

**Fig. S1.** Representative FACS analysis of various immune cell subtypes in the peripheral blood of the patients receiving allo-HSCT. (A) Immature myeloid-derived suppressor cells (I-MDSCs), (B) monocytic myeloid-derived suppressor cells (M-MDSCs), (C) CD3 T cells, (D) CD4 and CD8 T cells, (E) mucosal-associated invariant T cells (MAIT cells), (F) regulatory T cells (Treg), (G) natural killer (NK) and natural killer T (NKT)-like cells, (H) invariant NKT (iNKT) cells, (I) natural-killer receptor group 2, member D (NKG2D)-expressing NK cells, and (J) NKG2D-expressing NKT cells.

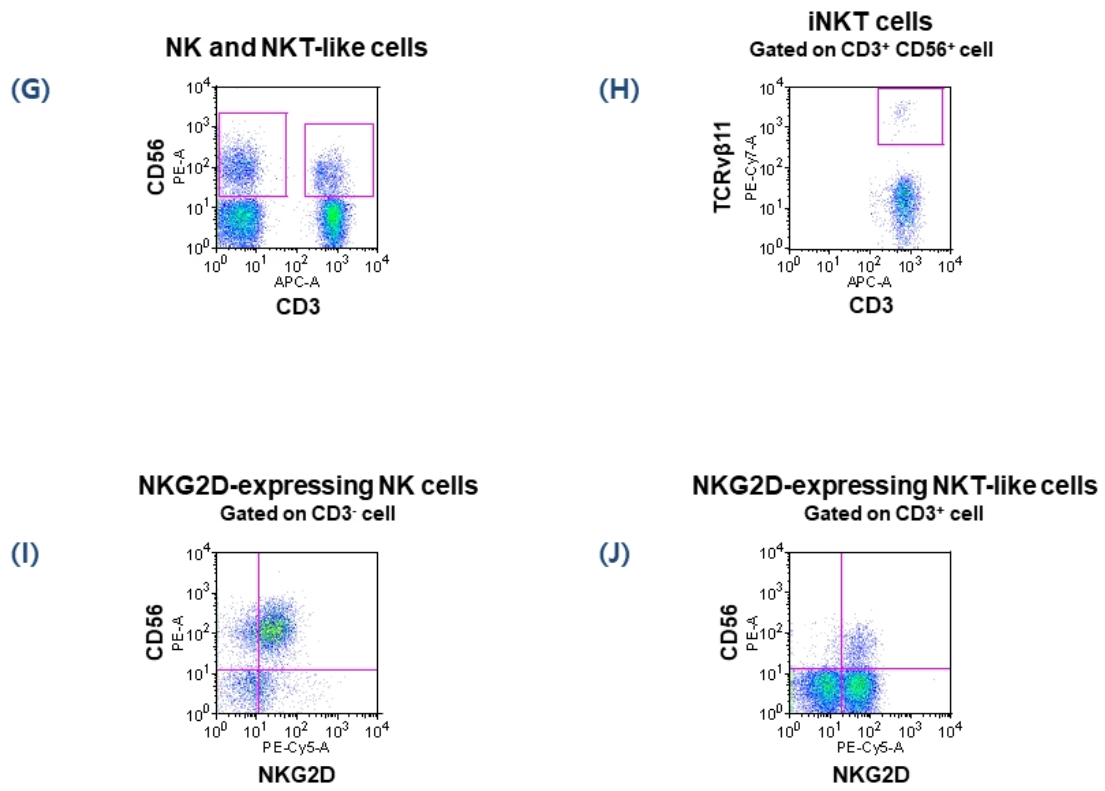
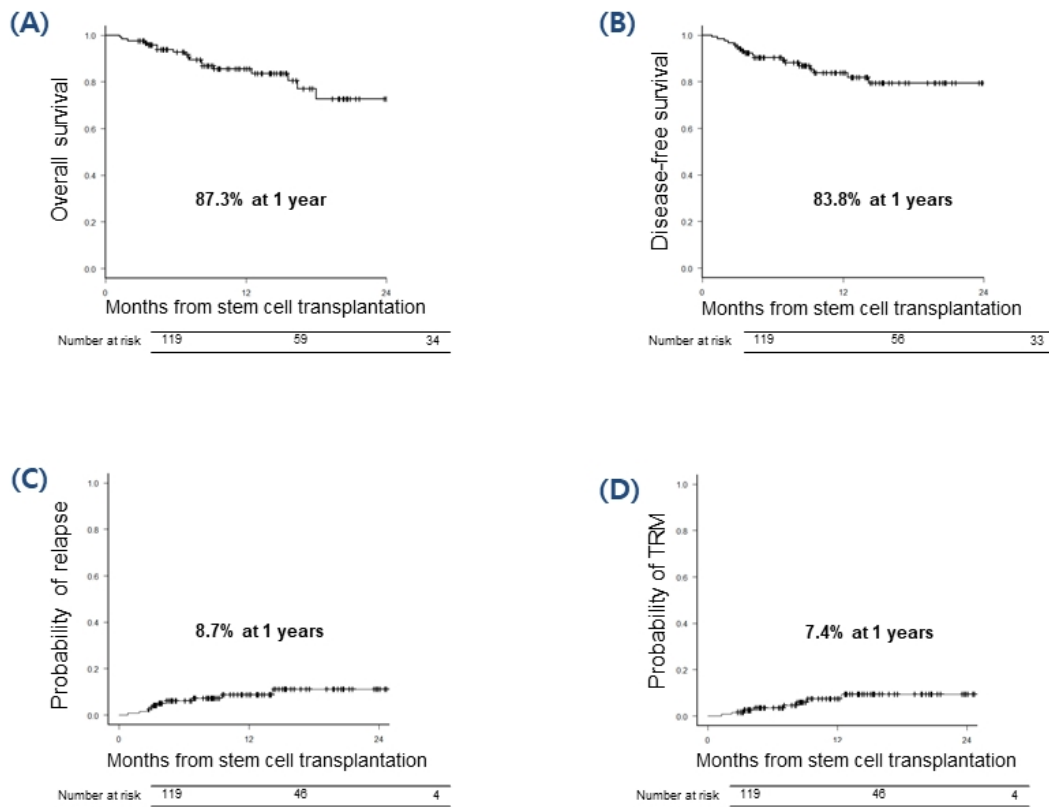
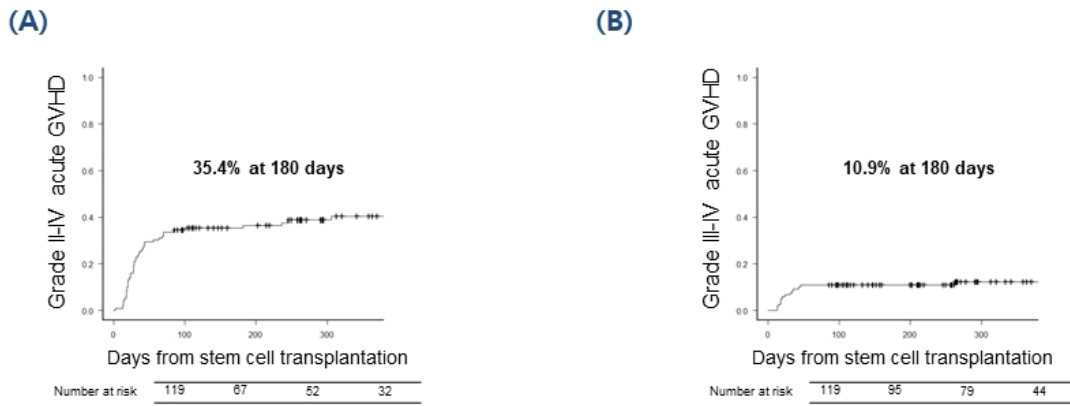


Fig. S1. Continued.



**Fig. S2.** Transplant outcomes. (A) overall survival, (B) disease-free survival, (C) cumulative incidence (CI) of relapse, (D) CI of treatment-related mortality (TRM).



**Fig. S3.** Cumulative incidences of acute graft-versus-host disease (GVHD) of total patients. (A) Grade II-IV acute GVHD, (B) Grade III-IV acute GVHD.

**Table S1.** Univariate analyses of factors affecting GVHD outcomes

Variables (N=119)	N	Grade III-IV acute GVHD at 180 days (95%CI)	p-value
<b>A. Clinical variables</b>			
Patient age (years)			0.077
<40	43	18.6% (8.6~31.5)	
≥40	76	6.6% (2.4~13.7)	
Donor age (years)			0.807
≤35	53	13.2% (5.7~23.8)	
>35	58	10.3% (4.2~19.8)	
Unavailable (double cord transplant)	8		
Disease			0.941
AML	74	10.8% (5.0~19.1)	
ALL	44	11.4% (4.1~22.7)	
Mixed phenotype acute leukemia	1	0.0%	
HLA match			0.473
Full-matched HLA	86	15.2% (5.4~29.5)	
Mismatched HLA	33	9.3% (4.3~16.6)	
Comorbidity (HCT-CI <sup>†</sup> )			0.759
Low to intermediate (score <3) (N, %)	81	11.1% (5.4~19.1)	
High (score ≥3) (N, %)	38	10.5% (3.3~22.7)	
Conditioning intensity			0.464
Myeloablative	84	11.9% (6.1~19.9)	
Reduced intensity	35	8.6% (2.1~20.8)	
Stem cell source			0.780
Bone marrow	18	5.6% (0.3~23.1)	
Peripheral blood	93	12.9% (7.0~20.6)	
Unavailable (double cord transplant)	8		
Infused dose of CD34 ( $\times 10^6$ /kg)			0.971
<5.7 (median)	59	10.2% (4.1~19.5)	
≥5.7 (median)	60	11.7% (5.1~21.2)	
Infused dose of CD3 ( $\times 10^6$ /kg)			0.562
<339.9 (median)	59	11.9% (5.2~21.6)	
≥339.9 (median)	60	10.0% (4.0~19.2)	
ATG use			0.378
0~2.5 mg/kg	88	9.1% (4.2~16.2)	
5.0~10.0 mg/kg	31	16.1% (5.8~31.2)	
TBI use			0.777
Yes	96	10.4% (5.3~17.5)	
No	23	13.0% (3.1~30.2)	
Donor type			0.383
Sibling	48	6.2% (1.6~15.6)	
Unrelated	40	17.5% (7.6~30.8)	
Haploidentical	23	13.0% (3.1~30.2)	
Double cord blood	8	0.0%	
GVHD prophylaxis			0.978
Methotrexate + cyclosporine	45	33.3% (20.0~47.2)	
Methotrexate + tacrolimus	66	36.4% (24.9~48.0)	
Mycophenolate mofetil + tacrolimus	8	37.5% (7.2~69.4)	

**Table S1.** Continued

Variables (N=119)	N	Grade III-IV acute GVHD at 180 days (95%CI)	p-value
<b>B. Experimental variables (post-transplant immune cell populations)</b>			
CD3 <sup>+</sup> T cells			0.297
≤61.5	95	11.6 (6.1~18.9)	
>61.5	22	4.5 (0.3~19.4)	
Unknown	2		
CD4 <sup>+</sup> T cells			0.368
≤1.45	30	16.7 (5.9~32.1)	
>1.45	89	9.0 (4.2~16.1)	
CD8 <sup>+</sup> T cells			0.044
≤5.8	26	23.1 (9.1~40.7)	
>5.8	93	7.5 (3.3~14.1)	
CD56 <sup>+</sup> cells			0.116
≤1.15	32	11.9 (5.2~21.6)	
>1.15	85	8.6 (3.1~17.6)	
Unknown	2		
Natural killer cells (CD3 <sup>-</sup> CD56 <sup>+</sup> )			0.765
≤8.1	59	11.9 (5.2~21.6)	
>8.1	58	8.6 (3.1~17.6)	
Unknown	2		
NKT-like cells (CD3 <sup>+</sup> CD56 <sup>+</sup> )			0.806
≤2	50	12.0 (4.8~22.7)	
>2	67	9.0 (4.2-3.6~17.3)	
Unknown	2		
Regulatory T cells (CD25 <sup>+</sup> CD127 <sup>low</sup> in CD3 <sup>+</sup> CD4 <sup>+</sup> cells)			0.229
≤0.83	36	16.7 (6.7~30.6)	
>0.83	40	7.5 (1.9~18.4)	
Unknown	43		
Invariant NKT cells (NKT-like cell marking Vβ11 <sup>+</sup> CD3 <sup>+</sup> )			0.028
≤0.027	39	17.9 (7.8~31.5)	
>0.027	78	6.4 (2.4~13.4)	
Unknown	2		
NKG2D expression on NK cells			0.203
≤5.6 (5.8)	61	13.1 (6.1~22.9)	
>5.6 (5.8)	56	7.1 (2.3~15.9)	
Unknown	2		
NKG2D expression on NKT-like cells,			0.650
≤0.42	33	9.1 (2.3~21.9)	
>0.42	84	10.7 (5.2~18.4)	
Unknown	2		
MAIT cells (CD8 <sup>+</sup> CD161 <sup>+</sup> Vα7.2 <sup>+</sup> )			0.144
≤0.17	25	20.0 (7.1~37.6)	
>0.17	94	8.5 (4.0~15.3)	
I-MDSC (HLA-DR <sup>-</sup> LIN <sup>-</sup> CD11b <sup>+</sup> CD33 <sup>+</sup> )			0.087
≤0.11	60	6.7 (2.1~14.9)	
>0.11	59	15.3 (7.5~25.6)	
M-MDSC (HLA-DR <sup>-</sup> CD14 <sup>+</sup> )			0.030
≤0.27	62	17.7 (9.4~28.2)	
>0.27	57	3.5 (0.6~10.8)	

GVHD: graft-versus-host disease, AML: acute myeloid leukemia, ALL: acute lymphoblastic leukemia, ATG: anti-thymocyte globulin, TBI: total body irradiation, HCT-CI: hematopoietic cell transplantation-comorbidity index, NKG2D: natural killer group 2, member D, MAIT: mucosal associated invariant T cell, I-MDSCs: immature myeloid-derived suppressor cells, M-MDSCs: monocytic myeloid-derived suppressor cells.

<sup>†</sup>HCT-CI was defined by Sorror et al. (21).

**Table S2.** Univariate analyses for association clinical factors with iNKT cells and M-MDSC cells

Variables (N=119)	Invariant NKT Cells (Mean±SD)	p-value	M-MDSC Cells (Mean±SD)	p-value
Patient age (years)		0.655		0.647
<40	0.374±0.749%		0.289±0.660%	
≥40	0.474±1.345%		0.243±0.417%	
Donor age (years)		0.172		0.015
≤35	0.522±1.547%		0.398±0.735%	
>35	0.229±0.417%		0.153±0.159%	
Unavailable (double cord transplant)				
Disease		0.560		0.216
AML	0.389±1.307%		0.577±0.811%	
ALL or Mixed phenotype acute leukemia	0.519±0.856%		0.907±2.039%	
HLA match		0.268		0.002
Full-matched HLA	0.657±1.736%		1.354±2.385%	
Mismatched HLA	0.354±0.847%		0.452±0.619%	
Comorbidity (HCT-CI <sup>†</sup> )		0.143		0.044
Low to intermediate (score <3) (N, %)	0.328±0.737%		0.524±0.748%	
High (score ≥3) (N, %)	0.664±1.730%		1.080±2.213%	
Conditioning intensity		0.363		0.556
Myeloablative	0.373±0.754%		0.653±1.559%	
Reduced intensity	0.586±1.788%		0.820±0.962%	
Stem cell source		0.924		0.742
Bone marrow	0.346±0.412%		0.765±0.925%	
Peripheral blood	0.373±1.207%		0.642±1.521%	
Unavailable (double cord transplant)				
Infused dose of CD34 (×10 <sup>6</sup> /kg)		0.455		0.500
<5.7 (median)	0.517±1.008%		0.719±0.873%	
≥5.7 (median)	0.356±1.299%		0.685±1.793%	
Infused dose of CD3 (×10 <sup>6</sup> /kg)		0.777		0.894
<339.9 (median)	0.468±1.005%		0.614±0.738%	
≥339.9 (median)	0.407±1.297%		0.789±1.848%	
ATG use		0.660		0.801
0~2.5 mg/kg	0.409±0.857%		0.682±1.531%	
5.0~10.0 mg/kg	0.518±1.785%		0.760±0.999%	
TBI use		0.989		0.175
Yes	0.436±1.262%		0.343±0.360%	
No	0.440±0.590%		0.788±1.547%	
Donor type		<0.001		0.002
Sibling	0.315±0.453%		0.458±0.640%	
Unrelated	0.393±1.170%		0.758±2.132%	
Haploidentical	0.439±1.828%		0.921±1.110%	
Double cord blood	1.367±1.432%		1.254±0.738%	
GVHD prophylaxis		<0.001		0.006
Methotrexate+cyclosporine	0.299±0.457%		0.451±0.655%	
Methotrexate+tacrolimus	0.418±1.406%		0.806±1.777%	
Mycophenolate mofetil+tacrolimus	1.367±1.432%		1.254±0.738%	

GVHD: graft-versus-host disease, AML: acute myeloid leukemia, ALL: acute lymphoblastic leukemia, ATG: anti-thymocyte globulin, TBI: total body irradiation, HCT-CI: hematopoietic cell transplantation-comorbidity index, M-MDSCs: monocytic myeloid-derived suppressor cells.

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