Table S1: Interactions between transcobalamin II (TCII) and hydroxycobalamin [*c*-lactam] (HCCL) or natural cobalamins common for every ligand used in the molecular docking study.

TCII	HCCL			Hydroxycobalamin			Methylcobalamin			Adenosylcobalamin		
Residue	**Residue**	**Type**	**Length [Å]**	**Residue**	**Type**	**Length [Å]**	**Residue**	**Type**	**Length [Å]**	**Residue**	**Type**	**Length [Å]**
Asn224	acetamide	conventional hydrogen bond	1.96	acetamide	conventional hydrogen bond	2.06	acetamide	conventional hydrogen bond	2.02	acetamide	conventional hydrogen bond	2.21
	acetamide	conventional hydrogen bond	2.20	acetamide	conventional hydrogen bond	2.11	acetamide	conventional hydrogen bond	2.16	acetamide	conventional hydrogen bond	2.23
Asp176	acetamide	conventional hydrogen bond	2.02	acetamide	conventional hydrogen bond	2.00	acetamide	conventional hydrogen bond	2.06	acetamide	conventional hydrogen bond	2.03
	acetamide	conventional hydrogen bond	2.62	acetamide	conventional hydrogen bond	2.43	acetamide	conventional hydrogen bond	2.48	acetamide	conventional hydrogen bond	2.60
Gln138	carbonyl	conventional hydrogen bond	2.44	carbonyl	conventional hydrogen bond	2.6	carbonyl	conventional hydrogen bond	2.74	carbonyl	conventional hydrogen bond	2.95
Gln273	acetamide	conventional hydrogen bond	2.18	acetamide	conventional hydrogen bond	2.44	acetamide	conventional hydrogen bond	2.33	acetamide	conventional hydrogen bond	2.71
Gln86	phosphate	conventional hydrogen bond	1.64	phosphate	conventional hydrogen bond	1.83	phosphate	conventional hydrogen bond	1.70	phosphate	conventional hydrogen bond	1.56
Leu358	phosphate	conventional hydrogen bond	2.07	phosphate	conventional hydrogen bond	2.09	phosphate	conventional hydrogen bond	2.00	phosphate	conventional hydrogen bond	1.92
Leu363	propamide	conventional hydrogen bond	2.29	propamide	conventional hydrogen bond	2.11	acetamide	conventional hydrogen bond	1.90	propamide	conventional hydrogen bond	2.12
	propamide	conventional hydrogen bond	2.71	propamide	conventional hydrogen bond	2.68	propamide	conventional hydrogen bond	2.26	propamide	conventional hydrogen bond	2.65
Leu379	methyl	alkyl	4.71	methyl	alkyl	4.60	methyl	Alkyl	4.48	methyl	alkyl	4.52
Met270	methyl	alkyl	4.66	methyl	alkyl	4.75	methyl	Alkyl	4.66	methyl	alkyl	5.02
Phe376	methyl	π-alkyl	3.41	methyl	π-alkyl	3.70	methyl	π-alkyl	3.84	methyl	π-alkyl	4.00
	methyl	π-alkyl	3.94	methyl	π-alkyl	3.84	methyl	π-alkyl	3.85	methyl	π-alkyl	4.17
Ser357	phosphate	carbon hydrogen bond	2.52	phosphate	carbon hydrogen bond	2.65	phosphate	carbon hydrogen bond	2.73	phosphate	carbon hydrogen bond	2.74
Trp409	methyl	π-alkyl	2.62	methyl	π-alkyl	4.45	methyl	π-alkyl	4.24	methyl	π-alkyl	3.80
	methyl	π-alkyl	4.85	methyl	π-alkyl	4.50	methyl	π-alkyl	4.94	methyl	π-alkyl	4.88
Tyr137	acetamide	conventional hydrogen bond	2.41	acetamide	conventional hydrogen bond	2.42	acetamide	conventional hydrogen bond	2.54	acetamide	conventional hydrogen bond	2.69
	methyl	π-alkyl	4.65	methyl	π-alkyl	4.71	methyl	π-alkyl	4.78	methyl	π-alkyl	4.87

Table S2: Differences in the interactions between transcobalamin II (TCII) and ligands used in the molecular docking study.

TCII	HCCL			Hydroxycobalamin			Methylcobalamin			Adenosylcobalamin		
Residue	**Residue**	**Type**	**Length [Å]**	**Residue**	**Type**	**Length [Å]**	**Residue**	**Type**	**Length [Å]**	**Residue**	**Type**	**Length [Å]**
Gln138	-	-	-	hydroxyl	conventional hydrogen bond	2.74	-	-	-	-	-	-
	-	-	-	hydroxyl	conventional hydrogen bond	2.49	-	-	-	-	-	-
Gln273	acetamide	conventional hydrogen bond	2.41	acetamide	conventional hydrogen bond	2.19	acetamide	conventional hydrogen bond	2.70	-	-	-
Gln378	γ-lactam ring	conventional hydrogen bond	2.70	-	-	-	-	-	-	-	-	-
	-	-	-	acetamide	carbon hydrogen bond	2.67	acetamide	carbon hydrogen bond	2.47	acetamide	carbon hydrogen bond	2.95
Gly390	-	-	-	propamide	conventional hydrogen bond	2.54	-	-	-	propamide	conventional hydrogen bond	2.57
Leu141	-	-	-	methyl	alkyl	5.39	methyl	alkyl	5.27	methyl	alkyl	5.25
Leu358	-	-	-	-	-	-	-	-	-	methyl	alkyl	5.41
Leu379	-	-	-	acetamide	conventional hydrogen bond	2.18	acetamide	conventional hydrogen bond	2.08	acetamide	conventional hydrogen bond	1.85
	-	-	-	acetamide	conventional hydrogen bond	2.18	acetamide	conventional hydrogen bond	1.88	-	-	-
Leu387	-	-	-	acetamide	conventional hydrogen bond	1.91	acetamide	conventional hydrogen bond	2.07	-	-	-
Leu388	propamide	conventional hydrogen bond	2.26	-	-	-	propamide	conventional hydrogen bond	2.22	propamide	conventional hydrogen bond	2.91
Leu89	-	-	-	methyl	alkyl	5.25	methyl	alkyl	4.92	methyl	alkyl	4.62
Phe376	-	-	-	-	-	-	-	-	-	pyrolidine	π-alkyl	5.07
	-	-	-	-	-	-	-	-	-	pyroline	π-alkyl	5.40
	-	-	-	-	-	-	-	-	-	propamide	π-alkyl	5.10
Ser135	-	-	-	-	-	-	propamide	carbon hydrogen bond	2.56	propamide	carbon hydrogen bond	2.60
Thr134	-	-	-	-	-	-	-	-	-	propamide	carbon hydrogen bond	2.98

Trp377	propamide	conventional hydrogen bond	2.60	propamide	conventional hydrogen bond	2.71	-	-	-	propamide	conventional hydrogen bond	2.77
	-	-	-	-	-	-	acetamide	conventional hydrogen Bond	2.50	-	-	-
Trp409	propamide	conventional hydrogen bond	2.49	-	-	-	-	-	-	-	-	-
	methyl	π-alkyl	1.96	-	-	-	methyl	π-alkyl	4.23	methyl	π-alkyl	3.80
	-	-	-	-	-	-	-	-	-	pyroline	π-alkyl	5.23
Tyr226	-	-	-	propamide	π -donor hydrogen bond	2.95	-	-	-	-	-	-
Tyr362	-	-	-	methyl	π-alkyl	5.33	methyl	π-alkyl	5.30	methyl	π-alkyl	5.23
	-	-	-	-	-	-	-	-	-	methyl	π-alkyl	5.10