

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
 Data File : BF118006.D
 Acq On : 26 Nov 2019 14:49
 Operator : JU
 Sample : K5999-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IDLEWILD-BH-03A

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-BF111319.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	2.175	9	15	20	rVB	638390	846952	36.24%	3.045%
2	5.104	508	513	523	rVB	395221	487060	20.84%	1.751%
3	5.510	577	582	585	rBV	2464931	2337280	100.00%	8.403%
4	6.522	749	754	766	rVB	2354704	2213536	94.71%	7.958%
5	6.663	774	778	781	rBV	2704045	2321858	99.34%	8.347%
6	6.893	813	817	820	rBV	987506	751962	32.17%	2.703%
7	7.051	840	844	847	rBV	2568980	2087386	89.31%	7.505%
8	7.457	908	913	916	rBV	1736155	1553807	66.48%	5.586%
9	8.181	1032	1036	1039	rBV	1409538	1049608	44.91%	3.774%
10	9.257	1215	1219	1222	rBV	2743050	2330717	99.72%	8.379%
11	9.498	1256	1260	1262	rBV	56126	49406	2.11%	0.178%
12	9.598	1274	1277	1280	rBV	504011	384392	16.45%	1.382%
13	9.651	1282	1286	1290	rVB	359008	280344	11.99%	1.008%
14	9.775	1305	1307	1309	rBV	38228	31611	1.35%	0.114%
15	9.804	1309	1312	1314	rVB2	54431	50479	2.16%	0.181%
16	9.945	1329	1336	1338	rBV	1076259	1072448	45.88%	3.856%
17	9.963	1338	1339	1341	rVB	532587	244160	10.45%	0.878%
18	10.569	1438	1442	1445	rBV	58199	56406	2.41%	0.203%
19	10.692	1458	1463	1464	rBV2	36408	28594	1.22%	0.103%
20	10.733	1464	1470	1477	rVB2	1447347	1692543	72.42%	6.085%
21	10.933	1499	1504	1510	rBV8	21492	35822	1.53%	0.129%
22	11.198	1546	1549	1553	rVB	66138	54744	2.34%	0.197%
23	11.375	1576	1579	1583	rBV4	28650	35484	1.52%	0.128%
24	11.433	1586	1589	1592	rVV	850337	800145	34.23%	2.877%
25	11.457	1592	1593	1599	rVV	147564	123266	5.27%	0.443%
26	11.510	1599	1602	1604	rVV	55661	44509	1.90%	0.160%
27	11.733	1636	1640	1641	rBV3	27720	38094	1.63%	0.137%
28	11.922	1670	1672	1674	rBV3	41655	41326	1.77%	0.149%
29	11.957	1675	1678	1683	rVV2	424218	451425	19.31%	1.623%
30	12.051	1692	1694	1696	rBV2	51404	53259	2.28%	0.191%
31	12.233	1723	1725	1727	rBV	36800	29504	1.26%	0.106%
32	12.657	1794	1797	1800	rBV	458386	421481	18.03%	1.515%
33	12.686	1800	1802	1804	rVB2	86165	79441	3.40%	0.286%
34	12.751	1810	1813	1817	rBV	190583	209425	8.96%	0.753%

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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-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.886	1833	1836	1841	rVB	420877	388908	16.64%	1.398%
36	13.027	1856	1860	1863	rBV	2527572	2136210	91.40%	7.680%
37	13.216	1889	1892	1894	rBV	107901	129107	5.52%	0.464%
38	13.945	2012	2016	2021	rBV4	176916	346001	14.80%	1.244%
39	14.063	2033	2036	2037	rBV	266142	234353	10.03%	0.843%
40	14.092	2037	2041	2043	rVV2	935113	1132186	48.44%	4.070%
41	14.116	2043	2045	2047	rVB	235737	171148	7.32%	0.615%
42	15.151	2218	2221	2228	rVB	254405	434384	18.59%	1.562%
43	15.598	2294	2297	2300	rBV	457628	554265	23.71%	1.993%

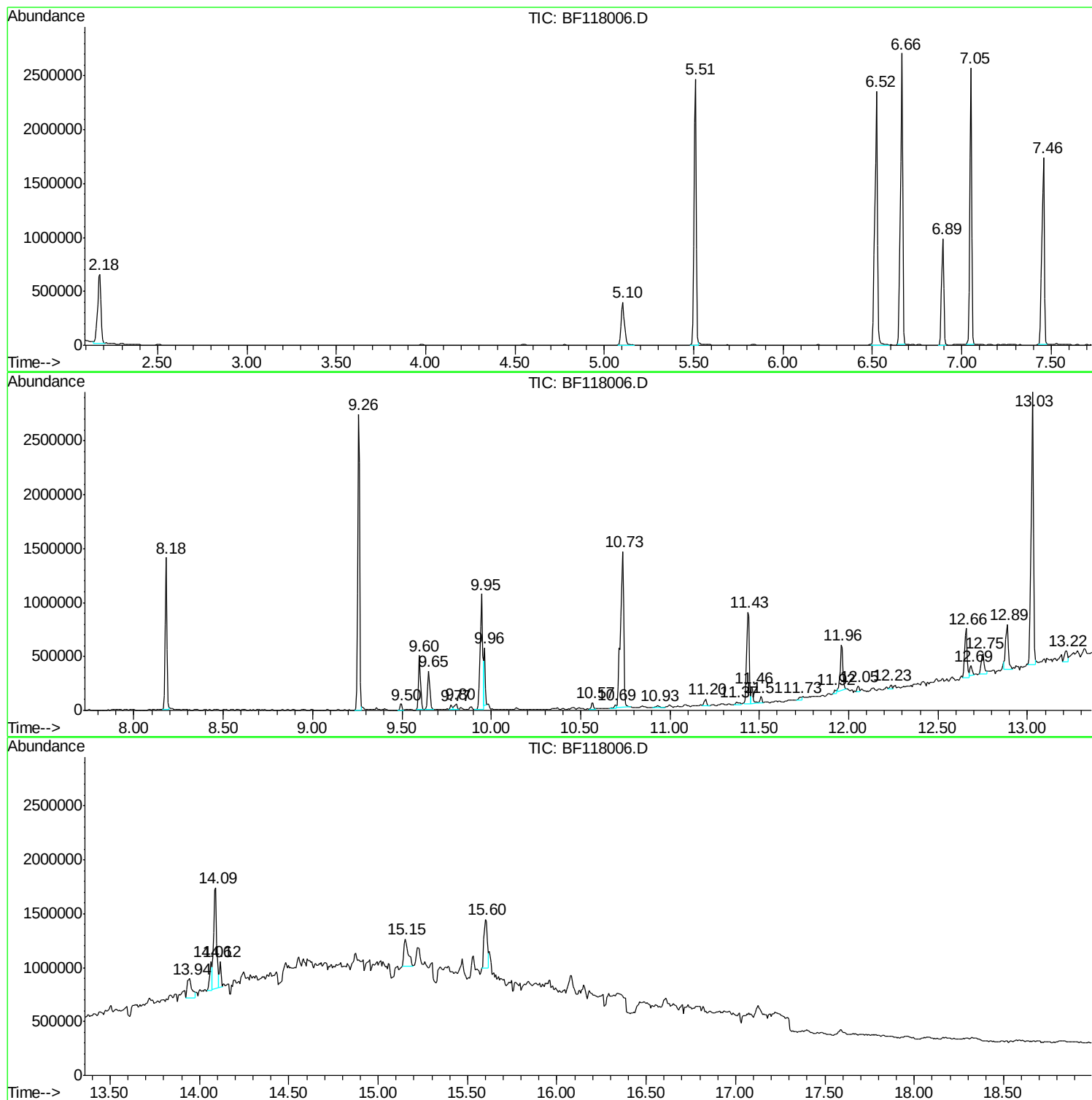
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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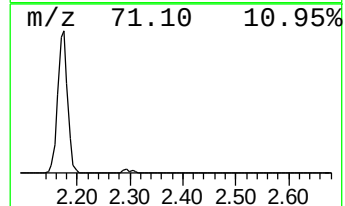
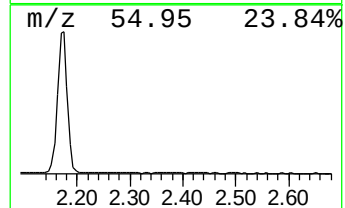
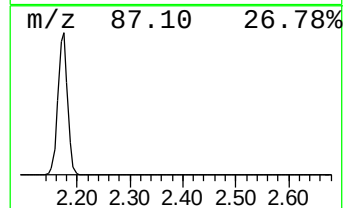
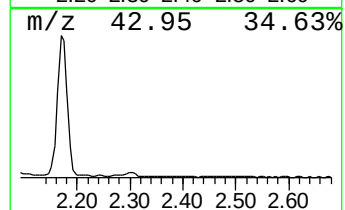
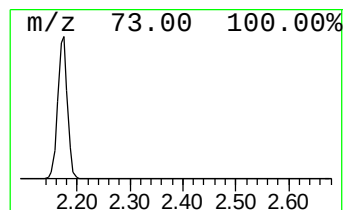
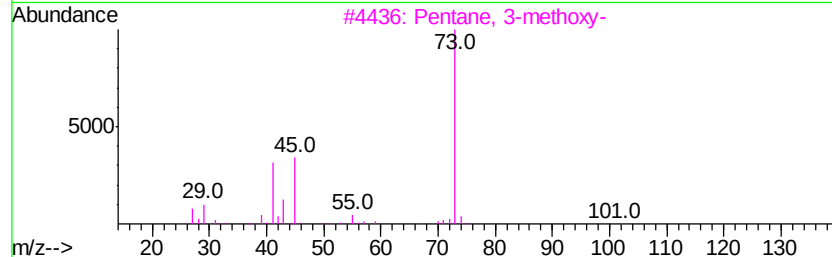
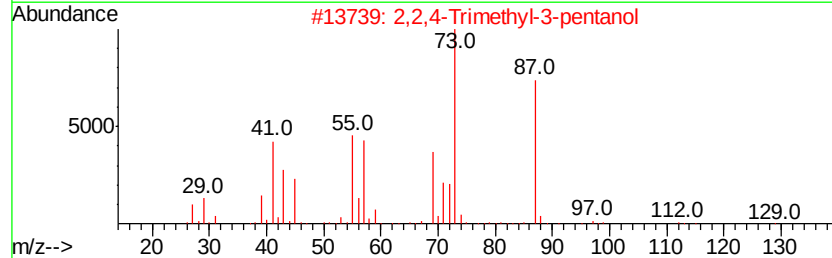
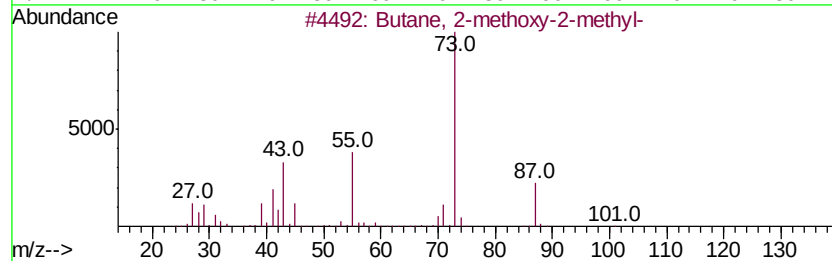
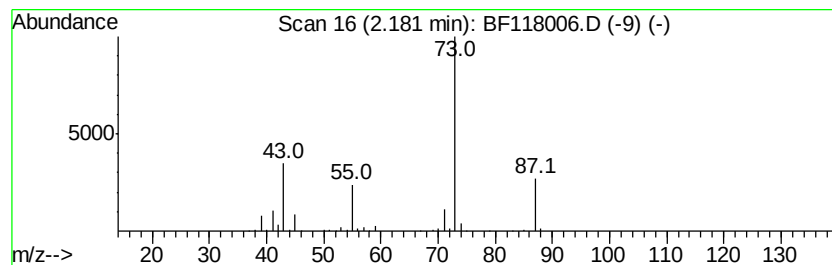
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	22.53 ng	846952	1,4-Dichlorobenzene-d4	6.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butane, 2-methoxy-2-methyl-	102 C6H14O	000994-05-8 83
2		2,2,4-Trimethyl-3-pentanol	130 C8H18O	005162-48-1 39
3		Pentane, 3-methoxy-	102 C6H14O	036839-67-5 23
4		Silane, tetramethyl-	88 C4H12Si	000075-76-3 17
5		1,3-Dioxolane, 2-methyl-	88 C4H8O2	000497-26-7 9



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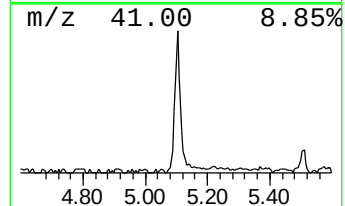
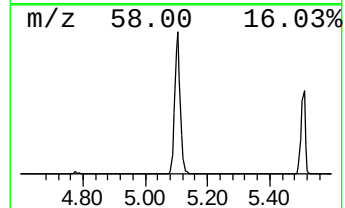
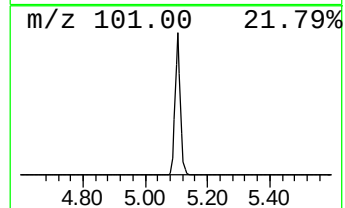
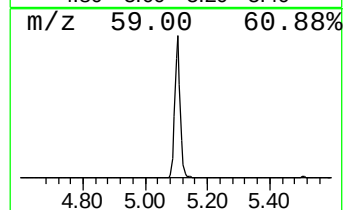
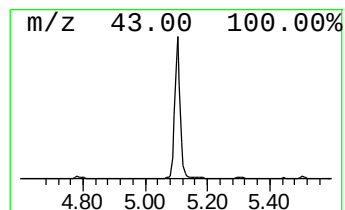
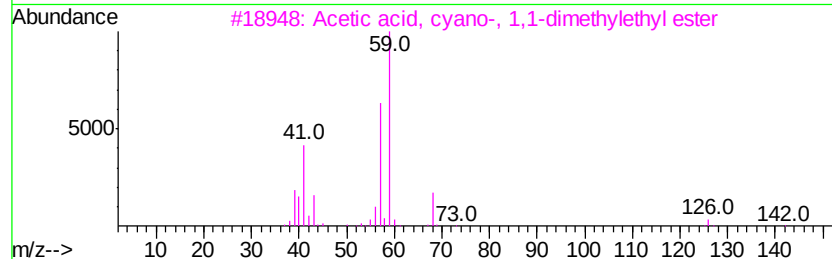
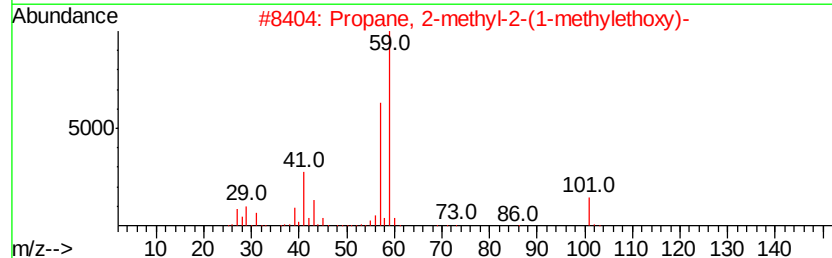
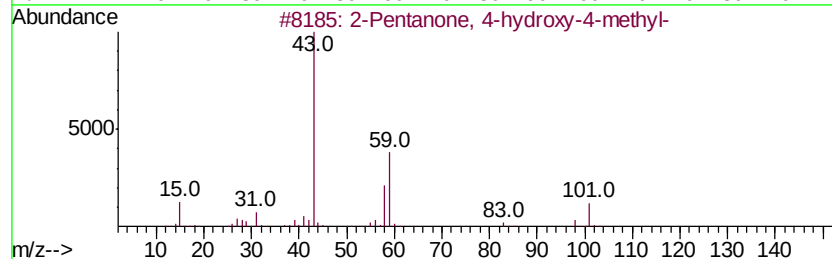
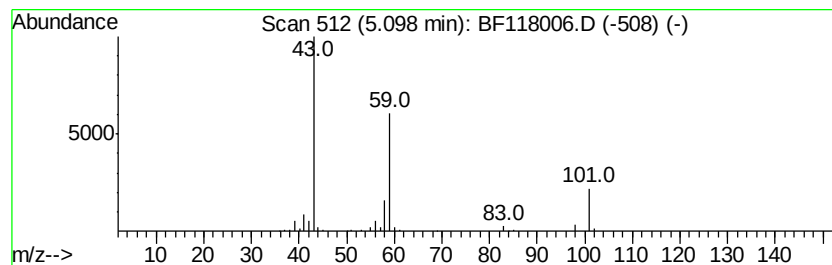
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	12.95 ng	487060	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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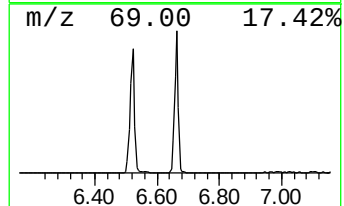
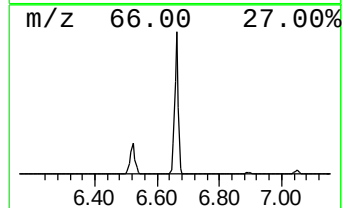
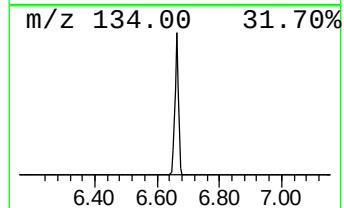
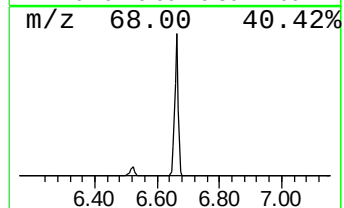
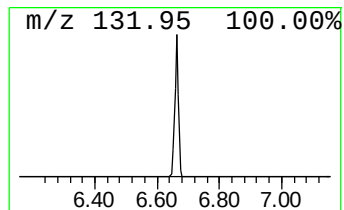
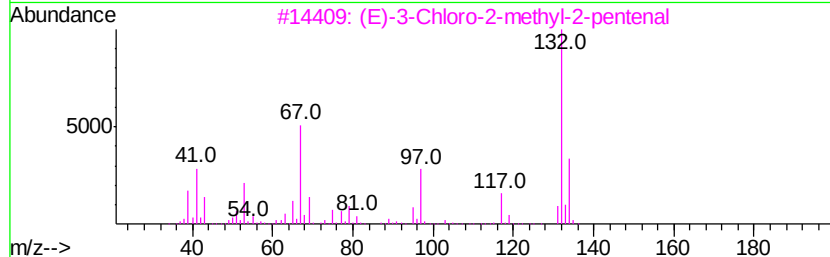
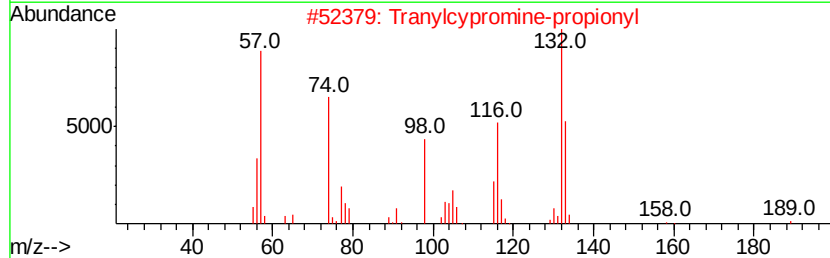
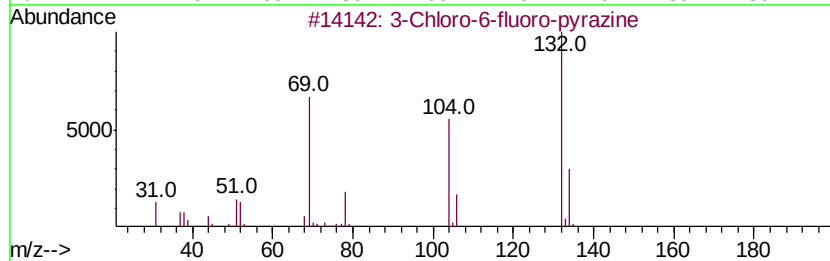
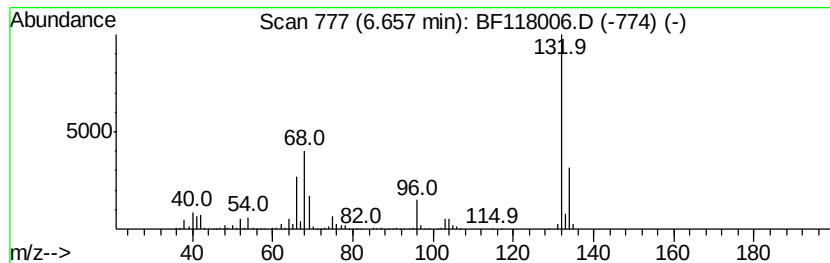
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	61.75 ng	2321860	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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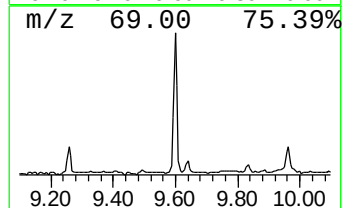
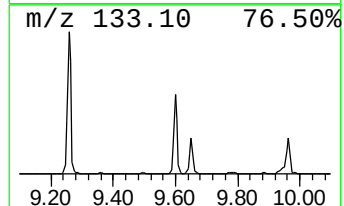
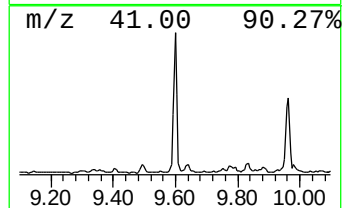
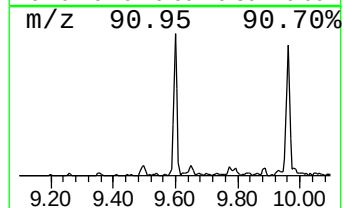
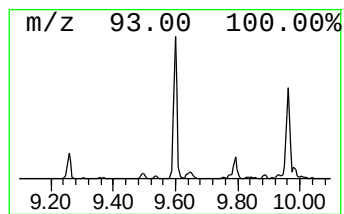
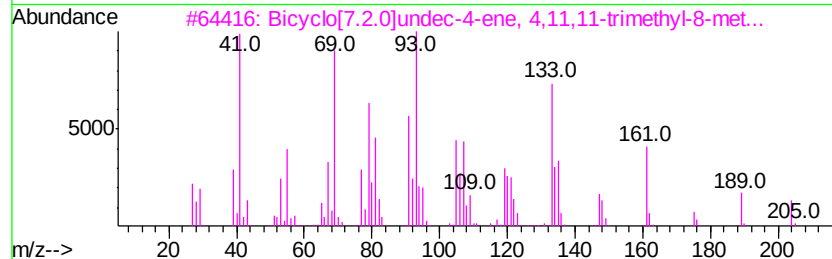
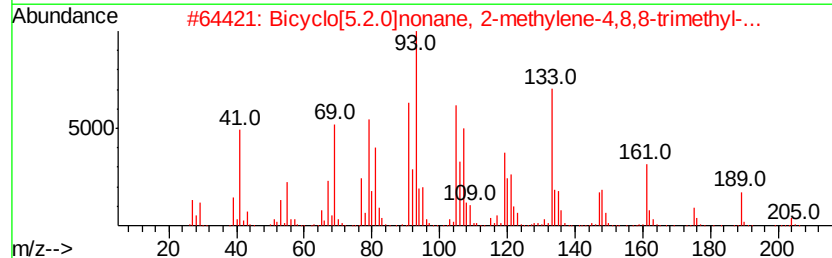
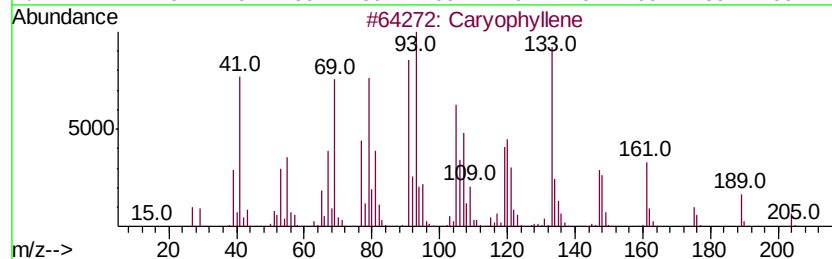
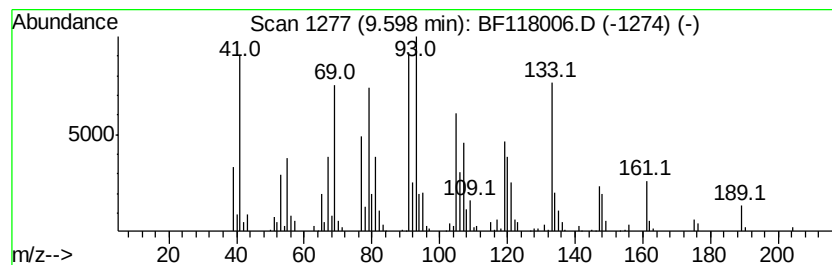
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Caryophyllene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.60	7.17 ng	384392	Acenaphthene-d10		9.95	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Carvophyllene	204	C15H24	000087-44-5	99
2		Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	93
3		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	91
4		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
5		Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	60



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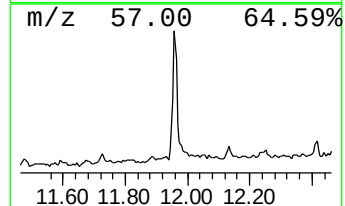
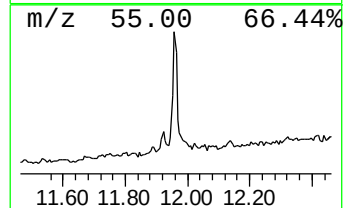
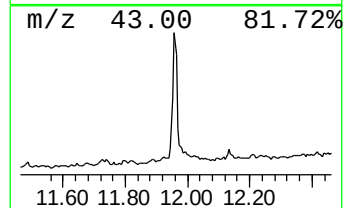
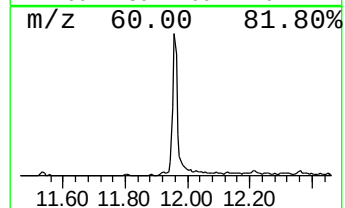
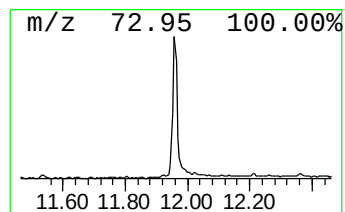
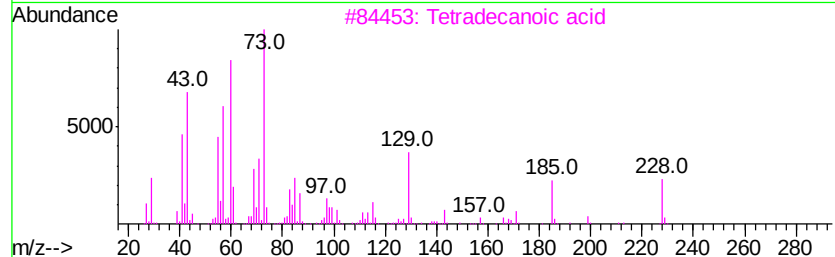
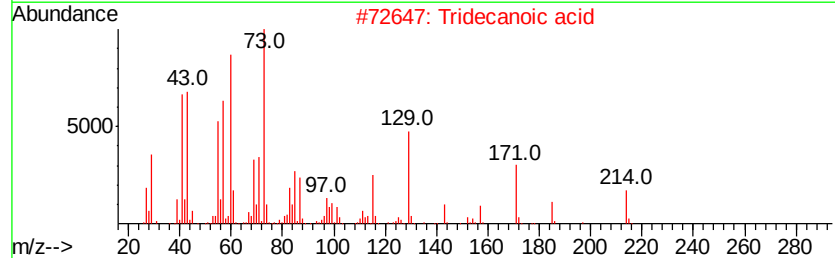
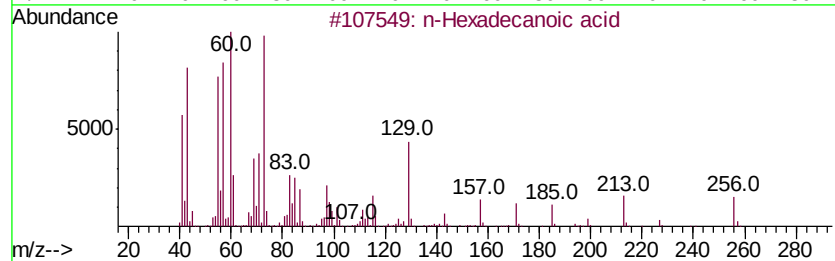
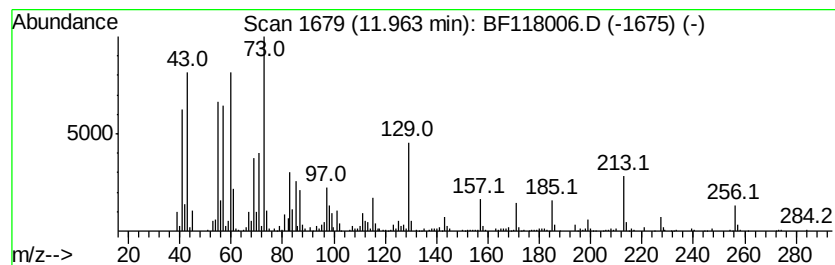
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.96	11.28 ng	451425	Phenanthrene-d10		11.43	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
5	Dodecanoic acid		200	C12H24O2	000143-07-7	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118006.D
Acq On : 26 Nov 2019 14:49
Operator : JU
Sample : K5999-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

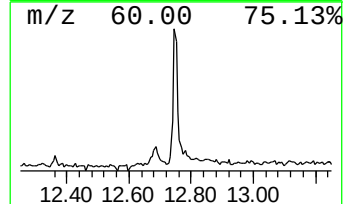
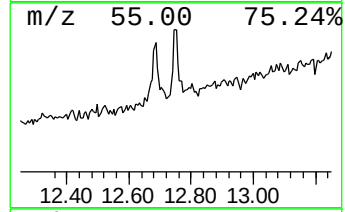
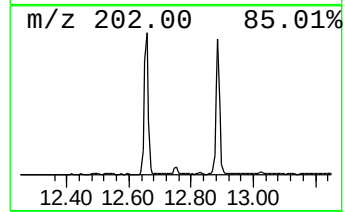
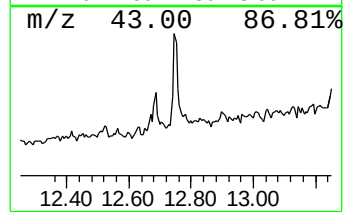
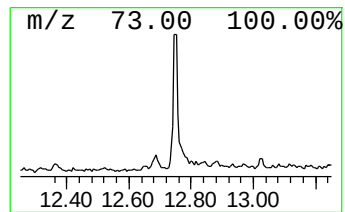
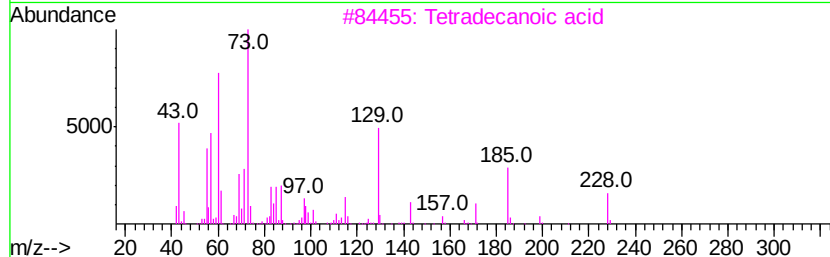
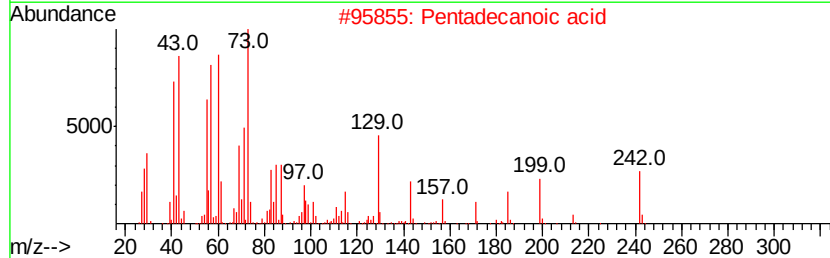
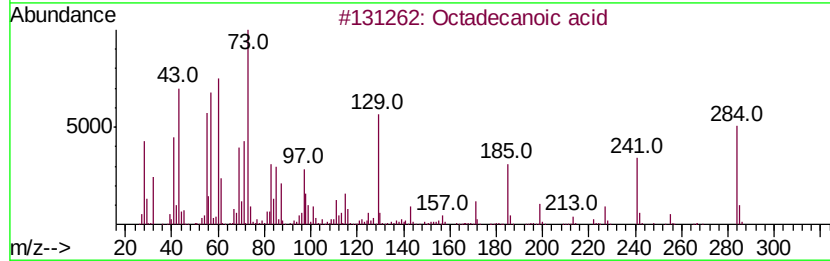
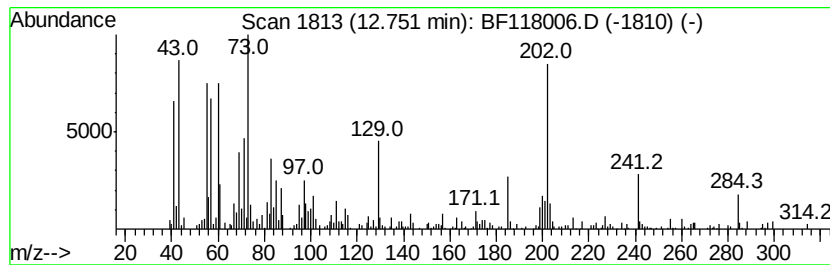
Instrument :
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ClientSampleId :
IDLEWILD-BH-03A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
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.	
12.75	5.23 ng	209425	Phenanthrene-d10		11.43	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	78
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	49
4	Undecanoic acid		186	C11H22O2	000112-37-8	46
5	Dodecanoic acid		200	C12H24O2	000143-07-7	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118006.D
Acq On : 26 Nov 2019 14:49
Operator : JU
Sample : K5999-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDLEWILD-BH-03A

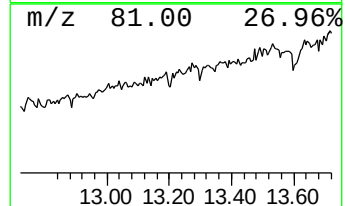
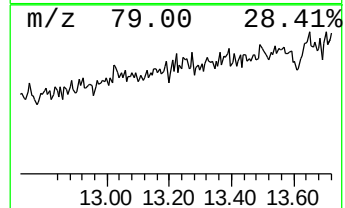
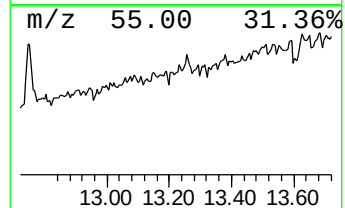
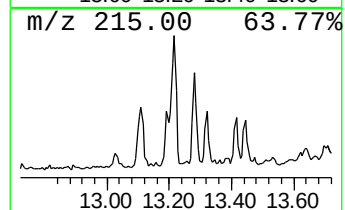
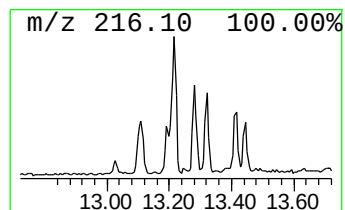
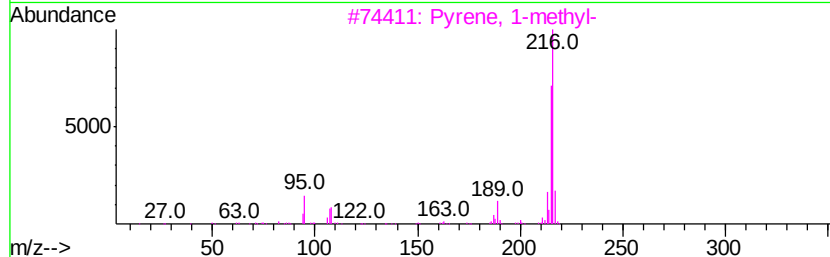
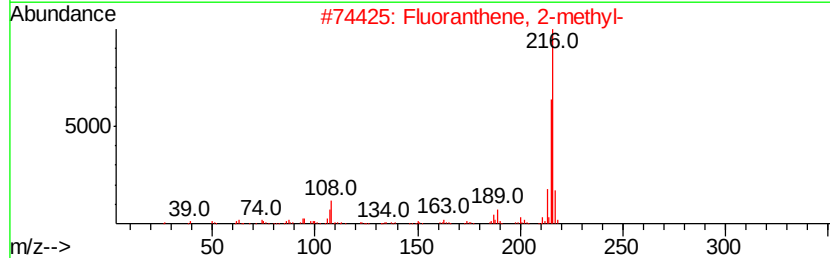
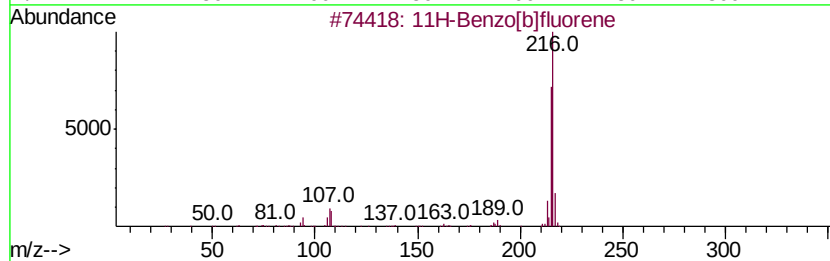
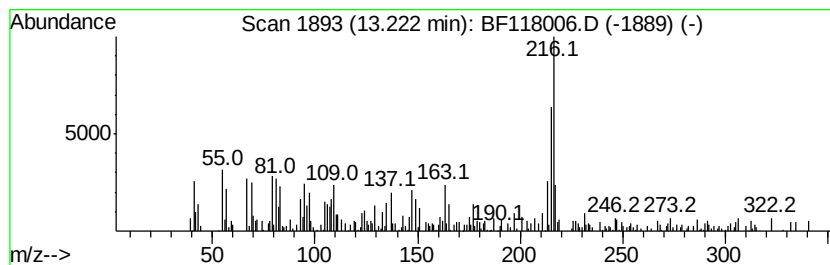
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.22	2.28 ng	129107	Chrysene-d12	14.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	89
3		Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4		Pyrene, 2-methyl-	216	C17H12	003442-78-2	81
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118006.D
Acq On : 26 Nov 2019 14:49
Operator : JU
Sample : K5999-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

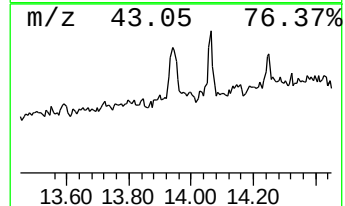
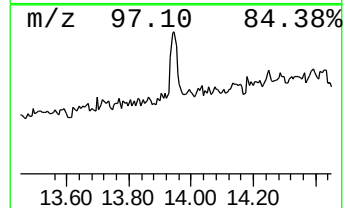
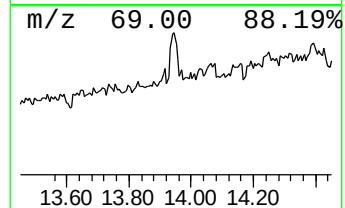
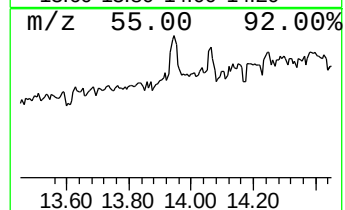
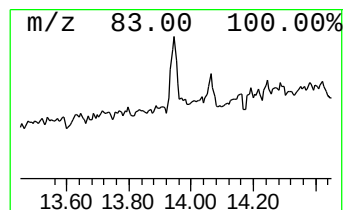
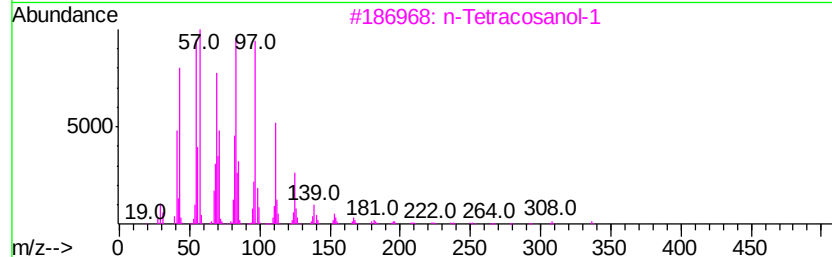
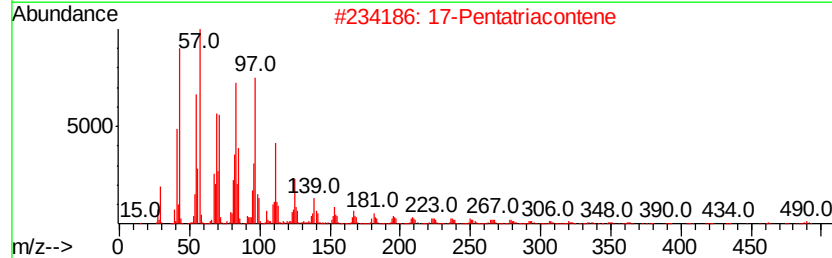
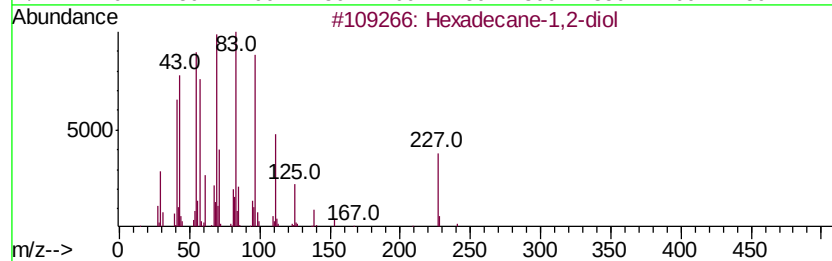
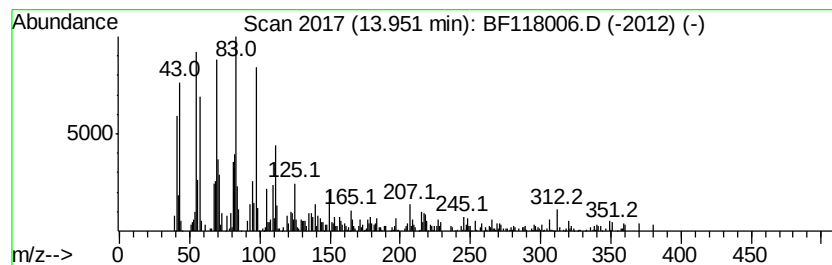
Instrument :
BNA_F
ClientSampleId :
IDLEWILD-BH-03A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane-1,2-diol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.95	6.11 ng	346001	Chrysene-d12		14.09
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane-1,2-diol	258	C16H34O2	006920-24-7	74
2	17-Pentatriacontene	491	C35H70	006971-40-0	62
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	60
4	Behenic alcohol	326	C22H46O	000661-19-8	60
5	1-Hexadecanol	242	C16H34O	036653-82-4	55



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Sample : K5999-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.18	22.5	ng	846952	1	6.89	751962	20.0
2-Pentanone, 4-hy...	5.10	12.9	ng	487060	1	6.89	751962	20.0
unknown6.66	6.66	61.8	ng	2321860	1	6.89	751962	20.0
Caryophyllene	9.60	7.2	ng	384392	3	9.95	1072450	20.0
n-Hexadecanoic acid	11.96	11.3	ng	451425	4	11.43	800145	20.0
Octadecanoic acid	12.75	5.2	ng	209425	4	11.43	800145	20.0
11H-Benzo[b]fluorene	13.22	2.3	ng	129107	5	14.09	1132190	20.0
Hexadecane-1,2-diol	13.95	6.1	ng	346001	5	14.09	1132190	20.0