Cocrystals by Design: A Rational Coformer Selection Approach for Tackling the API Problems

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Table S1: Reported coformers in literature used in the formation of cocrystals

Drug	Coformer/API Name	Cocrystals	API:Coformer Ratio	Reference
Diclofenac (DIC)	4,4'-Bipyridine (4,4 BPY)	DIC-4,4 BPY Cocrystal	2:1	[1]
5-Fluorouracil (5-FU)	Urea (UA)	5-FU-UA Cocrystal	1:1	[2]
	Thiourea (TUA)	5-FU-TUA Cocrystal	1:1	
	Pyrazinamide (PZA)	5-FU-PZA Cocrystal	2:1	
Carbamazepine (CMP)	Saccharin (SAC)	CMP-SAC Cocrystal	1:1	[3]
Progesterone (PROG)	4-Hydroxybenzoic acid (4-HBA)	PROG-4-HBA Cocrystal	1:1, 1:2, 2:1	[4]
Isoniazid (INH)	2,5-Dihydroxybenzoic acid (2,5-DHBA)	INH-2,5-DHBA Cocrystal	1:1	[5]
	2,4-Dihydroxycinnamic acid (2,4-DHCA)	INH-2,4-DHCA Cocrystal	1:1	
Imidazopyridazine (IMP)	Succinic Acid (SA)	IMP-SA Cocrystal	2:1, 1:1	[6]
Itraconazole (ITZ)	Succinic Acid (SA)	ITZ-SA Cocrystals	2:1	[7]
	Fumaric acid (FA)	ITZ-FA Cocrystals	2:1	
Carbamazepine (CMP)	Nicotinamide (NTA)	CMP-NTA Cocrystals	1:1	
Itraconazole (ITZ)	Tartaric Acid (TA)	ITZ-TA Cocrystals	2:1	[8]

	Malic acid (MA)	ITZ-MA Cocrystals	2:1	
Myricetin (MYR)	Isonicotinamide (INA)	MYR-INA Cocrystals	1:2	[9]
	Caffeine (CAF)	MYR-CAF Cocrystals	1:1	
Adefovir dipivoxil (AD)	Saccharin (SAC)	AD-SAC Cocrystals	1:1	[10]
	Nicotinamide (NTA)	AD-NTA Cocrystals	1:1	
Theophylline (THP)	Citric acid (CTA)	THP-CTA Cocrystals	1:1	[11]
Carbamazepine (CBZ)	4 Amino benzoic acid (4ABA)	CBZ-4ABA Cocrystals	2:1	
Indomethacin (IMC)	Saccharin (SAC)	IMC-SAC Cocrystal	1:1	[12]
Anhydrous theophylline (TP)	Citric acid (CA)	TP-CA Cocrystals	1:1	
Carbamazepine (CBZ)	Saccharin (SAC)	CBZ–SAC Cocrystals	1:1	[13]
	Cinnamic acid	CBZ–CIN Cocrystals	1:1	
Carbamazepine (CBZ)	Nicotinamide (NTA)	CBZ-NTA Cocrystals	1:1	[14]
Meloxicam	Aspirin	MLX-APN Cocrystals	1:1	[15]
Efavirenz (EFV)	DL-alanine (ALA)	EFV-ALA Cocrystals	1:1	[16]
	Oxalic acid (OX)	EFV-OX Cocrystals	1:1	
	Maleic acid (MAL)	EFV-MAL Cocrystals	1:1	
	Nicotinamide (NIC)	EFV-NIC Cocrystals	1:1	
Hydrochlorothiazide	Nicotinamide (NCT)	HTZ-NCT Cocrystals	1:1	[17]
Myricetin (MYR)	Nicotinamide (NCT)	MYR-NCT Cocrystals	1:2	[18]
	Proline (PRO)	MYR-PRO Cocrystals	1:2	
Quercetin (QUE)	Caffeine (CAF)	QUE-CAF Cocrystals	1:1	
	Nicotinamide (NCT)	QUE-NCT Cocrystals	1:1	
	Theobromine (TBR)	QUE-TBR Cocrystals	1:1	
Curcumin (CUR)	Ascorbic acid (AA)	CUR-AA Cocrystals	-	[19]
Carvedilol (CAR)	Tartaric Acid (TA)	CAR-TA Cocrystals	1:1	[20]
Efavirenz (EFV)	Tartaric Acid (TA)	EFV-TA Cocrystals	1:1	[21]
	Adipic acid (ADP)	EFV-ADP Cocrystals	1:1	

Brexpiprazole (BPZ)	Fumaric acid (FUM)	BPZ-FUM Cocrystals	1:1	[22]
	Malonic acid (MAL)	BPZ-MAL Cocrystals	1:1	
	Succinic acid (SUC)	BPZ-SUC Cocrystals	1:1	
	Glutaric acid (GLU)	BPZ-GLU Cocrystals	1:1	
Aripiprazole (ARP)	Succinic acid (SA)	ARP-SA Cocrystals	1:1	[23]
	Nicotinamide (NCT)	ARP-NCT Cocrystals	1:1	
Ketoconazole (KTZ)	Succinic acid (SUC)	KTZ-SA Cocrystals	1:1	[24]
	Fumaric acid (FUM)	KTZ-FUM Cocrystals	1:1	
	Adipic acid (ADP)	KTZ-ADP Cocrystals	1:1	
Abiraterone acetate (ABI)	Succinic acid (SA)	ABI-SA Cocrystals	2:1	[25]
	Glutaric acid (GA)	ABI-GA Cocrystals	1:1	
	4-Hydroxy benzoic acid (4-HBA)	ABI-4-HBA Cocrystals	1:1	
	3,5-Dihydroxy benzoic acid (3,5-DHBA)	ABI-3,5-DHBA Cocrystals	1:1	
Sulfamethazine (SZ)	2-Chloro-4-nitrobenzoic acid (2C4N)	SZ-2C4N Cocrystals	1:1	[26]
	2-Chloro-5-nitrobenzoic acid (2C5N)	SZ-2C5N Cocrystals	1:1	
	Salicylic acid (2HBA)	SZ-2HBA Cocrystals	1:1	
	3-Hydroxybenzoic acid (3HBA)	SZ-3HBA Cocrystals	1:1	
	4-Bromobenzoic acid (4BRBA)	SZ-4BRBA Cocrystals	1:1	
	Benzoic acid (BA)	SZ-BA Cocrystals	1:1	
	Cinnamic acid (CA)	SZ-CA Cocrystals	1:1	
	Toluic acid (TA)	SZ-TA Cocrystals	1:1	
Acyclovir (ACV)	Succinic acid (SA)	ACV-SA Cocrystals	1:1	[27]
Fluoxetine (FHC)	Succinic acid (SA)	FHC-SA Cocrystals	1:1	
Entacapone (ETP)	Acetamide (ACT)	ETP-ACT Cocrystals	1:1	[28]
	Nicotinamide (NAM)	ETP-NAM Cocrystals	1:1	
	Isonicotinamide (INAM)	ETP-INAM Cocrystals	1:1	

	Pyrazinamide (PYZ)	ETP-PYZ Cocrystals	1:1	
	Isoniazid (INZ)	ETP-INZ Cocrystals	1:1	
Pyrazinamide (PZA)	4-Hydroxy benzoic acid (4-HBA)	PZA-4-HBA Cocrystals	1:1	[29]
	p-Coumaric acid (PCA)	PZA-PCA Cocrystals	-	
	Ferulic acid (FRA)	PZA-FRA Cocrystals	1:1	
	Sinapic acid (SPA)	PZA-SPA Cocrystals	1:1	
3,5-Dinitrobenzoic acid (DNBA)	3-cyanopyridine (3-CNP)	DNBA-3-CNP Cocrystals	1:1	[30]
	Flufenamic acid (FA)	DNBA-FA Cocrystals	1:1	
	Theophylline (THP)	DNBA-THP Cocrystals	1:1	
	Thiourea (TU)	DNBA-TU Cocrystals	1:1	
Theophylline (THP)	Glutaric acid (GA)	THP-GA Cocrystals	1:1	[31]
	Isonicotinamide (INAM)	THP-INAM Cocrystals	1:1	
	Benzamide (BZ)	THP-BZ Cocrystals	1:1	
Oxyresveratrol (OXY)	Nicotinamide (NCT)	OXY-NCT Cocrystals	1:1	[32]
	Proline (PRO)	OXY-PRO Cocrystals	1:1	

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