Electronic Supplementary Information

Non-zeolitic properties of the dipeptide $_L$-leucyl-$_L$-leucine as a result of the specific nanostructures formation

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- Experimental and calculated powder diffractograms;
- TG/DSC/MS data for the products of $_L$-leucyl-$_L$-leucine saturation with guest vapors;
- AFM images of the crystals obtained from a pyridine solution on the HOPG surface;
- SEM images of the initial film after saturation with vapor of dichloromethane and film obtained from a dichloromethane solution on the HOPG surface;
- Powder diffraction data.

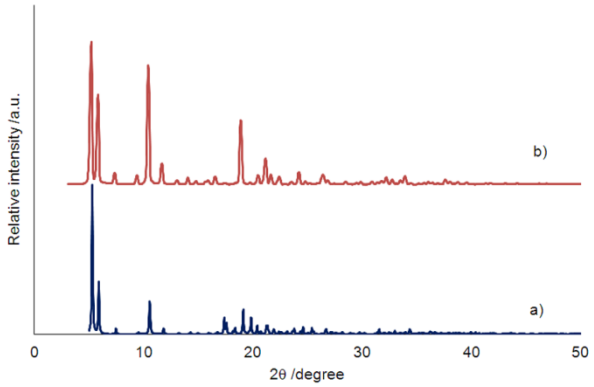

Figure. **S1**. X-ray powder diffractograms for: (a) Leu-Leu•0.87H_2O clathrate calculated from single crystal X-ray data [Chem. Eur. J. 2001, V.7, P.5153], (b) initial powder of Leu-Leu used in present work.

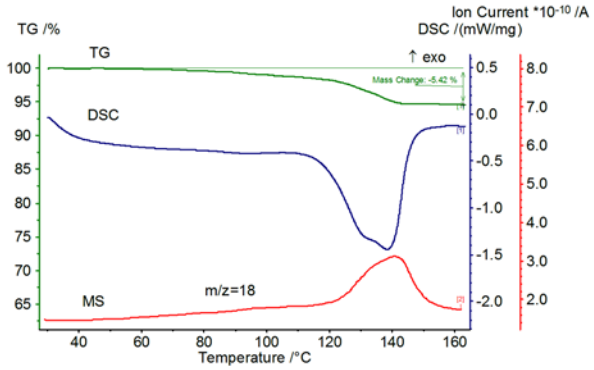

Figure. **S2**.The data of TG/DSC/MS analysis for the sample of Leu-Leu heated up to 130°C and saturated with water vapor for 3 days at 298K. Heating rate is 10 K min^{-1}.

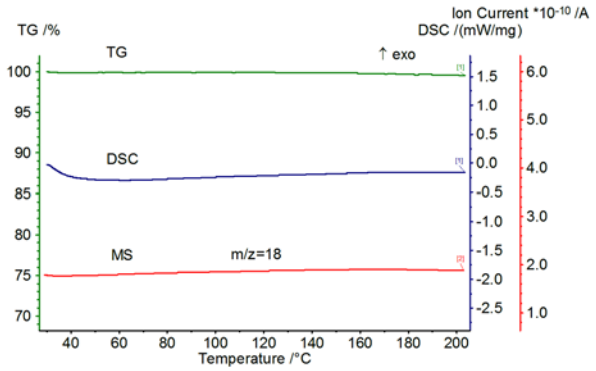

Figure. **S3**. The data of TG/DSC/MS analysis for the sample of Leu-Leu heated up to 180°C and stored at contact with water liquid water for 5 days at 298K. Heating rate is 10 K min^{-1}.

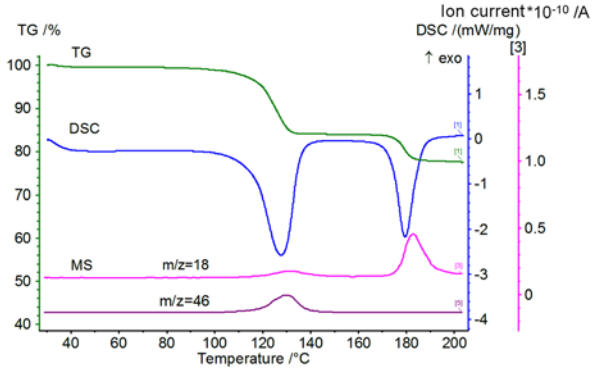

Figure. **S4**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of ethanol. Heating rate is 10 K min^{-1}.

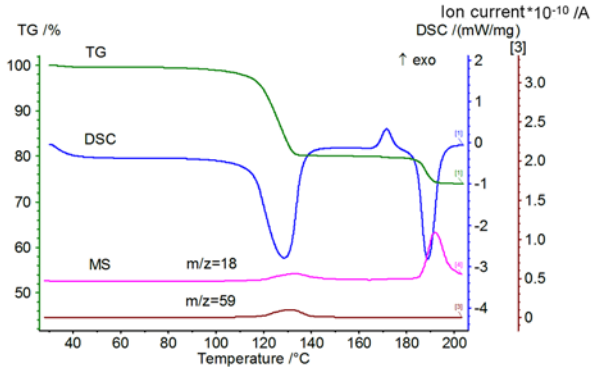

Figure. **S5**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of *n*-propanol. Heating rate is 10 K min^{-1}.

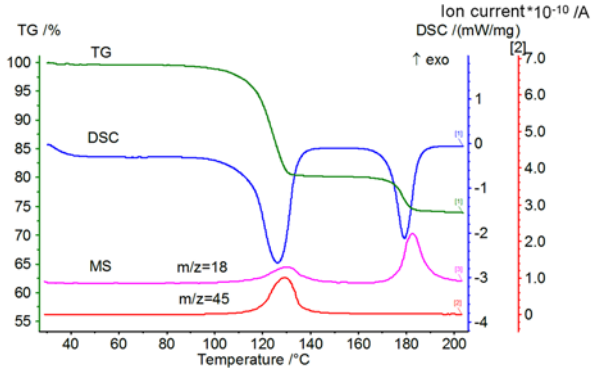

Figure. **S6**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of isopropanol. Heating rate is 10 K min^{-1}.

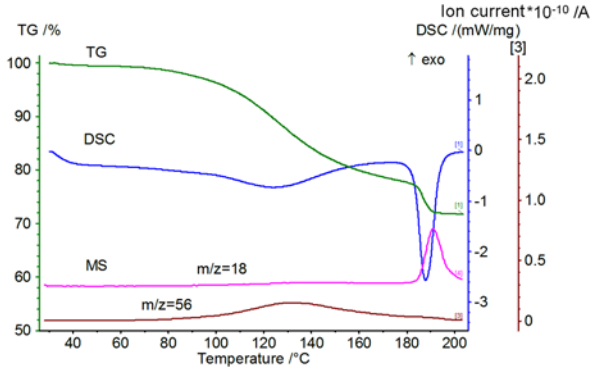

Figure. **S7**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of *n*-buthanol. Heating rate is 10 K min^{-1}.

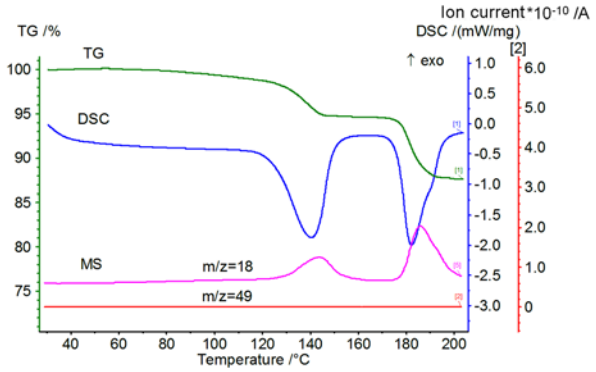

Figure. **S8**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of dichloromethane. Heating rate is 10 K min^{-1}.

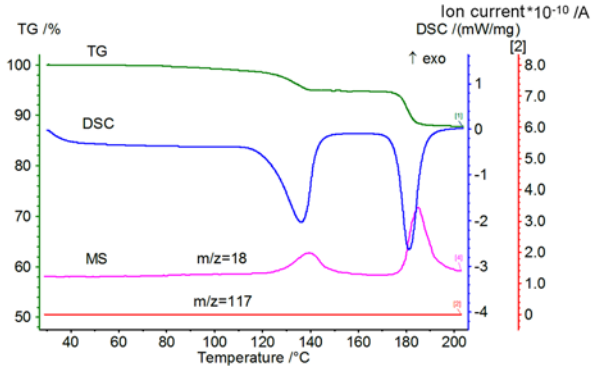

Figure. **S9**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of tetrachloromethane. Heating rate is 10 K min^{-1}.

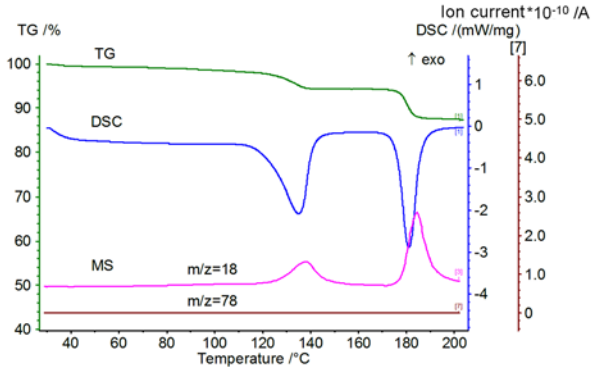

Figure. **S10**.The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of benzene. Heating rate is 10 K min^{-1}.

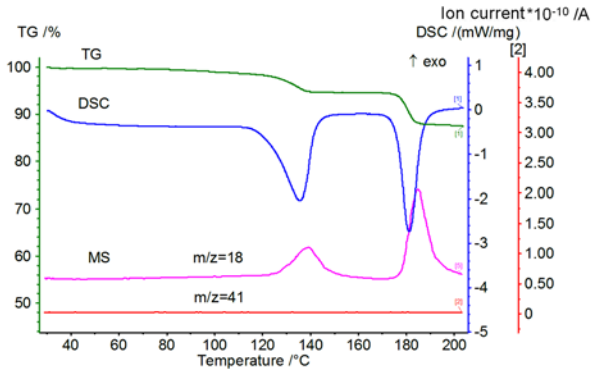

Figure. **S11**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of acetonitrile. Heating rate is 10 K min^{-1}.

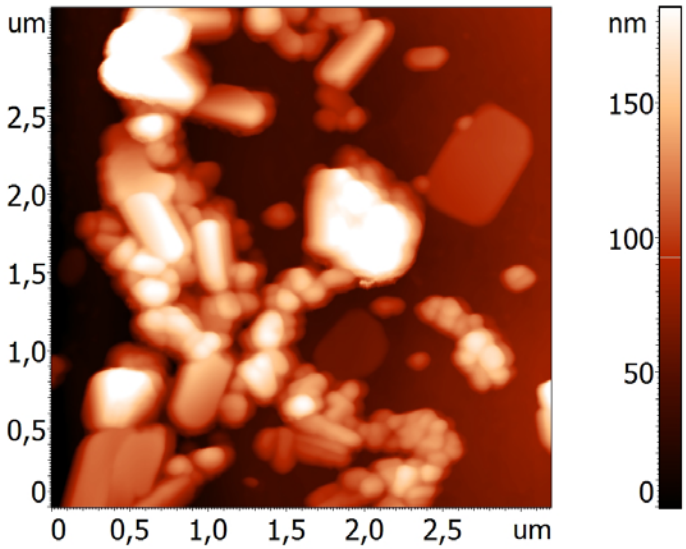

Figure. **S12**. AFM image of the Leu-Leu film deposited on the HOPG from methanol solution after the saturation with ethanol vapors for 2 hour.

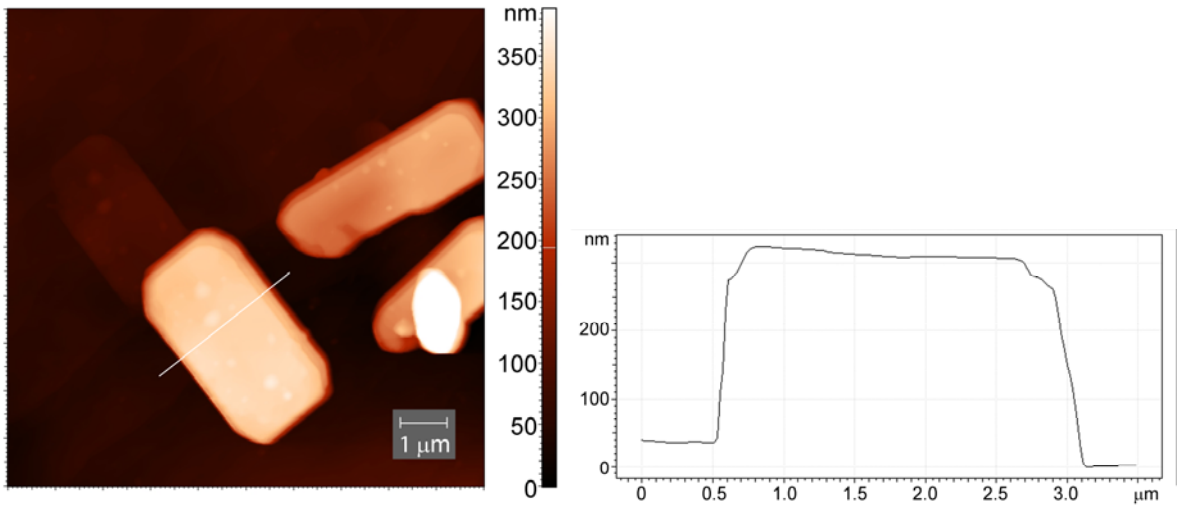

Figure. **S13**. 2D AFM images of the Leu-Leu crystals obtained from a pyridine solution on the HOPG surface, and cross-section by line.

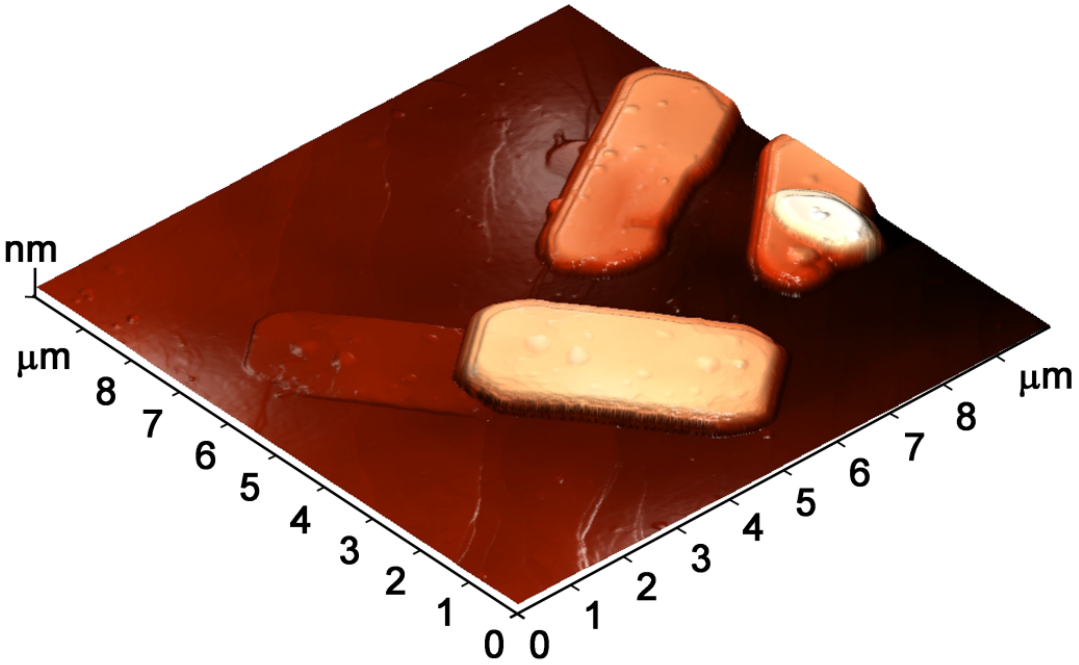

Figure. **S14**. 3D AFM images of the Leu-Leu crystals obtained from a pyridine solution on the HOPG surface.

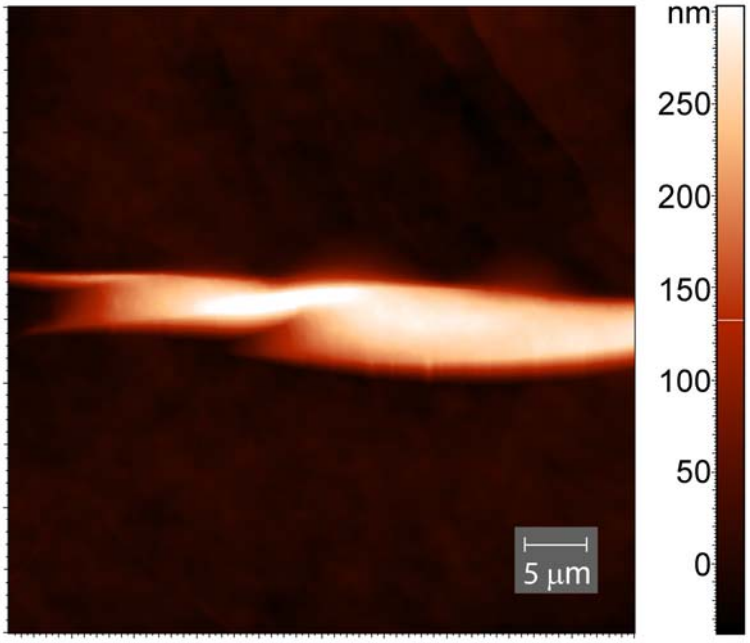

Figure. **S15**. AFM image of crystal which was formed on surface of Leu-Leu film after interaction with chloroform vapors.

Scanning electron microscopy

For scanning electron microscopy (SEM), films of dipeptide from methanol and dichloromethane solutions were prepared on the surfaces of HOPG as for AFM studies. The film from methanol solution was saturated with dichloromethane vapor for 200 min. SEM images were recorded using a scanning electron microscope Evo 50 (Carl Zeiss, Germany) at 20 kV.

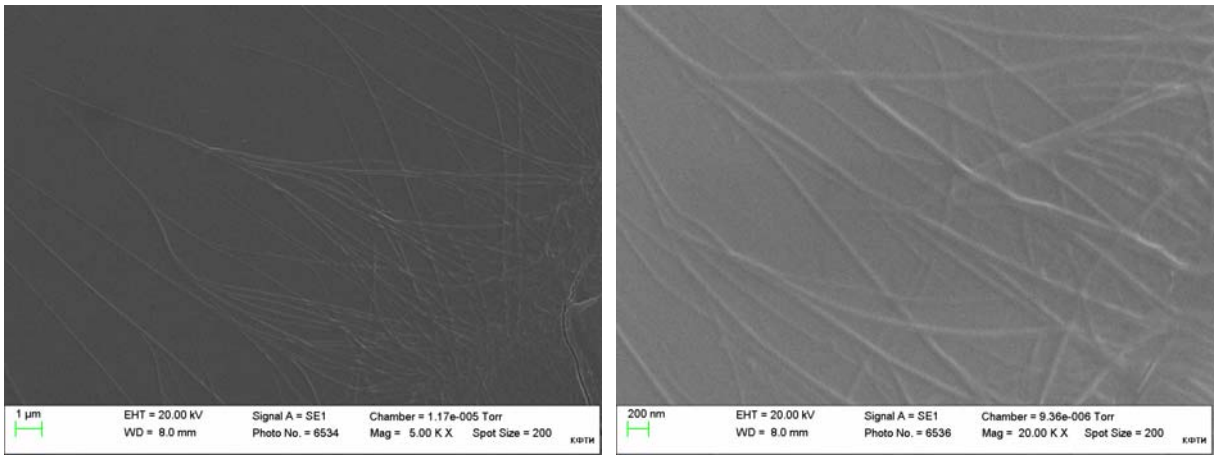

Figure. **S16**. SEM image (20 kV) of Leu-Leu film deposited on HOPG from methanol solution and saturated with dichloromethane vapor for 200 min.

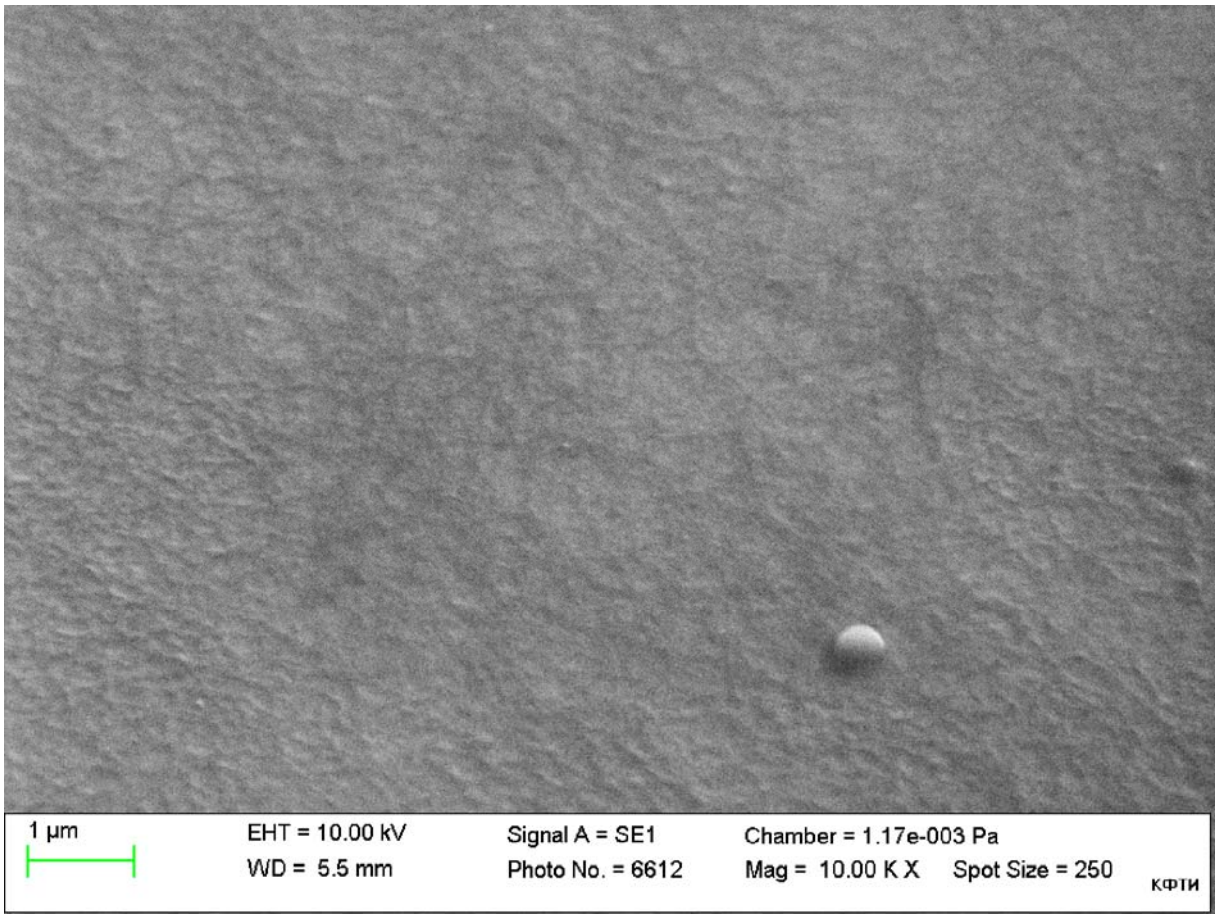

Figure. **S17**. SEM image (10 kV) of Leu-Leu film deposited on HOPG from dichloromethane solution.

Table. S1. Powder diffraction data of Leu-Leu initial powder.

№	2θ (deg)	d (Å)	Intensity
1	5.127(2)	17.221(8)	100
2	5.741(3)	15.382(8)	61.3
3	7.271(10)	12.148(17)	7.6
4	9.296(8)	9.506(8)	5.8
5	10.339(3)	8.549(2)	4.3
6	11.569(7)	7.643(5)	85.7
7	12.945(6)	6.833(3)	14.4
8	13.945(5)	6.345(2)	3
9	14.665(8)	6.035(3)	4.8
10	15.52(3)	5.705(10)	2.3
11	15.834(9)	5.592(3)	2.3
12	16.437(4)	5.3886(13)	2.2
13	17.405(10)	5.091(3)	5.9
14	18.32(5)	4.840(12)	0.9
15	18.7850(16)	4.7200(4)	47.5
16	19.66(3)	4.511(6)	0.6
17	20.376(6)	4.3548(12)	6.6
18	21.077(3)	4.2117(6)	21
19	21.543(6)	4.1215(11)	7.3
20	22.330(7)	3.9781(13)	7.2
21	23.419(11)	3.7956(17)	1.9
22	24.101(4)	3.6897(5)	9.1
23	24.640(15)	3.610(2)	0.5
24	24.780(14)	3.5901(19)	1.7
25	25.12(2)	3.542(3)	0.9
26	25.802(15)	3.450(2)	0.5
27	26.298(14)	3.3861(18)	4.5
28	26.44(2)	3.368(3)	5.2
29	26.744(7)	3.3307(9)	3.2
30	27.30(3)	3.264(3)	0.4
31	27.88(4)	3.197(4)	0.2
32	28.380(7)	3.1423(8)	1.8
33	29.36(2)	3.040(2)	0.9
34	29.742(16)	3.0015(16)	1.5
35	30.782(12)	2.9024(11)	1.9
36	31.26(2)	2.8589(18)	1.3
37	31.638(16)	2.8258(14)	2.8
38	32.086(7)	2.7873(6)	5.3
39	32.636(9)	2.7415(7)	3.1
40	33.02(5)	2.711(4)	0.3
41	33.396(12)	2.6809(9)	3
42	33.76(4)	2.653(3)	3.3
43	33.882(13)	2.6435(10)	2.8
44	34.37(3)	2.6068(19)	0.7
45	35.08(2)	2.5556(15)	0.4
46	35.52(2)	2.5253(15)	0.9
47	35.937(19)	2.4970(13)	1.7
48	36.33(2)	2.4709(13)	0.9
49	36.79(2)	2.4408(13)	0.7
50	37.507(9)	2.3960(5)	3.8
51	37.909(14)	2.3715(9)	1.9
52	38.31(3)	2.3476(17)	0.4

53	38.690(13)	2.3254(8)	1.7
54	39.459(14)	2.2818(8)	1.4
55	39.88(3)	2.2589(17)	0.2

Table. S2. Powder diffraction data of Leu-Leu sample after heating up to 130°C.

№	2θ (deg)	*d* (Å)	Intensity
1	6.852(6)	12.889(12)	100
2	6.9(6)	12.8(10)	7.4
3	7.115(6)	12.414(10)	35.5
4	7.785(6)	11.348(9)	53.9
5	13.524(16)	6.542(8)	6
6	14.03(2)	6.308(10)	2.3
7	17.319(10)	5.116(3)	8.5
8	18.61(3)	4.765(7)	4.7
9	20.51(2)	4.327(5)	4
10	24.20(4)	3.675(6)	1.9
11	32.78(19)	2.730(15)	0.6

Table. S3. Powder diffraction data of Leu-Leu sample after heating up to 130°C and saturated with vapors of water for 3 days at rt.

№	2θ (deg)	*d* (Å)	Intensity
1	4.183(9)	21.11(5)	3
2	5.0274(11)	17.563(4)	100
3	5.6476(19)	15.636(5)	51.5
4	7.180(6)	12.302(10)	8.5
5	8.492(10)	10.404(12)	1.6
6	9.221(4)	9.583(4)	4.4
7	10.2632(10)	8.6121(9)	58.5
8	11.4956(17)	7.6915(12)	11.8
9	12.885(3)	6.8651(13)	1.7
10	13.8916(14)	6.3698(6)	3.4
11	14.614(4)	6.0565(15)	1.5
12	15.491(6)	5.715(2)	1.4
13	15.753(5)	5.6209(16)	1.1
14	16.378(3)	5.4079(10)	4
15	17.258(18)	5.134(5)	1.4
16	18.16(4)	4.880(10)	1.9
17	18.730(3)	4.7338(7)	31.8
18	19.59(3)	4.527(7)	1.3
19	20.338(11)	4.363(2)	4.8
20	21.005(8)	4.2259(15)	13.4
21	21.470(12)	4.135(2)	4.6
22	22.288(15)	3.986(3)	3.5
23	23.362(8)	3.8046(13)	1.5
24	24.053(2)	3.6969(3)	7.2
25	24.660(5)	3.6072(8)	1.1
26	25.060(7)	3.5506(10)	0.9
27	25.728(13)	3.4598(17)	0.6
28	26.144(4)	3.4057(6)	1.1
29	26.299(4)	3.3860(5)	5.6

30	26.684(4)	3.3381(5)	2.3
31	27.228(17)	3.273(2)	0.5
32	27.85(2)	3.201(3)	0.3
33	28.345(6)	3.1461(6)	1.2
34	29.339(17)	3.0417(18)	0.6
35	29.720(13)	3.0036(13)	1
36	30.746(9)	2.9057(8)	1.5
37	31.224(15)	2.8623(13)	1
38	31.589(10)	2.8300(9)	1.8
39	32.042(5)	2.7911(4)	3.3
40	32.592(7)	2.7452(6)	2
41	32.92(4)	2.718(3)	0.4
42	33.336(8)	2.6856(6)	1.9
43	33.762(4)	2.6527(3)	4.3
44	34.327(19)	2.6103(14)	0.4
45	35.04(3)	2.559(2)	0.3
46	35.503(18)	2.5264(13)	0.5
47	35.902(15)	2.4993(10)	1
48	36.286(16)	2.4737(10)	0.6
49	36.784(17)	2.4414(11)	0.2
50	37.465(4)	2.3986(3)	2
51	37.904(8)	2.3718(5)	1.3
52	38.29(2)	2.3489(14)	0.4
53	38.614(8)	2.3298(5)	1
54	39.423(13)	2.2838(7)	1
55	39.82(3)	2.2620(15)	0.2

Table. S4. Powder diffraction data of Leu-Leu sample after heating up to 180°.

№	2θ (deg)	*d* (Å)	Intensity
1	6.989(6)	12.638(10)	100
2	14.00(3)	6.323(16)	1.5
3	16.58(5)	5.344(16)	1.5
4	18.00(13)	4.93(4)	3.3
5	18.87(11)	4.70(3)	2.9
6	20.71(6)	4.285(13)	2.6
7	27.5(2)	3.24(3)	0.5
8	31.5(3)	2.84(3)	1.1

Table. S5. Powder diffraction data of Leu-Leu sample after heating up to 180° and saturated with liquid water for 5 days at rt.

№	2θ (deg)	*d* (Å)	Intensity
1	7.037(6)	12.552(10)	100
2	12.39(3)	7.137(15)	1.9
3	14.03(4)	6.308(18)	3.4
4	16.62(3)	5.331(10)	3.7
5	17.9(2)	4.95(6)	2.6
6	18.83(7)	4.709(17)	13.8
7	20.69(7)	4.290(14)	6.8
8	23.6(2)	3.77(4)	1.9
9	31.82(15)	2.810(13)	1.8

10	45.8(3)	1.978(12)	0.2