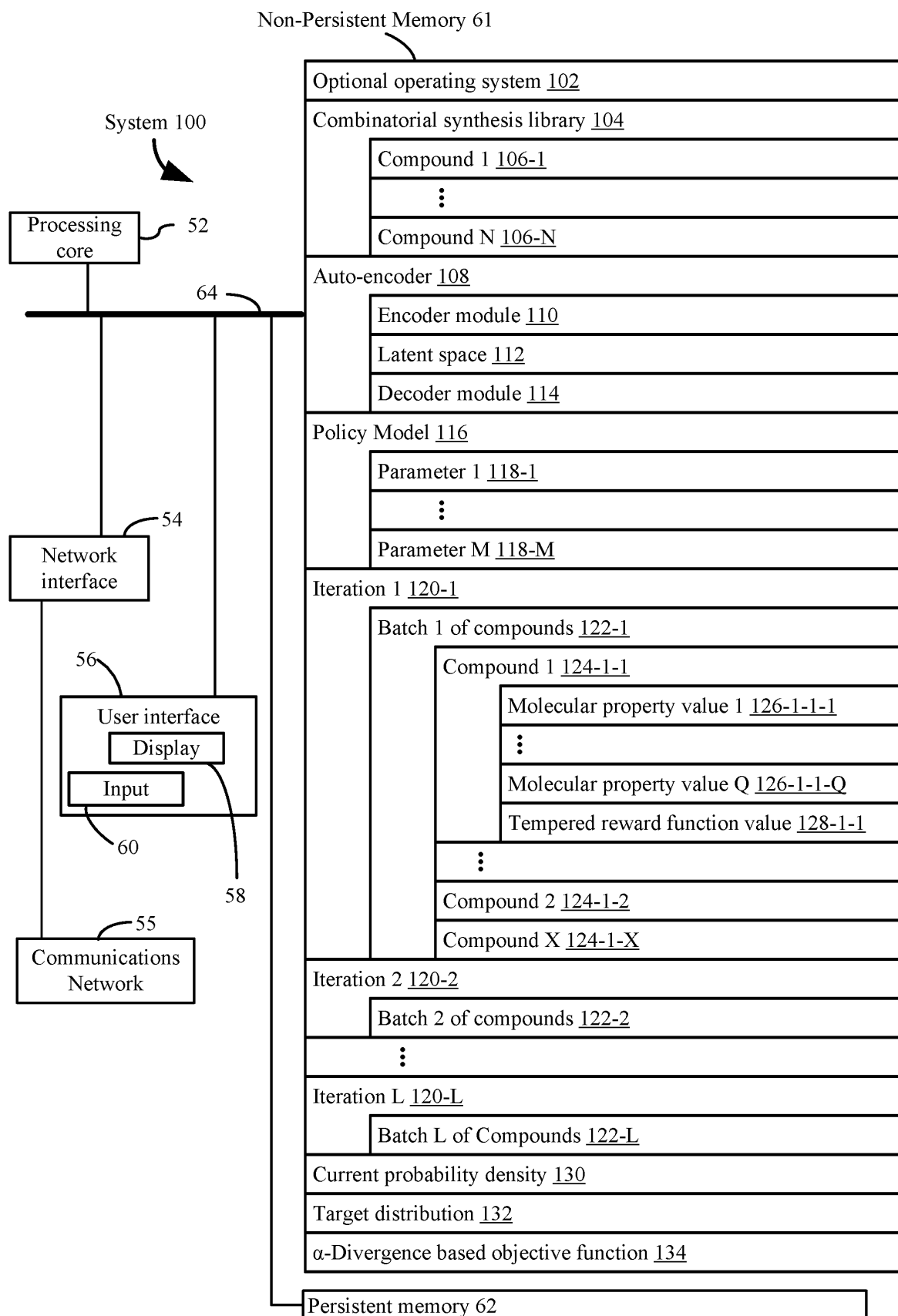


**Fig. 1**

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200 Computer-implemented methods for identifying a plurality of compounds in a combinatorial synthesis library that each satisfy a plurality of molecular properties are provided. The combinatorial synthesis library is accessible through a trained variational auto-encoder that comprises (i) an encoder module that maps a compound in the combinatorial synthesis library into a d -dimensional code in a learned d -dimensional latent space and (ii) a decoder module that retrieves a molecular structure of the compound, with a reconstruction likelihood greater than a threshold reconstruction likelihood, upon inputting the d -dimensional code into the decoder.

202 The threshold reconstruction likelihood is 50 percent or greater, 60 percent or greater, or between 60 percent and 80 percent.

204 A first molecular property in the plurality of molecular properties is a bioactivity prediction against a therapeutic target, and the first molecular property is satisfied for a respective compound in the plurality of compounds when a bioactivity classification module determines, based on a chemical structure of the respective compound, that the respective compound is an active compound against the therapeutic target.

206 A first molecular property in the plurality of molecular properties is a potency prediction against a therapeutic target, and the first molecular property is satisfied for a respective compound in the plurality of compounds when a potency prediction regression module determines, based on a chemical structure of the respective compound, that the respective compound has at least a threshold potency against the therapeutic target.

208 The plurality of compounds comprises 500 or more compounds, 1000 or more compounds, 10,000 or more compounds, or 100,000 or more compounds.

210 The combinatorial synthesis library represents more than 10,000 synthons and more than 10 three- or four- component reactions.

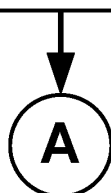


Fig. 2A

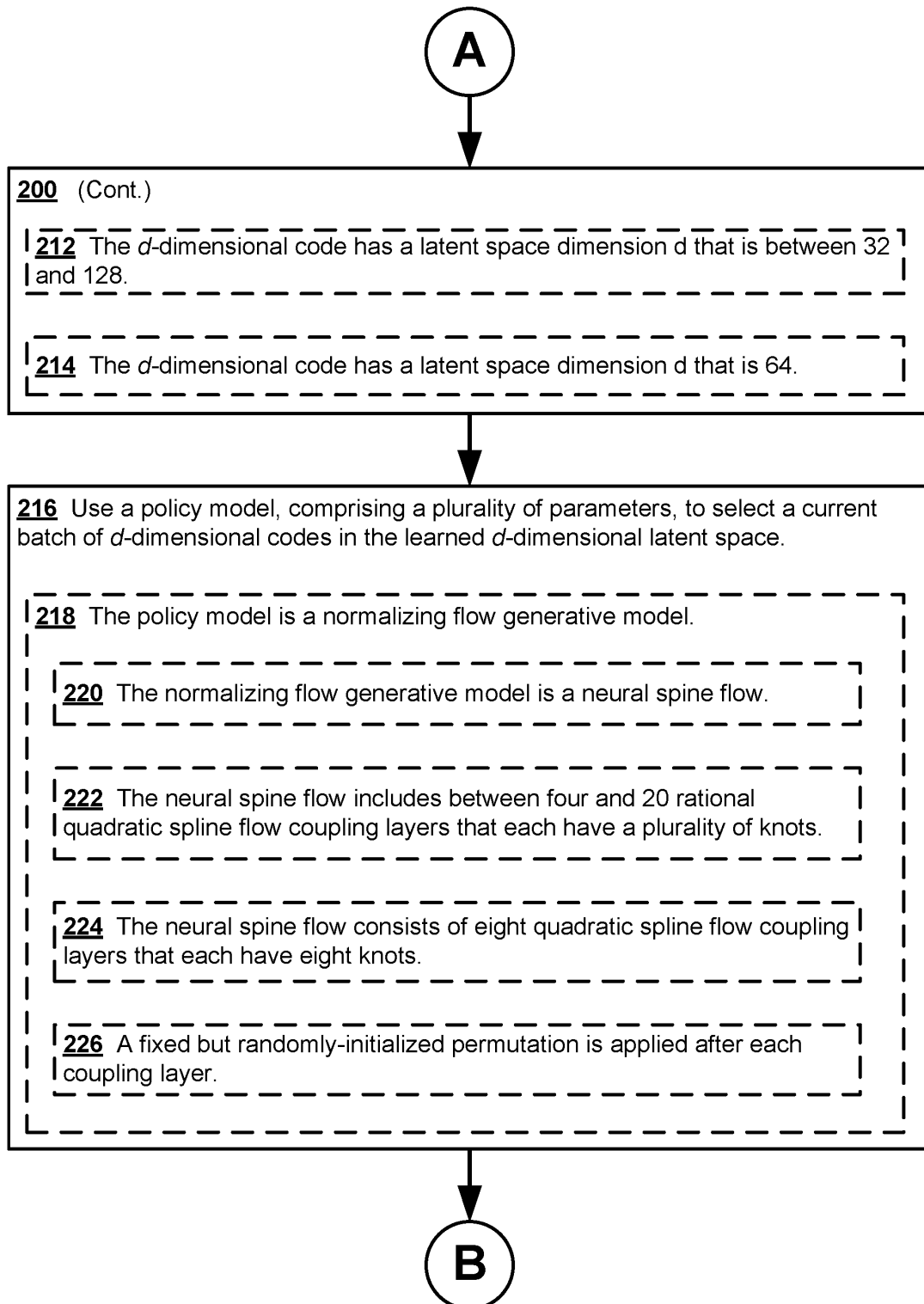


Fig. 2B

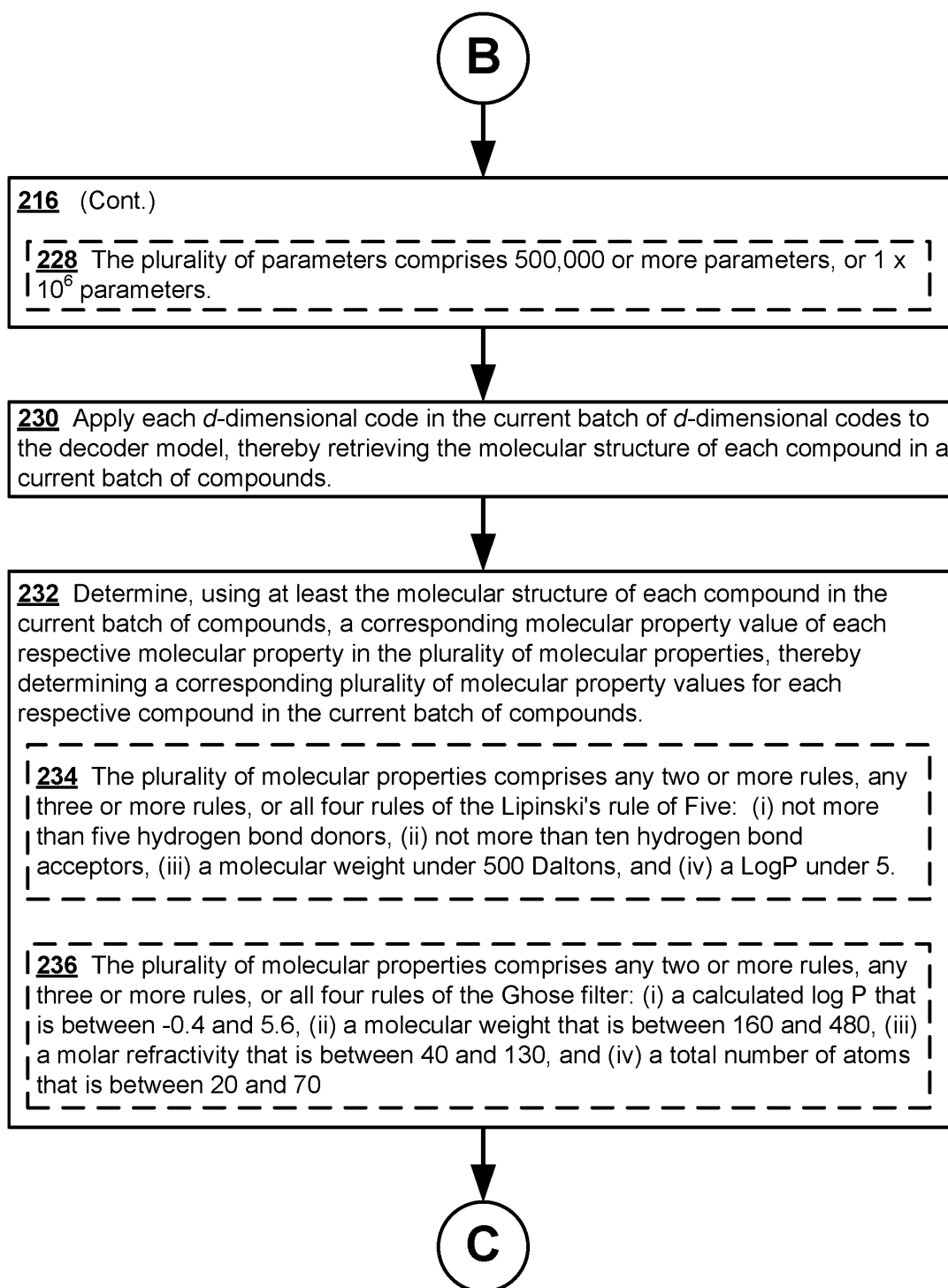


Fig. 2C

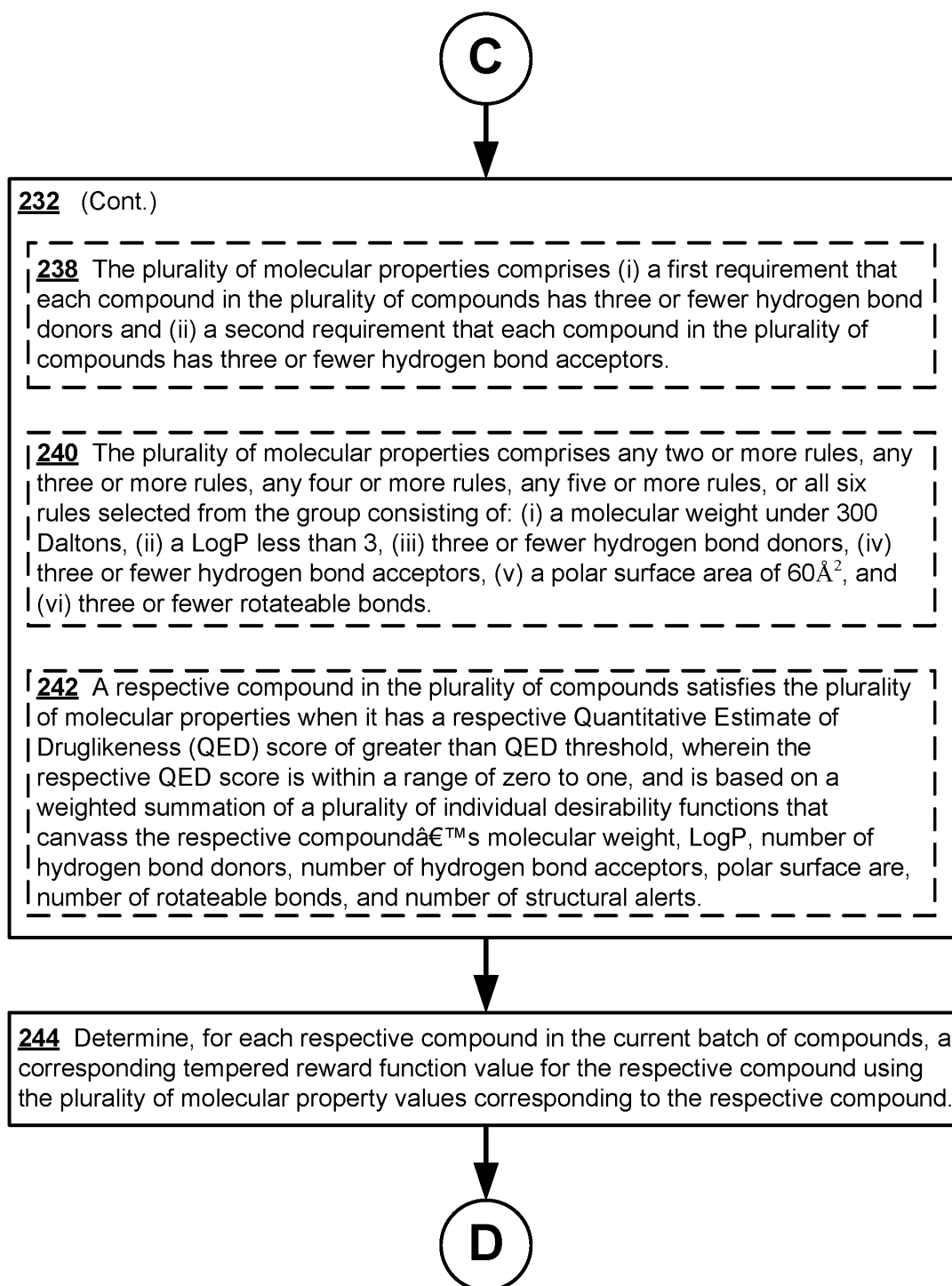


Fig. 2D

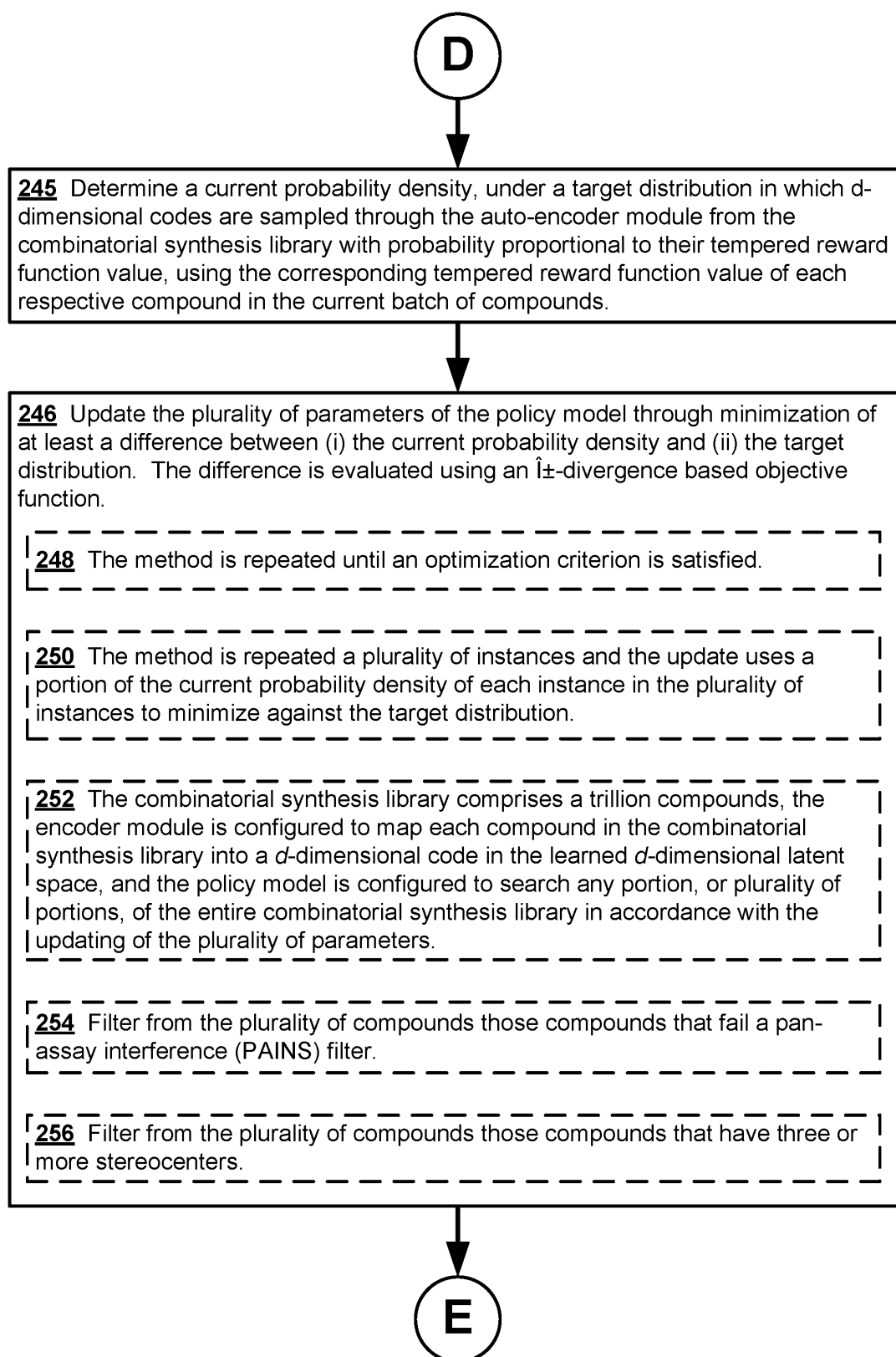


Fig. 2E



246 Cont.

258 Cluster the plurality of compounds based on structural similarity thereby forming a plurality of clusters and retaining, in the plurality of compounds, a subset of compounds in each cluster in the plurality of clusters.

260 Synthesize the plurality of compounds and test the synthesized plurality of compounds in a wet lab assay to determine whether they have bioactivity against a therapeutic target.

262 Synthesize the plurality of compounds and test the synthesized plurality of compounds in a wet lab assay to determine whether they have potency against a therapeutic target.

264 The therapeutic target is associated with a condition.

266 The condition is inflammation or pain.

268 The condition is a disease.

270 The condition is a cancer, hematologic disorder, autoimmune disease, inflammatory disease, immunological disorder, metabolic disorder, neurological disorder, genetic disorder, psychiatric disorder, gastroenterological disorder, renal disorder, cardiovascular disorder, dermatological disorder, respiratory disorder, viral infection, or other disease or disorder.

Fig. 2F

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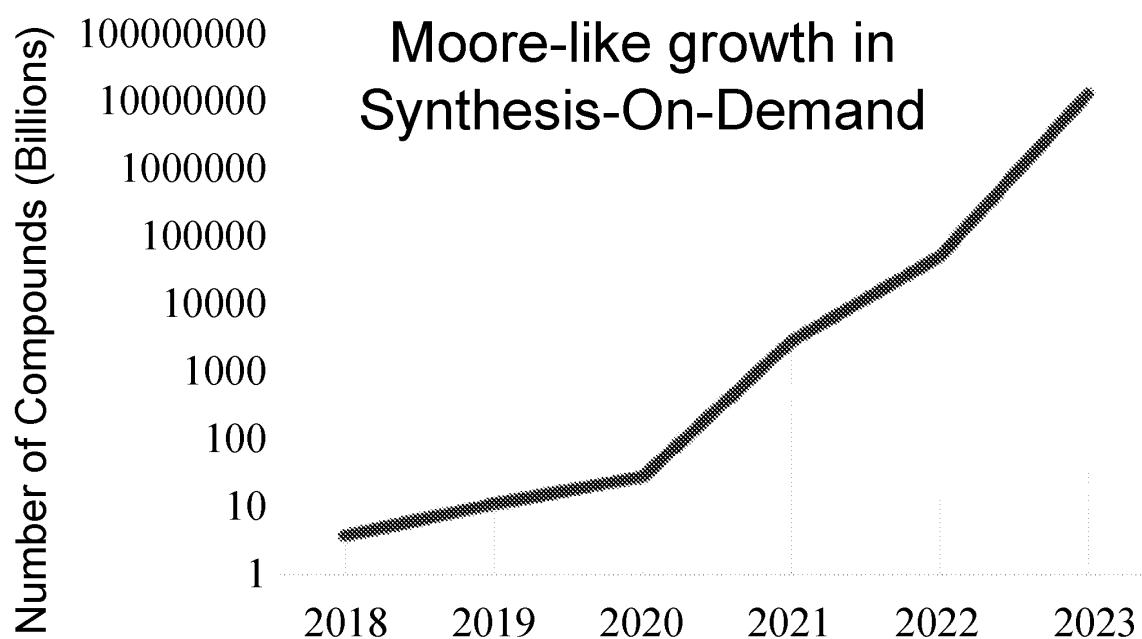


Fig. 3A
(Prior Art)

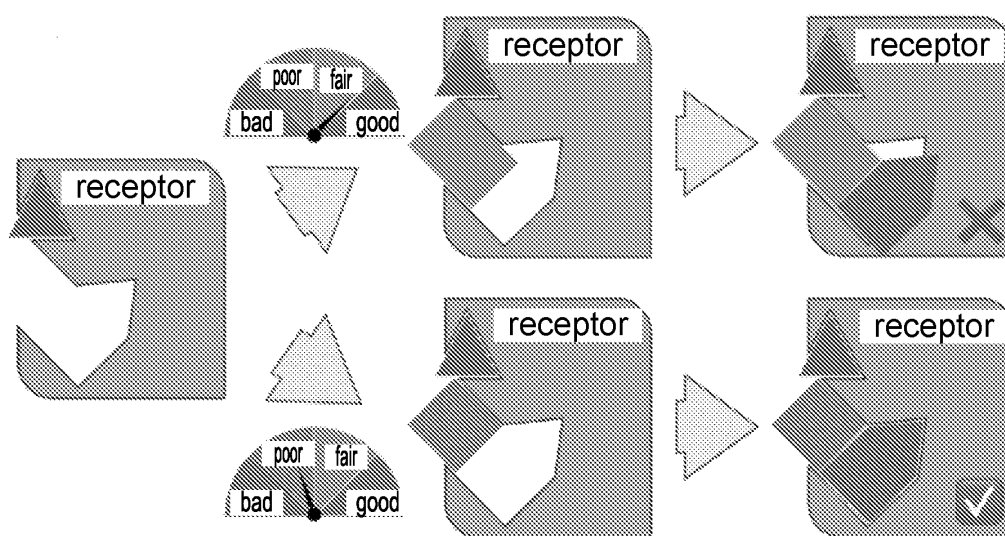


Fig. 3B
(Prior Art)

$$S(\triangle) + S(\diamond) + S(\nabla) \neq S(\triangle \diamond \nabla)$$

Fig. 3C
(Prior Art)

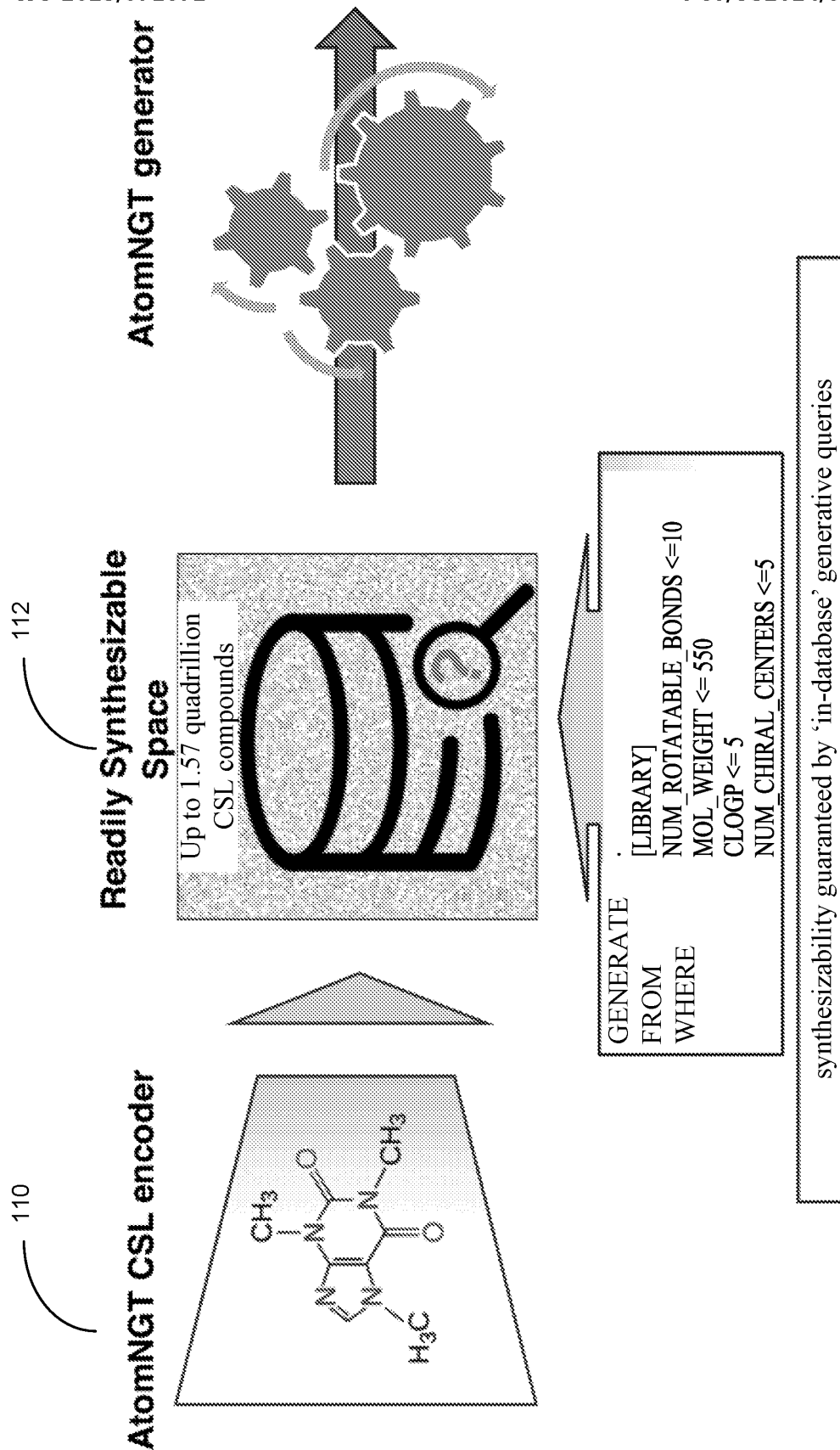


Fig. 4

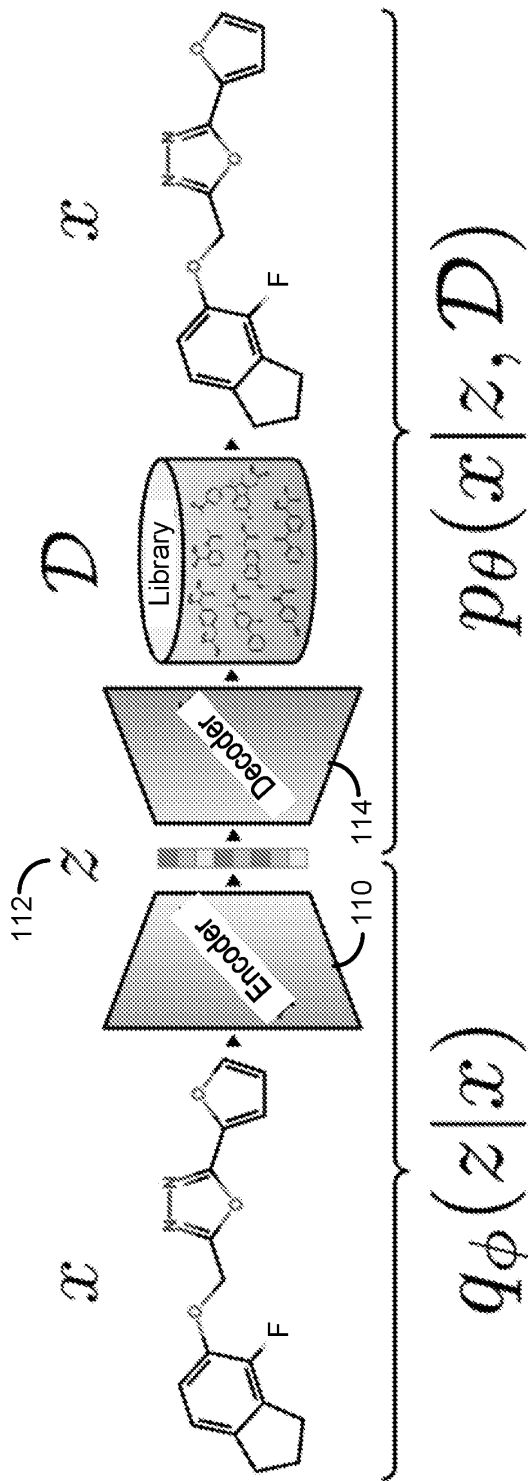


Fig. 5A

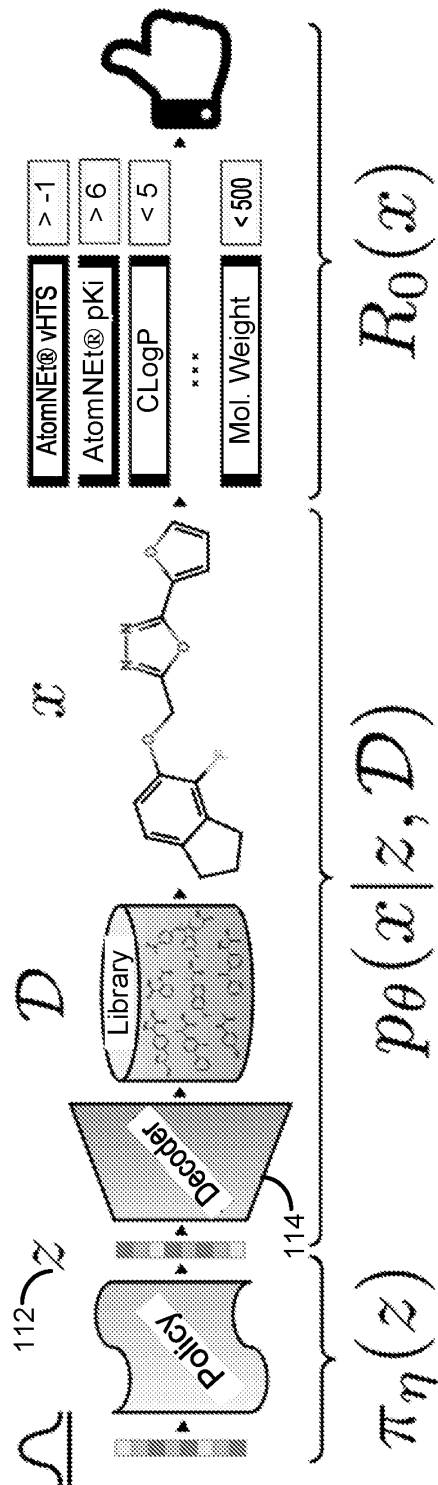
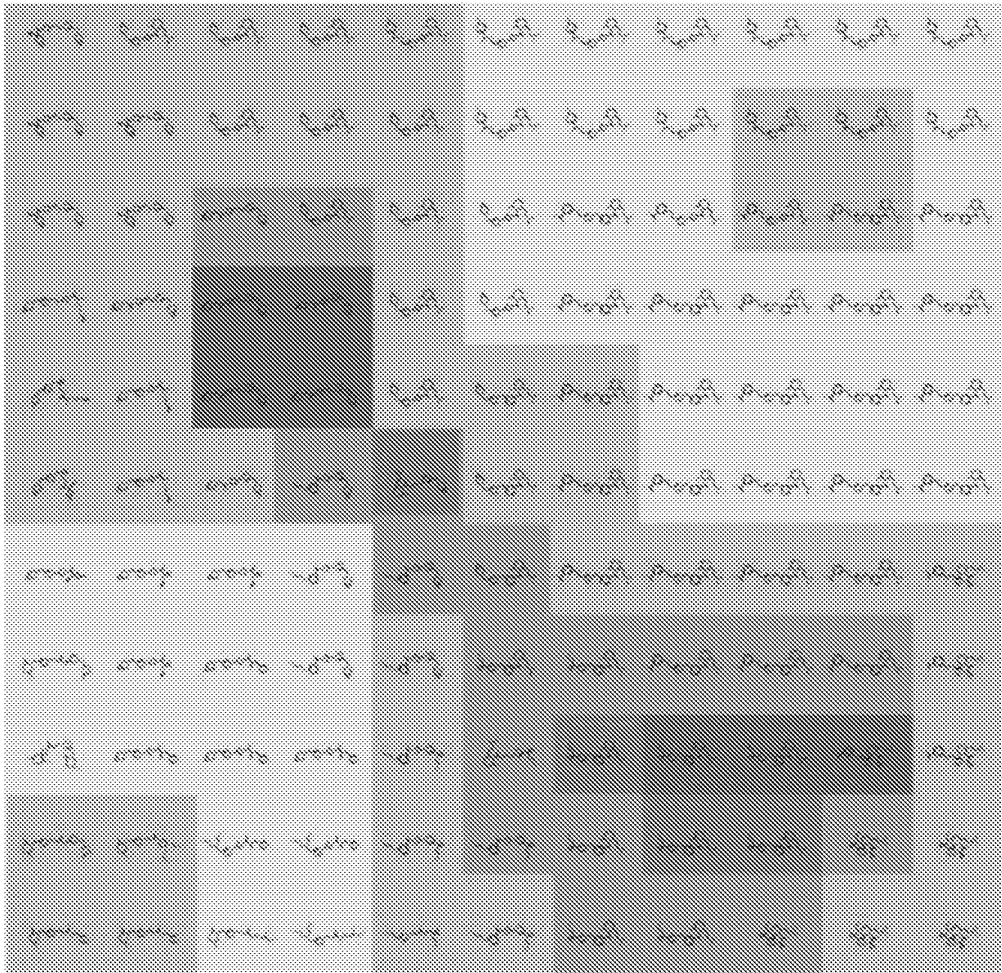


Fig. 5B



$$\pi_{\eta}(z) \propto \mathbb{E}_{p_{\theta}(x|z,\mathcal{D})}[R_0(x)]$$

Fig. 5C
SUBSTITUTE SHEET (RULE 26)

	Lipinski	Ghose	Lee	Rule-of-3	QED
Random (uniform)					
# satisfied clusters	223.4±9.5	189.8±21.9	2.2±1.3	0.2±0.4	7.2±2.6
% satisfied	2.27±0.09	1.92±0.21	0.02±0.01	0.01±0.01	0.07±0.03
Random (stratified)					
# satisfied clusters	1956.2±23.5	2075.8±23.2	30.6±7.3	0.8±0.6	121.8±10.5
% satisfied	29.47±0.43	31.51±0.46	0.40±0.03	0.02±0.02	1.36±0.10
HE (<i>k</i>=2000, <i>m</i>=20)					
# satisfied clusters	924.4±8.65	812.2±7.16	20.8±1.3	382.8±5.4	149.8±7.8
% satisfied	52.01±0.26	37.37±0.12	0.58±0.08	21.05±0.54	2.09±0.13
# evals	108,260	117,199	96,664	76,812	124,699
# capless evals	44,260	50,238	30,365	32,951	55,872
NGT (<i>α</i>=2, <i>i.i.d.</i>)					
# satisfied clusters	1504.6±29.2	1537.6±24.9	1251.4±47.5	119.6±2.6	992.8±26.7
% satisfied	26.61±0.37	20.46±0.33	17.57±0.44	11.15±0.18	23.87±0.36
% unique	98.40±0.21	99.82±0.02	99.56±0.03	67.34±0.11	97.80±0.14
NGT (<i>α</i>=2, <i>w/ d.s.</i>)					
# satisfied clusters	2705.8±21.7	4182.4±10.0	2490.4±17.5	156.2±6.8	1404.4±14.6
% satisfied	66.79±0.20	67.73±0.48	53.01±0.53	12.66±0.25	56.55±0.57
% unique	99.61±0.04	99.98±0.01	99.92±0.01	88.46±0.14	95.20±0.38

Fig. 6

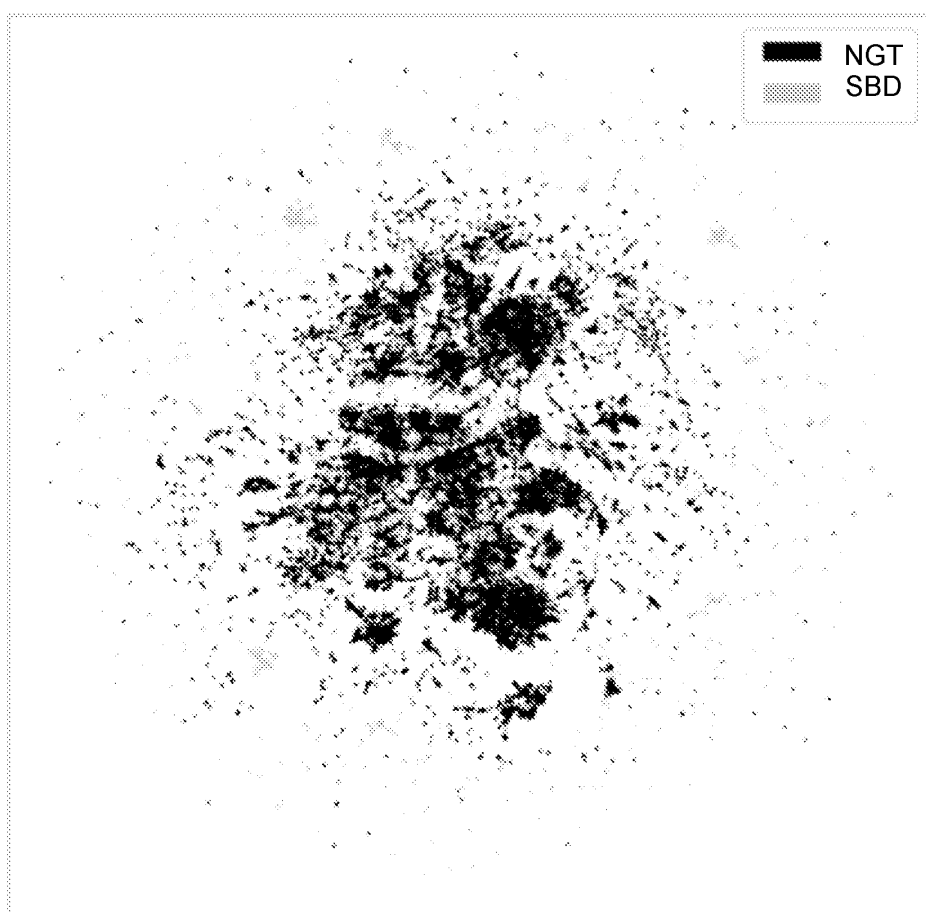
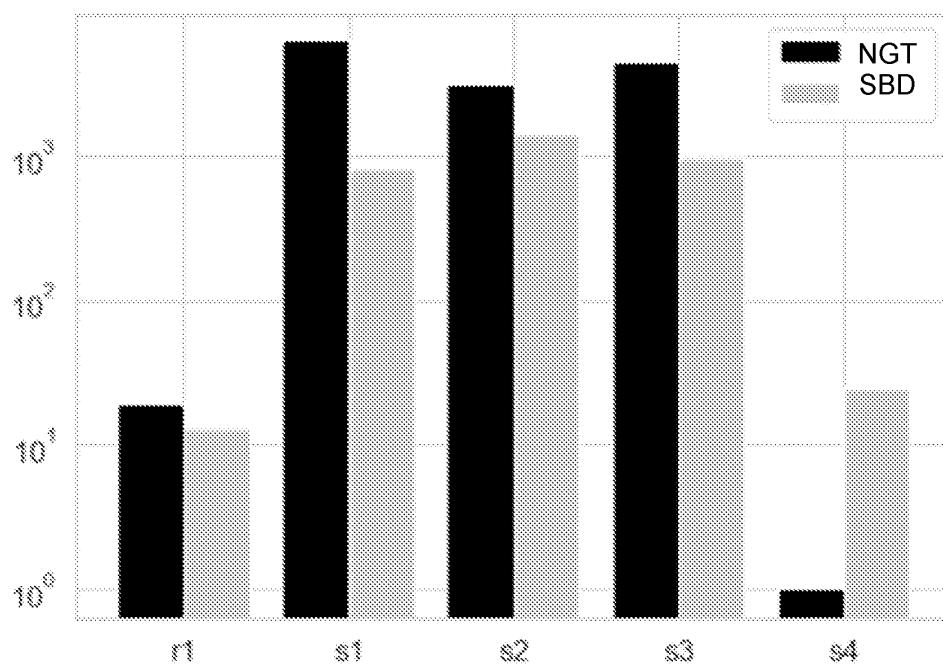


Fig. 7A

SUBSTITUTE SHEET (RULE 26)

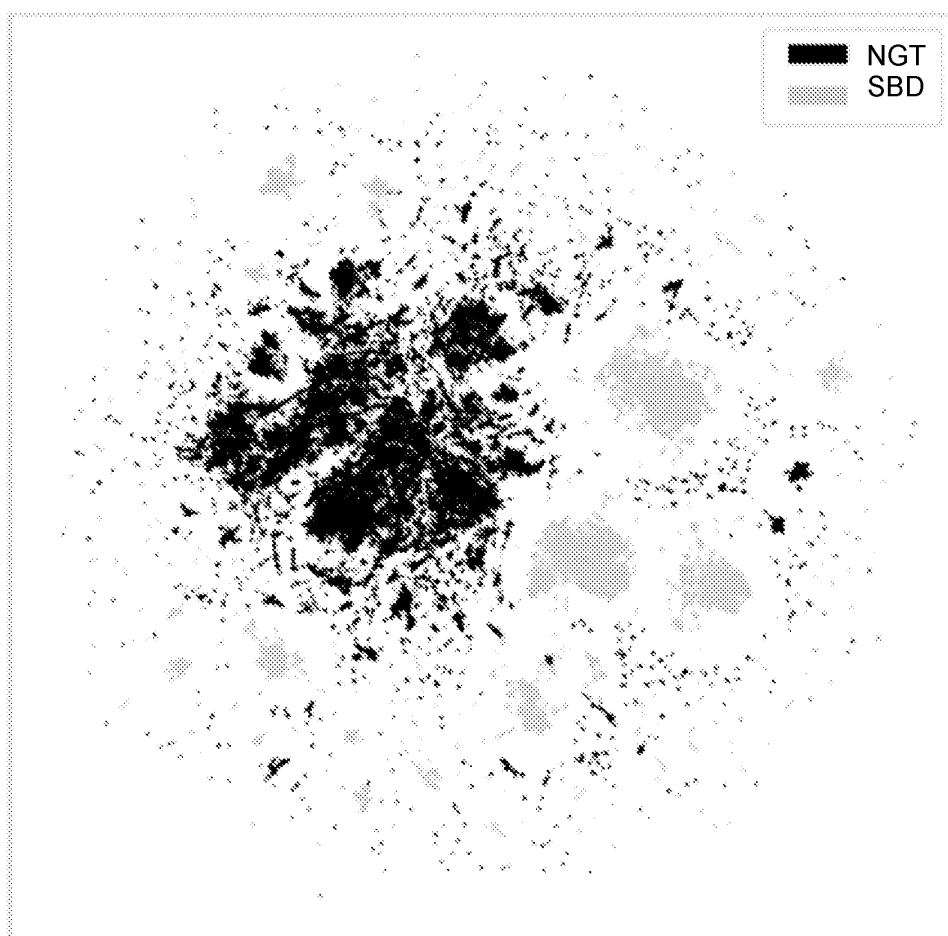
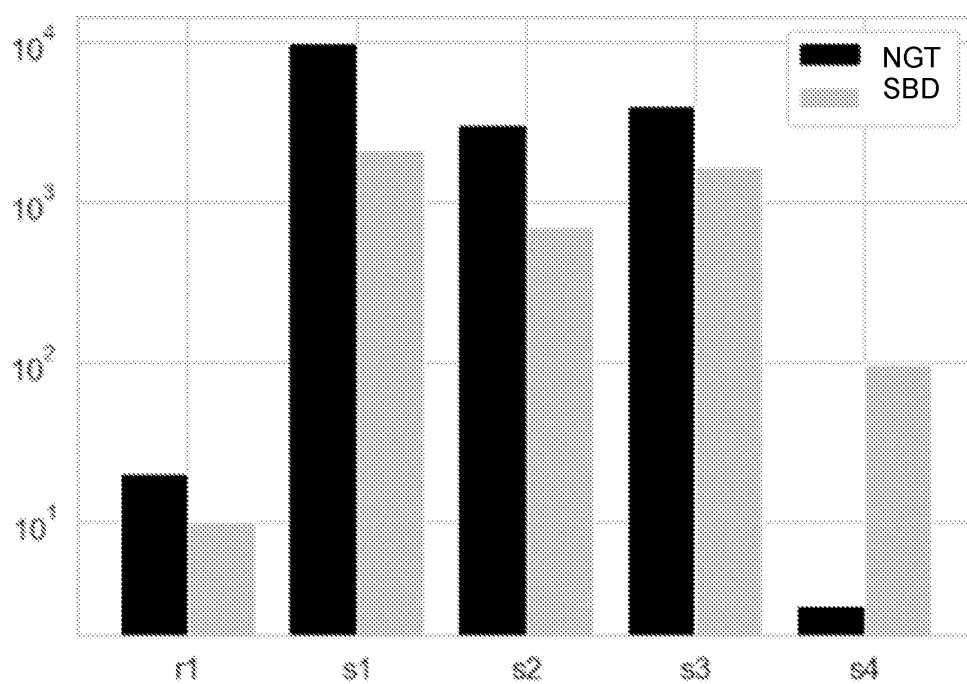


Fig. 7B

SUBSTITUTE SHEET (RULE 26)

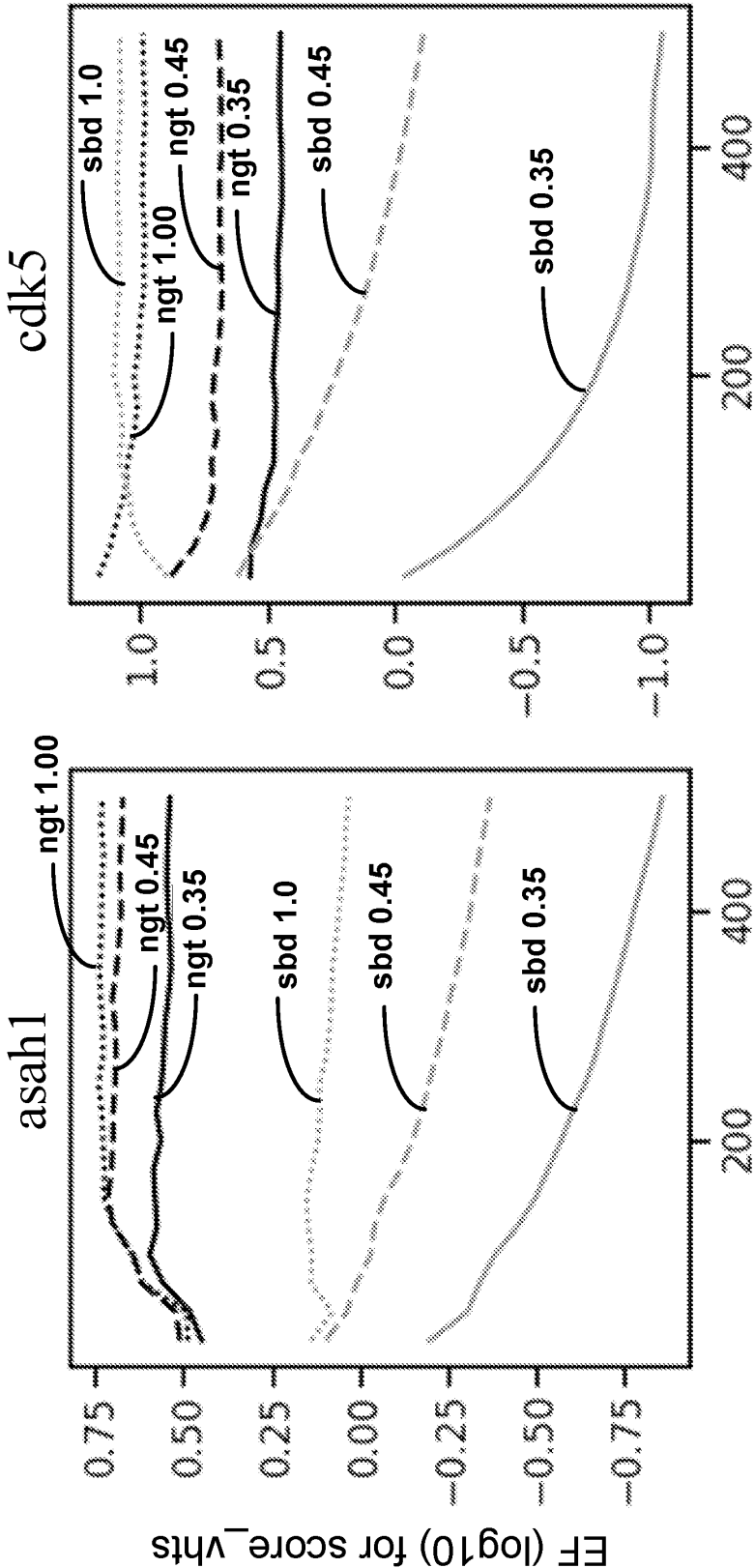


Fig. 7C

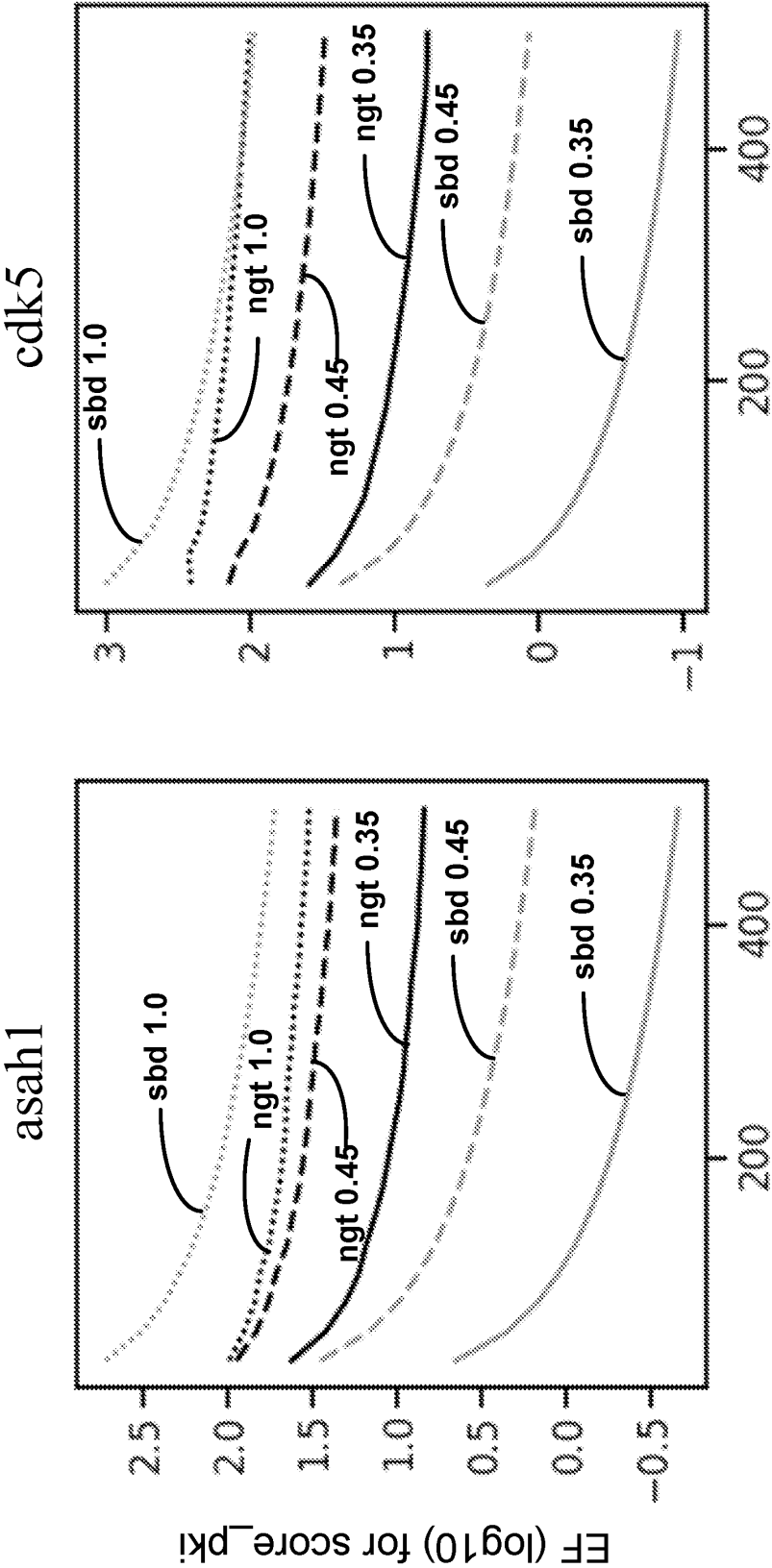


Fig. 7D

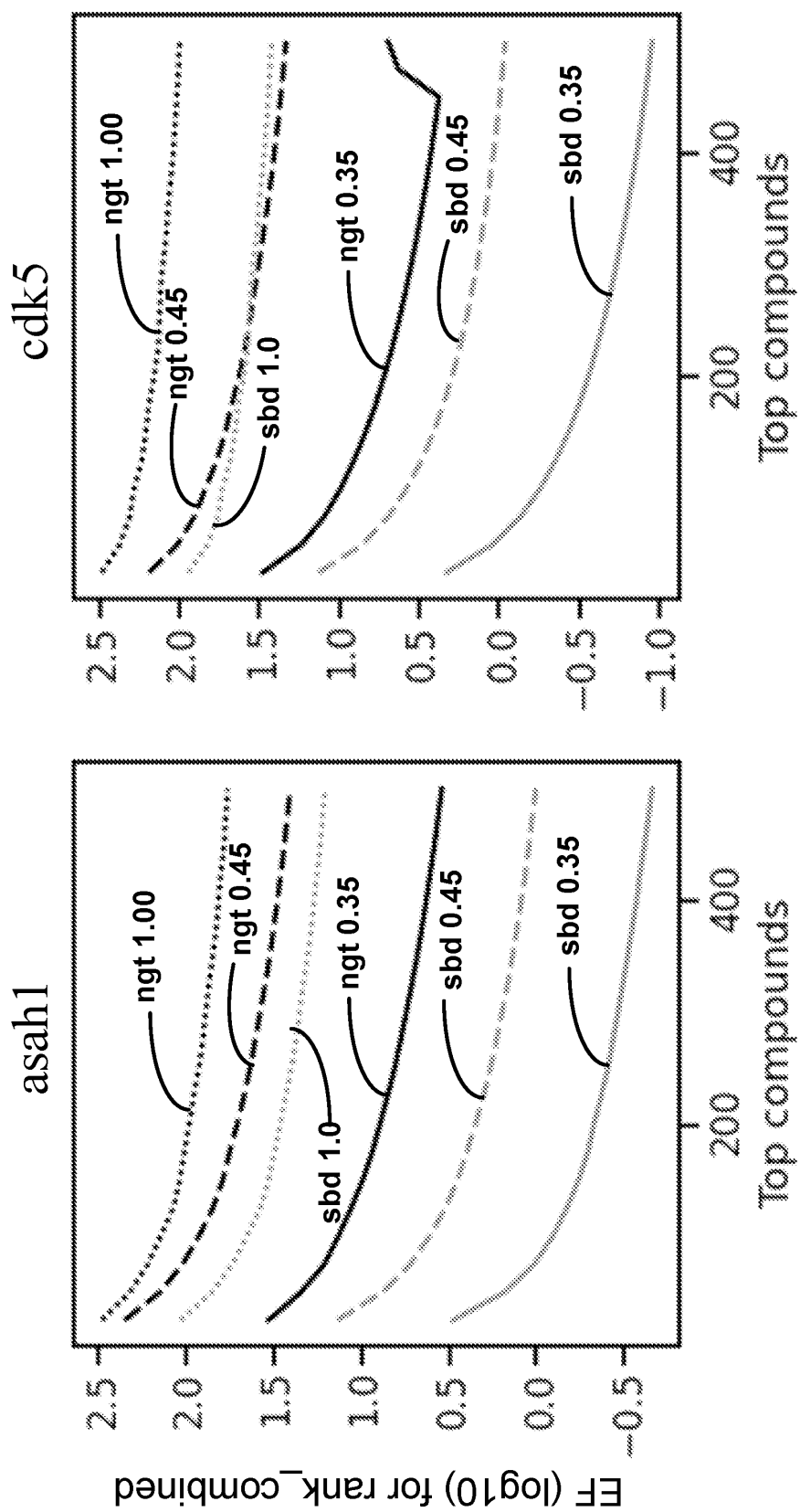


Fig. 7E



Fig. 8A
SUBSTITUTE SHEET (RULE 26)

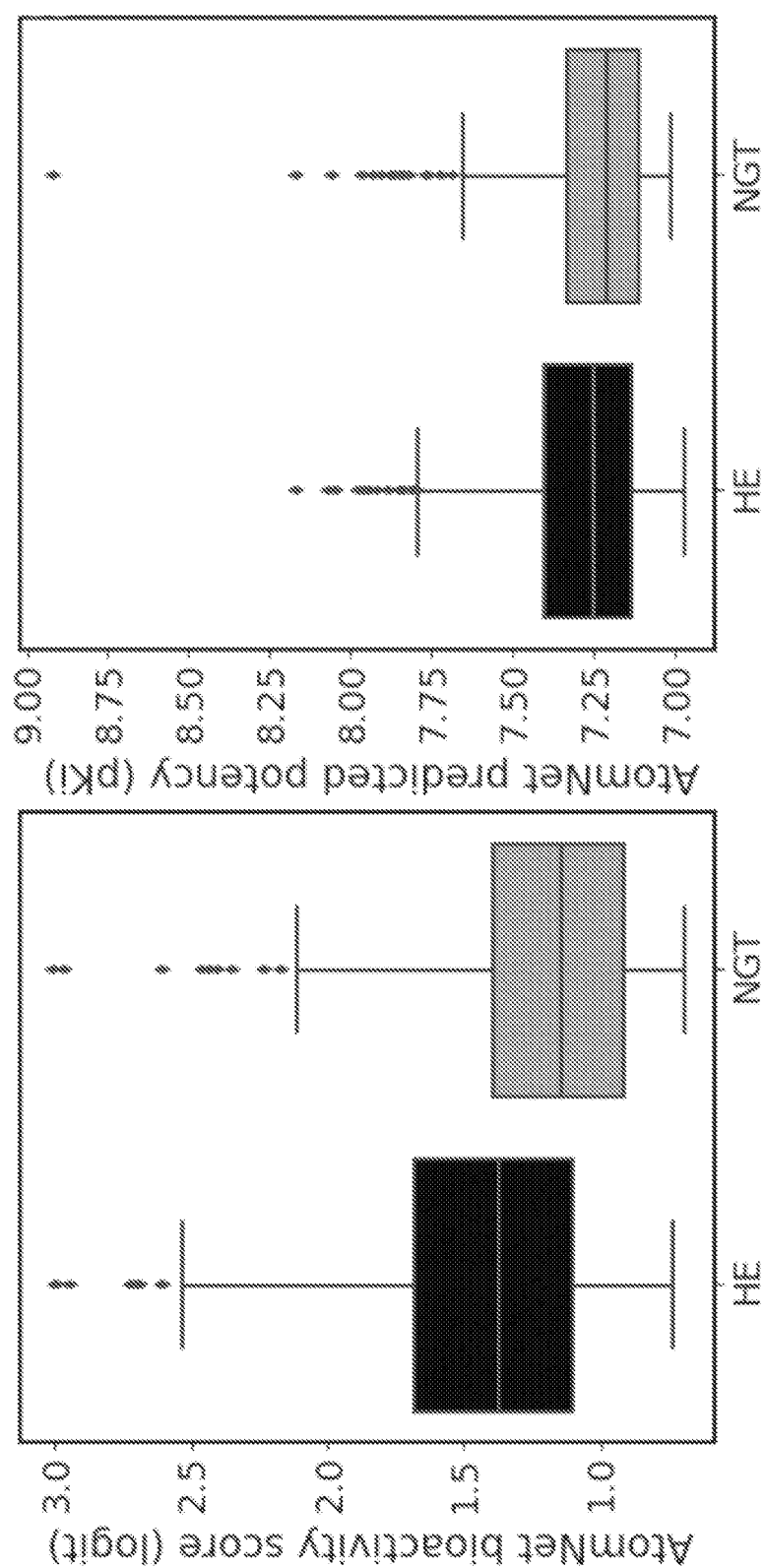


Fig. 8B

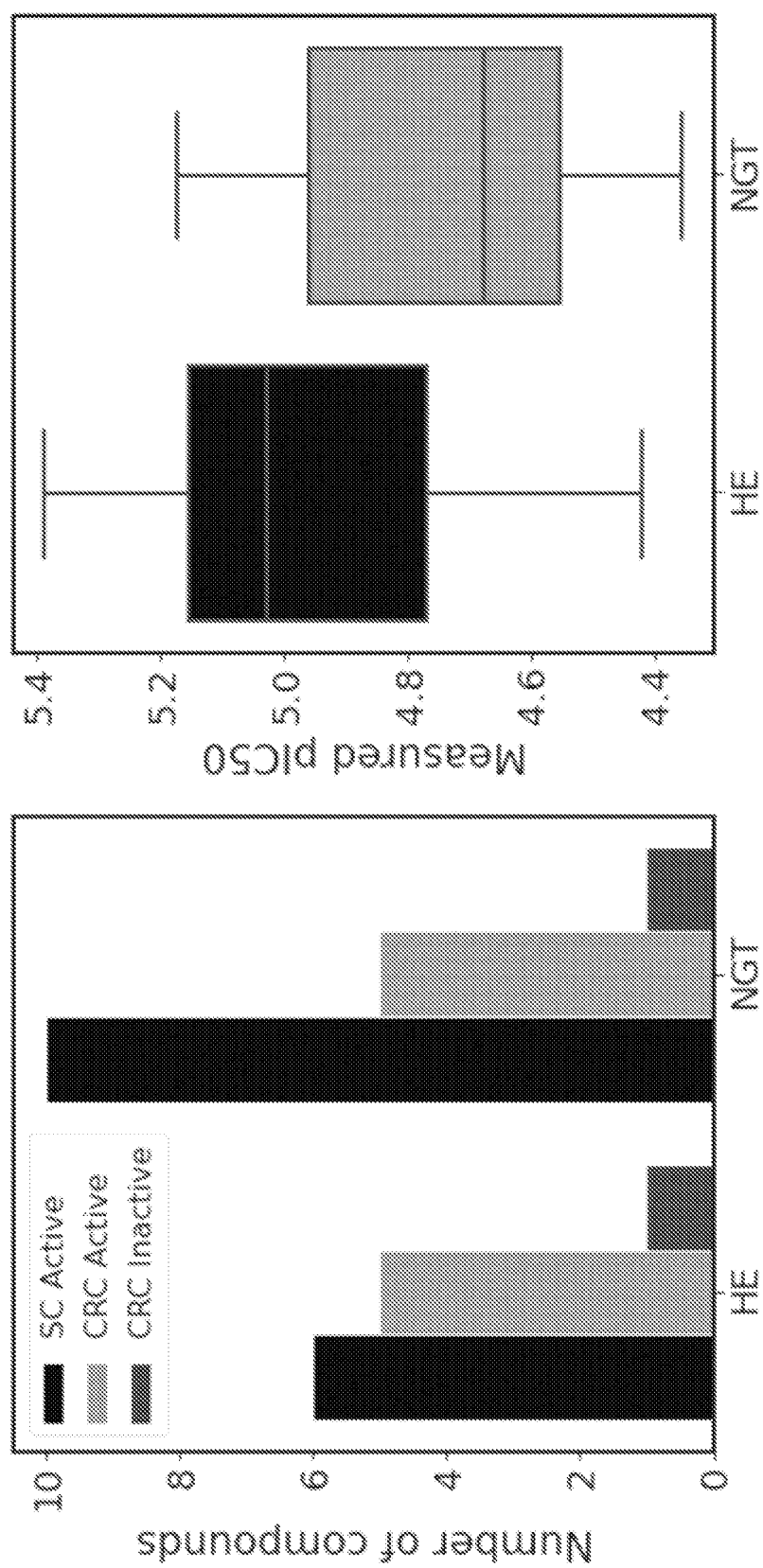


Fig. 8C

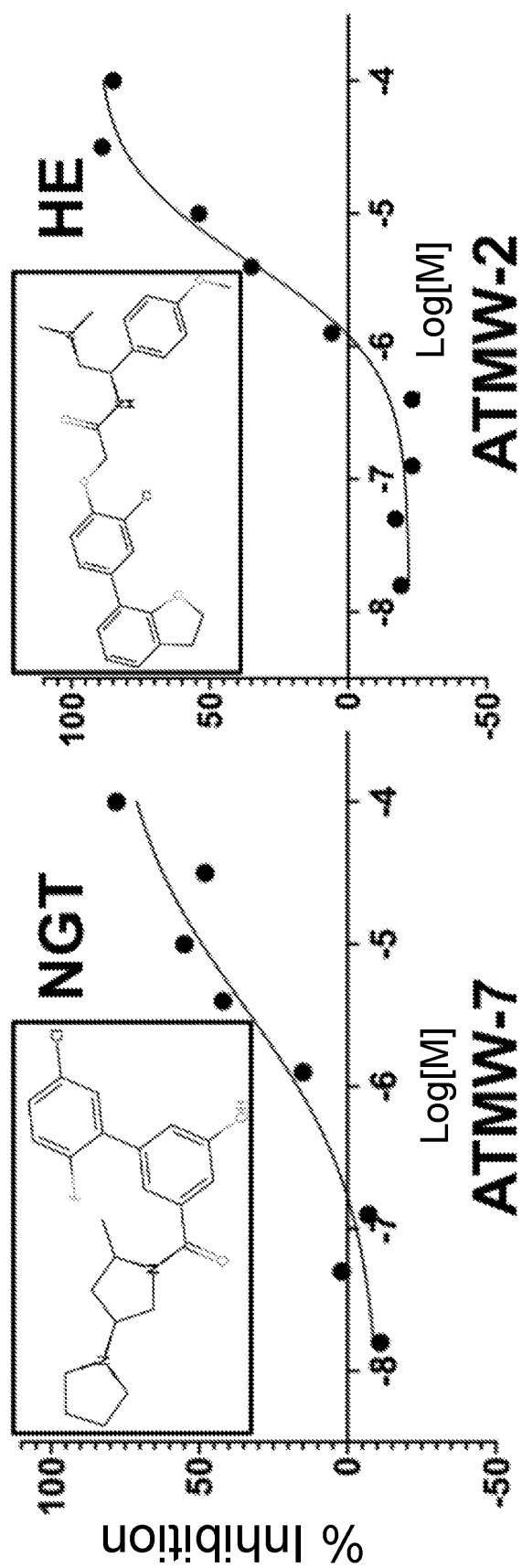


Fig. 8D

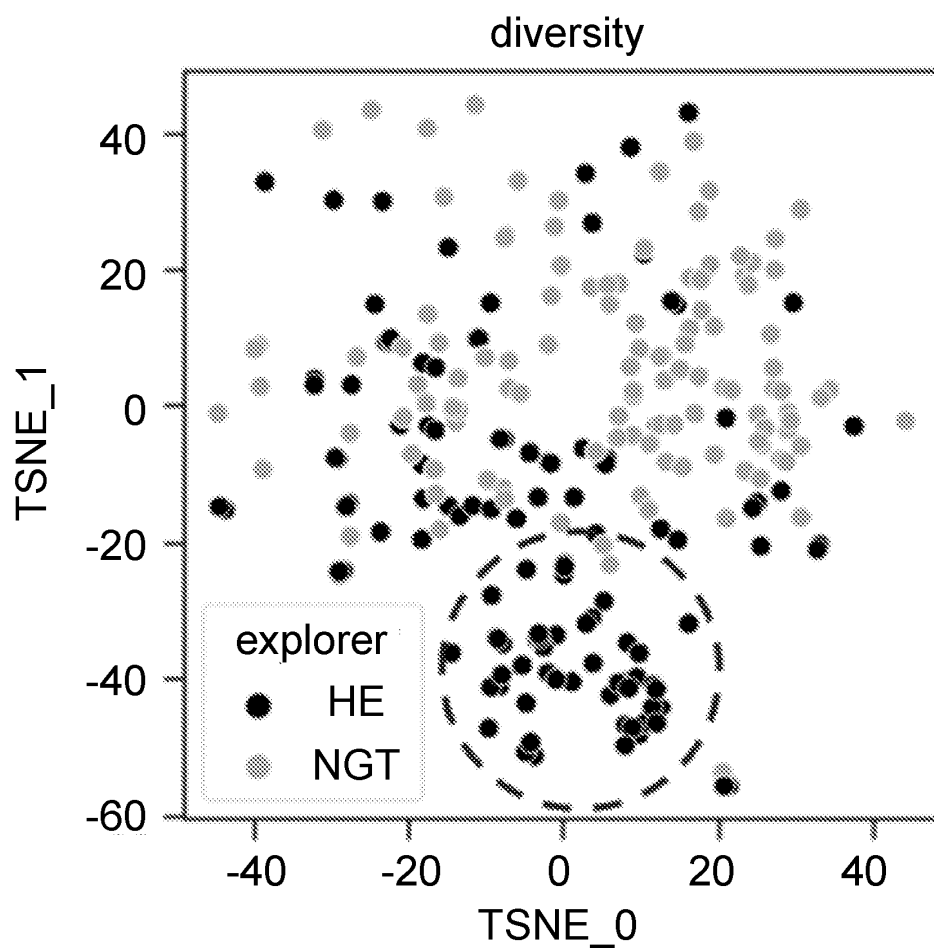


Fig. 8E
SUBSTITUTE SHEET (RULE 26)

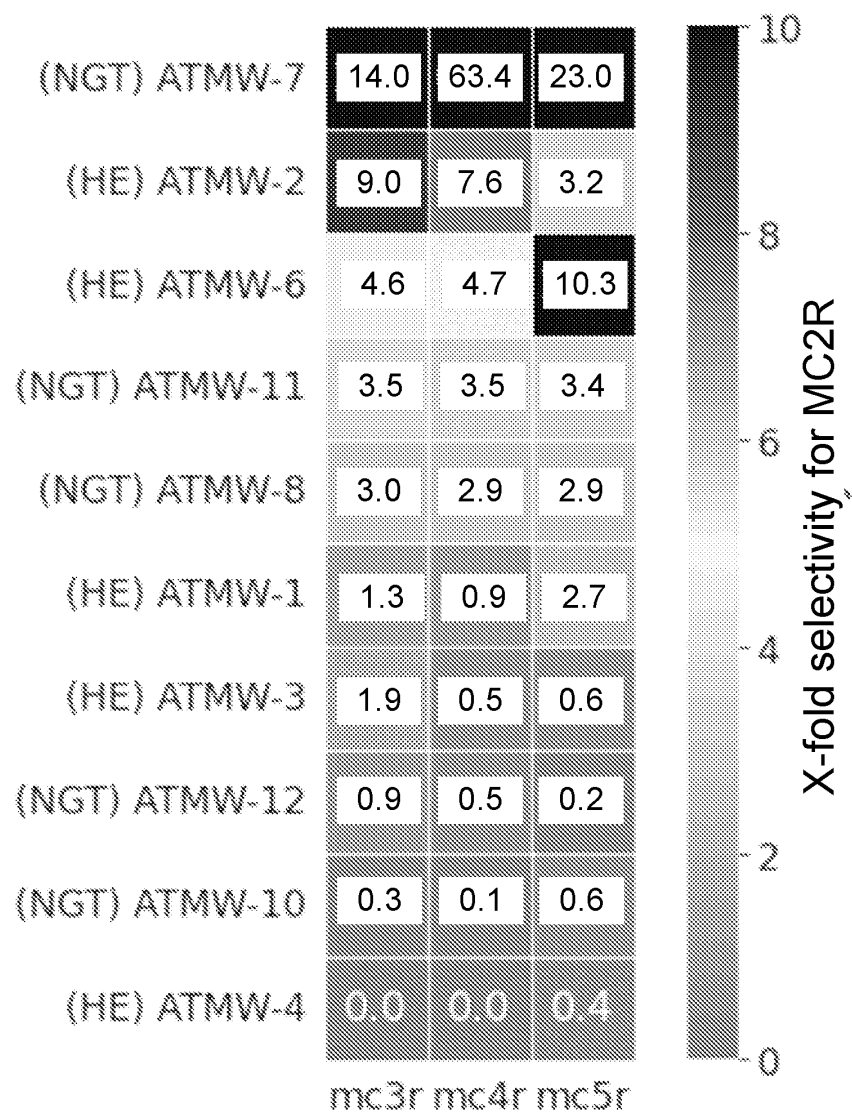
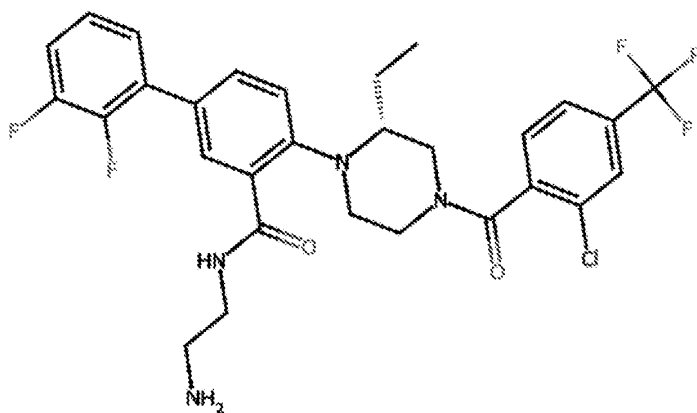


Fig. 8F

Fig. 8G
(Prior Art)

SUBSTITUTE SHEET (RULE 26)

```
def alpha_divergence(log_pi, log_reward, log_beta=None, alpha=2.0):
    # If behavior policy is unspecified, assume that it's on-policy
    log_beta = log_pi if log_beta is None else log_beta

    # Verify shapes, get batch size
    assert log_pi.shape == log_beta.shape == log_reward.shape
    n, = log_pi.shape

    # Get the log importance weights
    log_weights = log_pi - log_beta.detach()

    # Get the log (unnormalized) likelihood ratios
    log_ratios = log_reward.detach() - log_pi

    # Numerically stable estimator for the derived alpha-divergence
    logits = log_weights + alpha * log_ratios
    wavg = (logits.softmax(0) * log_ratios).sum(0)
    wlme = (logits - math.log(n)).logsumexp(0) / alpha
    return (wavg - wlme) / alpha
```

Fig. 9

	CDK5		ASAH1	
	NGT	HE	NGT	HE
Final Compounds	1,182,376	386,364	1,180,268	294,203
Compounds satisfying constraints	222,576	191,551	135,272	24,951
Taylor-Butina clusters				

Fig. 10

Property	Lipinski Rule of 5	Ghose	Lee	Rule-of-3	QED
Molecular Weight (MW)	< 500 Da	160 – 480 Da	–	< 300 Da	0.66
LogP	< 5	–0.4 – 5.6	–	≤ 3	0.46
Hydrogen Bond Donors (HBD)	< 5	–	≤ 3	≤ 3	0.61
Hydrogen Bond Acceptors (HBA)	< 10	–	≤ 3	≤ 3	0.05
Polar Surface Area (PSA)	–	–	–	≤ 60Å ²	0.06
Molar Refractivity	–	40 – 130	–	–	–
Total Number of Atoms	–	20 – 70	–	–	–
Rotatable Bonds	–	–	–	≤ 3	0.65
Number of Aromatic Rings	–	–	–	–	0.48
Number of Structural Alerts	–	–	–	–	0.95

Fig. 11

Compound	Provenance	MC2R	MC3R	MC4R	MC5R
ATMW-0168856 (10)	NGT	28	9	4	16
ATMW-0168991 (6)	HE	7	32	33	72
ATMW-0168987 (8)	NGT	11	33	32	31
ATMW-0168777 (2)	HE	4.1	37	31	13
ATMW-0168782 (3)	HE	17	33	8	10
ATMW-0168853 (11)	NGT	44	156	153	150
ATMW-0168922 (12)	NGT	21	19	10	4
ATMW-0168805 (1)	HE	38	50	36	102
ATMW-0168988 (7)	NGT	6.7	94	425	154
ATMW-0168760 (4)	HE	9.4	0	0	4

Fig. 12

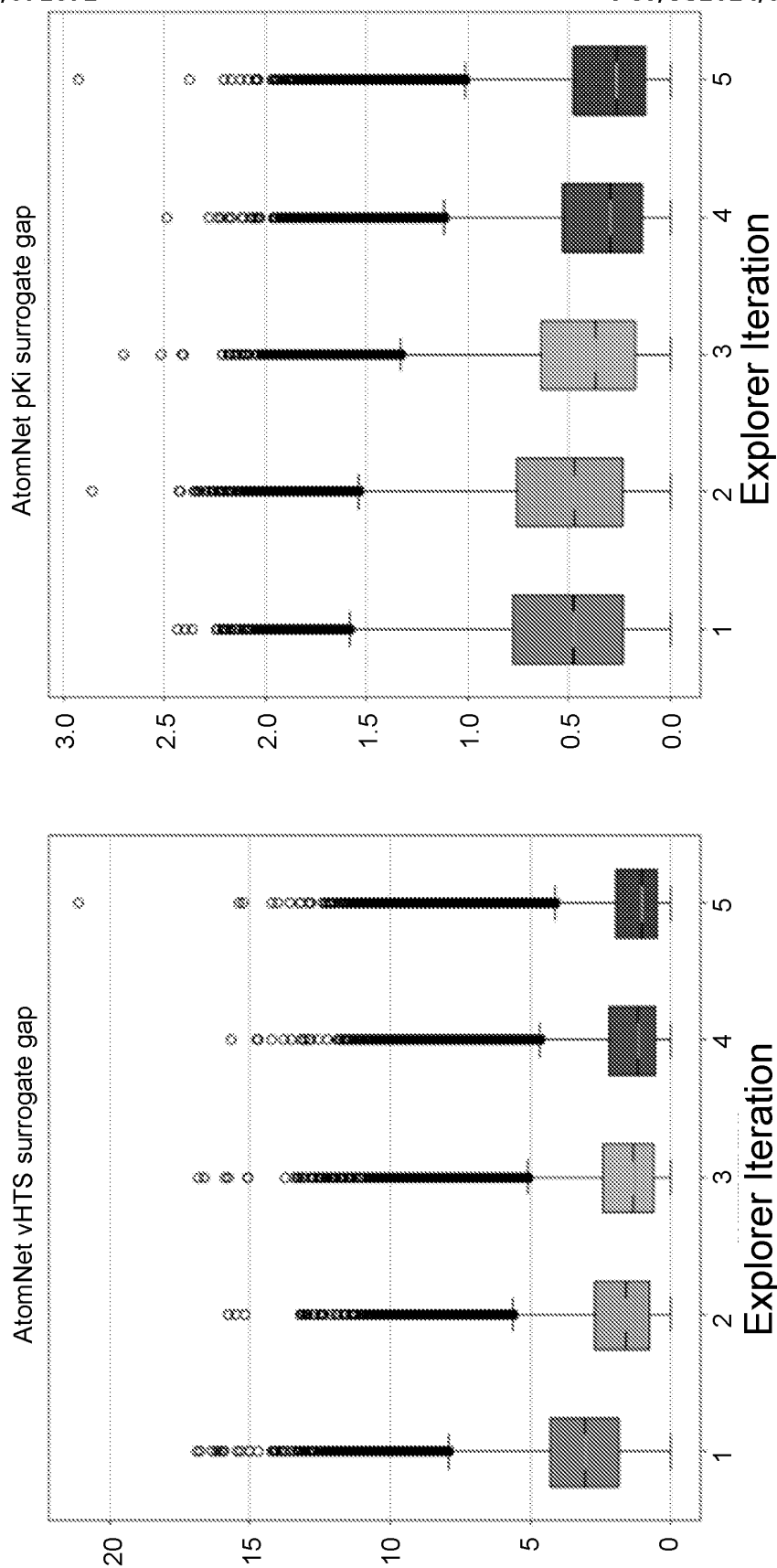


Fig. 13

(1)	(2)	(3)	(4)	(5)	(6)	(7)
1	HE	O=C(NCC(F)C(C1CC2(C1)CC21CCC1)N(C(=O)c1cc2c(cn1)CCCCC2)[C@H]1C[C@@H](N2CCCCC2)C1	60	T	CRC A 13	
2	HE	CCc1ccc(C(CN(C)NC(=O)COCc4c3OCC4jcc2C)cc1	76	T	CRC A 12	
3	HE	CCc1ccc(-c2cc(CN3CCN(c4ccc4C(N)=O)C3)c(OC)cc2F)sl	75	T	CRC A 14	
4	HE	CNc1cc(N2C[C@H](O)C[C@H]2CN2CC(c3ccc(-c4ccc(C5CC5)c4-c3)C2)ncn1	97	T	CRC A 1	
5	HE	CCc1ccc(-c2ccc(CC3CN(Cc4nc(C5CC5)no4)C3)c2)cc1C1	-111	T	CRC I 41	
6	HE	COCCN(C=O)C(C1CC2(C1)CC21CCC1)N(C(=O)c1cn(C)cn1)C1CCCN(c2cccc(C)c2)C1	72	T	CRC A 13	
7	NGT	CC1CC(N2CCCC2)CN1C(=O)c1ccc(-c2cc(C)ccc2F)cl	56	T	CRC A 55	
8	NGT	O=C1NCCO2ccc(CNCC3(c4ccc(C=C5CCSC5)s4)CCC3)cc21	75	T	CRC A 111	
9	NGT	CCn1ccc2c(NC3CCOC3)c(CNS(=O)=O)c3cc(C4=C(COC4)c(F)cc3C)c(C)nc21	-69	T	CRC I 65	
10	NGT	Cc1ccc(-c2cc(C)cc2)cc1(C(=O)NC2CN(C3CCCC3)C2)CC1	76	T	CRC A 43	
11	NGT	CCc1cc(Cc(-c2c(C)C(C(=O)NC3CCCN3CCCC)c(C)c2C)cc1C	52	T	CRC A 46	
12	NGT	CCCN1CC(NC(=O)[C@H]2C[C@H]2C[C@H]2c2ccc(-c3cc(C)ccc3OC)c2C)C1	83	T	CRC A 88	
13	NGT	CC(C)c1cc(S(=O)=O)NC2CCN(c3ccc3F)C2)ccc1-c1cn(C2CCCC2)n1	-70	T	SC A 83	
14	HE	CNC(=O)C(C1=Cc2cc(C)ccc2OC1)N(C(=O)COCc1ccc1F)C1CCN(C2CC2)CC1	69	T	SC A 13	
15	NGT	CCCN(S(=O)=O)NC(CO)c1ccc(-c2cc(C)c(Cc2C)cc1C(F)F	68	T	SC A 92	
16	HE	CN(C)[C@H]1CCCC[C@H]1N(C)C(=O)CCOc1ccc(C)cc1-c1ccc2c1OCCCC2	66	T	SC A 9	
17	NGT	CCc1ccc(C=C2CCCC2)cc1C1(C(=O)NCC(c2cn(C)nn2)N2CCCC2)CC1	65	T	SC A 80	
18	HE	CC(C)N1CCCC(C(=O)N(C)C2(c3ccc3)CC2)C(C(=O)NC2CCCC2)C2CC3(C2)CC32CCCC2)C1	64	T	SC A 13	
19	NGT	CC(NS(=O)=O)c1cc(C=Cc2ccc(C)ccc2)nn1C1c1ccc(SC(F)F)cc1	60	T	SC A 91	
20	HE	Cc1ccc(C(C(=O)NCC(C)N(C(=O)C2CC(c3ccc(C)cc3)C2)C2CCN(C3CC3)CC2)ncn1	58	T	SC A 13	
21	NGT	CC(C)c1cc(-c2c(F)ccc(S(=O)=O)NC3CN(C)C4(CCCC4)C3)c2F)ccc1O	56	T	SC A 0	
22	NGT	CCc1ccc(-c2cc(F)c(C)cc2C)cc1C1(C(=O)Nc2mme(C3CCCC3)nh2)CC1	55	T	SC A 100	
23	HE	CC(=O)NCCC(=O)N(C1CCN(C2CCCC2)C1)C(C(=O)Nc1ccc(F)cc1)C1CC2(C1)CC21CCC1	54	T	SC A 13	
24	NGT	Cc1cc(-c2cc(S(=O)=O)NC(C)c3c(C)nn(C)c3C)cc(C)c2C)ccc1F	53	T	SC A 2	
25	NGT	Cn1ccc1[C@H]1CN(C(=O)c2cc(C)cc(C(=O)C3CCCC3)c2F)C1C[C@H]1CN(C(=O)C1CCC1	52	T	SC A 50	
26	NGT	CCc1ccc(C(C)(C)C(=O)N2CCCC(CNS(N)=O)=O)C2)ccc1C=C(C)CC1CCC1	51	T	SC A 54	
27	NGT	CCCN(C)S(=O)=O)N1CCCC(C2(c3ccc(-c4cc(C)ccc4O)cc3)CC2)C1	-51	T	SC A 13	
28	HE	CCc1nccn1CC(C)NS(=O)=O)c1ccc(-c2cc(C)cc(C)cc1C	50	T	SC A 2	
29	NGT	CCCN(CCN1CCCCC1)C(=O)c1cc(C2=CCCCC2)c(F)cc1O	50	T	SC A 51	
30	NGT	Cc1ccc(CCC(=O)NCC2CCC3(CCC3)CN2C)c(-c2cn(C)C(C)c2F)cl	50	T	SC A 110	
31	HE	Cc1c(C)ccc1-c1cc(C(=O)N(C)C[C@H]2CCCC[C@H]2NS(=O)=O)C2CC2)ccc1F	48	F	SCI 35	
32	HE	CCCCN(C(=O)C1CN(C(C)CCO1)C(C(=O)NC1CC(F)C1)c1ccc2ccc(O)cc12	47	F	SCI 13	
33	NGT	Cc1cc(S(=O)=O)NCC(C)Cn2ccc2C)cc(-c2ccc(O)c(C)cc2)c1C	47	F	SCI 2	
34	HE	CCc1cc(F)cc(-c2ccc(CCS(=O)=O)NC(C)CN3CCCC3=O)cc2cl	-46	F	SCI 36	
35	HE	CNC(=O)N1CCCC(NS(=O)=O)c2cc(C)c(Cc(-c3ccc(COC(C)C)c3)c2)CC1	44	F	SCI 2	
36	HE	CCNC(=O)N1CCN(C(=O)c2ccc(-c3ccc(C)c(C)cc3)c2C)CC1	43	F	SCI 13	
37	NGT	Cc1cc(C)c(-c2cc(S(=O)=O)NCC(C)C(C)Cn3ccc3)c(C)cc2C)cc1C	43	F	SCI 113	
38	NGT	Cc1ccc(-c2ccc3c(c2)CCC3N2CCN(S(=O)=O)c3c(C)nn(C(F)F)c3C)CC2)ccc1O	-43	F	SCI 87	
39	NGT	Cc1nc(C2CCCC(C(=O)c3ccc(F)c(-c4cc(C)ccc4F)c3)C2)nh1	40	F	SCI 55	
40	NGT	Cc1cc(C)c(S(=O)=O)NC2CCCCN(C)C2)cc1-c1cc(C)cs1	39	F	SCI 90	
41	HE	CC(C)N1CCOC(C(=O)N(C)C2CCCCC2)C(C(=O)NC2CCCC2)c2cccc(C(C)(F)c2)C1	38	F	SCI 13	
42	NGT	O=C(c1ccc2ccc(F)ccc2nc1-c1ccc(CN2C(C)O)cc1)N1CC(C)C23CC(C2)C3)C1	38	F	SCI 99	
43	HE	CC1ccc(-c2cc(C)c(SCC(=O)NC3CN(C)CC3c3ccc3)cc2C)cl	37	F	SCI 32	
44	HE	CC(C)nc1cc(S(=O)=O)N2CCN(c3cccc3-c3cc(O)cc(C(C)C)c3)CC2)cn1	-37	F	SCI 2	

Fig. 14A

[illegible]

Fig. 14C

(1)	(2)	(3)	(4)	(5)	(6)	(7)
335	NGT	Cc1c(C=CCO)cccc1C1(C(=O)N2CCN(S(=O)(=O)N3CCC(C)CC3)CC2)CC1	-10	F	SCI	58
336	NGT	O=C(c1cc(F)c(O)cc1-c1cc(CN2CCCC2)ccc1F)N1CCCC1C1CCCC1	-10	F	SCI	109
337	NGT	Cc1cc(-c2cc(S(=O)(=O)NC3C4(CCN4C)C3)cc(C)c2C)ccc1C	-10	F	SCI	2
338	HE	CNN(C)C(=O)N1CCN(C(=O)C2(-c4ccc(-c5ccc5)cc4)ccc3)CCC2)CC1	9	F	SCI	33
339	NGT	CCC1CN(C(=O)c2cc3c(cc2C=CCe2cInH)lc2)n(C)c(=O)n3C(C)CC)CN1Cc1cccc1	9	F	SCI	56
340	NGT	O=C(NC1CCN(c2cccc2-c2cnc(N3CCCC(O)C3)nc2C1)C1CC2(CCC2)C1	9	F	SCI	84
341	NGT	CC(=Cc1cc(C(=O)NC2C3C=CCN2CCC3c(C)c(S(N)(=O)=O)c1)C1CC1	9	F	SCI	13
342	HE	Cc1nccc(C(=O)NO)N(C)CC2ccc(O)c(C1)c2C(=O)CC(C)C1c1C	9	F	SCI	13
343	HE	CCC(CN(C(=O)c1ccc(C#CC2CC2)cc1)C(C(=O)NC(C)C1(n2ccnn2)CC1))N1CCCC1	9	F	SCI	22
344	NGT	Cc1cc(-c2cc(S(=O)(=O)N3CC(N4CCCC(C(F)F)CC4)C3)cc(C)c2C)c(F)cn1	9	F	SCI	22
345	HE	Cc1ccc(CNC2CCN(c3ccc4nn4n3)C2)c(F)c1C=Cc1cc(F)cc(F)c1	-9	F	SCI	17
346	HE	Cc1nnc(C)cc1C(C(=O)NC1CCG1)N(C)C1(N(C)CCS1)C(=O)c1cc(C)c(C)c(C)c1	-9	F	SCI	63
347	NGT	CCC(C)C(C)C(NS(=O)(=O)c1cc(C)CC(C)C)CCc1C1CC2	-9	F	SCI	13
348	NGT	Cc1ccc(O)c(-c2ccc3c(c2O)CCN(CC(=O)N(C2CC2)C2CCS(=O)(=O)C2)C3)c1	-9	F	SCI	73
349	NGT	CC1c2cc(C)ccc2CCN1C(=O)c1cc2c(c(-c3ccc4g(c3)NCCNC4=O)c1)OCCO2	-9	F	SCI	79
350	HE	CNN(C)C(C)C(C(=O)NO)N(C)CC1ccc2c(c1)CCO2C(=O)c1cc2c(cn1)CCC2	-9	F	SCI	27
351	HE	Cc1nnc(C)cc1C(C(=O)N3C1CC1)N(C)C1(N(C)CCS1)C(=O)c1cc(C)c(C)c1	-9	F	SCI	13
352	HE	Cc1cc(-c2ccc(C(=O)CCC(=O)N3C3cccc3N3C1[C@@H](O)C3)ccc2)c(F)cc1F	8	F	SCI	20
353	HE	CC(C)C(NC(=O)C(C1CCOCC1)N(C(=O)c1nInH)lc2ccc(Cl)cc12)C1CCN(CC2CC2)CC1	8	F	SCI	25
354	NGT	Cc1m(-c2ncc2)cc1-c1ccc1S(=O)(=O)N1CCN(C)C1c2cccc2)C1	8	F	SCI	77
355	HE	Cc1cc(-c2cc(C(=O)N3CCC(N4CCN(C)C)CC4)C3)c(Cl)c([N+](=O)[O-])c2)ccc1Cl	-8	F	SCI	43
356	HE	CNC(=O)c1cc(C)cc(C)c1)N(C(=O)CC(C)C1CCCC1)N(C)C1ccc(OC)c(O)c1	-8	F	SCI	44
357	NGT	CCCN(CCC)S(=O)(=O)N1CCN(C(=O)c2c(C)c(C=Cc3ccc(O)ccc3)c(C)c2C)CC1	-8	F	SCI	49
358	NGT	Cc1cc(NC(=O)C2CC3CN(c4cccc4)CC3C2)ccc1C=C1CCCCS1	-8	F	SCI	47
359	NGT	Cc1nccc(-c2ccc(CN(CCN(C)C)CC3CCN(c4c(F)ccc4F)C3=O)cc2)c1C	-8	F	SCI	97
360	HE	CCC(CN(C(=O)c1ccc(C#CC2CC2)cc1)C(C(=O)NC)C1(n2ccnn2)CC1)N1CCCC1	-8	F	SCI	22
361	NGT	Cc1nccc(-c2cc(C)ccc2F)c(C)C1CNC(=O)C1CC2(C)CS(=O)(=O)C2	7	F	SCI	2
362	NGT	Cc1nccc(-c2cc(C(=O)N3C1C@H14C1C@H1O)C1C@H14C3)cc(C)c2C)cc1C	7	F	SCI	2
363	NGT	Cc1m(C)C)cc1-c1(F)ccc2c1N(C(=O)C)C(NS(=O)=O)c1c(C)nn(C)c1C(C)C2	7	F	SCI	0
364	NGT	CN(C)CCN(Cc1ccc(-c2ccc(-n3ccc3)ccc2)cc1)C1CCN(c2c(F)ccc2F)C1=O	7	F	SCI	97
365	HE	C1CN(=O)C(C2CC(C(F)F)CC2)N(C(=O)CCn2cnn2)C2CCN(C3CCCC3)C2)CC1	7	F	SCI	13
366	HE	CCC(NC(=O)C1CC(C)CCCC1)c1cc(F)cc(C2=CCOC2)c1	-7	F	SCI	0
367	HE	Cc1cc(C#N)cc(C)c1C(C(=O)NC1CCCC1)c1cc(C)cc(C)cc1)C(C)CN1CCCC1	-7	F	SCI	28
368	HE	Cc1ccc(-c2ccnc(C(=O)NCC3(N4CCOCC4)CCN(C)CC3)c2F)cc1C	-7	F	SCI	13
369	HE	Cc1cc(NC(=O)C2(CN(C)C)CCCC2)cc1-c2cn(C)C(C)Cnc2C)c1	-7	F	SCI	0
370	HE	Cc1m(C)C)cc1-c1ncc2cccc2c1NCC1CCCC1N1CCN(C)CC1	-7	F	SCI	0
371	NGT	Cc1c(C=CC(C)O)cccc1S(=O)(=O)N1CCn2cnn2C2CC2(C)C)C1	-7	F	SCI	60
372	NGT	CNN1CCCC1CN(Cc1ccc(O)cc1)C(=O)CCn1cc(-c2ccc(N)cc2F)c(C)n1	-7	F	SCI	2
373	NGT	CCCN1CC1C1S(=O)(=O)NC1CCS(=O)(=O)c2ccc(C3=CCC(F)C3)cc21	-7	F	SCI	95
374	HE	Cc1cc(C)cc(-c2ccc(C3(C(=O)N)CC45CCCC(N)CC4)C5)CCC3)cc2c1	6	F	SCI	13
375	HE	CNNC(=O)C(c1ccc1)N(C(=O)C1CC2CC(C)C2)c1C1CCN(C2CCCCC2)CC1	6	F	SCI	13
376	NGT	Cc1c(C=CC(C)C)cccc1S(=O)(=O)NC(C)C)C1(CO)CC=CC1	6	F	SCI	66
377	NGT	Cc1nd(S(=O)(=O)N2CCCC(C)C(=O)N3CCCC3)C2)c(C=Cc2ccc(O)cc2)n1C	6	F	SCI	68
378	NGT	O=C(NCC1(N2CCOCC2)CCOCC1)C1(c2ccc(-c3ccc(F)c(C(F)c3)ccc2F)CCC1	6	F	SCI	13
379	HE	CCc1nc(C)en2cc(-c3c(C)nn(C)c3)CS(=O)(=O)N3CC(C)OCC(C4CC4)C3)cc12	-6	F	SCI	5

Fig. 14D

(1)	(2)	(3)	(4)	(5)	(6)	(7)
180	HE	CC1CCN(CCOc2ccc(-c3ccc(C(=O)N4CCN(C(=O)C(C)(O)C(F)(F)F)CC4)cc3)c2)CC1	-6	F	SCI	11
181	HE	COc1cc(-c2ccc(Cl)c(C)c2)cc(N2CCN(S(=O)(=O)c3c(C)noc3C)CC2)n1	-6	F	SCI	16
182	NGT	CC(=Cc1cc2c(cc1C(=O)N(C)C1C(C)C(C)C1C3cccc3)CC1Cm(C)c(=O)n2C)c1ccnn1C	-6	F	SCI	56
183	HE	CC(C)(O)NC(=O)C(c1ccc(C2CC2)c1N)CC1CCCN(CCC1)C2C(=O)c1cc(Cl)n[nH]c1=O	-6	F	SCI	24
184	NGT	CCC=Cc1cc(C2(C(=O)NC3CCCN4CCCC34)CC2)ccc1C	-6	F	SCI	35
185	NGT	CCc1cc(-c2cc(S(=O)(=O)NCC(C)Cn3ccc3C)cc(C)c2C)ccc1O	-6	F	SCI	2
186	HE	CCc1ncc(C(C(=O)NC)N(C2CCCN2C2C(=O)c2ccc(C3CC(F)(F)F)C3)c2)cn1	-6	F	SCI	13
187	HE	CCc1cccc(-c2ccc(NC(=O)NCCC(=O)N3CCN(c4nc(SC)ns4)CC3)cc2)c1	5	F	SCI	31
188	HE	COc1ncc(-c2cc(F)c(CNCCC3(CN)=O)CCCC3)cc2C1)cc1C1	5	F	SCI	2
189	NGT	CCCN1CCN(c2ccc(CN(C)S(=O)(=O)Cc3cc(F)ccc3C3=CC4(CCC4)C3)nn2)CC1	5	F	SCI	61
190	NGT	Ce1nn2c(c1-e1ccc3c(c1C)CCO3)CN(S(=O)(=O)c1CCC(C(=O)C3CCCC3)C1)CC2	5	F	SCI	112
191	HE	CO[C@@H]1[C@H](C[C@H](CNc2ccc3nccc(C4=CCCC(F)CC4)c3s2)N(c2nccc(C)n2)C1	-5	F	SCI	3
192	HE	Cc1ccc(-c2cc(C)c(F)c(C)c2)cc1S(=O)(=O)NC(C)(C)c1cn(C(C)C)nn1	-5	F	SCI	4
193	HE	Cc1cc(N2CCCC(NC(=O)CCc3ccc(-c4ccc(C)c4)ccc3F)CC2)nc(C)n1	-5	F	SCI	8
194	HE	CNC(=O)C(COC(C)C)N(C)(C(=O)c1ccc(SC(F)F)cc1)[C@H]1C[C@@H](N2CCCC2)C1	-5	F	SCI	13
195	HE	CCNC(=O)C(c1ccc(C)cc(C)c1)N(C(=O)CCc1cccc1C#N)C1CCN(C2CCCC2)C1	-5	F	SCI	13
196	HE	CCOC(=O)c1ccc(-c2ccc(O)cc2CN[C@@H]2CC[C@H](C(=O)N3CCCC3)C2)s1	-5	F	SCI	40
197	HE	CN1CCC2(CC1)CCN(c1ccc(CCO)c(-c3nccc(C)(F)F)c3)en1)CC2CO	4	F	SCI	15
198	HE	CC(C)N1C2CCCC1CC(NC(=O)CNS(=O)(=O)c1ccc(-c3ccc(F)cc3CO)c1)C2	4	F	SCI	21
199	HE	O=C(NCC12CCCC(NC1)C2)C1(c2ccc(-c3ccc3F)cc2)CCC1	4	F	SCI	13
200	HE	Cc1cc(Cl)ccc1-e1ccnc(C(=O)N2CCN(C)C)C3(C)COC3)C2)c1F	4	F	SCI	34
201	HE	CNC(=O)C(c1cccc1N(C)C1CCN(C)CC1)N(C(C)(C)C(=O)c1cn(C)cn1	4	F	SCI	13
202	NGT	Cc1ccc(O)c(-c2cc(C)cc3ccc(CNS(=O)(=O)c4c(C)nn(C3CC5)c4C)nc23)c1	4	F	SCI	2
203	NGT	Cc1nccc(-c2ccc(C)c(C)(C)(C(=O)N3CCC(C)(CCO)C3)c2)c1	4	F	SCI	75
204	HE	CCNC(=O)C(C1CCC(c2ccc2)CC1)N(C(=O)c1enc(C#N)s1)C1CCN(C2CC2)CC1	4	F	SCI	13
205	HE	CO[C@@H]1[C@H](C[C@H](CNCc2cc(OC(F)F)ccc2C2=CCC(F)(F)CC2)N(c2nccc(C)n2)C1	4	F	SCI	3
206	NGT	O=C1NCCOe2cc(-c3ccc(Cl)C@@H)4C[C@@H]4S(=O)(=O)NC4CCN(c5ncc5)CC4)cc3)ccc21	4	F	SCI	2
207	HE	CCN1CCCC1CN(C(=O)C1C(C)C(=O)NC1CCC1)C1CCC(c2ccc2)CC1	-4	F	SCI	13
208	HE	O=C(CNC(=O)c1ccc(C2=CCCC2)c1)N1CCCCN(C(=O)C2CCCC2)C1	-4	F	SCI	30
209	HE	COc1nc(Cc2=CCC(F)(F)CC2)cc1CNC[C@H]1[C@H](C@@H)(OC)CN1c1nccc(C)n1	-4	F	SCI	3
210	NGT	COCC(CN1CCOCC1)NS(=O)(=O)c1c(F)ccc(C=CC(C)(C)c1F	-4	F	SCI	28
211	HE	CNC(=O)C(c1c(C)cc(C#N)cc1CN(C(=O)c1ccc(C(C)C)cc1)C(C)CN1CCOCC1	-4	F	SCI	13
212	HE	CNC(=O)C(c1ccc(C(C)F)c1)N(C(=O)C1CN(C(C)C)ccc1)C1CCCC1	-4	F	SCI	0
213	HE	Cc1nn(CCF)c(C)c1-e1ccc(C)N2CCCC(C)CC2)c(Cl)c1	3	F	SCI	37
214	HE	COc1cc(C(=O)N2CCN(C)CC2CC(C)C)cc(-c2cc(C)ccc2CO)c1	3	F	SCI	35
215	NGT	CC(=Cc1cc(C2(=O)N)C(C@@H)3CCCC[C@H]3NS(=O)(=O)C3CC3)CC2)ccc1F)CC1CCCC1	3	F	SCI	13
216	HE	CNC(=O)C(c1ccc(C)cc(C)c1OC)N(C(=O)Cn1en1)C1CCN(C2CCCC2)CC1	3	F	SCI	0
217	NGT	Cc1nn(CCF)c(C)c1-e1ccc(F)c(S(=O)(=O)N2CCN(C3CCCC3)C(C)C2)c1	3	F	SCI	28
218	NGT	CC#Cc1cccc(-c2ccc(Cl)C@@H)3C[C@H]3S(=O)(=O)NC3CCN(c4nccn4)CC3)c2)c1	3	F	SCI	38
219	HE	Cc1ccc(-c2ccc3[nH]c(=O)cc(C)N4COC[C@H]4C(=O)C5CCN6CCCCN65)C4)c3c2)cc1C	2	F	SCI	2
220	HE	CC(C)c1cc(-c2ccc(F)c(CN3CCN(S(=O)(=O)c4cnn(C)CC5CC5)c4)CC3)c2)enc1F	-3	F	SCI	64
221	NGT	CCc1cc(-c2cc3c(c(S(=O)(=O)N4CCN(C)C(=O)NCCOC)CC4)c2)OCC3)ccc1O	-3	F	SCI	72
222	NGT	Cc1nn(C(F)F)c(C)c1S(=O)(=O)NCC(CO)Cc1ccc(F)c(C=Cc2ccc(F)c(F)c2)c1	-3	F	SCI	13
223	NGT	COCCN(CCO)C1CN(S(=O)(=O)C2c(C)cc(-c3cc(C)ccc3O)cc2F)C1	2	F	SCI	13
224	NGT	Cc1nn2c(c1-e1en(C)c3ccc(F)cc13)CN(C(=O)c1ccc(S(=O)(=O)NC(C)CO)cc1)CC2	2	F	SCI	72

Fig. 14E

(1)	(2)	(3)	(4)	(5)	(6)	(7)
225	HE	Cc1c(C(C(=O)NC2(C)CC2)N(CC2CCN(C3CC3)CC2)C(=O)c2ccc(C(N)=O)c2)ccc2c1CCCC	2	F	SCI	102
226	NGT	CC(C)C(NS(=O)(=O)NCc1ccc(C=CC2CCCC2)cc1)C1(CO)CC=CC1	-2	F	SCI	66
227	NGT	Cc1cc(O)c(C(=O)N2C3C=CCC2CCC3)cc1-c1cm(C(O)C)nc1C	-2	F	SCI	85
228	NGT	C1CC2CC1(C(=O)Nc1ccc3ccc(C4=CCC(F)C4)c3c1)C2	-2	F	SCI	93
229	HE	Cc1nc2(c[nH]1)CCC(N(C(=O)c1cmm(C)c1)C(C(=O)NC(C)(C)C)c1cccc(OCCC3CCC3)c1)C2	-2	F	SCI	103
230	HE	C1(C)CCOc1ccc(-c2cc(C)c1cc3c2CN(C(=O)C2(N(C)C)Cc4cccc4C2)CC3)c1	1	F	SCI	19
231	HE	Cc1cc(C(C(=O)NC(C)(C)C)N(CC2(N(C)C)CCSC2)C(=O)c2nc3cccc3[nH]2)ccc2c1CCCC2	1	F	SCI	13
232	HE	Cc1ccc(CO)c(-c2ccc(S(=O)(=O)NC(C)(C)C)c3cm(C(C)C)nn3)c(C)cc2F)c1	1	F	SCI	4
233	HE	Cc1ccc(-c2ccc(CCC3CN(C4cnc(N5CCCC5)nc4)C3)c(C)cc2)c1	1	F	SCI	42
234	NGT	Cc1cc1CCCC(C(C=O)N2CCCCC2c2nm(C)cc2-c2ccc(O)c(F)c2F)C1	1	F	SCI	0
235	NGT	CC(=Cc1ccc2c(c1)CCN(CCN1C1C@H)C1[C@@H](C)C1)C2)c1ccnn1C	1	F	SCI	56
236	NGT	CC(Cn1cc(-c2c(C)ccc(C(=O)N3CCCCC3)CCNS(C)(=O)=O)c2F)c(C)nl	1	F	SCI	86
237	NGT	Cc1nn(C(C)C)cc1-c1c(F)ccc2c1CN(C(=O)CN1CCCC3(C)C3)S1(=O)=O)C(C)C2	1	F	SCI	0
238	NGT	Cc1ccc(-c2c(C)C)nm(C(C)C)c2C(=O)NC2CN(CCC3CC3)C2)c(C)cc1Cl	1	F	SCI	46
239	NGT	CCC=Cc1cc(F)cc1C1(C(=O)NC2CN(CCC2)CC3)CC1	1	F	SCI	35
240	NGT	Cc1ccc(C2(CNS(=O)=O)c3cc(-c4ccc(CN5CCN(C6CC6)CC5)cc4)cnm3C)CC2)c(C)c1	1	F	SCI	106
241	HE	CCC(NC(=O)C1(CN(C)C)CCCC1)c1cc(F)cc(-c2ccc(F)cc2CCO)c1	-1	F	SCI	0
242	HE	COc1ncc(-c2c(C)cnccc2(C(=O)N2CCN(C(C)C(=O)C3(C)CCCC3)C2)cc1C	-1	F	SCI	7
243	HE	CCCOc1ncc(-c2cccc2C(C)C)C(=O)N2CCN3(CCC4)C(C@H)3C2)c1	-1	F	SCI	2
244	HE	COc1ccc(-c2cccc(C(=O)N3CCN(C)C)C4(COCC4)C3)c2Cl)cc1F	-1	F	SCI	34
245	NGT	CNC(C[C@@H]1CCCCN(C)[C@@H]1)C1c1ccnn1C(C(=O)c1c(C=C2CCCSC2)cnm1C1CCCC1	-1	F	SCI	45
246	NGT	COc(=O)c1ccc(C=C2sccc2CC(C(=O)N2CC3CCN3CC2)CC1	-1	F	SCI	55
247	NGT	Cc1nn(CCC2)C(C)C1S(=O)(=O)NC1COc2ccc(-c3cc(F)cc3F)cc2C1	-1	F	SCI	2
248	HE	Cc1c(CCN(S(=O)(=O)c2cmm(C3CC3)c2)ccc1-c1cnc(F)c(C)C)c1	0	F	SCI	2
249	HE	Cc1ccc(-c2cc(O)cc(C(F)F)c2)c2nnc(C3CCN(C4CCN(C)CC4)C(C)C3)c2c1	0	F	SCI	2
250	NGT	Cc1ccc(C)c(-c2nccc(C(C)C(=O)N3CCN4C[C@@H](F)C[C@@H]4C3)c2)cc1C	0	F	SCI	71
251	NGT	Cc1ccc(C(CO)N2CCN(C(C)C)c3cc(-c4nccc1C[C@@H]5CCCN5C)c4)c(C)ccc2c1	0	F	SCI	76
252	NGT	COc1c(F)cc(C(C)C)cc1C1(C(=O)NC2CC3CCCC3)C2)N3CCC1	0	F	SCI	105

Fig. 14F