B3clf: A Resampling-Integrated Machine Learning Framework to Predict Blood-Brain Barrier Permeability

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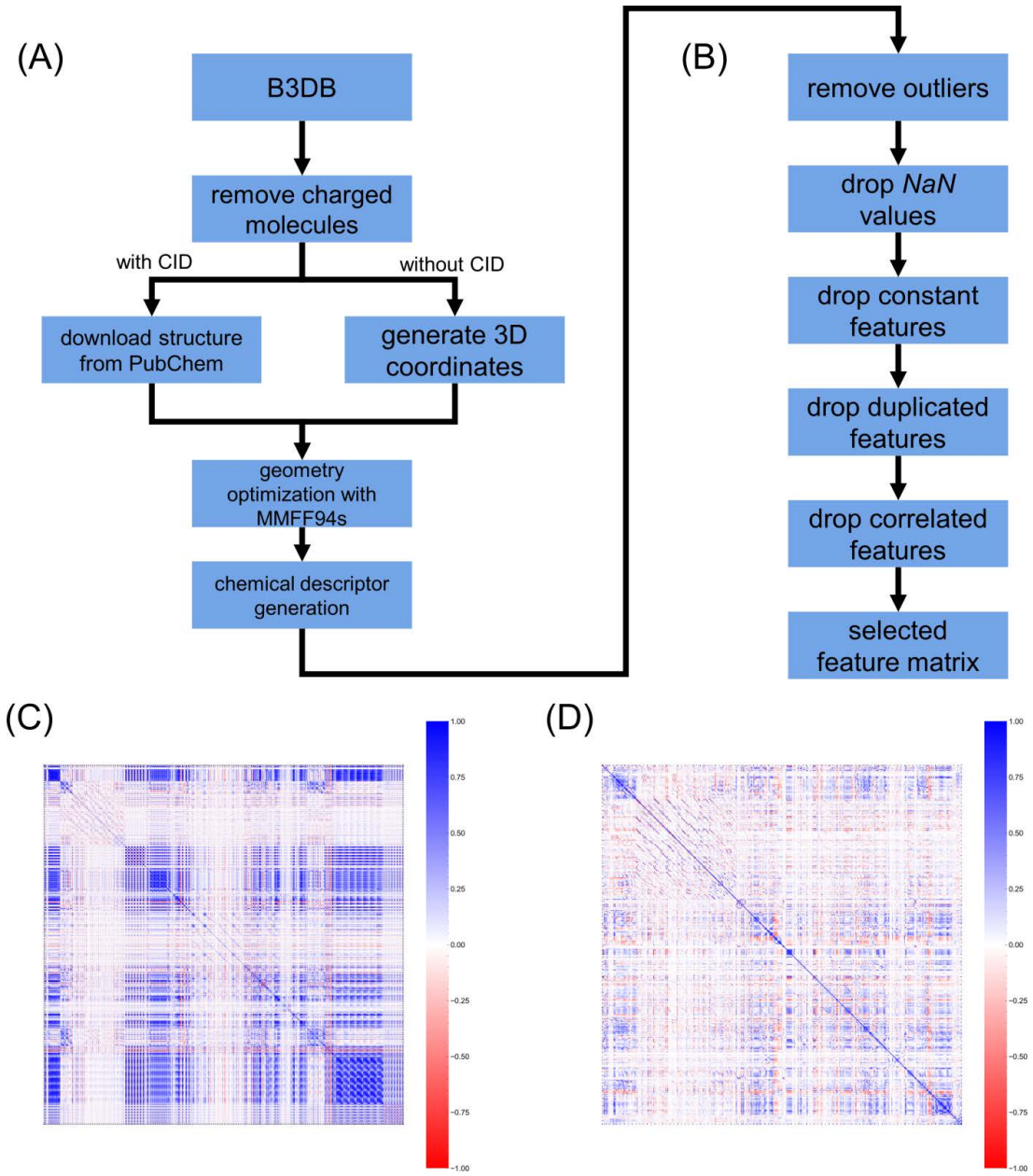

Fig. SI. 1 Workflow for (A) dataset preparation, (B) molecular feature generation, (C) and (D) feature filtering

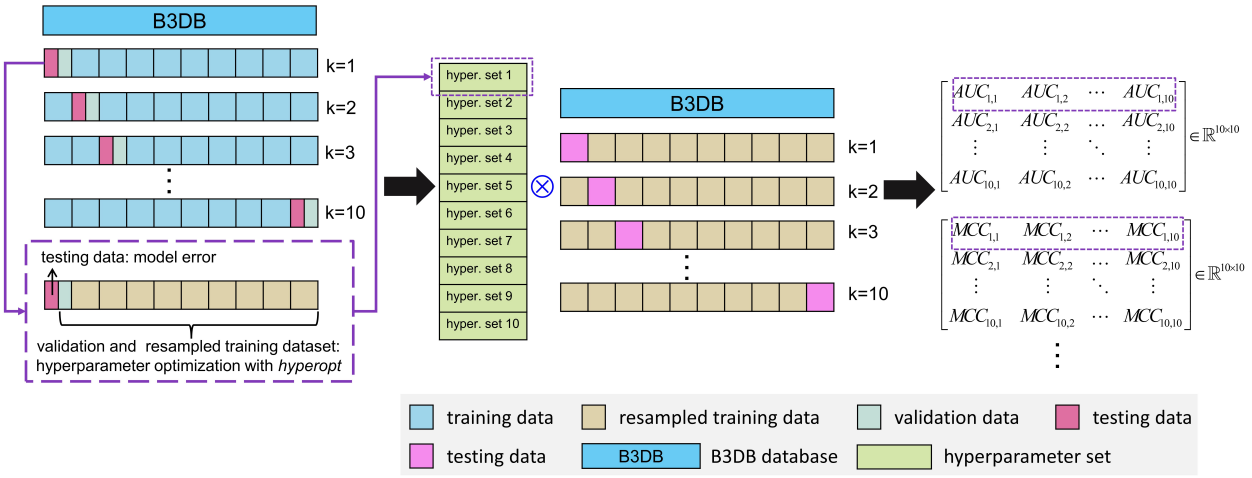

Fig. SI. 2 Two-stage stratified 10-fold cross-validation workflow for hyperparameter selection and model evaluation

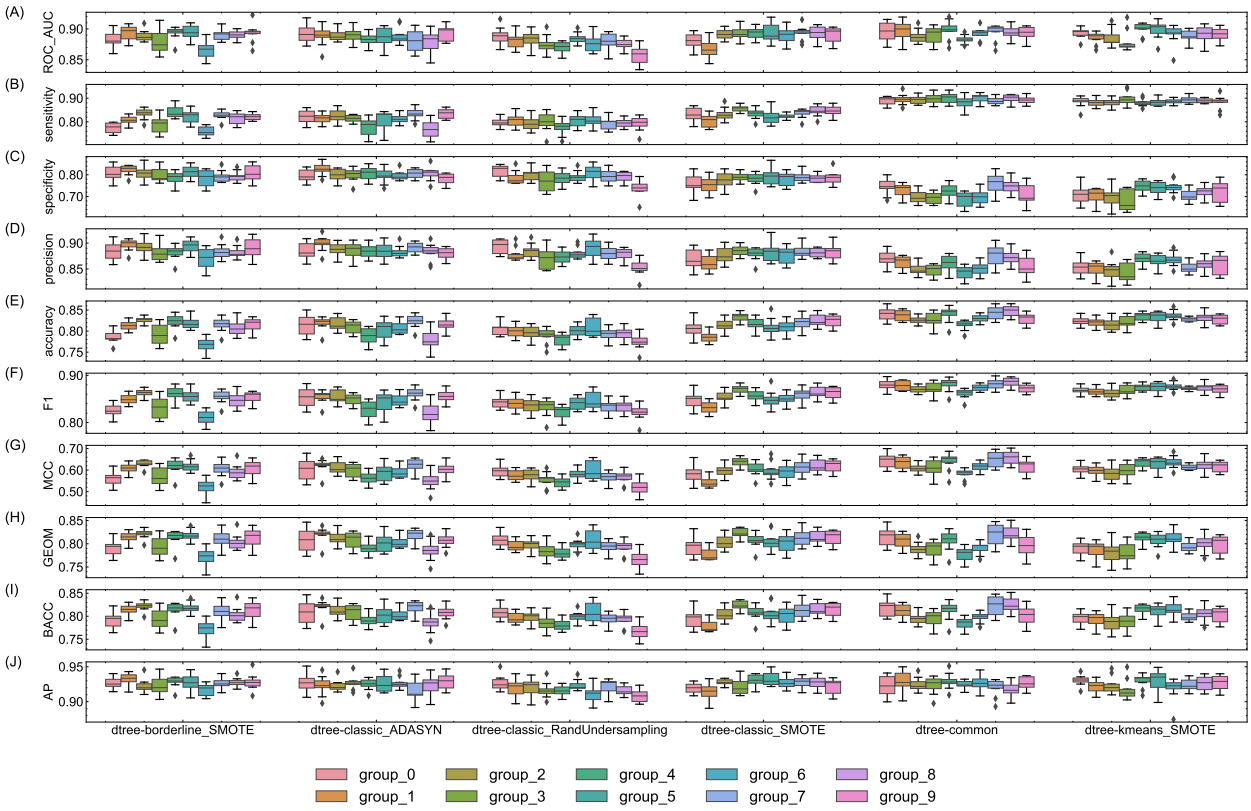

Fig. SI. 3 Model performances of decision trees based classifiers for 10 groups of hyperparameters

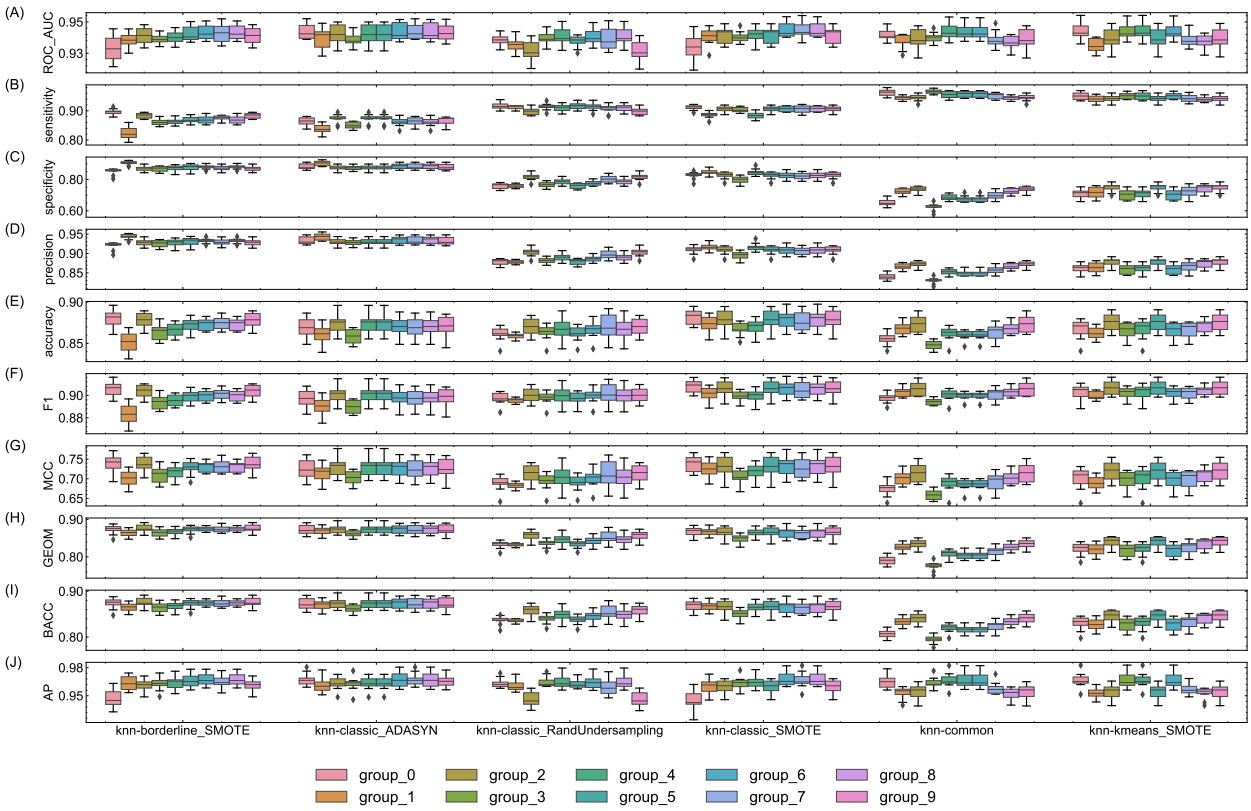

Fig. SI. 4 Model performances of kNN based classifiers for 10 groups of hyperparameters

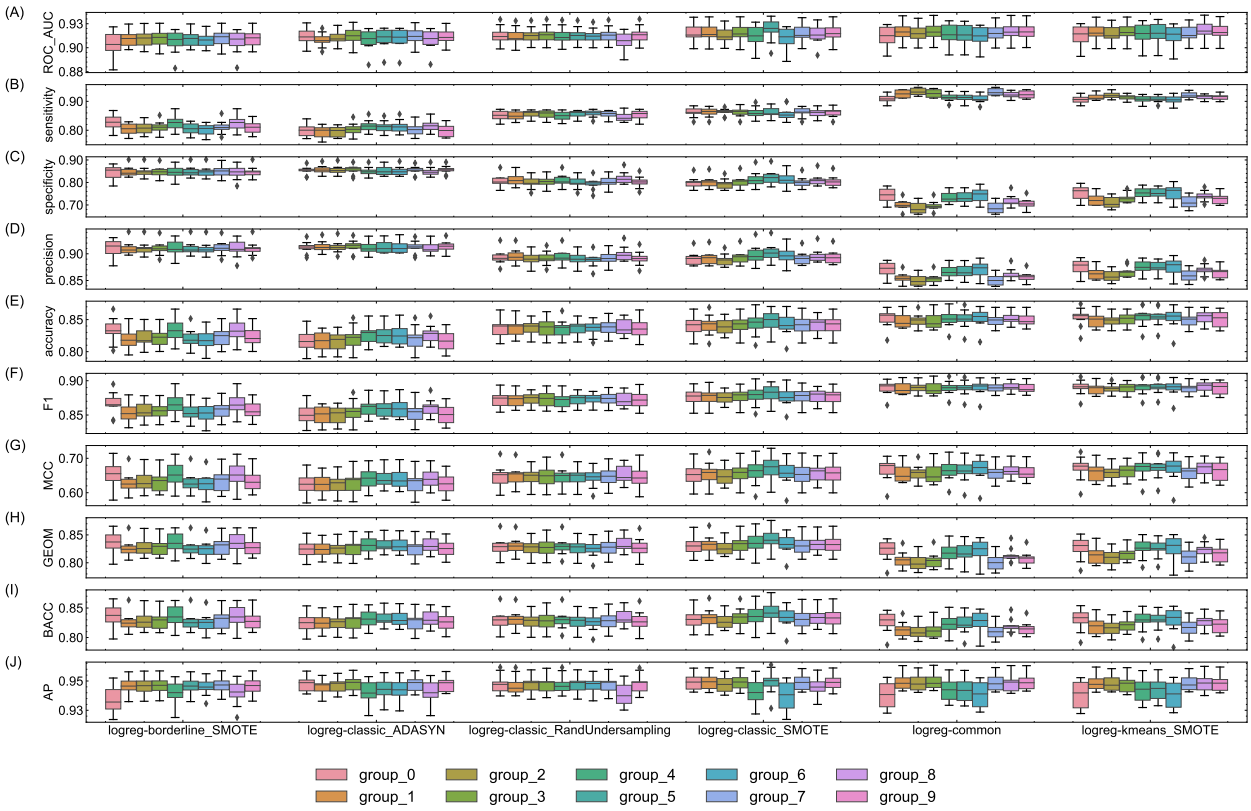

Fig. SI. 5 Model performances of logistical regression based classifiers for 10 groups of hyperparameters

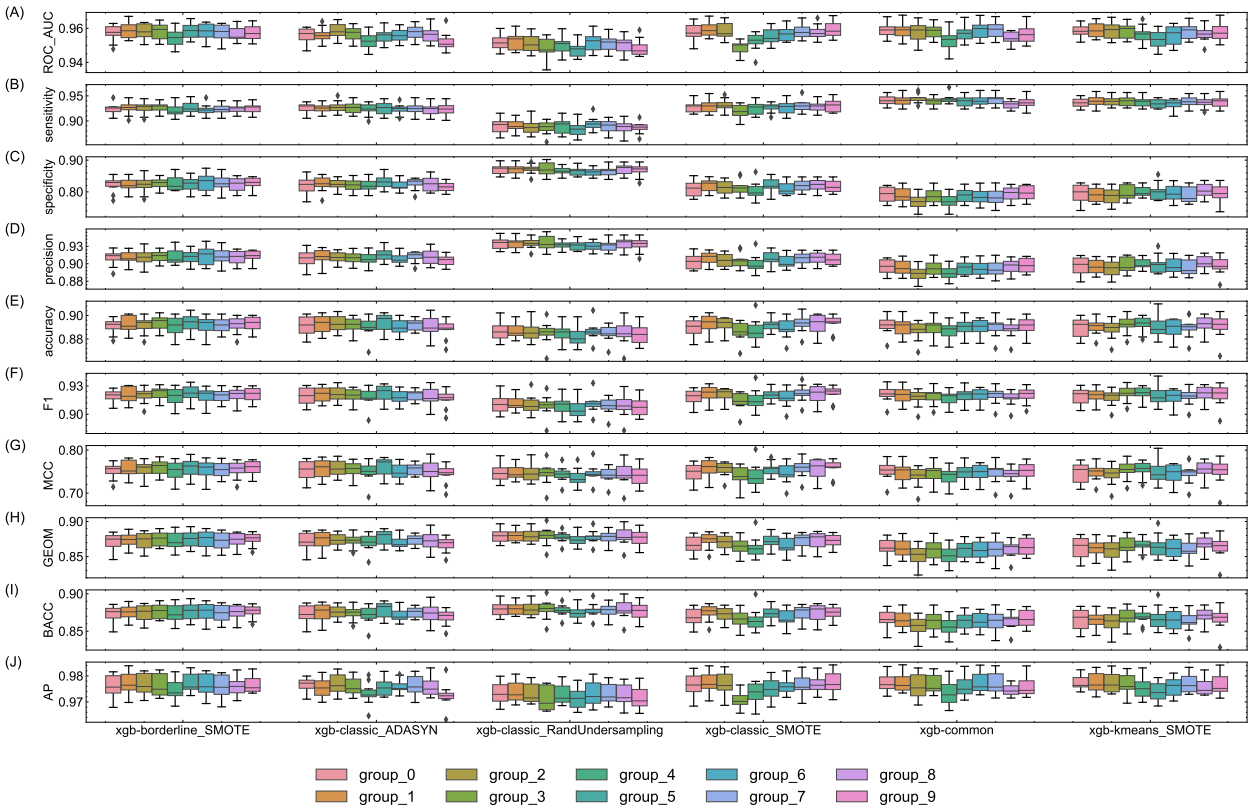

Fig. SI. 6 Model performances of XGBoost based classifiers for 10 groups of hyperparameters

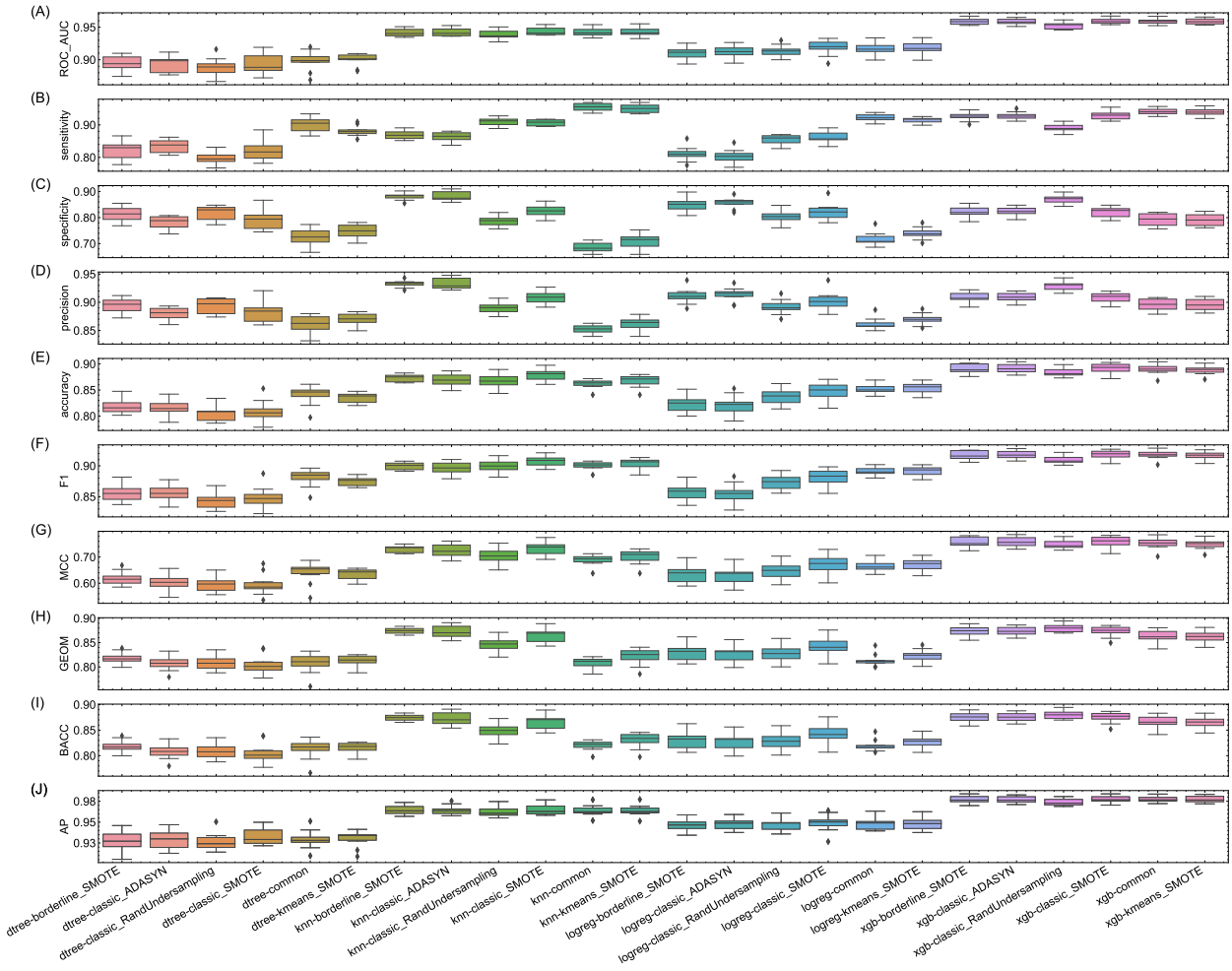

Fig. SI. 7 Summary of model performance across all classification model–sampling strategy combinations

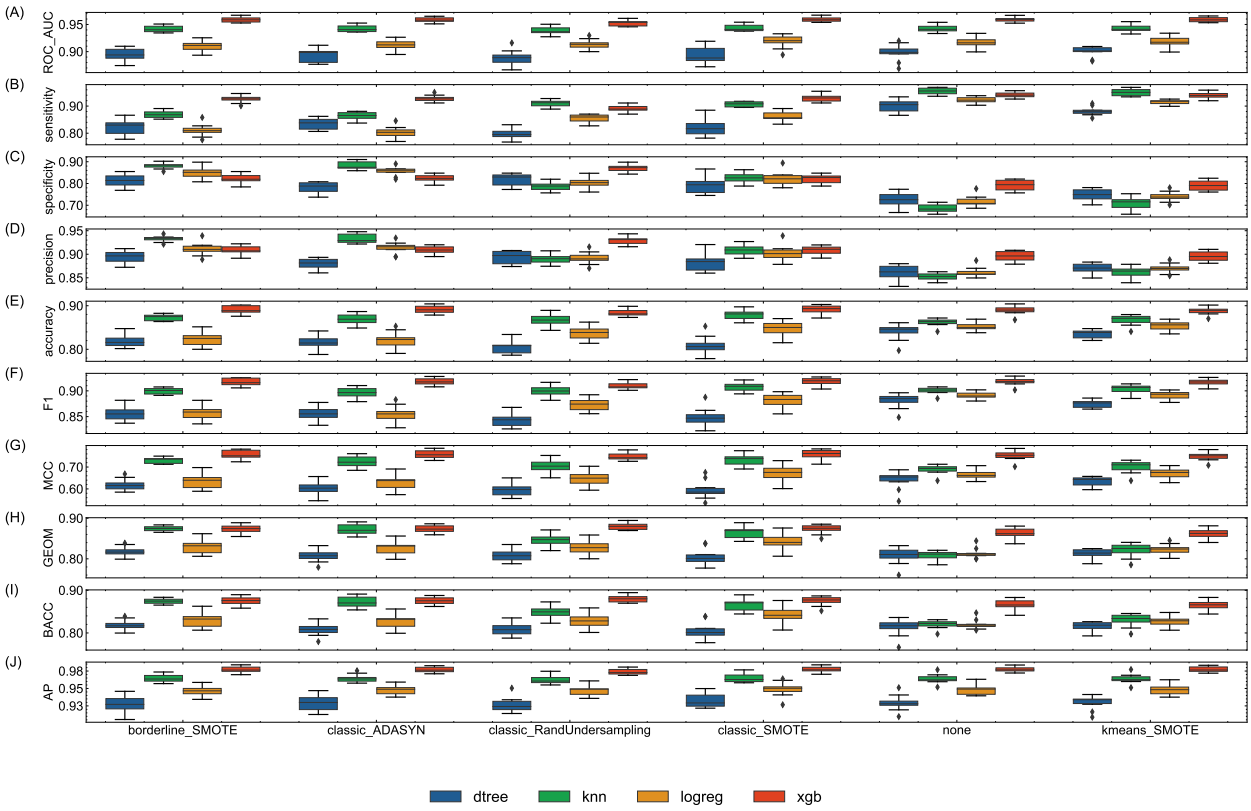

Fig. SI. 8 Summary of model performance across all classification model–sampling strategy combinations, organized by sampling strategies

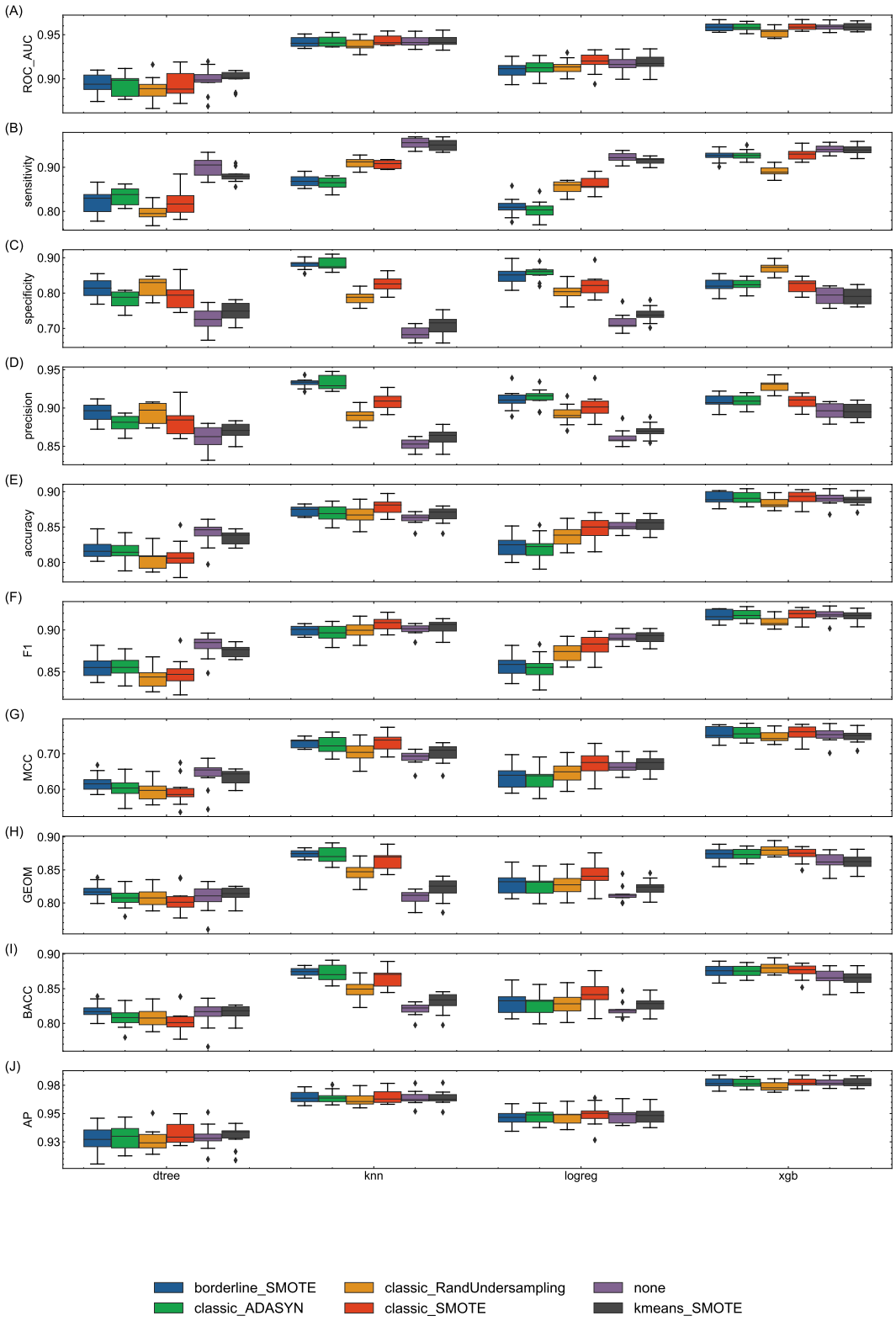

Fig. SI. 9 Summary of model performance across all classification model–sampling strategy combinations, organized by classification algorithms

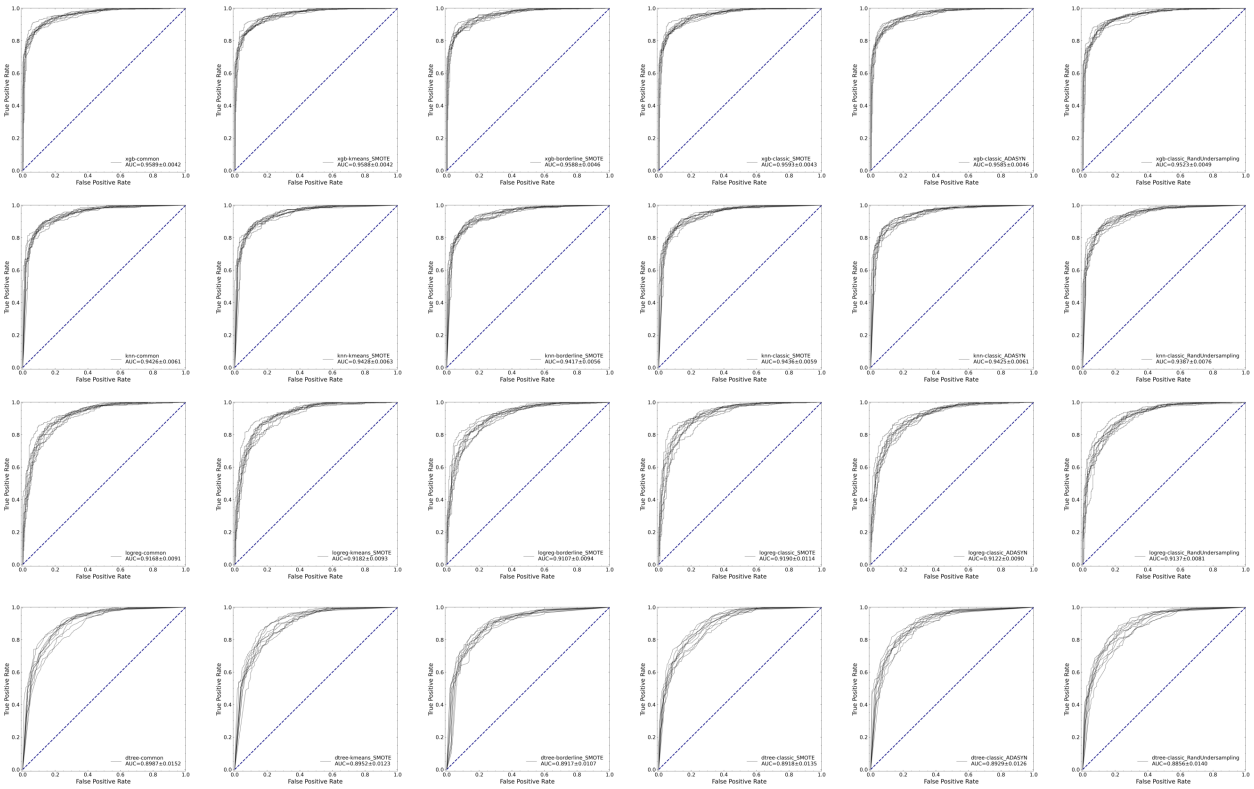

Fig. SI. 10 Receiver operating characteristic (ROC) curves of all classification model–sampling strategy combinations

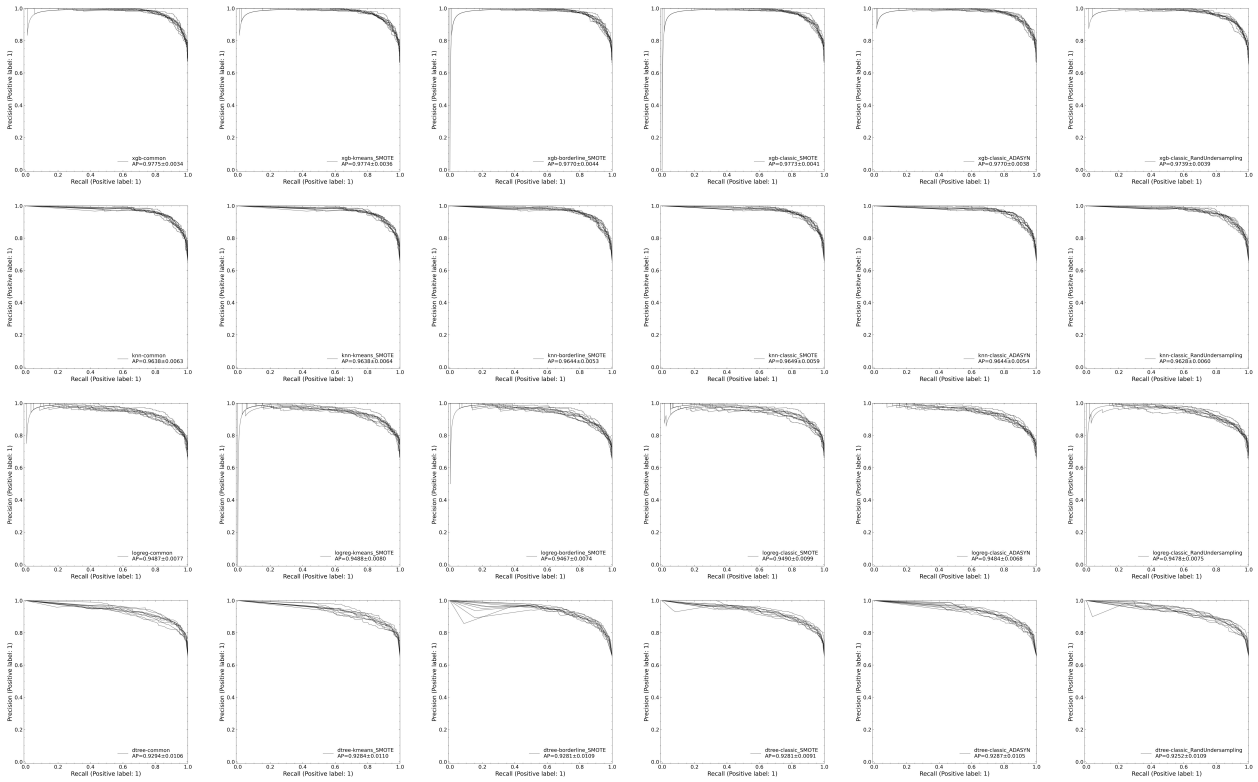

Fig. SI. 11 Precision-recall curves of all classification model–sampling strategy combinations

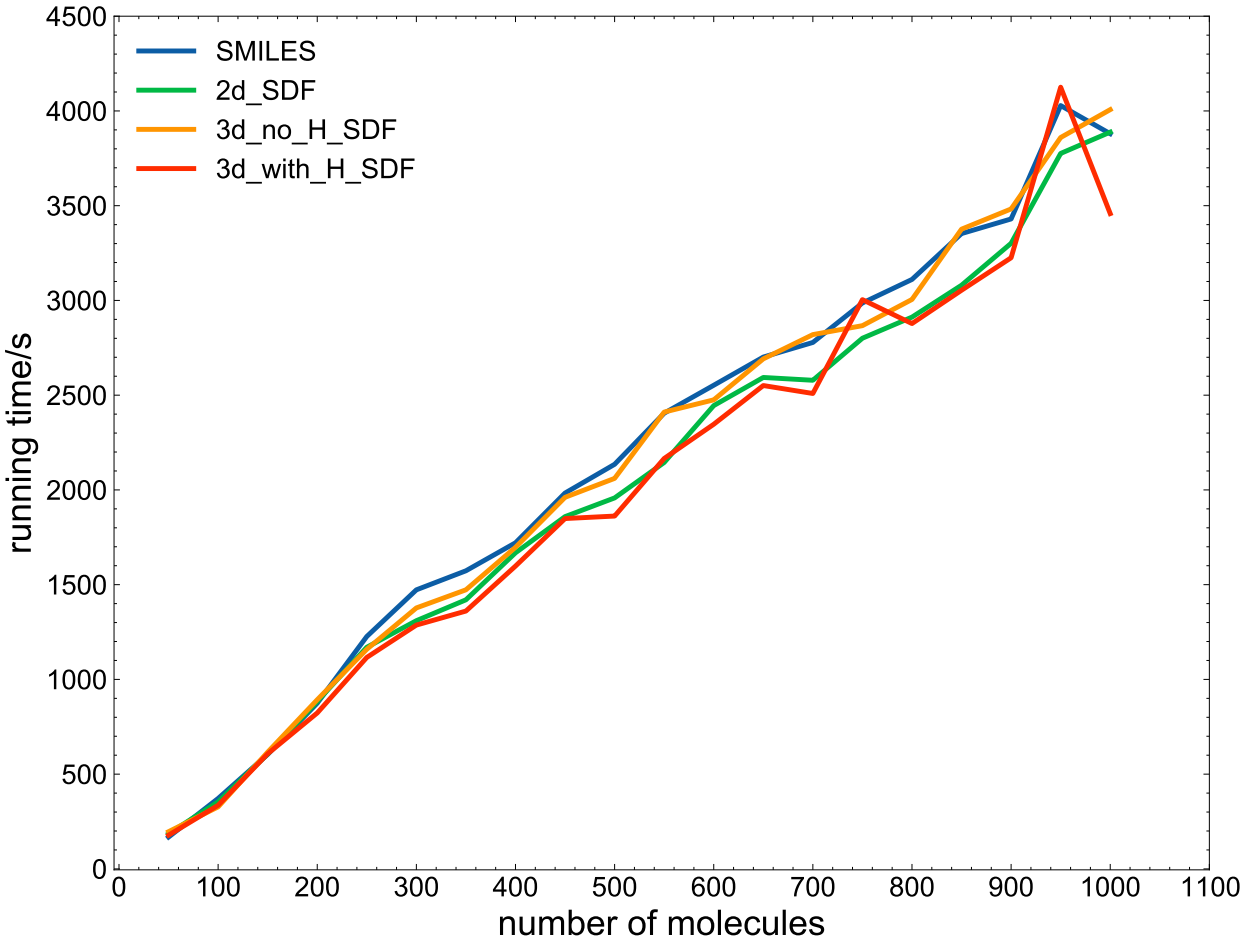

Fig. SI. 12 Relationship between number of molecules and running time in executing `B3clf` calculations

Table SI. 1 External dataset with compound identifiers and BBB permeability labels. For the most updated version of the extended B3DB dataset, please refer to https://github.com/theochem/B3DB.

Compound Name	SMILES	CID	Class
(3S)-3-acetyloxy-4-(trimethylazaniumyl)butanoate	CC(=O)O[C@@H](CC(=O)[O-])C[N+](C)(C)C	18230	BBB+
N-[2-(5-methoxy-1H-indol-3-yl)ethyl]acetamide	COc1ccc2[nH]cc(CCNC(C)=O)c2c1	896	BBB+
(2S)-2-acetamido-4-methylpentanoic acid	CC(=O)N[C@@H](CC(C)C)C(=O)O	70912	BBB+
adamantan-1-amine	N[C@]12C[C@H]3C[C@H](C[C@H](C3)C1)C2	2130	BBB+
4-amino-N-[[(2R)-1-ethylpyrrolidin-2-yl]methyl]-5-ethylsulfonyl-2-methoxybenzamide	CCN1CCC[C@@H]1CNC(=O)c1cc(S(=O)(=O)CC)c(N)cc1OC	5746246	BBB+
(1S)-1-[(1R,2R,4R)-2-bicyclo[2.2.1]hept-5-enyl]-1-phenyl-3-piperidin-1-ylpropan-1-ol	O[C@](CCN1CCCCC1)(c1ccccc1)[C@@H]1C[C@@H]2C=C[C@H]1C2	12149109	BBB+
(2S)-1-butyl-N-(2,6-dimethylphenyl)piperidine-2-carboxamide	CCCCN1CCCC[C@H]1C(=O)Nc1c(C)cccc1C	92253	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
(2R,5S)-2-methylspiro[1,3-oxathiolane-5,3'-1-azabicyclo[2.2.2]octane]	C[C@@H]1O[C@]2(CS1)CN1CCC2CC1	11041760	BBB+
7-chloro-4-hydroxy-N-methyl-5-phenyl-3H-1,4-benzodiazepin-2-imine	C/N=C1/CN(O)C(c2ccccc2)=c2cc(Cl)ccc2=N1	2712	BBB+
(11bS)-10-chloro-11b-(2-chlorophenyl)-2,3,5,7-tetrahydro-[1,3]oxazolo[3,2-d][1,4]benzodiazepin-6-one	O=C1CN2CCO[C@]2(c2ccccc2Cl)c2cc(Cl)ccc2N1	25271643	BBB+
5-(2,4-difluorophenyl)-2-hydroxybenzoic acid	O=C(O)c1cc(-c2ccc(F)cc2F)ccc1O	3059	BBB+
10-[(2R)-2-(dimethylamino)propyl]-N,N-dimethylphenothiazine-2-sulfonamide	C[C@H](CN1c2ccccc2Sc2ccc(S(=O)(=O)N(C)C)cc21)N(C)C	76960728	BBB+
diethylcarbamothioylsulfanyl N,N-diethylcarbamodithioate	CCN(CC)C(=S)SSC(=S)N(CC)CC	3117	BBB+
(2R)-N-ethyl-1-[3-(trifluoromethyl)phenyl]propan-2-amine	CCN[C@H](C)Cc1cccc(C(F)(F)F)c1	65801	BBB+
[(2R)-2,3-dihydroxypropyl] 2-[[8-(trifluoromethyl)quinolin-4-yl]amino]benzoate	O=C(OC[C@H](O)CO)c1ccccc1Nc1ccnc2c(C(F)(F)F)cccc12	76958517	BBB+

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Compound Name	SMILES	CID	Class
[(2R)-2,3-dihydroxypropyl] 2-[(7-chloroquinolin-4-yl)amino]benzoate	O=C(OC[C@H](O)CO)c1ccccc1Nc1ccnc2cc(Cl)ccc12	969495	BBB+
N-methyl-3-(1-tetracyclo[6.6.2.02,7.09,14]hexadeca-2,4,6,9,11,13-hexaenyl)propan-1-amine	CNCCC[C@]12CC[C@H](c3cccc31)c1ccccc12	4011	BBB+
[(1R,3R,5R)-6,6,9-trimethyl-9-azabicyclo[3.3.1]nonan-3-yl] 2-hydroxy-2,2-dithiophen-2-ylacetate	CN1[C@@H]2CCC(C)(C)[C@H]1C[C@H](OC(=O)C(O)(c1cccs1)c1cccs1)C2	68667	BBB+
(3S,5R)-3,5-dimethyladamantan-1-amine	C[C@]12C[C@@H]3C[C@](C)(C1)C[C@@](N)(C3)C2	1263681	BBB+
(2R)-N-(2,6-dimethylphenyl)-1-methylpiperidine-2-carboxamide	Cc1cccc(C)c1NC(=O)[C@H]1CCCCN1C	6918904	BBB+
(6R)-6-(dimethylamino)-4,4-diphenylheptan-3-one	CCC(=O)C(C[C@@H](C)N(C)C)(c1ccccc1)c1ccccc1	22267	BBB+
(3R)-1-methyl-3-(9H-thioxanthen-9-ylmethyl)piperidine	CN1CCC[C@H](CC2c3ccccc3Sc3ccccc32)C1	44163540	BBB+

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Compound Name	SMILES	CID	Class
2-[(S)-benzhydrylsulfinyl]acetamide	NC(=O)C[S@](=O)C(c1ccccc1)c1ccccc1	11173366	BBB+
(8aR)-1'-[3-(2-chloro-5,6-dihydrobenzo[b][1]benzazepin-11-yl)propyl]spiro[1,5,6,7,8,8a-hexahydroimidazo[1,2-a]pyridine-3,4'-piperidine]-2-one	O=C1N[C@H]2CCCCN2C12CCN(CCCN1c3ccccc3CCc3ccc(Cl)cc31)CC2	12831242	BBB+
[3-(dimethylcarbamoyloxy)phenyl]-trimethylazanium	CN(C)C(=O)Oc1cccc([N+](C)(C)C)c1	4456	BBB+
N-(1,5-dimethyl-3-oxo-2-phenylpyrazol-4-yl)pyridine-3-carboxamide	Cc1c(NC(=O)c2cccnc2)c(=O)n(-c2ccccc2)n1C	4487	BBB+
N-(4-ethoxyphenyl)acetamide	CCOc1ccc(NC(C)=O)cc1	4754	BBB+
(2R)-N-(2-methylphenyl)-2-(propylamino)propanamide	CCCN[C@H](C)C(=O)Nc1ccccc1C	12444990	BBB+
3-methyl-1-(5-oxohexyl)-7-propylpurine-2,6-dione	CCCn1cnc2c1c(=O)n(CCCCC(C)=O)c(=O)n2C	4938	BBB+
(1-methylpyridin-1-ium-3-yl) N,N-dimethylcarbamate	CN(C)C(=O)Oc1ccc[n+](C)c1	4991	BBB+
2-hydroxybenzamide	NC(=O)c1ccccc1O	5147	BBB+

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Compound Name	SMILES	CID	Class
2-(2-hydroxybenzoyl)oxybenzoic acid	O=C(Oc1ccccc1C(=O)O)c1ccccc1O	5161	BBB+
[(1R,2R,4S,5S)-9-methyl-3-oxa-9-azatricyclo[3.3.1.02,4]nonan-7-yl] (2R)-3-hydroxy-2-phenylpropanoate	CN1[C@@H]2C[C@H](OC(=O)[C@@H](CO)c3ccccc3)C[C@H]1[C@@H]1O[C@@H]12	673473	BBB+
2-(dimethylamino)ethyl 4-(butylamino)benzoate	CCCCNc1ccc(C(=O)OCCN(C)C)cc1	5411	BBB+
2,2,2-trichloroethyl dihydrogen phosphate	O=P(O)(O)OCC(Cl)(Cl)Cl	5563	BBB+
(1R)-1-cyclohexyl-1-phenyl-3-piperidin-1-ylpropan-1-ol	O[C@@](CCN1CCCCC1)(c1ccccc1)C1CCCCC1	207843	BBB+
(3S,4R)-3-ethyl-4-[(3-methylimidazol-4-yl)methyl]oxolan-2-one	CC[C@@H]1C(=O)OC[C@@H]1Cc1cncn1C	5910	BBB+
pyridine-3,4-diamine	Nc1ccncc1N	5918	BBB+
[(3R)-2-(carbamoyloxymethyl)-2,3-dimethylpentyl] carbamate	CC[C@@H](C)C(C)(COC(N)=O)COC(N)=O	57066553	BBB+
(2S)-2-aminobutanoic acid	CC[C@H](N)C(=O)O	80283	BBB+

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Compound Name	SMILES	CID	Class
(5S)-5-ethyl-3,5-dimethyl-1,3-oxazolidine-2,4-dione	CC[C@]1(C)OC(=O)N(C)C1=O	51380896	BBB+
2-(diethylamino)ethyl 4-amino-2-chlorobenzoate	CCN(CC)CCOC(=O)c1ccc(N)cc1Cl	8612	BBB+
(5R)-5-[(2S)-hex-3-yn-2-yl]-1-methyl-5-prop-2-enyl-1,3-diazinane-2,4,6-trione	C=CC[C@@]1([C@@H](C)C#CCC)C(=O)NC(=O)N(C)C1=O	51397655	BBB+
(6aR,9R)-N-[(2S)-1-hydroxybutan-2-yl]-4,7-dimethyl-6,6a,8,9-tetrahydroindolo[4,3-fg]quinoline-9-carboxamide	CC[C@@H](CO)NC(=O)[C@@H]1C=C2c3cccc4c3c(cn4C)C[C@H]2N(C)C1	9681	BBB+
(1R,9S)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one	O=c1cccc2n1C[C@@H]1CNC[C@H]2C1	10235	BBB+
2-[(R)-(4-butylsulfanylphenyl)-phenylmethyl]sulfanyl-N,N-dimethylethanamine	CCCCSc1ccc([C@H](SCCN(C)C)c2ccccc2)cc1	76959957	BBB+
3-ethyl-5,5-dimethyl-1,3-oxazolidine-2,4-dione	CCN1C(=O)OC(C)(C)C1=O	10630	BBB+
(2S)-N-carbamoyl-2-propan-2-ylpent-4-enamide	C=CC[C@H](C(=O)NC(N)=O)C(C)C	76961142	BBB+

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Compound Name	SMILES	CID	Class
2-(2-methylpropylamino)ethyl 3-aminobenzoate	CC(C)CNCCOC(=O)c1cccc(N)c1	11115	BBB+
ethyl 1-[(3S)-3-hydroxy-3-phenylpropyl]-4-phenylpiperidine-4-carboxylate	CCOC(=O)C1(c2ccccc2)CCN(CC[C@H](O)c2ccccc2)CC1	92215562	BBB+
[[(2R,3S,4R,5R)-5-(4-amino-2-oxopyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy-hydroxyphosphoryl] 2-(trimethylazaniumyl)ethyl phosphate	C[N+](C)(C)CCO[P@](=O)([O-])O[P@@](=O)(O)OC[C@H]1O[C@@H](n2ccc(N)nc2=O)[C@H](O)[C@@H]1O	13804	BBB+
2-[[[(2R,3S,4R,5R)-5-(4-amino-2-oxopyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy-hydroxyphosphoryl]oxy-hydroxyphosphoryl]oxyethyl-trimethylazanium	C[N+](C)(C)CCO[P@@](=O)(O)O[P@@](=O)(O)OC[C@H]1O[C@@H](n2ccc(N)nc2=O)[C@H](O)[C@@H]1O	13805	BBB+
(3R)-4-amino-3-phenylbutanoic acid	NC[C@H](CC(=O)O)c1ccccc1	685622	BBB+
(3R)-N-(4-ethoxyphenyl)-3-hydroxybutanamide	CCOc1ccc(NC(=O)C[C@@H](C)O)cc1	6918884	BBB+

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Compound Name	SMILES	CID	Class
(1S,2S,3R,4R)-N-ethyl-3-phenylbicyclo[2.2.1]heptan-2-amine	CCN[C@H]1[C@H]2CC[C@H](C2)[C@@H]1c1ccccc1	76960649	BBB+
(1S,9S,13S)-1,13-dimethyl-10-(2-phenylethyl)-10-azatricyclo[7.3.1.02,7]trideca-2(7),3,5-trien-4-ol	C[C@@H]1[C@@H]2Cc3ccc(O)cc3[C@@]1(C)CCN2CCc1ccccc1	3048356	BBB+
2-[2-[4-[(2R)-2-methyl-3-phenothiazin-10-ylpropyl]piperazin-1-yl]ethoxy]ethanol	C[C@H](CN1CCN(CCOCCO)CC1)CN1c2ccccc2Sc2ccccc21	9932302	BBB+
5-[(2R)-2-hydroxypropyl]-5-prop-2-enyl-1,3-diazinane-2,4,6-trione	C=CCC1(C[C@@H](C)O)C(=O)NC(=O)NC1=O	76968709	BBB+
(5S)-5-(2-bromoprop-2-enyl)-1-methyl-5-propan-2-yl-1,3-diazinane-2,4,6-trione	C=C(Br)C[C@]1(C(C)C)C(=O)NC(=O)N(C)C1=O	76963951	BBB+
5-[(1R,5S)-3-bicyclo[3.2.1]oct-2-enyl]-5-ethyl-1,3-diazinane-2,4,6-trione	CCC1(C2=C[C@@H]3CC[C@H](C2)C3)C(=O)NC(=O)NC1=O	71307002	BBB+
1,3-dimethyl-7-[2-[[(2R)-1-phenylpropan-2-yl]amino]ethyl]purine-2,6-dione	C[C@H](Cc1ccccc1)NCCn1cnc2c1c(=O)n(C)c(=O)n2C	25271663	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
(2R,3R)-2-ethyl-3-methylpentanamide	CC[C@@H](C)[C@@H](CC)C(N)=O	36689722	BBB+
(4-acetamidophenyl) 2-acetyloxybenzoate	CC(=O)Nc1ccc(OC(=O)c2ccccc2OC(C)=O)cc1	21102	BBB+
(2R)-N,N,2-trimethyl-3-(2-tricyclo[9.4.0.03,8]pentadeca-1(15),3,5,7,11,13-hexaenyl)propan-1-amine	C[C@H](CC1c2ccccc2CCc2cccc21)CN(C)C	36690126	BBB+
2-(butylamino)-N-(2-chloro-6-methylphenyl)acetamide	CCCCNCC(=O)Nc1c(C)cccc1Cl	22379	BBB+
methyl (2S)-2-amino-3-(3,4-dihydroxyphenyl)propanoate	COC(=O)[C@@H](N)Cc1ccc(O)c(O)c1	23497	BBB+
(1S,2R)-2-phenylcyclopropan-1-amine	N[C@H]1C[C@@H]1c1ccccc1	26070	BBB+
N-methyl-1-(1-tetracyclo[6.6.2.02,7.09,14]hexadeca-2,4,6,9,11,13-hexaenyl)methanamine	CNC[C@]12CC[C@H](c3ccccc31)c1ccccc12	28425	BBB+
3-(diethylamino)propyl (1S,2S,4R)-2-phenylbicyclo[2.2.1]heptane-2-carboxylate	CCN(CC)CCCOC(=O)[C@@]1(c2ccccc2)C[C@@H]2CC[C@H]1C2	76965001	BBB+

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Compound Name	SMILES	CID	Class
2-[(1R)-1-(2,6-dichlorophenoxy)ethyl]-4,5-dihydro-1H-imidazole	C[C@@H](Oc1c(Cl)cccc1Cl)C1=NCCN1	3038503	BBB+
(3S)-3-(1-benzylpiperidin-4-yl)-3-phenylpiperidine-2,6-dione	O=C1CC[C@@](c2ccccc2)(C2CCN(Cc3ccccc3)CC2)C(=O)N1	30843	BBB+
2,4,6-trimethyl-1,3,5-trioxane	C[C@H]1O[C@@H](C)O[C@@H](C)O1	31264	BBB+
methyl 4-methyl-3-[[(2S)-2-(propylamino)propanoyl]amino]thiophene-2-carboxylate	CCCN[C@@H](C)C(=O)Nc1c(C)csc1C(=O)OC	6604377	BBB+
3-(12H-[1]benzofuro[3,2-c][1]benzoxepin-6-ylidene)-N,N-dimethylpropan-1-amine	CN(C)CCC=C1c2ccccc2OCc2c1oc1ccccc21	36846	BBB+
(2S)-N-(2,6-dimethylphenyl)-2-[ethyl(propyl)amino]butanamide	CCCN(CC)[C@@H](CC)C(=O)Nc1c(C)cccc1C	12862484	BBB+
(3R)-7-chloro-5-(2-fluorophenyl)-3-hydroxy-1-(2-hydroxyethyl)-3H-1,4-benzodiazepin-2-one	O=C1[C@@H](O)N=C(c2ccccc2F)c2cc(Cl)ccc2N1CCO	76967234	BBB+
4-[[(4-chlorophenyl)-(5-fluoro-2-hydroxyphenyl)methylidene]amino]butanamide	NC(=O)CCC/N=C(\c1ccc(Cl)cc1)c1cc(F)ccc1O	44115	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
5-ethyl-5-prop-2-enyl-1,3-diazinane-2,4,6-trione	C=CCC1(CC)C(=O)NC(=O)NC 1=O	48542	BBB+
(6S)-6-[propyl(2-thiophen-2-ylethyl)amino]-5,6,7,8-tetrahydronaphthalen-1-ol	CCCN(CCc1cccs1)[C@H]1CCc2 c(O)cccc2C1	59227	BBB+
4-[4-(2-oxo-3-propanoylbenzimidazol-1-yl)piperidin-1-yl]-2,2-diphenylbutanenitrile	CCC(=O)n1c(=O)n(C2CCN(CC C(C#N)(c3ccccc3)c3ccccc3)CC2)c2ccccc21	61791	BBB+
[(3S)-3,6-dihydroxy-1-propan-2-yl-2,3-dihydroindol-5-yl]iminourea	CC(C)N1C[C@@H](O)c2cc(/N =N/C(N)=O)c(O)cc21	135565885	BBB+
(1S)-2-[bis[(2R)-butan-2-yl]amino]-1-[1-[(2-chlorophenyl)methyl]pyrrol-2-yl]ethanol	CC[C@@H](C)N(C[C@H](O)c 1cccn1Cc1ccccc1Cl)[C@H](C)C C	76961195	BBB+
3-(2-chlorophenothiazin-10-yl)-N,N-diethylpropan-1-amine	CCN(CC)CCCN1c2ccccc2Sc2ccc (Cl)cc21	65750	BBB+
2,3-diacetyloxybenzoic acid	CC(=O)Oc1cccc(C(=O)O)c1OC (C)=O	68093	BBB+

Continued on next page

Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
(2-methoxyphenyl) 2-acetyloxybenzoate	COc1ccccc1OC(=O)c1ccccc1OC(C)=O	68749	BBB+
3-acetamidopropane-1-sulfonic acid	CC(=O)NCCCS(=O)(=O)O	71158	BBB+
N-[(2R)-4-[4-(4-fluorophenyl)piperazin-1-yl]butan-2-yl]pyridine-3-carboxamide	C[C@H](CCN1CCN(c2ccc(F)cc2)CC1)NC(=O)c1cccnc1	76956128	BBB+
ethyl (6S)-1,6-dimethyl-4-oxo-6,7,8,9-tetrahydropyrido[1,2-a]pyrimidin-1-ium-3-carboxylate	CCOC(=O)c1c[n+](C)c2n(c1=O)[C@@H](C)CCC2	15584873	BBB+
(6R)-6-(methylamino)-6,7,8,9-tetrahydro-5H-carbazole-3-carboxamide	CN[C@@H]1CCc2[nH]c3ccc(C(N)=O)cc3c2C1	77992	BBB+
N-[2-(7-methoxynaphthalen-1-yl)ethyl]acetamide	COc1ccc2cccc(CCNC(C)=O)c2c1	82148	BBB+
(2R,5R)-2-methylspiro[1,3-oxathiolane-5,3'-1-azabicyclo[2.2.2]octane]	C[C@@H]1O[C@@]2(CS1)CN1CCC2CC1	83898	BBB+
11-[(3R)-1-azabicyclo[2.2.2]octan-3-yl]-5,6-dihydrobenzo[b][1]benzazepine	c1ccc2c(c1)CCc1ccccc1N2[C@H]1CN2CCC1CC2	76957954	BBB+

Continued on next page

Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
(8S,10S,13S,14S,16R,17S)-17-[2-[4-(2,6-dipyrrolidin-1-ylpyrimidin-4-yl)piperazin-1-yl]acetyl]-10,13,16-trimethyl-6,7,8,12,14,15,16,17-octahydrocyclopenta[a]phenanthren-3-one	C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)C3=CC[C@]2(C)[C@H]1C(=O)CN1CCN(c2cc(N3CCCC3)nc(N3CCCC3)n2)CC1	104903	BBB+
1,3,4,6-tetramethyl-3a,6a-dihydroimidazo[4,5-d]imidazole-2,5-dione	CN1C(=O)N(C)[C@H]2[C@@H]1N(C)C(=O)N2C	122282	BBB+
4-[(1R)-2-(dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol	CN(C)C[C@@H](c1ccc(O)cc1)C1(O)CCCCC1	12018336	BBB+
(2S)-2-[[4-[(3-fluorophenyl)methoxy]phenyl]methylamino]propanamide	C[C@H](NCc1ccc(OCc2cccc(F)c2)cc1)C(N)=O	131682	BBB+
[(1R,2R,4S,5S)-9-methyl-3-oxa-9-azatricyclo[3.3.1.02,4]nonan-7-yl] (2S)-3-hydroxy-2-phenylpropanoate	CN1[C@@H]2C[C@H](OC(=O)[C@H](CO)c3ccccc3)C[C@H]1[C@@H]1O[C@@H]12	3000322	BBB+
(1R,12S)-5,8,14-triazatetracyclo[10.3.1.02,11.04,9]hexadeca-2,4,6,8,10-pentaene	c1cnc2cc3c(cc2n1)[C@@H]1CNC[C@H]3C1	5310966	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
(2S)-N-(2,6-dimethylphenyl)-1-propylpiperidine-2-carboxamide	CCCN1CCCC[C@H]1C(=O)Nc1c(C)cccc1C	175805	BBB+
(1S,5R)-3-(6H-benzo[c][1]benzothiepin-11-ylidene)-8-methyl-8-azabicyclo[3.2.1]octane	CN1[C@@H]2CC[C@H]1CC(=C1c3ccccc3CSc3ccccc31)C2	3034047	BBB+
(1S,2R,6S,7R)-4-[[(1R,2R)-2-[[4-(1,2-benzothiazol-3-yl)piperazin-1-yl]methyl]cyclohexyl]methyl]-4-azatricyclo[5.2.1.02,6]decane-3,5-dione	O=C1[C@@H]2[C@H]3CC[C@H](C3)[C@@H]2C(=O)N1C[C@@H]1CCCC[C@H]1CN1CCN(c2nsc3ccccc23)CC1	213046	BBB+
(2R)-2-acetamido-N-benzyl-3-methoxypropanamide	COC[C@@H](NC(C)=O)C(=O)NCc1ccccc1	219078	BBB+
(1R,9R,13R)-1,13-dimethyl-10-(2-phenylethyl)-10-azatricyclo[7.3.1.02,7]trideca-2(7),3,5-trien-4-ol	C[C@H]1[C@H]2Cc3ccc(O)cc3[C@]1(C)CCN2CCc1ccccc1	443405	BBB+
methyl (1R,2R,3S,5S)-3-benzoyloxy-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylate	COC(=O)[C@H]1[C@@H](OC(=O)c2ccccc2)C[C@@H]2CC[C@H]1N2C	446220	BBB+
2,3,5,6,7,8-hexahydro-1H-cyclopenta[b]quinolin-9-amine	Nc1c2c(nc3c1CCC3)CCCC2	604519	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
[(1S,2R,4S,5R)-9-methyl-3-oxa-9-azatricyclo[3.3.1.02,4]nonan-7-yl] (2R)-3-hydroxy-2-phenylpropanoate	CN1[C@@H]2C[C@H](OC(=O)[C@@H](CO)c3ccccc3)C[C@H]1[C@H]1O[C@H]12	638340	BBB+
2-[(1R,6R)-3-methyl-6-prop-1-en-2-ylcyclohex-2-en-1-yl]-5-pentylbenzene-1,3-diol	C=C(C)[C@@H]1CCC(C)=C[C@H]1c1c(O)cc(CCCCC)cc1O	644019	BBB+
[(2R)-2,3-dihydroxypropyl] 2-(trimethylazaniumyl)ethyl phosphate	C[N+](C)(C)CCO[P@](=O)([O-])OC[C@H](O)CO	657272	BBB+
(1S,9R)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one	O=c1cccc2n1C[C@H]1CNC[C@@H]2C1	683511	BBB+
(1S,5R)-3-benzhydryloxy-8-methyl-8-azabicyclo[3.2.1]octane	CN1[C@@H]2CC[C@H]1C[C@H](OC(c1ccccc1)c1ccccc1)C2	1201549	BBB+
2-[(R)-benzhydrylsulfinyl]-N-hydroxyacetamide	O=C(C[S@@](=O)C(c1ccccc1)c1ccccc1)NO	25271624	BBB+
(2R,6R)-9-chloro-4-methyl-13-oxa-4-azatetracyclo[12.4.0.02,6.07,12]octadeca-1(18),7(12),8,10,14,16-hexaene	CN1C[C@H]2c3ccccc3Oc3ccc(Cl)cc3[C@@H]2C1	3036780	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
(2S)-2-amino-5-(2,5-dioxo-4,4-diphenylimidazolidin-1-yl)pentanoic acid	N[C@@H](CCCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O)C(=O)O	93482134	BBB+
(3,4-dihydroxy-5-nitrophenyl)-(4-methylphenyl)methanone	Cc1ccc(C(=O)c2cc(O)c(O)c([N+](=O)[O-])c2)cc1	4659569	BBB+
8-[(E)-2-(3,4-dimethoxyphenyl)ethenyl]-1,3-diethyl-7-methylpurine-2,6-dione	CCn1c(=O)c2c(nc(/C=C/c3ccc(OC)c(OC)c3)n2C)n(CC)c1=O	5311037	BBB+
5-[(1S)-1-(2,3-dimethylphenyl)ethyl]-1H-imidazole	Cc1cccc([C@H](C)c2cnc[nH]2)c1C	5311068	BBB+
(E,3R)-1-(1,3-benzodioxol-5-yl)-4,4-dimethylpent-1-en-3-ol	CC(C)(C)[C@H](O)/C=C/c1ccc2c(c1)OCO2	38988294	BBB+
(3E)-3-(12H-[1]benzofuro[3,2-c][1]benzoxepin-6-ylidene)-N,N-dimethylpropan-1-amine	CN(C)CC/C=C1\c2ccccc2OCc2c1oc1ccccc21	6434185	BBB+
(3Z)-3-(12H-[1]benzofuro[3,2-c][1]benzoxepin-6-ylidene)-N,N-dimethylpropan-1-amine	CN(C)CC/C=C1/c2ccccc2OCc2c1oc1ccccc21	6436540	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
[(2S)-2-(2-chlorophenyl)-2-hydroxyethyl] carbamate	NC(=O)OC[C@@H](O)c1ccccc1Cl	6918474	BBB+
(3R)-3-acetyloxy-4-(trimethylazaniumyl)butanoate	CC(=O)O[C@H](CC(=O)[O-])C[N+](C)(C)C	7045767	BBB+
(2S)-2-[(4R)-2-oxo-4-propylpyrrolidin-1-yl]butanamide	CCC[C@@H]1CC(=O)N([C@@H](CC)C(N)=O)C1	9837243	BBB+
3-[(2R,3R)-1-(dimethylamino)-2-methylpentan-3-yl]phenol	CC[C@@H](c1cccc(O)c1)[C@@H](C)CN(C)C	9838022	BBB+
4-[2-[(6-ethoxy-1H-benzimidazol-2-yl)sulfanyl]ethyl]morpholine	CCOc1ccc2nc(SCCN3CCOCC3)[nH]c2c1	9862937	BBB+
methyl 3-[(4S)-8-bromo-1-methyl-6-pyridin-2-yl-4H-imidazo[1,2-a][1,4]benzodiazepin-4-yl]propanoate	COC(=O)CC[C@@H]1N=C(c2ccccn2)c2cc(Br)ccc2-n2c(C)cnc21	9867812	BBB+
(5S)-5-hydroxy-5,6-dihydrobenzo[b][1]benzazepine-11-carboxamide	NC(=O)N1c2ccccc2C[C@H](O)c2ccccc21	9881504	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
[(1S,2R,4S,5R)-9-methyl-3-oxa-9-azatricyclo[3.3.1.02,4]nonan-7-yl] (2S)-3-hydroxy-2-phenylpropanoate	CN1[C@@H]2C[C@H](OC(=O)[C@H](CO)c3ccccc3)C[C@H]1[C@H]1O[C@H]12	3081743	BBB+
2-(2-oxo-1-phenyl-5-pyridin-2-ylpyridin-3-yl)benzonitrile	N#Cc1ccccc1-c1cc(-c2ccccn2)cn(-c2ccccc2)c1=O	9924495	BBB+
1-[3-[3-(4-chlorophenyl)propoxy]propyl]piperidine	Clc1ccc(CCCOCCCN2CCCCC2)cc1	9948102	BBB+
1-[2-(2,4-dimethylphenyl)sulfanylphenyl]piperazine	Cc1ccc(Sc2ccccc2N2CCNCC2)c(C)c1	9966051	BBB+
1-[(4-fluorophenyl)methyl]-1-(1-methylpiperidin-4-yl)-3-[[4-(2-methylpropoxy)phenyl]methyl]urea	CC(C)COc1ccc(CNC(=O)N(Cc2ccc(F)cc2)C2CCN(C)CC2)cc1	10071196	BBB+
[(2R)-2-amino-3-phenylpropyl] carbamate	NC(=O)OC[C@H](N)Cc1ccccc1	10130337	BBB+
N-[[(1R,2R)-2-(2,3-dihydro-1-benzofuran-4-yl)cyclopropyl]methyl]propanamide	CCC(=O)NC[C@@H]1C[C@H]1c1cccc2c1CCO2	10220503	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
3-[4-[2-[4-(2,3-dichlorophenyl)piperazin-1-yl]ethyl]cyclohexyl]-1,1-dimethylurea	CN(C)C(=O)N[C@H]1CC[C@@H](CCN2CCN(c3cccc(Cl)c3Cl)CC2)CC1	11154555	BBB+
(2S)-2,6-diamino-N-[(2S)-1-phenylpropan-2-yl]hexanamide	C[C@@H](Cc1ccccc1)NC(=O)[C@@H](N)CCCCN	11597698	BBB+
[(1R)-1-(2-chlorophenyl)-2-(tetrazol-2-yl)ethyl] carbamate	NC(=O)O[C@@H](Cn1ncnn1)c1ccccc1Cl	11962412	BBB+
7-[4-[4-(1-benzothiophen-4-yl)piperazin-1-yl]butoxy]-1H-quinolin-2-one	O=c1ccc2ccc(OCCCCN3CCN(c4cccc5sccc45)CC3)cc2[nH]1	11978813	BBB+
ethyl (1R,2S)-2-(dimethylamino)-1-phenylcyclohex-3-ene-1-carboxylate	CCOC(=O)[C@@]1(c2ccccc2)CCC=C[C@@H]1N(C)C	12546498	BBB+
(2S,5S)-2-methylspiro[1,3-oxathiolane-5,3'-1-azabicyclo[2.2.2]octane]	C[C@H]1O[C@]2(CS1)CN1CCC2CC1	18642481	BBB+
(1R,5S)-3-benzhydryloxy-8-ethyl-8-azabicyclo[3.2.1]octane	CCN1[C@@H]2CC[C@H]1C[C@H](OC(c1ccccc1)c1ccccc1)C2	20055089	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
(6S,8R,9S,10R,13S,14S,17R)-17-acetyl-17-hydroxy-10,13-dimethyl-6-(trifluoromethyl)-2,6,7,8,9,11,12,14,15,16-decahydro-1H-cyclopenta[a]phenanthren-3-one	CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3C[C@H](C(F)(F)F)C4=CC(=O)CC[C@]4(C)[C@H]3CC[C@@]21C	20055352	BBB+
[(2R,3R,11bR)-9,10-dimethoxy-3-(2-methylpropyl)-2,3,4,6,7,11b-hexahydro-1H-benzo[a]quinolizin-2-yl] (2S)-2-amino-3-methylbutanoate	COc1cc2c(cc1OC)[C@H]1C[C@@H](OC(=O)[C@@H](N)C(C)C)[C@H](CC(C)C)CN1CC2	24795069	BBB+
[(7R)-4-(5-chloro-1,3-benzoxazol-2-yl)-7-methyl-1,4-diazepan-1-yl]-[5-methyl-2-(triazol-2-yl)phenyl]methanone	Cc1ccc(-n2nccn2)c(C(=O)N2CCN(c3nc4cc(Cl)ccc4o3)CC[C@H]2C)c1	24965990	BBB+
[[(2R,3S,4R,5R)-5-(4-amino-2-oxopyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy-oxidophosphoryl] 2-(trimethylazaniumyl)ethyl phosphate	C[N+](C)(C)CCO[P+]([O-])([O-])O[P+]([O-])([O-])OC[C@H]1O[C@@H](n2ccc(N)nc2=O)[C@H](O)[C@@H]1O	25202509	BBB+
5-chloro-N-ethyl-4-hydroxy-1-methyl-2-oxo-N-phenylquinoline-3-carboxamide	CCN(C(=O)c1c(O)c2c(Cl)cccc2n(C)c1=O)c1ccccc1	54677946	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
2-[(1R,5S,6S)-6-(aminomethyl)-3-ethyl-6-bicyclo[3.2.0]hept-3-enyl]acetic acid	CCC1=C[C@@H]2[C@H](C1)C[C@]2(CN)CC(=O)O	59509752	BBB+
[(1S,3S,5S)-6,6,9-trimethyl-9-azabicyclo[3.3.1]nonan-3-yl] 2-hydroxy-2,2-dithiophen-2-ylacetate	CN1[C@H]2CCC(C)(C)[C@@H]1C[C@@H](OC(=O)C(O)(c1ccccs1)c1cccs1)C2	90471539	BBB+
[(1R,3R,5S)-6,6,9-trimethyl-9-azabicyclo[3.3.1]nonan-3-yl] 2-hydroxy-2,2-dithiophen-2-ylacetate	CN1[C@@H]2CCC(C)(C)[C@@H]1C[C@H](OC(=O)C(O)(c1cccs1)c1cccs1)C2	118984411	BBB+
(4R)-6-chloro-N-ethyl-4-methyl-4-phenyl-1H-3,1-benzoxazin-2-imine	CC/N=C1\Nc2ccc(Cl)cc2[C@@](C)(c2ccccc2)O1	135564606	BBB+
5-[3-(2,5-dichloro-4,6-dimethyl-1-oxidopyridin-1-ium-3-yl)-1,2,4-oxadiazol-5-yl]-3-nitrobenzene-1,2-diol	Cc1c(Cl)c(C)[n+]([O-])c(Cl)c1-c1noc(-c2cc(O)c(O)c([N+](=O)[O-])c2)n1	135565903	BBB+
N'-[(4-methoxyphenyl)methyl]-N,N-dimethyl-N'-pyridin-2-ylethane-1,2-diamine	COc1ccc(CN(CCN(C)C)c2ccccn2)cc1	4992	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
2-[(S)-(4-chlorophenyl)-pyridin-2-ylmethoxy]-N,N-dimethylethanamine	CN(C)CCO[C@@H](c1ccc(Cl)cc1)c1ccccn1	170336	BBB+
(2S)-N,N,2-trimethyl-3-phenothiazin-10-ylpropan-1-amine	C[C@@H](CN(C)C)CN1c2ccccc2Sc2ccccc21	6604496	BBB+
(3S)-N,N-dimethyl-3-phenyl-3-pyridin-2-ylpropan-1-amine	CN(C)CC[C@@H](c1ccccc1)c1ccccn1	667440	BBB+
1-benzhydryl-4-methylpiperazine	CN1CCN(C(c2ccccc2)c2ccccc2)CC1	6726	BBB+
1-[(R)-(4-chlorophenyl)-phenylmethyl]-4-methylpiperazine	CN1CCN([C@H](c2ccccc2)c2ccc(Cl)cc2)CC1	688438	BBB+
1-[(R)-(4-chlorophenyl)-phenylmethyl]-4-[(3-methylphenyl)methyl]piperazine	Cc1cccc(CN2CCN([C@H](c3ccccc3)c3ccc(Cl)cc3)CC2)c1	23307231	BBB+
2-benzhydryloxy-N,N-dimethylethanamine	CN(C)CCOC(c1ccccc1)c1ccccc1	3100	BBB+
(3S)-3-(4-bromophenyl)-N,N-dimethyl-3-pyridin-2-ylpropan-1-amine	CN(C)CC[C@@H](c1ccc(Br)cc1)c1ccccn1	16960	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
N'-[(4-chlorophenyl)methyl]-N,N-dimethyl-N'-pyridin-2-ylethane-1,2-diamine	CN(C)CCN(Cc1ccc(Cl)cc1)c1ccccn1	25295	BBB+
N,N-dimethyl-2-[(1R)-1-phenyl-1-pyridin-2-ylethoxy]ethanamine	CN(C)CCO[C@](C)(c1ccccc1)c1ccccn1	6852255	BBB+
N'-benzyl-N,N-dimethyl-N'-pyridin-2-ylethane-1,2-diamine	CN(C)CCN(Cc1ccccc1)c1ccccn1	5587	BBB+
N,N-dimethyl-2-[3-[(1R)-1-pyridin-2-ylethyl]-1H-inden-2-yl]ethanamine	C[C@H](C1=C(CCN(C)C)Cc2ccccc21)c1ccccn1	12963076	BBB+
1-methyl-4-(2-tricyclo[9.4.0.03,8]pentadeca-1(15),3,5,7,9,11,13-heptaenylidene)piperidine	CN1CCC(=C2c3ccccc3C=Cc3ccccc32)CC1	2913	BBB+
N-benzyl-N-(4,5-dihydro-1H-imidazol-2-ylmethyl)aniline	c1ccc(CN(CC2=NCCN2)c2ccccc2)cc1	2200	BBB+
(3S)-3-(4-chlorophenyl)-N,N-dimethyl-3-pyridin-2-ylpropan-1-amine	CN(C)CC[C@@H](c1ccc(Cl)cc1)c1ccccn1	33036	BBB+
(2R)-2-[2-[(1R)-1-(4-chlorophenyl)-1-phenylethoxy]ethyl]-1-methylpyrrolidine	CN1CCC[C@@H]1CCO[C@](C)(c1ccccc1)c1ccc(Cl)cc1	26987	BBB+

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
2-[2-[4-[(R)-(4-chlorophenyl)-phenylmethyl]piperazin-1-yl]ethoxy]ethanol	OCCOCCN1CCN([C@H](c2ccccc2)c2ccc(Cl)cc2)CC1	1548974	BBB+
N,N-dimethyl-2-[(S)-(2-methylphenyl)-phenylmethoxy]ethanamine	Cc1ccccc1[C@@H](OCCN(C)C)c1ccccc1	736041	BBB+
2-[(R)-(4-bromophenyl)-phenylmethoxy]-N,N-dimethylethanamine	CN(C)CCO[C@H](c1ccccc1)c1ccc(Br)cc1	45266805	BBB+
2-[(E)-1-(4-methylphenyl)-3-pyrrolidin-1-ylprop-1-enyl]pyridine	Cc1ccc(/C(=C\CN2CCCC2)c2ccccn2)cc1	5282443	BBB+
(2R)-2-(3-fluoro-4-phenylphenyl)propanoic acid	Fc2cc(ccc2c1ccccc1)[C@H](C(=O)O)C	92337	BBB-
3-[(E)-3-anilino-3-oxoprop-1-enyl]-4,6-dichloro-1H-indole-2-carboxylic acid	OC(C1=C(/C=C/C(NC2=CC=CC=C2)=O)C3=C(Cl)C=C(Cl)C=C3N1)=O	6450546	BBB-
4-(2-aminoethyl)benzene-1,2-diol	NCCc1cc(O)c(O)cc1	681	BBB-

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Table SI. 1 – continued from previous page

Compound Name	SMILES	CID	Class
[(1S,2S,3R,4S,7R,9S,10S,12R,15S)-4,12-diacetyloxy-15-[(2R,3S)-3-benzamido-2-hydroxy-3-phenylpropanoyl]oxy-1,9-dihydroxy-10,14,17,17-tetramethyl-11-oxo-6-oxatetracyclo[11.3.1.03,10.04,7]heptadec-13-en-2-yl] benzoate	CC1=C2[C@@]([C@]([C@H]([C@@H]3[C@]4([C@H](OC4)C[C@@H]([C@]3(C(=O)[C@@H]2OC(=O)C)C)O)OC(=O)C)OC(=O)c5ccccc5)(C[C@@H]1OC(=O)[C@H](O)[C@@H](NC(=O)c6ccccc6)c7ccccc7)O)(C)C	36314	BBB-

Table SI. 2 Evaluation metrics results of all classification model–sampling strategy combinations on the test dataset

model_name	ROC_AUC	sensitivity	specificity	precision	accuracy	F1	MCC	GEOM	BACC	AP
dtree-kmeans_SMOTE	0.9000 ±0.0094	0.8814 ±0.0158	0.7472 ±0.0289	0.8692 ±0.0120	0.8352 ±0.0101	0.8751 ±0.0079	0.6332 ±0.0227	0.8113 ±0.0136	0.8143 ±0.0124	0.9300 ±0.0100
dtree-common	0.8982 ±0.0152	0.9005 ±0.0225	0.7241 ±0.0347	0.8615 ±0.0153	0.8397 ±0.0183	0.8804 ±0.0141	0.6399 ±0.0411	0.8072 ±0.0211	0.8123 ±0.0200	0.9291 ±0.0112
dtree-classic_SMOTE	0.8942 ±0.0159	0.8194 ±0.0301	0.7904 ±0.0372	0.8818 ±0.0182	0.8094 ±0.0203	0.8491 ±0.0174	0.5948 ±0.0412	0.8043 ±0.0203	0.8049 ±0.0204	0.9332 ±0.0105
dtree-classic_RandUndersampling	0.8892 ±0.0137	0.7983 ±0.0198	0.8178 ±0.0275	0.8931 ±0.0140	0.8050 ±0.0147	0.8429 ±0.0127	0.5948 ±0.0299	0.8078 ±0.0155	0.8081 ±0.0155	0.9265 ±0.0106
dtree-classic_ADASYN	0.8931 ±0.0124	0.8346 ±0.0208	0.7817 ±0.0246	0.8793 ±0.0118	0.8164 ±0.0152	0.8562 ±0.0129	0.6045 ±0.0308	0.8076 ±0.0154	0.8082 ±0.0152	0.9291 ±0.0116
dtree-borderline_SMOTE	0.8941 ±0.0121	0.8218 ±0.0276	0.8139 ±0.0285	0.8940 ±0.0130	0.8191 ±0.0147	0.8560 ±0.0137	0.6182 ±0.0266	0.8175 ±0.0129	0.8178 ±0.0128	0.9278 ±0.0127
knn-kmeans_SMOTE	0.9428 ±0.0067	0.9502 ±0.0132	0.7096 ±0.0306	0.8618 ±0.0123	0.8673 ±0.0123	0.9037 ±0.0087	0.7009 ±0.0291	0.8209 ±0.0176	0.8299 ±0.0155	0.9638 ±0.0068
knn-common	0.9426 ±0.0065	0.9547 ±0.0119	0.6853 ±0.0186	0.8524 ±0.0072	0.8619 ±0.0089	0.9006 ±0.0066	0.6888 ±0.0214	0.8088 ±0.0110	0.8200 ±0.0098	0.9638 ±0.0066
knn-classic_SMOTE	0.9436 ±0.0062	0.9067 ±0.0098	0.8248 ±0.0237	0.9079 ±0.0114	0.8785 ±0.0112	0.9073 ±0.0084	0.7312 ±0.0254	0.8647 ±0.0141	0.8658 ±0.0136	0.9649 ±0.0063
knn-classic_RandUndersampling	0.9387 ±0.0080	0.9100 ±0.0130	0.7860 ±0.0187	0.8900 ±0.0093	0.8673 ±0.0131	0.8999 ±0.0101	0.7037 ±0.0290	0.8457 ±0.0142	0.8480 ±0.0139	0.9628 ±0.0063
knn-classic_ADASYN	0.9425 ±0.0065	0.8636 ±0.0144	0.8820 ±0.0186	0.9331 ±0.0101	0.8700 ±0.0126	0.8970 ±0.0104	0.7256 ±0.0261	0.8727 ±0.0130	0.8728 ±0.0131	0.9644 ±0.0057
knn-borderline_SMOTE	0.9417 ±0.0059	0.8686 ±0.0134	0.8805 ±0.0129	0.9326 ±0.0061	0.8727 ±0.0071	0.8994 ±0.0063	0.7302 ±0.0130	0.8744 ±0.0059	0.8745 ±0.0059	0.9644 ±0.0056
logreg-kmeans_SMOTE	0.9182 ±0.0098	0.9145 ±0.0090	0.7398 ±0.0227	0.8700 ±0.0101	0.8543 ±0.0105	0.8917 ±0.0076	0.6719 ±0.0241	0.8225 ±0.0138	0.8272 ±0.0128	0.9488 ±0.0084
logreg-common	0.9168 ±0.0095	0.9219 ±0.0115	0.7183 ±0.0251	0.8617 ±0.0104	0.8518 ±0.0089	0.8907 ±0.0065	0.6650 ±0.0205	0.8136 ±0.0129	0.8201 ±0.0115	0.9487 ±0.0082
logreg-classic_SMOTE	0.9190 ±0.0120	0.8622 ±0.0192	0.8225 ±0.0315	0.9026 ±0.0163	0.8485 ±0.0168	0.8818 ±0.0135	0.6730 ±0.0363	0.8419 ±0.0187	0.8424 ±0.0186	0.9491 ±0.0105
logreg-classic_RandUndersampling	0.9137 ±0.0086	0.8548 ±0.0156	0.8025 ±0.0252	0.8918 ±0.0129	0.8368 ±0.0153	0.8728 ±0.0122	0.6465 ±0.0327	0.8281 ±0.0169	0.8286 ±0.0167	0.9478 ±0.0079
logreg-classic_ADASYN	0.9122 ±0.0095	0.8021 ±0.0226	0.8562 ±0.0202	0.9138 ±0.0121	0.8207 ±0.0190	0.8542 ±0.0165	0.6331 ±0.0366	0.8286 ±0.0183	0.8291 ±0.0182	0.9484 ±0.0072
logreg-borderline_SMOTE	0.9107 ±0.0099	0.8109 ±0.0226	0.8491 ±0.0247	0.9110 ±0.0137	0.8241 ±0.0179	0.8579 ±0.0155	0.6367 ±0.0353	0.8297 ±0.0176	0.8300 ±0.0177	0.9467 ±0.0078
xgb-kmeans_SMOTE	0.9588 ±0.0044	0.9392 ±0.0112	0.7919 ±0.0235	0.8958 ±0.0103	0.8885 ±0.0092	0.9170 ±0.0068	0.7498 ±0.0209	0.8623 ±0.0123	0.8656 ±0.0114	0.9774 ±0.0038
xgb-common	0.9589 ±0.0044	0.9409 ±0.0097	0.7923 ±0.0235	0.8961 ±0.0105	0.8897 ±0.0099	0.9179 ±0.0072	0.7524 ±0.0226	0.8633 ±0.0132	0.8666 ±0.0123	0.9775 ±0.0036
gb-classic_SMOTE	0.9593 ±0.0045	0.9292 ±0.0131	0.8205 ±0.0217	0.9079 ±0.0098	0.8917 ±0.0095	0.9184 ±0.0072	0.7585 ±0.0213	0.8730 ±0.0113	0.8748 ±0.0108	0.9773 ±0.0043
xgb-classic_RandUndersampling	0.9523 ±0.0052	0.8908 ±0.0117	0.8699 ±0.0172	0.9288 ±0.0085	0.8836 ±0.0081	0.9094 ±0.0066	0.7485 ±0.0173	0.8802 ±0.0089	0.8804 ±0.0088	0.9739 ±0.0041
xgb-classic_ADASYN	0.9585 ±0.0048	0.9275 ±0.0121	0.8233 ±0.0180	0.9090 ±0.0080	0.8916 ±0.0083	0.9181 ±0.0065	0.7583 ±0.0184	0.8737 ±0.0094	0.8754 ±0.0091	0.9770 ±0.0040
xgb-borderline_SMOTE	0.9588 ±0.0048	0.9259 ±0.0131	0.8237 ±0.0210	0.9091 ±0.0095	0.8906 ±0.0092	0.9173 ±0.0071	0.7564 ±0.0204	0.8732 ±0.0108	0.8748 ±0.0104	0.9770 ±0.0046