Panel	Short Description	Folder	File Path	Notes
Figure 1: Study Design and a Multi-parameter Disease Severity Metric (DSM).				
A	Patient overview	A3	overview/patient.and.sample.overview.Rmd	
B	Experiment overview	NA	NA	
C	DSM parameter hm	A3	dsm/citeseq.patient.dsm.Rmd	Produces the DSM end point file
D	DSM parameter model coef	A3	dsm/citeseq.patient.dsm.Rmd	
E	DSM severity box plot	A3	dsm/brescia.dsm.validation.Rmd	
Figure 2: A Multimodal Single Immune Cell Atlas of COVID-19 Reveals Cell Populations Associated with Disease and Disease Severity (DSM).				
A	CITE hm	A2	3.UMAPandProteinVis.Figure2.R	
B	UMAP	A2	3.UMAPandProteinVis.Figure2.R	
C	CITE hm	A2	3.UMAPandProteinVis.Figure2.R	
D-I	Mono UMAP	A2	3.UMAPandProteinVis.Figure2.R	
Figure 3: Cell-type-specific Gene Expression Signatures of COVID-19 Disease Status and Severity.				
A	COVIDvsHC bubble	A4	figures/gsea_bubble_plots.Rmd	
B	DSM bubble	A4	figures/gsea_bubble_plots.Rmd	
C	Mono IFN hm	A1	DEplot.subject.hm.Rmd	
D	Mono IFN trajecotry	A1	modulescore.TSO.Rmd	
E	TSO IFN coef	A1	NES.PC1groupTSO.interaction.Rmd	
F	pDC apopt hm	A1	DEplot.subject.hm.Rmd	
G	corr hm and scatters	A4	figures/fig3_heatmap_and_scatterplots.R	
Figure 4: Cell-type-specific Gene Expression Profiles of Select Signatures and Disease Severity Network				
A	severity network	A3	severity.network/severity.network.Rmd	
B	NK FA IL15 corr	A1	modulescore.corr.Rmd	
C	IL15 DSM corr	A1	modulescore.corr.Rmd	
D	NK FA hm	A1	DEplot.subject.hm.Rmd	
E	NK NFkB hm	A1	DEplot.subject.hm.Rmd	
F	NK IL1 hm	A1	DEplot.subject.hm.Rmd	
G	NK FA inflam corr	A1	modulescore.corr.Rmd	
H	NK IFNG	A1	DEplot.subject.hm.Rmd	
I	NK FA mTOR, IFNG corr	A1	modulescore.corr.Rmd	
J	NK FA trajectory	A1	modulescore.TSO.Rmd	
K	NK inflam trajectory	A1	modulescore.TSO.Rmd	
L	IL15 trajectory	A1	modulescore.corr.Rmd	
Figure 5: Single Cell and Clonal Expansion Analysis in CD4+ and CD8+ T cells and Exhaustion Assessment in Clonal CD8+ T cells.				
A	CD8 cluster hm	A2	4.TcellReclustering.R	
B	CD8 CITE hm	A2	4.TcellReclustering.R	
C	CD8 cluster FC	A4	figures/fig4_plot_cd4_8_fig4_cluster_volcano.R	
D	CD8 cluster overlap w celltypes	A2	4.TcellReclustering.R	
E	clonality DSM	A4	figures/clonality/plot_pcgroup_onset_assoc_for_paper.Rmd	
F	CD8 exhaustion marker FC	A4	figures/tcell_exhaustion/CITE_surface_marker_coefficients_with_pval.Rmd	
G	exhaustion gene GSEA curve	A4	figures/tcell_exhaustion/exhaustion_fgsea_plots.Rmd	
Figure 6: Analyses of Longitudinal Data and Timing Effects Suggest an Immune Response Juncture Whose Immune Profile is Predictive of Deceased-or-Recovery Outcomes.				
A	Mono cell trajectory	A1	cell.freq.plot.Rmd	
B	Mono Neut count	A3	critical.juncture/dsm.high.v.low.cytokine.Rmd	
C	NES TSO group	A1	NES.PC1onsetgroup.interaction.Rmd	
D	juncture bubble	A4	figures/gsea_bubble_plots.Rmd	
E	NK, mono juncture trajectory	A1	modulescore.TSO.Rmd	
F	cytokine trajectory DSM	A3	critical.juncture/dsm.high.v.low.cytokine.Rmd	
Figure 7: Divergence of Deceased and Recovered Patients at the Late Juncture.				
A	scheme	NA	NA	
B	Cytokine effect sizes	A3	critical.juncture/deceased.v.recovered.cytokine.Rmd	
C	prediction AUC	A3	critical.juncture/deceased.v.recovered.prediction.Rmd	
D	cytokine trajectory	A3	critical.juncture/deceased.v.recovered.cytokine.Rmd	
E	serology trajectory	A3	critical.juncture/deceased.v.recovered.cytokine.Rmd	
Supplementary Figures				
Figure S1: Subject treatment timeline				
A	subject reatment timeline	A3	overview/patient.and.sample.overview.Rmd	
B	CITESeq patient DSM boxplot by WHO Scores	A3	dsm/citeseq.patient.dsm.Rmd	
C	Validation cohort DSM boxplot by ICU Status	A3	dsm/brescia.dsm.validation.Rmd	
Figure S2: cell freq description				
A	flow CITE corr	A1	cell.freq.corr.Rmd	
B	cell freq DSM	A1	cell.freq.plot.Rmd	
C	cell freq hm	A1	cell.freq.plot.Rmd	
Figure S3: Cell-type-specific Gene Expression Signatures of COVID-19 Disease Status and Severity				
A	DSM-low TSO bubble	A4	figures/gsea_bubble_plots.Rmd	
B	DSM-high TSO bubble	A4	figures/gsea_bubble_plots.Rmd	
C	mono translation hm	A1	DEplot.subject.hm.Rmd	
D	mono translation trajectory	A1	modulescore.TSO.Rmd	
E	German data pDC apopt hm1	A1	Schulte-Schrepping/cohort1.DEsubject.hm.Rmd	
F	German data pDC apopt hm2	A1	Schulte-Schrepping/cohort2.DEsubject.hm.Rmd	
G	German data pDC apopt GSEA curve	A4	figures/validations/pdc_apoptosis/pdc_apoptosis_schulteschrepping.Rmd	
Figure S4: Cell-type-specific Gene Expression Signatures of COVID-19 Disease Status and Severity				
A	pDC apopt v. oxidative stress corr	A3	cytokine.geneset.correlation/citeseq.T0.cytokine.pathway.corr	

B	NK FA IL15 residual corr	A3	cytokine.geneset.correlation/citeseq.T0.cytokine.pathway.corr	
C	German data NK FA hm1	A1	Schulte-Schrepping/cohort1.DEsubject.hm.Rmd	
D	German data NK FA hm2	A1	Schulte-Schrepping/cohort2.DEsubject.hm.Rmd	
E	German data NK FA GSEA curve	A4	figures/validations/NK_fattyacid_gsea_curves_cohorts_1_2.R	
F	German data FA NFkB score corr	A1	Schulte-Schrepping/NK.modulescore.corr.Rmd	
G-H	Mono inflam hm	A1	DEplot.subject.hm.Rmd	
Figure S5: Exogeneous corticosteroid effect				
A	glucocorticoid GSEA curve	A4	dsm_steroid_enrichment.R	
B	related scores and glucocorticoid score corr	A3	cytokine.geneset.correlation/citeseq.T0.cytokine.pathway.corr	
C	related scores and TSC22D3 corr	A3	cytokine.geneset.correlation/citeseq.T0.cytokine.pathway.corr	
D	TSC22D3 boxplot	A1	steroiduse.TSC22D3.Rmd	
Figure S6: CD4 and CD8 exhaustion validation				
A	CD4 cluster hm	A2	4.TcellReclustering.R	
B	CD4 CITE hm	A2	4.TcellReclustering.R	
C	CD4 cluster FC	A4	figures/cd4_8_cluster_volcano.Rmd	
D	CD4 cluster overlap w celltypes	A2	4.TcellReclustering.R	
E	exhaustion marker RNA	A4	figures/tcell_exhaustion/RNA_surface_marker_coeff_with_pval.R	
F	CD39+PD1+ freq boxplot	A4	figures/tcell_exhaustion/cd39_pd1.Rmd	
G	exhaustion cutoff boxplot	A4	figures/tcell_exhaustion/cutoff_markers_grid.Rmd	
H	exhaustion LE enrichment	A4	figures/tcell_exhaustion/wherry_exhaustion_enrichment.Rmd	
I	German data exhaustion bubble	A4	figures/validations/exhaustion_plots.Rmd	
J	German data exhaustion GSEA curve	A4	figures/validations/exhaustion_plots.Rmd	
Figure S7: Supporting data for critical juncture analysis				
A	difference of difference bubble	A4	figures/gsea_bubble_plots.Rmd	
B	Deceased v. recovered neutrophils and monocytes	A3	critical.juncture/deceased.v.recovered.cytokine.Rmd	
C	Outcome and severity comparison ES corr	A3	critical.juncture/deceased.v.recovered.cytokine.Rmd	
D	Yale cohort validation ES corr	A3	critical.juncture/cytokine.critical.juncture.validation.Rmd	
Supplementary Tables				
S4	GSEA enrichment results -- FDR < .2	A4	figures/gsea_bubble_plots.Rmd	
S5	GSEA enrichment results -- all	A4	figures/gsea_bubble_plots.Rmd	