Supporting Information

5-Amino-3-(diethylamino)-5H-benzo[4,5]imidazo[1,2-b][1,2,4,6]thiatriazine 1,1-dioxide

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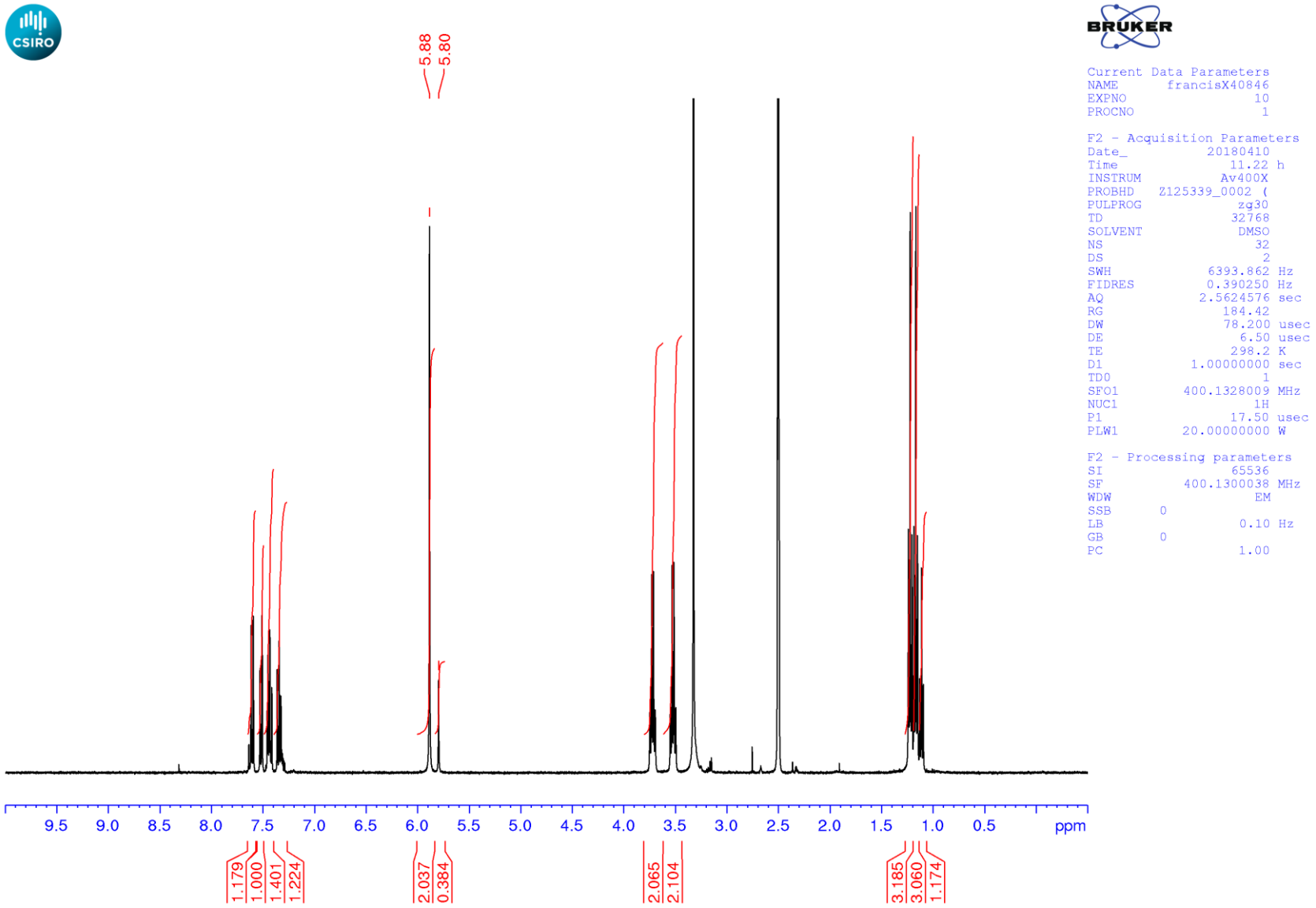
^{1}H-NMR spectrum of crude product (precipitate)

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TD                 32768
SOLVENT             DMSO
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TE                298.2 K
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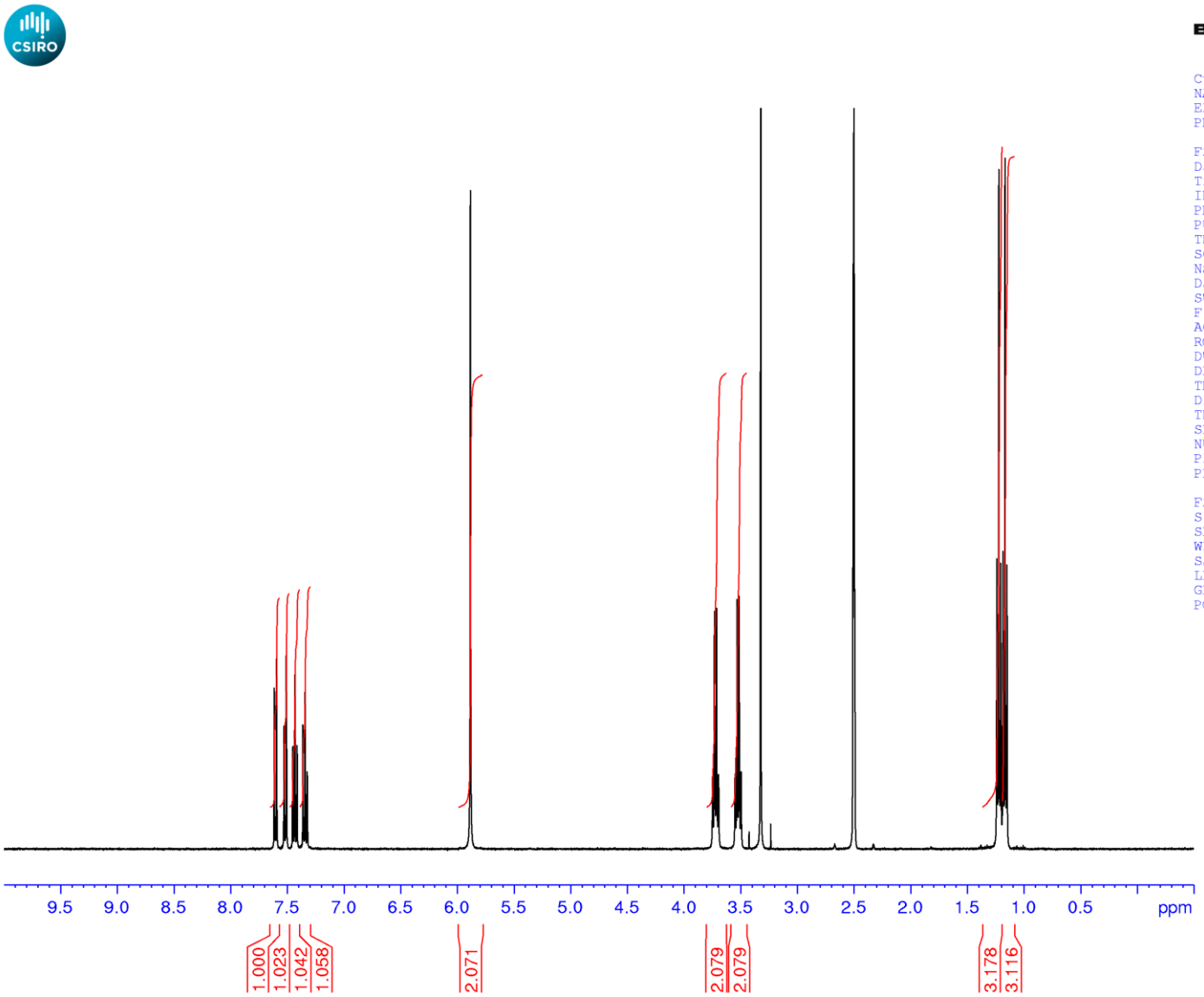
^{1}H-NMR spectrum of compound **6**

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P1                17.50 usec
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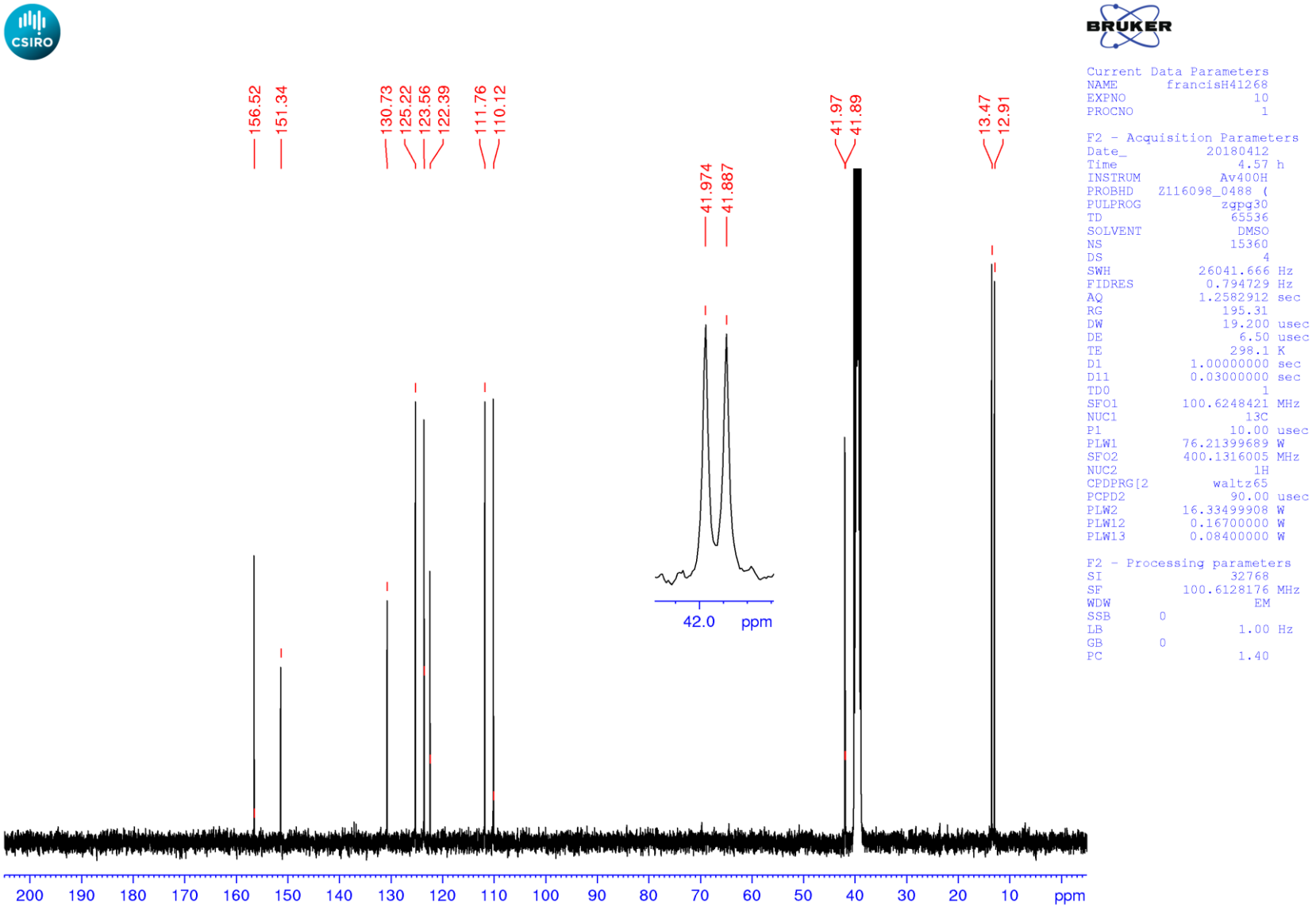
^{13}C-NMR spectrum of compound **6**

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TE                298.1 K
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SFO1        100.6248421 MHz
NUC1                13C
P1                10.00 usec
PLW1         76.21399689 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.33499908 W
PLW12         0.16700000 W
PLW13         0.08400000 W

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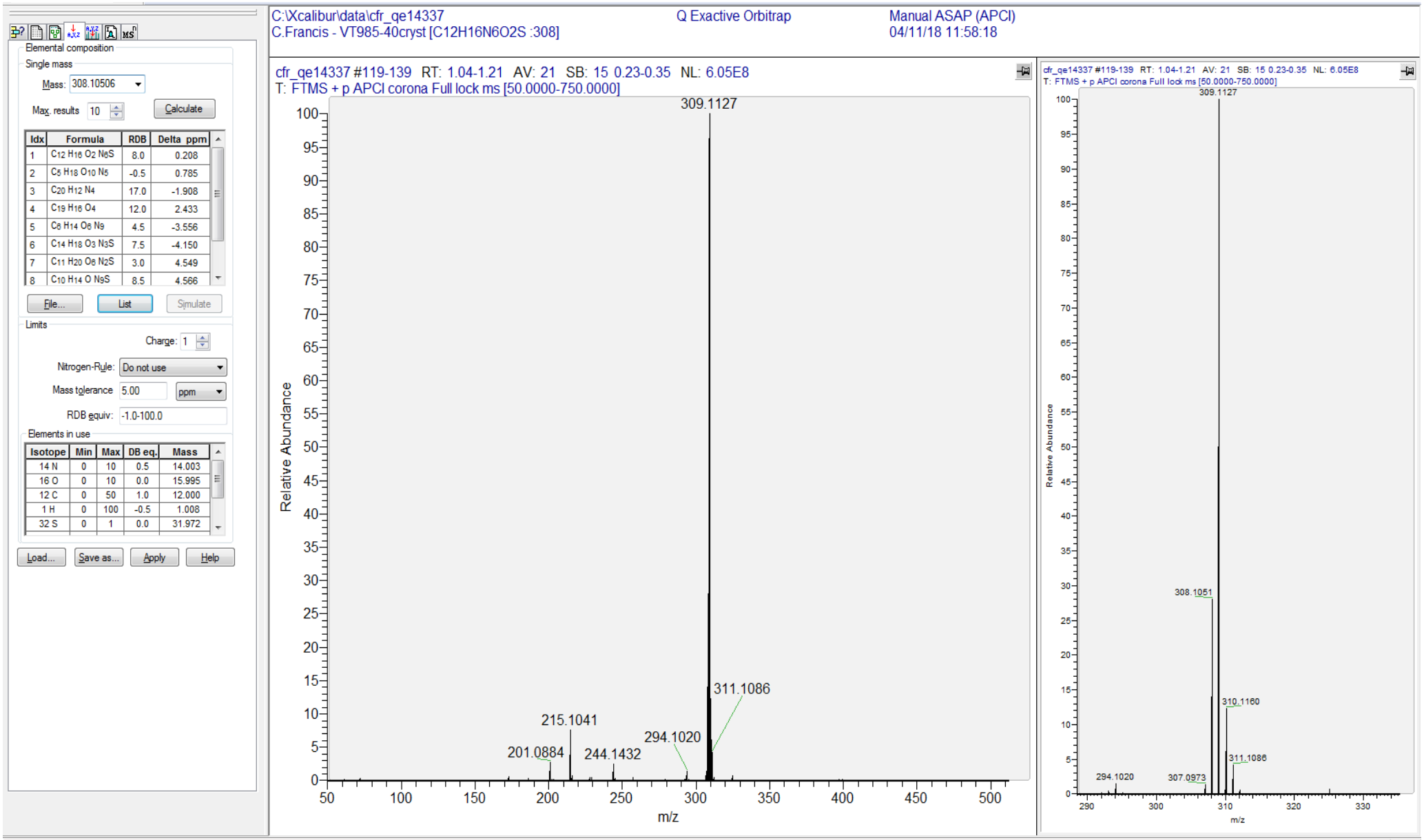
High resolution mass spectrum of compound **6**



[M]$^{+\cdot}$

m/z	Theo. Mass	Delta (ppm)	Composition
308.1051	**308.1050**	**0.21**	**C_{12} H_{16} O_2 N_6 S**
	308.1048	0.78	C5 H18 O10 N5
	308.1056	-1.91	C20 H12 N4
	308.1043	2.43	C19 H16 O4
	308.1062	-3.56	C6 H14 O6 N9
	308.1063	-4.15	C14 H18 O3 N3 S
	308.1037	4.55	C11 H20 O6 N2 S
	308.1037	4.57	C10 H14 O N9 S

[M+H]$^{+}$

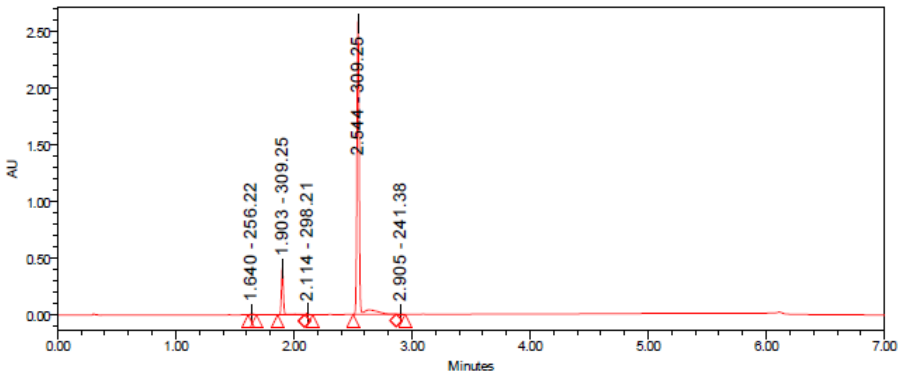
m/z	Theo. Mass	Delta (ppm)	Composition
309.1127	309.1126	0.05	C5 H19 O10 N5
	309.1128	**-0.52**	**C_{12} H_{17} O_2 N_6 S**
	309.1121	1.70	C19 H17 O4
	309.1135	-2.63	C20 H13 N4
	309.1115	3.81	C11 H21 O6 N2 S
	309.1115	3.82	C10 H15 O N9 S
	309.1140	-4.27	C6 H15 O6 N9
	309.1113	4.40	C3 H17 O9 N8
	309.1142	-4.86	C14 H19 O3 N3 S

LC-MS data for crude product (precipitate)

SAMPLE INFORMATION

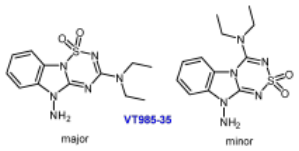
Sample Name:	VT985-35	Instrument:	Waters Acquity iClass PDA and QDa detectors
Vial:	1:A,5	Acquired By:	System
Injection #:	1	Sample Set Name:	MK_11_April2018
Injection Volume:	1.00 ul		
Run Time:	7.0 Minutes	Acquisition Method:	95% A1 to 100% B1 POSNEG
		Mobile Phase:	A1: 100% H2O / 0.1% FA B1: 100% ACN / 0.1% FA
Date Acquired:	11/04/2018 9:08:58 AM EST		
Date Processed:	11/04/2018 9:20:07 AM EST	Extracted Chromatogram:	PDA Spectrum PDA 254.0 nm

Auto-Scaled Chromatogram

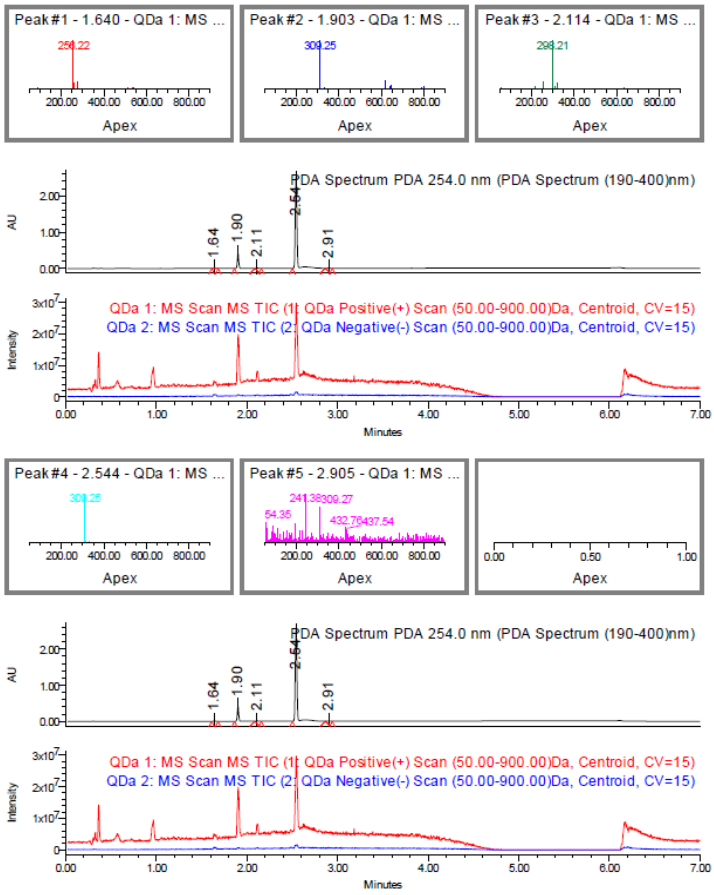


Peak Results

	RT	Area	% Area	Height	Base Peak (m/z)
1	1.640	18881	0.46	9635	256.22
2	1.903	494175	12.02	409297	309.25
3	2.114	15900	0.39	12401	298.21
4	2.544	3576078	86.98	2577062	309.25
5	2.905	6247	0.15	3331	241.38



Chemical Formula: $C_{12}H_{16}N_8O_2S$
Exact Mass: 308.11
Molecular Weight: 308.36
m/z: 308.11 (100.0%), 309.11 (13.0%), 310.10 (4.5%), 309.10 (2.2%)

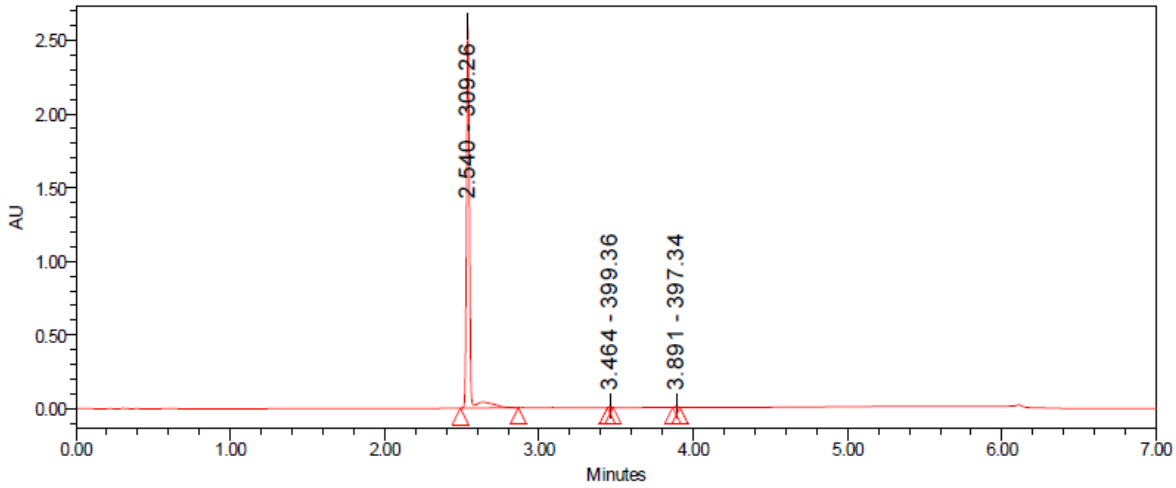


LC-MS data for compound **6**

SAMPLE INFORMATION

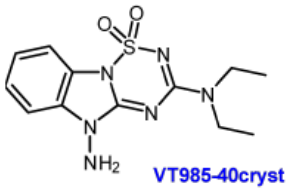
Sample Name:	**VT985-40cryst**	Instrument:	Waters Acquity iClass PDA and QDa detectors
Vial:	1:A,4	Acquired By:	System
Injection #:	1	Sample Set Name:	MK_11_April2018
Injection Volume:	0.50 ul		
Run Time:	7.0 Minutes	Acquisition Method:	95% A1 to 100% B1 POSNEG
		Mobile Phase:	A1: 100% H2O / 0.1% FA B1: 100% ACN / 0.1% FA
Date Acquired:	11/04/2018 9:00:28 AM EST		
Date Processed:	11/04/2018 9:10:01 AM EST	Extracted Chromatogram:	PDA Spectrum PDA 254.0 nm

Auto-Scaled Chromatogram

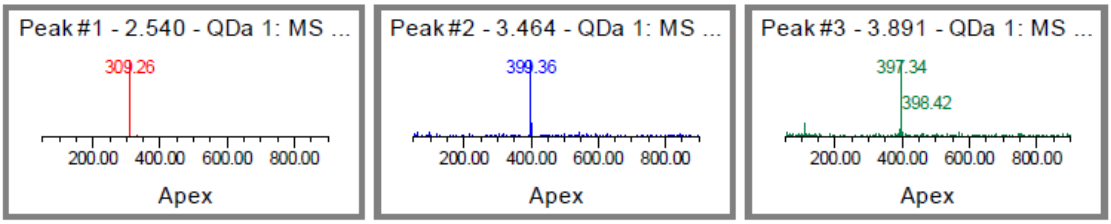


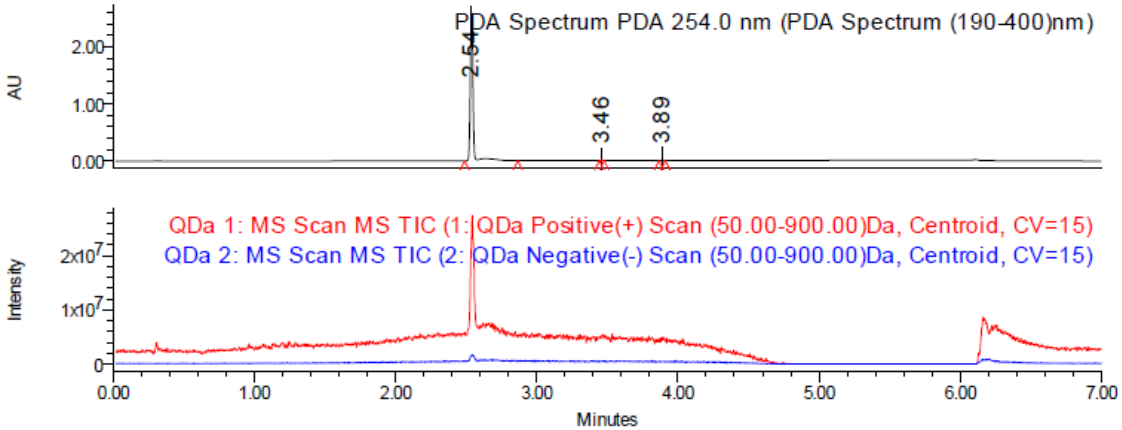
Peak Results

	RT	Area	% Area	Height	Base Peak (m/z)
1	2.540	3624941	99.46	2586768	309.26
2	3.464	9399	0.26	8874	399.36
3	3.891	10423	0.29	9162	397.34

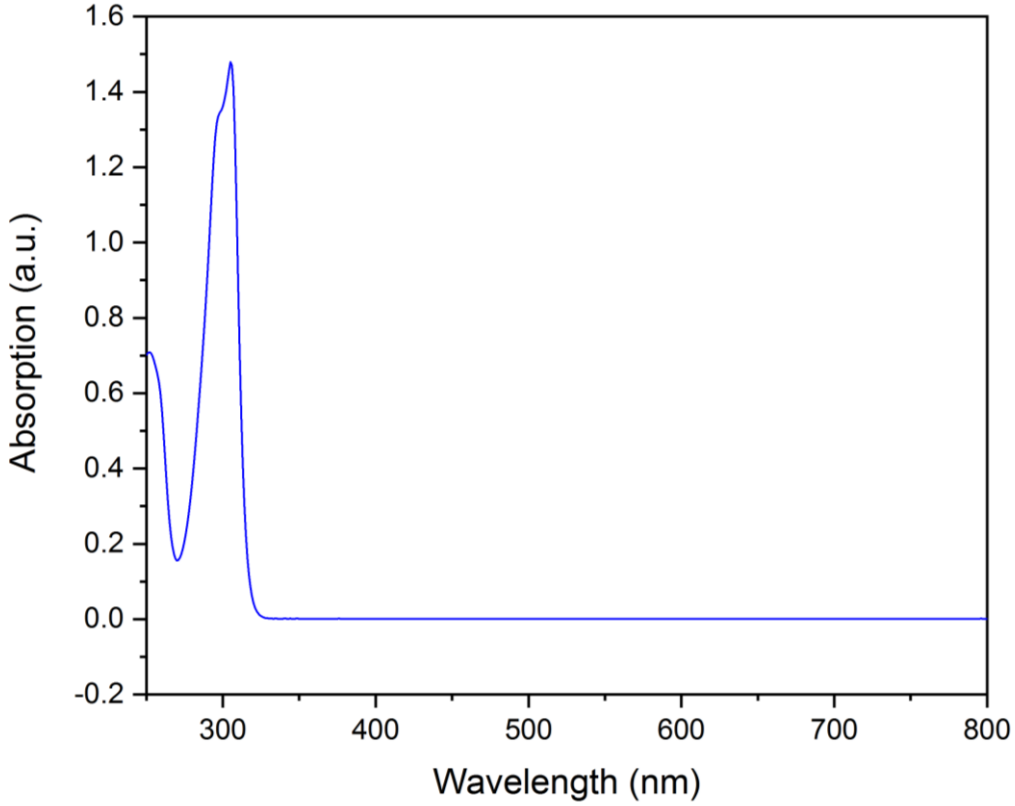


Chemical Formula: $C_{12}H_{16}N_6O_2S$
Exact Mass: 308.11
Molecular Weight: 308.36
m/z: 308.11 (100.0%), 309.11 (13.0%), 310.10 (4.5%), 309.10 (2.2%)

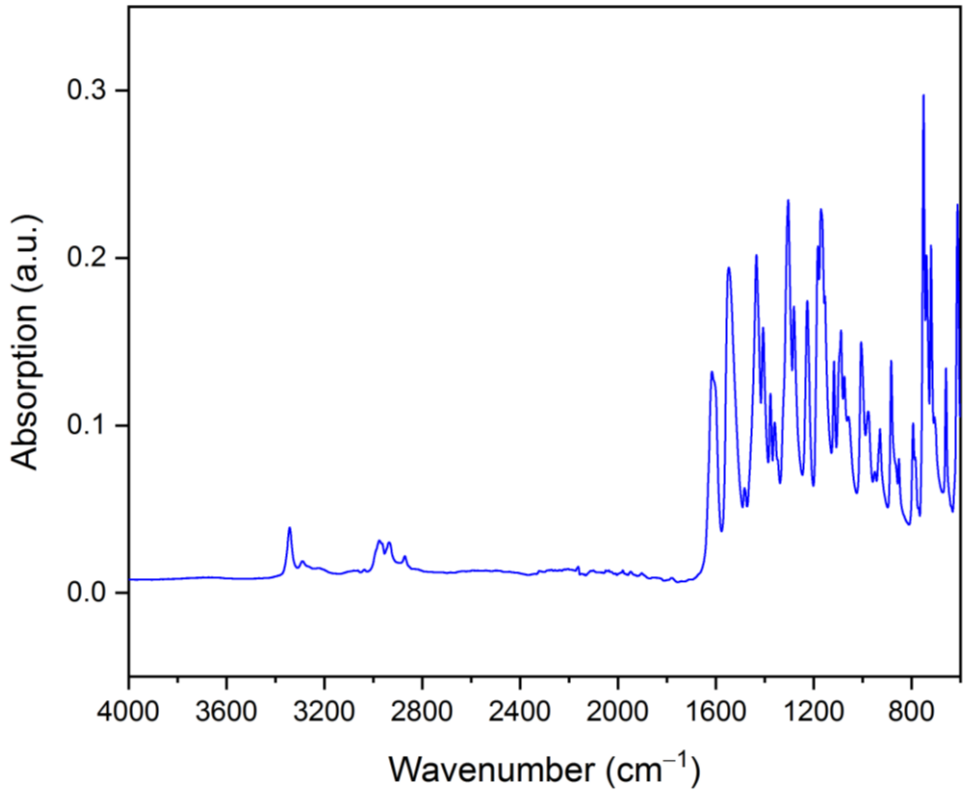




UV-vis spectrum of compound **6** (MeOH solution).



IR spectrum of compound **6** (solid sample on laminated diamond).



Single crystal and geometric data for compound **6**.

Table 1. Crystal data and structure refinement.

Identification code	K1_08ABA
Empirical formula	C_{12} H_{16} N_6 O_2 S
Formula weight	308.37
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *P*2(1)/*c*
Unit cell dimensions	a = 15.3907(2) Å alpha = 90 deg. b = 14.9210(2) Å beta = 114.4240(10) deg. c = 13.23680(10) Å gamma = 90 deg.
Volume	2767.73(6) $Å^3$
Z, Calculated density	8, 1.480 Mg/m^3
Absorption coefficient	0.249 mm^{-1}
F(000)	1296
Crystal size	0.300 x 0.300 x 0.150 mm
Theta range for data collection	1.453 to 27.494 deg.
Limiting indices	-19<=h<=19, -19<=k<=19, -14<=l<=16
Reflections collected / unique	25274 / 6221 [R(int) = 0.0459]
Completeness to theta = 25.242	99.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.96 and 0.95
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6221 / 0 / 395
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0431, wR2 = 0.1080
R indices (all data)	R1 = 0.0698, wR2 = 0.1220
Largest diff. peak and hole	0.319 and -0.503 $e.A^{-3}$

Table 2. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3).

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	1433(1)	5918(1)	4486(1)	18(1)
S(1A)	-3531(1)	5760(1)	-360(1)	18(1)
O(1)	1572(1)	6735(1)	4002(1)	25(1)
O(2A)	-2886(1)	5638(1)	779(1)	24(1)
O(2)	2152(1)	5726(1)	5571(1)	24(1)
O(1A)	-3288(1)	6462(1)	-931(1)	28(1)
N(2)	1220(1)	5094(1)	3713(1)	23(1)
N(2A)	-3784(1)	4854(1)	-985(1)	21(1)
N(3)	268(1)	4267(1)	2204(1)	20(1)
N(3A)	-4705(1)	4050(1)	-2527(1)	19(1)
N(4)	-507(1)	5115(1)	3038(1)	18(1)
N(4A)	-5482(1)	5134(1)	-1964(1)	18(1)
N(5)	-1173(1)	6119(1)	3902(1)	18(1)
N(5A)	-6144(1)	6246(1)	-1218(1)	18(1)
N(6)	-2144(1)	5993(1)	3228(1)	22(1)
N(6A)	-7111(1)	6158(1)	-1934(1)	24(1)
N(10)	398(1)	6044(1)	4628(1)	18(1)
N(10A)	-4590(1)	6044(1)	-354(1)	18(1)
C(3)	331(1)	4843(1)	3009(1)	18(1)
C(3A)	-4650(1)	4705(1)	-1815(1)	17(1)
C(4)	-428(1)	5702(1)	3804(1)	16(1)
C(4A)	-5409(1)	5753(1)	-1231(1)	16(1)
C(5)	-841(1)	6780(1)	4725(1)	18(1)
C(5A)	-5806(1)	6873(1)	-351(1)	18(1)
C(6)	-1330(1)	7404(1)	5064(2)	22(1)
C(6A)	-6287(1)	7510(1)	-16(2)	22(1)
C(7)	-780(1)	7998(1)	5878(2)	24(1)
C(7A)	-5726(1)	8041(1)	877(2)	24(1)
C(8)	213(1)	7966(1)	6341(2)	26(1)
C(8A)	-4740(1)	7940(1)	1407(2)	25(1)
C(9)	704(1)	7330(1)	6009(1)	23(1)
C(9A)	-4264(1)	7292(1)	1072(2)	23(1)
C(10)	152(1)	6745(1)	5184(1)	18(1)
C(10A)	-4823(1)	6766(1)	185(1)	17(1)
C(31)	-635(1)	3826(1)	1502(2)	23(1)
C(31A)	-5630(1)	3758(1)	-3386(1)	23(1)
C(32)	-1167(2)	4312(1)	420(2)	33(1)
C(32A)	-5928(2)	4284(1)	-4450(2)	32(1)
C(33)	1093(1)	4105(1)	1937(2)	24(1)
C(33A)	-3821(1)	3634(1)	-2478(2)	26(1)
C(34)	1726(1)	3341(1)	2584(2)	32(1)
C(34A)	-3283(2)	4225(1)	-2959(2)	34(1)

Table 3. Bond lengths [Å] and angles [deg].

S(1)-O(2)	1.4336(12)
S(1)-O(1)	1.4337(13)
S(1)-N(2)	1.5458(15)
S(1)-N(10)	1.6899(14)
S(1A)-O(1A)	1.4278(13)
S(1A)-O(2A)	1.4334(12)
S(1A)-N(2A)	1.5485(15)
S(1A)-N(10A)	1.6871(15)
N(2)-C(3)	1.352(2)
N(2A)-C(3A)	1.350(2)
N(3)-C(3)	1.341(2)
N(3)-C(31)	1.470(2)
N(3)-C(33)	1.472(2)
N(3A)-C(3A)	1.335(2)
N(3A)-C(33A)	1.472(2)
N(3A)-C(31A)	1.473(2)
N(4)-C(4)	1.307(2)
N(4)-C(3)	1.367(2)
N(4A)-C(4A)	1.309(2)
N(4A)-C(3A)	1.371(2)
N(5)-C(4)	1.357(2)
N(5)-C(5)	1.400(2)
N(5)-N(6)	1.401(2)
N(5A)-C(4A)	1.356(2)
N(5A)-C(5A)	1.402(2)
N(5A)-N(6A)	1.4023(19)
N(6)-H(6N)	0.88(2)
N(6)-H(7N)	0.89(2)
N(6A)-H(6AN)	0.89(2)
N(6A)-H(7AN)	0.91(2)
N(10)-C(4)	1.385(2)
N(10)-C(10)	1.417(2)
N(10A)-C(4A)	1.384(2)
N(10A)-C(10A)	1.418(2)
C(5)-C(6)	1.384(2)
C(5)-C(10)	1.392(2)
C(5A)-C(6A)	1.386(2)
C(5A)-C(10A)	1.390(2)
C(6)-C(7)	1.382(3)
C(6)-H(6)	0.9500
C(6A)-C(7A)	1.387(3)
C(6A)-H(6A)	0.9500
C(7)-C(8)	1.392(3)
C(7)-H(7)	0.9500
C(7A)-C(8A)	1.392(3)
C(7A)-H(7A)	0.9500
C(8)-C(9)	1.393(3)
C(8)-H(8)	0.9500
C(8A)-C(9A)	1.392(3)
C(8A)-H(8A)	0.9500
C(9)-C(10)	1.382(2)
C(9)-H(9)	0.9500
C(9A)-C(10A)	1.379(2)
C(9A)-H(9A)	0.9500
C(31)-C(32)	1.508(3)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(31A)-C(32A)	1.509(3)
C(31A)-H(31C)	0.9900
C(31A)-H(31D)	0.9900
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(32A)-H(32D)	0.9800
C(32A)-H(32E)	0.9800
C(32A)-H(32F)	0.9800
C(33)-C(34)	1.514(3)

C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(33A)-C(34A)	1.518(3)
C(33A)-H(33C)	0.9900
C(33A)-H(33D)	0.9900
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(34A)-H(34D)	0.9800
C(34A)-H(34E)	0.9800
C(34A)-H(34F)	0.9800

O(2)-S(1)-O(1)	114.94(8)
O(2)-S(1)-N(2)	111.64(8)
O(1)-S(1)-N(2)	114.28(8)
O(2)-S(1)-N(10)	106.44(7)
O(1)-S(1)-N(10)	106.05(7)
N(2)-S(1)-N(10)	102.16(8)
O(1A)-S(1A)-O(2A)	115.53(8)
O(1A)-S(1A)-N(2A)	114.91(8)
O(2A)-S(1A)-N(2A)	111.23(8)
O(1A)-S(1A)-N(10A)	106.44(8)
O(2A)-S(1A)-N(10A)	106.09(7)
N(2A)-S(1A)-N(10A)	101.04(8)
C(3)-N(2)-S(1)	123.59(13)
C(3A)-N(2A)-S(1A)	121.59(13)
C(3)-N(3)-C(31)	121.87(15)
C(3)-N(3)-C(33)	120.67(15)
C(31)-N(3)-C(33)	117.30(14)
C(3A)-N(3A)-C(33A)	119.32(15)
C(3A)-N(3A)-C(31A)	121.37(14)
C(33A)-N(3A)-C(31A)	119.28(14)
C(4)-N(4)-C(3)	115.74(15)
C(4A)-N(4A)-C(3A)	115.69(14)
C(4)-N(5)-C(5)	110.30(14)
C(4)-N(5)-N(6)	126.75(14)
C(5)-N(5)-N(6)	122.70(14)
C(4A)-N(5A)-C(5A)	110.11(14)
C(4A)-N(5A)-N(6A)	126.76(14)
C(5A)-N(5A)-N(6A)	123.12(14)
N(5)-N(6)-H(6N)	109.9(14)
N(5)-N(6)-H(7N)	108.4(13)
H(6N)-N(6)-H(7N)	111.5(19)
N(5A)-N(6A)-H(6AN)	108.9(13)
N(5A)-N(6A)-H(7AN)	107.5(14)
H(6AN)-N(6A)-H(7AN)	111.7(19)
C(4)-N(10)-C(10)	109.01(14)
C(4)-N(10)-S(1)	118.14(12)
C(10)-N(10)-S(1)	127.35(12)
C(4A)-N(10A)-C(10A)	109.22(14)
C(4A)-N(10A)-S(1A)	117.61(12)
C(10A)-N(10A)-S(1A)	129.71(12)
N(3)-C(3)-N(2)	116.41(15)
N(3)-C(3)-N(4)	116.97(15)
N(2)-C(3)-N(4)	126.62(16)
N(3A)-C(3A)-N(2A)	116.60(15)
N(3A)-C(3A)-N(4A)	117.23(15)
N(2A)-C(3A)-N(4A)	126.09(16)
N(4)-C(4)-N(5)	124.78(15)
N(4)-C(4)-N(10)	128.22(16)
N(5)-C(4)-N(10)	106.96(15)
N(4A)-C(4A)-N(5A)	125.13(15)
N(4A)-C(4A)-N(10A)	127.78(15)
N(5A)-C(4A)-N(10A)	107.08(14)
C(6)-C(5)-C(10)	122.01(16)
C(6)-C(5)-N(5)	130.83(16)
C(10)-C(5)-N(5)	107.12(15)
C(6A)-C(5A)-C(10A)	121.82(16)
C(6A)-C(5A)-N(5A)	130.81(16)
C(10A)-C(5A)-N(5A)	107.37(15)
C(7)-C(6)-C(5)	116.34(17)
C(7)-C(6)-H(6)	121.8

C(5)-C(6)-H(6)	121.8
C(5A)-C(6A)-C(7A)	116.00(17)
C(5A)-C(6A)-H(6A)	122.0
C(7A)-C(6A)-H(6A)	122.0
C(6)-C(7)-C(8)	121.94(17)
C(6)-C(7)-H(7)	119.0
C(8)-C(7)-H(7)	119.0
C(6A)-C(7A)-C(8A)	122.19(17)
C(6A)-C(7A)-H(7A)	118.9
C(8A)-C(7A)-H(7A)	118.9
C(7)-C(8)-C(9)	121.63(17)
C(7)-C(8)-H(8)	119.2
C(9)-C(8)-H(8)	119.2
C(9A)-C(8A)-C(7A)	121.44(17)
C(9A)-C(8A)-H(8A)	119.3
C(7A)-C(8A)-H(8A)	119.3
C(10)-C(9)-C(8)	116.29(17)
C(10)-C(9)-H(9)	121.9
C(8)-C(9)-H(9)	121.9
C(10A)-C(9A)-C(8A)	116.25(17)
C(10A)-C(9A)-H(9A)	121.9
C(8A)-C(9A)-H(9A)	121.9
C(9)-C(10)-C(5)	121.77(17)
C(9)-C(10)-N(10)	131.85(16)
C(5)-C(10)-N(10)	106.37(14)
C(9A)-C(10A)-C(5A)	122.29(17)
C(9A)-C(10A)-N(10A)	131.55(16)
C(5A)-C(10A)-N(10A)	106.15(14)
N(3)-C(31)-C(32)	112.69(16)
N(3)-C(31)-H(31A)	109.1
C(32)-C(31)-H(31A)	109.1
N(3)-C(31)-H(31B)	109.1
C(32)-C(31)-H(31B)	109.1
H(31A)-C(31)-H(31B)	107.8
N(3A)-C(31A)-C(32A)	112.96(15)
N(3A)-C(31A)-H(31C)	109.0
C(32A)-C(31A)-H(31C)	109.0
N(3A)-C(31A)-H(31D)	109.0
C(32A)-C(31A)-H(31D)	109.0
H(31C)-C(31A)-H(31D)	107.8
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31A)-C(32A)-H(32D)	109.5
C(31A)-C(32A)-H(32E)	109.5
H(32D)-C(32A)-H(32E)	109.5
C(31A)-C(32A)-H(32F)	109.5
H(32D)-C(32A)-H(32F)	109.5
H(32E)-C(32A)-H(32F)	109.5
N(3)-C(33)-C(34)	113.84(16)
N(3)-C(33)-H(33A)	108.8
C(34)-C(33)-H(33A)	108.8
N(3)-C(33)-H(33B)	108.8
C(34)-C(33)-H(33B)	108.8
H(33A)-C(33)-H(33B)	107.7
N(3A)-C(33A)-C(34A)	113.03(16)
N(3A)-C(33A)-H(33C)	109.0
C(34A)-C(33A)-H(33C)	109.0
N(3A)-C(33A)-H(33D)	109.0
C(34A)-C(33A)-H(33D)	109.0
H(33C)-C(33A)-H(33D)	107.8
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33A)-C(34A)-H(34D)	109.5
C(33A)-C(34A)-H(34E)	109.5

H(34D)-C(34A)-H(34E)	109.5
C(33A)-C(34A)-H(34F)	109.5
H(34D)-C(34A)-H(34F)	109.5
H(34E)-C(34A)-H(34F)	109.5

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) .

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
S(1)	14(1)	21(1)	15(1)	-2(1)	4(1)	0(1)
S(1A)	14(1)	23(1)	15(1)	-1(1)	4(1)	-1(1)
O(1)	26(1)	25(1)	26(1)	3(1)	11(1)	-3(1)
O(2A)	19(1)	33(1)	16(1)	-2(1)	2(1)	4(1)
O(2)	18(1)	32(1)	16(1)	-1(1)	1(1)	4(1)
O(1A)	27(1)	31(1)	26(1)	1(1)	12(1)	-9(1)
N(2)	18(1)	27(1)	23(1)	-9(1)	7(1)	1(1)
N(2A)	18(1)	23(1)	19(1)	-4(1)	6(1)	2(1)
N(3)	18(1)	22(1)	20(1)	-5(1)	8(1)	-1(1)
N(3A)	16(1)	21(1)	20(1)	-4(1)	8(1)	-1(1)
N(4)	18(1)	18(1)	17(1)	-2(1)	7(1)	-1(1)
N(4A)	17(1)	20(1)	15(1)	-2(1)	6(1)	0(1)
N(5)	15(1)	19(1)	17(1)	-3(1)	5(1)	0(1)
N(5A)	15(1)	21(1)	15(1)	-2(1)	3(1)	2(1)
N(6)	15(1)	27(1)	21(1)	-3(1)	4(1)	-1(1)
N(6A)	15(1)	32(1)	20(1)	-5(1)	2(1)	2(1)
N(10)	15(1)	20(1)	17(1)	-3(1)	6(1)	0(1)
N(10A)	16(1)	20(1)	17(1)	-3(1)	6(1)	0(1)
C(3)	19(1)	17(1)	17(1)	0(1)	7(1)	0(1)
C(3A)	19(1)	19(1)	15(1)	1(1)	8(1)	-2(1)
C(4)	15(1)	19(1)	15(1)	2(1)	5(1)	0(1)
C(4A)	15(1)	17(1)	13(1)	3(1)	4(1)	1(1)
C(5)	21(1)	19(1)	14(1)	1(1)	7(1)	-1(1)
C(5A)	21(1)	17(1)	15(1)	1(1)	7(1)	-1(1)
C(6)	25(1)	20(1)	22(1)	3(1)	12(1)	5(1)
C(6A)	24(1)	21(1)	22(1)	4(1)	9(1)	5(1)
C(7)	36(1)	20(1)	19(1)	1(1)	15(1)	6(1)
C(7A)	35(1)	19(1)	21(1)	-1(1)	15(1)	2(1)
C(8)	37(1)	22(1)	18(1)	-5(1)	11(1)	-3(1)
C(8A)	33(1)	23(1)	20(1)	-5(1)	11(1)	-5(1)
C(9)	27(1)	24(1)	17(1)	-2(1)	7(1)	-1(1)
C(9A)	25(1)	23(1)	20(1)	-1(1)	6(1)	-2(1)
C(10)	23(1)	17(1)	15(1)	1(1)	9(1)	2(1)
C(10A)	21(1)	15(1)	16(1)	1(1)	8(1)	2(1)
C(31)	22(1)	22(1)	26(1)	-9(1)	10(1)	-4(1)
C(31A)	20(1)	24(1)	24(1)	-8(1)	8(1)	-4(1)
C(32)	29(1)	35(1)	29(1)	-6(1)	6(1)	4(1)
C(32A)	34(1)	35(1)	22(1)	-4(1)	6(1)	1(1)
C(33)	25(1)	27(1)	23(1)	-4(1)	12(1)	2(1)
C(33A)	24(1)	27(1)	29(1)	-7(1)	15(1)	1(1)
C(34)	32(1)	38(1)	25(1)	0(1)	12(1)	9(1)
C(34A)	30(1)	41(1)	37(1)	-5(1)	21(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3).

	x	y	z	U(eq)
H(6)	-2008	7423	4754	26
H(6A)	-6960	7579	-375	26
H(7)	-1088	8442	6128	29
H(7A)	-6025	8488	1135	28
H(8)	564	8388	6898	31
H(8A)	-4384	8323	2011	30
H(9)	1381	7300	6331	28
H(9A)	-3592	7216	1435	28
H(31A)	-1046	3793	1912	28
H(31B)	-501	3206	1343	28
H(31C)	-6126	3822	-3097	28
H(31D)	-5588	3115	-3547	28
H(32A)	-1761	3992	-16	49
H(32B)	-1315	4923	572	49
H(32C)	-770	4336	2	49
H(32D)	-6545	4062	-4990	48
H(32E)	-5985	4920	-4301	48
H(32F)	-5447	4212	-4751	48
H(33A)	1480	4659	2087	29
H(33B)	858	3974	1134	29
H(33C)	-3982	3061	-2890	31
H(33D)	-3401	3497	-1695	31
H(34A)	2258	3271	2366	47
H(34B)	1976	3472	3380	47
H(34C)	1354	2786	2426	47
H(34D)	-2704	3916	-2904	50
H(34E)	-3690	4352	-3739	50
H(34F)	-3109	4789	-2543	50
H(6AN)	-7164(14)	6114(13)	-2628(18)	27(6)
H(6N)	-2348(16)	5500(15)	3429(17)	38(6)
H(7AN)	-7335(16)	5661(14)	-1726(17)	33(6)
H(7N)	-2220(14)	5964(13)	2521(18)	24(6)

Table 6. Hydrogen bonds [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(7N)...O(2A)	0.89(2)	2.16(2)	3.005(2)	158.2(17)
N(6)-H(6N)...O(2)#1	0.88(2)	2.20(2)	3.020(2)	153.4(19)
N(6A)-H(6AN)...O(2)#2	0.89(2)	2.25(2)	3.083(2)	156.4(17)
N(6A)-H(7AN)...O(2A)#3	0.91(2)	2.26(2)	3.086(2)	151.9(19)

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