Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

to

Explaining crystallization preferences of two polyphenolic diastereoisomers by crystal structure prediction.

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1. Known crystal structures of EPI and CAT

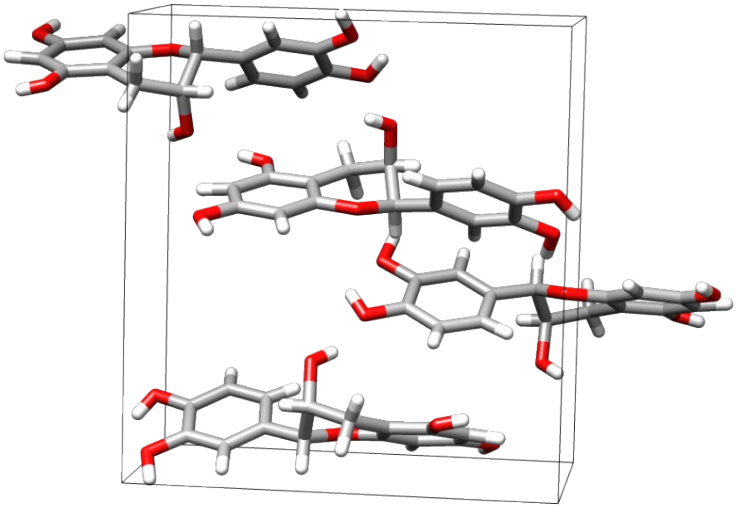

Figure S1. Experimental structure of EPI

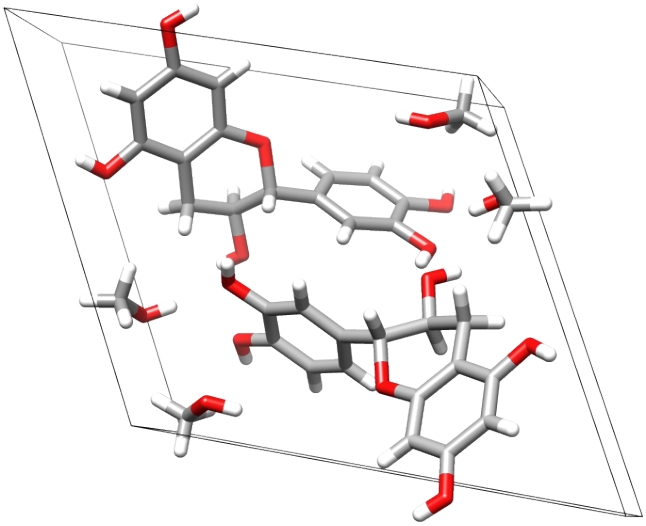

Figure S2. Experimental structure of CAT methanol solvate

2. Crystallization screening

The propensity of CAT to form different solvates were exploited via three different methods, yielding in most cases the same results: classic wet crystallization, mechanochemical grinding with 0.5:1, 1:1 and 2:1 stoichiometric ratios of solvents, and vapour diffusion of a solvent. All tested solvents were polar (at least partially), and included water, methanol, ethanol, isopropanol, n-butanol and acetone. In all cases the obtained phases after crystallization were examined with ^{13}C solid-state NMR. New solvents were obtained for methanol, ethanol, acetone and isopropanol. Their respective structures are currently under further studies.[1]

3. Comparison of 10000 and 2000-structure data sets for unsolvated EPI experimental structure and for all best EPI structures.

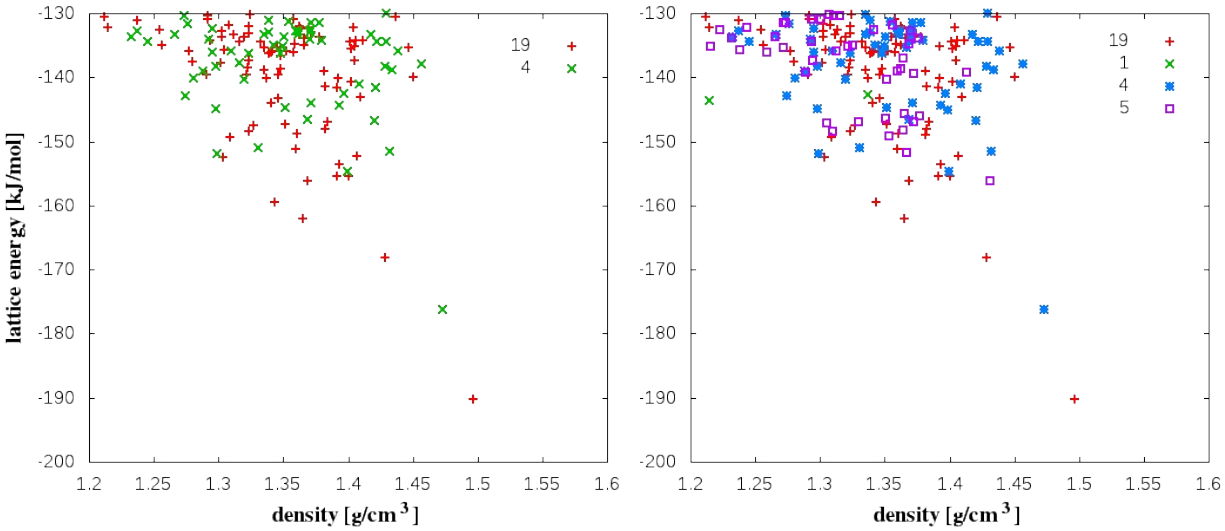

Figure S3. Comparison for 2000- (left) and 10000-structures (right) data sets used in the CSP search for EPI experimental structure. In 2000-structures set only two space groups were tested, in 10000-structures set – four space group were tested. Clearly all the most stable structures were found in the smaller set, with energies of the C2 and P1 structures found to be well above the global minimum.

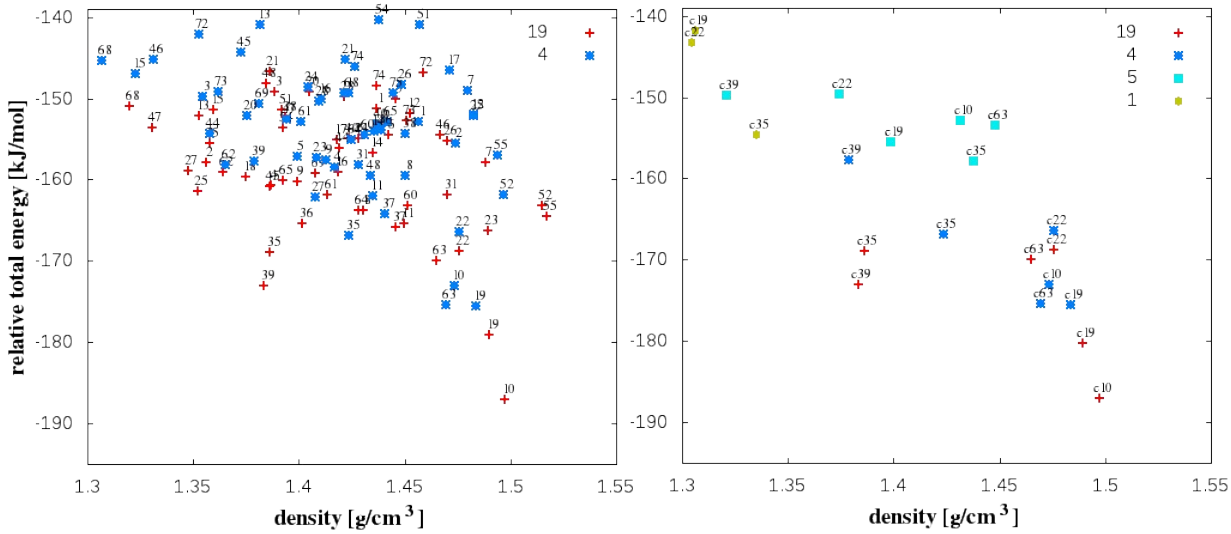

Figure S4. Comparison for 2000- (left) and 10000-structures (right) data sets used in the CSP search for EPI experimental structure. In 2000-structures set only two space groups were tested, in 10000-structures set – four space group were tested. The most stable structures were found in the smaller set, with energies of the C2 and P1 structures found to be well above the global minimum.

4. Procedure used for the comparison of the solvated and unsolvated structures of EPI and CAT

For the comparison of the unsolvated and differently solvated structures following equation and data were used:

$$E_{comp}^{\ tot} = E_{solv}^{\ tot} - N * (E_{methanol}^{\ intra} + E_{methanol}^{\ inter} - 3/2 * RT)$$

$E_{methanol}^{intra} = -303921\ kJ/mol$

$E_{methanol}^{inter} = -44.439\ kJ/mol$

$T = 300\ K$

5. Numerical data for CAT

Naming convention for the conformers

A following convention was used for the names of conformers: a letter 'e' or 'k' stands for epicatechin and catechin, respectively, followed by a number of conformer obtained after sorting the conformers from the lowest energy to the highest at the stage of the first MMFF optimization, and finally, after an underscore a space group in which certain structure was generated is given.

Table S1. Final numerical data obtained for the best structures of CAT in $P2_1$ and $P2_12_12_1$ space groups, together with relative energies obtained from the gas phase calculations (Eintra).

		unsolvated			2:1 solvates			1:1 solvates		
name	Eintra	density	Etotal	Einter	density	Etotal	Einter	density	Etotal	Einter
k10_19	5.91	1.4231	36.95	46.75	1.2763	18.99	35.80	1.3736	25.82	64.14
k10_4	5.91	1.3285	37.08	46.88	1.262	27.06	43.88	1.2805	16.94	55.27
k11_19	19.42	1.468	42.64	38.93	1.3417	24.42	27.73	1.3778	33.05	57.87
k11_4	19.42	1.3933	43.35	39.64	1.294	29.41	32.72	1.3033	32.05	56.87
k12_19	19.95	1.3895	39.26	35.01	1.3287	27.03	29.81	1.3564	24.54	48.82
k12_4	19.95	1.3964	40.17	35.92	1.361	24.90	27.67	1.3378	37.39	61.67
k13_19	21.07	1.4822	32.99	27.62	1.316	25.71	27.36	1.4504	36.22	59.38
k13_4	21.07	1.4037	48.37	43.00	1.2702	29.71	31.36	1.3631	31.65	54.81
k14_19	20.68	1.4712	31.77	26.79	1.3889	20.26	22.31	1.3885	28.83	52.39
k14_4	20.68	1.3603	35.71	30.74	1.3418	32.06	34.10	1.3553	25.86	49.42
k15_19	11.45	1.3439	23.30	27.55	1.3093	11.95	23.23	1.3691	7.32	40.10
k15_4	11.45	1.4623	21.60	25.85	1.365	6.86	18.13	1.3972	5.15	37.93
k16_19	13.03	1.3437	16.37	19.05	1.3165	2.99	12.69	1.3749	15.35	46.56
k16_4	13.03	1.4287	30.86	33.54	1.2412	13.85	23.55	1.3994	19.16	50.37
k17_19	13.40	1.3551	23.82	26.14	1.2632	19.58	28.90	1.3595	22.40	53.24
k17_4	13.40	1.3897	21.02	23.33	1.3016	20.30	29.63	1.3035	20.33	51.16
k18_19	0.00	1.5127	9.12	24.83	1.3545	12.26	34.98	1.35	7.78	52.01
k18_4	0.00	1.5004	13.00	28.71	1.326	7.18	29.90	1.435	4.30	48.54
k19_19	2.28	1.4222	22.37	35.80	1.3688	4.61	25.06	1.429	11.03	52.98
k19_4	2.28	1.4716	26.93	40.35	1.3127	10.51	30.96	1.4393	12.48	54.43
k1_19	2.67	1.5207	33.92	46.96	1.3545	22.85	42.90	1.3967	25.54	67.11
k1_4	2.67	1.4037	32.18	45.22	1.3671	15.70	35.75	1.4343	26.78	68.34
k20_19	15.57	1.5073	22.87	23.01	1.3215	21.44	28.60	1.3282	18.75	47.42
k20_4	15.56	1.3911	21.95	22.10	1.3023	15.90	23.06	1.319	24.82	53.49
k21_19	2.46	1.3637	13.94	27.19	1.3793	2.85	23.12	1.3752	12.24	54.02
k21_4	2.46	1.4502	30.94	44.19	1.3871	9.87	30.14	1.3758	5.99	47.77

k22_19	2.32	1.3579	24.90	38.28	1.2736	16.73	37.13	1.4473	21.76	63.67
k22_4	2.32	1.4264	20.33	33.72	1.31	15.78	36.18	1.3567	8.51	50.42
k23_19	17.47	1.4661	26.32	24.56	1.3383	12.17	17.42	1.3205	21.44	48.21
k23_4	17.47	1.3883	34.58	32.82	1.2904	24.46	29.72	1.3425	25.51	52.27
k24_19	3.52	1.4711	27.55	39.74	1.3546	19.84	39.05	1.3525	14.66	55.37
k24_4	3.52	1.4218	20.43	32.62	1.3111	17.94	37.15	1.3477	19.78	60.50
k25_19	18.57	1.3902	30.81	27.94	1.3352	18.96	23.11	1.327	30.43	56.09
k25_4	18.58	1.4522	39.27	36.40	1.3132	23.68	27.83	1.3297	23.88	49.54
k26_19	18.31	1.3281	45.35	42.75	1.32	21.63	26.05	1.3221	26.17	52.09
k26_4	18.30	1.4394	41.84	39.25	1.3306	23.10	27.52	1.3932	34.78	60.71
k27_19	6.56	1.3918	29.23	38.38	1.3528	14.51	30.68	1.2903	21.23	58.91
k27_4	6.56	1.3991	40.06	49.21	1.302	24.63	40.80	1.341	22.02	59.69
k28_19	6.40	1.4504	20.29	29.60	1.3292	14.05	30.38	1.3788	16.90	54.74
k28_4	6.40	1.4789	25.01	34.32	1.3425	17.01	33.34	1.3677	14.17	52.00
k29_19	6.78	1.3936	38.16	47.09	1.2916	12.61	28.56	1.2657	21.04	58.50
k29_4	6.78	1.3281	41.40	50.33	1.3129	17.00	32.94	1.3637	25.80	63.26
k2_19	17.12	1.5023	25.20	23.79	1.28	21.53	27.14	1.4127	26.66	53.78
k2_4	17.12	1.446	36.72	35.32	1.3486	11.55	17.16	1.3817	21.97	49.08
k30_19	21.40	1.3226	47.14	41.44	1.2844	21.03	22.36	1.3579	35.56	58.40
k30_4	21.40	1.4074	48.20	42.51	1.3129	18.99	20.31	1.3403	31.82	54.66
k31_19	17.23	1.3569	46.75	45.22	1.3543	27.09	32.58	1.3779	34.04	61.04
k31_4	17.23	1.384	49.66	48.14	1.254	40.70	46.19	1.3398	32.46	59.46
k32_19	35.89	1.4481	43.75	23.56	1.2272	32.28	19.11	1.4512	33.39	41.73
k32_4	35.89	1.368	53.96	33.78	1.3467	31.35	18.19	1.3945	43.25	51.59
k33_19	21.92	1.3688	46.13	39.91	1.3267	26.79	27.59	1.4489	28.06	50.37
k33_4	21.92	1.4032	54.38	48.17	1.2761	36.46	37.26	1.3808	25.14	47.45
k34_19	35.90	1.5071	46.47	26.28	1.3052	30.79	17.62	1.3905	39.47	47.80
k34_4	35.90	1.4248	51.42	31.23	1.3081	36.67	23.49	1.3766	27.33	35.67
k35_19	6.23	1.4395	33.98	43.46	1.3167	25.73	42.22	1.3846	23.09	61.09
k35_4	6.23	1.4264	36.01	45.49	1.3677	22.00	38.50	1.4028	34.37	72.37
k36_19	23.51	1.3469	42.48	34.68	1.3209	19.40	18.61	1.3148	12.56	33.28
k36_4	23.51	1.5082	45.08	37.28	1.3656	17.84	17.06	1.4052	18.35	39.08
k37_19	2.68	1.5208	34.01	47.04	1.348	22.54	42.59	1.3846	23.09	61.09
k37_4	2.68	1.4033	32.31	45.34	1.3671	15.71	35.76	1.4342	26.65	68.21
k38_19	16.79	1.3453	37.34	36.26	1.3044	22.72	28.66	1.3735	29.27	56.71
k38_4	16.79	1.3897	51.11	50.02	1.3384	14.00	19.94	1.4106	26.88	54.32
k39_19	18.28	1.4856	41.02	38.45	1.2374	25.92	30.36	1.359	27.87	53.82
k39_4	18.28	1.2747	47.70	45.13	1.3056	30.99	35.43	1.3011	37.60	63.55
k3_19	17.34	1.4812	31.32	29.69	1.2522	18.14	23.52	1.4204	17.94	44.84
k3_4	17.34	1.4458	30.20	28.57	1.3704	17.17	22.56	1.4004	16.49	43.39
k40_19	23.75	1.3676	29.39	21.35	1.3273	22.48	21.46	1.3909	25.16	45.64
k40_4	23.75	1.4478	46.28	38.24	1.2883	10.85	9.83	1.2125	23.95	44.44
k41_19	18.95	1.3658	34.68	31.44	1.2582	32.43	36.21	1.4236	28.36	53.64
k41_4	18.95	1.4061	56.12	52.88	1.319	34.78	38.55	1.3368	31.85	57.13
k42_19	38.45	1.4745	44.66	21.91	1.2711	21.44	5.71	1.3722	28.71	34.49
k42_4	38.45	1.3883	39.49	16.75	1.3391	29.05	13.32	1.41	14.22	20.01

k43_19	38.26	1.3584	27.10	4.55	1.2752	24.26	8.73	1.407	30.28	36.26
k43_4	38.26	1.2496	50.03	27.48	1.3412	19.27	3.73	1.3857	22.11	28.09
k44_19	18.49	1.4455	47.58	44.80	1.3062	22.89	27.12	1.3041	34.99	60.73
k44_4	18.49	1.3917	48.86	46.08	1.2996	29.03	33.26	1.2845	36.13	61.87
k45_19	5.38	1.4421	23.83	34.16	1.3529	15.00	32.35	1.4195	10.11	48.96
k45_4	5.38	1.4554	14.50	24.83	1.3667	12.50	29.85	1.4185	8.52	47.37
k48_19	10.50	1.4053	31.23	36.44	1.2966	24.55	36.77	1.3514	21.88	55.61
k48_4	10.50	1.4629	40.30	45.50	1.2973	25.71	37.94	1.3476	26.82	60.54
k4_19	3.47	1.427	27.26	39.50	1.3183	14.54	33.79	1.4415	18.26	59.03
k4_4	3.47	1.4836	26.40	38.64	1.3655	20.65	39.91	1.4189	16.55	57.32
k51_19	10.57	1.4239	26.86	32.00	1.341	22.19	34.35	1.4375	23.54	57.21
k51_4	10.57	1.3793	38.27	43.41	1.3696	21.93	34.08	1.3764	21.21	54.87
k54_19	11.95	1.4997	38.31	42.07	1.3159	17.16	27.93	1.3249	26.16	58.44
k54_4	11.95	1.3795	36.49	40.25	1.3696	21.93	34.08	1.3071	24.84	57.13
k56_19	12.45	1.3643	35.73	38.99	1.3202	21.41	31.69	1.3626	23.74	55.52
k56_4	12.45	1.4069	43.94	47.20	1.2953	17.18	27.45	1.397	27.86	59.64
k58_19	31.72	1.374	27.16	20.27	1.3195	13.82	4.82	1.4299	19.66	32.17
k58_4	31.72	1.3377	19.88	13.00	1.3046	8.99	0.00	1.3755	22.07	34.59
k5_19	5.38	1.442	23.88	34.21	1.3529	15.02	32.36	1.4195	10.12	48.98
k5_4	5.38	1.4554	14.53	24.86	1.3666	12.53	29.88	1.4185	8.57	47.42
k60_19	15.28	1.4379	45.38	45.81	1.3243	20.64	31.87	1.3251	30.84	59.79
k60_4	15.28	1.3685	46.09	46.51	1.3273	15.52	22.75	1.3707	32.52	61.48
k61_19	18.34	1.4668	27.97	34.46	1.3254	24.42	25.03	1.4343	18.71	44.61
k61_4	18.34	1.454	23.89	30.39	1.3934	15.31	19.91	1.3963	23.99	49.88
k63_19	14.61	1.4185	41.87	42.97	1.2967	15.32	23.43	1.3646	24.23	53.85
k63_4	14.61	1.4409	36.89	37.98	1.2662	27.67	35.78	1.3285	23.82	53.44
k64_19	19.93	1.4416	35.82	31.60	1.314	8.73	11.52	1.3699	12.05	36.35
k64_4	19.93	1.3707	22.46	18.23	1.3257	9.52	12.31	1.4521	14.96	39.26
k65_19	16.97	1.3996	28.42	27.16	1.3133	22.16	27.91	1.347	25.08	52.35
k65_4	16.97	1.3978	51.66	50.40	1.3451	22.05	27.81	1.3345	34.66	61.92
k66_19	16.92	1.4488	33.91	32.70	1.3039	20.21	26.02	1.3225	26.48	53.80
k66_4	16.91	1.4168	48.29	47.09	1.3132	26.12	31.93	1.3107	34.63	61.95
k67_19	34.21	1.4422	50.52	32.01	1.3814	28.16	16.67	1.3837	34.81	44.83
k67_4	34.21	1.4479	49.23	30.72	1.3101	32.63	21.14	1.3909	45.75	55.77
k68_19	36.22	1.4344	33.98	13.46	1.2567	20.34	6.84	1.29	24.47	32.48
k68_4	36.22	1.4125	20.52	0.00	1.3251	26.03	12.53	1.3771	24.56	32.57
k6_19	6.23	1.4398	33.75	43.23	1.2884	24.49	40.98	1.3849	23.04	61.04
k6_4	6.23	1.4263	36.10	45.58	1.3145	18.42	34.92	1.4028	34.42	72.43
k72_19	22.13	1.3233	47.39	40.97	1.2881	17.31	17.90	1.3226	27.00	49.10
k72_4	22.13	1.4352	54.95	48.53	1.3106	32.44	33.03	1.3156	38.00	60.10
k74_19	24.00	1.3842	25.87	17.58	1.3251	18.34	17.07	1.4153	15.29	35.52
k74_4	24.00	1.4499	14.94	6.65	1.3047	22.99	21.72	1.3847	22.79	43.03
k77_19	34.98	1.38	46.77	27.50	1.303	26.63	14.38	1.3789	33.12	42.37
k77_4	34.98	1.3764	47.03	27.76	1.2942	39.46	27.21	1.3111	37.91	47.16
k78_19	23.75	1.3676	20.27	21.35	1.3535	14.08	13.06	1.3908	25.19	45.68
k78_4	23.75	1.4478	37.17	38.25	1.3008	15.16	14.14	1.3925	28.80	49.29

k79_19	21.40	1.3226	47.17	41.47	1.2825	24.72	26.04	1.3581	35.53	58.36
k79_4	21.40	1.4073	48.18	42.48	1.3129	18.98	20.30	1.3403	31.81	54.65
k7_19	5.76	1.4193	18.25	28.21	1.3375	13.27	30.24	1.4535	11.18	49.66
k7_4	5.76	1.378	23.51	33.46	1.365	7.94	24.91	1.367	0.00	38.48
k80_19	23.51	1.3469	42.47	34.67	1.3209	19.38	18.60	1.3147	12.55	33.28
k80_4	23.51	1.5082	45.12	37.32	1.3655	17.82	17.04	1.4052	18.34	39.06
k82_19	28.62	1.3698	52.92	40.01	1.2285	32.82	26.93	1.3327	33.83	49.44
k82_4	28.62	1.4322	43.79	30.88	1.2803	23.77	17.87	1.3562	30.91	46.53
k83_19	28.69	1.4267	48.45	35.46	1.2284	15.99	10.02	1.3687	21.63	37.17
k83_4	28.70	1.378	49.07	36.09	1.3016	18.67	12.69	1.2866	28.22	43.76
k89_19	32.94	1.3717	52.36	35.12	1.3123	29.29	19.07	1.3557	31.69	42.98
k89_4	32.94	1.4322	56.04	38.80	1.28	36.30	26.08	1.3237	41.81	53.10
k8_19	6.26	1.4624	29.70	39.15	1.351	19.79	36.25	1.4284	17.48	55.45
k8_4	6.26	1.4587	30.61	40.06	1.227	25.43	41.89	1.3946	24.58	62.56
k90_19	33.23	1.4297	44.91	27.39	1.3409	25.70	15.20	1.3515	27.63	38.64
k90_4	33.22	1.3853	44.36	26.84	1.2898	27.84	17.34	1.2965	22.95	33.96
k9_19	6.05	1.4496	40.23	49.89	1.3086	23.10	39.77	1.4045	23.50	61.68
k9_4	6.05	1.3172	40.51	50.16	1.3821	24.63	41.30	1.3363	20.98	59.16
expr	33.14				1.3581	13.52	8.39	1.3418	20.21	0.00

Table S2. Final numerical data obtained for the best structures of CAT in C2 and P1 space groups

	2:1 solvates			2:1 solvates			1:1 solvates	
name	density	Etotal	name	density	Etotal	name	density	Etotal
k10s_5	1.2825	18.91	k10s_1	1.2844	15.60	k10s_1_1	1.2778	20.39
k14s_5	1.3111	28.86	k14s_1	1.288	28.62	k10s_1_5	1.2988	24.46
k15s_5	1.3015	17.98	k15s_1	1.2568	20.86	k15s_1_1	1.2949	41.56
k16s_5	1.2275	21.28	k16s_1	1.2391	23.18	k15s_1_5	1.392	21.57
k17s_5	1.2296	21.85	k17s_1	1.215	29.10	k16s_1_1	1.2819	44.71
k18s_5	1.301	14.41	k18s_1	1.2622	19.23	k16s_1_5	1.3617	23.01
k19s_5	1.3371	19.83	k19s_1	1.2861	30.91	k18s_1_1	1.3084	19.99
k1s_5	1.338	22.05	k1s_1	1.3051	24.18	k18s_1_5	1.3289	22.01
k20s_5	1.33	23.45	k20s_1	1.2938	22.66	k19s_1_1	1.3426	28.60
k21s_5	1.3207	17.83	k21s_1	1.3356	17.66	k19s_1_5	1.3179	17.74
k22s_5	1.2978	22.29	k22s_1	1.3468	17.98	k20s_1_1	1.3755	30.33
k23s_5	1.2506	24.49	k23s_1	1.3001	34.85	k20s_1_5	1.3234	19.62
k24s_5	1.2967	17.28	k24s_1	1.338	21.52	k21s_1_1	1.3278	38.63
k25s_5	1.1992	31.15	k25s_1	1.2866	34.27	k21s_1_5	1.4249	18.78
k26s_5	1.3011	31.34	k26s_1	1.2819	39.83	k22s_1_1	1.2984	25.00
k27s_5	1.2826	23.10	k27s_1	1.3071	19.75	k22s_1_5	1.3586	18.70
k28s_5	1.2599	23.00	k28s_1	1.3239	25.35	k24s_1_1	1.3077	33.13
k29s_5	1.2969	30.56	k29s_1	1.2905	25.82	k24s_1_5	1.3451	15.08
k2s_5	1.306	19.12	k2s_1	1.2944	22.35	k36s_1_1	1.3364	41.08
k30s_5	1.3378	34.22	k30s_1	1.3262	39.21	k36s_1_5	1.3458	36.25
k35s_5	1.2918	31.58	k35s_1	1.3498	25.02	k3s_1_1	1.2967	47.15
k36s_5	1.279	31.92	k36s_1	1.314	31.14	k3s_1_5	1.3809	24.11

k37s_5	1.3706	26.32	k37s_1	1.3048	24.31	k42s_1_1	1.3211	43.33
k38s_5	1.2557	32.18	k38s_1	1.318	22.49	k42s_1_5	1.3172	35.24
k3s_5	1.371	23.74	k3s_1	1.2738	38.61	k45s_1_1	1.3245	33.70
k40s_5	1.2968	24.14	k40s_1	1.2532	32.21	k45s_1_5	1.3747	19.42
k42s_5	1.2958	20.22	k42s_1	1.3087	38.24	k4s_1_1	1.3228	37.68
k43s_5	1.2343	30.84	k43s_1	1.2164	35.92	k4s_1_5	1.3952	25.31
k45s_5	1.3316	18.38	k45s_1	1.2949	37.85	k58s_1_1	1.3259	45.21
k4s_5	1.2815	21.31	k4s_1	1.2589	24.63	k58s_1_5	1.3699	28.29
k51s_5	1.3326	25.03	k51s_1	1.3342	21.26	k5s_1_1	1.3245	33.75
k54s_5	1.2515	23.83	k54s_1	1.2747	27.23	k5s_1_5	1.3747	19.44
k56s_5	1.1725	28.08	k56s_1	1.3454	24.62	k60s_1_1	1.2597	42.80
k58s_5	1.2485	18.13	k58s_1	1.2914	32.18	k60s_1_5	1.2908	39.15
k5s_5	1.2984	22.44	k5s_1	1.2948	37.87	k64s_1_1	1.3306	42.89
k60s_5	1.2805	26.90	k60s_1	1.2559	11.57	k64s_1_5	1.3407	32.34
k61s_5	1.3401	25.62	k61s_1	1.2828	27.40	k74s_1_1	1.2802	38.99
k63s_5	1.2694	31.85	k63s_1	1.3062	27.73	k74s_1_5	1.3589	31.57
k64s_5	1.3914	19.73	k64s_1	1.283	28.68	k7s_1_1	1.3374	28.86
k65s_5	1.2811	28.91	k65s_1	1.3318	29.49	k7s_1_5	1.3976	10.13
k66s_5	1.1966	34.87	k66s_1	1.2502	36.66	k80s_1_1	1.3364	41.05
k68s_5	1.2373	21.40	k68s_1	1.3293	23.83	k80s_1_5	1.3837	28.17
k6s_5	1.2979	26.96	k6s_1	1.3499	24.93	k8s_1_1	1.3635	26.32
k72s_5	1.2783	32.62	k72s_1	1.3207	39.67	k8s_1_5	1.392	22.16
k74s_5	1.297	29.33	k74s_1	1.3517	22.78			
k78s_5	1.3219	30.89	k78s_1	1.2532	32.22			
k79s_5	1.2931	33.54	k79s_1	1.3261	39.15			
k7s_5	1.3614	6.87	k7s_1	1.281	29.65			
k80s_5	1.2814	22.46	k80s_1	1.3141	31.13			
k83s_5	1.3401	31.54	k83s_1	1.3342	44.70			
k8s_5	1.2791	27.89	k8s_1	1.3038	32.25			

6. Numerical data for EPI

Table S3. Final numerical data obtained for the best structures of EPI in $P2_1$ and $P2_12_12_1$ space groups, together with relative energies obtained from the gas phase calculations (Eintra).

		unsolvated			2:1 solvates			1:1 solvates		
name	Eintra	density	Etotal	Einter	density	Etotal	Einter	density	Etotal	Einter
e1_19	5.10	1.4367	35.99	35.94	1.3373	30.56	29.34	1.2747	32.45	28.84
e10_19	5.05	1.497	0.00	0.00	1.3332	16.40	15.22	1.2917	30.16	26.60
e11_19	4.05	1.4499	22.87	23.87	1.3343	21.42	21.25	1.3352	27.73	25.18
e12_19	4.52	1.4523	37.68	38.21	1.3044	24.75	24.11	1.4192	23.62	20.58
e13_19	7.48	1.3526	38.05	35.62	1.3532	26.92	23.32	1.307	26.84	20.85
e14_19	4.35	1.4348	32.17	32.87	1.2718	23.43	22.96	1.3814	26.19	23.33
e15_19	6.26	1.3593	36.92	35.71	1.3539	29.76	27.37	1.4245	23.56	18.78
e16_19	5.12	1.4187	28.08	28.01	1.3774	26.30	25.06	1.3673	28.87	25.25
e17_19	9.56	1.4177	35.39	30.88	1.3276	22.46	16.79	1.4072	30.23	22.16

e18_19	8.68	1.375	29.05	25.42	1.3302	18.69	13.90	1.4111	28.46	21.27
e19_19	6.62	1.4897	8.99	7.42	1.2978	29.21	26.48	1.3842	31.32	26.19
e2_19	5.12	1.3561	27.50	27.43	1.2378	23.60	22.36	1.4065	27.90	24.27
e20_19	8.61	1.4046	40.87	37.31	1.3794	30.89	26.16	1.3046	30.68	23.56
e21_19	8.26	1.3862	43.11	39.90	1.3368	26.71	22.35	1.3775	31.89	25.13
e22_19	8.09	1.4759	20.76	17.72	1.3222	29.27	25.05	1.3159	28.19	21.59
e23_19	8.65	1.4892	25.49	21.89	1.3206	21.94	17.17	1.443	23.38	16.22
e24_19	24.24	1.4279	38.21	19.02	1.2861	36.91	16.55	1.33	38.64	15.88
e25_19	24.12	1.3521	31.42	12.35	1.2917	33.06	12.82	1.3816	36.45	13.81
e26_19	26.87	1.4699	41.59	19.77	1.3472	32.31	9.32	1.4045	33.68	8.30
e27_19	0.11	1.3477	27.07	32.01	1.3411	13.26	17.03	1.416	21.83	23.21
e28_19	26.99	1.4211	46.40	24.46	1.3167	34.84	11.73	1.4071	29.83	4.33
e3_19	7.16	1.3884	38.55	36.44	1.3164	31.37	28.09	1.3991	28.82	23.15
e31_19	1.89	1.47	28.97	32.13	1.2979	21.57	23.56	1.4228	21.73	21.33
e35_19	3.36	1.3862	20.06	21.75	1.3568	22.58	23.10	1.4506	10.45	8.58
e36_19	3.12	1.4015	22.95	24.88	1.3247	17.09	17.85	1.3288	27.37	25.74
e37_19	19.10	1.4459	28.65	14.60	1.2602	29.31	14.09	1.3324	32.87	15.26
e38_19	3.67	1.3936	38.51	39.89	1.2756	25.05	25.26	1.4143	21.95	19.77
e39_19	22.33	1.3833	20.71	3.43	1.2875	22.55	4.10	1.3045	20.94	0.10
e4_19	7.48	1.3866	26.03	23.60	1.3689	26.95	23.35	1.4294	26.37	20.38
e40_19	5.85	1.4236	38.46	37.66	1.3466	25.28	23.31	1.365	18.10	13.74
e44_19	7.62	1.4188	38.02	35.45	1.3088	20.68	16.93	1.3541	27.07	20.93
e45_19	7.58	1.386	30.38	27.85	1.377	15.51	11.80	1.3959	30.30	24.20
e46_19	23.69	1.4665	43.00	24.36	1.3462	25.32	5.52	1.2563	37.78	15.58
e47_19	26.69	1.3306	42.92	21.28	1.3054	26.85	4.04	1.2965	38.39	13.19
e48_19	23.23	1.3845	48.55	30.37	1.3573	27.31	7.96	1.3857	43.84	22.11
e5_19	9.85	1.4456	38.91	34.11	1.3315	30.36	24.39	1.3354	32.46	24.09
e51_19	23.72	1.3919	43.98	25.31	1.3123	33.98	14.14	1.4096	34.81	12.58
e52_19	25.52	1.5146	35.24	14.77	1.3358	36.19	14.56	1.3596	33.42	9.39
e54_19	14.43	1.3922	36.82	27.44	1.3959	36.34	25.79	1.3279	30.43	17.50
e55_19	25.77	1.5169	34.72	14.00	1.3599	31.79	9.90	1.3708	36.09	11.81
e6_19	8.42	1.4421	33.63	30.26	1.3336	21.34	16.79	1.3983	29.85	22.92
e60_19	18.43	1.4512	28.26	14.88	1.3269	31.07	16.52	1.3451	36.17	19.22
e61_19	19.13	1.4132	29.74	15.66	1.314	31.82	16.58	1.3441	34.32	16.68
e62_19	18.65	1.3643	35.75	22.15	1.2897	27.83	13.06	1.3202	21.03	3.87
e63_19	20.82	1.4647	22.43	6.66	1.3316	23.91	6.97	1.2889	33.05	13.72
e64_19	20.64	1.4284	32.79	17.20	1.3382	31.37	14.62	1.3515	28.81	9.67
e65_19	21.78	1.3923	32.60	15.87	1.3266	31.90	14.00	1.3542	30.67	10.37
e68_19	22.47	1.3198	46.12	28.70	1.3847	28.86	10.28	1.289	34.13	13.15
e69_19	24.68	1.4079	38.64	19.01	1.3616	33.87	13.07	1.3626	31.83	8.64
e7_19	9.80	1.4882	33.22	28.47	1.3058	23.18	17.26	1.3467	35.66	27.35
e72_19	33.66	1.459	51.66	23.05	1.3332	34.85	5.06	1.416	44.58	12.40
e73_19	34.35	1.4508	47.34	18.04	1.334	35.51	5.03	1.3936	37.18	4.32
e74_19	37.92	1.4368	52.92	20.05	1.3119	34.18	0.14	1.356	36.85	0.42
e75_19	38.72	1.358	43.64	9.97	1.3296	36.19	1.35	1.3072	43.20	5.97
e8_19	0.00	1.4304	23.18	28.23	1.3246	17.75	21.62	1.4284	20.07	21.56

e9_19	3.28	1.3992	28.67	30.44	1.4113	21.21	21.80	1.3453	25.11	23.32
e1_4	5.09	1.4563	34.31	34.27	1.3031	30.11	28.89	1.4303	35.47	31.86
e10_4	5.05	1.4734	15.13	15.13	1.3479	17.57	16.40	1.3724	21.18	17.62
e11_4	4.05	1.435	26.15	27.15	1.3261	20.44	20.28	1.368	34.30	31.74
e12_4	4.52	1.4826	38.89	39.42	1.3233	25.48	24.84	1.3905	26.09	23.06
e13_4	7.48	1.3819	51.55	49.12	1.3125	27.38	23.77	1.3679	34.23	28.24
e14_4	4.35	1.4357	35.08	35.78	1.3705	26.57	26.10	1.4007	33.60	30.74
e15_4	6.27	1.3228	41.66	40.44	1.3455	25.44	23.06	1.3222	29.98	25.20
e16_4	5.12	1.4107	38.43	38.36	1.3723	22.87	21.64	1.334	25.59	21.96
e17_4	9.56	1.4713	48.34	43.83	1.3289	32.48	26.80	1.387	26.28	18.20
e18_4	8.68	1.4235	43.72	40.09	1.3068	26.40	21.60	1.3099	29.05	21.86
e19_4	6.62	1.4839	12.29	10.72	1.3204	29.57	26.84	1.3886	28.04	22.91
e2_4	5.12	1.4739	32.60	32.53	1.2531	25.61	24.37	1.358	28.40	24.76
e20_4	8.61	1.3756	38.28	34.72	1.3477	31.02	26.27	1.3358	35.21	28.09
e21_4	8.25	1.422	46.71	43.51	1.305	28.86	24.49	1.3774	38.68	31.92
e22_4	8.10	1.4757	23.26	20.21	1.3279	25.80	21.58	1.3428	30.68	25.90
e23_4	8.65	1.4085	31.93	28.33	1.3629	29.34	24.57	1.3522	36.71	29.55
e24_4	24.24	1.4045	45.67	26.48	1.2625	31.80	11.44	1.3018	27.69	4.94
e25_4	24.13	1.4825	45.23	26.15	1.2851	38.24	18.00	1.3544	34.57	11.93
e26_4	26.87	1.4484	49.03	27.21	1.3631	41.15	18.16	1.2742	38.43	13.05
e27_4	0.11	1.4075	27.02	31.96	1.2613	20.90	24.67	1.3465	11.89	13.28
e28_4	26.99	1.4096	46.14	24.20	1.2885	41.76	18.65	1.3783	38.88	13.38
e3_4	7.16	1.3543	37.87	35.76	1.3275	31.12	27.84	1.419	34.46	28.78
e31_4	1.89	1.4283	32.67	35.83	1.2841	17.81	19.80	1.3258	20.71	20.30
e35_4	3.36	1.4237	20.90	22.59	1.2717	16.68	17.20	1.4625	12.22	10.35
e36_4	3.12	1.4389	36.28	38.21	1.3163	12.89	13.65	1.434	32.24	30.61
e37_4	19.10	1.4408	30.38	16.33	1.3742	15.22	0.00	1.324	24.12	6.51
e38_4	3.67	1.4505	35.30	36.68	1.3444	22.65	22.86	1.3709	28.74	26.56
e39_4	22.33	1.3789	38.08	20.80	1.2468	23.91	5.46	1.317	20.84	0.00
e4_4	7.48	1.4169	29.12	26.69	1.3086	23.53	19.93	1.3683	32.55	26.56
e40_4	5.85	1.437	40.59	39.79	1.3091	25.04	23.08	1.328	11.18	6.82
e44_4	7.62	1.3577	38.27	35.70	1.3657	17.65	13.90	1.4055	33.50	27.37
e45_4	7.59	1.3727	49.78	47.24	1.2541	21.19	17.49	1.3578	24.13	18.04
e46_4	23.69	1.3311	51.20	32.56	1.3307	26.03	6.22	1.3488	37.90	15.71
e47_4	26.69	1.3943	45.33	23.69	1.2841	37.36	14.55	1.3261	40.04	14.84
e48_4	23.23	1.4339	35.73	17.55	1.3273	34.22	14.87	1.3797	49.12	27.38
e5_4	9.86	1.3993	32.09	27.28	1.3422	31.25	25.28	1.2856	33.90	25.54
e51_4	23.73	1.4568	57.95	39.27	1.3694	38.60	18.76	1.3888	41.97	19.74
e52_4	25.51	1.4965	35.72	15.26	1.3351	35.85	14.22	1.3056	31.53	7.51
e54_4	14.43	1.438	52.15	42.77	1.3645	27.70	17.15	1.3825	42.44	29.50
e55_4	25.78	1.4937	42.49	21.77	1.3506	30.86	8.97	1.3791	32.36	8.08
e6_4	8.42	1.4215	41.28	37.91	1.2897	23.48	18.94	1.3715	39.18	32.24
e60_4	18.43	1.4312	38.07	24.69	1.3539	35.04	20.49	1.3439	39.97	23.02
e61_4	19.13	1.4009	39.11	25.03	1.3011	35.42	20.17	1.3236	34.12	16.48
e62_4	18.65	1.365	35.88	22.28	1.3266	21.50	6.74	1.4433	21.39	4.23
e63_4	20.82	1.4696	15.90	0.13	1.3212	37.66	20.72	1.3817	31.88	12.55

e64_4	20.63	1.4248	41.89	26.31	1.3291	24.62	7.86	1.3805	32.70	13.55
e65_4	21.78	1.4418	41.74	25.01	1.3331	25.40	7.50	1.2612	37.07	16.78
e68_4	22.46	1.3069	53.17	35.76	1.348	33.41	14.83	1.3427	39.43	18.46
e69_4	24.68	1.3811	48.75	29.12	1.3227	27.79	6.99	1.2642	28.09	4.90
e7_4	9.80	1.4797	42.91	38.16	1.3393	22.00	16.08	1.4119	33.45	25.14
e72_4	33.67	1.3526	57.29	28.67	1.3092	35.45	5.66	1.3616	47.46	15.27
e73_4	34.36	1.3617	47.96	18.65	1.2977	36.39	5.91	1.3243	43.64	10.77
e74_4	37.92	1.4267	55.44	22.57	1.3488	48.07	14.03	1.3239	52.79	16.36
e75_4	38.73	1.4444	52.87	19.20	1.2988	45.39	10.55	1.3427	47.47	10.24
e8_4	0.00	1.4501	27.81	32.86	1.2828	17.55	21.42	1.4405	25.31	26.79
e9_4	3.28	1.4129	29.73	31.50	1.3168	13.20	13.80	1.3975	21.45	19.66
expr	5.05	1.4968	0.00	0.00						

Table S4. Final numerical data obtained for the best structures of EPI in C2 and P1 space groups

	2:1 solvates			2:1 solvates			1:1 solvates	
name	density	Etotal	name	density	Etotal	name	density	Etotal
e10s_1	1.2366	29.98	e10s_5	1.2053	18.48	e10_1_1	1.3622	23.62
e11s_1	1.3334	27.35	e11s_5	1.2402	22.37	e10_1_5	1.3755	36.65
e12s_1	1.2522	28.58	e12s_5	1.2397	23.56	e11_1_1	1.2538	37.56
e13s_1	1.2667	38.67	e13s_5	1.2598	26.46	e11_1_5	1.2947	31.89
e14s_1	1.2834	29.01	e14s_5	1.2887	32.5	e12_1_1	1.2425	42.74
e15s_1	1.2749	31.84	e15s_5	1.2872	30.25	e12_1_5	1.347	29.25
e16s_1	1.3177	31.38	e16s_5	1.3166	29.04	e13_1_1	1.247	45.73
e17s_1	1.3113	29.21	e17s_5	1.3216	22.11	e13_1_5	1.2692	43.13
e18s_1	1.3267	32.78	e18s_5	1.2963	28.49	e14_1_1	1.305	48.23
e19s_1	1.2822	26.32	e19s_5	1.3146	28.9	e14_1_5	1.2725	38.81
e1s_1	1.3265	34.12	e1s_5	1.2626	25.8	e15_1_1	1.3092	43.55
e20s_1	1.3482	29.61	e20s_5	1.3066	28.41	e15_1_5	1.3556	46.30
e21s_1	1.3579	30.98	e21s_5	1.2449	30.24	e16_1_1	1.2802	41.38
e22s_1	1.3019	25.77	e22s_5	1.3058	35.3	e16_1_5	1.3459	37.61
e23s_1	1.2513	30.97	e23s_5	1.2184	20.6	e17_1_1	1.3032	38.04
e24s_1	1.2729	38.6	e24s_5	1.3251	37.3	e17_1_5	1.2993	44.60
e25s_1	1.3046	51.77	e25s_5	1.3972	36.7	e18_1_1	1.1783	44.04
e26s_1	1.2686	38.51	e26s_5	1.3943	37.82	e18_1_5	1.2951	42.52
e27s_1	1.2626	22.25	e27s_5	1.3107	17.28	e19_1_1	1.346	37.06
e28s_1	1.3487	46.74	e28s_5	1.2917	25.71	e19_1_5	1.2914	37.42
e2s_1	1.3094	34.1	e2s_5	1.2147	19.5	e2_1_1	1.2679	50.43
e31s_1	1.3801	18.83	e31s_5	1.2805	20.81	e2_1_5	1.2649	35.41
e35s_1	1.2292	18.63	e35s_5	1.3166	18.41	e22_1_1	1.337	31.62
e36s_1	1.2923	21.35	e36s_5	1.2542	12.11	e22_1_5	1.3147	41.02
e37s_1	1.2281	33.05	e37s_5	1.3323	24.2	e23_1_1	1.3703	39.40
e38s_1	1.293	25.56	e38s_5	1.2931	24.64	e23_1_5	1.2876	34.53
e39s_1	1.3329	19.16	e39s_5	1.2447	21.42	e24_1_1	1.2722	55.65
e3s_1	1.341	35.18	e3s_5	1.3319	21.38	e24_1_5	1.3301	46.28
e40s_1	1.2887	26.63	e40s_5	1.2944	18	e27_1_1	1.3091	43.51

e44s_1	1.3343	24.47	e44s_5	1.2952	27.97	e27_1_5	1.2791	23.95
e45s_1	1.3069	30.5	e45s_5	1.292	19.93	e28_1_1	1.3705	44.96
e46s_1	1.2847	37.29	e46s_5	1.2478	38.35	e28_1_5	1.2448	50.75
e47s_1	1.3118	27.33	e47s_5	1.2382	37.42	e3_1_1	1.341	48.07
e48s_1	1.316	46.07	e48s_5	1.2361	41.05	e3_1_5	1.3064	39.86
e4s_1	1.3186	28.51	e4s_5	1.2937	24.31	e31_1_1	1.3843	38.13
e54s_1	1.2885	33.53	e54s_5	1.2758	29.72	e31_1_5	1.3284	30.17
e55s_1	1.2853	30.91	e55s_5	1.3141	36.73	e35_1_1	1.4009	23.35
e5s_1	1.3087	31.12	e5s_5	1.1826	32.69	e35_1_5	1.3014	25.69
e60s_1	1.3348	46.76	e60s_5	1.3051	29.85	e36_1_1	1.2564	34.85
e61s_1	1.302	29.39	e61s_5	1.2526	29.95	e36_1_5	1.2439	25.89
e62s_1	1.2324	33.6	e62s_5	1.2378	27.87	e37_1_1	1.3211	45.44
e63s_1	1.2658	31.23	e63s_5	1.2269	38.1	e37_1_5	1.3955	34.94
e64s_1	1.3522	22.35	e64s_5	1.2623	22.98	e4_1_1	1.3235	37.79
e65s_1	1.3134	32.99	e65s_5	1.2271	34.56	e4_1_5	1.3337	34.93
e69s_1	1.2359	21.18	e69s_5	1.253	19.74	e54_1_1	1.2882	49.66
e6s_1	1.2925	36.35	e6s_5	1.2451	34.86	e54_1_5	1.3504	43.50
e75s_1	1.3497	43.81	e75s_5	1.2291	35.84	e6_1_1	1.2833	42.67
e7s_1	1.316	33.99	e7s_5	1.2966	26.71	e6_1_5	1.2913	40.90
e8s_1	1.323	28.62	e8s_5	1.3681	25.1	e62_1_1	1.3597	54.35
e9s_1	1.3223	17.39	e9s_5	1.3158	14.34	e62_1_5	1.3443	38.77
						e64_1_1	1.2795	30.78
						e64_1_5	1.258	37.21
						e69_1_1	1.3577	37.39
						e69_1_5	1.32	38.02
						e8_1_1	1.2389	44.07
						e8_1_5	1.2547	37.11
						e9_1_1	1.2845	37.10
						e9_1_5	1.2593	28.68
						e38_1_1	1.2951	40.81
						e38_1_5	1.3322	35.72
						e39_1_1	1.23	40.39
						e39_1_5	1.2931	41.92
						e40_1_1	1.2828	49.73
						e40_1_5	1.2919	33.90
						e44_1_1	1.2505	43.78
						e44_1_5	1.3804	38.75
						e45_1_1	1.234	52.31
						e45_1_5	1.3359	34.81

[1] Marta K. Dudek, Piotr Paluch, Justyna Sniechowska, Karol Nartowski, Graeme M. Day, Marek J. Potrzebowski. Joint solid-state NMR – crystal structure prediction approach to determine crystal structure of new catechin solvates (*in preparation*)