

Table S1. Peptides used in this study.**Fatty acid-XRR-NH₂**

Code	Fatty acid	X	Average mass	Monoisotopic mass	z	Calculated m/z		Measured m/z
						Average	Monoisotopic	
1	C8	-	455.598	455.333	1	456.61	456.34	456.41
					2	228.81	228.67	228.78
2	C10	-	483.651	483.365	1	484.66	484.37	484.48
					2	242.83	242.69	242.78
3	C12	-	511.704	511.396	1	512.71	512.40	512.47
					2	256.86	256.71	256.85
4	C14	-	539.757	539.427	1	540.77	540.43	540.52
					2	270.89	270.72	270.87
5	C16	-	567.810	567.458	1	568.82	568.47	568.57
					2	284.41	284.23	284.91
6	C18	-	595.863	595.489	1	596.87	596.50	596.59
					2	298.44	298.25	298.95
7	C8	A	526.676	526.370	1	527.68	527.38	527.47
					2	264.35	264.19	264.33
8	C10	A	554.729	554.402	1	555.74	555.41	555.53
					2	278.37	278.21	278.35
9	C12	A	582.782	582.433	1	583.79	583.44	583.53
					2	292.40	292.22	292.39
10	C14	A	610.836	610.464	1	611.84	611.47	611.61
					2	306.43	306.24	306.41
11	C8	C(Acm)	629.819	629.380	1	630.83	630.39	630.52
					2	315.92	315.70	315.85
12	C10	C(Acm)	657.872	657.411	1	658.88	658.42	658.52
					2	329.94	329.71	329.89
13	C12	C(Acm)	685.925	685.442	1	686.93	686.45	686.56
					2	343.97	343.73	343.93
14	C14	C(Acm)	713.978	713.473	1	714.99	714.48	714.60
					2	358.00	357.74	357.94
15	C8	D	570.685	570.360	1	571.69	571.37	571.49
					2	286.35	286.19	286.31
16	C10	D	598.739	598.391	1	599.75	599.40	599.52
					2	300.38	300.20	300.33
17	C12	D	626.792	626.423	1	627.80	627.43	627.55
					2	314.40	314.22	314.40
18	C14	D	654.845	654.454	1	655.85	655.46	655.58
					2	328.43	328.23	328.45
19	C8	E	584.712	584.376	1	585.72	585.38	585.51
					2	293.36	293.20	293.37
20	C10	E	612.765	612.407	1	613.77	613.41	613.53
					2	307.39	307.21	307.36
21	C12	E	640.818	640.438	1	641.83	641.45	641.57
					2	321.42	321.23	321.41

22	C14	E	668.872	668.470	1	669.88	669.48	669.60
					2	335.44	335.24	335.41
23	C8	F	602.772	602.402	1	603.78	603.41	603.53
					2	302.39	302.21	302.37
24	C10	F	630.825	630.433	1	631.83	631.44	631.56
					2	316.42	316.22	316.43
25	C12	F	658.878	658.464	1	659.89	659.47	659.57
					2	330.45	330.24	330.43
26	C14	F	686.932	686.496	1	687.94	687.50	687.62
					2	344.47	344.26	344.45
27	C8	G	512.649	512.355	1	513.66	513.36	513.47
					2	257.33	257.19	257.32
28	C10	G	540.703	540.386	1	541.71	541.39	541.50
					2	271.36	271.20	271.33
29	C12	G	568.756	568.417	1	569.76	569.43	569.55
					2	285.39	285.22	285.36
30	C14	G	596.809	596.449	1	597.82	597.46	597.58
					2	299.41	299.23	299.40
31	C8	H	592.737	592.392	1	593.75	593.40	593.46
					2	297.38	297.20	297.34
					3	198.59	198.47	198.57
32	C10	H	620.790	620.423	1	621.80	621.43	621.53
					2	311.40	311.22	311.38
					3	207.94	207.82	207.97
33	C12	H	648.844	648.455	1	649.85	649.46	649.54
					2	325.43	325.24	325.45
					3	217.29	217.16	217.29
34	C14	H	676.897	676.486	1	677.90	677.49	677.56
					2	339.46	339.25	339.42
					3	226.64	226.50	226.63
35	C8	I	568.756	568.417	1	569.76	569.43	569.54
					2	285.39	285.22	285.37
36	C10	I	596.809	596.449	1	597.82	597.46	597.58
					2	299.41	299.23	299.41
37	C12	I	624.862	624.480	1	625.87	625.49	625.60
					2	313.44	313.25	313.42
38	C14	I	652.915	652.511	1	653.92	653.52	653.60
					2	327.47	327.26	327.49
39	C8	K	583.773	583.428	1	584.78	584.44	584.64
					2	292.89	292.72	293.00
					3	195.60	195.48	195.66
40	C10	K	611.823	611.459	1	612.83	612.47	612.74
					2	306.92	306.74	307.06
					3	204.95	204.83	205.21
41	C12	K	639.877	639.491	1	640.88	640.50	640.79
					2	320.95	320.75	320.92
					3	214.30	214.17	214.51

42	C14	K	667.930	667.522	1	668.94	668.53	668.77
					2	334.97	334.77	335.10
					3	223.65	223.52	223.81
43	C8	L	568.756	568.417	1	569.76	569.43	569.54
					2	285.39	285.22	285.38
44	C10	L	596.809	596.449	1	597.82	597.46	597.57
					2	299.41	299.23	299.42
45	C12	L	624.862	624.480	1	625.87	625.49	625.60
					2	313.44	313.25	313.47
46	C14	L	652.915	652.511	1	653.92	653.52	653.63
					2	327.47	327.26	327.47
47	C8	M	586.794	586.374	1	587.80	587.38	587.49
					2	294.40	294.19	294.35
48	C10	M	614.847	614.405	1	615.86	615.41	615.52
					2	308.43	308.21	308.39
49	C12	M	642.900	642.436	1	643.91	643.44	643.55
					2	322.46	322.23	322.44
50	C14	M	670.953	670.468	1	671.96	671.48	671.59
					2	336.48	336.24	336.48
51	C8	M(O)	602.794	602.369	1	603.80	603.38	603.57
					2	302.40	302.19	302.43
52	C10	M(O)	630.847	630.400	1	631.85	631.41	631.63
					2	316.43	316.21	316.49
53	C12	M(O)	658.900	658.431	1	659.91	659.44	659.65
					2	330.46	330.22	330.45
54	C14	M(O)	686.953	686.463	1	687.96	687.47	687.64
					2	344.48	344.24	344.53
55	C8	M(O2)	618.793	618.364	1	619.80	619.37	619.62
					2	310.40	310.19	310.45
56	C10	M(O2)	646.846	646.395	1	647.85	647.40	647.63
					2	324.43	324.21	324.49
57	C12	M(O2)	674.899	674.426	1	675.91	675.43	675.61
					2	338.46	338.22	338.41
58	C14	M(O2)	702.952	702.457	1	703.96	703.47	703.63
					2	352.48	352.24	352.5
59	C8	N	569.701	569.376	1	570.71	570.38	570.51
					2	285.86	285.70	285.83
60	C10	N	597.754	597.407	1	598.76	598.42	598.56
					2	299.88	299.71	299.88
61	C12	N	625.807	625.439	1	626.81	626.45	626.57
					2	313.91	313.73	313.94
62	C14	N	653.860	653.470	1	654.87	654.48	654.59
					2	327.94	327.74	327.92
63	C8	Nle	568.756	568.417	1	569.76	569.43	569.55
					2	285.39	285.22	285.35
64	C10	Nle	596.809	596.449	1	597.82	597.46	597.58
					2	299.41	299.23	299.44

65	C12	Nle	624.862	624.480	1	625.87	625.49	625.59
					2	313.44	313.25	313.42
66	C14	Nle	652.915	652.511	1	653.92	653.52	653.59
					2	327.47	327.26	327.48
67	C8	Nva	554.729	554.402	1	555.74	555.41	555.53
					2	278.37	278.21	278.34
68	C10	Nva	582.782	582.433	1	583.79	583.44	583.57
					2	292.40	292.22	292.35
69	C12	Nva	610.835	610.464	1	611.84	611.47	611.6
					2	306.43	306.24	306.41
70	C14	Nva	638.888	638.496	1	639.90	639.50	639.65
					2	320.45	320.26	320.46
71	C8	P	552.713	552.386	1	553.72	553.39	553.52
					2	277.36	277.20	277.37
72	C10	P	580.766	580.417	1	581.77	581.43	581.54
					2	291.39	291.22	291.38
73	C12	P	608.819	608.449	1	609.83	609.46	609.59
					2	305.42	305.23	305.40
74	C14	P	636.873	636.480	1	637.88	637.49	637.62
					2	319.44	319.25	319.42
75	C8	Q	583.727	583.392	1	584.74	584.40	584.53
					2	292.87	292.70	292.88
76	C10	Q	611.780	611.423	1	612.79	612.43	612.55
					2	306.90	306.72	306.87
77	C12	Q	639.834	639.454	1	640.84	640.46	640.58
					2	320.92	320.74	320.97
78	C14	Q	667.887	667.486	1	668.89	668.49	668.61
					2	334.95	334.75	334.99
79	C8	R	611.784	611.434	1	612.79	612.44	612.56
					2	306.90	306.72	306.98
					3	204.94	204.82	205.36
80	C10	R	639.837	639.466	1	640.84	640.47	640.71
					2	320.93	320.74	320.99
					3	214.29	214.16	214.54
81	C12	R	667.890	667.497	1	668.90	668.50	668.79
					2	334.95	334.76	335.09
					3	223.64	223.51	223.78
82	C14	R	695.943	695.528	1	696.95	696.54	696.78
					2	348.98	348.77	349.05
					3	232.99	232.85	233.07
83	C8	S	542.675	542.365	1	543.68	543.37	543.47
					2	272.35	272.19	272.31
84	C10	S	570.728	570.397	1	571.74	571.40	571.55
					2	286.37	286.21	286.35
85	C12	S	598.782	598.428	1	599.79	599.44	599.55
					2	300.40	300.22	300.40
86	C14	S	626.835	626.459	1	627.84	627.47	627.57

					2	314.43	314.24	314.4
87	C8	T	556.702	556.381	1	557.71	557.39	557.53
					2	279.36	279.20	279.44
88	C10	T	584.755	584.412	1	585.76	585.42	585.61
					2	293.39	293.21	293.47
89	C12	T	612.808	612.444	1	613.82	613.45	613.66
					2	307.41	307.23	307.54
90	C14	T	640.861	640.475	1	641.87	641.48	641.71
					2	321.44	321.25	321.50
91	C8	V	554.729	554.402	1	555.74	555.41	555.54
					2	278.37	278.21	278.36
92	C10	V	582.782	582.433	1	583.79	583.44	583.57
					2	292.40	292.22	292.38
93	C12	V	610.835	610.464	1	611.84	611.47	611.61
					2	306.43	306.24	306.44
94	C14	V	638.888	638.496	1	639.90	639.50	639.63
					2	320.45	320.26	320.4
95	C8	W	641.808	641.413	1	642.82	642.42	642.54
					2	321.91	321.71	321.91
96	C10	W	669.861	669.444	1	670.87	670.45	670.57
					2	335.94	335.73	335.93
97	C12	W	697.914	697.475	1	698.92	698.48	698.62
					2	349.96	349.75	349.96
98	C14	W	725.967	725.506	1	726.98	726.51	726.64
					2	363.99	363.76	364.04
99	C8	Y	618.771	618.397	1	619.78	619.40	619.52
					2	310.39	310.21	310.39
100	C10	Y	646.824	646.428	1	647.83	647.44	647.58
					2	324.42	324.22	324.42
101	C12	Y	674.878	674.459	1	675.89	675.47	675.58
					2	338.45	338.24	338.43
102	C14	Y	702.931	702.490	1	703.94	703.50	703.61
					2	352.47	352.25	352.45
103	C6(2)	-	455.598	455.333	1	456.61	455.33	456.38
					2	228.81	228.67	228.73
104	C8(4)	-	511.704	511.396	1	512.71	512.40	512.45
					2	256.86	256.71	256.80
105	C10(6)	-	567.810	567.458	1	568.82	568.47	568.56
					2	284.41	284.23	284.86
106	C10-RFR-NH ₂		630.825	630.433	1	631.83	631.44	631.54
					2	316.42	316.22	316.40
107	C12-RFR-NH ₂		658.878	658.464	1	659.89	659.47	659.54
					2	330.45	330.24	330.42
108	C10-RRF-NH ₂		630.825	630.433	1	631.83	631.44	631.76
					2	316.42	316.22	316.52
109	C12-RRF-NH ₂		658.878	658.464	1	659.89	659.47	659.77
					2	330.45	330.24	330.52

Table S2. Antimicrobial and hemolytic activities, selectivity indexes and retention time of lipopeptides (1-105).

SA – *Staphylococcus aureus* ATCC 25923, PA – *Pseudomonas aeruginosa* ATCC 9027, CA – *Candida albicans* ATCC 10231
 SI – selectivity index (HC50/MIC)

Code	Name	X	tR' [min]	HC50 [µg/ml]	MIC SA [µg/ml] (SI)	MIC PA [µg/ml] (SI)	MIC CA [µg/ml] (SI)
1	C8-RR-NH ₂	Reference lipopeptides	14.46	-	>256	>256	>256
2	C10-RR-NH ₂		24.30	-	>256	>256	>256
3	C12-RR-NH ₂		32.58	>256	32 (>8)	128 (>2)	64 (>4)
4	C14-RR-NH ₂		39.79	68.43 (+/- 1.41)	8 (8.55)	32 (2.14)	8 (8.55)
5	C16-RR-NH ₂		46.51	22.91 (+/- 1.18)	8 (2.86)	16 (1.43)	4 (5.73)
6	C18-RR-NH ₂		53.39	25.19 (+/- 0.67)	16 (1.57)	64 (0.39)	4 (6.30)
7	C8-ARR-NH ₂	A	16.10	-	>256	>256	>256
8	C10-ARR-NH ₂	A	25.71	-	256	>256	>256
9	C12-ARR-NH ₂	A	33.76	-	64	128	128
10	C14-ARR-NH ₂	A	40.92	41.08 (+/- 0.62)	8 (5.14)	32 (1.28)	16 (2.57)
11	C8-C(Acm)RR-NH ₂	C(Acm)	17.91	-	>256	>256	>256
12	C10-C(Acm)RR-NH ₂	C(Acm)	26.58	-	>256	>256	>256
13	C12-C(Acm)RR-NH ₂	C(Acm)	34.30	-	64	128	128
14	C14-C(Acm)RR-NH ₂	C(Acm)	43.24	39.72 (+/- 1.25)	16 (2.48)	16 (2.48)	8 (4.97)
15	C8-DRR-NH ₂	D	15.64	-	>256	>256	>256
16	C10-DRR-NH ₂	D	25.10	-	>256	>256	>256
17	C12-DRR-NH ₂	D	33.17	-	256	>256	256
18	C14-DRR-NH ₂	D	40.25	49.95 (+/- 1.00)	64 (0.78)	128 (0.46)	32 (1.86)
19	C8-ERR-NH ₂	E	16.33	-	>256	>256	>256
20	C10-ERR-NH ₂	E	25.51	-	>256	>256	>256
21	C12-ERR-NH ₂	E	33.35	-	>256	>256	256
22	C14-ERR-NH ₂	E	40.17	59.51 (+/- 4.00)	64 (0.93)	128 (0.46)	32 (1.86)
23	C8-FRR-NH ₂	F	27.29	-	128	256	256
24	C10-FRR-NH ₂	F	34.68	>256	16 (>16)	32 (>8)	64 (>4)
25	C12-FRR-NH ₂	F	41.45	91.21 (+/-16.38)	4 (22.80)	8 (11.40)	8 (11.40)
26	C14-FRR-NH ₂	F	47.75	39.09 (+/- 1.18)	4 (9.77)	8 (4.89)	2 (19.55)
27	C8-GRR-NH ₂	G	15.16	-	>256	>256	>256
28	C10-GRR-NH ₂	G	24.94	-	256	>256	>256
29	C12-GRR-NH ₂	G	33.20	>256	32 (>8)	128 (>2)	64 (>4)
30	C14-GRR-NH ₂	G	40.53	31.94 (+/- 1.99)	8 (3.99)	32 (1.00)	16 (2.00)
31	C8-HRR-NH ₂	H	12.25	-	>256	>256	>256
32	C10-HRR-NH ₂	H	21.17	-	>256	>256	>256
33	C12-HRR-NH ₂	H	29.09	-	64	256	128
34	C14-HRR-NH ₂	H	35.80	50.31	16	64	16

				(+/- 0.52)	(3.14)	(0.79)	(3.14)
35	C8-IRR-NH ₂	I	24.02	-	>256	>256	>256
36	C10-IRR-NH ₂	I	31.95	-	64	64	128
37	C12-IRR-NH ₂	I	39.05	120.40 (+/- 1.55)	8 (15.05)	16 (7.53)	16 (7.53)
38	C14-IRR-NH ₂	I	45.65	78.92 (+/- 4.38)	4 (19.73)	4 (19.73)	4 (19.73)
39	C8-KRR-NH ₂	K	12.19	-	>256	>256	>256
40	C10-KRR-NH ₂	K	21.04	-	>256	>256	>256
41	C12-KRR-NH ₂	K	28.87	-	64	256	256
42	C14-KRR-NH ₂	K	35.66	212.08 (+/- 6.12)	8 (26.51)	64 (3.31)	32 (6.63)
43	C8-LRR-NH ₂	L	25.03	-	256	256	>256
44	C10-LRR-NH ₂	L	32.85	-	64	64	128
45	C12-LRR-NH ₂	L	39.82	112.81 (+/- 1.39)	8 (14.10)	16 (7.05)	16 (7.05)
46	C14-LRR-NH ₂	L	46.44	29.50 (+/- 1.05)	4 (7.38)	4 (7.38)	4 (7.38)
47	C8-MRR-NH ₂	M	22.49	-	>256	>256	>256
48	C10-MRR-NH ₂	M	30.74	-	128	128	256
49	C12-MRR-NH ₂	M	37.95	206.50 (+/- 9.14)	8 (25.81)	32 (6.45)	32 (6.45)
50	C14-MRR-NH ₂	M	44.69	35.11 (+/- 0.90)	4 (8.78)	8 (4.39)	4 (8.78)
51	C8-M(O)RR-NH ₂	M(O)	14.48	-	>256	>256	>256
52	C10-M(O)RR-NH ₂	M(O)	23.87	-	>256	>256	>256
53	C12-M(O)RR-NH ₂	M(O)	32.06	-	128	256	256
54	C14-M(O)RR-NH ₂	M(O)	39.18	116.28 (+/- 1.77)	32 (3.63)	64 (1.82)	32 (3.63)
55	C8-M(O ₂)RR-NH ₂	M(O ₂)	16.94	-	>256	>256	>256
56	C10-M(O ₂)RR-NH ₂	M(O ₂)	26.10	-	>256	>256	>256
57	C12-M(O ₂)RR-NH ₂	M(O ₂)	34.34	-	64	128	64
58	C14-M(O ₂)RR-NH ₂	M(O ₂)	41.17	70.11 (+/- 2.93)	16 (4.38)	32 (2.19)	16 (4.38)
59	C8-NRR-NH ₂	N	13.75	-	>256	>256	>256
60	C10-NRR-NH ₂	N	23.38	-	>256	>256	>256
61	C12-NRR-NH ₂	N	31.60	-	64	256	128
62	C14-NRR-NH ₂	N	38.71	64.37 (+/- 2.23)	16 (4.02)	32 (2.01)	16 (4.02)
63	C8-NleRR-NH ₂	Nle	25.43	-	>256	>256	>256
64	C10-NleRR-NH ₂	Nle	33.16	>256	32 (>8)	64 (>4)	64 (>4)
65	C12-NleRR-NH ₂	Nle	39.96	>256	8 (>32)	8 (>32)	16 (>16)
66	C14-NleRR-NH ₂	Nle	46.68	37.54 (+/- 1.39)	4 (9.39)	4 (9.39)	4 (9.39)
67	C8-NvaRR-NH ₂	Nva	22.11	-	>256	>256	>256
68	C10-NvaRR-NH ₂	Nva	30.44	-	128	128	256
69	C12-NvaRR-NH ₂	Nva	37.67	207.62 (+/- 5.27)	8 (25.95)	32 (6.49)	32 (6.49)
70	C14-NvaRR-NH ₂	Nva	44.53	42.04 (+/- 1.38)	4 (10.51)	8 (5.26)	4 (10.51)
71	C8-PRR-NH ₂	P	19.57	-	>256	>256	>256
72	C10-PRR-NH ₂	P	28.23	-	256	256	>256
73	C12-PRR-NH ₂	P	35.82	>256	32 (>8)	64 (>4)	64 (>4)

74	C14-PRR-NH ₂	P	42.61	53.41 (+/- 1.84)	16 (3.34)	16 (3.34)	8 (6.68)
75	C8-QRR-NH ₂	Q	13.93	-	>256	>256	>256
76	C10-QRR-NH ₂	Q	23.36	-	>256	>256	>256
77	C12-QRR-NH ₂	Q	31.42	-	128	256	128
78	C14-QRR-NH ₂	Q	38.52	72.31 (+/- 3.00)	16 (4.52)	32 (2.26)	32 (2.26)
79	C8-RRR-NH ₂	R	13.53	-	>256	>256	>256
80	C10-RRR-NH ₂	R	22.32	-	128	>256	256
81	C12-RRR-NH ₂	R	30.00	>256	16 (>16)	128 (>2)	128 (>2)
82	C14-RRR-NH ₂	R	36.76	211.32 (+/- 9.57)	4 (52.83)	32 (6.60)	16 (13.21)
83	C8-SRR-NH ₂	S	14.65	-	>256	>256	>256
84	C10-SRR-NH ₂	S	24.34	-	>256	>256	>256
85	C12-SRR-NH ₂	S	32.57	-	64	128	128
86	C14-SRR-NH ₂	S	39.72	41.54 (+/- 1.29)	16 (2.60)	32 (1.30)	32 (1.30)
87	C8-TRR-NH ₂	T	15.96	-	>256	>256	>256
88	C10-TRR-NH ₂	T	25.53	-	>256	>256	>256
89	C12-TRR-NH ₂	T	33.82	>256	32 (>8)	128 (>2)	64 (>4)
90	C14-TRR-NH ₂	T	40.80	43.43 (+/- 0.90)	8 (5.43)	32 (1.36)	8 (5.43)
91	C8-VRR-NH ₂	V	21.19	-	>256	>256	>256
92	C10-VRR-NH ₂	V	29.75	-	128	256	256
93	C12-VRR-NH ₂	V	37.17	246.30 (+/- 14.12)	16 (15.39)	32 (7.70)	32 (7.70)
94	C14-VRR-NH ₂	V	44.02	30.73 (+/- 0.41)	4 (7.68)	8 (3.84)	8 (3.84)
95	C8-WRR-NH ₂	W	27.14	-	128	128	256
96	C10-WRR-NH ₂	W	34.31	>256	16 (>16)	32 (>8)	32 (>8)
97	C12-WRR-NH ₂	W	40.79	42.42 (+/- 0.57)	4 (10.61)	8 (5.30)	8 (5.30)
98	C14-WRR-NH ₂	W	47.11	36.91 (+/- 0.89)	4 (9.23)	8 (4.61)	4 (9.23)
99	C8-YRR-NH ₂	Y	20.55	-	>256	>256	>256
100	C10-YRR-NH ₂	Y	28.79	-	64	128	128
101	C12-YRR-NH ₂	Y	36.17	123.08 (+/- 1.12)	8 (15.39)	16 (7.69)	32 (3.85)
102	C14-YRR-NH ₂	Y	42.73	46.52 (+/- 5.24)	4 (11.63)	8 (5.82)	4 (11.63)
103	C6(2)-RR-NH ₂	Branched lipopeptides	10.01	-	>256	>256	>256
104	C8(4)-RR-NH ₂		26.02	-	>256	256	>256
105	C10(6)-RR-NH ₂		39.62	200.25 (+/- 16.07)	4 (50.06)	8 (25.03)	16 (12.52)

Table S3. Molecular volume of selected lipopeptides.

Molar volume (with uncertainty of 7.0 cm³) was calculated with ChemSketch 2012 freeware software (Advanced Chemistry Development, Inc., Toronto, On, Canada, www.acdlabs.com, 2019).

Code	Sequence	Molar volume [cm ³]
1	C8-RR-NH ₂	347.9
2	C10-RR-NH ₂	380.0
3	C12-RR-NH ₂	412.1
4	C14-RR-NH ₂	444.2
5	C16-RR-NH ₂	476.3
6	C18-RR-NH ₂	508.4
7	C8-ARR-NH ₂	397.1
8	C10-ARR-NH ₂	429.2
9	C12-ARR-NH ₂	461.3
10	C14-ARR-NH ₂	493.4
23	C8-FRR-NH ₂	465.6
24	C10-FRR-NH ₂	497.7
25	C12-FRR-NH ₂	529.8
26	C14-FRR-NH ₂	561.9
27	C8-GRR-NH ₂	381.9
28	C10-GRR-NH ₂	414.0
29	C12-GRR-NH ₂	446.1
30	C14-GRR-NH ₂	478.2
35	C8-IRR-NH ₂	444.3
36	C10-IRR-NH ₂	476.4
37	C12-IRR-NH ₂	508.5
38	C14-IRR-NH ₂	540.6
43	C8-LRR-NH ₂	444.3
44	C10-LRR-NH ₂	476.4
45	C12-LRR-NH ₂	508.5
46	C14-LRR-NH ₂	540.6
63	C8-NleRR-NH ₂	445.2
64	C10-NleRR-NH ₂	477.3
65	C12-NleRR-NH ₂	509.4
66	C14-NleRR-NH ₂	541.5
67	C8-NvaRR-NH ₂	429.1
68	C10-NvaRR-NH ₂	461.2
69	C12-NvaRR-NH ₂	493.3
70	C14-NvaRR-NH ₂	525.4
71	C8-PRR-NH ₂	407.6
72	C10-PRR-NH ₂	439.7
73	C12-PRR-NH ₂	471.8
74	C14-PRR-NH ₂	503.9
91	C8-VRR-NH ₂	428.3
92	C10-VRR-NH ₂	460.4
93	C12-VRR-NH ₂	492.5
94	C14-VRR-NH ₂	524.6
95	C8-WRR-NH ₂	473.8
96	C10-WRR-NH ₂	505.9
97	C12-WRR-NH ₂	538.0
98	C14-WRR-NH ₂	570.1
99	C8-YRR-NH ₂	462.8
100	C10-YRR-NH ₂	494.9
101	C12-YRR-NH ₂	527.0
102	C14-YRR-NH ₂	559.1
103	C6(2)-RR-NH ₂	347.1
104	C8(4)-RR-NH ₂	411.2
105	C10(6)-RR-NH ₂	475.4

Peptide hydrophobicity vs antimicrobial activity

Antimicrobial activity against *Staphylococcus aureus* ATCC 25923

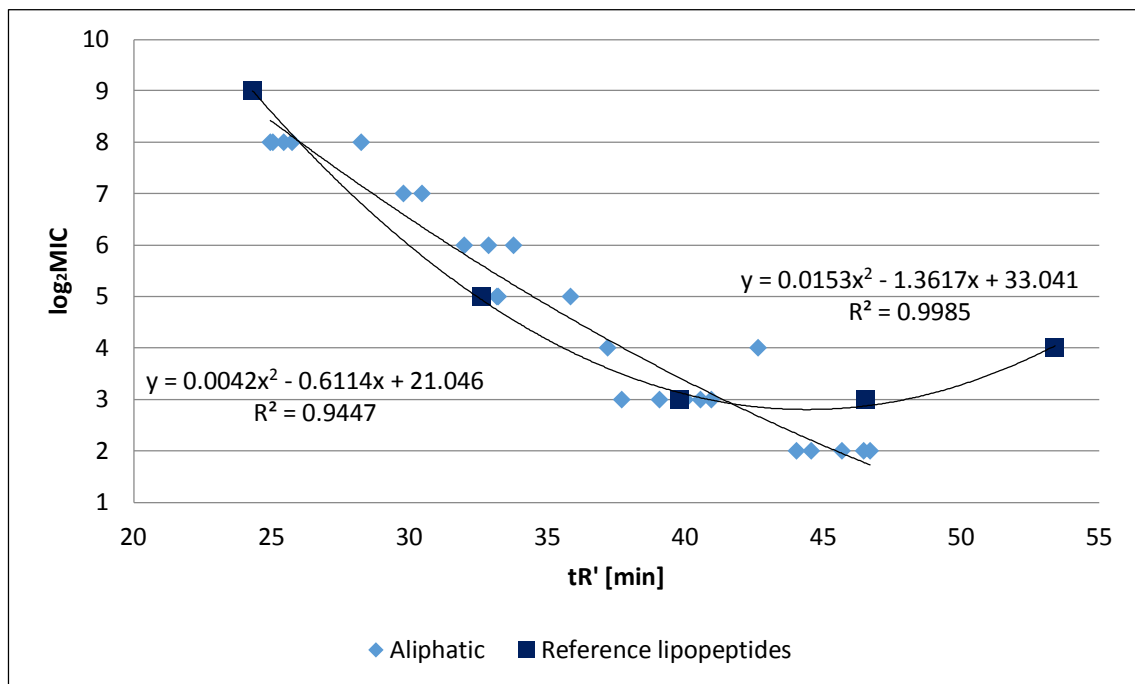


Figure S1. The \log_2MIC of lipopeptides with aliphatic amino acid residue against *S. aureus* vs tR' .

Aliphatic amino acid denotes Gly, Ala, Pro, Val, Leu, Ile, Nva, Nle.

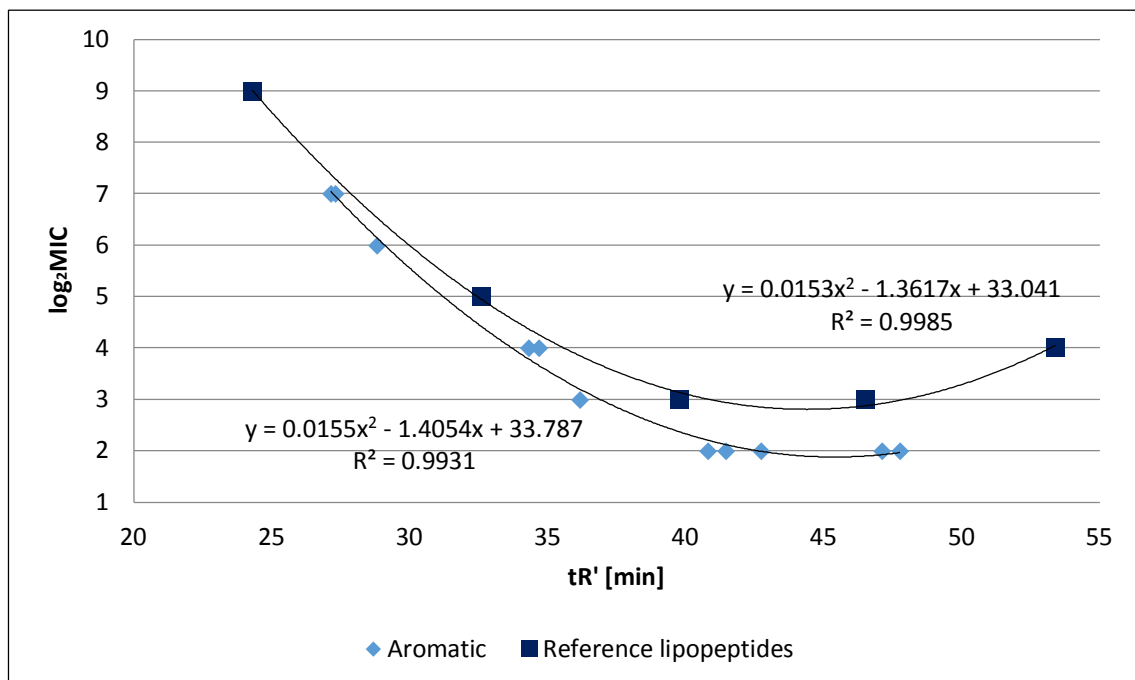


Figure S2. The \log_2MIC of lipopeptides with aromatic amino acid residue against *S. aureus* vs tR' .

Aromatic amino acid denotes Phe, Tyr, Trp.

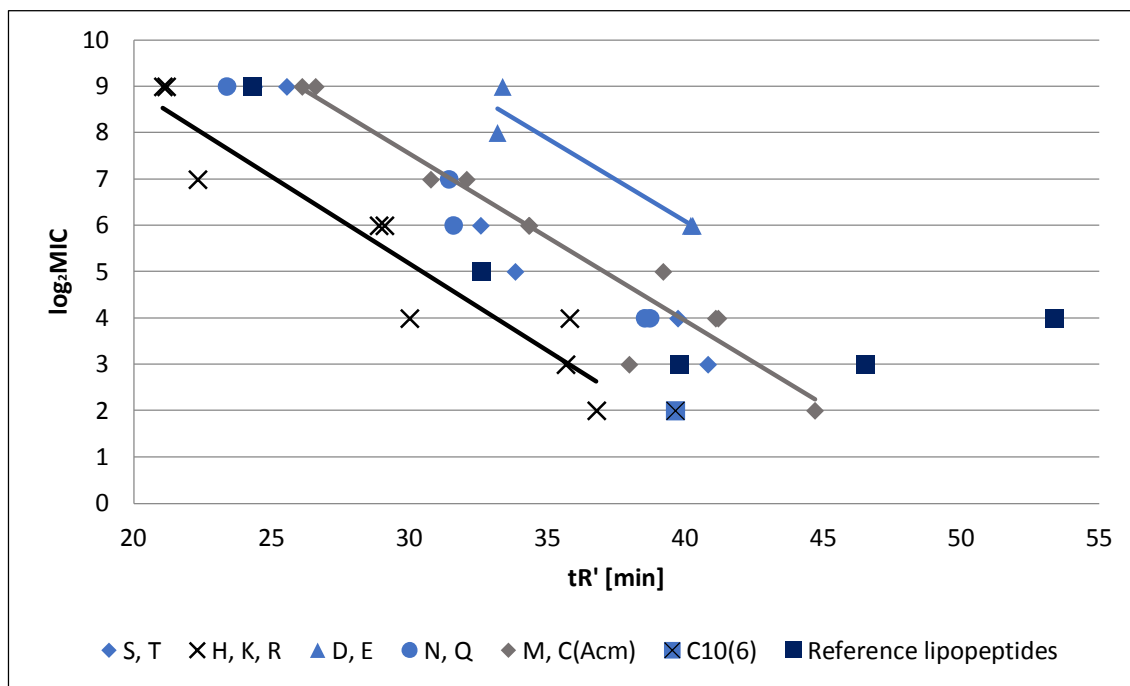


Figure S3. The \log_2 MIC of lipopeptides with remaining amino residues against *S. aureus* vs tR' .

Remaining amino acid residues denotes Ser, Thr, His, Lys, Arg, Asp, Glu, Asn, Gln, Met, Met(O), Met(O2), C(Acm), moreover branched lipopeptide is included C10(6)-RR-NH₂.

Antimicrobial activity against *Pseudomonas aeruginosa* ATCC 9027

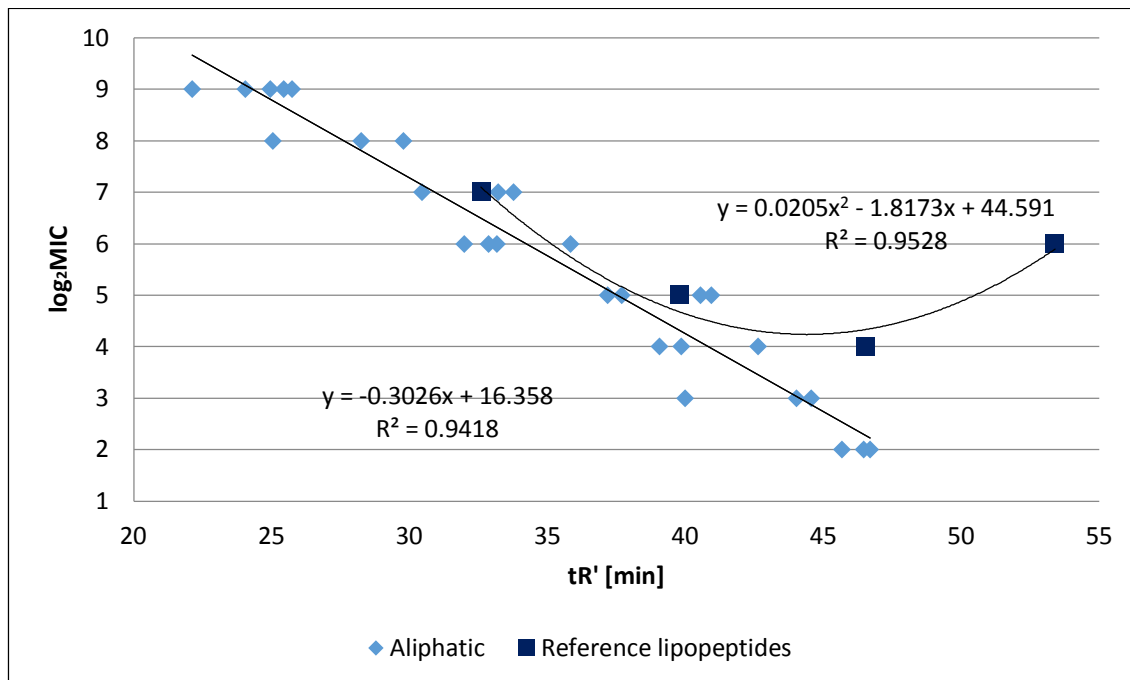


Figure S4. The \log_2 MIC of lipopeptides with aliphatic amino acid residue against *P. aeruginosa* vs tR' .

Aliphatic amino acid denotes Gly, Ala, Pro, Val, Leu, Ile, Nva, Nle.

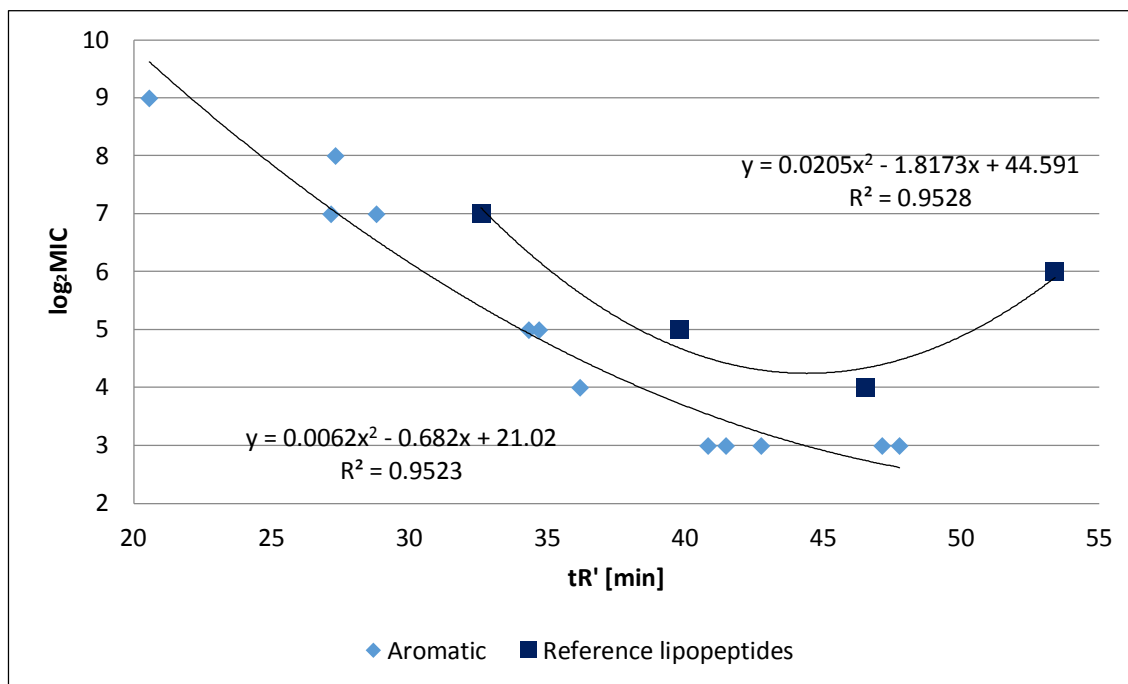


Figure S5. The log₂MIC of lipopeptides with aromatic amino acid residue against *P. aeruginosa* vs tR'.

Aromatic amino acid denotes Phe, Tyr, Trp.

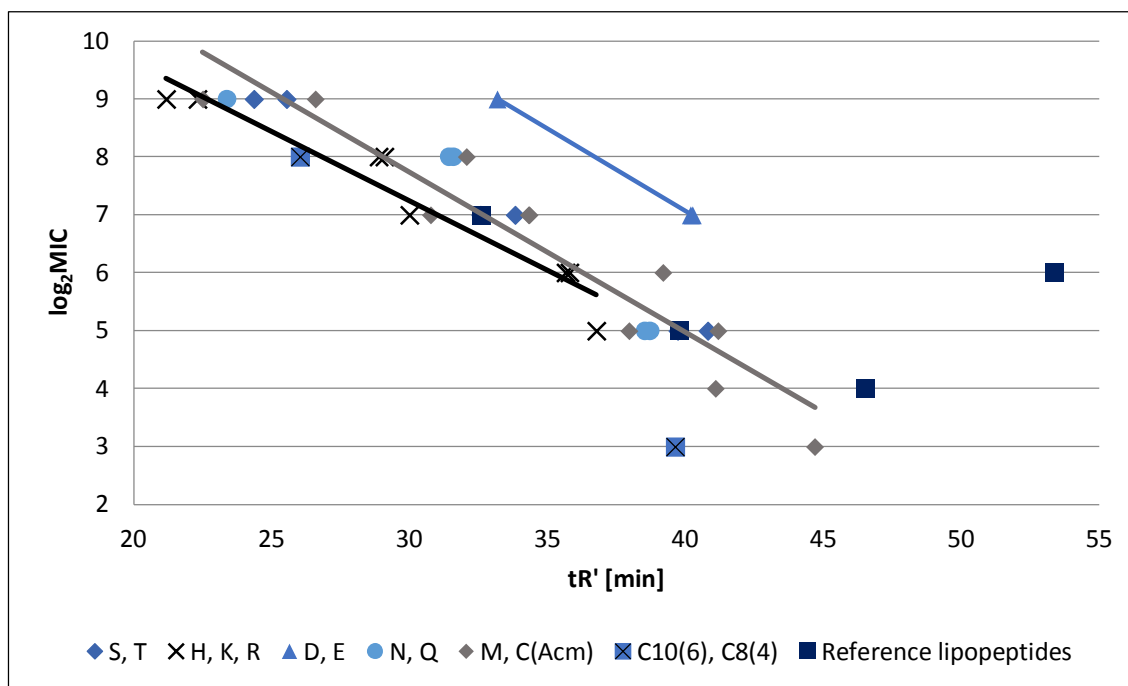


Figure S6. The log₂MIC of lipopeptides with remaining amino residues against *P. aeruginosa* vs tR'.

Remaining amino acid residues denotes Ser, Thr, His, Lys, Arg, Asp, Glu, Asn, Gln, Met, Met(O), Met(O₂), C(Acm), moreover branched lipopeptides are included – C10(6)-RR-NH₂ and C8(4)-RR-NH₂.

Antimicrobial activity against *Candida albicans* ATCC 10231

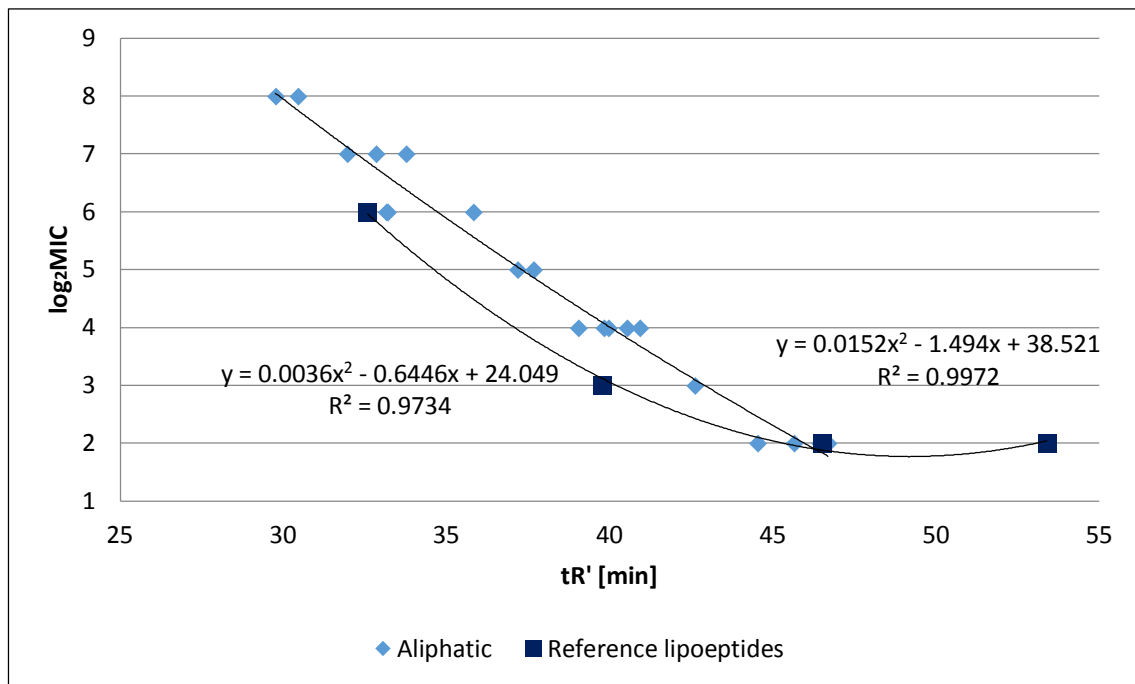


Figure S7. The \log_2 MIC of lipopeptides with aliphatic amino acid residue against *C. albicans* vs tR' .

Aliphatic amino acid denotes Gly, Ala, Pro, Val, Leu, Ile, Nva, Nle.

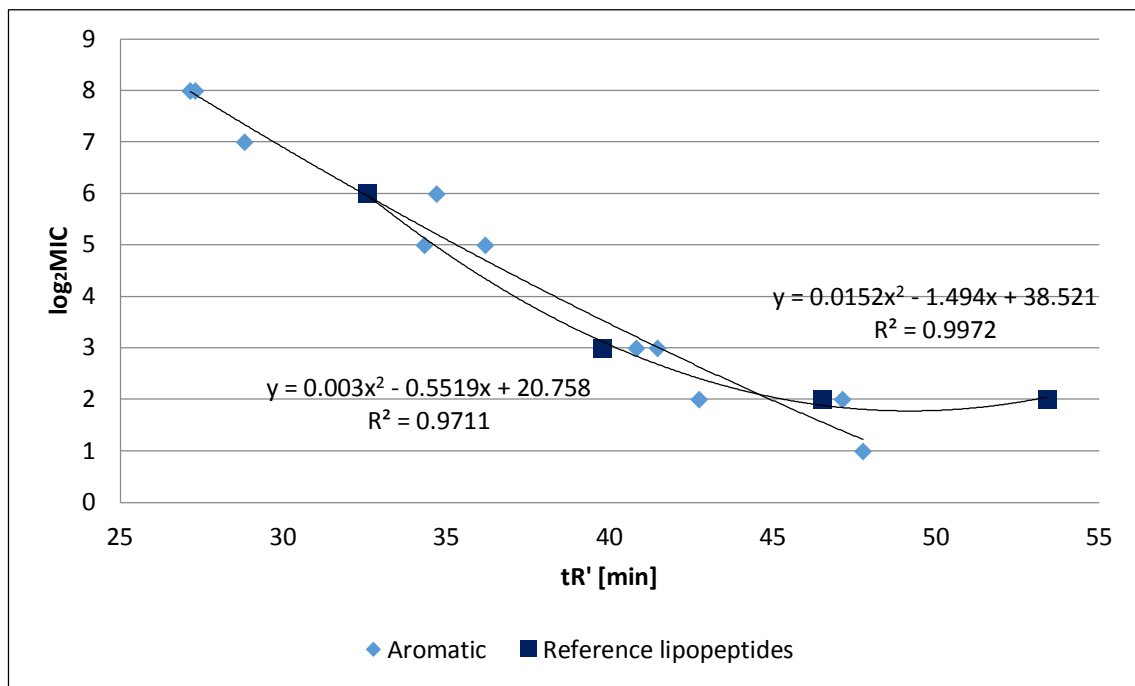


Figure S8. The \log_2 MIC of lipopeptides with aromatic amino acid residue against *C. albicans* vs tR' .

Aromatic amino acid denotes Phe, Tyr, Trp.

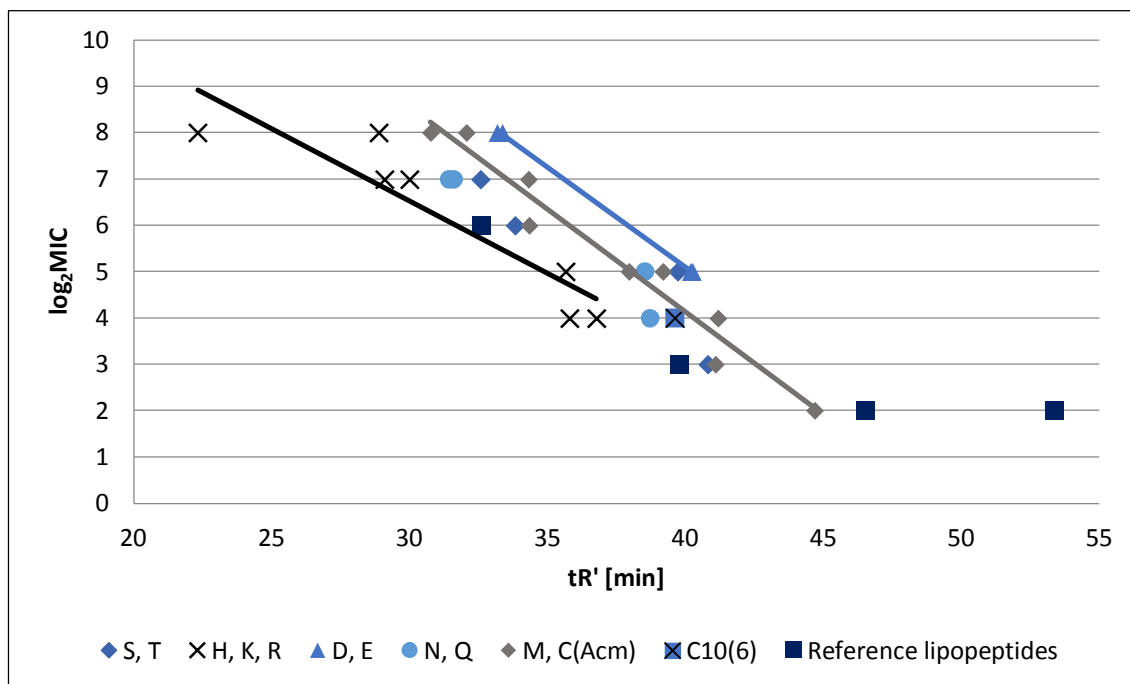


Figure S9. The log₂MIC of lipopeptides with remaining amino residues against *C. albicans* vs tR'.

Remaining amino acid residues denotes Ser, Thr, His, Lys, Arg, Asp, Glu, Asn, Gln, Met, Met(O), Met(O₂), C(Acm), moreover branched lipopeptide is included – C10(6)-RR-NH₂.