Enantioselective Total Synthesis of Lycopodine.

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Electronic Supplementary Information: Crystallographic Data

Figure 1. ORTEP Representation of X-Ray Crystallographic Analysis of Ketone **3**.

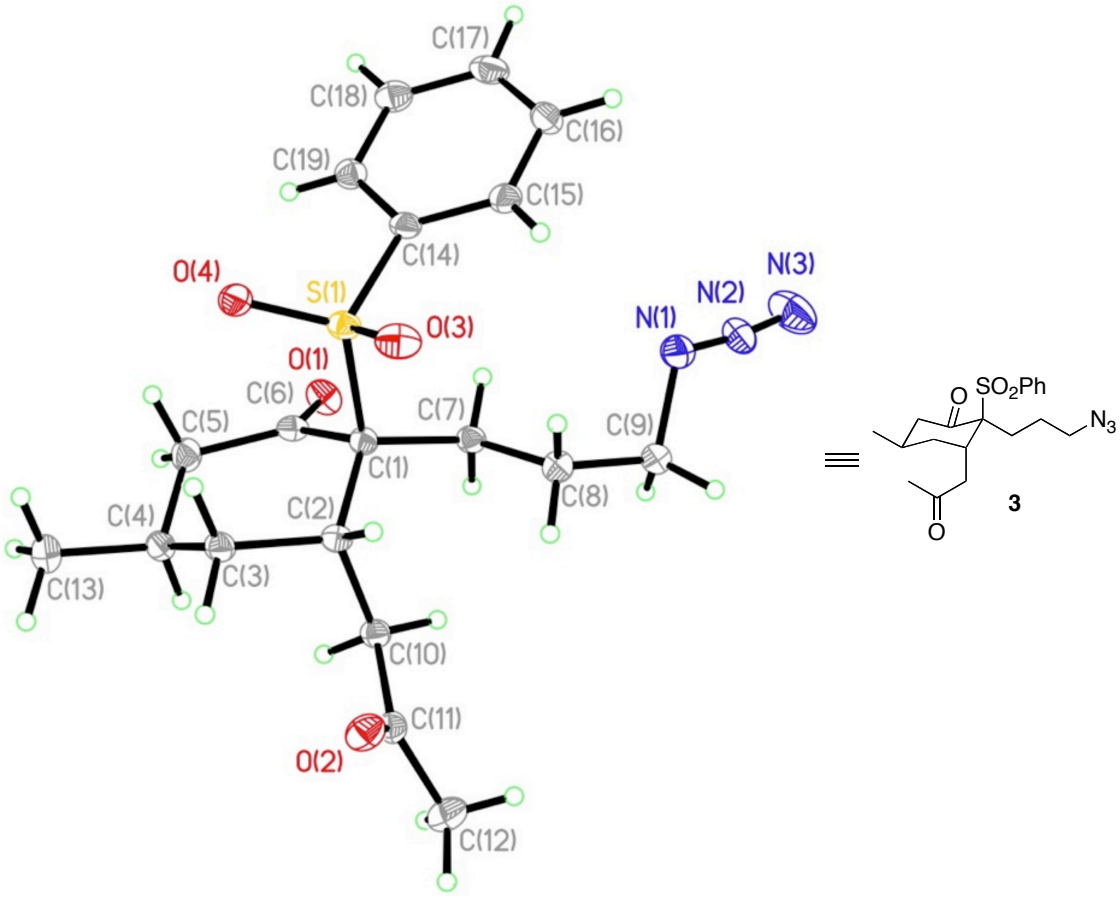

Table 1. Crystal data and structure refinement for rc28 (Compound **3**).

Identification code	rc28	
Empirical formula	C19 H25 N3 O4 S	
Formula weight	391.48	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 11.2466(8) Å	a= 90°.
	b = 11.9082(9) Å	b= 90°.
	c = 14.2975(10) Å	g = 90°.
Volume	1914.8(2) $Å^3$	
Z	4	
Density (calculated)	1.358 Mg/m^3	
Absorption coefficient	0.199 mm^{-1}	
F(000)	832	
Crystal size	0.32 x 0.16 x 0.14 mm^3	
Theta range for data collection	2.23 to 27.00°.	
Index ranges	-14<=h<=14, -15<=k<=15, -18<=l<=18	
Reflections collected	21488	
Independent reflections	4185 [R(int) = 0.0385]	
Completeness to theta = 27.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9726 and 0.9389	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4185 / 0 / 344	
Goodness-of-fit on F^2	1.086	
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0816	
R indices (all data)	R1 = 0.0424, wR2 = 0.0861	
Absolute structure parameter	0.00(6)	
Largest diff. peak and hole	0.255 and -0.169 $e.Å^{-3}$	

Figure 2. ORTEP Representation of X-Ray Crystallographic Analysis of Tricycle **19**.

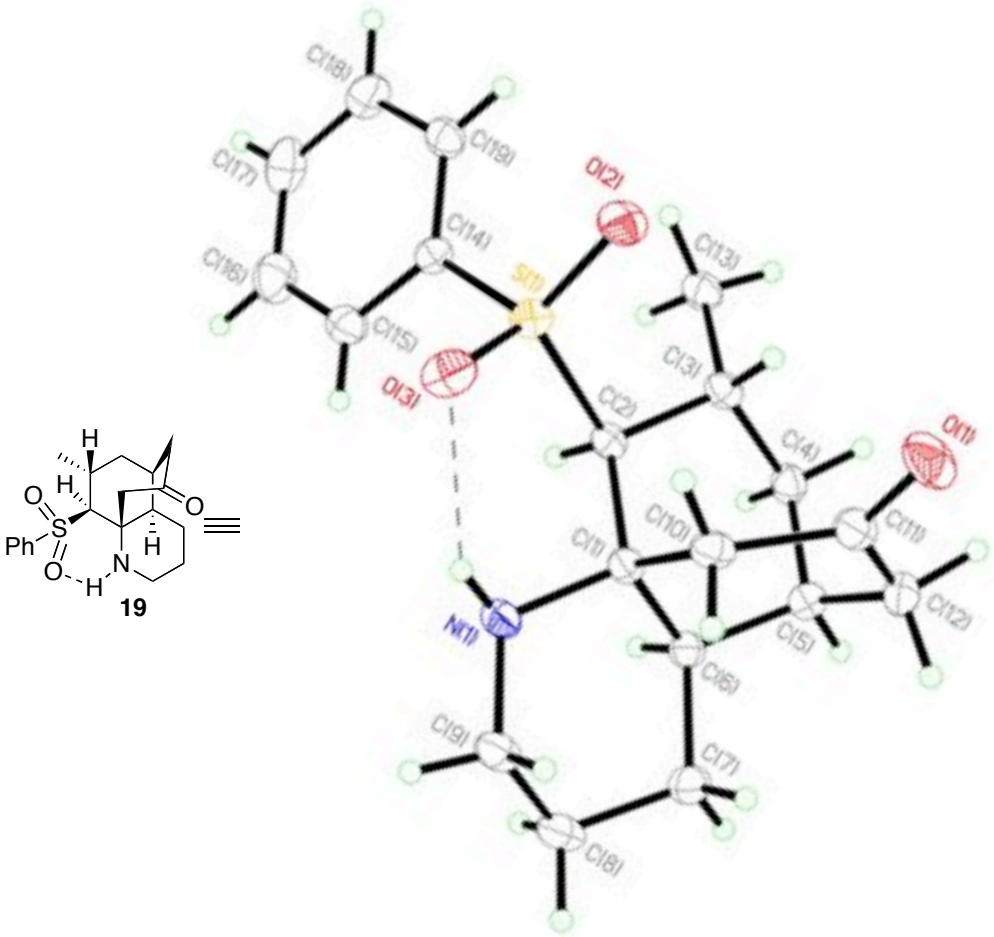

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Table 2. Crystal data and structure refinement for rc31 (Compound **19**).

Identification code	rc31	
Empirical formula	C19 H25 N O3 S	
Formula weight	347.46	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 9.3648(10) Å	a= 90°.
	b = 10.0518(11) Å	b= 90°.
	c = 18.751(2) Å	g = 90°.
Volume	1765.1(3) $Å^3$	
Z	4	
Density (calculated)	1.307 Mg/m^3	
Absorption coefficient	0.200 mm^{-1}	
F(000)	744	
Crystal size	0.22 x 0.13 x 0.03 mm^3	
Theta range for data collection	2.17 to 26.99°.	
Index ranges	-11<=h<=11, -12<=k<=12, -23<=l<=23	
Reflections collected	19903	
Independent reflections	3842 [R(int) = 0.0595]	
Completeness to theta = 26.99°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9940 and 0.9573	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3842 / 0 / 317	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0436, wR2 = 0.0799	
R indices (all data)	R1 = 0.0618, wR2 = 0.0876	
Absolute structure parameter	0.03(8)	
Largest diff. peak and hole	0.203 and -0.237 $e.Å^{-3}$	