Supplemental Materials for Crystallographic Data

Allantoin from lichen *Umbilicaria esculenta* (Miyoshi) Minks

Appearance: colorless prismatic crystal (in water)
Melting point: 219 °C–220 °C.
Solubility: soluble in DMSO
Molecular weight: 158.13
UV λ_{max} (in MeOH) (nm): 267, 335, 395.
IR ν_{max} (KBr) (cm^{-1}): 3425, 3340, 3125, 3060, 1810, 1740, 1680, 1560.
Positive FAB-MS: *m/z* 180.9 $[M + Na]^+$ in DMSO with NBR (Na).
^{1}H-NMR (600 MHz, DMSO-d_6) δ: 8.06 (1H, s, N_4-$\underline{H}_4$), 6.90 (1H, d, N_3-$\underline{H}_3$), 5.79 (2H, s, N1-$\underline{H}$1a, 1b), 5.25 (1H, t, N_2-$\underline{H}_2$), 3.35 (1H, s, C_3-$\underline{H}_3$).
^{13}C-NMR (125 MHz, DMSO-d_6) δ: 173.60 (C-4), 157.35 (C-2), 156.76 (C-1), 62.41 (C-3).
X-ray crystal data was listed in Table S1, S2, S3, S4 as below:
Molecular Formula: $C_4H_6N_4O_3$

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for allantoin from *U. esculenta*.

	x	y	z	U(eq)
O(1)	2350(1)	1073(2)	2462(1)	24(1)
O(2)	690(1)	3218(2)	4211(1)	24(1)
O(3)	6366(1)	2125(2)	4374(1)	28(1)
N(1)	1068(1)	3202(2)	1272(1)	25(1)
N(2)	2117(1)	5446(2)	2525(1)	21(1)
N(3)	4662(1)	4859(2)	3500(1)	25(1)
N(4)	3485(1)	2270(2)	4484(1)	22(1)
C(1)	2162(1)	3532(2)	4072(1)	19(1)
C(2)	4997(1)	3017(2)	4127(1)	21(1)
C(3)	2887(1)	5523(2)	3420(1)	20(1)
C(4)	1849(1)	3132(2)	2094(1)	19(1)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table S2. Anisotropic displacement parameters ($A^2 \times 10^3$) for allantoin from *U. esculenta*.

	U11	U22	U33	U23	U13	U12
O(1)	31(1)	15(1)	25(1)	1(1)	1(1)	3(1)
O(2)	22(1)	25(1)	27(1)	3(1)	4(1)	1(1)
O(3)	22(1)	30(1)	33(1)	6(1)	0(1)	4(1)
N(1)	33(1)	20(1)	22(1)	0(1)	-3(1)	-2(1)
N(2)	29(1)	13(1)	19(1)	2(1)	-2(1)	2(1)
N(3)	20(1)	26(1)	28(1)	8(1)	1(1)	-2(1)
N(4)	22(1)	22(1)	21(1)	5(1)	2(1)	2(1)
C(1)	24(1)	16(1)	18(1)	-1(1)	1(1)	1(1)
C(2)	23(1)	19(1)	21(1)	-1(1)	0(1)	-1(1)
C(3)	23(1)	16(1)	20(1)	0(1)	0(1)	-1(1)
C(4)	19(1)	17(1)	20(1)	0(1)	4(1)	0(1)

The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12]$.

Table S3. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for allantoin from *U. esculenta*.

	x	y	z	U (eq)
H(1A)	890	1787	973	30
H(1B)	742	4663	1043	30
H(2)	1820	6868	2257	25
H(3)	5409	5569	3182	30
H(4)	3402	1149	4911	26
H(5)	2740	7267	3669	23

Table S4. Torsion angles [°] for allantoin from *U. esculenta*.

C(2)-N(4)-C(1)-O(2)	176.91(11)	C(2)-N(3)-C(3)-N(2)	-127.97(10)
C(2)-N(4)-C(1)-C(3)	-5.23(12)	C(2)-N(3)-C(3)-C(1)	-4.66(12)
C(3)-N(3)-C(2)-O(3)	-177.01(11)	O(2)-C(1)-C(3)-N(2)	-51.28(14)
C(3)-N(3)-C(2)-N(4)	1.86(13)	N(4)-C(1)-C(3)-N(2)	130.83(9)
C(1)-N(4)-C(2)-O(3)	-178.74(11)	O(2)-C(1)-C(3)-N(3)	-176.34(11)
C(1)-N(4)-C(2)-N(3)	2.33(13)	N(4)-C(1)-C(3)-N(3)	5.78(11)
C(4)-N(2)-C(3)-N(3)	70.30(13)	C(3)-N(2)-C(4)-O(1)	-3.44(15)
C(4)-N(2)-C(3)-C(1)	-46.09(13)	C(3)-N(2)-C(4)-N(1)	177.58(10)

Symmetry transformations used to generate equivalent atoms.

Figure S1. [1]H-NMR spectrum of allantoin from *U. esculenta* (600 MHz, DMSO-d_6).

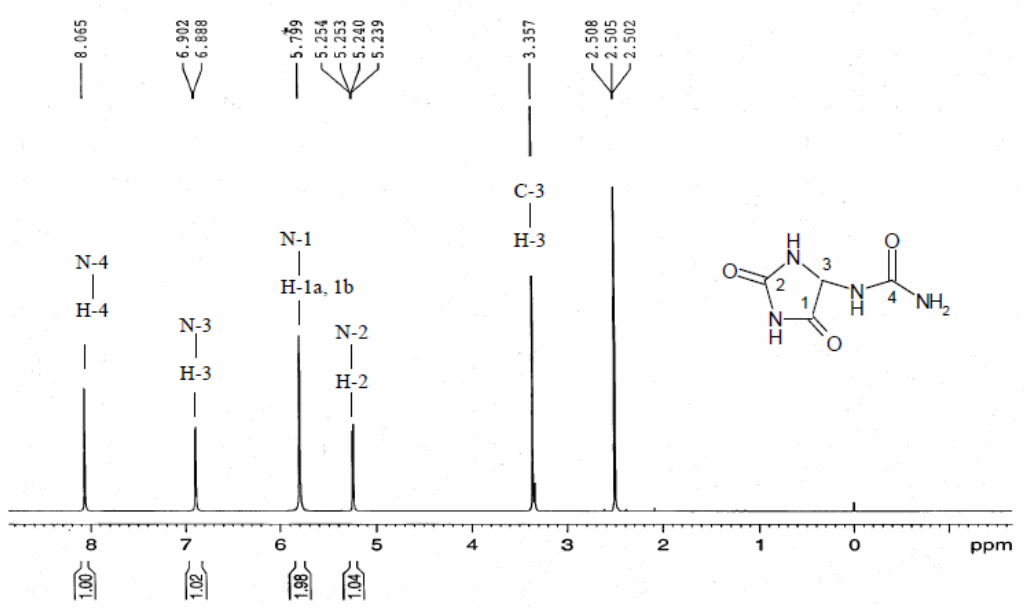

Figure S2. [13]C-NMR spectrum of allantoin from *U. esculenta* (125 MHz, DMSO-d_6).

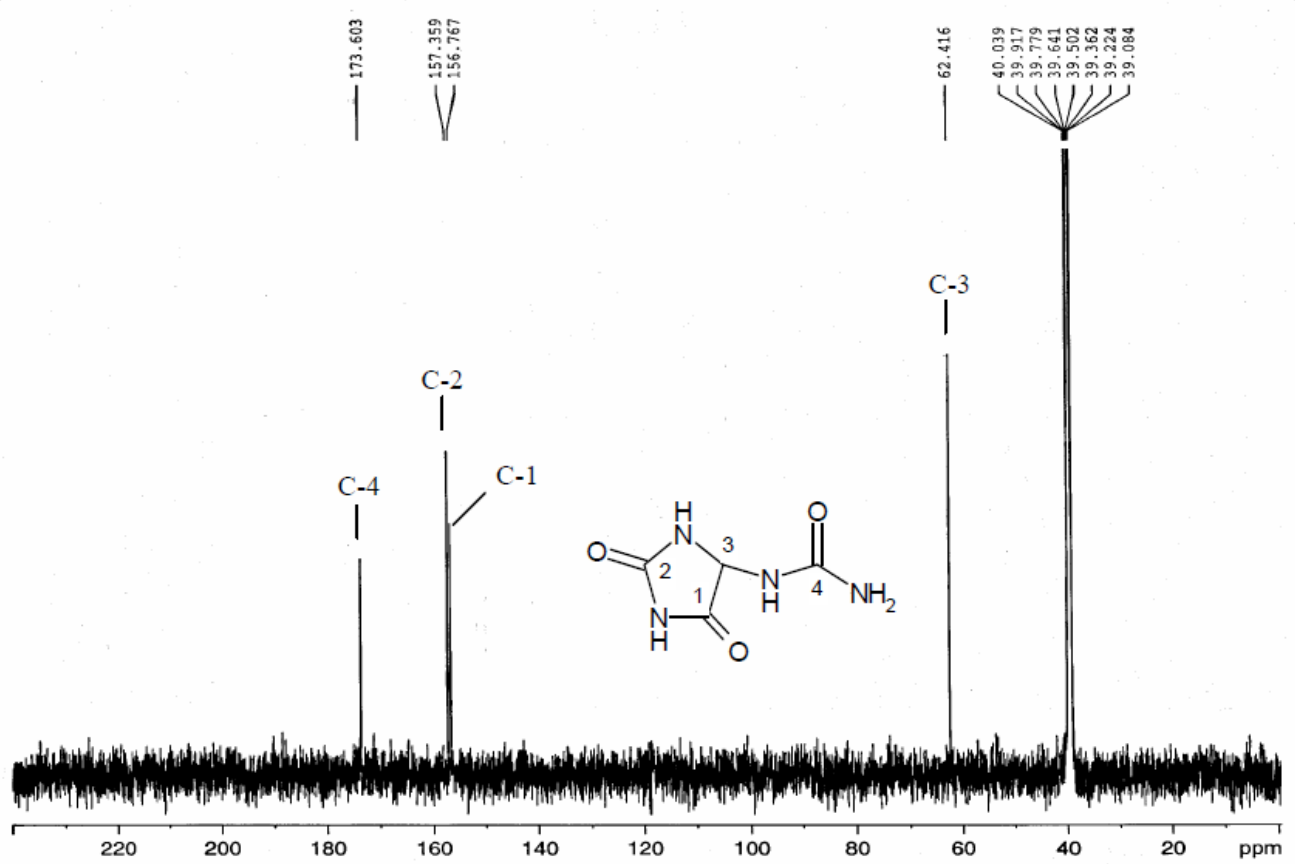

Figure S3. DEPT-spectrum of allantoin from *U. esculenta* (125 MHz, DMSO-d_6).

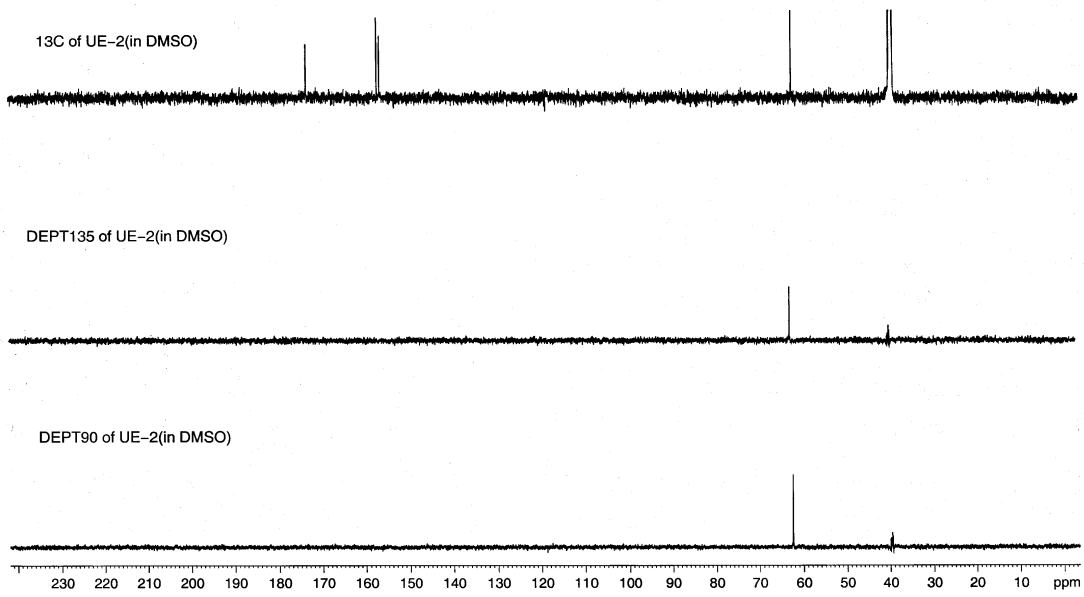

Figure S4. FAB-MS spectrum of allantoin in DMSO with NBA (Na).