Supplementary Information

Molecular screening for solid–solid phase transition by machine learning

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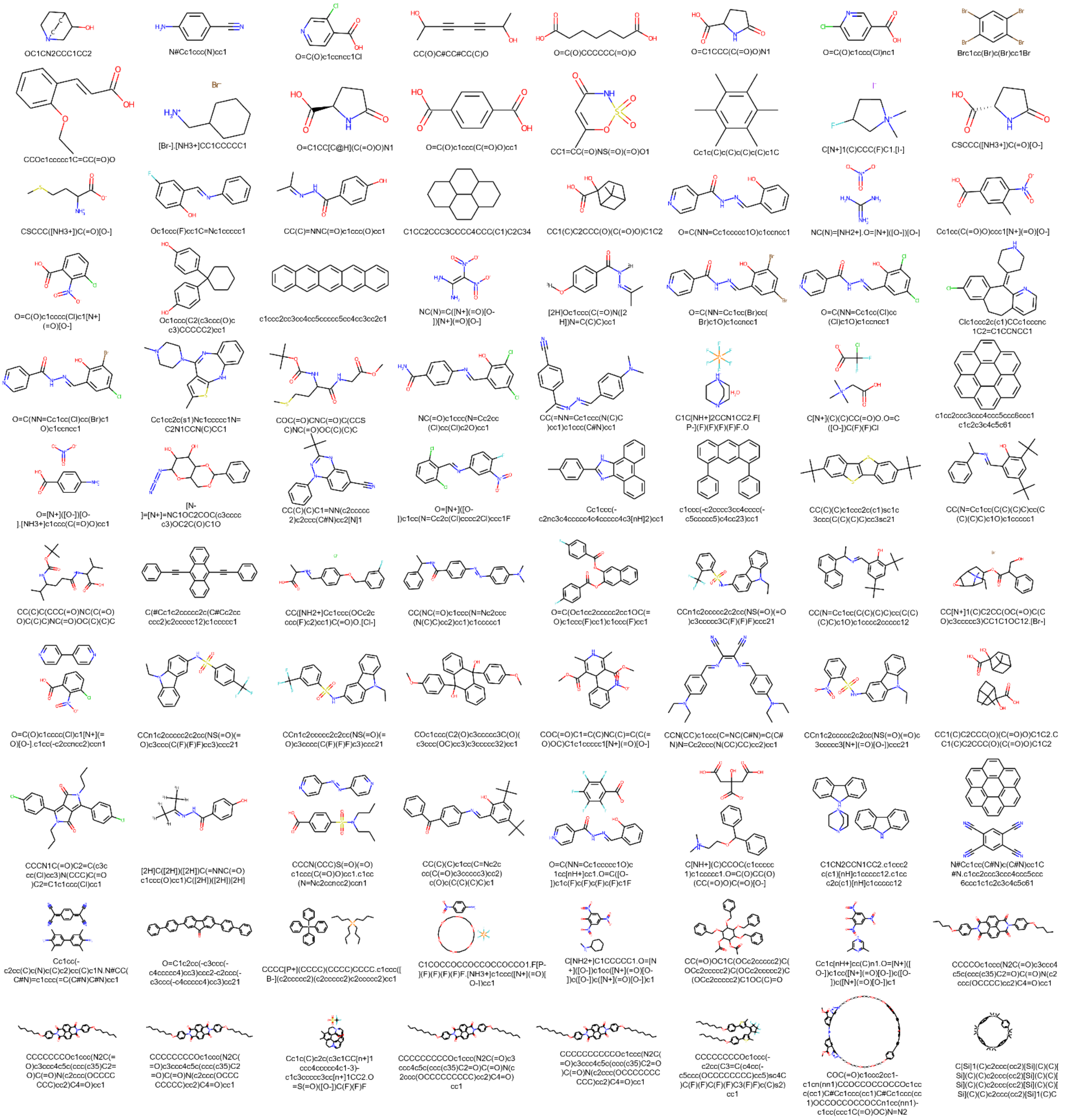
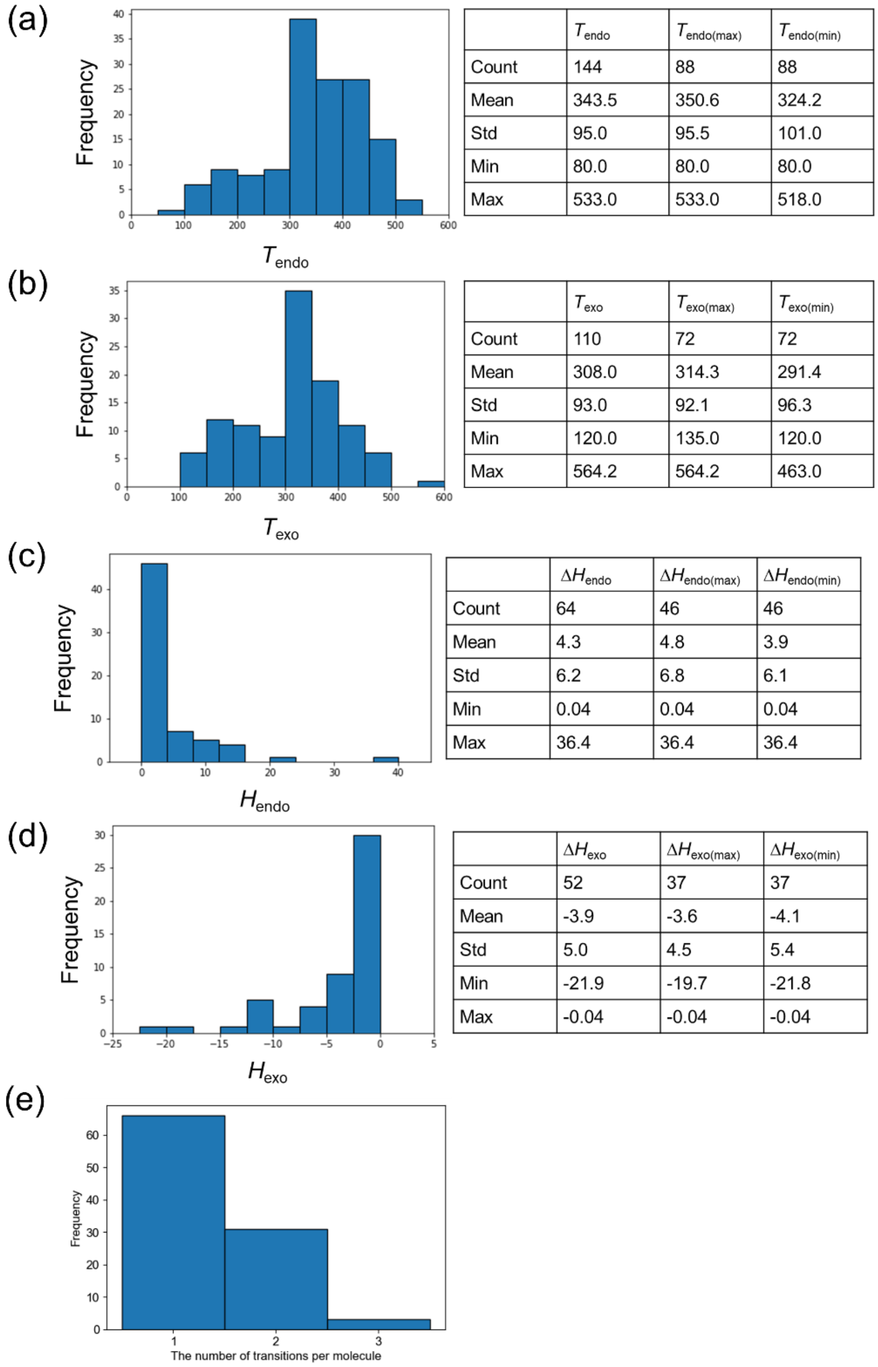


OC1CN2CCC1CC2
N#Cc1ccc(N)cc1
O=C(O)c1ccncc1Cl
CC(O)C#CC#CC(C)O
O=C(O)CCCCCC(=O)O
O=C1CCC(C(=O)O)N1
O=C(O)c1ccc(Cl)nc1
Brc1cc(Br)c(Br)cc1Br
CCOc1ccccc1C=CC(=O)O
[Br-].[NH3+]CC1CCCCC1
O=C1CC[C@H](C(=O)O)N1
O=C(O)c1ccc(C(=O)O)cc1
CC1=CC(=O)NS(=O)(=O)O1
Cc1c(C)c(C)c(C)c(C)c1C
C[N+]1(C)CCC(F)C1.[I-]
CSCCC([NH3+])C(=O)[O-]
CSCCC([NH3+])C(=O)[O-]
Oc1ccc(F)cc1C=Nc1ccccc1
CC(C)=NNC(=O)c1ccc(O)cc1
C1CC2CCC3CCCC4CCC(C1)C2C34
CC1(C)C2CCC(O)(C(=O)O)C1C2
O=C(NN=Cc1ccccc1O)c1ccncc1
NC(N)=[NH2+].O=[N+]([O-])[O-]
Cc1cc(C(=O)O)ccc1[N+](=O)[O-]
O=C(O)c1cccc(Cl)c1[N+](=O)[O-]
Oc1ccc(C2(c3ccc(O)cc3)CCCCC2)cc1
c1ccc2cc3cc4cc5ccccc5cc4cc3cc2c1
NC(N)=C([N+](=O)[O-])[N+](=O)[O-]
[2H]Oc1ccc(C(=O)N([2H])N=C(C)C)cc1
O=C(NN=Cc1cc(Br)cc(Br)c1O)c1ccncc1
O=C(NN=Cc1cc(Cl)cc(Cl)c1O)c1ccncc1
Clc1ccc2c(c1)CCc1cccnc1C2=C1CCNCC1
O=C(NN=Cc1cc(Cl)cc(Br)c1O)c1ccncc1
Cc1cc2c(s1)Nc1ccccc1N=C2N1CCN(C)CC1
COC(=O)CNC(=O)C(CCSC)NC(=O)OC(C)(C)C
NC(=O)c1ccc(N=Cc2cc(Cl)cc(Cl)c2O)cc1
CC(=NN=Cc1ccc(N(C)C)cc1)c1ccc(C#N)cc1
C1C[NH+]2CCN1CC2.F[P-](F)(F)(F)(F)F.O
C[N+](C)(C)CC(=O)O.O=C([O-])C(F)(F)Cl
c1cc2ccc3ccc4ccc5ccc6ccc1c1c2c3c4c5c61
O=[N+]([O-])[O-].[NH3+]c1ccc(C(=O)O)cc1
[N-]=[N+]=NC1OC2COC(c3ccccc3)OC2C(O)C1O
CC(C)(C)C1=NN(c2ccccc2)c2ccc(C#N)cc2[N]1
O=[N+]([O-])c1cc(N=Cc2c(Cl)cccc2Cl)ccc1F
Cc1ccc(-c2nc3c4ccccc4c4ccccc4c3[nH]2)cc1
c1ccc(-c2cccc3cc4cccc(-c5ccccc5)c4cc23)cc1
CC(C)(C)c1ccc2c(c1)sc1c3cc(C(C)(C)C)cc3sc21
CC(N=Cc1cc(C(C)(C)C)cc(C(C)(C)C)c1O)c1ccccc1
CC(C)C(CCC(=O)NC(C(=O)O)C(C)C)NC(=O)OC(C)(C)C
C(#Cc1c2ccccc2c(C#Cc2ccccc2)c2ccccc12)c1ccccc1
CC([NH2+]Cc1ccc(OCc2cccc(F)c2)cc1)C(=O)O.[Cl-]
CC(NC(=O)c1ccc(N=Nc2ccc(N(C)C)cc2)cc1)c1ccccc1
O=C(Oc1cc2ccccc2cc1OC(=O)c1ccc(F)cc1)c1ccc(F)cc1
CCn1c2ccccc2c2cc(NS(=O)(=O)c3ccccc3C(F)(F)F)ccc21
CC(N=Cc1cc(C(C)(C)C)cc(C(C)(C)C)c1O)c1cccc2ccccc12
CC[N+]1(C)C2CC(OC(=O)C(CO)c3ccccc3)CC1C1OC12.[Br-]
O=C(O)c1cccc(Cl)c1[N+](=O)[O-].c1cc(-c2ccncc2)ccn1
CCn1c2ccccc2c2cc(NS(=O)(=O)c3ccc(C(F)(F)F)cc3)ccc21
CCn1c2ccccc2c2cc(NS(=O)(=O)c3cccc(C(F)(F)F)c3)ccc21
COc1ccc(C2(O)c3ccccc3C(O)(c3ccc(OC)cc3)c3ccccc32)cc1
COC(=O)C1=C(C)NC(C)=C(C(=O)OC)C1c1ccccc1[N+](=O)[O-]
CCN(CC)c1ccc(C=NC(C#N)=C(C#N)N=Cc2ccc(N(CC)CC)cc2)cc1
CCn1c2ccccc2c2cc(NS(=O)(=O)c3ccccc3[N+](=O)[O-])ccc21
CC1(C)C2CCC(O)(C(=O)O)C1C2.CC1(C)C2CCC(O)(C(=O)O)C1C2
CCCN1C(=O)C2=C(c3ccc(Cl)cc3)N(CCC)C(=O)C2=C1c1ccc(Cl)cc1
[2H]C([2H])([2H])C(=NNC(=O)c1ccc(O)cc1)C([2H])([2H])[2H]
CCCN(CCC)S(=O)(=O)c1ccc(C(=O)O)cc1.c1cc(N=Nc2ccncc2)ccn1
CC(C)(C)c1cc(C=Nc2ccc(C(=O)c3ccccc3)cc2)c(O)c(C(C)(C)C)c1
O=C(NN=Cc1ccccc1O)c1cc[nH+]cc1.O=C([O-])c1c(F)c(F)c(F)c(F)c1F
C[NH+](C)CCOC(c1ccccc1)c1ccccc1.O=C(O)CC(O)(CC(=O)O)C(=O)[O-]
C1CN2CCN1CC2.c1ccc2c(c1)[nH]c1ccccc12.c1ccc2c(c1)[nH]c1ccccc12
N#Cc1cc(C#N)c(C#N)cc1C#N.c1cc2ccc3ccc4ccc5ccc6ccc1c1c2c3c4c5c61
Cc1cc(-c2cc(C)c(N)c(C)c2)cc(C)c1N.N#CC(C#N)=c1ccc(=C(C#N)C#N)cc1
O=C1c2cc(-c3ccc(-c4ccccc4)cc3)ccc2-c2ccc(-c3ccc(-c4ccccc4)cc3)cc21
CCCC[P+](CCCC)(CCCC)CCCC.c1ccc([B-](c2ccccc2)(c2ccccc2)c2ccccc2)cc1
C1COCCOCCOCCOCCOCCO1.F[P-](F)(F)(F)(F)F.[NH3+]c1ccc([N+](=O)[O-])cc1
C[NH2+]C1CCCCC1.O=[N+]([O-])c1cc([N+](=O)[O-])c([O-])c([N+](=O)[O-])c1
CC(=O)OC1C(OCc2ccccc2)C(OCc2ccccc2)C(OCc2ccccc2)C(OCc2ccccc2)C1OC(C)=O
Cc1c[nH+]cc(C)n1.O=[N+]([O-])c1cc([N+](=O)[O-])c([O-])c([N+](=O)[O-])c1
CCCCOc1ccc(N2C(=O)c3ccc4c5c(ccc(c35)C2=O)C(=O)N(c2ccc(OCCCC)cc2)C4=O)cc1
CCCCCCCOc1ccc(N2C(=O)c3ccc4c5c(ccc(c35)C2=O)C(=O)N(c2ccc(OCCCCCCC)cc2)C4=O)cc1
CCCCCCCCOc1ccc(N2C(=O)c3ccc4c5c(ccc(c35)C2=O)C(=O)N(c2ccc(OCCCCCCCC)cc2)C4=O)cc1
Cc1c(C)c2c(c3c1CC[n+]1ccc4ccccc4c1-3)-c1c3ccccc3cc[n+]1CC2.O=S(=O)([O-])C(F)(F)F
CCCCCCCCCOc1ccc(N2C(=O)c3ccc4c5c(ccc(c35)C2=O)C(=O)N(c2ccc(OCCCCCCCCC)cc2)C4=O)cc1
CCCCCCCCCCOc1ccc(N2C(=O)c3ccc4c5c(ccc(c35)C2=O)C(=O)N(c2ccc(OCCCCCCCCCC)cc2)C4=O)cc1
CCCCCCCCOc1ccc(-c2cc(C3=C(c4cc(-c5ccc(OCCCCCCCC)cc5)sc4C)C(F)(F)C(F)(F)C3(F)F)c(C)s2)cc1
COC(=O)c1ccc2cc1-c1cn(nn1)CCOCCOCCOCCOc1ccc(cc1)C#Cc1ccc(cc1)C#Cc1ccc(cc1)OCCOCCOCCOCCn1cc(nn1)-c1cc(ccc1C(=O)OC)N=N2
C[Si]1(C)c2ccc(cc2)[Si](C)(C)[Si](C)(C)c2ccc(cc2)[Si](C)(C)[Si](C)(C)c2ccc(cc2)[Si](C)(C)[Si](C)(C)c2ccc(cc2)[Si]1(C)C

Figure S1. Molecules collected as positive data.



	T_{endo}	$T_{endo(max)}$	$T_{endo(min)}$
Count	144	88	88
Mean	343.5	350.6	324.2
Std	95.0	95.5	101.0
Min	80.0	80.0	80.0
Max	533.0	533.0	518.0

	T_{exo}	$T_{exo(max)}$	$T_{exo(min)}$
Count	110	72	72
Mean	308.0	314.3	291.4
Std	93.0	92.1	96.3
Min	120.0	135.0	120.0
Max	564.2	564.2	463.0

	ΔH_{endo}	$\Delta H_{endo(max)}$	$\Delta H_{endo(min)}$
Count	64	46	46
Mean	4.3	4.8	3.9
Std	6.2	6.8	6.1
Min	0.04	0.04	0.04
Max	36.4	36.4	36.4

	ΔH_{exo}	$\Delta H_{exo(max)}$	$\Delta H_{exo(min)}$
Count	52	37	37
Mean	-3.9	-3.6	-4.1
Std	5.0	4.5	5.4
Min	-21.9	-19.7	-21.8
Max	-0.04	-0.04	-0.04

Figure S2. The distribution of positive dataset. (a,b) Statistics of transition temperature corresponding to (a) endothermic and (b) exothermic transitions. (c,d) Statistics of transition enthalpy corresponding to (c) endothermic and (d) exothermic transitions. (e) The distribution of the number of solid phase transitions per molecule.

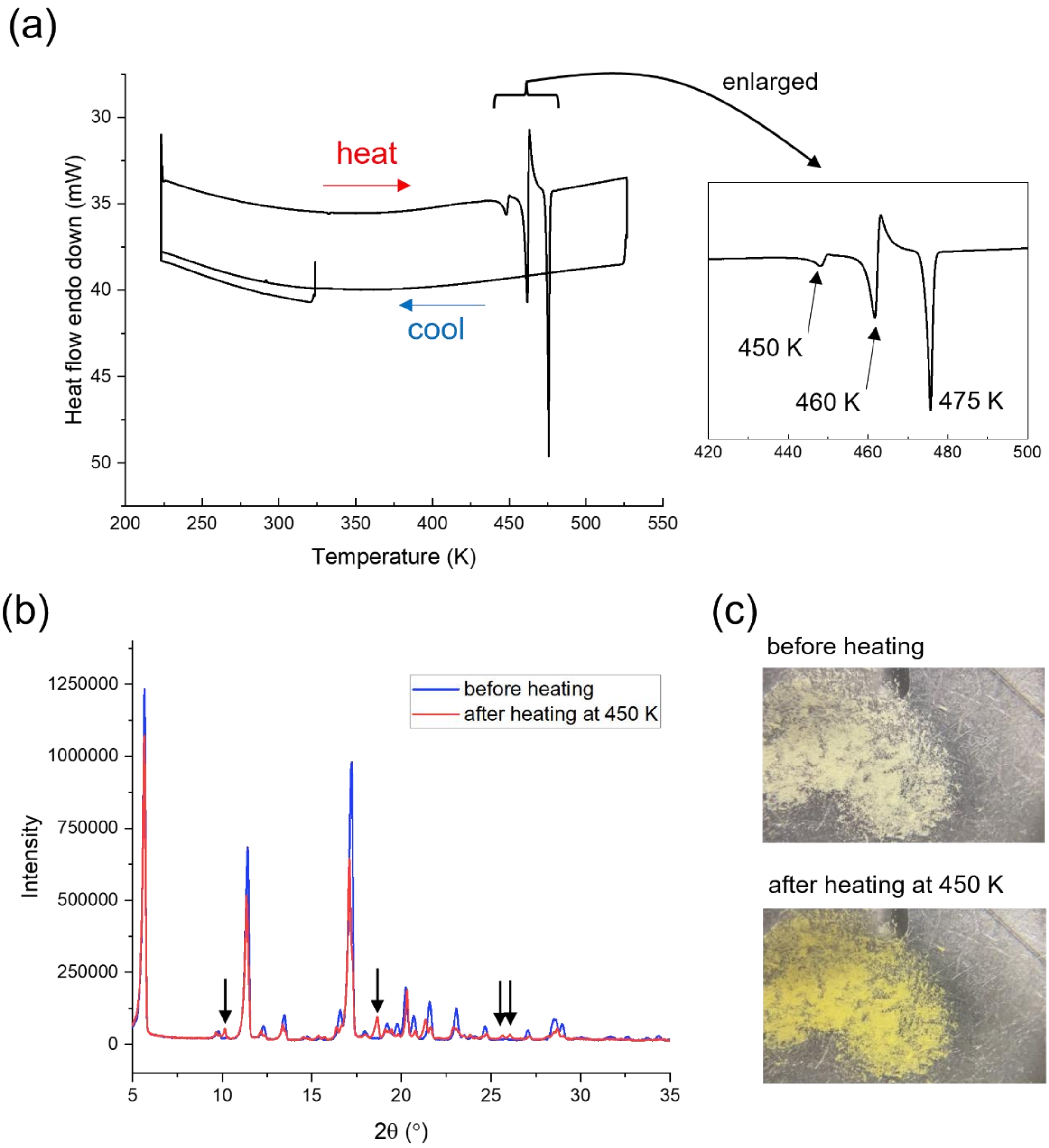


Figure S3. Crystal-to-crystal phase transition of the crystal of OCAPAK. (a) Thermal analysis by DSC. The crystal exhibited a crystal-to-crystal transition at 450 K, and an anomalous endothermic-exothermic peak at 460 K before melting at 475 K. (b) XRD patterns of the crystal before heating, and after heating at 450 K. Both measurements were performed at 293 K. Unique peaks after heating are indicated by arrows. The slight difference of XRD pattern before and after heating reflects the crystal-to-crystal phase transition. (c) Pictures of crystalline powder before and after heating. Crystal appearance did not change before and after heating, although slight color change was observed.

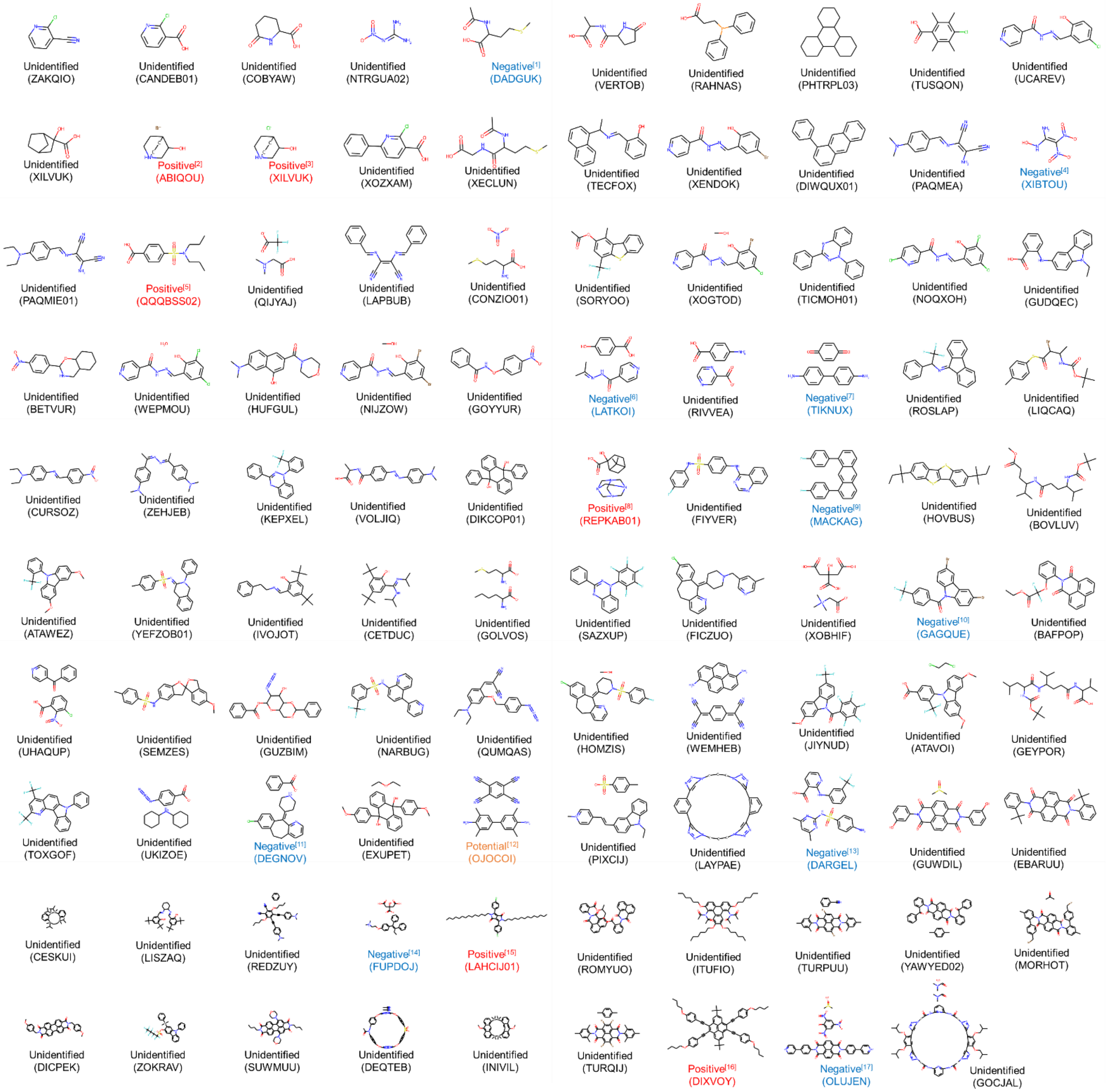


Figure S4. Molecular structures suggested by PU learning with *p* = 0.2. References are summarized in supplementary references.

Supplementary Tables

Table S1. Hyperparameters used for ML models in classification and regression.

ML models	Hyperparameters
Classification	
RF	n_estimaters:100, max_depth: None
NN	hidden_layer_sizes: (50,), activation: ‘relu’
SVM	kernel: ‘rbf’, gamma: 0.2
GBDT	n_estimaters:100, max_depth: 3
Regression	
NN	hidden_layer_sizes: (100,), activation: ‘relu’
RF	n_estimaters: 100, max_depth: None
TL-NN	(Search space)
	n_layers: {1, 10}, n_dim: {50, 100, 200, 300, 400, 500, 750, 1000}
ECFP	n_layers: 5, n_dim: 1000
Avalon	n_layers: 4, n_dim: 750
ErG	n_layers: 3, n_dim: 1000
MACCSKeys	n_layers: 4, n_dim: 1000
Estate	n_layers: 7, n_dim: 1000

Table S2. Comparison of true positive rate (TPR) between PU and BC. The value is the averaged TPR in 10-fold CV.

	PU				BC			
	RF	NN	SVM	GBDT	RF	NN	SVM	GBDT
Mordred	0.13	0.0	0.30	0.96	0.06	0.0	0.0	0.02
ECFP	0.22	0.27	0.39	0.62	0.14	0.13	0.01	0.06
Avalon	0.28	0.21	0.52	0.28	0.14	0.19	0.0	0.01
ErG	0.26	0.21	0.05	0.46	0.12	0.11	0.0	0.0
RDKit	0.20	0.01	0.0	0.74	0.06	0.0	0.0	0.01
MACCSKeys	0.15	0.21	0.20	0.04	0.10	0.14	0.0	0.0
Estate	0.16	0.03	0.0	0.14	0.10	0.0	0.0	0.0

Table S3. Comparison of TPR and SE between each combination of molecular descriptor and classification model. Each value is the average obtained from 10-fold CV.

	TPR				SE			
	RF	NN	SVM	GBDT	RF	NN	SVM	GBDT
Mordred	0.13	0.0	0.30	0.96	69.2	4936.1	1.0	1.0
ECFP	0.22	0.27	0.39	0.62	87.8	1110.4	12441.4	2.1
Avalon	0.28	0.21	0.52	0.28	90.6	2011.0	21990.2	113.3
ErG	0.26	0.21	0.05	0.46	72.9	384.8	64422.4	73.3
RDKit	0.20	0.01	0.0	0.74	248.8	8575.1	NaN*	1.0
MACCSKeys	0.15	0.21	0.20	0.04	67.0	333.7	13594.6	145.3
Estate	0.16	0.03	0.0	0.14	74.0	202.2	171825.4	111.6

* SE was not able to be calculated because n_{up} was zero in the combination of RDKit-SVM.

Table S4. Regression performance based on MAE when using molecular descriptors for each property. Each MAE value represents the mean and standard deviation on five 5-fold CVs. The letter "-" in TL-NN means the transfer wasn't succeeded due to the mismatch of input dimension. TL-NN is the best model among all the fine-tuning models.

	NN	TL-NN	RF	mean
$T_{\mathrm{endo(max)}}$ (K)				
Mordred	2.0×10^7 (2.4×10^7)	-	58.7 (8.1)	75.4
ECFP	227.8 (21.1)	76.7 (15.8)	71.6 (9.9)	75.4
Avalon	157.1 (25.0)	76.2 (11.8)	64.1 (12.5)	75.4
ErG	206.8 (19.4)	94.1 (21.7)	66.0 (13.2)	75.4
RDkitDesc	149.1 (34.4)	-	70.6 (13.1)	75.4
MACCSKeys	183.9 (29.9)	77.9 (10.6)	69.5 (14.3)	75.4
Estate	220.4 (25.3)	98.2 (20.5)	69.9 (11.7)	75.4
$T_{\mathrm{endo(min)}}$ (K)				
Mordred	2.4×10^7 (3.1×10^7)	-	64.9 (9.0)	80.3
ECFP	200.2 (24.7)	75.3 (9.8)	69.8 (14.3)	80.3
Avalon	143.1 (19.8)	75.2 (17.0)	71.3 (14.4)	80.3
ErG	188.6 (28.8)	98.9 (24.1)	68.0 (14.2)	80.3
RDkitDesc	147.5 (30.4)	-	71.1 (17.4)	80.3
MACCSKeys	167.9 (26.5)	80.9 (13.0)	69.9 (12.1)	80.3
Estate	197.9 (20.3)	96.3 (18.0)	74.3 (17.5)	80.3
$T_{\mathrm{exo(max)}}$ (K)				
Mordred	1.8×10^7 (2.5×10^7)	-	66.2 (14.4)	71.5
ECFP	196.9 (24.9)	78.3 (16.6)	70.5 (14.0)	71.5
Avalon	151.7 (21.0)	76.1 (19.1)	65.0 (16.4)	71.5
ErG	184.1 (31.0)	105.2 (28.0)	65.7 (16.2)	71.5
RDkitDesc	132.6 (43.7)	-	69.8 (17.3)	71.5
MACCSKeys	161.5 (26.1)	81.8 (14.2)	72.9 (11.6)	71.5
Estate	187.4 (27.6)	100.5 (20.1)	69.7 (12.9)	71.5

$T_{\text{exo(min)}}$ (K)				
Mordred	3.5×10^7 (3.7×10^7)	-	69.4 (12.8)	80.8
ECFP	173.0 (22.7)	76.2 (16.2)	70.8 (13.7)	80.8
Avalon	137.4 (22.3)	73.5 (16.8)	71.7 (16.1)	80.8
ErG	167.4 (30.2)	99.1 (22.7)	67.4 (13.9)	80.8
RDkitDesc	122.3 (37.2)	-	73.9 (11.2)	80.8
MACCSKeys	145.6 (25.0)	81.1 (16.4)	72.5 (11.8)	80.8
Estate	165.7 (24.5)	93.5 (22.3)	78.5 (16.3)	80.8
$\Delta H_{\text{endo(max)}}$ (kJ/mol)				
Mordred	2.4×10^7 (4.2×10^7)	-	5.3 (1.3)	4.6
ECFP	4.8 (1.7)	4.8 (2.1)	4.2 (1.4)	4.6
Avalon	4.3 (2.0)	4.8 (2.3)	5.3 (1.4)	4.6
ErG	5.8 (1.4)	4.7 (2.1)	4.5 (1.3)	4.6
RDkitDesc	10.1 (9.5)	-	5.2 (1.5)	4.6
MACCSKeys	4.8 (1.2)	4.7 (2.6)	4.6 (1.4)	4.6
Estate	5.9 (1.8)	4.8 (1.8)	4.4 (1.3)	4.6
$\Delta H_{\text{endo(min)}}$ (kJ/mol)				
Mordred	1.9×10^7 (2.3×10^7)	-	5.1 (1.3)	3.7
ECFP	4.3 (1.5)	3.9 (1.9)	4.5 (1.8)	3.7
Avalon	4.0 (1.3)	3.9 (1.6)	4.9 (1.4)	3.7
ErG	5.6 (1.9)	3.9 (2.3)	3.8 (1.4)	3.7
RDkitDesc	11.5 (11.1)	-	4.1 (1.2)	3.7
MACCSKeys	4.2 (2.0)	3.9 (2.0)	4.3 (1.7)	3.7
Estate	4.6 (1.3)	4.2 (1.8)	4.0 (1.8)	3.7
$\Delta H_{\text{exo(max)}}$ (kJ/mol)				
Mordred	1.2×10^7 (1.9×10^7)	-	3.7 (1.0)	3.2
ECFP	3.8 (0.8)	3.5 (1.6)	3.1 (1.2)	3.2
Avalon	3.3 (1.1)	3.5 (1.5)	3.2 (1.1)	3.2
ErG	6.5 (2.2)	3.6 (1.6)	3.5 (1.0)	3.2
RDkitDesc	12.6 (11.5)	-	3.9 (1.2)	3.2
MACCSKeys	4.6 (1.3)	3.5 (1.5)	3.8 (1.0)	3.2
Estate	5.0 (1.6)	3.6 (1.4)	3.7 (0.9)	3.2

$\Delta H_{\mathrm{exo(min)}}$ (kJ/mol)				
Mordred	1.5×10^7 (1.9×10^7)	-	4.3 (1.1)	3.9
ECFP	3.4 (0.9)	4.1 (1.7)	3.4 (1.3)	3.9
Avalon	3.2 (1.0)	4.1 (1.9)	3.3 (1.2)	3.9
ErG	6.4 (1.9)	4.1 (1.8)	3.9 (1.5)	3.9
RDkitDesc	8.7 (3.6)	-	4.3 (1.0)	3.9
MACCSKeys	4.5 (1.1)	4.1 (2.1)	4.5 (1.3)	3.9
Estate	5.1 (2.0)	4.2 (1.2)	4.5 (1.3)	3.9

Table S5. Top-10 ranked important features in the regression of each property. The value in bracket is the averaged value of feature importance.

Rank	$T_{\text{endo(max)}}$	$T_{\text{endo(min)}}$	$T_{\text{exo(max)}}$	$T_{\text{exo(min)}}$
1	**VSA_EState4** (0.044)	**ATSC2d** (0.044)	**ATSC1are** (0.022)	ATSC1se (0.039)
2	ATSC3p (0.034)	**AATS0p** (0.036)	**VSA_EState4** (0.021)	**VSA_EState4** (0.037)
3	**ATSC3v** (0.031)	**VSA_EState4** (0.034)	ATSC5dv (0.020)	**ATSC1are** (0.036)
4	SLogP_VSA2 (0.031)	JGI1 (0.030)	AATSC3m (0.019)	GATS1d (0.023)
5	**ATSC2d** (0.018)	AATSC1dv (0.028)	Xc-3d (0.018)	ATSC5d (0.017)
6	**AATS0p** (0.017)	GATS1p (0.023)	AATSC3Z (0.017)	JGI1 (0.017)
7	GATS3p (0.016)	**ATSC3v** (0.020)	VSA_Estate3 (0.014)	ATSC1pe (0.017)
8	GATS2d (0.015)	ATSC1se (0.019)	SssssC (0.014)	JGT10 (0.015)
9	Xc-3dv (0.013)	GATS3d (0.017)	Xc-3dv (0.013)	GATS1p (0.015)
10	GATS3v (0.013)	ATSC1pe (0.017)	EState_VSA1 (0.011)	AATSC0d (0.014)

Red bold: the descriptor commonly appeared in $T_{\text{endo(max)}}$, $T_{\text{endo(min)}}$, $T_{\text{exo(max)}}$, and $T_{\text{exo(min)}}$

Black bold: the descriptor commonly appeared in $T_{\text{endo(max)}}$ and $T_{\text{endo(min)}}$

Orange bold: the descriptor commonly appeared in $T_{\text{exo(max)}}$ and $T_{\text{exo(min)}}$

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