

# Synthesis and antimalarial and antituberculosis activities of a series of natural and unnatural 4-methoxy-6-styryl-pyran-2-ones, dihydro analogues and photo-dimers

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## Supplementary data

### Table of contents.

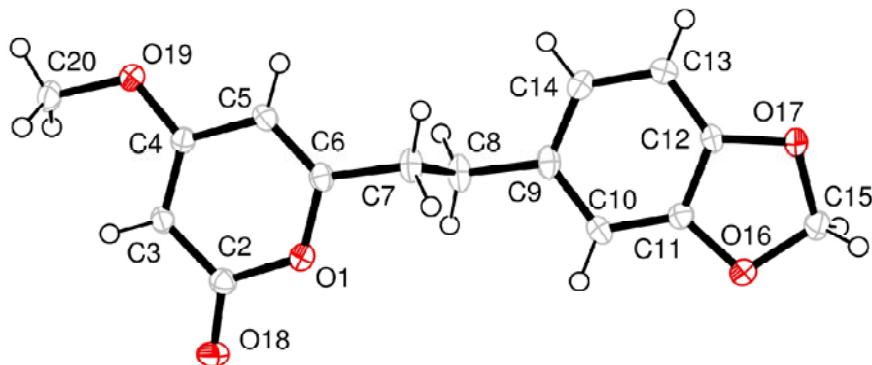
	page
General crystallography information	2
Crystal structure data for compound <b>2</b>	3
Crystal structure data for compound <b>3</b>	11
Crystal structure data for compound <b>14</b>	19
<sup>1</sup> H and <sup>13</sup> C NMR spectra of <b>1-5, 7, 12-35</b>	28

### **X-ray crystallography.**

Single crystal X-ray data for **2**, **3** and **14** were collected with a Bruker SMART-APEX II diffractometer. The data was integrated with SAINT.<sup>1</sup> Empirical absorption corrections were made with SADABS.<sup>2</sup> The structures were solved by direct methods (SHELXS-97) and refined by full-matrix least-squares methods against  $F^2$  (SHELXL-97).<sup>3</sup> All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically at calculated positions using a riding model.

- (1) *SAINT*; Bruker AXS Inc.: Madison, WI, 2000.
- (2) G. M. Sheldrick, *SADABS 2.0*; Universität Göttingen, Göttingen, Germany, 2000.
- (3) G. M. Sheldrick, *Acta Crystallogr. Sect. A* **2008**, *A64*, 112-122.

**Figure S1.** Crystal structure of **2** with ellipsoids drawn at the 50% probability level.



**Table S1.** Crystal data and structure refinement for **2**.

Identification code	shelxl	
Empirical formula	C <sub>15</sub> H <sub>14</sub> O <sub>5</sub>	
Formula weight	274.26	
Temperature	98(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.0036(2) Å	α = 90.8060(10)°
	b = 8.3760(3) Å	β = 105.8980(10)°
	c = 10.5599(3) Å	γ = 110.4210(10)°
Volume	633.31(3) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.438 Mg/m <sup>3</sup>	
Absorption coefficient	0.109 mm <sup>-1</sup>	
F(000)	288	
Crystal size	0.43 x 0.29 x 0.2 mm <sup>3</sup>	
Theta range for data collection	2.02 to 27.98°.	
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 10, -13 ≤ l ≤ 13	
Reflections collected	15272	
Independent reflections	3024 [R(int) = 0.0243]	
Completeness to theta = 27.98°	99.4 %	
Absorption correction	None	

Refinement method	Full-matrix least-squares on $F^2$
Data / restraints / parameters	3024 / 0 / 182
Goodness-of-fit on $F^2$	1.033
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 0.0342, wR2 = 0.0944
R indices (all data)	R1 = 0.0368, wR2 = 0.0974
Largest diff. peak and hole	0.336 and -0.240 e. $\text{\AA}^{-3}$

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

	x	y	z	U(eq)
O(1)	1891(1)	8019(1)	7566(1)	21(1)
O(19)	1577(1)	12762(1)	7927(1)	24(1)
O(16)	3166(1)	1779(1)	12057(1)	24(1)
C(5)	1524(1)	10196(1)	8783(1)	19(1)
O(17)	2646(1)	2476(1)	14006(1)	24(1)
C(10)	3397(1)	4549(1)	11174(1)	20(1)
C(14)	3091(1)	6587(1)	12660(1)	25(1)
C(3)	1922(1)	10614(1)	6600(1)	19(1)
C(11)	3200(1)	3437(1)	12118(1)	18(1)
C(12)	2915(1)	3861(1)	13292(1)	19(1)
C(2)	2041(1)	8959(1)	6493(1)	20(1)
O(18)	2268(1)	8270(1)	5567(1)	28(1)
C(4)	1685(1)	11221(1)	7715(1)	18(1)
C(6)	1624(1)	8638(1)	8666(1)	19(1)
C(13)	2852(2)	5431(1)	13604(1)	24(1)
C(8)	3479(1)	7438(1)	10453(1)	25(1)
C(7)	1535(1)	7416(1)	9685(1)	22(1)
C(9)	3347(1)	6172(1)	11465(1)	21(1)
C(20)	1756(2)	13863(1)	6891(1)	26(1)
C(15)	3193(1)	1304(1)	13364(1)	23(1)

**Table S3.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **2**.

---

O(1)-C(6)	1.3647(11)
O(1)-C(2)	1.3962(11)
O(19)-C(4)	1.3436(11)
O(19)-C(20)	1.4450(11)
O(16)-C(11)	1.3795(11)
O(16)-C(15)	1.4379(12)
C(5)-C(6)	1.3405(13)
C(5)-C(4)	1.4335(12)
C(5)-H(5)	0.9300
O(17)-C(12)	1.3780(11)
O(17)-C(15)	1.4345(12)
C(10)-C(11)	1.3775(13)
C(10)-C(9)	1.4065(14)
C(10)-H(10)	0.9300
C(14)-C(9)	1.3913(14)
C(14)-C(13)	1.4033(13)
C(14)-H(14)	0.9300
C(3)-C(4)	1.3615(12)
C(3)-C(2)	1.4276(13)
C(3)-H(3)	0.9300
C(11)-C(12)	1.3838(12)
C(12)-C(13)	1.3725(13)
C(2)-O(18)	1.2152(11)
C(6)-C(7)	1.4943(12)
C(13)-H(13)	0.9300
C(8)-C(9)	1.5134(12)
C(8)-C(7)	1.5383(14)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600

C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(6)-O(1)-C(2)	121.86(7)
C(4)-O(19)-C(20)	116.89(7)
C(11)-O(16)-C(15)	104.79(7)
C(6)-C(5)-C(4)	118.82(8)
C(6)-C(5)-H(5)	120.6
C(4)-C(5)-H(5)	120.6
C(12)-O(17)-C(15)	104.83(7)
C(11)-C(10)-C(9)	117.11(8)
C(11)-C(10)-H(10)	121.4
C(9)-C(10)-H(10)	121.4
C(9)-C(14)-C(13)	122.53(9)
C(9)-C(14)-H(14)	118.7
C(13)-C(14)-H(14)	118.7
C(4)-C(3)-C(2)	120.16(8)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(10)-C(11)-O(16)	128.05(8)
C(10)-C(11)-C(12)	122.16(9)
O(16)-C(11)-C(12)	109.74(8)
C(13)-C(12)-O(17)	128.13(8)
C(13)-C(12)-C(11)	122.15(9)
O(17)-C(12)-C(11)	109.68(8)
O(18)-C(2)-O(1)	115.85(8)
O(18)-C(2)-C(3)	127.04(9)
O(1)-C(2)-C(3)	117.11(8)
O(19)-C(4)-C(3)	125.17(8)
O(19)-C(4)-C(5)	114.40(8)
C(3)-C(4)-C(5)	120.43(8)
C(5)-C(6)-O(1)	121.62(8)
C(5)-C(6)-C(7)	126.32(9)
O(1)-C(6)-C(7)	112.03(8)
C(12)-C(13)-C(14)	116.12(9)
C(12)-C(13)-H(13)	121.9

C(14)-C(13)-H(13)	121.9
C(9)-C(8)-C(7)	111.11(8)
C(9)-C(8)-H(8A)	109.4
C(7)-C(8)-H(8A)	109.4
C(9)-C(8)-H(8B)	109.4
C(7)-C(8)-H(8B)	109.4
H(8A)-C(8)-H(8B)	108.0
C(6)-C(7)-C(8)	112.21(8)
C(6)-C(7)-H(7A)	109.2
C(8)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7B)	109.2
C(8)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9
C(14)-C(9)-C(10)	119.91(9)
C(14)-C(9)-C(8)	119.90(9)
C(10)-C(9)-C(8)	120.13(9)
O(19)-C(20)-H(20A)	109.5
O(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
O(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(17)-C(15)-O(16)	107.32(7)
O(17)-C(15)-H(15A)	110.3
O(16)-C(15)-H(15A)	110.3
O(17)-C(15)-H(15B)	110.3
O(16)-C(15)-H(15B)	110.3
H(15A)-C(15)-H(15B)	108.5

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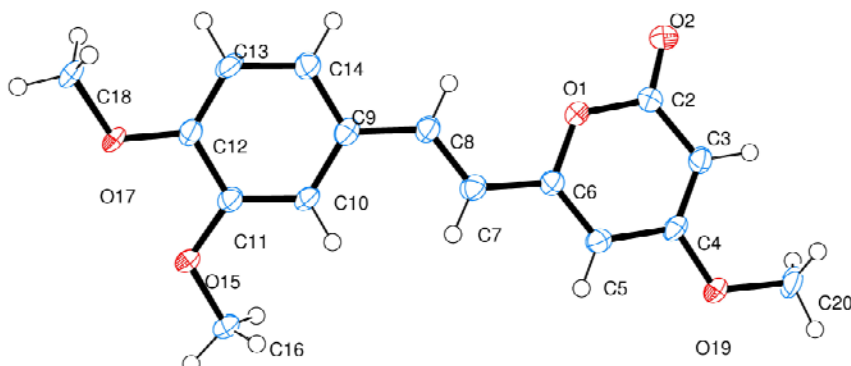
**Table S4.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **2**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
O(1)	26(1)	19(1)	22(1)	5(1)	8(1)	11(1)
O(19)	35(1)	19(1)	21(1)	4(1)	9(1)	13(1)
O(16)	33(1)	21(1)	22(1)	4(1)	10(1)	14(1)
C(5)	21(1)	22(1)	16(1)	4(1)	7(1)	8(1)
O(17)	37(1)	21(1)	22(1)	9(1)	14(1)	14(1)
C(10)	18(1)	26(1)	16(1)	5(1)	6(1)	8(1)
C(14)	30(1)	20(1)	28(1)	5(1)	8(1)	12(1)
C(3)	21(1)	19(1)	16(1)	5(1)	5(1)	7(1)
C(11)	17(1)	19(1)	19(1)	2(1)	5(1)	7(1)
C(12)	22(1)	20(1)	17(1)	6(1)	6(1)	8(1)
C(2)	19(1)	22(1)	18(1)	2(1)	5(1)	8(1)
O(18)	35(1)	30(1)	23(1)	0(1)	10(1)	17(1)
C(4)	18(1)	16(1)	18(1)	3(1)	4(1)	6(1)
C(6)	16(1)	21(1)	19(1)	6(1)	5(1)	6(1)
C(13)	32(1)	24(1)	20(1)	3(1)	10(1)	13(1)
C(8)	20(1)	28(1)	29(1)	15(1)	7(1)	9(1)
C(7)	20(1)	23(1)	25(1)	11(1)	7(1)	8(1)
C(9)	17(1)	23(1)	23(1)	9(1)	5(1)	7(1)
C(20)	35(1)	18(1)	24(1)	6(1)	5(1)	11(1)
C(15)	28(1)	22(1)	24(1)	7(1)	10(1)	13(1)

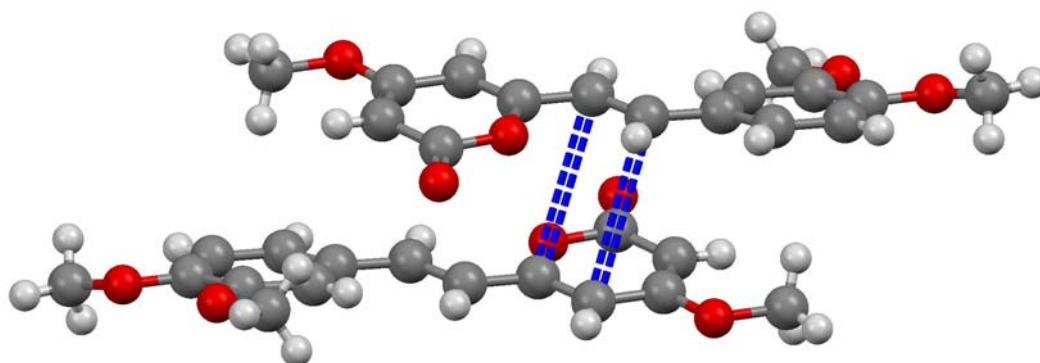
**Table S5.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **2**.

	x	y	z	U(eq)
H(5)	1353	10604	9543	23
H(10)	3556	4240	10378	24
H(14)	3078	7672	12841	30
H(3)	2006	11280	5906	23
H(13)	2663	5713	14395	29
H(8A)	4060	7149	9835	30
H(8B)	4258	8583	10901	30
H(7A)	753	6264	9251	27
H(7B)	963	7715	10305	27
H(20A)	2916	14040	6711	39
H(20B)	1733	14948	7174	39
H(20C)	738	13332	6102	39
H(15A)	2332	136	13307	28
H(15B)	4436	1376	13861	28

**Figure S2.** Crystal structure of **3** with ellipsoids drawn at the 50% probability level.



**Figure S3.** The packing of structure **3** with ellipsoids drawn at the 50 % probability level. Highlighted distances between C-7/C-8 (top) to C-5/C-6 (bottom) are 3.6 – 3.7 Å .



**Table S6.** Crystal data and structure refinement for **3**.

Identification code	shelxl	
Empirical formula	C <sub>16</sub> H <sub>16</sub> O <sub>5</sub>	
Formula weight	288.30	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6990(7) Å	α = 89.624(7)°
	b = 9.3889(8) Å	β = 68.010(6)°
	c = 10.0485(8) Å	γ = 67.643(6)°
Volume	694.90(10) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.378 Mg/m <sup>3</sup>	
Absorption coefficient	0.103 mm <sup>-1</sup>	
F(000)	304	
Crystal size	0.18 x 0.16 x 0.10 mm <sup>3</sup>	
Theta range for data collection	2.21 to 28.17°.	
Index ranges	-11<=h<=11, -12<=k<=12, -13<=l<=13	
Reflections collected	8711	
Independent reflections	3359 [R(int) = 0.0688]	
Completeness to theta = 28.17°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.990 and 0.990	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3359 / 0 / 193	
Goodness-of-fit on F <sup>2</sup>	1.084	
Final R indices [I>2sigma(I)]	R1 = 0.0730, wR2 = 0.2232	
R indices (all data)	R1 = 0.1357, wR2 = 0.2648	
Largest diff. peak and hole	0.394 and -0.367 e.Å <sup>-3</sup>	

**Table S7.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **3**. U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
C(2)	1839(5)	1892(4)	3537(4)	26(1)
C(3)	311(4)	1517(4)	3760(4)	23(1)
C(4)	-1192(4)	2136(4)	5004(4)	22(1)
C(5)	-1264(4)	3118(4)	6134(4)	23(1)
C(6)	203(4)	3421(4)	5938(3)	22(1)
C(7)	315(4)	4381(4)	6988(4)	24(1)
C(8)	1798(4)	4633(4)	6803(4)	24(1)
C(9)	1961(4)	5607(4)	7834(4)	24(1)
C(10)	437(4)	6637(4)	9032(3)	23(1)
C(11)	623(4)	7550(4)	9984(3)	22(1)
C(12)	2379(4)	7426(4)	9779(3)	23(1)
C(13)	3876(4)	6445(4)	8586(4)	26(1)
C(14)	3664(5)	5549(4)	7610(4)	26(1)
C(16)	-2564(4)	8830(4)	11306(4)	28(1)
C(18)	4191(4)	8033(4)	10776(4)	27(1)
C(20)	-2813(5)	1021(4)	4223(4)	29(1)
O(1)	1724(3)	2821(3)	4676(2)	25(1)
O(2)	3227(3)	1497(3)	2448(3)	39(1)
O(15)	-773(3)	8601(3)	11146(2)	27(1)
O(17)	2431(3)	8322(3)	10812(2)	25(1)
O(19)	-2747(3)	1939(3)	5331(2)	28(1)

**Table S8.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **3**.

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C(2)-O(2)	1.212(4)
C(2)-O(1)	1.394(4)
C(2)-C(3)	1.440(5)
C(3)-C(4)	1.348(4)
C(3)-H(3)	0.9300
C(4)-O(19)	1.353(4)
C(4)-C(5)	1.435(4)
C(5)-C(6)	1.355(5)
C(5)-H(5)	0.9300
C(6)-O(1)	1.365(4)
C(6)-C(7)	1.446(4)
C(7)-C(8)	1.344(5)
C(7)-H(7)	0.9300
C(8)-C(9)	1.466(4)
C(8)-H(8)	0.9300
C(9)-C(14)	1.392(5)
C(9)-C(10)	1.410(5)
C(10)-C(11)	1.382(4)
C(10)-H(10)	0.9300
C(11)-O(15)	1.361(4)
C(11)-C(12)	1.420(4)
C(12)-O(17)	1.365(4)
C(12)-C(13)	1.384(5)
C(13)-C(14)	1.402(5)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(16)-O(15)	1.435(4)
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(18)-O(17)	1.435(4)
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600

C(20)-O(19)	1.443(4)
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
O(2)-C(2)-O(1)	115.7(3)
O(2)-C(2)-C(3)	126.8(3)
O(1)-C(2)-C(3)	117.5(3)
C(4)-C(3)-C(2)	119.6(3)
C(4)-C(3)-H(3)	120.2
C(2)-C(3)-H(3)	120.2
C(3)-C(4)-O(19)	125.9(3)
C(3)-C(4)-C(5)	120.8(3)
O(19)-C(4)-C(5)	113.2(3)
C(6)-C(5)-C(4)	119.1(3)
C(6)-C(5)-H(5)	120.4
C(4)-C(5)-H(5)	120.4
C(5)-C(6)-O(1)	120.7(3)
C(5)-C(6)-C(7)	124.8(3)
O(1)-C(6)-C(7)	114.5(3)
C(8)-C(7)-C(6)	124.4(3)
C(8)-C(7)-H(7)	117.8
C(6)-C(7)-H(7)	117.8
C(7)-C(8)-C(9)	126.0(3)
C(7)-C(8)-H(8)	117.0
C(9)-C(8)-H(8)	117.0
C(14)-C(9)-C(10)	118.6(3)
C(14)-C(9)-C(8)	119.4(3)
C(10)-C(9)-C(8)	122.0(3)
C(11)-C(10)-C(9)	121.0(3)
C(11)-C(10)-H(10)	119.5
C(9)-C(10)-H(10)	119.5
O(15)-C(11)-C(10)	125.0(3)
O(15)-C(11)-C(12)	115.2(3)
C(10)-C(11)-C(12)	119.8(3)
O(17)-C(12)-C(13)	125.1(3)

O(17)-C(12)-C(11)	115.4(3)
C(13)-C(12)-C(11)	119.4(3)
C(12)-C(13)-C(14)	120.2(3)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(9)-C(14)-C(13)	120.9(3)
C(9)-C(14)-H(14)	119.5
C(13)-C(14)-H(14)	119.5
O(15)-C(16)-H(16A)	109.5
O(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
O(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(17)-C(18)-H(18A)	109.5
O(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
O(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(19)-C(20)-H(20A)	109.5
O(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
O(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(6)-O(1)-C(2)	122.1(3)
C(11)-O(15)-C(16)	116.0(2)
C(12)-O(17)-C(18)	116.7(2)
C(4)-O(19)-C(20)	116.6(3)

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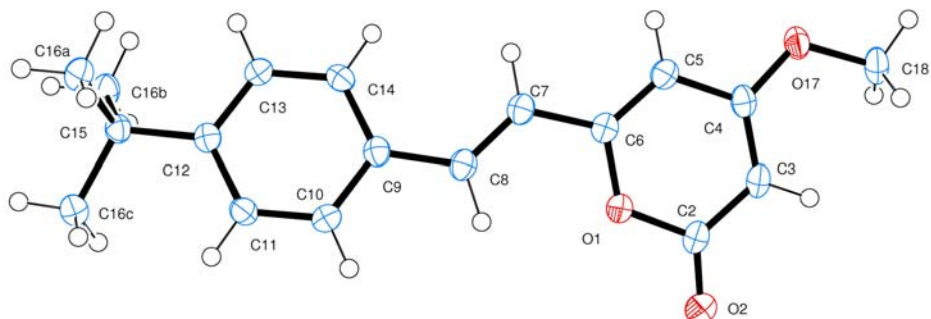
**Table S9.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **3**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
C(2)	23(2)	28(2)	24(2)	-2(1)	-5(1)	-12(1)
C(3)	24(2)	24(2)	25(2)	2(1)	-12(1)	-11(1)
C(4)	20(2)	22(2)	29(2)	6(1)	-14(1)	-11(1)
C(5)	20(2)	27(2)	23(2)	3(1)	-8(1)	-10(1)
C(6)	21(2)	23(2)	24(2)	2(1)	-10(1)	-9(1)
C(7)	22(2)	29(2)	24(2)	5(1)	-11(1)	-10(1)
C(8)	23(2)	25(2)	28(2)	2(1)	-12(1)	-10(1)
C(9)	24(2)	23(2)	29(2)	6(1)	-14(1)	-11(1)
C(10)	18(2)	27(2)	29(2)	3(1)	-11(1)	-11(1)
C(11)	20(2)	25(2)	24(2)	5(1)	-11(1)	-10(1)
C(12)	23(2)	26(2)	24(2)	4(1)	-12(1)	-13(1)
C(13)	18(2)	31(2)	34(2)	5(2)	-14(1)	-12(1)
C(14)	23(2)	26(2)	30(2)	1(1)	-13(1)	-8(1)
C(16)	16(2)	34(2)	34(2)	-2(2)	-10(1)	-10(1)
C(18)	21(2)	35(2)	33(2)	2(2)	-16(1)	-15(2)
C(20)	32(2)	33(2)	35(2)	2(2)	-20(2)	-20(2)
O(1)	20(1)	28(1)	28(1)	-2(1)	-7(1)	-13(1)
O(2)	27(1)	46(2)	36(2)	-10(1)	2(1)	-21(1)
O(15)	16(1)	36(1)	29(1)	-3(1)	-9(1)	-11(1)
O(17)	18(1)	35(1)	29(1)	0(1)	-12(1)	-14(1)
O(19)	21(1)	36(1)	30(1)	-3(1)	-10(1)	-15(1)

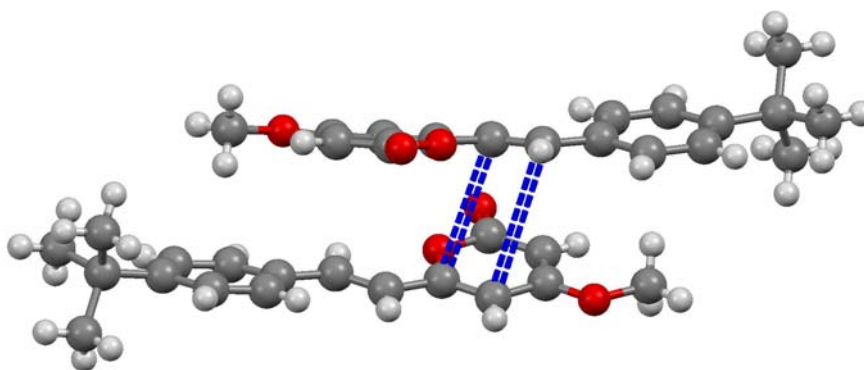
**Table S10.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **3**.

	x	y	z	U(eq)
H(3)	360	851	3049	28
H(5)	-2304	3540	6991	28
H(7)	-707	4856	7849	29
H(8)	2815	4144	5942	29
H(10)	-713	6704	9183	28
H(13)	5025	6380	8430	31
H(14)	4676	4908	6802	31
H(16A)	-2701	9070	10416	42
H(16B)	-3446	9677	12079	42
H(16C)	-2746	7895	11531	42
H(18A)	4810	6949	10804	40
H(18B)	4057	8653	11601	40
H(18C)	4883	8305	9899	40
H(20A)	-2650	1506	3367	44
H(20B)	-3968	953	4573	44
H(20C)	-1863	-8	3993	44

**Figure S4.** Crystal structure of **14** with ellipsoids drawn at the 50% probability level.



**Figure S5.** The packing of structure **14** with ellipsoids drawn at the 50 % probability level. Highlighted distances between C-7/C-8 (top) to C-5/C-6 (bottom) are 3.5 – 3.9 Å.



**Table S11.** Crystal data and structure refinement for **14**.

Identification code	shelxl	
Empirical formula	C18 H20 O3	
Formula weight	284.34	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 14.6633(5) Å	$\alpha = 90^\circ$
	b = 7.1228(3) Å	$\beta = 113.468(3)^\circ$
	c = 15.6152(6) Å	$\gamma = 90^\circ$
Volume	1496.01(10) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.262 Mg/m <sup>3</sup>	
Absorption coefficient	0.085 mm <sup>-1</sup>	
F(000)	608	
Crystal size	0.44 x 0.12 x 0.12 mm <sup>3</sup>	
Theta range for data collection	2.46 to 27.99°.	
Index ranges	-19<=h<=19, -9<=k<=9, -20<=l<=20	
Reflections collected	18895	
Independent reflections	3588 [R(int) = 0.0656]	
Completeness to theta = 27.99°	99.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3588 / 0 / 202	
Goodness-of-fit on F <sup>2</sup>	1.013	
Final R indices [I>2sigma(I)]	R1 = 0.0465, wR2 = 0.1007	
R indices (all data)	R1 = 0.0906, wR2 = 0.1190	
Largest diff. peak and hole	0.257 and -0.229 e.Å <sup>-3</sup>	

**Table S12.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **14**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
C(2)	3663(1)	7287(2)	1495(1)	25(1)
C(3)	4520(1)	7047(2)	2337(1)	25(1)
C(4)	4432(1)	6627(2)	3151(1)	23(1)
C(5)	3469(1)	6362(2)	3161(1)	24(1)
C(6)	2653(1)	6603(2)	2365(1)	22(1)
C(7)	1635(1)	6466(2)	2278(1)	24(1)
C(8)	842(1)	6669(2)	1470(1)	24(1)
C(9)	-203(1)	6689(2)	1326(1)	23(1)
C(10)	-919(1)	6661(2)	409(1)	25(1)
C(11)	-1922(1)	6790(2)	217(1)	24(1)
C(12)	-2269(1)	6984(2)	926(1)	21(1)
C(13)	-1544(1)	6958(2)	1847(1)	23(1)
C(14)	-544(1)	6818(2)	2043(1)	23(1)
C(15)	-3363(1)	7214(2)	739(1)	23(1)
C(16A)	-3721(1)	5462(2)	1094(1)	29(1)
C(16B)	-3515(1)	8954(2)	1252(1)	31(1)
C(16C)	-4014(1)	7475(2)	-304(1)	28(1)
C(18)	6181(1)	6709(2)	4037(1)	31(1)
O(1)	2737(1)	7051(2)	1545(1)	26(1)
O(2)	3635(1)	7700(2)	731(1)	34(1)
O(17)	5189(1)	6447(2)	3991(1)	28(1)

**Table S13.** Bond lengths [Å] and angles [°] for **14**.

---

C(2)-O(2)	1.2143(17)
C(2)-O(1)	1.4005(19)
C(2)-C(3)	1.421(2)
C(3)-C(4)	1.360(2)
C(3)-H(3)	0.9300
C(4)-O(17)	1.3456(18)
C(4)-C(5)	1.431(2)
C(5)-C(6)	1.350(2)
C(5)-H(5)	0.9300
C(6)-O(1)	1.3710(17)
C(6)-C(7)	1.448(2)
C(7)-C(8)	1.340(2)
C(7)-H(7)	0.961(16)
C(8)-C(9)	1.458(2)
C(8)-H(8)	0.997(15)
C(9)-C(10)	1.398(2)
C(9)-C(14)	1.399(2)
C(10)-C(11)	1.382(2)
C(10)-H(10)	0.9300
C(11)-C(12)	1.398(2)
C(11)-H(11)	0.9300
C(12)-C(13)	1.407(2)
C(12)-C(15)	1.520(2)
C(13)-C(14)	1.377(2)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(16C)	1.537(2)
C(15)-C(16B)	1.539(2)
C(15)-C(16A)	1.540(2)
C(16A)-H(16A)	0.9600
C(16A)-H(16B)	0.9600
C(16A)-H(16C)	0.9600
C(16B)-H(16D)	0.9600
C(16B)-H(16E)	0.9600

C(16B)-H(16F)	0.9600
C(16C)-H(16G)	0.9600
C(16C)-H(16H)	0.9600
C(16C)-H(16I)	0.9600
C(18)-O(17)	1.4400(19)
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
O(2)-C(2)-O(1)	115.48(14)
O(2)-C(2)-C(3)	127.51(15)
O(1)-C(2)-C(3)	117.00(13)
C(4)-C(3)-C(2)	120.85(15)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
O(17)-C(4)-C(3)	125.78(15)
O(17)-C(4)-C(5)	114.26(13)
C(3)-C(4)-C(5)	119.95(15)
C(6)-C(5)-C(4)	119.38(14)
C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3
C(5)-C(6)-O(1)	120.85(14)
C(5)-C(6)-C(7)	125.49(14)
O(1)-C(6)-C(7)	113.65(13)
C(8)-C(7)-C(6)	123.77(14)
C(8)-C(7)-H(7)	123.4(10)
C(6)-C(7)-H(7)	112.8(10)
C(7)-C(8)-C(9)	127.66(14)
C(7)-C(8)-H(8)	115.8(9)
C(9)-C(8)-H(8)	116.5(9)
C(10)-C(9)-C(14)	117.32(15)
C(10)-C(9)-C(8)	118.21(13)
C(14)-C(9)-C(8)	124.41(14)
C(11)-C(10)-C(9)	121.43(14)
C(11)-C(10)-H(10)	119.3
C(9)-C(10)-H(10)	119.3

C(10)-C(11)-C(12)	121.72(14)
C(10)-C(11)-H(11)	119.1
C(12)-C(11)-H(11)	119.1
C(11)-C(12)-C(13)	116.30(14)
C(11)-C(12)-C(15)	123.15(13)
C(13)-C(12)-C(15)	120.55(12)
C(14)-C(13)-C(12)	122.20(13)
C(14)-C(13)-H(13)	118.9
C(12)-C(13)-H(13)	118.9
C(13)-C(14)-C(9)	120.96(14)
C(13)-C(14)-H(14)	119.5
C(9)-C(14)-H(14)	119.5
C(12)-C(15)-C(16C)	112.33(12)
C(12)-C(15)-C(16B)	110.30(13)
C(16C)-C(15)-C(16B)	107.23(13)
C(12)-C(15)-C(16A)	109.20(13)
C(16C)-C(15)-C(16A)	108.80(13)
C(16B)-C(15)-C(16A)	108.92(13)
C(15)-C(16A)-H(16A)	109.5
C(15)-C(16A)-H(16B)	109.5
H(16A)-C(16A)-H(16B)	109.5
C(15)-C(16A)-H(16C)	109.5
H(16A)-C(16A)-H(16C)	109.5
H(16B)-C(16A)-H(16C)	109.5
C(15)-C(16B)-H(16D)	109.5
C(15)-C(16B)-H(16E)	109.5
H(16D)-C(16B)-H(16E)	109.5
C(15)-C(16B)-H(16F)	109.5
H(16D)-C(16B)-H(16F)	109.5
H(16E)-C(16B)-H(16F)	109.5
C(15)-C(16C)-H(16G)	109.5
C(15)-C(16C)-H(16H)	109.5
H(16G)-C(16C)-H(16H)	109.5
C(15)-C(16C)-H(16I)	109.5
H(16G)-C(16C)-H(16I)	109.5
H(16H)-C(16C)-H(16I)	109.5



O(17)-C(18)-H(18A)	109.5
O(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
O(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(6)-O(1)-C(2)	121.94(12)
C(4)-O(17)-C(18)	117.38(12)

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**Table S14.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **14**. The anisotropic displacement factor exponent takes the form:  $-2p^2[ h^2 a^* 2U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

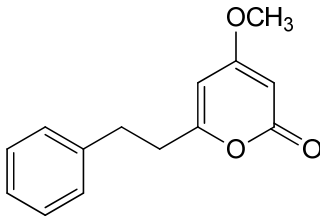
	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
C(2)	22(1)	24(1)	32(1)	-3(1)	13(1)	-1(1)
C(3)	17(1)	26(1)	33(1)	-4(1)	11(1)	-1(1)
C(4)	20(1)	18(1)	29(1)	-4(1)	8(1)	2(1)
C(5)	24(1)	23(1)	27(1)	0(1)	12(1)	-1(1)
C(6)	23(1)	18(1)	27(1)	-1(1)	11(1)	0(1)
C(7)	23(1)	21(1)	29(1)	-1(1)	12(1)	-1(1)
C(8)	22(1)	23(1)	29(1)	0(1)	11(1)	-2(1)
C(9)	21(1)	20(1)	26(1)	1(1)	9(1)	-1(1)
C(10)	26(1)	28(1)	24(1)	0(1)	12(1)	0(1)
C(11)	23(1)	26(1)	20(1)	1(1)	6(1)	-1(1)
C(12)	22(1)	17(1)	25(1)	0(1)	9(1)	-2(1)
C(13)	24(1)	22(1)	23(1)	0(1)	11(1)	-1(1)
C(14)	23(1)	24(1)	20(1)	0(1)	5(1)	-1(1)
C(15)	20(1)	25(1)	24(1)	-2(1)	8(1)	-2(1)
C(16A)	24(1)	33(1)	32(1)	1(1)	13(1)	-4(1)
C(16B)	25(1)	32(1)	36(1)	-5(1)	13(1)	1(1)
C(16C)	23(1)	33(1)	27(1)	1(1)	7(1)	0(1)
C(18)	17(1)	35(1)	37(1)	-5(1)	8(1)	2(1)
O(1)	21(1)	31(1)	25(1)	1(1)	9(1)	-1(1)
O(2)	30(1)	45(1)	30(1)	3(1)	15(1)	-1(1)
O(17)	18(1)	36(1)	28(1)	-1(1)	6(1)	2(1)

**Table S15.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **14**.

	x	y	z	U(eq)
H(3)	5148	7179	2331	30
H(5)	3406	6027	3710	29
H(10)	-716	6554	-82	30
H(11)	-2379	6747	-401	29
H(13)	-1747	7038	2339	27
H(14)	-88	6808	2661	28
H(16A)	-3628	4369	778	44
H(16B)	-4414	5596	971	44
H(16C)	-3346	5330	1753	44
H(16D)	-3141	8811	1911	46
H(16E)	-4208	9083	1128	46
H(16F)	-3291	10052	1036	46
H(16G)	-3795	8562	-533	43
H(16H)	-4694	7641	-388	43
H(16I)	-3960	6386	-643	43
H(18A)	6310	5803	3644	46
H(18B)	6652	6549	4669	46
H(18C)	6243	7952	3828	46
H(7)	1586(12)	6230(20)	2864(11)	31(4)
H(8)	989(12)	6860(20)	906(11)	26(4)

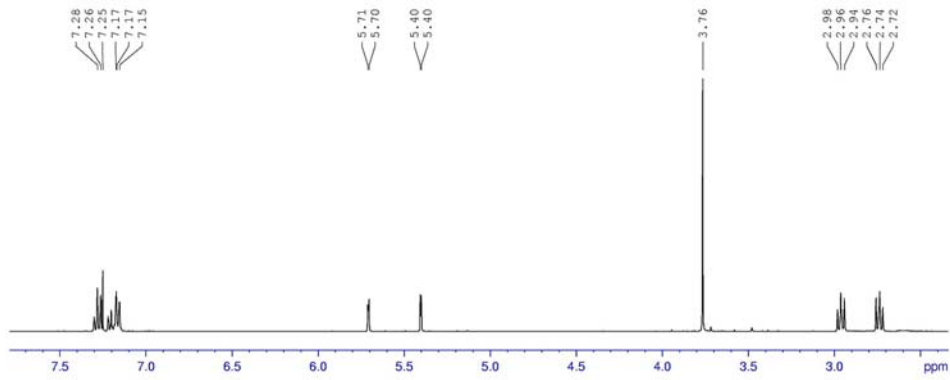
# Pyrone 1

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



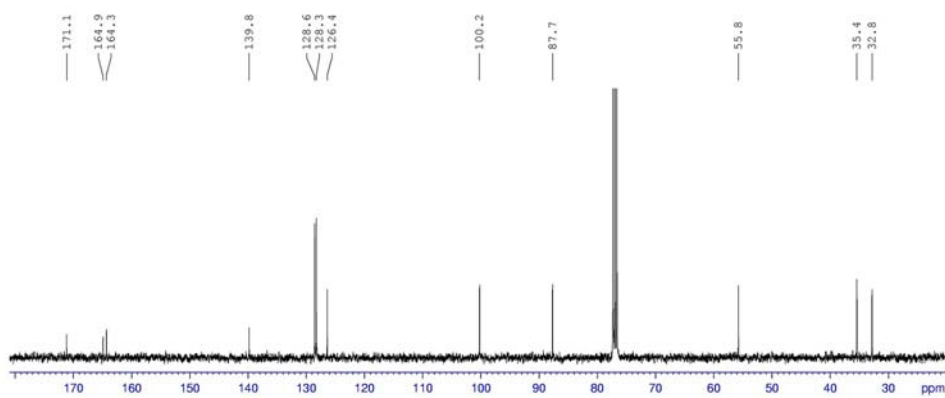
**1**

Pyrone 1 (STM6-73)



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EXPNO 20
PROCNO 1
Date_ 20080304
Time 21.55
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PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWS 8169.935 Hz
FIDRES 0.249327 Hz
AQ 2.0024517 sec
RG 456.1
SW 61.200 usec
DE 6.50 usec
TE 300.0 K
D1 0.1000000 sec
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NUC1 1H
P1 14.40 usec
PL1 2.20 dB
SFO1 400.1321007 MHz
SI 16384
SF 400.1300170 MHz
HWHM 0
SSB 0
LB 0.10 Hz
GB 0
PC 0.80
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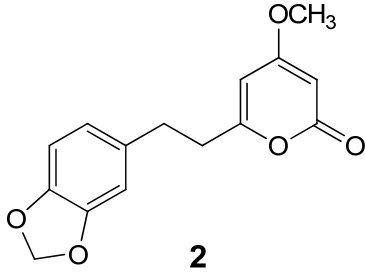
Pyrone 1 (STM6-73)



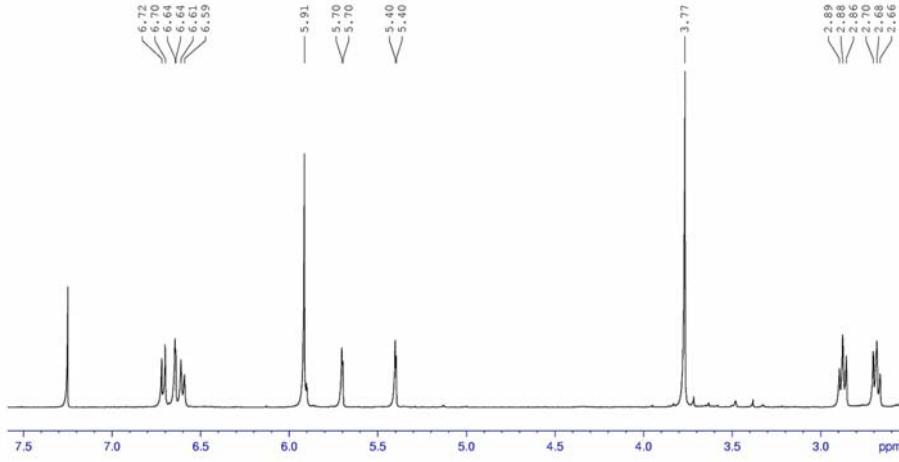
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TD 65536
SOLVENT CDCl3
NS 1000
DS 0
SWS 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 632
SW 20.850 usec
DE 8.50 usec
TE 300.0 K
D1 0.63167691 sec
d11 0.03000000 sec
d12 0.00002000 sec
----- CHANNEL f1 -----
NUC1 13C
P1 9.00 usec
PL1 -1.50 dB
SFO1 100.6238978 MHz
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 2.00 dB
PL12 19.10 dB
PL13 22.10 dB
SFO2 400.1318004 MHz
SI 132768
SF 100.6127732 MHz
HWHM 0
SSB 0
LB 2.00 Hz
GB 0
PC 0.80
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**Pyrone 2**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



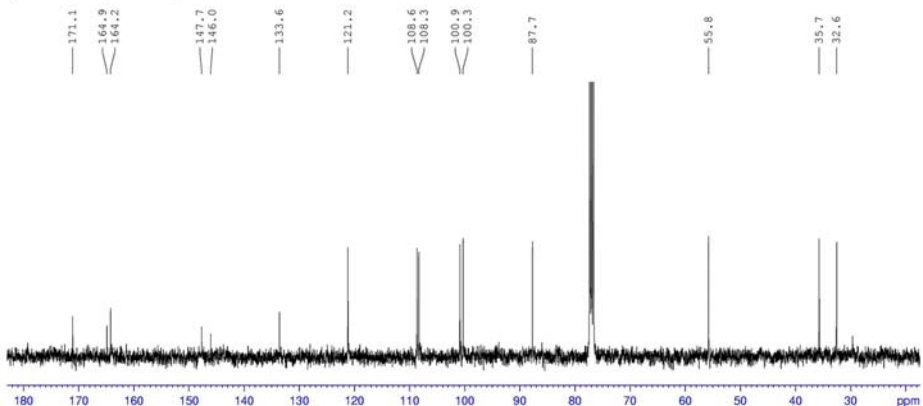
Pyrone 2 (SIM6-81)



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EXPNO    1
PROCNO    1
Date_     20080306
Time      17.54
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         0
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0447731 sec
RG         656.1
LW         62.400 usec
DE         6.50 usec
TE         300.0 K
D1         0.10000000 sec
D11        0.10000000 sec
D12        0.10000000 sec
D13        0.10000000 sec
D14        0.10000000 sec
D15        0.10000000 sec
D16        0.10000000 sec
D17        0.10000000 sec
D18        0.10000000 sec
D19        0.10000000 sec
D20        0.10000000 sec
D21        0.10000000 sec
D22        0.10000000 sec
D23        0.10000000 sec
D24        0.10000000 sec
D25        0.10000000 sec
D26        0.10000000 sec
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D28        0.10000000 sec
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D30        0.10000000 sec
D31        0.10000000 sec
D32        0.10000000 sec
D33        0.10000000 sec
D34        0.10000000 sec
D35        0.10000000 sec
D36        0.10000000 sec
D37        0.10000000 sec
D38        0.10000000 sec
D39        0.10000000 sec
D40        0.10000000 sec
D41        0.10000000 sec
D42        0.10000000 sec
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D52        0.10000000 sec
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D58        0.10000000 sec
D59        0.10000000 sec
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D61        0.10000000 sec
D62        0.10000000 sec
D63        0.10000000 sec
D64        0.10000000 sec
D65        0.10000000 sec
D66        0.10000000 sec
D67        0.10000000 sec
D68        0.10000000 sec
D69        0.10000000 sec
D70        0.10000000 sec
D71        0.10000000 sec
D72        0.10000000 sec
D73        0.10000000 sec
D74        0.10000000 sec
D75        0.10000000 sec
D76        0.10000000 sec
D77        0.10000000 sec
D78        0.10000000 sec
D79        0.10000000 sec
D80        0.10000000 sec
D81        0.10000000 sec
D82        0.10000000 sec
D83        0.10000000 sec
D84        0.10000000 sec
D85        0.10000000 sec
D86        0.10000000 sec
D87        0.10000000 sec
D88        0.10000000 sec
D89        0.10000000 sec
D90        0.10000000 sec
D91        0.10000000 sec
D92        0.10000000 sec
D93        0.10000000 sec
D94        0.10000000 sec
D95        0.10000000 sec
D96        0.10000000 sec
D97        0.10000000 sec
D98        0.10000000 sec
D99        0.10000000 sec
D100       0.10000000 sec
  
```

Pyrone 2 (SIM6-81)

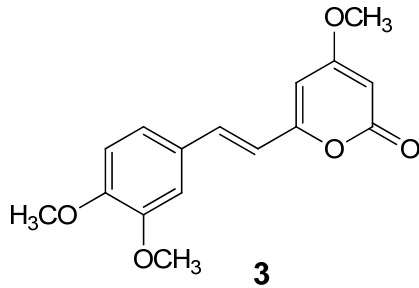


```

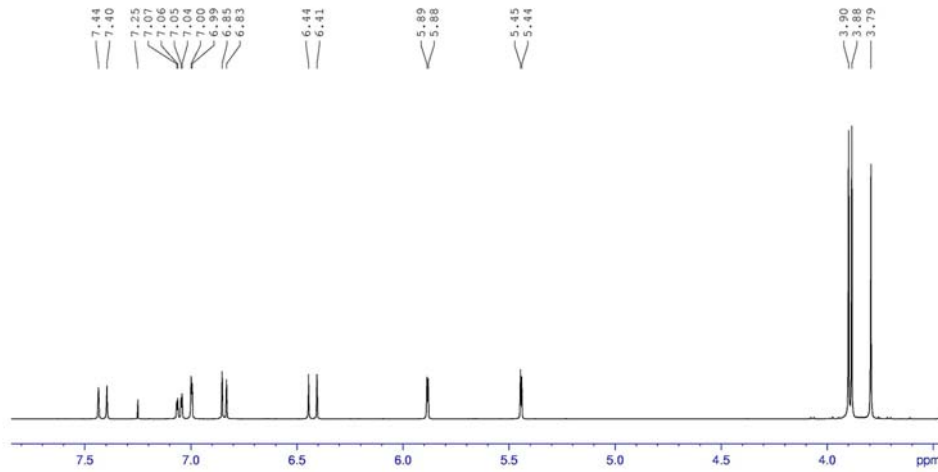
NAME      STM pyrone compd 2 6-81
EXPNO    1
PROCNO    1
Date_     20080326
Time      19.20
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2000
DS         0
SWH        24038.441 Hz
FIDRES     0.266738 Hz
AQ         1.3831988 sec
RG         6502
LW         20.800 usec
DE         6.50 usec
TE         300.0 K
D1         0.63167891 sec
D11        0.10000000 sec
D12        0.10000000 sec
D13        0.10000000 sec
D14        0.10000000 sec
D15        0.10000000 sec
D16        0.10000000 sec
D17        0.10000000 sec
D18        0.10000000 sec
D19        0.10000000 sec
D20        0.10000000 sec
D21        0.10000000 sec
D22        0.10000000 sec
D23        0.10000000 sec
D24        0.10000000 sec
D25        0.10000000 sec
D26        0.10000000 sec
D27        0.10000000 sec
D28        0.10000000 sec
D29        0.10000000 sec
D30        0.10000000 sec
D31        0.10000000 sec
D32        0.10000000 sec
D33        0.10000000 sec
D34        0.10000000 sec
D35        0.10000000 sec
D36        0.10000000 sec
D37        0.10000000 sec
D38        0.10000000 sec
D39        0.10000000 sec
D40        0.10000000 sec
D41        0.10000000 sec
D42        0.10000000 sec
D43        0.10000000 sec
D44        0.10000000 sec
D45        0.10000000 sec
D46        0.10000000 sec
D47        0.10000000 sec
D48        0.10000000 sec
D49        0.10000000 sec
D50        0.10000000 sec
D51        0.10000000 sec
D52        0.10000000 sec
D53        0.10000000 sec
D54        0.10000000 sec
D55        0.10000000 sec
D56        0.10000000 sec
D57        0.10000000 sec
D58        0.10000000 sec
D59        0.10000000 sec
D60        0.10000000 sec
D61        0.10000000 sec
D62        0.10000000 sec
D63        0.10000000 sec
D64        0.10000000 sec
D65        0.10000000 sec
D66        0.10000000 sec
D67        0.10000000 sec
D68        0.10000000 sec
D69        0.10000000 sec
D70        0.10000000 sec
D71        0.10000000 sec
D72        0.10000000 sec
D73        0.10000000 sec
D74        0.10000000 sec
D75        0.10000000 sec
D76        0.10000000 sec
D77        0.10000000 sec
D78        0.10000000 sec
D79        0.10000000 sec
D80        0.10000000 sec
D81        0.10000000 sec
D82        0.10000000 sec
D83        0.10000000 sec
D84        0.10000000 sec
D85        0.10000000 sec
D86        0.10000000 sec
D87        0.10000000 sec
D88        0.10000000 sec
D89        0.10000000 sec
D90        0.10000000 sec
D91        0.10000000 sec
D92        0.10000000 sec
D93        0.10000000 sec
D94        0.10000000 sec
D95        0.10000000 sec
D96        0.10000000 sec
D97        0.10000000 sec
D98        0.10000000 sec
D99        0.10000000 sec
D100       0.10000000 sec
  
```

**Pyrone 3**

<sup>1</sup>H 400 MHz, <sup>13</sup>C 100 MHz, CDCl<sub>3</sub>.



Pyrone 3 (STM7-29-1)

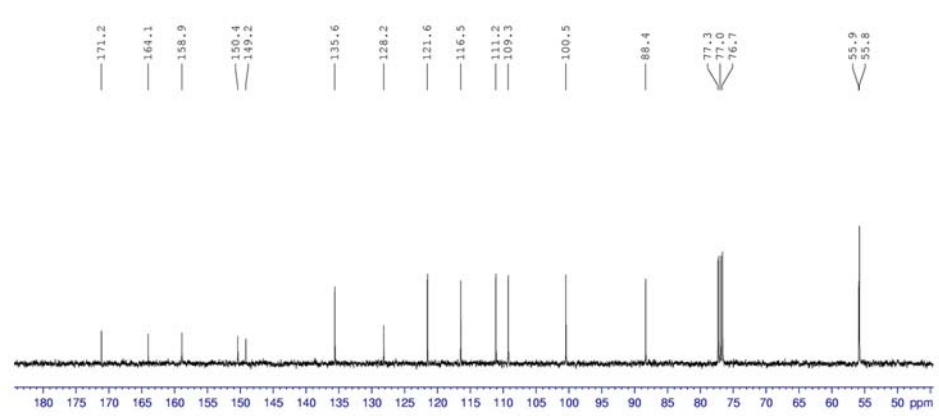


```

NAME      STM pyrone comp 3 7-29-1
EXPNO     1
PROCNO    1
Date_     20090922
Time      11.47
INSTRUM   spect
PROBHD    5 mm F400 EB/
PULPROG   zgpg30
TD        32768
SOLVENT   CDCl3
NS        32
DS        0
SWH       8012.820 Hz
FIDRES    0.244532 Hz
AQ        2.0447731 sec
RG        141
DM        62.400 usec
DE        6.20 usec
TE        300.0 K
D1        0.10000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      1H
P1        18.70 usec
PL1       0.50 dB
SFO1      400.1300007 MHz
SI        16384
SF        400.1300171 MHz
WDW       EM
SSB       0
GB        0.10 Hz
PC        0.60
    
```

Pyrone 3 (STM7-29-1)



```

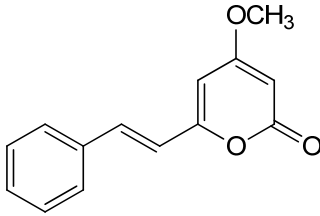
NAME      STM pyrone comp 3 7-29-1
EXPNO     2
PROCNO    1
Date_     20090922
Time      11.50
INSTRUM   spect
PROBHD    5 mm F400 EB/
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        138
DS        0
SWH       24038.440 Hz
FIDRES    0.366788 Hz
AQ        1.3451989 sec
RG        652
DM        20.000 usec
DE        6.10 usec
TE        300.0 K
D1        0.63100000 sec
d11       0.02000000 sec
DELTA     0.03100000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -1.20 dB
SFO1      100.6284667 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2       0.50 dB
PL12      15.56 dB
PL13      19.40 dB
SFO2      400.1318000 MHz
SI        52768
SF        100.6127719 MHz
WDW       EM
SSB       0
GB        2.00 Hz
PC        0.60
    
```

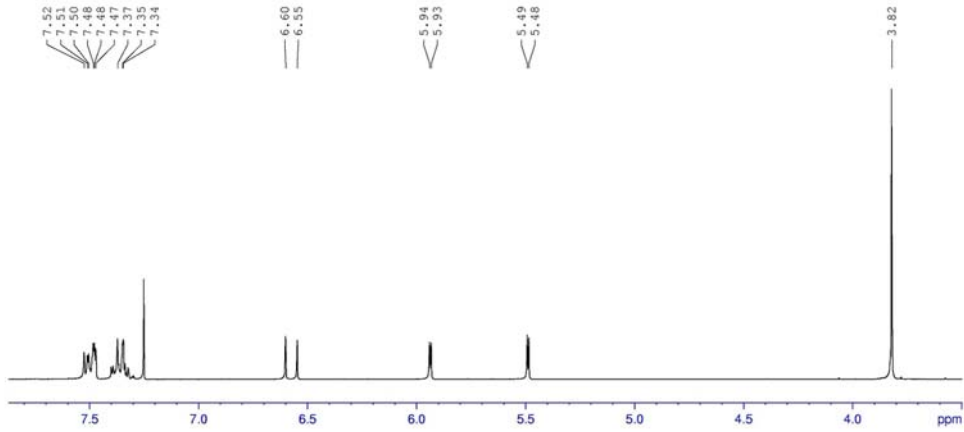
**Pyrone 4**

$^1\text{H}$  300 MHz,  $^{13}\text{C}$  75 MHz,  $\text{CDCl}_3$ .



**4**

Pyrone 4 (STM7-15)

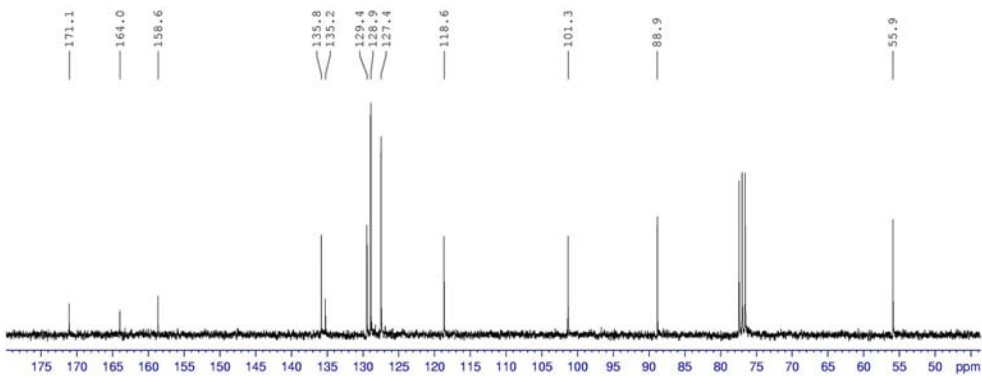


```

NAME      STM pyrone compd 4 7-15
EXPNO    1
PROCNO   1
Date_    20090903
Time     14.07
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       33
DS       0
SMB      5995.204 Hz
FIDRES   0.182959 Hz
AQ       2.7329011 sec
RG       512.7
SM       83.400 usec
DE       6.00 usec
TE       300.2 K
D1       0.10000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       22.90 usec
PL1     -0.90 dB
PL1W    44.18504333 W
SFO1    300.13506 MHz
SI      16384
SF      300.1300087 MHz
WDW      EM
SSB      0
LB      0.10 Hz
GB      0
PC      0.80
    
```

Pyrone 4 (STM4-150)



```

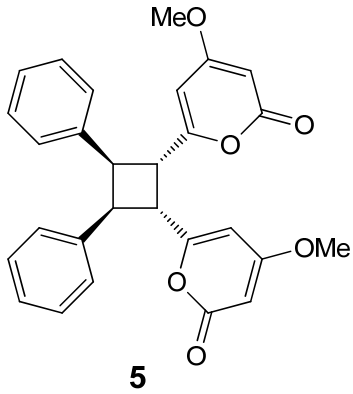
NAME      STM pyrone compd 4b 4-150
EXPNO    2
PROCNO   1
Date_    20061203
Time     15.23
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg2
TD       65536
SOLVENT  CDCl3
NS       412
DS       0
SMB      13985.411 Hz
FIDRES   0.274418 Hz
AQ       1.8219508 sec
RG       16384
SM       27.890 usec
DE       25.00 usec
TE       300.0 K
D1       0.1189371 sec
d11     0.83000000 sec
d12     0.00000000 sec

===== CHANNEL f1 =====
NUC1     13C
P1       5.44 usec
PL1     0.00 dB
PL1W    75.4760973 MHz

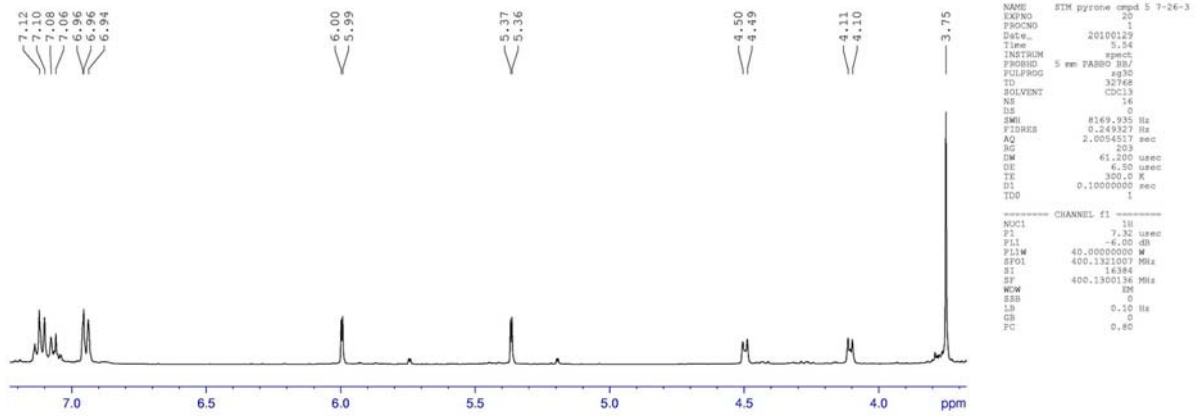
===== CHANNEL f2 =====
CPDPRG2  wa1414
NUC2     1H
PCPD2    100.00 usec
PL2     0.00 dB
PL2W    20.00 dB
PL13    24.40 dB
SFO2    300.1312003 MHz
SI      32768
SF      75.4671494 MHz
WDW      EM
SSB      0
LB      1.00 Hz
GB      0
PC      1.00
    
```

**Pyrone 5**

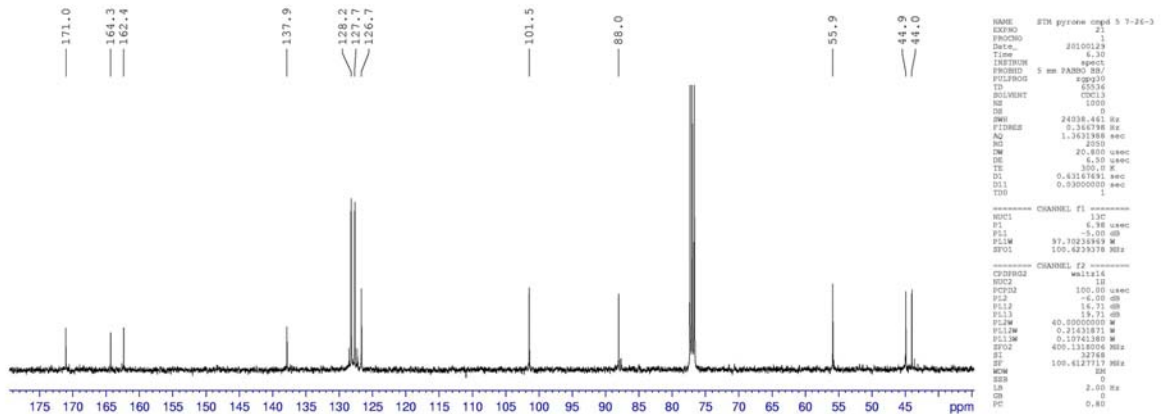
$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



Pyrone 5 (SIM7-26-3)



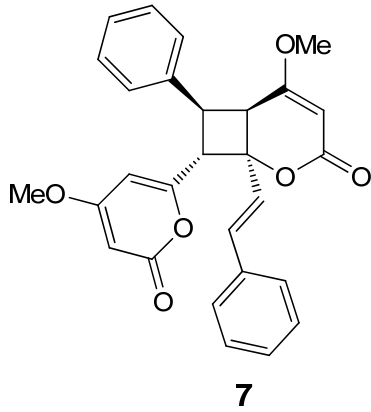
Pyrone 5 (SIM7-26-3)



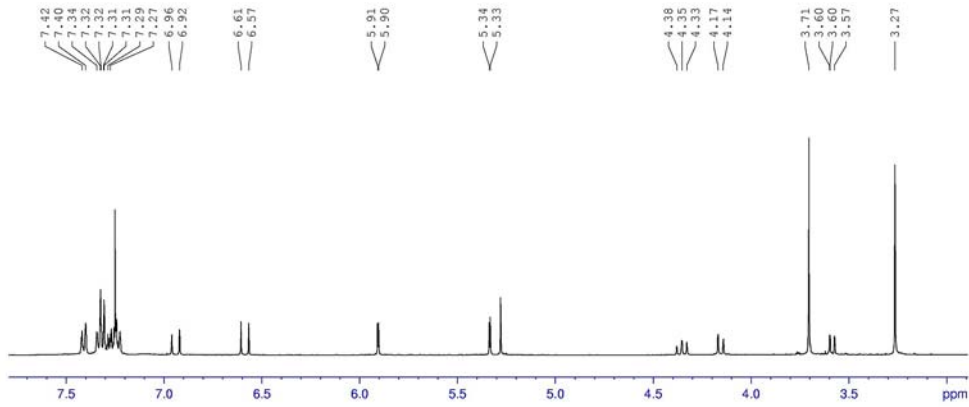


**Pyrone 7**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



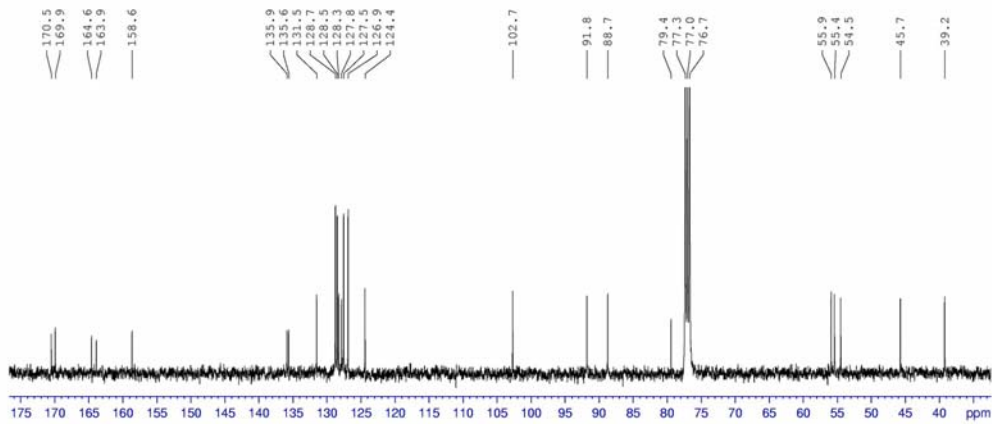
Pyrone 7 (STM7-26-8)



```

NAME      STM pyrone comp 7 7-26-8
EXPNO    20
PROCNO   20100208
Date_    17.10
Time     17.10
INSTRUM  spect
PROBHD   5 mm F400 BBO/
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       32
DS       0
SHE      8169.332 Hz
FIDRES   0.249327 Hz
AQ       2.0054517 sec
RG       287
AQ       2.0054517 sec
DE       61.200 usec
TE       300.2 K
D1       0.10000000 sec
TDO      1
----- CHANNEL f1 -----
NUC1     1H
P1       7.32 usec
PL1     -6.00 dB
PL12W   40.0000000 W
SFO1     400.132037 MHz
SI       16384
SF       400.1300338 MHz
WDW      EM
SSB      0
LB       0.10 Hz
GB       0
PC       0.80
    
```

Pyrone 7 (STM7-26-8)

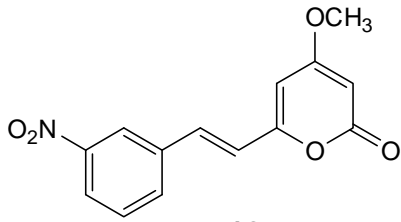


```

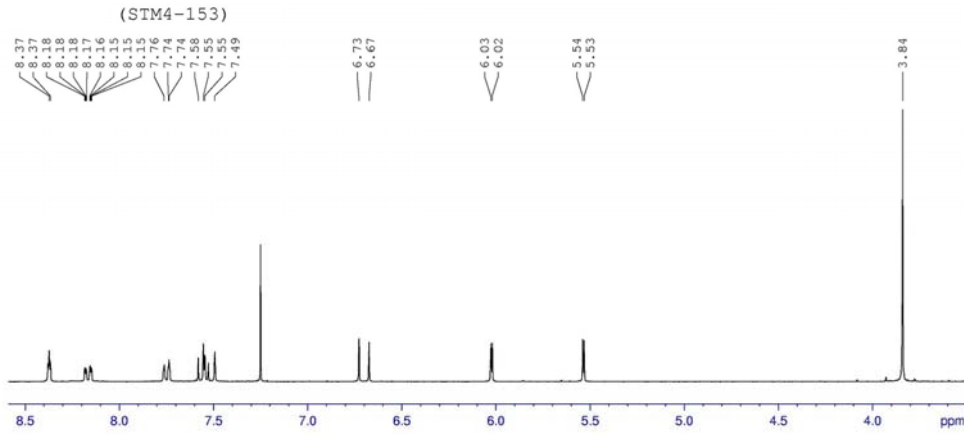
NAME      STM pyrone comp 7 7-26-8
EXPNO    21
PROCNO   20100208
Date_    14.11
Time     18.20
INSTRUM  spect
PROBHD   5 mm F400 BBO/
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       2000
DS       0
SHE      24038.442 Hz
FIDRES   0.266798 Hz
AQ       1.3431988 sec
RG       2000
AQ       1.3431988 sec
DE       20.000 usec
TE       300.2 K
D1       0.63167491 sec
D11      0.03000000 sec
TDO      1
----- CHANNEL f1 -----
NUC1     13C
P1       4.38 usec
PL1     -5.00 dB
PL12W   97.7023849 W
SFO1     100.6233378 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
P2       100.00 usec
PL2     -4.00 dB
PL12W   14.71 dB
PL13    19.71 dB
PL14    40.0000000 W
PL15W  0.21431871 W
PL16W  0.10741380 W
SFO2     400.132034 MHz
SF       100.6233378 MHz
WDW      EM
SSB      0
LB       2.00 Hz
GB       0
PC       0.80
    
```

**Pyrone 12**

$^1\text{H}$  300 MHz,  $^{13}\text{C}$  75 MHz,  $\text{CDCl}_3$ .



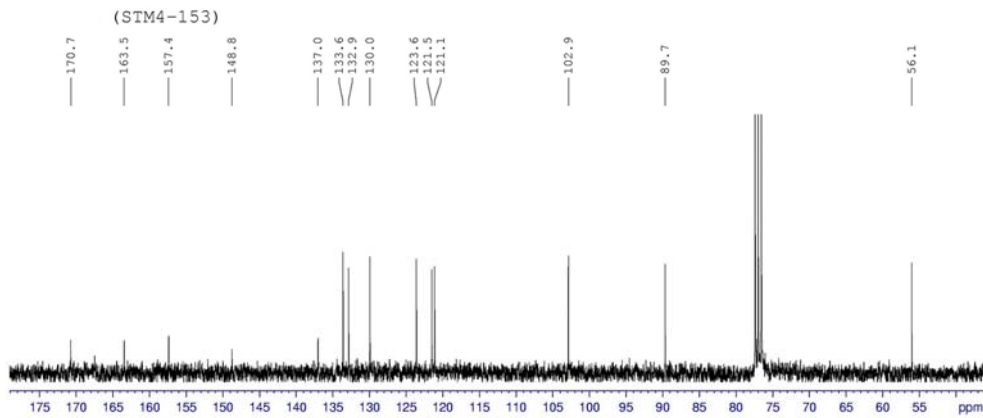
**12**



```

NAME      STM pyrone ompd 11 4-153
EXPNO    1
PROCNO   1
Date_    20061203
Time     16.15
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SWH       5995.204 Hz
FIDRES   0.182959 Hz
AQ        2.7329011 sec
RG        812.7
DM        83.400 usec
DE        8.00 usec
TE        300.2 K
D1        0.1000000 sec

----- CHANNEL f1 -----
NUC1      1H
P1         9.30 usec
PL1        0.00 dB
SFO1      300.1315004 MHz
SI         16384
SF         300.1300089 MHz
WDW        EM
SSB        0
LB         0.10 Hz
GB         0
PC         0.80
    
```



```

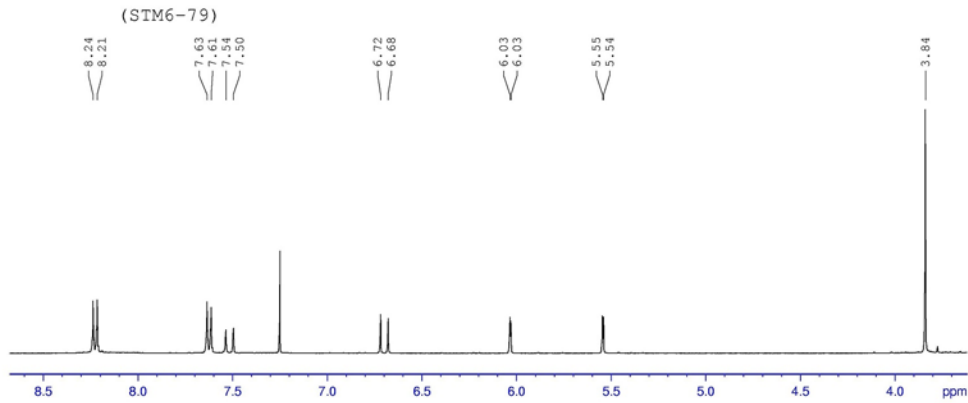
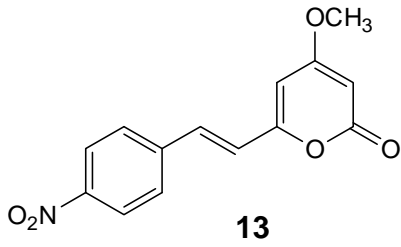
NAME      STM pyrone ompd 11 4-153
EXPNO    1
PROCNO   1
Date_    20061203
Time     16.20
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        719
DS        0
SWH       17985.611 Hz
FIDRES   0.278439 Hz
AQ        1.8213508 sec
RG        16384
DM        27.800 usec
DE        20.00 usec
TE        300.2 K
D1        0.17591171 sec
d11       0.00000000 sec
d12       0.00000000 sec

----- CHANNEL f1 -----
NUC1      13C
P1         5.44 usec
PL1        0.00 dB
SFO1      75.4760973 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2       1H
FIDRES   0.182959 Hz
PL2        0.00 dB
PL12      20.00 dB
PL13      20.00 dB
SFO2      300.1315005 MHz
SI         32768
SF         75.467493 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00
    
```

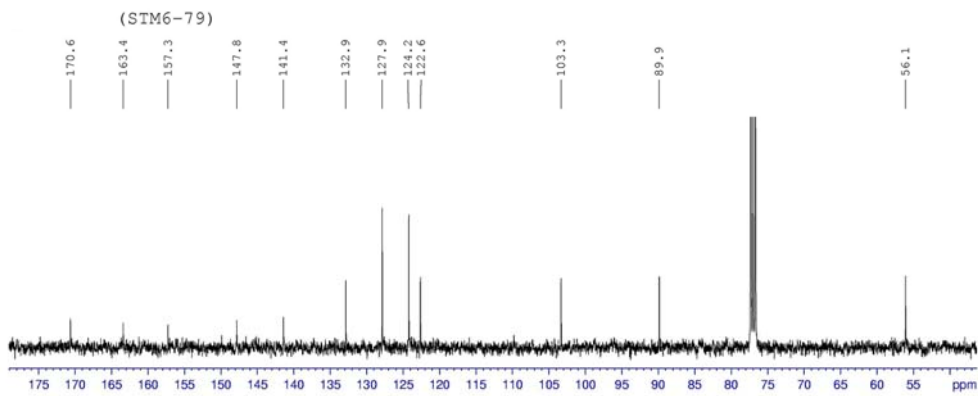
**Pyrone 13**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



```

NAME      STM pyrone comp 12 6-79-2c
EXPNO    2
PROCNO   1
Date_    20080326
Time     17.49
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zg30
TD        32768
SOLVENT  CDCl3
NS        0
DS        0
SWH       8017.875 Hz
FIDRES   0.244532 Hz
AQ        2.0447331 sec
RG        645.1
DW        62.400 usec
DE        6.50 usec
TE        300.2 K
SI        0
D1        0.10000000 sec
----- CHANNEL f1 -----
NUC1      1H
P1        14.40 usec
PL1       -2.20 dB
SFO1      400.1320007 MHz
SI        16384
SF        400.1300172 MHz
MCW       3M
SSB       0
LB        0.10 Hz
GB        0
PC        0.80
    
```

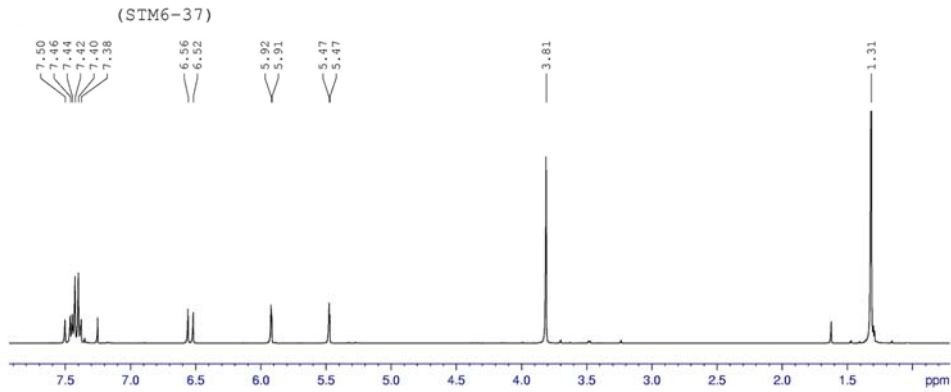
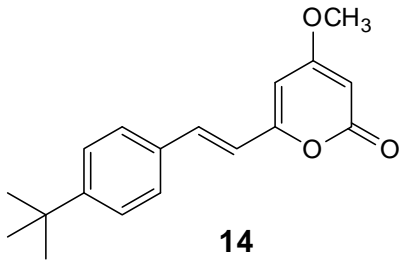


```

NAME      STM pyrone comp 12 6-79-2c
EXPNO    11
PROCNO   1
Date_    20080326
Time     19.01
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        0
DS        0
SWH       24039.461 Hz
FIDRES   0.360798 Hz
AQ        1.3637983 sec
RG        6502
DW        20.800 usec
DE        6.50 usec
TE        300.2 K
SI        0
D1        0.4316769 sec
d11      0.02000000 sec
d12      0.00000000 sec
----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -1.00 dB
SFO1      100.6230978 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    100.00 usec
PL2      -2.20 dB
PL12     17.10 dB
PL12     22.10 dB
SFO2      400.1310058 MHz
SI        16384
SF        100.6127774 MHz
MCW       3M
SSB       0
LB        0.10 Hz
GB        0
PC        0.80
    
```

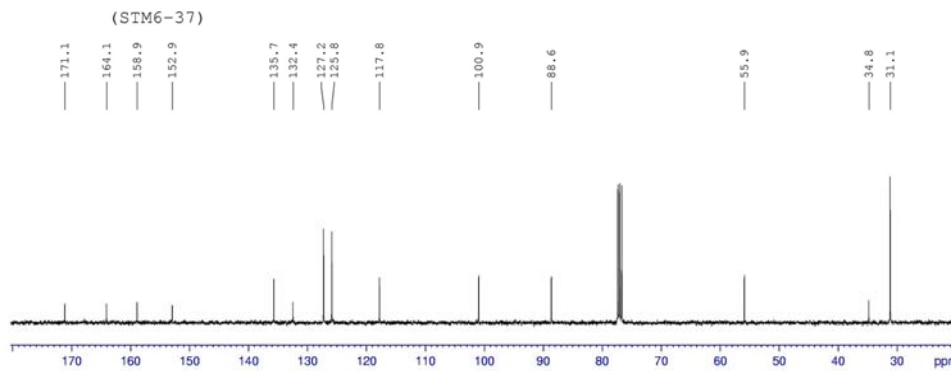
**Pyrone 14**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



```

NAME      STM pyrone cmpd 13 6-37-3
EXPNO    1
PROCNO    1
Date_     20071213
Time      18.28
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         512
DS         0
SWH        8105.935 Hz
FIDRES     0.259327 Hz
AQ         2.0054557 sec
RG         181
DW         61.700 usec
DE         6.50 usec
TE         300.0 K
TE        0.10000000 sec
----- CHANNEL f1 -----
NUC1       1H
P1         14.40 usec
PL1        0.00 dB
SFO1       400.1321007 MHz
SI         16384
SF         400.1300170 MHz
WDW        EM
SSB        0
LB         0.10 Hz
GB         0
PC         0.80
    
```

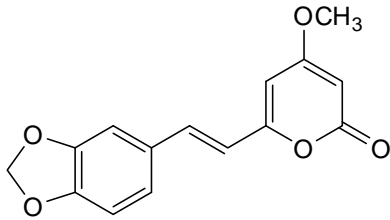


```

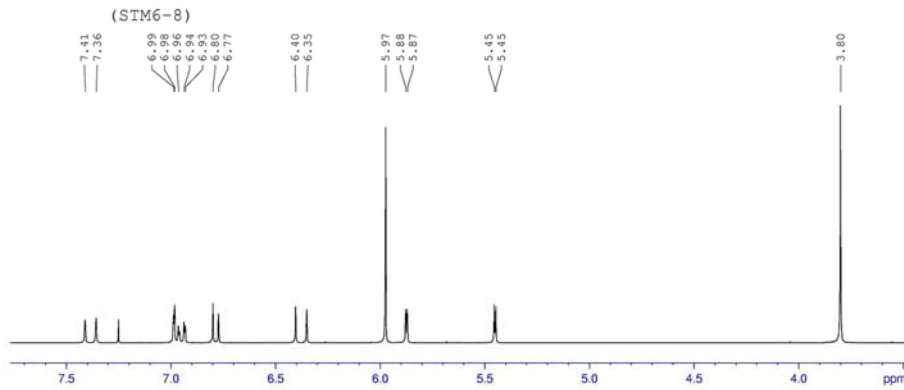
NAME      STM pyrone cmpd 13 6-37-3
EXPNO    1
PROCNO    1
Date_     20071213
Time      18.47
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         512
DS         0
SWH        24038.441 Hz
FIDRES     0.264796 Hz
AQ         1.3431983 sec
RG         4000
DW         20.800 usec
DE         6.50 usec
TE         300.0 K
TE        0.40167491 sec
D1         0.40167491 sec
d11        0.00000000 sec
d12        0.00000000 sec
----- CHANNEL f1 -----
NUC1       13C
P1         9.00 usec
PL1        -1.00 dB
SFO1       100.62838978 MHz
----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2       1H
PCPD2     100.00 usec
PL2        2.00 dB
PL12       17.10 dB
PL13       17.10 dB
SFO2       400.1321008 MHz
SI         32768
SF         100.6277233 MHz
WDW        EM
SSB        0
LB         0.10 Hz
GB         0
PC         0.80
    
```

**Pyrone 15**

$^1\text{H}$  300 MHz,  $^{13}\text{C}$  75 MHz,  $\text{CDCl}_3$ .

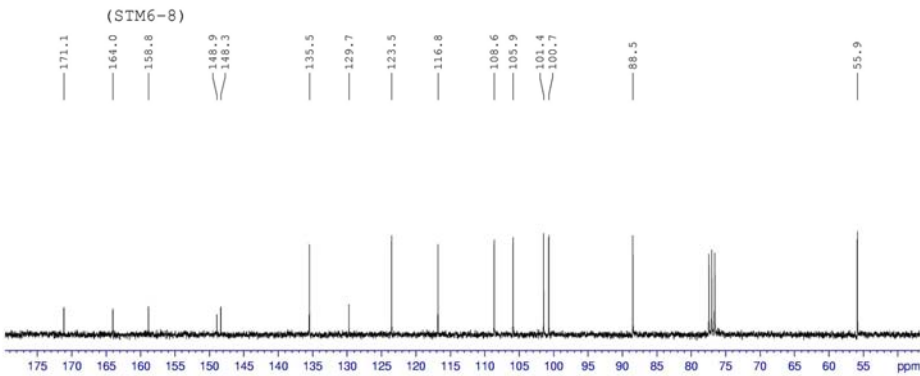


**15**



```

NAME      STM pyrone compd 14 6-8-1
EXPNO    1
PROCNO   1
Data_    20041123
Time     16.39
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SFO      5995.204 Hz
FIDRES   0.182959 Hz
AQ        2.7320011 sec
RG        362
SFO      83.400 MHz
DE        6.00 usec
TE        300.2 K
D1        0.10000000 sec
----- CHANNEL f1 -----
NUC1      1H
P1        9.30 usec
PL1       0.00 dB
SFO1     300.1315094 MHz
SI        16384
SF        300.1300009 MHz
WDW       EM
SSB       0
GB        0.10 Hz
CB        0
PC        0.40
    
```

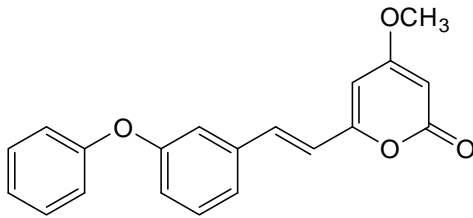


```

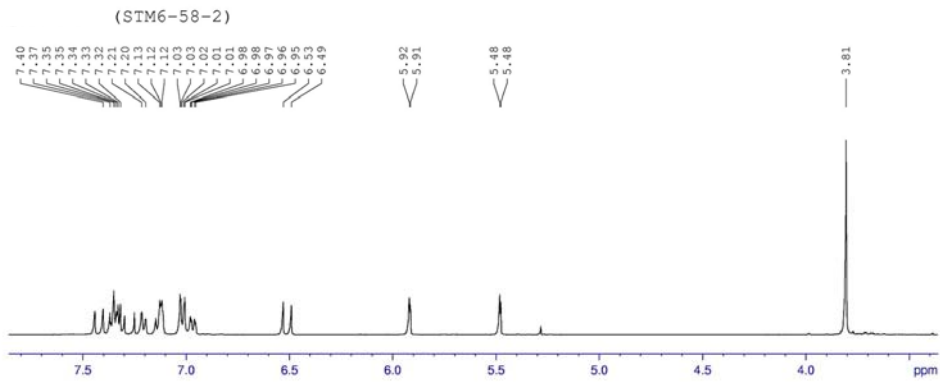
NAME      STM pyrone compd 14 6-8-1
EXPNO    1
PROCNO   1
Data_    20041123
Time     16.46
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        223
DS        0
SFO      17985.610 Hz
FIDRES   0.274439 Hz
AQ        1.8213000 sec
RG        6384
SFO      27.800 MHz
DE        20.00 usec
TE        300.2 K
D1        0.17500000 sec
D11       0.30000000 sec
d12       0.00000000 sec
----- CHANNEL f1 -----
NUC1      13C
P1        9.44 usec
PL1       0.00 dB
SFO1     75.4760973 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    180.00 usec
PL2      0.00 dB
PL12     20.00 dB
PL13     20.00 dB
SFO2     300.1312000 MHz
SI        22768
SF        75.4677510 MHz
WDW       EM
SSB       0
GB        1.00 Hz
CB        0
PC        1.00
    
```

**Pyrone 16**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .

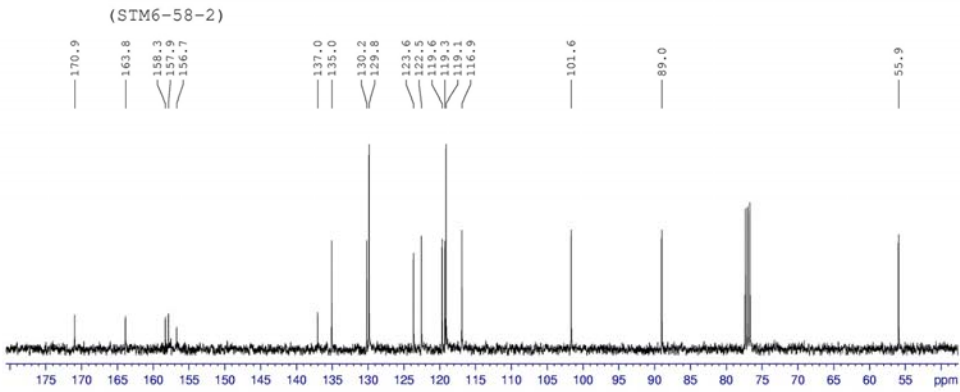


**16**



```

NAME      STM pyrone compd 15 6-58-2
EXPNO    2
PROCNO   1
Date_    20080311
Time     24.34
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zg30
TD        32768
SOLVENT  CDCl3
NS        14
DS        0
SHE      8012.020 Hz
FIDRES   0.244522 Hz
AQ        2.0447731 sec
RG        251.2
DM        62.400 usec
DE        6.50 usec
TE        300.2 K
D1        0.10000000 sec
----- CHANNEL f1 -----
NUC1      1H
P1        14.40 usec
PL1       2.20 dB
SFO1      400.1320007 MHz
SI        14384
SF        400.1300147 MHz
WDW       EM
SSB       0
LB        0.10 Hz
GB        0
PC        0.80
    
```

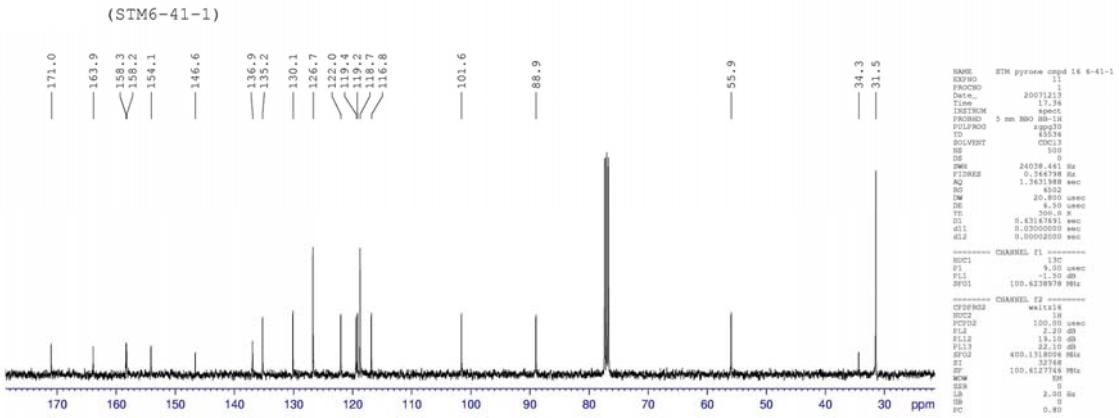
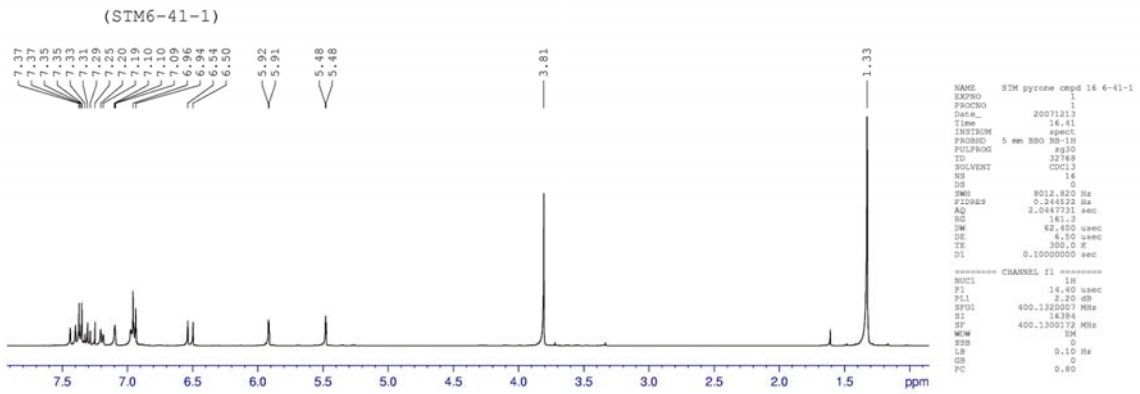
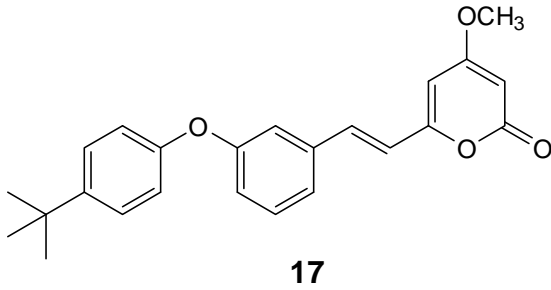


```

NAME      STM pyrone compd 15 6-58-2
EXPNO    2
PROCNO   1
Date_    20080311
Time     14.40
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD        4884
SOLVENT  CDCl3
NS        183
DS        0
SHE      24038.441 Hz
FIDRES   0.344788 Hz
AQ        1.2612388 sec
RG        1502
DM        20.800 usec
DE        6.50 usec
TE        300.2 K
D1        0.63154089 sec
d11      0.02000000 sec
d12      0.00002000 sec
----- CHANNEL f1 -----
NUC1      13C
P1        5.00 usec
PL1       -1.10 dB
SFO1      100.6238947 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    100.00 usec
PL2      2.20 dB
PL12     19.10 dB
PL13     22.10 dB
SFO2     400.1316000 MHz
SI        32768
SF        100.6127500 MHz
WDW       EM
SSB       0
LB        2.00 Hz
GB        0
PC        0.80
    
```

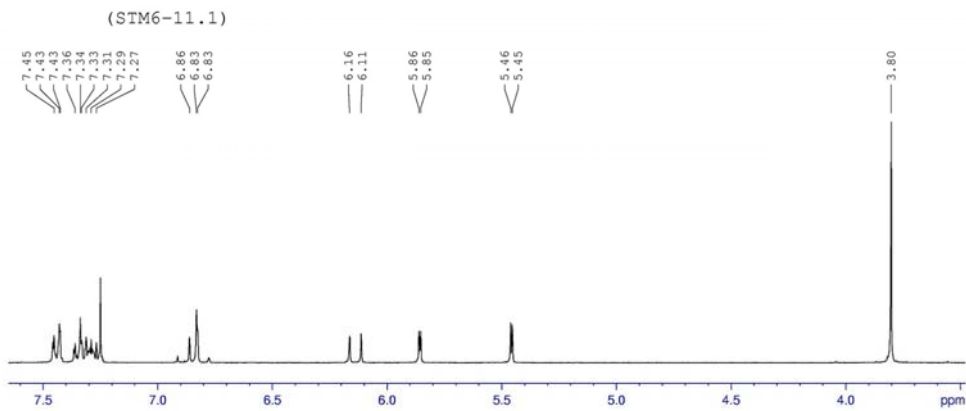
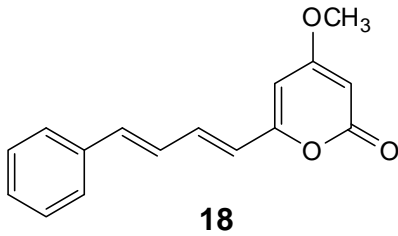
**Pyrone 17**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



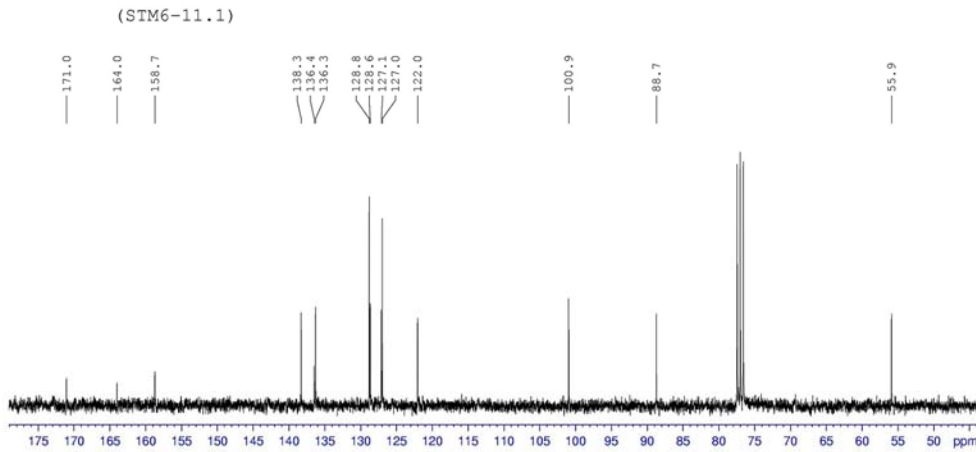
**Pyrone 18**

$^1\text{H}$  300 MHz,  $^{13}\text{C}$  75 MHz,  $\text{CDCl}_3$ .



```

NAME      STM pyrone cmpd 17 6-11-1
EXPNO    1
PROCNO   1
Date_    20061128
Time     15.38
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SWH       5990.204 Hz
F2RES    0.1192956 Hz
AQ        2.7329011 sec
RG        574.7
DW        83.400 usec
DE        4.00 usec
TE        300.0 K
D1        0.10000000 sec
===== CHANNEL f1 =====
NUC1      13C
P1        9.30 usec
PL1       0.00 dB
SFO1     300.1310006 MHz
SI        16384
SF        300.1300099 MHz
WDW       EM
SSB       0
LB        0.10 Hz
GB        0
PC        0.80
    
```



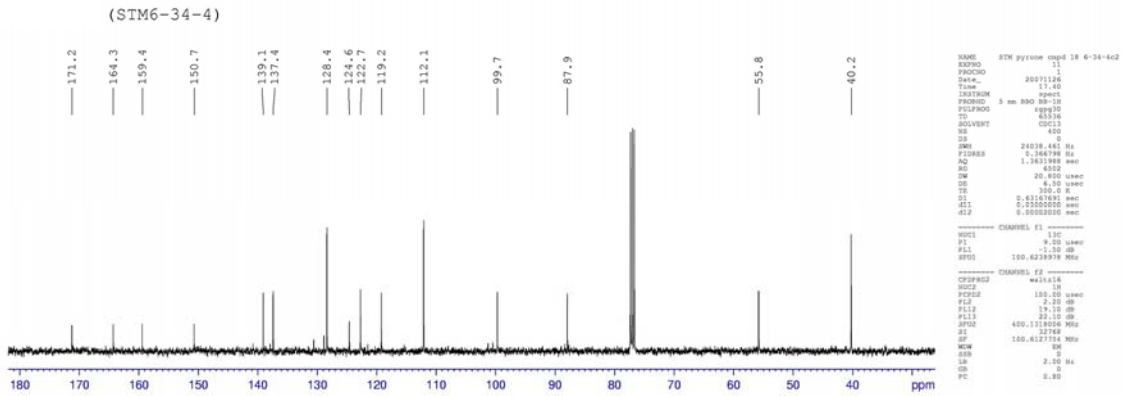
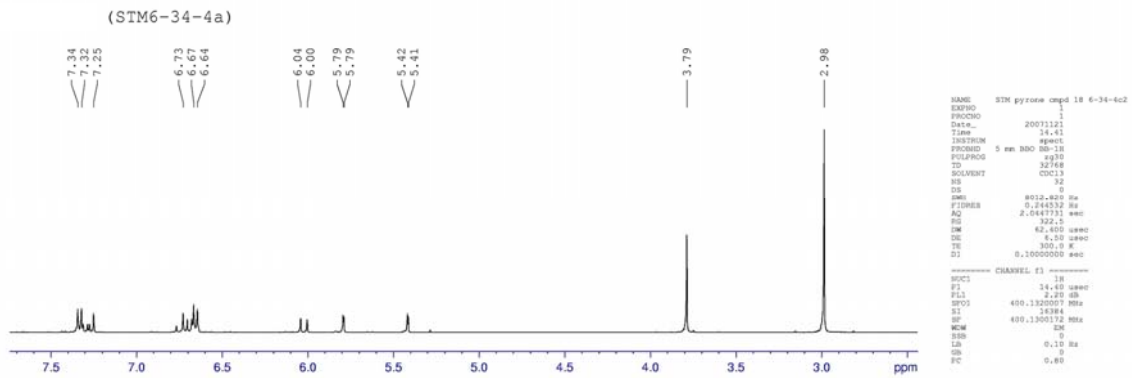
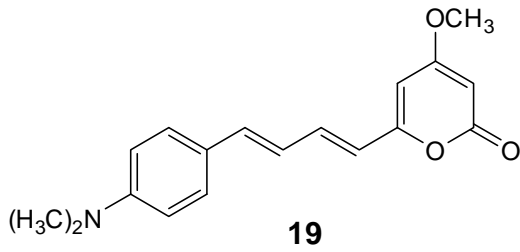
```

NAME      STM pyrone cmpd 17 6-11-1
EXPNO    1
PROCNO   1
Date_    20061127
Time     15.10
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        332
DS        0
SWH       17985.411 Hz
F2RES    0.274459 Hz
AQ        1.8219508 sec
RG        14284
DW        27.800 usec
DE        20.00 usec
TE        300.0 K
D1        0.1759371 sec
d11       0.03000000 sec
d12       0.00002000 sec
===== CHANNEL f1 =====
NUC1      13C
P1        9.14 usec
PL1       0.00 dB
SFO1     75.4760973 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    100.00 usec
PL2       0.00 dB
PL12     20.80 dB
PL13     24.49 dB
SFO2     300.1310005 MHz
SI        32768
SF        75.4677484 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
    
```



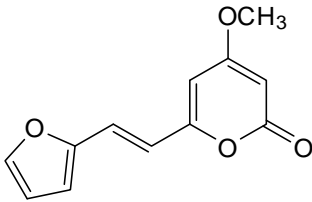
**Pyrone 19**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .

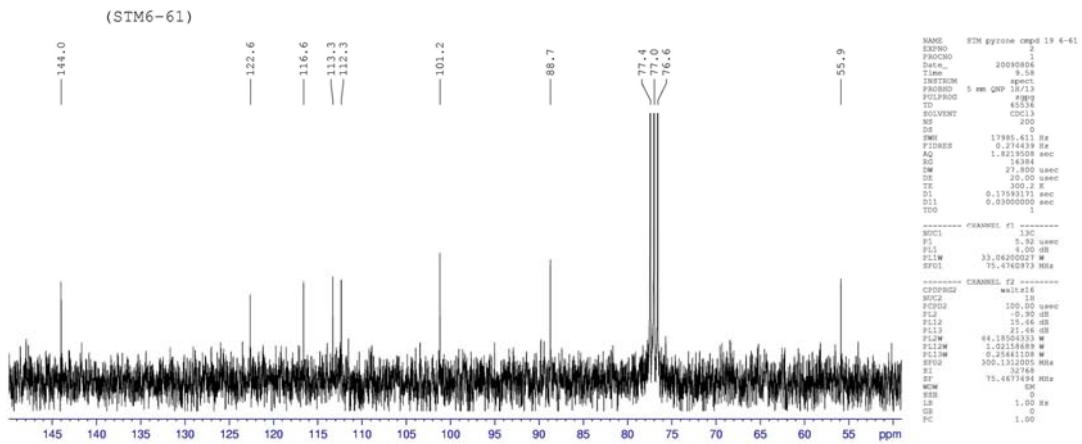
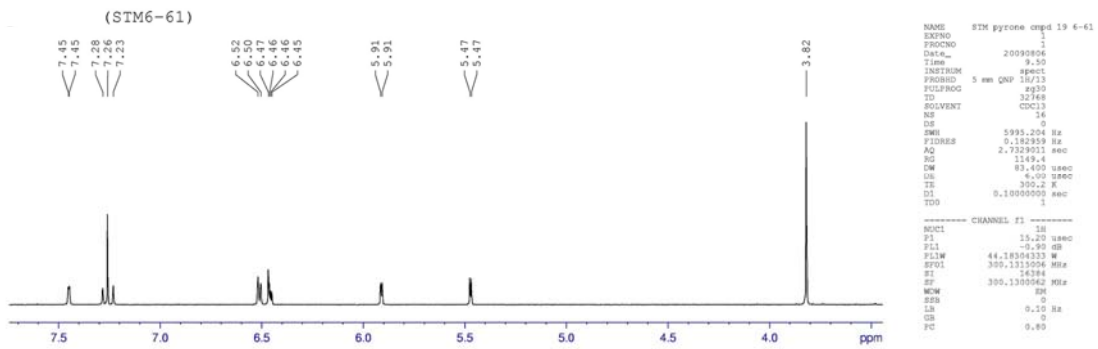


**Pyrone 20**

$^1\text{H}$  300 MHz,  $^{13}\text{C}$  75 MHz,  $\text{CDCl}_3$ .

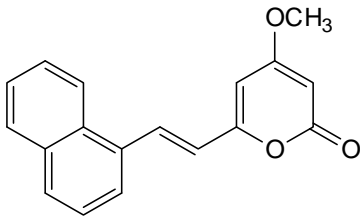


**20**

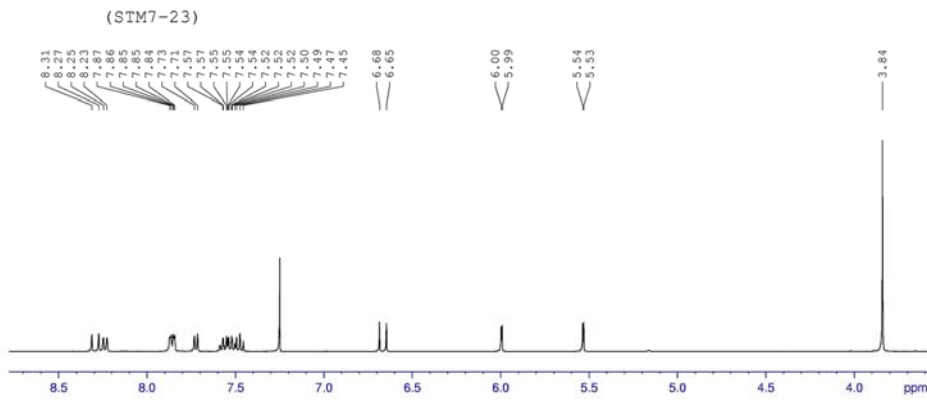


**Pyrone 21**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



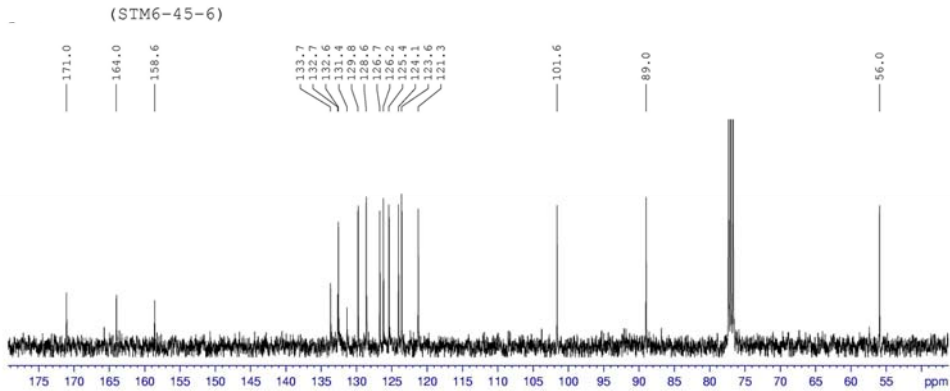
**21**



```

NAME STM pyrone cpd 20 6-45-6
EXPNO 1
PROCNO 1
Date_ 20080213
Time 15.58
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 445.1
DM 62.400 usec
DE 6.50 usec
TE 300.0 K
TL 0.1000000 sec
D1 0.1000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PL1 2.00 dB
SFO1 400.1320007 MHz
SI 16384
SF 400.1300177 MHz
WDW EM
SSB 0
LR 0.10 Hz
GB 0
PC 0.80
    
```



```

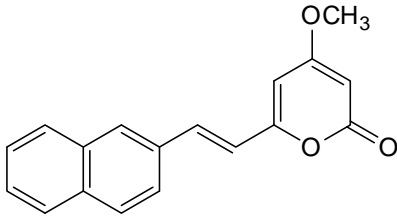
NAME STM pyrone cpd 20 6-45-6
EXPNO 1
PROCNO 1
Date_ 20080214
Time 22.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 650
DS 0
SWH 24039.441 Hz
FIDRES 0.244798 Hz
AQ 1.3431988 sec
RG 450
DM 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 0.4314743 sec
d11 0.0300000 sec
d12 0.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 1.50 dB
SFO1 100.6283970 MHz

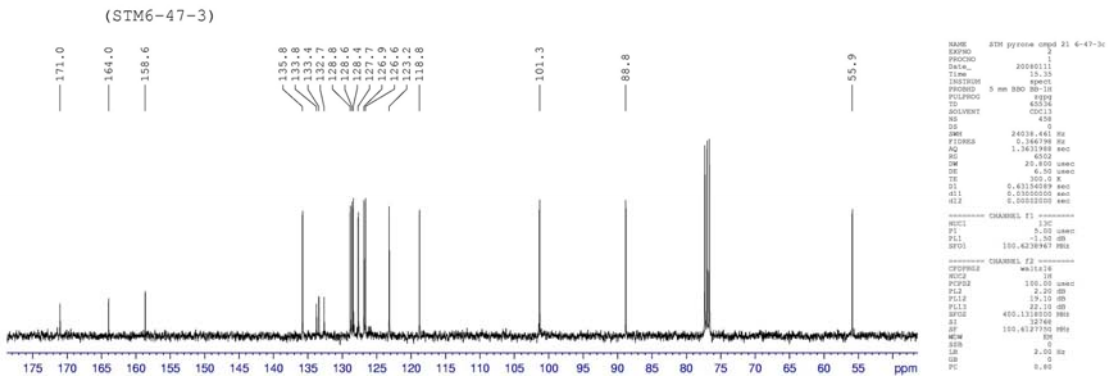
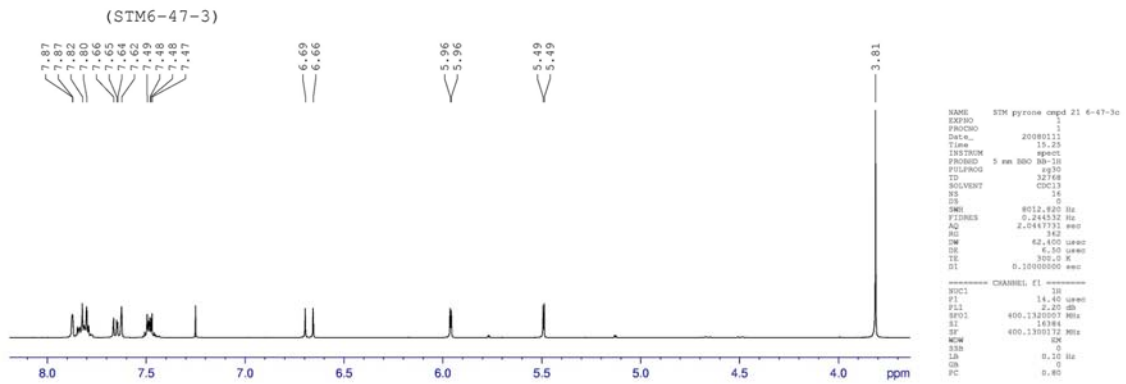
===== CHANNEL f2 =====
NUC2 1H
P2 100.00 usec
PL2 2.00 dB
PL12 19.10 dB
PL13 22.10 dB
SFO2 400.1318004 MHz
SI 32768
SF 100.6127724 MHz
WDW EM
SSB 0
LR 2.00 Hz
GB 0
PC 0.80
    
```

**Pyrone 22**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .

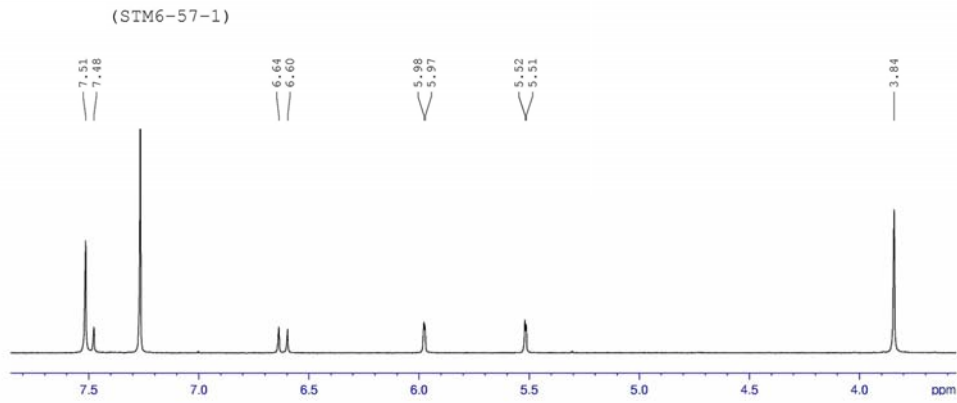
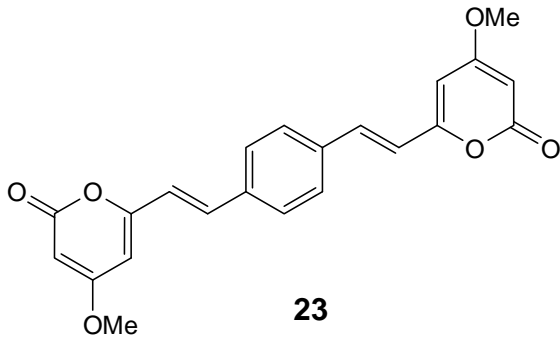


**22**



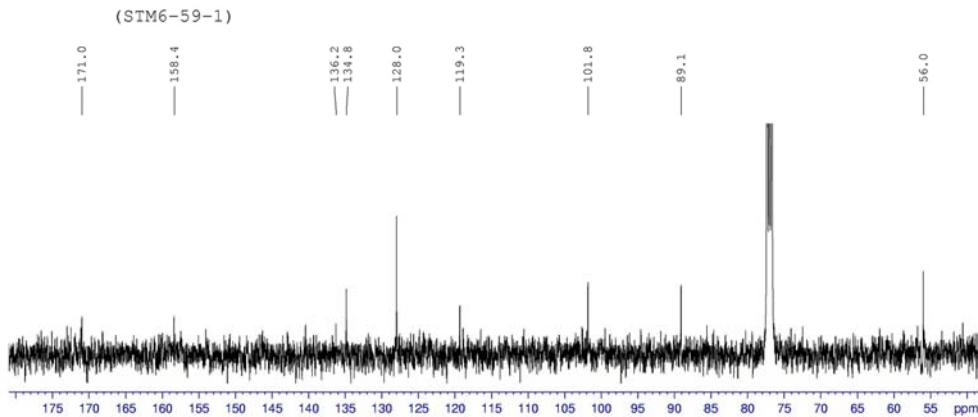
**Pyrone 23**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



```

NAME STM pyrone cmpd 22 6-57-1
EXPNO 10
PROCNO 1
DATE_ 20080214
Time 23.18
INSTRUM spect
PROBHD 5 mm BBO HP-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 0149.398 Hz
FIDRES 0.249327 Hz
AQ 2.0054513 sec
RG 512.3
DW 61.300 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PL1 2.00 dB
SFO1 400.1321007 MHz
SI 16384
SF 400.1300113 MHz
WWSW 0
SSB 0
LB 0.10 Hz
GB 0
PC 0.80
    
```

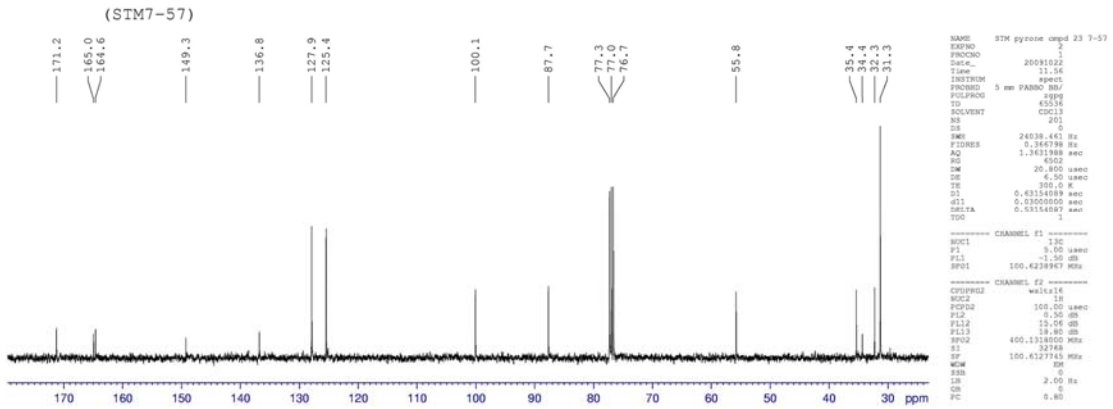
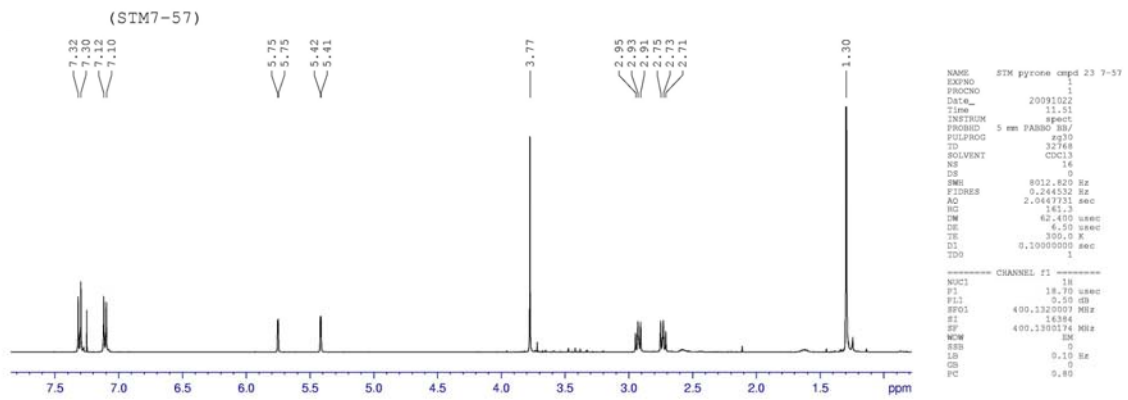
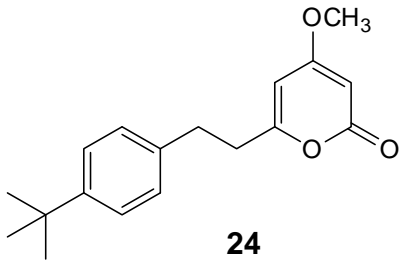


```

NAME STM pyrone cmpd 22b 6-59-1
EXPNO 21
PROCNO 1
DATE_ 20080220
Time 6.12
INSTRUM spect
PROBHD 5 mm BBO HP-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6500
DS 0
SWH 24030.461 Hz
FIDRES 0.366798 Hz
AQ 1.3431988 sec
RG 6502
DW 20.800 usec
DE 6.00 usec
TE 300.0 K
D1 0.63167691 sec
d11 0.03000000 sec
d12 0.00000000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -1.50 dB
SFO1 100.6218178 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 180.00 usec
PL2 2.00 dB
PL12 19.10 dB
PL13 22.10 dB
SFO2 400.1318004 MHz
SI 13768
SF 100.6217113 MHz
WWSW 0
SSB 0
LB 2.00 Hz
GB 0
PC 0.80
    
```

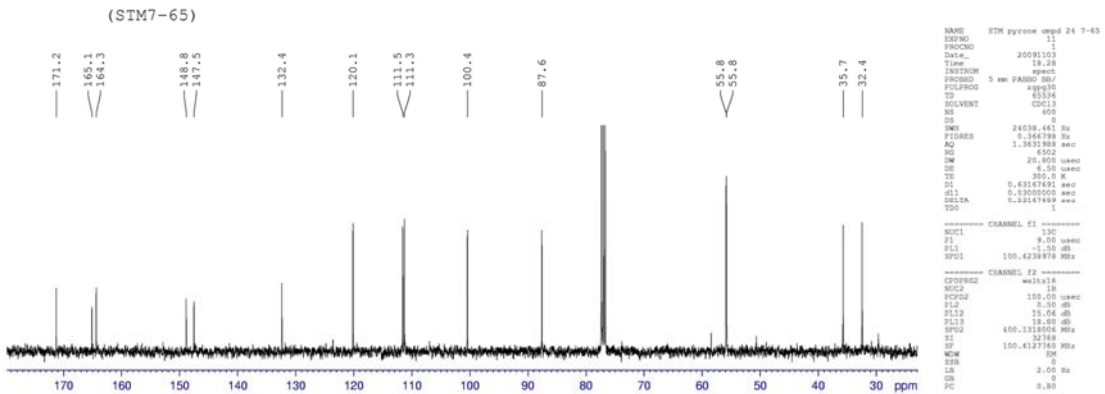
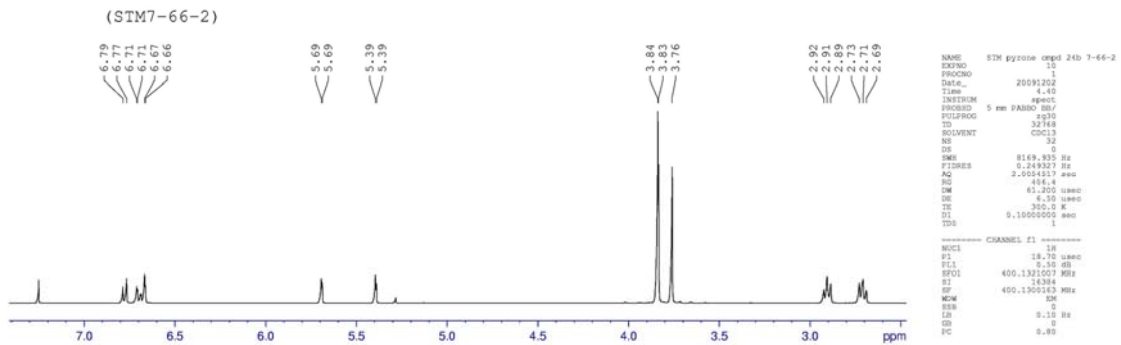
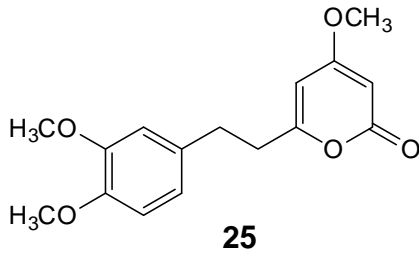
**Pyrone 24**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



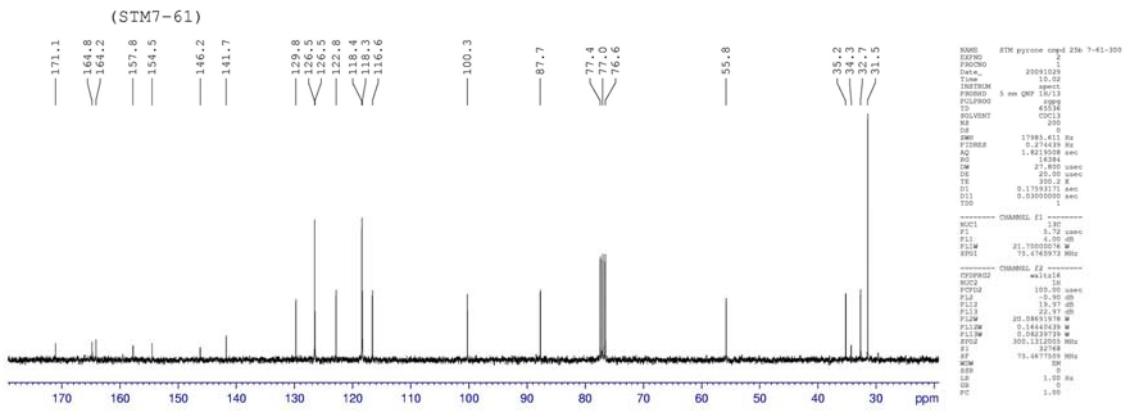
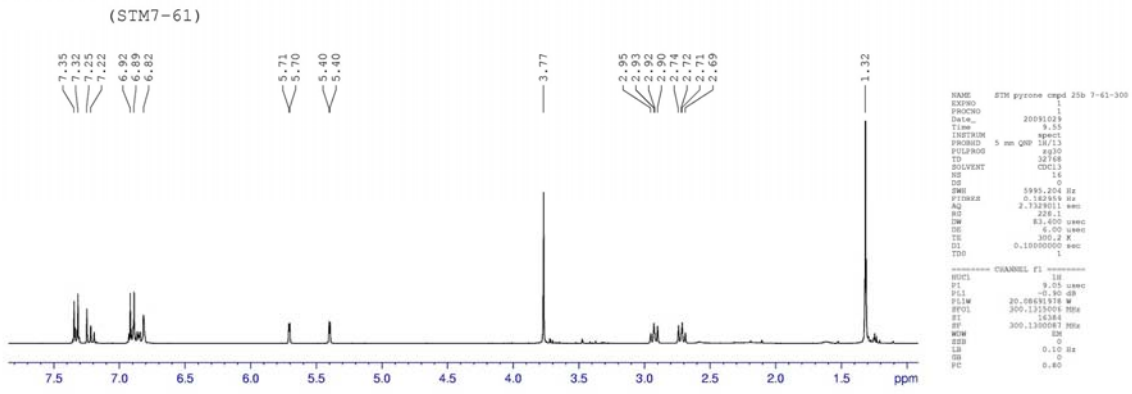
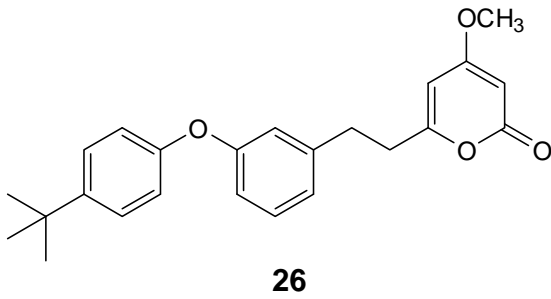
**Pyrone 25**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



**Pyrone 26**

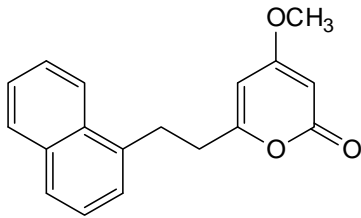
$^1\text{H}$  300 MHz,  $^{13}\text{C}$  75 MHz,  $\text{CDCl}_3$ .



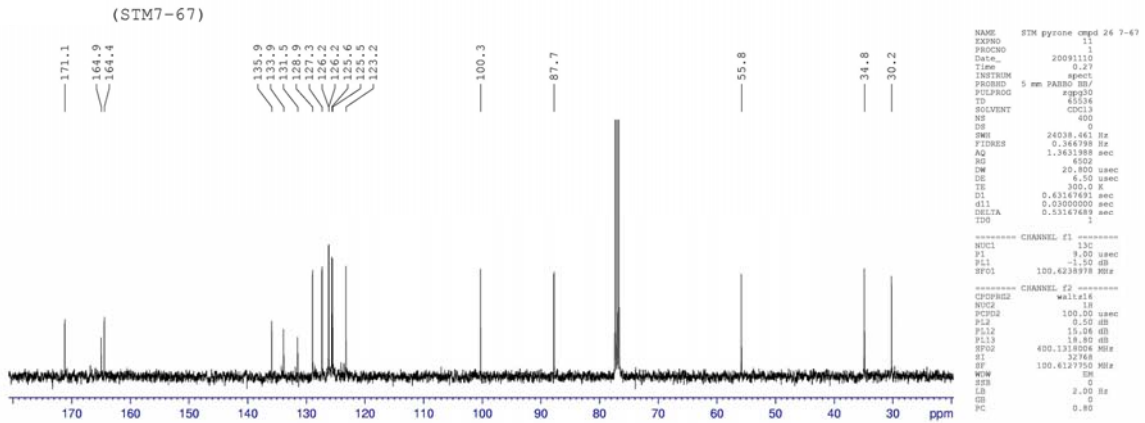
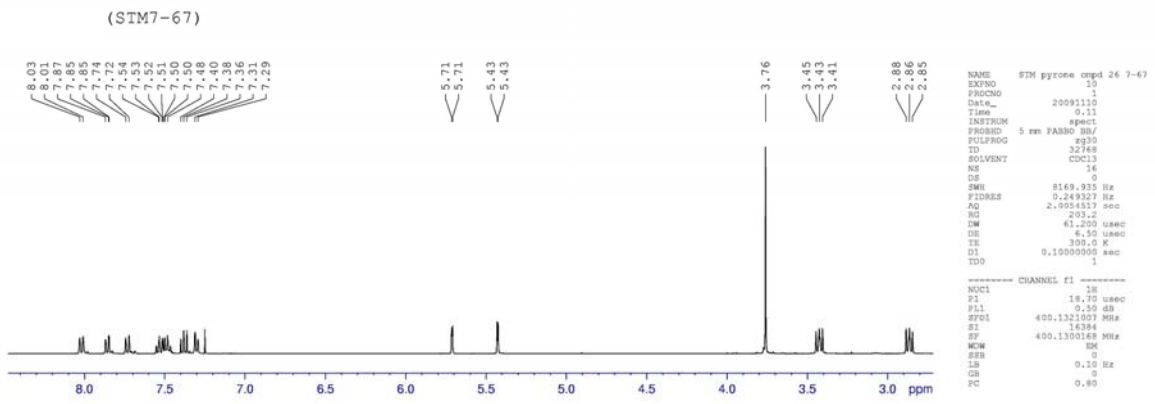


**Pyrone 27**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .

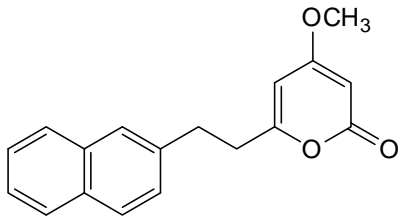


**27**



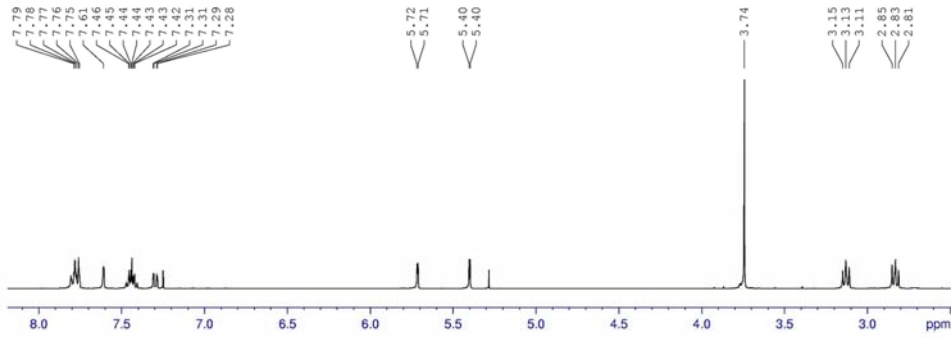
**Pyrone 28**

<sup>1</sup>H 400 MHz, <sup>13</sup>C 100 MHz, CDCl<sub>3</sub>.



**28**

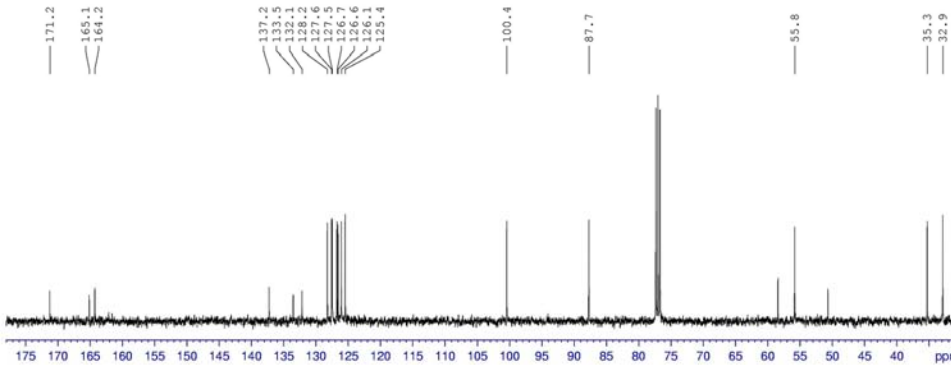
(SIM7-63-2)



```

NAME      STM pyrone comp 27b 7-63-2b
EXPNO    1
PROCNO   1
Date_    20091127
Time     14.54
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SWH       8012.820 Hz
FIDRES   0.244332 Hz
AQ        2.0147771 sec
RG         256
DM        62.400 usec
DE        6.50 usec
TE        300.0 K
D1        0.10000000 sec
TDO       1
----- CHANNEL f1 -----
NUC1      1H
P1        18.70 usec
PL1       0.00 dB
SFO1      400.1320000 MHz
SI        16384
SF         400.1300170 MHz
WDW       EM
SSB       0
LB        0.10 Hz
GB        0
PC        0.80
    
```

(SIM7-63)

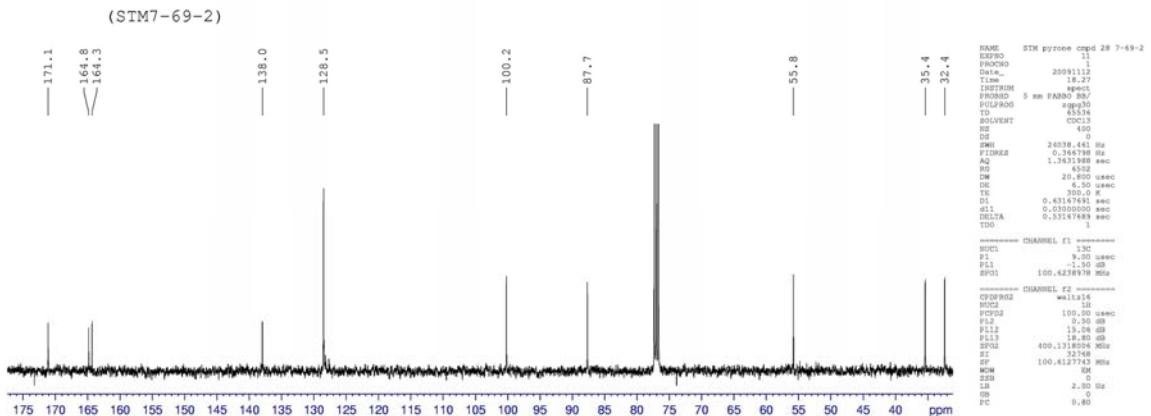
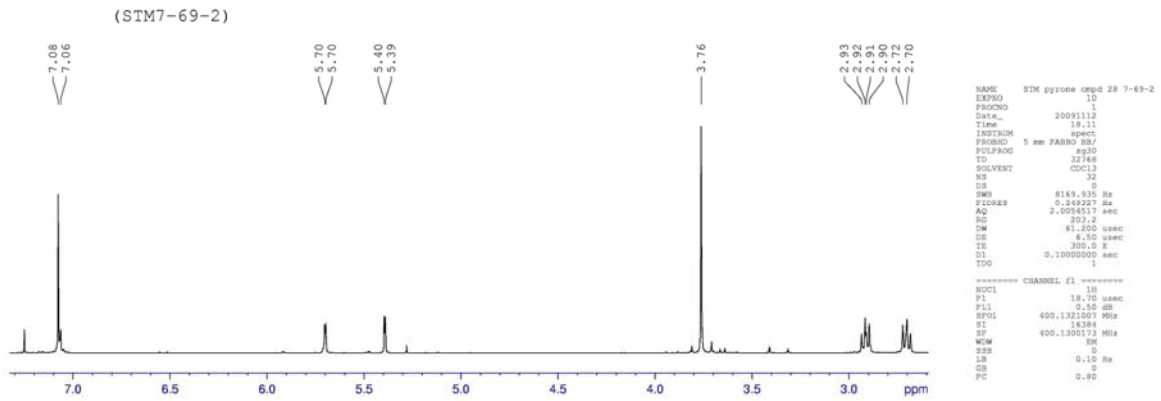
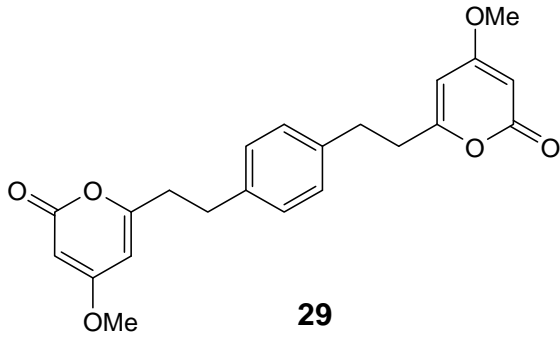


```

NAME      STM pyrone comp 27 7-63-2
EXPNO    2
PROCNO   1
Date_    20091105
Time     10.38
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        256
DS        0
SWH       24038.440 Hz
FIDRES   0.3449798 Hz
AQ        1.7401588 sec
RG         502
DM        20.400 usec
DE        6.50 usec
TE        300.0 K
D1        0.63154089 sec
d11       0.02000000 sec
DELTA    0.63154087 sec
TDO       1
----- CHANNEL f1 -----
NUC1      13C
P1        2.00 usec
PL1       -1.00 dB
SFO1      100.6288847 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    100.00 usec
PL2       0.10 dB
PL12     15.04 dB
PL13     18.80 dB
SFO2     400.1318000 MHz
SI        32768
SF        100.6127761 MHz
WDW       EM
SSB       0
LB        2.00 Hz
GB        0
PC        0.80
    
```

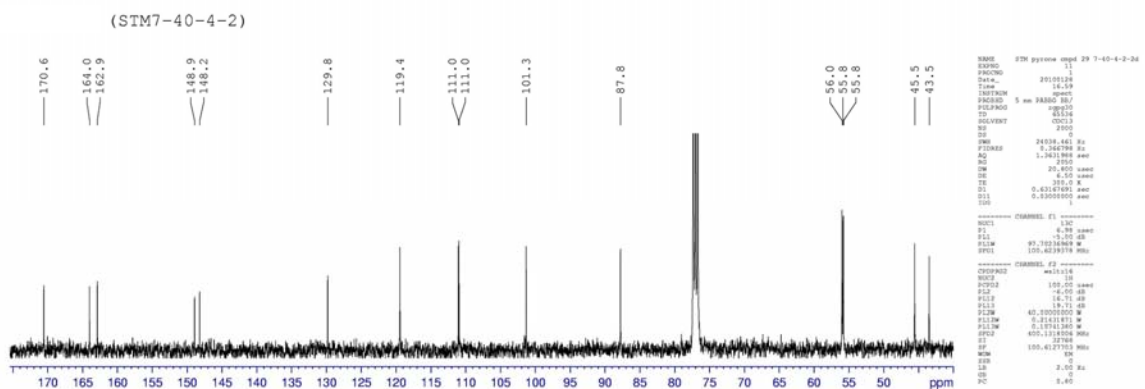
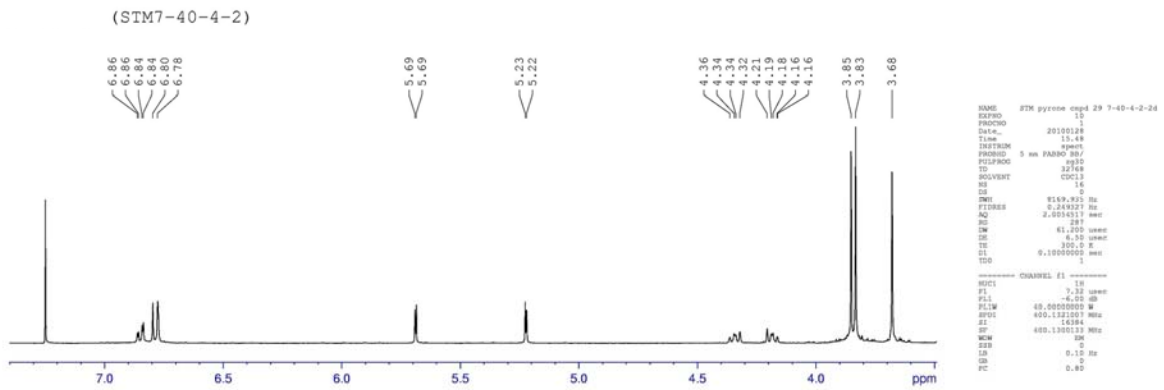
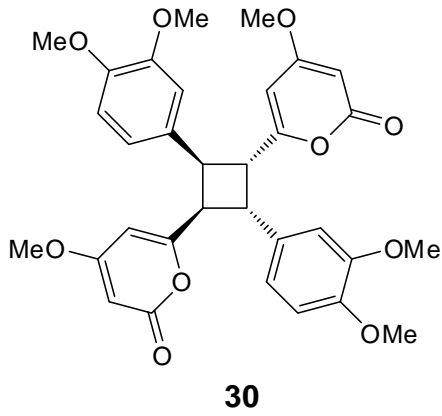
**Pyrone 29**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



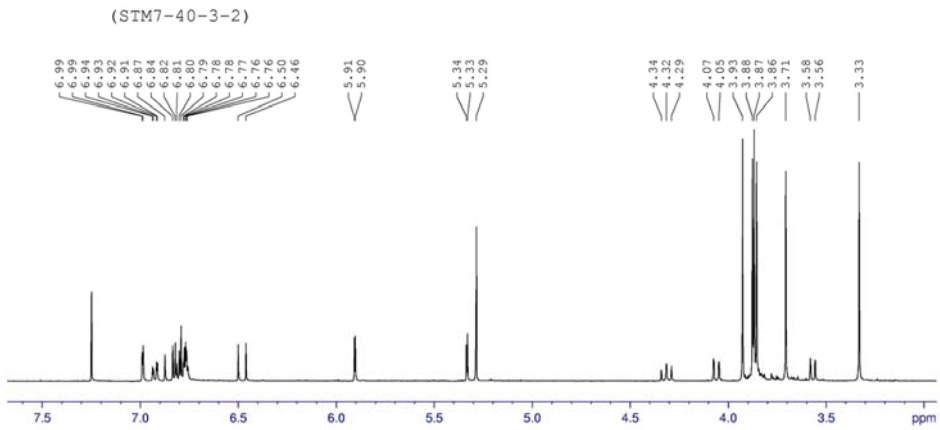
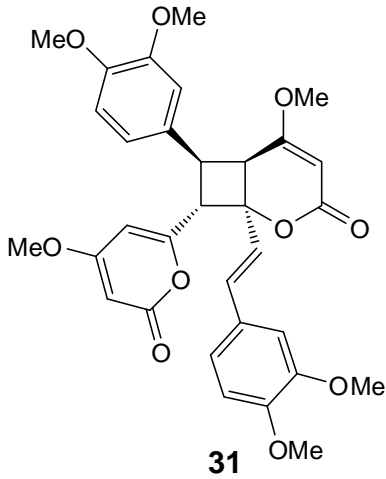
**Pyrone 30**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



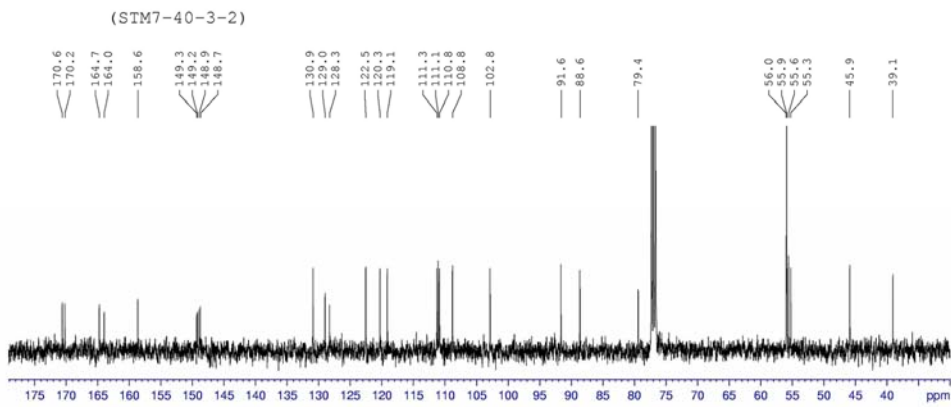
**Pyrone 31**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



```

NAME STM pyrone comp 30 7-40-3-2
EXPNO 1
PROCNO 1
Date_ 20091217
Time 16.33
INSTRUM spect
PROBHD 5 mm PABBO MM/
PULPROG zg30
TD 32768
SOLVENT CDCl3
SI 16
DS 0
SWH 8012.460 Hz
FIDRES 0.244532 Hz
AQ 2.0447771 sec
RG 642
DM 62.400 umec
DE 4.10 umec
TE 300.0 K
SI 0.10000000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 18.70 umec
PC1 0.10 dB
SFO1 400.1320007 MHz
SF 400.1300172 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 0.00
    
```

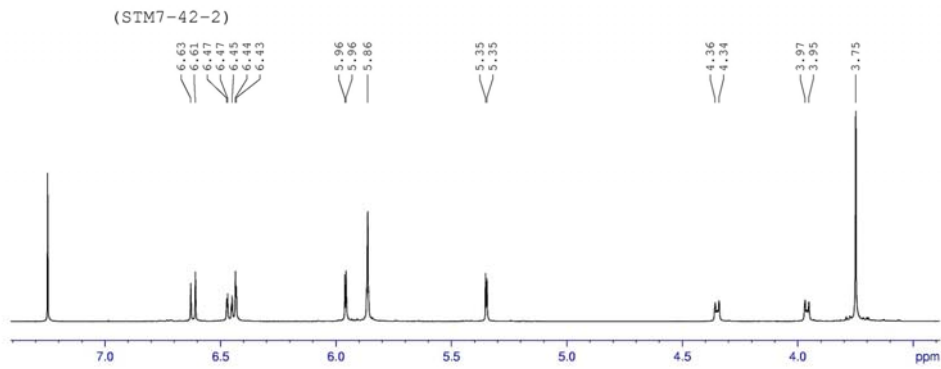
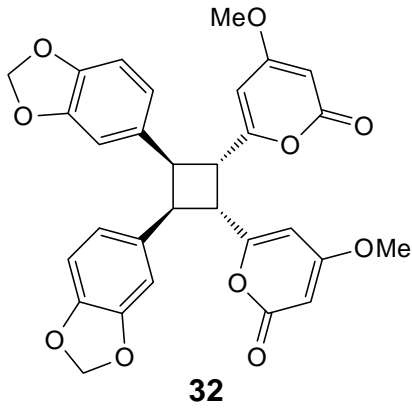


```

NAME STM pyrone comp 30 7-40-3-2
EXPNO 12
PROCNO 1
Date_ 20091221
Time 13.32
INSTRUM spect
PROBHD 5 mm PABBO MM/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
SI 192
DS 0
SWH 24038.460 Hz
FIDRES 0.248078 Hz
AQ 1.8619919 sec
RG 402
DM 20.800 umec
DE 6.30 umec
TE 300.0 K
SI 0.43140800 sec
d11 0.23000000 sec
SOLVA 1
TDS 1
----- CHANNEL f1 -----
NUC1 13C
P1 9.00 umec
PC1 1.10 dB
SFO1 100.6218894 MHz
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 180.00 umec
P112 0.25 dB
P112 19.08 dB
SFO2 400.1318000 MHz
SF 100.6127724 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 0.00
    
```

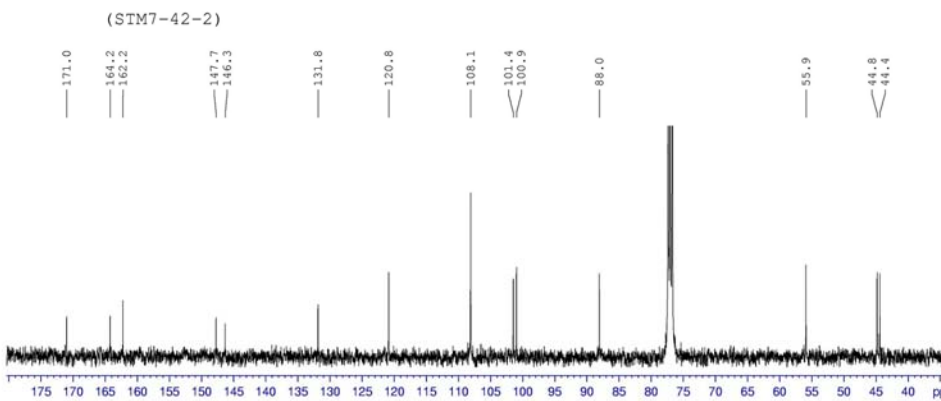
**Pyrone 32**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



```

NAME: STM pyrone cpd 31 7-42-2
EXPNO: 15
PROCNO: 20100204
Date_: 11.55
INSTRUM: spect
PROBHD: 5 mm PABBO BB/
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 8169.935 Hz
FIDRES: 0.249327 Hz
AQ: 2.004511 sec
RG: 322
DM: 61.000 usec
DE: 6.50 usec
TE: 300.2 K
D1: 0.1000000 sec
TD0: 1
----- CHANNEL f1 -----
NUC1: 1H
P1: 7.32 usec
PC1: -4.00 dB
PL1W: 40.0000000 W
SFO1: 400.132001 MHz
SI: 16384
SF: 400.130019 MHz
MCW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 0.80
    
```

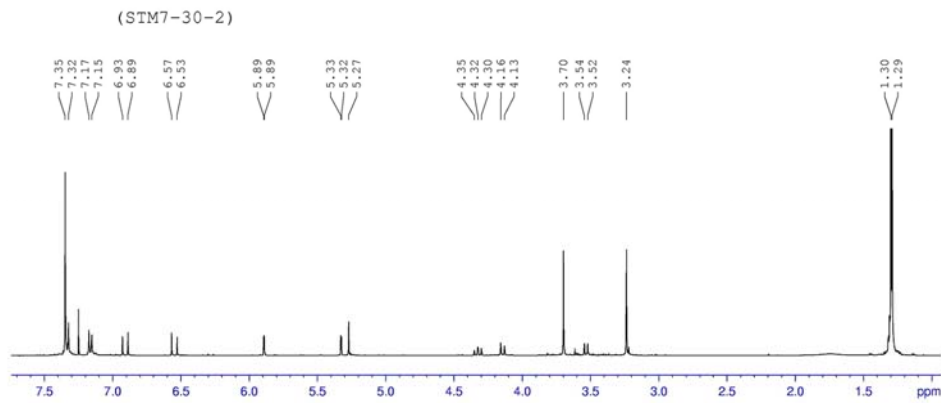
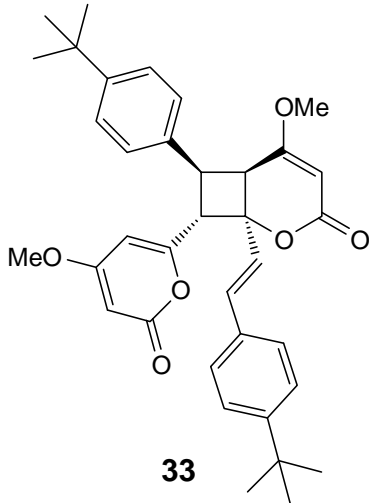


```

NAME: STM pyrone cpd 31 7-42-2
EXPNO: 15
PROCNO: 20100204
Date_: 11.55
INSTRUM: spect
PROBHD: 5 mm PABBO BB/
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 2000
DS: 0
SWH: 26038.48 Hz
FIDRES: 0.346798 Hz
AQ: 1.363398 sec
RG: 1024
DM: 20.000 usec
DE: 6.50 usec
TE: 300.2 K
D1: 0.4318761 sec
D11: 0.0300000 sec
TD0: 1
----- CHANNEL f1 -----
NUC1: 13C
P1: 6.38 usec
PC1: -5.00 dB
PL1W: 99.70276943 W
SFO1: 100.6293978 MHz
----- CHANNEL f2 -----
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 usec
P2: -6.00 dB
PL2: 16.71 dB
PL2W: 19.31 dB
PL3W: 40.0000000 W
SFO2: 0.1434871 MHz
PL3W: 0.10741381 W
SFO3: 400.1318024 MHz
SI: 16384
SF: 100.6127702 MHz
SSB: 0
LB: 2.00 Hz
GB: 0
PC: 0.80
    
```

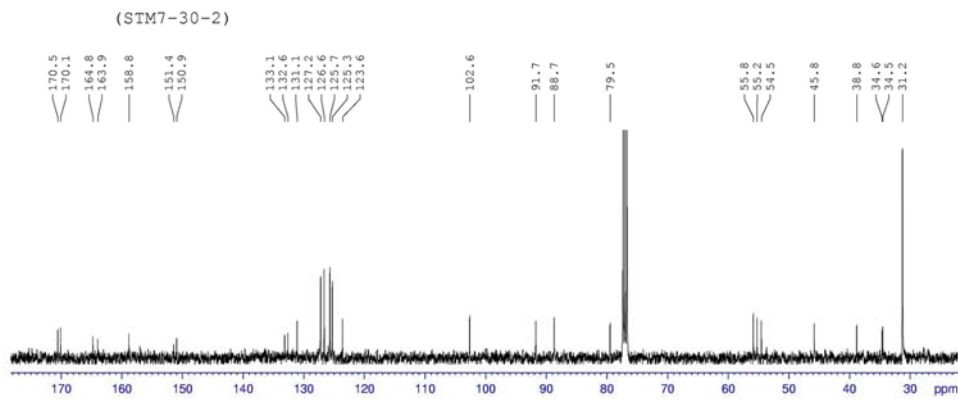
**Pyrone 33**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



```

NAME      SIM pyrone cpd 32 7-30-2
EXPNO    20
PROCNO   1
Date_    20100212
Time     12.39
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        32768
DS        4
SWH       8169.935 Hz
FIDRES   0.249327 Hz
AQ        4.1000001 sec
RG        181
DW        61.200 usec
DE        6.50 usec
TE        300.2 K
D1        0.1000000 sec
D11       1
D12       1
----- CHANNEL f1 -----
NUC1      1H
P1        7.22 usec
PL1       -6.00 dB
PULPROG  zgpg30
SFO1      400.132001 MHz
SI        16384
SF        400.1300139 MHz
WDW       EM
SSB       0
LB        0.10 Hz
GB        0
PC        0.80
    
```

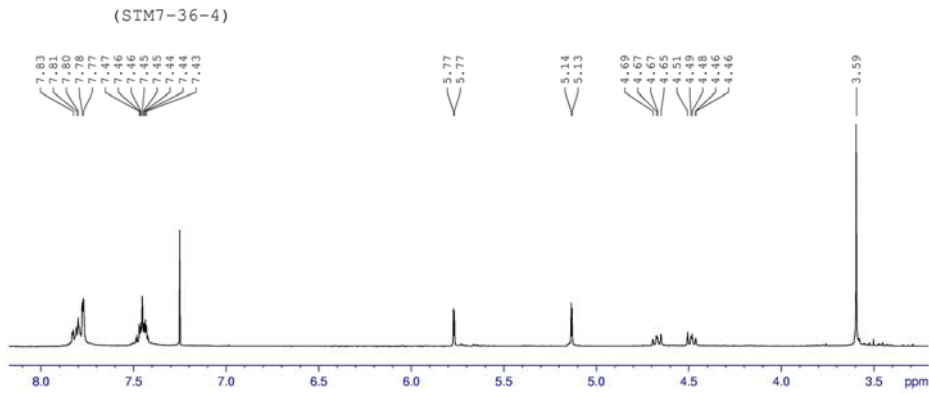
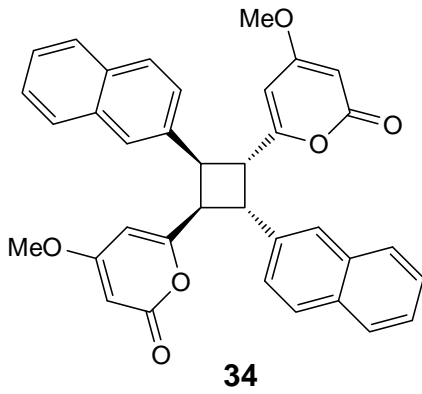


```

NAME      SIM pyrone cpd 32 7-30-2
EXPNO    11
PROCNO   1
Date_    20100212
Time     12.46
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        320
DS        4
SWH       24039.441 Hz
FIDRES   0.244798 Hz
AQ        1.3631988 sec
RG        2500
DW        20.800 usec
DE        6.50 usec
TE        300.2 K
D1        0.4316180 sec
D11       0.0300000 sec
D12       1
D13       1
----- CHANNEL f1 -----
NUC1      13C
P1        4.28 usec
PL1       -5.00 dB
PULPROG  zgpg30
SFO1      100.6263849 MHz
SI        100.6233378 MHz
SF        100.6233378 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPDPRG2 100.00 usec
PL2       -4.00 dB
PL12      14.71 dB
PL13      14.71 dB
PL14      14.71 dB
PL15      14.71 dB
PL16      14.71 dB
PL17      14.71 dB
PL18      14.71 dB
PL19      14.71 dB
PL20      14.71 dB
PL21      14.71 dB
PL22      14.71 dB
PL23      14.71 dB
PL24      14.71 dB
PL25      14.71 dB
PL26      14.71 dB
PL27      14.71 dB
PL28      14.71 dB
PL29      14.71 dB
PL30      14.71 dB
PL31      14.71 dB
PL32      14.71 dB
PL33      14.71 dB
PL34      14.71 dB
PL35      14.71 dB
PL36      14.71 dB
PL37      14.71 dB
PL38      14.71 dB
PL39      14.71 dB
PL40      14.71 dB
PL41      14.71 dB
PL42      14.71 dB
PL43      14.71 dB
PL44      14.71 dB
PL45      14.71 dB
PL46      14.71 dB
PL47      14.71 dB
PL48      14.71 dB
PL49      14.71 dB
PL50      14.71 dB
PL51      14.71 dB
PL52      14.71 dB
PL53      14.71 dB
PL54      14.71 dB
PL55      14.71 dB
PL56      14.71 dB
PL57      14.71 dB
PL58      14.71 dB
PL59      14.71 dB
PL60      14.71 dB
PL61      14.71 dB
PL62      14.71 dB
PL63      14.71 dB
PL64      14.71 dB
PL65      14.71 dB
PL66      14.71 dB
PL67      14.71 dB
PL68      14.71 dB
PL69      14.71 dB
PL70      14.71 dB
PL71      14.71 dB
PL72      14.71 dB
PL73      14.71 dB
PL74      14.71 dB
PL75      14.71 dB
PL76      14.71 dB
PL77      14.71 dB
PL78      14.71 dB
PL79      14.71 dB
PL80      14.71 dB
PL81      14.71 dB
PL82      14.71 dB
PL83      14.71 dB
PL84      14.71 dB
PL85      14.71 dB
PL86      14.71 dB
PL87      14.71 dB
PL88      14.71 dB
PL89      14.71 dB
PL90      14.71 dB
PL91      14.71 dB
PL92      14.71 dB
PL93      14.71 dB
PL94      14.71 dB
PL95      14.71 dB
PL96      14.71 dB
PL97      14.71 dB
PL98      14.71 dB
PL99      14.71 dB
PL100     14.71 dB
    
```

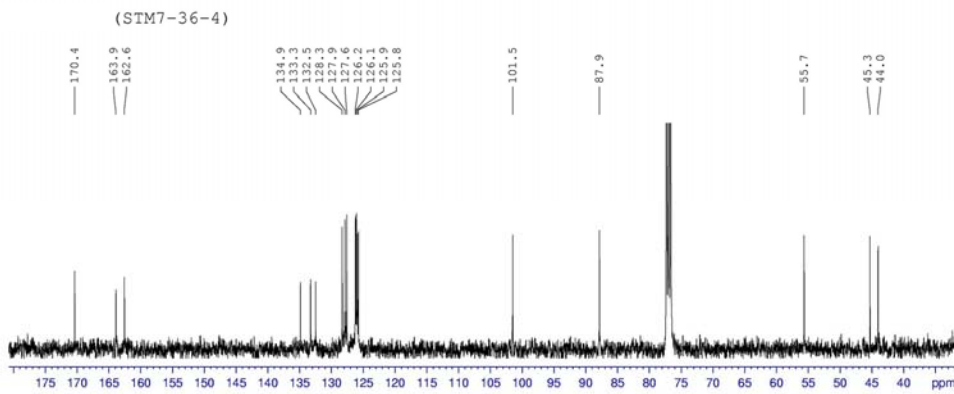
**Pyrone 34**

$^1\text{H}$  400 MHz,  $^{13}\text{C}$  100 MHz,  $\text{CDCl}_3$ .



```

NAME      STM pyrone cpd 33 7-36-4
EXPNO    1
PROCNO   1
Date_    20100208
Time     20.38
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        32
DS        0
SWH       8169.935 Hz
FIDRES   0.249327 Hz
AQ        2.0054517 sec
RG         257
SW        41.200 usec
DE        6.50 usec
TE        300.2 K
D1        0.10000000 sec
TDO       1
===== CHANNEL f1 =====
NUC1      1H
P1        7.12 usec
PL1       -6.00 dB
PL12      40.0000000 W
SFO1      400.1321007 MHz
SI        43984
SF        400.1320138 MHz
MCW       0
SE        0
LB        0.10 Hz
GB        0
PC        0.80
    
```



```

NAME      STM pyrone cpd 33 7-36-4
EXPNO    1
PROCNO   1
Date_    20100208
Time     21.48
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        2000
DS        0
SWH       24938.461 Hz
FIDRES   0.184578 Hz
AQ        1.3431988 sec
RG         250
SW        20.800 usec
DE        6.50 usec
TE        300.2 K
D1        0.6387891 sec
D11       0.03000000 sec
TDO       1
===== CHANNEL f1 =====
NUC1      13C
P1        8.88 usec
PL1       -6.00 dB
PL12      97.70236369 W
SFO1      100.6239378 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    100.00 usec
PL2      16.00 dB
PL12     16.01 dB
PL13     16.01 dB
PL14     16.01 dB
PL15     16.01 dB
PL16     16.01 dB
PL17     16.01 dB
PL18     16.01 dB
PL19     16.01 dB
PL20     16.01 dB
SFO2     400.1320138 MHz
SI        37768
SF        100.6127705 MHz
MCW       0
SE        0
LB        2.00 Hz
GB        0
PC        0.80
    
```



