Supporting Information

A Straightforward Synthesis of Functionalized *cis*-Perhydroisoquinolin-1-ones

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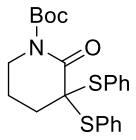
Contents

I) Copies of ^{1}H- and ^{13}C-NMR spectra



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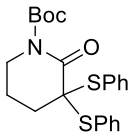

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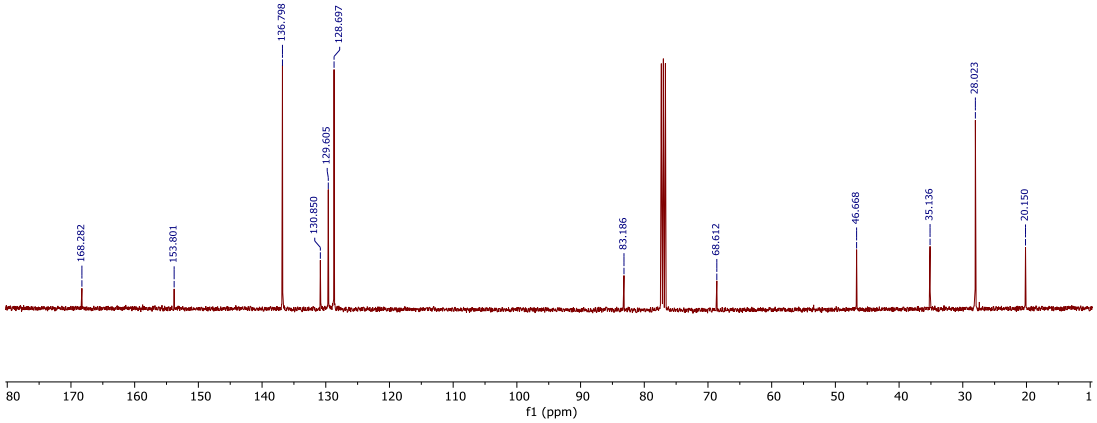

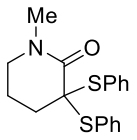

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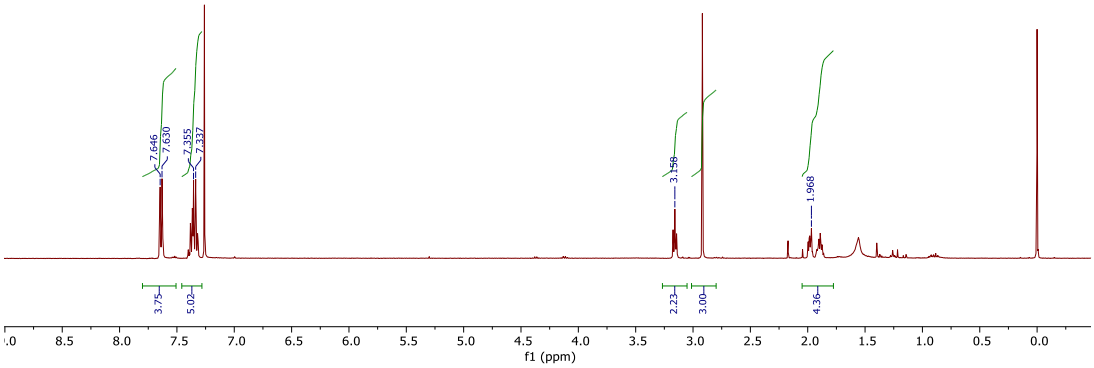

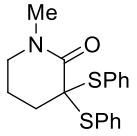

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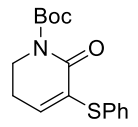

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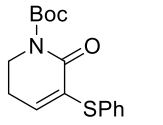

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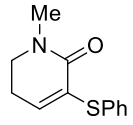

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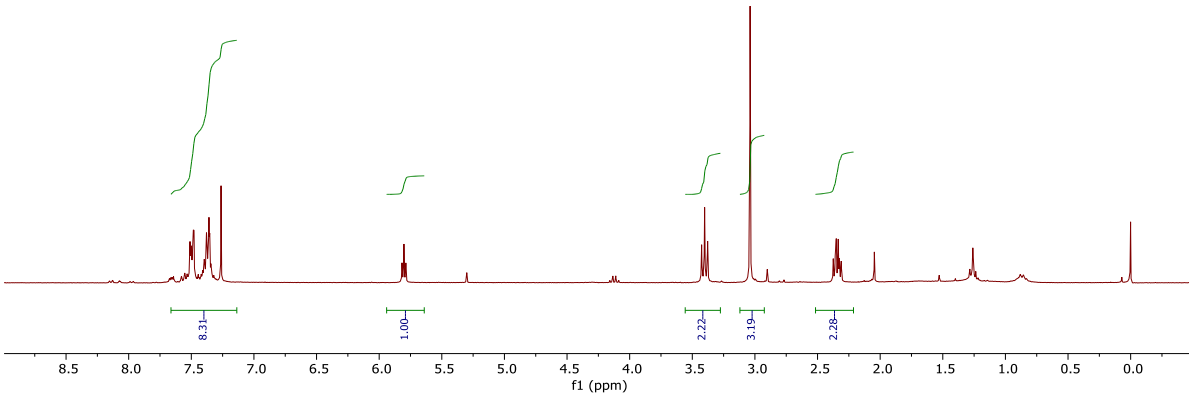

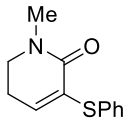

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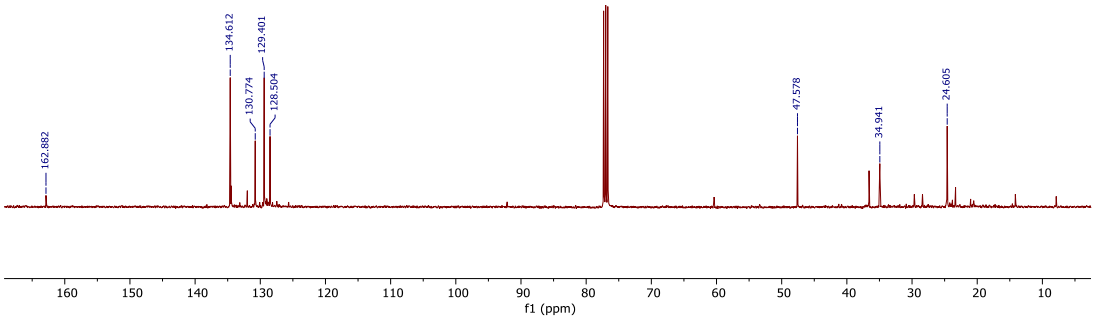

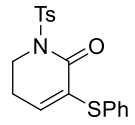

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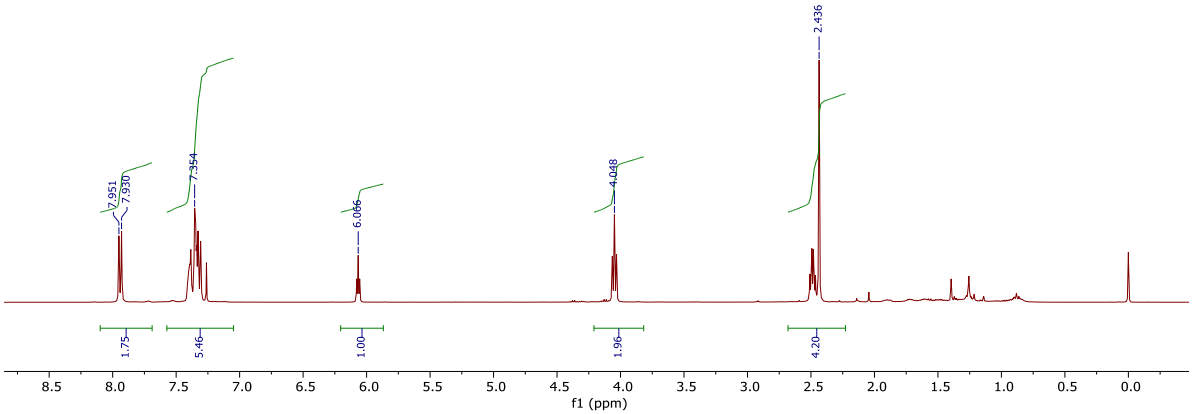

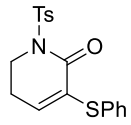

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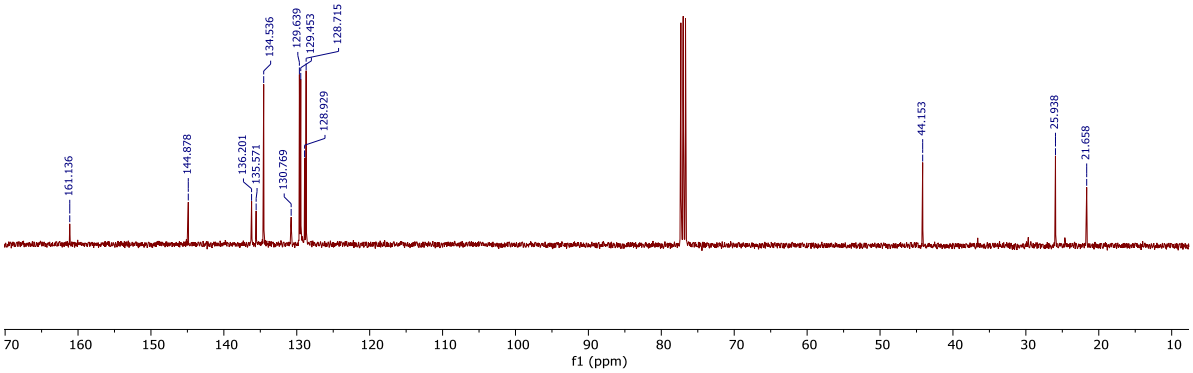

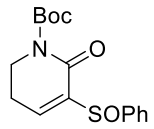

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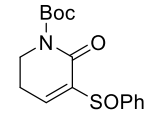

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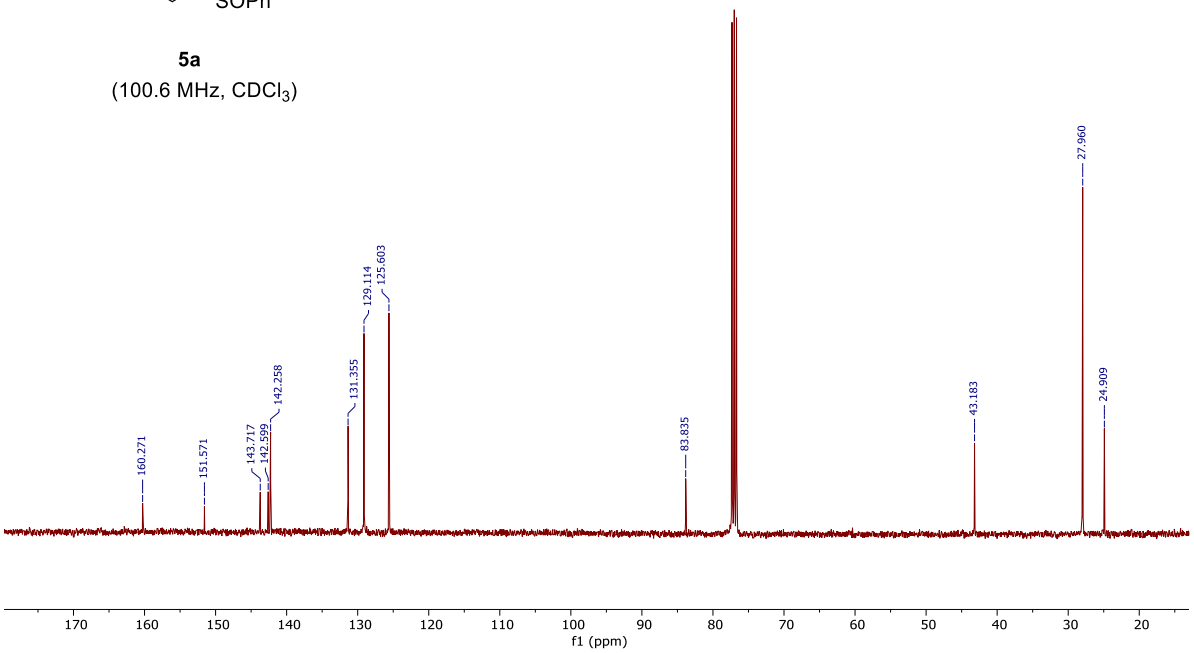

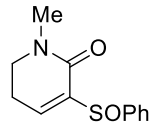

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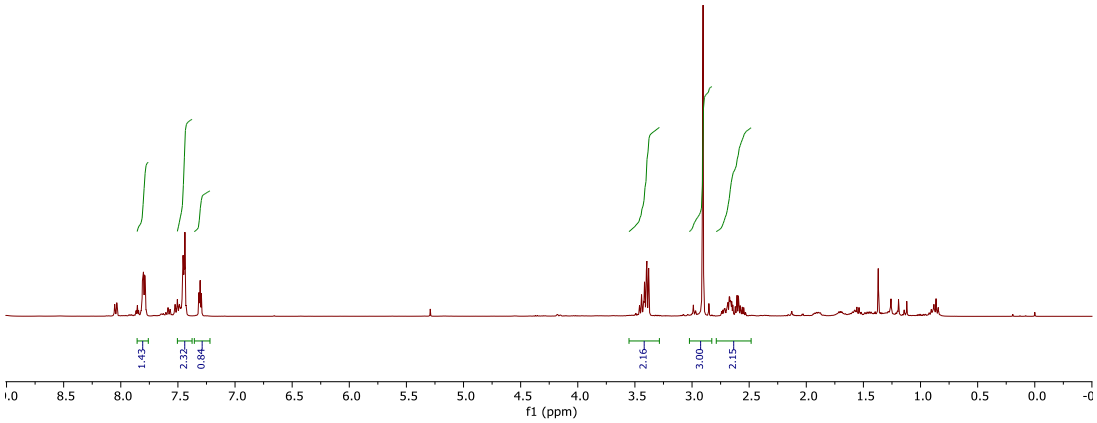

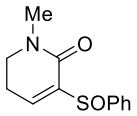

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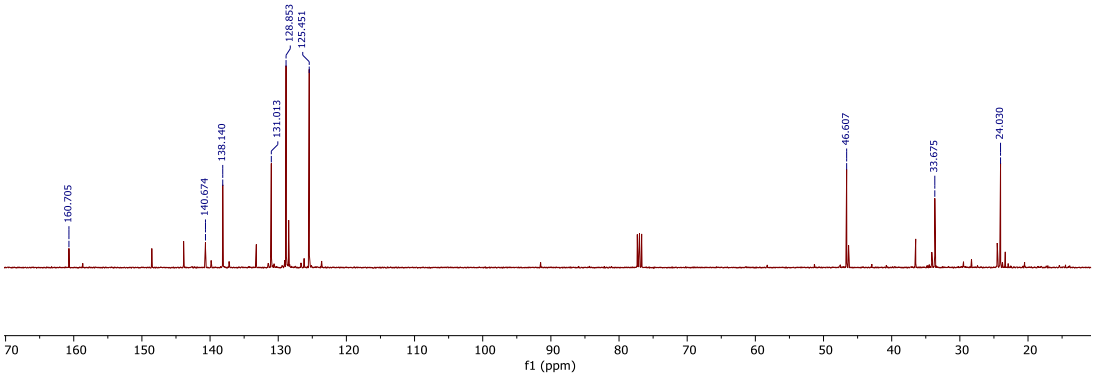

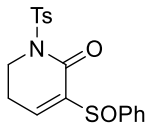

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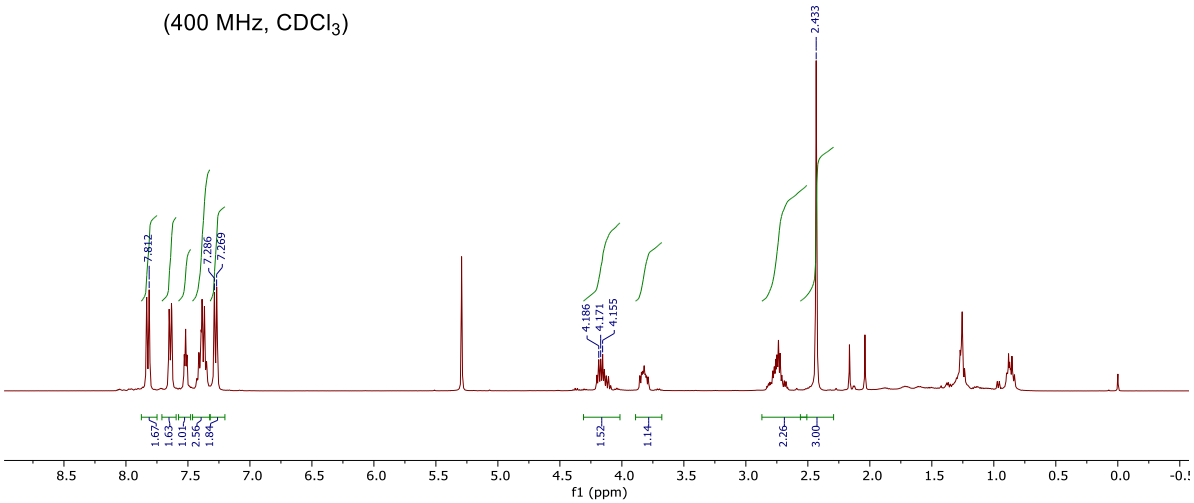

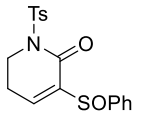

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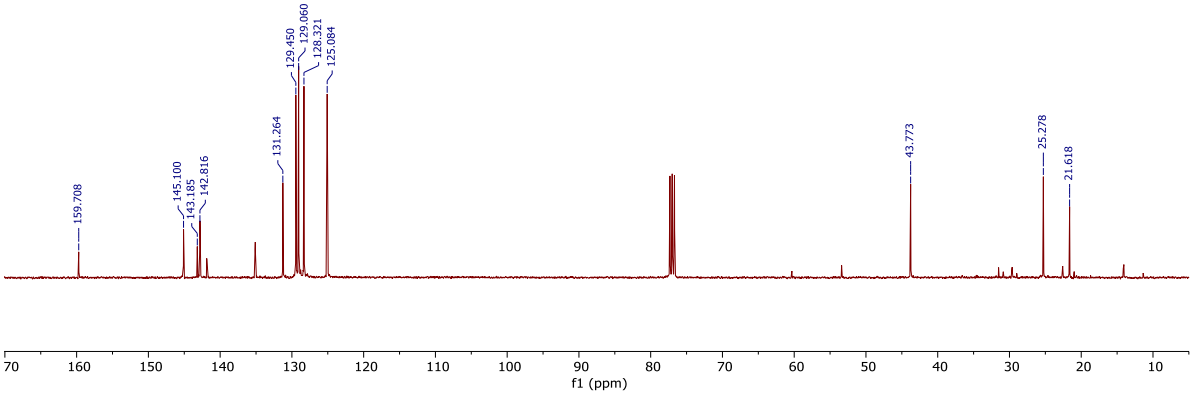

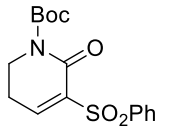

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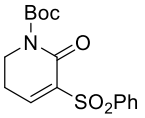

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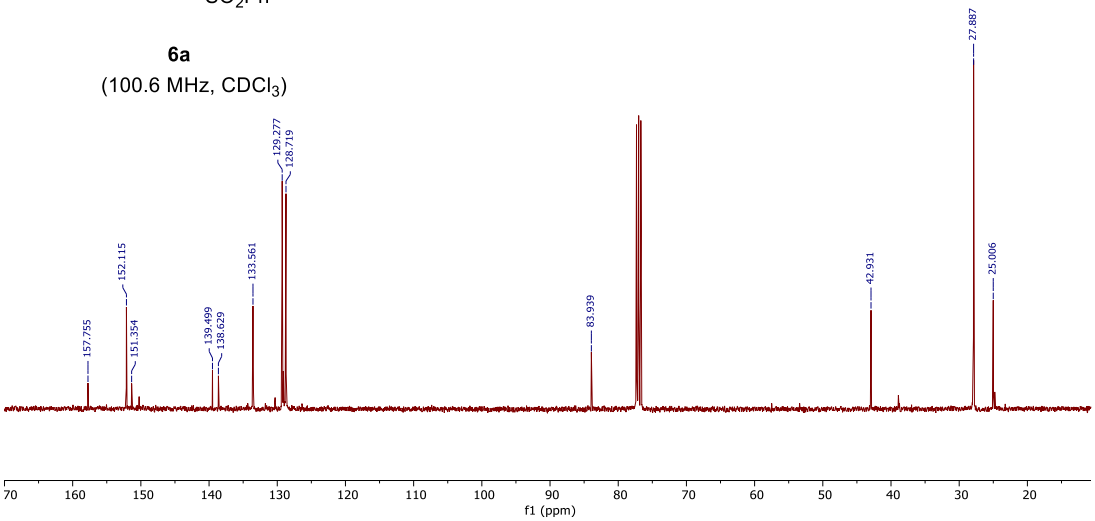

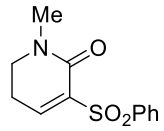

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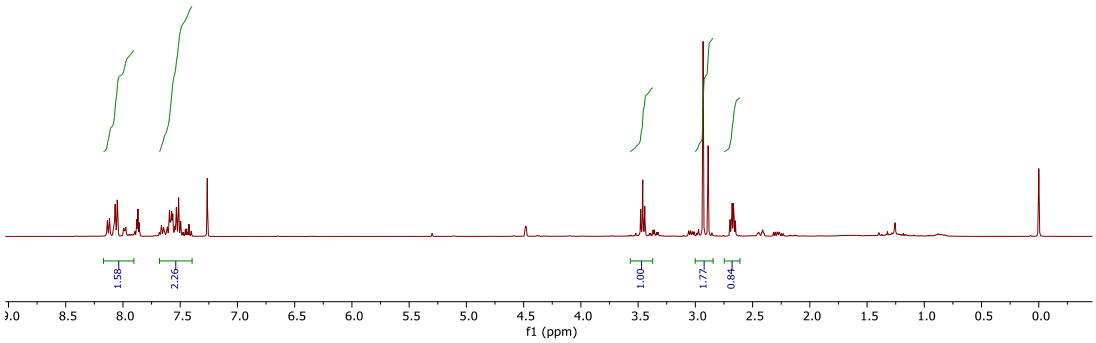

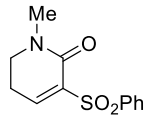

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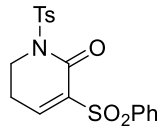

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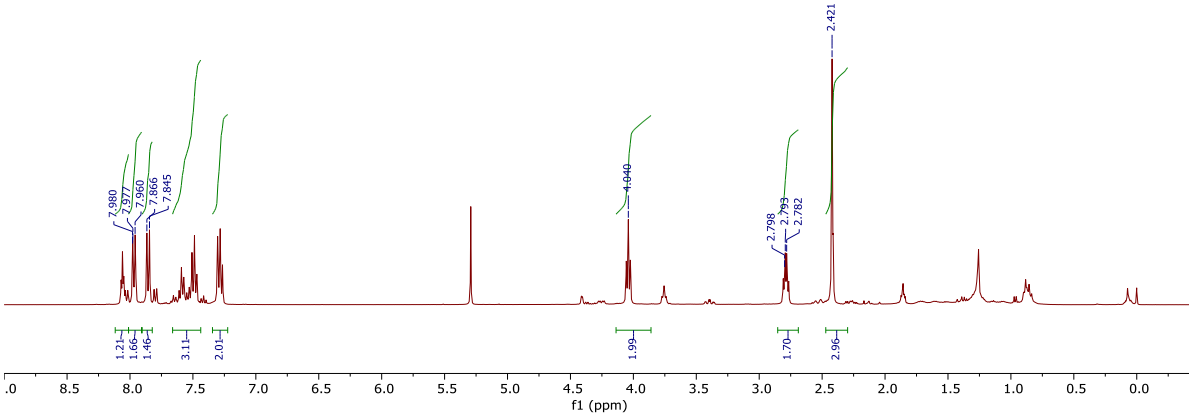

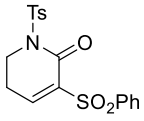

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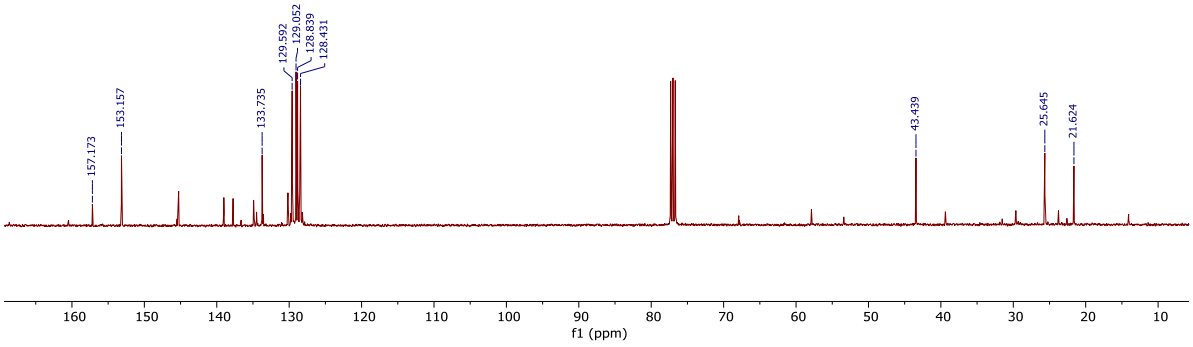

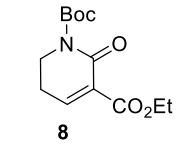

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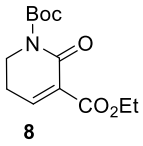

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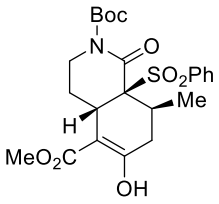

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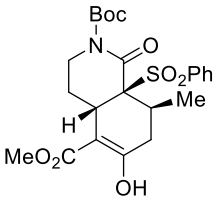

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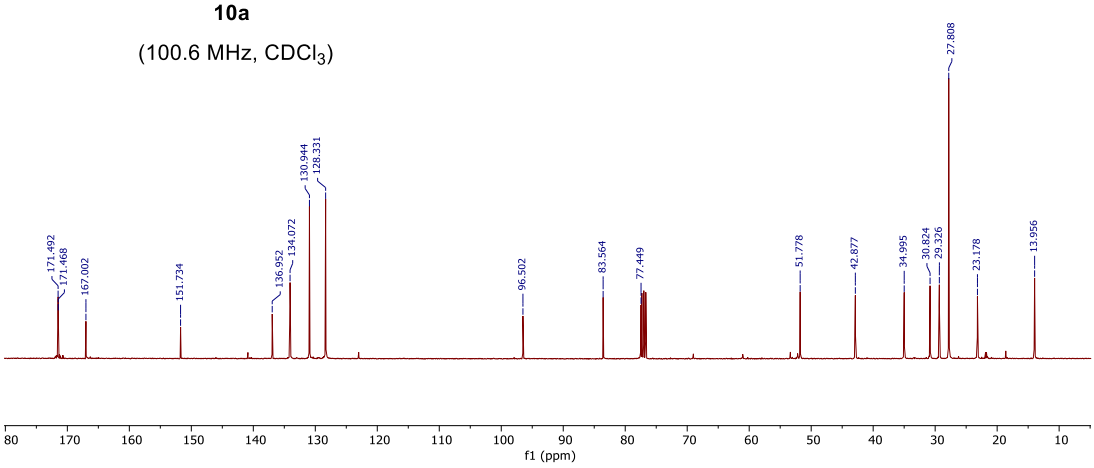

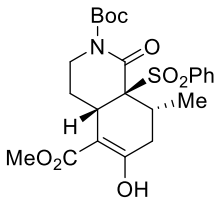

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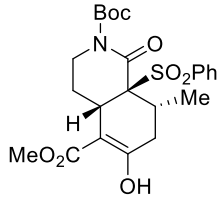

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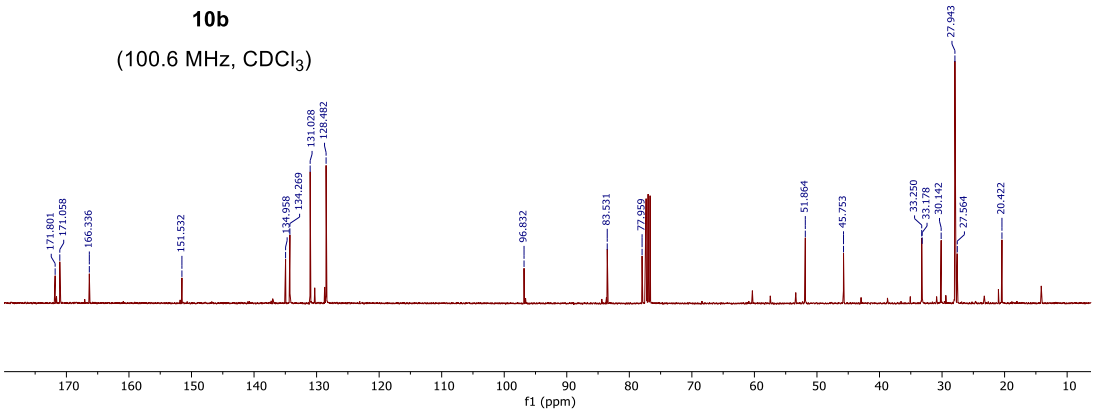

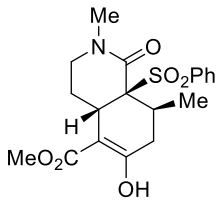

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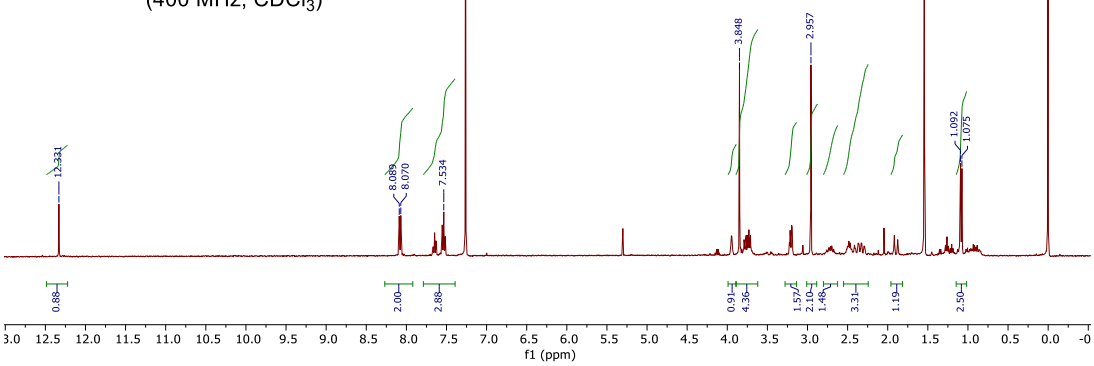

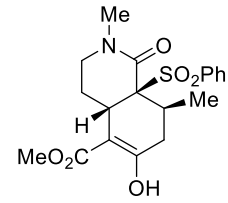

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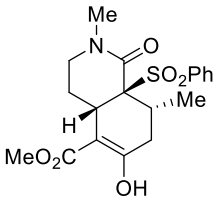

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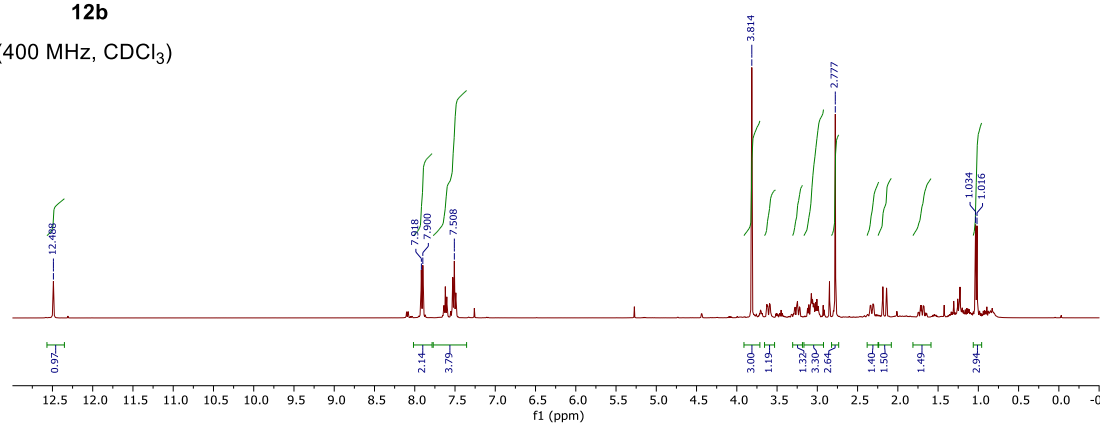

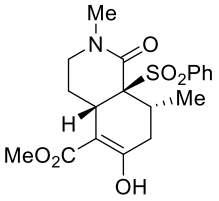

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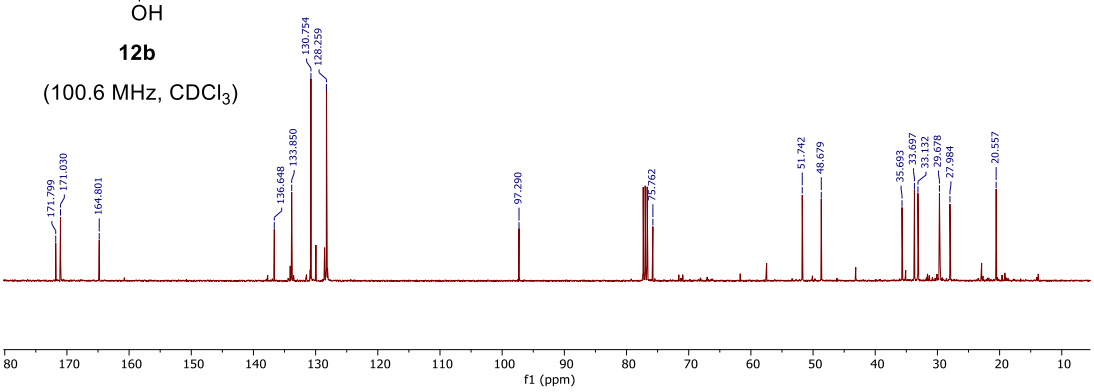

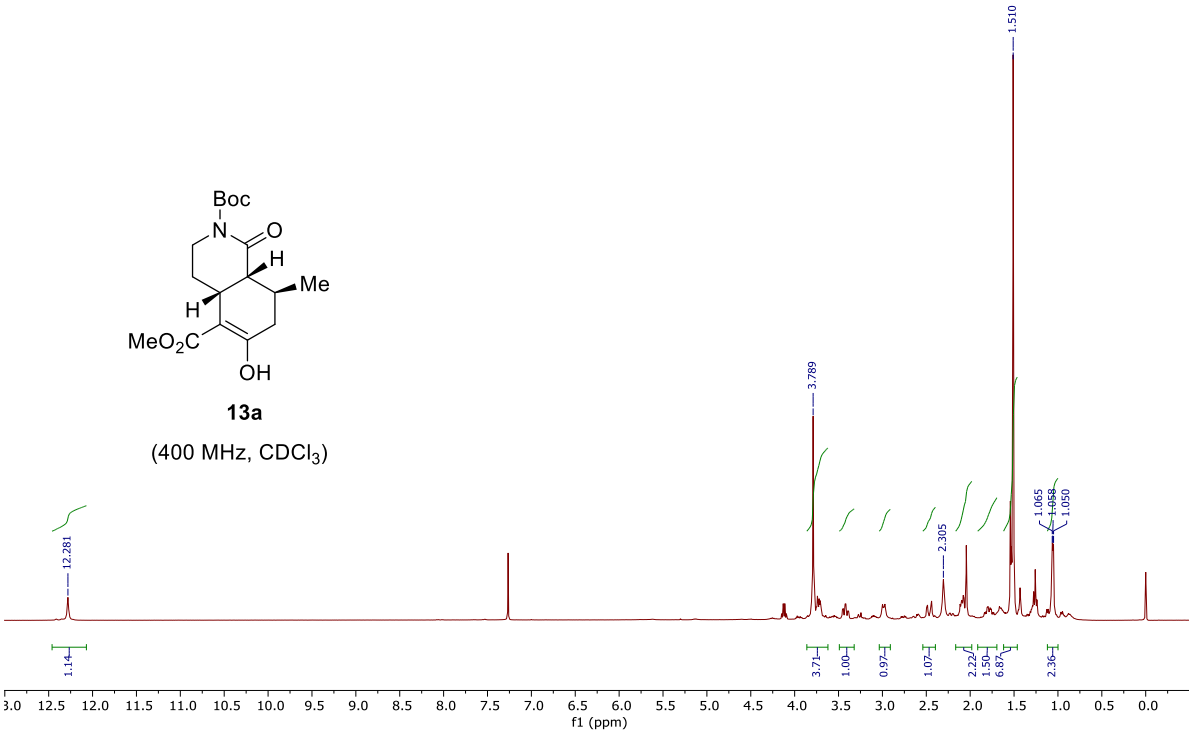
Boc
N
O
H
Me
H
MeO2C
OH
13a
(400 MHz, CDCl3)
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2.305
1.065
1.058
1.050
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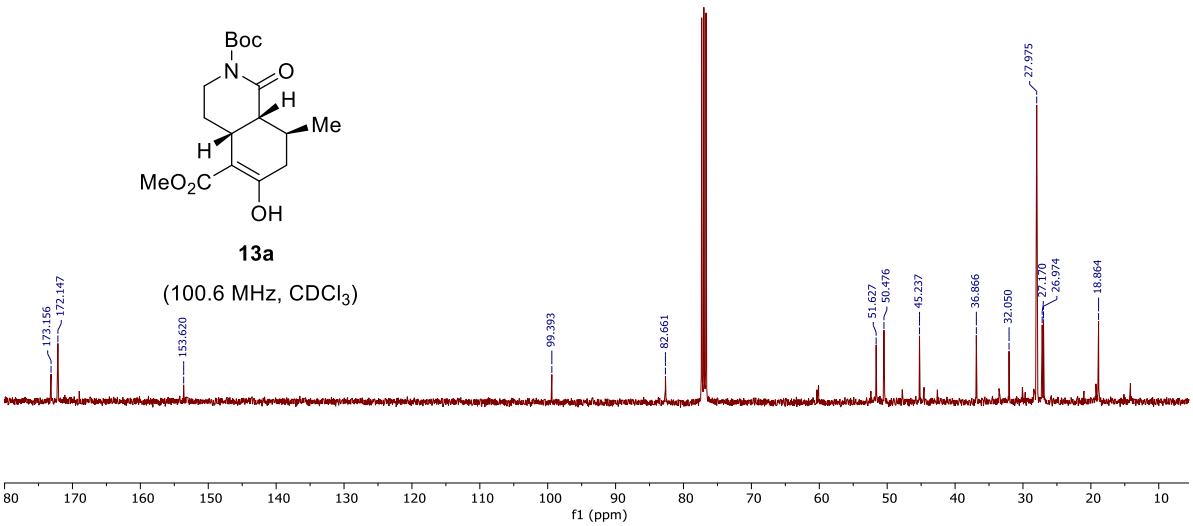
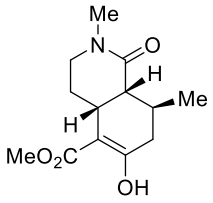
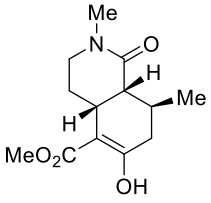
1.14
3.71
1.00
0.97
1.07
2.22
1.50
6.87
2.36
f1 (ppm)


Boc
N
O
H
Me
H
MeO2C
OH
13a
(100.6 MHz, CDCl3)
27.975
173.156
172.147
153.620
99.393
82.661
51.627
50.476
45.237
36.866
32.050
27.170
26.974
18.864
f1 (ppm)



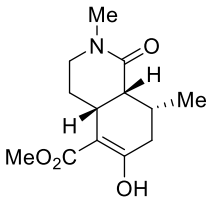
14a

(400 MHz, $CDCl_3$)



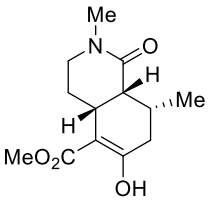
14a

(100.6 MHz, $CDCl_3$)



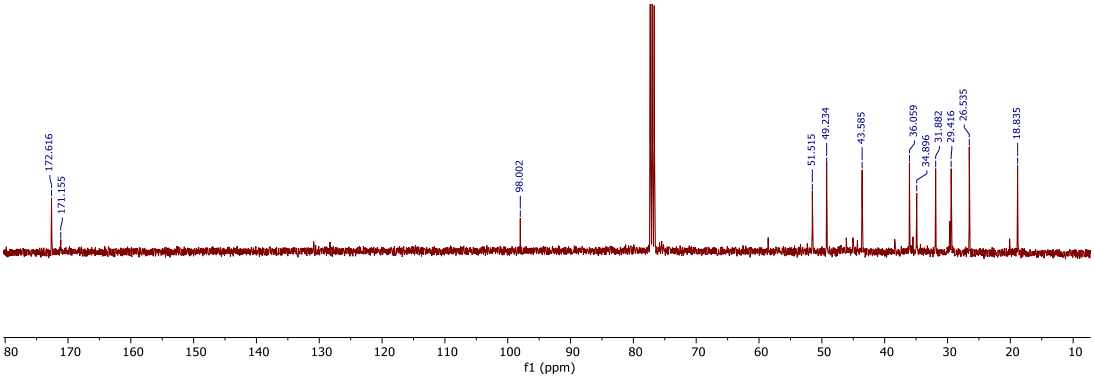
14b

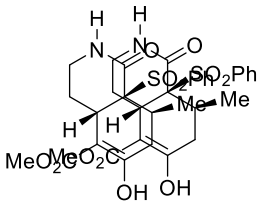
(400 MHz, $CDCl_3$)



14b

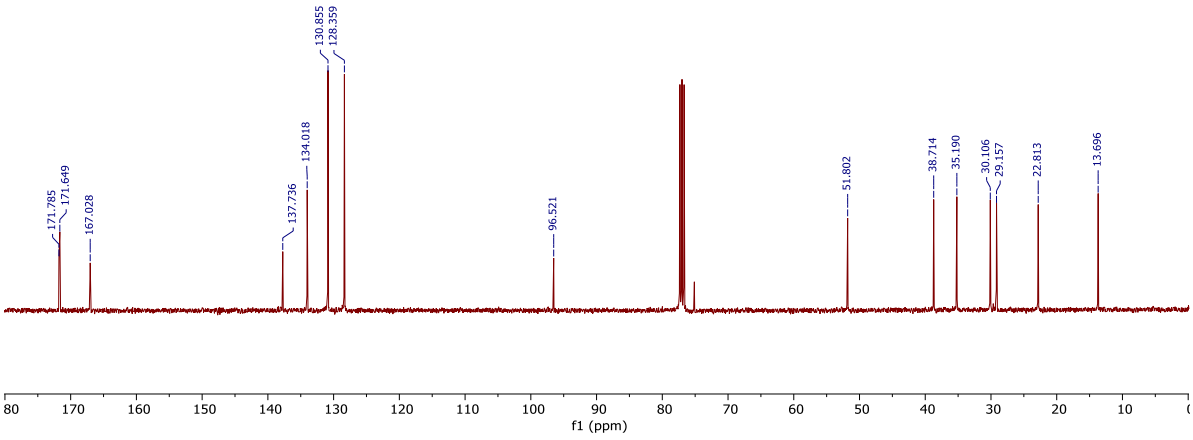
(100.6 MHz, $CDCl_3$)

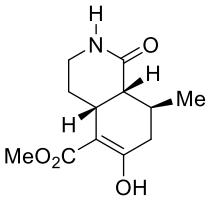




15 **15**

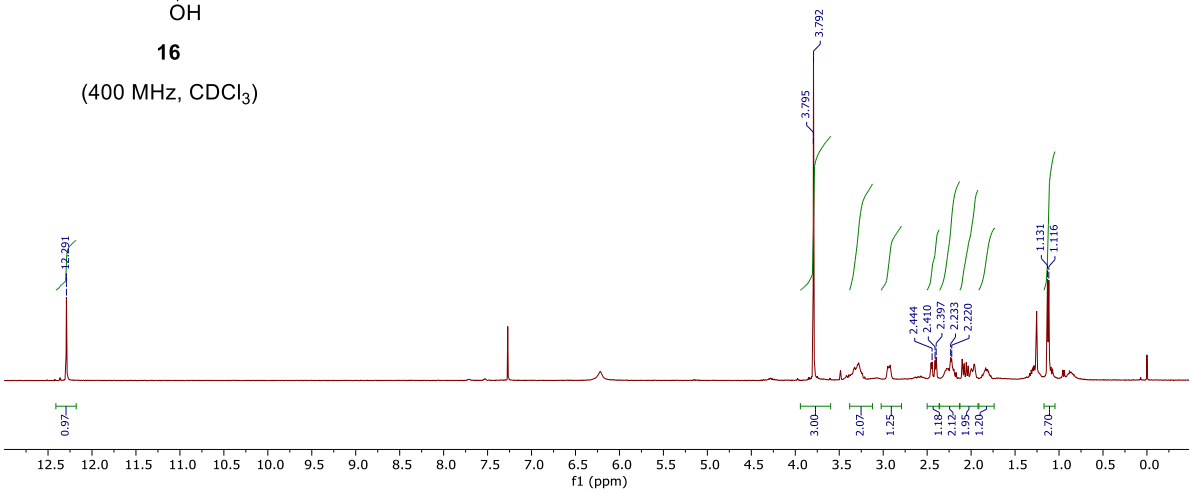
(400 MHz, $CDCl_3$) (100.6 MHz, $CDCl_3$)

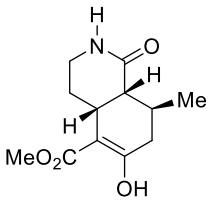




16

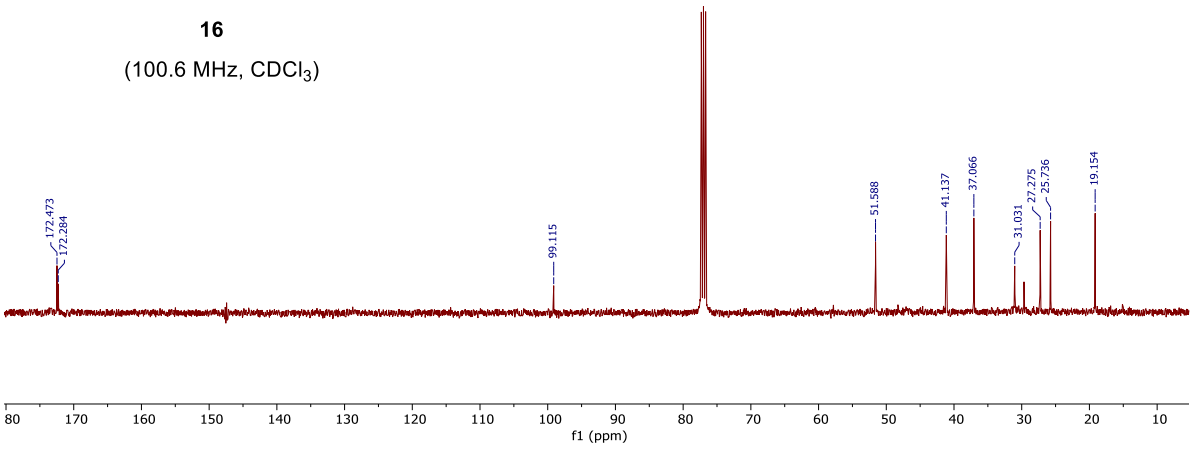
(400 MHz, $CDCl_3$)

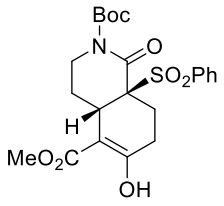




16

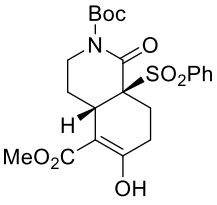
(100.6 MHz, $CDCl_3$)





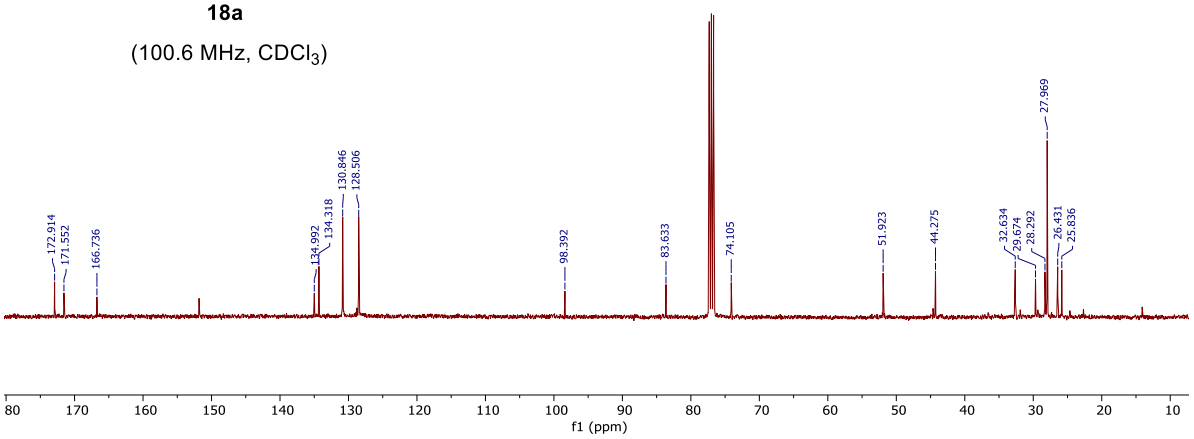
18a

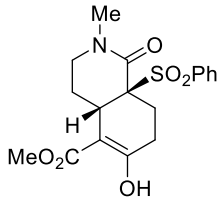
(400 MHz, $CDCl_3$)



18a

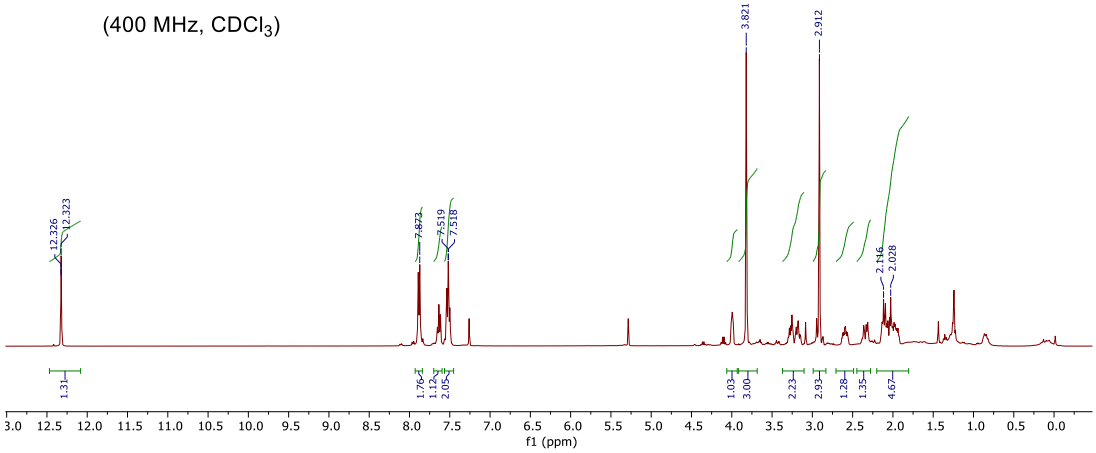
(100.6 MHz, $CDCl_3$)

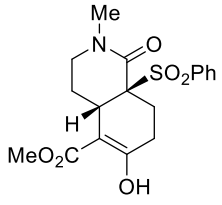




18b

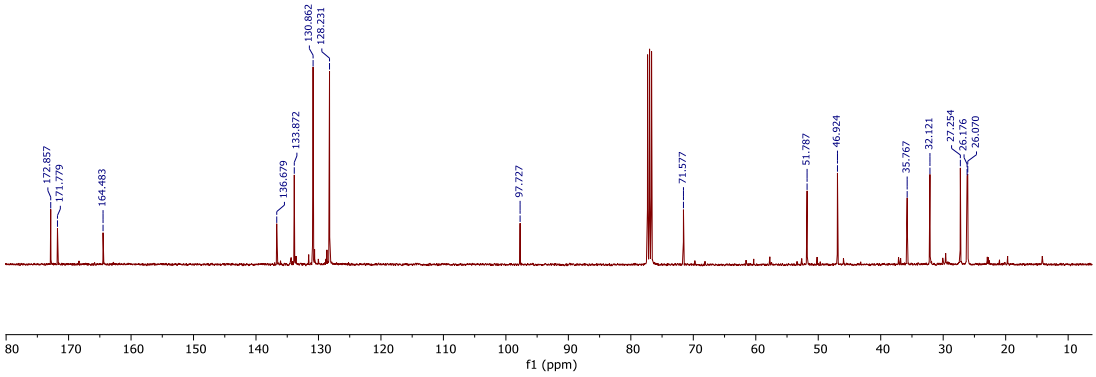
(400 MHz, $CDCl_3$)

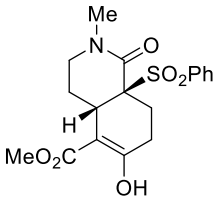




18b

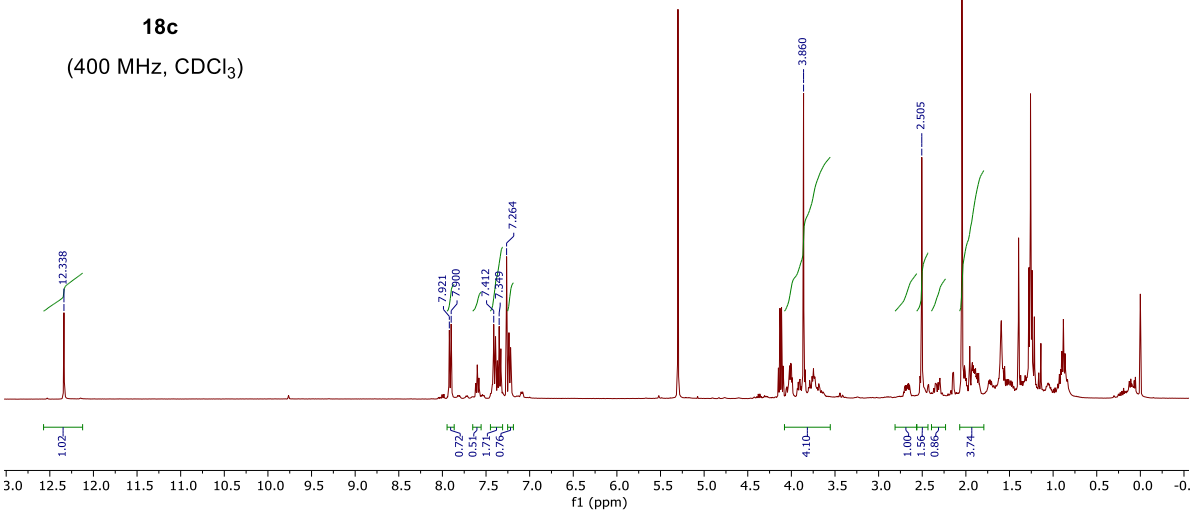
(100.6 MHz, $CDCl_3$)

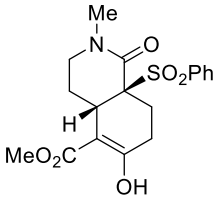




18c

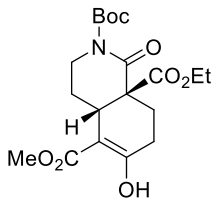
(400 MHz, $CDCl_3$)





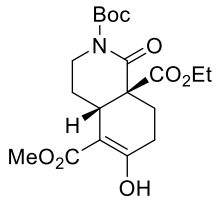
18c

(100.6 MHz, $CDCl_3$)



19

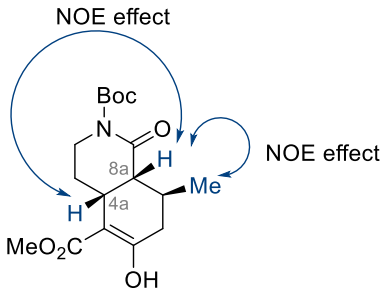
(400 MHz, $CDCl_3$)



19

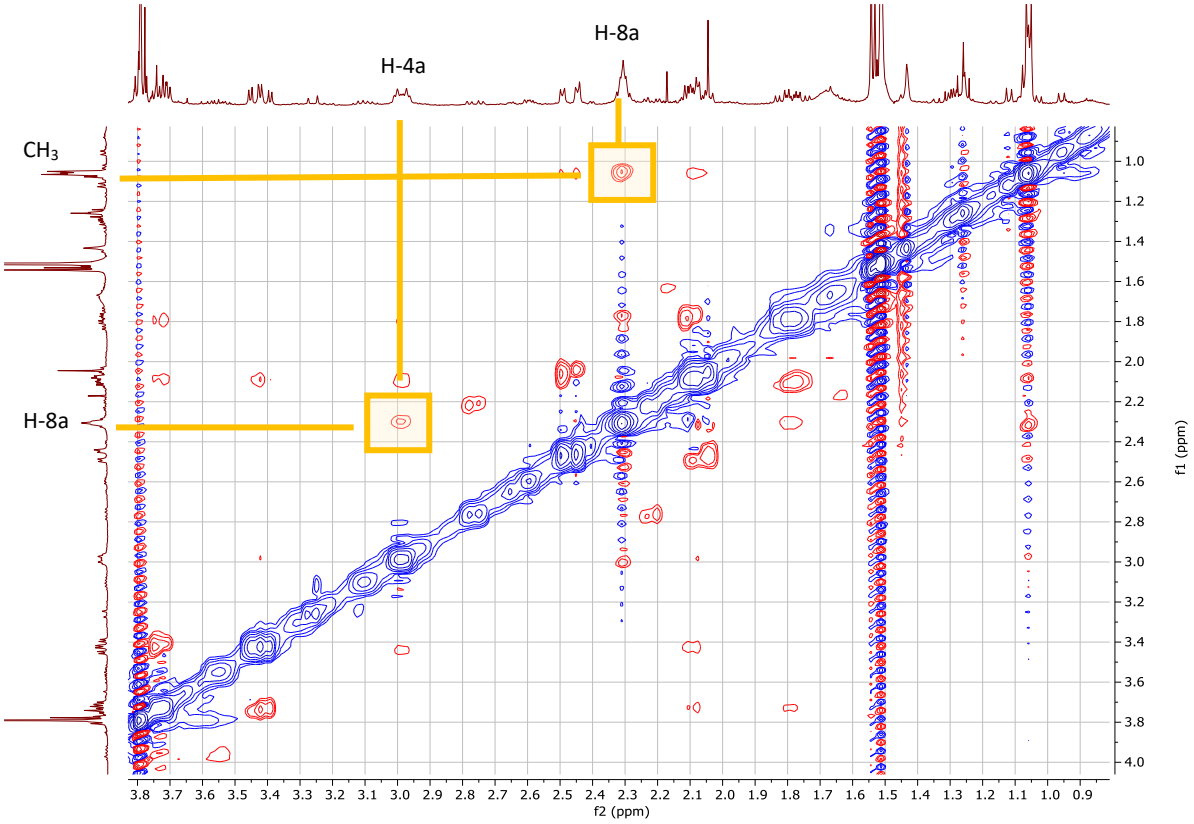
(100.6 MHz, $CDCl_3$)

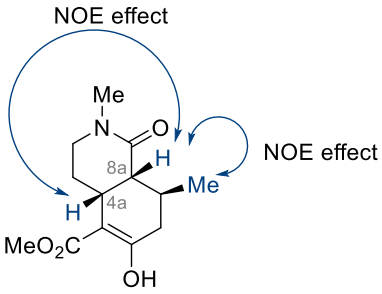
II) Copies of NOE NMR spectra **13a**, **14a**, and **14b**



13a

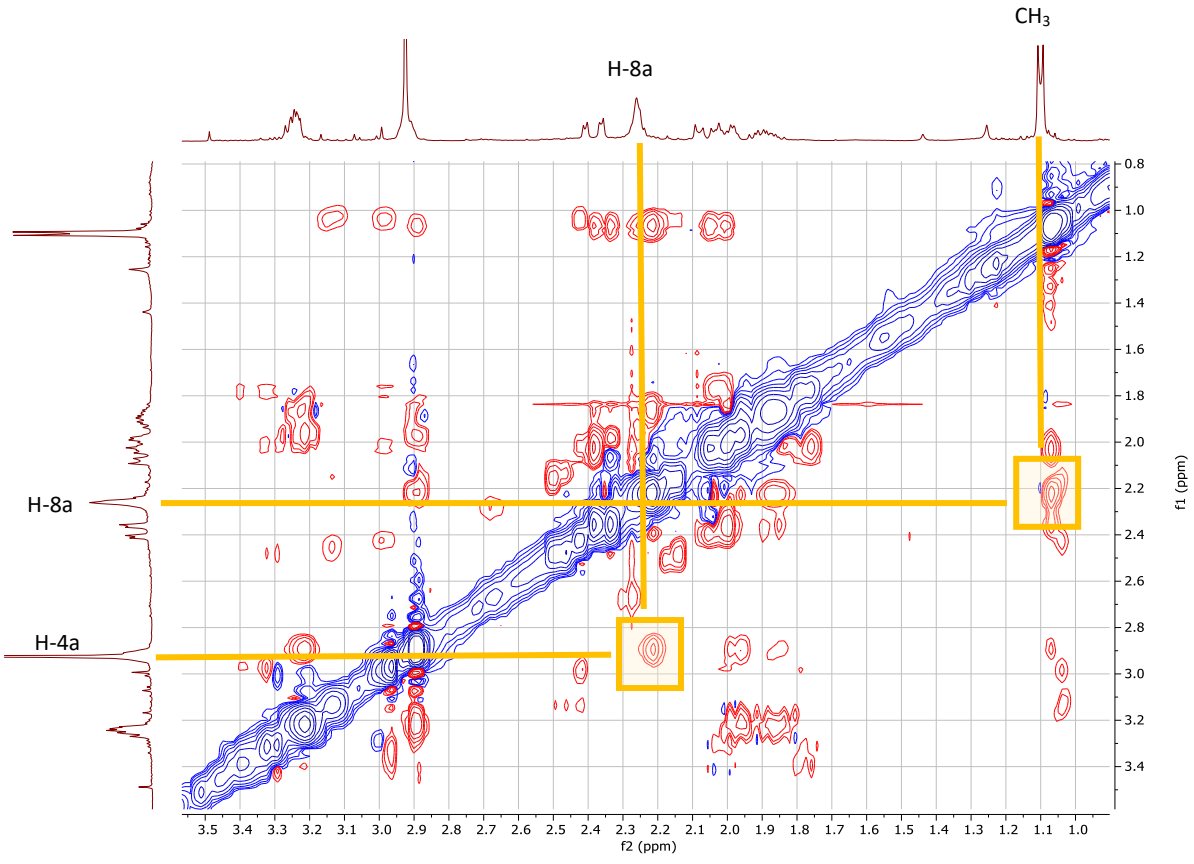
(400 MHz, $CDCl_3$)

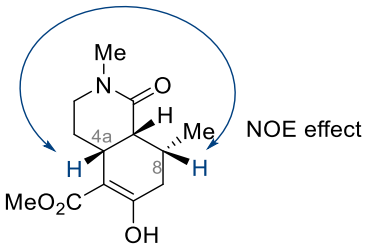




14a

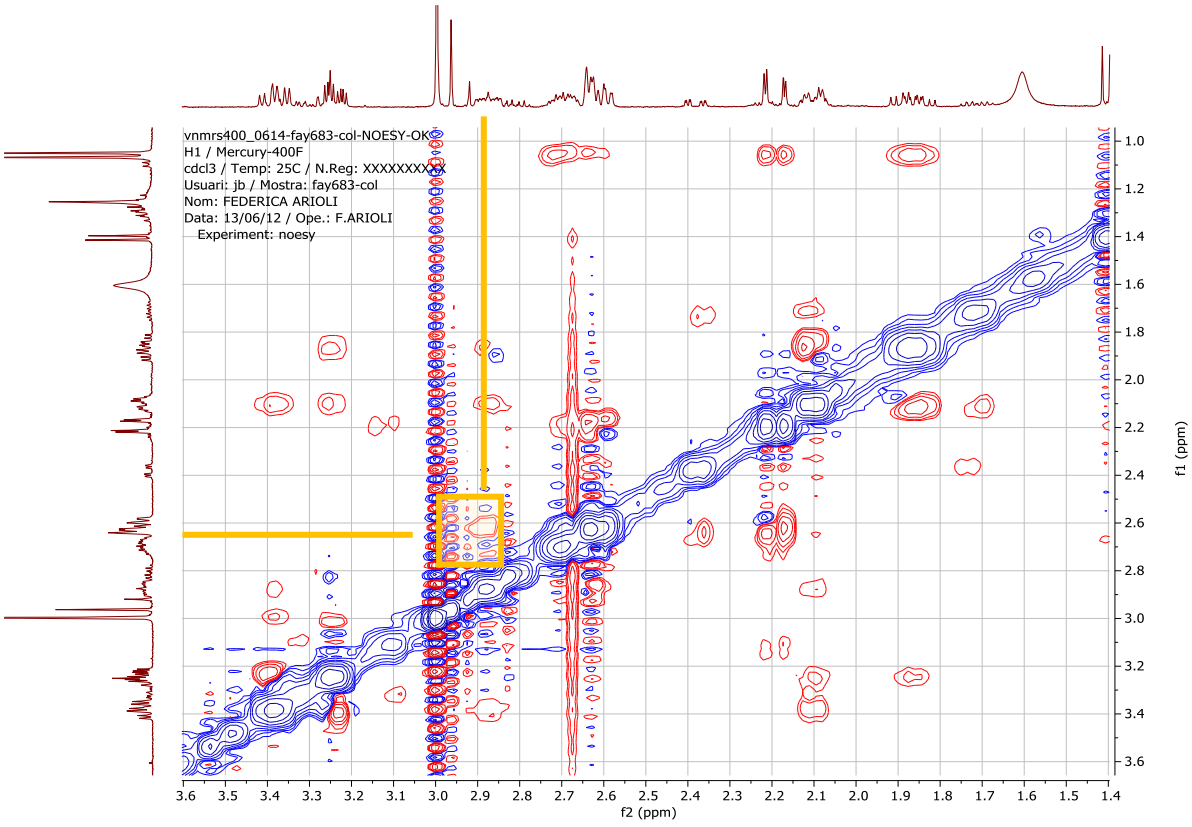
(400 MHz, $CDCl_3$)



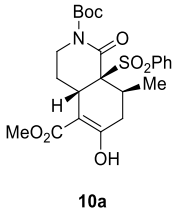


14b

(400 MHz, $CDCl_3$)



III) X- ray crystallographic data for compounds **10a**, **12a**, and **12b**



10a

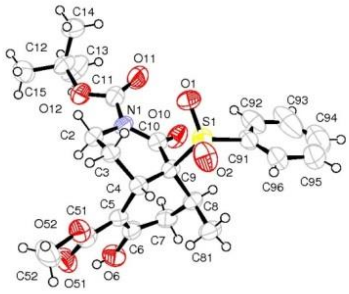


Table S1. Crystal data and structure refinement for compound **10a**.

Identification code	Jb95	
Empirical formula	C23 H29 N O8 S	
Formula weight	479.53	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.948(3) Å	= 90°.
	b = 10.790(3) Å	= 90°.
	c = 27.749(9) Å	= 90°.
Volume	2379.7(14) $Å^3$	
Z	4	
Density (calculated)	1.338 Mg/m^3	
Absorption coefficient	0.184 mm^{-1}	
F(000)	1016	
Crystal size	0.45 x 0.27 x 0.15 mm^3	
Theta range for data collection	1.47 to 24.96°.	
Index ranges	0<=h<=9, 0<=k<=12, 0<=l<=32	
Reflections collected	2468	
Independent reflections	2398 [R(int) = 0.0534]	
Completeness to theta = 24.96°	99.8 %	
Max. and min. transmission	0.9729 and 0.9218	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2398 / 0 / 304	
Goodness-of-fit on F^2	0.958	
Final R indices [I>2sigma(I)]	R1 = 0.0559, wR2 = 0.1214	
R indices (all data)	R1 = 0.1161, wR2 = 0.1470	
Absolute structure parameter	-0.1(2)	
Largest diff. peak and hole	0.220 and -0.256 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jb95. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6582(2)	1618(2)	4083(1)	57(1)
O(1)	8167(6)	1911(5)	3856(2)	75(2)
O(2)	6553(7)	1294(4)	4584(2)	76(2)
O(6)	1414(6)	5630(5)	4169(2)	79(2)
O(10)	5358(6)	3177(5)	3147(2)	68(2)
O(11)	8107(8)	4282(5)	2805(2)	89(2)
O(12)	8266(7)	6097(5)	3187(2)	70(1)
O(51)	2924(7)	6523(5)	4904(2)	80(2)
O(52)	4939(7)	5391(5)	5234(2)	68(1)
N(1)	6969(7)	4561(5)	3565(2)	53(2)
C(2)	7303(8)	5248(6)	4012(2)	53(2)
C(3)	7099(8)	4426(7)	4449(2)	53(2)
C(4)	5357(8)	3813(6)	4450(2)	46(2)
C(5)	3927(8)	4767(6)	4474(2)	47(2)
C(6)	2625(9)	4752(7)	4167(3)	58(2)
C(7)	2348(8)	3766(7)	3807(3)	60(2)
C(8)	3301(8)	2602(6)	3921(2)	48(2)
C(9)	5178(8)	2995(6)	4001(2)	45(2)
C(10)	5832(9)	3587(6)	3526(3)	51(2)
C(11)	7818(10)	4960(7)	3146(3)	62(2)
C(12)	9343(9)	6741(7)	2826(3)	62(2)
C(13)	8442(11)	6864(8)	2359(3)	99(3)
C(14)	11002(9)	6081(7)	2780(3)	77(2)
C(15)	9630(11)	7999(7)	3075(3)	85(3)
C(51)	3888(9)	5628(7)	4873(3)	59(2)
C(52)	4860(11)	6166(8)	5662(3)	94(3)
C(81)	2539(9)	1939(6)	4356(3)	62(2)
C(91)	5719(9)	355(7)	3758(3)	56(2)
C(92)	5774(11)	357(8)	3271(3)	80(3)
C(93)	5130(16)	-661(12)	3024(5)	127(5)
C(94)	4492(14)	-1639(14)	3279(7)	134(7)
C(95)	4475(14)	-1643(11)	3753(5)	123(5)
C(96)	5069(11)	-601(8)	4020(4)	92(3)

Table S3. Bond lengths [Å] and angles [°] for jb95.

S(1)-O(2)	1.436(5)
S(1)-O(1)	1.444(5)
S(1)-C(91)	1.771(7)
S(1)-C(9)	1.871(6)
O(6)-C(6)	1.350(8)
O(10)-C(10)	1.204(7)
O(11)-C(11)	1.218(8)
O(12)-C(11)	1.282(8)
O(12)-C(12)	1.488(8)
O(51)-C(51)	1.236(8)
O(52)-C(51)	1.329(8)
O(52)-C(52)	1.453(8)
N(1)-C(10)	1.391(8)
N(1)-C(11)	1.412(9)
N(1)-C(2)	1.469(7)
C(2)-C(3)	1.509(8)
C(3)-C(4)	1.534(9)
C(4)-C(9)	1.534(9)
C(4)-C(5)	1.535(9)
C(5)-C(6)	1.341(9)
C(5)-C(51)	1.446(9)
C(6)-C(7)	1.475(9)
C(7)-C(8)	1.500(9)
C(8)-C(81)	1.528(8)
C(8)-C(9)	1.567(8)
C(9)-C(10)	1.553(9)
C(12)-C(13)	1.488(10)
C(12)-C(14)	1.504(10)
C(12)-C(15)	1.540(10)
C(91)-C(92)	1.352(10)
C(91)-C(96)	1.364(11)
C(92)-C(93)	1.392(13)
C(93)-C(94)	1.368(18)
C(94)-C(95)	1.315(17)
C(95)-C(96)	1.427(14)
O(2)-S(1)-O(1)	119.4(3)
O(2)-S(1)-C(91)	107.5(4)
O(1)-S(1)-C(91)	106.5(3)
O(2)-S(1)-C(9)	107.5(3)
O(1)-S(1)-C(9)	107.0(3)
C(91)-S(1)-C(9)	108.6(3)
C(11)-O(12)-C(12)	123.2(6)
C(51)-O(52)-C(52)	118.5(6)
C(10)-N(1)-C(11)	118.5(6)

Table S3. *Cont*.

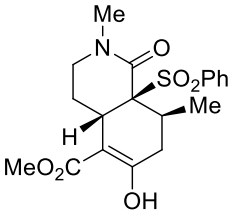
C(10)-N(1)-C(2)	124.4(6)
C(11)-N(1)-C(2)	117.1(6)
N(1)-C(2)-C(3)	111.2(5)
C(2)-C(3)-C(4)	110.7(5)
C(9)-C(4)-C(3)	109.2(5)
C(9)-C(4)-C(5)	110.7(5)
C(3)-C(4)-C(5)	112.3(5)
C(6)-C(5)-C(51)	118.6(6)
C(6)-C(5)-C(4)	122.4(6)
C(51)-C(5)-C(4)	118.7(6)
C(5)-C(6)-O(6)	122.6(7)
C(5)-C(6)-C(7)	123.6(7)
O(6)-C(6)-C(7)	113.8(6)
C(6)-C(7)-C(8)	112.7(6)
C(7)-C(8)-C(81)	111.0(6)
C(7)-C(8)-C(9)	106.5(5)
C(81)-C(8)-C(9)	113.1(5)
C(4)-C(9)-C(10)	114.9(5)
C(4)-C(9)-C(8)	111.0(5)
C(10)-C(9)-C(8)	108.1(5)
C(4)-C(9)-S(1)	107.7(4)
C(10)-C(9)-S(1)	103.3(4)
C(8)-C(9)-S(1)	111.7(4)
O(10)-C(10)-N(1)	123.3(6)
O(10)-C(10)-C(9)	119.1(6)
N(1)-C(10)-C(9)	117.6(6)
O(11)-C(11)-O(12)	126.2(8)
O(11)-C(11)-N(1)	123.2(7)
O(12)-C(11)-N(1)	110.6(7)
C(13)-C(12)-O(12)	110.5(6)
C(13)-C(12)-C(14)	112.9(7)
O(12)-C(12)-C(14)	109.9(6)
C(13)-C(12)-C(15)	112.5(7)
O(12)-C(12)-C(15)	101.3(6)
C(14)-C(12)-C(15)	109.0(6)
O(51)-C(51)-O(52)	119.2(7)
O(51)-C(51)-C(5)	124.6(7)
O(52)-C(51)-C(5)	116.1(7)
C(92)-C(91)-C(96)	123.1(8)
C(92)-C(91)-S(1)	119.6(7)
C(96)-C(91)-S(1)	117.2(7)
C(91)-C(92)-C(93)	118.6(10)
C(94)-C(93)-C(92)	119.4(13)
C(95)-C(94)-C(93)	121.5(15)

Table S3. *Cont*.

C(94)-C(95)-C(96)	120.9(14)
C(91)-C(96)-C(95)	116.4(10)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for jb95. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	51(1)	53(1)	66(1)	-1(1)	-10(1)	4(1)
O(1)	37(3)	78(4)	111(4)	-9(3)	2(3)	-2(3)
O(2)	96(4)	60(3)	72(3)	5(3)	-26(3)	18(3)
O(6)	43(3)	69(4)	125(5)	-7(3)	-6(3)	22(3)
O(10)	71(3)	77(4)	56(3)	2(3)	-7(3)	-29(3)
O(11)	93(4)	81(4)	94(4)	-14(3)	31(4)	-31(4)
O(12)	71(3)	55(3)	82(3)	10(3)	15(3)	-10(3)
O(51)	72(4)	63(3)	106(4)	-23(3)	-1(3)	13(3)
O(52)	65(3)	66(3)	72(3)	-17(3)	3(3)	-4(3)
N(1)	46(3)	61(4)	53(3)	-5(3)	6(3)	-13(3)
C(2)	44(4)	55(4)	60(5)	-3(4)	-2(4)	-7(4)
C(3)	38(4)	55(4)	67(5)	-10(4)	-3(3)	0(4)
C(4)	45(4)	46(4)	46(4)	5(3)	-2(3)	1(3)
C(5)	38(4)	50(4)	52(4)	-2(3)	3(3)	1(3)
C(6)	38(4)	52(5)	85(6)	-2(4)	1(4)	-2(4)
C(7)	33(4)	67(5)	78(5)	1(4)	-6(4)	7(4)
C(8)	35(3)	57(4)	52(4)	5(3)	-6(3)	-5(4)
C(9)	36(3)	43(4)	56(4)	14(3)	-5(3)	2(3)
C(10)	51(4)	54(5)	50(4)	4(4)	-2(4)	1(4)
C(11)	60(5)	60(5)	67(5)	-2(4)	2(4)	-9(4)
C(12)	52(4)	66(5)	68(5)	18(4)	3(4)	-12(5)
C(13)	93(6)	128(8)	76(5)	38(6)	-11(6)	-32(7)
C(14)	51(5)	79(6)	100(6)	0(5)	3(5)	3(5)
C(15)	89(6)	56(5)	109(7)	6(5)	26(6)	6(5)
C(51)	48(4)	62(5)	69(5)	2(4)	-1(4)	-8(4)
C(52)	82(6)	97(7)	105(7)	-48(6)	-6(6)	4(6)
C(81)	43(4)	67(5)	75(5)	10(4)	5(4)	-3(4)
C(91)	49(4)	52(5)	67(5)	-15(4)	-7(4)	6(4)
C(92)	79(6)	75(6)	86(6)	-9(5)	-4(5)	29(5)
C(93)	111(10)	124(10)	147(11)	-69(10)	-56(9)	58(9)
C(94)	63(7)	97(10)	242(19)	-73(14)	-36(11)	11(7)
C(95)	80(7)	68(7)	221(15)	-22(10)	28(10)	0(6)
C(96)	74(6)	58(5)	145(9)	-25(6)	21(7)	4(5)



12a

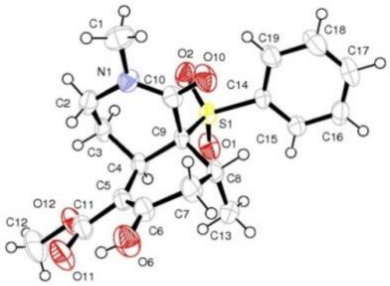


Table S5. Crystal data and structure refinement for compound **12a**.

Identification code	Jb94	
Empirical formula	C19 H23 N O6 S	
Formula weight	393.44	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.652(3) Å	= 80.94(4)°.
	b = 8.175(3) Å	= 79.28(4)°.
	c = 17.270(10) Å	= 62.69(4)°.
Volume	939.9(7) $Å^3$	
Z	2	
Density (calculated)	1.390 Mg/m^3	
Absorption coefficient	0.208 mm^{-1}	
F(000)	416	
Crystal size	0.45 x 0.39 x 0.21 mm^3	
Theta range for data collection	1.20 to 24.97°.	
Index ranges	-8<=h<=9, -9<=k<=9, 0<=l<=20	
Reflections collected	3556	
Independent reflections	3294 [R(int) = 0.0452]	
Completeness to theta = 24.97°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3294 / 0 / 248	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0451, wR2 = 0.1184	
R indices (all data)	R1 = 0.0607, wR2 = 0.1255	
Largest diff. peak and hole	0.314 and -0.267 $e.Å^{-3}$	

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jb94. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	3709(1)	3363(1)	2117(1)	36(1)
O(1)	3669(3)	4156(2)	2806(1)	51(1)
O(2)	5595(2)	2370(2)	1661(1)	54(1)
O(6)	-656(3)	-921(3)	3763(1)	65(1)
O(10)	2083(3)	1508(2)	1128(1)	53(1)
O(11)	1981(3)	-2493(3)	4700(1)	70(1)
O(12)	4294(3)	-1486(2)	4591(1)	56(1)
N(1)	4416(3)	-1052(3)	1677(1)	41(1)
C(1)	4852(4)	-1984(4)	963(2)	57(1)
C(2)	5500(3)	-2140(3)	2337(2)	44(1)
C(3)	5560(3)	-933(3)	2893(1)	41(1)
C(4)	3466(3)	526(3)	3162(1)	34(1)
C(5)	2184(3)	-372(3)	3618(1)	38(1)
C(6)	434(4)	-59(3)	3406(2)	44(1)
C(7)	-535(4)	1385(4)	2776(2)	48(1)
C(8)	266(3)	2822(3)	2617(1)	39(1)
C(9)	2551(3)	1748(3)	2428(1)	32(1)
C(10)	3009(3)	704(3)	1690(1)	37(1)
C(11)	2787(4)	-1558(3)	4340(2)	47(1)
C(12)	5003(5)	-2610(4)	5303(2)	77(1)
C(13)	-457(4)	4021(3)	3316(2)	52(1)
C(14)	2222(3)	5159(3)	1466(1)	34(1)
C(15)	820(3)	6827(3)	1746(1)	39(1)
C(16)	-290(4)	8206(3)	1218(2)	48(1)
C(17)	-6(4)	7926(3)	432(2)	52(1)
C(18)	1433(5)	6285(4)	157(2)	62(1)
C(19)	2573(4)	4898(3)	672(2)	51(1)

Table S7. Bond lengths [Å] and angles [°] for jb94.

S(1)-O(1)	1.4321(19)
S(1)-O(2)	1.437(2)
S(1)-C(14)	1.771(2)
S(1)-C(9)	1.868(2)
O(6)-C(6)	1.335(3)
O(10)-C(10)	1.226(3)
O(11)-C(11)	1.222(3)
O(12)-C(11)	1.333(3)
O(12)-C(12)	1.444(3)
N(1)-C(10)	1.343(3)
N(1)-C(1)	1.456(3)
N(1)-C(2)	1.462(3)
C(2)-C(3)	1.501(3)
C(3)-C(4)	1.533(3)
C(4)-C(5)	1.521(3)
C(4)-C(9)	1.545(3)
C(5)-C(6)	1.354(3)
C(5)-C(11)	1.459(3)
C(6)-C(7)	1.489(3)
C(7)-C(8)	1.525(3)
C(8)-C(13)	1.533(4)
C(8)-C(9)	1.551(3)
C(9)-C(10)	1.540(3)
C(14)-C(19)	1.378(3)
C(14)-C(15)	1.385(3)
C(15)-C(16)	1.382(3)
C(16)-C(17)	1.374(4)
C(17)-C(18)	1.374(4)
C(18)-C(19)	1.379(4)
O(1)-S(1)-O(2)	118.30(12)
O(1)-S(1)-C(14)	108.32(11)
O(2)-S(1)-C(14)	106.63(11)
O(1)-S(1)-C(9)	107.98(10)
O(2)-S(1)-C(9)	107.41(11)
C(14)-S(1)-C(9)	107.79(10)
C(11)-O(12)-C(12)	117.5(2)
C(10)-N(1)-C(1)	118.1(2)
C(10)-N(1)-C(2)	125.01(19)
C(1)-N(1)-C(2)	116.9(2)
N(1)-C(2)-C(3)	111.79(18)
C(2)-C(3)-C(4)	110.79(18)
C(5)-C(4)-C(3)	111.12(18)
C(5)-C(4)-C(9)	111.53(17)
C(3)-C(4)-C(9)	108.73(18)

Table S7. *Cont*.

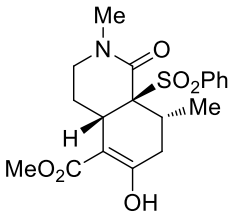
C(6)-C(5)-C(11)	117.4(2)
C(6)-C(5)-C(4)	122.8(2)
C(11)-C(5)-C(4)	119.7(2)
O(6)-C(6)-C(5)	124.1(2)
O(6)-C(6)-C(7)	113.0(2)
C(5)-C(6)-C(7)	122.8(2)
C(6)-C(7)-C(8)	111.30(19)
C(7)-C(8)-C(13)	110.2(2)
C(7)-C(8)-C(9)	106.62(18)
C(13)-C(8)-C(9)	115.0(2)
C(10)-C(9)-C(4)	114.97(17)
C(10)-C(9)-C(8)	107.96(18)
C(4)-C(9)-C(8)	110.73(18)
C(10)-C(9)-S(1)	104.17(15)
C(4)-C(9)-S(1)	107.67(14)
C(8)-C(9)-S(1)	111.17(15)
O(10)-C(10)-N(1)	121.7(2)
O(10)-C(10)-C(9)	118.9(2)
N(1)-C(10)-C(9)	119.39(19)
O(11)-C(11)-O(12)	122.3(2)
O(11)-C(11)-C(5)	124.5(2)
O(12)-C(11)-C(5)	113.2(2)
C(19)-C(14)-C(15)	121.0(2)
C(19)-C(14)-S(1)	118.64(18)
C(15)-C(14)-S(1)	120.24(18)
C(16)-C(15)-C(14)	118.6(2)
C(17)-C(16)-C(15)	120.6(2)
C(16)-C(17)-C(18)	120.2(2)
C(17)-C(18)-C(19)	120.1(3)
C(14)-C(19)-C(18)	119.4(2)

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for jb94. 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}
S(1)	36(1)	30(1)	42(1)	4(1)	-14(1)	-13(1)
O(1)	71(1)	44(1)	51(1)	5(1)	-31(1)	-32(1)
O(2)	33(1)	42(1)	74(1)	5(1)	-2(1)	-11(1)
O(6)	58(1)	64(1)	81(2)	20(1)	-17(1)	-38(1)
O(10)	68(1)	51(1)	42(1)	3(1)	-30(1)	-22(1)
O(11)	83(2)	62(1)	66(1)	28(1)	-20(1)	-40(1)
O(12)	75(1)	53(1)	44(1)	14(1)	-31(1)	-28(1)
N(1)	41(1)	36(1)	44(1)	-10(1)	-7(1)	-14(1)
C(1)	60(2)	59(2)	60(2)	-24(1)	3(1)	-31(1)
C(2)	36(1)	33(1)	56(2)	0(1)	-8(1)	-9(1)
C(3)	32(1)	36(1)	49(1)	9(1)	-18(1)	-9(1)
C(4)	37(1)	29(1)	34(1)	2(1)	-16(1)	-11(1)
C(5)	42(1)	32(1)	37(1)	2(1)	-11(1)	-14(1)
C(6)	46(1)	40(1)	47(2)	4(1)	-10(1)	-21(1)
C(7)	37(1)	53(2)	54(2)	8(1)	-18(1)	-20(1)
C(8)	31(1)	37(1)	42(1)	10(1)	-13(1)	-10(1)
C(9)	33(1)	27(1)	33(1)	3(1)	-13(1)	-10(1)
C(10)	41(1)	39(1)	37(1)	0(1)	-14(1)	-20(1)
C(11)	57(2)	37(1)	42(1)	4(1)	-15(1)	-17(1)
C(12)	104(3)	69(2)	57(2)	22(2)	-49(2)	-31(2)
C(13)	46(1)	38(1)	55(2)	0(1)	0(1)	-7(1)
C(14)	37(1)	26(1)	37(1)	2(1)	-10(1)	-13(1)
C(15)	41(1)	33(1)	41(1)	2(1)	-6(1)	-15(1)
C(16)	39(1)	32(1)	64(2)	7(1)	-9(1)	-11(1)
C(17)	61(2)	44(1)	59(2)	19(1)	-33(1)	-27(1)
C(18)	100(2)	49(2)	40(2)	7(1)	-24(2)	-35(2)
C(19)	75(2)	36(1)	38(1)	0(1)	-11(1)	-20(1)

Table S9. Hydrogen bonds for jb94 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(6)-H(6)...O(11)	0.82	1.84	2.553(3)	145.3



12b

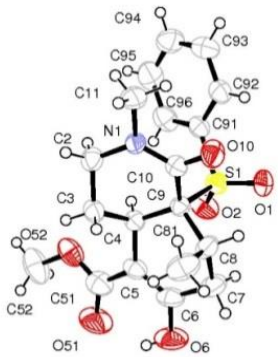


Table S10. Crystal data and structure refinement for compound **12b**.

Identification code	Jb96	
Empirical formula	C19 H23 N O6 S	
Formula weight	393.44	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.256(2) Å	α= 90°.
	b = 11.5211(14) Å	β= 90°.
	c = 19.717(3) Å	γ = 90°.
Volume	1875.4(6) $Å^3$	
Z	4	
Density (calculated)	1.393 Mg/m^3	
Absorption coefficient	0.209 mm^{-1}	
F(000)	832	
Crystal size	0.39 x 0.21 x 0.21 mm^3	
Theta range for data collection	2.05 to 24.97°.	
Index ranges	-9<=h<=9, 0<=k<=13, 0<=l<=23	
Reflections collected	3689	
Independent reflections	3289 [R(int) = 0.0455]	
Completeness to theta = 24.97°	100.0 %	
Max. and min. transmission	0.9574 and 0.9230	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3289 / 0 / 248	
Goodness-of-fit on F^2	0.971	
Final R indices [I>2sigma(I)]	R1 = 0.0492, wR2 = 0.0858	
R indices (all data)	R1 = 0.0944, wR2 = 0.0962	
Absolute structure parameter	-0.05(12)	
Largest diff. peak and hole	0.159 and -0.189 $e.Å^{-3}$	

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jb96. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2860(1)	4807(1)	6406(1)	46(1)
O(1)	1504(3)	4042(2)	6520(1)	59(1)
O(2)	3254(3)	5645(2)	6923(1)	59(1)
O(6)	6615(4)	4060(3)	8239(1)	83(1)
O(10)	3428(3)	2795(2)	5397(1)	57(1)
O(51)	8625(4)	5592(3)	7879(1)	92(1)
O(52)	8414(3)	6362(3)	6852(2)	64(1)
N(1)	5486(3)	3898(3)	5030(1)	39(1)
C(2)	6916(4)	4605(3)	5151(2)	47(1)
C(3)	7538(4)	4440(3)	5864(2)	43(1)
C(4)	6200(3)	4734(3)	6374(2)	37(1)
C(5)	6791(4)	4738(3)	7103(2)	46(1)
C(6)	6124(5)	4054(4)	7591(2)	54(1)
C(7)	4768(5)	3239(4)	7467(2)	60(1)
C(8)	4649(5)	2872(3)	6730(2)	49(1)
C(9)	4712(4)	3936(3)	6249(2)	36(1)
C(10)	4529(4)	3481(3)	5516(2)	39(1)
C(11)	5115(4)	3627(4)	4322(2)	55(1)
C(51)	8005(5)	5566(4)	7319(2)	62(1)
C(52)	9650(5)	7218(4)	7051(2)	87(2)
C(81)	5969(5)	1973(3)	6574(2)	68(1)
C(91)	2523(4)	5564(3)	5638(2)	43(1)
C(92)	1552(4)	5088(4)	5138(2)	50(1)
C(93)	1327(5)	5689(4)	4537(2)	59(1)
C(94)	2086(6)	6726(4)	4432(2)	70(1)
C(95)	3048(5)	7190(4)	4921(3)	71(1)
C(96)	3239(5)	6624(4)	5543(2)	58(1)

Table S12. Bond lengths [Å] and angles [°] for jb96.

S(1)-O(1)	1.442(2)
S(1)-O(2)	1.442(2)
S(1)-C(91)	1.770(4)
S(1)-C(9)	1.855(3)
O(6)-C(6)	1.341(4)
O(10)-C(10)	1.227(4)
O(51)-C(51)	1.218(4)
O(52)-C(51)	1.343(5)
O(52)-C(52)	1.472(5)
N(1)-C(10)	1.332(4)
N(1)-C(2)	1.454(4)
N(1)-C(11)	1.462(4)
C(2)-C(3)	1.509(4)
C(3)-C(4)	1.531(4)
C(4)-C(5)	1.519(4)
C(4)-C(9)	1.554(4)
C(5)-C(6)	1.359(5)
C(5)-C(51)	1.448(5)
C(6)-C(7)	1.482(6)
C(7)-C(8)	1.517(5)
C(8)-C(81)	1.534(5)
C(8)-C(9)	1.550(5)
C(9)-C(10)	1.544(5)
C(91)-C(96)	1.370(5)
C(91)-C(92)	1.384(5)
C(92)-C(93)	1.385(5)
C(93)-C(94)	1.365(5)
C(94)-C(95)	1.358(6)
C(95)-C(96)	1.398(5)
O(1)-S(1)-O(2)	118.26(15)
O(1)-S(1)-C(91)	108.21(16)
O(2)-S(1)-C(91)	108.10(17)
O(1)-S(1)-C(9)	109.62(15)
O(2)-S(1)-C(9)	107.13(15)
C(91)-S(1)-C(9)	104.70(15)
C(51)-O(52)-C(52)	116.6(3)
C(10)-N(1)-C(2)	124.4(3)
C(10)-N(1)-C(11)	119.0(3)
C(2)-N(1)-C(11)	116.6(3)
N(1)-C(2)-C(3)	111.0(3)
C(2)-C(3)-C(4)	109.8(3)
C(5)-C(4)-C(3)	113.0(3)
C(5)-C(4)-C(9)	113.9(3)
C(3)-C(4)-C(9)	109.6(3)

Table S12. Cont.

C(6)-C(5)-C(51)	117.0(3)
C(6)-C(5)-C(4)	122.6(3)
C(51)-C(5)-C(4)	120.2(3)
O(6)-C(6)-C(5)	123.3(4)
O(6)-C(6)-C(7)	112.9(4)
C(5)-C(6)-C(7)	123.8(3)
C(6)-C(7)-C(8)	112.5(3)
C(7)-C(8)-C(81)	109.5(3)
C(7)-C(8)-C(9)	111.3(3)
C(81)-C(8)-C(9)	112.8(3)
C(10)-C(9)-C(8)	107.5(3)
C(10)-C(9)-C(4)	115.2(3)
C(8)-C(9)-C(4)	113.4(3)
C(10)-C(9)-S(1)	105.0(2)
C(8)-C(9)-S(1)	107.3(2)
C(4)-C(9)-S(1)	107.8(2)
O(10)-C(10)-N(1)	122.2(3)
O(10)-C(10)-C(9)	118.1(3)
N(1)-C(10)-C(9)	119.5(3)
O(51)-C(51)-O(52)	120.0(4)
O(51)-C(51)-C(5)	125.0(4)
O(52)-C(51)-C(5)	115.0(3)
C(96)-C(91)-C(92)	120.5(4)
C(96)-C(91)-S(1)	119.2(3)
C(92)-C(91)-S(1)	120.3(3)
C(91)-C(92)-C(93)	119.2(4)
C(94)-C(93)-C(92)	120.5(4)
C(95)-C(94)-C(93)	120.3(4)
C(94)-C(95)-C(96)	120.4(4)
C(91)-C(96)-C(95)	119.1(4)

Table S13. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for jb96. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	38(1)	59(1)	40(1)	-3(1)	4(1)	3(1)
O(1)	38(1)	81(2)	58(2)	6(2)	11(1)	-8(2)
O(2)	58(2)	74(2)	46(2)	-27(1)	-6(1)	11(2)
O(6)	95(3)	119(3)	34(2)	-2(2)	-14(2)	16(2)
O(10)	59(2)	64(2)	49(2)	-11(1)	3(1)	-20(2)
O(51)	91(2)	128(3)	56(2)	-20(2)	-30(2)	-6(2)
O(52)	53(2)	64(2)	75(2)	-24(2)	-13(2)	-6(2)
N(1)	38(2)	49(2)	30(2)	-3(2)	2(1)	-5(2)
C(2)	47(2)	54(3)	42(2)	-5(2)	5(2)	-5(2)
C(3)	37(2)	50(2)	43(2)	-5(2)	0(2)	1(2)
C(4)	36(2)	40(2)	36(2)	-4(2)	1(2)	2(2)
C(5)	43(2)	57(3)	37(2)	-11(2)	-6(2)	8(2)
C(6)	60(3)	71(3)	32(2)	-6(2)	-7(2)	17(2)
C(7)	71(3)	72(3)	38(2)	10(2)	8(2)	5(3)
C(8)	52(2)	50(2)	43(2)	10(2)	9(2)	0(2)
C(9)	37(2)	39(2)	31(2)	-1(2)	2(2)	1(2)
C(10)	38(2)	40(2)	39(2)	-3(2)	-1(2)	3(2)
C(11)	56(3)	75(3)	34(2)	-7(2)	-1(2)	0(2)
C(51)	62(3)	74(3)	50(3)	-16(2)	-4(2)	9(3)
C(52)	57(3)	90(4)	114(4)	-48(3)	-3(3)	-13(3)
C(81)	97(3)	49(3)	58(3)	7(2)	6(2)	14(2)
C(91)	35(2)	45(2)	48(2)	-2(2)	-2(2)	5(2)
C(92)	42(2)	55(3)	54(2)	-3(2)	-1(2)	2(2)
C(93)	61(3)	66(3)	51(3)	-5(2)	-12(2)	15(2)
C(94)	67(3)	72(3)	71(3)	24(3)	-5(3)	16(3)
C(95)	64(3)	45(3)	105(4)	19(3)	-9(3)	-1(3)
C(96)	51(3)	47(3)	77(3)	-2(2)	-9(2)	6(2)