Supplementary data for 3-(4-fluorophenyl)-3-hydroxy-1-(2-hydroxyphenyl)propan-1-one 7b, 6pp., for M.J. Mphahlele and M.A. Fernandes, *S. Afr. J. Chem*., 2002, **55**, 97-110, <http://journals.sabinet.co.za/sajchem/>, <http://ejour.sabinet.co.za/images/ejour/chem/chem_v55_a9.pdf>.
Direct link to supp. material: <http://ejour.sabinet.co.za/images/ejour/chem/chem_v55_a9supp.pdf>.

Supplementary Table 1 Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for the non-hydrogen atoms of compound **7b**. *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor. Esd's are given in parentheses.

Atom	*x*	*y*	*z*	*U*(eq)
F1	–0.0672(2)	0.48244(12)	0.64854(13)	0.0909(7)
O1	0.1437(2)	0.98757(13)	0.57393(14)	0.0497(7)
O2	0.0350(2)	1.20852(13)	0.67528(13)	0.0625(7)
O3	0.2491(2)	1.37533(13)	0.75191(14)	0.0714(7)
C1	0.0884(3)	0.82252(18)	0.66644(17)	0.0430(8)
C2	–0.0218(3)	0.7687(2)	0.5766(2)	0.0682(10)
C3	–0.0736(4)	0.6548(2)	0.5703(2)	0.0775(11)
C4	–0.0153(3)	0.5957(2)	0.6539(2)	0.0599(10)
C5	0.0930(4)	0.6435(2)	0.7448(2)	0.0816(11)
C6	0.1438(3)	0.7581(2)	0.7491(2)	0.0736(11)
C7	0.1464(3)	0.94832(17)	0.67582(17)	0.0429(8)
C8	0.0454(3)	1.02330(17)	0.73099(18)	0.0505(8)
C9	0.1051(3)	1.14798(18)	0.74271(18)	0.0452(8)
C10	0.2474(3)	1.19580(18)	0.82841(18)	0.0438(8)
C11	0.3113(3)	1.30806(19)	0.82950(19)	0.0501(9)
C12	0.4443(3)	1.3543(2)	0.9108(2)	0.0654(10)
C13	0.5120(3)	1.2915(3)	0.9933(2)	0.0743(11)
C14	0.4493(3)	1.1804(2)	0.9945(2)	0.0694(11)
C15	0.3198(3)	1.1342(2)	0.91338(19)	0.0554(9)
F1'	0.3469(2)	0.41787(14)	0.19183(13)	0.0994(8)
O1'	0.6368(2)	0.07512(14)	0.52975(14)	0.0514(7)
O2'	0.5460(2)	0.05058(15)	0.74657(14)	0.0698(7)
O3'	0.7760(2)	0.03179(15)	0.91175(15)	0.0810(8)
C1'	0.5482(3)	0.25175(18)	0.45599(18)	0.0450(8)
C2'	0.4227(3)	0.2003(2)	0.3742(2)	0.0708(10)
C3'	0.3552(4)	0.2548(2)	0.2847(2)	0.0813(11)
C4'	0.4141(3)	0.3624(2)	0.2794(2)	0.0661(11)
C5'	0.5385(4)	0.4164(2)	0.3564(3)	0.0869(11)
C6'	0.6045(3)	0.3596(2)	0.4453(2)	0.0785(11)
C7'	0.6221(3)	0.19353(18)	0.55546(17)	0.0473(8)
C8'	0.5257(3)	0.2042(2)	0.63933(17)	0.0534(9)
C9'	0.6011(3)	0.1468(2)	0.73829(18)	0.0491(9)
C10'	0.7427(3)	0.20252(19)	0.82058(18)	0.0466(8)
C11'	0.8231(3)	0.1414(2)	0.9048(2)	0.0568(10)
C12'	0.9568(3)	0.1924(3)	0.9827(2)	0.0738(11)
C13'	1.0085(4)	0.3032(3)	0.9795(2)	0.0800(14)
C14'	0.9311(4)	0.3657(2)	0.8976(2)	0.0745(11)
C15'	0.8004(3)	0.3152(2)	0.82014(19)	0.0578(10)

Supplementary Table 2 Anisotropic displacement parameters (Å^2) for compound **7b**. The temperature factor has the form $\exp(-T)$, where $T = 2\pi^2 \sum_{ij} [h_i h_j U_{ij} a^*_i a^*_j]$ for anisotropic atoms; a^* are reciprocal axial lengths, and h values are the reflection indices. Esd's are given in parentheses.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	0.1115(13)	0.0418(9)	0.1036(13)	0.0128(8)	0.0031(10)	–0.0154(8)
O1	0.0595(13)	0.0463(10)	0.0499(12)	0.0084(8)	0.0244(11)	0.0090(9)
O2	0.0734(12)	0.0535(11)	0.0567(11)	0.0092(8)	0.0077(9)	0.0113(9)
O3	0.0851(13)	0.0426(10)	0.0847(14)	0.0201(9)	0.0152(10)	0.0032(9)
C1	0.0474(14)	0.0412(13)	0.0406(14)	0.0028(10)	0.0119(11)	0.0068(11)
C2	0.092(2)	0.0507(16)	0.0503(17)	0.0156(12)	–0.0011(15)	–0.0124(14)
C3	0.103(2)	0.0571(18)	0.0528(17)	0.0050(14)	–0.0083(16)	–0.0201(16)
C4	0.0707(18)	0.0361(14)	0.0681(18)	0.0054(13)	0.0114(15)	–0.0022(12)
C5	0.098(2)	0.0469(17)	0.079(2)	0.0201(14)	–0.0170(18)	–0.0017(15)
C6	0.081(2)	0.0501(17)	0.0668(19)	0.0089(13)	–0.0196(15)	–0.0072(14)
C7	0.0463(13)	0.0414(13)	0.0414(14)	0.0038(10)	0.0126(11)	0.0034(10)
C8	0.0551(15)	0.0476(14)	0.0499(15)	–0.0006(11)	0.0191(12)	–0.0005(11)
C9	0.0585(15)	0.0386(13)	0.0440(14)	0.0024(11)	0.0234(12)	0.0080(11)
C10	0.0552(15)	0.0373(13)	0.0426(14)	0.0025(10)	0.0193(12)	0.0066(11)
C11	0.0587(16)	0.0406(14)	0.0553(16)	0.0042(12)	0.0222(13)	0.0092(12)
C12	0.0683(18)	0.0498(16)	0.077(2)	–0.0061(14)	0.0238(16)	–0.0056(14)
C13	0.0699(19)	0.079(2)	0.0634(19)	–0.0059(16)	0.0048(15)	–0.0011(16)
C14	0.077(2)	0.072(2)	0.0549(18)	0.0118(14)	0.0073(15)	0.0103(16)
C15	0.0679(17)	0.0488(14)	0.0503(16)	0.0061(12)	0.0173(13)	0.0036(13)
F1'	0.1227(15)	0.0902(13)	0.0793(12)	0.0431(10)	0.0020(10)	0.0211(11)
O1'	0.0572(13)	0.0475(11)	0.0537(12)	0.0060(9)	0.0197(11)	0.0153(9)
O2'	0.0752(13)	0.0589(12)	0.0769(13)	0.0083(9)	0.0249(10)	–0.0047(10)
O3'	0.0904(14)	0.0739(14)	0.0864(14)	0.0440(11)	0.0240(11)	0.0130(11)
C1'	0.0464(14)	0.0434(14)	0.0457(14)	0.0027(11)	0.0134(11)	0.0054(11)
C2'	0.084(2)	0.0473(15)	0.0668(18)	0.0130(13)	–0.0064(16)	–0.0021(14)
C3'	0.094(2)	0.0609(19)	0.069(2)	0.0103(15)	–0.0148(16)	0.0034(16)
C4'	0.077(2)	0.0654(19)	0.0573(18)	0.0234(14)	0.0118(15)	0.0191(16)
C5'	0.096(2)	0.0622(19)	0.092(2)	0.0324(17)	0.0032(19)	–0.0154(17)
C6'	0.081(2)	0.0679(19)	0.070(2)	0.0196(15)	–0.0081(16)	–0.0192(16)
C7'	0.0493(14)	0.0455(14)	0.0460(14)	0.0046(11)	0.0101(11)	0.0063(11)
C8'	0.0542(15)	0.0599(16)	0.0460(15)	0.0019(12)	0.0121(12)	0.0141(12)
C9'	0.0569(16)	0.0491(15)	0.0468(15)	0.0046(11)	0.0221(12)	0.0120(12)
C10'	0.0609(15)	0.0461(14)	0.0386(14)	0.0055(11)	0.0211(12)	0.0139(12)
C11'	0.0665(18)	0.0616(17)	0.0525(17)	0.0169(13)	0.0280(14)	0.0170(14)
C12'	0.071(2)	0.097(2)	0.0538(18)	0.0157(16)	0.0108(16)	0.0240(18)
C13'	0.074(2)	0.104(3)	0.054(2)	–0.0152(18)	0.0106(16)	0.0066(19)
C14'	0.092(2)	0.0599(18)	0.068(2)	–0.0083(15)	0.0218(17)	–0.0026(16)
C15'	0.0819(19)	0.0450(15)	0.0472(16)	0.0030(11)	0.0172(14)	0.0122(13)

Supplementary Table 3 Hydrogen coordinates and isotropic displacement parameters (Å^2) for compound **7d**. The temperature factor has the form exp(–T), where T = $8\pi^2 U(\sin\theta/\lambda)^2$ for isotropic atoms. Esd's are given in parentheses.

Atom	*x*	*y*	*Z*	*U*(iso)
*H1A	0.204(3)	0.956(3)	0.543(3)	0.039(16)
H2	–0.06250	0.81010	0.51860	0.0820
H3	–0.14820	0.61940	0.50870	0.0930
H5	0.13210	0.60110	0.80230	0.0980
H6	0.21890	0.79250	0.81100	0.0880
H7	0.25720	0.95860	0.72080	0.0510
H12	0.48780	1.42820	0.90950	0.0790
H13	0.60000	1.32340	1.04840	0.0890
H14	0.49510	1.13760	1.05020	0.0830
H15	0.27870	1.05970	0.91480	0.0660
H31	0.17160	1.34020	0.70790	0.1070
H81	–0.06540	1.01310	0.68840	0.0610
H82	0.04980	0.99940	0.80200	0.0610
*H1B	0.057(3)	0.979(4)	0.529(3)	0.06(2)
H2'	0.38180	0.12660	0.37920	0.0850
*H1B'	0.549(3)	0.039(4)	0.503(4)	0.07(2)
H3'	0.27120	0.21820	0.22920	0.0970
H5'	0.57910	0.48980	0.35020	0.1040
H6'	0.69020	0.39630	0.49950	0.0940
H7'	0.72980	0.23110	0.58860	0.0570
H12'	1.01110	0.15090	1.03710	0.0890
H13'	1.09680	0.33770	1.03290	0.0960
H14'	0.96800	0.44110	0.89550	0.0890
H15'	0.74850	0.35740	0.76560	0.0690
H31'	0.69630	0.01040	0.86200	0.1220
H81'	0.51930	0.28460	0.66060	0.0640
H82'	0.41760	0.16950	0.60740	0.0640
*H1A'	0.689(4)	0.058(4)	0.487(3)	0.047(19)

Supplementary Table 4 Bond lengths (Å) for compound **7b**. Esd's are given in parentheses.

F1–C4	1.371(3)	C13–C14	1.388(4)
F1'–C4'	1.367(3)	C14–C15	1.366(4)
O1–C7	1.420(3)	C2–H2	0.9304
O2–C9	1.231(3)	C3–H3	0.9298
O3–C11	1.350(3)	C5–H5	0.9301
O1–H1A	0.82(3)	C6–H6	0.9304
O1–H1B	0.82(3)	C7–H7	0.9794
O3–H31	0.8198	C8–H82	0.9697
O1'–C7'	1.425(3)	C8–H81	0.9698
O2'–C9'	1.226(3)	C12–H12	0.9300
O3'–C11'	1.347(3)	C13–H13	0.9301
O1'–H1B'	0.82(4)	C14–H14	0.9295
O1'–H1A'	0.82(4)	C15–H15	0.9296
O3'–H31'	0.8203	C1'–C2'	1.369(3)
C1–C7	1.519(3)	C1'–C7'	1.515(3)
C1–C6	1.362(3)	C1'–C6'	1.363(3)
C1–C2	1.370(3)	C2'–C3'	1.379(4)
C2–C3	1.376(3)	C3'–C4'	1.350(3)
C3–C4	1.336(3)	C4'–C5'	1.343(4)
C4–C5	1.349(4)	C5'–C6'	1.386(4)
C5–C6	1.385(3)	C7'–C8'	1.525(3)
C7–C8	1.533(3)	C8'–C9'	1.508(3)
C8–C9	1.508(3)	C9'–C10'	1.473(3)
C9–C10	1.470(3)	C10'–C15'	1.390(3)
C10–C11	1.399(3)	C10'–C11'	1.408(3)
C10–C15	1.397(3)	C11'–C12'	1.385(4)
C11–C12	1.386(4)	C12'–C13'	1.360(5)
C12–C13	1.372(4)	C13'–C14'	1.389(4)
C14'–C15'	1.365(4)	C8'–H81'	0.9707
C2'–H2'	0.9307	C8'–H82'	0.9694
C3'–H3'	0.9303	C12'–H12'	0.9308
C5'–H5'	0.9305	C13'–H13'	0.9301
C6'–H6'	0.9305	C14'–H14'	0.9299
C7'–H7'	0.9803	C15'–H15'	0.9302

Supplementary Table 5 Bond angles (°) for compound **7b**. Esd's are given in parentheses.

C7–O1–H1B	116(3)	C10–C11–C12	120.6(2)
C7–O1–H1A	114(3)	C11–C12–C13	120.3(2)
C11–O3–H31	109.50	C12–C13–C14	120.0(2)
C7'–O1'–H1A'	118(3)	C13–C14–C15	119.7(2)
C7'–O1'–H1B'	112(3)	C10–C15–C14	121.8(2)
C11'–O3'–H31'	109.49	C3–C2–H2	119.30
C2–C1–C7	122.5(2)	C1–C2–H2	119.24
C6–C1–C7	120.6(2)	C2–C3–H3	120.47
C2–C1–C6	116.9(2)	C4–C3–H3	120.39
C1–C2–C3	121.5(2)	C4–C5–H5	121.26
C2–C3–C4	119.1(2)	C6–C5–H5	121.34
C3–C4–C5	122.4(2)	C5–C6–H6	118.66
F1–C4–C5	118.1(2)	C1–C6–H6	118.63
F1–C4–C3	119.5(2)	C1–C7–H7	108.08
C4–C5–C6	117.4(2)	O1–C7–H7	108.10
C1–C6–C5	122.7(2)	C8–C7–H7	108.09
O1–C7–C8	108.51(17)	C7–C8–H81	109.38
O1–C7–C1	112.80(17)	C7–C8–H82	109.37
C1–C7–C8	111.1(2)	H81–C8–H82	108.04
C7–C8–C9	111.2(2)	C9–C8–H81	109.37
C8–C9–C10	121.58(19)	C9–C8–H82	109.41
O2–C9–C8	118.0(2)	C11–C12–H12	119.91
O2–C9–C10	120.3(2)	C13–C12–H12	119.83
C9–C10–C11	120.3(2)	C12–C13–H13	119.95
C9–C10–C15	122.2(2)	C14–C13–H13	120.02
C11–C10–C15	117.5(2)	C15–C14–H14	120.12
O3–C11–C10	122.2(2)	C13–C14–H14	120.21
O3–C11–C12	117.1(2)	C10–C15–H15	119.08
C14–C15–H15	119.08	C13'–C14'–C15'	119.3(2)
C2'–C1'–C7'	122.4(2)	C10'–C15'–C14'	121.8(2)
C2'–C1'–C6'	117.1(2)	C1'–C2'–H2'	119.08
C6'–C1'–C7'	120.5(2)	C3'–C2'–H2'	119.14
C1'–C2'–C3'	121.8(2)	C2'–C3'–H3'	120.76
C2'–C3'–C4'	118.5(3)	C4'–C3'–H3'	120.77
C3'–C4'–C5'	122.3(2)	C4'–C5'–H5'	120.93
F1'–C4'–C3'	119.0(2)	C6'–C5'–H5'	121.02
F1'–C4'–C5'	118.6(2)	C1'–C6'–H6'	118.87
C4'–C5'–C6'	118.0(2)	C5'–C6'–H6'	118.90
C1'–C6'–C5'	122.2(2)	O1'–C7'–H7'	108.05
O1'–C7'–C1'	112.37(17)	C1'–C7'–H7'	108.04
O1'–C7'–C8'	108.25(18)	C8'–C7'–H7'	108.07
C1'–C7'–C8'	111.9(2)	C7'–C8'–H81'	109.33
C7'–C8'–C9'	111.4(2)	C7'–C8'–H82'	109.37
C8'–C9'–C10'	120.8(2)	C9'–C8'–H81'	109.32
O2'–C9'–C10'	120.6(2)	C9'–C8'–H82'	109.33
O2'–C9'–C8'	118.5(2)	H81'–C8'–H82'	107.99
C9'–C10'–C11'	119.7(2)	C11'–C12'–H12'	120.03
C9'–C10'–C15'	122.6(2)	C13'–C12'–H12'	120.10
C11'–C10'–C15'	117.7(2)	C12'–C13'–H13'	119.62
C10'–C11'–C12'	120.4(2)	C14'–C13'–H13'	119.46
O3'–C11'–C10'	121.9(2)	C13'–C14'–H14'	120.38
O3'–C11'–C12'	117.7(2)	C15'–C14'–H14'	120.34
C11'–C12'–C13'	119.9(3)	C10'–C15'–H15'	119.12
C12'–C13'–C14'	120.9(3)	C14'–C15'–H15'	119.08

Supplementary Table 6 Torsion angles (°) for compound **7d**. Esd's are given in parentheses.

C7–C1–C2–C3	–179.4(3)	C7'–C1'–C2'–C3'	179.2(3)
C6–C1–C7–O1	151.2(2)	C6'–C1'–C2'–C3'	–0.2(4)
C2–C1–C7–C8	92.6(3)	C6'–C1'–C7'–C8'	97.7(3)
C6–C1–C2–C3	–0.1(4)	C6'–C1'–C7'–O1'	–140.2(2)
C6–C1–C7–C8	–86.7(3)	C7'–C1'–C6'–C5'	–179.0(3)
C2–C1–C7–O1	–29.5(3)	C2'–C1'–C7'–O1'	40.5(3)
C2–C1–C6–C5	–0.1(4)	C2'–C1'–C6'–C5'	0.4(4)
C7–C1–C6–C5	179.2(3)	C2'–C1'–C7'–C8'	–81.6(3)
C1–C2–C3–C4	0.2(5)	C1'–C2'–C3'–C4'	–1.0(4)
C2–C3–C4–F1	179.5(3)	C2'–C3'–C4'–C5'	2.0(5)
C2–C3–C4–C5	0.0(5)	C2'–C3'–C4'–F1'	–179.2(2)
F1–C4–C5–C6	–179.8(2)	C3'–C4'–C5'–C6'	–1.8(5)
C3–C4–C5–C6	–0.2(5)	F1'–C4'–C5'–C6'	179.4(3)
C4–C5–C6–C1	0.3(4)	C4'–C5'–C6'–C1'	0.6(5)
O1–C7–C8–C9	–56.7(2)	C1'–C7'–C8'–C9'	–179.54(19)
C1–C7–C8–C9	178.70(18)	O1'–C7'–C8'–C9'	56.1(2)
C7–C8–C9–O2	98.7(3)	C7'–C8'–C9'–C10'	77.6(3)
C7–C8–C9–C10	–78.3(3)	C7'–C8'–C9'–O2'	–99.5(3)
C8–C9–C10–C11	172.3(2)	O2'–C9'–C10'–C11'	5.1(4)
C8–C9–C10–C15	–10.4(4)	O2'–C9'–C10'–C15'	–173.9(2)
O2–C9–C10–C15	172.7(2)	C8'–C9'–C10'–C11'	–171.9(2)
O2–C9–C10–C11	–4.7(4)	C8'–C9'–C10'–C15'	9.2(4)
C15–C10–C11–C12	1.7(4)	C15'–C10'–C11'–O3'	–179.9(2)
C15–C10–C11–O3	–179.2(2)	C15'–C10'–C11'–C12'	–1.2(4)
C9–C10–C11–O3	–1.7(4)	C9'–C10'–C11'–C12'	179.8(2)
C11–C10–C15–C14	–0.6(4)	C9'–C10'–C11'–O3'	1.1(4)
C9–C10–C15–C14	–178.1(2)	C11'–C10'–C15'–C14'	0.5(4)
C9–C10–C11–C12	179.2(2)	C9'–C10'–C15'–C14'	179.5(3)
O3–C11–C12–C13	178.8(2)	O3'–C11'–C12'–C13'	–179.6(3)
C10–C11–C12–C13	–2.1(4)	C10'–C11'–C12'–C13'	1.7(4)
C11–C12–C13–C14	1.3(4)	C11'–C12'–C13'–C14'	–1.4(5)
C12–C13–C14–C15	–0.2(4)	C12'–C13'–C14'–C15'	0.7(5)
C13–C14–C15–C10	–0.1(4)	C13'–C14'–C15'–C10'	–0.3(4)