

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
 Data File : BF091282.D
 Acq On : 23 Nov 2016 18:39
 Operator : UM/SJ
 Sample : H5718-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHOENIX-BPM

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-BF112316.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	1.767	4	7	17	rVB	2124568	2985778	41.04%	3.884%
2	1.904	17	19	41	rVB	2859308	5996006	82.42%	7.800%
3	2.178	41	43	69	rVB2	108809	445004	6.12%	0.579%
4	3.230	133	135	148	rBV2	39138	118078	1.62%	0.154%
5	5.081	293	297	305	rVB	1595728	2541514	34.94%	3.306%
6	5.493	329	333	335	rBV	4576205	7230199	99.39%	9.405%
7	6.510	418	422	424	rVB	5800677	7274857	100.00%	9.463%
8	6.647	431	434	436	rBV	6065563	6429114	88.37%	8.363%
9	6.876	452	454	456	rBV	1602079	1334801	18.35%	1.736%
10	7.036	465	468	470	rVB	5415673	5036416	69.23%	6.551%
11	7.436	500	503	506	rBV	3340929	4137098	56.87%	5.382%
12	8.156	564	566	569	rBV	1407894	1723339	23.69%	2.242%
13	9.242	658	661	664	rBV	6415349	6810038	93.61%	8.859%
14	9.630	693	695	698	rVB	938052	893350	12.28%	1.162%
15	9.916	717	720	722	rBV	2302496	2063773	28.37%	2.685%
16	10.339	754	757	758	rBV2	56146	102023	1.40%	0.133%
17	10.705	786	789	792	rBV	4851649	5253949	72.22%	6.834%
18	10.830	798	800	805	rVB	130805	158539	2.18%	0.206%
19	11.276	837	839	841	rBV	141871	121321	1.67%	0.158%
20	11.402	847	850	852	rVB	2204700	2198817	30.22%	2.860%
21	11.631	868	870	872	rBV	892338	701117	9.64%	0.912%
22	11.699	874	876	879	rVB	101195	122110	1.68%	0.159%
23	11.939	894	897	899	rBV	721906	839401	11.54%	1.092%
24	12.111	910	912	914	rBV	109128	91498	1.26%	0.119%
25	12.453	940	942	944	rBV	206948	213492	2.93%	0.278%
26	12.499	944	946	950	rVB	82675	85031	1.17%	0.111%
27	12.636	953	958	963	rBV2	49014	122366	1.68%	0.159%
28	12.716	963	965	972	rBV2	360218	549067	7.55%	0.714%
29	12.876	977	979	983	rVB	76577	96704	1.33%	0.126%
30	12.991	986	989	991	rBV	6431117	6600437	90.73%	8.586%
31	13.231	1006	1010	1012	rBV	72699	86458	1.19%	0.112%
32	13.882	1065	1067	1074	rBV	326387	383501	5.27%	0.499%
33	14.031	1077	1080	1083	rBV	2354321	2124660	29.21%	2.764%
34	14.899	1153	1156	1158	rVB	70361	84419	1.16%	0.110%

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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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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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35	15.471	1203	1206	1209	rBV	1628039	1920227	26.40%	2.498%
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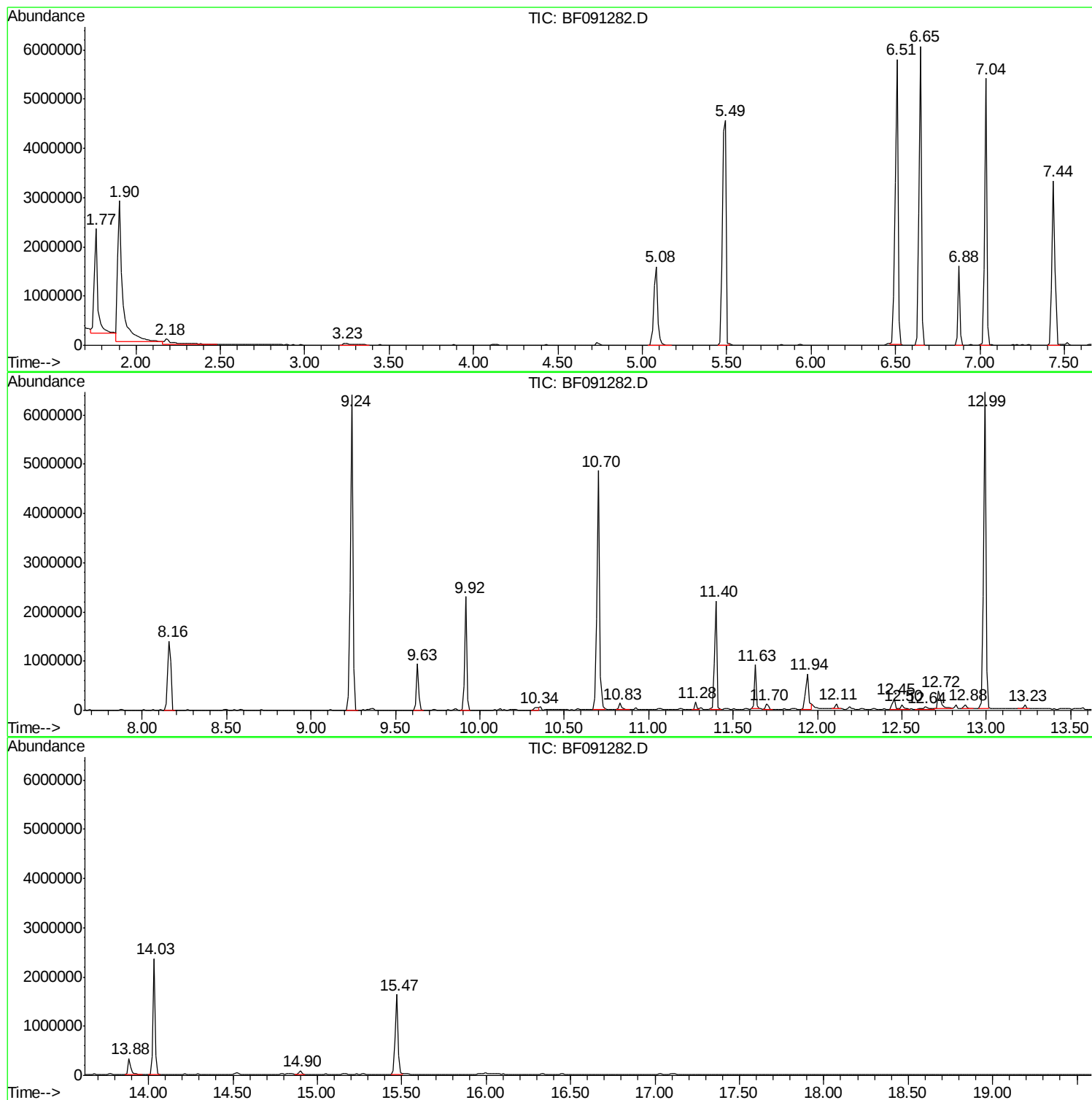
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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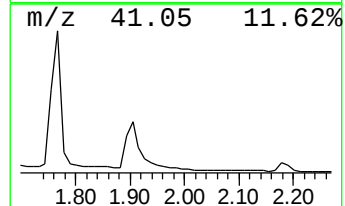
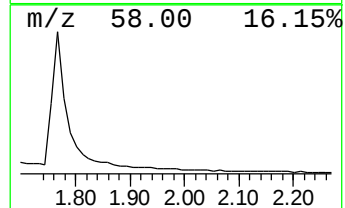
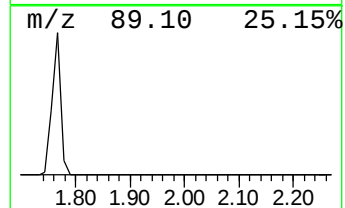
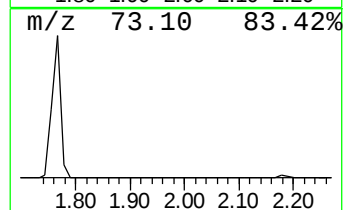
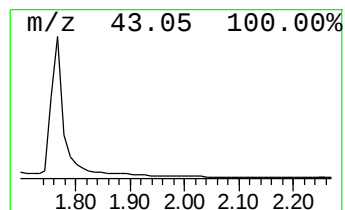
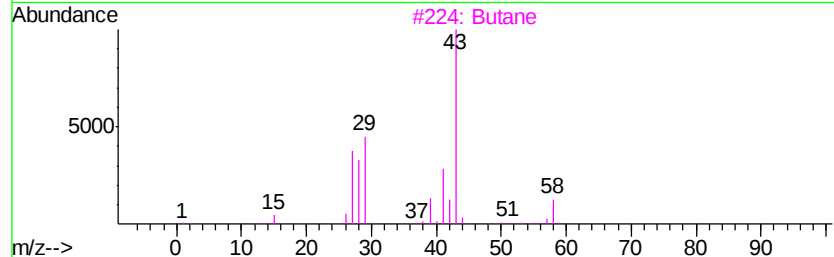
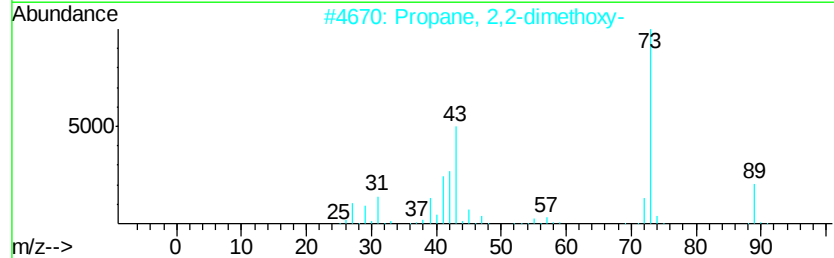
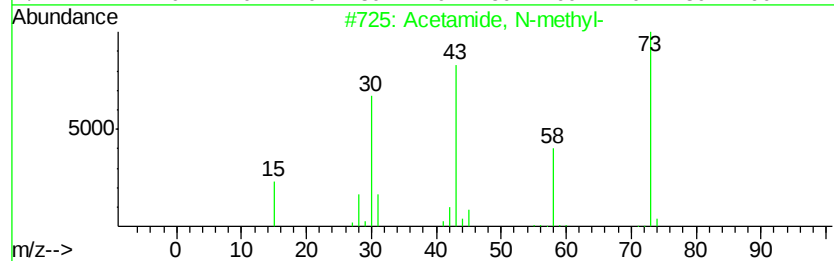
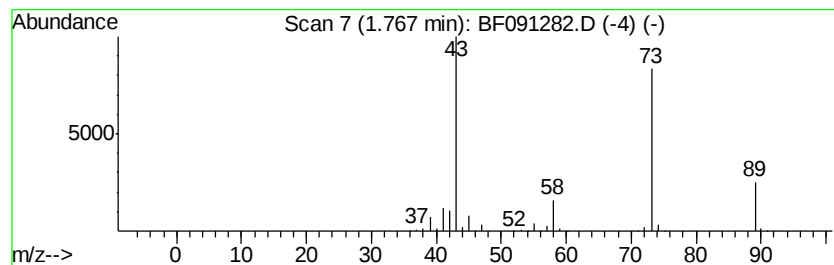
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.77	44.74 ng	2985780	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	46
2		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
3		Butane	58	C4H10	000106-97-8	27
4		Acetone	58	C3H6O	000067-64-1	9
5		Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	9



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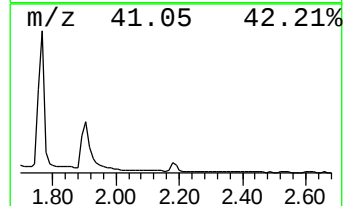
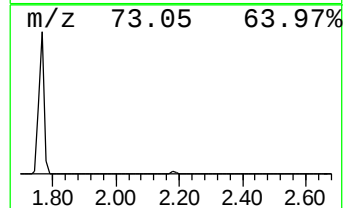
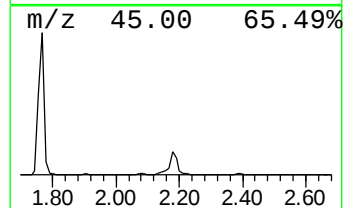
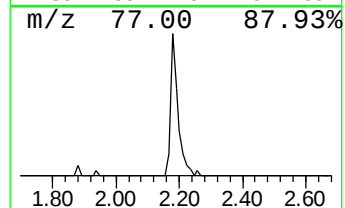
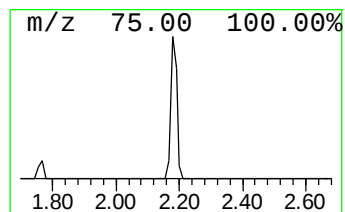
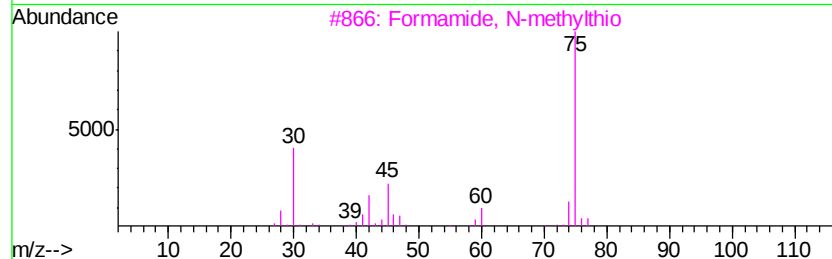
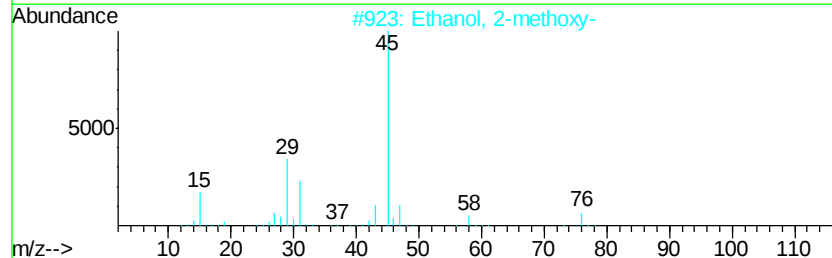
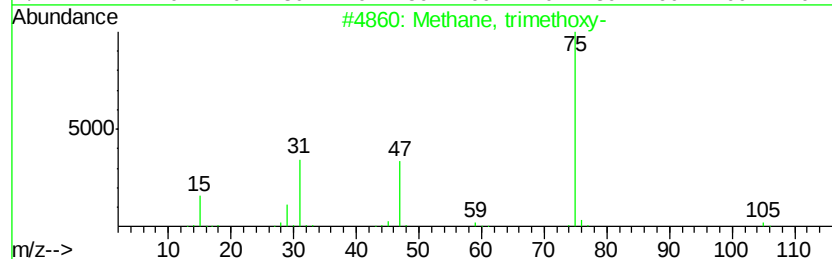
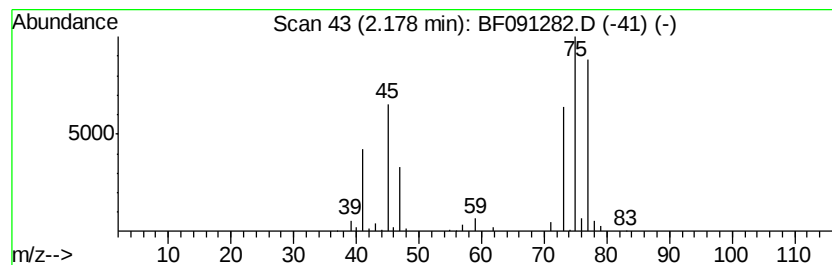
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown2.18 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	6.67 ng	445004	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methane, trimethoxy-	106	C4H10O3	000149-73-5	17
2		Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9
3		Formamide, N-methylthio	75	C2H5NS	018952-41-5	9
4		Ethanethioamide	75	C2H5NS	000062-55-5	9
5		1,2,4-Butanetriol	106	C4H10O3	003068-00-6	9



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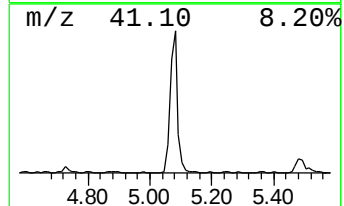
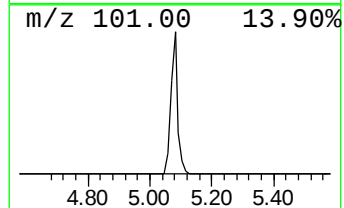
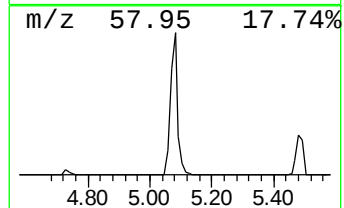
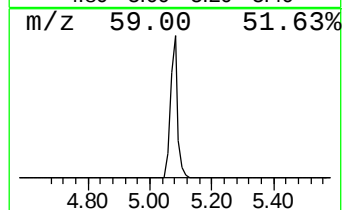
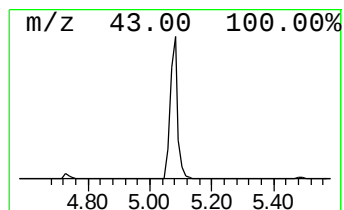
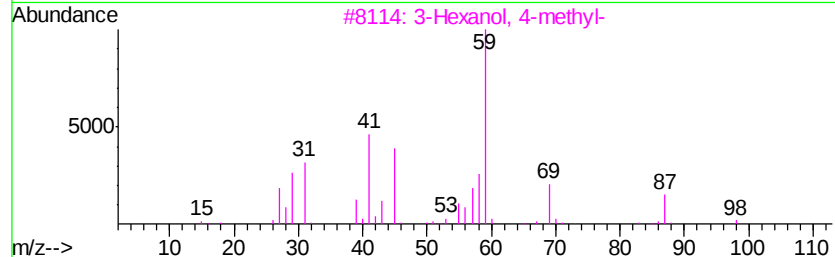
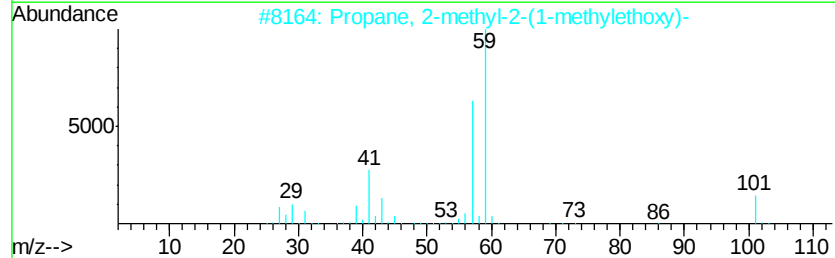
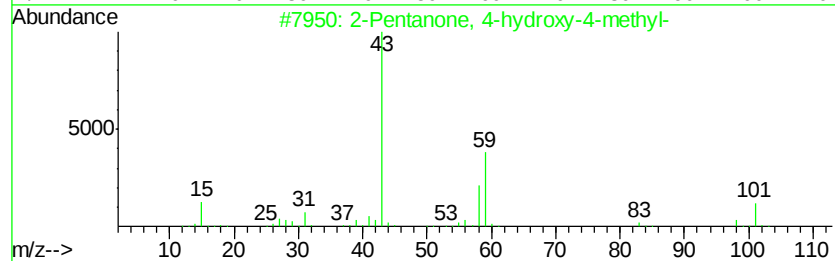
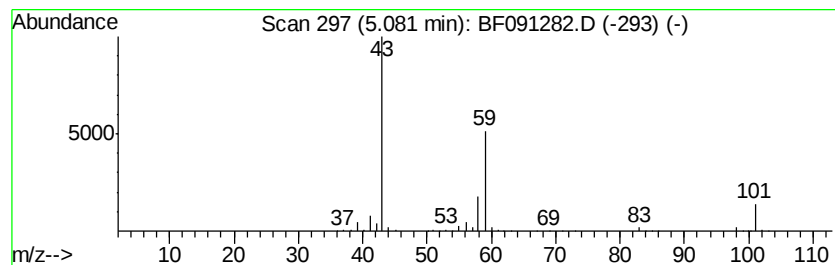
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	38.08 ng	2541510	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
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	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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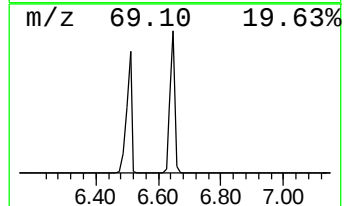
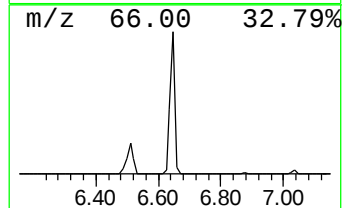
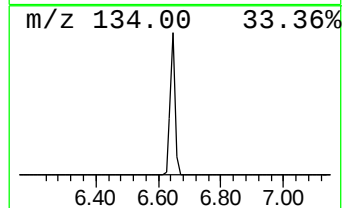
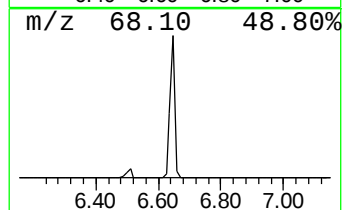
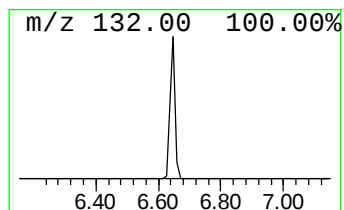
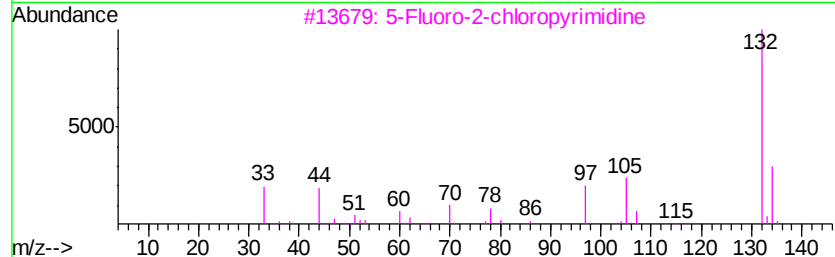
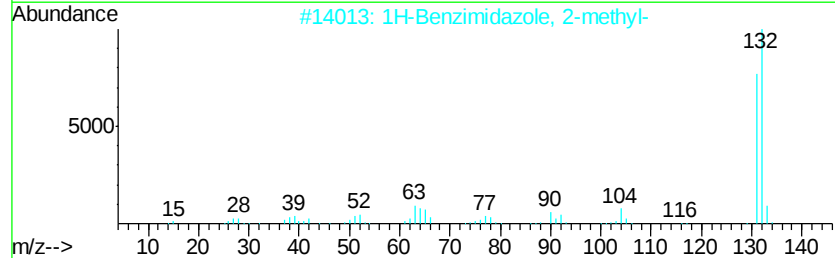
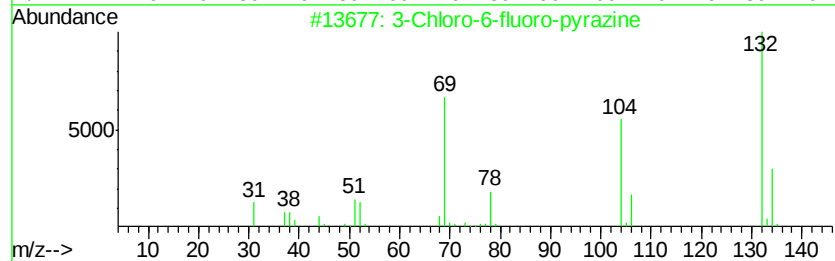
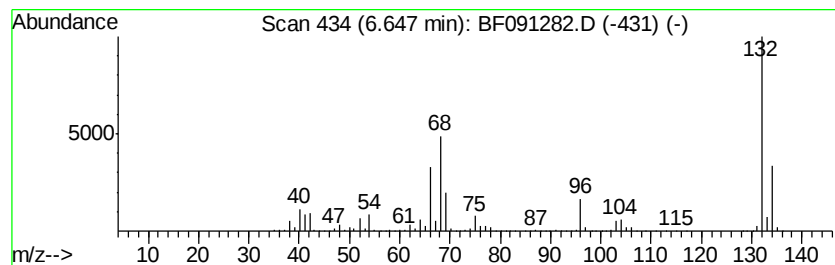
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	96.33 ng	6429110	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	25
3	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
4	(5-METHYL-2-PYRIDYL)ACETONITRILE			132	C8H8N2	1000241-93-9	10
5	Benzene, 1,2,4-trifluoro-			132	C6H3F3	000367-23-7	9



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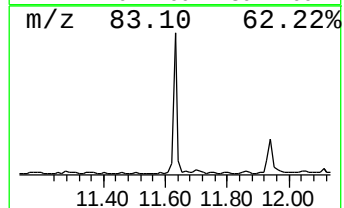
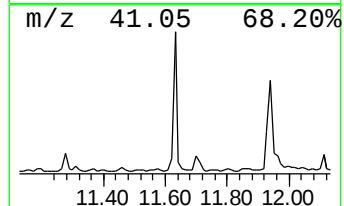
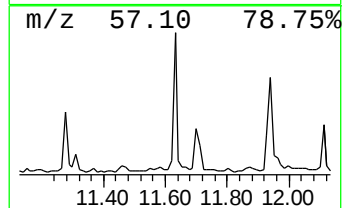
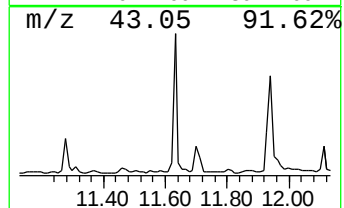
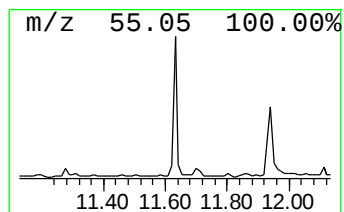
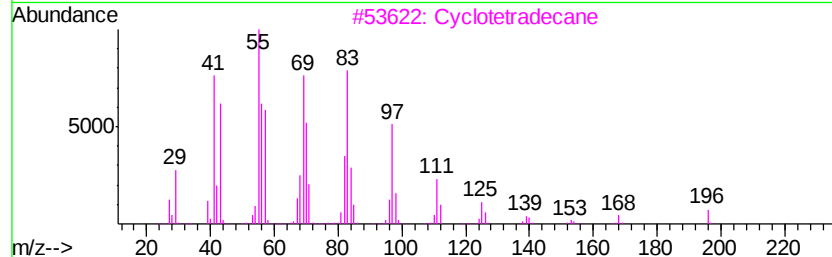
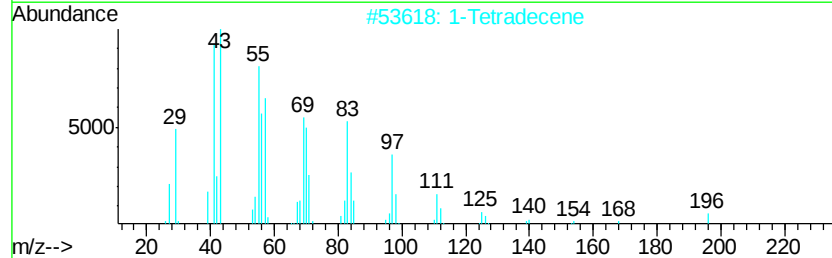
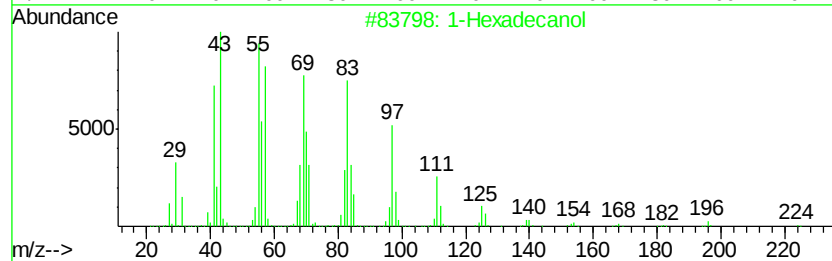
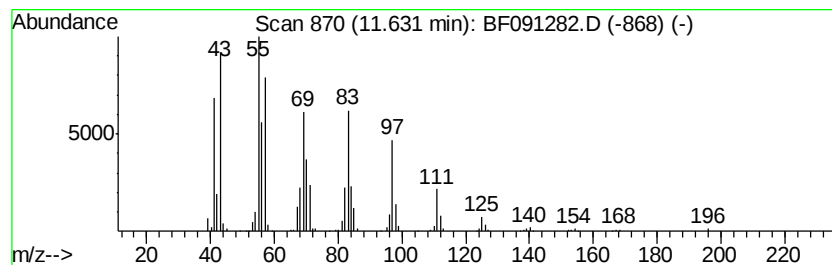
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Peak Number 7 1-Hexadecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.63	6.38 ng	701117	Phenanthrene-d10		11.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	1-Tetradecene	196	C14H28	001120-36-1	93
3	Cyclotetradecane	196	C14H28	000295-17-0	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	90
5	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	87



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BNA_F
ClientSampleId :
PHOENIX-BPM

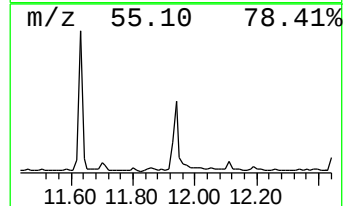
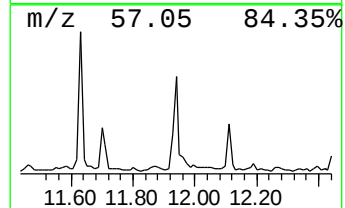
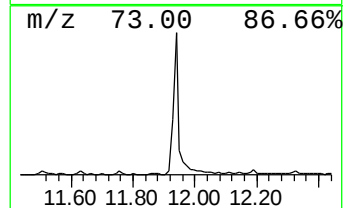
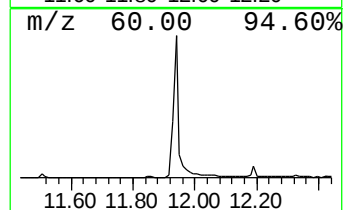
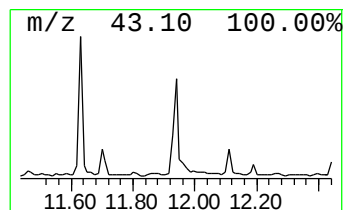
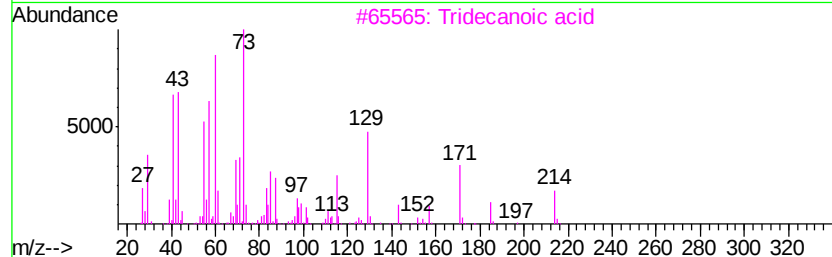
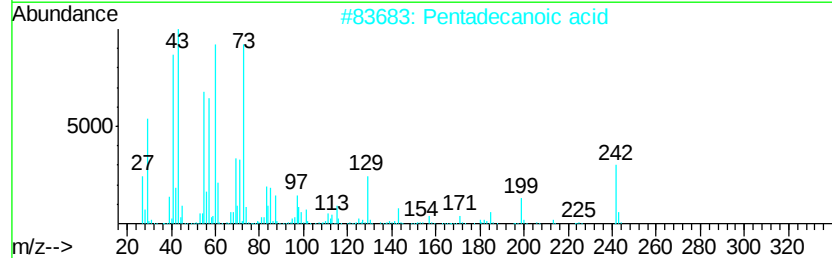
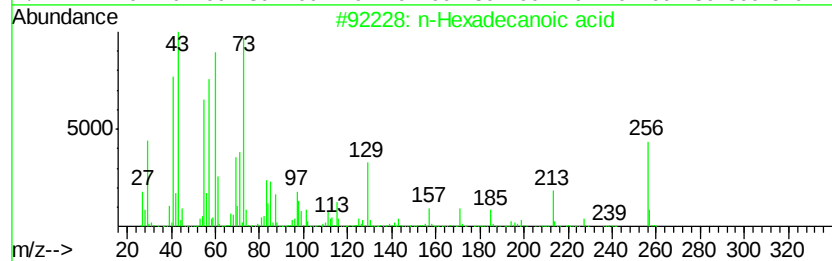
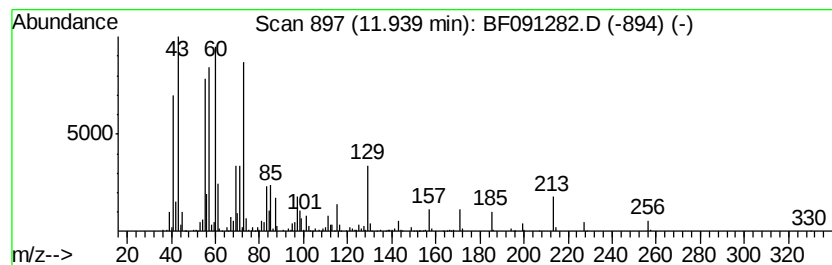
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	7.64 ng	839401	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091282.D
Acq On : 23 Nov 2016 18:39
Operator : UM/SJ
Sample : H5718-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

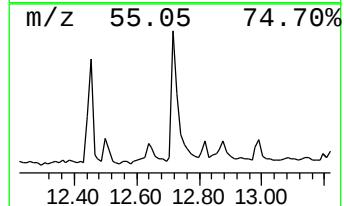
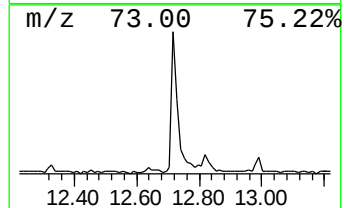
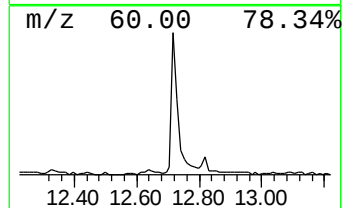
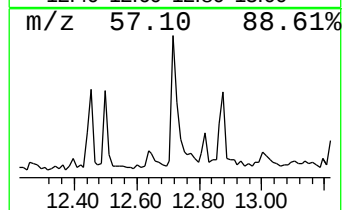
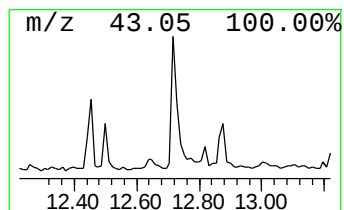
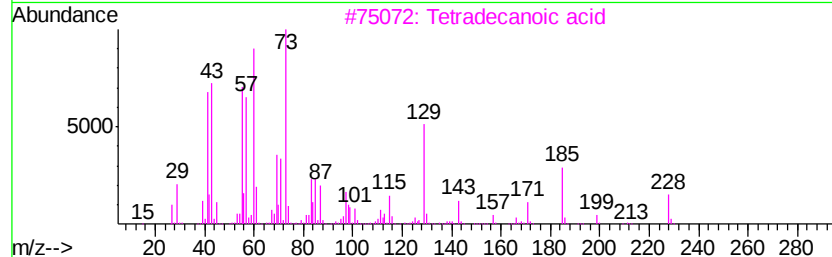
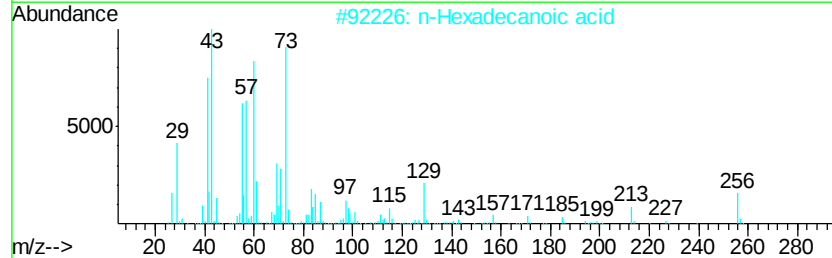
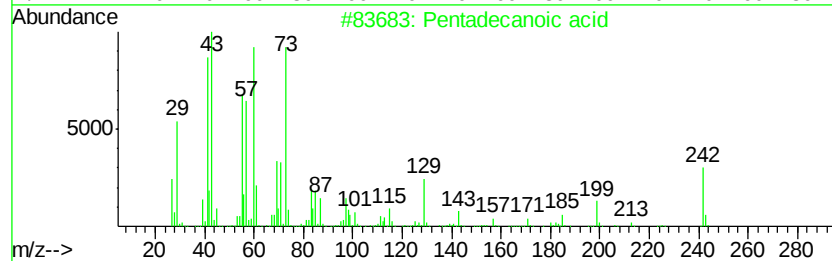
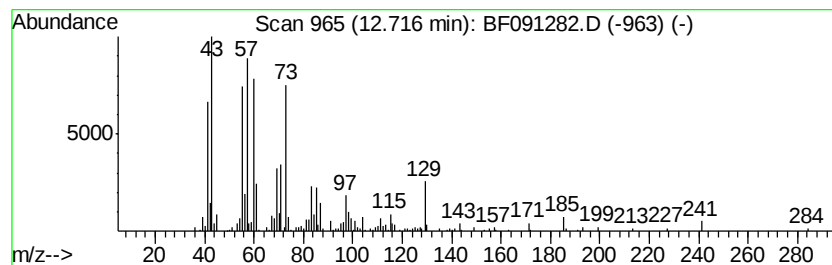
Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Pentadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.72	4.99 ng	549067	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	43
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091282.D
Acq On : 23 Nov 2016 18:39
Operator : UM/SJ
Sample : H5718-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

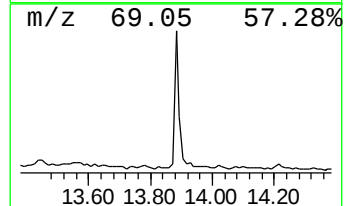
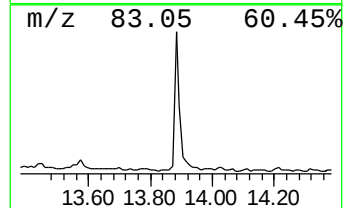
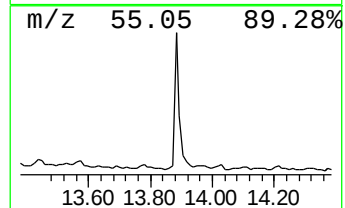
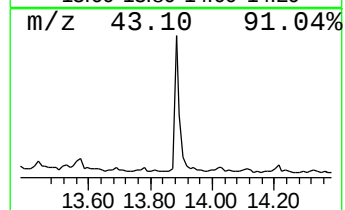
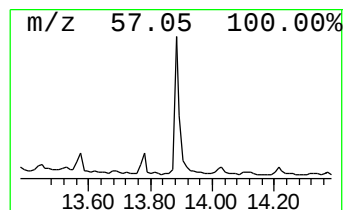
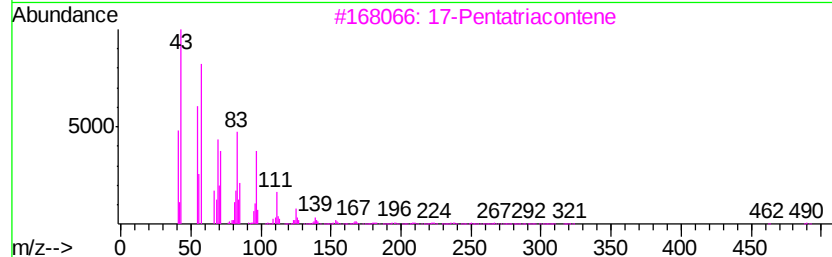
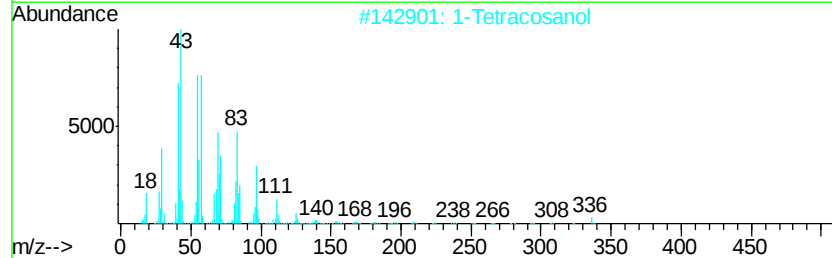
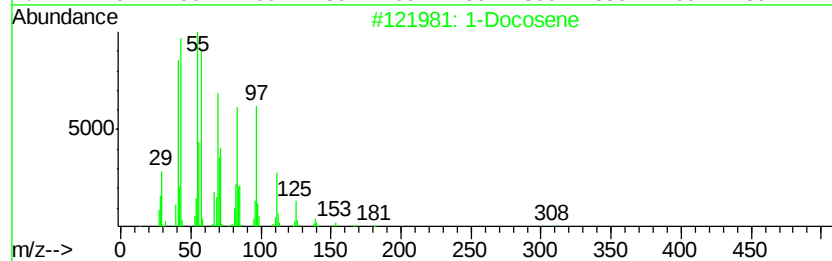
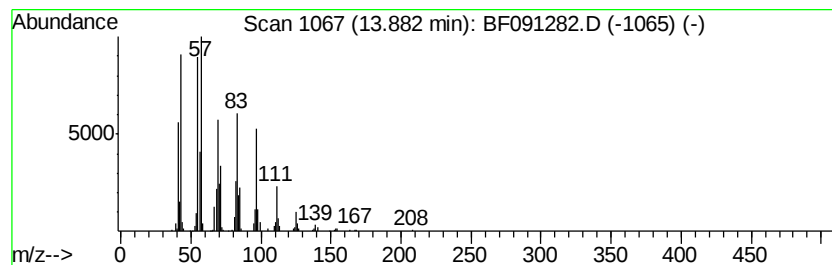
Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Docosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	3.61 ng	383501	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene	308 C22H44	001599-67-3	90
2	1-Tetracosanol	354 C24H50O	000506-51-4	87
3	17-Pentatriacontene	491 C35H70	006971-40-0	86
4	Dichloroacetic acid, tetradecyl ...	324 C16H30Cl2O2	083005-02-1	83
5	Pentafluoropropionic acid, hexad...	388 C19H33F5O2	006222-07-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091282.D
Acq On : 23 Nov 2016 18:39
Operator : UM/SJ
Sample : H5718-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown2.18	2.18	6.7	ng	445004	1	6.88	1334800	20.0
2-Pentanone, 4-hy...	5.08	38.1	ng	2541510	1	6.88	1334800	20.0
unknown6.65	6.65	96.3	ng	6429110	1	6.88	1334800	20.0
1-Hexadecanol	11.63	6.4	ng	701117	4	11.40	2198820	20.0
n-Hexadecanoic acid	11.94	7.6	ng	839401	4	11.40	2198820	20.0
Pentadecanoic acid	12.72	5.0	ng	549067	4	11.40	2198820	20.0
1-Docosene	13.88	3.6	ng	383501	5	14.03	2124660	20.0