

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF101217\
 Data File : BF099426.D
 Acq On : 13 Oct 2017 7:26
 Operator : SJ/JU
 Sample : I5731-04
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 100417-TIDO-F-U-S

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\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	2.128	4	7	30	rVB	241324	567090	21.50%	3.320%
2	5.069	504	507	517	rBV	162129	174124	6.60%	1.019%
3	5.475	572	576	590	rBV	930746	902023	34.19%	5.281%
4	6.481	744	747	760	rBV	630259	591012	22.40%	3.460%
5	6.622	767	771	775	rBV	1867097	1560931	59.17%	9.139%
6	6.851	807	810	814	rBV	714206	568115	21.53%	3.326%
7	7.010	833	837	840	rBV	2417832	2150251	81.51%	12.589%
8	7.422	901	907	910	rBV	1559215	1600950	60.68%	9.373%
9	8.133	1024	1028	1037	rBV	877833	707585	26.82%	4.143%
10	9.210	1206	1211	1214	rBV	2991285	2638159	100.00%	15.446%
11	9.886	1322	1326	1335	rBV	749814	625774	23.72%	3.664%
12	10.674	1457	1460	1470	rBV	776908	772489	29.28%	4.523%
13	11.374	1575	1579	1584	rBV	649591	547684	20.76%	3.207%
14	12.768	1812	1816	1819	rVB	76260	61216	2.32%	0.358%
15	12.957	1844	1848	1852	rBV	2145448	2053985	77.86%	12.026%
16	13.468	1932	1935	1939	rBV	64253	52089	1.97%	0.305%
17	13.839	1995	1998	2004	rBV	29833	33067	1.25%	0.194%
18	14.015	2024	2028	2035	rBV	671272	577347	21.88%	3.380%
19	15.098	2209	2212	2216	rBV	26165	28995	1.10%	0.170%
20	15.486	2272	2278	2290	rBV	348788	494603	18.75%	2.896%
21	15.909	2345	2350	2356	rVB	47359	66055	2.50%	0.387%
22	16.409	2430	2435	2442	rBV2	48401	88072	3.34%	0.516%
23	16.992	2529	2534	2542	rVB3	37098	74640	2.83%	0.437%
24	17.692	2646	2653	2663	rBV5	32018	82541	3.13%	0.483%
25	18.521	2784	2794	2803	rBV5	20842	61021	2.31%	0.357%

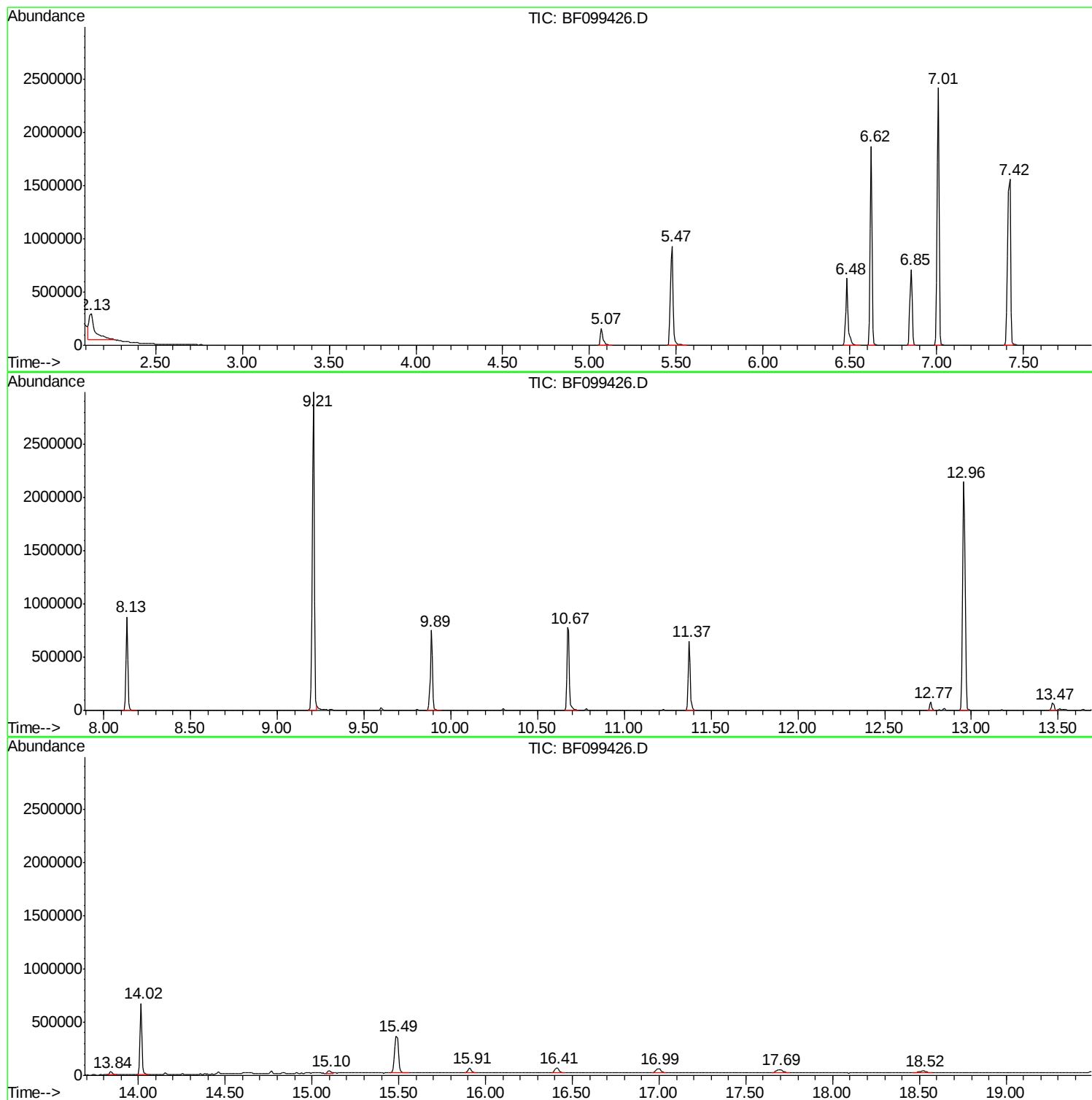
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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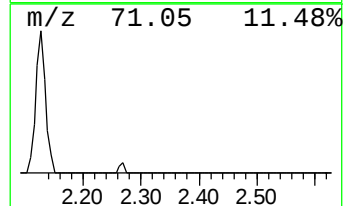
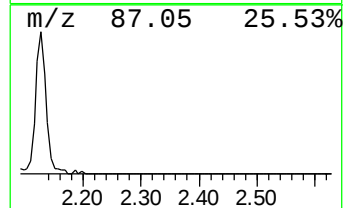
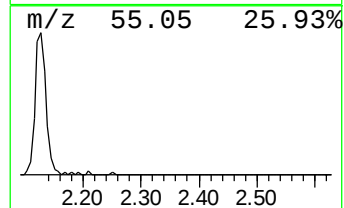
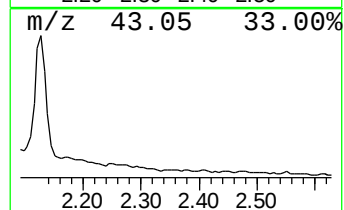
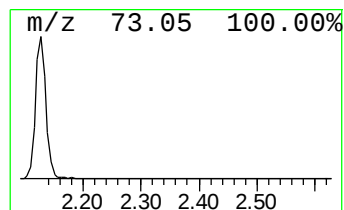
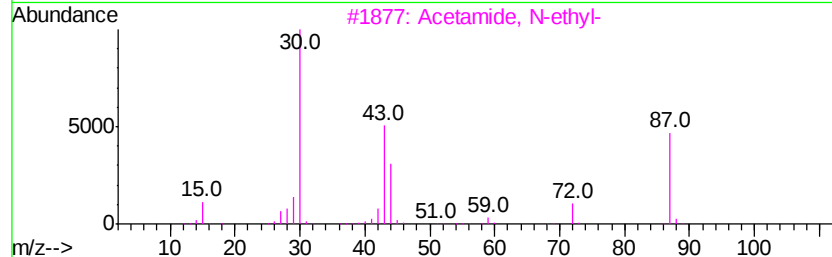
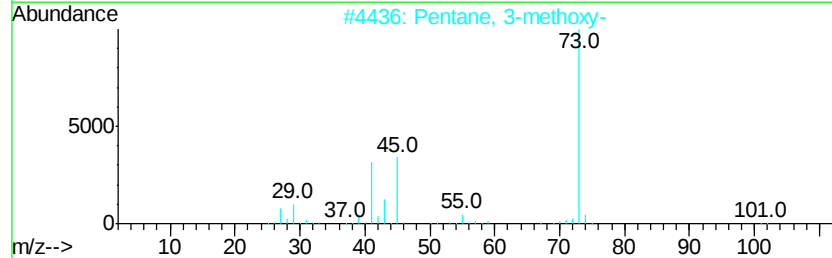
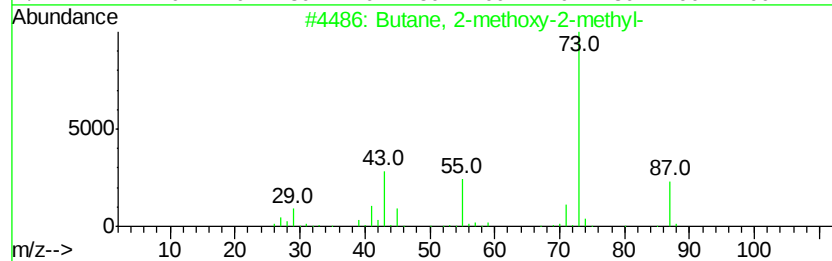
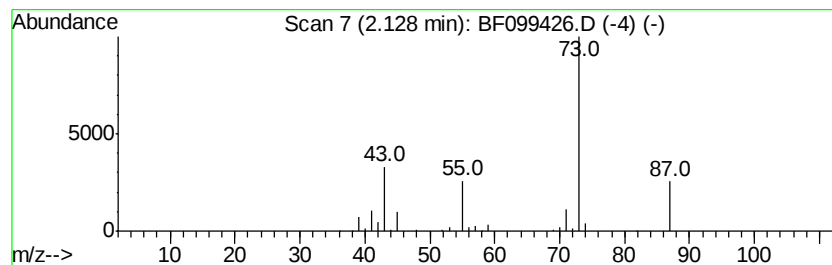
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	19.96 ng	567090	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	9



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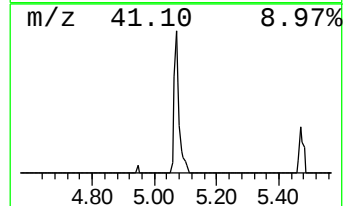
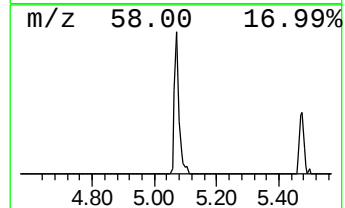
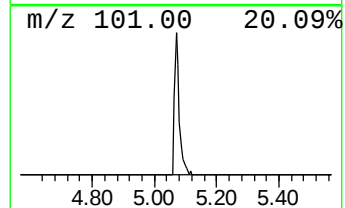
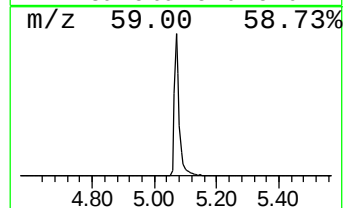
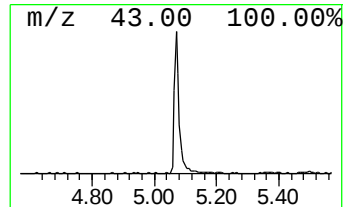
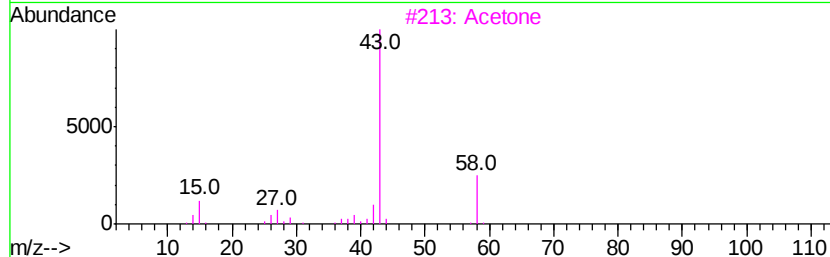
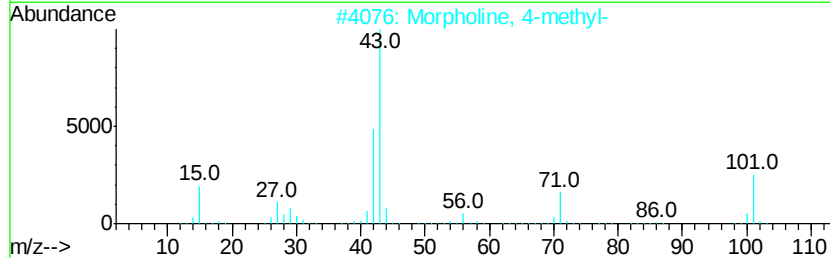
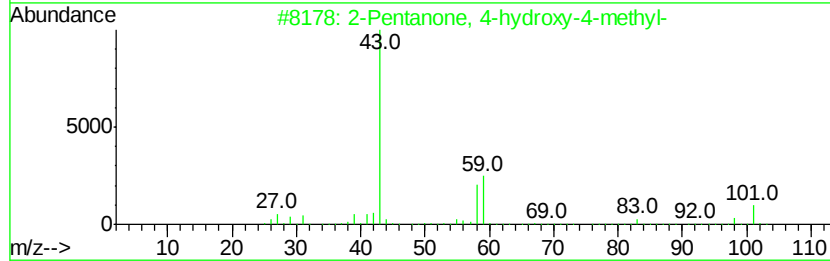
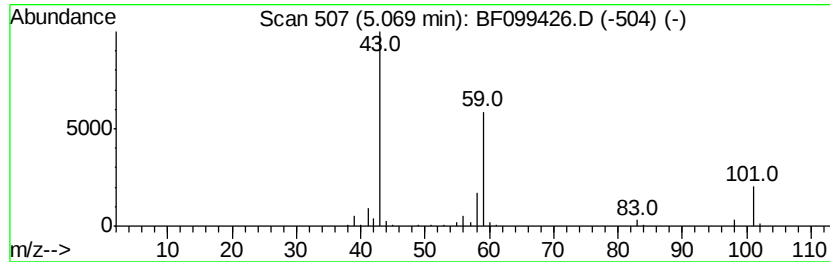
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	6.13 ng	174124	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		Acetone	58	C3H6O	000067-64-1	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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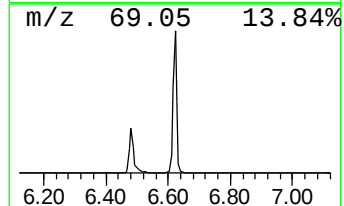
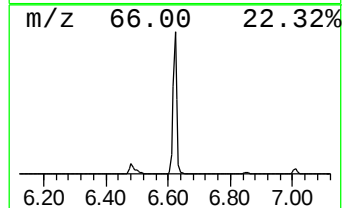
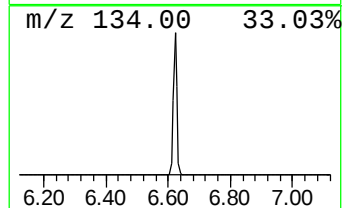
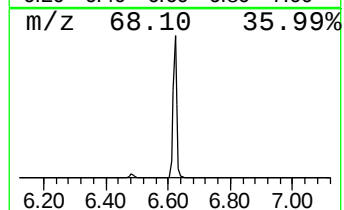
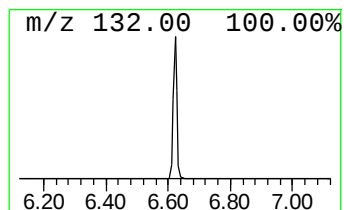
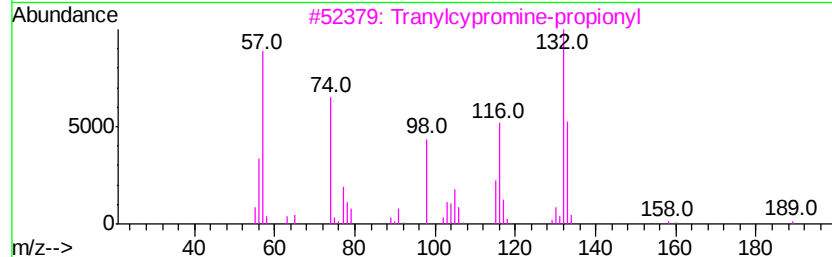
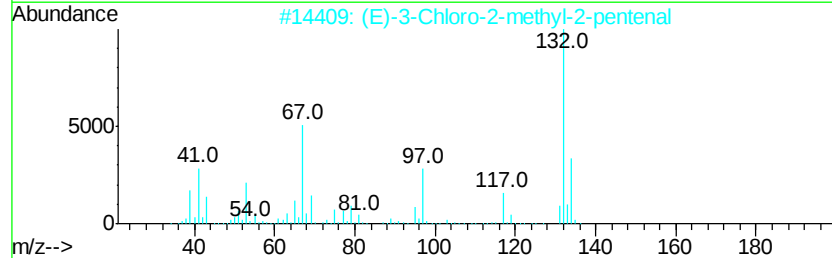
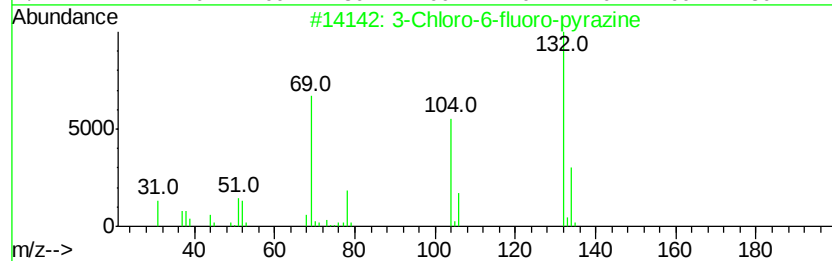
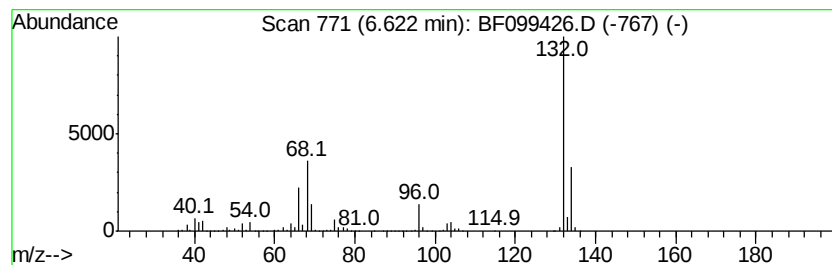
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Peak Number 3 unknown6.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	54.95 ng	1560930	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Xenon	132	Xe	007440-63-3	9



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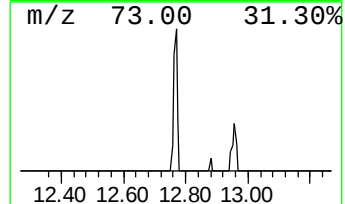
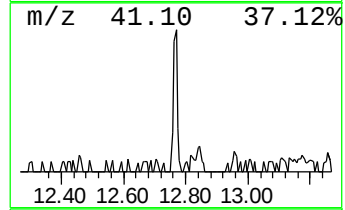
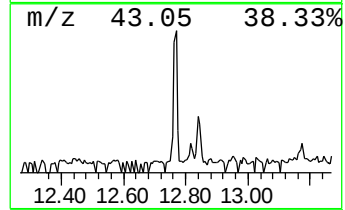
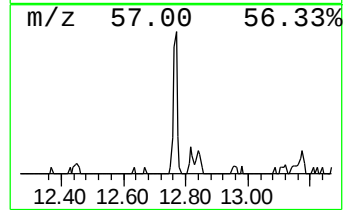
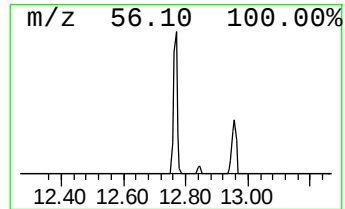
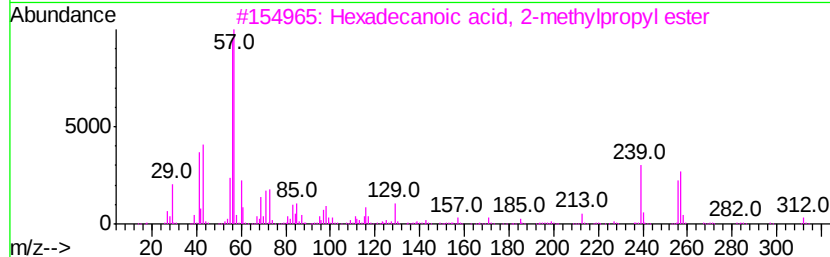
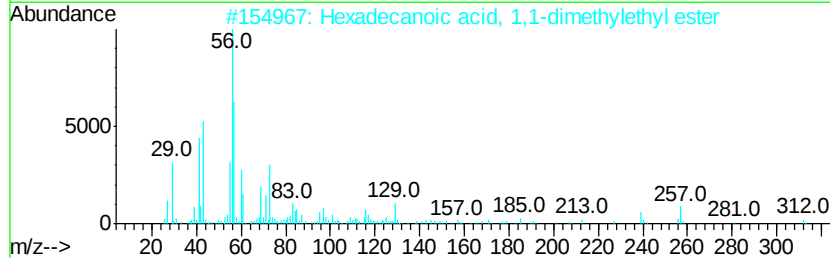
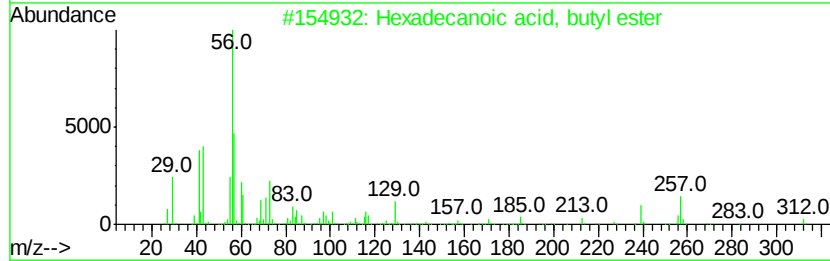
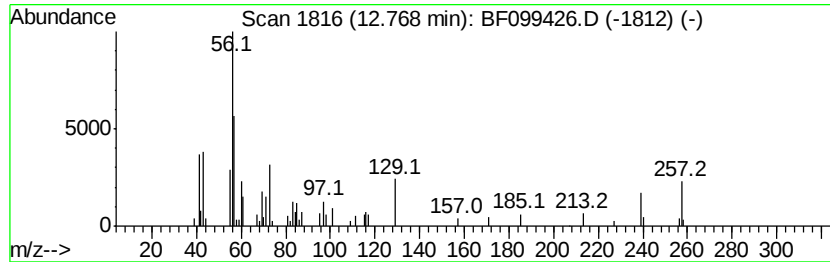
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.12 ng	61216	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	45
4		Nipecotic acid	129	C6H11NO2	000498-95-3	38
5		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	35



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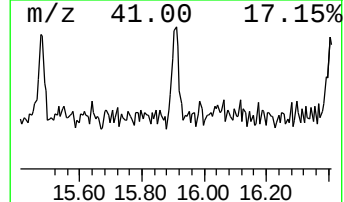
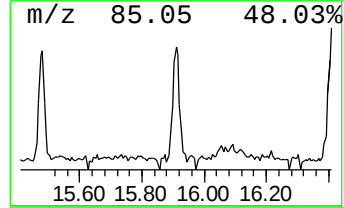
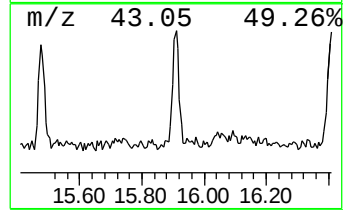
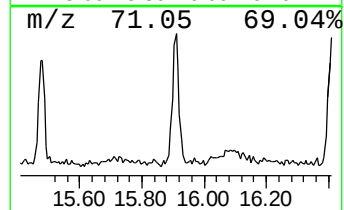
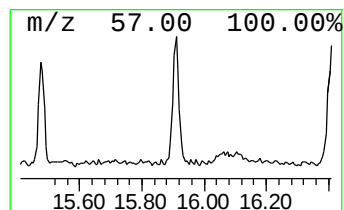
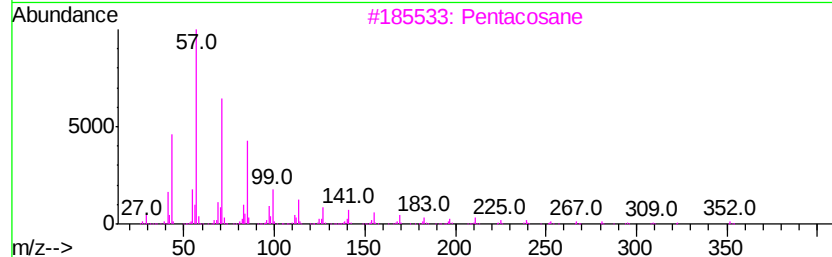
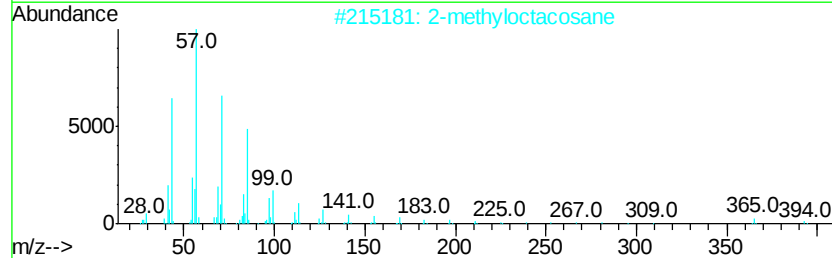
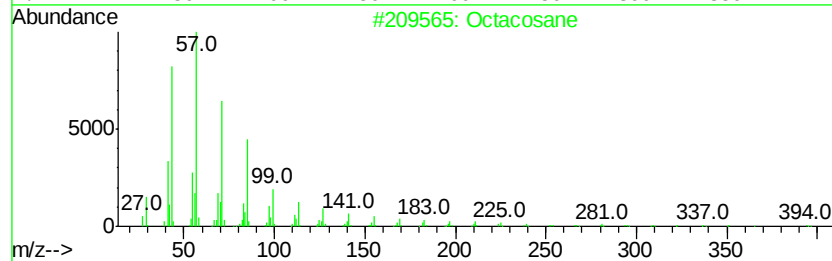
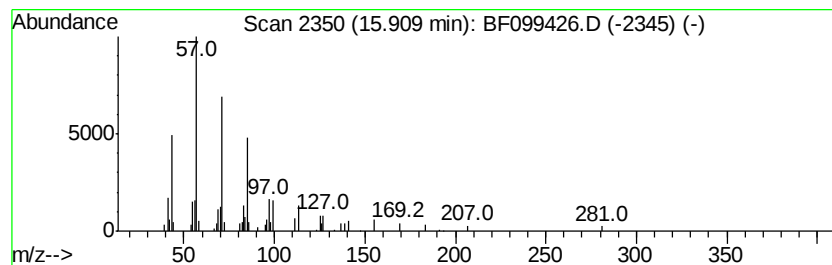
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Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.67 ng	66055	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		Heptacosane	380	C27H56	000593-49-7	91



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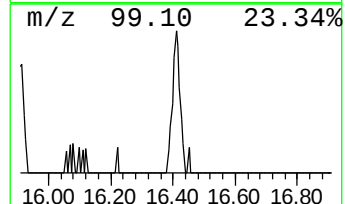
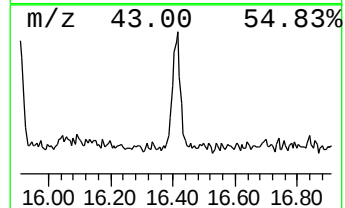
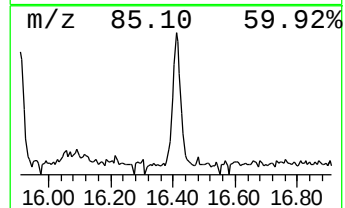
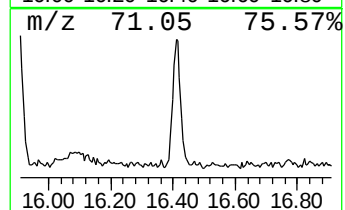
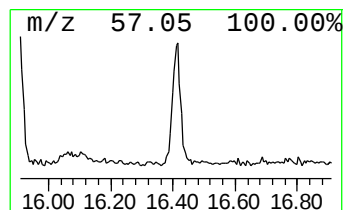
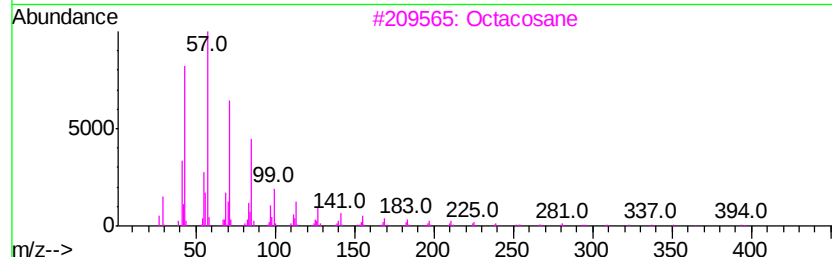
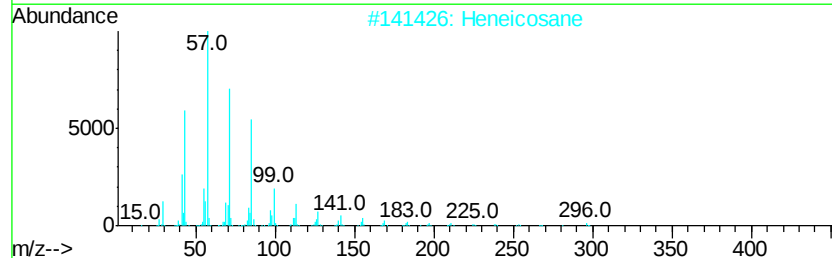
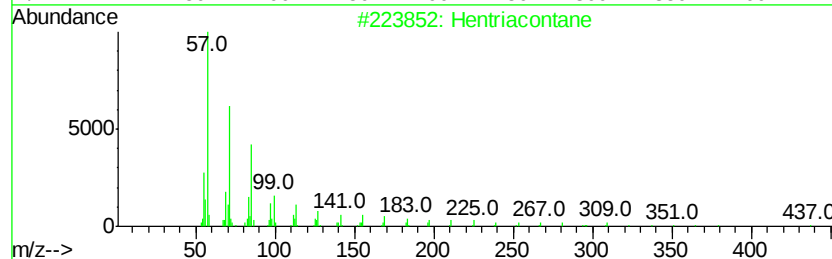
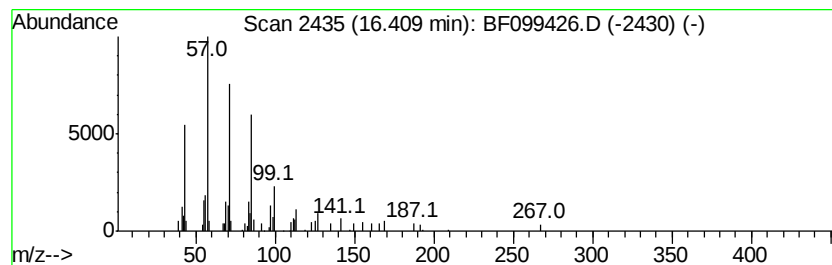
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	3.56 ng	88072	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		triacontane	422	C30H62	000638-68-6	91
5		Heptadecane	240	C17H36	000629-78-7	91



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099426.D
Acq On : 13 Oct 2017 7:26
Operator : SJ/JU
Sample : I5731-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

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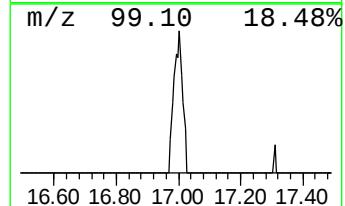
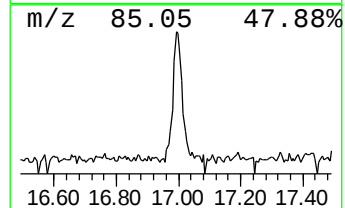
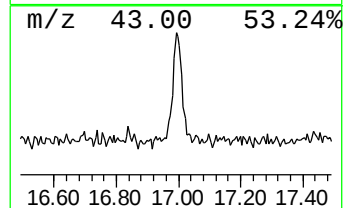
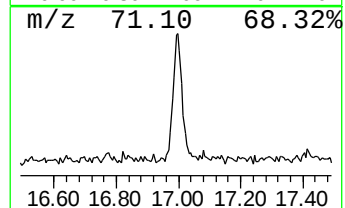
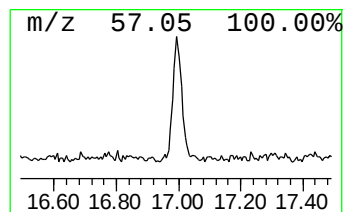
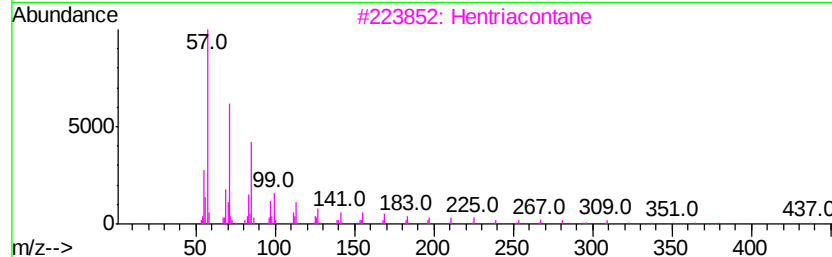
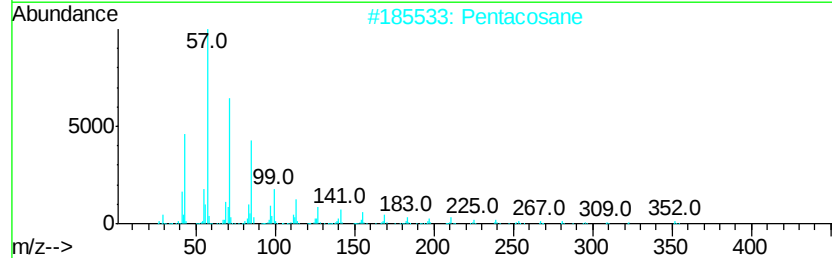
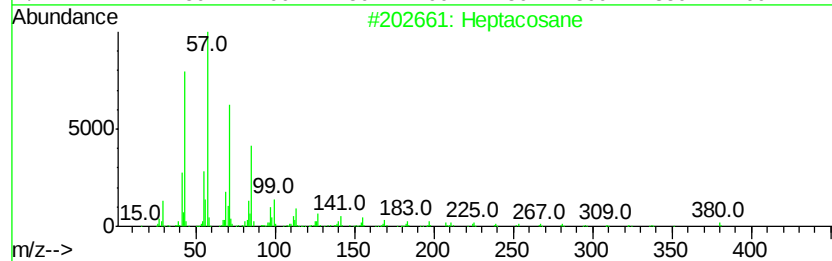
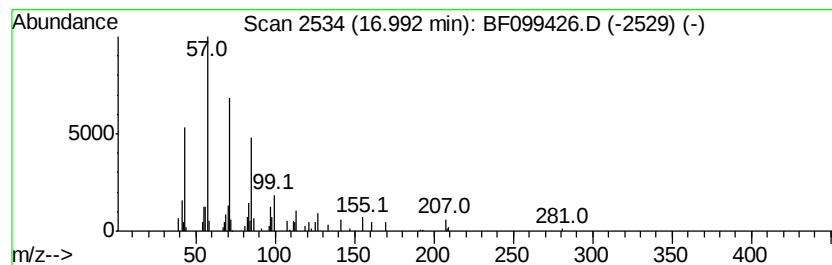
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.99	3.02 ng	74640	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Pentacosane		352	C25H52	000629-99-2	91
3	Hentriacontane		437	C31H64	000630-04-6	90
4	Hexacosane		366	C26H54	000630-01-3	87
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF101217\
Data File : BF099426.D
Acq On : 13 Oct 2017 7:26
Operator : SJ/JU
Sample : I5731-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
100417-TIDO-F-U-S

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...	2.13	20.0	ng	567090	1	6.85	568115	20.0
2-Pentanone, 4-hy...	5.07	6.1	ng	174124	1	6.85	568115	20.0
unknown6.62	6.62	55.0	ng	1560930	1	6.85	568115	20.0
Hexadecanoic acid...	12.77	2.1	ng	61216	5	14.02	577347	20.0
Octacosane	15.91	2.7	ng	66055	6	15.49	494603	20.0
Hentriacontane	16.41	3.6	ng	88072	6	15.49	494603	20.0
Heptacosane	16.99	3.0	ng	74640	6	15.49	494603	20.0