Supplementary Tables

Metal Isotope /Fluorochrome	Antigen	Clone	Manufacturer	
Barcoding and fluorescent				
89 _{Y or} 113 _{In}	CD45	30-F11	Biolegend	
Biotin	CD86	IT2.2	BD	
PE	CD223 (Lag3)	T47-530	BD	
Remaining surface stain				
115 _{In}	CD11c	Bu15	Biolegend	
141 _{Pr}	CD27	M-T271	BD	
142 _{Nd}	CD19	HIB19	BD	
143 _{Nd}	CD45RA	HI100	Biolegend	
¹⁴⁴ Nd	CCR5	HEK/1/8	Biolegend	
145 _{Nd}	CD4	RPA-T4	BD	
146 _{Nd}	CCR10	1B5	BD	
147 _{Sm}	CD20	2H7	Biolegend	
148 _{Nd}	CD16	3G8	BD	
¹⁴⁹ Sm	CD366 (Tim3)	7D3	BD	
150 _{Nd}	Biotin	1D4-C5	Biolegend	
151 _{Eu}	CD278 (ICOS)	DX29	BD	
152 _{Sm}	CD45RO	UCHL1	BD	
153 _{Eu}	CD62L	DREG	Biolegend	
154 _{Gd}	CD196 (CCR6)	11A9	BD	
155 _{Gd}	CD31	WM59	Biolegend	
156 _{Gd}	PE	PE00 1	Biolegend	
158 _{Gd}	CD194 (CCR4)	L291H4	Biolegend	
159 _{Tb}	CD197 (CCR7)	150503	RnD Systems	
160 _{Gd}	CD14	M5E2	Biolegend	
161 _{Dy}	CD274 (PD-L1)	29E.2A3	Biolegend	
163 _{Dy}	CD183 (CXCR3)	G025H7	Biolegend	
164 _{Er}	CD161	DX12	BD	
165 _{Ho}	CD127 (IL-7R)	A019D5	Biolegend	
166 _{Er}	CD185 (CXCR5)	RF8B2	BD	
167 _{Er}	CD38	HIT2	Biolegend	
168 _{Er}	CD8a	RPA-T8	BD	
169 _{Tm}	CD25	2A3	Fluidigm	
170 _{Er}	CD3	UCHT1	BD	

Supplementary table 1: Mass cytometry panel used for immunophenotyping.

171 _{Yb}	CD335 (NKp46)	9E2	Biolegend	
172 _{Yb}	CD57	HCD57	Fluidigm	
173 _{Yb}	Integrin β7	FIB504	BD	
174 _{Yb}	HLA-DR	L243	BD	
175 _{Lu}	CD279 (PD-1)	EH12.2H7	Biolegend	
176 _{Lu}	CD56	NCAM16	BD	
Intracellular stain				
162 _{Er}	FOXP3	PCH101	BD	
191/193 _{lr}	DNA Intercalator		Fluidigm	

Supplementary Figures

Supplementary figure 1. Gating Strategy. PBMCs were stained as per antibodies and steps outlined in Supplementary table S1 and subsequently analysed by mass cytometry. **A**) Cells were pre-gated prior to population analysis. Cells were first distinguished as positive for DNA-intercalated events (detected in channels 191 and 193) and negative for EQ-beads (detected in 140 channel), and with subsequent demarcation for exclusion of dead (cisplatin positive) cells and differential CD45 antibody staining to distinguish barcoded, concurrently analysed samples. **B**) The gating strategy allows for distinguishing major immune lineages and particular subsets of interest following haemopoietic stem cell transplantation immune reconstitution. **C**) Summarising the collective gated population occupancy as demarcated by populations in second row of Supplementary figure 1B (boxed in grey), with median frequency \pm sem across a batch of healthy controls (n = 4) and patients receiving HSCT alone (n = 10).

Supplementary figure 2. The mass cytometry immunophenotyping assay is robust across experimental batches. **A**) Correlation showing consistency of population frequencies for the 6 healthy control (HC) samples analysed across two different batches, with HC4 analysed in three independent batches. Colour identifies healthy control correlated across the frequency of major immune populations (Supplementary figure **1B**, row 2). Linear regression line is shown in black with the 95% confidence intervals shaded. Coefficient, *P*-value and slope was calculated on data from all healthy control batch comparisons. t-SNE shows good mixing of batches across clusters when analysed for **B**) scaled populations or **C**) frequencies of parental gates.

Supplementary figure 3. Density plot, CD3, CD4, CD8, CD19, CD56, HLA-DR and CD16 intensity of signal are shown across viSNE space occupancy from a time series of Patient 1 and Patient 2 who had divergent clinical outcomes following VST treatment. Day post-transplant annotated on Figure, with day post-VST infusion in brackets.

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Supplementary figure 1



Supplementary figure 2



Patient 1 - VST ineffective Patient 2 - VST effective Pre-VST infusion Day 171 post transplant Pre-VST infusion Day 83 post transplant Day 199 (28) Day 255 (84) Day 113 (30) Day 172 (89) Density CD3 CD4 CD8 CD19 CD56 HLA-DR +20 CD16 t-SNE2 -20 +20 -20 t-SNE1

Supplementary figure 3

Intensity

low

high