

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062219\
 Data File : BF115128.D
 Acq On : 22 Jun 2019 18:37
 Operator : HP/JU
 Sample : K3470-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-4

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF062119.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.495	254	265	273	rVB	107603	187818	4.46%	0.419%
2	4.460	424	429	433	rVB	101598	123368	2.93%	0.275%
3	5.207	551	556	559	rBV	3645731	3496080	83.02%	7.805%
4	6.242	727	732	735	rBV	3588253	3678182	87.34%	8.211%
5	6.284	735	739	744	rVB	75313	73845	1.75%	0.165%
6	6.378	750	755	758	rBV	4255936	3847720	91.37%	8.590%
7	6.613	791	795	798	rBV	1931277	1681691	39.93%	3.754%
8	6.766	817	821	824	rBV	3659694	3047156	72.36%	6.803%
9	7.166	884	889	892	rBV	2396596	2348014	55.75%	5.242%
10	7.413	928	931	935	rVB	50464	51500	1.22%	0.115%
11	7.889	1008	1012	1015	rBV	2806245	2226276	52.86%	4.970%
12	8.336	1084	1088	1094	rBV2	53460	68878	1.64%	0.154%
13	8.966	1191	1195	1198	rBV	4768026	4206990	99.90%	9.392%
14	9.360	1258	1262	1265	rBV	667642	530084	12.59%	1.183%
15	9.636	1305	1309	1313	rBV	2989814	2522883	59.91%	5.632%
16	9.907	1352	1355	1360	rBV	48059	53653	1.27%	0.120%
17	10.413	1437	1441	1444	rBV	2860331	2360712	56.06%	5.270%
18	11.107	1555	1559	1562	rBV	3216144	2693749	63.96%	6.014%
19	11.654	1650	1652	1660	rBV2	197775	215122	5.11%	0.480%
20	12.307	1760	1763	1766	rBV	142294	111797	2.65%	0.250%
21	12.365	1770	1773	1777	rVV3	56824	66713	1.58%	0.149%
22	12.436	1781	1785	1793	rBV	236619	328724	7.81%	0.734%
23	12.530	1797	1801	1804	rVB	142019	138507	3.29%	0.309%
24	12.689	1824	1828	1831	rBV	4816413	4211326	100.00%	9.401%
25	13.607	1980	1984	1991	rBV2	425917	566706	13.46%	1.265%
26	13.724	1999	2004	2007	rBV	2190710	1992792	47.32%	4.449%
27	13.930	2036	2039	2044	rBV	134681	128711	3.06%	0.287%
28	14.236	2088	2091	2101	rBV2	388469	539244	12.80%	1.204%
29	14.530	2137	2141	2144	rBV	242454	240936	5.72%	0.538%
30	14.712	2169	2172	2174	rBV	39841	46709	1.11%	0.104%
31	14.830	2188	2192	2198	rBV	271784	301076	7.15%	0.672%
32	15.083	2230	2235	2245	rBV	1642811	1898438	45.08%	4.238%
33	15.165	2245	2249	2256	rVB	227629	289613	6.88%	0.647%
34	15.548	2310	2314	2319	rBV	181788	280464	6.66%	0.626%

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.989	2385	2389	2397	rVB2	94798	161736	3.84%	0.361%
36	16.501	2473	2476	2482	rVB	47379	77142	1.83%	0.172%

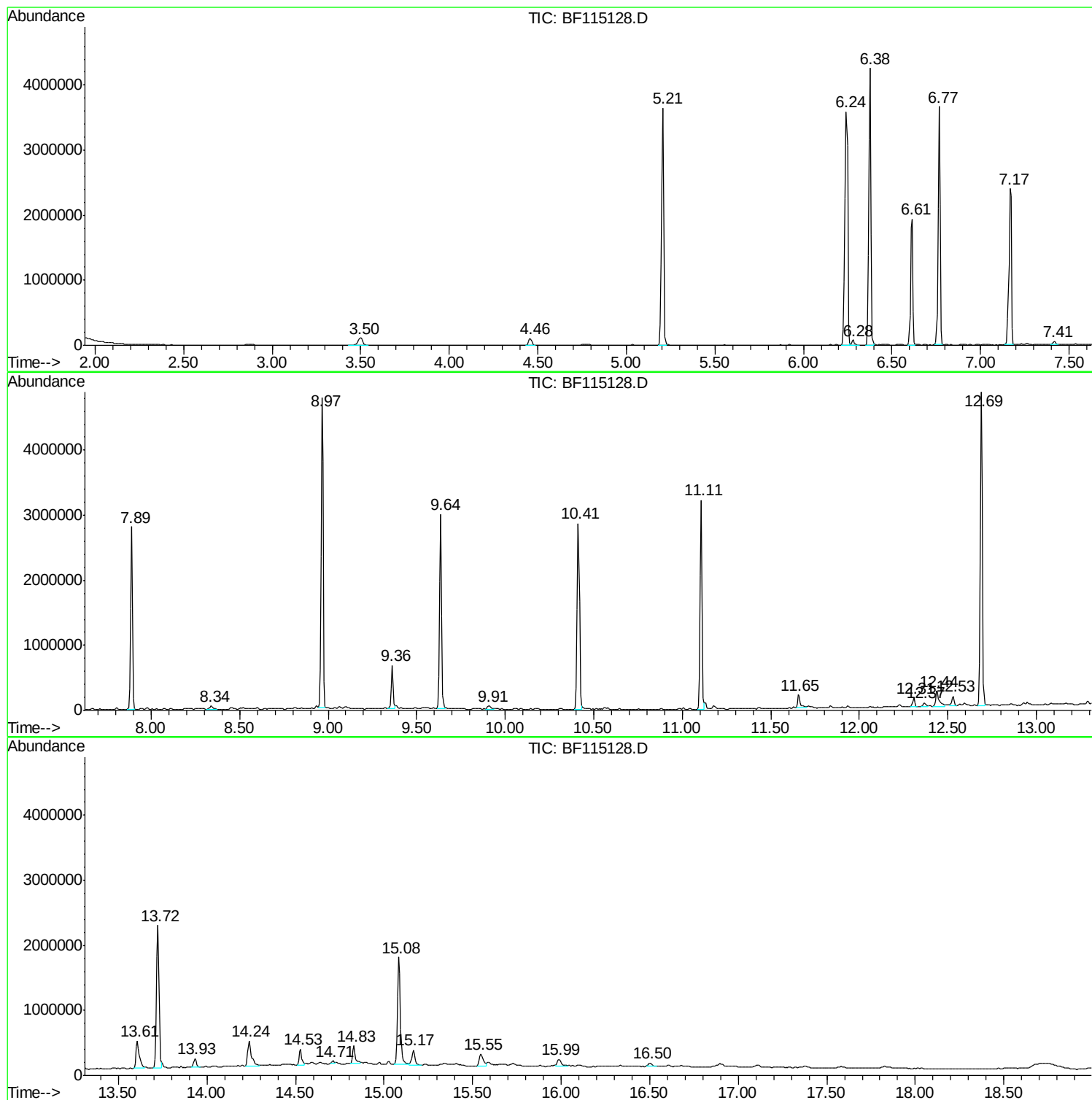
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF062119.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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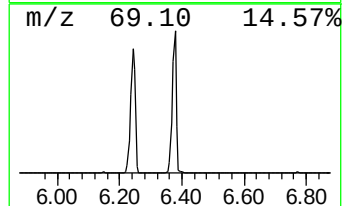
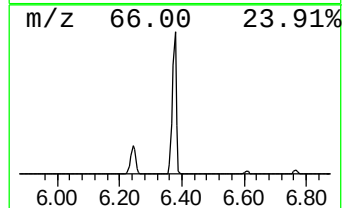
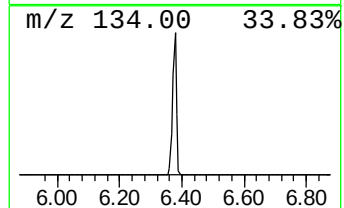
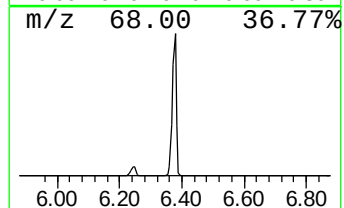
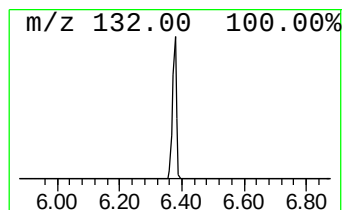
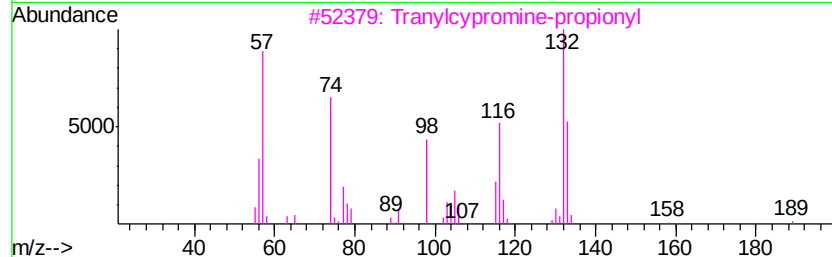
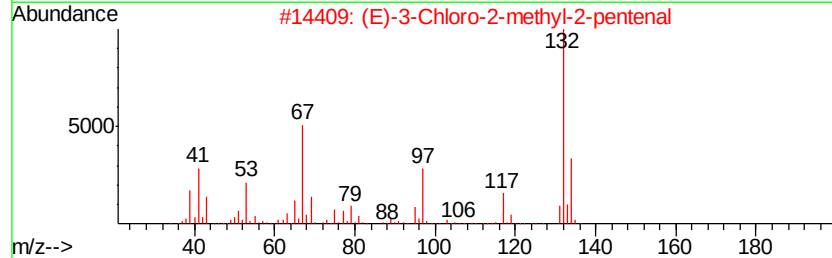
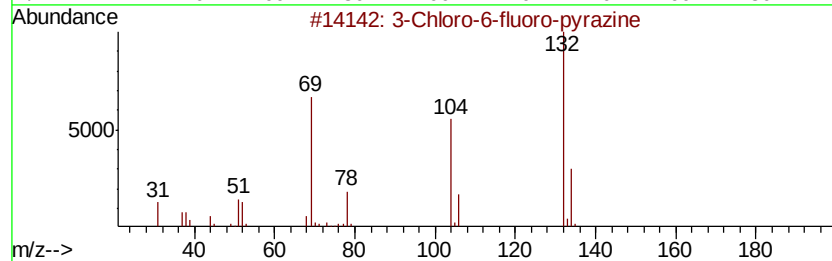
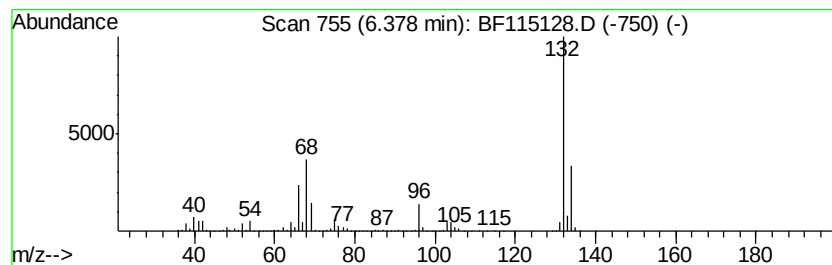
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF062119.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	45.76 ng	3847720	1,4-Dichlorobenzene-d4	6.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		2H-Cyclopentaf[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9



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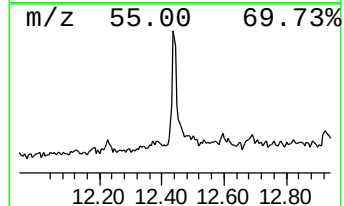
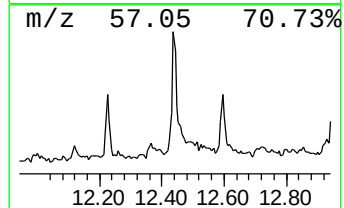
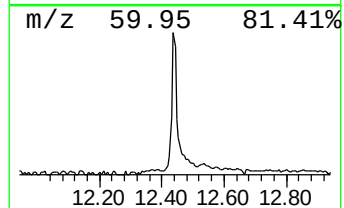
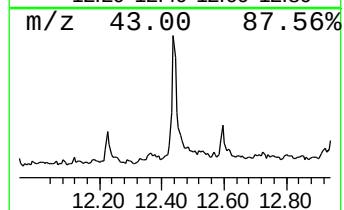
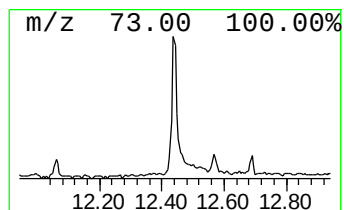
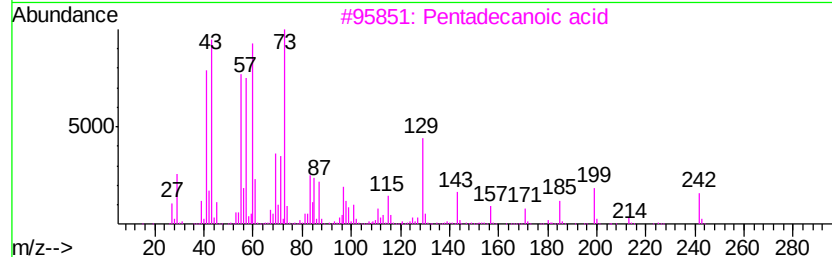
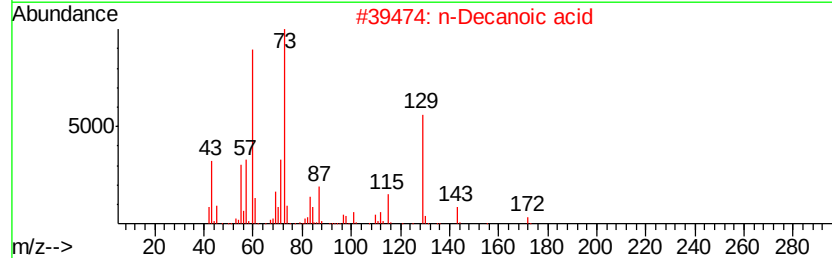
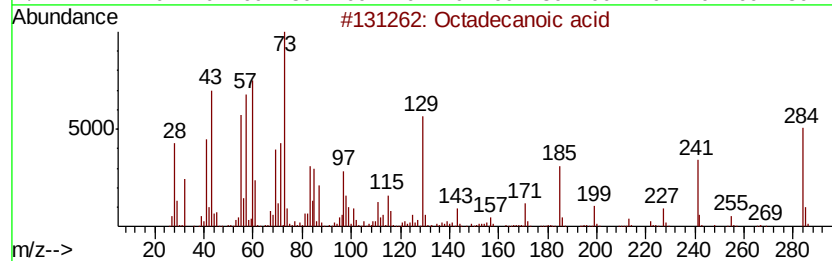
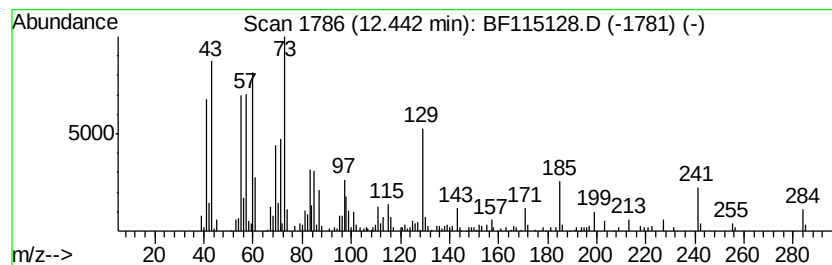
Instrument :
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ClientSampleId :
SAMPLE-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF062119.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.44	3.30 ng	328724	Chrysene-d12	13.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	87
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83



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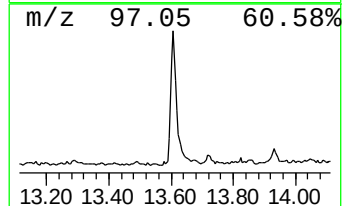
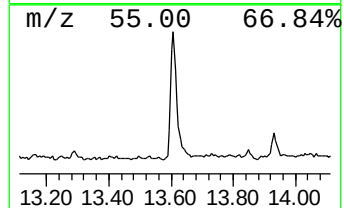
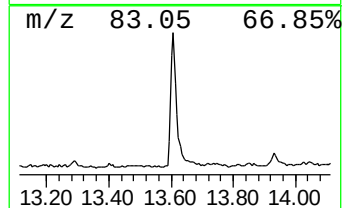
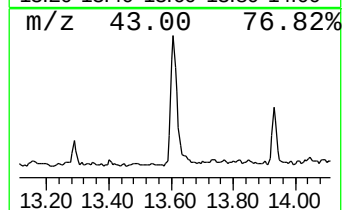
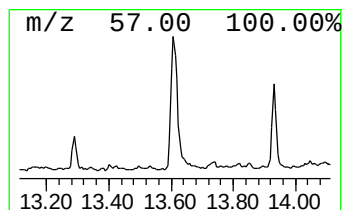
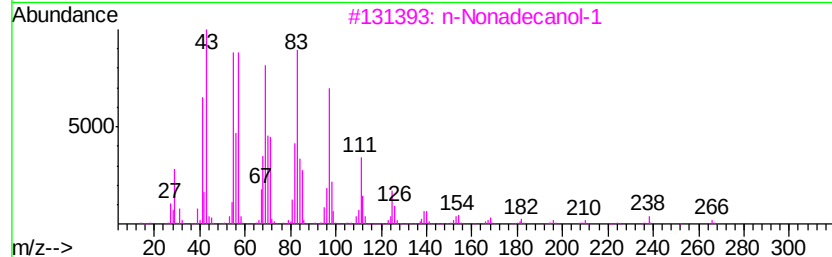
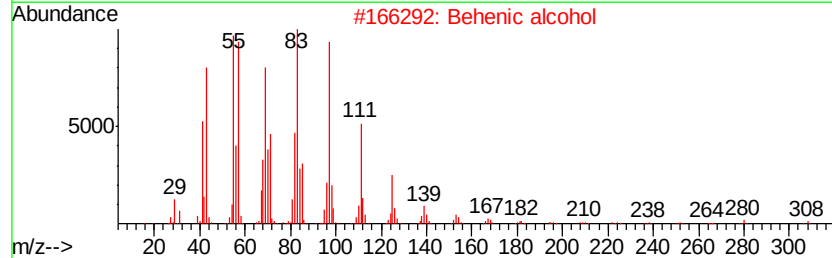
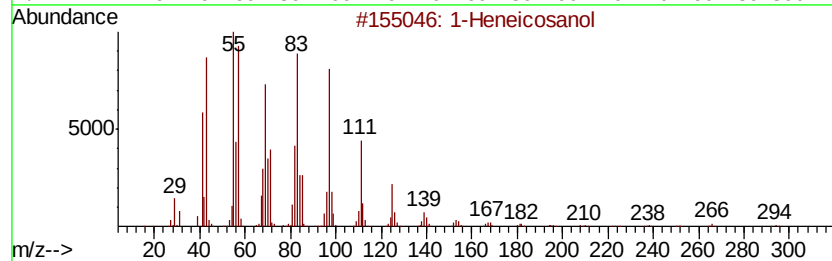
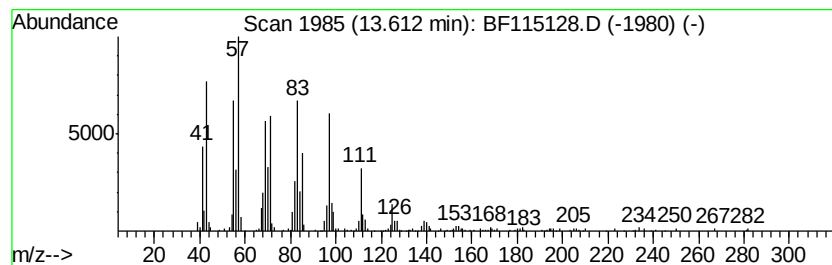
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.61	5.69 ng	566706	Chrysene-d12		13.72
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Cyclopentadecane	210	C15H30	000295-48-7	93



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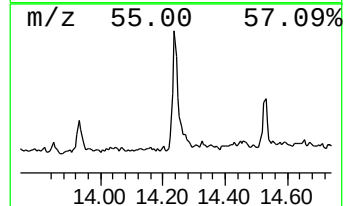
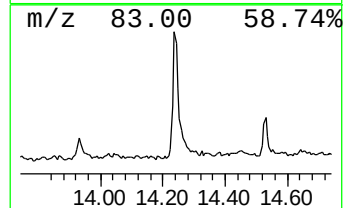
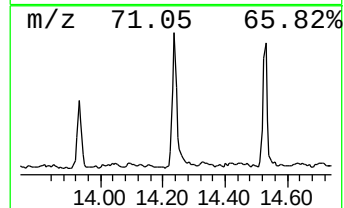
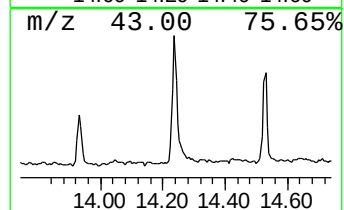
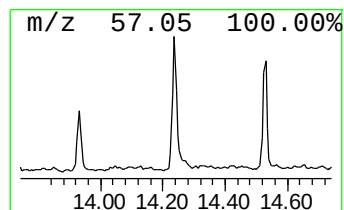
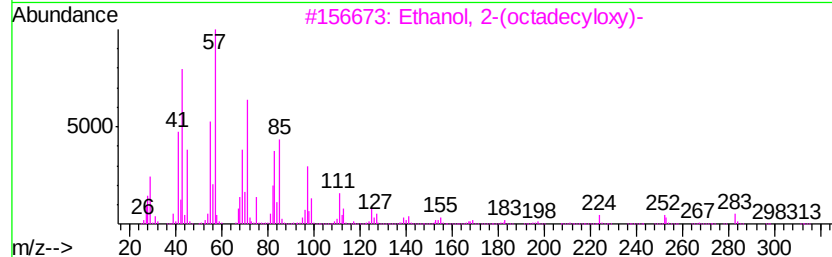
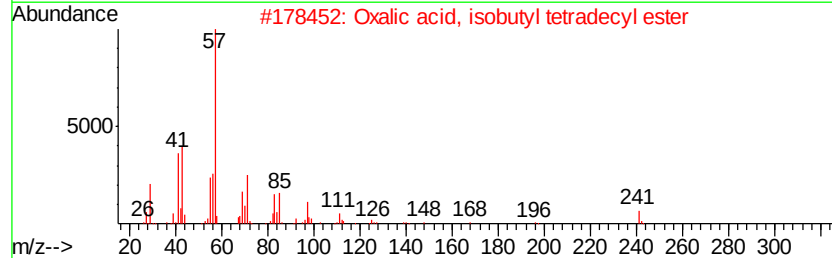
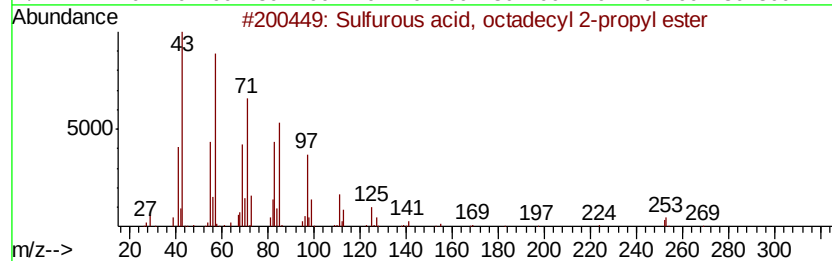
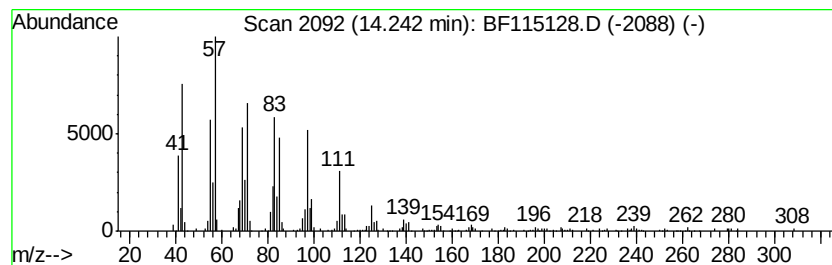
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Sulfurous acid, octadecyl 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	5.41 ng	539244	Chrysene-d12	13.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	91
2		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
3		Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	87
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	70
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70



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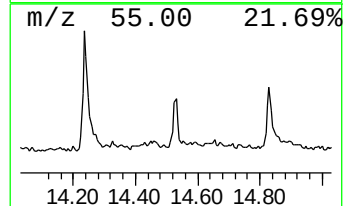
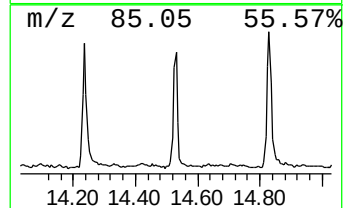
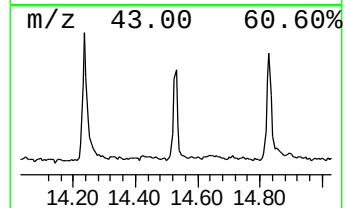
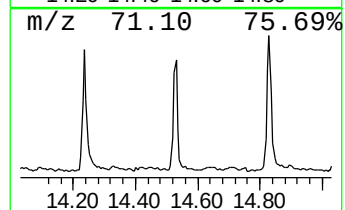
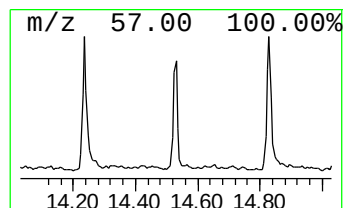
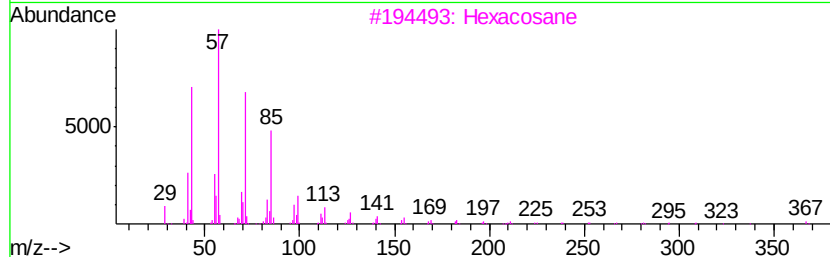
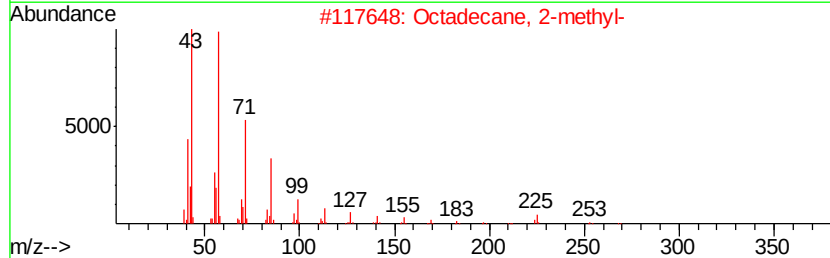
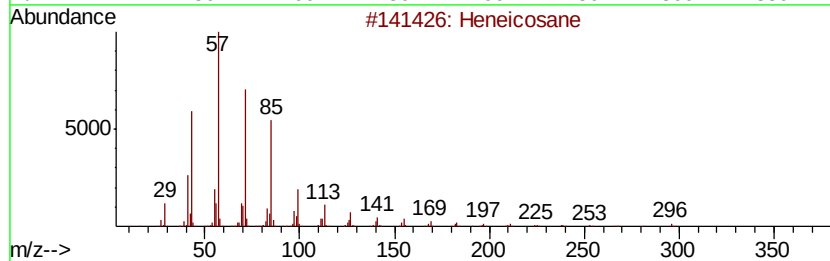
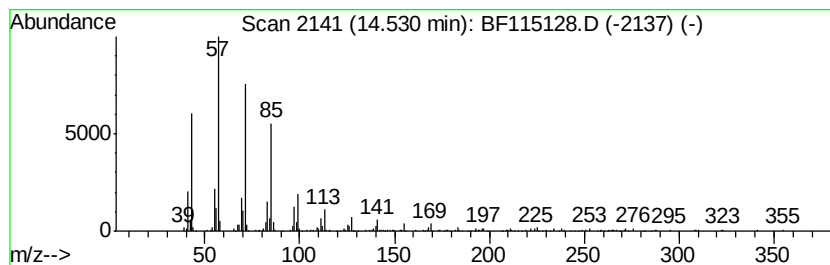
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Peak Number 7 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.54 ng	240936	Perylene-d12	15.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Tetracosane	338	C24H50	000646-31-1	91



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 Misc :
 ALS Vial : 18 Sample Multiplier: 1

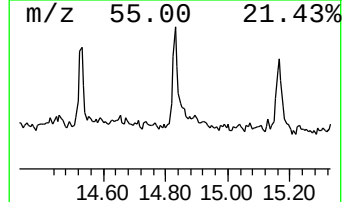
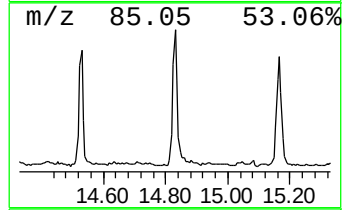
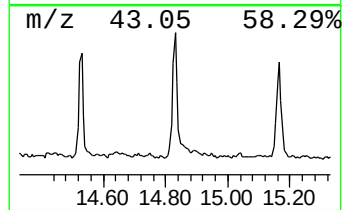
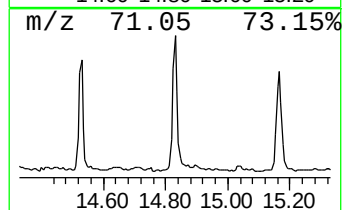
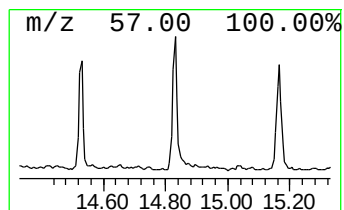
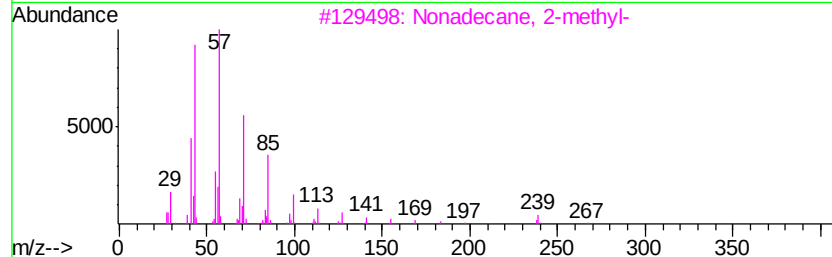
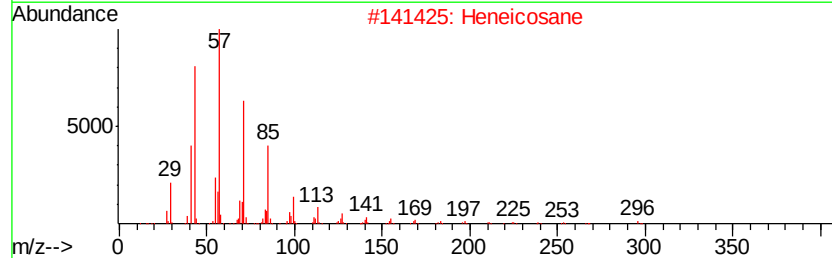
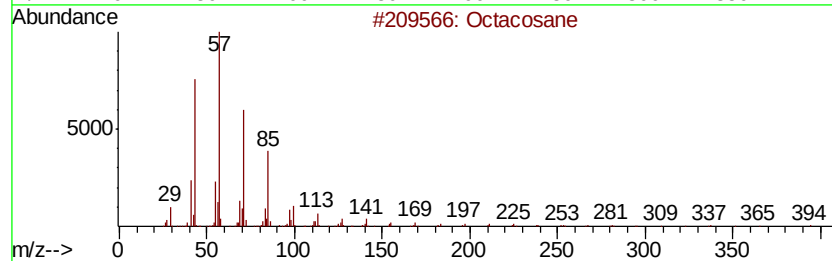
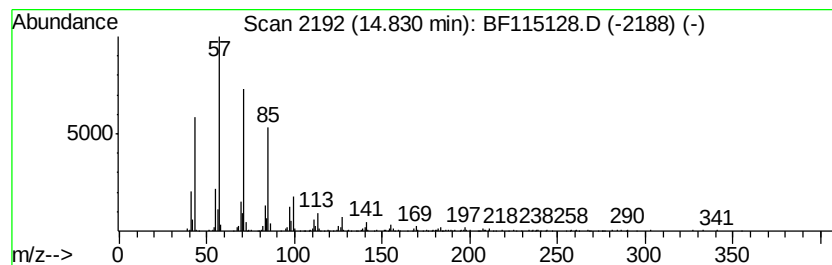
Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF062119.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 8 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.83	3.17 ng	301076	Perylene-d12		15.08
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062219\
 Data File : BF115128.D
 Acq On : 22 Jun 2019 18:37
 Operator : HP/JU
 Sample : K3470-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-4

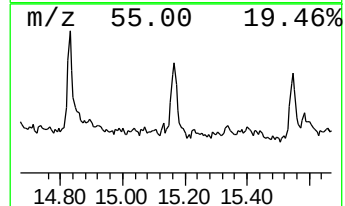
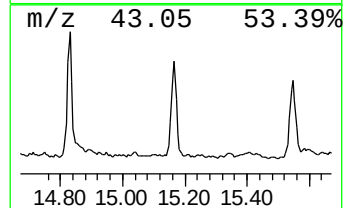
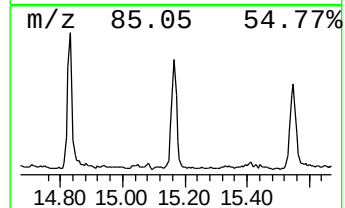
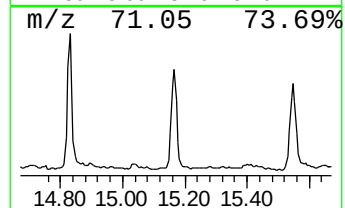
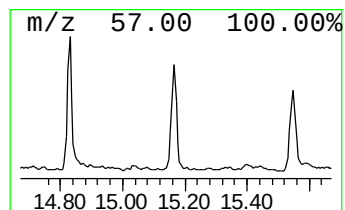
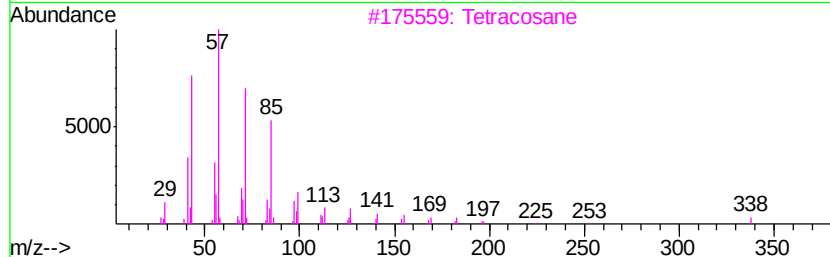
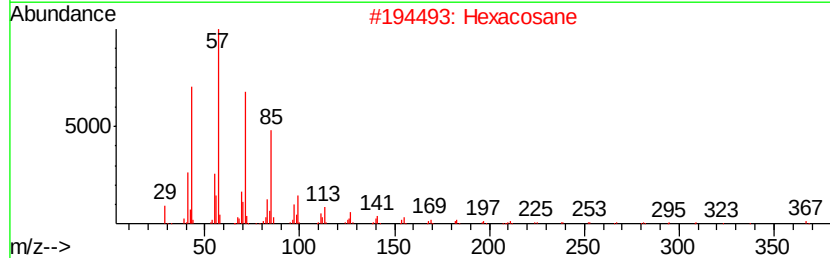
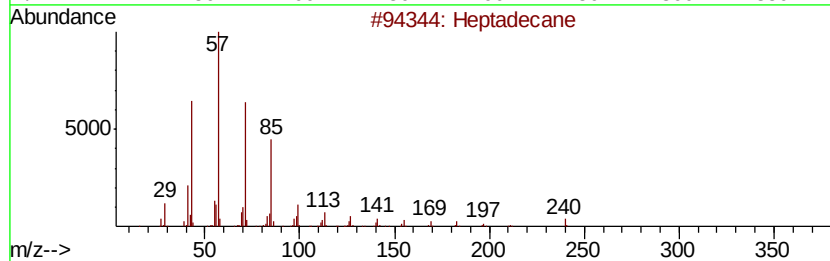
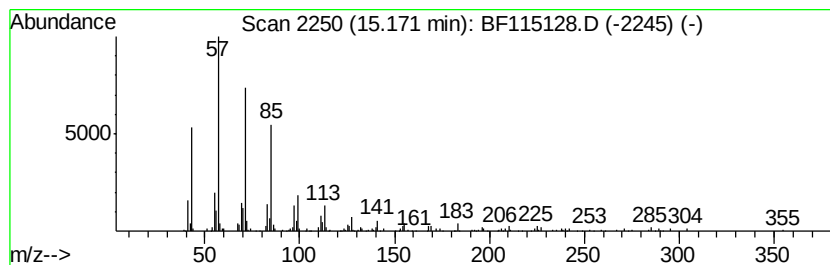
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 9 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	3.05 ng	289613	Perylene-d12	15.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	94
2	Hexacosane		366	C26H54	000630-01-3	91
3	Tetracosane		338	C24H50	000646-31-1	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	90
5	Octacosane		394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062219\
Data File : BF115128.D
Acq On : 22 Jun 2019 18:37
Operator : HP/JU
Sample : K3470-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-4

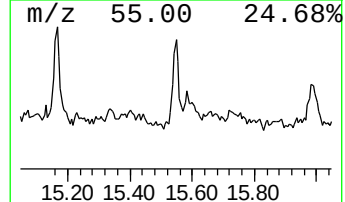
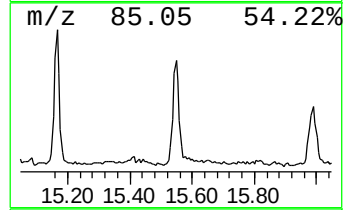
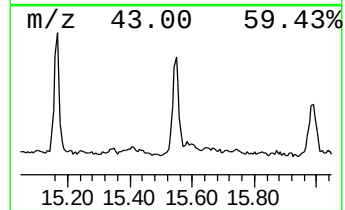
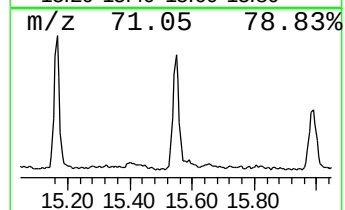
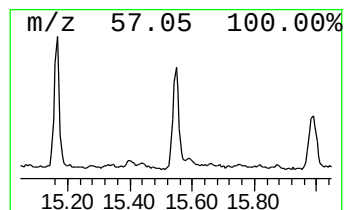
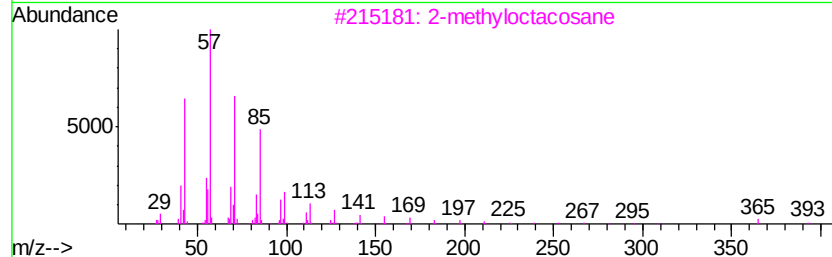
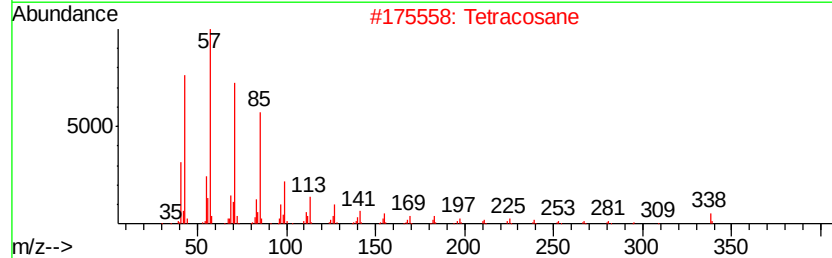
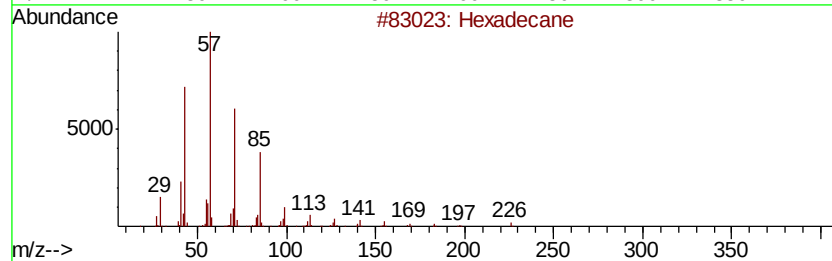
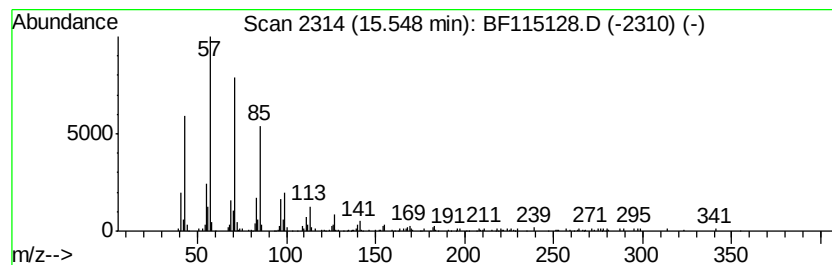
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	2.95 ng	280464	Perylene-d12	15.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	93
2		Tetracosane	338	C24H50	000646-31-1	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		2-methyltetracosane	352	C25H52	1000376-72-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062219\
Data File : BF115128.D
Acq On : 22 Jun 2019 18:37
Operator : HP/JU
Sample : K3470-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.38	6.38	45.8	ng	3847720	1	6.61	1681690	20.0
Octadecanoic acid	12.44	3.3	ng	328724	5	13.72	1992790	20.0
1-Heneicosanol	13.61	5.7	ng	566706	5	13.72	1992790	20.0
Sulfurous acid, o...	14.24	5.4	ng	539244	5	13.72	1992790	20.0
Heneicosane	14.53	2.5	ng	240936	6	15.08	1898440	20.0
Octacosane	14.83	3.2	ng	301076	6	15.08	1898440	20.0
Heptadecane	15.17	3.0	ng	289613	6	15.08	1898440	20.0
Hexadecane	15.55	3.0	ng	280464	6	15.08	1898440	20.0