

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
 Data File : BF098923.D
 Acq On : 28 Sep 2017 22:56
 Operator : SJ/JU
 Sample : I5475-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WS-20408-COMP

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	2.251	24	28	39	rVB	171707	246538	7.25%	0.826%
2	2.469	61	65	70	rVB	39529	54788	1.61%	0.184%
3	3.104	166	173	184	rVB	80060	130346	3.83%	0.437%
4	5.151	517	521	531	rVB	578564	781901	22.99%	2.620%
5	5.545	582	588	591	rBV	3288732	3369833	99.08%	11.290%
6	6.545	752	758	761	rBV	3013574	3343648	98.31%	11.202%
7	6.686	777	782	785	rBV	3495348	3401193	100.00%	11.395%
8	6.739	788	791	796	rVB	44709	37355	1.10%	0.125%
9	6.916	817	821	824	rBV	1057301	818315	24.06%	2.742%
10	7.075	843	848	851	rBV	2870483	2595896	76.32%	8.697%
11	7.480	911	917	920	rBV	2025769	2094653	61.59%	7.018%
12	8.198	1035	1039	1042	rBV	1242808	1023920	30.10%	3.430%
13	9.274	1216	1222	1225	rBV	3429514	3274445	96.27%	10.970%
14	9.663	1284	1288	1291	rBV	566875	456157	13.41%	1.528%
15	9.951	1333	1337	1341	rBV	1040816	958560	28.18%	3.211%
16	10.374	1406	1409	1412	rVB	63798	49522	1.46%	0.166%
17	10.739	1467	1471	1475	rBV	1491158	1494384	43.94%	5.007%
18	10.845	1486	1489	1496	rBV	78207	74831	2.20%	0.251%
19	11.439	1586	1590	1594	rBV	915476	759494	22.33%	2.545%
20	11.951	1674	1677	1681	rBV	62726	58375	1.72%	0.196%
21	13.021	1855	1859	1863	rBV	2300376	2172783	63.88%	7.279%
22	13.903	2006	2009	2017	rBV	232918	250029	7.35%	0.838%
23	14.080	2035	2039	2042	rBV	785045	688343	20.24%	2.306%
24	14.539	2112	2117	2123	rBV7	57367	102829	3.02%	0.345%
25	15.192	2225	2228	2236	rVB	64437	72910	2.14%	0.244%
26	15.574	2288	2293	2303	rVB	589738	818712	24.07%	2.743%
27	16.033	2366	2371	2376	rBV	101000	156725	4.61%	0.525%
28	16.550	2454	2459	2467	rVB	110520	210075	6.18%	0.704%
29	17.162	2558	2563	2573	rVB2	91225	189787	5.58%	0.636%
30	17.886	2682	2686	2696	rVB3	65670	161897	4.76%	0.542%

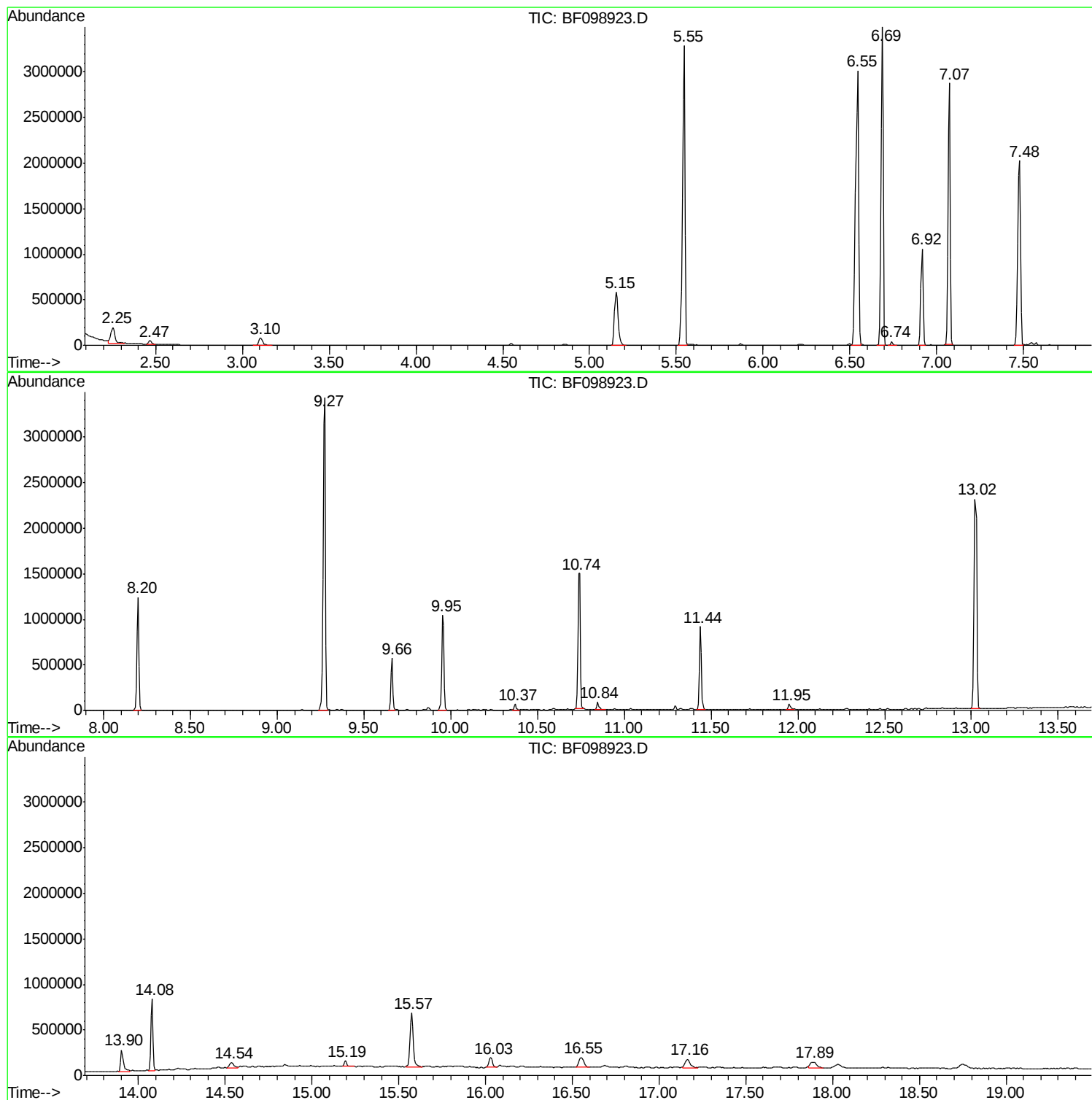
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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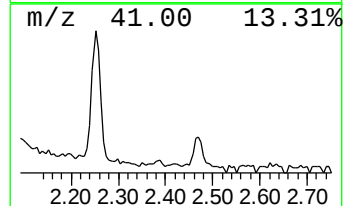
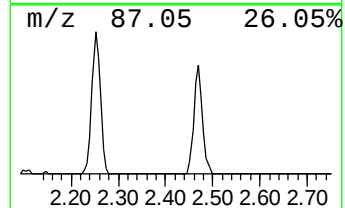
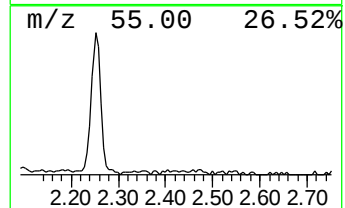
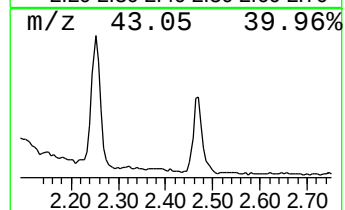
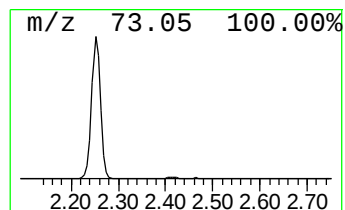
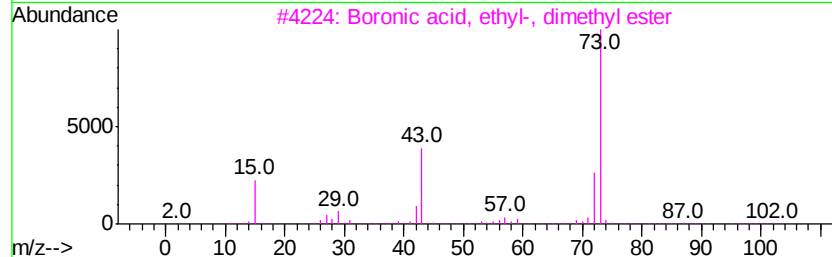
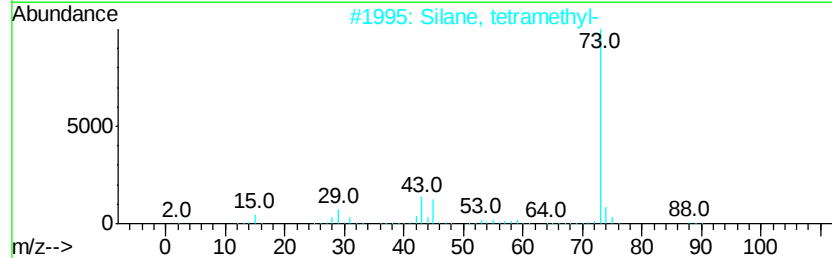
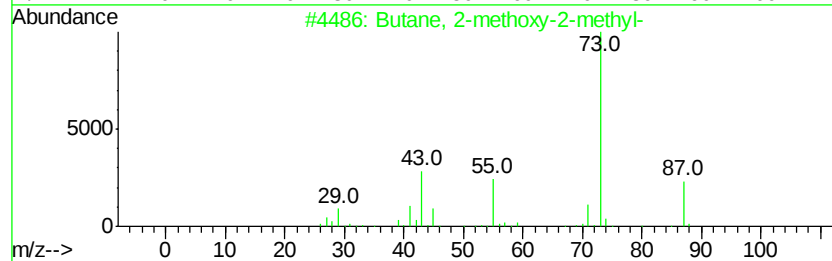
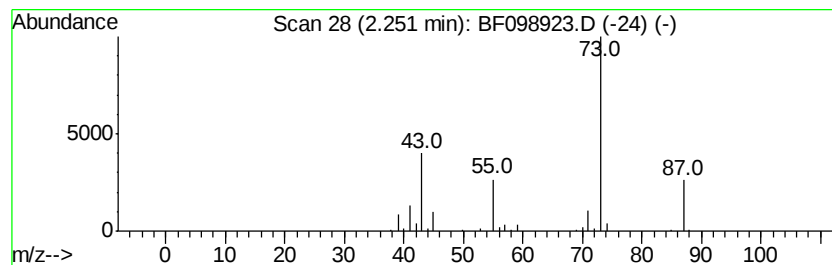
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	6.03 ng	246538	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
3		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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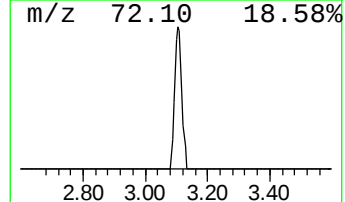
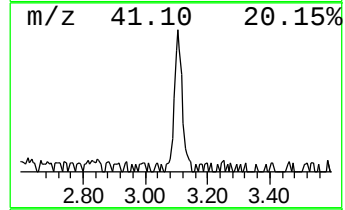
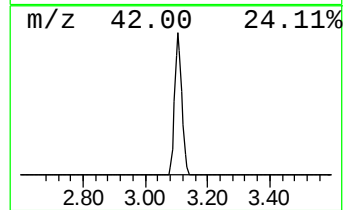
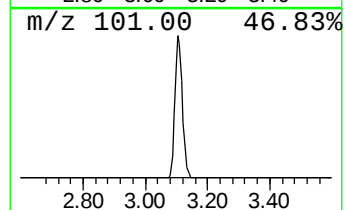
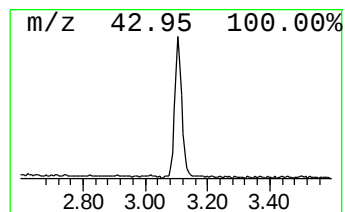
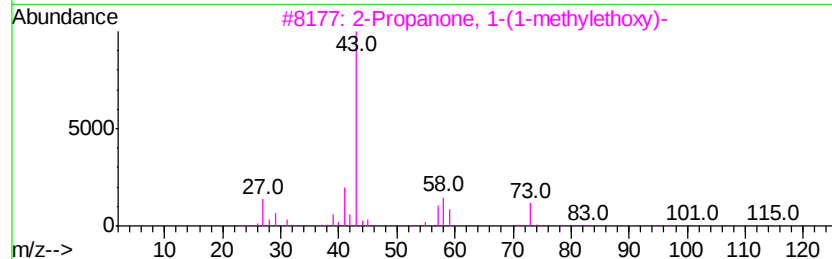
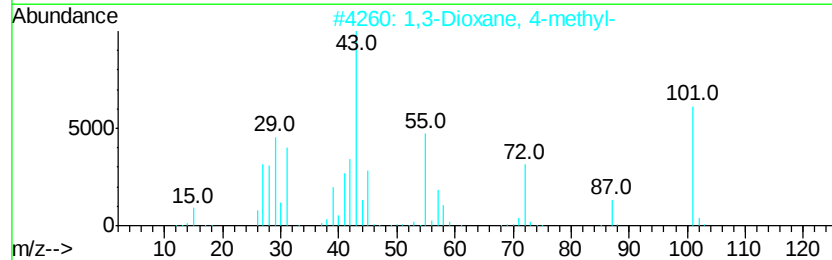
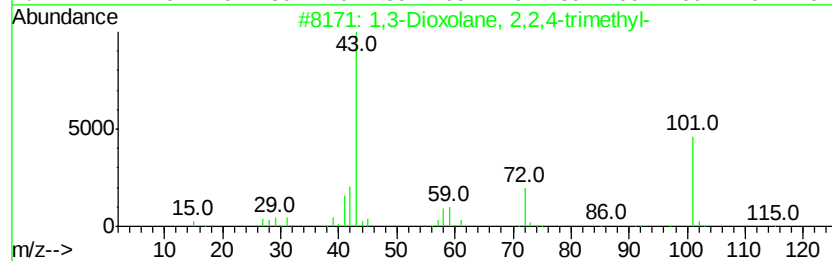
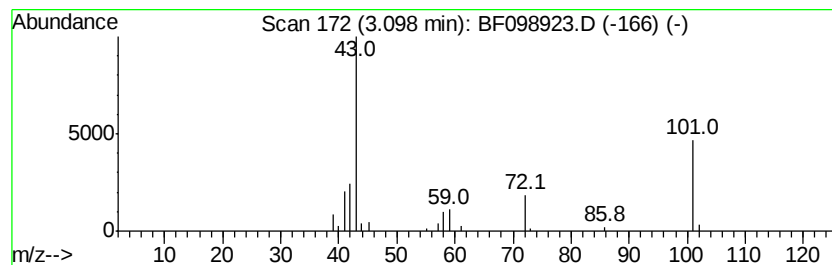
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Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.10	3.19 ng	130346	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	45
3			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	10
4			1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	10
5			2-Buten-1-ol, acetate	114	C6H10O2	000628-08-0	10



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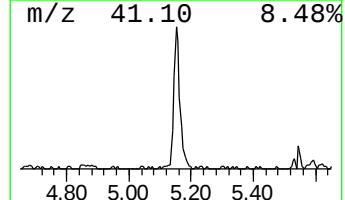
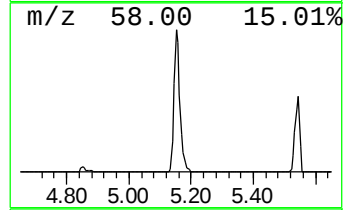
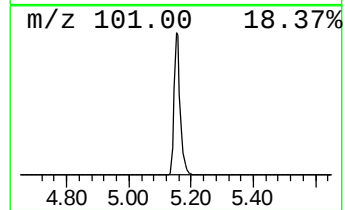
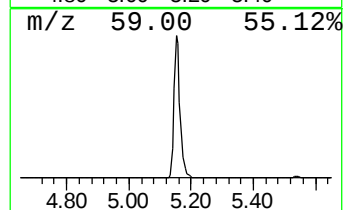
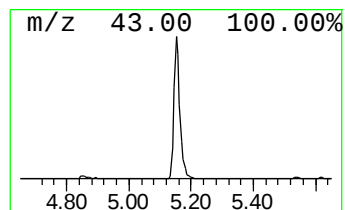
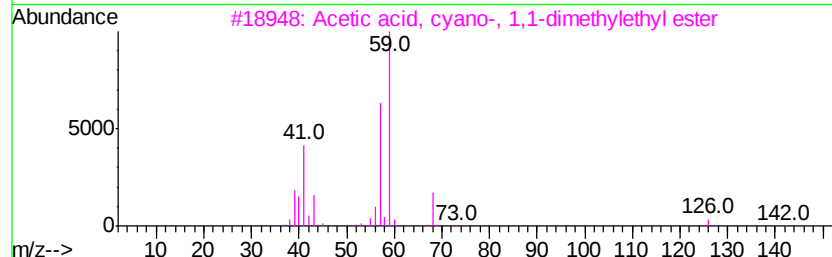
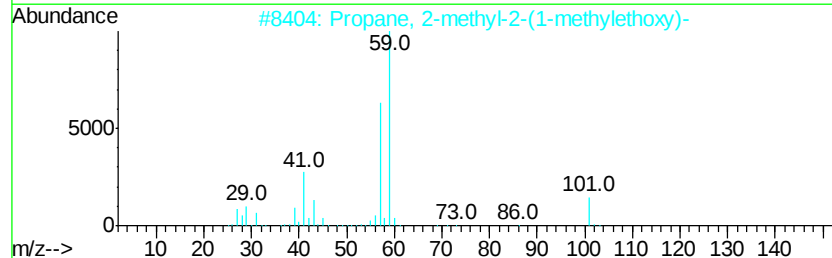
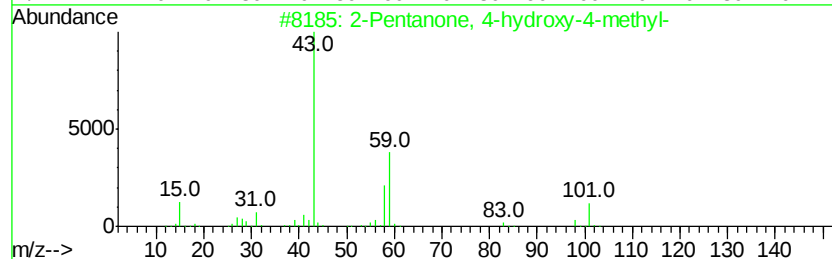
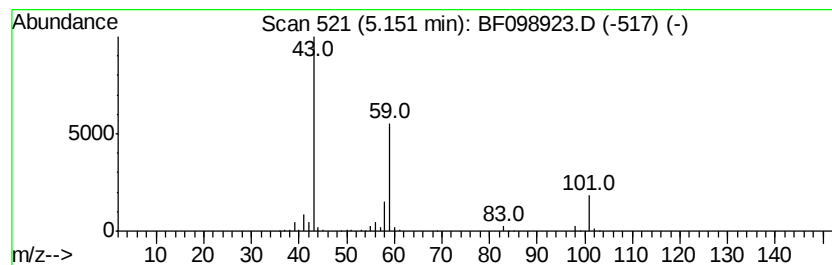
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	19.11 ng	781901	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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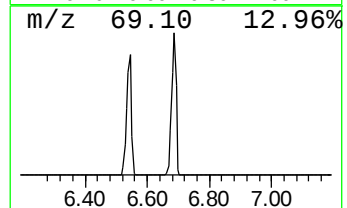
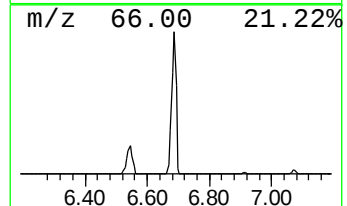
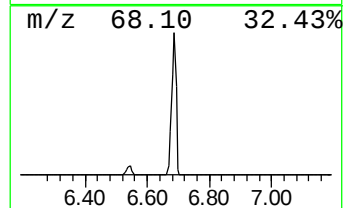
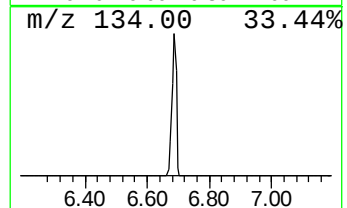
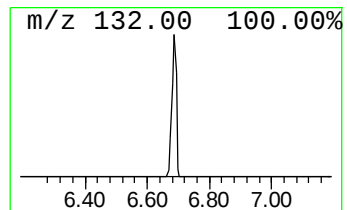
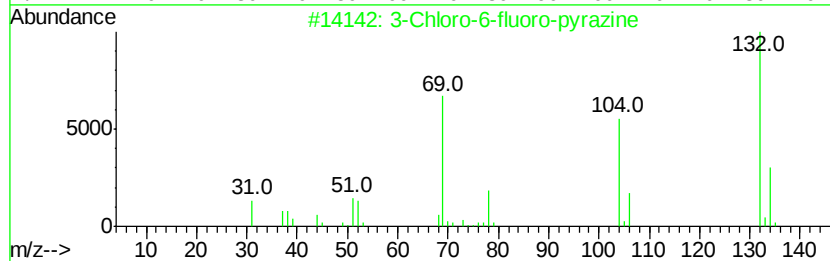
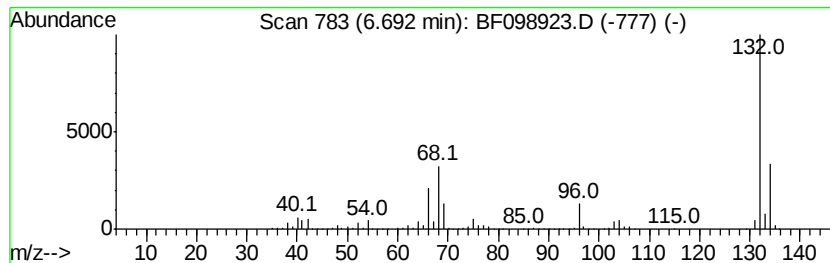
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	83.13 ng	3401190	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	17
3	5-Aminoindole			132	C8H8N2	005192-03-0	12
4	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9



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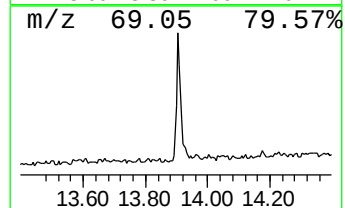
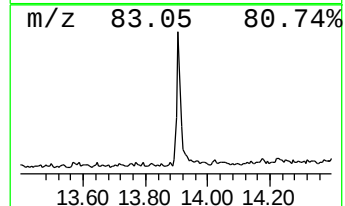
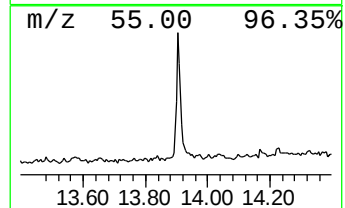
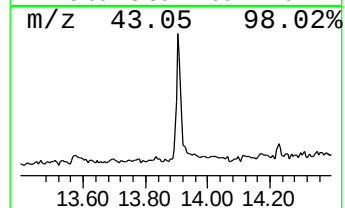
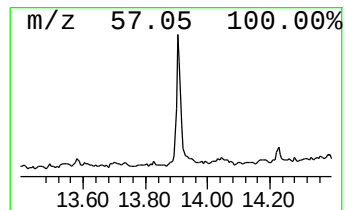
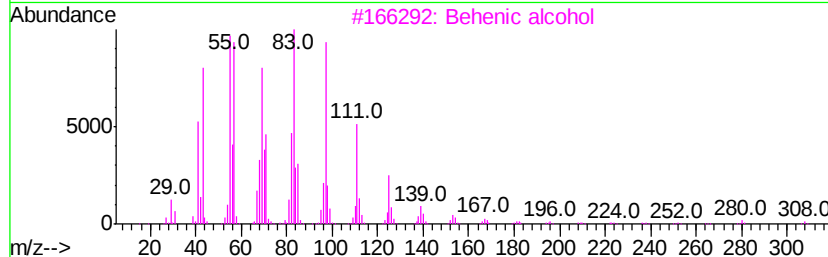
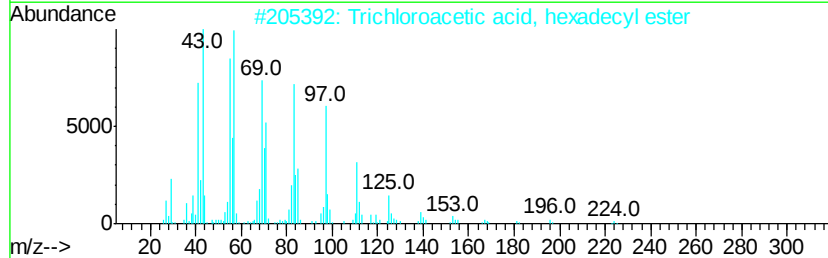
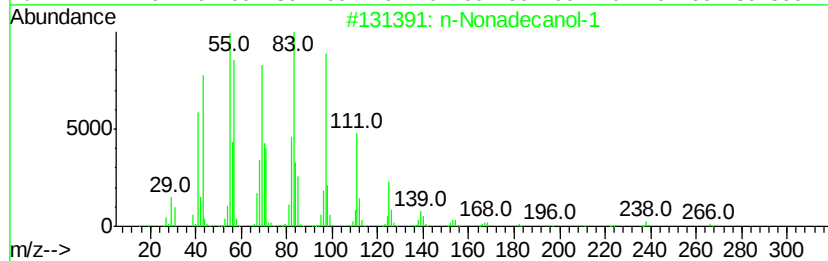
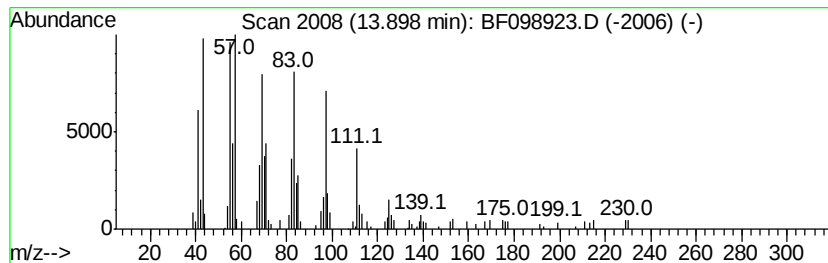
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	7.26 ng	250029	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		Cyclopentadecane	210	C15H30	000295-48-7	93
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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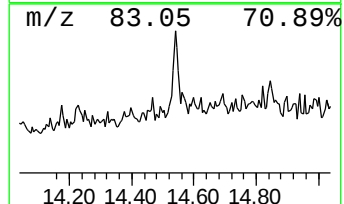
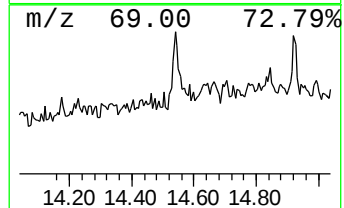
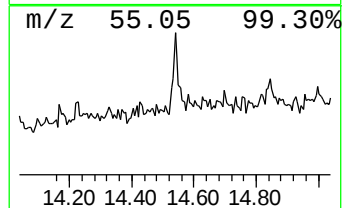
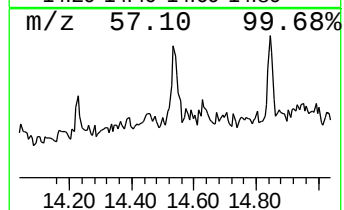
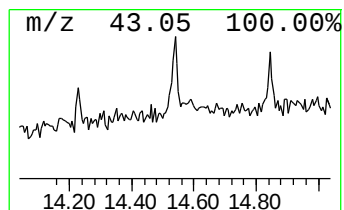
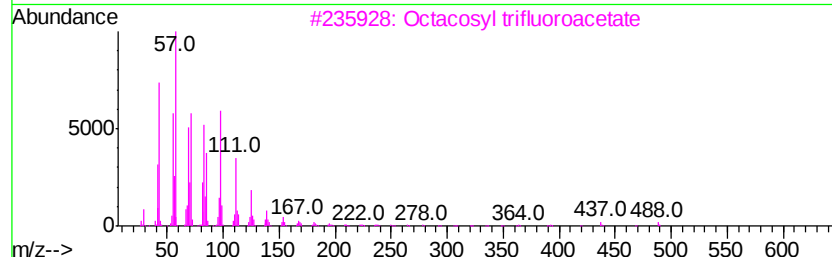
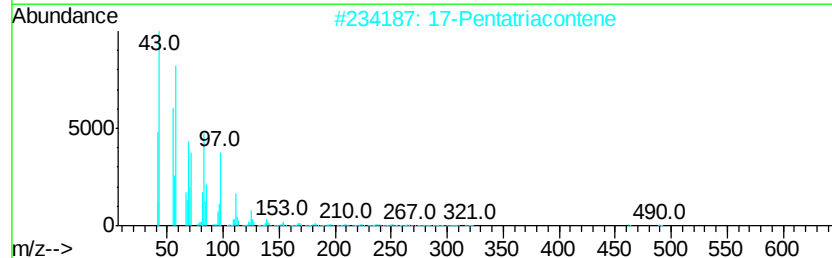
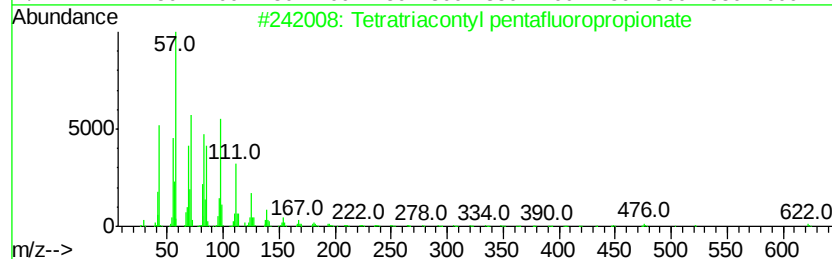
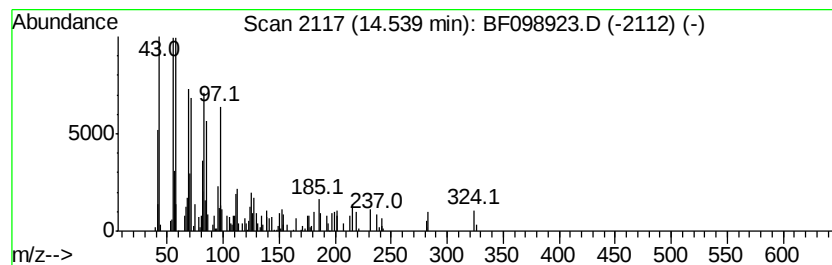
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratriacontyl pentafluoro... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	2.99 ng	102829	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	58
2		17-Pentatriacontene	491	C35H70	006971-40-0	58
3		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	58
4		Oxalic acid, allyl tetradecyl ester	326	C19H34O4	1000309-24-2	58
5		Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098923.D
Acq On : 28 Sep 2017 22:56
Operator : SJ/JU
Sample : I5475-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-20408-COMP

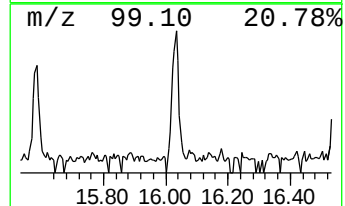
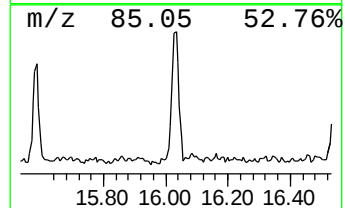
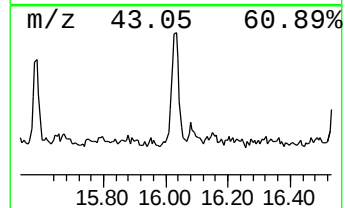
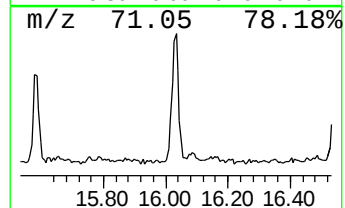
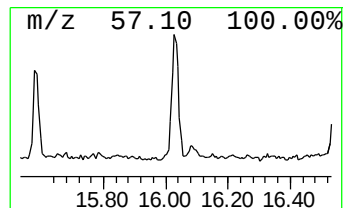
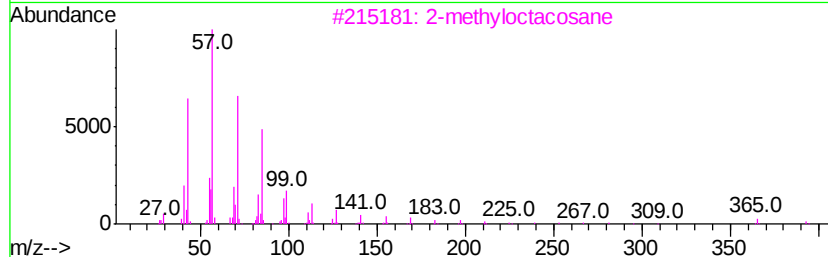
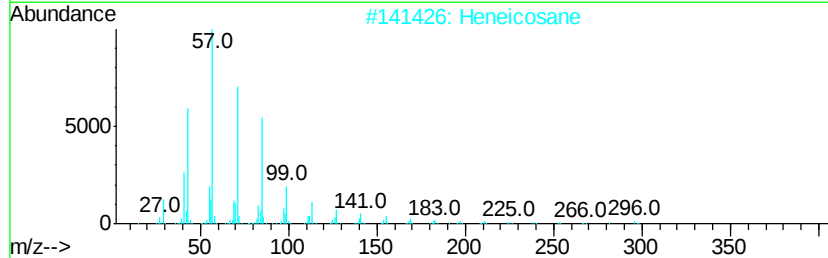
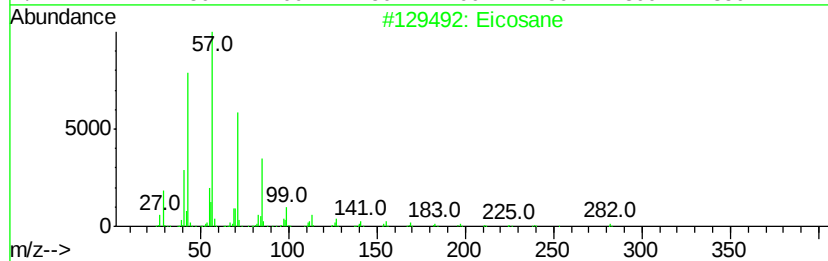
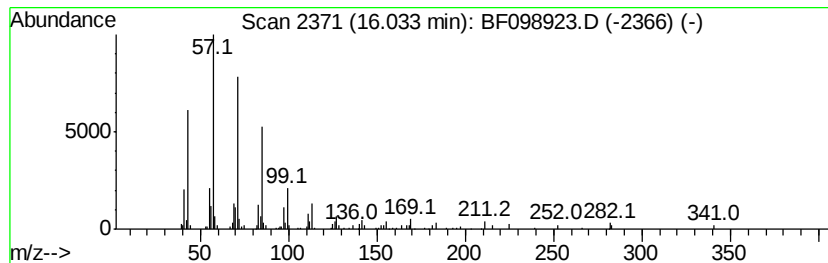
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	3.83 ng	156725	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptadecane	240	C17H36	000629-78-7	90
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098923.D
Acq On : 28 Sep 2017 22:56
Operator : SJ/JU
Sample : I5475-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-20408-COMP

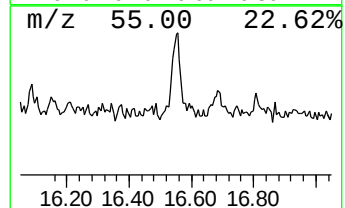
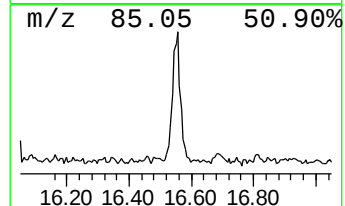
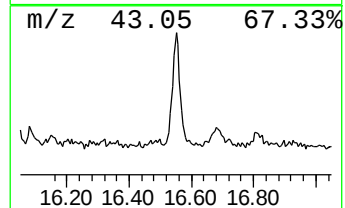
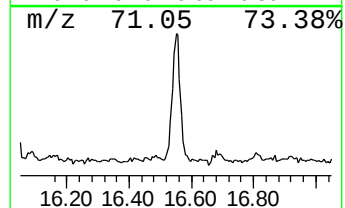
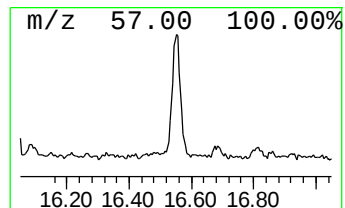
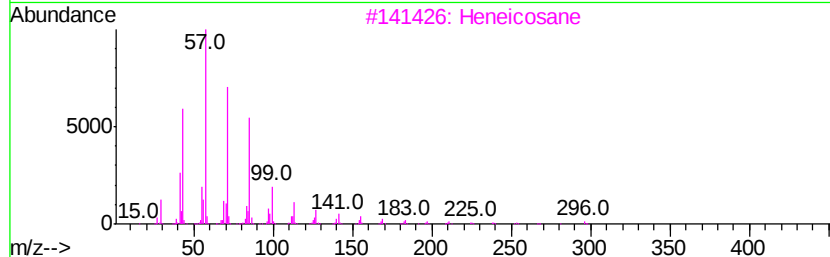
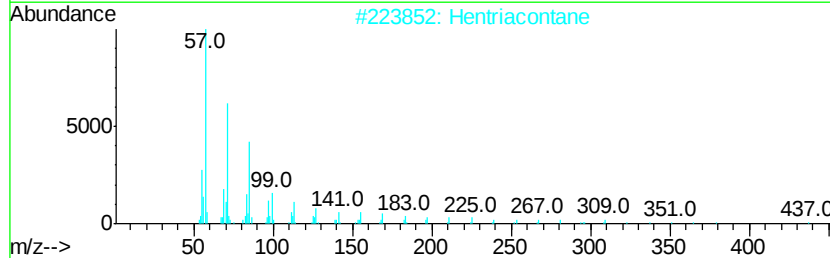
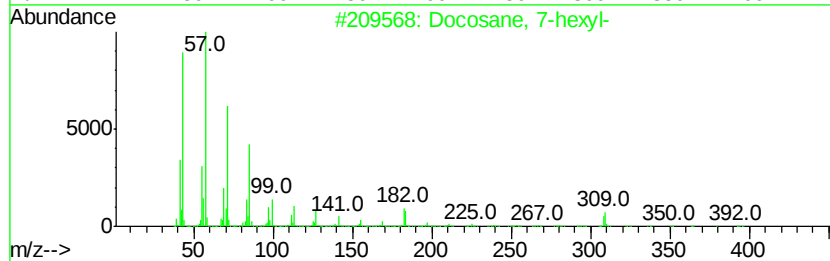
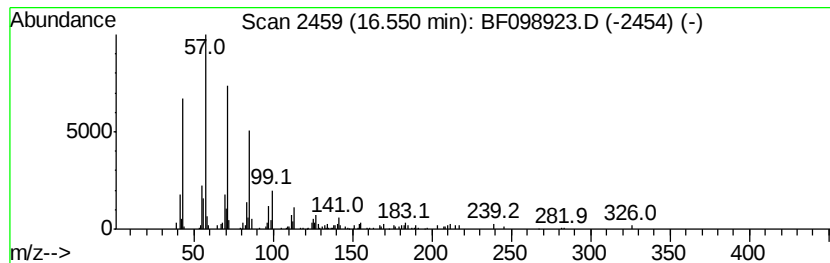
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	5.13 ng	210075	Perylene-d12	15.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098923.D
Acq On : 28 Sep 2017 22:56
Operator : SJ/JU
Sample : I5475-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-20408-COMP

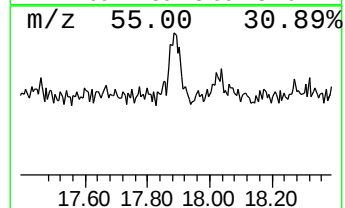
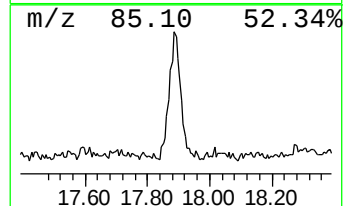
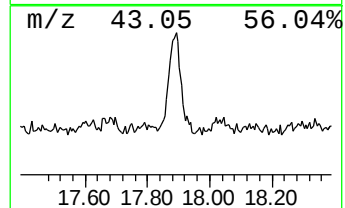
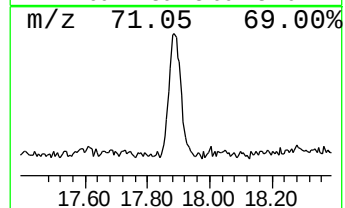
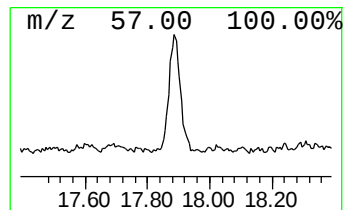
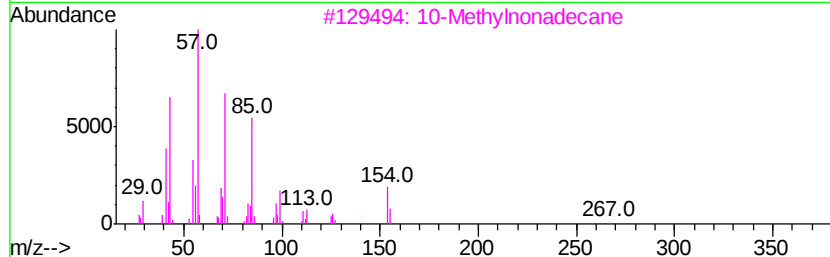
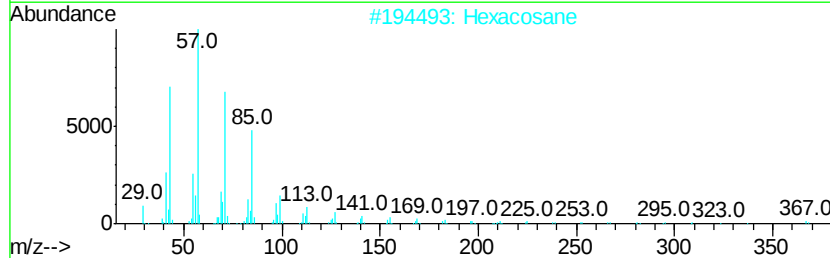
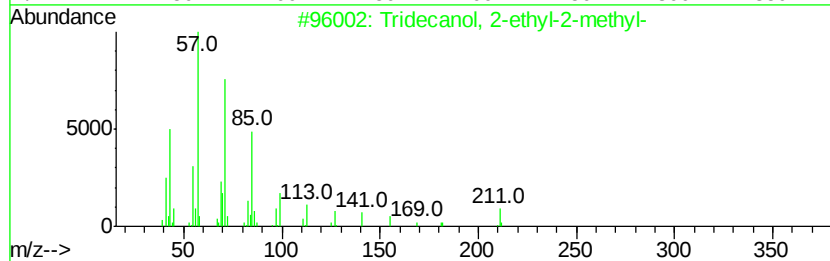
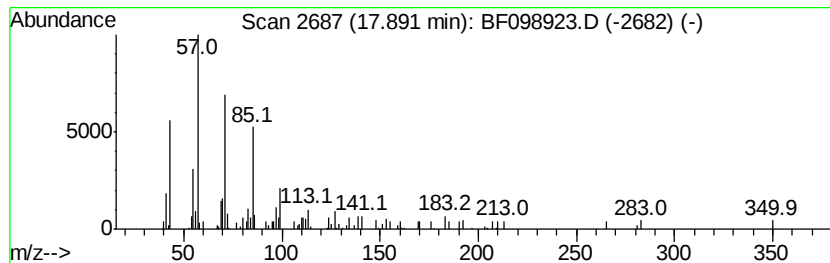
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tridecanol, 2-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	3.95 ng	161897	Perylene-d12	15.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	87
2			Hexacosane	366	C26H54	000630-01-3	87
3			10-Methylnonadecane	282	C20H42	056862-62-5	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			Hentriacontane	437	C31H64	000630-04-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098923.D
Acq On : 28 Sep 2017 22:56
Operator : SJ/JU
Sample : I5475-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-20408-COMP

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
Butane, 2-methoxy...	2.25	6.0	ng	246538	1	6.92	818315	20.0
1,3-Dioxolane, 2,...	3.10	3.2	ng	130346	1	6.92	818315	20.0
2-Pentanone, 4-hy...	5.15	19.1	ng	781901	1	6.92	818315	20.0
unknown6.69	6.69	83.1	ng	3401190	1	6.92	818315	20.0
n-Nonadecanol-1	13.90	7.3	ng	250029	5	14.08	688343	20.0
Tetratriacontyl p...	14.54	3.0	ng	102829	5	14.08	688343	20.0
Eicosane	16.03	3.8	ng	156725	6	15.57	818712	20.0
Docosane, 7-hexyl-	16.55	5.1	ng	210075	6	15.57	818712	20.0
Tridecanol, 2-eth...	17.89	4.0	ng	161897	6	15.57	818712	20.0