



SUPPLEMENTARY MATERIAL TO
**Importance of *N*-terminal proline for the promiscuous activity of
4-oxalocrotonate tautomerase (4-OT)**

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¹H-NMR DATA FOR COMPOUNDS 4–6

2,2-Dimethyl-4-nitro-3-phenylbutanal (4).¹ ¹H-NMR (200 MHz, CDCl₃,
 δ / ppm) 9.53 (1H, s), 7.40–7.13 (5H, m), 4.92–4.64 (2H, m), 3.78 (1H, dd, J_1 =
= 11.0 Hz & J_2 = 4.4 Hz), 1.14 (3H, s), 1.01 (3H, s).

2,2-Dimethyl-4-nitro-3-(2-thienyl)butanal (5).¹ ¹H-NMR (200 MHz, CDCl₃,
 δ / ppm) 9.54 (1H, s), 7.27–7.22 (1H, m), 7.00–6.91 (2H, m), 4.75–4.59 (2H, m),
4.14 (1H, dd, J_1 = 4.9 Hz & J_2 = 10.0 Hz), 1.21 (3H, s), 1.09 (3H, s).

3-(4-Chlorophenyl)-2,2-dimethyl-4-nitrobutanal (6).² ¹H-NMR (200 MHz,
CDCl₃, δ / ppm) 9.51 (1H, s), 7.32 (2H, d, J = 8.6 Hz), 7.15 (2H, d, J = 8.5 Hz),
4.83 (1H, dd, J_1 = 13.1 & J_2 = 11.2 Hz), 4.69 (1H, dd, J_1 = 13.1 & J_2 = 4.4 Hz),
3.77 (1H, dd, J_1 = 11.2 & J_2 = 4.4 Hz), 1.13 (3H, s), 1.02 (3H, s).

REFERENCES

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