

Supplemental Tables

Supplemental Table 1. Enrichment Results for Bayesian model building.

Output	Category %	1%	5%	10%	25%	50%	75%	90%	95%	99%
MLSMR All single point screen (N = 220463)	1.858%	19.2%	48.8%	63.9%	83.2%	94.5%	98.5%	99.6%	99.8%	100%
MLSMR dose response set (N = 2273)	20.897%	3.6%	16.4%	27.4%	53.7%	81.3%	95.2%	98.1%	98.9%	100%

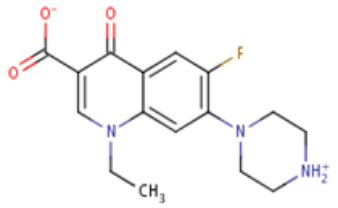
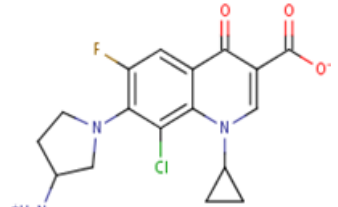
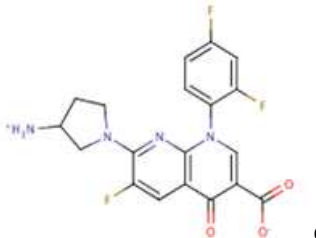
Supplemental Table 2. Percentile Results for Bayesian model building.

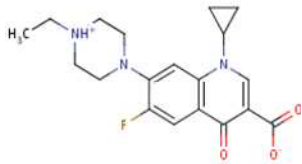
Model Name	99%	95%	90%	70%	50%	30%	10%	5%	1%
MLSMR All single point screen (N = 220463)	-22.270	-12.144	-6.647	-0.572	-0.572	24.019	30.094	35.591	45.717
	85%/15%	59%/41%	42%/58%	24%/76%	5%/95%	1%/99%	1%/99%	1%/99%	1%/99%
MLSMR dose response set (N = 2273)	-17.513	-11.417	-8.108	-4.450	-4.450	10.356	14.013	17.323	23.419
	90%/10%	72%/28%	59%/41%	42%/58%	15%/85%	4%/96%	2%/98%	1%/99%	1%/99%

Supplemental Table 3. Category Statistics Results for Bayesian model building

Output	Category N	Category Mean (\pmStdDev)	Noncategory N	Noncategory Mean (\pmStdDev)
MLSMR All single point screen (N = 220463)	4096	11.72 (\pm 14.47)	216367	-9.43 (\pm 12.49)
MLSMR dose response set (N = 2273)	475	2.95 (\pm 8.71)	1798	-6.25 (\pm 8.86)

Supplemental Table 4. Molecules in common between the NIAID and MLSMR dose response datasets

Molecule	Structure	CDD Number	TB Prathiparti MIC A: MIC (uM)	MTb (H37Rv) Inhibitory Dose Response: Activity Comment	MTb (H37Rv) Inhibitory Dose Response: IC50 (XLFit 205) (uM)	MTb (H37Rv) Inhibitory Dose Response: IC50 (XLFit 205) Std Dev	MTb (H37Rv) Inhibitory Dose Response: IC50 (XLFit 205) Hill Slope	MTb (H37Rv) Inhibitory Dose Response: IC50 (XLFit 205) Normalized Chi2	common name
1991		CDD-5200f	0.939449	Active	2.845	2601.67	24.377	7.44	norfloxacin
7759		CDD-5122f	0.0273	Active	< 0.391	> 9999.0	-0.964	0.79	
7807		CDD-5237f	2.47312	Active	1.29	0.043	1.857	2.22	



8322

CDD-51711

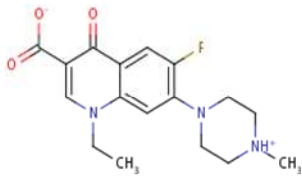
0.347801 Active

< 0.391

0.005

1.002

0.11 ENROFLOXACIN



8377

CDD-5199:

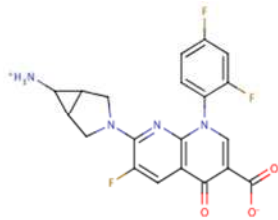
0.89992 Active

3.059

0.159

7.323

7.22



10848

CDD-5274:

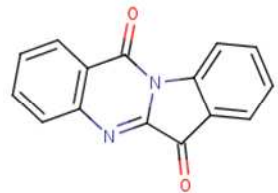
4.80355 Active

1.215

0.06

2.413

3.76



17287

CDD-5226:

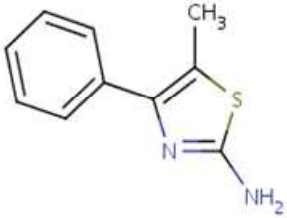
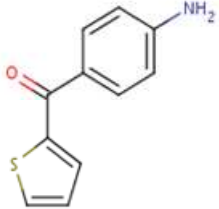
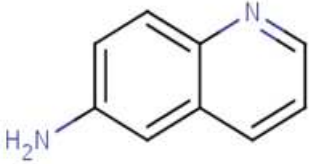

2.01417 Active

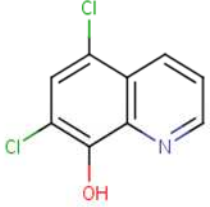
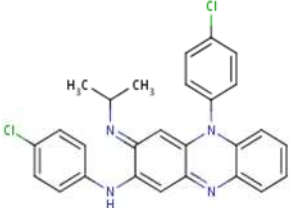
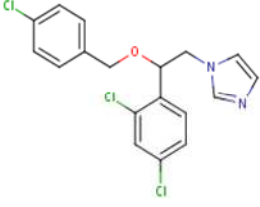
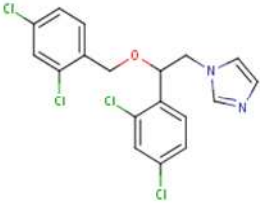
< 0.195

0

0.169

2.3

19675		CDD-5434i	32.8481 Weakly Active	> 100.0	61.031	0.988	16.84
20216		CDD-5261i	3.83735 Weakly Active	22.063	9.907	0.527	13.32
20623		CDD-1096i	21.6401 Weakly Active	37.939	8.772	0.777	8.46
44913		CDD-5137i	0.0799 Active	< 0.195	0	0.722	0.06

Chloroxine		CDD-1512:	0.887639 Active	0.779	13.502	22.696	1.84 CHLOROXINE
Clofazimine		CDD-809	0.126741 Active	< 0.391	0.03	1.173	0.55 Clofazimine
Econazole		CDD-234	0.314391 Active	3.744	0.453	5.27	11.11
Miconazole		CDD-444	4.80613 Active	2.846	16.023	15.778	5.13

Supplemental Figure 1. Example of a molecule in the CDD database showing the molecule page with calculated properties and links to the structure in different formats

CDD · CDD - Sean Ekins
Sean Ekins: [Your Account](#) [Log out](#)

Dashboard
Explore Data
Import Data
Share Data

Currently using CDD - Sean Ekins data and **1 shared data set** [i](#)
[Choose data sets ...](#)

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MOXIFLOXACIN

Available in **1** data set. Now viewing: MOXIFLOXACIN

Overview Batches 0 Plates 0 Protocols 3 Files 3

Definition [Edit definition and structure](#)

Name: MOXIFLOXACIN

Synonyms: 6 and moxifloxacin

Description:

Structure: [SMILES](#) [CXSMILES](#) [InChI](#) [InChIKey](#) [IUPAC](#) [i](#)

COc1c(N2C[C@@H]3CCCN[C@@H]3C2)c(F)cc2c1n(cc(C(O)=O)c2)

User-defined Fields [Edit user-defined fields](#)

No user-defined fields.

Lipinski Properties [i](#)

Molecular weight: 401.431 g/mol

log P: -1.75

H-bond donors: 2

H-bond acceptors: 8

Lipinski Rule of 5: Satisfied
4 of 4 within desirable range

Additional Properties [i](#)

Formula: C₂₁H₂₄FN₃O₄

pK_a: 9.42


Exact mass: 401.175 g/mol

Atom count: 53

Composition: C (62.83%), H (6.03%), F (4.73%), N (10.47%), O (15.94%)

Topological polar surface area (PSA): 82.11 Å²

Rotatable bonds: 4



CDD-460

[Find molecules with this structure](#)

[View ChemSpider page](#)

Owner: Sean Ekins

Created: March 21, 2008

Updated: March 21, 2008

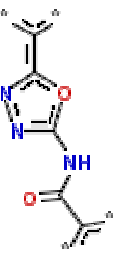
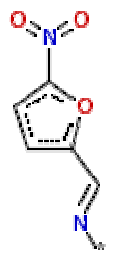
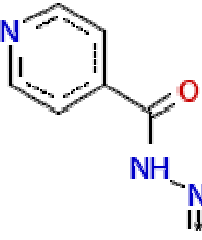
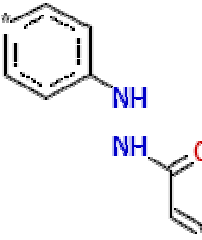
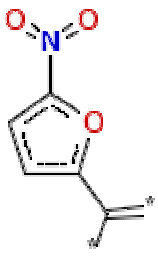
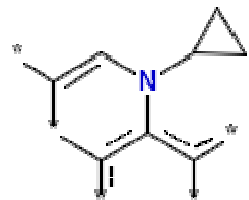
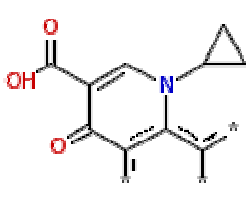
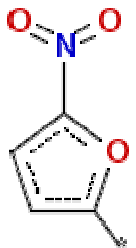
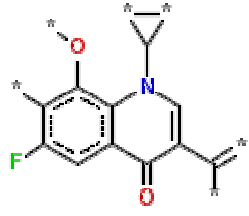
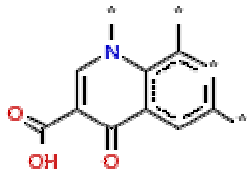
[Delete this molecule](#)

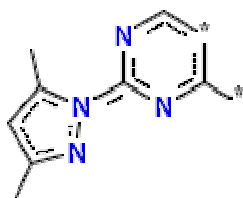
Collaborative Drug Discovery
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Supplemental Figure 2. MLSMR All single point screen (N = 220463) Bayesian model.

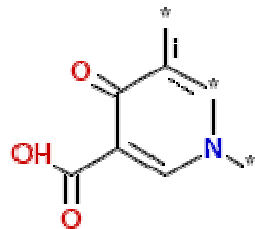
A. Simple descriptors with FCFP_6: features important for Actives, B. Simple descriptors with FCFP_6: features important for Inactives

A

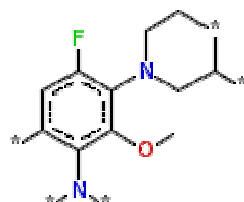
 <p>G1: 1704324327 73 out of 165 good Bayesian Score: 2.885</p>	 <p>G2: -2092491099 57 out of 120 good Bayesian Score: 2.873</p>	 <p>G3: -1230843627 75 out of 188 good Bayesian Score: 2.811</p>	 <p>G4: 940811929 35 out of 65 good Bayesian Score: 2.780</p>	 <p>G5: 563485513 123 out of 357 good Bayesian Score: 2.769</p>
 <p>G6: -1837273810 23 out of 27 good Bayesian Score: 2.764</p>	 <p>G7: 1682136030 22 out of 24 good Bayesian Score: 2.760</p>	 <p>G8: 1951066682 125 out of 386 good Bayesian Score: 2.716</p>	 <p>G9: 1286357304 20 out of 21 good Bayesian Score: 2.709</p>	 <p>G10: 192299924 31 out of 62 good Bayesian Score: 2.688</p>



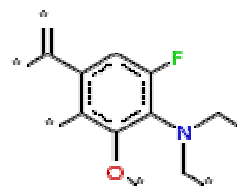
G11: -1943210977
40 out of 95 good
Bayesian Score: 2.682



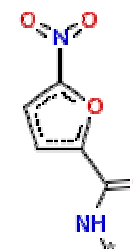
G12: 173580544
35 out of 80 good
Bayesian Score: 2.660



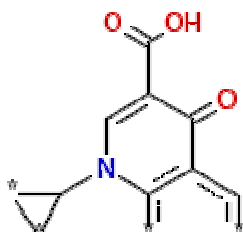
G13: 1410483689
18 out of 19 good
Bayesian Score: 2.636



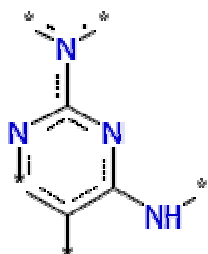
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18 out of 19 good
Bayesian Score: 2.636



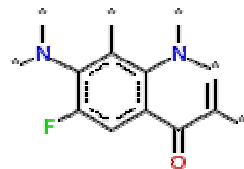
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32 out of 73 good
Bayesian Score: 2.627



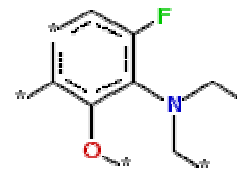
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32 out of 75 good
Bayesian Score: 2.611



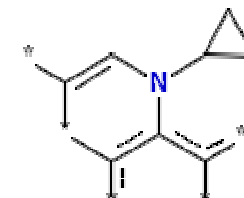
G17: 75474173
24 out of 49 good
Bayesian Score: 2.561



G18: -695845985
31 out of 84 good
Bayesian Score: 2.512

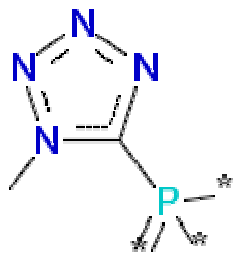
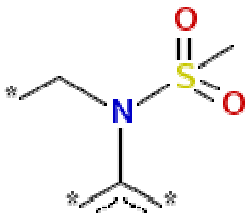
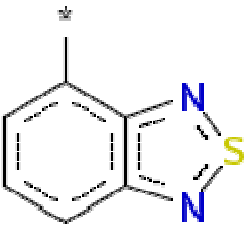
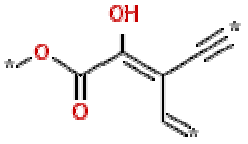
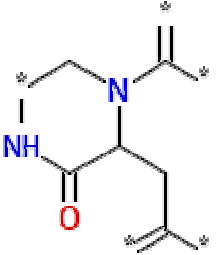
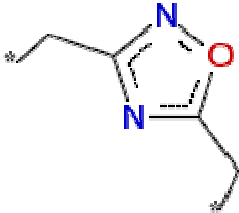
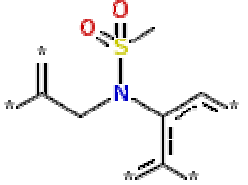
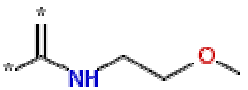
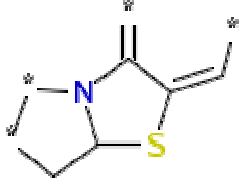
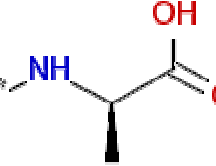
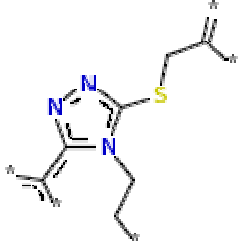
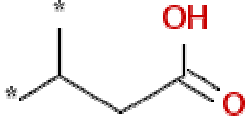
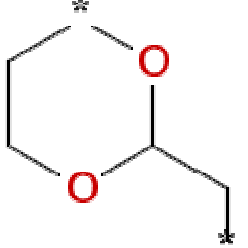
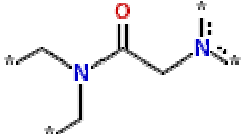
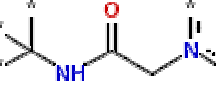


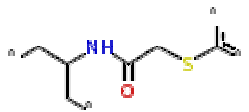
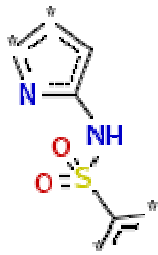
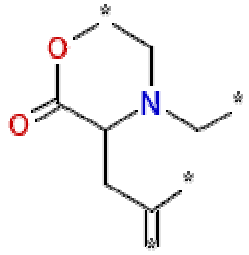
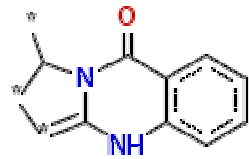
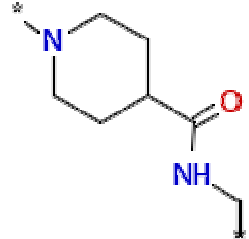
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19 out of 34 good
Bayesian Score: 2.498



G20: -2102761594
15 out of 17 good
Bayesian Score: 2.493

B.

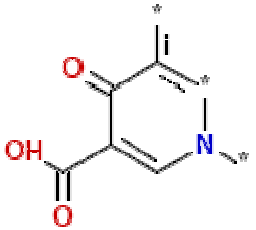
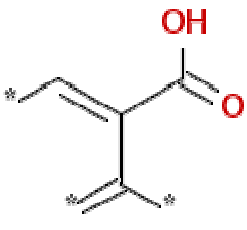
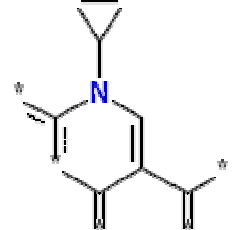
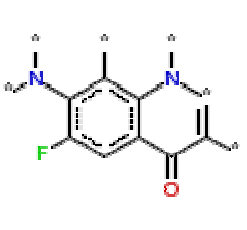
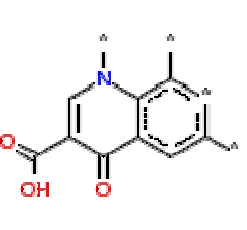
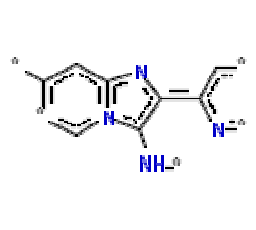
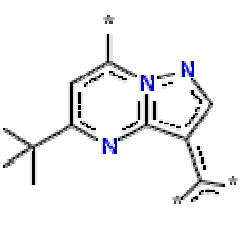
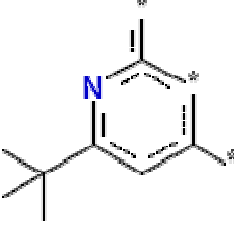
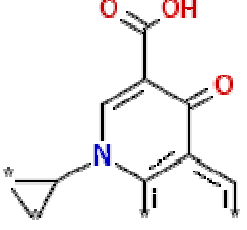
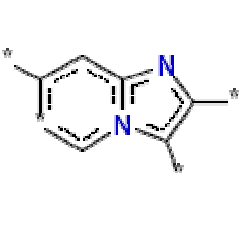
 <p>B1: 1444982751 0 out of 1158 good Bayesian Score: -3.135</p>	 <p>B2: 274564616 0 out of 1024 good Bayesian Score: -3.018</p>	 <p>B3: -1775057221 0 out of 982 good Bayesian Score: -2.978</p>	 <p>B4: 48625803 0 out of 740 good Bayesian Score: -2.712</p>	 <p>B5: 899570811 0 out of 738 good Bayesian Score: -2.709</p>
 <p>B6: -634714342 0 out of 735 good Bayesian Score: -2.705</p>	 <p>B7: -236386689 0 out of 691 good Bayesian Score: -2.648</p>	 <p>B8: -469395141 0 out of 686 good Bayesian Score: -2.641</p>	 <p>B9: -166879442 0 out of 672 good Bayesian Score: -2.622</p>	 <p>B10: 389859240 0 out of 667 good Bayesian Score: -2.615</p>
 <p>B11: -1512436476</p>	 <p>B12: 394124770</p>	 <p>B13: 745786291</p>	 <p>B14: 839269998</p>	 <p>B15: -922187952</p>

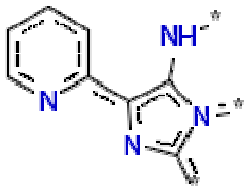
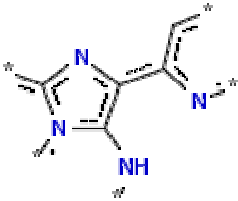
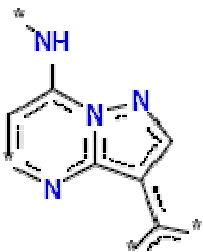
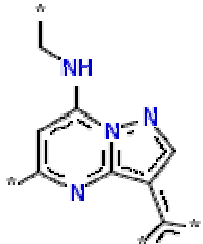
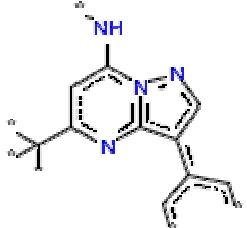
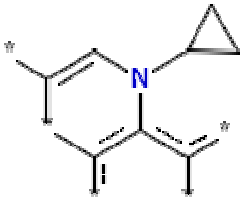
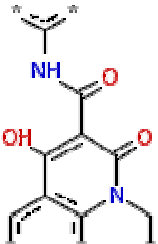
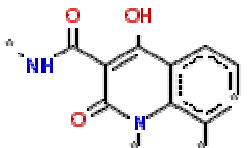
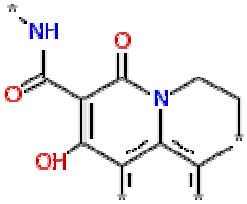
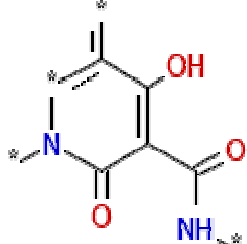
<p>0 out of 656 good Bayesian Score: -2.600</p>	<p>2 out of 2014 good Bayesian Score: -2.571</p>	<p>0 out of 632 good Bayesian Score: -2.565</p>	<p>0 out of 631 good Bayesian Score: -2.564</p>	<p>0 out of 615 good Bayesian Score: -2.540</p>
 <p>B16: -770014726 0 out of 613 good Bayesian Score: -2.537</p>	 <p>B17: 1955977916 0 out of 600 good Bayesian Score: -2.517</p>	 <p>B18: -1916257959 0 out of 597 good Bayesian Score: -2.513</p>	 <p>B19: 1967778163 0 out of 596 good Bayesian Score: -2.511</p>	 <p>B20: -50059269 0 out of 594 good Bayesian Score: -2.508</p>

Supplemental Figure 3. MLSMR dose response (N = 2273) model. A. Simple descriptors with FCFP_6: features important for Actives, B.

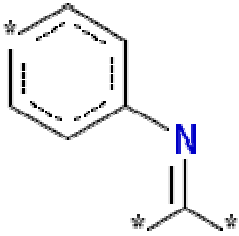
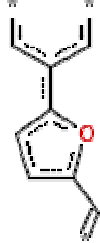
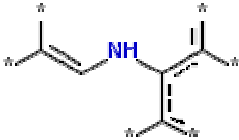
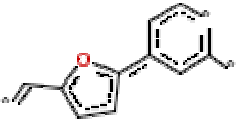
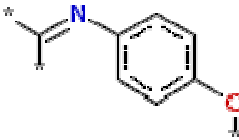
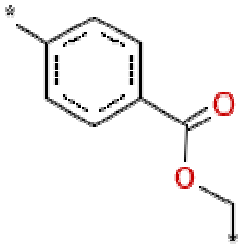
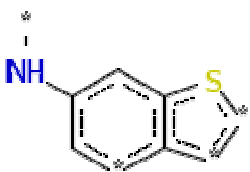
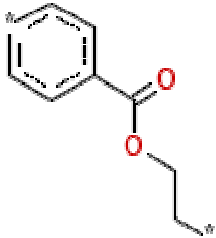
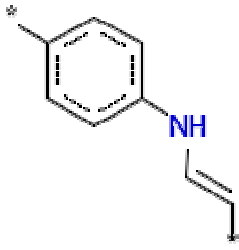
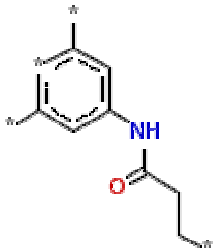
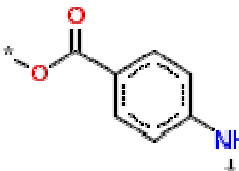
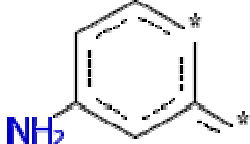
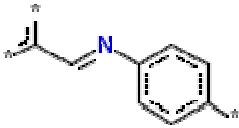
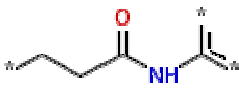
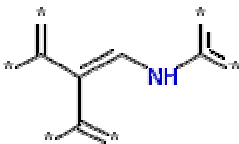
Simple descriptors with FCFP_6: features important for Inactives.

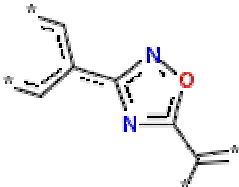
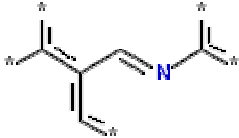
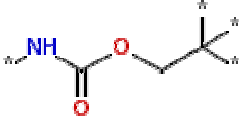
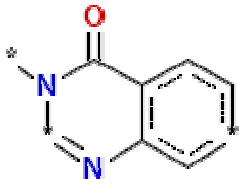
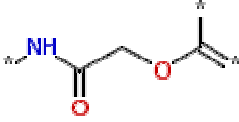
A.

 <p>G1: 173580544 10 out of 10 good Bayesian Score: 1.253</p>	 <p>G2: 1393614142 10 out of 10 good Bayesian Score: 1.253</p>	 <p>G3: -1646949305 9 out of 9 good Bayesian Score: 1.228</p>	 <p>G4: -695845985 9 out of 9 good Bayesian Score: 1.228</p>	 <p>G5: 192299924 8 out of 8 good Bayesian Score: 1.199</p>
 <p>G6: 126527349 8 out of 8 good Bayesian Score: 1.199</p>	 <p>G7: -1492853728 8 out of 8 good Bayesian Score: 1.199</p>	 <p>G8: 1363919920 8 out of 8 good Bayesian Score: 1.199</p>	 <p>G9: 1048446020 7 out of 7 good Bayesian Score: 1.163</p>	 <p>G10: -444825055 10 out of 12 good Bayesian Score: 1.125</p>

 <p>G11: -1087652354 8 out of 9 good Bayesian Score: 1.123</p>	 <p>G12: 867496812 8 out of 9 good Bayesian Score: 1.123</p>	 <p>G13: 1045438014 6 out of 6 good Bayesian Score: 1.119</p>	 <p>G14: -1151542701 6 out of 6 good Bayesian Score: 1.119</p>	 <p>G15: -28315240 6 out of 6 good Bayesian Score: 1.119</p>
 <p>G16: -1837273810 6 out of 6 good Bayesian Score: 1.119</p>	 <p>G17: 332551053 9 out of 11 good Bayesian Score: 1.092</p>	 <p>G18: -1237632426 9 out of 11 good Bayesian Score: 1.092</p>	 <p>G19: 443372493 9 out of 11 good Bayesian Score: 1.092</p>	 <p>G20: -811904132 9 out of 11 good Bayesian Score: 1.092</p>

B.

 <p>B1: -1699460258 0 out of 56 good Bayesian Score: -2.565</p>	 <p>B2: -1448737182 0 out of 42 good Bayesian Score: -2.303</p>	 <p>B3: 758147873 0 out of 41 good Bayesian Score: -2.281</p>	 <p>B4: -458381731 0 out of 37 good Bayesian Score: -2.189</p>	 <p>B5: -1185638464 0 out of 33 good Bayesian Score: -2.088</p>
 <p>B6: 262463794 2 out of 100 good Bayesian Score: -2.012</p>	 <p>B7: -768831192 0 out of 29 good Bayesian Score: -1.976</p>	 <p>B8: -1261000356 2 out of 96 good Bayesian Score: -1.973</p>	 <p>B9: -974330059 0 out of 27 good Bayesian Score: -1.915</p>	 <p>B10: 1904392374 1 out of 54 good Bayesian Score: -1.838</p>
				

<p>B11: 1764559217 2 out of 83 good Bayesian Score: -1.834</p>	<p>B12: -1247245120 0 out of 23 good Bayesian Score: -1.780</p>	<p>B13: 1447143601 0 out of 22 good Bayesian Score: -1.743</p>	<p>B14: -1944142687 2 out of 74 good Bayesian Score: -1.726</p>	<p>B15: -259532869 0 out of 20 good Bayesian Score: -1.665</p>
 <p>B16: -1968900341 0 out of 20 good Bayesian Score: -1.665</p>	 <p>B17: 838561463 0 out of 20 good Bayesian Score: -1.665</p>	 <p>B18: 220252777 0 out of 20 good Bayesian Score: -1.665</p>	 <p>B19: 562091192 0 out of 20 good Bayesian Score: -1.665</p>	 <p>B20: 1415248070 2 out of 67 good Bayesian Score: -1.633</p>

