

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040919\
 Data File : BF113669.D
 Acq On : 9 Apr 2019 18:59
 Operator : JU/SJ
 Sample : K2198-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OK-01-040819

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-BF040319.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	5.292	541	545	567	rBV	2100177	2389681	90.85%	9.915%
2	6.333	718	722	738	rBV	2355280	2524219	95.96%	10.473%
3	6.451	738	742	761	rVB	2629649	2534758	96.36%	10.517%
4	6.675	777	780	793	rVB	687722	684476	26.02%	2.840%
5	6.833	803	807	824	rBV	2204161	1940873	73.78%	8.053%
6	7.245	873	877	898	rBV	1592938	1585113	60.26%	6.577%
7	7.963	995	999	1019	rBV	803921	878132	33.38%	3.643%
8	9.033	1177	1181	1192	rBV	2936773	2630481	100.00%	10.914%
9	9.163	1199	1203	1213	rVB	101925	151141	5.75%	0.627%
10	9.427	1244	1248	1253	rBV	247107	246079	9.35%	1.021%
11	9.710	1292	1296	1308	rVB	969525	888369	33.77%	3.686%
12	10.498	1426	1430	1443	rBV	1507460	1528342	58.10%	6.341%
13	10.616	1448	1450	1455	rBV2	30531	40137	1.53%	0.167%
14	11.063	1520	1526	1529	rBV3	28543	36427	1.38%	0.151%
15	11.192	1544	1548	1557	rBV	821185	822574	31.27%	3.413%
16	11.486	1596	1598	1603	rVB2	26176	29834	1.13%	0.124%
17	11.727	1636	1639	1650	rBV2	314017	377349	14.35%	1.566%
18	12.280	1730	1733	1736	rVB	40487	40258	1.53%	0.167%
19	12.404	1742	1754	1757	rBV5	89248	278904	10.60%	1.157%
20	12.433	1757	1759	1768	rVB	102372	126498	4.81%	0.525%
21	12.510	1769	1772	1776	rBV3	67062	82892	3.15%	0.344%
22	12.633	1790	1793	1794	rBV	31684	31454	1.20%	0.131%
23	12.651	1794	1796	1799	rVB	43315	37950	1.44%	0.157%
24	12.768	1812	1816	1820	rBV	2263622	2116592	80.46%	8.782%
25	12.798	1820	1821	1825	rVB	46288	37332	1.42%	0.155%
26	13.004	1854	1856	1861	rBV2	39850	37838	1.44%	0.157%
27	13.345	1912	1914	1917	rVB	43097	33832	1.29%	0.140%
28	13.674	1968	1970	1973	rBV2	40655	38457	1.46%	0.160%
29	13.827	1992	1996	2004	rBV	842129	898209	34.15%	3.727%
30	14.292	2073	2075	2078	rVB	80141	62965	2.39%	0.261%
31	14.586	2123	2125	2128	rBV	85913	69467	2.64%	0.288%
32	14.651	2134	2136	2140	rVB	158353	139002	5.28%	0.577%
33	15.233	2231	2235	2241	rVB	621666	782272	29.74%	3.246%

LSC Area Percent Report

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Sample : K2198-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

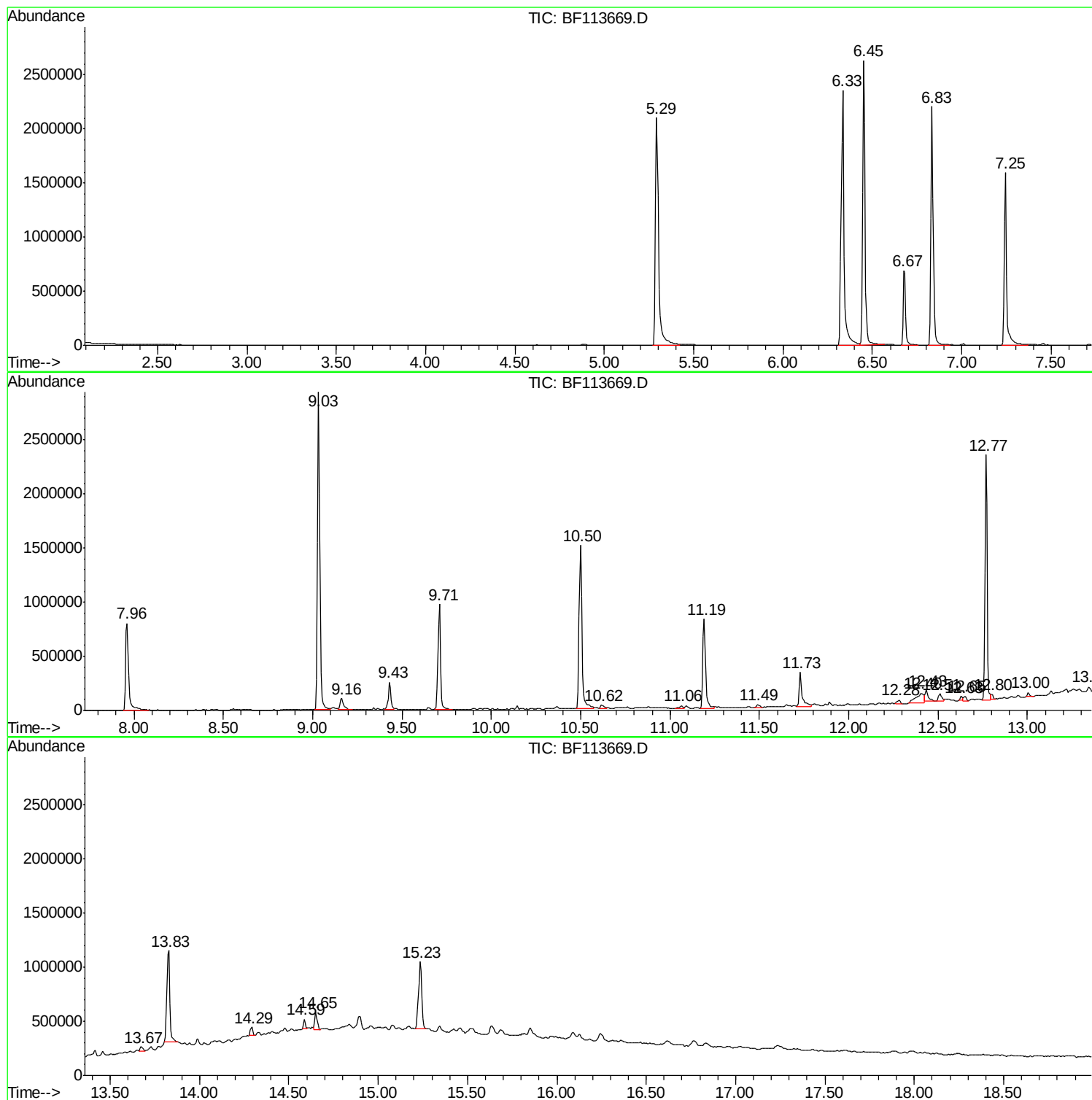
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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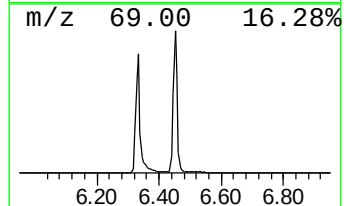
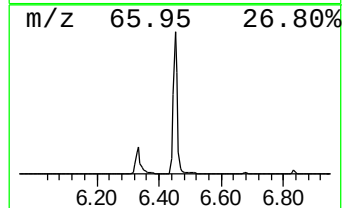
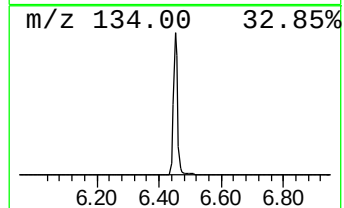
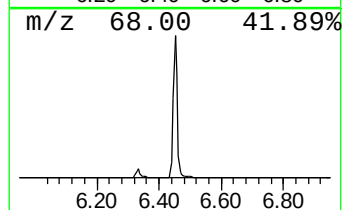
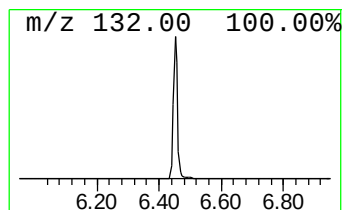
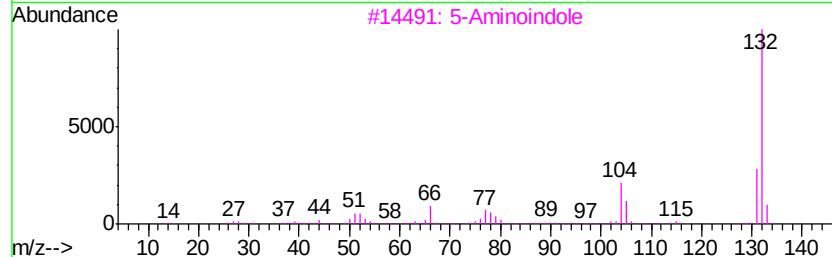
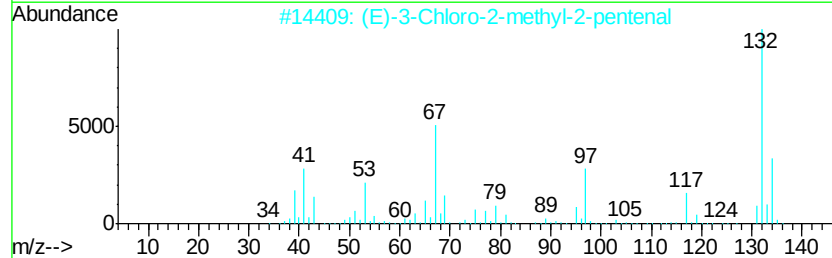
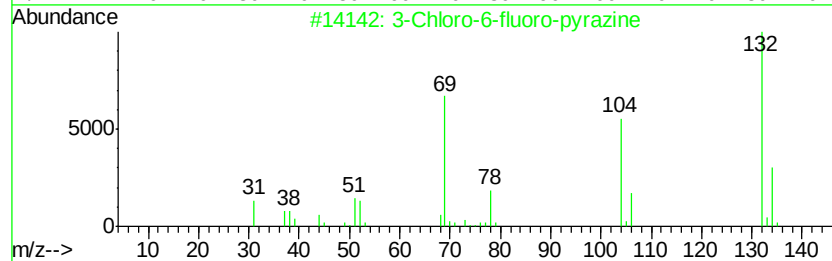
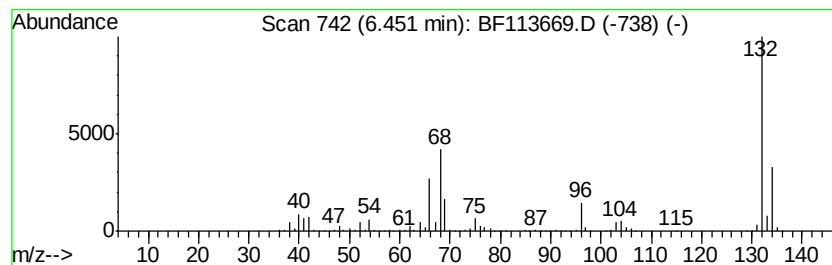
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	74.06 ng	2534760	1,4-Dichlorobenzene-d4	6.68

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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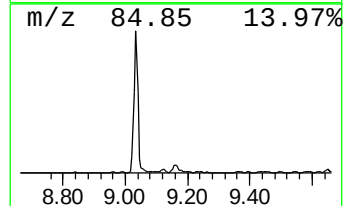
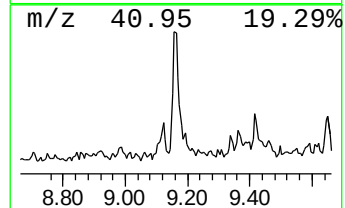
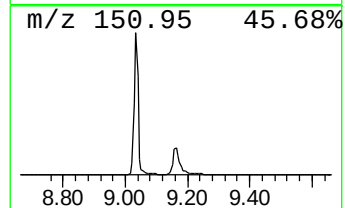
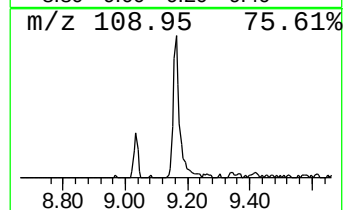
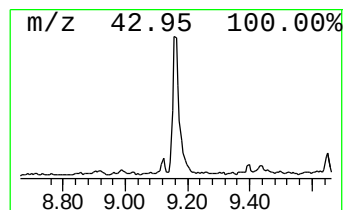
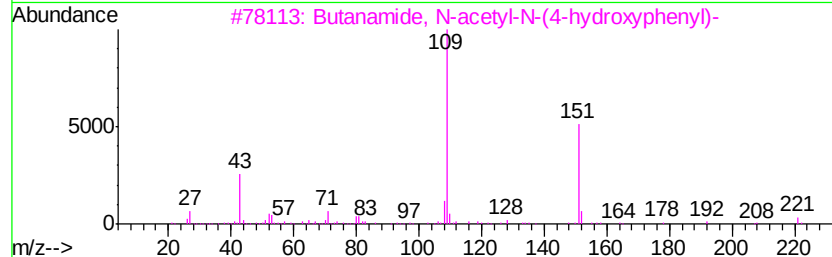
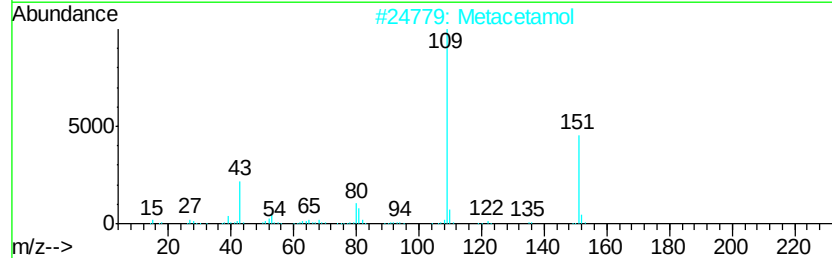
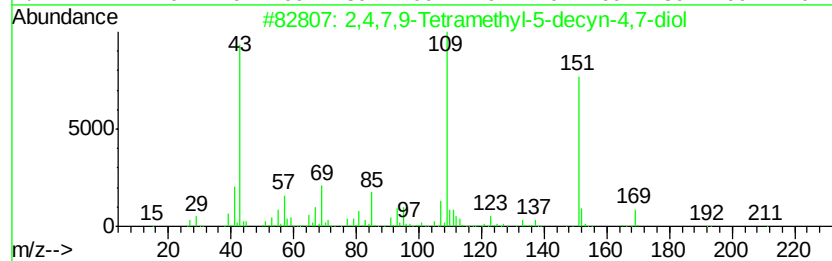
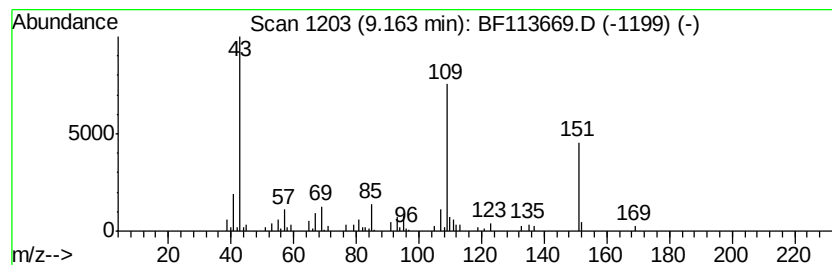
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.16	3.40 ng	151141	Acenaphthene-d10	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2		Metacetamol	151	C8H9NO2	000621-42-1	64
3		Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	59
4		3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
5		m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59



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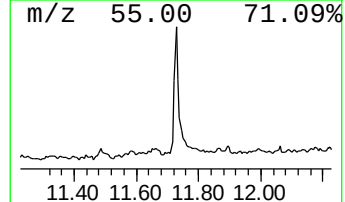
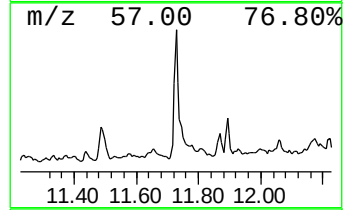
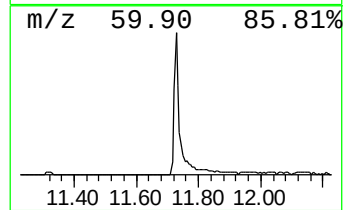
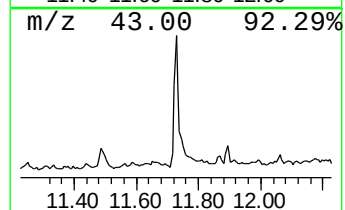
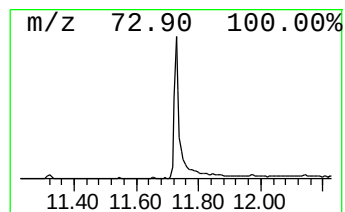
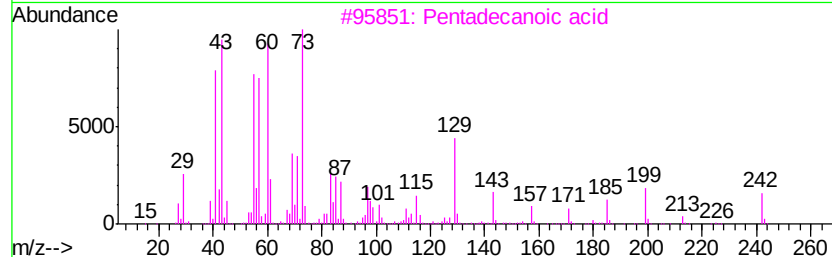
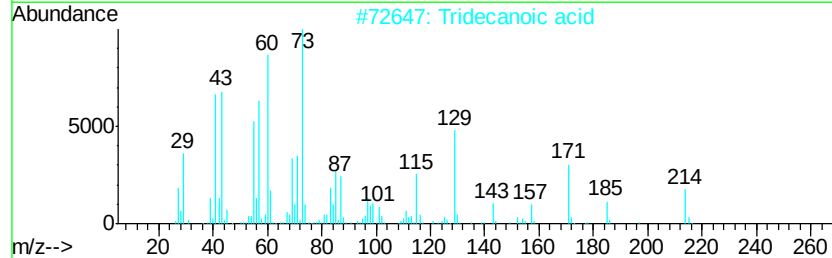
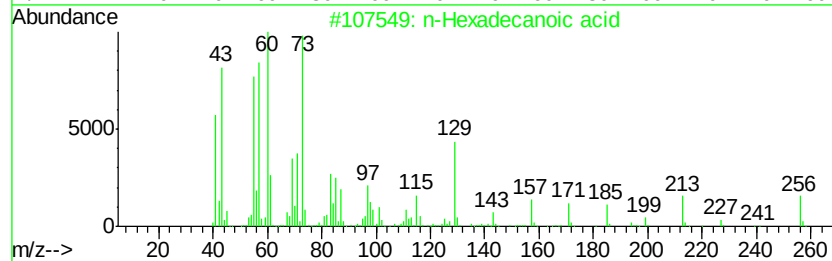
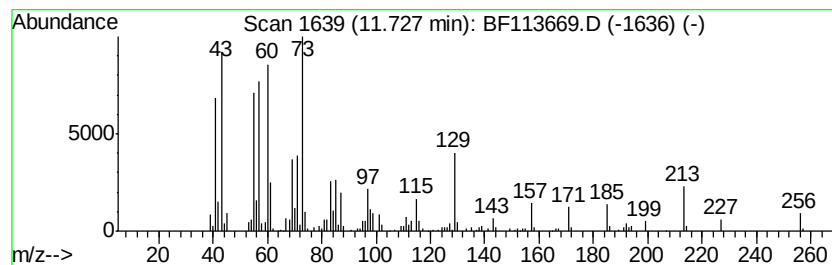
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	9.17 ng	377349	Phenanthrene-d10	11.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	68



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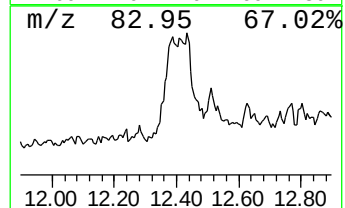
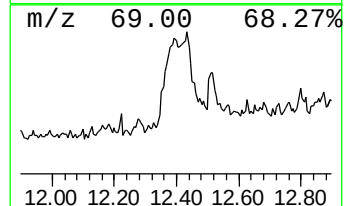
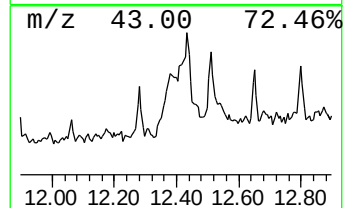
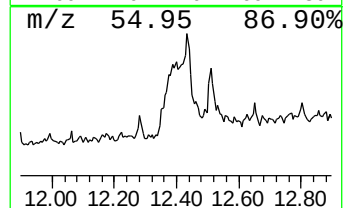
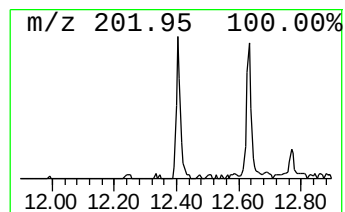
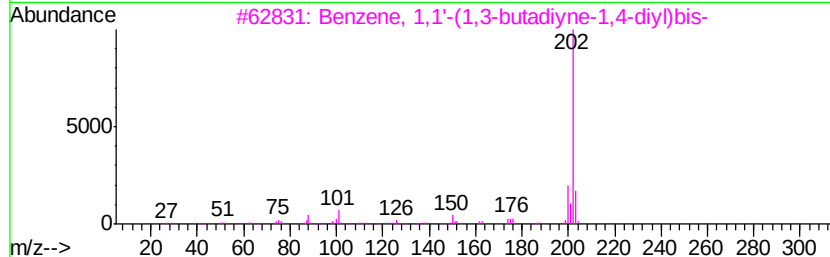
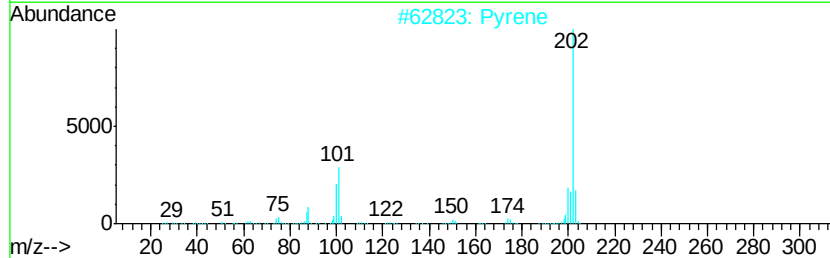
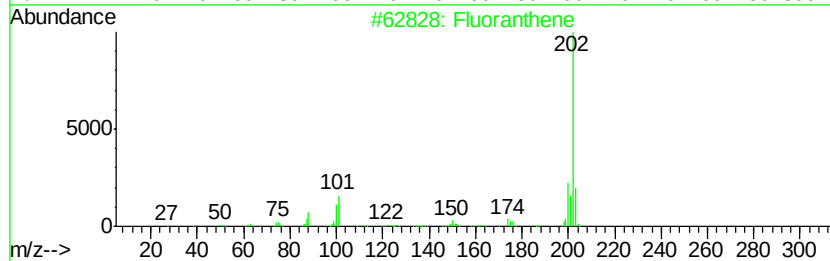
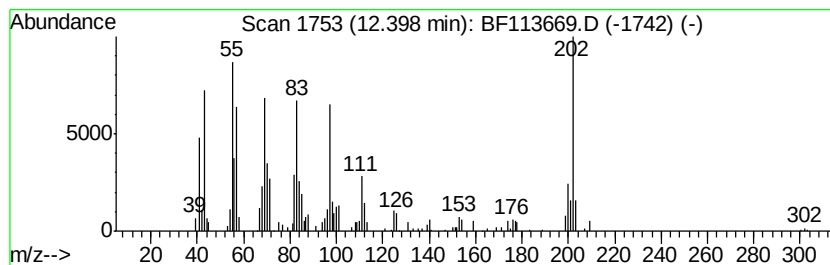
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown12.40 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.40	6.78 ng	278904	Phenanthrene-d10	11.19	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	70
2	Pyrene	202	C16H10	000129-00-0	49
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	49
4	Pyridazine-3,6(1H,2H)-dione, 1-(...	202	C11H10N2O2	034019-60-8	38
5	Di-1H-pyrrol-1-yl-isopropenylsilane	202	C11H14N2Si	1000306-57-7	38



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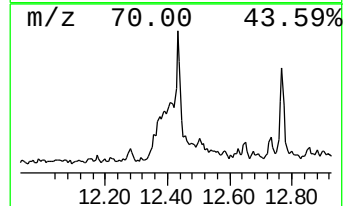
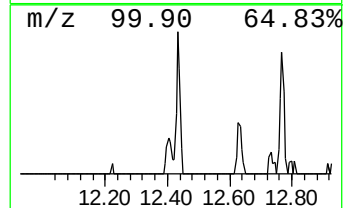
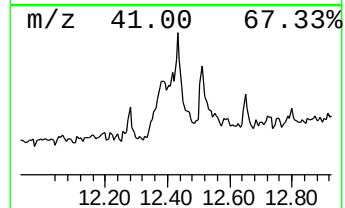
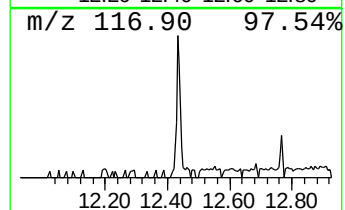
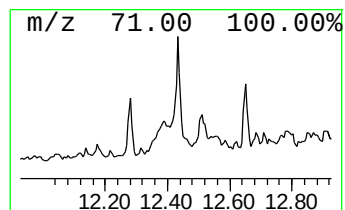
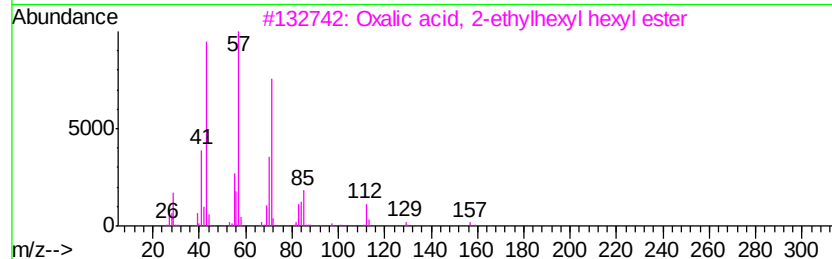
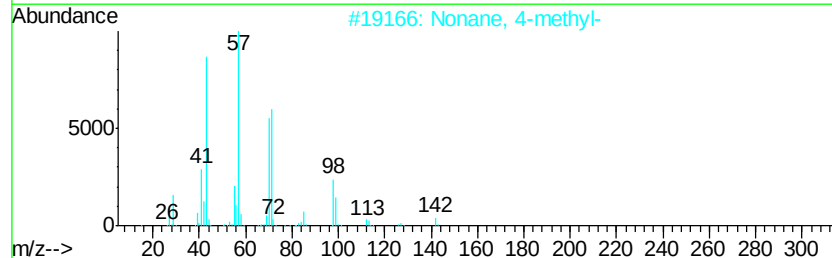
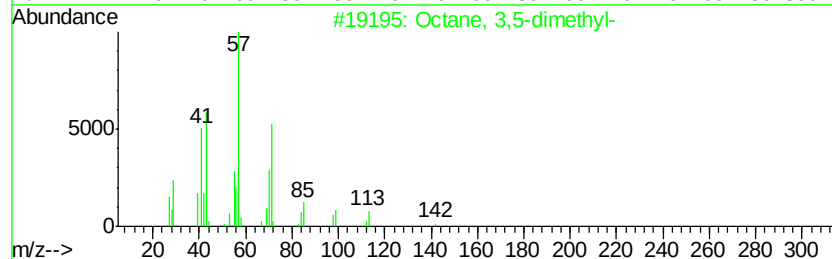
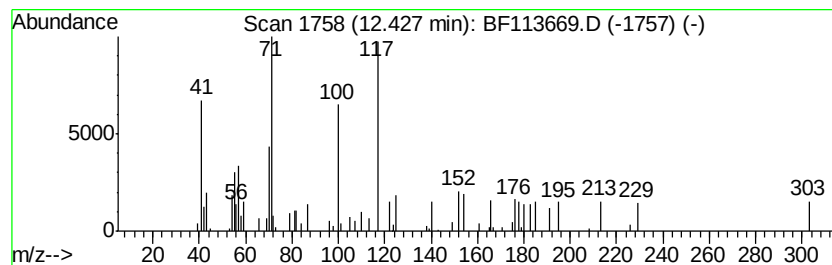
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Peak Number 6 unknown12.43 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	3.08 ng	126498	Phenanthrene-d10	11.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	35
2		Nonane, 4-methyl-	142	C10H22	017301-94-9	35
3		Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	27
4		Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	27
5		Oxalic acid, 2-ethylhexyl pentyl...	272	C15H28O4	1000309-38-7	27



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OK-01-040819

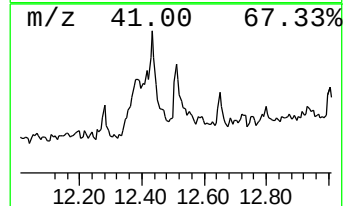
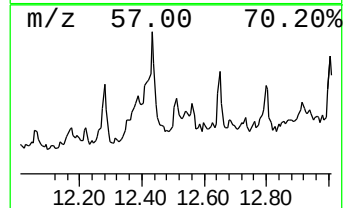
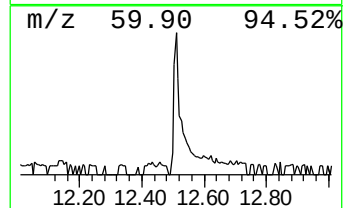
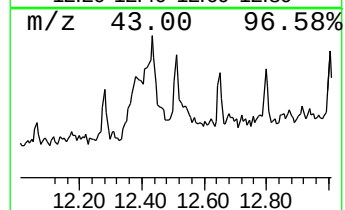
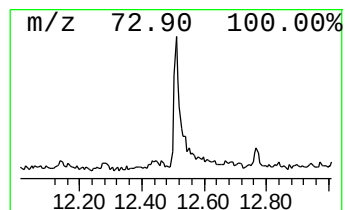
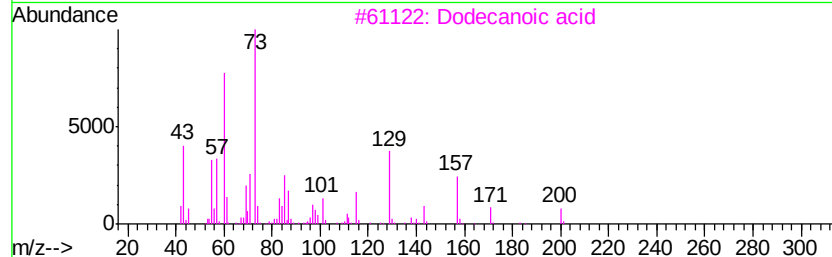
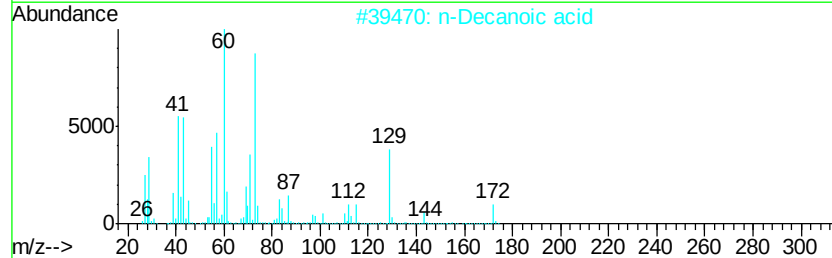
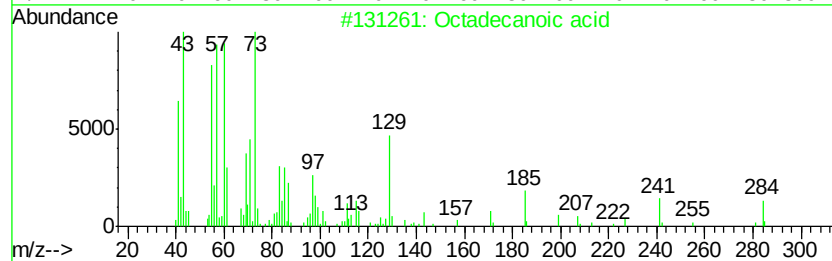
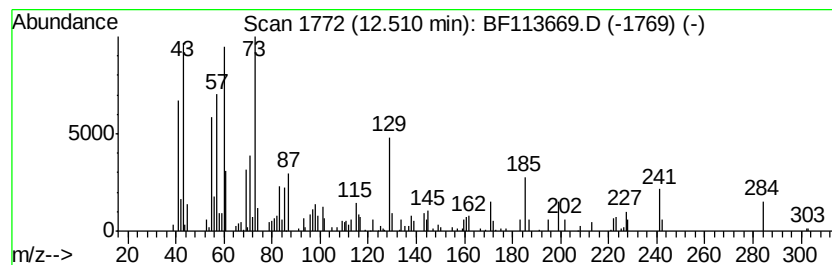
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	2.02 ng	82892	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	50
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47
5	Maltose	342	C12H22O11	000069-79-4	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040919\
Data File : BF113669.D
Acq On : 9 Apr 2019 18:59
Operator : JU/SJ
Sample : K2198-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

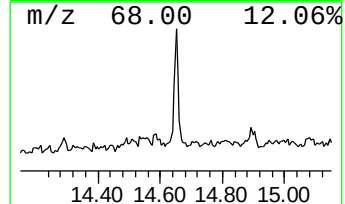
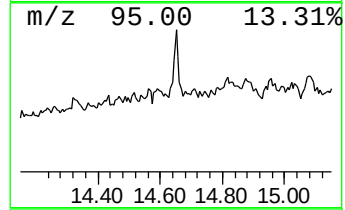
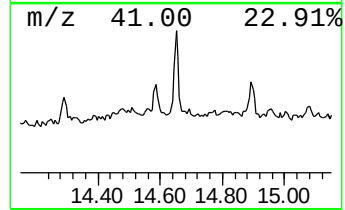
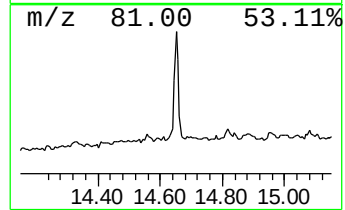
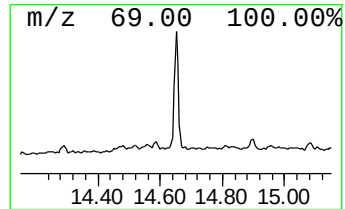
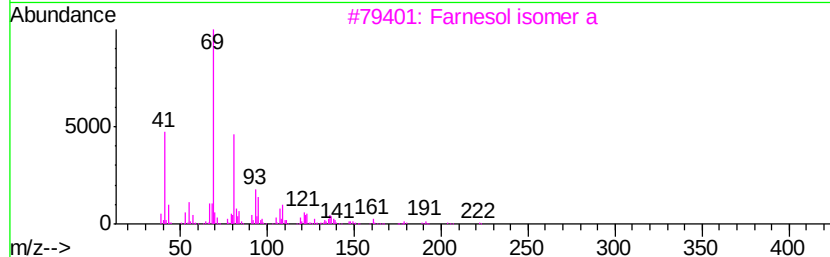
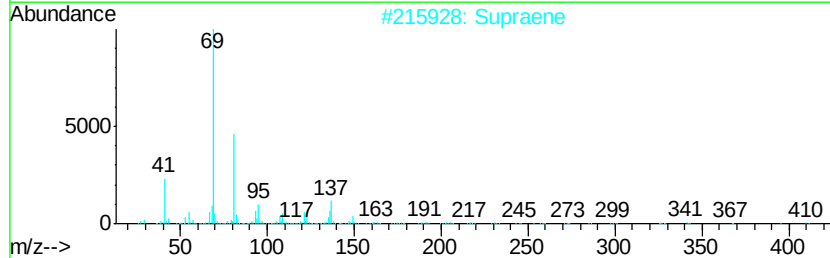
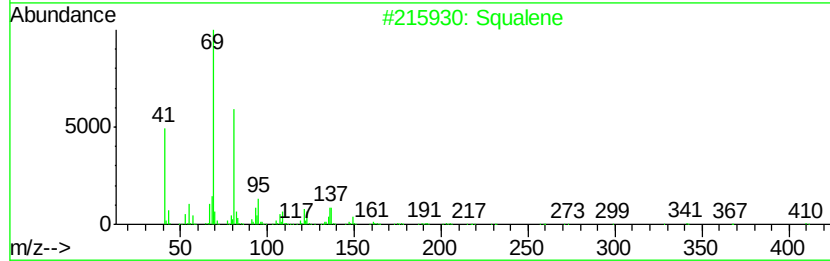
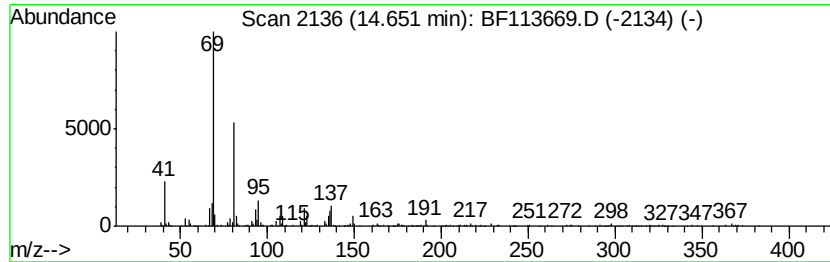
Instrument :
BNA_F
ClientSampleId :
OK-01-040819

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.65	3.55 ng	139002	Perylene-d12	15.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Farnesol isomer a	222	C15H26O	1000108-92-4	72
4	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040919\
Data File : BF113669.D
Acq On : 9 Apr 2019 18:59
Operator : JU/SJ
Sample : K2198-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-01-040819

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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
unknown6.45	6.45	74.1	ng	2534760	1	6.68	684476	20.0
2,4,7,9-Tetrameth...	9.16	3.4	ng	151141	3	9.71	888369	20.0
n-Hexadecanoic acid	11.73	9.2	ng	377349	4	11.19	822574	20.0
unknown12.40	12.40	6.8	ng	278904	4	11.19	822574	20.0
unknown12.43	12.43	3.1	ng	126498	4	11.19	822574	20.0
Octadecanoic acid	12.51	2.0	ng	82892	4	11.19	822574	20.0
Squalene	14.65	3.5	ng	139002	6	15.23	782272	20.0