

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
 Data File : BF125410.D
 Acq On : 9 Sep 2021 13:46
 Operator : JU/CG
 Sample : M3681-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BS-STOCK

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125410.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	12	19	37	rVB	1490542	2013792	39.98%	5.166%
2	5.516	578	583	586	rBV	4316486	4267742	84.72%	10.947%
3	6.522	748	754	757	rBV	3695787	4271741	84.80%	10.958%
4	6.881	812	815	819	rBV	1161002	1029753	20.44%	2.641%
5	7.451	906	912	915	rBV	2711749	2811587	55.82%	7.212%
6	8.069	1014	1017	1029	rBV	123669	225766	4.48%	0.579%
7	8.169	1029	1034	1037	rBV	1401912	1351632	26.83%	3.467%
8	9.245	1211	1217	1220	rBV	5006852	4712915	93.56%	12.089%
9	9.922	1327	1332	1336	rBV	1770873	1541351	30.60%	3.954%
10	10.122	1361	1366	1371	rBV3	35224	53267	1.06%	0.137%
11	10.716	1460	1467	1470	rBV	3697991	3392910	67.36%	8.703%
12	11.069	1521	1527	1537	rBV9	30542	61068	1.21%	0.157%
13	11.410	1581	1585	1589	rBV	1728716	1587581	31.52%	4.072%
14	11.933	1668	1674	1685	rBV2	690048	859381	17.06%	2.204%
15	12.080	1696	1699	1705	rVV	80639	92346	1.83%	0.237%
16	12.145	1705	1710	1725	rVB	43686	141695	2.81%	0.363%
17	12.716	1802	1807	1812	rBV	279566	297530	5.91%	0.763%
18	12.786	1812	1819	1827	rVB3	82095	232755	4.62%	0.597%
19	13.004	1850	1856	1859	rBV	4960817	5037323	100.00%	12.921%
20	13.610	1953	1959	1966	rVB2	133295	266016	5.28%	0.682%
21	13.845	1994	1999	2002	rBV	50607	64918	1.29%	0.167%
22	13.886	2002	2006	2008	rVV2	88424	114325	2.27%	0.293%
23	13.915	2008	2011	2026	rVB2	333113	639019	12.69%	1.639%
24	14.057	2031	2035	2038	rVB	1451061	1282490	25.46%	3.290%
25	14.210	2057	2061	2062	rBV	47522	51465	1.02%	0.132%
26	14.233	2062	2065	2072	rVB	159448	243373	4.83%	0.624%
27	14.510	2104	2112	2116	rBV	64747	89759	1.78%	0.230%
28	14.768	2151	2156	2161	rBV	153605	254118	5.04%	0.652%
29	14.821	2161	2165	2171	rVB	74833	93049	1.85%	0.239%
30	14.904	2175	2179	2181	rBV	52622	55396	1.10%	0.142%
31	15.168	2221	2224	2231	rVB	55334	72301	1.44%	0.185%
32	15.351	2249	2255	2263	rVB	125561	223184	4.43%	0.572%
33	15.545	2283	2288	2296	rVB	791458	1059939	21.04%	2.719%
34	16.004	2361	2366	2374	rVB	109399	206957	4.11%	0.531%
35	16.762	2489	2495	2502	rBV4	44456	107476	2.13%	0.276%
36	17.174	2562	2565	2575	rVB4	41775	101366	2.01%	0.260%

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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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.656	2643	2647	2654	rVB3	35251	77227	1.53%	0.198%
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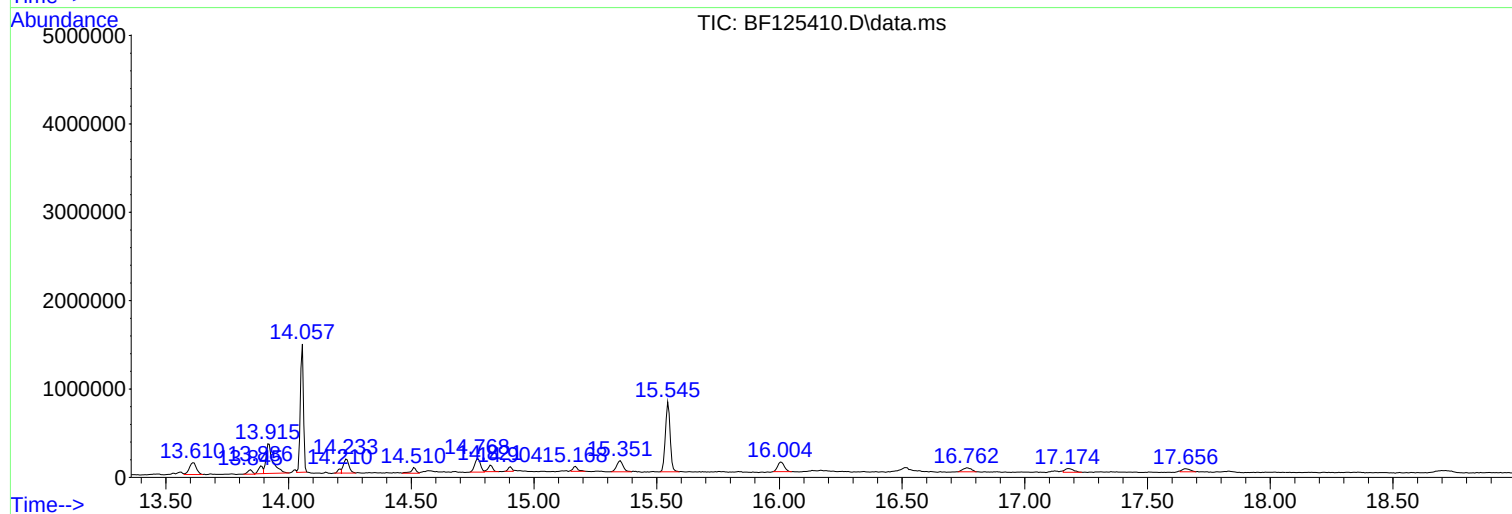
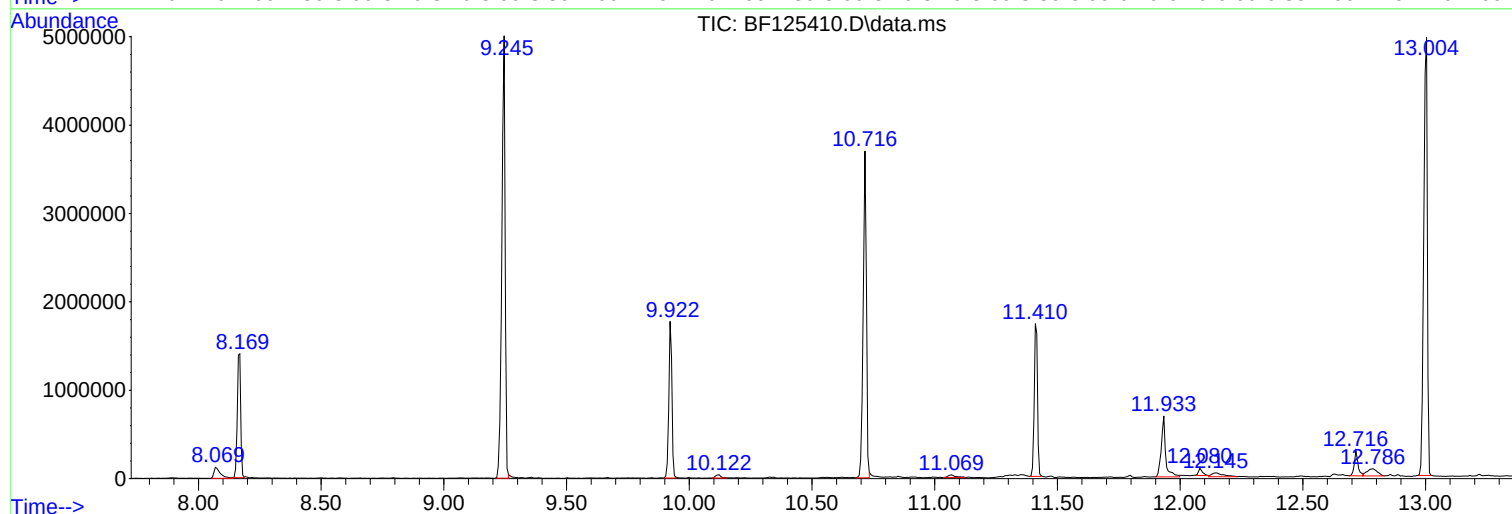
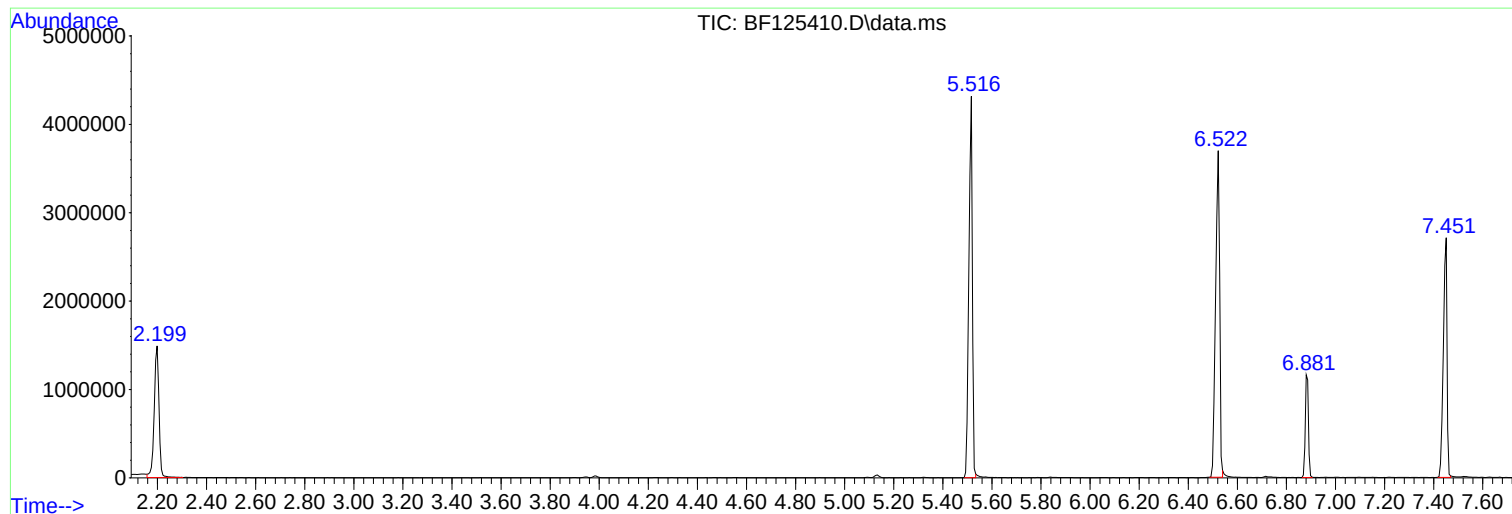
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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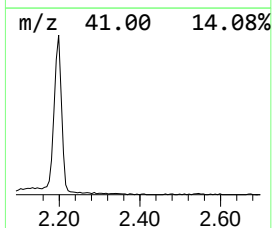
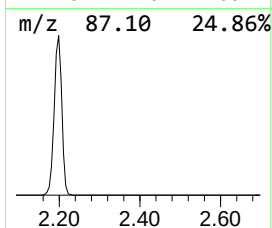
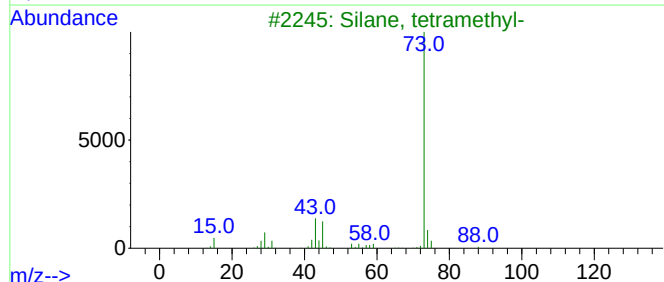
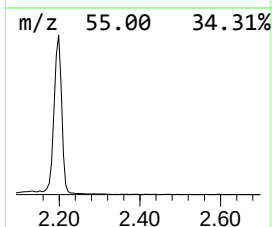
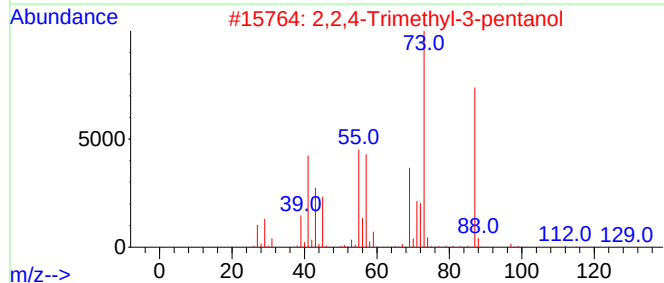
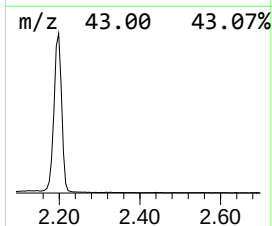
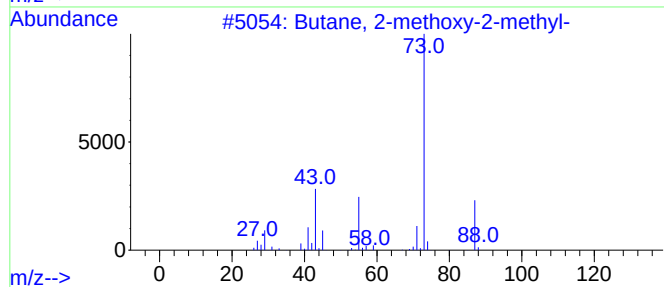
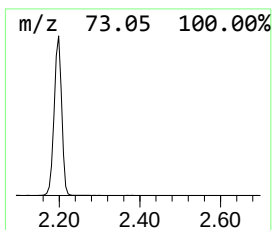
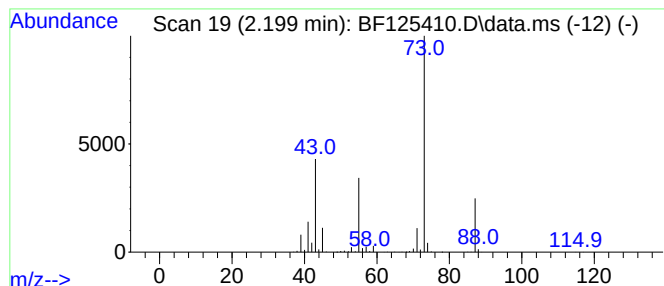
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.199	39.11 ng	2013790	1,4-Dichlorobenzene-d4	6.886

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	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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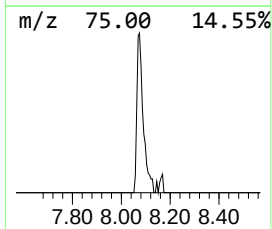
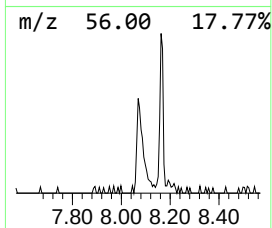
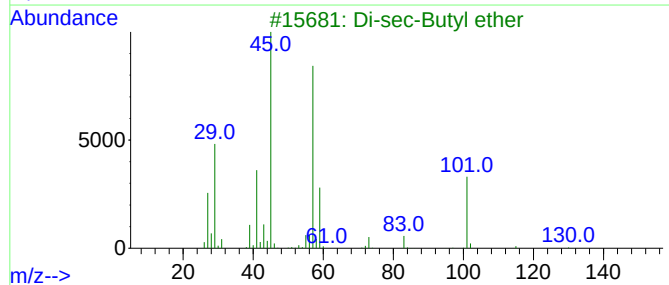
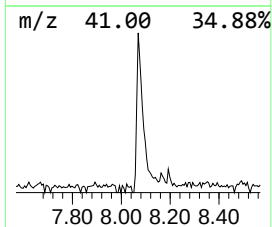
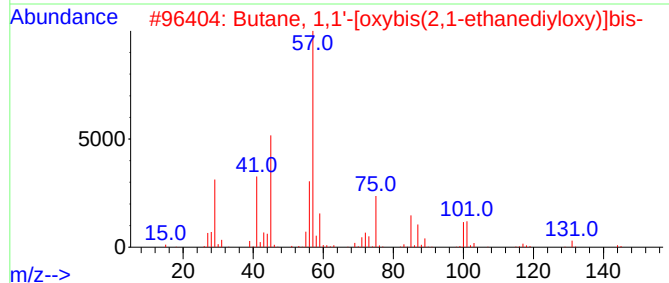
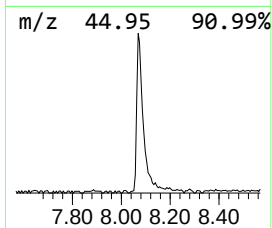
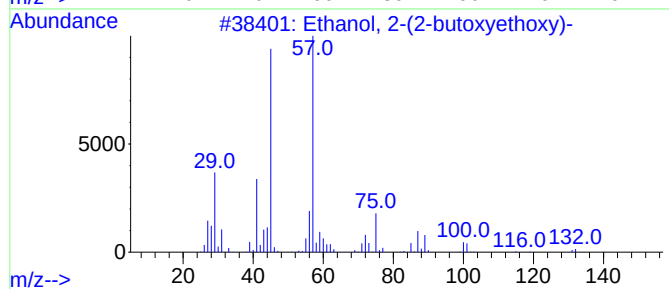
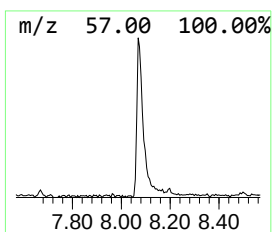
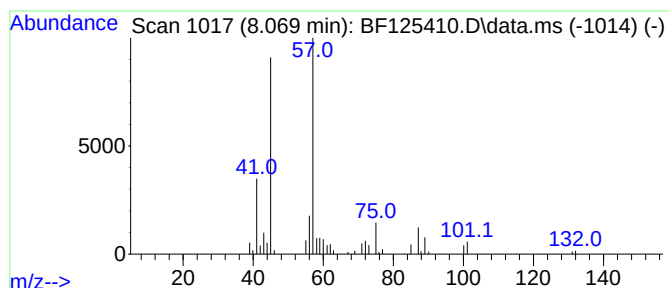
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.069	3.34 ng	225766	Naphthalene-d8	8.169	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	56
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47



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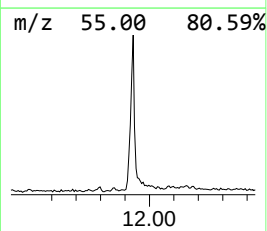
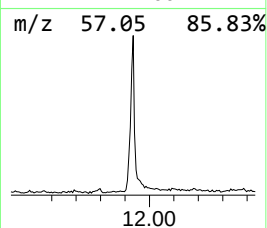
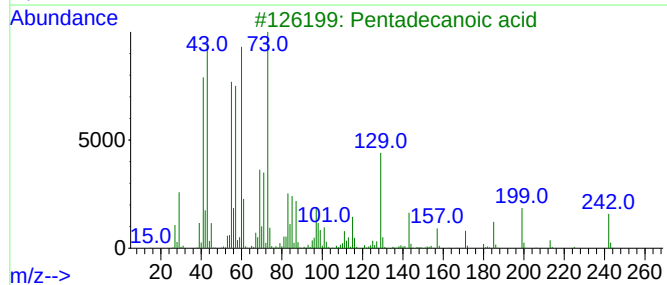
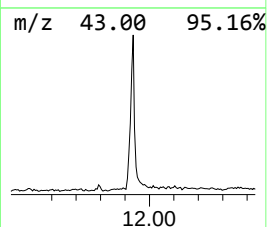
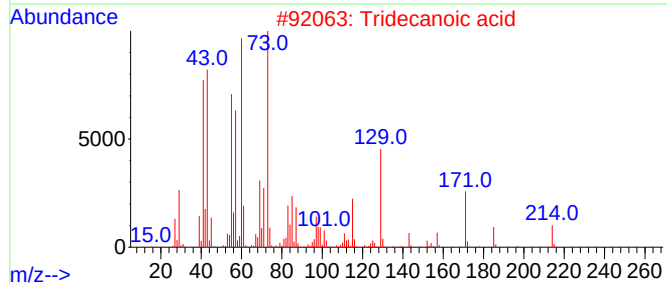
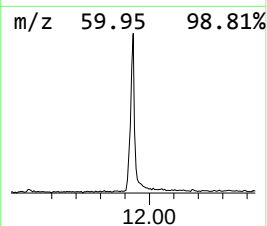
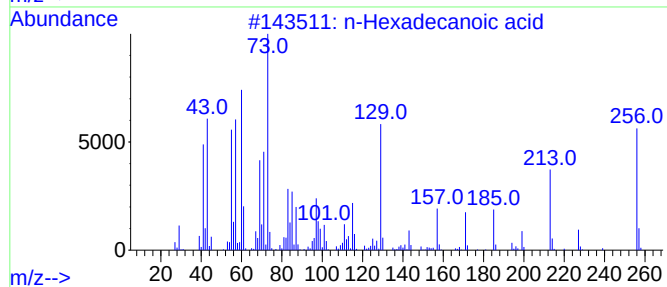
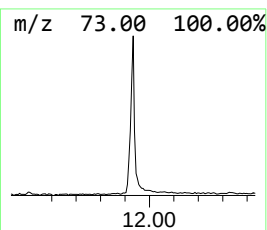
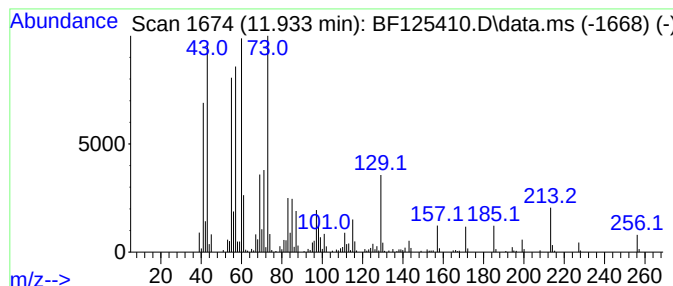
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	10.83 ng	859381	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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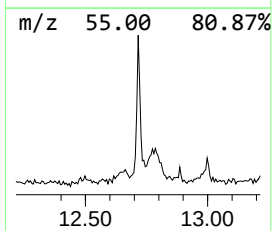
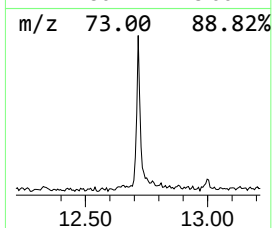
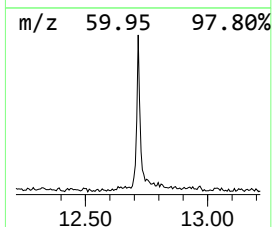
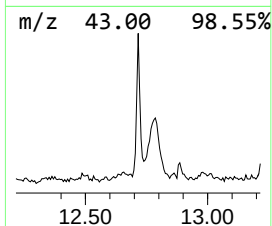
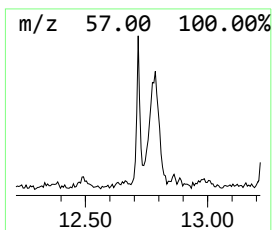
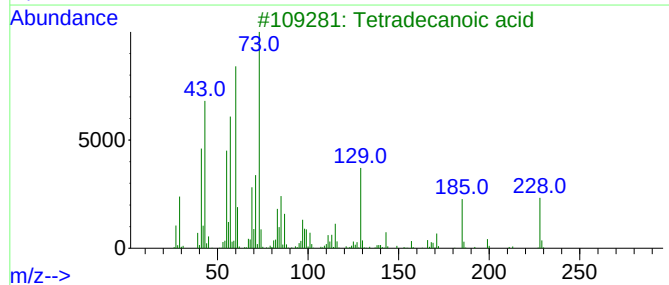
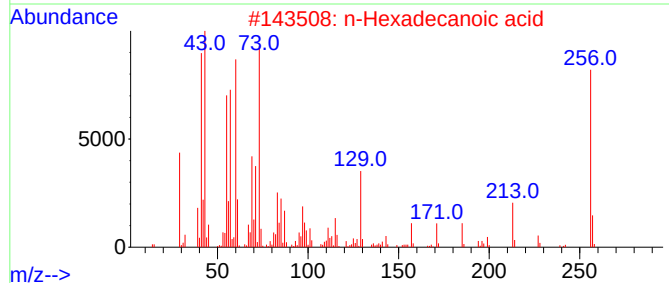
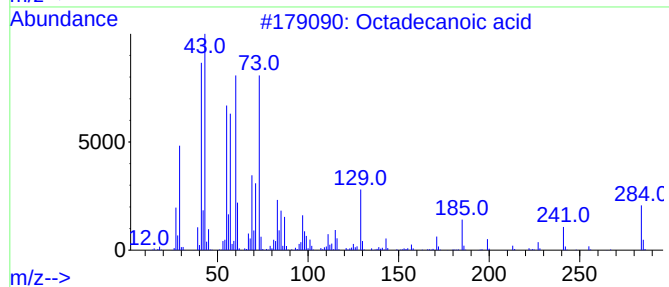
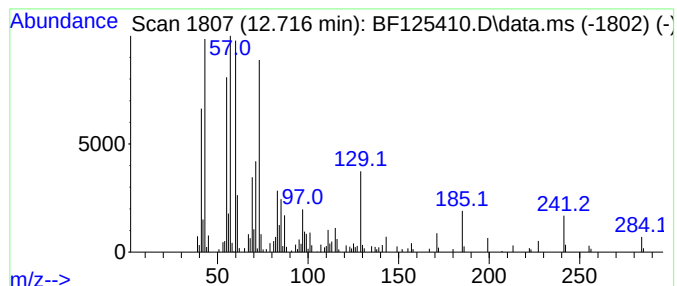
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	3.75 ng	297530	Phenanthrene-d10	11.410

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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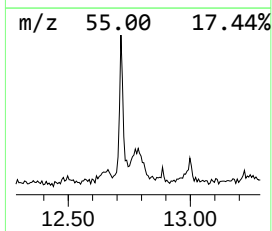
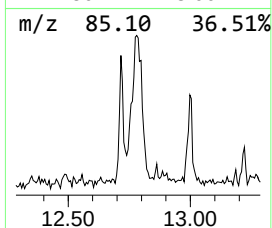
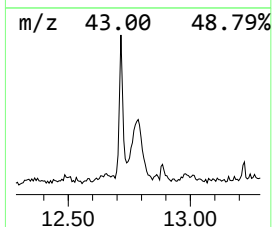
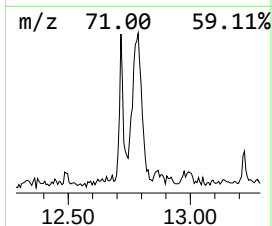
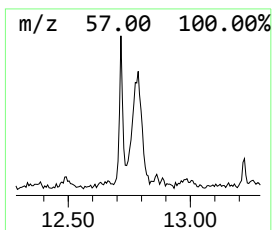
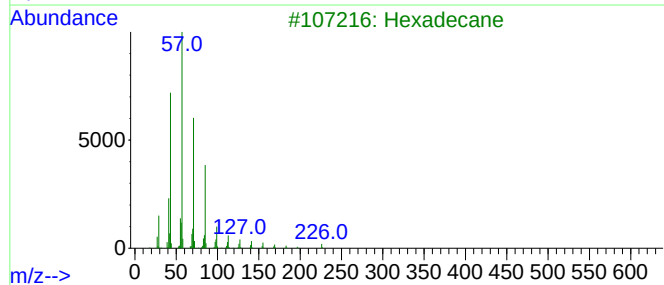
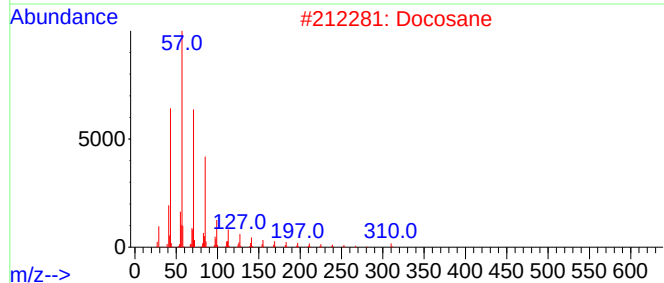
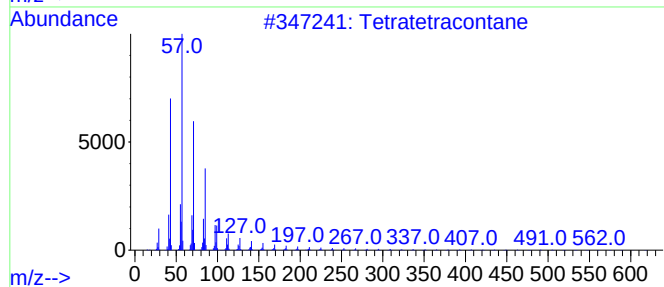
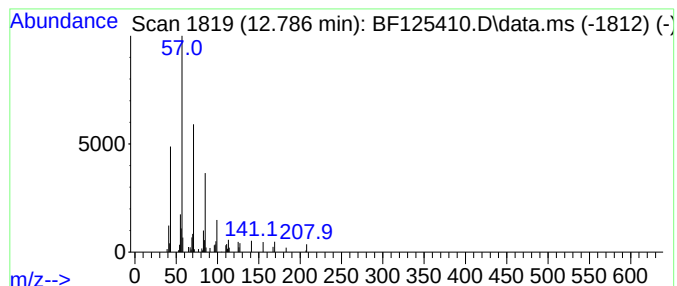
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetratetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	3.63 ng	232755	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	86
2			Docosane	310	C22H46	000629-97-0	86
3			Hexadecane	226	C16H34	000544-76-3	86
4			Heptacosane	380	C27H56	000593-49-7	86
5			Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125410.D
Acq On : 9 Sep 2021 13:46
Operator : JU/CG
Sample : M3681-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BS-STOCK

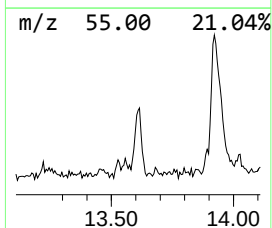
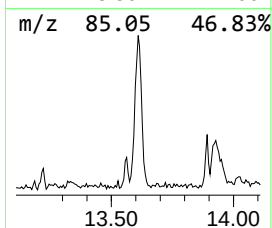
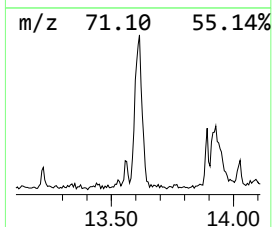
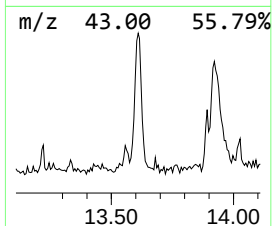
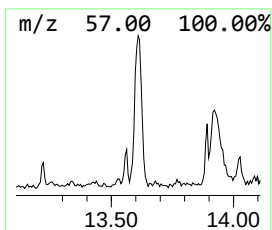
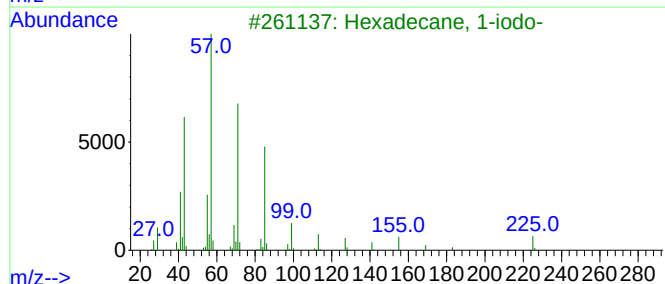
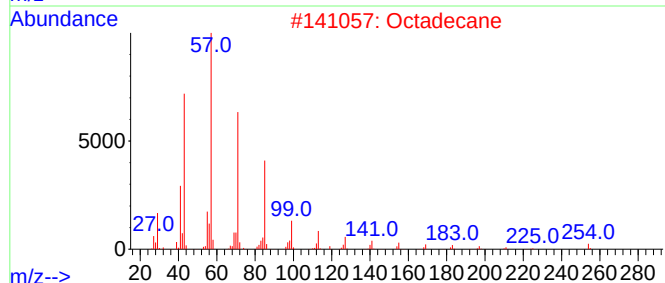
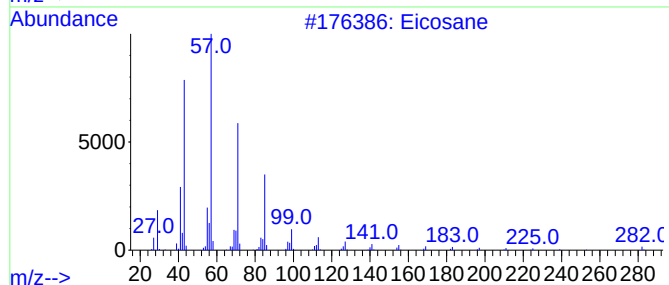
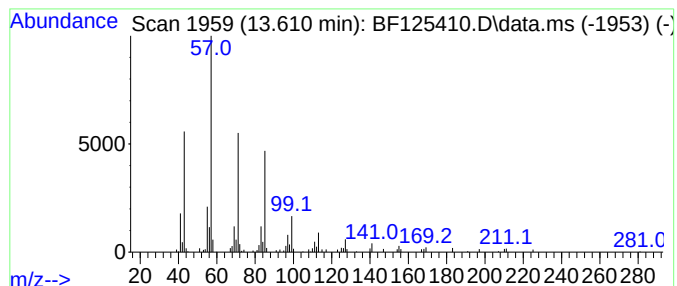
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.610	4.15 ng	266016	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	87
2			Octadecane	254	C18H38	000593-45-3	87
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
4			Hentriacontane	437	C31H64	000630-04-6	81
5			Heptacosane	380	C27H56	000593-49-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125410.D
Acq On : 9 Sep 2021 13:46
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Sample : M3681-01
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ALS Vial : 7 Sample Multiplier: 1

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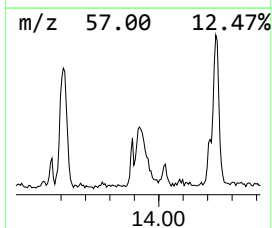
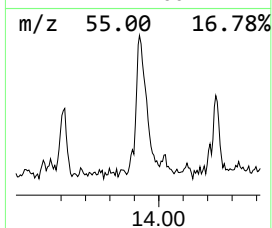
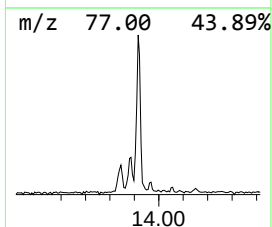
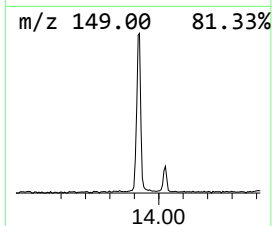
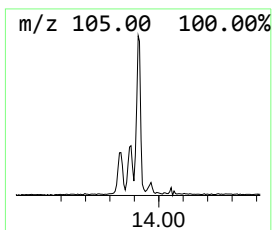
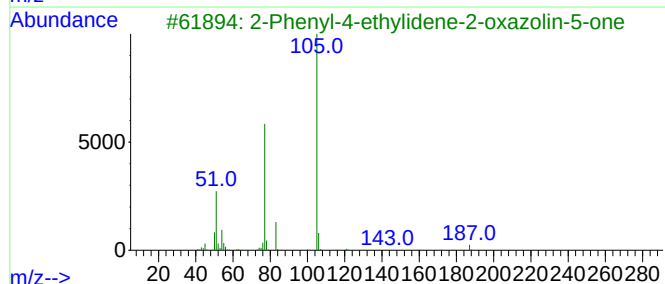
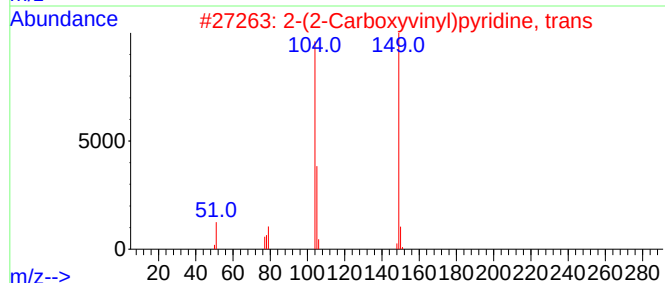
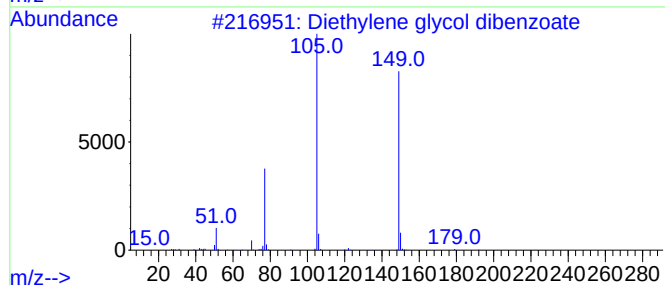
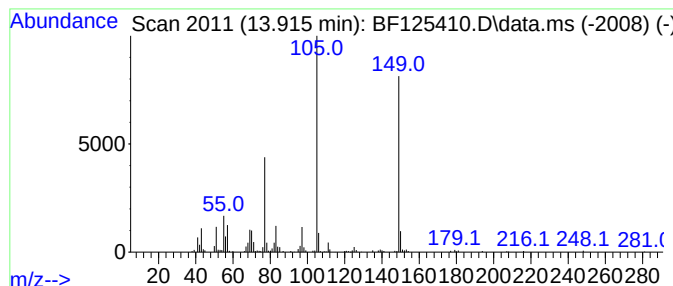
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	9.97 ng	639019	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	43
3			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	22
4			N-(Methoxymethyl)benzamide	165	C9H11NO2	013156-28-0	22
5			E-2-Hexenyl benzoate	204	C13H16O2	076841-70-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125410.D
Acq On : 9 Sep 2021 13:46
Operator : JU/CG
Sample : M3681-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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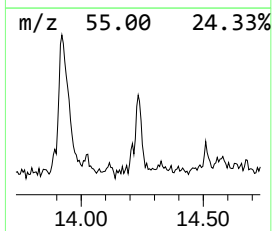
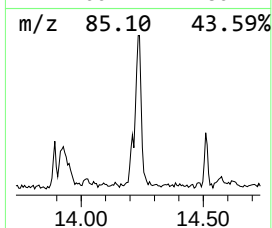
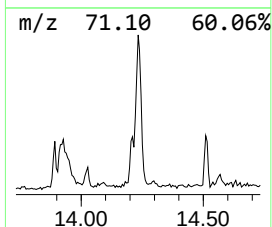
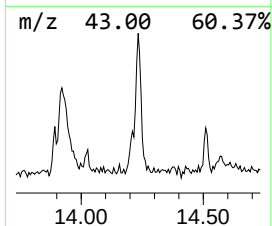
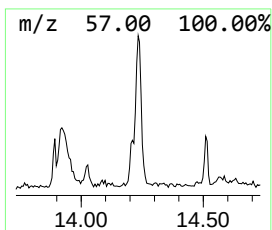
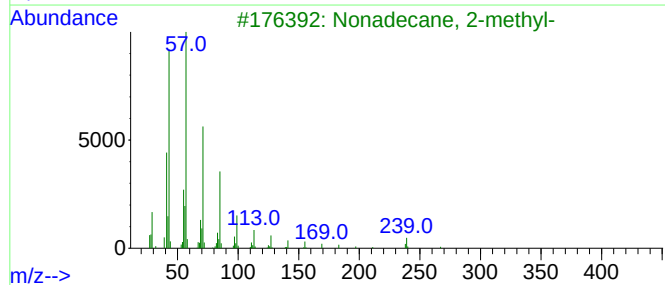
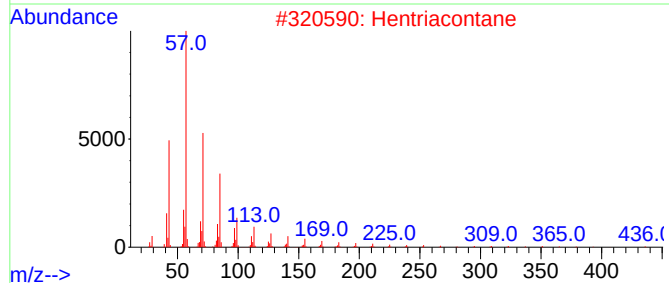
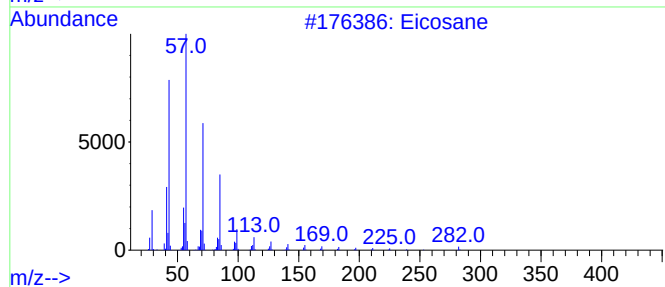
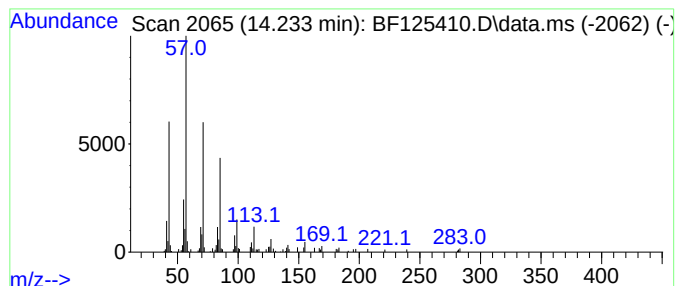
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	3.80 ng	243373	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	97
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125410.D
Acq On : 9 Sep 2021 13:46
Operator : JU/CG
Sample : M3681-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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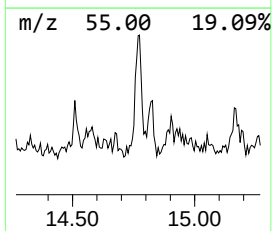
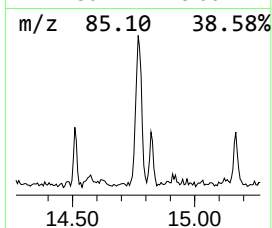
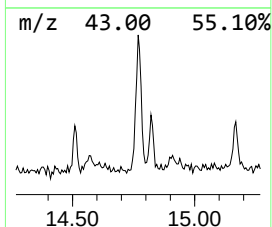
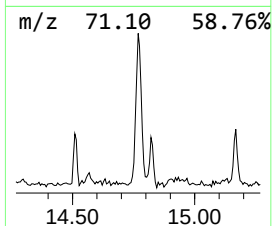
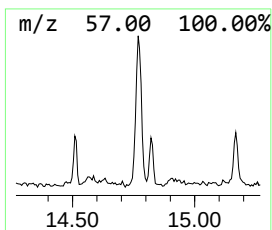
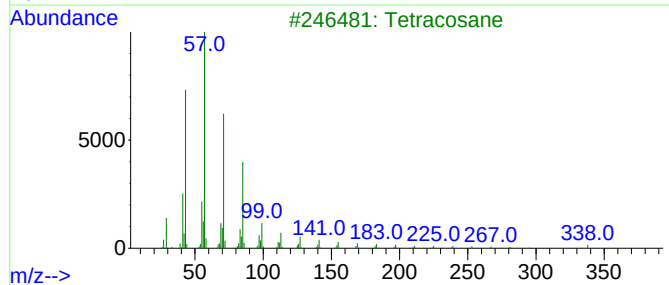
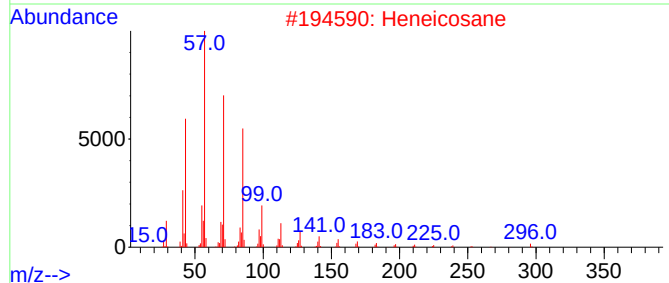
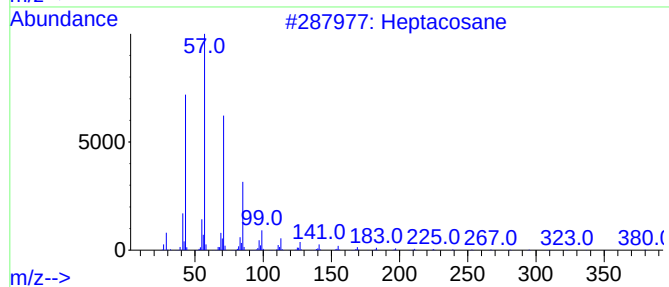
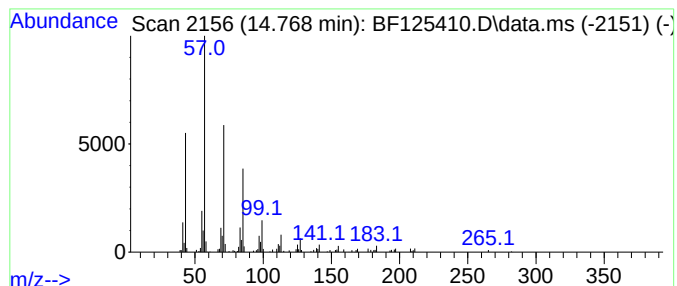
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	3.96 ng	254118	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Tetracosane	338	C24H50	000646-31-1	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Pentacosane	352	C25H52	000629-99-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125410.D
Acq On : 9 Sep 2021 13:46
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Sample : M3681-01
Misc :
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Instrument :
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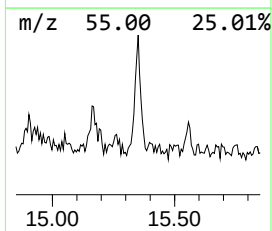
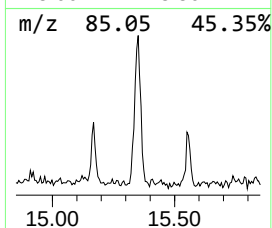
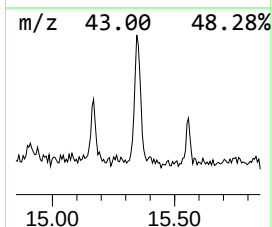
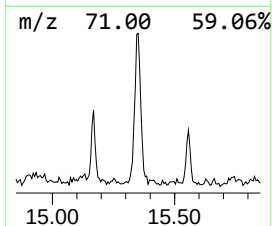
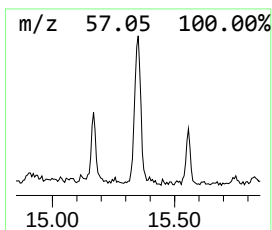
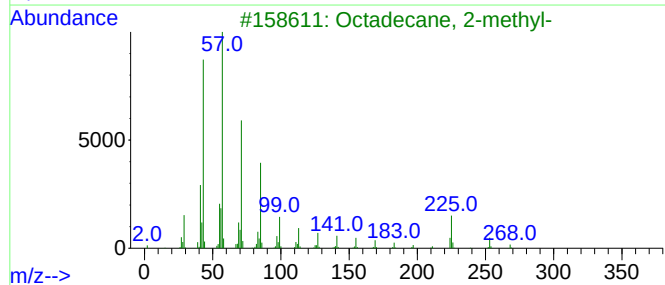
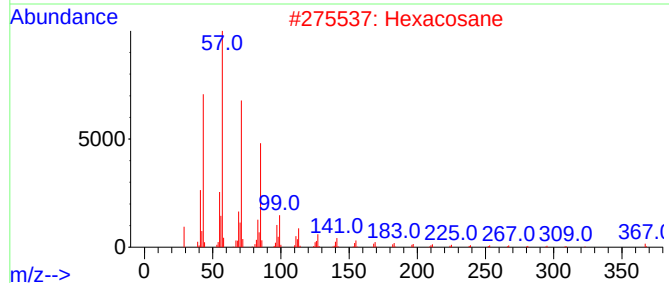
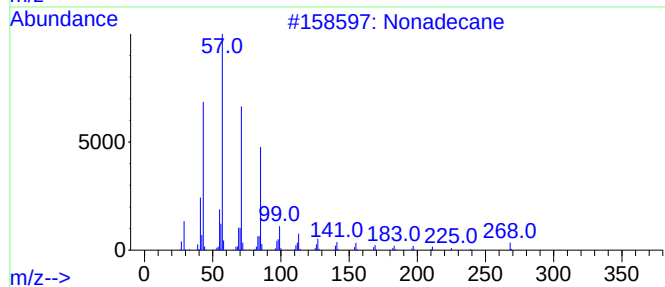
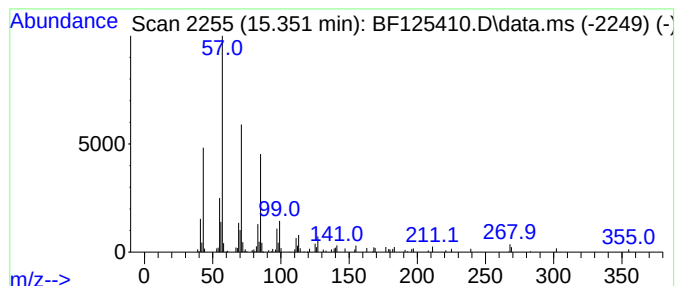
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	4.21 ng	223184	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	96
2			Hexacosane	366	C26H54	000630-01-3	90
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
4			Octacosane	394	C28H58	000630-02-4	87
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125410.D
Acq On : 9 Sep 2021 13:46
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Sample : M3681-01
Misc :
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Instrument :
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ClientSampled :
BS-STOCK

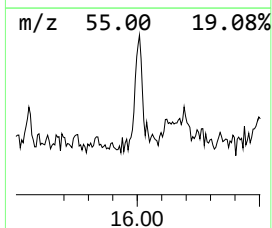
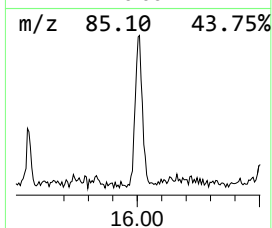
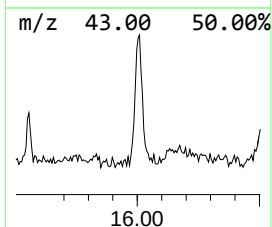
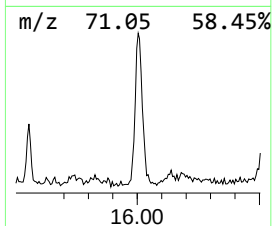
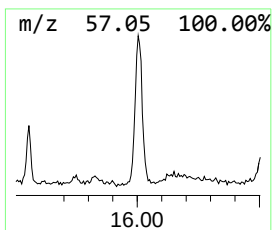
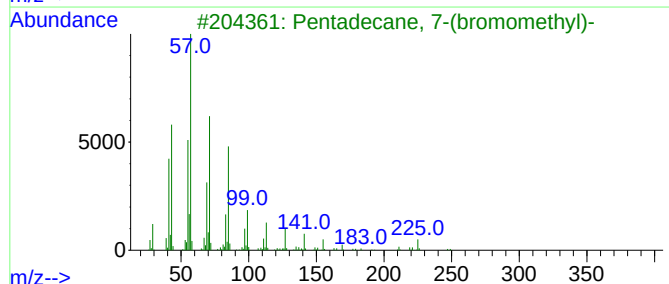
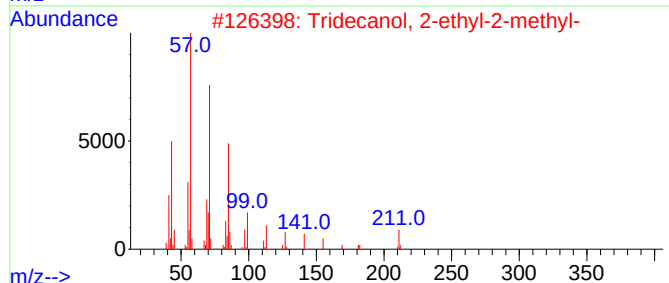
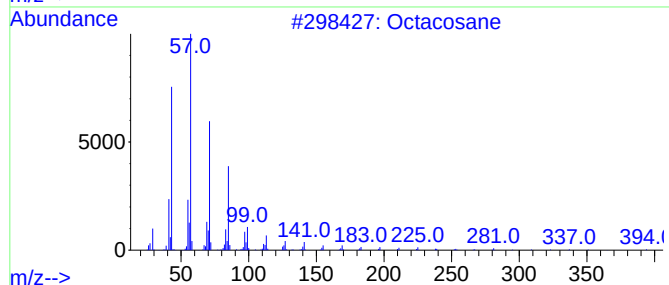
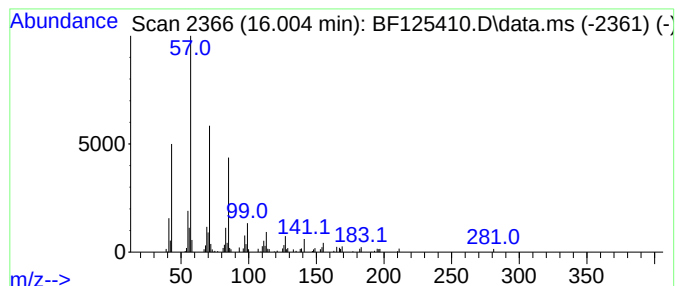
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.003	3.91 ng	206957	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	91
3			Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	91
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
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Sample : M3681-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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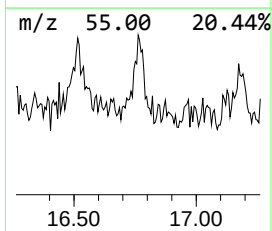
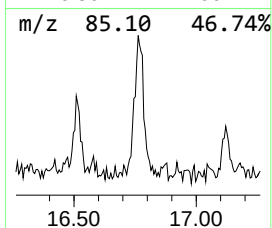
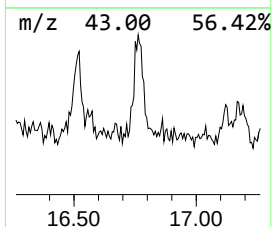
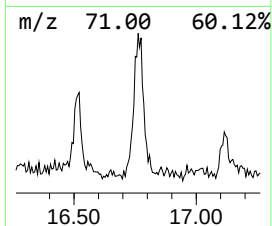
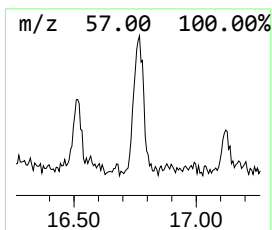
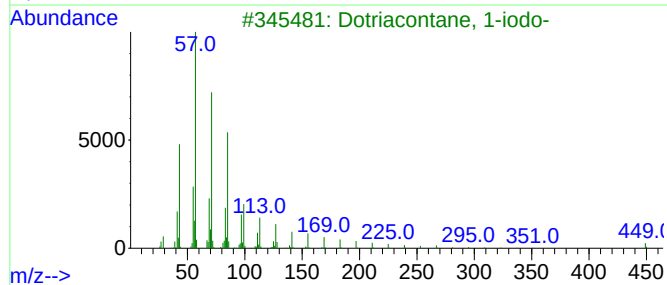
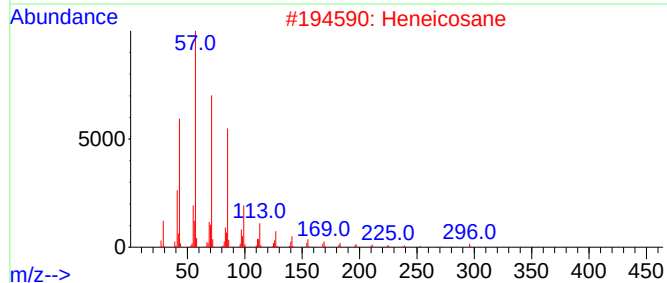
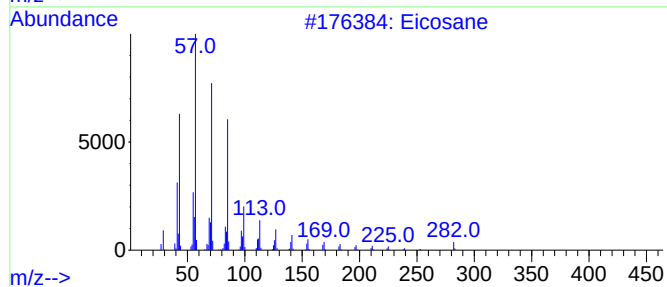
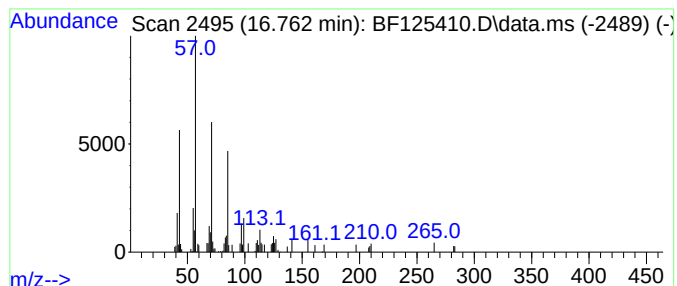
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	2.03 ng	107476	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Heneicosane	296	C21H44	000629-94-7	83
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	80
4			Hentriacontane	437	C31H64	000630-04-6	80
5			Triacontane	422	C30H62	000638-68-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125410.D
Acq On : 9 Sep 2021 13:46
Operator : JU/CG
Sample : M3681-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BS-STOCK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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
Butane, 2-metho...	2.199	39.1	ng	2013790	1	6.886	1029750	20.0
Ethanol, 2-(2-b...	8.069	3.3	ng	225766	2	8.169	1351630	20.0
n-Hexadecanoic ...	11.933	10.8	ng	859381	4	11.410	1587580	20.0
Octadecanoic acid	12.716	3.8	ng	297530	4	11.410	1587580	20.0
Tetratetracontane	12.786	3.6	ng	232755	5	14.057	1282490	20.0
Octadecane	13.610	4.2	ng	266016	5	14.057	1282490	20.0
Diethylene glyc...	13.915	10.0	ng	639019	5	14.057	1282490	20.0
Eicosane	14.233	3.8	ng	243373	5	14.057	1282490	20.0
Heptacosane	14.768	4.0	ng	254118	5	14.057	1282490	20.0
Nonadecane	15.351	4.2	ng	223184	6	15.545	1059940	20.0
Octacosane	16.003	3.9	ng	206957	6	15.545	1059940	20.0
Heneicosane	16.762	2.0	ng	107476	6	15.545	1059940	20.0