



POLITECNICO DI TORINO

Master Degree course in Computer Engineering

Master Degree Thesis

Drug-likeness Prediction and Fragment Extraction using Transformer-based Graph Neural Network on Traditional Chinese Medicine Molecules

Supervisors

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Chapter 1

Supplementary

Cluster ID	TM-MC ID(s)	Status	References
0	8175	Drug	[1]
1	92061	Drug	[2]
2	99068, 97699	Experiments Needed	
3	435768, 1588	Drug	[3] , [4]
4	7795, 30171	Non Drug	[5] , [6]
5	200226, 367327	Drug	[7]
6	93083, 93195	No Info	
7	91919, 60334	Experiments Needed	[8]
8	238616, 99487	Drug	[9]
9	37545, 37556	Experiments Needed	
10	301922, 75704	Drug	[10]
11	90413	Drug	[11]
12	98859, 98860	No Info	
13	40376, 16114	Drug	[12] , [13]
14	70344, 9175	Drug	[14] , [15]
15	13489, 91662	Experiments Needed	[16]
16	94471, 94476	Drug	[17] , [18]
17	C94886, 300375	Experiments Needed	
18	82436, 300710	Drug	[19]
19	20237, 20241	Experiments Needed	
20	10581, 70185	Drug	[20]
21	40443, 40451	Drug	[21]
22	60207, 95238	Drug	[22] , [23]
23	99736, 637110	Drug	[24] , [25]
24	C94926, 91073	No Info	
25	97927, 97932	Drug	[26]
26	4125, 50331	Drug	[27]

Cluster ID	TM-MC ID(s)	Status	References
27	93921	Drug	[28]
28	396771, 4774	Drug	[29], [30]
29	90351, 93487	Experiments Needed	
30	789921, 99649	Drug	[31], [32]
31	6769, 94776	Drug	[33]
32	38090, 20248	Drug	[34]
33	40609, 781460	Drug	[35], [36]
34	442431, 173158	Drug	[37], [38]
35	92584, 10458	Drug	[39]
36	33866,	Drug	[40]
37	81028, 10657	Drug	[41], [42]
38	95834	Drug	[43]
39	301029, 9202	Drug	[44], [45]
40	95098, 95092	No Info	
41	70336, 280934	Drug	[46]
42	30314, 302082	Experiments Needed	[47]
43	160006, 800013	Drug	[48], [49]
44	80, 83	Drug	[50]
45	92607, 2014	Drug	[51], [52]
46	301170, 239	Drug	[53]
47	274591, 93176	Drug	[54], [55]
48	90407, 94453	Drug	[56]
49	301696, 94138	Drug	[57]
50	991588, 12738	Drug	[58], [59]
51	92558, 37795	Drug	[60], [61]
52		No Info	
53	93569, 784642	Drug	[62], [63], [64]
54	50389	Drug	[65]
55	327183, 524143	Drug	[66], [67]
56	242253, 300055	Experiments Needed	
57	312763	Drug	[68]
58	303054, 95514	Experiments Needed	[69]
59	98960, 91111	Drug	[70], [71]
60	301324, 33534	Drug	[72]
61	301789, 300413	No Info	
62	94491, 90710	Experiments Needed	[73]
63	256	Drug	[74]
64	60166, 60167	Drug	[75]
65	302050	Drug	[76]
66	95482, 95483	Drug	[77]
67	30108, 33515	Drug	[78]
68	316526, 300375	No Info	

Cluster ID	TM-MC ID(s)	Status	References
69	50720, 301326	Drug	[79]
70	99927, 60157	No Info	
71	35762, 94542	Drug	[80]
72	93497, 601115	Drug	[81]
73	82861, 4528	Drug	[82]
74	99451, 274587	Drug	[83], [84]
75	436647, 105	Drug	[85]
76	95598, 37756	Drug	[86]
77	38827, 95230	No Info	
78	90444, 91703	Experiments Needed	
79	301359, 95144	No Info	
80	724099, 721282	Drug	[87]
81	799238, 559171	Drug	[88]
82	64971	Drug	[89]
83	30057, 93988	No Info	
84	302702, 701272	Drug	[90]
85	424827, 882759	Drug	[91], [92]
86	301898, 701272	Drug	[93], [94]
87	30108, 33515	Drug	[95]
88	471007, 471008	Drug	[96],
89	90637, 269022	Drug	[97]
90	92245, 92246	No Info	
91	400592, 302218	Drug	[98]
92	99860, 95673	Drug	[99]
93	97825, 95877	Drug	[100], [101]
94	38067, 1995	Drug	[102]
95	579073, 14291	Experiments Needed	
96	90745, 91337	Drug	[103]
97	301676	Drug	[104], [105]
98	300260, 94834	Drug	[106]
99	814524	Drug	[107],
100	464082	Drug	[108]
101	20274, 299003	Drug	[109], [110]
102	6267, 179	Drug	[111], [112]
103	94201, 94203	Drug	[113],
104	94632	Drug	[114]
105	12471, 300178	Drug	[115]
106	303524, 303523	Drug	[116], [117]
107	98567, 10712	Drug	[118], [119]
108	132407, 129626	Drug	[120], [121]
109	70296, 300463	Drug	[122]
110	157085, 50022	Drug	[123]
111	90345, 95352	No Info	
112	302242, 301907	Experiments Needed	[124]

Cluster ID	TM-MC ID(s)	Status	References
113	9017, 837672	Drug	[125], [126]
114	10556, 442173	Drug	[127]
115	359271, 1093201556	Drug	[128]
116	93201, 93203	Drug	[129]
117	300712, 95110	Drug	[130], [131]
118	301243, 37685	Experiments Needed	
119	94040	Drug	[132],
120	43, 25	Drug	[133]
121	60120, 1164	No Info	
122	301785, 99406	Drug	[134], [135]
123	95092, 95098	No Info	
124	9259, 70076	Drug	[136], [137]
125	68381, 545772	Drug	[138], [139]
126	566705, 59900	Drug	[140], [141]
127	93428, 905172	Drug	[142]
128	300420, 98912	Drug	[143], [144]
129	94273, 30293	Drug	[145], [141]
130	3306, 30016	Drug	[146], [147]
131	935013, 935011	Drug	[148]
132	90907, 441677	Drug	[149], [150]
133	300741, 300744	Drug	[151]
134	38521, 99863	No Info	
135	60080, 60083	Drug	[152], [153]
136	92023, 92019	No Info	
137	20281, 90663	Drug	[154]
138	300171	Drug	[155]
139	95497, 302046	Drug	[156], [157]
140	300178, 90517	Drug	[158]
141	440983	Drug	[159]
142	97773, 93954	Drug	[160], [161]
143	50433, 8203	Experiments Needed	
144	96884, 13252	Drug	[162], [163]
145	99734, 628136	Drug	[164]
146	38714, 443916	Experiments Needed	[165]

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