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Supporting information for article:

Single-crystal-to-single-crystal phase transition of 18β-glycyrrhetinic acid isopropyl ester

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Table S1 Unit cell parameters a, b, c [Å] and V [Å^3] during heating–cooling-heating cycles.

T[K]	a [Å]	b [Å]	c [Å]	V [Å^3]
300	11,8873	13,1470	18,8810	2950,8
310	11,9014	13,1577	18,8938	2958,7
315	11,9038	13,1561	18,8925	2958,7
320	11,9083	13,1591	18,8968	2961,2
325	11,9098	13,1577	18,8964	2961,2
330	13,1926	13,2794	17,1966	3012,7
340	13,1998	13,2812	17,2035	3015,9
330	13,1944	13,2813	17,1875	3011,9
320	13,1912	13,2780	17,1741	3008,1
310	13,1864	13,2739	17,1581	3003,3
300*	**13,1735**	**13,2527**	**17,1463**	**2993,5**
300*	**11,8943**	**13,1511**	**18,8868**	**2954,3**
290	11,8777	13,1434	18,8758	2946,8
285	11,8738	13,1419	18,8750	2945,3
280	11,8708	13,1406	18,8718	2943,8
290	11,8790	13,4232	18,8769	2947,2
300	11,8864	13,1471	18,8829	2950,9
310	11,8940	13,1485	18,8866	2953,7
325	11,9109	13,1578	18,8976	2961,7
330	13,1911	13,2719	17,1934	3010,1
335	13,1924	13,2734	17,2028	3012,3
340	13,1943	13,2740	17,2740	3014,4

* During the cooling cycle at 300 K, the phase transition occurred, and there is possible to assign two different unit cell parameters.

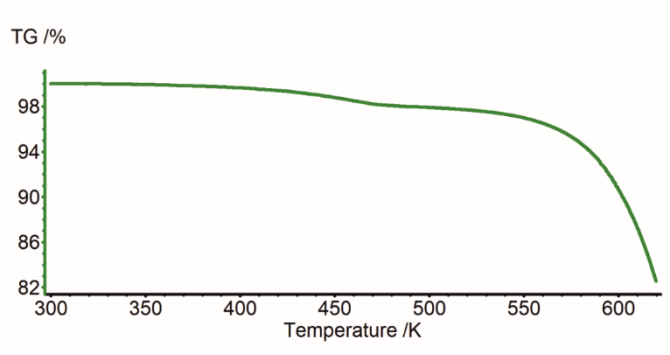

Figure S1 TGA thermogram of isopropyl-GE ester.

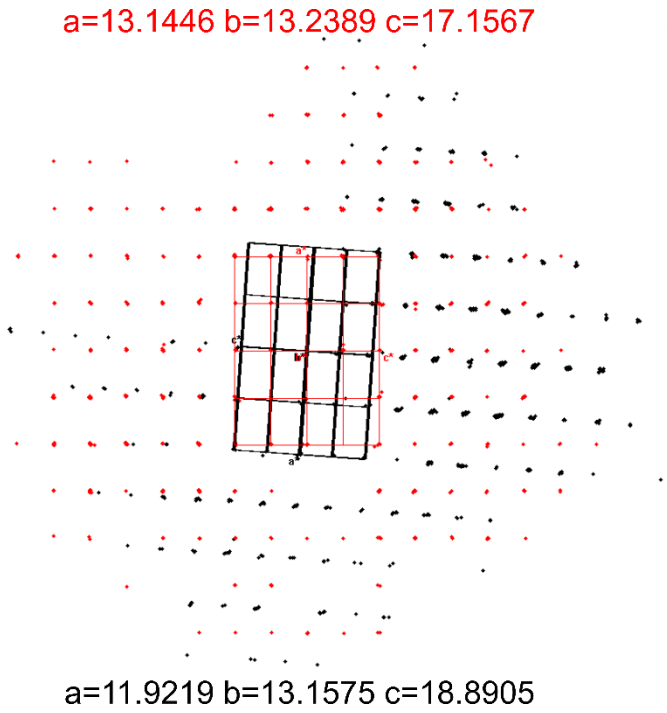

Figure S2 Ewald sphere at 300 K shown along b* during the cooling cycle. Two different unit cells are assigned. Starting phase, in red, is P-13-17, and the post-transition P-11-18 phase, in black.

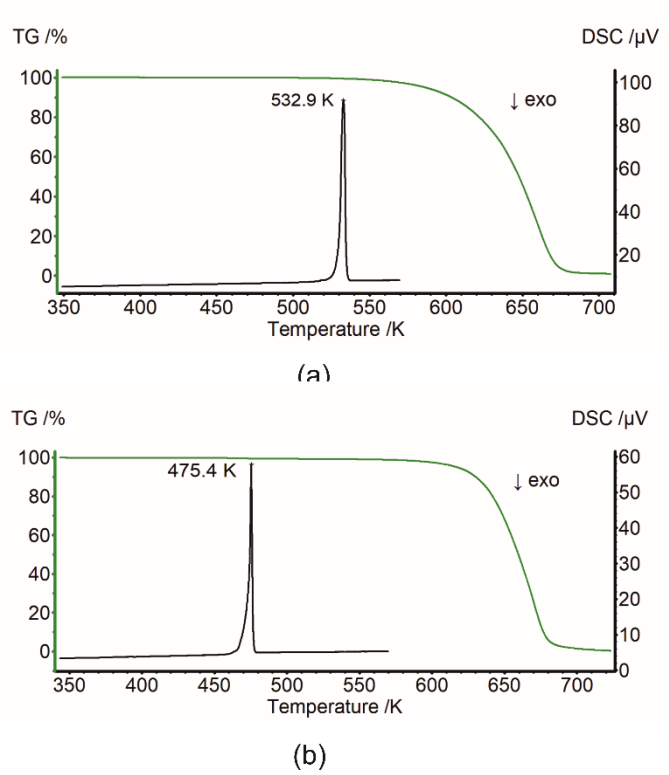

Figure S3 TGA (green) and DSC (black) thermograms of a) ethyl-GE and b) 2-morpholinoethyl-GE esters.

Table S2 Experimental details

For all structures: orthorhombic, $P2_12_12_1$, Z = 4. Experiments were carried out at 298 K with Cu Kα radiation using a SuperNova, Dual, Cu at home/near, Atlas. Absorption was corrected by multi-scan methods, CrysAlis PRO 1.171.41.93a (Rigaku Oxford Diffraction, 2020) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. H-atom parameters were constrained.

	(ethyl-GE)	(2-morpholinoethyl-GE)
Crystal data		
Chemical formula	$C_{32}H_{50}O_4$	$C_{36}H_{57}NO_5$
M_r	498.72	583.82
a, *b*, *c* (Å)	13.0243 (1), 12.9924 (1), 16.6941 (2)	12.9136 (2), 13.7752 (3), 18.7441 (4)
V (Å^3)	2824.92 (5)	3334.32 (10)
µ (mm^{-1})	0.58	0.60
Crystal size (mm)	0.60 × 0.20 × 0.15	0.40 × 0.15 × 0.05
Data collection		

T_{min}, T_{max}	0.880, 1.000	0.78, 1.00
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27501, 5167, 4966	64824, 6099, 5635
R_{int}	0.033	0.045
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.602	0.602
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$	0.039, 0.106	0.037, 0.100
S	1.04	1.04
No. of parameters	335	387
No. of restraints	2	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, -0.26	0.10, -0.16
Absolute structure	Flack x determined using 2119 quotients [(I+)-(I-)]/[(I+)+(I-)]	Flack x determined using 2381 quotients [(I+)-(I-)]/[(I+)+(I-)]
Absolute structure parameter	-0.05 (7)	-0.15 (7)

Computer programs: CrysAlis PRO 1.171.41.93a (Rigaku OD, 2020), SHELXT (Sheldrick, 2015), SHELXL 2018/3 (Sheldrick, 2015), Olex2 1.5 (Dolomanov et al., 2009), Flack (Parsons et al., 2013).