

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
 Data File : BF102673.D
 Acq On : 31 Jan 2018 23:41
 Operator : SJ/JU
 Sample : J1384-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OILY-STONES-1

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-BF012218.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	2.163	6	13	18	rVB3	62226	121790	3.57%	0.557%
2	4.298	372	376	383	rVB3	66521	119075	3.49%	0.545%
3	4.904	476	479	484	rBV	181807	243013	7.12%	1.112%
4	5.339	549	553	570	rBV	3139442	3271243	95.79%	14.965%
5	5.492	576	579	582	rBV	73460	83167	2.44%	0.380%
6	5.634	600	603	611	rVB3	63045	84337	2.47%	0.386%
7	6.139	685	689	693	rBV	107470	119378	3.50%	0.546%
8	6.381	726	730	740	rBV	2595115	3415043	100.00%	15.623%
9	6.492	745	749	754	rVB	3432151	3182631	93.19%	14.559%
10	6.710	782	786	790	rBV	950539	777525	22.77%	3.557%
11	6.869	808	813	816	rBV	2581166	2534246	74.21%	11.593%
12	7.022	834	839	841	rBV2	75221	83740	2.45%	0.383%
13	7.281	879	883	886	rBV	2034228	1874432	54.89%	8.575%
14	7.992	1001	1004	1008	rBV	1125551	875739	25.64%	4.006%
15	8.792	1135	1140	1148	rBV	384738	776494	22.74%	3.552%
16	9.069	1183	1187	1196	rBV	1921475	3335594	97.67%	15.259%
17	9.310	1223	1228	1231	rBV	148090	265509	7.77%	1.215%
18	9.751	1300	1303	1311	rBV	267288	696716	20.40%	3.187%

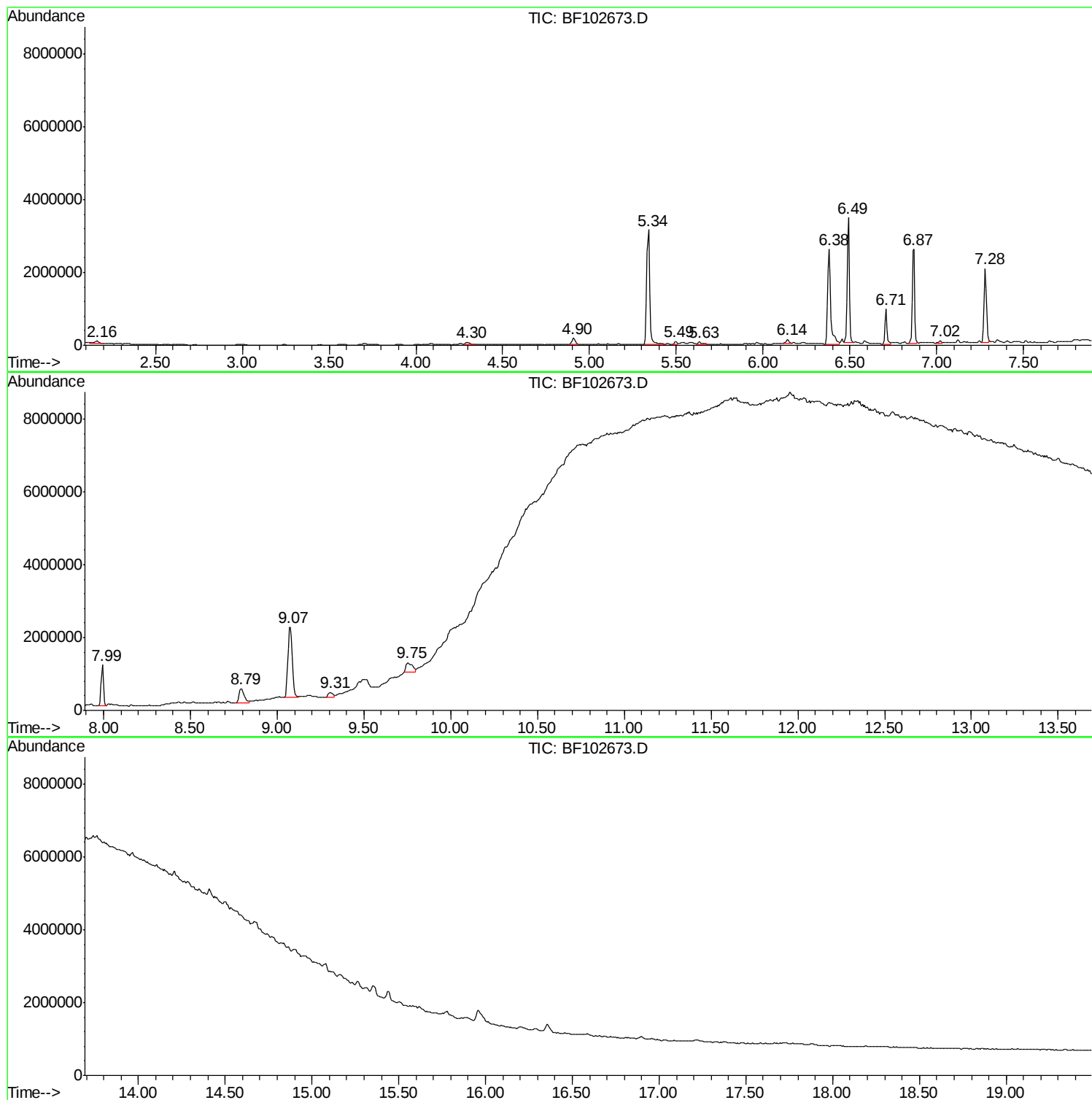
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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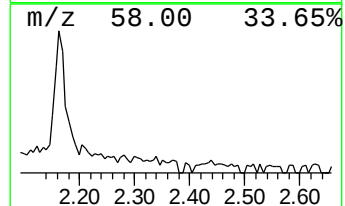
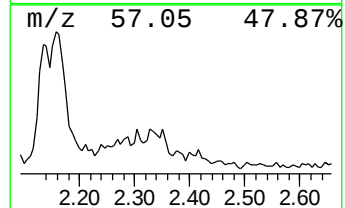
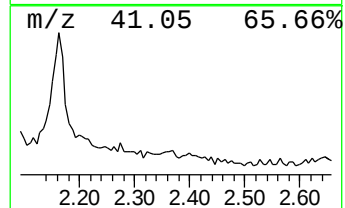
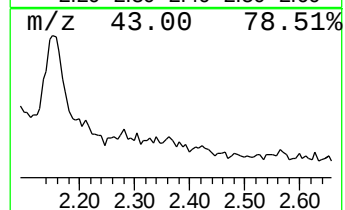
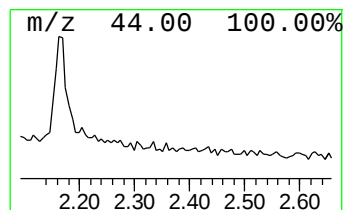
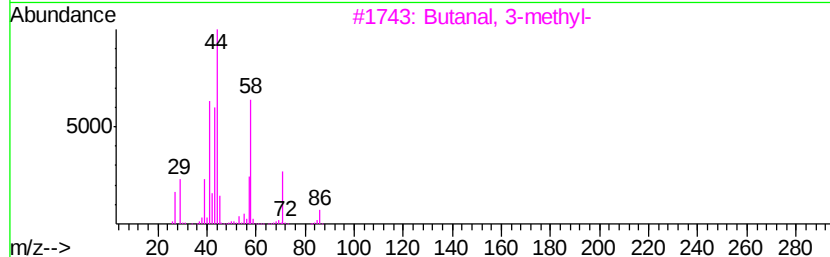
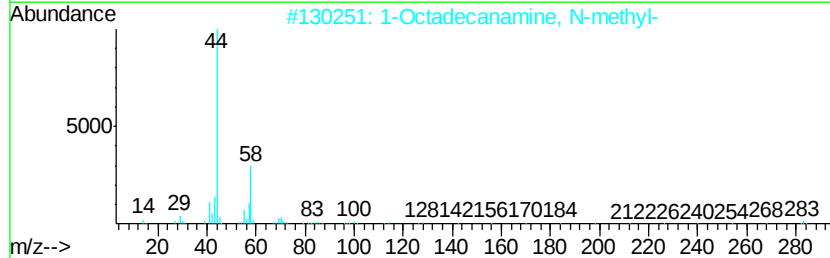
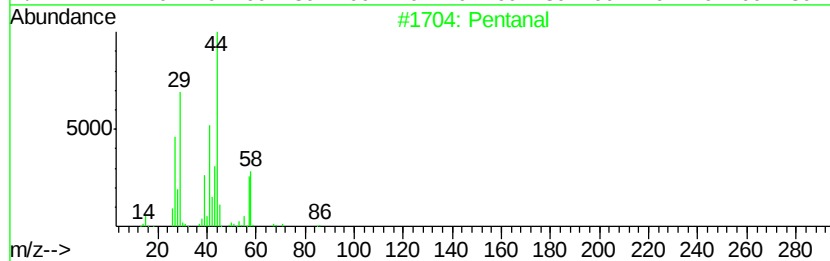
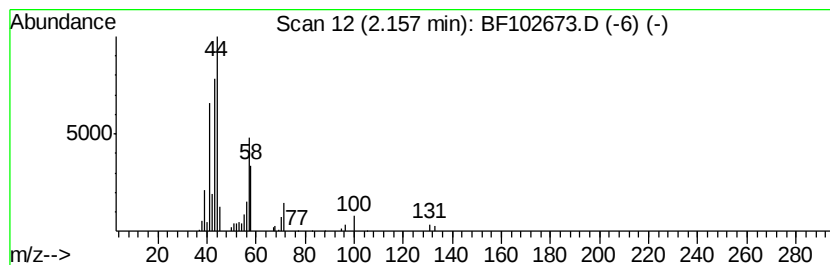
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	3.13 ng	121790	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal	86	C5H10O	000110-62-3	56
2		1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	50
3		Butanal, 3-methyl-	86	C5H10O	000590-86-3	38
4		Methylpent-4-enylamine	99	C6H13N	005831-72-1	38
5		4-Fluorohistamine	129	C5H8FN3	049872-60-8	38



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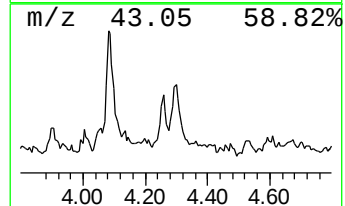
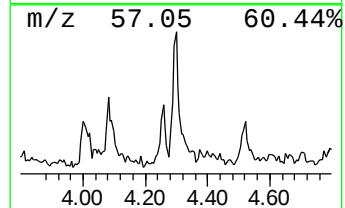
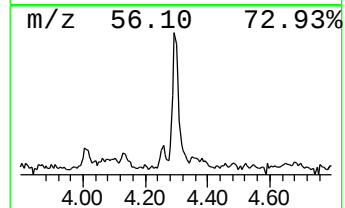
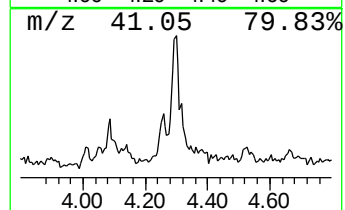
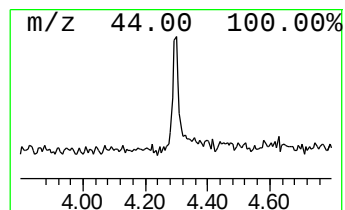
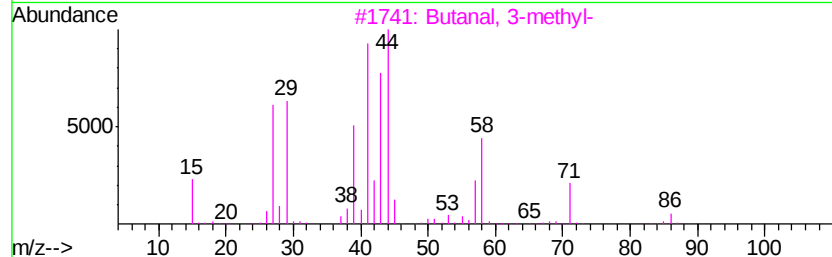
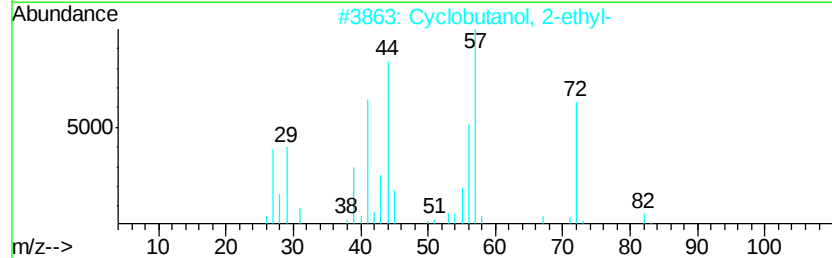
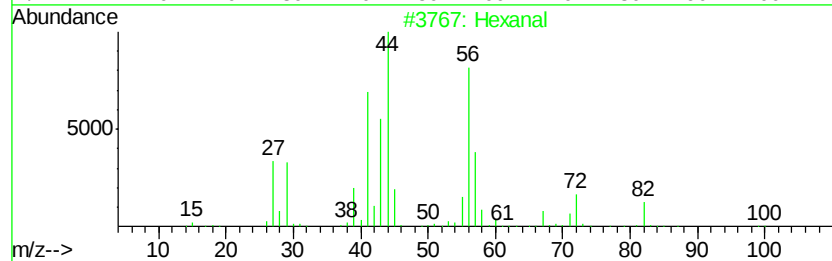
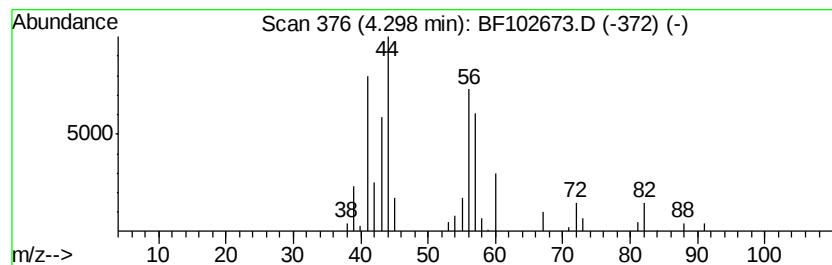
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	3.06 ng	119075	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	59
2			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	36
3			Butanal, 3-methyl-	86	C5H10O	000590-86-3	23
4			Pentanal	86	C5H10O	000110-62-3	23
5			Pentanal, 3-methyl-	100	C6H12O	015877-57-3	17



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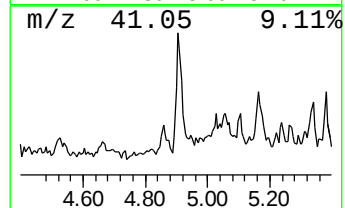
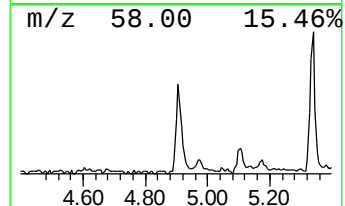
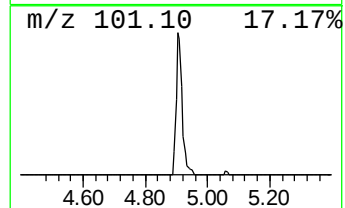
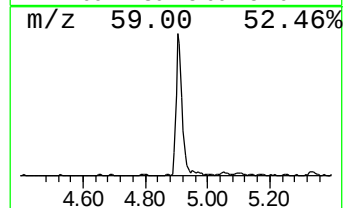
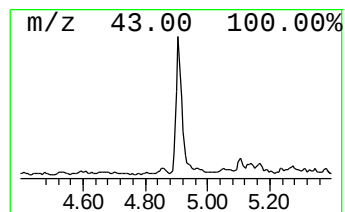
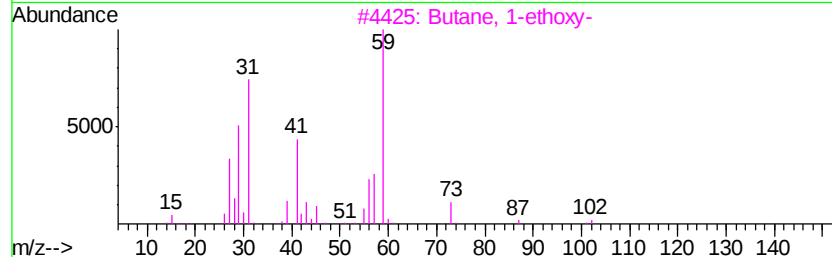
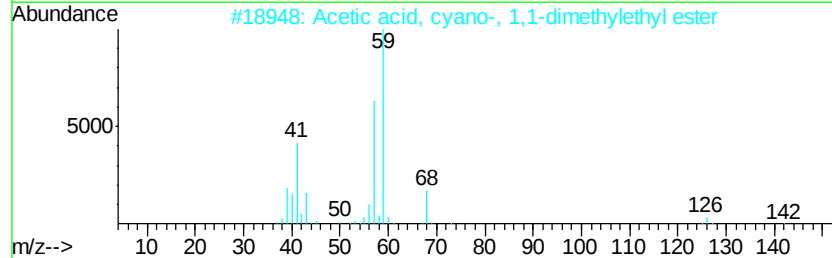
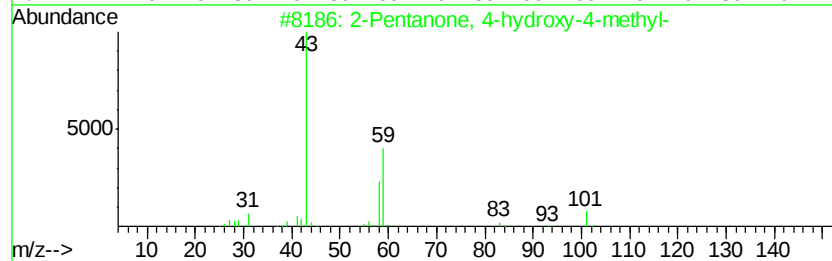
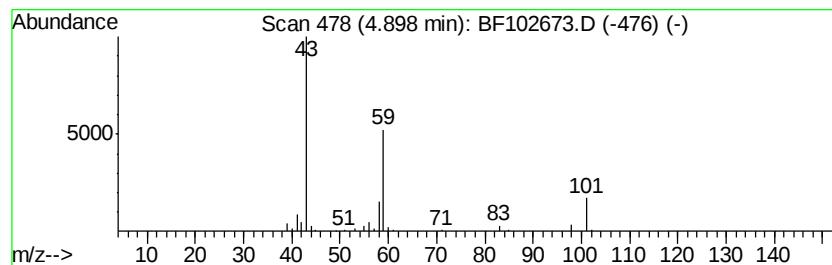
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	6.25 ng	243013	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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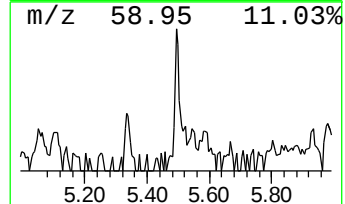
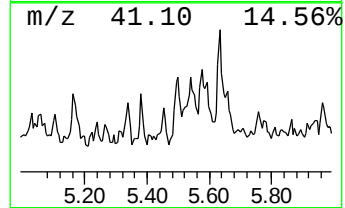
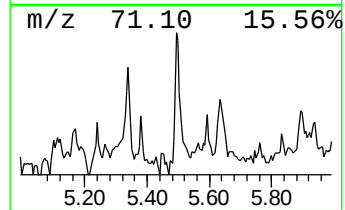
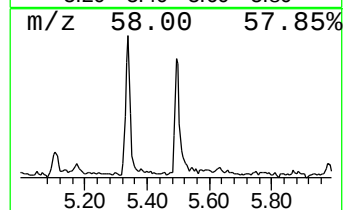
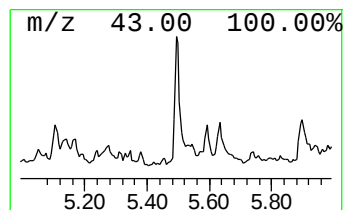
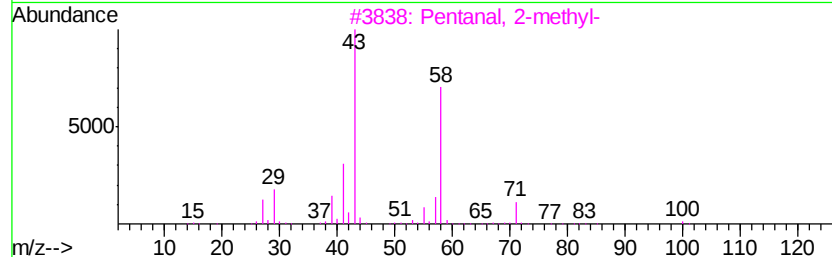
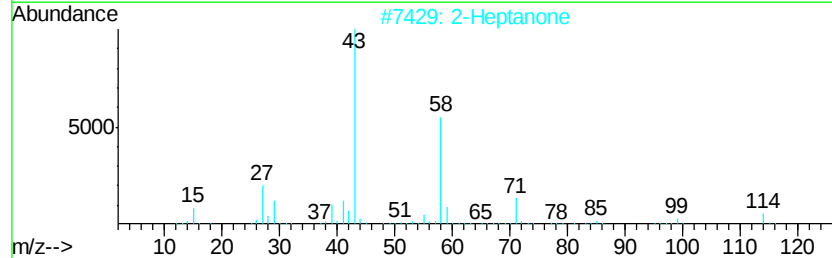
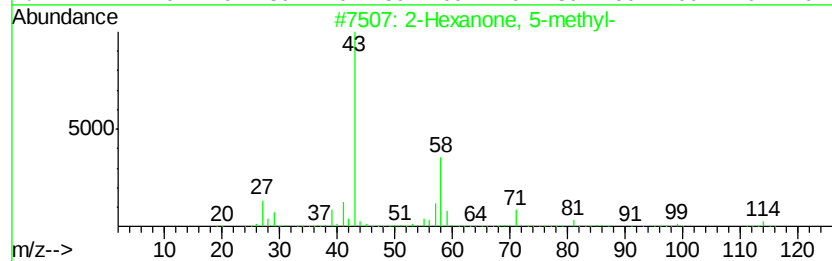
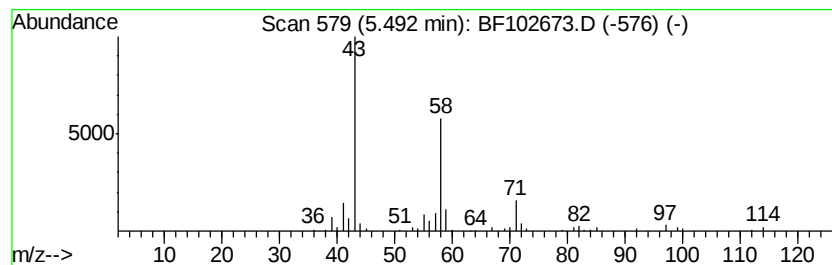
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hexanone, 5-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.49	2.14 ng	83167	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	87
2		2-Heptanone	114	C7H14O	000110-43-0	78
3		Pentanal, 2-methyl-	100	C6H12O	000123-15-9	59
4		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	50
5		2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	43



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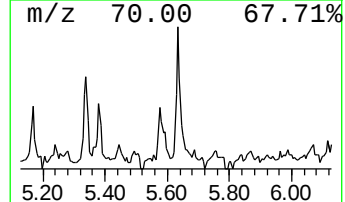
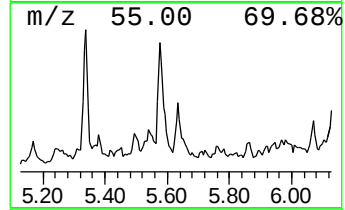
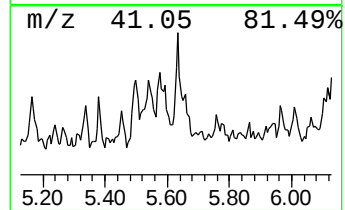
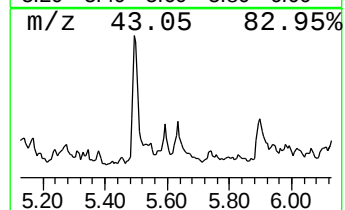
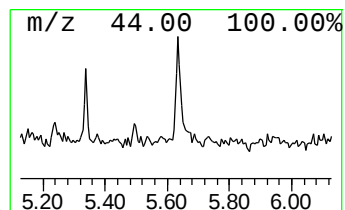
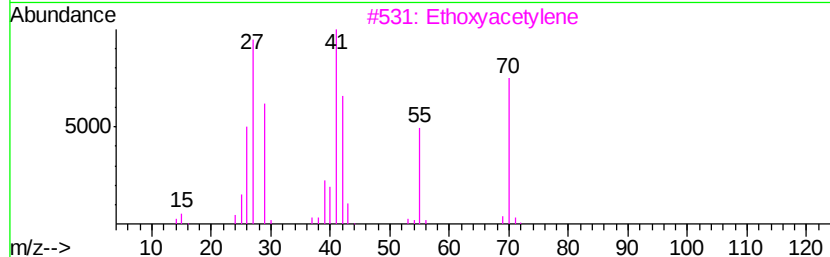
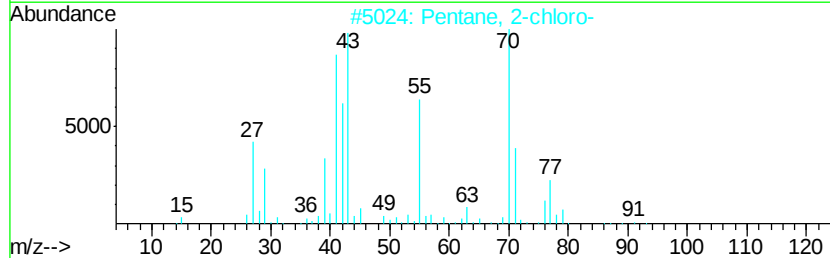
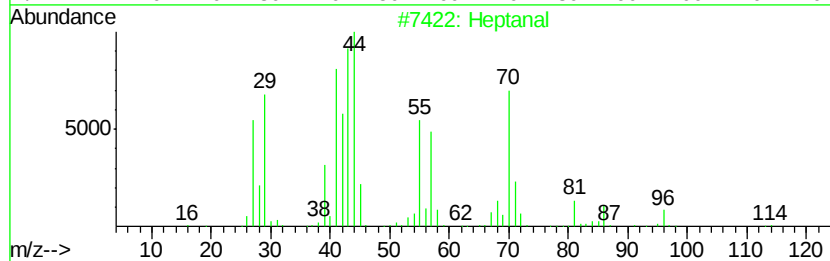
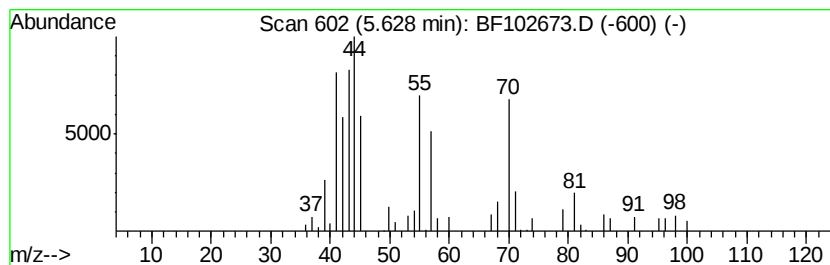
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.63	2.17 ng	84337	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptanal	114	C7H14O	000111-71-7	90
2		Pentane, 2-chloro-	106	C5H11Cl	000625-29-6	38
3		Ethoxvacetylvene	70	C4H6O	000927-80-0	35
4		2-Butene, 2-methyl-	70	C5H10	000513-35-9	35
5		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	35



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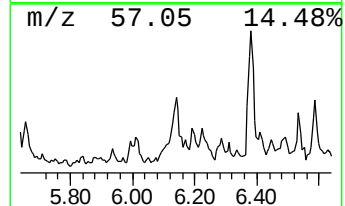
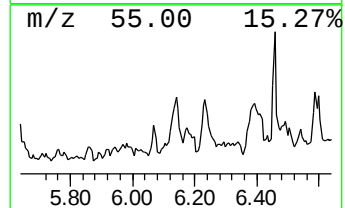
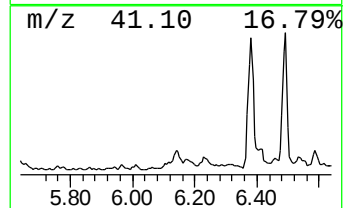
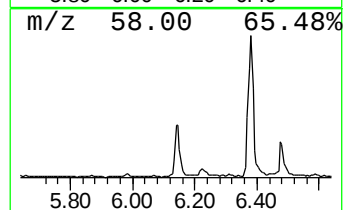
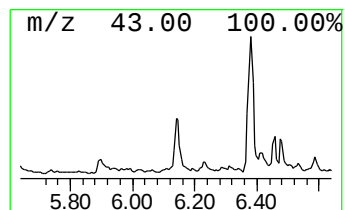
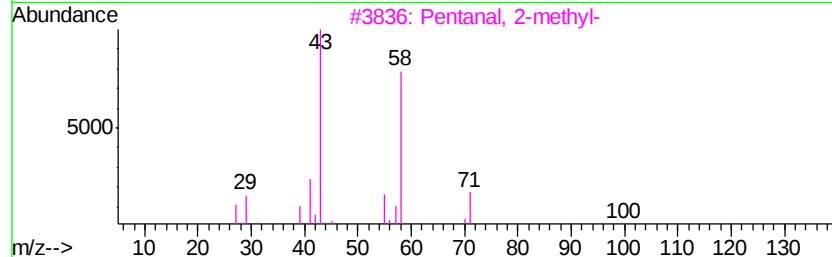
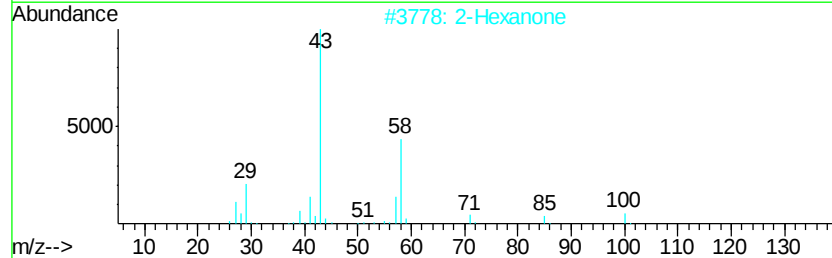
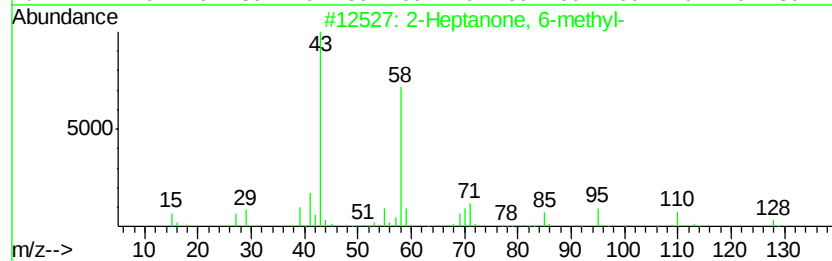
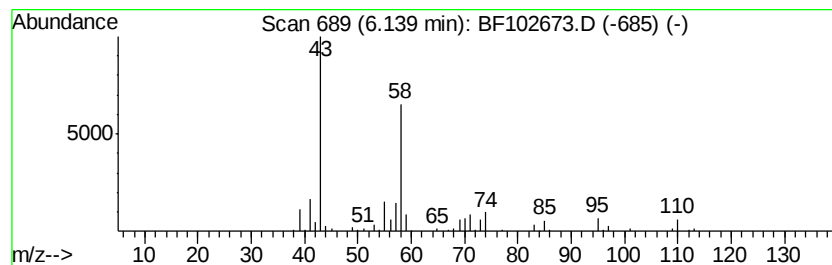
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Heptanone, 6-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	3.07 ng	119378	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	59
2			2-Hexanone	100	C6H12O	000591-78-6	53
3			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	40
4			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	33
5			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	33



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102673.D
Acq On : 31 Jan 2018 23:41
Operator : SJ/JU
Sample : J1384-02
Misc :
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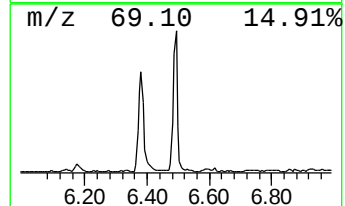
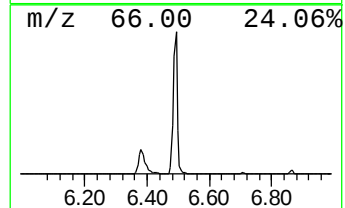
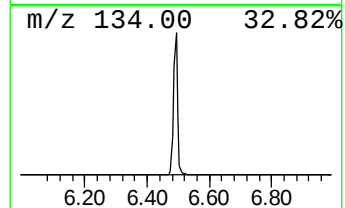
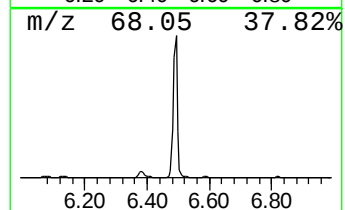
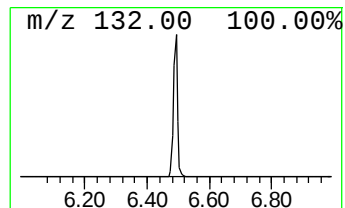
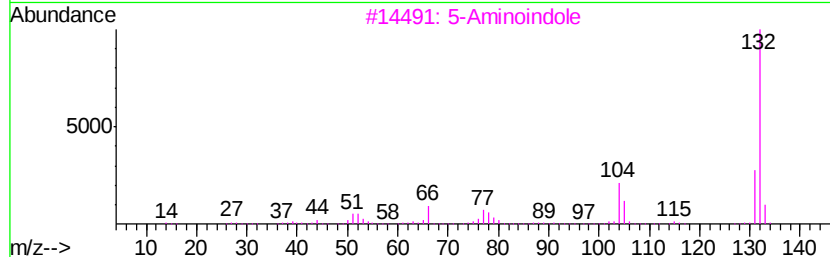
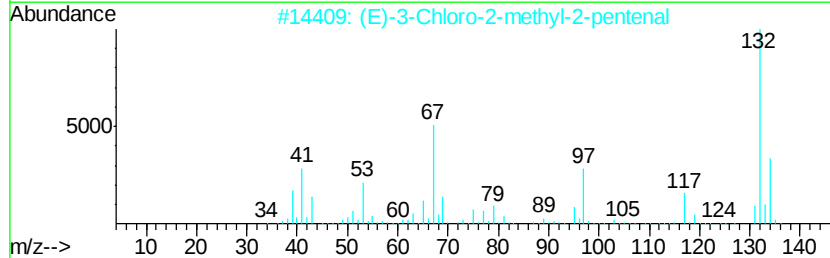
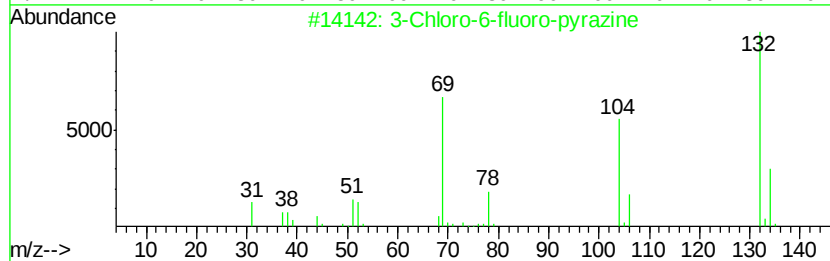
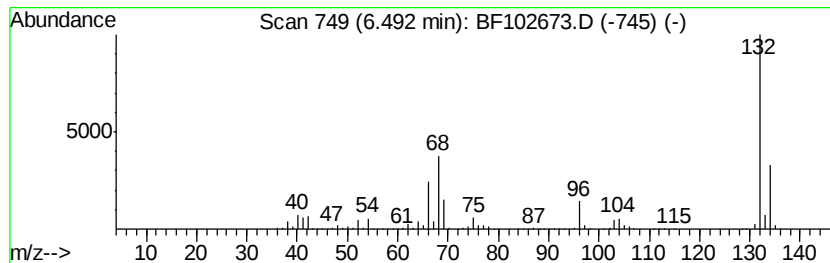
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	81.87 ng	3182630	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
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Sample : J1384-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OILY-STONES-1

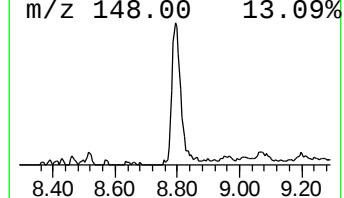
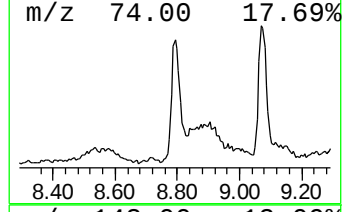
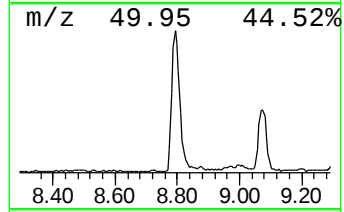
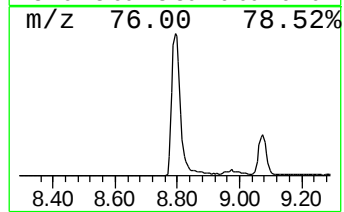
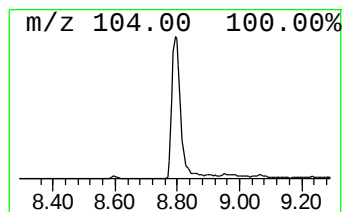
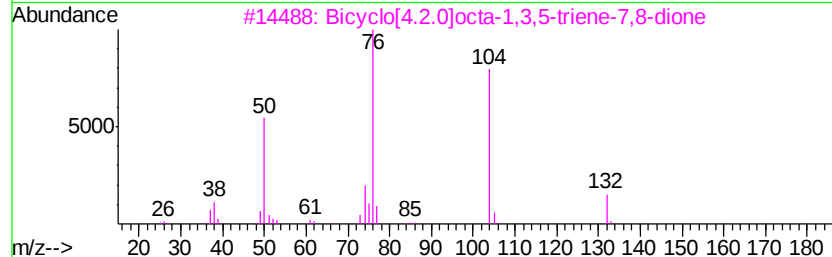
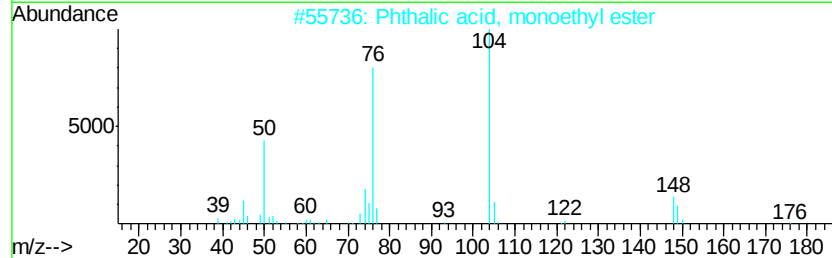
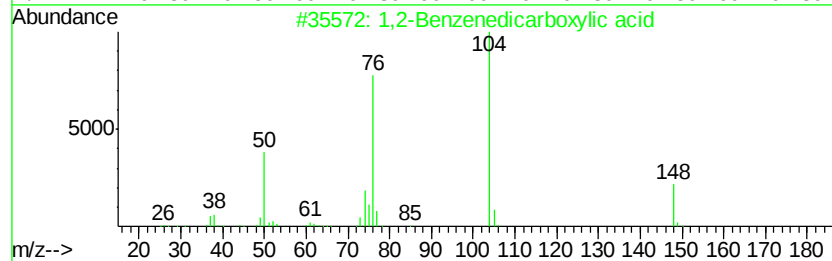
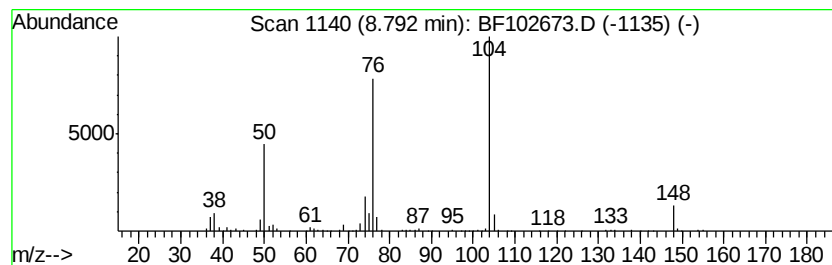
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,2-Benzenedicarboxylic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.79	17.73 ng	776494	Naphthalene-d8	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	90
2		Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	90
3		Bicyclo[4.2.0]octa-1,3,5-triene...	132	C8H4O2	006383-11-5	90
4		Phthalamic acid	165	C8H7NO3	000088-97-1	83
5		Phthalic anhydride	148	C8H4O3	000085-44-9	76



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Sample : J1384-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OILY-STONES-1

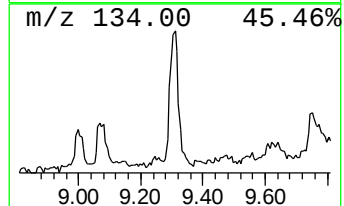
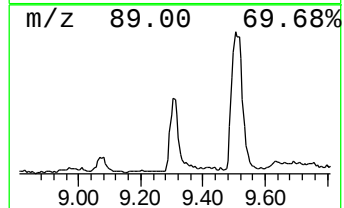
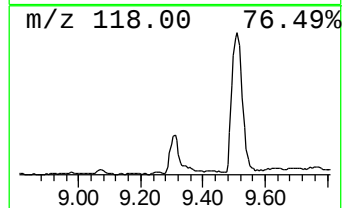
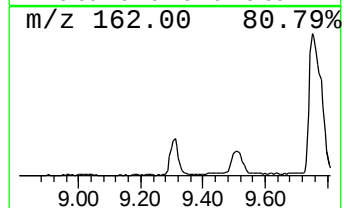
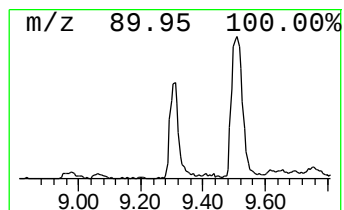
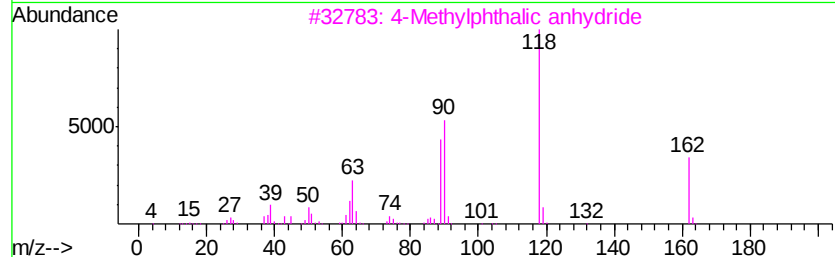
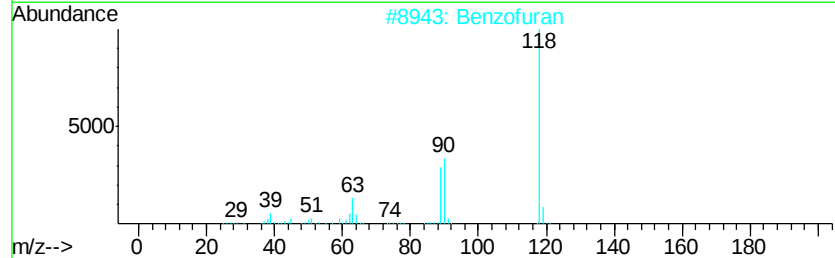
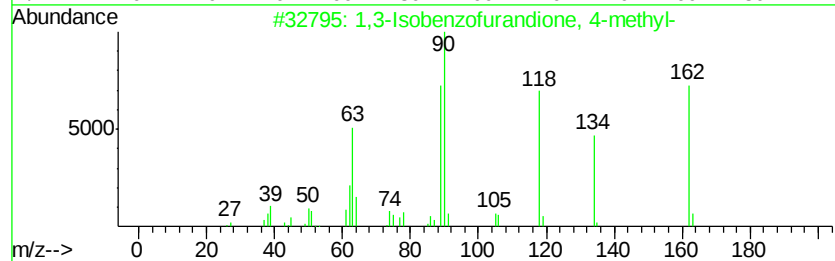
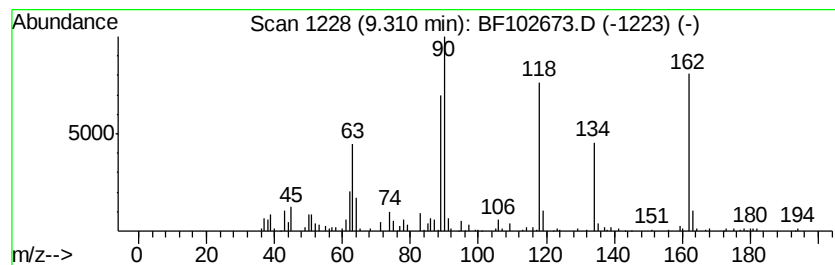
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,3-Isobenzofurandione, 4-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.31	7.62 ng	265509	Acenaphthene-d10	9.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Isobenzofurandione, 4-methyl-	162	C9H6O3	004792-30-7	95
2			Benzofuran	118	C8H6O	000271-89-6	95
3			4-Methylphthalic anhydride	162	C9H6O3	019438-61-0	87
4			3(2H)-Benzofuranone, 2,7-dimethyl-	162	C10H10O2	054365-79-6	80
5			Benzene, 1-isocyanato-4-nitro-	164	C7H4N2O3	000100-28-7	53



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 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OILY-STONES-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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
Pentanal	2.16	3.1	ng	121790	1	6.71	777525	20.0
Hexanal	4.30	3.1	ng	119075	1	6.71	777525	20.0
2-Pentanone, 4-hy...	4.90	6.3	ng	243013	1	6.71	777525	20.0
2-Hexanone, 5-met...	5.49	2.1	ng	83167	1	6.71	777525	20.0
Heptanal	5.63	2.2	ng	84337	1	6.71	777525	20.0
2-Heptanone, 6-me...	6.14	3.1	ng	119378	1	6.71	777525	20.0
unknown6.49	6.49	81.9	ng	3182630	1	6.71	777525	20.0
1,2-Benzenedicarb...	8.79	17.7	ng	776494	2	7.99	875739	20.0
1,3-Isobenzofuran...	9.31	7.6	ng	265509	3	9.75	696716	20.0