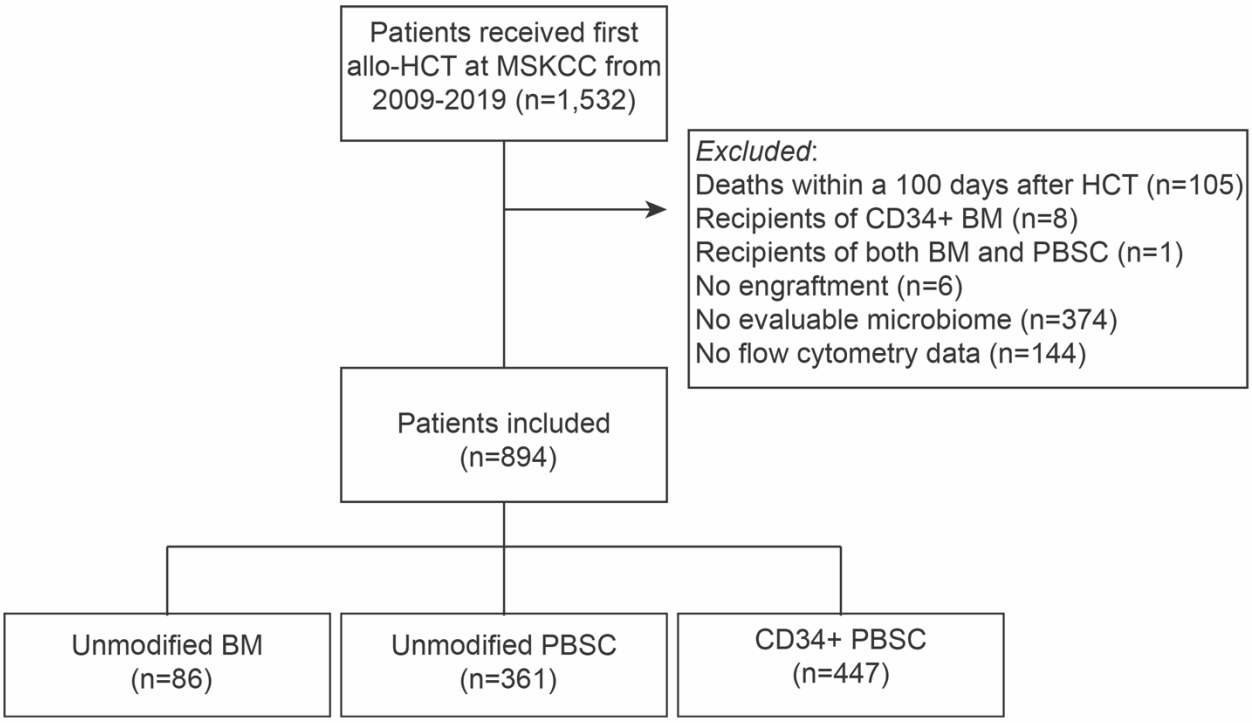
Figure S1. Consort flow diagram.



Allo-HCT: allogeneic hematopoietic cell transplant; BM: Bone marrow transplant; PBSC: Peripheral blood stem cell transplant.

Figure S2. Day 100 CD4 counts by GVHD prophylaxis regimen.
Lower limit of normal (LLN) = 429; upper limit of normal (ULN) = 1,331cells/μl.

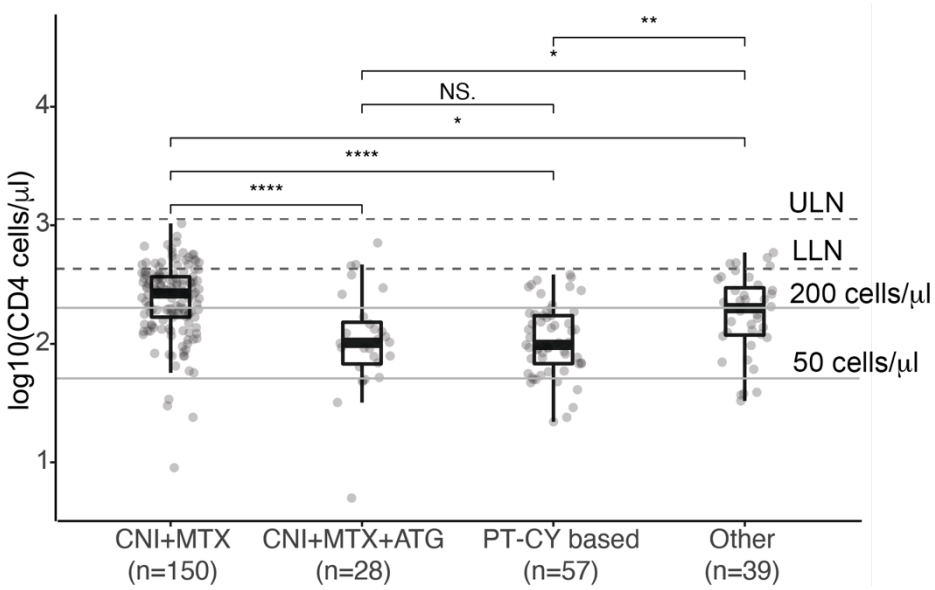


Figure S3. A-diversity per graft type (a) over time and (b) summarized at peri-engraftment period. Patients included: n=894 total, **(a)** Patients with available stool samples between day -30 and +40 from allo-HCT were included: 86 BM; 361 unmodified PBSC; 447 CD34+ PBSC. **(b)** Patients with available stool samples during the peri-engraftment period were included: 74 BM; 270 PBSC and 323 CD34+ selected. Median peri-engraftment α-diversity was calculated per patient.
HCT: hematopoietic cell transplant; BM: Bone marrow transplant; PBSC: Peripheral blood stem cell transplant.

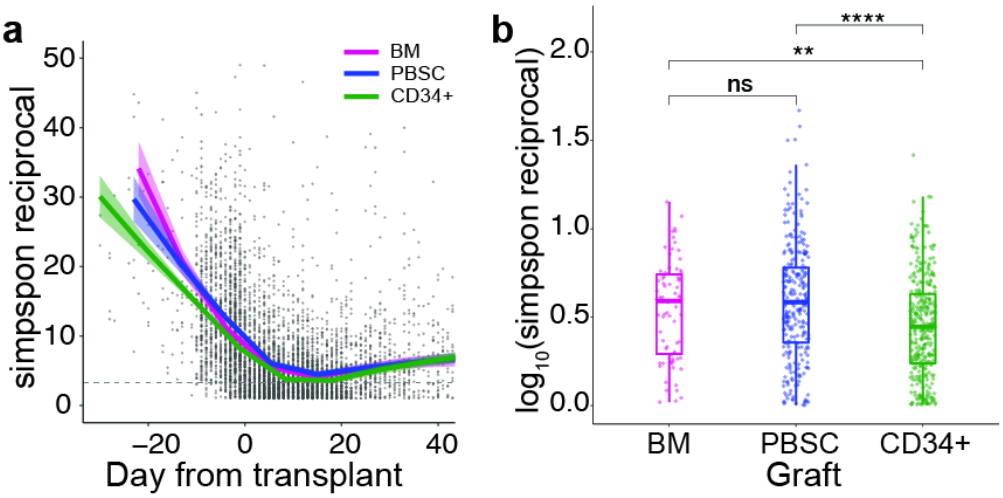


Figure S4: CD4 counts at day 100 and clinical outcomes after allo-HCT. CD4 recovery was defined as high, moderate and low using thresholds at 25th and 75th percentile at day 100 by graft type**. (a-b)** Overall survival for **(a)** BM, **(b)** PBSC and **(c)** CD34-selected PBSC recipients. **(d-f)** Cumulative incidence of non-relapse mortality of **(d)** BM, **(e)** PBSC and **(f)** CD34-selected PBSC recipients. HCT: allogeneic hematopoietic cell transplant; BM: bone marrow transplant; PBSC: peripheral blood stem cell transplant.

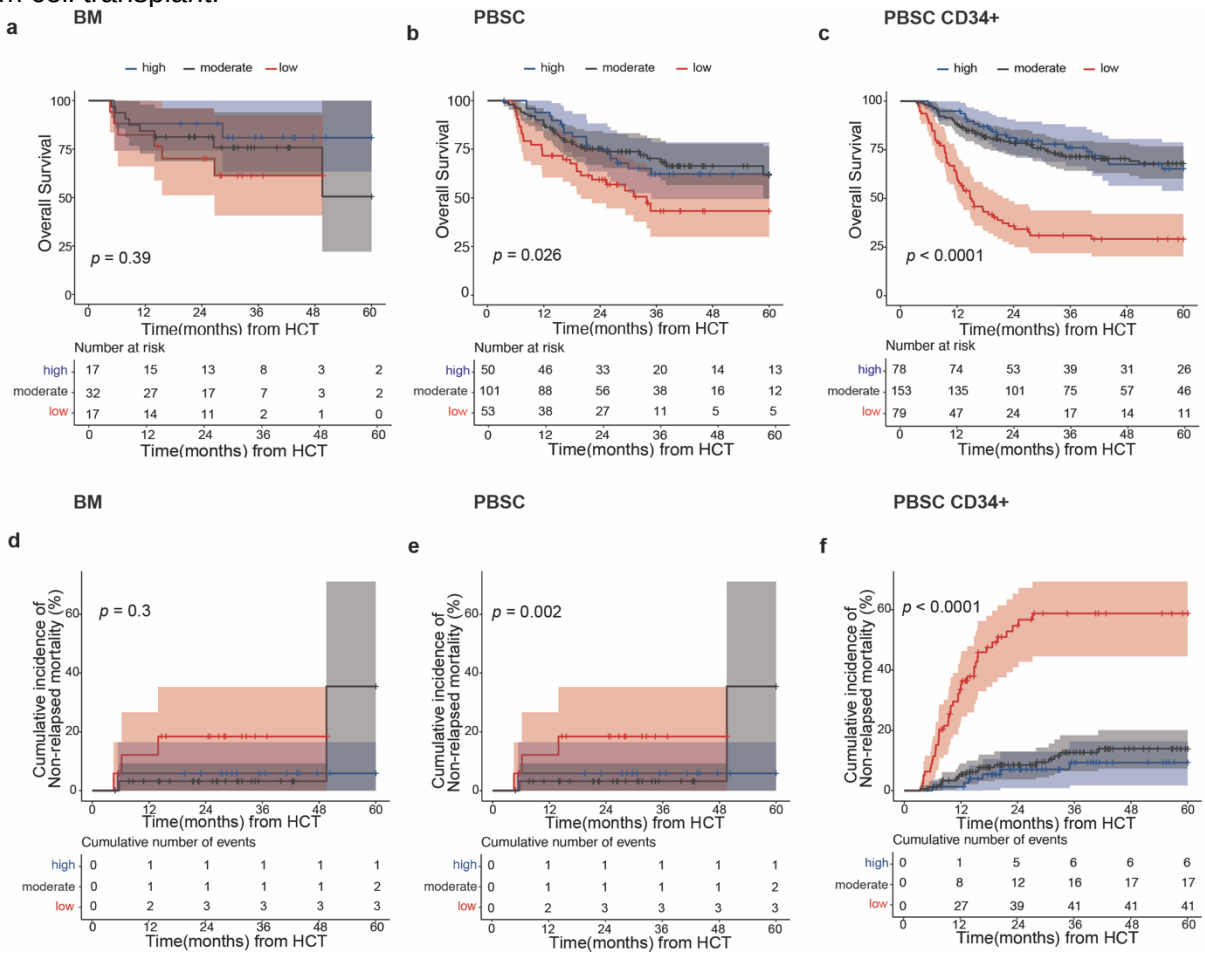


Figure S5. Overall survival **(a-c)** and non-relapse mortality **(d-f)** in patients with high and low peri-engraftment α-diversity in recipients of BM **(a,d)**, PBSC **(b,e)** and CD34-selected PBSC **(c,f)**.

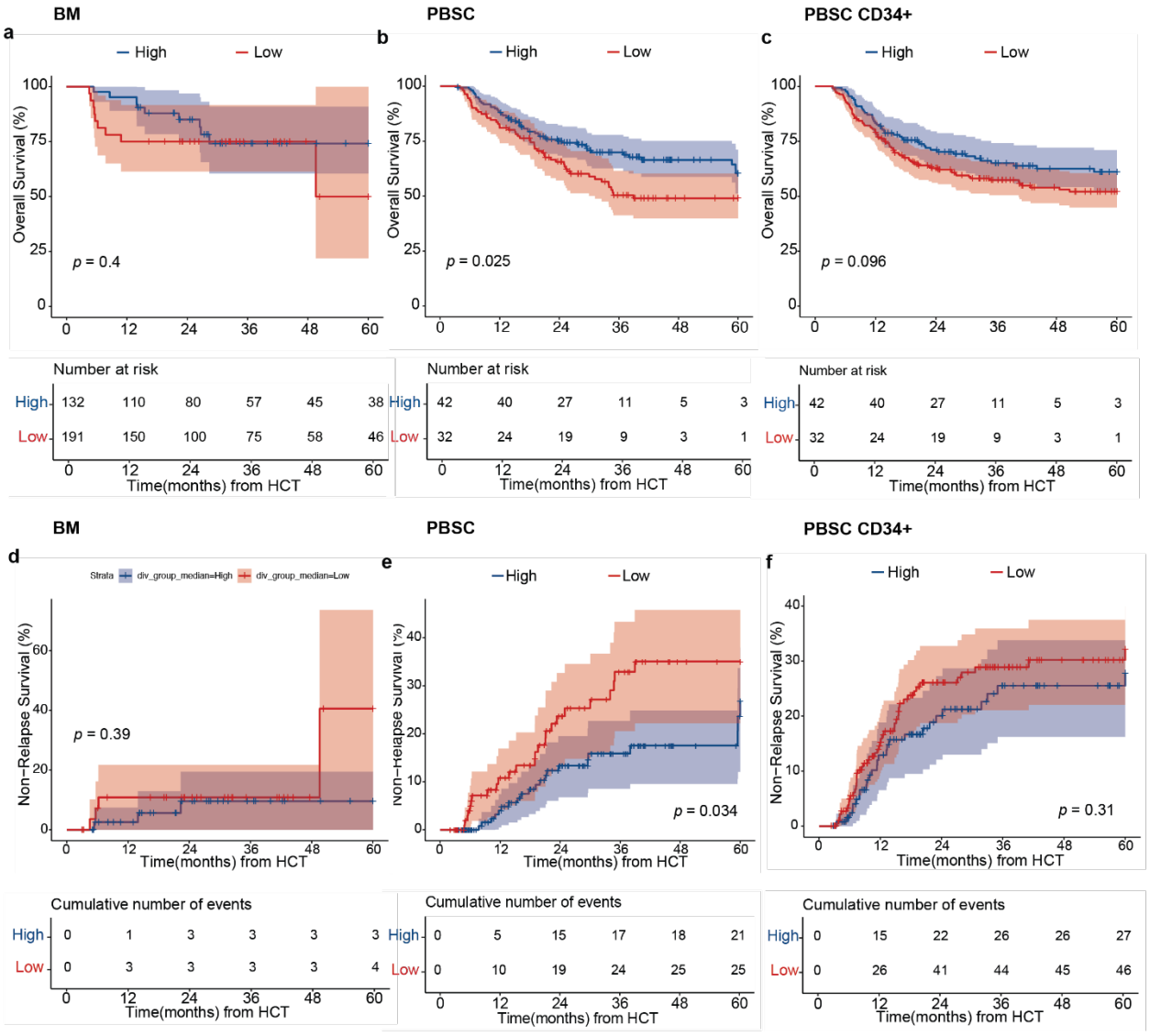
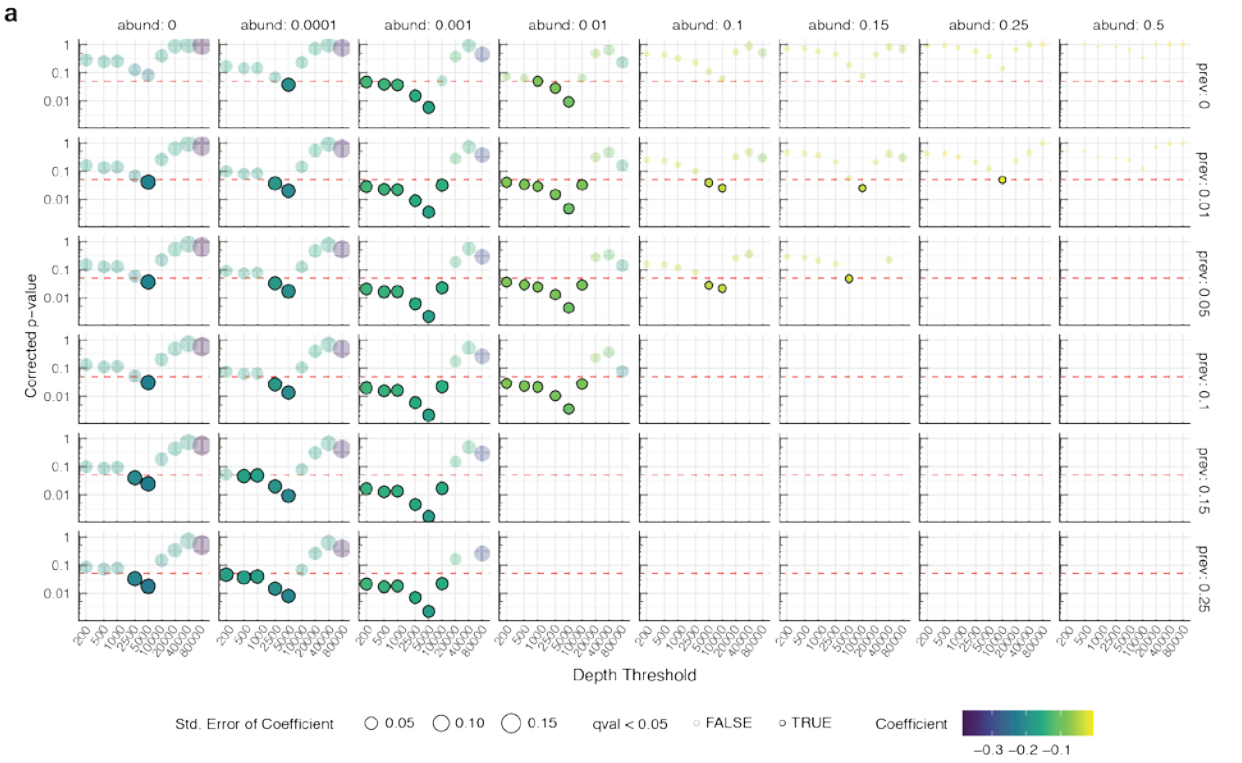
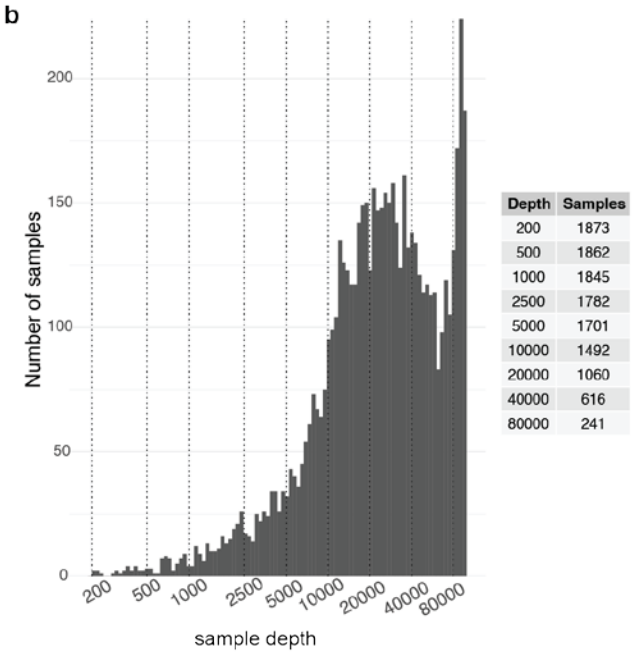


Figure S6: (a) Evaluation of the sensitivity of the MaAsLin2 results to selection of prevalence, abundance and minimum read depth thresholds. The association between Staphylococcus and CD4 count is detected across a range of reasonable thresholds. Above a minimum sample depth of ~10,000, too many samples are excluded to detect significant associations. Similarly, the absolute value of the coefficient decreases. The histogram in panel **(b)** shows the distribution of depths in this study, indicating the depth thresholds considered for this sensitivity analysis. The table in panel **(b)** shows the number of samples retained according to the various depth thresholds (assuming no prevalence of abundance filtering). **(c)** CD4 counts in patients with high and low Staphylococcus abundance (using the 75th percentile) in a univariate analysis. Lower limit of normal (LLN) = 429; upper limit of normal (ULN) = 1,331cells/ml.





Depth	Samples
200	1873
500	1862
1000	1845
2500	1782
5000	1701
10000	1492
20000	1060
40000	616
80000	241

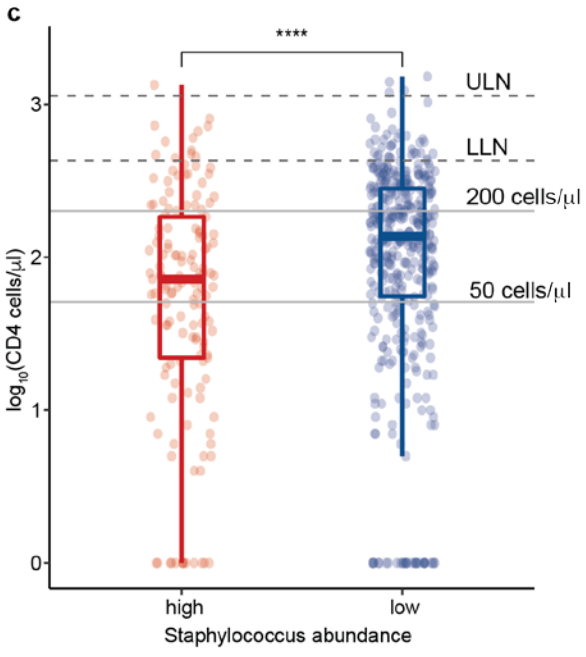


Table S1. Conditioning, Donor type and GvHD prophylaxis medications.

	BM (n=86)	PBSC (n=361)	PBSC CD34+ (n=447)	All (n=894)	
Conditioning					<0.001
Ablative	49 (57.0)	97 (26.9)	446 (99.8)	589 (65.9)	
Non-ablative	15 (17.4)	99 (27.4)	0 (0)	114 (12.8)	
Reduced intensity	22 (25.6)	165 (45.7)	1 (0.2)	191 (21.4)	
Donor type					<0.001
Matched related	17 (19.8)	124 (34.3)	147 (32.9)	288 (32.2)	
Mismatched related	0 (0)	2 (0.6)	2 (0.4)	4 (0.4)	
Haploidentical	24 (27.9)	20 (5.5)	0 (0)	44 (4.9)	
Matched unrelated	34 (39.5)	187 (51.8)	226 (50.6)	447 (50.0)	
Mismatched non-related	11 (12.8)	28 (7.8)	72 (16.1)	111(12.4)	
GvHD prophylaxis regimen					<0.001
CNI + MMF, n (%)	0 (0)	5 (1.4)	1 (0.2)	6 (0.7)	
CNI + MTX, n (%)	34 (39.5)	228 (63.2)	0 (0)	262 (29.3)	
CNI + MTX + ATG, n (%)	5 (5.8)	35 (9.7)	NA*	40 (4.5)	
Post-transplant cyclophosphamide-based, n (%)	41 (47.7)	36 (10.0)	1 (0.2)	78 (8.7)	
Others, n (%)	6 (7.0)	57 (15.8)	10 (2.2)	72 (8.1)	
CD34-selection, No additional drugs, n (%)	0 (0)	0 (0)	435 (97.3)	436 (48.8)	

Others included: CNI monotherapy (n=9), CNI + sirolimus (n=4), CNI +/- sirolimus + MMF + MTX (n=57), CNI/sirolimus + MMF + MTX + ATG (n=2). Six patients that received a PT-CY-based regimen also received ATG.
GvHD: graft versus host disease, BM: Bone marrow transplant; PBSC: Peripheral blood stem cell transplant, CNI: calcineurin inhibitor, MMF: mycophenolate mofetil, MTX: methotrexate

Table S2. High dose (HD) steroids: defined as equal or more than 1mg/kg of prednisone-equivalent given for 7-days continuously between HCT day and flow cytometry test in peri-100 and peri-180 day periods.

	BM	PBSC	PBSC CD34+	All
Peri-100 day	(n=73)	(n=270)	(n=429)	(n=772)
HD steroids, n (%)	21 (29)	88 (33)	60 (14)	169 (22)
Peri-180 day	(n=63)	(n=262)	(n=390)	(n=715)
HD steroids, n (%)	21 (32)	88 (31)	65 (15)	174 (24)

HCT: allogeneic hematopoietic cell transplant; BM: Bone marrow transplant; PBSC: Peripheral blood stem cell transplant.

Table S3. High dose (HD) steroids: defined as any dose equal or more than 1mg/kg of prednisone equivalent, given at least once, 7-days before the flow cytometry in peri-100 and peri-180 day periods.

	BM	PBSC	PBSC CD34+	All
Peri-100 day	(n=83)	(n=284)	(n=465)	(n=823)
HD steroids n (%)	2 (2.4)	3 (1.1)	4 (0.9)	9 (1.1)
Peri-180 day	(n=63)	(n=262)	(n=390)	(n=715)
HD steroids n (%)	0 (0)	3 (1.1)	2 (0.5)	5 (0.7)

HCT: allogeneic hematopoietic cell transplant; BM: Bone marrow transplant; PBSC: Peripheral blood stem cell transplant.

Table S4. Lymphocyte subset counts.

	All (cells/ml)	BM	PBSC	CD34+
CD4	153	114	227	61
CD8	112	89	225	48
CD19	212	47	59	287
NK	247	212	180	322

Table S5. Engraftment day and median peri-engraftment diversity per graft source.

	Median Engraftment day	Median peri-engraftment diversity (simpson reciprocal)
BM	17 (+/- 4.6 SD)	4.0 (+/- 2.8 SD)
PBSC	12 (+/- 4.1 SD)	3.8 (+/- 5.6 SD)
CD34+ PBSC	10 (+/- 1.0 SD)	2.8 (+/- 2.5 SD)
All	11 (+/-3.6 SD)	3.3 (+/- 4.0 SD)

BM: Bone marrow transplant; PBSC: Peripheral blood stem cell transplant; SD: standard deviation.
Patients receiving CD34+ PBSC had statistically significantly lower diversity than patients receiving PBSC (p-val <0.001) or BM (p-val=0.002); however, patients receiving either PBSC or BM had similar median diversity (p-val=0.8).

Table S6. Clinical characteristics of patients with high and low Staphylococcus abundance (higher or lower than 75th percentile) in the peri-engraftment period.

	Staphylococcus abundance		*p*-val
	Low (n=450)	High (n=155)	
Age: median (IQR)	58 (47, 66)	57 (50, 64)	0.6
Sex: males, n (%)	274 (61)	90 (58)	0.5
Disease			
Lymphoma	79 (18)	10 (6.5)	0.004
MDS/MPN	106 (24)	39 (25)	
Leukemia	215 (48)	87 (56)	
Multiple Myeloma	40 (8.9)	18 (12)	
Non-malignant	10 (2.2)	1 (0.6)	
Intensity			<0.001
Reduced intensity	92 (20)	19 (13)	
Non-ablative	59 (13)	6 (3.9)	
Ablative	299 (66)	129 (83)	
Graft			<0.001
BM	50 (11)	18(12)	
PBSC	180 (40)	29 (19)	
CD34-selected	220 (49)	108 (70)	
Overall GVHD	179 (39.8)	62 (40)	0.3
Grade 0-1	318 (70.7)	104 (67.1)	
Grade 2-4	132 (29.3)	51 (32.9)	
Lower gut GVHD	43 (9.6)	12 (7.7)	0.4
Grade 0-1	433 (96.2)	148 (95.5)	
Grade 2-4	17 (3.8)	7 (4.5)	