

Supplementary information

Table S1. Crystal data and detail of experimental data collection and refinement for a monohydrated molecular salt of GABA and L-tartaric acid

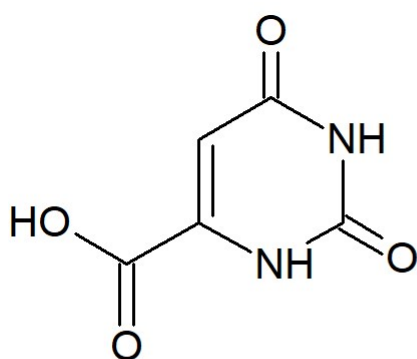
GABA L-tartaric acid monohydrate	
Crystal data	
Chemical formula	C ₄ H ₅ O ₆ ·C ₄ H ₁₀ NO ₂ ·H ₂ O
<i>M_r</i>	271.22
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.1846 (2), 27.8403 (8), 7.4558 (2)
μ (°)	109.007 (3)
<i>V</i> (Å ³)	1213.76 (7)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.14
Crystal size (mm)	0.45 × 0.18 × 0.03
Data collection	
Diffractometer	Xcalibur, Ruby, Gemini ultra
Absorption correction	Multi-scan <i>CrysAlis PRO</i> , Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 <i>CrysAlis171 .NET</i>) (compiled Aug 13 2014,18:06:01) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
<i>T_{min}</i> , <i>T_{max}</i>	0.919, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	15413, 4952, 4034
<i>R_{int}</i>	0.043
(sin Θ/λ) _{max} (Å ⁻¹)	0.625
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.048, 0.100, 1.02
No. of reflections	4952
No. of parameters	341
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.48, -0.32

Table S2. Selected hydrogen-bond parameters

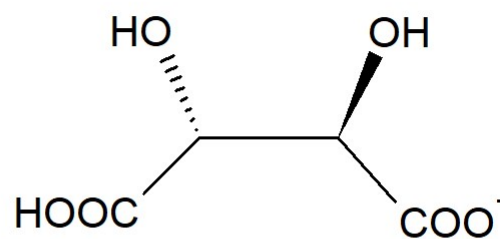
<i>D</i> —H··· <i>A</i>	<i>D</i> —H (Å)	H··· <i>A</i> (Å)	<i>D</i> ··· <i>A</i> (Å)	<i>D</i> —H··· <i>A</i> (°)
O12—H12···O16 ⁱ	0.82	1.69	2.509 (4)	177.0
O13—H13···O26	0.82	2.06	2.768 (4)	144.6
O14—H14···O11 ⁱⁱ	0.82	2.19	2.819 (4)	133.7
O21—H21···O26 ⁱ	0.82	1.82	2.633 (4)	169.4
N11—H11A···O15	0.89	1.88	2.749 (4)	165.5
N11—H11B···O16 ⁱⁱ	0.89	1.89	2.779 (4)	177.5
N11—H11C···O14 ⁱⁱⁱ	0.89	1.95	2.827 (4)	166.2
N12—H12A···O25	0.89	1.92	2.789 (4)	163.8

N12—H12B···O24 ⁱⁱⁱ	0.89	1.97	2.856 (4)	170.8
O27—H27···O1 ^{iv}	0.82	1.85	2.667 (5)	173.2
O17—H17···O2 ^v	0.82	1.79	2.601 (6)	171.7
O1—H1A···O18 ^{vi}	0.85	1.98	2.824 (6)	170.1
O1—H1B···O11 ⁱⁱ	0.85	2.01	2.833 (4)	162.5
O2—H2A···O28	0.85	2.01	2.824 (6)	161.0
O2—H2B···O22 ⁱⁱⁱ	0.85	2.35	3.002 (5)	134.3
O2—H2B···O23 ⁱⁱⁱ	0.85	2.09	2.864 (5)	150.9
O23—H23A···N12 ^{vii}	0.82	2.52	3.014 (5)	120.2

Symmetry code(s): (i) $x, y, z-1$; (ii) $x-1, y, z$; (iii) $x, y, z+1$; (iv) $-x+1, y-1/2, -z+1$; (v) $-x+2, y+1/2, -z+2$; (vi) $x-1, y, z-1$; (vii) $x+1, y, z$.



a



b

Scheme S1. Orotic and L-tartaric acids

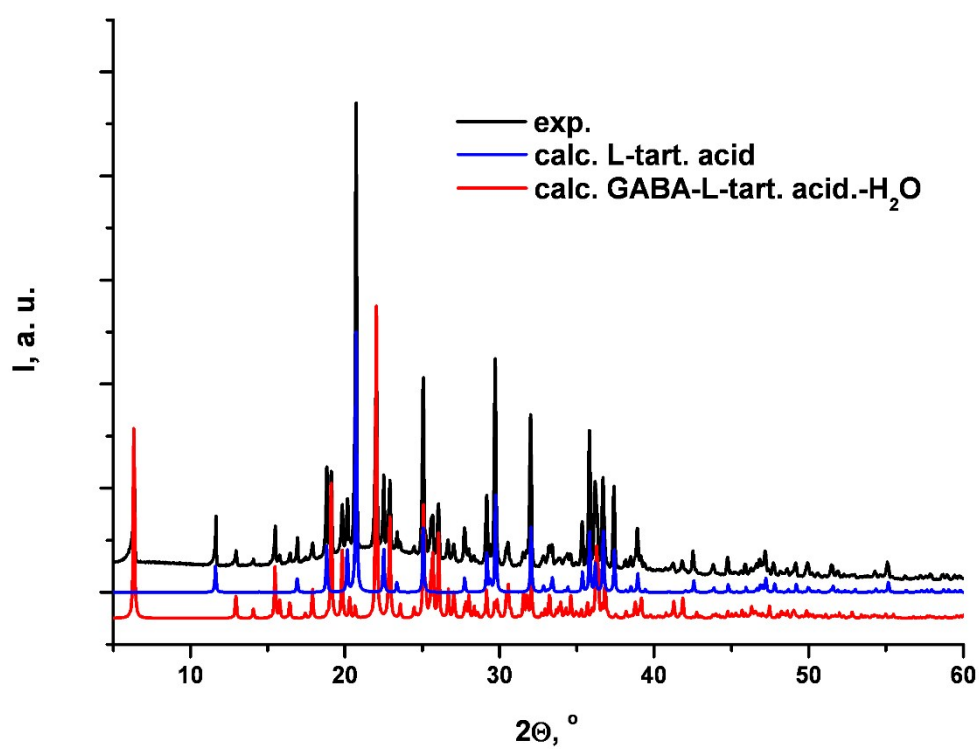


Fig. S1. Manual liquid-assisted grinding of equimolar amounts of GABA, L-tartaric acid and water by mortar and pestle. Experimental XRPD pattern shown black; theoretically calculated XRPD patterns for L-tartaric acid and hydrated salt of GABA with L-tartaric acid are put in blue and red, respectively.

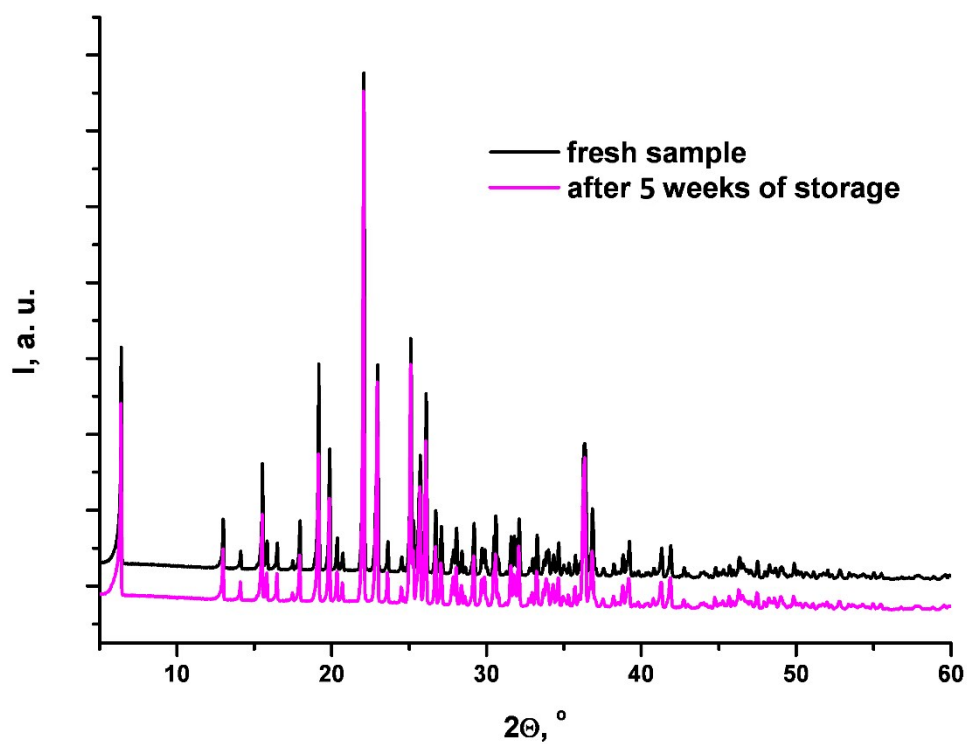


Fig. S2. Results of storage experiments of the hydrated molecular salt during 2 weeks. XRPD patterns of initial powder and the same sample after 5 weeks of storage in open vial are shown in black and magenta, respectively. There is no evidence of dehydration.

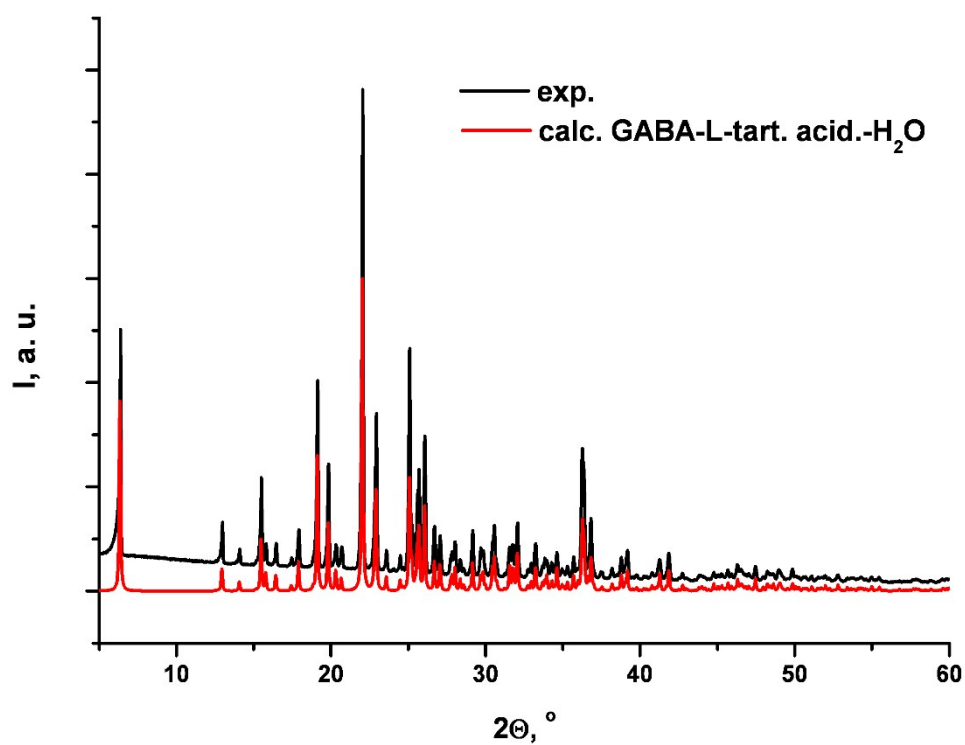


Fig. S3. Intense manual grinding of the hydrated molecular salt of GABA with L-tartaric acid (black). Theoretically calculated XRPD patterns of the hydrated salt shown red. Stability of the compound is demonstrated.

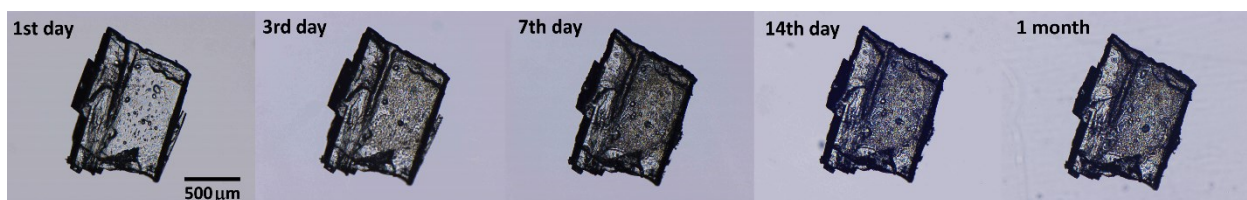


Fig. S4. A single crystal of the hydrated molecular salt of GABA with L-tartaric acid on storage on air during 1 month. No dehydration was observed (see results of phase analysis by XRPD). Some visual turbidity of the crystal after several days of storage is common for any freshly prepared crystal.

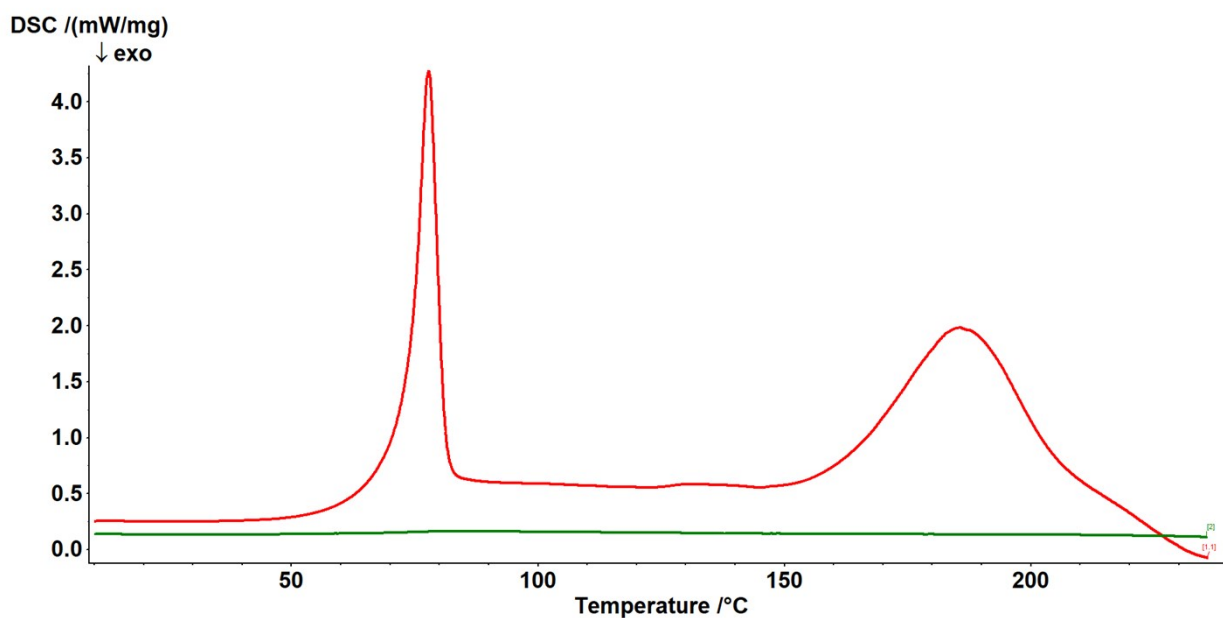


Fig. S5. Results of DSC experiments with hydrated molecular salt of GABA with L-tartaric acid in an open crucible. First heating run: red line. Second heating run: green line.

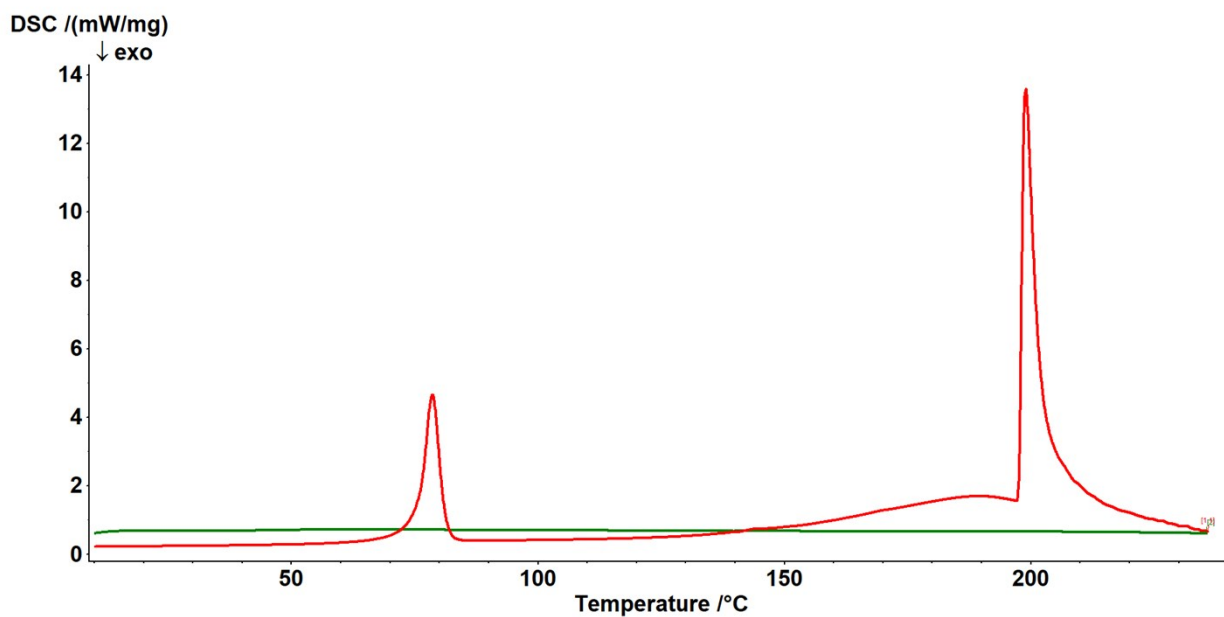


Fig. S6. Results of the DSC experiments with the hydrated molecular salt of GABA with L-tartaric acid in a closed crucible. First heating run: red line. Second heating run: green line.

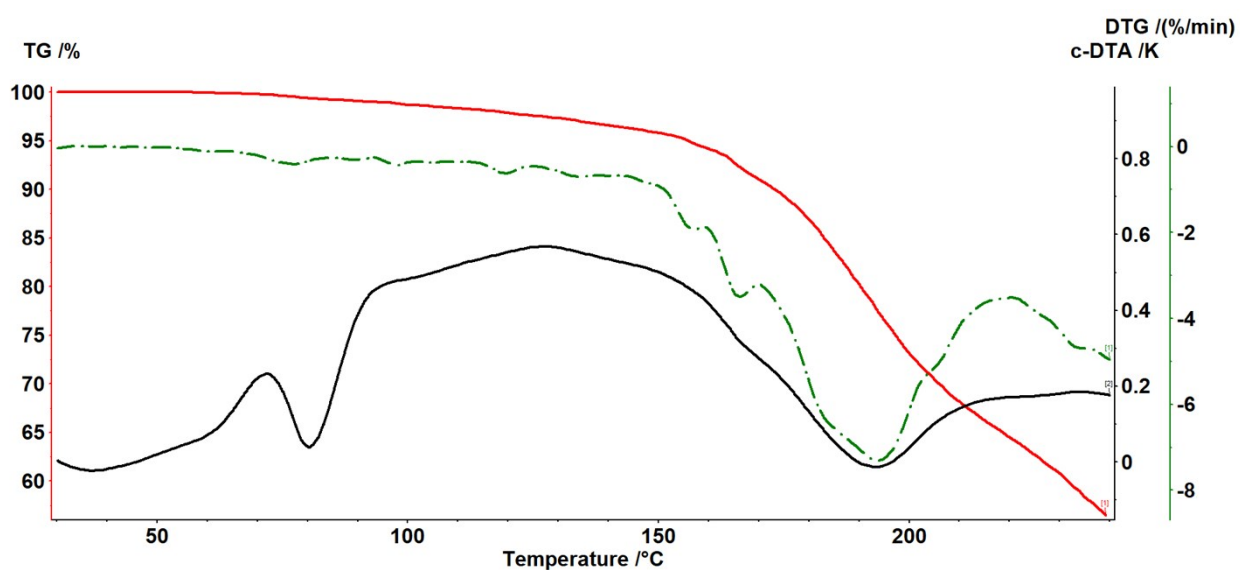


Fig. S7. Results of the TG experiments with the hydrated molecular salt of GABA with L-tartaric acid. Total mass, % : red line. Derivative of mass loss, %/min: green dashed line. C-DTA, K: black line.