

Supplemental Information for: **Mixed cyclo di-amino acids structured edible oils: A potential hardstock fat mimic**

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Table S1: The Hansen solubility parameters of each solvents tested for CdAA self-assembly.

Solvents	δ_d (MPa^{1/2})	δ_p (MPa^{1/2})	δ_h (MPa^{1/2})
Salicylaldehyde	19.0	10.5	12.0
Dimethyl sulfoxide	18.4	16.4	10.2
O-xylene	17.8	1.0	3.1
Isobutyl alcohol	15.1	5.7	15.9
Triethylene glycol	16.0	12.5	18.6
Butylamine	16.2	4.5	8.0
Hexanoic acid	16.3	4.2	11.5
Dichlorotoluene	19.8	9.8	2.5
Tetramethylurea	16.7	8.2	11.0
Carbon tetrachloride	17.8	0	0.6
Benzyl methacrylate	16.8	4.1	4.1
Chloroform	17.8	3.1	5.7
Triethylamine	15.5	0.4	1.0
Hexane	14.9	0.001	0.001
Benzene	18.4	0.001	2.0
Acetone	15.5	10.4	7.0
Acetonitrile	15.3	18.0	6.1
Pyridine	19.0	8.8	5.9
Toluene	18.0	1.4	2.0
Dichloromethane	17.0	7.3	7.1
Ethanol	15.8	8.8	19.4
Dimethyl formamide	17.4	13.7	11.3
Water	15.8	16.0	42.3
Triolein	16.6	2.1	2.3
Canola oil	16.5	2.1	2.6

Table S2: Gelation outcomes of 5 wt.% CdAA gelators in solvents (gel (G), precipitate (P), solution (S)).

	Leu-Glu	Phe-Leu	Phe-Tyr	Ser-Asp	Lys-Glu	Gln-Tyr
Salicylaldehyde	G	G	G	S	G	G
Dimethyl sulfoxide	S	S	S	S	P	S
O-xylene	G	G	P	P	P	G
Isobutyl alcohol	P	G	P	P	P	P
Triethylene glycol	S	G	P	S	P	S
Butylamine	S	S	P	S	P	S
Hexanoic acid	S	S	P	S	P	G
Dichlorotoluene	G	S	P	P	S	P
Tetramethylurea	S	S	P	S	P	S
Carbon tetrachloride	P	G	P	P	P	P
Benzyl methacrylate	G	G	P	P	P	G
Acetophenone	G	G	P	P	P	G
Chloroform	P	G	P	P	P	P
Triethylamine	S	P	P	P	P	P
Hexane	P	P	P	P	P	P
Benzene	P	G	P	P	P	S
Acetone	P	G	P	P	P	G
Acetonitrile	G	G	P	P	P	G
Pyridine	S	S	G	S	P	G
Toluene	P	G	P	P	P	P
Dichloromethane	P	G	P	P	P	P
Ethanol	P	G	G	S	P	G
Dimethyl formamide	S	S	P	S	P	G
Water	P	G	P	S	S	G
Triolein	S	G	P	P	P	P
Canola oil	P	G	P	P	P	P

Table S3: CdAAs gelation results reported in literature and tested in sufficient solvents to determine the Hansen coordinates of the minimum enclosing sphere containing either gels (G), solutions (S), or precipitate (P)).

	Leu-Leu	Phe-Phe	Tyr-Tyr	Trp-Trp	Gly-Ala	Gly-Val	Gly-Leu	Gly-Phe	Val-Val	Val-Leu	Leu-Leu	Phe-Leu	Phe-Phe	Tyr-Lys
Dimethyl sulfoxide	S	P	S	S										G
O-xylene	P	P	P	P										
Tetramethylurea	S	P	S	P										
Chloroform	P	P	P	G	P	P	P	P	S	G	S	S	P	
Hexane	P	P	P	P										
Benzene	G	P	P	P	P	P	P	P	S	P	G	S	P	
Acetone					P	P	P	P	P	P	S	S	P	P
Acetonitrile	G	P	P	P										
Pyridine	S	P	S	S										
Toluene	P	P	P	P	P	P	P	P	S	S	G	G	P	
Ethanol					P	G	S	P	P	S	S	S		P
Dimethyl	S	P	S	S										G
Water	P	P	G	P										G
Triolein					P	G	G	G	S	P	P	G	P	
Canola oil	P	P	P	P										
Benzaldehyde	G	P	P	S										
Ethyl acetate	G	P	P	P	P	P	P	P	P	S	P	S	P	
Isopropanol	G	P	G	P										
Propylene glycol	G	P	G	S										
Ethylene glycol	G	P	P	S										
Hexanol	G	P	P	P										P
Glycerol	P	P	G	P										
Methanol					P	S	S	P	P	S	S	S	P	
Tetrachloromethane					P	P	P	P	S	P	S	P	P	
Cyclohexane					P	P	P	P	P	P	P	P	P	
Methoxybenzene					P	G	S	S	P	P	P	G	P	
Chlorobenzene					P	P	S	P	P	P	P	G	P	
Nitrobenzene					S	G	S	G	P	P	P	G	P	
Tricaprylin					P	G	P	G	P	P	P	G	P	
Soybean oil					P	G	G	G	P	P	G	G	P	
Silicone oil					G	G	G	G	S	G	G	G	G	
Dimethylacetamide														G
Piperidine														G
Butanol														P

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2) K. Hanabusa, M. Matsumoto, M. Kimura, A. Kakehi and H. Shirai, *J Colloid Interface Sci*, 2000, 224, 231-244.

3) Z. Xie, A. Zhang, L. Ye and Z. G. Feng, *Soft Matter*, 2009, 5;1474-1482.

Table S4: The radius and coordinates for the center of the sphere enclosing all CdAA-solvent solution (s), gel (g), and precipitate (p) outcomes in Hansen space.

	State	$2\delta_d$ (MPa ^{1/2})	δ_p (MPa ^{1/2})	δ_h (MPa ^{1/2})	Radius (MPa ^{1/2})
Mixed	S	32.7	9.5	22.2	21.2
	G	35.5	6.3	7.3	6.8
	P	31.9	7.1	8.4	11.2
Leu-Glu	S	31.9	6.9	9.5	8.9
	G	33.1	9.5	4.6	9.0
	P	30.7	8.0	21.2	22.6
Phe-Leu	S	35.9	9.6	8.5	7.0
	G	33.6	8.0	21.5	22.4
	P	30.4	0.2	0.5	0.81
Phe-Tyr	S	N/A	N/A	N/A	N/A
	G	34.8	8.8	12.6	7.5
	P	30.7	8.0	21.2	22.6
Ser-Asp	S	34.8	12.4	24.1	18.8
	G	N/A	N/A	N/A	N/A
	P	32.1	7.9	6.1	10.2
Lys-Glu	S	35.6	12.9	22.4	20.5
	G	N/A	N/A	N/A	N/A
	P	31.8	7.0	8.7	11.3
Gln-Tyr	S	34.4	6.3	10.3	10.7
	G	33.6	8.5	22.7	21.1
	P	32.9	5.2	7.0	9.3
Leu-Leu	S	36.1	11.7	9.2	4.8
	G	34.7	7.3	13.1	13.4
	P	30.7	8.1	21.1	22.6
Phe-Phe	S	N/A	N/A	N/A	N/A
	G	N/A	N/A	N/A	N/A
	P	30.7	8.0	21.2	22.6
Tyr-Tyr	S	36.1	11.7	9.2	4.8
	G	31.6	11.1	29.3	13.9
	P	31.9	5.6	13.0	14.3
Trp-Trp	S	36.4	9.2	15.7	10.8
	G	N/A	N/A	N/A	N/A
	P	30.7	8.0	21.2	22.6
Gly-Ala	S	N/A	N/A	N/A	N/A
	G	N/A	N/A	N/A	N/A
	P	32.4	6.4	11.3	12.8
Gly-Val	S	N/A	N/A	N/A	N/A
	G	33.6	6.4	10.6	9.4
	P	33.3	5.2	3.8	6.5
Gly-Leu	S	34.1	8.3	12.1	11.6
	G	33.1	2.1	2.5	0.01
	P	33.3	5.2	3.8	6.5
Gly-Phe	S	N/A	N/A	N/A	N/A
	G	36.5	5.3	3.4	4.9
	P	32.4	6.1	11.3	12.8
Val-Val	S	35.6	1.6	3.2	3.0
	G	N/A	N/A	N/A	N/A
	P	31.9	6.2	11.3	12.8
Val-Leu	S	35.1	6.9	12.2	11.9
	G	N/A	N/A	N/A	N/A
	P	34.1	5.7	3.5	6.6
Tyr-Lys	S	N/A	N/A	N/A	N/A
	G	33.0	10.6	25.5	17.8
	P	31.3	9.6	13.2	6.3

Table S5: Gelation results for 5 wt.% mixed CdAAs in canola oil (precipitate (P), gel (G)).

Number of CdAAs	Leu-Glu	Phe-Tyr	Ser-Asp	Lys-Glu	Gln-Tyr	Outcome
2	X	X				P
	X		X			P
				X	X	P
			X		X	P
			X	X		P
3			X	X	X	P
	X	X	X			P
4		X	X	X	X	G
	X		X	X	X	G
	X	X		X	X	G
	X	X	X		X	G
	X	X	X	X		G
5	X	X	X	X	X	G