

Sample_ID	EMSL_ID	Target Vol for FTICRMS (mL)	Vol SPE Extract needed (uL) to make FTICRMS sample	Vol Methanol needed to finish FTICRMS dilution (uL)	Target Eluate Mass for FTICRMS (g)	Target MeOH Mass to finish FTICRMS dilution (g)	Actual FTICRMS Eluate mass (g)	Actual FTICRMS MeOH mass (g)
TMP_0.A.5_EXP	EUP60985_01	0.45	450	0	0.3564	0.0000		
TMP_0.A.1_EXP	EUP60985_02	0.45	436	14	0.3454	11.0325		
TMP_0.A.2_EXP	EUP60985_03	0.45	442	8	0.3499	6.5775		
TMP_0.A.3_EXP	EUP60985_04	0.45	347	103	0.2750	81.4103		
TMP_0.A.4_EXP	EUP60985_05	0.45	450	0	0.3564	0.0000		
TMP_0.A.6_EXP	EUP60985_06	0.45	282	168	0.2236	132.8395		
TMP_0.B.1_EXP	EUP60985_07	0.45	443	7	0.3509	5.5235		
TMP_0.B.3_EXP	EUP60985_08	0.45	450	0	0.3564	0.0000		
TMP_0.B.4_EXP	EUP60985_09	0.45	450	0	0.3564	0.0000		
TMP_0.B.5_EXP	EUP60985_10	0.45	450	0	0.3564	0.0000		
TMP_0.B.6_EXP	EUP60985_11	0.45	310	140	0.2459	110.5123		
TMP_0.C.1_EXP	EUP60985_12	0.45	358	92	0.2839	72.5789		
TMP_0.C.3_EXP	EUP60985_13	0.45	450	0	0.3564	0.0000		
TMP_0.C.4_EXP	EUP60985_14	0.45	292	158	0.2314	124.9992		
TMP_0.C.5_EXP	EUP60985_15	0.45	284	166	0.2248	131.6210		
TMP_01.A.1_EXP	EUP60985_16	0.45	351	99	0.2780	78.3981		
TMP_01.A.2_EXP	EUP60985_17	0.45	450	0	0.3564	0.0000		
TMP_01.A.3_EXP	EUP60985_18	0.45	383	67	0.3033	53.0979		
TMP_01.A.4_EXP	EUP60985_19	0.45	440	10	0.3481	8.2998		
TMP_01.A.5_EXP	EUP60985_20	0.45	450	0	0.3564	0.0000		
TMP_01.A.6_EXP	EUP60985_21	0.45	310	140	0.2452	111.2432		
TMP_01.B.1_EXP	EUP60985_22	0.45	339	111	0.2685	87.9001		
TMP_01.B.2_EXP	EUP60985_23	0.45	450	0	0.3564	0.0000		
TMP_01.B.3_EXP	EUP60985_24	0.45	383	67	0.3035	52.9119		
TMP_01.B.4_EXP	EUP60985_25	0.45	450	0	0.3564	0.0000		
TMP_01.B.5_EXP	EUP60985_26	0.45	450	0	0.3564	0.0000		
TMP_01.B.6_EXP	EUP60985_27	0.45	280	170	0.2221	134.3443		

Sample_ID	EMSL_ID	Target Vol for FTICRMS (mL)	Vol SPE Extract needed (uL) to make FTICRMS sample	Vol Methanol needed to finish FTICRMS dilution (uL)	Target Eluate Mass for FTICRMS (g)	Target MeOH Mass to finish FTICRMS dilution (g)	Actual FTICRMS Eluate mass (g)	Actual FTICRMS MeOH mass (g)
TMP_01.C.1_EXP	EUP60985_28	0.45	360	90	0.2855	70.9418		
TMP_01.C.2_EXP	EUP60985_29	0.45	450	0	0.3564	0.0000		
TMP_01.C.3_EXP	EUP60985_30	0.45	396	54	0.3135	42.9159		
TMP_01.C.4_EXP	EUP60985_31	0.45	431	19	0.3413	15.1403		
TMP_01.C.5_EXP	EUP60985_32	0.45	450	0	0.3564	0.0000		
TMP_1.A.2_EXP	EUP60985_33	0.45	363	87	0.2873	69.1191		
TMP_1.A.3_EXP	EUP60985_34	0.45	404	46	0.3200	36.4046		
TMP_1.A.4_EXP	EUP60985_35	0.45	450	0	0.3564	0.0000		
TMP_1.A.5_EXP	EUP60985_36	0.45	371	79	0.2939	62.5522		
TMP_1.A.6_EXP	EUP60985_37	0.45	450	0	0.3564	0.0000		
TMP_1.B.1_EXP	EUP60985_38	0.45	391	59	0.3096	46.8374		
TMP_1.B.2_EXP	EUP60985_39	0.45	375	75	0.2973	59.1102		
TMP_1.B.3_EXP	EUP60985_40	0.45	440	10	0.3482	8.2692		
TMP_1.B.4_EXP	EUP60985_41	0.45	438	12	0.3467	9.7626		
TMP_1.B.5_EXP	EUP60985_42	0.45	418	32	0.3310	25.4102		
TMP_1.B.6_EXP	EUP60985_43	0.45	287	163	0.2276	128.8301		
TMP_1.C.1_EXP	EUP60985_44	0.45	342	108	0.2705	85.9190		
TMP_1.C.2_EXP	EUP60985_45	0.45	377	73	0.2988	57.6746		
TMP_1.C.3_EXP	EUP60985_46	0.45	443	7	0.3506	5.8031		
TMP_1.C.4_EXP	EUP60985_47	0.45	450	0	0.3564	0.0000		
TMP_1.C.5_EXP	EUP60985_48	0.45	434	16	0.3438	12.6516		
TMP_100.A.1_EXP	EUP60985_49	0.45	450	0	0.3564	0.0000		
TMP_100.A.2_EXP	EUP60985_50	0.45	376	74	0.2978	58.6630		
TMP_100.A.3_EXP	EUP60985_51	0.45	355	95	0.2809	75.5585		
TMP_100.A.4_EXP	EUP60985_52	0.45	257	193	0.2034	153.0295		
TMP_100.A.5_EXP	EUP60985_53	0.45	276	174	0.2188	137.6812		
TMP_100.A.6_EXP	EUP60985_54	0.45	430	20	0.3405	15.9619		

Sample_ID	EMSL_ID	Target Vol for FTICRMS (mL)	Vol SPE Extract needed (uL) to make FTICRMS sample	Vol Methanol needed to finish FTICRMS dilution (uL)	Target Eluate Mass for FTICRMS (g)	Target MeOH Mass to finish FTICRMS dilution (g)	Actual FTICRMS Eluate mass (g)	Actual FTICRMS MeOH mass (g)
TMP_100.B.1_EXP	EUP60985_55	0.45	450	0	0.3564	0.0000		
TMP_100.B.2_EXP	EUP60985_56	0.45	330	120	0.2612	95.1983		
TMP_100.B.3_EXP	EUP60985_57	0.45	302	148	0.2390	117.4576		
TMP_100.B.4_EXP	EUP60985_58	0.45	221	229	0.1747	181.7582		
TMP_100.B.5_EXP	EUP60985_59	0.45	414	36	0.3276	28.8602		
TMP_100.B.6_EXP	EUP60985_60	0.45	425	25	0.3363	20.1254		
TMP_100.C.1_EXP	EUP60985_61	0.45	484	-34	0.3833	-26.8787		
TMP_100.C.2_EXP	EUP60985_62	0.45	329	121	0.2606	95.8858		
TMP_100.C.3_EXP	EUP60985_63	0.45	361	89	0.2862	70.2817		
TMP_100.C.4_EXP	EUP60985_64	0.45	223	227	0.1765	179.9521		
TMP_100.C.5_EXP	EUP60985_65	0.45	441	9	0.3491	7.3792		
TMP_25.A.1_EXP	EUP60985_66	0.45	450	0	0.3564	0.0000		
TMP_25.A.2_EXP	EUP60985_67	0.45	310	140	0.2457	110.7564		
TMP_25.A.3_EXP	EUP60985_68	0.45	274	176	0.2171	139.3837		
TMP_25.A.4_EXP	EUP60985_69	0.45	227	223	0.1798	176.6837		
TMP_25.A.5_EXP	EUP60985_70	0.45	432	18	0.3418	14.6100		
TMP_25.A.6_EXP	EUP60985_71	0.45	338	112	0.2677	88.7713		
TMP_25.B.2_EXP	EUP60985_72	0.45	333	117	0.2640	92.4117		
TMP_25.B.3_EXP	EUP60985_73	0.45	257	193	0.2034	153.0295		
TMP_25.B.4_EXP	EUP60985_74	0.45	244	206	0.1932	163.2122		
TMP_25.B.5_EXP	EUP60985_75	0.45	450	0	0.3564	0.0000		
TMP_25.B.6_EXP	EUP60985_76	0.45	356	94	0.2823	74.1168		
TMP_25.C.1_EXP	EUP60985_77	0.45	299	151	0.2371	119.3461		
TMP_25.C.3_EXP	EUP60985_78	0.45	270	180	0.2138	142.6182		
TMP_25.C.5_EXP	EUP60985_79	0.45	386	64	0.3054	51.0394		
TMP_5.A.1_EXP	EUP60985_80	0.45	403	47	0.3192	37.2558		
TMP_5.A.2_EXP	EUP60985_81	0.45	450	0	0.3564	0.0000		

Sample_ID	EMSL_ID	Target Vol for FTICRMS (mL)	Vol SPE Extract needed (uL) to make FTICRMS sample	Vol Methanol needed to finish FTICRMS dilution (uL)	Target Eluate Mass for FTICRMS (g)	Target MeOH Mass to finish FTICRMS dilution (g)	Actual FTICRMS Eluate mass (g)	Actual FTICRMS MeOH mass (g)
TMP_5.A.3_EXP	EUP60985_82	0.45	362	88	0.2871	69.3482		
TMP_5.A.4_EXP	EUP60985_83	0.45	450	0	0.3564	0.0000		
TMP_5.A.5_EXP	EUP60985_84	0.45	335	115	0.2655	90.9248		
TMP_5.A.6_EXP	EUP60985_85	0.45	429	21	0.3399	16.5463		
TMP_5.B.1_EXP	EUP60985_86	0.45	315	135	0.2497	106.7917		
TMP_5.B.2_EXP	EUP60985_87	0.45	450	0	0.3564	0.0000		
TMP_5.B.3_EXP	EUP60985_88	0.45	362	88	0.2866	69.8676		
TMP_5.B.4_EXP	EUP60985_89	0.45	450	0	0.3564	0.0000		
TMP_5.B.5_EXP	EUP60985_90	0.45	337	113	0.2668	89.6369		
TMP_5.B.6_EXP	EUP60985_91	0.45	450	0	0.3564	0.0000		
TMP_5.C.1_EXP	EUP60985_92	0.45	416	34	0.3294	27.0621		
TMP_5.C.2_EXP	EUP60985_93	0.45	450	0	0.3564	0.0000		
TMP_5.C.3_EXP	EUP60985_94	0.45	289	161	0.2290	127.4879		
TMP_5.C.4_EXP	EUP60985_95	0.45	387	63	0.3067	49.7148		
TMP_5.C.5_EXP	EUP60985_96	0.45	340	110	0.2696	86.8031		
TMP_5.C.6_EXP	EUP60985_97	0.45	450	0	0.3564	0.0000		
PB-100.A	EUP60985_98	0.45	450	0	0.3564	0.0000		
PB-100.B	EUP60985_99	0.45	450	0	0.3564	0.0000		
PB-25.B	EUP60985_100	0.45	450	0	0.3564	0.0000		
PB-25.A	EUP60985_101	0.45	450	0	0.3564	0.0000		
PB-100.C	EUP60985_102	0.45	450	0	0.3564	0.0000		
PB-25.C	EUP60985_103	0.45	450	0	0.3564	0.0000		
PB-5.A	EUP60985_104	0.45	450	0	0.3564	0.0000		
PB-5.B	EUP60985_105	0.45	450	0	0.3564	0.0000		
PB-5.C	EUP60985_106	0.45	450	0	0.3564	0.0000		
PB-01.A	EUP60985_107	0.45	450	0	0.3564	0.0000		
PB-1.C	EUP60985_108	0.45	450	0	0.3564	0.0000		

[illegible]