

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
 Data File : BF113419.D
 Acq On : 29 Mar 2019 17:57
 Operator : JU/SJ
 Sample : K2139-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S7B(12-20)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-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	573	rBV	2850809	2976391	73.79%	8.408%
2	6.351	720	725	742	rBV	2975996	3246884	80.50%	9.173%
3	6.475	742	746	749	rBV	3409328	3061747	75.91%	8.650%
4	6.698	781	784	793	rBV	1058501	929852	23.05%	2.627%
5	6.857	807	811	827	rBV	2787508	2454695	60.86%	6.935%
6	7.263	876	880	906	rBV	2035557	2034619	50.44%	5.748%
7	7.981	999	1002	1019	rBV	1197596	1229938	30.49%	3.475%
8	9.057	1181	1185	1197	rBV	3875298	3623511	89.84%	10.237%
9	9.145	1198	1200	1217	rVB3	31031	58431	1.45%	0.165%
10	9.451	1249	1252	1262	rVB	189144	208561	5.17%	0.589%
11	9.733	1296	1300	1312	rVB	1375063	1415079	35.08%	3.998%
12	10.516	1429	1433	1448	rBV	1937427	2231058	55.31%	6.303%
13	11.210	1547	1551	1564	rBV	1602669	1567356	38.86%	4.428%
14	11.745	1639	1642	1654	rBV2	112112	216054	5.36%	0.610%
15	12.421	1754	1757	1762	rBV	81419	82378	2.04%	0.233%
16	12.527	1772	1775	1786	rBV3	91772	182490	4.52%	0.516%
17	12.610	1786	1789	1792	rVV	146263	143704	3.56%	0.406%
18	12.645	1792	1795	1798	rVB	79283	73142	1.81%	0.207%
19	12.792	1815	1820	1823	rBV	4078911	4033397	100.00%	11.395%
20	12.816	1823	1824	1830	rVB	230415	152531	3.78%	0.431%
21	13.333	1908	1912	1915	rBV	152861	143475	3.56%	0.405%
22	13.692	1970	1973	1976	rBV	65845	58125	1.44%	0.164%
23	13.792	1980	1990	1991	rVV6	35825	99895	2.48%	0.282%
24	13.839	1991	1998	2011	rVB	1513034	1821245	45.15%	5.145%
25	14.010	2023	2027	2033	rVB	85074	85840	2.13%	0.243%
26	14.310	2075	2078	2082	rVB	154009	133160	3.30%	0.376%
27	14.604	2124	2128	2132	rBV	218640	197322	4.89%	0.557%
28	14.668	2136	2139	2143	rBV	162640	160946	3.99%	0.455%
29	14.845	2165	2169	2176	rBV	80079	144102	3.57%	0.407%
30	14.915	2177	2181	2185	rBV	223545	228936	5.68%	0.647%
31	15.127	2213	2217	2223	rBV2	44022	58251	1.44%	0.165%
32	15.239	2231	2236	2255	rVB	1078013	1751110	43.42%	4.947%
33	15.656	2302	2307	2313	rBV	199683	286765	7.11%	0.810%
34	16.115	2380	2385	2393	rBV	125819	213452	5.29%	0.603%

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ClientSampleId :
S7B(12-20)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

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35	16.651	2472	2476	2483	rVB2	49584	93136	2.31%	0.263%
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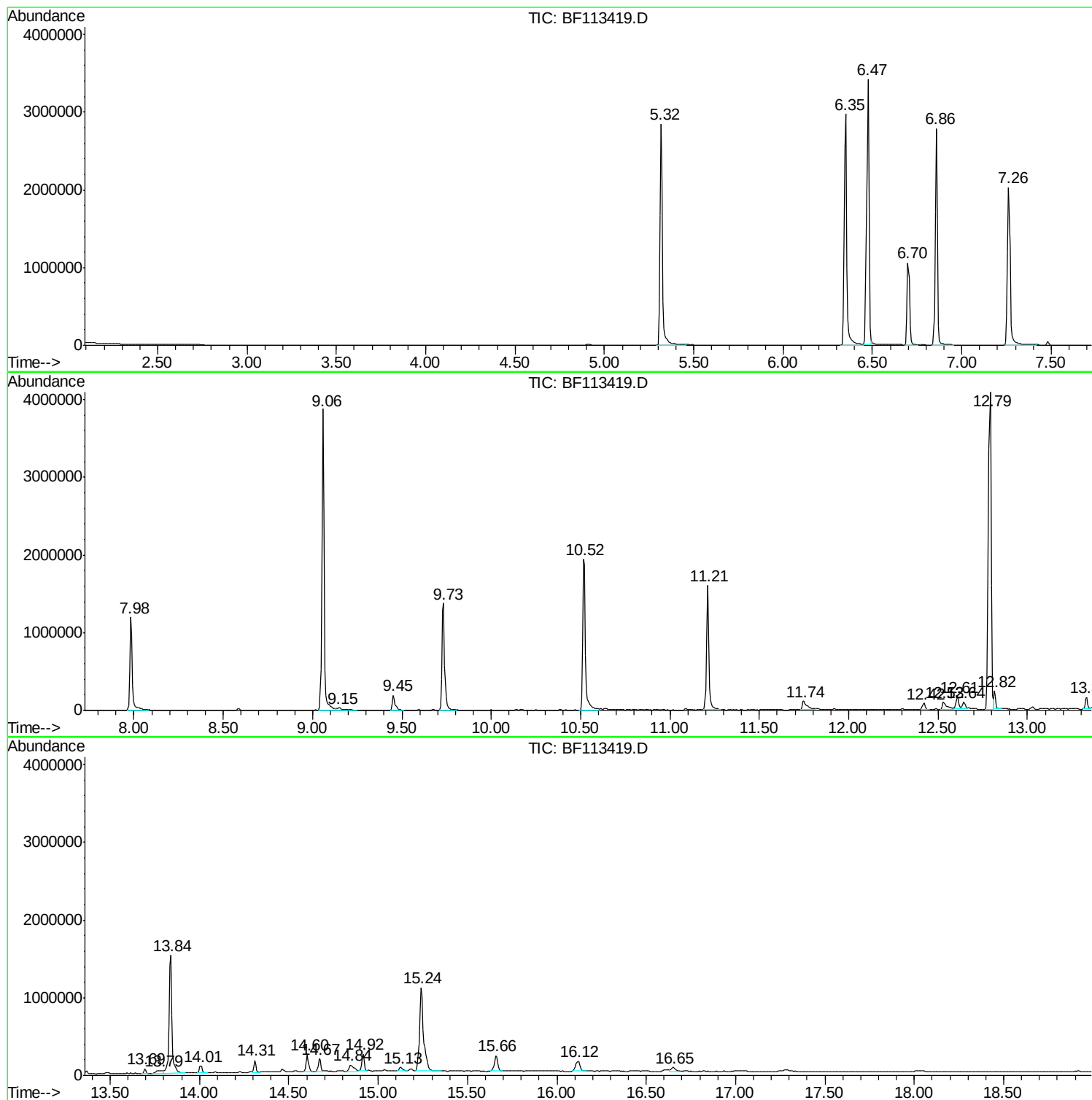
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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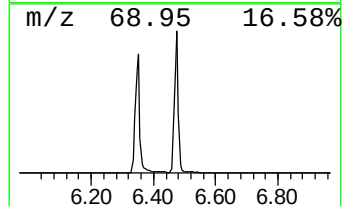
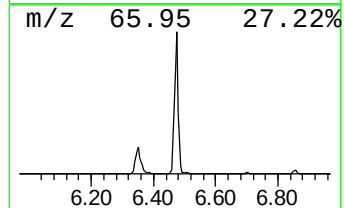
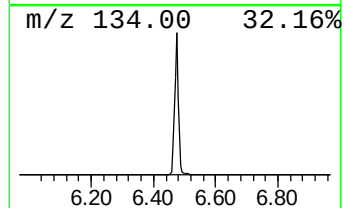
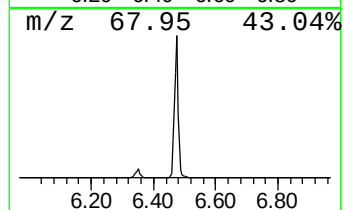
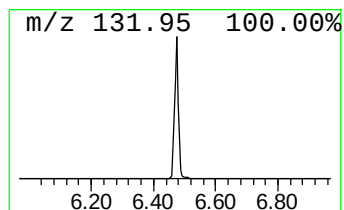
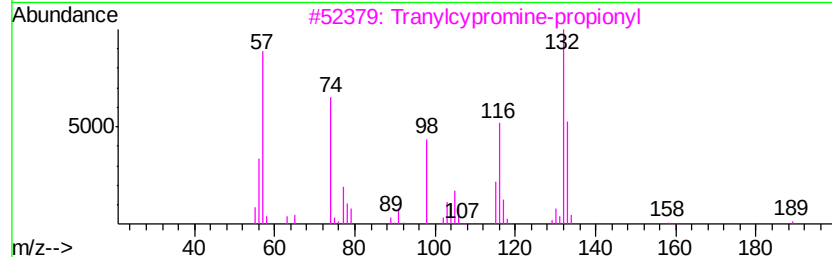
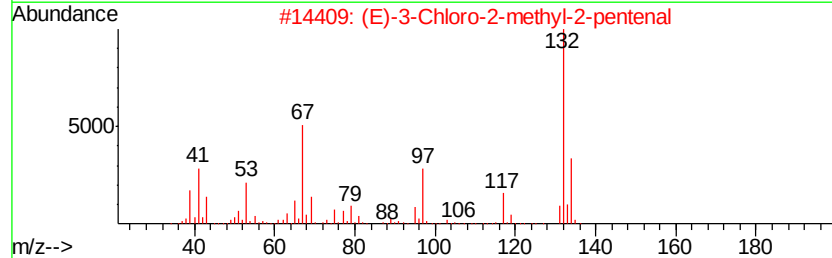
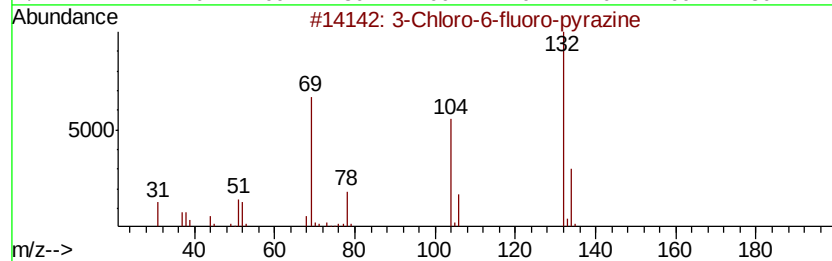
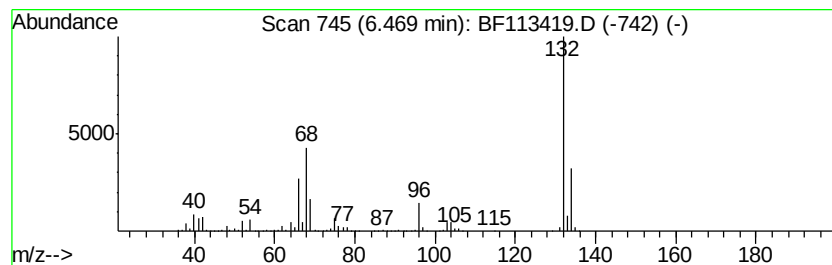
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	65.85 ng	3061750	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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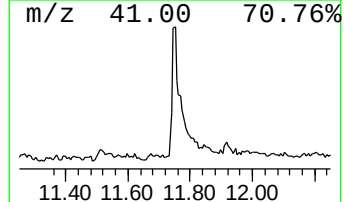
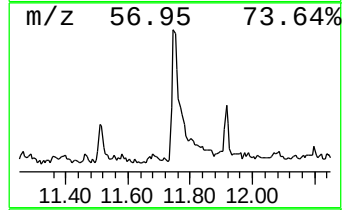
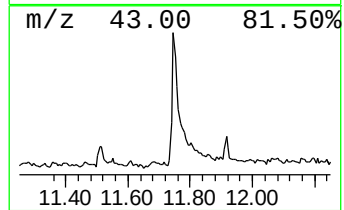
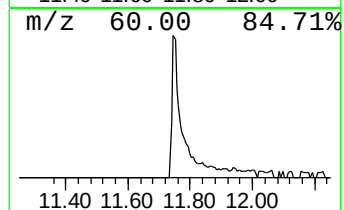
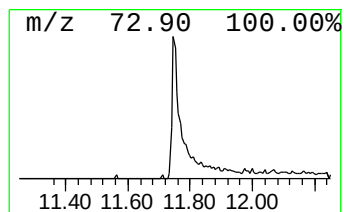
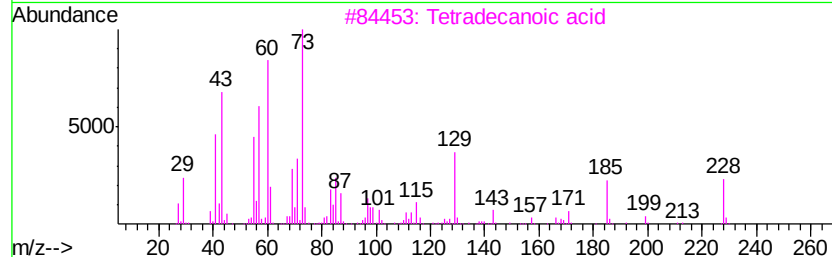
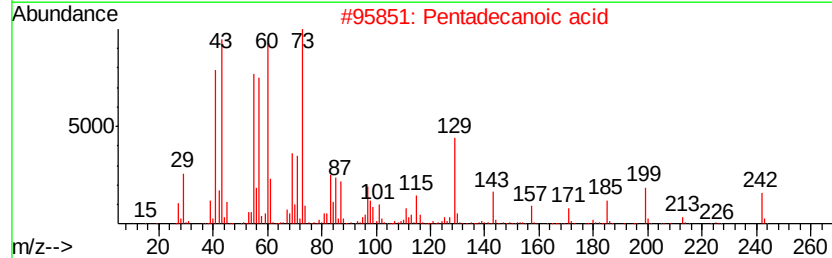
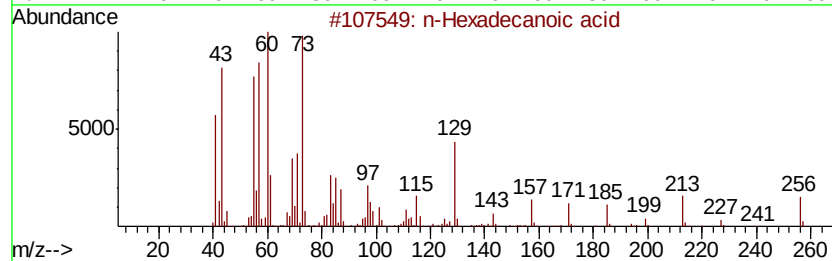
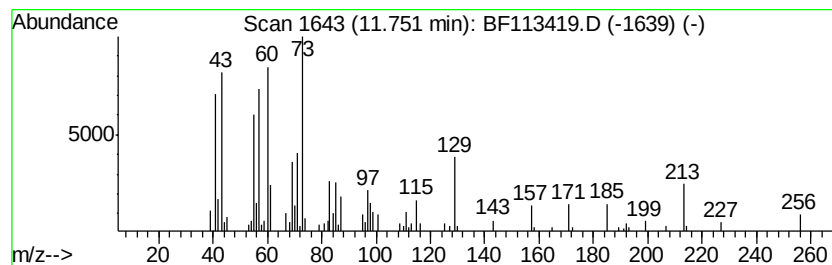
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.75	2.76 ng	216054	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	11



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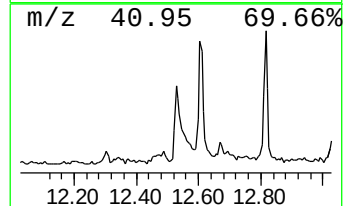
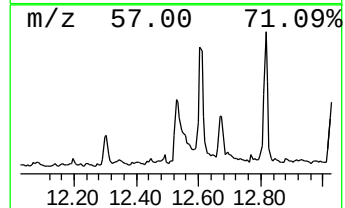
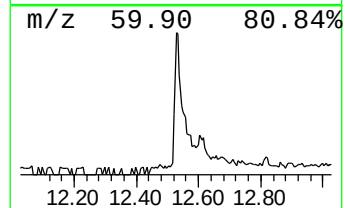
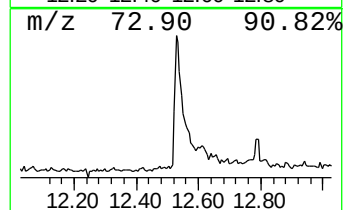
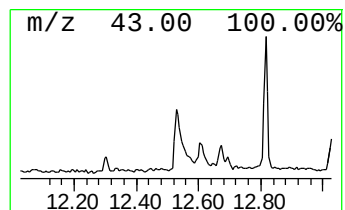
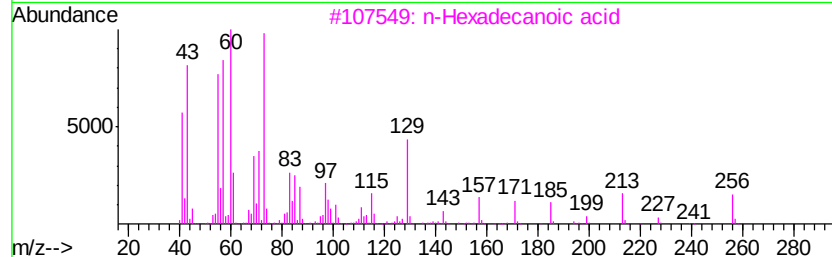
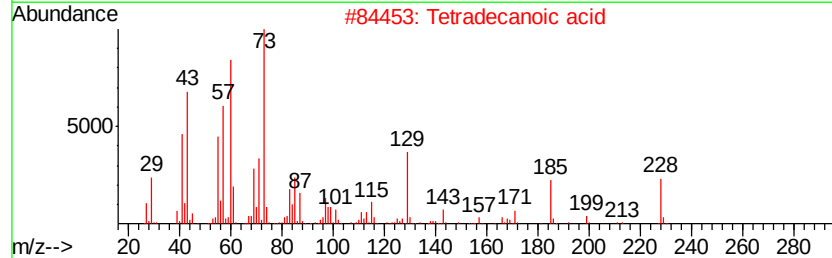
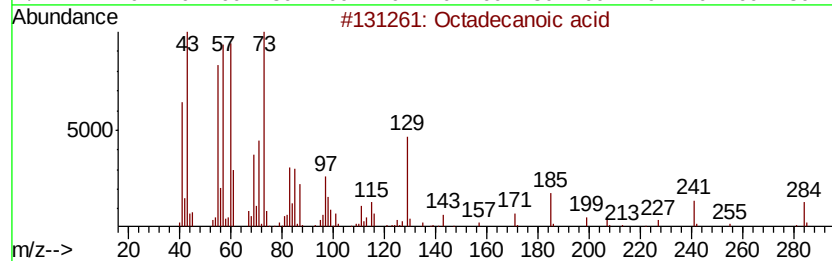
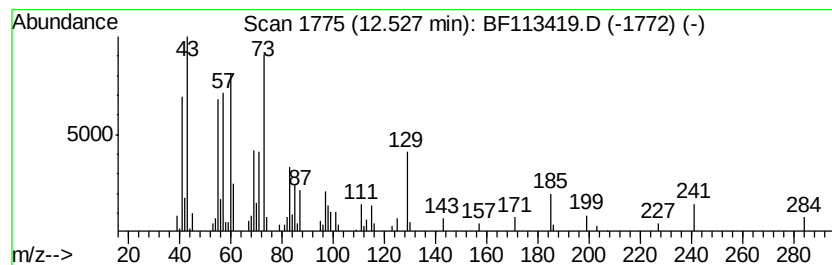
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.53	2.00 ng	182490	Chrysene-d12		13.84
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



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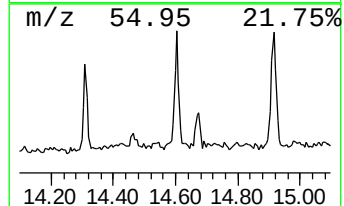
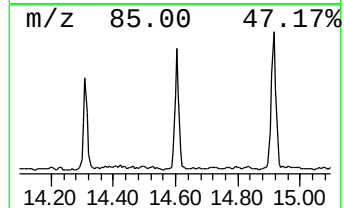
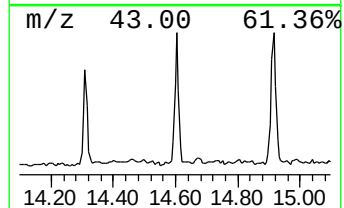
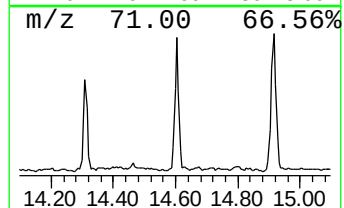
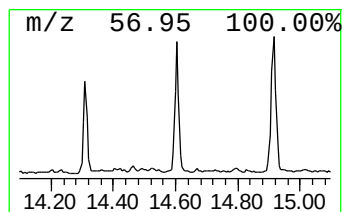
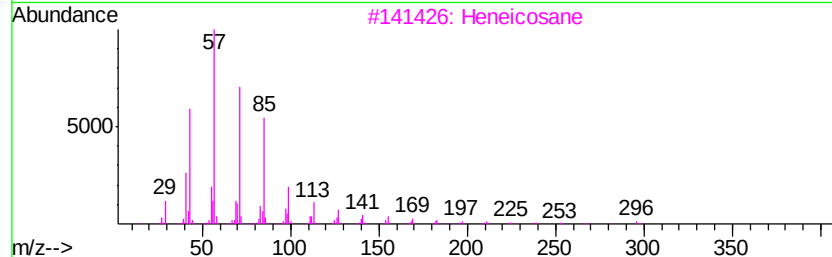
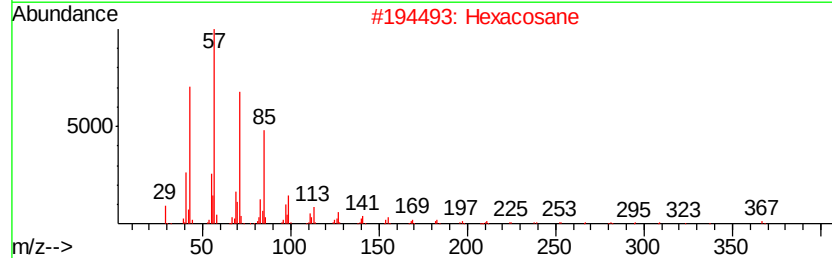
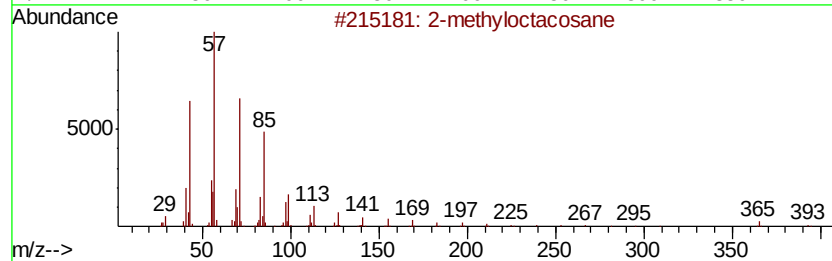
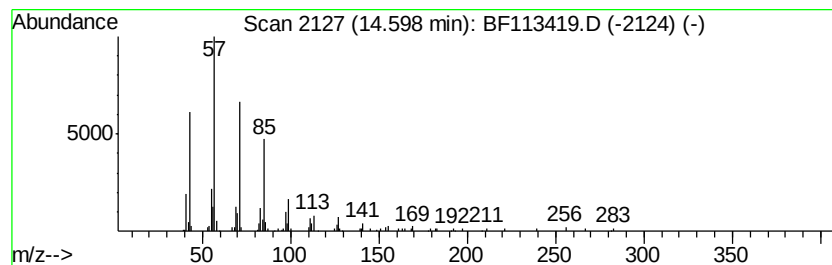
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.25 ng	197322	Perylene-d12	15.24

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	triacontane	422	C30H62	000638-68-6	91
5	Heptadecane	240	C17H36	000629-78-7	91



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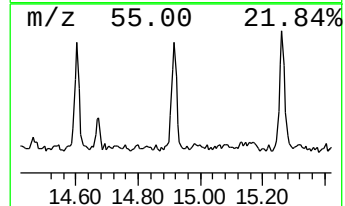
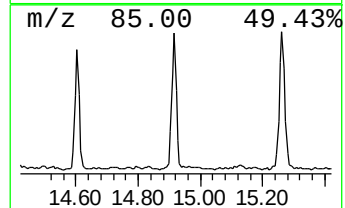
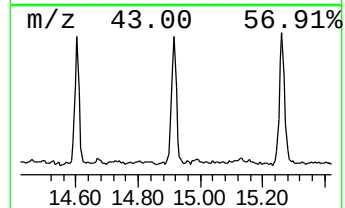
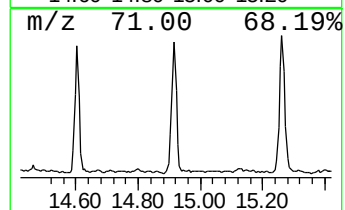
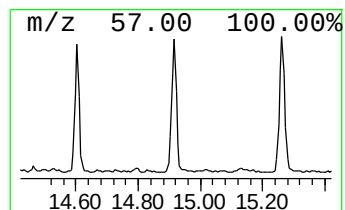
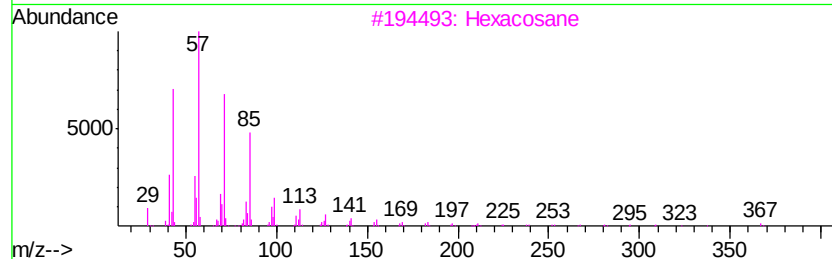
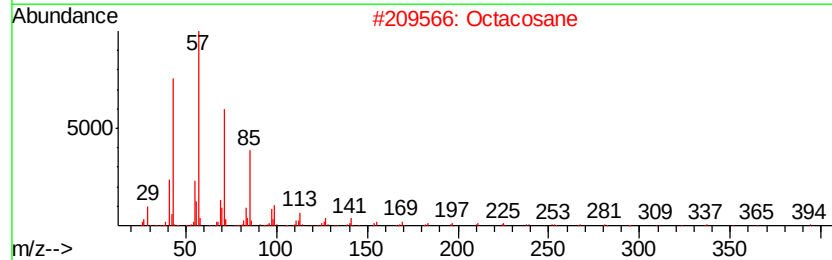
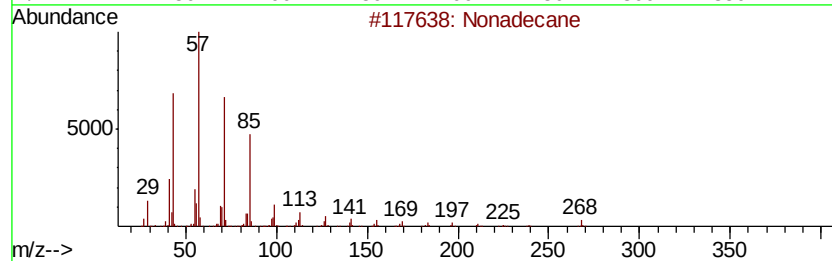
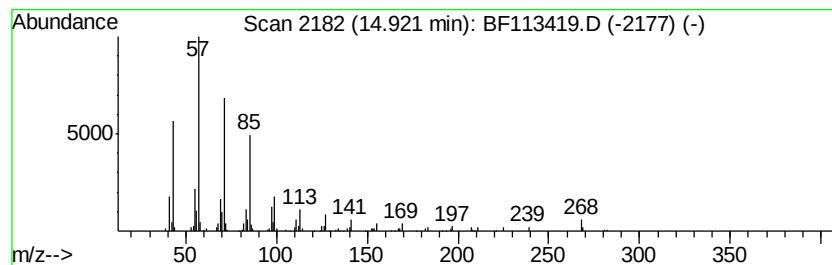
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.61 ng	228936	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	94
2	Octacosane		394	C28H58	000630-02-4	91
3	Hexacosane		366	C26H54	000630-01-3	91
4	Heneicosane		296	C21H44	000629-94-7	91
5	Pentacosane		352	C25H52	000629-99-2	90



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ClientSampleId :
S7B(12-20)COMP

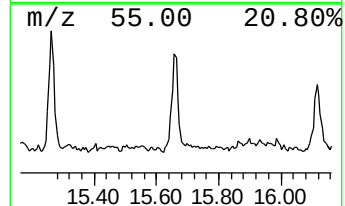
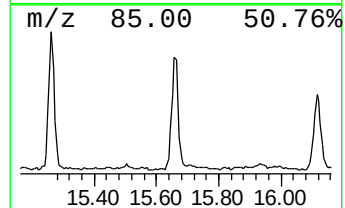
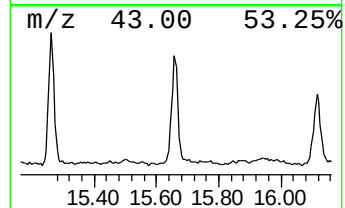
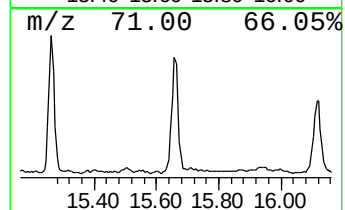
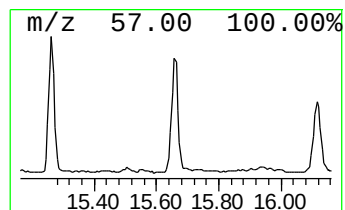
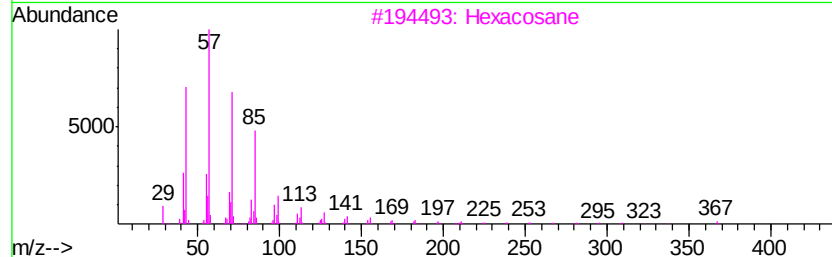
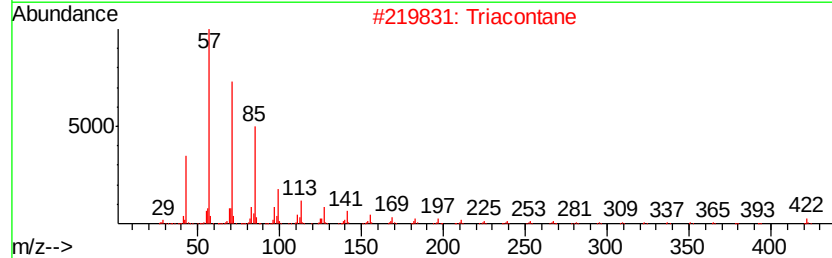
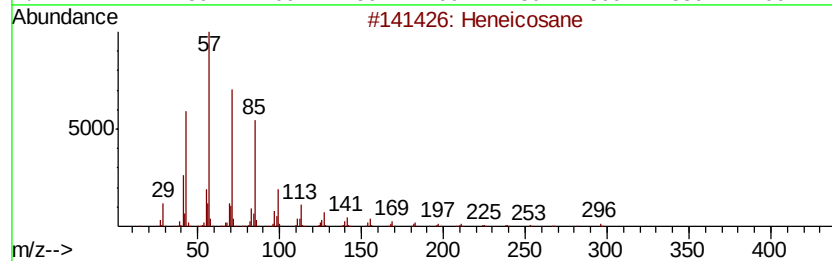
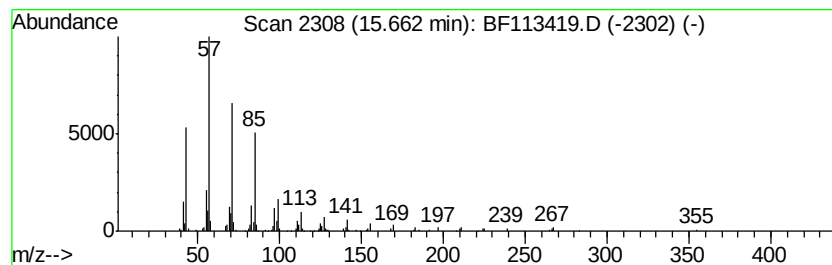
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	3.28 ng	286765	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Triacontane		422	C30H62	000638-68-6	91
3	Hexacosane		366	C26H54	000630-01-3	90
4	Heptadecane		240	C17H36	000629-78-7	87
5	Octadecane		254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
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Acq On : 29 Mar 2019 17:57
Operator : JU/SJ
Sample : K2139-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

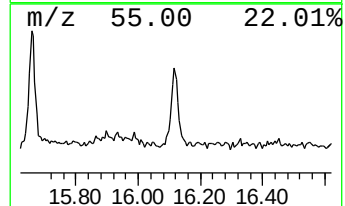
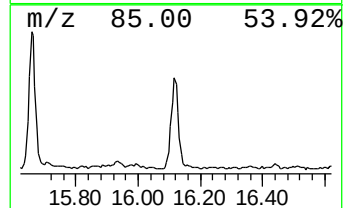
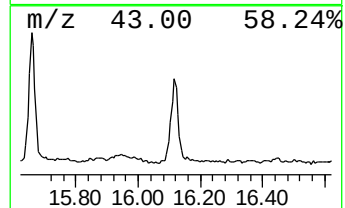
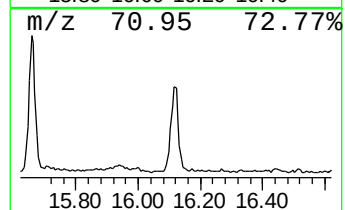
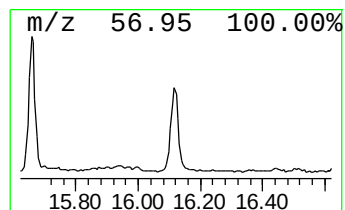
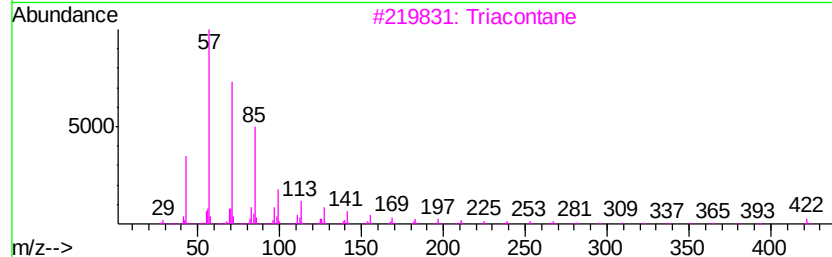
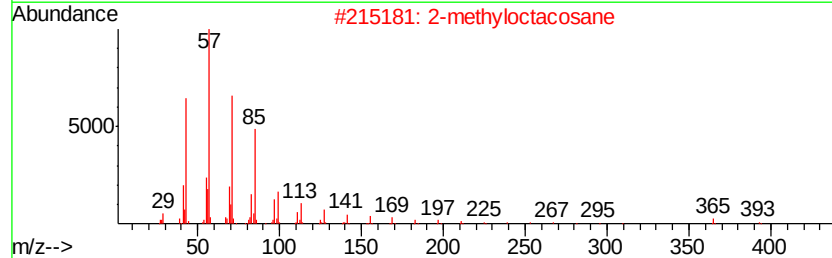
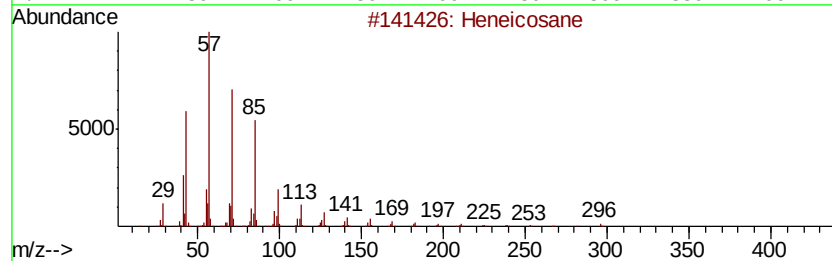
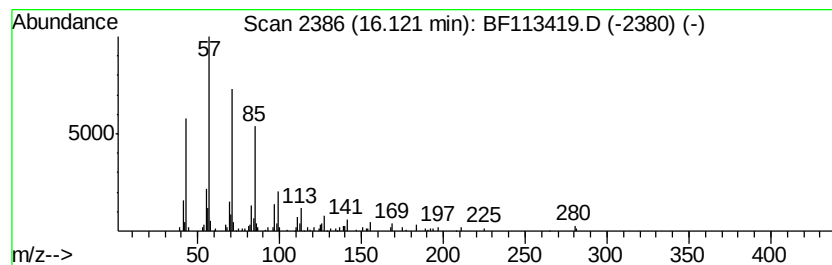
Instrument :
BNA_F
ClientSampleId :
S7B(12-20)COMP

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 8 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.44 ng	213452	Perylene-d12	15.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296	C21H44	000629-94-7 91
2	2-methyloctacosane	408	C29H60	1000376-72-8 91
3	Triacontane	422	C30H62	000638-68-6 91
4	Hexacosane	366	C26H54	000630-01-3 90
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1 90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113419.D
Acq On : 29 Mar 2019 17:57
Operator : JU/SJ
Sample : K2139-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S7B(12-20)COMP

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
unknown6.47	6.47	65.8	ng	3061750	1	6.70	929852	20.0
n-Hexadecanoic acid	11.75	2.8	ng	216054	4	11.21	1567360	20.0
Octadecanoic acid	12.53	2.0	ng	182490	5	13.84	1821250	20.0
2-methyloctacosane	14.60	2.3	ng	197322	6	15.24	1751110	20.0
Nonadecane	14.92	2.6	ng	228936	6	15.24	1751110	20.0
Heneicosane	15.66	3.3	ng	286765	6	15.24	1751110	20.0
Triacontane	16.12	2.4	ng	213452	6	15.24	1751110	20.0