ELECTRONIC SUPPLEMENTARY INFORMATION

for the paper entitled

Protection from Neurodegeneration in the 6-Hydroxydopamine (6-OHDA) Model of Parkinson's with Novel 1-Hydroxypyridin-2-one Metal Chelators

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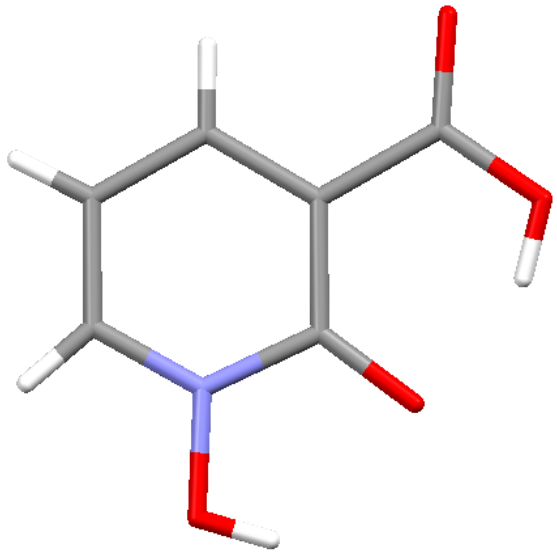

Figure 1. Mercury plot of acid **9**. CCDC 983801 contains the supplementary crystallographic data for this structure. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44)1223-336-033; or deposit@ccdc.cam.ac.uk.

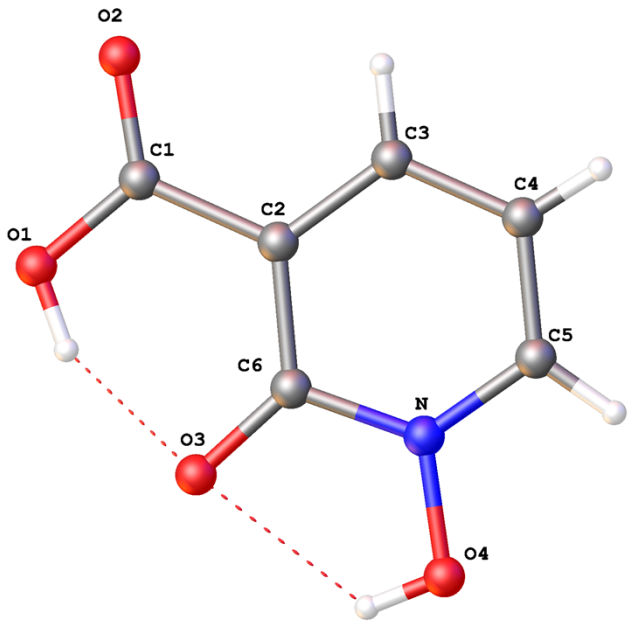

Figure 2. Olex 2 representation of acid **9**. Hydrogen bonds are shown by dotted lines. CCDC 983801 contains the supplementary crystallographic data for this structure. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44)1223-336-033; or deposit@ccdc.cam.ac.uk.

Table 1. Crystal data and structure refinement for acid **9**.

Chemical formula (moiety)	$C_6H_5NO_4$	
Chemical formula (total)	$C_6H_5NO_4$	
Formula weight	155.11	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	orthorhombic, $Pca2_1$	
Unit cell parameters	a = 15.1813(16) Å	α = 90°
	b = 3.8432(5) Å	β = 90°
	c = 10.5335(14) Å	γ = 90°
Cell volume	614.57(13) $Å^3$	
Z	4	
Calculated density	1.676 g/cm^3	
Absorption coefficient μ	0.144 mm^{-1}	
F(000)	320	
Crystal colour and size	colourless, 0.34 × 0.04 × 0.04 mm^3	
Reflections for cell refinement	1593 (θ range 3.3 to 28.6°)	
Data collection method	Xcalibur, Atlas, Gemini ultra	
	thick-slice ω scans	
θ range for data collection	3.3 to 28.6°	
Index ranges	h –18 to 19, k –5 to 4, l –14 to 12	
Completeness to θ = 25.0°	99.8 %	
Reflections collected	3871	
Independent reflections	1255 (R_{int} = 0.0364)	

Reflections with $F^2>2\sigma$	1194
Absorption correction	semi-empirical from equivalents
Min. and max. transmission	0.9526 and 0.9943
Structure solution	direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting parameters a, b	0.0707, 0.0988
Data / restraints / parameters	1255 / 1 / 121
Final R indices [$F^2>2\sigma$]	R1 = 0.0392, wR2 = 0.1036
R indices (all data)	R1 = 0.0416, wR2 = 0.1067
Goodness-of-fit on F^2	1.052
Absolute structure parameter	2.1(13)
Extinction coefficient	0.006(4)
Largest and mean shift/su	0.000 and 0.000
Largest diff. peak and hole	0.25 and –0.23 e $Å^{-3}$

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for ndt4. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	0.12404(9)	0.3127(4)	0.38014(15)	0.0259(4)
O(2)	0.14148(10)	0.6051(5)	0.55736(17)	0.0317(4)
O(3)	0.25619(9)	0.0243(4)	0.27351(13)	0.0230(4)
O(4)	0.42567(10)	–0.0830(4)	0.26178(17)	0.0290(4)
N	0.39057(11)	0.1050(4)	0.36073(17)	0.0199(4)
C(1)	0.17364(13)	0.4337(6)	0.4733(2)	0.0205(5)
C(2)	0.26934(13)	0.3524(5)	0.4662(2)	0.0180(4)
C(3)	0.32612(13)	0.4741(6)	0.5582(2)	0.0200(4)
C(4)	0.41616(13)	0.4040(6)	0.5504(2)	0.0222(5)
C(5)	0.44693(13)	0.2175(6)	0.4494(2)	0.0219(5)
C(6)	0.30084(13)	0.1545(5)	0.3618(2)	0.0183(4)

Table 3. Bond lengths [Å] and angles [°] for acid **9**.

O(1)–H(1)	0.86(3)	O(1)–C(1)	1.322(3)
O(2)–C(1)	1.207(3)	O(3)–C(6)	1.255(3)
O(4)–H(4)	0.82(4)	O(4)–N	1.376(2)
N–C(5)	1.338(3)	N–C(6)	1.375(3)
C(1)–C(2)	1.488(3)	C(2)–C(3)	1.379(3)
C(2)–C(6)	1.420(3)	C(3)–H(3)	0.91(3)
C(3)–C(4)	1.396(3)	C(4)–H(4A)	0.90(3)
C(4)–C(5)	1.365(3)	C(5)–H(5)	0.92(3)

H(1)–O(1)–C(1)	110(2)	H(4)–O(4)–N	104(2)
O(4)–N–C(5)	116.79(16)	O(4)–N–C(6)	117.55(17)
C(5)–N–C(6)	125.64(17)	O(1)–C(1)–O(2)	120.42(18)
O(1)–C(1)–C(2)	116.43(18)	O(2)–C(1)–C(2)	123.14(19)
C(1)–C(2)–C(3)	120.25(19)	C(1)–C(2)–C(6)	118.71(17)
C(3)–C(2)–C(6)	121.03(17)	C(2)–C(3)–H(3)	119.8(17)
C(2)–C(3)–C(4)	120.4(2)	H(3)–C(3)–C(4)	119.9(17)
C(3)–C(4)–H(4A)	124.0(16)	C(3)–C(4)–C(5)	118.84(19)
H(4A)–C(4)–C(5)	117.1(16)	N–C(5)–C(4)	119.64(18)
N–C(5)–H(5)	110.3(17)	C(4)–C(5)–H(5)	130.0(17)
O(3)–C(6)–N	118.26(19)	O(3)–C(6)–C(2)	127.27(17)
N–C(6)–C(2)	114.47(16)		

Table 4. Anisotropic displacement parameters ($Å^2$) for acid **9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	0.0146(7)	0.0382(9)	0.0249(8)	–0.0068(8)	–0.0019(7)	0.0016(6)
O(2)	0.0165(6)	0.0470(11)	0.0315(9)	–0.0122(8)	–0.0017(7)	0.0074(7)
O(3)	0.0187(6)	0.0303(8)	0.0201(8)	–0.0035(7)	–0.0036(6)	0.0015(5)
O(4)	0.0173(7)	0.0432(10)	0.0264(8)	–0.0115(9)	0.0001(7)	0.0052(6)
N	0.0155(7)	0.0241(9)	0.0200(8)	–0.0004(8)	0.0016(7)	0.0025(6)
C(1)	0.0146(8)	0.0263(10)	0.0206(10)	0.0010(9)	–0.0012(8)	–0.0001(8)
C(2)	0.0141(8)	0.0196(9)	0.0205(10)	0.0027(9)	–0.0002(8)	0.0002(7)
C(3)	0.0186(9)	0.0211(10)	0.0202(10)	0.0000(9)	0.0000(8)	0.0000(8)
C(4)	0.0160(9)	0.0259(11)	0.0247(10)	0.0015(9)	–0.0044(9)	–0.0025(8)
C(5)	0.0134(9)	0.0254(11)	0.0269(10)	0.0025(10)	–0.0015(8)	–0.0013(8)
C(6)	0.0140(8)	0.0199(9)	0.0210(10)	0.0037(9)	–0.0014(8)	–0.0006(7)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for acid **9**.

	x	y	z	U
H(1)	0.156(2)	0.188(8)	0.330(3)	0.041(9)
H(4)	0.383(2)	–0.130(8)	0.218(3)	0.042(9)
H(3)	0.3048(17)	0.605(6)	0.624(3)	0.024(6)
H(4A)	0.4560(18)	0.481(7)	0.606(2)	0.025(6)
H(5)	0.5040(19)	0.160(6)	0.427(3)	0.026(7)

Table 6. Torsion angles [°] for acid **9**.

O(1)–C(1)–C(2)–C(3)	178.8(2)	O(1)–C(1)–C(2)–C(6)	0.1(3)
O(2)–C(1)–C(2)–C(3)	–0.1(3)	O(2)–C(1)–C(2)–C(6)	–178.7(2)
C(1)–C(2)–C(3)–C(4)	–178.7(2)	C(6)–C(2)–C(3)–C(4)	–0.1(3)
C(2)–C(3)–C(4)–C(5)	0.9(3)	O(4)–N–C(5)–C(4)	–179.67(19)
C(6)–N–C(5)–C(4)	–1.3(3)	C(3)–C(4)–C(5)–N	–0.3(3)
O(4)–N–C(6)–O(3)	0.5(3)	O(4)–N–C(6)–C(2)	–179.65(17)
C(5)–N–C(6)–O(3)	–177.9(2)	C(5)–N–C(6)–C(2)	2.0(3)
C(1)–C(2)–C(6)–O(3)	–2.7(3)	C(1)–C(2)–C(6)–N	177.41(18)
C(3)–C(2)–C(6)–O(3)	178.7(2)	C(3)–C(2)–C(6)–N	–1.2(3)

Table 7. Hydrogen bonds for acid **9** [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O(1)–H(1)...O(3)	0.86(3)	1.75(3)	2.552(2)	153(3)
O(4)–H(4)...O(2A)	0.82(4)	2.01(3)	2.667(2)	137(3)
O(4)–H(4)...O(3)	0.82(4)	2.10(4)	2.609(2)	120(3)

Symmetry operations for equivalent atoms

A –x+1/2,y–1,z–1/2