Electronic Supplementary Material (ESI) for CrystEngComm

Crystal architecture and physicochemical properties of felodipine solvates

Artem O. Surov, Katarzyna A. Solanko, Andrew D. Bond,
Annette Bauer-Brandl, and German L. Perlovich

Supporting Information

S1. CSD Analysis for felodipine-like molecules

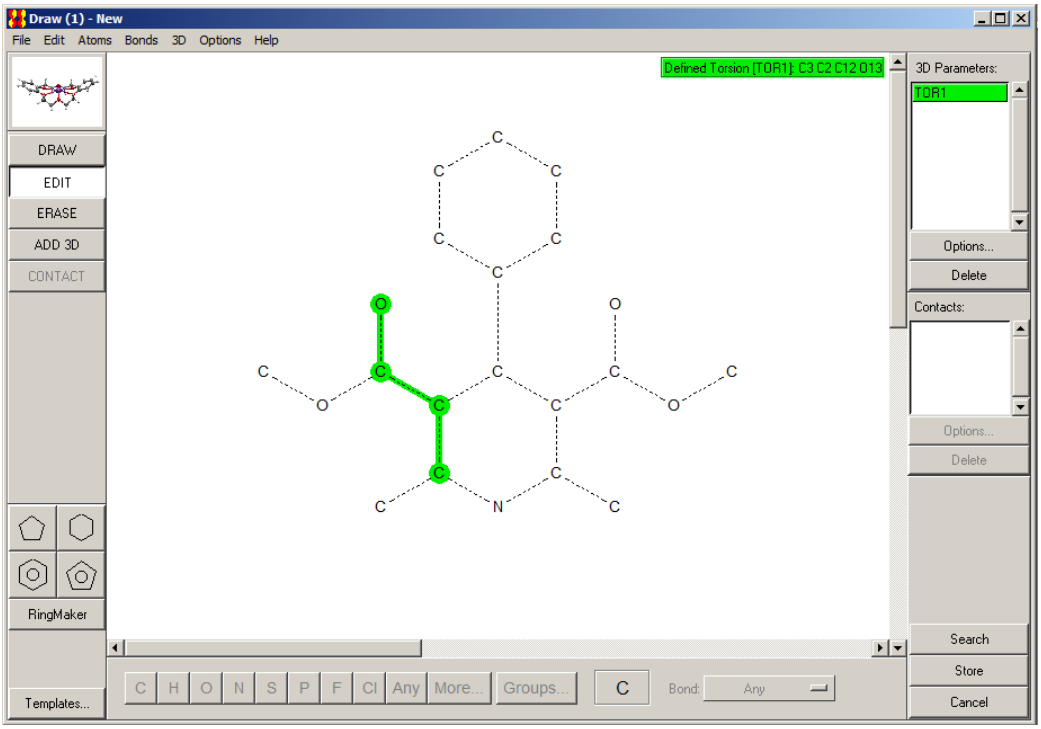

Figure S1. Molecular fragment used in a Conquest search of the CSD

CSD Version 5.34 (Nov 2012), best representative set according to *R*-factor (379018 entries)

Search constraints: 3-D coordinates determined, only organics

Result: 155 hits

Restrict to Me and Et groups on the ester, and methyl groups either side of N: 83 hits

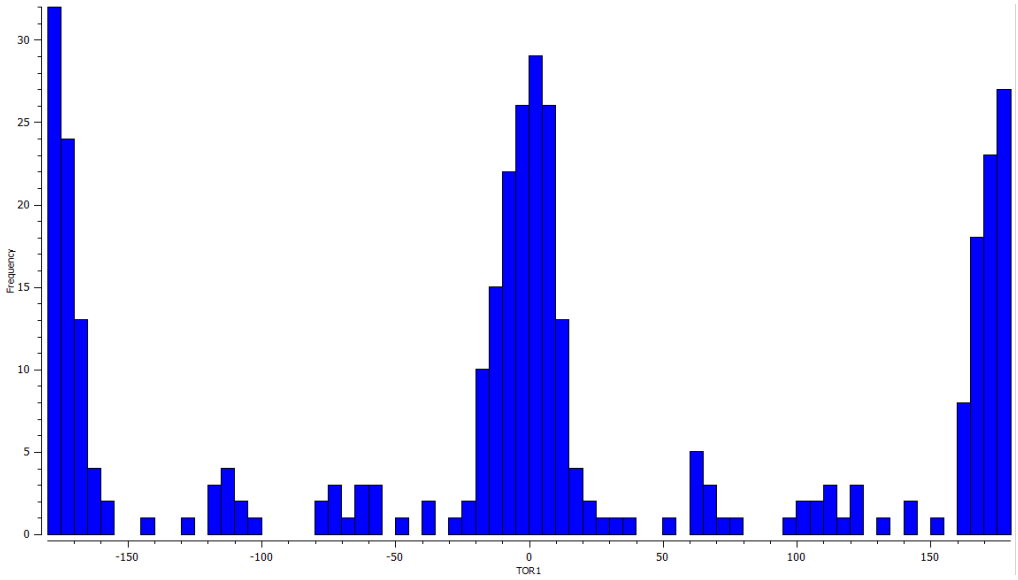

Figure S2. Distribution of torsion angle τ_1 from the retrieved CSD set (83 hits).

S2. Simulated and measured PXRD patterns

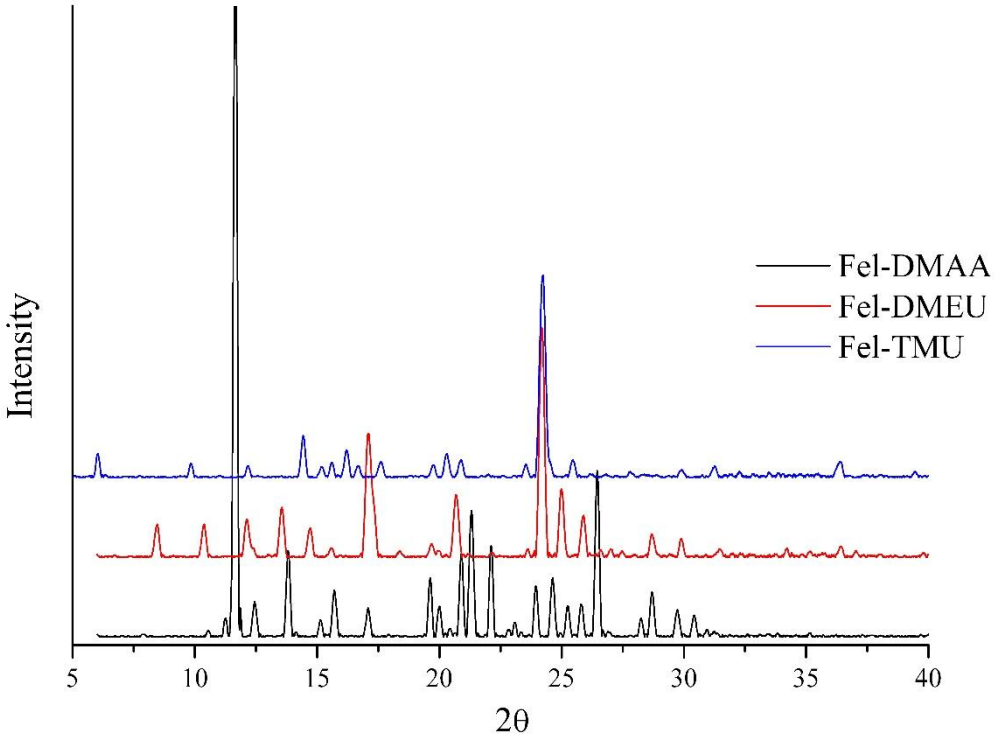

Figure S3. Measured PXRD patterns of the felodipine solvates

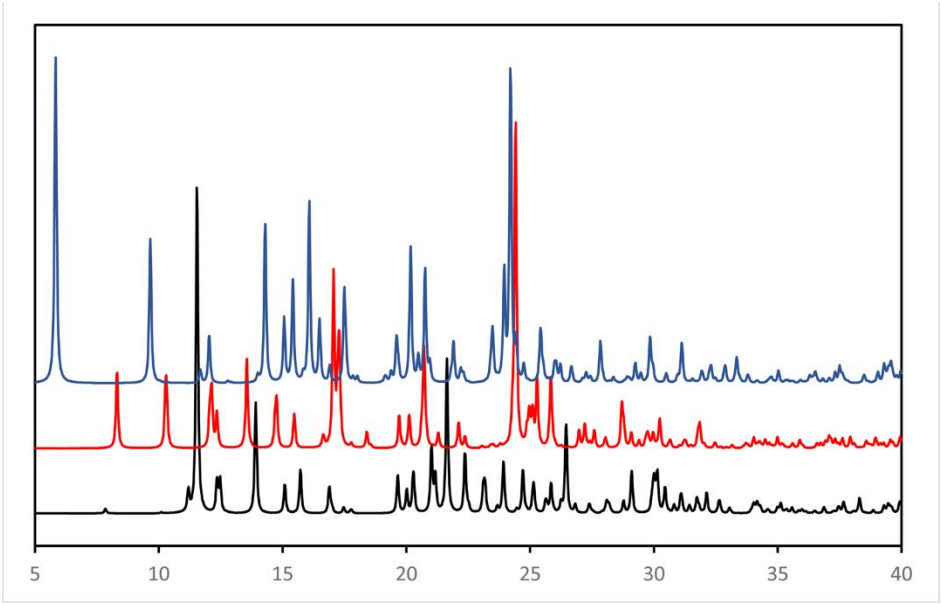

Figure S4. Simulated PXRD patterns of the felodipine solvates

The measured PXRD pattern of [Fel+TMU] appears to be subject to preferred orientation, enhancing intensity of the peak at 2θ ≈24°. The peak positions are otherwise well matched.

S3 HSM pictures for [Fel+TMU] and [Fel+DMEU]

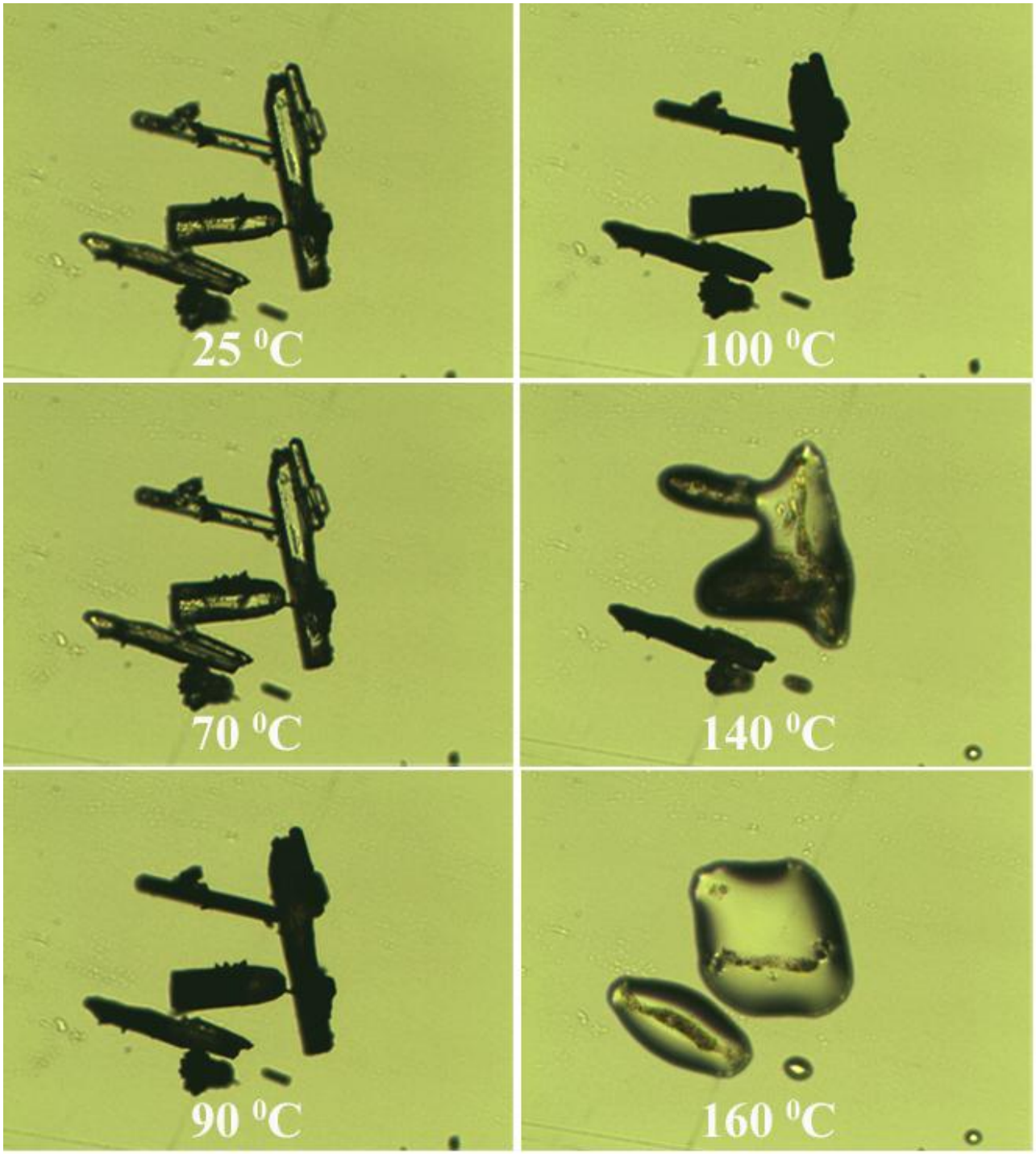

Figure S5. Photomicrographs of **[Fel+TMU]** showing thermal decomposition of the solvate and the subsequent dissolution process.

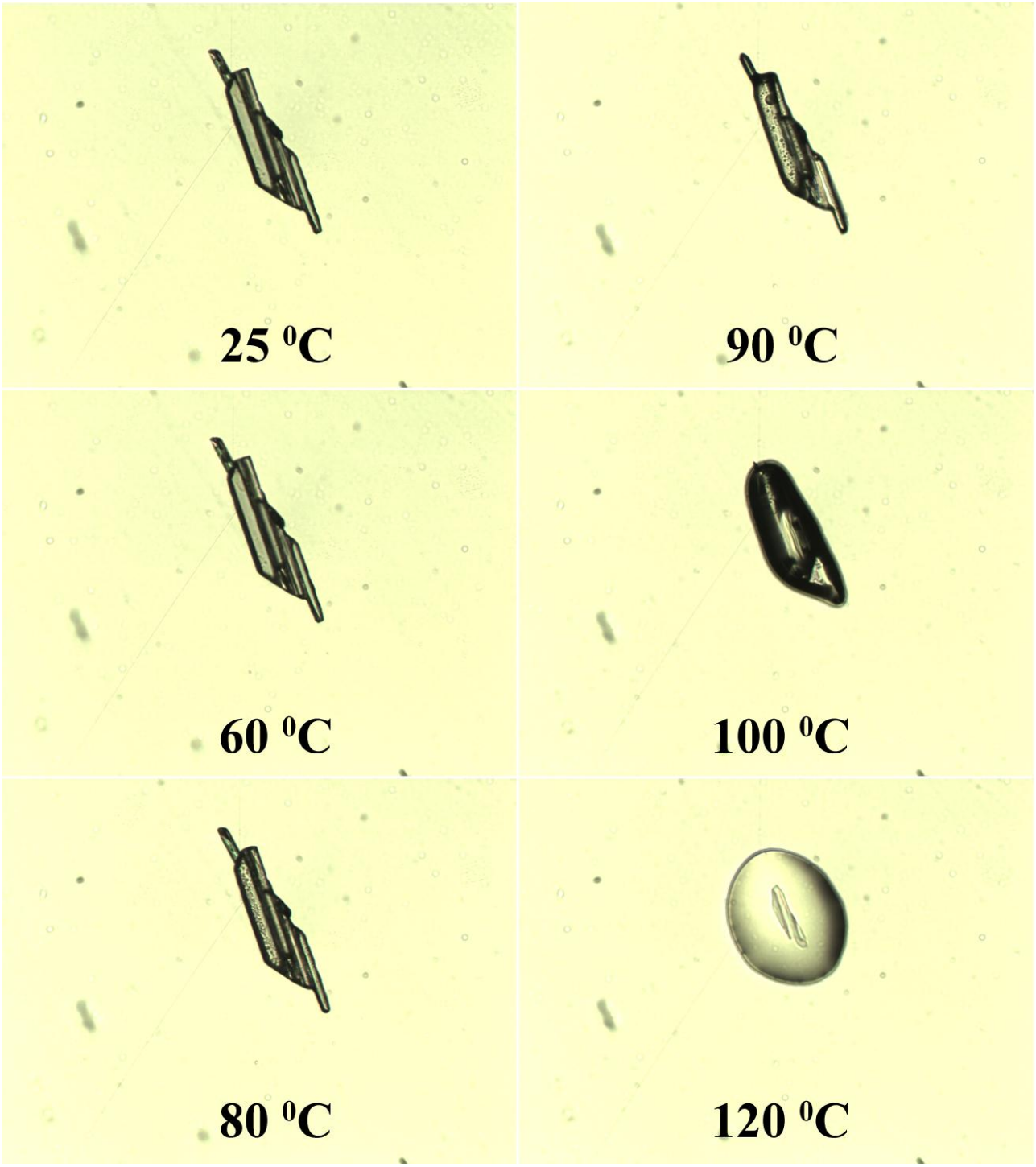

Figure S6. Photomicrographs of **[Fel+DMEU]** showing thermal decomposition of the solvate and the subsequent dissolution process.

S4 TGA traces of the felodipine solvates

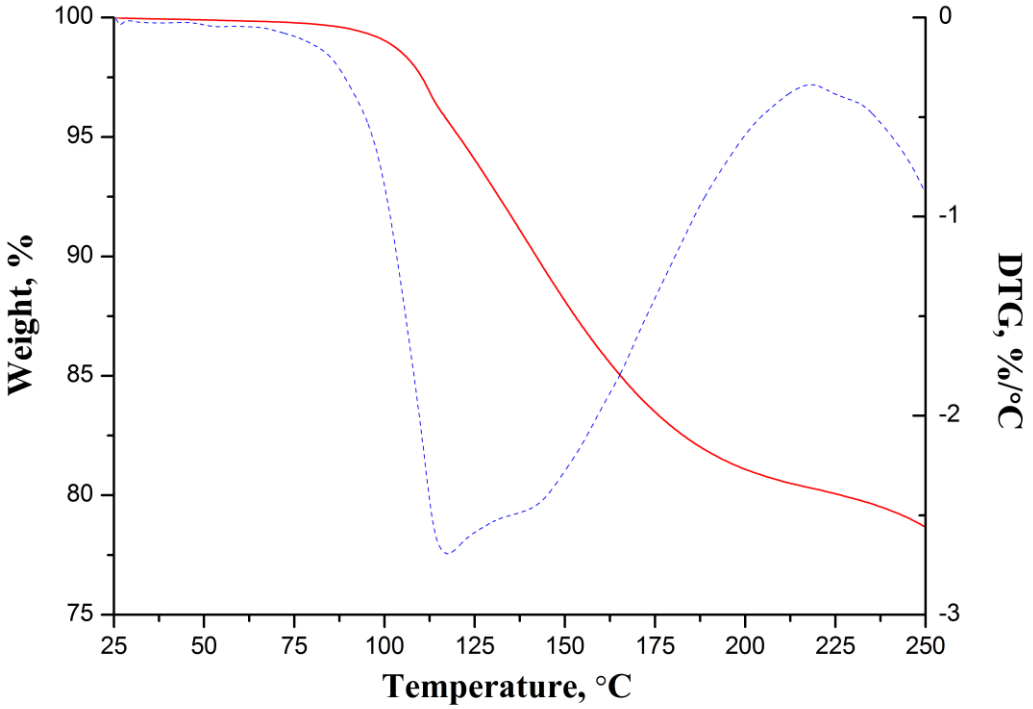

Figure S7. TGA trace of **[Fel+DMAA]** solvate

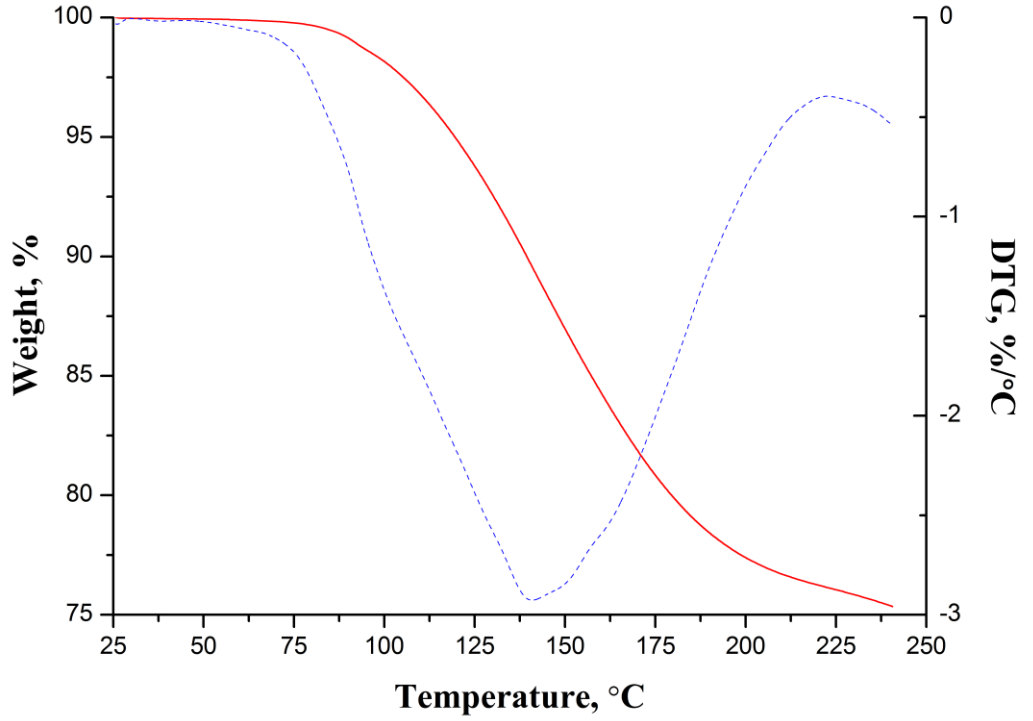

Figure S8. TGA trace of **[Fel+TMU]** solvate

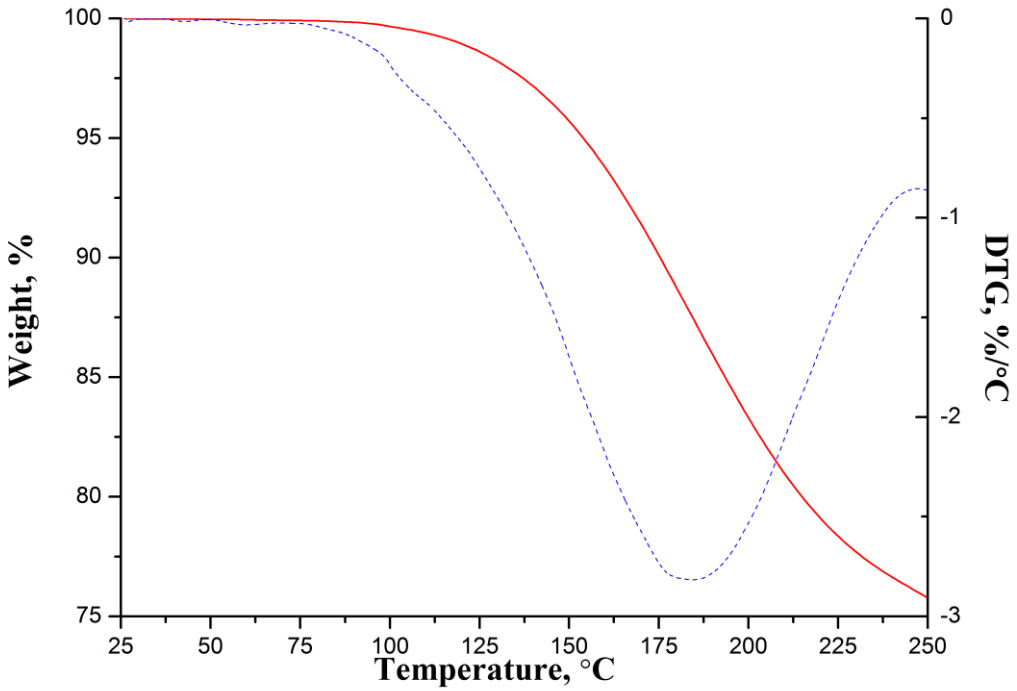

Figure S9. TGA trace of **[Fel+DMEU]** solvate

Table S1. The weight, g (mg), solution concentrations, m (mol kg^{-1}), and solution enthalpies, ΔH^0_{sol} ($kJ \cdot mol^{-1}$), of felodipine and its solvates in respective solvents at 298 K.

Dimethylacetamide (DMAA)					
Felodipine			[Fel+DMAA]		
mg	$m \cdot 10^{-3}$	ΔH^0_{sol}	mg	$m \cdot 10^{-3}$	ΔH^0_{sol}
12.5	0.72	11.5	28.7	1.38	29.2
48.9	2.83	10.6	51.3	2.46	29.8
17.1	0.98	11.0	84.2	4.04	31.0
34.5	1.99	10.7	24.9	1.17	29.2
			54.5	2.56	29.7
	$\Delta H^{m,298}_{sol}$	=10.9±0.2		$\Delta H^{m,298}_{sol}$	=29.8±0.3
Dimethylethyleneurea (DMEU)					
Felodipine			[Fel+DMEU]		
mg	$m \cdot 10^{-3}$	ΔH^0_{sol}	mg	$m \cdot 10^{-3}$	ΔH^0_{sol}
13.8	0.72	7.9	26.9	1.05	25.9
31.8	1.65	7.4	64.9	2.54	25.1
61.2	3.17	7.2	36.3	1.52	25.8
18.4	0.98	6.9	76.0	3.19	25.7
43.4	2.33	7.1	84.8	3.41	27.0
	$\Delta H^{m,298}_{sol}$	=7.3±0.2		$\Delta H^{m,298}_{sol}$	=25.9±0.3
Tetramethylurea (TMU)					
Felodipine			[Fel+TMU]		
mg	$m \cdot 10^{-3}$	ΔH^0_{sol}	mg	$m \cdot 10^{-3}$	ΔH^0_{sol}
11.8	0.67	3.9	15.0	0.67	22.1
27.7	1.59	4.0	46.3	2.06	23.6
47.4	2.72	4.3	66.0	2.93	23.4
22.9	1.33	4.1	19.6	0.88	23.8
45.9	2.65	4.3	39.3	1.77	22.7
			64.7	2.91	22.4
	$\Delta H^{m,298}_{sol}$	=4.1±0.1		$\Delta H^{m,298}_{sol}$	=23.0±0.3