Supporting Information for:

Quantification of D-Ala-D-Lac terminated peptidoglycan structure in vancomycin-resistant *Enterococcus faecalis* using a combined solid-state NMR and mass spectrometry analysis

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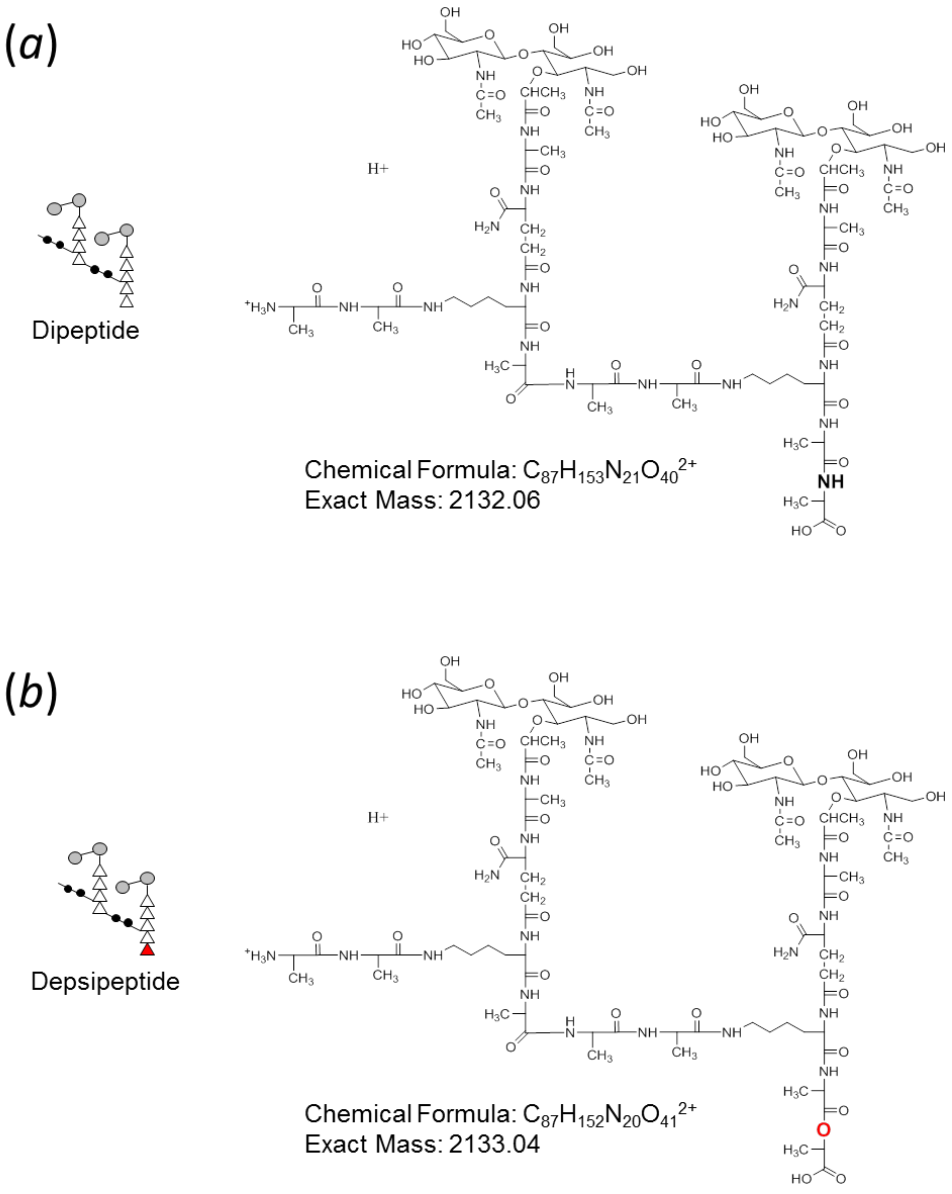
KEYWORDS: Vancomycin, REDOR, *E. faecalis*, Peptidoglycan, and solid-state NMR.



Supplementary Figure S1. (a) Chemical structure of a PG dimer with a pentapeptide stem terminating in D-Ala-D-Ala from vancomycin-resistant *E. faecalis* (ATCC 51299) grown in absence of vancomycin. (b) Chemical structure of a PG dimer with a pentapeptide stem terminating in D-Ala-D-Lac from vancomycin-resistant *E. faecalis* grown in presence of vancomycin (6 μg/mL).

Supplementary Table S1. List of peptidoglycan fragments observed by LC-MS for vancomycin-resistant *E. faecalis* (ATCC 51299) grown in absence of vancomycin during the exponential growth phase (OD_{600} 0.6). Chemical formula shown are for non-ionized peptidoglycan fragments.

Chemical Formula	Charge Obs.	Calculated (m/z)	Observed[1] (m/z)	Scaled integral[1]	Observed[2] m/z	Scaled integral[2]	Observed[3] m/z	Scaled integral[3]
C41H71N9O20	2	463.7375	463.7178	447	463.7178	676	463.7178	579
C39H70N9O19	2	484.7428	484.7287	6634	484.7287	5819	484.7287	5241
C42H75N10O20	2	520.2613	520.2299	9960	520.2200	9268	520.2200	10324
C47H81N11O22	2	534.7746	534.7697	21398	534.7697	19110	534.7697	18118
C44H77N10O21	2	541.2666	541.2915	39512	541.2915	46283	541.2915	38861
C45H80N11O21	2	555.7799	555.7808	6400	555.7705	6553	555.7705	6319
C47H82N11O22	2	576.7852	576.8089	30515	576.7984	27483	576.7984	24854
C83H143N19O39	3	649.6599	649.6593	241794	649.6593	288311	649.6593	264532
C83H143N19O39	2	973.9862	973.9894	136465	973.9894	147705	973.9894	110714
C81H142N19O38	3	663.6634	663.6667	2873710	663.6667	3271206	663.6667	2885170
C81H142N19O38	2	994.9915	995.0037	3517480	995.0037	3589885	995.0037	3321445
C81H142N19O38	1	1988.9758	1988.9984	11906	1988.9984	14281	1988.9984	12878
C86H148N20O40	3	673.3390	673.3409	63263	673.3409	59571	673.3409	77303
C86H148N20O40	2	1009.5048	1009.5031	28309	1009.5031	39483	1009.5031	32686
C83H144N19O39	3	677.6670	677.6758	362929	677.6758	389742	677.6758	365868
C83H144N19O39	2	1015.9968	1016.0197	446557	1016.0197	494266	1016.0197	404279
C84H147N20O39	3	687.3425	687.3481	806433	687.3481	892086	687.3481	731617
C84H147N20O39	2	1030.5101	1030.5168	607893	1030.5168	615535	1030.5168	528643
C89H153N21O41	3	697.0180	697.0199	533224	697.0199	593223	697.0199	564200
C89H153N21O41	2	1045.0234	1045.0317	137847	1045.0317	146790	1045.0175	134022
C86H149N20O40	3	701.3460	701.3607	180926	701.3607	162305	701.3607	222672
C87H152N21O40	3	711.0215	711.0255	6588213	711.0255	6844143	711.0255	6299936
C87H152N21O40	2	1066.0286	1066.0393	4289477	1066.0393	4568330	1066.0393	3540535
C89H154N21O41	3	725.0250	725.0293	193347	725.0293	231622	725.0293	184973
C89H154N21O41	2	1087.0339	1087.0400	91320	1087.0400	90624	1087.0400	80893
C125H215N29O58	4	742.6211	742.6517	140831	742.6279	144291	742.6279	140831
C125H215N29O58	3	989.8258	989.8596	336790	989.8322	491136	989.8184	295785
C123H214N29O57	4	753.1238	753.1351	905646	753.1231	930088	753.1231	859448
C123H214N29O57	3	1003.8293	1003.8375	3393731	1003.8375	3701847	1003.8375	3393823
C123H214N29O57	2	1505.2403	1505.2425	204061	1505.2425	210740	1505.2425	197147
C128H220N30O59	4	760.3804	760.4135	83700	760.3895	76629	760.3775	76359
C128H220N30O59	3	1013.5048	1013.5441	81477	1013.5024	59489	1013.5024	81261
C125H216N29O58	4	763.6264	763.6437	222873	763.6437	272307	763.6316	285042
C125H216N29O58	3	1017.8328	1017.8436	456649	1017.8436	459953	1017.8436	425309
C125H216N29O58	2	1526.2456	1526.2691	45150	1526.2691	35775	1526.2691	48069
C126H219N30O58	4	770.8831	770.8877	244108	770.8877	244158	770.8877	201911
C126H219N30O58	3	1027.5083	1027.5055	805735	1027.5055	692226	1027.5055	1122453
C126H219N30O58	2	1540.7588	1540.7507	41517	1540.7507	51975	1540.7507	63011

C131H225N31O60	4	778.1397	778.1418	327079	778.1539	283500	778.1418	272770
C131H225N31O60	3	1037.1838	1037.2271	421811	1037.1989	398875	1037.1848	407398
C129H224N31O59	4	788.6423	788.6511	1157533	788.6511	1247761	788.6388	1120764
C129H224N31O59	3	1051.1874	1051.1945	4701929	1051.1945	4843200	1051.1945	5171673
C129H224N31O59	2	1576.2774	1576.2742	289585	1576.2742	305282	1576.2742	289260
C131H226N31O60	3	1065.1909	1065.2269	76806	1065.2126	79128	1065.2269	59425
C167H287N39O77	4	997.7455	997.7877	74974	997.7601	75153	997.7463	68375
C167H287N39O77	3	1329.9916	1330.0541	68177	1329.9904	57197	1329.9904	70747
C165H286N39O76	4	1008.2482	1008.2550	1330279	1008.2550	1239789	1008.2550	1249994
C165H286N39O76	3	1343.9951	1343.9912	582757	1343.9912	648261	1343.9912	640974
C170H292N40O78	4	1015.5048	1015.5466	156051	1015.5048	82037	1015.5048	98394
C170H292N40O78	3	1353.6706	1353.7245	32922	1353.6602	26541	1353.6602	28884
C167H288N39O77	4	1018.7508	1018.7492	193790	1018.7632	234437	1018.7632	220166
C167H288N39O77	3	1357.9986	1358.0170	160069	1358.0170	131095	1358.0170	123630
C168H291N40O77	4	1026.0074	1026.0085	418962	1026.0085	391427	1026.0085	368087
C168H291N40O77	3	1367.6742	1367.6717	145388	1367.6556	163152	1367.6717	131164
C173H297N41O79	4	1033.2641	1033.3077	330082	1033.2796	305294	1033.2656	344194
C173H297N41O79	3	1377.3497	1377.4092	66677	1377.3606	63408	1377.3444	46727
C171H296N41O78	4	1043.7667	1043.7619	1447687	1043.7619	1929308	1043.7619	1412777
C171H296N41O78	3	1391.3532	1391.3635	516607	1391.3473	548238	1391.3473	511333
C173H298N41O79	4	1054.2694	1054.2686	143438	1054.2686	110148	1054.2686	91491

[1,2,3] Observed peaks (m/z) and their corresponding integrals in three independent measurements.

Supplementary Table S2. List of peptidoglycan fragments observed by LC-MS for vancomycin-resistant *E. faecalis* (ATCC 51299) grown in absence of vancomycin during the stationary growth phase (OD_{600} > 1.0). Chemical formula shown are for non-ionized peptidoglycan fragments.

Chemical Formula	Charge Obs.	Calculated (m/z)	Observed[1] (m/z)	Scaled integral[1]	Observed[2] m/z	Scaled integral[2]	Observed[3] m/z	Scaled integral[3]
C39H70N9O19	2	484.7428	484.7328	3825	484.7136	3794	484.7136	3261
C44H76N10O21	2	499.2560	499.2390	12526	499.2195	11112	499.2195	12123
C41H72N9O20	2	505.7480	505.7472	17777	505.7374	15951	505.7276	15962
C42H75N10O20	2	520.2613	520.2137	6147	520.2038	8567	520.2038	5948
C47H81N11O22	2	534.7746	534.7630	6628	534.7530	7054	534.7428	6949
C44H77N10O21	2	541.2666	541.2645	4407	541.2543	4400	541.2441	5516
C45H80N11O21	2	555.7799	555.7738	5033	555.7635	5041	555.7532	4157
C47H82N11O22	2	576.7852	576.7490	18718	576.7385	34097	576.7280	27531
C83H143N19O39	3	649.6599	649.6613	69068	649.6502	83796	649.6390	78303
C83H143N19O39	2	973.9862	973.9999	52259	973.9726	49851	973.9590	56795
C81H142N19O38	3	663.6634	663.6685	905565	663.6685	954386	663.6685	898929
C81H142N19O38	2	994.9915	995.0002	1618058	995.0002	1631511	995.0002	1676440
C81H142N19O38	1	1988.9758	1988.9947	3187	1988.9947	3704	1988.9947	4495
C86H148N20O40	3	673.3390	673.3425	33084	673.3312	33055	673.3199	30331
C86H148N20O40	2	1009.5048	1009.5133	35230	1009.4855	32814	1009.4716	39402
C83H144N19O39	3	677.6670	677.6773	204501	677.6773	286480	677.6773	218086
C83H144N19O39	2	1015.9968	1016.0019	420071	1016.0019	346105	1016.0019	386513
C84H147N20O39	3	687.3425	687.3496	512511	687.3496	526170	687.3496	541000
C84H147N20O39	2	1030.5101	1030.5266	578959	1030.5266	607029	1030.5266	592330
C89H153N21O41	3	697.0180	697.0212	212483	697.0096	210566	696.9981	210171
C89H153N21O41	2	1045.0234	1044.9850	72461	1044.9992	71087	1044.9850	72461
C86H149N20O40	3	701.3460	701.3504	107657	701.3504	111273	701.3504	99164
C87H152N21O40	3	711.0215	711.0266	3072508	711.0266	3083289	711.0266	2826401
C87H152N21O40	2	1066.0286	1066.0346	2552988	1066.0346	2576393	1066.0346	2609712
C89H154N21O41	3	725.0250	725.0302	187538	725.0302	211078	725.0302	253437
C89H154N21O41	2	1087.0339	1087.0493	149278	1087.0493	149192	1087.0493	151790
C125H215N29O58	4	742.6211	742.6286	26214	742.6048	33292	742.6048	25983
C125H215N29O58	3	989.8258	989.8287	171323	989.8013	170646	989.7875	160370
C123H214N29O57	4	753.1238	753.1356	196401	753.1116	197456	753.0996	207928
C123H214N29O57	3	1003.8293	1003.8338	2155397	1003.8062	2279513	1003.7923	2197304
C123H214N29O57	2	1505.2403	1505.2462	102483	1505.2124	121434	1505.1956	121968
C128H220N30O59	4	760.3804	760.3898	20902	760.3658	20523	760.3538	17784
C128H220N30O59	3	1013.5048	1013.5125	43648	1013.4708	43081	1013.4708	39139
C125H216N29O58	3	1017.8328	1017.8397	690630	1017.8119	722741	1017.8180	695179
C125H216N29O58	2	1526.2456	1526.2557	36666	1526.2044	28262	1526.2044	51941
C126H219N30O58	4	770.8831	770.8880	85893	770.8758	100360	770.8637	86822

C126H219N30O58	3	1027.5083	1027.5154	965190	1027.4874	928349	1027.4734	1005702
C126H219N30O58	2	1540.7588	1540.7713	47666	1540.7199	50000	1540.7027	55500
C127H218N29O59	3	1031.8363	1031.8445	140192	1031.8164	139087	1031.8024	72684
C131H225N31O60	4	778.1397	778.1175	73898	778.1296	87003	778.1175	80707
C131H225N31O60	3	1037.1838	1037.1948	293623	1037.1666	304181	1037.1525	316007
C128H221N30O59	3	1041.5118	1041.4736	142918	1041.4878	134224	1041.4736	149221
C128H221N30O59	2	1561.7641	1561.7847	3009	1561.7157	6392	1561.7157	8073
C129H224N31O59	4	788.6423	788.6510	500224	788.6265	469973	788.6142	489812
C129H224N31O59	3	1051.1874	1051.2041	4660766	1051.1617	4834726	1051.1475	5016835
C129H224N31O59	2	1576.2774	1576.2944	209182	1576.2442	233681	1576.2251	248433
C131H226N31O60	3	1065.1909	1065.1937	434055	1065.1652	442245	1065.1509	451662
C131H226N31O60	2	1597.2827	1597.3036	17345	1597.2513	27976	1597.2338	18210
C133H228N31O61	3	1079.1944	1079.2039	67928	1079.1752	91979	1079.1608	39435
C167H287N39O77	4	997.7455	997.7566	64081	997.7290	59870	997.7152	58818
C167H287N39O77	3	1329.9916	1330.0127	29667	1329.9490	39006	1329.9490	23406
C165H286N39O76	4	1008.2482	1008.2513	793986	1008.2236	804403	1008.2097	635153
C165H286N39O76	3	1343.9951	1344.0133	410496	1343.9653	586172	1343.9493	403651
C170H292N40O78	4	1015.5048	1015.5149	38079	1015.4731	30502	1015.4731	50379
C170H292N40O78	3	1353.6706	1353.6823	16174	1353.6180	26154	1353.6180	21961
C167H288N39O77	4	1018.7508	1018.7592	161973	1018.7174	174808	1018.7174	142061
C167H288N39O77	3	1357.9986	1358.0230	114344	1357.9585	104432	1357.9425	96472
C168H291N40O77	4	1026.0074	1026.0185	333957	1025.9765	371712	1025.9765	509946
C168H291N40O77	3	1367.6742	1367.6775	163616	1367.6453	144828	1367.6291	169231
C169H290N39O78	4	1029.2534	1029.2656	43908	1029.2376	84253	1029.2236	67623
C169H290N39O78	3	1372.0022	1372.0082	47034	1371.9597	18355	1371.9597	19488
C173H297N41O79	4	1033.2641	1033.2754	210812	1033.2473	295431	1033.2333	214325
C173H297N41O79	3	1377.3497	1377.3663	53793	1377.3177	49636	1377.3015	58011
C170H293N40O78	4	1036.5101	1036.5200	31790	1036.4919	19288	1036.4637	35209
C170H293N40O78	3	1381.6777	1381.6777	0	1381.6311	21360	1381.6346	0
C171H296N41O78	4	1043.7667	1043.7715	1697590	1043.7433	1597997	1043.7293	1567770
C171H296N41O78	3	1391.3532	1391.3691	568098	1391.3202	657280	1391.3040	633849
C173H298N41O79	4	1054.2694	1054.2783	252507	1054.2498	252555	1054.2357	163122
C173H298N41O79	3	1405.3567	1405.3609	95321	1405.3117	72738	1405.2953	45125
C175H300N41O80	4	1064.7720	1064.7662	20137	1064.7519	35368	1064.7378	28409

[1,2,3] Observed peaks (m/z) and their corresponding integrals in three independent measurements.

Supplementary Table S3. List of peptidoglycan fragments observed by LC-MS for vancomycin-resistant *E. faecalis* (ATCC 51299) grown in presence of vancomycin (6 μg/mL) during the exponential growth phase (OD_{600} 0.6). Chemical formula shown are for non-ionized peptidoglycan fragments.

Chemical Formula	Charge Obs.	Calculated (m/z)	Observed[1] (m/z)	Scaled integral[1]	Observed[2] m/z	Scaled integral[2]	Observed[3] m/z	Scaled integral[3]
C41H71N9O20	2	463.7375	463.7106	671	463.7012	1081	463.7012	747
C39H70N9O19	2	484.7428	484.7211	27966	484.7307	28976	484.7307	14348
C44H76N10O21	2	499.2560	499.2175	3438	499.2175	3084	499.2175	1943
C42H75N10O20	2	520.2613	520.2617	55362	520.2617	50957	520.2716	43916
C47H81N11O22	2	534.7746	534.8016	3560	534.8016	8151	534.8016	7501
C47H80N10O23	2	535.2666	535.2561	2013	535.2359	3602	535.2359	3145
C44H77N10O21	2	541.2666	541.2831	18540	541.2831	18057	541.2932	17237
C45H80N11O21	2	555.7799	555.7516	1692	555.7516	1448	555.7516	1395
C45H79N10O22	2	556.2719	556.2559	4254	556.2559	4914	556.2559	4884
C47H82N11O22	2	576.7852	576.7579	1631	576.7579	1771	576.7579	1833
C47H81N10O23	2	577.2772	577.2613	3093	577.2718	4264	577.2718	2688
C83H143N19O39	3	649.6599	649.6603	171032	649.6603	164780	694.6580	137087
C83H143N19O39	2	973.9862	973.9877	97972	973.9877	91597	973.9877	82206
C81H142N19O38	3	663.6634	663.6676	1477601	663.6676	1501173	663.6676	1301409
C81H142N19O38	2	994.9915	994.9881	1735321	994.9881	1814267	994.9881	1955810
C86H148N20O40	3	673.3390	673.3417	201959	673.3417	163178	673.3417	176763
C86H148N20O40	2	1009.5048	1009.5012	66646	1009.5151	64195	1009.5151	49003
C83H144N19O39	3	677.6670	677.6652	117166	677.6652	169580	677.6652	144424
C83H144N19O39	2	1015.9968	1016.0038	317272	1016.0038	266705	1016.0038	220349
C84H147N20O39	3	687.3425	687.3488	2375431	687.3488	2245791	687.3488	2088858
C84H147N20O39	2	1030.5101	1030.5145	2463621	1030.5145	2492171	1030.5145	1801819
C89H153N21O41	3	697.0180	697.0205	26910	697.0205	27493	697.0205	30761
C89H153N21O41	2	1045.0234	1045.0296	13922	1045.0296	17671	1045.0296	9403
C89H152N20O42	3	697.3460	697.3433	39355	697.3548	27778	697.3548	34868
C89H152N20O42	2	1045.5154	1045.5094	3514	1045.5094	2705	1045.5375	0
C86H149N20O40	2	1051.5154	1051.5178	225492	1051.5178	231409	1051.5178	173406
C87H152N21O40	3	711.0215	711.0260	278888	711.0260	296145	711.0260	271687
C87H152N21O40	2	1066.0286	1066.0369	167783	1066.0369	193689	1066.0369	162886
C87H151N20O41	3	711.3495	711.3519	135823	711.3519	90245	711.3519	95479
C87H151N20O41	2	1066.5206	1066.5216	95967	1066.5216	112004	1066.5216	96908
C89H154N21O41	3	725.0250	725.0297	51550	725.0297	43064	725.0297	46018
C89H154N21O41	2	1087.0339	1087.0518	26374	1087.0518	25687	1087.0518	31277
C89H153N20O42	3	725.3530	725.3417	0	725.3417	0	725.3417	2241
C125H215N29O58	4	742.6211	742.6282	52023	742.6282	61668	742.6282	48454
C125H215N29O58	3	989.8258	989.8304	228495	989.8304	213964	989.8304	234433
C123H214N29O57	4	753.1238	753.1233	480556	753.1233	468579	753.1233	422016

C123H214N29O57	3	1003.8293	1003.8355	1885033	1003.8355	1900721	1003.8355	1626272
C123H214N29O57	2	1505.2403	1505.2358	95798	1505.2528	96309	1505.2528	56325
C128H220N30O59	4	760.3804	760.3776	117901	760.3776	99038	760.3896	89601
C128H220N30O59	3	1013.5048	1013.5003	200311	1013.5003	179509	1013.5142	170992
C125H216N29O58	4	763.6264	763.6317	68883	763.6317	43135	763.6317	59284
C125H216N29O58	3	1017.8328	1017.8277	314070	1017.8277	334968	1017.8416	281297
C125H216N29O58	2	1526.2456	1526.2452	7350	1526.2281	14579	1526.2623	4629
C126H219N30O58	4	770.8831	770.8878	459857	770.8878	419544	770.8878	456507
C126H219N30O58	3	1027.5083	1027.5174	2320544	1027.5174	2191730	1027.5174	2149093
C126H219N30O58	2	1540.7588	1540.7609	126052	1540.7609	122412	1540.7609	63599
C131H225N31O60	4	778.1397	778.1417	23061	778.1417	23845	778.1417	16441
C131H225N31O60	3	1037.1838	1037.1686	64026	1037.1827	45019	1037.1968	27496
C131H224N30O61	4	778.3857	778.3854	19159	778.3854	16414	773.3856	14987
C131H224N30O61	3	1037.5118	1037.5063	0	1037.5063	0	1037.5203	8351
C128H221N30O59	3	1041.5118	1041.5040	197187	1041.5040	292900	1041.5180	241437
C128H221N30O59	2	1561.7641	1561.7743	12159	1561.7743	11710	1561.7743	4694
C129H224N31O59	4	788.6423	788.6388	40613	788.6510	78225	788.6510	53685
C129H224N31O59	3	1051.1874	1051.1922	334431	1051.1924	290749	1051.1922	330972
C129H224N31O59	2	1576.2774	1576.2669	16428	1576.2842	13837	1576.2842	4513
C129H223N30O60	3	1051.5154	1051.5178	141179	1051.5178	152626	1051.5178	129992
C130H223N30O60	3	1055.5154	1055.5141	120888	1055.5141	163031	1055.5283	82233
C131H226N31O60	3	1065.1909	1065.1959	76806	1065.2102	79128	1065.2102	59425
C167H287N39O77	4	997.7455	997.7445	115478	997.7445	129187	997.7445	100998
C167H287N39O77	3	1329.9916	1329.9854	26171	1330.0014	25683	1330.0014	25039
C165H286N39O76	4	1008.2482	1008.2393	893695	1008.2532	892054	1008.2532	710345
C165H286N39O76	3	1343.9951	1343.9862	463306	1344.0022	294207	1344.0022	374707
C170H292N40O78	4	1015.5048	1015.5029	120491	1015.4889	98821	1015.5029	57445
C170H292N40O78	3	1353.6706	1353.6551	49279	1353.6712	34261	1353.6872	23547
C167H288N39O77	4	1018.7508	1018.4963	52623	1018.7472	44491	1018.7472	41006
C167H288N39O77	3	1357.9986	1357.9796	49390	1357.9958	43717	1357.9958	0
C168H291N40O77	4	1026.0074	1026.0065	787829	1026.0065	701257	1026.0065	931282
C168H291N40O77	3	1367.6742	1367.6665	288917	1367.6665	275457	1367.6826	239057
C173H297N41O79	4	1033.2641	1033.2915	16889	1033.2775	25552	1033.2775	25928
C173H297N41O79	3	1377.3497	1377.3229	4081	1377.3391	6742	1377.3552	8283
C173H296N40O80	4	1033.5101	1033.5021	5694	1033.5021	0	1033.5161	10936
C173H296N40O80	3	1377.6777	1377.6631	280	1377.6793	5858	1377.6793	1552
C170H293N40O78	4	1036.5101	1036.5080	137564	1036.5080	143837	1036.5080	90992
C170H293N40O78	3	1381.6777	1381.6687	17969	1381.6687	33934	1381.6687	17416
C171H296N41O78	4	1043.7667	1043.7595	114556	1043.7595	131193	1043.7595	61187
C171H296N41O78	3	1391.3532	1391.3418	15617	1391.3582	10732	1391.3582	4869
C173H298N41O79	4	1054.2694	1054.2694	0	1054.2694	0	1054.2804	4691

[1,2,3] Observed peaks (m/z) and their corresponding integrals in three independent measurements.

Supplementary Table S4. List of peptidoglycan fragments observed by LC-MS for vancomycin-resistant *E. faecalis* (ATCC 51299) grown in presence of vancomycin (6 μg/mL) during the stationary growth phase (OD_{600} > 1.0). Chemical formula shown are for non-ionized peptidoglycan fragments.

Chemical Formula	Charge Obs.	Calculated (m/z)	Observed[1] (m/z)	Scaled integral[1]	Observed[2] m/z	Scaled integral[2]	Observed[3] m/z	Scaled integral[3]
C41H71N9O20	2	463.7375	463.6990	11045	463.6990	11742	463.7084	10627
C39H70N9O19	2	484.7428	484.7191	22461	484.7191	20683	484.7287	21090
C44H76N10O21	2	499.2560	499.2253	5278	499.2253	6270	499.2253	3781
C41H72N9O20	2	505.7480	505.7237	20271	505.7237	18022	505.7335	16204
C42H75N10O20	2	520.2613	520.2399	160426	520.2399	144727	520.2498	152752
C47H81N11O22	2	534.7746	534.7697	61034	534.7697	61111	534.7797	54205
C47H80N10O23	2	535.2666	535.2645	37547	535.2544	35925	535.2746	34159
C44H77N10O21	2	541.2666	541.3016	188023	541.3016	185352	541.3118	182454
C45H80N11O21	2	555.7799	555.7911	41204	555.7911	45365	555.8014	43690
C45H79N10O22	2	556.2719	556.2750	39334	556.2750	46949	556.2853	49855
C47H82N11O22	2	576.7852	576.7774	18328	576.7774	15609	576.7879	17319
C47H81N10O23	2	577.2772	577.2704	32087	577.2704	32331	577.2809	31355
C83H143N19O39	3	649.6599	649.6593	43292	649.6593	43766	649.6705	58182
C83H143N19O39	2	973.9862	973.9758	35787	973.9758	41972	974.0030	40457
C81H142N19O38	3	663.6634	663.6667	403892	663.6667	352004	663.6667	378640
C81H142N19O38	2	994.9915	994.9899	1016054	994.9899	1107781	994.9899	973420
C86H148N20O40	3	673.3390	673.3409	61976	673.3409	60310	673.3522	58463
C86H148N20O40	2	1009.5048	1009.5031	38340	1009.5031	43796	1009.5170	37385
C83H144N19O39	3	677.6670	677.6643	210227	677.6643	92763	677.6643	81013
C83H144N19O39	2	1015.9968	1015.9919	207871	1015.9919	216118	1015.9919	168872
C84H147N20O39	3	687.3425	687.3481	698214	687.3481	682818	687.3481	650380
C84H147N20O39	2	1030.5101	1030.5028	1066519	1030.5028	1279767	1030.5028	1228354
C89H153N21O41	3	697.0180	697.0199	11692	697.0199	12387	697.0314	13495
C89H153N21O41	2	1045.0234	1045.0175	4927	1045.0175	6313	1045.0459	5625
C89H152N20O42	2	1045.5154	1045.4975	560	1045.5116	299	1045.5257	399
C86H149N20O40	2	1051.5154	1051.5201	126543	1051.5201	146556	1051.5201	120885
C87H152N21O40	3	711.0215	711.0255	95613	711.0255	85890	711.0255	93832
C87H152N21O40	2	1066.0286	1066.0251	71088	1066.0251	74886	1066.0251	70315
C87H151N20O41	3	711.3495	711.3515	68886	711.3515	36393	711.3515	36860
C87H151N20O41	2	1066.5206	1066.5240	81339	1066.5240	78136	1066.5240	78263
C88H151N20O41	2	1072.5206	1072.5209	27005	1072.5209	35935	1072.5209	19899
C89H154N21O41	3	725.0250	725.0411	40551	725.0411	29508	725.0411	28167
C89H154N21O41	2	1087.0339	1087.0544	11356	1087.0544	15723	1087.0544	14658
C89H153N20O42	3	725.3530	725.3531	207738	725.3531	164034	725.3531	161808
C89H153N20O42	2	1087.5259	1087.5439	123355	1087.5439	119805	1087.5439	119086
C125H215N29O58	4	742.6211	742.6160	16529	742.6160	11110	742.6279	10036

C125H215N29O58	3	989.8258	989.8184	91157	989.8184	88515	989.8322	92124
C123H214N29O57	4	753.1238	753.1231	52641	753.1231	42036	753.1351	50084
C123H214N29O57	3	1003.8293	1003.8236	872072	1003.8236	925506	1003.8512	877802
C123H214N29O57	2	1505.2403	1505.2425	50141	1505.2425	46334	1505.2594	55901
C128H220N30O59	4	760.3804	760.3775	15215	760.3775	11226	760.3895	15508
C128H220N30O59	3	1013.5048	1013.5024	102146	1013.5024	96269	1013.5162	104676
C125H216N29O58	3	1017.8328	1017.8297	229148	1017.8297	226122	1017.8436	217742
C125H216N29O58	2	1526.2456	1526.2351	11918	1526.2351	10998	1526.2691	14235
C126H219N30O58	4	770.8831	770.8877	89550	770.8756	81161	770.8998	75994
C126H219N30O58	3	1027.5083	1027.5055	1126725	1027.5055	1097979	1027.5195	1088561
C126H219N30O58	2	1540.7588	1540.7507	65560	1540.7507	66674	1540.7850	68382
C127H218N29O59	3	1031.8363	1031.8363	0	1031.8205	24372	1031.7994	0
C131H225N31O60	4	778.1397	778.1418	8861	778.1418	7739	778.1539	8408
C131H225N31O60	3	1037.1838	1037.1708	4074	1037.1848	5818	1037.1989	11505
C128H221N30O59	3	1041.5118	1041.5061	190734	1041.5203	158653	1041.5343	174629
C128H221N30O59	2	1561.7641	1561.7644	8236	1561.7644	9656	1561.7816	11748
C129H224N31O59	4	788.6423	788.6388	7671	788.6388	3650	788.6511	3619
C129H224N31O59	3	1051.1874	1051.1803	76275	1051.1803	75975	1051.2086	65467
C129H224N31O59	2	1576.2774	1576.2568	2407	1576.2742	2864	1576.2915	2878
C129H223N30O60	3	1051.5154	1051.5060	65347	1051.5060	66485	1051.5343	69445
C130H223N30O60	3	1055.5154	1055.5165	35225	1055.5165	22391	1055.5307	22981
C131H226N31O60	3	1065.1909	1065.1841	71383	1065.1984	20873	1065.2126	49031
C131H225N30O61	3	1065.5189	1065.5261	58616	1065.5261	102532	1065.5404	81662
C131H225N30O61	2	1597.7747	1597.7722	4578	1597.7722	0	1597.8246	3804
C132H225N30O61	3	1069.5189	1069.4777	10914	1069.5205	16277	1069.5205	9091
C133H227N30O62	3	1079.5224	1079.5244	19510	1079.5244	15145	1079.5531	12821
C167H287N39O77	4	997.7455	997.7325	22421	997.7325	20347	997.7739	18087
C167H287N39O77	3	1329.9916	1329.9904	11286	1329.9585	14754	1330.0062	12486
C165H286N39O76	4	1008.2482	1008.2411	241404	1008.2411	232314	1008.2689	193818
C165H286N39O76	3	1343.9951	1343.9912	157703	1343.9912	161446	1344.0072	167857
C170H292N40O78	4	1015.5048	1015.4909	9625	1015.4909	18099	1015.5188	26947
C170H292N40O78	3	1353.6706	1353.6602	16062	1353.6442	20969	1353.6763	14540
C167H288N39O77	4	1018.7508	1018.7492	58472	1018.7492	51226	1018.7632	50899
C167H288N39O77	3	1357.9986	1358.0008	37753	1357.9848	27509	1358.0170	25174
C168H291N40O77	4	1026.0074	1026.0085	298029	1025.9946	288150	1026.0225	299408
C168H291N40O77	3	1367.6742	1367.6717	169462	1367.6717	175897	1367.6879	153137
C169H290N39O78	4	1029.2534	1029.2416	12398	1029.2557	12334	1029.2557	10801
C169H290N39O78	3	1372.0022	1372.0024	7810	1371.9862	11225	1372.0348	8547
C173H296N40O80	4	1033.5101	1033.5041	12312	1033.5041	3037	1033.5182	8231
C173H296N40O80	3	1377.6777	1377.6685	748	1377.6685	3729	1337.6861	1569
C170H293N40O78	4	1036.5101	1036.5101	30467	1036.5101	29998	1036.5242	30731
C170H293N40O78	3	1381.6777	1381.6742	25801	1381.6580	28851	1381.6903	35309
C171H296N41O78	4	1043.7667	1043.7619	20269	1043.7619	24828	1043.7759	35480
C171H296N41O78	3	1391.3532	1391.3473	11098	1391.3473	15220	1391.3635	17371
C171H295N40O79	4	1044.0127	1044.0016	5336	1044.0298	6591	1044.0298	8384
C171H295N40O79	3	1391.6812	1391.6730	7681	1391.6730	5675	1391.6892	11435
C172H295N40O79	4	1047.0127	1047.0087	18412	1047.0087	8854	1047.0369	12574
C172H295N40O79	3	1395.6812	1395.6664	2972	1395.6664	4033	1395.6826	7664

C173H298N41O79	4	1054.2694	1054.2686	16808	1054.2686	12278	1054.2827	18620
C173H298N41O79	3	1405.3567	1405.3882	6193	1405.2738	6971	1405.3555	6644
C173H297N40O80	4	1054.5154	1054.5238	7815	1054.5095	12174	1054.5380	5903
C173H297N40O80	3	1405.6847	1405.6829	4108	1405.6665	4335	1405.6992	9314

[1,2,3] Observed peaks (m/z) and their corresponding integrals in three independent measurements.