

Supporting Information

Total synthesis and evaluation of melleumin A, a cyclic depsipeptide from the myxomycete *Physarum melleum*

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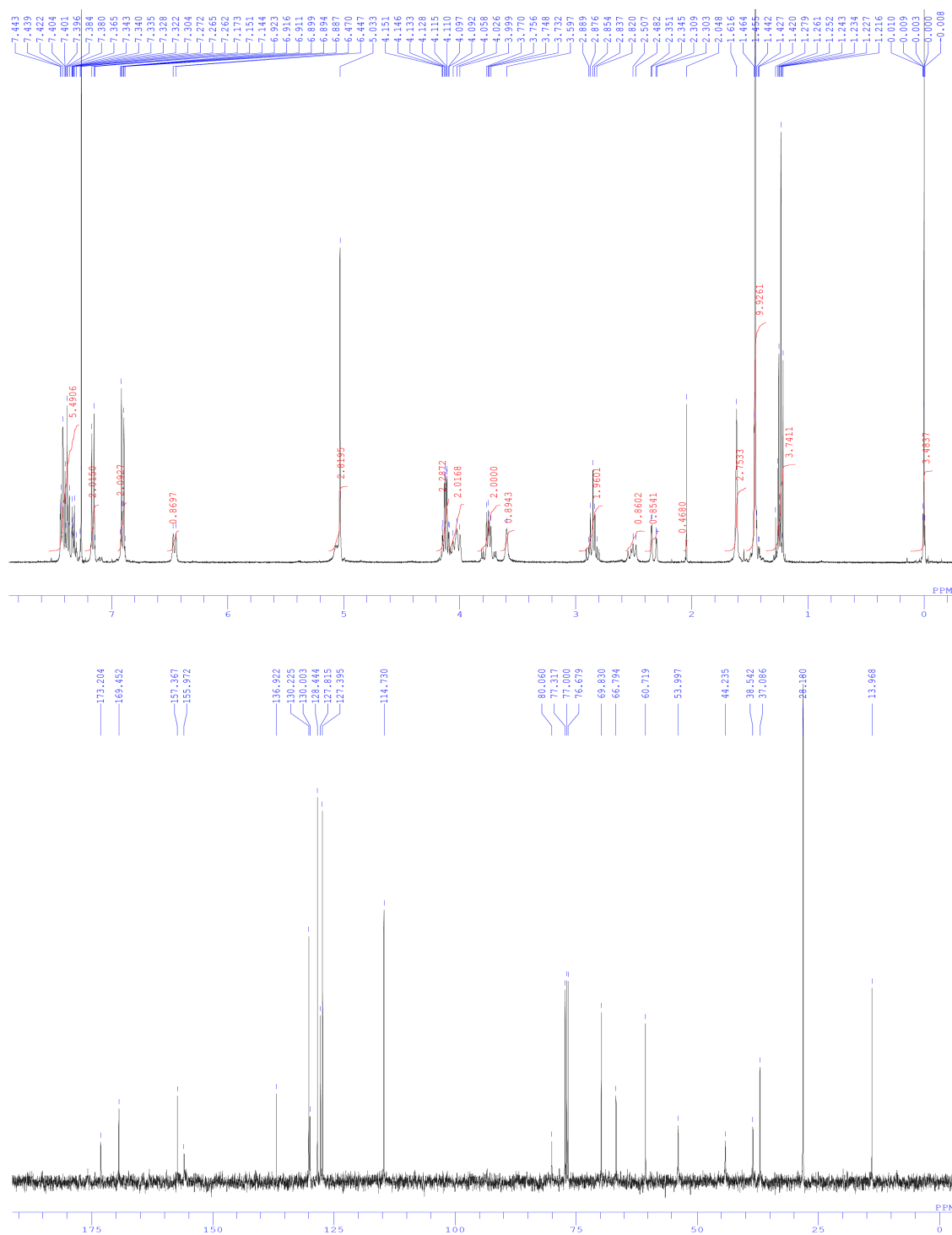
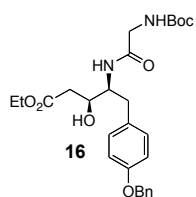
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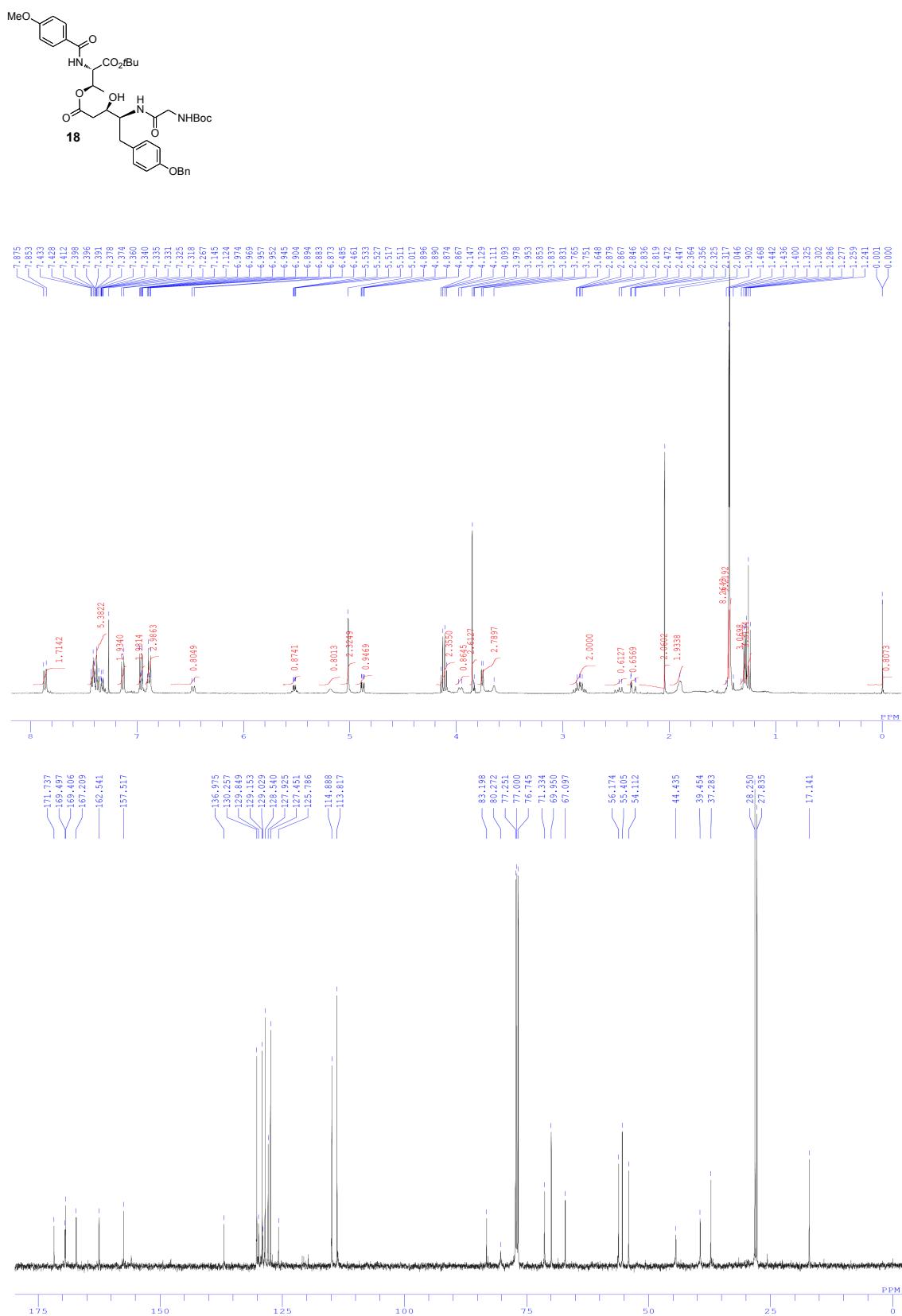
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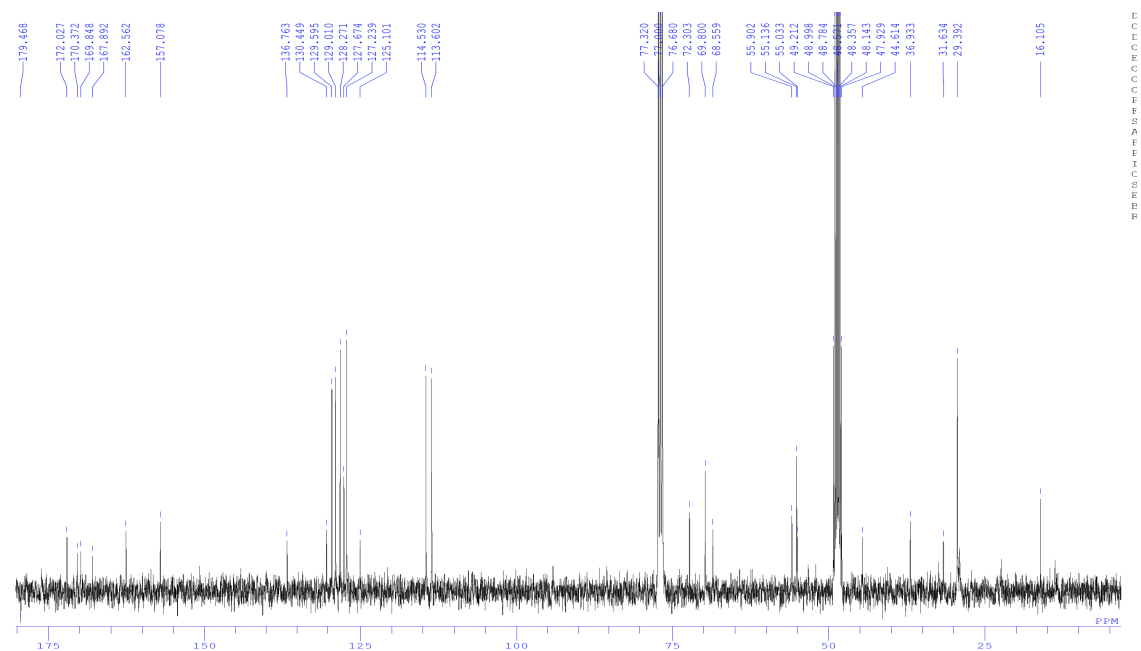
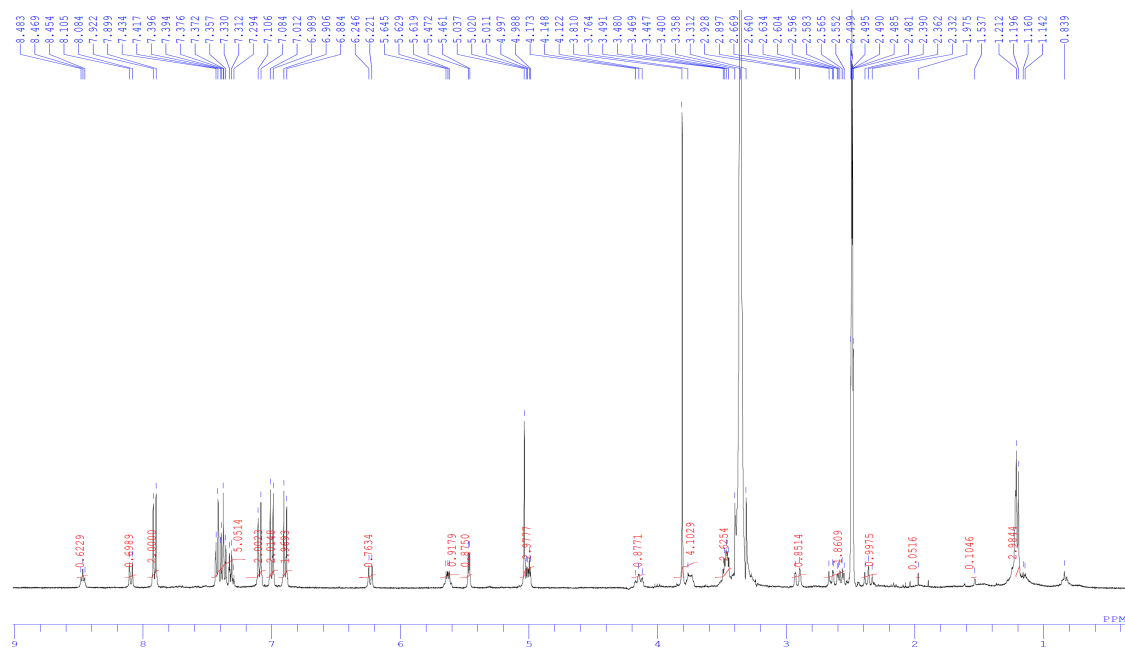
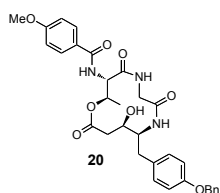
S2~17 ^1H and ^{13}C NMR spectra.

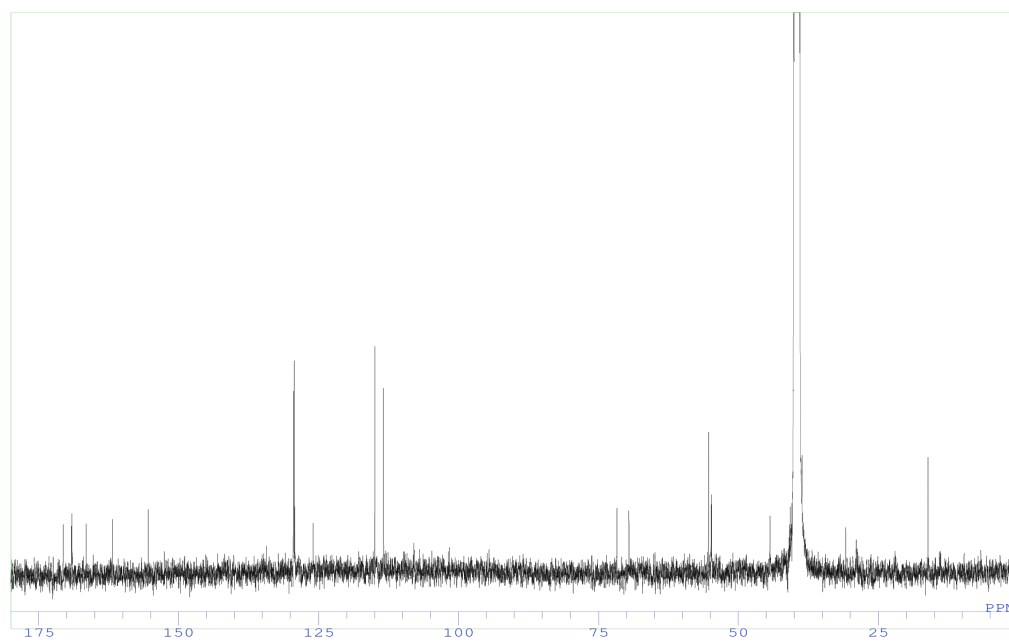
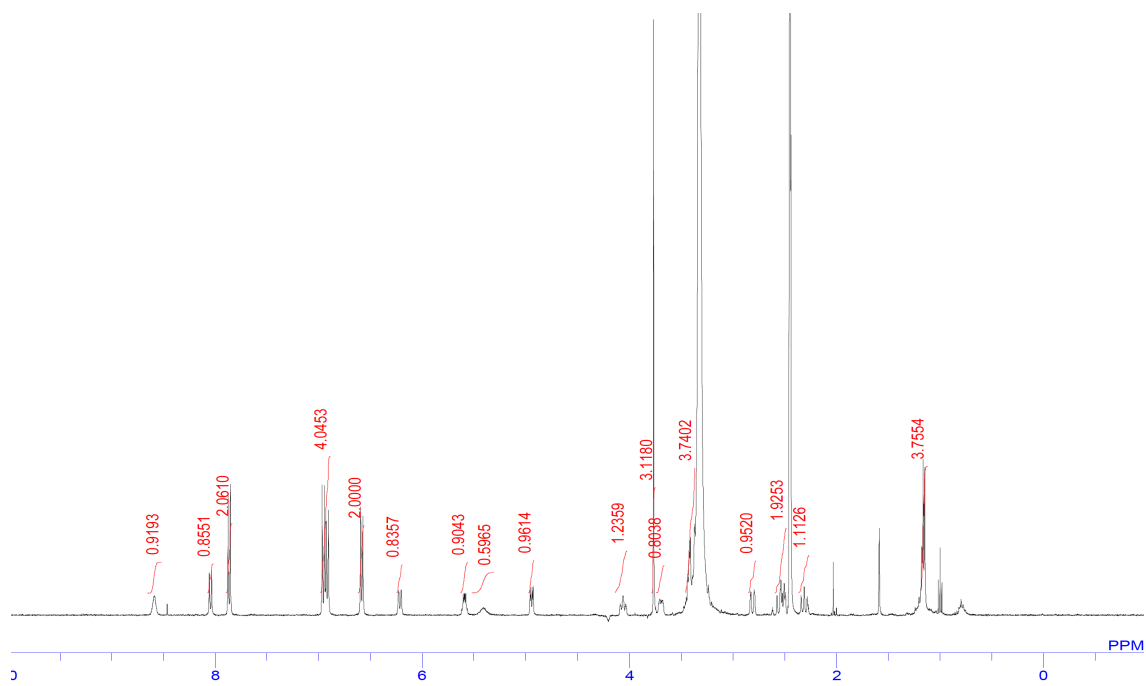
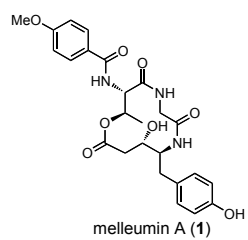
S15 COSY and HMBC of compound **26**.

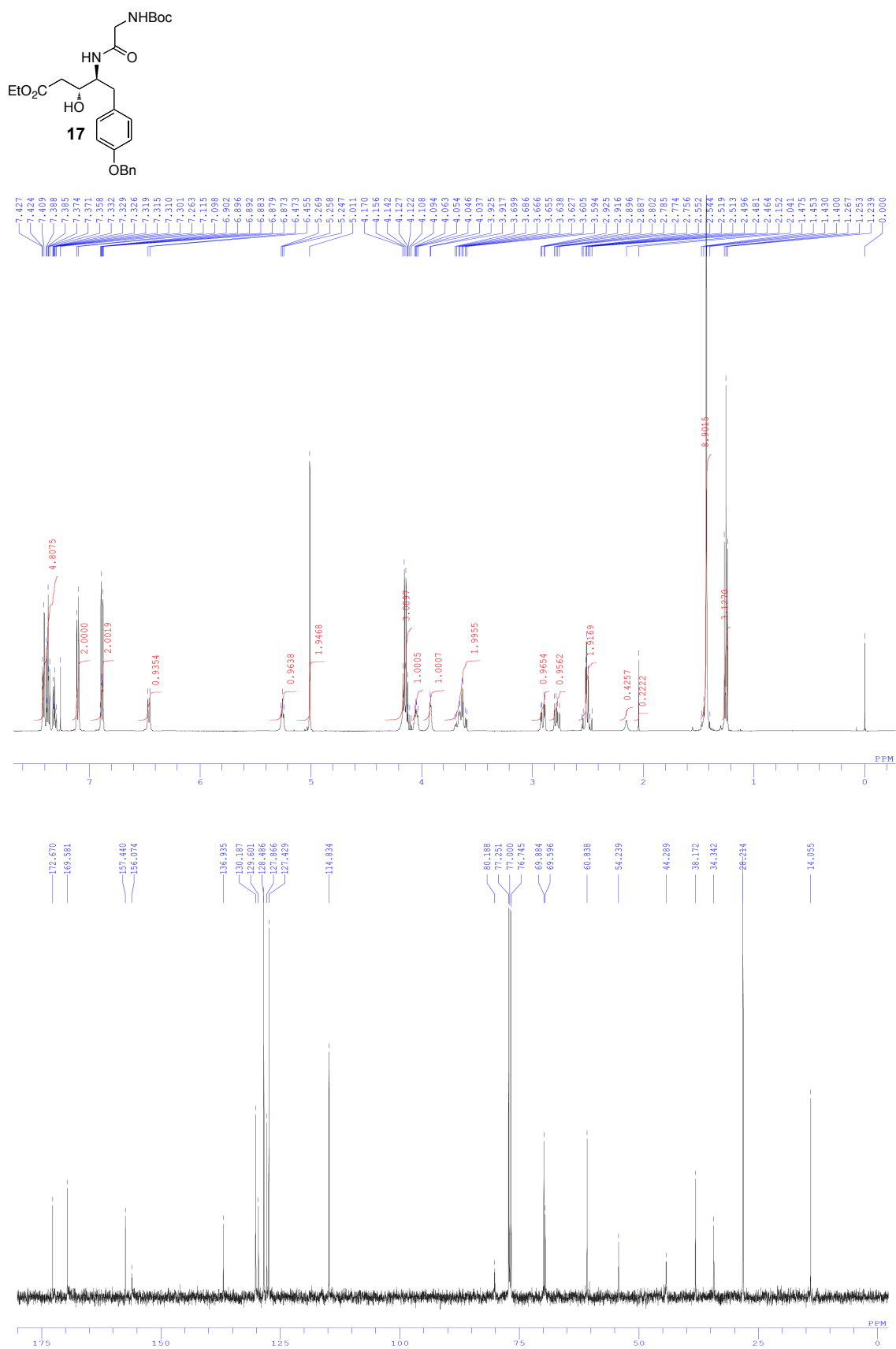
S18~ X-ray Structure Report.

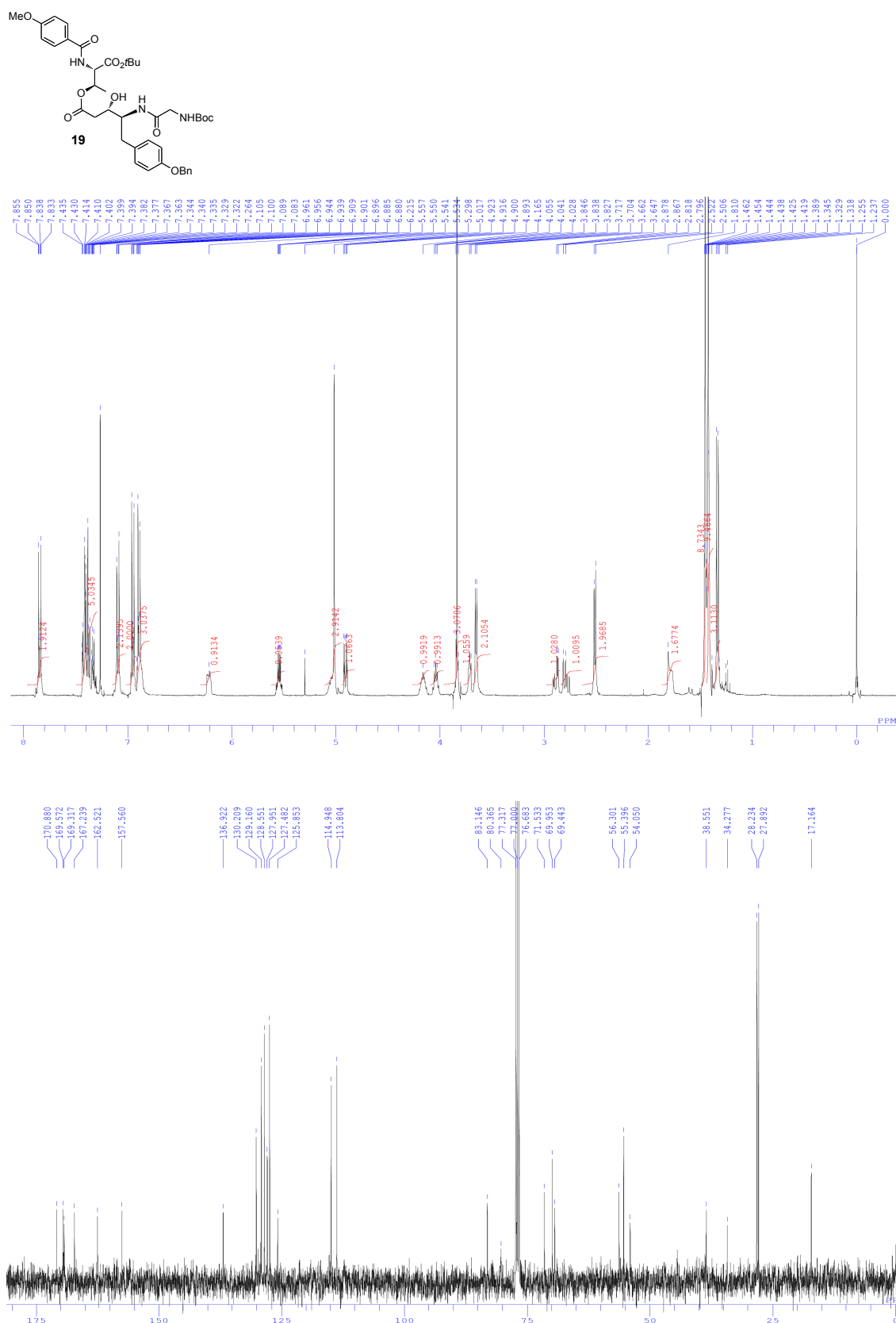


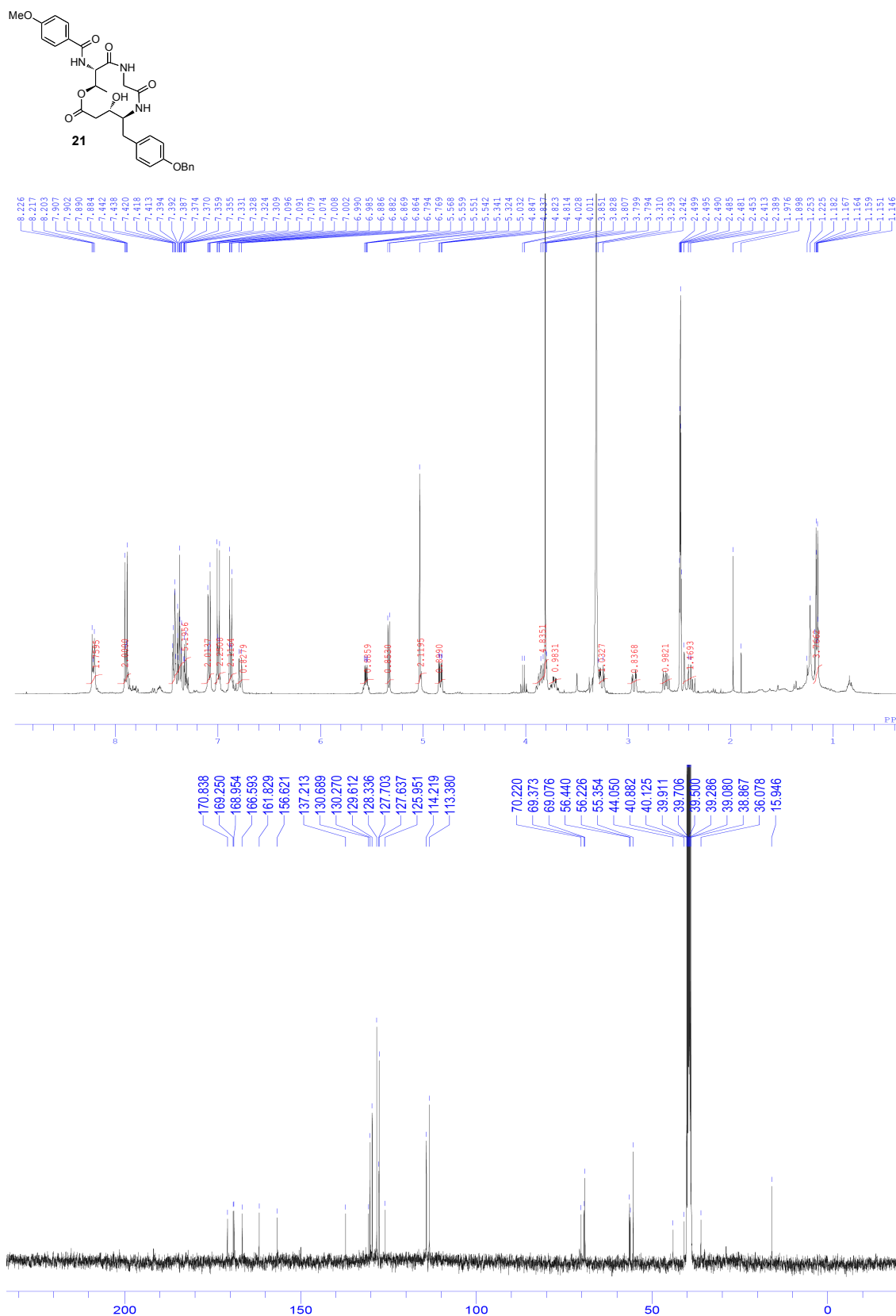


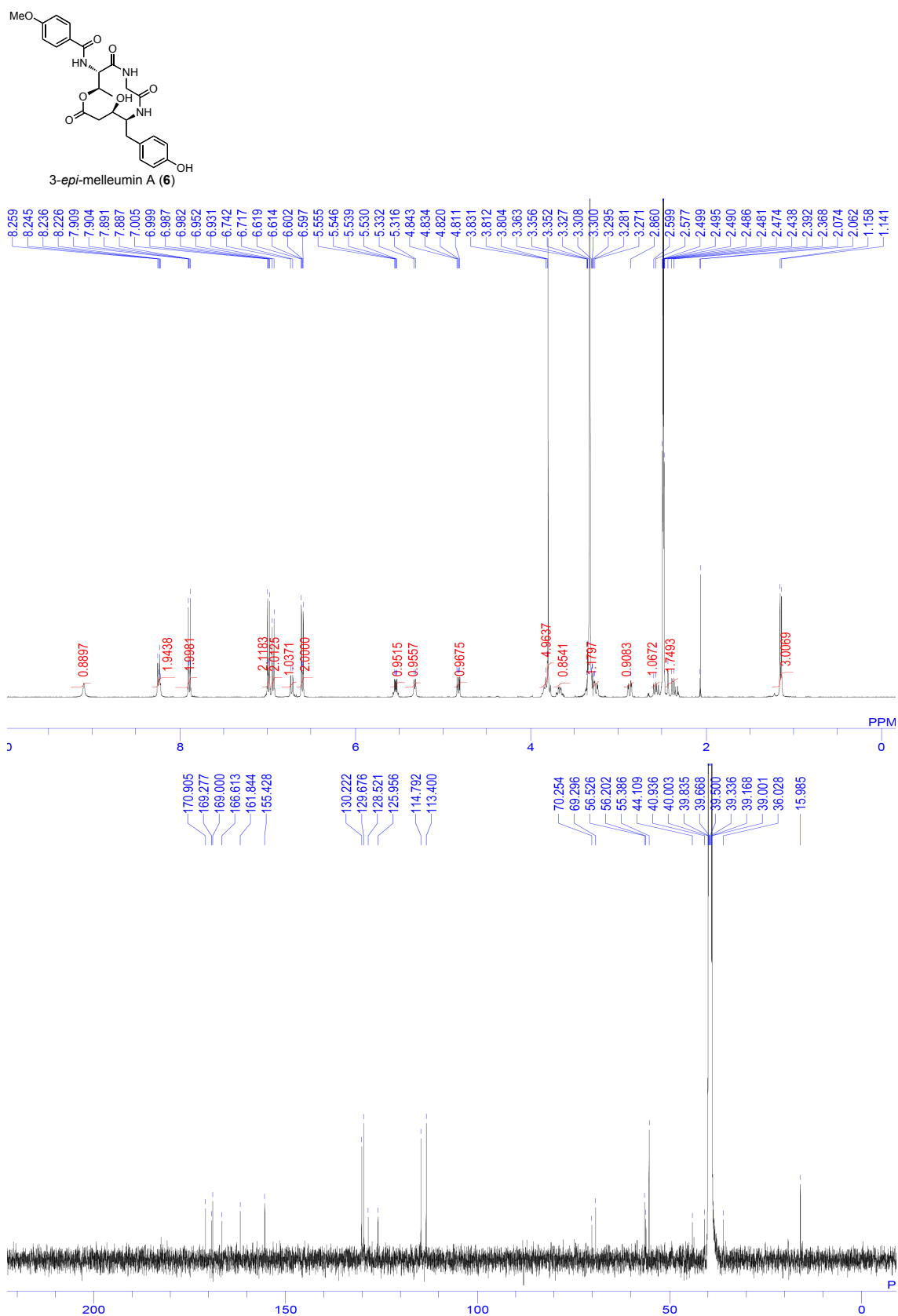


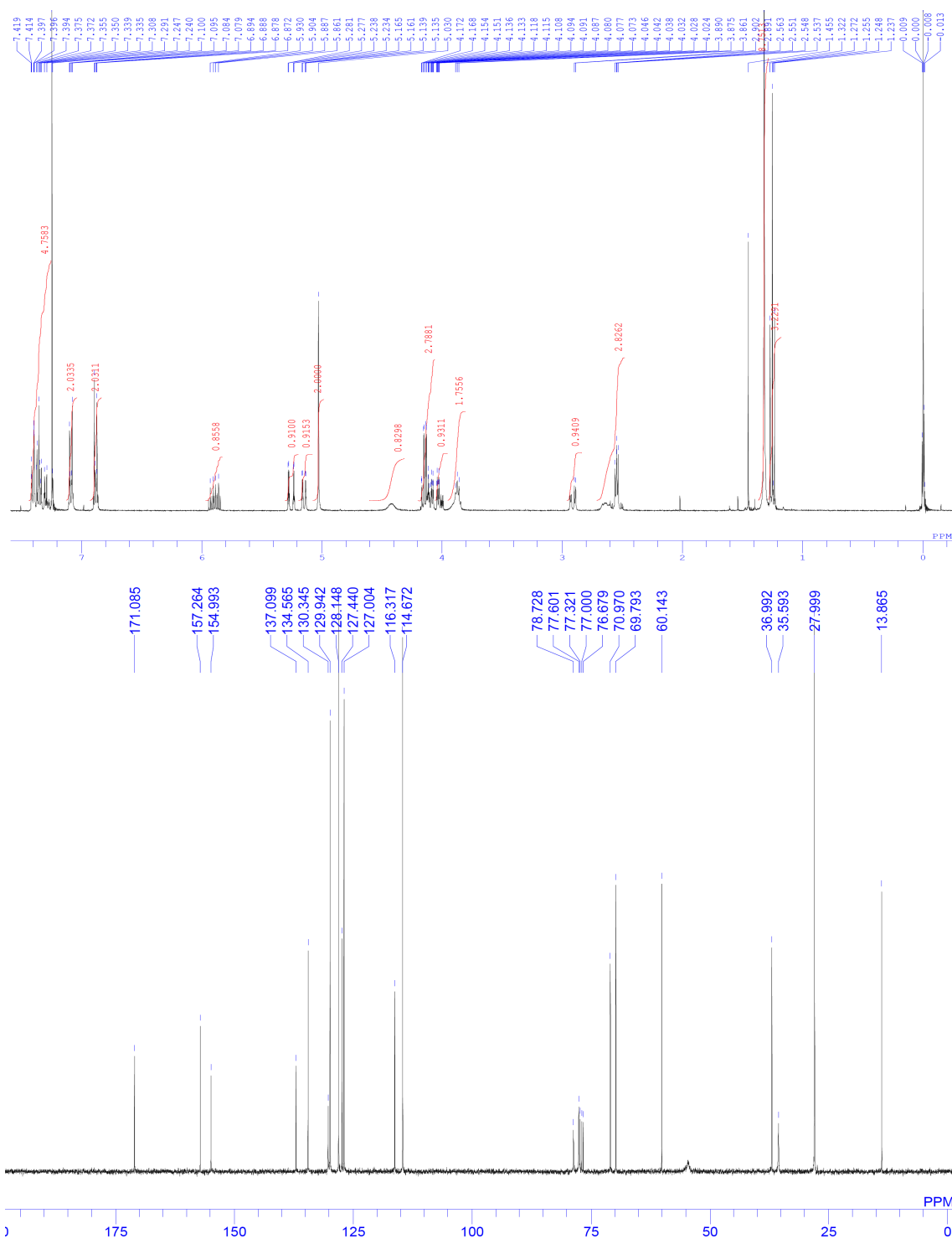
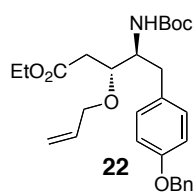


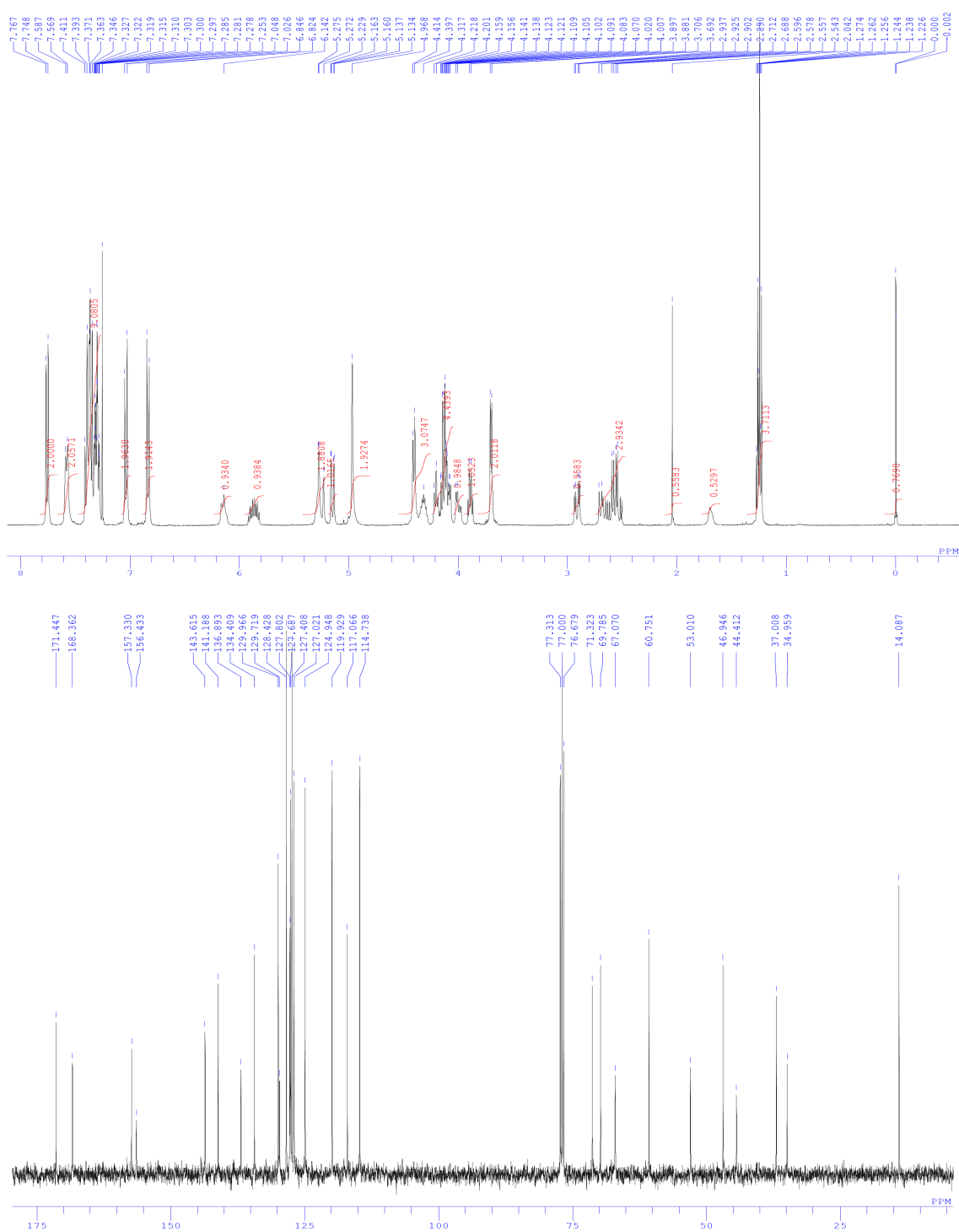
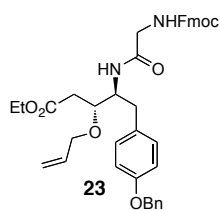


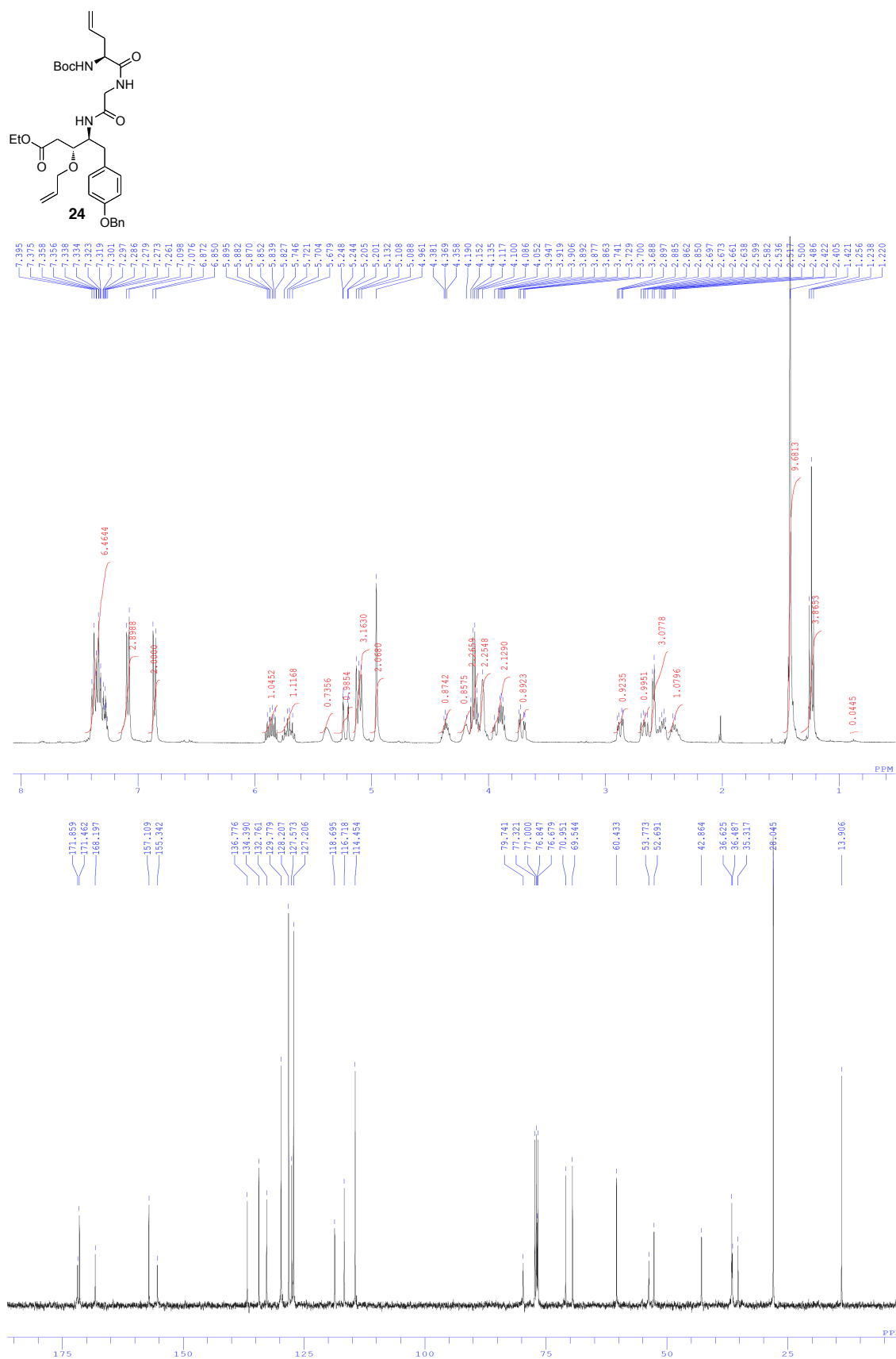


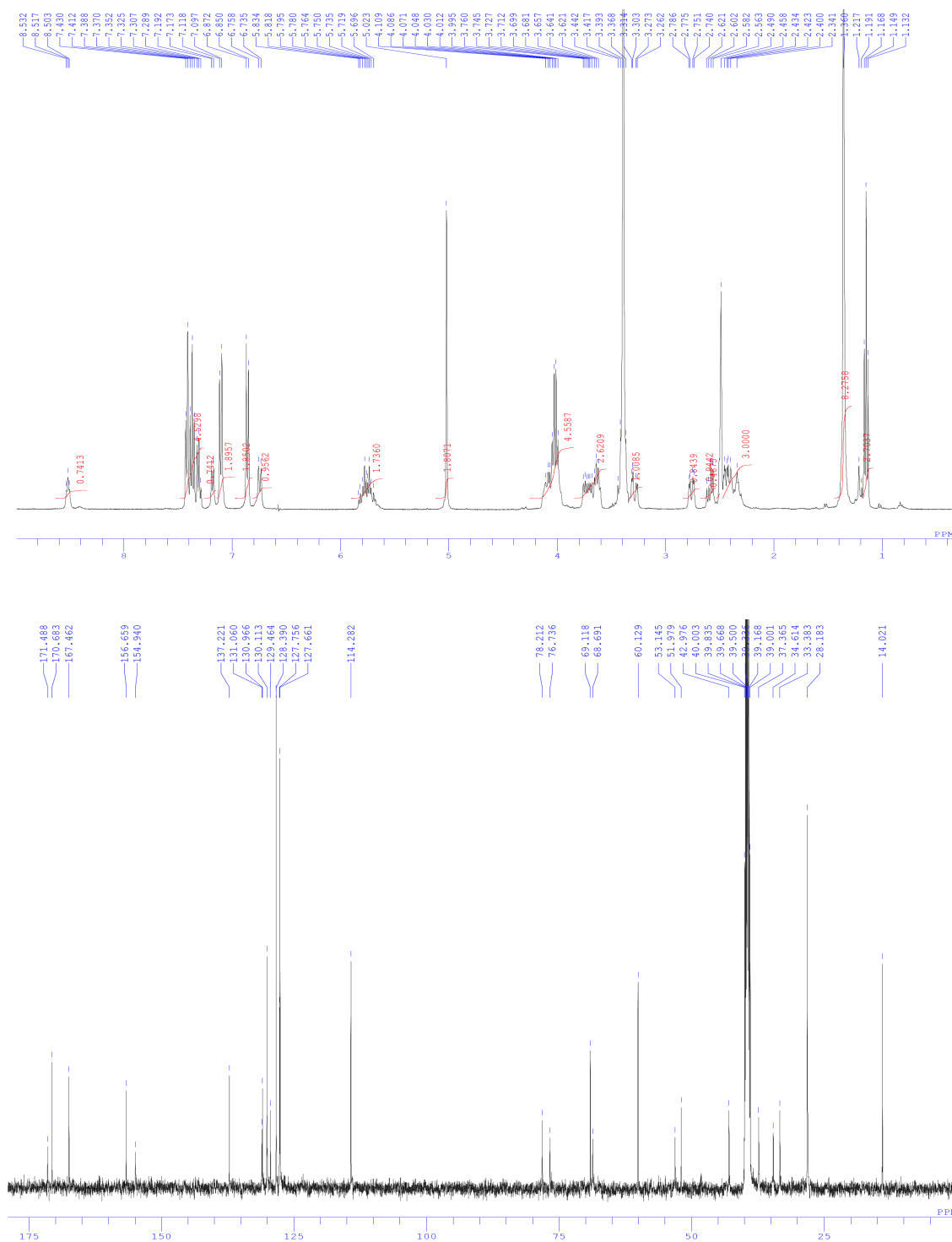
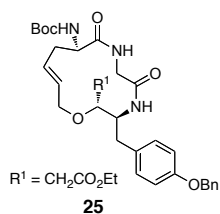


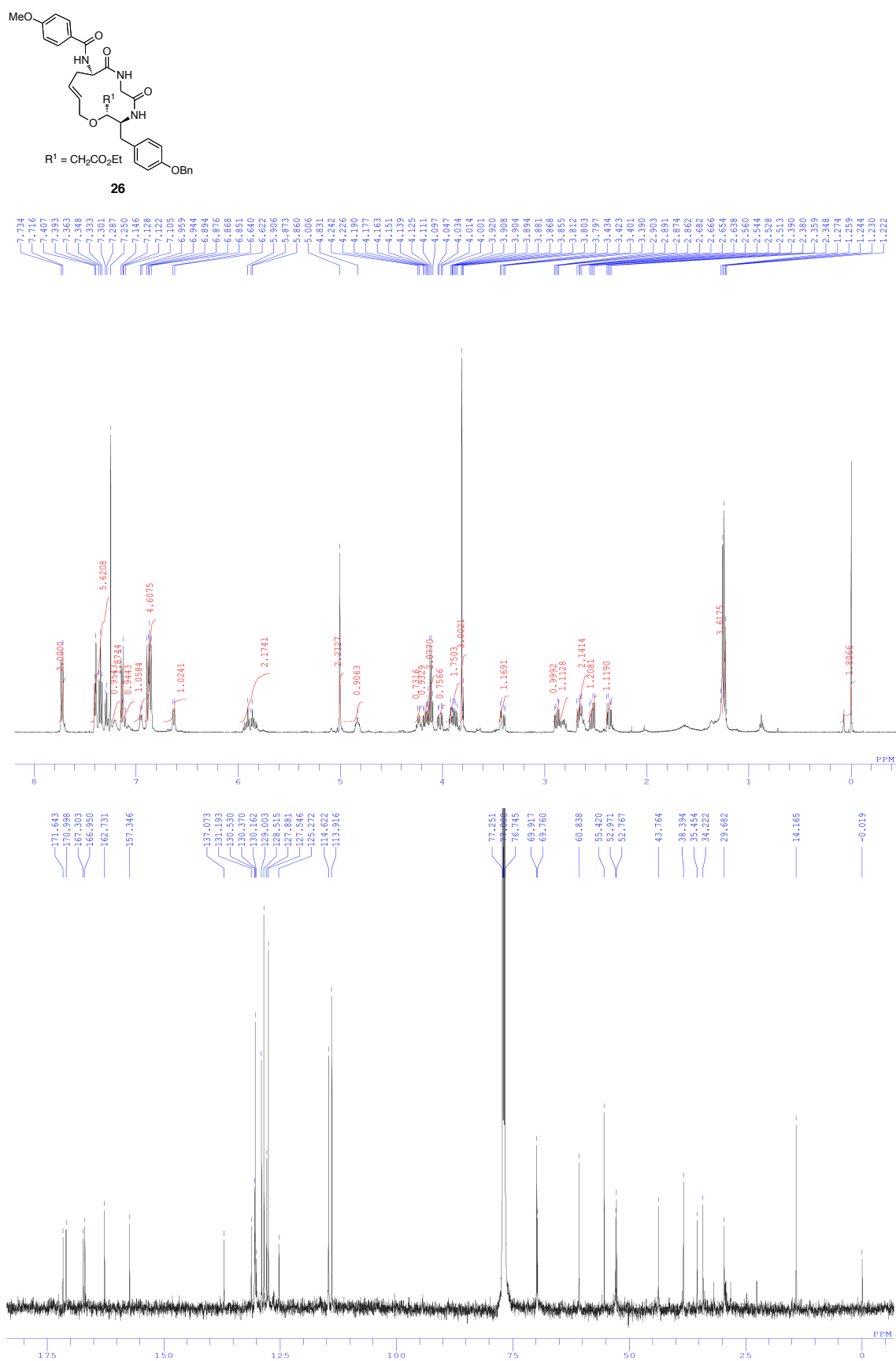


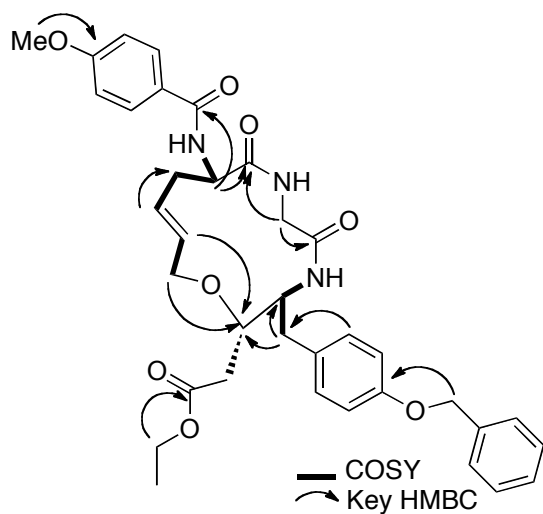




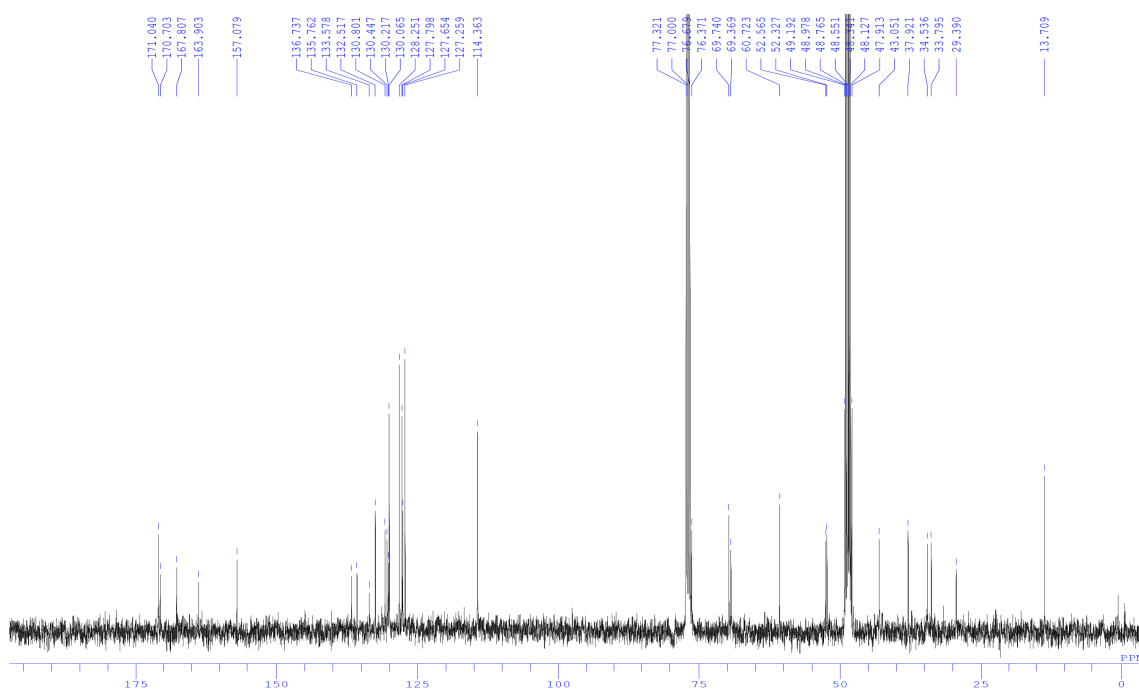
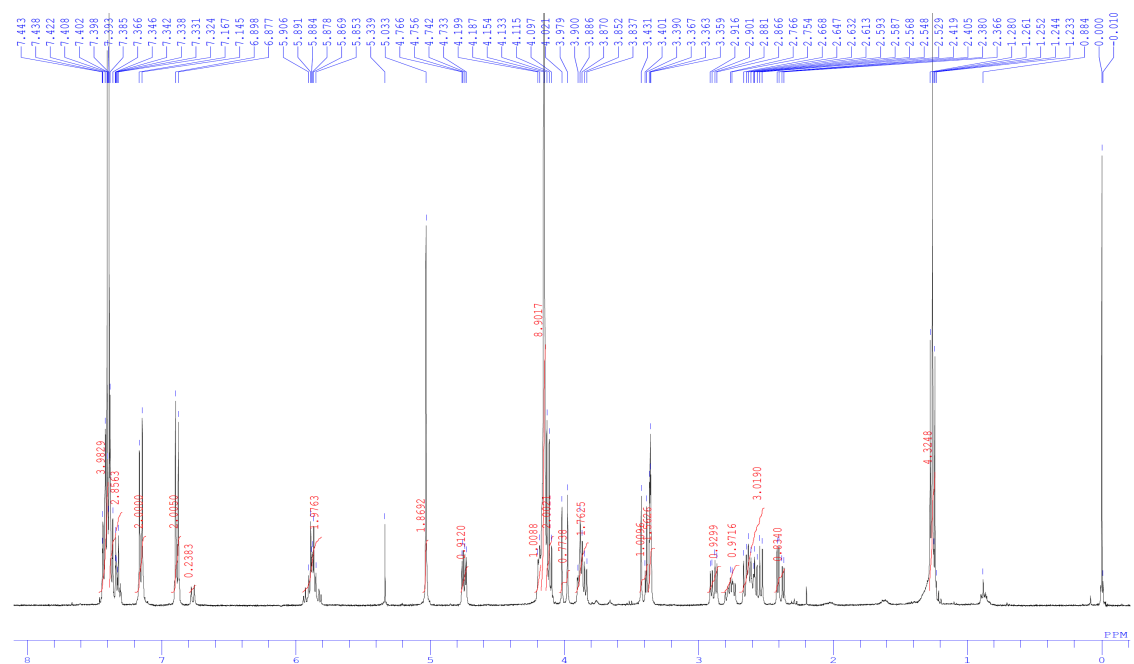
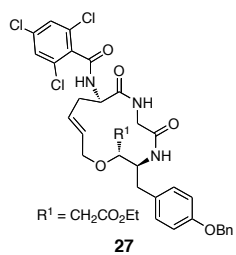


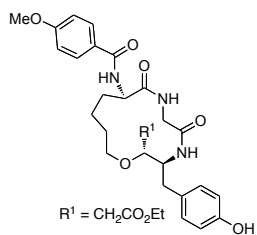




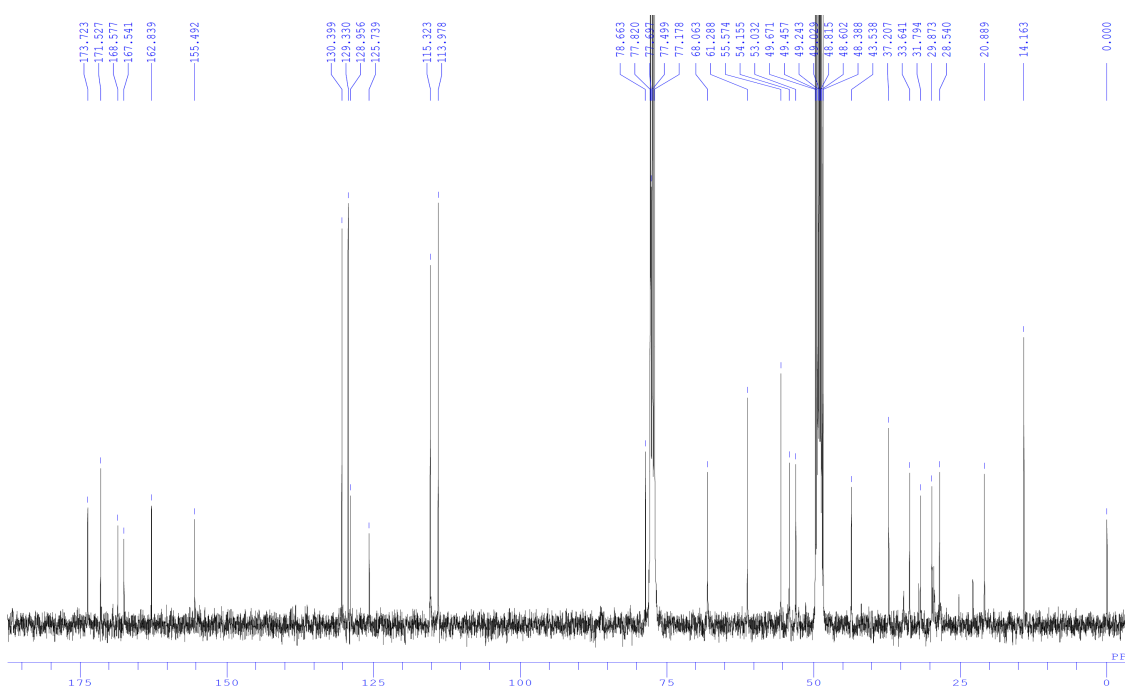
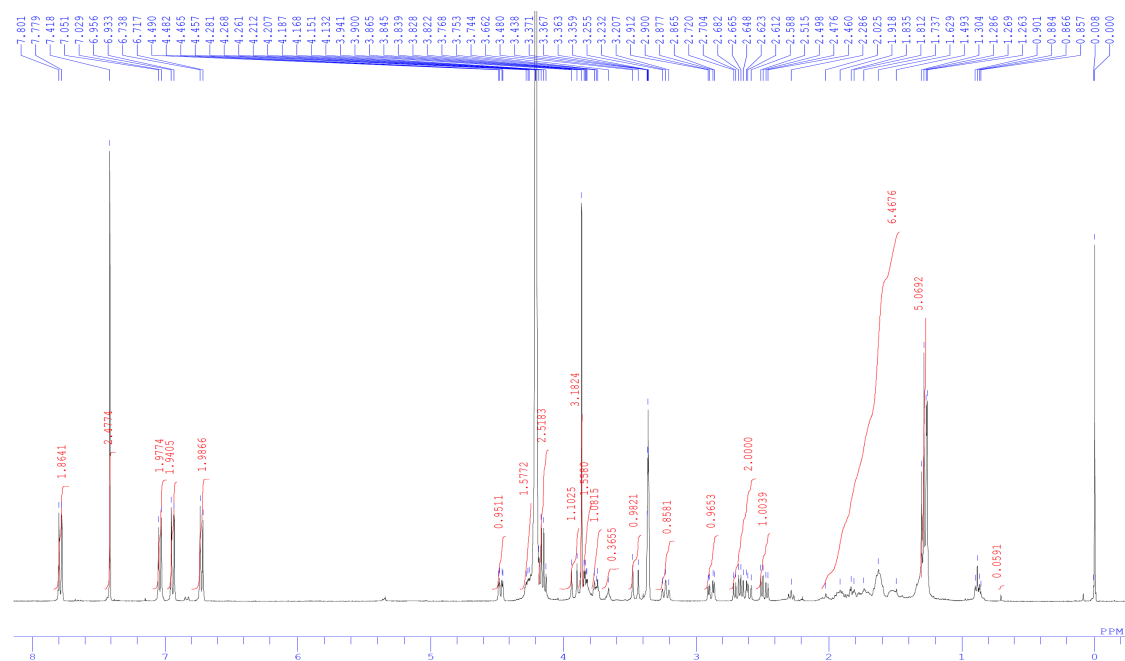


^1H - ^1H COSY and HMBC correlations of **26**

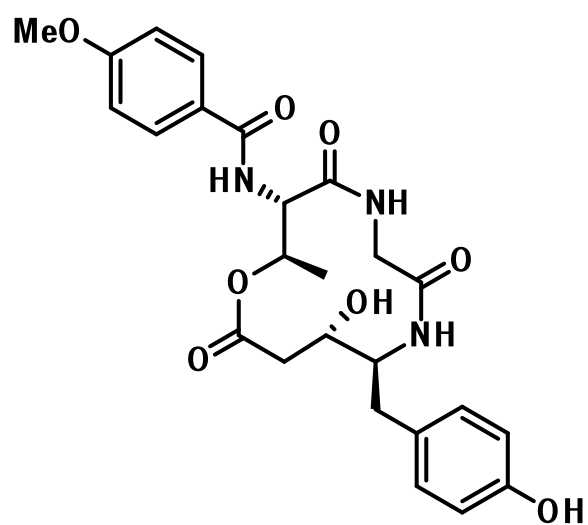




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X-ray Structure Report



melleumin A

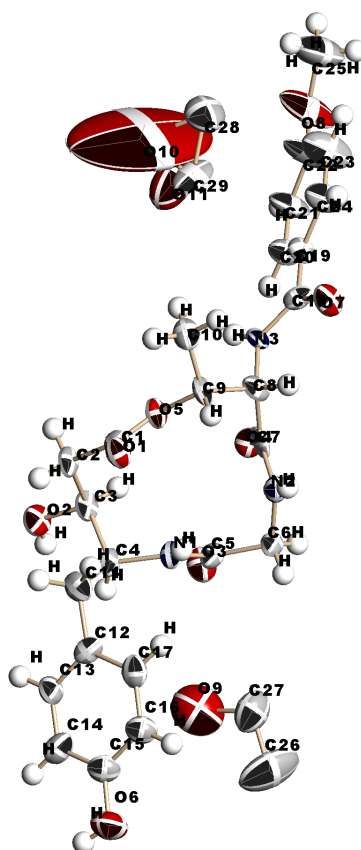


Table 1. Crystal data and structure refinement.

Empirical formula	C ₂₅ H ₂₉ N ₃ O ₈	
Formula weight	499.51	
Temperature	298 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 10.9532(17) Å	α = 90°
	b = 7.9598(13) Å	β = 96.705(2)°
	c = 17.259(3) Å	γ = 90°
Volume	1494.4(4) Å ³	
Z	2	
Density (calculated)	1.110 Mg/m ³	
Absorption coefficient	0.084 mm ⁻¹	
F(000)	528	
Crystal size	0.45 x 0.20 x 0.15 mm ³	
Theta range for data collection	1.19 to 19.09°.	
Index ranges	-7 ≤ h ≤ 10, -7 ≤ k ≤ 7, -15 ≤ l ≤ 15	
Reflections collected	3934	
Independent reflections	2341 [R(int) = 0.0250]	
Completeness to theta = 19.09–	99.5 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9039 and 0.8988	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2341 / 1 / 396	
Goodness-of-fit on F ²	0.929	
Final R indices [I > 2σ(I)]	R1 = 0.0693, wR2 = 0.1875	
R indices (all data)	R1 = 0.0761, wR2 = 0.1984	
Absolute structure parameter	0(3)	
Extinction coefficient	0.064(9)	
Largest diff. peak and hole	1.165 and -0.313 e.Å ⁻³	
Detector	Rigaku Saturn	
Goniometer	Rigaku AFC10	
Radiation	MoKα	