

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
 Data File : BF139445.D
 Acq On : 19 Sep 2024 00:32
 Operator : RC/JU
 Sample : P4009-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DN-B-34B

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139445.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	7	16	23	rVB	749685	1191796	79.31%	9.800%
2	5.098	502	511	519	rVB	72747	109833	7.31%	0.903%
3	5.498	573	579	584	rBV	1147358	1495447	99.51%	12.297%
4	6.504	744	750	763	rVB	1108999	1502744	100.00%	12.357%
5	6.881	808	814	819	rBV	296348	375437	24.98%	3.087%
6	7.439	903	909	914	rBV	755082	950863	63.28%	7.819%
7	7.692	948	952	958	rVB	27715	33225	2.21%	0.273%
8	8.157	1023	1031	1039	rBV	323769	413918	27.54%	3.404%
9	8.745	1127	1131	1135	rBV	14732	17091	1.14%	0.141%
10	9.233	1209	1214	1219	rBV	1178100	1426344	94.92%	11.729%
11	9.310	1223	1227	1232	rVB	12381	15556	1.04%	0.128%
12	9.910	1324	1329	1334	rBV	303771	368023	24.49%	3.026%
13	10.310	1394	1397	1407	rVB	22482	33254	2.21%	0.273%
14	10.622	1442	1450	1455	rBV	100701	123890	8.24%	1.019%
15	10.698	1458	1463	1468	rVV	611070	756288	50.33%	6.219%
16	10.745	1468	1471	1477	rVB	11615	16357	1.09%	0.135%
17	11.398	1577	1582	1591	rBV2	274051	436744	29.06%	3.591%
18	11.886	1661	1665	1666	rBV3	15356	18726	1.25%	0.154%
19	11.921	1666	1671	1682	rVV3	143970	238260	15.85%	1.959%
20	12.010	1682	1686	1694	rVB4	12828	27483	1.83%	0.226%
21	12.604	1783	1787	1800	rBV	91731	165984	11.05%	1.365%
22	12.704	1800	1804	1812	rBV	36751	60836	4.05%	0.500%
23	12.792	1815	1819	1822	rBV	54222	70768	4.71%	0.582%
24	12.833	1822	1826	1831	rVB	67026	93601	6.23%	0.770%
25	12.980	1845	1851	1858	rBV	963481	1283475	85.41%	10.554%
26	13.457	1928	1932	1937	rBV	96926	132054	8.79%	1.086%
27	13.515	1938	1942	1946	rVB	74363	90493	6.02%	0.744%
28	13.880	2000	2004	2014	rBV	69972	124292	8.27%	1.022%
29	14.033	2024	2030	2038	rVB2	228472	363967	24.22%	2.993%
30	15.504	2275	2280	2291	rVB	134597	224033	14.91%	1.842%

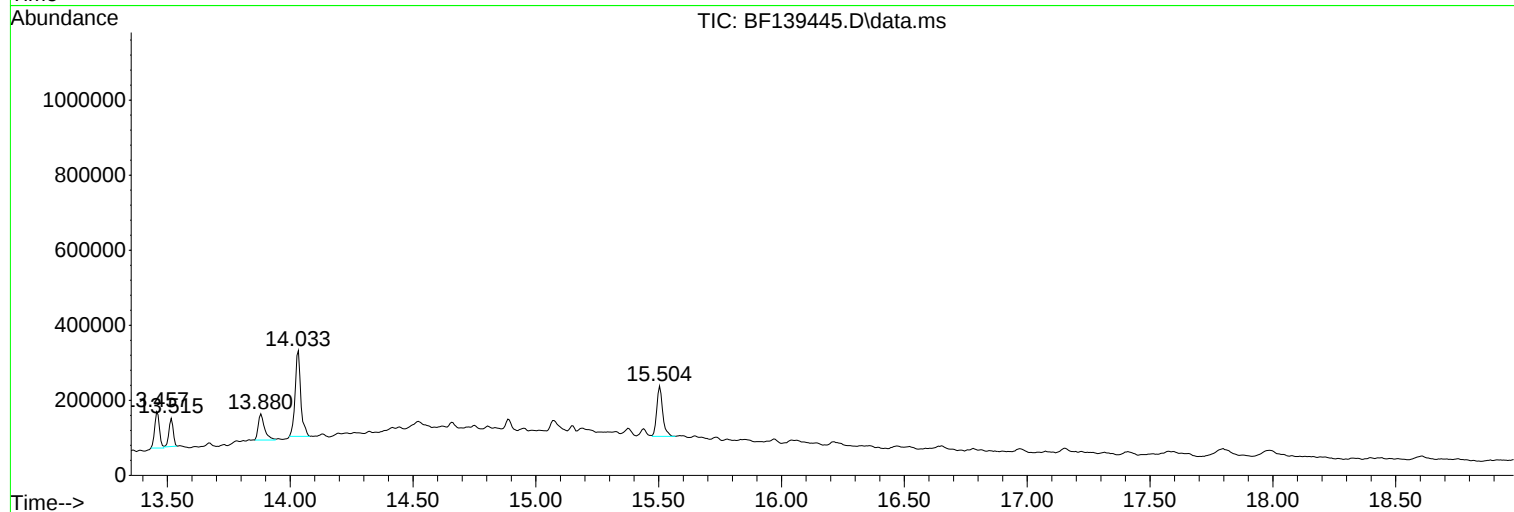
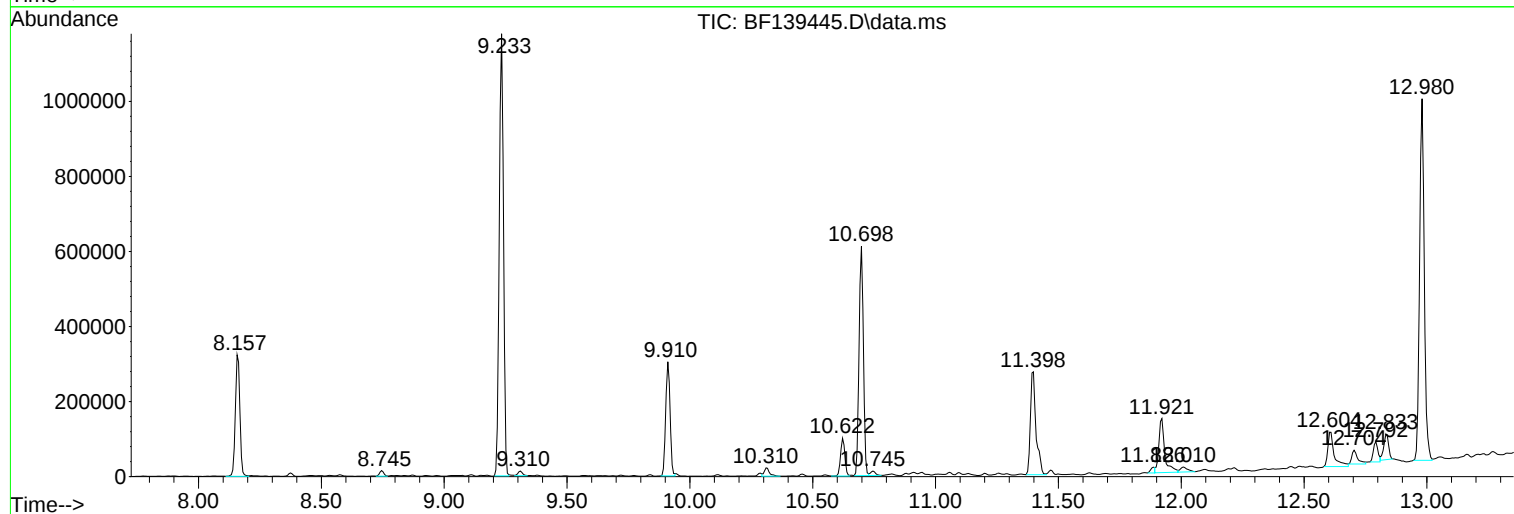
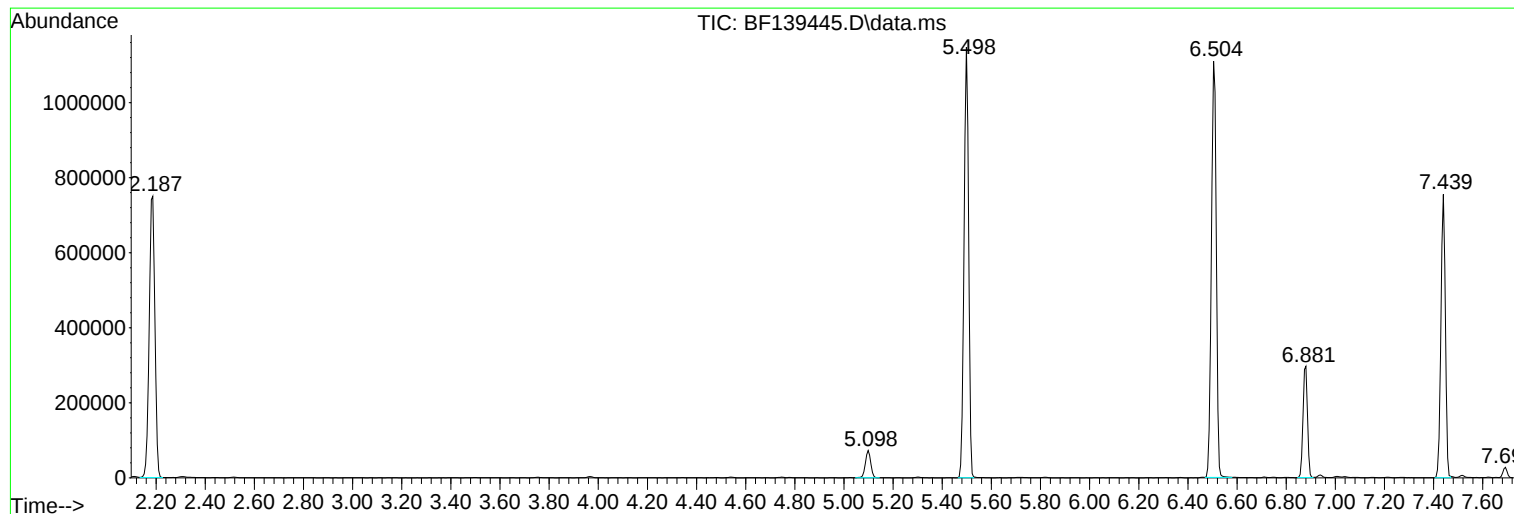
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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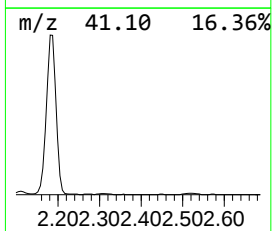
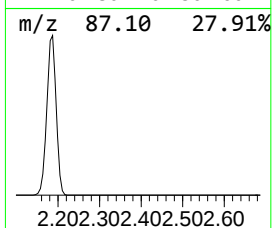
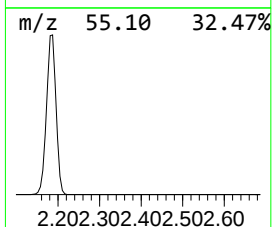
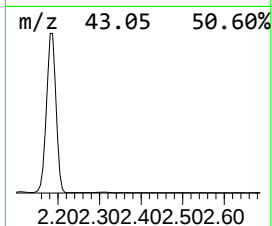
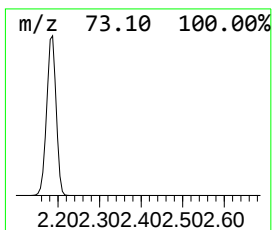
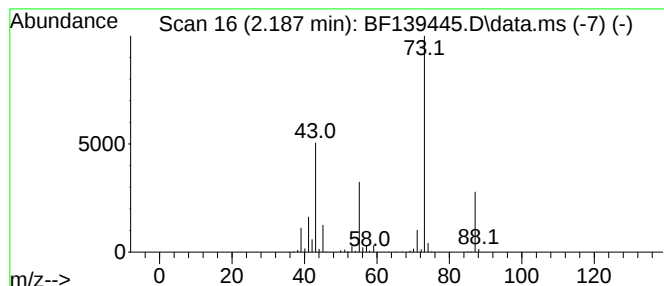
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	63.49 ng	1191800	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11B02	007318-82-3	10
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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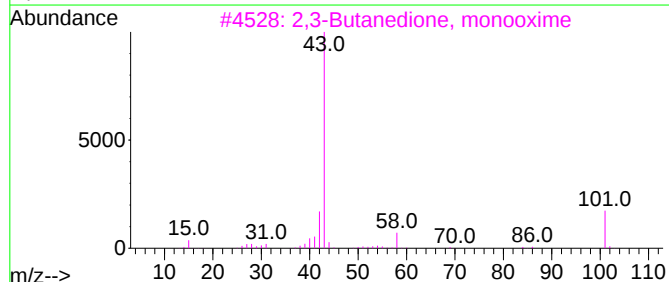
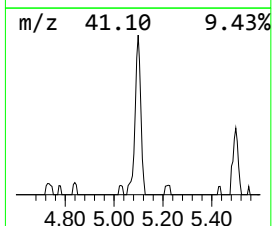
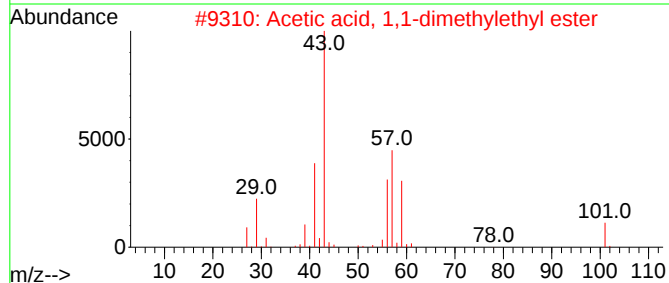
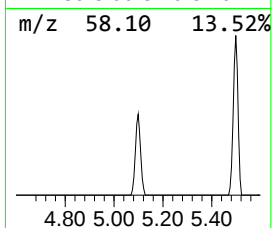
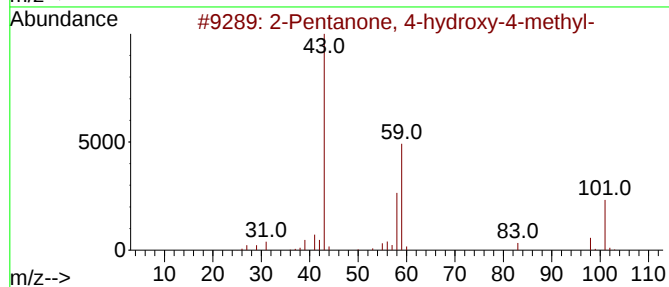
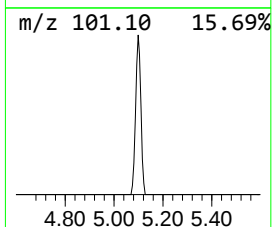
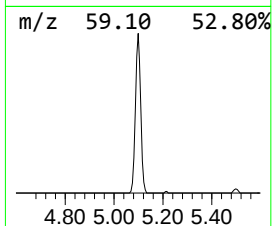
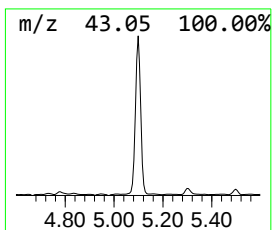
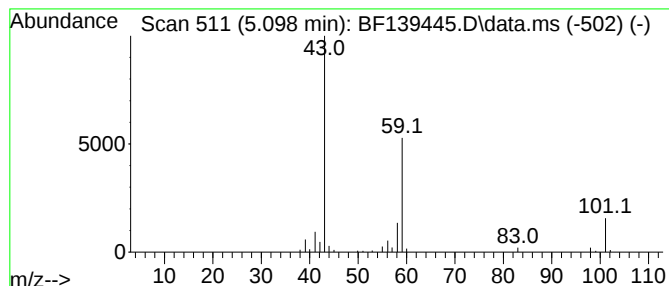
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	5.85 ng	109833	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Diacetamide	101	C4H7NO2	000625-77-4	9



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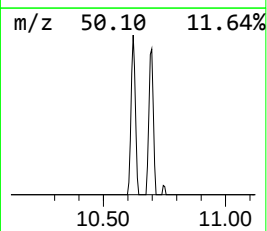
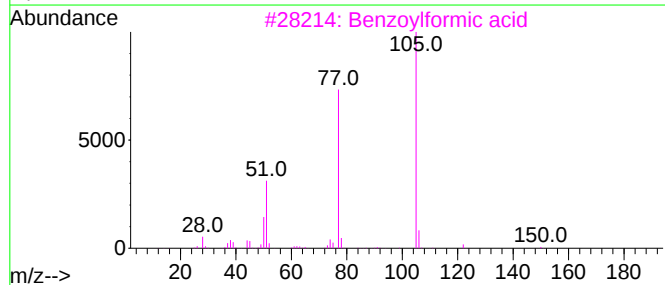
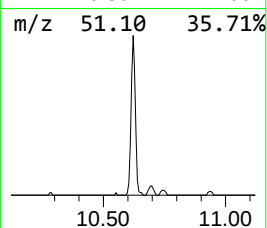
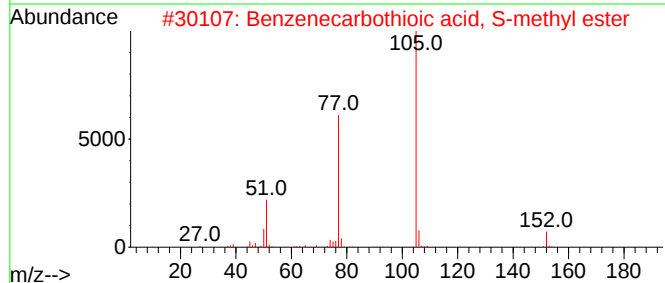
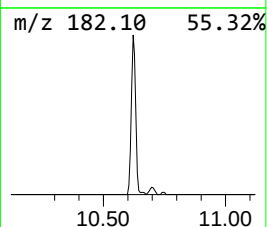
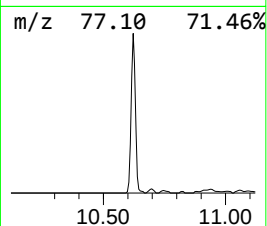
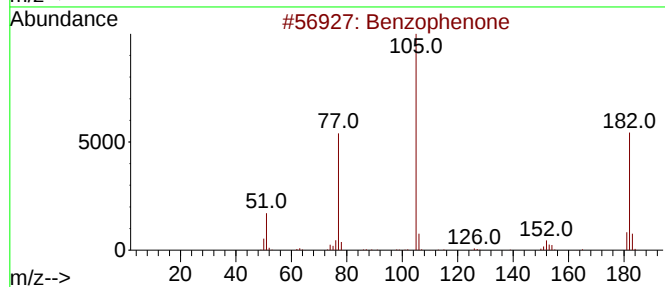
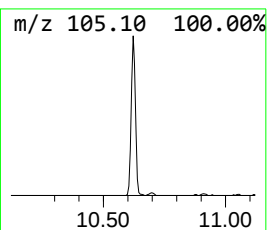
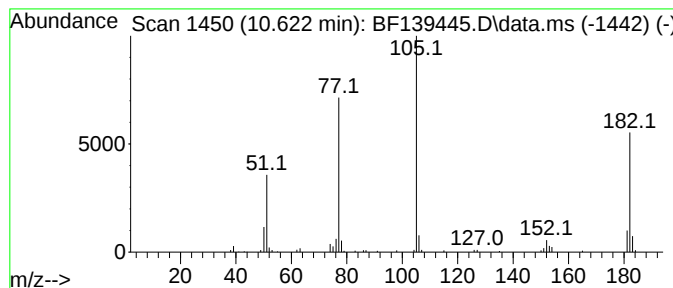
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.621	6.73 ng	123890	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	64
3			Benzoylformic acid	150	C8H6O3	000611-73-4	49
4			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	47
5			N-cyanobenzamide	146	C8H6N2O	015150-25-1	47



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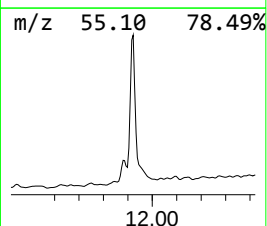
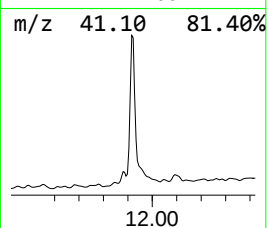
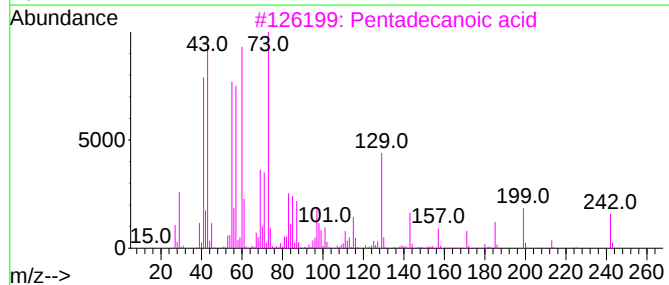
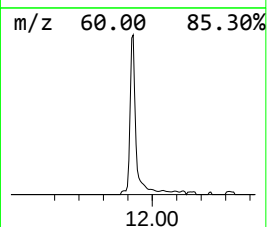
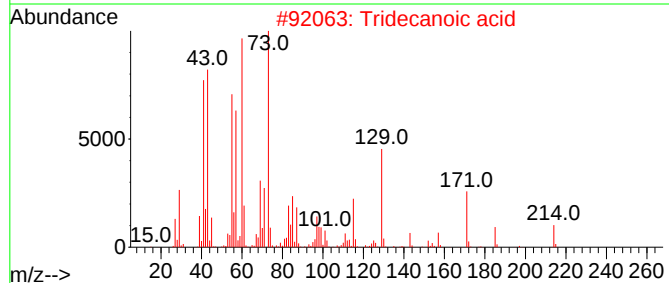
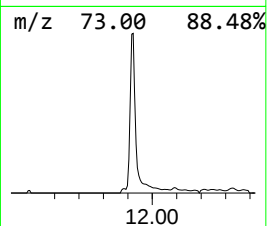
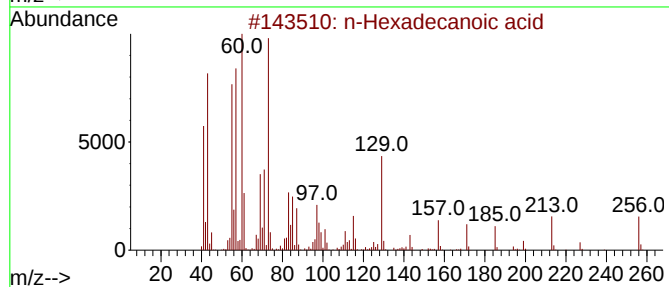
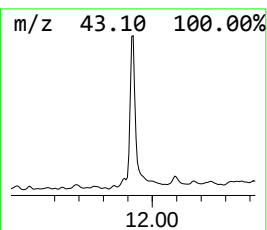
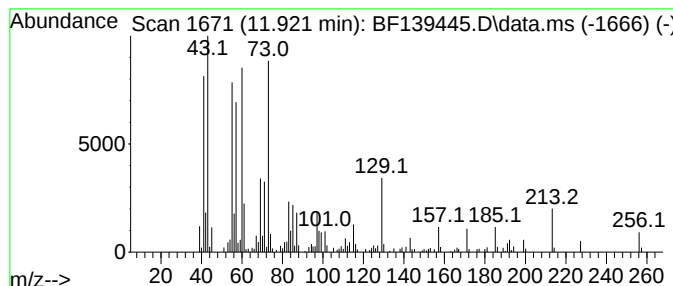
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	10.91 ng	238260	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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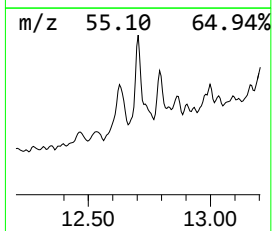
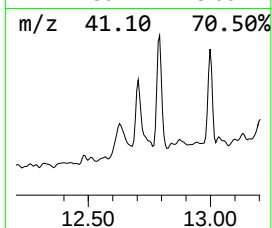
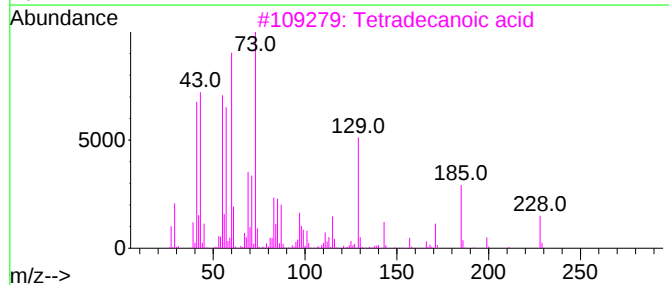
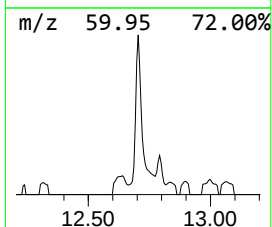
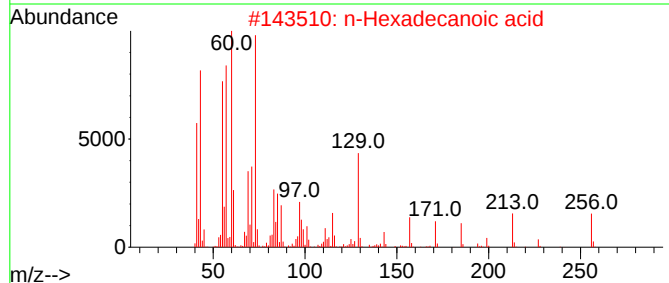
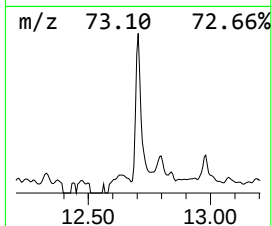
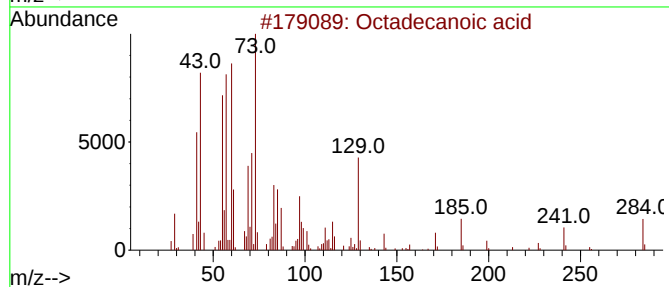
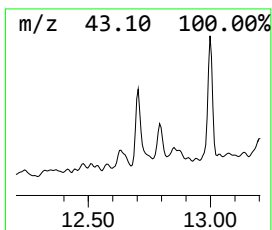
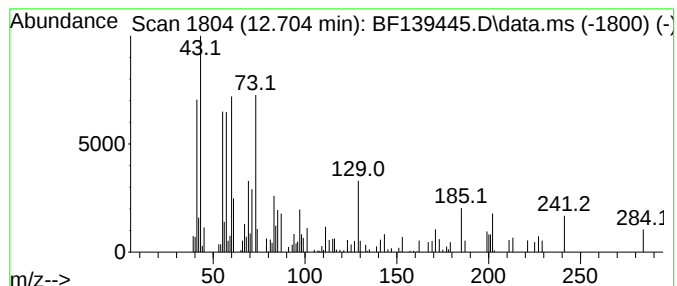
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	2.79 ng	60836	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4			Dodecanoic acid	200	C12H24O2	000143-07-7	50
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	49



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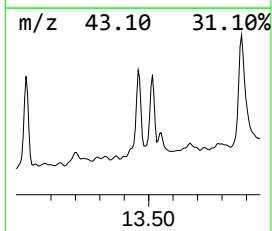
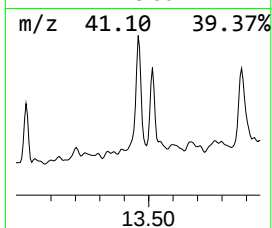
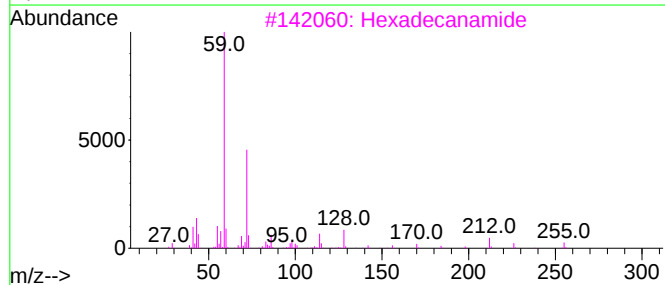
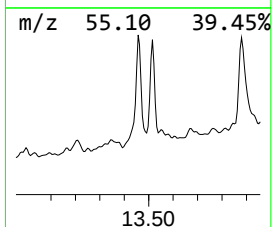
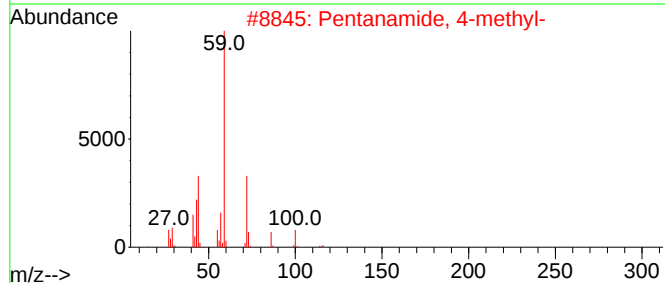
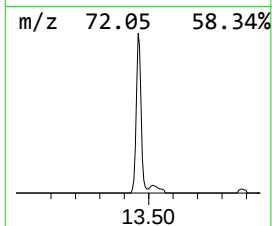
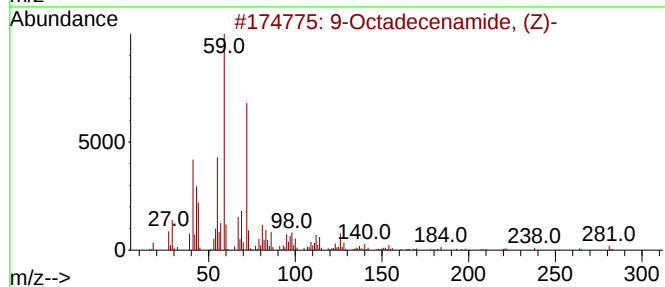
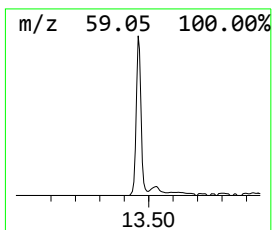
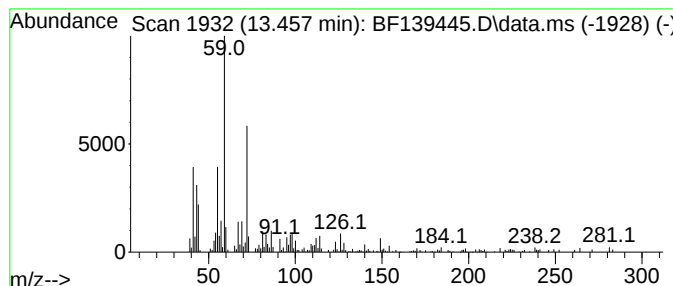
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	7.26 ng	132054	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	72
3		Hexadecanamide	255	C16H33NO	000629-54-9	64
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Palmitoleamide	253	C16H31NO	106010-22-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139445.D
Acq On : 19 Sep 2024 00:32
Operator : RC/JU
Sample : P4009-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DN-B-34B

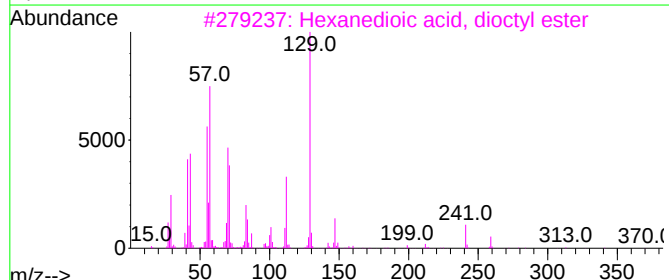
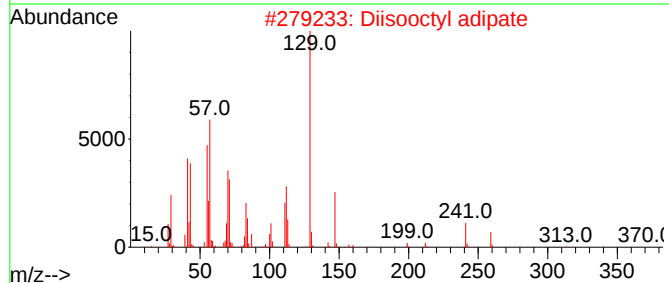
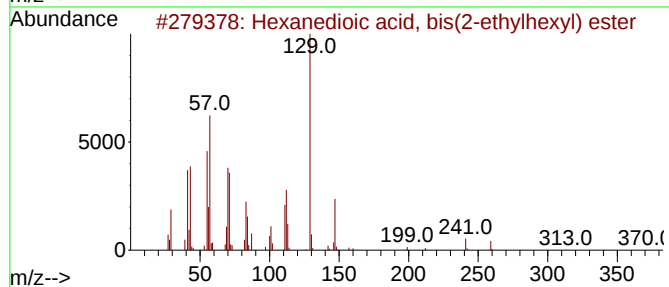
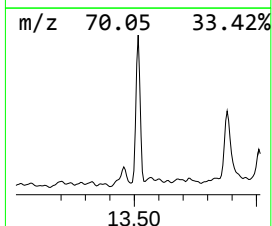
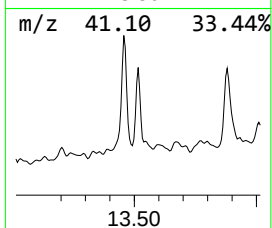
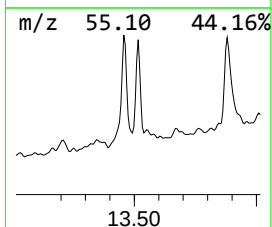
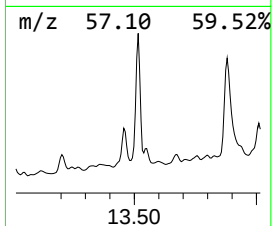
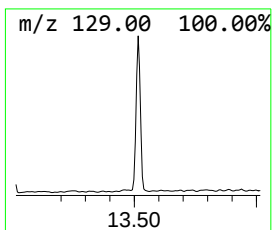
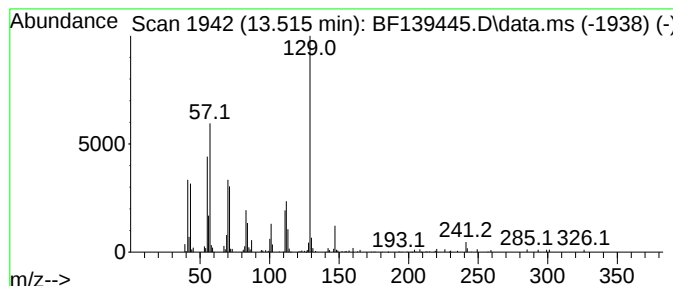
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexanedioic acid, bis(2-eth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.515	4.97 ng	90493	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2			Diisooctyl adipate	370	C22H42O4	001330-86-5	91
3			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	87
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58
5			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139445.D
Acq On : 19 Sep 2024 00:32
Operator : RC/JU
Sample : P4009-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DN-B-34B

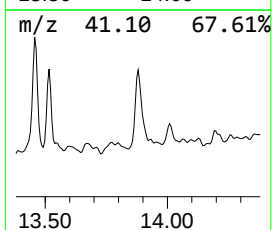
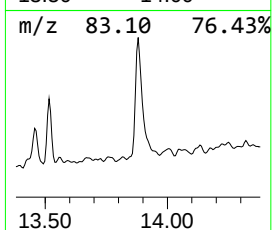
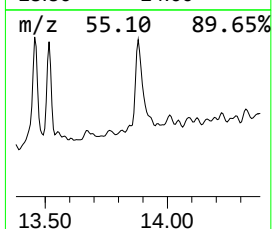
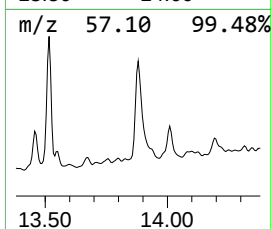
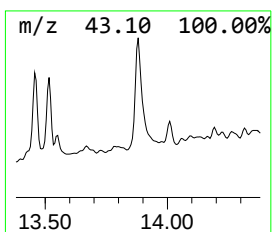
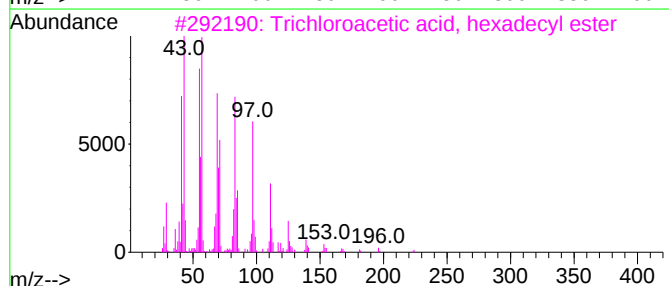
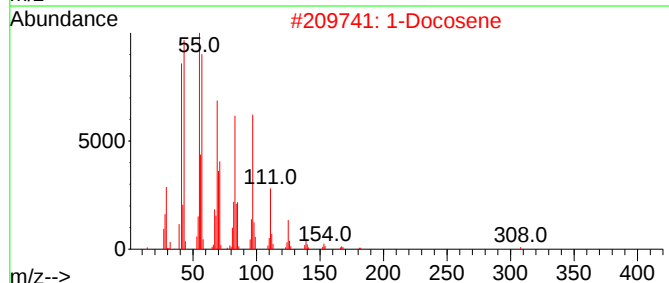
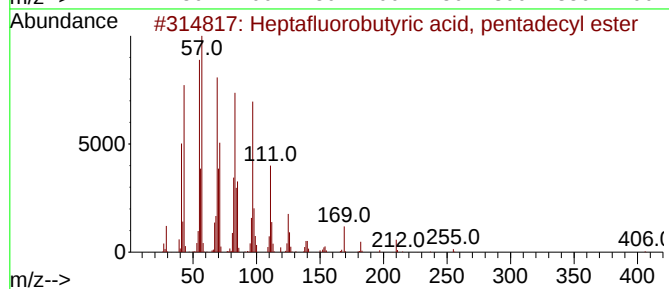
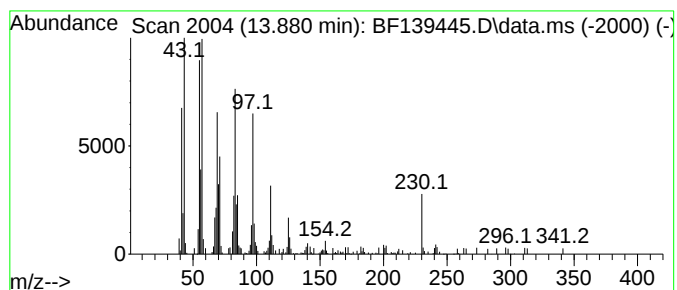
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	6.83 ng	124292	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2			1-Docosene	308	C22H44	001599-67-3	93
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139445.D
Acq On : 19 Sep 2024 00:32
Operator : RC/JU
Sample : P4009-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DN-B-34B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.187	63.5	ng	1191800	1	6.881	375437	20.0
2-Pentanone, 4-...	5.098	5.8	ng	109833	1	6.881	375437	20.0
Benzophenone	10.621	6.7	ng	123890	3	9.910	368023	20.0
n-Hexadecanoic ...	11.922	10.9	ng	238260	4	11.398	436744	20.0
Octadecanoic acid	12.704	2.8	ng	60836	4	11.398	436744	20.0
9-Octadecenamid...	13.457	7.3	ng	132054	5	14.033	363967	20.0
Hexanedioic aci...	13.515	5.0	ng	90493	5	14.033	363967	20.0
Heptafluorobuty...	13.880	6.8	ng	124292	5	14.033	363967	20.0