

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
 Data File : BF112986.D
 Acq On : 12 Mar 2019 6:11
 Operator : JU/SJ
 Sample : K1817-19
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-028-B099-030619

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	3.663	262	268	273	rVB	24907	37877	2.08%	0.207%
2	5.328	547	551	568	rBV	1256114	1211478	66.43%	6.619%
3	6.363	723	727	735	rBV	1391104	1355717	74.34%	7.407%
4	6.492	746	749	753	rBV	1460295	1354626	74.28%	7.401%
5	6.728	786	789	793	rBV	709742	569039	31.20%	3.109%
6	6.887	812	816	825	rVB	1105735	983151	53.91%	5.372%
7	7.287	880	884	891	rBV	841197	777657	42.64%	4.249%
8	7.339	891	893	897	rVB	37144	34757	1.91%	0.190%
9	8.010	1004	1007	1015	rBV	726377	720362	39.50%	3.936%
10	9.086	1186	1190	1205	rBV	1579938	1528189	83.80%	8.349%
11	9.480	1254	1257	1263	rBV	121503	118030	6.47%	0.645%
12	9.763	1301	1305	1318	rVB	1003308	980949	53.79%	5.359%
13	10.545	1434	1438	1457	rBV	1296388	1336892	73.31%	7.304%
14	11.239	1552	1556	1572	rBV	1215653	1259208	69.05%	6.880%
15	11.774	1644	1647	1657	rBV3	176615	215730	11.83%	1.179%
16	12.445	1757	1761	1765	rBV	97825	89282	4.90%	0.488%
17	12.498	1765	1770	1776	rVV5	18586	27292	1.50%	0.149%
18	12.557	1776	1780	1791	rVV5	41581	76147	4.18%	0.416%
19	12.669	1793	1799	1803	rBV	83293	105349	5.78%	0.576%
20	12.816	1820	1824	1834	rBV	2061778	1823644	100.00%	9.964%
21	13.063	1861	1866	1870	rBV3	28780	35519	1.95%	0.194%
22	13.304	1903	1907	1912	rVB3	79169	78013	4.28%	0.426%
23	13.404	1921	1924	1926	rBV	21777	20013	1.10%	0.109%
24	13.733	1974	1980	1991	rBV2	115858	213289	11.70%	1.165%
25	13.863	1997	2002	2014	rBV	1093726	1164057	63.83%	6.360%
26	14.045	2029	2033	2039	rBV	53350	64238	3.52%	0.351%
27	14.345	2081	2084	2086	rBV	103317	96410	5.29%	0.527%
28	14.368	2086	2088	2092	rVB4	31933	41635	2.28%	0.227%
29	14.639	2131	2134	2138	rBV	105286	104129	5.71%	0.569%
30	14.710	2143	2146	2149	rVB	35061	36743	2.01%	0.201%
31	14.774	2154	2157	2161	rVB	66241	63039	3.46%	0.344%
32	14.874	2170	2174	2181	rBV	40456	81812	4.49%	0.447%
33	14.957	2184	2188	2192	rVV	215523	243138	13.33%	1.328%
34	14.998	2192	2195	2205	rVB4	52226	104077	5.71%	0.569%

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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	15.151	2219	2221	2227	rVB2	21428	23146	1.27%	0.126%
36	15.210	2228	2231	2235	rVV	20369	27316	1.50%	0.149%
37	15.268	2236	2241	2245	rVV	610768	791213	43.39%	4.323%
38	15.310	2245	2248	2257	rVB	106967	157592	8.64%	0.861%
39	15.715	2312	2317	2323	rBV	140282	191949	10.53%	1.049%
40	16.115	2381	2385	2390	rBV8	27432	48240	2.65%	0.264%
41	16.186	2393	2397	2404	rVB2	37557	62615	3.43%	0.342%
42	16.445	2439	2441	2450	rVB10	28329	49452	2.71%	0.270%

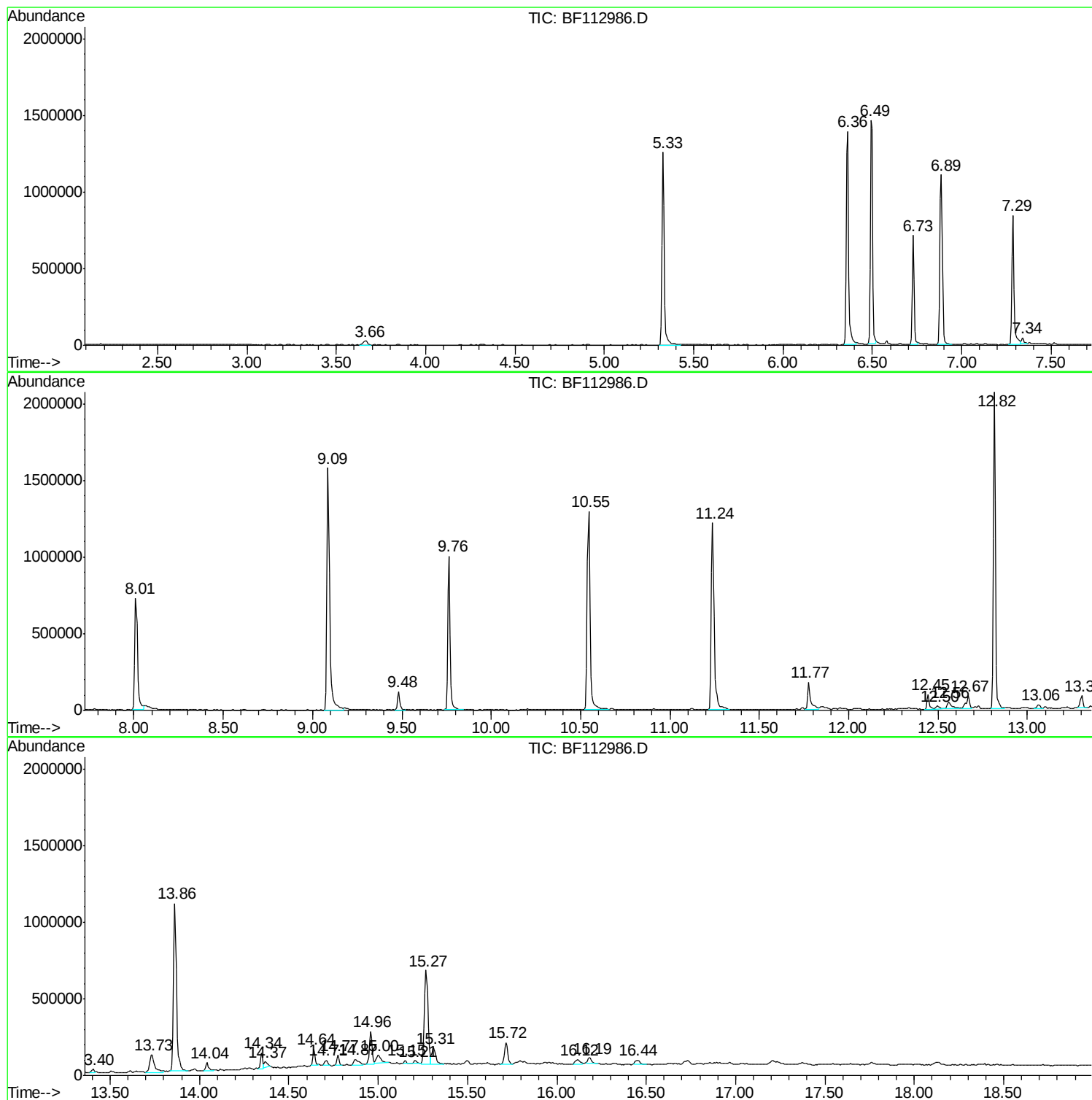
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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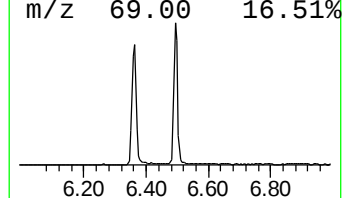
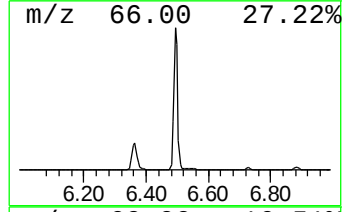
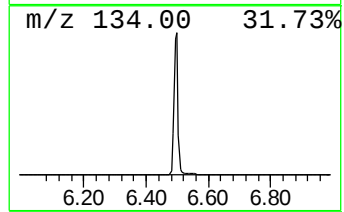
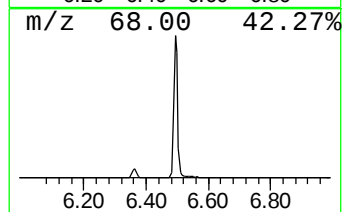
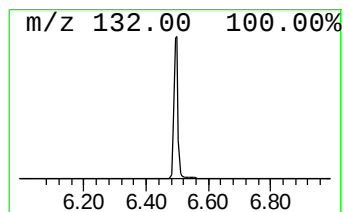
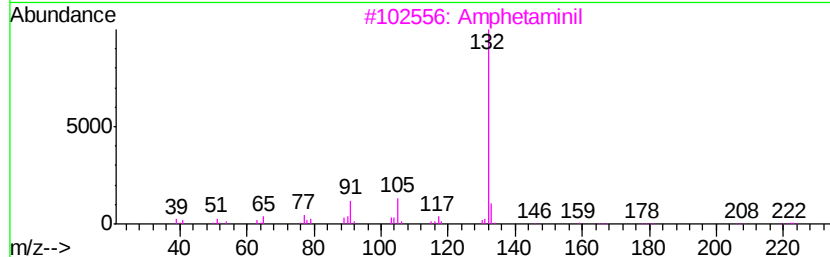
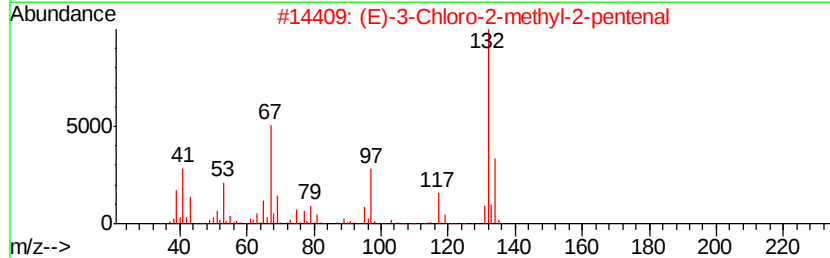
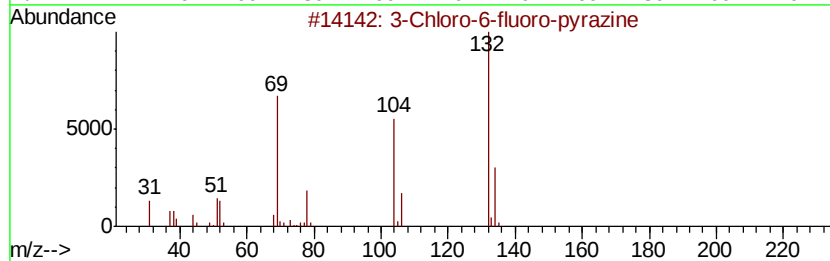
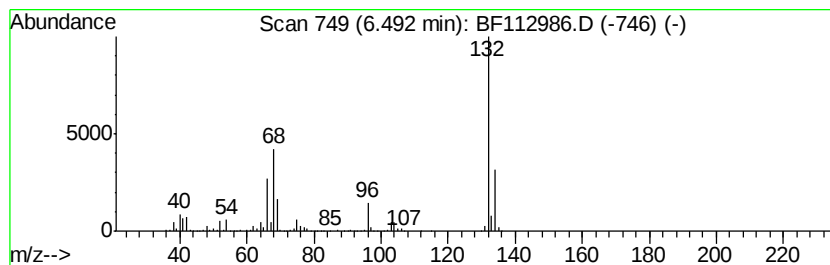
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	47.61 ng	1354630	1,4-Dichlorobenzene-d4	6.73

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		Amphetaminil	250	C17H18N2	017590-01-1	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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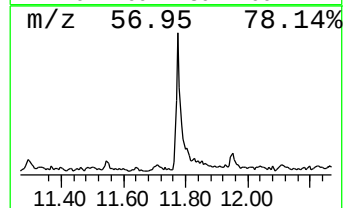
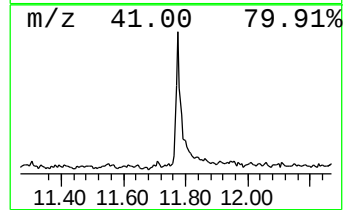
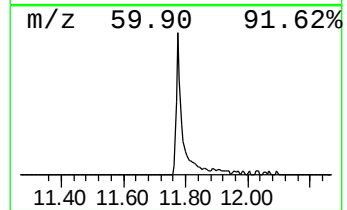
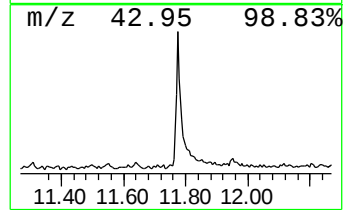
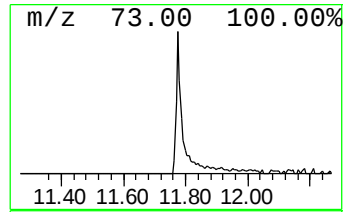
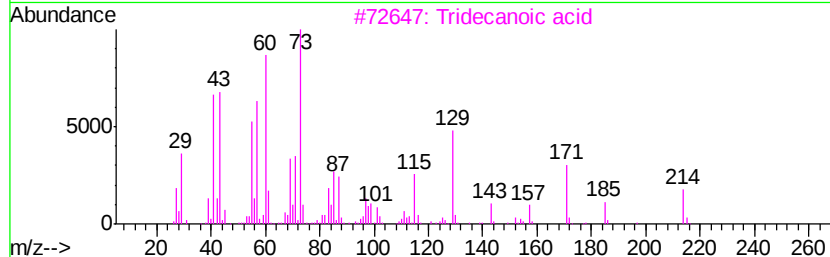
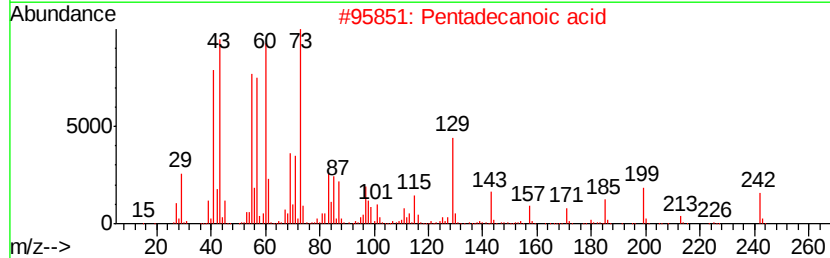
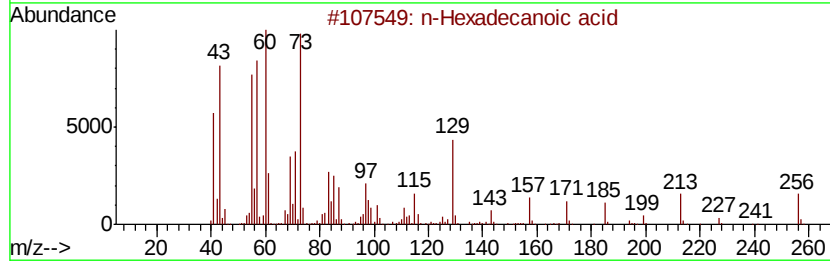
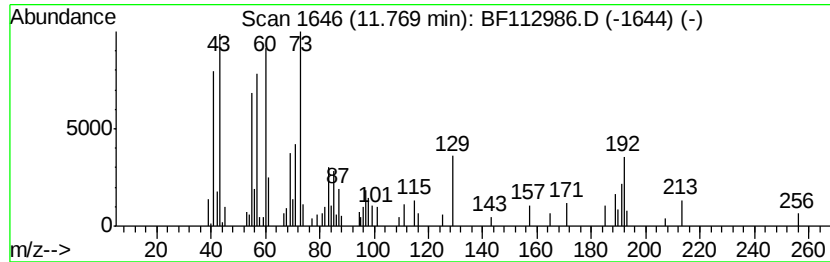
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.77	3.43 ng	215730	Phenanthrene-d10		11.24
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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	15



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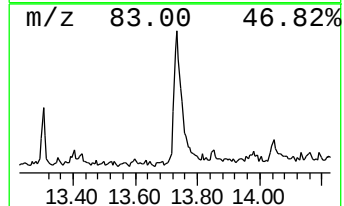
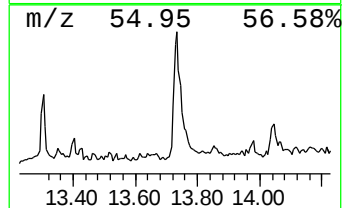
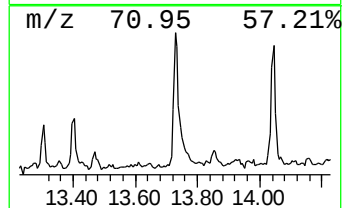
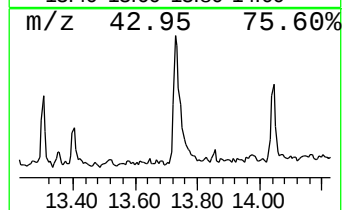
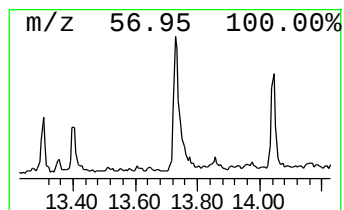
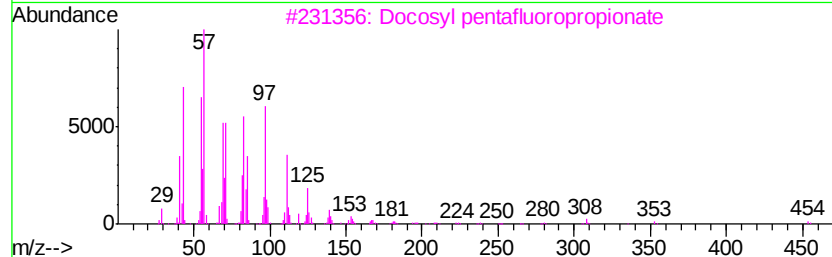
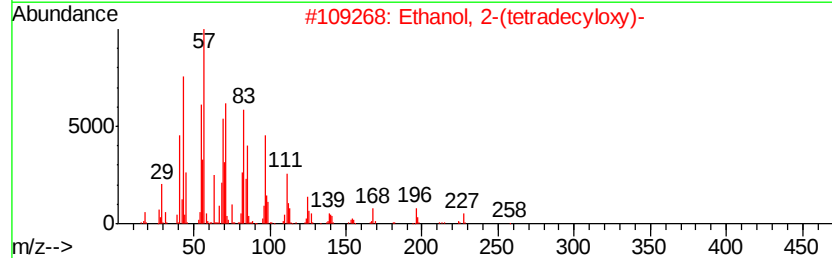
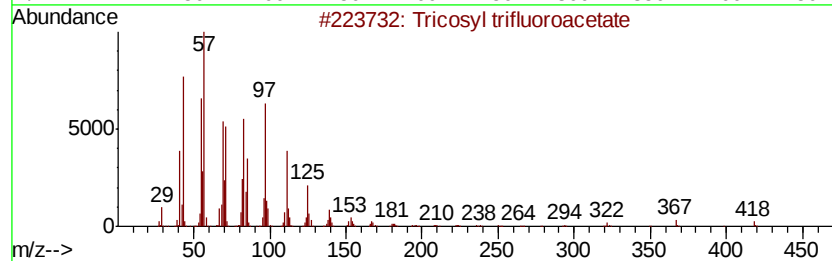
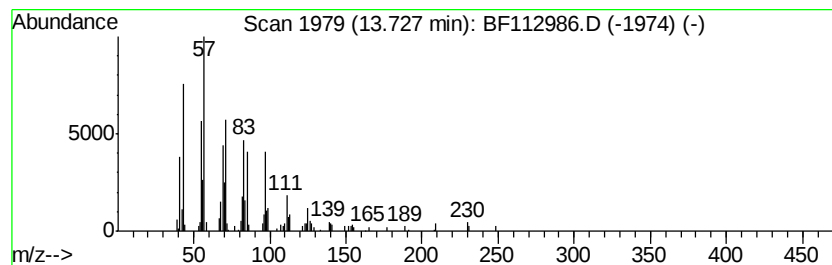
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tricosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.73	3.66 ng	213289	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	90
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87



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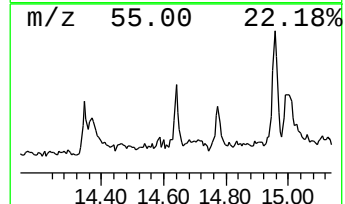
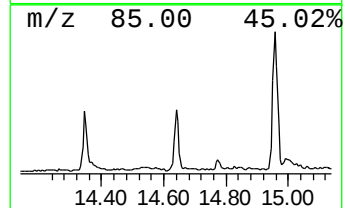
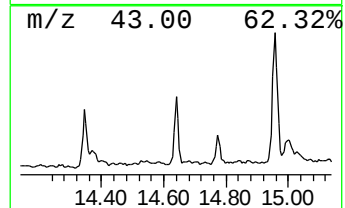
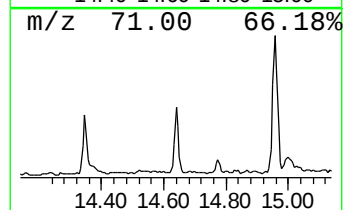
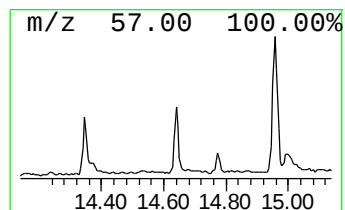
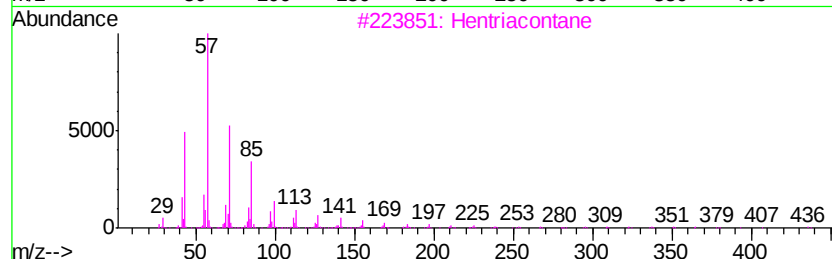
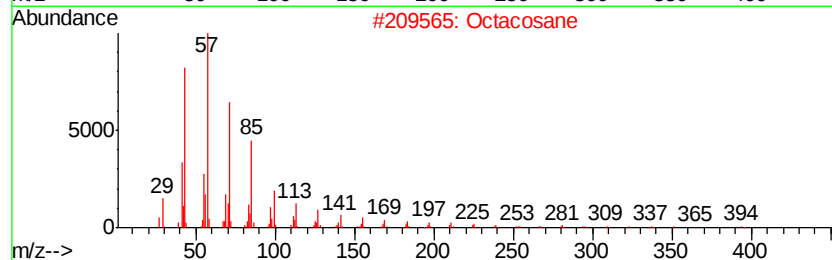
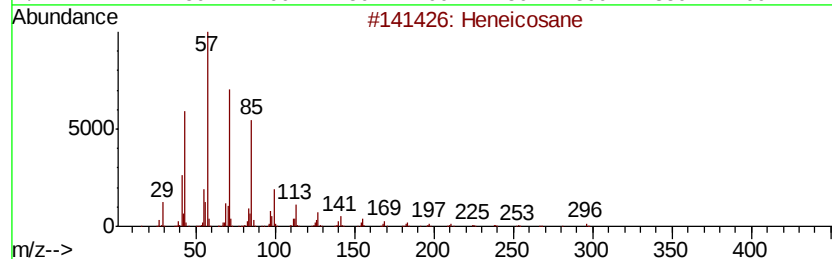
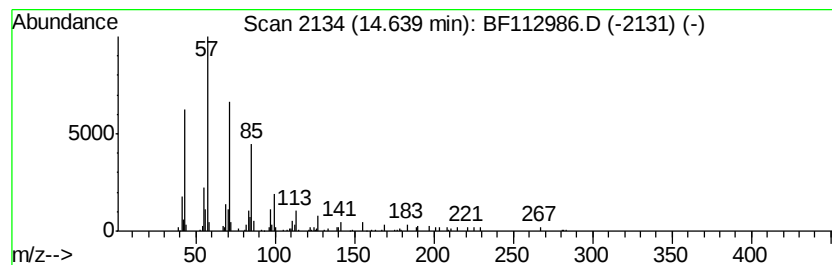
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.63 ng	104129	Perylene-d12	15.27

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	Hentriacontane		437	C31H64	000630-04-6	91
4	Triacontane		422	C30H62	000638-68-6	91
5	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	90



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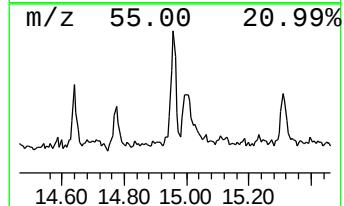
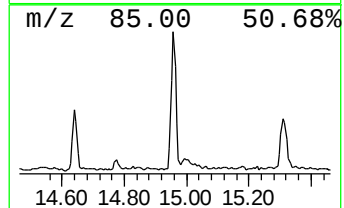
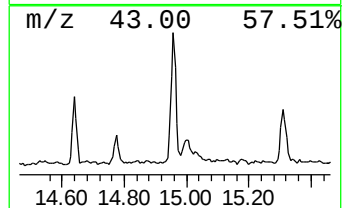
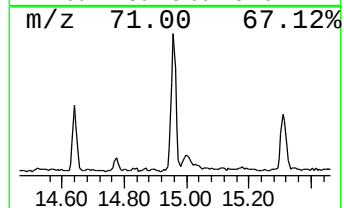
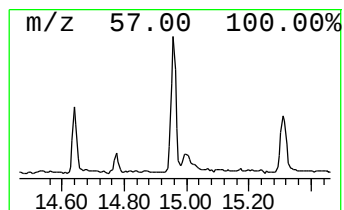
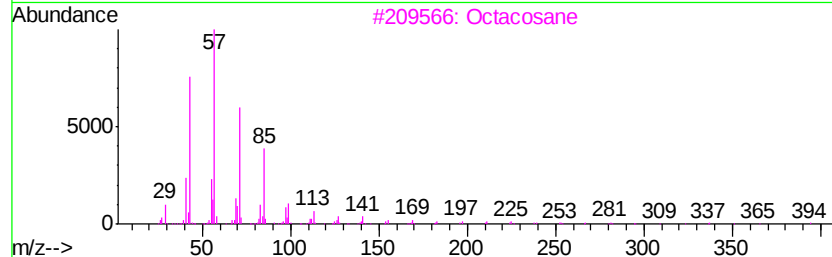
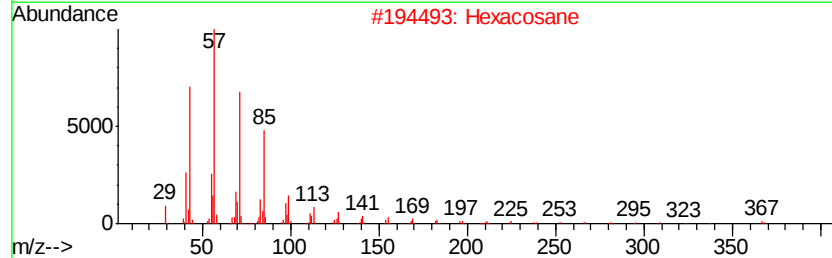
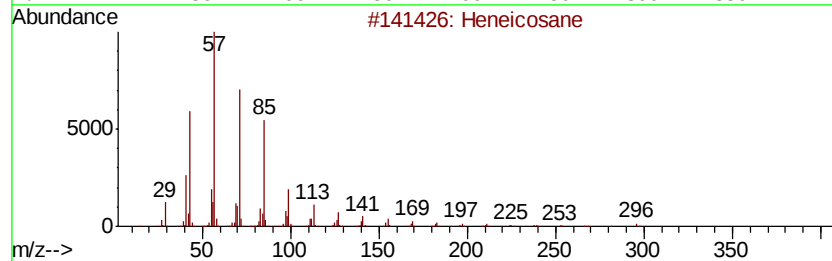
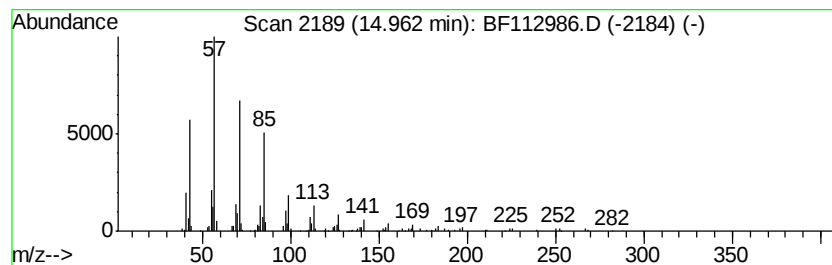
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown14.96 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	6.15 ng	243138	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Nonadecane	268	C19H40	000629-92-5	90
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112986.D
Acq On : 12 Mar 2019 6:11
Operator : JU/SJ
Sample : K1817-19
Misc :
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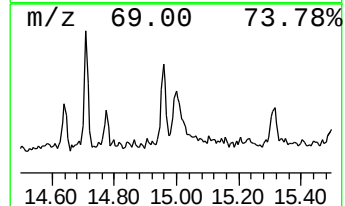
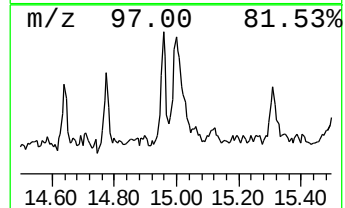
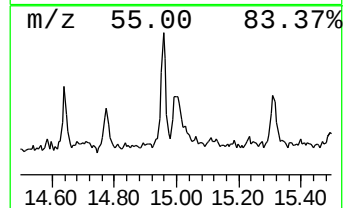
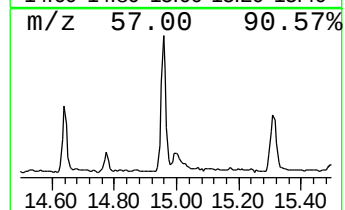
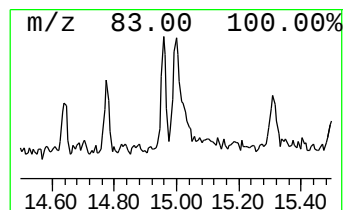
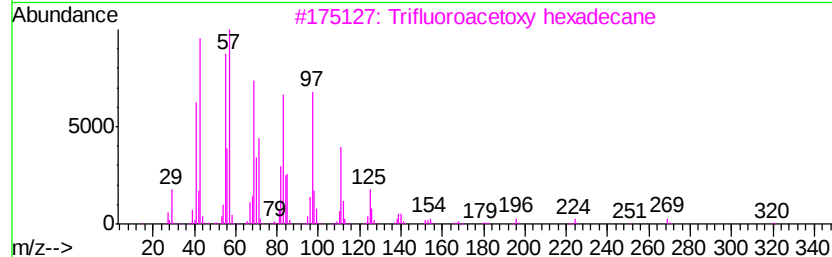
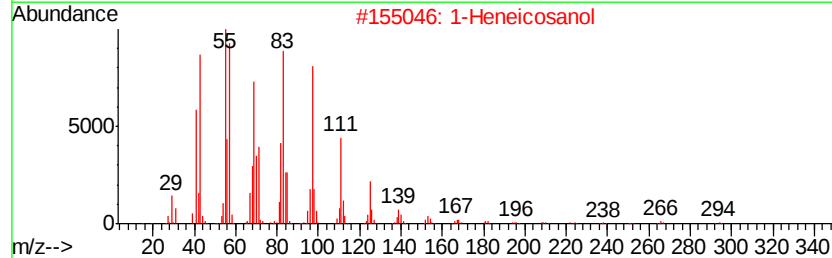
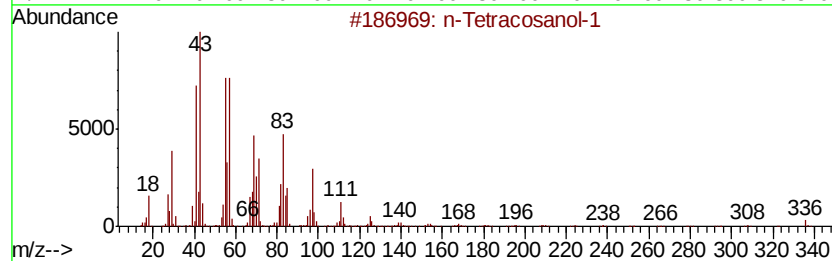
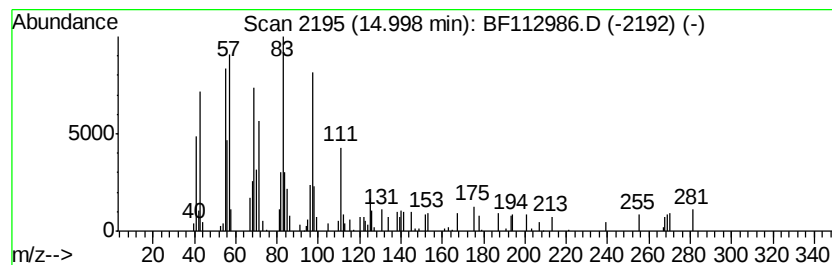
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Tetracosanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.63 ng	104077	Perylene-d12	15.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Tetracosanol-1	354 C24H50O	000506-51-4	86
2	1-Heneicosanol	312 C21H44O	015594-90-8	76
3	Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3	74
4	Behenic alcohol	326 C22H46O	000661-19-8	68
5	n-Nonadecanol-1	284 C19H40O	001454-84-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112986.D
Acq On : 12 Mar 2019 6:11
Operator : JU/SJ
Sample : K1817-19
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PST-028-B099-030619

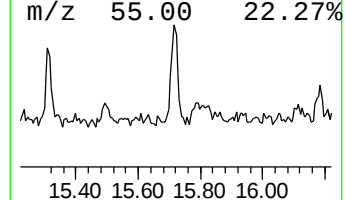
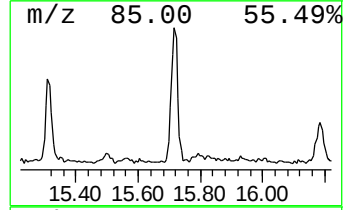
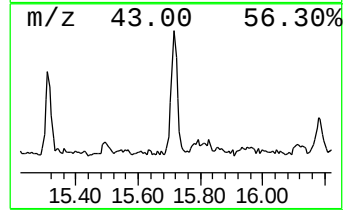
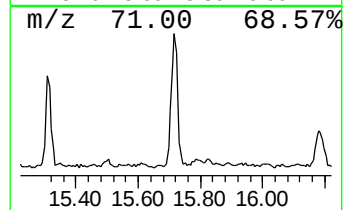
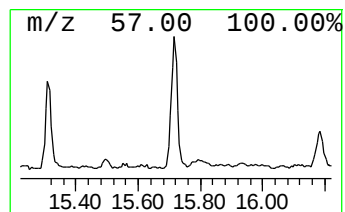
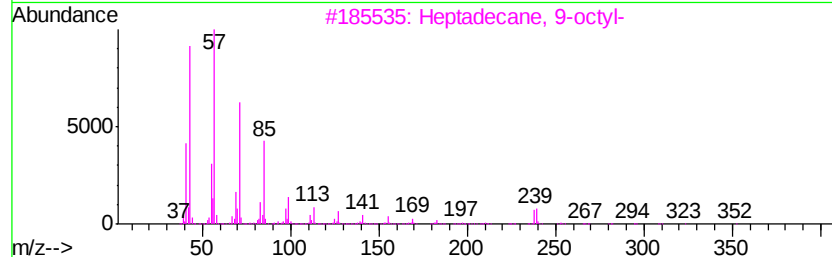
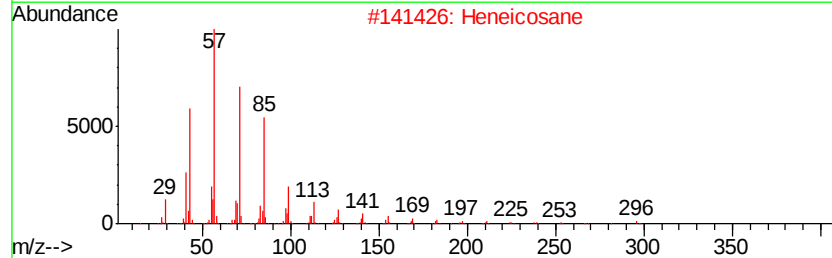
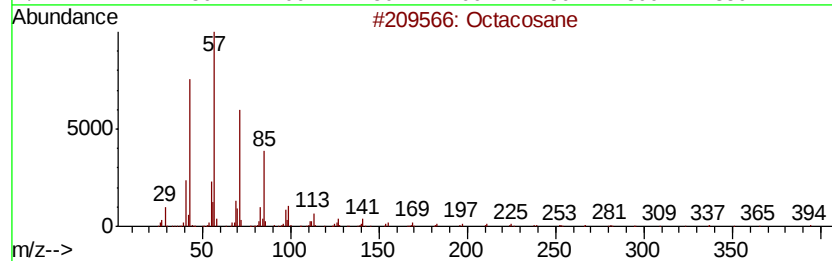
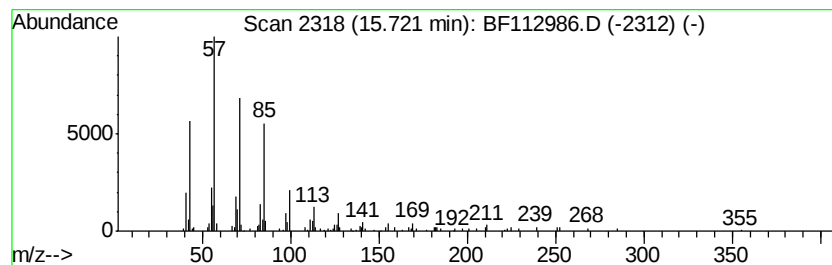
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	4.85 ng	191949	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Triacontane		422	C30H62	000638-68-6	91
5	Hexacosane		366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
Data File : BF112986.D
Acq On : 12 Mar 2019 6:11
Operator : JU/SJ
Sample : K1817-19
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-B099-030619

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	47.6	ng	1354630	1	6.73	569039	20.0
n-Hexadecanoic acid	11.77	3.4	ng	215730	4	11.24	1259210	20.0
Tricosyl trifluor...	13.73	3.7	ng	213289	5	13.86	1164060	20.0
Heneicosane	14.64	2.6	ng	104129	6	15.27	791213	20.0
unknown14.96	14.96	6.2	ng	243138	6	15.27	791213	20.0
n-Tetracosanol-1	15.00	2.6	ng	104077	6	15.27	791213	20.0
Octacosane	15.72	4.8	ng	191949	6	15.27	791213	20.0