

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
 Data File : BF098795.D
 Acq On : 25 Sep 2017 21:04
 Operator : SJ/JU
 Sample : I5388-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-016

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-BF092317.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	2.228	20	24	29	rVB	39859	56291	1.43%	0.224%
2	5.134	514	518	529	rVB	307903	355818	9.02%	1.416%
3	5.528	581	585	588	rBV	2154522	1965156	49.82%	7.818%
4	6.528	750	755	760	rBV	1984266	2024202	51.31%	8.053%
5	6.681	776	781	784	rBV	2261302	2049584	51.96%	8.154%
6	6.910	817	820	824	rBV	971352	815160	20.66%	3.243%
7	7.069	843	847	850	rBV	1811805	1490673	37.79%	5.931%
8	7.469	910	915	918	rBV	1294686	1175208	29.79%	4.675%
9	8.192	1034	1038	1042	rBV	1284152	1121216	28.42%	4.461%
10	9.269	1216	1221	1224	rBV	2403128	2102433	53.29%	8.364%
11	9.657	1283	1287	1290	rBV	148781	108036	2.74%	0.430%
12	9.951	1332	1337	1340	rBV	1400089	1229905	31.18%	4.893%
13	10.739	1465	1471	1474	rBV	1681889	1583448	40.14%	6.300%
14	11.439	1585	1590	1593	rBV	1466774	1298223	32.91%	5.165%
15	11.951	1673	1677	1682	rBV	157090	136769	3.47%	0.544%
16	12.739	1807	1811	1820	rBV	53031	64361	1.63%	0.256%
17	13.027	1854	1860	1863	rBV	3707490	3944903	100.00%	15.695%
18	13.904	2005	2009	2017	rBV	295533	300800	7.63%	1.197%
19	14.074	2034	2038	2042	rVB	1339491	1169732	29.65%	4.654%
20	14.533	2112	2116	2122	rBV2	86687	104500	2.65%	0.416%
21	14.921	2179	2182	2186	rVB	42195	42788	1.08%	0.170%
22	15.192	2224	2228	2232	rBV	208863	232058	5.88%	0.923%
23	15.562	2286	2291	2308	rVB	697167	947578	24.02%	3.770%
24	16.027	2365	2370	2375	rBV	174401	247482	6.27%	0.985%
25	16.080	2375	2379	2385	rVV2	35384	50231	1.27%	0.200%
26	16.550	2454	2459	2465	rVB2	37863	67546	1.71%	0.269%
27	17.162	2558	2563	2570	rVB3	45694	92902	2.35%	0.370%
28	17.615	2636	2640	2643	rBV5	29024	51650	1.31%	0.205%
29	17.662	2644	2648	2653	rVV4	62421	126951	3.22%	0.505%
30	18.150	2727	2731	2736	rVB5	29951	49561	1.26%	0.197%
31	18.509	2785	2792	2797	rBV9	46905	130334	3.30%	0.519%

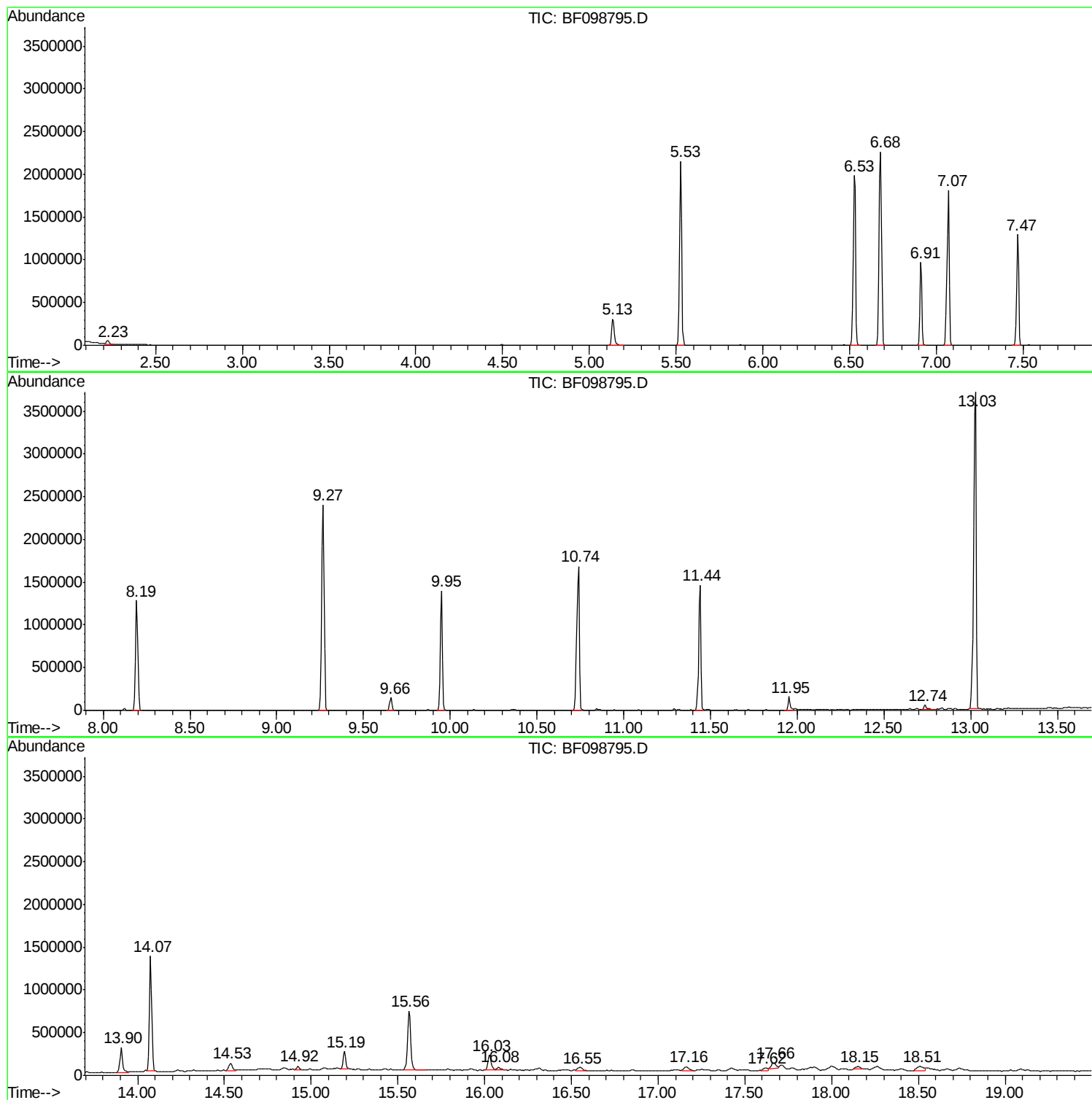
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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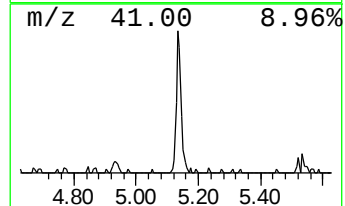
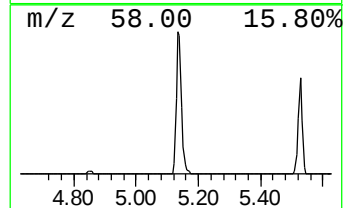
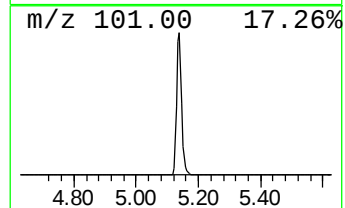
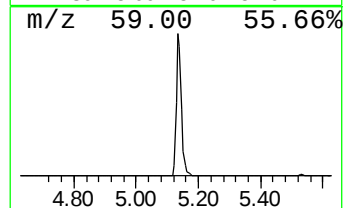
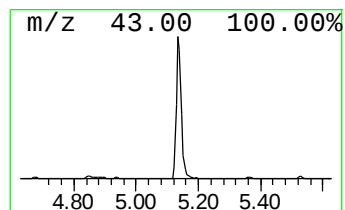
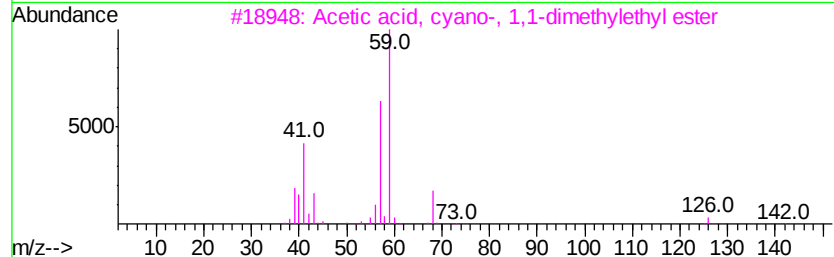
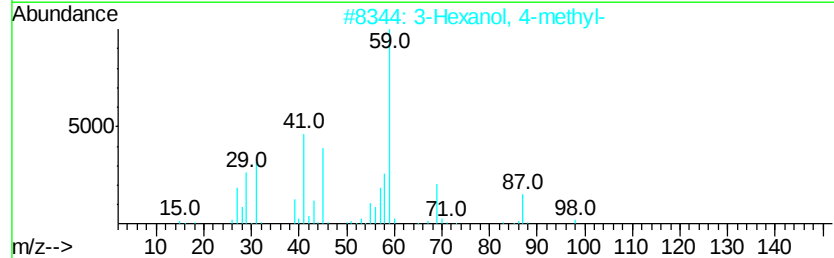
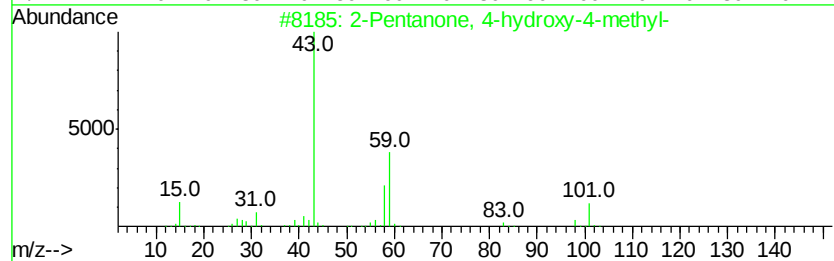
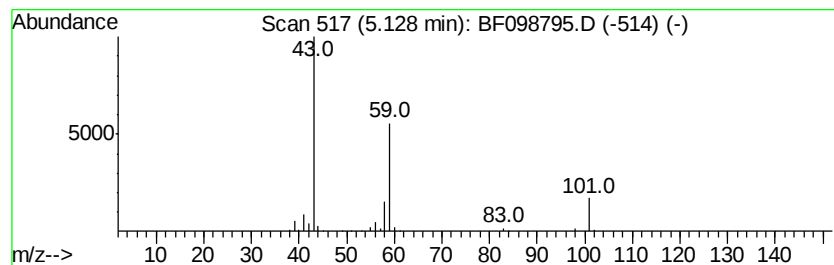
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	8.73 ng	355818	1,4-Dichlorobenzene-d4	6.91

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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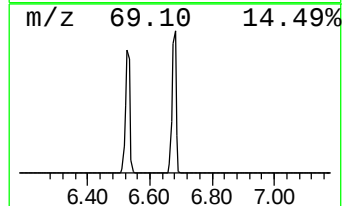
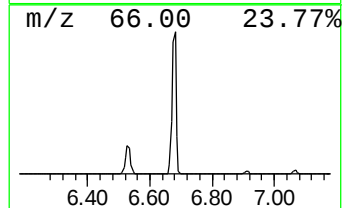
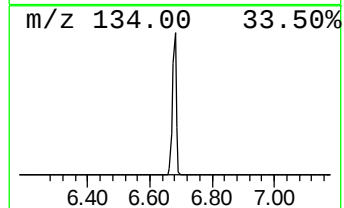
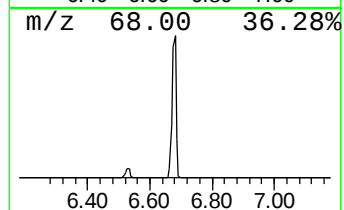
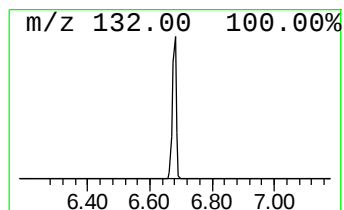
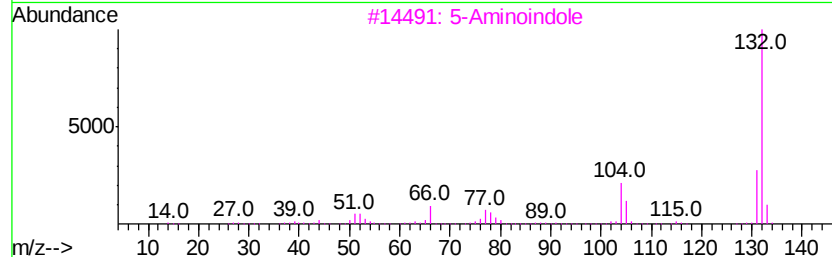
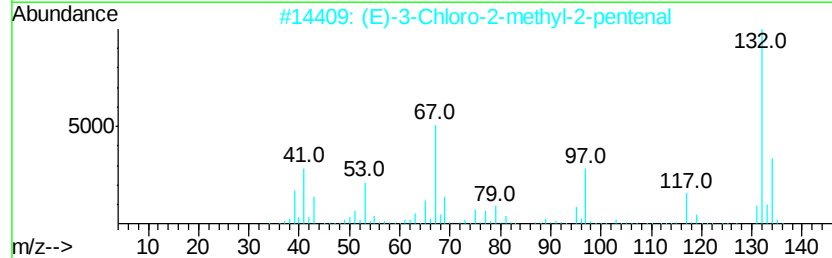
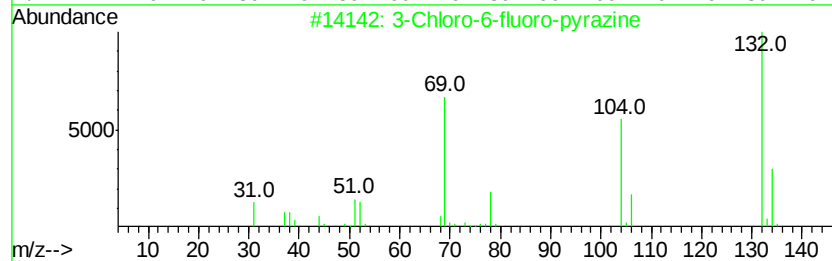
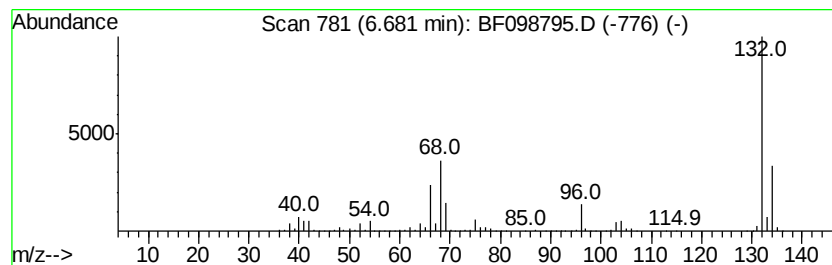
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Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	50.29 ng	2049580	1,4-Dichlorobenzene-d4	6.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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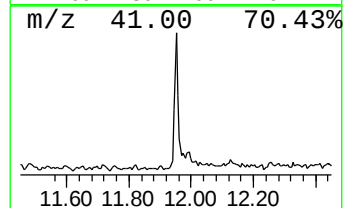
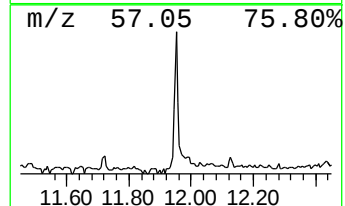
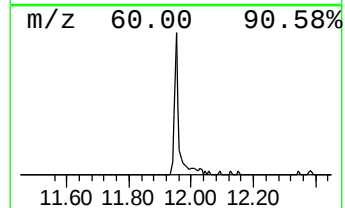
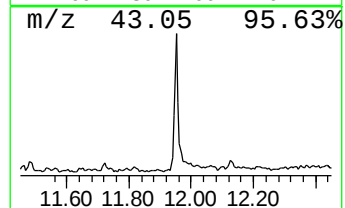
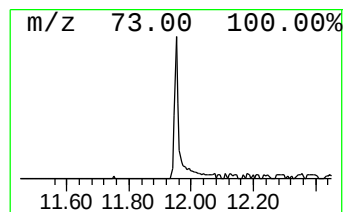
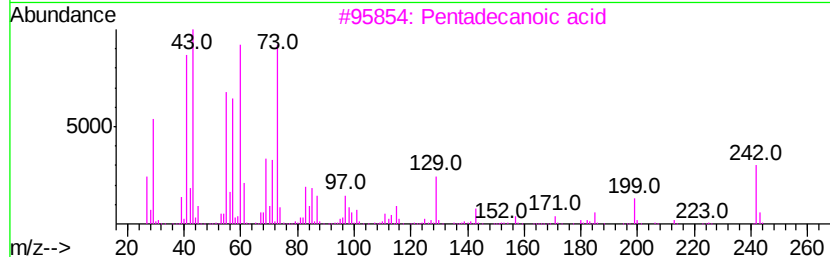
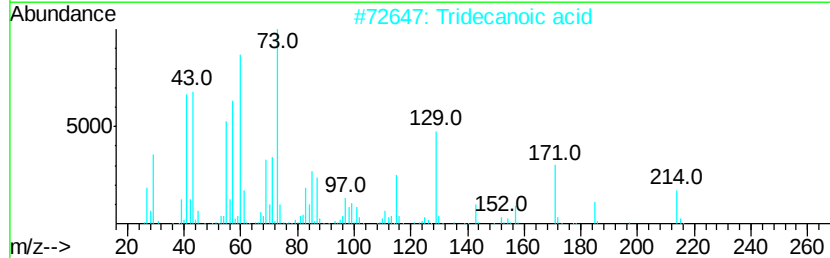
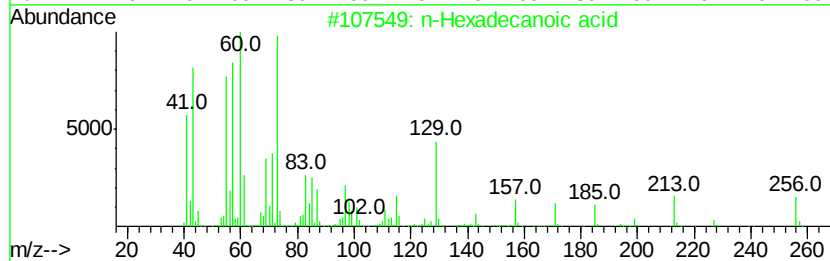
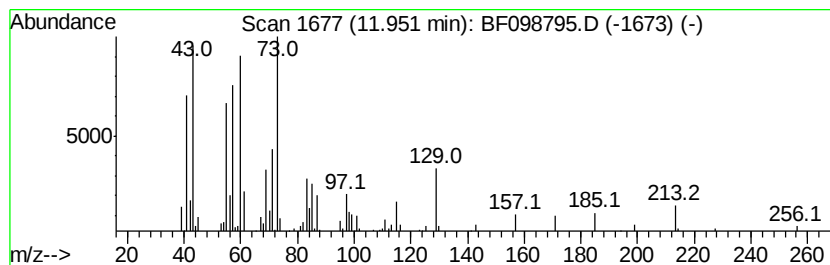
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.95	2.11 ng	136769	Phenanthrene-d10	11.44	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	25



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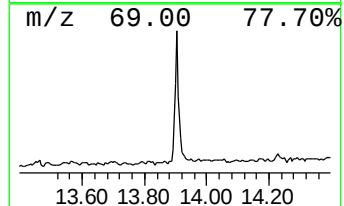
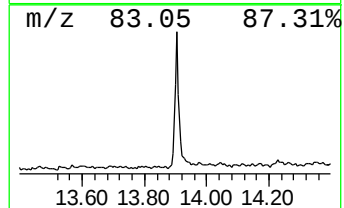
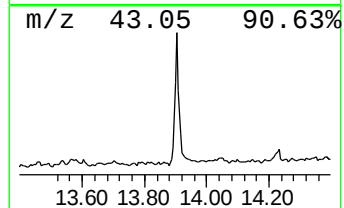
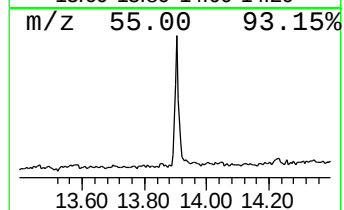
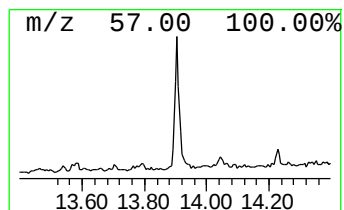
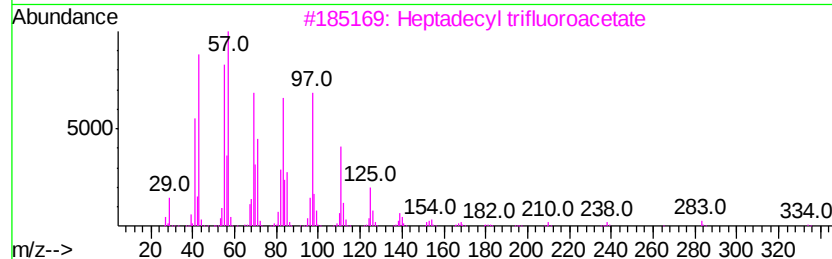
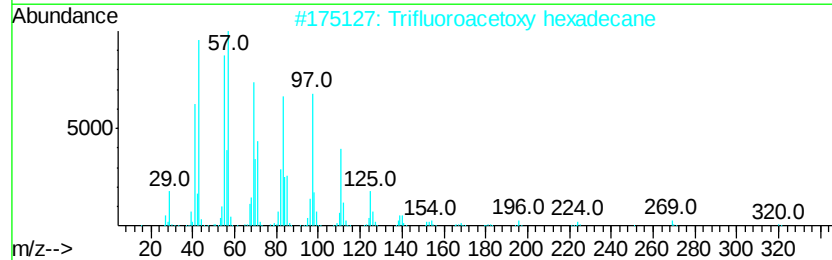
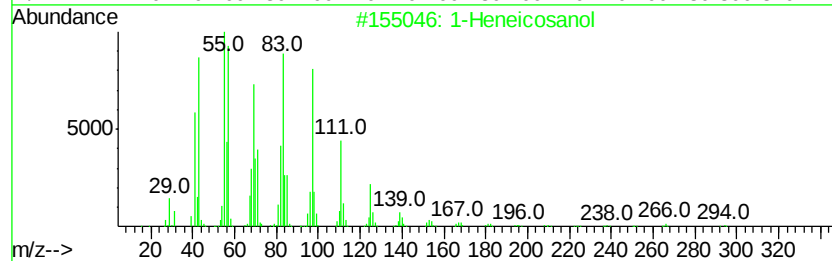
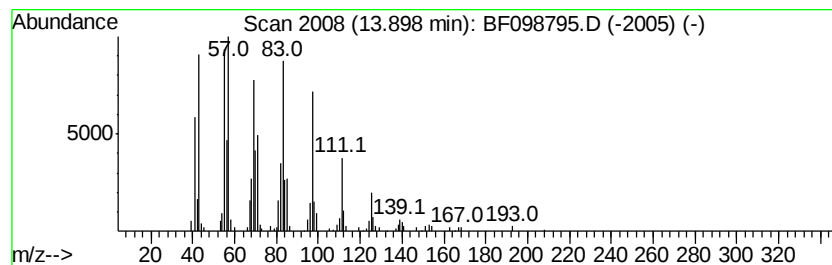
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	5.14 ng	300800	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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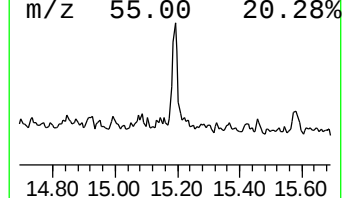
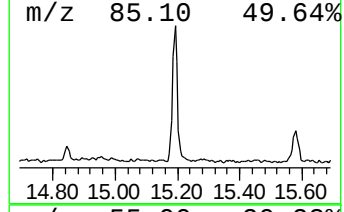
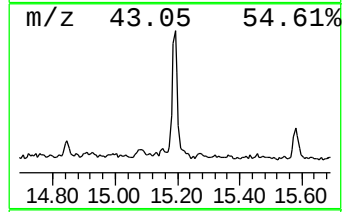
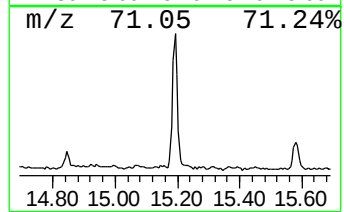
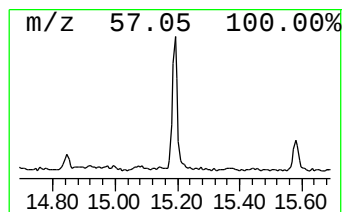
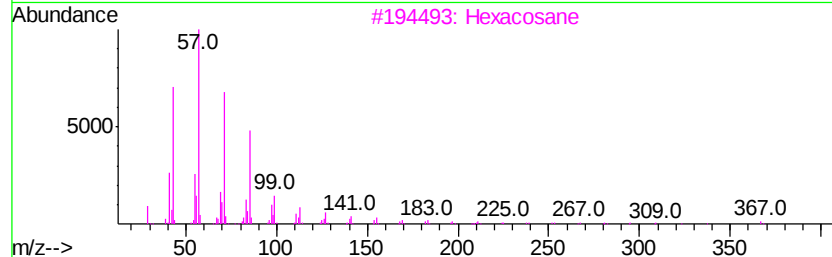
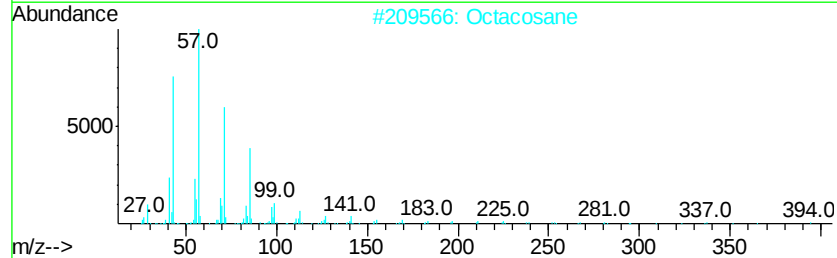
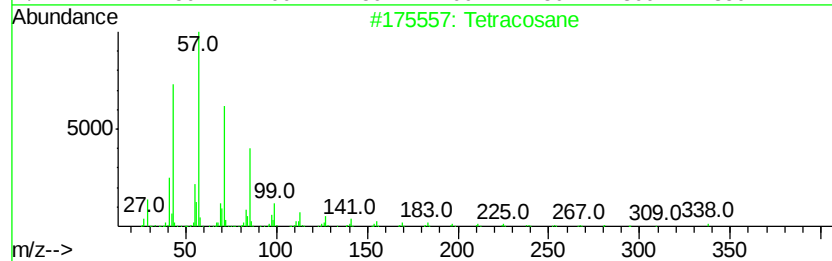
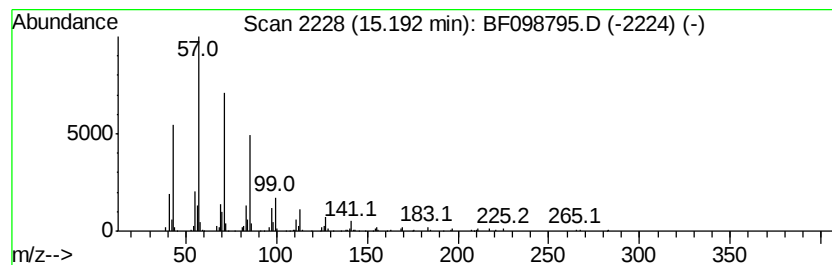
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Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	4.90 ng	232058	Perylene-d12	15.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetracosane	338 C24H50	000646-31-1 91
2		Octacosane	394 C28H58	000630-02-4 91
3		Hexacosane	366 C26H54	000630-01-3 91
4		Tetratetracontane	619 C44H90	007098-22-8 91
5		Heneicosane, 11-(1-ethylpropyl)-	366 C26H54	055282-11-6 91



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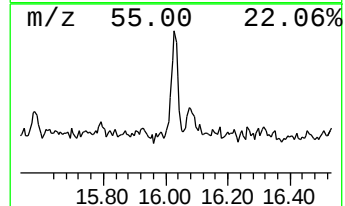
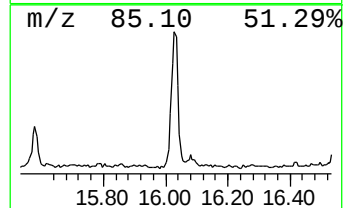
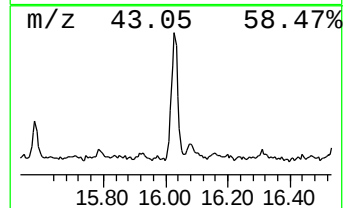
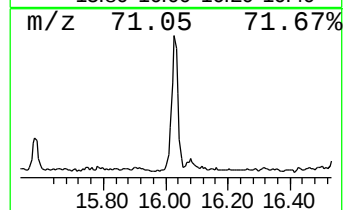
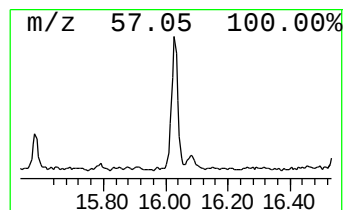
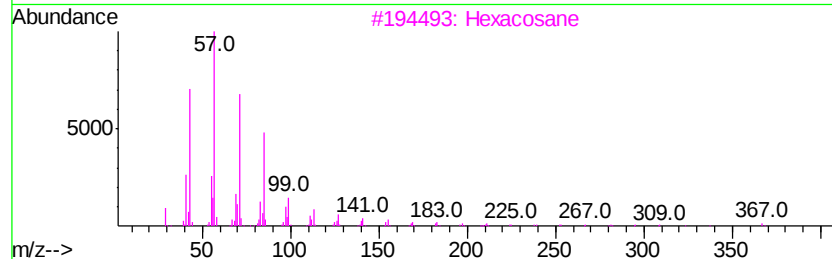
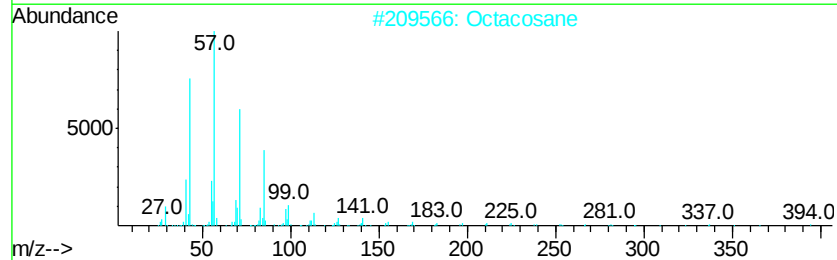
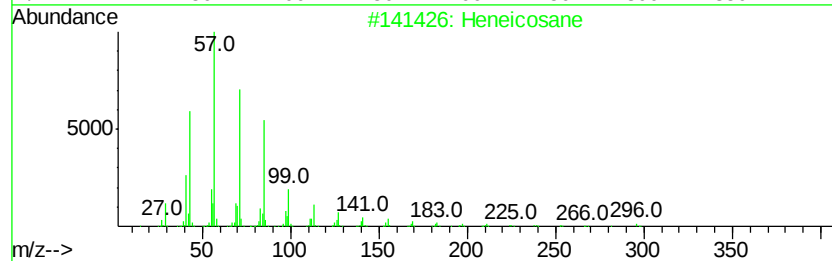
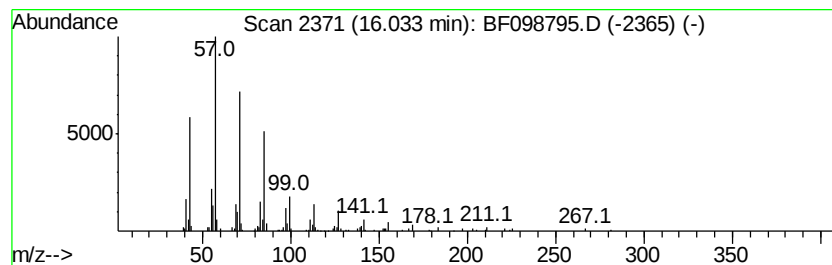
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	5.22 ng	247482	Perylene-d12	15.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098795.D
Acq On : 25 Sep 2017 21:04
Operator : SJ/JU
Sample : I5388-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-016

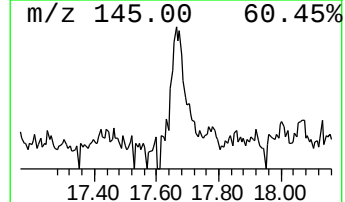
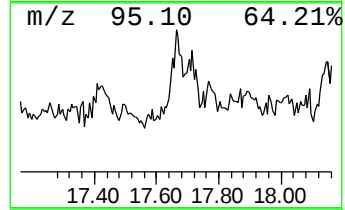
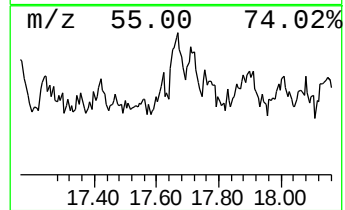
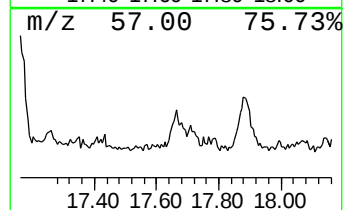
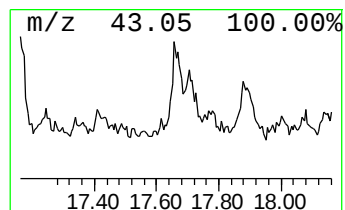
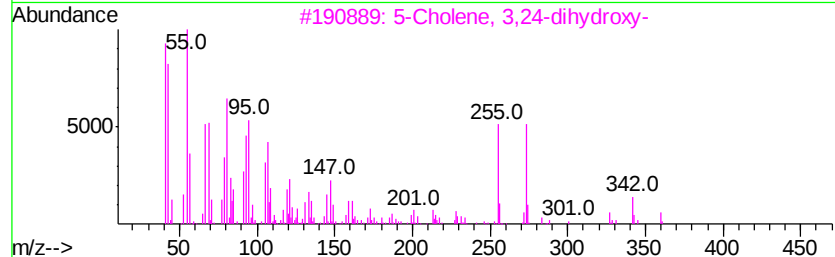
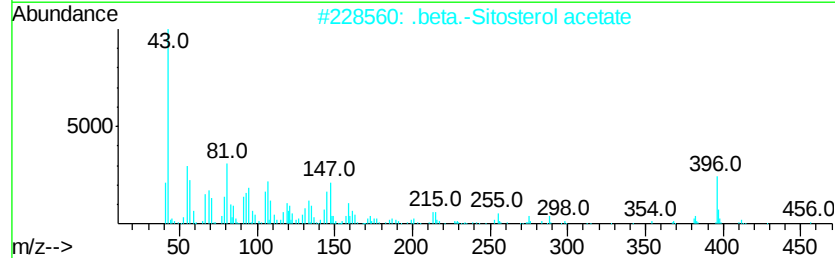
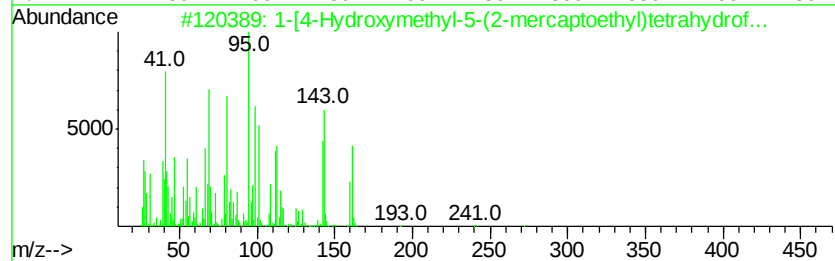
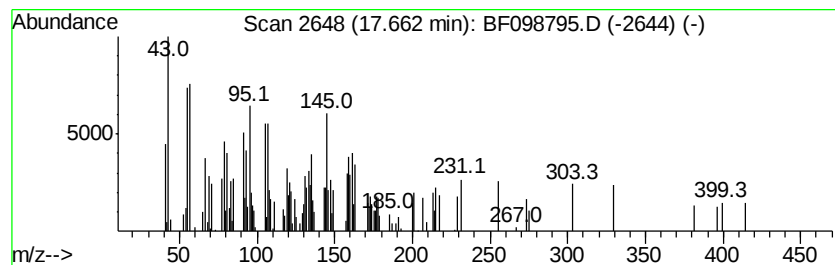
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-[4-Hydroxymethyl-5-(2-mer... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.66	2.68 ng	126951	Perylene-d12	15.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-[4-Hydroxymethyl-5-(2-mercapto...	272	C11H16N2O4S	128453-39-4	56
2		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	38
3		5-Cholene, 3,24-dihydroxy-	360	C24H40O2	1000251-69-2	27
4		Ledene oxide-(II)	220	C15H24O	1000159-36-7	14
5		Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098795.D
Acq On : 25 Sep 2017 21:04
Operator : SJ/JU
Sample : I5388-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

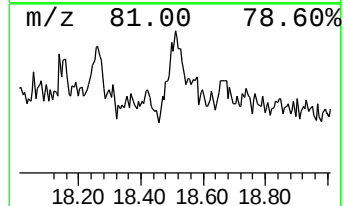
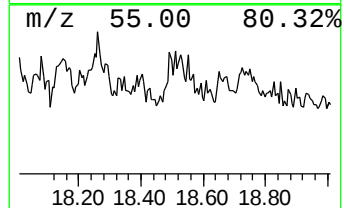
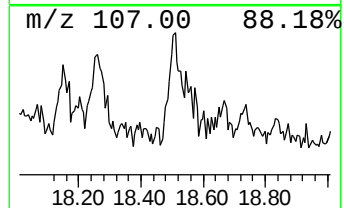
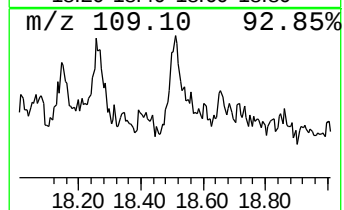
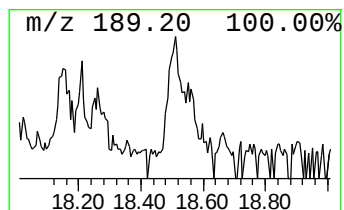
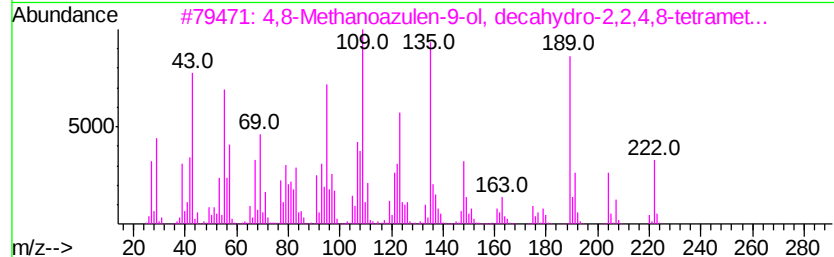
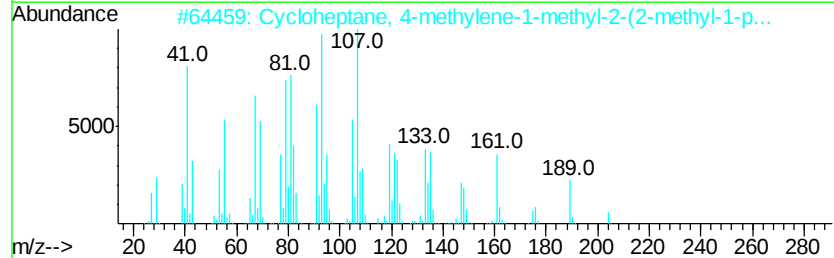
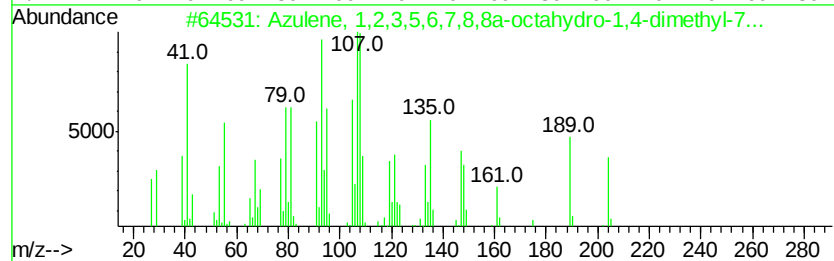
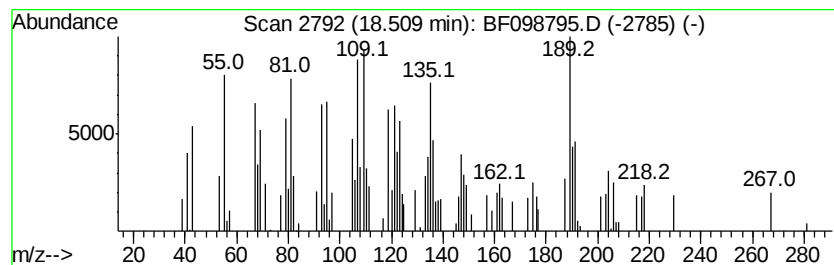
Instrument :
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ClientSampleId :
FK-PS-01-016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Azulene, 1,2,3,5,6,7,8,8a-o... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.51	2.75 ng	130334	Perylene-d12	15.56		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	55
2		Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	53
3		4,8-Methanoazulen-9-ol, decahvd...	222	C15H26O	004586-22-5	41
4		Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	38
5		(-)-1,2,2.alpha.,3,3,4,6,7,8,8.a...	204	C15H24	1000365-86-7	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098795.D
Acq On : 25 Sep 2017 21:04
Operator : SJ/JU
Sample : I5388-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.13	8.7	ng	355818	1	6.91	815160	20.0
unknown6.68	6.68	50.3	ng	2049580	1	6.91	815160	20.0
n-Hexadecanoic acid	11.95	2.1	ng	136769	4	11.44	1298220	20.0
1-Heneicosanol	13.90	5.1	ng	300800	5	14.07	1169730	20.0
Tetracosane	15.19	4.9	ng	232058	6	15.56	947578	20.0
Heneicosane	16.03	5.2	ng	247482	6	15.56	947578	20.0
1-[4-Hydroxymethy...	17.66	2.7	ng	126951	6	15.56	947578	20.0
Azulene, 1,2,3,5,...	18.51	2.8	ng	130334	6	15.56	947578	20.0