

SUPPLEMENTARY INFORMATION

Thymine Cocrystals Based on DNA-Inspired Binding Motifs

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Table S1. CSD Entries for Single and Multicomponent Crystals Containing Thymine

Table S2. CSD Entries for Single and Multicomponent Crystals Containing Adenine

Table S3. CSD Entries for Single and Multicomponent Crystals Containing Guanine

Table S4. CSD Entries for Single and Multicomponent Crystals Containing Cytosine

Fig. S1. Optical micrographs of the three cocrystals: (a) **T:DAP**, (b) **T:TAP·H₂O**, and (c) **T:DAHP·3H₂O**.

Fig. S2. Hot stage microscopy of **T:DAHP·3H₂O** in air. Progressive water loss upon heating causes the crystal to turn opaque. At temperatures >250°C, the polycrystalline material appears to decompose and/or melt. Scale bar =140 μm.

Fig. S3. Possible tautomeric forms of (7), (8) and (9).

Fig. S4. TGA of (top) **T:DAP**, (middle) **T:TAP·H₂O**, and (bottom) **T:DAHP·3H₂O**.

Table S5. Hydrogen Bond Distances in cocrystals of (a) **T:DAP**, (b) **T:TAP·H₂O** and (c) **T:DHAP·3H₂O**.

Table S1. CSD Entries for Single and Multicomponent Crystals Containing Thymine

charge	REFCODE	# components	name
0	THYMIN THYMIN01 THYMIN02 THYMIN03	1	Thymine
0	OGIYEK	2	5-Methylpyrimidine-2,4(1H,3H)-dione benzene-1,2-diol
0	OGIYIO	2	bis(5-Methylpyrimidine-2,4(1H,3H)-dione) benzene-1,3-diol
0	OGIYOU	2	bis(5-Methylpyrimidine-2,4(1H,3H)-dione) benzene-1,4-diol
0	OGIYUA	2	5-Methylpyrimidine-2,4(1H,3H)-dione bis(benzene-1,2,3-triol)
0	THYBNZ10	2	Thymine-p-benzoquinone complex
0	THYMEL	3	Thymine N,N-diethylmelamine monohydrate
0	THYMMH	2	Thymine monohydrate
0	WNSAO WNSAO01	3	Thymine hydrogen peroxide solvate hydrate
0	WUPGOE*	3	5-Methylpyrimidine-2,4(1H,3H)-dione 9H-purin-6-amine dihydrate
0	WUPGUK*	3	5-Methylpyrimidine-2,4(1H,3H)-dione 9H-purin-6-amine tetrahydrate
0	YAFGEU	2	thymine hydrogen peroxide
0	YUXHAC	3	2,4-dihydroxybenzoic acid 5-methylpyrimidine-2,4(1H,3H)-dione monohydrate

Table S2. CSD Entries for Single and Multicomponent Crystals Containing Adenine

charge	REFCODE	# components	name
0	KOBFUD KOBFUD01	1	Adenine
0	ADRBFT10	3	Adenine-riboflavin trihydrate
0	BERNAP	3	6-Isopropylpyrimidine-2,4(1H,3H)-dione 9H-purin-6-amine dihydrate
0	COFBUU	2	Adenine bis(N-methyl-2-pyrrolidone)
0	DXCADM10	3	Deoxycorticosterone-adenine monohydrate
0	FUSVAQ	2	Adenine trihydrate
0	JOZZED	2	Adenine hydrogen peroxide
0	KORGUV	3	adenine 2,4,6-trinitrophenol methanol solvate
0	LOLCUL	3	bis(9H-Purin-6-amine) adipic acid methanol solvate
0	MUBRAD	2	tris(2-Hydroxybenzoic acid) 9H-purin-6-amine
0	OCIQUM	4	Adeninium tri-iodide di-iodine monohydrate
0	SEQVIV	2	9H-Purin-6-amine succinic acid
0	TAZWOH	2	9H-purin-6-amine benzoic acid
0	WUPGOE*	3	5-Methylpyrimidine-2,4(1H,3H)-dione 9H-purin-6-amine dihydrate
0	WUPGUK*	3	5-Methylpyrimidine-2,4(1H,3H)-dione 9H-purin-6-amine tetrahydrate
0, 1+	BETNOD	4	tris(Adenine) phthalic acid hexahydrate
0, 1+	EVIFIY	4	Adeninium adenine perchlorate dihydrate
0, 1+	PANSAA	4	6-Amino-9H-purin-1-ium hydrogen maleate hemikis(9H-purin-6-amine) monohydrate
0, 1+	VIGVEM	4	Adenine-adeninium tetrafluoroborate dihydrate
1+	ADALEW	3	Adenine (4,6,6,3-di-t-butyl-4,6,5-dimethyl-4,6(1,2)-dibenzene-1,3,2-dioxaphosphacyclohexaphane 2,2-dioxide) methanol solvate
1+	ADENBH	3	Adeninium hydrobromide hemihydrate
1+	ADENCH	3	Adenine hydrochloride hemihydrate
1+	ADENOH	3	bis(Adeninium nitrate) monohydrate
1+	ADENPH	2	Adeninium phosphate
1+	ADESUL	3	Adeninium hemisulfate monohydrate
1+	BEZSII	3	bis(Adeninium) hydrogen phosphate dihydrate
1+	BOTSIN	4	9H-Adenin-1-ium oxalate hemikis(oxalic acid) monohydrate
1+	BUDJAM	4	Adeninium 3-carboxyanilinium diperchlorate trihydrate
1+	BUDVUR	2	Adenine 1-(2-carboxyethyl)-uracil
1+	IKAFOQ	2	6-amino-9H-purin-1-ium perchlorate
1+	LEZHIH	3	bis(Adenine) 7-hydroxy-8-(phenylazo)-1,3-naphthalene-disulfonate pentahydrate
1+	LICGIO	4	bis(adeninium) phthalate phthalic acid hydrate

1+	LOLDAS	2	Adeninium 2,6-dihydroxybenzoate
1+	LOLDEW	3	Adeninium 2,6-dihydroxybenzoate monohydrate
1+	LOLDIA	3	Adeninium 2-hydroxybenzoate methanol solvate
1+	LOLDOG	4	Adeninium hydroxonium 3,5-dihydroxybenzoate hydroxide
1+	LOSHUY	3	bis(Adeninium) hexafluoro-silicate dihydrate
1+	MUCCOD*	3	Adeninium cytosinium sulfate
1+	PIDQIC	3	tetrakis(Adeninium) p-sulfonatocalix(4)arene tetradecahydrate clathrate
1+	RIGMEA	4	Adeninium phenylacetate phenylacetic acid monohydrate
1+	RIGMIE	3	Adeninium 3-carboxypropionate monohydrate
1+	ROPMIU	3	bis(Adenin-1-ium) selenate dihydrate
1+	SEQTUF	3	6-amino-9H-purin-1-ium 3-carboxyacrylate methanol solvate
1+	SEQVAN	2	6-amino-9H-purin-1-ium 3-carboxyacrylate
1+	SEQVER	2	6-amino-7H-purin-3-ium 3-carboxyacrylate
1+	SIXZUW	3	bis(6-amino-9H-purin-1-ium) (1-Hydroxy-1-(hydroxyphosphinato)-2-(1H-imidazol-3-ium-1-yl)ethyl)phosphonate tetrahydrate
1+	SIYBAF	3	bis(6-amino-9H-purin-1-ium) (1-hydroxy-2-(1H-imidazol-3-ium-1-yl)ethane-1,1-diyl)bis(hydrogen (phosphonate)) hexahydrate
1+	TINYIZ	3	Bis(adeninium) chloranilate dihydrate
1+	TUDLOT	3	2-Aminopurinium 2-fluorobenzoate monohydrate
1+	UWAMEM	3	Adeninium salicylate monohydrate
1+	UWAMUC	3	Adeninium sulfosalicylate monohydrate
1+	VITMES	4	bis(Adeninium) dihydrogen benzene-1,2,4,5-tetracarboxylate benzene-1,2,4,5-tetracarboxylic acid dihydrate
1+	XIVBOV	3	Adenin-1-ium hydrogen isophthalate dimethylformamide solvate
1+	YANQAH	3	6-amino-7H-purin-3-ium 2,6-dioxo-2H,6H-[1,2]oxaselenolo[4,3,2-hi][2,1]benzoxaselenol-8-ide monohydrate
2+	ADENDH ADENDH01	2	Adenine dihydrochloride
2+	ADENSL	2	Adeninium sulfate
2+	AHEWIT	4	Adenine-1,7-di-ium chloride pentaiodide monohydrate
2+	AHEWOZ	4	Adenine-1,7-di-ium bromide pentaiodide monohydrate
2+	AHEWUF	3	Adenine-1,7-di-ium hexaiodide dihydrate
2+	BIDRUB	2	Adenine dinitrate
2+	BOTSEJ	3	9H-Adenine-1,7-diium hemikis(oxalate) chloride
2+	COFBII	2	Adeninium bis(trichloro-acetate)

2+	COFBOO COFBOO10	2	Adeninium bis(monochloro-acetate)
2+	DUJHUN	3	6-amino-9H-purine-1,7-dium bis(4-chlorobenzenesulfonate) monohydrate
2+	DUMYIU	3	6-Amino-9H-purine-1,7-dium bis(4-methylbenzenesulfonate) monohydrate
2+	EFADAS	3	bis(adeninium) bis(hydrogen sulfate) sulfate
2+	GADWEO	3	Adeninium diperchlorate monohydrate

Table S3. CSD Entries for Single and Multicomponent Crystals Containing Guanine

charge	REFCODE	# components	name
0	KEMDOW	1	2-amino-1,7-dihydro-6H-purin-6-one
0	GUANMH10	2	Guanine monohydrate
0,1+	KIRPUY	4	tris(2-Amino-6-oxo-6,7-dihydro-1H-purin-9-ium) hydrogen sulfate sulfate 2-amino-1,9-dihydro-6H-purin-6-one
1+	DUKKOJ	3	bis(Guaninium) hydrogen phosphate hydrate
1+	ELEYID ELEYID01	3	Guaninium hydrogenphosphite dihydrate
1+	GUANBM	3	Guanine hydrobromide monohydrate
1+	GUANCD	3	Guanine hydrochloride dihydrate
1+	GUANCH01	3	Guanine hydrochloride monohydrate
1+	GUNPIC10	3	Guanine picrate monohydrate
1+	HUMNEI	3	Guaninium dinitrate dihydrate
1+	HUSBEC	3	Guaninium sulfate monohydrate
1+	KIRQAF	3	2-Amino-6-oxo-6,9-dihydro-1H-purin-7-ium sulfate hydrate
1+	KIRQEJ	3	2-Amino-6-oxo-6,9-dihydro-1H-purin-7-ium sulfate hydrate
1+	RIFWOT	3	Guaninium hydrogen phosphite monohydrate
1+	RIFWUZ	3	Guaninium dihydrogen phosphate monohydrate
2+	GODYUT	2	2-Amino-1,6-dihydro-6-oxo-9H-purine-3,7-di-ium dichloride
2+	JEJLEQ*	4	Cytosinium guaninium 25,26,27,28-tetrahydroxy-5,11,17,23-tetrasulfonatecalix(4)arene cytosinium clathrate octahydrate

Table S4. CSD Entries for Single and Multicomponent Crystals Containing Cytosine

charge	REFCODE	# components	name
0	CYTSIN CYTSIN01 CYTSIN02	1	Cytosine
0	CUVDIH	3	4-Aminopyrimidin-2(1H)-one oxalic acid hemihydrate
0	CUVDON	2	Malonic acid 4-aminopyrimidin-2(1H)-one
0	CUVDUT	2	4-Aminopyrimidin-2(1H)-one succinic acid
0	CYTFUR CYTFUR01	3	Cytosine 5-fluorouracil complex monohydrate
0	CYTOSM EXOHOQ	2	Cytosine monohydrate
0	CYTSCA	4	Cytosine calcium chloride hydrate
0	INOCYT	2	Inosine-cytosine complex
0	IYIWEU	2	5,7-dihydroxy-2-phenyl-4H-chromen-4-one cytosine
0	PUJWUO	2	Cytosine 1,10-phenanthroline
0	QOBCER	3	2-amino-5-isopropyl-6-methylpyrimidin-4(3H)-one 4-aminopyrimidin-2(1H)-one monohydrate
0	QOBCOB	2	2-amino-6-phenylpyrimidin-4(3H)-one 4-aminopyrimidin-2(1H)-one
0	ZEYNOI	2	bis(Cytosine) fumaric acid
0,1+	CYTRES10	4	bis(Cytosine) gamma-resorcylic acid complex monohydrate
0,1+	DOTGOJ	5	2-oxo-2,3-dihydro-4(1H)-aminopyrimidinium 3-oxido-6-oxo-1,6-dihydro-pyridazine 2-oxo-1,2-dihydro-4-aminopyrimidine 6-hydroxy-3(2H)-pyridazinone dihydrate
0,1+	DUJCAN	3	Cytosinium cytosine hydrogen maleate
0,1+	DUZNOC	4	4-amino-2-oxo-2,3-dihydropyrimidin-1-ium isonicotinate 4-aminopyrimidin-2(1H)-one dihydrate
0,1+	EFUNUP	4	4-amino-2-oxo-2,3-dihydropyrimidin-1-ium 4-amino-2-oxo-2,3-dihydropyrimidine 4-nitrobenzoate monohydrate
0,1+	EPAMAK	5	Cytosinium 4-hydroxybenzoate cytosine bis(4-hydroxybenzoic acid) cytosine dihydrate
0,1+	GATMOF	5	6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium 5-nitro-2,4-dioxo-3,4-dihydro-2H-pyrimidin-1-ide 5-nitropyrimidine-2,4(1H,3H)-dione 4-aminopyrimidin-2(1H)-one dihydrate
0,1+	GITYEN	3	Dicytosine trichloroacetate
0,1+	KEVSAG	4	Cytosine cytosinium dicyano(2,3,5,6-tetrafluoro-4-(dicyano(methoxy)methyl)phenyl)methanide monohydrate
0,1+	LIWSIU	3	Cytosinium cytosine 2,5-diethyl-7,7,8,8-tetracyanoquinodimethane

0,1+	LIWSOA	4	Cytosine cytosinium dicyano(4-(dicyano(methoxy)methyl)phenyl)methanide methanol solvate
0,1+	ODICOU	3	Cytosinium cytosine 7,7,8,8-tetracyanoquinodimethane
0,1+	OYERIU	4	Cytosinium dihydrogen citrate bis(cytosine) monohydrate
0,1+	TAZWUN	4	cytosinium benzoate cytosine benzoic acid
0,1+	UWANAJ	4	Cytosinium sulfosalicylate cytosine monohydrate
0,1+	VISVIE	3	6-amino-2-oxo-2,3-dihydropyrimidin-1-ium 4-aminopyrimidin-2(1H)-one tribromoacetate
0,1+	XICRIM	4	Cytosinium 4-amino-2-hydroxybenzoate cytosine monohydrate
0,1+	XOMZUW	3	2-Oxo-2,3-dihydropyrimidin-4(1H)-iminium 4-aminopyrimidin-2(1H)-one 5-chlorothiophene-2-carboxylate
0,1+	YUMGOD	3	Cytosinium cytosine hexafluorophosphate
0,1+	ZAZGEO	3	2-Oxo-2,3-dihydropyrimidin-4(1H)-iminium 2-((2,3-dimethylphenyl)amino)benzoate 4-aminopyrimidin-2(1H)-one
0,1+	ZEGFAU	4	Cytosinium 4-hydroxyphenylacetate cytosine monohydrate
0,1+	ZEGFEY	4	Cytosinium 4-aminobenzoate cytosine monohydrate
0,1+	ZEYJOE	4	6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium 4-aminopyrimidin-2(1H)-one bromide monohydrate
0,1+	ZEYJUK	4	6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium 4-aminopyrimidin-2(1H)-one chloride monohydrate
0,1+	ZEYKAR	3	6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium 4-aminopyrimidin-2(1H)-one 3-oxo-3H-1,2-benzothiazol-2-ide 1,1-dioxide
0,1+	ZEYKEV	3	6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium 4-aminopyrimidin-2(1H)-one 2,6-dinitrophenolate
0,1+	ZEYLEW	4	Cytosinium hydrogen adamantane-1,3-dicarboxylate cytosine monohydrate
0,1+	ZEYLIA	4	Cytosinium acetylenedicarboxylate cytosine monohydrate
1+	ACITEM	3	Cytosinium cytosine tetrafluoroborate
1+	ADALAS	3	Cytosine (4S6!,6S3!-di-t-butyl-4S4!,6S5!-dimethyl-4,6(1,2)-dibenzena-1,3,2-dioxaphosphacyclohexaphane 2,2-dioxide) methanol solvate
1+	CASCIJ	3	Cytosinium hydrogen oxalate monohydrate
1+	CIRVUV	3	Cytosinium 3,5-dicarboxybenzoate monohydrate
1+	CIRWAC	4	tetrakis(Cytosinium) 4,6-dicarboxybenzene-1,3-dicarboxylate 3,6-dicarboxybenzene-1,4-dicarboxylate dihydrate
1+	CTSGLM	3	Cytosine N,N-phthaloyl-DL-glutamic acid dihydrate

1+	CUKCUH	2	Cytosinium hydrogen sulfate
1+	CUKDAO	2	Cytosinium perchlorate
1+	CYTBGL	3	Cytosine-N-benzoylglycine monohydrate
1+	CYTFGL	2	Cytosine N-formylglycine
1+	CYTOSC CYTOSC03	2	Cytosine hydrochloride
1+	CYTPIC	2	Cytosine picrate
1+	DOTGID	3	2-Oxo-2,3-dihydro-4(1H)-amino-pyrimidinium 2,4-dioxo-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate dihydrate
1+	DUZNIW	3	4-Amino-2-oxo-2,3-dihydropyrimidin-1-ium nicotinate monohydrate
1+	EFUNOJ	2	4-amino-2-oxo-2,3-dihydropyrimidin-1-ium 3-carboxypropanoate
1+	ENODIV	3	4-amino-2-oxo-2,3-dihydropyrimidin-1-ium 1-hydroxy-2-(1H,3H-imidazol-3-ium-1-yl)ethylidenediphosphonate trihydrate
1+	FICXIZ	2	Cytosinium 3,5-dinitrosalicylate
1+	JAYNIG	2	Cytosinium dihydrogenmonophosphate
1+	JEJLEQ*	4	Cytosinium guaninium 25,26,27,28-tetrahydroxy-5,11,17,23-tetrasulfonatecalix(4)arene cytosinium clathrate octahydrate
1+	JOXBAB	3	Cytosin-3-ium pyrazine-2-carboxylate monohydrate
1+	KEQPEC	3	4-Aminopyrimidinio-2(1H)-one 2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone monohydrate
1+	KINTOS	2	6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium 2-((3-(3,4-dimethoxyphenyl)acryloyl)amino)benzoate
1+	LEZHON	3	bis(Cytosine) 7-hydroxy-8-(phenylazo)-1,3-naphthalene-disulfonate monohydrate
1+	MUCCOD*	3	Adeninium cytosinium sulfate
1+	NEQHIC	3	2-Oxo-2,3-dihydropyrimidin-4(1H)-iminium 2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylate dihydrate
1+	OCIRAT	3	bis(Cytosinium) bis(pentaiodide) trihydrate
1+	OJERIE	2	Cytosinium nitrate
1+	OYEREQ	2	catena-(tetrakis(Cytosinium) dihydrogen bis(adipate))
1+	ROFLAZ	2	Cytosinium hydrogen maleate
1+	SEGZUZ	2	Cytosine trichloroacetate
1+	SOXFAN	2	Cytosinium dihydrogen phosphite
1+	TAQJAZ	3	bis(6-amino-2-oxo-2,3-dihydropyrimidin-1-ium) 2,3-dihydroxybutanedioate monohydrate
1+	TAZXAU	2	cytosinium isophthalate
1+	TAZXEY	2	cytosinium phthalate
1+	UWAMIQ	2	Cytosinium salicylate
1+	WIGGAW	2	6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium 3-((2-hydroxybenzylidene)amino)benzoate
1+	XAVTIZ	2	Cytosinium furosemide

1+	XICPUW	2	2-Oxo-2,3-dihydropyrimidin-4(1H)-iminium (2-(2-((2,6-dichlorophenyl)amino)phenyl)acetoxy)acetate
1+	XICROS	2	cytosinium 4-amino-2-hydroxybenzoate
1+	XIYLUO	2	2-Oxo-2,3-dihydropyrimidin-4(1H)-iminium hydrogen selenite
1+	ZEGDOG	2	Cytosinium 2,5-dihydroxybenzoate
1+	ZEGDUM	3	Cytosinium 3,5-dinitrobenzoate trihydrate
1+	ZEYDAK	2	6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium 2,6-dinitrophenolate
1+	ZEYDEO ZEYDEO01	2	2-Oxo-2,3-dihydropyrimidin-4(1H)-iminium 4-methyl-3,5-dinitrobenzoate
1+	ZEYDIS	2	bis(6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium) but-2-ynedioate
1+	ZEYDOY	2	2-Oxo-2,3-dihydropyrimidin-4(1H)-iminium 3-carboxyacrylate
1+	ZEYJAQ	3	6-Amino-2-oxo-2,3-dihydropyrimidin-1-ium carboxyacetate monohydrate
1+	ZEYLAS	2	Cytosinium hydrogen malonate
1+	ZEYPOK ZEYPOK01	2	2-Oxo-2,3-dihydropyrimidin-4(1H)-iminium bromide

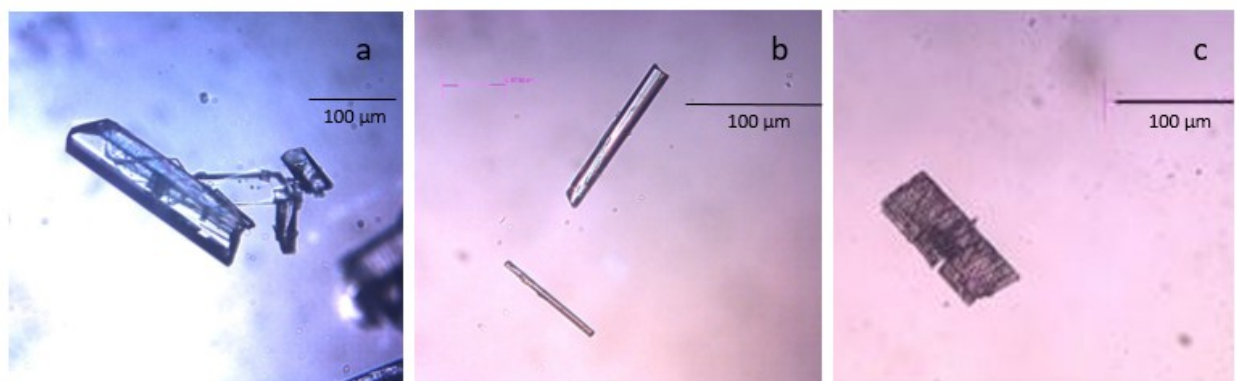


Fig. S1. Optical micrographs of the three cocrystals: (a) **T:DAP**, (b) **T:TAP·H₂O**, and (c) **T:DAHP·3H₂O**.

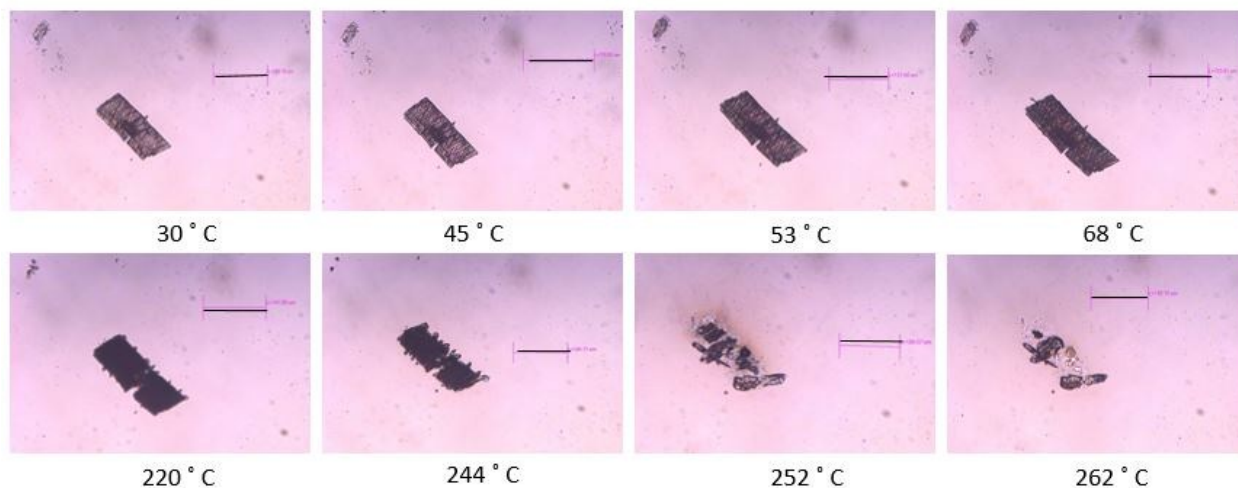


Fig. S2. Hot stage microscopy of **T:DAHP·3H₂O** in air. Progressive water loss upon heating causes the crystal to turn opaque. At temperatures >250°C, the polycrystalline material appears to decompose and/or melt. Scale bar =140 μm .

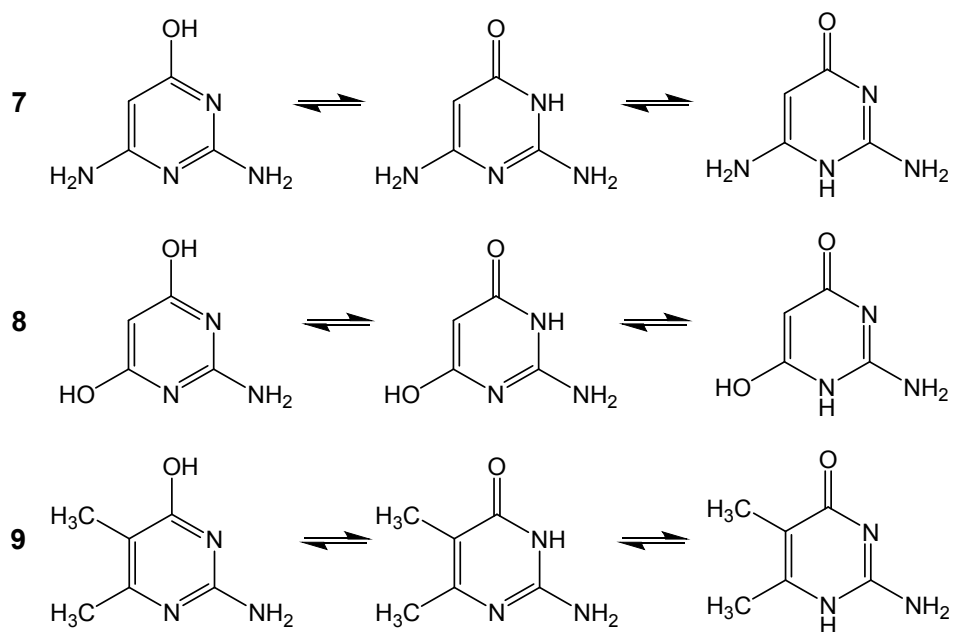
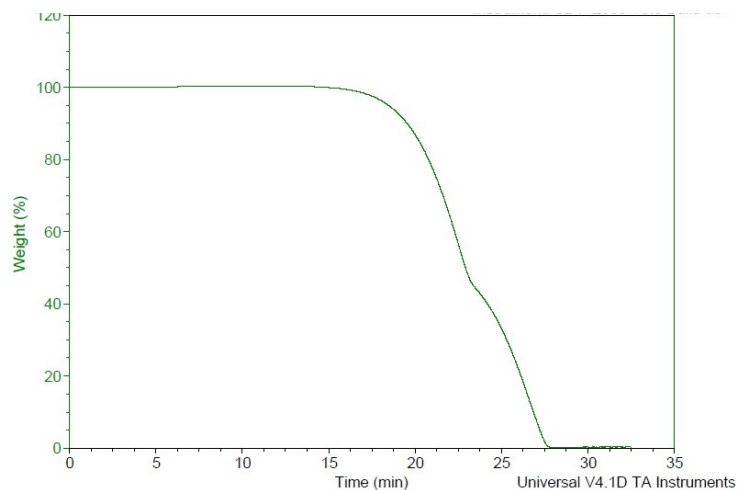
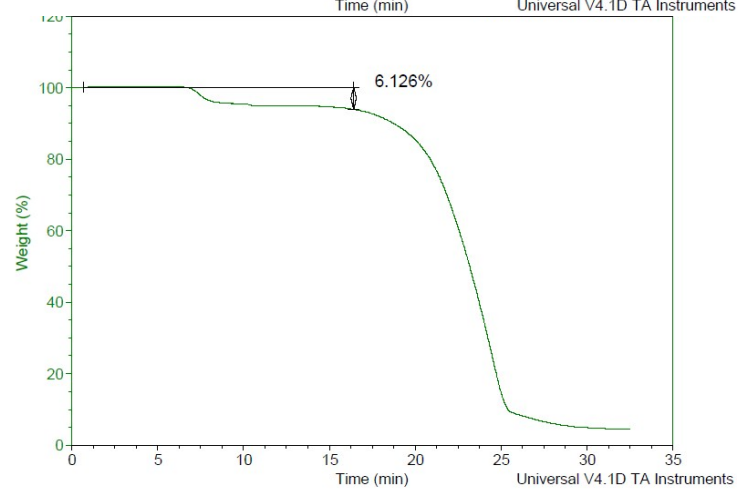


Fig. S3. Possible tautomeric forms of (7), (8) and (9).

T:DAP



T:TAP·H₂O



T:DAHP·3H₂O

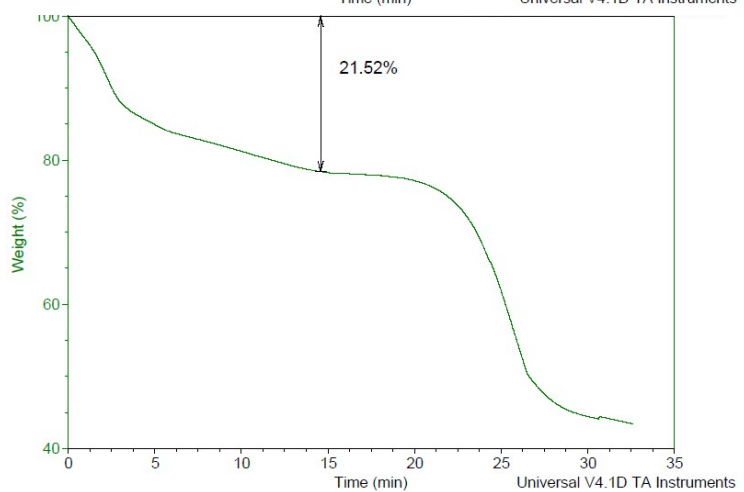


Fig. S4. TGA of (top) **T:DAP**, (middle) **T:TAP·H₂O**, and (bottom) **T:DAHP·3H₂O**.

Table S5. Hydrogen Bond Distances in cocrystals of (a) **T:DAP**, (b) **T:TAP·H₂O** and (c) **T:DHAP·3H₂O**.

(a) T:DAP

D-H	A	distance (H..A) Å	distance (D..A) Å	angle
N1-H1A	N5	2.103	2.962	175.74°
N2-H2A	O2	1.967	2.816	169.10°
N4-H4A	N3	2.159	3.017	175.30°
N4-H4B	O2	2.071	2.930	176.67°
N6-H6A	O1	2.104	2.963	176.55°
N6-H6B	O1	2.099	2.909	156.78°

(b) T:TAP·H₂O

D-H	A	distance (H..A) Å	distance (D..A) Å	angle
N1A-H1AA	N5B	2.07	2.913	159.76°
N2A-H2AA	O3A	1.96	2.824	168.10°
N4A-H4AA	O2A	2.25	2.924	132.02°
N4A-H4AB	O2B	2.03	2.936	178.76°
N6A-H6AA	O1B	2.14	3.036	171.54°
N6A-H6AB	O1B	2.15	2.963	155.61°
N7A-H7AA	O3B	2.17	2.942	143.32°
N1B-H1BA	N5A	2.10	2.928	156.81°
N2B-H2BA	O3B	1.98	2.834	164.50°
N4B-H4BA	O2B	2.27	2.973	135.02°
N4B-H4BB	O2A	2.05	2.939	176.70°
N6B-H6BA	O1A	2.16	3.044	169.19°
N6B-H6BB	O1A	2.13	2.956	157.42°
N7B-H7BA	O3A	2.15	2.945	142.02°
N7B-H7BB	N5A	2.52	3.225	141.12°
O3A-H3AB	N3A	2.09	2.879	159.20°
O3A-H3AC	O2A	1.99	2.816	164.20°
O3B-H3BC	O2B	2.07	2.847	152.20°
O3B-H3BB	N3B	2.06	2.859	158.19°

(c) T:DAHP·3H₂O

D-H	A	distance (H..A) Å	distance (D..A) Å	angle
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N15-H15A	O3	2.061	2.834	143.66°
N8-H8	O6	1.809	2.658	174.07°
N9-H9	O2	2.092	2.934	176.11°
O11-H11A	O6	1.786	2.658	176.37°
O11-H11B	O1	1.939	2.788	177.52°
N4-H4	O2	1.955	2.853	175.55°
O1-H1A	O5	1.955	2.831	179.11°
O5-H5A	O11	1.922	2.793	168.07°
N7-H7A	O3	2.297	3.138	166.94°
N7-H7B	O1	2.121	3.011	166.45°
N15-H15B	N10	2.105	2.958	175.37°
O5-H5B	O11	1.905	2.763	167.63°
O1-H1B	O5	1.981	2.805	177.26°