Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

SUPPORTING INFORMATION

Advanced and novel one-pot synthetic method for diverse benzo[*c*[chromen-6-ones by transition-metal free mild base-promoted domino reactions of substituted 2-hydroxychalcones with β-ketoesters and its application to polysubstituted terphenyls

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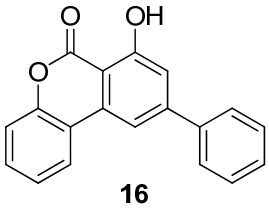

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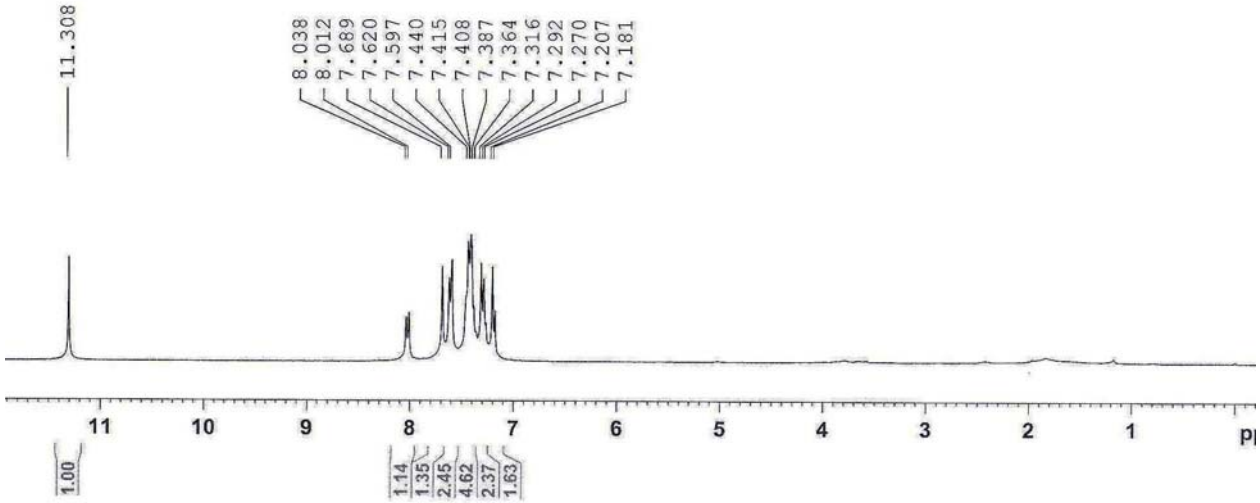

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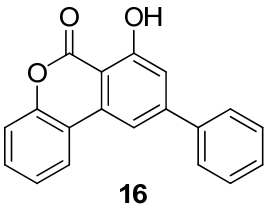

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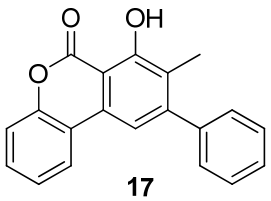

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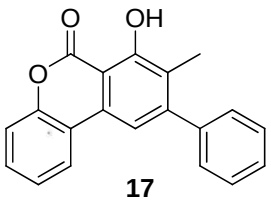

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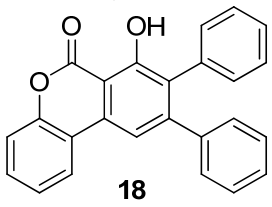

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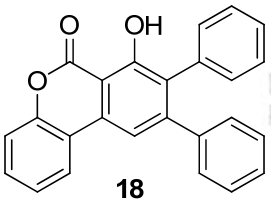

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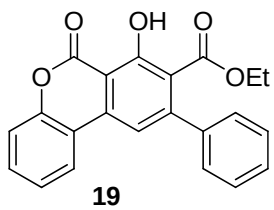

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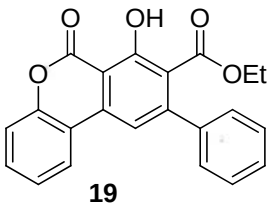

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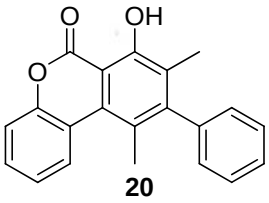

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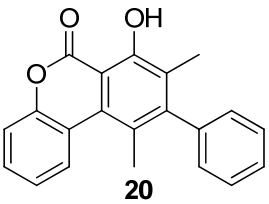

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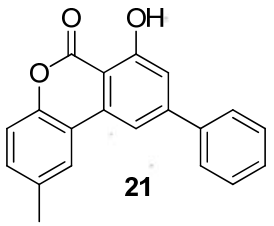

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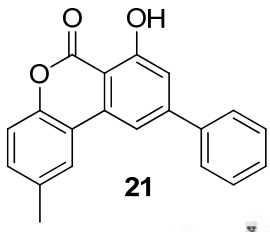

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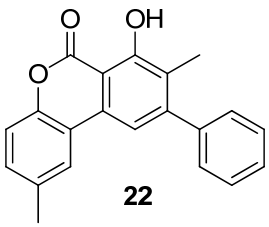

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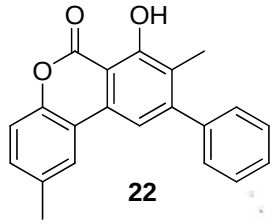

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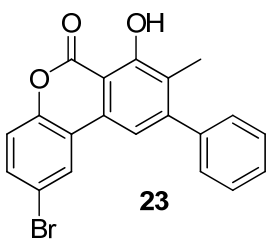

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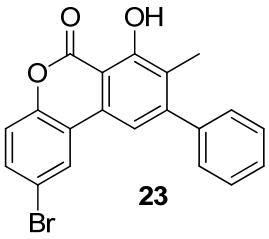

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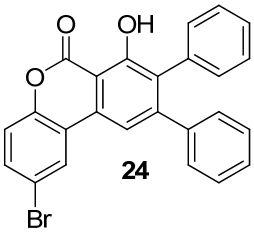

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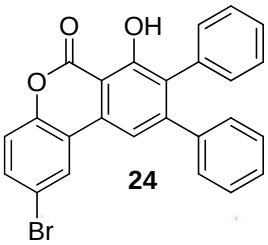

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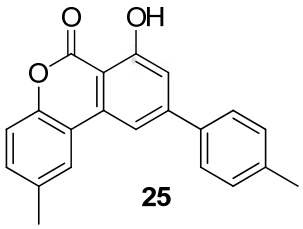

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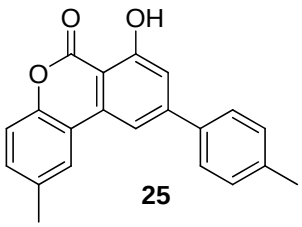

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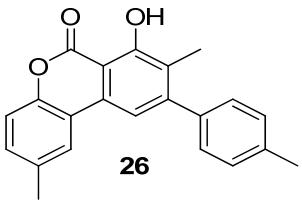

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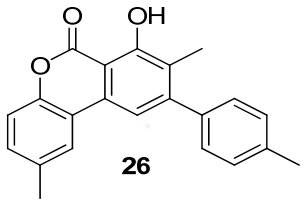

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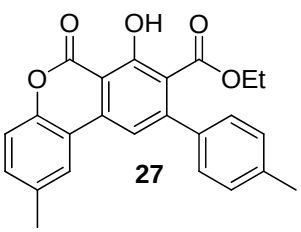

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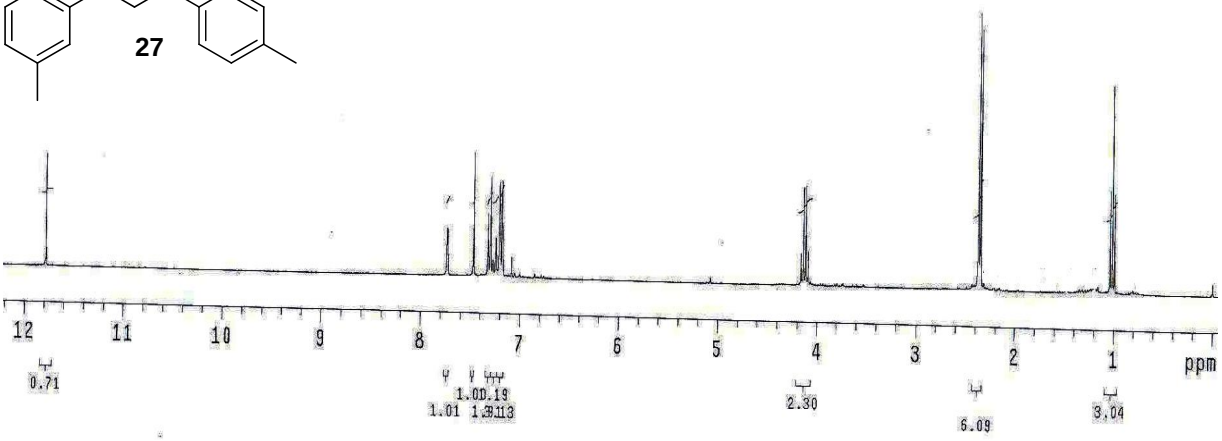

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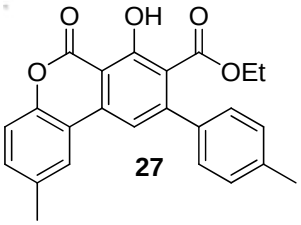

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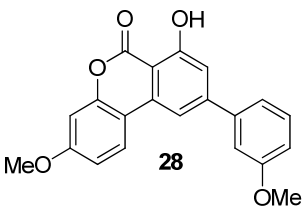

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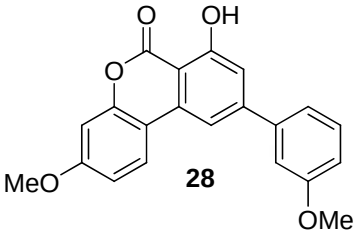

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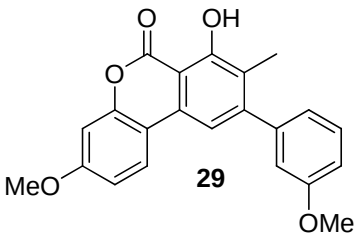

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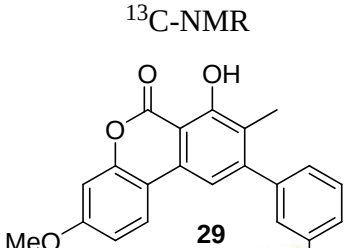

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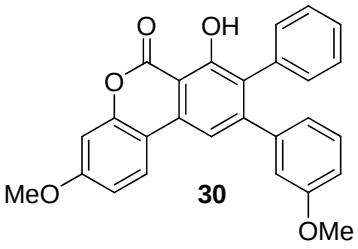

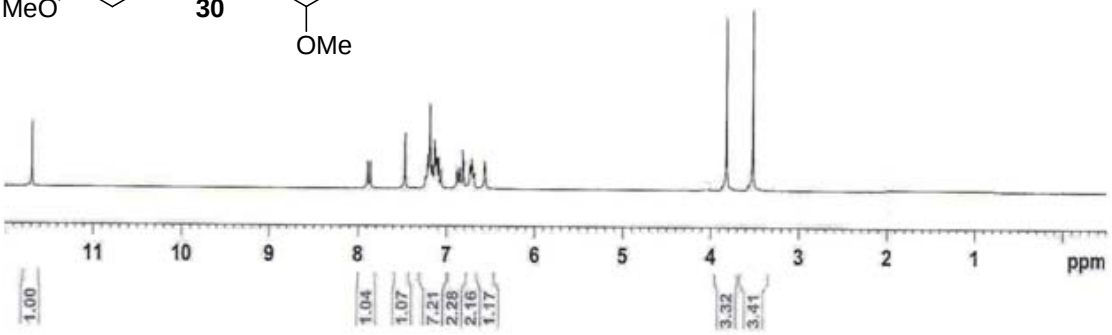

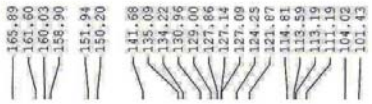

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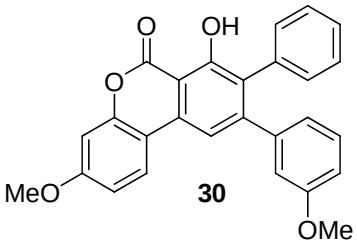

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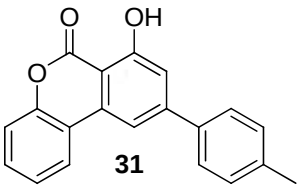

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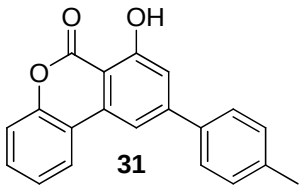

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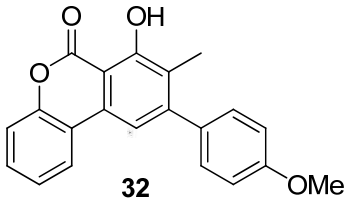

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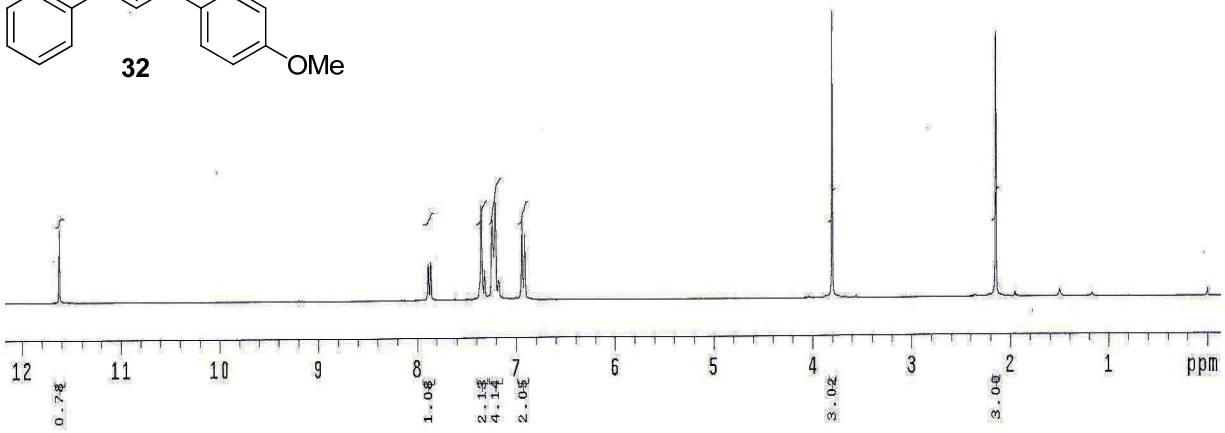

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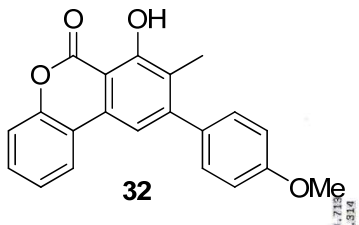

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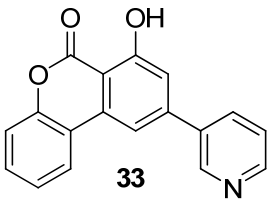

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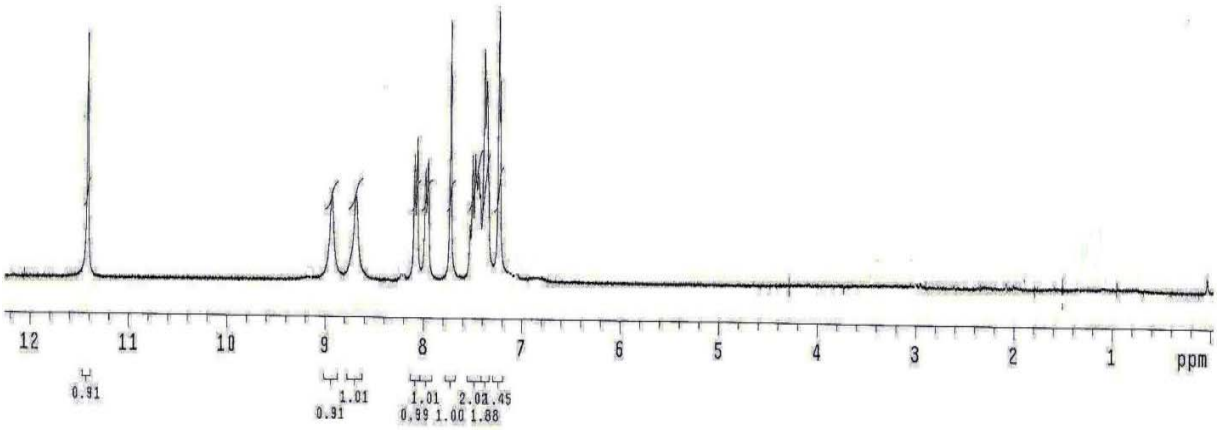

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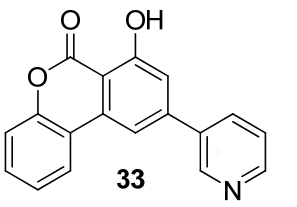

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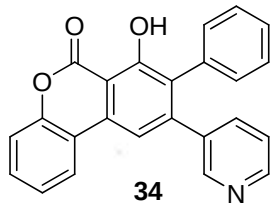

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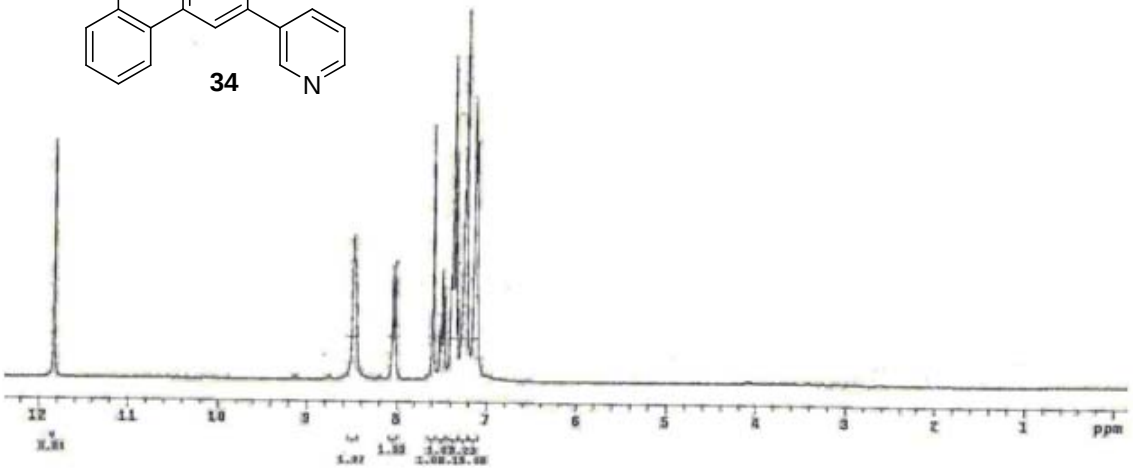

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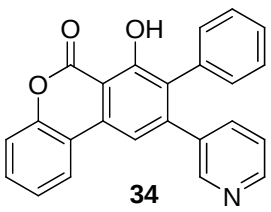

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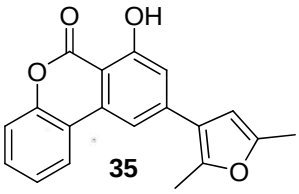

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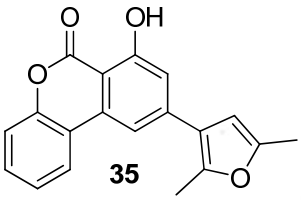

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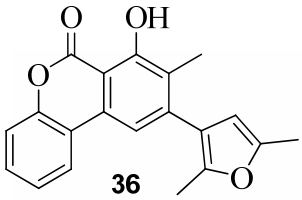

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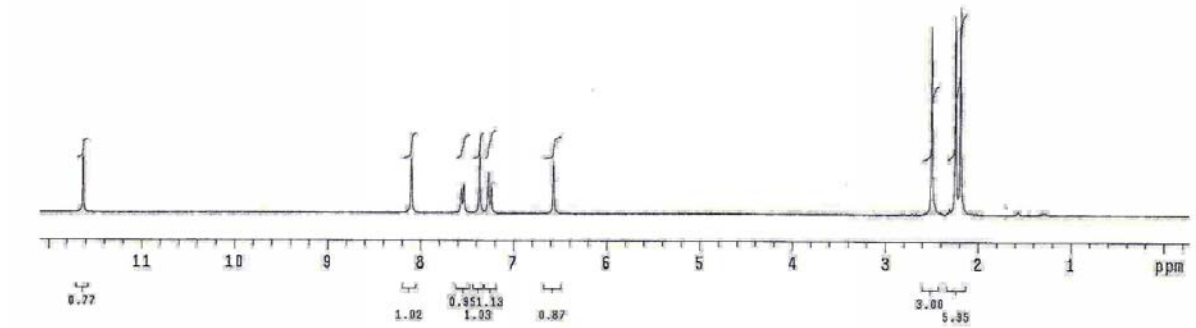

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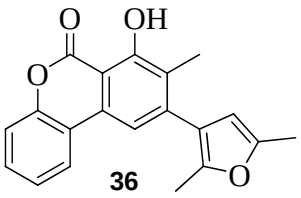

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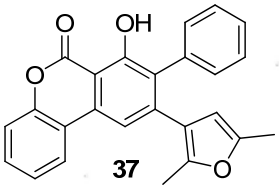

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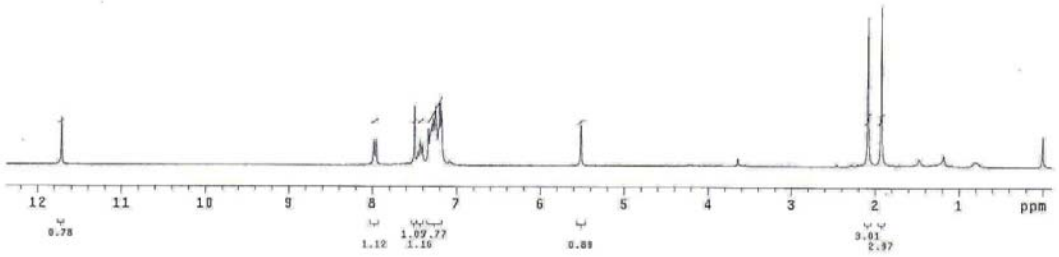

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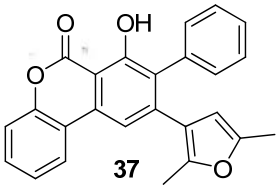

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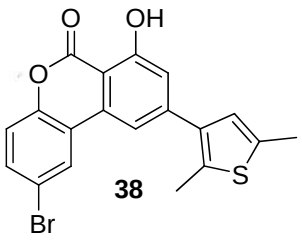

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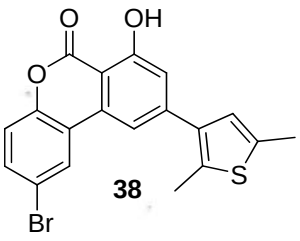

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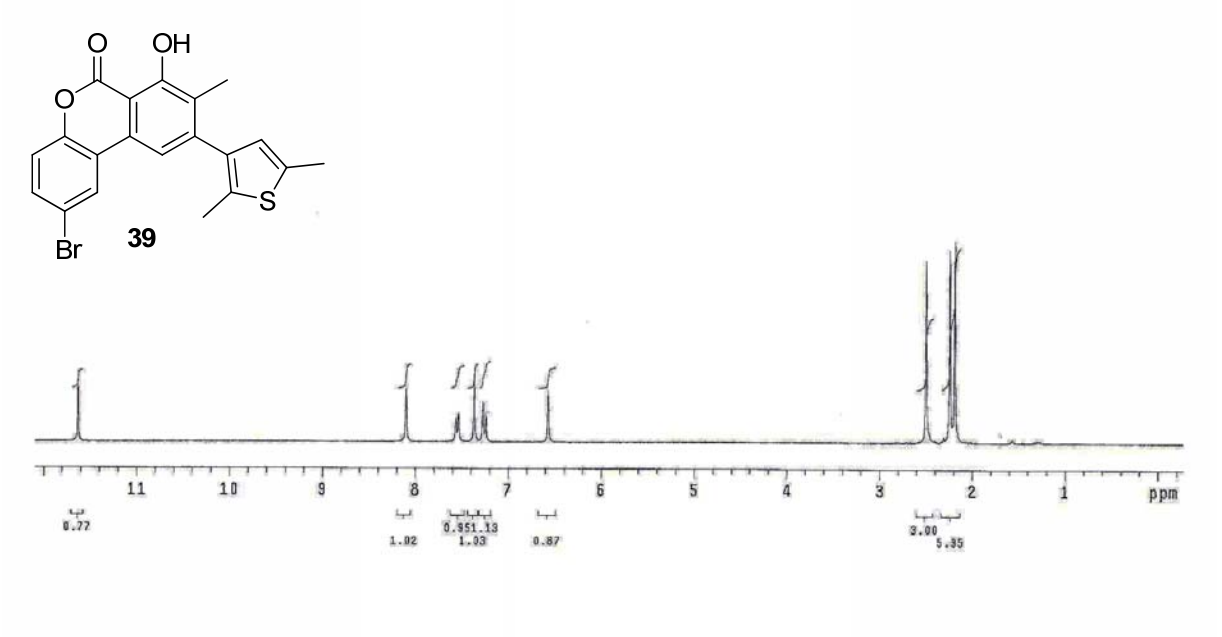

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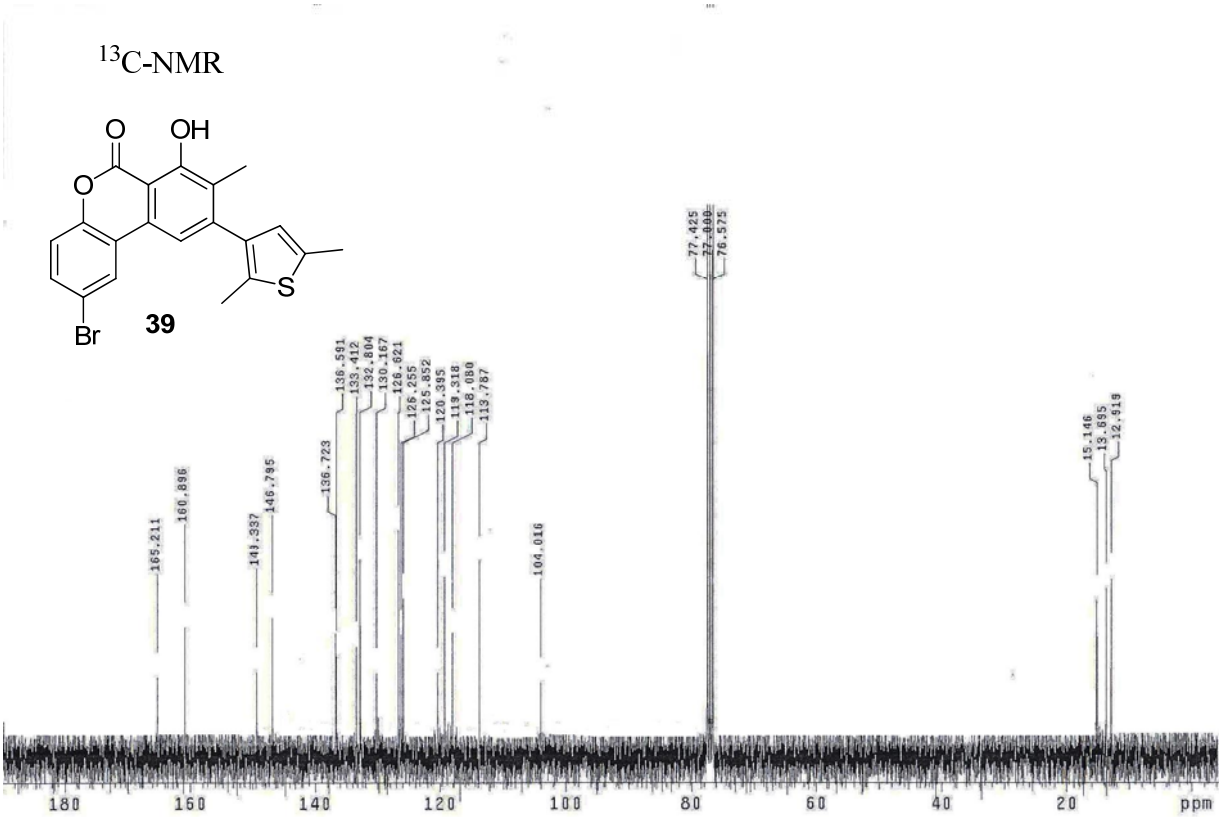
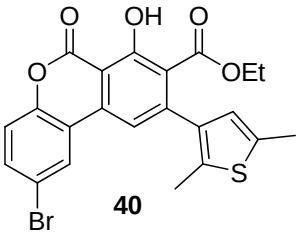
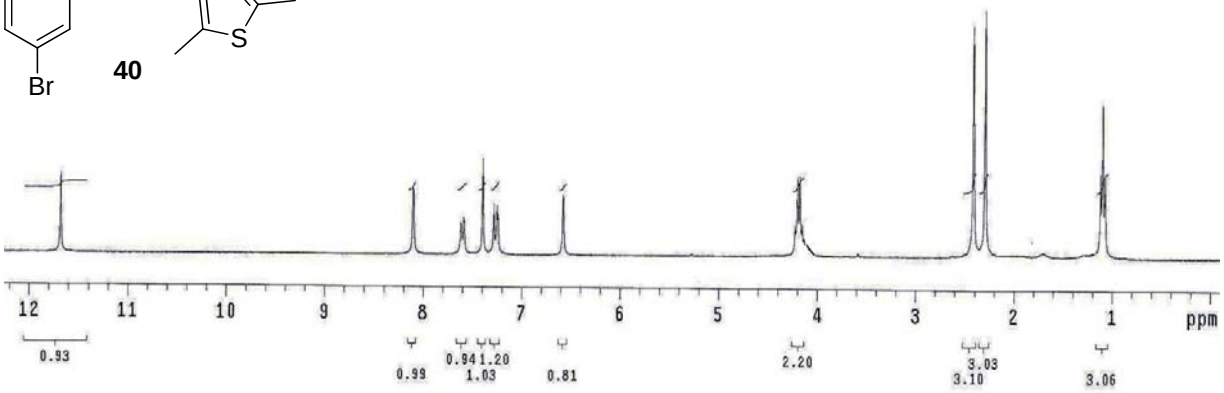


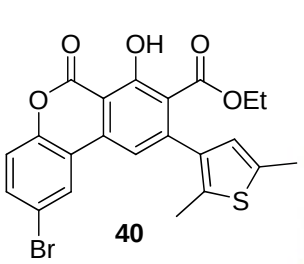
^{1}H-NMR



40



^{13}C-NMR



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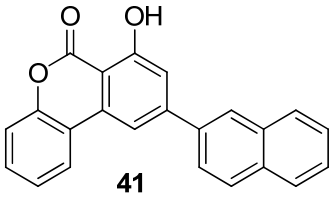
^{1}H-NMR



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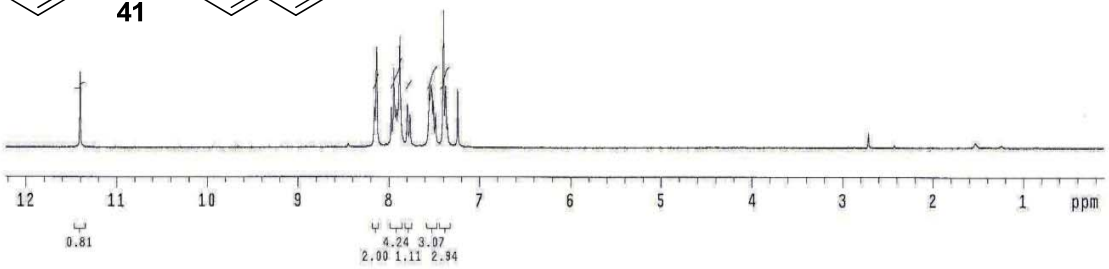
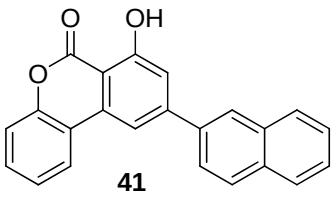
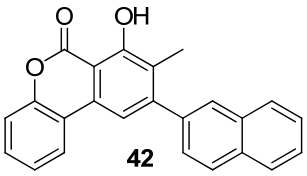


^{13}C-NMR



41

^{1}H-NMR



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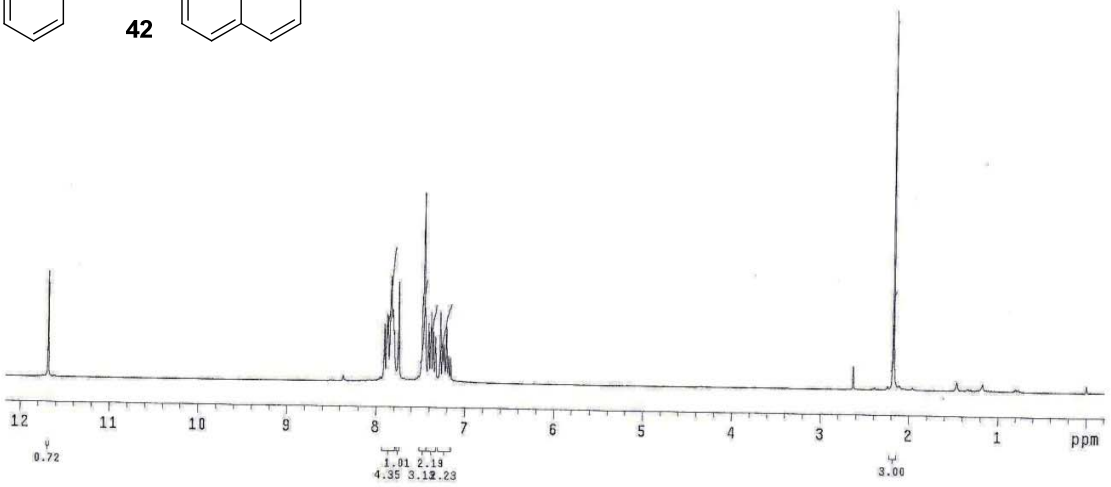
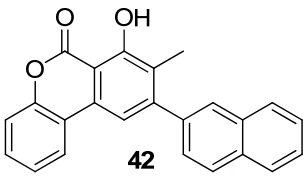
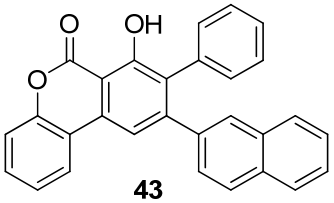


^{13}C-NMR



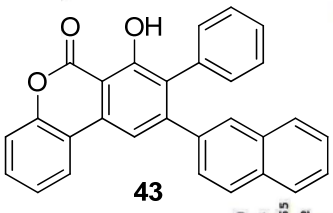
42

^{1}H-NMR



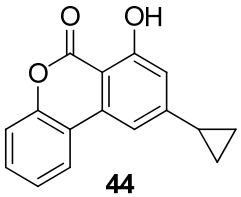
43

^{13}C-NMR

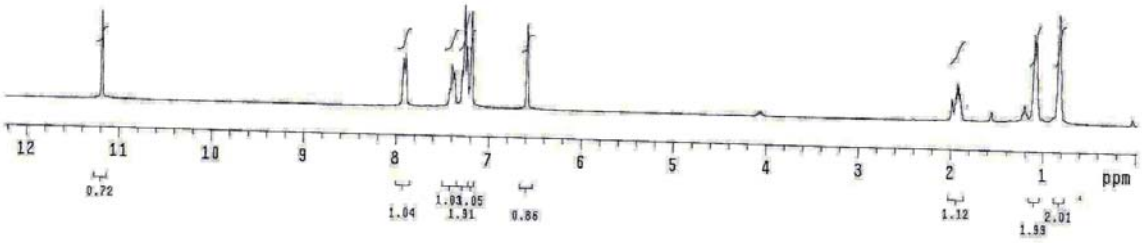


43

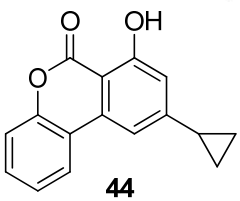
^{1}H-NMR



44

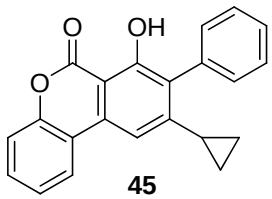


^{13}C-NMR

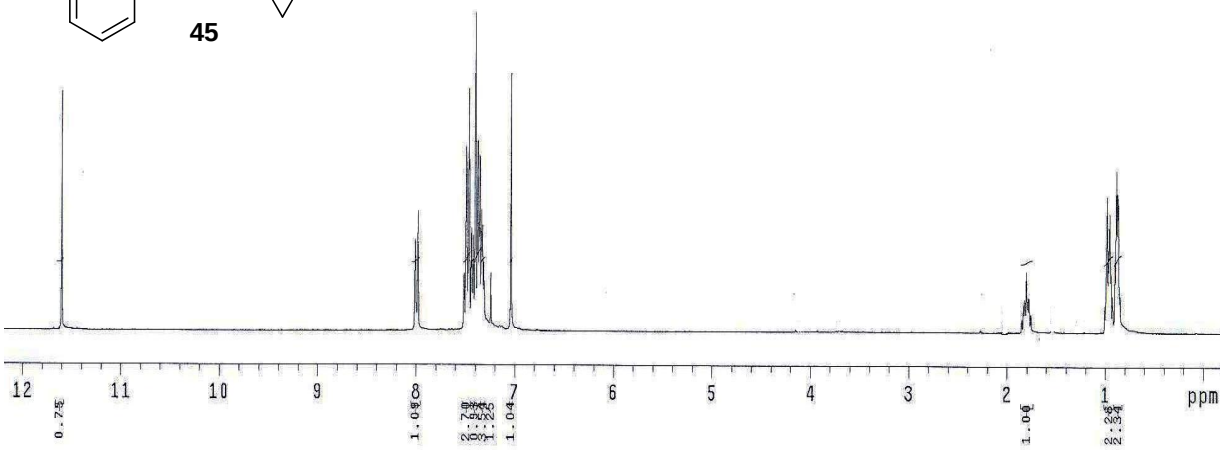


44

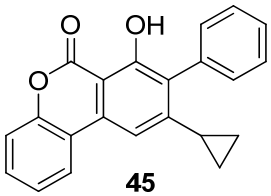
^{1}H-NMR



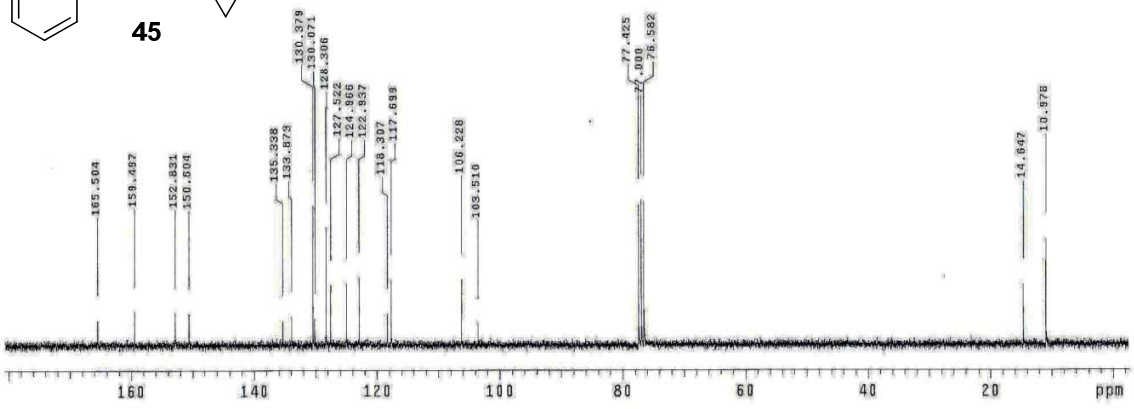
45



^{13}C-NMR

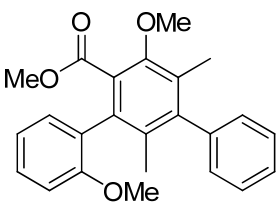


45



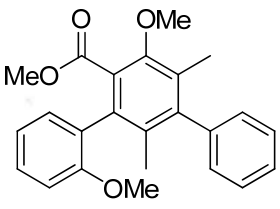
^{1}H NMR and ^{13}C NMR Spectra of compounds 49-54

^{1}H-NMR



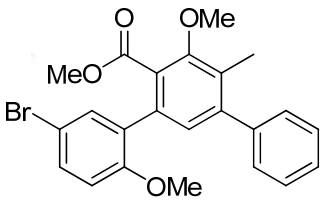
49

^{13}C-NMR



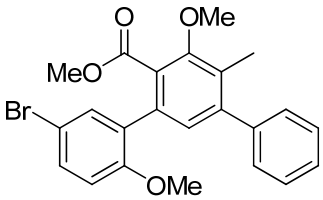
49

^{1}H-NMR

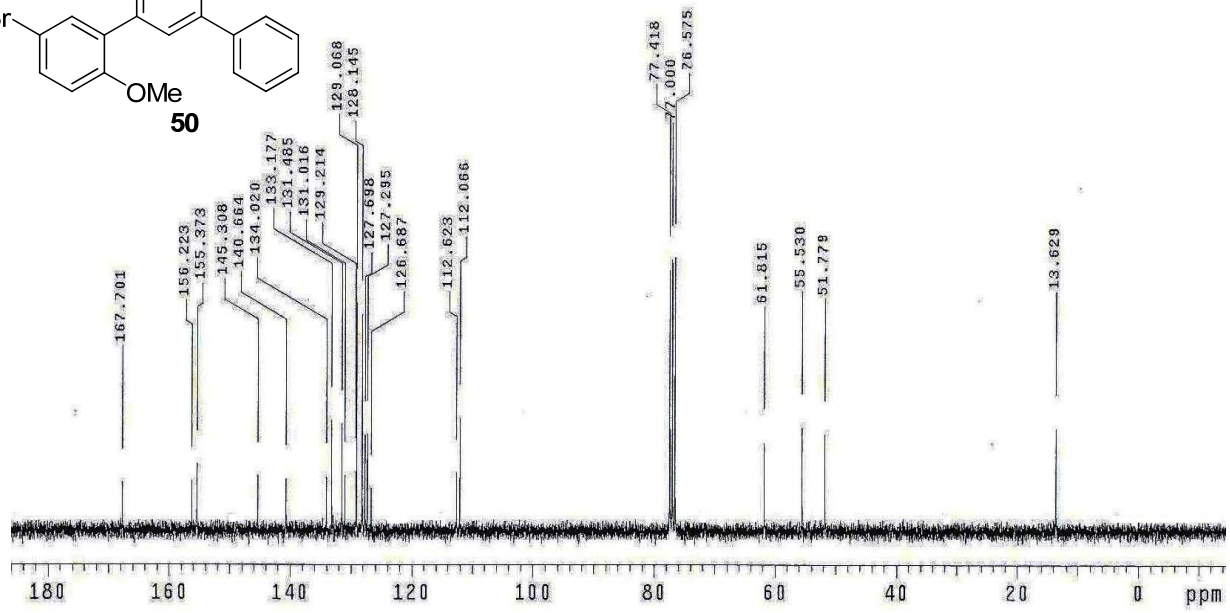


50

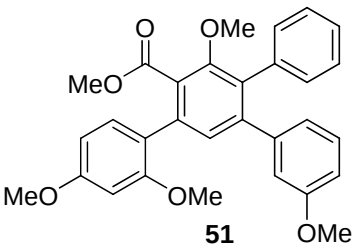
^{13}C-NMR



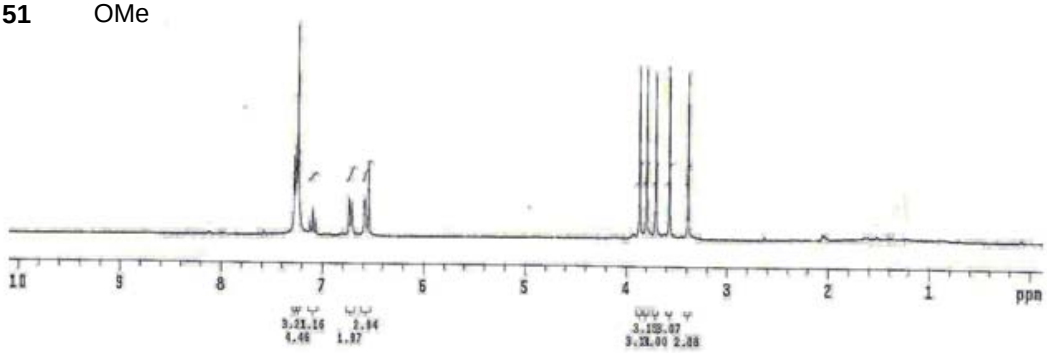
50



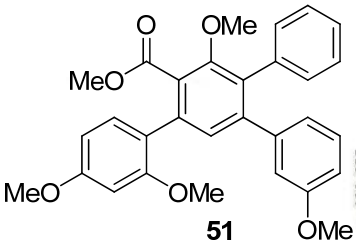
^{1}H-NMR



51

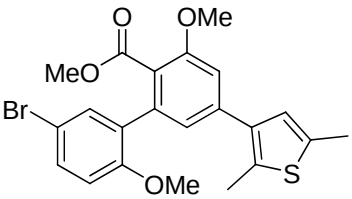


^{13}C-NMR

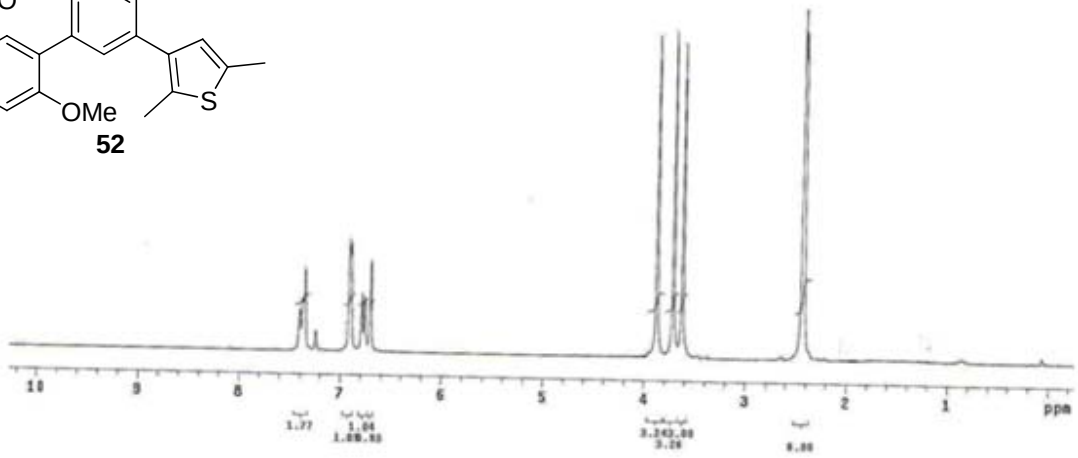


51

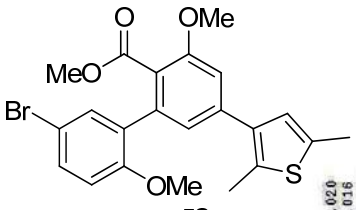
^{1}H-NMR



52

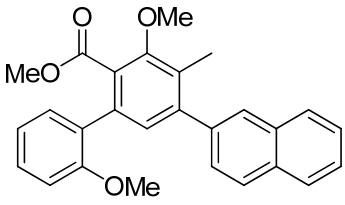


^{13}C-NMR

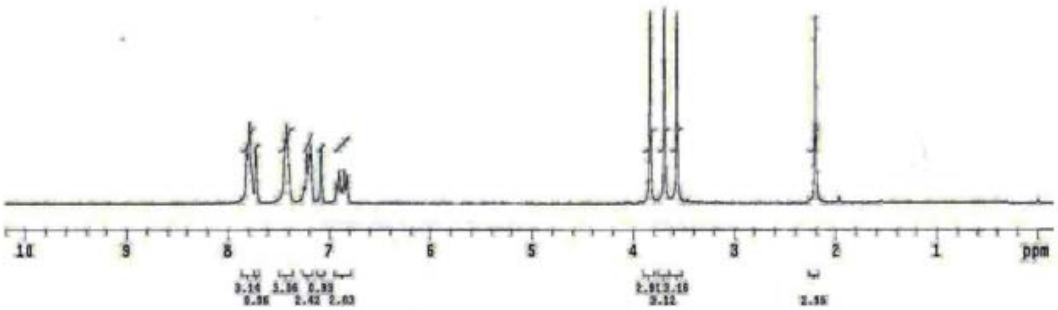


52

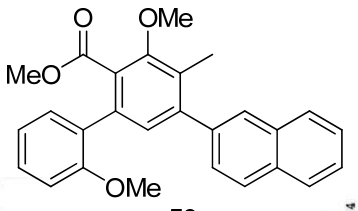
^{1}H-NMR



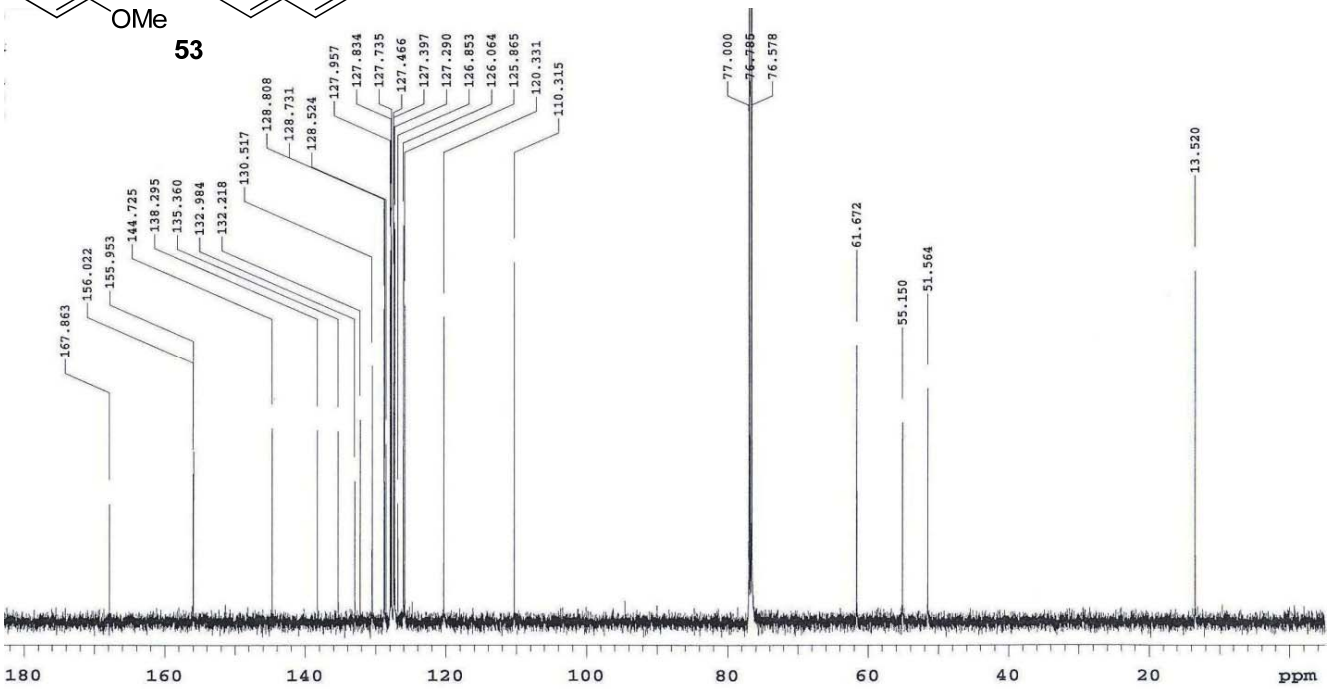
53



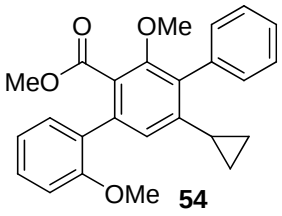
^{13}C-NMR



53

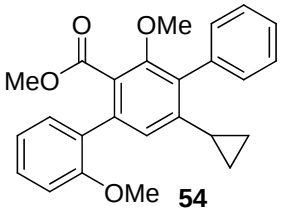


^{1}H-NMR

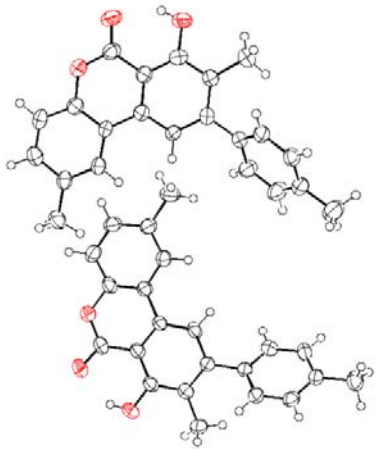


54

^{13}C-NMR



54



X-ray data of compound 26

Table 1. Crystal data and structure refinement for No6.

Identification code	No6	
Empirical formula	C_{44} H_{36} O_6	
Formula weight	660.73	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.8607(14) Å	= 83.181(3)°.
	b = 11.4179(14) Å	= 80.292(3)°.
	c = 15.2714(19) Å	= 61.859(2)°.
Volume	1644.3(4) $Å^3$	
Z	2	
Density (calculated)	1.335 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	696	
Crystal size	0.42 x 0.22 x 0.18 mm^3	
Theta range for data collection	1.35 to 26.08°.	
Index ranges	-8<=h<=13, -13<=k<=14, -18<=l<=18	
Reflections collected	10459	
Independent reflections	6463 [R(int) = 0.0454]	
Completeness to theta = 26.08°	99.2 %	

Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6463 / 0 / 459
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0642, wR2 = 0.1559
R indices (all data)	R1 = 0.1161, wR2 = 0.2354
Largest diff. peak and hole	0.307 and -0.429 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)
for No6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	-613(3)	2167(3)	3992(2)	58(1)
C(1)	-273(4)	3052(3)	3788(2)	43(1)
O(2)	-1096(2)	4220(2)	4189(1)	46(1)
C(2)	-775(4)	5278(3)	4045(2)	39(1)
C(3)	-1659(4)	6385(3)	4533(2)	43(1)
C(4)	-1393(4)	7456(3)	4428(2)	45(1)
C(5)	-240(3)	7446(3)	3848(2)	38(1)
C(6)	15(4)	8637(3)	3764(2)	52(1)
C(7)	609(3)	6327(3)	3380(2)	38(1)
C(8)	381(3)	5213(3)	3450(2)	32(1)
C(9)	1239(3)	4009(3)	2954(2)	34(1)
C(10)	919(3)	2946(3)	3141(2)	36(1)
C(11)	1712(4)	1773(3)	2672(2)	40(1)
O(3)	1450(3)	716(2)	2843(2)	53(1)
C(12)	2810(3)	1659(3)	1992(2)	36(1)
C(13)	3651(4)	355(3)	1544(2)	48(1)
C(14)	3048(3)	2762(3)	1784(2)	35(1)
C(15)	2311(3)	3895(3)	2273(2)	35(1)
C(16)	4070(3)	2778(3)	994(2)	37(1)
C(17)	5127(4)	3092(3)	1057(2)	46(1)

C(18)	6020(4)	3147(4)	308(2)	55(1)
C(19)	5872(4)	2912(3)	-532(2)	45(1)
C(20)	6866(4)	2942(4)	-1335(2)	66(1)
C(21)	4794(3)	2620(3)	-593(2)	41(1)
C(22)	3908(3)	2549(3)	155(2)	41(1)
O(4)	4320(3)	11448(2)	4171(2)	52(1)
C(23)	4652(4)	10348(3)	3910(2)	43(1)
O(5)	3857(2)	9759(2)	4299(1)	46(1)
C(24)	4168(4)	8482(3)	4087(2)	40(1)
C(25)	3321(4)	7964(4)	4566(2)	49(1)
C(26)	3562(4)	6718(3)	4389(2)	47(1)
C(27)	4649(4)	5967(3)	3746(2)	42(1)
C(28)	4908(4)	4598(4)	3556(2)	56(1)
C(29)	5473(3)	6516(3)	3289(2)	39(1)
C(30)	5265(3)	7785(3)	3444(2)	36(1)
C(31)	6100(3)	8413(3)	2967(2)	36(1)
C(32)	5797(3)	9675(3)	3223(2)	36(1)
C(33)	6592(4)	10306(3)	2794(2)	40(1)
O(6)	6375(3)	11487(2)	3053(2)	51(1)
C(34)	7652(4)	9727(3)	2092(2)	39(1)
C(35)	8534(4)	10410(3)	1701(2)	49(1)
C(36)	7883(3)	8512(3)	1808(2)	36(1)
C(37)	7140(3)	7855(3)	2260(2)	36(1)
C(38)	8872(3)	7896(3)	1001(2)	35(1)
C(39)	8788(3)	8616(3)	194(2)	39(1)
C(40)	9636(3)	8014(3)	-569(2)	42(1)
C(41)	10610(4)	6682(3)	-554(2)	40(1)
C(42)	11524(4)	6028(4)	-1398(2)	52(1)
C(43)	10722(4)	5965(3)	251(2)	43(1)
C(44)	9852(3)	6561(3)	1019(2)	40(1)

Table 3. Bond lengths [Å] and angles [°] for No6.

O(1)-C(1)	1.221(4)
C(1)-O(2)	1.355(4)
C(1)-C(10)	1.454(4)
O(2)-C(2)	1.392(4)
C(2)-C(3)	1.383(4)
C(2)-C(8)	1.396(4)
C(3)-C(4)	1.369(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.402(4)
C(4)-H(4)	0.9500
C(5)-C(7)	1.369(4)
C(5)-C(6)	1.499(5)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-C(8)	1.396(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.461(4)
C(9)-C(15)	1.392(4)
C(9)-C(10)	1.398(4)
C(10)-C(11)	1.407(4)
C(11)-O(3)	1.354(4)
C(11)-C(12)	1.409(4)
O(3)-H(3A)	0.8400
C(12)-C(14)	1.392(4)
C(12)-C(13)	1.505(4)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.387(4)
C(14)-C(16)	1.500(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.375(4)
C(16)-C(22)	1.392(4)

C(17)-C(18)	1.385(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.392(5)
C(18)-H(18)	0.9500
C(19)-C(21)	1.379(5)
C(19)-C(20)	1.499(5)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.385(4)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
O(4)-C(23)	1.229(4)
C(23)-O(5)	1.353(4)
C(23)-C(32)	1.444(4)
O(5)-C(24)	1.398(4)
C(24)-C(30)	1.383(4)
C(24)-C(25)	1.384(5)
C(25)-C(26)	1.373(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.395(5)
C(26)-H(26)	0.9500
C(27)-C(29)	1.376(4)
C(27)-C(28)	1.507(5)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.400(4)
C(29)-H(29)	0.9500
C(30)-C(31)	1.460(4)
C(31)-C(37)	1.386(4)
C(31)-C(32)	1.408(4)
C(32)-C(33)	1.406(4)
C(33)-O(6)	1.351(4)
C(33)-C(34)	1.395(4)
O(6)-H(6)	0.8400

C(34)-C(36)	1.397(4)
C(34)-C(35)	1.511(4)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(37)	1.398(4)
C(36)-C(38)	1.488(4)
C(37)-H(37)	0.9500
C(38)-C(44)	1.388(4)
C(38)-C(39)	1.388(4)
C(39)-C(40)	1.382(4)
C(39)-H(39)	0.9500
C(40)-C(41)	1.384(5)
C(40)-H(40)	0.9500
C(41)-C(43)	1.384(4)
C(41)-C(42)	1.516(4)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(44)	1.393(4)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500

O(1)-C(1)-O(2)	116.6(3)
O(1)-C(1)-C(10)	124.9(3)
O(2)-C(1)-C(10)	118.5(3)
C(1)-O(2)-C(2)	121.9(3)
C(3)-C(2)-O(2)	116.0(3)
C(3)-C(2)-C(8)	122.3(3)
O(2)-C(2)-C(8)	121.7(3)
C(4)-C(3)-C(2)	118.8(3)
C(4)-C(3)-H(3)	120.6
C(2)-C(3)-H(3)	120.6
C(3)-C(4)-C(5)	121.5(3)
C(3)-C(4)-H(4)	119.2
C(5)-C(4)-H(4)	119.2

C(7)-C(5)-C(4)	117.6(3)
C(7)-C(5)-C(6)	122.9(3)
C(4)-C(5)-C(6)	119.5(3)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-C(8)	123.4(3)
C(5)-C(7)-H(7)	118.3
C(8)-C(7)-H(7)	118.3
C(7)-C(8)-C(2)	116.3(3)
C(7)-C(8)-C(9)	125.5(3)
C(2)-C(8)-C(9)	118.2(3)
C(15)-C(9)-C(10)	118.4(3)
C(15)-C(9)-C(8)	123.0(3)
C(10)-C(9)-C(8)	118.4(3)
C(9)-C(10)-C(11)	120.2(3)
C(9)-C(10)-C(1)	121.0(3)
C(11)-C(10)-C(1)	118.8(3)
O(3)-C(11)-C(10)	122.0(3)
O(3)-C(11)-C(12)	117.0(3)
C(10)-C(11)-C(12)	121.0(3)
C(11)-O(3)-H(3A)	109.5
C(14)-C(12)-C(11)	117.5(3)
C(14)-C(12)-C(13)	124.4(3)
C(11)-C(12)-C(13)	118.1(3)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(12)	121.4(3)
C(15)-C(14)-C(16)	118.0(3)

C(12)-C(14)-C(16)	120.6(3)
C(14)-C(15)-C(9)	121.2(3)
C(14)-C(15)-H(15)	119.4
C(9)-C(15)-H(15)	119.4
C(17)-C(16)-C(22)	118.0(3)
C(17)-C(16)-C(14)	122.1(3)
C(22)-C(16)-C(14)	119.8(3)
C(16)-C(17)-C(18)	120.7(3)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
C(17)-C(18)-C(19)	121.7(3)
C(17)-C(18)-H(18)	119.1
C(19)-C(18)-H(18)	119.1
C(21)-C(19)-C(18)	117.3(3)
C(21)-C(19)-C(20)	121.4(3)
C(18)-C(19)-C(20)	121.3(3)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-C(22)	121.1(3)
C(19)-C(21)-H(21)	119.4
C(22)-C(21)-H(21)	119.4
C(21)-C(22)-C(16)	121.1(3)
C(21)-C(22)-H(22)	119.4
C(16)-C(22)-H(22)	119.4
O(4)-C(23)-O(5)	116.1(3)
O(4)-C(23)-C(32)	124.7(3)
O(5)-C(23)-C(32)	119.2(3)
C(23)-O(5)-C(24)	121.4(2)
C(30)-C(24)-C(25)	122.6(3)
C(30)-C(24)-O(5)	121.6(3)
C(25)-C(24)-O(5)	115.7(3)
C(26)-C(25)-C(24)	118.8(3)

C(26)-C(25)-H(25)	120.6
C(24)-C(25)-H(25)	120.6
C(25)-C(26)-C(27)	121.2(3)
C(25)-C(26)-H(26)	119.4
C(27)-C(26)-H(26)	119.4
C(29)-C(27)-C(26)	118.0(3)
C(29)-C(27)-C(28)	121.1(3)
C(26)-C(27)-C(28)	120.9(3)
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-C(30)	122.8(3)
C(27)-C(29)-H(29)	118.6
C(30)-C(29)-H(29)	118.6
C(24)-C(30)-C(29)	116.4(3)
C(24)-C(30)-C(31)	118.9(3)
C(29)-C(30)-C(31)	124.7(3)
C(37)-C(31)-C(32)	118.3(3)
C(37)-C(31)-C(30)	123.7(3)
C(32)-C(31)-C(30)	118.0(3)
C(33)-C(32)-C(31)	119.9(3)
C(33)-C(32)-C(23)	119.4(3)
C(31)-C(32)-C(23)	120.6(3)
O(6)-C(33)-C(34)	117.3(3)
O(6)-C(33)-C(32)	121.4(3)
C(34)-C(33)-C(32)	121.3(3)
C(33)-O(6)-H(6)	109.5
C(33)-C(34)-C(36)	118.2(3)
C(33)-C(34)-C(35)	118.7(3)
C(36)-C(34)-C(35)	123.1(3)
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5

C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-C(37)	120.5(3)
C(34)-C(36)-C(38)	122.0(3)
C(37)-C(36)-C(38)	117.4(3)
C(31)-C(37)-C(36)	121.6(3)
C(31)-C(37)-H(37)	119.2
C(36)-C(37)-H(37)	119.2
C(44)-C(38)-C(39)	117.9(3)
C(44)-C(38)-C(36)	120.9(3)
C(39)-C(38)-C(36)	121.1(3)
C(40)-C(39)-C(38)	121.0(3)
C(40)-C(39)-H(39)	119.5
C(38)-C(39)-H(39)	119.5
C(39)-C(40)-C(41)	121.3(3)
C(39)-C(40)-H(40)	119.4
C(41)-C(40)-H(40)	119.4
C(40)-C(41)-C(43)	118.1(3)
C(40)-C(41)-C(42)	120.9(3)
C(43)-C(41)-C(42)	121.0(3)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-C(44)	120.8(3)
C(41)-C(43)-H(43)	119.6
C(44)-C(43)-H(43)	119.6
C(38)-C(44)-C(43)	120.9(3)
C(38)-C(44)-H(44)	119.6
C(43)-C(44)-H(44)	119.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for No6. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2\ a^{*2} U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	70(2)	63(2)	56(2)	-2(1)	7(1)	-48(2)
C(1)	48(2)	50(2)	36(2)	0(2)	-1(2)	-29(2)
O(2)	46(2)	50(1)	43(1)	-5(1)	6(1)	-26(1)
C(2)	41(2)	42(2)	33(2)	1(1)	-4(2)	-20(2)
C(3)	35(2)	54(2)	30(2)	-5(2)	3(2)	-14(2)
C(4)	48(2)	41(2)	38(2)	-7(1)	-3(2)	-14(2)
C(5)	30(2)	45(2)	36(2)	-7(1)	-5(1)	-13(2)
C(6)	64(3)	43(2)	47(2)	-14(2)	1(2)	-24(2)
C(7)	40(2)	41(2)	29(2)	-7(1)	3(2)	-18(2)
C(8)	28(2)	38(2)	28(2)	-3(1)	0(1)	-13(1)
C(9)	35(2)	35(2)	32(2)	1(1)	-6(1)	-16(1)
C(10)	37(2)	39(2)	31(2)	-1(1)	-4(1)	-18(2)
C(11)	45(2)	42(2)	38(2)	3(1)	-8(2)	-26(2)
O(3)	69(2)	46(1)	54(2)	0(1)	1(1)	-38(1)
C(12)	37(2)	35(2)	35(2)	-2(1)	-5(2)	-15(2)
C(13)	49(2)	40(2)	51(2)	-9(2)	-3(2)	-17(2)
C(14)	33(2)	37(2)	34(2)	-4(1)	-2(1)	-13(2)
C(15)	32(2)	38(2)	36(2)	-3(1)	0(1)	-19(2)
C(16)	37(2)	33(2)	39(2)	-7(1)	0(2)	-15(1)
C(17)	57(2)	61(2)	36(2)	-7(2)	-2(2)	-39(2)
C(18)	55(2)	73(3)	52(2)	-8(2)	0(2)	-44(2)
C(19)	47(2)	49(2)	41(2)	-6(2)	3(2)	-26(2)
C(20)	73(3)	81(3)	53(2)	-5(2)	7(2)	-49(3)
C(21)	42(2)	43(2)	37(2)	-8(1)	-2(2)	-19(2)
C(22)	36(2)	44(2)	46(2)	-11(2)	2(2)	-21(2)
O(4)	56(2)	44(1)	54(1)	-21(1)	5(1)	-20(1)
C(23)	47(2)	37(2)	42(2)	-13(2)	-2(2)	-17(2)
O(5)	51(2)	43(1)	47(1)	-14(1)	8(1)	-26(1)
C(24)	44(2)	37(2)	40(2)	-12(1)	-3(2)	-18(2)
C(25)	49(2)	57(2)	42(2)	-9(2)	8(2)	-29(2)
C(26)	55(2)	51(2)	45(2)	-3(2)	-1(2)	-35(2)

C(27)	46(2)	48(2)	39(2)	-3(2)	-2(2)	-27(2)
C(28)	70(3)	51(2)	60(2)	-4(2)	-5(2)	-41(2)
C(29)	42(2)	41(2)	36(2)	-5(1)	-2(2)	-20(2)
C(30)	40(2)	36(2)	34(2)	-4(1)	-4(2)	-20(2)
C(31)	40(2)	32(2)	35(2)	-6(1)	-3(2)	-17(2)
C(32)	40(2)	32(2)	35(2)	-5(1)	-4(2)	-16(2)
C(33)	47(2)	31(2)	43(2)	-8(1)	-5(2)	-18(2)
O(6)	62(2)	39(1)	60(2)	-16(1)	2(1)	-28(1)
C(34)	43(2)	37(2)	40(2)	-6(1)	-3(2)	-20(2)
C(35)	54(2)	49(2)	53(2)	-9(2)	3(2)	-34(2)
C(36)	38(2)	37(2)	36(2)	-5(1)	-3(2)	-20(2)
C(37)	38(2)	32(2)	40(2)	-11(1)	-4(2)	-16(2)
C(38)	36(2)	37(2)	38(2)	-6(1)	-1(2)	-21(2)
C(39)	36(2)	40(2)	42(2)	-5(1)	-2(2)	-19(2)
C(40)	45(2)	49(2)	41(2)	-5(2)	0(2)	-31(2)
C(41)	43(2)	43(2)	38(2)	-9(1)	4(2)	-23(2)
C(42)	53(2)	58(2)	49(2)	-18(2)	0(2)	-27(2)
C(43)	38(2)	40(2)	47(2)	-14(2)	1(2)	-13(2)
C(44)	42(2)	36(2)	43(2)	0(1)	-9(2)	-18(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for No6.

	x	y	z	U(eq)
H(3)	-2438	6403	4934	52
H(4)	-2003	8224	4755	54
H(6A)	770	8527	3276	77
H(6B)	291	8728	4321	77
H(6C)	-848	9436	3639	77
H(7)	1395	6309	2986	45
H(3A)	753	900	3238	79
H(13A)	3189	354	1046	72
H(13B)	3710	-374	1973	72
H(13C)	4601	238	1322	72
H(15)	2543	4607	2140	42
H(17)	5246	3273	1619	56
H(18)	6753	3350	370	66
H(20A)	7242	2120	-1650	98
H(20B)	7642	3022	-1148	98
H(20C)	6363	3706	-1730	98
H(21)	4656	2466	-1158	49
H(22)	3178	2340	95	50
H(25)	2586	8463	5011	58
H(26)	2978	6359	4709	56
H(28A)	4285	4673	3133	84
H(28B)	4715	4151	4110	84
H(28C)	5891	4081	3301	84
H(29)	6215	6012	2850	47
H(6)	5671	11778	3445	77
H(35A)	9466	9747	1449	73
H(35B)	8636	10865	2168	73
H(35C)	8072	11061	1232	73

H(37)	7353	7005	2079	43
H(39)	8138	9535	167	47
H(40)	9547	8525	-1115	50
H(42A)	12400	5268	-1245	78
H(42B)	11744	6672	-1783	78
H(42C)	11019	5721	-1710	78
H(43)	11401	5055	280	52
H(44)	9931	6047	1563	48

Table 6. Torsion angles [°] for No6.

O(1)-C(1)-O(2)-C(2)	176.7(3)
C(10)-C(1)-O(2)-C(2)	-4.5(5)
C(1)-O(2)-C(2)-C(3)	-176.6(3)
C(1)-O(2)-C(2)-C(8)	2.7(5)
O(2)-C(2)-C(3)-C(4)	179.4(3)
C(8)-C(2)-C(3)-C(4)	0.1(5)
C(2)-C(3)-C(4)-C(5)	-0.8(5)
C(3)-C(4)-C(5)-C(7)	0.7(5)
C(3)-C(4)-C(5)-C(6)	-179.4(3)
C(4)-C(5)-C(7)-C(8)	0.2(5)
C(6)-C(5)-C(7)-C(8)	-179.8(3)
C(5)-C(7)-C(8)-C(2)	-0.8(5)
C(5)-C(7)-C(8)-C(9)	178.8(3)
C(3)-C(2)-C(8)-C(7)	0.7(5)
O(2)-C(2)-C(8)-C(7)	-178.6(3)
C(3)-C(2)-C(8)-C(9)	-179.0(3)
O(2)-C(2)-C(8)-C(9)	1.8(4)
C(7)-C(8)-C(9)-C(15)	-7.3(5)
C(2)-C(8)-C(9)-C(15)	172.3(3)
C(7)-C(8)-C(9)-C(10)	176.2(3)
C(2)-C(8)-C(9)-C(10)	-4.1(4)
C(15)-C(9)-C(10)-C(11)	2.8(5)
C(8)-C(9)-C(10)-C(11)	179.4(3)

C(15)-C(9)-C(10)-C(1)	-174.3(3)
C(8)-C(9)-C(10)-C(1)	2.3(4)
O(1)-C(1)-C(10)-C(9)	-179.4(3)
O(2)-C(1)-C(10)-C(9)	2.0(5)
O(1)-C(1)-C(10)-C(11)	3.5(5)
O(2)-C(1)-C(10)-C(11)	-175.2(3)
C(9)-C(10)-C(11)-O(3)	178.9(3)
C(1)-C(10)-C(11)-O(3)	-3.9(5)
C(9)-C(10)-C(11)-C(12)	-2.0(5)
C(1)-C(10)-C(11)-C(12)	175.2(3)
O(3)-C(11)-C(12)-C(14)	177.2(3)
C(10)-C(11)-C(12)-C(14)	-1.9(5)
O(3)-C(11)-C(12)-C(13)	-3.2(4)
C(10)-C(11)-C(12)-C(13)	177.6(3)
C(11)-C(12)-C(14)-C(15)	5.1(5)
C(13)-C(12)-C(14)-C(15)	-174.5(3)
C(11)-C(12)-C(14)-C(16)	-172.2(3)
C(13)-C(12)-C(14)-C(16)	8.3(5)
C(12)-C(14)-C(15)-C(9)	-4.3(5)
C(16)-C(14)-C(15)-C(9)	173.0(3)
C(10)-C(9)-C(15)-C(14)	0.3(5)
C(8)-C(9)-C(15)-C(14)	-176.2(3)
C(15)-C(14)-C(16)-C(17)	54.1(4)
C(12)-C(14)-C(16)-C(17)	-128.5(4)
C(15)-C(14)-C(16)-C(22)	-121.9(3)
C(12)-C(14)-C(16)-C(22)	55.4(4)
C(22)-C(16)-C(17)-C(18)	-1.4(5)
C(14)-C(16)-C(17)-C(18)	-177.6(3)
C(16)-C(17)-C(18)-C(19)	1.1(6)
C(17)-C(18)-C(19)-C(21)	0.0(6)
C(17)-C(18)-C(19)-C(20)	-178.5(3)
C(18)-C(19)-C(21)-C(22)	-0.8(5)
C(20)-C(19)-C(21)-C(22)	177.8(3)
C(19)-C(21)-C(22)-C(16)	0.4(5)
C(17)-C(16)-C(22)-C(21)	0.7(5)
C(14)-C(16)-C(22)-C(21)	176.9(3)

O(4)-C(23)-O(5)-C(24)	-177.1(3)
C(32)-C(23)-O(5)-C(24)	3.8(5)
C(23)-O(5)-C(24)-C(30)	-2.8(5)
C(23)-O(5)-C(24)-C(25)	176.5(3)
C(30)-C(24)-C(25)-C(26)	-1.1(5)
O(5)-C(24)-C(25)-C(26)	179.6(3)
C(24)-C(25)-C(26)-C(27)	0.8(5)
C(25)-C(26)-C(27)-C(29)	-0.3(5)
C(25)-C(26)-C(27)-C(28)	179.9(3)
C(26)-C(27)-C(29)-C(30)	0.1(5)
C(28)-C(27)-C(29)-C(30)	179.8(3)
C(25)-C(24)-C(30)-C(29)	0.8(5)
O(5)-C(24)-C(30)-C(29)	-179.9(3)
C(25)-C(24)-C(30)-C(31)	179.7(3)
O(5)-C(24)-C(30)-C(31)	-1.0(5)
C(27)-C(29)-C(30)-C(24)	-0.3(5)
C(27)-C(29)-C(30)-C(31)	-179.1(3)
C(24)-C(30)-C(31)-C(37)	-174.2(3)
C(29)-C(30)-C(31)-C(37)	4.6(5)
C(24)-C(30)-C(31)-C(32)	3.7(5)
C(29)-C(30)-C(31)-C(32)	-177.6(3)
C(37)-C(31)-C(32)-C(33)	-3.3(5)
C(30)-C(31)-C(32)-C(33)	178.8(3)
C(37)-C(31)-C(32)-C(23)	175.3(3)
C(30)-C(31)-C(32)-C(23)	-2.7(5)
O(4)-C(23)-C(32)-C(33)	-1.5(5)
O(5)-C(23)-C(32)-C(33)	177.6(3)
O(4)-C(23)-C(32)-C(31)	180.0(3)
O(5)-C(23)-C(32)-C(31)	-0.9(5)
C(31)-C(32)-C(33)-O(6)	-176.7(3)
C(23)-C(32)-C(33)-O(6)	4.7(5)
C(31)-C(32)-C(33)-C(34)	2.4(5)
C(23)-C(32)-C(33)-C(34)	-176.2(3)
O(6)-C(33)-C(34)-C(36)	-179.3(3)
C(32)-C(33)-C(34)-C(36)	1.6(5)
O(6)-C(33)-C(34)-C(35)	3.2(5)

C(32)-C(33)-C(34)-C(35)	-175.9(3)
C(33)-C(34)-C(36)-C(37)	-4.6(5)
C(35)-C(34)-C(36)-C(37)	172.7(3)
C(33)-C(34)-C(36)-C(38)	172.8(3)
C(35)-C(34)-C(36)-C(38)	-9.8(5)
C(32)-C(31)-C(37)-C(36)	0.2(5)
C(30)-C(31)-C(37)-C(36)	178.1(3)
C(34)-C(36)-C(37)-C(31)	3.8(5)
C(38)-C(36)-C(37)-C(31)	-173.8(3)
C(34)-C(36)-C(38)-C(44)	133.0(3)
C(37)-C(36)-C(38)-C(44)	-49.5(4)
C(34)-C(36)-C(38)-C(39)	-51.0(5)
C(37)-C(36)-C(38)-C(39)	126.6(3)
C(44)-C(38)-C(39)-C(40)	1.2(5)
C(36)-C(38)-C(39)-C(40)	-175.0(3)
C(38)-C(39)-C(40)-C(41)	-1.0(5)
C(39)-C(40)-C(41)-C(43)	-0.4(5)
C(39)-C(40)-C(41)-C(42)	179.3(3)
C(40)-C(41)-C(43)-C(44)	1.6(5)
C(42)-C(41)-C(43)-C(44)	-178.1(3)
C(39)-C(38)-C(44)-C(43)	0.0(5)
C(36)-C(38)-C(44)-C(43)	176.2(3)
C(41)-C(43)-C(44)-C(38)	-1.4(5)

Symmetry transformations used to generate equivalent atoms: