

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
 Data File : BF088136.D
 Acq On : 18 Jun 2016 16:12
 Operator : UM/SJ
 Sample : H3501-09
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SED3-0-6

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-BF060716.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	1.667	6	7	11	rVV	60620	77333	3.79%	0.413%
2	1.724	11	12	15	rVB	26337	28931	1.42%	0.155%
3	1.781	15	17	23	rBV	603229	840452	41.24%	4.494%
4	1.873	23	25	38	rVB2	71524	205357	10.08%	1.098%
5	2.067	38	42	50	rVB5	15721	61107	3.00%	0.327%
6	2.261	56	59	67	rVB2	17115	39067	1.92%	0.209%
7	3.347	151	154	159	rBV	11078	26529	1.30%	0.142%
8	4.844	283	285	291	rVB	87345	142635	7.00%	0.763%
9	4.970	291	296	300	rBV	14091	37701	1.85%	0.202%
10	5.290	322	324	327	rBV	1634562	1757978	86.27%	9.399%
11	6.353	414	417	419	rBV	1585105	2037851	100.00%	10.895%
12	6.456	424	426	429	rVV	1509309	1856451	91.10%	9.926%
13	6.684	444	446	449	rBV	698290	583708	28.64%	3.121%
14	6.753	449	452	455	rVV4	34268	55581	2.73%	0.297%
15	6.844	458	460	462	rVB	1771752	1697545	83.30%	9.076%
16	7.107	479	483	484	rBV2	13192	27848	1.37%	0.149%
17	7.176	487	489	493	rVB	13785	27730	1.36%	0.148%
18	7.256	493	496	498	rBV	1125366	1083898	53.19%	5.795%
19	7.370	504	506	512	rVB4	15080	31403	1.54%	0.168%
20	7.507	516	518	525	rVB2	11201	28754	1.41%	0.154%
21	7.736	535	538	540	rBV	22692	31085	1.53%	0.166%
22	7.976	556	559	561	rBV	667403	723822	35.52%	3.870%
23	8.262	581	584	586	rBV	14726	23760	1.17%	0.127%
24	8.330	588	590	595	rVB3	13620	29140	1.43%	0.156%
25	8.685	619	621	625	rVB2	21239	31155	1.53%	0.167%
26	8.753	625	627	629	rBV	23096	26624	1.31%	0.142%
27	8.913	639	641	644	rVB2	11570	22031	1.08%	0.118%
28	8.982	644	647	650	rBV4	12402	23196	1.14%	0.124%
29	9.050	650	653	655	rBV	2197289	2031388	99.68%	10.861%
30	9.119	655	659	662	rBV3	13568	30999	1.52%	0.166%
31	9.199	665	666	671	rVB2	17017	31458	1.54%	0.168%
32	9.336	674	678	680	rBV3	16657	22045	1.08%	0.118%
33	9.450	684	688	690	rBV2	206132	280352	13.76%	1.499%
34	9.542	694	696	698	rBV	48951	64567	3.17%	0.345%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.668	703	707	709 rBV	16576	24599	1.21%	0.132%
36	9.725	709	712	714 rBV	687385	690316	33.87%	3.691%
37	10.056	739	741	744 rBV4	13405	23445	1.15%	0.125%
38	10.148	745	749	752 rBV3	38146	95749	4.70%	0.512%
39	10.239	755	757	758 rBV	27648	26709	1.31%	0.143%
40	10.365	764	768	773 rBV5	41424	110556	5.43%	0.591%
41	10.445	773	775	778 rBV	89687	93902	4.61%	0.502%
42	10.513	778	781	783 rBV	948038	989223	48.54%	5.289%
43	10.548	783	784	785 rVV	47954	39259	1.93%	0.210%
44	10.582	785	787	790 rVB3	21660	35077	1.72%	0.188%
45	10.639	790	792	794 rBV2	39041	60533	2.97%	0.324%
46	10.959	818	820	822 rBV	53224	50275	2.47%	0.269%
47	11.085	829	831	832 rBV	54124	70408	3.46%	0.376%
48	11.199	839	841	844 rBV	621323	592567	29.08%	3.168%
49	11.759	888	890	892 rBV2	189769	242687	11.91%	1.298%
50	12.788	978	980	983 rBV	1010656	1209537	59.35%	6.467%
51	13.839	1070	1072	1075 rVB	301013	329301	16.16%	1.761%

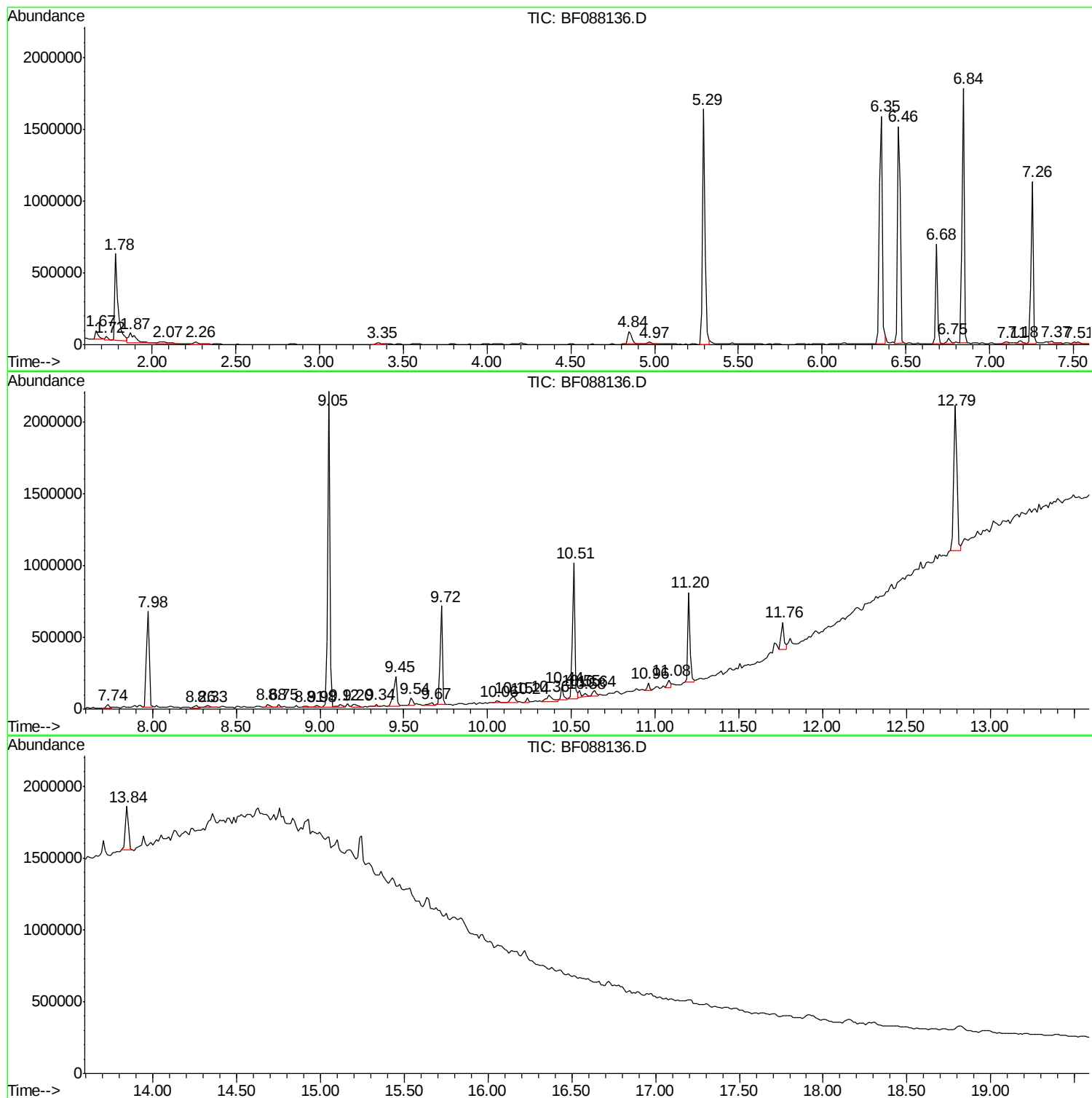
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Instrument :
BNA_F
ClientSampled :
SED3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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Sample : H3501-09
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED3-0-6

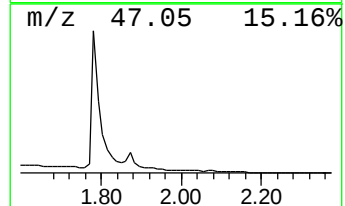
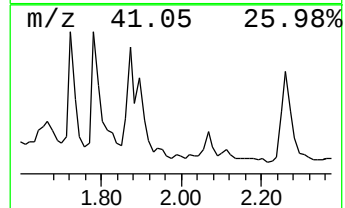
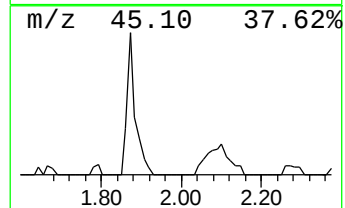
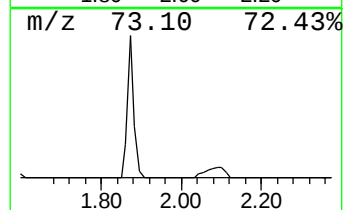
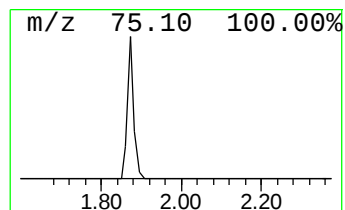
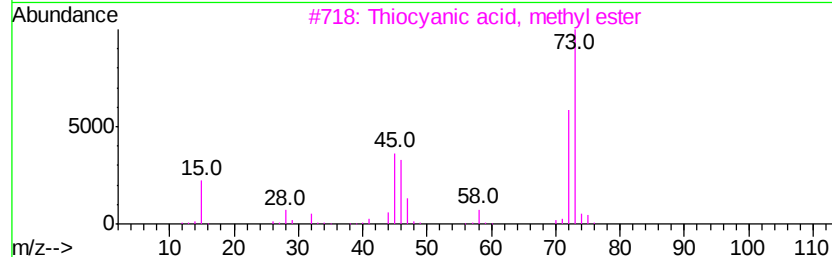
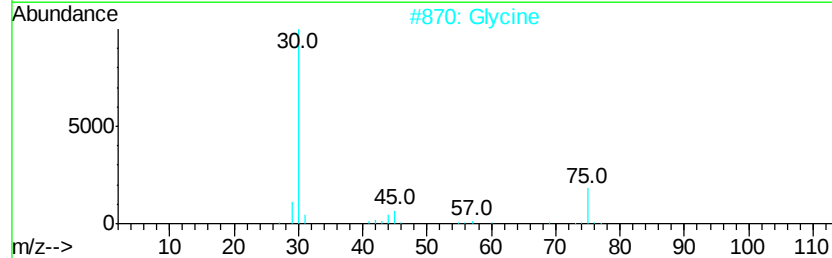
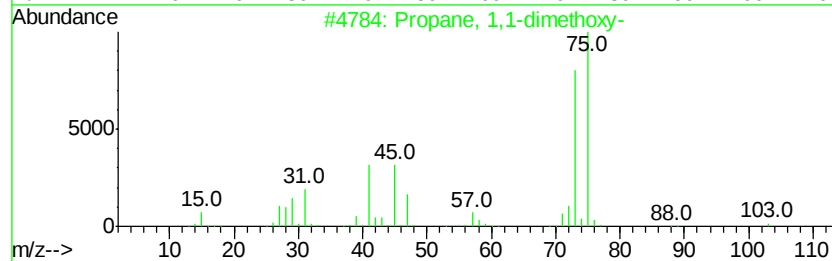
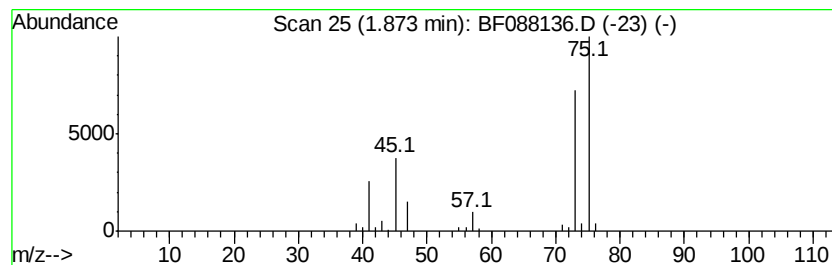
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.87	7.04 ng	205357	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		Glycine	75	C2H5NO2	000056-40-6	9
3		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
4		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	5



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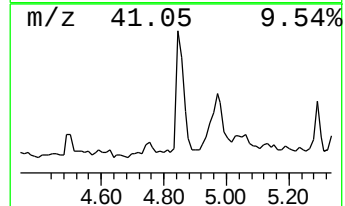
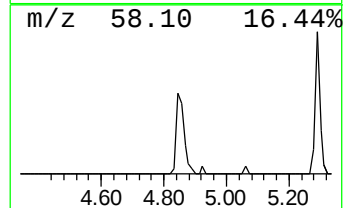
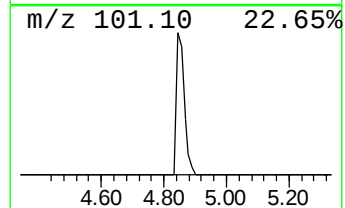
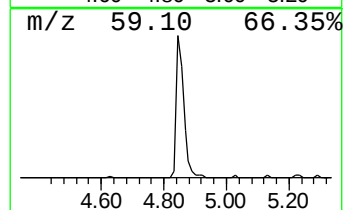
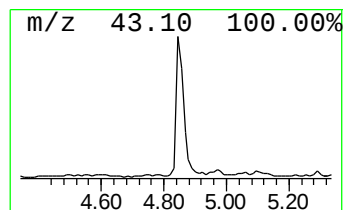
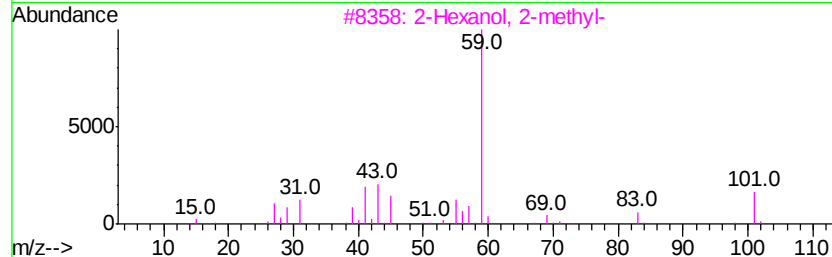
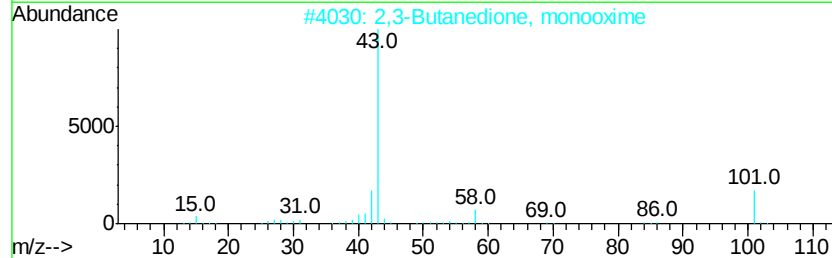
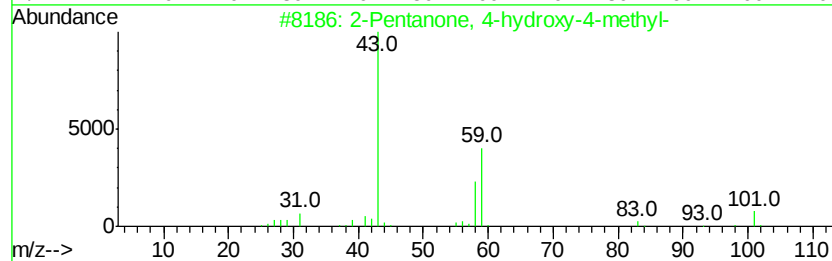
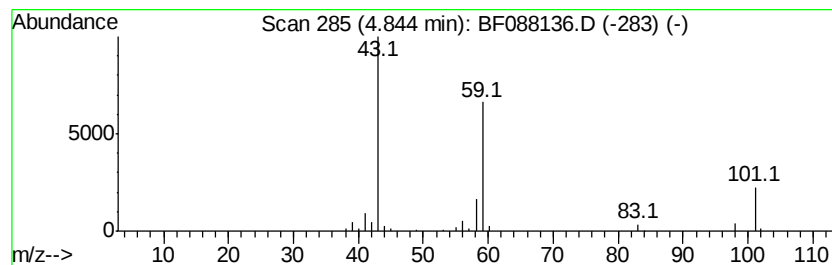
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	4.89 ng	142635	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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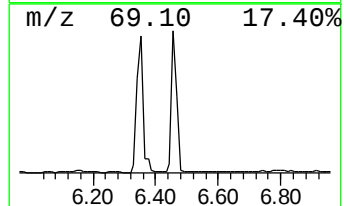
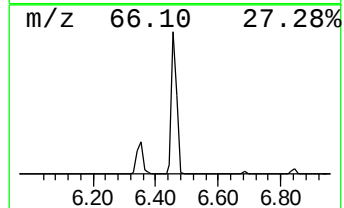
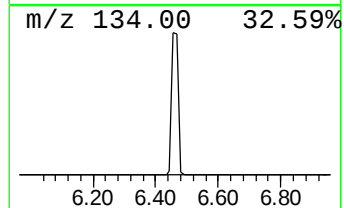
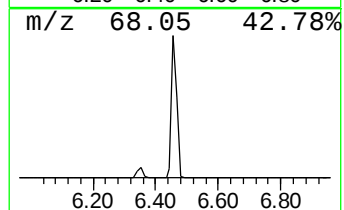
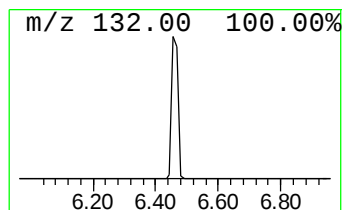
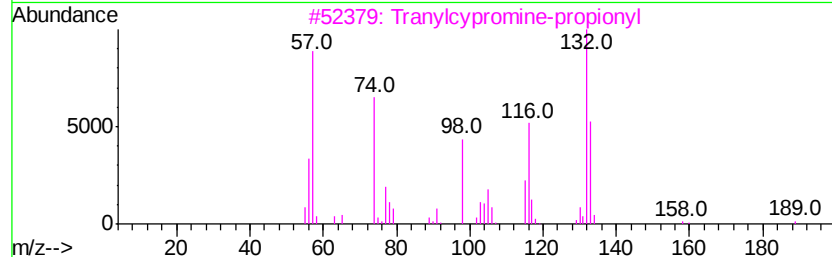
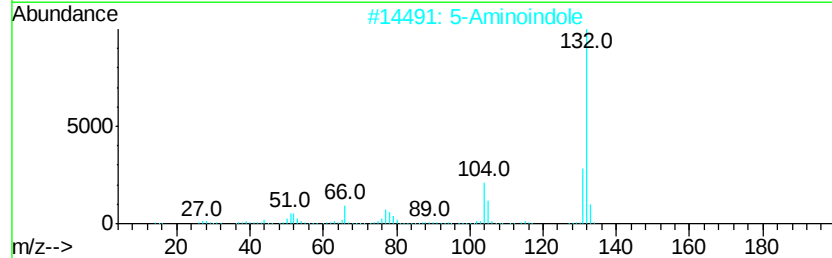
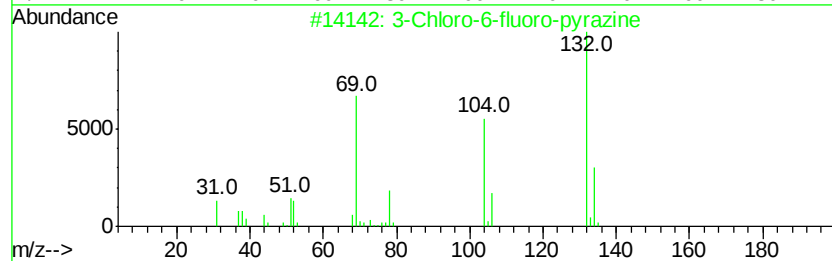
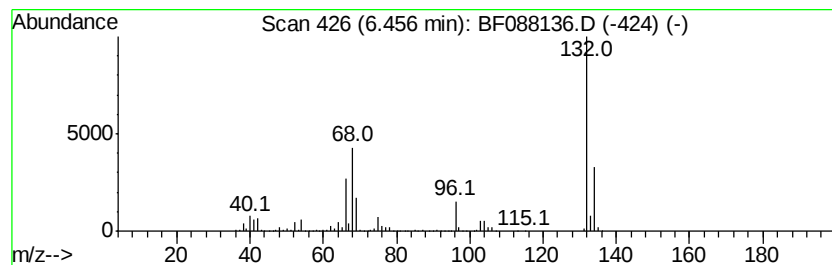
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	63.61 ng	1856450	1,4-Dichlorobenzene-d4	6.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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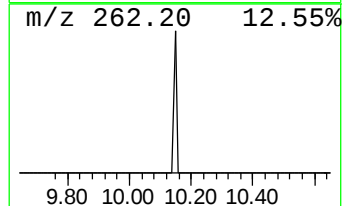
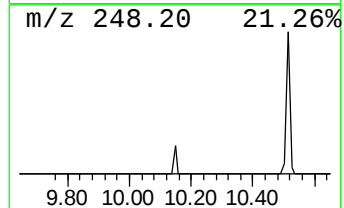
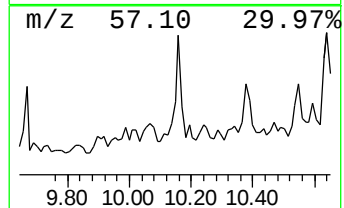
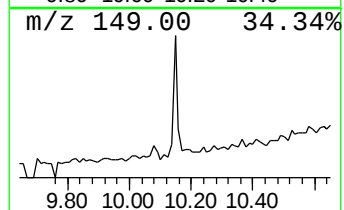
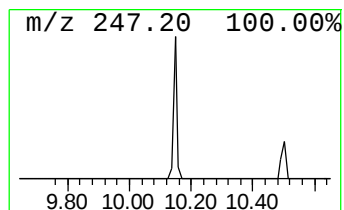
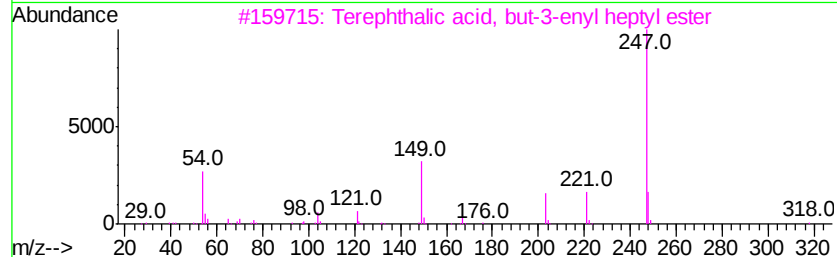
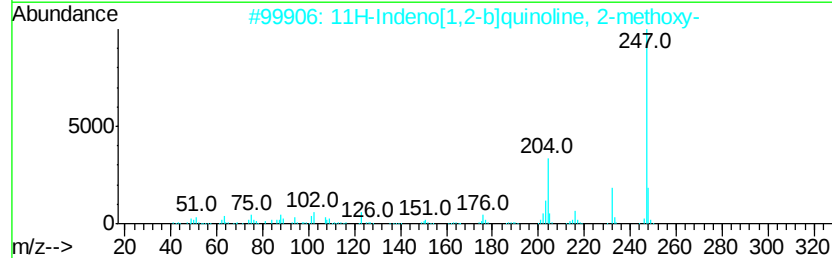
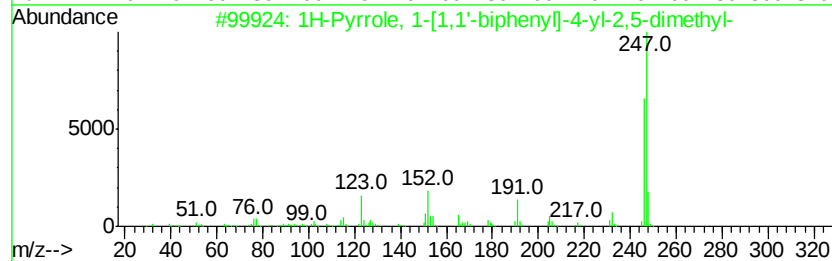
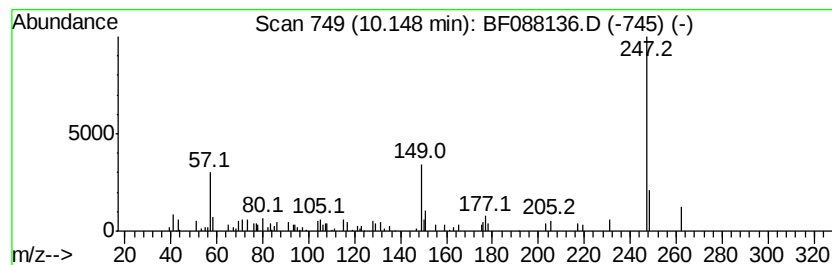
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 1H-Pyrrole, 1-[1,1'-bipheny... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	2.77 ng	95749	Acenaphthene-d10	9.72
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1H-Pyrrole, 1-[1,1'-biphenyl]-4-...	247 C18H17N	1000319-18-2	53
2	11H-Indeno[1,2-b]quinoline, 2-me...	247 C17H13NO	035639-27-1	50
3	Terephthalic acid, but-3-enyl he...	318 C19H26O4	1000356-33-7	42
4	Terephthalic acid, 2-chloropheny...	374 C21H23ClO4	1000324-04-1	42
5	1,1,9,9,9a-Pentamethyl-1,8,9,9a-...	262 C15H22N2O2	1000188-31-8	42



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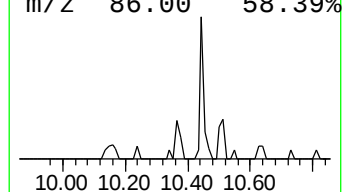
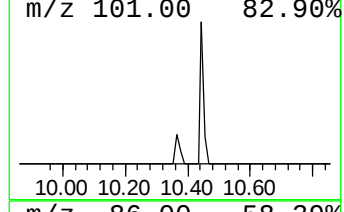
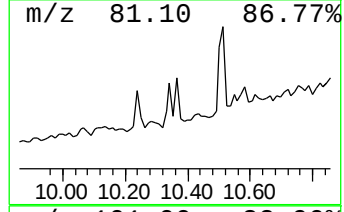
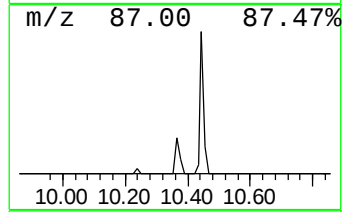
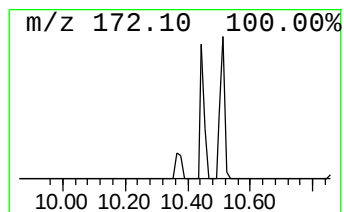
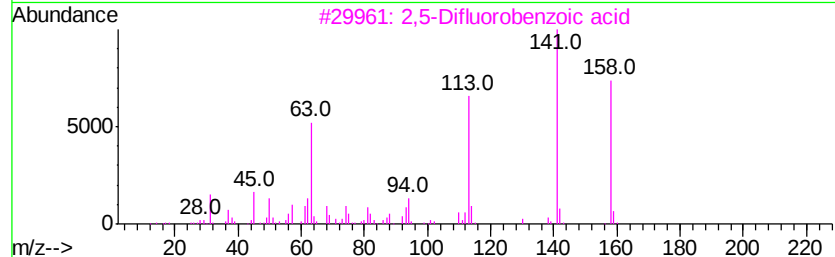
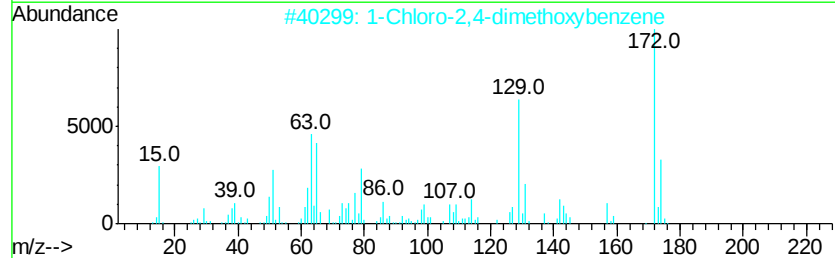
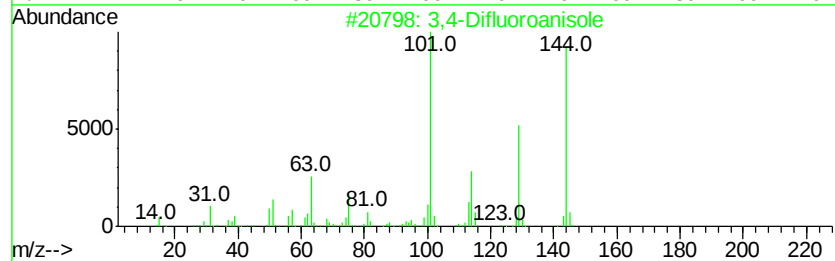
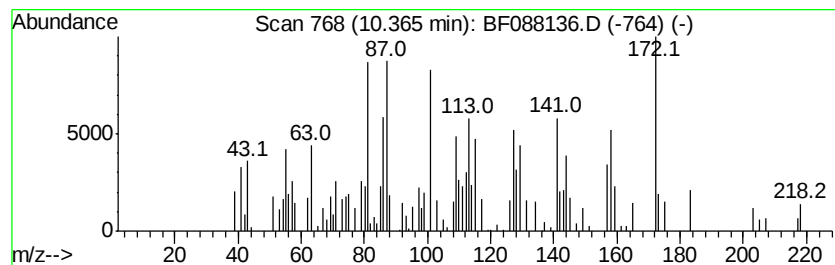
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown10.36 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.36	3.20 ng	110556	Acenaphthene-d10	9.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Difluoroanisole	144	C7H6F2O	115144-40-6	38
2	1-Chloro-2,4-dimethoxybenzene	172	C8H9ClO2	007051-13-0	38
3	2,5-Difluorobenzoic acid	158	C7H4F2O2	002991-28-8	27
4	1-Naphthalenecarboxaldehyde, 2-h...	172	C11H8O2	000708-06-5	11
5	Benzaldehyde, 3,5-difluoro-2-met...	172	C8H6F2O2	131782-50-8	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088136.D
Acq On : 18 Jun 2016 16:12
Operator : UM/SJ
Sample : H3501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED3-0-6

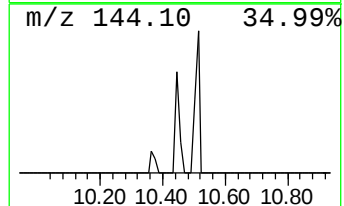
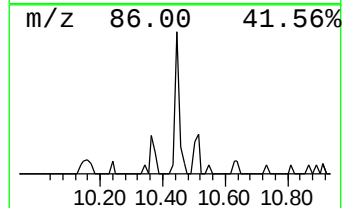
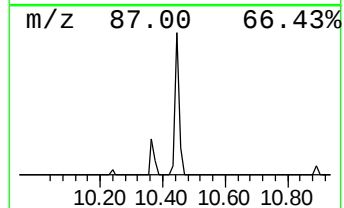
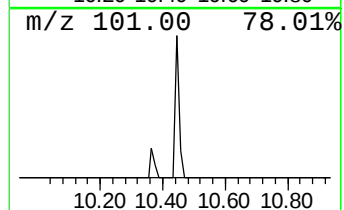
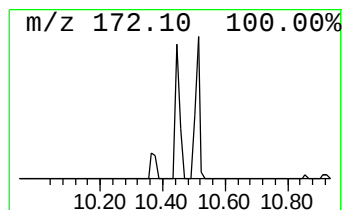
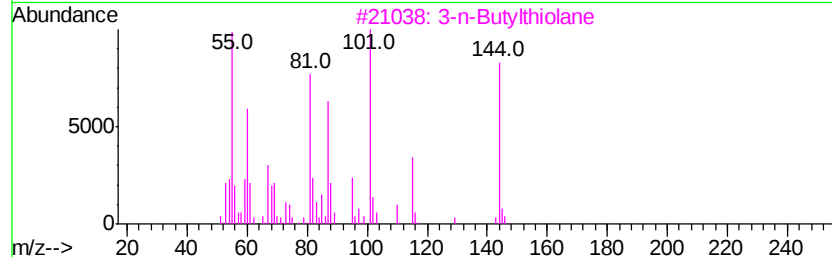
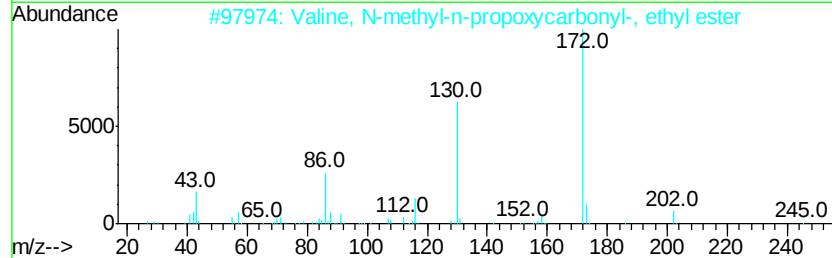
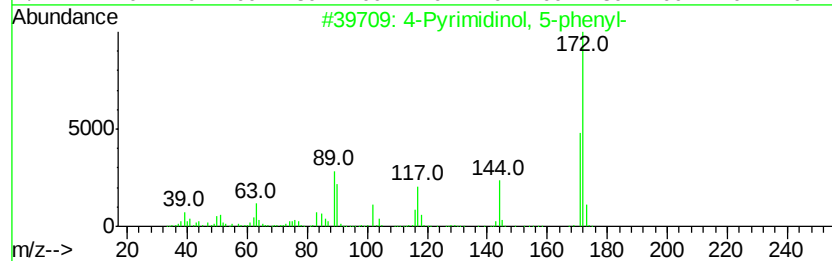
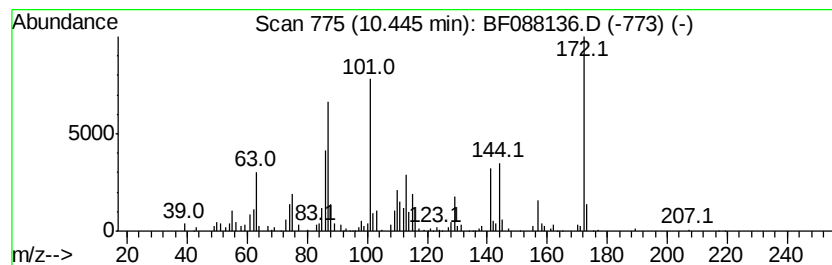
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.44 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.72 ng	93902	Acenaphthene-d10	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Pyrimidinol, 5-phenyl-	172	C10H8N2O	022433-69-8	22
2		Valine, N-methyl-n-propoxycarbon...	245	C12H23NO4	1000328-91-4	14
3		3-n-Butylthiolane	144	C8H16S	001551-24-2	14
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	14
5		Succinic acid, butyl undecyl ester	328	C19H36O4	1000324-86-2	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088136.D
Acq On : 18 Jun 2016 16:12
Operator : UM/SJ
Sample : H3501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

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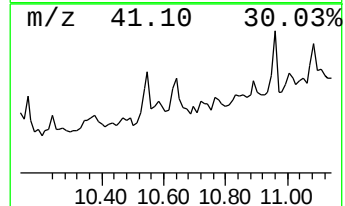
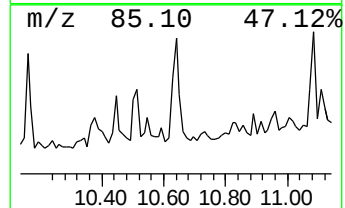
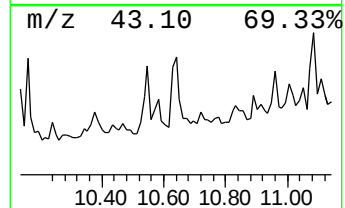
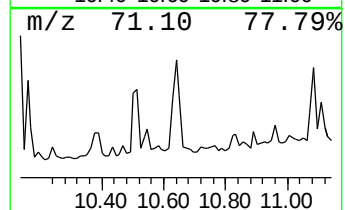
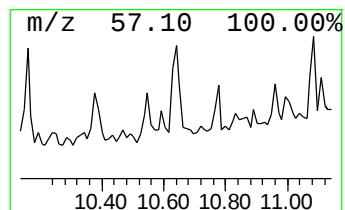
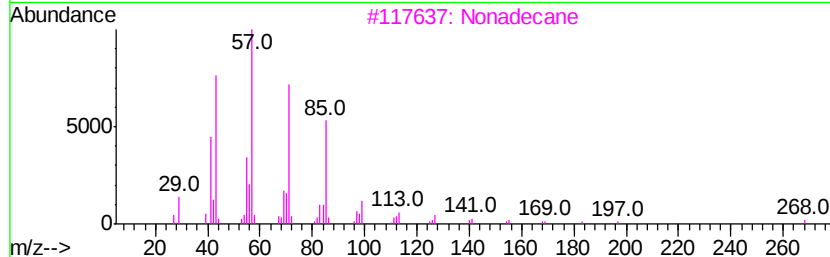
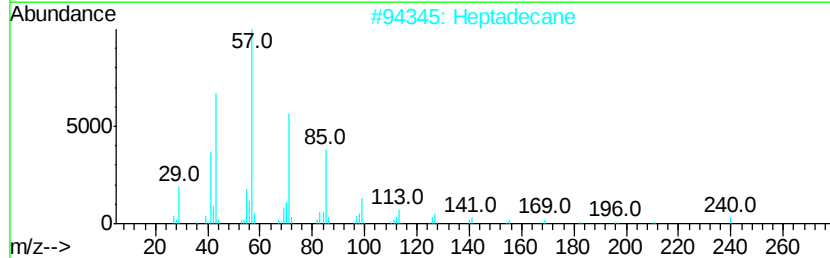
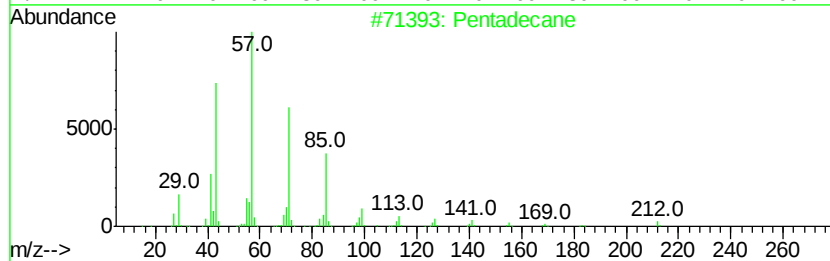
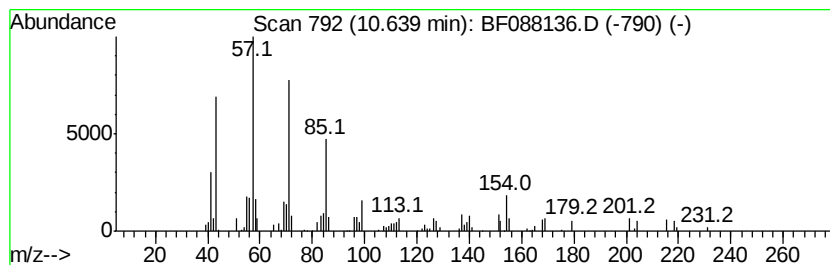
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	2.04 ng	60533	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	80
2		Heptadecane	240	C17H36	000629-78-7	80
3		Nonadecane	268	C19H40	000629-92-5	80
4		Tetracosane	338	C24H50	000646-31-1	80
5		Hexadecane	226	C16H34	000544-76-3	80



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Data File : BF088136.D
Acq On : 18 Jun 2016 16:12
Operator : UM/SJ
Sample : H3501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

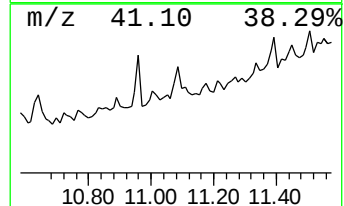
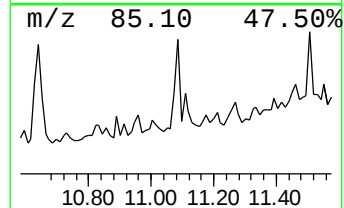
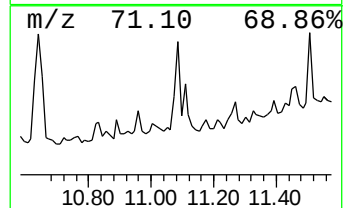
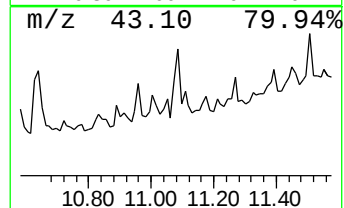
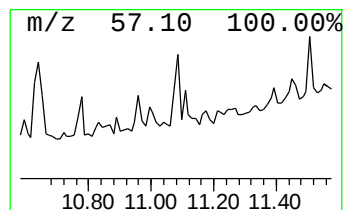
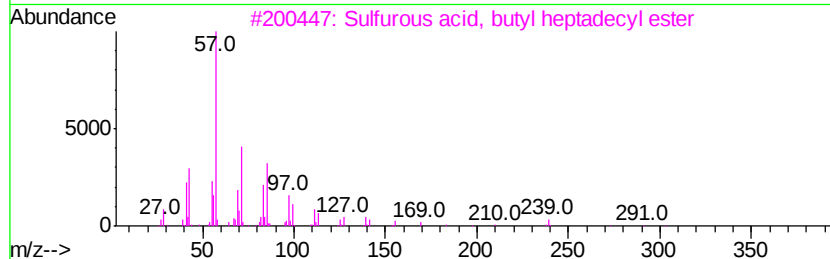
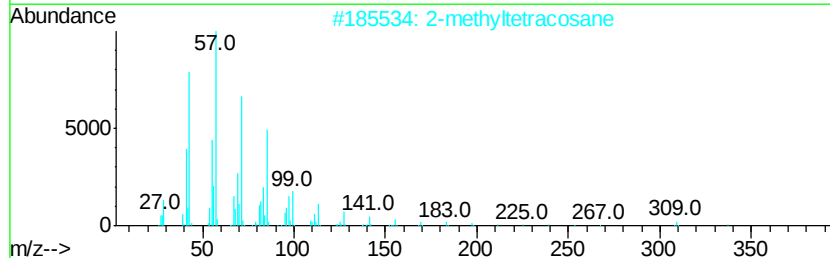
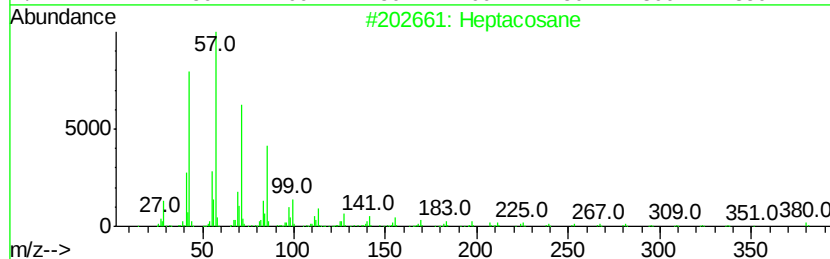
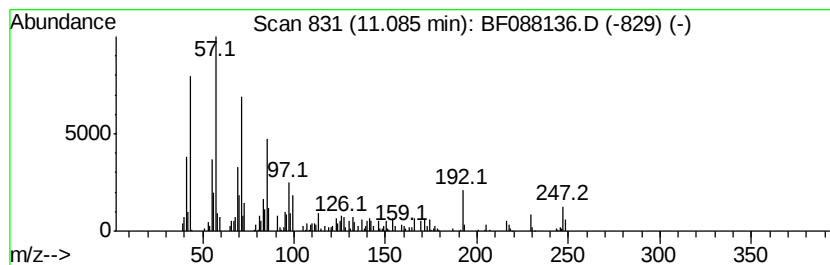
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	2.38 ng	70408	Phenanthrene-d10	11.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	58
2	2-methyltetracosane	352 C25H52	1000376-72-6	58
3	Sulfurous acid, butyl heptadecyl...	376 C21H44O3S	1000309-18-4	53
4	Tetradecane	198 C14H30	000629-59-4	52
5	Eicosane, 10-methyl-	296 C21H44	054833-23-7	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088136.D
Acq On : 18 Jun 2016 16:12
Operator : UM/SJ
Sample : H3501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

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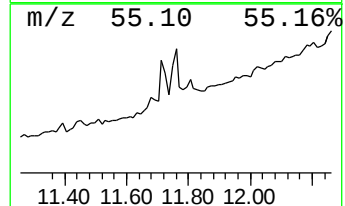
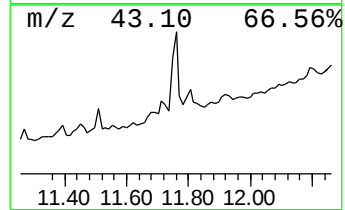
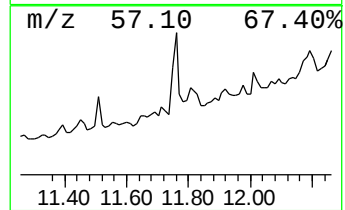
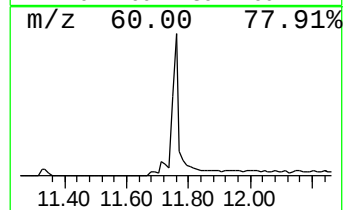
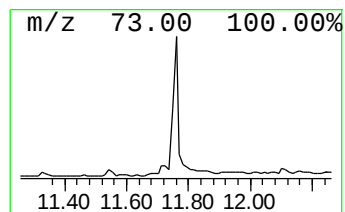
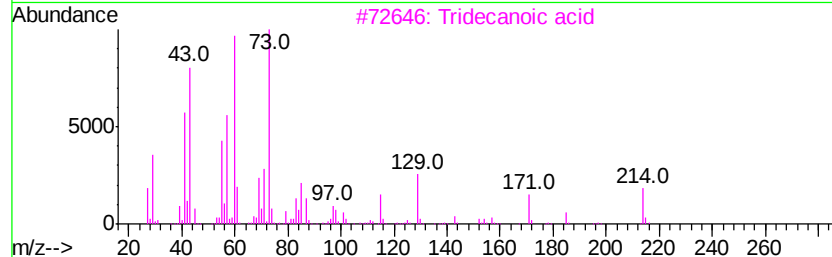
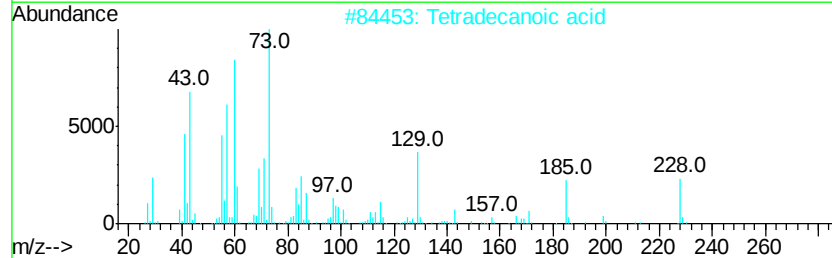
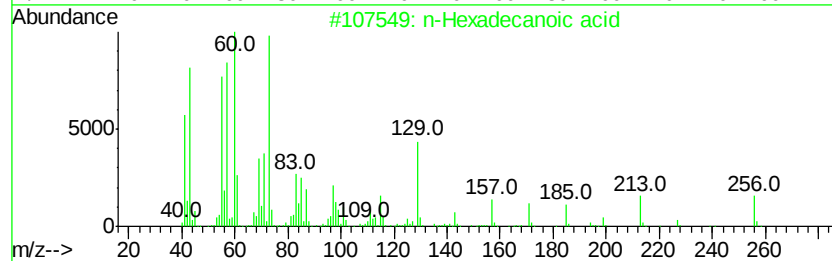
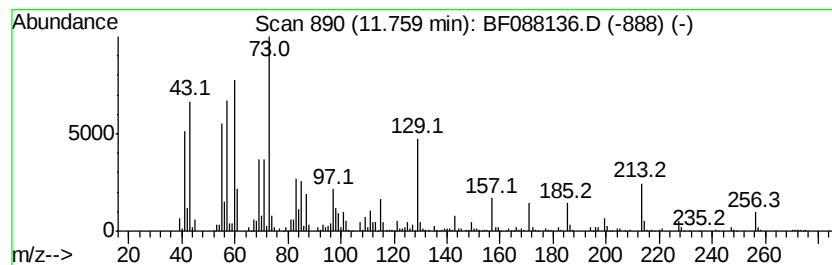
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	8.19 ng	242687	Phenanthrene-d10	11.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088136.D
Acq On : 18 Jun 2016 16:12
Operator : UM/SJ
Sample : H3501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
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2-Pentanone, 4-hy...	4.84	4.9	ng	142635	1	6.68	583708	20.0
unknown6.46	6.46	63.6	ng	1856450	1	6.68	583708	20.0
1H-Pyrrole, 1-[1,...	10.15	2.8	ng	95749	3	9.72	690316	20.0
unknown10.36	10.36	3.2	ng	110556	3	9.72	690316	20.0
unknown10.44	10.44	2.7	ng	93902	3	9.72	690316	20.0
Pentadecane	10.64	2.0	ng	60533	4	11.20	592567	20.0
Heptacosane	11.08	2.4	ng	70408	4	11.20	592567	20.0
n-Hexadecanoic acid	11.76	8.2	ng	242687	4	11.20	592567	20.0