Supplementary Information

to

Structure and Thermotropic Phase Behavior of a Homologous Series of *N*-Acylglycines: Neuroactive and Antinociceptive Constituents of Biomembranes

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Running title: Structure and phase behavior of *N*-acylglycines

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Table S1: Assignment of resonances in the IR spectra of NAGs in KBr pellet.

Acyl chain length	Amide(cm^{-1})			Carboxylic acid moiety	Aliphatic C-H (cm^{-1}) vibration bands		
	C=O Amide-1	N-H(def) Amide-2	N-H stretch		C-H stretch	C-H scissoring	C-H rocking
8	~1645	~1560	~3310	~1707, ~1744	~2922,~2853	~1467	~696
9	~1644	~1559	~3327	~1705, ~1748	~2920,~2853	~1467	~696
10	~1645	~1559	~3310	~1705, ~1748	~2919,~2849	~1468	~694
11	~1645	~1559	~3320	~1703, ~1742	~2920,~2851	~1464	~693
12	~1645	~1559	~3326	~1705, ~1742	~2919,~2849	~1464	~689
13	~1645	~1557	~3326	~1703, ~1740	~2919,~2849	~1471	~687
14	~ 1644	~1549	~3314	~1700	~2921,~2849	~1466	~673
15	~1644	~1561	~3328	~1705, ~1742	~2919,~2849	~1464	~691
16	~1645	~1561	~3328	~1705, ~1740	~2919,~2849	~1474	~687
17	~1645	~1557	~3329	~1705, ~1742	~2919,~2849	~1464	~687
18	~1645	~1559	~3329	~1707, ~1747	~2919,~2849	~1464	~685
19	~1645	~1557	~3333	~1705, ~1740	~2919,~2849	~1462	~689
20	~1645	~1559	~3333	~1705, ~1740	~2919,~2849	~1462	~685

Table S2: ^{1}H-NMR spectral data of NAGs were recorded in $CDCl_3$ with traces of CD_3OD solvent.

Acyl chain length	Hydrophobic moiety				Amino acid group	
	CH_3	$(CH_2)_n$	CH_2-C-CO	CH_2–CO	N-H	N-CH_2-CO
8	0.99,t	1.26,m	1.62,q	2.22,t	6.59,s	3.95,s
9	0.87,t	1.27,m	1.63,q	2.23,t	6.35,s	3.99,s
10	0.87,t	1.27,m	1.61,q	2.24,t	6.44,s	3.98,s
11	0.86,t	1.24,m	1.62,q	2.22,t	6.32,s	3.98,s
12	0.85,t	1.22,m	1.60,q	2.21,t	6.54,s	3.95,s
13	0.87,t	1.25,m	1.62,q	2.23,t	6.46,s	3.99,s
14	0.87,t	1.24,m	1.63,q	2.23,t	6.35,s	3.99,s
15	0.84,t	1.27,m	1.59,q	2.18,t	6.16,s	3.96,s
16	0.80,t	1.17,m	1.55,q	2.15,t	6.39,s	3.92,s
17	0.80,t	1.21,m	1.55,q	2.15,t	6.29,s	3.91,s
18	0.82,t	1.19,m	1.58,q	2.23,t	6.28,s	3.93,s
19	0.83,t	1.20,m	1.60,q	2.19,t	6.49,s	4.19,s
20	0.85,t	1.23,m	1.60,q	2.22,t	6.92,s	3.94,s

Table S3: ^{13}C-NMR spectral data of *N*-acylglycines in CD_3OD (solvent). Chemical shift values are given in ppm (δ scale).

Acyl chain length	Glycine Moiety		Acyl chain						
	NH-CH_2-COOH	-CH_2-COOH	C=O	(C=O)-CH_2-	(C=O)-CH_2-CH_2-	-CH_3	-CH_2–CH_3	CH_2–C_2H_5	$(CH_2)_n$ multiple peaks in the range
C8	40.34	171.74	175.42	35.47	25.49	13.05	22.32	31.53	28.83
C9	40.34	171.68	175.36	35.42	25.46	13.05	22.33	31.62	29.05-28.92
C10	40.36	171.74	175.39	35.46	25.50	13.11	22.38	31.70	29.25-28.92
C11	40.37	171.76	175.42	35.47	25.52	13.12	22.40	31.73	29.37-28.92
C12	40.38	171.74	175.42	35.47	25.52	13.11	22.41	31.75	29.42-28.92
C13	40.43	171.79	175.43	35.52	25.55	13.13	22.44	31.78	29.46-28.96
C14	40.37	171.76	175.40	35.46	25.51	13.09	22.39	31.73	29.43-28.90
C15	40.39	171.78	175.42	35.49	25.52	13.11	22.42	31.75	29.47-28.93
C16	40.37	171.66	175.30	35.44	25.40	12.96	22.26	31.62	29.32-28.83
C17	40.37	171.75	175.41	35.44	25.49	13.07	22.38	31.71	29.42-28.89
C18	40.20	171.57	175.27	35.30	25.34	12.93	22.23	31.57	29.27-28.75
C19	40.23	171.67	175.37	35.36	25.39	12.99	22.32	31.67	29.42-28.92
C20	40.70	172.07	175.75	35.79	25.84	13.43	22.74	32.07	29.77-29.24

Table S4: Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for *N*-myristoylglycine. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor [$U(eq) = \frac{1}{3} \sum_i \sum_j U_{ij} a_{i*} a_{j*} a_i a_j \cos(ai, aj)$].

Atom	X	Y	Z	U(eq)
C(1)	2312(1)	2320(6)	3834(4)	42(1)
C(2)	2173(1)	2173(6)	2811(4)	44(1)
C(3)	1950(1)	1494(5)	4339(4)	33(1)
C(4)	1820(1)	2807(5)	5123(4)	37(1)
C(5)	1680(1)	1778(6)	4271(4)	41(1)
C(6)	1545(1)	3007(6)	5041(4)	42(1)
C(7)	1406(1)	1899(6)	4219(4)	47(1)
C(8)	1268(1)	3085(6)	4975(4)	46(1)
C(9)	1131(1)	1937(7)	4152(5)	49(1)
C(10)	993(1)	3092(7)	4893(5)	50(1)
C(11)	855(1)	1937(7)	4074(5)	52(1)
C(12)	717(1)	3078(7)	4802(5)	54(1)
C(13)	580(1)	1926(7)	3976(5)	57(1)
C(14)	442(1)	3029(8)	4694(5)	62(1)
C(15)	305(1)	1874(9)	3870(6)	76(1)
C(16)	167(1)	2967(11)	4606(7)	103(2)
N(1)	2049(1)	3180(4)	3714(3)	39(1)
O(1)	2415(1)	996(6)	3095(3)	72(1)
O(2)	2329(1)	3589(6)	5175(3)	69(1)
O(3)	1963(1)	-1021(4)	4266(3)	51(1)

Table S5: Selected bond distances (Å) and bond angles (degrees) for the *N*-myristoylglycine

Bond distances		Bond angles	
C(1)-C(2)	1.487(4)	C(3)-N(1)-C(2)	121.9(2)
C(3)-C(4)	1.502(3)	C(3)-C(4)-C(5)	111.8(2)
C(4)-C(5)	1.516(4)	C(4)-C(5)-C(6)	113.8(2)
C(5)-C(6)	1.518(4)	C(5)-C(6)-C(7)	113.4(2)
C(6)-C(7)	1.513(4)	C(6)-C(7)-C(8)	114.4(3)
C(7)-C(8)	1.521(4)	C(7)-C(8)-C(9)	113.7(3)
C(8)-C(9)	1.512(4)	C(8)-C(9)-C(10)	114.5(3)
C(9)-C(10)	1.515(4)	C(9)-C(10)-C(11)	114.4(3)
C(10)-C(11)	1.509(4)	C(10)-C(11)-C(12)	114.8(3)
C(11)-C(12)	1.512(4)	C(11)-C(12)-C(13)	114.6(3)
C(12)-C(13)	1.506(4)	C(12)-C(13)-C(14)	115.3(3)
C(13)-C(14)	1.504(4)	C(13)-C(14)-C(15)	115.2(3)
C(14)-C(15)	1.504(5)	C(14)-C(15)-C(16)	115.0(4)
C(15)-C(16)	1.506(5)	N(1)-C(2)-C(1)	114.7(3)
N(1)-C(2)	1.438(3)	N(1)-C(3)-C(4)	116.8(2)
N(1)-C(3)	1.329(3)	O(1)-C(1)-C(2)	112.6(3)
O(1)-C(1)	1.297(3)	O(2)-C(1)-O(1)	123.2(3)
O(2)-C(1)	1.203(4)	O(2)-C(1)-C(2)	124.1(3)
O(3)-C(3)	1.229(3)	O(3)-C(3)-N(1)	121.9(2)
		O(3)-C(3)-C(4)	121.3(2)

Table S6: Selected torsion angles (degrees) for the *N*-myristoylglycine

C(2) N(1) C(3) O(3)	4.14
C(2) N(1) C(3) C(4)	-175.07
C(3) N(1) C(2) C(1)	-106.11
C(3) C(4) C(5) C(6)	178.95
C(4) C(5) C(6) C(7)	-178.21
C(5) C(6) C(7) C(8)	179.63
C(6) C(7) C(8) C(9)	-179.43
C(7) C(8) C(9) C(10)	179.89
C(8) C(9) C(10) C(11)	-179.81
C(9) C(10) C(11) C(12)	-179.93
C(10) C(11) C(12) C(13)	179.81
C(11) C(12) C(13) C(14)	179.67
C(12) C(13) C(14) C(15)	-179.91
C(13) C(14) C(15) C(16)	179.46
N(1) C(3) C(4) C(5)	124.54
O(1) C(1) C(2) N(1)	169.47
O(2) C(1) C(2) N(1)	-12.56
O(3) C(3) C(4) C(5)	-54.67

Table S7: Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for the *N*-palmitoylglycine. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor [$U(eq) = \frac{1}{3} \sum_i \sum_j U_{ij} a_{i*} a_{j*} a_i a_j \cos(ai, aj)$].

Atom	X	Y	Z	U(eq)
C(1)	339(1)	4845(8)	-984(6)	38(1)
C(2)	590(1)	4656(8)	-1882(5)	40(1)
C(3)	991(1)	3993(6)	-142(5)	30(1)
C(4)	1225(1)	5313(7)	775(5)	32(1)
C(5)	1477(1)	4292(7)	35(5)	37(1)
C(6)	1721(1)	5506(8)	943(5)	38(1)
C(7)	1971(1)	4406(8)	248(5)	40(1)
C(8)	2218(1)	5583(8)	1132(6)	43(1)
C(9)	2467(1)	4443(8)	445(6)	43(1)
C(10)	2714(1)	5582(9)	1320(6)	47(1)
C(11)	2962(1)	4443(8)	630(6)	46(1)
C(12)	3211(1)	5554(9)	1490(6)	51(1)
C(13)	3458(1)	4465(9)	800(6)	52(1)
C(14)	3707(1)	5521(10)	1643(7)	55(1)
C(15)	3954(1)	4468(10)	959(7)	61(1)
C(16)	4202(1)	5472(11)	1802(7)	66(1)
C(17)	4449(1)	4461(14)	1102(8)	84(2)
C(18)	4696(1)	5366(15)	1960(10)	105(2)
N(1)	813(1)	5674(6)	-870(4)	36(1)
O(1)	152(1)	3489(7)	-1835(5)	69(1)
O(2)	310(1)	6074(7)	348(5)	68(1)
O(3)	969(1)	1487(5)	-230(4)	48(1)

Table S8: Selected bond distances (Å) and bond angles (degrees) for the *N*-palmitoylglycine

Bond distances		**Bond angles**	
C(1)-C(2)	1.492(5)	C(3)-N(1)-C(2)	121.7(3)
C(1)-O(1)	1.311(5)	C(3)-C(4)-C(5)	111.3(3)
C(3)-O(3)	1.226(4)	C(4)-C(5)-C(6)	113.6(3)
C(4)-C(3)	1.505(5)	C(6)-C(7)-C(8)	114.6(3)
C(5)-C(4)	1.520(5)	C(7)-C(6)-C(5)	113.5(3)
C(6)-C(5)	1.520(5)	C(8)-C(9)-C(10)	114.8(4)
C(8)-C(7)	1.516(5)	C(9)-C(8)-C(7)	114.1(3)
C(8)-C(9)	1.510(5)	C(11)-C(10)-C(9)	114.7(4)
C(10)-C(9)	1.511(5)	C(12)-C(11)-C(10)	115.4(4)
C(10)-C(11)	1.507(5)	C(13)-C(12)-C(11)	115.9(4)
C(12)-C(11)	1.505(5)	C(14)-C(13)-C(12)	116.8(4)
C(12)-C(13)	1.496(5)	C(14)-C(15)-C(16)	117.7(4)
C(14)-C(13)	1.494(5)	C(15)-C(14)-C(13)	117.2(4)
C(14)-C(15)	1.483(6)	C(17)-C(16)-C(15)	117.9(5)
C(16)-C(15)	1.483(6)	C(18)-C(17)-C(16)	118.5(6)
C(16)-C(17)	1.482(7)	N(1)-C(2)-C(1)	114.6(3)
C(18)-C(17)	1.467(7)	N(1)-C(3)-C(4)	116.6(3)
		O(1)-C(1)-C(2)	111.8(4)
		O(2)-C(1)-O(1)	123.5(4)
		O(2)-C(1)-C(2)	124.7(3)
		O(3)-C(3)-N(1)	122.0(3)
		O(3)-C(3)-C(4)	121.3(3)

Table S9: Selected torsion angles (degrees) for the *N*-palmitoylglycine

C(2) N(1) C(3) C(4)	175.7(3)
C(2) N(1) C(3) O(3)	-3.3(6)
C(3) N(1) C(2) C(1)	106.6(4)
C(3) C(4) C(5) C(6)	-178.6(3)
C(4) C(5) C(6) C(7)	177.9(3)
C(5) C(6) C(7) C(8)	-180.0(3)
C(6) C(7) C(8) C(9)	179.2(3)
C(7) C(8) C(9) C(10)	-179.6(3)
C(8) C(9) C(10) C(11)	-179.9(4)
C(9) C(10) C(11) C(12)	-179.9(4)
C(10) C(11) C(12) C(13)	-179.2(4)
C(11) C(12) C(13) C(14)	-179.5(4)
C(12) C(13) C(14) C(15)	-179.6(4)
C(13) C(14) C(15) C(16)	-179.2(4)
C(14) C(15) C(16) C(17)	-179.0(5)
C(15) C(16) C(17) C(18)	-178.0(6)
N(1) C(3) C(4) C(5)	-123.9(3)
O(1) C(1) C(2) N(1)	-169.5(3)
O(2) C(1) C(2) N(1)	10.5(6)
O(3) C(3) C(4) C(5)	55.1(5)

Table S10: *d*-Spacing values of NAGs determined from PXRD data.

Chain length	d_1	d_2	d_3	d_4	d_5	d_6	d_7	d_8	d_{avg}
C8	31.203	31.325	-	30.825	30.982	-	-	-	31.084±0.223
C9	35.411	33.686	-	34.371	-	-	33.949	-	34.354±0.759
C10	37.493	37.193	36.499	36.544	-	-	36.287	-	36.803±0.513
C11	38.463	38.474	38.489	38.591	-	-	38.799	-	38.563±0.141
C12	43.739	42.911	42.382	42.232	-	41.788	41.764	-	42.469±0.753
C13	-	45.537	45.242	44.880	-	44.776	44.416	-	44.970±0.433
C14	-	48.505	47.825	47.127	-	47.294	-	-	47.688±0.621
C15	-	51.588	50.529	50.450	-	49.744	-	-	50.578±0.760
C16	-	52.808	52.510	52.066	-	51.854	-	-	52.310±0.430
C17	-	56.482	56.257	55.457	-	55.267	-	54.951	55.683±0.657
C18	-	58.328	57.961	57.788	-	57.392	-	56.945	57.683±0.389
C19	-	61.124	60.583	61.358	59.854	59.820	-	60.102	60.474±0.658
C20	-	63.740	63.451	-	62.709	62.319	-	62.185	62.881±0.688

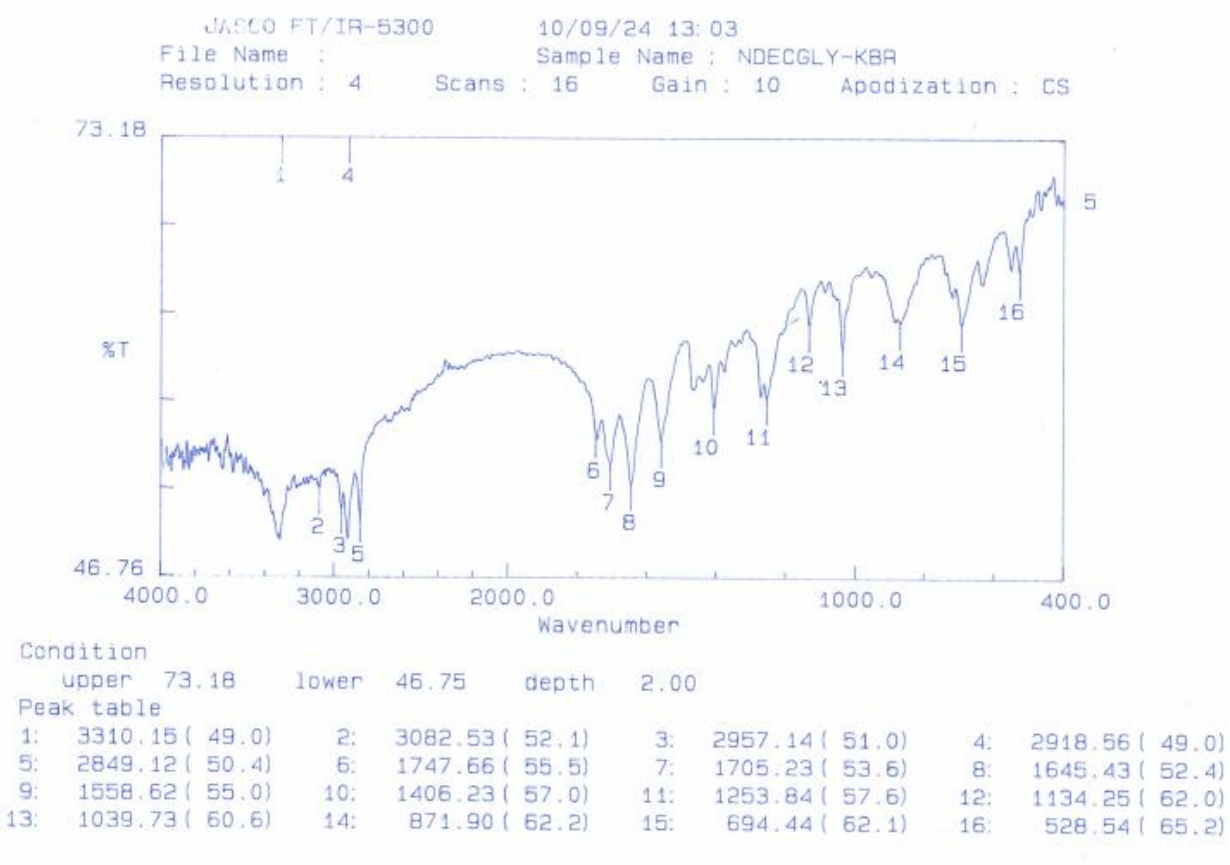


Fig. S1: FTIR spectrum of *N*-decanoylglycine. The sample was prepared as a KBr pellet.

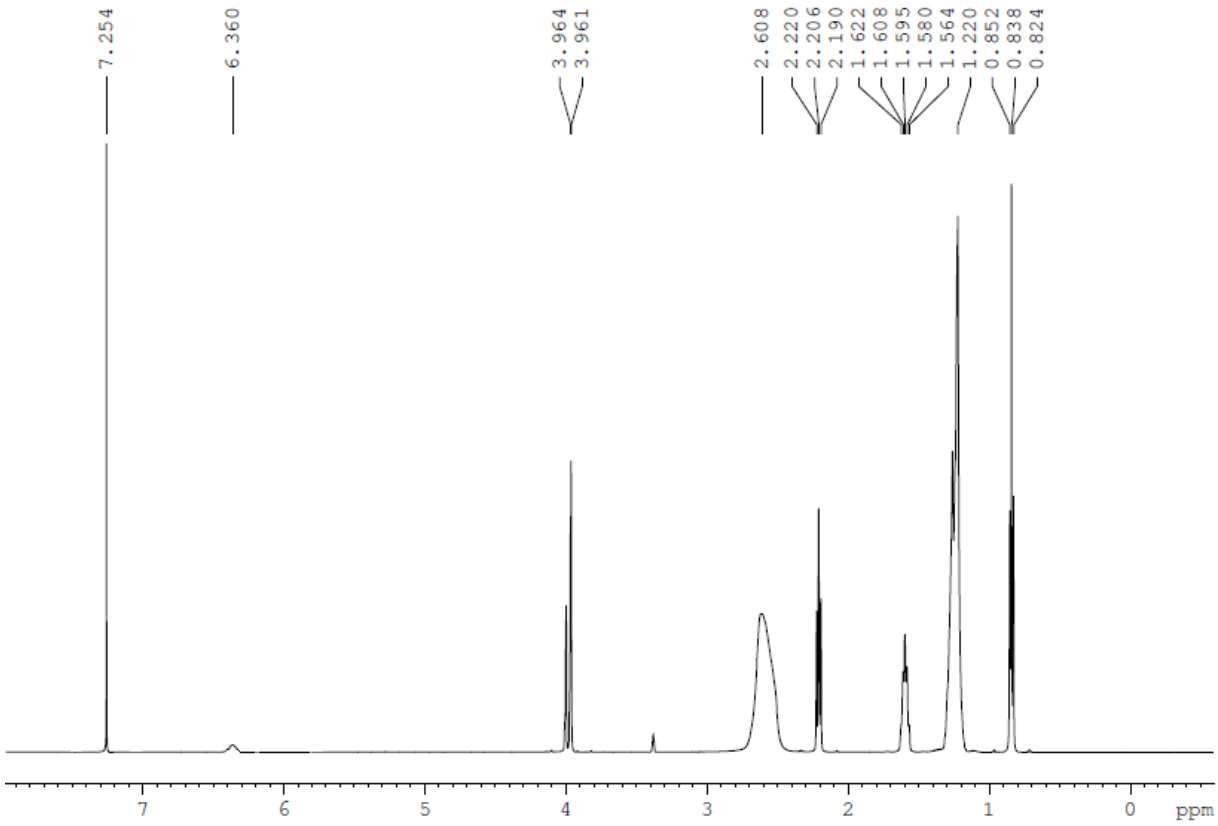


Fig. S2: ^{1}H NMR spectrum of *N*-decanoylglycine in $CDCl_3$ containing a trace of CD_3OD.

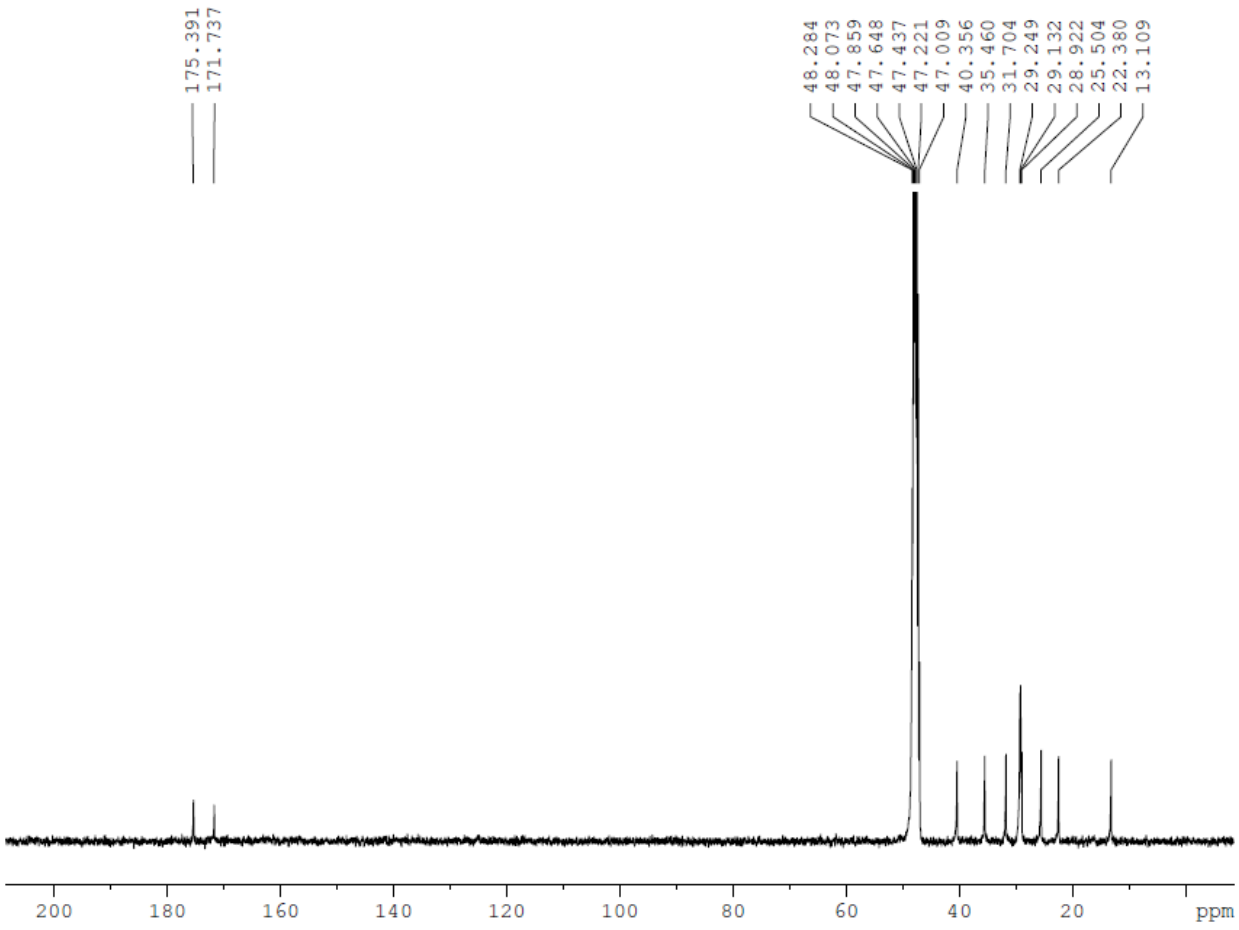
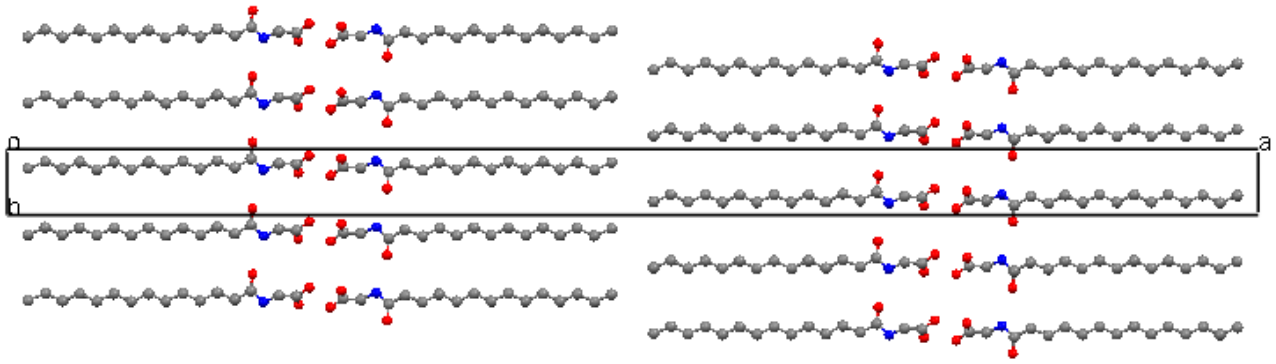


Fig. S3. ^{13}C NMR spectrum of *N*-decanoylglycine in CD_3OD.

Fig. S4.

A).



B).

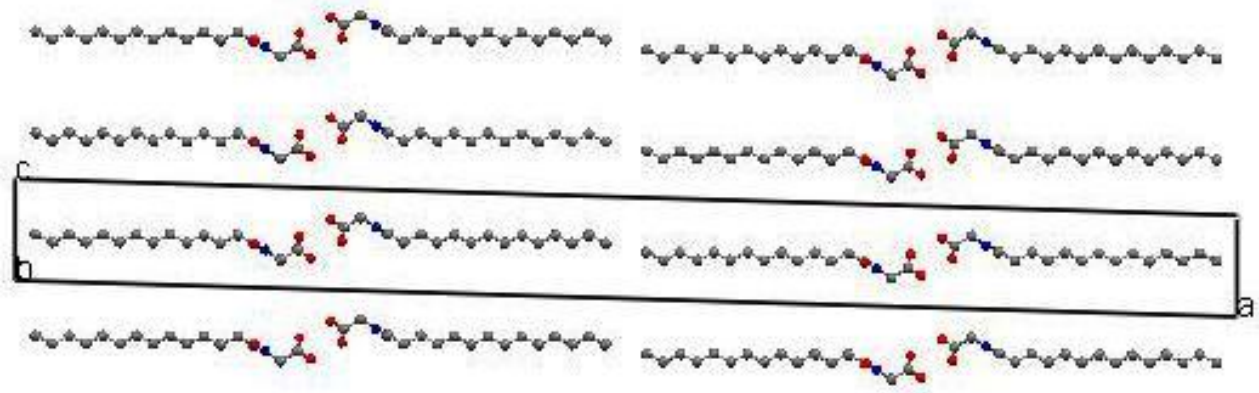
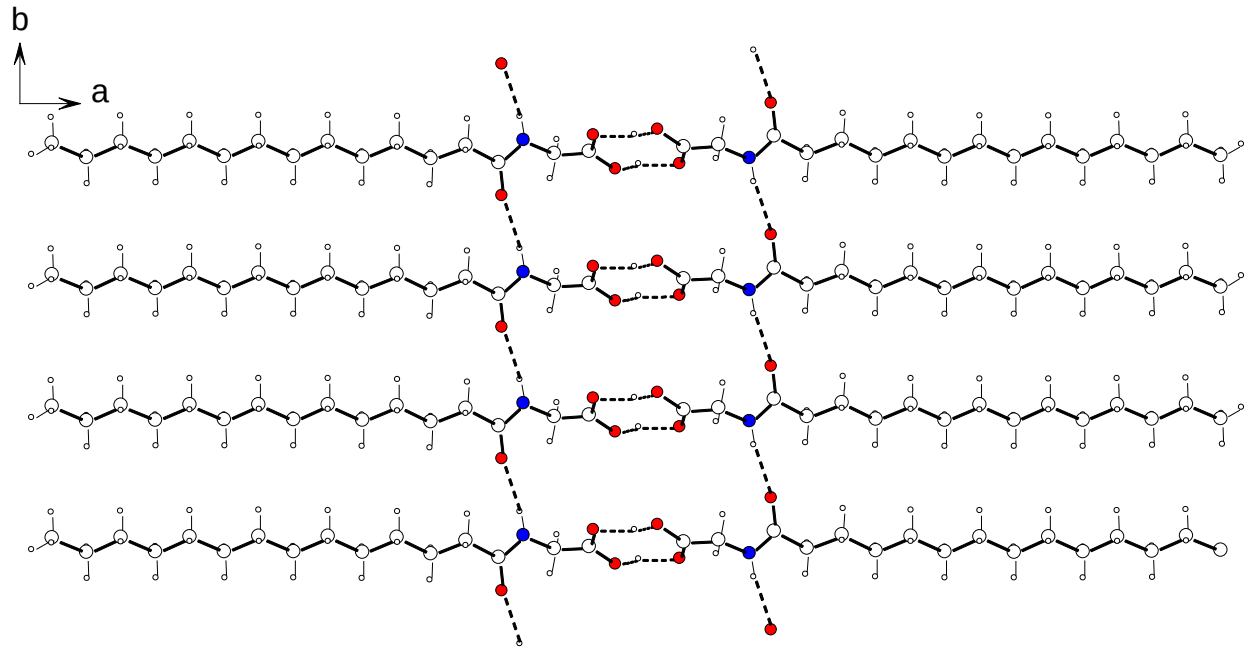


Fig. S4: Packing diagram of *N*-myristoylglycine viewed down the *c*-axis (A) and *b*-axis (B).

Fig. S5.

A)



B)

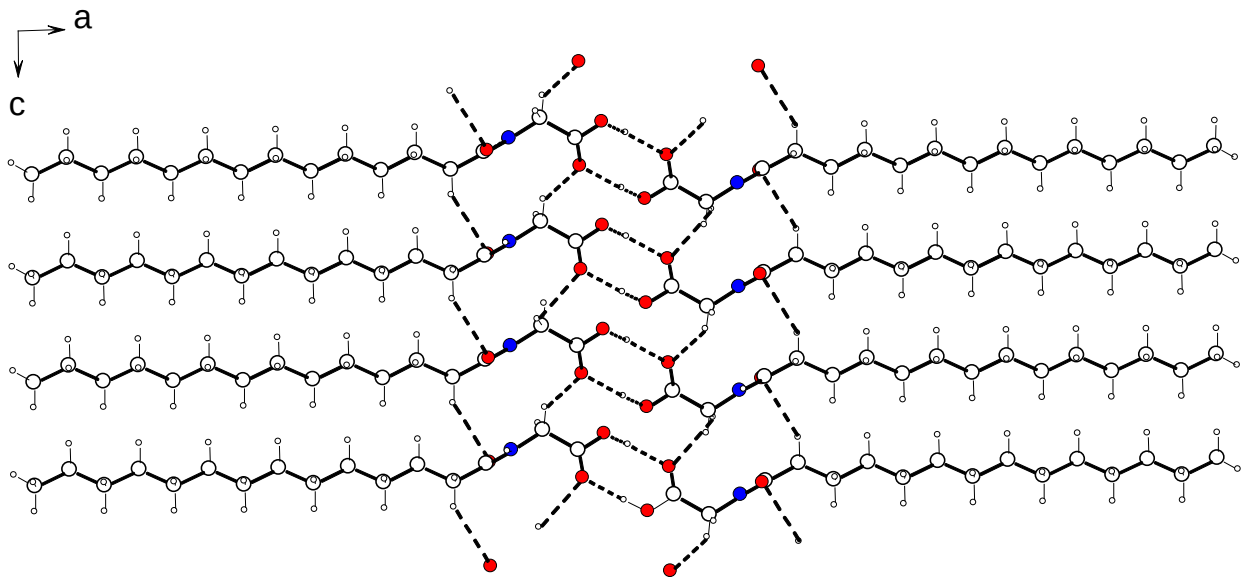


Fig. S5: Hydrogen bonding pattern in the crystal lattice of *N*-myristoylglycine. (A) A view of the bilayer down the *c*-axis displaying N-H・・・O and O-H・・・O type hydrogen bonding. (B) A view of the bilayer down the *b*-axis displaying C-H・・・O and O-H・・・O type hydrogen bonding. Carbon atoms are shown as open circles, nitrogen atoms are shown in blue and oxygen atoms are in red. Additional details regarding these hydrogen bonds are given below.

Hydrogen bonding in the crystal structure of *N*-myristoylglycine. The H-atoms on C2 form two different types of C-H···O hydrogen bonds with O2. These bonds are formed between O2 (oxygen atom of carboxylic carbonyl group) of one molecule with two different H-atoms (H2A and H2B) on C2 (carbon atom α- to carboxylic carbonyl) of an adjacent molecule in the same layer. All the C2(H2A)···O2 bonds are identical, with a C2(H2A)–O2 distance of 3.249 Å (3), an H2A···O2 distance of 2.4 Å, and C2-H2A···O2 angle of 145.8^{o}. Similarly, all the C2(H2B)···O2 bonds are also identical, with a C2(H2B)–O2 distance of 3.762Å, an H2B···O2 distance of 3.062 Å, and C2-H2B···O2 angle of 130.2^{o}.

In a similar way, two different types of C-H···O hydrogen bonds are seen between H-atoms on C4 and O3. These bonds are formed between O3 (oxygen atom of amide carbonyl group) of one molecule with different H-atoms on C4 (carbon atom α- to amide carbonyl) of adjacent molecule in the same layer. All the C4(H4A)···O3 bonds are identical, with a C4(H4A)–O3 distance of 5.241 Å (3), an H4A···O3 distance of 4.611 Å, and C4-H4A···O3 angle of 126.1^{o}. All the C2(H2B)···O2 bonds are also identical, with a C4(H4B)–O3 distance of 3.505Å, an H4B···O3 distance of 2.635 Å, and C4-H4B···O3 angle of 149.4^{o}.

Fig. S6.

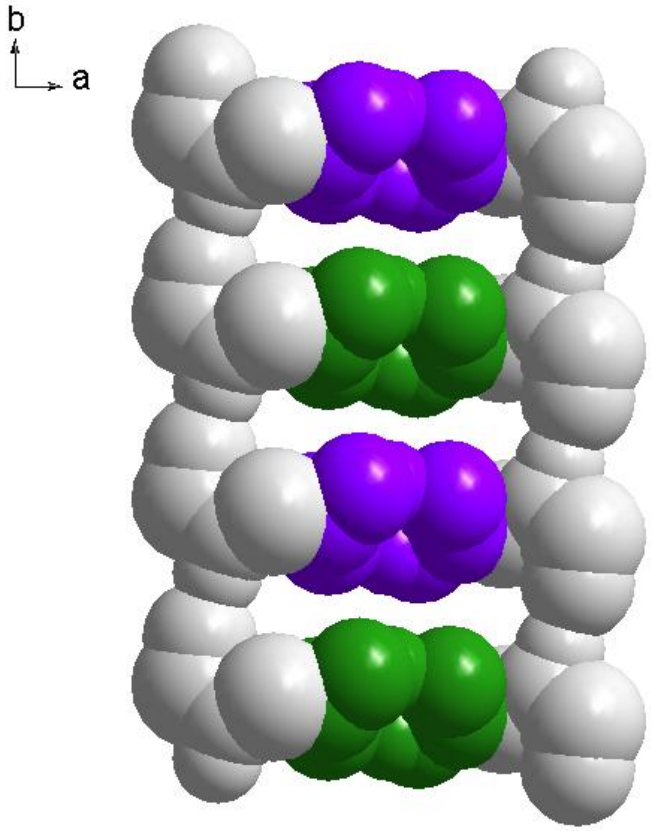


Fig. S6: A space filling model of H-bonding pattern of *N*-palmitoylglycine viewed down the *c*-axis. The donut-shaped hydrogen bonded carboxylic acid dimers are shown in green and blue whereas the other atoms are shown in light grey.

Fig. S7.

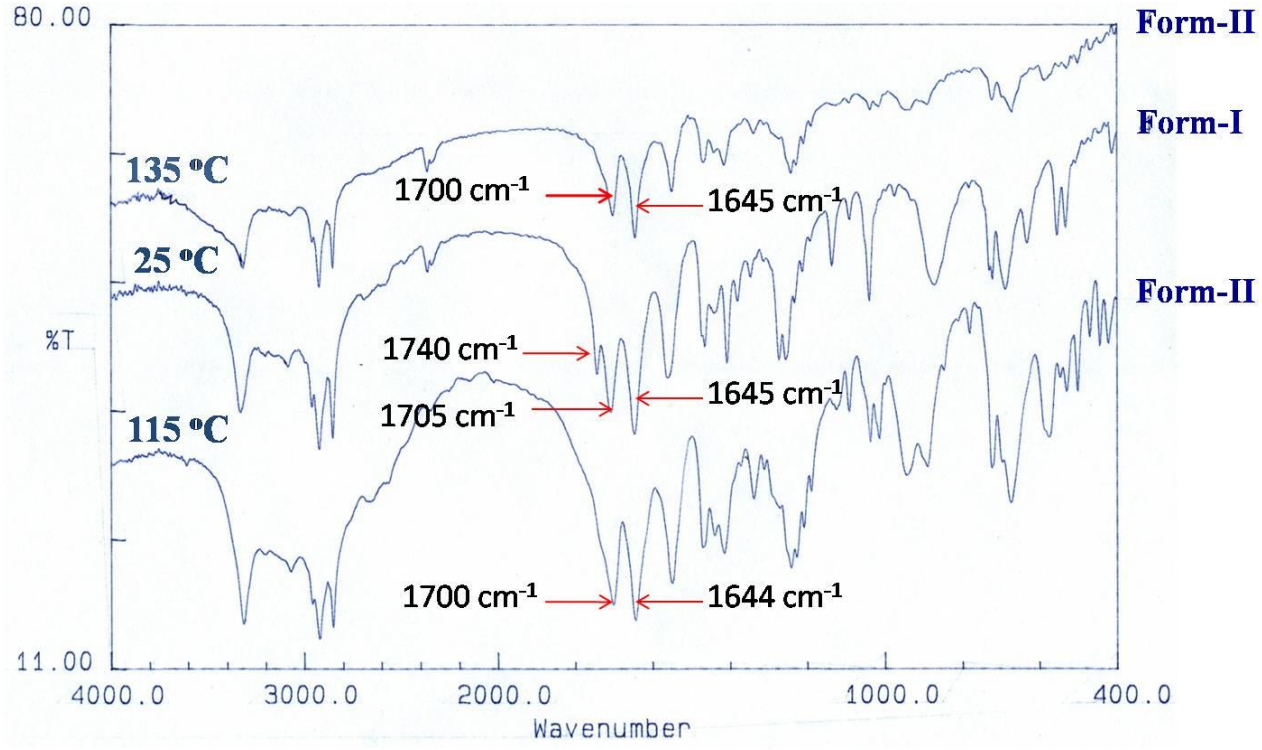


Fig. S7. FTIR spectra of *N*-palmitoylglycine recorded after heating to the temperature indicated followed by cooling to room temperature.

Fig. S8.

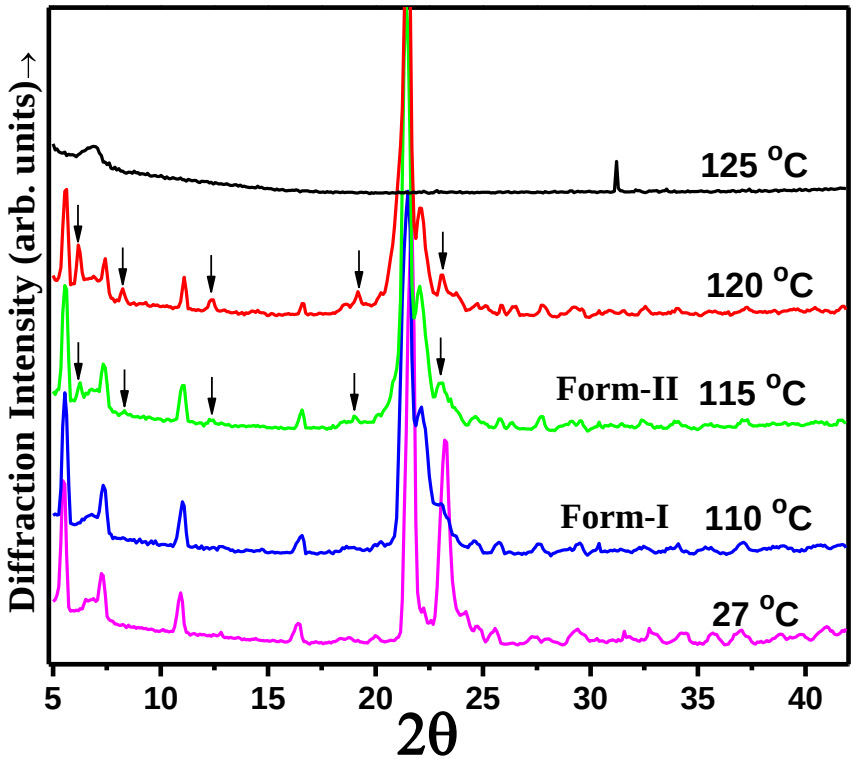


Fig. S8: Variable-temperature powder X-ray diffraction (VT-PXRD) profiles of *N*-pentadecanoylglycine. The temperature at which the data was collected is indicated against each diffraction profile. Additional peaks that appeared after the minor transition are indicated with arrows.

Fig. S9.

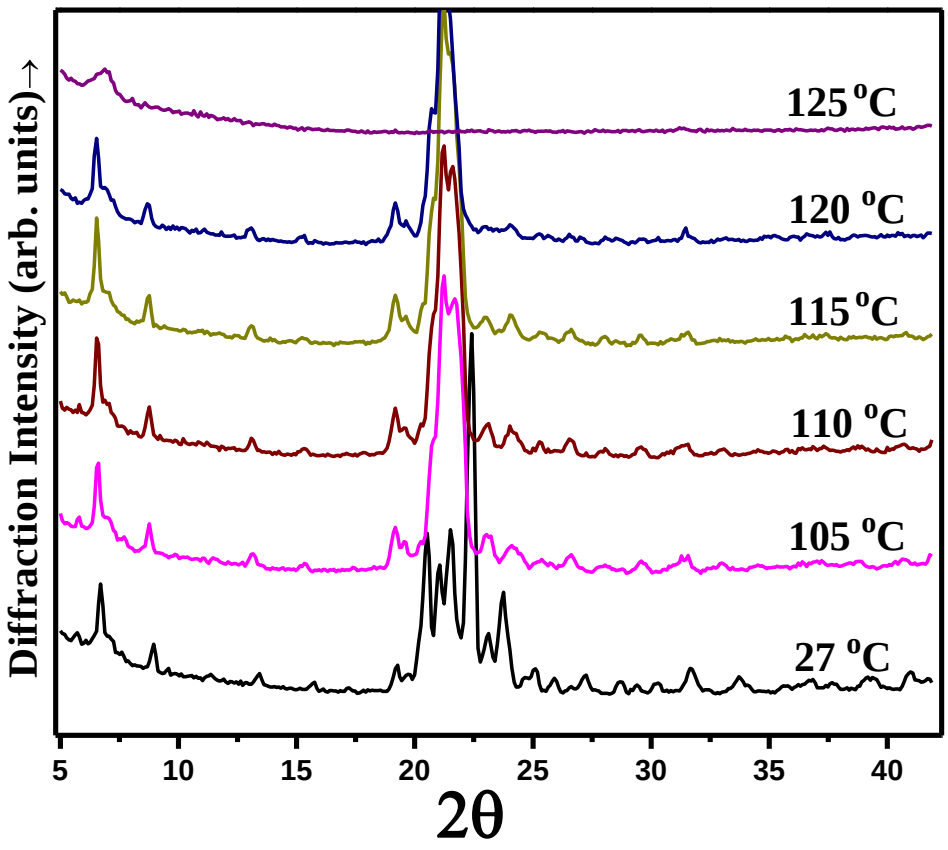


Fig. S9: Variable-temperature powder X-ray diffraction (VT-PXRD) profiles of *N*-myristoylglycine. The temperature at which the data was collected is indicated against each diffraction profile.