10, 11
3	-	150.8	2, 11
4	-	87.8	6
5	-	197.1	6, 9
6	6.35 (d, *J* = 1.5 Hz, 1H)	129.5	9
7	-	175.6	6, 9
8	-	83.1	2, 6, 9, 10, 11
9	2.21 (d, *J* = 1.5 Hz, 3H)	16.8	6
10	0.66 (s, 3H)	24.0	2, 11
11	1.29 (s, 3H)	25.0	10
12	-	143.0	13, 14
13	7.91 – 7.81 (m, 1H)	115.5	14, 15
14	7.17 – 7.09 (m, 1H)	121.6	13
15	7.17 – 7.09 (m, 1H)	120.9	16
16	7.51 – 7.44 (m, 2H)	117.9	14, 15
17	-	133.8	15, 16
18	7.48 (s, 1H)	-	-
19	6.08 (s, 1H)	-	-

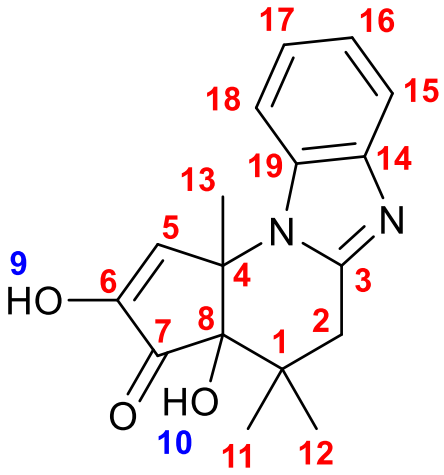


Table S2. Assignment of NMR signals and 2D NMR (HMBC) correlations for compound 5a

№	^{1}H	^{13}C	HMBC
1	-	38.4	2, 10, 11, 12
2	3.11 (d, *J* = 16 Hz, 1H) 2.56 (d, *J* = 17.1 Hz, 1H)	34.3	11, 12
3	-	150.6	2
4	-	63.7	5, 10, 13
5	7.17 – 7.09 (m, 1H)	127.4	13
6	-	152.8	-
7	-	202.0	5, 10
8	-	81.4	2, 5, 10, 11, 12, 13
9	10.3 (br.s, 1H)	-	-
10	6.23 (s, 1H)	-	-
11	1.22 (s, 3H)	22.6	12
12	0.56 (s, 3H)	25.0	11
13	1.62 (s, 3H)	26.7	5
14	-	143.2	2, 15, 16
15	7.91 – 7.81 (m, 1H)	112.0	16, 18
16	7.26 – 7.19 (m, 1H)	121.5	15, 17, 18
17	7.17 – 7.09 (m, 1H)	121.4	15, 18
18	7.59 – 7.54 (m, 1H)	118.8	16
19	-	132.1	18, 16

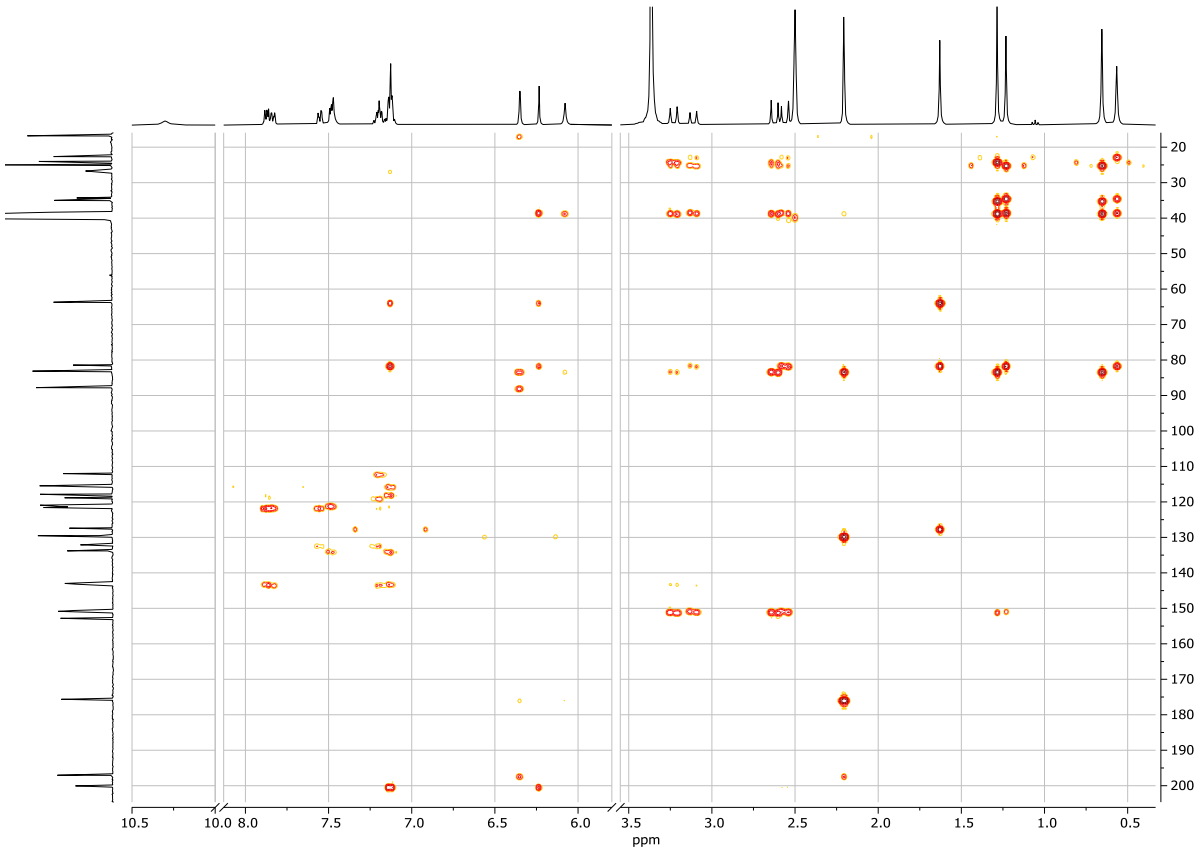


Figure S5. 2D NMR spectrum (HMBC) of mixture of **4a** and **5a** in DMSO-d_6

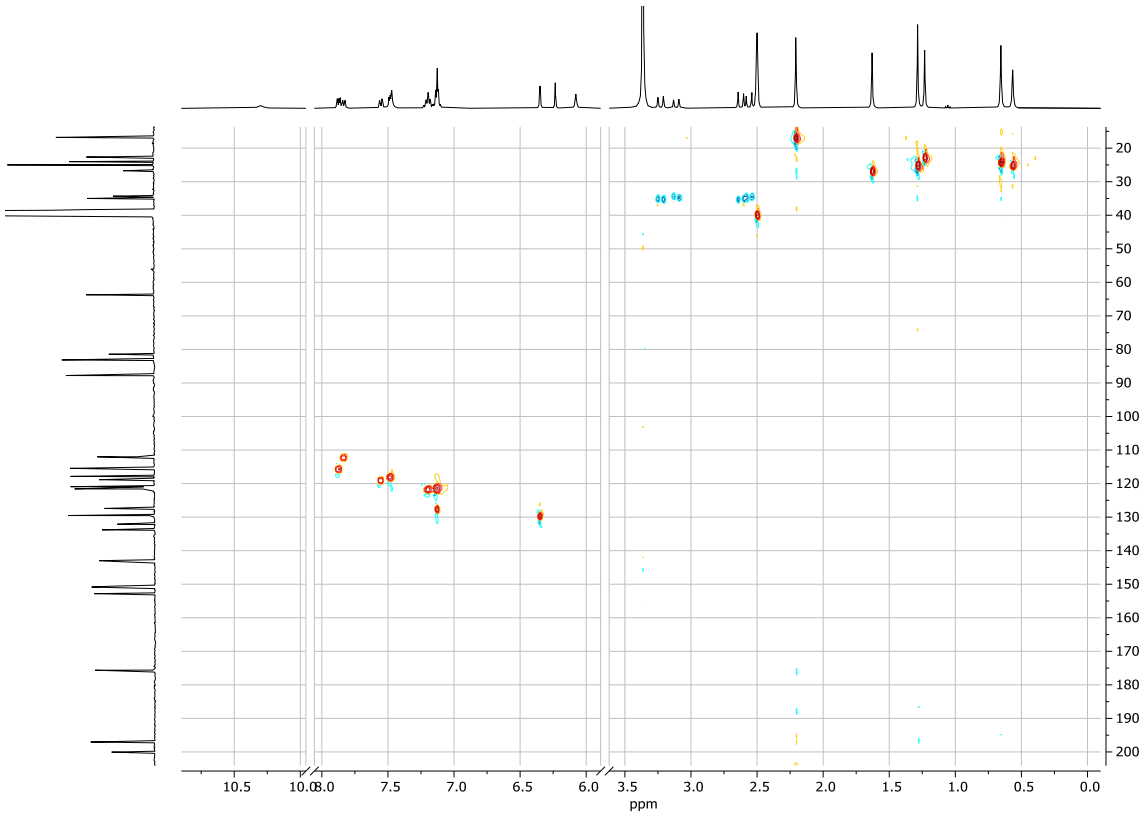
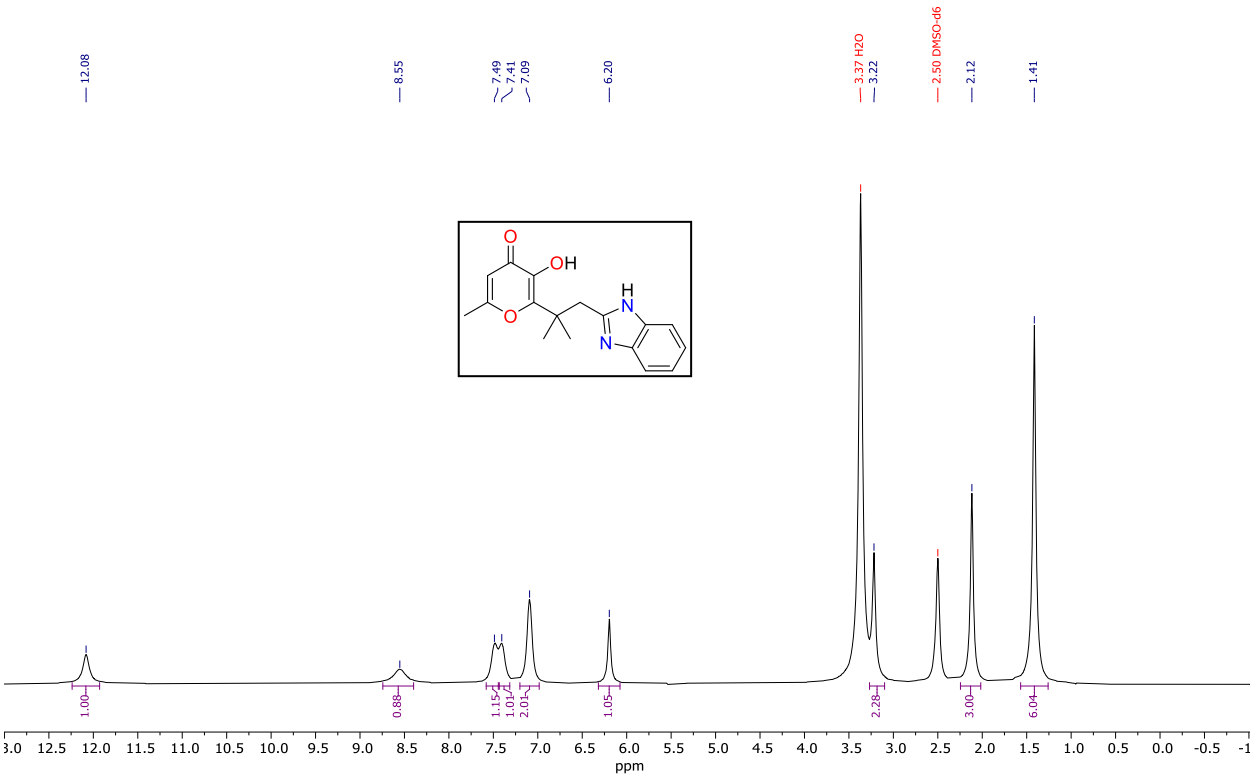


Figure S6. 2D NMR spectrum (HSQC) of mixture of **4a** and **5a** in DMSO-d_6

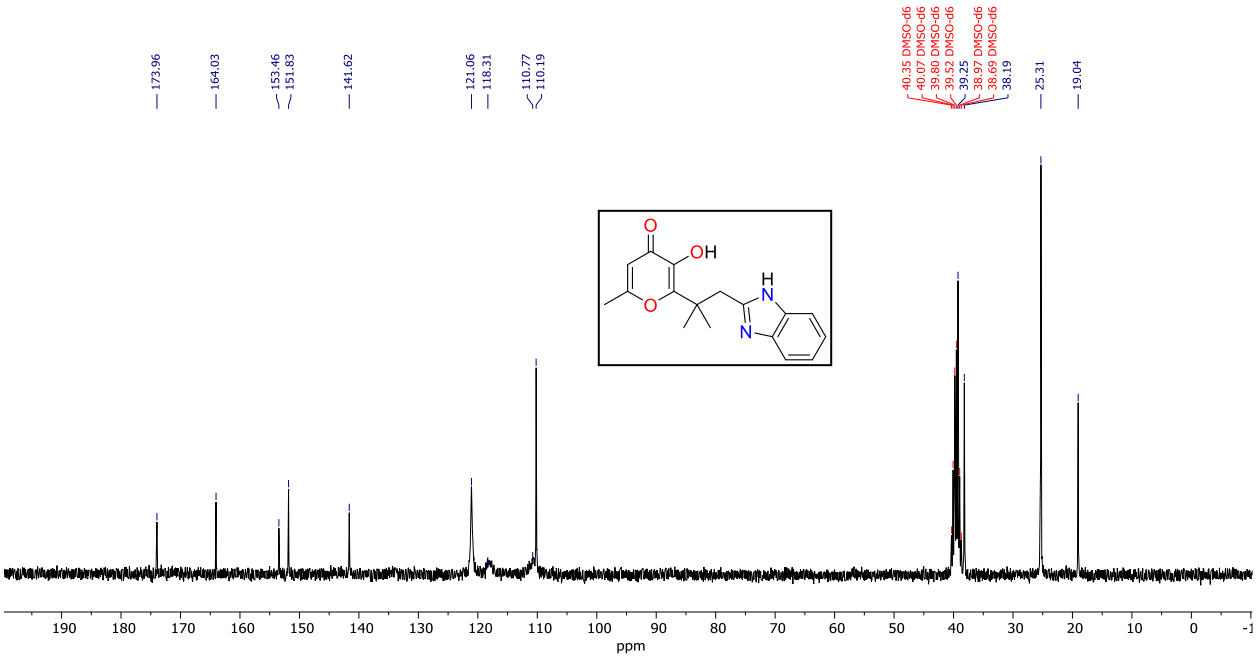
4. Copies of ^{1}H and ^{13}C NMR spectra

4.1. Starting compounds **3**

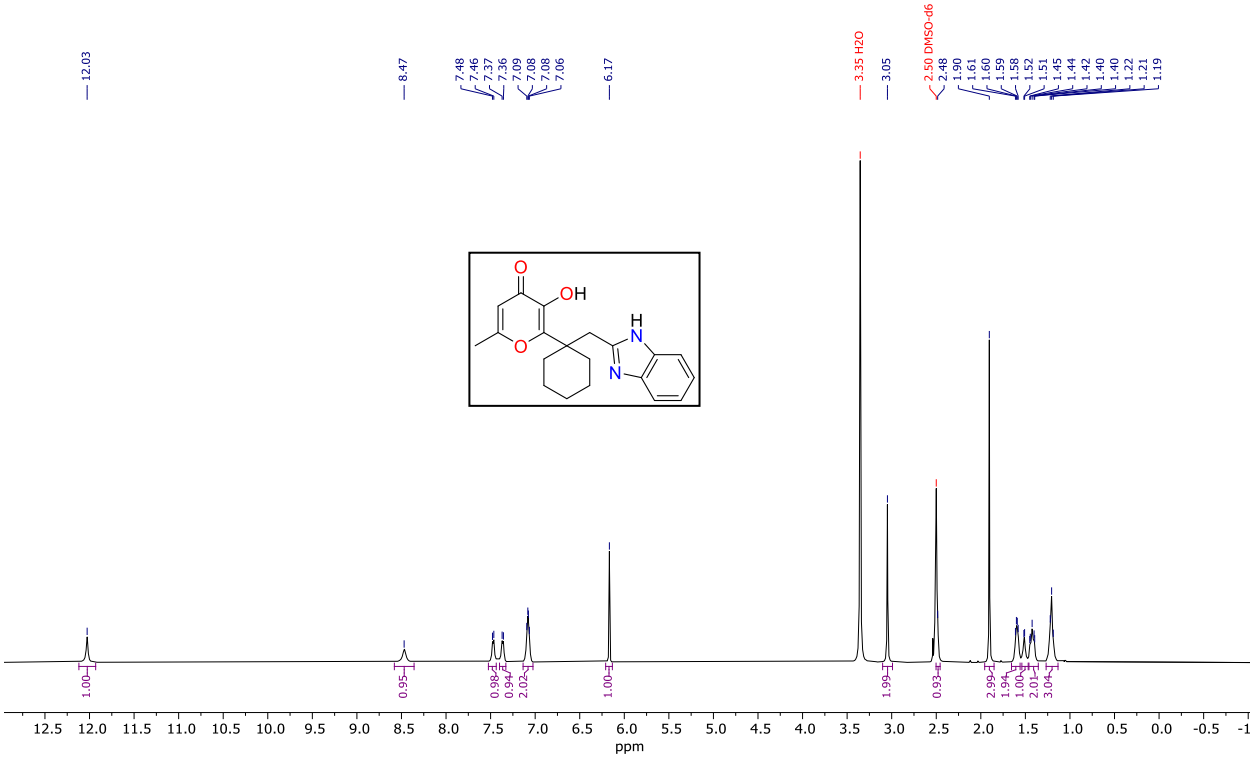
^{1}H NMR spectrum (300 MHz) of **3a** in DMSO-d_6



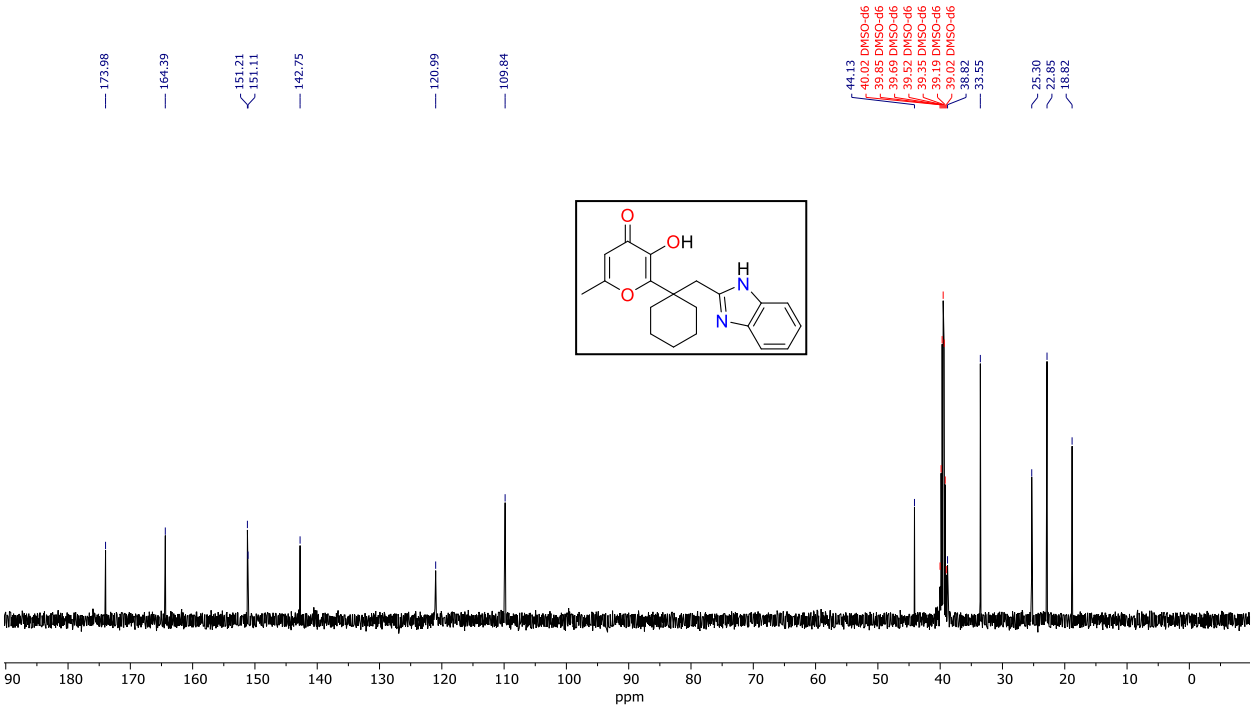
^{13}C {^{1}H} NMR spectrum (75 MHz) of **3a** in DMSO-d_6



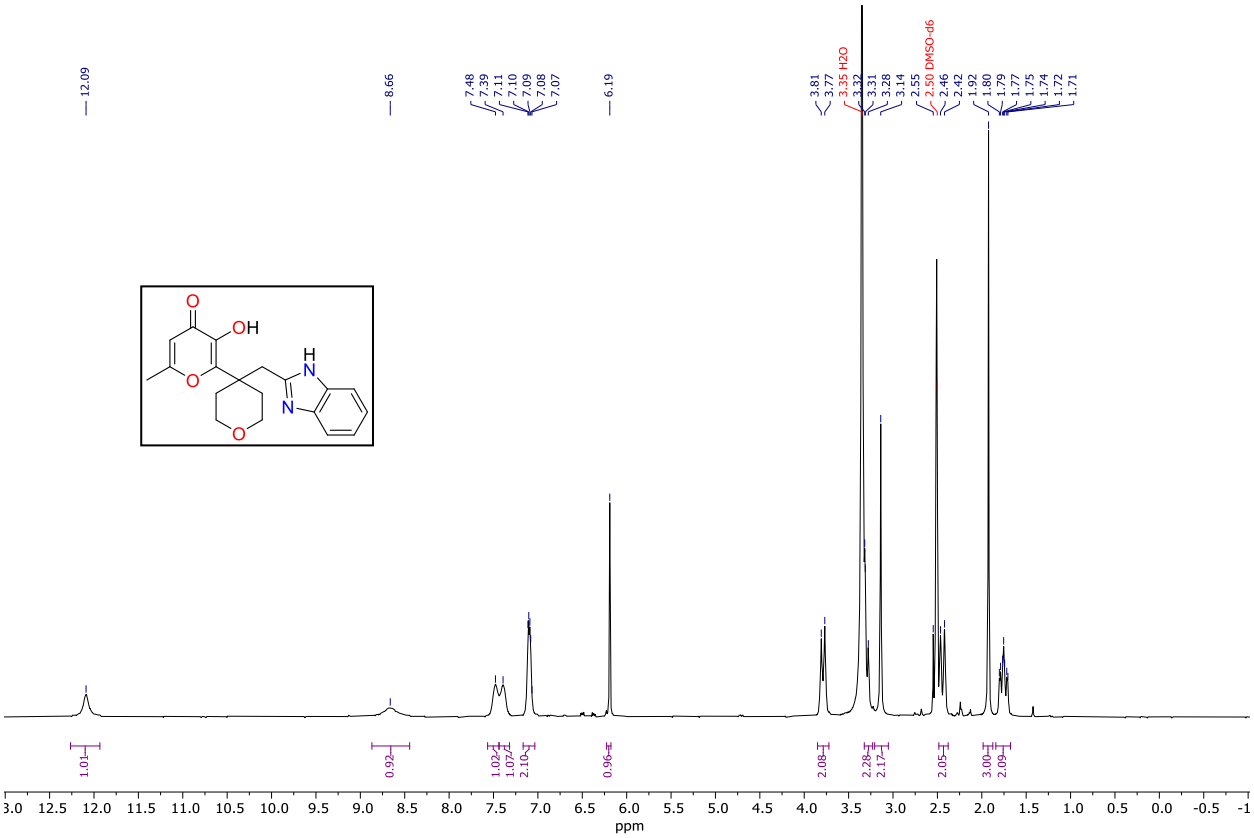
^{1}H NMR spectrum (500 MHz) of **3b** in DMSO-d_6



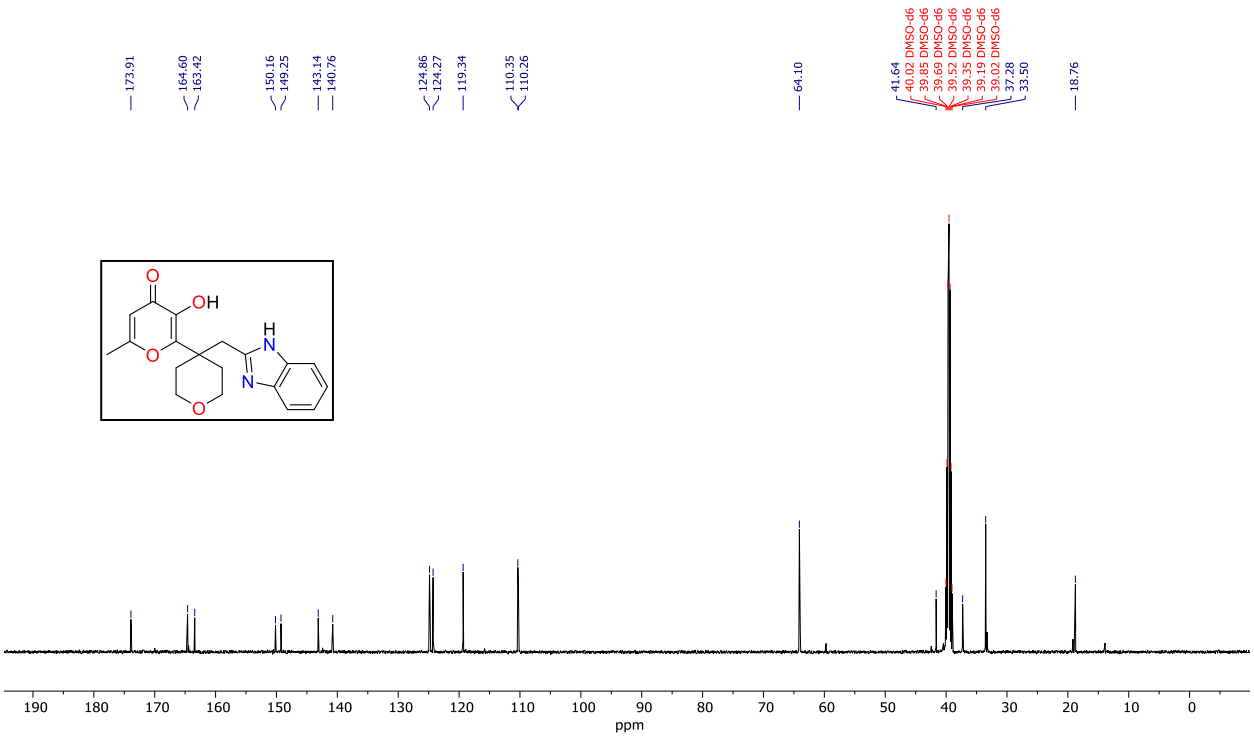
^{13}C {^{1}H} NMR spectrum (126 MHz) of **3b** in DMSO-d_6



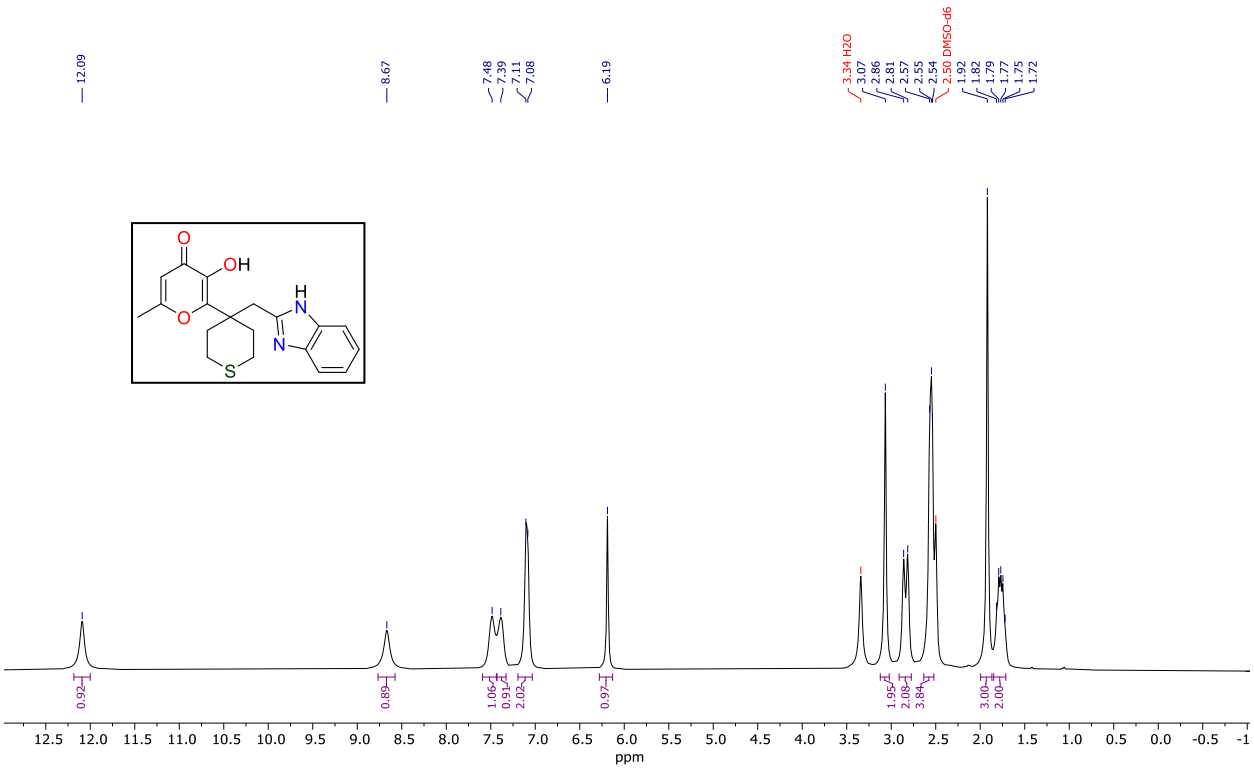
^{1}H NMR spectrum (300 MHz) of **3c** in DMSO-d_6



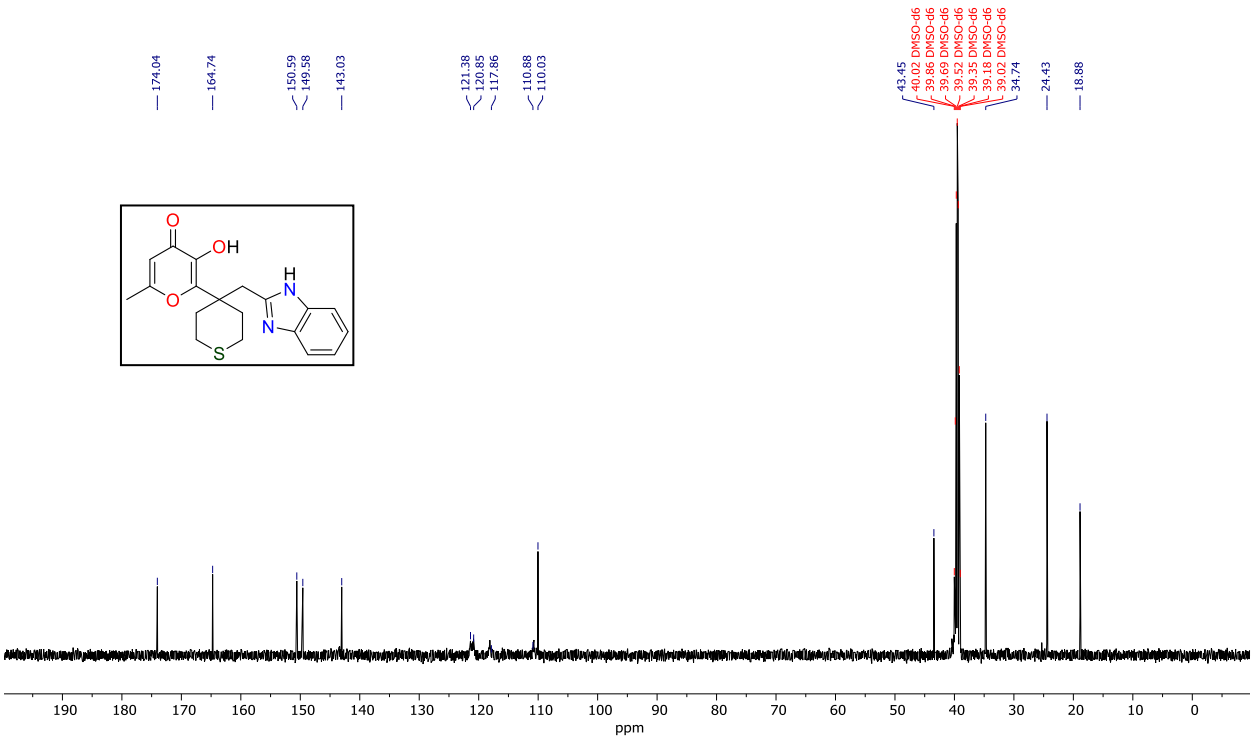
^{13}C {^{1}H} NMR spectrum (126 MHz) of **3c** in DMSO-d_6



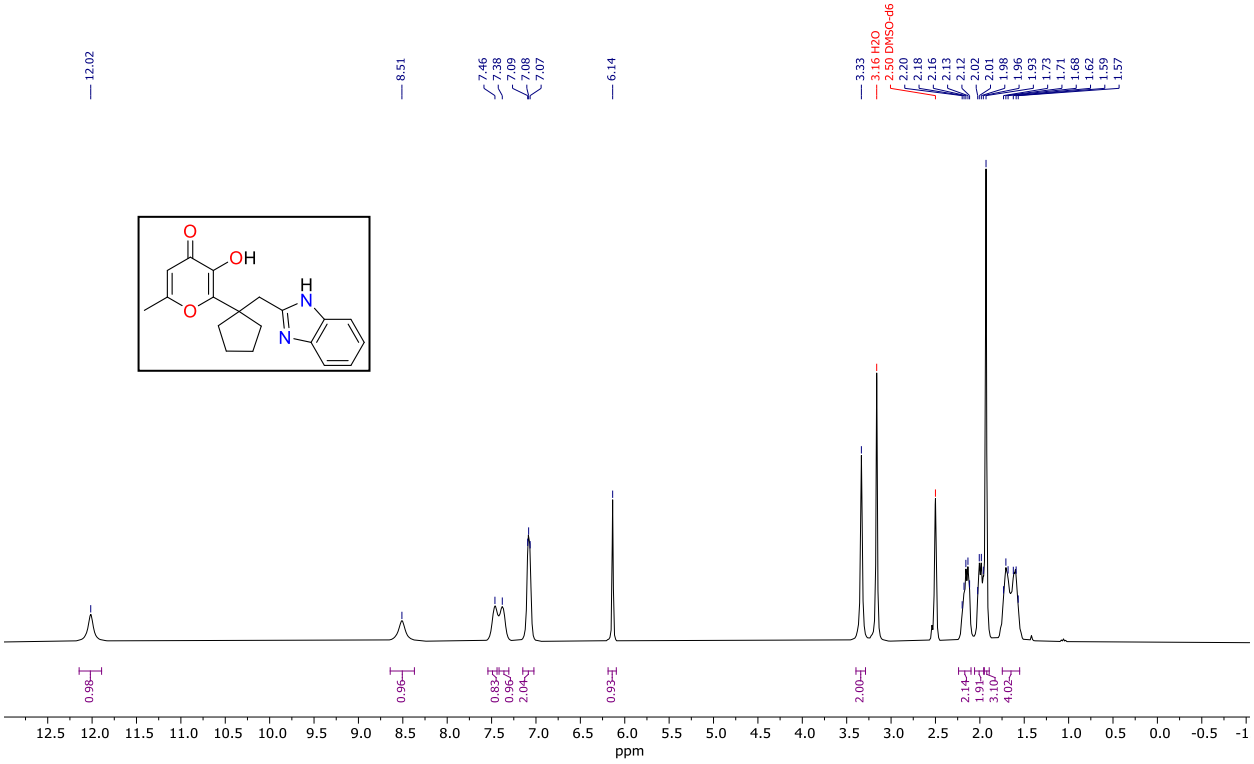
^{1}H NMR spectrum (300 MHz) of **3d** in DMSO-d_6



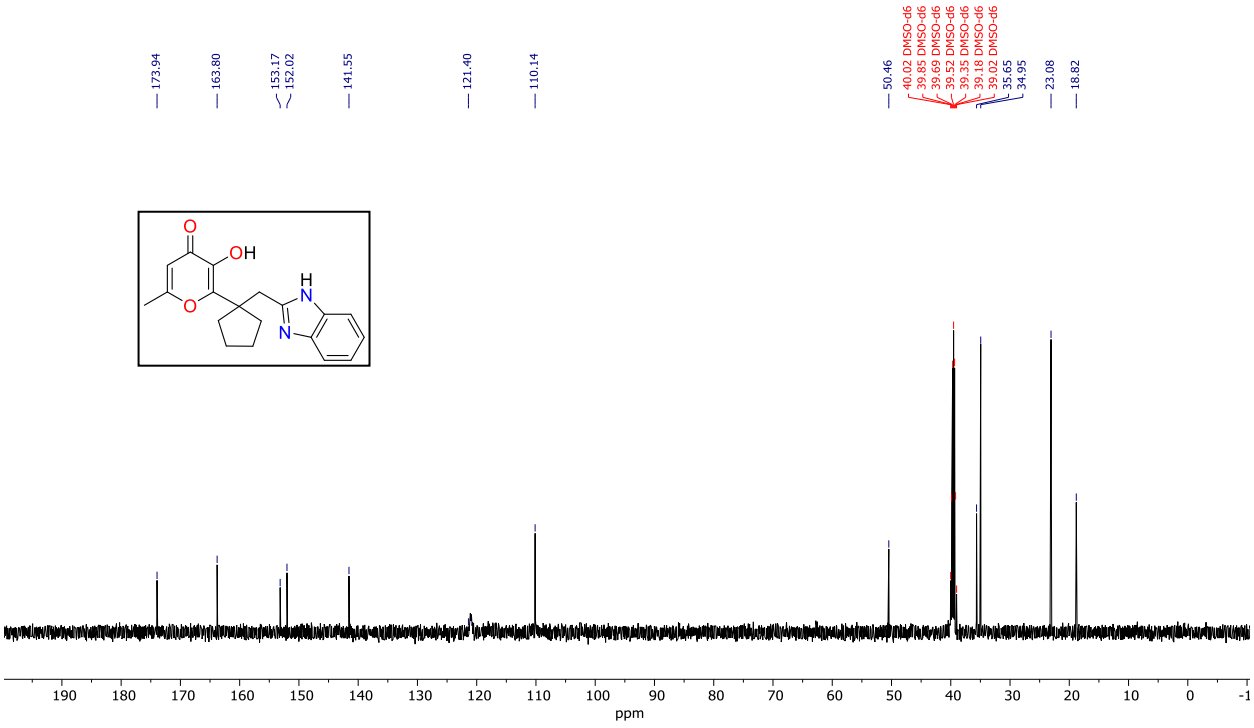
^{13}C {^{1}H} NMR spectrum (126 MHz) of **3d** in DMSO-d_6



^{1}H NMR spectrum (300 MHz) of **3e** in DMSO-d_6

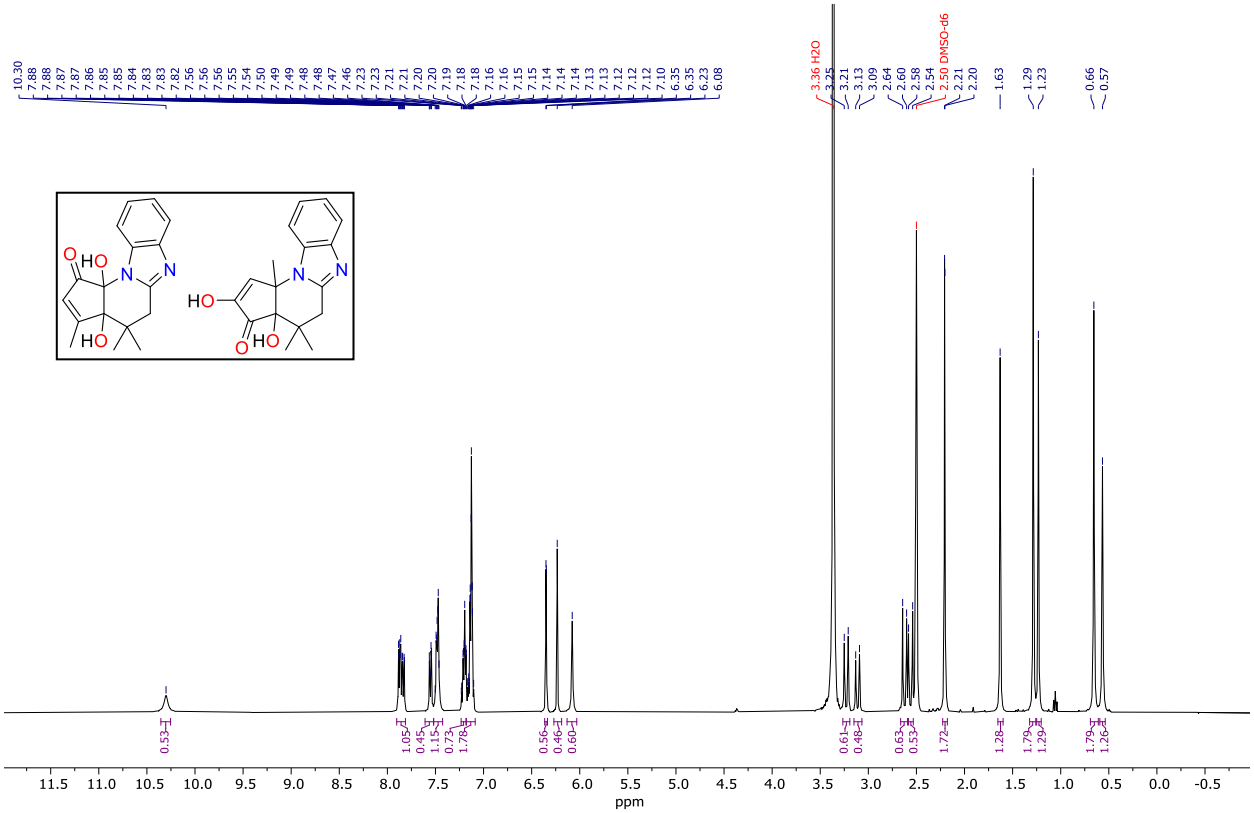


^{13}C {^{1}H} NMR spectrum (126 MHz) of **3e** in DMSO-d_6

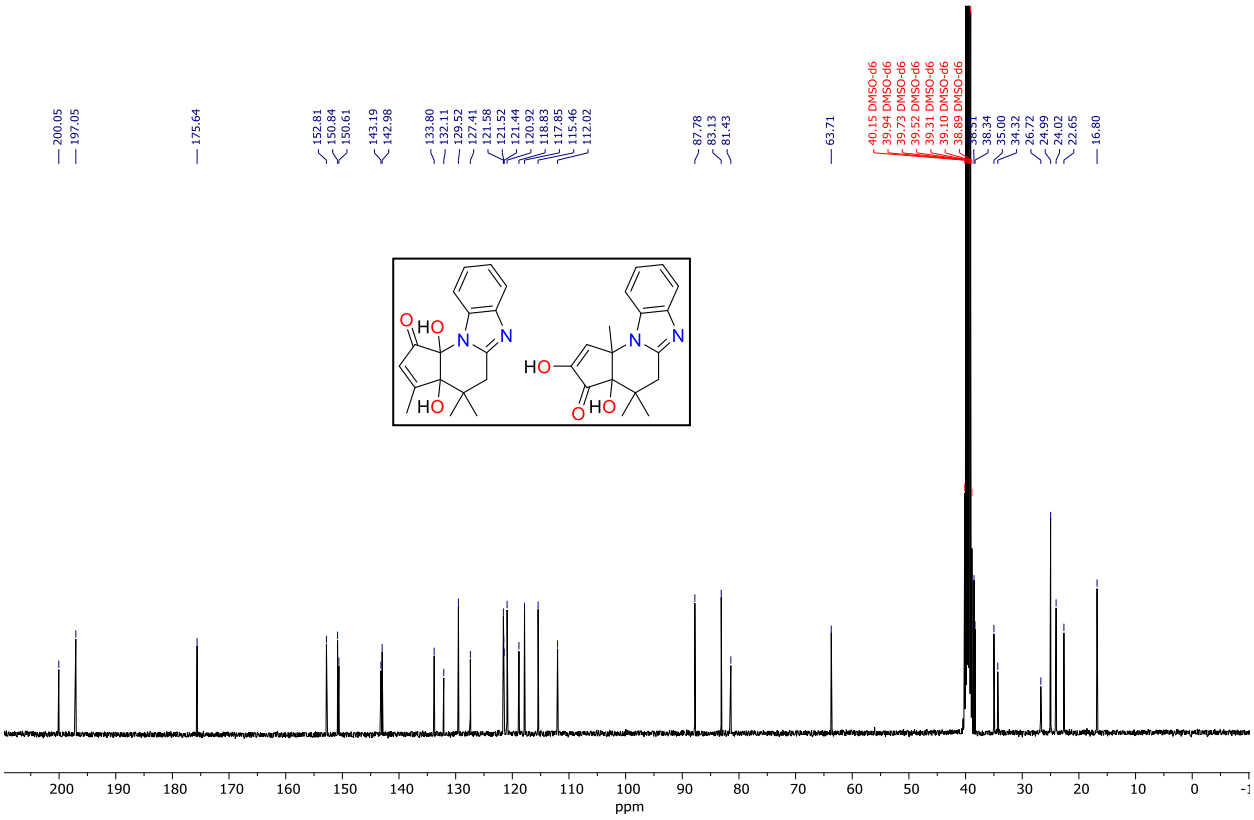


4.2. Mixture of photoproducts **4** and **5**

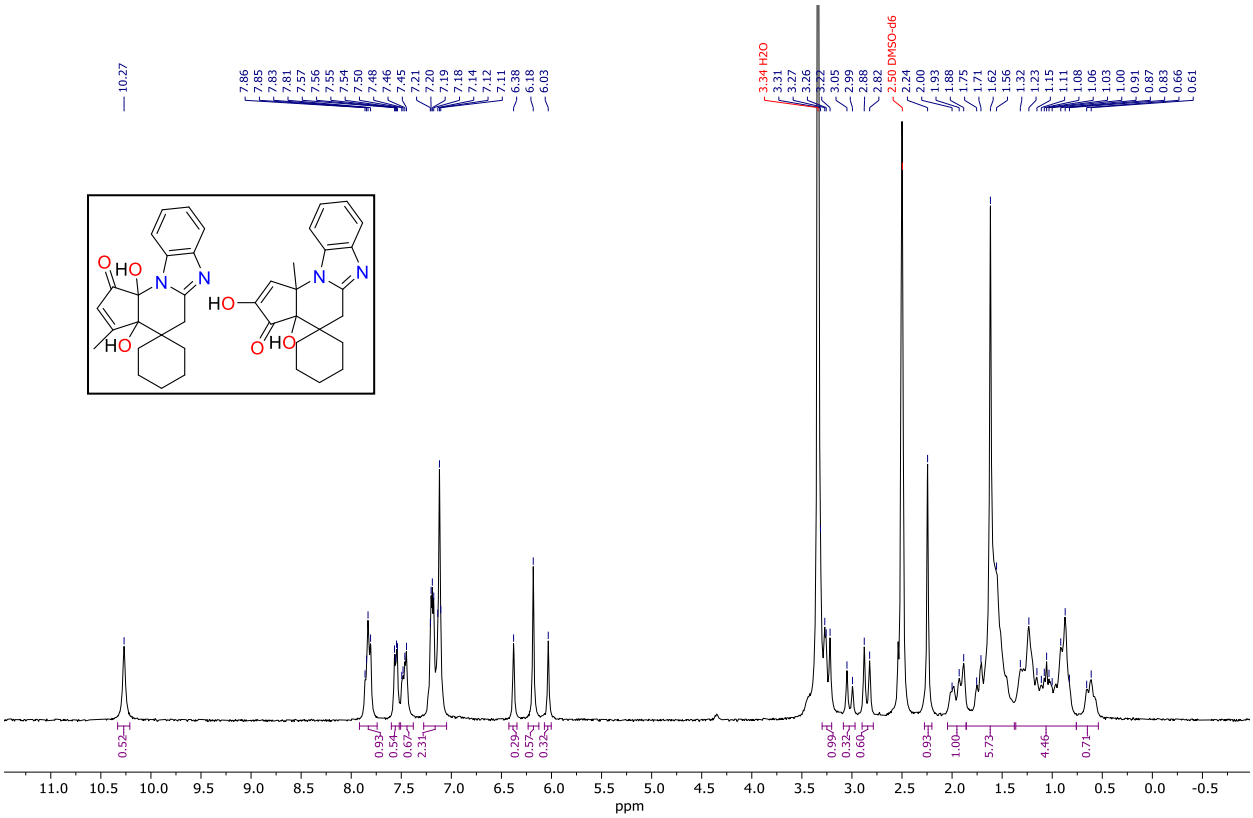
^{1}H NMR spectrum (400 MHz) of mixture of **4a** and **5a** in DMSO-d_6



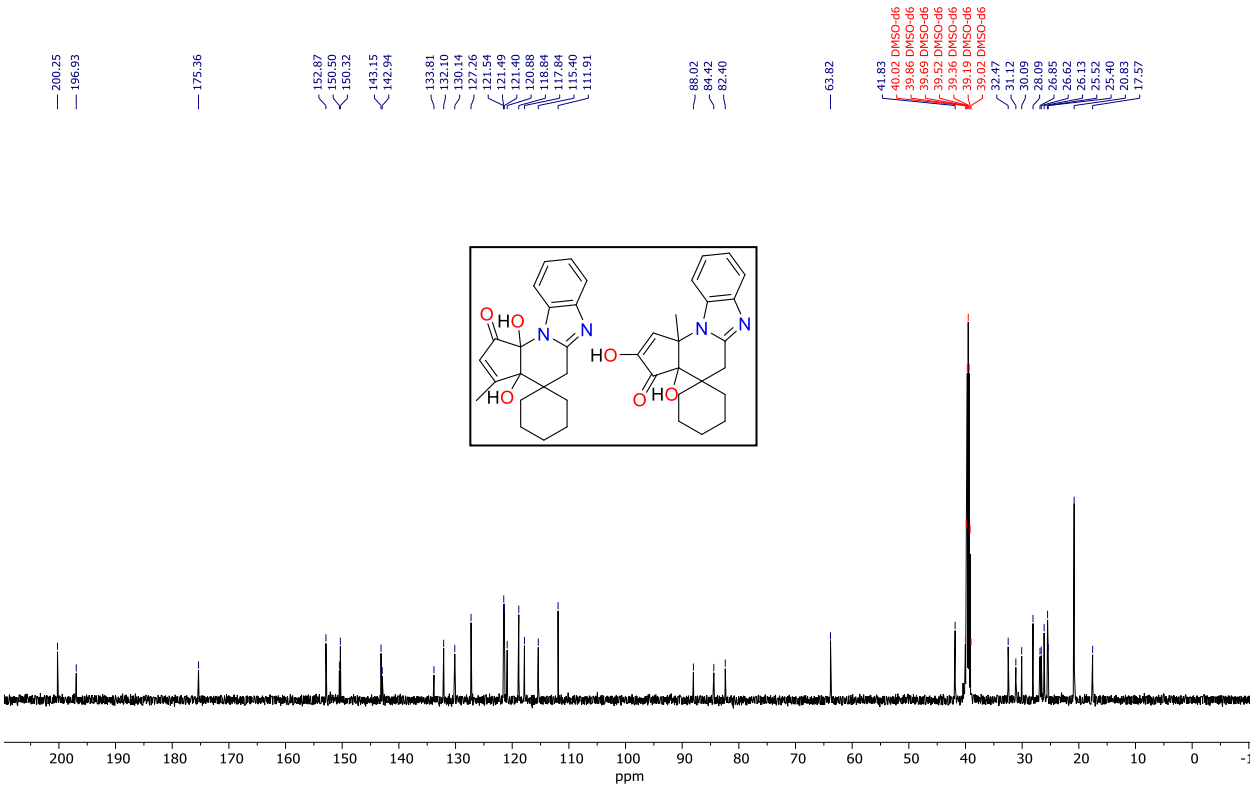
^{13}C {^{1}H} NMR spectrum (101 MHz) of mixture of **4a** and **5a** in DMSO-d_6



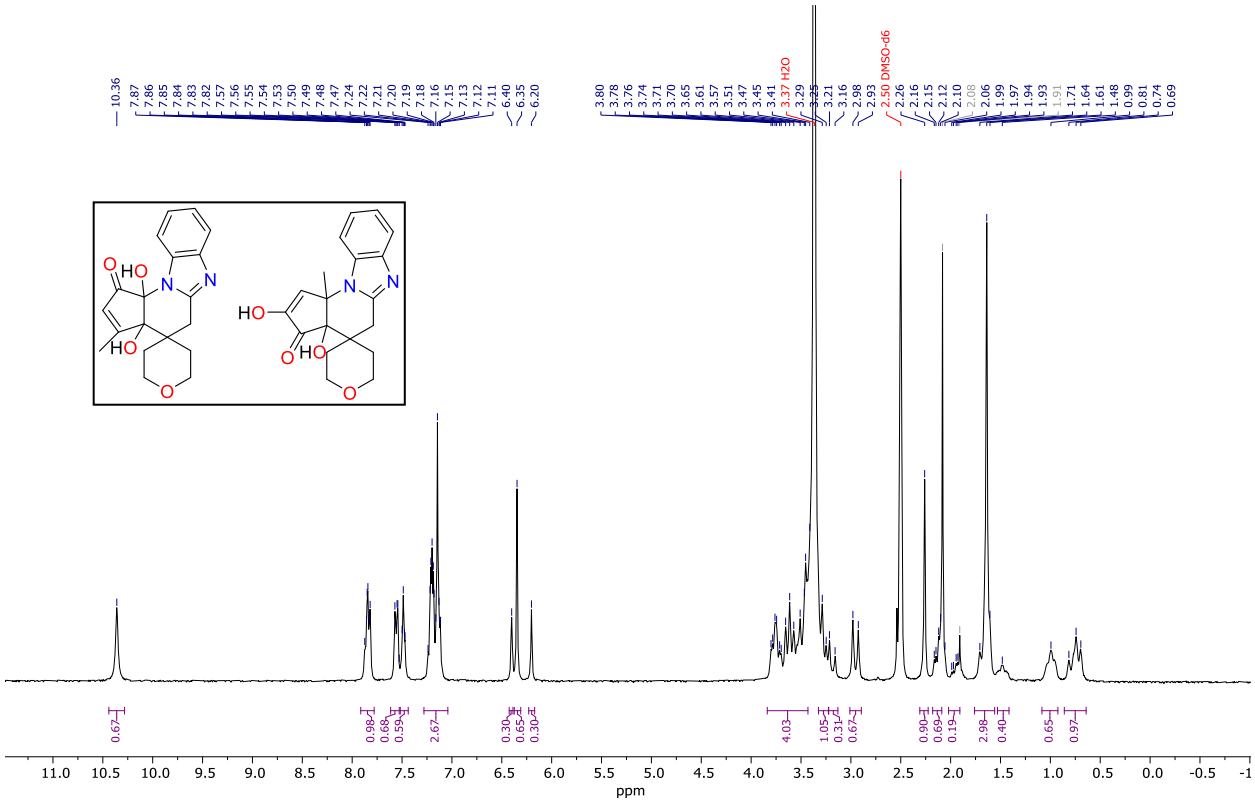
^{1}H NMR spectrum (300 MHz) of mixture of **4b** and **5b** in DMSO-d_6



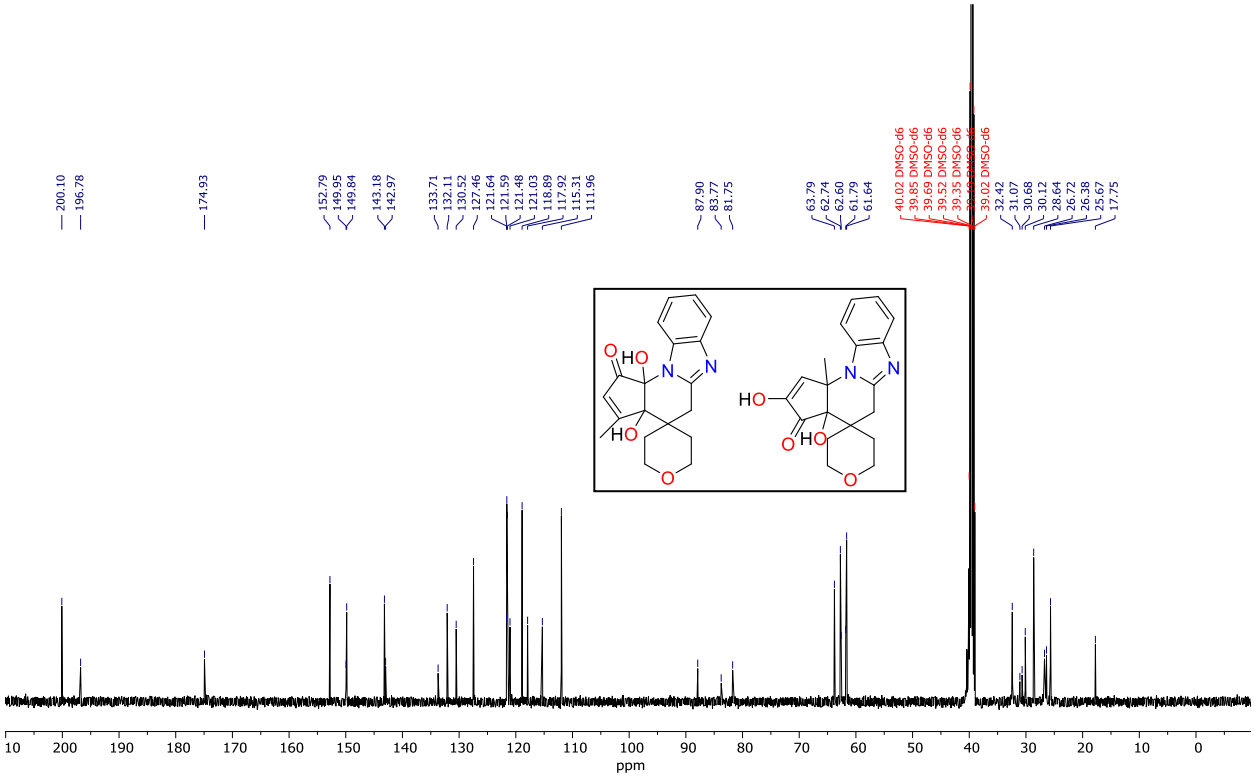
^{13}C {^{1}H} NMR spectrum (126 MHz) of mixture of **4b** and **5b** in DMSO-d_6



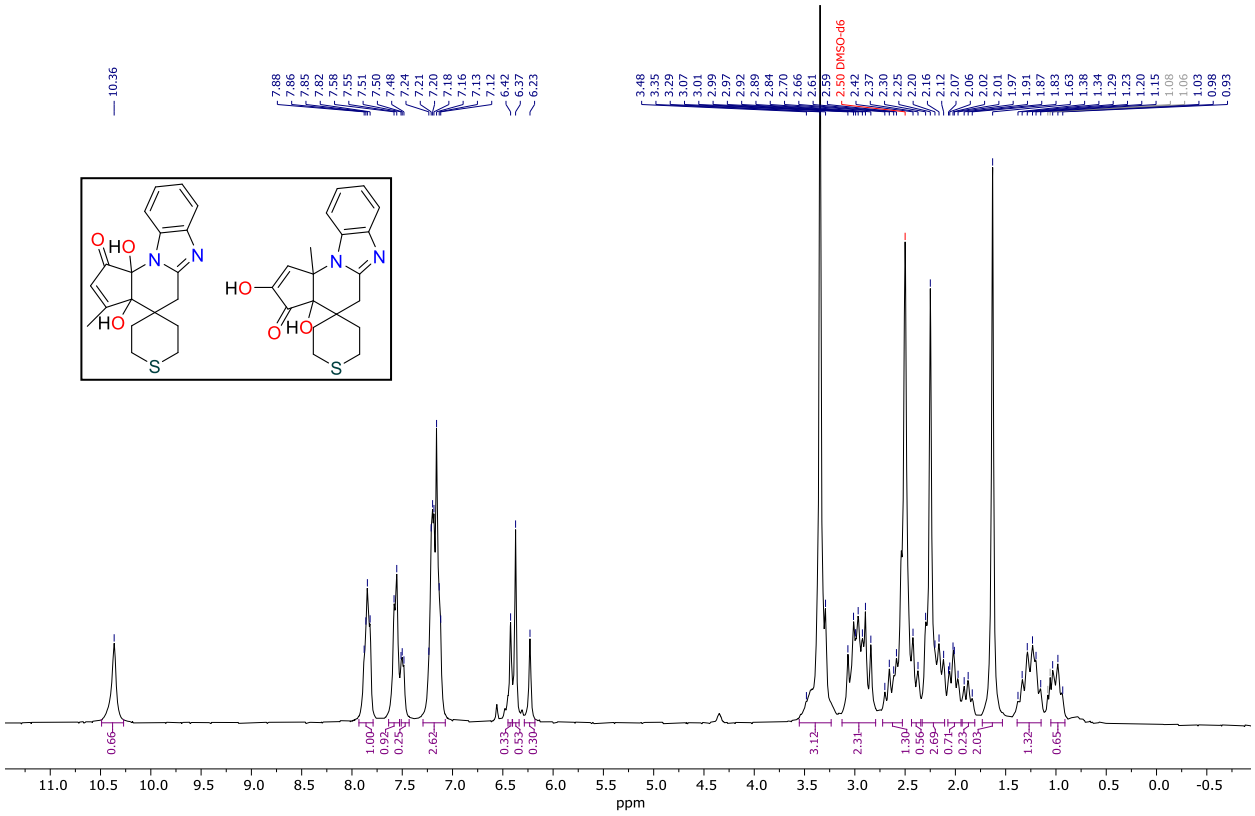
^{1}H NMR spectrum (300 MHz) of mixture of **4c** and **5c** in DMSO-d_6



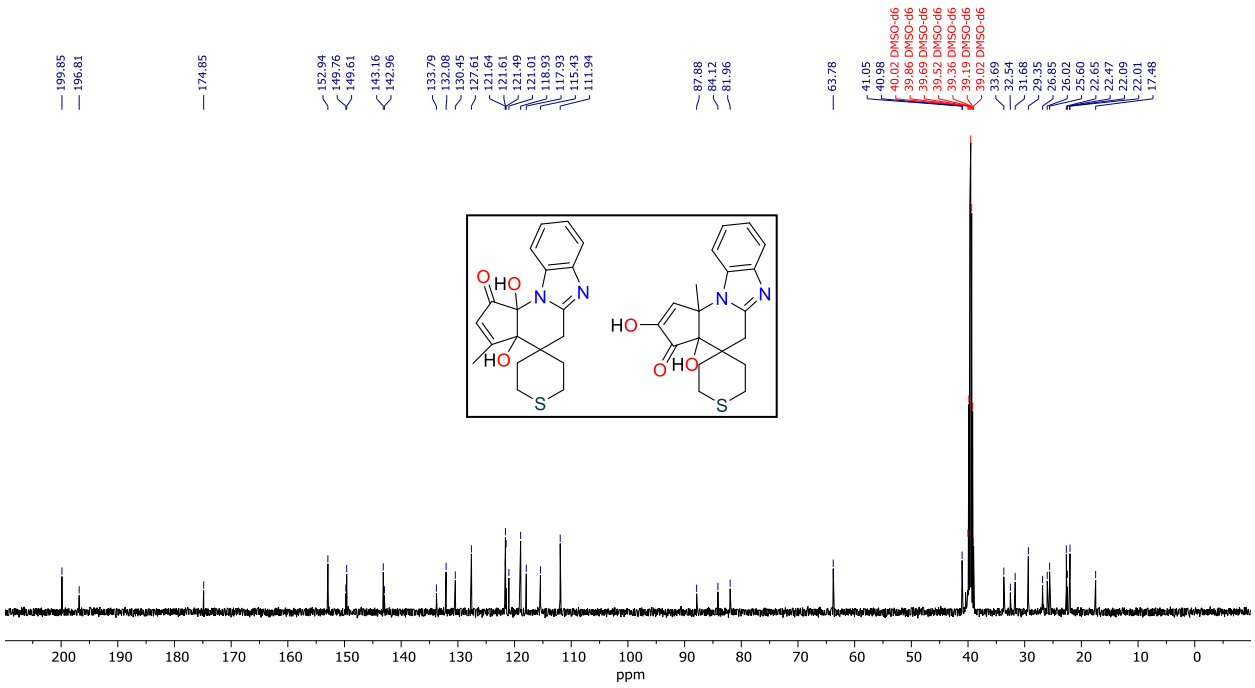
^{13}C {^{1}H} NMR spectrum (126 MHz) of mixture of **4c** and **5c** in DMSO-d_6



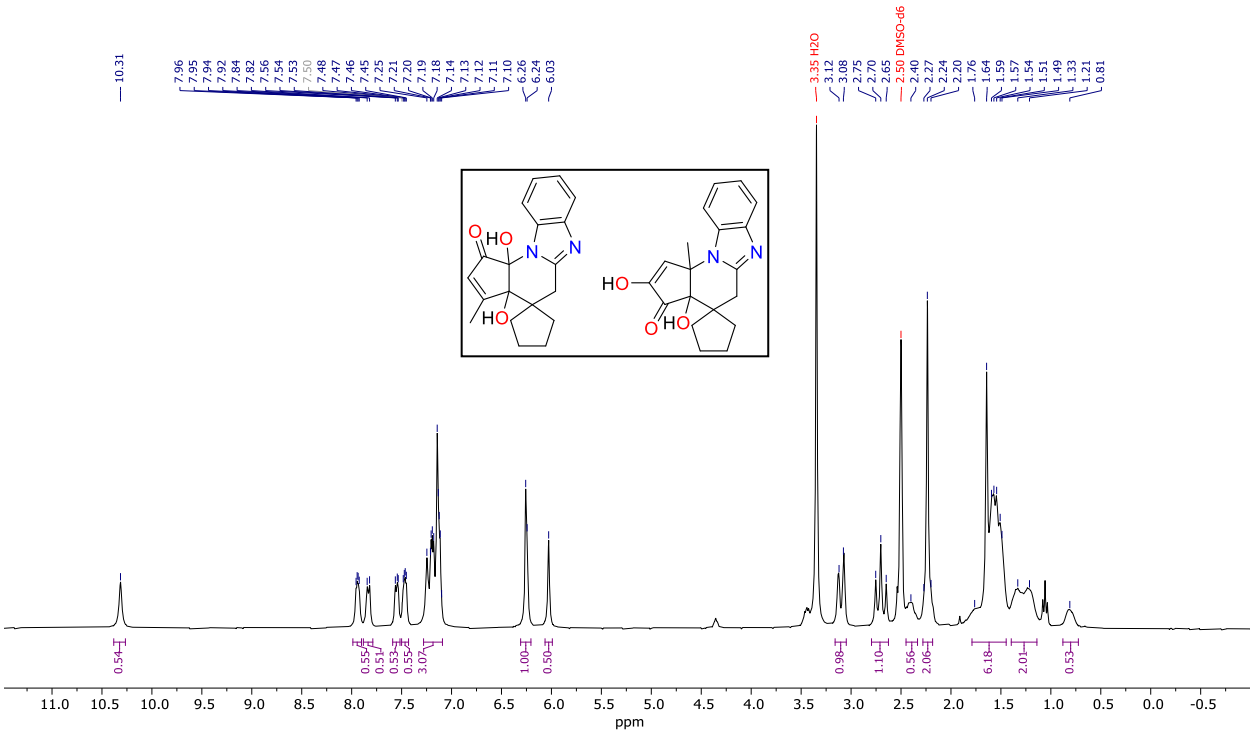
^{1}H NMR spectrum (300 MHz) of mixture of **4d** and **5d** in DMSO-d_6



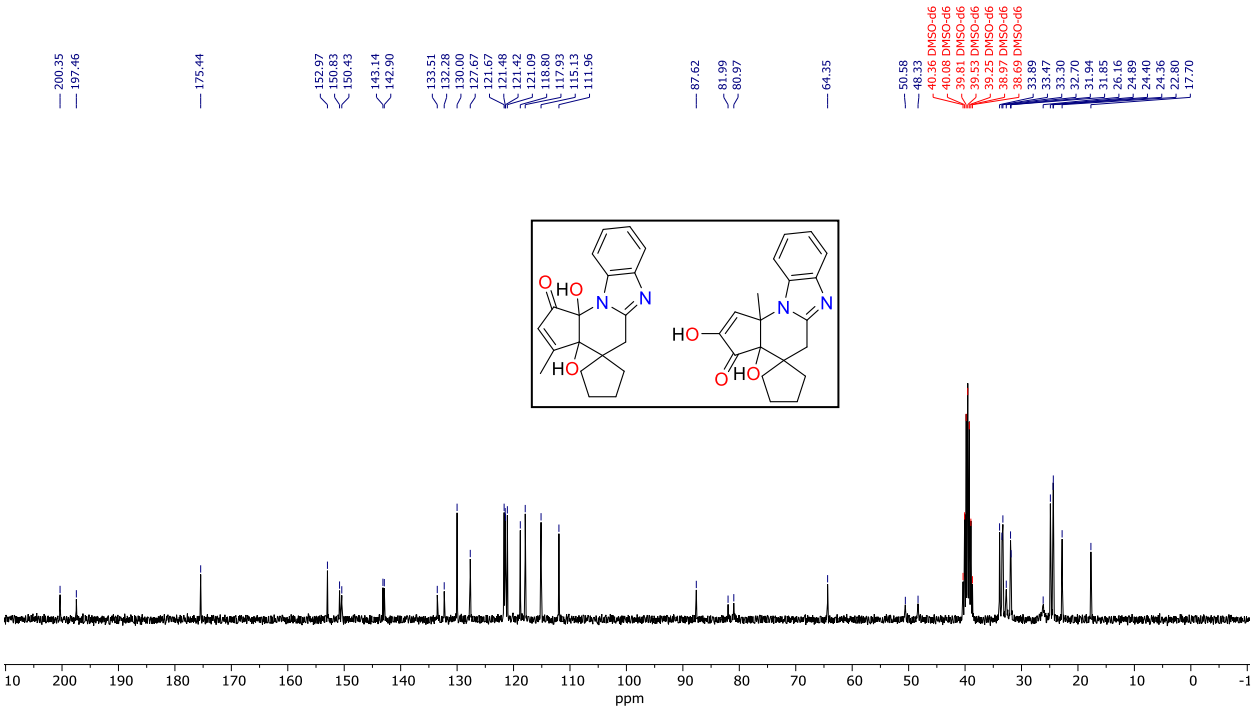
^{13}C {^{1}H} NMR spectrum (126 MHz) of mixture of **4d** and **5d** in DMSO-d_6



^{1}H NMR spectrum (300 MHz) of mixture of **4e** and **5e** in DMSO-d_6

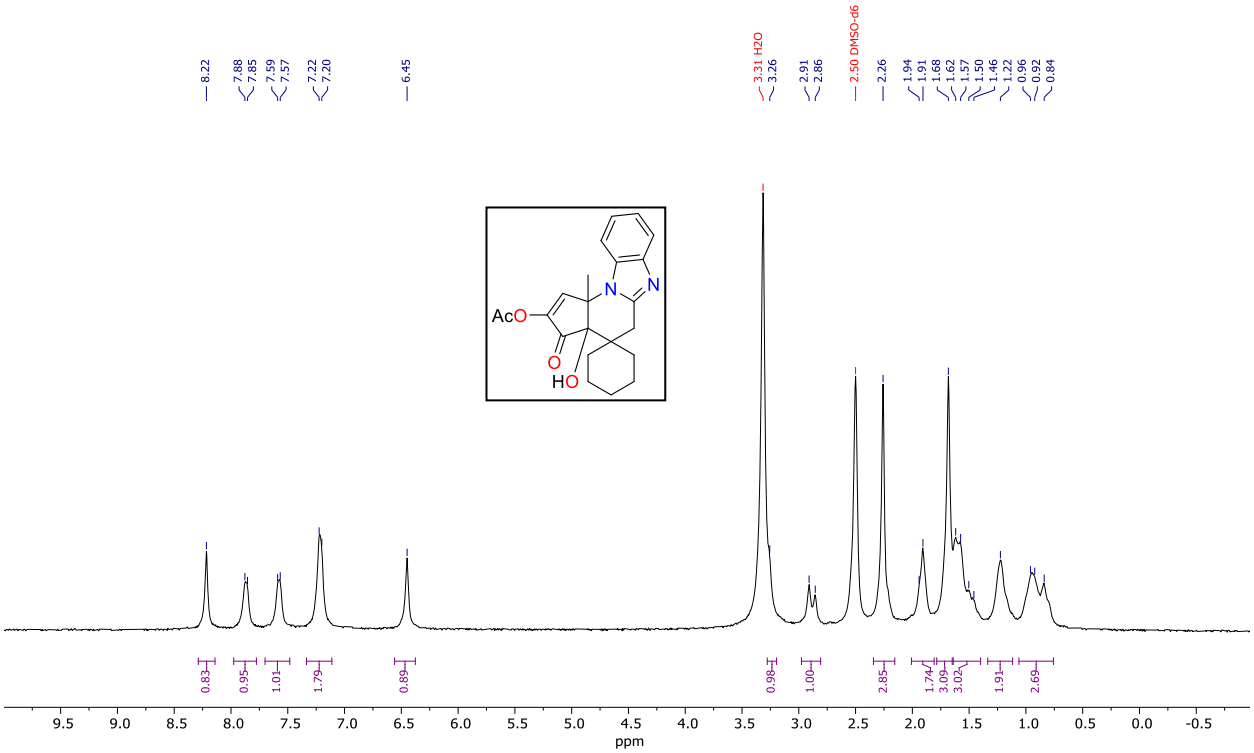


^{13}C {^{1}H} NMR spectrum (75 MHz) of mixture of **4e** and **5e** in DMSO-d_6

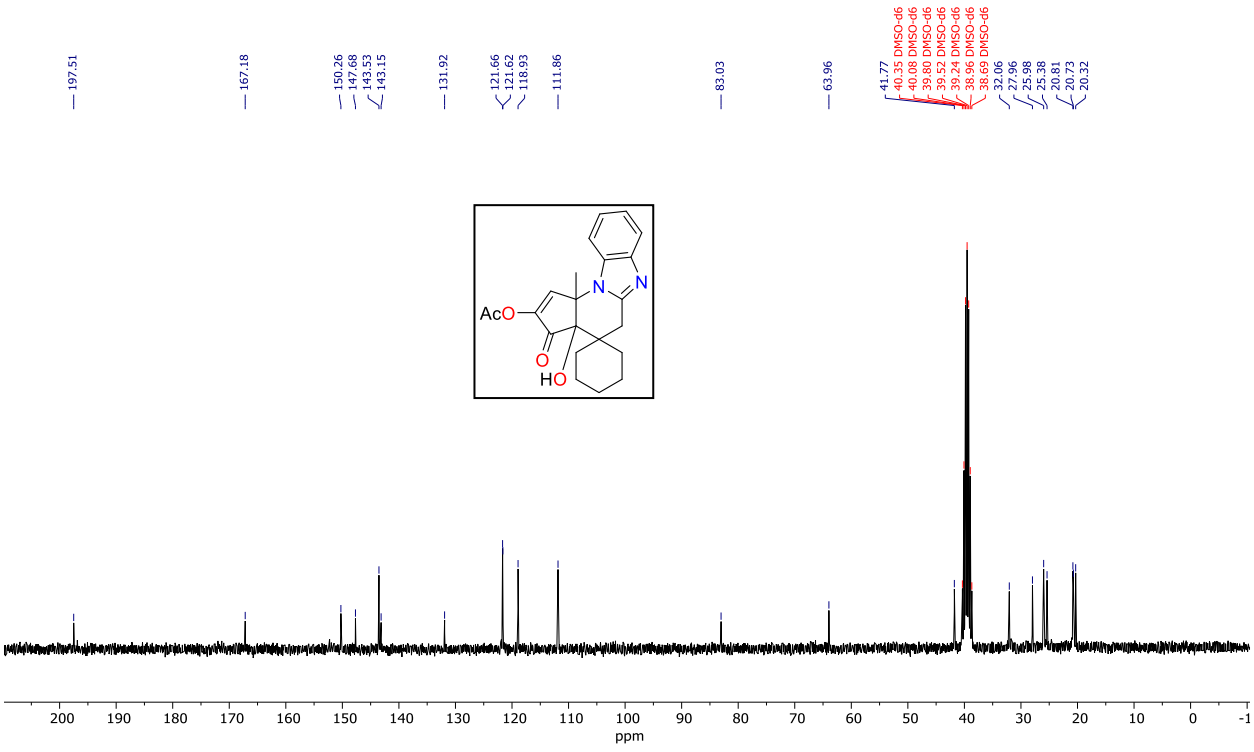


4.3. Derivatization products **10-13**

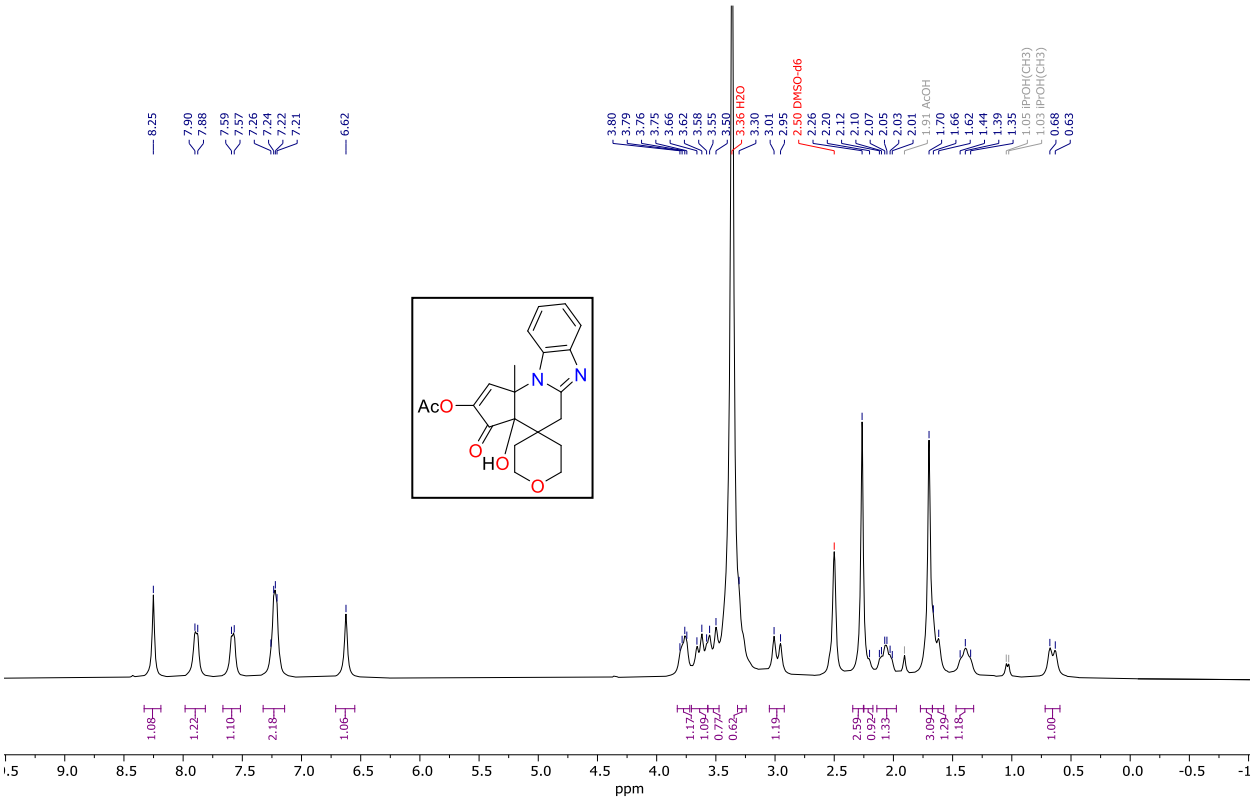
^{1}H NMR spectrum (300 MHz) of **10a** in DMSO-d_6



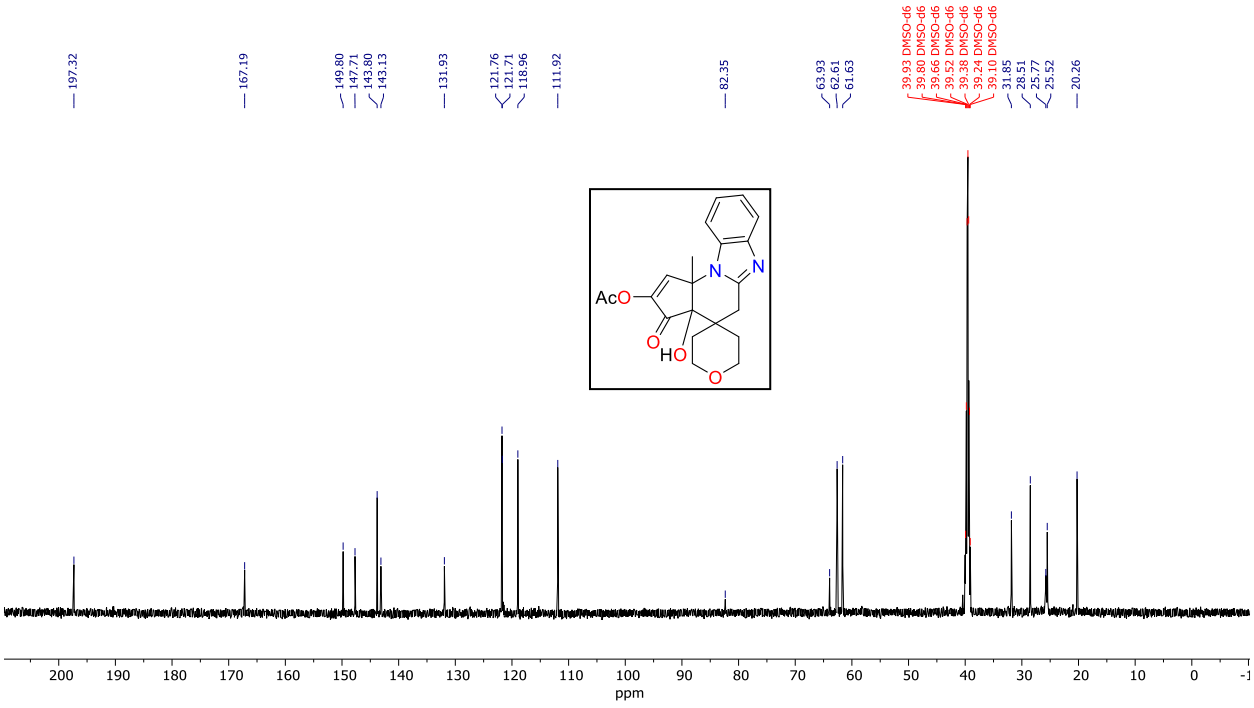
^{13}C {^{1}H} NMR spectrum (75 MHz) of **10a** in DMSO-d_6



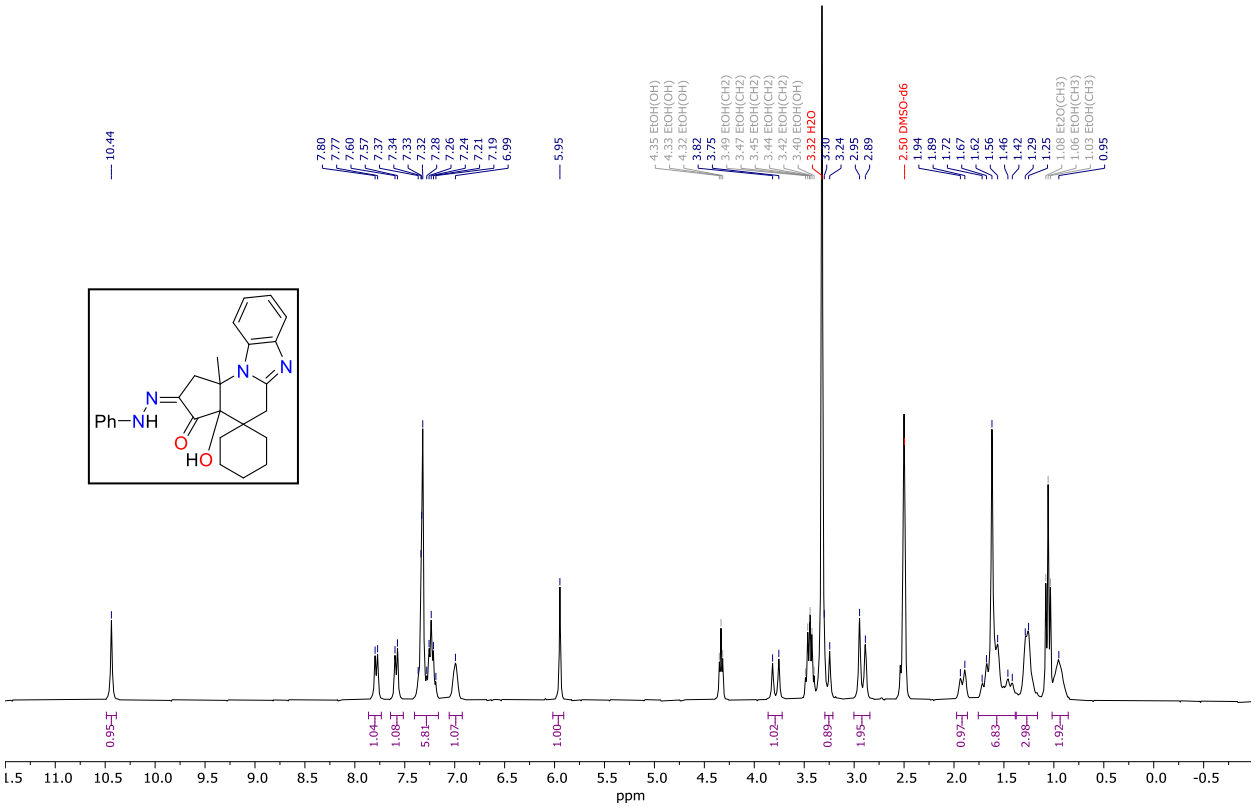
^{1}H NMR spectrum (300 MHz) of **10b** in DMSO-d_6



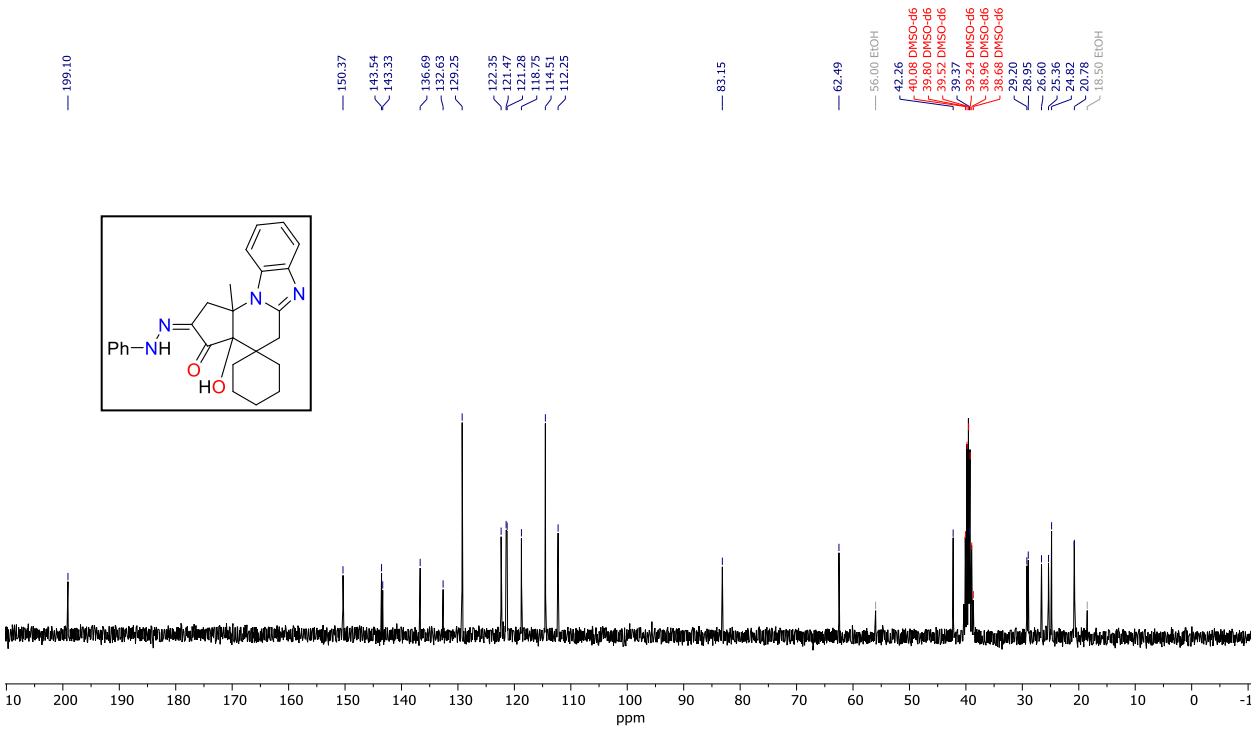
^{13}C {^{1}H} NMR spectrum (151 MHz) of **10b** in DMSO-d_6



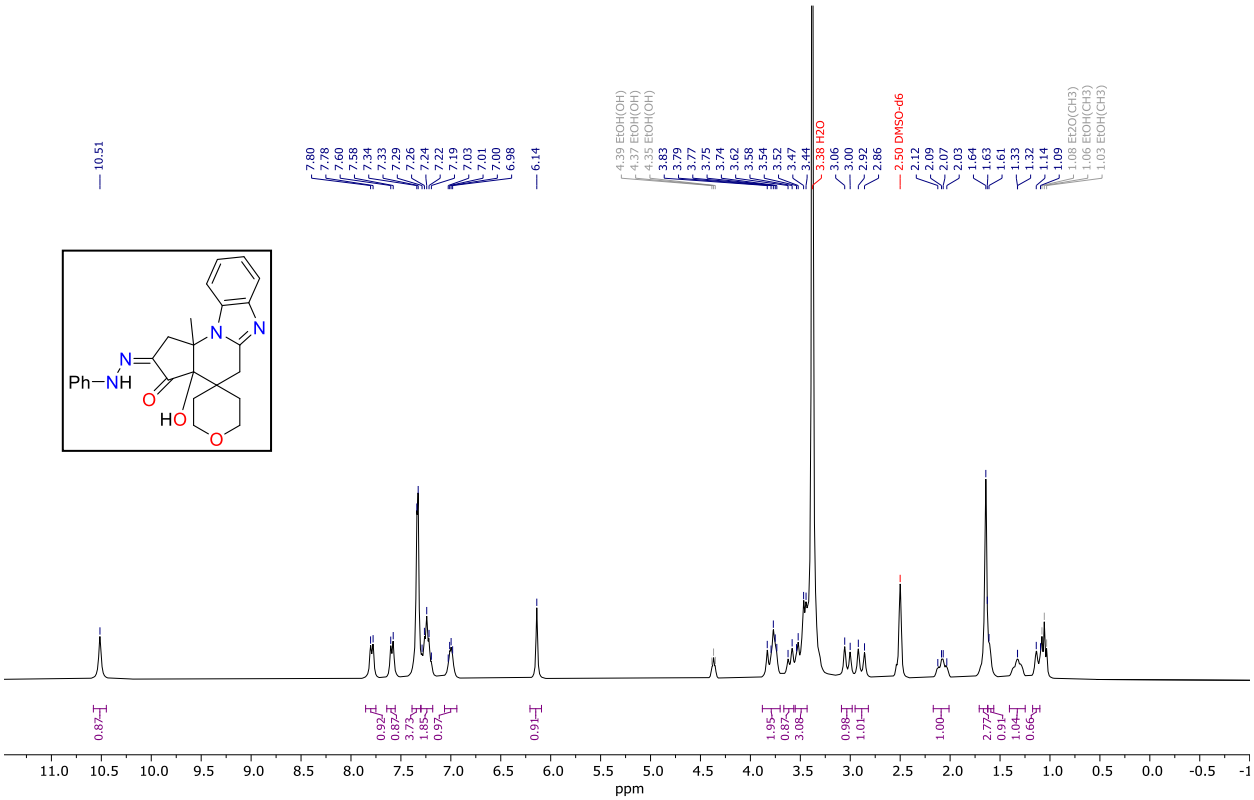
^{1}H NMR spectrum (300 MHz) of **11a** in DMSO-d_6



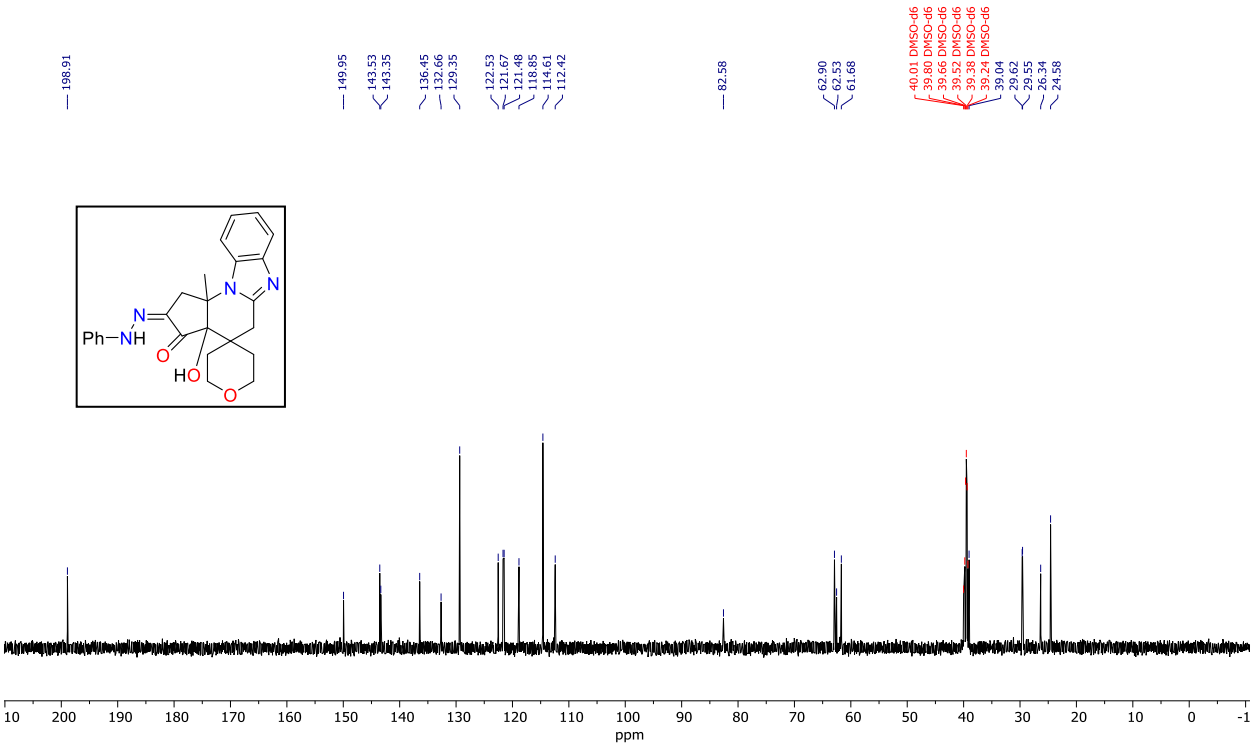
^{13}C {^{1}H} NMR spectrum (75 MHz) of **11a** in DMSO-d_6



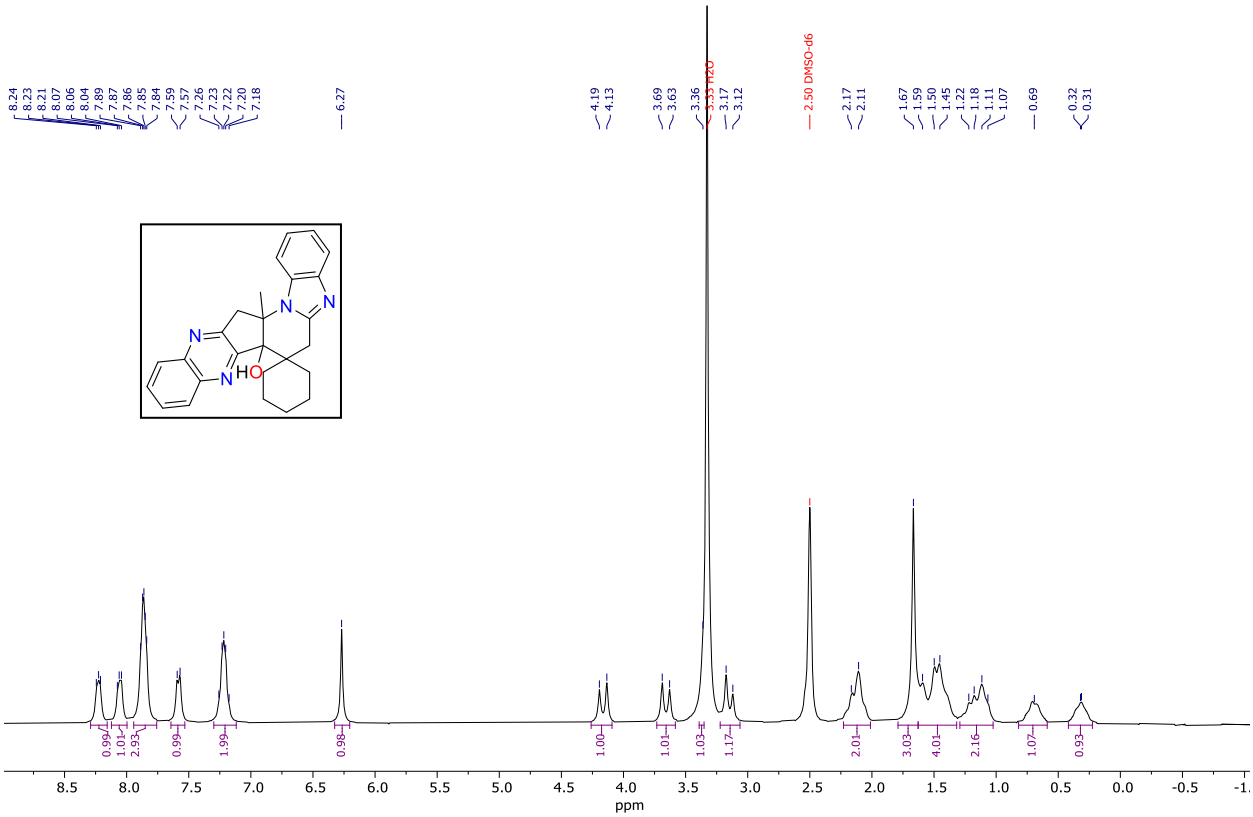
^{1}H NMR spectrum (300 MHz) of **11b** in DMSO-d_6



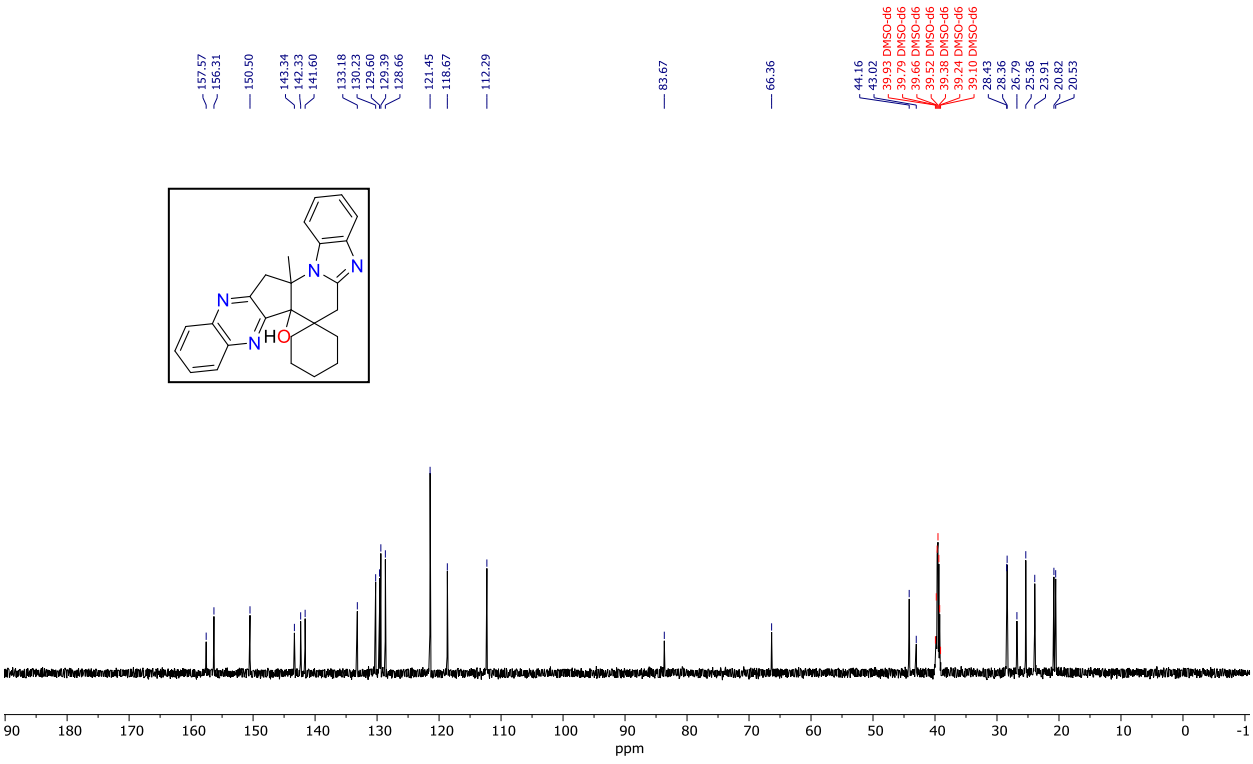
^{13}C {^{1}H} NMR spectrum (151 MHz) of **11b** in DMSO-d_6



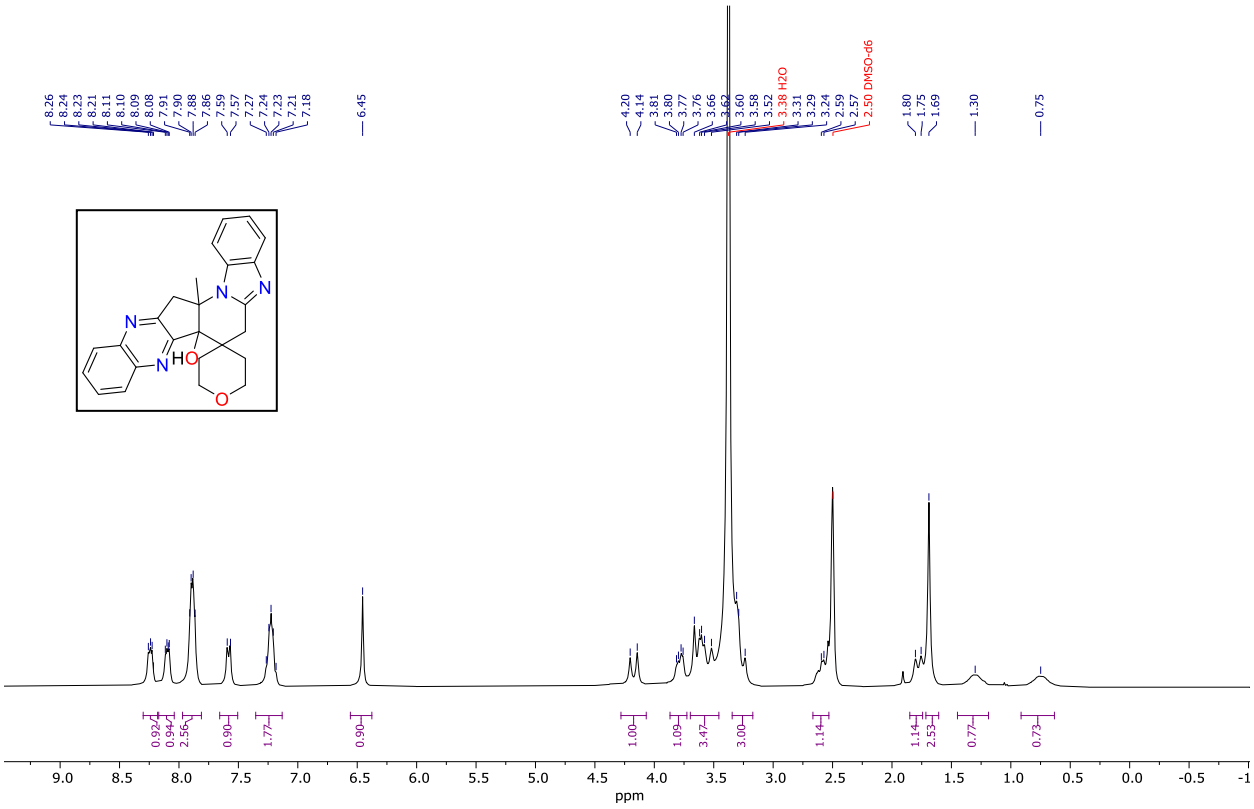
^{1}H NMR spectrum (300 MHz) of **12a** in DMSO-d_6



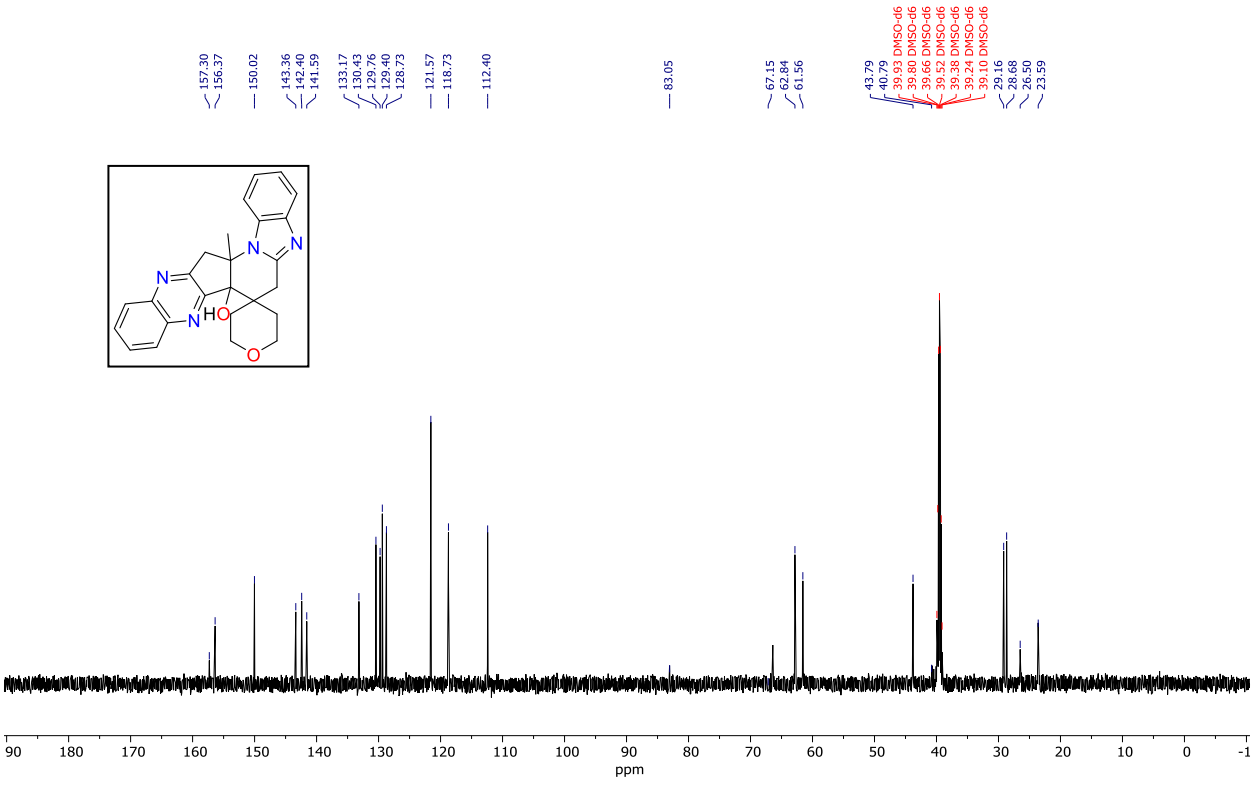
^{13}C {^{1}H} NMR spectrum (151 MHz) of **12a** in DMSO-d_6



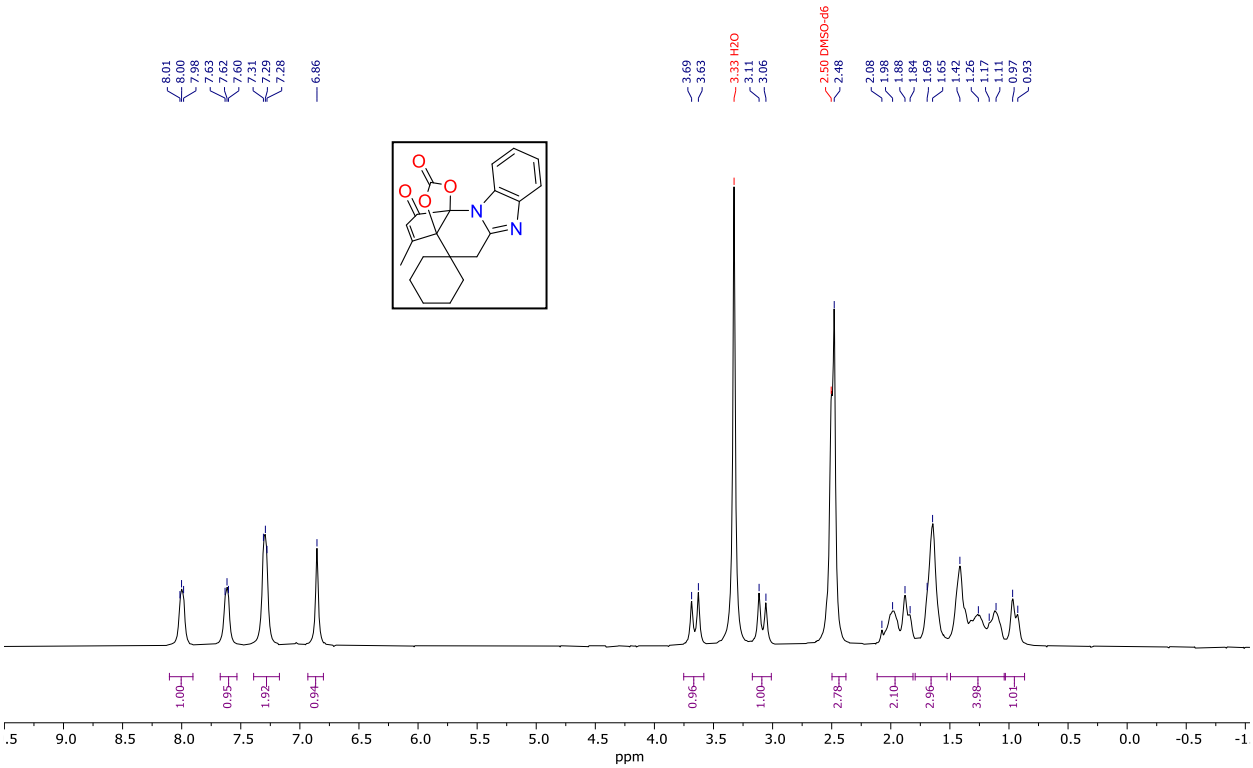
^{1}H NMR spectrum (300 MHz) of **12b** in DMSO-d_6



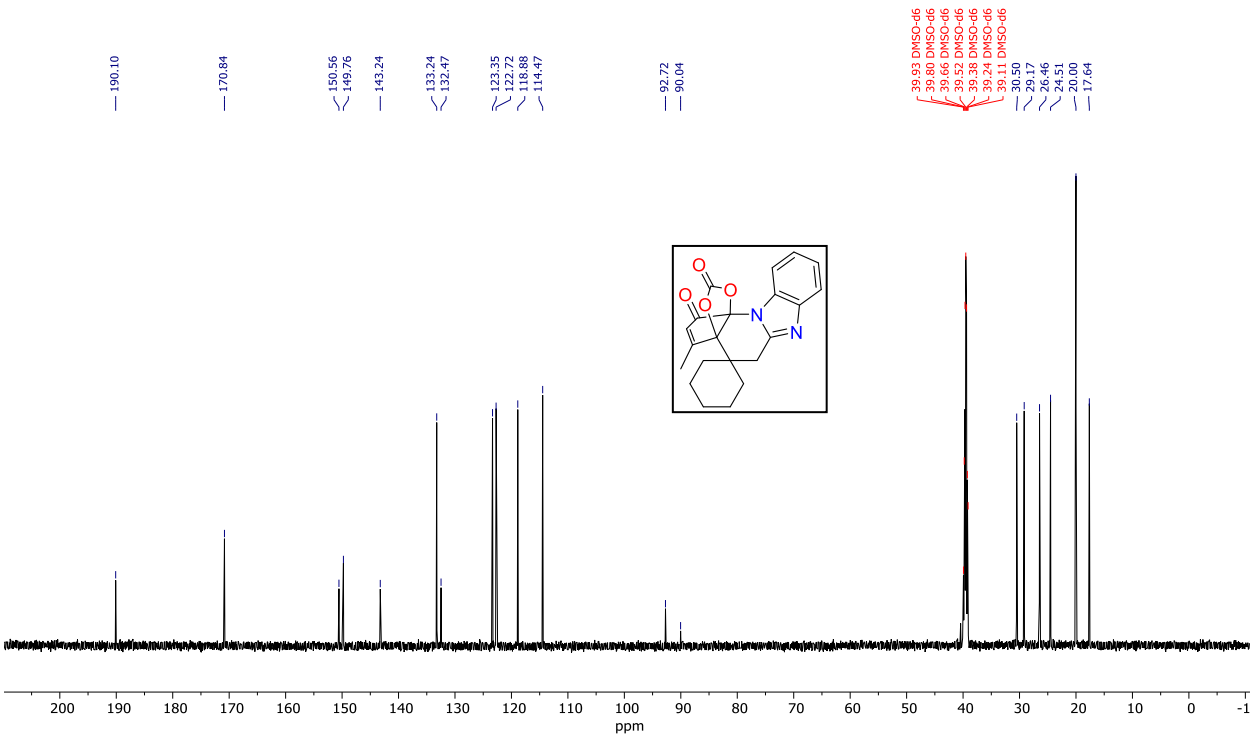
^{13}C {^{1}H} NMR spectrum (151 MHz) of **12b** in DMSO-d_6



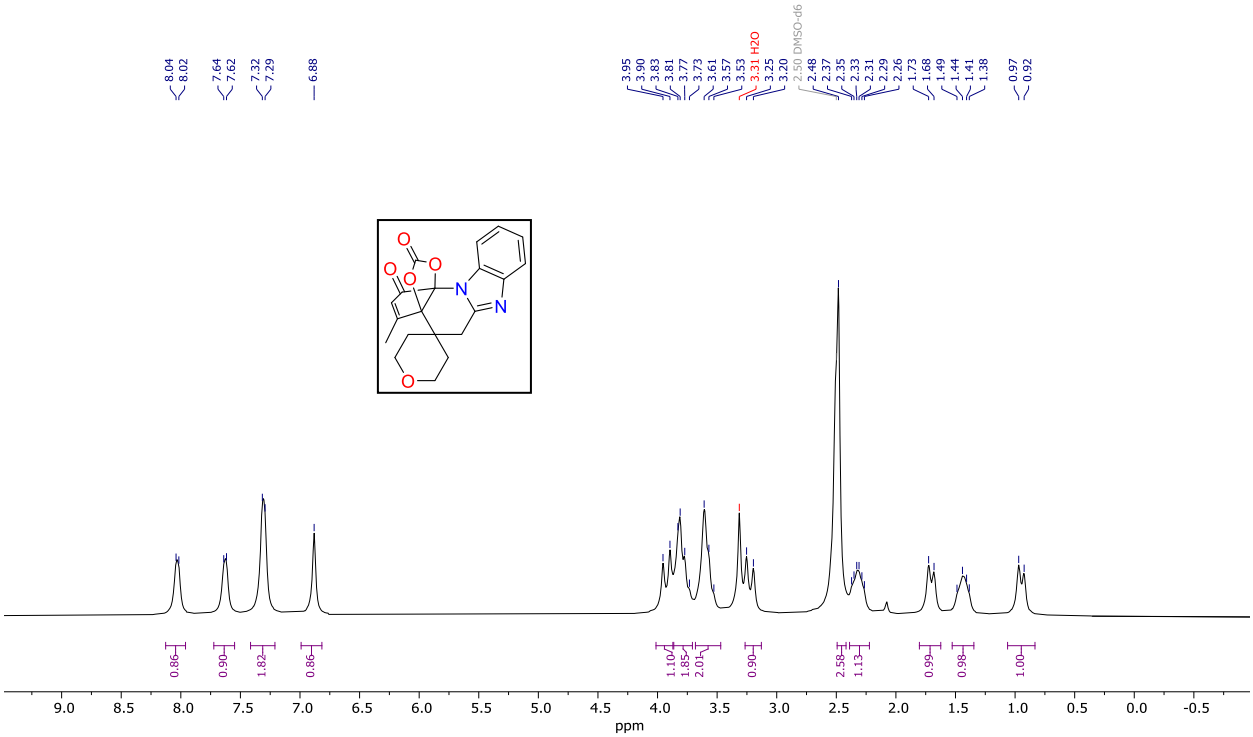
^{1}H NMR spectrum (300 MHz) of **13a** in DMSO-d_6



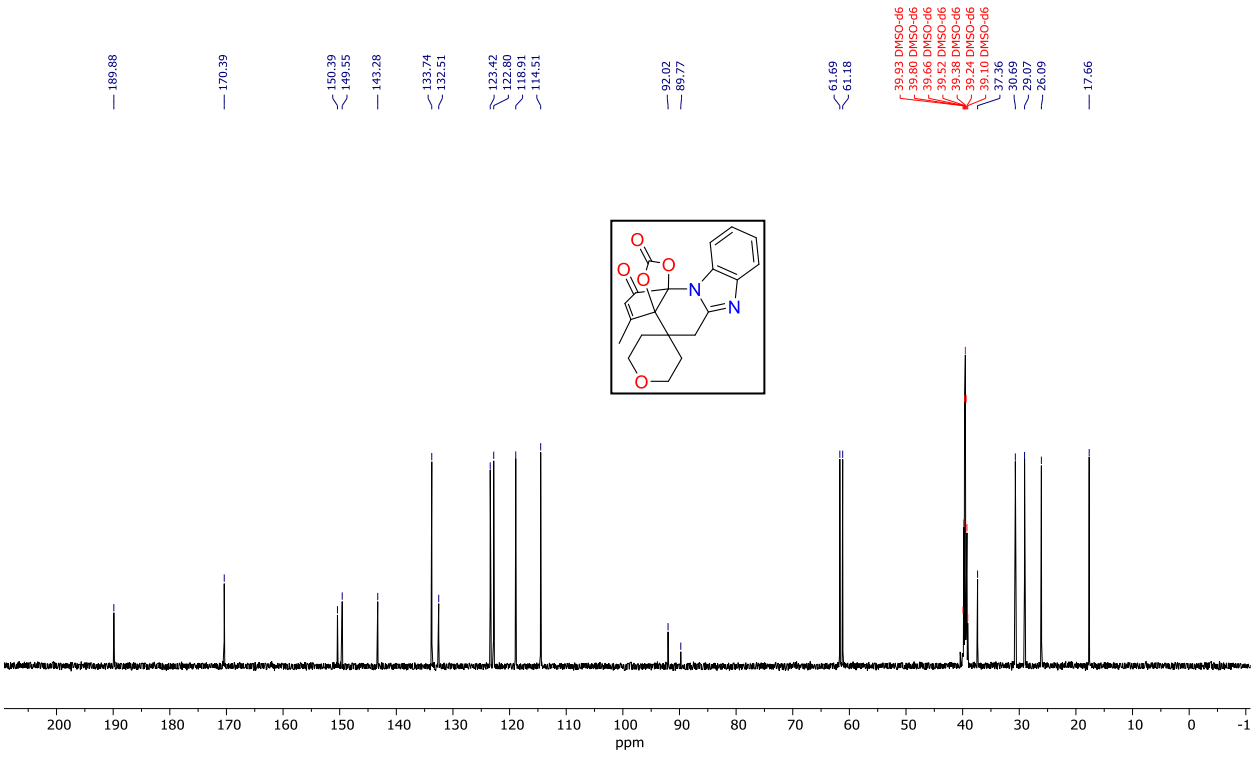
^{13}C {^{1}H} NMR spectrum (151 MHz) of **13a** in DMSO-d_6



^{1}H NMR spectrum (300 MHz) of **13b** in DMSO-d_6

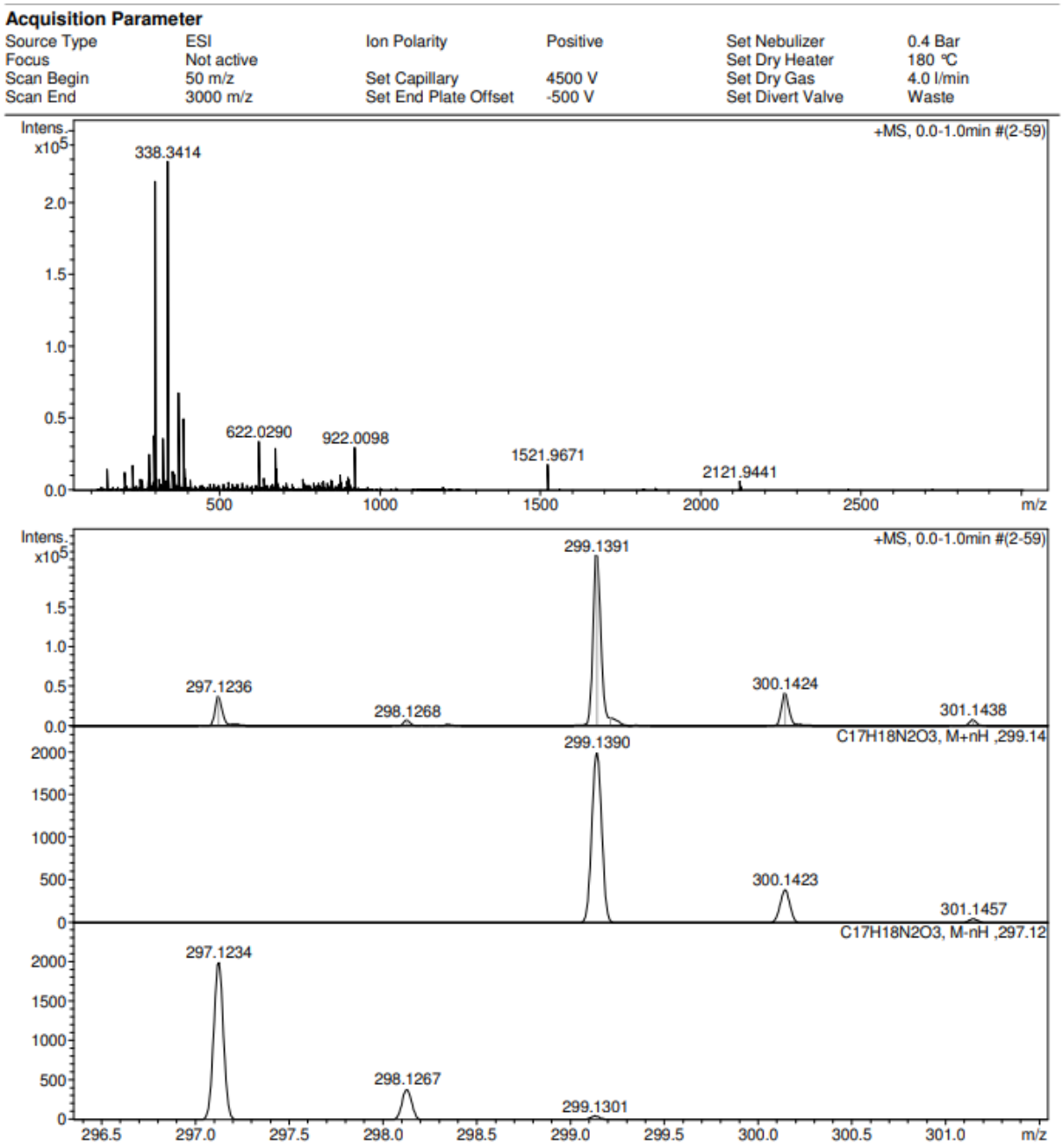


^{13}C {^{1}H} NMR spectrum (151 MHz) of **13b** in DMSO-d_6



5. Copies of HRMS for all compounds

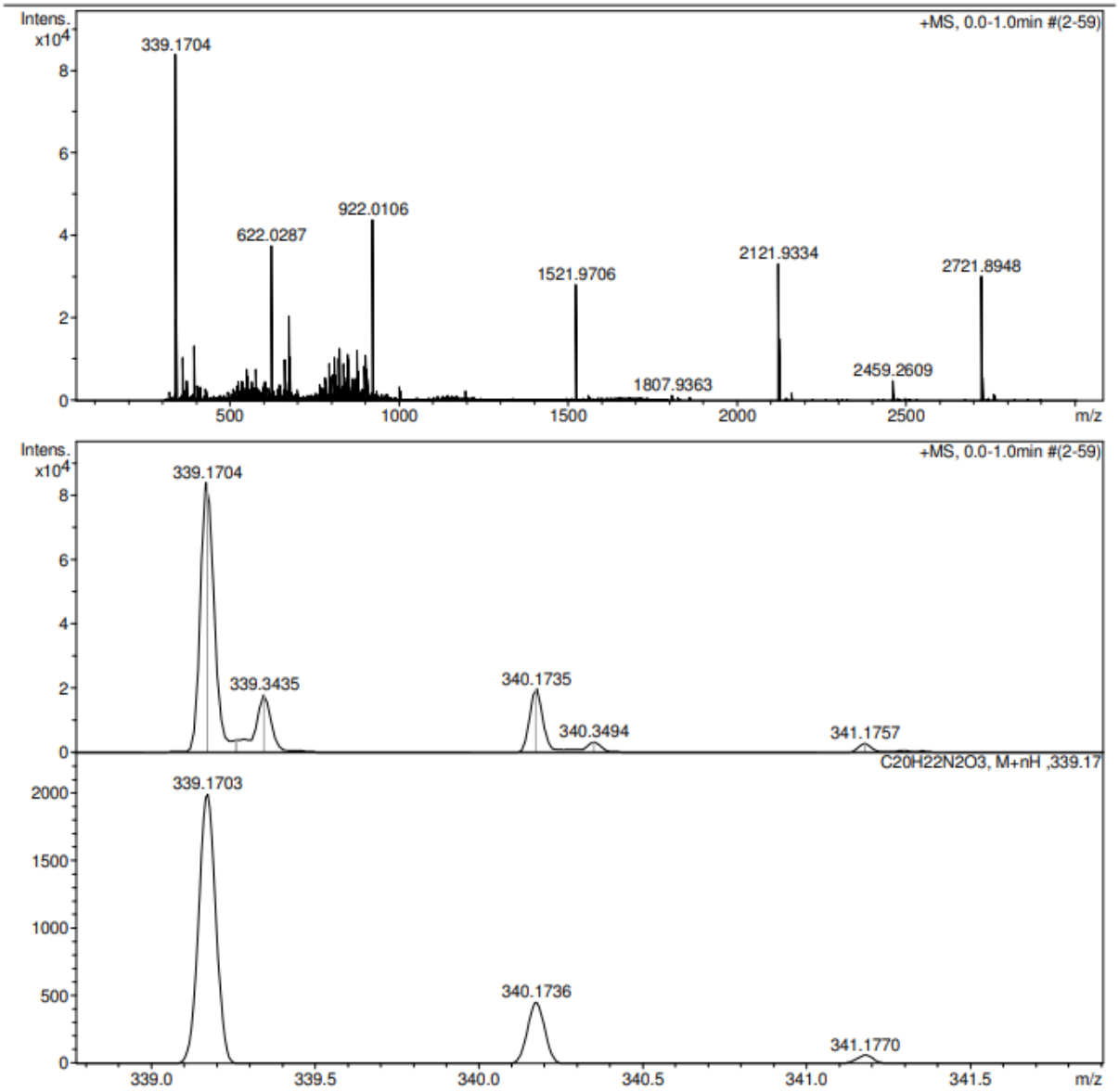
HRMS for compound **3a**



HRMS for compound **3b**

Acquisition Parameter

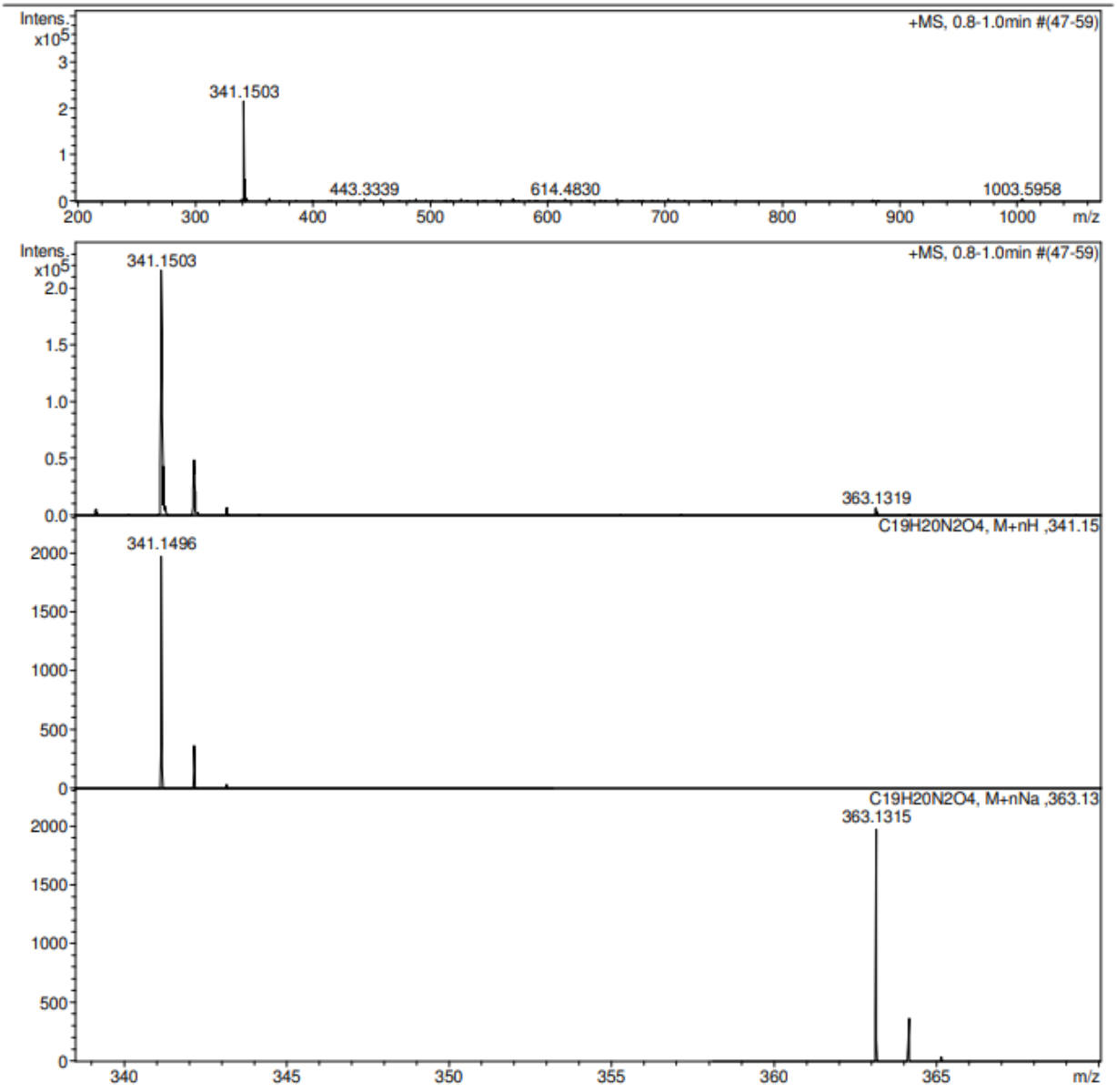
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **3c**

Acquisition Parameter

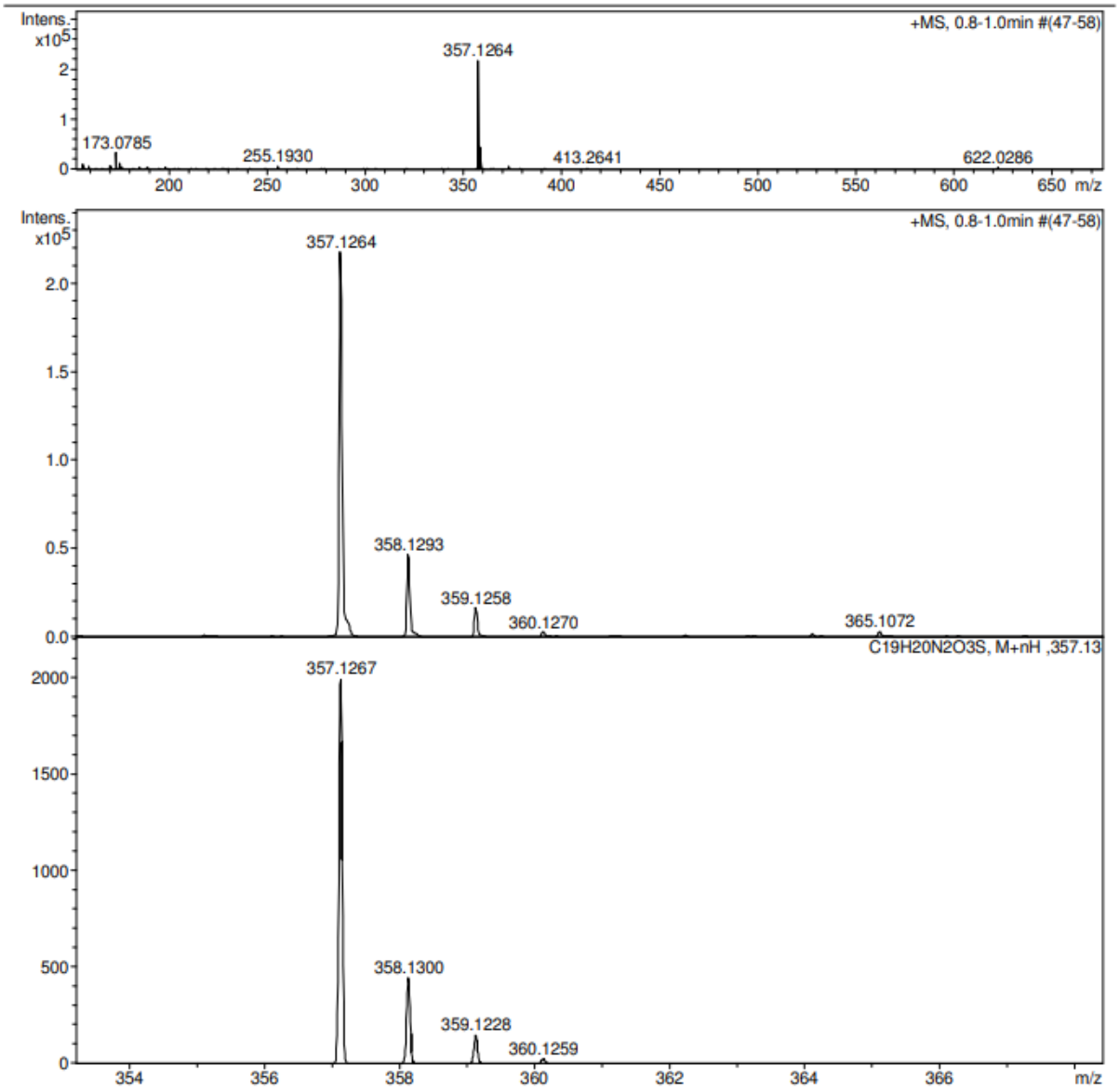
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **3d**

Acquisition Parameter

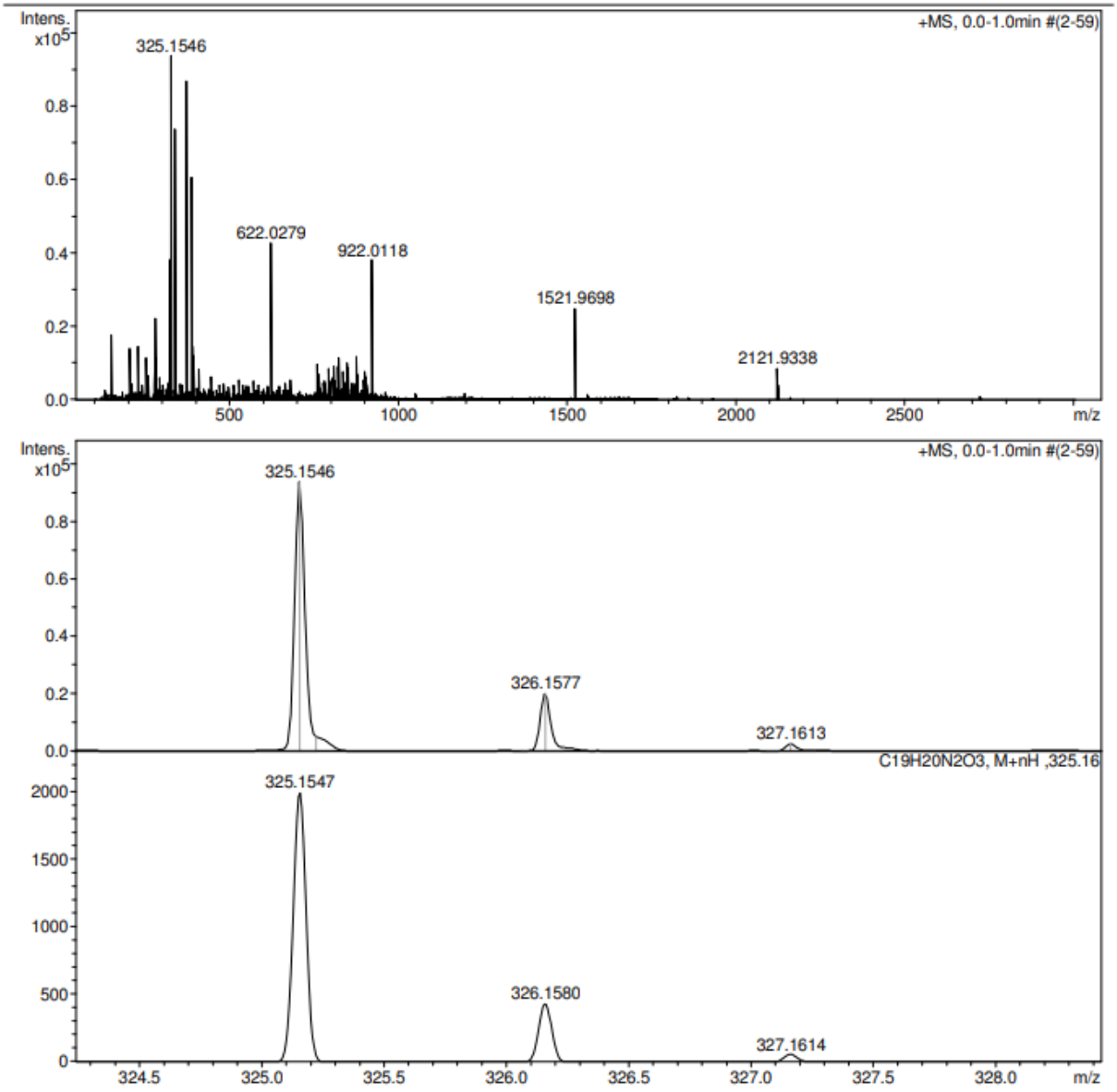
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **3e**

Acquisition Parameter

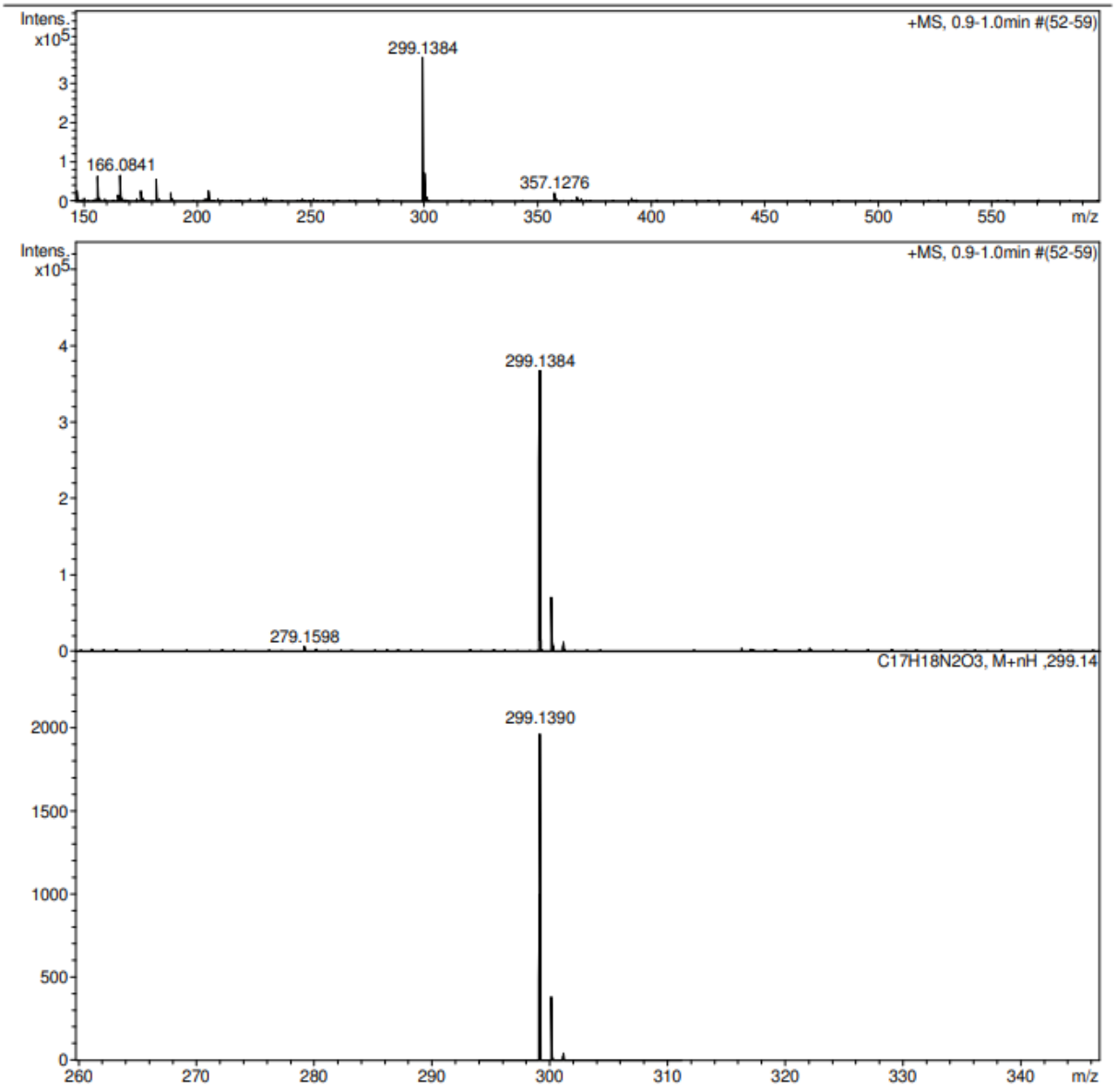
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



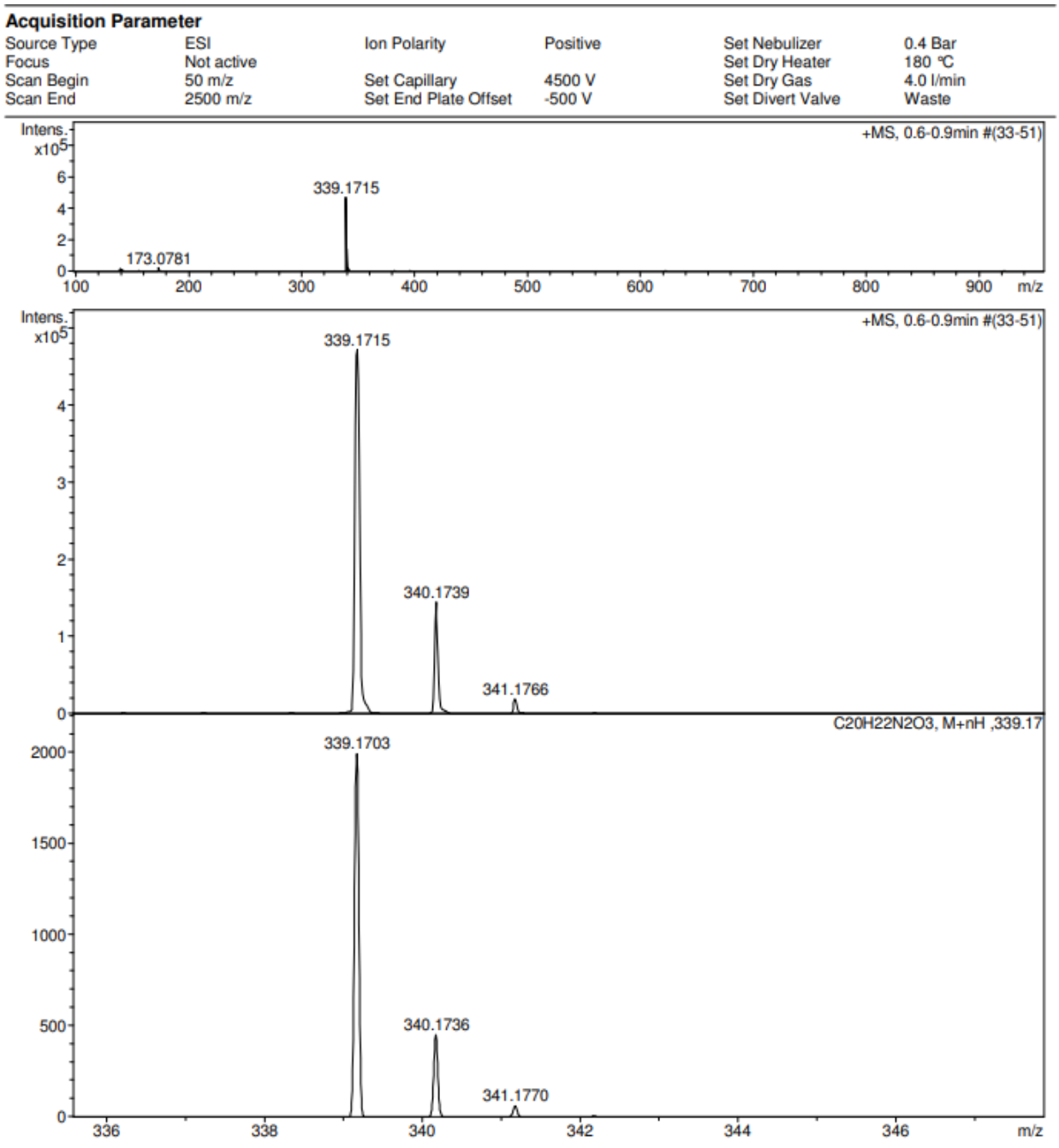
HRMS for mixture of isomers **4a** and **5a**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



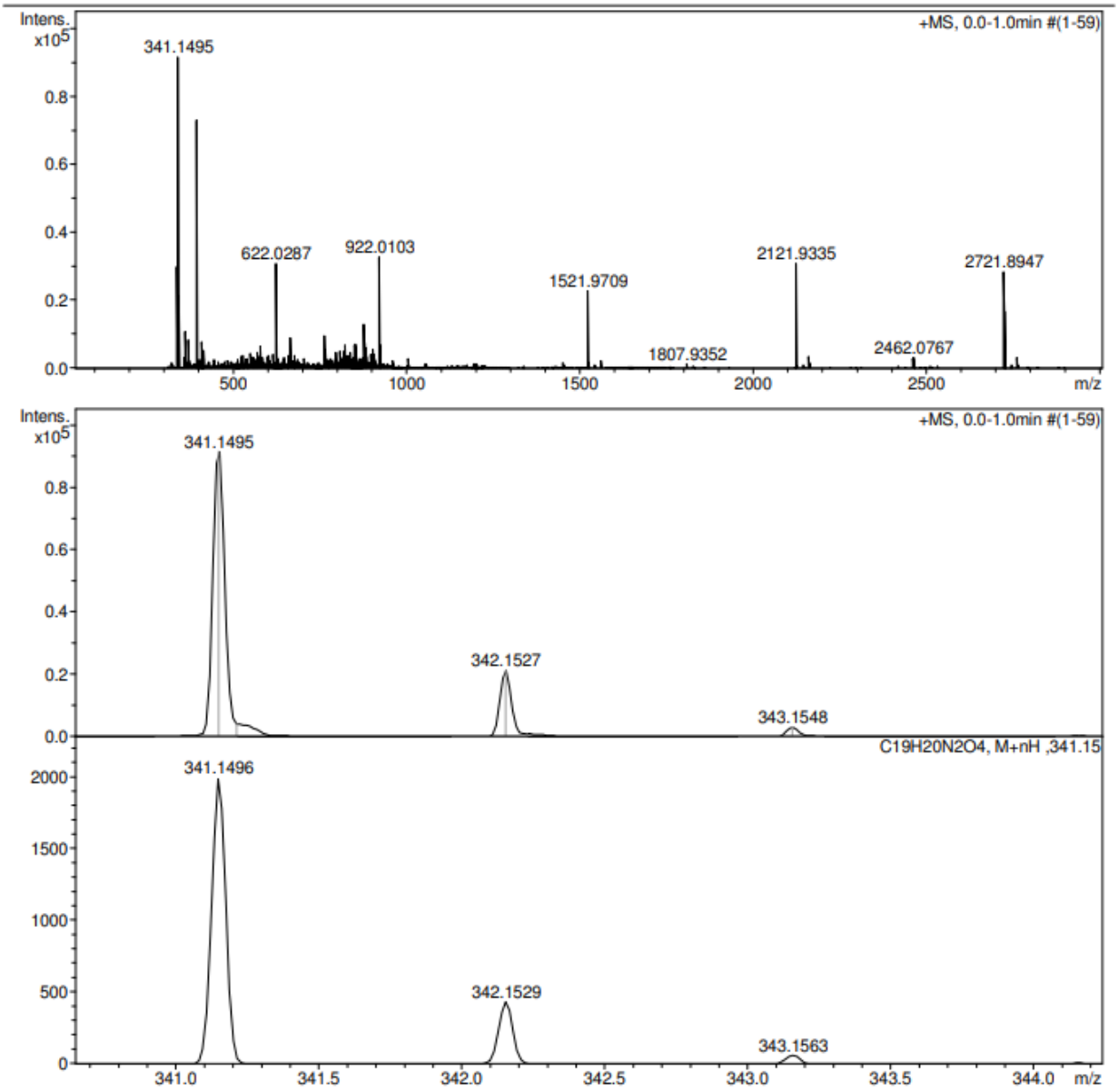
HRMS for mixture of isomers **4b** and **5b**



HRMS for mixture of isomers **4c** and **5c**

Acquisition Parameter

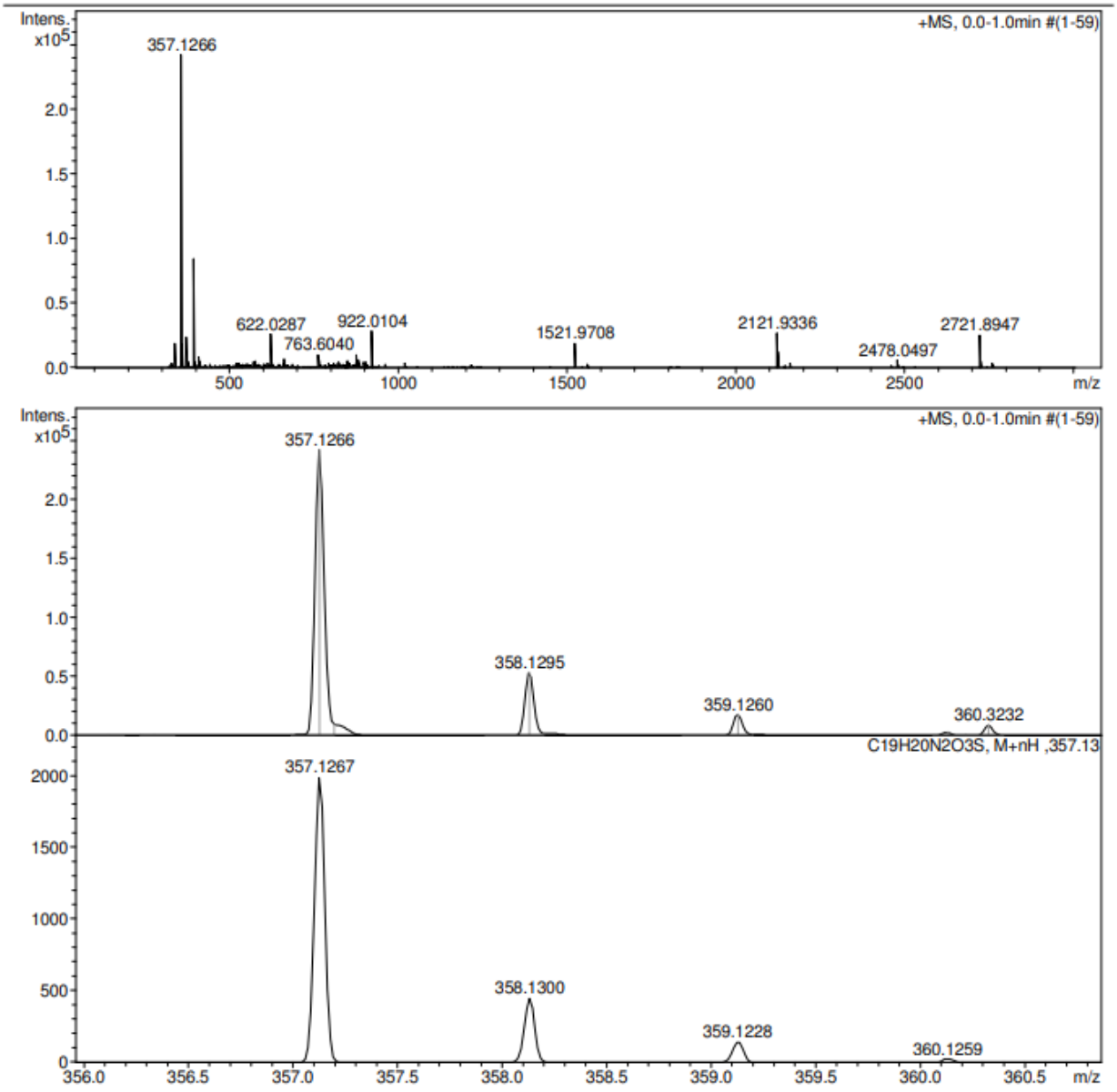
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for mixture of isomers **4d** and **5d**

Acquisition Parameter

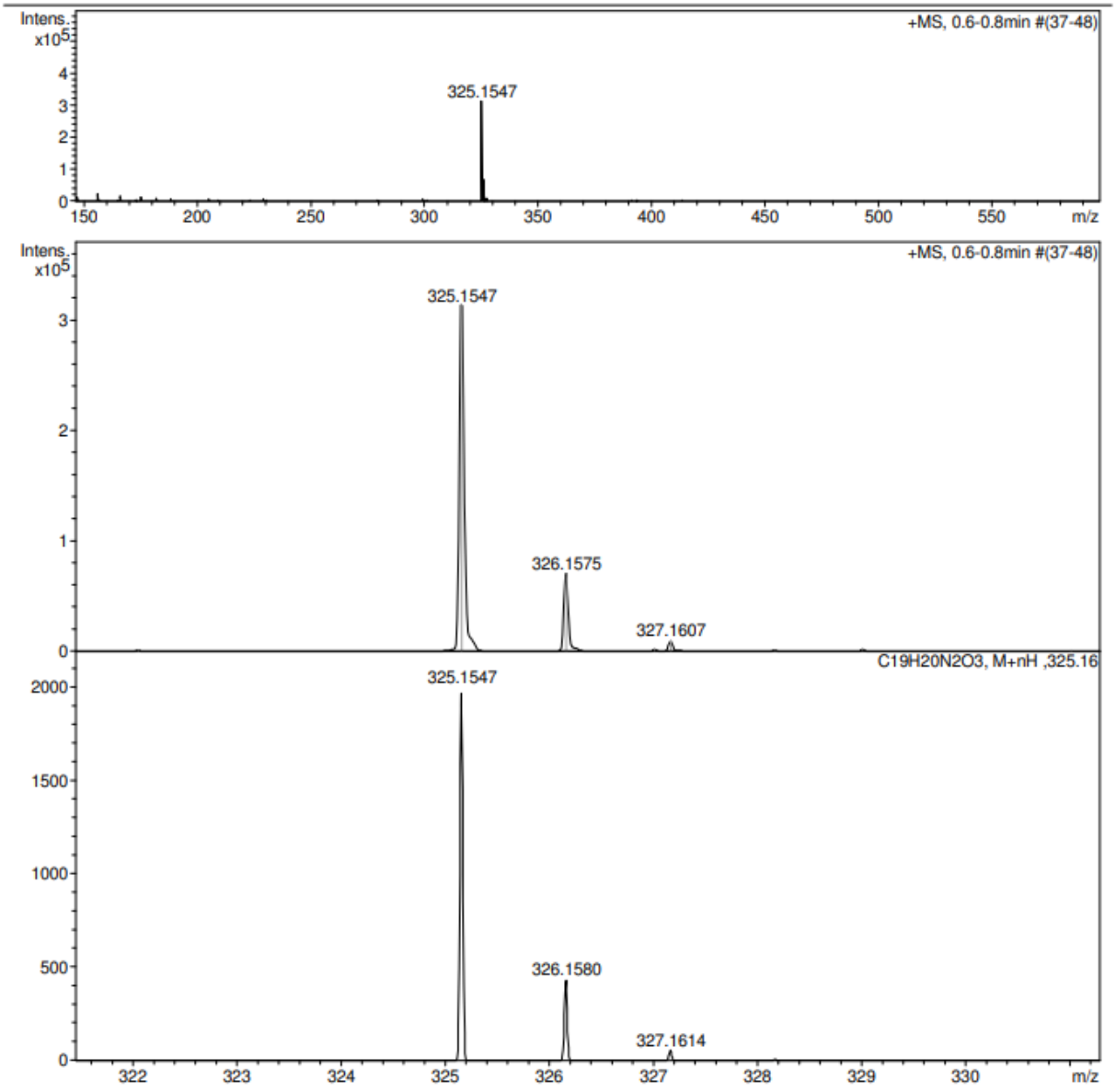
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for mixture of isomers **4e** and **5e**

Acquisition Parameter

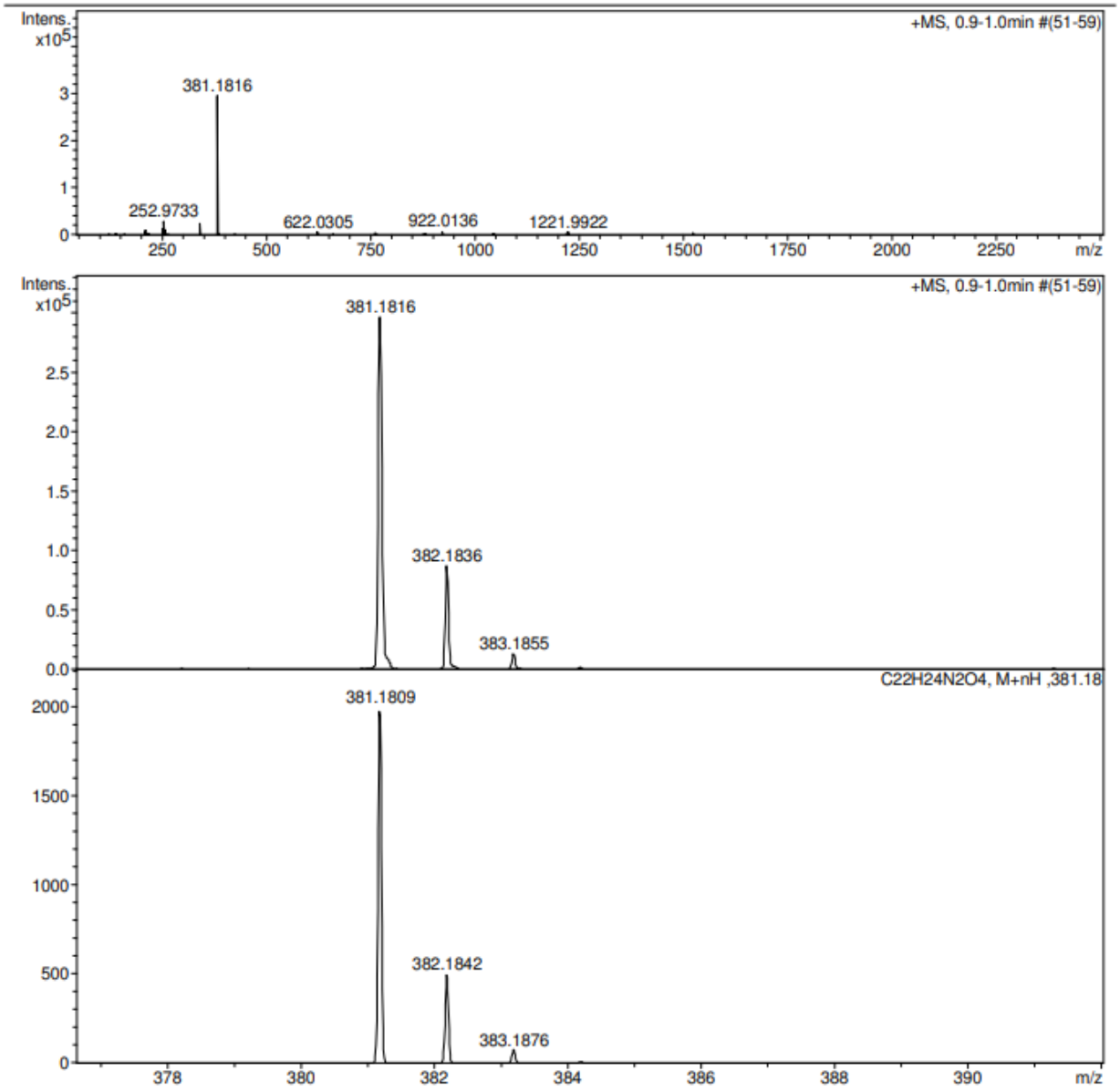
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **10a**

Acquisition Parameter

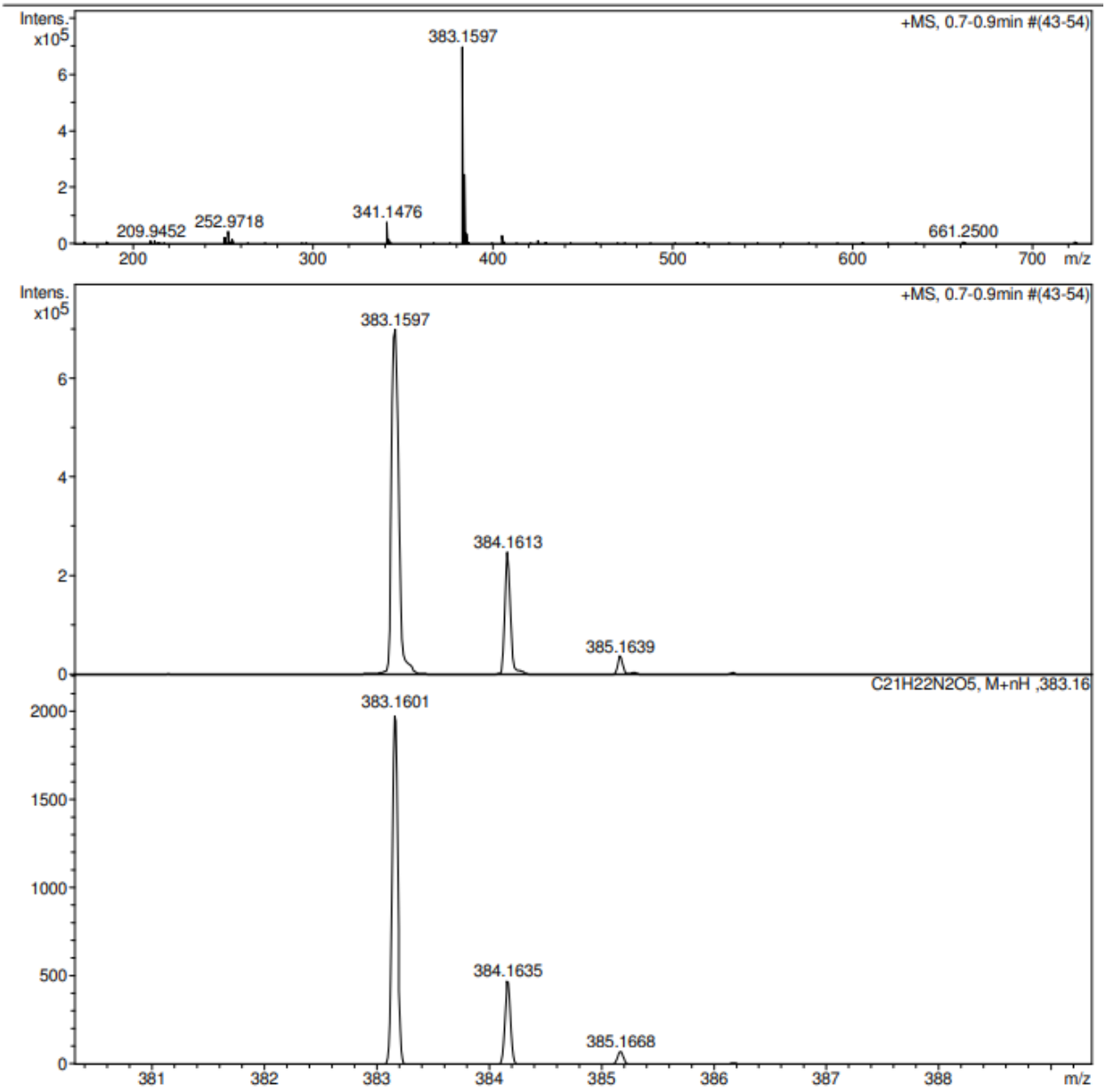
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **10b**

Acquisition Parameter

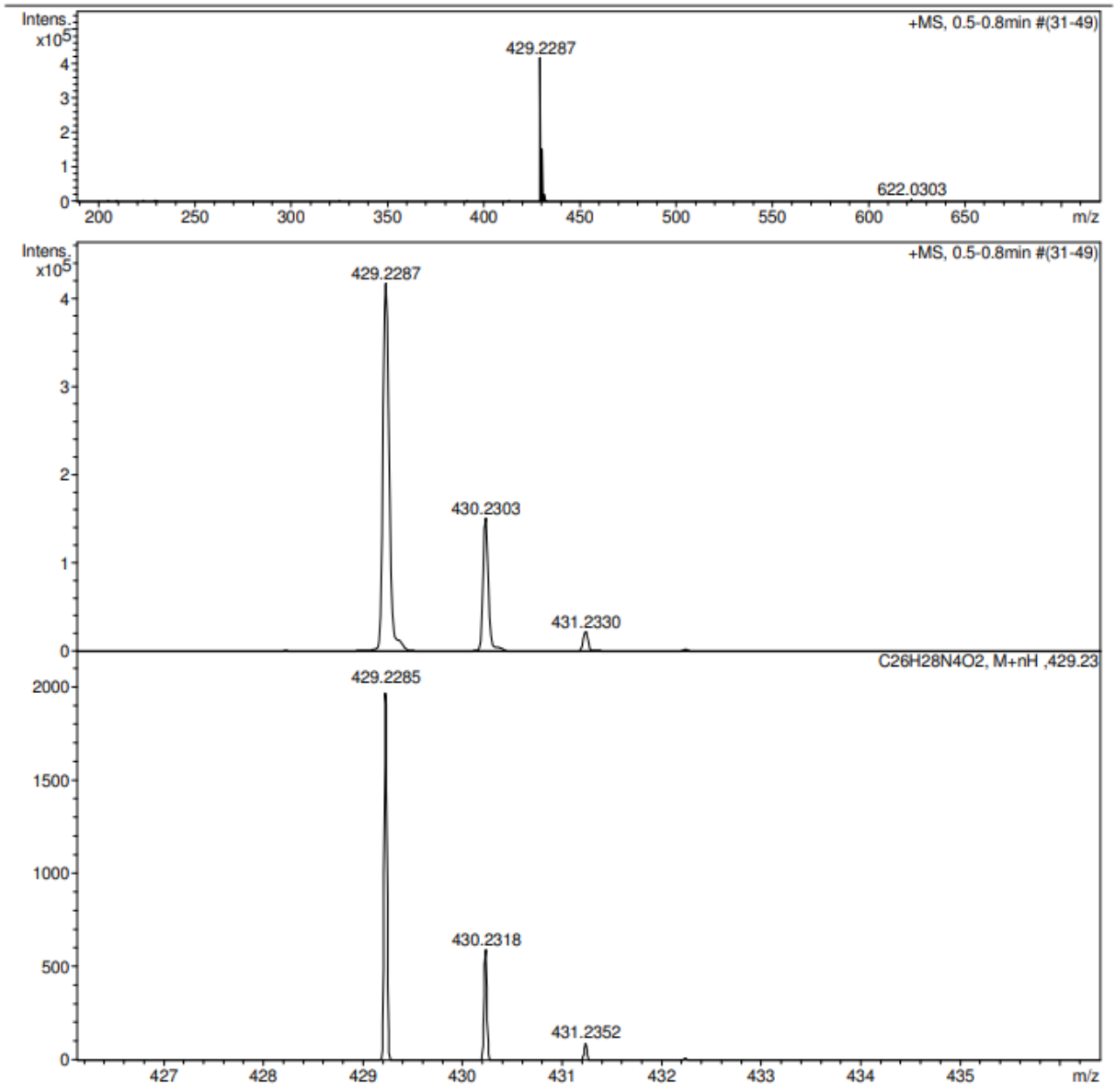
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **11a**

Acquisition Parameter

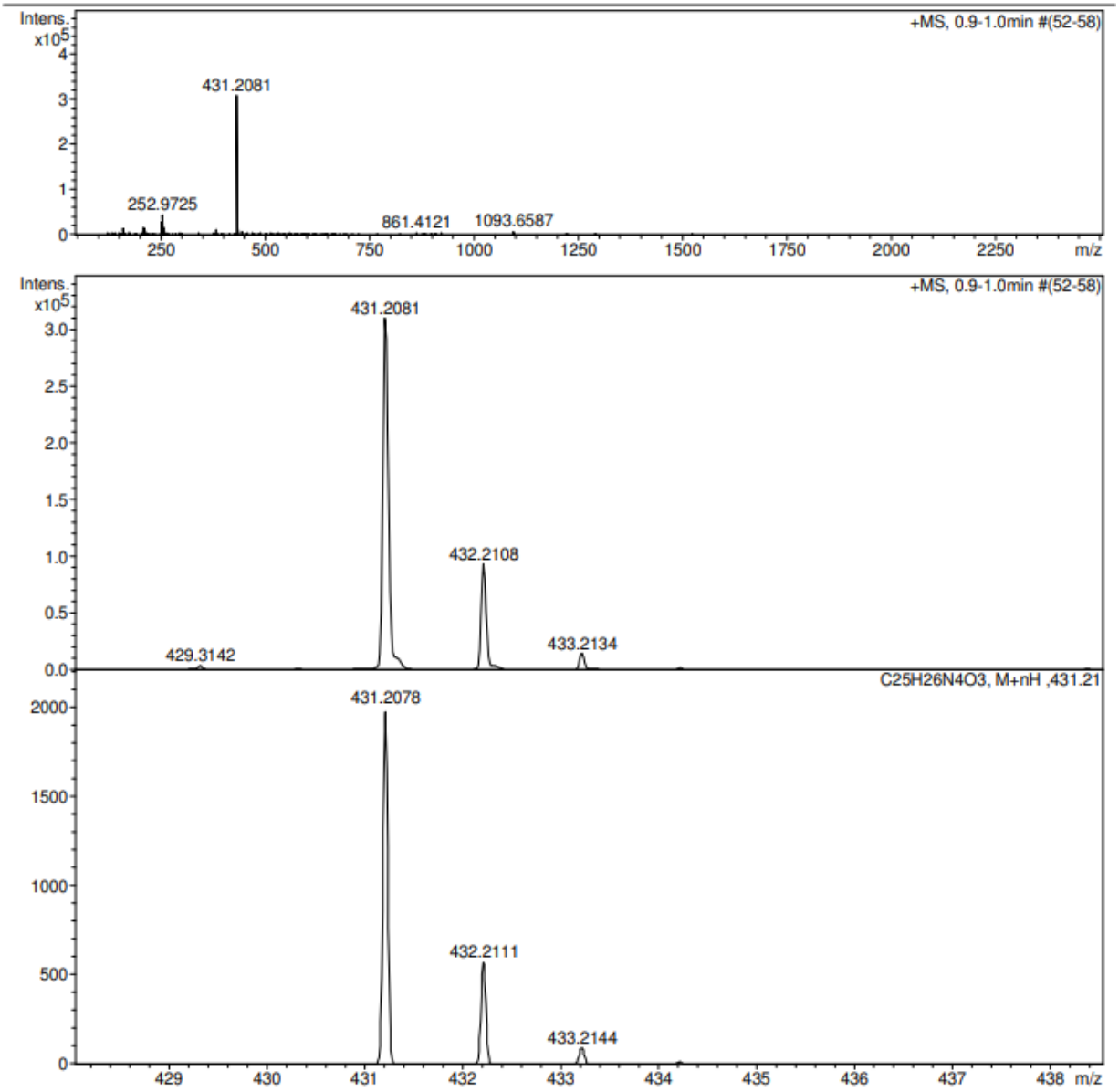
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **11b**

Acquisition Parameter

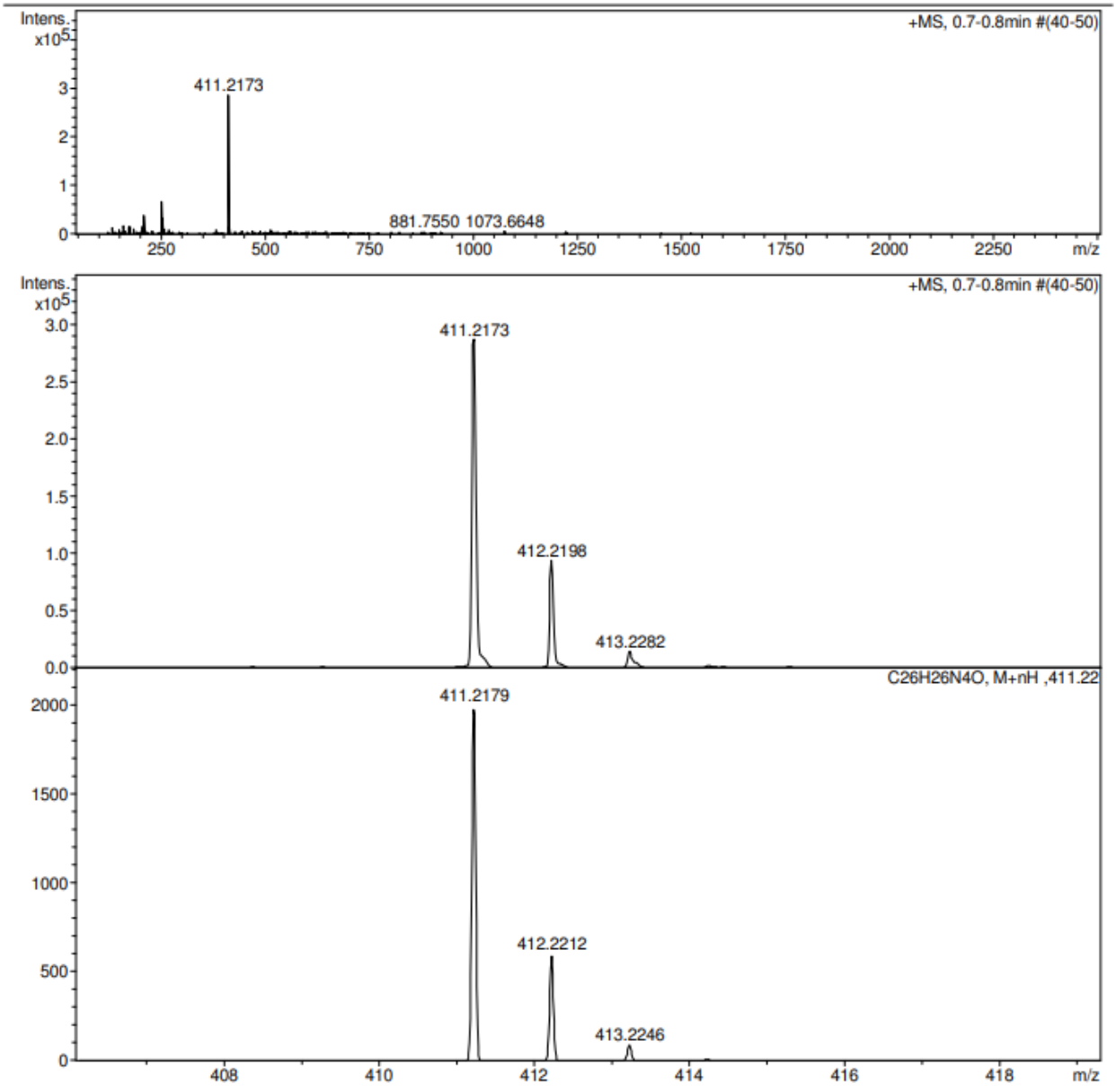
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **12a**

Acquisition Parameter

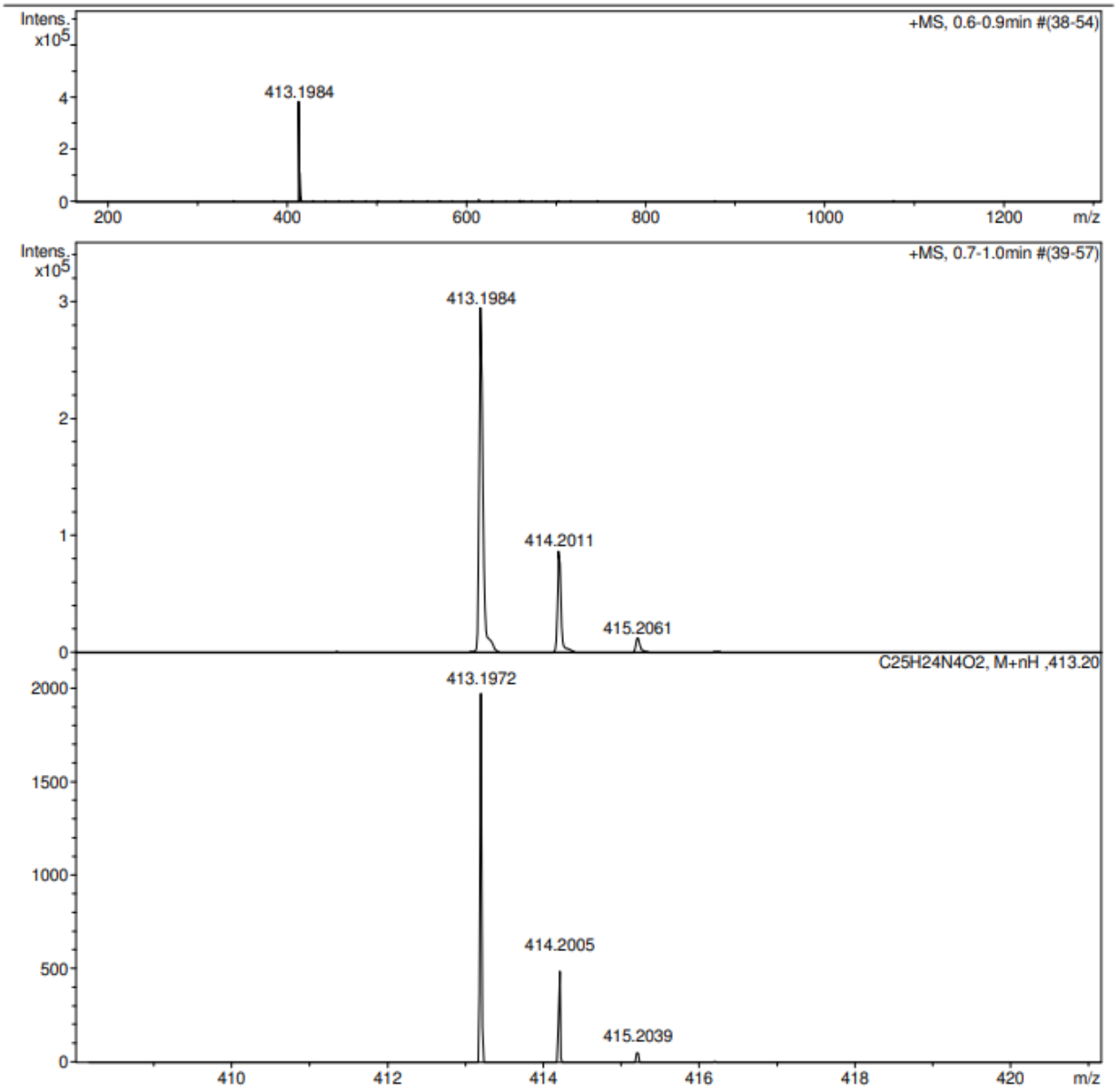
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **12b**

Acquisition Parameter

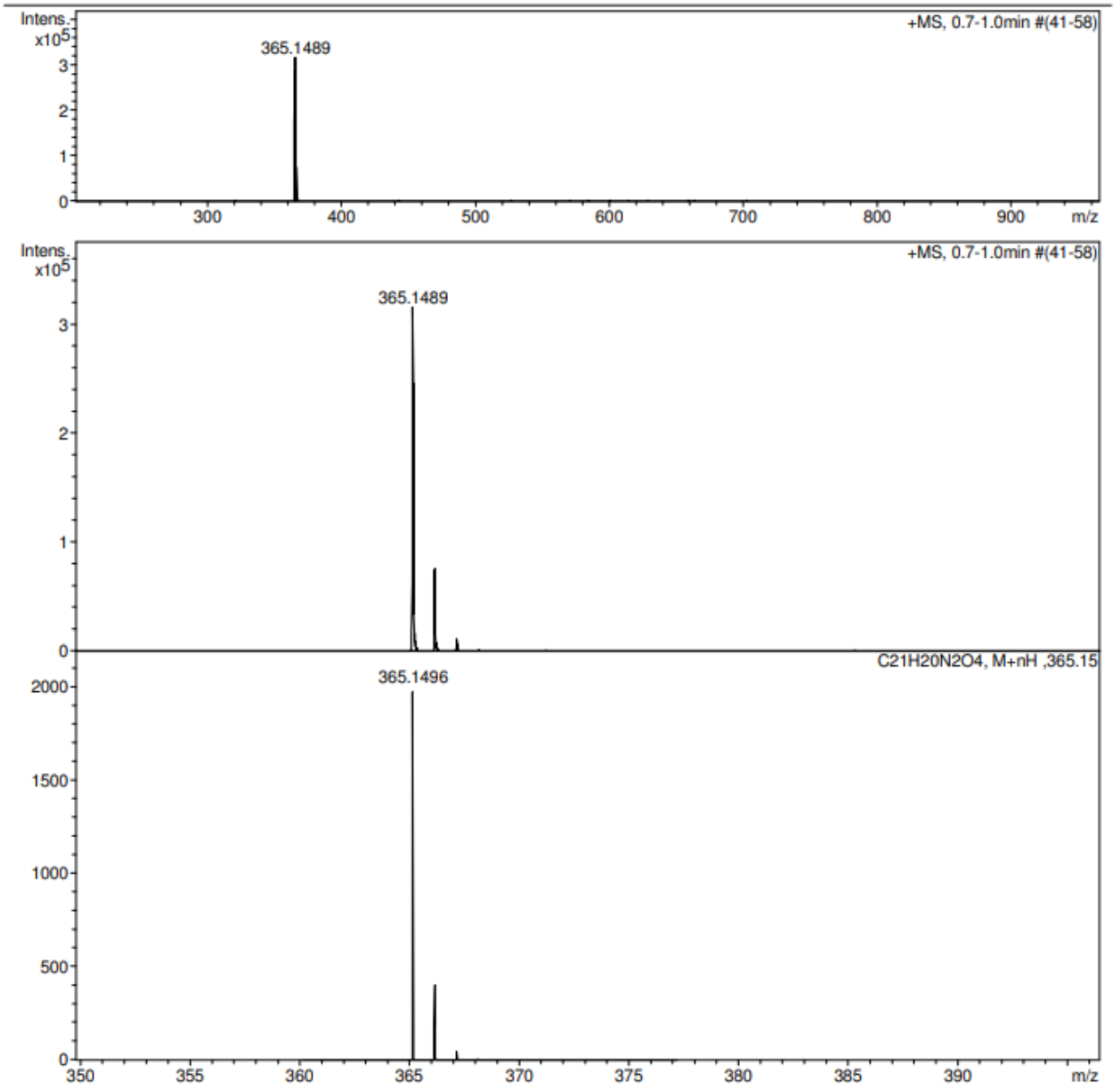
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **13a**

Acquisition Parameter

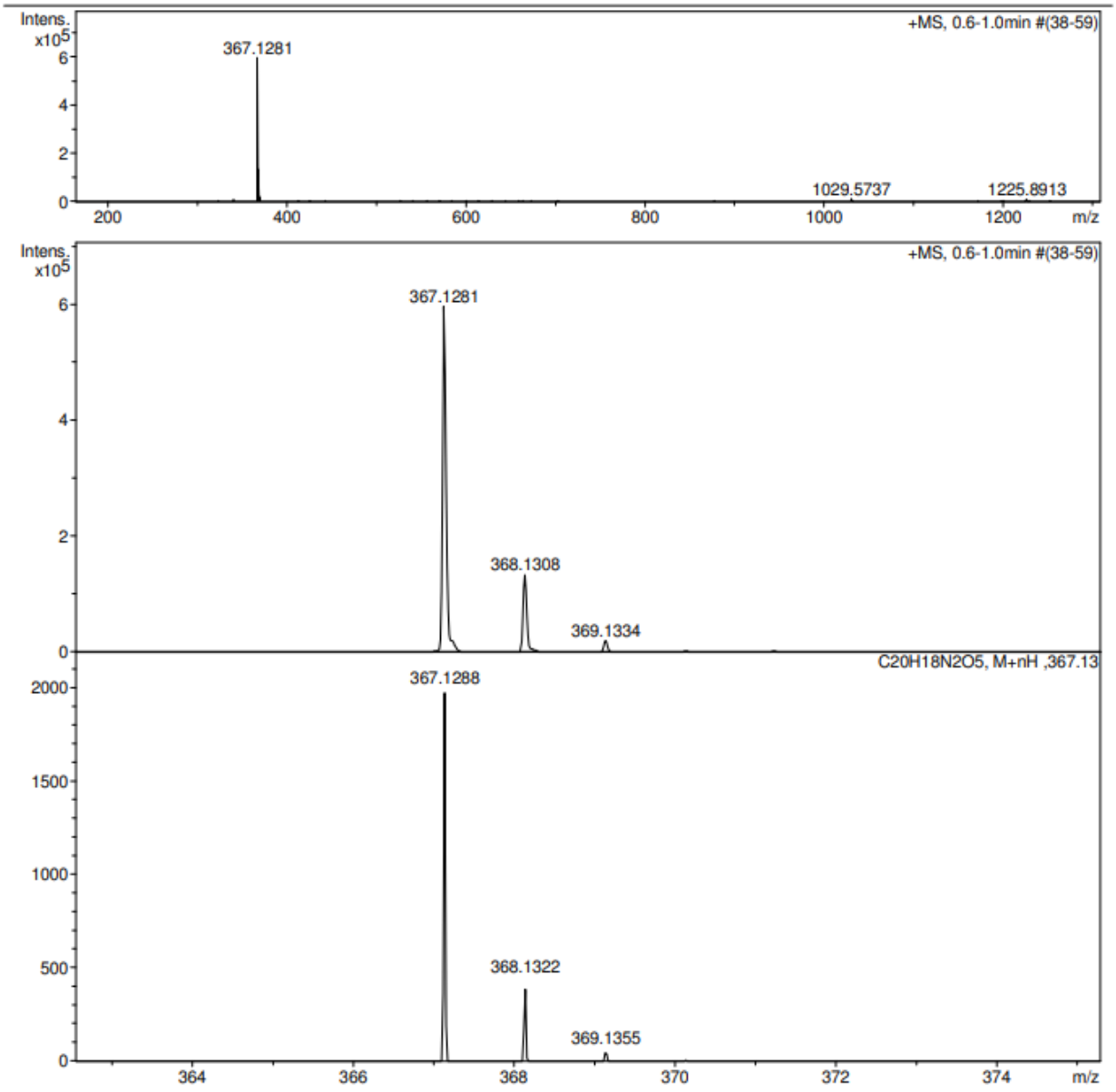
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



HRMS for compound **13b**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



6. X-ray crystallographic data and refinement details

6.1. Compound **4b** (1)

X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix600HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[1] The structure was solved by direct methods using SHELXT[2] and refined on F^2 using SHELXL-2018[3] in the OLEX2 program.[4] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. Locations of hydroxy H-atoms (H1A, H1B, H2A and H2B) were found from the electron density-difference map; these hydrogen atoms were refined with individual isotropic displacement parameters. All other hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters.

Table S3. Crystal data and structure refinement for **4b** (1).

Identification code	**4b** (1)	
Empirical formula	C21.50 H25 N2 O3.50	
Formula weight	367.43	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 22.38682(16) Å	a= 90°.
	b = 12.13681(9) Å	b= 93.0248(6)°.
	c = 13.54889(7) Å	g = 90°.
Volume	3676.17(4) $Å^3$	
Z	8	
Density (calculated)	1.328 g/cm^3	
Absorption coefficient	0.731 mm^{-1}	
F(000)	1568	
Crystal size	0.21 x 0.13 x 0.08 mm^3	
Theta range for data collection	3.266 to 78.500°.	
Index ranges	-28<=h<=28, -15<=k<=15, -12<=l<=16	
Reflections collected	103526	
Independent reflections	7887 [R(int) = 0.0528]	
Observed reflections	7522	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.86655	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	7887 / 0 / 504
Goodness-of-fit on F^2	1.187
Final R indices [I>2sigma(I)]	R1 = 0.0718, wR2 = 0.2347
R indices (all data)	R1 = 0.0749, wR2 = 0.2380
Largest diff. peak and hole	0.470 and -0.335 e.Å^{-3}
CCDC	**2233462**

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **4b** (1). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1A)	5160(1)	7124(2)	1535(2)	21(1)
O(2A)	4054(1)	7104(2)	2010(2)	22(1)
O(3A)	5755(1)	9445(2)	1908(2)	28(1)
N(1A)	5339(1)	7630(2)	3157(2)	17(1)
N(2A)	5432(1)	7199(2)	4760(2)	18(1)
C(1A)	5058(1)	7468(2)	4017(2)	17(1)
C(2A)	5997(1)	7157(2)	4366(2)	18(1)
C(3A)	6552(1)	6888(3)	4822(2)	23(1)
C(4A)	7043(1)	6882(3)	4245(3)	26(1)
C(5A)	6983(2)	7122(3)	3230(3)	28(1)
C(6A)	6439(1)	7389(3)	2763(2)	25(1)
C(7A)	5947(1)	7417(2)	3358(2)	19(1)
C(8A)	5045(1)	7954(2)	2223(2)	17(1)
C(9A)	4349(1)	8101(2)	2274(2)	18(1)
C(10A)	4230(1)	8979(2)	1477(2)	21(1)
C(11A)	4729(1)	9533(3)	1275(2)	22(1)
C(12A)	5249(1)	9083(2)	1819(2)	20(1)
C(13A)	3627(2)	9142(3)	979(2)	28(1)
C(14A)	4149(1)	8445(2)	3324(2)	17(1)
C(15A)	4398(1)	7549(2)	4033(2)	18(1)
C(16A)	3460(1)	8464(3)	3346(2)	22(1)
C(17A)	3241(1)	8856(3)	4345(2)	26(1)
C(18A)	3500(2)	9981(3)	4629(3)	28(1)
C(19A)	4184(1)	9968(3)	4628(2)	24(1)
C(20A)	4394(1)	9590(2)	3624(2)	19(1)

O(1B)	93(1)	7121(2)	8307(2)	23(1)
O(2B)	-1024(1)	7126(2)	7644(2)	23(1)
O(3B)	692(1)	9464(2)	7985(2)	32(1)
N(1B)	271(1)	7622(2)	6713(2)	18(1)
N(2B)	353(1)	7167(2)	5126(2)	20(1)
C(1B)	-15(1)	7451(2)	5807(2)	18(1)
C(2B)	921(1)	7129(3)	5614(2)	21(1)
C(3B)	1475(1)	6874(3)	5238(2)	25(1)
C(4B)	1971(2)	6897(3)	5888(3)	28(1)
C(5B)	1923(2)	7152(3)	6889(3)	30(1)
C(6B)	1377(1)	7408(3)	7275(3)	26(1)
C(7B)	880(1)	7402(2)	6608(2)	20(1)
C(8B)	-20(1)	7950(2)	7600(2)	19(1)
C(9B)	-717(1)	8116(2)	7431(2)	20(1)
C(10B)	-824(1)	8990(3)	8214(2)	23(1)
C(11B)	-322(2)	9533(3)	8507(2)	24(1)
C(12B)	193(1)	9083(3)	8030(2)	23(1)
C(13B)	-1428(2)	9178(3)	8611(3)	30(1)
C(14B)	-911(1)	8474(2)	6350(2)	19(1)
C(15B)	-674(1)	7561(3)	5680(2)	20(1)
C(16B)	-650(1)	9606(3)	6102(2)	21(1)
C(17B)	-842(1)	9989(3)	5056(2)	25(1)
C(18B)	-1523(2)	10040(3)	4914(3)	31(1)
C(19B)	-1803(1)	8927(3)	5153(3)	28(1)
C(20B)	-1600(1)	8531(3)	6196(2)	23(1)
O(4)	2675(2)	6127(3)	3815(2)	65(1)
C(21)	2572(2)	5420(3)	3204(3)	28(1)
C(22)	2127(2)	4538(4)	3385(4)	44(1)
C(23)	2876(2)	5381(3)	2246(3)	32(1)

Table S5. Bond lengths [Å] and angles [°] for **4b** (1)

O(1A)-H(1A)	0.84(5)	C(16A)-C(17A)	1.538(4)
O(1A)-C(8A)	1.405(3)	C(17A)-H(17A)	0.9900
O(2A)-H(2A)	0.85(5)	C(17A)-H(17B)	0.9900
O(2A)-C(9A)	1.416(3)	C(17A)-C(18A)	1.524(5)
O(3A)-C(12A)	1.214(4)	C(18A)-H(18A)	0.9900
N(1A)-C(1A)	1.367(4)	C(18A)-H(18B)	0.9900
N(1A)-C(7A)	1.398(4)	C(18A)-C(19A)	1.532(4)
N(1A)-C(8A)	1.451(3)	C(19A)-H(19A)	0.9900
N(2A)-C(1A)	1.316(4)	C(19A)-H(19B)	0.9900
N(2A)-C(2A)	1.401(4)	C(19A)-C(20A)	1.533(4)
C(1A)-C(15A)	1.483(4)	C(20A)-H(20A)	0.9900
C(2A)-C(3A)	1.396(4)	C(20A)-H(20B)	0.9900
C(2A)-C(7A)	1.400(4)	O(1B)-H(1B)	0.91(5)
C(3A)-H(3A)	0.9500	O(1B)-C(8B)	1.402(4)
C(3A)-C(4A)	1.383(5)	O(2B)-H(2B)	0.86(5)
C(4A)-H(4A)	0.9500	O(2B)-C(9B)	1.421(4)
C(4A)-C(5A)	1.405(5)	O(3B)-C(12B)	1.213(4)
C(5A)-H(5A)	0.9500	N(1B)-C(1B)	1.370(4)
C(5A)-C(6A)	1.382(5)	N(1B)-C(7B)	1.402(4)
C(6A)-H(6A)	0.9500	N(1B)-C(8B)	1.452(4)
C(6A)-C(7A)	1.399(4)	N(2B)-C(1B)	1.314(4)
C(8A)-C(9A)	1.574(4)	N(2B)-C(2B)	1.402(4)
C(8A)-C(12A)	1.553(4)	C(1B)-C(15B)	1.482(4)
C(9A)-C(10A)	1.530(4)	C(2B)-C(3B)	1.400(4)
C(9A)-C(14A)	1.571(4)	C(2B)-C(7B)	1.395(4)
C(10A)-C(11A)	1.343(4)	C(3B)-H(3B)	0.9500
C(10A)-C(13A)	1.491(4)	C(3B)-C(4B)	1.381(5)
C(11A)-H(11A)	0.9500	C(4B)-H(4B)	0.9500
C(11A)-C(12A)	1.452(4)	C(4B)-C(5B)	1.400(5)
C(13A)-H(13A)	0.9800	C(5B)-H(5B)	0.9500
C(13A)-H(13B)	0.9800	C(5B)-C(6B)	1.390(5)
C(13A)-H(13C)	0.9800	C(6B)-H(6B)	0.9500
C(14A)-C(15A)	1.536(4)	C(6B)-C(7B)	1.396(4)
C(14A)-C(16A)	1.544(4)	C(8B)-C(9B)	1.579(4)
C(14A)-C(20A)	1.541(4)	C(8B)-C(12B)	1.559(4)
C(15A)-H(15A)	0.9900	C(9B)-C(10B)	1.528(4)
C(15A)-H(15B)	0.9900	C(9B)-C(14B)	1.567(4)
C(16A)-H(16A)	0.9900	C(10B)-C(11B)	1.345(5)
C(16A)-H(16B)	0.9900	C(10B)-C(13B)	1.498(4)

C(11B)-H(11B)	0.9500	N(2A)-C(1A)-N(1A)	112.6(3)
C(11B)-C(12B)	1.455(4)	N(2A)-C(1A)-C(15A)	126.8(3)
C(13B)-H(13D)	0.9800	C(3A)-C(2A)-N(2A)	129.8(3)
C(13B)-H(13E)	0.9800	C(3A)-C(2A)-C(7A)	120.5(3)
C(13B)-H(13F)	0.9800	C(7A)-C(2A)-N(2A)	109.7(3)
C(14B)-C(15B)	1.544(4)	C(2A)-C(3A)-H(3A)	121.1
C(14B)-C(16B)	1.538(4)	C(4A)-C(3A)-C(2A)	117.8(3)
C(14B)-C(20B)	1.547(4)	C(4A)-C(3A)-H(3A)	121.1
C(15B)-H(15C)	0.9900	C(3A)-C(4A)-H(4A)	119.5
C(15B)-H(15D)	0.9900	C(3A)-C(4A)-C(5A)	121.0(3)
C(16B)-H(16C)	0.9900	C(5A)-C(4A)-H(4A)	119.5
C(16B)-H(16D)	0.9900	C(4A)-C(5A)-H(5A)	118.9
C(16B)-C(17B)	1.531(4)	C(6A)-C(5A)-C(4A)	122.2(3)
C(17B)-H(17C)	0.9900	C(6A)-C(5A)-H(5A)	118.9
C(17B)-H(17D)	0.9900	C(5A)-C(6A)-H(6A)	121.8
C(17B)-C(18B)	1.529(4)	C(5A)-C(6A)-C(7A)	116.3(3)
C(18B)-H(18C)	0.9900	C(7A)-C(6A)-H(6A)	121.8
C(18B)-H(18D)	0.9900	N(1A)-C(7A)-C(2A)	105.0(2)
C(18B)-C(19B)	1.530(5)	N(1A)-C(7A)-C(6A)	132.8(3)
C(19B)-H(19C)	0.9900	C(6A)-C(7A)-C(2A)	122.2(3)
C(19B)-H(19D)	0.9900	O(1A)-C(8A)-N(1A)	107.1(2)
C(19B)-C(20B)	1.538(5)	O(1A)-C(8A)-C(9A)	109.1(2)
C(20B)-H(20C)	0.9900	O(1A)-C(8A)-C(12A)	109.4(2)
C(20B)-H(20D)	0.9900	N(1A)-C(8A)-C(9A)	113.4(2)
O(4)-C(21)	1.206(5)	N(1A)-C(8A)-C(12A)	114.7(2)
C(21)-C(22)	1.490(5)	C(12A)-C(8A)-C(9A)	103.0(2)
C(21)-C(23)	1.498(5)	O(2A)-C(9A)-C(8A)	110.0(2)
C(22)-H(22A)	0.9800	O(2A)-C(9A)-C(10A)	110.9(2)
C(22)-H(22B)	0.9800	O(2A)-C(9A)-C(14A)	107.7(2)
C(22)-H(22C)	0.9800	C(10A)-C(9A)-C(8A)	100.5(2)
C(23)-H(23A)	0.9800	C(10A)-C(9A)-C(14A)	114.1(2)
C(23)-H(23B)	0.9800	C(14A)-C(9A)-C(8A)	113.6(2)
C(23)-H(23C)	0.9800	C(11A)-C(10A)-C(9A)	112.2(3)
C(8A)-O(1A)-H(1A)	109(3)	C(11A)-C(10A)-C(13A)	125.8(3)
C(9A)-O(2A)-H(2A)	107(3)	C(13A)-C(10A)-C(9A)	122.0(3)
C(1A)-N(1A)-C(7A)	107.1(2)	C(10A)-C(11A)-H(11A)	124.4
C(1A)-N(1A)-C(8A)	125.1(2)	C(10A)-C(11A)-C(12A)	111.2(3)
C(7A)-N(1A)-C(8A)	127.8(2)	C(12A)-C(11A)-H(11A)	124.4
C(1A)-N(2A)-C(2A)	105.6(2)	O(3A)-C(12A)-C(8A)	125.1(3)
N(1A)-C(1A)-C(15A)	120.5(2)	O(3A)-C(12A)-C(11A)	129.3(3)

C(11A)-C(12A)-C(8A)	105.5(2)	H(19A)-C(19A)-H(19B)	108.0
C(10A)-C(13A)-H(13A)	109.5	C(20A)-C(19A)-H(19A)	109.4
C(10A)-C(13A)-H(13B)	109.5	C(20A)-C(19A)-H(19B)	109.4
C(10A)-C(13A)-H(13C)	109.5	C(14A)-C(20A)-H(20A)	109.1
H(13A)-C(13A)-H(13B)	109.5	C(14A)-C(20A)-H(20B)	109.1
H(13A)-C(13A)-H(13C)	109.5	C(19A)-C(20A)-C(14A)	112.4(2)
H(13B)-C(13A)-H(13C)	109.5	C(19A)-C(20A)-H(20A)	109.1
C(15A)-C(14A)-C(9A)	105.5(2)	C(19A)-C(20A)-H(20B)	109.1
C(15A)-C(14A)-C(16A)	109.1(2)	H(20A)-C(20A)-H(20B)	107.9
C(15A)-C(14A)-C(20A)	111.2(2)	C(8B)-O(1B)-H(1B)	107(3)
C(16A)-C(14A)-C(9A)	110.7(2)	C(9B)-O(2B)-H(2B)	108(3)
C(20A)-C(14A)-C(9A)	111.3(2)	C(1B)-N(1B)-C(7B)	106.9(2)
C(20A)-C(14A)-C(16A)	108.9(2)	C(1B)-N(1B)-C(8B)	125.0(2)
C(1A)-C(15A)-C(14A)	111.5(2)	C(7B)-N(1B)-C(8B)	128.1(2)
C(1A)-C(15A)-H(15A)	109.3	C(1B)-N(2B)-C(2B)	105.3(2)
C(1A)-C(15A)-H(15B)	109.3	N(1B)-C(1B)-C(15B)	120.4(3)
C(14A)-C(15A)-H(15A)	109.3	N(2B)-C(1B)-N(1B)	112.9(3)
C(14A)-C(15A)-H(15B)	109.3	N(2B)-C(1B)-C(15B)	126.7(3)
H(15A)-C(15A)-H(15B)	108.0	C(3B)-C(2B)-N(2B)	129.4(3)
C(14A)-C(16A)-H(16A)	109.0	C(7B)-C(2B)-N(2B)	110.0(3)
C(14A)-C(16A)-H(16B)	109.0	C(7B)-C(2B)-C(3B)	120.6(3)
H(16A)-C(16A)-H(16B)	107.8	C(2B)-C(3B)-H(3B)	121.3
C(17A)-C(16A)-C(14A)	112.7(2)	C(4B)-C(3B)-C(2B)	117.5(3)
C(17A)-C(16A)-H(16A)	109.0	C(4B)-C(3B)-H(3B)	121.3
C(17A)-C(16A)-H(16B)	109.0	C(3B)-C(4B)-H(4B)	119.3
C(16A)-C(17A)-H(17A)	109.3	C(3B)-C(4B)-C(5B)	121.4(3)
C(16A)-C(17A)-H(17B)	109.3	C(5B)-C(4B)-H(4B)	119.3
H(17A)-C(17A)-H(17B)	108.0	C(4B)-C(5B)-H(5B)	119.1
C(18A)-C(17A)-C(16A)	111.4(3)	C(6B)-C(5B)-C(4B)	121.9(3)
C(18A)-C(17A)-H(17A)	109.3	C(6B)-C(5B)-H(5B)	119.1
C(18A)-C(17A)-H(17B)	109.3	C(5B)-C(6B)-H(6B)	121.9
C(17A)-C(18A)-H(18A)	109.5	C(5B)-C(6B)-C(7B)	116.3(3)
C(17A)-C(18A)-H(18B)	109.5	C(7B)-C(6B)-H(6B)	121.9
C(17A)-C(18A)-C(19A)	110.9(3)	C(2B)-C(7B)-N(1B)	104.9(3)
H(18A)-C(18A)-H(18B)	108.0	C(2B)-C(7B)-C(6B)	122.3(3)
C(19A)-C(18A)-H(18A)	109.5	C(6B)-C(7B)-N(1B)	132.7(3)
C(19A)-C(18A)-H(18B)	109.5	O(1B)-C(8B)-N(1B)	107.3(2)
C(18A)-C(19A)-H(19A)	109.4	O(1B)-C(8B)-C(9B)	109.4(2)
C(18A)-C(19A)-H(19B)	109.4	O(1B)-C(8B)-C(12B)	109.7(2)
C(18A)-C(19A)-C(20A)	111.0(3)	N(1B)-C(8B)-C(9B)	113.5(2)

N(1B)-C(8B)-C(12B)	114.2(2)	C(17B)-C(16B)-H(16D)	109.1
C(12B)-C(8B)-C(9B)	102.8(2)	C(16B)-C(17B)-H(17C)	109.4
O(2B)-C(9B)-C(8B)	110.3(2)	C(16B)-C(17B)-H(17D)	109.4
O(2B)-C(9B)-C(10B)	110.5(2)	H(17C)-C(17B)-H(17D)	108.0
O(2B)-C(9B)-C(14B)	108.1(2)	C(18B)-C(17B)-C(16B)	111.0(3)
C(10B)-C(9B)-C(8B)	100.3(2)	C(18B)-C(17B)-H(17C)	109.4
C(10B)-C(9B)-C(14B)	114.2(2)	C(18B)-C(17B)-H(17D)	109.4
C(14B)-C(9B)-C(8B)	113.2(2)	C(17B)-C(18B)-H(18C)	109.5
C(11B)-C(10B)-C(9B)	112.6(3)	C(17B)-C(18B)-H(18D)	109.5
C(11B)-C(10B)-C(13B)	125.2(3)	C(17B)-C(18B)-C(19B)	110.7(3)
C(13B)-C(10B)-C(9B)	122.2(3)	H(18C)-C(18B)-H(18D)	108.1
C(10B)-C(11B)-H(11B)	124.6	C(19B)-C(18B)-H(18C)	109.5
C(10B)-C(11B)-C(12B)	110.8(3)	C(19B)-C(18B)-H(18D)	109.5
C(12B)-C(11B)-H(11B)	124.6	C(18B)-C(19B)-H(19C)	109.3
O(3B)-C(12B)-C(8B)	125.5(3)	C(18B)-C(19B)-H(19D)	109.3
O(3B)-C(12B)-C(11B)	129.1(3)	C(18B)-C(19B)-C(20B)	111.5(3)
C(11B)-C(12B)-C(8B)	105.3(3)	H(19C)-C(19B)-H(19D)	108.0
C(10B)-C(13B)-H(13D)	109.5	C(20B)-C(19B)-H(19C)	109.3
C(10B)-C(13B)-H(13E)	109.5	C(20B)-C(19B)-H(19D)	109.3
C(10B)-C(13B)-H(13F)	109.5	C(14B)-C(20B)-H(20C)	109.1
H(13D)-C(13B)-H(13E)	109.5	C(14B)-C(20B)-H(20D)	109.1
H(13D)-C(13B)-H(13F)	109.5	C(19B)-C(20B)-C(14B)	112.4(3)
H(13E)-C(13B)-H(13F)	109.5	C(19B)-C(20B)-H(20C)	109.1
C(15B)-C(14B)-C(9B)	105.3(2)	C(19B)-C(20B)-H(20D)	109.1
C(15B)-C(14B)-C(20B)	108.9(2)	H(20C)-C(20B)-H(20D)	107.8
C(16B)-C(14B)-C(9B)	111.3(2)	O(4)-C(21)-C(22)	120.2(4)
C(16B)-C(14B)-C(15B)	111.5(2)	O(4)-C(21)-C(23)	122.5(3)
C(16B)-C(14B)-C(20B)	108.5(2)	C(22)-C(21)-C(23)	117.3(3)
C(20B)-C(14B)-C(9B)	111.3(2)	C(21)-C(22)-H(22A)	109.5
C(1B)-C(15B)-C(14B)	111.5(2)	C(21)-C(22)-H(22B)	109.5
C(1B)-C(15B)-H(15C)	109.3	C(21)-C(22)-H(22C)	109.5
C(1B)-C(15B)-H(15D)	109.3	H(22A)-C(22)-H(22B)	109.5
C(14B)-C(15B)-H(15C)	109.3	H(22A)-C(22)-H(22C)	109.5
C(14B)-C(15B)-H(15D)	109.3	H(22B)-C(22)-H(22C)	109.5
H(15C)-C(15B)-H(15D)	108.0	C(21)-C(23)-H(23A)	109.5
C(14B)-C(16B)-H(16C)	109.1	C(21)-C(23)-H(23B)	109.5
C(14B)-C(16B)-H(16D)	109.1	C(21)-C(23)-H(23C)	109.5
H(16C)-C(16B)-H(16D)	107.8	H(23A)-C(23)-H(23B)	109.5
C(17B)-C(16B)-C(14B)	112.5(3)	H(23A)-C(23)-H(23C)	109.5
C(17B)-C(16B)-H(16C)	109.1	H(23B)-C(23)-H(23C)	109.5

Table S6. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4b** (1). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1A)	32(1)	20(1)	11(1)	-1(1)	2(1)	4(1)
O(2A)	26(1)	18(1)	21(1)	-4(1)	-1(1)	-3(1)
O(3A)	27(1)	28(1)	29(1)	4(1)	0(1)	-6(1)
N(1A)	19(1)	23(1)	9(1)	1(1)	0(1)	1(1)
N(2A)	22(1)	21(1)	12(1)	0(1)	0(1)	0(1)
C(1A)	22(1)	17(1)	12(1)	0(1)	2(1)	1(1)
C(2A)	22(1)	17(1)	16(1)	-2(1)	0(1)	0(1)
C(3A)	27(2)	24(2)	19(1)	-2(1)	-2(1)	2(1)
C(4A)	21(1)	28(2)	29(2)	1(1)	-2(1)	1(1)
C(5A)	22(2)	32(2)	30(2)	4(1)	8(1)	2(1)
C(6A)	25(2)	31(2)	20(1)	4(1)	6(1)	1(1)
C(7A)	19(1)	19(1)	19(1)	0(1)	2(1)	1(1)
C(8A)	23(1)	18(1)	10(1)	0(1)	0(1)	0(1)
C(9A)	21(1)	17(1)	15(1)	-2(1)	-1(1)	-1(1)
C(10A)	27(2)	20(1)	15(1)	-4(1)	0(1)	4(1)
C(11A)	30(2)	19(1)	16(1)	2(1)	1(1)	3(1)
C(12A)	27(2)	19(1)	14(1)	-1(1)	3(1)	-1(1)
C(13A)	30(2)	31(2)	24(2)	2(1)	-6(1)	6(1)
C(14A)	19(1)	17(1)	16(1)	-1(1)	0(1)	-1(1)
C(15A)	20(1)	20(1)	14(1)	0(1)	2(1)	-1(1)
C(16A)	20(1)	23(1)	23(2)	0(1)	0(1)	-1(1)
C(17A)	23(1)	30(2)	27(2)	3(1)	7(1)	2(1)
C(18A)	31(2)	27(2)	27(2)	-1(1)	9(1)	5(1)
C(19A)	29(2)	22(2)	20(1)	-4(1)	4(1)	-1(1)
C(20A)	23(1)	16(1)	16(1)	-3(1)	1(1)	-1(1)
O(1B)	33(1)	23(1)	13(1)	2(1)	-2(1)	4(1)
O(2B)	25(1)	20(1)	24(1)	4(1)	4(1)	-2(1)
O(3B)	27(1)	29(1)	40(1)	-6(1)	1(1)	-5(1)
N(1B)	19(1)	24(1)	12(1)	-1(1)	-1(1)	2(1)
N(2B)	21(1)	25(1)	14(1)	0(1)	1(1)	1(1)
C(1B)	21(1)	21(1)	14(1)	2(1)	-1(1)	1(1)
C(2B)	21(1)	22(1)	20(1)	4(1)	1(1)	2(1)
C(3B)	26(2)	28(2)	22(2)	4(1)	6(1)	3(1)
C(4B)	21(1)	28(2)	37(2)	5(1)	4(1)	3(1)
C(5B)	20(2)	30(2)	38(2)	0(1)	-5(1)	2(1)

C(6B)	25(2)	28(2)	26(2)	-1(1)	-4(1)	1(1)
C(7B)	19(1)	20(1)	21(1)	1(1)	0(1)	1(1)
C(8B)	24(1)	19(1)	14(1)	0(1)	2(1)	0(1)
C(9B)	22(1)	18(1)	18(1)	2(1)	3(1)	-3(1)
C(10B)	29(2)	22(1)	18(1)	2(1)	4(1)	3(1)
C(11B)	32(2)	19(1)	21(1)	-4(1)	2(1)	1(1)
C(12B)	26(2)	23(2)	21(1)	-2(1)	-1(1)	-2(1)
C(13B)	30(2)	32(2)	29(2)	-4(1)	10(1)	3(1)
C(14B)	18(1)	21(1)	18(1)	2(1)	1(1)	0(1)
C(15B)	20(1)	24(1)	17(1)	-1(1)	0(1)	-1(1)
C(16B)	21(1)	21(1)	23(2)	3(1)	1(1)	-1(1)
C(17B)	24(2)	25(2)	26(2)	8(1)	1(1)	0(1)
C(18B)	27(2)	32(2)	34(2)	10(1)	-5(1)	2(1)
C(19B)	20(1)	30(2)	32(2)	3(1)	-2(1)	1(1)
C(20B)	20(1)	22(1)	28(2)	1(1)	2(1)	-1(1)
O(4)	90(3)	66(2)	40(2)	-23(2)	26(2)	-42(2)
C(21)	31(2)	25(2)	28(2)	2(1)	-1(1)	-3(1)
C(22)	42(2)	36(2)	58(3)	-4(2)	14(2)	-11(2)
C(23)	32(2)	32(2)	32(2)	-3(1)	3(1)	-3(1)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4b** (1)

	x	y	z	U(eq)
H(1A)	5235(19)	7410(40)	990(40)	31
H(2A)	4290(20)	6720(40)	1680(30)	33
H(3A)	6590	6714	5506	28
H(4A)	7427	6714	4539	31
H(5A)	7329	7099	2852	34
H(6A)	6401	7545	2075	30
H(11A)	4739	10140	833	26
H(13A)	3670	9383	297	43
H(13B)	3408	9703	1335	43
H(13C)	3405	8445	979	43
H(15A)	4285	7721	4713	22
H(15B)	4217	6830	3842	22
H(16A)	3297	8959	2818	26
H(16B)	3303	7714	3207	26

H(17A)	2799	8900	4304	32
H(17B)	3361	8314	4863	32
H(18A)	3375	10185	5295	34
H(18B)	3340	10542	4155	34
H(19A)	4345	9464	5151	28
H(19B)	4340	10716	4776	28
H(20A)	4837	9568	3652	22
H(20B)	4262	10134	3112	22
H(1B)	90(20)	7440(40)	8910(40)	35
H(2B)	-770(20)	6680(40)	7930(30)	34
H(3B)	1509	6693	4561	30
H(4B)	2354	6737	5652	34
H(5B)	2273	7149	7316	35
H(6B)	1344	7578	7954	32
H(11B)	-305	10128	8962	29
H(13D)	-1380	9450	9291	45
H(13E)	-1651	8483	8601	45
H(13F)	-1648	9723	8200	45
H(15C)	-863	6851	5841	24
H(15D)	-786	7737	4981	24
H(16C)	-782	10156	6584	26
H(16D)	-208	9567	6166	26
H(17C)	-672	10727	4937	30
H(17D)	-683	9472	4568	30
H(18C)	-1637	10244	4222	37
H(18D)	-1679	10614	5352	37
H(19C)	-1687	8374	4662	33
H(19D)	-2244	8995	5106	33
H(20C)	-1770	7792	6309	28
H(20D)	-1758	9040	6691	28
H(22A)	2315	3815	3314	67
H(22B)	1787	4607	2905	67
H(22C)	1988	4613	4056	67
H(23A)	2576	5432	1695	48
H(23B)	3096	4686	2202	48
H(23C)	3156	6000	2216	48

Table S8. Torsion angles [°] for **4b** (1)

O(1A)-C(8A)-C(9A)-O(2A)	26.8(3)	C(7A)-N(1A)-C(8A)-O(1A)	58.6(4)
O(1A)-C(8A)-C(9A)-C(10A)	-90.2(3)	C(7A)-N(1A)-C(8A)-C(9A)	179.0(3)
O(1A)-C(8A)-C(9A)-C(14A)	147.6(2)	C(7A)-N(1A)-C(8A)-C(12A)	-63.0(4)
O(1A)-C(8A)-C(12A)-O(3A)	-85.0(4)	C(7A)-C(2A)-C(3A)-C(4A)	-0.3(5)
O(1A)-C(8A)-C(12A)-C(11A)	90.8(3)	C(8A)-N(1A)-C(1A)-N(2A)	-178.7(3)
O(2A)-C(9A)-C(10A)-C(11A)	-136.1(3)	C(8A)-N(1A)-C(1A)-C(15A)	4.1(4)
O(2A)-C(9A)-C(10A)-C(13A)	41.9(4)	C(8A)-N(1A)-C(7A)-C(2A)	179.1(3)
O(2A)-C(9A)-C(14A)-C(15A)	65.5(3)	C(8A)-N(1A)-C(7A)-C(6A)	-3.7(5)
O(2A)-C(9A)-C(14A)-C(16A)	-52.4(3)	C(8A)-C(9A)-C(10A)-C(11A)	-19.8(3)
O(2A)-C(9A)-C(14A)-C(20A)	-173.7(2)	C(8A)-C(9A)-C(10A)-C(13A)	158.2(3)
N(1A)-C(1A)-C(15A)-C(14A)	-35.5(4)	C(8A)-C(9A)-C(14A)-C(15A)	-56.6(3)
N(1A)-C(8A)-C(9A)-O(2A)	-92.5(3)	C(8A)-C(9A)-C(14A)-C(16A)	-174.5(2)
N(1A)-C(8A)-C(9A)-C(10A)	150.6(2)	C(8A)-C(9A)-C(14A)-C(20A)	64.2(3)
N(1A)-C(8A)-C(9A)-C(14A)	28.4(3)	C(9A)-C(8A)-C(12A)-O(3A)	159.1(3)
N(1A)-C(8A)-C(12A)-O(3A)	35.4(4)	C(9A)-C(8A)-C(12A)-C(11A)	-25.1(3)
N(1A)-C(8A)-C(12A)-C(11A)	-148.8(2)	C(9A)-C(10A)-C(11A)-C(12A)	4.3(4)
N(2A)-C(1A)-C(15A)-C(14A)	147.7(3)	C(9A)-C(14A)-C(15A)-C(1A)	59.1(3)
N(2A)-C(2A)-C(3A)-C(4A)	178.2(3)	C(9A)-C(14A)-C(16A)-C(17A)	-177.0(2)
N(2A)-C(2A)-C(7A)-N(1A)	0.7(3)	C(9A)-C(14A)-C(20A)-C(19A)	177.6(2)
N(2A)-C(2A)-C(7A)-C(6A)	-176.9(3)	C(10A)-C(9A)-C(14A)-C(15A)	-170.9(2)
C(1A)-N(1A)-C(7A)-C(2A)	-1.4(3)	C(10A)-C(9A)-C(14A)-C(16A)	71.1(3)
C(1A)-N(1A)-C(7A)-C(6A)	175.9(3)	C(10A)-C(9A)-C(14A)-C(20A)	-50.2(3)
C(1A)-N(1A)-C(8A)-O(1A)	-120.9(3)	C(10A)-C(11A)-C(12A)-O(3A)	-170.7(3)
C(1A)-N(1A)-C(8A)-C(9A)	-0.5(4)	C(10A)-C(11A)-C(12A)-C(8A)	13.7(3)
C(1A)-N(1A)-C(8A)-C(12A)	117.5(3)	C(12A)-C(8A)-C(9A)-O(2A)	142.9(2)
C(1A)-N(2A)-C(2A)-C(3A)	-178.4(3)	C(12A)-C(8A)-C(9A)-C(10A)	26.0(3)
C(1A)-N(2A)-C(2A)-C(7A)	0.3(3)	C(12A)-C(8A)-C(9A)-C(14A)	-96.2(3)
C(2A)-N(2A)-C(1A)-N(1A)	-1.2(3)	C(13A)-C(10A)-C(11A)-C(12A)	-173.6(3)
C(2A)-N(2A)-C(1A)-C(15A)	175.8(3)	C(14A)-C(9A)-C(10A)-C(11A)	102.1(3)
C(2A)-C(3A)-C(4A)-C(5A)	-1.0(5)	C(14A)-C(9A)-C(10A)-C(13A)	-79.9(3)
C(3A)-C(2A)-C(7A)-N(1A)	179.5(3)	C(14A)-C(16A)-C(17A)-C(18A)	55.3(3)
C(3A)-C(2A)-C(7A)-C(6A)	1.9(5)	C(15A)-C(14A)-C(16A)-C(17A)	67.3(3)
C(3A)-C(4A)-C(5A)-C(6A)	1.0(5)	C(15A)-C(14A)-C(20A)-C(19A)	-65.1(3)
C(4A)-C(5A)-C(6A)-C(7A)	0.5(5)	C(16A)-C(14A)-C(15A)-C(1A)	178.1(2)
C(5A)-C(6A)-C(7A)-N(1A)	-178.8(3)	C(16A)-C(14A)-C(20A)-C(19A)	55.2(3)
C(5A)-C(6A)-C(7A)-C(2A)	-1.9(5)	C(16A)-C(17A)-C(18A)-C(19A)	-55.0(4)
C(7A)-N(1A)-C(1A)-N(2A)	1.7(3)	C(17A)-C(18A)-C(19A)-C(20A)	55.8(4)
C(7A)-N(1A)-C(1A)-C(15A)	-175.5(3)	C(18A)-C(19A)-C(20A)-C(14A)	-57.0(3)

C(20A)-C(14A)-C(15A)-C(1A)	-61.7(3)
C(20A)-C(14A)-C(16A)-C(17A)	-54.2(3)
O(1B)-C(8B)-C(9B)-O(2B)	-27.0(3)
O(1B)-C(8B)-C(9B)-C(10B)	89.6(3)
O(1B)-C(8B)-C(9B)-C(14B)	-148.3(2)
O(1B)-C(8B)-C(12B)-O(3B)	88.4(4)
O(1B)-C(8B)-C(12B)-C(11B)	-89.7(3)
O(2B)-C(9B)-C(10B)-C(11B)	136.3(3)
O(2B)-C(9B)-C(10B)-C(13B)	-42.3(4)
O(2B)-C(9B)-C(14B)-C(15B)	-65.2(3)
O(2B)-C(9B)-C(14B)-C(16B)	173.9(2)
O(2B)-C(9B)-C(14B)-C(20B)	52.7(3)
N(1B)-C(1B)-C(15B)-C(14B)	34.4(4)
N(1B)-C(8B)-C(9B)-O(2B)	92.7(3)
N(1B)-C(8B)-C(9B)-C(10B)	-150.7(2)
N(1B)-C(8B)-C(9B)-C(14B)	-28.6(3)
N(1B)-C(8B)-C(12B)-O(3B)	-32.0(4)
N(1B)-C(8B)-C(12B)-C(11B)	149.9(3)
N(2B)-C(1B)-C(15B)-C(14B)	-147.6(3)
N(2B)-C(2B)-C(3B)-C(4B)	-179.9(3)
N(2B)-C(2B)-C(7B)-N(1B)	-0.7(3)
N(2B)-C(2B)-C(7B)-C(6B)	178.7(3)
C(1B)-N(1B)-C(7B)-C(2B)	1.2(3)
C(1B)-N(1B)-C(7B)-C(6B)	-178.0(3)
C(1B)-N(1B)-C(8B)-O(1B)	120.1(3)
C(1B)-N(1B)-C(8B)-C(9B)	-0.8(4)
C(1B)-N(1B)-C(8B)-C(12B)	-118.1(3)
C(1B)-N(2B)-C(2B)-C(3B)	-179.7(3)
C(1B)-N(2B)-C(2B)-C(7B)	-0.1(3)
C(2B)-N(2B)-C(1B)-N(1B)	0.9(3)
C(2B)-N(2B)-C(1B)-C(15B)	-177.3(3)
C(2B)-C(3B)-C(4B)-C(5B)	0.8(5)
C(3B)-C(2B)-C(7B)-N(1B)	178.9(3)
C(3B)-C(2B)-C(7B)-C(6B)	-1.7(5)
C(3B)-C(4B)-C(5B)-C(6B)	-0.9(5)
C(4B)-C(5B)-C(6B)-C(7B)	-0.2(5)
C(5B)-C(6B)-C(7B)-N(1B)	-179.3(3)
C(5B)-C(6B)-C(7B)-C(2B)	1.5(5)
C(7B)-N(1B)-C(1B)-N(2B)	-1.4(4)
C(7B)-N(1B)-C(1B)-C(15B)	176.9(3)
C(7B)-N(1B)-C(8B)-O(1B)	-58.7(4)
C(7B)-N(1B)-C(8B)-C(9B)	-179.6(3)
C(7B)-N(1B)-C(8B)-C(12B)	63.1(4)
C(7B)-C(2B)-C(3B)-C(4B)	0.5(5)
C(8B)-N(1B)-C(1B)-N(2B)	179.6(3)
C(8B)-N(1B)-C(1B)-C(15B)	-2.1(4)
C(8B)-N(1B)-C(7B)-C(2B)	-179.8(3)
C(8B)-N(1B)-C(7B)-C(6B)	0.9(6)
C(8B)-C(9B)-C(10B)-C(11B)	19.8(3)
C(8B)-C(9B)-C(10B)-C(13B)	-158.7(3)
C(8B)-C(9B)-C(14B)-C(15B)	57.3(3)
C(8B)-C(9B)-C(14B)-C(16B)	-63.6(3)
C(8B)-C(9B)-C(14B)-C(20B)	175.2(2)
C(9B)-C(8B)-C(12B)-O(3B)	-155.3(3)
C(9B)-C(8B)-C(12B)-C(11B)	26.6(3)
C(9B)-C(10B)-C(11B)-C(12B)	-3.3(4)
C(9B)-C(14B)-C(15B)-C(1B)	-59.5(3)
C(9B)-C(14B)-C(16B)-C(17B)	-178.9(2)
C(9B)-C(14B)-C(20B)-C(19B)	177.6(3)
C(10B)-C(9B)-C(14B)-C(15B)	171.3(2)
C(10B)-C(9B)-C(14B)-C(16B)	50.4(3)
C(10B)-C(9B)-C(14B)-C(20B)	-70.8(3)
C(10B)-C(11B)-C(12B)-O(3B)	166.7(3)
C(10B)-C(11B)-C(12B)-C(8B)	-15.3(4)
C(12B)-C(8B)-C(9B)-O(2B)	-143.5(2)
C(12B)-C(8B)-C(9B)-C(10B)	-26.9(3)
C(12B)-C(8B)-C(9B)-C(14B)	95.3(3)
C(13B)-C(10B)-C(11B)-C(12B)	175.2(3)
C(14B)-C(9B)-C(10B)-C(11B)	-101.6(3)
C(14B)-C(9B)-C(10B)-C(13B)	79.9(4)
C(14B)-C(16B)-C(17B)-C(18B)	57.7(4)
C(15B)-C(14B)-C(16B)-C(17B)	63.9(3)
C(15B)-C(14B)-C(20B)-C(19B)	-66.7(3)
C(16B)-C(14B)-C(15B)-C(1B)	61.3(3)
C(16B)-C(14B)-C(20B)-C(19B)	54.8(3)
C(16B)-C(17B)-C(18B)-C(19B)	-55.7(4)
C(17B)-C(18B)-C(19B)-C(20B)	54.8(4)
C(18B)-C(19B)-C(20B)-C(14B)	-55.5(4)
C(20B)-C(14B)-C(15B)-C(1B)	-179.0(2)
C(20B)-C(14B)-C(16B)-C(17B)	-56.0(3)

Table S9. Hydrogen bonds for **4b** (1) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1A)-H(1A)...N(2A)#1	0.84(5)	1.81(5)	2.643(3)	170(4)
O(2A)-H(2A)...O(1A)	0.85(5)	2.02(4)	2.591(3)	124(4)
O(1B)-H(1B)...N(2B)#2	0.91(5)	1.79(5)	2.648(3)	158(4)
O(2B)-H(2B)...O(1B)	0.86(5)	2.05(4)	2.612(3)	122(4)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+3/2,z-1/2 #2 x,-y+3/2,z+1/2

6.2. Compound **4b** (2)

X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix600HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_a-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[1] The structure was solved by direct methods using SHELXT[2] and refined on F^2 using SHELXL-2018[3] in the OLEX2 program.[4] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. Locations of hydroxy H-atoms were found from the electron density-difference map; these hydrogen atoms were refined with individual isotropic displacement parameters. All other hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters.

Table S10. Crystal data and structure refinement for **4b** (2).

Identification code	**4b** (2)	
Empirical formula	C20 H22 N2 O3	
Formula weight	338.39	
Temperature	100.0(1) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 11.68226(12) Å	a= 90°.
	b = 9.54123(6) Å	b= 110.8694(11)°.
	c = 15.99352(16) Å	g = 90°.
Volume	1665.73(3) $Å^3$	
Z	4	

Density (calculated)	1.349 g/cm^3
Absorption coefficient	0.737 mm^{-1}
F(000)	720
Crystal size	0.33 x 0.24 x 0.07 mm^3
Theta range for data collection	2.957 to 79.481°.
Index ranges	-14<=h<=14, -11<=k<=9, -20<=l<=20
Reflections collected	6684
Independent reflections	6684 [R(int) = 0]
Observed reflections	6666
Completeness to theta = 67.684°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.41618
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6684 / 7 / 467
Goodness-of-fit on F^2	1.067
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.1411
R indices (all data)	R1 = 0.0548, wR2 = 0.1412
Absolute structure parameter	0.01(13)
Extinction coefficient	0.0095(13)
Largest diff. peak and hole	0.533 and -0.349 e.Å^{-3}
CCDC	**2233466**

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **4b** (2). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1A)	4324(2)	5090(2)	659(1)	14(1)
O(2A)	6646(2)	4987(2)	1749(1)	14(1)
O(3A)	3820(2)	7643(2)	-604(1)	17(1)
N(1A)	4352(2)	7304(2)	1286(1)	13(1)
N(2A)	4225(2)	8663(3)	2393(1)	16(1)
C(1A)	4957(2)	7955(3)	2083(2)	13(1)
C(2A)	3054(2)	8435(3)	1770(2)	15(1)
C(3A)	1915(2)	8903(3)	1773(2)	20(1)
C(4A)	876(2)	8454(4)	1082(2)	22(1)
C(5A)	942(2)	7573(3)	399(2)	18(1)
C(6A)	2063(2)	7119(3)	377(2)	16(1)

C(7A)	3104(2)	7571(3)	1072(2)	13(1)
C(8A)	4898(2)	6399(3)	797(2)	12(1)
C(9A)	6340(2)	6238(3)	1245(2)	12(1)
C(10A)	6692(2)	6153(3)	403(2)	13(1)
C(11A)	5792(2)	6591(3)	-338(2)	16(1)
C(12A)	4714(2)	6990(3)	-143(2)	13(1)
C(13A)	7906(2)	5624(3)	437(2)	19(1)
C(14A)	6988(2)	7464(3)	1898(2)	12(1)
C(15A)	6288(2)	7687(3)	2542(2)	14(1)
C(16A)	8323(2)	7040(3)	2464(2)	15(1)
C(17A)	9017(2)	8214(3)	3097(2)	18(1)
C(18A)	9021(2)	9567(3)	2592(2)	21(1)
C(19A)	7715(2)	9993(3)	2015(2)	19(1)
C(20A)	7018(2)	8824(3)	1385(2)	15(1)
O(1B)	4304(2)	105(2)	3961(1)	14(1)
O(2B)	6642(2)	-1(2)	4097(1)	14(1)
O(3B)	3805(2)	2707(2)	4945(1)	17(1)
N(1B)	4367(2)	2313(2)	3346(1)	13(1)
N(2B)	4294(2)	3697(3)	2199(1)	15(1)
C(1B)	4997(2)	2965(3)	2886(2)	12(1)
C(2B)	3105(2)	3492(3)	2193(2)	15(1)
C(3B)	1999(2)	4032(3)	1600(2)	20(1)
C(4B)	936(2)	3639(3)	1742(2)	20(1)
C(5B)	964(2)	2735(3)	2442(2)	19(1)
C(6B)	2056(2)	2202(3)	3036(2)	17(1)
C(7B)	3121(2)	2620(3)	2901(2)	14(1)
C(8B)	4884(2)	1413(3)	4120(2)	11(1)
C(9B)	6337(2)	1246(3)	4452(1)	12(1)
C(10B)	6652(2)	1139(3)	5466(2)	14(1)
C(11B)	5742(2)	1581(3)	5729(2)	16(1)
C(12B)	4689(2)	2016(3)	4960(2)	14(1)
C(13B)	7857(2)	605(3)	6088(2)	18(1)
C(14B)	6988(2)	2486(3)	4161(2)	12(1)
C(15B)	6334(2)	2703(3)	3144(1)	13(1)
C(16B)	6957(2)	3840(3)	4680(2)	13(1)
C(17B)	7667(2)	5032(3)	4449(2)	17(1)
C(18B)	9002(2)	4639(3)	4621(2)	19(1)
C(19B)	9067(2)	3289(3)	4118(2)	18(1)
C(20B)	8340(2)	2100(3)	4338(2)	15(1)

Table S12. Bond lengths [Å] and angles [°] for **4b** (2).

O(1A)-H(1A)	0.88(3)	C(16A)-H(16B)	0.9900
O(1A)-C(8A)	1.397(3)	C(16A)-C(17A)	1.534(4)
O(2A)-H(2A)	0.88(3)	C(17A)-H(17A)	0.9900
O(2A)-C(9A)	1.413(3)	C(17A)-H(17B)	0.9900
O(3A)-C(12A)	1.214(3)	C(17A)-C(18A)	1.524(4)
N(1A)-C(1A)	1.367(3)	C(18A)-H(18A)	0.9900
N(1A)-C(7A)	1.398(3)	C(18A)-H(18B)	0.9900
N(1A)-C(8A)	1.456(3)	C(18A)-C(19A)	1.530(4)
N(2A)-C(1A)	1.317(3)	C(19A)-H(19A)	0.9900
N(2A)-C(2A)	1.393(3)	C(19A)-H(19B)	0.9900
C(1A)-C(15A)	1.487(3)	C(19A)-C(20A)	1.528(4)
C(2A)-C(3A)	1.406(3)	C(20A)-H(20A)	0.9900
C(2A)-C(7A)	1.404(3)	C(20A)-H(20B)	0.9900
C(3A)-H(3A)	0.9500	O(1B)-H(1B)	0.89(3)
C(3A)-C(4A)	1.388(4)	O(1B)-C(8B)	1.399(3)
C(4A)-H(4A)	0.9500	O(2B)-H(2B)	0.88(3)
C(4A)-C(5A)	1.401(4)	O(2B)-C(9B)	1.417(3)
C(5A)-H(5A)	0.9500	O(3B)-C(12B)	1.219(3)
C(5A)-C(6A)	1.391(3)	N(1B)-C(1B)	1.362(3)
C(6A)-H(6A)	0.9500	N(1B)-C(7B)	1.404(3)
C(6A)-C(7A)	1.392(3)	N(1B)-C(8B)	1.449(3)
C(8A)-C(9A)	1.585(3)	N(2B)-C(1B)	1.314(3)
C(8A)-C(12A)	1.547(3)	N(2B)-C(2B)	1.399(3)
C(9A)-C(10A)	1.542(3)	C(1B)-C(15B)	1.488(3)
C(9A)-C(14A)	1.572(3)	C(2B)-C(3B)	1.401(3)
C(10A)-C(11A)	1.341(3)	C(2B)-C(7B)	1.401(4)
C(10A)-C(13A)	1.489(3)	C(3B)-H(3B)	0.9500
C(11A)-H(11A)	0.9500	C(3B)-C(4B)	1.391(4)
C(11A)-C(12A)	1.452(3)	C(4B)-H(4B)	0.9500
C(13A)-H(13A)	0.9800	C(4B)-C(5B)	1.404(4)
C(13A)-H(13B)	0.9800	C(5B)-H(5B)	0.9500
C(13A)-H(13C)	0.9800	C(5B)-C(6B)	1.388(4)
C(14A)-C(15A)	1.541(3)	C(6B)-H(6B)	0.9500
C(14A)-C(16A)	1.552(3)	C(6B)-C(7B)	1.394(3)
C(14A)-C(20A)	1.542(4)	C(8B)-C(9B)	1.596(3)
C(15A)-H(15A)	0.9900	C(8B)-C(12B)	1.552(3)
C(15A)-H(15B)	0.9900	C(9B)-C(10B)	1.533(3)
C(16A)-H(16A)	0.9900	C(9B)-C(14B)	1.564(3)

C(10B)-C(11B)	1.342(3)	C(4A)-C(3A)-H(3A)	121.3
C(10B)-C(13B)	1.495(3)	C(3A)-C(4A)-H(4A)	119.0
C(11B)-H(11B)	0.9500	C(3A)-C(4A)-C(5A)	122.1(2)
C(11B)-C(12B)	1.456(3)	C(5A)-C(4A)-H(4A)	119.0
C(13B)-H(13D)	0.9800	C(4A)-C(5A)-H(5A)	119.4
C(13B)-H(13E)	0.9800	C(6A)-C(5A)-C(4A)	121.3(2)
C(13B)-H(13F)	0.9800	C(6A)-C(5A)-H(5A)	119.4
C(14B)-C(15B)	1.544(3)	C(5A)-C(6A)-H(6A)	121.8
C(14B)-C(16B)	1.543(4)	C(5A)-C(6A)-C(7A)	116.5(2)
C(14B)-C(20B)	1.547(3)	C(7A)-C(6A)-H(6A)	121.8
C(15B)-H(15C)	0.9900	N(1A)-C(7A)-C(2A)	104.3(2)
C(15B)-H(15D)	0.9900	C(6A)-C(7A)-N(1A)	132.7(2)
C(16B)-H(16C)	0.9900	C(6A)-C(7A)-C(2A)	123.0(2)
C(16B)-H(16D)	0.9900	O(1A)-C(8A)-N(1A)	109.75(19)
C(16B)-C(17B)	1.528(3)	O(1A)-C(8A)-C(9A)	111.0(2)
C(17B)-H(17C)	0.9900	O(1A)-C(8A)-C(12A)	106.20(19)
C(17B)-H(17D)	0.9900	N(1A)-C(8A)-C(9A)	114.41(19)
C(17B)-C(18B)	1.530(3)	N(1A)-C(8A)-C(12A)	111.7(2)
C(18B)-H(18C)	0.9900	C(12A)-C(8A)-C(9A)	103.36(18)
C(18B)-H(18D)	0.9900	O(2A)-C(9A)-C(8A)	110.6(2)
C(18B)-C(19B)	1.534(4)	O(2A)-C(9A)-C(10A)	111.2(2)
C(19B)-H(19C)	0.9900	O(2A)-C(9A)-C(14A)	106.55(18)
C(19B)-H(19D)	0.9900	C(10A)-C(9A)-C(8A)	100.48(18)
C(19B)-C(20B)	1.531(4)	C(10A)-C(9A)-C(14A)	113.83(19)
C(20B)-H(20C)	0.9900	C(14A)-C(9A)-C(8A)	114.2(2)
C(20B)-H(20D)	0.9900	C(11A)-C(10A)-C(9A)	112.8(2)
C(8A)-O(1A)-H(1A)	111(2)	C(11A)-C(10A)-C(13A)	125.0(2)
C(9A)-O(2A)-H(2A)	110(2)	C(13A)-C(10A)-C(9A)	122.2(2)
C(1A)-N(1A)-C(7A)	107.04(19)	C(10A)-C(11A)-H(11A)	124.5
C(1A)-N(1A)-C(8A)	126.21(19)	C(10A)-C(11A)-C(12A)	110.9(2)
C(7A)-N(1A)-C(8A)	126.5(2)	C(12A)-C(11A)-H(11A)	124.5
C(1A)-N(2A)-C(2A)	104.7(2)	O(3A)-C(12A)-C(8A)	124.7(2)
N(1A)-C(1A)-C(15A)	119.0(2)	O(3A)-C(12A)-C(11A)	128.9(2)
N(2A)-C(1A)-N(1A)	113.2(2)	C(11A)-C(12A)-C(8A)	106.4(2)
N(2A)-C(1A)-C(15A)	127.4(2)	C(10A)-C(13A)-H(13A)	109.5
N(2A)-C(2A)-C(3A)	129.6(2)	C(10A)-C(13A)-H(13B)	109.5
N(2A)-C(2A)-C(7A)	110.6(2)	C(10A)-C(13A)-H(13C)	109.5
C(7A)-C(2A)-C(3A)	119.8(2)	H(13A)-C(13A)-H(13B)	109.5
C(2A)-C(3A)-H(3A)	121.3	H(13A)-C(13A)-H(13C)	109.5
C(4A)-C(3A)-C(2A)	117.3(2)	H(13B)-C(13A)-H(13C)	109.5

C(15A)-C(14A)-C(9A)	107.64(19)	C(19A)-C(20A)-H(20B)	109.3
C(15A)-C(14A)-C(16A)	107.93(18)	H(20A)-C(20A)-H(20B)	107.9
C(15A)-C(14A)-C(20A)	110.9(2)	C(8B)-O(1B)-H(1B)	107(3)
C(16A)-C(14A)-C(9A)	109.9(2)	C(9B)-O(2B)-H(2B)	114(2)
C(20A)-C(14A)-C(9A)	111.70(18)	C(1B)-N(1B)-C(7B)	107.0(2)
C(20A)-C(14A)-C(16A)	108.7(2)	C(1B)-N(1B)-C(8B)	126.2(2)
C(1A)-C(15A)-C(14A)	113.85(18)	C(7B)-N(1B)-C(8B)	126.7(2)
C(1A)-C(15A)-H(15A)	108.8	C(1B)-N(2B)-C(2B)	104.7(2)
C(1A)-C(15A)-H(15B)	108.8	N(1B)-C(1B)-C(15B)	119.3(2)
C(14A)-C(15A)-H(15A)	108.8	N(2B)-C(1B)-N(1B)	113.45(19)
C(14A)-C(15A)-H(15B)	108.8	N(2B)-C(1B)-C(15B)	127.1(2)
H(15A)-C(15A)-H(15B)	107.7	N(2B)-C(2B)-C(3B)	128.8(2)
C(14A)-C(16A)-H(16A)	109.1	N(2B)-C(2B)-C(7B)	110.5(2)
C(14A)-C(16A)-H(16B)	109.1	C(7B)-C(2B)-C(3B)	120.7(2)
H(16A)-C(16A)-H(16B)	107.9	C(2B)-C(3B)-H(3B)	121.6
C(17A)-C(16A)-C(14A)	112.3(2)	C(4B)-C(3B)-C(2B)	116.9(2)
C(17A)-C(16A)-H(16A)	109.1	C(4B)-C(3B)-H(3B)	121.6
C(17A)-C(16A)-H(16B)	109.1	C(3B)-C(4B)-H(4B)	119.1
C(16A)-C(17A)-H(17A)	109.3	C(3B)-C(4B)-C(5B)	121.8(2)
C(16A)-C(17A)-H(17B)	109.3	C(5B)-C(4B)-H(4B)	119.1
H(17A)-C(17A)-H(17B)	107.9	C(4B)-C(5B)-H(5B)	119.2
C(18A)-C(17A)-C(16A)	111.7(2)	C(6B)-C(5B)-C(4B)	121.7(2)
C(18A)-C(17A)-H(17A)	109.3	C(6B)-C(5B)-H(5B)	119.2
C(18A)-C(17A)-H(17B)	109.3	C(5B)-C(6B)-H(6B)	121.8
C(17A)-C(18A)-H(18A)	109.5	C(5B)-C(6B)-C(7B)	116.3(2)
C(17A)-C(18A)-H(18B)	109.5	C(7B)-C(6B)-H(6B)	121.8
C(17A)-C(18A)-C(19A)	110.7(2)	C(2B)-C(7B)-N(1B)	104.3(2)
H(18A)-C(18A)-H(18B)	108.1	C(6B)-C(7B)-N(1B)	133.1(2)
C(19A)-C(18A)-H(18A)	109.5	C(6B)-C(7B)-C(2B)	122.6(2)
C(19A)-C(18A)-H(18B)	109.5	O(1B)-C(8B)-N(1B)	110.24(19)
C(18A)-C(19A)-H(19A)	109.0	O(1B)-C(8B)-C(9B)	111.1(2)
C(18A)-C(19A)-H(19B)	109.0	O(1B)-C(8B)-C(12B)	106.06(18)
H(19A)-C(19A)-H(19B)	107.8	N(1B)-C(8B)-C(9B)	114.44(18)
C(20A)-C(19A)-C(18A)	112.7(2)	N(1B)-C(8B)-C(12B)	112.0(2)
C(20A)-C(19A)-H(19A)	109.0	C(12B)-C(8B)-C(9B)	102.46(18)
C(20A)-C(19A)-H(19B)	109.0	O(2B)-C(9B)-C(8B)	109.84(19)
C(14A)-C(20A)-H(20A)	109.3	O(2B)-C(9B)-C(10B)	111.6(2)
C(14A)-C(20A)-H(20B)	109.3	O(2B)-C(9B)-C(14B)	107.33(18)
C(19A)-C(20A)-C(14A)	111.81(19)	C(10B)-C(9B)-C(8B)	100.63(17)
C(19A)-C(20A)-H(20A)	109.3	C(10B)-C(9B)-C(14B)	114.0(2)

C(14B)-C(9B)-C(8B)	113.42(19)	C(14B)-C(16B)-H(16D)	109.2
C(11B)-C(10B)-C(9B)	113.1(2)	H(16C)-C(16B)-H(16D)	107.9
C(11B)-C(10B)-C(13B)	124.2(2)	C(17B)-C(16B)-C(14B)	111.99(19)
C(13B)-C(10B)-C(9B)	122.7(2)	C(17B)-C(16B)-H(16C)	109.2
C(10B)-C(11B)-H(11B)	124.7	C(17B)-C(16B)-H(16D)	109.2
C(10B)-C(11B)-C(12B)	110.5(2)	C(16B)-C(17B)-H(17C)	109.1
C(12B)-C(11B)-H(11B)	124.7	C(16B)-C(17B)-H(17D)	109.1
O(3B)-C(12B)-C(8B)	124.7(2)	C(16B)-C(17B)-C(18B)	112.4(2)
O(3B)-C(12B)-C(11B)	128.8(2)	H(17C)-C(17B)-H(17D)	107.9
C(11B)-C(12B)-C(8B)	106.5(2)	C(18B)-C(17B)-H(17C)	109.1
C(10B)-C(13B)-H(13D)	109.5	C(18B)-C(17B)-H(17D)	109.1
C(10B)-C(13B)-H(13E)	109.5	C(17B)-C(18B)-H(18C)	109.6
C(10B)-C(13B)-H(13F)	109.5	C(17B)-C(18B)-H(18D)	109.6
H(13D)-C(13B)-H(13E)	109.5	C(17B)-C(18B)-C(19B)	110.4(2)
H(13D)-C(13B)-H(13F)	109.5	H(18C)-C(18B)-H(18D)	108.1
H(13E)-C(13B)-H(13F)	109.5	C(19B)-C(18B)-H(18C)	109.6
C(15B)-C(14B)-C(9B)	107.71(19)	C(19B)-C(18B)-H(18D)	109.6
C(15B)-C(14B)-C(20B)	108.35(17)	C(18B)-C(19B)-H(19C)	109.3
C(16B)-C(14B)-C(9B)	111.49(18)	C(18B)-C(19B)-H(19D)	109.3
C(16B)-C(14B)-C(15B)	110.9(2)	H(19C)-C(19B)-H(19D)	108.0
C(16B)-C(14B)-C(20B)	108.6(2)	C(20B)-C(19B)-C(18B)	111.5(2)
C(20B)-C(14B)-C(9B)	109.8(2)	C(20B)-C(19B)-H(19C)	109.3
C(1B)-C(15B)-C(14B)	113.05(18)	C(20B)-C(19B)-H(19D)	109.3
C(1B)-C(15B)-H(15C)	109.0	C(14B)-C(20B)-H(20C)	108.9
C(1B)-C(15B)-H(15D)	109.0	C(14B)-C(20B)-H(20D)	108.9
C(14B)-C(15B)-H(15C)	109.0	C(19B)-C(20B)-C(14B)	113.3(2)
C(14B)-C(15B)-H(15D)	109.0	C(19B)-C(20B)-H(20C)	108.9
H(15C)-C(15B)-H(15D)	107.8	C(19B)-C(20B)-H(20D)	108.9
C(14B)-C(16B)-H(16C)	109.2	H(20C)-C(20B)-H(20D)	107.7

Table S13. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4b** (2). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1A)	18(1)	11(1)	15(1)	0(1)	10(1)	-2(1)
O(2A)	18(1)	10(1)	15(1)	1(1)	8(1)	2(1)
O(3A)	18(1)	15(1)	18(1)	4(1)	7(1)	-1(1)

N(1A)	14(1)	14(1)	14(1)	0(1)	10(1)	2(1)
N(2A)	16(1)	17(1)	18(1)	0(1)	12(1)	1(1)
C(1A)	15(1)	11(1)	17(1)	-1(1)	10(1)	0(1)
C(2A)	17(1)	16(1)	19(1)	0(1)	13(1)	2(1)
C(3A)	18(1)	24(2)	24(1)	-4(1)	15(1)	2(1)
C(4A)	15(1)	28(2)	28(1)	-2(1)	13(1)	1(1)
C(5A)	12(1)	22(2)	23(1)	2(1)	9(1)	-1(1)
C(6A)	16(1)	17(1)	18(1)	3(1)	9(1)	0(1)
C(7A)	14(1)	11(1)	19(1)	2(1)	11(1)	0(1)
C(8A)	16(1)	10(1)	14(1)	0(1)	10(1)	1(1)
C(9A)	14(1)	9(1)	15(1)	-1(1)	9(1)	2(1)
C(10A)	18(1)	9(1)	17(1)	-3(1)	12(1)	-3(1)
C(11A)	21(1)	15(1)	16(1)	0(1)	12(1)	0(1)
C(12A)	18(1)	10(1)	14(1)	-1(1)	8(1)	-3(1)
C(13A)	18(1)	22(1)	21(1)	-4(1)	12(1)	-1(1)
C(14A)	12(1)	9(1)	16(1)	-1(1)	7(1)	1(1)
C(15A)	14(1)	17(1)	15(1)	-3(1)	9(1)	1(1)
C(16A)	14(1)	13(1)	20(1)	-1(1)	7(1)	3(1)
C(17A)	15(1)	20(2)	19(1)	-5(1)	6(1)	-1(1)
C(18A)	21(1)	18(2)	27(1)	-6(1)	14(1)	-6(1)
C(19A)	25(1)	10(1)	24(1)	-1(1)	11(1)	-2(1)
C(20A)	20(1)	12(1)	17(1)	1(1)	10(1)	0(1)
O(1B)	18(1)	10(1)	18(1)	-2(1)	12(1)	-3(1)
O(2B)	17(1)	9(1)	20(1)	1(1)	13(1)	2(1)
O(3B)	18(1)	15(1)	24(1)	-5(1)	14(1)	-1(1)
N(1B)	14(1)	13(1)	15(1)	1(1)	9(1)	-1(1)
N(2B)	15(1)	16(1)	16(1)	1(1)	8(1)	1(1)
C(1B)	12(1)	10(1)	16(1)	1(1)	9(1)	0(1)
C(2B)	16(1)	13(1)	18(1)	-1(1)	9(1)	0(1)
C(3B)	17(1)	21(2)	20(1)	1(1)	6(1)	1(1)
C(4B)	16(1)	20(2)	22(1)	-1(1)	6(1)	2(1)
C(5B)	16(1)	16(1)	28(1)	-6(1)	12(1)	-2(1)
C(6B)	18(1)	16(1)	22(1)	-1(1)	12(1)	-2(1)
C(7B)	13(1)	12(1)	18(1)	-2(1)	7(1)	-1(1)
C(8B)	15(1)	8(1)	15(1)	1(1)	11(1)	-1(1)
C(9B)	14(1)	10(1)	14(1)	2(1)	8(1)	2(1)
C(10B)	19(1)	10(1)	17(1)	-1(1)	11(1)	-4(1)
C(11B)	22(1)	15(1)	16(1)	-2(1)	12(1)	-2(1)
C(12B)	18(1)	10(1)	18(1)	-1(1)	12(1)	-1(1)
C(13B)	20(1)	19(1)	18(1)	3(1)	9(1)	-1(1)

C(14B)	12(1)	10(1)	17(1)	1(1)	9(1)	1(1)
C(15B)	13(1)	15(1)	16(1)	3(1)	9(1)	1(1)
C(16B)	16(1)	11(1)	17(1)	-1(1)	10(1)	0(1)
C(17B)	20(1)	11(1)	23(1)	1(1)	11(1)	-2(1)
C(18B)	18(1)	14(1)	26(1)	3(1)	9(1)	-3(1)
C(19B)	12(1)	20(2)	26(1)	4(1)	12(1)	1(1)
C(20B)	15(1)	14(1)	21(1)	3(1)	11(1)	2(1)

Table S14. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4b** (2).

	x	y	z	U(eq)
H(1A)	4390(30)	4690(40)	1172(19)	16
H(2A)	6350(30)	4260(30)	1400(20)	17
H(3A)	1859	9504	2231	25
H(4A)	95	8753	1070	26
H(5A)	206	7280	-58	22
H(6A)	2115	6531	-87	19
H(11A)	5851	6635	-915	19
H(13A)	7864	5379	-169	28
H(13B)	8128	4792	820	28
H(13C)	8527	6354	681	28
H(15A)	6393	6845	2924	17
H(15B)	6656	8491	2938	17
H(16A)	8308	6196	2820	18
H(16B)	8764	6797	2058	18
H(17A)	8629	8389	3546	22
H(17B)	9872	7912	3420	22
H(18A)	9513	9434	2206	25
H(18B)	9405	10324	3025	25
H(19A)	7263	10257	2410	23
H(19B)	7748	10827	1656	23
H(20A)	7415	8633	944	18
H(20B)	6169	9137	1054	18
H(1B)	4400(30)	-250(40)	3480(20)	16
H(2B)	6440(30)	-780(30)	4310(20)	16
H(3B)	1975	4639	1123	23
H(4B)	170	3992	1355	24

H(5B)	216	2482	2510	23
H(6B)	2077	1586	3508	20
H(11B)	5781	1606	6332	19
H(13D)	7769	274	6642	28
H(13E)	8464	1361	6227	28
H(13F)	8130	-172	5803	28
H(15C)	6713	3508	2951	16
H(15D)	6458	1861	2825	16
H(16C)	6095	4133	4537	16
H(16D)	7314	3649	5330	16
H(17C)	7647	5866	4812	21
H(17D)	7261	5284	3811	21
H(18C)	9442	4502	5270	23
H(18D)	9408	5411	4419	23
H(19C)	8736	3471	3466	21
H(19D)	9934	3001	4283	21
H(20C)	8740	1842	4976	18
H(20D)	8365	1269	3974	18

Table S15. Torsion angles [°] for **4b** (2).

O(1A)-C(8A)-C(9A)-O(2A)	-26.8(3)	N(2A)-C(2A)-C(3A)-C(4A)	-176.7(3)
O(1A)-C(8A)-C(9A)-C(10A)	90.7(2)	N(2A)-C(2A)-C(7A)-N(1A)	-1.1(3)
O(1A)-C(8A)-C(9A)-C(14A)	-146.99(18)	N(2A)-C(2A)-C(7A)-C(6A)	176.9(2)
O(1A)-C(8A)-C(12A)-O(3A)	85.9(3)	C(1A)-N(1A)-C(7A)-C(2A)	1.9(3)
O(1A)-C(8A)-C(12A)-C(11A)	-93.6(2)	C(1A)-N(1A)-C(7A)-C(6A)	-175.8(3)
O(2A)-C(9A)-C(10A)-C(11A)	133.1(2)	C(1A)-N(1A)-C(8A)-O(1A)	123.0(2)
O(2A)-C(9A)-C(10A)-C(13A)	-46.4(3)	C(1A)-N(1A)-C(8A)-C(9A)	-2.5(3)
O(2A)-C(9A)-C(14A)-C(15A)	-73.2(2)	C(1A)-N(1A)-C(8A)-C(12A)	-119.5(3)
O(2A)-C(9A)-C(14A)-C(16A)	44.1(2)	C(1A)-N(2A)-C(2A)-C(3A)	177.9(3)
O(2A)-C(9A)-C(14A)-C(20A)	164.80(18)	C(1A)-N(2A)-C(2A)-C(7A)	-0.2(3)
N(1A)-C(1A)-C(15A)-C(14A)	34.2(3)	C(2A)-N(2A)-C(1A)-N(1A)	1.5(3)
N(1A)-C(8A)-C(9A)-O(2A)	98.1(2)	C(2A)-N(2A)-C(1A)-C(15A)	-171.7(3)
N(1A)-C(8A)-C(9A)-C(10A)	-144.4(2)	C(2A)-C(3A)-C(4A)-C(5A)	-0.3(5)
N(1A)-C(8A)-C(9A)-C(14A)	-22.1(3)	C(3A)-C(2A)-C(7A)-N(1A)	-179.4(2)
N(1A)-C(8A)-C(12A)-O(3A)	-33.8(4)	C(3A)-C(2A)-C(7A)-C(6A)	-1.4(4)
N(1A)-C(8A)-C(12A)-C(11A)	146.8(2)	C(3A)-C(4A)-C(5A)-C(6A)	-0.8(5)
N(2A)-C(1A)-C(15A)-C(14A)	-152.9(3)	C(4A)-C(5A)-C(6A)-C(7A)	0.8(4)

C(5A)-C(6A)-C(7A)-N(1A)	177.7(3)
C(5A)-C(6A)-C(7A)-C(2A)	0.3(4)
C(7A)-N(1A)-C(1A)-N(2A)	-2.3(3)
C(7A)-N(1A)-C(1A)-C(15A)	171.6(2)
C(7A)-N(1A)-C(8A)-O(1A)	-50.9(3)
C(7A)-N(1A)-C(8A)-C(9A)	-176.4(2)
C(7A)-N(1A)-C(8A)-C(12A)	66.6(3)
C(7A)-C(2A)-C(3A)-C(4A)	1.3(4)
C(8A)-N(1A)-C(1A)-N(2A)	-177.2(2)
C(8A)-N(1A)-C(1A)-C(15A)	-3.4(4)
C(8A)-N(1A)-C(7A)-C(2A)	176.8(2)
C(8A)-N(1A)-C(7A)-C(6A)	-0.9(4)
C(8A)-C(9A)-C(10A)-C(11A)	16.0(3)
C(8A)-C(9A)-C(10A)-C(13A)	-163.5(2)
C(8A)-C(9A)-C(14A)-C(15A)	49.2(3)
C(8A)-C(9A)-C(14A)-C(16A)	166.52(19)
C(8A)-C(9A)-C(14A)-C(20A)	-72.8(2)
C(9A)-C(8A)-C(12A)-O(3A)	-157.2(3)
C(9A)-C(8A)-C(12A)-C(11A)	23.3(3)
C(9A)-C(10A)-C(11A)-C(12A)	-1.6(3)
C(9A)-C(14A)-C(15A)-C(1A)	-55.5(3)
C(9A)-C(14A)-C(16A)-C(17A)	178.30(19)
C(9A)-C(14A)-C(20A)-C(19A)	-176.58(19)
C(10A)-C(9A)-C(14A)-C(15A)	163.9(2)
C(10A)-C(9A)-C(14A)-C(16A)	-78.8(2)
C(10A)-C(9A)-C(14A)-C(20A)	41.9(3)
C(10A)-C(11A)-C(12A)-O(3A)	166.3(3)
C(10A)-C(11A)-C(12A)-C(8A)	-14.3(3)
C(12A)-C(8A)-C(9A)-O(2A)	-140.3(2)
C(12A)-C(8A)-C(9A)-C(10A)	-22.7(2)
C(12A)-C(8A)-C(9A)-C(14A)	99.5(2)
C(13A)-C(10A)-C(11A)-C(12A)	177.9(3)
C(14A)-C(9A)-C(10A)-C(11A)	-106.5(2)
C(14A)-C(9A)-C(10A)-C(13A)	73.9(3)
C(14A)-C(16A)-C(17A)-C(18A)	-56.2(3)
C(15A)-C(14A)-C(16A)-C(17A)	-64.6(3)
C(15A)-C(14A)-C(20A)-C(19A)	63.3(3)
C(16A)-C(14A)-C(15A)-C(1A)	-174.0(2)
C(16A)-C(14A)-C(20A)-C(19A)	-55.2(3)
C(16A)-C(17A)-C(18A)-C(19A)	53.7(3)
C(17A)-C(18A)-C(19A)-C(20A)	-54.0(3)
C(18A)-C(19A)-C(20A)-C(14A)	55.9(3)
C(20A)-C(14A)-C(15A)-C(1A)	67.0(3)
C(20A)-C(14A)-C(16A)-C(17A)	55.8(2)
O(1B)-C(8B)-C(9B)-O(2B)	28.8(2)
O(1B)-C(8B)-C(9B)-C(10B)	-89.0(2)
O(1B)-C(8B)-C(9B)-C(14B)	148.85(18)
O(1B)-C(8B)-C(12B)-O(3B)	-87.8(3)
O(1B)-C(8B)-C(12B)-C(11B)	91.8(2)
O(2B)-C(9B)-C(10B)-C(11B)	-133.1(2)
O(2B)-C(9B)-C(10B)-C(13B)	47.3(3)
O(2B)-C(9B)-C(14B)-C(15B)	70.8(2)
O(2B)-C(9B)-C(14B)-C(16B)	-167.35(17)
O(2B)-C(9B)-C(14B)-C(20B)	-47.0(2)
N(1B)-C(1B)-C(15B)-C(14B)	-34.5(3)
N(1B)-C(8B)-C(9B)-O(2B)	-96.9(2)
N(1B)-C(8B)-C(9B)-C(10B)	145.3(2)
N(1B)-C(8B)-C(9B)-C(14B)	23.2(3)
N(1B)-C(8B)-C(12B)-O(3B)	32.5(4)
N(1B)-C(8B)-C(12B)-C(11B)	-147.9(2)
N(2B)-C(1B)-C(15B)-C(14B)	151.2(3)
N(2B)-C(2B)-C(3B)-C(4B)	179.0(3)
N(2B)-C(2B)-C(7B)-N(1B)	0.7(3)
N(2B)-C(2B)-C(7B)-C(6B)	-177.7(2)
C(1B)-N(1B)-C(7B)-C(2B)	-1.3(3)
C(1B)-N(1B)-C(7B)-C(6B)	176.8(3)
C(1B)-N(1B)-C(8B)-O(1B)	-124.1(2)
C(1B)-N(1B)-C(8B)-C(9B)	2.0(4)
C(1B)-N(1B)-C(8B)-C(12B)	118.0(3)
C(1B)-N(2B)-C(2B)-C(3B)	-179.9(3)
C(1B)-N(2B)-C(2B)-C(7B)	0.2(3)
C(2B)-N(2B)-C(1B)-N(1B)	-1.1(3)
C(2B)-N(2B)-C(1B)-C(15B)	173.4(3)
C(2B)-C(3B)-C(4B)-C(5B)	-0.5(4)
C(3B)-C(2B)-C(7B)-N(1B)	-179.2(2)
C(3B)-C(2B)-C(7B)-C(6B)	2.5(4)
C(3B)-C(4B)-C(5B)-C(6B)	0.9(5)
C(4B)-C(5B)-C(6B)-C(7B)	0.4(4)
C(5B)-C(6B)-C(7B)-N(1B)	-179.8(3)
C(5B)-C(6B)-C(7B)-C(2B)	-2.0(4)

C(7B)-N(1B)-C(1B)-N(2B)	1.6(3)	C(10B)-C(9B)-C(14B)-C(15B)	-165.08(19)
C(7B)-N(1B)-C(1B)-C(15B)	-173.4(2)	C(10B)-C(9B)-C(14B)-C(16B)	-43.2(3)
C(7B)-N(1B)-C(8B)-O(1B)	52.3(3)	C(10B)-C(9B)-C(14B)-C(20B)	77.2(2)
C(7B)-N(1B)-C(8B)-C(9B)	178.4(2)	C(10B)-C(11B)-C(12B)-O(3B)	-164.8(3)
C(7B)-N(1B)-C(8B)-C(12B)	-65.5(3)	C(10B)-C(11B)-C(12B)-C(8B)	15.7(3)
C(7B)-C(2B)-C(3B)-C(4B)	-1.1(4)	C(12B)-C(8B)-C(9B)-O(2B)	141.7(2)
C(8B)-N(1B)-C(1B)-N(2B)	178.6(2)	C(12B)-C(8B)-C(9B)-C(10B)	23.9(2)
C(8B)-N(1B)-C(1B)-C(15B)	3.6(4)	C(12B)-C(8B)-C(9B)-C(14B)	-98.3(2)
C(8B)-N(1B)-C(7B)-C(2B)	-178.3(2)	C(13B)-C(10B)-C(11B)-C(12B)	-179.2(2)
C(8B)-N(1B)-C(7B)-C(6B)	-0.2(5)	C(14B)-C(9B)-C(10B)-C(11B)	105.1(2)
C(8B)-C(9B)-C(10B)-C(11B)	-16.6(3)	C(14B)-C(9B)-C(10B)-C(13B)	-74.5(3)
C(8B)-C(9B)-C(10B)-C(13B)	163.8(2)	C(14B)-C(16B)-C(17B)-C(18B)	-56.9(3)
C(8B)-C(9B)-C(14B)-C(15B)	-50.7(3)	C(15B)-C(14B)-C(16B)-C(17B)	-64.0(2)
C(8B)-C(9B)-C(14B)-C(16B)	71.1(2)	C(15B)-C(14B)-C(20B)-C(19B)	65.7(3)
C(8B)-C(9B)-C(14B)-C(20B)	-168.48(18)	C(16B)-C(14B)-C(15B)-C(1B)	-65.7(3)
C(9B)-C(8B)-C(12B)-O(3B)	155.6(3)	C(16B)-C(14B)-C(20B)-C(19B)	-54.8(3)
C(9B)-C(8B)-C(12B)-C(11B)	-24.8(3)	C(16B)-C(17B)-C(18B)-C(19B)	54.9(3)
C(9B)-C(10B)-C(11B)-C(12B)	1.2(3)	C(17B)-C(18B)-C(19B)-C(20B)	-53.5(3)
C(9B)-C(14B)-C(15B)-C(1B)	56.6(3)	C(18B)-C(19B)-C(20B)-C(14B)	55.3(3)
C(9B)-C(14B)-C(16B)-C(17B)	176.00(19)	C(20B)-C(14B)-C(15B)-C(1B)	175.3(2)
C(9B)-C(14B)-C(20B)-C(19B)	-176.90(19)	C(20B)-C(14B)-C(16B)-C(17B)	54.9(3)

Table S16. Hydrogen bonds for **4b** (2) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1A)-H(1A)...N(2B)	0.88(3)	1.93(3)	2.810(3)	172(3)
O(2A)-H(2A)...O(3A)#1	0.88(3)	1.96(3)	2.818(3)	163(3)
O(1B)-H(1B)...N(2A)#2	0.89(3)	1.97(3)	2.833(3)	165(3)
O(2B)-H(2B)...O(3B)#3	0.88(3)	1.96(3)	2.823(3)	166(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z #2 x,y-1,z #3 -x+1,y-1/2,-z+1

6.3. Compound **4c**

X-ray diffraction data were collected at 100K on a Rigaku Synergy S diffractometer equipped with a HyPix600HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_a-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[1] The structure was solved by direct methods using SHELXT[2] and refined on F^2 using SHELXL-2018[3] in the OLEX2 program.[4] Positions of all atoms were found from the electron density-difference map. Atoms were refined with individual anisotropic (non-hydrogen atoms) or isotropic (hydrogen atoms) displacement parameters.

Table S17. Crystal data and structure refinement for **4c**.

Identification code	**4c**	
Empirical formula	C19 H20 N2 O4	
Formula weight	340.37	
Temperature	100.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 11.38512(6) Å	a= 90°.
	b = 9.48447(4) Å	b= 110.6652(6)°.
	c = 15.80604(8) Å	g = 90°.
Volume	1596.950(14) $Å^3$	
Z	4	
Density (calculated)	1.416 g/cm^3	
Absorption coefficient	0.822 mm^{-1}	
F(000)	720	
Crystal size	0.34 x 0.17 x 0.08 mm^3	
Theta range for data collection	2.988 to 79.491°.	
Index ranges	-14<=h<=14, -10<=k<=12, -20<=l<=20	
Reflections collected	41676	
Independent reflections	6778 [R(int) = 0.0282]	
Observed reflections	6769	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.83418 and 0.83014	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6778 / 1 / 610	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0275, wR2 = 0.0730	
R indices (all data)	R1 = 0.0276, wR2 = 0.0731	

Absolute structure parameter	-0.03(4)
Extinction coefficient	0.0048(4)
Largest diff. peak and hole	0.274 and -0.157 e.Å^{-3}
CCDC	**2233460**

Table S18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **4c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1A)	6797(1)	5003(1)	4146(1)	14(1)
O(2A)	4409(1)	5075(1)	4025(1)	14(1)
O(3A)	3841(1)	7551(2)	5055(1)	18(1)
O(4A)	9242(1)	9514(2)	4792(1)	24(1)
N(1A)	4347(1)	8692(2)	2247(1)	16(1)
N(2A)	4450(1)	7320(2)	3423(1)	13(1)
C(1A)	6473(2)	6239(2)	4515(1)	12(1)
C(2A)	4998(2)	6392(2)	4196(1)	12(1)
C(3A)	4783(2)	6937(2)	5057(1)	14(1)
C(4A)	5884(2)	6521(2)	5819(1)	17(1)
C(5A)	6811(2)	6112(2)	5542(1)	15(1)
C(6A)	8052(2)	5566(2)	6152(1)	20(1)
C(7A)	7147(2)	7488(2)	4221(1)	12(1)
C(8A)	7152(2)	8845(2)	4764(1)	15(1)
C(9A)	7981(2)	9984(2)	4588(1)	20(1)
C(10A)	9272(2)	8349(2)	4227(1)	21(1)
C(11A)	8526(2)	7094(2)	4372(1)	17(1)
C(12A)	6460(2)	7751(2)	3203(1)	15(1)
C(13A)	5085(2)	7985(2)	2951(1)	13(1)
C(14A)	3132(2)	8439(2)	2240(1)	16(1)
C(15A)	1975(2)	8888(2)	1619(1)	20(1)
C(16A)	898(2)	8427(2)	1750(1)	21(1)
C(17A)	951(2)	7534(2)	2470(1)	20(1)
C(18A)	2090(2)	7095(2)	3098(1)	17(1)
C(19A)	3170(2)	7573(2)	2966(1)	15(1)
O(1B)	6775(1)	15(1)	1768(1)	15(1)
O(2B)	4368(1)	67(1)	695(1)	14(1)
O(3B)	3774(1)	2643(1)	-584(1)	17(1)

O(4B)	9075(1)	4650(1)	2371(1)	21(1)
N(1B)	4319(1)	3663(2)	2471(1)	16(1)
N(2B)	4399(1)	2293(2)	1341(1)	13(1)
C(1B)	6421(2)	1253(2)	1241(1)	13(1)
C(2B)	4939(2)	1396(2)	828(1)	12(1)
C(3B)	4710(2)	1992(2)	-132(1)	14(1)
C(4B)	5790(2)	1595(2)	-360(1)	16(1)
C(5B)	6737(2)	1157(2)	375(1)	14(1)
C(6B)	7957(2)	603(2)	368(1)	19(1)
C(7B)	7082(2)	2505(2)	1880(1)	13(1)
C(8B)	7023(2)	3878(2)	1339(1)	15(1)
C(9B)	7795(2)	5049(2)	1940(1)	19(1)
C(10B)	9173(2)	3457(2)	2942(1)	19(1)
C(11B)	8482(2)	2178(2)	2412(1)	16(1)
C(12B)	6417(2)	2695(2)	2571(1)	15(1)
C(13B)	5045(2)	2948(2)	2137(1)	13(1)
C(14B)	3098(2)	3430(2)	1866(1)	16(1)
C(15B)	1948(2)	3892(2)	1903(1)	20(1)
C(16B)	866(2)	3454(2)	1222(1)	22(1)
C(17B)	907(2)	2576(2)	520(1)	20(1)
C(18B)	2035(2)	2117(2)	466(1)	17(1)
C(19B)	3126(2)	2566(2)	1151(1)	14(1)

Table S19. Bond lengths [Å] and angles [°] for **4c**.

O(1A)-H(1A)	0.84(3)	C(1A)-C(5A)	1.535(2)
O(1A)-C(1A)	1.415(2)	C(1A)-C(7A)	1.569(2)
O(2A)-H(2A)	0.91(3)	C(2A)-C(3A)	1.554(2)
O(2A)-C(2A)	1.398(2)	C(3A)-C(4A)	1.453(2)
O(3A)-C(3A)	1.219(2)	C(4A)-H(4A)	1.00(3)
O(4A)-C(9A)	1.427(2)	C(4A)-C(5A)	1.334(3)
O(4A)-C(10A)	1.429(2)	C(5A)-C(6A)	1.494(3)
N(1A)-C(13A)	1.317(2)	C(6A)-H(6A)	1.03(3)
N(1A)-C(14A)	1.400(2)	C(6A)-H(6B)	0.90(4)
N(2A)-C(2A)	1.455(2)	C(6A)-H(6C)	0.99(3)
N(2A)-C(13A)	1.364(2)	C(7A)-C(8A)	1.546(2)
N(2A)-C(19A)	1.400(2)	C(7A)-C(11A)	1.548(2)
C(1A)-C(2A)	1.581(2)	C(7A)-C(12A)	1.542(2)

C(8A)-H(8A)	0.99(3)	C(4B)-H(4B)	1.00(3)
C(8A)-H(8B)	0.98(2)	C(4B)-C(5B)	1.342(3)
C(8A)-C(9A)	1.524(3)	C(5B)-C(6B)	1.489(2)
C(9A)-H(9A)	0.96(2)	C(6B)-H(6D)	1.02(3)
C(9A)-H(9B)	0.99(3)	C(6B)-H(6E)	0.95(3)
C(10A)-H(10A)	0.98(3)	C(6B)-H(6F)	0.94(4)
C(10A)-H(10B)	0.97(3)	C(7B)-C(8B)	1.547(2)
C(10A)-C(11A)	1.527(3)	C(7B)-C(11B)	1.548(2)
C(11A)-H(11A)	1.00(3)	C(7B)-C(12B)	1.543(2)
C(11A)-H(11B)	0.95(3)	C(8B)-H(8C)	1.00(3)
C(12A)-H(12A)	0.95(3)	C(8B)-H(8D)	0.99(3)
C(12A)-H(12B)	0.98(3)	C(8B)-C(9B)	1.523(2)
C(12A)-C(13A)	1.489(2)	C(9B)-H(9C)	0.98(3)
C(14A)-C(15A)	1.403(2)	C(9B)-H(9D)	1.00(2)
C(14A)-C(19A)	1.399(2)	C(10B)-H(10C)	0.97(2)
C(15A)-H(15A)	0.96(3)	C(10B)-H(10D)	0.99(2)
C(15A)-C(16A)	1.385(3)	C(10B)-C(11B)	1.526(3)
C(16A)-H(16A)	0.96(2)	C(11B)-H(11C)	0.98(3)
C(16A)-C(17A)	1.403(3)	C(11B)-H(11D)	1.02(3)
C(17A)-H(17A)	0.97(3)	C(12B)-H(12C)	0.97(3)
C(17A)-C(18A)	1.389(3)	C(12B)-H(12D)	0.94(3)
C(18A)-H(18A)	0.98(3)	C(12B)-C(13B)	1.487(2)
C(18A)-C(19A)	1.394(2)	C(14B)-C(15B)	1.402(2)
O(1B)-H(1B)	0.85(3)	C(14B)-C(19B)	1.406(2)
O(1B)-C(1B)	1.414(2)	C(15B)-H(15B)	0.95(3)
O(2B)-H(2B)	0.85(3)	C(15B)-C(16B)	1.383(3)
O(2B)-C(2B)	1.400(2)	C(16B)-H(16B)	0.98(3)
O(3B)-C(3B)	1.221(2)	C(16B)-C(17B)	1.403(3)
O(4B)-C(9B)	1.425(2)	C(17B)-H(17B)	0.97(3)
O(4B)-C(10B)	1.427(2)	C(17B)-C(18B)	1.386(3)
N(1B)-C(13B)	1.316(2)	C(18B)-H(18B)	0.98(3)
N(1B)-C(14B)	1.398(2)	C(18B)-C(19B)	1.396(2)
N(2B)-C(2B)	1.453(2)	C(1A)-O(1A)-H(1A)	111.4(19)
N(2B)-C(13B)	1.363(2)	C(2A)-O(2A)-H(2A)	111(2)
N(2B)-C(19B)	1.396(2)	C(9A)-O(4A)-C(10A)	110.14(14)
C(1B)-C(2B)	1.585(2)	C(13A)-N(1A)-C(14A)	104.73(14)
C(1B)-C(5B)	1.536(2)	C(13A)-N(2A)-C(2A)	125.89(14)
C(1B)-C(7B)	1.569(2)	C(13A)-N(2A)-C(19A)	107.10(14)
C(2B)-C(3B)	1.551(2)	C(19A)-N(2A)-C(2A)	126.67(14)
C(3B)-C(4B)	1.449(2)	O(1A)-C(1A)-C(2A)	110.29(13)

O(1A)-C(1A)-C(5A)	111.49(14)
O(1A)-C(1A)-C(7A)	106.12(13)
C(5A)-C(1A)-C(2A)	100.73(13)
C(5A)-C(1A)-C(7A)	113.97(14)
C(7A)-C(1A)-C(2A)	114.33(14)
O(2A)-C(2A)-N(2A)	110.12(13)
O(2A)-C(2A)-C(1A)	111.25(14)
O(2A)-C(2A)-C(3A)	104.68(13)
N(2A)-C(2A)-C(1A)	114.57(14)
N(2A)-C(2A)-C(3A)	112.38(14)
C(3A)-C(2A)-C(1A)	103.24(13)
O(3A)-C(3A)-C(2A)	124.52(15)
O(3A)-C(3A)-C(4A)	129.29(16)
C(4A)-C(3A)-C(2A)	106.16(14)
C(3A)-C(4A)-H(4A)	122.4(16)
C(5A)-C(4A)-C(3A)	111.06(15)
C(5A)-C(4A)-H(4A)	126.5(16)
C(4A)-C(5A)-C(1A)	113.02(15)
C(4A)-C(5A)-C(6A)	124.57(16)
C(6A)-C(5A)-C(1A)	122.41(15)
C(5A)-C(6A)-H(6A)	111.1(16)
C(5A)-C(6A)-H(6B)	111(2)
C(5A)-C(6A)-H(6C)	111.3(18)
H(6A)-C(6A)-H(6B)	109(3)
H(6A)-C(6A)-H(6C)	105(3)
H(6B)-C(6A)-H(6C)	109(3)
C(8A)-C(7A)-C(1A)	111.75(13)
C(8A)-C(7A)-C(11A)	108.12(14)
C(11A)-C(7A)-C(1A)	110.31(14)
C(12A)-C(7A)-C(1A)	108.09(13)
C(12A)-C(7A)-C(8A)	110.26(14)
C(12A)-C(7A)-C(11A)	108.26(13)
C(7A)-C(8A)-H(8A)	110.6(15)
C(7A)-C(8A)-H(8B)	108.9(15)
H(8A)-C(8A)-H(8B)	109(2)
C(9A)-C(8A)-C(7A)	111.66(14)
C(9A)-C(8A)-H(8A)	109.4(15)
C(9A)-C(8A)-H(8B)	107.1(14)
O(4A)-C(9A)-C(8A)	112.09(16)
O(4A)-C(9A)-H(9A)	109.3(14)
O(4A)-C(9A)-H(9B)	109.0(17)
C(8A)-C(9A)-H(9A)	110.0(15)
C(8A)-C(9A)-H(9B)	109.4(16)
H(9A)-C(9A)-H(9B)	107(2)
O(4A)-C(10A)-H(10A)	105.1(16)
O(4A)-C(10A)-H(10B)	110.6(16)
O(4A)-C(10A)-C(11A)	111.77(15)
H(10A)-C(10A)-H(10B)	106(2)
C(11A)-C(10A)-H(10A)	111.3(16)
C(11A)-C(10A)-H(10B)	111.9(15)
C(7A)-C(11A)-H(11A)	113.1(15)
C(7A)-C(11A)-H(11B)	110.6(14)
C(10A)-C(11A)-C(7A)	112.11(15)
C(10A)-C(11A)-H(11A)	105.9(16)
C(10A)-C(11A)-H(11B)	108.4(14)
H(11A)-C(11A)-H(11B)	106(2)
C(7A)-C(12A)-H(12A)	112.8(14)
C(7A)-C(12A)-H(12B)	107.8(15)
H(12A)-C(12A)-H(12B)	108(2)
C(13A)-C(12A)-C(7A)	113.64(13)
C(13A)-C(12A)-H(12A)	109.4(14)
C(13A)-C(12A)-H(12B)	104.6(14)
N(1A)-C(13A)-N(2A)	113.22(15)
N(1A)-C(13A)-C(12A)	126.79(15)
N(2A)-C(13A)-C(12A)	119.70(15)
N(1A)-C(14A)-C(15A)	129.43(17)
C(19A)-C(14A)-N(1A)	110.41(15)
C(19A)-C(14A)-C(15A)	120.13(16)
C(14A)-C(15A)-H(15A)	122.1(16)
C(16A)-C(15A)-C(14A)	117.50(18)
C(16A)-C(15A)-H(15A)	120.4(16)
C(15A)-C(16A)-H(16A)	119.9(15)
C(15A)-C(16A)-C(17A)	121.69(17)
C(17A)-C(16A)-H(16A)	118.4(15)
C(16A)-C(17A)-H(17A)	119.4(16)
C(18A)-C(17A)-C(16A)	121.48(17)
C(18A)-C(17A)-H(17A)	119.1(16)
C(17A)-C(18A)-H(18A)	121.1(14)
C(17A)-C(18A)-C(19A)	116.52(17)
C(19A)-C(18A)-H(18A)	122.4(14)

C(14A)-C(19A)-N(2A)	104.49(15)	C(12B)-C(7B)-C(1B)	107.44(13)
C(18A)-C(19A)-N(2A)	132.79(17)	C(12B)-C(7B)-C(8B)	110.92(14)
C(18A)-C(19A)-C(14A)	122.65(16)	C(12B)-C(7B)-C(11B)	107.88(13)
C(1B)-O(1B)-H(1B)	107.3(18)	C(7B)-C(8B)-H(8C)	111.1(16)
C(2B)-O(2B)-H(2B)	110(2)	C(7B)-C(8B)-H(8D)	110.4(16)
C(9B)-O(4B)-C(10B)	110.58(14)	H(8C)-C(8B)-H(8D)	105(2)
C(13B)-N(1B)-C(14B)	104.93(14)	C(9B)-C(8B)-C(7B)	111.44(14)
C(13B)-N(2B)-C(2B)	125.83(14)	C(9B)-C(8B)-H(8C)	107.5(15)
C(13B)-N(2B)-C(19B)	107.15(14)	C(9B)-C(8B)-H(8D)	111.6(16)
C(19B)-N(2B)-C(2B)	126.88(14)	O(4B)-C(9B)-C(8B)	111.85(15)
O(1B)-C(1B)-C(2B)	110.77(13)	O(4B)-C(9B)-H(9C)	106.4(14)
O(1B)-C(1B)-C(5B)	111.63(14)	O(4B)-C(9B)-H(9D)	110.0(13)
O(1B)-C(1B)-C(7B)	106.07(13)	C(8B)-C(9B)-H(9C)	112.3(15)
C(5B)-C(1B)-C(2B)	100.83(13)	C(8B)-C(9B)-H(9D)	109.1(14)
C(5B)-C(1B)-C(7B)	114.13(14)	H(9C)-C(9B)-H(9D)	107(2)
C(7B)-C(1B)-C(2B)	113.54(13)	O(4B)-C(10B)-H(10C)	110.7(14)
O(2B)-C(2B)-N(2B)	110.16(13)	O(4B)-C(10B)-H(10D)	104.9(15)
O(2B)-C(2B)-C(1B)	110.78(14)	O(4B)-C(10B)-C(11B)	111.89(15)
O(2B)-C(2B)-C(3B)	105.83(13)	H(10C)-C(10B)-H(10D)	107.2(19)
N(2B)-C(2B)-C(1B)	114.76(13)	C(11B)-C(10B)-H(10C)	110.3(14)
N(2B)-C(2B)-C(3B)	111.97(14)	C(11B)-C(10B)-H(10D)	111.7(15)
C(3B)-C(2B)-C(1B)	102.79(13)	C(7B)-C(11B)-H(11C)	107.5(14)
O(3B)-C(3B)-C(2B)	124.59(15)	C(7B)-C(11B)-H(11D)	111.0(14)
O(3B)-C(3B)-C(4B)	128.87(16)	C(10B)-C(11B)-C(7B)	111.82(15)
C(4B)-C(3B)-C(2B)	106.53(14)	C(10B)-C(11B)-H(11C)	110.8(15)
C(3B)-C(4B)-H(4B)	123.7(15)	C(10B)-C(11B)-H(11D)	107.1(15)
C(5B)-C(4B)-C(3B)	110.93(15)	H(11C)-C(11B)-H(11D)	109(2)
C(5B)-C(4B)-H(4B)	125.3(15)	C(7B)-C(12B)-H(12C)	108.5(14)
C(4B)-C(5B)-C(1B)	112.61(15)	C(7B)-C(12B)-H(12D)	111.1(15)
C(4B)-C(5B)-C(6B)	124.68(16)	H(12C)-C(12B)-H(12D)	108(2)
C(6B)-C(5B)-C(1B)	122.69(15)	C(13B)-C(12B)-C(7B)	112.99(14)
C(5B)-C(6B)-H(6D)	112.4(15)	C(13B)-C(12B)-H(12C)	106.8(14)
C(5B)-C(6B)-H(6E)	110.1(18)	C(13B)-C(12B)-H(12D)	109.5(15)
C(5B)-C(6B)-H(6F)	112(2)	N(1B)-C(13B)-N(2B)	113.25(15)
H(6D)-C(6B)-H(6E)	105(2)	N(1B)-C(13B)-C(12B)	127.21(15)
H(6D)-C(6B)-H(6F)	110(3)	N(2B)-C(13B)-C(12B)	119.27(15)
H(6E)-C(6B)-H(6F)	107(3)	N(1B)-C(14B)-C(15B)	129.77(17)
C(8B)-C(7B)-C(1B)	111.31(13)	N(1B)-C(14B)-C(19B)	110.06(15)
C(8B)-C(7B)-C(11B)	107.78(14)	C(15B)-C(14B)-C(19B)	120.15(16)
C(11B)-C(7B)-C(1B)	111.47(14)	C(14B)-C(15B)-H(15B)	121.7(16)

C(16B)-C(15B)-C(14B)	117.57(18)	C(18B)-C(17B)-H(17B)	117.6(16)
C(16B)-C(15B)-H(15B)	120.7(16)	C(17B)-C(18B)-H(18B)	121.6(14)
C(15B)-C(16B)-H(16B)	119.3(15)	C(17B)-C(18B)-C(19B)	116.55(17)
C(15B)-C(16B)-C(17B)	121.67(17)	C(19B)-C(18B)-H(18B)	121.8(14)
C(17B)-C(16B)-H(16B)	119.0(15)	N(2B)-C(19B)-C(14B)	104.57(15)
C(16B)-C(17B)-H(17B)	120.6(16)	C(18B)-C(19B)-N(2B)	133.04(16)
C(18B)-C(17B)-C(16B)	121.71(17)	C(18B)-C(19B)-C(14B)	122.34(15)

Table S20. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4c**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1A)	17(1)	10(1)	17(1)	-1(1)	7(1)	0(1)
O(2A)	17(1)	11(1)	14(1)	-1(1)	6(1)	-2(1)
O(3A)	19(1)	16(1)	22(1)	-5(1)	9(1)	0(1)
O(4A)	19(1)	21(1)	28(1)	-3(1)	6(1)	-6(1)
N(1A)	16(1)	17(1)	12(1)	1(1)	4(1)	0(1)
N(2A)	12(1)	13(1)	14(1)	2(1)	4(1)	1(1)
C(1A)	14(1)	10(1)	12(1)	-1(1)	4(1)	1(1)
C(2A)	15(1)	10(1)	13(1)	1(1)	5(1)	-1(1)
C(3A)	18(1)	11(1)	15(1)	-2(1)	8(1)	-4(1)
C(4A)	21(1)	15(1)	14(1)	-1(1)	6(1)	-1(1)
C(5A)	19(1)	10(1)	14(1)	0(1)	4(1)	-2(1)
C(6A)	20(1)	21(1)	15(1)	4(1)	3(1)	0(1)
C(7A)	13(1)	10(1)	15(1)	1(1)	5(1)	1(1)
C(8A)	18(1)	12(1)	16(1)	-2(1)	6(1)	-1(1)
C(9A)	23(1)	14(1)	25(1)	-1(1)	10(1)	-2(1)
C(10A)	16(1)	21(1)	27(1)	2(1)	9(1)	0(1)
C(11A)	14(1)	16(1)	21(1)	2(1)	5(1)	2(1)
C(12A)	16(1)	16(1)	13(1)	2(1)	6(1)	2(1)
C(13A)	16(1)	12(1)	12(1)	-1(1)	5(1)	0(1)
C(14A)	16(1)	15(1)	15(1)	-1(1)	4(1)	0(1)
C(15A)	19(1)	21(1)	17(1)	2(1)	2(1)	2(1)
C(16A)	14(1)	22(1)	20(1)	-4(1)	-1(1)	2(1)
C(17A)	16(1)	18(1)	25(1)	-5(1)	6(1)	-1(1)
C(18A)	17(1)	15(1)	20(1)	-1(1)	6(1)	0(1)
C(19A)	15(1)	12(1)	15(1)	-1(1)	2(1)	1(1)

O(1B)	17(1)	10(1)	15(1)	1(1)	3(1)	1(1)
O(2B)	16(1)	12(1)	13(1)	0(1)	5(1)	-2(1)
O(3B)	17(1)	15(1)	17(1)	4(1)	3(1)	1(1)
O(4B)	18(1)	17(1)	26(1)	-1(1)	5(1)	-3(1)
N(1B)	16(1)	16(1)	15(1)	-1(1)	7(1)	-1(1)
N(2B)	13(1)	14(1)	12(1)	-1(1)	4(1)	1(1)
C(1B)	13(1)	12(1)	13(1)	1(1)	4(1)	2(1)
C(2B)	14(1)	11(1)	12(1)	-1(1)	4(1)	0(1)
C(3B)	18(1)	12(1)	12(1)	-1(1)	3(1)	-3(1)
C(4B)	21(1)	16(1)	13(1)	-1(1)	7(1)	-2(1)
C(5B)	17(1)	11(1)	16(1)	-3(1)	8(1)	-3(1)
C(6B)	16(1)	24(1)	20(1)	-4(1)	7(1)	0(1)
C(7B)	12(1)	12(1)	12(1)	0(1)	2(1)	1(1)
C(8B)	17(1)	12(1)	15(1)	0(1)	4(1)	0(1)
C(9B)	19(1)	14(1)	21(1)	-2(1)	3(1)	0(1)
C(10B)	15(1)	17(1)	20(1)	-1(1)	1(1)	1(1)
C(11B)	14(1)	14(1)	18(1)	0(1)	2(1)	2(1)
C(12B)	16(1)	16(1)	12(1)	-2(1)	4(1)	0(1)
C(13B)	16(1)	11(1)	12(1)	0(1)	6(1)	-2(1)
C(14B)	16(1)	15(1)	16(1)	1(1)	6(1)	-1(1)
C(15B)	22(1)	19(1)	23(1)	-1(1)	11(1)	2(1)
C(16B)	17(1)	23(1)	28(1)	5(1)	10(1)	2(1)
C(17B)	15(1)	22(1)	21(1)	5(1)	5(1)	-1(1)
C(18B)	16(1)	17(1)	16(1)	1(1)	4(1)	-1(1)
C(19B)	14(1)	14(1)	17(1)	4(1)	6(1)	2(1)

Table S21. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4c**.

	x	y	z	U(eq)
H(1A)	6540(30)	4270(30)	4328(19)	29(7)
H(2A)	4500(30)	4670(40)	3530(20)	37(8)
H(4A)	5900(20)	6540(30)	6453(19)	27(6)
H(6A)	8000(30)	5210(30)	6755(19)	33(7)
H(6B)	8650(30)	6230(40)	6270(20)	51(9)
H(6C)	8320(30)	4740(40)	5880(20)	43(8)
H(8A)	6290(20)	9210(30)	4613(17)	21(6)

H(8B)	7500(20)	8630(30)	5409(16)	18(5)
H(9A)	7640(20)	10280(30)	3968(17)	17(6)
H(9B)	7980(30)	10820(30)	4960(19)	32(7)
H(10A)	10170(20)	8110(30)	4391(17)	24(6)
H(10B)	8990(20)	8640(30)	3597(17)	21(6)
H(11A)	9000(20)	6740(30)	5000(18)	27(7)
H(11B)	8560(20)	6360(30)	3972(16)	15(5)
H(12A)	6820(20)	8510(30)	2976(16)	15
H(12B)	6530(20)	6890(30)	2879(17)	19(6)
H(15A)	1920(20)	9490(30)	1120(19)	30(7)
H(16A)	90(20)	8710(30)	1340(16)	21(6)
H(17A)	180(20)	7220(30)	2535(17)	25(6)
H(18A)	2120(20)	6460(30)	3598(16)	18(6)
H(1B)	6540(20)	-690(30)	1408(18)	23(6)
H(2B)	4470(30)	-320(30)	1200(20)	33(7)
H(4B)	5820(20)	1670(30)	-986(18)	25(6)
H(6D)	7930(30)	350(30)	-268(19)	29(7)
H(6E)	8160(30)	-250(40)	690(20)	38(8)
H(6F)	8620(30)	1230(40)	640(20)	49(9)
H(8C)	7360(20)	3730(30)	842(17)	23(6)
H(8D)	6140(20)	4170(30)	1029(18)	25(6)
H(9C)	7800(20)	5910(30)	1601(16)	19(6)
H(9D)	7420(20)	5300(30)	2406(16)	15(5)
H(10C)	8870(20)	3680(30)	3423(15)	12(5)
H(10D)	10090(20)	3280(30)	3227(16)	18(6)
H(11C)	8510(20)	1390(30)	2818(17)	20(6)
H(11D)	8940(20)	1890(30)	1984(17)	23(6)
H(12C)	6510(20)	1830(30)	2919(16)	14(5)
H(12D)	6780(20)	3430(30)	2977(17)	17(6)
H(15B)	1910(20)	4510(30)	2366(19)	29(7)
H(16B)	50(20)	3760(30)	1232(16)	23(6)
H(17B)	140(30)	2270(30)	53(19)	24(6)
H(18B)	2060(20)	1490(30)	-23(16)	17

Table S22. Torsion angles [°] for **4c**.

O(1A)-C(1A)-C(2A)-O(2A)	28.47(18)	O(1A)-C(1A)-C(2A)-C(3A)	140.24(14)
O(1A)-C(1A)-C(2A)-N(2A)	-97.25(17)	O(1A)-C(1A)-C(5A)-C(4A)	-133.01(16)

O(1A)-C(1A)-C(5A)-C(6A)	46.3(2)
O(1A)-C(1A)-C(7A)-C(8A)	-165.88(13)
O(1A)-C(1A)-C(7A)-C(11A)	-45.57(17)
O(1A)-C(1A)-C(7A)-C(12A)	72.62(16)
O(2A)-C(2A)-C(3A)-O(3A)	-84.4(2)
O(2A)-C(2A)-C(3A)-C(4A)	93.79(15)
O(3A)-C(3A)-C(4A)-C(5A)	-168.19(19)
O(4A)-C(10A)-C(11A)-C(7A)	56.3(2)
N(1A)-C(14A)-C(15A)-C(16A)	176.98(19)
N(1A)-C(14A)-C(19A)-N(2A)	0.71(19)
N(1A)-C(14A)-C(19A)-C(18A)	-176.72(17)
N(2A)-C(2A)-C(3A)-O(3A)	35.1(2)
N(2A)-C(2A)-C(3A)-C(4A)	-146.70(15)
C(1A)-C(2A)-C(3A)-O(3A)	159.10(17)
C(1A)-C(2A)-C(3A)-C(4A)	-22.73(18)
C(1A)-C(7A)-C(8A)-C(9A)	170.93(14)
C(1A)-C(7A)-C(11A)-C(10A)	-171.66(14)
C(1A)-C(7A)-C(12A)-C(13A)	54.08(19)
C(2A)-N(2A)-C(13A)-N(1A)	175.97(15)
C(2A)-N(2A)-C(13A)-C(12A)	1.8(3)
C(2A)-N(2A)-C(19A)-C(14A)	-175.32(16)
C(2A)-N(2A)-C(19A)-C(18A)	1.7(3)
C(2A)-C(1A)-C(5A)-C(4A)	-16.0(2)
C(2A)-C(1A)-C(5A)-C(6A)	163.33(16)
C(2A)-C(1A)-C(7A)-C(8A)	72.33(17)
C(2A)-C(1A)-C(7A)-C(11A)	-167.35(14)
C(2A)-C(1A)-C(7A)-C(12A)	-49.17(18)
C(2A)-C(3A)-C(4A)-C(5A)	13.8(2)
C(3A)-C(4A)-C(5A)-C(1A)	1.8(2)
C(3A)-C(4A)-C(5A)-C(6A)	-177.48(17)
C(5A)-C(1A)-C(2A)-O(2A)	-89.41(15)
C(5A)-C(1A)-C(2A)-N(2A)	144.88(14)
C(5A)-C(1A)-C(2A)-C(3A)	22.36(17)
C(5A)-C(1A)-C(7A)-C(8A)	-42.80(19)
C(5A)-C(1A)-C(7A)-C(11A)	77.52(17)
C(5A)-C(1A)-C(7A)-C(12A)	-164.30(14)
C(7A)-C(1A)-C(2A)-O(2A)	147.94(13)
C(7A)-C(1A)-C(2A)-N(2A)	22.2(2)
C(7A)-C(1A)-C(2A)-C(3A)	-100.29(15)
C(7A)-C(1A)-C(5A)-C(4A)	106.88(17)
C(7A)-C(1A)-C(5A)-C(6A)	-73.8(2)
C(7A)-C(8A)-C(9A)-O(4A)	-57.2(2)
C(7A)-C(12A)-C(13A)-N(1A)	154.45(17)
C(7A)-C(12A)-C(13A)-N(2A)	-32.2(2)
C(8A)-C(7A)-C(11A)-C(10A)	-49.18(19)
C(8A)-C(7A)-C(12A)-C(13A)	-68.34(19)
C(9A)-O(4A)-C(10A)-C(11A)	-61.3(2)
C(10A)-O(4A)-C(9A)-C(8A)	61.93(19)
C(11A)-C(7A)-C(8A)-C(9A)	49.35(19)
C(11A)-C(7A)-C(12A)-C(13A)	173.57(15)
C(12A)-C(7A)-C(8A)-C(9A)	-68.83(18)
C(12A)-C(7A)-C(11A)-C(10A)	70.26(19)
C(13A)-N(1A)-C(14A)-C(15A)	-177.32(19)
C(13A)-N(1A)-C(14A)-C(19A)	0.6(2)
C(13A)-N(2A)-C(2A)-O(2A)	-123.24(17)
C(13A)-N(2A)-C(2A)-C(1A)	3.1(2)
C(13A)-N(2A)-C(2A)-C(3A)	120.49(17)
C(13A)-N(2A)-C(19A)-C(14A)	-1.73(19)
C(13A)-N(2A)-C(19A)-C(18A)	175.32(19)
C(14A)-N(1A)-C(13A)-N(2A)	-1.8(2)
C(14A)-N(1A)-C(13A)-C(12A)	171.92(17)
C(14A)-C(15A)-C(16A)-C(17A)	-0.6(3)
C(15A)-C(14A)-C(19A)-N(2A)	178.87(16)
C(15A)-C(14A)-C(19A)-C(18A)	1.4(3)
C(15A)-C(16A)-C(17A)-C(18A)	1.4(3)
C(16A)-C(17A)-C(18A)-C(19A)	-0.8(3)
C(17A)-C(18A)-C(19A)-N(2A)	-177.23(19)
C(17A)-C(18A)-C(19A)-C(14A)	-0.6(3)
C(19A)-N(2A)-C(2A)-O(2A)	49.2(2)
C(19A)-N(2A)-C(2A)-C(1A)	175.51(15)
C(19A)-N(2A)-C(2A)-C(3A)	-67.1(2)
C(19A)-N(2A)-C(13A)-N(1A)	2.3(2)
C(19A)-N(2A)-C(13A)-C(12A)	-171.90(15)
C(19A)-C(14A)-C(15A)-C(16A)	-0.8(3)
O(1B)-C(1B)-C(2B)-O(2B)	-28.95(18)
O(1B)-C(1B)-C(2B)-N(2B)	96.57(17)
O(1B)-C(1B)-C(2B)-C(3B)	-141.61(14)
O(1B)-C(1B)-C(5B)-C(4B)	134.41(16)
O(1B)-C(1B)-C(5B)-C(6B)	-44.2(2)
O(1B)-C(1B)-C(7B)-C(8B)	167.10(13)

O(1B)-C(1B)-C(7B)-C(11B)	46.72(17)	C(7B)-C(1B)-C(2B)-C(3B)	99.18(15)
O(1B)-C(1B)-C(7B)-C(12B)	-71.28(15)	C(7B)-C(1B)-C(5B)-C(4B)	-105.33(17)
O(2B)-C(2B)-C(3B)-O(3B)	86.4(2)	C(7B)-C(1B)-C(5B)-C(6B)	76.0(2)
O(2B)-C(2B)-C(3B)-C(4B)	-92.58(15)	C(7B)-C(8B)-C(9B)-O(4B)	57.69(19)
O(3B)-C(3B)-C(4B)-C(5B)	166.73(19)	C(7B)-C(12B)-C(13B)-N(1B)	-151.23(17)
O(4B)-C(10B)-C(11B)-C(7B)	-56.4(2)	C(7B)-C(12B)-C(13B)-N(2B)	35.1(2)
N(1B)-C(14B)-C(15B)-C(16B)	-177.50(19)	C(8B)-C(7B)-C(11B)-C(10B)	50.21(19)
N(1B)-C(14B)-C(19B)-N(2B)	-0.3(2)	C(8B)-C(7B)-C(12B)-C(13B)	64.92(19)
N(1B)-C(14B)-C(19B)-C(18B)	177.47(16)	C(9B)-O(4B)-C(10B)-C(11B)	60.72(19)
N(2B)-C(2B)-C(3B)-O(3B)	-33.6(2)	C(10B)-O(4B)-C(9B)-C(8B)	-61.50(19)
N(2B)-C(2B)-C(3B)-C(4B)	147.38(14)	C(11B)-C(7B)-C(8B)-C(9B)	-50.73(18)
C(1B)-C(2B)-C(3B)-O(3B)	-157.33(17)	C(11B)-C(7B)-C(12B)-C(13B)	-177.25(15)
C(1B)-C(2B)-C(3B)-C(4B)	23.68(17)	C(12B)-C(7B)-C(8B)-C(9B)	67.16(18)
C(1B)-C(7B)-C(8B)-C(9B)	-173.26(13)	C(12B)-C(7B)-C(11B)-C(10B)	-69.63(19)
C(1B)-C(7B)-C(11B)-C(10B)	172.64(14)	C(13B)-N(1B)-C(14B)-C(15B)	177.35(19)
C(1B)-C(7B)-C(12B)-C(13B)	-56.95(19)	C(13B)-N(1B)-C(14B)-C(19B)	-0.9(2)
C(2B)-N(2B)-C(13B)-N(1B)	-178.07(16)	C(13B)-N(2B)-C(2B)-O(2B)	123.30(17)
C(2B)-N(2B)-C(13B)-C(12B)	-3.5(3)	C(13B)-N(2B)-C(2B)-C(1B)	-2.5(2)
C(2B)-N(2B)-C(19B)-C(14B)	177.27(16)	C(13B)-N(2B)-C(2B)-C(3B)	-119.22(17)
C(2B)-N(2B)-C(19B)-C(18B)	-0.1(3)	C(13B)-N(2B)-C(19B)-C(14B)	1.37(18)
C(2B)-C(1B)-C(5B)-C(4B)	16.76(19)	C(13B)-N(2B)-C(19B)-C(18B)	-176.04(19)
C(2B)-C(1B)-C(5B)-C(6B)	-161.90(16)	C(14B)-N(1B)-C(13B)-N(2B)	1.9(2)
C(2B)-C(1B)-C(7B)-C(8B)	-71.03(17)	C(14B)-N(1B)-C(13B)-C(12B)	-172.13(17)
C(2B)-C(1B)-C(7B)-C(11B)	168.59(13)	C(14B)-C(15B)-C(16B)-C(17B)	0.3(3)
C(2B)-C(1B)-C(7B)-C(12B)	50.59(18)	C(15B)-C(14B)-C(19B)-N(2B)	-178.76(16)
C(2B)-C(3B)-C(4B)-C(5B)	-14.3(2)	C(15B)-C(14B)-C(19B)-C(18B)	-1.0(3)
C(3B)-C(4B)-C(5B)-C(1B)	-2.0(2)	C(15B)-C(16B)-C(17B)-C(18B)	-0.8(3)
C(3B)-C(4B)-C(5B)-C(6B)	176.59(17)	C(16B)-C(17B)-C(18B)-C(19B)	0.5(3)
C(5B)-C(1B)-C(2B)-O(2B)	89.34(15)	C(17B)-C(18B)-C(19B)-N(2B)	177.47(18)
C(5B)-C(1B)-C(2B)-N(2B)	-145.14(14)	C(17B)-C(18B)-C(19B)-C(14B)	0.4(3)
C(5B)-C(1B)-C(2B)-C(3B)	-23.32(16)	C(19B)-N(2B)-C(2B)-O(2B)	-51.9(2)
C(5B)-C(1B)-C(7B)-C(8B)	43.78(19)	C(19B)-N(2B)-C(2B)-C(1B)	-177.71(15)
C(5B)-C(1B)-C(7B)-C(11B)	-76.60(18)	C(19B)-N(2B)-C(2B)-C(3B)	65.6(2)
C(5B)-C(1B)-C(7B)-C(12B)	165.40(14)	C(19B)-N(2B)-C(13B)-N(1B)	-2.1(2)
C(7B)-C(1B)-C(2B)-O(2B)	-148.16(13)	C(19B)-N(2B)-C(13B)-C(12B)	172.41(15)
C(7B)-C(1B)-C(2B)-N(2B)	-22.6(2)	C(19B)-C(14B)-C(15B)-C(16B)	0.6(3)

Table S23. Hydrogen bonds for **4c** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1A)-H(1A)...O(3A)#1	0.84(3)	2.02(3)	2.8592(19)	171(3)
O(2A)-H(2A)...N(1B)	0.91(3)	1.87(3)	2.7677(19)	167(3)
O(1B)-H(1B)...O(3B)#2	0.85(3)	2.00(3)	2.8507(19)	172(2)
O(2B)-H(2B)...N(1A)#3	0.85(3)	1.95(3)	2.7864(19)	169(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y-1/2,-z+1 #2 -x+1,y-1/2,-z #3 x,y-1,z

6.4. Compound **10b**

X-ray diffraction data were collected at 100K on a Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[1] The structure was solved by direct methods using SHELXT[2] and refined on F^2 using SHELXL-2018[3] in the OLEX2 program.[4] Positions of all atoms were found from the electron density-difference map. Atoms were refined with individual anisotropic (non-hydrogen atoms) or isotropic (hydrogen atoms) displacement parameters.

Table S24. Crystal data and structure refinement for **10b**.

Identification code	**10b**	
Empirical formula	C21 H22 N2 O5	
Formula weight	382.40	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 8.16824(5) Å	a= 90°.
	b = 16.10854(12) Å	b= 91.7049(6)°.
	c = 13.62304(8) Å	g = 90°.
Volume	1791.71(2) $Å^3$	
Z	4	

Density (calculated)	1.418 g/cm^3
Absorption coefficient	0.841 mm^{-1}
F(000)	808
Crystal size	0.690 x 0.371 x 0.138 mm^3
Theta range for data collection	4.251 to 79.526°.
Index ranges	-10<=h<=10, -20<=k<=20, -14<=l<=17
Reflections collected	21964
Independent reflections	3879 [R(int) = 0.0305]
Observed reflections	3770
Completeness to theta = 67.684°	100.0 %
Absorption correction	Analytical
Max. and min. transmission	0.921 and 0.724
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3879 / 0 / 342
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0359, wR2 = 0.0922
R indices (all data)	R1 = 0.0368, wR2 = 0.0929
Extinction coefficient	0.0023(3)
Largest diff. peak and hole	0.389 and -0.286 e.Å^{-3}
CCDC	**2233471**

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

	x	y	z	U(eq)
O(1)	6863(1)	5711(1)	8997(1)	20(1)
O(2)	9290(1)	5087(1)	8820(1)	38(1)
O(3)	6559(1)	4058(1)	9956(1)	20(1)
O(4)	4059(1)	3093(1)	8917(1)	16(1)
O(5)	9850(1)	2462(1)	7680(1)	22(1)
N(1)	4197(1)	2928(1)	5486(1)	16(1)
N(2)	4126(1)	3871(1)	6697(1)	14(1)
C(1)	6103(1)	5013(1)	8611(1)	16(1)
C(2)	6066(1)	4208(1)	9128(1)	15(1)
C(3)	5185(1)	3588(1)	8429(1)	13(1)

C(4)	4217(1)	4192(1)	7710(1)	13(1)
C(5)	5170(1)	4996(1)	7795(1)	15(1)
C(6)	8537(1)	5671(1)	9104(1)	19(1)
C(7)	9198(2)	6436(1)	9588(1)	20(1)
C(8)	6443(1)	3023(1)	7882(1)	14(1)
C(9)	7785(1)	3531(1)	7384(1)	15(1)
C(10)	9079(1)	2973(1)	6947(1)	19(1)
C(11)	8676(1)	1937(1)	8128(1)	20(1)
C(12)	7315(1)	2427(1)	8613(1)	17(1)
C(13)	5405(1)	2521(1)	7125(1)	15(1)
C(14)	4569(1)	3090(1)	6412(1)	14(1)
C(15)	3419(1)	3645(1)	5133(1)	15(1)
C(16)	2705(1)	3804(1)	4207(1)	17(1)
C(17)	2001(1)	4579(1)	4051(1)	19(1)
C(18)	2010(1)	5182(1)	4794(1)	19(1)
C(19)	2696(1)	5029(1)	5719(1)	18(1)
C(20)	3380(1)	4246(1)	5878(1)	14(1)
C(21)	2472(1)	4341(1)	8059(1)	16(1)

Table S26. Bond lengths [Å] and angles [°] for **10b**.

O(1)-C(1)	1.3811(13)	C(1)-C(5)	1.3289(16)
O(1)-C(6)	1.3724(14)	C(2)-C(3)	1.5438(14)
O(2)-C(6)	1.1941(16)	C(3)-C(4)	1.5760(14)
O(3)-C(2)	1.2102(14)	C(3)-C(8)	1.5757(14)
O(4)-H(4)	0.89(2)	C(4)-C(5)	1.5137(14)
O(4)-C(3)	1.3999(13)	C(4)-C(21)	1.5352(14)
O(5)-C(10)	1.4263(14)	C(5)-H(5)	0.950(16)
O(5)-C(11)	1.4286(14)	C(6)-C(7)	1.4918(16)
N(1)-C(14)	1.3140(14)	C(7)-H(7A)	0.962(19)
N(1)-C(15)	1.3960(14)	C(7)-H(7B)	0.98(2)
N(2)-C(4)	1.4737(13)	C(7)-H(7C)	0.95(2)
N(2)-C(14)	1.3688(14)	C(8)-C(9)	1.5411(14)
N(2)-C(20)	1.3921(13)	C(8)-C(12)	1.5433(14)
C(1)-C(2)	1.4774(16)	C(8)-C(13)	1.5439(14)

C(9)-H(9A)	0.977(15)
C(9)-H(9B)	0.978(16)
C(9)-C(10)	1.5224(15)
C(10)-H(10A)	1.006(16)
C(10)-H(10B)	1.008(16)
C(11)-H(11A)	0.975(16)
C(11)-H(11B)	1.016(15)
C(11)-C(12)	1.5296(16)
C(12)-H(12A)	0.992(15)
C(12)-H(12B)	0.998(15)
C(13)-H(13A)	1.001(16)
C(13)-H(13B)	0.981(17)
C(13)-C(14)	1.4870(14)
C(15)-C(16)	1.3983(15)
C(15)-C(20)	1.4030(15)
C(16)-H(16)	0.944(16)
C(16)-C(17)	1.3873(16)
C(17)-H(17)	0.953(15)
C(17)-C(18)	1.4033(17)
C(18)-H(18)	0.988(16)
C(18)-C(19)	1.3855(16)
C(19)-H(19)	0.968(16)
C(19)-C(20)	1.3951(15)
C(21)-H(21A)	0.968(15)
C(21)-H(21B)	0.962(16)
C(21)-H(21C)	0.953(16)
C(6)-O(1)-C(1)	115.94(9)
C(3)-O(4)-H(4)	114.4(12)
C(10)-O(5)-C(11)	110.65(8)
C(14)-N(1)-C(15)	104.90(9)
C(14)-N(2)-C(4)	125.56(9)
C(14)-N(2)-C(20)	106.51(9)
C(20)-N(2)-C(4)	127.38(9)
O(1)-C(1)-C(2)	123.29(10)
C(5)-C(1)-O(1)	125.15(10)
C(5)-C(1)-C(2)	111.17(10)
O(3)-C(2)-C(1)	127.52(10)
O(3)-C(2)-C(3)	125.60(10)
C(1)-C(2)-C(3)	106.80(9)
O(4)-C(3)-C(2)	112.08(8)
O(4)-C(3)-C(4)	108.77(8)
O(4)-C(3)-C(8)	110.06(8)
C(2)-C(3)-C(4)	101.55(8)
C(2)-C(3)-C(8)	111.52(8)
C(8)-C(3)-C(4)	112.60(8)
N(2)-C(4)-C(3)	112.07(8)
N(2)-C(4)-C(5)	112.51(9)
N(2)-C(4)-C(21)	108.89(8)
C(5)-C(4)-C(3)	103.48(8)
C(5)-C(4)-C(21)	108.82(9)
C(21)-C(4)-C(3)	110.97(8)
C(1)-C(5)-C(4)	111.28(10)
C(1)-C(5)-H(5)	126.5(9)
C(4)-C(5)-H(5)	121.8(9)
O(1)-C(6)-C(7)	110.76(10)
O(2)-C(6)-O(1)	121.57(11)
O(2)-C(6)-C(7)	127.67(11)
C(6)-C(7)-H(7A)	109.5(11)
C(6)-C(7)-H(7B)	107.9(12)
C(6)-C(7)-H(7C)	109.2(12)
H(7A)-C(7)-H(7B)	108.8(16)
H(7A)-C(7)-H(7C)	111.4(15)
H(7B)-C(7)-H(7C)	109.9(16)
C(9)-C(8)-C(3)	112.59(9)
C(9)-C(8)-C(12)	107.06(8)
C(9)-C(8)-C(13)	111.63(9)
C(12)-C(8)-C(3)	110.38(8)
C(12)-C(8)-C(13)	109.79(9)
C(13)-C(8)-C(3)	105.42(8)
C(8)-C(9)-H(9A)	108.3(9)
C(8)-C(9)-H(9B)	111.3(9)
H(9A)-C(9)-H(9B)	108.7(12)
C(10)-C(9)-C(8)	111.70(9)
C(10)-C(9)-H(9A)	108.4(9)
C(10)-C(9)-H(9B)	108.4(9)
O(5)-C(10)-C(9)	111.35(9)
O(5)-C(10)-H(10A)	108.6(9)
O(5)-C(10)-H(10B)	106.9(9)
C(9)-C(10)-H(10A)	113.3(9)
C(9)-C(10)-H(10B)	109.0(9)

H(10A)-C(10)-H(10B)	107.5(12)	N(1)-C(15)-C(20)	109.91(9)
O(5)-C(11)-H(11A)	105.6(9)	C(16)-C(15)-C(20)	120.58(10)
O(5)-C(11)-H(11B)	109.0(8)	C(15)-C(16)-H(16)	121.0(10)
O(5)-C(11)-C(12)	112.65(9)	C(17)-C(16)-C(15)	117.59(10)
H(11A)-C(11)-H(11B)	109.1(12)	C(17)-C(16)-H(16)	121.4(10)
C(12)-C(11)-H(11A)	109.7(9)	C(16)-C(17)-H(17)	118.9(9)
C(12)-C(11)-H(11B)	110.6(8)	C(16)-C(17)-C(18)	121.25(10)
C(8)-C(12)-H(12A)	109.7(9)	C(18)-C(17)-H(17)	119.9(9)
C(8)-C(12)-H(12B)	110.3(9)	C(17)-C(18)-H(18)	119.8(9)
C(11)-C(12)-C(8)	111.68(9)	C(19)-C(18)-C(17)	121.76(11)
C(11)-C(12)-H(12A)	110.2(9)	C(19)-C(18)-H(18)	118.4(9)
C(11)-C(12)-H(12B)	109.2(9)	C(18)-C(19)-H(19)	121.9(9)
H(12A)-C(12)-H(12B)	105.6(12)	C(18)-C(19)-C(20)	116.86(10)
C(8)-C(13)-H(13A)	107.6(9)	C(20)-C(19)-H(19)	121.2(9)
C(8)-C(13)-H(13B)	113.5(9)	N(2)-C(20)-C(15)	105.19(9)
H(13A)-C(13)-H(13B)	109.9(13)	N(2)-C(20)-C(19)	132.90(10)
C(14)-C(13)-C(8)	110.19(9)	C(19)-C(20)-C(15)	121.91(10)
C(14)-C(13)-H(13A)	108.6(9)	C(4)-C(21)-H(21A)	108.4(8)
C(14)-C(13)-H(13B)	107.0(9)	C(4)-C(21)-H(21B)	109.7(9)
N(1)-C(14)-N(2)	113.47(9)	C(4)-C(21)-H(21C)	109.0(9)
N(1)-C(14)-C(13)	126.42(10)	H(21A)-C(21)-H(21B)	109.5(12)
N(2)-C(14)-C(13)	120.11(9)	H(21A)-C(21)-H(21C)	110.8(13)
N(1)-C(15)-C(16)	129.49(10)	H(21B)-C(21)-H(21C)	109.4(13)

Table S27. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10b**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	15(1)	16(1)	28(1)	-8(1)	-1(1)	-2(1)
O(2)	17(1)	37(1)	60(1)	-26(1)	2(1)	1(1)
O(3)	19(1)	27(1)	14(1)	-2(1)	-2(1)	-1(1)
O(4)	15(1)	20(1)	13(1)	4(1)	-1(1)	-3(1)
O(5)	16(1)	21(1)	28(1)	4(1)	0(1)	3(1)
N(1)	17(1)	15(1)	14(1)	-1(1)	-2(1)	1(1)
N(2)	17(1)	13(1)	11(1)	0(1)	-1(1)	2(1)
C(1)	14(1)	15(1)	19(1)	-5(1)	3(1)	-2(1)
C(2)	11(1)	19(1)	14(1)	-4(1)	2(1)	0(1)
C(3)	13(1)	15(1)	11(1)	1(1)	0(1)	-1(1)
C(4)	15(1)	13(1)	11(1)	-1(1)	0(1)	0(1)
C(5)	16(1)	13(1)	17(1)	-1(1)	3(1)	1(1)
C(6)	16(1)	22(1)	19(1)	-3(1)	2(1)	-2(1)
C(7)	18(1)	20(1)	22(1)	-2(1)	1(1)	-6(1)
C(8)	14(1)	13(1)	13(1)	0(1)	-1(1)	1(1)
C(9)	16(1)	14(1)	15(1)	0(1)	1(1)	0(1)
C(10)	18(1)	18(1)	20(1)	0(1)	2(1)	2(1)
C(11)	18(1)	17(1)	24(1)	3(1)	-2(1)	2(1)
C(12)	17(1)	16(1)	16(1)	3(1)	-3(1)	1(1)
C(13)	17(1)	12(1)	14(1)	0(1)	-2(1)	1(1)
C(14)	14(1)	13(1)	14(1)	-1(1)	-1(1)	0(1)
C(15)	15(1)	16(1)	14(1)	0(1)	1(1)	0(1)
C(16)	18(1)	20(1)	13(1)	-1(1)	-1(1)	-1(1)
C(17)	18(1)	24(1)	14(1)	4(1)	-2(1)	1(1)
C(18)	20(1)	18(1)	19(1)	4(1)	1(1)	3(1)
C(19)	21(1)	15(1)	16(1)	0(1)	1(1)	3(1)
C(20)	15(1)	16(1)	12(1)	1(1)	1(1)	0(1)
C(21)	15(1)	19(1)	15(1)	0(1)	1(1)	1(1)

Table S28. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **10b**.

	x	y	z	U(eq)
H(4)	4420(20)	2906(12)	9498(14)	39(5)
H(5)	4996(19)	5439(10)	7345(11)	23(4)
H(7A)	10370(20)	6400(11)	9649(13)	35(4)
H(7B)	8910(20)	6911(13)	9167(15)	45(5)
H(7C)	8720(20)	6499(12)	10210(15)	44(5)
H(9A)	8318(18)	3886(9)	7880(11)	18(3)
H(9B)	7321(19)	3883(10)	6861(11)	21(4)
H(10A)	8635(19)	2607(10)	6404(11)	21(4)
H(10B)	9962(19)	3330(10)	6665(11)	23(4)
H(11A)	9290(19)	1619(10)	8624(11)	23(4)
H(11B)	8198(18)	1542(9)	7614(11)	19(3)
H(12A)	6505(18)	2042(9)	8893(11)	19(3)
H(12B)	7790(18)	2743(10)	9184(11)	20(3)
H(13A)	4552(19)	2214(10)	7493(11)	22(4)
H(13B)	6050(20)	2130(10)	6742(12)	25(4)
H(16)	2714(19)	3400(10)	3705(12)	23(4)
H(17)	1519(18)	4702(10)	3422(11)	20(4)
H(18)	1515(19)	5732(10)	4663(11)	24(4)
H(19)	2682(19)	5440(10)	6237(12)	23(4)
H(21A)	2541(17)	4557(9)	8722(11)	15(3)
H(21B)	1924(18)	4738(10)	7636(11)	20(3)
H(21C)	1885(19)	3829(10)	8038(11)	22(4)

Table S29. Torsion angles [°] for **10b**.

O(1)-C(1)-C(2)-O(3)	5.87(17)	C(4)-C(3)-C(8)-C(12)	-178.25(8)
O(1)-C(1)-C(2)-C(3)	-177.09(9)	C(4)-C(3)-C(8)-C(13)	-59.75(11)
O(1)-C(1)-C(5)-C(4)	-166.65(9)	C(5)-C(1)-C(2)-O(3)	-167.27(11)
O(3)-C(2)-C(3)-O(4)	40.84(14)	C(5)-C(1)-C(2)-C(3)	9.76(12)
O(3)-C(2)-C(3)-C(4)	156.78(10)	C(6)-O(1)-C(1)-C(2)	66.65(14)
O(3)-C(2)-C(3)-C(8)	-83.07(13)	C(6)-O(1)-C(1)-C(5)	-121.18(12)
O(4)-C(3)-C(4)-N(2)	-97.13(10)	C(8)-C(3)-C(4)-N(2)	25.14(12)
O(4)-C(3)-C(4)-C(5)	141.40(8)	C(8)-C(3)-C(4)-C(5)	-96.33(10)
O(4)-C(3)-C(4)-C(21)	24.85(11)	C(8)-C(3)-C(4)-C(21)	147.12(9)
O(4)-C(3)-C(8)-C(9)	-176.28(8)	C(8)-C(9)-C(10)-O(5)	-59.15(12)
O(4)-C(3)-C(8)-C(12)	-56.71(11)	C(8)-C(13)-C(14)-N(1)	148.79(11)
O(4)-C(3)-C(8)-C(13)	61.79(10)	C(8)-C(13)-C(14)-N(2)	-30.40(13)
O(5)-C(11)-C(12)-C(8)	55.68(12)	C(9)-C(8)-C(12)-C(11)	-50.89(12)
N(1)-C(15)-C(16)-C(17)	179.75(11)	C(9)-C(8)-C(13)-C(14)	-61.05(11)
N(1)-C(15)-C(20)-N(2)	-1.07(12)	C(10)-O(5)-C(11)-C(12)	-59.18(12)
N(1)-C(15)-C(20)-C(19)	178.87(10)	C(11)-O(5)-C(10)-C(9)	60.54(12)
N(2)-C(4)-C(5)-C(1)	-140.43(9)	C(12)-C(8)-C(9)-C(10)	52.90(11)
C(1)-O(1)-C(6)-O(2)	4.63(17)	C(12)-C(8)-C(13)-C(14)	-179.61(9)
C(1)-O(1)-C(6)-C(7)	-176.14(10)	C(13)-C(8)-C(9)-C(10)	-67.27(11)
C(1)-C(2)-C(3)-O(4)	-136.26(9)	C(13)-C(8)-C(12)-C(11)	70.46(11)
C(1)-C(2)-C(3)-C(4)	-20.33(10)	C(14)-N(1)-C(15)-C(16)	-176.95(11)
C(1)-C(2)-C(3)-C(8)	99.83(10)	C(14)-N(1)-C(15)-C(20)	1.48(12)
C(2)-C(1)-C(5)-C(4)	6.34(13)	C(14)-N(2)-C(4)-C(3)	10.27(14)
C(2)-C(3)-C(4)-N(2)	144.53(8)	C(14)-N(2)-C(4)-C(5)	126.40(11)
C(2)-C(3)-C(4)-C(5)	23.06(10)	C(14)-N(2)-C(4)-C(21)	-112.88(11)
C(2)-C(3)-C(4)-C(21)	-93.50(9)	C(14)-N(2)-C(20)-C(15)	0.26(11)
C(2)-C(3)-C(8)-C(9)	-51.23(11)	C(14)-N(2)-C(20)-C(19)	-179.68(12)
C(2)-C(3)-C(8)-C(12)	68.34(11)	C(15)-N(1)-C(14)-N(2)	-1.35(12)
C(2)-C(3)-C(8)-C(13)	-173.17(8)	C(15)-N(1)-C(14)-C(13)	179.42(10)
C(3)-C(4)-C(5)-C(1)	-19.25(11)	C(15)-C(16)-C(17)-C(18)	0.26(17)
C(3)-C(8)-C(9)-C(10)	174.38(9)	C(16)-C(15)-C(20)-N(2)	177.51(10)
C(3)-C(8)-C(12)-C(11)	-173.76(9)	C(16)-C(15)-C(20)-C(19)	-2.54(16)
C(3)-C(8)-C(13)-C(14)	61.50(11)	C(16)-C(17)-C(18)-C(19)	-1.04(18)
C(4)-N(2)-C(14)-N(1)	172.71(9)	C(17)-C(18)-C(19)-C(20)	0.04(17)
C(4)-N(2)-C(14)-C(13)	-8.00(16)	C(18)-C(19)-C(20)-N(2)	-178.34(11)
C(4)-N(2)-C(20)-C(15)	-171.55(10)	C(18)-C(19)-C(20)-C(15)	1.72(16)
C(4)-N(2)-C(20)-C(19)	8.51(19)	C(20)-N(2)-C(4)-C(3)	-179.40(9)
C(4)-C(3)-C(8)-C(9)	62.18(11)	C(20)-N(2)-C(4)-C(5)	-63.27(13)

C(20)-N(2)-C(4)-C(21)	57.45(13)	C(20)-C(15)-C(16)-C(17)	1.47(16)
C(20)-N(2)-C(14)-N(1)	0.71(12)	C(21)-C(4)-C(5)-C(1)	98.81(10)
C(20)-N(2)-C(14)-C(13)	179.99(9)		

Table S30. Hydrogen bonds for **10b** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4)...N(1)#1	0.89(2)	1.91(2)	2.6978(12)	146.0(17)

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z+1/2

6.5. Compound **11a**

X-ray diffraction data were collected at 100K on a Rigaku Synergy S diffractometer equipped with a HyPix600HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[1] The structure was solved by direct methods using SHELXT[2] and refined on F^2 using SHELXL-2018[3] in the OLEX2 program.[4] Positions of all atoms were found from the electron density-difference map. Atoms were refined with individual anisotropic (non-hydrogen atoms) or isotropic (hydrogen atoms) displacement parameters.

Table S31. Crystal data and structure refinement for **11a**.

Identification code	**11a**	
Empirical formula	C28 H34 N4 O3	
Formula weight	474.59	
Temperature	100.0(1) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.48626(8) Å	α= 90°.
	b = 24.4487(2) Å	β= 102.1288(8)°.

	c = 12.18602(9) Å γ = 90°.
Volume	2471.89(4) $Å^3$
Z	4
Density (calculated)	1.275 g/cm^3
Absorption coefficient	0.670 mm^{-1}
F(000)	1016
Crystal size	0.46 x 0.06 x 0.05 mm^3
Theta range for data collection	3.616 to 79.523°.
Index ranges	-10<=h<=10, -31<=k<=30, -13<=l<=15
Reflections collected	31875
Independent reflections	5343 [R(int) = 0.0324]
Observed reflections	5026
Completeness to theta = 67.684°	99.9 %
Absorption correction	Analytical
Max. and min. transmission	0.969 and 0.844
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5343 / 0 / 453
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0399, wR2 = 0.1035
R indices (all data)	R1 = 0.0416, wR2 = 0.1048
Extinction coefficient	0.00118(19)
Largest diff. peak and hole	0.340 and -0.242 $e.Å^{-3}$
CCDC	**2233463**

Table S32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **11a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4111(1)	3947(1)	5508(1)	23(1)
O(2)	5468(1)	2935(1)	4921(1)	24(1)
N(1)	5656(1)	2118(1)	6627(1)	20(1)
N(2)	5737(1)	1775(1)	7487(1)	21(1)
N(3)	2337(1)	3617(1)	7515(1)	19(1)
N(4)	-175(1)	3951(1)	7272(1)	22(1)
C(1)	3695(1)	3440(1)	5909(1)	19(1)
C(2)	4838(1)	2974(1)	5732(1)	20(1)

C(3)	5013(1)	2595(1)	6687(1)	20(1)
C(4)	4245(1)	2827(1)	7591(1)	21(1)
C(5)	3844(1)	3429(1)	7223(1)	19(1)
C(6)	985(1)	3791(1)	6777(1)	20(1)
C(7)	895(1)	3789(1)	5543(1)	22(1)
C(8)	1928(1)	3322(1)	5223(1)	20(1)
C(9)	6325(1)	1241(1)	7415(1)	21(1)
C(10)	6472(2)	904(1)	8353(1)	27(1)
C(11)	7044(2)	376(1)	8310(1)	34(1)
C(12)	7452(2)	176(1)	7338(1)	33(1)
C(13)	7294(2)	515(1)	6407(1)	28(1)
C(14)	6745(2)	1047(1)	6437(1)	24(1)
C(15)	5226(1)	3799(1)	7796(1)	24(1)
C(16)	2019(1)	3675(1)	8587(1)	20(1)
C(17)	2910(1)	3557(1)	9659(1)	22(1)
C(18)	2189(2)	3676(1)	10553(1)	24(1)
C(19)	637(2)	3897(1)	10392(1)	26(1)
C(20)	-261(2)	4001(1)	9324(1)	24(1)
C(21)	451(1)	3888(1)	8416(1)	21(1)
C(22)	1259(1)	2764(1)	5493(1)	22(1)
C(23)	-379(2)	2624(1)	4738(1)	27(1)
C(24)	-292(2)	2645(1)	3500(1)	29(1)
C(25)	301(2)	3203(1)	3204(1)	27(1)
C(26)	1932(1)	3346(1)	3955(1)	23(1)
O(3)	7049(1)	4409(1)	6083(1)	25(1)
C(27)	7207(2)	4986(1)	6242(1)	33(1)
C(28)	7408(2)	5159(1)	7453(1)	37(1)

Table S33. Bond lengths [Å] and angles [°] for **11a**.

O(1)-H(1)	0.92(2)	N(3)-C(6)	1.3682(14)
O(1)-C(1)	1.4047(13)	N(3)-C(16)	1.3948(14)
O(2)-C(2)	1.2218(14)	N(4)-C(6)	1.3172(15)
N(1)-N(2)	1.3340(13)	N(4)-C(21)	1.3924(14)
N(1)-C(3)	1.2955(15)	C(1)-C(2)	1.5410(15)
N(2)-H(2)	0.912(17)	C(1)-C(5)	1.5797(15)
N(2)-C(9)	1.4053(15)	C(1)-C(8)	1.5821(15)
N(3)-C(5)	1.4726(14)	C(2)-C(3)	1.4698(15)

C(3)-C(4)	1.5041(15)	C(23)-C(24)	1.5266(18)
C(4)-H(4A)	1.008(16)	C(24)-H(24A)	1.003(18)
C(4)-H(4B)	0.991(16)	C(24)-H(24B)	1.017(16)
C(4)-C(5)	1.5541(15)	C(24)-C(25)	1.5223(19)
C(5)-C(15)	1.5288(16)	C(25)-H(25A)	1.005(18)
C(6)-C(7)	1.4890(15)	C(25)-H(25B)	0.984(17)
C(7)-H(7A)	0.990(16)	C(25)-C(26)	1.5313(17)
C(7)-H(7B)	0.997(16)	C(26)-H(26A)	1.009(16)
C(7)-C(8)	1.5386(15)	C(26)-H(26B)	0.995(16)
C(8)-C(22)	1.5413(16)	O(3)-H(3)	0.92(2)
C(8)-C(26)	1.5465(15)	O(3)-C(27)	1.4251(16)
C(9)-C(10)	1.3940(16)	C(27)-H(27A)	0.995(19)
C(9)-C(14)	1.3963(16)	C(27)-H(27B)	1.01(2)
C(10)-H(10)	0.956(17)	C(27)-C(28)	1.5102(19)
C(10)-C(11)	1.3846(19)	C(28)-H(28A)	1.01(2)
C(11)-H(11)	0.986(19)	C(28)-H(28B)	1.04(2)
C(11)-C(12)	1.3896(19)	C(28)-H(28C)	1.01(2)
C(12)-H(12)	0.971(17)	C(1)-O(1)-H(1)	112.2(12)
C(12)-C(13)	1.3874(19)	C(3)-N(1)-N(2)	118.41(10)
C(13)-H(13)	0.979(17)	N(1)-N(2)-H(2)	122.0(10)
C(13)-C(14)	1.3861(18)	N(1)-N(2)-C(9)	119.73(9)
C(14)-H(14)	0.979(17)	C(9)-N(2)-H(2)	118.2(10)
C(15)-H(15A)	1.001(18)	C(6)-N(3)-C(5)	126.05(9)
C(15)-H(15B)	0.969(17)	C(6)-N(3)-C(16)	106.53(9)
C(15)-H(15C)	0.994(16)	C(16)-N(3)-C(5)	127.38(9)
C(16)-C(17)	1.3958(16)	C(6)-N(4)-C(21)	105.17(9)
C(16)-C(21)	1.4029(16)	O(1)-C(1)-C(2)	113.14(9)
C(17)-H(17)	0.967(15)	O(1)-C(1)-C(5)	113.26(9)
C(17)-C(18)	1.3878(16)	O(1)-C(1)-C(8)	104.87(9)
C(18)-H(18)	0.999(16)	C(2)-C(1)-C(5)	102.14(8)
C(18)-C(19)	1.3985(18)	C(2)-C(1)-C(8)	110.26(9)
C(19)-H(19)	0.983(16)	C(5)-C(1)-C(8)	113.42(9)
C(19)-C(20)	1.3876(17)	O(2)-C(2)-C(1)	124.41(10)
C(20)-H(20)	1.001(16)	O(2)-C(2)-C(3)	127.13(11)
C(20)-C(21)	1.3949(16)	C(3)-C(2)-C(1)	108.45(9)
C(22)-H(22A)	1.004(15)	N(1)-C(3)-C(2)	119.69(10)
C(22)-H(22B)	0.991(16)	N(1)-C(3)-C(4)	129.28(10)
C(22)-C(23)	1.5357(16)	C(2)-C(3)-C(4)	110.83(10)
C(23)-H(23A)	0.995(17)	C(3)-C(4)-H(4A)	112.6(9)
C(23)-H(23B)	0.981(17)	C(3)-C(4)-H(4B)	109.7(9)

C(3)-C(4)-C(5)	104.32(9)	C(9)-C(14)-H(14)	119.7(10)
H(4A)-C(4)-H(4B)	108.1(13)	C(13)-C(14)-C(9)	119.31(11)
C(5)-C(4)-H(4A)	110.6(9)	C(13)-C(14)-H(14)	121.0(10)
C(5)-C(4)-H(4B)	111.6(9)	C(5)-C(15)-H(15A)	110.1(10)
N(3)-C(5)-C(1)	110.58(9)	C(5)-C(15)-H(15B)	111.4(10)
N(3)-C(5)-C(4)	112.00(9)	C(5)-C(15)-H(15C)	109.6(9)
N(3)-C(5)-C(15)	109.03(9)	H(15A)-C(15)-H(15B)	109.2(13)
C(4)-C(5)-C(1)	105.98(9)	H(15A)-C(15)-H(15C)	108.4(13)
C(15)-C(5)-C(1)	110.07(9)	H(15B)-C(15)-H(15C)	108.1(13)
C(15)-C(5)-C(4)	109.14(9)	N(3)-C(16)-C(17)	133.01(11)
N(3)-C(6)-C(7)	121.45(10)	N(3)-C(16)-C(21)	105.21(10)
N(4)-C(6)-N(3)	113.21(10)	C(17)-C(16)-C(21)	121.77(10)
N(4)-C(6)-C(7)	125.34(10)	C(16)-C(17)-H(17)	123.3(9)
C(6)-C(7)-H(7A)	107.9(9)	C(18)-C(17)-C(16)	116.70(11)
C(6)-C(7)-H(7B)	107.7(9)	C(18)-C(17)-H(17)	119.9(9)
C(6)-C(7)-C(8)	110.31(9)	C(17)-C(18)-H(18)	117.6(9)
H(7A)-C(7)-H(7B)	107.6(12)	C(17)-C(18)-C(19)	121.94(11)
C(8)-C(7)-H(7A)	110.2(9)	C(19)-C(18)-H(18)	120.5(9)
C(8)-C(7)-H(7B)	112.9(9)	C(18)-C(19)-H(19)	119.1(9)
C(7)-C(8)-C(1)	105.00(9)	C(20)-C(19)-C(18)	121.18(11)
C(7)-C(8)-C(22)	110.35(9)	C(20)-C(19)-H(19)	119.7(9)
C(7)-C(8)-C(26)	110.27(9)	C(19)-C(20)-H(20)	121.6(9)
C(22)-C(8)-C(1)	113.53(9)	C(19)-C(20)-C(21)	117.62(11)
C(22)-C(8)-C(26)	108.95(9)	C(21)-C(20)-H(20)	120.8(9)
C(26)-C(8)-C(1)	108.67(9)	N(4)-C(21)-C(16)	109.86(10)
C(10)-C(9)-N(2)	118.01(10)	N(4)-C(21)-C(20)	129.39(11)
C(10)-C(9)-C(14)	120.21(11)	C(20)-C(21)-C(16)	120.75(11)
C(14)-C(9)-N(2)	121.77(10)	C(8)-C(22)-H(22A)	111.7(8)
C(9)-C(10)-H(10)	119.0(10)	C(8)-C(22)-H(22B)	109.0(9)
C(11)-C(10)-C(9)	119.55(12)	H(22A)-C(22)-H(22B)	107.1(12)
C(11)-C(10)-H(10)	121.5(10)	C(23)-C(22)-C(8)	113.39(10)
C(10)-C(11)-H(11)	119.2(11)	C(23)-C(22)-H(22A)	107.5(9)
C(10)-C(11)-C(12)	120.73(12)	C(23)-C(22)-H(22B)	108.0(9)
C(12)-C(11)-H(11)	120.1(11)	C(22)-C(23)-H(23A)	111.2(10)
C(11)-C(12)-H(12)	119.8(10)	C(22)-C(23)-H(23B)	109.0(10)
C(13)-C(12)-C(11)	119.30(12)	H(23A)-C(23)-H(23B)	108.6(14)
C(13)-C(12)-H(12)	120.9(10)	C(24)-C(23)-C(22)	111.06(10)
C(12)-C(13)-H(13)	120.2(10)	C(24)-C(23)-H(23A)	107.9(10)
C(14)-C(13)-C(12)	120.89(12)	C(24)-C(23)-H(23B)	109.0(10)
C(14)-C(13)-H(13)	118.9(10)	C(23)-C(24)-H(24A)	110.1(10)

C(23)-C(24)-H(24B)	109.4(9)	C(25)-C(26)-H(26B)	110.9(9)
H(24A)-C(24)-H(24B)	106.6(13)	H(26A)-C(26)-H(26B)	107.4(13)
C(25)-C(24)-C(23)	110.56(10)	C(27)-O(3)-H(3)	107.4(13)
C(25)-C(24)-H(24A)	111.1(10)	O(3)-C(27)-H(27A)	104.8(11)
C(25)-C(24)-H(24B)	109.0(9)	O(3)-C(27)-H(27B)	110.3(11)
C(24)-C(25)-H(25A)	110.0(10)	O(3)-C(27)-C(28)	113.45(11)
C(24)-C(25)-H(25B)	110.0(10)	H(27A)-C(27)-H(27B)	108.5(15)
C(24)-C(25)-C(26)	111.48(10)	C(28)-C(27)-H(27A)	110.9(10)
H(25A)-C(25)-H(25B)	104.5(13)	C(28)-C(27)-H(27B)	108.7(12)
C(26)-C(25)-H(25A)	111.2(10)	C(27)-C(28)-H(28A)	108.0(11)
C(26)-C(25)-H(25B)	109.5(10)	C(27)-C(28)-H(28B)	110.6(12)
C(8)-C(26)-H(26A)	108.1(9)	C(27)-C(28)-H(28C)	109.5(11)
C(8)-C(26)-H(26B)	108.0(9)	H(28A)-C(28)-H(28B)	108.4(16)
C(25)-C(26)-C(8)	113.38(10)	H(28A)-C(28)-H(28C)	107.8(16)
C(25)-C(26)-H(26A)	108.8(9)	H(28B)-C(28)-H(28C)	112.5(16)

Table S34. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C6BNIMNH2NH2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	24(1)	22(1)	22(1)	4(1)	4(1)	-1(1)
O(2)	24(1)	31(1)	19(1)	2(1)	7(1)	3(1)
N(1)	19(1)	22(1)	18(1)	1(1)	2(1)	0(1)
N(2)	24(1)	22(1)	17(1)	1(1)	5(1)	2(1)
N(3)	20(1)	21(1)	17(1)	0(1)	4(1)	3(1)
N(4)	22(1)	24(1)	19(1)	-1(1)	4(1)	3(1)
C(1)	21(1)	20(1)	17(1)	1(1)	4(1)	0(1)
C(2)	18(1)	24(1)	18(1)	0(1)	2(1)	-1(1)
C(3)	19(1)	23(1)	18(1)	1(1)	3(1)	2(1)
C(4)	22(1)	22(1)	18(1)	2(1)	5(1)	3(1)
C(5)	18(1)	22(1)	18(1)	1(1)	4(1)	2(1)
C(6)	22(1)	20(1)	20(1)	0(1)	3(1)	1(1)
C(7)	22(1)	23(1)	18(1)	0(1)	3(1)	4(1)
C(8)	20(1)	22(1)	17(1)	0(1)	3(1)	2(1)
C(9)	18(1)	22(1)	22(1)	1(1)	3(1)	0(1)
C(10)	34(1)	26(1)	24(1)	3(1)	11(1)	2(1)

C(11)	46(1)	28(1)	33(1)	10(1)	16(1)	6(1)
C(12)	40(1)	21(1)	40(1)	4(1)	16(1)	6(1)
C(13)	32(1)	27(1)	30(1)	-2(1)	13(1)	1(1)
C(14)	26(1)	25(1)	22(1)	2(1)	6(1)	2(1)
C(15)	23(1)	28(1)	20(1)	0(1)	4(1)	-2(1)
C(16)	22(1)	20(1)	19(1)	-1(1)	6(1)	0(1)
C(17)	22(1)	23(1)	20(1)	1(1)	4(1)	1(1)
C(18)	28(1)	26(1)	18(1)	0(1)	4(1)	1(1)
C(19)	28(1)	30(1)	20(1)	-1(1)	8(1)	2(1)
C(20)	23(1)	28(1)	23(1)	-1(1)	7(1)	3(1)
C(21)	23(1)	21(1)	19(1)	-1(1)	4(1)	1(1)
C(22)	22(1)	23(1)	21(1)	-1(1)	3(1)	0(1)
C(23)	23(1)	29(1)	29(1)	-1(1)	2(1)	-1(1)
C(24)	26(1)	33(1)	26(1)	-6(1)	-2(1)	2(1)
C(25)	27(1)	34(1)	18(1)	-1(1)	1(1)	6(1)
C(26)	24(1)	28(1)	17(1)	1(1)	4(1)	4(1)
O(3)	23(1)	24(1)	25(1)	1(1)	2(1)	0(1)
C(27)	45(1)	24(1)	28(1)	4(1)	4(1)	0(1)
C(28)	53(1)	26(1)	30(1)	-2(1)	2(1)	0(1)

Table S35. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **11a**.

	x	y	z	U(eq)
H(1)	5170(20)	4037(8)	5791(16)	47(5)
H(2)	5484(19)	1881(7)	8146(14)	30(4)
H(4A)	4984(19)	2815(6)	8356(14)	29(4)
H(4B)	3259(19)	2617(6)	7627(13)	26(4)
H(7A)	1295(18)	4147(7)	5335(13)	26(4)
H(7B)	-264(19)	3760(6)	5164(13)	25(4)
H(10)	6190(20)	1045(7)	9016(15)	35(4)
H(11)	7140(20)	139(8)	8976(16)	43(5)
H(12)	7850(20)	-195(7)	7320(14)	35(4)
H(13)	7580(20)	380(7)	5717(14)	33(4)
H(14)	6650(20)	1289(7)	5787(14)	31(4)
H(15A)	6260(20)	3675(7)	7609(14)	34(4)
H(15B)	5031(19)	4177(7)	7567(13)	28(4)

H(15C)	5337(19)	3780(7)	8623(14)	29(4)
H(17)	3969(18)	3391(6)	9797(12)	21(3)
H(18)	2817(19)	3597(6)	11326(14)	28(4)
H(19)	178(19)	3977(6)	11051(13)	28(4)
H(20)	-1380(20)	4150(7)	9202(13)	30(4)
H(22A)	1129(18)	2744(6)	6292(13)	22(3)
H(22B)	2034(18)	2473(6)	5396(13)	25(4)
H(23A)	-1230(20)	2885(7)	4857(14)	33(4)
H(23B)	-690(20)	2254(7)	4918(14)	32(4)
H(24A)	-1370(20)	2558(7)	3017(15)	38(4)
H(24B)	482(19)	2353(7)	3340(13)	27(4)
H(25A)	-530(20)	3490(7)	3253(14)	35(4)
H(25B)	390(20)	3208(7)	2413(14)	33(4)
H(26A)	2767(19)	3079(7)	3801(13)	28(4)
H(26B)	2284(19)	3719(7)	3783(13)	27(4)
H(3)	7980(30)	4250(8)	6479(17)	52(5)
H(27A)	6200(20)	5141(7)	5776(15)	42(5)
H(27B)	8150(20)	5126(8)	5945(17)	51(5)
H(28A)	7480(20)	5569(8)	7482(16)	47(5)
H(28B)	6410(30)	5037(9)	7773(18)	59(6)
H(28C)	8450(20)	5009(8)	7902(17)	50(5)

Table S36. Torsion angles [°] for **11a**.

O(1)-C(1)-C(2)-O(2)	-35.27(15)	N(2)-N(1)-C(3)-C(4)	-2.93(18)
O(1)-C(1)-C(2)-C(3)	145.13(9)	N(2)-C(9)-C(10)-C(11)	179.88(12)
O(1)-C(1)-C(5)-N(3)	87.56(11)	N(2)-C(9)-C(14)-C(13)	-178.98(11)
O(1)-C(1)-C(5)-C(4)	-150.86(9)	N(3)-C(6)-C(7)-C(8)	30.70(15)
O(1)-C(1)-C(5)-C(15)	-32.96(13)	N(3)-C(16)-C(17)-C(18)	179.51(12)
O(1)-C(1)-C(8)-C(7)	-62.25(10)	N(3)-C(16)-C(21)-N(4)	0.77(13)
O(1)-C(1)-C(8)-C(22)	177.13(9)	N(3)-C(16)-C(21)-C(20)	-179.59(11)
O(1)-C(1)-C(8)-C(26)	55.73(11)	N(4)-C(6)-C(7)-C(8)	-149.00(11)
O(2)-C(2)-C(3)-N(1)	-12.99(18)	C(1)-C(2)-C(3)-N(1)	166.59(10)
O(2)-C(2)-C(3)-C(4)	171.71(11)	C(1)-C(2)-C(3)-C(4)	-8.70(12)
N(1)-N(2)-C(9)-C(10)	176.65(11)	C(1)-C(8)-C(22)-C(23)	-173.82(9)
N(1)-N(2)-C(9)-C(14)	-3.71(16)	C(1)-C(8)-C(26)-C(25)	176.40(10)
N(1)-C(3)-C(4)-C(5)	175.31(11)	C(2)-C(1)-C(5)-N(3)	-150.43(9)
N(2)-N(1)-C(3)-C(2)	-177.24(10)	C(2)-C(1)-C(5)-C(4)	-28.85(11)

C(2)-C(1)-C(5)-C(15)	89.04(10)	C(8)-C(1)-C(2)-C(3)	-97.80(10)
C(2)-C(1)-C(8)-C(7)	175.65(9)	C(8)-C(1)-C(5)-N(3)	-31.81(12)
C(2)-C(1)-C(8)-C(22)	55.03(12)	C(8)-C(1)-C(5)-C(4)	89.77(11)
C(2)-C(1)-C(8)-C(26)	-66.37(11)	C(8)-C(1)-C(5)-C(15)	-152.33(9)
C(2)-C(3)-C(4)-C(5)	-9.97(12)	C(8)-C(22)-C(23)-C(24)	55.88(14)
C(3)-N(1)-N(2)-C(9)	175.58(10)	C(9)-C(10)-C(11)-C(12)	-0.8(2)
C(3)-C(4)-C(5)-N(3)	144.91(9)	C(10)-C(9)-C(14)-C(13)	0.65(18)
C(3)-C(4)-C(5)-C(1)	24.25(11)	C(10)-C(11)-C(12)-C(13)	0.5(2)
C(3)-C(4)-C(5)-C(15)	-94.26(10)	C(11)-C(12)-C(13)-C(14)	0.4(2)
C(5)-N(3)-C(6)-N(4)	-178.31(10)	C(12)-C(13)-C(14)-C(9)	-1.0(2)
C(5)-N(3)-C(6)-C(7)	1.95(17)	C(14)-C(9)-C(10)-C(11)	0.24(19)
C(5)-N(3)-C(16)-C(17)	-3.8(2)	C(16)-N(3)-C(5)-C(1)	-178.54(10)
C(5)-N(3)-C(16)-C(21)	177.58(10)	C(16)-N(3)-C(5)-C(4)	63.51(14)
C(5)-C(1)-C(2)-O(2)	-157.35(11)	C(16)-N(3)-C(5)-C(15)	-57.39(14)
C(5)-C(1)-C(2)-C(3)	23.05(11)	C(16)-N(3)-C(6)-N(4)	-0.51(13)
C(5)-C(1)-C(8)-C(7)	61.82(11)	C(16)-N(3)-C(6)-C(7)	179.75(10)
C(5)-C(1)-C(8)-C(22)	-58.81(12)	C(16)-C(17)-C(18)-C(19)	0.92(18)
C(5)-C(1)-C(8)-C(26)	179.79(9)	C(17)-C(16)-C(21)-N(4)	-178.06(11)
C(6)-N(3)-C(5)-C(1)	-1.19(15)	C(17)-C(16)-C(21)-C(20)	1.58(18)
C(6)-N(3)-C(5)-C(4)	-119.15(12)	C(17)-C(18)-C(19)-C(20)	0.7(2)
C(6)-N(3)-C(5)-C(15)	119.96(12)	C(18)-C(19)-C(20)-C(21)	-1.20(19)
C(6)-N(3)-C(16)-C(17)	178.46(13)	C(19)-C(20)-C(21)-N(4)	179.65(12)
C(6)-N(3)-C(16)-C(21)	-0.18(12)	C(19)-C(20)-C(21)-C(16)	0.09(18)
C(6)-N(4)-C(21)-C(16)	-1.07(13)	C(21)-N(4)-C(6)-N(3)	0.97(13)
C(6)-N(4)-C(21)-C(20)	179.34(12)	C(21)-N(4)-C(6)-C(7)	-179.30(11)
C(6)-C(7)-C(8)-C(1)	-59.04(12)	C(21)-C(16)-C(17)-C(18)	-2.04(17)
C(6)-C(7)-C(8)-C(22)	63.66(12)	C(22)-C(8)-C(26)-C(25)	52.24(13)
C(6)-C(7)-C(8)-C(26)	-175.93(9)	C(22)-C(23)-C(24)-C(25)	-56.16(14)
C(7)-C(8)-C(22)-C(23)	68.62(12)	C(23)-C(24)-C(25)-C(26)	56.08(14)
C(7)-C(8)-C(26)-C(25)	-69.01(13)	C(24)-C(25)-C(26)-C(8)	-55.38(14)
C(8)-C(1)-C(2)-O(2)	81.80(13)	C(26)-C(8)-C(22)-C(23)	-52.58(12)

Table S37. Hydrogen bonds for **11a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(3)	0.92(2)	1.81(2)	2.6920(12)	161.4(18)
N(2)-H(2)...O(2)#1	0.912(17)	2.212(17)	3.1041(12)	166.0(14)
O(3)-H(3)...N(4)#2	0.92(2)	1.81(2)	2.7332(13)	179(2)

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z+1/2 #2 x+1,y,z

6.6. Compound **12b**

X-ray diffraction data were collected at 100K on a Rigaku Synergy S diffractometer equipped with a HyPix600HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[1] The structure was solved by direct methods using SHELXT[2] and refined on F^2 using SHELXL-2018[3] in the OLEX2 program.[4] Positions of all atoms were found from the electron density-difference map. Atoms were refined with individual anisotropic (non-hydrogen atoms) or isotropic (hydrogen atoms) displacement parameters. The position of hydroxy atom H1 was restrained at the distance of 0.85(2)Å from O1, and Uiso(H1)=1.5 Ueq(O1).

Table S38. Crystal data and structure refinement for **12b.**

Identification code	**12b**	
Empirical formula	C25 H24 N4 O2	
Formula weight	412.48	
Temperature	100.0(1) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	I2/a	
Unit cell dimensions	a = 18.1847(2) Å	α= 90°.
	b = 9.88774(11) Å	β= 106.5529(13)°.
	c = 27.3603(4) Å	γ = 90°.
Volume	4715.65(11) $Å^3$	
Z	8	

Density (calculated)	1.162 g/cm^3
Absorption coefficient	0.604 mm^{-1}
F(000)	1744
Crystal size	0.28 x 0.18 x 0.10 mm^3
Theta range for data collection	3.370 to 79.678°.
Index ranges	-23<=h<=17, -12<=k<=12, -34<=l<=34
Reflections collected	32398
Independent reflections	5013 [R(int) = 0.0370]
Observed reflections	4797
Completeness to theta = 67.684°	99.7 %
Absorption correction	Analytical
Max. and min. transmission	0.948 and 0.877
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5013 / 1 / 376
Goodness-of-fit on F^2	1.092
Final R indices [I>2sigma(I)]	R1 = 0.0563, wR2 = 0.1405
R indices (all data)	R1 = 0.0577, wR2 = 0.1413
Extinction coefficient	0.00065(6)
Largest diff. peak and hole	0.498 and -0.213 e.Å^{-3}
CCDC	**2233468**

Table S39. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **12b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4289(1)	8374(1)	6371(1)	37(1)
O(2)	2424(1)	5092(1)	6782(1)	32(1)
N(1)	5041(1)	7003(2)	8099(1)	32(1)
N(2)	5363(1)	6701(2)	7374(1)	29(1)
N(3)	4997(1)	4177(2)	5804(1)	28(1)
N(4)	3826(1)	6193(2)	5593(1)	32(1)
C(1)	4416(1)	6991(2)	6492(1)	28(1)
C(2)	3814(1)	6604(2)	6782(1)	27(1)
C(3)	4035(1)	7440(2)	7277(1)	30(1)
C(4)	4810(1)	7061(2)	7598(1)	29(1)
C(5)	5281(1)	6713(2)	6823(1)	29(1)
C(6)	5501(1)	5306(2)	6649(1)	30(1)

C(7)	4954(1)	5121(2)	6131(1)	26(1)
C(8)	4357(1)	6103(2)	6030(1)	27(1)
C(9)	5806(1)	7814(2)	6715(1)	37(1)
C(10)	5808(1)	6604(2)	8218(1)	31(1)
C(11)	6342(1)	6431(2)	8694(1)	36(1)
C(12)	7075(1)	6020(2)	8707(1)	38(1)
C(13)	7269(1)	5769(2)	8255(1)	36(1)
C(14)	6751(1)	5946(2)	7778(1)	33(1)
C(15)	6019(1)	6386(2)	7769(1)	30(1)
C(16)	4430(1)	4188(2)	5354(1)	30(1)
C(17)	4396(1)	3147(2)	4996(1)	34(1)
C(18)	3818(1)	3124(3)	4548(1)	43(1)
C(19)	3270(1)	4174(3)	4427(1)	48(1)
C(20)	3296(1)	5205(3)	4764(1)	46(1)
C(21)	3856(1)	5219(2)	5240(1)	32(1)
C(22)	3004(1)	6994(2)	6458(1)	30(1)
C(23)	2388(1)	6517(2)	6696(1)	33(1)
C(24)	3152(1)	4704(2)	7114(1)	30(1)
C(25)	3807(1)	5075(2)	6894(1)	27(1)

Table S40. Bond lengths [Å] and angles [°] for **12b**.

O(1)-H(1)	0.884(17)	C(2)-C(3)	1.540(3)
O(1)-C(1)	1.411(2)	C(2)-C(22)	1.537(3)
O(2)-C(23)	1.426(2)	C(2)-C(25)	1.544(2)
O(2)-C(24)	1.428(2)	C(3)-H(3A)	1.01(2)
N(1)-C(4)	1.314(3)	C(3)-H(3B)	0.99(2)
N(1)-C(10)	1.395(3)	C(3)-C(4)	1.482(3)
N(2)-C(4)	1.368(2)	C(5)-C(6)	1.559(3)
N(2)-C(5)	1.472(3)	C(5)-C(9)	1.530(3)
N(2)-C(15)	1.398(3)	C(6)-H(6A)	1.01(3)
N(3)-C(7)	1.311(2)	C(6)-H(6B)	1.00(2)
N(3)-C(16)	1.363(2)	C(6)-C(7)	1.492(3)
N(4)-C(8)	1.308(3)	C(7)-C(8)	1.425(2)
N(4)-C(21)	1.376(3)	C(9)-H(9A)	1.03(3)
C(1)-C(2)	1.571(3)	C(9)-H(9B)	1.04(3)
C(1)-C(5)	1.599(3)	C(9)-H(9C)	1.04(3)
C(1)-C(8)	1.519(3)	C(10)-C(11)	1.395(3)

C(10)-C(15)	1.406(3)
C(11)-H(11)	0.95(3)
C(11)-C(12)	1.385(3)
C(12)-H(12)	1.02(3)
C(12)-C(13)	1.401(3)
C(13)-H(13)	1.01(2)
C(13)-C(14)	1.386(3)
C(14)-H(14)	0.98(3)
C(14)-C(15)	1.395(3)
C(16)-C(17)	1.410(3)
C(16)-C(21)	1.429(3)
C(17)-H(17)	1.03(3)
C(17)-C(18)	1.367(3)
C(18)-H(18)	0.97(3)
C(18)-C(19)	1.412(4)
C(19)-H(19)	1.01(3)
C(19)-C(20)	1.366(4)
C(20)-H(20)	1.00(3)
C(20)-C(21)	1.406(3)
C(22)-H(22A)	0.98(3)
C(22)-H(22B)	0.99(3)
C(22)-C(23)	1.523(3)
C(23)-H(23A)	1.03(2)
C(23)-H(23B)	0.96(2)
C(24)-H(24A)	1.03(2)
C(24)-H(24B)	1.03(2)
C(24)-C(25)	1.523(3)
C(25)-H(25A)	1.00(2)
C(25)-H(25B)	0.99(2)
C(1)-O(1)-H(1)	113.0(19)
C(23)-O(2)-C(24)	111.19(14)
C(4)-N(1)-C(10)	104.96(16)
C(4)-N(2)-C(5)	125.85(16)
C(4)-N(2)-C(15)	106.50(16)
C(15)-N(2)-C(5)	127.59(16)
C(7)-N(3)-C(16)	115.75(16)
C(8)-N(4)-C(21)	115.32(16)
O(1)-C(1)-C(2)	105.32(14)
O(1)-C(1)-C(5)	111.63(15)
O(1)-C(1)-C(8)	113.32(16)
C(2)-C(1)-C(5)	112.86(15)
C(8)-C(1)-C(2)	112.64(14)
C(8)-C(1)-C(5)	101.32(14)
C(3)-C(2)-C(1)	105.56(14)
C(3)-C(2)-C(25)	111.43(16)
C(22)-C(2)-C(1)	109.82(16)
C(22)-C(2)-C(3)	109.88(15)
C(22)-C(2)-C(25)	107.47(14)
C(25)-C(2)-C(1)	112.68(14)
C(2)-C(3)-H(3A)	113.6(13)
C(2)-C(3)-H(3B)	108.9(13)
H(3A)-C(3)-H(3B)	104.1(18)
C(4)-C(3)-C(2)	110.60(15)
C(4)-C(3)-H(3A)	108.4(13)
C(4)-C(3)-H(3B)	111.2(13)
N(1)-C(4)-N(2)	113.57(17)
N(1)-C(4)-C(3)	126.64(18)
N(2)-C(4)-C(3)	119.78(18)
N(2)-C(5)-C(1)	112.11(15)
N(2)-C(5)-C(6)	110.17(16)
N(2)-C(5)-C(9)	108.38(15)
C(6)-C(5)-C(1)	106.12(14)
C(9)-C(5)-C(1)	109.66(16)
C(9)-C(5)-C(6)	110.41(16)
C(5)-C(6)-H(6A)	110.4(14)
C(5)-C(6)-H(6B)	112.1(14)
H(6A)-C(6)-H(6B)	107.5(19)
C(7)-C(6)-C(5)	103.87(15)
C(7)-C(6)-H(6A)	110.4(14)
C(7)-C(6)-H(6B)	112.6(13)
N(3)-C(7)-C(6)	125.64(16)
N(3)-C(7)-C(8)	122.90(17)
C(8)-C(7)-C(6)	111.45(16)
N(4)-C(8)-C(1)	125.50(16)
N(4)-C(8)-C(7)	123.20(17)
C(7)-C(8)-C(1)	111.29(16)
C(5)-C(9)-H(9A)	110.3(15)
C(5)-C(9)-H(9B)	107.1(14)
C(5)-C(9)-H(9C)	111.4(14)
H(9A)-C(9)-H(9B)	110(2)

H(9A)-C(9)-H(9C)	110(2)	C(20)-C(19)-H(19)	116.3(17)
H(9B)-C(9)-H(9C)	108(2)	C(19)-C(20)-H(20)	119.1(15)
N(1)-C(10)-C(15)	110.00(17)	C(19)-C(20)-C(21)	120.7(2)
C(11)-C(10)-N(1)	129.57(19)	C(21)-C(20)-H(20)	120.0(15)
C(11)-C(10)-C(15)	120.43(19)	N(4)-C(21)-C(16)	121.25(18)
C(10)-C(11)-H(11)	119(2)	N(4)-C(21)-C(20)	119.67(19)
C(12)-C(11)-C(10)	117.9(2)	C(20)-C(21)-C(16)	119.05(19)
C(12)-C(11)-H(11)	123(2)	C(2)-C(22)-H(22A)	107.2(14)
C(11)-C(12)-H(12)	119.1(14)	C(2)-C(22)-H(22B)	110.5(14)
C(11)-C(12)-C(13)	120.9(2)	H(22A)-C(22)-H(22B)	108(2)
C(13)-C(12)-H(12)	120.0(14)	C(23)-C(22)-C(2)	112.03(16)
C(12)-C(13)-H(13)	118.1(13)	C(23)-C(22)-H(22A)	110.8(14)
C(14)-C(13)-C(12)	122.3(2)	C(23)-C(22)-H(22B)	108.4(14)
C(14)-C(13)-H(13)	119.6(13)	O(2)-C(23)-C(22)	111.77(15)
C(13)-C(14)-H(14)	121.3(15)	O(2)-C(23)-H(23A)	109.1(13)
C(13)-C(14)-C(15)	116.5(2)	O(2)-C(23)-H(23B)	105.9(14)
C(15)-C(14)-H(14)	122.2(15)	C(22)-C(23)-H(23A)	111.8(13)
N(2)-C(15)-C(10)	104.95(16)	C(22)-C(23)-H(23B)	108.8(14)
C(14)-C(15)-N(2)	133.05(19)	H(23A)-C(23)-H(23B)	109.3(19)
C(14)-C(15)-C(10)	122.01(19)	O(2)-C(24)-H(24A)	106.2(12)
N(3)-C(16)-C(17)	119.64(17)	O(2)-C(24)-H(24B)	110.7(13)
N(3)-C(16)-C(21)	121.37(17)	O(2)-C(24)-C(25)	111.80(16)
C(17)-C(16)-C(21)	118.98(18)	H(24A)-C(24)-H(24B)	109.1(18)
C(16)-C(17)-H(17)	116.1(14)	C(25)-C(24)-H(24A)	109.0(12)
C(18)-C(17)-C(16)	120.4(2)	C(25)-C(24)-H(24B)	109.9(13)
C(18)-C(17)-H(17)	123.5(14)	C(2)-C(25)-H(25A)	109.3(13)
C(17)-C(18)-H(18)	117.7(16)	C(2)-C(25)-H(25B)	111.1(14)
C(17)-C(18)-C(19)	120.6(2)	C(24)-C(25)-C(2)	111.50(15)
C(19)-C(18)-H(18)	121.7(16)	C(24)-C(25)-H(25A)	106.6(12)
C(18)-C(19)-H(19)	123.4(17)	C(24)-C(25)-H(25B)	108.1(13)
C(20)-C(19)-C(18)	120.2(2)	H(25A)-C(25)-H(25B)	110.3(18)

Table S41. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **12b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	44(1)	16(1)	55(1)	2(1)	23(1)	1(1)

O(2)	20(1)	28(1)	46(1)	4(1)	7(1)	1(1)
N(1)	33(1)	23(1)	40(1)	-4(1)	11(1)	-4(1)
N(2)	24(1)	24(1)	38(1)	-4(1)	8(1)	-5(1)
N(3)	26(1)	20(1)	40(1)	-1(1)	11(1)	-1(1)
N(4)	30(1)	28(1)	38(1)	4(1)	11(1)	5(1)
C(1)	28(1)	16(1)	41(1)	-1(1)	11(1)	0(1)
C(2)	23(1)	19(1)	39(1)	-2(1)	9(1)	0(1)
C(3)	28(1)	22(1)	42(1)	-4(1)	13(1)	0(1)
C(4)	26(1)	20(1)	42(1)	-6(1)	11(1)	-5(1)
C(5)	24(1)	24(1)	38(1)	-6(1)	10(1)	-6(1)
C(6)	20(1)	28(1)	42(1)	-5(1)	7(1)	-1(1)
C(7)	24(1)	18(1)	38(1)	-1(1)	10(1)	-3(1)
C(8)	26(1)	19(1)	38(1)	2(1)	10(1)	-1(1)
C(9)	34(1)	33(1)	45(1)	-5(1)	15(1)	-13(1)
C(10)	32(1)	20(1)	42(1)	-3(1)	11(1)	-8(1)
C(11)	40(1)	27(1)	40(1)	-1(1)	9(1)	-7(1)
C(12)	36(1)	30(1)	45(1)	2(1)	3(1)	-9(1)
C(13)	27(1)	26(1)	54(1)	1(1)	8(1)	-6(1)
C(14)	27(1)	24(1)	49(1)	-3(1)	10(1)	-7(1)
C(15)	28(1)	20(1)	42(1)	-3(1)	8(1)	-7(1)
C(16)	28(1)	25(1)	36(1)	1(1)	11(1)	-2(1)
C(17)	33(1)	29(1)	40(1)	-2(1)	11(1)	-3(1)
C(18)	45(1)	47(1)	37(1)	-6(1)	12(1)	-7(1)
C(19)	39(1)	68(2)	34(1)	-3(1)	3(1)	2(1)
C(20)	38(1)	58(1)	40(1)	4(1)	9(1)	12(1)
C(21)	31(1)	32(1)	36(1)	3(1)	11(1)	3(1)
C(22)	27(1)	20(1)	42(1)	2(1)	9(1)	6(1)
C(23)	26(1)	28(1)	44(1)	4(1)	9(1)	6(1)
C(24)	22(1)	24(1)	43(1)	3(1)	9(1)	1(1)
C(25)	21(1)	19(1)	39(1)	1(1)	7(1)	2(1)

Table S42. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **12b**.

	x	y	z	U(eq)
H(1)	4484(15)	8640(30)	6125(9)	55
H(3A)	3663(13)	7340(20)	7488(9)	33(6)

H(3B)	4010(13)	8410(20)	7188(9)	31(6)
H(6A)	5424(13)	4570(30)	6888(9)	37(6)
H(6B)	6049(13)	5270(20)	6646(9)	34(6)
H(9A)	6370(16)	7570(30)	6885(10)	47(7)
H(9B)	5701(13)	7870(30)	6321(10)	40(6)
H(9C)	5685(14)	8750(30)	6845(10)	43(7)
H(11)	6188(19)	6590(30)	8994(13)	73(10)
H(12)	7478(14)	5920(30)	9050(10)	41(6)
H(13)	7806(13)	5450(20)	8282(8)	33(6)
H(14)	6892(14)	5750(30)	7466(10)	42(7)
H(17)	4810(14)	2410(30)	5099(9)	42(7)
H(18)	3806(15)	2370(30)	4317(10)	47(7)
H(19)	2864(16)	4250(30)	4088(11)	56(8)
H(20)	2878(15)	5900(30)	4683(9)	44(7)
H(22A)	2928(14)	6590(30)	6120(10)	39(6)
H(22B)	2959(13)	7990(30)	6414(9)	38(6)
H(23A)	2427(13)	7000(20)	7034(9)	33(6)
H(23B)	1894(13)	6690(20)	6462(9)	32(6)
H(24A)	3134(12)	3660(20)	7149(8)	28(5)
H(24B)	3240(13)	5140(20)	7468(9)	36(6)
H(25A)	3720(12)	4560(20)	6569(9)	28(5)
H(25B)	4292(13)	4790(20)	7140(9)	32(6)

Table S43. Torsion angles [°] for **12b**.

O(1)-C(1)-C(2)-C(3)	-64.53(18)	N(2)-C(5)-C(6)-C(7)	143.73(15)
O(1)-C(1)-C(2)-C(22)	53.87(19)	N(3)-C(7)-C(8)-N(4)	-3.9(3)
O(1)-C(1)-C(2)-C(25)	173.64(15)	N(3)-C(7)-C(8)-C(1)	175.21(16)
O(1)-C(1)-C(5)-N(2)	94.86(18)	N(3)-C(16)-C(17)-C(18)	178.25(19)
O(1)-C(1)-C(5)-C(6)	-144.83(16)	N(3)-C(16)-C(21)-N(4)	-4.0(3)
O(1)-C(1)-C(5)-C(9)	-25.6(2)	N(3)-C(16)-C(21)-C(20)	178.20(19)
O(1)-C(1)-C(8)-N(4)	-43.7(2)	C(1)-C(2)-C(3)-C(4)	-62.52(19)
O(1)-C(1)-C(8)-C(7)	137.17(16)	C(1)-C(2)-C(22)-C(23)	174.37(15)
O(2)-C(24)-C(25)-C(2)	57.2(2)	C(1)-C(2)-C(25)-C(24)	-172.77(16)
N(1)-C(10)-C(11)-C(12)	179.84(19)	C(1)-C(5)-C(6)-C(7)	22.16(19)
N(1)-C(10)-C(15)-N(2)	1.6(2)	C(2)-C(1)-C(5)-N(2)	-23.5(2)
N(1)-C(10)-C(15)-C(14)	-178.31(16)	C(2)-C(1)-C(5)-C(6)	96.77(17)

C(2)-C(1)-C(5)-C(9)	-143.97(16)	C(8)-C(1)-C(5)-C(6)	-23.92(18)
C(2)-C(1)-C(8)-N(4)	75.7(2)	C(8)-C(1)-C(5)-C(9)	95.33(17)
C(2)-C(1)-C(8)-C(7)	-103.40(17)	C(9)-C(5)-C(6)-C(7)	-96.60(18)
C(2)-C(3)-C(4)-N(1)	-144.17(18)	C(10)-N(1)-C(4)-N(2)	1.4(2)
C(2)-C(3)-C(4)-N(2)	34.5(2)	C(10)-N(1)-C(4)-C(3)	-179.88(17)
C(2)-C(22)-C(23)-O(2)	-56.6(2)	C(10)-C(11)-C(12)-C(13)	-0.8(3)
C(3)-C(2)-C(22)-C(23)	-69.9(2)	C(11)-C(10)-C(15)-N(2)	-177.67(16)
C(3)-C(2)-C(25)-C(24)	68.8(2)	C(11)-C(10)-C(15)-C(14)	2.4(3)
C(4)-N(1)-C(10)-C(11)	177.34(19)	C(11)-C(12)-C(13)-C(14)	1.5(3)
C(4)-N(1)-C(10)-C(15)	-1.8(2)	C(12)-C(13)-C(14)-C(15)	-0.2(3)
C(4)-N(2)-C(5)-C(1)	-8.6(2)	C(13)-C(14)-C(15)-N(2)	178.35(18)
C(4)-N(2)-C(5)-C(6)	-126.54(18)	C(13)-C(14)-C(15)-C(10)	-1.8(3)
C(4)-N(2)-C(5)-C(9)	112.56(19)	C(15)-N(2)-C(4)-N(1)	-0.4(2)
C(4)-N(2)-C(15)-C(10)	-0.75(19)	C(15)-N(2)-C(4)-C(3)	-179.24(16)
C(4)-N(2)-C(15)-C(14)	179.16(19)	C(15)-N(2)-C(5)-C(1)	174.56(16)
C(5)-N(2)-C(4)-N(1)	-177.79(16)	C(15)-N(2)-C(5)-C(6)	56.6(2)
C(5)-N(2)-C(4)-C(3)	3.4(3)	C(15)-N(2)-C(5)-C(9)	-64.3(2)
C(5)-N(2)-C(15)-C(10)	176.57(16)	C(15)-C(10)-C(11)-C(12)	-1.0(3)
C(5)-N(2)-C(15)-C(14)	-3.5(3)	C(16)-N(3)-C(7)-C(6)	179.30(17)
C(5)-C(1)-C(2)-C(3)	57.49(18)	C(16)-N(3)-C(7)-C(8)	0.1(3)
C(5)-C(1)-C(2)-C(22)	175.89(14)	C(16)-C(17)-C(18)-C(19)	3.1(3)
C(5)-C(1)-C(2)-C(25)	-64.3(2)	C(17)-C(16)-C(21)-N(4)	174.60(18)
C(5)-C(1)-C(8)-N(4)	-163.44(17)	C(17)-C(16)-C(21)-C(20)	-3.2(3)
C(5)-C(1)-C(8)-C(7)	17.45(19)	C(17)-C(18)-C(19)-C(20)	-2.2(4)
C(5)-C(6)-C(7)-N(3)	168.95(17)	C(18)-C(19)-C(20)-C(21)	-1.5(4)
C(5)-C(6)-C(7)-C(8)	-11.8(2)	C(19)-C(20)-C(21)-N(4)	-173.7(2)
C(6)-C(7)-C(8)-N(4)	176.79(17)	C(19)-C(20)-C(21)-C(16)	4.1(3)
C(6)-C(7)-C(8)-C(1)	-4.1(2)	C(21)-N(4)-C(8)-C(1)	-175.59(17)
C(7)-N(3)-C(16)-C(17)	-175.03(17)	C(21)-N(4)-C(8)-C(7)	3.4(3)
C(7)-N(3)-C(16)-C(21)	3.6(3)	C(21)-C(16)-C(17)-C(18)	-0.4(3)
C(8)-N(4)-C(21)-C(16)	0.3(3)	C(22)-C(2)-C(3)-C(4)	179.13(16)
C(8)-N(4)-C(21)-C(20)	178.10(19)	C(22)-C(2)-C(25)-C(24)	-51.7(2)
C(8)-C(1)-C(2)-C(3)	171.49(15)	C(23)-O(2)-C(24)-C(25)	-60.1(2)
C(8)-C(1)-C(2)-C(22)	-70.11(19)	C(24)-O(2)-C(23)-C(22)	59.6(2)
C(8)-C(1)-C(2)-C(25)	49.7(2)	C(25)-C(2)-C(3)-C(4)	60.1(2)
C(8)-C(1)-C(5)-N(2)	-144.23(15)	C(25)-C(2)-C(22)-C(23)	51.5(2)

6.7. Compound **13a**

X-ray diffraction data were collected at 100K on a Rigaku Synergy S diffractometer equipped with a HyPix600HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[1] The structure was solved by direct methods using SHELXT[2] and refined on F^2 using SHELXL-2018[3] in the OLEX2 program.[4] Positions of all atoms were found from the electron density-difference map. Atoms were refined with individual anisotropic (non-hydrogen atoms) or isotropic (hydrogen atoms) displacement parameters.

Table S44. Crystal data and structure refinement for **13a**.

Identification code	**13a**	
Empirical formula	C21 H20 N2 O4	
Formula weight	364.39	
Temperature	100.0(1) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 7.48251(7) Å	α= 107.8011(13)°.
	b = 8.97191(13) Å	β= 96.7797(9)°.
	c = 13.67021(19) Å	γ = 98.0759(10)°.
Volume	852.40(2) $Å^3$	
Z	2	
Density (calculated)	1.420 g/cm^3	
Absorption coefficient	0.813 mm^{-1}	
F(000)	384	
Crystal size	0.28 x 0.15 x 0.08 mm^3	
Theta range for data collection	3.446 to 79.456°.	
Index ranges	-7<=h<=9, -11<=k<=11, -17<=l<=17	
Reflections collected	18947	
Independent reflections	3679 [R(int) = 0.0308]	
Observed reflections	3503	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Analytical	
Max. and min. transmission	0.947 and 0.845	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3679 / 0 / 325	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.1038	

R indices (all data)	R1 = 0.0389, wR2 = 0.1049
Extinction coefficient	0.0025(7)
Largest diff. peak and hole	0.344 and -0.240 e.Å^{-3}
CCDC	**2233465**

Table S45. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **13a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3097(1)	1421(1)	5601(1)	19(1)
O(2)	1687(1)	3406(1)	5473(1)	19(1)
O(3)	847(1)	983(1)	4248(1)	25(1)
O(4)	3929(1)	6736(1)	6328(1)	28(1)
N(1)	547(1)	4137(1)	8620(1)	18(1)
N(2)	1866(1)	4519(1)	7295(1)	16(1)
C(1)	1793(2)	1848(1)	5033(1)	19(1)
C(2)	2908(2)	4098(1)	6472(1)	16(1)
C(3)	4058(2)	2772(1)	6493(1)	17(1)
C(4)	4297(2)	5488(1)	6377(1)	20(1)
C(5)	6000(2)	4917(1)	6245(1)	22(1)
C(6)	5883(2)	3409(1)	6236(1)	20(1)
C(7)	7303(2)	2419(2)	5956(1)	27(1)
C(8)	4154(2)	2238(1)	7472(1)	17(1)
C(9)	2185(2)	2042(1)	7703(1)	18(1)
C(10)	1494(1)	3559(1)	7904(1)	16(1)
C(11)	204(2)	5562(1)	8485(1)	17(1)
C(12)	-758(2)	6642(1)	9065(1)	20(1)
C(13)	-1004(2)	7943(1)	8758(1)	22(1)
C(14)	-324(2)	8148(1)	7885(1)	21(1)
C(15)	678(2)	7104(1)	7313(1)	19(1)
C(16)	966(1)	5818(1)	7647(1)	16(1)
C(17)	4787(2)	619(1)	7274(1)	21(1)
C(18)	5056(2)	159(1)	8267(1)	24(1)
C(19)	6370(2)	1463(2)	9155(1)	26(1)
C(20)	5724(2)	3058(1)	9374(1)	23(1)
C(21)	5484(2)	3524(1)	8385(1)	19(1)

Table S46. Bond lengths [Å] and angles [°] for **13a**.

O(1)-C(1)	1.3449(14)	C(17)-H(17A)	0.993(17)
O(1)-C(3)	1.4559(13)	C(17)-H(17B)	0.994(16)
O(2)-C(1)	1.3602(14)	C(17)-C(18)	1.5338(17)
O(2)-C(2)	1.4533(13)	C(18)-H(18A)	1.005(16)
O(3)-C(1)	1.1887(14)	C(18)-H(18B)	1.005(18)
O(4)-C(4)	1.2091(15)	C(18)-C(19)	1.5282(17)
N(1)-C(10)	1.2990(15)	C(19)-H(19A)	1.001(19)
N(1)-C(11)	1.4000(14)	C(19)-H(19B)	1.005(17)
N(2)-C(2)	1.4305(14)	C(19)-C(20)	1.5290(17)
N(2)-C(10)	1.3921(14)	C(20)-H(20A)	0.999(18)
N(2)-C(16)	1.4134(14)	C(20)-H(20B)	1.013(17)
C(2)-C(3)	1.5678(15)	C(20)-C(21)	1.5313(16)
C(2)-C(4)	1.5554(15)	C(21)-H(21A)	0.990(16)
C(3)-C(6)	1.5262(15)	C(21)-H(21B)	0.980(17)
C(3)-C(8)	1.5514(15)	C(1)-O(1)-C(3)	111.11(8)
C(4)-C(5)	1.4489(17)	C(1)-O(2)-C(2)	110.56(8)
C(5)-H(5)	0.955(18)	C(10)-N(1)-C(11)	104.96(9)
C(5)-C(6)	1.3392(17)	C(10)-N(2)-C(2)	122.25(9)
C(6)-C(7)	1.4893(16)	C(10)-N(2)-C(16)	105.91(9)
C(7)-H(7A)	1.01(2)	C(16)-N(2)-C(2)	131.79(9)
C(7)-H(7B)	0.982(19)	O(1)-C(1)-O(2)	111.33(9)
C(7)-H(7C)	0.987(19)	O(3)-C(1)-O(1)	124.80(10)
C(8)-C(9)	1.5398(15)	O(3)-C(1)-O(2)	123.87(11)
C(8)-C(17)	1.5464(15)	O(2)-C(2)-C(3)	103.05(8)
C(8)-C(21)	1.5432(15)	O(2)-C(2)-C(4)	106.62(9)
C(9)-H(9A)	0.972(15)	N(2)-C(2)-O(2)	110.02(9)
C(9)-H(9B)	0.983(17)	N(2)-C(2)-C(3)	115.61(9)
C(9)-C(10)	1.4829(15)	N(2)-C(2)-C(4)	115.74(9)
C(11)-C(12)	1.3950(16)	C(4)-C(2)-C(3)	104.69(9)
C(11)-C(16)	1.4036(15)	O(1)-C(3)-C(2)	102.84(8)
C(12)-H(12)	0.965(17)	O(1)-C(3)-C(6)	108.54(9)
C(12)-C(13)	1.3845(16)	O(1)-C(3)-C(8)	107.99(8)
C(13)-H(13)	0.999(17)	C(6)-C(3)-C(2)	103.11(9)
C(13)-C(14)	1.4023(17)	C(6)-C(3)-C(8)	116.54(9)
C(14)-H(14)	0.991(18)	C(8)-C(3)-C(2)	116.76(9)
C(14)-C(15)	1.3924(16)	O(4)-C(4)-C(2)	124.97(11)
C(15)-H(15)	0.965(16)	O(4)-C(4)-C(5)	127.97(11)
C(15)-C(16)	1.3973(15)	C(5)-C(4)-C(2)	106.73(9)

C(4)-C(5)-H(5)	120.8(10)	C(15)-C(14)-H(14)	118.6(10)
C(6)-C(5)-C(4)	112.55(10)	C(14)-C(15)-H(15)	122.2(9)
C(6)-C(5)-H(5)	126.5(10)	C(14)-C(15)-C(16)	116.58(11)
C(5)-C(6)-C(3)	111.99(10)	C(16)-C(15)-H(15)	121.2(9)
C(5)-C(6)-C(7)	124.87(11)	C(11)-C(16)-N(2)	104.24(9)
C(7)-C(6)-C(3)	123.06(10)	C(15)-C(16)-N(2)	134.49(10)
C(6)-C(7)-H(7A)	108.9(12)	C(15)-C(16)-C(11)	121.20(10)
C(6)-C(7)-H(7B)	109.8(11)	C(8)-C(17)-H(17A)	108.3(10)
C(6)-C(7)-H(7C)	110.1(11)	C(8)-C(17)-H(17B)	111.7(9)
H(7A)-C(7)-H(7B)	109.2(16)	H(17A)-C(17)-H(17B)	106.7(13)
H(7A)-C(7)-H(7C)	108.1(16)	C(18)-C(17)-C(8)	112.18(10)
H(7B)-C(7)-H(7C)	110.7(15)	C(18)-C(17)-H(17A)	110.8(10)
C(9)-C(8)-C(3)	105.85(9)	C(18)-C(17)-H(17B)	107.0(9)
C(9)-C(8)-C(17)	108.51(9)	C(17)-C(18)-H(18A)	109.4(9)
C(9)-C(8)-C(21)	111.63(9)	C(17)-C(18)-H(18B)	106.8(10)
C(17)-C(8)-C(3)	111.96(9)	H(18A)-C(18)-H(18B)	107.9(13)
C(21)-C(8)-C(3)	109.17(9)	C(19)-C(18)-C(17)	111.70(10)
C(21)-C(8)-C(17)	109.70(9)	C(19)-C(18)-H(18A)	110.1(9)
C(8)-C(9)-H(9A)	108.6(9)	C(19)-C(18)-H(18B)	110.8(10)
C(8)-C(9)-H(9B)	112.6(9)	C(18)-C(19)-H(19A)	112.0(10)
H(9A)-C(9)-H(9B)	107.6(13)	C(18)-C(19)-H(19B)	109.3(9)
C(10)-C(9)-C(8)	111.28(9)	C(18)-C(19)-C(20)	111.11(10)
C(10)-C(9)-H(9A)	109.8(9)	H(19A)-C(19)-H(19B)	106.8(14)
C(10)-C(9)-H(9B)	106.9(10)	C(20)-C(19)-H(19A)	108.8(10)
N(1)-C(10)-N(2)	113.78(10)	C(20)-C(19)-H(19B)	108.6(10)
N(1)-C(10)-C(9)	126.50(10)	C(19)-C(20)-H(20A)	109.3(10)
N(2)-C(10)-C(9)	119.72(10)	C(19)-C(20)-H(20B)	110.7(10)
N(1)-C(11)-C(16)	111.00(10)	C(19)-C(20)-C(21)	110.68(10)
C(12)-C(11)-N(1)	127.64(10)	H(20A)-C(20)-H(20B)	105.5(13)
C(12)-C(11)-C(16)	121.36(10)	C(21)-C(20)-H(20A)	109.5(10)
C(11)-C(12)-H(12)	121.6(10)	C(21)-C(20)-H(20B)	111.0(10)
C(13)-C(12)-C(11)	117.64(11)	C(8)-C(21)-H(21A)	107.5(9)
C(13)-C(12)-H(12)	120.7(10)	C(8)-C(21)-H(21B)	110.1(9)
C(12)-C(13)-H(13)	119.6(10)	C(20)-C(21)-C(8)	112.65(9)
C(12)-C(13)-C(14)	120.74(11)	C(20)-C(21)-H(21A)	108.1(9)
C(14)-C(13)-H(13)	119.7(10)	C(20)-C(21)-H(21B)	109.8(9)
C(13)-C(14)-H(14)	119.1(10)	H(21A)-C(21)-H(21B)	108.6(13)
C(15)-C(14)-C(13)	122.33(11)		

Table S47. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **13a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	21(1)	14(1)	19(1)	2(1)	-2(1)	2(1)
O(2)	21(1)	16(1)	18(1)	5(1)	1(1)	3(1)
O(3)	28(1)	20(1)	20(1)	4(1)	-4(1)	0(1)
O(4)	34(1)	16(1)	40(1)	11(1)	16(1)	6(1)
N(1)	18(1)	17(1)	19(1)	7(1)	1(1)	2(1)
N(2)	17(1)	14(1)	19(1)	6(1)	3(1)	3(1)
C(1)	20(1)	17(1)	19(1)	6(1)	2(1)	2(1)
C(2)	17(1)	14(1)	17(1)	4(1)	2(1)	2(1)
C(3)	16(1)	12(1)	18(1)	1(1)	0(1)	1(1)
C(4)	23(1)	15(1)	19(1)	3(1)	5(1)	0(1)
C(5)	19(1)	21(1)	23(1)	5(1)	3(1)	-1(1)
C(6)	18(1)	21(1)	18(1)	3(1)	1(1)	2(1)
C(7)	21(1)	27(1)	31(1)	7(1)	6(1)	7(1)
C(8)	17(1)	13(1)	19(1)	4(1)	-1(1)	3(1)
C(9)	18(1)	14(1)	21(1)	6(1)	0(1)	1(1)
C(10)	15(1)	15(1)	18(1)	6(1)	-1(1)	0(1)
C(11)	16(1)	16(1)	18(1)	5(1)	0(1)	2(1)
C(12)	20(1)	22(1)	18(1)	6(1)	3(1)	4(1)
C(13)	21(1)	19(1)	23(1)	4(1)	2(1)	6(1)
C(14)	21(1)	16(1)	26(1)	7(1)	2(1)	4(1)
C(15)	19(1)	17(1)	22(1)	8(1)	2(1)	3(1)
C(16)	15(1)	14(1)	18(1)	4(1)	1(1)	3(1)
C(17)	23(1)	15(1)	23(1)	4(1)	-2(1)	5(1)
C(18)	27(1)	17(1)	27(1)	7(1)	-3(1)	6(1)
C(19)	27(1)	22(1)	26(1)	8(1)	-5(1)	6(1)
C(20)	25(1)	20(1)	21(1)	4(1)	-3(1)	3(1)
C(21)	18(1)	14(1)	21(1)	3(1)	-1(1)	1(1)

Table S48. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **13a**.

	x	y	z	U(eq)
H(5)	7030(20)	5560(20)	6130(13)	30(4)
H(7A)	8180(30)	2950(30)	5609(17)	51(5)
H(7B)	6720(20)	1360(20)	5473(14)	36(4)
H(7C)	8000(20)	2340(20)	6591(15)	36(4)
H(9A)	1400(20)	1226(18)	7108(12)	20(3)
H(9B)	2090(20)	1710(20)	8318(13)	26(4)
H(12)	-1200(20)	6515(19)	9676(13)	24(4)
H(13)	-1680(20)	8740(20)	9161(13)	30(4)
H(14)	-560(20)	9070(20)	7668(13)	31(4)
H(15)	1130(20)	7237(19)	6706(13)	23(4)
H(17A)	3870(20)	-200(20)	6721(13)	27(4)
H(17B)	5970(20)	633(19)	7012(12)	24(4)
H(18A)	3840(20)	-62(19)	8484(12)	25(4)
H(18B)	5550(20)	-860(20)	8080(13)	31(4)
H(19A)	6510(20)	1190(20)	9813(14)	34(4)
H(19B)	7620(20)	1590(20)	8957(13)	27(4)
H(20A)	6650(20)	3900(20)	9927(13)	29(4)
H(20B)	4550(20)	3020(20)	9672(13)	29(4)
H(21A)	6690(20)	3655(18)	8164(12)	20(3)
H(21B)	5060(20)	4540(20)	8535(12)	24(4)

Table S49. Torsion angles [°] for **13a**.

O(1)-C(3)-C(6)-C(5)	118.29(11)	O(4)-C(4)-C(5)-C(6)	-173.16(12)
O(1)-C(3)-C(6)-C(7)	-58.71(14)	N(1)-C(11)-C(12)-C(13)	-176.96(11)
O(1)-C(3)-C(8)-C(9)	-70.81(10)	N(1)-C(11)-C(16)-N(2)	-2.39(12)
O(1)-C(3)-C(8)-C(17)	47.24(11)	N(1)-C(11)-C(16)-C(15)	175.01(10)
O(1)-C(3)-C(8)-C(21)	168.91(8)	N(2)-C(2)-C(3)-O(1)	109.92(10)
O(2)-C(2)-C(3)-O(1)	-10.14(10)	N(2)-C(2)-C(3)-C(6)	-137.26(9)
O(2)-C(2)-C(3)-C(6)	102.69(9)	N(2)-C(2)-C(3)-C(8)	-8.10(13)
O(2)-C(2)-C(3)-C(8)	-128.16(9)	N(2)-C(2)-C(4)-O(4)	-52.14(16)
O(2)-C(2)-C(4)-O(4)	70.59(14)	N(2)-C(2)-C(4)-C(5)	134.01(10)
O(2)-C(2)-C(4)-C(5)	-103.27(10)	C(1)-O(1)-C(3)-C(2)	8.00(11)

C(1)-O(1)-C(3)-C(6)	-100.78(10)	C(8)-C(9)-C(10)-N(1)	-138.33(11)
C(1)-O(1)-C(3)-C(8)	132.03(9)	C(8)-C(9)-C(10)-N(2)	41.04(13)
C(1)-O(2)-C(2)-N(2)	-114.35(10)	C(8)-C(17)-C(18)-C(19)	-54.87(13)
C(1)-O(2)-C(2)-C(3)	9.47(11)	C(9)-C(8)-C(17)-C(18)	-68.86(12)
C(1)-O(2)-C(2)-C(4)	119.40(9)	C(9)-C(8)-C(21)-C(20)	65.81(12)
C(2)-O(2)-C(1)-O(1)	-4.98(12)	C(10)-N(1)-C(11)-C(12)	-179.65(11)
C(2)-O(2)-C(1)-O(3)	174.95(11)	C(10)-N(1)-C(11)-C(16)	0.65(12)
C(2)-N(2)-C(10)-N(1)	179.34(9)	C(10)-N(2)-C(2)-O(2)	99.63(11)
C(2)-N(2)-C(10)-C(9)	-0.11(15)	C(10)-N(2)-C(2)-C(3)	-16.54(14)
C(2)-N(2)-C(16)-C(11)	-179.57(11)	C(10)-N(2)-C(2)-C(4)	-139.45(10)
C(2)-N(2)-C(16)-C(15)	3.5(2)	C(10)-N(2)-C(16)-C(11)	3.08(11)
C(2)-C(3)-C(6)-C(5)	9.69(13)	C(10)-N(2)-C(16)-C(15)	-173.80(12)
C(2)-C(3)-C(6)-C(7)	-167.30(11)	C(11)-N(1)-C(10)-N(2)	1.48(12)
C(2)-C(3)-C(8)-C(9)	44.38(12)	C(11)-N(1)-C(10)-C(9)	-179.12(10)
C(2)-C(3)-C(8)-C(17)	162.43(9)	C(11)-C(12)-C(13)-C(14)	0.78(17)
C(2)-C(3)-C(8)-C(21)	-75.91(11)	C(12)-C(11)-C(16)-N(2)	177.89(10)
C(2)-C(4)-C(5)-C(6)	0.45(14)	C(12)-C(11)-C(16)-C(15)	-4.72(17)
C(3)-O(1)-C(1)-O(2)	-2.43(12)	C(12)-C(13)-C(14)-C(15)	-2.48(18)
C(3)-O(1)-C(1)-O(3)	177.65(11)	C(13)-C(14)-C(15)-C(16)	0.57(17)
C(3)-C(2)-C(4)-O(4)	179.36(11)	C(14)-C(15)-C(16)-N(2)	179.41(11)
C(3)-C(2)-C(4)-C(5)	5.51(12)	C(14)-C(15)-C(16)-C(11)	2.95(16)
C(3)-C(8)-C(9)-C(10)	-59.82(11)	C(16)-N(2)-C(2)-O(2)	-77.35(13)
C(3)-C(8)-C(17)-C(18)	174.69(9)	C(16)-N(2)-C(2)-C(3)	166.48(10)
C(3)-C(8)-C(21)-C(20)	-177.52(9)	C(16)-N(2)-C(2)-C(4)	43.57(16)
C(4)-C(2)-C(3)-O(1)	-121.50(9)	C(16)-N(2)-C(10)-N(1)	-3.00(12)
C(4)-C(2)-C(3)-C(6)	-8.68(11)	C(16)-N(2)-C(10)-C(9)	177.55(9)
C(4)-C(2)-C(3)-C(8)	120.48(10)	C(16)-C(11)-C(12)-C(13)	2.72(17)
C(4)-C(5)-C(6)-C(3)	-6.65(15)	C(17)-C(8)-C(9)-C(10)	179.86(9)
C(4)-C(5)-C(6)-C(7)	170.29(11)	C(17)-C(8)-C(21)-C(20)	-54.50(13)
C(6)-C(3)-C(8)-C(9)	166.79(9)	C(17)-C(18)-C(19)-C(20)	55.64(14)
C(6)-C(3)-C(8)-C(17)	-75.16(12)	C(18)-C(19)-C(20)-C(21)	-55.95(14)
C(6)-C(3)-C(8)-C(21)	46.50(12)	C(19)-C(20)-C(21)-C(8)	56.37(13)
C(8)-C(3)-C(6)-C(5)	-119.60(11)	C(21)-C(8)-C(9)-C(10)	58.85(12)
C(8)-C(3)-C(6)-C(7)	63.41(14)	C(21)-C(8)-C(17)-C(18)	53.33(13)

7. References

1. CrysAlisPro. Version 1.171.41. *Rigaku Oxford Diffraction*, **2021**.

2. Sheldrick, G. M. SHELXT - Integrated space-group and crystal-structure determination. *Acta Cryst.* **2015**, A71(1), 3-8.

3. Sheldrick, G. M. Crystal structure refinement with SHELXL. *Acta Cryst.* **2015**, C71, 1, 3-8.

4. Dolomanov O.V.; Bourhis L.J.; Gildea R.J.; Howard J.A.K.; Puschmann H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009**, 42, 2, 229-341.