| | | | | Number of Hidden | | | | | | | | |
|-------|-----------------------|--------------|--------------|---------------------|-----------|-----------|--------|----------|---------|--------|--------------|-----------|
| | | | | Nodes | | | | | Micro | | | |
| | | | | per | Test Mean | Macro | Macro | Macro | Precisi | Micro | | Composite |
| | | Network | Number of | Hidden | Accuracy | Precision | Recall | F1 Score | on | Recall | Micro | Index |
| Index | Feature | Architecture | Hidden Layer | Layer | (%) | (%) | (%) | (%) | (%) | (%) | F1 Score (%) | |
| 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 |

| Network Netw | | | | | | | | | | | | | |
|--|-------|---------------|--------------|--------------|--------|-----------|-----------|--------|-------|---------|--------|--------------|-----------|
| Network Number of Hidden Accuracy Precision Recall El Score On Recall Micro Index | | | | | Hidden | | | | | Micro | | | |
| Note Festure Architecture Hidden Layer Layer C50 C51 C51 | | | | | per | Test Mean | Macro | Macro | Macro | Precisi | Micro | | Composite |
| ST Mono_cADMET 1,512 1 512 57.3 46.9 19.9 24.7 57.3 57.3 57.3 46.4 | | | Network | Number of | Hidden | Accuracy | Precision | Recall | | on | Recall | Micro | Index |
| 18 | Index | | Architecture | Hidden Layer | Layer | (%) | (%) | (%) | (%) | (%) | (%) | F1 Score (%) | (%) |
| 99 Mono c-ADMET [2,128] 2 128 49 235 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 [2,512] 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 49.5 37.2 44 Mono c-ADMET [3,128] 3 128 49.5 128 49.5 24.3 11.1 12.7 49.5 49.5 49.5 49.5 37.2 44 Mono c-ADMET [3,128] 3 128 49.5 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 64.8 55.9 46.6 Mono c-ADMET [3,1024] 3 1024 68.1 53.6 45.2 46.1 68.1 68.1 68.1 68.1 68.1 68.0 46 Mono c-ADMET [3,1024] 4 128 49 18.7 10.5 11.6 49 49 49 49 49 63.6 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 [4,256] 4 256 56.8 36.6 20.3 22.9 56.8 56.8 56.8 45.5 49 Mono c-ADMET [4,1024] 4 1024 67.5 50.1 44.7 44.8 67.5 67.5 67.5 60.5 10 Mono c-ADMET [4,1024] 4 1024 67.5 50.1 44.7 44.8 67.5 67.5 67.5 60.5 10 Mono c-MOIDES [1,128] 1 128 48.1 131.9 12.9 15.2 48.1 48.1 48.1 37.1 15.1 Mono c-MOIDES [1,128] 1 128 48.1 131.9 12.9 15.2 48.1 48.1 48.1 37.1 15.1 Mono c-MOIDES [1,128] 1 128 48.1 131.9 12.9 15.2 48.1 48.1 48.1 37.1 15.1 Mono c-MOIDES [1,128] 1 128 48.1 31.9 12.9 15.2 48.1 48.1 48.1 37.1 15.1 15.1 15.2 58.6 58.6 58.4 25.1 30.7 58.6 58.6 58.6 49.3 58.5 59.6 Mono c-MOIDES [1,128] 2 128 51.4 32.6 13.8 16.5 13.4 51.4 51.4 51.4 51.4 51.4 51.4 51.4 51 | | Mono_c-ADMET | [1,512] | 1 | 512 | 57.3 | | 19.9 | | 57.3 | 57.3 | 57.3 | 46.4 |
| A0 Mono_CADMET (2,256) 2 256 57.5 43 21 25.3 57.5 57.5 46.8 | | Mono_c-ADMET | | | | | | | | | | | |
| 41 Mono_c-ADMET | | Mono_c-ADMET | | | | | | | | | | | |
| A2 Mono_c-ADMET | | Mono_c-ADMET | | | | | | | | | | | |
| Mono_c-ADMET (3,128) 3 128 49.5 24.3 11.1 12.7 49.5 49.5 37.2 | | Mono_c-ADMET | | | | 64.9 | 54.5 | 32.3 | 37.1 | 64.9 | 64.9 | 64.9 | 55.7 |
| ## Mono_c-ADMET | | Mono_c-ADMET | | | | | | | | | | | |
| 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 49 36.6 48 Mono_c-ADMET [4,128] 4 128 49 18.7 10.5 11.6 49 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 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 53.6 43.1 52 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 63 55.2 55 Mono_c-MolDes [2,128] 2 128 51.4 32.6 13.8 16 51.4 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 73.5 67.2 58 Mono_c-MolDes [2,128] 3 128 51.4 25 13.7 14.8 51.4 51.4 51.4 39.6 59 Mono_c-MolDes [2,512] 2 512 73.5 69.4 49.1 54.6 73.5 73.5 73.5 73.5 67.2 58 Mono_c-MolDes [3,128] 3 128 51.4 25 13.7 14.8 51.4 51.4 51.4 39.6 59 Mono_c-MolDes [3,128] 3 128 51.4 25 13.7 14.8 51.4 51.4 51.4 39.6 59 Mono_c-MolDes [3,128] 3 128 51.4 25 13.7 14.8 51.4 51.4 51.4 39.2 50 Mono_c-MolDes [3,128] 3 128 51.4 25 13.7 14.8 51.4 51.4 51.4 39.2 51.4 51.4 51.4 51.4 51.4 51.4 51.4 51.4 | | Mono_c-ADMET | | | | | | 11.1 | | | | 49.5 | - |
| 46 Mono_c-ADMET [3,1024] 3 1024 68.1 53.6 45.2 46.1 68.1 68.1 60.8 47 Mono_c-ADMET [4,128] 4 128 49 18.7 10.5 11.6 49 49 36.6 48 Mono_c-ADMET [4,526] 4 256 56.8 36.6 20.3 22.9 56.8 56.9 56.9 56.0 56.0 56.0 56.0 56.0 56.0 56.0 57.5 67.5 67.5 60.0 56.0 56.0 56.0 58.6 58.4 25.1 30.7 58.6 58.6 49.3 36.3 63.2 53.6 58.6 58.6 58.6 | | Mono_c-ADMET | [3,256] | | | 57.7 | 39.2 | 21.4 | | | 57.7 | 57.7 | 46.6 |
| 47 Mono_c-ADMET [4,128] 4 128 49 18.7 10.5 11.6 49 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 66.4 46.6 33.7 35.9 66.4 64.4 64.4 64.5 4.9 50 Mono_c-ADMET [4,1024] 4 1024 67.5 50.1 44.7 44.8 67.5 67.5 67.5 67.5 60 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 [1,512] 1 256 53.6 43.3 18.3 22.1 53.6 53.6 53.6 53.6 43.3 18.3 22.1 53.6 53.6 53.6 53.6 43.3 18.3 22.1 53.6 53.6 53.6 53.6 49.3 53 Mono_c-MolDes [1,512] 1 512 58.6 58.4 25.1 30.7 58.6 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 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 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 58 Mono_c-MolDes [3,128] 3 128 51.4 25 13.7 14.8 51.4 51.4 51.4 51.4 51.4 51.4 51.4 51.4 | | Mono_c-ADMET | | | | | | | | | | | |
| 48 Mono_c-ADMET [4,256] 4 256 56.8 36.6 20.3 22.9 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 54.9 50 Mono_c-ADMET [4,1024] 4 1024 67.5 50.1 44.7 44.8 67.5 67.5 60.0 51 Mono_c-MolDes [1,128] 1 128 48.1 31.9 12.9 15.2 48.1 48.1 37.1 52 Mono_c-MolDes [1,512] 1 512 58.6 58.4 25.1 30.7 58.6 58.6 43.1 53 Mono_c-MolDes [1,512] 1 1024 63 64.1 33.1 39.7 63 63 63 55.2 54 Mono_c-MolDes [2,128] 2 128 51.4 32.6 13.8 16 51.4 51.4 39.4 | | Mono_c-ADMET | | | | | | | | | | | |
| 49 Mono_c-ADMET [4,512] 4 512 64.4 46.6 33.7 35.9 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 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 49.3 54 Mono_c-MolDes [1,1024] 1 1024 63 64.1 33.1 39.7 63 63 65 58.6 49.3 55 Mono_c-MolDes [2,258] 2 256 63.2 55.1 30 34.6 63.2 <td></td> <td>Mono_c-ADMET</td> <td></td> <td>4</td> <td></td> <td></td> <td></td> <td>10.5</td> <td></td> <td></td> <td></td> <td>49</td> <td>36.6</td> | | Mono_c-ADMET | | 4 | | | | 10.5 | | | | 49 | 36.6 |
| 50 Mono_c-ADMET [4,1024] 4 1024 67.5 50.1 44.7 44.8 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 [1,526] 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 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 63.2 53.7 75.5 69.4 49.1 54.6 73.5 73.5 73.5 73.5 73.5 <td>48</td> <td>Mono_c-ADMET</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>20.3</td> <td></td> <td></td> <td></td> <td>56.8</td> <td></td> | 48 | Mono_c-ADMET | | | | | | 20.3 | | | | 56.8 | |
| 51 Mono_c-MolDes [1,128] 1 128 48.1 31.9 12.9 15.2 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 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 55.2 55.7 Mono_c-MolDes [2,256] 2 256 63.2 55.1 30 34.6 63.2 63.2 53.7 57.5 57.5 73.5 69.4 49.1 54.6 73.5 73.5 67.2 73.5 69.4 49. | | Mono_c-ADMET | | | | | | | | | | | |
| 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 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 53.7 57 Mono_c-MolDes [2,512] 2 512 73.5 69.4 49.1 54.6 73.5 73.5 67.2 58 Mono_c-MolDes [2,128] 3 128 51.4 25 13.7 14.8 51.4 51.4 | | Mono_c-ADMET | | | | | | | | | | 67.5 | |
| 53 Mono_c-MolDes [1,512] 1 512 58.6 58.4 25.1 30.7 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 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 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 <td>51</td> <td>Mono_c-MolDes</td> <td>[1,128]</td> <td>1</td> <td></td> <td>48.1</td> <td>31.9</td> <td>12.9</td> <td>15.2</td> <td>48.1</td> <td>48.1</td> <td>48.1</td> <td>37.1</td> | 51 | Mono_c-MolDes | [1,128] | 1 | | 48.1 | 31.9 | 12.9 | 15.2 | 48.1 | 48.1 | 48.1 | 37.1 |
| 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 53.7 57 Mono_c-MolDes [2,512] 2 512 73.5 69.4 49.1 54.6 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 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 [3,512] 3 512 76.2 72.6 58.1 61.1 76.2 7 | | Mono_c-MolDes | <u> </u> | 1 | 256 | 53.6 | | | 22.1 | 53.6 | 53.6 | 53.6 | 43.1 |
| 55 Mono_c-MolDes [2,128] 2 128 51.4 32.6 13.8 16 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 53.7 57 Mono_c-MolDes [2,512] 2 512 73.5 69.4 49.1 54.6 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 39.2 60 Mono_c-MolDes [3,556] 3 256 64.6 49.6 30 33.8 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 77.2 76. | 53 | Mono_c-MolDes | | 1 | 512 | 58.6 | 58.4 | 25.1 | 30.7 | 58.6 | 58.6 | 58.6 | 49.3 |
| 56 Mono_c-MolDes [2,256] 2 256 63.2 55.1 30 34.6 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 67.2 58 Mono_c-MolDes [2,1024] 2 1024 80.8 78.2 66.6 69.8 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 39.2 60 Mono_c-MolDes [3,556] 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 71.2 62 Mono_c-MolDes [4,128] 4 128 52.3 20.6 14.1 14.6 52.3 52.3 39.8 | 54 | Mono_c-MolDes | | 1 | 1024 | 63 | 64.1 | 33.1 | 39.7 | 63 | 63 | 63 | 55.2 |
| 57 Mono_c-MolDes [2,512] 2 512 73.5 69.4 49.1 54.6 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 39.2 60 Mono_c-MolDes [3,256] 3 256 64.6 49.6 30 33.8 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 71.2 62 Mono_c-MolDes [3,1024] 3 1024 83.7 78.9 73.4 74.6 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 39.8 | | Mono_c-MolDes | [2,128] | 2 | | 51.4 | | 13.8 | 16 | 51.4 | 51.4 | 51.4 | |
| 58 Mono_c-MolDes [2,1024] 2 1024 80.8 78.2 66.6 69.8 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 39.2 60 Mono_c-MolDes [3,256] 3 256 64.6 49.6 30 33.8 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 71.2 62 Mono_c-MolDes [3,1024] 3 1024 83.7 78.9 73.4 74.6 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 39.8 64 Mono_c-MolDes [4,256] 4 256 64.6 42.4 28.6 31.1 64.6 64.6 53.4 | 56 | Mono_c-MolDes | | | 256 | | | 30 | 34.6 | 63.2 | 63.2 | 63.2 | |
| 59 Mono_c-MolDes [3,128] 3 128 51.4 25 13.7 14.8 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 54.3 61 Mono_c-MolDes [3,512] 3 512 76.2 72.6 58.1 61.1 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 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 53.4 65 Mono_c-MolDes [4,512] 4 512 77.4 72.5 62.5 63.7 77.4 77.4 77.4 <td< td=""><td></td><td>Mono_c-MolDes</td><td></td><td>2</td><td>512</td><td>73.5</td><td></td><td>49.1</td><td>54.6</td><td>73.5</td><td>73.5</td><td>73.5</td><td>67.2</td></td<> | | Mono_c-MolDes | | 2 | 512 | 73.5 | | 49.1 | 54.6 | 73.5 | 73.5 | 73.5 | 67.2 |
| 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 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 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 | | Mono_c-MolDes | | | 1024 | 80.8 | | | 69.8 | 80.8 | 80.8 | 80.8 | |
| 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 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 | 59 | Mono_c-MolDes | | | | | | 13.7 | 14.8 | 51.4 | 51.4 | 51.4 | 39.2 |
| 62 Mono_c-MolDes [3,1024] 3 1024 83.7 78.9 73.4 74.6 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 63.4 65 Mono_c-MolDes [4,512] 4 512 77.4 72.5 62.5 63.7 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 82.8 67 Mono_SSP [1,128] 1 128 72.4 70.9 41.1 47.5 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 77.3 69 Mono_SSP [1,512] 1 512 87 90.2 79.1 <td>60</td> <td>Mono_c-MolDes</td> <td></td> <td></td> <td></td> <td>64.6</td> <td>49.6</td> <td>30</td> <td>33.8</td> <td>64.6</td> <td>64.6</td> <td>64.6</td> <td>54.3</td> | 60 | Mono_c-MolDes | | | | 64.6 | 49.6 | 30 | 33.8 | 64.6 | 64.6 | 64.6 | 54.3 |
| 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 53.4 65 Mono_c-MolDes [4,512] 4 512 77.4 72.5 62.5 63.7 77.4 77.4 77.4 77.8 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 64.1 68 Mono_SSP [1,256] 1 256 81.3 83.9 63.6 69.5 81.3 81.3 77.3 69 Mono_SSP [1,512] 1 512 87 90.2 79.1 82.7 87 87 85.5 70 Mono_SSP [1,1024] 1 1024 90.4 | 61 | Mono_c-MolDes | [3,512] | 3 | 512 | 76.2 | | | 61.1 | 76.2 | 76.2 | 76.2 | 71.2 |
| 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 82.8 67 Mono_SSP [1,128] 1 128 72.4 70.9 41.1 47.5 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 77.3 69 Mono_SSP [1,512] 1 512 87 90.2 79.1 82.7 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 | | Mono_c-MolDes | • • • | 3 | 1024 | 83.7 | 78.9 | 73.4 | 74.6 | 83.7 | 83.7 | 83.7 | 80.7 |
| 65 Mono_c-MolDes [4,512] 4 512 77.4 72.5 62.5 63.7 77.4 | 63 | Mono_c-MolDes | | 4 | 128 | 52.3 | 20.6 | 14.1 | 14.6 | 52.3 | 52.3 | 52.3 | 39.8 |
| 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 87.3 69 Mono_SSP [1,512] 1 512 87 90.2 79.1 82.7 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 | 64 | Mono_c-MolDes | | 4 | 256 | 64.6 | 42.4 | 28.6 | 31.1 | 64.6 | 64.6 | 64.6 | 53.4 |
| 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 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 | 65 | Mono_c-MolDes | [4,512] | 4 | | 77.4 | | 62.5 | 63.7 | 77.4 | 77.4 | 77.4 | |
| 68 Mono_SSP [1,256] 1 256 81.3 83.9 63.6 69.5 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 | 66 | Mono_c-MolDes | | 4 | 1024 | | 79.8 | 78.9 | 79.1 | 84.6 | 84.6 | 84.6 | 82.8 |
| 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 | 67 | Mono_SSP | | 1 | 128 | 72.4 | 70.9 | 41.1 | 47.5 | 72.4 | 72.4 | 72.4 | 64.1 |
| 70 Mono_SSP [1,1024] 1 1024 90.4 92.3 87.1 89 90.4 90.4 90.4 89.9 | 68 | Mono_SSP | [1,256] | 1 | 256 | 81.3 | 83.9 | 63.6 | 69.5 | 81.3 | 81.3 | 81.3 | |
| | 69 | Mono_SSP | | 1 | | 87 | | | 82.7 | 87 | 87 | 87 | 85.5 |
| | 70 | Mono_SSP | [1,1024] | 1 | 1024 | 90.4 | | 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 | 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 | 72 | Mono_SSP | [2,256] | 2 | 256 | 82.9 | 80 | 66.1 | 69.8 | 82.9 | 82.9 | 82.9 | 78.5 |

| | | | | Number of | | | | | | | | |
|----------|--------------------|---------------------|-------------------|--------------|-------------|-----------|--------|----------|-------------|--------|-----------------------|-----------|
| | | | | Hidden | | | | | | | | |
| | | | | Nodes | Total Marco | Maria | | | Micro | B.61 | | C |
| | | Materials | Nemakanas | per | Test Mean | Macro | Macro | Macro | Precisi | | D. Giova | Composite |
| Lord ave | Factoria | Network | Number of | Hidden | Accuracy | Precision | Recall | F1 Score | on (o/) | Recall | Micro F1 Score (%) | Index |
| 73 | Feature SCD | Architecture | Hidden Layer 2 | Layer 512 | 90.1 | 90.7 | (%) | (%) | (%) 90.1 | (%) | 90.1 | 89.5 |
| 74 | Mono_SSP | [2,512] [2,1024] | 2 | 1024 | 94.4 | 93.6 | 92.2 | 92.5 | 94.4 | 90.1 | 94.4 | 93.7 |
| 75 | Mono_SSP Mono_SSP | [3,128] | 3 | 1024 | 71 | 42.5 | 31.2 | 33.4 | 71 | 71 | 71 | 58.4 |
| 76 | Mono_SSP | [3,128] | 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 | [4,128] | 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 | [1,126] | 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 |
| | L _{1,2} | . /] | | | - **= | | | | | J | | |

| land ou | Foothing | Network | Number of | Number of Hidden Nodes per Hidden | Test Mean Accuracy | Macro Precision | Macro Recall | Macro F1 Score | Micro Precisi on | Recall | Micro | Composite Index |
|---------|----------|--------------|--------------|---|-----------------------|--------------------|-----------------|-------------------|------------------------|--------|--------------|--------------------|
| | Feature | Architecture | Hidden Layer | Layer | (%) | (%) | (%) | (%) | (%) | (%) | F1 Score (%) | |
| 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 |