

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
 Data File : BF136835.D
 Acq On : 29 Dec 2023 18:15
 Operator : CG\JU
 Sample : 05897-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-37a

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136835.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	497	500	510	rVB	25115	32194	1.87%	0.253%
2	5.428	564	568	571	rBV	1632274	1399368	81.41%	10.998%
3	6.428	733	738	741	rBV	1564237	1387540	80.72%	10.905%
4	6.481	744	747	751	rVB	35315	32468	1.89%	0.255%
5	6.781	794	798	801	rBV	523412	401775	23.37%	3.158%
6	7.345	889	894	897	rBV	964822	936393	54.48%	7.359%
7	8.057	1011	1015	1018	rBV	678364	528968	30.77%	4.157%
8	9.133	1194	1198	1201	rBV	2014195	1718852	100.00%	13.508%
9	9.816	1310	1314	1317	rBV	706998	595852	34.67%	4.683%
10	10.610	1445	1449	1452	rBV	1145068	1018345	59.25%	8.003%
11	11.304	1564	1567	1571	rBV	698181	607271	35.33%	4.773%
12	11.839	1655	1658	1674	rBV	131385	195799	11.39%	1.539%
13	12.498	1767	1770	1774	rBV	22122	20129	1.17%	0.158%
14	12.633	1790	1793	1801	rBV5	23811	39944	2.32%	0.314%
15	12.904	1834	1839	1842	rBV	1696110	1473678	85.74%	11.582%
16	13.127	1873	1877	1881	rBV3	25704	37859	2.20%	0.298%
17	13.251	1894	1898	1903	rBV2	53369	58877	3.43%	0.463%
18	13.427	1924	1928	1931	rBV4	15921	23082	1.34%	0.181%
19	13.810	1990	1993	1997	rVB	230042	185016	10.76%	1.454%
20	13.880	1997	2005	2012	rBV8	42210	142845	8.31%	1.123%
21	13.963	2015	2019	2028	rVB	433474	454506	26.44%	3.572%
22	14.033	2028	2031	2034	rBV3	28616	45065	2.62%	0.354%
23	14.127	2043	2047	2050	rVB2	19850	19788	1.15%	0.156%
24	14.251	2063	2068	2070	rBV2	19843	26139	1.52%	0.205%
25	14.433	2095	2099	2103	rBV	171105	166726	9.70%	1.310%
26	14.527	2107	2115	2118	rBV7	31731	87023	5.06%	0.684%
27	14.745	2148	2152	2155	rBV5	14964	19756	1.15%	0.155%
28	14.810	2159	2163	2169	rVB4	30765	44427	2.58%	0.349%
29	14.892	2174	2177	2180	rVB2	25213	25298	1.47%	0.199%
30	15.086	2206	2210	2215	rVB	66582	75462	4.39%	0.593%
31	15.210	2221	2231	2234	rBV7	50330	152796	8.89%	1.201%
32	15.439	2265	2270	2279	rBV	270780	369029	21.47%	2.900%
33	15.680	2309	2311	2316	rVB5	18483	22906	1.33%	0.180%
34	15.751	2319	2323	2327	rVB6	11409	20737	1.21%	0.163%
35	15.921	2348	2352	2360	rVB	38810	58204	3.39%	0.457%
36	16.045	2367	2373	2379	rBV6	35703	97499	5.67%	0.766%

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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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.698	2480	2484	2489	rBV5	13315	28602	1.66%	0.225%
38	16.745	2489	2492	2498	rVB6	12709	22010	1.28%	0.173%
39	16.998	2529	2535	2540	rBV9	17339	32702	1.90%	0.257%
40	17.062	2540	2546	2553	rVV7	16013	35667	2.08%	0.280%
41	17.792	2664	2670	2682	rVB7	29458	83716	4.87%	0.658%

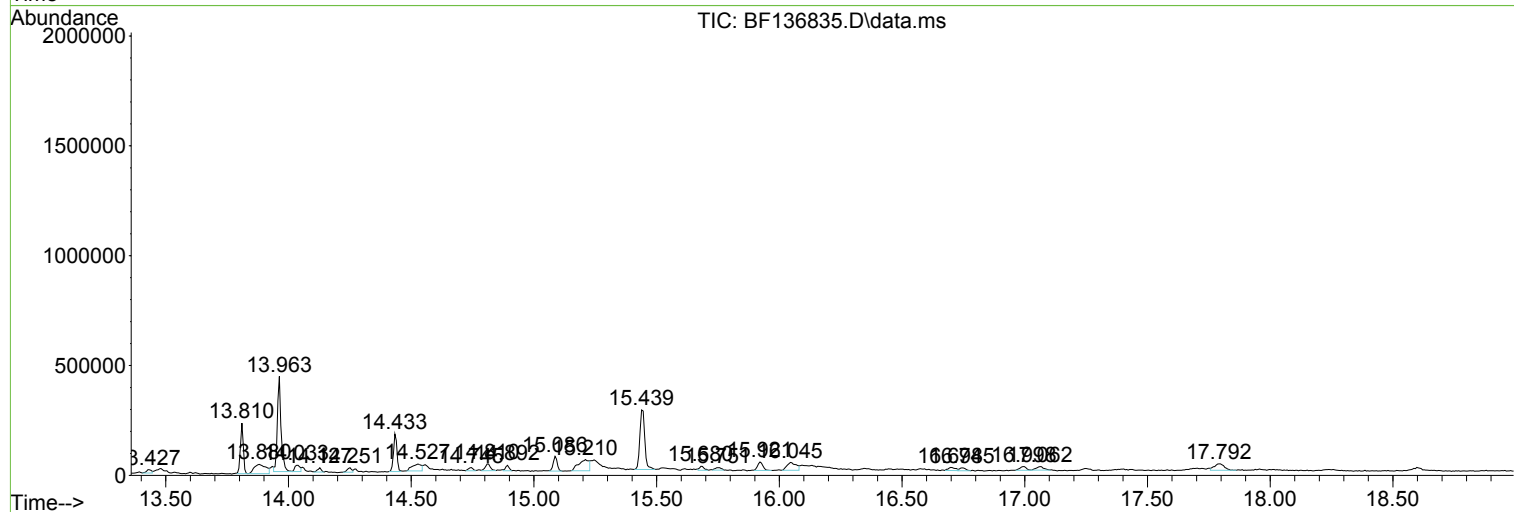
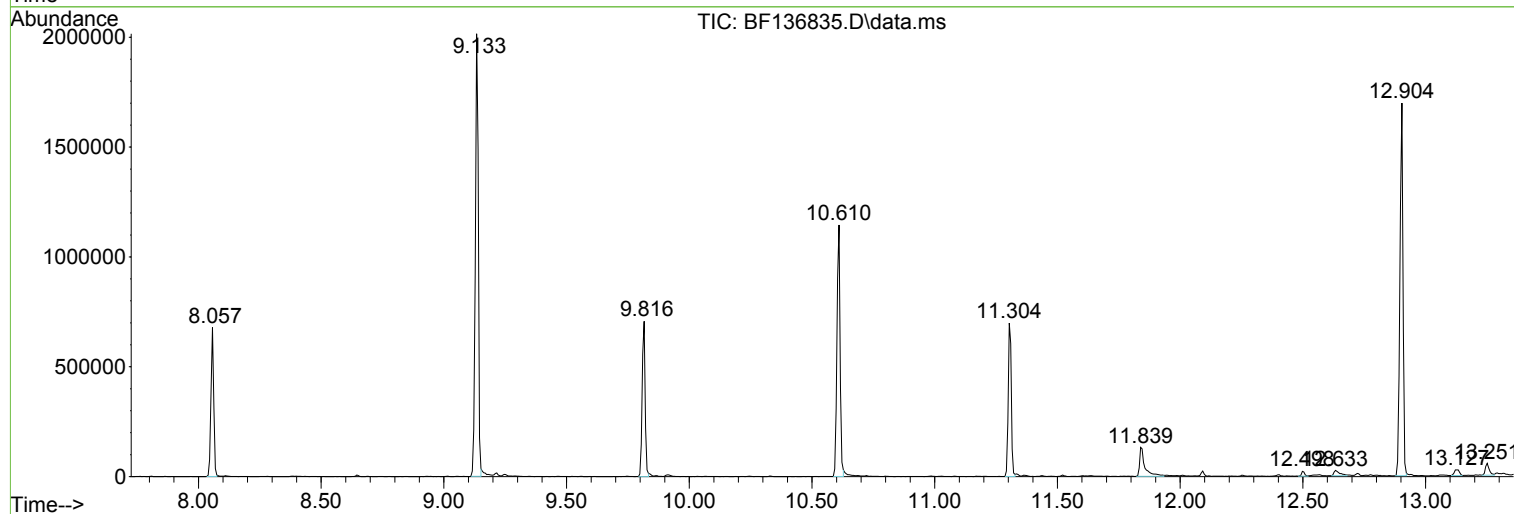
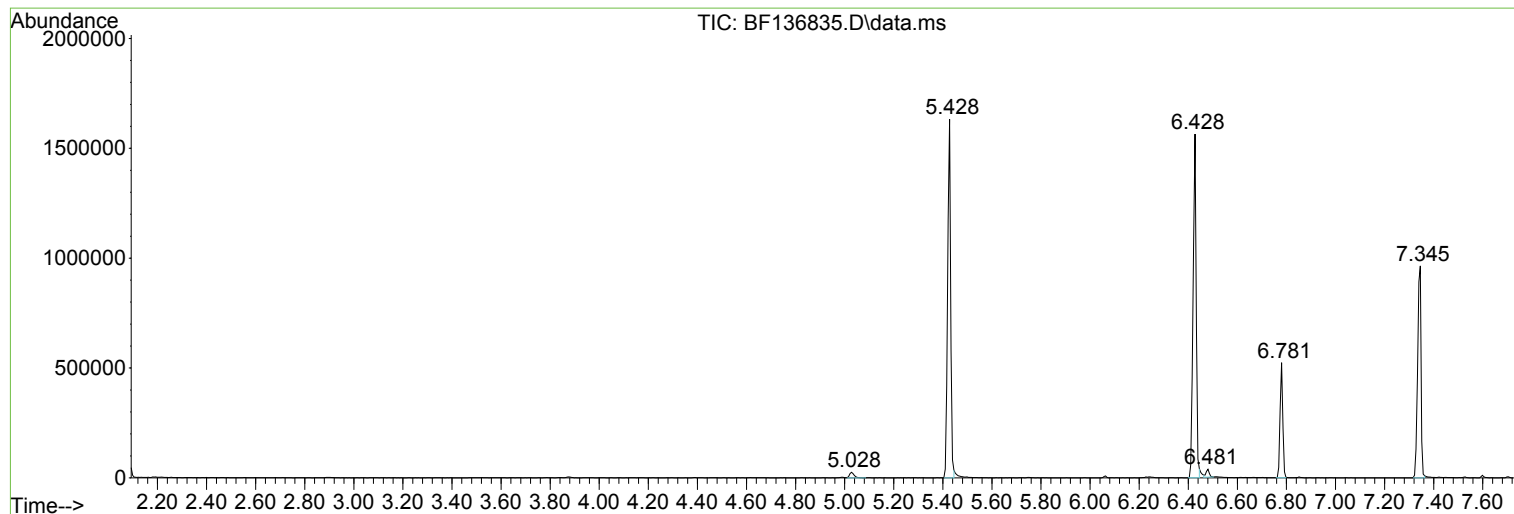
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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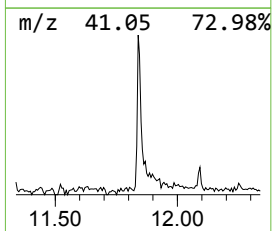
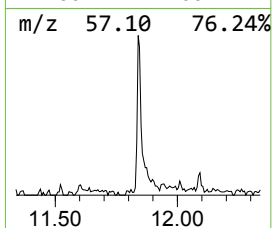
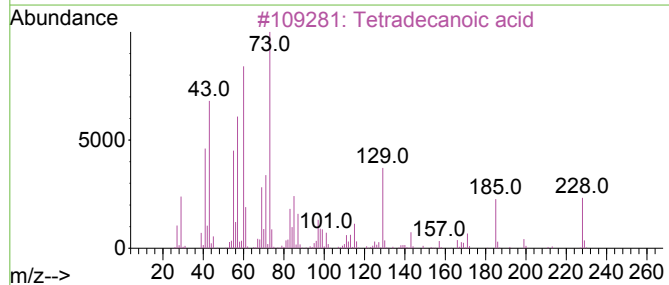
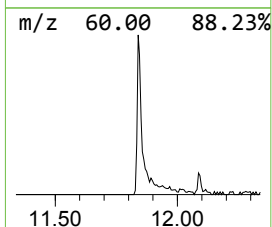
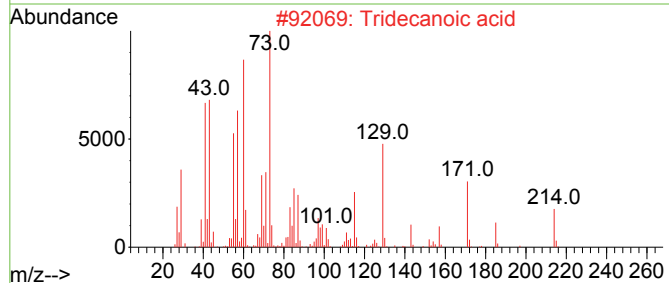
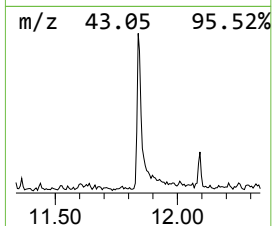
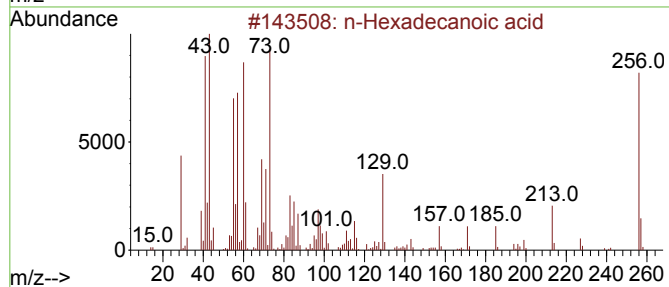
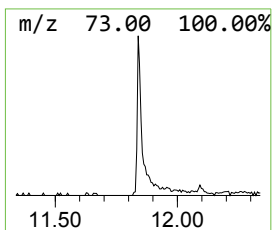
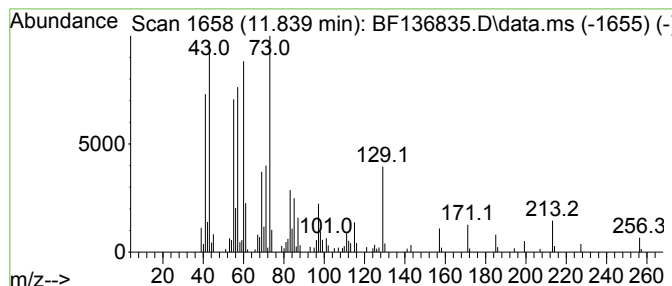
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	6.45 ng	195799	Phenanthrene-d10	11.304

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	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	20



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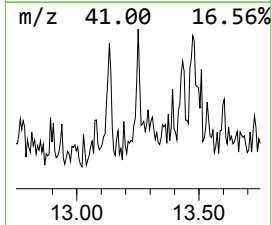
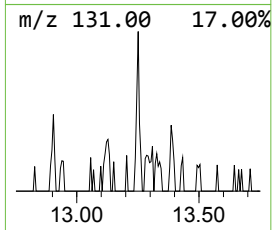
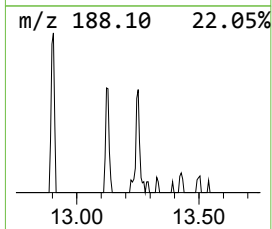
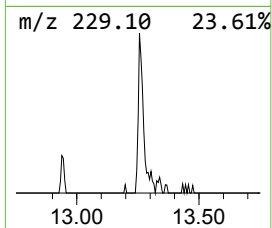
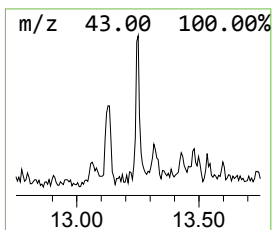
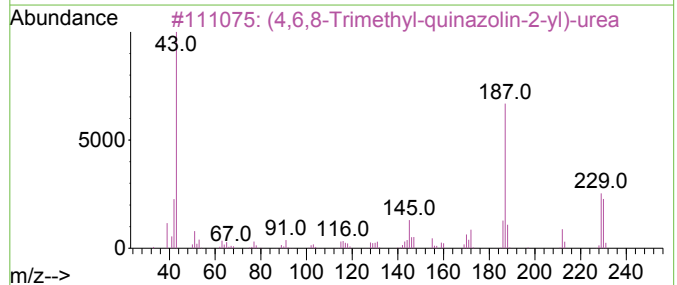
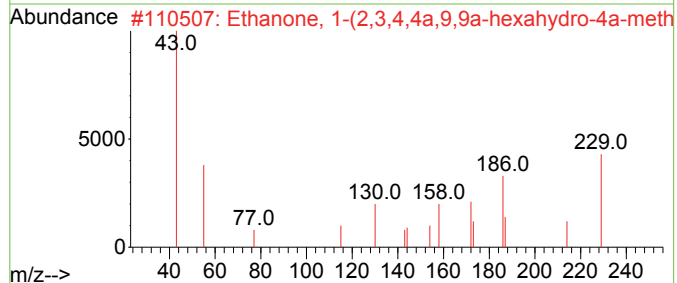
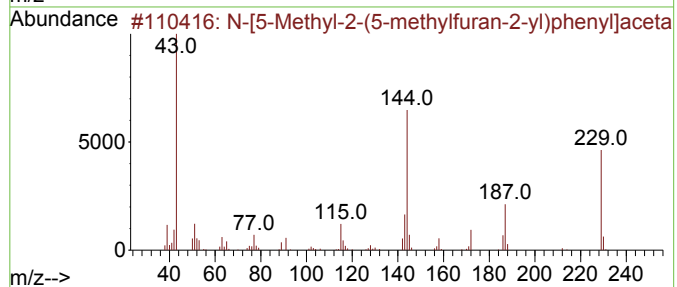
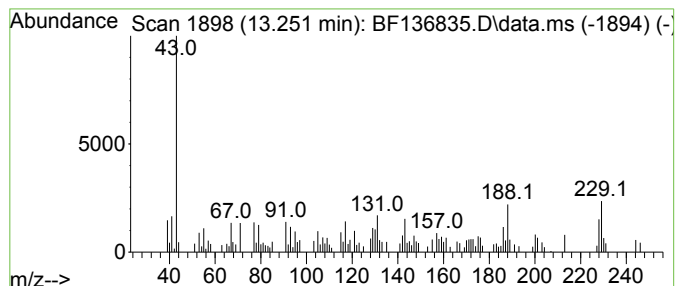
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown13.251 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.251	2.59 ng	58877	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[5-Methyl-2-(5-methylfuran-2-y...	229	C14H15NO2	1000388-78-0	43
2	Ethanone, 1-(2,3,4,4a,9,9a-hexah...	229	C15H19NO	053155-57-0	27
3	(4,6,8-Trimethyl-quinazolin-2-yl...	230	C12H14N4O	1000300-42-2	25
4	(3aR,4aR,5R,7S,7aS)-5-hydroxy-5,...	306	C17H22O5	1223748-08-0	22
5	Carbamic acid, (3-chloro-4-hydro...	229	C10H12ClNO3	028705-96-6	17



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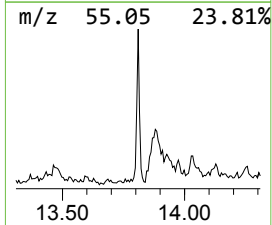
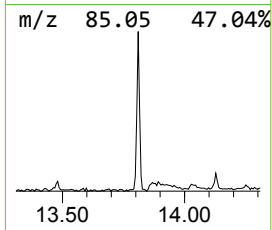
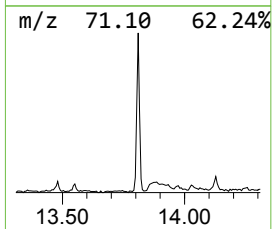
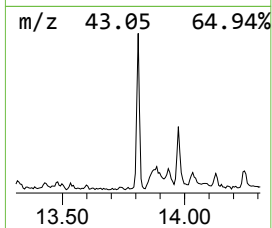
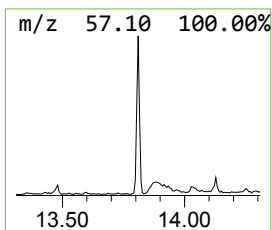
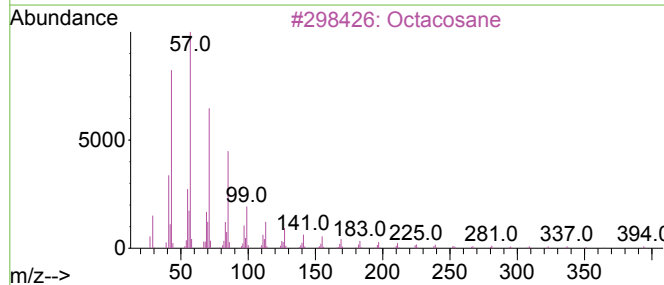
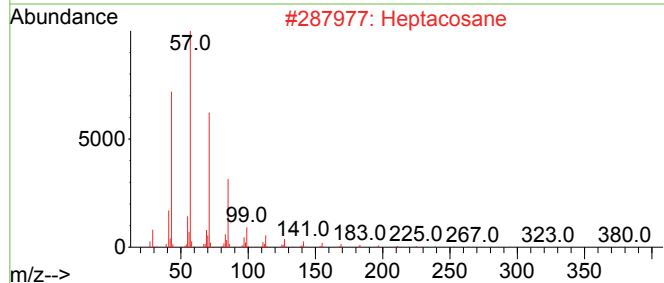
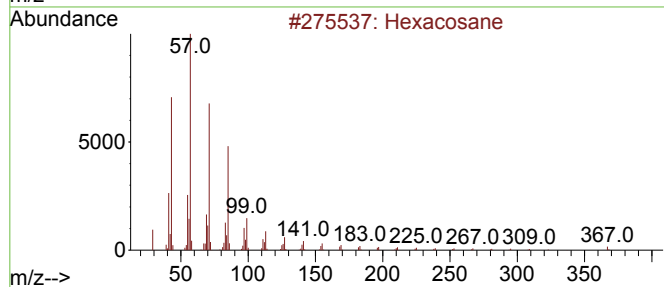
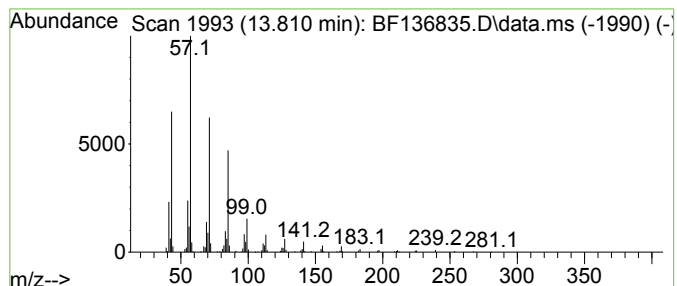
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	8.14 ng	185016	Chrysene-d12	13.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Octadecane	254	C18H38	000593-45-3	91



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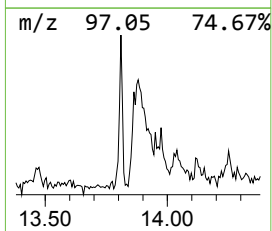
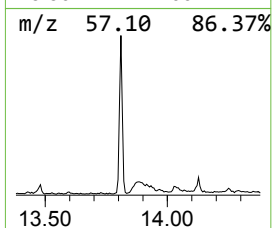
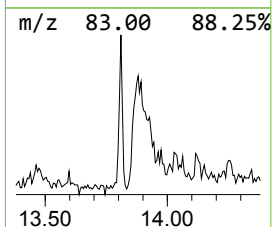
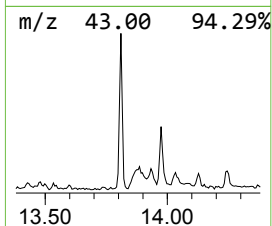
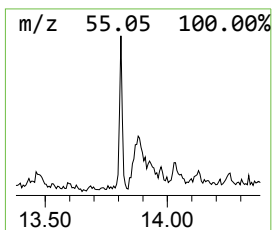
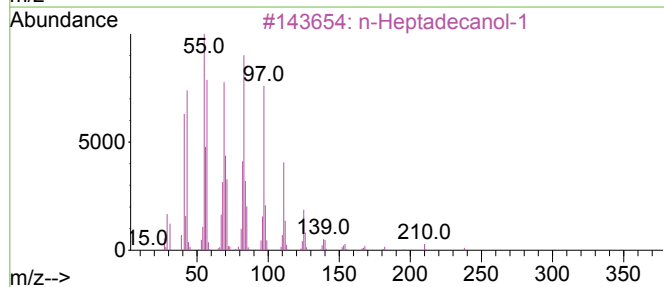
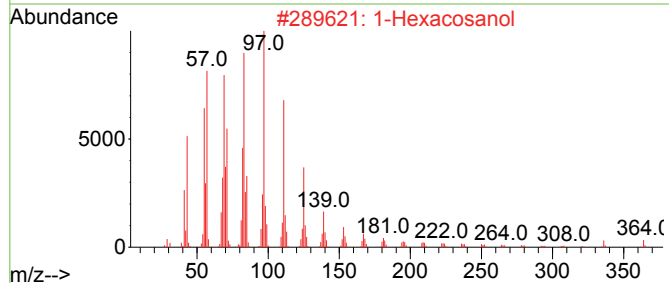
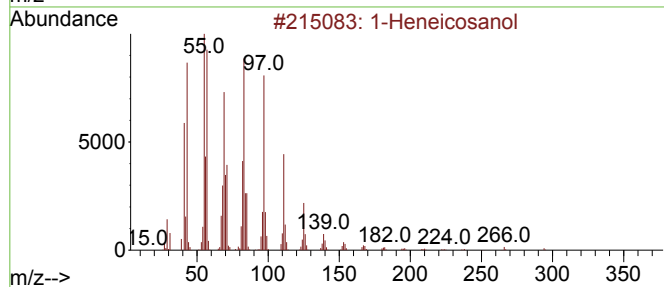
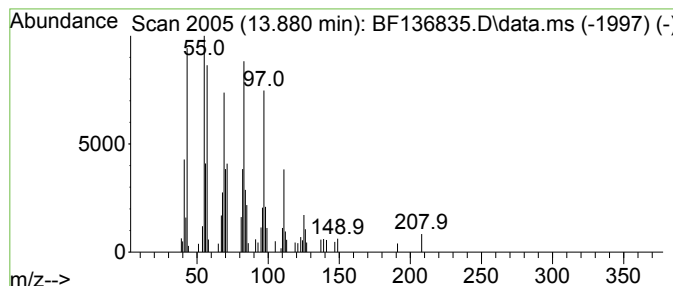
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	6.29 ng	142845	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Hexacosanol	382	C26H54O	000506-52-5	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91



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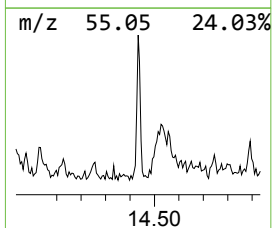
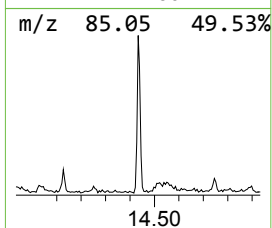
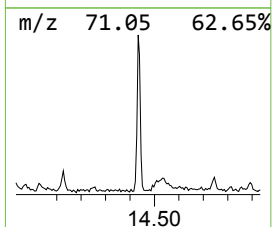
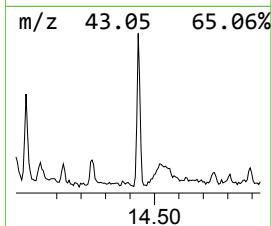
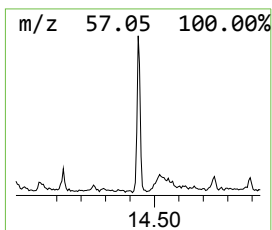
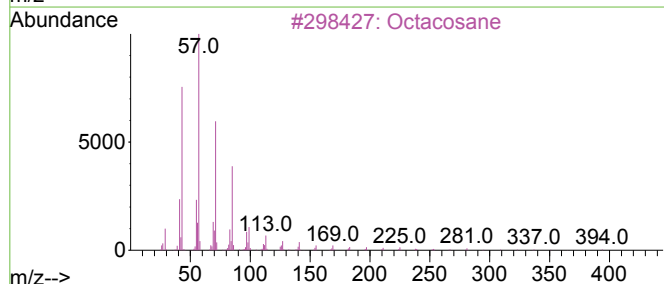
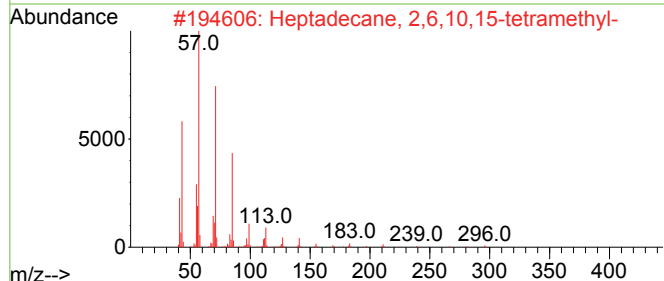
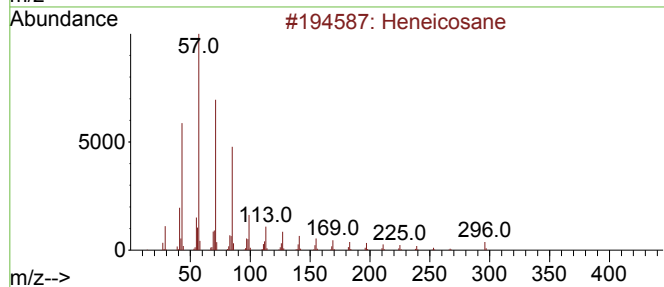
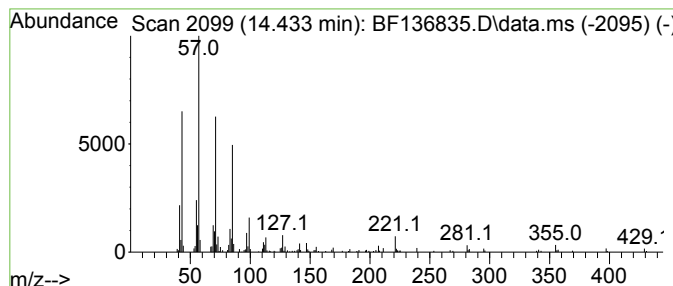
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	7.34 ng	166726	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3			Octacosane	394	C28H58	000630-02-4	83
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83
5			Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136835.D
Acq On : 29 Dec 2023 18:15
Operator : CG\JU
Sample : 05897-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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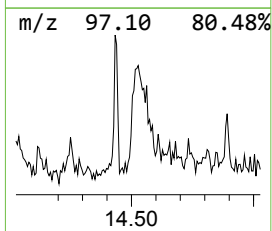
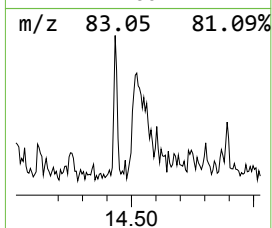
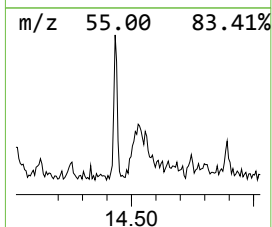
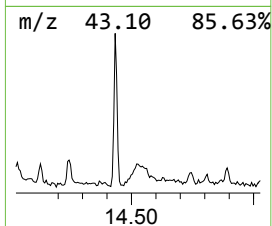
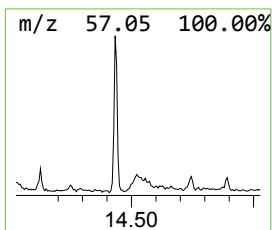
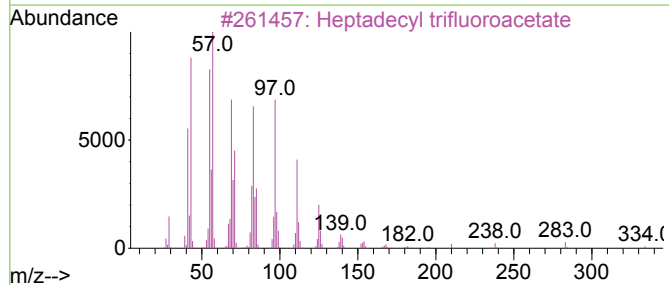
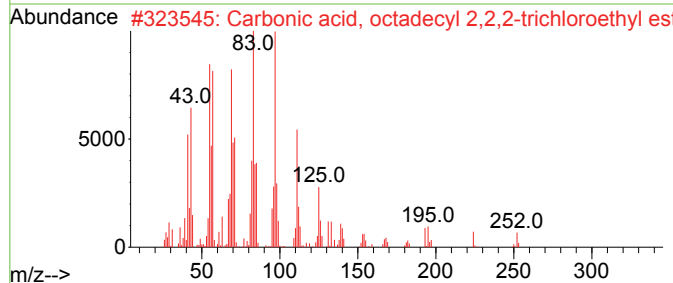
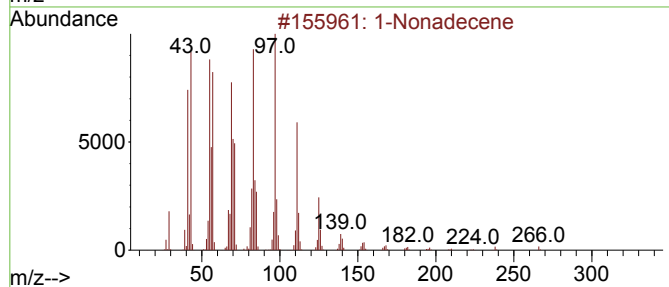
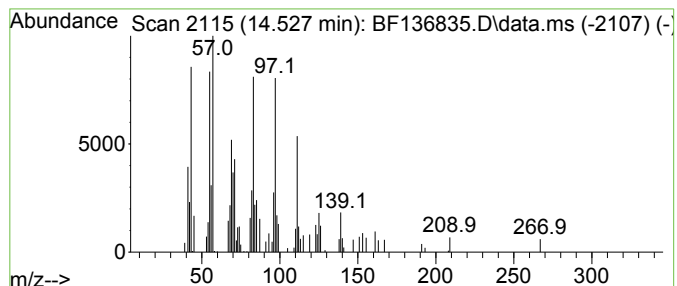
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	3.83 ng	87023	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	90
2	Carbonic acid, octadecyl 2,2,2-t...			444	C21H39Cl3O3	1000314-56-3	87
3	Heptadecyl trifluoroacetate			352	C19H35F3O2	1010351-87-0	87
4	Octacosanol			410	C28H58O	000557-61-9	83
5	n-Tetracosanol-1			354	C24H50O	000506-51-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136835.D
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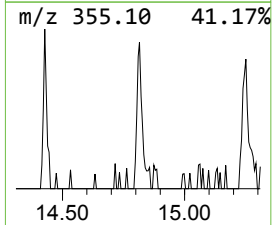
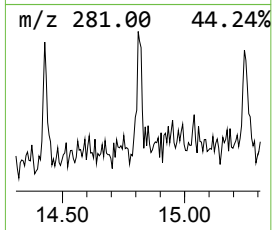
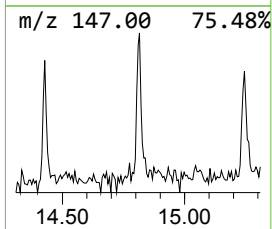
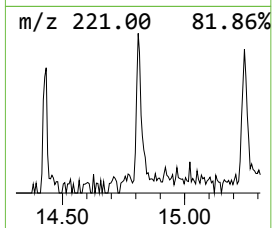
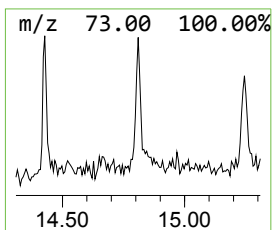
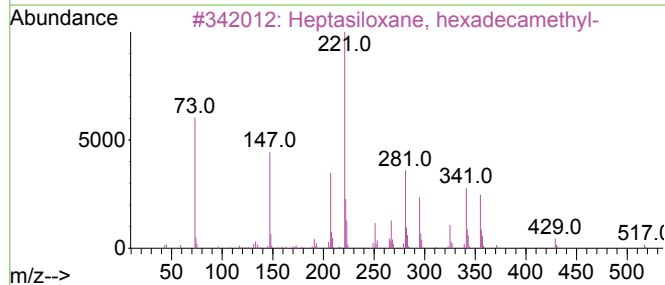
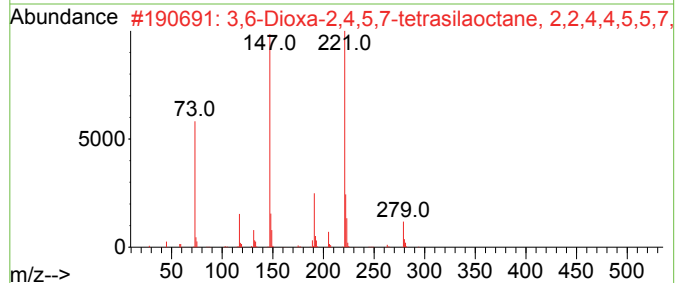
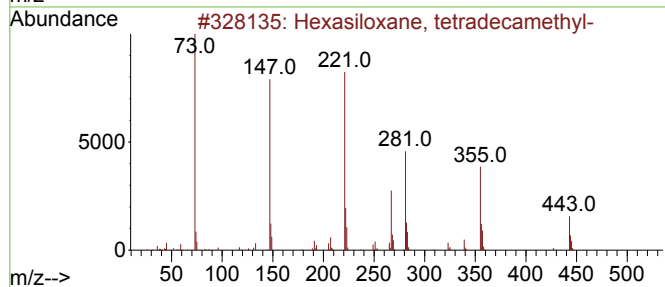
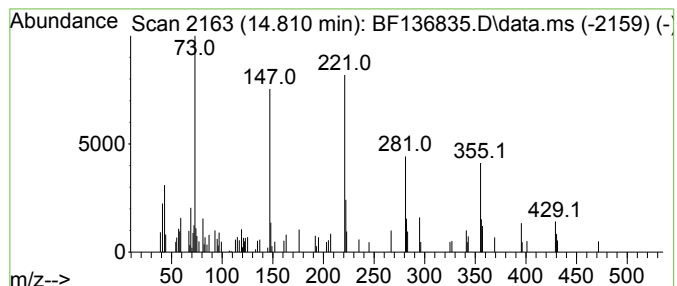
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexasiloxane, tetradecamethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.810	2.41 ng	44427	Perylene-d12	15.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	32
4	2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O2S2Si4	959295-06-8	25
5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136835.D
Acq On : 29 Dec 2023 18:15
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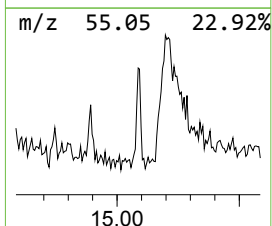
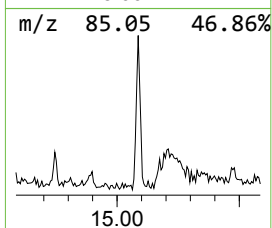
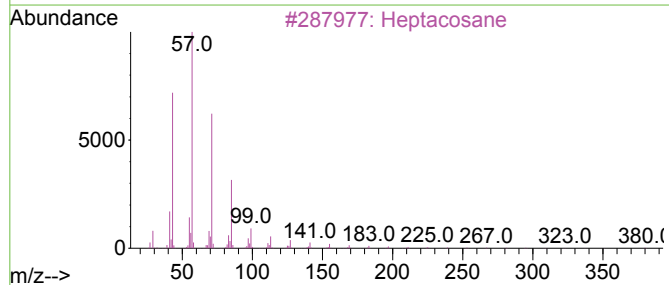
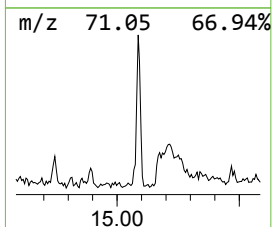
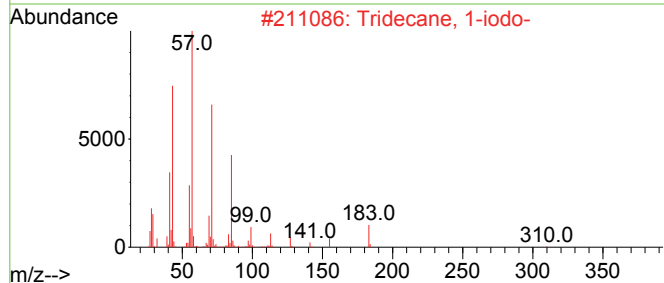
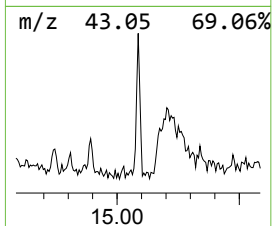
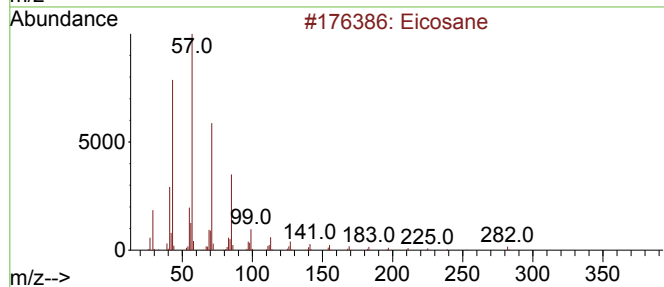
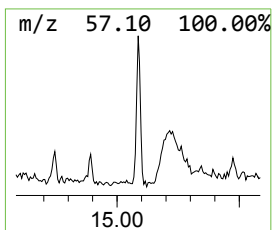
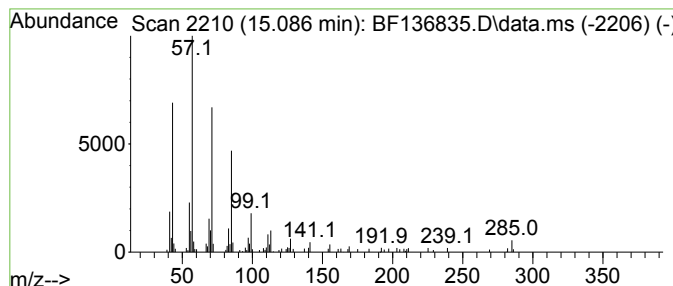
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	4.09 ng	75462	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
3			Heptacosane	380	C27H56	000593-49-7	83
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
5			Hexacosane	366	C26H54	000630-01-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136835.D
Acq On : 29 Dec 2023 18:15
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
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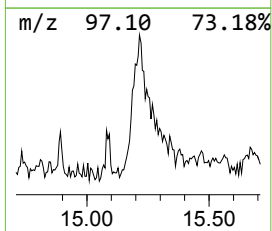
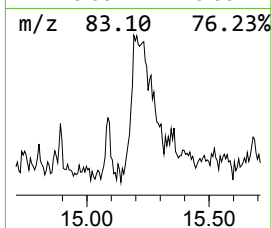
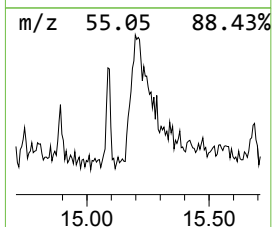
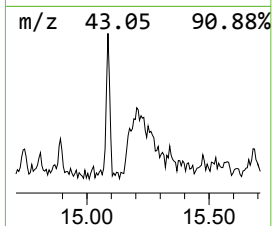
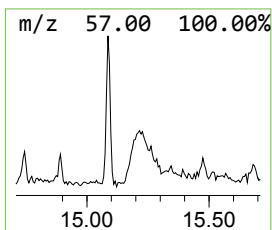
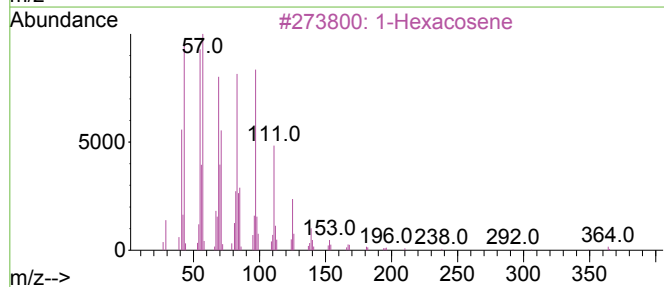
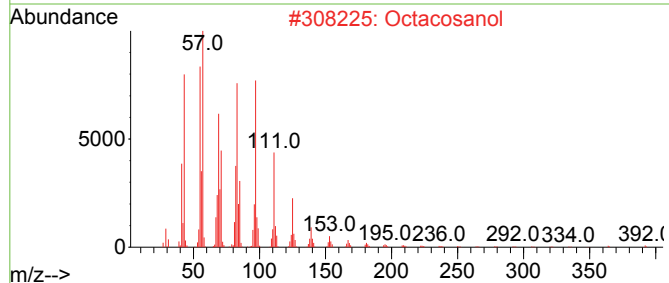
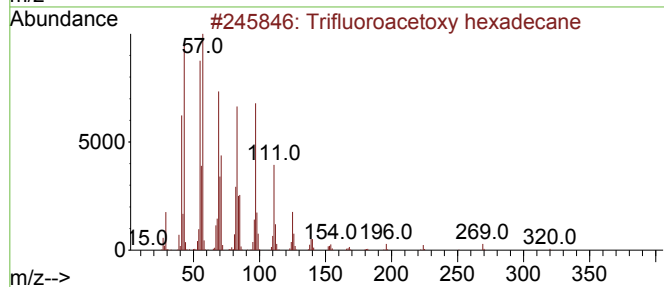
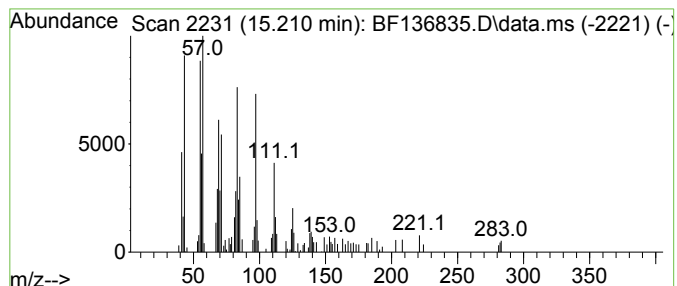
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	8.28 ng	152796	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2			Octacosanol	410	C28H58O	000557-61-9	94
3			1-Hexacosene	364	C26H52	018835-33-1	93
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136835.D
Acq On : 29 Dec 2023 18:15
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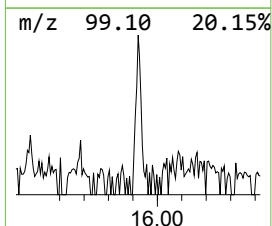
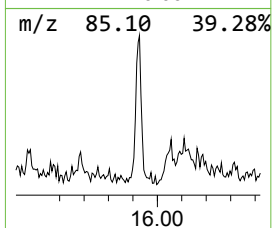
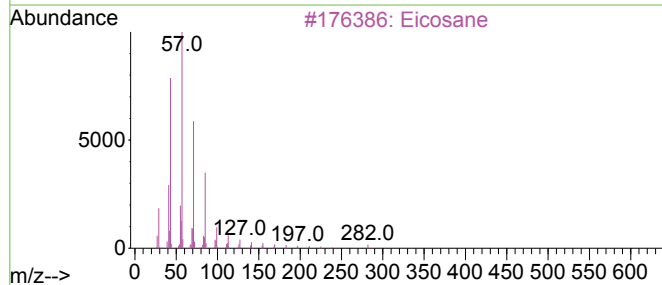
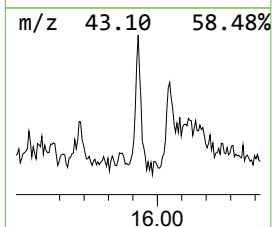
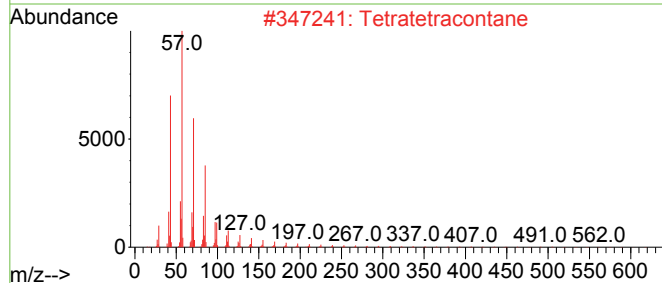
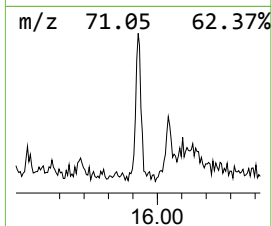
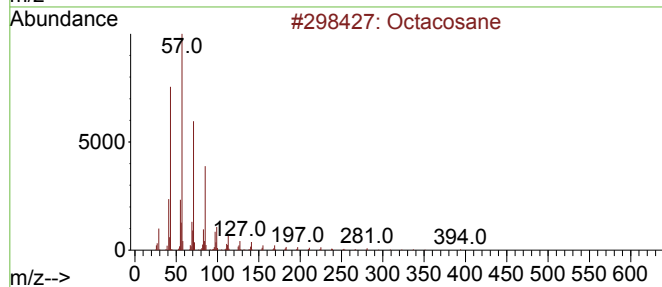
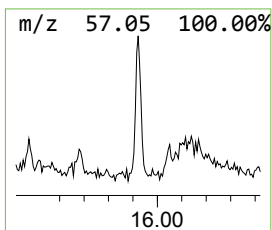
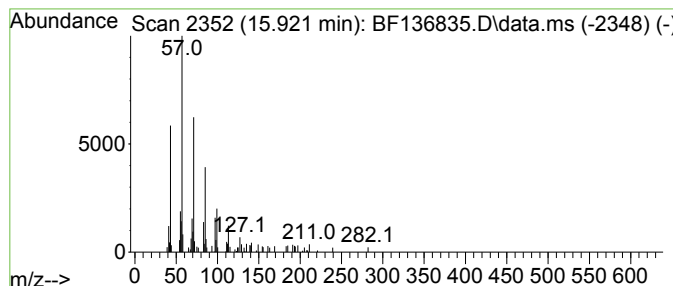
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	3.15 ng	58204	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	83
2			Tetratetracontane	619	C44H90	007098-22-8	83
3			Eicosane	282	C20H42	000112-95-8	81
4			Hentriacontane	437	C31H64	000630-04-6	74
5			Hexacosane	366	C26H54	000630-01-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136835.D
Acq On : 29 Dec 2023 18:15
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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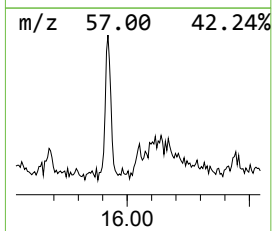
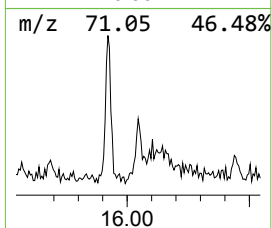
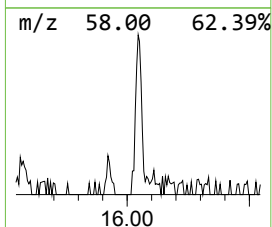
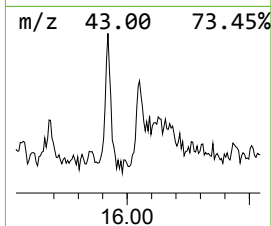
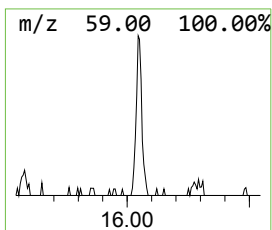
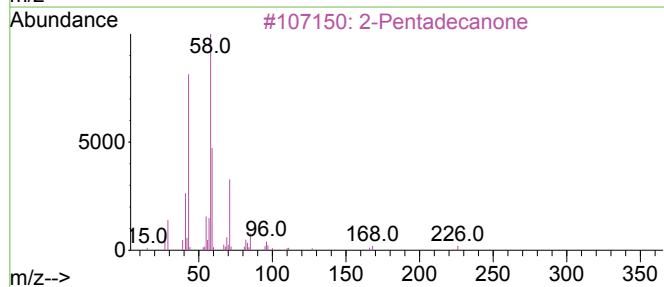
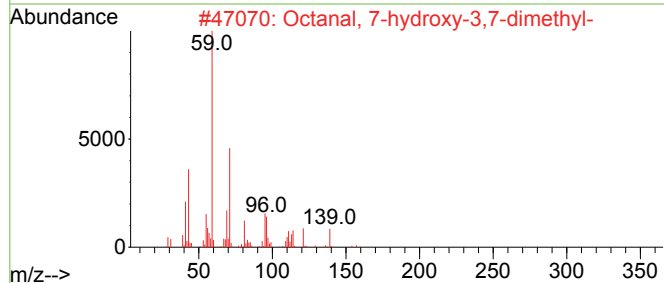
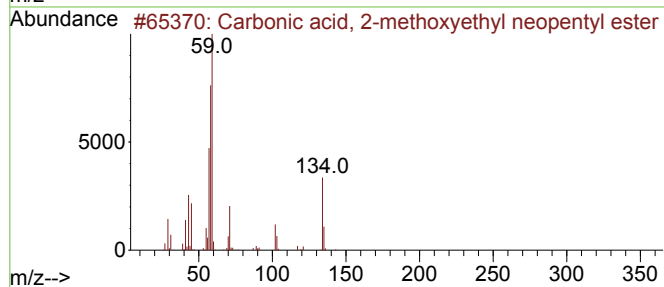
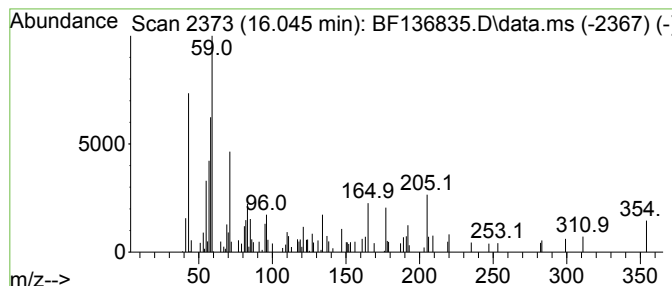
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown16.045 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.045	5.28 ng	97499	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-methoxyethyl ne...	190	C9H18O4	1000331-42-7	43
2			Octanal, 7-hydroxy-3,7-dimethyl-	172	C10H20O2	000107-75-5	35
3			2-Pentadecanone	226	C15H30O	002345-28-0	35
4			6-Hydroxy-6-methyl-2-heptanone	144	C8H16O2	1000432-37-3	35
5			2-Nonadecanone	282	C19H38O	000629-66-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136835.D
Acq On : 29 Dec 2023 18:15
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ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
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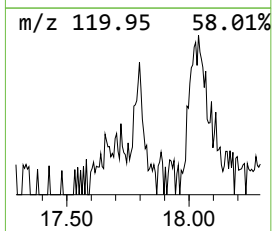
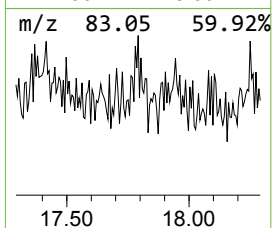
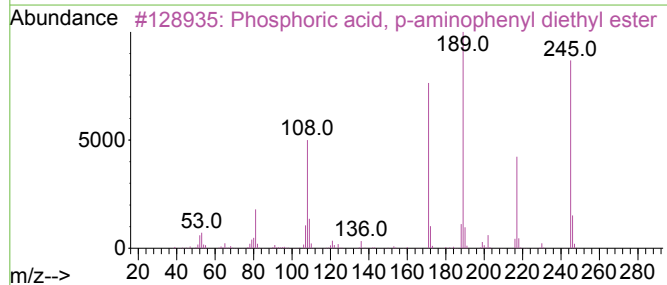
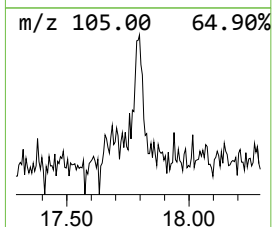
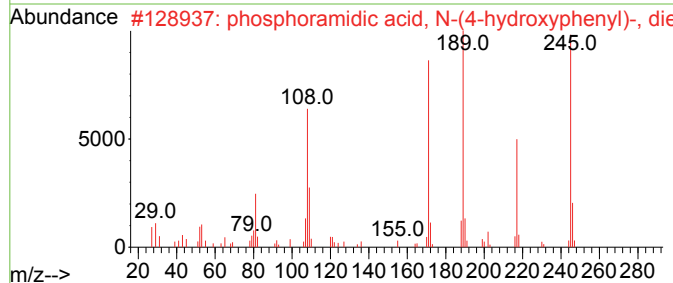
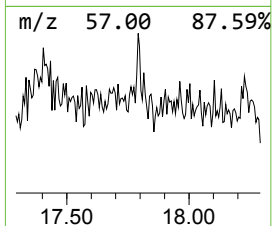
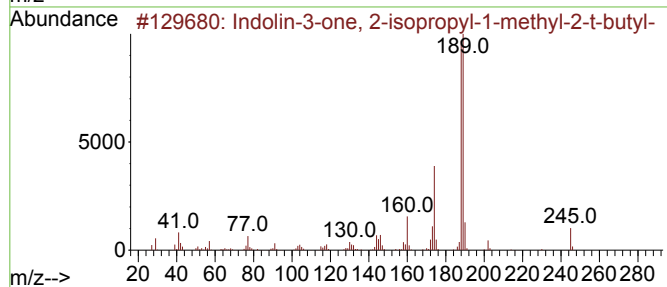
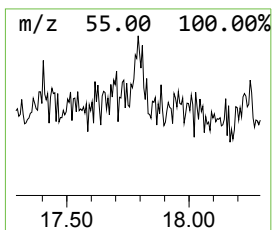
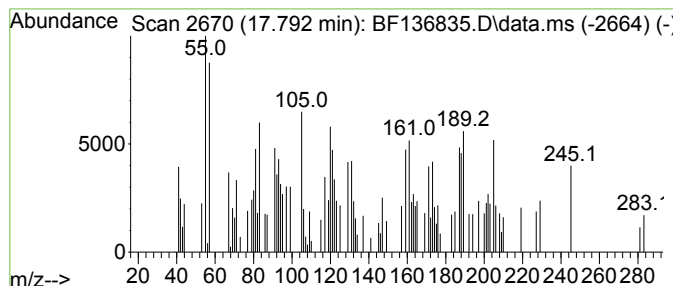
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.792 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.792	4.54 ng	83716	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indolin-3-one, 2-isopropyl-1-met...	245	C16H23NO	163064-70-8	22
2			phosphoramidic acid, N-(4-hydrox...	245	C10H16NO4P	1000401-27-7	14
3			Phosphoric acid, p-aminophenyl d...	245	C10H16NO4P	014984-58-8	14
4			4(1H)-Quinolinone, 3-methoxy-1-m...	189	C11H11NO2	052381-20-1	11
5			3-Bromo-5-cyclopropyl-1H-1,2,4-t...	187	C5H6BrN3	082767-64-4	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136835.D
Acq On : 29 Dec 2023 18:15
Operator : CG\JU
Sample : 05897-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-37a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.839	6.5	ng	195799	4	11.304	607271	20.0
unknown13.251	13.251	2.6	ng	58877	5	13.963	454506	20.0
Hexacosane	13.810	8.1	ng	185016	5	13.963	454506	20.0
1-Heneicosanol	13.880	6.3	ng	142845	5	13.963	454506	20.0
Heneicosane	14.433	7.3	ng	166726	5	13.963	454506	20.0
1-Nonadecene	14.527	3.8	ng	87023	5	13.963	454506	20.0
Hexasiloxane, t...	14.810	2.4	ng	44427	6	15.439	369029	20.0
Eicosane	15.086	4.1	ng	75462	6	15.439	369029	20.0
Trifluoroacetox...	15.210	8.3	ng	152796	6	15.439	369029	20.0
Octacosane	15.921	3.1	ng	58204	6	15.439	369029	20.0
unknown16.045	16.045	5.3	ng	97499	6	15.439	369029	20.0
unknown17.792	17.792	4.5	ng	83716	6	15.439	369029	20.0