

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
 Data File : BF096419.D
 Acq On : 2 Jul 2017 16:40
 Operator : SJ/MA
 Sample : I3950-18
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B6-10-12

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:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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	4.934	479	484	494	rVB	524827	713267	18.52%	2.429%
2	5.351	550	555	558	rBV	3347578	3851717	100.00%	13.117%
3	6.375	723	729	732	rBV	3166331	3523750	91.49%	12.001%
4	6.504	746	751	754	rBV	3394937	3398578	88.24%	11.574%
5	6.734	786	790	793	rBV	1146208	894603	23.23%	3.047%
6	6.893	812	817	820	rBV	2624225	2316200	60.13%	7.888%
7	7.292	879	885	888	rBV	2008274	2117192	54.97%	7.210%
8	7.392	897	902	907	rVB3	52591	65009	1.69%	0.221%
9	8.016	1004	1008	1011	rBV	1584195	1294254	33.60%	4.408%
10	9.092	1186	1191	1194	rBV	3082684	2740961	71.16%	9.335%
11	9.186	1201	1207	1210	rBV3	48822	44925	1.17%	0.153%
12	9.481	1254	1257	1261	rBV	679098	601270	15.61%	2.048%
13	9.710	1293	1296	1301	rVB	85052	70621	1.83%	0.241%
14	9.769	1301	1306	1309	rBV	1253761	1171141	30.41%	3.988%
15	10.210	1378	1381	1384	rVB	111172	84791	2.20%	0.289%
16	10.551	1434	1439	1442	rBV	1786885	1647533	42.77%	5.611%
17	10.680	1458	1461	1468	rVV	93891	104279	2.71%	0.355%
18	11.128	1534	1537	1541	rBV	61155	52243	1.36%	0.178%
19	11.245	1553	1557	1560	rBV	1049412	878645	22.81%	2.992%
20	11.780	1644	1648	1652	rBV3	96582	100402	2.61%	0.342%
21	12.451	1759	1762	1766	rBV	84997	71545	1.86%	0.244%
22	12.651	1793	1796	1798	rBV2	34110	40486	1.05%	0.138%
23	12.674	1798	1800	1803	rVB	71392	61090	1.59%	0.208%
24	12.827	1822	1826	1829	rBV	1832330	1656584	43.01%	5.642%
25	13.310	1903	1908	1916	rBV	137550	152862	3.97%	0.521%
26	13.380	1916	1920	1924	rBV3	30663	41609	1.08%	0.142%
27	13.727	1976	1979	1984	rBV	207877	221475	5.75%	0.754%
28	13.874	1999	2004	2006	rBV	780871	765294	19.87%	2.606%
29	14.363	2084	2087	2092	rVV2	40115	57274	1.49%	0.195%
30	15.280	2239	2243	2250	rBV	421167	524934	13.63%	1.788%
31	15.339	2250	2253	2256	rVB2	32930	43448	1.13%	0.148%
32	15.751	2319	2323	2326	rBV2	39085	55249	1.43%	0.188%

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Misc :
ALS Vial : 16 Sample Multiplier: 1

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ClientSampleId :
B6-10-12

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:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

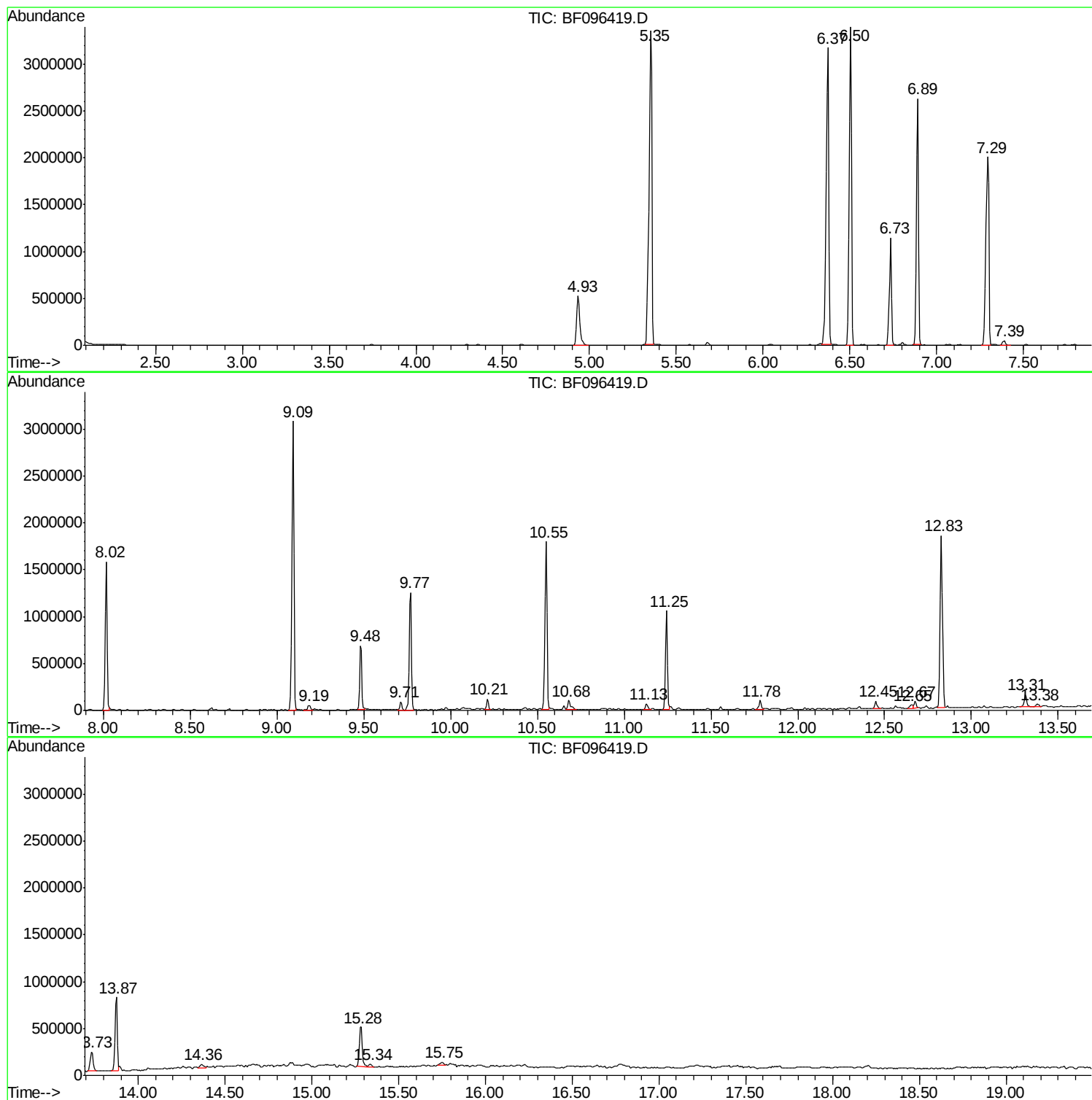
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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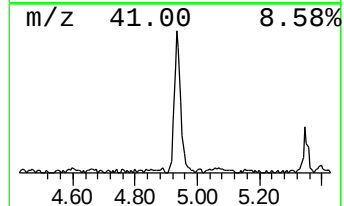
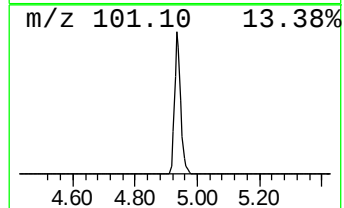
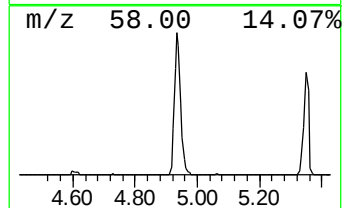
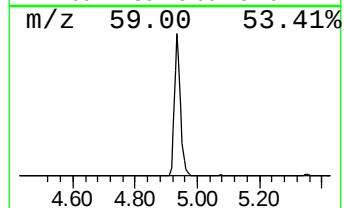
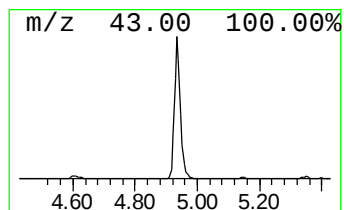
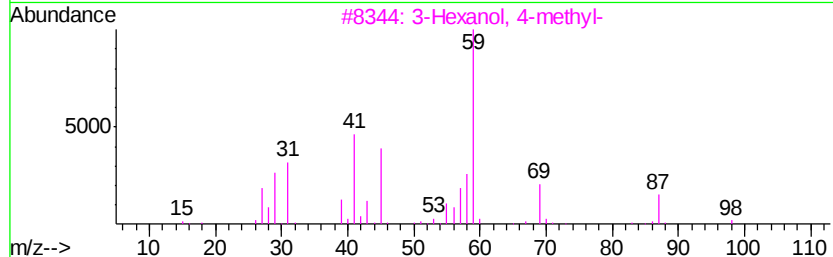
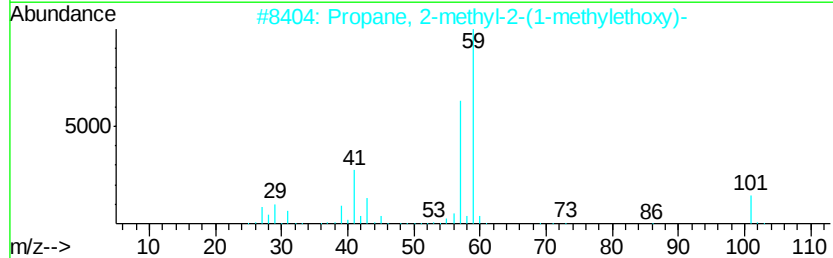
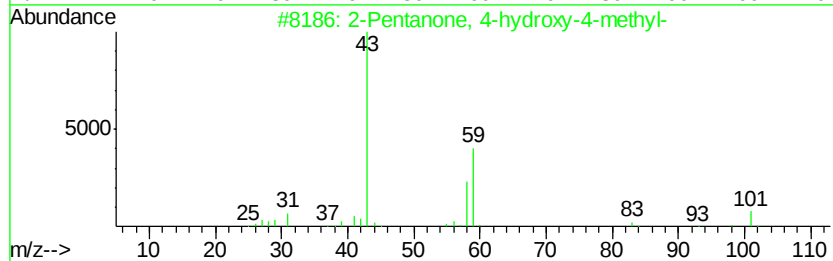
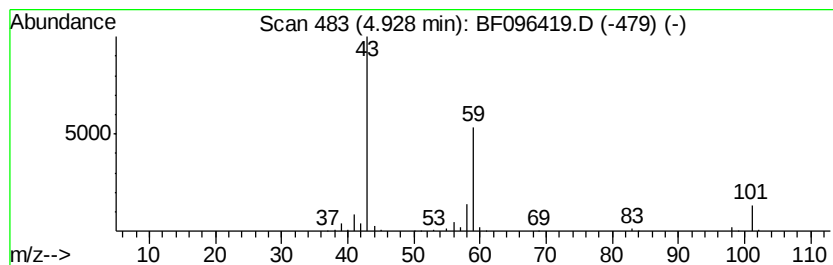
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	15.95 ng	713267	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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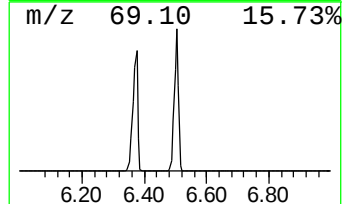
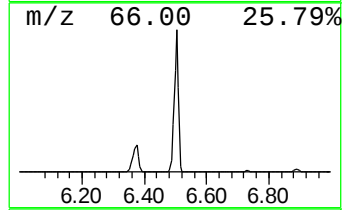
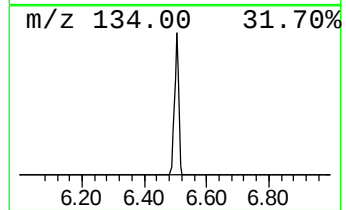
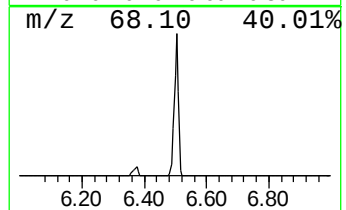
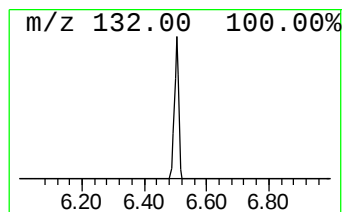
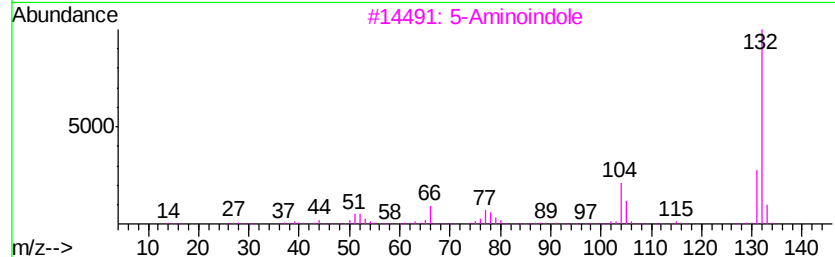
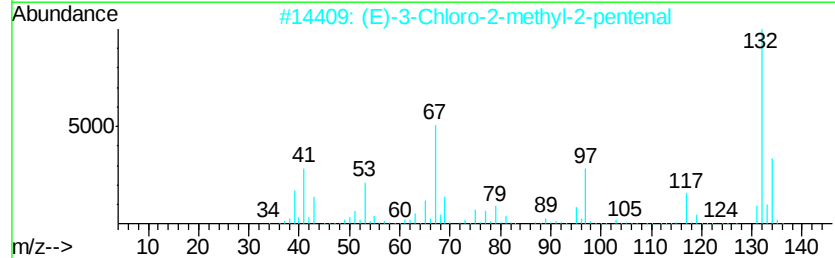
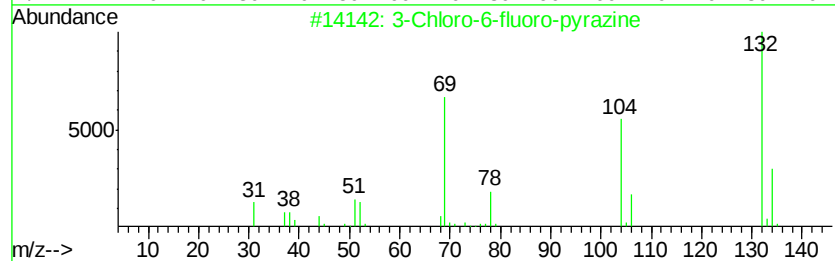
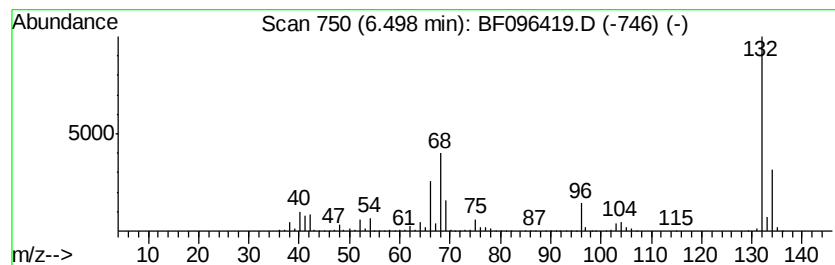
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	75.98 ng	3398580	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	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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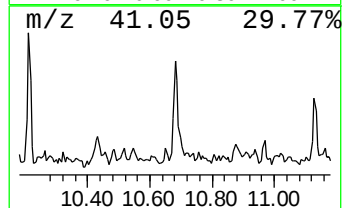
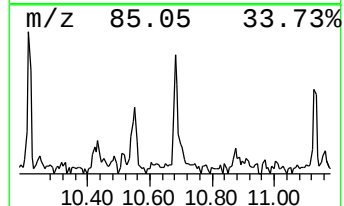
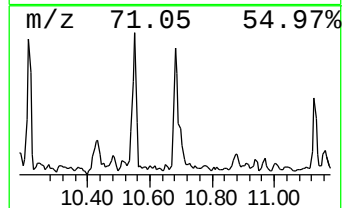
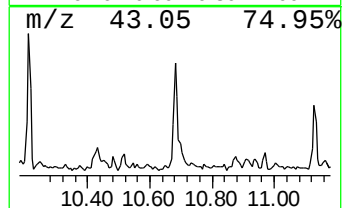
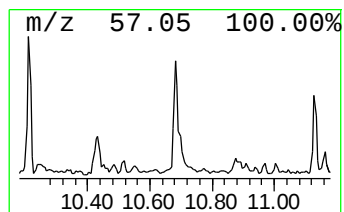
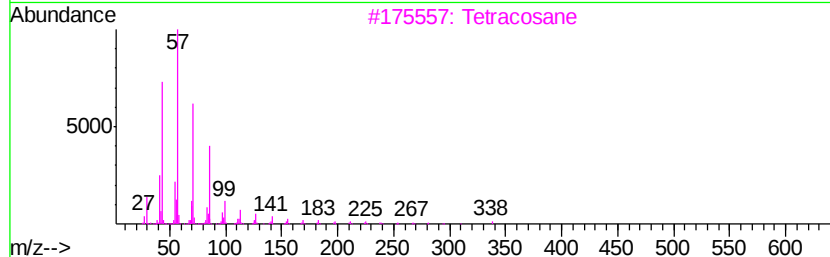
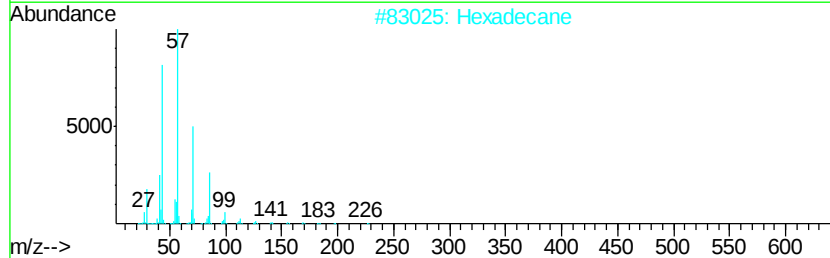
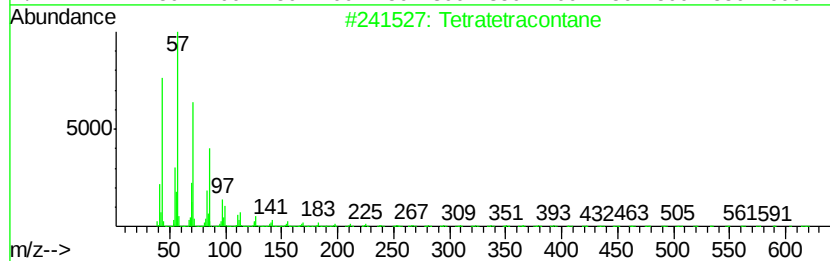
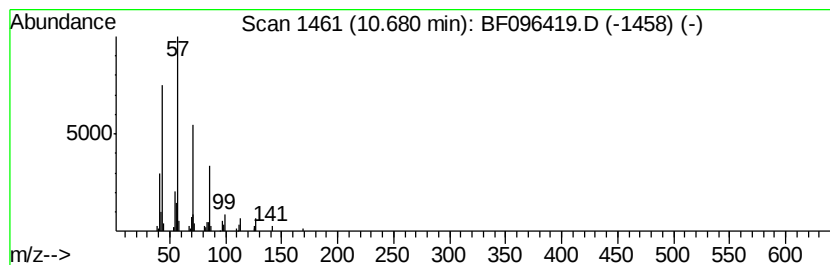
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.37 ng	104279	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	90
2		Hexadecane	226	C16H34	000544-76-3	86
3		Tetracosane	338	C24H50	000646-31-1	86
4		Heneicosane	296	C21H44	000629-94-7	86
5		Heptacosane	380	C27H56	000593-49-7	86



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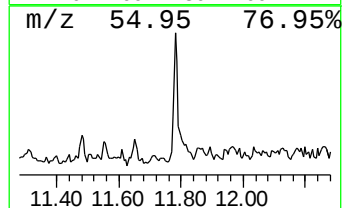
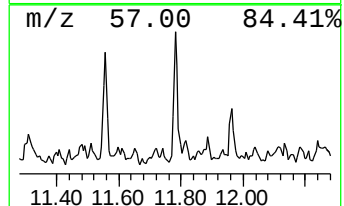
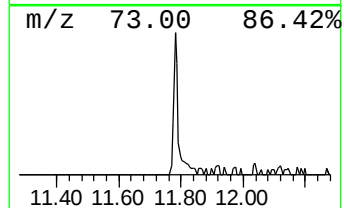
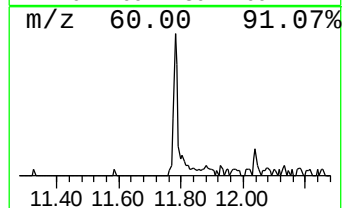
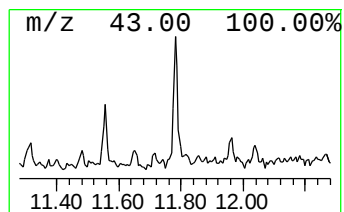
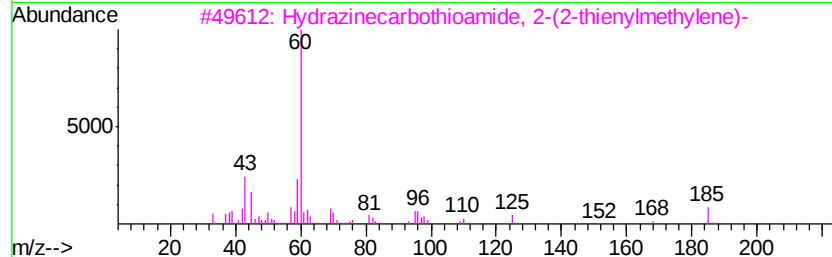
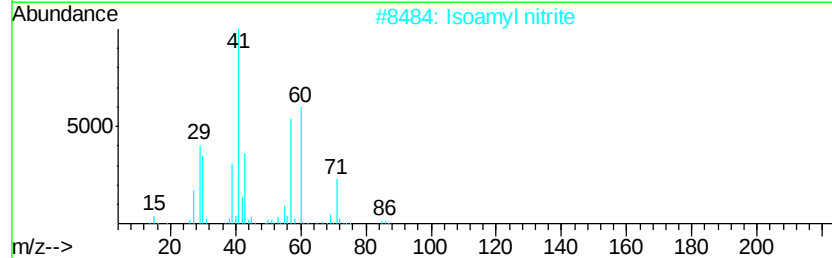
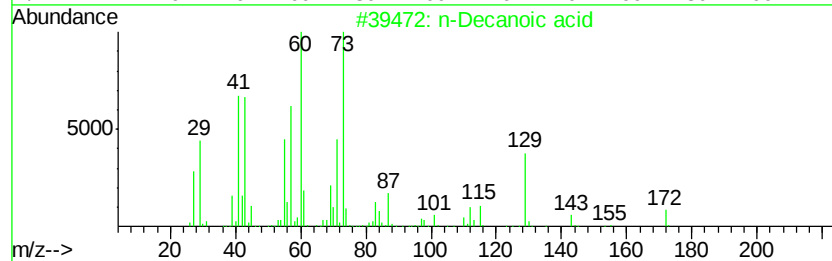
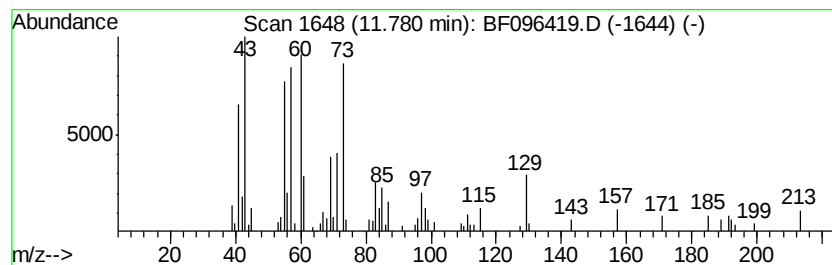
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Decanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.29 ng	100402	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	53
2		Isoamyl nitrite	117	C5H11NO2	000110-46-3	38
3		Hydrazinecarbothioamide, 2-(2-th...	185	C6H7N3S2	005351-91-7	22
4		Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	22
5		Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	18



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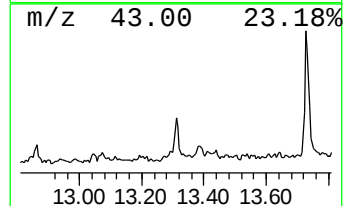
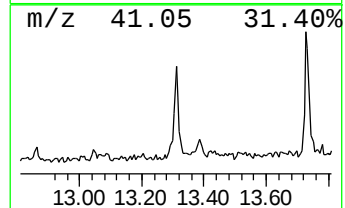
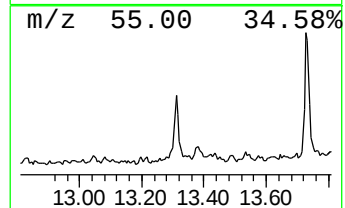
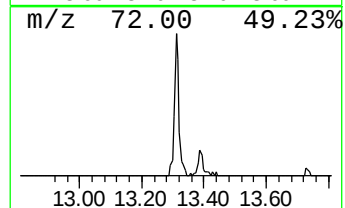
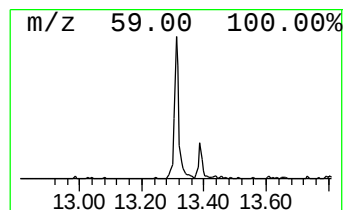
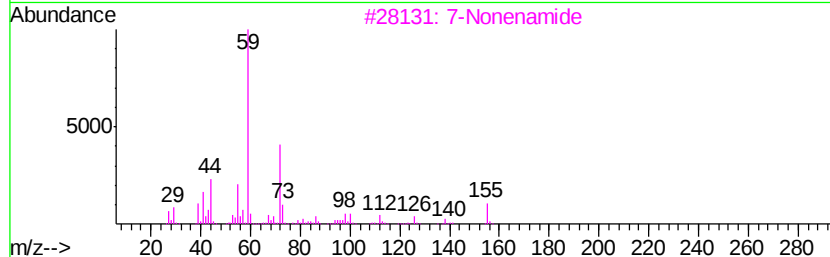
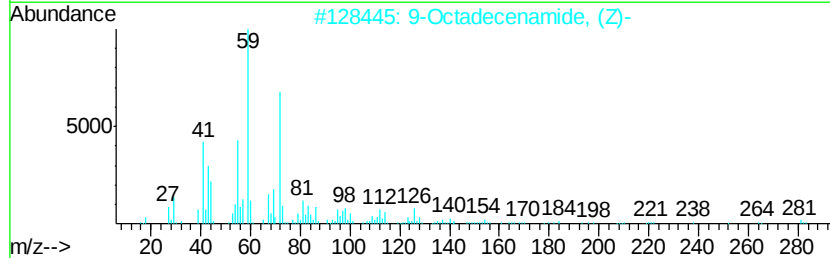
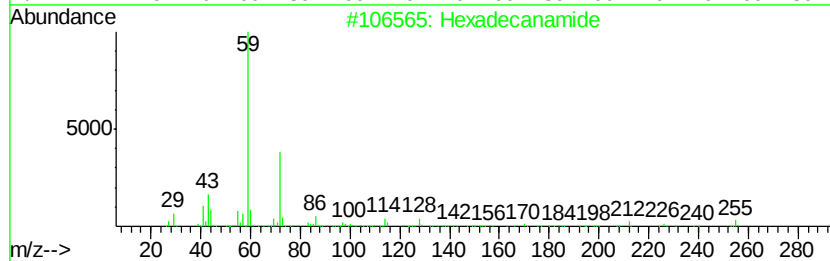
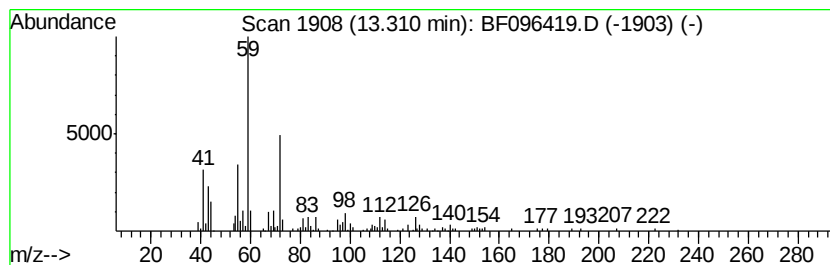
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.31	3.99 ng	152862	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide		255	C16H33NO	000629-54-9	72
2	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	68
3	7-Nonenamide		155	C9H17NO	090949-53-4	64
4	Nonanamide		157	C9H19NO	001120-07-6	53
5	Dodecanamide		199	C12H25NO	001120-16-7	53



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B6-10-12

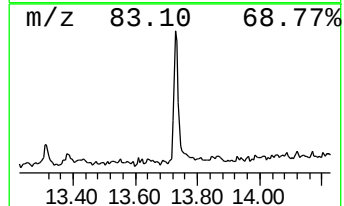
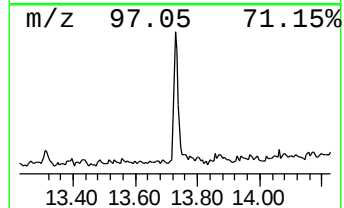
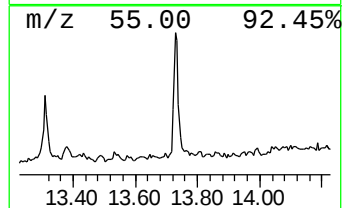
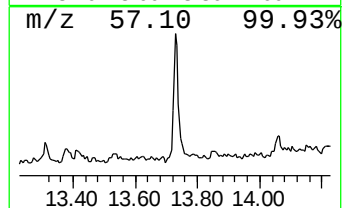
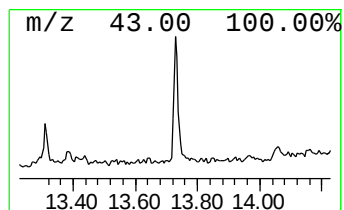
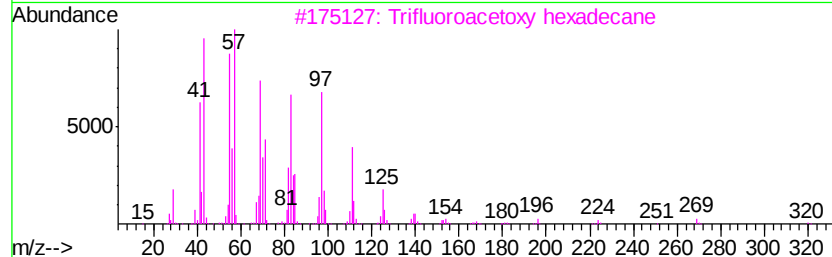
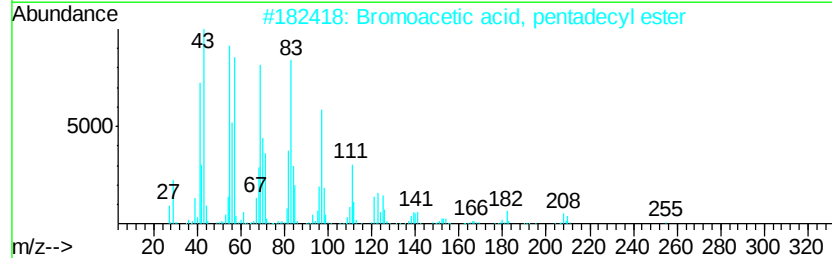
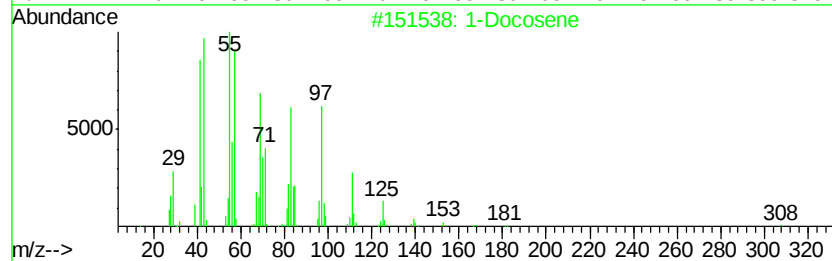
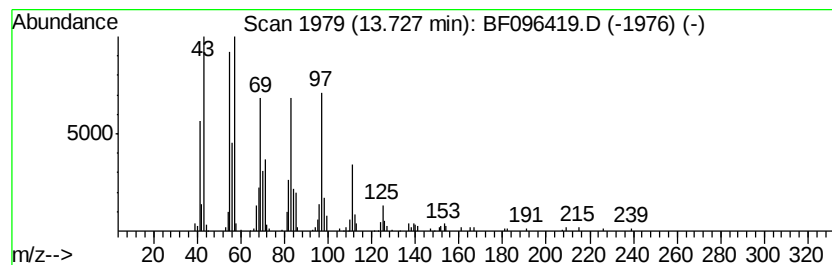
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	5.79 ng	221475	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	94
2	Bromoacetic acid, pentadecyl ester		348	C17H33BrO2	131143-01-6	91
3	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	91
4	Pentafluoropropionic acid, tetra...		360	C17H29F5O2	006222-06-6	91
5	1-Octadecanol		270	C18H38O	000112-92-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096419.D
Acq On : 2 Jul 2017 16:40
Operator : SJ/MA
Sample : I3950-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

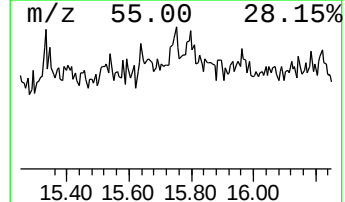
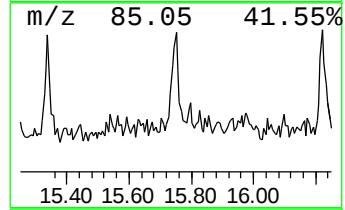
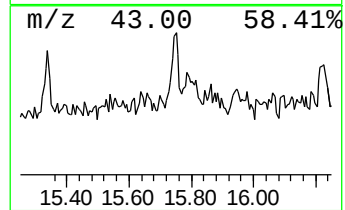
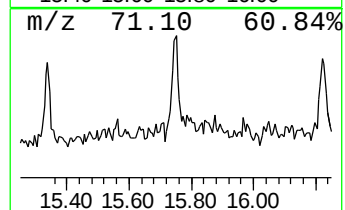
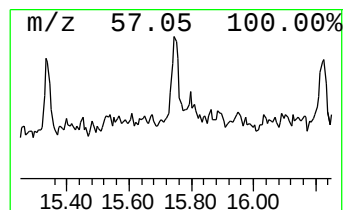
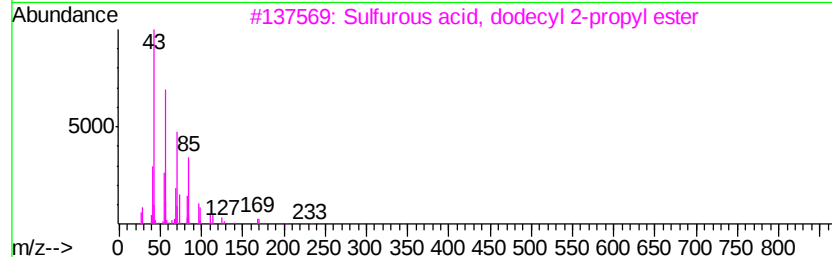
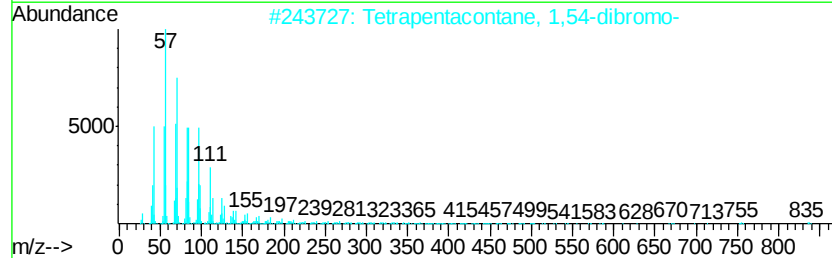
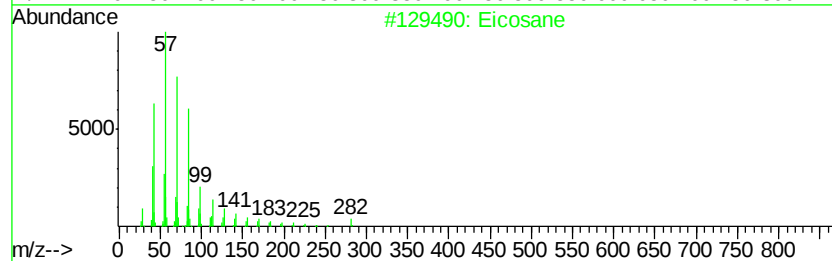
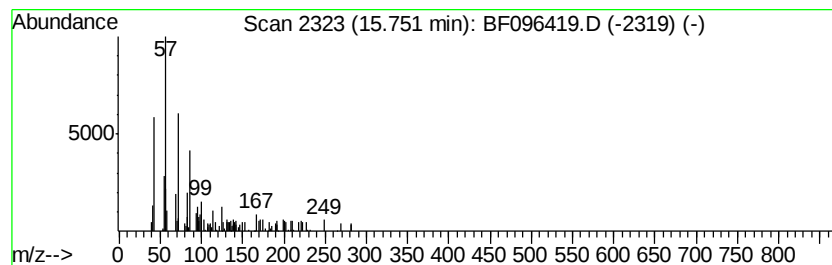
Instrument :
BNA_F
ClientSampleId :
B6-10-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	2.10 ng	55249	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 86
2	Tetrapentacontane, 1,54-dibromo-		915 C54H108Br2	1000156-09-4 59
3	Sulfurous acid, dodecyl 2-propyl...		292 C15H32O3S	1000309-12-3 53
4	Tridecane, 1-iodo-		310 C13H27I	035599-77-0 50
5	Pentadecane, 2,6,10-trimethyl-		254 C18H38	003892-00-0 50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096419.D
Acq On : 2 Jul 2017 16:40
Operator : SJ/MA
Sample : I3950-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B6-10-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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
2-Pentanone, 4-hy...	4.93	15.9	ng	713267	1	6.73	894603	20.0
unknown6.50	6.50	76.0	ng	3398580	1	6.73	894603	20.0
Tetratetracontane	10.68	2.4	ng	104279	4	11.25	878645	20.0
n-Decanoic acid	11.78	2.3	ng	100402	4	11.25	878645	20.0
Hexadecanamide	13.31	4.0	ng	152862	5	13.87	765294	20.0
1-Docosene	13.73	5.8	ng	221475	5	13.87	765294	20.0
Eicosane	15.75	2.1	ng	55249	6	15.29	524934	20.0