Supplementary Material

Tert-Butylation of naphthalene-2,6-diol and 6-methoxynaphthalen-2-ol

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Dedicated to Professor Oleg A. Rakitin on the occasion of his 65th birthday

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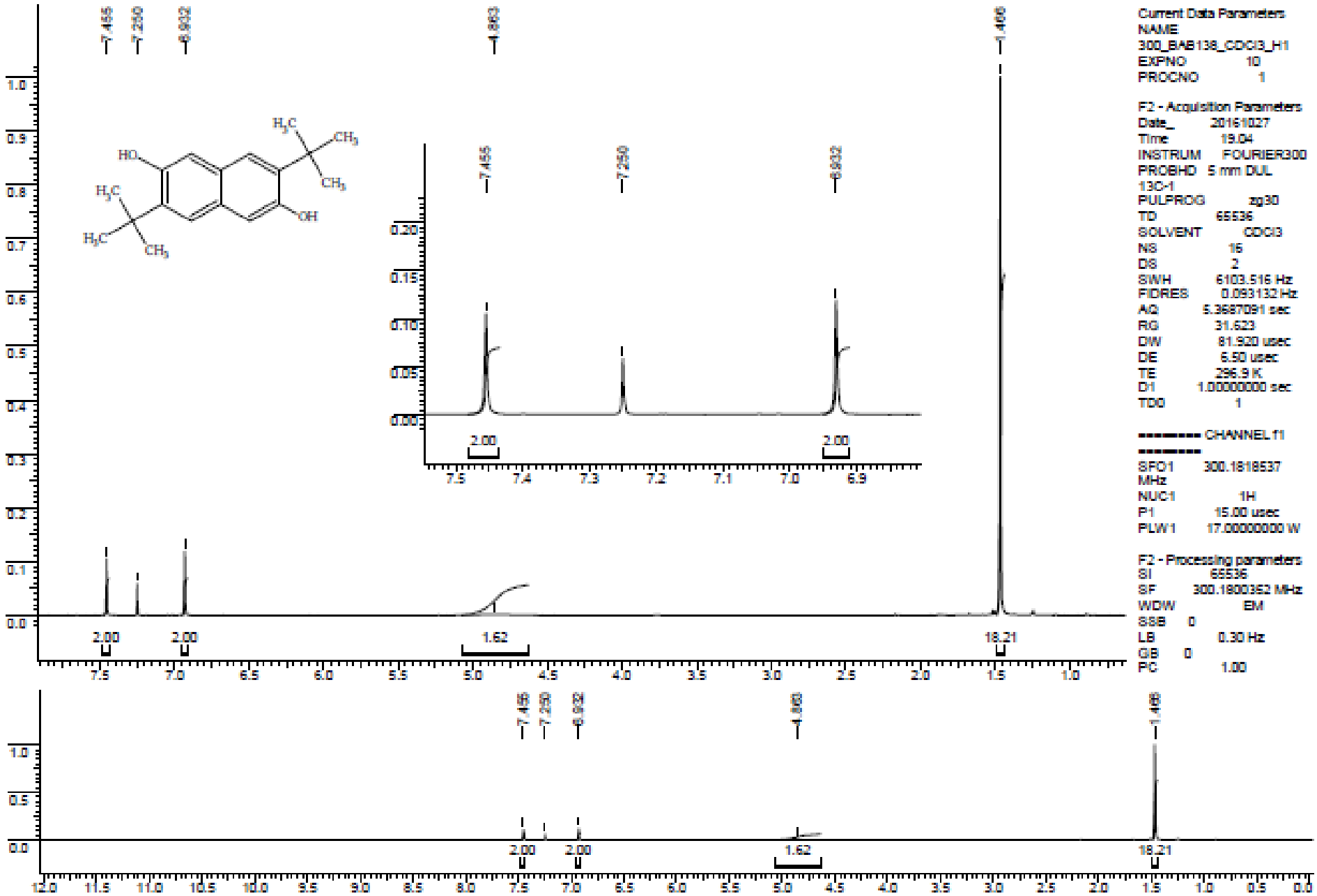
3,7-di-tert-butylnaphthalene-2,6-diol (2)



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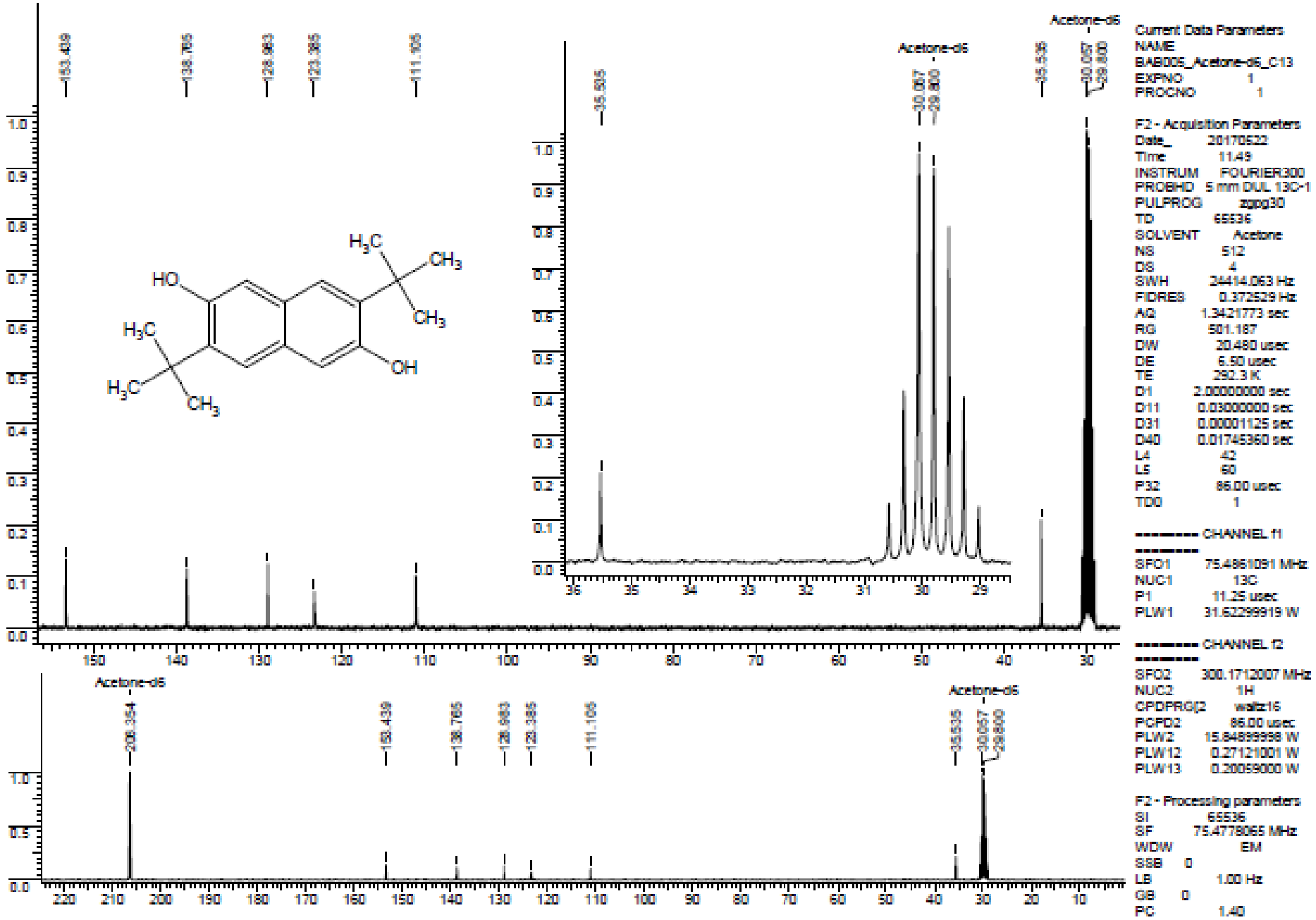
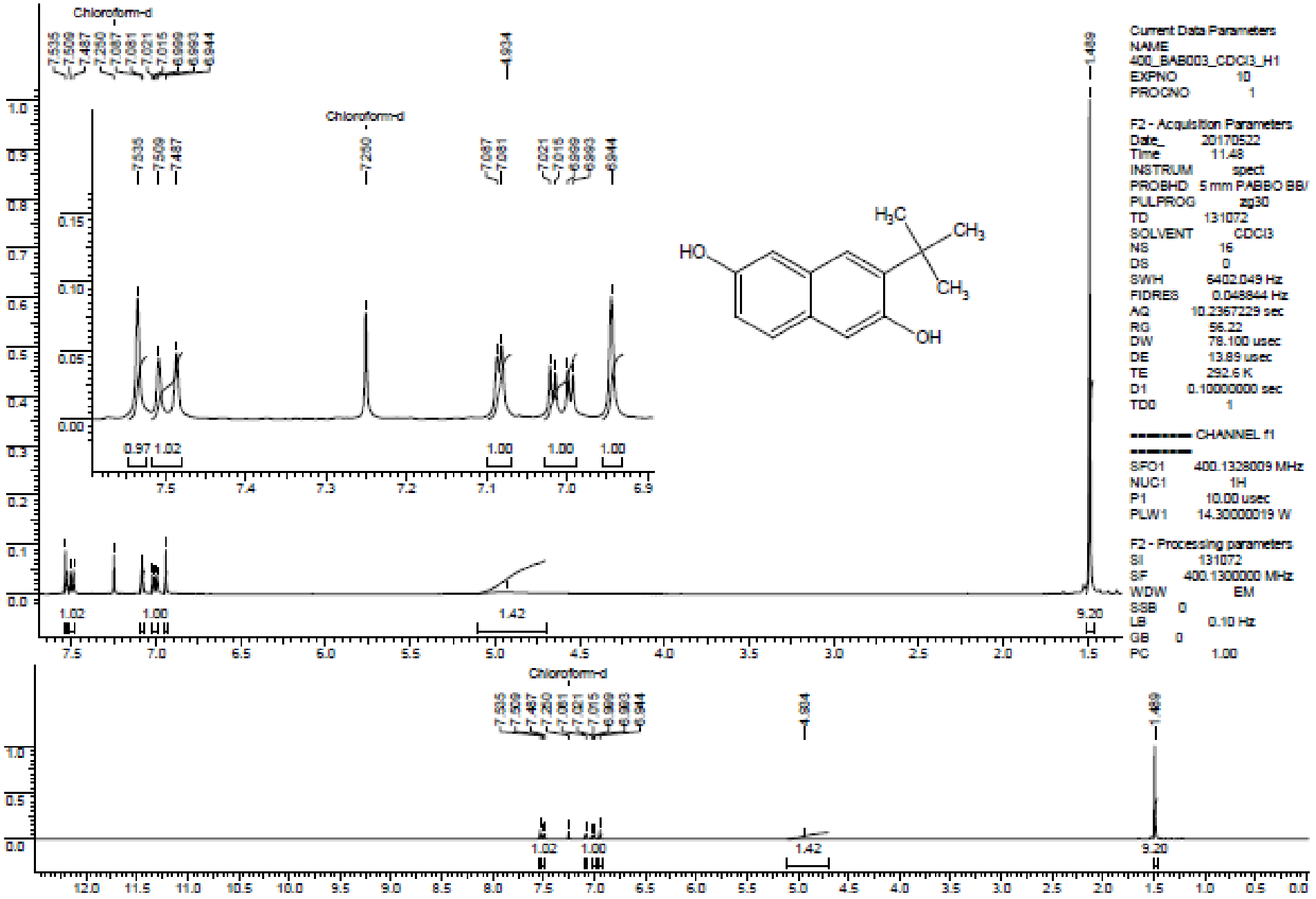


3-tert-butylnaphthalene-2,6-diol (3)



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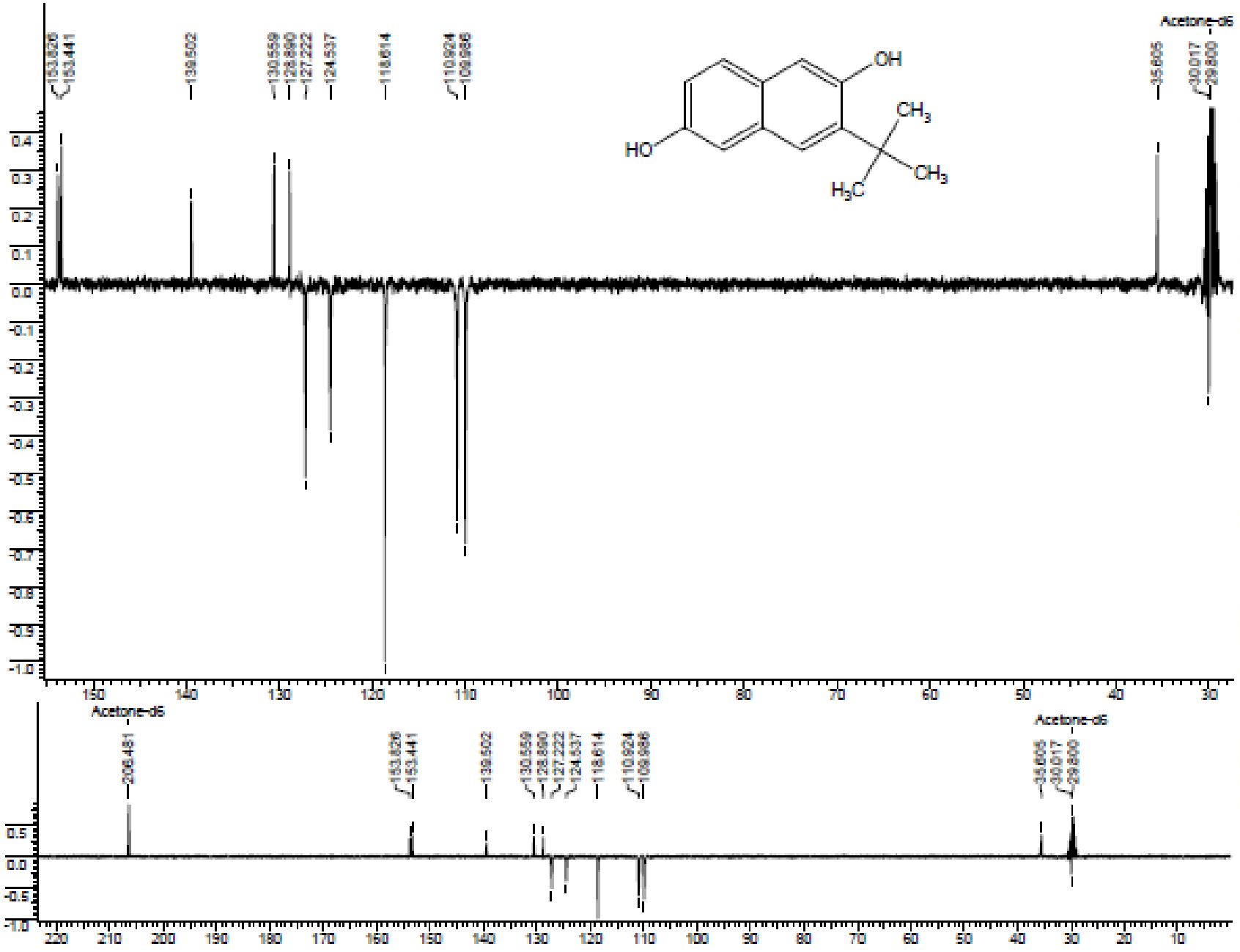
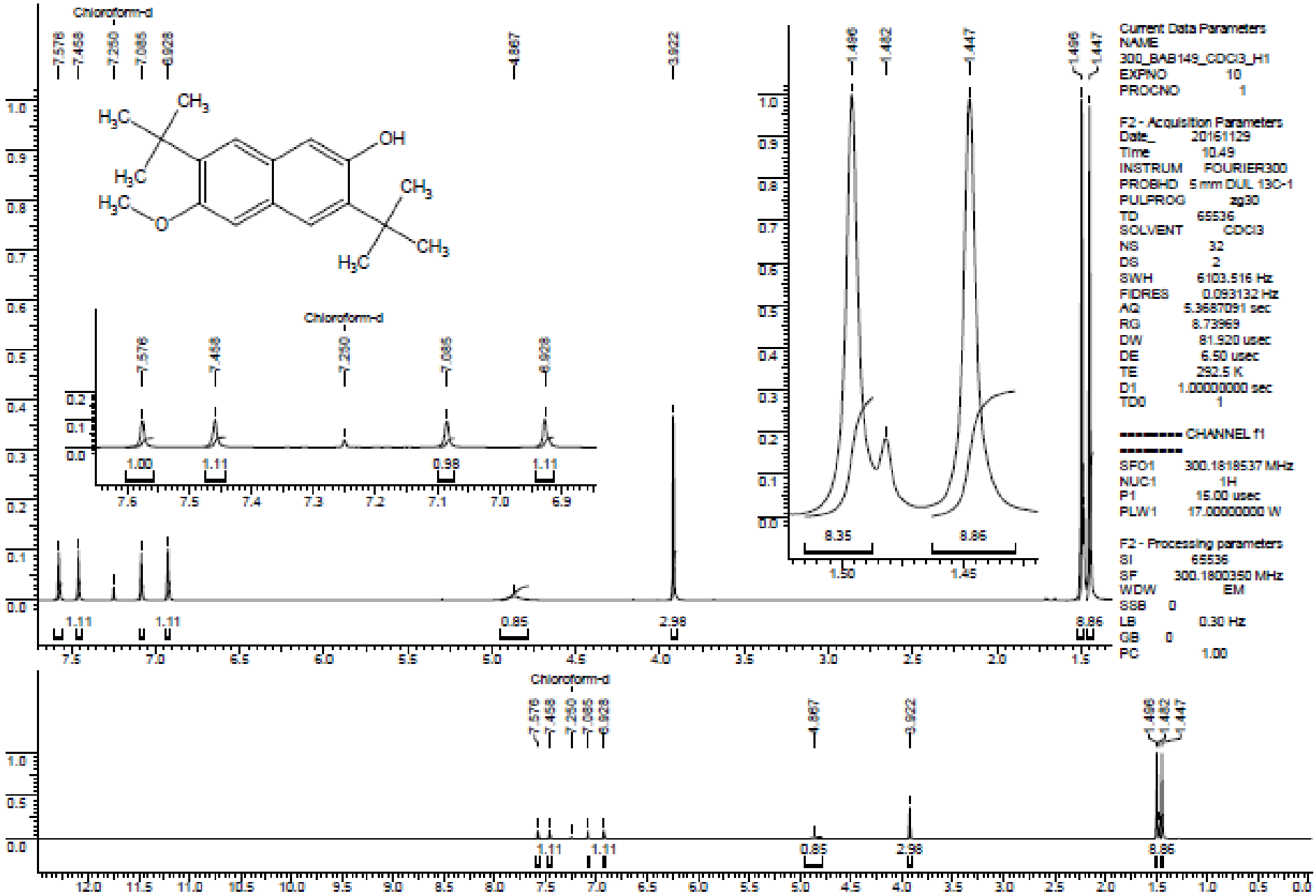


3,7-di-tert-butyl-6-methoxynaphthalen-2-ol (5)



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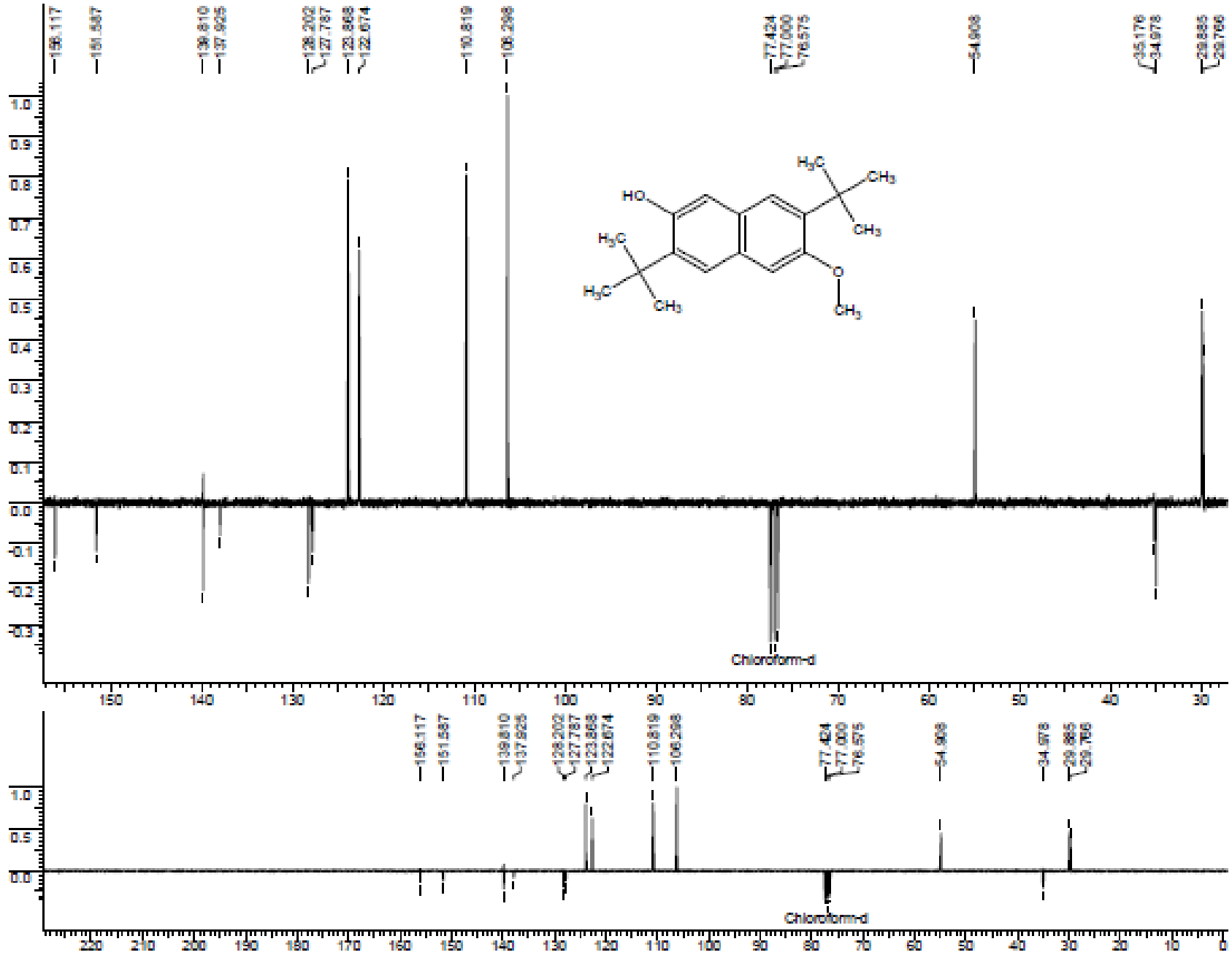

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PROCNO 1

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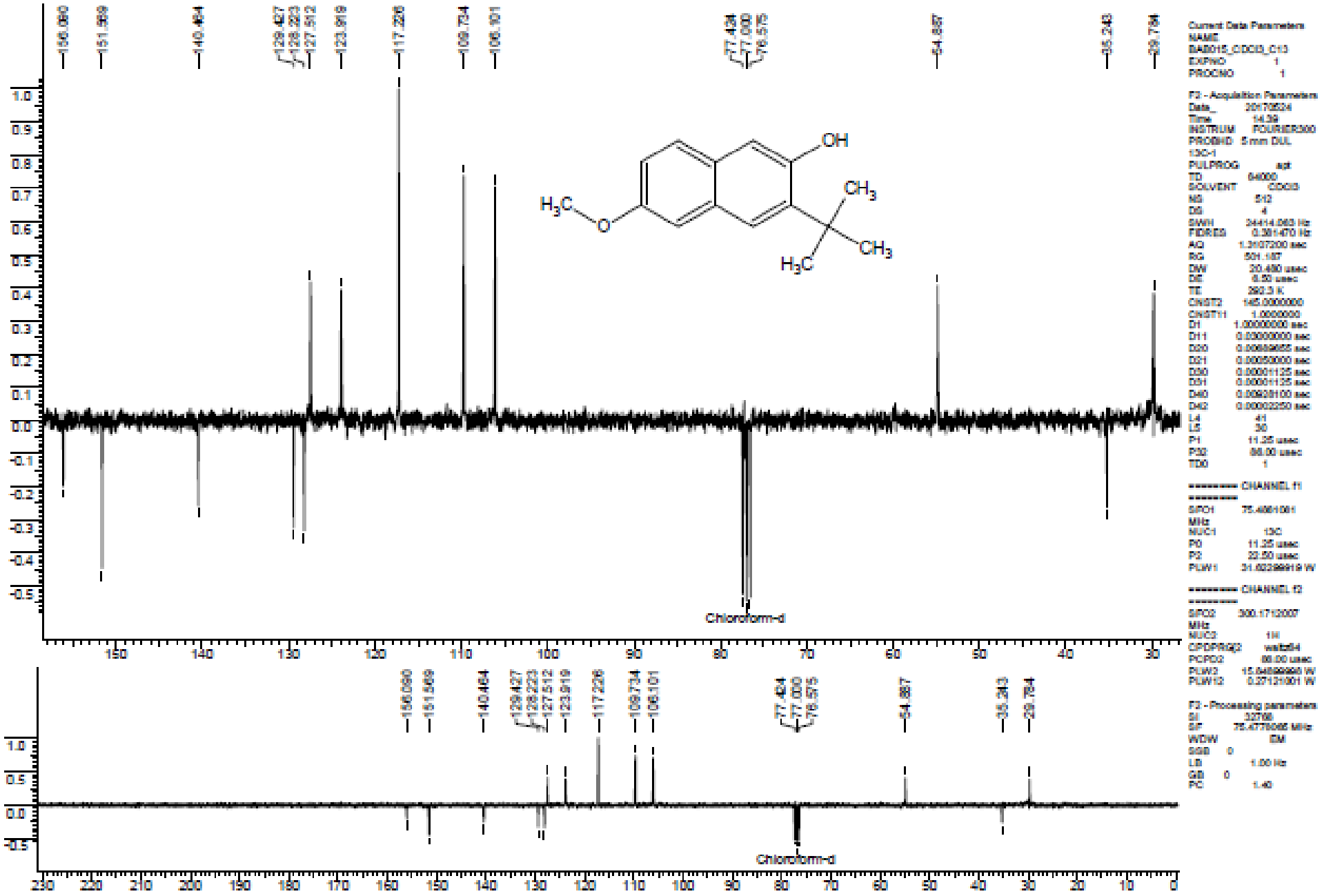
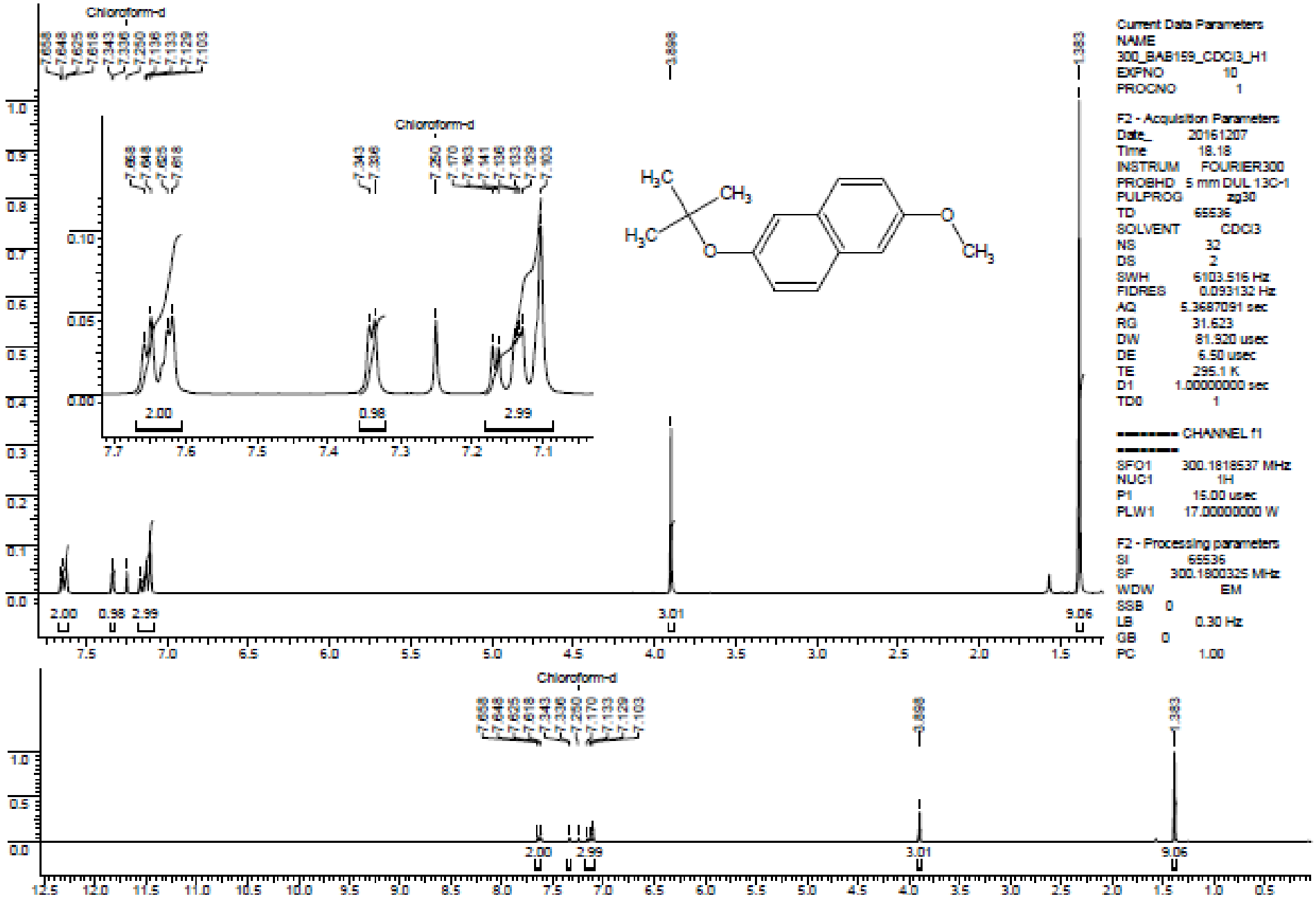
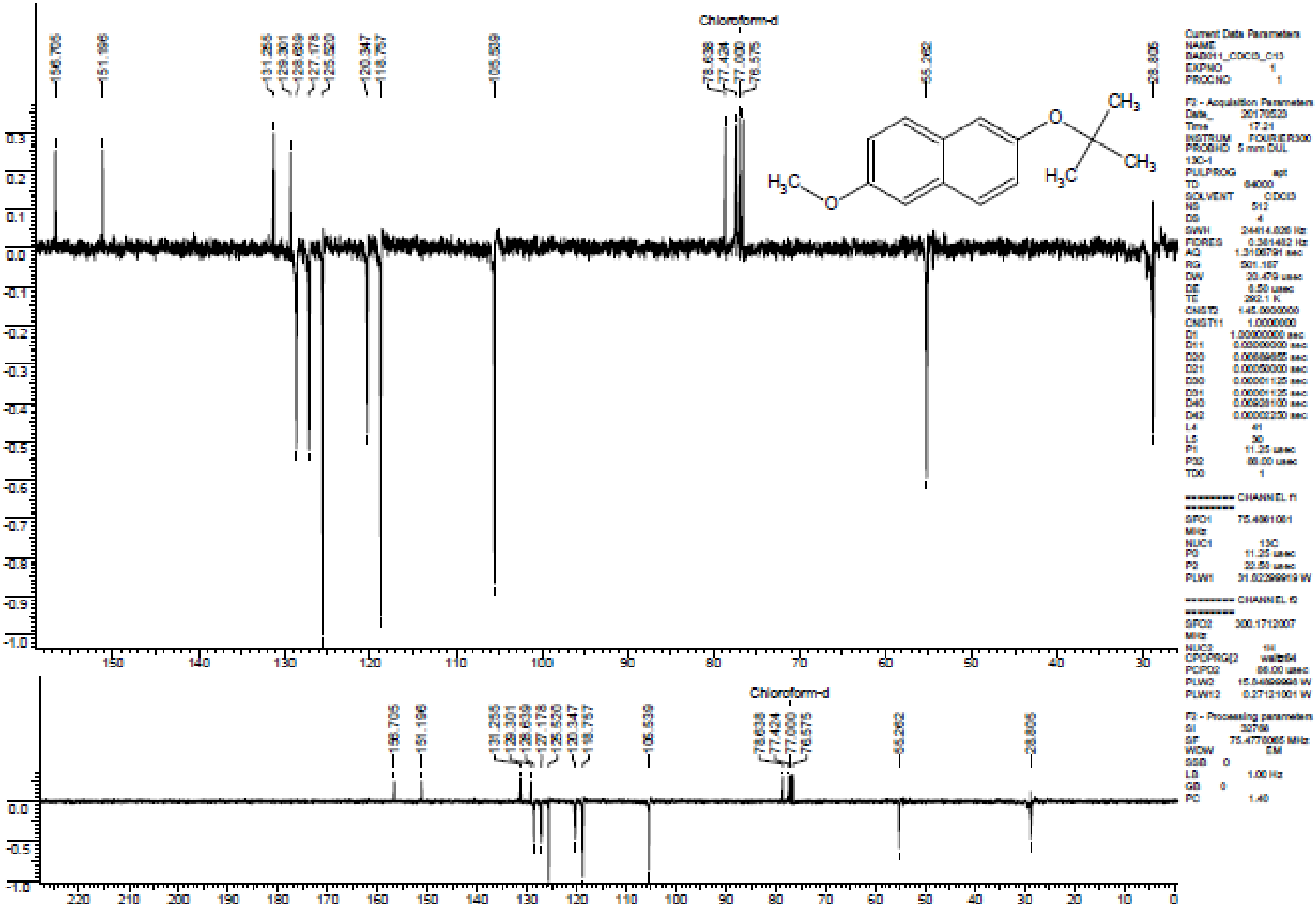
3-tert-butyl-6-methoxynaphthalen-2-ol (6)



2-tert-butoxy-6-methoxynaphthalene (7)



2-tert-butoxy-6-methoxynaphthalene (7)



X-ray measurements:

Single crystals of **2** and **3** were grown by slow evaporation of $CHCl_3$ solutions, while a single crystal of **5** was obtained by evaporation of a hexane solution. Crystallographic studies were undertaken on single crystal mounted in paratone, mounted on the goniometer head with a nylon loop and studied on an Agilent SuperNova Dual three-circle diffractometer using Cu-Kα (λ = 1.540598 Å) or Mo-Kα (λ = 0.7093187 Å) radiation and a CCD detector. Measurements were typically made at 150(1) K with temperatures maintained using an Oxford Cryostream unless otherwise stated. Data were collected, integrated and corrected for absorption using a numerical absorption correction based on Gaussian integration over a multifaceted crystal model within CrysAlisPro.[1S]The structures were solved by direct methods and refined against F2 within SHELXL-2013.[2S]A summary of crystallographic data are available as ESI and the structures deposited with the Cambridge Structural Database (CCDC deposition numbers 1558768 (**2**), 1558766(**3**), and 1558767 (**5**)). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data for compound 2

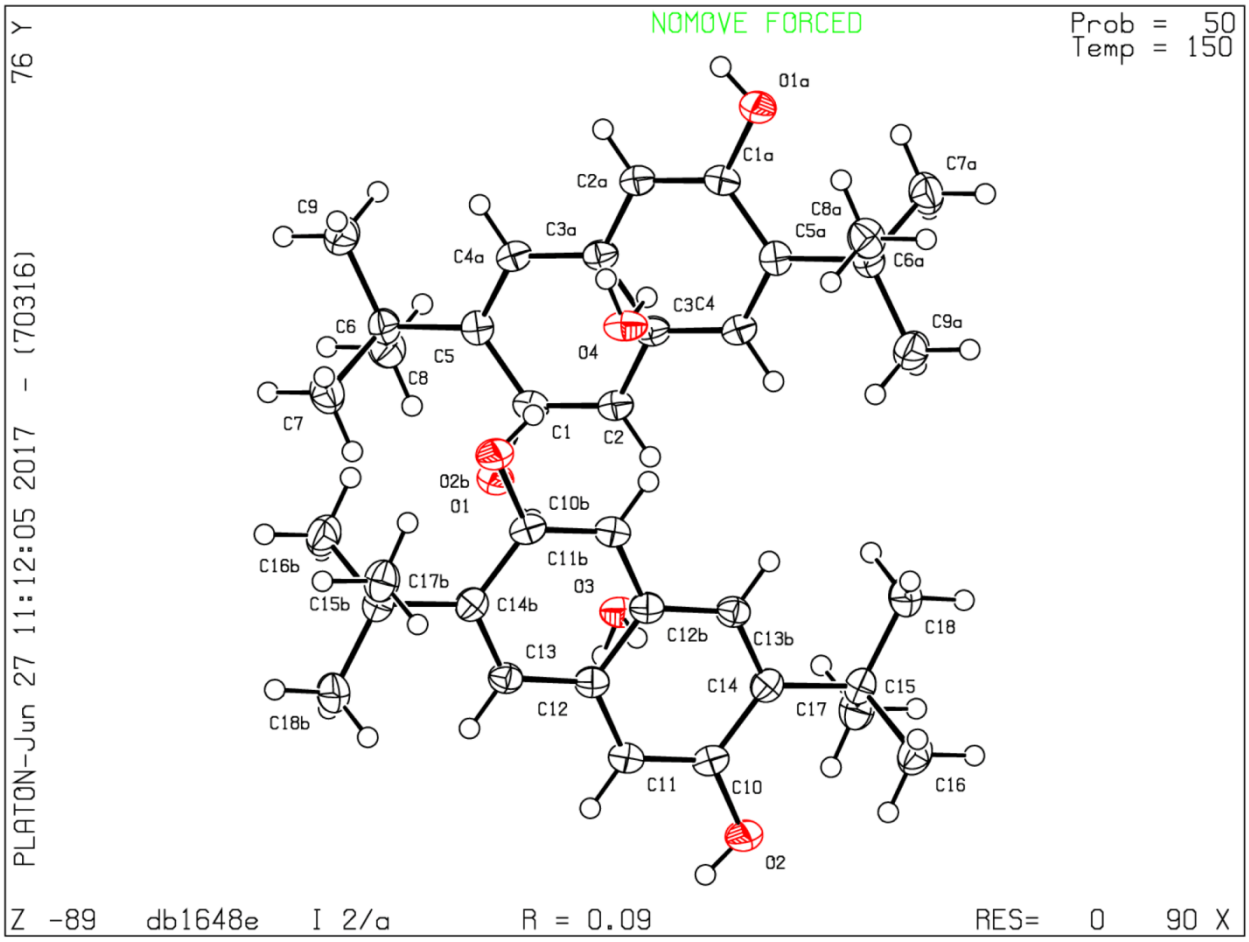


Table S1. Crystal data and structure refinement for **2**.

Identification code	1558768 (**2**)
Empirical formula	C36 H52 O6
Formula weight	580.77
Temperature	150(2) K
Wavelength	1.54184 Å
Crystal system	Monoclinic

Space group	I 2/a	
Unit cell dimensions	a = 12.2515(4) Å	α= 90°.
	b = 11.0764(3) Å	β= 104.115(4)°.
	c = 24.8986(10) Å	γ = 90°.
Volume	3276.8(2) $Å^3$	
Z	4	
Density (calculated)	1.177 Mg/m^3	
Absorption coefficient	0.622 mm^{-1}	
F(000)	1264	
Crystal size	0.260 x 0.182 x 0.068 mm^3	
Theta range for data collection	3.661 to 73.864°.	
Index ranges	-15<=h<=14, -8<=k<=13, -30<=l<=30	
Reflections collected	9291	
Independent reflections	4729 [R(int) = 0.0329]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.52751	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4729 / 0 / 206	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0897, wR2 = 0.2341	
R indices (all data)	R1 = 0.1000, wR2 = 0.2576	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.738 and -0.338 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	4045(2)	3711(2)	5591(1)	26(1)
C(2)	4151(2)	3637(2)	5055(1)	26(1)
C(3)	4754(2)	4512(2)	4830(1)	24(1)
C(4)	4899(2)	4440(2)	4282(1)	25(1)
C(5)	4510(2)	4722(2)	5941(1)	24(1)
C(6)	4335(3)	4844(2)	6531(1)	29(1)
C(7)	4902(3)	3778(3)	6885(1)	38(1)

C(8)	3074(3)	4881(2)	6514(2)	34(1)
C(9)	4863(3)	6013(3)	6811(1)	38(1)
C(10)	3458(2)	-1278(2)	4407(1)	26(1)
C(11)	4096(2)	-1366(2)	4942(1)	26(1)
C(12)	4919(2)	-491(2)	5170(1)	25(1)
C(13)	5616(2)	-574(2)	5716(1)	25(1)
C(14)	3573(2)	-271(2)	4061(1)	26(1)
C(15)	2825(3)	-132(2)	3470(1)	27(1)
C(16)	3040(3)	-1192(3)	3115(1)	38(1)
C(17)	1571(3)	-114(2)	3490(2)	34(1)
C(18)	3058(3)	1047(3)	3196(1)	37(1)
O(1)	3496(1)	2839(2)	5808(1)	33(1)
O(2)	2693(1)	-2156(2)	4188(1)	34(1)
O(3)	2500	1141(2)	5000	30(1)
O(4)	7500	3854(2)	5000	31(1)

Table S3. Bond lengths [Å] and angles [°] for **2**.

C(1)-O(1)	1.362(3)
C(1)-C(2)	1.374(3)
C(1)-C(5)	1.447(3)
C(2)-C(3)	1.415(3)
C(2)-H(2)	0.9500
C(3)-C(3)#1	1.414(4)
C(3)-C(4)	1.421(3)
C(4)-C(5)#1	1.375(3)
C(4)-H(4)	0.9500
C(5)-C(4)#1	1.375(3)
C(5)-C(6)	1.541(4)
C(6)-C(7)	1.535(4)
C(6)-C(8)	1.535(5)
C(6)-C(9)	1.537(4)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-O(2)	1.368(3)
C(10)-C(11)	1.374(3)
C(10)-C(14)	1.438(3)
C(11)-C(12)	1.413(3)
C(11)-H(11)	0.9500
C(12)-C(12)#2	1.420(5)
C(12)-C(13)	1.421(3)
C(13)-C(14)#2	1.379(3)
C(13)-H(13)	0.9500
C(14)-C(13)#2	1.379(3)
C(14)-C(15)	1.539(4)
C(15)-C(18)	1.531(4)
C(15)-C(16)	1.532(4)
C(15)-C(17)	1.549(5)

C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
O(1)-H(1A)	0.8400
O(2)-H(2A)	0.8400
O(3)-H(3)	0.85(4)
O(4)-H(4A)	0.87(4)

O(1)-C(1)-C(2)	121.00(19)
O(1)-C(1)-C(5)	118.0(2)
C(2)-C(1)-C(5)	121.0(2)
C(1)-C(2)-C(3)	121.7(2)
C(1)-C(2)-H(2)	119.1
C(3)-C(2)-H(2)	119.1
C(3)#1-C(3)-C(2)	118.4(3)
C(3)#1-C(3)-C(4)	118.8(2)
C(2)-C(3)-C(4)	122.9(2)
C(5)#1-C(4)-C(3)	123.5(2)
C(5)#1-C(4)-H(4)	118.2
C(3)-C(4)-H(4)	118.2
C(4)#1-C(5)-C(1)	116.6(2)
C(4)#1-C(5)-C(6)	122.3(2)
C(1)-C(5)-C(6)	121.1(2)
C(7)-C(6)-C(8)	110.3(3)
C(7)-C(6)-C(9)	107.8(3)
C(8)-C(6)-C(9)	107.4(3)
C(7)-C(6)-C(5)	109.3(2)
C(8)-C(6)-C(5)	110.5(3)
C(9)-C(6)-C(5)	111.5(2)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5

H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5
C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(2)-C(10)-C(11)	120.6(2)
O(2)-C(10)-C(14)	118.0(2)
C(11)-C(10)-C(14)	121.4(2)
C(10)-C(11)-C(12)	121.4(2)
C(10)-C(11)-H(11)	119.3
C(12)-C(11)-H(11)	119.3
C(11)-C(12)-C(12)#2	118.4(3)
C(11)-C(12)-C(13)	122.8(2)
C(12)#2-C(12)-C(13)	118.7(2)
C(14)#2-C(13)-C(12)	123.2(2)
C(14)#2-C(13)-H(13)	118.4
C(12)-C(13)-H(13)	118.4
C(13)#2-C(14)-C(10)	116.8(2)
C(13)#2-C(14)-C(15)	121.4(2)
C(10)-C(14)-C(15)	121.9(2)
C(18)-C(15)-C(16)	108.6(3)
C(18)-C(15)-C(14)	112.2(2)
C(16)-C(15)-C(14)	109.2(2)
C(18)-C(15)-C(17)	107.3(2)
C(16)-C(15)-C(17)	109.8(3)
C(14)-C(15)-C(17)	109.6(3)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(1)-O(1)-H(1A)	109.5
C(10)-O(2)-H(2A)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x+1,-y,-z+1

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	25(1)	22(1)	32(1)	2(1)	7(1)	0(1)
C(2)	24(1)	21(1)	31(1)	-1(1)	6(1)	0(1)
C(3)	21(1)	21(1)	30(1)	-1(1)	5(1)	2(1)
C(4)	22(1)	22(1)	30(1)	-3(1)	5(1)	0(1)
C(5)	21(1)	27(1)	26(1)	0(1)	7(1)	4(1)
C(6)	31(2)	31(1)	24(1)	1(1)	8(1)	0(1)
C(7)	43(2)	41(2)	29(1)	5(1)	5(1)	5(1)
C(8)	33(2)	40(2)	35(2)	1(1)	16(1)	1(1)
C(9)	46(2)	39(2)	31(1)	-6(1)	13(1)	-8(1)
C(10)	24(1)	22(1)	32(1)	-4(1)	7(1)	-1(1)
C(11)	26(1)	22(1)	32(1)	1(1)	9(1)	0(1)
C(12)	23(1)	23(1)	29(1)	0(1)	8(1)	2(1)
C(13)	25(1)	22(1)	29(1)	0(1)	9(1)	1(1)
C(14)	24(1)	27(1)	27(1)	-3(1)	8(1)	2(1)
C(15)	26(1)	31(1)	24(1)	-4(1)	5(1)	2(1)

C(16)	47(2)	38(2)	29(1)	-7(1)	9(1)	3(1)
C(17)	28(2)	42(2)	31(2)	-1(1)	2(1)	3(1)
C(18)	42(2)	39(1)	27(1)	4(1)	1(1)	-2(1)
O(1)	40(1)	28(1)	33(1)	0(1)	13(1)	-9(1)
O(2)	37(1)	28(1)	35(1)	-1(1)	3(1)	-10(1)
O(3)	28(1)	22(1)	41(1)	0	14(1)	0
O(4)	23(1)	21(1)	47(1)	0	4(1)	0

Crystal data for compound 3

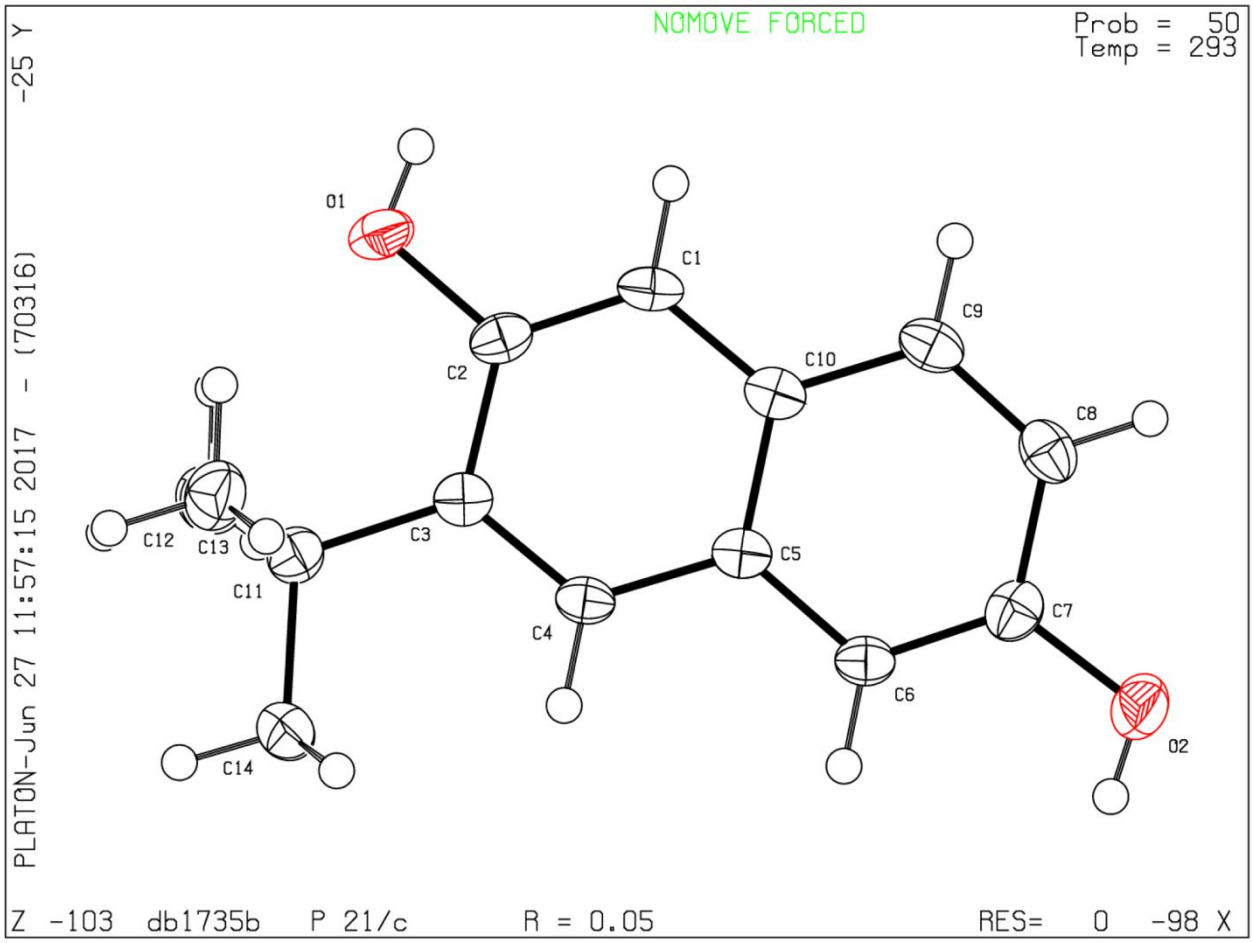


Table S5. Crystal data and structure refinement for **3**.

Identification code	1558766 (**3)**	
Empirical formula	C14 H16 O2	
Formula weight	216.27	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 6.4201(3) Å	α= 90°.

	b = 7.1231(5) Å	β= 94.017(6)°.
	c = 25.2730(14) Å	γ = 90°.
Volume	1152.92(12) $Å^3$	
Z	4	
Density (calculated)	1.246 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	464	
Crystal size	0.775 x 0.646 x 0.135 mm^3	
Theta range for data collection	2.972 to 29.635°.	
Index ranges	-6<=h<=8, -9<=k<=7, -33<=l<=34	
Reflections collected	5223	
Independent reflections	2724 [R(int) = 0.0187]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.340	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2724 / 0 / 145	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1102	
R indices (all data)	R1 = 0.0707, wR2 = 0.1240	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.222 and -0.223 $e.Å^{-3}$	

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 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)
O(1)	11338(2)	4645(2)	1190(1)	33(1)
O(2)	4243(2)	2605(2)	3480(1)	39(1)
C(5)	6799(2)	3215(2)	2225(1)	20(1)
C(12)	9232(2)	1617(3)	528(1)	37(1)
C(4)	6514(2)	2866(2)	1673(1)	21(1)
C(3)	7961(2)	3323(2)	1318(1)	22(1)
C(11)	7572(2)	2953(2)	721(1)	26(1)
C(10)	8679(2)	4083(2)	2426(1)	22(1)
C(2)	9848(2)	4192(2)	1535(1)	23(1)

C(9)	8974(2)	4437(2)	2978(1)	25(1)
C(1)	10174(2)	4554(2)	2065(1)	23(1)
C(6)	5270(2)	2723(2)	2579(1)	22(1)
C(7)	5613(2)	3077(2)	3109(1)	26(1)
C(14)	5447(2)	2025(3)	591(1)	32(1)
C(8)	7476(2)	3949(2)	3310(1)	27(1)
C(13)	7596(2)	4824(2)	419(1)	35(1)

Table S7. Bond lengths [Å] and angles [°] for **3**.

O(1)-C(2)	1.3767(15)
O(1)-H(1A)	0.8200
O(2)-C(7)	1.3712(16)
O(2)-H(10)	0.8200
C(5)-C(4)	1.4168(18)
C(5)-C(6)	1.4177(18)
C(5)-C(10)	1.4184(19)
C(12)-C(11)	1.534(2)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(4)-C(3)	1.3747(18)
C(4)-H(4)	0.9300
C(3)-C(2)	1.4350(19)
C(3)-C(11)	1.5331(19)
C(11)-C(14)	1.5313(19)
C(11)-C(13)	1.537(2)
C(10)-C(1)	1.4106(18)
C(10)-C(9)	1.4175(19)
C(2)-C(1)	1.3647(19)
C(9)-C(8)	1.365(2)
C(9)-H(9)	0.9300
C(1)-H(1)	0.9300
C(6)-C(7)	1.3662(19)
C(6)-H(6)	0.9300
C(7)-C(8)	1.410(2)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600

C(8)-H(8)	0.9300
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600

C(2)-O(1)-H(1A)	109.5
C(7)-O(2)-H(10)	109.5
C(4)-C(5)-C(6)	122.12(12)
C(4)-C(5)-C(10)	118.48(12)
C(6)-C(5)-C(10)	119.40(12)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(3)-C(4)-C(5)	123.69(12)
C(3)-C(4)-H(4)	118.2
C(5)-C(4)-H(4)	118.2
C(4)-C(3)-C(2)	116.33(12)
C(4)-C(3)-C(11)	121.98(12)
C(2)-C(3)-C(11)	121.69(12)
C(14)-C(11)-C(3)	111.59(11)
C(14)-C(11)-C(12)	106.97(13)
C(3)-C(11)-C(12)	110.57(11)
C(14)-C(11)-C(13)	107.85(12)
C(3)-C(11)-C(13)	109.42(12)
C(12)-C(11)-C(13)	110.38(12)
C(1)-C(10)-C(9)	123.01(12)
C(1)-C(10)-C(5)	118.22(12)
C(9)-C(10)-C(5)	118.78(13)
C(1)-C(2)-O(1)	120.71(12)
C(1)-C(2)-C(3)	121.61(12)
O(1)-C(2)-C(3)	117.67(12)
C(8)-C(9)-C(10)	120.63(13)
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7
C(2)-C(1)-C(10)	121.67(12)
C(2)-C(1)-H(1)	119.2
C(10)-C(1)-H(1)	119.2

C(7)-C(6)-C(5)	120.19(13)
C(7)-C(6)-H(6)	119.9
C(5)-C(6)-H(6)	119.9
C(6)-C(7)-O(2)	123.90(13)
C(6)-C(7)-C(8)	120.59(13)
O(2)-C(7)-C(8)	115.51(12)
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(9)-C(8)-C(7)	120.41(13)
C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **3**. The anisotropicdisplacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	21(1)	40(1)	37(1)	-6(1)	8(1)	-8(1)
O(2)	48(1)	39(1)	30(1)	-4(1)	13(1)	-17(1)
C(5)	20(1)	14(1)	27(1)	1(1)	-1(1)	2(1)
C(12)	30(1)	43(1)	38(1)	-12(1)	3(1)	7(1)
C(4)	17(1)	19(1)	27(1)	1(1)	-2(1)	0(1)
C(3)	20(1)	17(1)	27(1)	1(1)	1(1)	4(1)
C(11)	22(1)	29(1)	26(1)	-1(1)	3(1)	3(1)
C(10)	21(1)	14(1)	28(1)	0(1)	-3(1)	3(1)

C(2)	18(1)	19(1)	32(1)	1(1)	4(1)	2(1)
C(9)	25(1)	19(1)	31(1)	-3(1)	-4(1)	1(1)
C(1)	17(1)	18(1)	34(1)	-3(1)	-2(1)	-2(1)
C(6)	22(1)	16(1)	28(1)	-1(1)	1(1)	-2(1)
C(7)	31(1)	19(1)	29(1)	2(1)	7(1)	0(1)
C(14)	26(1)	42(1)	26(1)	-4(1)	-1(1)	-2(1)
C(8)	35(1)	21(1)	24(1)	-2(1)	-3(1)	1(1)
C(13)	34(1)	41(1)	30(1)	6(1)	4(1)	2(1)

Crystal data for compound 5

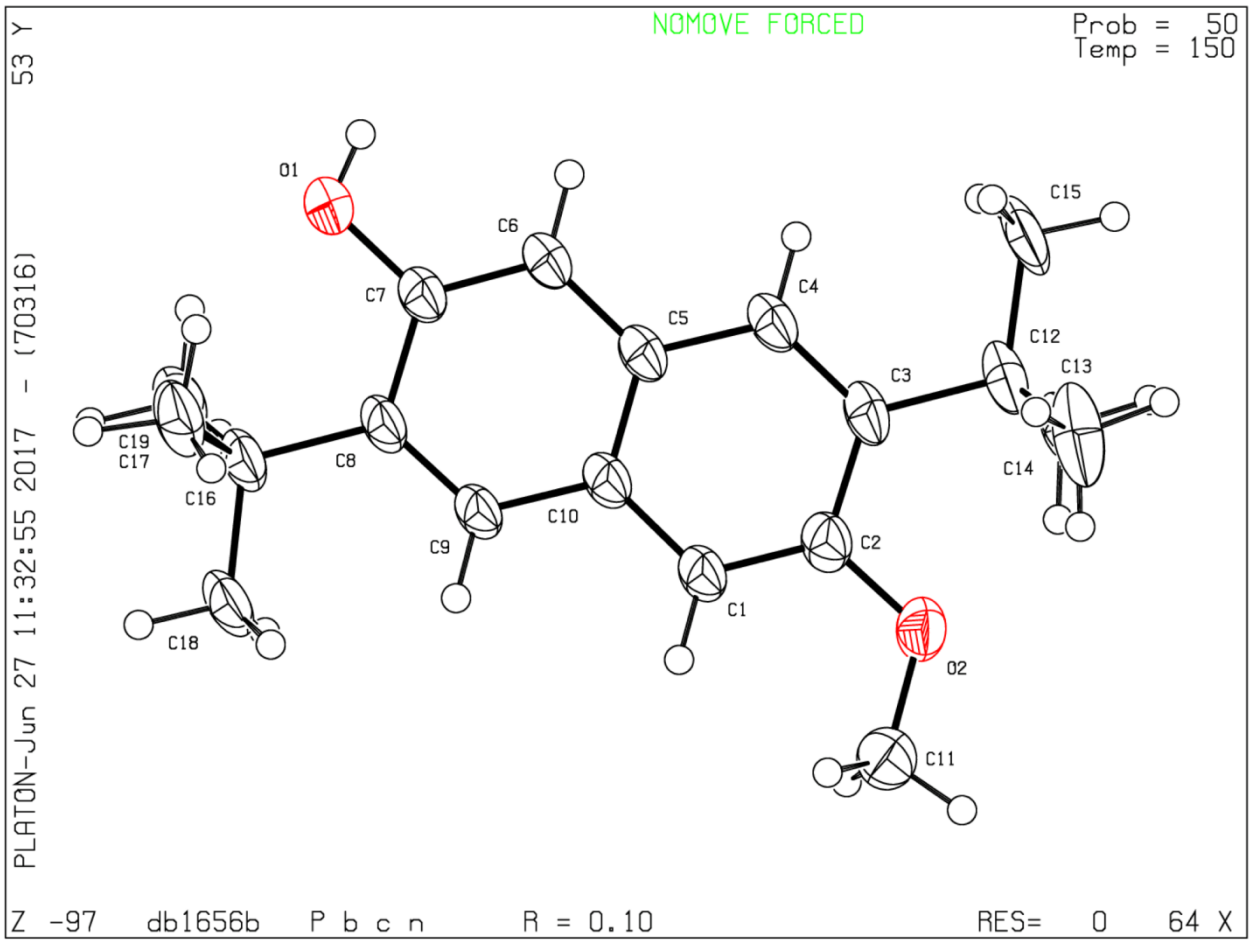


Table S9. Crystal data and structure refinement for **5**.

Identification code	1558767 (**5**)	
Empirical formula	C19 H26 O2	
Formula weight	286.40	
Temperature	150(2) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	P b c n	
Unit cell dimensions	a = 21.420(2) Å	α= 90°.

	b = 6.4137(6) Å	β= 90°.
	c = 24.380(2) Å	γ = 90°.
Volume	3349.3(6) $Å^3$	
Z	8	
Density (calculated)	1.136 Mg/m^3	
Absorption coefficient	0.557 mm^{-1}	
F(000)	1248	
Crystal size	0.940 x 0.157 x 0.084 mm^3	
Theta range for data collection	3.626 to 70.134°.	
Index ranges	-18<=h<=25, -7<=k<=7, -29<=l<=23	
Reflections collected	8334	
Independent reflections	3165 [R(int) = 0.0777]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.28053	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3165 / 0 / 198	
Goodness-of-fit on F^2	1.096	
Final R indices [I>2sigma(I)]	R1 = 0.0968, wR2 = 0.2641	
R indices (all data)	R1 = 0.1214, wR2 = 0.2853	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.282 and -0.383 $e.Å^{-3}$	

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	855(2)	9630(6)	1287(1)	38(1)
C(2)	912(2)	8899(6)	766(2)	37(1)
C(3)	1279(2)	9975(6)	363(1)	37(1)
C(4)	1594(2)	11745(6)	539(1)	36(1)
C(5)	1549(2)	12515(6)	1083(1)	34(1)
C(6)	1864(2)	14336(6)	1260(1)	37(1)
C(7)	1791(2)	15066(6)	1787(1)	36(1)
C(8)	1393(2)	14034(6)	2176(1)	37(1)
C(9)	1099(2)	12264(5)	1995(1)	36(1)

C(10)	1168(2)	11461(6)	1460(1)	35(1)
C(11)	264(2)	5969(7)	971(2)	51(1)
C(12)	1304(2)	9254(7)	-233(2)	45(1)
C(13)	1559(3)	6991(10)	-263(2)	71(2)
C(14)	649(2)	9325(7)	-485(1)	44(1)
C(15)	1715(3)	10664(11)	-585(2)	79(2)
C(16)	1318(2)	14873(6)	2764(1)	42(1)
C(17)	1948(2)	14796(8)	3062(2)	56(1)
C(18)	855(2)	13527(7)	3090(2)	51(1)
C(19)	1057(3)	17098(6)	2754(2)	55(1)
O(1)	2097(2)	16822(4)	1963(1)	48(1)
O(2)	619(1)	7134(4)	583(1)	46(1)

Table S11. Bond lengths [Å] and angles [°] for **5**.

C(1)-C(2)	1.361(5)
C(1)-C(10)	1.417(5)
C(1)-H(1)	0.9500
C(2)-O(2)	1.368(5)
C(2)-C(3)	1.434(5)
C(3)-C(4)	1.389(5)
C(3)-C(12)	1.527(5)
C(4)-C(5)	1.419(5)
C(4)-H(4)	0.9500
C(5)-C(10)	1.402(5)
C(5)-C(6)	1.415(5)
C(6)-C(7)	1.376(5)
C(6)-H(6)	0.9500
C(7)-O(1)	1.373(4)
C(7)-C(8)	1.437(5)
C(8)-C(9)	1.371(5)
C(8)-C(16)	1.539(5)
C(9)-C(10)	1.409(5)
C(9)-H(9)	0.9500
C(11)-O(2)	1.424(5)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800

C(11)-H(11C)	0.9800
C(12)-C(15)	1.525(7)
C(12)-C(14)	1.532(6)
C(12)-C(13)	1.552(7)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(19)	1.532(6)
C(16)-C(17)	1.533(7)
C(16)-C(18)	1.536(6)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
O(1)-H(1A)	0.8400

C(2)-C(1)-C(10)	121.4(3)
C(2)-C(1)-H(1)	119.3
C(10)-C(1)-H(1)	119.3
C(1)-C(2)-O(2)	123.2(3)
C(1)-C(2)-C(3)	121.5(3)
O(2)-C(2)-C(3)	115.3(3)
C(4)-C(3)-C(2)	116.7(3)
C(4)-C(3)-C(12)	121.6(3)
C(2)-C(3)-C(12)	121.7(4)
C(3)-C(4)-C(5)	122.7(3)
C(3)-C(4)-H(4)	118.6
C(5)-C(4)-H(4)	118.6
C(10)-C(5)-C(6)	118.4(3)

C(10)-C(5)-C(4)	119.0(3)
C(6)-C(5)-C(4)	122.6(3)
C(7)-C(6)-C(5)	120.6(3)
C(7)-C(6)-H(6)	119.7
C(5)-C(6)-H(6)	119.7
O(1)-C(7)-C(6)	121.2(3)
O(1)-C(7)-C(8)	116.9(3)
C(6)-C(7)-C(8)	121.9(3)
C(9)-C(8)-C(7)	116.1(3)
C(9)-C(8)-C(16)	122.8(3)
C(7)-C(8)-C(16)	121.1(3)
C(8)-C(9)-C(10)	123.5(3)
C(8)-C(9)-H(9)	118.2
C(10)-C(9)-H(9)	118.2
C(5)-C(10)-C(9)	119.4(3)
C(5)-C(10)-C(1)	118.7(3)
C(9)-C(10)-C(1)	121.9(3)
O(2)-C(11)-H(11A)	109.5
O(2)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(2)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(15)-C(12)-C(3)	112.1(4)
C(15)-C(12)-C(14)	106.6(4)
C(3)-C(12)-C(14)	109.8(3)
C(15)-C(12)-C(13)	109.0(4)
C(3)-C(12)-C(13)	109.9(4)
C(14)-C(12)-C(13)	109.3(4)
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(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5

H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(19)-C(16)-C(17)	111.0(4)
C(19)-C(16)-C(18)	107.3(4)
C(17)-C(16)-C(18)	107.7(3)
C(19)-C(16)-C(8)	110.4(3)
C(17)-C(16)-C(8)	109.7(3)
C(18)-C(16)-C(8)	110.7(3)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(7)-O(1)-H(1A)	109.5
C(2)-O(2)-C(11)	117.6(3)

Symmetry transformations used to generate equivalent atoms:

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **5**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	57(2)	37(2)	21(2)	3(1)	-1(2)	-2(2)
C(2)	48(2)	39(2)	26(2)	2(1)	-7(2)	2(1)
C(3)	38(2)	53(2)	20(2)	-4(1)	-4(2)	4(2)
C(4)	36(2)	52(2)	20(2)	1(1)	0(1)	1(1)
C(5)	39(2)	43(2)	20(2)	2(1)	-2(1)	2(1)
C(6)	46(2)	44(2)	21(2)	1(1)	2(2)	-1(1)
C(7)	45(2)	40(2)	22(2)	1(1)	0(1)	-1(1)
C(8)	54(2)	40(2)	17(2)	2(1)	1(2)	1(1)
C(9)	53(2)	36(2)	18(2)	4(1)	0(1)	0(1)
C(10)	46(2)	40(2)	20(2)	3(1)	-2(1)	0(1)
C(11)	68(3)	45(2)	38(2)	4(2)	-5(2)	-7(2)
C(12)	40(2)	73(3)	23(2)	-14(2)	1(2)	6(2)
C(13)	66(3)	104(4)	43(2)	-32(3)	-10(2)	34(3)
C(14)	49(2)	66(3)	17(2)	-7(2)	-4(2)	3(2)
C(15)	64(3)	152(6)	22(2)	-30(3)	14(2)	-39(3)
C(16)	64(3)	45(2)	18(2)	-1(1)	3(2)	1(2)
C(17)	75(3)	71(3)	23(2)	-6(2)	-3(2)	2(2)
C(18)	81(3)	54(2)	19(2)	1(2)	9(2)	1(2)
C(19)	88(3)	46(2)	29(2)	-2(2)	12(2)	6(2)
O(1)	67(2)	48(2)	28(1)	-6(1)	7(1)	-14(1)
O(2)	67(2)	41(1)	31(1)	-4(1)	-6(1)	-6(1)

References:

1S - CrysAlisPro, Agilent Technologies, Version 1.171.37.33 (release 27-03-2014 CrysAlis171.NET)

2S - G. M. Sheldrick, *SHELX-2013: Program for the Solution of Crystal Structures* **2013** University of Göttingen.