

Table S1. Crystal data and structure refinement for CN-debranone stereoisomers.

Feature	R-CN-debranone	S-CN-debranone
Empirical formula	C ₁₂ H ₉ NO ₃	C ₁₂ H ₉ NO ₃
Formula weight	215.20	215.20
Temperature	100(2) K	100(2) K
Wavelength	1.54178 Å	1.54178 Å
Crystal system	Orthorhombic	Orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
Unit cell dimensions	<i>a</i> = 3.87580(10) Å <i>b</i> = 11.1080(3) Å <i>c</i> = 23.4431(7) Å	<i>a</i> = 3.87530(10) Å <i>b</i> = 11.1070(2) Å <i>c</i> = 23.4321(3) Å
Volume	1009.28(5) Å ³	1008.59(3) Å ³
<i>Z</i>	4	4
Density (calculated)	1.416 Mg/m ³	1.417 Mg/m ³
μ	0.860 mm ⁻¹	0.860 mm ⁻¹
Crystal size	0.55 x 0.22 x 0.15 mm ³	0.38 x 0.05 x 0.05 mm ³
θ range for data collection	3.77 to 67.19°	3.77 to 67.22°
Index ranges	-4 ≤ <i>h</i> ≤ 4, -13 ≤ <i>k</i> ≤ 13, -28 ≤ <i>l</i> ≤ 27	-4 ≤ <i>h</i> ≤ 4, -12 ≤ <i>k</i> ≤ 13, -27 ≤ <i>l</i> ≤ 28
Reflections collected	19709	7582
Independent reflections	1808 [<i>R</i> (int) = 0.0385]	1804 [<i>R</i> (int) = 0.0200]
Completeness to θ = 67.19°	99.9 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max./min. transmission	1.00/0.93	1.00/0.79
Refinement method	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	1808 / 0 / 146	1804 / 0 / 147
Goodness-of-fit on <i>F</i> ²	1.113	1.077
Final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> 1 = 0.0375, <i>wR</i> 2 = 0.1027	<i>R</i> 1 = 0.0271, <i>wR</i> 2 = 0.0713
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0378, <i>wR</i> 2 = 0.1030	<i>R</i> 1 = 0.0274, <i>wR</i> 2 = 0.0718
Absolute structure parameter	-0.1(3)	0.04(17)
Largest diff. peak and hole	0.258 and -0.236 e.Å ⁻³	0.151 and -0.178 e.Å ⁻³