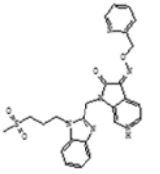
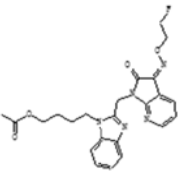
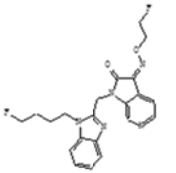
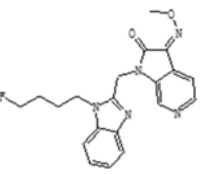
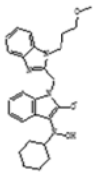
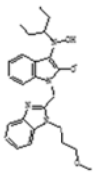
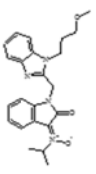
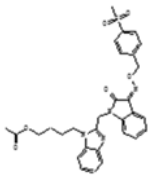
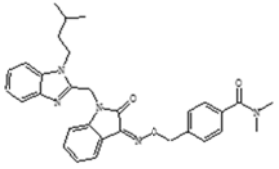
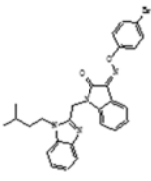
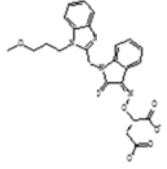
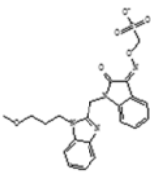
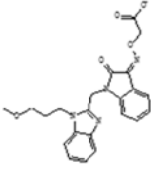
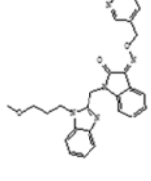
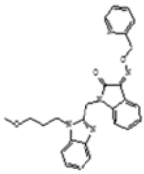
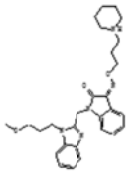
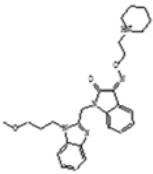
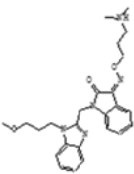
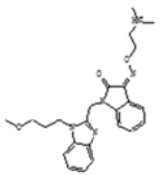
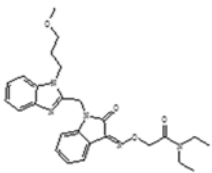
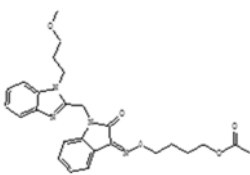
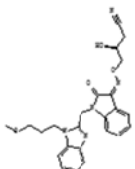
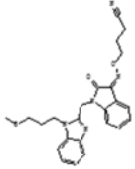
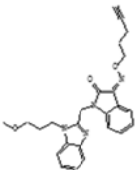
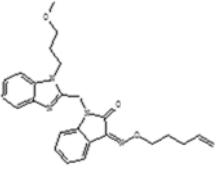
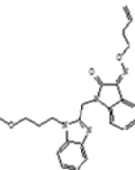
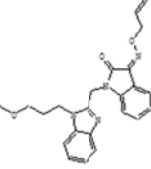
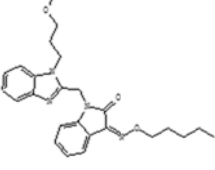


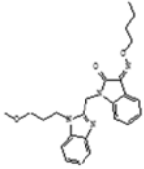
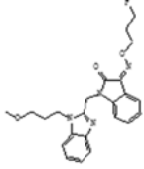
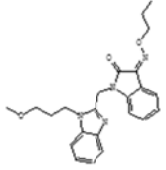
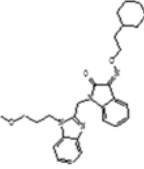
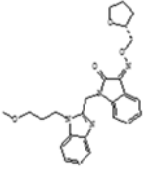
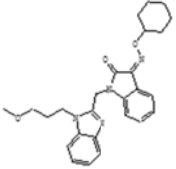
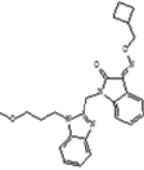
Table S1. Structures and bioactivities

ID	Structure	ACS Registry Number	pEC50	CoMFA	CoMSIA
G1-1		1187776-07-3	7.5376	7.6866	7.5514
G1-2		1187776-06-2	7.2628	7.6737	7.2973
G1-3		1187776-05-1	7.2083	7.3624	7.4020
G1-4		1187776-04-0	6.9747	7.4232	7.0470
G1-5*		1187776-03-9	6.5452	6.5680	6.2370
G1-6*		1187776-02-8	6.0467	6.3659	6.5209
G1-7		1187776-01-7	6.6383	6.8704	6.6906

G1-8		1187775-94-5	8.3010	8.2893	8.1056
G1-9		1187775-93-4	8.0458	8.1423	7.9182
G1-10		1187775-91-2	6.1518	6.1437	6.7625
G1-11*		1187775-90-1	7.7212	7.6439	6.8944
G1-12*		1187775-89-8	7.3372	7.4745	7.8387
G1-13*		1187775-88-7	6.5302	6.5031	6.4473
G1-14		1187775-87-6	6.8508	6.7963	6.7634

G1-15		1187775-86-5	6.6234	6.4887	6.4580
G1-16		1187775-85-4	6.5376	6.6688	6.4382
G1-17*		1187775-84-3	6.1662	6.1603	6.0602
G1-18		1187775-83-2	6.6198	6.7638	6.5285
G1-19		1187775-82-1	6.4318	6.3484	6.1742
G1-20		1187775-81-0	7.5850	7.6263	7.6951
G1-21		1187775-80-9	7.2076	7.1145	7.3191

G1-22		1187775-79-6	7.1871	7.2868	7.2314
G1-23		1187775-78-5	7.1024	6.7242	6.8044
G1-24		1187775-77-4	7.1938	7.0635	6.9119
G1-25*		1187775-76-3	6.7167	6.7016	6.7091
G1-26		1187775-75-2	6.5850	6.6339	6.8360
G1-27		1187775-74-1	6.3686	6.5914	6.7963
G1-28		1187775-73-0	6.7258	6.7366	6.6168

G1-29		1187775-71-8	6.5834	6.9735	6.7778
G1-30		1187775-70-7	6.9031	6.8960	6.8587
G1-31		1187775-69-4	6.8327	7.0454	7.0583
G1-32		1187775-68-3	6.4157	6.5803	5.9417
G1-33		1187775-67-2	6.8182	7.1620	6.4352
G1-34		1187775-66-1	6.1858	6.5901	6.5309
G1-36*		1187775-64-9	6.6091	7.0244	6.5386

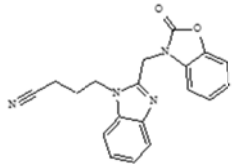
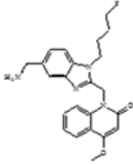
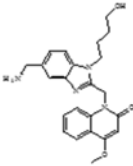
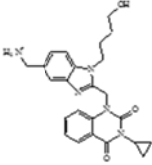
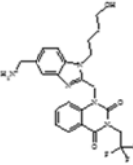
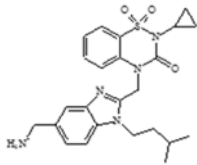
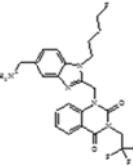
G1-37*	A complex organic molecule featuring a central benzimidazole ring system. It has a propyl group at the 2-position, a 2-(propylamino)ethyl group at the 5-position, and a 2-(propylamino)ethyl group at the 7-position.	1187775-63-8	7.0177	6.8227	6.5359
G1-38	A complex organic molecule featuring a central benzimidazole ring system. It has a propyl group at the 2-position, a 2-(propylamino)ethyl group at the 5-position, and a 2-(propylamino)ethyl group at the 7-position.	1187775-62-7	6.0292	6.2816	6.4571
G1-39	A complex organic molecule featuring a central benzimidazole ring system. It has a propyl group at the 2-position, a 2-(propylamino)ethyl group at the 5-position, and a 2-(propylamino)ethyl group at the 7-position.	1187775-61-6	6.5901	6.4169	6.6358
G1-40*	A complex organic molecule featuring a central benzimidazole ring system. It has a propyl group at the 2-position, a 2-(propylamino)ethyl group at the 5-position, and a 2-(propylamino)ethyl group at the 7-position.	1187775-60-5	7.1487	7.4811	7.1206
G1-41	A complex organic molecule featuring a central benzimidazole ring system. It has a propyl group at the 2-position, a 2-(propylamino)ethyl group at the 5-position, and a 2-(propylamino)ethyl group at the 7-position.	1187775-59-2	7.2291	6.7645	6.8833
G1-42	A complex organic molecule featuring a central benzimidazole ring system. It has a propyl group at the 2-position, a 2-(propylamino)ethyl group at the 5-position, and a 2-(propylamino)ethyl group at the 7-position.	1187775-58-1	7.5229	7.3559	7.2004
G1-43	A complex organic molecule featuring a central benzimidazole ring system. It has a propyl group at the 2-position, a 2-(propylamino)ethyl group at the 5-position, and a 2-(propylamino)ethyl group at the 7-position.	1187775-57-0	7.5229	7.7732	7.2677

G1-44*	<p>The chemical structure of G1-44* features a central benzimidazole ring system. One nitrogen atom is substituted with a 3-hydroxypropyl group (-CH₂-CH₂-CH₂-OH). The other nitrogen atom is substituted with a 2-(2-methylphenyl)ethyl group. The benzimidazole ring is fused to a benzene ring.</p>	1187775-56-9	8.0000	7.5606	7.5466
G2-45	<p>The chemical structure of G2-45 features a central benzimidazole ring system. One nitrogen atom is substituted with a 2-(2-methylphenyl)ethyl group. The other nitrogen atom is substituted with a 2-(2-aminoethyl)ethyl group (-CH₂-CH₂-CH₂-NH₂). The benzimidazole ring is fused to a benzene ring.</p>	950668-30-1	5.4318	5.1612	5.8135
G2-46	<p>The chemical structure of G2-46 features a central benzimidazole ring system. One nitrogen atom is substituted with a 2-(2-methylphenyl)ethyl group. The other nitrogen atom is substituted with a 2-(2-hydroxyethyl)ethyl group (-CH₂-CH₂-CH₂-OH). The benzimidazole ring is fused to a benzene ring.</p>	950668-29-8	3.6091	3.4015	3.4902
G2-47*	<p>The chemical structure of G2-47* features a central benzimidazole ring system. One nitrogen atom is substituted with a 2-(2-methylphenyl)ethyl group. The other nitrogen atom is substituted with a 2-(2-aminoethyl)ethyl group. The benzimidazole ring is fused to a benzene ring.</p>	950668-28-7	3.6383	3.5819	3.8798
G2-48	<p>The chemical structure of G2-48 features a central benzimidazole ring system. One nitrogen atom is substituted with a 2-(2-methylphenyl)ethyl group. The other nitrogen atom is substituted with a 2-(2-aminoethyl)ethyl group. The benzimidazole ring is fused to a benzene ring.</p>	950668-27-6	3.7167	3.7811	3.4434
G2-49	<p>The chemical structure of G2-49 features a central benzimidazole ring system. One nitrogen atom is substituted with a 2-(2-methylphenyl)ethyl group. The other nitrogen atom is substituted with a 2-(2-aminoethyl)ethyl group. The benzimidazole ring is fused to a benzene ring.</p>	950668-26-5	3.9101	4.1585	3.7609
G2-50	<p>The chemical structure of G2-50 features a central benzimidazole ring system. One nitrogen atom is substituted with a 2-(2-methylphenyl)ethyl group. The other nitrogen atom is substituted with a 2-(2-aminoethyl)ethyl group. The benzimidazole ring is fused to a benzene ring.</p>	950668-25-4	3.6234	3.5870	3.7399

G2-51*	A complex organic molecule featuring a central benzimidazole ring system. It has a 2-ethylbutyl group at position 2, a 2,4-dimethylphenyl group at position 1, and a 4-cyanophenyl group at position 5.	950668-24-3	7.3565	7.1395	7.7145
G2-52*	A complex organic molecule featuring a central benzimidazole ring system. It has a 2-ethylbutyl group at position 2, a 2,4-dimethylphenyl group at position 1, and a 4-(dimethylamino)phenyl group at position 5.	950668-23-2	3.7375	3.7192	3.7270
G2-53	A complex organic molecule featuring a central benzimidazole ring system. It has a 2-ethylbutyl group at position 2, a 2,4-dimethylphenyl group at position 1, and a 4-(2-oxoethyl)phenyl group at position 5.	950668-22-1	3.6383	3.6529	3.6300
G2-54	A complex organic molecule featuring a central benzimidazole ring system. It has a 2-ethylbutyl group at position 2, a 2,4-dimethylphenyl group at position 1, and a 4-(2-thiazolyl)phenyl group at position 5.	950668-20-9	3.6478	3.6794	3.5271
G2-55	A complex organic molecule featuring a central benzimidazole ring system. It has a 2-ethylbutyl group at position 2, a 2,4-dimethylphenyl group at position 1, and a 4-(2-oxoethyl)phenyl group at position 5.	950668-19-6	3.5784	3.4963	3.6669
G2-56	A complex organic molecule featuring a central benzimidazole ring system. It has a 2-ethylbutyl group at position 2, a 2,4-dimethylphenyl group at position 1, and a 4-(2-thiazolyl)phenyl group at position 5.	950668-18-5	3.6216	3.8179	4.1753
G3-57	A complex organic molecule featuring a central benzimidazole ring system. It has a 2-ethylbutyl group at position 2, a 2,4-dimethylphenyl group at position 1, and a 4-(2-oxoethyl)phenyl group at position 5.	948864-12-8	6.5800	6.6549	6.3910

G3-59*	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring containing a nitrogen atom. It has a propyl chain with a terminal hydroxyl group and a side chain with a terminal epoxide ring.	948864-09-3	7.2596	7.3086	7.1315
G3-60*	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring containing a nitrogen atom. It has a propyl chain with a terminal hydroxyl group and a side chain with a terminal epoxide ring.	948864-08-2	5.8729	6.0247	6.1544
G3-61	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring containing a nitrogen atom. It has a propyl chain with a terminal hydroxyl group and a side chain with a terminal epoxide ring.	948864-07-1	7.3372	7.2162	7.6456
G3-62*	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring containing a nitrogen atom. It has a propyl chain with a terminal hydroxyl group and a side chain with a terminal epoxide ring.	948864-06-0	6.2596	6.5877	6.3927
G3-63	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring containing a nitrogen atom. It has a propyl chain with a terminal hydroxyl group and a side chain with a terminal epoxide ring.	948864-05-9	6.7696	6.8355	6.4081
G3-64	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring containing a nitrogen atom. It has a propyl chain with a terminal hydroxyl group and a side chain with a terminal epoxide ring.	948864-04-8	8.0458	8.2855	7.5388
G3-65	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring containing a nitrogen atom. It has a propyl chain with a terminal hydroxyl group and a side chain with a terminal epoxide ring.	948864-03-7	6.5850	6.7511	6.8913

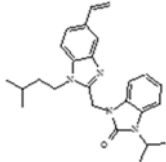
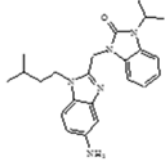
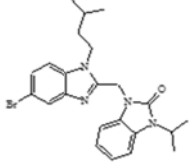
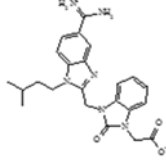
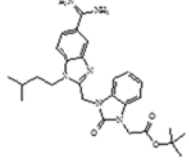
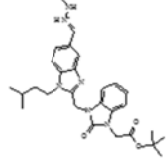
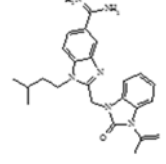
G3-66*	A complex polycyclic molecule featuring a central benzene ring fused to a five-membered ring containing a nitrogen atom. This is further fused to a six-membered ring with a carbonyl group. A side chain includes a phenyl ring and a propyl group.	948864-02-6	5.7430	5.4755	5.9697
G3-67*	A complex polycyclic molecule similar to G3-66*, but with a different side chain configuration, including a phenyl ring and a propyl group.	948864-01-5	5.2808	5.6159	5.9190
G3-68*	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring with a nitrogen atom, and a six-membered ring with a carbonyl group. It has a side chain with a phenyl ring, a propyl group, and a methyl group.	948864-00-4	6.5406	6.8086	6.4386
G3-70	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring with a nitrogen atom, and a six-membered ring with a carbonyl group. It has a side chain with a phenyl ring and a propyl group.	948863-98-7	7.0862	6.6725	7.0044
G3-71	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring with a nitrogen atom, and a six-membered ring with a carbonyl group. It has a side chain with a phenyl ring and a propyl group.	948863-97-6	7.4437	7.3471	7.3730
G3-72*	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring with a nitrogen atom, and a six-membered ring with a carbonyl group. It has a side chain with a phenyl ring and a propyl group.	948863-96-5	6.3410	6.0634	6.8082
G3-73*	A complex polycyclic molecule with a central benzene ring fused to a five-membered ring with a nitrogen atom, and a six-membered ring with a carbonyl group. It has a side chain with a phenyl ring and a propyl group.	948863-95-4	5.9559	6.3684	6.5975

G3-75		948863-93-2	5.6003	5.6240	6.1504
G3-76		792184-48-6	8.0458	8.0646	7.9461
G3-77		791583-23-8	8.0969	8.2849	7.9852
G3-78*		785773-56-0	7.7447	7.5549	7.7862
G3-79		778572-60-4	7.6778	7.6503	7.9842
G3-80		775576-32-4	8.5229	8.5926	8.2905
G3-81		765267-71-8	8.0969	8.1651	8.4326

G3-82		754182-82-6	8.0458	8.0235	7.9132
G3-83		752980-90-8	7.9586	7.8149	7.9096
G2-84*		751477-81-3	6.0862	6.2409	6.1049
G3-85		749845-87-2	6.1035	6.4728	6.6149
G2-86		748766-54-3	6.1457	6.2680	6.1463
G1-87		735259-03-7	7.7959	7.8028	7.6718
G2-88		720662-44-2	3.6716	3.5154	3.8490

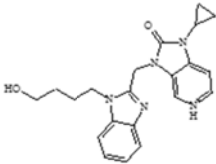
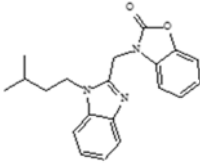
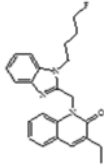
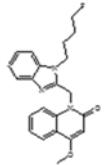
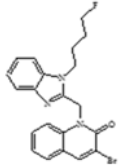
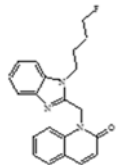
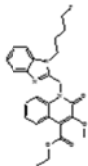
G2-89*	A complex polycyclic molecule featuring a central benzimidazole core. It has a 2-cyanoethyl group at position 2, an isobutyl group at position 3, and a 2-isobutyl-1H-benzimidazol-5-ylmethyl group at position 4. The benzimidazole ring is fused to a benzene ring.	554458-79-6	3.6308	3.4332	3.9202
G2-90	A complex polycyclic molecule similar to G2-89*, but with a 2-isobutyl-1H-benzimidazol-5-ylmethyl group at position 2 and a 2-cyanoethyl group at position 3.	554458-75-2	3.6180	3.8595	3.8214
G2-91	A complex polycyclic molecule similar to G2-89*, but with a 2-isobutyl-1H-benzimidazol-5-ylmethyl group at position 2 and a 2-methoxyethyl group at position 3.	554458-74-1	5.1249	4.9855	5.2147
G2-92	A complex polycyclic molecule similar to G2-89*, but with a 2-isobutyl-1H-benzimidazol-5-ylmethyl group at position 2 and a 2-hydroxyethyl group at position 3.	554458-70-7	6.0862	6.1719	6.2187
G2-93*	A complex polycyclic molecule similar to G2-89*, but with a 2-isobutyl-1H-benzimidazol-5-ylmethyl group at position 2 and a 2-methoxyethyl group at position 3. It also has a 2-methoxyethyl group at position 4.	554458-69-4	3.6383	3.8557	4.3869
G2-95	A complex polycyclic molecule similar to G2-89*, but with a 2-isobutyl-1H-benzimidazol-5-ylmethyl group at position 2 and a 2-isobutyl-1H-benzimidazol-5-ylmethyl group at position 3.	554458-48-9	4.6655	5.0741	4.6760
G2-96	A complex polycyclic molecule similar to G2-89*, but with a 2-isobutyl-1H-benzimidazol-5-ylmethyl group at position 2 and a 2-isobutyl-1H-benzimidazol-5-ylmethyl group at position 3. It also has a 2-hydroxyethyl group at position 4.	554458-47-8	6.9547	6.8241	6.8359

G2-100*	A complex organic molecule featuring a central benzimidazole ring system. It has a 2,4,6-trimethylphenyl group attached to the benzimidazole nitrogen, a 2-ethylbutyl group attached to the imidazole nitrogen, and a 4-(2,4,6-trimethylphenyl)phenyl group attached to the imidazole ring. A 2-aminoethyl group is attached to the benzimidazole ring at the 5-position.	554457-86-2	6.1586	5.7461	6.0448
G2-101	A complex organic molecule similar to G2-100*, but with a 2-aminoethyl group attached to the benzimidazole ring at the 6-position.	554457-64-6	5.1481	5.0281	5.3778
G2-102	A complex organic molecule similar to G2-100*, but with a 2-aminoethyl group attached to the benzimidazole ring at the 7-position.	554457-62-4	7.2441	7.4337	7.2810
G2-103*	A complex organic molecule similar to G2-100*, but with a 2-aminoethyl group attached to the benzimidazole ring at the 8-position.	554457-61-3	3.7399	3.6330	3.2739
G2-104	A complex organic molecule similar to G2-100*, but with a 2-aminoethyl group attached to the benzimidazole ring at the 9-position.	554457-59-9	6.8729	6.9305	7.0508
G2-105	A complex organic molecule similar to G2-100*, but with a 2-aminoethyl group attached to the benzimidazole ring at the 10-position.	554457-54-4	7.0223	7.1461	6.9213
G2-106	A complex organic molecule similar to G2-100*, but with a 2-aminoethyl group attached to the benzimidazole ring at the 11-position.	554457-49-7	6.1599	6.6069	6.6736

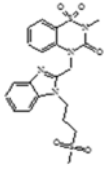
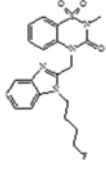
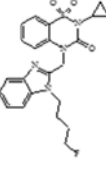
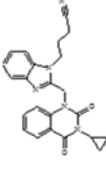
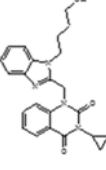
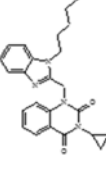
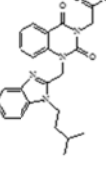
G2-107		554457-48-6	6.2007	6.3430	6.7126
G2-108		554457-47-5	6.9031	6.9343	7.0865
G2-109		554457-45-3	7.7447	7.7088	7.4076
G2-110*		554457-30-6	7.5086	7.5610	7.7921
G2-111		554457-29-3	8.0458	7.9796	8.1423
G2-112		554457-28-2	7.7959	7.9648	7.5246
G2-113*		554457-22-6	8.3979	8.0013	8.3632

G2-114		554457-21-5	8.3010	8.0123	8.4416
G2-115*		554457-20-4	7.3279	7.1798	7.5286
G2-116		554457-19-1	5.3635	5.4791	5.4485
G2-117		554457-18-0	6.9318	6.9451	6.6343
G2-118		554457-17-9	6.4401	6.2259	6.6273
G2-119*		554457-16-8	7.2441	7.7042	7.7880
G2-120		554457-14-6	6.7799	6.5717	6.7258

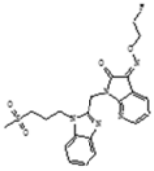
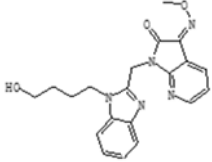
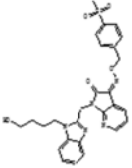
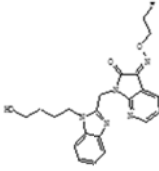
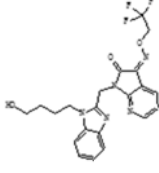
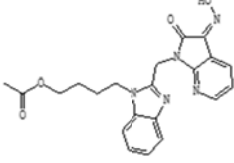
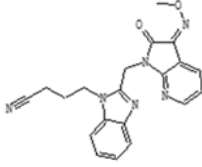
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G2-122		554457-12-4	7.3010	7.0466	7.2119
G2-123		554457-11-3	3.6234	3.7764	3.5886
G2-124*		554457-10-2	6.1397	6.1344	6.6869
G2-125		554457-09-9	6.2000	5.8298	6.3516
G2-126		554457-08-8	8.6990	8.7043	8.3397
G2-127		554457-07-7	6.3224	6.1842	6.4143

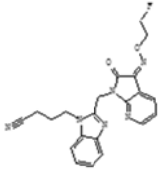
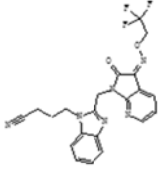
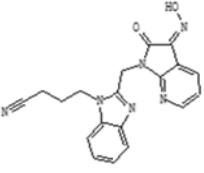
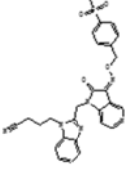
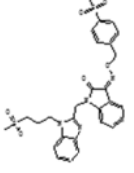
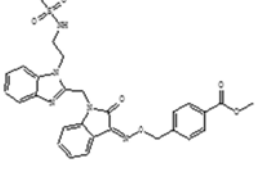
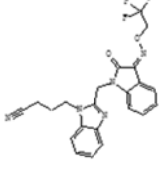
G2-128		543700-68-1	7.6778	7.6678	7.9162
G3-129		443987-52-8	7.3565	7.0565	7.4366
G3-130		443987-46-0	6.0448	6.1097	6.1749
G3-131		443987-44-8	6.6757	6.8096	7.0038
G3-132		443987-43-7	6.1035	6.1294	6.0340
G3-133*		443987-42-6	5.6373	5.4474	5.9468
G3-134		443987-41-5	6.8327	6.9162	6.7686

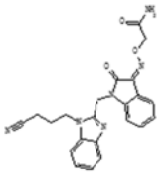
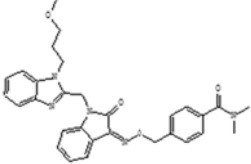
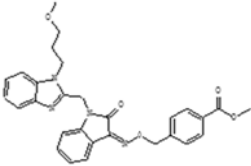
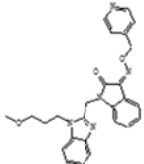
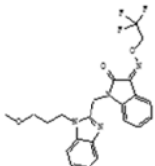
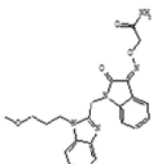
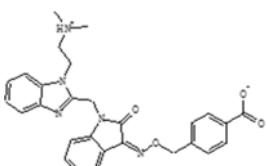
G3-135*	A complex polycyclic molecule featuring a central benzimidazole ring system. It is substituted with a phenyl group, a propyl chain, and a 1,2,4-triazole ring fused to a benzene ring.	443987-40-4	4.5864	4.5669	4.4791
G3-136	A complex polycyclic molecule similar to G3-135*, but with a different substitution pattern on the benzimidazole ring, including a propyl chain and a 1,2,4-triazole ring.	443987-32-4	5.1152	5.3793	4.9215
G3-138	A complex polycyclic molecule similar to G3-135*, but with a different substitution pattern on the benzimidazole ring, including a propyl chain and a 1,2,4-triazole ring.	443987-28-8	6.6402	6.3486	6.7532
G3-139	A complex polycyclic molecule similar to G3-135*, but with a different substitution pattern on the benzimidazole ring, including a propyl chain and a 1,2,4-triazole ring.	443987-27-7	5.9905	5.8269	6.5165
G3-140	A complex polycyclic molecule similar to G3-135*, but with a different substitution pattern on the benzimidazole ring, including a propyl chain and a 1,2,4-triazole ring.	443987-26-6	5.8729	6.1659	5.8642
G3-141*	A complex polycyclic molecule similar to G3-135*, but with a different substitution pattern on the benzimidazole ring, including a propyl chain and a 1,2,4-triazole ring.	443987-25-5	6.5622	6.7989	6.9010
G3-142	A complex polycyclic molecule similar to G3-135*, but with a different substitution pattern on the benzimidazole ring, including a propyl chain and a 1,2,4-triazole ring.	443987-21-1	7.7212	7.7220	7.5760

G3-143		443987-20-0	5.2418	5.4513	4.9915
G3-144		443987-19-7	7.4318	7.2872	7.1334
G3-145		443987-18-6	6.3645	6.6924	6.5601
G3-146		443987-09-5	6.7670	6.3699	6.7636
G3-147		443987-08-4	7.6021	7.5968	7.5269
G3-148		443987-07-3	7.3010	7.5059	7.3239
G3-149		443987-06-2	8.0458	7.9815	7.3401

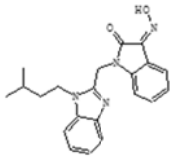
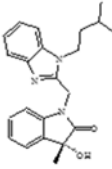
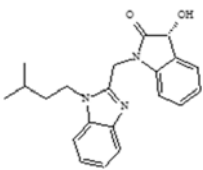
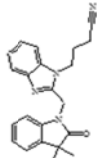
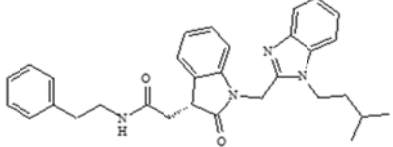
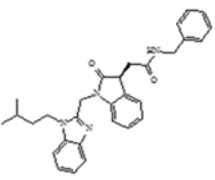
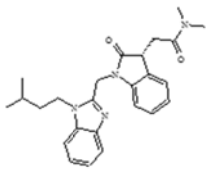
G3-150*	A complex molecule featuring a central benzimidazole ring system. One nitrogen is substituted with a tert-butyl group, and the other with a propyl group. The benzimidazole is linked via a methylene bridge to a pyridin-2(1H)-one ring, which is further substituted with a propyl ester group.	443987-05-1	5.7317	5.9483	5.8633
G3-151	A complex molecule with a central benzimidazole ring system. It features a propyl ester group and a 4-(2-fluorophenyl)butyl chain attached to the benzimidazole ring.	443987-04-0	6.3788	6.2187	6.3501
G1-152	A complex molecule with a central benzimidazole ring system. It features a propyl ester group and a 4-(2-fluorophenyl)butyl chain. The pyridinone ring has a hydroxyl group (HO) at the 2-position.	443986-99-0	7.7471	7.6304	7.8738
G1-153	A complex molecule with a central benzimidazole ring system. It features a propyl ester group and a 4-(2-fluorophenyl)butyl chain. The pyridinone ring has a hydroxyl group (HO) at the 2-position.	443986-96-7	7.5100	7.5310	7.8171
G1-154	A complex molecule with a central benzimidazole ring system. It features a propyl ester group and a 4-(2-fluorophenyl)butyl chain. The pyridinone ring has a hydroxyl group (HO) at the 2-position.	443986-94-5	7.9066	7.6229	7.9381
G1-155	A complex molecule with a central benzimidazole ring system. It features a propyl ester group and a 4-(2-fluorophenyl)butyl chain. The pyridinone ring has a hydroxyl group (HO) at the 2-position.	443986-93-4	7.2660	7.5551	7.7376
G1-156	A complex molecule with a central benzimidazole ring system. It features a propyl ester group and a 4-(2-fluorophenyl)butyl chain. The pyridinone ring has a hydroxyl group (HO) at the 2-position.	443986-91-2	7.9031	7.6198	7.9786

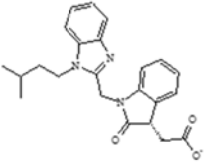
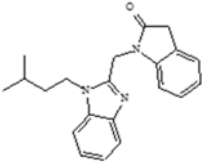
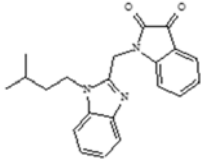
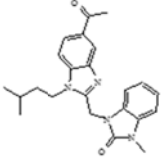
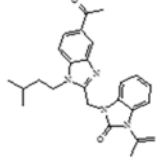
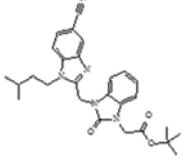
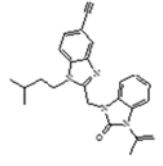
G1-157		443986-85-4	7.5346	7.4212	7.4933
G1-158		443986-84-3	7.5058	7.4216	7.5226
G1-159		443986-83-2	8.1367	8.0295	8.1325
G1-160		443986-82-1	7.3655	7.4100	7.4475
G1-161		443986-81-0	7.0980	7.1129	6.9815
G1-162		443986-80-9	7.3036	7.2556	7.4774
G1-163		443986-78-5	7.0325	7.1163	7.2751

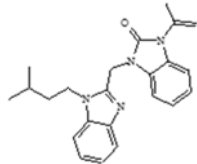
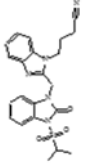
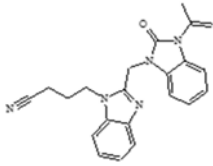
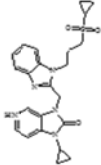
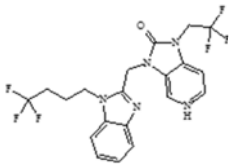
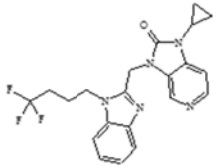
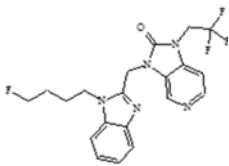
G1-164		443986-77-4	7.2418	7.3672	7.3564
G1-165		443986-76-3	6.9508	6.9553	7.4274
G1-166*		443986-75-2	7.6440	7.4963	7.7432
G1-167*		443986-71-8	4.9922	5.0407	4.7678
G1-168		443986-70-7	4.9749	5.1087	4.5344
G1-169*		443986-40-1	7.2924	7.4514	7.6497
G1-170*		443986-39-8	7.1805	7.2874	7.5792

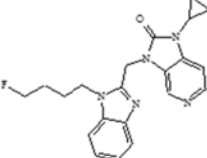
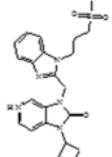
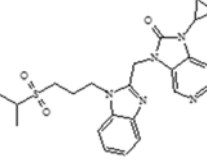
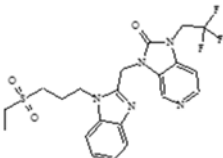
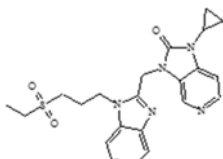
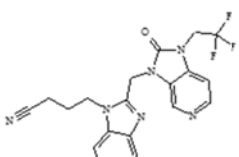
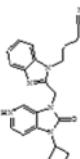
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G1-172		443986-35-4	7.5229	7.4733	7.4197
G1-173*		443986-33-2	7.3010	7.3116	7.2327
G1-174		443986-30-9	6.6162	6.6848	6.5086
G1-175		443986-29-6	7.1805	7.1901	7.1607
G1-176		443986-28-5	6.8125	6.6797	6.7510
G1-177		443986-23-0	7.7825	7.9118	7.7001

G1-178		443986-22-9	7.6383	7.4658	7.4717
G1-179		443986-20-7	5.9469	5.9630	6.2163
G1-180		443986-19-4	7.9208	8.0308	8.0360
G1-181		443986-15-0	7.6383	7.7728	7.5344
G1-182		443986-08-1	6.6946	6.6250	6.6454
G1-183		443986-07-0	6.4260	6.3651	6.6107
G1-184		443986-05-8	7.0605	7.2311	7.2095

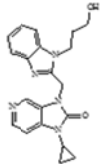
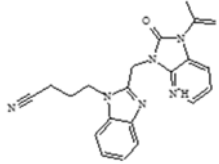
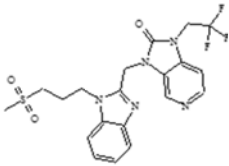
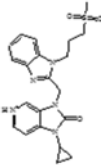
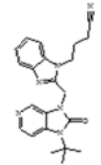
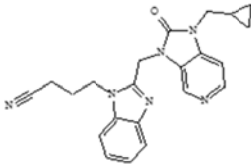
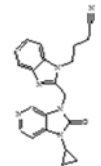
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G3-186		443985-86-2	7.0132	7.1859	7.0583
G3-187		443985-85-1	6.7852	6.5615	6.9803
G3-188		443985-82-8	7.7212	7.4593	7.8902
G3-189*		443985-80-6	6.4214	6.4250	6.4841
G3-190		443985-79-3	6.9586	6.8908	6.9148
G3-191		443985-78-2	6.6882	6.7500	6.6649

G3-192		443985-77-1	6.1518	6.1026	6.2727
G3-193*		443985-76-0	7.4948	7.2612	7.6503
G3-194*		443985-74-8	6.6383	6.9948	5.9464
G2-195		406944-77-2	6.7144	6.3843	6.5188
G2-196*		406944-75-0	6.7471	6.3261	6.2753
G2-197		406944-73-8	5.5935	5.6564	5.2523
G2-198		406944-70-5	7.2441	7.2010	6.8546

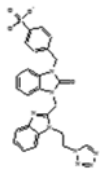
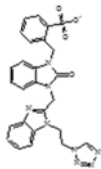
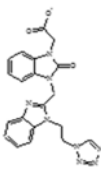
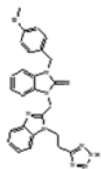
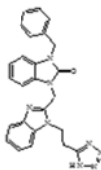
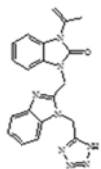
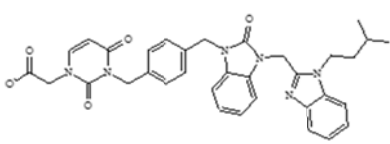
G2-199		406940-52-1	8.3979	8.2568	7.9406
G2-200		928164-16-3	7.1871	6.9642	7.3041
G2-205		406942-50-5	8.3010	8.2653	8.0175
G2-206		380604-55-7	7.7696	7.5222	7.8324
G2-212*		380604-26-2	7.2924	7.5672	7.4348
G2-213		380604-25-1	8.2218	7.9770	7.9818
G2-214		380604-23-9	7.8239	7.3315	8.3220

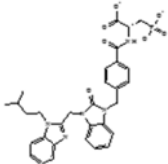
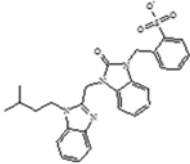
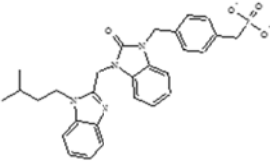
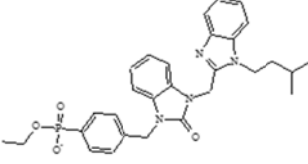
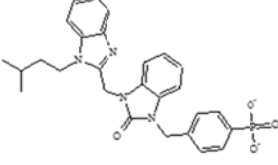
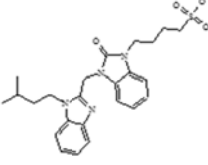
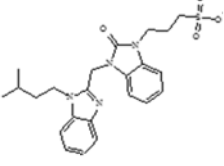
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G2-217		380604-02-4	6.6861	6.6212	6.7424
G2-218		380604-00-2	7.9586	7.8253	8.3535
G2-219		380603-98-5	8.2218	8.4693	8.4820
G2-220		380603-86-1	7.8239	7.7603	8.1157
G2-221		380603-79-2	7.7959	7.9515	7.6418

G2-222		380603-57-6	8.0969	8.0563	8.1364
G2-223		380603-55-4	8.1549	7.9633	8.1695
G2-224*		380603-45-2	7.4318	7.2945	7.5456
G2-225		380603-32-7	6.5143	6.4865	6.1597
G2-226		380603-27-0	8.0969	7.9867	8.4777
G2-227*		380603-22-5	6.9245	7.0565	6.6121
G2-228		380603-19-0	7.8697	8.2063	8.1766
G2-229		380603-16-7	7.6778	7.6650	7.3947

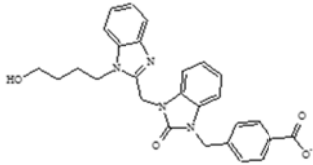
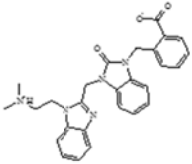
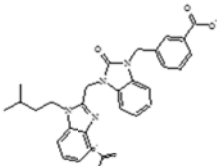
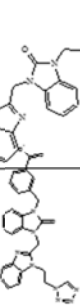
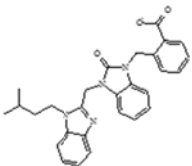
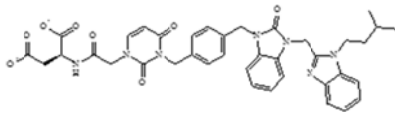
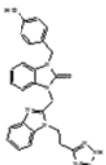
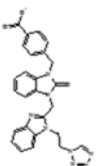
G2-230		380603-10-1	7.3665	7.3422	7.1020
G2-232		380602-63-1	8.5229	8.2046	8.0551
G2-233		380602-60-8	7.8239	7.9638	7.9570
G2-234		380602-59-5	8.3010	8.2436	8.3723
G2-236*		380602-55-1	7.5229	7.3713	7.6157
G2-237		380602-54-0	8.5229	8.4141	8.3353
G2-238		380602-53-9	8.0000	7.9942	7.8698

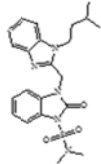
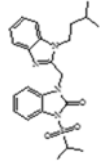
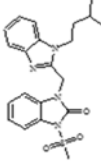
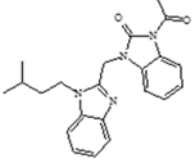
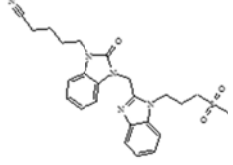
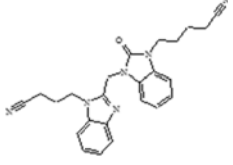
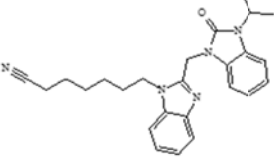
G2-239*	A complex heterocyclic molecule featuring a central benzimidazole core. It has a 4-cyanophenyl group attached to one nitrogen, a 2-(4-methyl-1H-imidazol-5-yl)ethyl group attached to the other nitrogen, and a 2-phenylethyl group attached to the 2-position of the benzimidazole ring.	380602-52-8	8.3979	8.0150	8.1401
G2-240	A complex heterocyclic molecule similar to G2-239*, but with a 2-(4-methyl-1H-imidazol-5-yl)ethyl group instead of a 2-phenylethyl group.	380602-51-7	8.2218	8.4524	8.1001
G2-241	A complex heterocyclic molecule similar to G2-239*, but with a 4-(methylsulfonyl)phenyl group instead of a 2-phenylethyl group.	380602-35-7	7.1249	7.2302	7.4416
G2-242*	A complex heterocyclic molecule similar to G2-239*, but with a 4-ethynylphenyl group instead of a 2-phenylethyl group.	380602-34-6	6.2062	6.3480	6.3619
G2-243	A complex heterocyclic molecule featuring a central benzimidazole core. It has a 2-(4-methyl-1H-imidazol-5-yl)ethyl group attached to one nitrogen, a 2-(2-hydroxyethyl)phenyl group attached to the other nitrogen, and a 2-phenylethyl group attached to the 2-position of the benzimidazole ring.	380602-33-5	6.6253	6.7043	6.8455
G2-244	A complex heterocyclic molecule similar to G2-239*, but with a 2-phenylethyl group instead of a 2-(4-methyl-1H-imidazol-5-yl)ethyl group.	380602-31-3	5.2434	5.0109	5.2084
G2-245	A complex heterocyclic molecule similar to G2-239*, but with a 2-(4-methyl-1H-imidazol-5-yl)ethyl group instead of a 2-phenylethyl group.	380602-28-8	6.6946	6.7663	6.7109

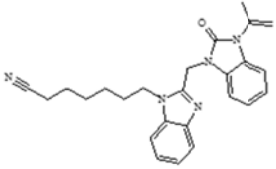
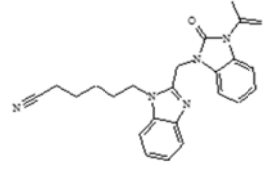
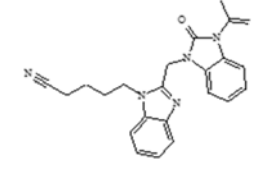
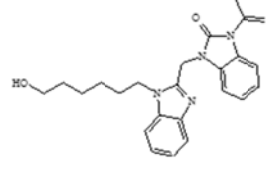
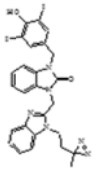
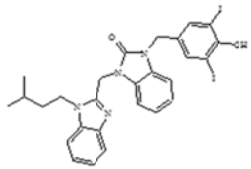
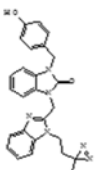
G2-248		880550-47-0	6.4342	6.4988	6.5548
G2-249		880550-46-9	7.8861	8.0408	7.7675
G2-250		880550-45-8	6.8097	6.7889	7.0977
G2-251		880550-44-7	6.4776	6.3759	6.6596
G2-252		880550-43-6	6.9431	6.8895	6.6962
G2-253*		880550-42-5	5.0738	5.1317	5.5766
G2-254		880550-41-4	8.5229	8.3743	8.4644

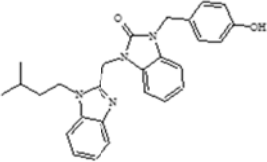
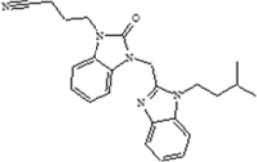
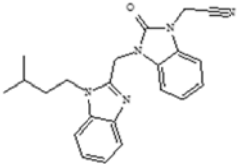
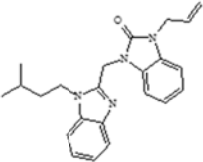
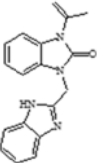
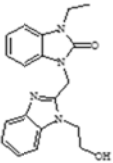
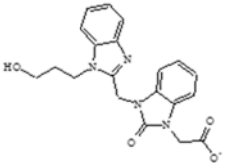
G2-255		880550-40-3	7.4685	7.5401	7.7183
G2-256		880550-39-0	8.1549	8.1639	7.9712
G2-257		880550-38-9	7.2924	7.4157	7.1191
G2-258*		880550-37-8	7.3188	7.2304	7.6679
G2-259		880550-36-7	7.5686	7.5407	7.4776
G2-260		880550-35-6	7.2840	7.4040	7.2676
G2-261		880550-34-5	7.4202	7.4295	7.4274

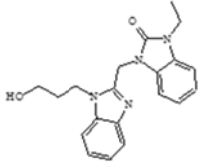
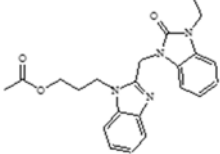
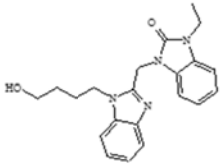
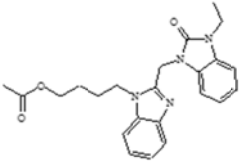
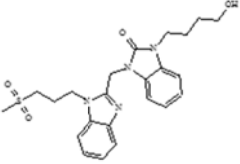
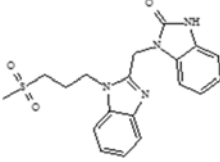
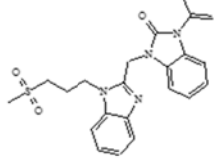
G2-262		880550-33-4	7.8861	7.8953	8.3039
G2-263		880550-32-3	6.6289	7.0212	6.5866
G2-264		880550-31-2	6.3010	6.2740	6.1939
G2-265*		880550-30-1	5.9158	6.0213	5.8942
G2-266		880550-29-8	6.2125	6.5345	5.4260
G2-267		880550-28-7	7.8239	7.5358	7.6140
G2-268		880550-27-6	6.7878	6.7625	6.8163

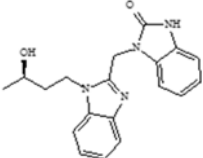
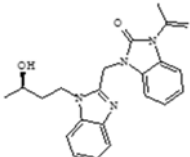
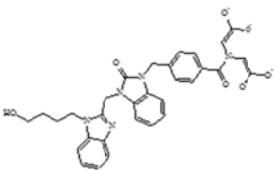
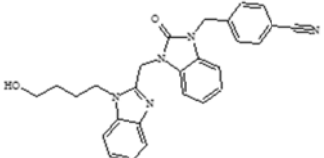
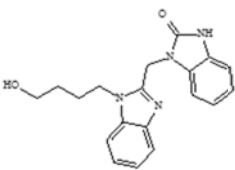
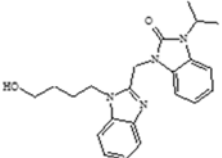
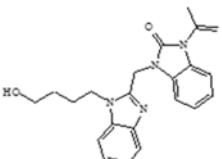
G2-269		792899-80-0	8.3979	8.0936	8.4428
G2-270		777846-71-6	6.8962	7.0364	6.9811
G2-271		769112-50-7	8.0000	7.9514	7.5618
G2-272		767280-09-1	8.1549	7.9130	8.0635
G2-273		755746-27-1	7.9586	7.8903	7.6748
G2-274*		750563-87-2	8.0969	8.0031	8.0089
G2-276		724420-50-2	7.2007	7.1996	6.9591
G2-277*		688736-16-5	7.8539	7.8772	8.4553

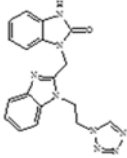
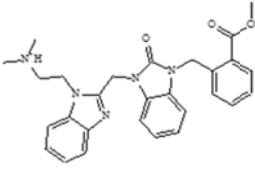
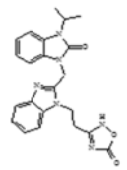
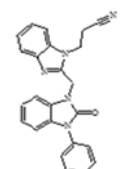
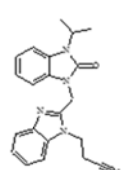
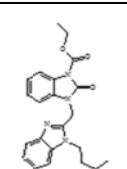
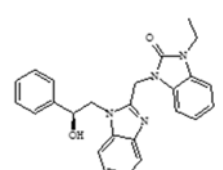
G2-278		682755-77-7	7.2076	7.4273	7.0991
G2-279		682755-75-5	7.1871	6.9496	7.1415
G2-280		682755-73-3	8.1549	8.3981	7.6490
G2-281		682755-71-1	6.1487	6.0042	6.3438
G2-282		682755-63-1	7.1487	7.3246	7.3185
G2-283		682755-59-5	7.6021	7.5059	7.4675
G2-284		682755-57-3	8.3010	8.3613	8.2790

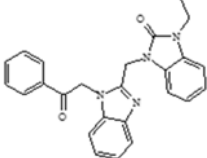
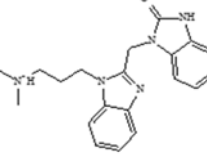
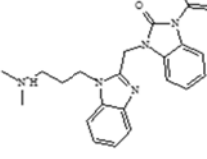
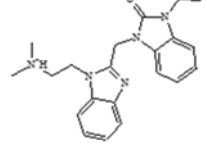
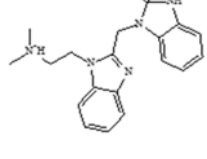
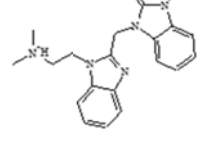
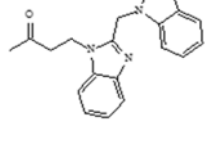
G2-285		682755-55-1	8.2218	8.0403	8.0790
G2-286*		682755-53-9	7.8861	8.0527	7.7739
G2-287		682755-51-7	7.5686	7.2953	7.7504
G2-288		682755-40-4	6.9431	7.2151	6.9164
G2-289*		682755-02-8	7.4202	7.2333	7.0473
G2-290		682754-99-0	6.1637	6.4011	6.7394
G2-291		682754-96-7	8.3979	8.3494	8.4518

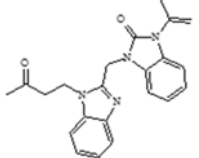
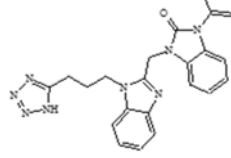
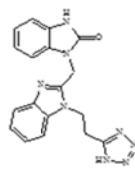
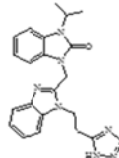
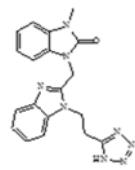
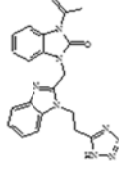
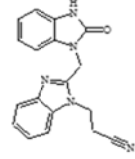
G2-292		682754-93-4	7.7447	7.6885	8.0926
G2-293		682754-87-6	7.3979	7.6563	7.2514
G2-294		682754-84-3	7.5528	7.6882	7.7397
G2-295		682754-81-0	7.7959	7.9428	7.4316
G2-296		406944-83-0	6.1249	6.3277	6.2251
G2-297		406944-48-7	6.6402	6.7253	6.9595
G2-298		406944-42-1	5.7144	5.6872	5.4458

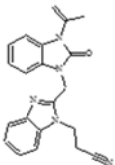
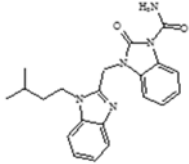
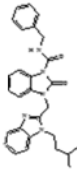
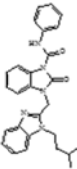
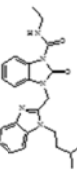
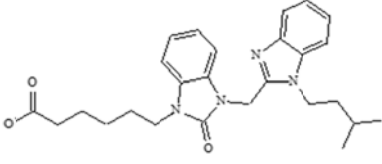
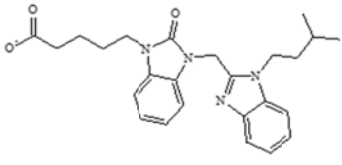
G2-299		406944-40-9	8.0000	7.6325	7.7468
G2-300*		406944-39-6	7.7447	7.4651	7.6569
G2-301		406944-37-4	7.8539	7.6865	7.8925
G2-302		406944-36-3	7.6778	7.1992	7.7475
G2-303		406944-27-2	7.0362	6.8508	7.1645
G2-304*		406944-25-0	5.8271	5.6133	5.8193
G2-305		406944-22-7	7.5229	7.5729	7.7578

G2-306		406944-10-3	6.3809	6.3045	6.6018
G2-307		406944-09-0	7.5528	7.4656	7.6806
G2-308*		406944-05-6	7.2441	7.2193	6.9986
G2-309		406944-01-2	7.2757	7.0268	7.2244
G2-310		406943-97-3	6.7620	6.7611	6.6927
G2-311		406943-96-2	7.9586	7.6619	7.9142
G2-312		406943-95-1	8.3979	8.2780	8.1736

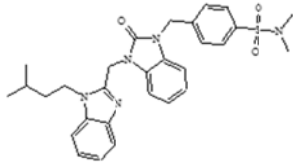
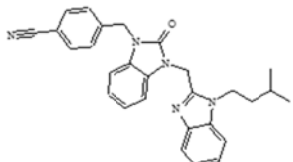
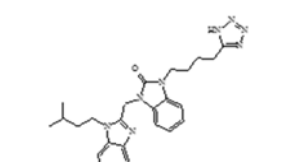
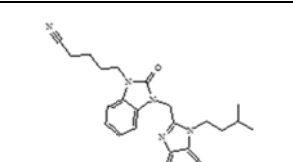
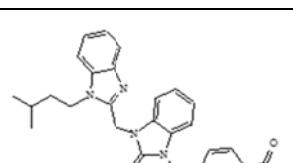
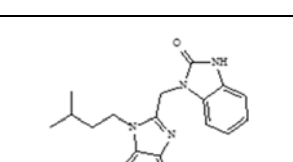
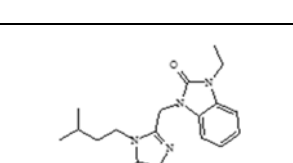
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G2-314		406943-32-6	7.7212	7.6192	7.3257
G2-316		406943-23-5	7.6778	7.5575	8.0865
G2-317*		406943-21-3	8.3010	8.0140	7.1719
G2-318		406943-20-2	8.0969	7.9262	7.5989
G2-319*		406943-16-6	6.5258	6.4333	6.0490
G2-320		406943-07-5	7.4318	7.3194	7.6095

G2-321		406943-05-3	6.9508	6.9215	6.6647
G2-322		406942-99-2	5.7786	6.1191	5.5992
G2-323		406942-98-1	7.1249	6.6986	7.2639
G2-324*		406942-73-2	7.8539	7.6354	7.4643
G2-325		406942-72-1	7.2076	6.9047	6.9431
G2-326		406942-71-0	7.9586	8.0928	7.8874
G2-327		406942-69-6	6.7190	6.5973	6.9841

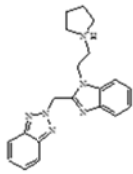
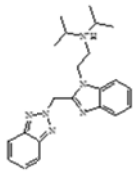
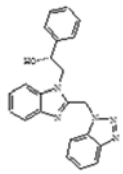
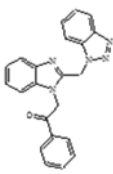
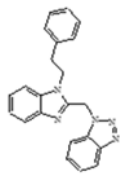
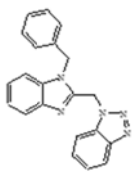
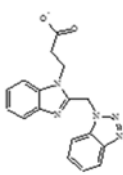
G2-328		406942-68-5	8.3010	8.3698	8.2921
G2-329		406942-51-6	7.8539	7.7106	7.5260
G2-331		406941-92-2	5.9970	6.1100	6.4835
G2-332		406941-91-1	7.8239	7.9149	8.1584
G2-333		406941-90-0	6.2269	6.3821	6.0873
G2-334*		406941-89-7	5.0738	5.1340	5.1399
G2-335		406941-88-6	7.0044	7.2208	6.7888

G2-336		406941-87-5	7.8239	7.8592	7.4385
G2-337		406941-82-0	7.3010	7.4335	7.2861
G2-338*		406941-75-1	7.0655	6.6516	7.0629
G2-339		406941-74-0	7.3872	7.5709	7.1532
G2-340		406941-73-9	7.2840	7.6446	7.3698
G2-341		406941-27-3	7.8239	7.7272	7.6058
G2-342		406941-26-2	8.0969	8.2544	7.9404

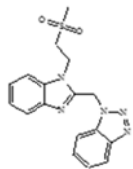
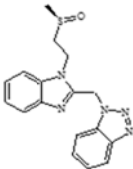
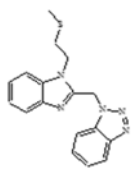
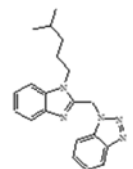
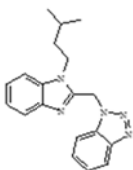
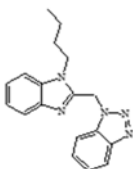
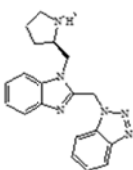
G2-343*	A complex organic molecule featuring a central benzimidazole ring system. It has an isobutyl group on the left nitrogen, a 2-oxo-1,2-diphenylethan-1-yl group on the right nitrogen, and a 4-oxo-4-(3-oxopropyl)butanoate group at the 2-position.	406941-25-1	7.1249	7.1769	7.1704
G2-344	A complex organic molecule similar to G2-343*, but with a 2-oxo-1,2-diphenylethan-1-yl group at the 2-position instead of a butanoate derivative.	406941-20-6	6.1831	6.0223	6.3718
G2-345	A complex organic molecule with a central benzimidazole ring system, an isobutyl group on the left nitrogen, and a 2-oxo-1,2-diphenylethan-1-yl group on the right nitrogen. It also features a 2-oxo-1,2-diphenylethan-1-yl group at the 2-position.	406941-15-9	8.2218	8.3546	8.0672
G2-346	A complex organic molecule with a central benzimidazole ring system. It has an isobutyl group on the left nitrogen, a 2-oxo-1,2-diphenylethan-1-yl group on the right nitrogen, and a 6-cyano-1-hexyl group at the 2-position.	406941-00-2	7.6021	7.4315	7.6682
G2-347	A complex organic molecule with a central benzimidazole ring system. It has an isobutyl group on the left nitrogen, a 2-oxo-1,2-diphenylethan-1-yl group on the right nitrogen, and a 2-oxo-1,2-diphenylethan-1-yl group at the 2-position. It also features a 2-oxo-1,2-diphenylethan-1-yl group at the 2-position.	406940-96-3	6.3979	6.5638	6.5030
G2-348*	A complex organic molecule with a central benzimidazole ring system. It has an isobutyl group on the left nitrogen, a 2-oxo-1,2-diphenylethan-1-yl group on the right nitrogen, and a 2-oxo-1,2-diphenylethan-1-yl group at the 2-position. It also features a 2-oxo-1,2-diphenylethan-1-yl group at the 2-position.	406940-95-2	6.5346	6.8861	7.0256
G2-349	A complex organic molecule with a central benzimidazole ring system. It has an isobutyl group on the left nitrogen, a 2-oxo-1,2-diphenylethan-1-yl group on the right nitrogen, and a 2-oxo-1,2-diphenylethan-1-yl group at the 2-position. It also features a 2-oxo-1,2-diphenylethan-1-yl group at the 2-position.	406940-91-8	8.0458	7.8845	8.1090

G2-350		406940-90-7	8.3979	8.2360	8.2507
G2-351		406940-88-3	7.9208	7.9457	8.0481
G2-352		406940-77-0	7.8239	7.8237	7.9100
G2-353		406940-76-9	7.4559	7.0688	7.2769
G2-356		406940-56-5	7.9586	8.1317	8.0631
G2-357*		406940-54-3	7.2441	7.0369	7.1116
G2-358		406940-53-2	7.9586	8.0197	7.4856

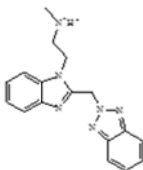
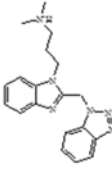
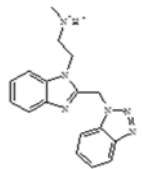
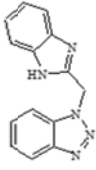
G3-360*	The structure shows a benzimidazole ring system with a methyl group on the nitrogen and a 2-phenyl-1H-benzimidazol-5-ylmethyl group attached to the 2-position of the benzimidazole ring.	574732-09-5	4.3233	4.0925	4.8520
G3-361	The structure shows a benzimidazole ring system with a methyl group on the nitrogen and a 2-(1H-benzotriazol-4-ylmethyl)benzimidazole group attached to the 2-position of the benzimidazole ring.	574732-08-4	4.2882	4.4274	4.4740
G3-366	The structure shows a benzimidazole ring system with a methyl group on the nitrogen and a 2-(1H-benzotriazol-4-ylmethyl)benzimidazole group attached to the 2-position of the benzimidazole ring.	574731-93-4	4.8097	4.7256	5.3148
G3-367	The structure shows a benzimidazole ring system with a methyl group on the nitrogen and a 2-(1H-benzotriazol-4-ylmethyl)benzimidazole group attached to the 2-position of the benzimidazole ring.	256366-13-9	5.5702	5.5378	5.7965
G3-368	The structure shows a benzimidazole ring system with a methyl group on the nitrogen and a 2-(1H-benzotriazol-4-ylmethyl)benzimidazole group attached to the 2-position of the benzimidazole ring.	256366-07-1	6.3565	6.4078	6.6007
G3-369	The structure shows a benzimidazole ring system with a methyl group on the nitrogen and a 2-(1H-benzotriazol-4-ylmethyl)benzimidazole group attached to the 2-position of the benzimidazole ring.	256366-06-0	5.9586	5.7527	5.8977
G3-370	The structure shows a benzimidazole ring system with a methyl group on the nitrogen and a 2-(1H-benzotriazol-4-ylmethyl)benzimidazole group attached to the 2-position of the benzimidazole ring.	256366-05-9	5.5850	5.6077	5.3354

G3-371		256366-04-8	6.3768	6.4864	6.4396
G3-372		256366-03-7	6.5850	6.6053	6.2998
G3-373		256366-02-6	6.2291	6.2270	6.1637
G3-374*		256366-01-5	5.6576	5.8714	5.7849
G3-375		256366-00-4	6.1135	6.2197	6.3603
G3-376		256365-98-7	4.9788	4.5203	5.1260
G3-377		256365-95-4	4.7423	4.6408	4.6929

G3-378*	<p>The structure shows a central benzimidazole ring system. One nitrogen is substituted with a 2,2,4,4-tetramethyl-1,3-dioxane-5-carbonyl group. The other nitrogen is substituted with a 1H-benzotriazol-4-ylmethyl group.</p>	256365-94-3	5.3655	5.4292	5.1005
G3-379	<p>The structure shows a central benzimidazole ring system. One nitrogen is substituted with a 2-aminoethyl group. The other nitrogen is substituted with a 1H-benzotriazol-4-ylmethyl group.</p>	256365-93-2	5.6778	5.9557	5.4784
G3-380	<p>The structure shows a central benzimidazole ring system. One nitrogen is substituted with a 2-aminoethyl group. The other nitrogen is substituted with a 1H-benzotriazol-4-ylmethyl group.</p>	256365-90-9	6.9208	6.6459	6.6588
G3-381	<p>The structure shows a central benzimidazole ring system. One nitrogen is substituted with a 2-aminoethyl group. The other nitrogen is substituted with a 1H-benzotriazol-4-ylmethyl group.</p>	256365-89-6	6.2840	6.5546	6.4583
G3-382*	<p>The structure shows a central benzimidazole ring system. One nitrogen is substituted with a 2-aminoethyl group. The other nitrogen is substituted with a 1H-benzotriazol-4-ylmethyl group.</p>	256365-88-5	6.6778	7.0122	6.6567
G3-383	<p>The structure shows a central benzimidazole ring system. One nitrogen is substituted with a 2-aminoethyl group. The other nitrogen is substituted with a 1H-benzotriazol-4-ylmethyl group.</p>	256365-86-3	5.4815	5.4113	5.5467
G3-384	<p>The structure shows a central benzimidazole ring system. One nitrogen is substituted with a 2-hydroxyethyl group. The other nitrogen is substituted with a 1H-benzotriazol-4-ylmethyl group.</p>	256365-83-0	5.1135	5.3208	5.3247

G3-385		256365-78-3	6.6021	6.7447	6.8153
G3-386*		256365-77-2	6.3665	6.4973	6.3293
G3-387		256365-76-1	6.5229	6.3333	6.8134
G3-388		256365-74-9	6.7212	6.4671	6.6927
G3-389		256365-72-7	7.0000	6.9225	6.7537
G3-390		256365-71-6	7.1805	6.9695	6.6531
G3-391		256365-70-5	6.0000	6.1495	6.0794

G3-392		256365-69-2	5.1331	5.1499	5.1593
G3-393		256365-68-1	5.5528	5.5456	5.5949
G3-394*		256365-67-0	5.9586	6.4371	5.6768
G3-395		256365-66-9	6.2218	6.6841	6.5662
G3-396		256365-62-5	5.1739	5.0185	5.2766
G3-399		6075-17-8	6.3279	6.5549	6.7315
G3-400*		5914-83-0	6.6576	6.4458	6.2927

G3-401		5823-63-2	6.7447	6.6509	6.2367
G3-403*		5823-61-0	5.9586	5.9402	5.7287
G3-404		5823-60-9	6.8539	6.8284	6.8621
G3-405		5823-54-1	4.5072	4.8298	4.6215

* Test set

Table S2. Selected descriptors in the VS-RF classification

Descriptor	Definition	Class
D299	The largest eigenvalue	Eigenvalue-based indices
D347	Molecular topological path index of order 07	Walk and path counts
D490	Moran topological structure autocorrelation length-4 weighted by atomic van der Waals volumes	2D autocorrelation
D503	Moran topological structure autocorrelation length-1 weighted by atomic polarizabilities	2D autocorrelation
D513	Molecular topological order-3 charge index	Topological charge indices
D528	Mean molecular topological order-8 charge index	Topological charge indices