

## Supporting Information

### **NEW MONOTERPENOID INDOLE ALKALOIDS FROM *GELSEMIUM ELEGANS***

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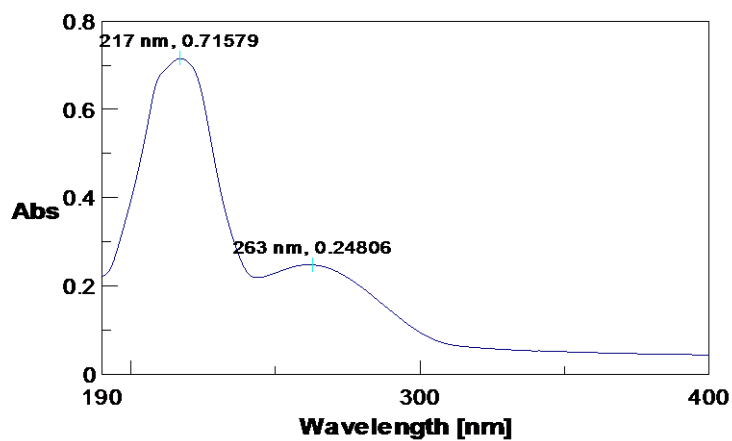
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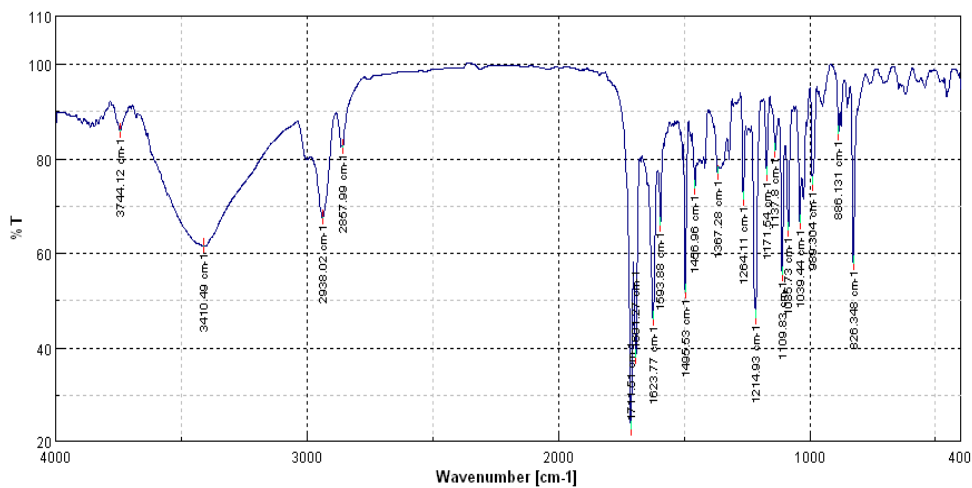
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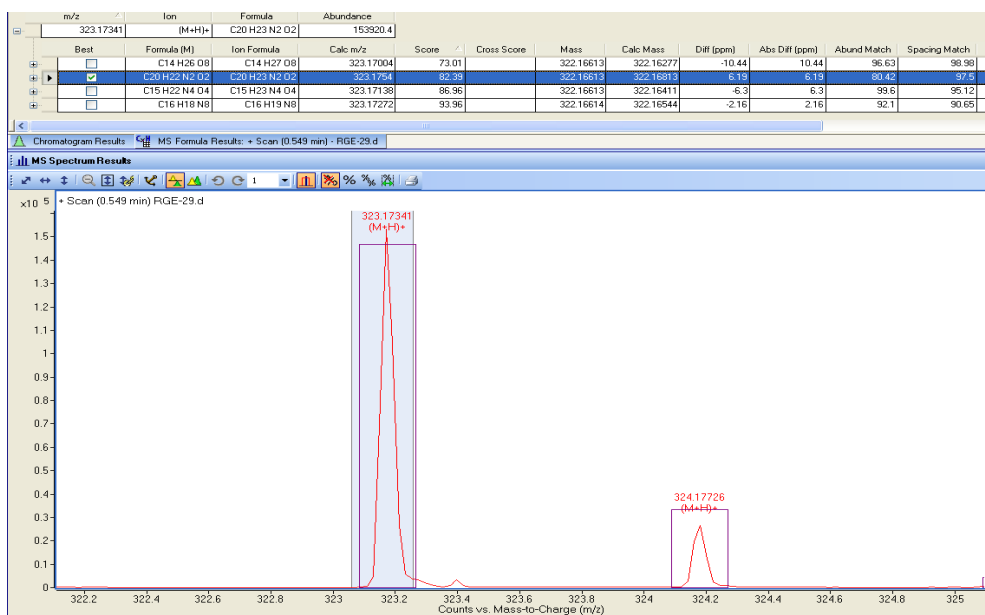
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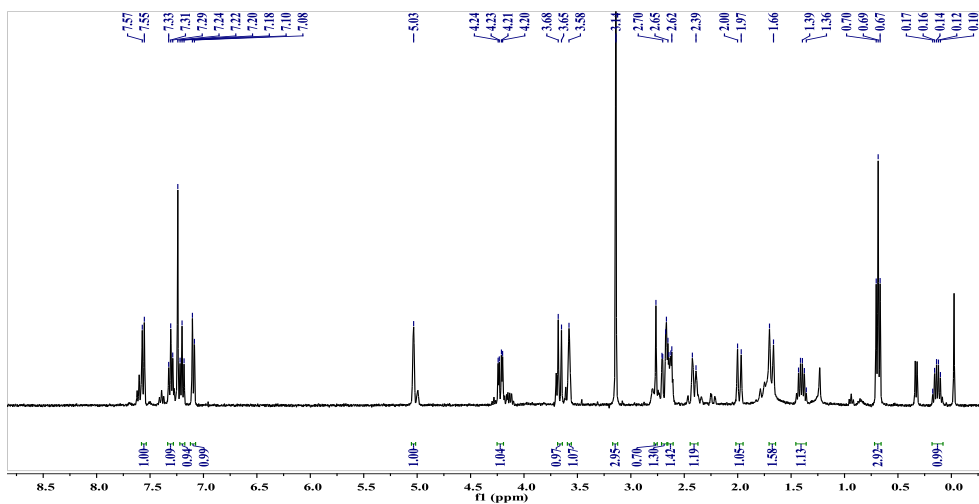
UV spectrum of 1 (CH<sub>3</sub>OH)



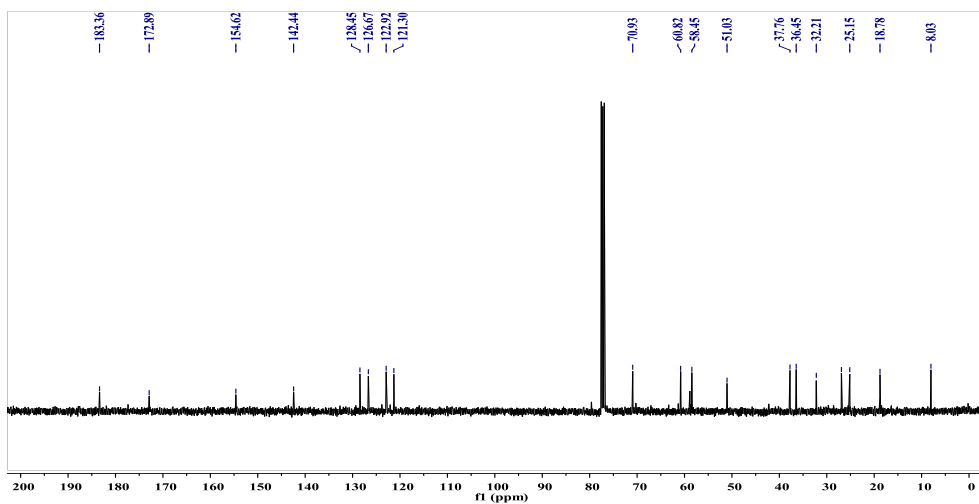
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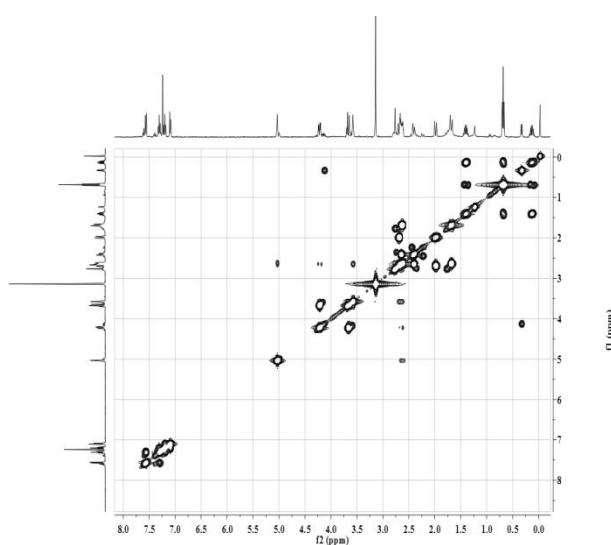
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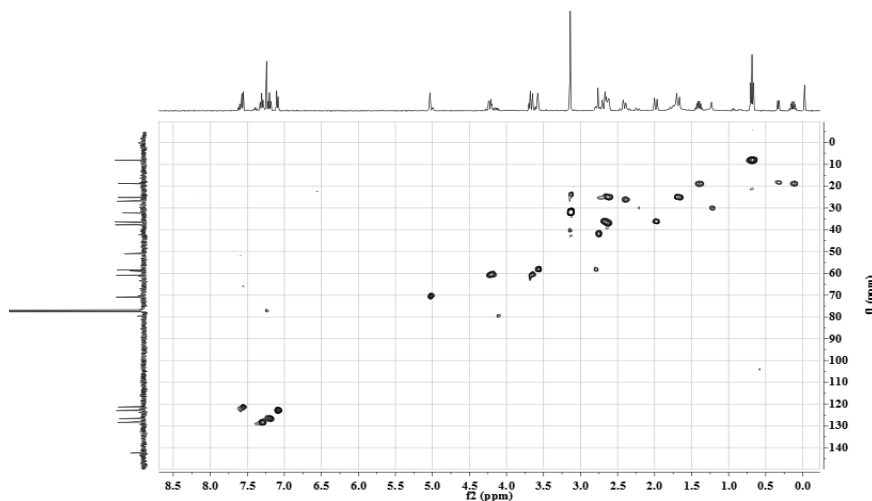
$^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$



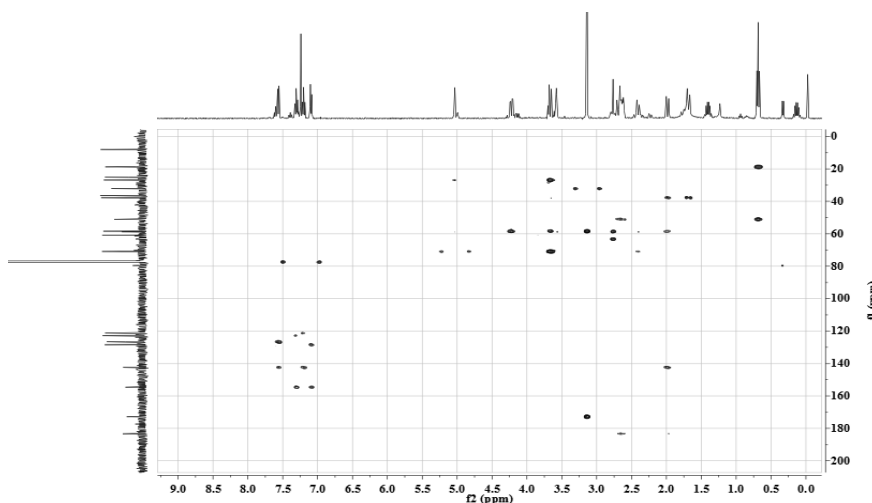
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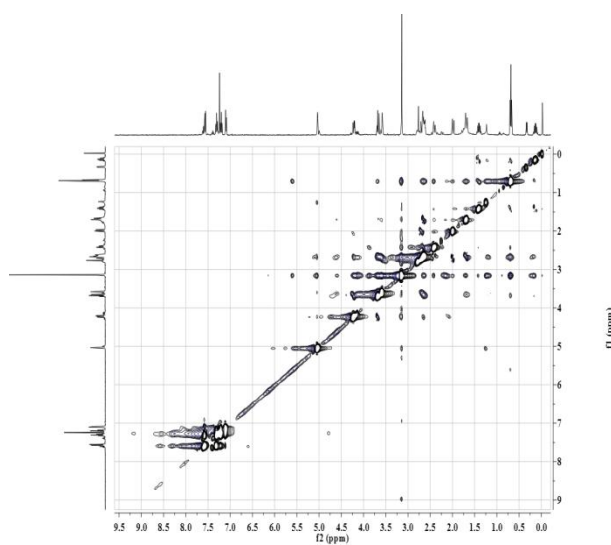
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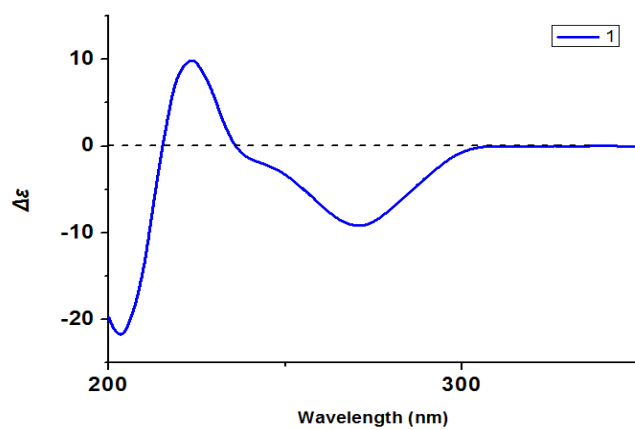
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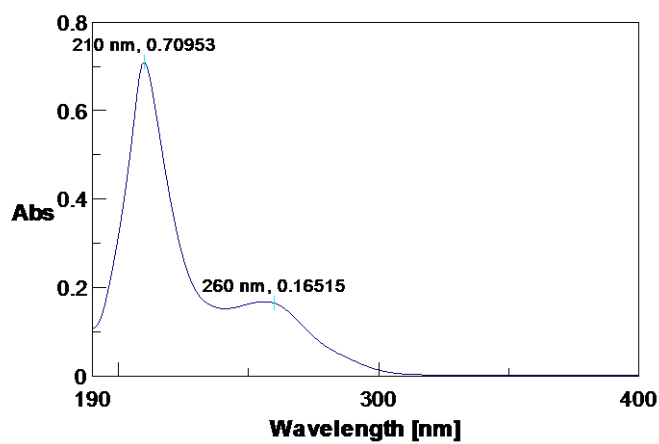
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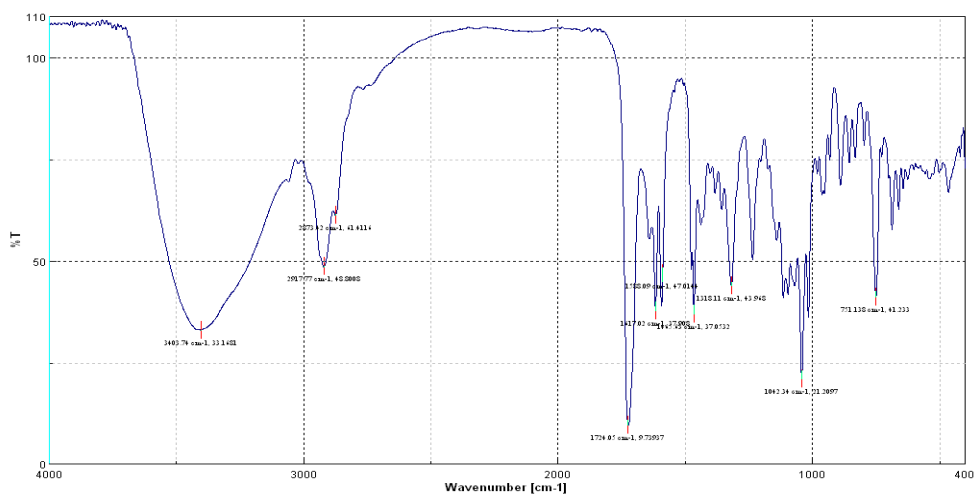
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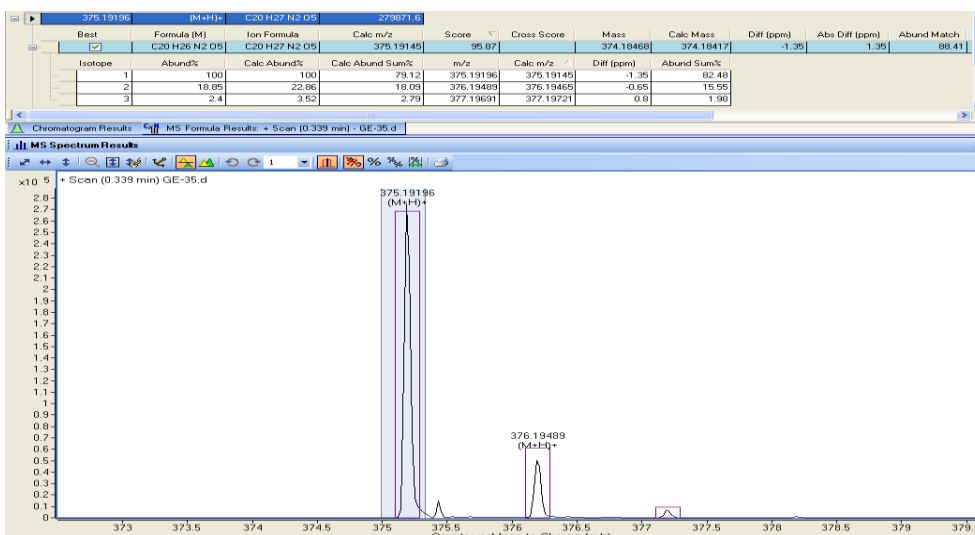
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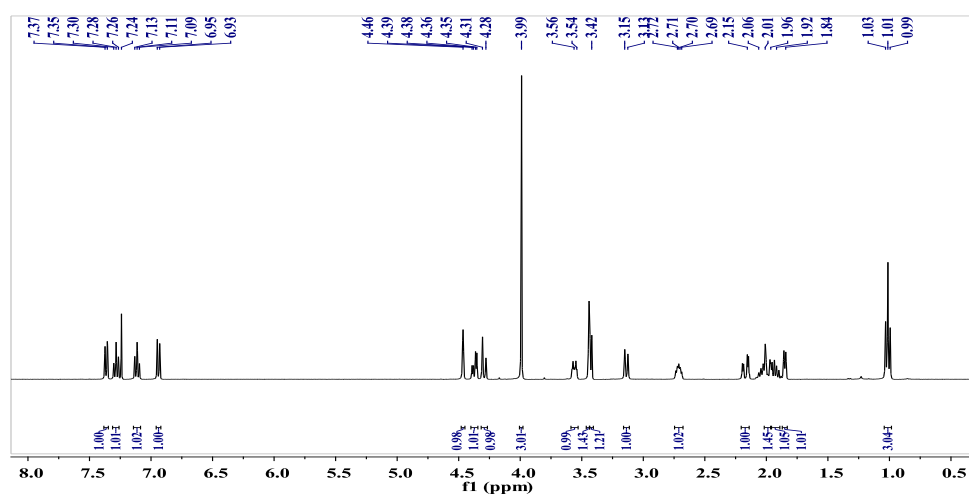
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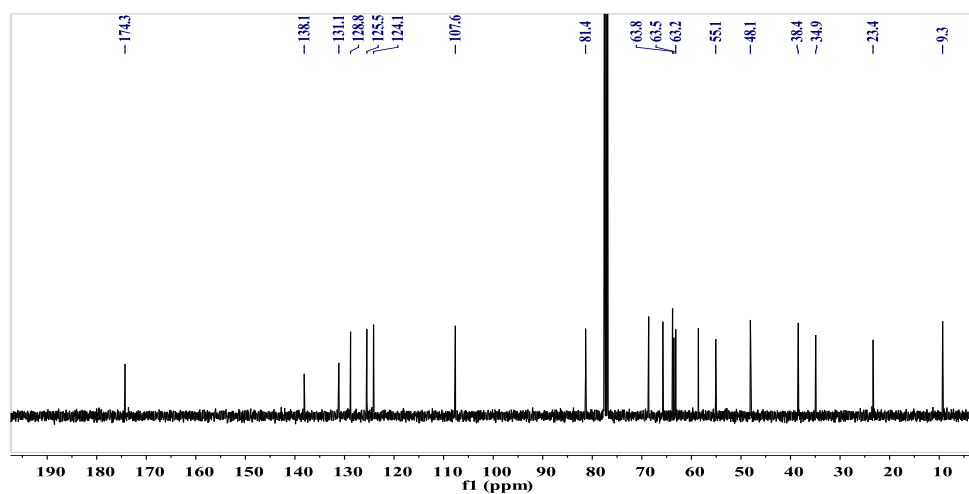
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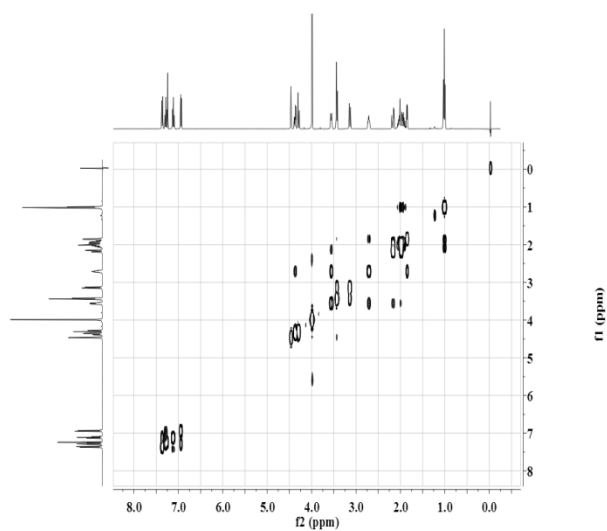
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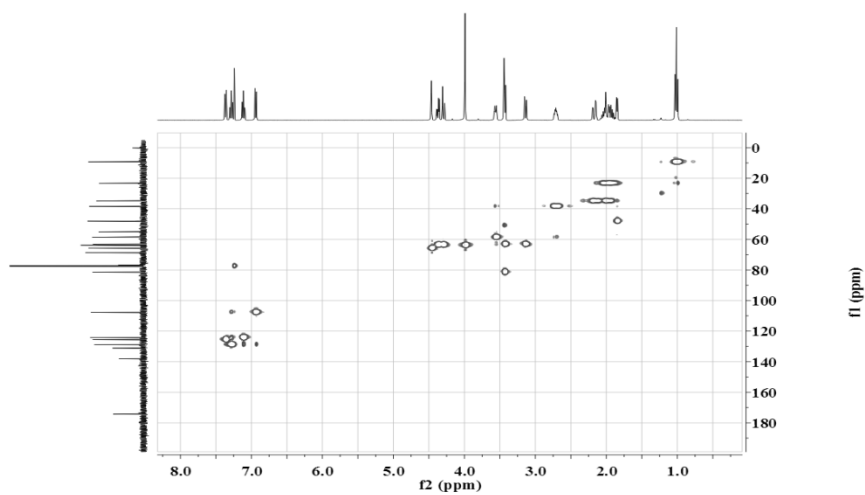
<sup>1</sup>H NMR spectrum of **2** in CDCl<sub>3</sub>



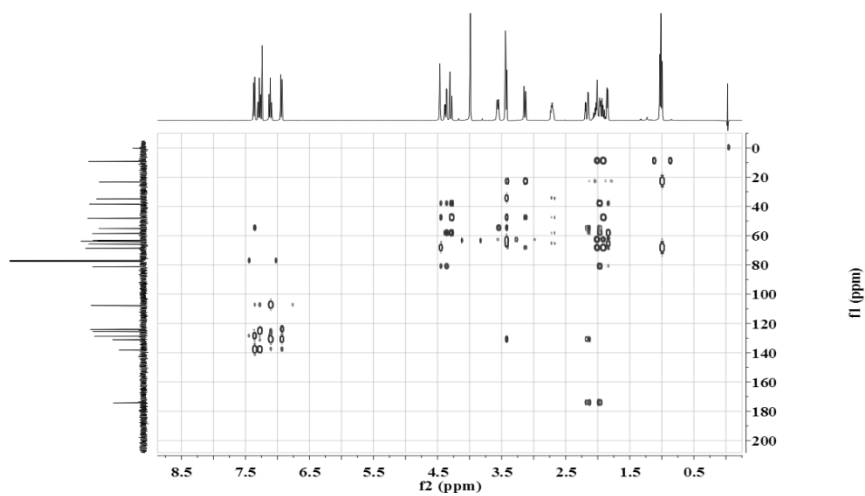
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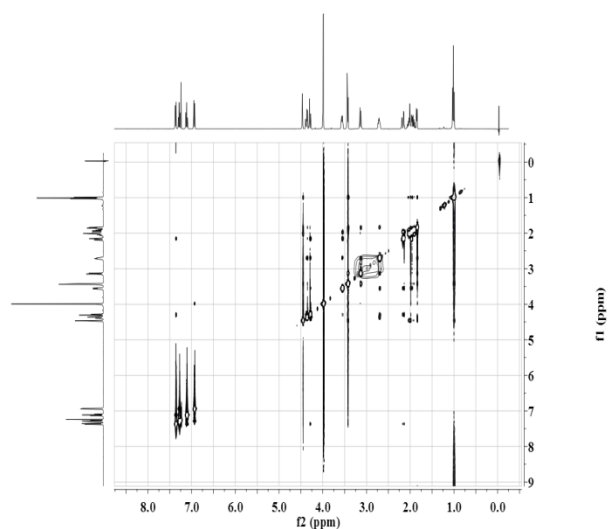
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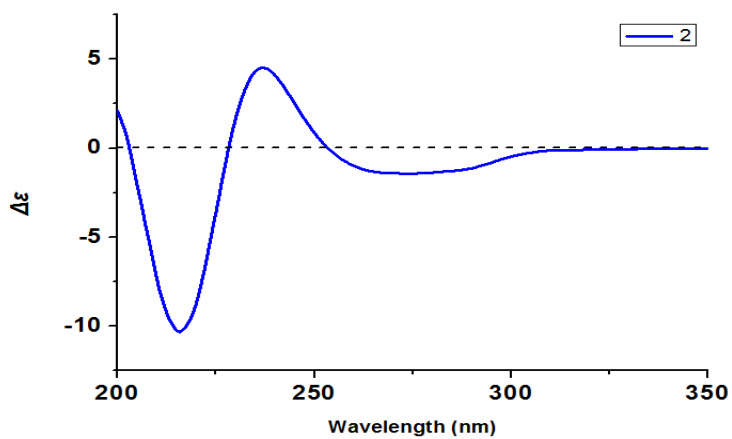
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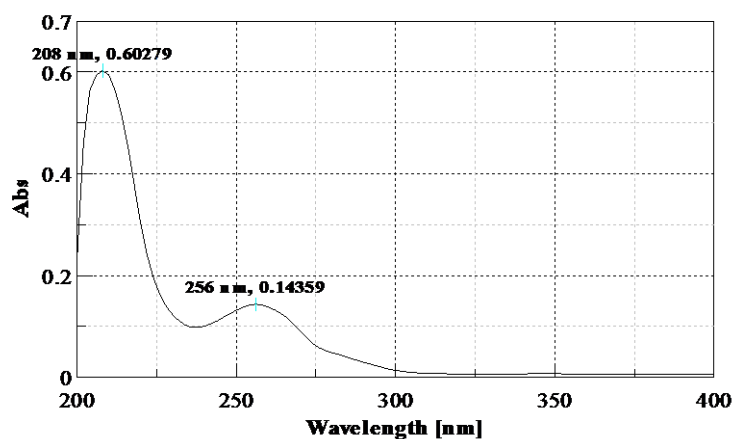
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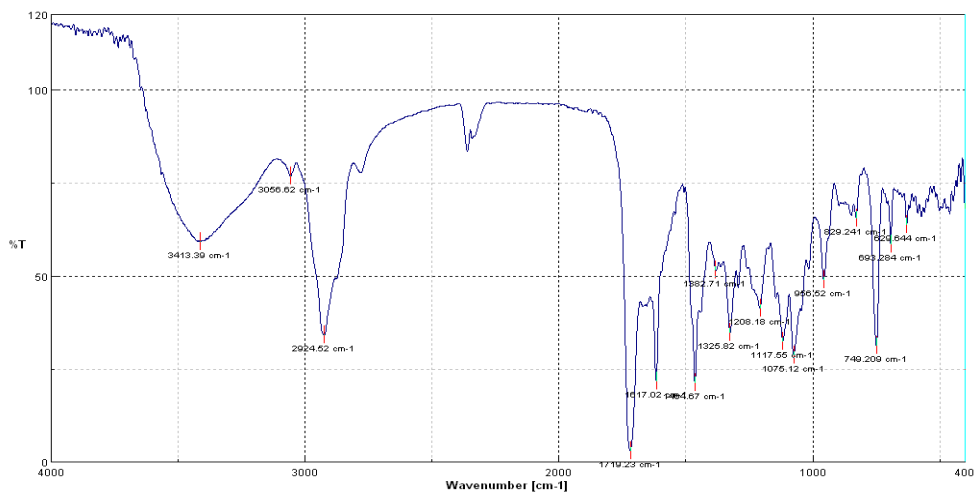
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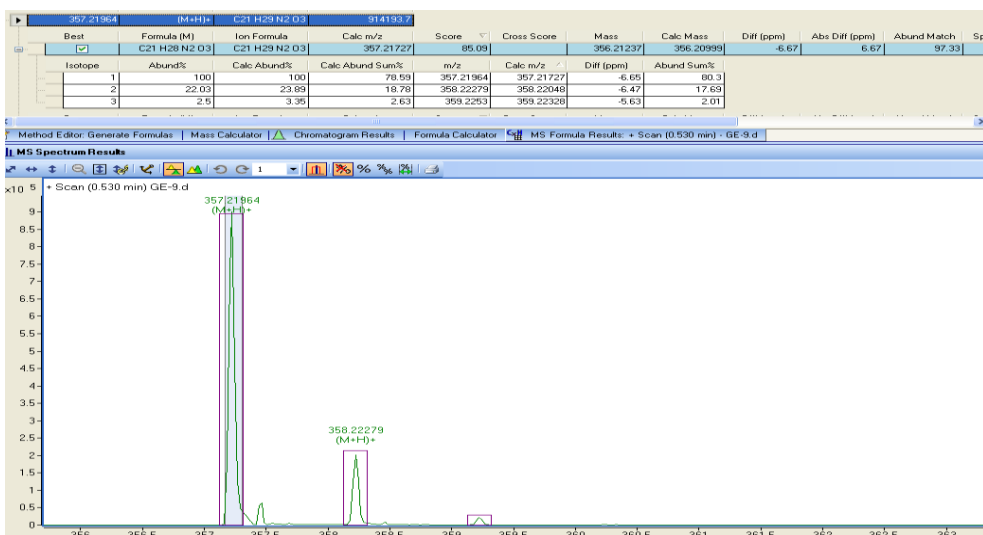
CD spectrum of **2** ( $\text{CH}_3\text{CN}$ )



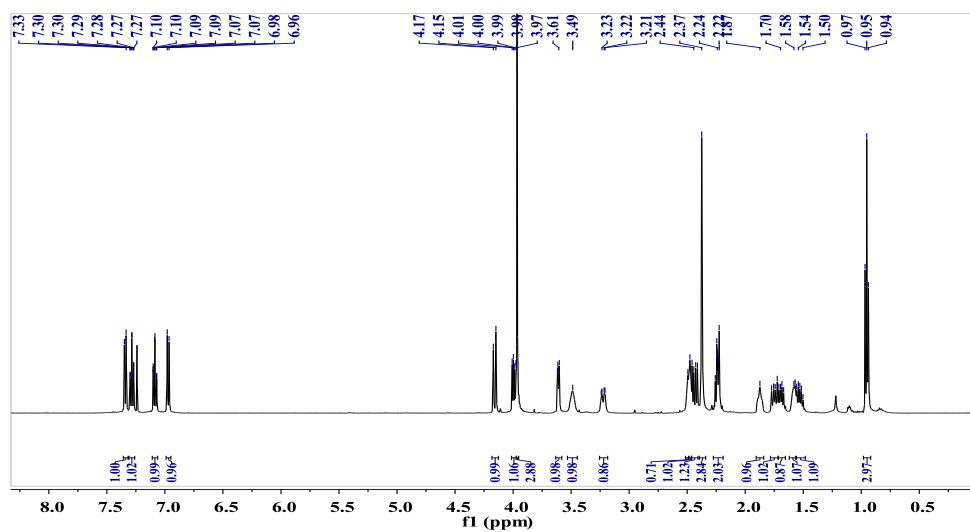
UV spectrum of **3** ( $\text{CH}_3\text{OH}$ )



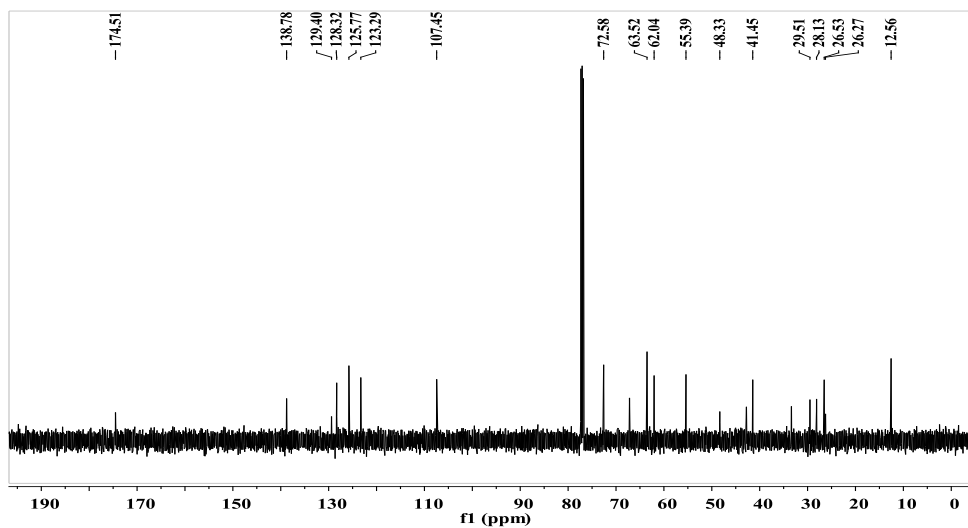
IR spectrum of **3** (KBr disc)



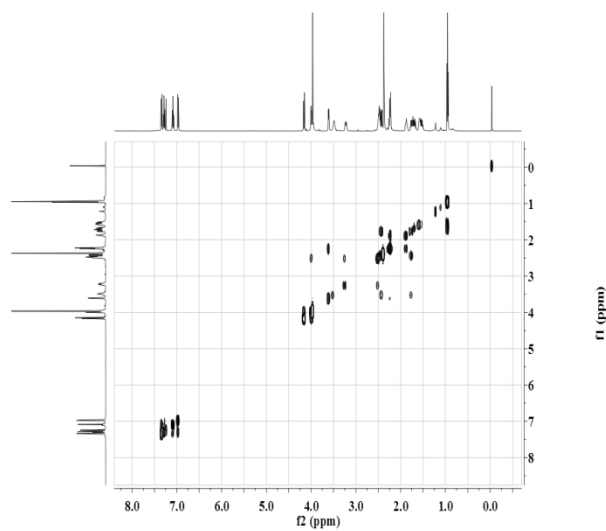
HR-ESI-MS spectrum of **3**



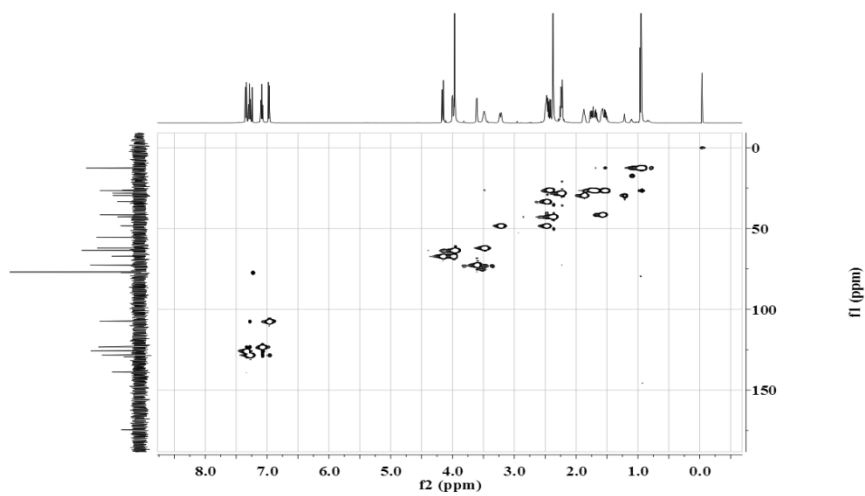
<sup>1</sup>H NMR spectrum of **3** in CDCl<sub>3</sub>



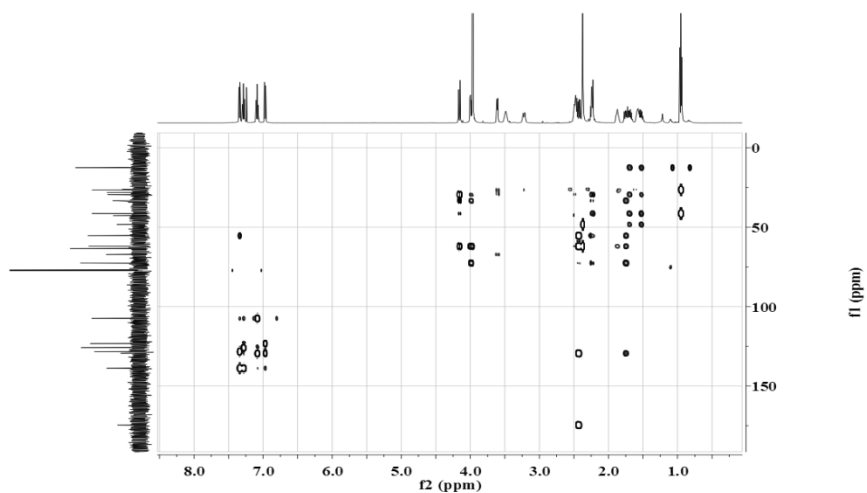
$^{13}\text{C}$  NMR spectrum of **3** in  $\text{CDCl}_3$



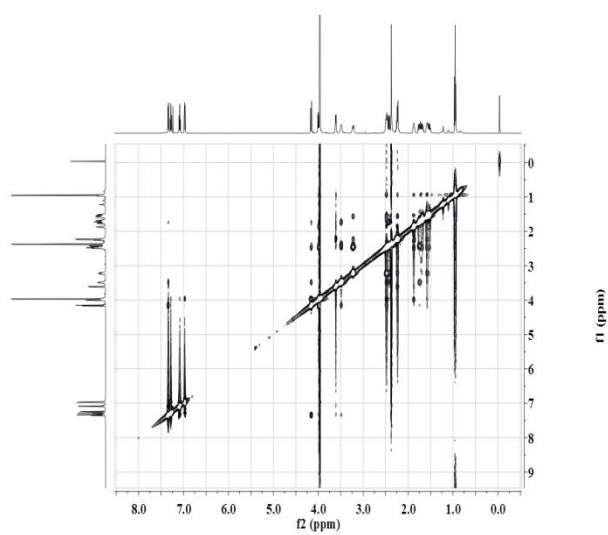
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3** in  $\text{CDCl}_3$



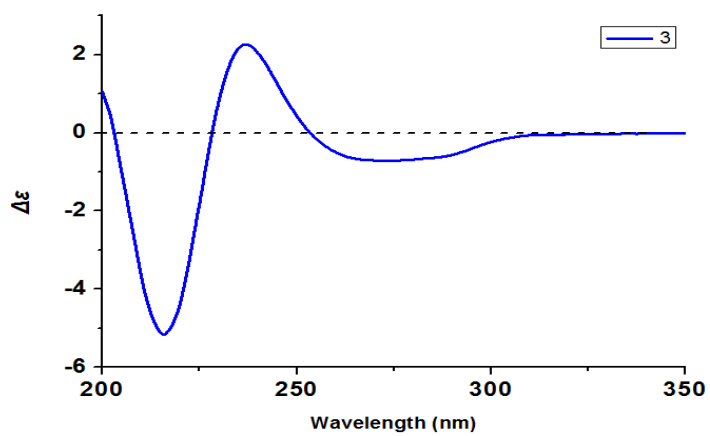
HSQC spectrum of **3** in  $\text{CDCl}_3$



HMBC spectrum of **3** in  $\text{CDCl}_3$

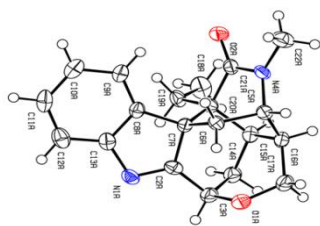


NOESY spectrum of **3** in  $\text{CDCl}_3$



CD spectrum of **3** ( $\text{CH}_3\text{CN}$ )

## Single crystal X-ray data and structure of **1**



**1**

**Table 1.** Crystal data and structure refinement for **1**.

Identification code	1	
Empirical formula	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>	
Formula weight	322.40	
Temperature	293(2) K	
Wavelength	1.54184 Å	
Crystal system, space group	?, ?	
Unit cell dimensions	a = 7.5745(3) Å	alpha = 74.991(3) deg.
	b = 8.1556(3) Å	beta = 84.522(3) deg.
	c = 14.9064(5) Å	gamma = 71.324(3) deg.
Volume	842.51(5) Å <sup>3</sup>	
Z, Calculated density	2, 1.271 Mg/m <sup>3</sup>	
Absorption coefficient	0.657 mm <sup>-1</sup>	
F(000)	344	
Crystal size	? x ? x ? mm	
Theta range for data collection	5.90 to 62.97 deg.	
Limiting indices	-8 ≤ h ≤ 8, -9 ≤ k ≤ 9, -17 ≤ l ≤ 17	
Reflections collected / unique	5068 / 5068 [R(int) = 0.0000]	
Completeness to theta = 62.97	98.7 %	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	5068 / 3 / 434	
Goodness-of-fit on F <sup>2</sup>	1.044	
Final R indices [I > 2σ(I)]	R1 = 0.0368, wR2 = 0.0840	
R indices (all data)	R1 = 0.0392, wR2 = 0.0862	
Absolute structure parameter	0.0(2)	
Extinction coefficient	0.0054(4)	
Largest diff. peak and hole	0.507 and -0.150 e.Å <sup>-3</sup>	

**Table 2.** Atomic coordinates ( × 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> × 10<sup>3</sup>) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U<sub>ij</sub> tensor.

	x	y	z	U(eq)
O(2A)	-1787(2)	-6539(2)	-2224(1)	35(1)

N(4B)	1526(3)	-9771(3)	-5064(1)	25(1)
O(2B)	-587(2)	-11214(2)	-4407(1)	34(1)
O(1B)	-411(2)	-3878(2)	-6043(1)	29(1)
N(4A)	287(3)	-5388(3)	-1804(1)	25(1)
C(21A)	-1256(3)	-5886(3)	-1680(2)	26(1)
C(13B)	-4368(3)	-6119(3)	-6937(2)	24(1)
C(14B)	-2158(3)	-4860(3)	-4649(2)	25(1)
C(3B)	-2218(3)	-3992(3)	-5677(2)	26(1)
C(15A)	-901(3)	-6331(3)	33(2)	27(1)
N(1A)	-5338(3)	-2029(3)	73(1)	29(1)
C(6A)	-1325(3)	-2732(3)	-1283(2)	24(1)
N(1B)	-4251(3)	-4583(2)	-6671(1)	26(1)
O(1A)	-843(2)	-3314(2)	730(1)	35(1)
C(2B)	-2792(3)	-5128(3)	-6169(2)	22(1)
C(20B)	-1629(3)	-7957(3)	-4934(2)	21(1)
C(7B)	-1722(3)	-7108(3)	-6022(2)	22(1)
C(5A)	464(3)	-4315(3)	-1185(2)	25(1)
C(7A)	-2978(3)	-3452(3)	-898(2)	22(1)
C(19B)	-3530(3)	-8059(3)	-4535(2)	24(1)
C(5B)	1649(3)	-8024(3)	-5604(2)	26(1)
C(6B)	317(3)	-7422(3)	-6412(2)	25(1)
C(2A)	-3637(3)	-3066(3)	40(2)	25(1)
C(16A)	726(3)	-5503(3)	-203(2)	27(1)
C(21B)	-191(3)	-9831(3)	-4771(2)	24(1)
C(8A)	-4757(3)	-2422(3)	-1438(2)	25(1)
C(16B)	1102(3)	-6765(3)	-4950(2)	26(1)
C(12A)	-7806(4)	-473(3)	-1138(2)	37(1)
C(19A)	-3970(3)	-6284(3)	-612(2)	29(1)
C(22B)	3062(4)	-11367(3)	-5100(2)	39(1)
C(13A)	-6051(4)	-1578(3)	-851(2)	28(1)
C(18B)	-3715(4)	-8418(4)	-3474(2)	34(1)
C(10B)	-4091(4)	-9315(3)	-7313(2)	30(1)
C(3A)	-2443(4)	-3968(3)	874(2)	30(1)
C(9B)	-2759(4)	-9257(3)	-6744(2)	28(1)
C(10A)	-6986(4)	-1121(3)	-2643(2)	37(1)
C(8B)	-2910(3)	-7648(3)	-6560(2)	24(1)
C(9A)	-5220(4)	-2188(3)	-2342(2)	30(1)
C(15B)	-824(3)	-6794(3)	-4500(2)	23(1)
C(14A)	-1851(4)	-5968(3)	948(2)	31(1)
C(12B)	-5671(3)	-6173(3)	-7508(2)	30(1)
C(18A)	-3456(4)	-8321(4)	-303(2)	44(1)
C(17A)	895(4)	-4541(4)	523(2)	32(1)
C(22A)	1409(4)	-5403(4)	-2656(2)	41(1)
C(17B)	1111(4)	-4864(3)	-5420(2)	28(1)
C(20A)	-2311(3)	-5539(3)	-783(2)	22(1)
C(11B)	-5512(4)	-7797(4)	-7690(2)	32(1)
C(11A)	-8267(4)	-258(3)	-2046(2)	37(1)

**Table 3.** Bond lengths [Å] and angles [deg] for **1**.

O(2A)-C(21A)	1.235(3)
N(4B)-C(21B)	1.343(3)
N(4B)-C(22B)	1.451(3)
N(4B)-C(5B)	1.471(3)
O(2B)-C(21B)	1.235(3)
O(1B)-C(17B)	1.436(3)
O(1B)-C(3B)	1.446(3)

N(4A)-C(21A)	1.337(3)
N(4A)-C(22A)	1.460(3)
N(4A)-C(5A)	1.468(3)
C(21A)-C(20A)	1.535(3)
C(13B)-C(12B)	1.381(3)
C(13B)-C(8B)	1.402(3)
C(13B)-N(1B)	1.438(3)
C(14B)-C(3B)	1.511(3)
C(14B)-C(15B)	1.549(3)
C(14B)-H(14C)	0.9700
C(14B)-H(14D)	0.9700
C(3B)-C(2B)	1.501(3)
C(3B)-H(3B)	0.9800
C(15A)-C(14A)	1.533(3)
C(15A)-C(16A)	1.557(4)
C(15A)-C(20A)	1.561(3)
C(15A)-H(15A)	0.9800
N(1A)-C(2A)	1.300(3)
N(1A)-C(13A)	1.441(3)
C(6A)-C(5A)	1.531(3)
C(6A)-C(7A)	1.550(3)
C(6A)-H(6AA)	0.9700
C(6A)-H(6AB)	0.9700
N(1B)-C(2B)	1.285(3)
O(1A)-C(17A)	1.438(3)
O(1A)-C(3A)	1.450(3)
C(2B)-C(7B)	1.525(3)
C(20B)-C(19B)	1.524(3)
C(20B)-C(21B)	1.541(3)
C(20B)-C(15B)	1.567(3)
C(20B)-C(7B)	1.588(3)
C(7B)-C(8B)	1.490(3)
C(7B)-C(6B)	1.563(3)
C(5A)-C(16A)	1.522(3)
C(5A)-H(5A)	0.9800
C(7A)-C(2A)	1.516(3)
C(7A)-C(8A)	1.517(3)
C(7A)-C(20A)	1.579(3)
C(19B)-C(18B)	1.534(3)
C(19B)-H(19C)	0.9700
C(19B)-H(19D)	0.9700
C(5B)-C(6B)	1.522(3)
C(5B)-C(16B)	1.532(3)
C(5B)-H(5B)	0.9800
C(6B)-H(6BA)	0.9700
C(6B)-H(6BB)	0.9700
C(2A)-C(3A)	1.490(3)
C(16A)-C(17A)	1.528(3)
C(16A)-H(16A)	0.9800
C(8A)-C(9A)	1.375(3)
C(8A)-C(13A)	1.384(3)
C(16B)-C(17B)	1.529(3)
C(16B)-C(15B)	1.551(3)
C(16B)-H(16B)	0.9800
C(12A)-C(13A)	1.380(4)
C(12A)-C(11A)	1.383(4)
C(12A)-H(12A)	0.9300
C(19A)-C(18A)	1.532(3)
C(19A)-C(20A)	1.537(3)
C(19A)-H(19A)	0.9700

C(19A)-H(19B)	0.9700
C(22B)-H(22D)	0.9600
C(22B)-H(22E)	0.9600
C(22B)-H(22F)	0.9600
C(18B)-H(18D)	0.9600
C(18B)-H(18E)	0.9600
C(18B)-H(18F)	0.9600
C(10B)-C(11B)	1.382(4)
C(10B)-C(9B)	1.398(3)
C(10B)-H(10B)	0.9300
C(3A)-C(14A)	1.524(4)
C(3A)-H(3A)	0.9800
C(9B)-C(8B)	1.377(3)
C(9B)-H(9B)	0.9300
C(10A)-C(9A)	1.384(3)
C(10A)-C(11A)	1.397(4)
C(10A)-H(10A)	0.9300
C(9A)-H(9A)	0.9300
C(15B)-H(15B)	0.9800
C(14A)-H(14A)	0.9700
C(14A)-H(14B)	0.9700
C(12B)-C(11B)	1.386(4)
C(12B)-H(12B)	0.9300
C(18A)-H(18A)	0.9600
C(18A)-H(18B)	0.9600
C(18A)-H(18C)	0.9600
C(17A)-H(17A)	0.9700
C(17A)-H(17B)	0.9700
C(22A)-H(22A)	0.9600
C(22A)-H(22B)	0.9600
C(22A)-H(22C)	0.9600
C(17B)-H(17C)	0.9700
C(17B)-H(17D)	0.9700
C(11B)-H(11B)	0.9300
C(11A)-H(11A)	0.9300
C(21B)-N(4B)-C(22B)	122.3(2)
C(21B)-N(4B)-C(5B)	115.83(19)
C(22B)-N(4B)-C(5B)	119.4(2)
C(17B)-O(1B)-C(3B)	114.97(18)
C(21A)-N(4A)-C(22A)	122.2(2)
C(21A)-N(4A)-C(5A)	115.43(19)
C(22A)-N(4A)-C(5A)	119.8(2)
O(2A)-C(21A)-N(4A)	124.3(2)
O(2A)-C(21A)-C(20A)	123.5(2)
N(4A)-C(21A)-C(20A)	112.14(19)
C(12B)-C(13B)-C(8B)	121.4(2)
C(12B)-C(13B)-N(1B)	127.2(2)
C(8B)-C(13B)-N(1B)	111.3(2)
C(3B)-C(14B)-C(15B)	108.27(18)
C(3B)-C(14B)-H(14C)	110.0
C(15B)-C(14B)-H(14C)	110.0
C(3B)-C(14B)-H(14D)	110.0
C(15B)-C(14B)-H(14D)	110.0
H(14C)-C(14B)-H(14D)	108.4
O(1B)-C(3B)-C(2B)	107.71(18)
O(1B)-C(3B)-C(14B)	111.81(19)
C(2B)-C(3B)-C(14B)	108.04(19)
O(1B)-C(3B)-H(3B)	109.7
C(2B)-C(3B)-H(3B)	109.7
C(14B)-C(3B)-H(3B)	109.7

C(14A)-C(15A)-C(16A)	109.9(2)
C(14A)-C(15A)-C(20A)	111.3(2)
C(16A)-C(15A)-C(20A)	109.37(19)
C(14A)-C(15A)-H(15A)	108.8
C(16A)-C(15A)-H(15A)	108.8
C(20A)-C(15A)-H(15A)	108.8
C(2A)-N(1A)-C(13A)	105.82(19)
C(5A)-C(6A)-C(7A)	108.39(18)
C(5A)-C(6A)-H(6AA)	110.0
C(7A)-C(6A)-H(6AA)	110.0
C(5A)-C(6A)-H(6AB)	110.0
C(7A)-C(6A)-H(6AB)	110.0
H(6AA)-C(6A)-H(6AB)	108.4
C(2B)-N(1B)-C(13B)	106.15(18)
C(17A)-O(1A)-C(3A)	116.03(19)
N(1B)-C(2B)-C(3B)	124.3(2)
N(1B)-C(2B)-C(7B)	115.2(2)
C(3B)-C(2B)-C(7B)	120.3(2)
C(19B)-C(20B)-C(21B)	110.81(19)
C(19B)-C(20B)-C(15B)	113.42(19)
C(21B)-C(20B)-C(15B)	107.11(18)
C(19B)-C(20B)-C(7B)	111.24(18)
C(21B)-C(20B)-C(7B)	107.56(17)
C(15B)-C(20B)-C(7B)	106.41(17)
C(8B)-C(7B)-C(2B)	99.80(18)
C(8B)-C(7B)-C(6B)	112.82(18)
C(2B)-C(7B)-C(6B)	111.9(2)
C(8B)-C(7B)-C(20B)	116.48(19)
C(2B)-C(7B)-C(20B)	107.42(17)
C(6B)-C(7B)-C(20B)	108.13(18)
N(4A)-C(5A)-C(16A)	107.67(19)
N(4A)-C(5A)-C(6A)	106.66(18)
C(16A)-C(5A)-C(6A)	112.7(2)
N(4A)-C(5A)-H(5A)	109.9
C(16A)-C(5A)-H(5A)	109.9
C(6A)-C(5A)-H(5A)	109.9
C(2A)-C(7A)-C(8A)	99.01(18)
C(2A)-C(7A)-C(6A)	111.19(19)
C(8A)-C(7A)-C(6A)	113.01(19)
C(2A)-C(7A)-C(20A)	108.71(18)
C(8A)-C(7A)-C(20A)	115.92(18)
C(6A)-C(7A)-C(20A)	108.62(18)
C(20B)-C(19B)-C(18B)	115.3(2)
C(20B)-C(19B)-H(19C)	108.4
C(18B)-C(19B)-H(19C)	108.4
C(20B)-C(19B)-H(19D)	108.4
C(18B)-C(19B)-H(19D)	108.4
H(19C)-C(19B)-H(19D)	107.5
N(4B)-C(5B)-C(6B)	106.86(19)
N(4B)-C(5B)-C(16B)	107.24(19)
C(6B)-C(5B)-C(16B)	112.47(19)
N(4B)-C(5B)-H(5B)	110.1
C(6B)-C(5B)-H(5B)	110.1
C(16B)-C(5B)-H(5B)	110.1
C(5B)-C(6B)-C(7B)	109.01(19)
C(5B)-C(6B)-H(6BA)	109.9
C(7B)-C(6B)-H(6BA)	109.9
C(5B)-C(6B)-H(6BB)	109.9
C(7B)-C(6B)-H(6BB)	109.9
H(6BA)-C(6B)-H(6BB)	108.3

N(1A)-C(2A)-C(3A)	123.3(2)
N(1A)-C(2A)-C(7A)	115.5(2)
C(3A)-C(2A)-C(7A)	120.9(2)
C(5A)-C(16A)-C(17A)	113.4(2)
C(5A)-C(16A)-C(15A)	108.58(19)
C(17A)-C(16A)-C(15A)	111.8(2)
C(5A)-C(16A)-H(16A)	107.6
C(17A)-C(16A)-H(16A)	107.6
C(15A)-C(16A)-H(16A)	107.6
O(2B)-C(21B)-N(4B)	124.6(2)
O(2B)-C(21B)-C(20B)	123.3(2)
N(4B)-C(21B)-C(20B)	112.1(2)
C(9A)-C(8A)-C(13A)	119.6(2)
C(9A)-C(8A)-C(7A)	132.4(2)
C(13A)-C(8A)-C(7A)	107.9(2)
C(17B)-C(16B)-C(5B)	113.6(2)
C(17B)-C(16B)-C(15B)	111.50(19)
C(5B)-C(16B)-C(15B)	108.85(19)
C(17B)-C(16B)-H(16B)	107.6
C(5B)-C(16B)-H(16B)	107.6
C(15B)-C(16B)-H(16B)	107.6
C(13A)-C(12A)-C(11A)	117.3(2)
C(13A)-C(12A)-H(12A)	121.3
C(11A)-C(12A)-H(12A)	121.3
C(18A)-C(19A)-C(20A)	115.2(2)
C(18A)-C(19A)-H(19A)	108.5
C(20A)-C(19A)-H(19A)	108.5
C(18A)-C(19A)-H(19B)	108.5
C(20A)-C(19A)-H(19B)	108.5
H(19A)-C(19A)-H(19B)	107.5
N(4B)-C(22B)-H(22D)	109.5
N(4B)-C(22B)-H(22E)	109.5
H(22D)-C(22B)-H(22E)	109.5
N(4B)-C(22B)-H(22F)	109.5
H(22D)-C(22B)-H(22F)	109.5
H(22E)-C(22B)-H(22F)	109.5
C(12A)-C(13A)-C(8A)	122.6(2)
C(12A)-C(13A)-N(1A)	125.7(2)
C(8A)-C(13A)-N(1A)	111.6(2)
C(19B)-C(18B)-H(18D)	109.5
C(19B)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(19B)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5
C(11B)-C(10B)-C(9B)	121.1(2)
C(11B)-C(10B)-H(10B)	119.5
C(9B)-C(10B)-H(10B)	119.5
O(1A)-C(3A)-C(2A)	107.3(2)
O(1A)-C(3A)-C(14A)	111.1(2)
C(2A)-C(3A)-C(14A)	107.4(2)
O(1A)-C(3A)-H(3A)	110.3
C(2A)-C(3A)-H(3A)	110.3
C(14A)-C(3A)-H(3A)	110.3
C(8B)-C(9B)-C(10B)	118.2(2)
C(8B)-C(9B)-H(9B)	120.9
C(10B)-C(9B)-H(9B)	120.9
C(9A)-C(10A)-C(11A)	120.6(2)
C(9A)-C(10A)-H(10A)	119.7
C(11A)-C(10A)-H(10A)	119.7

C(9B)-C(8B)-C(13B)	120.3(2)
C(9B)-C(8B)-C(7B)	132.1(2)
C(13B)-C(8B)-C(7B)	107.55(19)
C(8A)-C(9A)-C(10A)	119.0(2)
C(8A)-C(9A)-H(9A)	120.5
C(10A)-C(9A)-H(9A)	120.5
C(14B)-C(15B)-C(16B)	109.44(19)
C(14B)-C(15B)-C(20B)	111.05(19)
C(16B)-C(15B)-C(20B)	109.62(18)
C(14B)-C(15B)-H(15B)	108.9
C(16B)-C(15B)-H(15B)	108.9
C(20B)-C(15B)-H(15B)	108.9
C(3A)-C(14A)-C(15A)	108.8(2)
C(3A)-C(14A)-H(14A)	109.9
C(15A)-C(14A)-H(14A)	109.9
C(3A)-C(14A)-H(14B)	109.9
C(15A)-C(14A)-H(14B)	109.9
H(14A)-C(14A)-H(14B)	108.3
C(13B)-C(12B)-C(11B)	118.0(2)
C(13B)-C(12B)-H(12B)	121.0
C(11B)-C(12B)-H(12B)	121.0
C(19A)-C(18A)-H(18A)	109.5
C(19A)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(19A)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5
H(18B)-C(18A)-H(18C)	109.5
O(1A)-C(17A)-C(16A)	113.4(2)
O(1A)-C(17A)-H(17A)	108.9
C(16A)-C(17A)-H(17A)	108.9
O(1A)-C(17A)-H(17B)	108.9
C(16A)-C(17A)-H(17B)	108.9
H(17A)-C(17A)-H(17B)	107.7
N(4A)-C(22A)-H(22A)	109.5
N(4A)-C(22A)-H(22B)	109.5
H(22A)-C(22A)-H(22B)	109.5
N(4A)-C(22A)-H(22C)	109.5
H(22A)-C(22A)-H(22C)	109.5
H(22B)-C(22A)-H(22C)	109.5
O(1B)-C(17B)-C(16B)	113.5(2)
O(1B)-C(17B)-H(17C)	108.9
C(16B)-C(17B)-H(17C)	108.9
O(1B)-C(17B)-H(17D)	108.9
C(16B)-C(17B)-H(17D)	108.9
H(17C)-C(17B)-H(17D)	107.7
C(21A)-C(20A)-C(19A)	110.93(19)
C(21A)-C(20A)-C(15A)	108.54(18)
C(19A)-C(20A)-C(15A)	113.12(19)
C(21A)-C(20A)-C(7A)	106.79(18)
C(19A)-C(20A)-C(7A)	111.32(19)
C(15A)-C(20A)-C(7A)	105.82(17)
C(10B)-C(11B)-C(12B)	120.9(2)
C(10B)-C(11B)-H(11B)	119.5
C(12B)-C(11B)-H(11B)	119.5
C(12A)-C(11A)-C(10A)	120.7(2)
C(12A)-C(11A)-H(11A)	119.6
C(10A)-C(11A)-H(11A)	119.6

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Symmetry transformations used to generate equivalent atoms:

**Table 4.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **1**. The anisotropic displacement factor exponent takes the form:  $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	U11	U22	U33	U23	U13	U12
O(2A)	33(1)	38(1)	40(1)	-23(1)	-1(1)	-10(1)
N(4B)	20(1)	23(1)	31(1)	-8(1)	-3(1)	-4(1)
O(2B)	35(1)	21(1)	45(1)	-5(1)	0(1)	-9(1)
O(1B)	28(1)	32(1)	32(1)	-10(1)	2(1)	-15(1)
N(4A)	22(1)	28(1)	26(1)	-12(1)	6(1)	-6(1)
C(21A)	21(1)	24(1)	31(1)	-9(1)	-1(1)	-4(1)
C(13B)	25(1)	27(1)	22(1)	-7(1)	4(1)	-12(1)
C(14B)	25(1)	23(1)	31(1)	-13(1)	3(1)	-7(1)
C(3B)	23(1)	23(1)	33(1)	-11(1)	4(1)	-7(1)
C(15A)	23(1)	28(1)	27(1)	-3(1)	-1(1)	-7(1)
N(1A)	28(1)	24(1)	36(1)	-15(1)	3(1)	-6(1)
C(6A)	25(1)	19(1)	26(1)	-6(1)	1(1)	-5(1)
N(1B)	27(1)	22(1)	28(1)	-5(1)	0(1)	-4(1)
O(1A)	33(1)	40(1)	38(1)	-19(1)	-3(1)	-13(1)
C(2B)	23(1)	24(1)	21(1)	-5(1)	4(1)	-10(1)
C(20B)	19(1)	22(1)	24(1)	-6(1)	-1(1)	-7(1)
C(7B)	21(1)	20(1)	25(1)	-5(1)	-1(1)	-7(1)
C(5A)	23(1)	25(1)	31(1)	-11(1)	1(1)	-9(1)
C(7A)	22(1)	20(1)	25(1)	-6(1)	-3(1)	-6(1)
C(19B)	21(1)	25(1)	27(1)	-4(1)	1(1)	-10(1)
C(5B)	22(1)	31(1)	28(1)	-11(1)	1(1)	-11(1)
C(6B)	21(1)	28(1)	28(1)	-11(1)	2(1)	-7(1)
C(2A)	29(1)	24(1)	29(1)	-11(1)	5(1)	-13(1)
C(16A)	21(1)	28(1)	30(1)	-7(1)	-4(1)	-5(1)
C(21B)	27(1)	22(1)	26(1)	-10(1)	-4(1)	-6(1)
C(8A)	23(1)	20(1)	32(1)	-4(1)	-4(1)	-6(1)
C(16B)	25(1)	26(1)	28(1)	-10(1)	-1(1)	-7(1)
C(12A)	30(2)	25(1)	54(2)	-10(1)	4(1)	-7(1)
C(19A)	20(1)	30(1)	40(1)	-14(1)	5(1)	-9(1)
C(22B)	33(2)	32(1)	53(2)	-22(1)	-1(1)	-3(1)
C(13A)	25(1)	20(1)	40(2)	-8(1)	-1(1)	-8(1)
C(18B)	32(2)	40(2)	32(1)	-10(1)	5(1)	-15(1)
C(10B)	35(2)	31(1)	31(1)	-11(1)	-2(1)	-16(1)
C(3A)	27(1)	41(2)	24(1)	-9(1)	1(1)	-12(1)
C(9B)	27(1)	29(1)	30(1)	-8(1)	0(1)	-11(1)
C(10A)	37(2)	35(1)	39(2)	-1(1)	-12(1)	-15(1)
C(8B)	23(1)	28(1)	19(1)	-4(1)	1(1)	-8(1)
C(9A)	24(1)	31(1)	35(1)	-5(1)	-5(1)	-8(1)
C(15B)	26(1)	23(1)	22(1)	-7(1)	-1(1)	-7(1)
C(14A)	27(1)	38(1)	29(1)	-8(1)	0(1)	-11(1)
C(12B)	21(1)	39(1)	29(1)	-9(1)	-2(1)	-7(1)
C(18A)	37(2)	33(2)	68(2)	-16(1)	3(2)	-18(1)
C(17A)	26(1)	41(2)	32(1)	-10(1)	-2(1)	-12(1)
C(22A)	42(2)	49(2)	36(2)	-19(1)	11(1)	-18(1)
C(17B)	26(1)	26(1)	37(1)	-13(1)	0(1)	-9(1)
C(20A)	21(1)	18(1)	27(1)	-7(1)	-2(1)	-5(1)
C(11B)	28(1)	45(2)	28(1)	-14(1)	-1(1)	-13(1)
C(11A)	24(2)	25(1)	57(2)	-2(1)	-8(1)	-7(1)

**Table 5.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **1**.

	x	y	z	U(eq)
H(14C)	-3396	-4870	-4417	31
H(14D)	-1714	-4197	-4315	31
H(3B)	-3127	-2796	-5794	31
H(15A)	-390	-7623	106	32
H(6AA)	-1524	-2102	-1931	28
H(6AB)	-1224	-1908	-938	28
H(5A)	1544	-3885	-1374	30
H(19C)	-3807	-8996	-4730	29
H(19D)	-4463	-6943	-4802	29
H(5B)	2925	-8134	-5839	31
H(6BA)	616	-8327	-6763	30
H(6BB)	439	-6327	-6823	30
H(16A)	1887	-6483	-200	32
H(16B)	2017	-7241	-4451	31
H(12A)	-8646	103	-737	44
H(19A)	-4779	-5783	-141	35
H(19B)	-4677	-5881	-1180	35
H(22D)	2770	-12392	-4717	58
H(22E)	4170	-11282	-4878	58
H(22F)	3263	-11482	-5730	58
H(18D)	-4950	-8465	-3287	51
H(18E)	-3489	-7478	-3272	51
H(18F)	-2822	-9536	-3199	51
H(10B)	-4019	-10393	-7440	36
H(3A)	-3140	-3694	1434	36
H(9B)	-1796	-10279	-6496	34
H(10A)	-7324	-977	-3249	44
H(9A)	-4359	-2738	-2745	36
H(15B)	-665	-7324	-3832	28
H(14A)	-2934	-6388	1067	37
H(14B)	-996	-6599	1458	37
H(12B)	-6626	-5150	-7762	36
H(18A)	-4571	-8666	-221	66
H(18B)	-2802	-8736	274	66
H(18C)	-2673	-8836	-768	66
H(17A)	1376	-5422	1090	39
H(17B)	1787	-3894	300	39
H(22A)	1133	-6166	-2980	61
H(22B)	2708	-5840	-2504	61
H(22C)	1125	-4214	-3044	61
H(17C)	1059	-4231	-4944	34
H(17D)	2274	-4915	-5763	34
H(11B)	-6375	-7865	-8072	39
H(11A)	-9442	469	-2261	44

**Table 6.** Torsion angles [deg] for **1**.

C(22A)-N(4A)-C(21A)-O(2A)	6.5(4)
C(5A)-N(4A)-C(21A)-O(2A)	167.9(2)
C(22A)-N(4A)-C(21A)-C(20A)	-173.1(2)
C(5A)-N(4A)-C(21A)-C(20A)	-11.6(3)
C(17B)-O(1B)-C(3B)-C(2B)	-108.2(2)
C(17B)-O(1B)-C(3B)-C(14B)	10.4(3)
C(15B)-C(14B)-C(3B)-O(1B)	-62.2(2)
C(15B)-C(14B)-C(3B)-C(2B)	56.1(2)

C(12B)-C(13B)-N(1B)-C(2B)	-177.4(2)
C(8B)-C(13B)-N(1B)-C(2B)	0.7(3)
C(13B)-N(1B)-C(2B)-C(3B)	-174.8(2)
C(13B)-N(1B)-C(2B)-C(7B)	-0.2(3)
O(1B)-C(3B)-C(2B)-N(1B)	-118.8(2)
C(14B)-C(3B)-C(2B)-N(1B)	120.3(2)
O(1B)-C(3B)-C(2B)-C(7B)	66.8(3)
C(14B)-C(3B)-C(2B)-C(7B)	-54.1(3)
N(1B)-C(2B)-C(7B)-C(8B)	-0.4(3)
C(3B)-C(2B)-C(7B)-C(8B)	174.5(2)
N(1B)-C(2B)-C(7B)-C(6B)	119.2(2)
C(3B)-C(2B)-C(7B)-C(6B)	-65.9(3)
N(1B)-C(2B)-C(7B)-C(20B)	-122.3(2)
C(3B)-C(2B)-C(7B)-C(20B)	52.6(3)
C(19B)-C(20B)-C(7B)-C(8B)	-39.7(3)
C(21B)-C(20B)-C(7B)-C(8B)	81.8(2)
C(15B)-C(20B)-C(7B)-C(8B)	-163.67(19)
C(19B)-C(20B)-C(7B)-C(2B)	71.1(2)
C(21B)-C(20B)-C(7B)-C(2B)	-167.4(2)
C(15B)-C(20B)-C(7B)-C(2B)	-52.8(2)
C(19B)-C(20B)-C(7B)-C(6B)	-167.94(18)
C(21B)-C(20B)-C(7B)-C(6B)	-46.4(2)
C(15B)-C(20B)-C(7B)-C(6B)	68.1(2)
C(21A)-N(4A)-C(5A)-C(16A)	67.4(3)
C(22A)-N(4A)-C(5A)-C(16A)	-130.7(2)
C(21A)-N(4A)-C(5A)-C(6A)	-53.8(3)
C(22A)-N(4A)-C(5A)-C(6A)	108.1(2)
C(7A)-C(6A)-C(5A)-N(4A)	65.8(2)
C(7A)-C(6A)-C(5A)-C(16A)	-52.1(3)
C(5A)-C(6A)-C(7A)-C(2A)	105.6(2)
C(5A)-C(6A)-C(7A)-C(8A)	-144.08(19)
C(5A)-C(6A)-C(7A)-C(20A)	-14.0(2)
C(21B)-C(20B)-C(19B)-C(18B)	74.8(2)
C(15B)-C(20B)-C(19B)-C(18B)	-45.7(3)
C(7B)-C(20B)-C(19B)-C(18B)	-165.57(19)
C(21B)-N(4B)-C(5B)-C(6B)	-55.0(2)
C(22B)-N(4B)-C(5B)-C(6B)	107.7(2)
C(21B)-N(4B)-C(5B)-C(16B)	65.8(2)
C(22B)-N(4B)-C(5B)-C(16B)	-131.5(2)
N(4B)-C(5B)-C(6B)-C(7B)	65.1(2)
C(16B)-C(5B)-C(6B)-C(7B)	-52.3(3)
C(8B)-C(7B)-C(6B)-C(5B)	-143.42(19)
C(2B)-C(7B)-C(6B)-C(5B)	105.0(2)
C(20B)-C(7B)-C(6B)-C(5B)	-13.1(2)
C(13A)-N(1A)-C(2A)-C(3A)	-174.5(2)
C(13A)-N(1A)-C(2A)-C(7A)	0.0(3)
C(8A)-C(7A)-C(2A)-N(1A)	-1.9(3)
C(6A)-C(7A)-C(2A)-N(1A)	117.2(2)
C(20A)-C(7A)-C(2A)-N(1A)	-123.3(2)
C(8A)-C(7A)-C(2A)-C(3A)	172.8(2)
C(6A)-C(7A)-C(2A)-C(3A)	-68.1(3)
C(20A)-C(7A)-C(2A)-C(3A)	51.4(3)
N(4A)-C(5A)-C(16A)-C(17A)	-178.95(19)
C(6A)-C(5A)-C(16A)-C(17A)	-61.6(3)
N(4A)-C(5A)-C(16A)-C(15A)	-54.1(2)
C(6A)-C(5A)-C(16A)-C(15A)	63.3(3)
C(14A)-C(15A)-C(16A)-C(5A)	-126.9(2)
C(20A)-C(15A)-C(16A)-C(5A)	-4.5(3)
C(14A)-C(15A)-C(16A)-C(17A)	-1.1(3)
C(20A)-C(15A)-C(16A)-C(17A)	121.3(2)

C(22B)-N(4B)-C(21B)-O(2B)	8.9(3)
C(5B)-N(4B)-C(21B)-O(2B)	171.0(2)
C(22B)-N(4B)-C(21B)-C(20B)	-171.5(2)
C(5B)-N(4B)-C(21B)-C(20B)	-9.4(3)
C(19B)-C(20B)-C(21B)-O(2B)	3.5(3)
C(15B)-C(20B)-C(21B)-O(2B)	127.7(2)
C(7B)-C(20B)-C(21B)-O(2B)	-118.3(2)
C(19B)-C(20B)-C(21B)-N(4B)	-176.13(18)
C(15B)-C(20B)-C(21B)-N(4B)	-52.0(2)
C(7B)-C(20B)-C(21B)-N(4B)	62.1(2)
C(2A)-C(7A)-C(8A)-C(9A)	-178.7(3)
C(6A)-C(7A)-C(8A)-C(9A)	63.6(3)
C(20A)-C(7A)-C(8A)-C(9A)	-62.7(4)
C(2A)-C(7A)-C(8A)-C(13A)	3.0(2)
C(6A)-C(7A)-C(8A)-C(13A)	-114.7(2)
C(20A)-C(7A)-C(8A)-C(13A)	119.0(2)
N(4B)-C(5B)-C(16B)-C(17B)	-178.5(2)
C(6B)-C(5B)-C(16B)-C(17B)	-61.3(3)
N(4B)-C(5B)-C(16B)-C(15B)	-53.6(2)
C(6B)-C(5B)-C(16B)-C(15B)	63.6(3)
C(11A)-C(12A)-C(13A)-C(8A)	1.5(4)
C(11A)-C(12A)-C(13A)-N(1A)	-177.4(2)
C(9A)-C(8A)-C(13A)-C(12A)	-0.9(4)
C(7A)-C(8A)-C(13A)-C(12A)	177.7(2)
C(9A)-C(8A)-C(13A)-N(1A)	178.1(2)
C(7A)-C(8A)-C(13A)-N(1A)	-3.3(3)
C(2A)-N(1A)-C(13A)-C(12A)	-178.9(2)
C(2A)-N(1A)-C(13A)-C(8A)	2.1(3)
C(17A)-O(1A)-C(3A)-C(2A)	-106.7(2)
C(17A)-O(1A)-C(3A)-C(14A)	10.4(3)
N(1A)-C(2A)-C(3A)-O(1A)	-118.3(2)
C(7A)-C(2A)-C(3A)-O(1A)	67.5(3)
N(1A)-C(2A)-C(3A)-C(14A)	122.2(2)
C(7A)-C(2A)-C(3A)-C(14A)	-52.1(3)
C(11B)-C(10B)-C(9B)-C(8B)	0.7(4)
C(10B)-C(9B)-C(8B)-C(13B)	0.1(4)
C(10B)-C(9B)-C(8B)-C(7B)	-177.5(2)
C(12B)-C(13B)-C(8B)-C(9B)	-0.8(4)
N(1B)-C(13B)-C(8B)-C(9B)	-179.1(2)
C(12B)-C(13B)-C(8B)-C(7B)	177.3(2)
N(1B)-C(13B)-C(8B)-C(7B)	-0.9(3)
C(2B)-C(7B)-C(8B)-C(9B)	178.6(2)
C(6B)-C(7B)-C(8B)-C(9B)	59.7(3)
C(20B)-C(7B)-C(8B)-C(9B)	-66.3(3)
C(2B)-C(7B)-C(8B)-C(13B)	0.7(2)
C(6B)-C(7B)-C(8B)-C(13B)	-118.2(2)
C(20B)-C(7B)-C(8B)-C(13B)	115.9(2)
C(13A)-C(8A)-C(9A)-C(10A)	-0.6(4)
C(7A)-C(8A)-C(9A)-C(10A)	-178.8(2)
C(11A)-C(10A)-C(9A)-C(8A)	1.6(4)
C(3B)-C(14B)-C(15B)-C(16B)	54.8(2)
C(3B)-C(14B)-C(15B)-C(20B)	-66.4(3)
C(17B)-C(16B)-C(15B)-C(14B)	-1.1(3)
C(5B)-C(16B)-C(15B)-C(14B)	-127.2(2)
C(17B)-C(16B)-C(15B)-C(20B)	120.9(2)
C(5B)-C(16B)-C(15B)-C(20B)	-5.1(2)
C(19B)-C(20B)-C(15B)-C(14B)	-58.7(2)
C(21B)-C(20B)-C(15B)-C(14B)	178.68(19)
C(7B)-C(20B)-C(15B)-C(14B)	63.9(2)
C(19B)-C(20B)-C(15B)-C(16B)	-179.80(19)

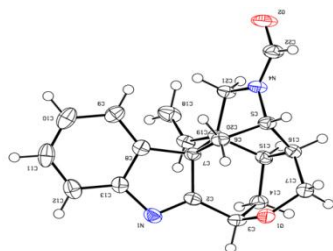
C(21B)-C(20B)-C(15B)-C(16B)	57.6(2)
C(7B)-C(20B)-C(15B)-C(16B)	-57.2(2)
O(1A)-C(3A)-C(14A)-C(15A)	-61.7(3)
C(2A)-C(3A)-C(14A)-C(15A)	55.4(3)
C(16A)-C(15A)-C(14A)-C(3A)	54.4(3)
C(20A)-C(15A)-C(14A)-C(3A)	-66.9(3)
C(8B)-C(13B)-C(12B)-C(11B)	0.8(4)
N(1B)-C(13B)-C(12B)-C(11B)	178.8(2)
C(3A)-O(1A)-C(17A)-C(16A)	45.5(3)
C(5A)-C(16A)-C(17A)-O(1A)	73.4(3)
C(15A)-C(16A)-C(17A)-O(1A)	-49.8(3)
C(3B)-O(1B)-C(17B)-C(16B)	46.8(3)
C(5B)-C(16B)-C(17B)-O(1B)	72.5(3)
C(15B)-C(16B)-C(17B)-O(1B)	-50.9(3)
O(2A)-C(21A)-C(20A)-C(19A)	5.8(3)
N(4A)-C(21A)-C(20A)-C(19A)	-174.61(19)
O(2A)-C(21A)-C(20A)-C(15A)	130.7(2)
N(4A)-C(21A)-C(20A)-C(15A)	-49.7(2)
O(2A)-C(21A)-C(20A)-C(7A)	-115.7(2)
N(4A)-C(21A)-C(20A)-C(7A)	63.9(2)
C(18A)-C(19A)-C(20A)-C(21A)	72.8(3)
C(18A)-C(19A)-C(20A)-C(15A)	-49.5(3)
C(18A)-C(19A)-C(20A)-C(7A)	-168.5(2)
C(14A)-C(15A)-C(20A)-C(21A)	177.9(2)
C(16A)-C(15A)-C(20A)-C(21A)	56.3(2)
C(14A)-C(15A)-C(20A)-C(19A)	-58.5(3)
C(16A)-C(15A)-C(20A)-C(19A)	179.9(2)
C(14A)-C(15A)-C(20A)-C(7A)	63.6(2)
C(16A)-C(15A)-C(20A)-C(7A)	-58.0(2)
C(2A)-C(7A)-C(20A)-C(21A)	-167.35(19)
C(8A)-C(7A)-C(20A)-C(21A)	82.3(2)
C(6A)-C(7A)-C(20A)-C(21A)	-46.2(2)
C(2A)-C(7A)-C(20A)-C(19A)	71.4(2)
C(8A)-C(7A)-C(20A)-C(19A)	-39.0(3)
C(6A)-C(7A)-C(20A)-C(19A)	-167.4(2)
C(2A)-C(7A)-C(20A)-C(15A)	-51.9(2)
C(8A)-C(7A)-C(20A)-C(15A)	-162.2(2)
C(6A)-C(7A)-C(20A)-C(15A)	69.3(2)
C(9B)-C(10B)-C(11B)-C(12B)	-0.7(4)
C(13B)-C(12B)-C(11B)-C(10B)	-0.1(4)
C(13A)-C(12A)-C(11A)-C(10A)	-0.5(4)
C(9A)-C(10A)-C(11A)-C(12A)	-1.0(4)

Symmetry transformations used to generate equivalent atoms:

**Table 7.** Hydrogen bonds for **1** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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## Single crystal X-ray data and structure of **4**



**4**

**Table 1.** Crystal data and structure refinement for **4**.

Identification code	4
Empirical formula	C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Formula weight	320.38
Temperature	293(2) K
Wavelength	1.54184 Å
Crystal system, space group	?, ?
Unit cell dimensions	a = 7.6859(2) Å    alpha = 90 deg. b = 7.71266(16) Å    beta = 105.195(3) deg. c = 13.5130(3) Å    gamma = 90 deg.
Volume	773.03(3) Å <sup>3</sup>
Z, Calculated density	2, 1.376 Mg/m <sup>3</sup>
Absorption coefficient	0.715 mm <sup>-1</sup>
F(000)	340
Crystal size	? x ? x ? mm
Theta range for data collection	3.39 to 62.77 deg.
Limiting indices	-8 ≤ h ≤ 8, -8 ≤ k ≤ 8, -15 ≤ l ≤ 15
Reflections collected / unique	12477 / 2466 [R(int) = 0.0369]
Completeness to theta = 62.77	99.6 %
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2466 / 1 / 226
Goodness-of-fit on F <sup>2</sup>	1.045
Final R indices [I > 2σ(I)]	R1 = 0.0267, wR2 = 0.0658
R indices (all data)	R1 = 0.0288, wR2 = 0.0676
Absolute structure parameter	0.0(2)
Extinction coefficient	0.0095(7)
Largest diff. peak and hole	0.211 and -0.108 e.Å <sup>-3</sup>

**Table 2.** Atomic coordinates ( × 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> × 10<sup>3</sup>) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U<sub>ij</sub> tensor.

	x	y	z	U(eq)
N(1)	-3007(2)	6026(2)	4337(1)	28(1)
N(4)	-170(2)	5866(2)	1152(1)	25(1)
O(1)	1199(2)	4604(2)	4473(1)	30(1)
O(2)	-462(2)	6361(2)	-534(1)	46(1)
C(2)	-1869(2)	5408(2)	3880(1)	24(1)
C(3)	-609(2)	3944(2)	4289(1)	28(1)
C(5)	886(2)	5936(2)	2226(1)	24(1)
C(6)	-151(2)	7097(2)	2786(1)	25(1)
C(7)	-1944(2)	6192(2)	2833(1)	23(1)
C(8)	-3473(2)	7446(2)	2760(1)	25(1)
C(9)	-4307(2)	8633(2)	2016(1)	33(1)
C(10)	-5723(3)	9626(2)	2182(2)	40(1)
C(11)	-6229(2)	9485(2)	3089(2)	39(1)
C(12)	-5375(2)	8341(2)	3849(1)	35(1)
C(13)	-4016(2)	7314(2)	3668(1)	26(1)
C(14)	-994(2)	2495(2)	3495(1)	28(1)
C(15)	-837(2)	3247(2)	2471(1)	24(1)
C(16)	1083(2)	4081(2)	2643(1)	25(1)
C(17)	2175(2)	4002(2)	3769(1)	29(1)
C(18)	-5445(3)	3875(3)	1006(1)	38(1)
C(19)	-4187(2)	3965(2)	1873(1)	26(1)
C(20)	-2300(2)	4653(2)	2030(1)	22(1)
C(21)	-2024(2)	5269(2)	1001(1)	25(1)
C(22)	433(2)	6371(2)	363(1)	32(1)

**Table 3.** Bond lengths [Å] and angles [deg] for **4**.

N(1)-C(2)	1.287(2)
N(1)-C(13)	1.428(2)
N(4)-C(22)	1.327(2)
N(4)-C(21)	1.460(2)
N(4)-C(5)	1.4661(19)
O(1)-C(17)	1.436(2)
O(1)-C(3)	1.439(2)
O(2)-C(22)	1.227(2)
C(2)-C(3)	1.496(2)
C(2)-C(7)	1.526(2)
C(3)-C(14)	1.524(2)
C(3)-H(3)	0.9800
C(5)-C(6)	1.525(2)
C(5)-C(16)	1.530(2)
C(5)-H(5)	0.9800
C(6)-C(7)	1.561(2)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-C(8)	1.505(2)
C(7)-C(20)	1.583(2)
C(8)-C(9)	1.386(2)
C(8)-C(13)	1.399(2)
C(9)-C(10)	1.396(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.385(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.382(3)

C(11)-H(11)	0.9300
C(12)-C(13)	1.383(3)
C(12)-H(12)	0.9300
C(14)-C(15)	1.534(2)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(20)	1.563(2)
C(15)-C(16)	1.570(2)
C(15)-H(15)	0.9800
C(16)-C(17)	1.534(2)
C(16)-H(16)	0.9800
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.310(2)
C(18)-H(18A)	0.98(2)
C(18)-H(18B)	1.00(2)
C(19)-C(20)	1.507(2)
C(19)-H(19)	0.9300
C(20)-C(21)	1.536(2)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-H(22)	0.9300
C(2)-N(1)-C(13)	106.20(13)
C(22)-N(4)-C(21)	120.93(13)
C(22)-N(4)-C(5)	124.39(14)
C(21)-N(4)-C(5)	114.61(12)
C(17)-O(1)-C(3)	114.83(12)
N(1)-C(2)-C(3)	123.93(14)
N(1)-C(2)-C(7)	115.62(14)
C(3)-C(2)-C(7)	120.35(14)
O(1)-C(3)-C(2)	107.41(14)
O(1)-C(3)-C(14)	112.44(13)
C(2)-C(3)-C(14)	107.82(13)
O(1)-C(3)-H(3)	109.7
C(2)-C(3)-H(3)	109.7
C(14)-C(3)-H(3)	109.7
N(4)-C(5)-C(6)	106.68(12)
N(4)-C(5)-C(16)	107.82(13)
C(6)-C(5)-C(16)	112.32(13)
N(4)-C(5)-H(5)	110.0
C(6)-C(5)-H(5)	110.0
C(16)-C(5)-H(5)	110.0
C(5)-C(6)-C(7)	109.85(12)
C(5)-C(6)-H(6A)	109.7
C(7)-C(6)-H(6A)	109.7
C(5)-C(6)-H(6B)	109.7
C(7)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
C(8)-C(7)-C(2)	98.90(12)
C(8)-C(7)-C(6)	113.11(13)
C(2)-C(7)-C(6)	113.30(12)
C(8)-C(7)-C(20)	116.44(12)
C(2)-C(7)-C(20)	107.24(12)
C(6)-C(7)-C(20)	107.64(12)
C(9)-C(8)-C(13)	119.74(15)
C(9)-C(8)-C(7)	132.60(15)
C(13)-C(8)-C(7)	107.64(14)
C(8)-C(9)-C(10)	118.57(17)
C(8)-C(9)-H(9)	120.7
C(10)-C(9)-H(9)	120.7

C(11)-C(10)-C(9)	120.67(17)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(12)-C(11)-C(10)	121.29(18)
C(12)-C(11)-H(11)	119.4
C(10)-C(11)-H(11)	119.4
C(11)-C(12)-C(13)	117.90(17)
C(11)-C(12)-H(12)	121.1
C(13)-C(12)-H(12)	121.1
C(12)-C(13)-C(8)	121.76(16)
C(12)-C(13)-N(1)	126.63(15)
C(8)-C(13)-N(1)	111.61(14)
C(3)-C(14)-C(15)	108.13(14)
C(3)-C(14)-H(14A)	110.1
C(15)-C(14)-H(14A)	110.1
C(3)-C(14)-H(14B)	110.1
C(15)-C(14)-H(14B)	110.1
H(14A)-C(14)-H(14B)	108.4
C(14)-C(15)-C(20)	112.81(13)
C(14)-C(15)-C(16)	108.35(13)
C(20)-C(15)-C(16)	109.04(13)
C(14)-C(15)-H(15)	108.9
C(20)-C(15)-H(15)	108.9
C(16)-C(15)-H(15)	108.9
C(5)-C(16)-C(17)	112.23(14)
C(5)-C(16)-C(15)	109.29(13)
C(17)-C(16)-C(15)	112.25(13)
C(5)-C(16)-H(16)	107.6
C(17)-C(16)-H(16)	107.6
C(15)-C(16)-H(16)	107.6
O(1)-C(17)-C(16)	113.55(13)
O(1)-C(17)-H(17A)	108.9
C(16)-C(17)-H(17A)	108.9
O(1)-C(17)-H(17B)	108.9
C(16)-C(17)-H(17B)	108.9
H(17A)-C(17)-H(17B)	107.7
C(19)-C(18)-H(18A)	123.2(12)
C(19)-C(18)-H(18B)	122.1(12)
H(18A)-C(18)-H(18B)	114.8(16)
C(18)-C(19)-C(20)	127.05(16)
C(18)-C(19)-H(19)	116.5
C(20)-C(19)-H(19)	116.5
C(19)-C(20)-C(21)	109.72(12)
C(19)-C(20)-C(15)	112.28(13)
C(21)-C(20)-C(15)	107.68(12)
C(19)-C(20)-C(7)	110.37(12)
C(21)-C(20)-C(7)	110.40(12)
C(15)-C(20)-C(7)	106.32(12)
N(4)-C(21)-C(20)	109.43(12)
N(4)-C(21)-H(21A)	109.8
C(20)-C(21)-H(21A)	109.8
N(4)-C(21)-H(21B)	109.8
C(20)-C(21)-H(21B)	109.8
H(21A)-C(21)-H(21B)	108.2
O(2)-C(22)-N(4)	124.64(16)
O(2)-C(22)-H(22)	117.7
N(4)-C(22)-H(22)	117.7

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Symmetry transformations used to generate equivalent atoms:

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

	U11	U22	U33	U23	U13	U12
N(1)	30(1)	33(1)	22(1)	-5(1)	9(1)	0(1)
N(4)	26(1)	32(1)	17(1)	1(1)	6(1)	-5(1)
O(1)	32(1)	37(1)	20(1)	-2(1)	4(1)	7(1)
O(2)	40(1)	77(1)	22(1)	14(1)	8(1)	-7(1)
C(2)	28(1)	27(1)	18(1)	-3(1)	7(1)	-2(1)
C(3)	35(1)	32(1)	18(1)	5(1)	9(1)	4(1)
C(5)	24(1)	29(1)	18(1)	0(1)	3(1)	-3(1)
C(6)	29(1)	25(1)	21(1)	0(1)	5(1)	-2(1)
C(7)	27(1)	23(1)	18(1)	0(1)	6(1)	1(1)
C(8)	26(1)	22(1)	26(1)	-5(1)	4(1)	-2(1)
C(9)	36(1)	26(1)	33(1)	2(1)	3(1)	1(1)
C(10)	35(1)	24(1)	53(1)	-1(1)	0(1)	2(1)
C(11)	26(1)	29(1)	58(1)	-14(1)	5(1)	1(1)
C(12)	28(1)	38(1)	38(1)	-14(1)	9(1)	-3(1)
C(13)	25(1)	26(1)	26(1)	-7(1)	4(1)	-1(1)
C(14)	35(1)	26(1)	25(1)	4(1)	10(1)	2(1)
C(15)	29(1)	22(1)	21(1)	-3(1)	10(1)	-1(1)
C(16)	28(1)	26(1)	20(1)	-2(1)	7(1)	2(1)
C(17)	30(1)	33(1)	24(1)	0(1)	7(1)	5(1)
C(18)	32(1)	53(1)	29(1)	-4(1)	10(1)	-13(1)
C(19)	32(1)	26(1)	22(1)	-1(1)	11(1)	-3(1)
C(20)	26(1)	24(1)	17(1)	-1(1)	8(1)	-1(1)
C(21)	26(1)	31(1)	18(1)	-1(1)	7(1)	-4(1)
C(22)	29(1)	42(1)	26(1)	8(1)	10(1)	-4(1)

**Table 5.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for **4**.

	x	y	z	U(eq)
H(3)	-816	3525	4934	34
H(5)	2078	6432	2271	29
H(6A)	-417	8196	2430	30
H(6B)	580	7324	3476	30
H(9)	-3932	8764	1420	39
H(10)	-6333	10391	1677	47
H(11)	-7161	10173	3190	46
H(12)	-5705	8264	4462	41
H(14A)	-2196	2037	3422	33
H(14B)	-134	1559	3710	33
H(15)	-960	2303	1972	28
H(16)	1738	3413	2239	29
H(17A)	2549	2813	3938	35
H(17B)	3255	4698	3853	35
H(18A)	-6660(30)	3410(30)	954(15)	40(5)
H(18B)	-5240(30)	4300(30)	341(16)	47(6)
H(19)	-4493	3559	2453	31
H(21A)	-2267	4324	511	30
H(21B)	-2853	6207	731	30
H(22)	1618	6760	500	38

**Table 6.** Torsion angles [deg] for **4**.

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C(13)-N(1)-C(2)-C(3)	-176.31(15)
C(13)-N(1)-C(2)-C(7)	0.00(18)
C(17)-O(1)-C(3)-C(2)	-108.43(15)
C(17)-O(1)-C(3)-C(14)	10.03(18)
N(1)-C(2)-C(3)-O(1)	-117.54(17)
C(7)-C(2)-C(3)-O(1)	66.32(17)
N(1)-C(2)-C(3)-C(14)	121.06(17)
C(7)-C(2)-C(3)-C(14)	-55.1(2)
C(22)-N(4)-C(5)-C(6)	120.60(17)
C(21)-N(4)-C(5)-C(6)	-56.32(17)
C(22)-N(4)-C(5)-C(16)	-118.55(17)
C(21)-N(4)-C(5)-C(16)	64.53(17)
N(4)-C(5)-C(6)-C(7)	67.88(15)
C(16)-C(5)-C(6)-C(7)	-50.05(16)
N(1)-C(2)-C(7)-C(8)	-1.02(18)
C(3)-C(2)-C(7)-C(8)	175.44(14)
N(1)-C(2)-C(7)-C(6)	118.98(16)
C(3)-C(2)-C(7)-C(6)	-64.56(19)
N(1)-C(2)-C(7)-C(20)	-122.38(15)
C(3)-C(2)-C(7)-C(20)	54.07(19)
C(5)-C(6)-C(7)-C(8)	-145.37(13)
C(5)-C(6)-C(7)-C(2)	103.10(14)
C(5)-C(6)-C(7)-C(20)	-15.30(15)
C(2)-C(7)-C(8)-C(9)	179.53(17)
C(6)-C(7)-C(8)-C(9)	59.4(2)
C(20)-C(7)-C(8)-C(9)	-66.1(2)
C(2)-C(7)-C(8)-C(13)	1.61(16)
C(6)-C(7)-C(8)-C(13)	-118.53(14)
C(20)-C(7)-C(8)-C(13)	116.00(15)
C(13)-C(8)-C(9)-C(10)	-2.3(2)
C(7)-C(8)-C(9)-C(10)	179.96(16)
C(8)-C(9)-C(10)-C(11)	2.9(3)
C(9)-C(10)-C(11)-C(12)	-1.2(3)
C(10)-C(11)-C(12)-C(13)	-1.1(3)
C(11)-C(12)-C(13)-C(8)	1.7(3)
C(11)-C(12)-C(13)-N(1)	-178.19(15)
C(9)-C(8)-C(13)-C(12)	0.1(2)
C(7)-C(8)-C(13)-C(12)	178.30(15)
C(9)-C(8)-C(13)-N(1)	179.94(14)
C(7)-C(8)-C(13)-N(1)	-1.83(18)
C(2)-N(1)-C(13)-C(12)	-178.97(17)
C(2)-N(1)-C(13)-C(8)	1.16(18)
O(1)-C(3)-C(14)-C(15)	-63.12(17)
C(2)-C(3)-C(14)-C(15)	55.09(17)
C(3)-C(14)-C(15)-C(20)	-64.77(17)
C(3)-C(14)-C(15)-C(16)	56.04(16)
N(4)-C(5)-C(16)-C(17)	179.94(13)
C(6)-C(5)-C(16)-C(17)	-62.81(17)
N(4)-C(5)-C(16)-C(15)	-54.87(15)
C(6)-C(5)-C(16)-C(15)	62.39(15)
C(14)-C(15)-C(16)-C(5)	-128.55(13)
C(20)-C(15)-C(16)-C(5)	-5.42(16)
C(14)-C(15)-C(16)-C(17)	-3.36(18)

C(20)-C(15)-C(16)-C(17)	119.77(14)
C(3)-O(1)-C(17)-C(16)	46.02(19)
C(5)-C(16)-C(17)-O(1)	74.45(18)
C(15)-C(16)-C(17)-O(1)	-49.11(19)
C(18)-C(19)-C(20)-C(21)	0.1(2)
C(18)-C(19)-C(20)-C(15)	-119.55(19)
C(18)-C(19)-C(20)-C(7)	122.02(19)
C(14)-C(15)-C(20)-C(19)	-57.91(17)
C(16)-C(15)-C(20)-C(19)	-178.33(12)
C(14)-C(15)-C(20)-C(21)	-178.80(13)
C(16)-C(15)-C(20)-C(21)	60.78(15)
C(14)-C(15)-C(20)-C(7)	62.87(16)
C(16)-C(15)-C(20)-C(7)	-57.55(15)
C(8)-C(7)-C(20)-C(19)	-39.89(18)
C(2)-C(7)-C(20)-C(19)	69.70(16)
C(6)-C(7)-C(20)-C(19)	-168.07(12)
C(8)-C(7)-C(20)-C(21)	81.58(16)
C(2)-C(7)-C(20)-C(21)	-168.83(13)
C(6)-C(7)-C(20)-C(21)	-46.60(16)
C(8)-C(7)-C(20)-C(15)	-161.90(13)
C(2)-C(7)-C(20)-C(15)	-52.31(16)
C(6)-C(7)-C(20)-C(15)	69.91(14)
C(22)-N(4)-C(21)-C(20)	176.06(15)
C(5)-N(4)-C(21)-C(20)	-6.90(18)
C(19)-C(20)-C(21)-N(4)	-177.62(13)
C(15)-C(20)-C(21)-N(4)	-55.14(16)
C(7)-C(20)-C(21)-N(4)	60.53(17)
C(21)-N(4)-C(22)-O(2)	-1.1(3)
C(5)-N(4)-C(22)-O(2)	-177.87(17)

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Symmetry transformations used to generate equivalent atoms:

**Table 7.** Hydrogen bonds for **4** [Å and deg.].

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D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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