Supplementary Information for the Article
Crystal packing in the 2-R,4-oxo-[1,3-*a/b*]-naphthodioxanes – Hirshfeld surface analysis and melting point correlation

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Crystal and Refinement Data

1-H. $C_{12}H_8O_3$, M = 200.2 g mol^{-1}. Monoclinic, space group $P2_1/c$ (no. 14), a = 20.0779(8), b = 6.2280(3), c = 7.2121(3) Å, β = 100.161(4)º, V = 887.7 Å^3. D_c (Z = 4) = 1.498 g cm^{-3}. μ_{Mo} = 0.108 mm^{-1}; specimen: 0.31 x 0.21 x 0.15 mm^3; $T_{min/max}$ = 0.92. $2\theta_{max}$ = 75º; N_t = 9430, N = 4379 (R_{int} = 0.026), N_o = 2657. $R1$ = 0.054, $wR2$ = 0.121 (a = 0.054), S = 1.00. $|\Delta\rho_{max}|$ = 0.60(7) e Å^{-3}. CCDC-846991.

1-Me. $C_{13}H_{10}O_3$, M = 214.2 g mol^{-1}. Monoclinic, space group $P2_1/c$ (no. 14), a = 10.7746(4), b = 15.6168(5), c = 6.1107(2) Å, β = 98.201(3)°, V = 1017.7 Å^3. D_c (Z = 4) = 1.398 g cm^{-3}. μ_{Mo} = 0.100 mm^{-1}; specimen: 0.21 x 0.19 x 0.18 mm^3; $T_{min/max}$ = 0.99. $2\theta_{max}$ = 75°; N_t = 11513, N = 5059 (R_{int} = 0.032), N_o = 2714. $R1$ = 0.051, $wR2$ = 0.098 (a = 0.029), S = 1.00. $|\Delta\rho_{max}|$ = 0.046(6) e Å^{-3}. CCDC-846997.

1-Et. $C_{14}H_{12}O_3$, M = 228.2 g mol^{-1}. Monoclinic, space group $P2_1/n$ (no. 14, variant), a = 9.0829(2), b = 8.4907(2), c = 14.0688(3) Å, β = 96.172(2)º, V = 1078.7 Å^3. D_c (Z = 4) = 1.405 g cm^{-3}. μ_{Mo} = 0.099 mm^{-1}; specimen: 0.40 x 0.39 x 0.30 mm^3; $T_{min/max}$ = 1.00. $2\theta_{max}$ = 82º; N_t = 29349, N = 6938 (R_{int} = 0.035), N_o = 4419. $R1$ = 0.055, $wR2$ = 0.155 (a = 0.087), S = 1.00. $|\Delta\rho_{max}|$ = 0.86(9) e Å^{-3}. CCDC-846990.

1-iPr. $C_{15}H_{14}O_3$, M = 242.3 g mol^{-1}. Orthorhombic, space group $P2_12_12_1$ (no. 19), a = 7.8319(2), b = 12.3938(5), c = 24.6888(7) Å, V = 2396.5 Å^3. D_c (Z = 8) = 1.343 g cm^{-3}. μ_{Mo} = 0.093 mm^{-1}; specimen: 0.35 x 0.21 x 0.11 mm^3; $T_{min/max}$ = 0.89. $2\theta_{max}$ = 56º; N_t = 35712, N = 5793 (R_{int} = 0.053), N_o = 4557. $R1$ = 0.072, $wR2$ = 0.172 (a = 0.070, b = 3.4), S = 1.01. $|\Delta\rho_{max}|$ = 0.35(6) e Å^{-3}. CCDC-846995.

1-nBu. $C_{16}H_{16}O_3$, M = 256.3 g mol^{-1}. Monoclinic, space group $C2/c$ (no. 15), a = 11.8830(2), b = 14.6412(3), c = 15.4699(3) Å, β = 108.565(2)º, V = 2551.4 Å^3. D_c (Z = 8) = 1.334 g cm^{-3}. μ_{Mo} = 0.091 mm^{-1}; specimen: 0.36 x 0.26 x 0.18 mm^3; $T_{min/max}$ = 0.99. $2\theta_{max}$ = 75º; N_t = 26764, N = 6411 (R_{int} = 0.032), N_o = 3924. $R1$ = 0.046, $wR2$ = 0.111 (a = 0.050), S = 1.01. $|\Delta\rho_{max}|$ = 0.57(6) e Å^{-3}. CCDC-846989.

1-CCl$_3$. $C_{13}H_7Cl_3O_3$, M = 317.5 g mol^{-1}. Triclinic, space group $P\bar{1}$ (no. 2), a = 5.8452(3), b = 9.3279(3), c = 12.1599(6) Å, α = 109.289(4), β = 99.692(4), γ = 93.069(4)º, V = 612.6 Å^3. D_c (Z = 2) = 1.72$_1$ g cm^{-3}. μ_{Mo} = 0.75 mm^{-1}; specimen: 0.40 x 0.31 x 0.25 mm^3; $T_{min/max}$ = 0.99. $2\theta_{max}$ = 82º; N_t = 16108, N = 7835 (R_{int} = 0.020), N_o = 6261. $R1$ = 0.028, $wR2$ = 0.075 (a = 0.040), S = 1.00. $|\Delta\rho_{max}|$ = 0.63(8) e Å^{-3}. CCDC-846994.

1-diox. $C_{17}H_{16}O_5$, M = 300.3 g mol^{-1}. Monoclinic, space group $P2_1$ (no. 4), a = 10.6142(2), b = 5.8945(1), c = 11.1109(2) Å, β = 90.093(2)º, V = 695.2 Å^3. D_c (Z = 2) = 1.435 g cm^{-3}. μ_{Mo} = 0.106 mm^{-1}; specimen: 0.43 x 0.29 x 0.17 mm^3; $T_{min/max}$ = 0.99. $2\theta_{max}$ = 75º; N_t = 25466, N = 6986 (R_{int} = 0.027), N_o = 6072. $R1$ = 0.033, $wR2$ = 0.084 (a = 0.059), S = 1.01. $|\Delta\rho_{max}|$ = 0.46(6) e Å^{-3}. CCDC-846987.

2-Et. $C_{14}H_{12}O_3$, M = 228.2 g mol^{-1}. Orthorhombic, space group $Pna2_1$ (no. 33), a = 7.5217(2), b = 15.7302(4), c = 9.0870(2) Å, V = 1075.2 Å^3. D_c (Z = 4) = 1.410 g cm^{-3}. μ_{Mo} = 0.099 mm^{-1}; specimen: 0.29 x 0.20 x 0.12 mm^3; $T_{min/max}$ = 0.99. $2\theta_{max}$ = 75º; N_t = 21092, N = 5368 (R_{int} = 0.037), N_o = 4080. $R1$ = 0.044, $wR2$ = 0.095 (a = 0.045), S = 1.00. $|\Delta\rho_{max}|$ = 0.45(6) e Å^{-3}. CCDC-846996.

2-iPr. $C_{15}H_{14}O_3$, M = 242.3 g mol^{-1}. Monoclinic, space group $C2/c$ (no. 15), a = 22.438(1), b = 7.1267(2), c = 16.9373(7) Å, β = 117.532(6)º, V = 2401.7 Å^3. D_c (Z = 8) = 1.340 g cm^{-3}. μ_{Mo} = 0.093 mm^{-1}; specimen: 0.32 x 0.23 x 0.11 mm^3; $T_{min/max}$ = 0.98. $2\theta_{max}$ = 75º; N_t = 24817, N = 6027 (R_{int} = 0.033), N_o = 3786. $R1$ = 0.048, $wR2$ = 0.114 (a = 0.053), S = 1.00. $|\Delta\rho_{max}|$ = 0.51(6) e Å^{-3}. CCDC-846988.

2-nBu. $C_{16}H_{16}O_3$, M = 256.3 g mol^{-1}. Monoclinic, space group Pc (no. 7), a = 8.1408(2), b = 10.6093(2), c = 15.5627(3) Å, β = 95.408(2)º, V = 1338.1 Å^3. D_c (Z = 4) = 1.272 g cm^{-3}. μ_{Mo} = 0.087 mm^{-1}; specimen: 0.30 x 0.27 x 0.25 mm^3; $T_{min/max}$ = 0.99. $2\theta_{max}$ = 75º; N_t = 29410, N = 12825 (R_{int} = 0.028), N_o = 8996. $R1$ = 0.045, $wR2$ = 0.096 (a = 0.050), S = 1.00. $|\Delta\rho_{max}|$ = 0.48(5) e Å^{-3}. CCDC-846992.

2-diox. $C_{17}H_{16}O_5$, M = 300.3 g mol^{-1}. Orthorhombic, space group $P2_12_12_1$ (no. 19), a = 6.5117(1), b = 10.3653(2), c = 21.8661(4) Å, V = 1475.9 Å^3. D_c (Z = 4) = 1.351 g cm^{-3}. μ_{Mo} = 0.100 mm^{-1}; specimen: 0.37 x 0.28 x 0.12 mm^3; $T_{min/max}$ = 0.92. $2\theta_{max}$ = 75º; N_t = 31913, N = 4217 (R_{int} = 0.049), N_o = 3010. $R1$ = 0.057, $wR2$ = 0.114 (a = 0.056), S = 1.01. $|\Delta\rho_{max}|$ = 0.53(6) e Å^{-3}. CCDC-846993.

Table S1 Non-hydrogen atom geometries, **1-R**, **2-R**

(a) **1-R**

1-R	**1-H**	**1-Me**	**1-Et**	**1-nBu**	**1-iPr** (mols. 1,2)*	**1-CCl$_3$**	**1-diox**	< >
Distances/Å								
O(1)-C(2)	1.423(1)	1.419(1)	1.415(1)	1.418(1)	1.401(4), 1.418(4)	1.3954(9)	1.407(1)	1.413(10)
O(1)-C(14)	1.372(1)	1.376(1)	1.371(1)	1.380(1)	1.387(5), 1.376(5)	1.3782(8)	1.376(1)	1.376(3)
C(2)-O(3)	1.437(1)	1.445(1)	1.447(1)	1.444(1)	1.451(5), 1.434(5)	1.4259(9)*	1.439(1)	1.442(4)
C(2)-C(15)		1.494(1)	1.506(1)	1.502(1)	1.504(6), 1.508(5)	1.5377(10)*	1.520(1)*	1.503(5)
O(3)-C(4)	1.360(1)	1.360(1)	1.360(1)	1.362(1)	1.363(5), 1.366(5)	1.3719(9)*	1.360(1)	1.360(1)
C(4)-C(5)	1.484(1)	1.475(1)	1.471(1)	1.474(1)	1.477(5), 1.472(5)	1.4706(10)	1.478(1)	1.476(5)
C(4)-O(4)	1.202(1)	1.206(1)	1.209(1)	1.208(1)	1.199(5), 1.198(6)	1.2039(10)	1.208(1)	1.206(3)
C(5)-C(6)	1.376(1)	1.376(1)	1.379(1)	1.375(1)	1.358(6), 1.367(6)	1.3810(10)	1.378(1)	1.378(2)
C(5)-C(14)	1.419(1)	1.415(1)	1.420(1)	1.419(1)	1.414(6), 1.408(6)	1.4153(10)	1.420(1)	1.417(4)
C(6)-C(7)	1.419(1)	1.411(1)	1.414(1)	1.412(1)	1.414(5), 1.407(5)	1.4110(11)	1.418(1)	1.414(4)
C(7)-C(8)	1.422(1)	1.420(1)	1.421(1)	1.417(1)	1.411(6), 1.411(6)	1.4258(10)	1.423(1)	1.422(3)
C(7)-C(12)	1.430(2)	1.425(1)	1.433(1)	1.430(1)	1.428(6), 1.417(6)	1.4263(11)	1.429(1)	1.429(3)
C(8)-C(9)	1.373(2)	1.364(1)	1.372(1)	1.369(1)	1.359(6), 1.350(6)	1.3702(12)	1.375(1)	1.369(4)
C(9)-C(10)	1.411(2)	1.410(2)	1.409(1)	1.412(1)	1.396(6), 1.393(6)	1.415(1)	1.417(2)	1.412(3)
C(10)-C(11)	1.376(2)	1.370(1)	1.374(1)	1.365(1)	1.357(6), 1.352(8)	1.3707(11)	1.373(1)	1.372(4)
C(11)-C(12)	1.425(1)	1.421(1)	1.419(1)	1.424(1)	1.415(5), 1.427(6)	1.4189(11)	1.423(1)	1.422(3)
C(12)-C(13)	1.418(2)	1.420(1)	1.415(1)	1.417(1)	1.410(6), 1.392(6)	1.4165(10)	1.416(1)	1.417(2)
C(13)-C(14)	1.372(1)	1.368(1)	1.366(1)	1.365(1)	1.359(5), 1.365(6)	1.3657(10)	1.370(1)	1.368(3)
Angles/degrees								
C(2)-O(1)-C(14)	111.98(8)	112.19(7)	110.98(6)	112.36(6)	111.7(3), 111.0(3)	112.95(5)	111.76(8)	
O(1)-C(2)-O(3)	111.66(8)	110.86(7)	110.03(6)	110.38(6)	110.9(3), 111.0(3)	112.74(6)	111.70(7)	

O(1)-C(2)-C(15)		108.77(8)	110.14(6)	108.84(6)	110.6(4), 110.2(3)	107.12(6)	108.46(8)	
O(3)-C(2)-C(15)		107.52(8)	108.34(7)	107.89(6)	107.6(3), 108.4(3)	107.07(5)	105.58(7)	
C(2)-O(3)-C(4)	116.50(8)	116.31(8)	115.12(6)	116.06(6)	115.7(3), 115.8(3)	117.94(6)	118.05(7)	
O(3)-C(4)-C(5)	115.48(9)	115.23(9)	115.51(7)	115.39(6)	116.1(3), 115.4(4)	115.78(6)	115.77(8)	115.5(2)
O(3)-C(4)-O(4)	119.43(9)	119.27(9)	119.02(7)	119.06(7)	118.5(4), 118.9(4)	118.05(7)	118.51(8)	118.9(5)
C(5)-C(4)-O(4)	124.85(9)	125.41(9)	125.40(8)	125.40(8)	125.3(4), 125.6(4)	126.13(7)	125.71(9)	125.5(4)
C(4)-C(5)-C(6)	120.50(9)	120.20(9)	121.03(7)	120.81(7)	121.2(4), 120.6(4)	121.46(6)	121.42(8)	120.9(5)
C(4)-C(5)-C(14)	119.20(9)	119.83(9)	118.74(7)	119.28(7)	119.2(4), 119.3(4)	119.23(6)	118.49(8)	119.1(5)
C(6)-C(5)-C(14)	119.98(9)	119.78(9)	120.07(7)	119.68(7)	119.5(4), 119.9(4)	119.26(7)	120.03(8)	119.8(3)
C(5)-C(6)-C(7)	120.52(10)	120.66(9)	120.23(7)	120.82(7)	121.4(4), 121.3(4)	120.66(7)	120.27(9)	120.5(2)
C(6)-C(7)-C(8)	121.71(10)	121.52(9)	121.70(7)	122.02(7)	122.5(4), 122.5(4)	121.89(7)	121.96(9)	121.8(2)
C(6)-C(7)-C(12)	118.93(9)	118.98(9)	119.11(7)	118.72(7)	118.6(4), 117.8(4)	119.02(6)	119.07(8)	119.0(1)
C(8)-C(7)-C(12)	119.34(9)	119.50(9)	119.18(8)	119.25(7)	118.9(4), 119.7(4)	119.09(7)	118.97(8)	119.2(2)
C(7)-C(8)-C(9)	120.49(11)	120.55(10)	120.35(8)	120.70(8)	120.7(4), 121.2(5)	120.20(7)	120.72(9)	120.5(2)
C(8)-C(9)-C(10)	120.42(10)	120.23(10)	120.42(8)	119.98(8)	120.4(4), 119.8(5)	120.63(7)	120.11(9)	120.3(2)
C(9)-C(10)-C(11)	120.64(10)	120.70(10)	120.85(8)	121.13(8)*	121.1(4), 121.1(4)	120.48(8)	120.68(9)	120.7(1)
C(10)-C(11)-C(12)	120.60(11)	120.75(10)	120.38(8)	120.42(8)	120.5(4), 121.3(5)	120.53(7)	120.52(9)	120.5(1)
C(11)-C(12)-C(7)	118.50(9)	118.26(9)	119.36(7)	118.52(7)	118.4(4), 116.9(4)	119.04(7)	118.97(8)	118.8(4)
C(11)-C(12)-C(13)	121.85(10)	122.00(9)	121.78(8)	121.72(7)	122.8(4), 122.9(5)	121.14(7)	121.32(9)	121.6(4)
C(13)-C(12)-C(7)	119.64(9)	119.74(9)	118.75(9)*	119.75(7)	118.8(3), 120.2(4)	119.82(7)	119.70(8)	119.73(7)
C(12)-C(13)-C(14)	119.72(10)	119.38(9)	120.04(7)	119.53(7)	120.6(4), 120.7(4)	119.19(7)	119.73(8)	119.6(3)
O(1)-C(14)-C(5)	118.96(9)	118.78(9)	118.77(7)	118.54(7)	118.3(3), 118.7(4)	118.51(6)	119.05(8)	118.8(2)
O(1)-C(14)-C(13)	119.76(9)	119.69(9)	120.19(7)	119.99(7)	120.5(4), 121.2(4)	119.37(6)	119.73(8)	119.8(3)
C(5)-C(14)-C(13)	121.20(9)	121.45(9)	121.03(7)	121.44(7)	121.4(4), 120.1(4)	122.03(6)	121.19(8)	121.4(4)
Torsion angles/degrees								
C(14)-O(1)-C(2)-O(3)	57.6(1)	57.60(10)	61.23(8)	58.20(8)	60.1(4), –60.5(4)	55.76(8)	57.88(10)	
O(1)-C(2)-O(3)-C(4)	–53.1(1)	–54.97(10)	–57.17(9)	–55.67(8)	–54.2(4), 54.4(5)	–47.02(8)	–48.2(1)	
C(2)-O(3)-C(4)-C(5)	18.8(1)	22.66(11)	19.34(10)	20.76(9)	20.2(5), –17.6(6)	15.07(9)	13.1(1)	
O(3)-C(4)-C(5)-C(14)	9.7(1)	5.3(1)	12.6(1)	10.3(1)	6.2(5), –11.7(6)	7.04(10)	11.2(1)	
C(4)-C(5)-C(14)-O(1)	–3.8(1)	–1.1(1)	–7.4(1)	–6.5(1)	0.8(5), 4.3(6)	2.71(10)	–.0.1(1)	
C(5)-C(14)-O(1)-C(2)	–29.6(1)	–30.6(1)	–29.63(10)	–28.01(9)	–34.0(5), 31.4(5)	–34.06(9)	–34.5(1)	
Atom deviations (δÅ) from the C_{10} naphthyl plane								
$\chi^2(C_{10})$	442	303	11511	930	66, 100	1082	1133	
δO(1)	0.071(1)	0.072(1)	–0.166(1)	–0.039(1)	0.092(5), –0.022(5)	0.115(1)	0.024(1)	
δC(2)	–0.518(2)	–0.544(1)	–0.854(1)	–0.637(1)	–0.583(6), –0.719(6)	–0.544(1)	–0.700(1)	
δO(3)	0.101(1)	0.057(1)	–0.130(1)	0.063(1)	–0.025(5), –0.099(6)	–0.104(1)	–0.201(1)	
δC(4)	0.170(1)	0.081(1)	0.098(1)	0.176(1)	0.036(5), 0.076(7)	0.002(1)	0.006(1)	
δO(4)	0.451(2)	0.232(2)	0.417(2)	0.471(1)	0.188(5), 0.351(8)	0.142(2)	0.203(2)	
δC(15)		–0.330(2)	–0.971(2)	–0.536(1)	–0.457(8), –0.731(7)	–0.204(2)	–0.490(2)	

*Values marked are excluded from the calculation of the mean (< >), being more than 3σ deviant from the mean of the remainder; all values of the less precise determination of **1-iPr** are also excluded.

(b) **2-R**

2-R	**2-Et**	**2n-Bu** (mols.1,2)	**2-iPr**	**2-diox**	< >
Distances/Å					
O(1)-C(2)	1.419(1)	1.423(2), 1.426(2)	1.4188(9)	1.417(2)	1.421(4)
O(1)-C(13)	1.365(1)	1.367(2), 1.363(2)	1.3588(9)	1.371(2)	1.365(5)
C(2)-O(3)	1.440(1)	1.443(2), 1.438(2)	1.4404(9)	1.424(2)*	1.440(2)
C(2)-C(15)	1.508(2)	1.502(2), 1.500(2)	1.5112(11)	1.507(2)	1.506(5)
O(3)-C(4)	1.366(1)	1.364(2), 1.362(2)	1.3662(10)	1.372(2)	1.366(4)
C(4)-C(14)	1.464(1)	1.465(2), 1.468(2)	1.4674(12)	1.464(2)	1.466(2)
C(4)-O(4)	1.207(1)	1.216(2), 1.214(2)	1.2094(9)	1.204(2)	1.210(5)
C(14)-C(5)	1.421(1)	1.421(2), 1.419(2)	1.422(1)	1.429(2)*	1.421(1)
C(14)-C(13)	1.380(1)	1.382(2), 1.374(2)	1.380(1)	1.377(2)	1.379(3)
C(5)-C(6)	1.361(2)	1.357(2), 1.360(2)	1.358(1)	1.360(3)	1.359(2)
C(6)-C(7)	1.424(2)	1.428(2), 1.424(2)	1.430(1)	1.420(3)	1.425(4)
C(7)-C(8)	1.422(2)	1.416(2), 1.414(2)	1.417(1)	1.421(3)	1.418(3)
C(7)-C(12)	1.421(1)	1.423(2), 1.424(2)	1.415(1)*	1.423(2)	1.423(1)
C(8)-C(9)	1.374(2)	1.369(2), 1.369(2)	1.371(2)	1.369(3)	1.370(2)
C(9)-C(10)	1.406(2)	1.407(2), 1.414(2)*	1.401(1)	1.403(3)	1.404(3)
C(10)-C(11)	1.372(2)	1.375(2), 1.373(2)	1.373(1)	1.372(2)	1.373(1)
C(11)-C(12)	1.419(2)*	1.412(2), 1.414(2)	1.413(1)	1.413(2)	1.413(1)
C(12)-C(13)	1.420(2)	1.420(2), 1.423(2)	1.423(1)	1.419(2)	1.421(2)
Angles/degrees					
C(2)-O(1)-C(13)	114.75(8)	111.3(1), 111.3(1)	113.01(6)	111.9(1)	
O(1)-C(2)-O(3)	111.98(8)	109.8(1), 110.3(1)	110.65(6)	111.5(1)	
O(1)-C(2)-C(15)	106.99(8)	109.5(1), 109.3(1)	108.61(6)	106.8(1)	
O(3)-C(2)-C15)	108.58(9)	108.4(1), 108.1(1)	108.67(6)	107.8(1)	108.3(4)
C(2)-O(3)-C(4)	116.92(8)*	115.4(1), 115.4(1)	115.69(6)	115.3(1)	115.5(2)
O(3)-C(4)-C(14)	115.80(9)	116.0(1), 115.8(1)	115.38(7)	115.1(1)	115.6(4)
O(3)-C(4)-O(4)	118.65(10)	119.0(1), 119.2(1)	118.44(8)	118.4(2)	118.7(4)
C(14)-C(4)-O(4)	125.39(10)	124.9(1), 124.8(1)	125.99(8)	126.4(2)	125.5(7)
C(14)-C(5)-C(6)	120.34(9)	120.3(1), 119.8(1)*	120.25(8)	120.3(2)	120.3(1)
C(5)-C(6)-C(7)	120.77(10)	120.7(1), 120.7(1)	121.26(8)*	120.9(2)	120.8(1)
C(6)-C(7)-C(8)	121.86(10)	122.3(1), 121.7(1)	122.78(8)	122.5(2)	122.2(4)
C(6)-C(7)-C(12)	119.88(10)	120.0(1), 120.2(1)	119.36(8)*	120.0(2)	120.0(1)
C(8)-C(7)-C(12)	118.25(9)	117.7(1), 118.1(1)	117.86(8)	117.5(2)	117.9(3)
C(7)-C(8)-C(9)	120.72(10)	121.1(1), 120.9(1)	121.00(9)	121.3(2)	121.0(2)
C(8)-C(9)-C(10)	120.66(11)	120.7(1), 120.5(1)	120.54(8)	120.5(2)	120.6(1)
C(9)-C(10)-C(11)	120.26(10)	120.2(1), 120.4(1)	120.30(9)	120.5(2)	120.3(1)
C(10)-C(11)-C(12)	120.34(10)	120.0(1), 119.7(1)	119.96(9)	119.9(2)	120.0(2)
C(11)-C(12)-C(13)	122.57(9)	122.1(1), 122.3(1)	121.82(7)	122.3(2)	122.2(3)
C(11)-C(12)-C(7)	119.76(9)*	120.4(1), 120.4(1)	120.32(7)	120.4(2)	120.4(1)
C(13)-C(12)-C(7)	117.67(9)	117.5(1), 117.4(1)	117.86(7)	117.3(2)	117.6(2)
C(12)-C(13)-O(1)	117.13(8)	117.9(1), 117.9(1)	117.03(7)	117.4(1)	117.5(4)

C(12)-C(13)-C(14)	121.76(9)	121.7(1), 121.3(1)	121.97(7)	122.3(1)	121.8(4)
O(1)-C(13)-C(14)	121.03(9)	120.4(1), 120.7(1)	120.94(7)	120.3(1)	120.7(3)
C(4)-C(14)-C(5)	120.58(9)	121.2(1), 120.3(1)	121.19(7)	120.7(2)	120.8(4)
C(4)-C(14)-C(13)	119.49(9)	118.4(1), 118.5(1)	118.99(7)	119.8(1)	119.0(6)
C(5)-C(14)-C(13)	119.58(10)	119.8(1), 120.5(1)	119.28(8)	119.1(2)	119.7(5)
Torsion angles/degrees					
C(14)-C(13)-O(1)-C(2)	–22.5(2)	–28.3(2), 26.2(2)	–23.9(1)	–25.9(2)	
C(13)-O(1)-C(2)-O(3)	47.9(1)	58.7(1), –57.6(1)	53.8(1)	55.6(2)	
O(1)-C(2)-O(3)-C(4)	–50.4(1)	–54.8(2), 54.7(2)	–55.00(9)	–55.7(2)	
C(2)-O(3)-C(4)-C(14)	25.2(1)	18.6(2), –18.8(2)	23.98(10)	23.6(2)	
O(3)-C(4)-C(14)-C(13)	1.7(2)	13.0(2), –13.2(2)	–167.76(8)	6.7(2)	
C(4)-C(14)-C(13)-O(1)	–3.1(2)	–7.9(2), 9.1(2)	–7.2(1)	–5.3(2)	
Atom deviations (δÅ) from the C_{10} naphthyl plane					
$\chi^2(C_{10})$	32	719, 594	752	257	
δO(1)	0.071(1)	–0.005(2), –0.037(2)	0.028(1)	–0.046(2)	
δC(2)	–0.358(2)	–0.591(2), 0.502(2)	–0.448(2)	0.514(3)	
δO(3)	0.229(2)	0.124(2), –0.217(2)	0.256(2)	–0.121(2)	
δC(4)	0.137(1)	0.238(2), –0.289(2	0.239(1)	–0.121(2)	
δO(4)	0.259(1)	0.594(2), –0.647(3)	0.488(1)	–0.284(2)	
δC(15)	0.094(2)	–0.503(3), 0.357(3)	–0.208(2)	0.260(3)	

*See part (a).

Table S2 Mean skeletal geometries

Values for the less precise determination of **1-iPr** are excluded from the calculations

(a) The naphthyl groups

	1-R	**2-R**
Distances/Å		
C(5)-C(6)	1.378(2)	1.359(2)
C(5)-C(14)	1.417(4)	1.421(1)
C(6)-C(7)	1.414(4)	1.425(4)
C(7)-C(8)	1.422(3)	1.418(3)
C(7)-C(12)	1.429(3)	1.423(1)
C(8)-C(9)	1.369(4)	1.370(2)
C(9)-C(10)	1.412(3)	1.404(3)
C(10)-C(11)	1.372(4)	1.373(1)
C(11)-C(12)	1.422(3)	1.413(1)
C(12)-C(13)	1.417(2)	1.421(2)
C(13)-C(14)	1.368(3)	1.379(3)

Angles/degrees		
C(6)-C(5)-C(14)	119.8(3)	120.3(1)
C(5)-C(6)-C(7)	120.5(2)	120.8(1)
C(6)-C(7)-C(8)	121.8(2)	122.2(4)
C(6)-C(7)-C(12)	119.0(1)	120.0(1)
C(8)-C(7)-C(12)	119.2(2)	117.9(3)
C(7)-C(8)-C(9)	120.5(4)	121.0(2)
C(8)-C(9)-C(10)	120.3(2)	120.6(1)
C(9)-C(10)-C(11)	120.7(1)	120.3(1)
C(10)-C(11)-C(12)	120.5(1)	120.0(2)
C(11)-C(12)-C(7)	118.8(4)	120.4(1)
C(11)-C(12)-C(13)	121.6(4)	122.2(3)
C(7)-C(12)-C(13)	119.73(7)	117.6(2)
C(12)-C(13)-C(14)	119.6(4)	121.8(4)
C(5)-C(14)-C(13)	121.4(4)	119.7(5)

Individual values deviant from the mean by more than 3σ and not included in the calculations are: **1-Et**: C(13)-C(12)-C(7) 118.75(9); **1-nBu**: C(9)-C(10)-C(11) 121.13(8)º; **2-nBu** (mol. 2): C(9)-C(10) 1.414(2) Å; C(14)-C(5)-C(6) 119.8(1)º; **2-iPr**: C(7)-C(12) 1.415(1) Å; C(5)-C(6)-C(7) 121.26(8); C(6)-C(7)-C(12) 119.36(8)º; **2-diox**: C(5)-C(14) 1.429(2) Å.

(b) The six-membered dioxo rings

	1-R	**2-R**
Distances/Å		
O(1)-C(2)	1.413(10)	1.421(4)
O(1)-C(14/13)	1.376(3)	1.365(5)
C(2)-O(3)	1.442(4)	1.440(2)
C(2)-C(15)	1.503(5)	1.506(5)
O(3)-C(4)	1.360(1)	1.366(4)
C(4)-C(5/14)	1.476(5)	1.466(2)
C(4)-O(4)	1.206(3)	1.210(5)
C(5)-C(14)	1.417(4)	(1.421(1))
C(13)-C(14)	(1.368(3))	1.379(3)

Angles/degrees		
C(2)-O(1)-C(14/13)		
O(1)-C(2)-O(3)	(see Table 1(c): individual values)	
O(1)-C(2)-C(15)		
C(2)-O(3)-C(4)		115.5(2)
O(3)-C(4)-C(5/14)	115.5(2)	115.6(4)
O(3)-C(4)-O(4)	118.9(5)	118.7(4)
C(5/14)-C(4)-O(4)	125.5(4)	125.5(7)
C(4)-C(5/14)-C(14/13)	119.1(5)	119.0(6)
C(4)-C(5/14)-C(6/5)	120.9(5)	120.8(4)
C(5/14)-C(14/13)-O(1)	118.3(2)	120.7(3)
O(1)-C(14/13)-C(13/12)	119.8(3)	117.5(4)

Individual values deviant from the mean by more than 3σ and not included in the calculations are (Å): **1-CCl$_3$**: C(2)-C(15) 1.5377(10); C(2)-O(3) 1.4259(9); O(3)-C(4) 1.3719(9); **1-diox**: C(2)-C(15) 1.520(1); **2-Et**: C(2)-O(3)-C(14) 116.92(8)º; **2-diox**: C(2)-O(3) 1.424(2).

Individual values (**1-R**, R = H, Me, Et, nBu, CCl$_3$, diox; **2-R**, R = Et, nBu (mols. 1,2), *i*Pr, diox) are (degrees): C(2)-O(1)-C(14/13): 111.98(8), 112.19(7), 110.98(6), 112.36(6), 112.95(5), 111.76(8); 114.75(8), 111.3(1), 111.3(1), 113.01(6), 111.9(1); O(1)-C(2)-O(3): 111.66(8), 110.86(7), 110.03(6), 110.38(6), 112.74(6), 111.70(7); 111.98(8), 109.8(1), 110.3(1), 110.65(6), 111.5(1); C(15)-C(2)-O(1): –, 108.77(8), 110.14(6), 108.84(6), 107.12(6), 108.46(8); 106.99(8), 109.5(1), 109.3(1), 108.61(8), 106.8(1); C(15)-C(2)-O(3): –, 107.52(8), 108.34(7), 107.89(6), 107.07(5), 105.58(7); 108.58(9), 108.4(1), 108.1(1), 108.67(6), 107.8(1), 108.3(4).

(c) The six-membered dioxo rings: individual values

(i) **1-R**

1-R	**1H**	**1-Me**	**1-Et**	**1-*n*Bu**	**1-CCl$_3$**	**1-diox**
Angles/deg						
C(2)-O(1)-C(14)	111.98(8)	112.19(7)	110.98(6)	112.36(6)	112.95(5)	111.76(8)
O(1)-C(2)-O(3)	111.66(8)	110.86(7)	110.03(6)	110.38(6)	112.74(6)	111.70(7)
O(1)-C(2)-C(15)		108.77(8)	110.14(6)	108.84(6)	107.12(6)	108.46(8)
O(3)-C(2)-C(15)		107.52(8)	108.34(7)	107.89(6)	107.07(5)	105.58(7)
C(2)-O(3)-C(4)	116.50(8)	116.31(8)	115.12(6)	116.06(6)	117.94(6)	118.05(7)
Torsion angles/degrees						
C(14)-O(1)-C(2)-O(3)	57.6(1)	57.60(10)	61.23(8)	58.20(8)	55.76(8)	57.88(10)
O(1)-C(2)-O(3)-C(4)	–53.1(1)	–54.97(10)	–57.17(9)	–55.67(8)	–47.02(8)	–48.2(1)
C(2)-O(3)-C(4)-C(5)	18.8(1)	22.66(11)	19.34(10)	20.76(9)	15.07(9)	13.1(1)
O(3)-C(4)-C(5)-C(14)	9.7(1)	5.3(1)	12.6(1)	10.3(1)	7.04(10)	11.2(1)

C(4)-C(5)-C(14)-O(1)	–3.8(1)	–1.1(1)	–7.4(1)	–6.5(1)	2.71(10)	–.0.1(1)
C(5)-C(14)-O(1)-C(2)	–29.6(1)	–30.6(1)	–29.63(10)	–28.01(9)	–34.06(9)	–34.5(1)

Atom deviations (δÅ) from the C_{10} naphthyl plane

$\chi^2(C_{10})$	442	303	11511	930	1082	1133
δO(1)	0.071(1)	0.072(1)	–0.166(1)	–0.039(1)	0.115(1)	0.024(1)
δC(2)	–0.518(2)	–0.544(1)	–0.854(1)	–0.637(1)	–0.544(1)	–0.700(1)
δO(3)	0.101(1)	0.057(1)	–0.130(1)	0.063(1)	–0.104(1)	–0.201(1)
δC(4)	0.170(1)	0.081(1)	0.098(1)	0.176(1)	0.002(1)	0.006(1)
δO(4)	0.451(2)	0.232(2)	0.417(2)	0.471(1)	0.142(2)	0.203(2)
δC(15)		–0.330(2)	–0.971(2)	–0.536(1)	–0.204(2)	–0.490(2)

(ii) **2-R**

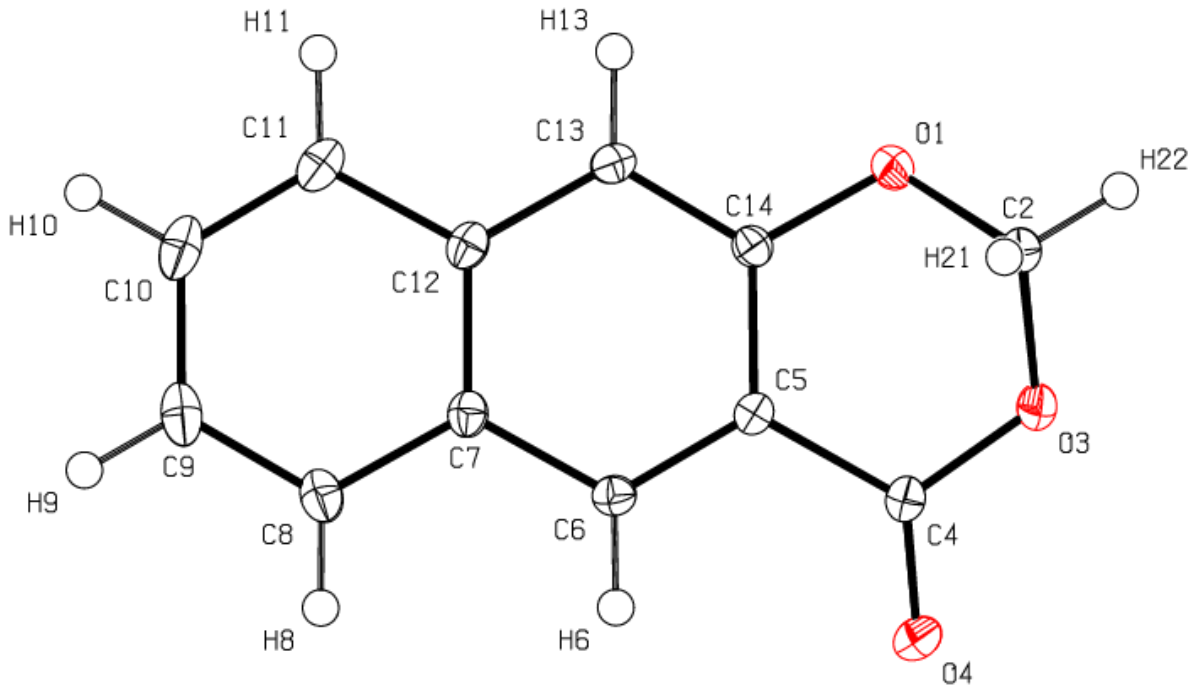
2-R	**2-Et**	**2n-Bu** (mols.1,2)	**2-iPr**	**2-diox**
Angles/degrees				
C(2)-O(1)-C(13)	114.75(8)	111.3(1), 111.3(1)	113.01(6)	111.9(1)
O(1)-C(2)-O(3)	111.98(8)	109.8(1), 110.3(1)	110.65(6)	111.5(1)
O(1)-C(2)-C(15)	106.99(8)	109.5(1), 109.3(1)	108.61(6)	106.8(1)
Torsion angles/degrees				
C(14)-C(13)-O(1)-C(2)	–22.5(2)	–28.3(2), 26.2(2)	–23.9(1)	–25.9(2)
C(13)-O(1)-C(2)-O(3)	47.9(1)	58.7(1), –57.6(1)	53.8(1)	55.6(2)
O(1)-C(2)-O(3)-C(4)	–50.4(1)	–54.8(2), 54.7(2)	–55.00(9)	–55.7(2)
C(2)-O(3)-C(4)-C(14)	25.2(1)	18.6(2), –18.8(2)	23.98(10)	23.6(2)
O(3)-C(4)-C(14)-C(13)	1.7(2)	13.0(2), –13.2(2)	–167.76(8)	6.7(2)
C(4)-C(14)-C(13)-O(1)	–3.1(2)	–7.9(2), 9.1(2)	–7.2(1)	–5.3(2)
Atom deviations (δÅ) from the C_{10} naphthyl plane				
$\chi^2(C_{10})$	32	719, 594	752	257
δO(1)	0.071(1)	–0.005(2), –0.037(2)	0.028(1)	–0.046(2)
δC(2)	–0.358(2)	–0.591(2), 0.502(2)	–0.448(2)	0.514(3)
δO(3)	0.229(2)	0.124(2), –0.217(2)	0.256(2)	–0.121(2)
δC(4)	0.137(1)	0.238(2), –0.289(2	0.239(1)	–0.121(2)
δO(4)	0.259(1)	0.594(2), –0.647(3)	0.488(1)	–0.284(2)
δC(15)	0.094(2)	–0.503(3), 0.357(3)	–0.208(2)	0.260(3)

(d) the five-membered dioxo rings: individual values

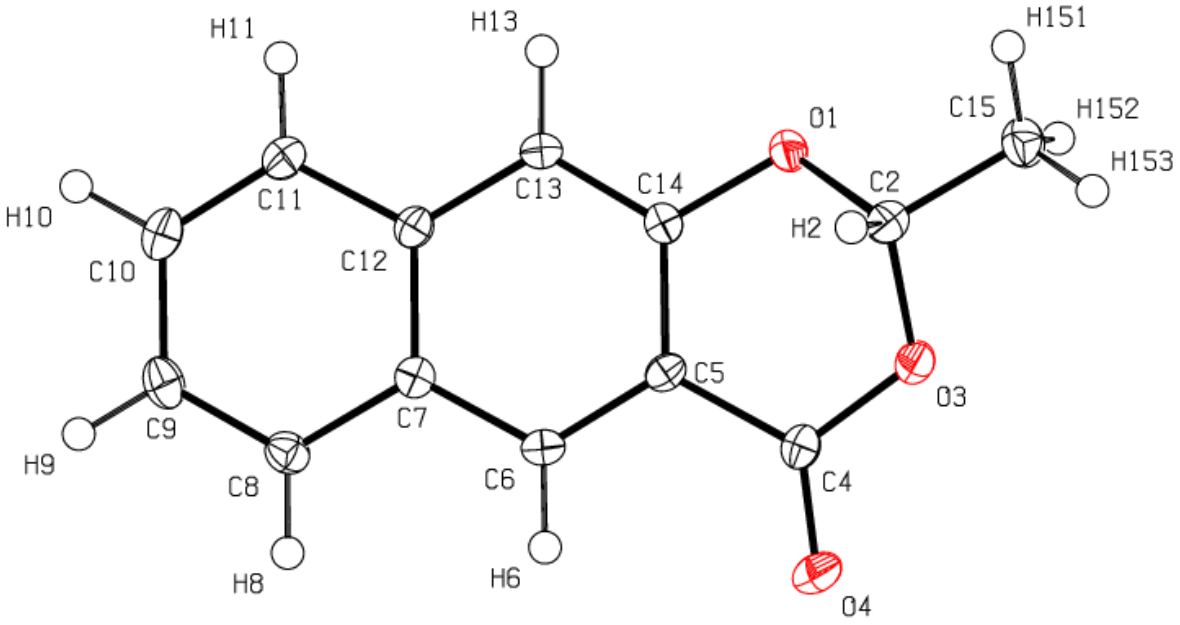
	1-diox	**2-diox**	< >
Distances/Å			
C(15)-O(19)	1.425(2)	1.427(1)	1.426(1)
C(15)-C(16)	1.533(2)	1.519(1)	1.526(10)
C(16)-O(17)	1.429(2)	1.433(1)	1.431(3)
O(17)-C(18)	1.424(2)	1.426(1)	1.425(1)
C(18)-O(19)	1.427(2)	1.427(1)	1.427(1)
Angles/degrees			
O(19)-C(15)-C(16)	104.6(1)	103.54(8)	104.1(8)
C(15)-C(16)-O(17)	103.7(1)	102.62(8)	103.2(8)
C(16)-O(17)-C(18)	106.0(1)	105.53(7)	105.8(4)
O(17)-C(18)-O(19)	104.8(1)	105.55(7)	105.2(6)

C(18)-O(19)-C(15)	108.7(1)	109.03(7)	108.9(2)
Torsion angles/degrees			
O(19)-C(15)-C(16)-O(17)	–14.9(2)	–30.3(1)	
C(15)-C(16)-O(17)-C(18)	31.1(2)	37.6(1)	
C(16)-O(17)-C(18)-O(19)	–35.8(2)	–30.5(1)	
O(17)-C(18)-O(19)-C(15)	26.0(2)	10.5(1)	
C(18)-O(19)-C(15)-C(16)	–6.6(2)	12.3(1)	

Fig. S1 Molecular projections of all investigated compounds with anisotropic displacement parameters for non-hydrogen atoms shown at a 50% probability amplitude level, hydrogen atoms are of arbitrary radii



a) **1-H**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C13
C11
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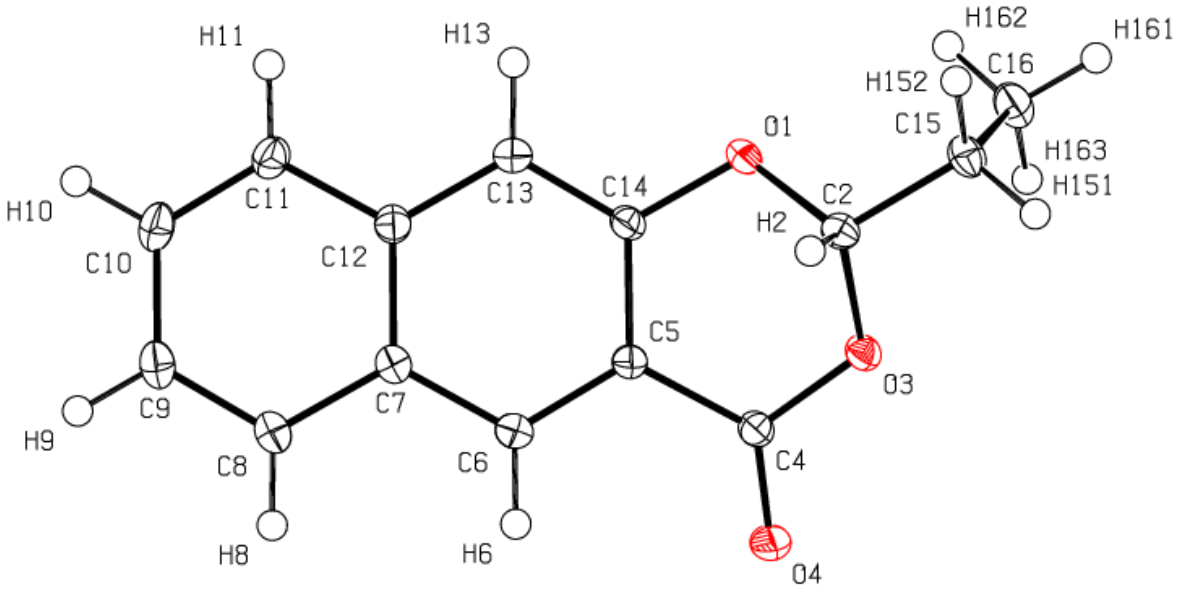
C9
C7
H9
C8
C6
C4
H8
H6
O4

b) **1-Me**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C13
C10
C12
C5
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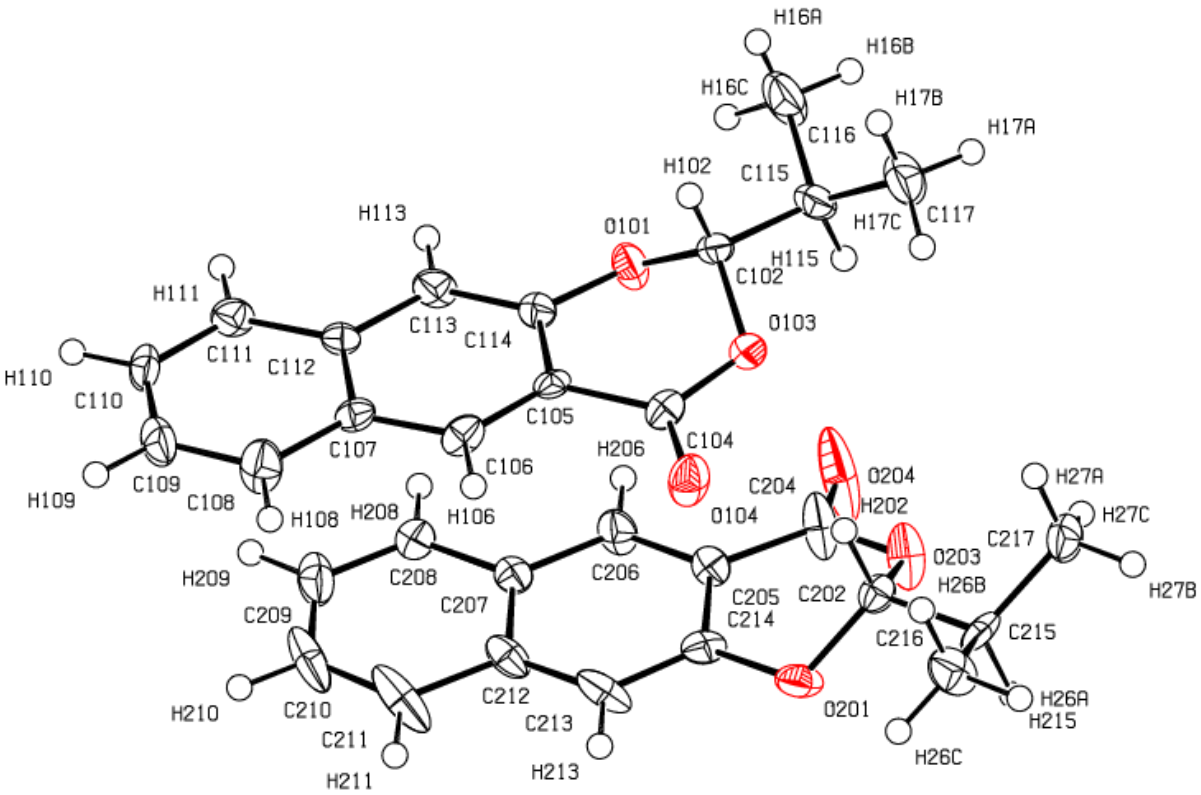
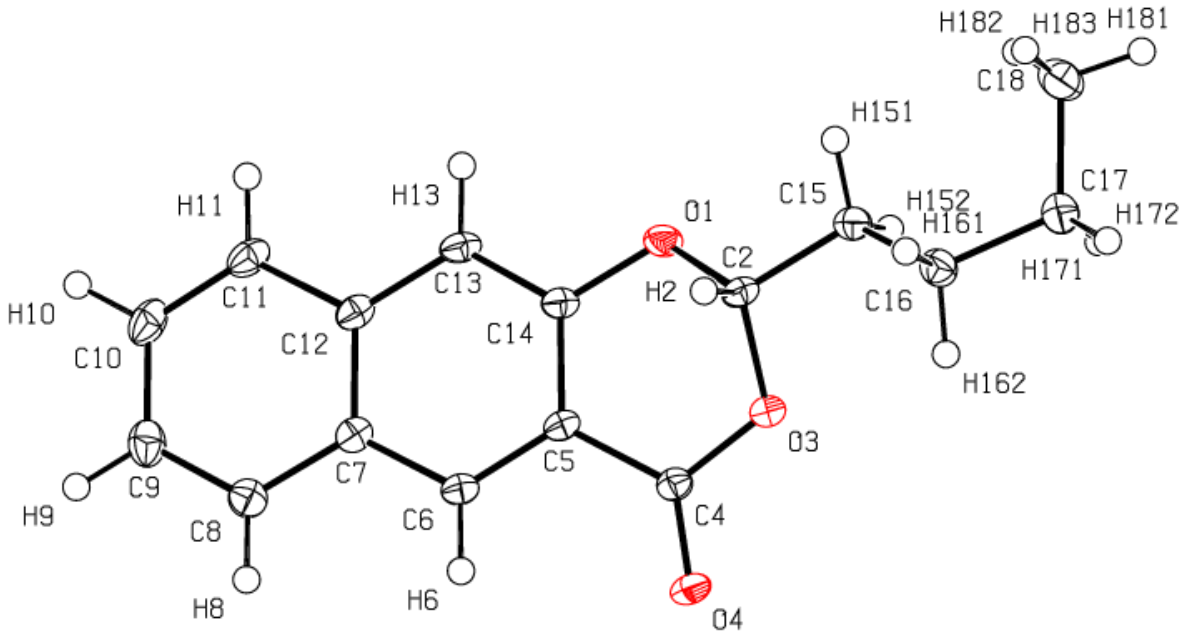
C9
C7
H9
C8
C6
C4
H8
H6
O4

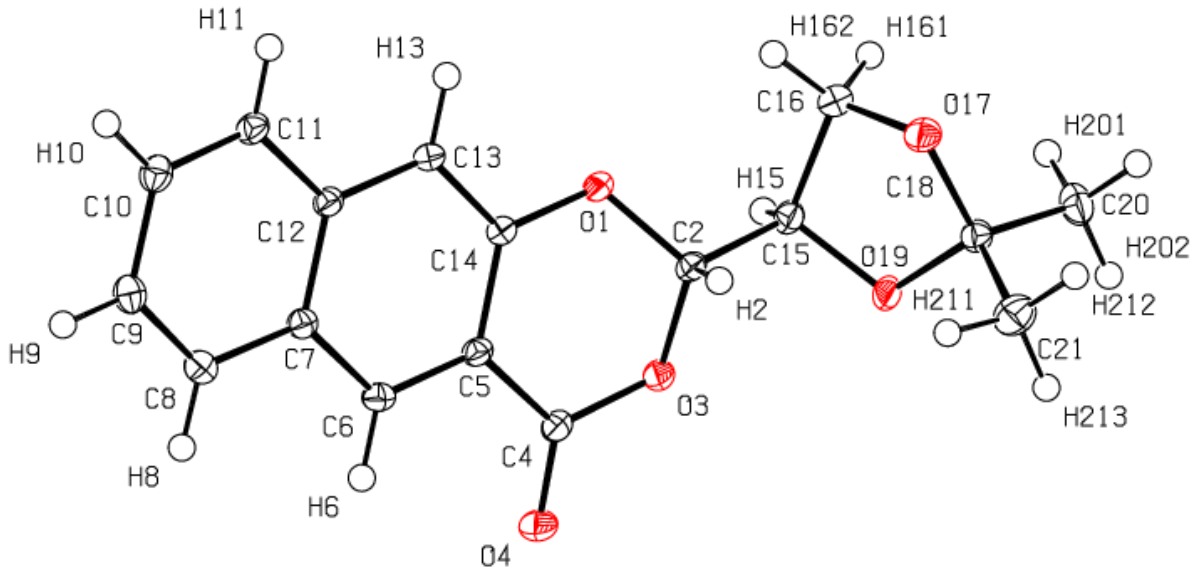
c) **1-Et**



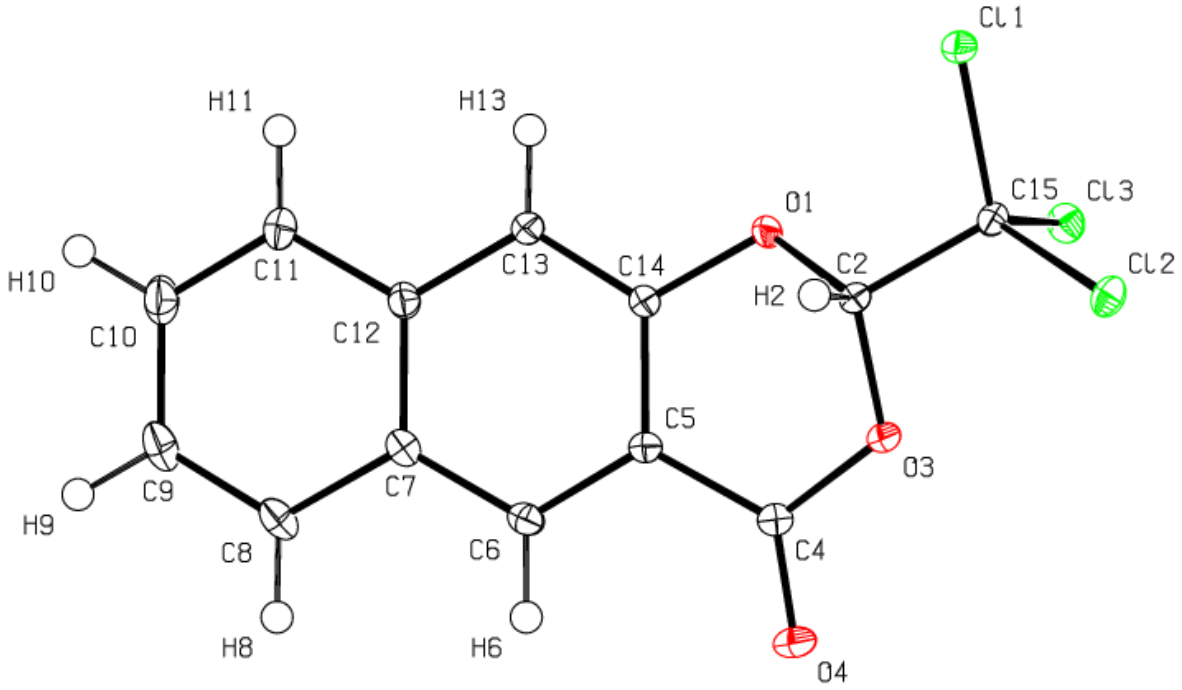
d) **1-iPr**



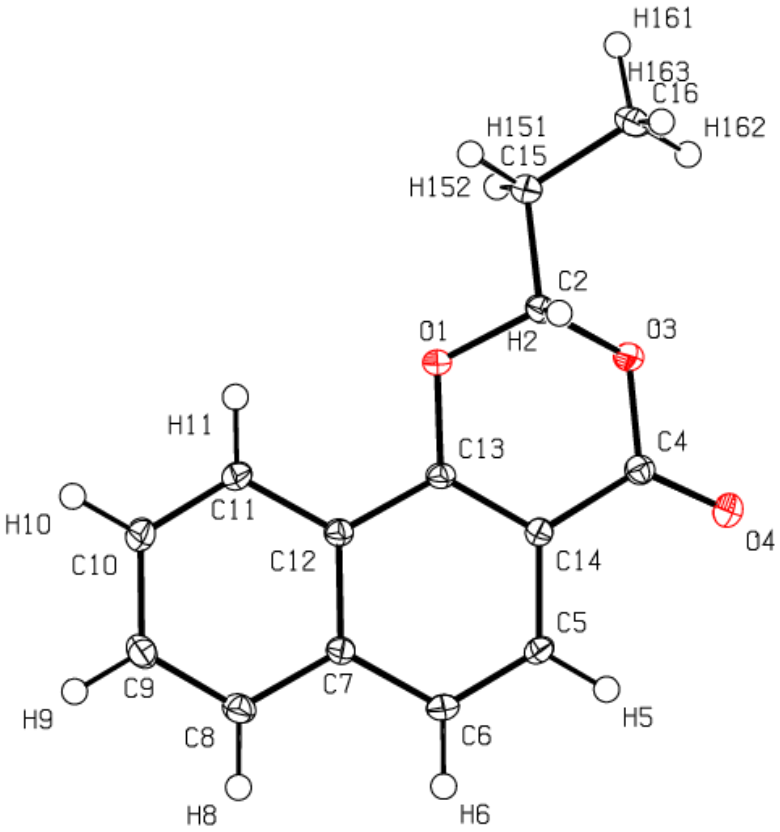
e) **1-nBu**



f) **1-diox**



g) **1-CCl_3**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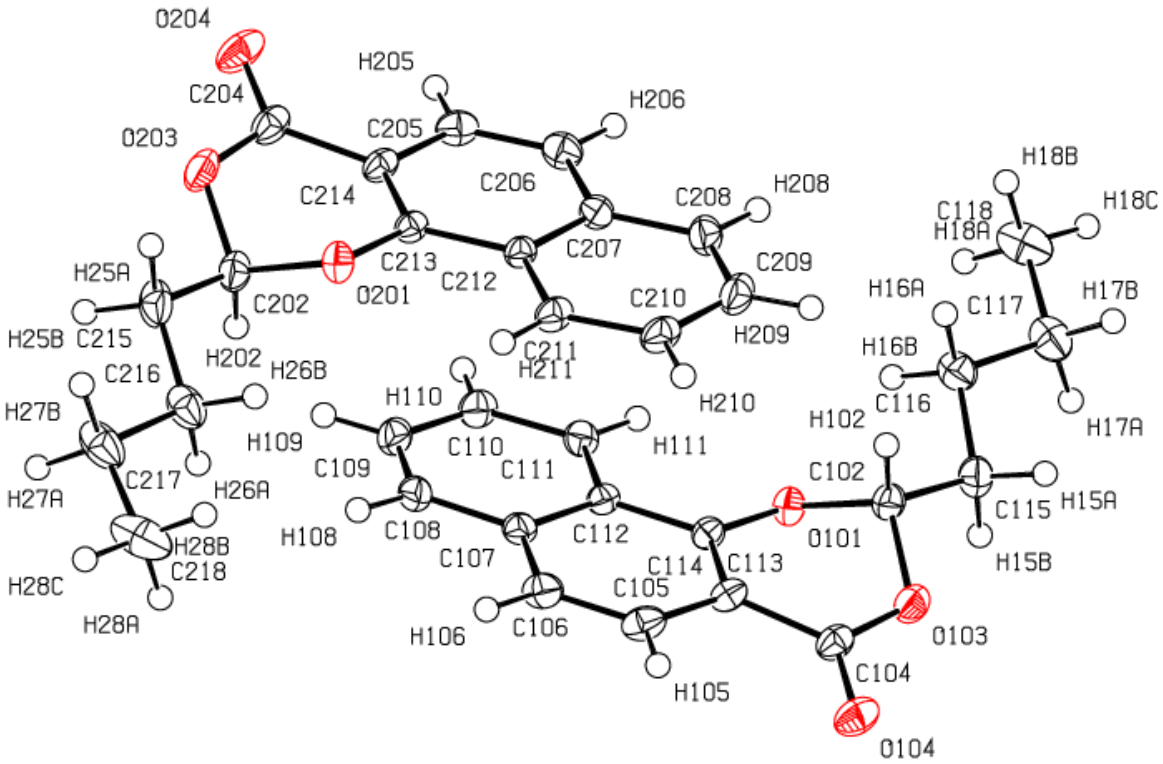
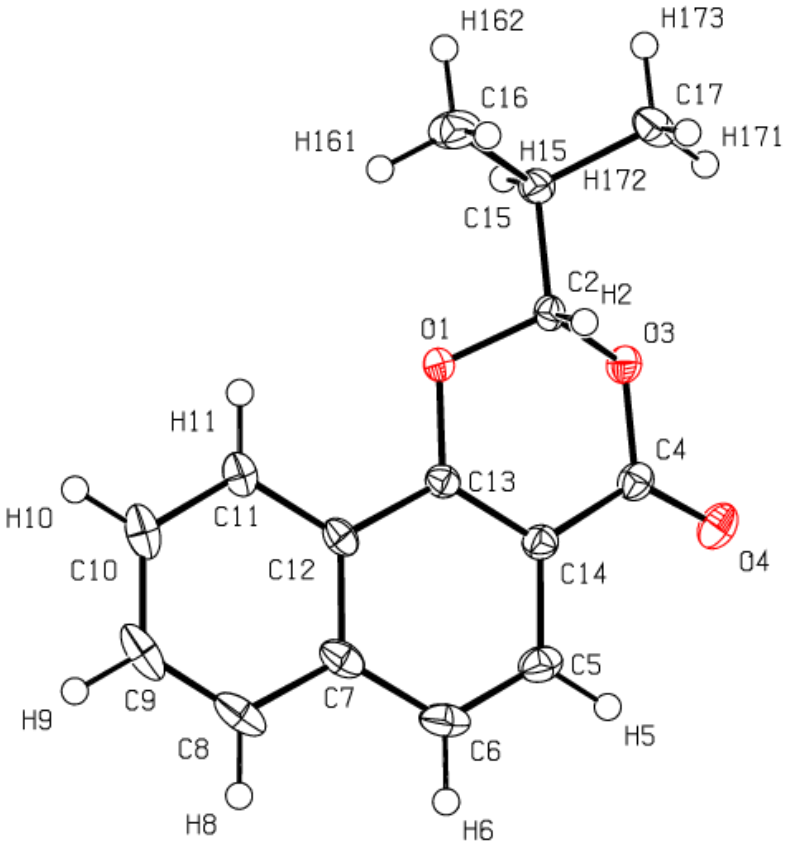
O4
C10
C12
C14
C5
C9
C7
H9
H5
C8
C6
H8
H6

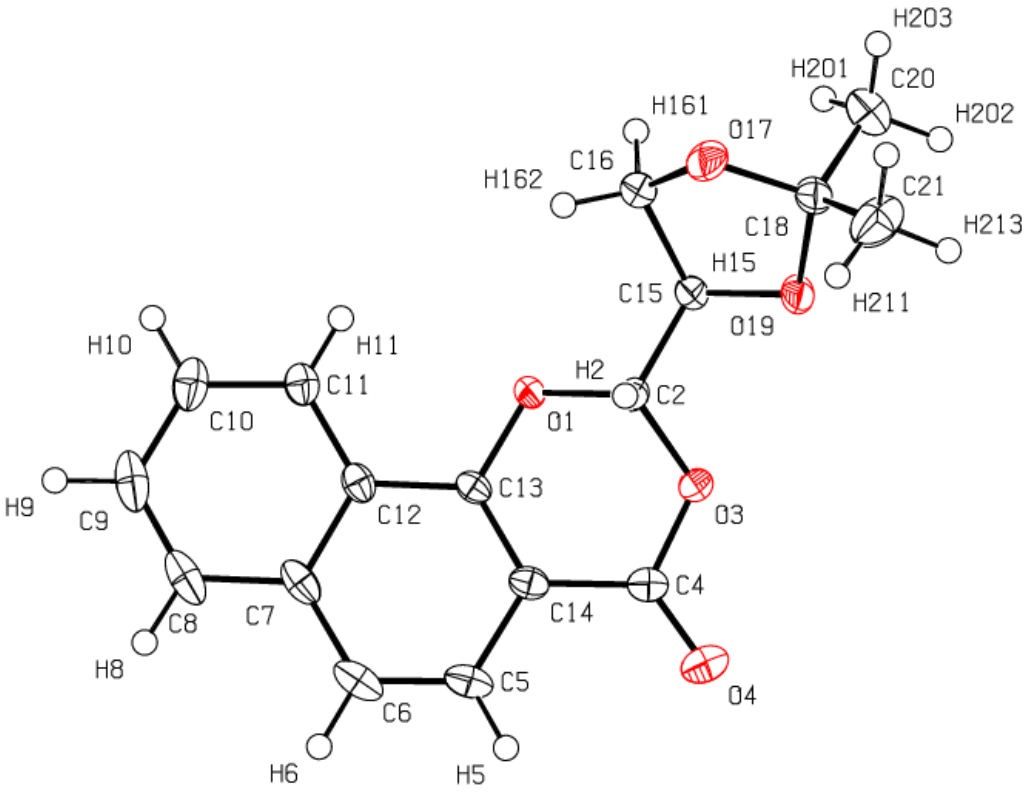
h) **2-Et**


O204
H205
C204
H206
C205
O203
C206
H208
C214
C208
H18B
C118
H18C
H18A
C213
C207
C209
H25A
C212
O201
C210
H16A
C117
H17B
C202
H25B
C215
H209
H16B
H202
H26B
C211
H211
C216
H110
C116
H27B
H102
H109
C110
H111
H17A
C109
C111
C102
H27A
C217
H26A
C115
H15A
H108
C108
C112
O101
H28B
C107
C114
C113
H15B
H28C
C218
C105
O103
H106
C106
C104
H28A
H105
O104

i) **2-nBu**

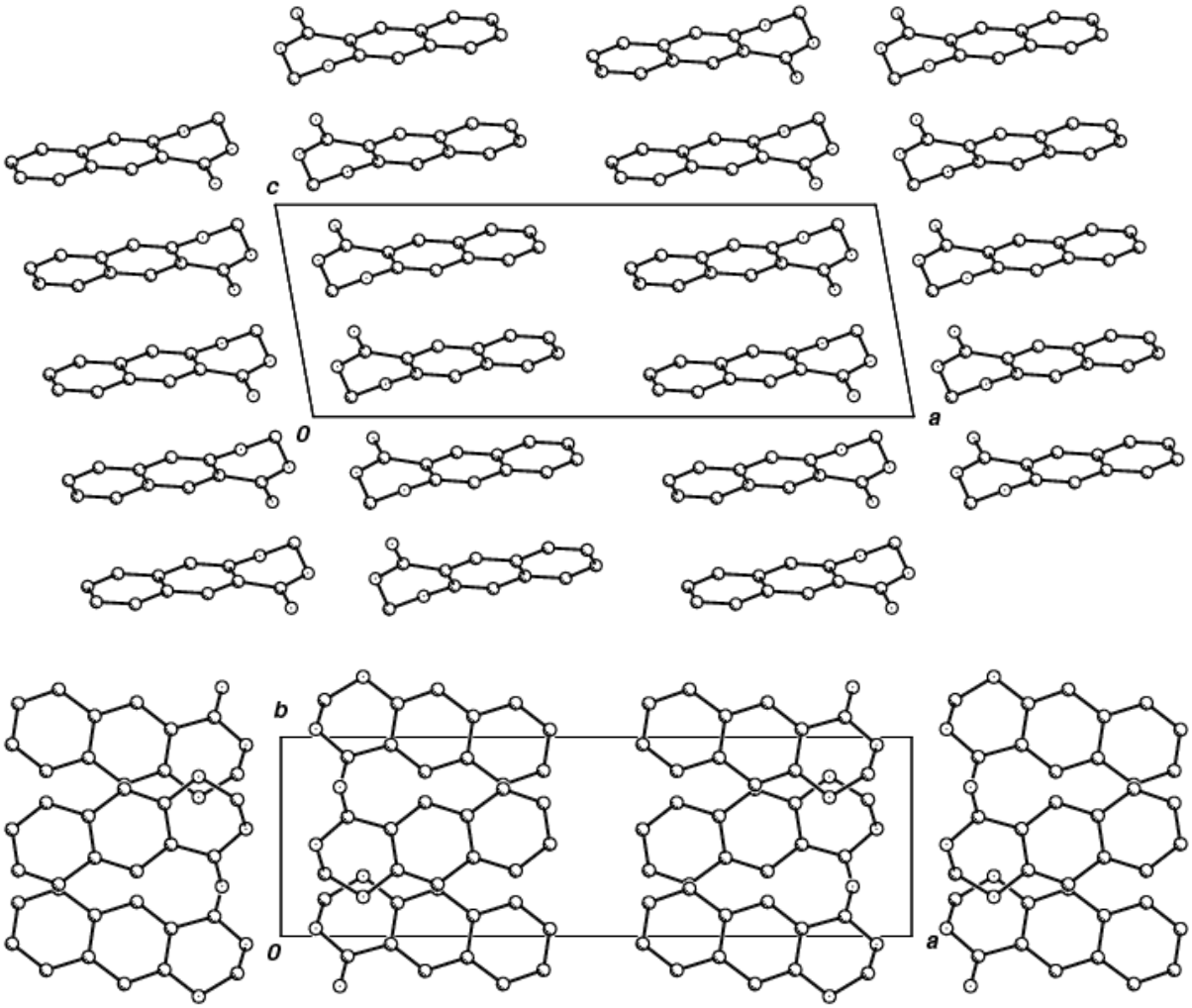


j) **2-iPr**

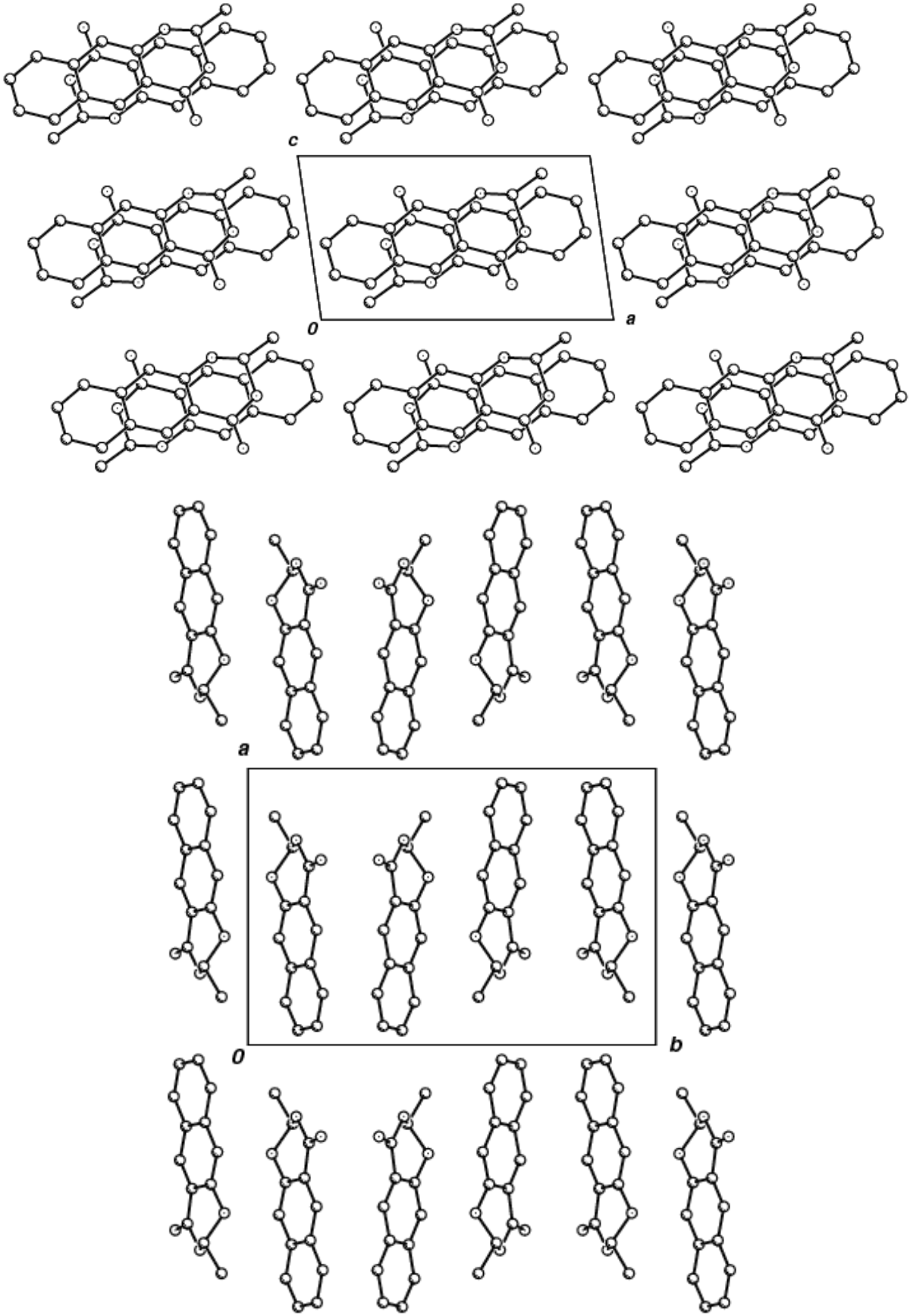


k) **2-diox**

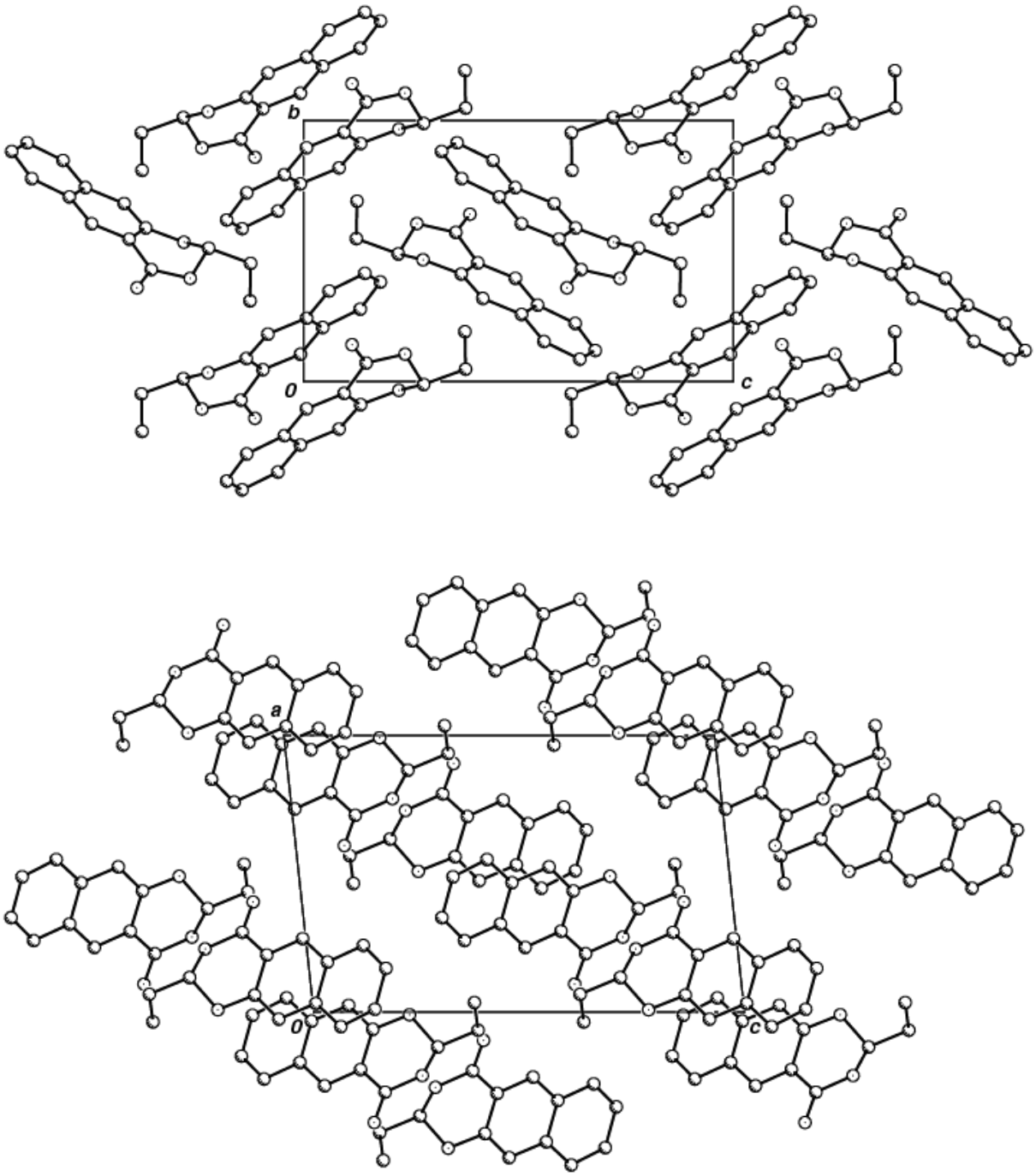
Fig S2 Packing diagrams of all compounds studied



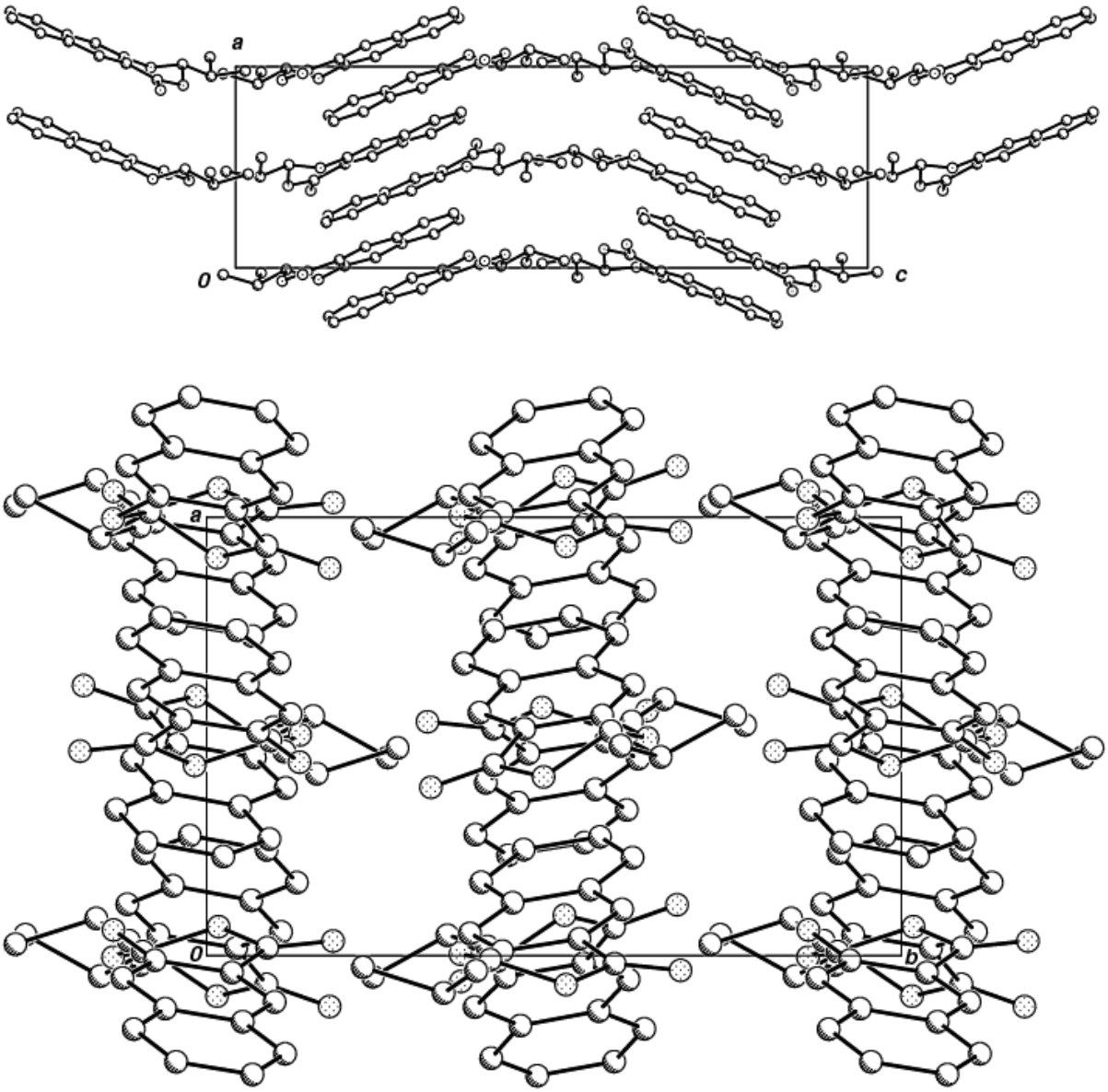
a) **1-H**, projections along *b* (above) and *c* (below)



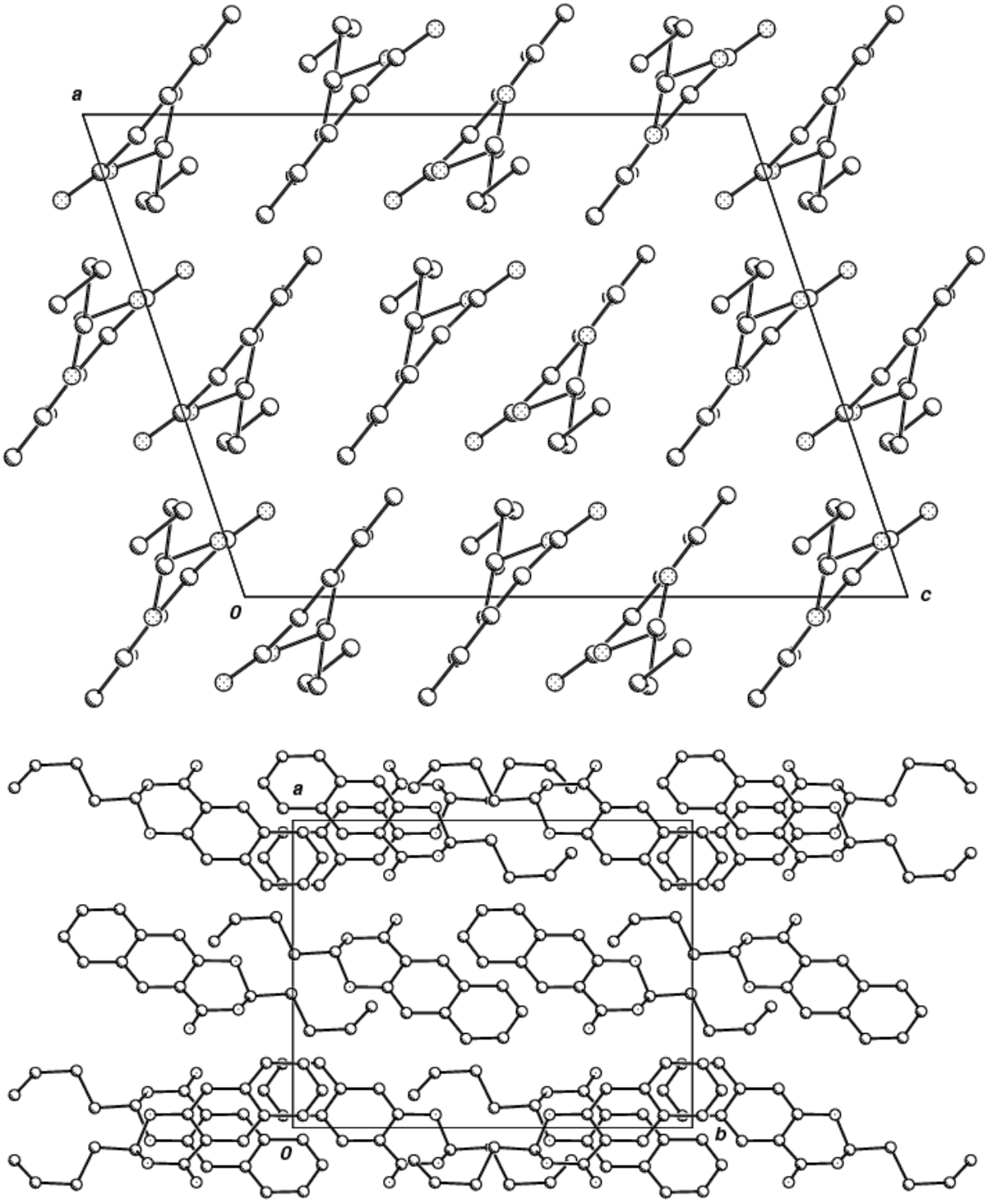
b) **1-Me**, projections along *b* (above) and *c* (below)



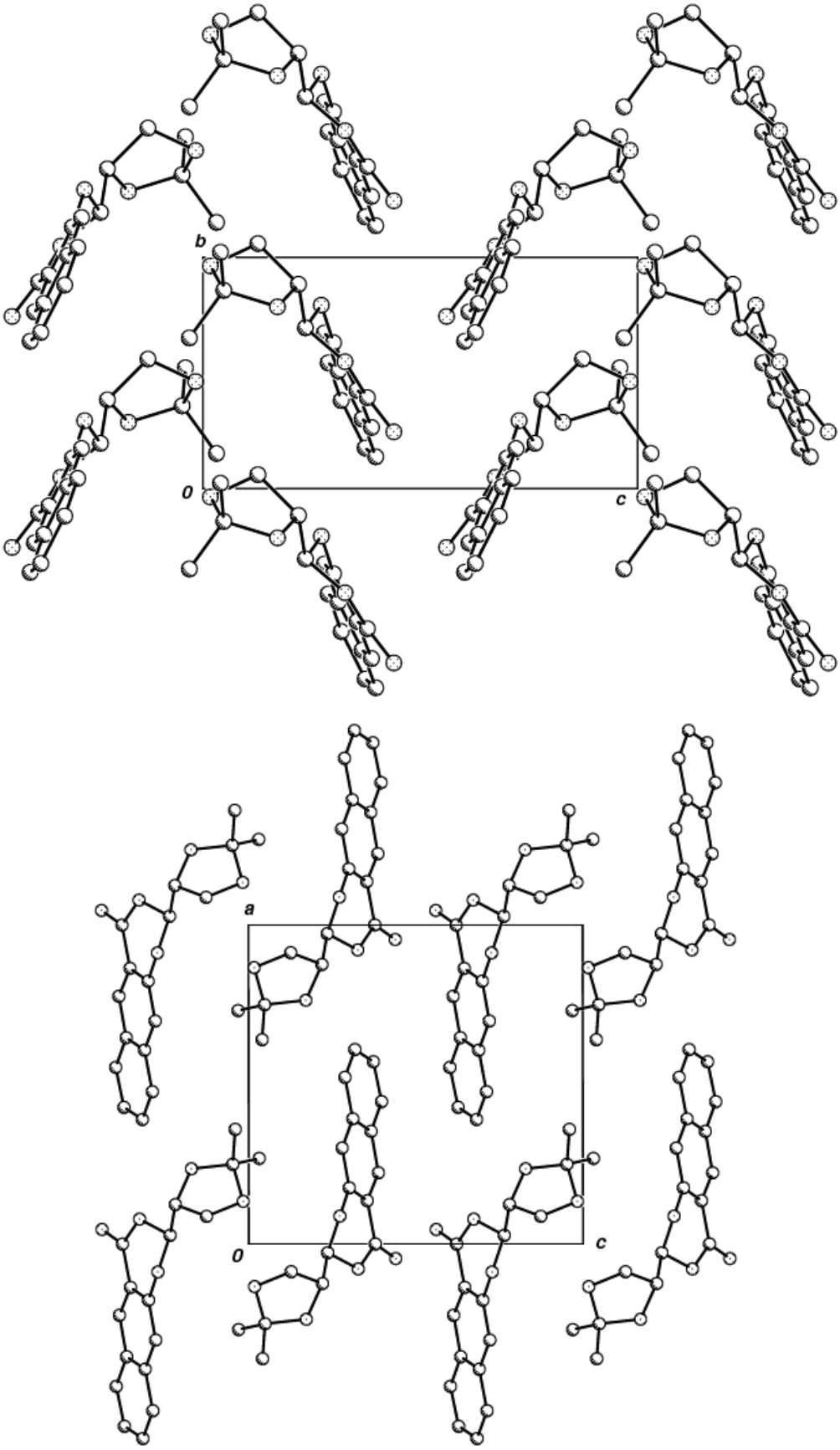
c) **1-Et**, projections along *a* (above) and *b* (below)



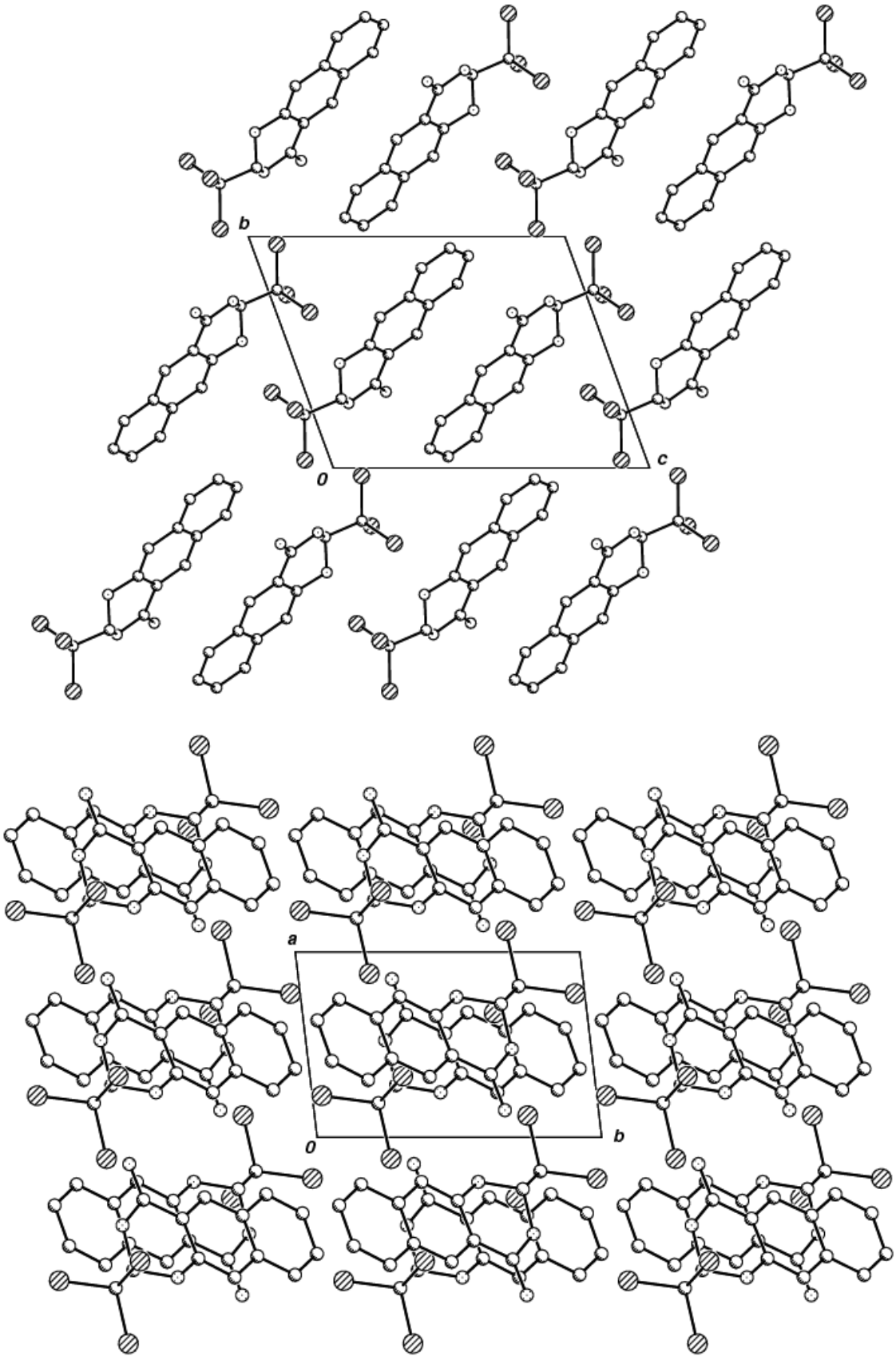
d) **1-iPr**, projections along *b* (above) and *c* (below)



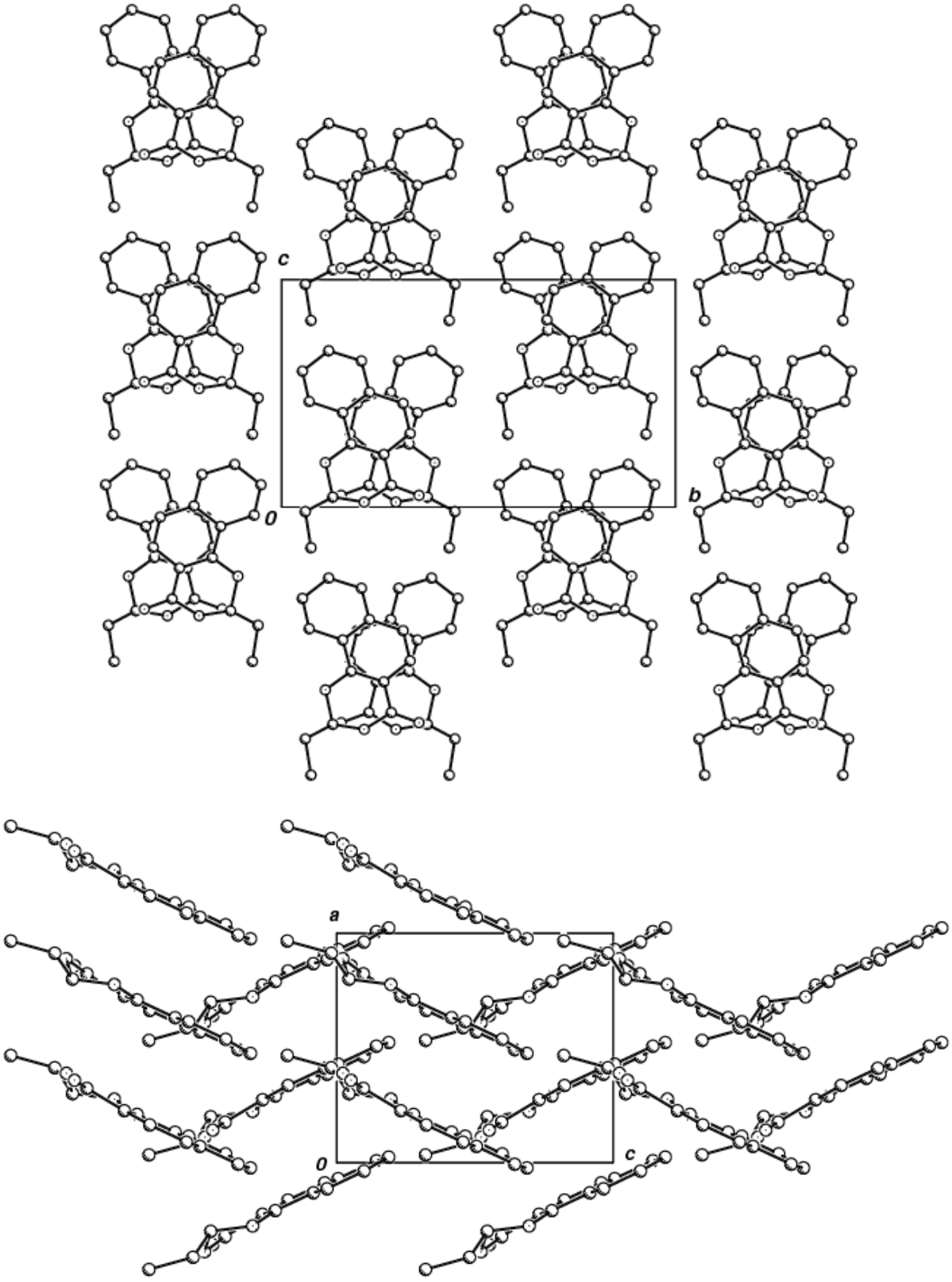
e) **1-nBu**, projections along *b* (above) and *c* (below)



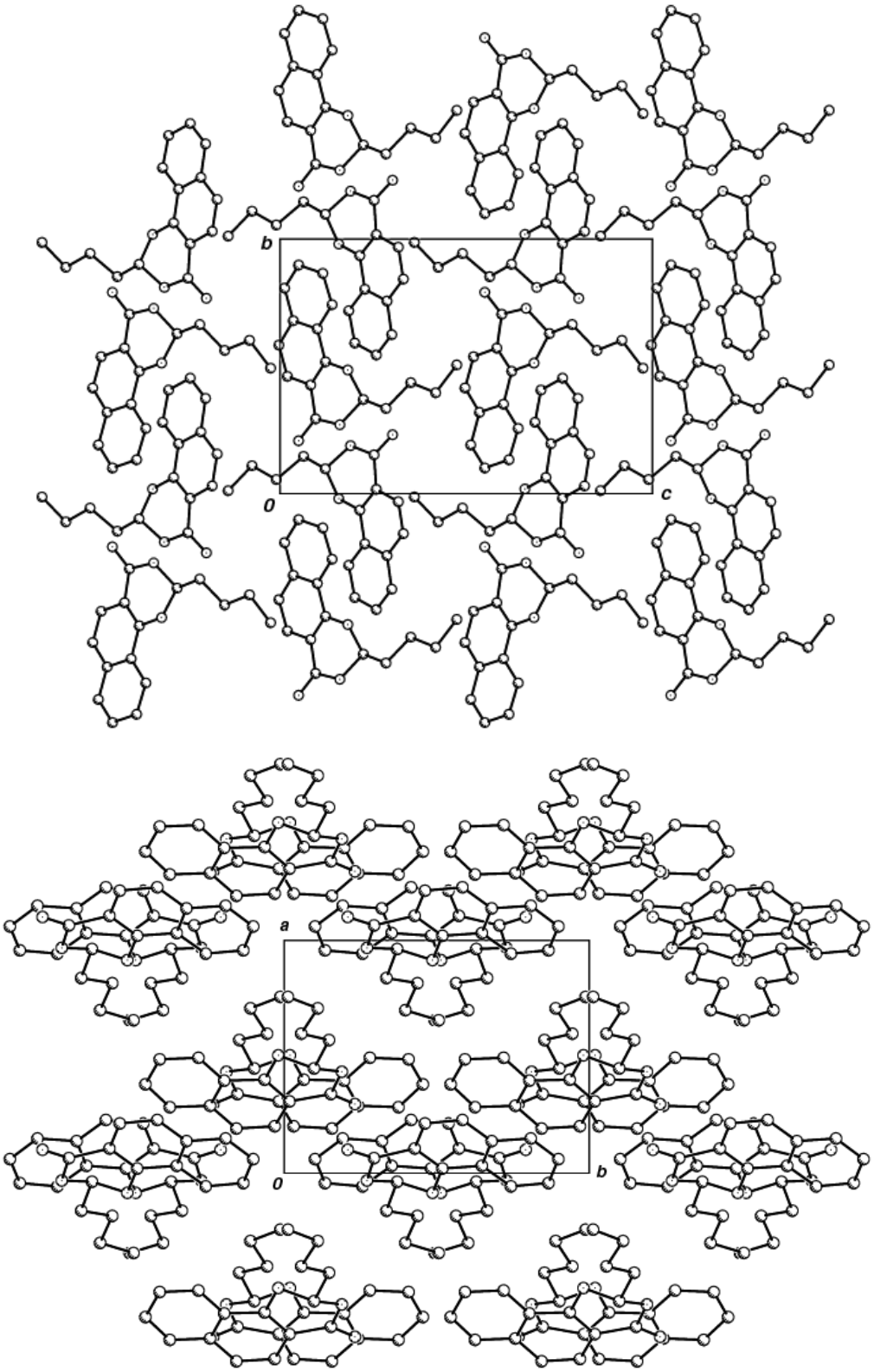
f) **1-diox**, projections along *a* (above) and *b* (below)



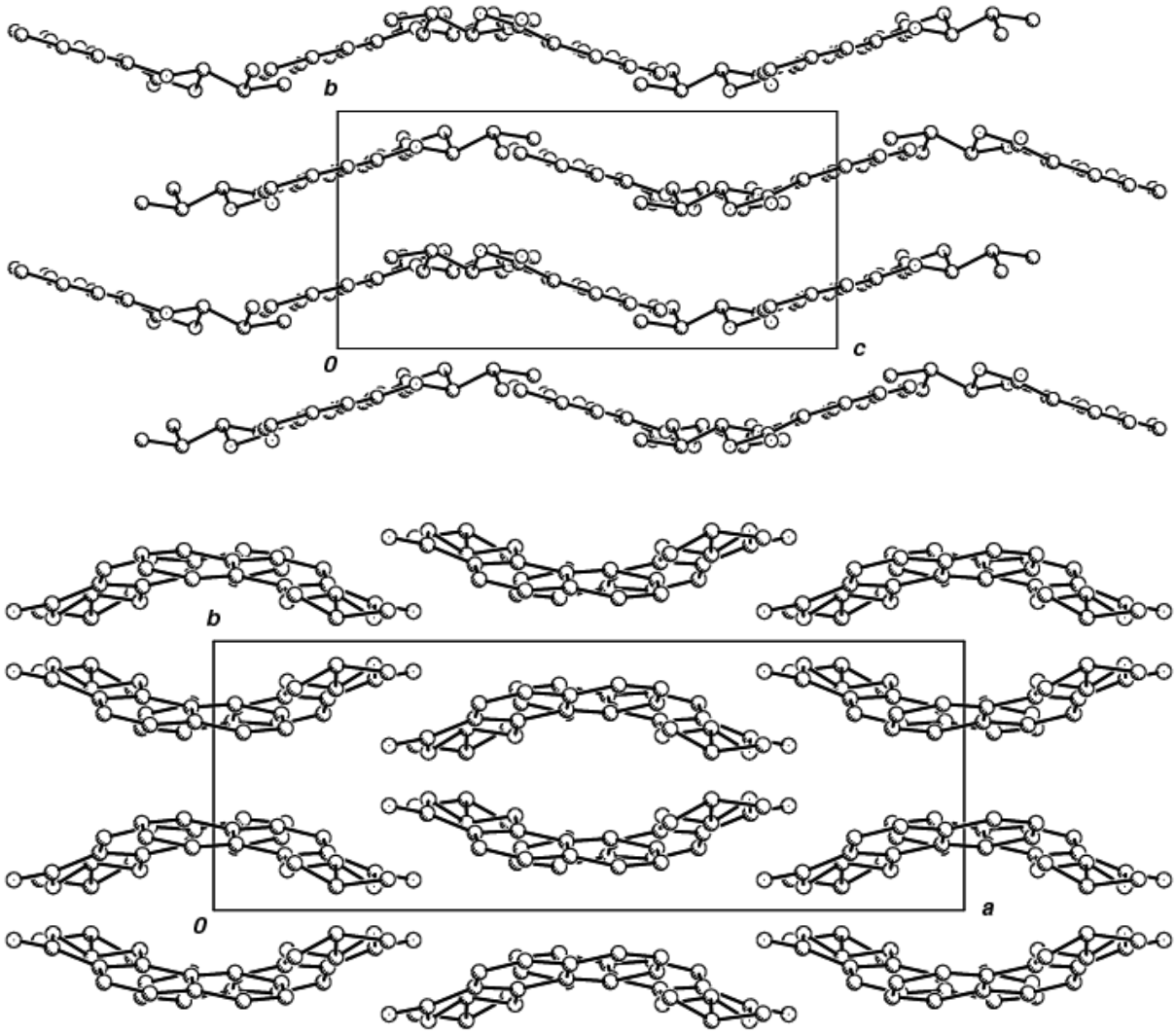
g) **1-CCl$_3$**, projections along *a* (above) and *c* (below)



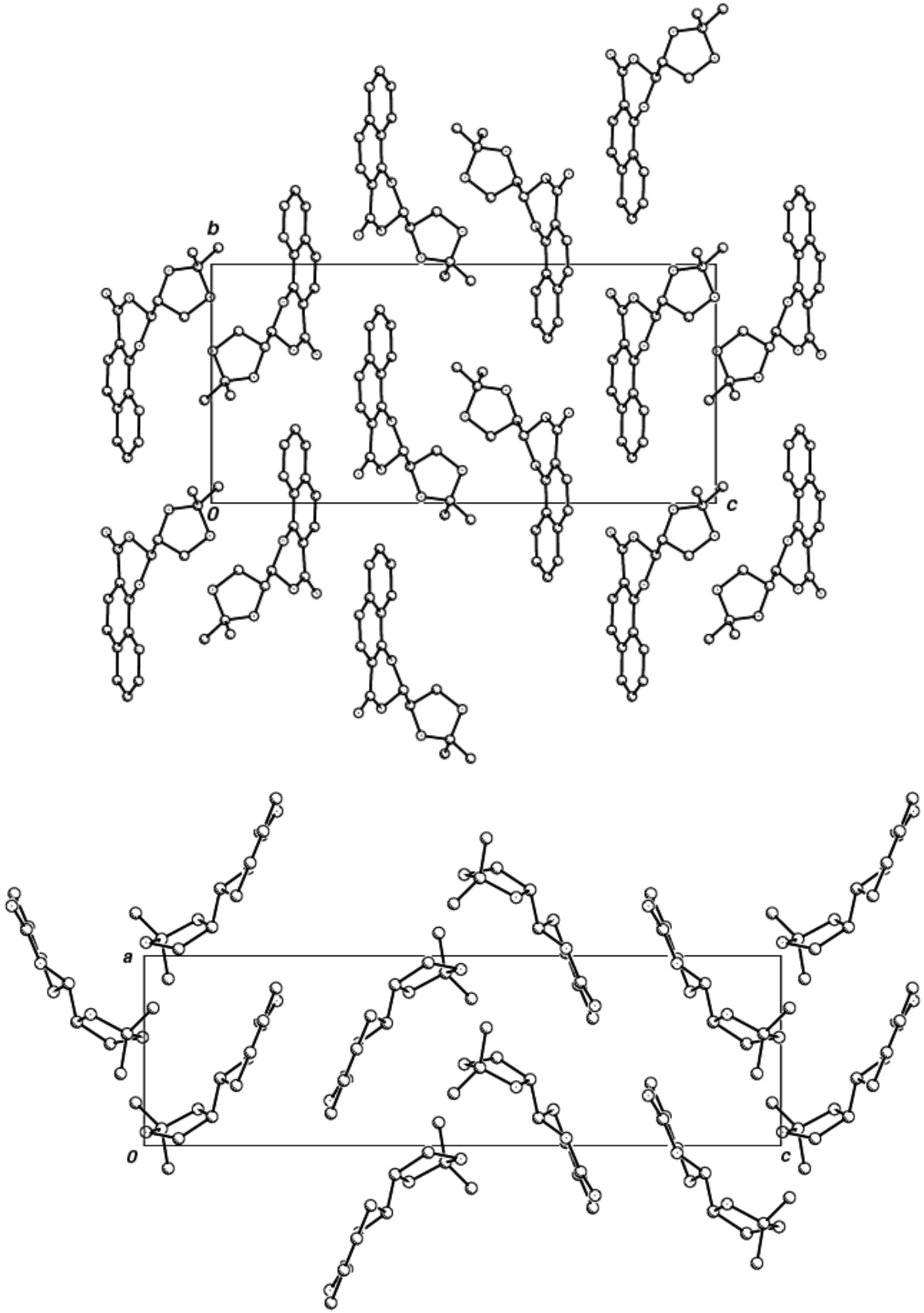
h) **2-Et**, projections along *a* (above) and *b* (below)



i) **2-nBu**, projections along *a* (above) and *c* (below)

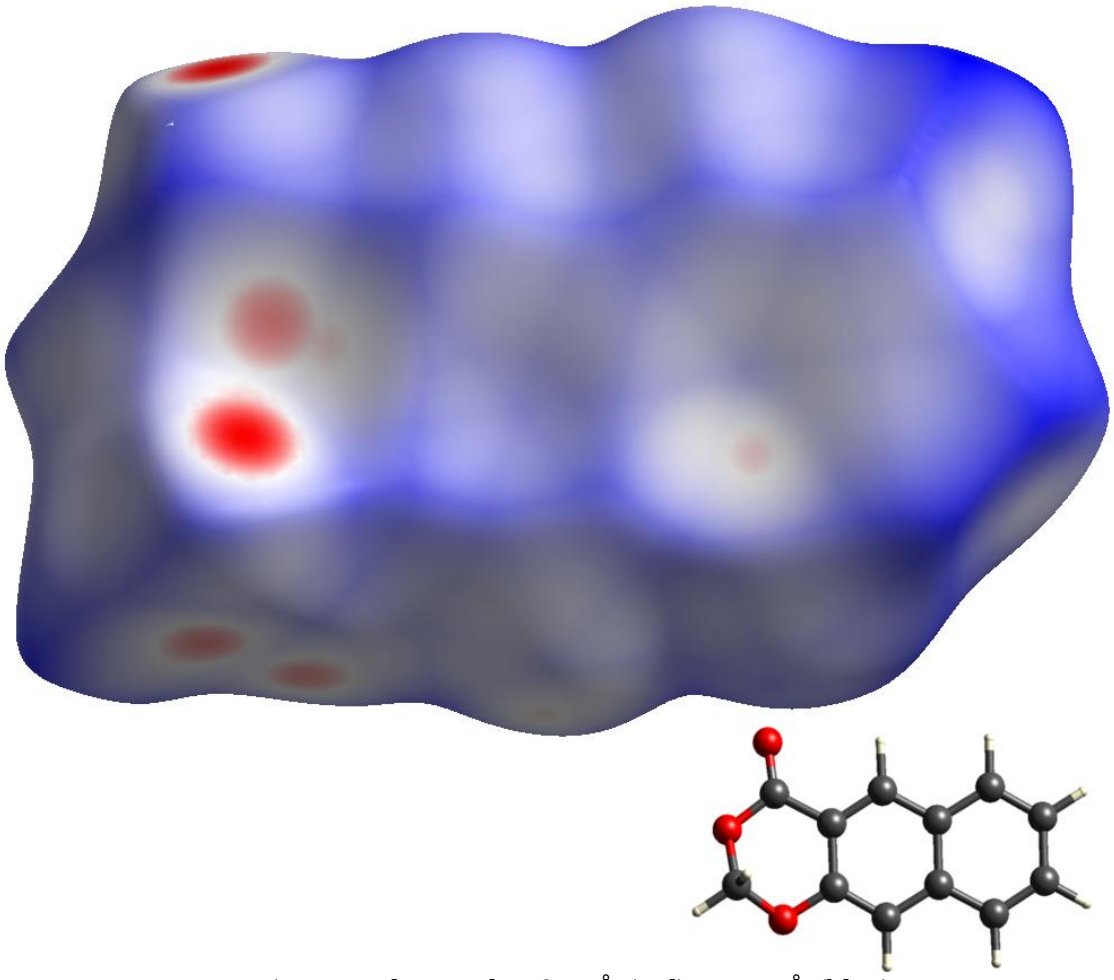


j) **2-iPr**, projections along *a* (above) and *c* (below)

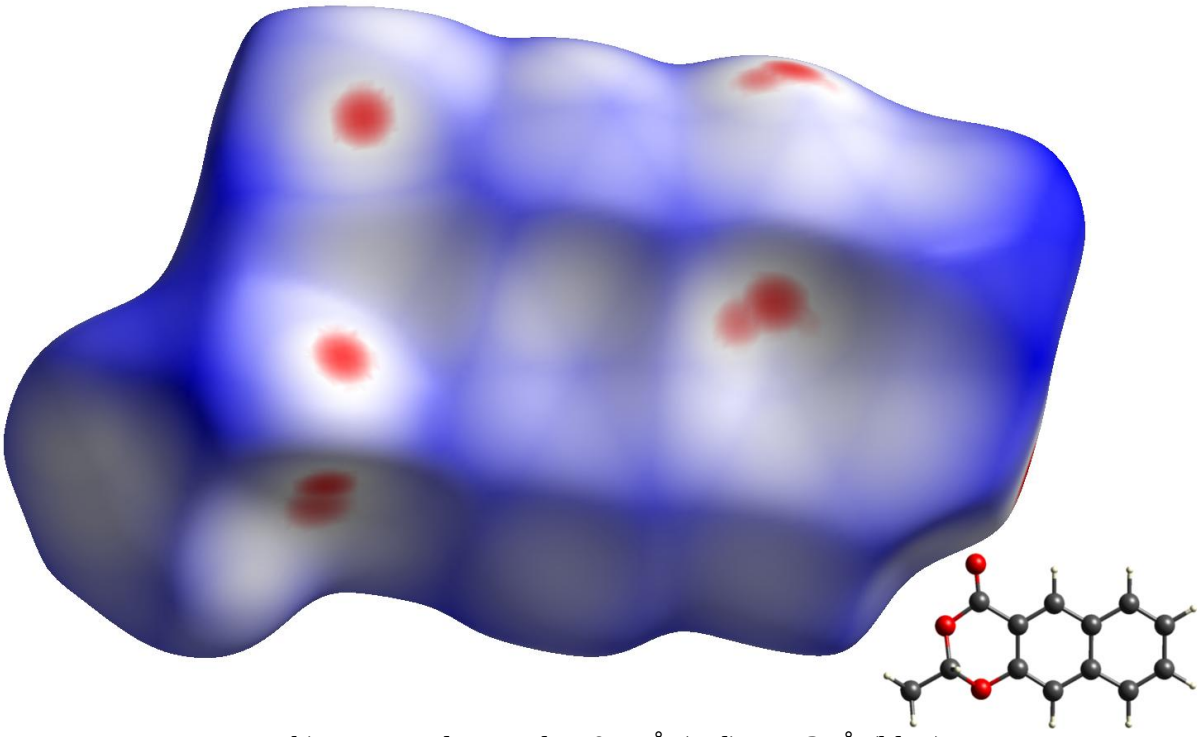


k) **2-diox**, projections along *a* (above) and *b* (below)

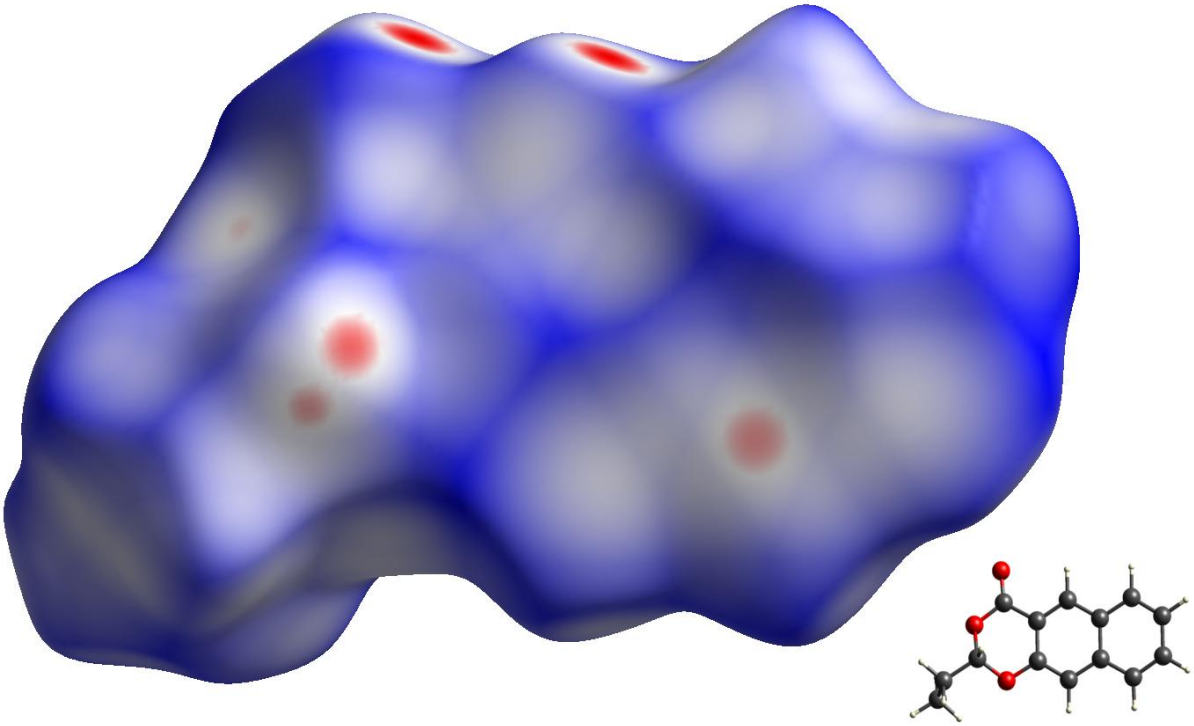
Fig. S3 Hirshfeld surface representations with the geometric function d_{norm} plotted onto it for all compounds investigated



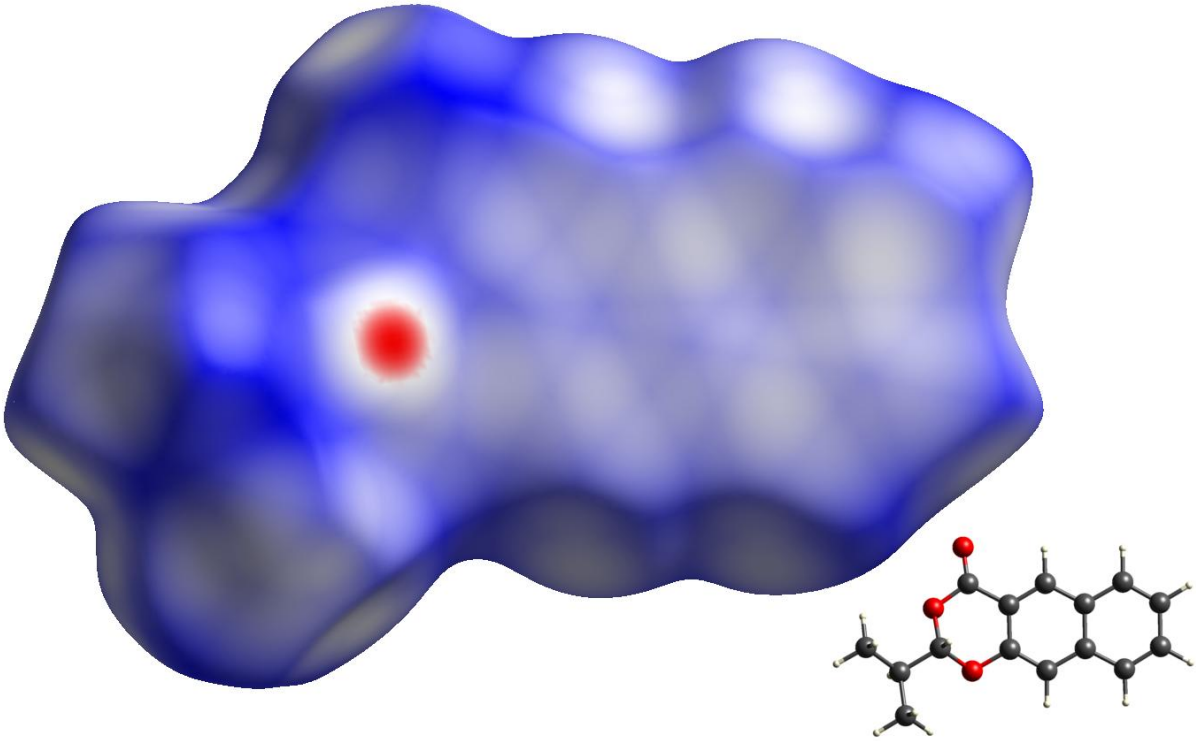
a) **1-H**, colour code: -0.25Å (red) to 1.24Å (blue)



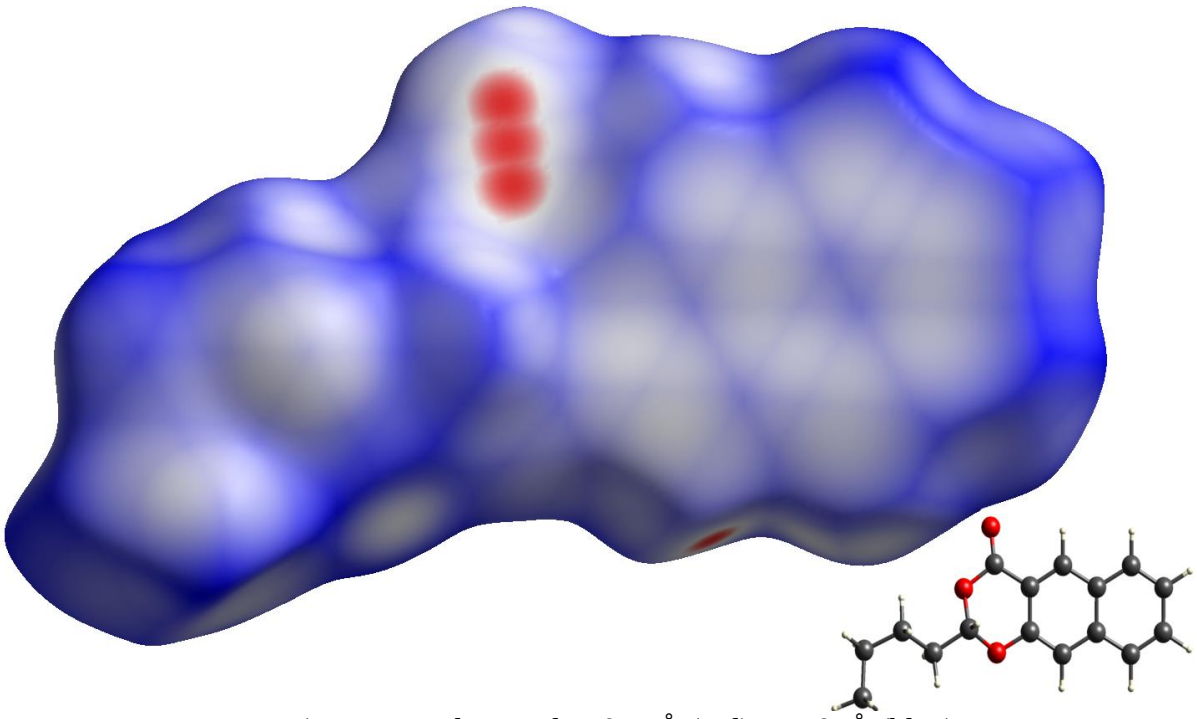
b) **1-Me**, colour code: -0.15Å (red) to 1.31Å (blue)



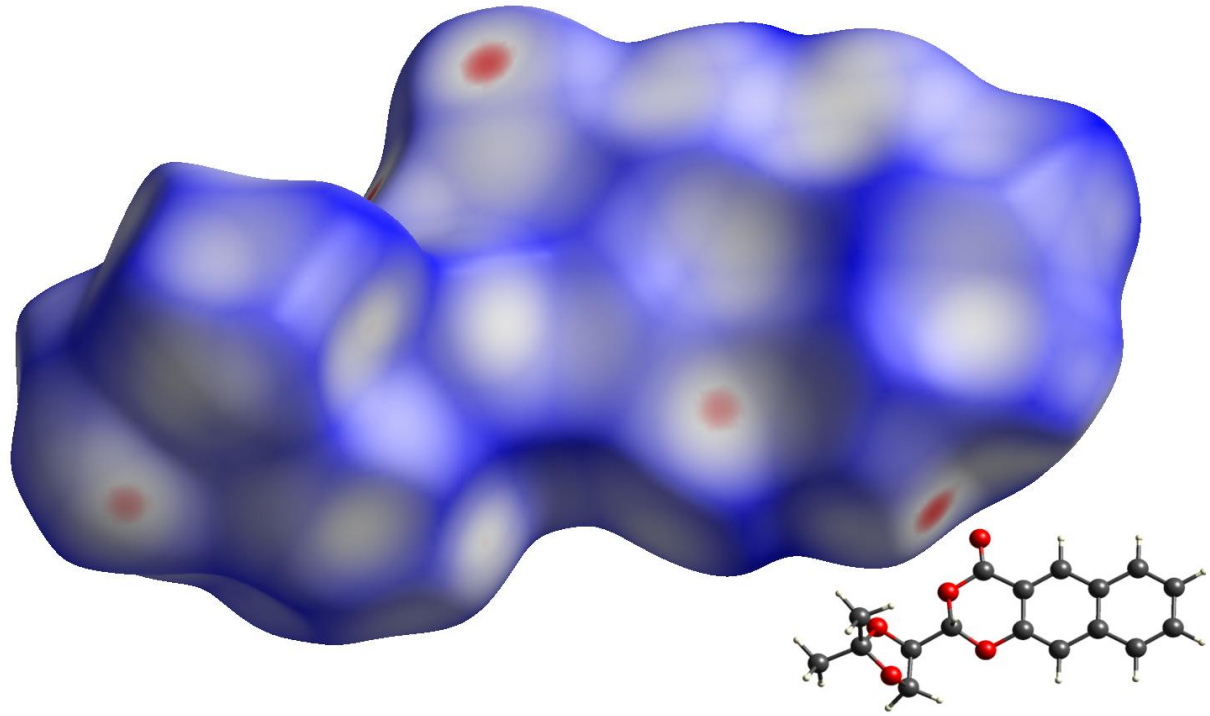
c) **1-Et**, colour code: -0.15Å (red) to 1.20Å (blue)



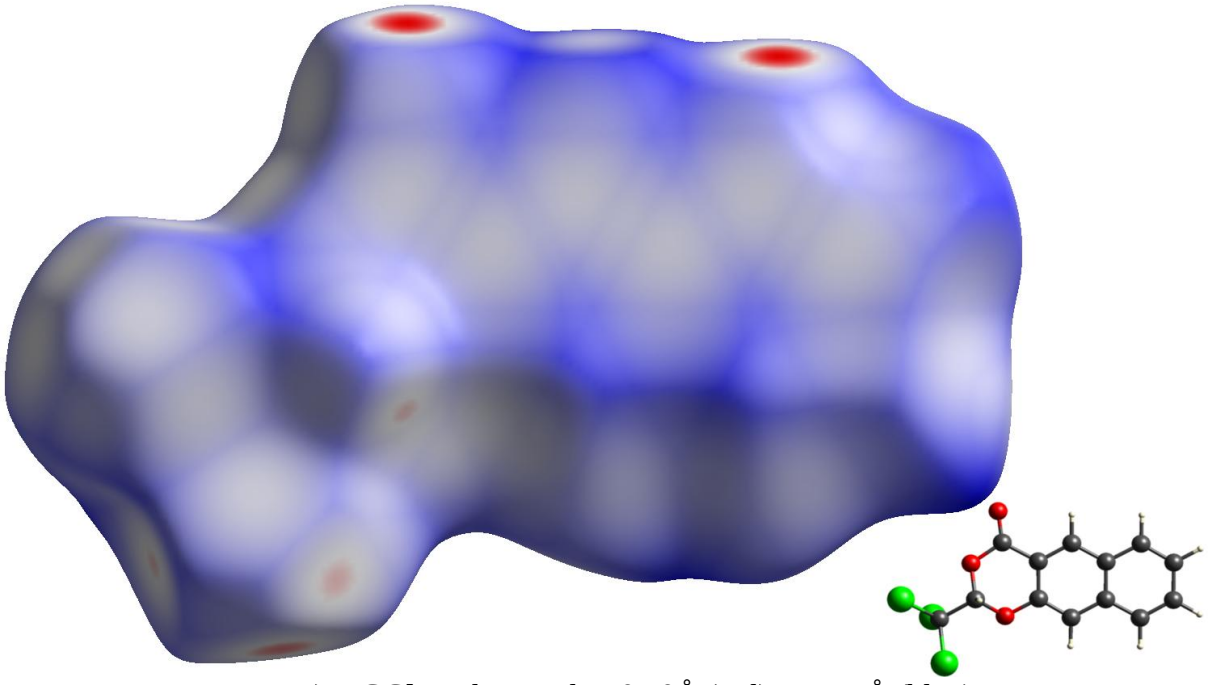
d) **1-iPr**, colour code: -0.21Å (red) to 1.14Å (blue). The Hirshfeld surface of the second molecule of the asymmetric unit is similar and therefore not shown.



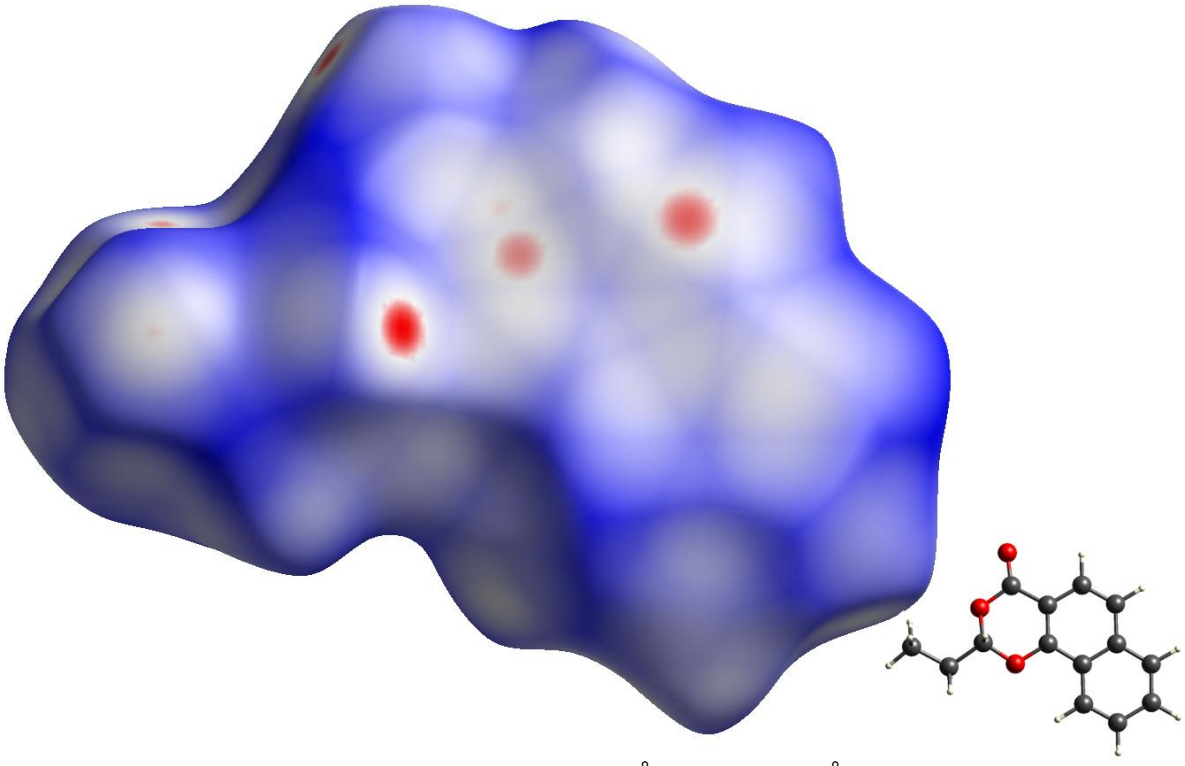
e) **1-nBu**, colour code: -0.15Å (red) to 1.05Å (blue)



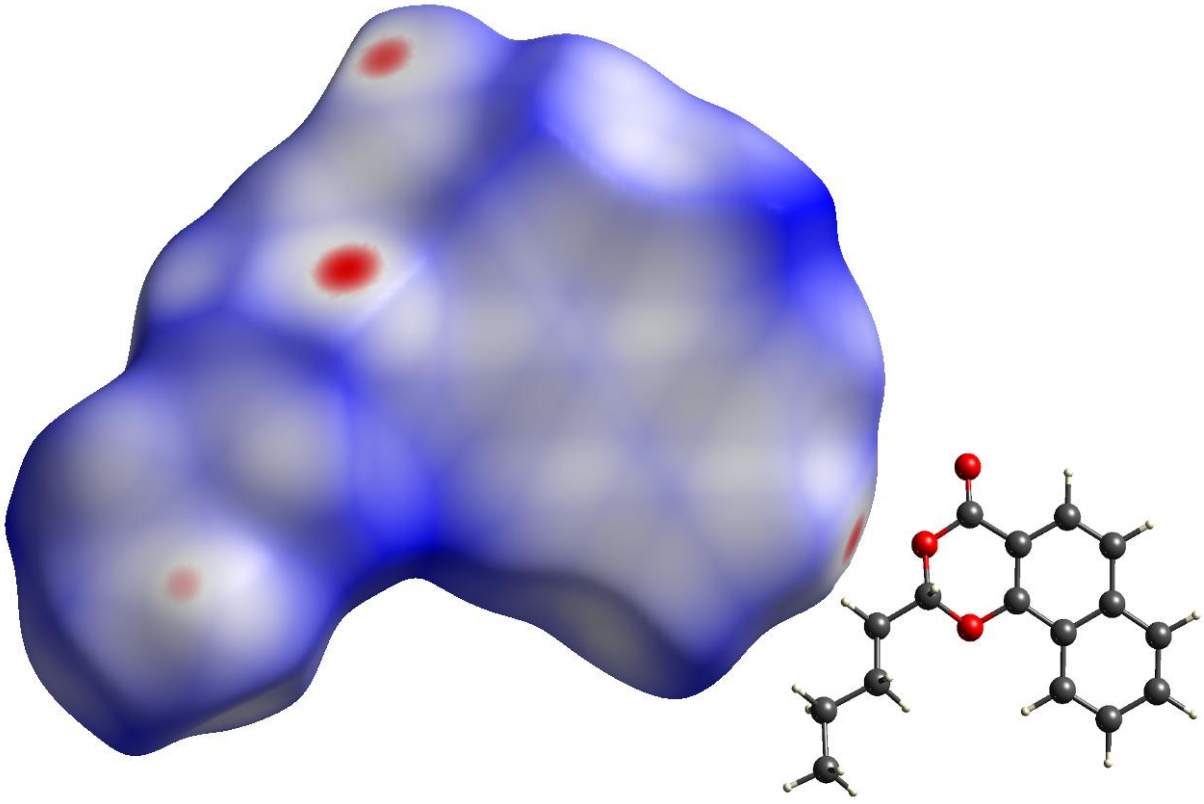
f) **1-diox**, colour code: -0.18Å (red) to 1.09Å (blue)



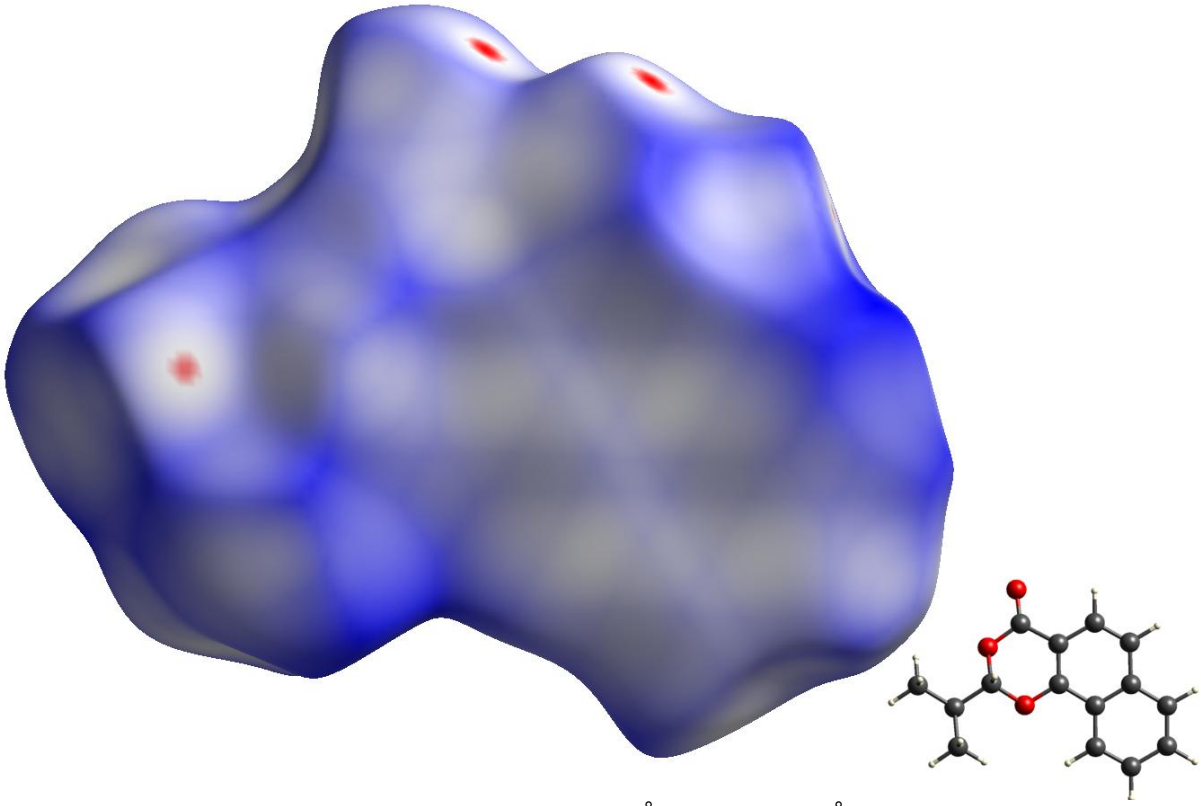
g) **1-CCl_3**, colour code: -0.20Å (red) to 1.22Å (blue)



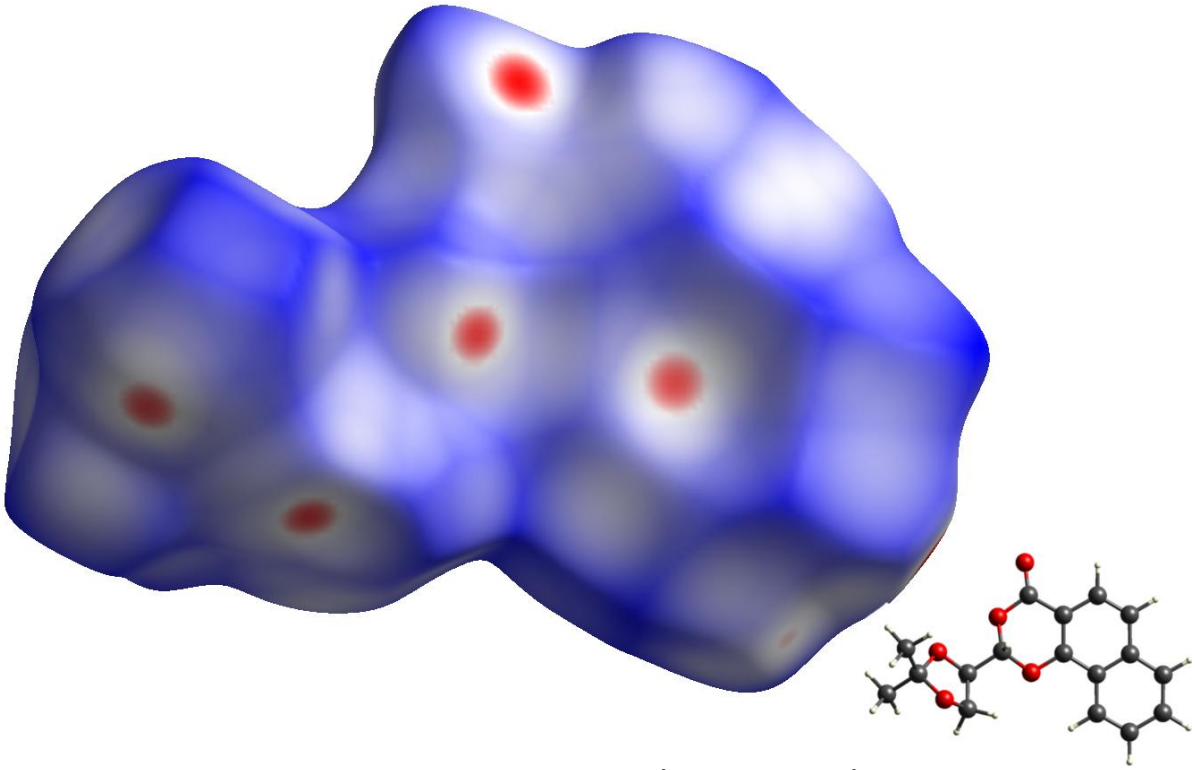
h) **2-Et**, colour code: -0.11Å (red) to 1.09Å (blue)



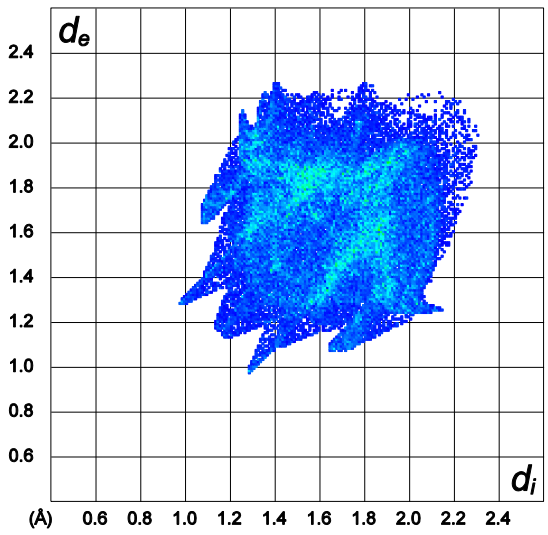
i) **2-nBu**, colour code: -0.22Å (red) to 1.44Å (blue). The Hirshfeld surface of the second molecule of the asymmetric unit is similar and therefore not shown.



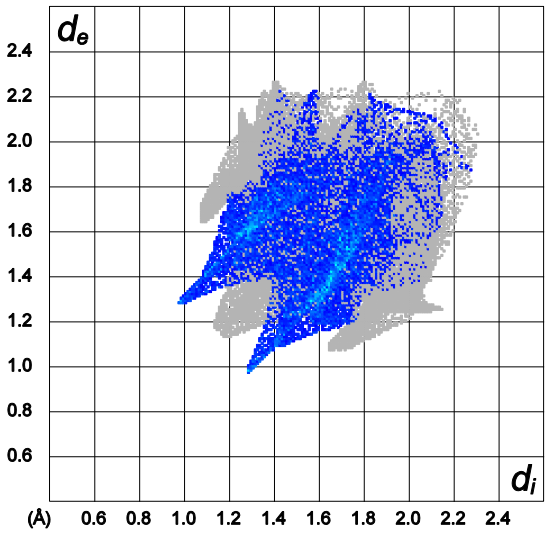
j) **2-iPr**, colour code: -0.06Å (red) to 1.30Å (blue)



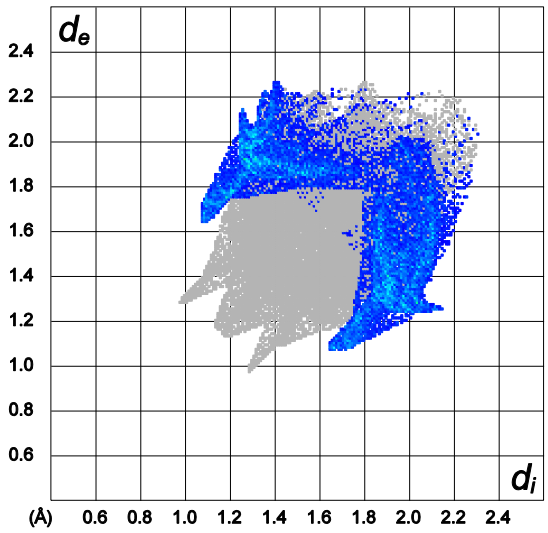
k) **2-diox**, colour code: -0.20Å (red) to 1.34Å (blue)



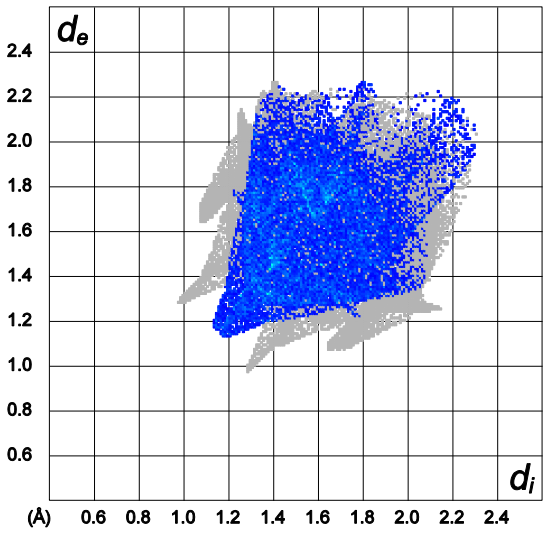
a) all contacts accounted for



b) reduced to contributions of the contact type O...H (24% of all contacts)



c) reduced to contributions of the contact type C...H (29% of all contacts)



d) reduced to contributions of the contact type H...H (36% of all contacts)

Fig. S4 Hirshfeld fingerprint plots of compound **1-H** (*cf.* Fig. 3 in the main article)