

SupplementaryMaterial S5.

Average cell subtype-wise performance results for cell subtype predictions of moSCminer with its variant and the baseline methods based on 5-fold cross-validation.

| GSE136718 | Cell subtype | moSCminer (omics-attn) | moSCminer (no-attn) | RF | SVM | LR | NB |
|-----------|--------------|------------------------|---------------------|--------------|--------------|--------------|-------|
| Accuracy | 2cell | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.971 |
| | 4cell | 0.991 | 0.962 | 0.971 | 0.976 | 0.971 | 0.924 |
| | 8cell | 0.995 | 0.995 | 1.000 | 0.995 | 0.991 | 0.910 |
| | ICM | 1.000 | 1.000 | 1.000 | 1.000 | 0.995 | 0.929 |
| | Late4cell | 0.991 | 0.962 | 0.971 | 0.971 | 0.967 | 0.933 |
| | Morula | 0.995 | 0.995 | 1.000 | 1.000 | 0.995 | 0.943 |
| | TE | 1.000 | 1.000 | 1.000 | 1.000 | 0.995 | 0.924 |
| | Zygote | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.981 |
| F1-score | 2cell | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.870 |
| | 4cell | 0.977 | 0.906 | 0.930 | 0.937 | 0.928 | 0.808 |
| | 8cell | 0.960 | 0.987 | 1.000 | 0.985 | 0.973 | 0.736 |
| | ICM | 1.000 | 1.000 | 1.000 | 1.000 | 0.987 | 0.784 |
| | Late4cell | 0.953 | 0.780 | 0.847 | 0.825 | 0.798 | 0.565 |
| | Morula | 0.982 | 0.978 | 1.000 | 1.000 | 0.978 | 0.671 |
| | TE | 1.000 | 1.000 | 1.000 | 1.000 | 0.978 | 0.576 |
| | Zygote | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.820 |
| ROC-AUC | 2cell | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.967 |
| | 4cell | 0.986 | 0.952 | 0.982 | 0.985 | 0.982 | 0.921 |
| | 8cell | 0.967 | 0.988 | 1.000 | 0.997 | 0.994 | 0.900 |
| | ICM | 1.000 | 1.000 | 1.000 | 1.000 | 0.997 | 0.869 |
| | Late4cell | 0.981 | 0.894 | 0.879 | 0.858 | 0.842 | 0.760 |
| | Morula | 0.997 | 0.997 | 1.000 | 1.000 | 0.980 | 0.789 |
| | TE | 1.000 | 1.000 | 1.000 | 1.000 | 0.980 | 0.819 |
| | Zygote | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.867 |

| GSE154762 | Cell subtype | moSCminer (omics-attn) | moSCminer (no-attn) | RF | SVM | LR | NB |
|-----------|--------------|------------------------|---------------------|-------|--------------|--------------|-------|
| Accuracy | FGO | 0.993 | 0.984 | 0.992 | 0.989 | 0.984 | 0.922 |
| | GO1 | 0.994 | 0.971 | 0.986 | 0.983 | 0.972 | 0.940 |
| | GO2 | 0.992 | 0.971 | 0.983 | 0.982 | 0.971 | 0.950 |
| | Granulosa | 0.991 | 0.984 | 0.990 | 0.994 | 0.993 | 0.912 |
| | Immune | 0.997 | 0.999 | 0.999 | 1.000 | 1.000 | 0.980 |
| | MI | 0.982 | 0.945 | 0.976 | 0.961 | 0.949 | 0.859 |
| | MII | 0.989 | 0.954 | 0.981 | 0.971 | 0.963 | 0.891 |
| | StromaC1 | 0.998 | 0.912 | 0.953 | 0.920 | 0.911 | 0.797 |
| StromaC2 | 0.993 | 0.911 | 0.954 | 0.923 | 0.909 | 0.786 | |
| F1-score | FGO | 0.953 | 0.911 | 0.965 | 0.932 | 0.907 | 0.560 |
| | GO1 | 0.922 | 0.712 | 0.861 | 0.829 | 0.741 | 0.537 |
| | GO2 | 0.870 | 0.600 | 0.741 | 0.740 | 0.607 | 0.504 |
| | Granulosa | 0.954 | 0.910 | 0.941 | 0.973 | 0.963 | 0.613 |
| | Immune | 0.978 | 0.978 | 0.921 | 1.000 | 1.000 | 0.160 |
| | MI | 0.950 | 0.844 | 0.928 | 0.884 | 0.854 | 0.544 |
| | MII | 0.942 | 0.768 | 0.898 | 0.848 | 0.808 | 0.505 |
| | StromaC1 | 0.995 | 0.790 | 0.890 | 0.808 | 0.784 | 0.468 |
| StromaC2 | 0.982 | 0.780 | 0.882 | 0.810 | 0.781 | 0.457 | |
| ROC-AUC | FGO | 0.986 | 0.944 | 0.961 | 0.949 | 0.944 | 0.763 |
| | GO1 | 0.981 | 0.913 | 0.965 | 0.946 | 0.919 | 0.874 |
| | GO2 | 0.946 | 0.754 | 0.811 | 0.840 | 0.760 | 0.765 |
| | Granulosa | 0.956 | 0.926 | 0.980 | 0.991 | 0.968 | 0.818 |
| | Immune | 0.999 | 0.999 | 0.930 | 1.000 | 1.000 | 0.550 |
| | MI | 0.984 | 0.914 | 0.963 | 0.936 | 0.920 | 0.715 |
| | MII | 0.951 | 0.873 | 0.933 | 0.914 | 0.885 | 0.744 |
| | StromaC1 | 0.999 | 0.872 | 0.936 | 0.882 | 0.865 | 0.661 |
| StromaC2 | 0.992 | 0.859 | 0.918 | 0.877 | 0.863 | 0.661 | |

| GSE140203 | Cell subtype | moSCminer (omics-attn) | moSCminer (no-attn) | RF | SVM | LR | NB |
|------------------|---------------------------|---------------------------|------------------------|-------|-------|-------|-------|
| Accuracy | Basal | 0.998 | 0.966 | 0.994 | 0.927 | 0.953 | 0.802 |
| | Dermal Fibroblast | 0.999 | 0.994 | 0.997 | 0.993 | 0.995 | 0.971 |
| | Dermal Papilla | 0.998 | 0.995 | 0.996 | 0.995 | 0.995 | 0.969 |
| | Dermal Sheath | 0.999 | 0.997 | 0.996 | 0.996 | 0.996 | 0.966 |
| | Endothelial | 0.999 | 0.994 | 0.998 | 0.993 | 0.993 | 0.976 |
| | Granular | 0.999 | 0.993 | 0.995 | 0.992 | 0.992 | 0.970 |
| | Hair Shaft-cuticle-cortex | 0.998 | 0.987 | 0.997 | 0.983 | 0.986 | 0.972 |
| | IRS | 0.999 | 0.989 | 0.997 | 0.985 | 0.987 | 0.969 |
| | Infundibulum | 0.997 | 0.964 | 0.984 | 0.947 | 0.958 | 0.887 |
| | Isthmus | 0.999 | 0.991 | 0.998 | 0.986 | 0.989 | 0.919 |
| | K6+ Bulge Companion Layer | 0.999 | 0.994 | 0.997 | 0.991 | 0.993 | 0.982 |
| | Macrophage DC | 1.000 | 0.997 | 0.998 | 0.995 | 0.996 | 0.982 |
| | Medulla | 0.998 | 0.985 | 0.996 | 0.982 | 0.984 | 0.964 |
| | Melanocyte | 1.000 | 0.999 | 0.998 | 0.999 | 0.999 | 0.989 |
| | ORS | 0.999 | 0.993 | 0.998 | 0.992 | 0.992 | 0.979 |
| | Schwann Cell | 0.999 | 0.998 | 0.999 | 0.996 | 0.997 | 0.852 |
| | Sebaceous Gland | 1.000 | 0.999 | 0.999 | 0.998 | 0.998 | 0.978 |
| | Spinous | 0.997 | 0.971 | 0.994 | 0.955 | 0.966 | 0.910 |
| | TAC-1 | 0.995 | 0.959 | 0.972 | 0.944 | 0.952 | 0.908 |
| | TAC-2 | 0.998 | 0.981 | 0.995 | 0.979 | 0.980 | 0.969 |
| ahighCD34+ bulge | 0.999 | 0.986 | 0.998 | 0.978 | 0.983 | 0.906 | |
| alowCD34+ bulge | 0.998 | 0.981 | 0.997 | 0.975 | 0.978 | 0.943 | |
| F1-score | Basal | 0.995 | 0.929 | 0.987 | 0.858 | 0.905 | 0.651 |
| | Dermal Fibroblast | 0.980 | 0.918 | 0.955 | 0.898 | 0.922 | 0.286 |
| | Dermal Papilla | 0.968 | 0.884 | 0.909 | 0.884 | 0.892 | 0.281 |
| | Dermal Sheath | 0.945 | 0.873 | 0.804 | 0.834 | 0.845 | 0.126 |
| | Endothelial | 0.976 | 0.901 | 0.958 | 0.869 | 0.877 | 0.330 |
| | Granular | 0.924 | 0.503 | 0.576 | 0.373 | 0.391 | 0.105 |
| | Hair Shaft-cuticle-cortex | 0.978 | 0.822 | 0.953 | 0.769 | 0.806 | 0.578 |
| | IRS | 0.969 | 0.726 | 0.909 | 0.635 | 0.676 | 0.397 |
| | Infundibulum | 0.987 | 0.865 | 0.941 | 0.801 | 0.841 | 0.330 |
| | Isthmus | 0.979 | 0.775 | 0.941 | 0.629 | 0.716 | 0.228 |
| | K6+ Bulge Companion Layer | 0.969 | 0.811 | 0.903 | 0.689 | 0.763 | 0.273 |
| | Macrophage DC | 0.977 | 0.805 | 0.828 | 0.625 | 0.728 | 0.075 |
| | Medulla | 0.967 | 0.755 | 0.930 | 0.671 | 0.718 | 0.162 |
| | Melanocyte | 0.961 | 0.900 | 0.837 | 0.884 | 0.873 | 0.378 |
| | ORS | 0.982 | 0.896 | 0.959 | 0.877 | 0.878 | 0.539 |
| | Schwann Cell | 0.941 | 0.724 | 0.823 | 0.456 | 0.542 | 0.035 |
| | Sebaceous Gland | 0.992 | 0.887 | 0.847 | 0.839 | 0.851 | 0.273 |
| | Spinous | 0.987 | 0.853 | 0.972 | 0.763 | 0.823 | 0.195 |
| | TAC-1 | 0.978 | 0.804 | 0.881 | 0.742 | 0.777 | 0.285 |
| | TAC-2 | 0.965 | 0.685 | 0.919 | 0.615 | 0.648 | 0.283 |
| ahighCD34+ bulge | 0.991 | 0.853 | 0.973 | 0.767 | 0.814 | 0.449 | |
| alowCD34+ bulge | 0.985 | 0.836 | 0.973 | 0.788 | 0.811 | 0.107 | |
| ROC-AUC | Basal | 0.996 | 0.955 | 0.989 | 0.919 | 0.946 | 0.789 |
| | Dermal Fibroblast | 0.988 | 0.971 | 0.985 | 0.950 | 0.959 | 0.585 |
| | Dermal Papilla | 0.983 | 0.928 | 0.968 | 0.930 | 0.930 | 0.616 |
| | Dermal Sheath | 0.965 | 0.919 | 0.837 | 0.890 | 0.896 | 0.570 |
| | Endothelial | 0.990 | 0.946 | 0.974 | 0.917 | 0.933 | 0.602 |
| | Granular | 0.967 | 0.698 | 0.703 | 0.629 | 0.648 | 0.585 |
| | Hair Shaft-cuticle-cortex | 0.988 | 0.909 | 0.955 | 0.879 | 0.897 | 0.760 |
| | IRS | 0.982 | 0.860 | 0.917 | 0.809 | 0.818 | 0.736 |
| | Infundibulum | 0.994 | 0.934 | 0.987 | 0.900 | 0.920 | 0.602 |
| | Isthmus | 0.984 | 0.876 | 0.944 | 0.785 | 0.830 | 0.736 |
| | K6+ Bulge Companion Layer | 0.975 | 0.910 | 0.912 | 0.812 | 0.863 | 0.607 |
| | Macrophage DC | 0.978 | 0.865 | 0.855 | 0.747 | 0.830 | 0.570 |
| | Medulla | 0.983 | 0.867 | 0.950 | 0.804 | 0.842 | 0.552 |
| | Melanocyte | 0.967 | 0.927 | 0.861 | 0.902 | 0.907 | 0.784 |
| | ORS | 0.988 | 0.945 | 0.961 | 0.925 | 0.933 | 0.694 |
| | Schwann Cell | 0.953 | 0.806 | 0.853 | 0.658 | 0.712 | 0.665 |
| | Sebaceous Gland | 0.992 | 0.937 | 0.868 | 0.888 | 0.894 | 0.818 |

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|------------------|--------------|-------|-------|-------|-------|-------|
| Spinous | 0.994 | 0.918 | 0.990 | 0.861 | 0.902 | 0.554 |
| TAC-1 | 0.992 | 0.893 | 0.982 | 0.871 | 0.886 | 0.586 |
| TAC-2 | 0.980 | 0.824 | 0.925 | 0.770 | 0.795 | 0.597 |
| ahighCD34+ bulge | 0.993 | 0.927 | 0.974 | 0.868 | 0.893 | 0.844 |
| alowCD34+ bulge | 0.994 | 0.916 | 0.978 | 0.888 | 0.906 | 0.529 |
