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Supporting information for article:

Using structural mimics for accessing and exploring structural landscapes of poorly soluble molecular solids

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Content

1.1 PXRD data

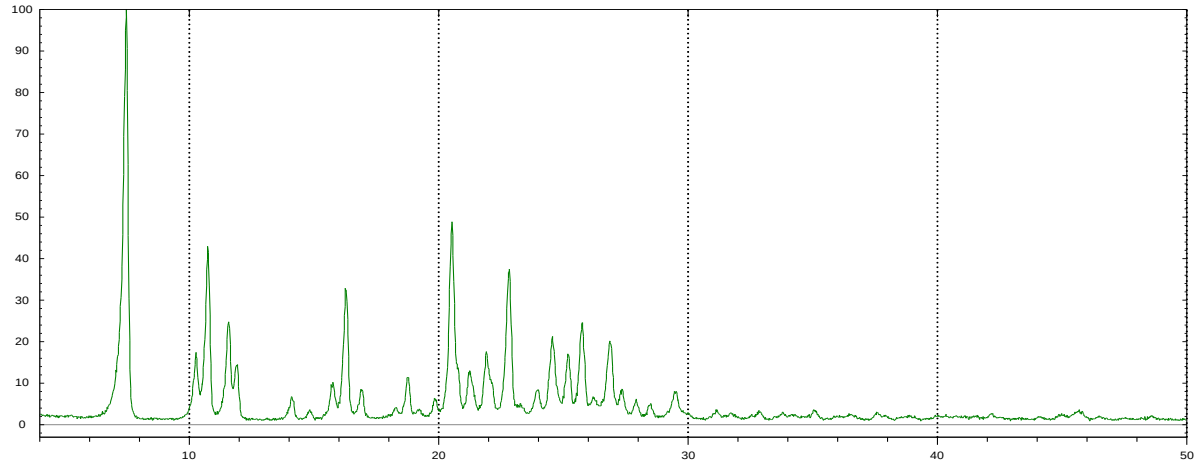

Figure S1 Powder pattern of $(EM)_2$:dodecanedioic co-crystal obtained through solvothermal method.

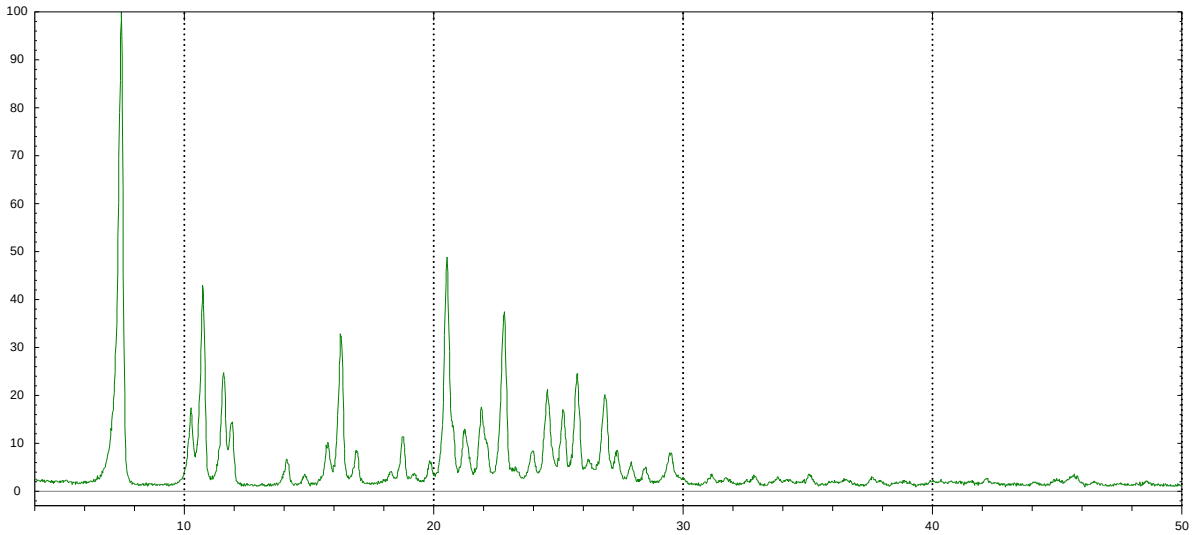

Figure S2 Stimulated powder pattern of $(EM)_2$:dodecanedioic co-crystal analysis

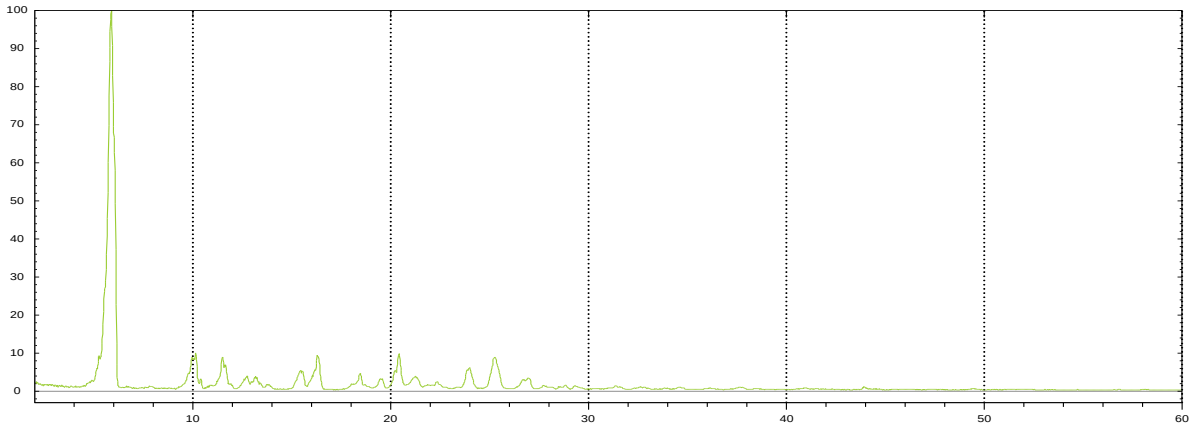

Figure S3 Powder patter of $(EM)_2$:suberic acid co-crystal obtained through solvothermal method

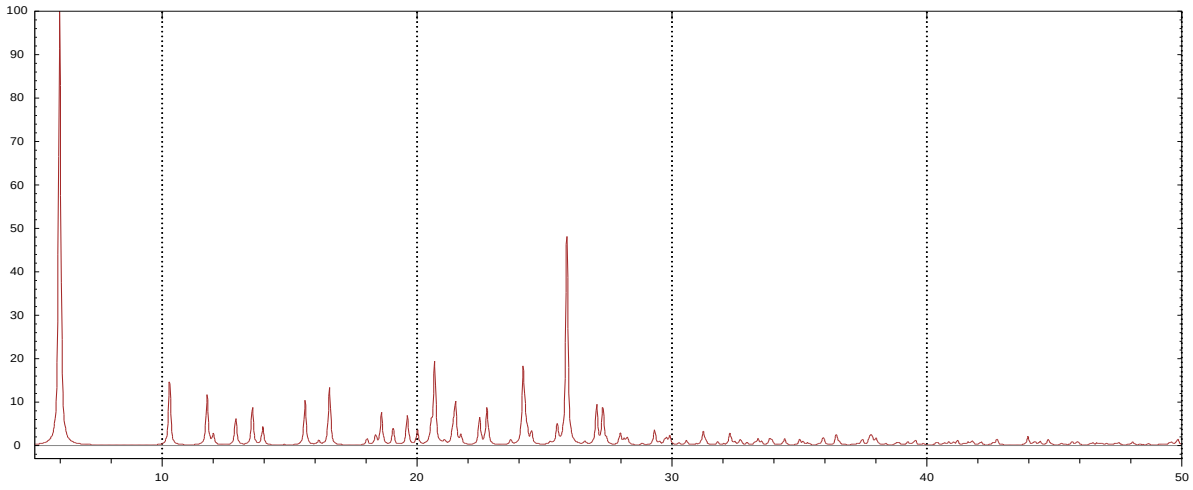

Figure S4 Stimulated powder pattern of $(EM)_2$:suberic acid co-crystal

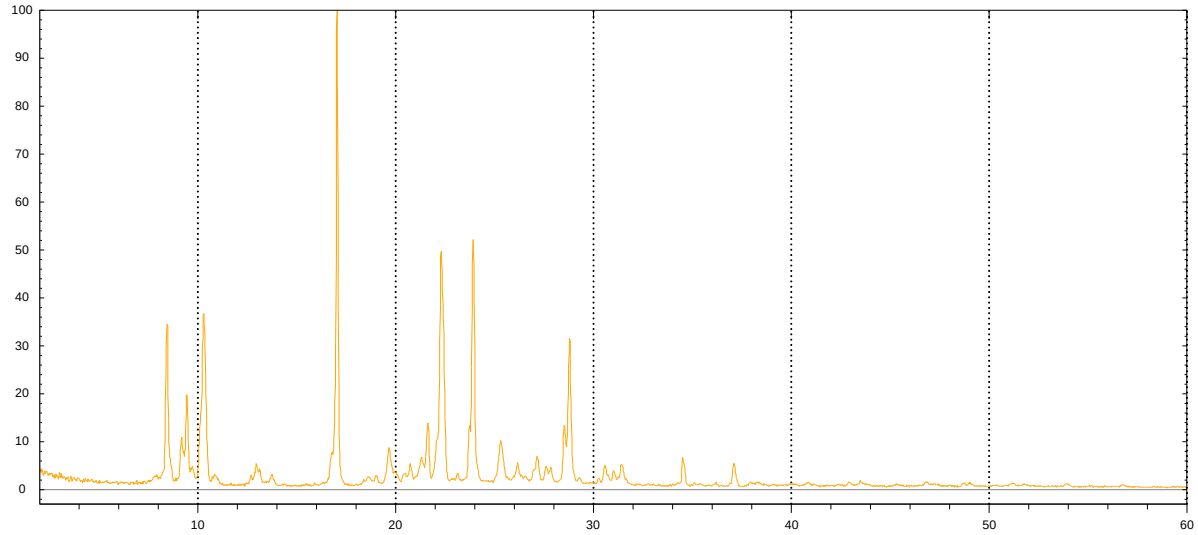

Figure S5 Powder pattern of $(EM)_2$:succinic co-crystal obtained through solvothermal method

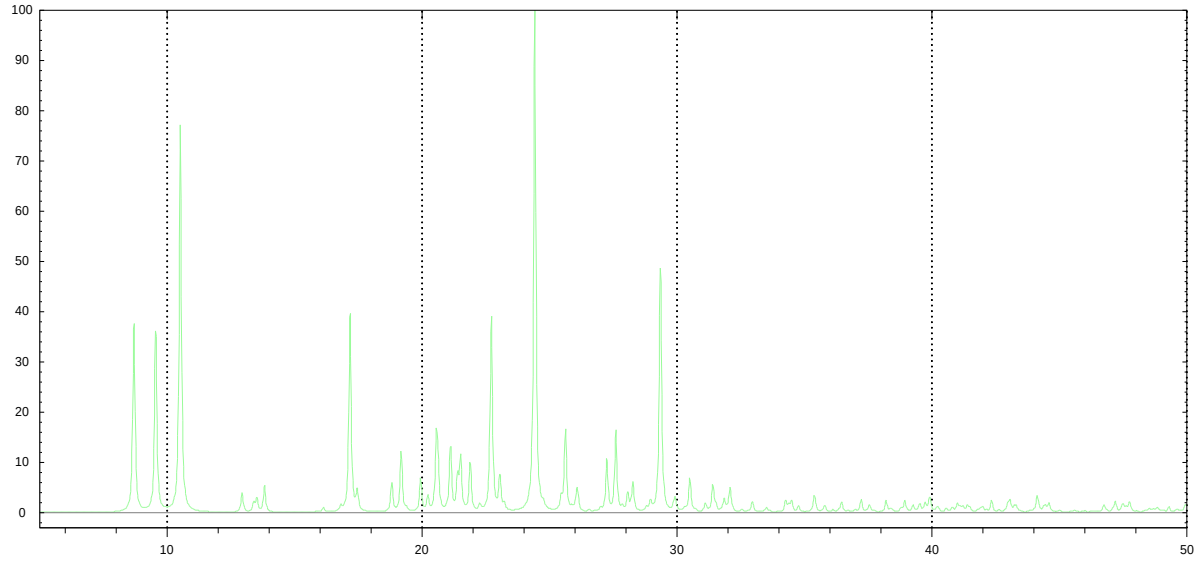

Figure S6 Stimulated powder pattern of $(EM)_2$:succinic co-crystal

1.2 Crystallographic data

Table S1 Crystallographic data of the co-crystals

Code	**EMH^+:Cl^-**	**$(EMH^+)_2$:ADP^- :ADP.MeOH**	**(EM_2):Succinic acid**	**(EM_2):Suberic acid**	**(EM_2):Dodecanedioicacid**
Formula moiety	$C_{18}H_{16}N_3O_2$, Cl	$(C_{18}H_{16}N_3O_2)_2$, $C_6H_8O_4$, $C_6H_{10}O_4$, CH_4O	$C_{18}H_{15}N_3O_2$, $0.5(C_4H_6O_4)$	$C_{18}H_{15}N_3O_2$, $0.5(C_8H_{14}O_4)$	$C_{18}H_{15}N_3O_2$, $0.5(C_{12}H_{22}O_4)$
Empirical formula	$C_{18}H_{16}ClN_3O_2$	$C_{49}H_{54}N_6O_{13}$	$C_{20}H_{18}N_3O_4$	$C_{22}H_{22}N_3O_4$	$C_{24}H_{26}N_3O_4$
Molecular weight	341.79	934.98	364.37	392.42	420.48

Color, Habit	Colorless, Blocks	Colorless, Blocks	Colorless, Blocks	Colorless, Blocks	Colorless, Blocks
Crystal system	Orthorhombic	Triclinic	Monoclinic	Triclinic	Monoclinic
Space group, *Z*	*Pbca*, 8	$P\bar{1}$, 2	*P*2(1)/*c*, 4	$P\bar{1}$, 2	*P*2(1)/*c*, 4
a, Å	9.507(2)	9.304(4)	10.145(4)	7.889(4)	7.5496(16)
b, Å	7.9958(17)	15.756(8)	18.472(7)	9.157(4)	16.434(4)
c, Å	43.262(9)	15.829(7)	9.421(3)	14.832(7)	17.094(4)
α, º	90	94.54(2)	90	86.153(19)	90
β, º	90	93.95(2)	91.423(19)	83.38(2)	93.547(12)
γ, º	90	104.56(2)	90	69.517(18)	90
Volume, Å^3	3288.6(12)	2229.4(18)	1764.9(11)	996.6(8)	2116.8(8)
Density, g/cm^3	1.381	1.393	1.371	1.308	1.319
T, ºK	130(2)	130(2)	130(2)	130(2)	130(2)
Crystal size, min x mid x max	0.152 x 0.301 x 0.487	0.172 x 0.298 x 0.440	0.157 x 0.242 x 0.274	0.122 x 0.196 x 0.278	0.084 x 0.168 x 0.262
X-ray wavelength, Å	0.71073	0.71073	0.71073	0.71073	0.71073
μ, mm^{-1}	0.248	0.102	0.097	0.091	0.091
Trans min / max	0.89 / 0.96	0.96 / 0.98	0.97 / 0.98	0.97 / 0.99	0.98 / 0.99
θ_{min}, º	0.94	1.30	2.01	1.38	1.72
θ_{max}, º	26.79	26.60	26.05	25.60	25.20
Reflections					
collected	44653	35562	28660	15029	36479
independent	3440	8806	3419	3506	3787
observed	2741	4654	2215	2377	2480
R_{int}	0.0531	0.1147	0.0942	0.0610	0.0966
Threshold expression	> 2σ(*I*)	> 2σ(*I*)	> 2σ(*I*)	> 2σ(*I*)	> 2σ(*I*)
No. parameters	227	646	255	272	291

No. restraints	0	5	1	1	1
R_1 (observed)	0.0384	0.0645	0.0474	0.0490	0.0571
wR_2 (all)	0.1060	0.1981	0.1311	0.1510	0.1577
Goodness of fit (all)	1.123	1.022	1.029	1.069	1.034
ρ_{max}, ρ_{min}, e Å^{-3}	0.286, -0.395	0.478, -0.380	0.261, -0.227	0.327, -0.332	0.357, -0.233
Completeness to 2θ limit	0.982	0.943	0.979	0.936	0.994

1.3 Crystallography Experimental Details

All datasets were collected on a Bruker Kappa APEX II system using MoKα radiation. Data were collected using APEX2 software.[i] Initial cell constants were found by small widely separated "matrix" runs. Data collection strategies were determined using COSMO.[ii] Scan speed and scan widths were chosen based on scattering power and peak rocking curves. All datasets were collected at -143 °C using an Oxford Cryostream low-temperature device.

Unit cell constants and orientation matrix were improved by least-squares refinement of reflections thresholded from the entire dataset. Integration was performed with SAINT,[iii] using this improved unit cell as a starting point. Precise unit cell constants were calculated in SAINT from the final merged dataset. Lorenz and polarization corrections were applied. Multi-scan absorption corrections were performed with SADABS.[iv]

Data were reduced with SHELXTL.[v] The structures were solved in all cases by direct methods without incident. Except as noted, hydrogen atoms were located in idealized positions and were treated with a riding model. All non-hydrogen atoms were assigned anisotropic thermal parameters. Refinements continued to convergence, using the recommended weighting schemes.

EMH^+:Cl^- – Coordinates of the quinazoline proton H1 and an amine proton H11 were allowed to refine.

$(EMH^+)_2$:ADP^-:ADP.MeOH – Coordinates of the quinazoline protons H1 and H24; amine protons H11 and H34; carboxylic acid protons H57 and H62; and methanol proton H68 were allowed to refine.

(EM_2):Succinic acid – Coordinates of an amine proton H11 and the carboxylic acid proton H25 were allowed to refine.

(EM_2):Suberic acid – Coordinates of an amine proton H11 and the carboxylic acid proton H24 were allowed to refine.

(EM_2):Dodecanedioic acid – Coordinates of an amine proton H11 and the carboxylic acid proton H25 were allowed to refine.

1.4 References

[i] APEX2 v2013.10-0, © 2013, Bruker Analytical X-ray Systems, Madison, WI.

[ii] COSMO v1.61, © 1999 - 2009, Bruker Analytical X-ray Systems, Madison, WI.

[iii] SAINT v8.34a, © 1997 - 2013, Bruker Analytical X-ray Systems, Madison, WI.

[iv] SADABS v2012/1, © 2012, Bruker Analytical X-ray Systems, Madison, WI.

[v] SHELXTL v2008/4, © 2008, Bruker Analytical X-ray Systems, Madison, WI.