

## Supporting Information

### Solvent-Free Modafinil Acid Cocrystallization through Green Melt-based Approach

Timothy Joseph Hutagaol <sup>a</sup>, Jianmin Zhou <sup>a,b</sup>, Ziyi Liu <sup>a,b</sup>, Zhenguo Gao <sup>a,b,c\*</sup>, Junbo Gong <sup>a,b</sup>

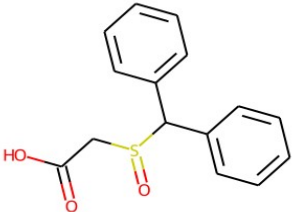
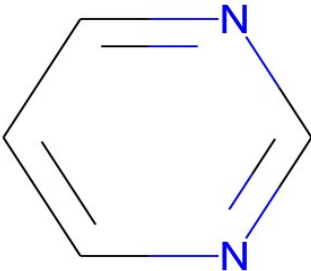
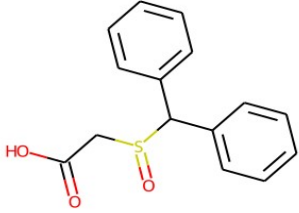
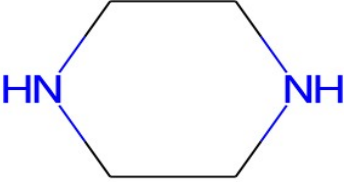
<sup>a</sup> School of Chemical Engineering and Technology, State Key Laboratory of Chemical Engineering, Tianjin University, The Co-Innovation Center of Chemistry and Chemical Engineering of Tianjin, Tianjin, 300072, P. R. China

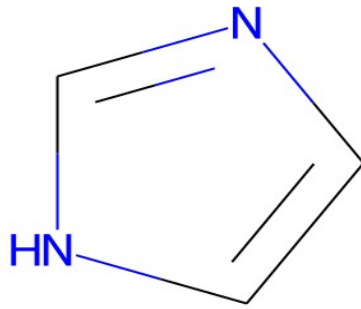
<sup>b</sup> Haihe Laboratory of Sustainable Chemical Transformations, Tianjin 300192, P. R. China

<sup>c</sup> Shanxi Research Institute of Huairou Laboratory, Taiyuan, Shanxi 030032, P. R. China

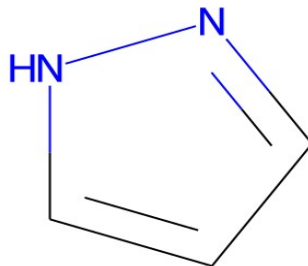
\*Corresponding author: Zhenguo Gao; Email: [zhenguogao@tju.edu.cn](mailto:zhenguogao@tju.edu.cn)

#### T1. CCPT Cocrystal Prediction Score

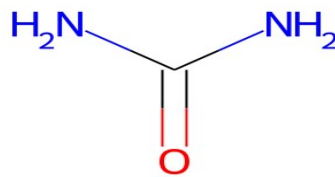
Modafinil Acid	Coformer Compound	Score
		39.67306137
		37.67663574



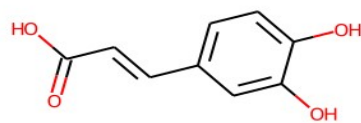
36.7094841



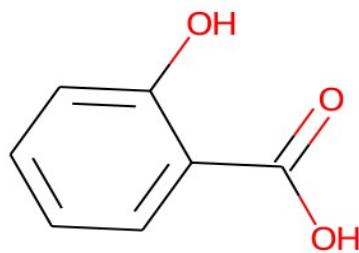
36.25755692



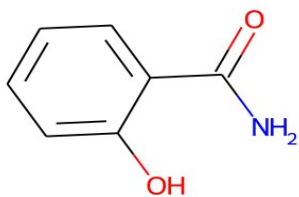
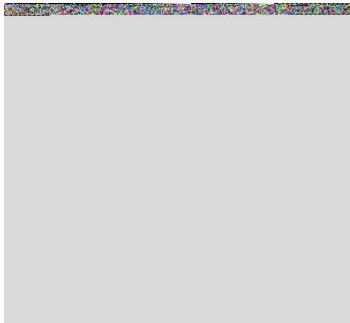
35.81337357



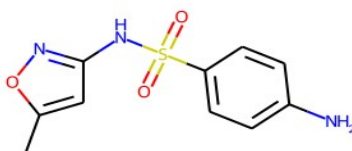
30.74576187



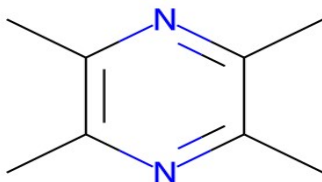
29.89514923



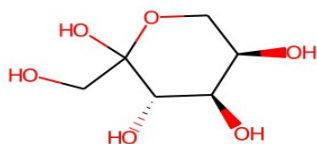
29.31505394



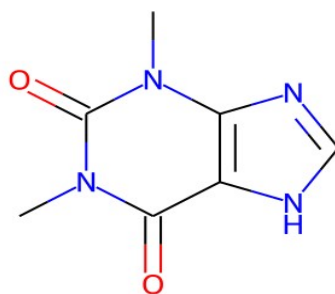
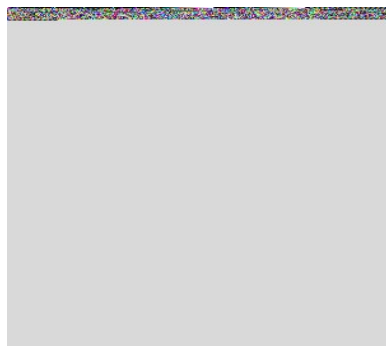
28.36584854



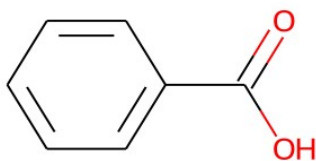
26.62135315



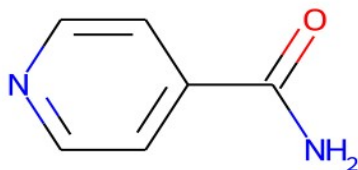
26.05613899



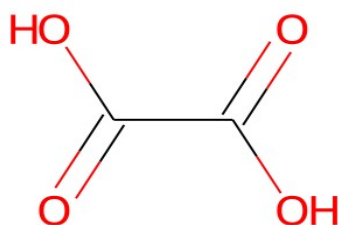
24.82731819



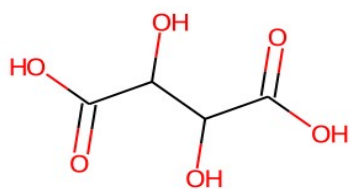
24.79765129



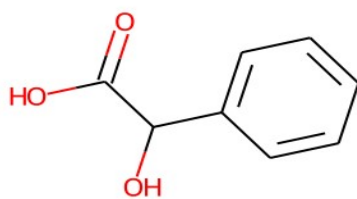
23.77697372



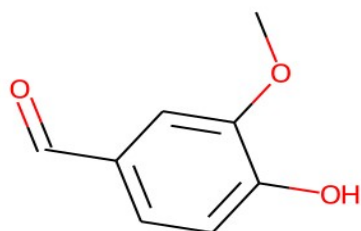
21.91519165



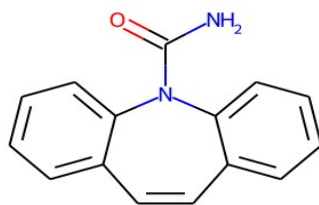
21.21183205



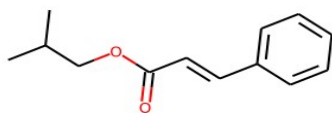
19.9114933



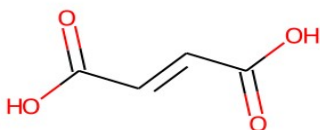
16.02734756



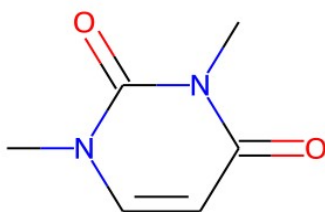
15.25044632



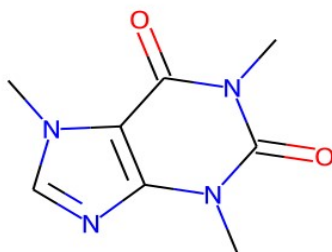
14.20041275



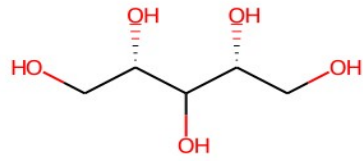
8.832574844



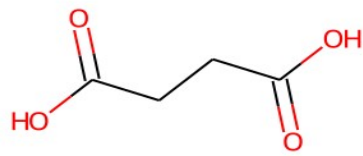
2.06095171



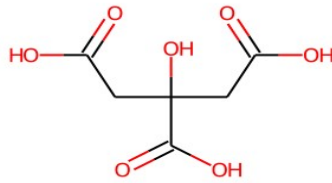
-9.772455215



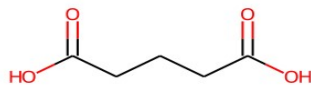
-17.88008499



-21.58124924



-22.80604553



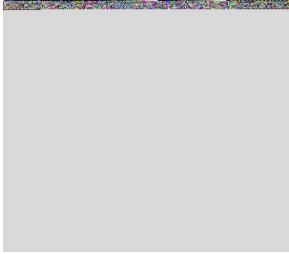
-43.89781952



29.89514923



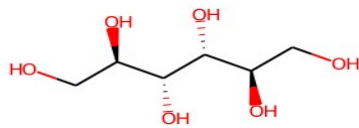
29.31505394



24.79765129



23.77697372



-0.858127356

---

## T2 Molecular Complementarity Coformer Screening Descriptor Criteria

Coformer	Hit Rate%	PASS/FAIL Criteria
2-amino-5-methylbenzoic_acid	100	PASS
3-methylpyridine	100	PASS
4-acetamidobenzoic_acid	100	PASS
4-aminobenzoic_acid	100	PASS
4-hydroxybenzoic_acid	100	PASS
D-alanine	0	FAIL
D-glucuronic_acid	0	FAIL
D-pantothenol	100	PASS
EDTA	0	FAIL
L-arginine	0	FAIL
L-aspartic_acid	0	FAIL
L-aspartic_acid_z	0	FAIL
L-glutamic_acid	0	FAIL
L-glutamic_acid_z	0	FAIL
L-glutamine	0	FAIL
L-glutathione	100	PASS
L-lactic_acid	0	FAIL
L-leucine	100	PASS
L-methionine	100	PASS
L-phenylalanine	100	PASS
L-proline	100	PASS
L-serine	0	FAIL
L-tartaric_acid	0	FAIL
L-tryptophan	100	PASS
L-tyrosine	100	PASS
N,N-dimethylacetamide	100	PASS
N-ethylacetamide	100	PASS
acesulfame	0	FAIL
acetic_acid	0	FAIL
acetophenone_oxime	100	PASS
acetylenedicarboxylic_acid	0	FAIL
adipic_acid	100	PASS
alitame	100	PASS
apigenin	100	PASS
azelaic_acid	0	FAIL
benzoic_acid	100	PASS
biotin	100	PASS
caprolactam	100	PASS
capsaicin	0	FAIL
cholic_acid	0	FAIL

---

<b>citric_acid</b>	0	FAIL
<b>ethylparaben</b>	100	PASS
<b>folic_acid</b>	0	FAIL
<b>fumaric_acid</b>	0	FAIL
<b>gentisic_acid</b>	100	PASS
<b>glutaric_acid</b>	100	PASS
<b>glycine</b>	0	FAIL
<b>glycolic_acid</b>	0	FAIL
<b>hesperetin</b>	100	PASS
<b>hippuric_acid</b>	100	PASS
<b>hydrocinnamic_acid</b>	100	PASS
<b>imidazole</b>	100	PASS
<b>isonicotinamide</b>	100	PASS
<b>ketoglutaric_acid</b>	0	FAIL
<b>lactobionic_acid</b>	0	FAIL
<b>lactose</b>	0	FAIL
<b>maleic_acid</b>	0	FAIL
<b>malic_acid</b>	0	FAIL
<b>malonic_acid</b>	0	FAIL
<b>maltitol</b>	0	FAIL
<b>mannitol</b>	0	FAIL
<b>methanesulfonic_acid</b>	0	FAIL
<b>methylparaben</b>	100	PASS
<b>monobutyryn</b>	100	PASS
<b>nicotinamide</b>	100	PASS
<b>oxalic_acid</b>	0	FAIL
<b>pamoic_acid</b>	100	PASS
<b>phthalamide</b>	100	PASS
<b>pimelic_acid</b>	0	FAIL
<b>piperazine</b>	100	PASS
<b>propylparaben</b>	100	PASS
<b>pyrazine</b>	100	PASS
<b>riboflavin</b>	100	PASS
<b>salicylic acid</b>	100	PASS
<b>salicylamide</b>	100	PASS
<b>suberic_acid</b>	0	FAIL
<b>succinic_acid</b>	0	FAIL
<b>t-butylamine</b>	0	FAIL
<b>t-butylhydroxyanisole</b>	100	PASS
<b>theophylline</b>	0	FAIL
<b>thymidine</b>	100	PASS
<b>triphenylacetic_acid</b>	100	PASS
<b>urea</b>	0	FAIL
<b>valerolactam</b>	100	PASS

---

xanthine

0

FAIL

**T2 Molecular Complementarity Cofomer Screening Descriptor Results (continued)**

<b>Cofomer Conformation</b>	<b>S/L axis ratio</b>	<b> S/L axis  (pass &lt; 0.275)</b>	<b>S/L axis ratio pass/fail</b>
<b>2-amino-5-methylbenzoic_acid</b>	0.408	0.103	pass
<b>3-methylpyridine</b>	0.502	0.01	pass
<b>4-acetamidobenzoic_acid</b>	0.32	0.191	pass
<b>4-aminobenzoic_acid</b>	0.355	0.156	pass
<b>4-hydroxybenzoic_acid</b>	0.357	0.154	pass
<b>D-alanine</b>	0.767	0.255	pass
<b>D-glucuronic_acid</b>	0.676	0.165	pass
<b>D-pantothenol</b>	0.562	0.051	pass
<b>EDTA</b>	0.486	0.025	pass
<b>L-arginine</b>	0.464	0.048	pass
<b>L-aspartic_acid</b>	0.656	0.145	pass
<b>L-aspartic_acid_z</b>	0.621	0.11	pass
<b>L-glutamic_acid</b>	0.563	0.052	pass
<b>L-glutamic_acid_z</b>	0.564	0.053	pass
<b>L-glutamine</b>	0.659	0.148	pass
<b>L-glutathione</b>	0.478	0.033	pass
<b>L-lactic_acid</b>	0.774	0.263	pass
<b>L-leucine</b>	0.656	0.144	pass
<b>L-methionine</b>	0.531	0.02	pass
<b>L-phenylalanine</b>	0.483	0.028	pass
<b>L-proline</b>	0.716	0.205	pass
<b>L-serine</b>	0.691	0.18	pass
<b>L-tartaric_acid</b>	0.671	0.16	pass
<b>L-tryptophan</b>	0.53	0.019	pass
<b>L-tyrosine</b>	0.571	0.06	pass
<b>Molecule Name</b>	0.344	0.167	pass
<b>N-ethylacetamide</b>	0.478	0.033	pass
<b>acesulfame</b>	0.648	0.137	pass
<b>acetic_acid</b>	0.69	0.179	pass
<b>acetophenone_oxime</b>	0.442	0.069	pass
<b>acetylenedicarboxylic_acid</b>	0.415	0.096	pass
<b>adipic_acid</b>	0.361	0.15	pass
<b>alitame</b>	0.605	0.094	pass
<b>apigenin</b>	0.25	0.261	pass
<b>azelaic_acid</b>	0.262	0.249	pass
<b>benzoic_acid</b>	0.382	0.129	pass
<b>biotin</b>	0.471	0.04	pass
<b>caprolactam</b>	0.697	0.186	pass
<b>capsaicin</b>	0.319	0.192	pass

<b>cholic_acid</b>	0.405	0.106	pass
<b>citric_acid</b>	0.617	0.106	pass
<b>ethylparaben</b>	0.383	0.128	pass
<b>folic_acid</b>	0.365	0.146	pass
<b>fumaric_acid</b>	0.382	0.129	pass
<b>gentisic_acid</b>	0.398	0.113	pass
<b>glutaric_acid</b>	0.386	0.125	pass
<b>glycine</b>	0.577	0.066	pass
<b>glycolic_acid</b>	0.599	0.088	pass
<b>hesperetin</b>	0.575	0.064	pass
<b>hippuric_acid</b>	0.489	0.022	pass
<b>hydrocinnamic_acid</b>	0.67	0.159	pass
<b>imidazole</b>	0.552	0.041	pass
<b>isonicotinamide</b>	0.412	0.099	pass
<b>ketoglutaric_acid</b>	0.39	0.121	pass
<b>lactobionic_acid</b>	0.661	0.15	pass
<b>lactose</b>	0.515	0.004	pass
<b>maleic_acid</b>	0.411	0.101	pass
<b>malic_acid</b>	0.521	0.01	pass
<b>malonic_acid</b>	0.53	0.019	pass
<b>maltitol</b>	0.679	0.168	pass
<b>mannitol</b>	0.753	0.242	pass
<b>methanesulfonic_acid</b>	0.938	0.427	fail
<b>methylparaben</b>	0.402	0.109	pass
<b>monobutylin</b>	0.485	0.026	pass
<b>nicotinamide</b>	0.386	0.125	pass
<b>oxalic_acid</b>	0.52	0.009	pass
<b>pamoic_acid</b>	0.602	0.091	pass
<b>phthalamide</b>	0.567	0.056	pass
<b>pimelic_acid</b>	0.323	0.188	pass
<b>piperazine</b>	0.697	0.186	pass
<b>propylparaben</b>	0.371	0.14	pass
<b>pyrazine</b>	0.547	0.036	pass
<b>riboflavin</b>	0.502	0.009	pass
<b>saccharin</b>	0.629	0.118	pass
<b>sorbic_acid</b>	0.379	0.132	pass
<b>suberic_acid</b>	0.295	0.216	pass
<b>succinic_acid</b>	0.444	0.067	pass
<b>t-butylamine</b>	0.889	0.378	fail
<b>t-butylhydroxyanisole</b>	0.606	0.095	pass
<b>theophylline</b>	0.425	0.087	pass
<b>thymidine</b>	0.646	0.135	pass
<b>triphenylacetic_acid</b>	0.74	0.229	pass
<b>urea</b>	0.547	0.036	pass

valerolactam	0.651	0.14	pass
xanthine	0.384	0.127	pass

## T2 Molecular Complementarity Coformer Screening Descriptor Results (continued)

Coformer Conformation	Overall PASS/FAIL	M/L axis	M/L  (pass < 0.31)	M/L axis ratio pass/fail	S axis (Å)	S axis (Å)  (pass < 3.23)	S axis (Å) pass/fail
2-amino-5-methylbenzoic_acid	PASS	0.766	0.013	pass	4.169	2.587	pass
3-methylpyridine	PASS	0.807	0.027	pass	4.167	2.589	pass
4-acetamidobenzoic_acid	PASS	0.536	0.244	pass	4.174	2.582	pass
4-aminobenzoic_acid	PASS	0.671	0.108	pass	3.54	3.216	pass
4-hydroxybenzoic_acid	PASS	0.675	0.104	pass	3.54	3.216	pass
D-alanine	FAIL	0.944	0.165	pass	5.087	1.669	pass
D-glucuronic_acid	FAIL	0.776	0.004	pass	6.455	0.301	pass
D-pantothenol	PASS	0.582	0.198	pass	6.932	0.176	pass
EDTA	FAIL	0.681	0.098	pass	6.595	0.161	pass
L-arginine	FAIL	0.577	0.203	pass	5.881	0.874	pass
L-aspartic_acid	FAIL	0.896	0.116	pass	5.344	1.412	pass
L-aspartic_acid_z	FAIL	0.789	0.009	pass	5.373	1.383	pass
L-glutamic_acid	FAIL	0.746	0.034	pass	5.501	1.254	pass
L-glutamic_acid_z	FAIL	0.702	0.078	pass	5.536	1.22	pass
L-glutamine	FAIL	0.774	0.005	pass	5.887	0.869	pass
L-glutathione	PASS	0.84	0.06	pass	6.835	0.079	pass
L-lactic_acid	FAIL	0.897	0.117	pass	5.399	1.357	pass
L-leucine	PASS	0.853	0.074	pass	5.688	1.068	pass
L-methionine	PASS	0.681	0.099	pass	5.459	1.297	pass
L-phenylalanine	PASS	0.577	0.203	pass	5.567	1.188	pass
L-proline	PASS	0.783	0.003	pass	5.744	1.012	pass
L-serine	FAIL	0.922	0.142	pass	5.064	1.692	pass
L-tartaric_acid	FAIL	0.964	0.184	pass	5.335	1.421	pass
L-tryptophan	PASS	0.689	0.09	pass	6.018	0.737	pass
L-tyrosine	PASS	0.668	0.112	pass	6.27	0.486	pass
Molecule Name	PASS	0.593	0.187	pass	3.54	3.216	pass
N-ethylacetamide	PASS	0.683	0.097	pass	4.169	2.587	pass
acesulfame	FAIL	0.998	0.219	pass	5.267	1.489	pass
acetic_acid	FAIL	0.865	0.085	pass	4.175	2.581	pass
acetophenone_oxime	PASS	0.774	0.006	pass	4.181	2.574	pass
acetylenedicarboxylic_acid	FAIL	0.657	0.123	pass	3.737	3.019	pass
adipic_acid	PASS	0.475	0.305	pass	4.161	2.594	pass
alitame	PASS	0.652	0.128	pass	7.989	1.233	pass
apigenin	PASS	0.638	0.142	pass	3.549	3.206	pass
azelaic_acid	FAIL	0.351	0.429	fail	4.167	2.589	pass

<b>benzoic_acid</b>	PASS	0.723	0.056	pass	3.541	3.215	pass
<b>biotin</b>	PASS	0.664	0.116	pass	6.324	0.432	pass
<b>caprolactam</b>	PASS	0.953	0.173	pass	5.535	1.221	pass
<b>capsaicin</b>	FAIL	0.445	0.334	fail	6.494	0.262	pass
<b>cholic_acid</b>	FAIL	0.453	0.326	fail	7.399	0.644	pass
<b>citric_acid</b>	FAIL	0.673	0.107	pass	6.253	0.502	pass
<b>ethylparaben</b>	PASS	0.636	0.144	pass	4.371	2.384	pass
<b>folic_acid</b>	FAIL	0.42	0.36	fail	8.015	1.26	pass
<b>fumaric_acid</b>	FAIL	0.617	0.163	pass	3.54	3.216	pass
<b>gentisic_acid</b>	PASS	0.868	0.088	pass	3.548	3.208	pass
<b>glutaric_acid</b>	PASS	0.527	0.252	pass	4.167	2.589	pass
<b>glycine</b>	FAIL	0.745	0.035	pass	4.364	2.391	pass
<b>glycolic_acid</b>	FAIL	0.786	0.006	pass	4.182	2.573	pass
<b>hesperetin</b>	PASS	0.682	0.098	pass	7.492	0.737	pass
<b>hippuric_acid</b>	PASS	0.578	0.202	pass	5.866	0.89	pass
<b>hydrocinnamic_acid</b>	PASS	0.805	0.025	pass	6.032	0.724	pass
<b>imidazole</b>	PASS	0.942	0.162	pass	3.54	3.215	pass
<b>isonicotinamide</b>	PASS	0.772	0.008	pass	3.551	3.205	pass
<b>ketoglutaric_acid</b>	FAIL	0.574	0.206	pass	4.171	2.584	pass
<b>lactobionic_acid</b>	FAIL	0.706	0.074	pass	8.159	1.404	pass
<b>lactose</b>	FAIL	0.687	0.092	pass	6.591	0.164	pass
<b>maleic_acid</b>	FAIL	0.69	0.09	pass	3.575	3.18	pass
<b>malic_acid</b>	FAIL	0.653	0.127	pass	4.874	1.881	pass
<b>malonic_acid</b>	FAIL	0.697	0.083	pass	4.15	2.606	pass
<b>maltitol</b>	FAIL	0.846	0.067	pass	8.056	1.301	pass
<b>mannitol</b>	FAIL	0.859	0.08	pass	6.684	0.072	pass
<b>methanesulfonic_acid</b>	FAIL	0.994	0.215	pass	5.261	1.495	pass
<b>methylparaben</b>	PASS	0.666	0.113	pass	4.23	2.526	pass
<b>monobutyrim</b>	PASS	0.729	0.05	pass	5.161	1.594	pass
<b>nicotinamide</b>	PASS	0.724	0.056	pass	3.548	3.208	pass
<b>oxalic_acid</b>	FAIL	0.844	0.065	pass	3.54	3.216	pass
<b>pamoic_acid</b>	PASS	0.725	0.055	pass	7.963	1.208	pass
<b>phthalamide</b>	PASS	0.953	0.173	pass	5.027	1.728	pass
<b>pimelic_acid</b>	FAIL	0.433	0.347	fail	4.18	2.576	pass
<b>piperazine</b>	PASS	0.92	0.14	pass	4.979	1.777	pass
<b>propylparaben</b>	PASS	0.532	0.247	pass	4.913	1.843	pass
<b>pyrazine</b>	PASS	0.938	0.158	pass	3.55	3.205	pass
<b>riboflavin</b>	PASS	0.833	0.053	pass	6.995	0.239	pass
<b>saccharin</b>	PASS	0.929	0.149	pass	5.577	1.179	pass
<b>sorbic_acid</b>	PASS	0.499	0.28	pass	4.166	2.589	pass
<b>suberic_acid</b>	FAIL	0.393	0.387	fail	4.161	2.594	pass
<b>succinic_acid</b>	FAIL	0.581	0.199	pass	4.189	2.567	pass
<b>t-butylamine</b>	FAIL	0.923	0.144	pass	5.972	0.783	pass
<b>t-butylhydroxyanisole</b>	PASS	0.743	0.037	pass	6.735	0.02	pass

theophylline	FAIL	0.884	0.105	pass	4.194	2.561	pass
thymidine	PASS	0.7	0.08	pass	7.542	0.786	pass
triphenylacetic_acid	PASS	0.967	0.188	pass	8.323	1.567	pass
urea	FAIL	0.865	0.086	pass	3.54	3.216	pass
valerolactam	PASS	0.851	0.071	pass	5.134	1.621	pass
xanthine	FAIL	0.824	0.044	pass	3.545	3.211	pass

## T2 Molecular Complementarity Cofomer Screening Descriptor Results (continued)

Cofomer Conformation	DM (Debye)	DM (Debye)  (pass < 5.94)	DM (Debye)   pass/fail	FNO	FNO  (pass < 0.294)	FNO pass/fail
2-amino-5-methylbenzoic_acid	1.361	0.988	pass	0.273	0.115	pass
3-methylpyridine	1.437	0.911	pass	0.143	0.015	pass
4-acetamidobenzoic_acid	1.612	0.736	pass	0.308	0.15	pass
4-aminobenzoic_acid	0.849	1.499	pass	0.3	0.142	pass
4-hydroxybenzoic_acid	2.205	0.144	pass	0.3	0.142	pass
D-alanine	3.343	0.995	pass	0.5	0.342	fail
D-glucuronic_acid	3.657	1.309	pass	0.538	0.381	fail
D-pantothenol	4.265	1.917	pass	0.357	0.199	pass
EDTA	3.05	0.701	pass	0.5	0.342	fail
L-arginine	2.027	0.322	pass	0.5	0.342	fail
L-aspartic_acid	1.186	1.162	pass	0.556	0.398	fail
L-aspartic_acid_z	15.846	13.498	fail	0.556	0.398	fail
L-glutamic_acid	1.697	0.651	pass	0.5	0.342	fail
L-glutamic_acid_z	15.835	13.486	fail	0.5	0.342	fail
L-glutamine	0.564	1.784	pass	0.5	0.342	fail
L-glutathione	0.646	1.702	pass	0.45	0.292	pass
L-lactic_acid	2.587	0.239	pass	0.5	0.342	fail
L-leucine	3.422	1.074	pass	0.333	0.175	pass
L-methionine	2.085	0.264	pass	0.333	0.175	pass
L-phenylalanine	1.37	0.978	pass	0.25	0.092	pass
L-proline	1.545	0.804	pass	0.375	0.217	pass
L-serine	4.362	2.014	pass	0.571	0.414	fail
L-tartaric_acid	3.295	0.946	pass	0.6	0.442	fail
L-tryptophan	0.932	1.416	pass	0.267	0.109	pass
L-tyrosine	1.737	0.611	pass	0.308	0.15	pass
Molecule Name	0.88	1.468	pass	0.182	0.024	pass
N-ethylacetamide	1.656	0.693	pass	0.333	0.175	pass
acesulfame	2.386	0.038	pass	0.5	0.342	fail
acetic_acid	0.86	1.489	pass	0.5	0.342	fail
acetophenone_oxime	1.223	1.125	pass	0.2	0.042	pass
acetylenedicarboxylic_acid	0.428	1.92	pass	0.5	0.342	fail

<b>adipic_acid</b>	0.013	2.336	pass	0.4	0.242	pass
<b>alitame</b>	1.98	0.368	pass	0.318	0.16	pass
<b>apigenin</b>	0.493	1.856	pass	0.25	0.092	pass
<b>azelaic_acid</b>	0.928	1.42	pass	0.308	0.15	pass
<b>benzoic_acid</b>	0.991	1.357	pass	0.222	0.064	pass
<b>biotin</b>	1.638	0.711	pass	0.313	0.155	pass
<b>caprolactam</b>	2.061	0.287	pass	0.25	0.092	pass
<b>capsaicin</b>	2.166	0.183	pass	0.182	0.024	pass
<b>cholic_acid</b>	4.539	2.191	pass	0.172	0.015	pass
<b>citric_acid</b>	1.783	0.566	pass	0.538	0.381	fail
<b>ethylparaben</b>	3.594	1.245	pass	0.25	0.092	pass
<b>folic_acid</b>	2.021	0.328	pass	0.406	0.248	pass
<b>fumaric_acid</b>	2.637	0.288	pass	0.5	0.342	fail
<b>gentisic_acid</b>	2.843	0.495	pass	0.364	0.206	pass
<b>glutaric_acid</b>	2.449	0.1	pass	0.444	0.287	pass
<b>glycine</b>	1.007	1.341	pass	0.6	0.442	fail
<b>glycolic_acid</b>	1.422	0.927	pass	0.6	0.442	fail
<b>hesperetin</b>	5.599	3.25	pass	0.273	0.115	pass
<b>hippuric_acid</b>	2.176	0.172	pass	0.308	0.15	pass
<b>hydrocinnamic_acid</b>	0.852	1.496	pass	0.182	0.024	pass
<b>imidazole</b>	1.319	1.03	pass	0.4	0.242	pass
<b>isonicotinamide</b>	1.272	1.077	pass	0.333	0.175	pass
<b>ketoglutaric_acid</b>	1.37	0.978	pass	0.5	0.342	fail
<b>lactobionic_acid</b>	8.72	6.372	fail	0.5	0.342	fail
<b>lactose</b>	4.554	2.206	pass	0.478	0.32	fail
<b>maleic_acid</b>	4.208	1.859	pass	0.5	0.342	fail
<b>malic_acid</b>	3.291	0.942	pass	0.556	0.398	fail
<b>malonic_acid</b>	1.699	0.65	pass	0.571	0.414	fail
<b>maltitol</b>	7.131	4.782	pass	0.478	0.32	fail
<b>mannitol</b>	4.66	2.312	pass	0.5	0.342	fail
<b>methanesulfonic_acid</b>	2.599	0.25	pass	0.6	0.442	fail
<b>methylparaben</b>	1.291	1.057	pass	0.273	0.115	pass
<b>monobutyryn</b>	3.488	1.139	pass	0.364	0.206	pass
<b>nicotinamide</b>	2.435	0.086	pass	0.333	0.175	pass
<b>oxalic_acid</b>	2.623	0.275	pass	0.667	0.509	fail
<b>pamoic_acid</b>	0.233	2.115	pass	0.207	0.049	pass
<b>phthalamide</b>	2.875	0.526	pass	0.333	0.175	pass
<b>pimelic_acid</b>	1.664	0.684	pass	0.364	0.206	pass
<b>piperazine</b>	0.001	2.348	pass	0.333	0.175	pass
<b>propylparaben</b>	2.286	0.062	pass	0.231	0.073	pass
<b>pyrazine</b>	0	2.348	pass	0.333	0.175	pass
<b>riboflavin</b>	3.978	1.63	pass	0.37	0.212	pass
<b>saccharin</b>	2.141	0.208	pass	0.333	0.175	pass
<b>sorbic_acid</b>	1.028	1.321	pass	0.25	0.092	pass

---

<b>suberic_acid</b>	0.01	2.339	pass	0.333	0.175	pass
<b>succinic_acid</b>	1.076	1.273	pass	0.5	0.342	fail
<b>t-butylamine</b>	0.771	1.577	pass	0.2	0.042	pass
<b>t-butylhydroxyanisole</b>	0.688	1.66	pass	0.154	0.004	pass
<b>theophylline</b>	0.736	1.612	pass	0.462	0.304	fail
<b>thymidine</b>	4.421	2.072	pass	0.412	0.254	pass
<b>triphenylacetic_acid</b>	3.073	0.724	pass	0.091	0.067	pass
<b>urea</b>	1.44	0.908	pass	0.75	0.592	fail
<b>valerolactam</b>	2.028	0.321	pass	0.286	0.128	pass
<b>xanthine</b>	1.202	1.147	pass	0.545	0.388	fail

---

### T3 Excess Enthalpy Computational Results ( $H_{ex}$ )

<b>Cofomer</b>	<b>Cofomer Ranking</b>	<b>H_ex[kcal/mol]</b>
Oxalic acid	2.0	-2.954825
1,3,5-trihydroxybenzene	3.0	-2.799725
1,3,5-trihydroxybenzene	61.0	-2.355095
4,4-biphenol	5.0	-2.251965
1,3-dihydroxybenzene	4.0	-2.22683
1-naphthol	1.0	-2.18447
Citric acid	75.0	-2.096455
Caffeic Acid	47.0	-1.758385
Maleic acid	40.0	-1.429405
salicyclic acid	16.0	-1.318445
Succinic acid	69.0	-1.018895
3-cyanophenol	6.0	-0.792715
4-cyanophenol	7.0	-0.619655
benzoic acid	26.0	-0.616155
Glutaric acid	74.0	-0.613015
ethine	8.0	-0.5671
N,N-dimethylacetamid	9.0	-0.467125
chloroform	10.0	-0.46157
dimethylsulfoxide	11.0	-0.454585
ch2cl2	12.0	-0.38096
H2S	13.0	-0.339
O2	14.0	-0.337435
aceticacid	15.0	-0.313905
salicylamide	62.0	-0.30981
N2	17.0	-0.26738

---

bicalutamide	79.0	-0.24997
1,2-bis(4-pyridyl)ethane	63.0	-0.221575
propyne	18.0	-0.21726
propanone	19.0	-0.19655
1,3-dimethyluracil	20.0	-0.1916
CO2	21.0	-0.185465
butanone	22.0	-0.13166
dioxane	23.0	-0.12839
4,4'-bipyridine	24.0	-0.119535
trans-1,2-bis(4-dipyridyl)ethylene	50.0	-0.11687
Tetrahydrofuran	25.0	-0.113755
5-hydroxyisoquinoline	27.0	-0.092535
ethylacetate	51.0	-0.09165
Paracetamol	66.0	-0.08152
Pyrazole	28.0	-0.06335
3-hydroxypyridine	29.0	-0.060765
Pyrimidine	30.0	-0.05502
Vanillin	67.0	-0.050325
4-phenylpyridine	31.0	-0.049065
2,3,5,6-tetramethylpyrazine	32.0	-0.033215
carbonmonoxide	33.0	0.010035
4-methyl-2-pentanone	57.0	0.01093
acetonitrile	34.0	0.045595
1-cyanonaphthalene	35.0	0.05355
4-pyridinecarbonitrile	36.0	0.064005
3-cyanopyridine	37.0	0.070505
Carbamazepine	60.0	0.095515

---

---

1,4-dicyanobenzene	38.0	0.095775
1,3-dicyanobenzene	39.0	0.09824
Theophylline	41.0	0.117675
PVC	77.0	0.12384
Piperazine	42.0	0.168235
toluene	43.0	0.188335
Cinnamic acid	78.0	0.194
water	44.0	0.240205
propene	45.0	0.25425
CH4	46.0	0.255795
isonicotinamide	64.0	0.299325
ethane	48.0	0.32012
Imidazole	49.0	0.332375
Urea	65.0	0.339235
methanol	52.0	0.43003
ethanol	53.0	0.43315
D-fructopyranose	80.0	0.436215
propane	54.0	0.45813
1-propanol	68.0	0.47973
ethyleneglycol	72.0	0.496185
2-propanol	55.0	0.496415
CCl4	56.0	0.501245
1-butanol	73.0	0.52779
isobutane	58.0	0.52983
butane	59.0	0.538635
1-pentanol	76.0	0.57583
mannitol	83.0	0.597615
Xylitol	82.0	0.686335

---

---

1-octanol	81.0	0.749195
1-hexadecanol	84.0	1.0178
SF6	70.0	1.07676

---

#### T4. Hansen Solubility Parameter Results ( $\Delta\delta_i$ )

COSMOQuick predicts miscibility of API and coformer through Hansen solubility parameter (HSP) model and hydrogen bonding contributions of dispersion ( $\delta_d$ ), polar ( $\delta_p$ ), and hydrogen bonding ( $\delta_h$ ). Manual calculation from each of hydrogen bonding total solubility parameter,  $\delta_t$  are calculated with equation below:

$$\delta_t = \sqrt{(\delta_d^2 + \delta_p^2 + \delta_h^2)}$$

Compound	$\delta_d$	$\delta_p$	$\delta_h$	$\delta_t$
<b>Pyrazole</b>	18.77322664	5.54310668	7.75066001	4.239299032
<b>Succinic acid</b>	17.12187336	12.36820952	22.95403332	5.900855435
<b>Urea</b>	18.66475524	17.67501992	22.60313324	8.937433068
<b>Vanillin</b>	19.24346664	9.58553339	12.2293534	0.558802436
<b>2,3,5,6-tetramethylpyrazine</b>	18.93787332	6.51815333	6.62550668	4.196737704
<b>Isonicotinamide</b>	19.83464656	14.43869336	13.03194663	2.487467631
<b>Theophylline</b>	19.46954	13.55249341	12.39651346	1.4733793
<b>Benzoic acid</b>	19.85212	7.10066	10.97915324	1.521238055
<b>Carbamazepine</b>	20.22008672	11.05924666	12.60337334	0.975530774
<b>D-fructopyranose</b>	17.86628672	10.42657995	22.31719324	5.137441605
<b>Citric acid</b>	18.39889512	15.7186934	25.40754652	9.795212013
<b>Salicylic acid</b>	18.89833988	8.12237336	13.85173996	0.493383788
<b>Maleic acid</b>	17.42398	11.78112472	21.27283332	4.622876787
<b>Piperazine</b>	17.64418668	5.6790933	8.43567331	4.927472801
<b>Salicylamide</b>	18.95727996	10.16691994	13.09594668	0.108102218
<b>Mannitol</b>	13.99137336	9.25473997	27.45759336	6.884122039
<b>Caffeic acid</b>	18.88592668	8.40279333	17.64047324	1.88243751
<b>Xylitol</b>	17.98564668	12.7586933	28.63416668	10.84876335
<b>1,3-dimethyluracil</b>	19.58035328	11.30177987	8.51660001	1.133483703

<b>Glutaric acid</b>	17.14839996	12.14601332	20.98627336	4.406376012
<b>Cinnamic acid</b>	17.98155332	4.78679999	4.21465999	6.213267207
<b>Imidazole</b>	20.05511996	14.40674096	14.33846668	3.262004226
<b>2,3-dihydroxybutanedioic acid</b>	16.9850666	13.66679333	26.87741992	9.314967074
<b>Pyrimidine</b>	19.72997336	9.33724672	8.91169338	1.715407089
<b>Oxalic acid</b>	17.0799666	17.37136008	26.3317266	10.58028708
<b>3-cyanophenol</b>	19.98021332	11.93819989	12.92667327	1.331438025
<b>1,2-bis(4-pyridyl)ethane</b>	19.35344008	7.50296665	7.35365335	3.271350055
<b>trans-1,2-bis(4-dipyridyl)ethylene</b>	19.46542008	7.38621999	8.04660001	2.971851805
<b>4,4'-bipyridine</b>	19.6192534	7.60889998	7.14309997	3.070010069
<b>4-phenylpyridine</b>	19.95288	7.06706666	5.45785334	3.432635952
<b>4-pyridinecarbonitrile</b>	19.79666004	11.72653994	10.0122934	0.19925718
<b>3-cyanopyridine</b>	19.87971344	12.1720666	10.07004671	0.099889497
<b>1-cyanonaphthalene</b>	20.1111466	8.81365998	5.14312	2.740442629
<b>1-naphthol</b>	19.84418668	6.37207333	12.37933994	1.051042365
<b>1,3-dicyanobenzene</b>	19.92822	14.32692664	7.88277999	0.486143748
<b>1,4-dicyanobenzene</b>	19.92187332	13.9718999	7.31852663	0.117365226
<b>1,3,5-trihydroxybenzene</b>	19.1311	9.58726003	19.30518	3.527816386
<b>4,4-biphenol</b>	19.57990668	9.45268002	14.8740066	1.050764247
<b>1,3-dihydroxybenzene</b>	19.45106668	8.91450003	17.74567324	2.505469836
<b>bicalutamide</b>	19.5246134	13.50342012	13.36025993	1.948190391
<b>3-hydroxypyridine</b>	19.96201992	11.02802	18.31501312	3.957207364
<b>5-hydroxyisoquinoline</b>	19.85749992	10.64785992	18.58307984	3.914250621
<b>4-cyanophenol</b>	19.92549996	14.06397323	13.1042067	2.394085265
<b>1-hexadecanol</b>	16.28820668	3.66762	8.26987335	6.660487905

<b>Paracetamol</b>	18.40496664	10.23887332	15.23060668	0.698925943
<b>CCl4</b>	17.02672	4.05138573	0.25638	7.788432824
<b>toluene</b>	18.12055336	1.53714667	2.20385334	6.973708195
<b>chloroform</b>	17.42837332	4.16910664	5.00202001	6.687291013
<b>water</b>	16.21935064	17.27807619	25.34473264	9.405656899
<b>1-octanol</b>	15.95663332	5.10407333	11.22444668	5.126732058
<b>1-pentanol</b>	15.86908656	5.74172	13.76912672	3.51203324
<b>ethyleneglycol</b>	16.87202664	11.31738006	25.11576948	7.011634571
<b>1-butanol</b>	15.90185988	5.81462667	15.62044656	2.255957873
<b>1-propanol</b>	15.9108466	6.99722	16.8354066	1.094314516
<b>ethanol</b>	15.695	8.50189998	18.49297332	0.40985102
<b>ch2cl2</b>	16.91586652	7.10505334	6.63725334	5.781334018
<b>2-propanol</b>	15.71431328	6.67912003	16.26231984	1.712458869
<b>methanol</b>	15.1372266	11.26026675	19.79657332	2.054151683
<b>aceticacid</b>	15.2951734	9.21440663	13.57783344	2.860158549
<b>dimethylsulfoxide</b>	17.80159328	16.55738672	10.36657999	1.136941367
<b>N,N-dimethylacetamid</b>	16.73524	12.31542681	9.01604663	2.642292458
<b>4-methyl-2-pentanone</b>	15.41596004	6.48145333	4.51560667	7.970391499
<b>butanone</b>	15.83687336	9.56544006	5.64962668	5.947562917
<b>propanone</b>	15.46038664	11.3044201	7.27880668	4.803506708
<b>acetonitrile</b>	15.2462868	16.74816665	7.41137334	1.462186066
<b>ethylacetate</b>	15.72590668	6.29512	7.28429331	6.853478307
<b>thf</b>	17.05585312	6.07534667	6.90978	5.913100179
<b>dioxane</b>	17.34798668	4.83574668	8.08738666	5.550486354
<b>PVC</b>	18.11744676	7.39690668	6.32369333	4.726762238
<b>O2</b>	14.91224668	2.60827999	1.55226667	10.07438616
<b>N2</b>	14.13333344	1.46378667	1.56226667	10.99783323
<b>CO2</b>	15.38702672	6.54075334	4.30586667	8.02732698

---

<b>carbonmonoxide</b>	13.41376004	13.63273338	11.88912675	2.772808739
<b>CH4</b>	14.22037336	0.65427333	0.45871333	11.04958828
<b>ethane</b>	14.79004676	0.60966666	0.36754	10.48522455
<b>propyne</b>	14.77817336	4.89016667	4.22220665	9.163687531
<b>propene</b>	14.38415904	2.08588	1.16014667	10.7115548
<b>propane</b>	13.70703348	0.22415334	0.09783333	11.58317858
<b>SF6</b>	14.89656672	2.17836665	0.02697333	10.23737112
<b>ethine</b>	13.88644008	5.00618665	8.7956734	8.10929186
<b>butane</b>	14.04292668	0.14513334	0.10714667	11.24830846
<b>isobutane</b>	14.30778012	0.37902667	0.02157333	10.97957795
<b>H2S</b>	16.67465996	6.58028667	9.59420001	4.960322338

---

## T5. Overlapping Coformer Screening Results through GNN-based and In-silico Tools

<b>Two-way Overlap</b>	
<b><math>H_{ex} \cap HSP</math></b>	1,3,5-Trihydroxybenzene, 1,3-Dihydroxybenzene, 1,3-Dimethyluracil, 1-Naphthol, 2,3,5,6-Tetramethylpyrazine, 3-Cyanophenol, 3-Hydroxypyridine, 4,4'-Bipyridine, 4,4-Biphenol, 4-Cyanophenol, 4-Phenylpyridine, 5-Hydroxyisoquinoline, Acetic acid, Benzoic acid, Bicalutamide, Butanone, Caffeic acid, Chloroform, Dichloromethane, Dimethyl sulfoxide, Dioxane, Ethyl acetate, Glutaric acid, H <sub>2</sub> S, Maleic acid, N,N-Dimethylacetamide, Paracetamol, Propanone, Pyrazole, Pyrimidine, Salicylic acid, Salicylamide, Succinic acid, Tetrahydrofuran, trans-1,2-Bis(4-pyridyl)ethylene, Vanillin
<b><math>H_{ex} \cap MC</math></b>	Benzoic acid, Glutaric acid, Salicylic acid, Salicylamide
<b><math>H_{ex} \cap CCPT</math></b>	1,3,5-Trihydroxybenzene, 1,3-Dihydroxybenzene, 1,3-Dimethyluracil, 1-Naphthol, 2,3,5,6-Tetramethylpyrazine, 3-Cyanophenol, 3-Hydroxypyridine, 4,4'-Bipyridine, 4,4-Biphenol, 4-Cyanophenol, 4-Phenylpyridine, 5-Hydroxyisoquinoline, Acetic acid, Benzoic acid, Bicalutamide, Butanone, Caffeic acid, Carbamazepine, Chloroform, Cinnamic acid, Citric acid, Dichloromethane, Dimethyl sulfoxide, Dioxane, Ethyl acetate, Fumaric acid, Glutaric acid, H <sub>2</sub> S, Imidazole, Isonicotinamide, Maleic acid, Mannitol, N,N-Dimethylacetamide, Oxalic acid, Paracetamol, Piperazine, Propanone, Pyrazole, Pyrimidine, Salicylic acid, Salicylamide, Succinic acid, Tartaric acid, Tetrahydrofuran, Theophylline, trans-1,2-Bis(4-pyridyl)ethylene, Urea Vanillin,
<b><math>HSP \cap MC</math></b>	Benzoic acid, Glutaric acid, Imidazole, Isonicotinamide, Piperazine, Salicylic acid, Salicylamide
<b><math>HSP \cap CCPT</math></b>	1,3,5-Trihydroxybenzene, 1,3-Dihydroxybenzene, 1,3-Dimethyluracil, 1-Naphthol, 2,3,5,6-Tetramethylpyrazine, 3-Cyanophenol, 3-Hydroxypyridine, 4,4'-Bipyridine, 4,4-Biphenol, 4-Cyanophenol 4-Phenylpyridine, 5-Hydroxyisoquinoline, Acetic acid,

	Benzoic acid, Bicalutamide, Butanone, Caffeic acid, Carbamazepine, Chloroform, Cinnamic acid, Citric acid, Dichloromethane, Dimethyl sulfoxide, Dioxane, Ethyl acetate, Fumaric acid, Glutaric acid, H <sub>2</sub> S, Imidazole, Isonicotinamide, Maleic acid, Mannitol, N,N-Dimethylacetamide, Oxalic acid, Paracetamol, Piperazine, Propanone, Pyrazole, Pyrimidine, Salicylic acid, Salicylamide, Succinic acid, Tartaric acid, Tetrahydrofuran, Theophylline, trans-1,2-Bis(4-pyridyl)ethylene, Urea Vanillin
<b>CCPT ∩ MC</b>	Benzoic acid, Glutaric acid, Imidazole, Isonicotinamide, Piperazine, Pyrazole, Pyrazine, Salicylic acid
<b>Three-way Overlap</b>	
<b>MC ∩ HSP ∩ CCPT</b>	Benzoic acid, Glutaric acid, Imidazole, Isonicotinamide
<b>MC ∩ HSP ∩ H<sub>ex</sub></b>	Benzoic acid, glutaric acid, salicylic acid, salicylamide
<b>HSP ∩ H<sub>ex</sub> ∩ CCPT</b>	Pyrazole, salicylic acid, 2,3,5,6-tetramethylpyrazine, benzoic acid, vanillin, 1,3-dimethyluracil, glutaric acid, mannitol
<b>MC ∩ H<sub>ex</sub> ∩ CCPT</b>	Pyrazole, salicylic acid, benzoic acid, glutaric acid
<b>Four-way Overlap</b>	
<b>MC ∩ HSP ∩ CCPT ∩ H<sub>ex</sub></b>	Benzoic acid, glutaric acid, salicylic acid

**T6.** Crystallographic data of 2:3:1 Modafinil Acid – Isonicotinamide – H<sub>2</sub>O Cocrystal Hydrate

Identification	Cocrystal Hydrate MODI
Empirical formula	C <sub>102</sub> H <sub>102</sub> N <sub>12</sub> O <sub>20</sub> S <sub>4</sub>
Formula weight	1944.19
Temperature/K	100.00(10)
Crystal System	TRICLINIC
Space Group	<i>P</i> - <i>1</i>
<i>a</i> /Å	8.7434(4)

---

$b/\text{Å}$	10.8237(5)
$c/\text{Å}$	25.1996(11)
$\alpha/^\circ$	84.465(4)
$\beta/^\circ$	80.705(4)
$\gamma/^\circ$	71.166(4)
Volume/ $\text{Å}^3$	2224.96(18)
$Z$	1
$\rho_{\text{calc}}(\text{g}/\text{cm}^3)$	1.451
$\mu/\text{mm}^{-1}$	1.675
Radiation	Cu K $\alpha$ ( $\lambda = 1.54184$ )
$2\theta$ range for data collection/ $^\circ$	3.556 to 150.916
Reflections collected	31221
Goodness-of-fit on $F^2$	1.116
Final R indexes $[I \geq 2\sigma(I)]$	$R_1 = 0.1076$ , $WR_2 = 0.2696$
Final R indexes [all data]	$R_1 = 0.1271$ , $WR_2 = 0.2821$
CCPT deposition	2537722

---

**S1. Comparison of X-ray powder diffraction data of modafinil acid crystal system and combined with other coformers.**

**S2 Thermal analysis results through DSC of modafinil acid crystal system and various combination with other cofomers**

