

#	Organism: Genus / Species / Strain Identity	Sample Prep.	MS File Name (data format: raw)	File Size (Byte)	Date - Time
1	<i>Escherichia coli</i> ATCC 47076 / DSM 18039 (K12 MG1655)	S-Trap	0168_2018_RKI_ZBS6_MS1_Lasch_Escherichia_coli_DSM_18039.raw	1,052,299,686	20.02.2018 - 20:04
2	<i>Acinetobacter baumannii</i> DSM 30007	S-Trap	0174_2018_RKI_ZBS6_MS1_Lasch_Acinetobacter_baumannii_DSM_30007.raw	1,057,217,066	21.02.2018 - 19:27
3	<i>Mycobacteroides abscessus</i> DSM 44196	S-Trap	0201_2018_RKI_ZBS6_MS1_Lasch_Mycobacteroides_abscessus_DSM_44196.raw	1,077,581,349	24.02.2018 - 06:38
4	<i>Burkholderia cepacia</i> ATCC 25416	S-Trap	0207_2018_RKI_ZBS6_MS1_Lasch_Burkholderia_cepacia_ATCC_25416.raw	1,146,941,042	25.02.2018 - 05:57
5	<i>Vibrio cholerae</i> NIH 41	S-Trap	0241_2018_RKI_ZBS6_MS1_Lasch_Vibrio_cholerae_NIH_41.raw	1,069,658,776	03.03.2018 - 05:38
6	<i>Yersinia pseudotuberculosis</i> DSM 8992	S-Trap	0279_2018_RKI_ZBS6_MS1_Lasch_Yersinia_pseudotuberculosis_DSM_8992.raw	1,072,549,555	11.03.2018 - 08:12
7	<i>Bacillus cereus</i> DSM 31	S-Trap	0326_2018_RKI_ZBS6_MS1_Lasch_Bacillus_cereus_DSM_31.raw	1,066,939,710	16.03.2018 - 18:07
8	<i>Pseudomonas aeruginosa</i> ATCC 27853	S-Trap	0332_2018_RKI_ZBS6_MS1_Lasch_Pseudomonas_aeruginosa_ATCC_27853.raw	1,052,225,433	17.03.2018 - 18:06
9	<i>Bacillus velezensis</i> DSM 23117 / FZB42	SPEED	1680_2018_RKI_ZBS6_MS1_Lasch_Bacillus_velezensis_FZB42.raw	1,483,673,971	19.10.2018 - 03:22
10	<i>Citrobacter freundii</i> DSM 30039	SPEED	0050_2019_RKI_ZBS6_MS1_Lasch_Citrobacter_freundii_DSM_30039.raw	1,244,054,563	15.01.2019 - 17:30
11	<i>Pseudomonas aeruginosa</i> ATCC 27853	SPEED	0051_2019_RKI_ZBS6_MS1_Lasch_Pseudomonas_aeruginosa_ATCC_27853.raw	1,313,167,212	15.01.2019 - 20:21
12	<i>Staphylococcus aureus</i> DSM 20231 / NCTC 8532	SPEED	0052_2019_RKI_ZBS6_MS1_Lasch_Staphylococcus_aureus_DSM_20231.raw	1,116,008,577	15.01.2019 - 23:11
13	<i>Enterococcus faecalis</i> DSM 20371	SPEED	0053_2019_RKI_ZBS6_MS1_Lasch_Enterococcus_faecalis_DSM_20371.raw	1,116,153,015	16.01.2019 - 02:02
14	<i>Staphylococcus epidermidis</i> DSM 1798	SPEED	0055_2019_RKI_ZBS6_MS1_Lasch_Staphylococcus_epidermidis_DSM_1798.raw	1,313,866,323	16.01.2019 - 07:44
15	<i>Burkholderia thailandensis</i> E131, [1 st BR, 1 st TR]	SPEED	0165_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E131.raw	1,156,941,593	02.02.2019 - 10:09
16	<i>Burkholderia thailandensis</i> E153, [1 st BR, 1 st TR]	SPEED	0166_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E153.raw	1,164,078,449	02.02.2019 - 13:00
17	<i>Burkholderia thailandensis</i> LMG 20219, [1 st BR, 1 st TR]	SPEED	0167_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_LMG_20219.raw	1,153,559,866	02.02.2019 - 15:51
18	<i>Burkholderia oklahomensis</i> DSM 21774, [1 st BR, 1 st TR]	SPEED	0168_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_oklahomensis_DSM_21774.raw	1,141,416,968	02.02.2019 - 18:42
19	<i>Burkholderia thailandensis</i> E131, [1 st BR, 2 nd TR]	SPEED	0169_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E131.raw	1,181,883,087	02.02.2019 - 22:10
20	<i>Burkholderia thailandensis</i> E153, [1 st BR, 2 nd TR]	SPEED	0170_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E153.raw	1,177,542,036	03.02.2019 - 01:01
21	<i>Burkholderia thailandensis</i> LMG 20219, [1 st BR, 2 nd TR]	SPEED	0171_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_LMG_20219.raw	1,164,885,759	03.02.2019 - 03:52
22	<i>Burkholderia oklahomensis</i> DSM 21774, [1 st BR, 2 nd TR]	SPEED	0172_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_oklahomensis_DSM_21774.raw	1,164,733,055	03.02.2019 - 06:43
23	<i>Burkholderia thailandensis</i> E131, [1 st BR, 3 rd TR]	SPEED	0173_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E131.raw	1,145,786,358	03.02.2019 - 10:12
24	<i>Burkholderia thailandensis</i> E153, [1 st BR, 3 rd TR]	SPEED	0174_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E153.raw	1,153,007,263	03.02.2019 - 13:03
25	<i>Burkholderia thailandensis</i> LMG 20219, [1 st BR, 3 rd TR]	SPEED	0175_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_LMG_20219.raw	1,157,753,760	03.02.2019 - 15:54
26	<i>Burkholderia oklahomensis</i> DSM 21774, [1 st BR, 3 rd TR]	SPEED	0176_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_oklahomensis_DSM_21774.raw	1,169,738,416	03.02.2019 - 18:45
27	<i>Burkholderia thailandensis</i> E125, [1 st BR, 1 st TR]	SPEED	0189_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E125.raw	1,162,988,859	07.02.2019 - 07:44

28	<i>Burkholderia thailandensis</i> E125, [1 st BR, 2 nd TR]	SPEED	0190_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E125.raw	1,164,218,762	07.02.2019 - 10:34
29	<i>Burkholderia thailandensis</i> E125, [1 st BR, 3 rd TR]	SPEED	0191_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E125.raw	1,166,340,542	07.02.2019 - 13:25
30	<i>Burkholderia thailandensis</i> DSM 13276, [1 st BR, 1 st TR]	SPEED	0192_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_DSM_13276.raw	1,121,033,003	07.02.2019 - 16:16
31	<i>Burkholderia thailandensis</i> DSM 13276, [1 st BR, 2 nd TR]	SPEED	0193_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_DSM_13276.raw	1,109,181,902	07.02.2019 - 19:07
32	<i>Burkholderia thailandensis</i> DSM 13276, [1 st BR, 3 rd TR]	SPEED	0194_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_DSM_13276.raw	1,109,840,636	07.02.2019 - 21:58
33	<i>Burkholderia oklahomensis</i> DSM 21774, [2 nd BR, 1 st TR]	SPEED	0243_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_oklahomensis_DSM_21774.raw	1,416,482,756	14.02.2019 - 18:30
34	<i>Burkholderia thailandensis</i> E153, [2 nd BR, 1 st TR]	SPEED	0244_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E153.raw	1,382,404,301	14.02.2019 - 21:22
35	<i>Burkholderia thailandensis</i> E131, [2 nd BR, 1 st TR]	SPEED	0245_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E131.raw	1,369,310,379	15.02.2019 - 00:14
36	<i>Burkholderia thailandensis</i> E125, [2 nd BR, 1 st TR]	SPEED	0246_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_E125.raw	1,349,846,078	15.02.2019 - 03:05
37	<i>Burkholderia thailandensis</i> LMG 20219, [2 nd BR, 1 st TR]	SPEED	0247_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_LMG_20219.raw	1,411,765,658	15.02.2019 - 05:56
38	<i>Burkholderia thailandensis</i> DSM 13276, [2 nd BR, 1 st TR]	SPEED	0248_2019_RKI_ZBS6_MS1_Lasch_Burkholderia_thailandensis_DSM_13276.raw	1,370,910,435	15.02.2019 - 08:47
39	<i>Mycobacteroides abscessus</i> DSM 44196	SPEED	0739_2019_RKI_ZBS6_MS1_Lasch_Mycobacteroides_abscessus_DSM_44196.raw	1,259,891,056	29.04.2019 - 19:25

R – biological replicate, TR – technical replicate

Nano-LC tandem MS measurements: Nano-LC tandem MS (nLC-MS²) measurements of pathogenic bacteria were partly carried out within the scope of other proteomics projects. Desalted digests were analyzed on an EASY-nanoLC 1200 device (Thermo Fisher Scientific, Bremen, Germany) coupled online to a Q Exactive™ Plus mass spectrometer (Thermo Fisher Scientific, Bremen, Germany). 1 µg peptides were separated on a 50 cm Acclaim™ PepMap™ column (75 µm inner diameter, i.d., 100 Å C18, 2 µm; Thermo Fisher Scientific, Bremen, Germany) using a linear 120 min gradient of 3 to 28 % acetonitrile (ACN) in 0.1 % FA at 200 nL/min flow rate. Column temperature was kept at 40°C using a butterfly heater (Phoenix S&T, Chester, PA, USA). The mass spectrometer was operated in a data-dependent manner in the m/z range of 300 – 1,650. Full scan spectra were recorded with a resolution of 70,000 using an automatic gain control (AGC) target value of 3×10^6 with a maximum injection time of 20 ms. Up to the 10 most intense 2+ – 5+ charged ions were selected for higher-energy c-trap dissociation (HCD) with a normalized collision energy (NCE) of 25 %. Fragment spectra were recorded at an isolation width of 2 Th and a resolution of 17,500@200 m/z using an AGC target value of 1×10^5 with a maximum injection time of 50 ms. The minimum AGC MS² target value was set to 1×10^4 . Once fragmented, peaks were dynamically excluded from precursor selection for 30 s within a 10 ppm window. Peptides were ionized using electrospray with a stainless steel emitter, i.d. 30 µm, (Proxeon, Odense, Denmark) at a spray voltage of 2.0 kV and a heated capillary temperature of 275°C.