

## List of experimentally characterized TBDTs and of TBDTs with predicted substrate used for classification

All TBDTs used for the analysis of the CLANs results are given. *Italic* indicates TBDTs with predicted substrate. The left columns give the numbers used in Figure 1, the second column the Cluster (see Figure 1A), the third column gives the assigned name, the fourth column the GenBank ID, the fifth column the source species, the sixth column the identified siderophores recognized by the according protein, the seventh column the siderophore classification and the eighth column representative references for the substrate and substrate classification (o.a.: only annotated). '[metal]' in column 6 indicates that the type of transported metal ion is known, but the according metallophore has not yet been identified.

No.	Cluster	Name	GenBank	Species	Substrate	Siderophore/Substrate Classification	Ref.
1	11	OprC	1498191	<i>Pseudomonas aeruginosa</i>	Copper chelate	Unknown	[34]
2	12	BfeA	538279	<i>Bordetella pertussis</i>	enterobactin	Catecholate	[35, 36]
3	12	PirA	2981053	<i>Pseudomonas aeruginosa</i>	enterobactin	Catecholate	[36, 37]
4	12	PfeA	548479	<i>Pseudomonas aeruginosa</i>	enterobactin	Catecholate	[36, 38]
5	12	FepA	2507463	<i>Escherichia coli</i> K12	enterobactin	Catecholate	[36, 39]
6	12	IroN	2738252	<i>Salmonella enterica</i>	salmochelins	glycosylated Catecholate	[40, 41]
7	12	CfrA	112360090	<i>Campylobacter jejuni</i>	enterobactin	Catecholate	[36, 42]
8	12	CirA	2507462	<i>Escherichia coli</i> K12	2,3-dihydroxybenzoylserine(DHBS)	Catecholate-Carboxylate	[43, 44]
9	12	IrgA	12644182	<i>Vibrio cholerae</i>	Enterobactin	Catecholate	[36, 45]
10	12	BfrA	1314835	<i>Bordetella bronchiseptica</i>	2,3-dihydroxybenzoylserine(DHBS)	Catecholate-Carboxylate	[44, 46]
11	18	HutR	147671724	<i>Vibrio cholerae</i>	haem	Porphyrine	[47]
12	18	HuvA	12697532	<i>Listonella anguillarum</i>	haem	Porphyrine	[48]
13	18	HutA	529727	<i>Vibrio cholerae</i>	haem	Porphyrine	[49]
14	18	PhuR	3044098	<i>Pseudomonas aeruginosa</i>	haem	Porphyrine	[37]
15	18	PfhR	4838477	<i>Pseudomonas fluorescens</i>	haem	Porphyrine	[37]
16	132	HpuB	11386826	<i>Neisseria meningitidis</i>	haem	Porphyrine	[50]
17	108	HmbR	687640	<i>Neisseria meningitidis</i>	haem	Porphyrine	[51]
18	17	HgbA	28194090	<i>Actinobacillus pleuropneumoniae</i>	haem	Porphyrine	[52]
19	86	HemR	6016198	<i>Yersinia enterocolitica</i>	haem	Porphyrine	[53]
20	86	HmuR	2501236	<i>Yersinia pestis</i>	haem	Porphyrine	[54]
21	86	ChuA	1763009	<i>Escherichia coli</i> O157:H7	haem	Porphyrine	[55]
22	86	ShuA	1655877	<i>Shigella dysenteriae</i>	haem	Porphyrine	[56]
23	86	HxuC	1170441	<i>Haemophilus influenzae</i>	haem	Porphyrine	[57]
24	48	TdhA	33151615	<i>Haemophilus ducreyi</i> 35000HP	haem	Porphyrine	[58]
25	152	HasR	34787214	<i>Serratia marcescens</i>	haem	Porphyrine	[59]

No.	Cluster	Name	GenBank	Species	Substrate	Siderophore/Substrate Classification	Ref.
26	107	MhuA	50403825	Moraxella catarrhalis	haem	Porphyrine	[60]
27	15	FetA_FrpB	4768684	Neisseria gonorrhoeae	enterobactin	Catecholate	[36,61]
28	59	VctA	18476494	Vibrio cholerae	enterobactin	Catecholate	[36, 62]
29	16	LbpA	915278	Neisseria gonorrhoeae	lactoferrin	Fe(III)-binding protein	[22, 63]
30	16	TbpA	150361	Neisseria gonorrhoeae	transferrin	Fe(III)-binding protein	[22, 64]
31	112	FrpB4	15646121	Helicobacter pylori 26695	[Nickel]	unknown	[14]
32	4	BtuB	416728	Escherichia coli K12	Vitamin B12	Porphyrine	[65]
33	4	XCC3067	21232497	Xanthomonas campestris pv. campestris str. ATCC 33913	Vitamin B12	Porphyrine	[66]
34	4	PA1271	15596468	Pseudomonas aeruginosa PAO1	Vitamin B12	Porphyrine	[66]
35	4	BPSL0976	53718618	Burkholderia pseudomallei K96243	Vitamin B12	Porphyrine	[66]
36	4	RS02718	17547119	Ralstonia solanacearum GMI1000	Vitamin B12	Porphyrine	[66]
37	165	CC1750	109897435	Pseudoalteromonas atlantica T6c	Vitamin B12	Porphyrine	[66]
38	4	VC0156	15640186	Vibrio cholera	Vitamin B12	Porphyrine	[66]
39	160	RSP_2402	77462960	Rhodobacter sphaeroides 2.4.1	Vitamin B12	Porphyrine	[66]
40	40	MxcH	162452159	Sorangium cellulosum 'So ce 56'	Myxochelin	Catecholate	[67, 68]
41	10	IutA	1170593	Escherichia coli	aerobactin	Citrate-Hydroxamate	[69, 70]
42	10	RhtA	6685883	Sinorhizobium meliloti	Rhizobactin 1021	Citrate-Hydroxamate	[71, 72]
43	166	SO_0815	24372404	Shewanella oneidensis MR-1	Vitamin B12	Porphyrine	[66]
44	82	RumA	1247762	Morganella morganii	ferric rhizoferrin	Carboxylate	[73, 74]
45	82	FecA	729471	Escherichia coli K12	diferic dicitrate	Citrate	[75, 76]
46	25	PA2911	15598107	Pseudomonas aeruginosa PAO1	Vitamin B12	Porphyrine	[66]
47	25	RPA0407	39933484	Rhodopseudomonas palustris CGA009	Vitamin B12	Porphyrine	[66]
48	0	VciA	147673813	Vibrio cholerae O395	unknown	unknown	[77]
49	0	PiuA_Fiu	115587765	Pseudomonas aeruginosa	pyochelin	Phenolate	[78, 79]
50	0	FoxA	1169726	Yersinia enterocolitica	desferrioxamine	Hydroxamate	[80, 81]
51	0	FegA	1518696	Bradyrhizobium japonicum	desferrioxamine	Hydroxamate	[82, 81]
52	0	FctA	871032	Erwinia chrysanthemi	chrysobactin	Catecholate	[83, 84]
53	0	FmtA	53719389	Burkholderia pseudomallei K96243	ferric malleobactin	Hydroxamate	[85, 86]
54	0	OrbA	76810798	Burkholderia pseudomallei	ferric ornibactin	Citrate-Hydroxamate	[87, 88] <sup>a</sup>
55	0	FhuA	2507464	Escherichia coli K12	ferrichrome	Hydroxamate	[89, 90]
56	0	OptS	116050410	Pseudomonas aeruginosa	desferrioxamine	Hydroxamate	[81, 91]
57	0	BfrI	33592999	Bordetella pertussis Tohama I	unknown	unknown	o.a.
58	-	BfrZ	6850914	Bordetella bronchiseptica	unknown	unknown	[92]
59	-	PrhA	17549099	Ralstonia solanacea rum	transducer without transport function	unknown	[93]
60	6	PbuA	1172035	Pseudomonas sp. M114	pseudobactin M114	Citrate-Catecholate-Hydroxamate	[94, 95]
61	6	FpvA	12230910	Pseudomonas aeruginosa	pyoverdine	Catecholate-Hydroxamate	[96, 97]
62	6	PupA	45723	Pseudomonas putida WCS358	pseudobactin A	Citrate-Catecholate-Hydroxamate	[95, 98]
63	6	PupB	585759	Pseudomonas putida WCS358	pseudobactin A	Citrate-Catecholate-Hydroxamate	[95, 99]
64	6	FauA	4589285	Bordetella pertussis	alcaligin	Hydroxamate	[100, 101]
65	6	FhuE	2507465	Escherichia coli K12	Coprogen, ferrioxamine B, rhodoturolic acid	Hydroxamates	[102-105]
66	6	FptA	1169730	Pseudomonas aeruginosa	pyochelin	Phenolate	[79, 106]
67	9	Bcep18194_b2436	78063283	Burkholderia sp. 383	Thiamin	Vitamin B1	[107]

No.	Cluster	Name	GenBank	Species	Substrate	Siderophore/Substrate Classification	Ref.
68	9	XCC0674	21230149	<i>X. campestris</i> pv. <i>Campestris</i> str. ATCC 33913	Thiamin	Vitamin B1	[107]
69	7	FatA	132510	Listonella anguillarum	anguibactin	Catecholate-Hydroxamate	[108, 109]
70	7	BauA	49175779	Acinetobacter baumannii	anguibactin	Catecholate-Hydroxamate	[109, 110]
71	7	FcuA	11696551	Yersinia enterocolitica	anguibactin	Catecholate-Hydroxamate	[111, 109]
72	79	FyuA	517234	Yersinia enterocolitica	yersiniabactin	Phenolate	[112, 113]
73	79	IrpC	17380443	Yersinia pestis	yersiniabactin	Phenolate	[113, 114]
74	140	ViuA	267356	Vibrio cholerae	vibriobactin	Catecholate	[115, 116]
75	118	SO_2715	24374256	<i>Shewanella oneidensis</i> MR-1	Thiamin	Vitamin B1	[107]
76	118	CPS_0067	71281279	<i>Colwellia psychrerythraea</i> 34H	Thiamin	Vitamin B1	[107]
77	45	SftP	6019468	<i>Pseudomonas putida</i>	hexylsulfate		[117]
78	64	SuxA	21232787	<i>Xanthomonas campestris</i> pv. <i>campestris</i> str. ATCC 33913	sucrose	disaccharide	[15]
79	64	Sfri_3988	114565138	<i>Shewanella frigidimarina</i> NCIMB 400	sucrose	disaccharide	[15]
80	52	bl16948	27382059	<i>Bradyrhizobium japonicum</i> USDA 110	[Nickel]	Unknown	
81	52	Daro_1684	71907314	<i>Dechloromonas aromatica</i> RCB	[Cobalt]	Unknown	[118]
82	52	Daro_3944	71909555	<i>Dechloromonas aromatic</i> RCB	[Nickel]	Unknown	[118]
83	9	BF0615	53711906	<i>Bacteroides fragilis</i> YCH46	Thiamin	Vitamin B1	[107]
84	9	PG1899	34541505	<i>Porphyromonas gingivalis</i> W83	Thiamin	Vitamin B1	[107]
85	26	RagA	110636973	<i>Cytophaga hutchinsonii</i> ATCC 33406	digested proteins	Polypeptides	[19] <sup>b</sup>
86	26	RagA	110636966	<i>Cytophaga hutchinsonii</i> ATCC 33406	digested proteins	Polypeptides	[19] <sup>b</sup>
87	26	SusC	29349110	<i>Bacteroides thetaiotaomicron</i> VPI-5482	Malto-oligo-saccharides /starch	Oligo-/Polysaccharides	[18]
88	26	CsuF	29348741	<i>Bacteroides thetaiotaomicron</i> VPI-5482	Chondroitin sulfate / hyaluronic acid	unbranched polysaccharides (GlcA GalNAc) / unbranched polymer of N-acetyl-glucosamine + glucuronic acid	[17, 119, 120]
89	26	OmpW	29348978	<i>Bacteroides thetaiotaomicron</i> VPI-5482	unknown	unknown	[121]
90	63	MalA	16126526	<i>Caulobacter crescentus</i> CB15	Maltodextrins	starch hydrolysate	[16]
91	63	SO_3514	24375018	<i>Shewanella oneidensis</i> MR-1	Chito-oligosaccharides	N-acetylglucosamine oligomer	[122, 123]
92	63	Sden_2708	91794059	<i>Shewanella denitrificans</i> OS217	Chito-oligosaccharides	N-acetylglucosamine oligomer	[122, 123]
93	63	CPS_1021	71281574	<i>Colwellia psychrerythraea</i> 34H	Chito-oligosaccharides	N-acetylglucosamine oligomer	[122, 123]
94	63	CC_0446	16124701	<i>Caulobacter crescentus</i> CB15	Chito-oligosaccharides	N-acetylglucosamine oligomer	[122, 123]
95	63	XCC0120	21229598	<i>X. campestris</i> pv. <i>campestris</i> str. ATCC 33913	Pectin	heteropolysaccharide	[15]
96	63	XCC2944	21232375	<i>X. campestris</i> pv. <i>campestris</i> str. ATCC 33913	Chito-oligosaccharides	N-acetylglucosamine oligomer	[122, 123]
97	72	XCC4120	21233542	<i>X. campestris</i> pv. <i>campestris</i> str. ATCC 33913	Xylan	heteropolysaccharide	[15]
98	41	BF1991	53713281	<i>Bacteroides fragilis</i> YCH46	Fibronectin	extracellular matrix glycoprotein	[124]

<sup>a</sup> ...we have marked one sequence (54; annotated as OrbA in GenBank) with 79% similarity and 67% identity to the one described in the reference (*Burkholderia cepacia*, gi|11230853, [87]); sequences with a higher similarity/identity are in the same cluster, too.

<sup>b</sup> ...we have marked two sequences (85, 86; annotated as RagA in GenBank) with 65% similarity and 31% identity to the one described in the reference (*Porphyromonas gingivalis* W83, gi|34540042, [19]).