Electronic Supplementary Material (ESI) for CrystEngComm.

A user-friendly application for predicting the outcome of co-crystallizations

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Following are the definitions required to understand the flowchart:

- *m,m1,m2*: molecules
- *x,y*: co-formers
- *acceptors*: # of hydrogen-bond acceptors
- *donors*: # of hydrogen-bond donors
- *KDS*: Known Data Set
- *Known_positives(m)*: The set of co-formers which experimentally form co-crystals with molecule m in *KDS*
- *Known_negatives(m)*: The set of co-formers which experimentally do not form co-crystals with molecule m in *KDS*
- *Conflict(m1,m2)*: There exists at least a co-former, x in *known_positives(m1)* and in *known_negatives(m2)*, or vice-versa
- *rank(k)*: Rank of *k* based on match, where k is a molecule or a co-former. Lower the match, lower will be the rank.

Outputs:

- **Most likely**: The set of co-formers which *will most likely* form a co-crystal
- **Likely**: The set of co-formers which *may* form a co-crystal
- **Least likely**: The set of co-formers which *will least likely* form a co-crystal

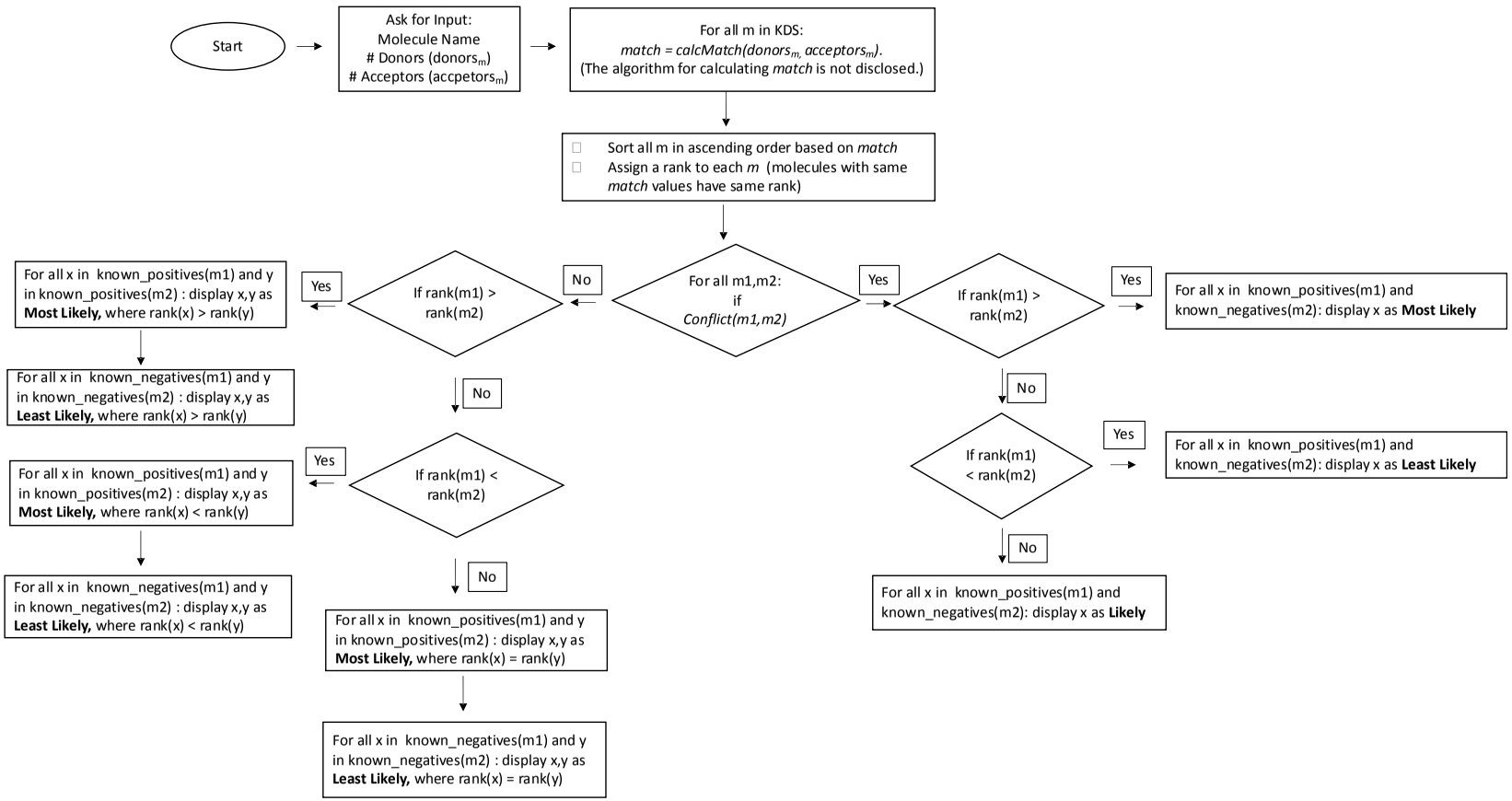
Start
Ask for Input:
Molecule Name
Donors (donors$_m$)
Acceptors (accpetors$_m$)
For all m in KDS:
match = calcMatch(donors$_m$, acceptors$_m$).
(The algorithm for calculating *match* is not disclosed.)
Sort all m in ascending order based on *match*
Assign a rank to each *m* (molecules with same *match* values have same rank)
For all m1,m2:
if
Conflict(m1,m2)
No
Yes
If rank(m1) > rank(m2)
For all x in known_positives(m1) and y in known_positives(m2) : display x,y as **Most Likely,** where rank(x) > rank(y)
For all x in known_negatives(m1) and y in known_negatives(m2) : display x,y as **Least Likely,** where rank(x) > rank(y)
No
Yes
If rank(m1) < rank(m2)
For all x in known_positives(m1) and y in known_positives(m2) : display x,y as **Most Likely,** where rank(x) < rank(y)
For all x in known_negatives(m1) and y in known_negatives(m2) : display x,y as **Least Likely,** where rank(x) < rank(y)
No
For all x in known_positives(m1) and y in known_positives(m2) : display x,y as **Most Likely,** where rank(x) = rank(y)
For all x in known_negatives(m1) and y in known_negatives(m2) : display x,y as **Least Likely,** where rank(x) = rank(y)
Yes
If rank(m1) > rank(m2)
For all x in known_positives(m1) and known_negatives(m2): display x as **Most Likely**
No
Yes
If rank(m1) < rank(m2)
For all x in known_positives(m1) and known_negatives(m2): display x as **Least Likely**
No
For all x in known_positives(m1) and known_negatives(m2): display x as **Likely**

Figure S1. Flow chart of the algorithm.

The database consists of a wide variety of compounds. Figure S2 lists a few examples. Experiments on the test compounds are not included in the database because we do not want the test compounds to affect the accuracy of CoForm in predicting the co-crystal screening results.

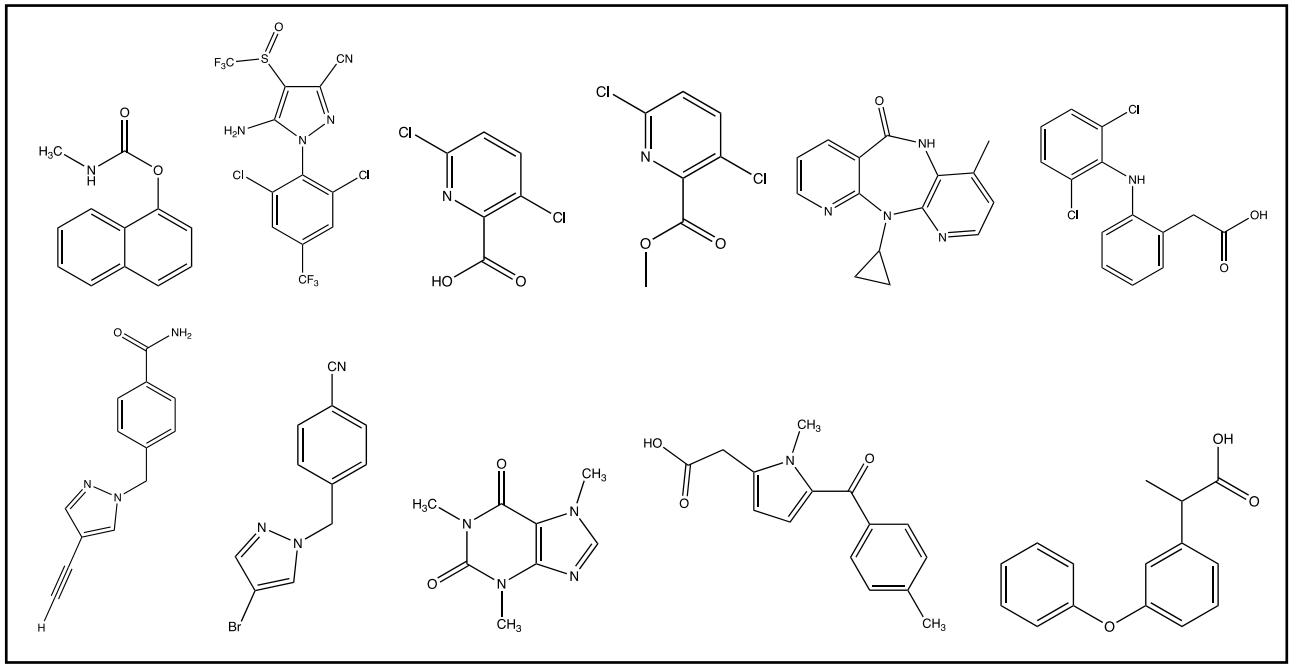

Figure S2. Few examples of compounds present in the training dataset.

Table S1. List of co-formers.

OGI list co-formers	Conventionally used co-formers
3-Hydroxy-2-naphthoic acid	1-Bromo-4- iodotetrafluorobenzene
4-Hydroxybenzoic acid	1,2-Bis(4-pyridyl)ethane
Adipic acid	1,2-Bis(4-pyridyl)ethylene
Apigenin	1,4-Dihydroxybenzene
Benzenesulfonic acid	1,4-Diiodobenzene
Benzoic acid	1,4-Diiodotetrafluorobenzene
Caffeine	2-Amino-3,5-dibromopyridine
Cholic acid	2-Amino-3-hydroxypyridine
Citric acid	2-Amino-4,6-dimethylpyrimidine
D-glucuronic acid	2-Amino-4-chloro-6-methylpyrimidine
EDTA	2-Amino-4-hydroxy-6-methylpyrimidine
Folic acid	2-Amino-4-methylpyrimidine
Fumaric acid	2-Amino-5-chloropyridine
Glutaric acid	2-Aminopyridine
Glycine	2-Aminopyrimidine
Glycolic acid	2-Chlorocyanoxime
Hydrocinnamic acid	2-Fluorocyanoxime
Isonicotinamide	2,4,6-Triaminopyrimidine
L-Glutamic acid	2,6-Diaminopyridine
L-Mandelic acid	2,6-Difluorobenzoic acid

L-Proline	3-Aminobenzoic acid
L-Serine	3-Aminopyridine
L-Tartaric acid	3-Benzoylpyridine
Maleic acid	3-Hydroxypyridine
Malic acid	3-Nitrobenzoic acid
Malonic acid	3,4-Dichlorobenzoic acid
Maltitol	3,5-Dinitrobenzoic acid
Mannitol	4,4’-Bipyridine
Nicotinamide	4-Aminobenzoic acid
Oxalic acid	4-Aminopyridine
Pamoic acid	4-Benzoylpyridine
Phosphoric acid	4-Bromocyanoxime
Piperazine	4-Bromotetrafluorobenzoic acid
Riboflavin	4-Chloro-2_6-diaminopyrimidine
Saccharin	4-Cyanobenzoic acid
Salicylic acid	4-Fluorocyanoxime
Sorbic acid	4-Hydroxybenzoic acid
Succinic acid	4-iodotetrafluorobenzoic acid
Theophylline	4-Nitrobenzoic acid
Urea	4-Phenylpyridine
Xanthine	4,4-Bisphenol
	4,4'-Dipyridyl
	4,4'-Trimethylenedipyridine
	Azelic acid
	Cyanoxime
	Dodecanedioic acid
	Pentafluorobenzoic acid
	Pimelic acid
	Sebacic acid
	Suberic acid

Table S2. Comparison between HBP/ MC vs. CoForm.

HBP/ MC	**CoForm**
• Based on crystal structures present in the CSD. • Select a sampling dataset which is comparable to the defined functional groups of the target and co-former[1]. • Understand the descriptors on which the calculations are based. • Each calculation takes 15-20 mins.	• It is a data-driven predictive application based on experimental data from attempted co-crystallization experiments. • Two inputs required: # of hydrogen-bond donors and # of hydrogen-bond acceptors. • It takes 10- 15 seconds to provide a list of co-formers which will likely or not likely form co-crystal.

Liquid assisted grinding experiments were performed with loratadine and desloratadine in combination with 41 co-formers. The target and the co-former were added in a 1:1 molar ratio to a spotting plate with a few methanol drops. The mixture was ground for 30-40 seconds or until the solvent was evaporated entirely.[2] An IR spectrum was then recorded of the resulting solid or a glue-like material to determine if the ground mixture consisted of peaks from both the starting materials and/or consequently, any shift in the stretches. A shift greater than 3 cm^{-1} in several modes in the infra-red spectrum was characterized as "YES" to co-crystallization, and consistent un-changed peaks were labeled as "NO" to co-crystallization[3], Table S3. There are three reported co-crystals of loratadine[4,5,6] and one with desloratadine,[7] which matches our experimental screening outcomes.

Table S3. IR analysis of the solids obtained from solvent assisted grinding of loratadine and desloratadine.

IR data (cm^{-1})	**Loratadine**		**Desloratadine**	
	1699, 1472, 1432, 1381, 1354, 1320, 1273		1584, 1477, 1434, 1419, 1176, 1100, 1085	
Co-former	**Ground mixture**	**Results**	**Ground mixture**	**Results**
3-Hydroxy-2-naphthoic acid 1655, 1626, 1597, 1513, 1463, 1439	1683, 1632, 1591, 1474, 1422, 1394, 1322, 1276, 1227, 1172	Yes	1671, 1621, 1588, 1568, 1476, 1436, 1418, 1384, 1243, 1114	Yes
4-Hydroxybenzoic acid 1667, 1605, 1592, 1509, 1445, 1411	1676, 1600, 1582, 1452, 1420, 1322, 1278, 1232, 1177, 1124	Yes	1706, 1619, 1561, 1476, 1437, 1415, 1383, 1275, 1170, 1097	Yes
Adipic acid 1683, 1461, 1426, 1407, 1267, 1187	1689, 1477, 1418, 1384, 1326, 1301, 1277, 1220, 1175, 1112	Yes	1588, 1566, 1480, 1454, 1376, 1328, 1297, 1248, 1218, 1139	Yes
Apigenin 1649, 1604, 1586, 1554, 1491, 1442	1649, 1604, 1586, 1554, 1491, 1442, 1351, 1267, 1241	No	1706, 1582, 1567, 1476, 1424, 1336, 1159, 1116, 1106	Yes
Benzenesulfonic acid 1663, 1445, 1092, 1031, 1009, 986	1730, 1689, 1646, 1578, 1503, 1426, 1394, 1343, 1304, 1273	Yes	1731, 1646, 1578, 1540, 1497, 1455, 1394, 1343, 1246, 1225	Yes
Benzoic acid 1677, 1602, 1581, 1452, 1419, 1323	1700, 1471, 1430, 1226, 1218, 1151, 1111, 1066, 1015, 992	Yes	1425, 1328, 1147, 1100, 1091, 1075, 1049, 1009, 968, 958	Yes
Caffeine 1694, 1639, 1545, 1454, 1428, 1357	1691, 1648, 1562, 1418, 1332, 1220, 1205, 1152, 1112, 995	Yes	1696, 1646, 1564, 1463, 1436, 1416, 1332, 1258, 1202, 1150	Yes
Cholic acid 1712, 1247, 1090, 1077, 1043, 979	1691, 1643, 1425, 1276, 1222, 1112, 995	Yes	1621, 1590, 1542, 1507, 1475, 1437, 1420, 1365, 1341, 1325	Yes
Citric acid 1741, 1691, 1425, 1391, 1358, 1235	1700, 1698, 1470, 1432, 1360, 1349, 1278, 1259, 1221	Yes	1642, 1586, 1566, 1475, 1435, 1421, 1331, 1282, 1246, 1236	Yes
D-Glucuronic acid 1703, 1456, 1362, 1347, 1249, 1224	1700, 1430, 1382, 1280, 1227, 1177, 1112, 1077, 1017, 993	No	1426, 1280, 1259, 1075, 1018, 950, 877, 864	Yes
EDTA 1690, 1412, 1386, 1309, 1253, 1092	1678, 1655, 1639, 1617, 1572, 1559, 1476, 1445, 1429, 1399	Yes	1705, 1616, 1576, 1474, 1450, 1349, 1260, 1198, 1140, 1117	Yes
Folic acid 1688, 1602, 1481, 1451, 1410, 1336	1688, 1434, 1278, 1219, 1170, 1097, 1086, 1056, 994	No	1624, 1567, 1475, 1436, 1422, 1318, 1081, 1039, 999, 952	Yes
Fumaric acid 1653, 1406, 1315, 1270, 1226, 1172	1692, 1663, 1642, 1561, 1476, 1438, 1420, 1220, 1187, 1113	Yes	1707, 1661, 1560, 1528, 1481, 1436, 1311, 1282, 1239, 1223	Yes
Glutaric acid 1682, 1466, 1430, 1406, 1301, 1264	1693, 1559, 1470, 1431, 1321, 1273, 1219, 1170, 1114, 1081	Yes	1644, 1560, 1475, 1436, 1421, 1366, 1270, 1246, 1173, 1083	Yes
Glycine 1607, 1577, 1500, 1441, 1409, 1315	1678, 1473, 1433, 1384, 1324, 1277, 1227, 1170, 1094, 1022	No	1711, 1574, 1476, 1438, 1422, 1382, 1254, 1171, 1088	Yes
Glycolic acid 1701, 1428, 1226, 1081, 925, 683	1701, 1428, 1226, 1081, 925, 683, 884, 850	No	1655, 1627, 1608, 1578, 1514, 1476, 1468, 1437, 1382	Yes
Hydrocinnamic acid 1692, 1426, 1406, 1299, 1216, 927	1695, 1509, 1472, 1430, 1304, 1224, 1114, 995	Yes	1581, 1555, 1518, 1477, 1434, 1396, 1340, 1309, 1154, 1073	Yes
Isonicotinamide 1653, 1621, 1594, 1546, 1388, 1290	1690, 1635, 1602, 1480, 1417, 1330, 1275, 1225, 1191, 1177	Yes	1687, 1661, 1601, 1474, 1438, 1401, 1332, 1178	Yes
L-Glutamic acid 1641, 1499, 1407, 1350, 1302, 1251	1689, 1482, 1463, 1381, 1354, 1320, 1273	Yes	1716, 1645, 1589, 1579, 1473, 1421, 1359, 1340	Yes

L-Mandelic acid 1708, 1491, 1455, 1241, 1187, 1096	1693, 1684, 1638, 1473, 1429, 1374, 1321, 1272, 1227, 1201	Yes	1553, 1439, 1417, 1379, 1345, 1309, 1293, 1264, 1239, 1182	Yes
L-Proline 1608, 1565, 1541, 1473, 1447, 1374	1649, 1604, 1586, 1554, 1491, 1442, 1351, 1267, 1241	No	1554, 1476, 1436, 1421, 1394, 1332, 1076, 1001, 973, 944	Yes
L-Serine 1582, 1466, 1408, 1382, 1337, 1301	1696, 1620, 1590, 1540, 1523, 1508, 1413, 1394, 1383, 1333	Yes	1585, 1563, 1519, 1506, 1476, 1438, 1420, 1332, 1272	Yes
L-Tartaric acid 1732, 1706, 1442, 1251, 1211, 1181	1688, 1654, 1473, 1422, 1382, 1321, 1275, 1224, 1114, 1084	Yes	1707, 1561, 1551, 1477, 1439, 1385, 1231, 1150, 1116	Yes
Maleic acid 1703, 1558, 1458, 1428, 1257, 1216	1664, 1605, 1586, 1475, 1436, 1386, 1356, 1276, 1221, 1159	Yes	1583, 1556,1458, 1440, 1364, 1267, 1235, 1160	No
Malic acid 1737, 1682, 1438, 1407, 1355, 1279	1693, 1682, 1650, 1604, 1572, 1556, 1472, 1421, 1351, 1267	Yes	1646, 1603, 1571, 1549, 1515, 1472, 1430, 1359, 1296, 1270	Yes
Malonic acid 1691, 1432, 1387, 1301, 1214, 1163	1667, 1647, 1420, 1386, 1273, 1224, 1161, 1112, 1085, 995	Yes	1703, 1692, 1631, 1577, 1560, 1437, 1425, 1376, 1355, 1311	Yes
Maltitol 1149, 1047, 1016, 992, 968, 903	1695, 1472, 1432, 1381, 1354, 1320, 1273	No	1584, 1477, 1434, 1419, 1176, 1100, 1083, 1006, 993	No
Mannitol 1712, 1538, 1455, 1415, 1387, 1251	1701, 1667, 1466, 1446, 1429, 1375, 1360, 1222, 1203, 1156	Yes	1712, 1538, 1455, 1415, 1387, 1251	No
Nicotinamide 1673, 1617, 1595, 1484, 1421, 1391	1695, 1415, 1387, 1311, 1277, 1212, 1166, 1107, 968, 862	Yes	1882, 1645, 1633, 1579, 1564, 1440, 1415, 1401, 1379, 1308	Yes
Oxalic acid 1677, 1161, 1128, 826, 779	1690, 1619, 1586, 1544, 1424, 1386, 1320, 1276, 1218, 1170	Yes	1587, 1475, 1434, 1419, 1176, 1100, 1085	No
Pamoic acid 1649, 1452, 1428, 1308, 1290, 1204	1691, 1652, 1596, 1552, 1473, 1432, 1356, 1323, 1226	Yes	1697, 1647, 1546, 1479, 1428, 1357, 1284, 1237, 1087	Yes
Phosphoric acid N/A	1690, 1676, 1582, 1474, 1434, 1383, 1278, 1226, 1178, 1112	Yes	1581, 1473, 1439, 1422, 1394, 1369, 1356, 1310, 1272, 1185	Yes
Piperazine 1648, 1456, 1322, 1270, 1127, 1084	1698, 1645, 1456, 1426, 1383, 1326, 1277, 1221, 1169	No	1584, 1477, 1434, 1419, 1176, 1100, 1085	No
Riboflavin 1730, 1645, 1578, 1536, 1503, 1395	1730, 1645, 1578, 1536, 1503, 1395, 1343, 1241, 1178	No	1730, 1645, 1578, 1536, 1503, 1395, 1343, 1241, 1178	No
Saccharin 1714, 1591, 1458, 1332, 1295, 1255	1694, 1649, 1453, 1429, 1306, 1293, 1206, 1171, 1112, 1093	Yes	1650, 1639, 1625, 1608, 1579, 1558, 1508, 1444, 1432, 1384	Yes
Salicylic acid 1652, 1608, 1480, 1440, 1292, 1233	1674, 1625, 1587, 1463, 1425, 1384, 1324, 1276, 1219, 1171	Yes	1682, 1625, 1599, 1560, 1540, 1469, 1425, 1349, 1260, 1243	Yes
Sorbic acid 1672, 1634, 1608, 1411, 1374, 1314	1688, 1477, 1432, 1384, 1325, 1277, 1222, 1173, 1115, 1025	Yes	1730, 1707, 1654, 1576, 1555, 1538, 1519, 1505, 1441, 1417	Yes
Succinic acid 1679, 1411, 1307, 1197, 1156, 1131	1688, 1627, 1579, 1512, 1431, 1380, 1318, 1276, 1224, 1116	Yes	1648, 1561, 1512, 1456, 1437, 1399, 1366, 1314, 1271	Yes
Theophylline 1700, 1659, 1555, 1481, 1441, 1313	1679, 1624, 1600, 1554, 1475, 1434, 1275, 1223, 1160, 1112	Yes	1679, 1651, 1624, 1591, 1553, 1476, 1436, 1411, 1398, 1364	Yes
Urea 1674, 1590, 1550, 1454, 1148, 1118	1695, 1670, 1470, 1434, 1226, 1161, 1120, 1086	No	1645, 1609, 1591, 1569, 1516, 1478, 1443, 1388, 1213, 1162	Yes
Xanthine 1692, 1650, 1564, 1454, 1436, 1415	1695, 1433, 1280, 1225, 1196, 1168, 1115, 995	No	1694, 1669, 1615, 1570, 1559, 1528, 1438, 1422, 1408	No
Experimental supramolecular yield		64%		83%

CoForm was used to predict the co-crystal screening outcome for Loratadine and Desloratadine, Table S4.

Table S4. CoForm co-crystal screening outputs for loratadine and desloratadine.

Co-former	Loratadine	Desloratadine
3-Hydroxy-2-naphthoic acid	Yes	Yes
4-Hydroxybenzoic acid	Yes	Yes
Adipic acid	No	Yes
Apigenin	Yes	Yes
Benzenesulfonic acid	Yes	Yes
Benzoic acid	Yes	Yes
Caffeine	Yes	Yes
Cholic acid	Yes	Yes
Citric acid	Yes	Yes
D-glucuronic acid	No	Yes
EDTA	Yes	Yes
Folic acid	No	No
Fumaric acid	No	Yes
Glutaric acid	Yes	Yes
Glycine	Yes	Yes
Glycolic acid	No	No
Hydrocinnamic acid	Yes	Yes
Isonicotinamide	Yes	No
L-glutamic acid	Yes	Yes
L-mandelic acid	No	Yes
L-proline	No	Yes
L-serine	Yes	Yes
L-tartaric acid	Yes	Yes
Maleic acid	Yes	Yes
Malic acid	Yes	Yes
Malonic acid	No	Yes
Maltitol	No	Yes
Mannitol	Yes	Yes
Nicotinamide	Yes	Yes
Oxalic acid	No	Yes
Pamoic acid	Yes	Yes
Phosphoric acid	Yes	Yes
Piperazine	Yes	Yes
Riboflavin	No	Yes
Saccharin	Yes	Yes
Salicylic acid	Yes	Yes
Sorbic acid	Yes	No
Succinic acid	No	Yes
Theophylline	Yes	Yes
Urea	No	No
Xanthine	Yes	Yes

The relevant HBP values for each API and co-formers are tabulated in Table S5. A $\Delta_{propensity} \geq 0$, was assigned as a "YES" to co-crystallization, and if $\Delta_{propensity} < 0$, it was assigned as a "NO" to co-crystallization[8,9].

Table S5. Hydrogen-bond propensity (HBP) calculations for loratadine and desloratadine.

Co-former	Homomeric interactions	Heteromeric interactions	$\Delta_{propensity}$ =Hetero-Homo	Homomeric interactions	Heteromeric interactions	$\Delta_{propensity}$ =Hetero-Homo
3-Hydroxy-2-naphthoic acid	0.23	0.47	0.24	0.4	0.31	-0.09
4-Hydroxybenzoic acid	0.28	0.51	0.23	0.35	0.41	0.06
Adipic acid	0.42	0.66	0.24	0.45	0.45	0
Apigenin	0.31	0.41	0.1	0.4	0.4	0
Benzenesulfonic acid	0.47	0.59	0.12	0.47	0.47	0
Benzoic acid	0.27	0.43	0.16	0.35	0.35	0
Caffeine	-	-	N/A	0.25	0.8	0.55
Cholic acid	0.45	0.64	0.19	0.54	0.6	0.06
Citric acid	0.33	0.53	0.2	0.37	0.52	0.15
D-glucuronic acid	0.53	0.56	0.03	0.49	0.53	0.04
EDTA	0.4	0.67	0.27	0.42	0.45	0.03
Folic acid	0.56	0.7	0.14	0.54	0.45	-0.09
Fumaric acid	0.46	0.59	0.13	0.42	0.41	-0.01
Glutaric acid	0.43	0.67	0.24	0.45	0.44	-0.01
Glycine	0.64	0.72	0.08	0.67	0.53	-0.14
Glycolic acid	0.53	0.6	0.07	0.54	0.6	0.06
Hydrocinnamic acid	0.37	0.58	0.21	0.35	0.35	0
Isonicotinamide	0.56	0.47	-0.09	0.58	0.4	-0.18
L-glutamic acid	0.56	0.7	0.14	0.6	0.52	-0.08
L-mandelic acid	0.34	0.58	0.24	0.44	0.51	0.07
L-proline	0.49	0.59	0.1	0.45	0.47	0.02
L-serine	0.62	0.62	0	0.61	0.61	0
L-tartaric acid	0.42	0.61	0.19	0.45	0.54	0.09
Maleic acid	0.45	0.59	0.14	0.42	0.41	-0.01
Malic acid	0.45	0.62	0.17	0.48	0.55	0.07
Malonic acid	0.5	0.67	0.17	0.5	0.44	-0.06
Maltitol	0.74	0.68	-0.06	0.7	0.76	0.06
Mannitol	0.36	0.48	0.12	0.38	0.59	0.21
Nicotinamide	0.57	0.48	-0.09	0.58	0.4	-0.18
Oxalic acid	0.17	0.21	0.04	0.41	0.28	-0.13
Pamoic acid	0.22	0.48	0.26	0.43	0.33	-0.1
Phosphoric acid	0.87	0.53	-0.34	0.86	0.82	-0.04
Piperazine	0.62	0.58	-0.04	0.47	0.41	-0.06
Riboflavin	0.66	0.5	-0.16	0.66	0.55	-0.11
Saccharin	0.44	0.46	0.02	0.41	0.33	-0.08
Salicylic acid	0.25	0.5	0.25	0.41	0.34	-0.07
Sorbic acid	0.44	0.58	0.14	0.41	0.4	-0.01
Succinic acid	0.44	0.67	0.23	0.46	0.42	-0.04
Theophylline	0.26	0.32	0.06	0.33	0.49	0.16
Urea	0.97	0.93	-0.04	0.97	0.84	-0.13
Xanthine	0.67	0.5	-0.17	0.64	0.56	-0.08

The relevant MC values for each API and co-formers are tabulated in Table S6. A hit rate% $\geq$ 40, was assigned as a "YES" to co-crystallization, and if hit rate% <40, it was assigned as a "NO" to co-crystallization[10].

Table S6. Molecular Complementarity (MC) calculations for loratadine and desloratadine.

Co-former	Loratadine hit rate %	Desloratadine hit rate %
3-Hydroxy-2-naphthoic acid	50	50
4-Hydroxybenzoic acid	0	0
Adipic acid	84	0
Apigenin	0	0
Benzenesulfonic acid	0	0
Benzoic acid	0	0
Caffiene	20	0
Cholic acid	60	0
Citric acid	0	0
D-glucuronic acid	0	0
EDTA	0	0
Folic acid	100	0
Fumaric acid	0	0
Glutaric acid	67	67
Glycine	0	0
Glycolic acid	0	0
Hydrocinnamic acid	0	0
Isonicotinamide	84	60
L-glutamic acid	0	0
L-mandelic acid	0	0
L-proline	100	100
L-serine	60	100
L-tartaric acid	0	0
Maleic acid	0	0
Malic acid	0	0
Malonic acid	0	0
Maltitol	0	0
Mannitol	0	0
Nicotinamide	20	0
Oxalic acid	0	0
Pamoic acid	0	0
Phosphoric acid	100	100
Piperazine	0	0
Riboflavin	100	100
Saccharin	64	90
Salicylic acid	60	25
Sorbic acid	50	50
Succinic acid	20	0
Theophylline	0	0
Urea	0	0
Xanthine	0	0

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