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Supporting information for article:

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to

S1. Structural variety of heterosynthons in linezolid cocrystals with modified thermal properties

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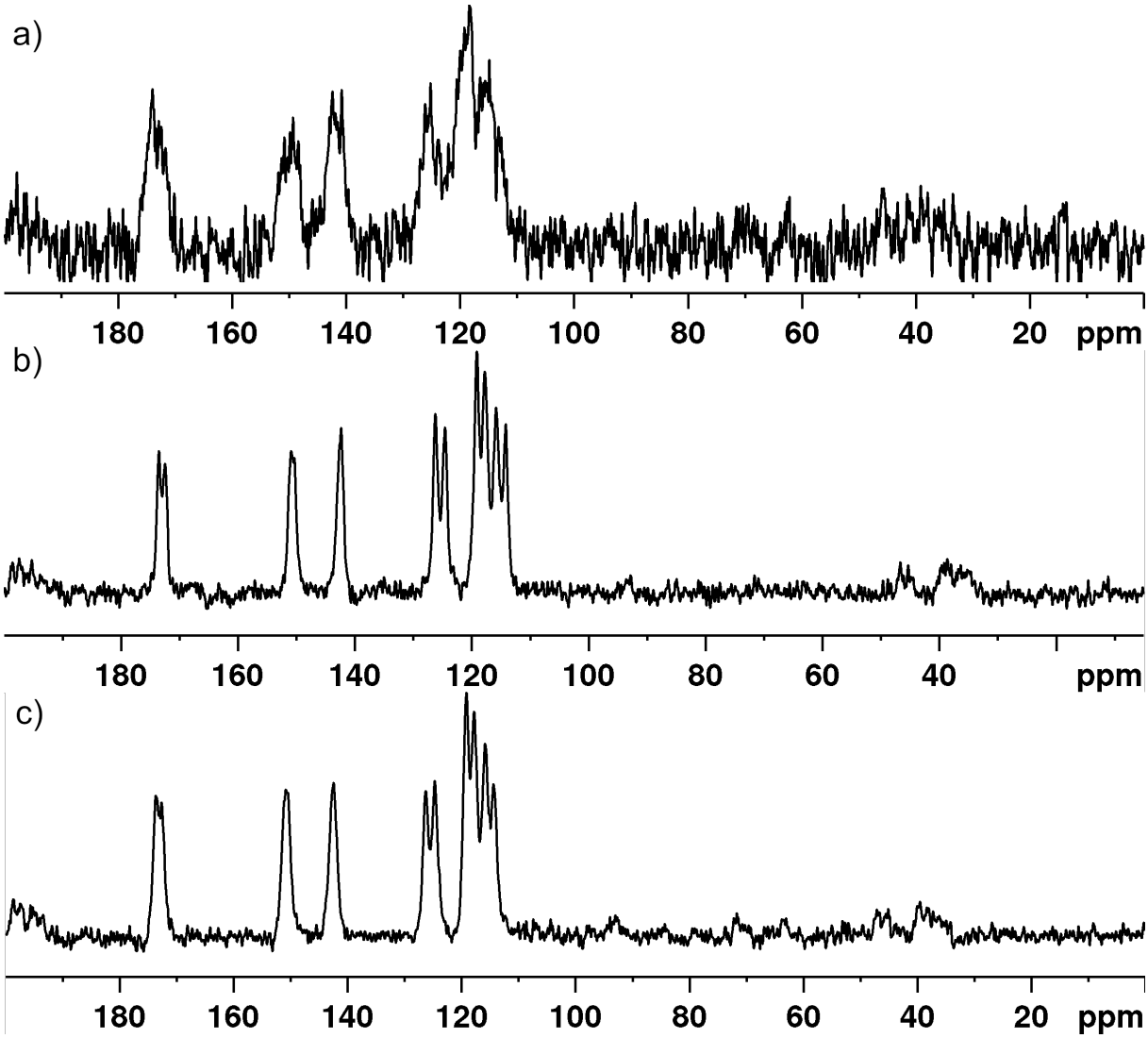


Figure S1. ^{13}C CPMAS spectra of 3,4-DHBA registered with a spinning speed of 8 kHz: (a) commercial, amorphous sample, (b) commercial sample recrystallized from water, corresponding to 3,4-DHBA monohydrate and (c) commercial sample ground for 1h with 100 μL of water.

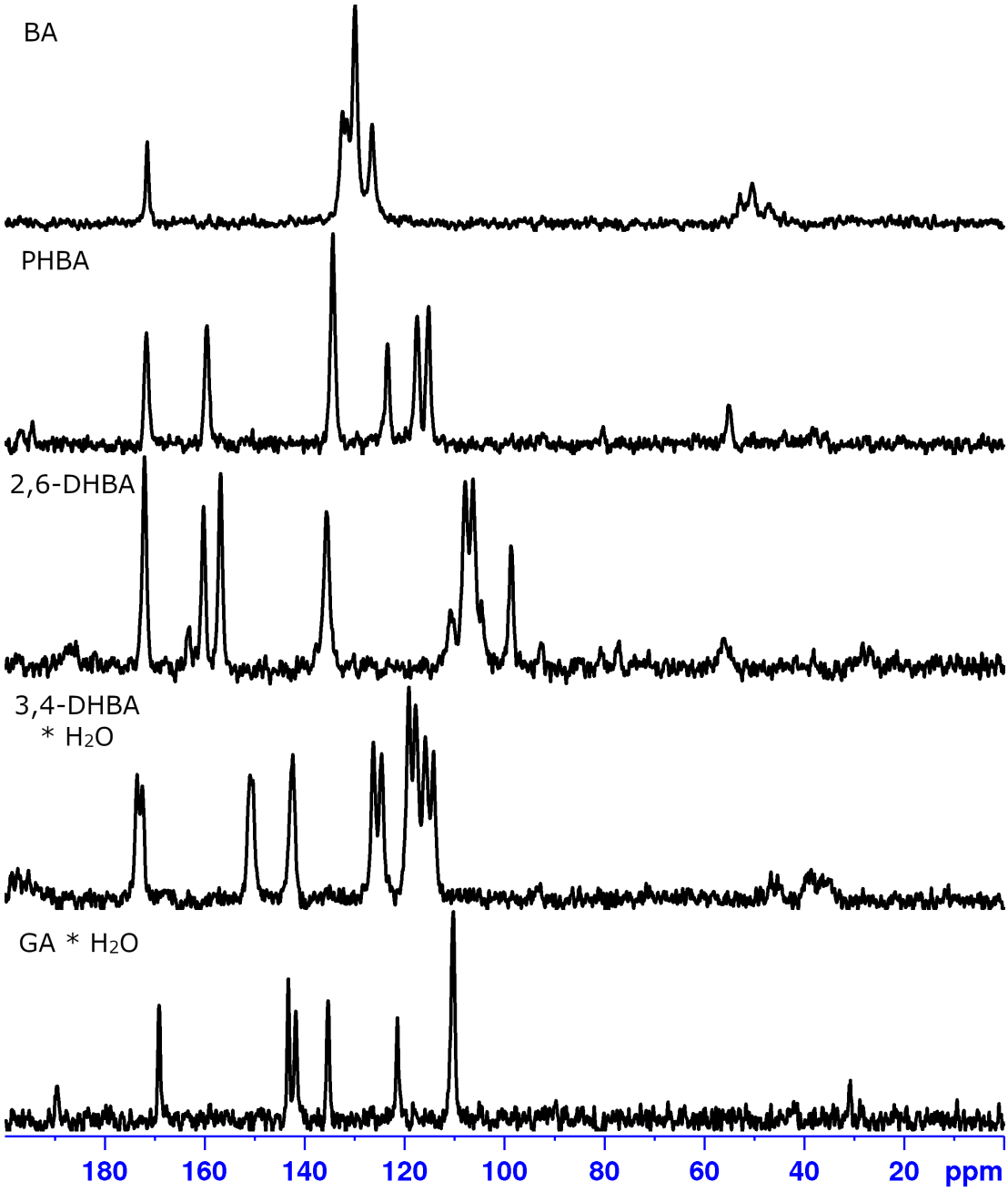
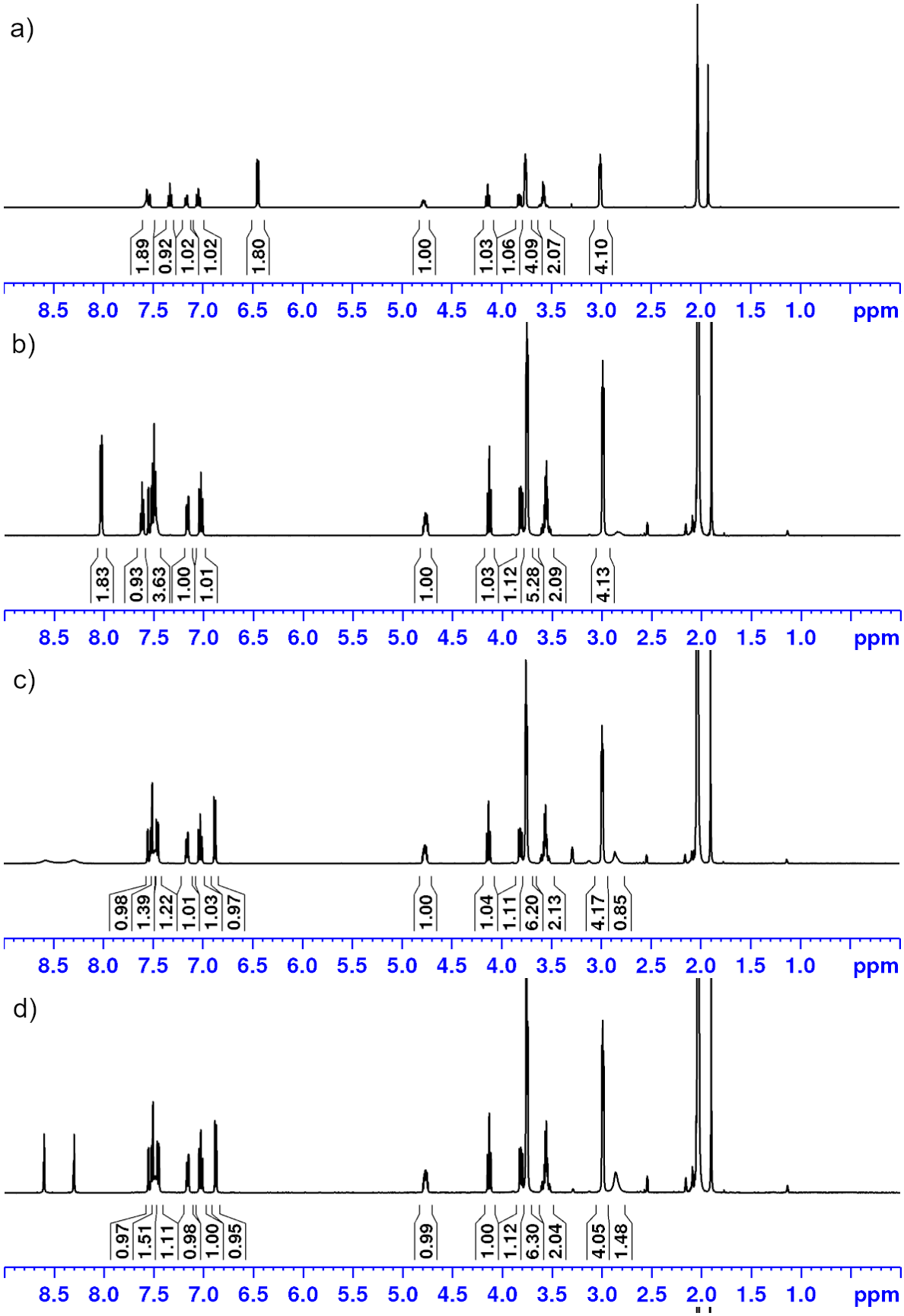


Figure S2. ^{13}C CPMAS spectra of coformers in their crystalline forms as used to obtained cocrystals with LIN.


a)
1.89
0.92
1.02
1.02
1.80
1.00
1.03
1.06
4.09
2.07
4.10
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
b)
1.83
0.93
3.63
1.00
1.01
1.00
1.03
1.12
5.28
2.09
4.13
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
c)
0.98
1.39
1.22
1.01
1.03
0.97
1.00
1.04
1.11
6.20
2.13
4.17
0.85
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
d)
0.97
1.51
1.11
0.98
1.00
0.95
0.99
1.00
1.12
6.30
2.04
4.05
1.48
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

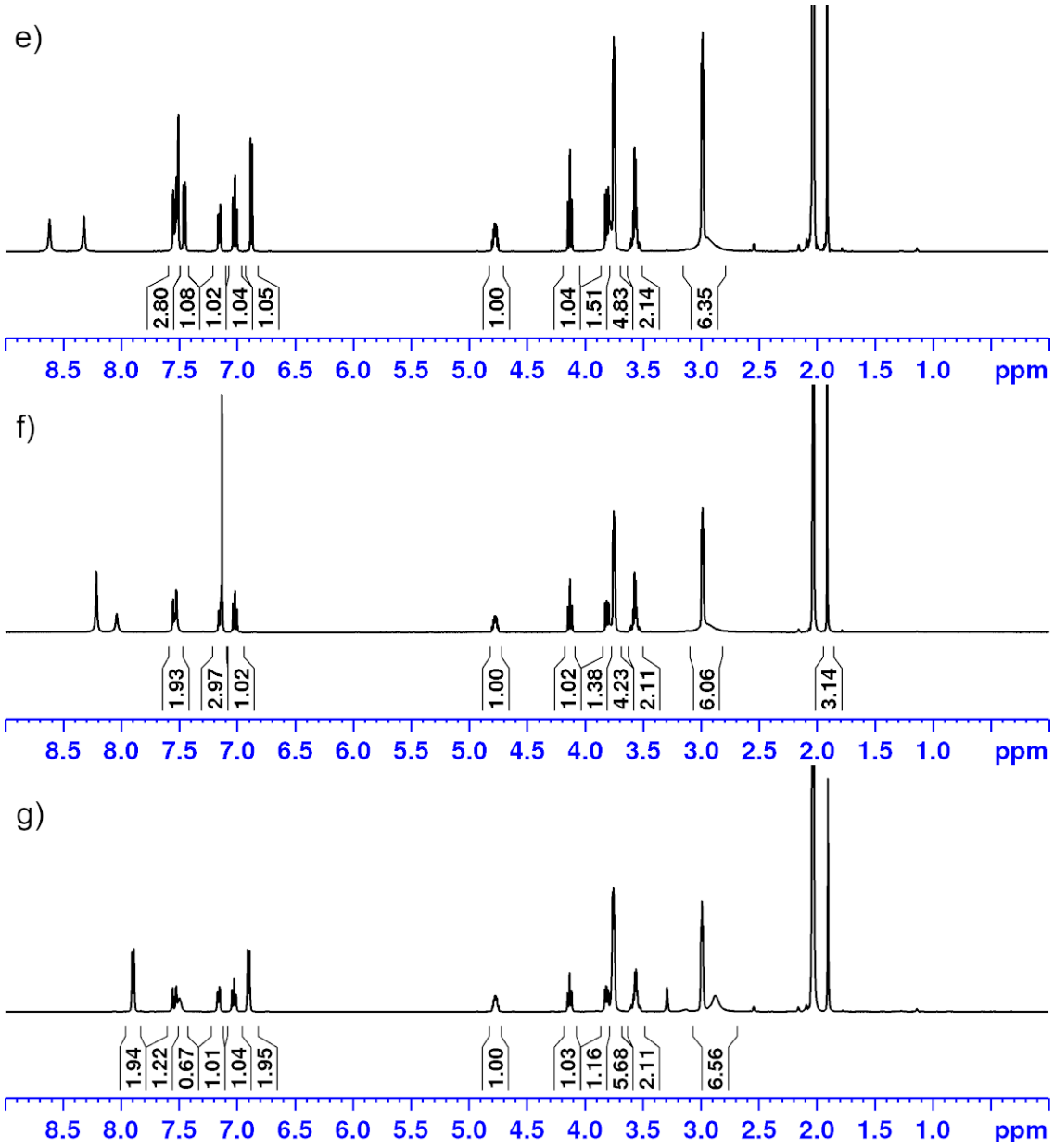


Figure S3. ^{1}H NMR spectra in anhydrous acetone-d_6 of cocrystals of LIN with 2,6-DHBA (a), BA (b), 3,4-DHBA (c, d, e), GA (f) and PHBA (g).

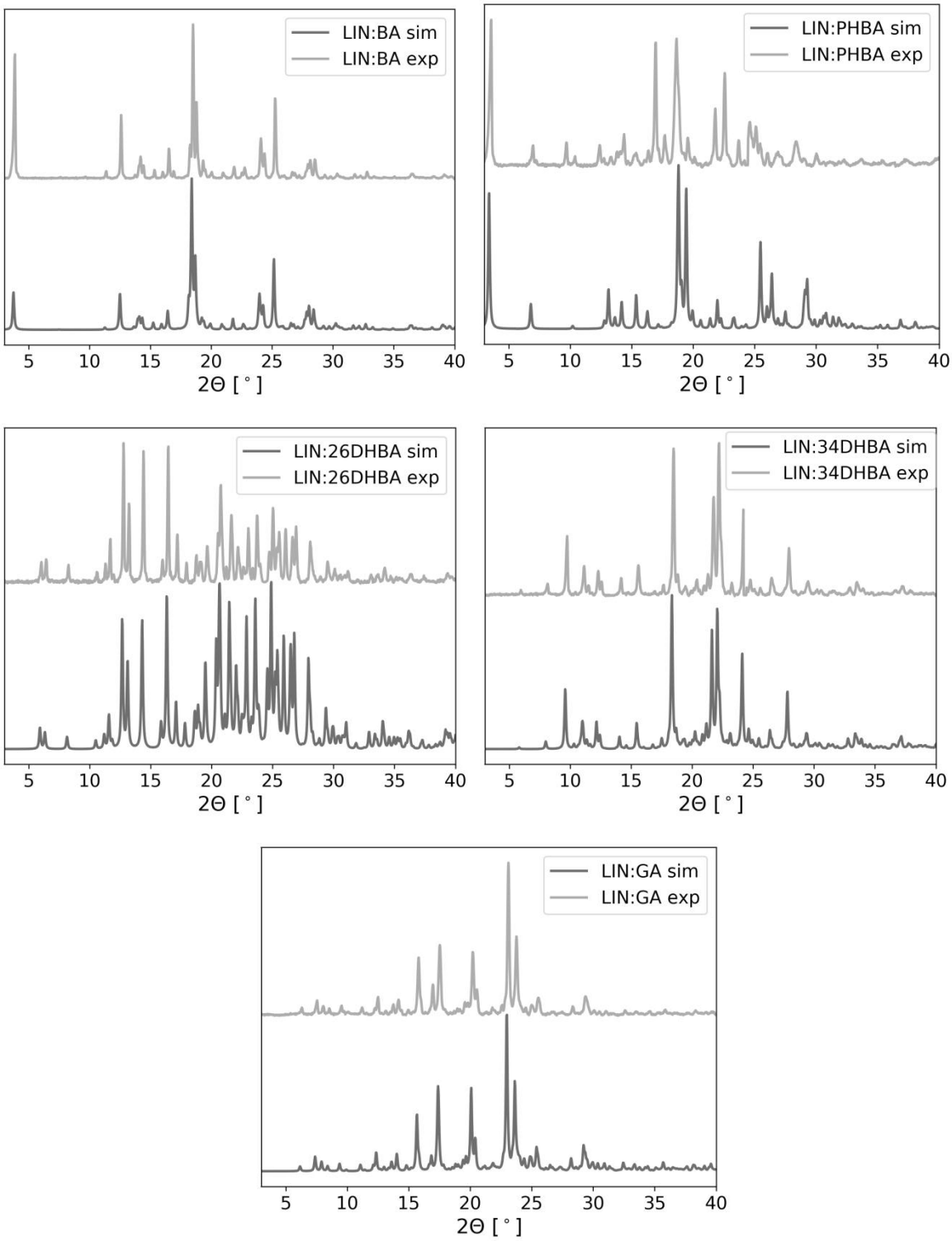


Figure S4. A comparison of the experimental powder X-Ray diffractograms for LIN:BA, LIN:PHBA:H_2O, LIN:2,6-DHBA, LIN:3,4-DHBA:H_2O and LIN:GA:H_2O samples obtained after mechanochemical grinding of LIN form II with appropriate coformers and simulated PXRD patterns for the crystallographic solutions from single crystal X-ray diffraction experiments.

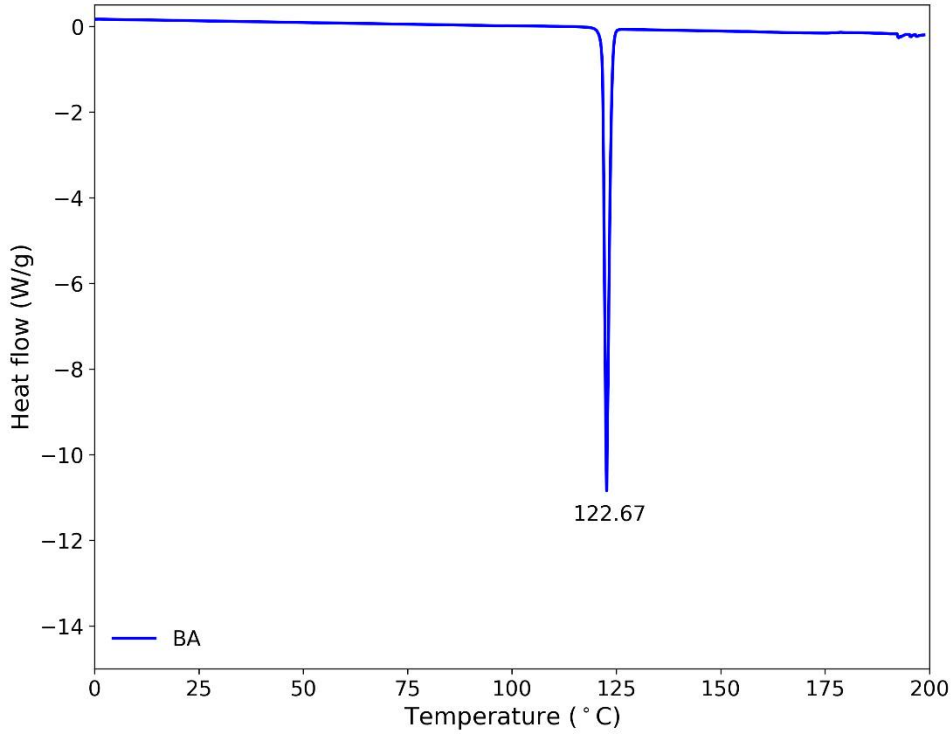


Figure S5. DSC curve for pure benzoic acid used for the mechanochemical preparation of LIN:BA cocrystal

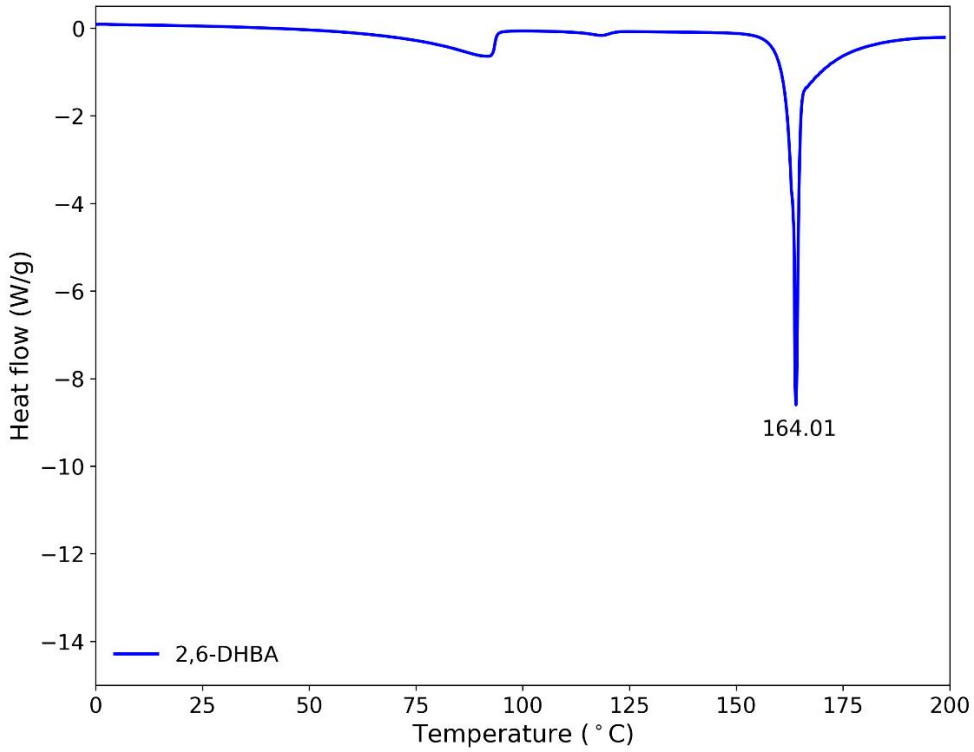


Figure S6. DSC curve for pure 2,6-dihydroxybenzoic acid used for the mechanochemical preparation of LIN:2,6-DHBA cocrystal

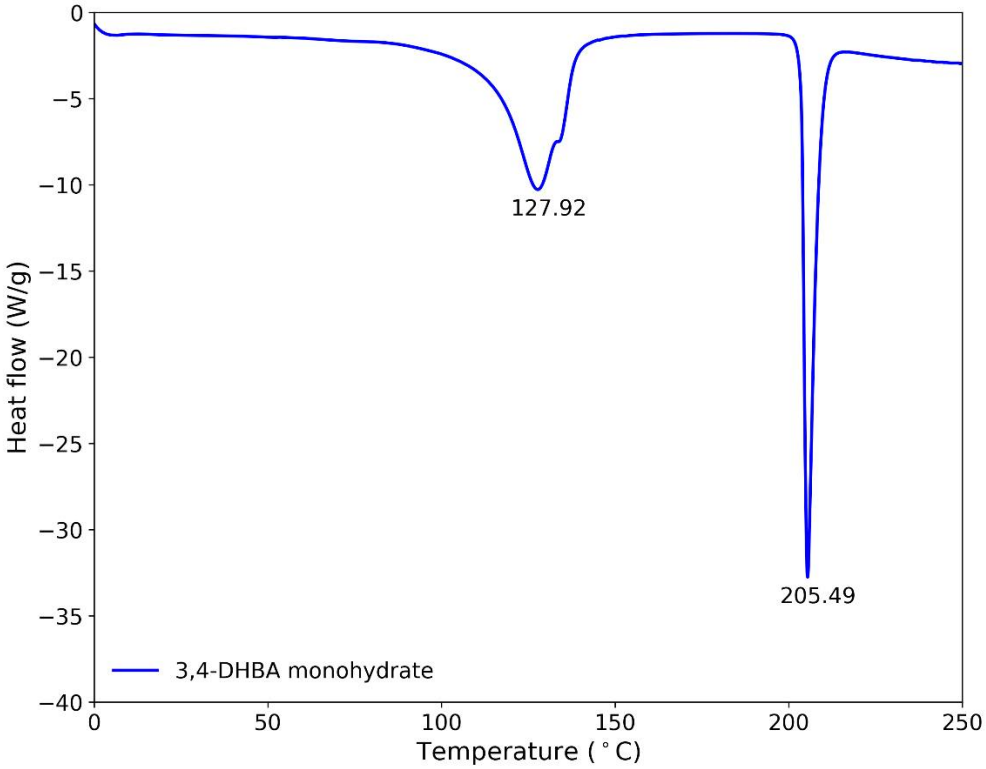


Figure S7. DSC curve for pure monohydrate of 3,4-dihydroxybenzoic acid used for the mechanochemical preparation of LIN:3,4-DHBA:H_2O cocrystal

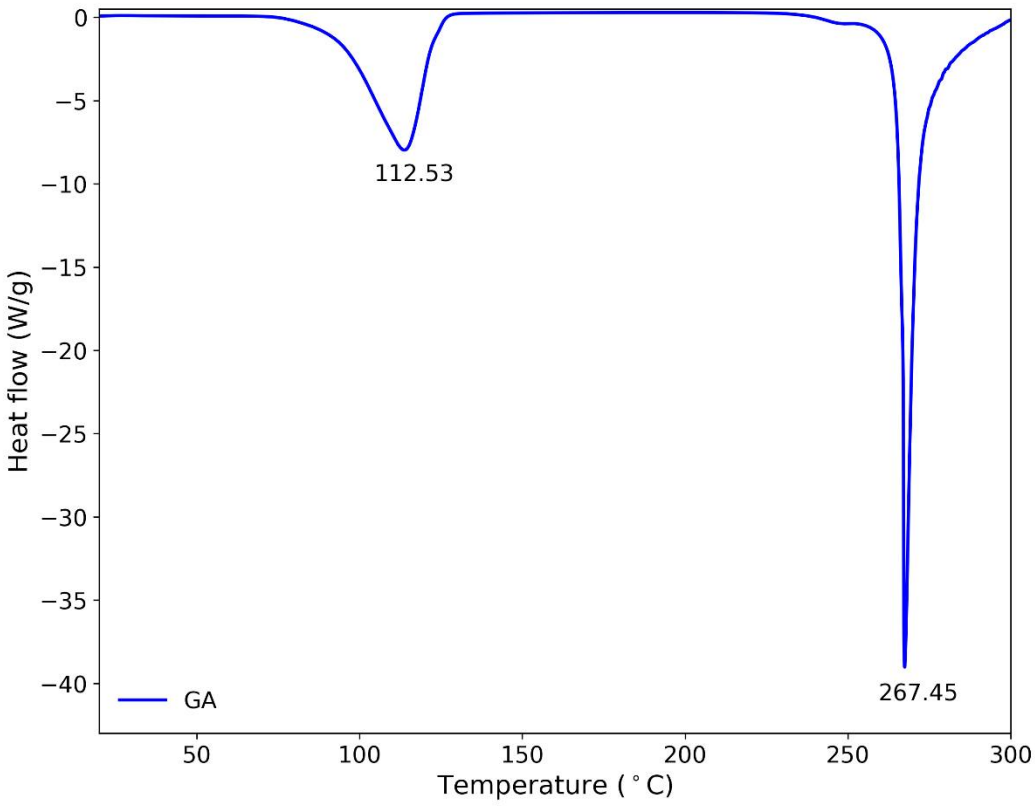


Figure S8. DSC curve for pure monohydrate of gallic acid used for the mechanochemical preparation of LIN:GA:H_2O cocrystal

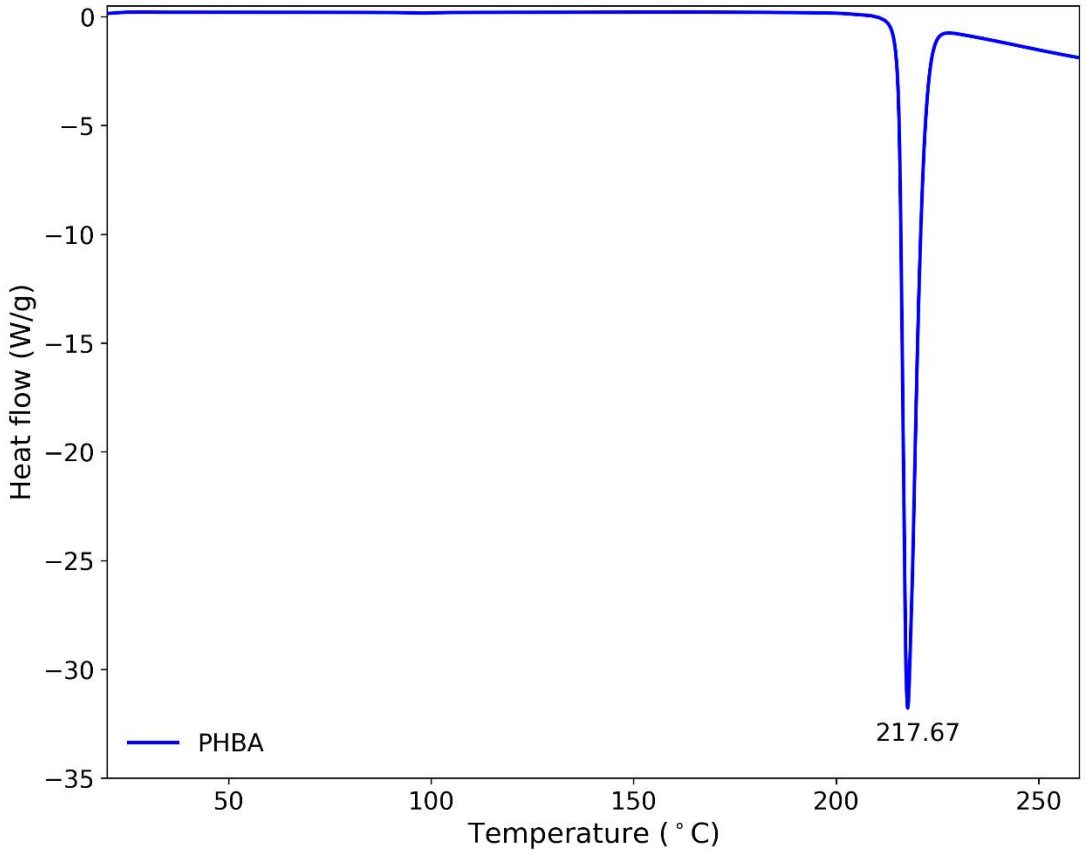


Figure S9. DSC curve for pure p-hydroxybenzoic acid used for the mechanochemical preparation of LIN:PHBA:H_2O cocrystal.

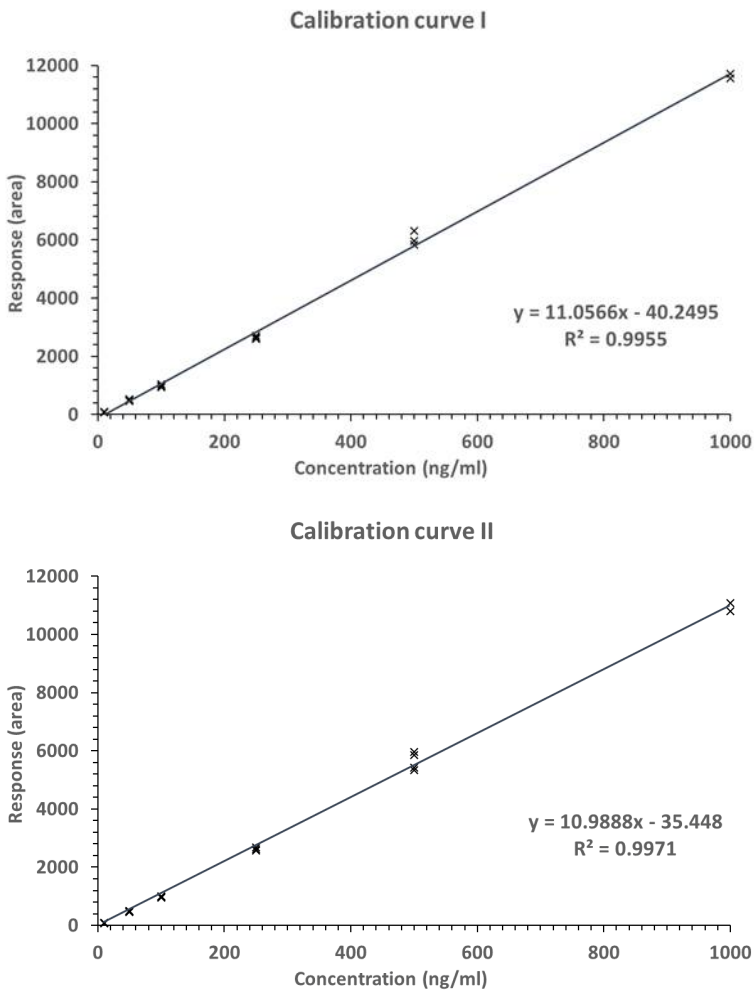


Figure S10. Calibration curves from MS measurements used for the calculations of water solubility of LIN.

Table S1. Numerical data used to calculate water solubility of the obtained cocrystals.

	time [h]	Concentration of LIN in each sample [ng/ml][a]								Mean concentration [ng/ml]	Solubility [mg/ml]	RSD [%][b]
LIN_II	**12h**	260.5	252.5	255.5	254.3	250.3	264.6	245.2	252.8	**255.0**	**2.55**	**2.10**
		259.7	251.1	256.0	254.8	250.8	265.7	252.9	253.3			
	24h	288.7	296.9	292.7	276.7	302.3	286.0	309.0	311.4	**293.9**	**2.94**	**4.34**
		290.7	286.9	275.9	274.5	302.4	286.5	310.8	310.3			
	36h	277.4	273.3	272.6	254.1	266.9	274.9	267.8	272.4	**270.3**	**2.70**	**2.71**
		278.7	275.2	273.6	255.0	264.0	275.3	267.8	275.0			
	48h	263.6	261.3	243.6	248.8	274.7	271.7	272.6	276.7	**264.6**	**2.65**	**4.37**
		265.5	260.3	244.0	253.5	274.3	272.3	274.0	276.2			
LIN:BA	**12h**	259.4	257.9	270.0	273.0	241.9	245.1	254.4	254.3	**256.3**	**2.56**	**3.70**
		259.8	258.3	263.4	269.3	244.9	245.6	250.3	252.9			
	24h	313.5	315.8	315.5	324.1	316.3	318.2	327.9	330.5	**321.9**	**3.22**	**1.76**
		320.5	326.1	315.9	324.5	321.0	322.4	327.5	330.8			
	36h	313.2	321.4	320.6	317.4	310.0	302.6	313.4	299.0	**313.0**	**3.13**	**3.47**
		333.2	328.1	317.7	321.7	310.4	303.0	294.5	301.7			
	48h	304.5	279.8	285.9	282.9	275.2	275.7	275.3	273.0	**281.3**	**2.81**	**3.30**
		301.2	281.7	282.5	281.8	275.6	276.1	275.7	273.4			
LIN:PHBA:H_2O	**12h**	176.9	177.3	170.4	172.0	174.8	174.0	170.3	170.0	**173.3**	**1.73**	**1.71**
		175.3	171.1	173.8	173.2							
	24h	205.0	205.8	208.2	203.1	197.1	198.0	194.4	201.0	**201.1**	**2.01**	**2.09**
		204.6	202.9	205.6	202.8	195.6	197.6	197.1	198.5			
	36h	221.5	213.2	216.4	223.0	215.0	208.0	227.4	219.6	**217.8**	**2.18**	**2.72**
		221.1	212.7	216.0	222.6	214.5	207.6	227.0	219.2			
	48h	198.1	198.8	195.4	192.4	190.2	187.7	179.4	185.0	**190.3**	**1.90**	**3.43**
		198.3	194.8	195.0	191.9	189.7	187.3	178.9	181.8			
LIN:2,6-DHBA	**12h**	248.4	260.8	262.2	266.6	266.0	269.4	259.9	262.9	**262.2**	**2.62**	**2.35**
		263.6	254.1	257.1	261.6	265.5	273.3	256.8	267.7			
	24h	257.7	269.2	268.2	277.5	281.1	274.3	278.4	277.2	**273.8**	**2.74**	**2.31**
		277.9	276.9	274.2	272.6							
	36h	280.0	284.8	278.0	280.6	282.3	284.5	278.5	282.3	**280.5**	**2.80**	**0.97**
		276.8	280.9	276.5	280.7							
	48h	286.7	293.2	294.3	298.4	313.3	306.8	289.0	297.6	**298.0**	**2.98**	**2.46**
		297.3	303.4	296.3	299.7							
LIN:3,4-DHBA:H_2O	**12h**	340.4	335.6	338.6	340.8	337.6	344.3	343.7	349.9	**341.3**	**3.41**	**1.11**
		341.8	338.9	339.5	343.9							
	24h	415.6	413.3	416.4	418.1	420.9	426.7	435.1	409.6	**419.9**	**4.20**	**1.97**
		415.6	410.0	425.6	431.7							
	36h	349.7	352.0	358.6	348.2	342.4	359.7	338.9	346.2	**350.8**	**3.51**	**2.46**
		350.1	332.0	357.8	363.6	353.7	357.6					
	48h	337.0	330.1	329.5	324.6	325.0	333.7	320.5	326.5	**332.7**	**3.33**	**1.75**
		338.1	337.2	334.4	339.2	335.6	333.0	341.3	337.2			
LIN:GA:H_2O	**12h**	174.3	173.8	179.8	178.4	167.4	160.1	164.9	165.1	**173.7**	**1.74**	**4.14**
		179.8	179.3	185.5	184.1	172.7	170.4	172.8	170.3			
	24h	231.7	227.4	218.4	215.7	227.7	234.2	224.6	224.5	**226.2**	**2.26**	**2.59**
		224.1	227.9	225.4	222.6	235.1	235.9	220.4	222.8			
	36h	212.7	215.0	212.2	203.3	183.8	185.0	189.8	188.8	**200.4**	**2.00**	**6.36**
		219.5	209.0	211.8	213.4	188.0	187.0	192.2	194.9			
	48h	188.5	189.9	187.1	186.8	194.9	192.4	194.5	190.5	**192.3**	**1.92**	**2.20**
		191.6	193.0	201.1	197.5							

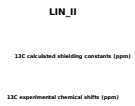
[a] Concentration of linezolid in samples after dilution; [b] Relative Standard Deviation

Table S2. Numerical data from the calculations of stabilization energies of the studied cocrystals. N and n denote number of molecules in a crystallographic unit cell and number of molecules in a formula unit, respectively.

	crystal structures	CCDC refcodes or deposition numbers	E^{total} (kJ/mol)	N	E^{total} / N (kJ/mol)	$E^{coformer} + E^{LIN}$ / n
pure components	BA	BENZAC13	-802469	4	-200617.22	-394323.96
	PHBA	JOZZIH01	-971971	4	-242992.74	-292183.58 (max) -292184.74 (min)
	3,4-DHBA*H_2O	BIJDON03	-1323525	4	-330881.33	-358458.22
	3,4-DHBA	WUYNUA	-1712090	6	-285348.37	
	2,6-DHBA	LEZJAB01	-1141401	4	-285350.37	-436690.53
	GA*H_2O	KONTIQ01	-1492996	4	-373249.04	-320426.58
	LIN II	TIYQAU01	-2352123	4	-588030.69	
						E^{stab} (kJ/ mol of molecules)
cocrystals	LIN:BA	1993998	-1577296	4	-394324.01	-0.05
	LIN:PHBA:H_2O	1997194	-3506298	12	-292191.51	-2.98 – -1.81
	LIN:3,4-DHBA:H_2O	1994000	-7169307	21	-358465.34	-7.13
	LIN:2,6-DHBA	1994001	-3493622	8	-436702.70	-12.17
	LIN:GA:H_2O	1993999	-7690305	24	-320429.36	-2.78

Table S3. Experimental (δ_{exp}) and theoretical ^{13}C chemical shifts (δ_{calc}) and shielding constants (σ_{calc}) for LIN form II and III, together with the regression curve calculated after plotting δ_{exp} *vs.* σ_{calc} and RMSD values for (δ_{exp} and δ_{calc}) pairs.

LIN form II				LIN form III			
atom	δ_{exp} (ppm)	σ_{calc} (ppm)	δ_{calc} (ppm)	atom	δ_{exp} (ppm)	σ_{calc} (ppm)	δ_{calc} (ppm)
C1	23.75	149.87	22.37	C1A	21.44	152.52	18.78
C2	170.35	0.59	169.71	C2A	170.47	0.74	169.49
C3	43.63	128.27	43.69	C3A	42.95	128.26	42.87
C4	73.50	95.48	76.06	C4A	72.65	94.67	76.22
C5	48.59	122.89	49.00	C5A	47.81	122.19	48.89
C6	157.30	14.49	155.99	C6A	154.51	16.66	153.68
C7	134.13	38.04	132.75	C7A	133.28	38.43	132.06
C8	109.57	61.51	109.58	C8A	106.24	65.53	105.15
C9	157.30	9.84	160.58	C10A	136.00	33.85	136.61
C10	138.80	32.28	138.43	C11A	117.46	52.51	118.08
C11	119.93	51.55	119.41	C12A	113.86	55.27	115.34
C12	118.87	53.47	117.52	C1B	20.98	153.40	17.90
C13	52.52	122.71	49.18	C2B	170.94	-0.35	170.57
C14	67.01	104.9	66.76	C3B	42.85	128.69	42.44
C15	67.01	101.07	70.54	C4B	72.65	94.91	75.98
C16	52.52	118.64	53.20	C5B	47.81	122.09	48.99
				C6B	154.51	16.60	153.74
				C7B	133.28	38.04	132.45
				C8B	105.16	67.10	103.59
				C10B	136.00	34.03	136.43
				C11B	119.55	50.59	119.99
				C12B	112.93	56.75	113.87
regression curve	$\delta_{calc} = (\sigma_{calc} - 172.54) / -1.0132$			$\delta_{calc} = (\sigma_{calc} - 171.43) / -1.0071$			
RMSD	**1.76**			**1.59**			



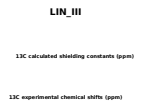


Figure S11. Experimental ^{13}C chemical shifts *vs.* calculated shielding constants for LIN forms II and III

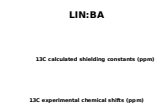
Table S4. Experimental (δ_{exp}) and theoretical ^{13}C chemical shifts (δ_{calc}) and shielding constants (σ_{calc}) for the cocrystals of LIN, together with the regression curve calculated after plotting δ_{exp} *vs.* σ_{calc} and RMSD values for (δ_{exp} and δ_{calc}) pairs.

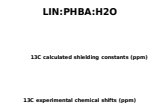
	LIN:BA			**LIN:PHBA:H_2O**			**LIN:2,6-DHBA:H_2O**		
atom	δ_{exp} (ppm)	σ_{calc} (ppm)	δ_{calc} (ppm)	δ_{exp} (ppm)	σ_{calc} (ppm)	δ_{calc} (ppm)	δ_{exp} (ppm)	σ_{calc} (ppm)	δ_{calc} (ppm)
C1	21.54	152.00	19.33	22.04	151.80	19.30	22.09	152.48	20.12
C2	175.37	-5.22	173.66	175.54	-5.76	174.08	174.93	-3.54	172.47
C3	42.89	127.57	43.31	43.04	127.52	43.15	46.76	124.87	47.09
C4	67.73	100.54	69.84	68.2	99.32	70.85	70.41	98.60	72.74
C5	47.41	123.32	47.48	47.11	123.83	46.78	48.88	122.36	49.54
C6	153.02	17.97	150.90	152.93	17.17	151.55	153.3	16.73	152.68
C7	133.1	36.65	132.56	135.09	33.61	135.40	130.27	41.48	128.51
C8	105.16	66.37	103.39	105.67	64.59	104.97	106.71	64.94	105.60
C9	156.3	10.10	158.62	156.5	9.52	159.07	155.65	10.62	158.65
C10	134.15	35.39	133.80	130.57	38.62	130.48	136.99	33.35	136.45
C11	118.35	51.74	117.75	118.8	50.08	119.22	119.42	51.33	118.89
C12	112.42	57.31	112.28	113.71	56.24	113.17	111.77	59.50	110.92
C13	53.27	117.01	53.68	51.26	118.32	52.19	52.22	121.62	50.26
C14	66.92	102.90	67.53	66.42	101.18	69.03	68.46	100.80	70.59
C15	68.71	98.80	71.55	66.42	100.91	69.29	68.46	100.41	70.97
C16	49.31	124.01	46.80	49.43	123.86	46.75	52.22	119.02	52.80
C1'	128.74	41.00	128.29	120.91	50.23	119.08	102.29	69.04	101.60
C2'	129.61	37.61	131.62	133.37	36.99	132.08	159.3	8.66	160.56
C3'	127.11	41.47	127.83	112.99	57.32	112.11	106.71	64.86	105.68
C4'	134.15	35.13	134.05	160.34	6.14	162.39	134.37	35.77	134.09
C5'	127.11	41.96	127.35	115.17	54.54	114.84	107.68	64.18	106.35
C6'	128.74	39.72	129.55	133.37	35.02	134.02	163.31	4.08	165.03
C7'	169.39	-0.77	169.29	169.21	0.05	168.37	171.19	-2.82	171.77
regression curve	$\delta_{calc} = (\sigma_{calc} - 171.69) / -1.0187$			$\delta_{calc} = (\sigma_{calc} - 171.45) / -1.0118$			$\delta_{calc} = (\sigma_{calc} - 173.09) / -1.0241$		
RMSD	**1.42**			**1.62**			**1.53**		

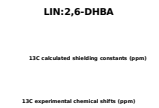
Table S4 continuation

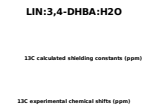
	LIN:3,4-DHBA:H_2O			LIN:GA:H_2O						
atom	δ_{exp} (ppm)	σ_{calc} (ppm)	δ_{calc} (ppm)	δ_{exp} (ppm)	σ_{calc} (ppm)	δ_{calc} (ppm)	atom	δ_{exp} (ppm)	σ_{calc} (ppm)	δ_{calc} (ppm)
C1A	23.99	149.31	23.28	21.36	152.56	19.30	C1C	21.73	151.17	20.67
C2A	173.44	-5.10	174.42	173.61	-2.29	171.55	C2C	173.61	-3.03	172.27
C3A	43.10	128.61	43.54	42.71	129.52	41.95	C3C	45.26	126.09	45.32
C4A	72.70	96.14	75.32	72.89	95.42	75.48	C4C	72.89	95.68	75.22
C5A	49.23	123.35	48.69	48.10	122.68	48.68	C5C	48.10	123.15	48.22
C6A	152.89	18.27	151.55	154.33	16.94	152.64	C6C	154.67	16.42	153.15
C7A	133.74	37.44	132.78	132.66	37.90	132.03	C7C	132.66	39.28	130.68
C8A	104.00	67.87	103.00	108.49	62.40	107.94	C8C	108.49	62.69	107.66
C9A	155.56	9.98	159.66	156.27	10.78	158.70	C9C	156.27	10.80	158.68
C10A	133.91	36.41	133.79	135.84	35.34	134.55	C10C	136.10	34.05	135.82
C11A	117.97	52.33	118.21	118.48	52.59	117.59	C11C	115.88	54.36	115.85
C12A	110.35	59.92	110.78	111.19	58.73	111.55	C12C	111.19	59.07	111.22
C13A	51.17	121.25	50.74	54.33	118.28	53.00	C13C	54.60	117.86	53.42
C14A	66.81	102.88	68.73	67.23	102.11	68.90	C14C	66.91	102.62	68.40
C15A	67.08	101.25	70.32	66.91	102.35	68.67	C15C	67.23	101.99	69.02
C16A	46.39	126.88	45.23	48.10	124.55	46.84	C16C	48.10	124.27	47.11
C1'A	122.17	47.94	122.50	118.29	52.80	117.38	C1'C	118.49	52.46	117.72
C2'A	115.61	55.16	115.44	110.50	60.66	109.65	C2'C	110.50	60.13	110.18
C3'A	143.76	23.54	146.39	145.79	21.80	147.86	C3'C	145.42	21.91	147.75
C4'A	153.18	16.16	153.61	139.04	27.87	141.89	C4'C	139.04	28.13	141.64
C5'A	116.55	52.56	117.98	145.24	22.52	147.15	C5'C	145.42	21.94	147.72
C6'A	127.02	42.64	127.69	107.96	64.04	106.33	C6'C	108.22	63.02	107.33
C7'A	173.72	-5.21	174.53	176.61	-5.04	174.25	C7'C	176.61	-4.79	174.00
C1B	23.20	150.60	22.01	21.73	151.41	20.43	C1D	21.73	151.60	20.24
C2B	177.44	-6.81	176.10	177.09	-6.48	175.67	C2D	173.61	-3.08	172.32
C3B	44.10	127.52	44.61	44.21	127.38	44.06	C3D	44.21	127.56	43.88
C4B	72.70	96.33	75.14	73.29	94.77	76.12	C4D	72.89	95.43	75.47
C5B	47.50	124.22	47.84	48.10	124.83	46.56	C5D	48.10	123.20	48.17
C6B	151.70	20.59	149.28	154.67	16.66	152.92	C6D	154.33	17.04	152.54
C7B	132.24	39.27	130.99	132.66	38.95	131.00	C7D	132.66	38.47	131.47
C8B	104.53	66.78	104.06	108.22	63.59	106.77	C8D	107.42	64.85	105.54
C9B	155.56	10.68	158.98	156.27	9.92	159.54	C9D	156.27	10.05	159.41
C10B	134.16	35.89	134.30	136.10	34.15	135.72	C10D	136.10	34.25	135.62
C11B	116.02	53.61	116.95	115.88	54.36	115.85	C11D	118.49	52.01	118.16
C12B	111.19	59.69	111.00	111.19	58.83	111.45	C12D	111.19	58.77	111.51
C13B	50.64	123.56	48.48	54.60	117.68	53.59	C13D	54.60	117.25	54.02
C14B	66.81	102.97	68.64	66.12	103.50	67.54	C14D	67.59	101.20	69.80
C15B	67.08	102.06	69.53	67.59	100.99	70.00	C15D	66.91	102.57	68.45
C16B	47.50	126.36	45.74	48.10	124.26	47.12	C16D	48.10	123.72	47.66
C1'B	120.62	50.57	119.93	117.75	53.20	116.99	C1'D	118.29	52.82	117.36
C2'B	116.02	53.21	117.35	110.05	61.37	108.96	C2'D	110.50	60.18	110.13
C3'B	143.53	23.70	146.23	145.42	21.99	147.67	C3'D	145.24	22.39	147.28
C4'B	153.18	14.28	155.45	139.04	27.53	142.23	C4'D	139.04	28.15	141.62
C5'B	116.55	53.00	117.55	145.79	21.63	148.03	C5'D	145.24	22.95	146.73
C6'B	125.97	44.26	126.11	107.42	64.80	105.58	C6'D	107.96	64.04	106.33

C7'B	175.13	-5.29	174.61	176.87	-5.35	174.56	C7'D	176.87	-5.31	174.52
regression curve	$\delta_{calc} = (\sigma_{calc} - 173.09) / -1.0261$					$\delta_{calc} = (\sigma_{calc} - 172.19) / -1.0171$				
RMSD	**1.61**					**1.65**				


LIN:BA
13C calculated shielding constants (ppm)
13C experimental chemical shifts (ppm)


LIN:PHBA:H2O
13C calculated shielding constants (ppm)
13C experimental chemical shifts (ppm)


LIN:2,6-DHBA
13C calculated shielding constants (ppm)
13C experimental chemical shifts (ppm)


LIN:3,4-DHBA:H2O
13C calculated shielding constants (ppm)
13C experimental chemical shifts (ppm)

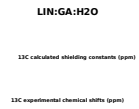


Figure S12. Experimental ^{13}C chemical shifts *vs.* calculated shielding constants for the cocrystals of LIN.

Table S5. D…A and D-H…A distances (in Å), as well as D-H…A angle values (in °) oberved in the analyzed crystal structures of LIN.

Crystal structure	HB interaction	D…A distance	D-H…A distance	D-H…A angle
LIN_II	NH…O=C_{ring}	2.995	2.214	176.23
LIN_III	NH…O=C_{ring} (1)	2.970	2.068	167.46
	NH…O=C_{ring} (2)	2.972	2.040	149.12
LIN:BA	NH…O=$C_{carboxylic}$	2.834	2.039	153.27
	$OH_{carboxylic}$…O=C_{amide}	2.618	1.808	168.74
LIN:PHBA:H_2O	NH…O=$C_{carboxylic}$	2.809	2.021	148.36
	$OH_{carboxylic}$…O=C_{amide}	2.601	1.794	160.70
	OH_{phenol}…OH_{water}	2.683	1.981	140.52
	OH_{water}…O_{morph}	2.825	2.120	137.99
	OH_{water}…N_{morph}	2.971	2.122	165.81
LIN:2,6-DHBA	NH…O=C_{ring}	2.922	2.064	175.07
	$OH_{carboxylic}$…O=C_{amide}	2.564	1.745	175.41
	OH_{phenol}…$OH_{carboxylic}$	2.608	1.902	143.55
	OH_{phenol}…O=$C_{carboxylic}$	2.567	1.877	141.19
LIN:3,4-DHBA:H_2O	NH…O=C_{amide} (1)	3.092	2.279	157.74
	NH…O=C_{amide} (2)	3.056	2.235	159.83
	OH_{phenol}…O=C_{amide} (1)	2.713	1.950	154.56
	OH_{phenol}…O=C_{amide} (2)	2.689	1.911	158.13
	OH_{phenol}…O_{morph} (1)	2.684	1.915	155.80
	OH_{phenol}…O_{morph} (2)	2.739	2.011	147.53
	$OH_{carboxylic}$…O=$C_{carboxylic}$ (1)	2.615	1.830	159.72
	$OH_{carboxylic}$…O=$C_{carboxylic}$ (2)	2.638	1.842	163.33
	OH_{water}…O=$C_{carboxylic}$	2.905	2.075	165.01
	OH_{water}…OH_{water}	2.915	2.117	155.95
	OH_{water}…$OH_{carboxylic}$	3.198	2.546	134.37
LIN:GA:H_2O	NH…O=C_{ring} (1)	2.931	2.081	150.69

$NH\ldots O{=}C_{ring}$ (2)	3.031	2.188	166.47
$NH\ldots O{=}C_{ring}$ (3)	2.973	2.124	169.38
$NH\ldots O{=}C_{ring}$ (4)	3.270	2.182	147.55
$OH_{phenol}\ldots O{=}C_{amide}$ (1)	2.728	2.031	142.61
$OH_{phenol}\ldots O{=}C_{amide}$ (2)	2.719	2.032	141.12
$OH_{phenol}\ldots O{=}C_{amide}$ (3)	2.793	2.095	142.86
$OH_{phenol}\ldots O{=}C_{amide}$ (4)	2.830	2.134	142.64
$OH_{phenol}\ldots O_{morph}$ (1)	2.765	1.962	166.30
$OH_{phenol}\ldots O_{morph}$ (2)	2.759	1.969	161.80
$OH_{phenol}\ldots O_{morph}$ (3)	2.699	1.882	173.97
$OH_{phenol}\ldots O_{morph}$ (4)	2.701	1.904	163.78
$OH_{water}\ldots O{=}C_{amide}$ (1)	2.763	1.940	162.73
$OH_{water}\ldots O{=}C_{amide}$ (2)	2.753	1.909	172.46
$OH_{water}\ldots O{=}C_{amide}$ (3)	2.787	1.956	165.52
$OH_{water}\ldots O{=}C_{amide}$ (3')	2.863	2.020	171.86
$OH_{water}\ldots O{=}C_{amide}$ (4)	2.823	1.975	174.09
$OH_{water}\ldots O{=}C_{amide}$ (4')	2.828	1.860	177.47
$OH_{carboxylic}\ldots O{=}C_{carboxylic}$ (1)	2.594	1.777	173.70
$OH_{carboxylic}\ldots O{=}C_{carboxylic}$ (2)	2.638	1.821	174.71
$OH_{carboxylic}\ldots O{=}C_{carboxylic}$ (3)	2.598	1.782	173.99
$OH_{carboxylic}\ldots O{=}C_{carboxylic}$ (4)	2.646	1.831	172.81
$OH_{phenol}\ldots OH_{water}$ (1)	2.749	2.000	151.62
$OH_{phenol}\ldots OH_{water}$ (2)	2.624	1.836	160.77
$OH_{phenol}\ldots OH_{water}$ (3)	2.617	1.840	157.79
$OH_{phenol}\ldots OH_{water}$ (4)	2.786	2.013	156.87
$OH_{water}\ldots OH_{water}$ (1)	2.824	1.975	178.37
$OH_{water}\ldots OH_{water}$ (2)	2.825	1.989	167.70

Table S6. A comparison of the torsion angle values (in °) for all confromations of LIN found in the analysed crystal structures.

	NH_{amide}-C3-C4-O	C6-N_{oxa}-C7-C8	C9-C10-N_{morph}-C13
LIN_II	-63.23	-134.16	-68.77
LIN_III mol A	-61.31	-5.51	-65.32
LIN_III mol B	-61.72	+20.91	+61.20
LIN:BA	-173.07	-20.06	+69.25
LIN:PHBA:H_2O	-172.95	-20.16	-65.34
LIN:2,6-DHBA	-65.18	+179.85	+57.05
LIN:3,4-DHBA:H_2O mol A	-63.30	+12.28	-67.27
LIN:3,4-DHBA:H_2O mol B	-70.79	-2.08	+60.42
LIN:GA:H_2O mol A	-66.39	-8.77	-68.66
LIN:GA:H_2O mol B	-60.01	+20.71	+63.48
LIN:GA:H_2O mol C	-67.43	-13.75	-63.97
LIN:GA:H_2O mol D	-60.27	+21.95	+66.97