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Supplementary Information

Nucleation Control and Separation of Ethyl Maltol Polymorphs under Different Growth Conditions through Solution Crystallization Process in Selected Solvent Environments

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Single Crystal X-ray diffraction (SCXRD) data on Form-I, Form-II, and Form-III polymorphs of ethyl maltol (Table S1 to S18).

Table S1. Non-hydrogen atoms with anisotropic atomic displacement parameters (Å^2) for Form-I polymorph

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0511(13)	0.0457(13)	0.0431(13)	0.0000(11)	0.0118(10)	-0.0042(11)
O2	0.0569(14)	0.0407(12)	0.0507(14)	-0.0002(11)	0.0219(11)	0.0009(11)
O3	0.0708(16)	0.0350(12)	0.0480(15)	-0.0042(11)	0.0192(12)	-0.0083(12)
C4	0.0404(18)	0.0306(17)	0.0311(17)	0.0016(13)	0.0034(15)	0.0022(14)
C3	0.0362(18)	0.0349(17)	0.0308(17)	0.0078(14)	-0.0016(15)	0.0051(15)
C5	0.0434(19)	0.0336(17)	0.0329(17)	0.0006(15)	0.0028(15)	0.0028(15)
C2	0.049(2)	0.0315(16)	0.0391(19)	-0.0042(14)	0.0038(16)	0.0042(15)
C1	0.059(2)	0.0367(18)	0.048(2)	-0.0032(17)	0.0019(18)	-0.0076(16)
C6	0.052(2)	0.052(2)	0.047(2)	-0.0039(16)	0.0131(17)	0.0106(17)
C7	0.092(3)	0.058(2)	0.045(2)	-0.0065(18)	0.015(2)	0.002(2)

Table S2. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for Form-I Polymorph

	x/a	y/b	z/c	U(eq)
H3	0.3506	0.1255	0.6939	0.076
H2	0.5809	0.7525	0.7190	0.048
H1	0.8981	0.7768	0.6462	0.058
H6A	0.7566	0.0697	0.5746	0.06
H6B	1.0123	0.1991	0.5623	0.06
H7A	0.4883	0.2392	0.4919	0.097
H7B	0.7470	0.1492	0.4622	0.097
H7C	0.7423	0.3710	0.4799	0.097

Table S3. Atomic coordinates and equivalent isotropic atomic displacement Parameters (Å^2) for Form-I polymorph

	x/a	y/b	z/c	U(eq)
O1	0.8659(4)	0.5143(3)	0.60844(10)	0.0462(6)
O2	0.3071(4)	0.4387(3)	0.74249(11)	0.0484(6)
O3	0.4224(5)	0.1370(3)	0.65887(10)	0.0504(7)
C4	0.5477(6)	0.3127(4)	0.65726(13)	0.0340(7)
C3	0.4762(6)	0.4662(4)	0.70131(14)	0.0342(7)
C5	0.7323(6)	0.3398(4)	0.61284(14)	0.0367(8)
C2	0.6187(6)	0.6453(4)	0.69321(14)	0.0400(8)
C1	0.8048(7)	0.6595(4)	0.64908(15)	0.0480(9)
C6	0.8127(7)	0.1991(4)	0.56224(14)	0.0497(9)
C7	0.6860(8)	0.2437(5)	0.49273(15)	0.0649(11)

Table S4. Bond lengths (Å) for Form-I polymorph

O1-C1	1.343(3)	O1-C5	1.372(3)
O2-C3	1.235(3)	O3-C4	1.355(3)
O3-H3	0.82	C4-C5	1.337(4)
C4-C3	1.442(4)	C3-C2	1.430(4)
C5-C6	1.484(4)	C2-C1	1.329(4)
C2-H2	0.93	C1-H1	0.93
C6-C7	1.511(4)	C6-H6A	0.97
C6-H6B	0.97	C7-H7A	0.96
C7-H7B	0.96	C7-H7C	0.96

Table S5. Bond angles (°) for Form-I polymorph

C1-O1-C5	118.7(2)	C4-O3-H3	109.5
C5-C4-O3	118.1(2)	C5-C4-C3	121.6(3)
O3-C4-C3	120.3(2)	O2-C3-C2	124.5(3)
O2-C3-C4	121.0(3)	C2-C3-C4	114.5(3)
C4-C5-O1	121.0(2)	C4-C5-C6	127.2(3)
O1-C5-C6	111.8(2)	C1-C2-C3	120.4(3)
C1-C2-H2	119.8	C3-C2-H2	119.8
C2-C1-O1	123.8(3)	C2-C1-H1	118.1
O1-C1-H1	118.1	C5-C6-C7	113.3(2)
C5-C6-H6A	108.9	C7-C6-H6A	108.9
C5-C6-H6B	108.9	C7-C6-H6B	108.9
H6A-C6-H6B	107.7	C6-C7-H7A	109.5
C6-C7-H7B	109.5	H7A-C7-H7B	109.5
C6-C7-H7C	109.5	H7A-C7-H7C	109.5

H7B-C7-H7C	109.5		

Table S6. Torsion angles (°) for Form-I polymorph

C5-C4-C3-O2	-179.4(3)	O3-C4-C3-O2	2.3(4)
C5-C4-C3-C2	-0.2(4)	O3-C4-C3-C2	-178.5(3)
O3-C4-C5-O1	179.8(2)	C3-C4-C5-O1	1.4(4)
O3-C4-C5-C6	2.1(4)	C3-C4-C5-C6	-176.2(3)
C1-O1-C5-C4	-1.0(4)	C1-O1-C5-C6	177.0(2)
O2-C3-C2-C1	177.6(3)	C4-C3-C2-C1	-1.6(4)
C3-C2-C1-O1	2.1(5)	C5-O1-C1-C2	-0.8(4)
C4-C5-C6-C7	103.4(4)	O1-C5-C6-C7	-74.4(3)

Table S7. Non-hydrogen atoms with anisotropic atomic displacement parameters ($Å^2$) for Form-II polymorph

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O3	0.0353(4)	0.0359(4)	0.0718(6)	-0.0161(4)	-0.0119(4)	0.0193(3)
O1	0.0525(5)	0.0348(4)	0.0544(5)	-0.0040(3)	-0.0062(4)	0.0261(4)
O2	0.0379(4)	0.0400(5)	0.0704(6)	-0.0001(4)	-0.0079(4)	0.0228(4)
C2	0.0287(5)	0.0304(5)	0.0367(5)	0.0000(4)	0.0026(4)	0.0138(4)
C1	0.0285(5)	0.0329(5)	0.0377(5)	0.0040(4)	0.0040(4)	0.0145(4)
C3	0.0371(5)	0.0350(5)	0.0357(5)	0.0006(4)	0.0012(4)	0.0196(4)
C5	0.0339(5)	0.0363(5)	0.0416(6)	-0.0021(4)	-0.0029(4)	0.0125(4)
C6	0.0478(7)	0.0504(7)	0.0469(6)	0.0004(5)	-0.0065(5)	0.0312(6)
C4	0.0457(6)	0.0329(5)	0.0504(7)	-0.0068(5)	-0.0041(5)	0.0151(5)

C7	0.0476(7)	0.0699(9)	0.0747(9)	0.0146(7)	0.0054(6)	0.0369(7)

Table S8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for Form-II Polymorph

	x/a	**y/b**	**z/c**	**U(eq)**
H3	0.5734	0.6699	0.3801	0.07
H5	0.7304	0.8657	0.6909	0.047
H6A	0.4771	0.7457	0.2806	0.054
H6B	0.5089	0.8310	0.2674	0.054
H4	0.6837	0.9395	0.6495	0.054
H7A	0.4184	0.7418	0.5336	0.091
H7B	0.3945	0.7794	0.3953	0.091
H7C	0.4535	0.8277	0.5314	0.091

Table S9. Atomic coordinates and equivalent isotropic atomic displacement Parameters (Å^2) for Form-II polymorph

	x/a	**y/b**	**z/c**	**U(eq)**
O3	0.54633(4)	0.68699(4)	0.39718(12)	0.0470(3)
O1	0.59834(5)	0.87239(4)	0.51082(11)	0.0453(2)
O2	0.67413(4)	0.73064(4)	0.58150(12)	0.0479(3)
C2	0.58598(5)	0.75526(5)	0.46398(13)	0.0323(2)
C1	0.65185(5)	0.77502(5)	0.56092(13)	0.0334(2)
C3	0.56209(6)	0.80376(6)	0.44108(13)	0.0352(3)
C5	0.68730(6)	0.84860(6)	0.62813(14)	0.0395(3)
C6	0.49551(7)	0.79072(7)	0.34614(16)	0.0454(3)
C4	0.65956(7)	0.89260(6)	0.60217(16)	0.0450(3)
C7	0.43492(8)	0.78433(9)	0.4622(2)	0.0607(4)

Table S10. Bond lengths (Å) for Form-II polymorph

O3-C2	1.3515(12)	O3-H3	0.82
O1-C4	1.3423(15)	O1-C3	1.3624(13)
O2-C1	1.2427(13)	C2-C3	1.3512(14)
C2-C1	1.4459(14)	C1-C5	1.4373(14)
C3-C6	1.4837(15)	C5-C4	1.3293(17)
C5-H5	0.93	C6-C7	1.5162(19)
C6-H6A	0.97	C6-H6B	0.97
C4-H4	0.93	C7-H7A	0.96
C7-H7B	0.96	C7-H7C	0.96

Table S11. Bond angles (°) for Form-II polymorph

C2-O3-H3	109.5	C4-O1-C3	119.36(9)
C3-C2-O3	118.78(9)	C3-C2-C1	121.01(9)
O3-C2-C1	120.19(9)	O2-C1-C5	124.68(10)
O2-C1-C2	121.14(9)	C5-C1-C2	114.18(9)
C2-C3-O1	121.31(10)	C2-C3-C6	126.67(10)
O1-C3-C6	112.01(9)	C4-C5-C1	121.13(10)
C4-C5-H5	119.4	C1-C5-H5	119.4
C3-C6-C7	112.38(11)	C3-C6-H6A	109.1
C7-C6-H6A	109.1	C3-C6-H6B	109.1
C7-C6-H6B	109.1	H6A-C6-H6B	107.9
C5-C4-O1	122.99(10)	C5-C4-H4	118.5
O1-C4-H4	118.5	C6-C7-H7A	109.5
C6-C7-H7B	109.5	H7A-C7-H7B	109.5

C6-C7-H7C	109.5	H7A-C7-H7C	109.5
H7B-C7-H7C	109.5		

Table S12. Torsion angles (°) for Form-II polymorph

C3-C2-C1-O2	-179.66(10)	O3-C2-C1-O2	1.62(15)
C3-C2-C1-C5	0.33(14)	O3-C2-C1-C5	-178.38(9)
O3-C2-C3-O1	177.55(9)	C1-C2-C3-O1	-1.18(15)
O3-C2-C3-C6	-0.78(17)	C1-C2-C3-C6	-179.52(10)
C4-O1-C3-C2	0.91(16)	C4-O1-C3-C6	179.47(10)
O2-C1-C5-C4	-179.22(11)	C2-C1-C5-C4	0.78(15)
C2-C3-C6-C7	108.44(14)	O1-C3-C6-C7	-70.03(13)
C1-C5-C4-O1	-1.11(18)	C3-O1-C4-C5	0.25(17)

Table S13. Non-hydrogen atoms with anisotropic atomic displacement parameters (Å^2) for Form-III polymorph

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0483(7)	0.0986(10)	0.0488(7)	-0.0272(7)	-0.0153(5)	-0.0217(6)
O3	0.0503(7)	0.0777(8)	0.0501(7)	-0.0225(6)	-0.0100(5)	-0.0143(6)
O2	0.0546(7)	0.0954(10)	0.0449(7)	-0.0169(6)	-0.0178(5)	-0.0188(6)
C1	0.0455(8)	0.0566(9)	0.0510(9)	-0.0255(7)	-0.0155(7)	-0.0024(7)
C2	0.0409(8)	0.0533(9)	0.0479(8)	-0.0227(7)	-0.0154(6)	-0.0035(6)
C3	0.0438(8)	0.0505(9)	0.0487(9)	-0.0201(7)	-0.0185(7)	-0.0020(6)
C4	0.0467(9)	0.0621(10)	0.0589(10)	-0.0244(8)	-0.0243(7)	-0.0042(7)
C6	0.0622(11)	0.0774(12)	0.0481(9)	-0.0281(8)	-0.0173(8)	-0.0086(9)
C5	0.0438(9)	0.0782(12)	0.0654(11)	-0.0279(9)	-0.0165(8)	-0.0127(8)

C7	0.0882(14)	0.0794(14)	0.0706(13)	-0.0165(10)	-0.0409(11)	-0.0076(11)

Table S14. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for Form-III Polymorph

	x/a	**y/b**	**z/c**	**U(eq)**
H1	-0.0019	0.0600	0.7938	0.095
H4	0.5924	0.1567	0.7802	0.064
H6A	0.1516	0.2161	0.2767	0.073
H6B	0.3611	0.2926	0.1187	0.073
H5	0.7419	0.3044	0.4421	0.074
H7A	0.0486	0.5295	0.2794	0.12
H7B	0.1085	0.5484	0.0536	0.12
H7C	0.2580	0.6060	0.1220	0.12

Table S15. Atomic coordinates and equivalent isotropic atomic displacement Parameters (Å^2) for Form-III polymorph

	x/a	**y/b**	**z/c**	**U(eq)**
O1	0.04608(17)	0.1032(2)	0.66783(17)	0.0636(4)
O3	0.52265(17)	0.30608(18)	0.34480(17)	0.0611(4)
O2	0.22952(18)	0.0360(2)	0.95314(17)	0.0669(4)
C1	0.3323(2)	0.2495(2)	0.4085(2)	0.0498(4)
C2	0.2331(2)	0.1591(2)	0.6107(2)	0.0462(4)
C3	0.3227(2)	0.1186(2)	0.7675(2)	0.0469(4)
C4	0.5233(2)	0.1792(2)	0.6890(3)	0.0537(4)
C6	0.2521(3)	0.3060(3)	0.2342(3)	0.0610(5)
C5	0.6112(3)	0.2672(3)	0.4876(3)	0.0619(5)
C7	0.1583(3)	0.5165(3)	0.1661(3)	0.0801(6)

Table S16. Bond lengths (Å) for Form-III polymorph

O1-C2	1.3490(18)	O1-H1	0.82
O3-C5	1.346(2)	O3-C1	1.3641(19)
O2-C3	1.2374(19)	C1-C2	1.344(2)
C1-C6	1.489(2)	C2-C3	1.442(2)
C3-C4	1.430(2)	C4-C5	1.322(2)
C4-H4	0.93	C6-C7	1.506(3)
C6-H6A	0.97	C6-H6B	0.97
C5-H5	0.93	C7-H7A	0.96
C7-H7B	0.96	C7-H7C	0.96

Table S17. Bond angles (°) for Form-III polymorph

C2-O1-H1	109.5	C5-O3-C1	118.95(13)
C2-C1-O3	120.71(14)	C2-C1-C6	126.25(15)
O3-C1-C6	113.00(14)	C1-C2-O1	119.01(13)
C1-C2-C3	121.64(14)	O1-C2-C3	119.35(13)
O2-C3-C4	124.49(14)	O2-C3-C2	121.05(14)
C4-C3-C2	114.47(14)	C5-C4-C3	120.40(15)
C5-C4-H4	119.8	C3-C4-H4	119.8
C1-C6-C7	111.51(15)	C1-C6-H6A	109.3
C7-C6-H6A	109.3	C1-C6-H6B	109.3
C7-C6-H6B	109.3	H6A-C6-H6B	108.0
C4-C5-O3	123.82(15)	C4-C5-H5	118.1
O3-C5-H5	118.1	C6-C7-H7A	109.5
C6-C7-H7B	109.5	H7A-C7-H7B	109.5

C6-C7-H7C	109.5	H7A-C7-H7C	109.5
H7B-C7-H7C	109.5		

Table S18. Torsion angles (°) for Form-III polymorph

C5-O3-C1-C2	1.0(2)	C5-O3-C1-C6	178.75(15)
O3-C1-C2-O1	-179.21(14)	C6-C1-C2-O1	3.4(3)
O3-C1-C2-C3	0.1(2)	C6-C1-C2-C3	-177.36(15)
C1-C2-C3-O2	179.71(16)	O1-C2-C3-O2	-1.0(2)
C1-C2-C3-C4	-1.0(2)	O1-C2-C3-C4	178.29(14)
O2-C3-C4-C5	-179.85(17)	C2-C3-C4-C5	0.9(2)
C2-C1-C6-C7	92.9(2)	O3-C1-C6-C7	-84.66(18)
C3-C4-C5-O3	0.2(3)	C1-O3-C5-C4	-1.1(3)