Supporting Information

for

Gold-Catalyzed Synthesis of 2-sulfenylspiroindolenines via Spirocyclizations

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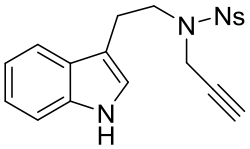
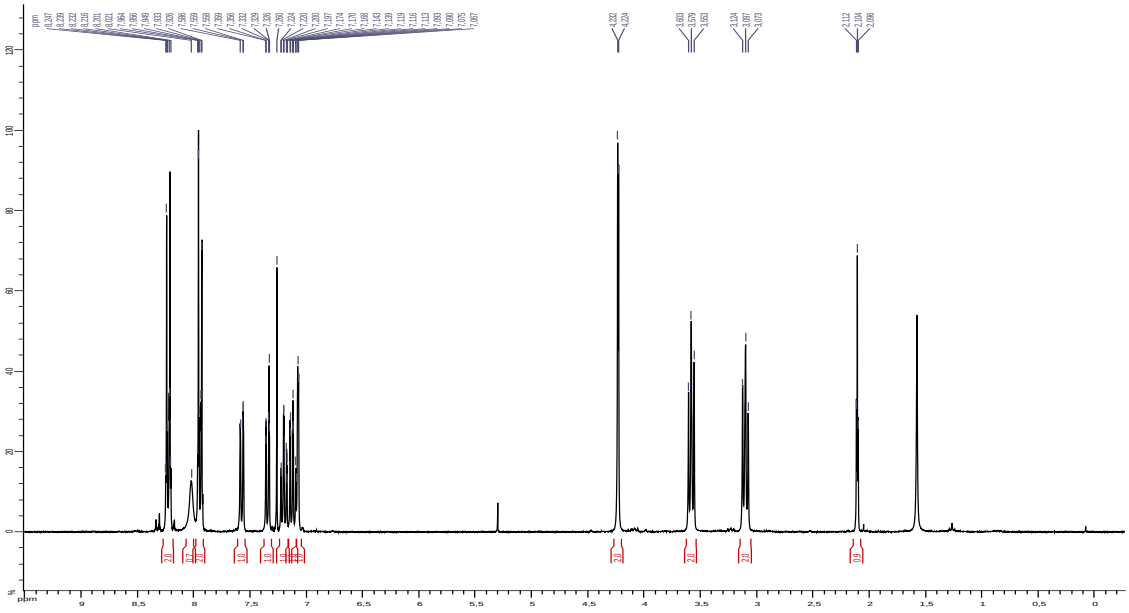
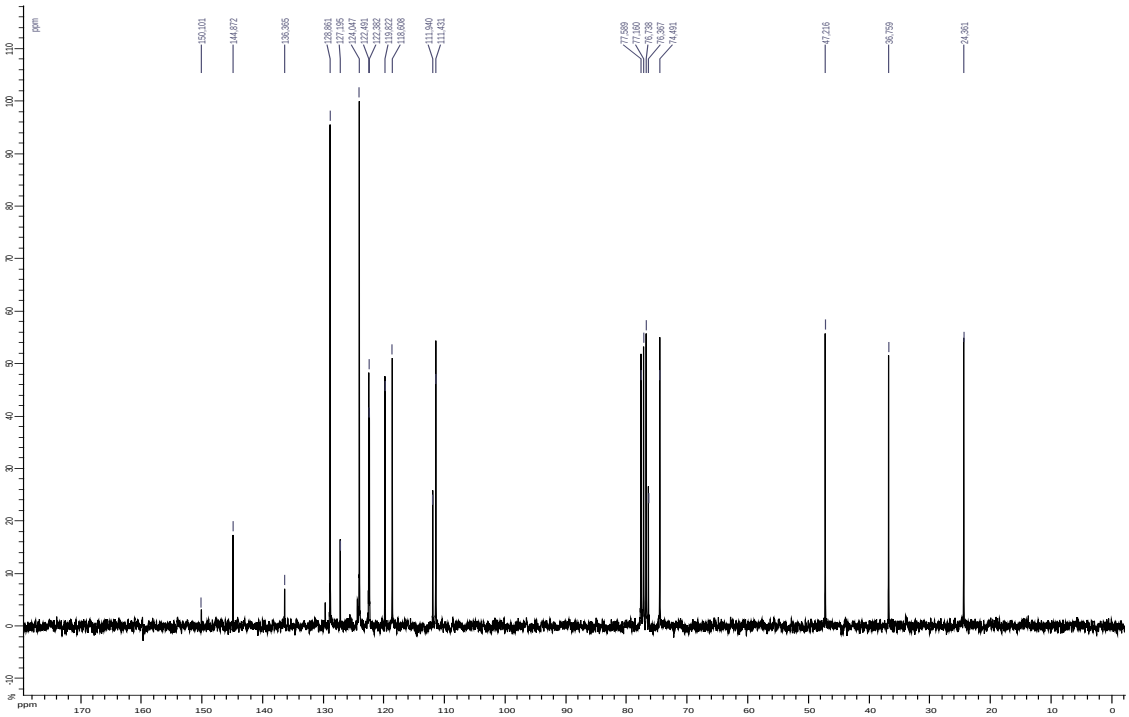
1. NMR Spectra

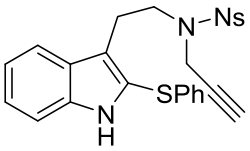


6a ^{1}**H NMR (CDCl$_3$, 300 MHz)**

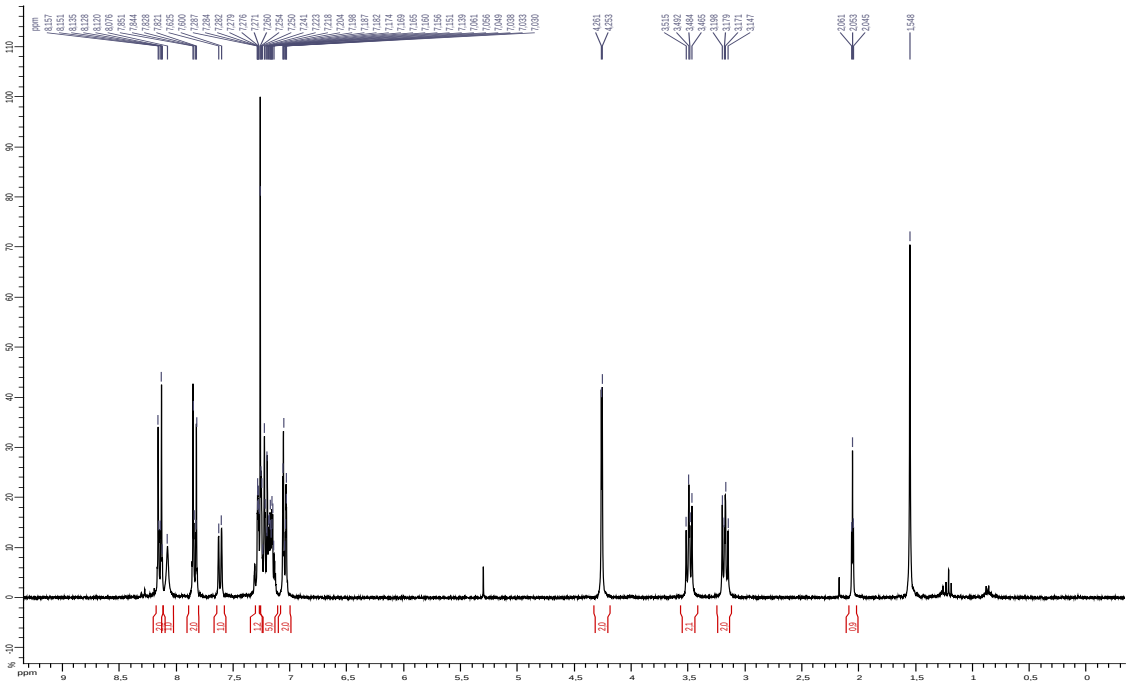


^{13}**C NMR (CDCl$_3$, 75 MHz)**

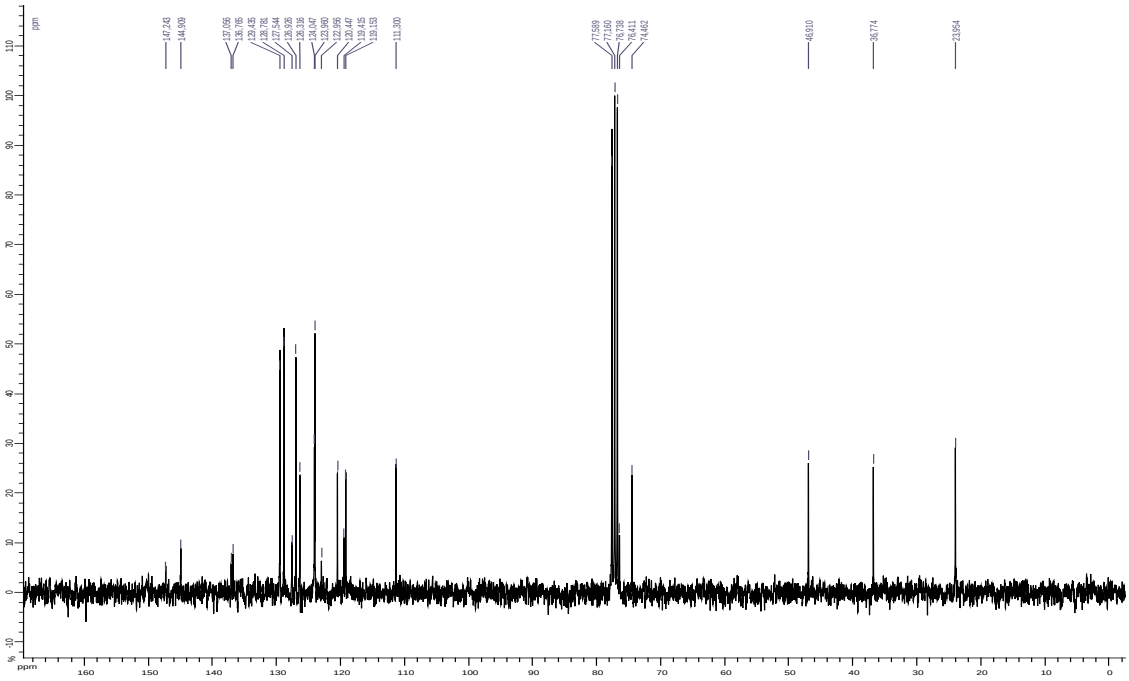


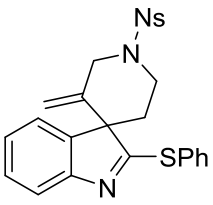


7a **^{1}H NMR ($CDCl_3$, 300 MHz)**

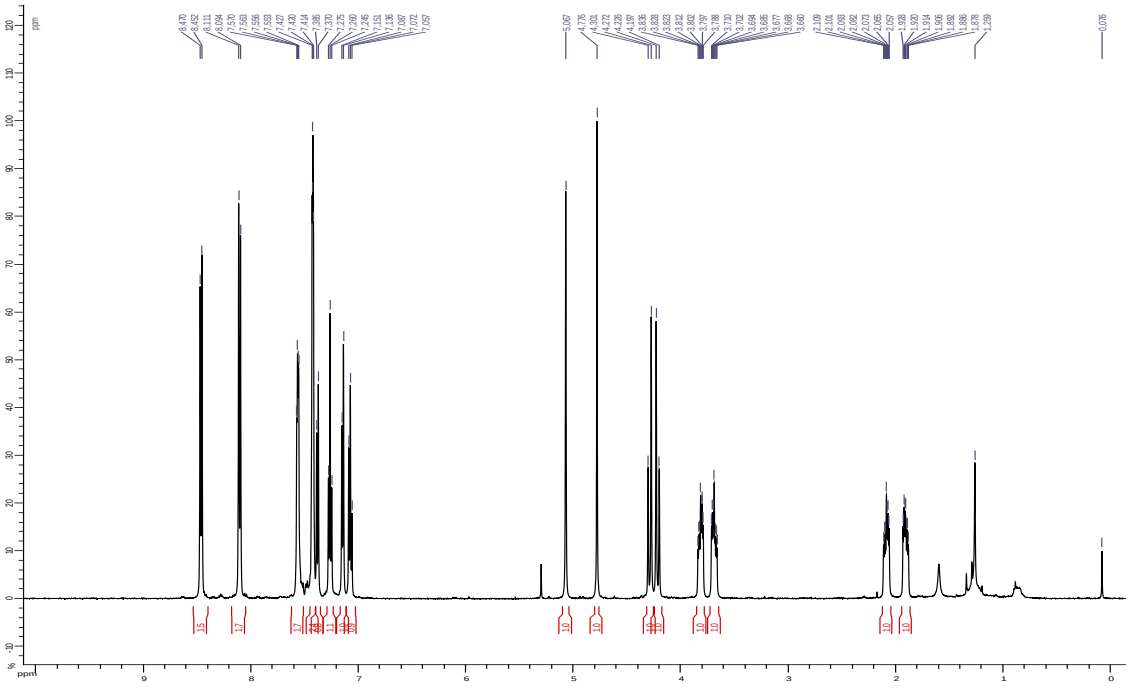


^{13}C NMR ($CDCl_3$, 75 MHz)

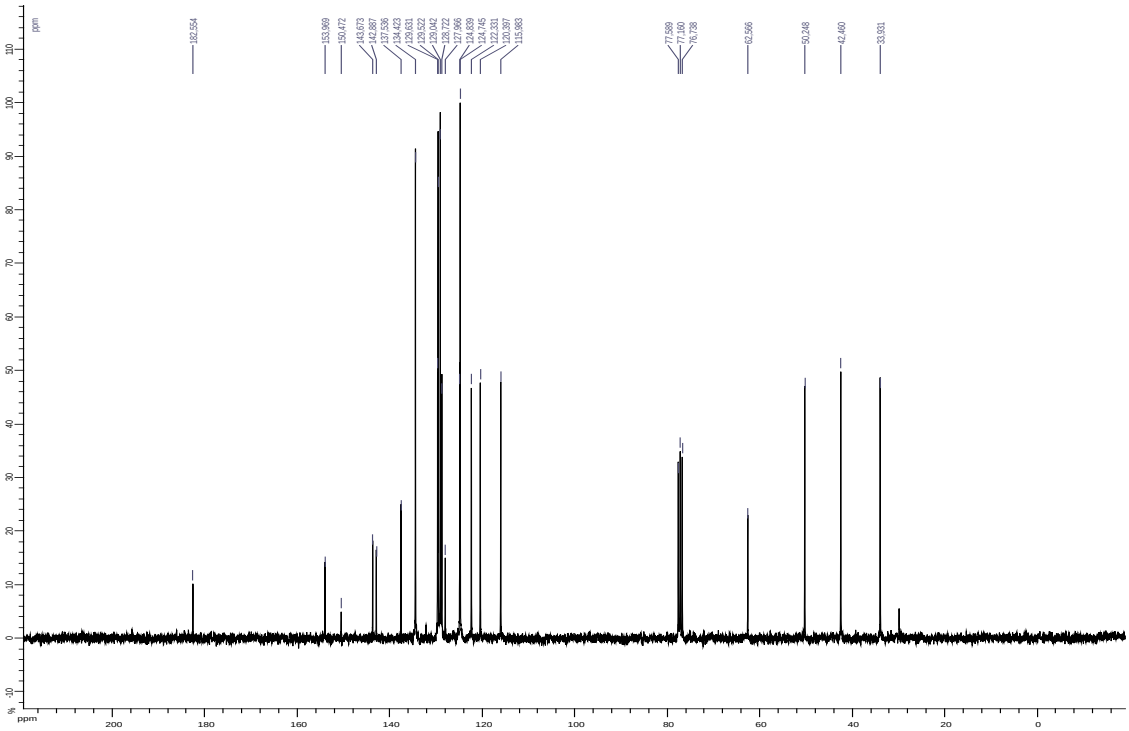


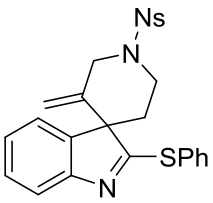


4a **^{1}H NMR ($CDCl_3$, 500 MHz)**

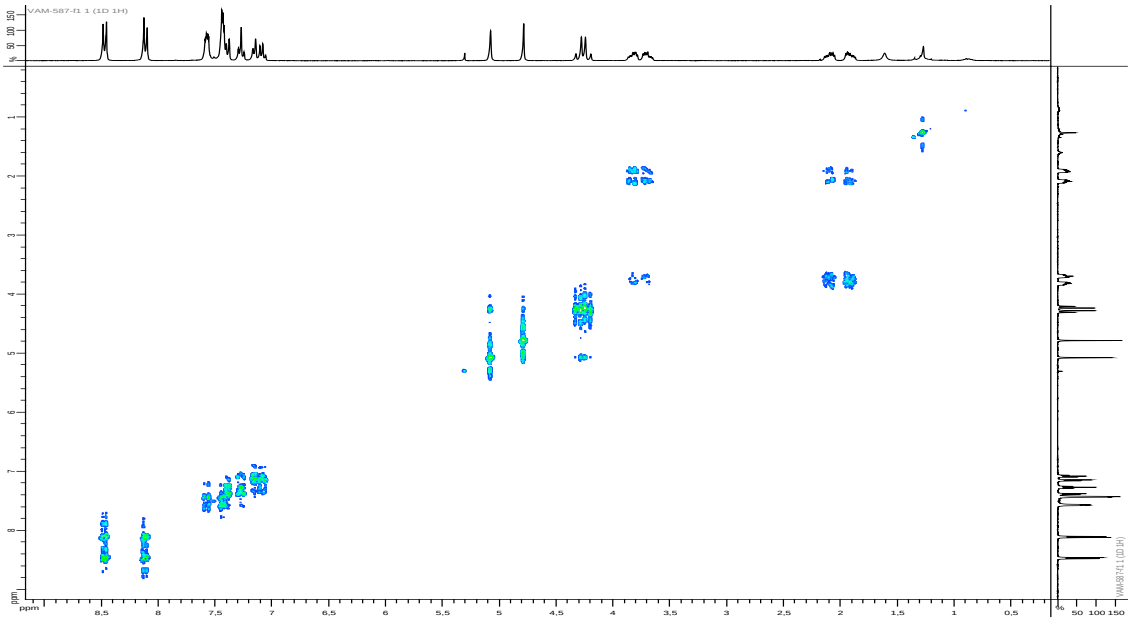


^{13}C NMR ($CDCl_3$, 75 MHz)

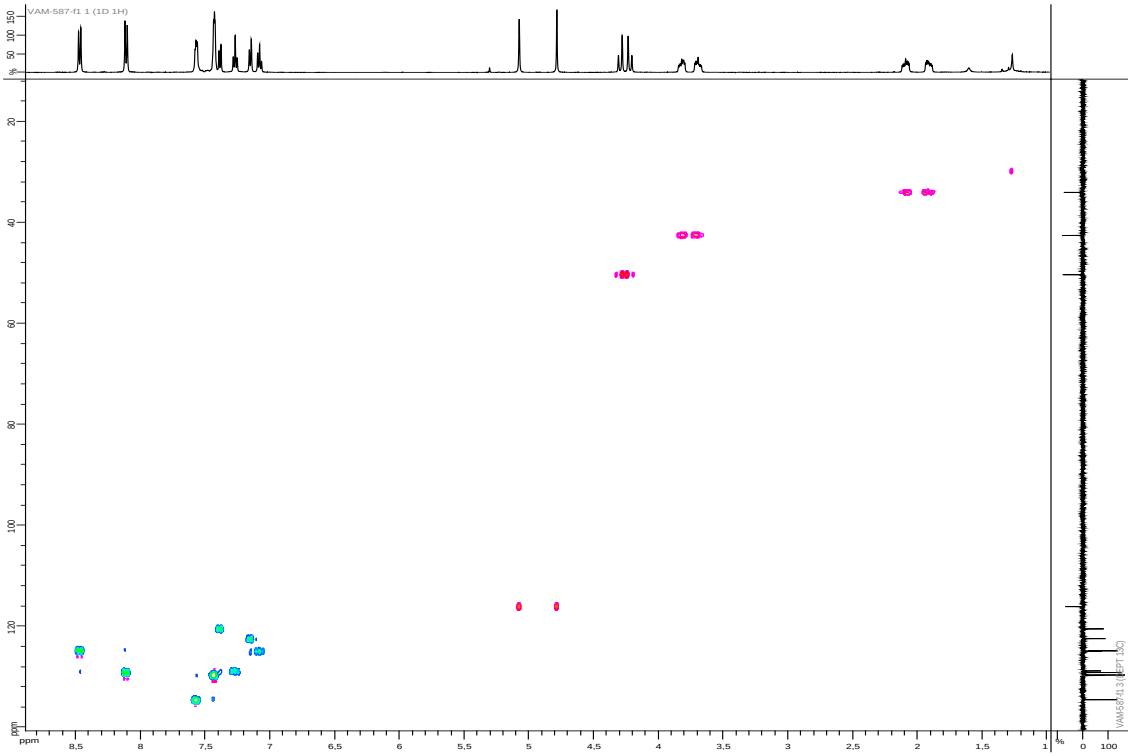


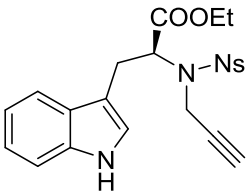


4a COSY (500 MHz, $CDCl_3$)

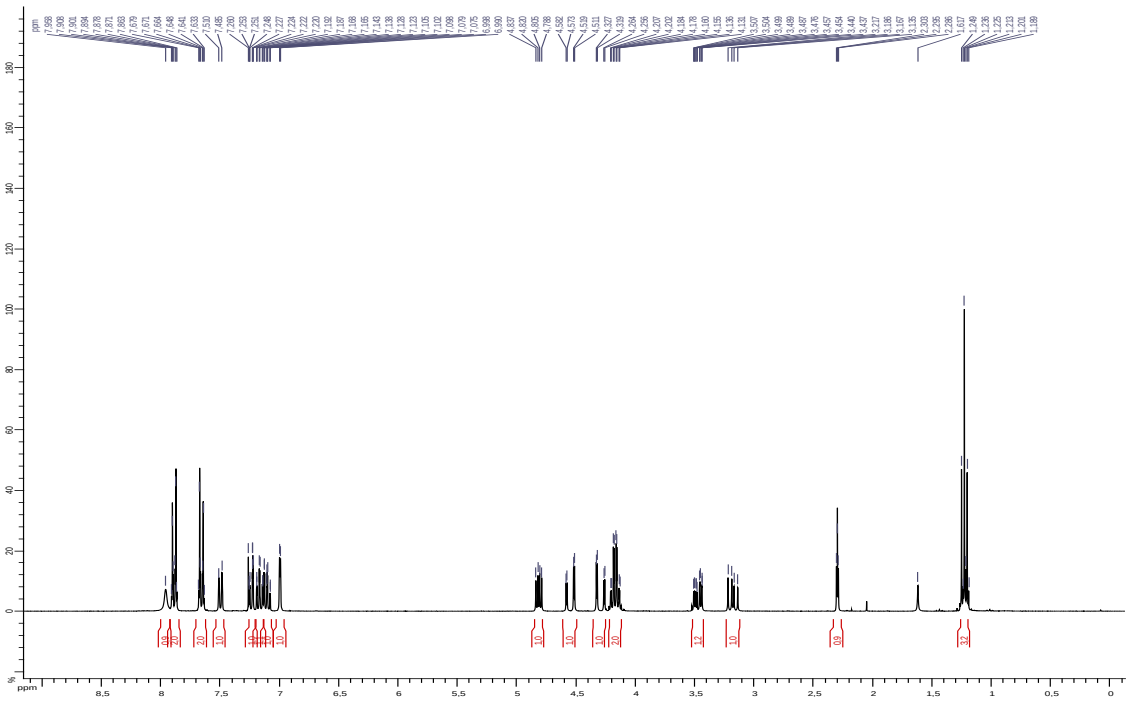


HSQC ($CDCl_3$)

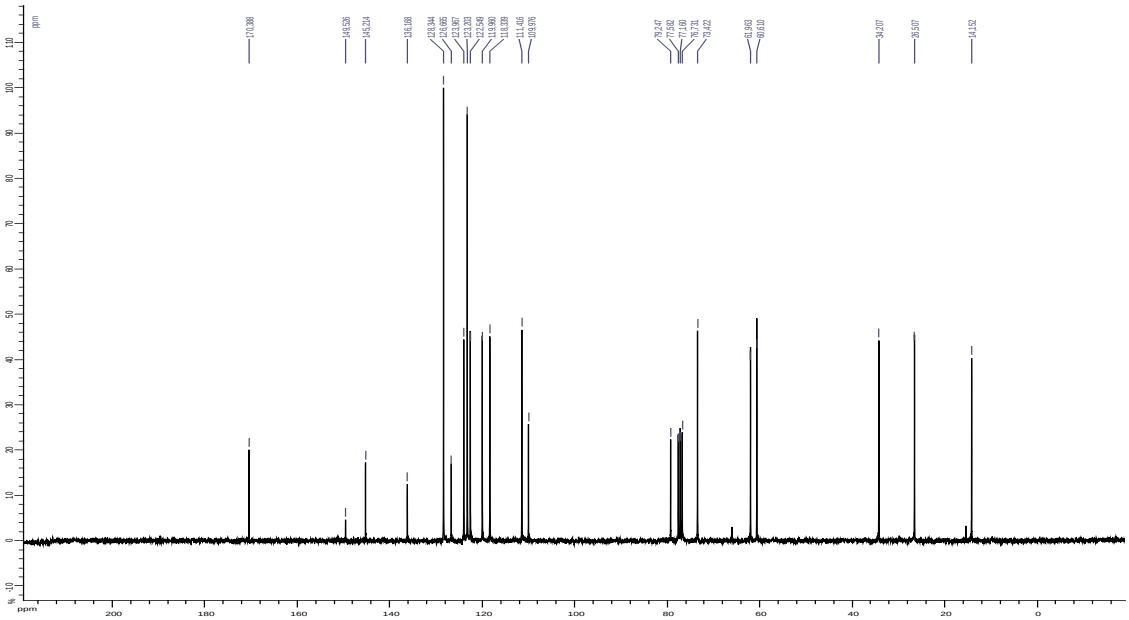


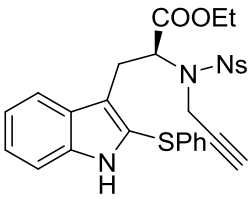


6b **^{1}H NMR ($CDCl_3$, 300 MHz**

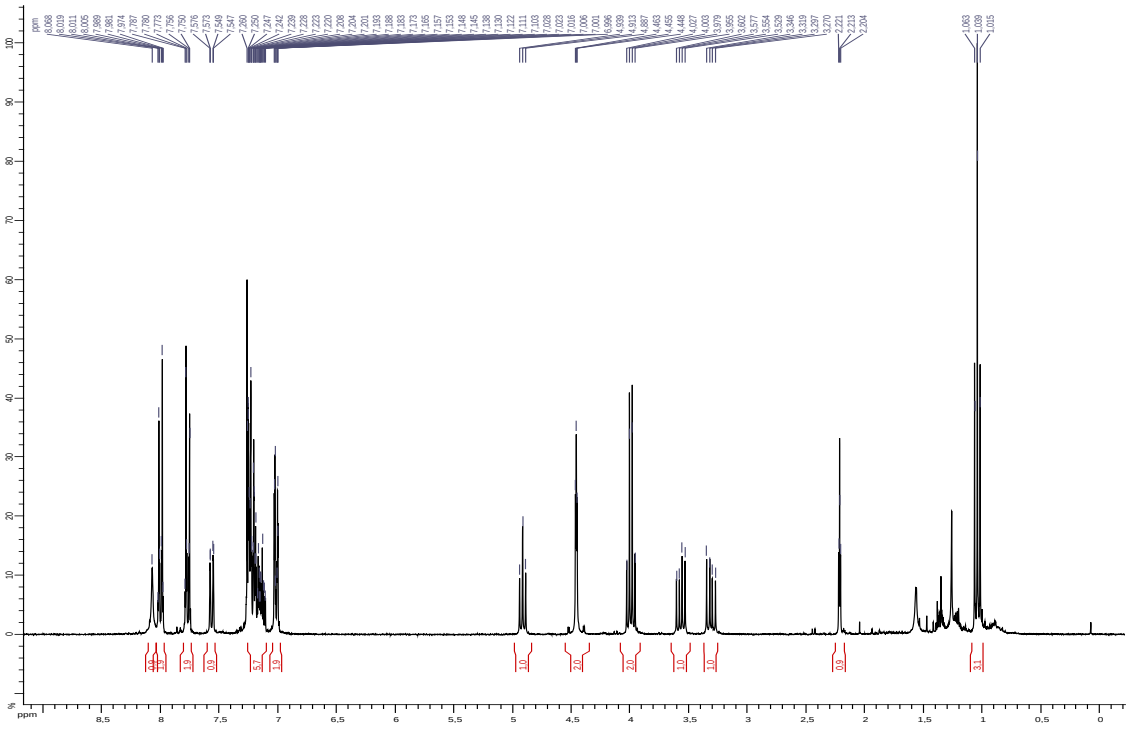


^{13}C NMR ($CDCl_3$, 75 MHz)

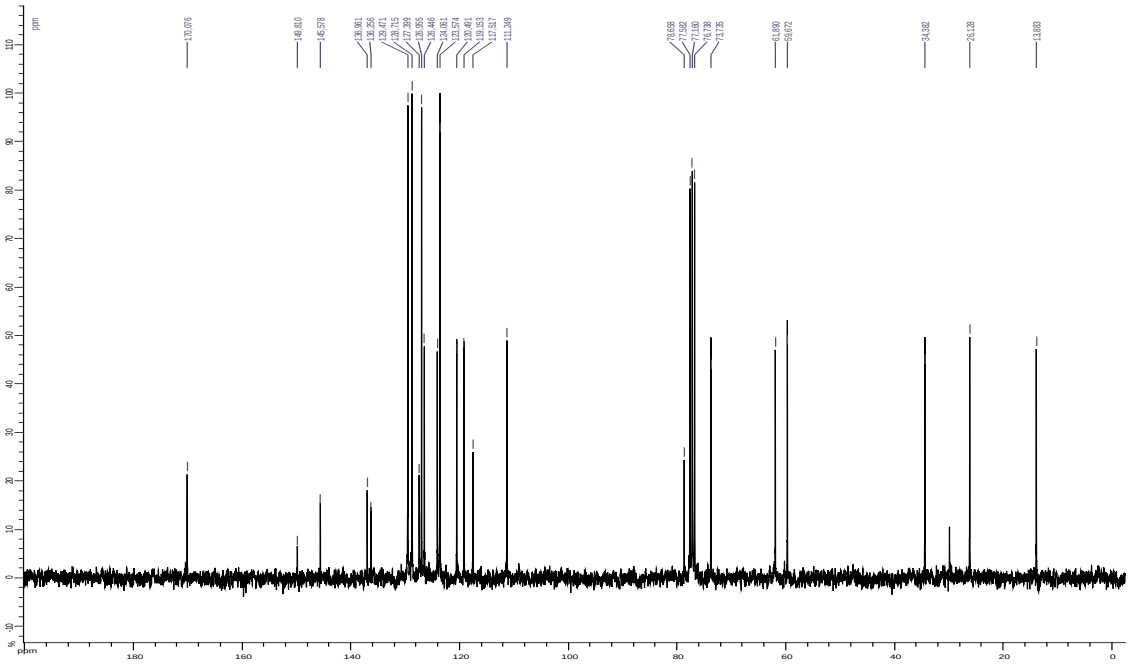


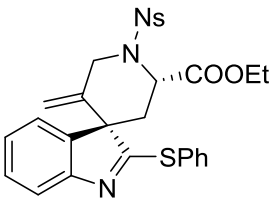


7b **^{1}H NMR ($CDCl_3$, 300 MHz)**

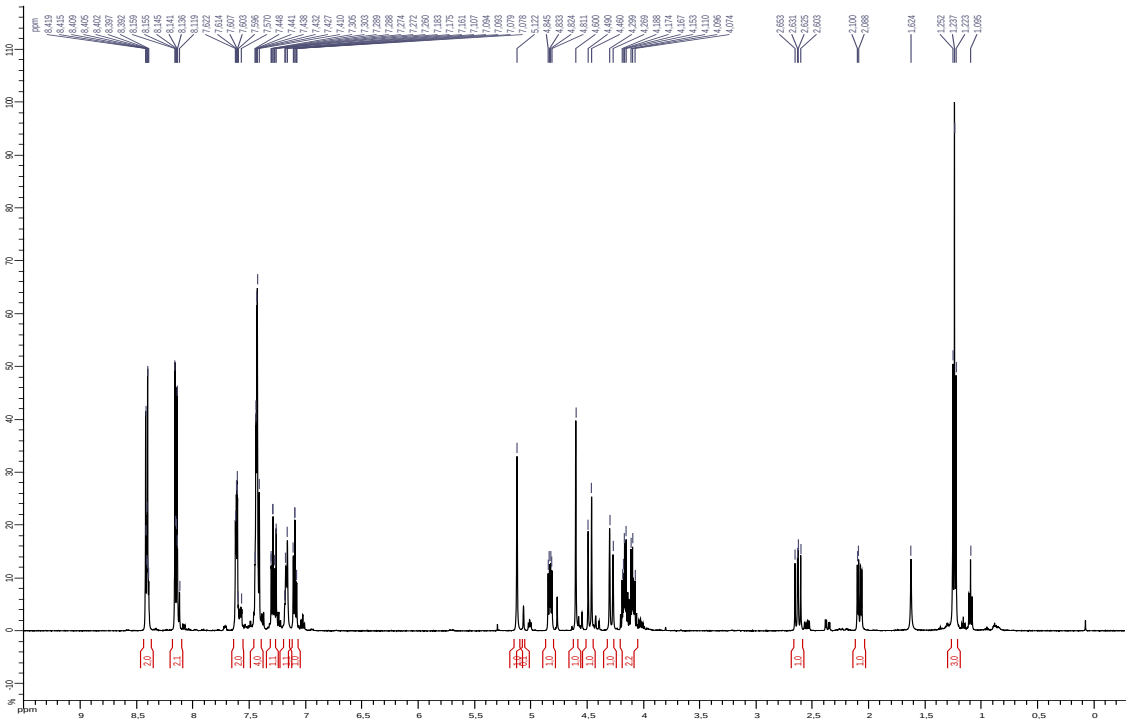


^{13}C NMR ($CDCl_3$, 75 MHz)

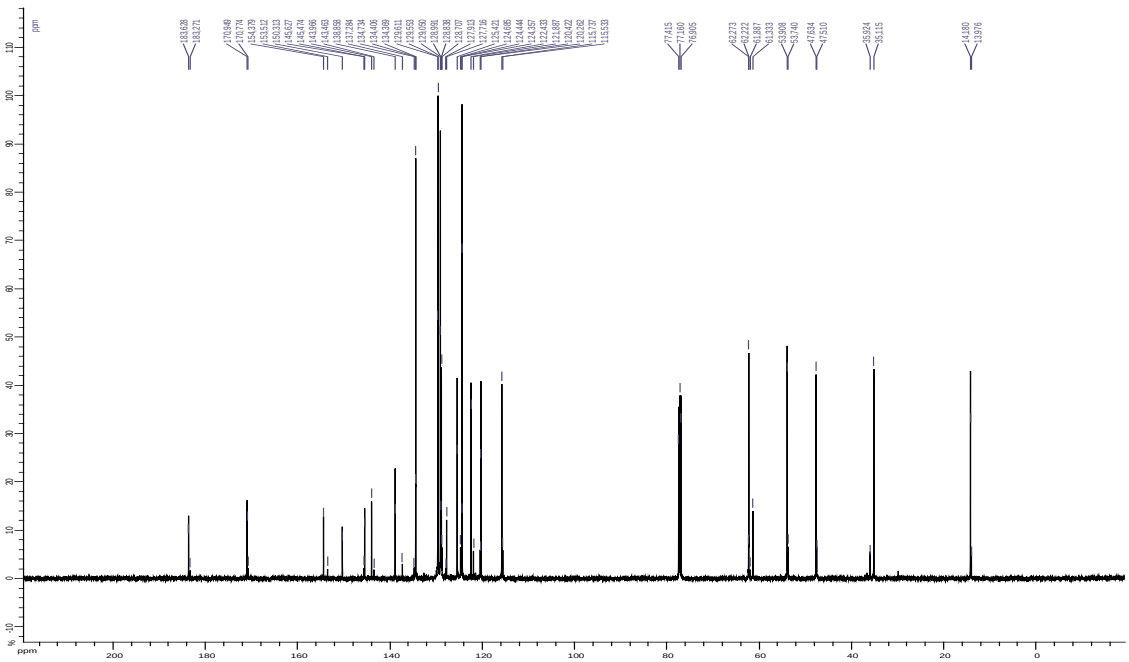


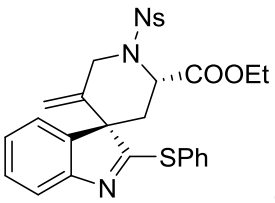


4b **^{1}H NMR ($CDCl_3$, 500 MHz**

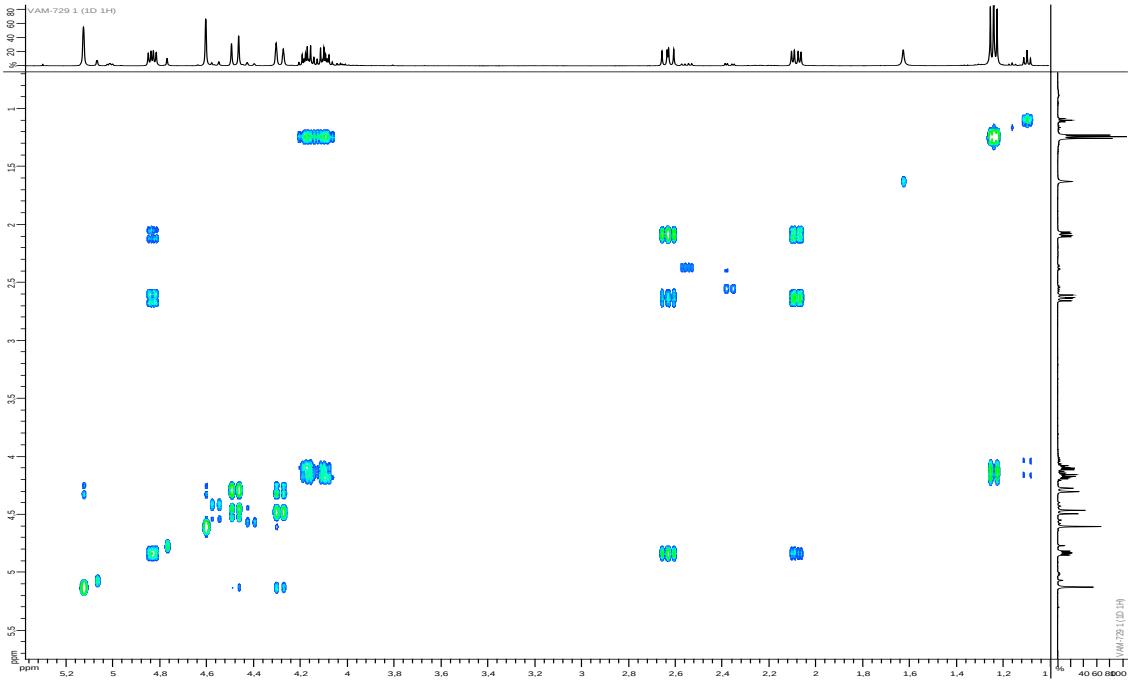


^{13}C NMR ($CDCl_3$, 125 MHz)

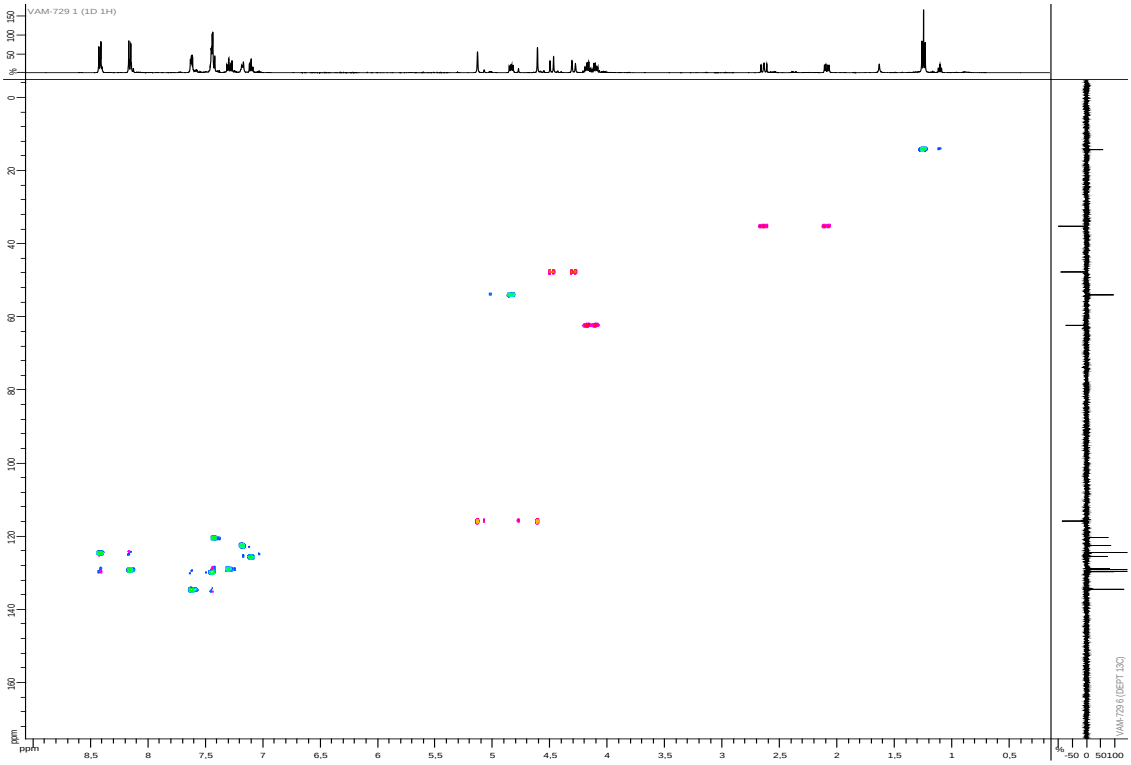


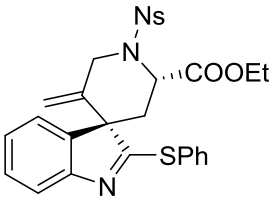


4b **COSY (500 MHz, $CDCl_3$)**

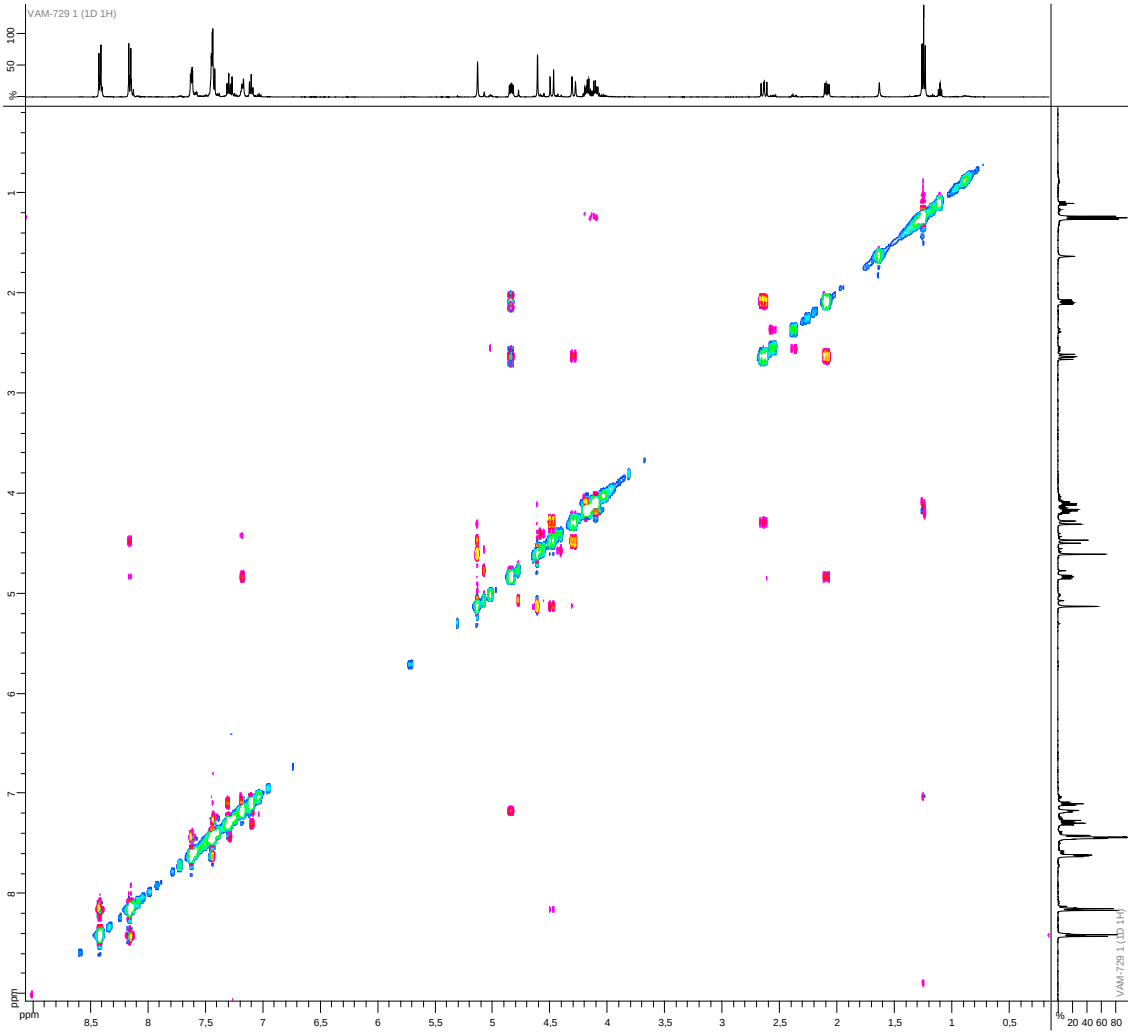


HSQC ($CDCl_3$)





4b **NOESY (500 Mz, $CDCl_3$)**



2. X-ray Crystallography

A tiny pale-yellow crystal (0.10 x 0.08 x 0.05 mm^3) was attached to the nylon cord of HR loop with paratone-N oil. Measurements were made on a Rigaku XtaLabPro PILATUS3R 200K - equipped diffractometer (0.6 mA, 50 kV) using monochromated Mo Kα radiation (λ = 0.71073 Å) at 293 K. The initial orientation and unit cell were indexed [1] using a least-squares analysis of a random set of reflections collected from three series of 0.5° width scans, 30 seconds per frame, and 10 frames per series that were well distributed in reciprocal space. For data collection, the frame length was adjusted to 45 seconds per frame to give a predicted resolution of 0.80 Å (θ -0.30° ; crystal-to-detector distance 28mm), and seven ω-scan frame series were collected with 0.5° width scans and a total of 832 frames at varying κ, and φ angles. Cell refinement and data reduction were performed with the Rigaku CrysAlisPro 1.171.39.7b software [1], which corrects for beam inhomogeneity, possible crystal decay, and Lorentz and polarization effects. Data processing and a multi-scan absorption correction was applied using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm [1]. The structure was solved using Intrinsic Phasing methods [2] and all non-hydrogen atoms were refined anisotropically using the ShelXLE [3] graphical user interface and SHELXL-2016/6 [4], that implemented full-matrix least-squares methods on 315 parameters, with the following weighted scheme: $w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 0.0852P]$ where $P = [\max(F_o^2,0) + 2F_o^2]/3$. Hydrogen atoms (except for those in the methylene group), located from difference Fourier synthesis were included at geometrically idealized positions using an appropriate riding model and coupled isotropic temperature factors. Methylene H atoms were allowed to freely refine their position and isotropic temperature factors. Ortep-type figure was made using Mercury [5].

Crystal data for $C_{25}\ H_{21}\ N_3\ O_4\ S_2$ (M = 491.57 g mol^{-1}): triclinic, space group P-1 (no. 2), a = 8.9028(5) Å, b = 11.8142(8) Å, c = 12.1707(7) Å, α = 108.385(6)°, β = 105.925(5)°, γ = 96.572(5)°, V = 1139.46(13) $Å^3$, Z = 2, T = 293(2) K, μ (MoKα) = 0.273 mm^{-1} , Dcalc = 1.433 g cm^{-3} , 15186 reflections measured (3.374 ≤ θ ≤ 25.350 °), 4165 unique (Rint = 0.074, Rsigma = 0.0712) which were used in all calculations except for 4 low-resolution reflections shaded by the beamstop. The final R1 was 0.0518 (I > 2σ (I)) and wR2 was 0.1458 (all data). CCDC 1578923 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html .

Supplementary materials: Table S1: Atomic coordinates and equivalent isotropic displacement parameters of ***VAM-587***, Table S2: Bond lengths [Å] and angles [°] for ***VAM-587***, Table S3: Anisotropic displacement parameters for ***VAM-587***, Table S4: Hydrogen coordinates and isotropic displacement parameters for ***VAM-587***. Table S5: Torsion angles [°] for ***VAM-587.***

References

1 Rigaku OD (2015). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, Oxfordshire, England.

2 Sheldrick, G.M. SHELXT—Integrated space-group and crystal-structure determination. Acta Cryst. A 2015, 71, 3–8.

3 Hübschle, C.B.; Sheldrick, G.M.; Dittrich, B. ShelXle: A Qt graphical user interface for SHELXL. J. Appl. Cryst. 2011, 44, 1281–1284.

4 Sheldrick, G.M. Crystal structure refinement with SHELXL. Acta Cryst. C 2015, 71, 3–8.

5 Macrae, C.F.; Bruno, I.J.; Chisholm, J.A.; Edgington, P.R.; McCabe, P.; Pidcock, E.; Rodriguez-Monge, L.; Taylor, R.; Streek, J.V.; Wood, P.A. Mercury CSD 2.0—New features for the visualization and investigation of crystal structures. J. Appl. Cryst. 2008, 41, 466–470.

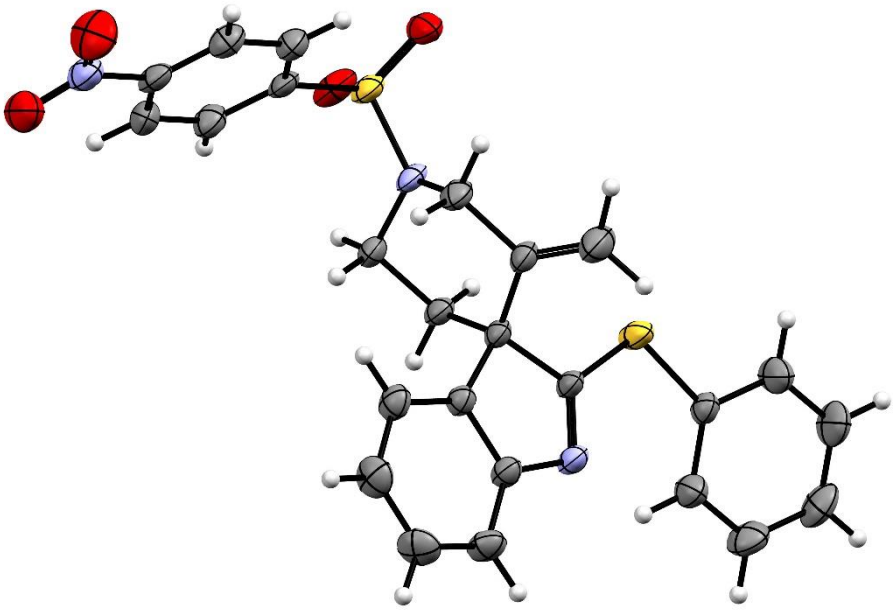


Figure xx Ortep plot of ***VAM-587***. Ellipsoids are drawn at 30% of probability.

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ***VAM-587***. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(2)	328(1)	3078(1)	1317(1)	55(1)
S(1)	2431(1)	1091(1)	5386(1)	66(1)
O(2)	-669(3)	1936(2)	473(2)	76(1)
O(1)	-331(3)	4000(2)	1989(2)	70(1)
N(1)	5610(3)	1862(2)	5915(2)	49(1)
N(2)	1708(3)	2799(2)	2324(2)	48(1)
O(3)	4292(3)	6257(3)	-1019(3)	96(1)
N(3)	3586(3)	5206(3)	-1506(3)	68(1)
O(4)	3501(4)	4548(3)	-2518(3)	104(1)
C(2)	4010(3)	2232(2)	4177(2)	40(1)
C(9)	3074(3)	1295(3)	2906(2)	47(1)
C(11)	2767(4)	3814(2)	3424(2)	48(1)
C(14)	2930(3)	755(2)	6738(2)	46(1)
C(12)	3213(3)	3342(2)	4465(2)	45(1)
C(8)	6629(3)	2431(3)	5435(2)	46(1)
C(10)	2518(4)	1811(3)	1903(2)	55(1)
C(3)	5784(3)	2641(2)	4396(2)	43(1)
C(22)	2048(4)	3480(3)	-1297(3)	58(1)
C(1)	4174(3)	1728(2)	5225(2)	43(1)
C(20)	1285(3)	3718(3)	485(2)	47(1)
C(21)	1304(4)	2981(3)	-646(3)	55(1)
C(7)	8284(3)	2751(3)	5918(3)	59(1)

C(25)	2002(4)	4952(3)	975(3)	57(1)
C(23)	2766(3)	4688(3)	-798(3)	52(1)
C(4)	6619(4)	3179(3)	3817(3)	55(1)
C(15)	4256(4)	1328(3)	7767(3)	68(1)
C(24)	2758(4)	5441(3)	324(3)	61(1)
C(6)	9095(4)	3311(3)	5340(3)	69(1)
C(5)	8285(4)	3503(3)	4305(3)	68(1)
C(17)	3259(5)	163(4)	8803(3)	77(1)
C(16)	4410(5)	1031(4)	8790(3)	77(1)
C(19)	1797(4)	-117(3)	6748(3)	75(1)
C(13)	2812(5)	128(3)	2633(4)	77(1)
C(18)	1954(5)	-412(4)	7788(4)	89(1)

Table S2. Bond lengths [Å] and angles [°] for ***VAM-587***.

S(2)-O(2)	1.419(2)
S(2)-O(1)	1.432(2)
S(2)-N(2)	1.625(2)
S(2)-C(20)	1.770(3)
S(1)-C(1)	1.734(3)
S(1)-C(14)	1.766(3)
N(1)-C(1)	1.283(3)
N(1)-C(8)	1.420(3)
N(2)-C(11)	1.468(4)
N(2)-C(10)	1.471(4)
O(3)-N(3)	1.201(4)
N(3)-O(4)	1.207(4)
N(3)-C(23)	1.492(4)
C(2)-C(3)	1.521(4)
C(2)-C(9)	1.521(4)
C(2)-C(1)	1.548(3)
C(2)-C(12)	1.551(4)
C(9)-C(13)	1.289(4)
C(9)-C(10)	1.521(4)
C(11)-C(12)	1.514(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(14)-C(19)	1.362(4)
C(14)-C(15)	1.375(4)
C(12)-H(12A)	0.9700

C(12)-H(12B)	0.9700
C(8)-C(7)	1.385(4)
C(8)-C(3)	1.395(4)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(3)-C(4)	1.384(4)
C(22)-C(23)	1.358(4)
C(22)-C(21)	1.381(4)
C(22)-H(22)	0.9300
C(20)-C(21)	1.383(4)
C(20)-C(25)	1.386(4)
C(21)-H(21)	0.9300
C(7)-C(6)	1.384(4)
C(7)-H(7)	0.9300
C(25)-C(24)	1.381(4)
C(25)-H(25)	0.9300
C(23)-C(24)	1.377(4)
C(4)-C(5)	1.394(4)
C(4)-H(4)	0.9300
C(15)-C(16)	1.372(4)
C(15)-H(15)	0.9300
C(24)-H(24)	0.9300
C(6)-C(5)	1.370(5)
C(6)-H(6)	0.9300
C(5)-H(5)	0.9300
C(17)-C(18)	1.357(5)
C(17)-C(16)	1.371(5)

C(17)-H(17)	0.9300
C(16)-H(16)	0.9300
C(19)-C(18)	1.392(5)
C(19)-H(19)	0.9300
C(13)-H(13A)	1.09(4)
C(13)-H(13B)	1.03(4)
C(18)-H(18)	0.9300

O(2)-S(2)-O(1)	120.62(16)
O(2)-S(2)-N(2)	107.39(13)
O(1)-S(2)-N(2)	106.68(12)
O(2)-S(2)-C(20)	106.62(13)
O(1)-S(2)-C(20)	107.48(14)
N(2)-S(2)-C(20)	107.45(12)
C(1)-S(1)-C(14)	108.94(13)
C(1)-N(1)-C(8)	106.1(2)
C(11)-N(2)-C(10)	112.5(2)
C(11)-N(2)-S(2)	119.55(17)
C(10)-N(2)-S(2)	119.08(17)
O(3)-N(3)-O(4)	124.7(3)
O(3)-N(3)-C(23)	117.0(3)
O(4)-N(3)-C(23)	118.3(3)
C(3)-C(2)-C(9)	114.4(2)
C(3)-C(2)-C(1)	97.95(19)
C(9)-C(2)-C(1)	114.2(2)
C(3)-C(2)-C(12)	111.3(2)
C(9)-C(2)-C(12)	110.5(2)

C(1)-C(2)-C(12)	107.9(2)
C(13)-C(9)-C(10)	119.7(3)
C(13)-C(9)-C(2)	124.5(3)
C(10)-C(9)-C(2)	115.7(2)
N(2)-C(11)-C(12)	108.0(2)
N(2)-C(11)-H(11A)	110.1
C(12)-C(11)-H(11A)	110.1
N(2)-C(11)-H(11B)	110.1
C(12)-C(11)-H(11B)	110.1
H(11A)-C(11)-H(11B)	108.4
C(19)-C(14)-C(15)	119.1(3)
C(19)-C(14)-S(1)	114.0(2)
C(15)-C(14)-S(1)	126.8(2)
C(11)-C(12)-C(2)	113.3(2)
C(11)-C(12)-H(12A)	108.9
C(2)-C(12)-H(12A)	108.9
C(11)-C(12)-H(12B)	108.9
C(2)-C(12)-H(12B)	108.9
H(12A)-C(12)-H(12B)	107.7
C(7)-C(8)-C(3)	122.2(3)
C(7)-C(8)-N(1)	125.1(2)
C(3)-C(8)-N(1)	112.7(2)
N(2)-C(10)-C(9)	109.3(2)
N(2)-C(10)-H(10A)	109.8
C(9)-C(10)-H(10A)	109.8
N(2)-C(10)-H(10B)	109.8
C(9)-C(10)-H(10B)	109.8

H(10A)-C(10)-H(10B)	108.3
C(4)-C(3)-C(8)	119.3(3)
C(4)-C(3)-C(2)	133.3(2)
C(8)-C(3)-C(2)	107.4(2)
C(23)-C(22)-C(21)	118.8(3)
C(23)-C(22)-H(22)	120.6
C(21)-C(22)-H(22)	120.6
N(1)-C(1)-C(2)	115.7(2)
N(1)-C(1)-S(1)	126.40(19)
C(2)-C(1)-S(1)	117.83(18)
C(21)-C(20)-C(25)	120.9(3)
C(21)-C(20)-S(2)	119.7(2)
C(25)-C(20)-S(2)	119.5(2)
C(22)-C(21)-C(20)	119.7(3)
C(22)-C(21)-H(21)	120.2
C(20)-C(21)-H(21)	120.2
C(6)-C(7)-C(8)	117.6(3)
C(6)-C(7)-H(7)	121.2
C(8)-C(7)-H(7)	121.2
C(24)-C(25)-C(20)	119.0(3)
C(24)-C(25)-H(25)	120.5
C(20)-C(25)-H(25)	120.5
C(22)-C(23)-C(24)	122.6(3)
C(22)-C(23)-N(3)	118.0(3)
C(24)-C(23)-N(3)	119.4(3)
C(3)-C(4)-C(5)	118.4(3)
C(3)-C(4)-H(4)	120.8

C(5)-C(4)-H(4)	120.8
C(16)-C(15)-C(14)	120.0(3)
C(16)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0
C(23)-C(24)-C(25)	119.0(3)
C(23)-C(24)-H(24)	120.5
C(25)-C(24)-H(24)	120.5
C(5)-C(6)-C(7)	121.0(3)
C(5)-C(6)-H(6)	119.5
C(7)-C(6)-H(6)	119.5
C(6)-C(5)-C(4)	121.5(3)
C(6)-C(5)-H(5)	119.2
C(4)-C(5)-H(5)	119.2
C(18)-C(17)-C(16)	119.4(3)
C(18)-C(17)-H(17)	120.3
C(16)-C(17)-H(17)	120.3
C(17)-C(16)-C(15)	120.9(3)
C(17)-C(16)-H(16)	119.5
C(15)-C(16)-H(16)	119.5
C(14)-C(19)-C(18)	120.8(3)
C(14)-C(19)-H(19)	119.6
C(18)-C(19)-H(19)	119.6
C(9)-C(13)-H(13A)	119.7(19)
C(9)-C(13)-H(13B)	123.8(19)
H(13A)-C(13)-H(13B)	116(3)
C(17)-C(18)-C(19)	119.8(3)
C(17)-C(18)-H(18)	120.1

C(19)-C(18)-H(18)	120.1

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ***VAM-587***. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(2)	48(1)	80(1)	48(1)	45(1)	9(1)	13(1)
S(1)	40(1)	103(1)	66(1)	61(1)	4(1)	-1(1)
O(2)	64(1)	95(2)	60(1)	48(1)	-2(1)	-11(1)
O(1)	64(1)	114(2)	66(1)	60(1)	32(1)	48(1)
N(1)	39(1)	68(2)	53(1)	40(1)	12(1)	14(1)
N(2)	55(1)	56(1)	38(1)	29(1)	7(1)	19(1)
O(3)	82(2)	117(2)	93(2)	65(2)	18(2)	-7(2)
N(3)	55(2)	93(2)	67(2)	53(2)	11(1)	9(2)
O(4)	125(3)	137(3)	75(2)	55(2)	54(2)	21(2)
C(2)	42(1)	48(2)	40(1)	28(1)	12(1)	12(1)
C(9)	56(2)	49(2)	45(2)	28(1)	14(1)	16(1)
C(11)	54(2)	48(2)	47(2)	28(1)	12(1)	16(1)
C(14)	48(2)	52(2)	48(2)	30(1)	17(1)	10(1)
C(12)	44(2)	56(2)	42(1)	29(1)	10(1)	14(1)
C(8)	40(1)	58(2)	50(2)	30(1)	16(1)	16(1)
C(10)	68(2)	57(2)	38(1)	24(1)	9(1)	13(2)
C(3)	42(1)	48(2)	46(1)	25(1)	16(1)	12(1)
C(22)	65(2)	70(2)	48(2)	30(2)	21(2)	23(2)

C(1)	37(1)	54(2)	46(1)	33(1)	10(1)	9(1)
C(20)	45(2)	62(2)	42(2)	34(1)	6(1)	17(1)
C(21)	63(2)	58(2)	48(2)	28(2)	13(1)	13(2)
C(7)	41(2)	83(2)	62(2)	36(2)	16(1)	20(2)
C(25)	70(2)	60(2)	45(2)	27(1)	16(1)	17(2)
C(23)	46(2)	76(2)	48(2)	41(2)	13(1)	20(2)
C(4)	56(2)	66(2)	60(2)	37(2)	26(2)	15(2)
C(15)	64(2)	78(2)	58(2)	38(2)	8(2)	-3(2)
C(24)	64(2)	57(2)	63(2)	36(2)	9(2)	6(2)
C(6)	41(2)	92(3)	78(2)	31(2)	27(2)	13(2)
C(5)	59(2)	84(2)	80(2)	40(2)	40(2)	12(2)
C(17)	98(3)	101(3)	71(2)	61(2)	45(2)	41(2)
C(16)	82(2)	102(3)	47(2)	37(2)	11(2)	18(2)
C(19)	64(2)	92(3)	70(2)	47(2)	14(2)	-10(2)
C(13)	94(3)	67(2)	65(2)	32(2)	9(2)	22(2)
C(18)	94(3)	104(3)	92(3)	68(2)	35(2)	-1(2)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ***VAM-587***.

	x	y	z	U(eq)
H(11A)	2223	4477	3631	57
H(11B)	3722	4120	3276	57
H(12A)	2255	3107	4646	55
H(12B)	3943	3998	5191	55
H(10A)	3430	2125	1713	65
H(10B)	1787	1170	1165	65
H(22)	2057	2998	-2064	69
H(21)	819	2153	-966	66
H(7)	8832	2596	6605	71
H(25)	1974	5444	1732	68
H(4)	6081	3321	3118	66
H(15)	5048	1916	7770	81
H(24)	3254	6266	638	73
H(6)	10205	3560	5658	83
H(5)	8860	3859	3920	82
H(17)	3373	-29	9502	92
H(16)	5307	1425	9485	92
H(19)	907	-520	6050	90
H(18)	1166	-1002	7787	107
H(13A)	2130(40)	-480(30)	1700(30)	83(11)
H(13B)	3240(40)	-280(30)	3250(30)	82(10)

Table S5. Torsion angles [°] for ***VAM-587***.

O(2)-S(2)-N(2)-C(11)	-170.5(2)
O(1)-S(2)-N(2)-C(11)	-39.9(2)
C(20)-S(2)-N(2)-C(11)	75.1(2)
O(2)-S(2)-N(2)-C(10)	44.6(3)
O(1)-S(2)-N(2)-C(10)	175.2(2)
C(20)-S(2)-N(2)-C(10)	-69.7(2)
C(3)-C(2)-C(9)-C(13)	92.9(4)
C(1)-C(2)-C(9)-C(13)	-18.8(4)
C(12)-C(2)-C(9)-C(13)	-140.6(3)
C(3)-C(2)-C(9)-C(10)	-83.4(3)
C(1)-C(2)-C(9)-C(10)	164.9(2)
C(12)-C(2)-C(9)-C(10)	43.1(3)
C(10)-N(2)-C(11)-C(12)	-64.9(3)
S(2)-N(2)-C(11)-C(12)	148.1(2)
C(1)-S(1)-C(14)-C(19)	-157.7(3)
C(1)-S(1)-C(14)-C(15)	26.7(3)
N(2)-C(11)-C(12)-C(2)	56.7(3)
C(3)-C(2)-C(12)-C(11)	81.8(3)
C(9)-C(2)-C(12)-C(11)	-46.4(3)
C(1)-C(2)-C(12)-C(11)	-171.9(2)
C(1)-N(1)-C(8)-C(7)	179.4(3)
C(1)-N(1)-C(8)-C(3)	-0.8(3)
C(11)-N(2)-C(10)-C(9)	61.0(3)
S(2)-N(2)-C(10)-C(9)	-151.9(2)
C(13)-C(9)-C(10)-N(2)	133.6(3)

C(2)-C(9)-C(10)-N(2)	-49.9(3)
C(7)-C(8)-C(3)-C(4)	0.5(4)
N(1)-C(8)-C(3)-C(4)	-179.3(3)
C(7)-C(8)-C(3)-C(2)	-177.3(3)
N(1)-C(8)-C(3)-C(2)	2.9(3)
C(9)-C(2)-C(3)-C(4)	58.1(4)
C(1)-C(2)-C(3)-C(4)	179.3(3)
C(12)-C(2)-C(3)-C(4)	-67.9(4)
C(9)-C(2)-C(3)-C(8)	-124.6(2)
C(1)-C(2)-C(3)-C(8)	-3.4(3)
C(12)-C(2)-C(3)-C(8)	109.4(2)
C(8)-N(1)-C(1)-C(2)	-1.7(3)
C(8)-N(1)-C(1)-S(1)	-179.5(2)
C(3)-C(2)-C(1)-N(1)	3.3(3)
C(9)-C(2)-C(1)-N(1)	124.6(3)
C(12)-C(2)-C(1)-N(1)	-112.2(3)
C(3)-C(2)-C(1)-S(1)	-178.75(19)
C(9)-C(2)-C(1)-S(1)	-57.4(3)
C(12)-C(2)-C(1)-S(1)	65.8(3)
C(14)-S(1)-C(1)-N(1)	4.6(3)
C(14)-S(1)-C(1)-C(2)	-173.2(2)
O(2)-S(2)-C(20)-C(21)	-16.5(3)
O(1)-S(2)-C(20)-C(21)	-147.2(2)
N(2)-S(2)-C(20)-C(21)	98.4(2)
O(2)-S(2)-C(20)-C(25)	163.4(2)
O(1)-S(2)-C(20)-C(25)	32.7(3)
N(2)-S(2)-C(20)-C(25)	-81.8(2)

C(23)-C(22)-C(21)-C(20)	0.9(4)
C(25)-C(20)-C(21)-C(22)	0.0(4)
S(2)-C(20)-C(21)-C(22)	179.9(2)
C(3)-C(8)-C(7)-C(6)	0.8(5)
N(1)-C(8)-C(7)-C(6)	-179.4(3)
C(21)-C(20)-C(25)-C(24)	-0.7(4)
S(2)-C(20)-C(25)-C(24)	179.4(2)
C(21)-C(22)-C(23)-C(24)	-1.2(5)
C(21)-C(22)-C(23)-N(3)	179.1(3)
O(3)-N(3)-C(23)-C(22)	-175.8(3)
O(4)-N(3)-C(23)-C(22)	3.9(4)
O(3)-N(3)-C(23)-C(24)	4.4(4)
O(4)-N(3)-C(23)-C(24)	-175.8(3)
C(8)-C(3)-C(4)-C(5)	-0.6(4)
C(2)-C(3)-C(4)-C(5)	176.5(3)
C(19)-C(14)-C(15)-C(16)	-1.0(5)
S(1)-C(14)-C(15)-C(16)	174.4(3)
C(22)-C(23)-C(24)-C(25)	0.5(5)
N(3)-C(23)-C(24)-C(25)	-179.8(3)
C(20)-C(25)-C(24)-C(23)	0.5(5)
C(8)-C(7)-C(6)-C(5)	-2.0(5)
C(7)-C(6)-C(5)-C(4)	2.0(5)
C(3)-C(4)-C(5)-C(6)	-0.6(5)
C(18)-C(17)-C(16)-C(15)	0.2(6)
C(14)-C(15)-C(16)-C(17)	0.3(6)
C(15)-C(14)-C(19)-C(18)	1.2(6)
S(1)-C(14)-C(19)-C(18)	-174.8(3)

C(16)-C(17)-C(18)-C(19)	0.0(6)
C(14)-C(19)-C(18)-C(17)	-0.8(6)

Symmetry transformations used to generate equivalent atoms: