

## APPENDIX 1

Ethyl 5-(2-hydroxy-5-isopropylbenzoyl)-2-methylbenzoate (6)

**Anal. Calcd. For C<sub>20</sub>H<sub>22</sub>O<sub>4</sub>: C, 73.60; H, 6.79; Found: C, 73.46; H, 7.00.**

5-(3-Hydroxy-5,5,8,8-tetramethyl-5,6,7,8-tetrahydronaphthalene-2-carbonyl)-2-methylbenzoic acid (10)

**Anal. Calcd. For C<sub>23</sub>H<sub>26</sub>O<sub>4</sub>: C, 75.38, H, 7.15; Found: C, 75.09, H, 7.34.**

APPENDIX 2

X-RAY CRYSTAL DATA FOR COMPOUND 5

Table 1. Refined Positional Parameters for Compound 5

Atom	x	y	z	U <sub>eq</sub> , Å <sup>2</sup>
C1	0.1119(2)	0.7628(2)	0.19503(11)	0.0239(3)
H1	0.0258	0.6834	0.2195	0.032
C2	0.0516(2)	0.8144(2)	0.10365(12)	0.0289(3)
H2	-0.0735	0.7695	0.0662	0.039
C3	0.1796(2)	0.9341(2)	0.06796(11)	0.0275(3)
H3	0.1411	0.9665	0.0039	0.037
C4	0.3620(2)	1.0051(2)	0.12590(11)	0.0248(3)
H4	0.4446	1.0876	0.1033	0.033
C5	0.4238(2)	0.9540(2)	0.21830(11)	0.0212(3)
C6	0.3004(2)	0.8277(2)	0.25194(10)	0.0195(3)
C7	0.3730(2)	0.7703(2)	0.34532(10)	0.0200(3)
C8	0.2740(2)	0.61625(14)	0.36262(10)	0.0191(3)
C9	0.3023(2)	0.60092(14)	0.48278(10)	0.0186(3)
H9	0.3661	0.6892	0.5506	0.025
C10	0.2380(2)	0.45760(14)	0.50453(10)	0.0180(3)
C11	0.1406(2)	0.32261(14)	0.40217(10)	0.0192(3)
C12	0.1122(2)	0.3399(2)	0.28268(11)	0.0226(3)
H12	0.0473	0.2524	0.2146	0.030
C13	0.1774(2)	0.4827(2)	0.26207(11)	0.0214(3)
H13	0.1568	0.4899	0.1809	0.028
C14	0.2834(2)	0.4450(2)	0.62979(10)	0.0187(3)
H14	0.2697	0.3451	0.6323	0.025
C15	0.3421(2)	0.5620(2)	0.74012(11)	0.0214(3)
H15	0.3450	0.6625	0.7447	0.029
C16	0.4020(2)	0.5335(2)	0.85446(10)	0.0196(3)
C17	0.0703(2)	0.1647(2)	0.41889(11)	0.0258(3)
H17a	0.0063	0.0890	0.3394	0.039
H17b	-0.0183	0.1671	0.4867	0.039
H17c	0.1780	0.1368	0.4413	0.039
O1	0.60489(12)	1.02943(11)	0.27190(8)	0.0316(3)
H1a	0.6235	0.9966	0.3299	0.047
O2	0.52546(12)	0.85028(10)	0.41123(7)	0.0260(2)
O3	0.38904(12)	0.40266(10)	0.85837(7)	0.0253(2)
O4	0.47421(14)	0.66172(10)	0.95269(7)	0.0295(3)
H4a	0.5138	0.6395	1.0113	0.044
$U_{eq} = \frac{1}{3} [U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos \gamma + 2U_{13}aa^*cc^* \cos \beta + 2U_{23}bb^*cc^* \cos \alpha]$				

**Table 2. Refined Thermal Parameters (U's) for Compound 5**

Atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>23</sub>	U <sub>13</sub>	U <sub>12</sub>
C1	0.0239(7)	0.0246(8)	0.0271(6)	0.0134(6)	0.0037(5)	0.0075(6)
C2	0.0249(7)	0.0337(9)	0.0325(7)	0.0154(6)	-0.0042(6)	0.0089(6)
C3	0.0361(8)	0.0292(8)	0.0244(6)	0.0141(6)	-0.0010(6)	0.0139(6)
C4	0.0336(7)	0.0207(8)	0.0226(6)	0.0102(5)	0.0047(5)	0.0087(6)
C5	0.0241(7)	0.0193(7)	0.0190(6)	0.0038(5)	0.0014(5)	0.0075(5)
C6	0.0244(7)	0.0193(7)	0.0166(6)	0.0058(5)	0.0024(5)	0.0091(5)
C7	0.0248(7)	0.0206(7)	0.0152(6)	0.0036(5)	0.0020(5)	0.0102(6)
C8	0.0204(6)	0.0217(7)	0.0188(6)	0.0084(5)	0.0008(5)	0.0093(5)
C9	0.0202(6)	0.0186(7)	0.0160(6)	0.0026(5)	-0.0008(5)	0.0075(5)
C10	0.0173(6)	0.0220(7)	0.0178(6)	0.0080(5)	0.0016(5)	0.0087(5)
C11	0.0181(6)	0.0205(7)	0.0203(6)	0.0065(5)	0.0010(5)	0.0078(5)
C12	0.0246(7)	0.0213(7)	0.0189(6)	0.0022(5)	-0.0049(5)	0.0065(6)
C13	0.0248(6)	0.0259(8)	0.0159(6)	0.0075(5)	-0.0010(5)	0.0101(6)
C14	0.0173(6)	0.0191(7)	0.0218(6)	0.0100(5)	0.0018(5)	0.0050(5)
C15	0.0255(7)	0.0214(7)	0.0213(6)	0.0101(5)	0.0007(5)	0.0091(5)
C16	0.0206(6)	0.0209(7)	0.0172(6)	0.0069(5)	0.0030(5)	0.0055(5)
C17	0.0293(7)	0.0232(8)	0.0235(6)	0.0069(5)	-0.0039(5)	0.0059(6)
O1	0.0302(5)	0.0275(6)	0.0348(5)	0.0157(4)	-0.0083(4)	-0.0020(4)
O2	0.0295(5)	0.0227(5)	0.0244(4)	0.0077(4)	-0.0069(4)	0.0045(4)
O3	0.0354(5)	0.0203(5)	0.0204(4)	0.0093(4)	-0.0051(4)	0.0045(4)
O4	0.0510(6)	0.0214(5)	0.0166(4)	0.0062(4)	-0.0072(4)	0.0103(4)

The form of the anisotropic displacement parameter is:

$$\exp[-2\pi^2(a^2U_{11}h^2+b^2U_{22}k^2+c^2U_{33}l^2+2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)].$$

**Table 3. Bond Distances in Compound 5, Å**

C1-C2	1.377(2)	C1-C6	1.403(2)	C2-C3	1.390(2)
C3-C4	1.371(2)	C4-C5	1.389(2)	C5-O1	1.3509(14)
C5-C6	1.410(2)	C6-C7	1.477(2)	C7-O2	1.2408(14)
C7-C8	1.491(2)	C8-C9	1.394(2)	C8-C13	1.395(2)
C9-C10	1.392(2)	C10-C11	1.414(2)	C10-C14	1.468(2)
C11-C12	1.395(2)	C11-C17	1.498(2)	C12-C13	1.382(2)
C14-C15	1.330(2)	C15-C16	1.466(2)	C16-O3	1.229(2)
C16-O4	1.3173(14)				

**Table 4. Bond Angles in Compound 5, °**

C2-C1-C6	121.38(12)	C1-C2-C3	119.31(11)	C4-C3-C2	120.87(11)
C3-C4-C5	120.14(12)	O1-C5-C4	117.09(11)	O1-C5-C6	122.63(10)
C4-C5-C6	120.27(11)	C1-C6-C5	117.89(10)	C1-C6-C7	122.90(11)
C5-C6-C7	119.21(10)	O2-C7-C6	119.63(11)	O2-C7-C8	117.38(10)
C6-C7-C8	122.96(10)	C9-C8-C13	118.25(11)	C9-C8-C7	117.22(10)
C13-C8-C7	123.95(10)	C10-C9-C8	122.09(11)	C9-C10-C11	119.41(10)
C9-C10-C14	120.17(10)	C11-C10-C14	120.28(11)	C12-C11-C10	117.86(11)
C12-C11-C17	120.16(10)	C10-C11-C17	121.98(10)	C13-C12-C11	122.21(11)
C12-C13-C8	120.18(10)	C15-C14-C10	126.52(12)	C14-C15-C16	120.32(12)
O3-C16-O4	122.81(10)	O3-C16-C15	123.43(11)	O4-C16-C15	113.75(11)

**APPENDIX 3**  
**X-RAY CRYSTAL DATA FOR COMPOUND 10**

**Table 5. Refined Positional Parameters for Compound 10**

Atom	x	y	z	U <sub>eq</sub> , Å <sup>2</sup>
C1	0.4930(3)	0.6135(2)	0.7317(2)	0.0289(6)
H1	0.5819	0.6203	0.7860	0.038
C2	0.4131(3)	0.7246(2)	0.7119(2)	0.0276(5)
C3	0.2774(3)	0.7135(2)	0.6305(2)	0.0270(5)
C4	0.2262(3)	0.5926(2)	0.5775(2)	0.0293(6)
H4	0.1344	0.5852	0.5266	0.039
C5	0.3077(3)	0.4821(2)	0.5980(2)	0.0290(6)
C6	0.4476(3)	0.4920(2)	0.6746(2)	0.0279(6)
C7	0.5373(3)	0.3762(2)	0.6943(2)	0.0305(6)
C8	0.6993(3)	0.3865(2)	0.7534(2)	0.0291(6)
C9	0.7503(3)	0.2848(2)	0.8209(2)	0.0277(5)
H9	0.6806	0.2179	0.8340	0.037
C10	0.9037(3)	0.2799(2)	0.8698(2)	0.0285(6)
C11	1.0104(3)	0.3808(2)	0.8532(2)	0.0311(6)
C12	0.9575(3)	0.4820(2)	0.7849(2)	0.0327(6)
H12	1.0261	0.5501	0.7730	0.044
C13	0.8059(3)	0.4849(2)	0.7339(2)	0.0311(6)
H13	0.7756	0.5529	0.6866	0.041
C14	0.9476(3)	0.1612(2)	0.9320(2)	0.0303(6)
C15	1.1780(3)	0.3870(3)	0.9032(3)	0.0417(7)
H15a	1.1851	0.3768	0.9908	0.063
H15b	1.2247	0.4691	0.8877	0.063
H15c	1.2306	0.3191	0.8628	0.063
C16	0.4831(3)	0.8526(2)	0.7718(2)	0.0309(6)
C17	0.3628(3)	0.9573(2)	0.7654(2)	0.0367(6)
H17a	0.2909	0.9436	0.8273	0.049
H17b	0.4147	1.0413	0.7850	0.049
C18	0.2745(3)	0.9569(2)	0.6400(2)	0.0377(6)
H18a	0.3466	0.9713	0.5783	0.050
H18b	0.2054	1.0279	0.6400	0.050
C19	0.1805(3)	0.8308(2)	0.6031(2)	0.0297(6)
C20	0.6211(3)	0.8926(3)	0.7021(3)	0.0477(7)
H20a	0.6959	0.8271	0.7068	0.071
H20b	0.6669	0.9729	0.7390	0.071
H20c	0.5871	0.9027	0.6169	0.071
C21	0.5378(3)	0.8409(2)	0.9083(3)	0.0428(7)
H21a	0.4542	0.8074	0.9508	0.064
H21b	0.5720	0.9246	0.9454	0.064
H21c	0.6216	0.7835	0.9143	0.064
C22	0.0384(3)	0.8234(2)	0.6776(3)	0.0403(7)
H22a	0.0712	0.8196	0.7640	0.060

H22b	-0.0241	0.7474	0.6495	0.060
H22c	-0.0206	0.8986	0.6658	0.060
C23	0.1268(3)	0.8304(2)	0.4655(3)	0.0440(7)
H23a	0.0746	0.9082	0.4496	0.066
H23b	0.0577	0.7570	0.4425	0.066
H23c	0.2145	0.8257	0.4178	0.066
O1	0.2489(2)	0.3687(2)	0.5419(2)	0.0389(5)
H1a	0.2982	0.3092	0.5688	0.058
O2	0.4807(2)	0.2675(2)	0.6596(2)	0.0420(5)
O3	1.0850(2)	0.1404(2)	0.9621(2)	0.0594(6)
O4	0.8387(2)	0.0812(2)	0.9499(2)	0.0520(6)
H4a	0.8750	0.0140	0.9729	0.078
$U_{eq} = \frac{1}{3} [U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha]$				

**Table 6. Refined Thermal Parameters (U's) for Compound 10**

Atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>23</sub>	U <sub>13</sub>	U <sub>12</sub>
C1	0.0241(12)	0.0307(12)	0.0313(13)	0.0053(10)	-0.0038(10)	0.0027(10)
C2	0.0230(11)	0.0291(12)	0.0314(13)	0.0062(10)	0.0029(10)	0.0033(9)
C3	0.0251(12)	0.0278(11)	0.0295(13)	0.0078(10)	0.0055(10)	0.0055(9)
C4	0.0225(12)	0.0340(12)	0.0309(13)	0.0074(10)	0.0041(10)	0.0031(10)
C5	0.0270(12)	0.0270(11)	0.0327(14)	0.0067(10)	-0.0022(10)	-0.0009(9)
C6	0.0248(12)	0.0275(11)	0.0320(13)	0.0086(10)	-0.0006(10)	0.0034(9)
C7	0.0310(13)	0.0297(12)	0.0311(13)	0.0075(10)	-0.0005(11)	0.0031(10)
C8	0.0292(13)	0.0264(11)	0.0319(13)	0.0049(10)	0.0004(10)	0.0061(10)
C9	0.0253(12)	0.0284(11)	0.0301(13)	0.0070(10)	0.0025(10)	0.0034(9)
C10	0.0284(12)	0.0290(12)	0.0290(13)	0.0073(10)	0.0012(10)	0.0072(10)
C11	0.0286(13)	0.0328(12)	0.0333(14)	0.0082(10)	0.0036(10)	0.0077(10)
C12	0.0301(13)	0.0297(12)	0.040(2)	0.0100(10)	0.0054(11)	0.0032(10)
C13	0.0332(13)	0.0268(11)	0.0349(14)	0.0088(10)	0.0035(11)	0.0087(10)
C14	0.0267(12)	0.0293(12)	0.0352(14)	0.0078(10)	0.0000(11)	0.0022(10)
C15	0.0293(14)	0.0434(14)	0.054(2)	0.0190(12)	0.0016(12)	0.0039(11)
C16	0.0263(12)	0.0280(11)	0.0382(14)	0.0035(10)	0.0000(11)	0.0051(10)
C17	0.0334(14)	0.0302(12)	0.046(2)	0.0024(11)	-0.0024(12)	0.0055(11)
C18	0.0377(14)	0.0306(12)	0.046(2)	0.0075(11)	0.0019(12)	0.0073(11)
C19	0.0261(12)	0.0288(12)	0.0347(13)	0.0072(10)	-0.0011(10)	0.0080(10)
C20	0.0342(14)	0.0394(14)	0.070(2)	0.0002(13)	0.0103(14)	-0.0029(11)
C21	0.041(2)	0.0382(14)	0.047(2)	-0.0054(12)	-0.0098(13)	0.0117(12)
C22	0.0317(13)	0.0363(13)	0.056(2)	0.0127(12)	0.0074(12)	0.0134(11)
C23	0.048(2)	0.0378(13)	0.047(2)	0.0079(12)	-0.0050(13)	0.0134(12)
O1	0.0369(10)	0.0270(8)	0.0503(11)	0.0021(8)	-0.0119(8)	0.0033(7)
O2	0.0405(10)	0.0262(9)	0.0572(12)	0.0070(8)	-0.0128(9)	0.0031(8)
O3	0.0339(11)	0.0482(11)	0.098(2)	0.0371(11)	-0.0114(11)	0.0066(9)
O4	0.0360(11)	0.0405(10)	0.082(2)	0.0322(10)	-0.037(10)	0.0037(9)

The form of the anisotropic displacement parameter is:

$$\exp[-2\pi^2(a^*U_{11}h^2+b^*U_{22}k^2+c^*U_{33}l^2+2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)].$$

**Table 7. Bond Distances in Compound 10, Å**

C1-C2	1.388(3)	C1-C6	1.399(3)	C2-C3	1.411(3)
C2-C16	1.525(3)	C3-C4	1.390(3)	C3-C19	1.538(3)
C4-C5	1.391(3)	C5-O1	1.353(3)	C5-C6	1.412(3)
C6-C7	1.475(3)	C7-O2	1.238(3)	C7-C8	1.497(3)
C8-C9	1.387(3)	C8-C13	1.392(3)	C9-C10	1.399(3)
C10-C11	1.403(3)	C10-C14	1.488(3)	C11-C12	1.392(3)
C11-C15	1.511(3)	C12-C13	1.390(3)	C14-O3	1.244(3)
C14-O4	1.271(3)	C16-C20	1.531(3)	C16-C21	1.531(4)
C16-C17	1.539(3)	C17-C18	1.504(4)	C18-C19	1.530(3)
C19-C23	1.526(4)	C19-C22	1.536(3)		

**Table 8. Bond Angles in Compound 10, °**

C2-C1-C6	123.8(2)	C1-C2-C3	117.9(2)	C1-C2-C16	118.2(2)
C3-C2-C16	123.8(2)	C4-C3-C2	119.3(2)	C4-C3-C19	118.9(2)
C2-C3-C19	121.7(2)	C3-C4-C5	122.2(2)	O1-C5-C4	117.9(2)
O1-C5-C6	122.6(2)	C4-C5-C6	119.5(2)	C1-C6-C5	117.3(2)
C1-C6-C7	122.7(2)	C5-C6-C7	120.0(2)	O2-C7-C6	120.4(2)
O2-C7-C8	118.2(2)	C6-C7-C8	121.4(2)	C9-C8-C13	118.1(2)
C9-C8-C7	117.7(2)	C13-C8-C7	123.8(2)	C8-C9-C10	121.8(2)
C9-C10-C11	120.2(2)	C9-C10-C14	116.9(2)	C11-C10-C14	122.8(2)
C12-C11-C10	117.3(2)	C12-C11-C15	117.8(2)	C10-C11-C15	124.9(2)
C13-C12-C11	122.4(2)	C12-C13-C8	120.2(2)	O3-C14-O4	121.9(2)
O3-C14-C10	121.2(2)	O4-C14-C10	116.9(2)	C2-C16-C20	108.4(2)
C2-C16-C21	111.4(2)	C20-C16-C21	109.0(2)	C2-C16-C17	110.3(2)
C20-C16-C17	109.8(2)	C21-C16-C17	107.8(2)	C18-C17-C16	112.6(2)
C17-C18-C19	113.3(2)	C23-C19-C18	108.1(2)	C23-C19-C22	109.0(2)
C18-C19-C22	110.0(2)	C23-C19-C3	111.1(2)	C18-C19-C3	110.7(2)
C22-C19-C3	108.1(2)				