

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032819\
 Data File : BF113378.D
 Acq On : 28 Mar 2019 17:09
 Operator : JU/SJ
 Sample : K2107-11
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

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-BF032519.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	5.316	545	549	568	rBV	2609366	2728653	65.90%	7.398%
2	6.351	720	725	742	rBV	2653627	2960234	71.49%	8.026%
3	6.475	742	746	749	rBV	3308227	2878276	69.52%	7.804%
4	6.704	781	785	794	rBV	917100	862663	20.83%	2.339%
5	6.857	807	811	827	rBV	2391187	2100327	50.73%	5.695%
6	7.263	876	880	901	rBV	1923153	1852162	44.73%	5.022%
7	7.980	999	1002	1023	rBV	1109542	1144267	27.64%	3.102%
8	9.057	1181	1185	1206	rBV	3518777	3443353	83.16%	9.336%
9	9.457	1249	1253	1261	rBV	146948	165684	4.00%	0.449%
10	9.733	1296	1300	1312	rBV	1419573	1340391	32.37%	3.634%
11	10.516	1429	1433	1452	rBV	1960602	2236695	54.02%	6.064%
12	11.210	1547	1551	1561	rBV	1606960	1502249	36.28%	4.073%
13	11.745	1638	1642	1658	rBV2	168765	317674	7.67%	0.861%
14	12.527	1771	1775	1788	rBV	193940	347285	8.39%	0.942%
15	12.792	1815	1820	1823	rBV	4340532	4140479	100.00%	11.226%
16	13.698	1970	1974	1977	rBV	75478	74352	1.80%	0.202%
17	13.757	1977	1984	1994	rVV3	146568	586051	14.15%	1.589%
18	13.839	1994	1998	2011	rVB	1637409	1749345	42.25%	4.743%
19	14.009	2023	2027	2031	rBV	172159	165190	3.99%	0.448%
20	14.315	2075	2079	2082	rVB	336930	338845	8.18%	0.919%
21	14.609	2124	2129	2136	rBV	723560	785283	18.97%	2.129%
22	14.921	2177	2182	2189	rVB	905917	1063805	25.69%	2.884%
23	15.239	2231	2236	2239	rBV	1066027	1563318	37.76%	4.239%
24	15.268	2239	2241	2250	rVB	936075	1002649	24.22%	2.718%
25	15.662	2303	2308	2320	rVB	624997	931945	22.51%	2.527%
26	16.121	2381	2386	2395	rBV	271194	467297	11.29%	1.267%
27	16.656	2473	2477	2484	rVB2	74435	134154	3.24%	0.364%

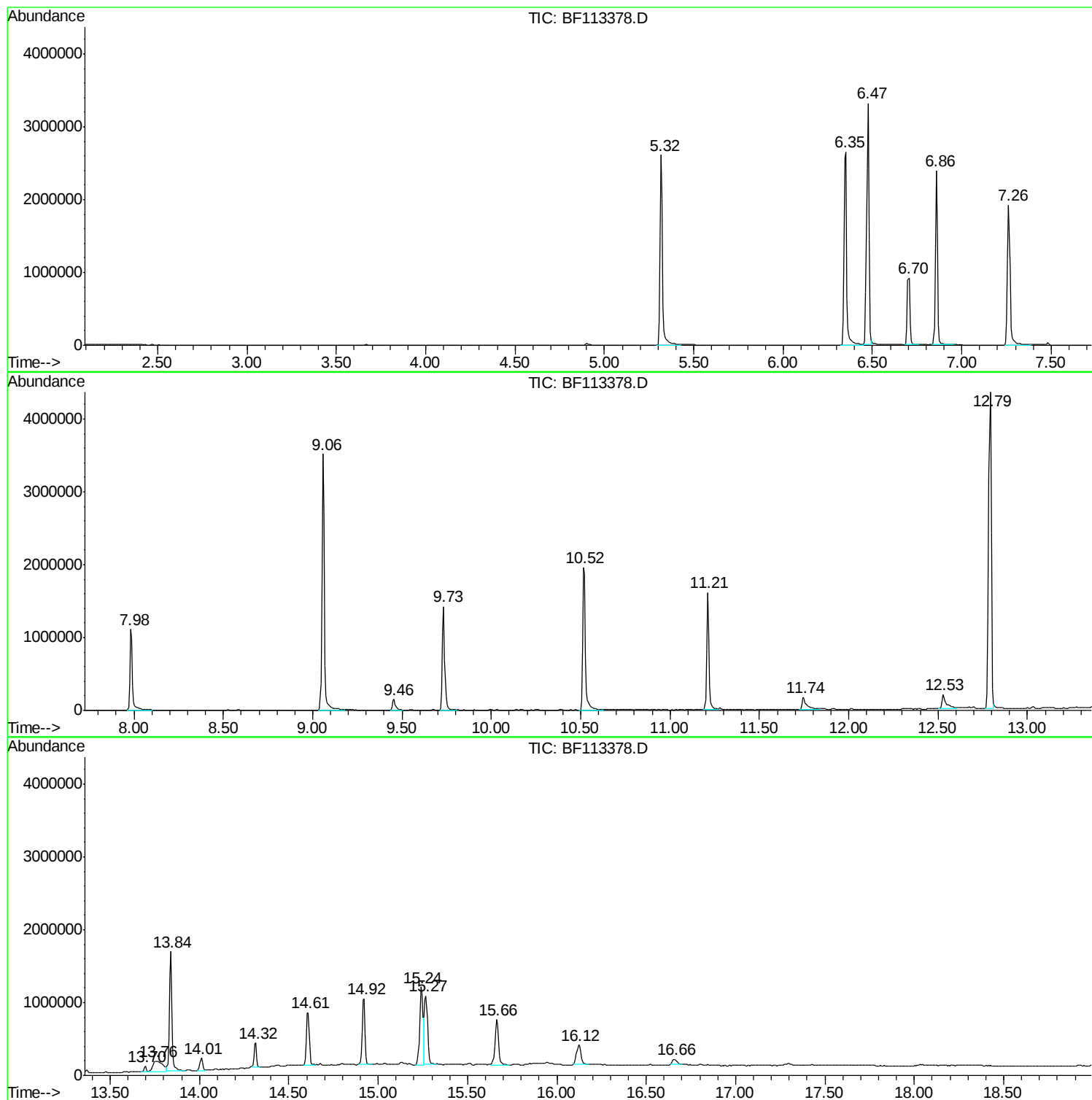
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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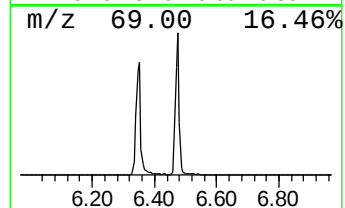
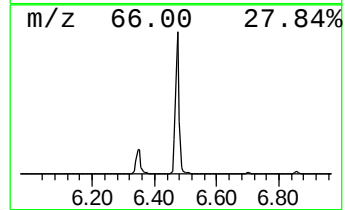
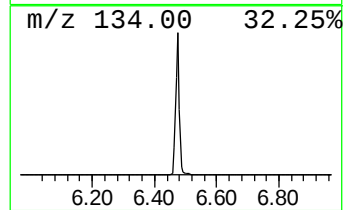
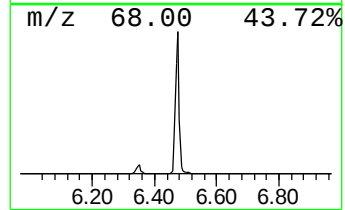
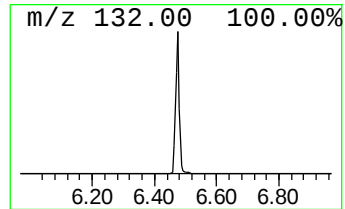
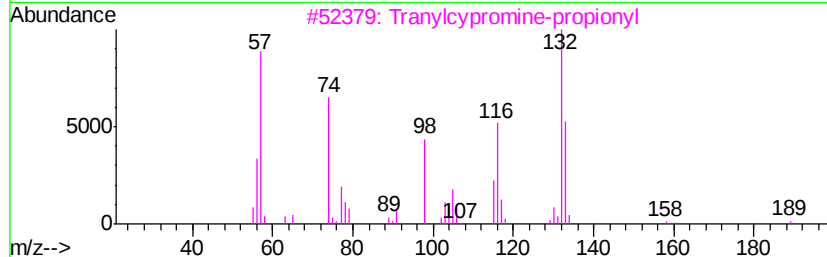
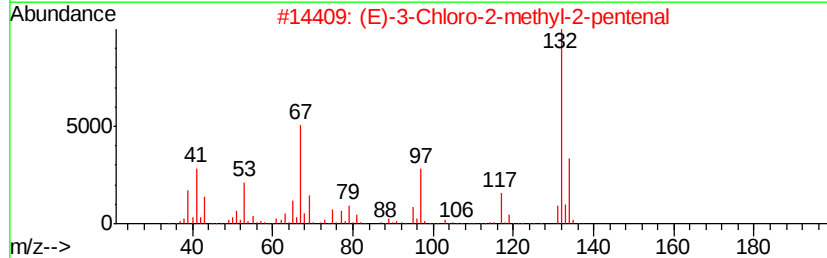
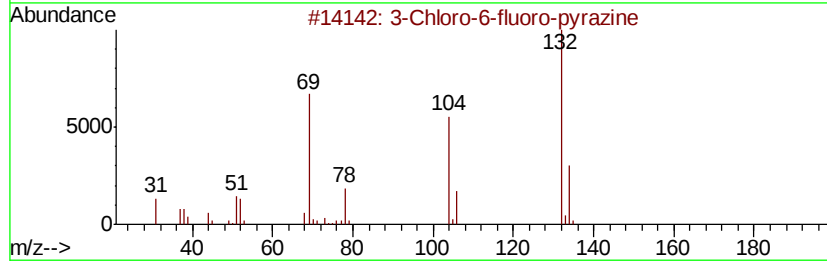
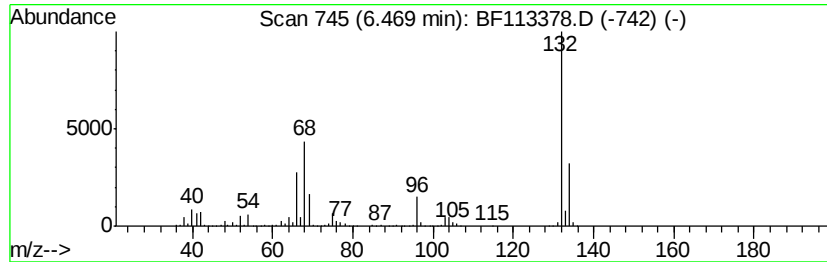
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	66.73 ng	2878280	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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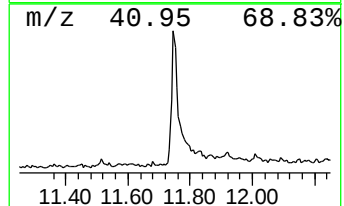
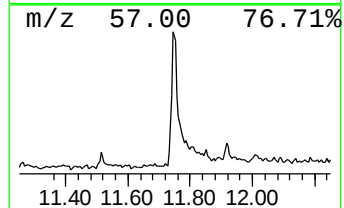
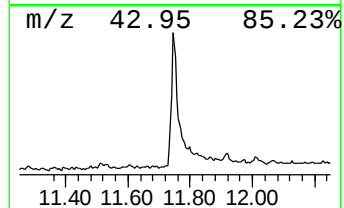
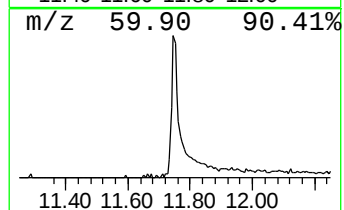
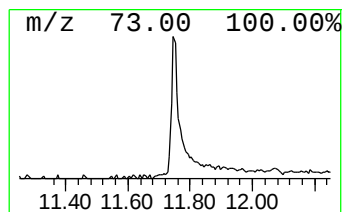
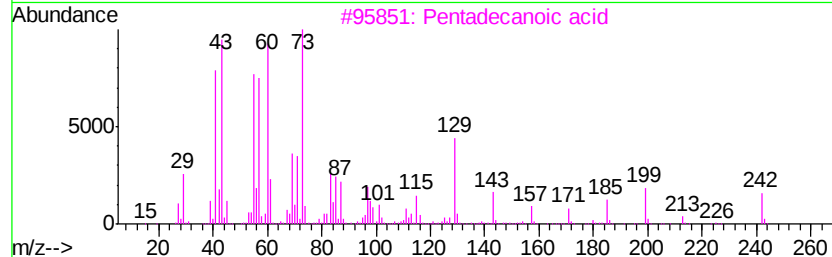
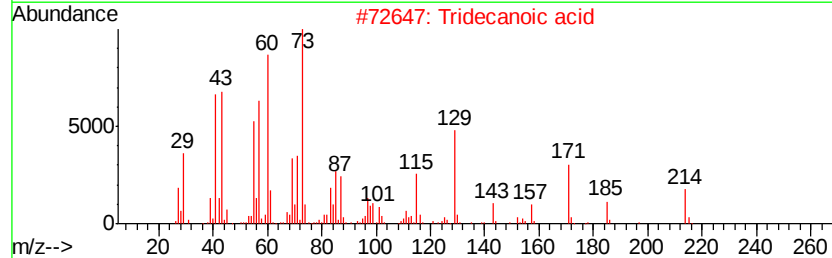
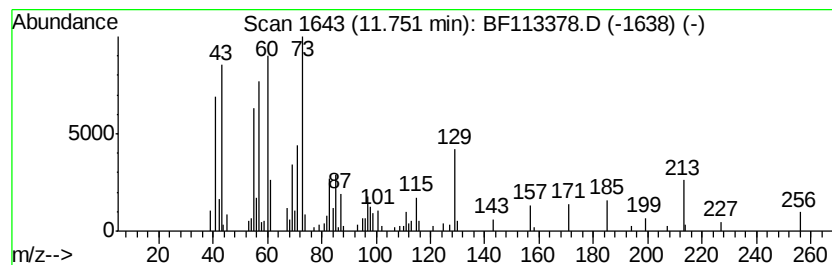
Instrument :
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TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.75	4.23 ng	317674	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	18



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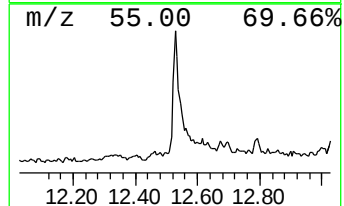
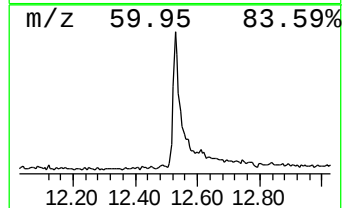
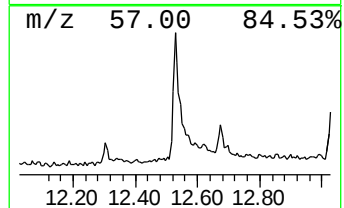
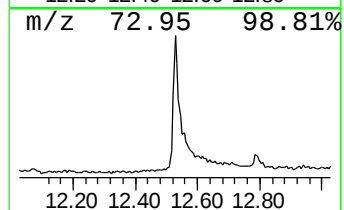
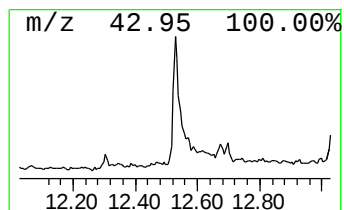
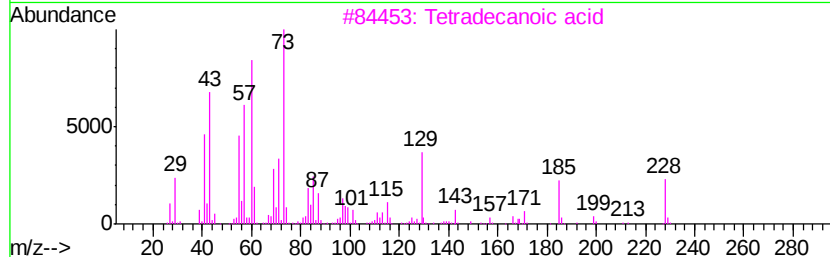
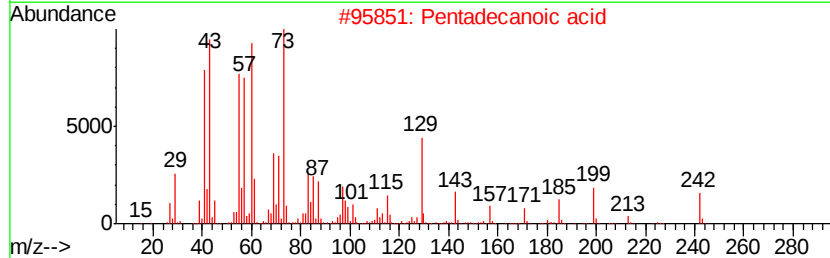
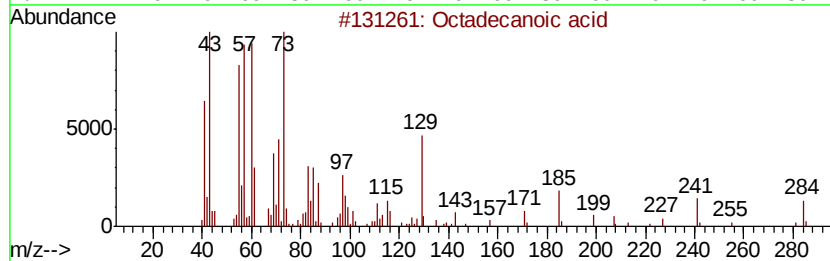
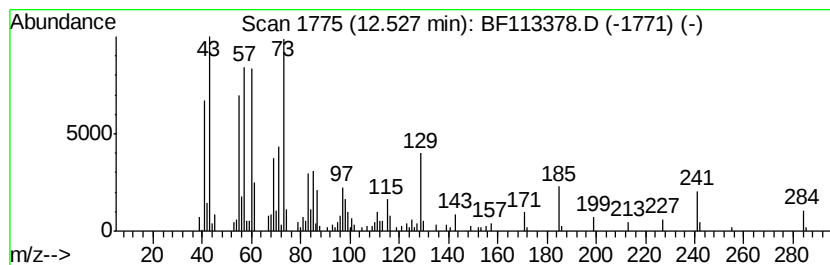
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	3.97 ng	347285	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	18



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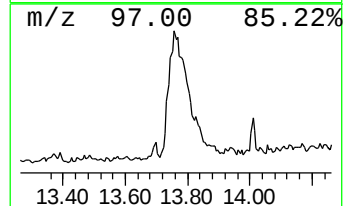
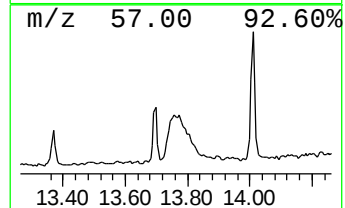
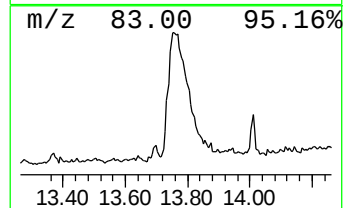
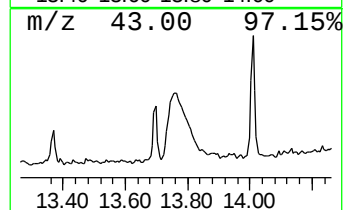
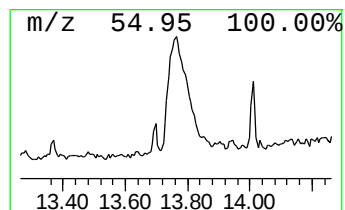
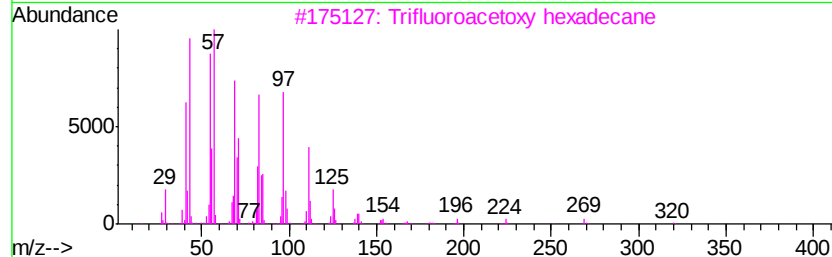
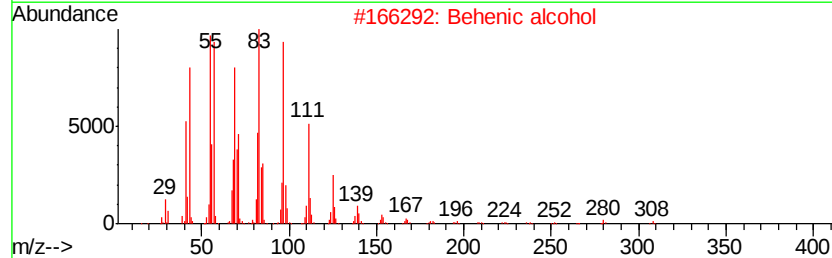
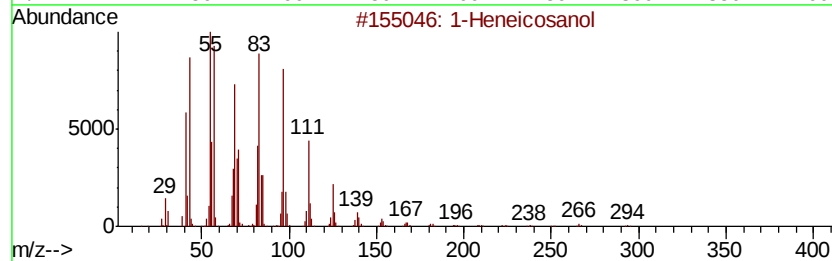
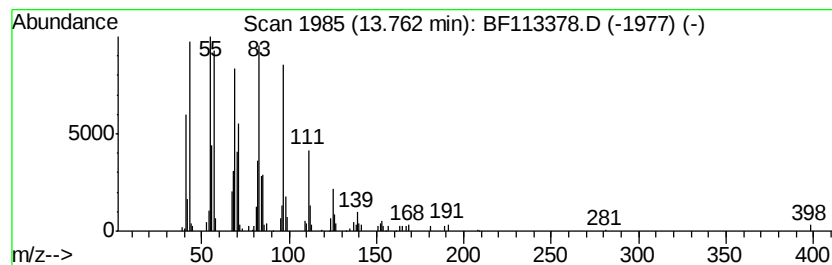
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Peak Number 5 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	6.70 ng	586051	Chrysene-d12	13.84
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	93
2	Behenic alcohol	326 C22H46O	000661-19-8	93
3	Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3	93
4	3-Eicosene, (E)-	280 C20H40	074685-33-9	91
5	n-Nonadecanol-1	284 C19H40O	001454-84-8	90



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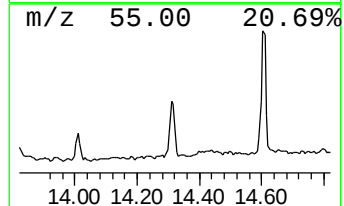
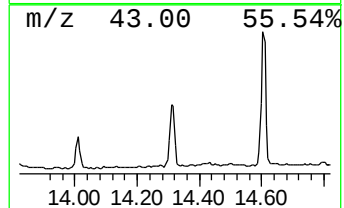
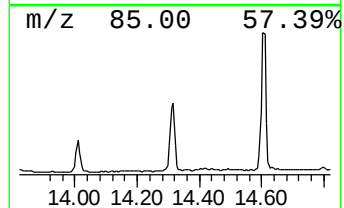
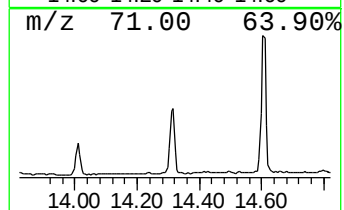
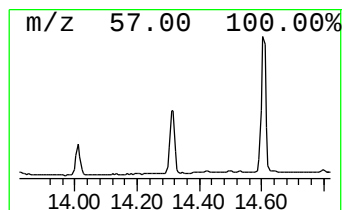
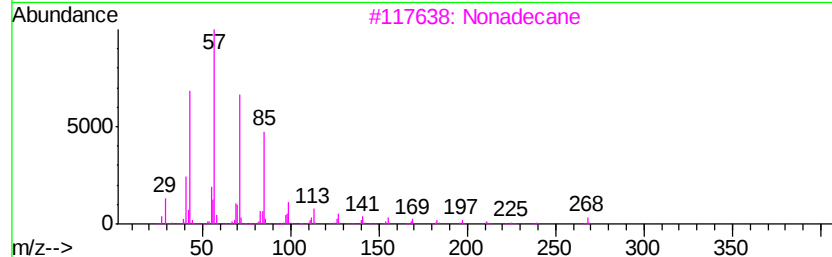
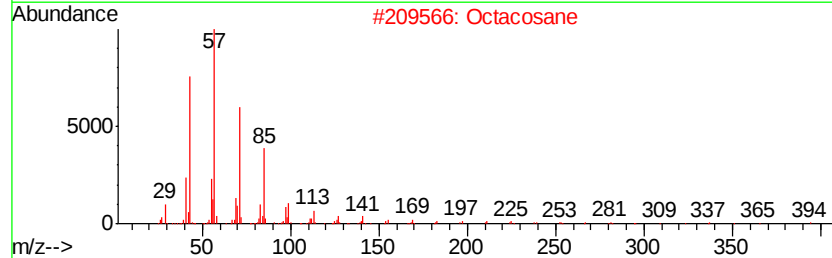
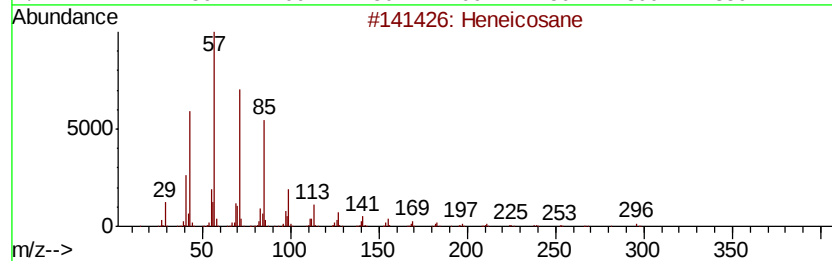
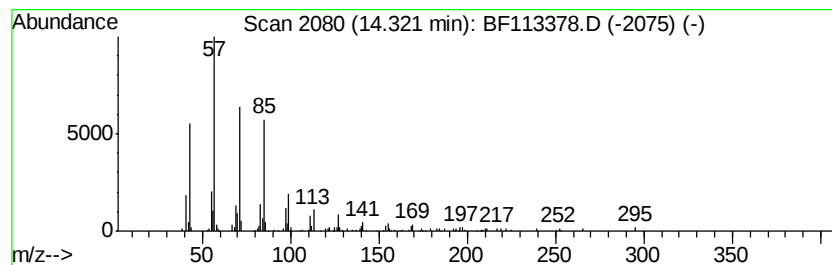
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 6 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	3.87 ng	338845	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Nonadecane		268	C19H40	000629-92-5	87
4	Tetratetracontane		619	C44H90	007098-22-8	87
5	2-Bromotetradecane		276	C14H29Br	074036-95-6	86



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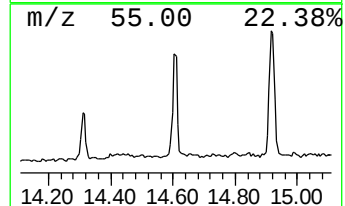
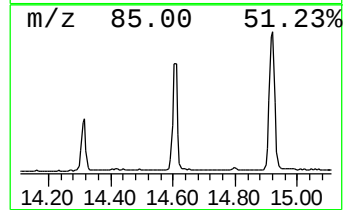
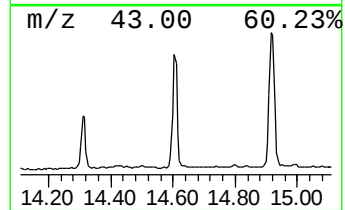
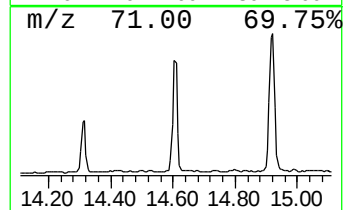
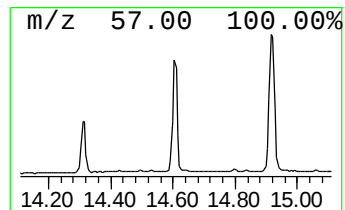
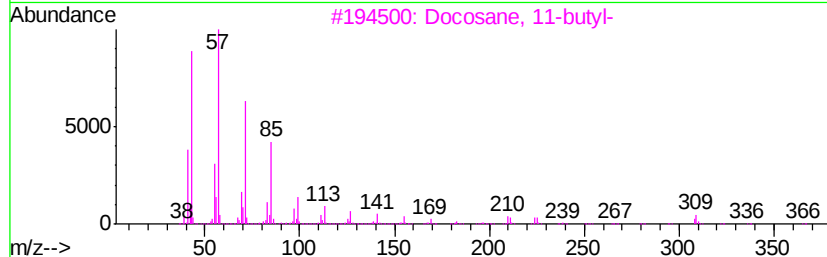
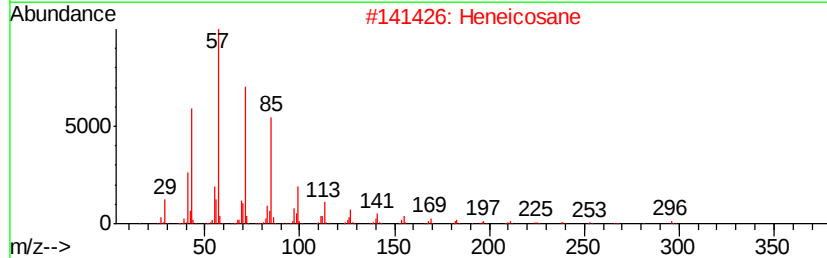
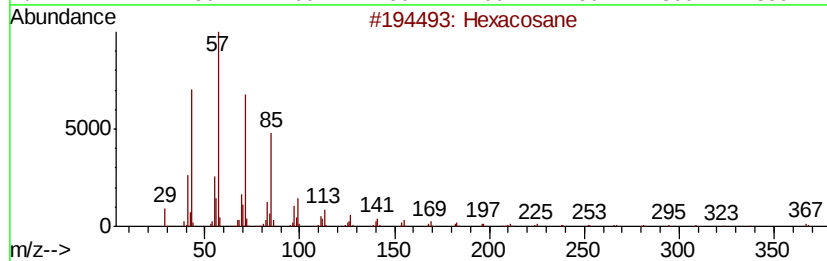
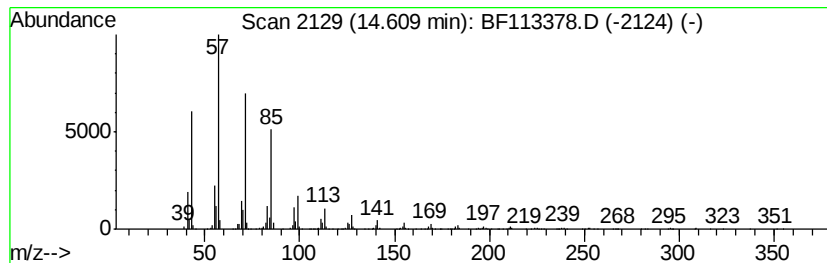
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	10.05 ng	785283	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032819\
Data File : BF113378.D
Acq On : 28 Mar 2019 17:09
Operator : JU/SJ
Sample : K2107-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

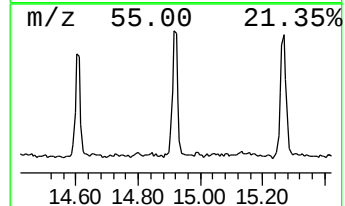
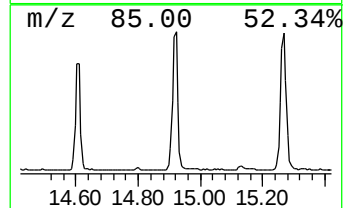
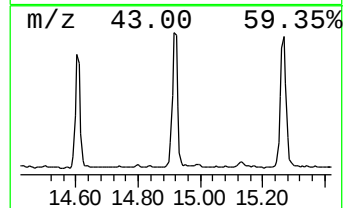
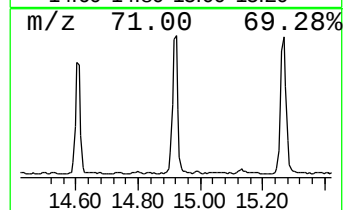
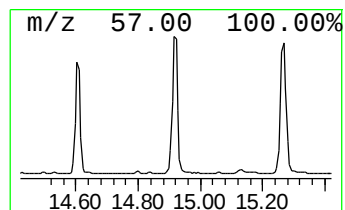
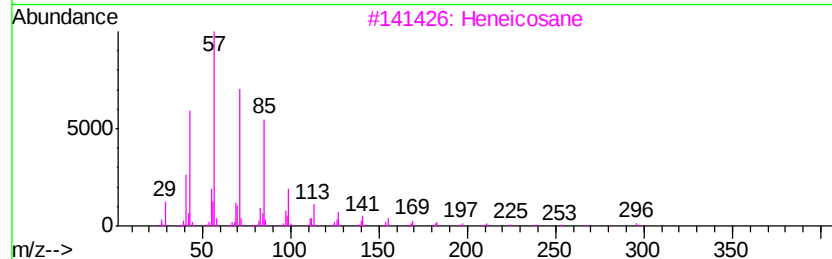
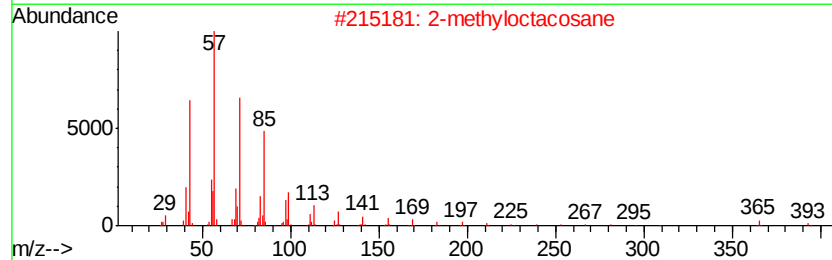
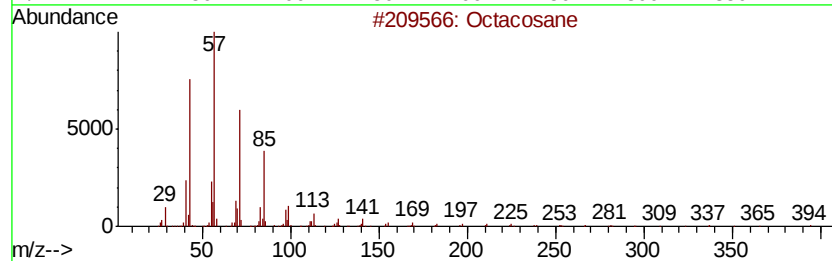
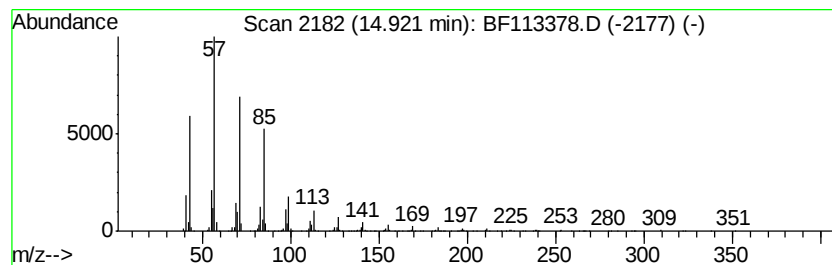
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	13.61 ng	1063810	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Hexacosane		366	C26H54	000630-01-3	91
5	Tetracosane		338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032819\
Data File : BF113378.D
Acq On : 28 Mar 2019 17:09
Operator : JU/SJ
Sample : K2107-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

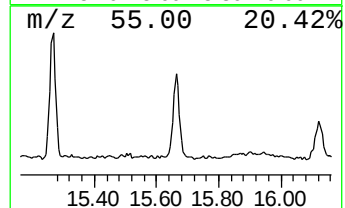
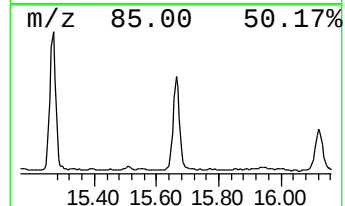
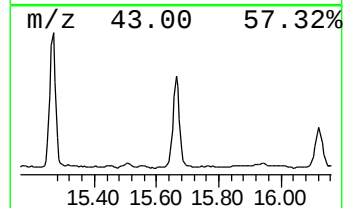
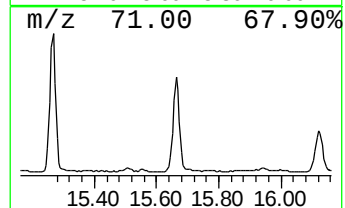
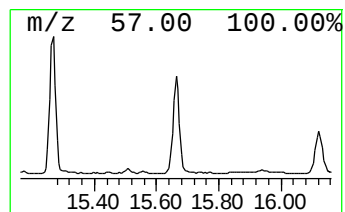
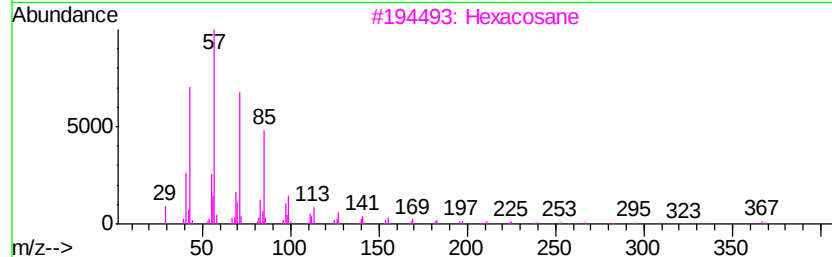
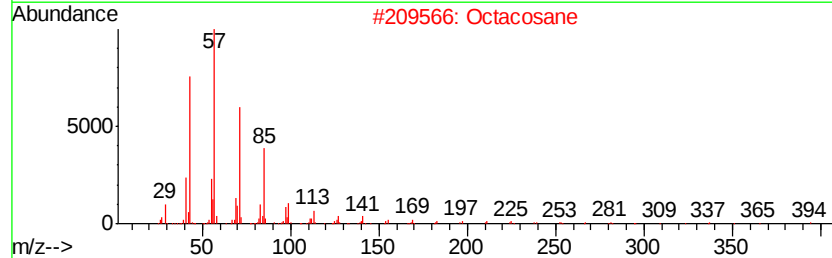
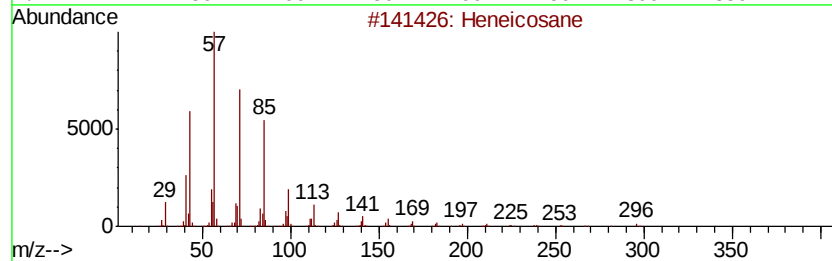
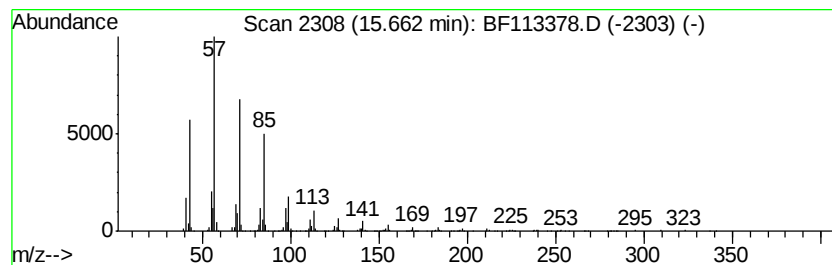
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane, 11-(1-ethylpro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	11.92 ng	931945	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Hexacosane		366	C26H54	000630-01-3	91
4	Docosane, 11-butyl-		366	C26H54	013475-76-8	90
5	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032819\
Data File : BF113378.D
Acq On : 28 Mar 2019 17:09
Operator : JU/SJ
Sample : K2107-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

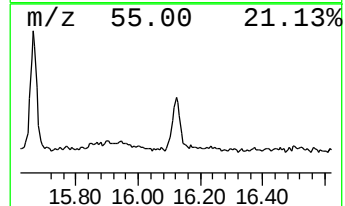
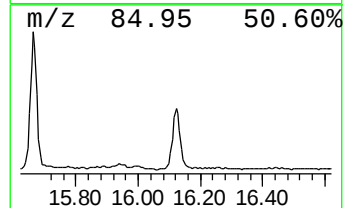
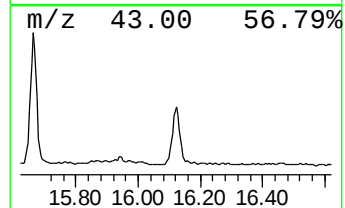
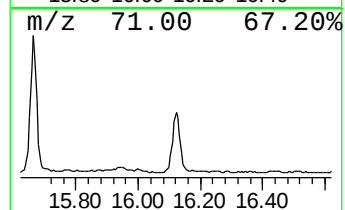
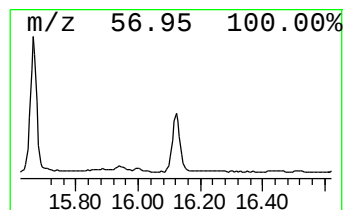
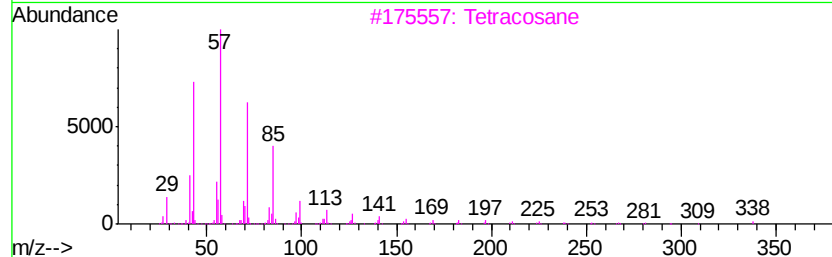
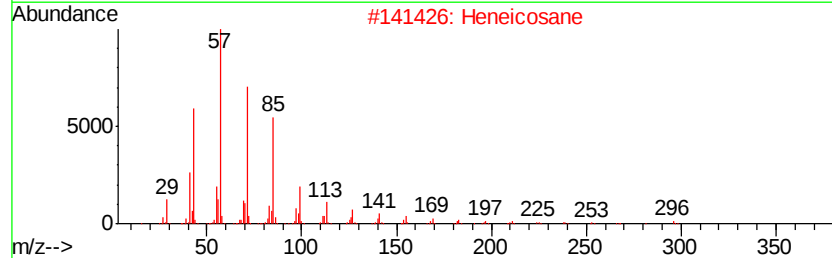
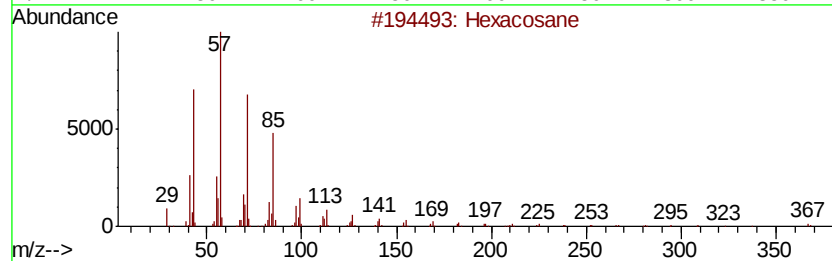
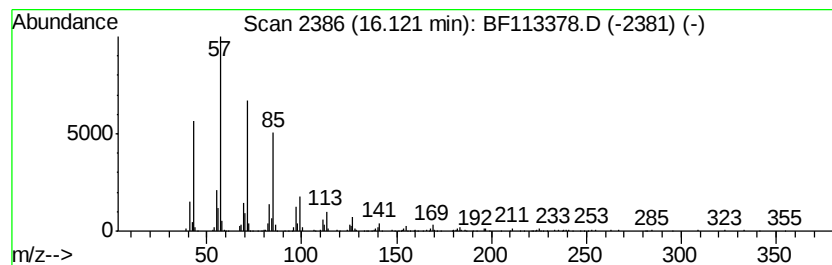
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	5.98 ng	467297	Perylene-d12	15.24

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Heneicosane	296	C21H44	000629-94-7	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032819\
Data File : BF113378.D
Acq On : 28 Mar 2019 17:09
Operator : JU/SJ
Sample : K2107-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.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
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n-Hexadecanoic acid	11.75	4.2	ng	317674	4	11.21	1502250	20.0
Octadecanoic acid	12.53	4.0	ng	347285	5	13.84	1749350	20.0
1-Heneicosanol	13.76	6.7	ng	586051	5	13.84	1749350	20.0
Heneicosane	14.32	3.9	ng	338845	5	13.84	1749350	20.0
Hexacosane	14.61	10.1	ng	785283	6	15.24	1563320	20.0
Octacosane	14.92	13.6	ng	1063810	6	15.24	1563320	20.0
Heneicosane, 11-(...	15.66	11.9	ng	931945	6	15.24	1563320	20.0
2-methyloctacosane	16.12	6.0	ng	467297	6	15.24	1563320	20.0