Index	Feature	Network Architecture	Number of Hidden Layer	Number of Hidden Nodes per Hidden Layer	Test Mean Accuracy (%)	Macro Precision (%)	Macro Recall (%)	Macro F1 Score (%)	Micro Precision (%)	Micro Recall (%)	Micro F1 Score (%)	Composite Index (%)
1	Duo_c-MolDes_ c-ADMET	[1,128]	1	128	61	49.5	23.2	27.4	61	61	61	49.8
2	Duo_c-MolDes_ c-ADMET	[1,256]	1	256	70.4	69.4	36.5	43.1	70.4	70.4	70.4	61.3
3	Duo_c-MolDes_ c-ADMET	[1,512]	1	512	78.2	77.7	52.7	58.9	78.2	78.2	78.2	71.8
4	Duo_c-MolDes_ c-ADMET	[1,1024]	1	1024	82.9	81.6	64.1	68.7	82.9	82.9	82.9	78.1
5	Duo_c-MolDes_ c-ADMET	[2,128]	2	128	62.2	41.1	21.1	24.1	62.2	62.2	62.2	49.5
6	Duo_c-MolDes_ c-ADMET	[2,256]	2	256	75.4	63	45.4	49.7	75.4	75.4	75.4	66.8
7	Duo_c-MolDes_ c-ADMET	[2,512]	2	512	84.6	84.4	72.2	75.3	84.6	84.6	84.6	81.5
8	Duo_c-MolDes_ c-ADMET	[2,1024]	2	1024	90.4	89.2	85.1	86.2	90.4	90.4	90.4	89
9	Duo_c-MolDes_ c-ADMET	[3,128]	3	128	62.5	29.1	20.1	21.5	62.5	62.5	62.5	48.8
10	Duo_c-MolDes_ c-ADMET	[3,256]	3	256	75.6	60.3	44.8	47.4	75.6	75.6	75.6	66.2
11	Duo_c-MolDes_ c-ADMET	[3,512]	3	512	86.6	84	78.2	79	86.6	86.6	86.6	84.1
12	Duo_c-MolDes_ c-ADMET	[3,1024]	3	1024	81.7	68.3	60.7	61.5	81.7	81.7	81.7	75
13	Duo_SSP_ c-ADMET	[1,128]	1	128	76.5	71.5	46.8	52.8	76.5	76.5	76.5	68.6
14	Duo_SSP_ c-ADMET	[1,256]	1	256	84.8	88.8	71	76.5	84.8	84.8	84.8	82.1
15	Duo_SSP_ c-ADMET	[1,512]	1	512	89.3	93.1	85.2	87.8	89.3	89.3	89.3	88.8
16	Duo_SSP_ c-ADMET	[1,1024]	1	1024	92.5	94.4	89.7	91.5	92.5	92.5	92.5	92.2
17	Duo_SSP_ c-ADMET	[2,128]	2	128	75.2	54.1	38.5	42.1	75.2	75.2	75.2	64.2
18	Duo_SSP_ c-ADMET	[2,256]	2	256	85.3	82.5	71	73.8	85.3	85.3	85.3	81.4
19	Duo_SSP_ c-ADMET	[2,512]	2	512	92.1	92.9	89.1	90.1	92.1	92.1	92.1	91.4
20	Duo_SSP_ c-ADMET	[2,1024]	2	1024	95.1	94.2	93.9	93.9	95.1	95.1	95.1	94.7
21	Duo_SSP_ c-ADMET	[3,128]	3	128	74	45.3	33.7	35.7	74	74	74	61.2
22	Duo_SSP_ c-ADMET	[3,256]	3	256	84.8	76.9	67.2	68.7	84.8	84.8	84.8	79.5
23	Duo_SSP_ c-ADMET	[3,512]	3	512	92.4	91	91.8	90.6	92.4	92.4	92.4	91.8
24	Duo_SSP_ c-MolDes	[1,128]	1	128	75.4	74	47.7	53.8	75.4	75.4	75.4	68.2
25	Duo_SSP_ c-MolDes	[1,256]	1	256	83.5	87.8	69.8	75.2	83.5	83.5	83.5	80.8
26	Duo_SSP_ c-MolDes	[1,512]	1	512	88.7	91	84.7	86.7	88.7	88.7	88.7	88
27	Duo_SSP_ c-MolDes	[1,1024]	1	1024	91.5	91.9	87.7	88.9	91.5	91.5	91.5	90.6
28	Duo_SSP_ c-MolDes	[2,128]	2	128	73.7	55.6	36.9	40.6	73.7	73.7	73.7	62.7
29	Duo_SSP_ c-MolDes	[2,256]	2	256	84.6	85.8	70.9	74.4	84.6	84.6	84.6	81.2
30	Duo_SSP_ c-MolDes	[2,512]	2	512	91.7	91.3	89.4	89.6	91.7	91.7	91.7	91
31	Duo_SSP_ c-MolDes	[2,1024]	2	1024	94.8	94.2	93.1	93.3	94.8	94.8	94.8	94.3
32	Duo_SSP_ c-MolDes	[3,128]	3	128	73.8	45	33.1	34.8	73.8	73.8	73.8	60.8
33	Duo_SSP_ c-MolDes	[3,256]	3	256	84.3	80.6	67.6	70.4	84.3	84.3	84.3	79.7
34	Duo_SSP_ c-MolDes	[3,512]	3	512	91.9	88.8	90.8	89	91.9	91.9	91.9	90.9
35	Mono_c-ADMET	[1,128]	1	128	47	29.6	9.7	11.7	47	47	47	35.3
36	Mono_c-ADMET	[1,256]	1	256	52.6	40	13.5	17	52.6	52.6	52.6	40.8

Index	Feature	Network Architecture	Number of Hidden Layer	Number of Hidden Nodes per Hidden Layer	Test Mean Accuracy (%)	Macro Precision (%)	Macro Recall (%)	Macro F1 Score (%)	Micro Precision (%)	Micro Recall (%)	Micro F1 Score (%)	Composite Index (%)
37	Mono_c-ADMET	[1,512]	1	512	57.3	46.9	19.9	24.7	57.3	57.3	57.3	46.4
38	Mono_c-ADMET	[1,1024]	1	1024	61.6	56.2	29.7	35.2	61.6	61.6	61.6	52.8
39	Mono_c-ADMET	[2,128]	2	128	49	23.5	10.3	12.2	49	49	49	36.7
40	Mono_c-ADMET	[2,256]	2	256	57.5	43	21	25.3	57.5	57.5	57.5	46.8
41	Mono_c-ADMET	[2,512]	2	512	64.9	54.5	32.3	37.1	64.9	64.9	64.9	55.7
42	Mono_c-ADMET	[2,1024]	2	1024	68.6	53.7	43.3	45.8	68.6	68.6	68.6	61
43	Mono_c-ADMET	[3,128]	3	128	49.5	24.3	11.1	12.7	49.5	49.5	49.5	37.2
44	Mono_c-ADMET	[3,256]	3	256	57.7	39.2	21.4	24.4	57.7	57.7	57.7	46.6
45	Mono_c-ADMET	[3,512]	3	512	64.8	49.6	34.8	38	64.8	64.8	64.8	55.9
46	Mono_c-ADMET	[3,1024]	3	1024	68.1	53.6	45.2	46.1	68.1	68.1	68.1	60.8
47	Mono_c-ADMET	[4,128]	4	128	49	18.7	10.5	11.6	49	49	49	36.6
48	Mono_c-ADMET	[4,256]	4	256	56.8	36.6	20.3	22.9	56.8	56.8	56.8	45.5
49	Mono_c-ADMET	[4,512]	4	512	64.4	46.6	33.7	35.9	64.4	64.4	64.4	54.9
50	Mono_c-ADMET	[4,1024]	4	1024	67.5	50.1	44.7	44.8	67.5	67.5	67.5	60
51	Mono_c-MolDes	[1,128]	1	128	48.1	31.9	12.9	15.2	48.1	48.1	48.1	37.1
52	Mono_c-MolDes	[1,256]	1	256	53.6	43.3	18.3	22.1	53.6	53.6	53.6	43.1
53	Mono_c-MolDes	[1,512]	1	512	58.6	58.4	25.1	30.7	58.6	58.6	58.6	49.3
54	Mono_c-MolDes	[1,1024]	1	1024	63	64.1	33.1	39.7	63	63	63	55.2
55	Mono_c-MolDes	[2,128]	2	128	51.4	32.6	13.8	16	51.4	51.4	51.4	39.6
56	Mono_c-MolDes	[2,256]	2	256	63.2	55.1	30	34.6	63.2	63.2	63.2	53.7
57	Mono_c-MolDes	[2,512]	2	512	73.5	69.4	49.1	54.6	73.5	73.5	73.5	67.2
58	Mono_c-MolDes	[2,1024]	2	1024	80.8	78.2	66.6	69.8	80.8	80.8	80.8	77.1
59	Mono_c-MolDes	[3,128]	3	128	51.4	25	13.7	14.8	51.4	51.4	51.4	39.2
60	Mono_c-MolDes	[3,256]	3	256	64.6	49.6	30	33.8	64.6	64.6	64.6	54.3
61	Mono_c-MolDes	[3,512]	3	512	76.2	72.6	58.1	61.1	76.2	76.2	76.2	71.2
62	Mono_c-MolDes	[3,1024]	3	1024	83.7	78.9	73.4	74.6	83.7	83.7	83.7	80.7
63	Mono_c-MolDes	[4,128]	4	128	52.3	20.6	14.1	14.6	52.3	52.3	52.3	39.8
64	Mono_c-MolDes	[4,256]	4	256	64.6	42.4	28.6	31.1	64.6	64.6	64.6	53.4
65	Mono_c-MolDes	[4,512]	4	512	77.4	72.5	62.5	63.7	77.4	77.4	77.4	72.8
66	Mono_c-MolDes	[4,1024]	4	1024	84.6	79.8	78.9	79.1	84.6	84.6	84.6	82.8
67	Mono_SSP	[1,128]	1	128	72.4	70.9	41.1	47.5	72.4	72.4	72.4	64.1
68	Mono_SSP	[1,256]	1	256	81.3	83.9	63.6	69.5	81.3	81.3	81.3	77.3
69	Mono_SSP	[1,512]	1	512	87	90.2	79.1	82.7	87	87	87	85.5
70	Mono_SSP	[1,1024]	1	1024	90.4	92.3	87.1	89	90.4	90.4	90.4	89.9
71	Mono_SSP	[2,128]	2	128	71.8	54.2	35.1	38.7	71.8	71.8	71.8	60.8
72	Mono_SSP	[2,256]	2	256	82.9	80	66.1	69.8	82.9	82.9	82.9	78.5

Index	Feature	Network Architecture	Number of Hidden Layer	Number of Hidden Nodes per Hidden Layer	Test Mean Accuracy (%)	Macro Precision (%)	Macro Recall (%)	Macro F1 Score (%)	Micro Precision (%)	Micro Recall (%)	Micro F1 Score (%)	Composite Index (%)
73	Mono_SSP	[2,512]	2	512	90.1	90.7	87.8	88.4	90.1	90.1	90.1	89.5
74	Mono_SSP	[2,1024]	2	1024	94.4	93.6	92.2	92.5	94.4	94.4	94.4	93.7
75	Mono_SSP	[3,128]	3	128	71	42.5	31.2	33.4	71	71	71	58.4
76	Mono_SSP	[3,256]	3	256	82.3	75.3	66	67.1	82.3	82.3	82.3	77.3
77	Mono_SSP	[3,512]	3	512	91.7	90	91.2	89.9	91.7	91.7	91.7	91.1
78	Mono_SSP	[3,1024]	3	1024	95	91.5	93.7	92.3	95	95	95	94.1
79	Mono_SSP	[4,128]	4	128	69.4	35.2	27.5	28.5	69.4	69.4	69.4	55.8
80	Mono_SSP	[4,256]	4	256	81.7	65.7	60.5	60.7	81.7	81.7	81.7	74.7
81	Mono_SSP	[4,512]	4	512	91.2	89.4	89	88.2	91.2	91.2	91.2	90.2
82	Mono_SSP	[4,1024]	4	1024	92.8	88.6	93.2	90.2	92.8	92.8	92.8	91.9
83	Triple	[1,128]	1	128	78.7	77	52.1	58.6	78.7	78.7	78.7	72
84	Triple	[1,256]	1	256	86.1	89	74.2	78.7	86.1	86.1	86.1	83.7
85	Triple	[1,512]	1	512	90.5	93.5	87.2	89.3	90.5	90.5	90.5	90.1
86	Triple	[1,1024]	1	1024	93	94.1	90.5	91.9	93	93	93	92.6
87	Triple	[2,128]	2	128	77.2	56.3	42	45.3	77.2	77.2	77.2	66.6
88	Triple	[2,256]	2	256	86.2	84.9	72.4	75.5	86.2	86.2	86.2	82.6
89	Triple	[2,512]	2	512	92.7	93.6	90.7	91.7	92.7	92.7	92.7	92.4
90	Triple	[2,1024]	2	1024	95.3	94.4	93.8	93.9	95.3	95.3	95.3	94.8
91	Triple	[3,128]	3	128	76	45.8	36	37.5	76	76	76	63.2
92	Triple	[3,256]	3	256	85.9	80.5	71	72.7	85.9	85.9	85.9	81.5
93	Triple	[3,512]	3	512	93.2	92	92.1	91.4	93.2	93.2	93.2	92.6
94	Triple	[3,1024]	3	1024	95.7	93.1	94.5	93.6	95.7	95.7	95.7	95
95	Triple	[4,128]	4	128	74.6	38.5	31.2	31.5	74.6	74.6	74.6	60.3
96	Triple	[4,256]	4	256	85.4	68.9	62.6	63.1	85.4	85.4	85.4	78
97	Triple	[4,512]	4	512	93.1	89.4	91.1	89.5	93.1	93.1	93.1	91.9
98	Triple	[4,1024]	4	1024	95.7	93.4	95.1	94.1	95.7	95.7	95.7	95.2
99	Triple	[5,128]	5	128	73.8	31.9	27.6	27.2	73.8	73.8	73.8	58.3
100	Triple	[5,256]	5	256	84.5	64.5	59.4	60	84.5	84.5	84.5	76.3
101	Triple	[5,512]	5	512	92.6	87.9	91.6	88.4	92.6	92.6	92.6	91.2
102	Triple	[5,1024]	5	1024	95.4	92.7	94.8	93.5	95.4	95.4	95.4	94.8
103	Triple	[6,128]	6	128	72.8	25	25.2	24	72.8	72.8	72.8	56.5
104	Triple	[6,256]	6	256	84.4	59	56.6	56.3	84.4	84.4	84.4	75
105	Triple	[6,512]	6	512	92.2	86.3	88.3	86	92.2	92.2	92.2	90.1
106	Triple	[6,1024]	6	1024	95.6	91.7	95.1	93.2	95.6	95.6	95.6	94.8
107	Triple	[7,128]	7	128	71.9	22.6	22.7	22	71.9	71.9	71.9	55.2
108	Triple	[7,256]	7	256	84.1	57.1	55.7	55.2	84.1	84.1	84.1	74.4

Index	Feature	Network Architecture	Number of Hidden Layer	Number of Hidden Nodes per Hidden Layer	Test Mean Accuracy (%)	Macro Precision (%)	Macro Recall (%)	Macro F1 Score (%)	Micro Precision (%)	Micro Recall (%)	Micro F1 Score (%)	Composite Index (%)
109	Triple	[7,512]	7	512	92.3	85.8	89.1	86	92.3	92.3	92.3	90.2
110	Triple	[7,1024]	7	1024	95.6	91.6	94.7	92.8	95.6	95.6	95.6	94.7
111	Triple	[8,128]	8	128	72.6	23.6	22.4	21.4	72.6	72.6	72.6	55.5
112	Triple	[8,256]	8	256	83.6	55.4	52.1	52.5	83.6	83.6	83.6	73.3
113	Triple	[8,512]	8	512	92.2	85	88.2	85.2	92.2	92.2	92.2	89.9
114	Triple	[8,1024]	8	1024	95.3	91.7	94.6	92.8	95.3	95.3	95.3	94.5