

## Estimation of Melting Temperature of Molecular Co-crystals using Artificial Neural Network Model

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**Table S1.** The 61CCs used in this study, respective crystal packing density, electrostatic interaction percentages, van der Waals interaction percentages and the ratio of electrostatic interactions vs van der Waals interactions.

<b>Compound Code</b>	<b>Molecular weight</b>	<b>API<sub>MW</sub>/CF<sub>MW</sub></b>	<b>Cocrystal</b>	<b>Crystal packing density (CPD)</b>	<b>Eel</b>	<b>EvdW</b>	<b>Eel/EvdW</b>
CAF	194.19	-	-	-	-	-	-
THP	180.16	-	-	-	-	-	-
INA	122.12	-	-	-	-	-	-
NA	122.12	-	-	-	-	-	-
DLMA	134.087	1.343	THP:DLMA	1.544	-40.171	-27.705	1.449
DMA	134.087	1.343	THP:DMA	1.558	-37.752	-29.445	1.282
GTA	132.12	1.363	THP:GTA	1.489	-32.076	-28.090	1.142
GNA	154.12	1.168	THP:GNA	1.567	-28.709	-35.055	0.819
SA	138.121	1.304	THP:SA	1.534	-19.732	-35.686	0.553
PCA-I	164.16	1.097	THP:PCA-I	1.483	-27.997	-36.653	0.763
PCA-II	164.16	1.097	THP:PCA-II	1.491	-27.452	-36.485	0.752
SAC	183.18	0.983	THP:SAC	1.534	-17.837	-41.764	0.427
URE	60.06	2.999	THP:URE	1.46	-31.147	-21.581	1.443
GTA-I	132.12	1.469	CAF:GTA-I	1.482	-22.871	-36.197	0.631
GTA-II	132.12	1.469	CAF:GTA-II	1.486	-22.926	-36.586	0.627
PCA	164.16	1.182	CAF:PCA	1.478	-23.755	-39.991	0.594

4NAN	138.12	1.405	CAF:4NAN	1.453	-15.891	-37.526	0.423
2I4NAN	264.02	0.735	CAF:2I4NAN	1.822	-9.698	-39.665	0.244
2F5NAN	156.11	1.243	CAF:2F5NAN	1.492	-37.139	-15.727	2.361
4F3NAN	156.11	1.243	CAF:4F3NAN	1.474	-18.006	-34.230	0.526
4C3NAN	172.57	1.125	CAF:4C3NAN	1.545	-17.112	-40.058	0.427
2C5NAN	172.57	1.125	CAF:2C5NAN	1.522	-14.675	-38.694	0.379
4I3NAN	264.02	0.735	CAF:4I3NAN	1.799	-16.83	-38.541	0.436
24DNBA	212.12	0.915	CAF:24DNBA	1.533	-25.77	-36.070	0.714
2F5NBA	185.11	1.049	CAF:2F5NBA	1.492	-18.301	-39.233	0.466
SA	194.19	0.711	CAF:SA	1.49	-15.671	-39.307	0.398
SA-I	194.19	0.711	CAF:SA-I	1.476	-15.686	-39.304	0.399
OXA	90.03	1.356	INA:OXA	1.584	-50.455	-34.515	1.461
MLA	104.06	1.173	INA:MLA	1.49	-94.85	-31.480	3.013
SCA	118.09	1.034	INA:SCA	1.478	-48.93	-36.738	1.331
GTA	132.12	0.924	INA:GTA	1.399	-33.227	-23.667	1.403
ADA	146.14	0.835	INA:ADA	1.39	-31.782	-25.931	1.225
PIA	160.17	0.762	INA:PIA	1.331	-31.12	-27.489	1.132
SUA	174.2	0.701	INA:SUA	1.369	-32.649	-29.538	1.105
AZA	188.22	0.648	INA:AZA	1.283	-31.277	-30.528	1.024
FUA	116.07	1.052	INA:FUA	1.5	-46.579	-37.636	1.237
4KPIA	174.15	0.701	INA:4KPA	1.415	-50.001	-41.710	1.198
12BDA	279.21	0.437	INA:12BDA	1.392	-23.198	-39.661	0.584
SA	138.12	0.884	INA:SA	1.455	-24.521	-26.369	0.929
3HBA	138.12	0.884	INA:3HBA	1.451	-29.38	-24.614	1.193
4HBA	138.12	0.884	INA:4HBA	1.471	-28.419	-26.747	1.063
4FBA	140.11	0.871	INA:4FBA	1.453	-23.983	-25.183	0.952
3NBA	167.12	0.730	INA:3NBA	1.526	-26.345	-27.712	0.951
2HEA	114.142	1.069	INA:2HEA	1.285	-23.406	-24.777	0.944
CIA	148.158	0.824	INA:CIA	1.365	-23.025	-29.762	0.773
CAA	94.5	1.29	INA:CAA	1.517	-23.738	-20.266	1.171

2PPARS	150.17	0.813	INA:2PPARS	1.282	-19.991	-28.781	0.695
2PPAR	150.17	0.813	INA:2PPAR	1.27	-23.575	-24.894	0.947
DLMDA	152.15	0.802	INA:DLMDA	1.373	-30.669	-25.585	1.198
CFA	214.645	0.568	INA:CFA	1.356	-24.188	-30.092	0.803
REOL	110.1	1.109	INA:REOL	1.373	-44.658	-33.232	1.343
HQ	110.1	1.109	INA:HQ	1.378	-44.707	-32.084	1.393
3NNDMABA	165.19	0.739	INA: 3NNDMABA	1.329	-22.973	-28.996	0.792
35TFMBA	258.12	0.473	INA:35TFMBA	1.626	-22.633	-28.691	0.788
MEFA	296.148	0.412	INA:MEFA	1.438	-22.14	-40.442	0.547
FAMEE	144	0.848	INA:FAMEE	1.368	-23.56	-28.194	0.835
FUA	116.07	1.052	NA:FUA	1.462	-31.564	-22.893	1.378
GTA	132.12	0.924	NA:GTA	1.461	-31.412	-26.295	1.195
4HBAIL	138.12	0.884	NA:4HBAIL	1.418	-28.164	-25.566	1.101
EPB	166.15	0.734	NA:EPB	1.393	-20.549	-31.115	0.660
2C4NBA	201.56	0.6058	NA:2C4NBA	1.526	-26.611	-27.934	0.953
TOFA	261.707	0.466	NA:TOFA	1.409	-32.631	-54.947	0.594
MEFA	241.285	0.5061	NA:MEFA	1.338	-31.806	-54.125	0.588
NIFA	282.217	0.432	NA:NIFA	1.533	-24.304	-38.426	0.632
FURA	330.745	0.369	NA:FURA	1.54	-32.907	-43.108	0.763