Supporting Information

Formal Synthesis of (-)-Podophyllotoxin through the Photocyclization of an Axially Chiral 3,4-Bisbenzylidene Succinate Amide Ester - a Flow Photochemistry Approach

Kamil Lisiecki[†], Krzysztof K. Krawczyk[†], Piotr Roszkowski[†], Jan K. Maurin[‡§], Zbigniew Czarnocki[†]*

[†]Faculty of Chemistry, University of Warsaw, Pasteura 1, Warsaw 02-093, Poland

[‡]National Medicines Institute, Chełmska 30/34, Warsaw 00-725, Poland

[§]Institute of Atomic Energy, Otwock-Świerk 05-400, Poland

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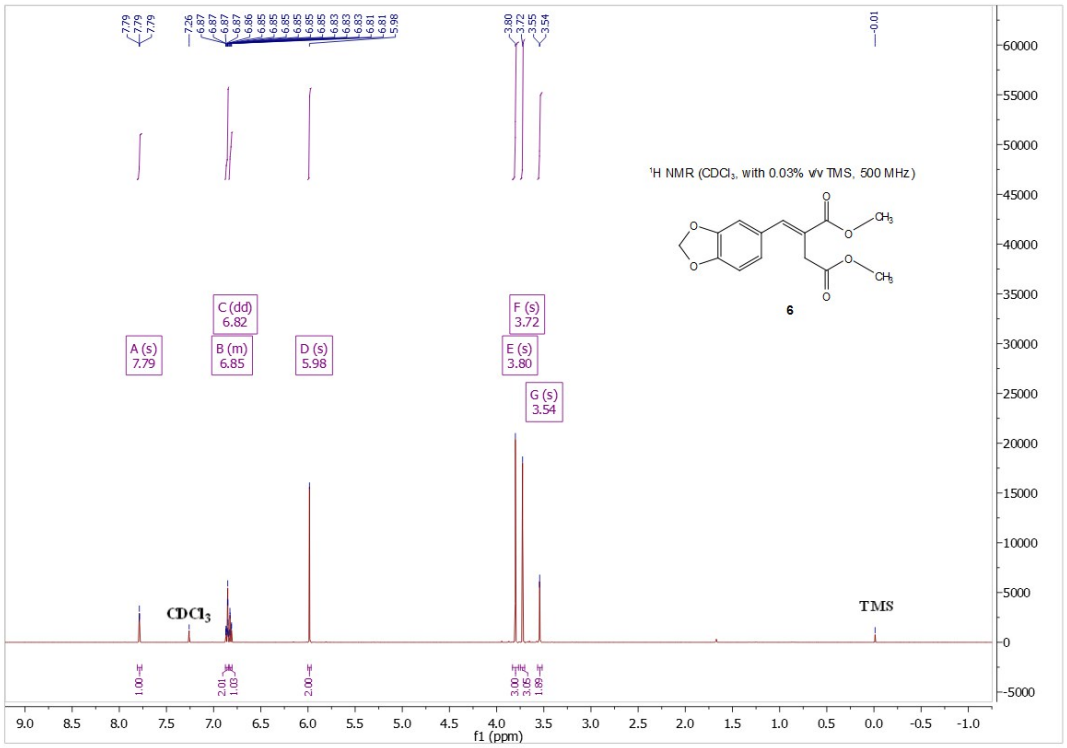

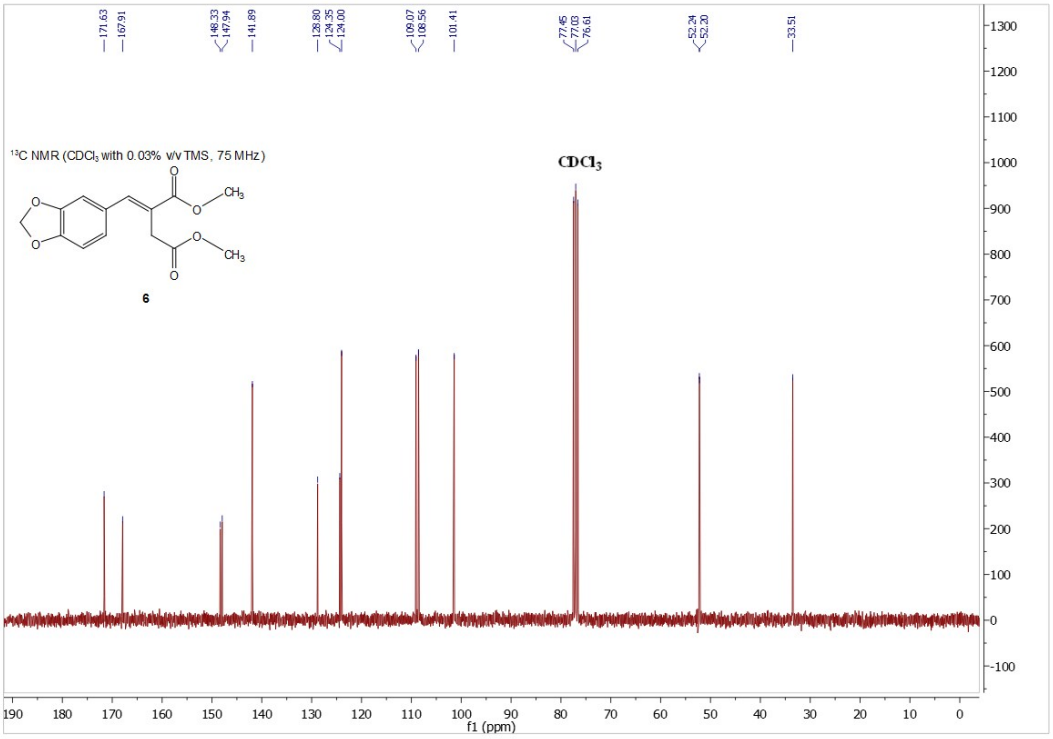

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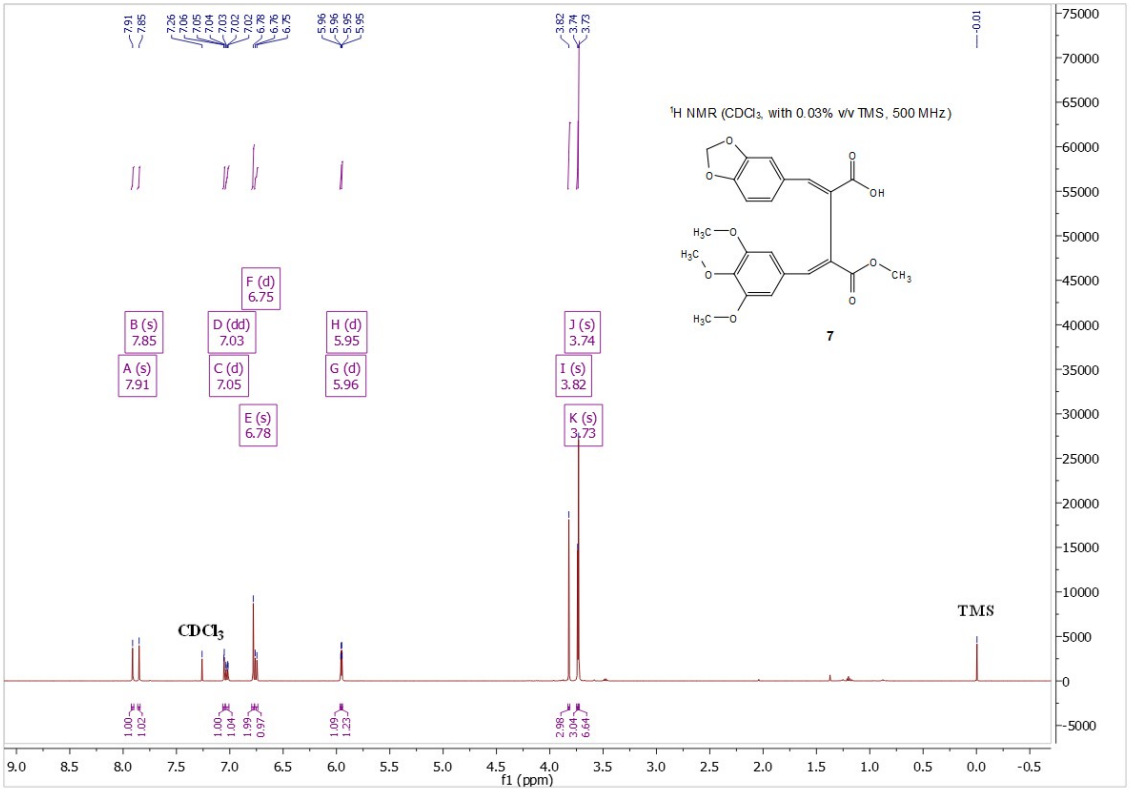

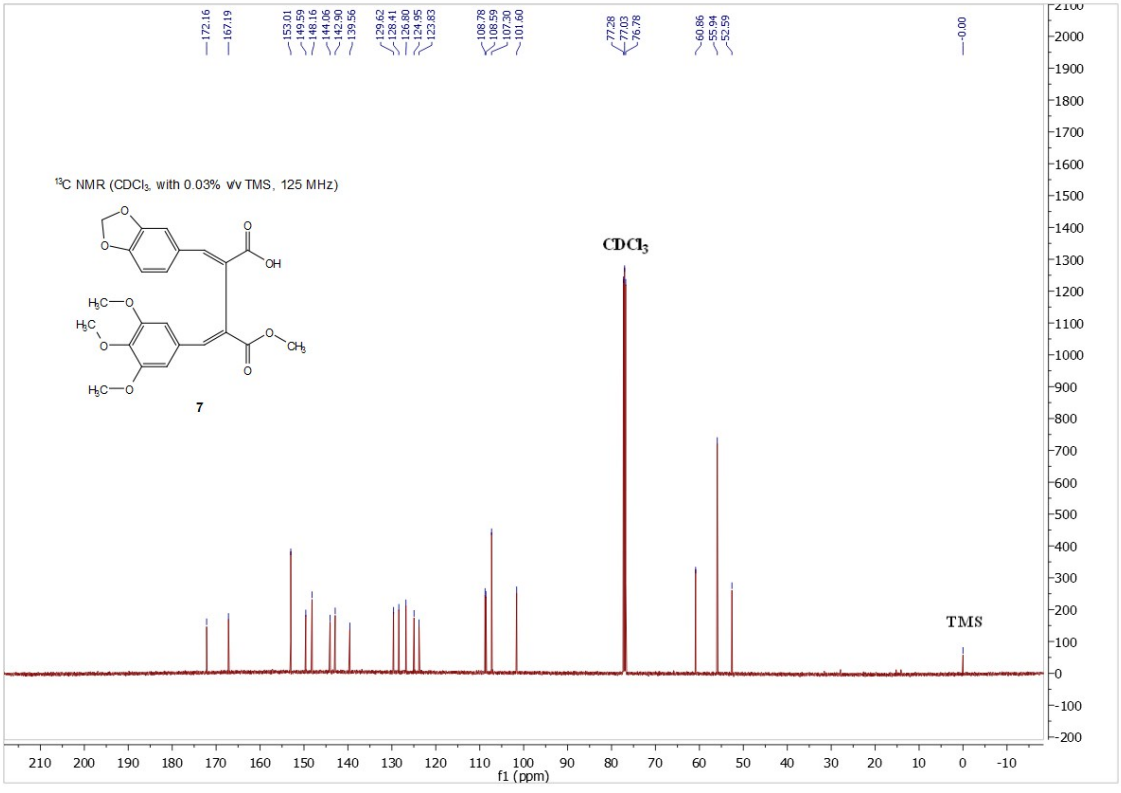

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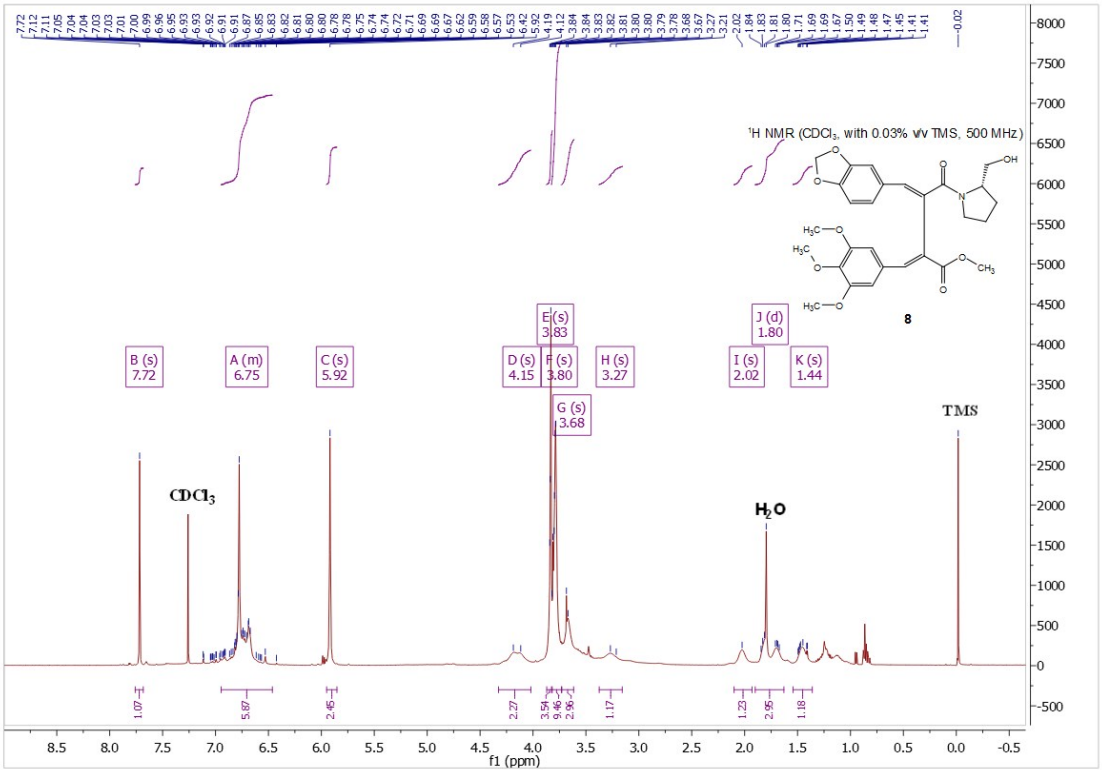

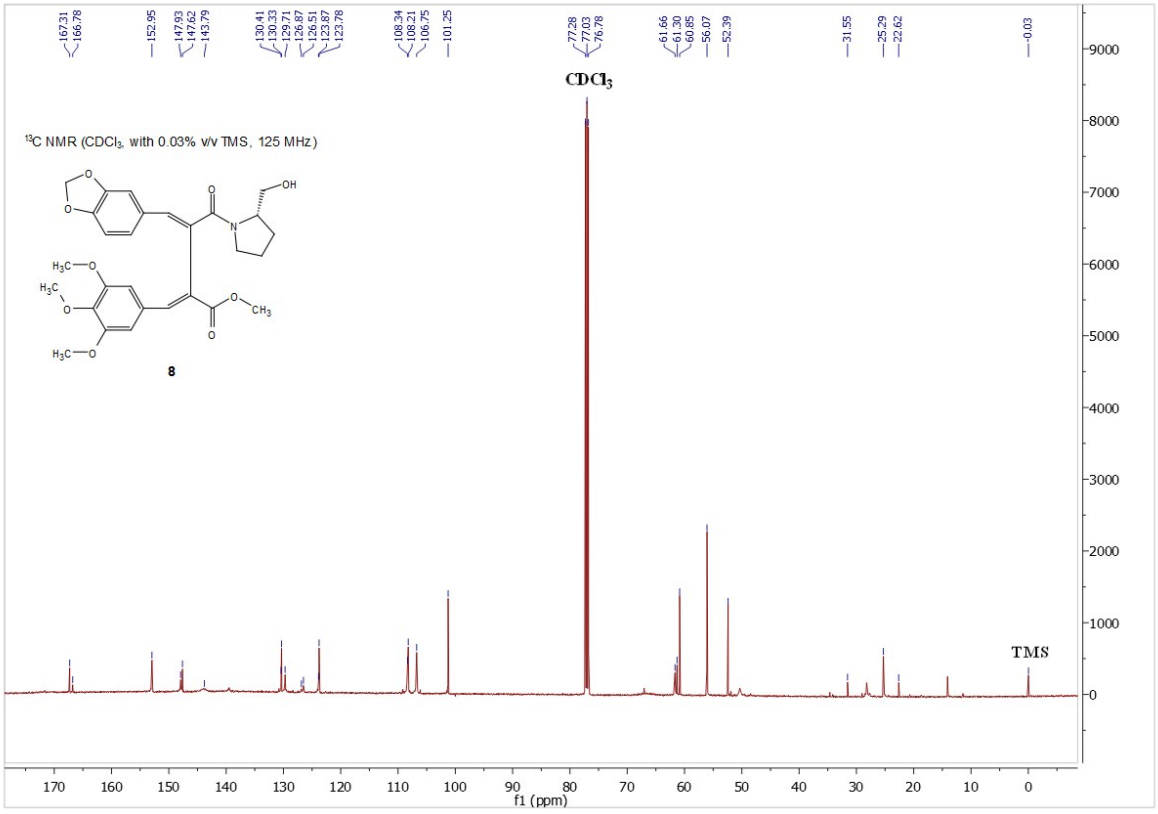

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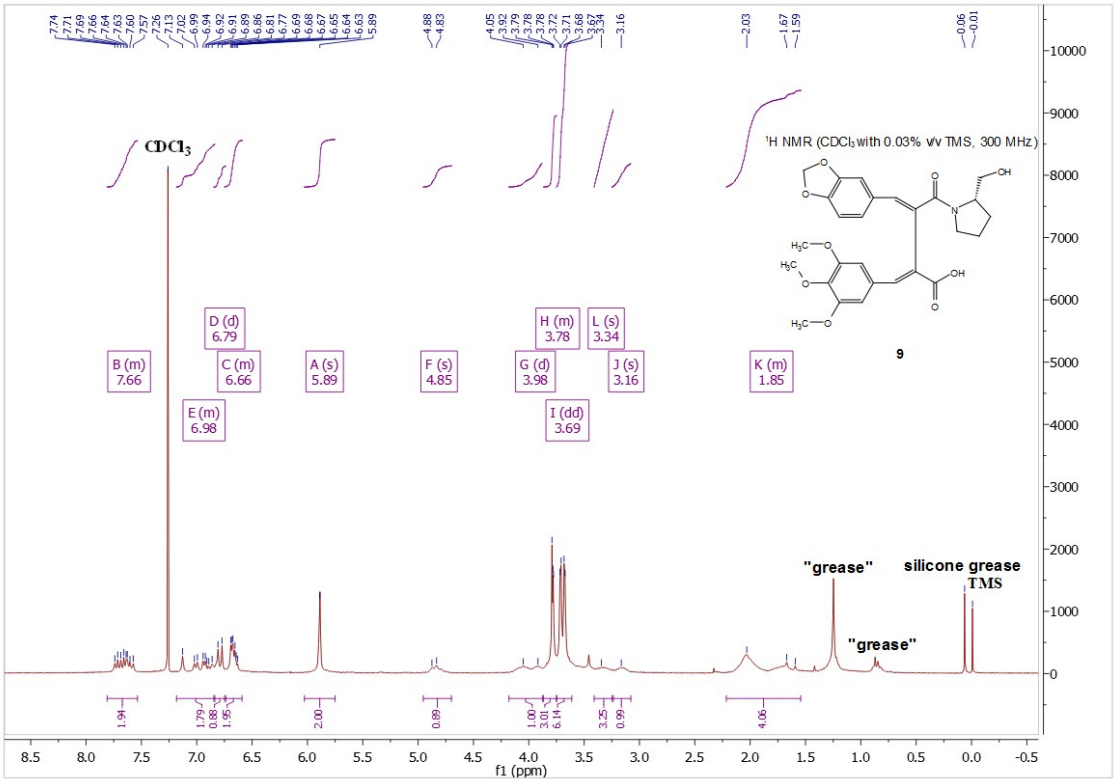

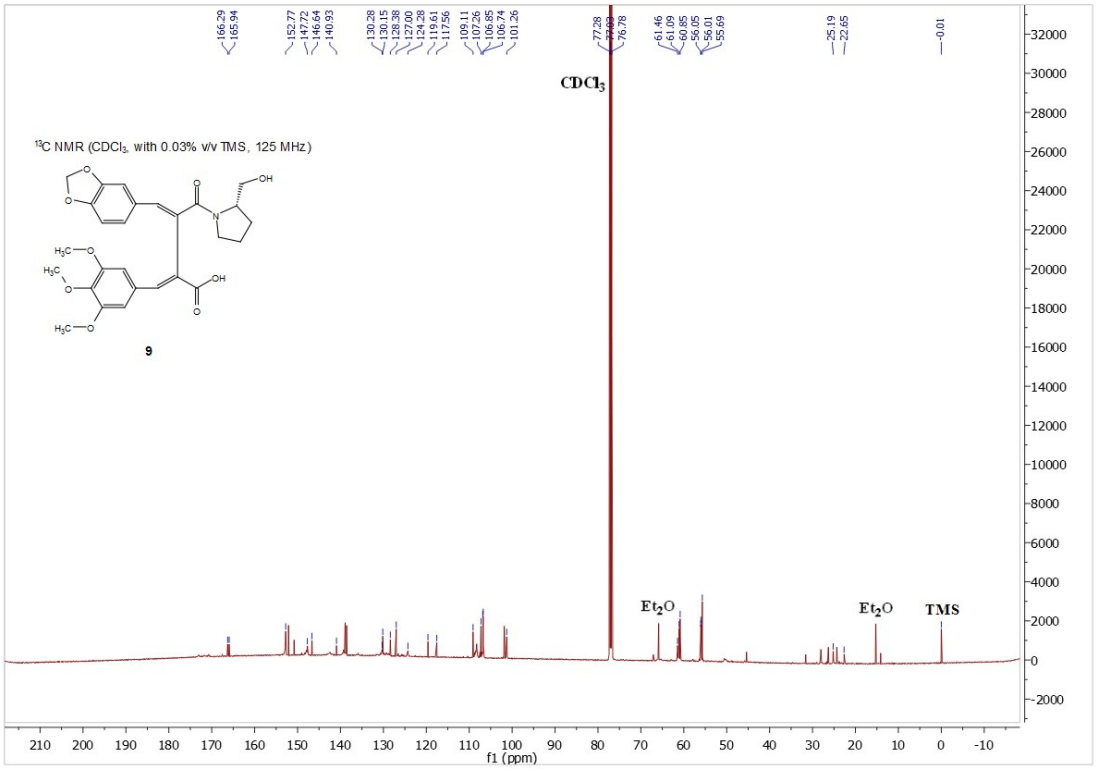

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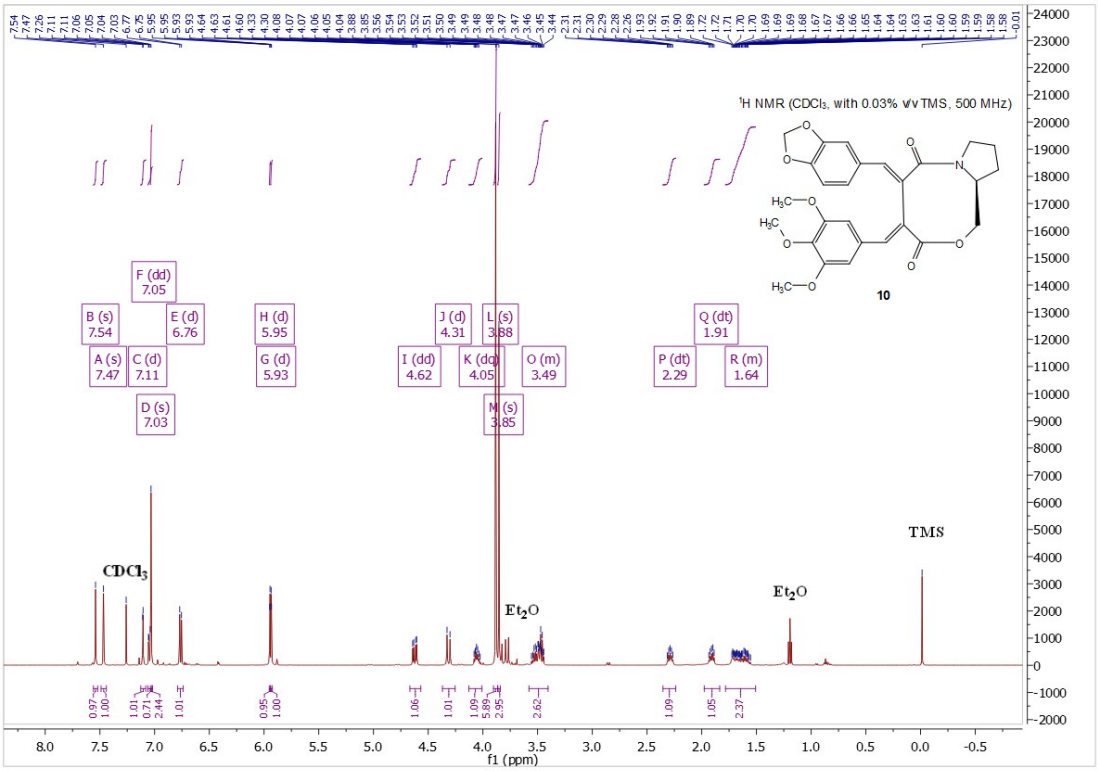
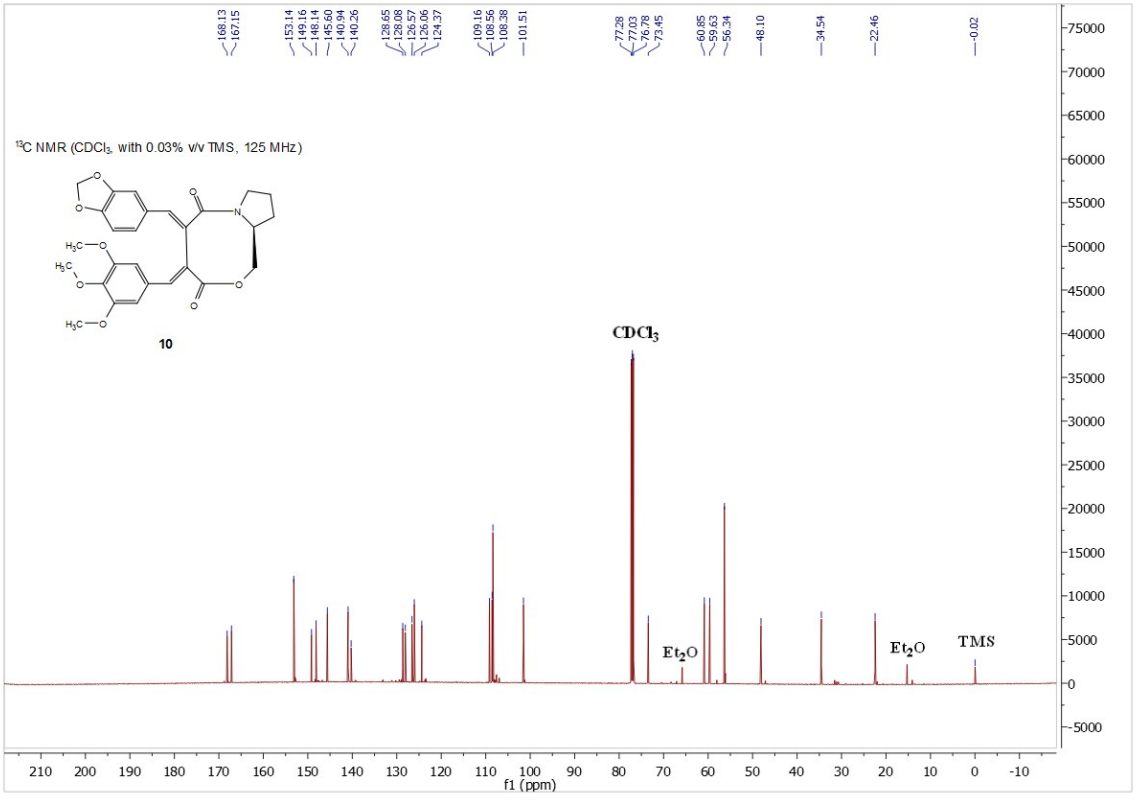
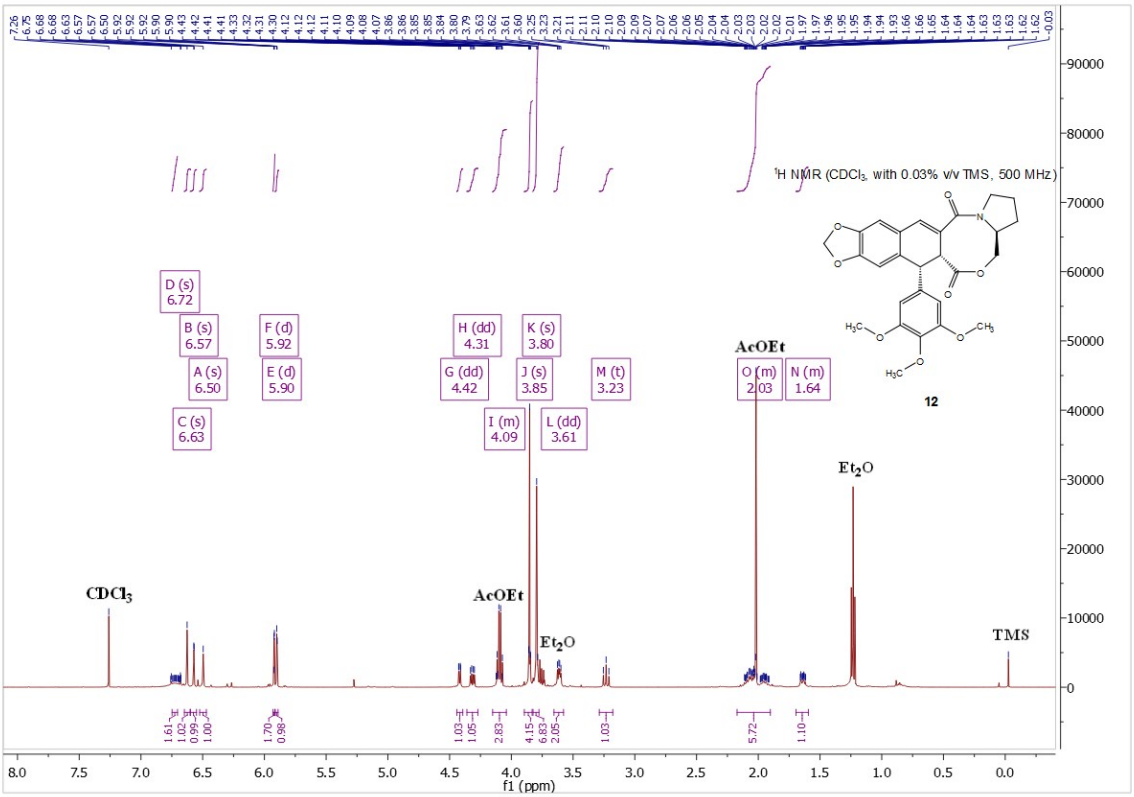
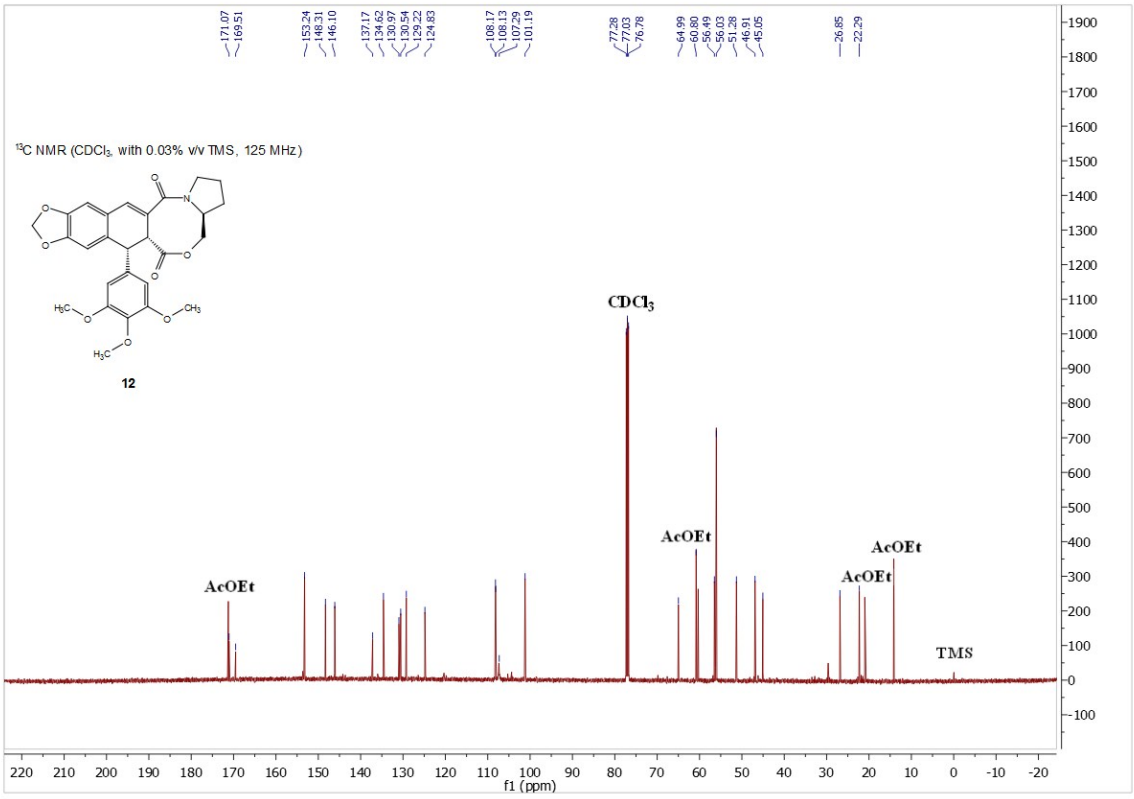
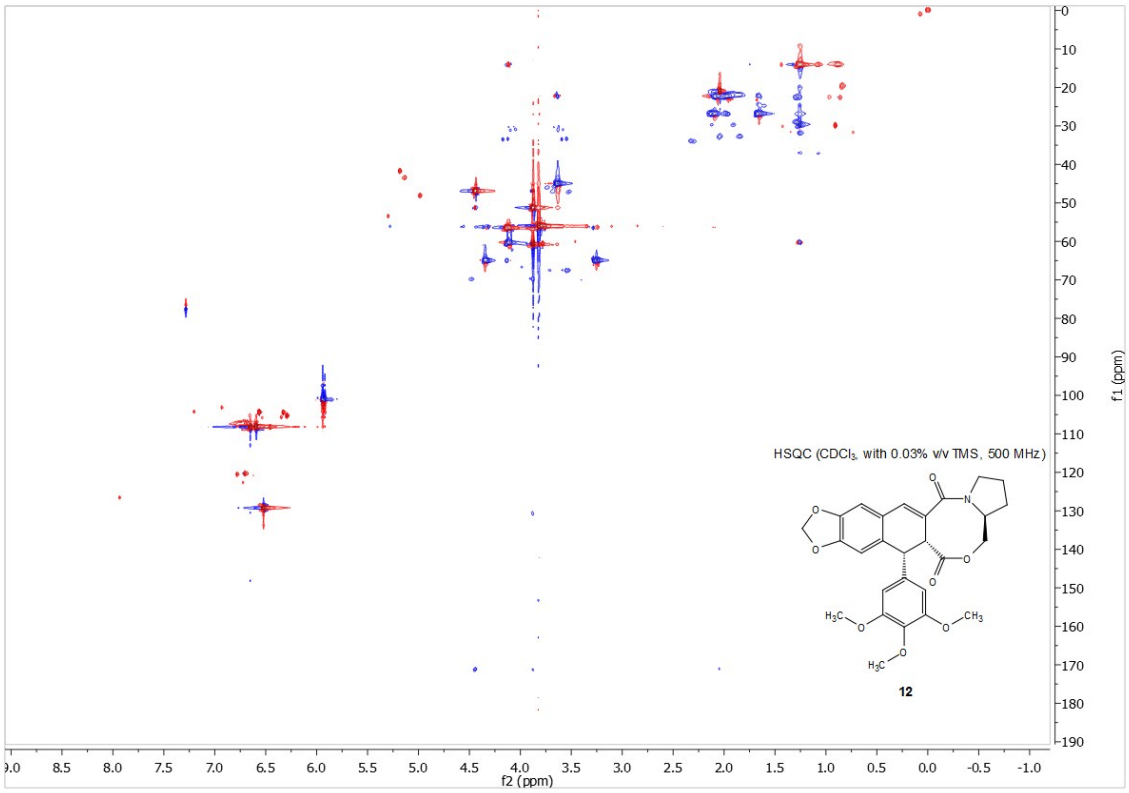


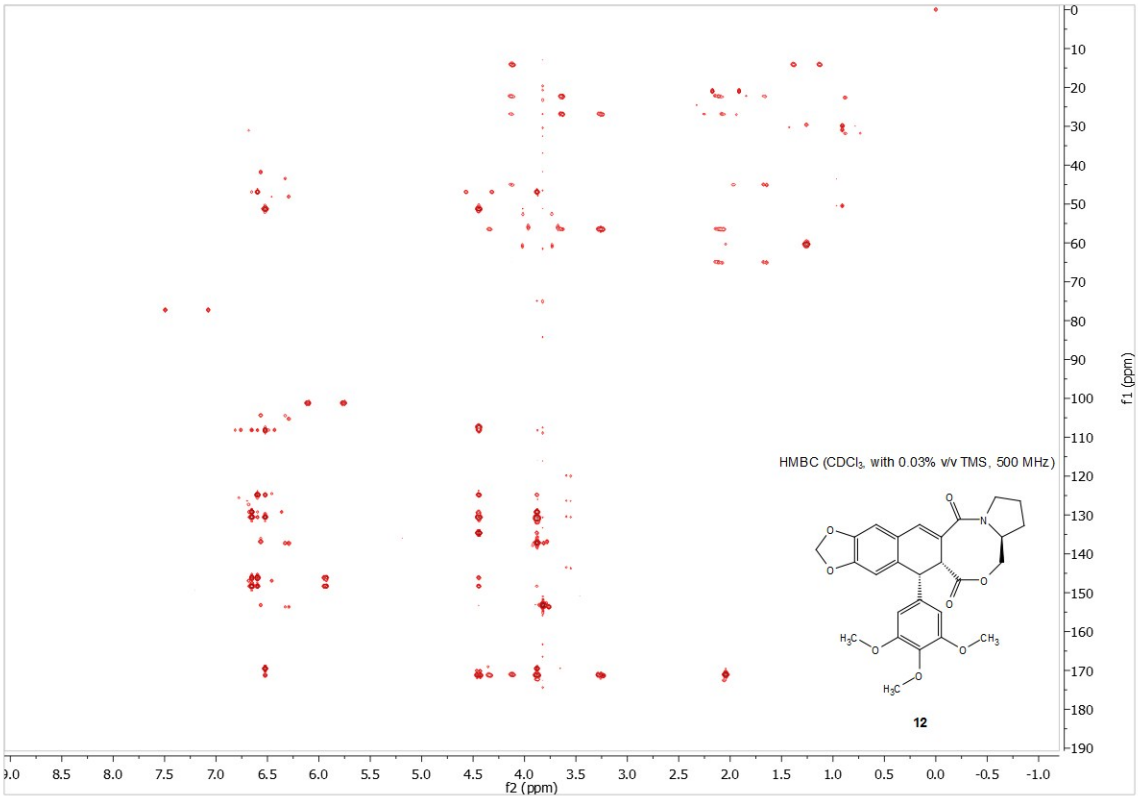


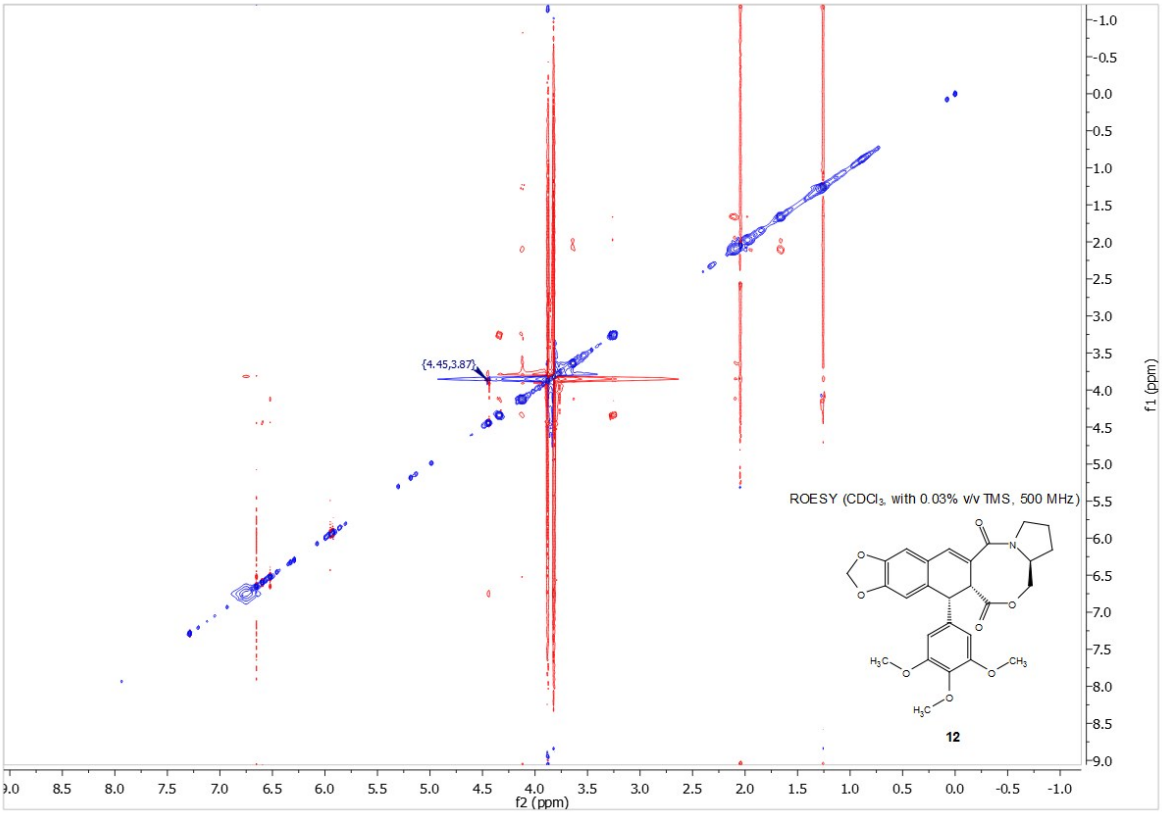
Copies of ^{1}H NMR, ^{13}C NMR, HSQC, HMBC and ROESY spectra of **12**



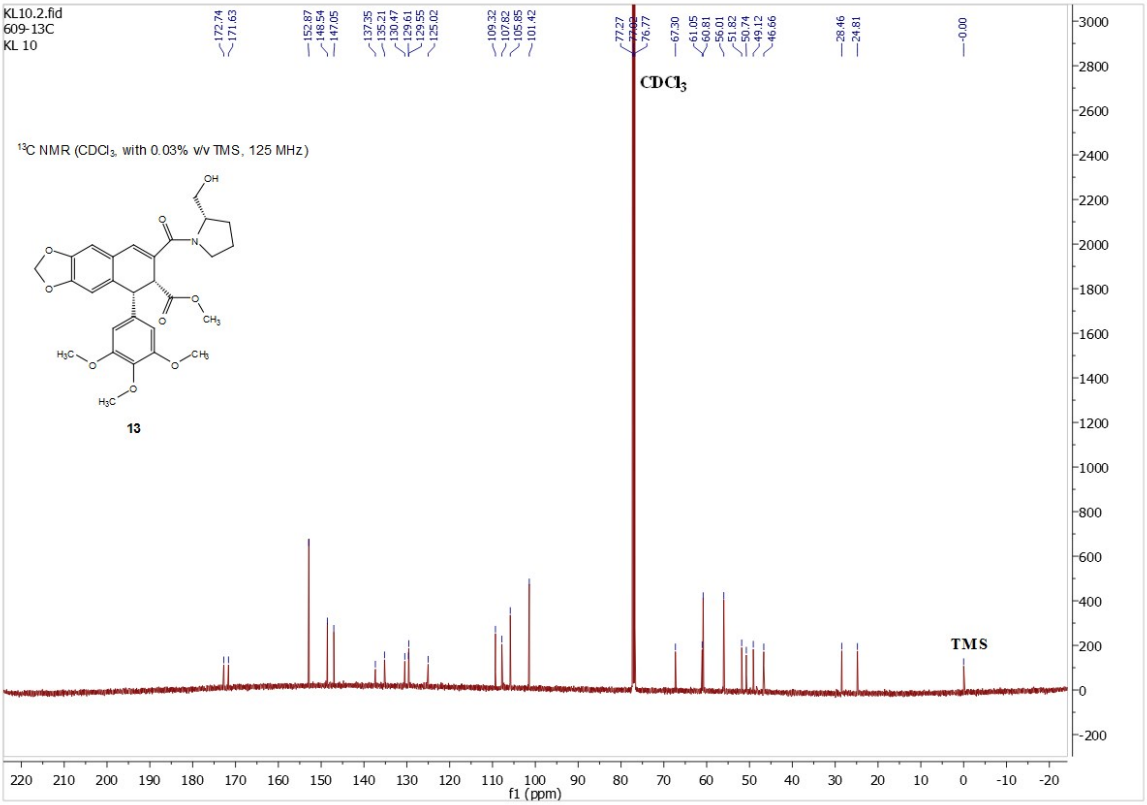


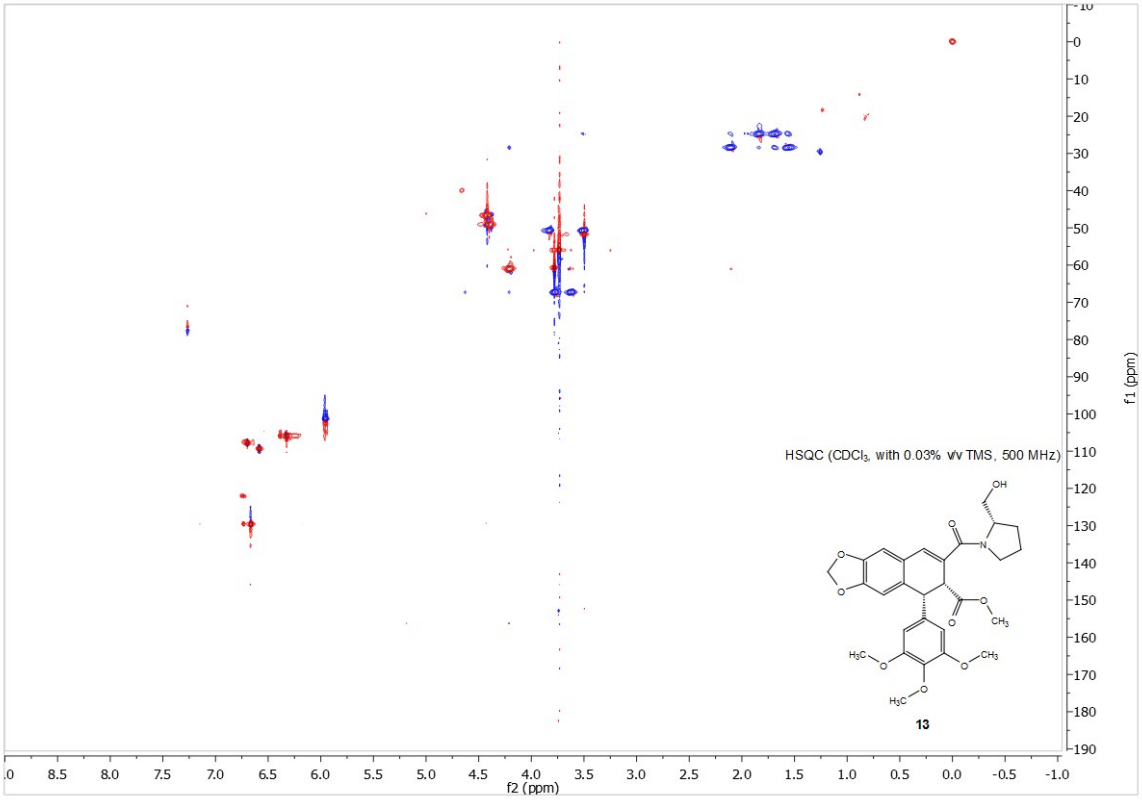

HSQC (CDCl3, with 0.03% v/v TMS, 500 MHz)
12
f1 (ppm)
f2 (ppm)

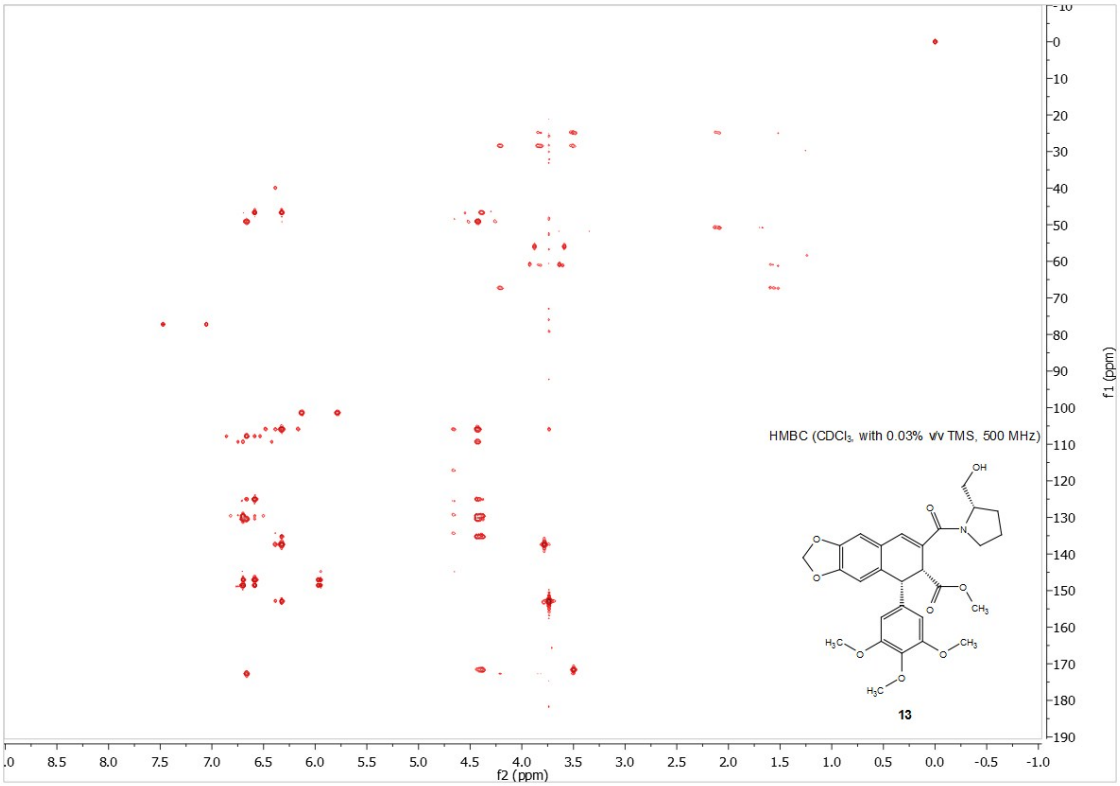

HMBC (CDCl3, with 0.03% v/v TMS, 500 MHz)
12
f1 (ppm)
f2 (ppm)

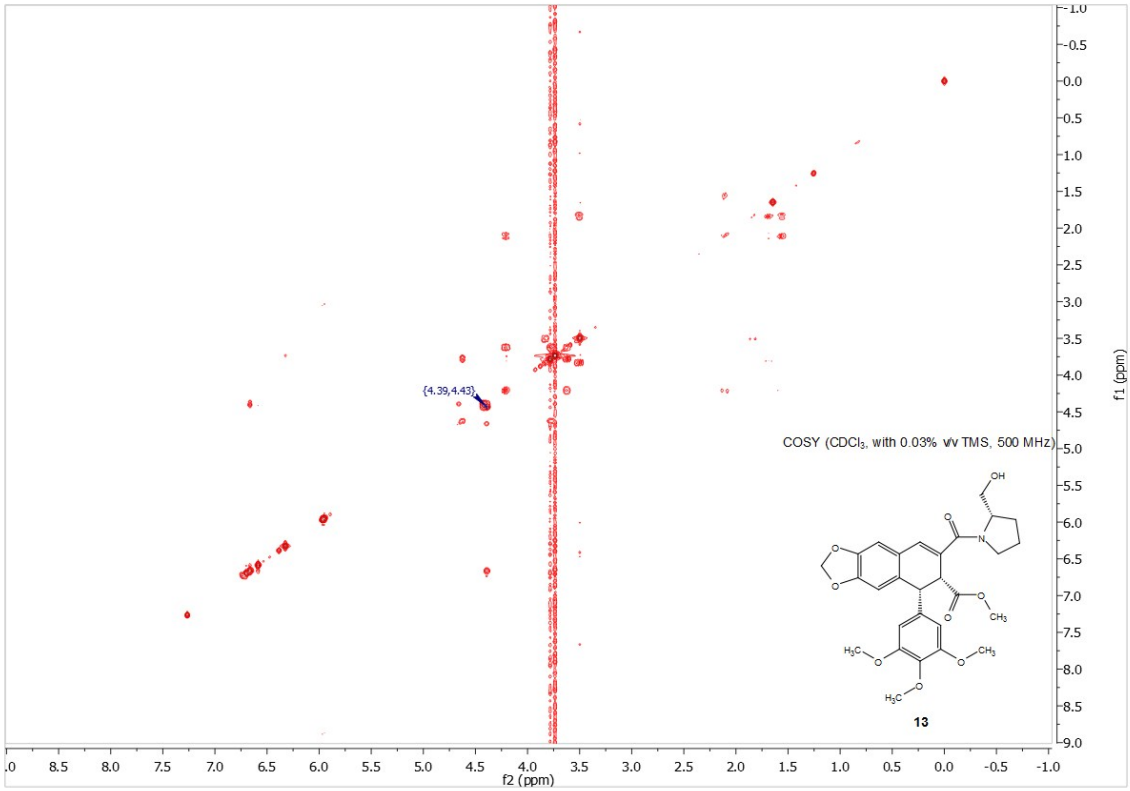


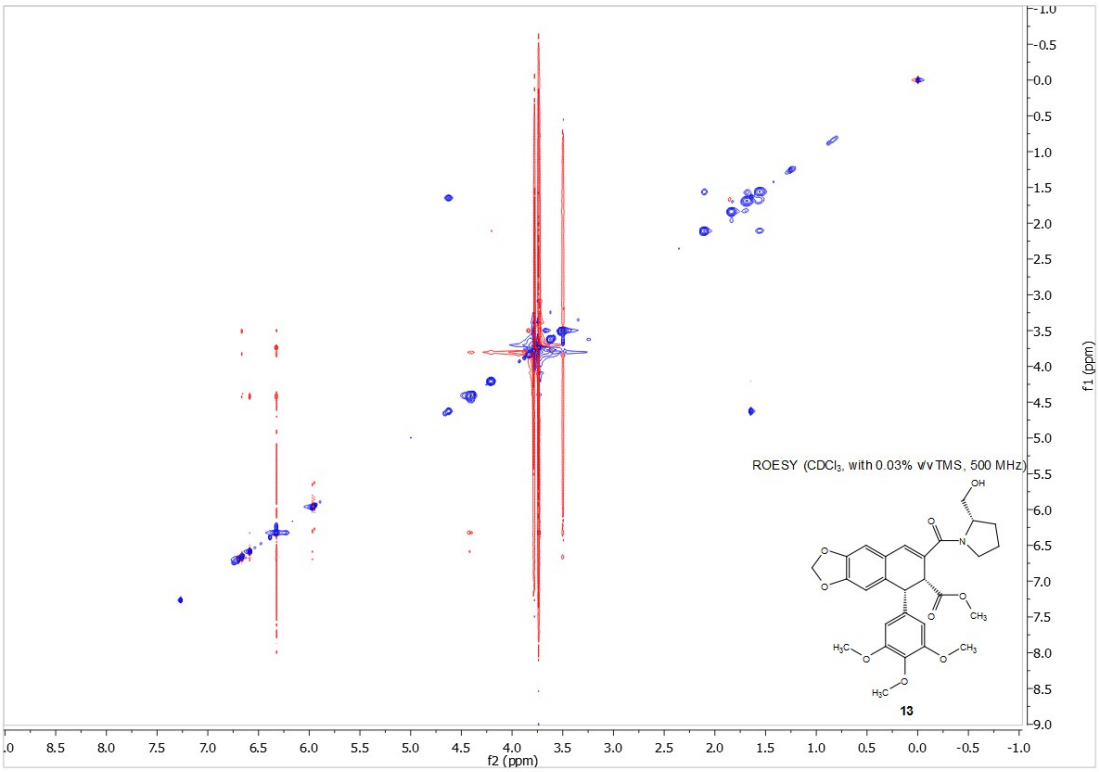
Copies of ^{1}H NMR, ^{13}C NMR, HSQC, HMBC, COSY and ROESY spectra of **13**


KL10.2.fid
609-13C
KL 10
172.74
171.63
152.87
148.54
147.05
137.35
135.21
130.47
129.61
129.55
125.02
109.32
107.82
105.85
101.42
77.27
77.06
76.77
67.30
61.05
60.81
56.01
51.82
50.74
49.12
46.66
28.46
24.81
-0.00
CDCl3
TMS
13C NMR (CDCl3, with 0.03% v/v TMS, 125 MHz)
13
f1 (ppm)

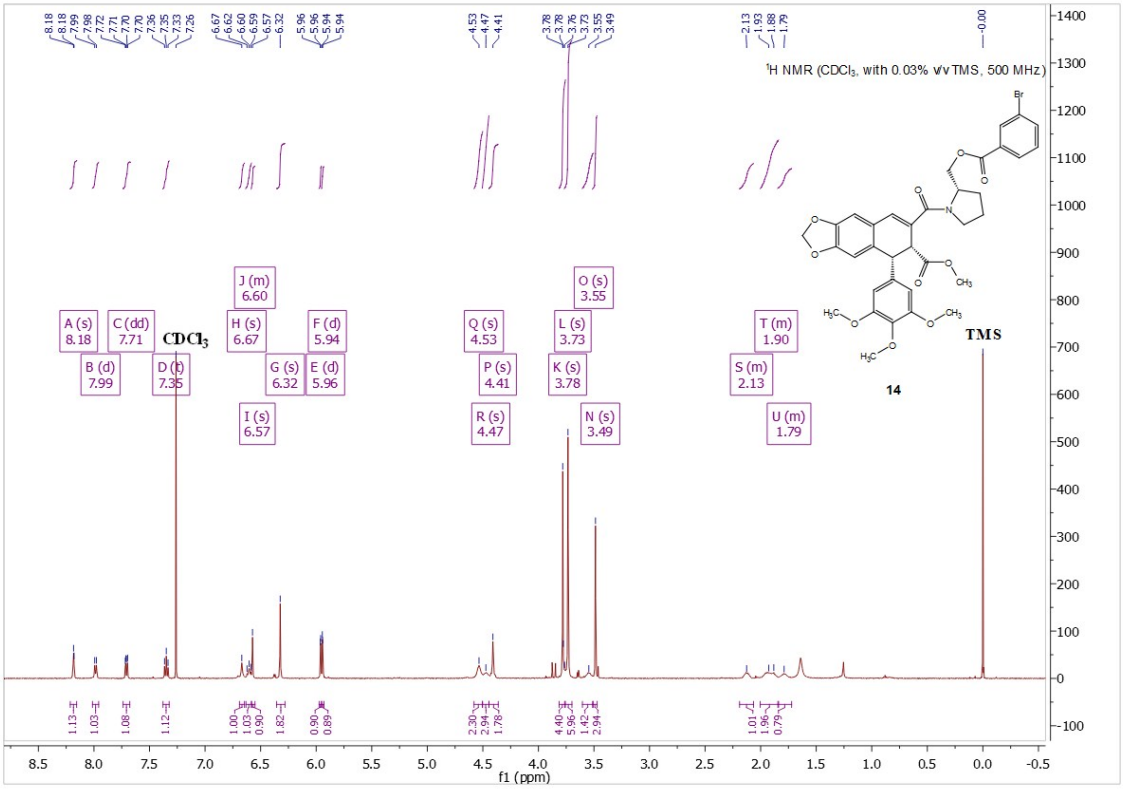

HSQC (CDCl3, with 0.03% v/v TMS, 500 MHz)
13
f2 (ppm)
f1 (ppm)

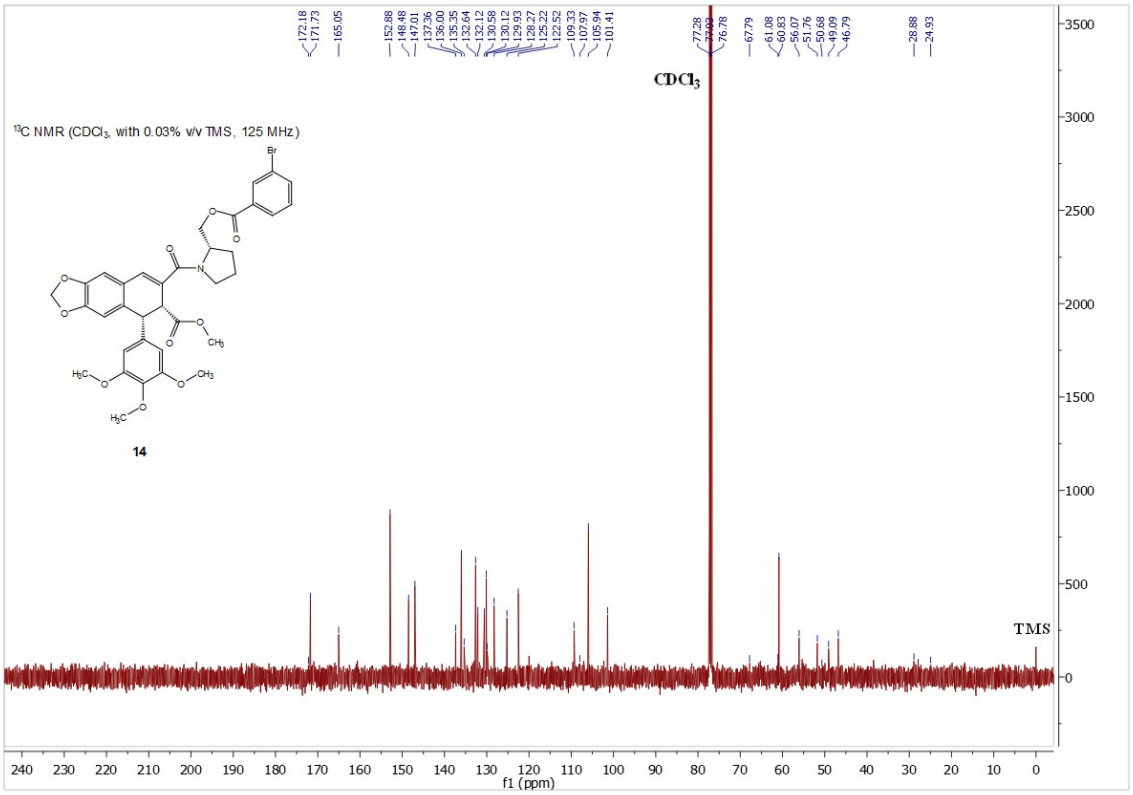

HMBC (CDCl3, with 0.03% v/v TMS, 500 MHz)
13
f2 (ppm)
f1 (ppm)


(4.39,4.43)
COSY (CDCl3, with 0.03% v/v TMS, 500 MHz)
13
f2 (ppm)
f1 (ppm)

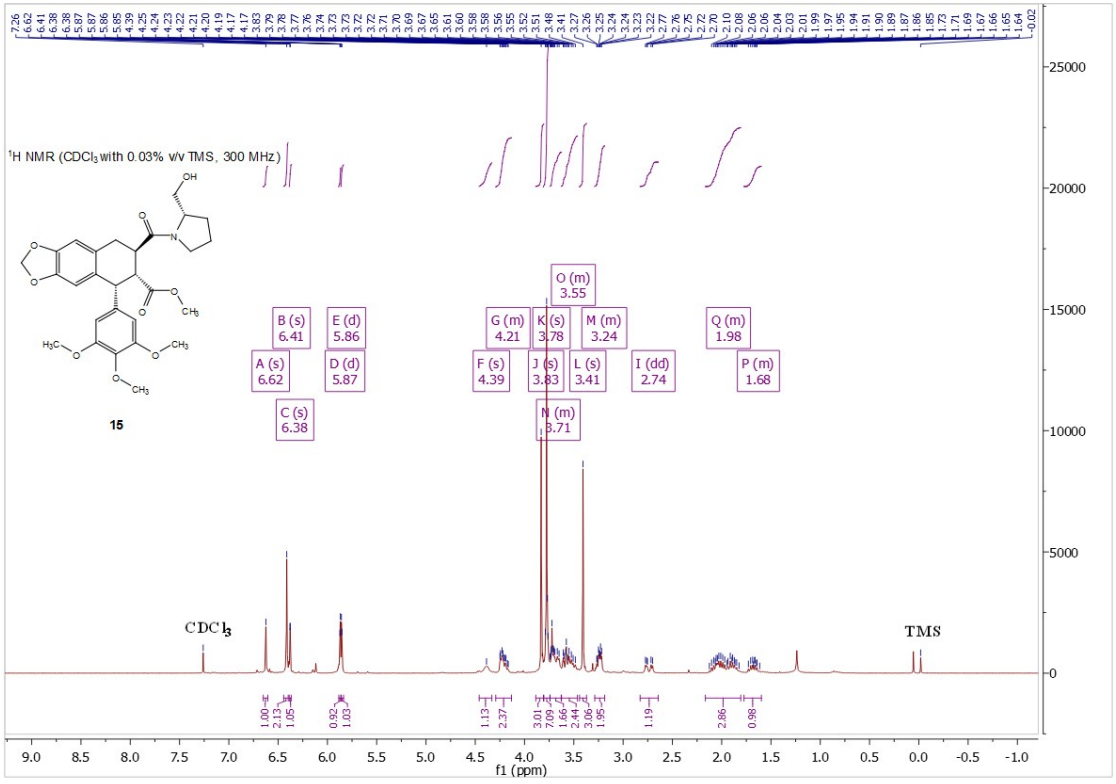


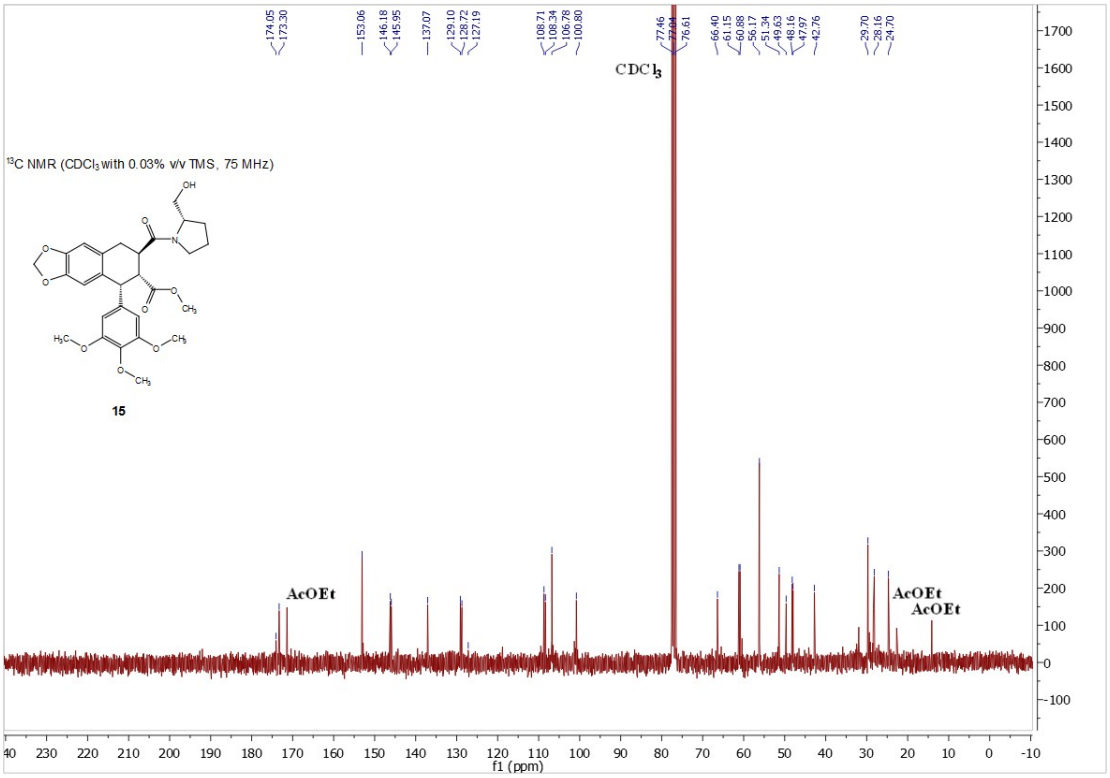
Copies of ^{1}H NMR and ^{13}C NMR spectra of **14**



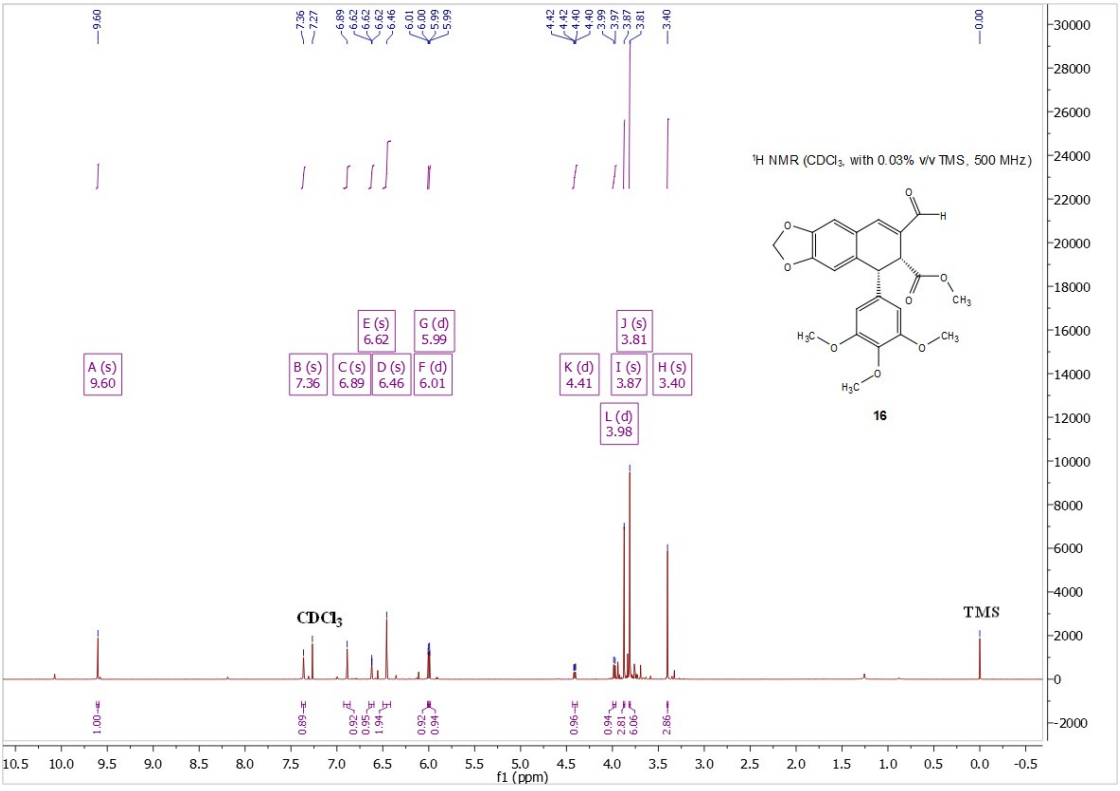


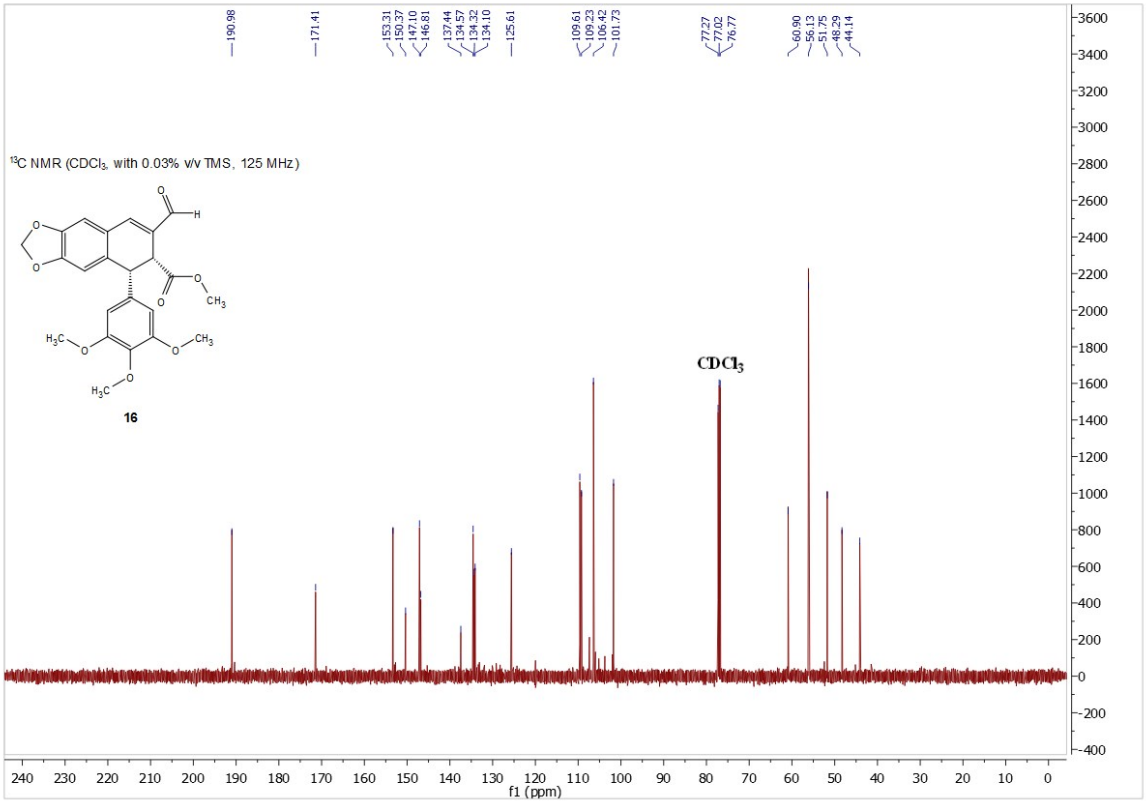
Copies of ^{1}H NMR and ^{13}C NMR spectra of **15**



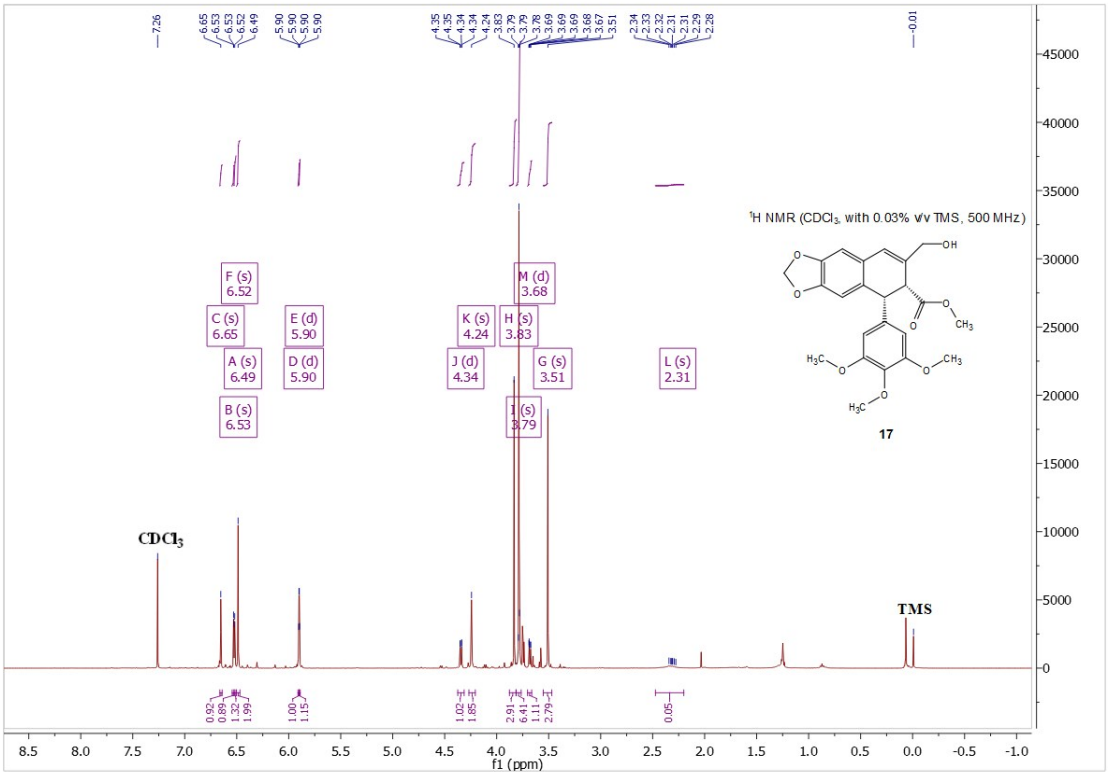


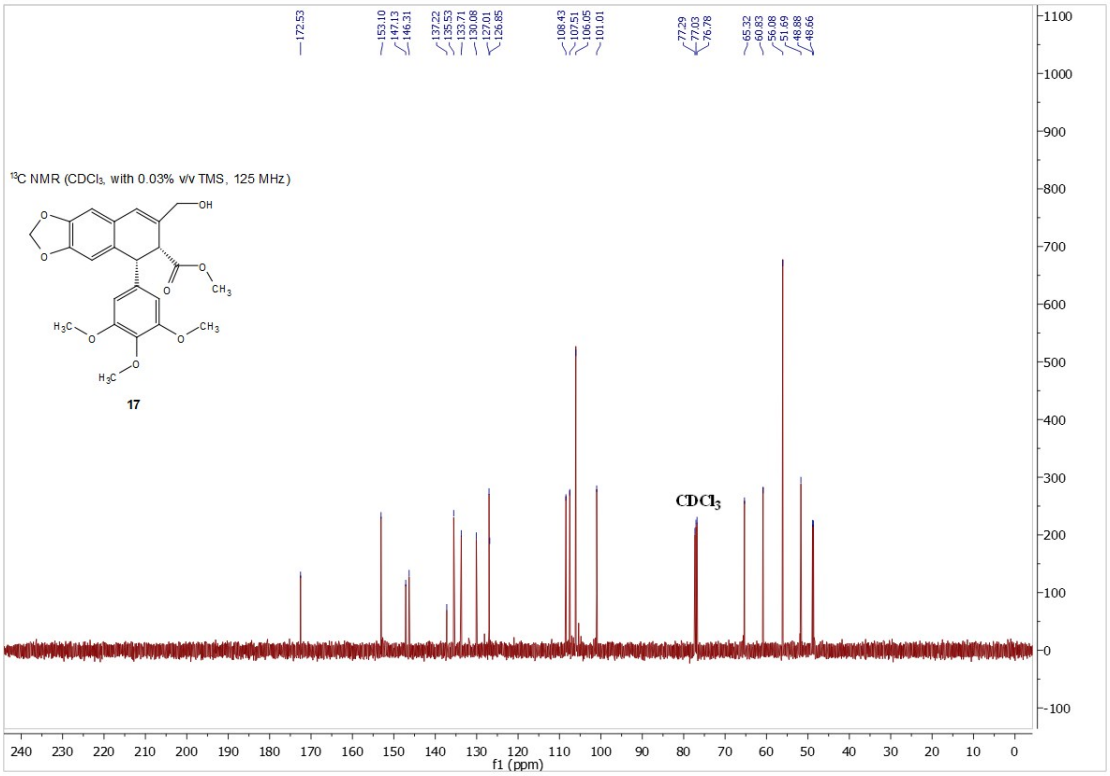
Copies of ^{1}H NMR and ^{13}C NMR spectra of **16**





Copies of ^{1}H NMR and ^{13}C NMR spectra of **17**





UV spectrum of 10, 12 and reaction mixture

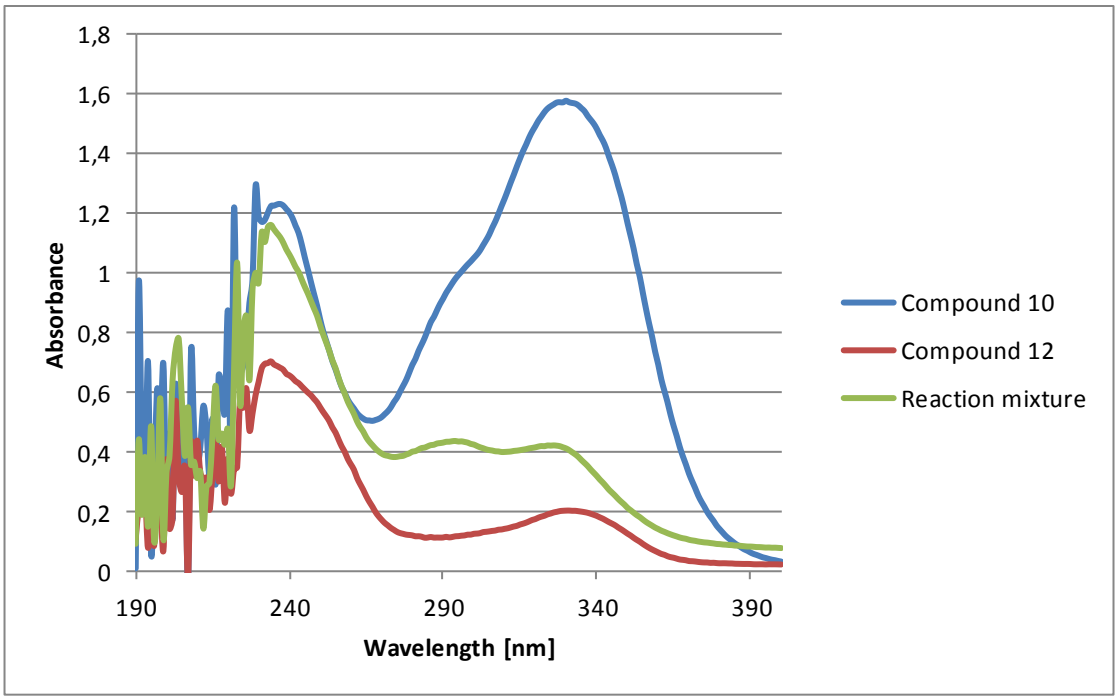


Figure S1. UV spectrum of **10**, **12** and reaction mixture (all samples at concentration 0.25 mM)

Photo of the system for “in-flow” photoreactions

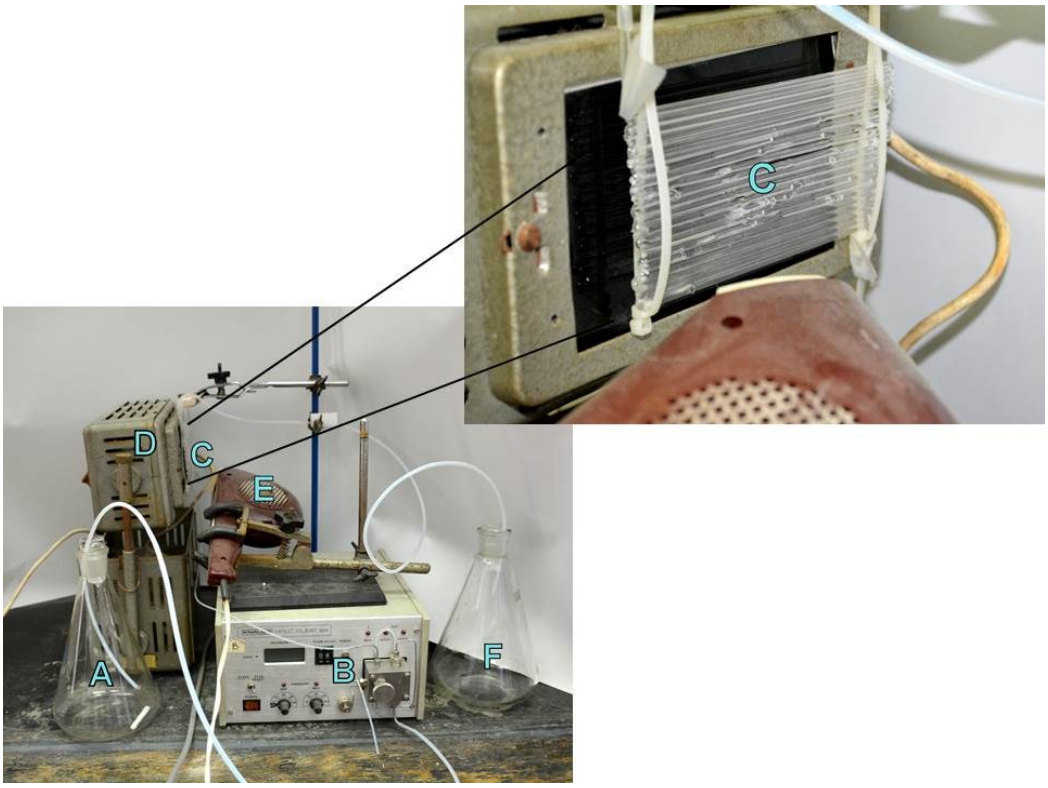


Figure S2. Photo showing the components of the system for “in-flow” photoreactions (A - substrate tank; B – HPLC pump; C - quartz reactor; D – UV source; E – cooler, F – product tank)

Emission spectrum of the employed UV-lamp

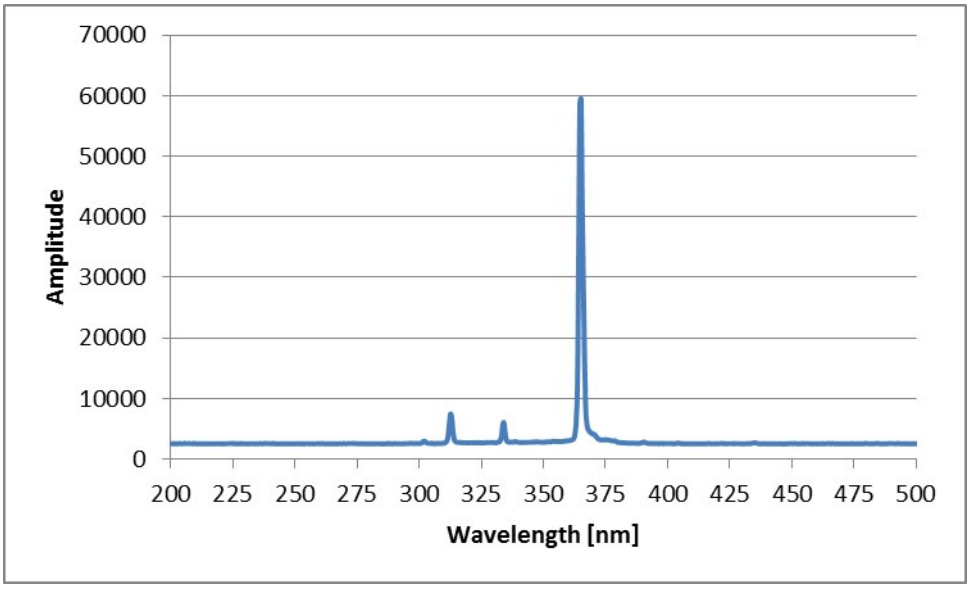


Figure S3. Emission spectrum of the employed UV-lamp (spectrum recorded by spectrometer SPM-002-ET Photon Control)

Details of X-Ray Crystal Structure analysis for 14

Table 1. Crystal data and structure refinement for ZC242abs.

Identification code	zc242abs	
Empirical formula	C35 H34 Br N O10	
Formula weight	708.54	
Temperature	293(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 9.1914(2) Å	α= 90°.
	b = 17.0779(3) Å	β= 98.692(2)°.
	c = 10.56690(20) Å	γ = 90°.
Volume	1639.64(6) $Å^3$	
Z	2	
Density (calculated)	1.435 Mg/m^3	
Absorption coefficient	2.218 mm^{-1}	
F(000)	732	
Crystal size	0.2908 x 0.1127 x 0.0200 mm^3	
Theta range for data collection	4.23 to 71.20°.	
Index ranges	-10<=h<=11, -18<=k<=20, -12<=l<=12	
Reflections collected	16482	
Independent reflections	5620 [R(int) = 0.0441]	
Completeness to theta = 71.20°	96.9 %	

Absorption correction	Analytical
Max. and min. transmission	0.957 and 0.679
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5620 / 1 / 425
Goodness-of-fit on F^2	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0590, wR2 = 0.1468
R indices (all data)	R1 = 0.0822, wR2 = 0.1643
Absolute structure parameter	-0.02(3)
Extinction coefficient	0.0011(3)
Largest diff. peak and hole	0.682 and -0.502 e.$Å^{-3}$

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

for ZC242abs. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	8320(2)	5541(1)	168(1)	181(1)
O(1)	5712(7)	-2477(3)	10167(4)	100(2)
O(2)	5382(6)	-1130(3)	10335(4)	93(1)
O(3)	2805(4)	-2229(2)	3364(3)	61(1)
O(4)	3126(4)	-3730(2)	2750(3)	57(1)
O(5)	5609(4)	-4506(2)	3489(3)	61(1)
O(6)	8247(4)	-1700(2)	3090(3)	68(1)
O(7)	9590(4)	-2634(2)	4198(4)	64(1)
O(8)	9866(4)	-182(3)	4403(4)	79(1)
O(9)	8590(5)	2026(2)	2396(4)	70(1)
O(10)	7247(6)	3016(3)	2960(5)	97(1)
N(1)	7490(5)	168(2)	3770(4)	54(1)
C(1)	6171(7)	-2094(3)	9149(5)	63(1)
C(2)	6772(6)	-2420(3)	8171(5)	61(1)
C(3)	7177(5)	-1917(3)	7242(4)	47(1)
C(4)	7737(5)	-2257(3)	6082(4)	48(1)

C(5)	8657(5)	-1658(3)	5404(4)	48(1)
C(6)	8061(5)	-835(3)	5384(4)	48(1)
C(7)	7351(6)	-604(3)	6309(4)	55(1)
C(8)	6964(5)	-1119(3)	7332(4)	53(1)
C(9)	6352(6)	-793(3)	8356(4)	58(1)
C(10)	5985(7)	-1297(4)	9248(5)	66(2)
C(11)	6499(5)	-2633(3)	5181(4)	43(1)
C(12)	5213(5)	-2230(3)	4733(4)	45(1)
C(13)	4100(5)	-2585(3)	3889(4)	47(1)
C(14)	4256(5)	-3355(3)	3495(4)	47(1)
C(15)	5538(5)	-3752(3)	3930(4)	47(1)
C(16)	6671(5)	-3401(3)	4769(4)	45(1)
C(17)	2523(6)	-1468(4)	3779(6)	66(1)
C(18)	2986(7)	-3587(4)	1427(5)	75(2)
C(19)	6894(7)	-4942(3)	3906(7)	75(2)
C(20)	8796(5)	-1976(3)	4110(5)	54(1)
C(21)	9637(7)	-3078(4)	3054(6)	80(2)
C(22)	8547(6)	-268(3)	4469(5)	53(1)
C(23)	7830(6)	715(3)	2778(5)	58(1)
C(24)	8085(8)	1523(4)	3364(5)	77(2)
C(25)	8083(6)	2755(4)	2295(5)	61(1)
C(26)	8678(6)	3213(3)	1298(5)	60(1)
C(27)	8303(8)	3994(4)	1149(6)	84(2)

C(28)	8876(10)	4459(4)	303(7)	95(2)
C(29)	9770(12)	4145(7)	-481(7)	117(4)
C(30)	10182(8)	3358(6)	-349(6)	96(2)
C(31)	9645(6)	2899(4)	535(5)	74(2)
C(33)	5211(8)	-1866(4)	10926(6)	87(2)
C(34)	6474(9)	682(5)	1778(5)	91(2)
C(35)	5253(8)	504(5)	2518(6)	94(2)
C(36)	5922(6)	-44(4)	3557(5)	64(1)

Table 3. Bond lengths [Å] and angles [°] for ZC242abs.

Br(1)-C(28)	1.918(8)
O(1)-C(1)	1.378(6)
O(1)-C(33)	1.434(8)
O(2)-C(10)	1.379(7)
O(2)-C(33)	1.423(8)
O(3)-C(13)	1.376(6)
O(3)-C(17)	1.409(7)
O(4)-C(14)	1.364(5)
O(4)-C(18)	1.406(6)
O(5)-C(15)	1.374(6)
O(5)-C(19)	1.409(7)
O(6)-C(20)	1.214(6)
O(7)-C(20)	1.335(6)
O(7)-C(21)	1.433(7)
O(8)-C(22)	1.234(6)
O(9)-C(25)	1.328(7)
O(9)-C(24)	1.463(6)
O(10)-C(25)	1.202(7)
N(1)-C(22)	1.352(6)
N(1)-C(36)	1.470(7)
N(1)-C(23)	1.472(6)

C(1)-C(2)	1.362(8)
C(1)-C(10)	1.378(8)
C(2)-C(3)	1.396(7)
C(2)-H(2)	0.9300
C(3)-C(8)	1.383(7)
C(3)-C(4)	1.514(7)
C(4)-C(11)	1.512(6)
C(4)-C(5)	1.568(7)
C(4)-H(4)	0.9800
C(5)-C(20)	1.495(7)
C(5)-C(6)	1.507(7)
C(5)-H(5)	0.9800
C(6)-C(7)	1.315(7)
C(6)-C(22)	1.484(7)
C(7)-C(8)	1.479(7)
C(7)-H(7)	0.9300
C(8)-C(9)	1.408(7)
C(9)-C(10)	1.356(7)
C(9)-H(9)	0.9300
C(11)-C(12)	1.387(6)
C(11)-C(16)	1.400(7)
C(12)-C(13)	1.390(6)
C(12)-H(12)	0.9300

C(13)-C(14)	1.393(7)
C(14)-C(15)	1.377(7)
C(15)-C(16)	1.396(7)
C(16)-H(16)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(23)-C(34)	1.508(8)
C(23)-C(24)	1.517(8)
C(23)-H(23)	0.9800
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-C(26)	1.482(8)
C(26)-C(27)	1.380(9)

C(26)-C(31)	1.394(8)
C(27)-C(28)	1.359(10)
C(27)-H(27)	0.9300
C(28)-C(29)	1.362(13)
C(29)-C(30)	1.398(14)
C(29)-H(29)	0.9300
C(30)-C(31)	1.366(9)
C(30)-H(30)	0.9300
C(31)-H(31)	0.9300
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(34)-C(35)	1.492(10)
C(34)-H(34A)	0.9700
C(34)-H(34B)	0.9700
C(35)-C(36)	1.502(8)
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700

C(1)-O(1)-C(33)	104.6(5)
C(10)-O(2)-C(33)	105.6(5)
C(13)-O(3)-C(17)	118.0(4)

C(14)-O(4)-C(18)	116.1(4)
C(15)-O(5)-C(19)	118.0(4)
C(20)-O(7)-C(21)	118.2(4)
C(25)-O(9)-C(24)	117.5(5)
C(22)-N(1)-C(36)	123.7(4)
C(22)-N(1)-C(23)	121.8(4)
C(36)-N(1)-C(23)	110.9(4)
C(2)-C(1)-C(10)	122.0(5)
C(2)-C(1)-O(1)	127.2(5)
C(10)-C(1)-O(1)	110.7(5)
C(1)-C(2)-C(3)	117.7(5)
C(1)-C(2)-H(2)	121.2
C(3)-C(2)-H(2)	121.2
C(8)-C(3)-C(2)	120.1(5)
C(8)-C(3)-C(4)	120.1(4)
C(2)-C(3)-C(4)	119.6(4)
C(11)-C(4)-C(3)	110.9(4)
C(11)-C(4)-C(5)	113.3(3)
C(3)-C(4)-C(5)	113.1(4)
C(11)-C(4)-H(4)	106.3
C(3)-C(4)-H(4)	106.3
C(5)-C(4)-H(4)	106.3
C(20)-C(5)-C(6)	114.1(4)

C(20)-C(5)-C(4)	107.9(4)
C(6)-C(5)-C(4)	113.3(4)
C(20)-C(5)-H(5)	107.1
C(6)-C(5)-H(5)	107.1
C(4)-C(5)-H(5)	107.1
C(7)-C(6)-C(22)	121.3(5)
C(7)-C(6)-C(5)	119.3(4)
C(22)-C(6)-C(5)	118.2(4)
C(6)-C(7)-C(8)	124.5(5)
C(6)-C(7)-H(7)	117.8
C(8)-C(7)-H(7)	117.8
C(3)-C(8)-C(9)	121.3(4)
C(3)-C(8)-C(7)	119.0(5)
C(9)-C(8)-C(7)	119.7(5)
C(10)-C(9)-C(8)	117.0(5)
C(10)-C(9)-H(9)	121.5
C(8)-C(9)-H(9)	121.5
C(9)-C(10)-C(1)	121.9(5)
C(9)-C(10)-O(2)	128.4(6)
C(1)-C(10)-O(2)	109.7(5)
C(12)-C(11)-C(16)	119.3(4)
C(12)-C(11)-C(4)	121.7(4)
C(16)-C(11)-C(4)	119.0(4)

C(13)-C(12)-C(11)	120.6(4)
C(13)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7
O(3)-C(13)-C(12)	125.1(4)
O(3)-C(13)-C(14)	114.7(4)
C(12)-C(13)-C(14)	120.3(4)
O(4)-C(14)-C(15)	120.0(4)
O(4)-C(14)-C(13)	120.8(4)
C(15)-C(14)-C(13)	119.1(4)
C(14)-C(15)-O(5)	115.5(4)
C(14)-C(15)-C(16)	121.3(4)
O(5)-C(15)-C(16)	123.2(4)
C(15)-C(16)-C(11)	119.4(4)
C(15)-C(16)-H(16)	120.3
C(11)-C(16)-H(16)	120.3
O(3)-C(17)-H(17A)	109.5
O(3)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(3)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(4)-C(18)-H(18A)	109.5
O(4)-C(18)-H(18B)	109.5

H(18A)-C(18)-H(18B)	109.5
O(4)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(5)-C(19)-H(19A)	109.5
O(5)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
O(5)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(6)-C(20)-O(7)	122.6(5)
O(6)-C(20)-C(5)	126.1(5)
O(7)-C(20)-C(5)	111.3(4)
O(7)-C(21)-H(21A)	109.5
O(7)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(7)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(8)-C(22)-N(1)	122.3(5)
O(8)-C(22)-C(6)	120.7(4)
N(1)-C(22)-C(6)	117.0(4)
N(1)-C(23)-C(34)	103.5(5)

N(1)-C(23)-C(24)	108.9(4)
C(34)-C(23)-C(24)	112.4(5)
N(1)-C(23)-H(23)	110.6
C(34)-C(23)-H(23)	110.6
C(24)-C(23)-H(23)	110.6
O(9)-C(24)-C(23)	107.1(4)
O(9)-C(24)-H(24A)	110.3
C(23)-C(24)-H(24A)	110.3
O(9)-C(24)-H(24B)	110.3
C(23)-C(24)-H(24B)	110.3
H(24A)-C(24)-H(24B)	108.5
O(10)-C(25)-O(9)	123.2(6)
O(10)-C(25)-C(26)	123.8(6)
O(9)-C(25)-C(26)	113.0(5)
C(27)-C(26)-C(31)	118.4(6)
C(27)-C(26)-C(25)	118.6(6)
C(31)-C(26)-C(25)	123.0(5)
C(28)-C(27)-C(26)	121.6(8)
C(28)-C(27)-H(27)	119.2
C(26)-C(27)-H(27)	119.2
C(29)-C(28)-C(27)	120.0(8)
C(29)-C(28)-Br(1)	120.8(7)
C(27)-C(28)-Br(1)	119.1(8)

C(28)-C(29)-C(30)	119.8(7)
C(28)-C(29)-H(29)	120.1
C(30)-C(29)-H(29)	120.1
C(31)-C(30)-C(29)	119.9(8)
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(31)-C(26)	120.2(7)
C(30)-C(31)-H(31)	119.9
C(26)-C(31)-H(31)	119.9
O(2)-C(33)-O(1)	109.4(5)
O(2)-C(33)-H(33A)	109.8
O(1)-C(33)-H(33A)	109.8
O(2)-C(33)-H(33B)	109.8
O(1)-C(33)-H(33B)	109.8
H(33A)-C(33)-H(33B)	108.3
C(35)-C(34)-C(23)	104.4(4)
C(35)-C(34)-H(34A)	110.9
C(23)-C(34)-H(34A)	110.9
C(35)-C(34)-H(34B)	110.9
C(23)-C(34)-H(34B)	110.9
H(34A)-C(34)-H(34B)	108.9
C(34)-C(35)-C(36)	104.6(6)
C(34)-C(35)-H(35A)	110.8

C(36)-C(35)-H(35A)	110.8
C(34)-C(35)-H(35B)	110.8
C(36)-C(35)-H(35B)	110.8
H(35A)-C(35)-H(35B)	108.9
N(1)-C(36)-C(35)	104.0(5)
N(1)-C(36)-H(36A)	111.0
C(35)-C(36)-H(36A)	111.0
N(1)-C(36)-H(36B)	111.0
C(35)-C(36)-H(36B)	111.0
H(36A)-C(36)-H(36B)	109.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ZC242abs. 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}
Br(1)	285(2)	73(1)	157(1)	44(1)	-61(1)	-42(1)
O(1)	177(5)	65(3)	67(2)	3(2)	52(3)	-29(3)
O(2)	143(4)	79(3)	62(2)	-2(2)	33(3)	-20(3)
O(3)	51(2)	49(2)	80(2)	-9(2)	-5(2)	8(2)
O(4)	56(2)	52(2)	62(2)	-6(2)	1(2)	-12(2)
O(5)	69(2)	38(2)	78(2)	-10(2)	11(2)	3(2)
O(6)	77(2)	68(3)	57(2)	2(2)	10(2)	8(2)
O(7)	59(2)	56(2)	78(2)	-3(2)	16(2)	9(2)
O(8)	51(2)	70(3)	117(3)	21(2)	22(2)	-2(2)
O(9)	100(3)	42(2)	75(2)	7(2)	31(2)	-6(2)
O(10)	118(4)	75(3)	109(3)	17(3)	55(3)	16(3)
N(1)	64(3)	39(2)	61(2)	9(2)	15(2)	0(2)
C(1)	92(4)	46(3)	48(2)	5(2)	2(2)	-13(3)
C(2)	77(3)	46(3)	57(3)	3(2)	4(2)	-9(3)
C(3)	57(3)	35(3)	45(2)	3(2)	-1(2)	-4(2)
C(4)	49(2)	37(3)	54(2)	5(2)	-3(2)	2(2)
C(5)	39(2)	45(3)	57(2)	6(2)	-4(2)	-3(2)
C(6)	49(2)	40(3)	54(2)	5(2)	3(2)	-4(2)

C(7)	69(3)	40(3)	53(3)	4(2)	4(2)	2(2)
C(8)	59(3)	49(3)	46(2)	9(2)	-8(2)	-2(2)
C(9)	80(3)	43(3)	50(3)	0(2)	10(2)	-2(3)
C(10)	86(4)	65(4)	46(3)	-5(2)	6(3)	-12(3)
C(11)	45(2)	41(3)	44(2)	3(2)	8(2)	-1(2)
C(12)	53(2)	31(2)	54(2)	1(2)	14(2)	0(2)
C(13)	42(2)	49(3)	50(2)	-3(2)	5(2)	-3(2)
C(14)	51(3)	37(3)	54(2)	-9(2)	9(2)	-3(2)
C(15)	57(3)	33(3)	52(2)	1(2)	16(2)	-2(2)
C(16)	51(2)	31(2)	55(2)	3(2)	10(2)	2(2)
C(17)	54(3)	53(3)	88(3)	-3(3)	4(3)	12(3)
C(18)	85(4)	70(4)	64(3)	-4(3)	-2(3)	-21(3)
C(19)	85(4)	37(3)	102(4)	-2(3)	12(3)	15(3)
C(20)	44(2)	54(3)	67(3)	-7(2)	12(2)	-2(2)
C(21)	75(4)	70(4)	100(4)	-21(3)	26(3)	4(3)
C(22)	60(3)	40(3)	60(3)	4(2)	10(2)	0(2)
C(23)	75(3)	48(4)	57(3)	7(2)	27(2)	0(3)
C(24)	125(5)	51(4)	57(3)	11(3)	17(3)	-27(4)
C(25)	65(3)	62(4)	56(3)	1(3)	4(2)	-9(3)
C(26)	73(3)	47(3)	53(3)	3(2)	-9(2)	-15(3)
C(27)	104(5)	75(5)	69(4)	7(3)	0(3)	-13(4)
C(28)	129(6)	63(5)	82(4)	17(4)	-20(4)	-36(4)
C(29)	146(8)	131(8)	66(4)	29(5)	-8(5)	-74(7)

C(30)	98(5)	126(8)	66(4)	10(4)	14(3)	-38(5)
C(31)	75(3)	91(5)	55(3)	-1(3)	11(3)	-22(3)
C(33)	110(5)	94(6)	60(3)	-2(3)	20(3)	-30(4)
C(34)	137(6)	75(5)	54(3)	15(3)	-7(3)	-25(4)
C(35)	92(5)	101(5)	83(4)	40(4)	-8(4)	-1(4)
C(36)	56(3)	67(4)	67(3)	17(3)	5(2)	3(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ZC242abs.

	x	y	z	U(eq)
H(2)	6908	-2958	8124	73
H(4)	8414	-2681	6400	58
H(5)	9649	-1645	5898	58
H(7)	7073	-80	6319	65
H(9)	6205	-256	8418	69
H(12)	5095	-1718	5000	54
H(16)	7533	-3676	5050	54
H(17A)	1592	-1290	3338	98
H(17B)	3287	-1121	3597	98
H(17C)	2499	-1473	4684	98
H(18A)	2165	-3877	992	112
H(18B)	3869	-3749	1118	112
H(18C)	2830	-3038	1266	112
H(19A)	6799	-5455	3532	113
H(19B)	7032	-4986	4822	113
H(19C)	7727	-4681	3648	113

H(21A)	10240	-3533	3254	120
H(21B)	10043	-2761	2443	120
H(21C)	8658	-3237	2699	120
H(23)	8697	539	2420	70
H(24A)	7180	1727	3604	93
H(24B)	8823	1500	4124	93
H(27)	7642	4208	1639	101
H(29)	10106	4453	-1102	140
H(30)	10820	3146	-862	116
H(31)	9925	2377	627	88
H(33A)	4183	-1949	11002	105
H(33B)	5776	-1872	11779	105
H(34A)	6310	1179	1336	109
H(34B)	6563	274	1155	109
H(35A)	4436	256	1975	113
H(35B)	4903	977	2879	113
H(36A)	5488	31	4329	77
H(36B)	5789	-586	3285	77

Table 6. Torsion angles [°] for ZC242abs.

C(33)-O(1)-C(1)-C(2)	178.5(6)
C(33)-O(1)-C(1)-C(10)	0.2(7)
C(10)-C(1)-C(2)-C(3)	-1.2(8)
O(1)-C(1)-C(2)-C(3)	-179.3(5)
C(1)-C(2)-C(3)-C(8)	0.0(7)
C(1)-C(2)-C(3)-C(4)	-175.2(4)
C(8)-C(3)-C(4)-C(11)	-103.0(5)
C(2)-C(3)-C(4)-C(11)	72.2(5)
C(8)-C(3)-C(4)-C(5)	25.6(6)
C(2)-C(3)-C(4)-C(5)	-159.3(4)
C(11)-C(4)-C(5)-C(20)	-37.7(5)
C(3)-C(4)-C(5)-C(20)	-165.0(4)
C(11)-C(4)-C(5)-C(6)	89.6(5)
C(3)-C(4)-C(5)-C(6)	-37.7(5)
C(20)-C(5)-C(6)-C(7)	153.1(4)
C(4)-C(5)-C(6)-C(7)	29.1(6)
C(20)-C(5)-C(6)-C(22)	-38.8(6)
C(4)-C(5)-C(6)-C(22)	-162.7(4)
C(22)-C(6)-C(7)-C(8)	-173.6(4)
C(5)-C(6)-C(7)-C(8)	-5.8(7)
C(2)-C(3)-C(8)-C(9)	0.5(7)

C(4)-C(3)-C(8)-C(9)	175.7(4)
C(2)-C(3)-C(8)-C(7)	-177.7(4)
C(4)-C(3)-C(8)-C(7)	-2.6(6)
C(6)-C(7)-C(8)-C(3)	-8.9(7)
C(6)-C(7)-C(8)-C(9)	172.8(5)
C(3)-C(8)-C(9)-C(10)	0.1(7)
C(7)-C(8)-C(9)-C(10)	178.4(5)
C(8)-C(9)-C(10)-C(1)	-1.3(8)
C(8)-C(9)-C(10)-O(2)	179.6(6)
C(2)-C(1)-C(10)-C(9)	1.9(9)
O(1)-C(1)-C(10)-C(9)	-179.7(5)
C(2)-C(1)-C(10)-O(2)	-178.9(5)
O(1)-C(1)-C(10)-O(2)	-0.5(8)
C(33)-O(2)-C(10)-C(9)	179.7(6)
C(33)-O(2)-C(10)-C(1)	0.6(7)
C(3)-C(4)-C(11)-C(12)	53.1(6)
C(5)-C(4)-C(11)-C(12)	-75.4(5)
C(3)-C(4)-C(11)-C(16)	-128.3(4)
C(5)-C(4)-C(11)-C(16)	103.2(5)
C(16)-C(11)-C(12)-C(13)	0.4(6)
C(4)-C(11)-C(12)-C(13)	179.0(4)
C(17)-O(3)-C(13)-C(12)	-5.0(7)
C(17)-O(3)-C(13)-C(14)	176.0(5)

C(11)-C(12)-C(13)-O(3)	-178.1(4)
C(11)-C(12)-C(13)-C(14)	0.8(7)
C(18)-O(4)-C(14)-C(15)	-100.6(6)
C(18)-O(4)-C(14)-C(13)	83.4(6)
O(3)-C(13)-C(14)-O(4)	-6.2(6)
C(12)-C(13)-C(14)-O(4)	174.7(4)
O(3)-C(13)-C(14)-C(15)	177.6(4)
C(12)-C(13)-C(14)-C(15)	-1.4(7)
O(4)-C(14)-C(15)-O(5)	4.4(6)
C(13)-C(14)-C(15)-O(5)	-179.5(4)
O(4)-C(14)-C(15)-C(16)	-175.3(4)
C(13)-C(14)-C(15)-C(16)	0.8(7)
C(19)-O(5)-C(15)-C(14)	-179.8(5)
C(19)-O(5)-C(15)-C(16)	-0.1(7)
C(14)-C(15)-C(16)-C(11)	0.4(7)
O(5)-C(15)-C(16)-C(11)	-179.3(4)
C(12)-C(11)-C(16)-C(15)	-1.0(6)
C(4)-C(11)-C(16)-C(15)	-179.6(4)
C(21)-O(7)-C(20)-O(6)	-7.9(7)
C(21)-O(7)-C(20)-C(5)	170.5(5)
C(6)-C(5)-C(20)-O(6)	-14.0(7)
C(4)-C(5)-C(20)-O(6)	112.8(6)
C(6)-C(5)-C(20)-O(7)	167.6(4)

C(4)-C(5)-C(20)-O(7)	-65.6(5)
C(36)-N(1)-C(22)-O(8)	163.2(5)
C(23)-N(1)-C(22)-O(8)	6.8(8)
C(36)-N(1)-C(22)-C(6)	-19.9(7)
C(23)-N(1)-C(22)-C(6)	-176.3(4)
C(7)-C(6)-C(22)-O(8)	117.9(6)
C(5)-C(6)-C(22)-O(8)	-50.0(7)
C(7)-C(6)-C(22)-N(1)	-59.1(6)
C(5)-C(6)-C(22)-N(1)	133.0(4)
C(22)-N(1)-C(23)-C(34)	146.5(5)
C(36)-N(1)-C(23)-C(34)	-12.7(6)
C(22)-N(1)-C(23)-C(24)	-93.8(6)
C(36)-N(1)-C(23)-C(24)	107.1(6)
C(25)-O(9)-C(24)-C(23)	140.4(5)
N(1)-C(23)-C(24)-O(9)	173.4(4)
C(34)-C(23)-C(24)-O(9)	-72.6(6)
C(24)-O(9)-C(25)-O(10)	0.5(8)
C(24)-O(9)-C(25)-C(26)	179.3(4)
O(10)-C(25)-C(26)-C(27)	2.5(8)
O(9)-C(25)-C(26)-C(27)	-176.3(5)
O(10)-C(25)-C(26)-C(31)	-179.9(6)
O(9)-C(25)-C(26)-C(31)	1.3(7)
C(31)-C(26)-C(27)-C(28)	-1.4(9)

C(25)-C(26)-C(27)-C(28)	176.3(5)
C(26)-C(27)-C(28)-C(29)	4.3(10)
C(26)-C(27)-C(28)-Br(1)	-179.2(5)
C(27)-C(28)-C(29)-C(30)	-4.6(11)
Br(1)-C(28)-C(29)-C(30)	178.9(5)
C(28)-C(29)-C(30)-C(31)	2.3(11)
C(29)-C(30)-C(31)-C(26)	0.5(9)
C(27)-C(26)-C(31)-C(30)	-0.9(8)
C(25)-C(26)-C(31)-C(30)	-178.5(5)
C(10)-O(2)-C(33)-O(1)	-0.5(7)
C(1)-O(1)-C(33)-O(2)	0.2(7)
N(1)-C(23)-C(34)-C(35)	29.9(7)
C(24)-C(23)-C(34)-C(35)	-87.4(6)
C(23)-C(34)-C(35)-C(36)	-36.3(8)
C(22)-N(1)-C(36)-C(35)	-168.1(5)
C(23)-N(1)-C(36)-C(35)	-9.4(7)
C(34)-C(35)-C(36)-N(1)	28.0(7)