

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
 Data File : BG017055.D
 Acq On : 11 May 2015 16:16
 Operator : TP/IZ
 Sample : G2176-20
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PS-26(3-5)

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_G\METHODS\8270-BG050515.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	2.720	3	5	21	rVB	5555074	6506403	100.00%	22.102%
2	2.855	24	28	37	rVB	163946	284127	4.37%	0.965%
3	2.937	37	42	46	rVB	143557	177080	2.72%	0.602%
4	4.864	363	370	378	rBV	79075	117638	1.81%	0.400%
5	5.346	445	452	461	rBV	1275730	1798373	27.64%	6.109%
6	6.950	717	725	732	rBV	1308981	2036446	31.30%	6.918%
7	7.291	775	783	792	rBV	1244952	1949162	29.96%	6.621%
8	7.749	854	861	870	rBV	216202	349769	5.38%	1.188%
9	8.072	909	916	923	rBV	866142	1356758	20.85%	4.609%
10	8.912	1052	1059	1066	rBV	751447	1223838	18.81%	4.157%
11	10.552	1330	1338	1345	rVB	282523	473070	7.27%	1.607%
12	13.025	1750	1759	1765	rBV	1734117	2542022	39.07%	8.635%
13	13.859	1896	1901	1906	rBV	97867	133916	2.06%	0.455%
14	14.406	1984	1994	2002	rVB2	434584	658000	10.11%	2.235%
15	15.898	2241	2248	2254	rBV	1746269	2409152	37.03%	8.184%
16	17.150	2454	2461	2467	rBV2	640324	843384	12.96%	2.865%
17	18.049	2610	2614	2623	rBV	187364	243206	3.74%	0.826%
18	19.330	2828	2832	2839	rBV2	71353	102214	1.57%	0.347%
19	19.782	2903	2909	2914	rBV	3468572	4149027	63.77%	14.094%
20	21.039	3120	3123	3130	rBV2	102779	142433	2.19%	0.484%
21	21.333	3167	3173	3178	rBV	808457	1004744	15.44%	3.413%
22	23.619	3555	3562	3569	rVB	494381	936656	14.40%	3.182%

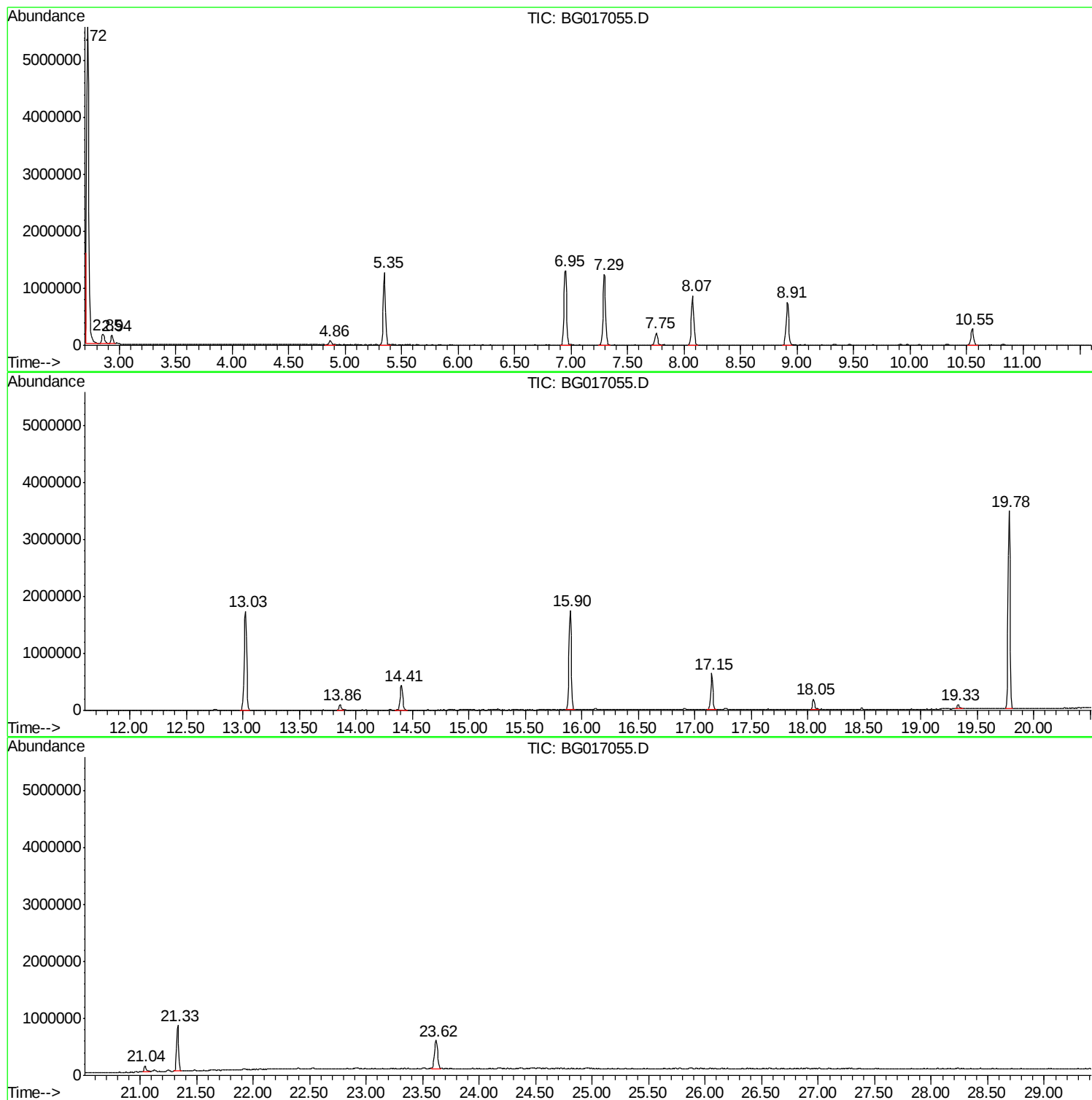
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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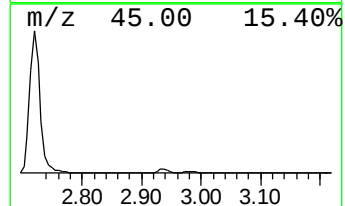
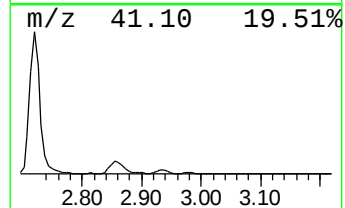
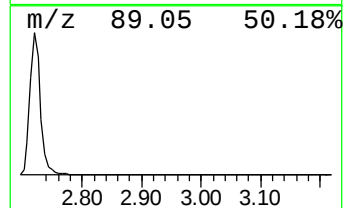
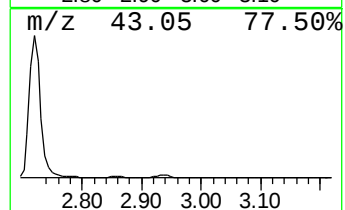
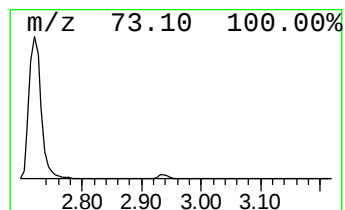
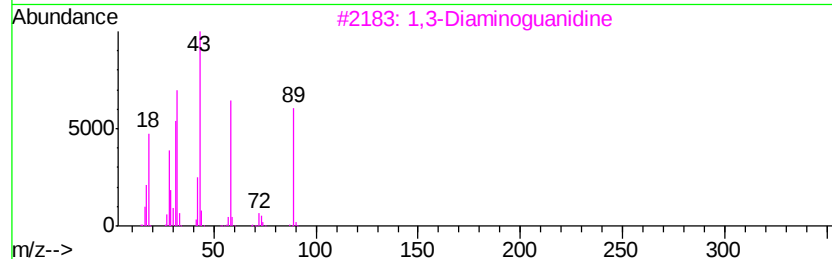
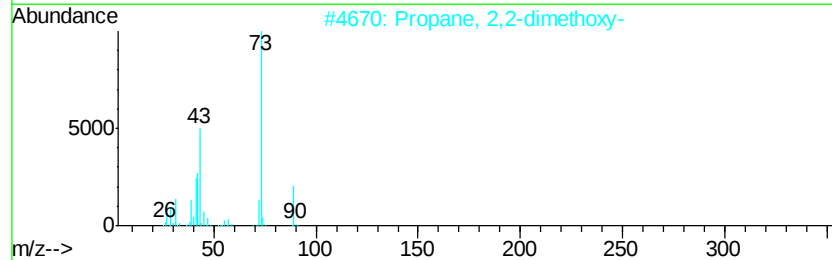
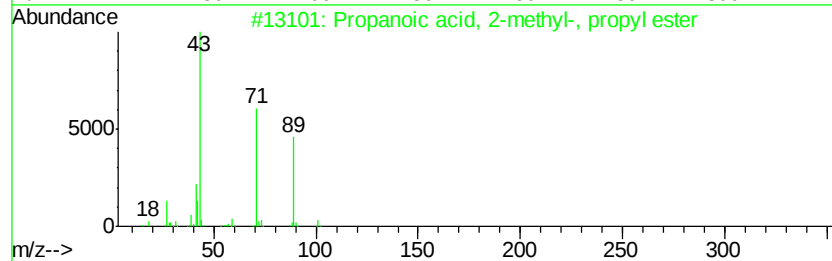
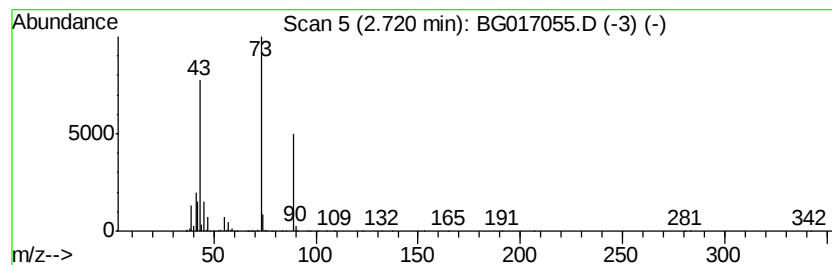
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanoic acid, 2-methyl-, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.72	372.04 ng	6506400	1,4-Dichlorobenzene-d4	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	50
2		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	42
3		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	40
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	12



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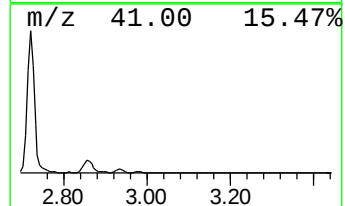
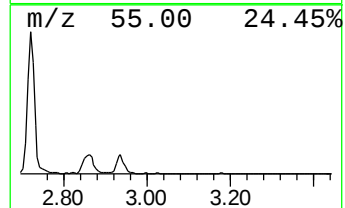
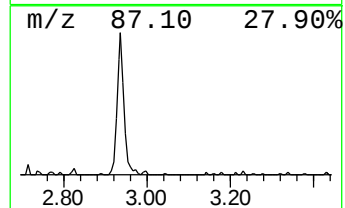
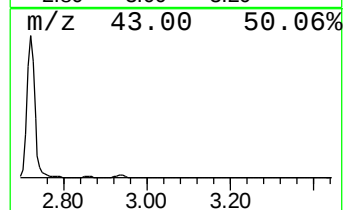
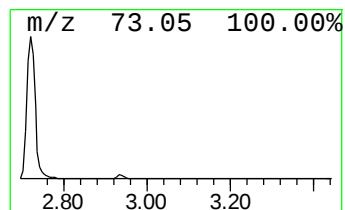
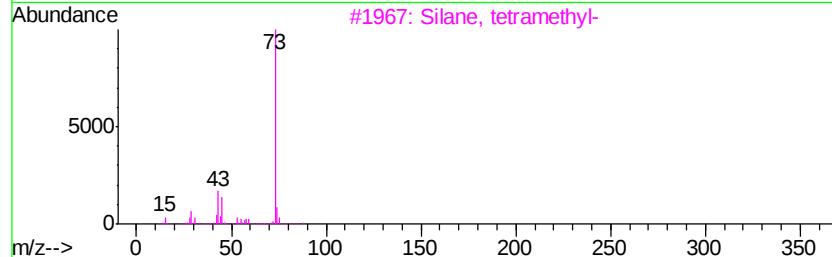
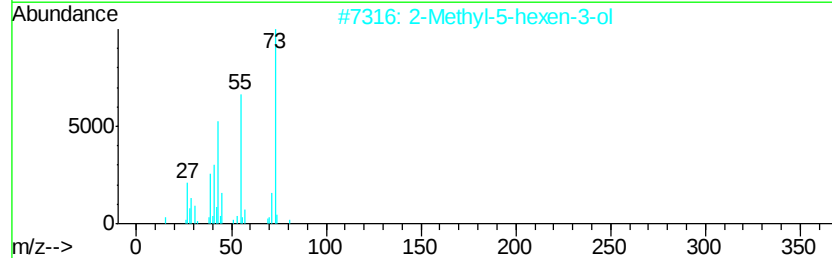
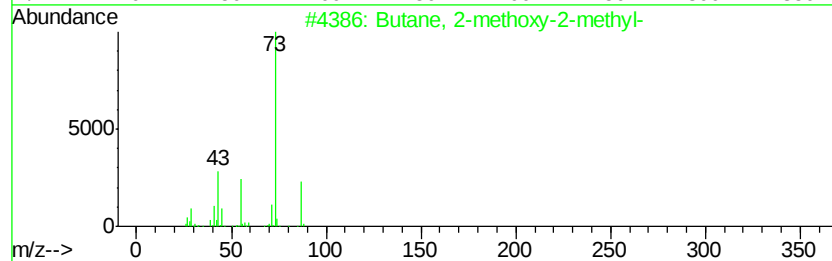
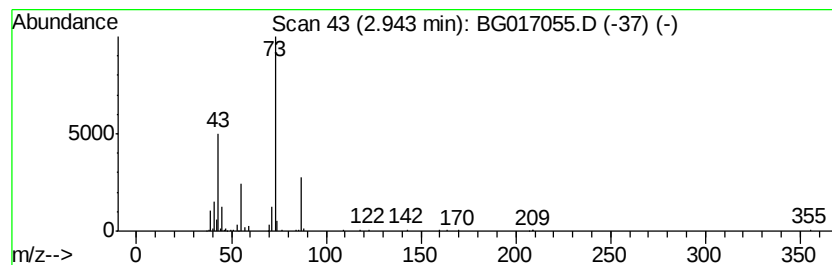
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.94	10.13 ng	177080	1,4-Dichlorobenzene-d4	7.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	22
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	17
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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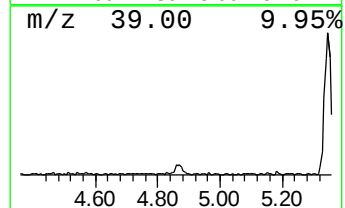
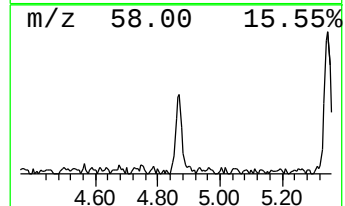
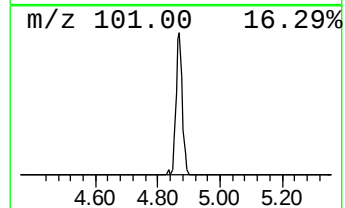
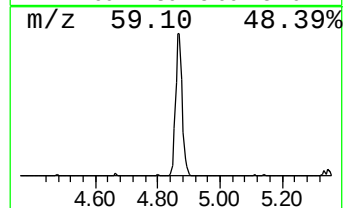
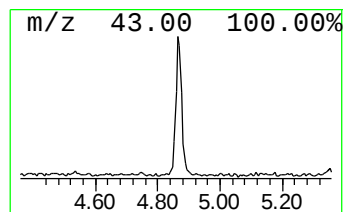
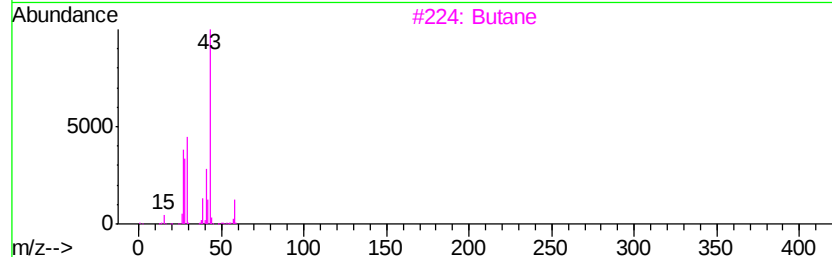
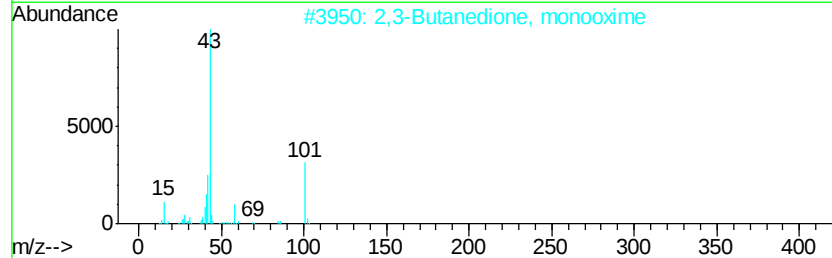
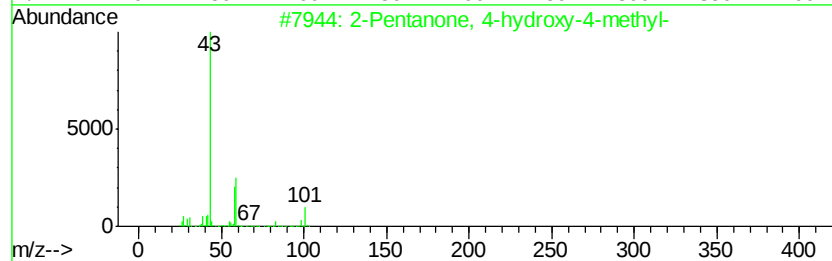
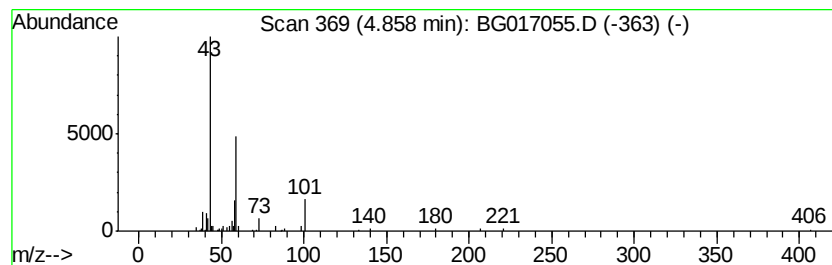
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	6.73 ng	117638	1,4-Dichlorobenzene-d4	7.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Butane	58	C4H10	000106-97-8	9
4			Heptanoic acid, 2,2-dimethyl-6-o...	186	C10H18O3	000926-27-2	9
5			Diacetamide	101	C4H7NO2	000625-77-4	9



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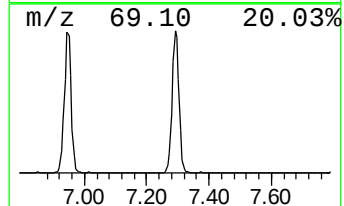
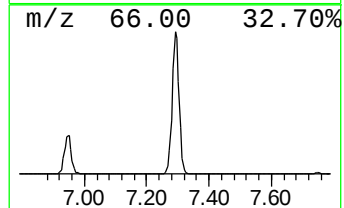
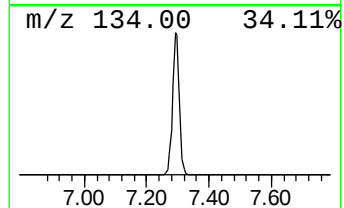
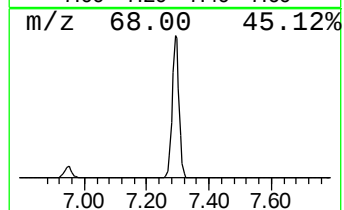
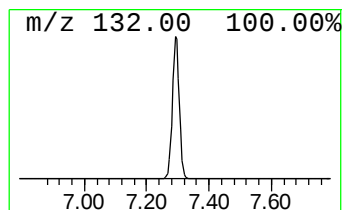
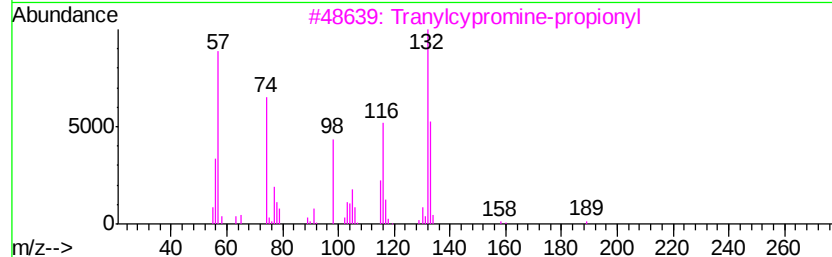
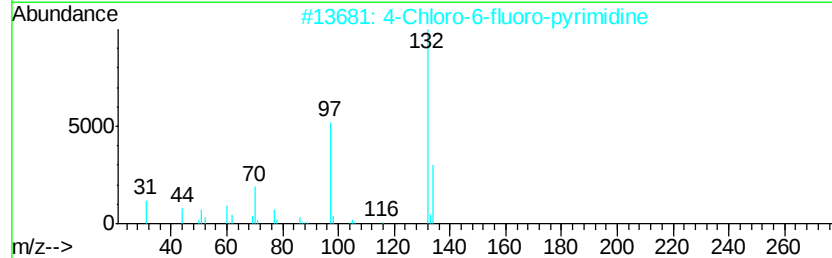
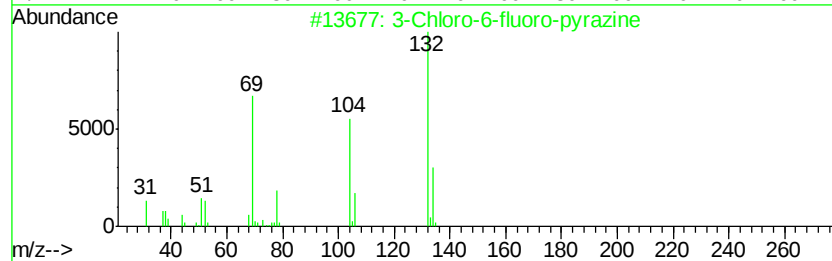
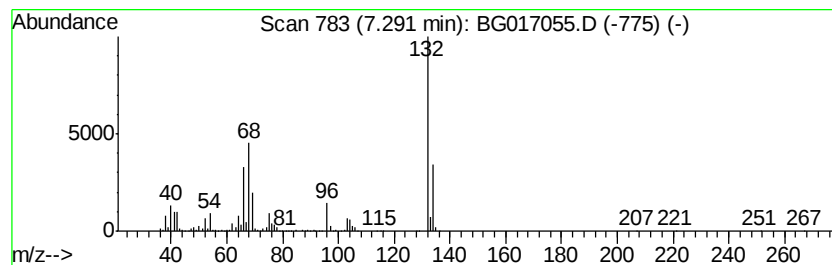
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown7.29 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	111.45 ng	1949160	1,4-Dichlorobenzene-d4	7.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	12



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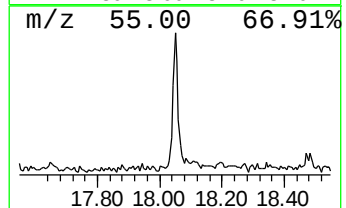
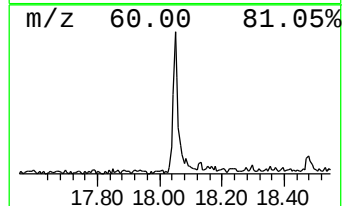
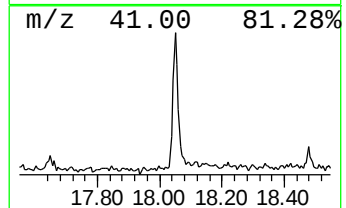
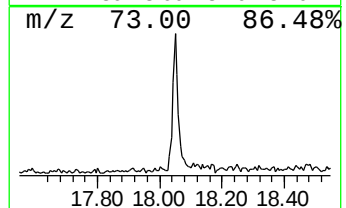
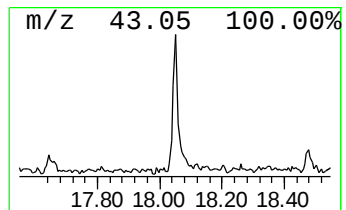
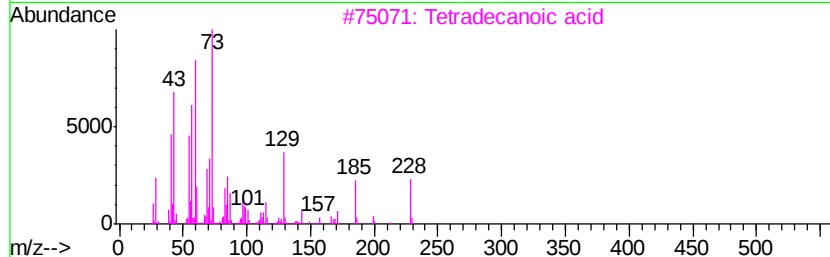
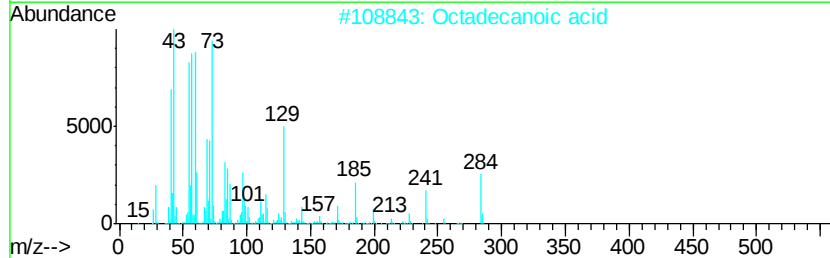
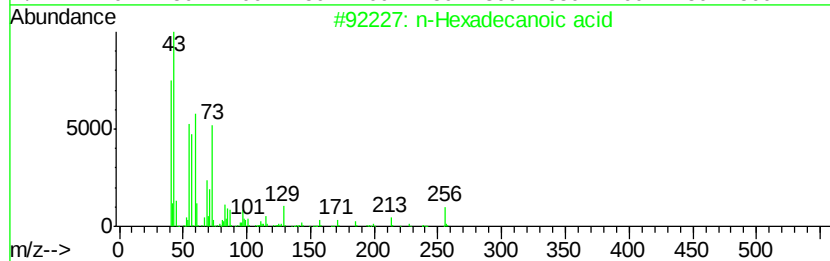
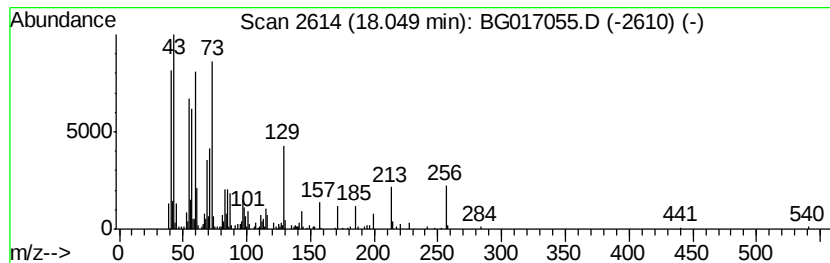
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	5.77 ng	243206	Phenanthrene-d10	17.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Octadecanoic acid	284	C18H36O2	000057-11-4	92
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	59
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	46



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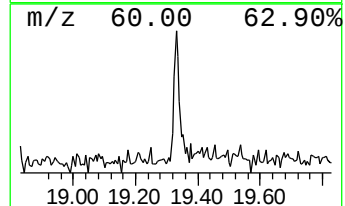
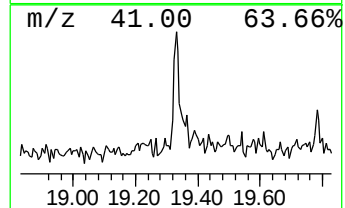
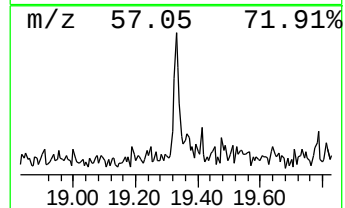
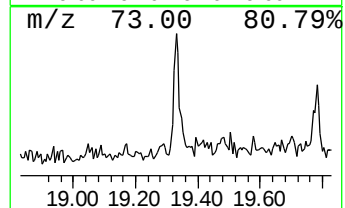
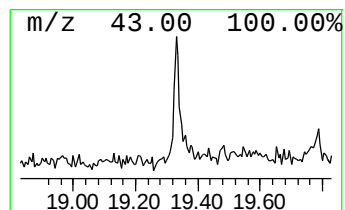
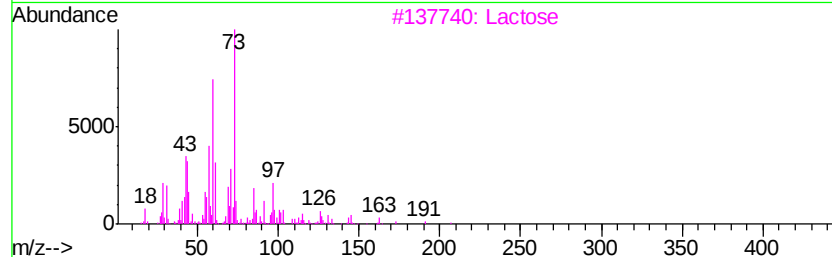
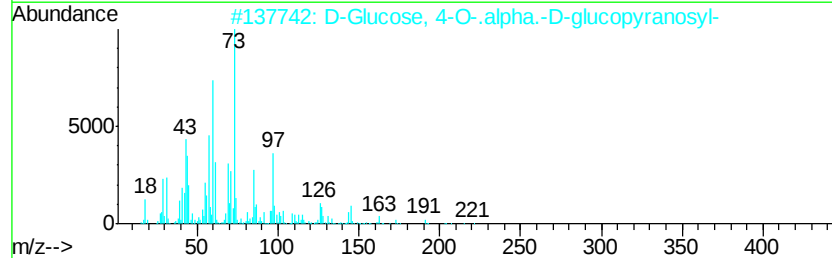
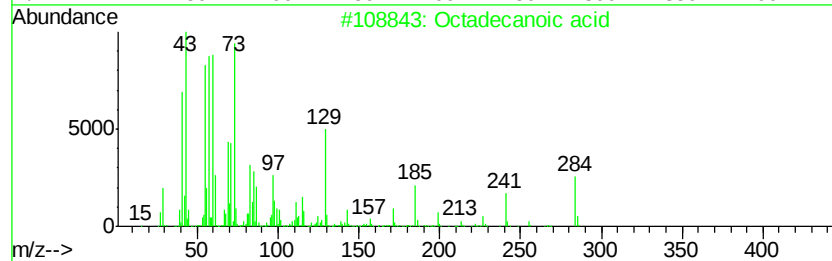
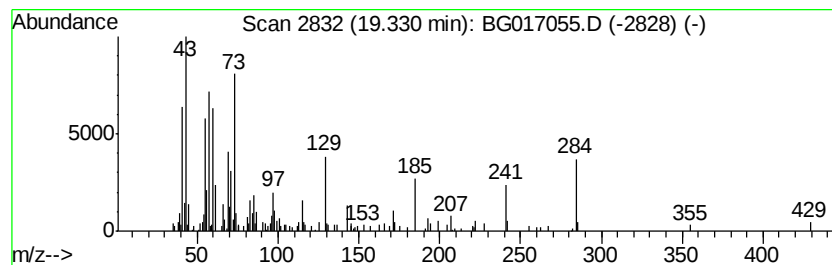
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	2.03 ng	102214	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2		D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	38
3		Lactose	342	C12H22O11	000063-42-3	38
4		n-Decanoic acid	172	C10H20O2	000334-48-5	35
5		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35



Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017055.D
Acq On : 11 May 2015 16:16
Operator : TP/IZ
Sample : G2176-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PS-26(3-5)

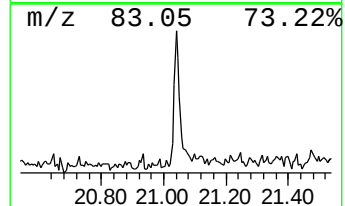
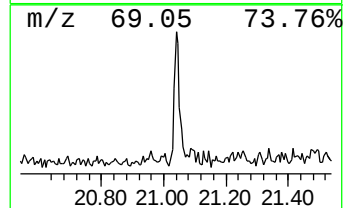
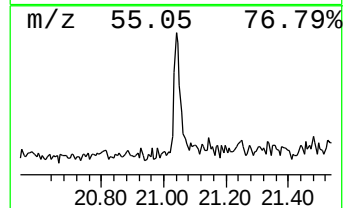
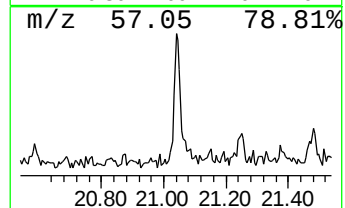
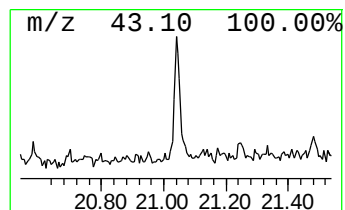
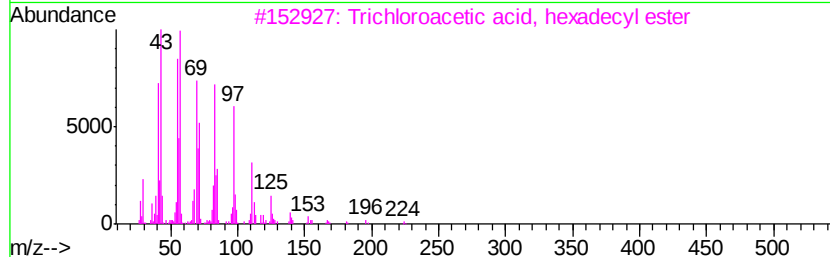
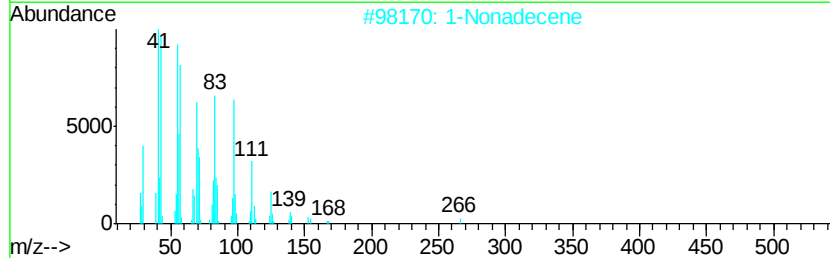
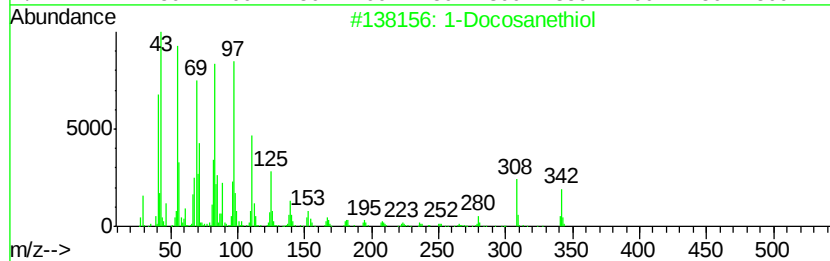
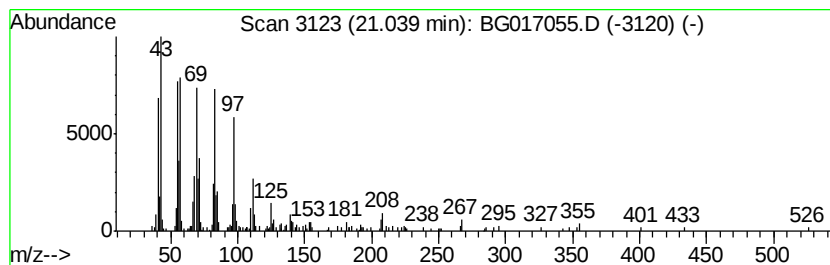
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Docosanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	2.84 ng	142433	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosanethiol	342	C22H46S	007773-83-3	95
2		1-Nonadecene	266	C19H38	018435-45-5	95
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	93
5		Cyclotetracosane	336	C24H48	000297-03-0	90



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051115\
Data File : BG017055.D
Acq On : 11 May 2015 16:16
Operator : TP/IZ
Sample : G2176-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PS-26(3-5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid, 2...	2.72	372.0	ng	6506400	1	7.75	349769	20.0
Butane, 2-methoxy...	2.94	10.1	ng	177080	1	7.75	349769	20.0
2-Pentanone, 4-hy...	4.86	6.7	ng	117638	1	7.75	349769	20.0
unknown7.29	7.29	111.5	ng	1949160	1	7.75	349769	20.0
n-Hexadecanoic acid	18.05	5.8	ng	243206	4	17.15	843384	20.0
Octadecanoic acid	19.33	2.0	ng	102214	5	21.33	1004740	20.0
1-Docosanethiol	21.04	2.8	ng	142433	5	21.33	1004740	20.0