

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
 Data File : BF117632.D
 Acq On : 30 Oct 2019 18:39
 Operator : JU
 Sample : K5539-09 2X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 162-94-(0-1)

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-BF101819.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	5.357	553	556	578	rBV	172259	305690	77.93%	6.830%
2	6.386	728	731	748	rBV	217523	367779	93.76%	8.217%
3	6.504	748	751	766	rVB	346452	392272	100.00%	8.764%
4	6.728	786	789	802	rVB	213386	200957	51.23%	4.490%
5	6.881	812	815	828	rBV	262882	261165	66.58%	5.835%
6	7.298	883	886	905	rBV	114788	199861	50.95%	4.465%
7	8.010	1004	1007	1032	rBV	213357	265581	67.70%	5.934%
8	9.080	1186	1189	1208	rBV	311195	343366	87.53%	7.671%
9	9.486	1255	1258	1263	rBV	25944	29210	7.45%	0.653%
10	9.763	1301	1305	1318	rBV	282606	287741	73.35%	6.429%
11	10.557	1437	1440	1455	rBB	125654	167110	42.60%	3.734%
12	11.251	1554	1558	1568	rBV	233890	259254	66.09%	5.792%
13	11.780	1645	1648	1655	rBV3	13137	19308	4.92%	0.431%
14	12.468	1762	1765	1769	rBV2	20382	22831	5.82%	0.510%
15	12.574	1778	1783	1786	rBV7	5184	8463	2.16%	0.189%
16	12.698	1799	1804	1808	rBV	22010	24832	6.33%	0.555%
17	12.827	1822	1826	1833	rBV	316240	281627	71.79%	6.292%
18	13.263	1898	1900	1902	rBV3	5219	4717	1.20%	0.105%
19	13.298	1903	1906	1912	rVB	81644	70144	17.88%	1.567%
20	13.574	1951	1953	1955	rBV3	6293	4816	1.23%	0.108%
21	13.721	1975	1978	1979	rBV3	8897	10163	2.59%	0.227%
22	13.739	1979	1981	1989	rVB7	25998	46430	11.84%	1.037%
23	13.857	1998	2001	2003	rBV	23244	18814	4.80%	0.420%
24	13.898	2003	2008	2018	rVV	240636	268763	68.51%	6.005%
25	13.968	2018	2020	2022	rBV3	7205	7653	1.95%	0.171%
26	14.039	2029	2032	2036	rBV5	16125	19934	5.08%	0.445%
27	14.345	2081	2084	2087	rBV2	23292	22481	5.73%	0.502%
28	14.639	2132	2134	2137	rBV3	25577	24054	6.13%	0.537%
29	14.709	2143	2146	2151	rVB	48691	45411	11.58%	1.015%
30	14.951	2185	2187	2195	rVB3	41754	66945	17.07%	1.496%
31	15.333	2245	2252	2259	rVB	141586	232028	59.15%	5.184%
32	15.709	2314	2316	2322	rVB3	20935	26926	6.86%	0.602%
33	15.951	2353	2357	2359	rBV5	15924	22139	5.64%	0.495%
34	16.351	2421	2425	2430	rBV8	13669	22081	5.63%	0.493%

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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	16.803	2496	2502	2510	rVB3	63784	121225	30.90%	2.708%
36	17.656	2645	2647	2649	rBV2	4690	4155	1.06%	0.093%

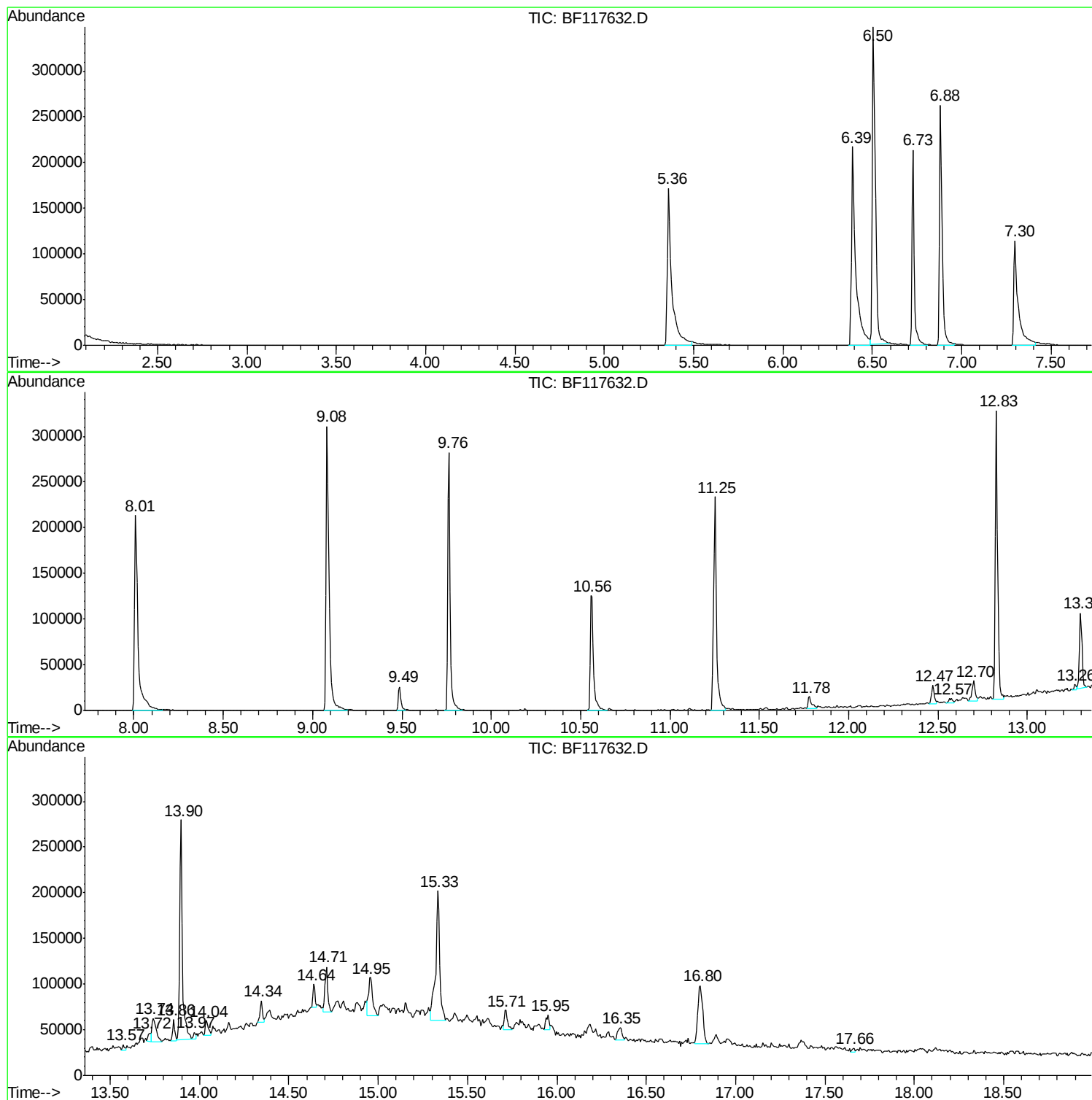
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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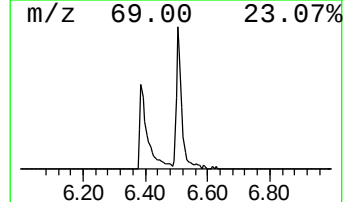
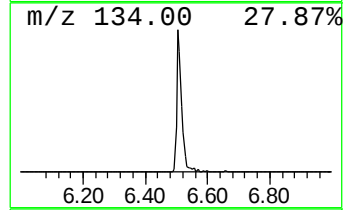
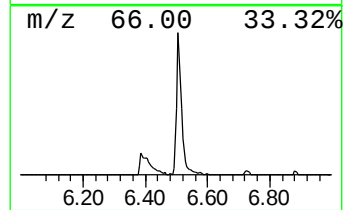
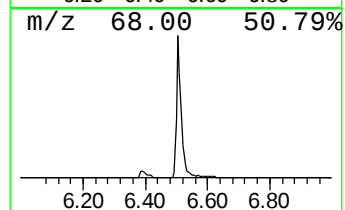
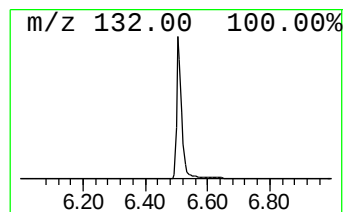
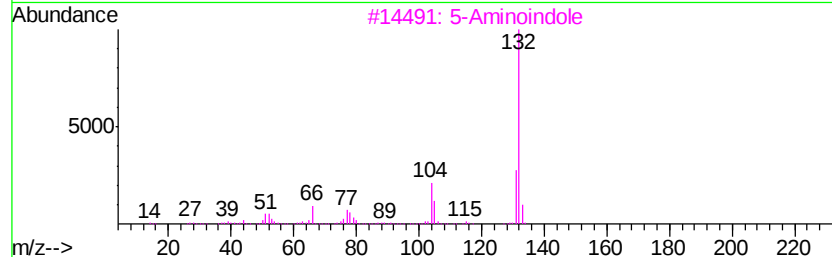
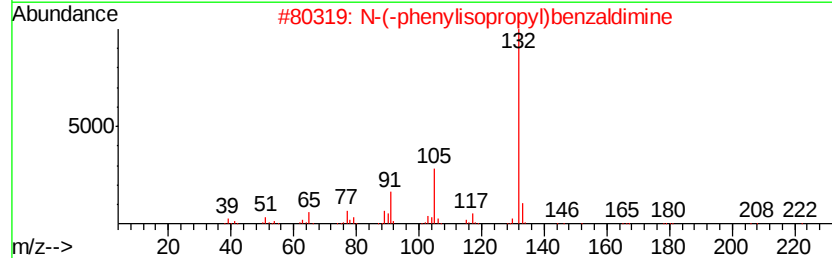
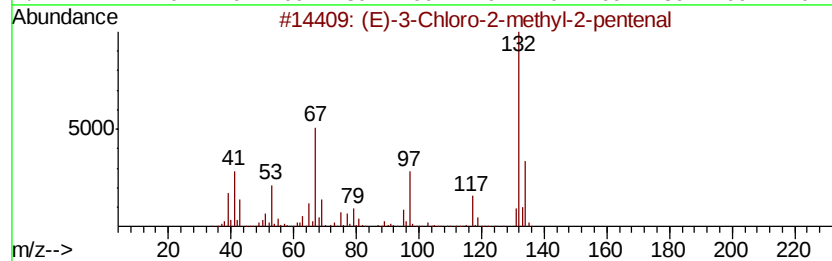
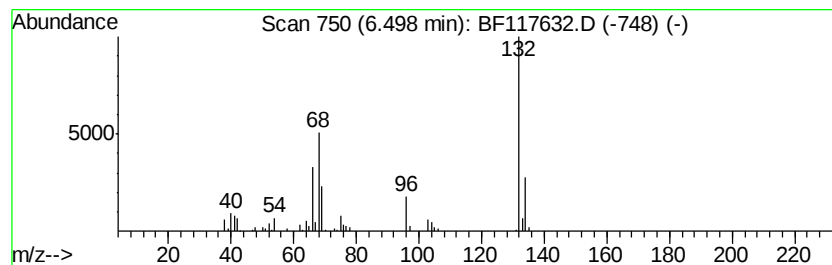
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	39.04 ng	392272	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		N-(-phenylisopropyl)benzalimine	223	C16H17N	1000379-01-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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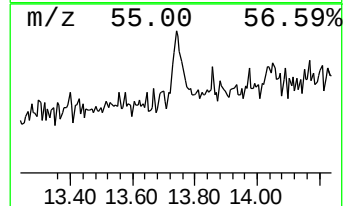
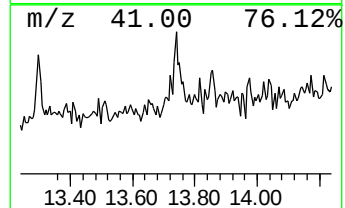
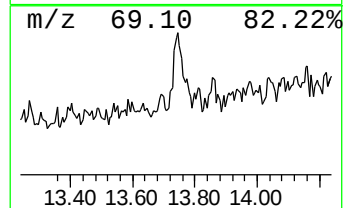
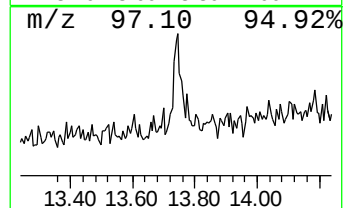
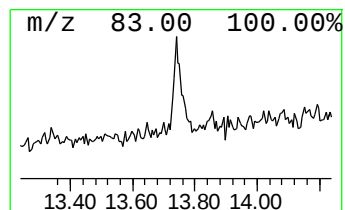
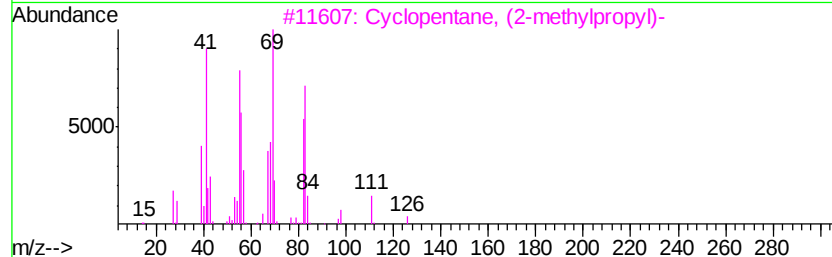
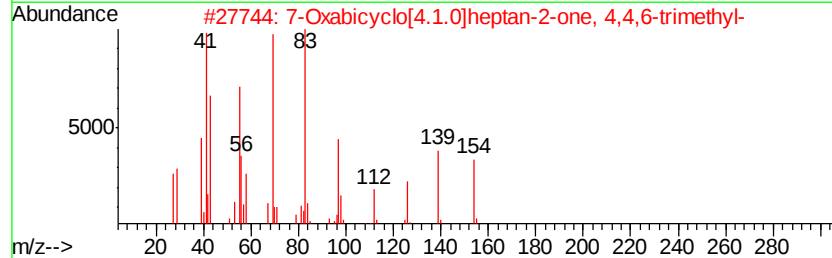
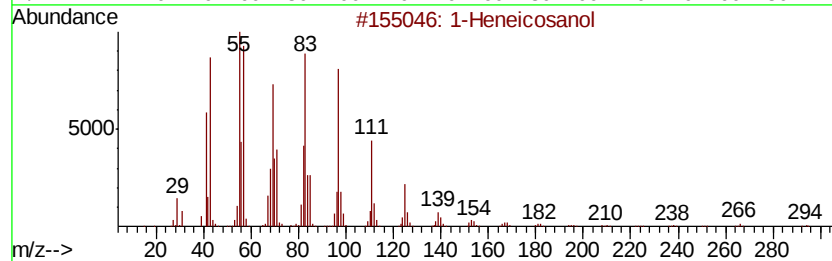
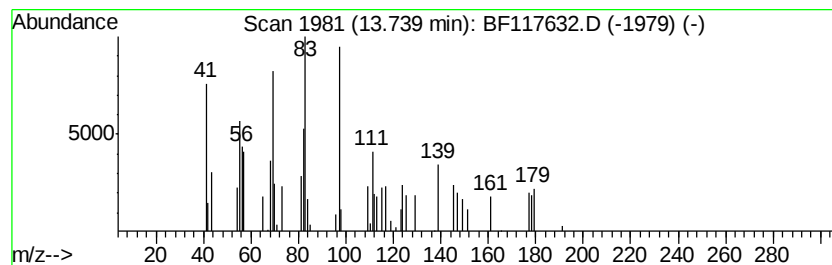
Instrument :
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ClientSampleId :
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Peak Number 3 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	3.46 ng	46430	Chrysene-d12	13.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	53
2	7-Oxabicyclo[4.1.0]heptan-2-one, ...	154	C9H14O2	010276-21-8	38
3	Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	35
4	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	27
5	3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	27



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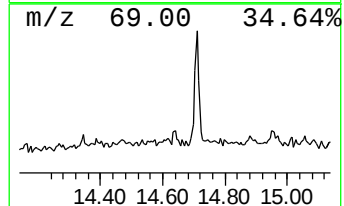
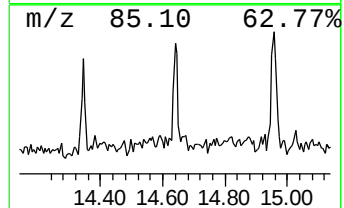
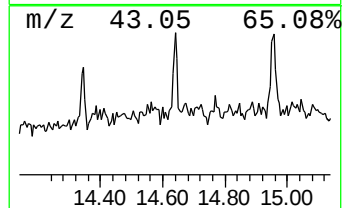
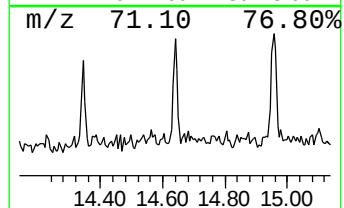
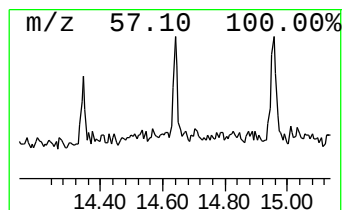
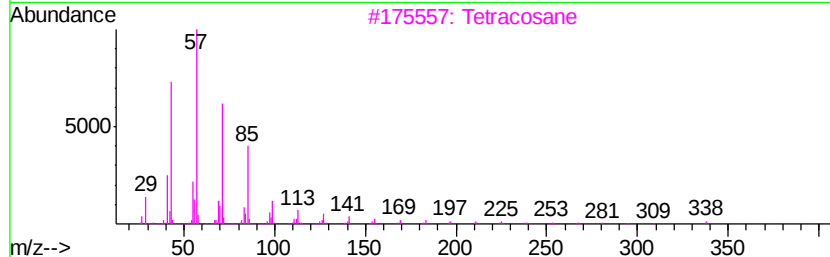
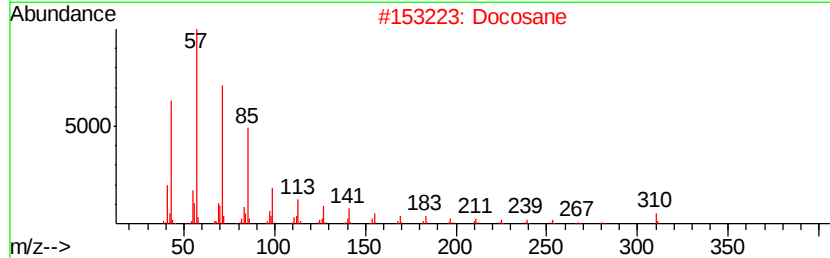
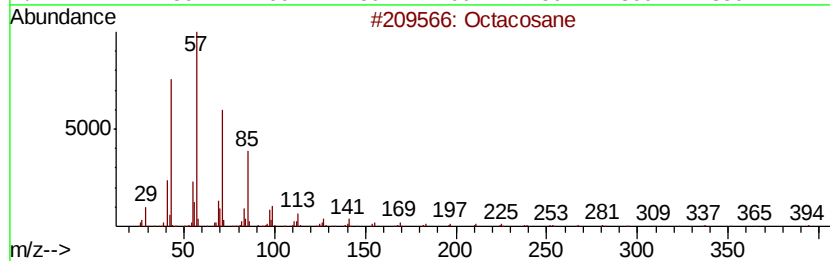
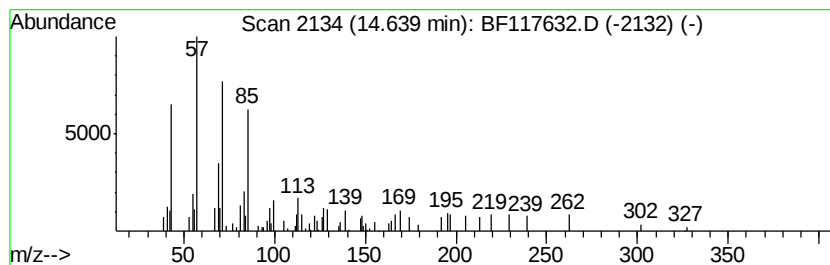
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.07 ng	24054	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	53
2	Docosane		310	C22H46	000629-97-0	53
3	Tetracosane		338	C24H50	000646-31-1	53
4	Undecane, 5-ethyl-5-propyl-		226	C16H34	002755-07-9	53
5	Hexadecane		226	C16H34	000544-76-3	53



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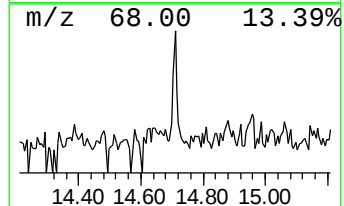
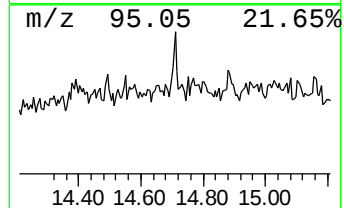
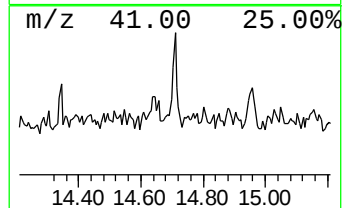
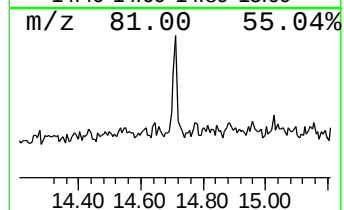
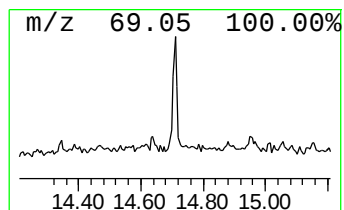
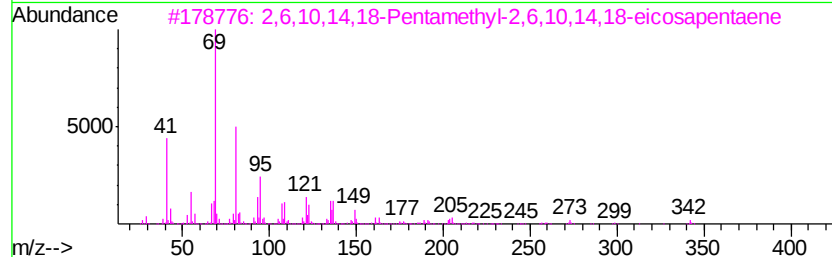
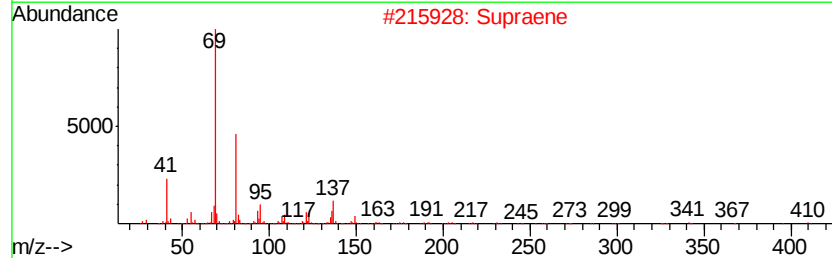
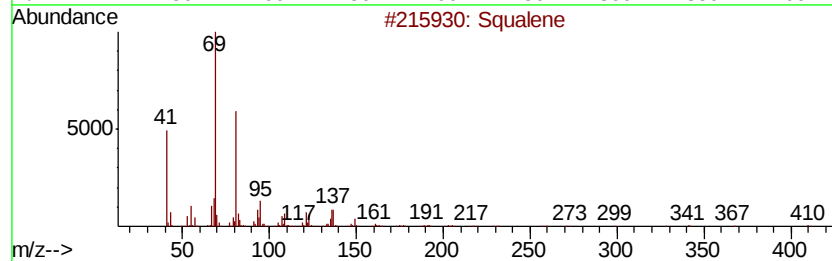
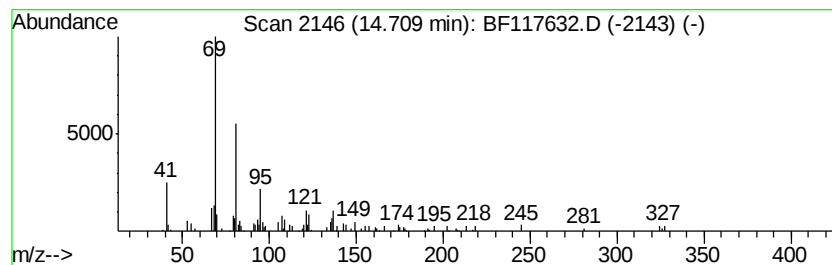
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.91 ng	45411	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	72
2		Supraene	410	C30H50	007683-64-9	64
3		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	64
4		2,5,9,13-Tetramethyl-tetradeca-4...	292	C19H32O2	055844-49-0	64
5		4,8,12-Tetradecatrilene, 5,9,13-...	248	C17H28O	066408-55-7	59



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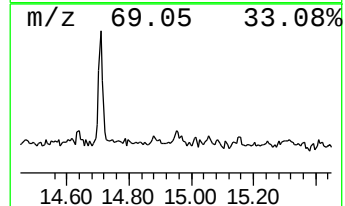
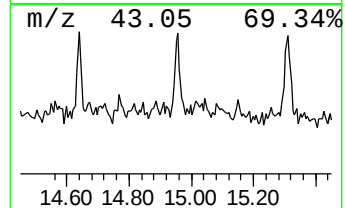
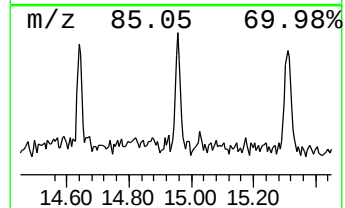
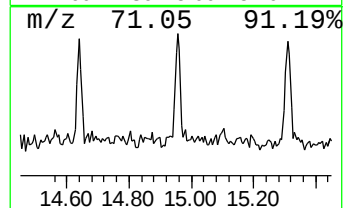
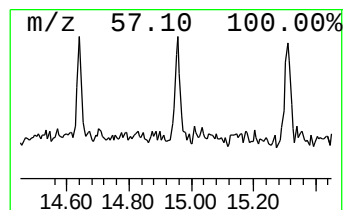
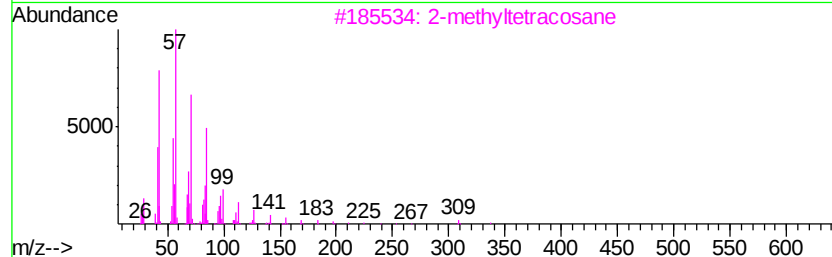
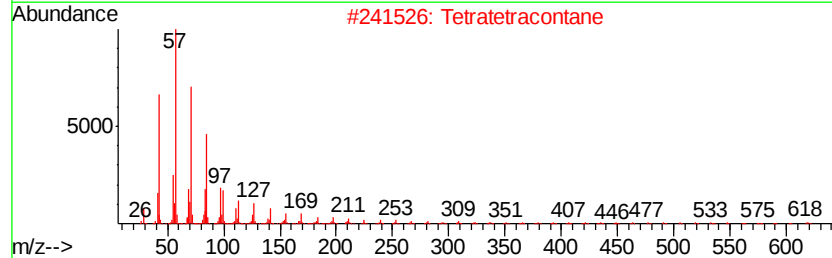
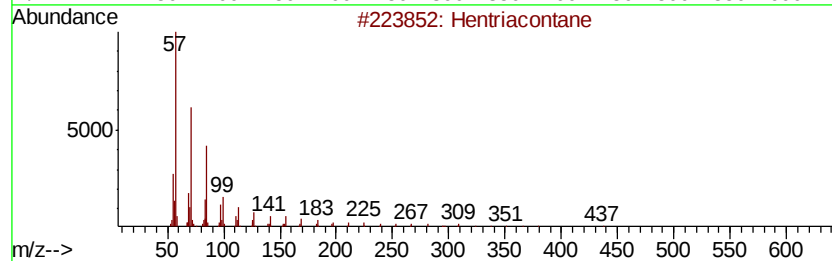
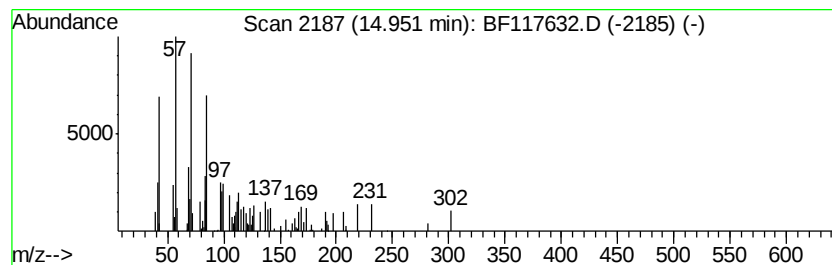
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	5.77 ng	66945	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	74
2	Tetratetracontane		619	C44H90	007098-22-8	72
3	2-methyltetracosane		352	C25H52	1000376-72-6	64
4	2-methyloctacosane		408	C29H60	1000376-72-8	64
5	Heptacosane		380	C27H56	000593-49-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117632.D
Acq On : 30 Oct 2019 18:39
Operator : JU
Sample : K5539-09 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
162-94-(0-1)

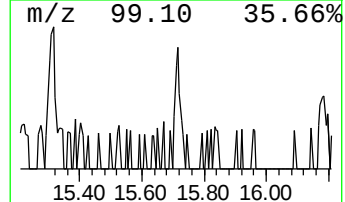
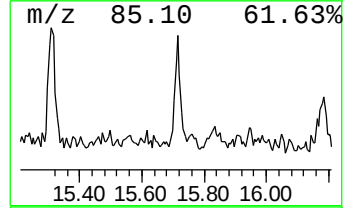
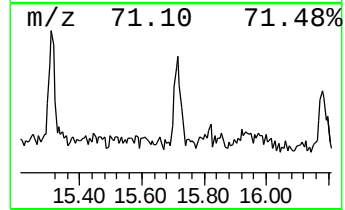
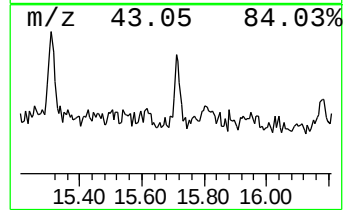
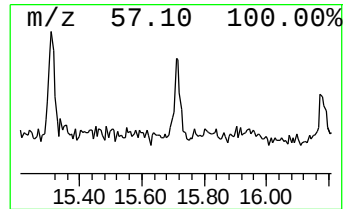
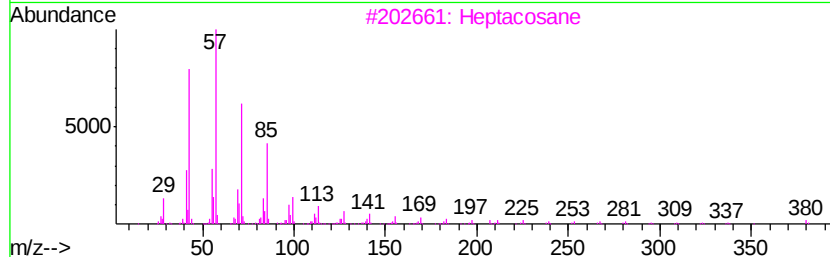
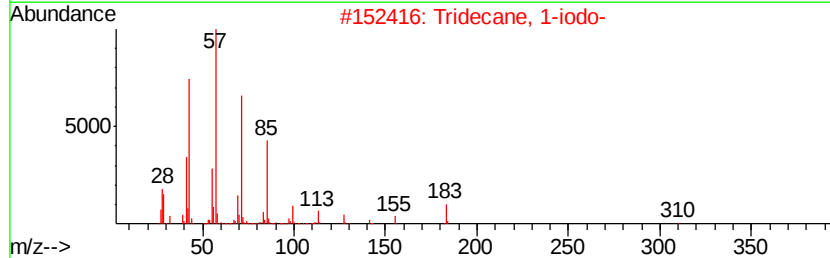
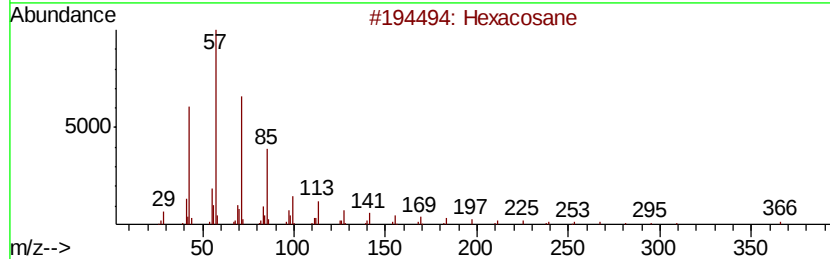
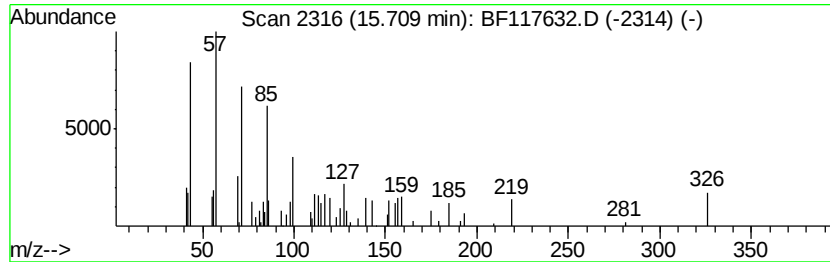
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.32 ng	26926	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	47
2	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	43
3	Heptacosane		380	C27H56	000593-49-7	43
4	1-Decanol, 2,2-dimethyl-		186	C12H26O	002370-15-2	43
5	2-Bromo dodecane		248	C12H25Br	013187-99-0	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
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Acq On : 30 Oct 2019 18:39
Operator : JU
Sample : K5539-09 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
162-94-(0-1)

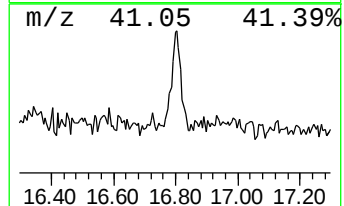
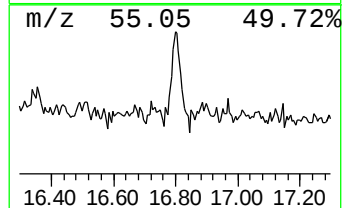
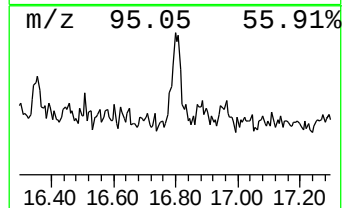
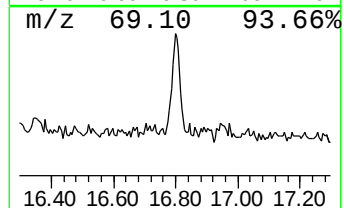
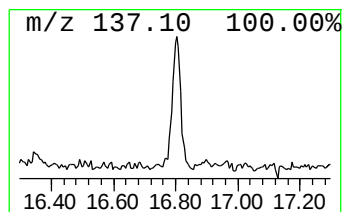
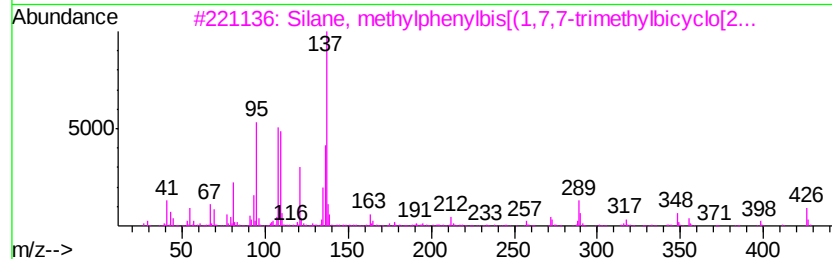
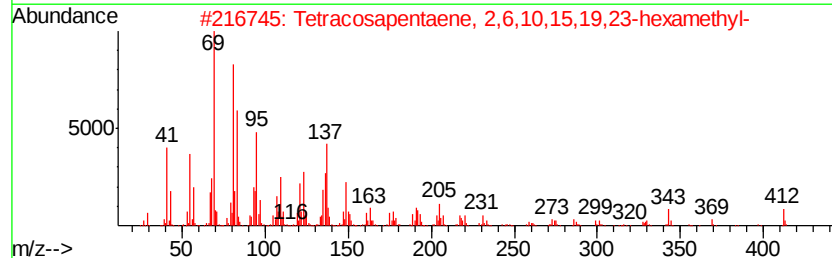
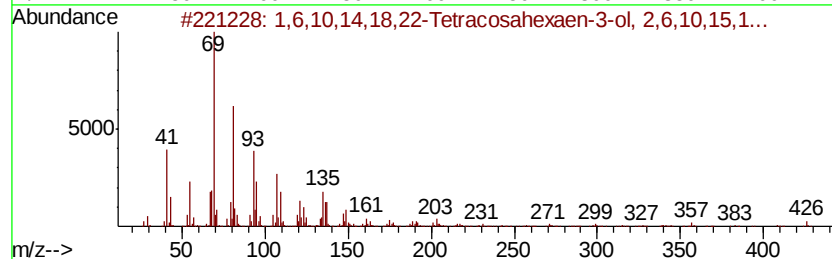
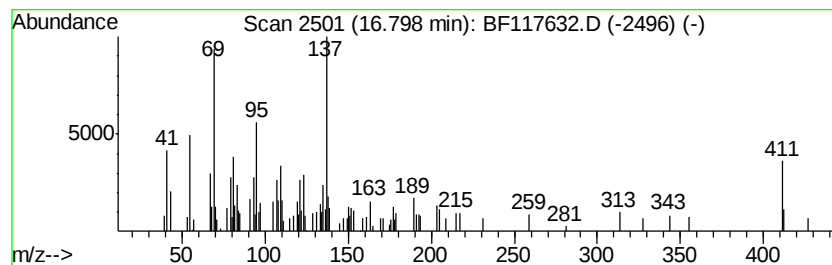
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.80 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	10.45 ng	121225	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H500	054159-46-5	49
2		Tetracosapentaene, 2,6,10,15,19,...	412	C30H52	026266-08-0	46
3		Silane, methylphenylbis[(1,7,7-t...	426	C27H42O2Si	074806-99-8	35
4		Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	35
5		3,6-Dimethyl-2,3,3a,4,5,7a-hexah...	152	C10H16O	070786-44-6	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
162-94-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.50	6.50	39.0	ng	392272	1	6.73	200957	20.0
1-Heneicosanol	13.74	3.5	ng	46430	5	13.90	268763	20.0
Octacosane	14.64	2.1	ng	24054	6	15.33	232028	20.0
Squalene	14.71	3.9	ng	45411	6	15.33	232028	20.0
Hentriacontane	14.95	5.8	ng	66945	6	15.33	232028	20.0
Hexacosane	15.71	2.3	ng	26926	6	15.33	232028	20.0
unknown16.80	16.80	10.4	ng	121225	6	15.33	232028	20.0