

Item name: 240422 - PIMT Methylation Assays - H4

Created time: 15:07:09 GMT Daylight Time

Analysis Information

Item name: 240422 - PIMT Methylation Assays - H4 Analysis Method Item name: 240422 - PIMT Methylation Assays - H4

Version: Analysis Method Version:

Modified date: Sample Set Created date: Apr 22, 2024 13:22:21 GMT Daylight Time

Modified by: Sample Set Instrument system name: XEVO-G2XSQTOF#NotSet

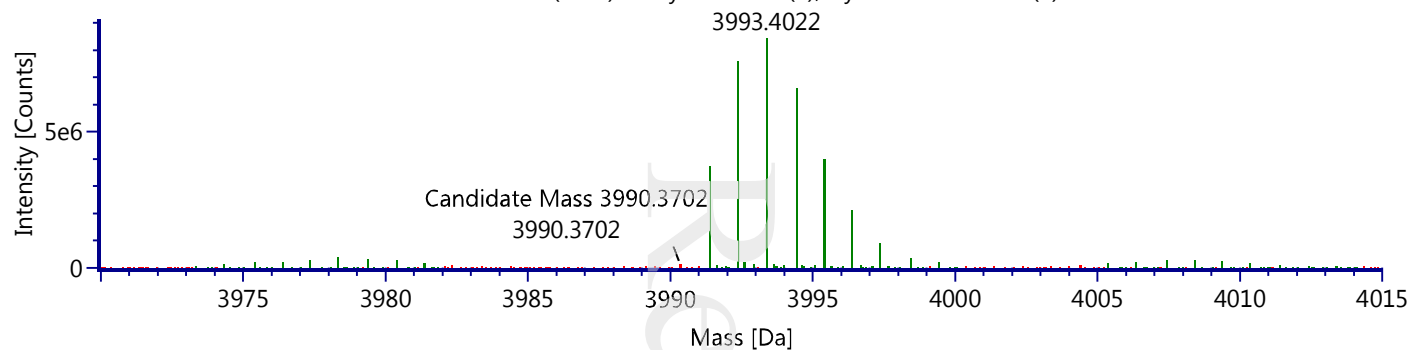
Folder: KCL/Manuel/Luis

Analysis injection list

.	Item name	Item description	Sample type	Replicate number	Sample position	Injection volume (µL)	Acquisition status	Limit status
1	240417_H4Iso_0		Unknown	1	1:1	3.00	Complete	No Checks Performed
2	240417_H4Iso_1		Unknown	1	1:2	3.00	Complete	No Checks Performed
3	240417_H4Iso_2		Unknown	1	1:3	3.00	Complete	No Checks Performed
4	240417_H4Iso_5		Unknown	1	1:4	3.00	Complete	No Checks Performed
5	240417_H4Iso_10		Unknown	1	1:5	3.00	Complete	No Checks Performed
6	240417_H4Iso_15		Unknown	1	1:6	3.00	Complete	No Checks Performed
7	240417_H4Iso_30		Unknown	1	1:7	3.00	Complete	No Checks Performed
8	240417_H4Iso_60		Unknown	1	1:8	3.00	Complete	No Checks Performed
9	240417_H4WT_0		Unknown	1	1:17	3.00	Complete	No Checks Performed
10	240417_H4WT_60		Unknown	1	1:18	3.00	Complete	No Checks Performed
11	240417_H4Iso_No PIMT_60		Unknown	1	1:19	3.00	Complete	No Checks Performed

Item name: 240417_H4Iso_0

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1)


H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	154090	4005.3817	4005.69900	-79.2
2	219195	4006.3829	4006.70230	-79.7
3	292840	4007.3993	4007.70570	-76.5
4	278664	4008.3848	4008.70900	-80.9
5	237106	4009.3875	4009.71240	-81.0
6	163440	4010.3980	4010.71570	-79.2
Sum	1345335.032	24047.334	24049.244	-476.547

H4D24 + H4isoD24

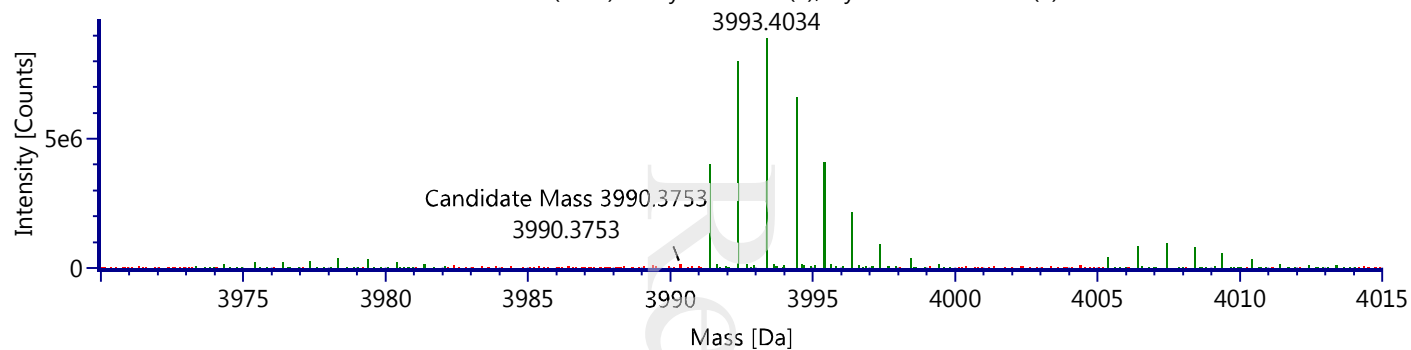
.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	3718798	3991.3984	3991.67240	-68.6
2	7605498	3992.4000	3992.67570	-69.1
3	8448217	3993.4022	3993.67910	-69.3
4	6619552	3994.4033	3994.68240	-69.9
5	4003711	3995.4023	3995.68580	-71.0
6	2109631	3996.4069	3996.68910	-70.6
7	900072	3997.4063	3997.69250	-71.6
8	357191	3998.4032	3998.69590	-73.2
9	188983	3999.4027	3999.69920	-74.1
Sum	33951651.796	35958.625	35961.172	-637.429

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	132112	3974.3631	3974.66040	-74.8
2	204275	3975.3744	3975.66380	-72.8
3	215608	3976.3675	3976.66720	-75.4
4	271311	3977.3721	3977.67050	-75.0
5	387006	3978.3656	3978.67390	-77.5
6	339209	3979.3695	3979.67720	-77.3
7	277737	3980.3711	3980.68060	-77.8
8	167072	3981.3698	3981.68390	-78.9
Sum	1994330.673	31822.953	31825.378	-609.493

Item name: 240417_H4Iso_1

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1)


H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	423957	4005.3997	4005.69900	-74.7
2	842194	4006.4100	4006.70230	-73.0
3	945278	4007.4130	4007.70570	-73.0
4	791703	4008.4040	4008.70900	-76.1
5	533021	4009.4127	4009.71240	-74.7
6	318984	4010.4084	4010.71570	-76.6
7	155005	4011.4097	4011.71910	-77.1
Sum	4010142.584	28058.857	28060.963	-525.338

H4D24 + H4isoD24

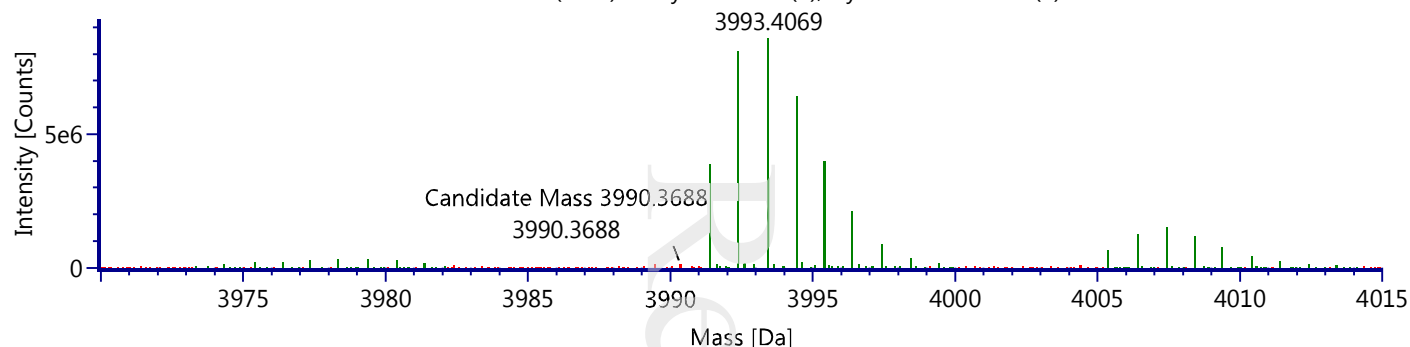
.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	3977665	3991.3997	3991.67240	-68.3
2	7990592	3992.4034	3992.67570	-68.2
3	8896654	3993.4034	3993.67910	-69.0
4	6589532	3994.4046	3994.68240	-69.6
5	4079529	3995.4049	3995.68580	-70.3
6	2162354	3996.4106	3996.68910	-69.7
7	886249	3997.4085	3997.69250	-71.0
8	374580	3998.4036	3998.69590	-73.1
9	157952	3999.4055	3999.69920	-73.4
Sum	35115106.792	35958.644	35961.172	-632.697

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	135612	3974.3742	3974.66040	-72.0
2	197452	3975.3703	3975.66380	-73.8
3	205396	3976.3694	3976.66720	-74.9
4	251058	3977.3781	3977.67050	-73.5
5	358320	3978.3719	3978.67390	-75.9
6	320607	3979.3731	3979.67720	-76.4
7	224376	3980.3721	3980.68060	-77.5
8	158163	3981.3700	3981.68390	-78.8
Sum	1850983.691	31822.979	31825.378	-602.891

Item name: 240417_H4Iso_2

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1)


H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	669386	4005.4070	4005.69900	-72.9
2	1262634	4006.4108	4006.70230	-72.8
3	1513199	4007.4164	4007.70570	-72.2
4	1178574	4008.4155	4008.70900	-73.2
5	761826	4009.4170	4009.71240	-73.7
6	421931	4010.4129	4010.71570	-75.5
7	226436	4011.4156	4011.71910	-75.7
8	119525	4012.4081	4012.72240	-78.3
Sum	6153511.237	32071.303	32073.686	-594.223

H4D24 + H4isoD24

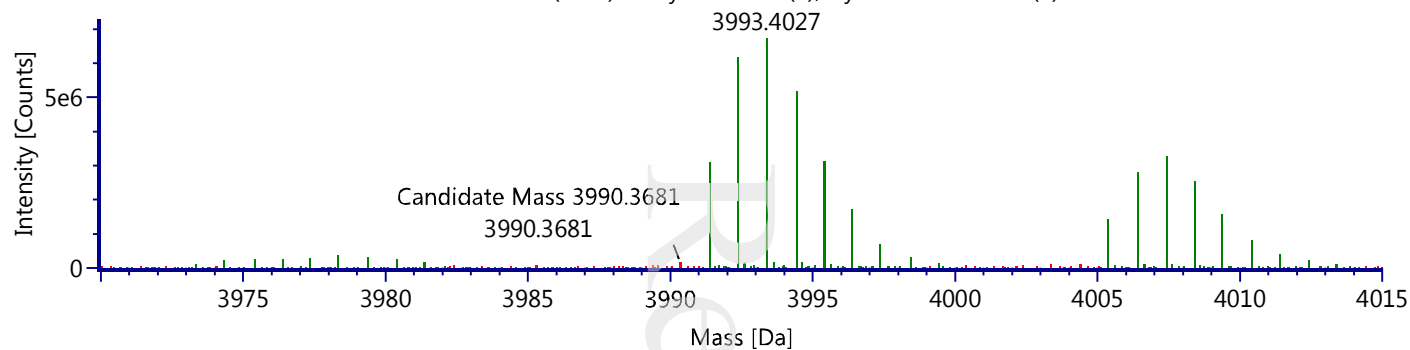
.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	3846410	3991.4017	3991.67240	-67.8
2	8098960	3992.4061	3992.67570	-67.5
3	8594461	3993.4069	3993.67910	-68.2
4	6408458	3994.4075	3994.68240	-68.8
5	3982135	3995.4093	3995.68580	-69.2
6	2115769	3996.4104	3996.68910	-69.7
7	848763	3997.4121	3997.69250	-70.1
8	360239	3998.4093	3998.69590	-71.7
9	157107	3999.3969	3999.69920	-75.6
Sum	34412301.811	35958.660	35961.172	-628.706

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	152361	3974.3670	3974.66040	-73.8
2	196988	3975.3777	3975.66380	-72.0
3	214776	3976.3741	3976.66720	-73.7
4	262905	3977.3760	3977.67050	-74.0
5	342311	3978.3732	3978.67390	-75.6
6	316651	3979.3773	3979.67720	-75.4
7	249777	3980.3780	3980.68060	-76.0
8	166128	3981.3703	3981.68390	-78.8
Sum	1901896.087	31822.994	31825.378	-599.260

Item name: 240417_H4Iso_5

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1)


H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	1424640	4005.4058	4005.69900	-73.2
2	2810724	4006.4130	4006.70230	-72.2
3	3277025	4007.4168	4007.70570	-72.1
4	2536726	4008.4135	4008.70900	-73.7
5	1550144	4009.4082	4009.71240	-75.9
6	809025	4010.4110	4010.71570	-76.0
7	395216	4011.4164	4011.71910	-75.5
8	207762	4012.4159	4012.72240	-76.4
9	115301	4013.4100	4013.72580	-78.7
Sum	13126563.484	36084.711	36087.411	-673.598

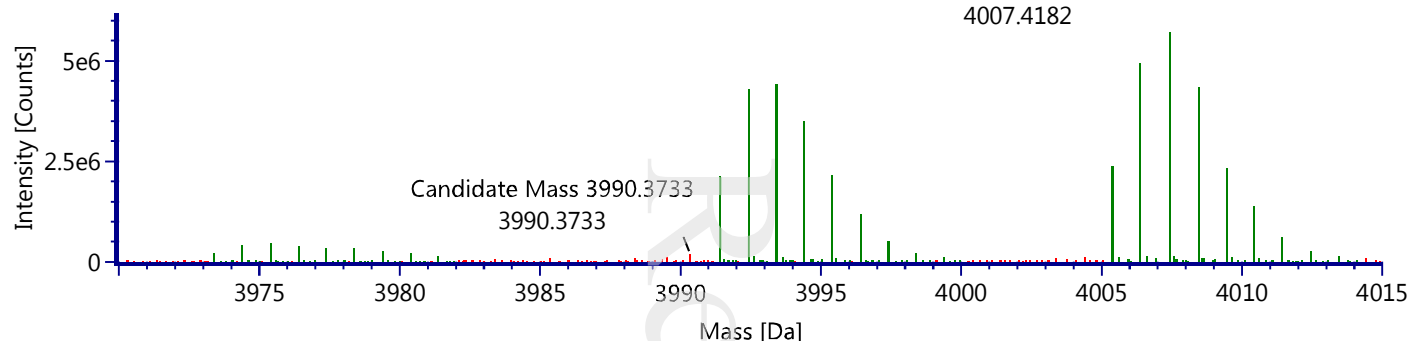
H4D24 + H4isoD24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	3091597	3991.3953	3991.67240	-69.4
2	6177336	3992.3984	3992.67570	-69.4
3	6737919	3993.4027	3993.67910	-69.2
4	5174156	3994.4007	3994.68240	-70.5
5	3122716	3995.4021	3995.68580	-71.0
6	1708876	3996.4062	3996.68910	-70.8
7	690418	3997.4043	3997.69250	-72.1
8	308236	3998.4046	3998.69590	-72.8
9	127674	3999.3863	3999.69920	-78.2
Sum	27138928.747	35958.601	35961.172	-643.602

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	199032	3974.3742	3974.66040	-72.0
2	253379	3975.3785	3975.66380	-71.8
3	233176	3976.3714	3976.66720	-74.4
4	270103	3977.3704	3977.67050	-75.4
5	362796	3978.3687	3978.67390	-76.7
6	289279	3979.3725	3979.67720	-76.6
7	234709	3980.3740	3980.68060	-77.0
8	139531	3981.3706	3981.68390	-78.7
Sum	1982003.874	31822.980	31825.378	-602.615

Item name: 240417_H4Iso_10

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1), Methyl D (1)
4007.4182


H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	2385446	4005.4082	4005.69900	-72.6
2	4926553	4006.4147	4006.70230	-71.8
3	5714605	4007.4182	4007.70570	-71.8
4	4330146	4008.4124	4008.70900	-74.0
5	2319256	4009.4143	4009.71240	-74.3
6	1384498	4010.4170	4010.71570	-74.5
7	599929	4011.4145	4011.71910	-75.9
8	274236	4012.4145	4012.72240	-76.7
9	147241	4013.4137	4013.72580	-77.8
Sum	22081910.190	36084.727	36087.411	-669.414

H4D24 + H4isoD24

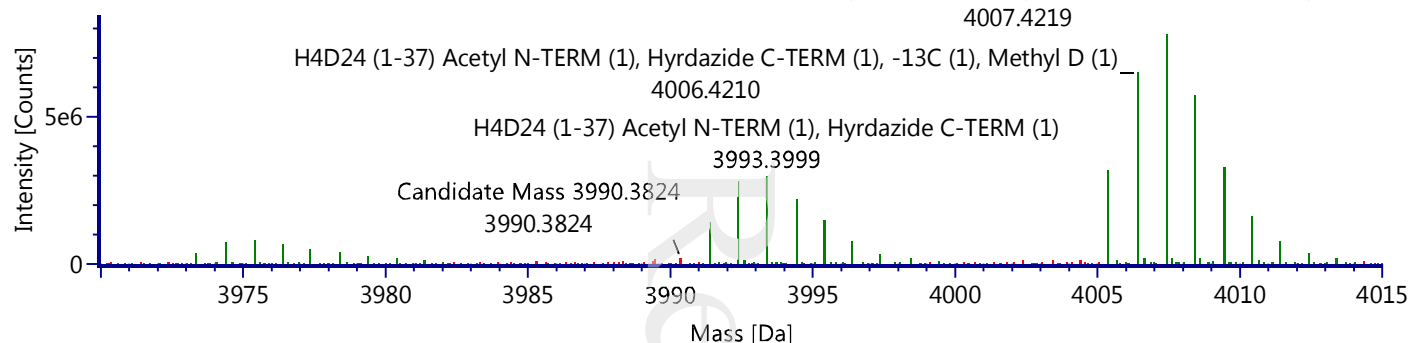
.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	2136082	3991.3921	3991.67240	-70.2
2	4297082	3992.3969	3992.67570	-69.8
3	4415649	3993.3971	3993.67910	-70.6
4	3478377	3994.4024	3994.68240	-70.1
5	2141118	3995.4000	3995.68580	-71.5
6	1184162	3996.4056	3996.68910	-70.9
7	508140	3997.4001	3997.69250	-73.1
8	210193	3998.3976	3998.69590	-74.6
9	104532	3999.3993	3999.69920	-75.0
Sum	18475335.046	35958.591	35961.172	-646.010

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	199505	3973.3804	3973.65710	-69.6
2	407083	3974.3806	3974.66040	-70.4
3	464825	3975.3827	3975.66380	-70.7
4	394081	3976.3797	3976.66720	-72.3
5	333676	3977.3840	3977.67050	-72.0
6	328308	3978.3683	3978.67390	-76.8
7	254502	3979.3697	3979.67720	-77.3
8	200869	3980.3724	3980.68060	-77.4
9	129261	3981.3694	3981.68390	-79.0
Sum	2712109.514	35796.387	35799.035	-665.627

Item name: 240417_H4Iso_15

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1), Methyl D (1)


H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	3168904	4005.4107	4005.69900	-72.0
2	6509165	4006.4210	4006.70230	-70.2
3	7812409	4007.4219	4007.70570	-70.8
4	5717506	4008.4189	4008.70900	-72.4
5	3282987	4009.4195	4009.71240	-73.1
6	1633902	4010.4162	4010.71570	-74.7
7	754337	4011.4215	4011.71910	-74.2
8	340981	4012.4210	4012.72240	-75.1
9	186674	4013.4161	4013.72580	-77.2
Sum	29406863.251	36084.767	36087.411	-659.562

H4D24 + H4isoD24

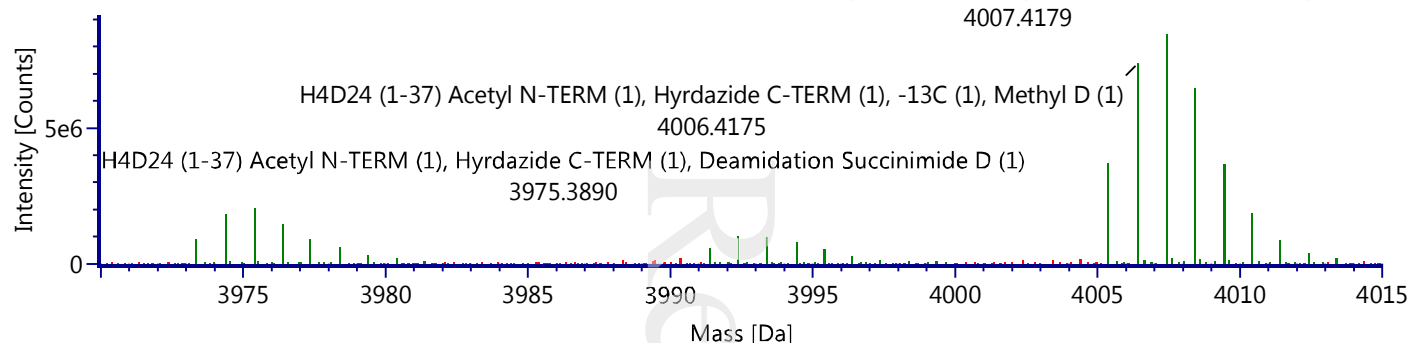
.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	1430211	3991.3958	3991.67240	-69.3
2	2815284	3992.3994	3992.67570	-69.2
3	2986012	3993.3999	3993.67910	-69.9
4	2193010	3994.4005	3994.68240	-70.6
5	1482755	3995.4026	3995.68580	-70.9
6	754192	3996.4081	3996.68910	-70.3
7	333212	3997.4053	3997.69250	-71.8
8	176901	3998.4048	3998.69590	-72.8
Sum	12171578.174	31959.216	31961.473	-564.866

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	371160	3973.3847	3973.65710	-68.6
2	739725	3974.3850	3974.66040	-69.3
3	803033	3975.3862	3975.66380	-69.8
4	642700	3976.3871	3976.66720	-70.4
5	490039	3977.3896	3977.67050	-70.6
6	378854	3978.3826	3978.67390	-73.2
7	248173	3979.3817	3979.67720	-74.2
8	172873	3980.3809	3980.68060	-75.3
9	117244	3981.3725	3981.68390	-78.2
Sum	3963800.654	35796.450	35799.035	-649.742

Item name: 240417_H4Iso_30

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1), Methyl D (1)


H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	3687192	4005.4106	4005.69900	-72.0
2	7386345	4006.4175	4006.70230	-71.1
3	8456889	4007.4179	4007.70570	-71.8
4	6474922	4008.4166	4008.70900	-73.0
5	3673544	4009.4211	4009.71240	-72.7
6	1864142	4010.4145	4010.71570	-75.1
7	848738	4011.4188	4011.71910	-74.9
8	397534	4012.4186	4012.72240	-75.7
9	195707	4013.4151	4013.72580	-77.4
Sum	32985012.898	36084.751	36087.411	-663.615

H4D24 + H4isoD24

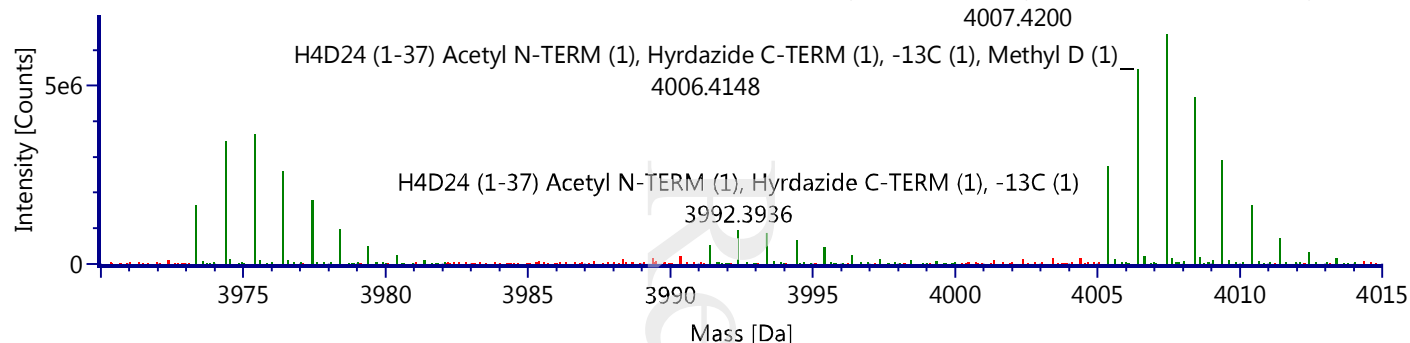
.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	567700	3991.3910	3991.67240	-70.5
2	1014165	3992.3920	3992.67570	-71.1
3	993151	3993.3926	3993.67910	-71.7
4	784361	3994.3937	3994.68240	-72.3
5	524401	3995.4000	3995.68580	-71.5
6	275974	3996.3904	3996.68910	-74.7
7	121773	3997.3899	3997.69250	-75.7
Sum	4281524.722	27960.750	27962.777	-507.575

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	889955	3973.3860	3973.65710	-68.2
2	1834549	3974.3854	3974.66040	-69.2
3	2025942	3975.3890	3975.66380	-69.1
4	1430721	3976.3887	3976.66720	-70.0
5	909655	3977.3884	3977.67050	-70.9
6	612689	3978.3874	3978.67390	-72.0
7	317157	3979.3877	3979.67720	-72.7
8	186803	3980.3745	3980.68060	-76.9
Sum	8207471.343	31815.087	31817.351	-569.185

Item name: 240417_H4Iso_60

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1), Methyl D (1)


H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	2738991	4005.4086	4005.69900	-72.5
2	5461823	4006.4148	4006.70230	-71.8
3	6444842	4007.4200	4007.70570	-71.3
4	4669416	4008.4143	4008.70900	-73.5
5	2887882	4009.4165	4009.71240	-73.8
6	1629674	4010.4189	4010.71570	-74.0
7	706323	4011.4181	4011.71910	-75.0
8	326514	4012.4202	4012.72240	-75.3
9	161624	4013.4094	4013.72580	-78.8
Sum	25027087.631	36084.741	36087.411	-666.064

H4D24 + H4isoD24

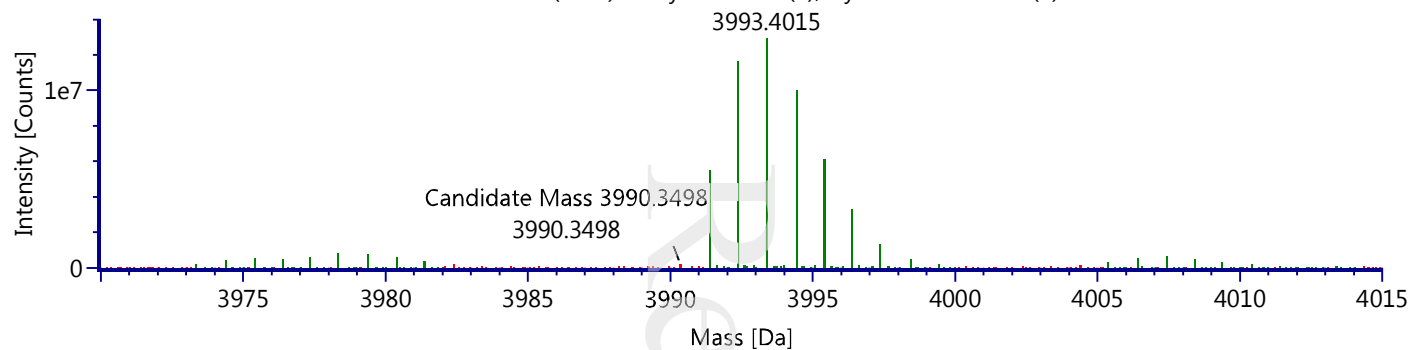
.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	519116	3991.3839	3991.67240	-72.3
2	928726	3992.3936	3992.67570	-70.7
3	872460	3993.3914	3993.67910	-72.0
4	649983	3994.3943	3994.68240	-72.1
5	459708	3995.4003	3995.68580	-71.5
6	240255	3996.3997	3996.68910	-72.4
7	126130	3997.3985	3997.69250	-73.5
Sum	3796377.306	27960.762	27962.777	-504.553

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	1637128	3973.3881	3973.65710	-67.7
2	3418282	3974.3921	3974.66040	-67.5
3	3646580	3975.3914	3975.66380	-68.5
4	2574515	3976.3958	3976.66720	-68.3
5	1775624	3977.3985	3977.67050	-68.4
6	967465	3978.3869	3978.67390	-72.1
7	480055	3979.3892	3979.67720	-72.4
8	248024	3980.3872	3980.68060	-73.7
9	111751	3981.3827	3981.68390	-75.7
Sum	14859425.390	35796.512	35799.035	-634.240

Item name: 240417_H4WT_0

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1)



H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	305827	4005.3957	4005.69900	-75.7
2	529694	4006.3983	4006.70230	-75.9
3	639268	4007.4073	4007.70570	-74.5
4	488433	4008.4045	4008.70900	-76.0
5	317660	4009.4172	4009.71240	-73.6
6	189920	4010.4049	4010.71570	-77.5
Sum	2470803.181	24047.428	24049.244	-453.138

H4D24 + H4isoD24

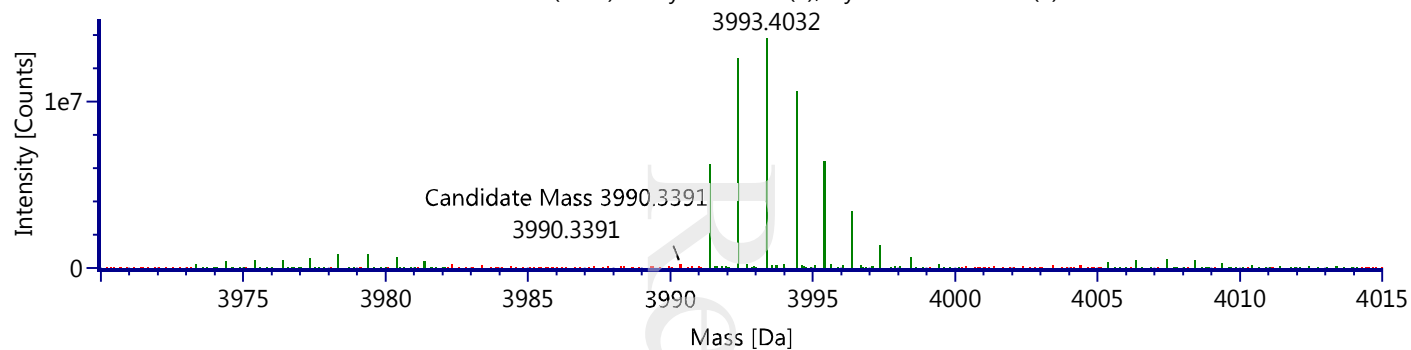
.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	5518958	3991.3971	3991.67240	-69.0
2	11610210	3992.4018	3992.67570	-68.6
3	12946755	3993.4015	3993.67910	-69.5
4	10015635	3994.4016	3994.68240	-70.3
5	6088168	3995.4040	3995.68580	-70.5
6	3298134	3996.4072	3996.68910	-70.5
7	1326601	3997.4022	3997.69250	-72.6
8	514913	3998.4049	3998.69590	-72.8
9	215085	3999.4089	3999.69920	-72.6
Sum	51534458.577	35958.629	35961.172	-636.432

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	192301	3973.3700	3973.65710	-72.3
2	413281	3974.3831	3974.66040	-69.8
3	526259	3975.3799	3975.66380	-71.4
4	451669	3976.3768	3976.66720	-73.0
5	598010	3977.3728	3977.67050	-74.8
6	783629	3978.3738	3978.67390	-75.4
7	760577	3979.3727	3979.67720	-76.5
8	570948	3980.3765	3980.68060	-76.4
9	358273	3981.3719	3981.68390	-78.4
Sum	4654946.891	35796.377	35799.035	-668.055

Item name: 240417_H4WT_60

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1)



H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	296571	4005.3953	4005.69900	-75.8
2	475326	4006.3965	4006.70230	-76.3
3	542474	4007.4093	4007.70570	-74.0
4	444970	4008.4070	4008.70900	-75.3
5	279985	4009.3985	4009.71240	-78.3
6	157799	4010.4129	4010.71570	-75.5
Sum	2197125.103	24047.419	24049.244	-455.273

H4D24 + H4isoD24

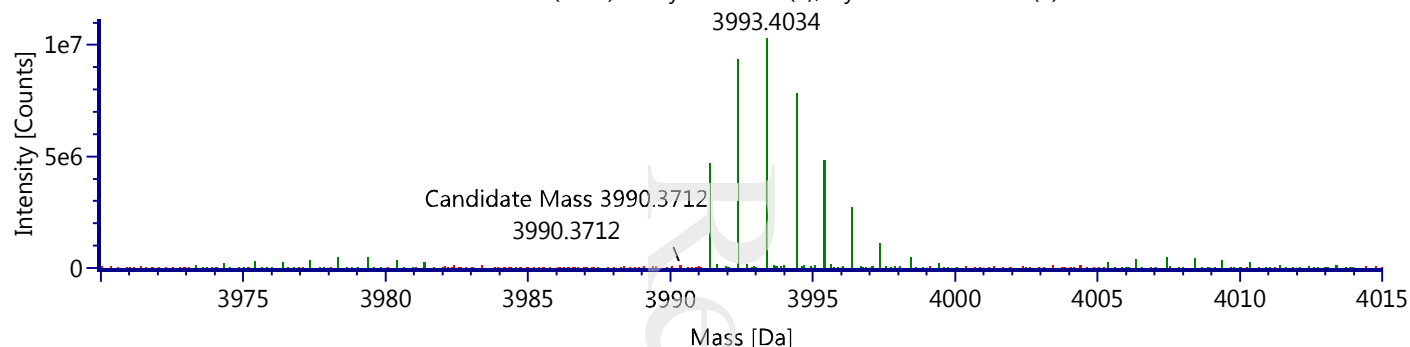
.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	6180894	3991.3987	3991.67240	-68.6
2	12595053	3992.4026	3992.67570	-68.4
3	13830901	3993.4032	3993.67910	-69.1
4	10617962	3994.4034	3994.68240	-69.8
5	6399098	3995.4006	3995.68580	-71.4
6	3438479	3996.4079	3996.68910	-70.4
7	1359673	3997.4007	3997.69250	-73.0
8	596581	3998.4010	3998.69590	-73.7
9	229091	3999.3936	3999.69920	-76.4
Sum	55247733.025	35958.612	35961.172	-640.808

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	184884	3973.3754	3973.65710	-70.9
2	392425	3974.3807	3974.66040	-70.4
3	428122	3975.3725	3975.66380	-73.3
4	428141	3976.3787	3976.66720	-72.5
5	582985	3977.3731	3977.67050	-74.8
6	786684	3978.3682	3978.67390	-76.8
7	787790	3979.3710	3979.67720	-76.9
8	605981	3980.3753	3980.68060	-76.7
9	364293	3981.3700	3981.68390	-78.8
Sum	4561305.485	35796.365	35799.035	-671.179

Item name: 240417_H4Iso_NoPIMT_60

H4D24 (1-37) Acetyl N-TERM (1), Hyrdazide C-TERM (1)


H4isoD24-Me

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	214007	4005.3827	4005.69900	-79.0
2	370110	4006.3912	4006.70230	-77.7
3	465036	4007.3967	4007.70570	-77.1
4	432713	4008.3902	4008.70900	-79.5
5	319668	4009.4012	4009.71240	-77.6
6	232725	4010.3968	4010.71570	-79.5
7	120954	4011.3967	4011.71910	-80.4
Sum	2155212.451	28058.756	28060.963	-550.748

H4D24 + H4isoD24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	4714880	3991.3999	3991.67240	-68.3
2	9356391	3992.4034	3992.67570	-68.2
3	10308461	3993.4034	3993.67910	-69.0
4	7842130	3994.4054	3994.68240	-69.3
5	4821577	3995.4036	3995.68580	-70.6
6	2691085	3996.4090	3996.68910	-70.1
7	1089169	3997.4046	3997.69250	-72.0
8	467808	3998.4083	3998.69590	-71.9
9	200195	3999.3999	3999.69920	-74.8
Sum	41491697.275	35958.638	35961.172	-634.361

H4succinimide24

.	Response	Observed mass (Da)	Expected mass (Da)	Mass error (ppm)
1	109412	3973.3867	3973.65710	-68.0
2	198258	3974.3750	3974.66040	-71.8
3	275739	3975.3728	3975.66380	-73.2
4	246704	3976.3743	3976.66720	-73.7
5	341051	3977.3731	3977.67050	-74.8
6	454052	3978.3657	3978.67390	-77.5
7	450265	3979.3733	3979.67720	-76.4
8	349081	3980.3739	3980.68060	-77.1
9	223445	3981.3653	3981.68390	-80.0
Sum	2648007.329	35796.360	35799.035	-672.413