

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032419\
 Data File : BF113264.D
 Acq On : 24 Mar 2019 13:26
 Operator : JU/SJ
 Sample : K2058-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S3B(5-15)COMP

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-BF022719.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	5.334	547	552	568	rBV	3514920	3975317	74.51%	7.083%
2	6.369	722	728	743	rBV	3667763	4680775	87.74%	8.340%
3	6.486	743	748	752	rBV	4134686	4286691	80.35%	7.638%
4	6.710	783	786	790	rBV	992575	851420	15.96%	1.517%
5	6.869	809	813	817	rBV	3409030	3066572	57.48%	5.464%
6	7.275	877	882	885	rBV	2440663	2619814	49.11%	4.668%
7	7.992	1000	1004	1011	rBV	1143175	1080085	20.25%	1.925%
8	9.075	1182	1188	1191	rBV	4637827	4644045	87.05%	8.275%
9	9.463	1250	1254	1265	rVB	307773	289162	5.42%	0.515%
10	9.745	1298	1302	1314	rVB	1419911	1310328	24.56%	2.335%
11	10.533	1431	1436	1450	rBV	3314210	3712976	69.60%	6.616%
12	11.227	1550	1554	1560	rBV	1432689	1470271	27.56%	2.620%
13	11.768	1639	1646	1665	rVB	1239102	1958173	36.70%	3.489%
14	12.545	1773	1778	1789	rVV	1229681	2004710	37.58%	3.572%
15	12.627	1789	1792	1795	rVV	147700	144735	2.71%	0.258%
16	12.810	1818	1823	1826	rBV	4889078	5334947	100.00%	9.506%
17	13.351	1912	1915	1917	rBV	74317	68036	1.28%	0.121%
18	13.386	1918	1921	1924	rVB	68204	66205	1.24%	0.118%
19	13.668	1964	1969	1972	rBV5	29836	77272	1.45%	0.138%
20	13.710	1973	1976	1979	rVV	245478	295905	5.55%	0.527%
21	13.745	1979	1982	1991	rVB2	202839	416186	7.80%	0.742%
22	13.857	1996	2001	2008	rBV	1559105	1623451	30.43%	2.893%
23	14.027	2025	2030	2036	rBV	836295	814354	15.26%	1.451%
24	14.333	2077	2082	2087	rVB	1479166	1542995	28.92%	2.749%
25	14.627	2127	2132	2136	rBV	2051983	2129033	39.91%	3.794%
26	14.692	2140	2143	2147	rVB	308762	313030	5.87%	0.558%
27	14.945	2180	2186	2195	rVB	1708604	2053337	38.49%	3.659%
28	15.156	2219	2222	2227	rVB2	42803	56332	1.06%	0.100%
29	15.262	2235	2240	2243	rBV	1007500	1451743	27.21%	2.587%
30	15.292	2243	2245	2256	rVB	1270569	1605343	30.09%	2.860%
31	15.698	2307	2314	2324	rVB	819440	1276592	23.93%	2.275%
32	16.156	2386	2392	2400	rVB	384036	688457	12.90%	1.227%
33	16.703	2479	2485	2490	rVB	108812	212872	3.99%	0.379%

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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S3B(5-15)COMP

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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

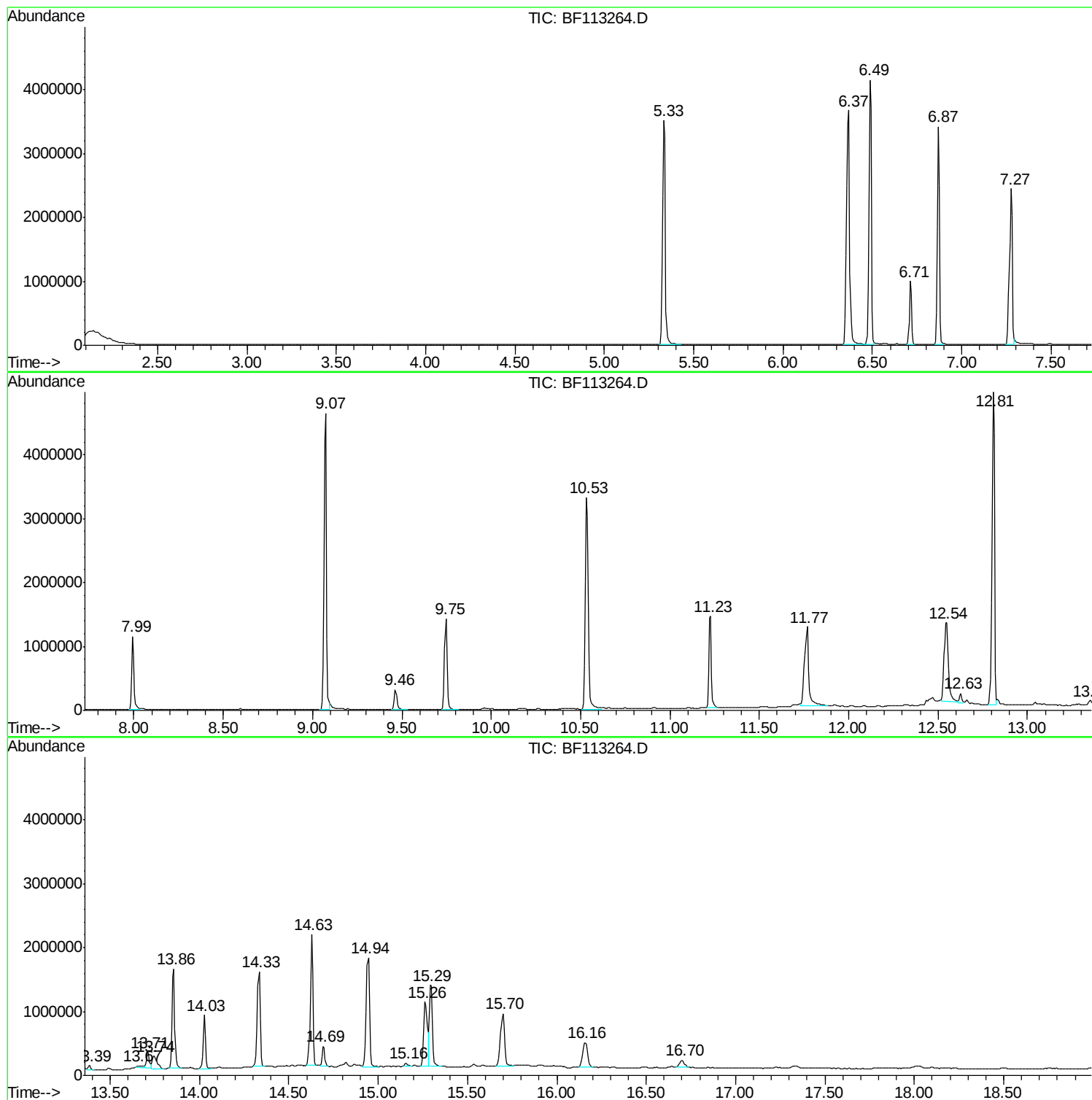
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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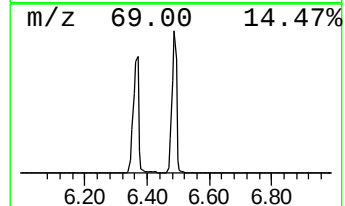
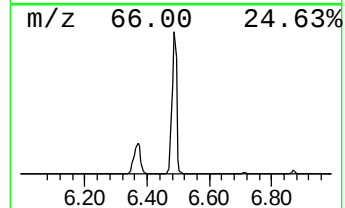
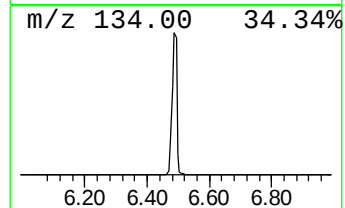
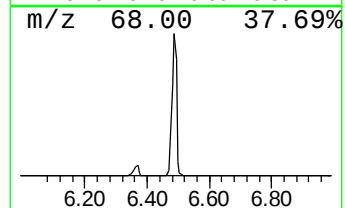
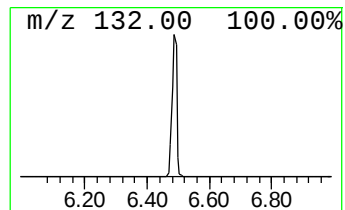
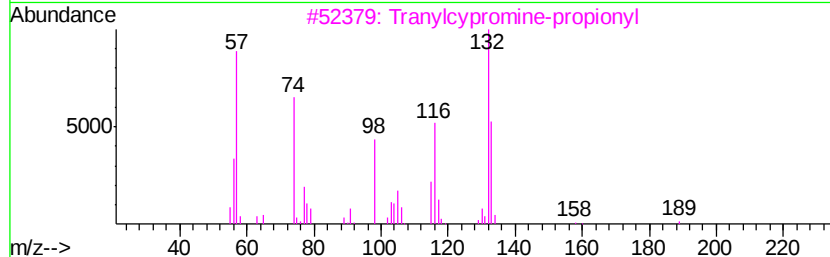
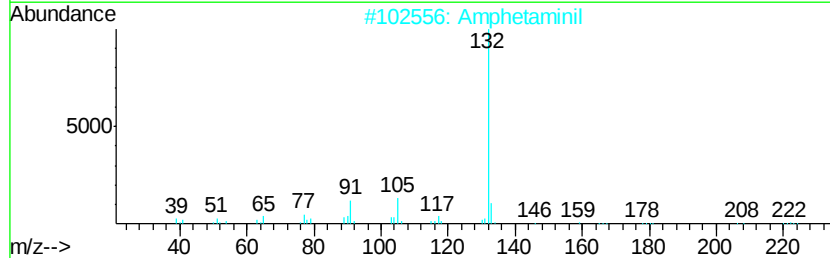
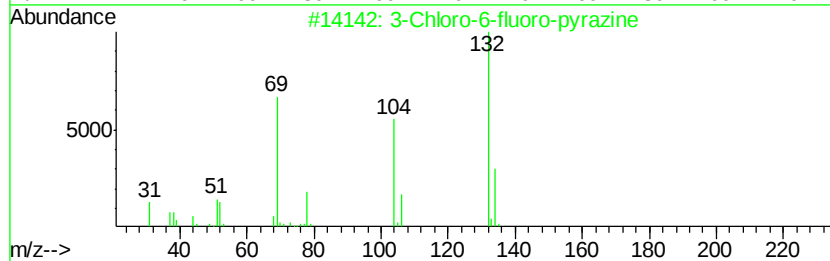
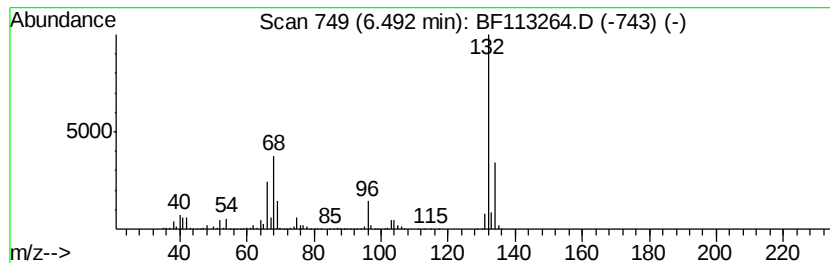
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	100.70 ng	4286690	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Amphetaminil	250	C17H18N2	017590-01-1	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12



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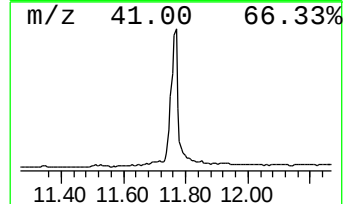
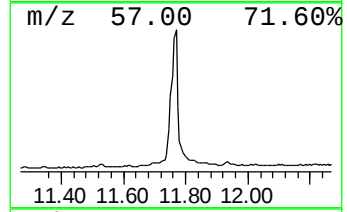
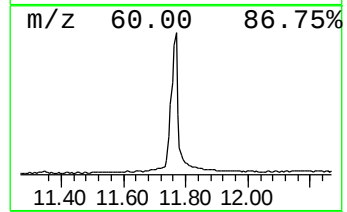
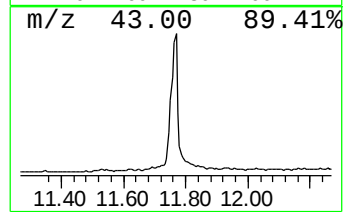
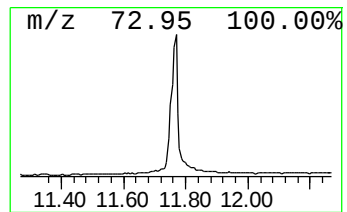
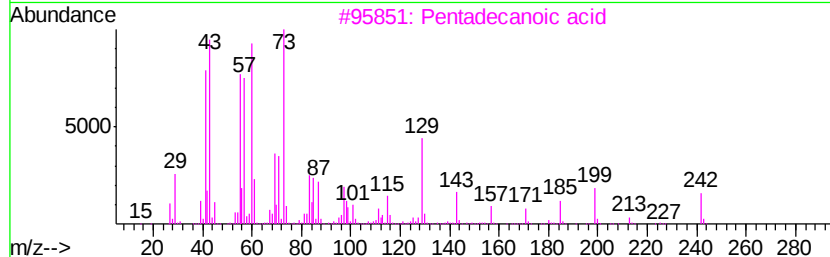
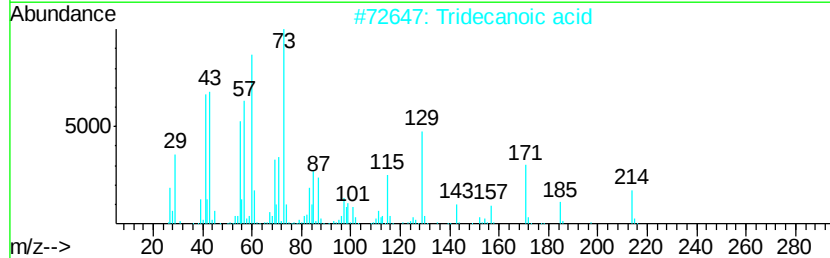
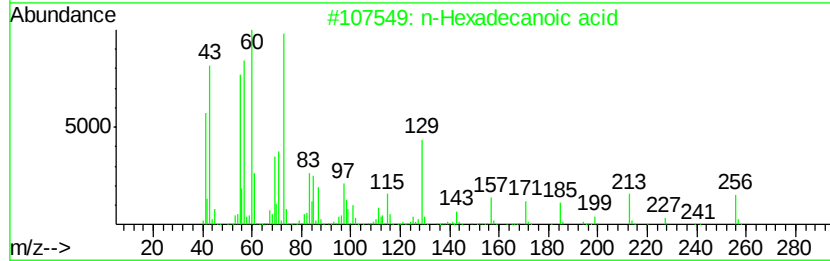
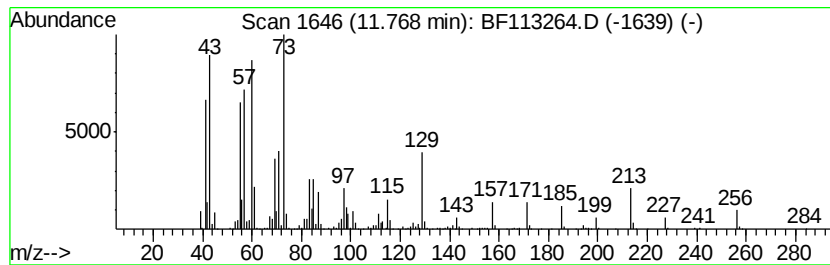
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	26.64 ng	1958170	Phenanthrene-d10	11.23	
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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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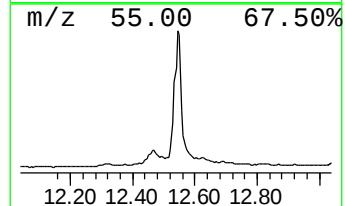
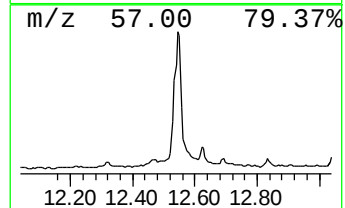
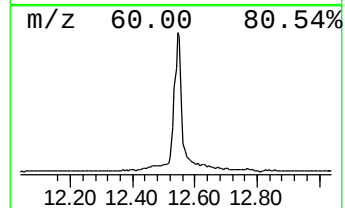
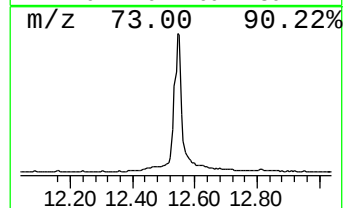
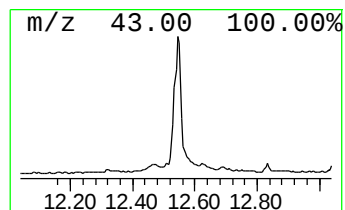
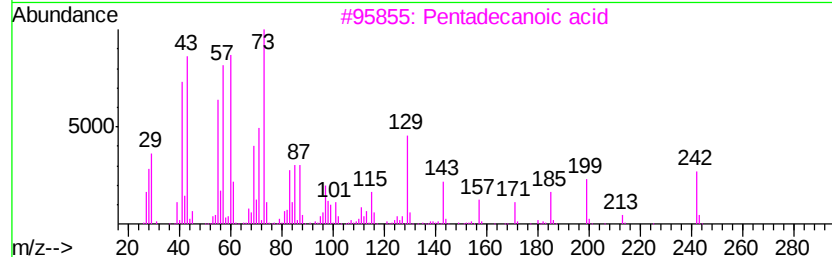
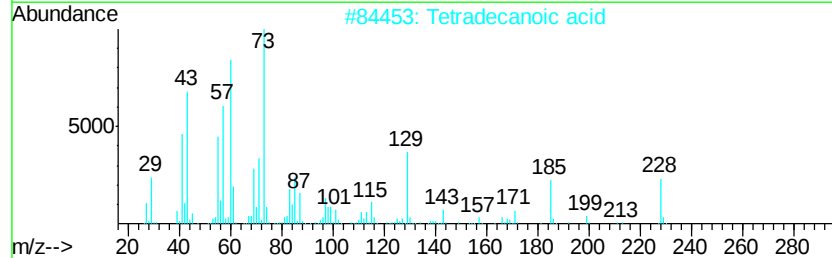
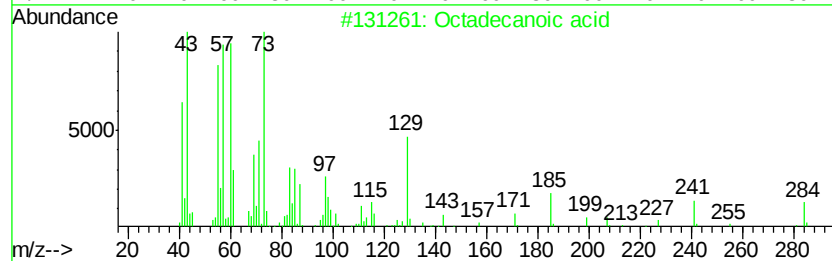
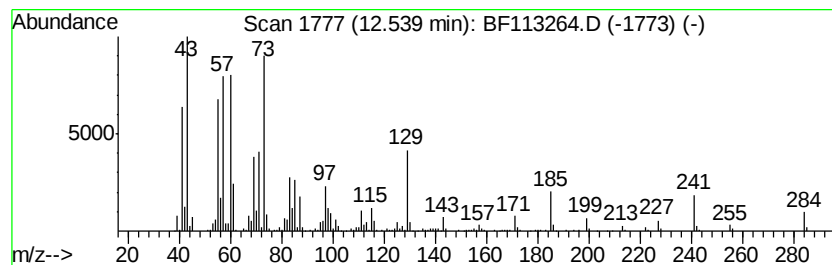
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	24.70 ng	2004710	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64



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ALS Vial : 5 Sample Multiplier: 1

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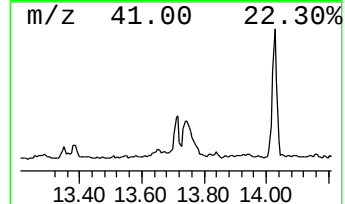
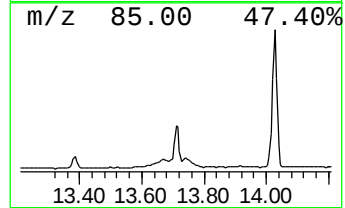
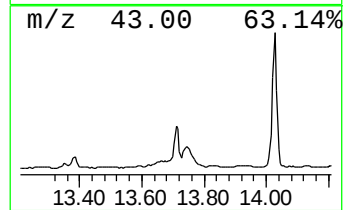
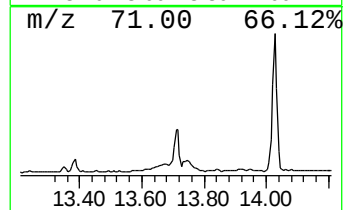
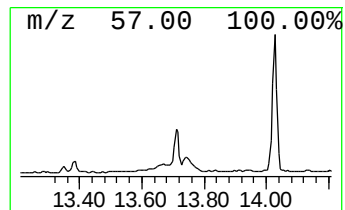
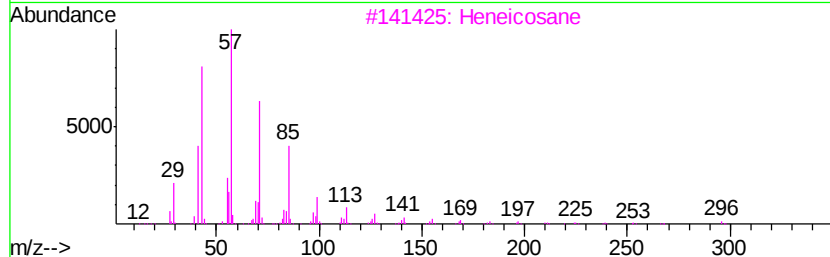
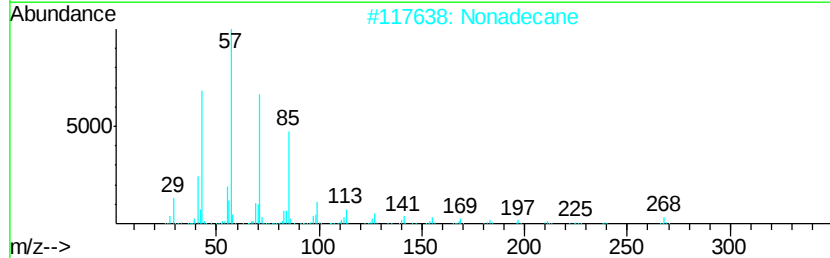
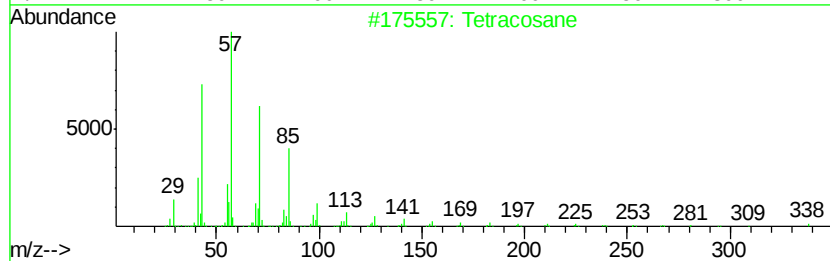
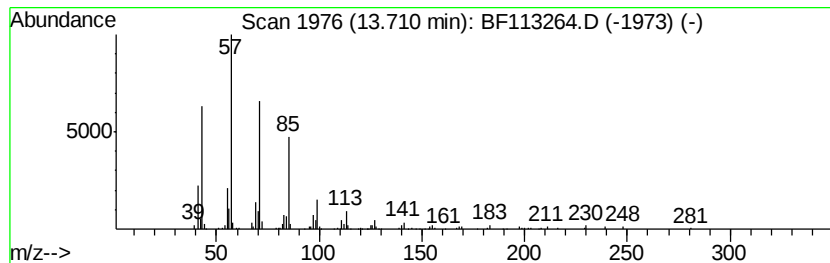
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	3.65 ng	295905	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Nonadecane	268	C19H40	000629-92-5	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Pentadecane	212	C15H32	000629-62-9	91
5		Heptadecane	240	C17H36	000629-78-7	90



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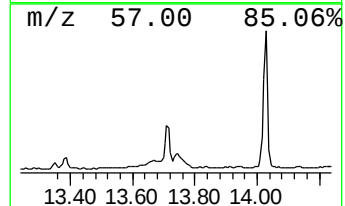
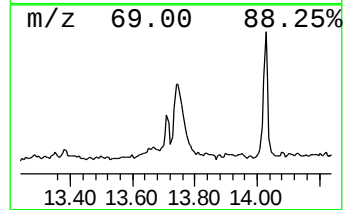
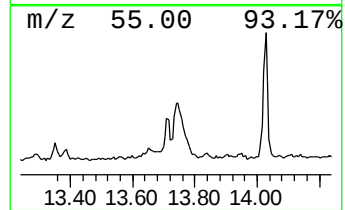
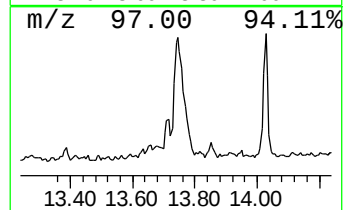
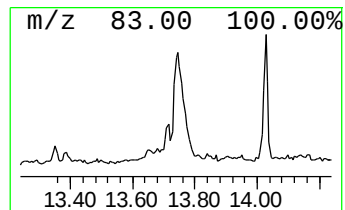
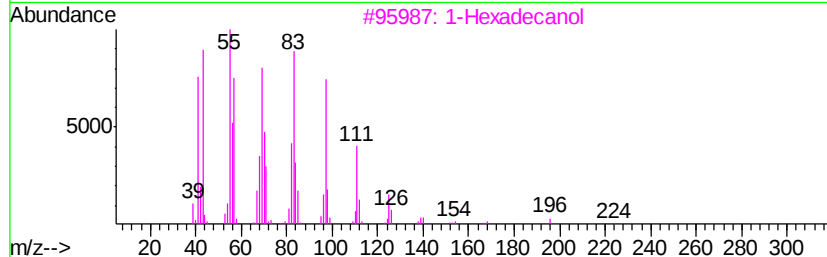
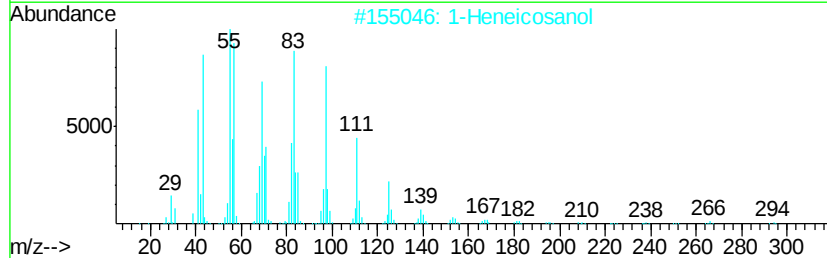
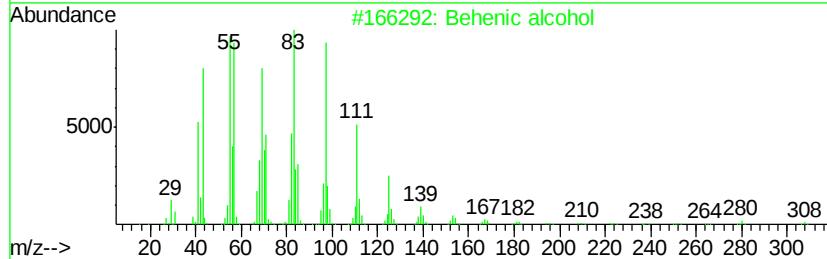
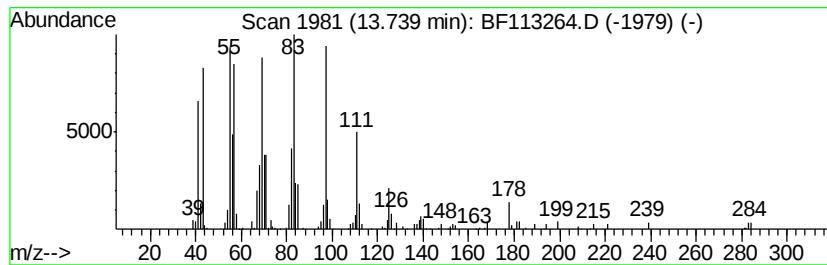
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Behenic alcohol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	5.13 ng	416186	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87



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Misc :
ALS Vial : 5 Sample Multiplier: 1

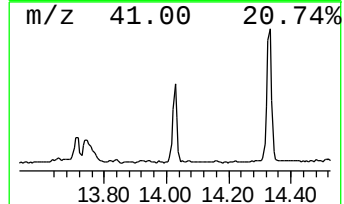
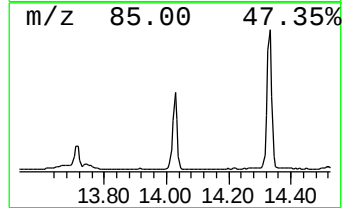
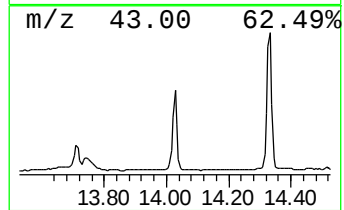
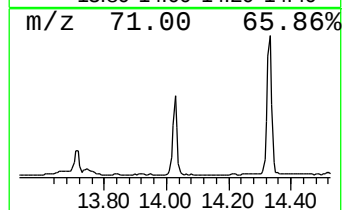
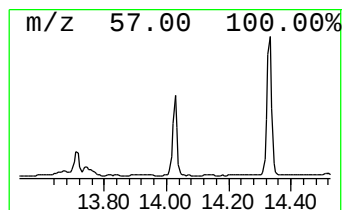
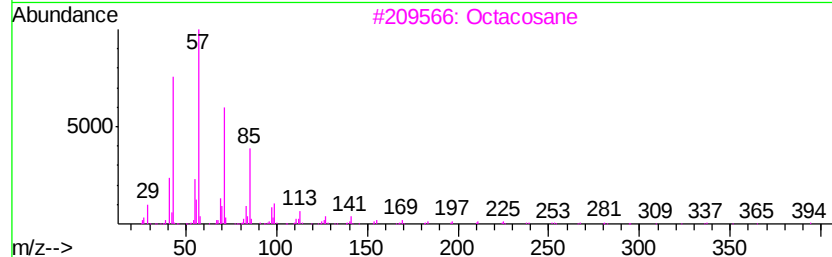
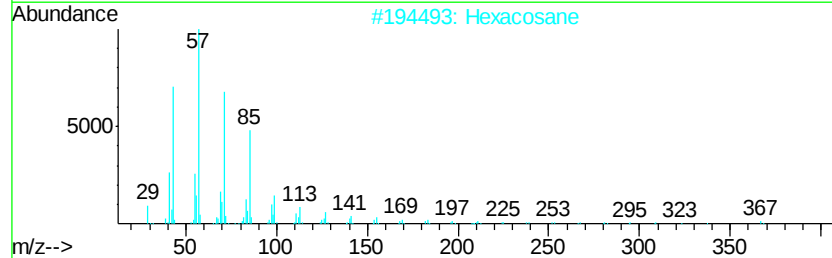
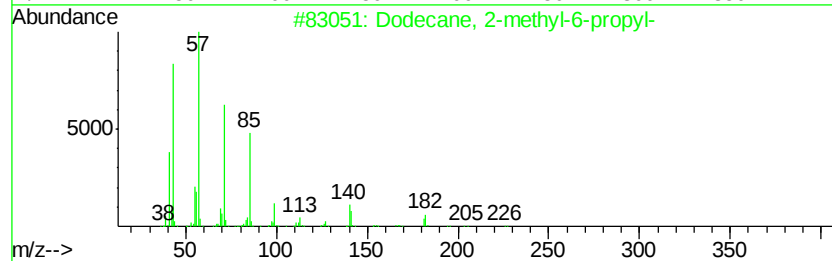
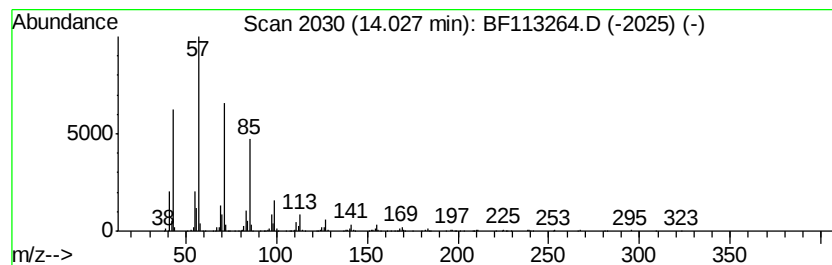
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ClientSampleId :
S3B(5-15)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecane, 2-methyl-6-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	10.03 ng	814354	Chrysene-d12	13.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecane, 2-methyl-6-propyl-	226 C16H34	055045-08-4	93
2	Hexacosane	366 C26H54	000630-01-3	91
3	Octacosane	394 C28H58	000630-02-4	91
4	Heneicosane	296 C21H44	000629-94-7	91
5	Heptacosane	380 C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032419\
Data File : BF113264.D
Acq On : 24 Mar 2019 13:26
Operator : JU/SJ
Sample : K2058-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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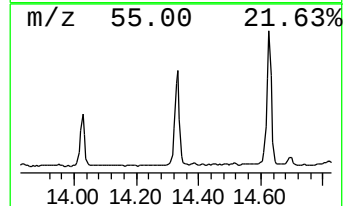
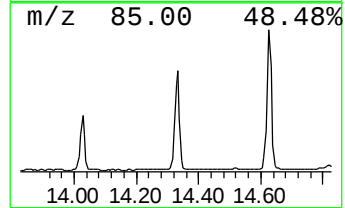
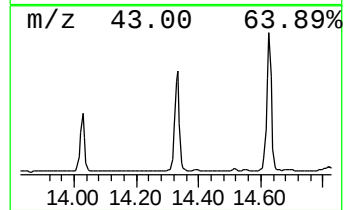
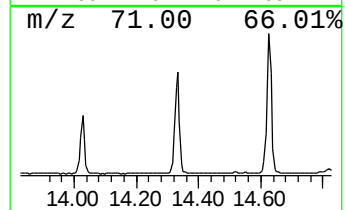
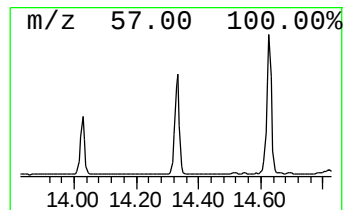
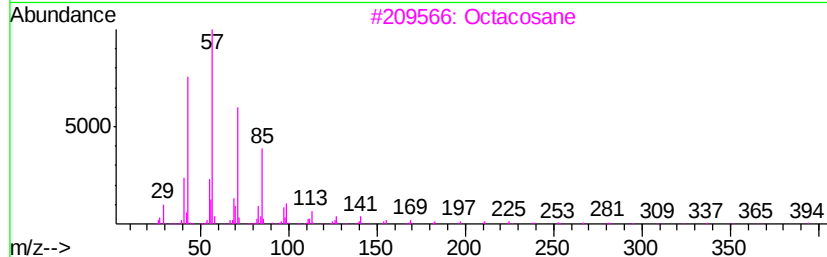
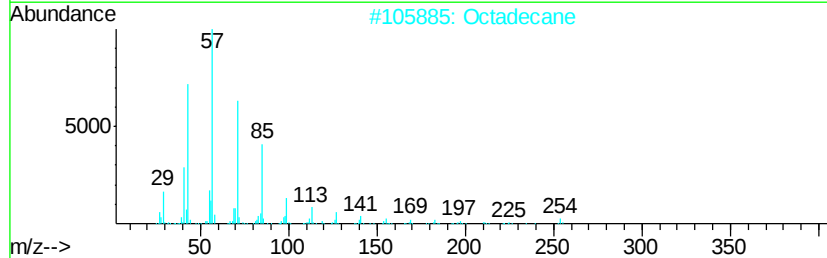
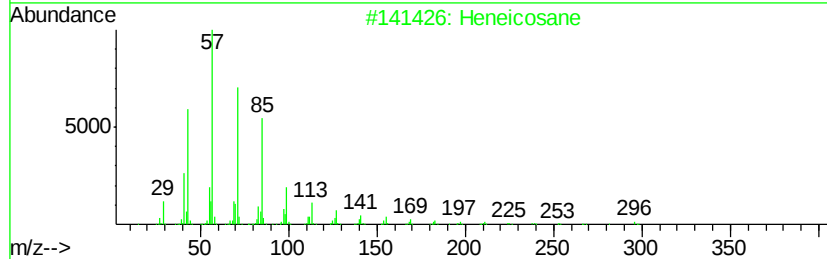
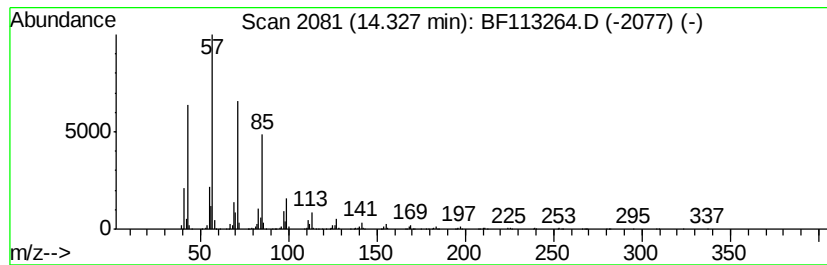
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	19.01 ng	1543000	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octadecane		254	C18H38	000593-45-3	91
3	Octacosane		394	C28H58	000630-02-4	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Docosane		310	C22H46	000629-97-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032419\
Data File : BF113264.D
Acq On : 24 Mar 2019 13:26
Operator : JU/SJ
Sample : K2058-01
Misc :
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ClientSampleId :
S3B(5-15)COMP

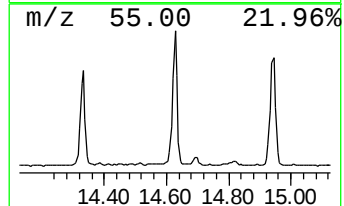
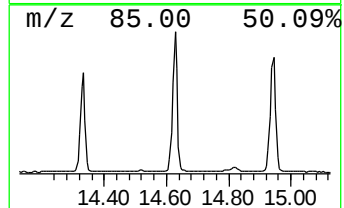
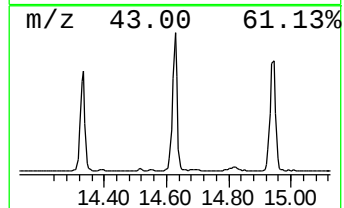
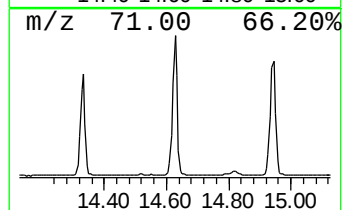
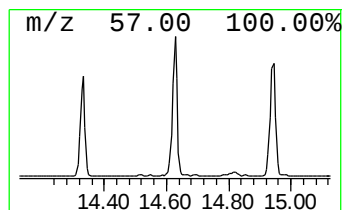
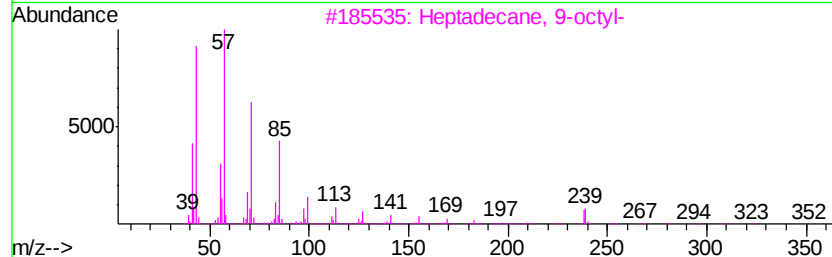
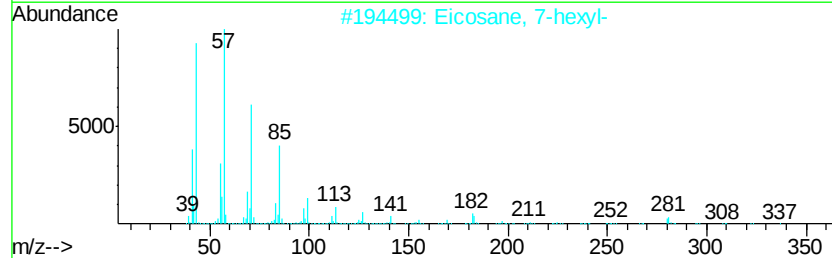
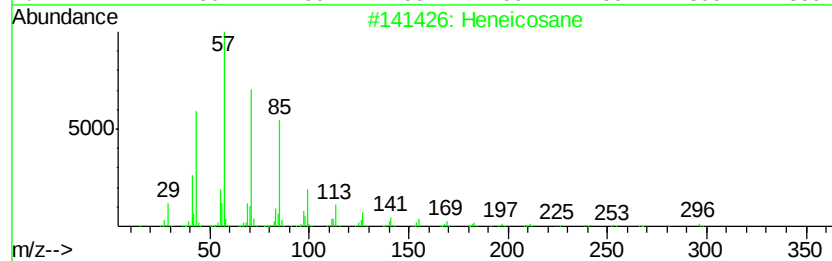
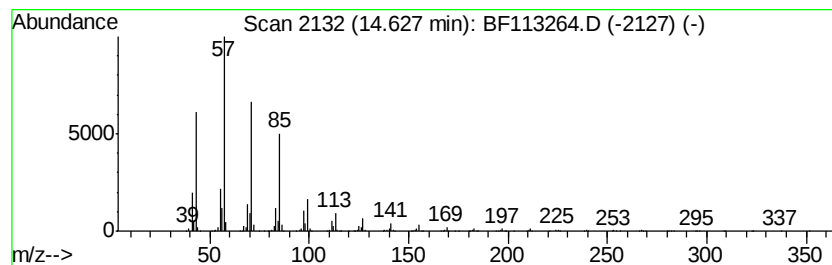
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	29.33 ng	2129030	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Octacosane	394	C28H58	000630-02-4	91
5		triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032419\
Data File : BF113264.D
Acq On : 24 Mar 2019 13:26
Operator : JU/SJ
Sample : K2058-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

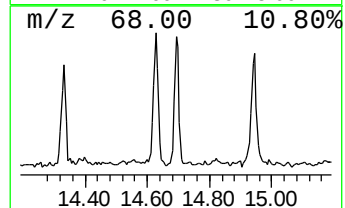
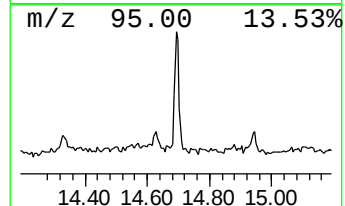
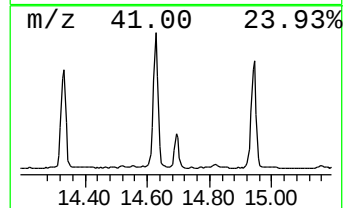
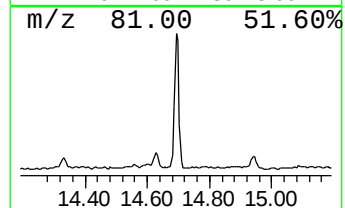
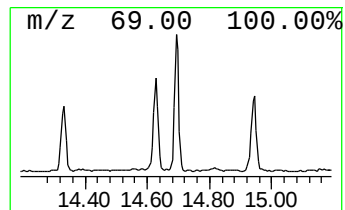
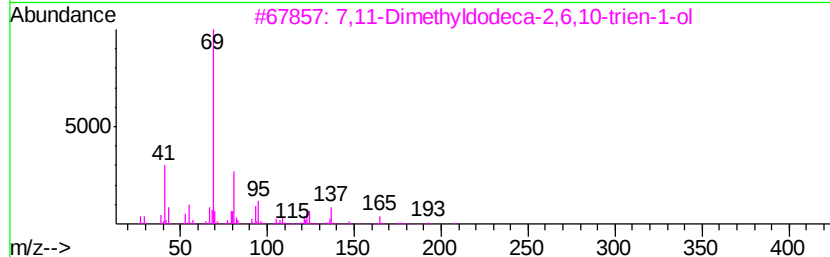
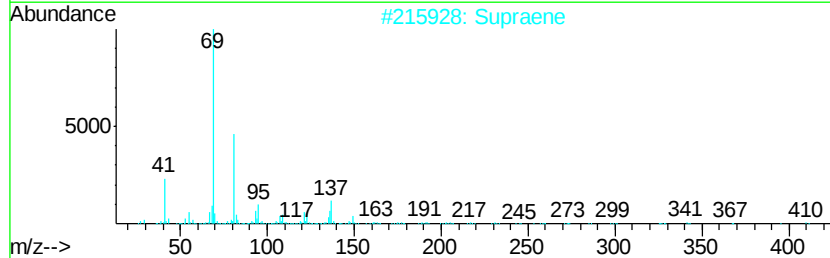
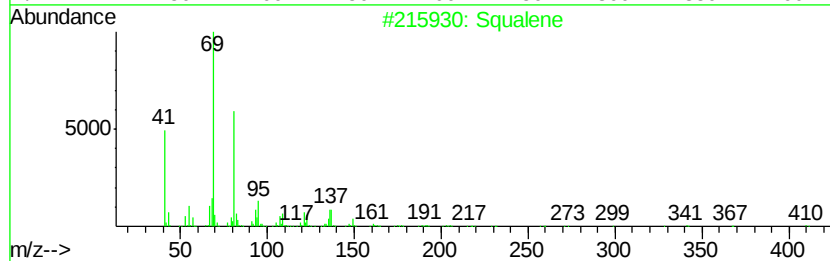
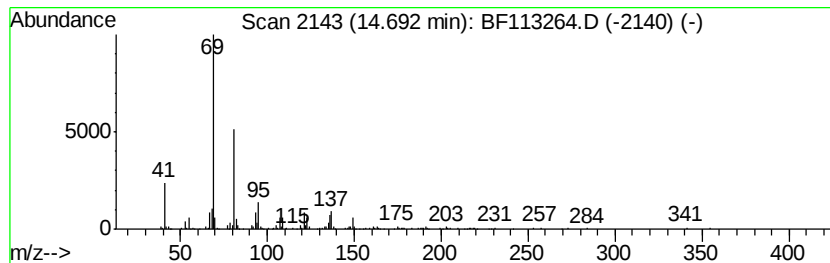
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	4.31 ng	313030	Perylene-d12	15.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	000111-02-4 91
2	Supraene		410 C30H50	007683-64-9 91
3	7,11-Dimethyldodeca-2,6,10-trien...		208 C14H240	125529-10-4 72
4	1,5-Heptadiene, 3,4-dimethyl-		124 C9H16	1000061-77-9 50
5	1,5-Heptadiene, 3,3,6-trimethyl-		138 C10H18	035387-63-4 50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032419\
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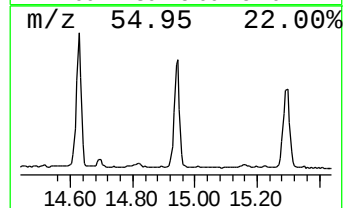
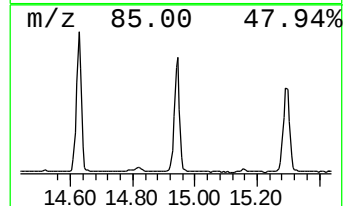
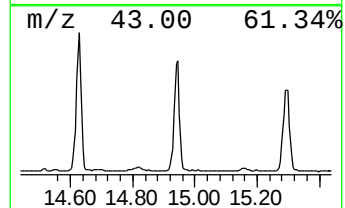
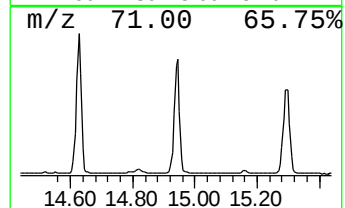
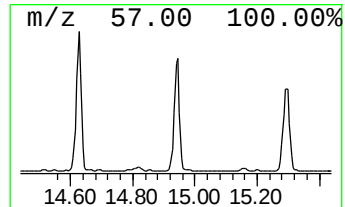
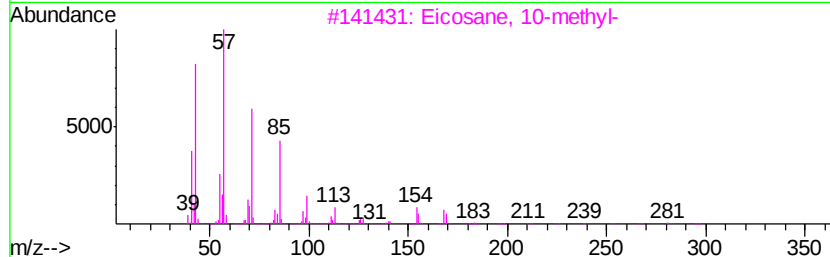
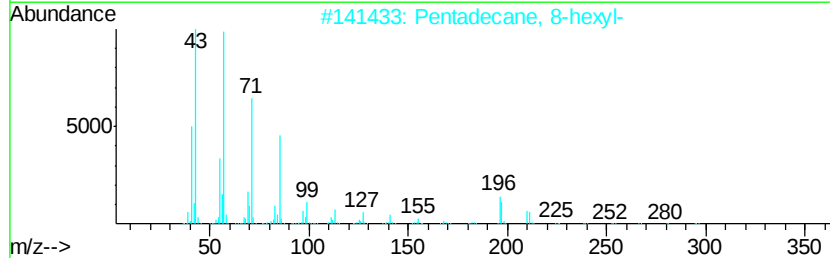
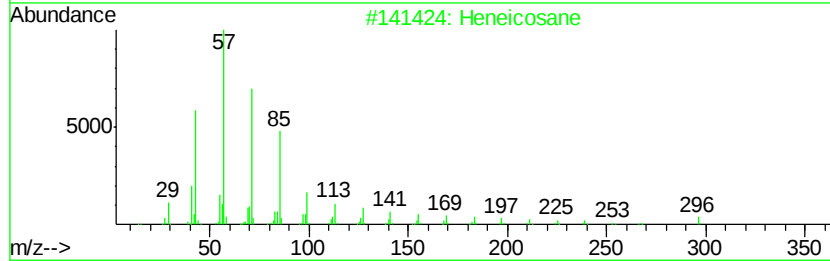
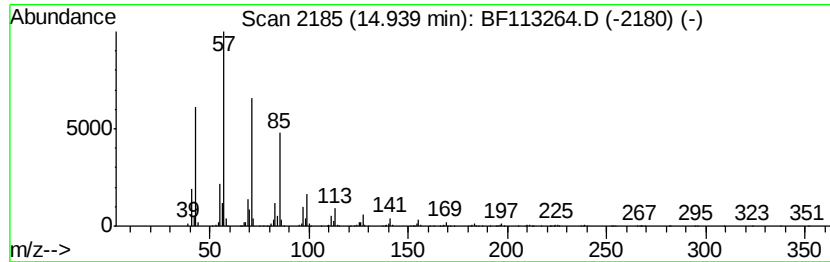
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane, 10-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	28.29 ng	2053340	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	98
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3		Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032419\
Data File : BF113264.D
Acq On : 24 Mar 2019 13:26
Operator : JU/SJ
Sample : K2058-01
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ALS Vial : 5 Sample Multiplier: 1

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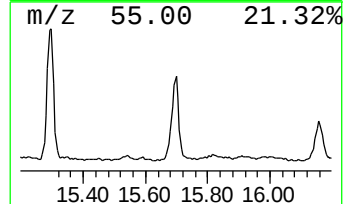
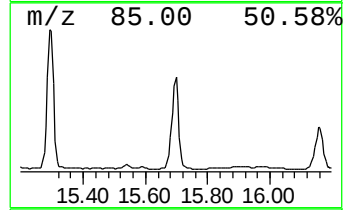
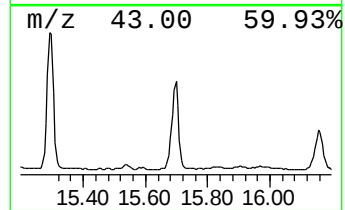
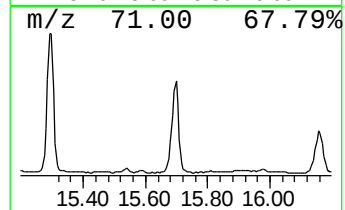
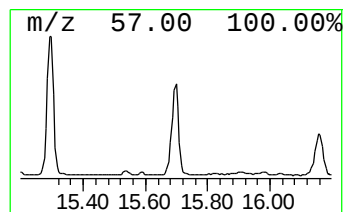
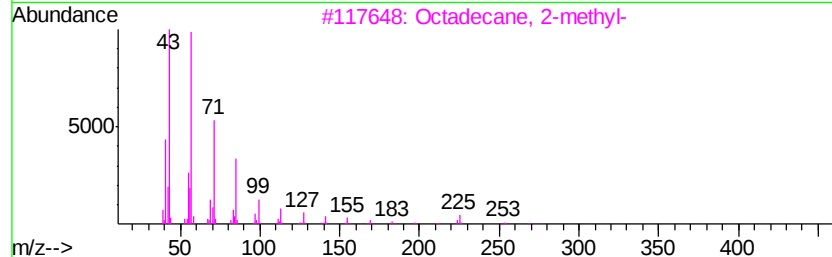
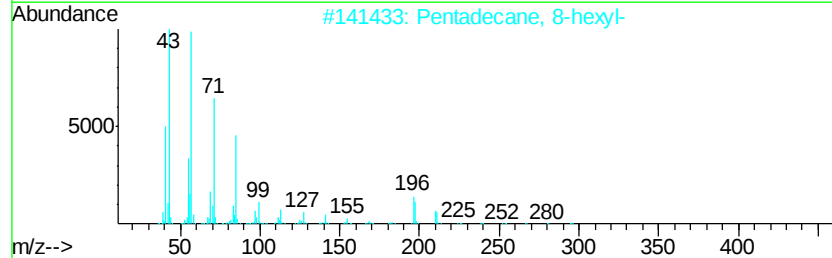
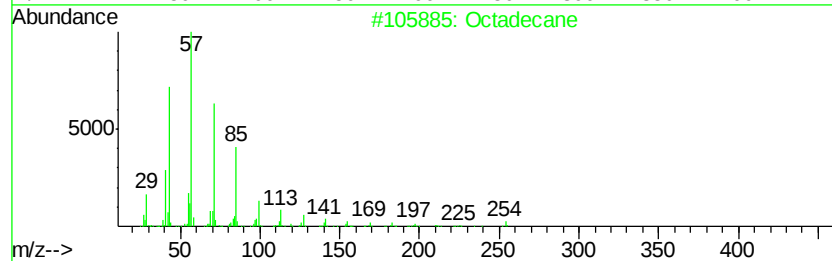
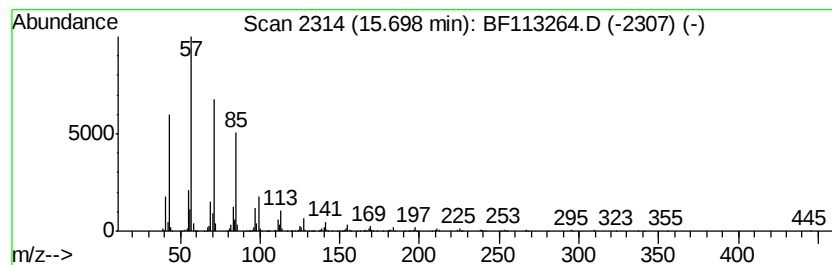
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	17.59 ng	1276590	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	95
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3		Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
5		Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032419\
Data File : BF113264.D
Acq On : 24 Mar 2019 13:26
Operator : JU/SJ
Sample : K2058-01
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ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId :
S3B(5-15)COMP

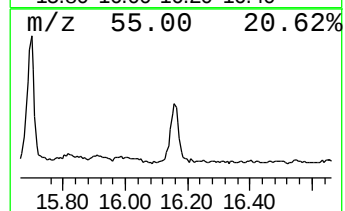
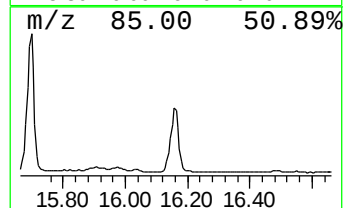
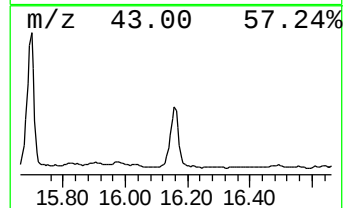
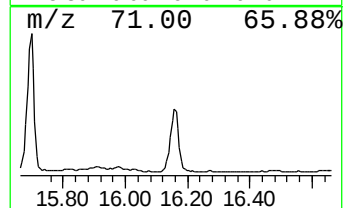
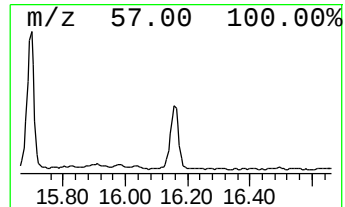
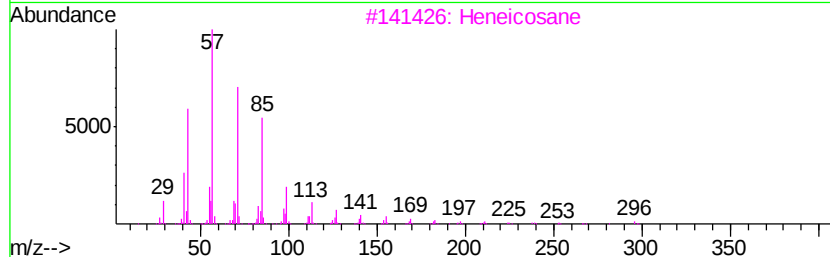
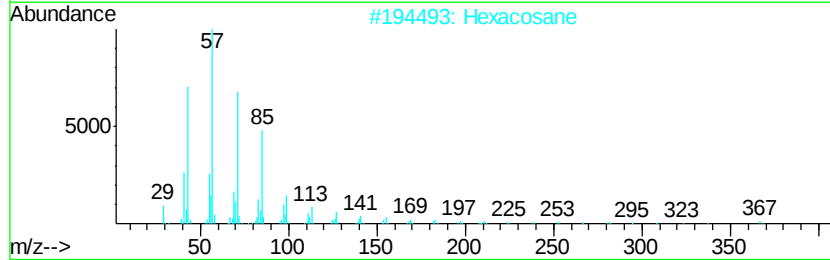
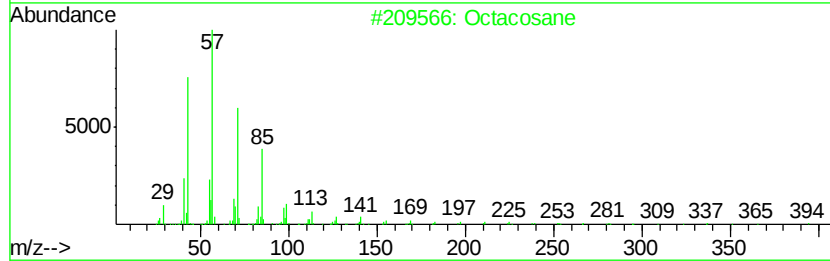
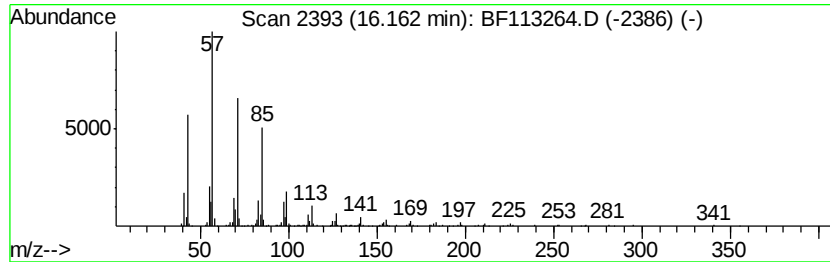
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Docosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	9.48 ng	688457	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Docosane	310	C22H46	000629-97-0	91



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 Data File : BF113264.D
 Acq On : 24 Mar 2019 13:26
 Operator : JU/SJ
 Sample : K2058-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S3B(5-15)COMP

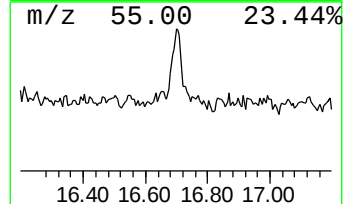
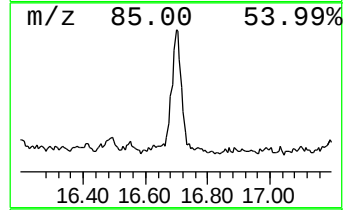
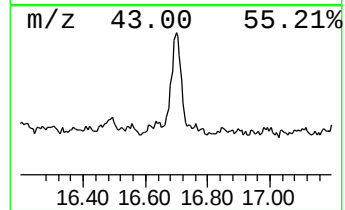
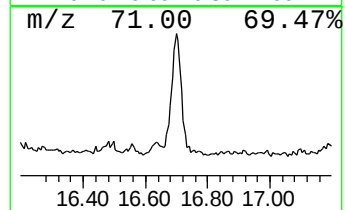
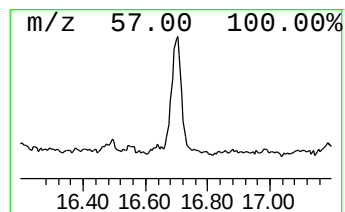
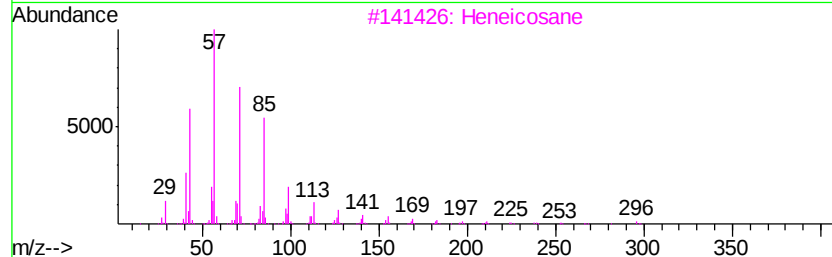
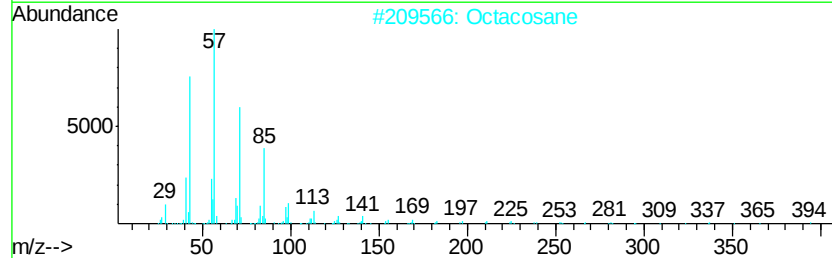
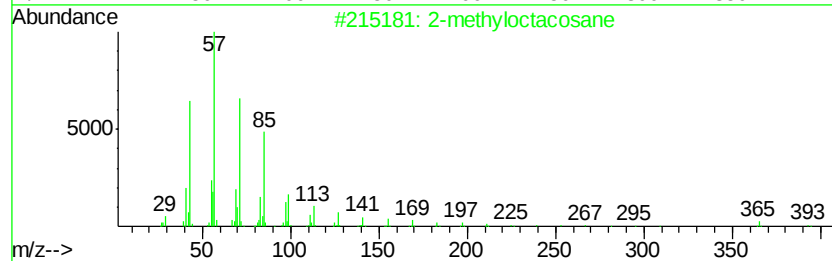
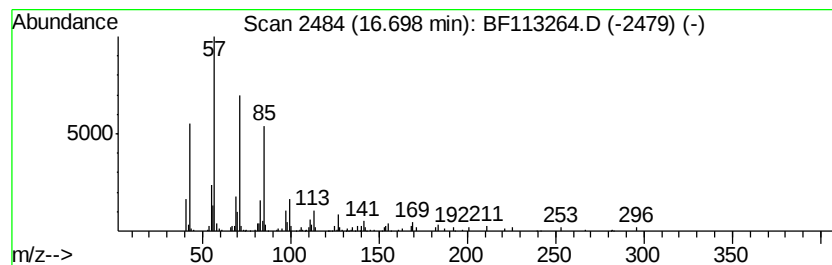
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 14 2-methyloctacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	2.93 ng	212872	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032419\
 Data File : BF113264.D
 Acq On : 24 Mar 2019 13:26
 Operator : JU/SJ
 Sample : K2058-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S3B(5-15)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.49	6.49	100.7	ng	4286690	1	6.71	851420	20.0
n-Hexadecanoic acid	11.77	26.6	ng	1958170	4	11.23	1470270	20.0
Octadecanoic acid	12.54	24.7	ng	2004710	5	13.86	1623450	20.0
Tetracosane	13.71	3.6	ng	295905	5	13.86	1623450	20.0
Behenic alcohol	13.74	5.1	ng	416186	5	13.86	1623450	20.0
Dodecane, 2-methy...	14.03	10.0	ng	814354	5	13.86	1623450	20.0
Heneicosane	14.33	19.0	ng	1543000	5	13.86	1623450	20.0
Eicosane, 7-hexyl-	14.63	29.3	ng	2129030	6	15.26	1451740	20.0
Squalene	14.69	4.3	ng	313030	6	15.26	1451740	20.0
Eicosane, 10-methyl-	14.94	28.3	ng	2053340	6	15.26	1451740	20.0
Octadecane	15.70	17.6	ng	1276590	6	15.26	1451740	20.0
Docosane	16.16	9.5	ng	688457	6	15.26	1451740	20.0
2-methyloctacosane	16.70	2.9	ng	212872	6	15.26	1451740	20.0