Supporting Information for

Novel Ascorbic Acid Co-Crystal Formulations for Improved Stability

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Table S1. selected bond lengths (Å) and bond angles (°).

C(1)-C(2)	1.515(9)	C(13)-C(14)	1.347(9)
C(2)-C(3)	1.378(9)	C(13)-C(16)	1.450(9)
C(2)-C(6)	1.397(9)	C(14)-C(15)	1.495(9)
C(3)-C(4)	1.384(9)	C(15)-C(17)	1.529(8)
C(5)-C(6)	1.383(9)	C(17)-C(18)	1.503(10)
C(19)-C(20)	1.389(10)	O(12)-C(12)	1.279(8)
C(20)-C(21)	1.382(9)	O(13)-C(12)	1.225(8)
C(21)-C(22)	1.390(9)	N(2)-C(7)	1.338(9)
C(21)-C(24)	1.517(9)	N(2)-C(11)	1.328(9)
C(22)-C(23)	1.387(10)	C(7)-C(8)	1.385(10)
N(1)-C(4)	1.333(8)	C(8)-C(9)	1.379(9)
N(1)-C(5)	1.341(8)	C(9)-C(10)	1.382(9)
N(3)-C(19)	1.344(9)	C(9)-C(12)	1.525(9)
N(3)-C(23)	1.331(9)	C(10)-C(11)	1.386(10)
O(1)-C(24)	1.237(8)	O(14)-C(29)	1.332(8)
O(2)-C(24)	1.260(7)	O(15)-C(30)	1.223(8)
O(3)-C(1)	1.235(8)	O(16)-C(27)	1.458(7)
O(4)-C(1)	1.275(8)	O(16)-C(30)	1.360(8)
O(5)-C(16)	1.215(7)	O(17)-C(26)	1.425(8)
O(6)-C(13)	1.346(8)	O(18)-C(28)	1.322(8)
O(7)-C(15)	1.444(7)	O(19)-C(25)	1.420(8)
O(7)-C(16)	1.355(8)	C(25)-C(26)	1.523(9)
O(8)-C(14)	1.335(8)	C(25)-C(27)	1.524(8)
O(9)-C(17)	1.409(8)	C(27)-C(28)	1.496(9)
O(10)-C(18)	1.401(11)	C(28)-C(29)	1.362(8)
O(11)-C(18)	1.281(13)	C(29)-C(30)	1.440(9)
O(22)-C(34)	1.314(8)	O(20)-C(31)	1.430(8)
O(23)-C(35)	1.353(7)	O(21)-C(32)	1.417(8)
C(32)-C(33)	1.521(8)	O(24)-C(36)	1.218(7)
C(33)-C(34)	1.501(9)	O(25)-C(33)	1.460(7)
C(34)-C(35)	1.357(8)	O(25)-C(36)	1.363(7)
C(35)-C(36)	1.440(9)	C(31)-C(32)	1.514(9)
C(23)-N(3)-C(19)	122.6(6)	C(10)-C(9)-C(12)	119.8(6)
N(3)-C(19)-C(20)	119.3(6)	C(9)-C(10)-C(11)	118.8(6)
C(21)-C(20)-C(19)	119.7(6)	N(2)-C(11)-C(10)	119.6(6)
C(20)-C(21)-C(22)	119.2(6)	O(12)-C(12)-C(9)	115.6(5)
C(20)-C(21)-C(24)	121.4(5)	O(13)-C(12)-O(12)	126.0(6)
C(22)-C(21)-C(24)	119.4(5)	O(13)-C(12)-C(9)	118.3(6)
C(23)-C(22)-C(21)	119.3(6)	C(30)-O(16)-C(27)	108.4(5)

N(3)-C(23)-C(22)	119.9(6)	O(19)-C(25)-C(26)	107.8(5)
O(1)-C(24)-O(2)	125.6(6)	O(19)-C(25)-C(27)	110.3(5)
O(1)-C(24)-C(21)	118.4(5)	C(26)-C(25)-C(27)	113.1(5)
O(2)-C(24)-C(21)	116.0(5)	O(17)-C(26)-C(25)	112.2(5)
C(4)-N(1)-C(5)	122.2(6)	O(16)-C(27)-C(25)	110.4(5)
O(3)-C(1)-O(4)	126.2(6)	O(16)-C(27)-C(28)	104.0(5)
O(3)-C(1)-C(2)	117.9(6)	C(28)-C(27)-C(25)	112.7(5)
O(4)-C(1)-C(2)	115.9(5)	O(18)-C(28)-C(27)	118.1(5)
C(3)-C(2)-C(1)	119.1(5)	O(18)-C(28)-C(29)	132.4(6)
C(3)-C(2)-C(6)	120.1(6)	C(29)-C(28)-C(27)	109.5(6)
C(6)-C(2)-C(1)	120.7(6)	O(14)-C(29)-C(28)	134.7(6)
C(2)-C(3)-C(4)	118.9(6)	O(14)-C(29)-C(30)	118.2(5)
N(1)-C(4)-C(3)	120.2(6)	C(28)-C(29)-C(30)	107.1(6)
N(1)-C(5)-C(6)	120.3(6)	O(15)-C(30)-O(16)	120.5(6)
C(5)-C(6)-C(2)	118.3(6)	O(15)-C(30)-C(29)	128.5(6)
C(16)-O(7)-C(15)	108.9(5)	O(16)-C(30)-C(29)	111.0(5)
O(6)-C(13)-C(14)	134.2(6)	C(36)-O(25)-C(33)	108.4(5)
O(6)-C(13)-C(16)	118.5(5)	O(20)-C(31)-C(32)	111.4(5)
C(14)-C(13)-C(16)	107.4(6)	O(21)-C(32)-C(31)	106.5(5)
O(8)-C(14)-C(13)	133.7(6)	O(21)-C(32)-C(33)	111.2(5)
O(8)-C(14)-C(15)	116.6(5)	C(31)-C(32)-C(33)	113.2(5)
C(13)-C(14)-C(15)	109.5(5)	O(25)-C(33)-C(32)	112.2(5)
O(7)-C(15)-C(14)	104.1(5)	O(25)-C(33)-C(34)	104.1(4)
O(7)-C(15)-C(17)	110.6(5)	C(34)-C(33)-C(32)	112.1(5)
C(14)-C(15)-C(17)	116.0(6)	O(22)-C(34)-C(33)	116.9(5)
O(5)-C(16)-O(7)	121.3(6)	O(22)-C(34)-C(35)	133.9(6)
O(5)-C(16)-C(13)	128.6(6)	C(35)-C(34)-C(33)	109.1(5)
O(7)-C(16)-C(13)	110.1(5)	O(23)-C(35)-C(34)	134.0(6)
O(9)-C(17)-C(15)	110.4(5)	O(23)-C(35)-C(36)	118.2(5)
O(9)-C(17)-C(18)	110.7(6)	C(34)-C(35)-C(36)	107.8(5)
C(18)-C(17)-C(15)	110.3(6)	O(24)-C(36)-O(25)	120.1(6)
O(10)-C(18)-C(17)	118.7(8)	O(24)-C(36)-C(35)	129.3(6)
O(11)-C(18)-C(17)	116.0(7)	O(25)-C(36)-C(35)	110.6(5)
C(9)-C(8)-C(7)	118.9(6)	C(11)-N(2)-C(7)	123.0(6)
C(8)-C(9)-C(10)	120.2(6)	N(2)-C(7)-C(8)	119.5(6)
C(8)-C(9)-C(12)	119.9(6)		

Table S2. Hydrogen bond length (Å) and bond angle (°).

Hydrogen bond	D…A	D—H…A	Hydrogen bond	D…A	D—H…A
N(1)—H(1)…O(24A)	2.710(7)	173	O(8)—H(8)…O(12B)	2.547(7)	147
N(2)—H(2)…O(15B)	2.705(7)	163	O(9)—H(9)…O(11B)	2.591(11)	138
N(3)—H(3)…O(5B)	2.766(8)	168	O(14)—H(14)…O(3C)	2.560(8)	159
O(6)—H(6)…O(13B)	2.647(7)	159	O(17)—H(17A)…O(18D)	2.759(7)	159
O(8)—H(8)…O(12B)	2.547(7)	147	O(18)—H(18)…O(4C)	2.459(7)	152
O(9)—H(9)…O(11B)	2.591(11)	138	O(19)—H(19)…O(17B)	2.700(7)	172
O(14)—H(14)…O(3C)	2.560(8)	159	O(20)—H(20)…O(12)	2.788(7)	153(11)
O(17)—H(17A)…O(18D)	2.759(7)	159	O(21)—H(21)…O(20B)	2.728(7)	173(7)
O(18)—H(18)…O(4C)	2.459(7)	152	O(22)—H(22)…O(2E)	2.524(7)	156
N(1)—H(1)…O(24A)	2.710(7)	173	O(23)—H(23)…O(1E)	2.622(7)	158
N(2)—H(2)…O(15B)	2.705(7)	163	O(6)—H(6)…O(13B)	2.647(7)	159
N(3)—H(3)…O(5B)	2.766(8)	168			

A: -1/2+x,-1/2+y,z; B: x,-1+y,z; C: 1-x,-1+y,1-z; D: 3/2-x,1/2+y,1-z; E: 1-x,-1+y,-z.