

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010719\
 Data File : BG038977.D
 Acq On : 7 Jan 2019 21:48
 Operator : JU/SJ
 Sample : K1012-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EO-02-010419-A

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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	3.199	13	19	24	rVB	44529	80237	3.71%	0.632%
2	3.487	64	68	77	rVB	42448	58128	2.68%	0.458%
3	3.916	136	141	148	rVB2	13929	22375	1.03%	0.176%
4	4.527	240	245	251	rBV	26817	42387	1.96%	0.334%
5	4.638	257	264	269	rBV	22948	36192	1.67%	0.285%
6	5.085	335	340	344	rBV	15437	25267	1.17%	0.199%
7	5.138	344	349	365	rVB	62406	107349	4.96%	0.846%
8	5.608	421	429	443	rVB	406235	683042	31.55%	5.380%
9	7.212	694	702	712	rBV	405422	703310	32.48%	5.539%
10	7.576	757	764	773	rBV	449983	808185	37.33%	6.365%
11	8.046	834	844	853	rVB	99471	169762	7.84%	1.337%
12	8.369	889	899	909	rBV	360302	634115	29.29%	4.994%
13	9.221	1036	1044	1056	rBV	281239	533163	24.62%	4.199%
14	10.860	1315	1323	1330	rBV	122029	225974	10.44%	1.780%
15	13.305	1727	1739	1746	rBV	824861	1348216	62.27%	10.619%
16	14.685	1967	1974	1984	rVB2	199281	334654	15.46%	2.636%
17	16.178	2221	2228	2240	rBV2	748380	1160197	53.58%	9.138%
18	16.801	2328	2334	2343	rBV2	71647	117759	5.44%	0.928%
19	17.429	2435	2441	2451	rBV2	264991	420445	19.42%	3.312%
20	18.311	2582	2591	2605	rBV	1161957	2165178	100.00%	17.054%
21	19.556	2799	2803	2812	rBV2	52126	82265	3.80%	0.648%
22	20.032	2878	2884	2893	rVB	1530714	2063773	95.32%	16.255%
23	21.712	3163	3170	3177	rVB	268753	454553	20.99%	3.580%
24	25.003	3721	3730	3743	rVB2	140153	419806	19.39%	3.307%

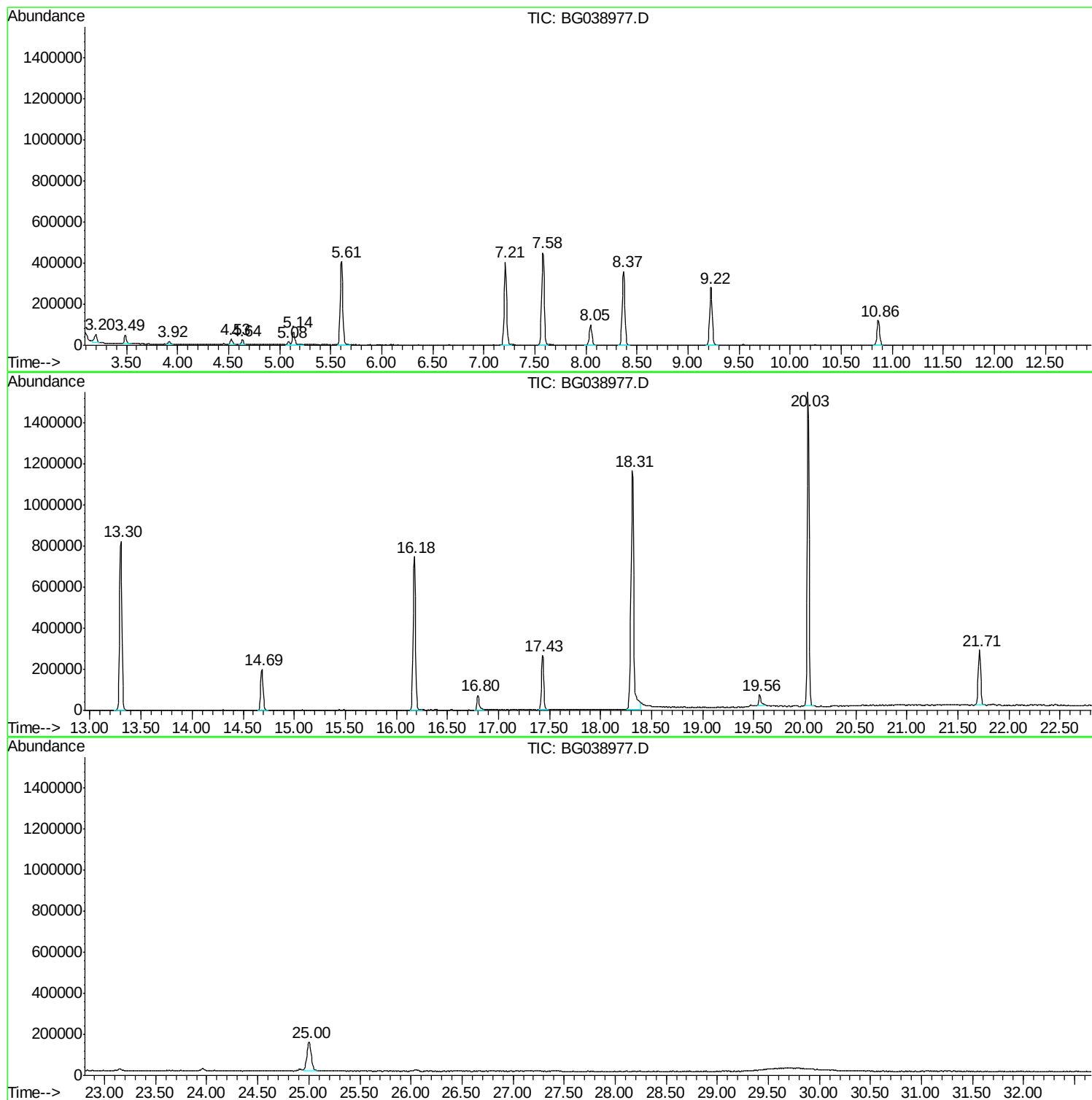
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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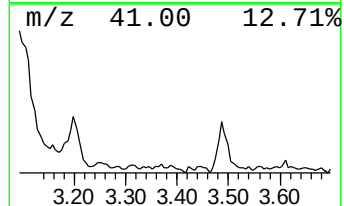
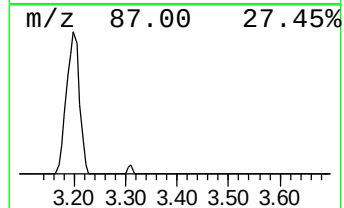
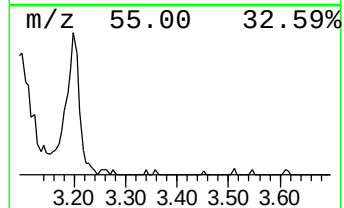
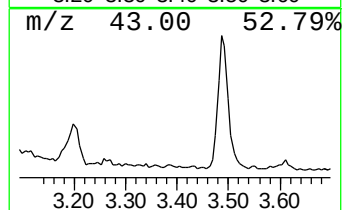
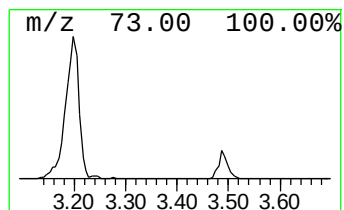
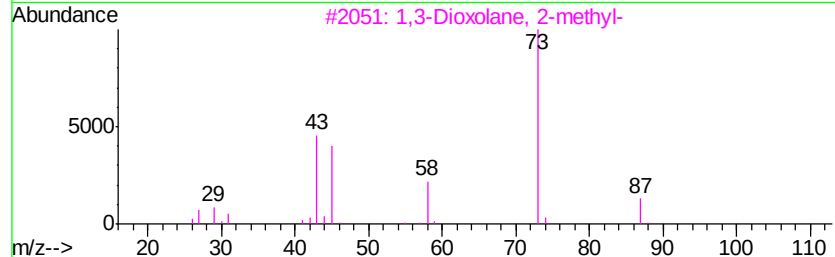
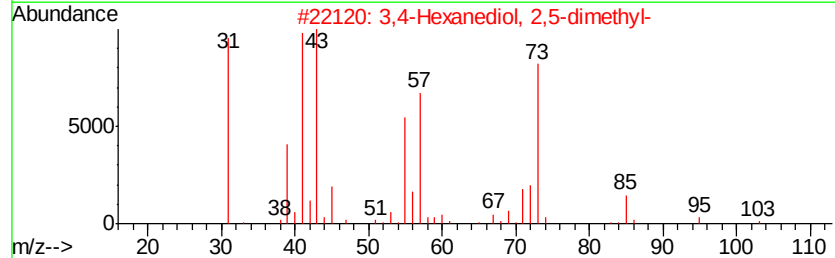
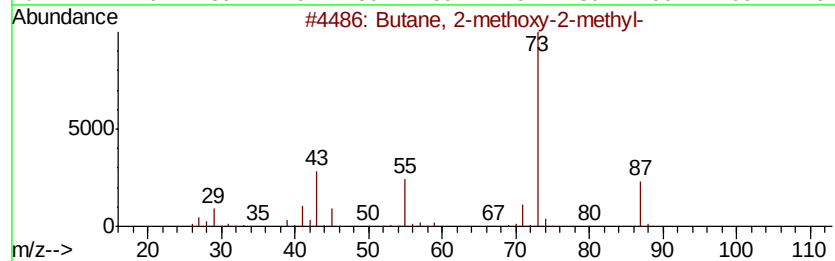
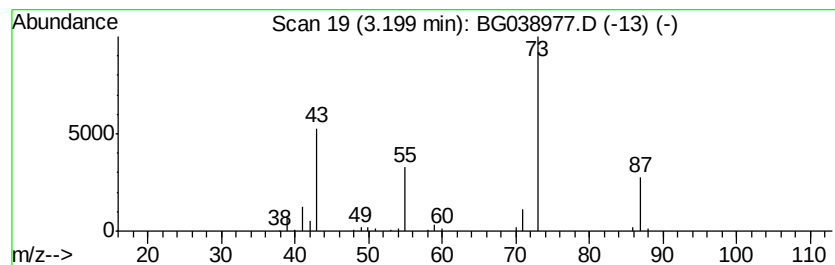
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.20	9.45 ng	80237	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2		3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	9
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	7
5		Pentane, 2-methyl-	86	C6H14	000107-83-5	7



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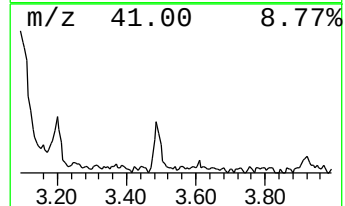
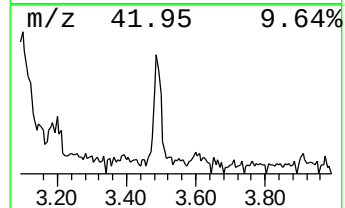
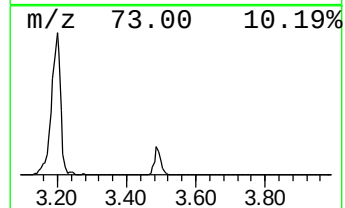
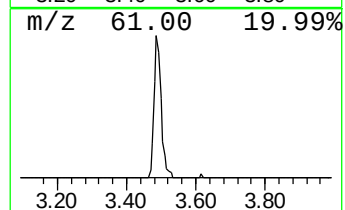
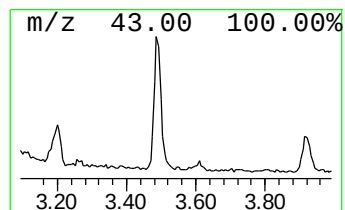
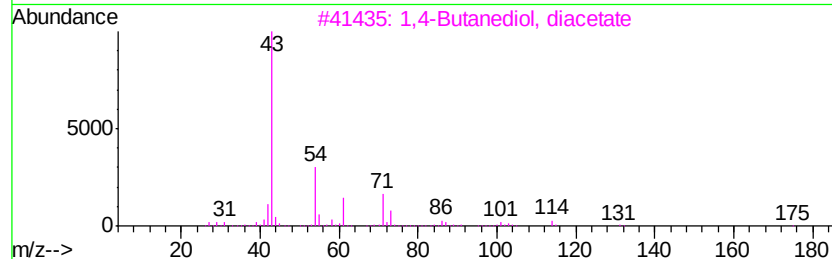
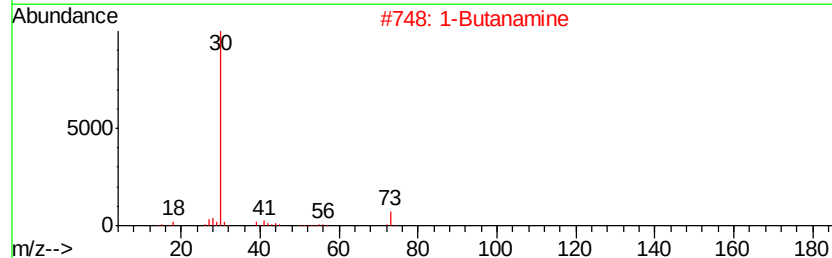
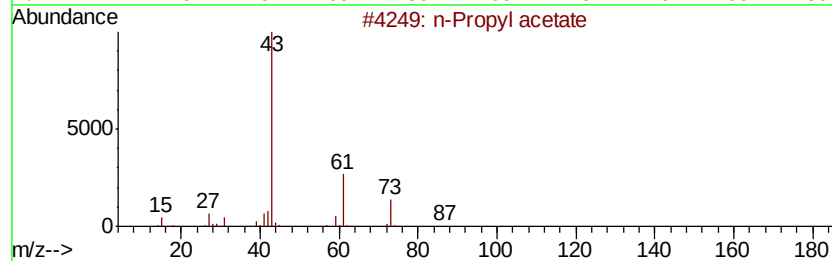
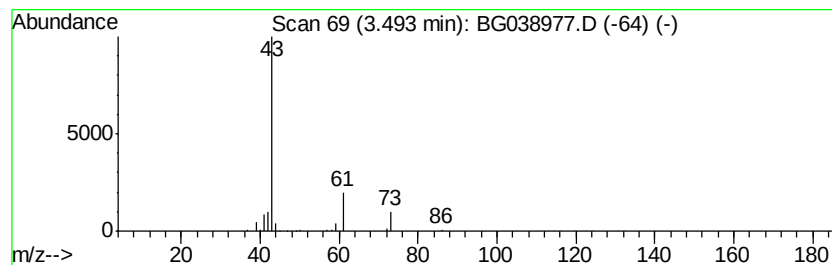
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.49	6.85 ng	58128	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2		1-Butanamine	73	C4H11N	000109-73-9	4
3		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4
4		Hydrogen azide	43	HN3	007782-79-8	4
5		Isobutylamine	73	C4H11N	000078-81-9	3



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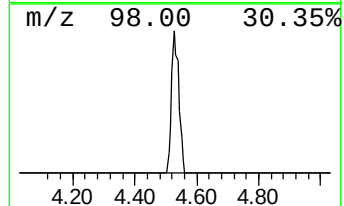
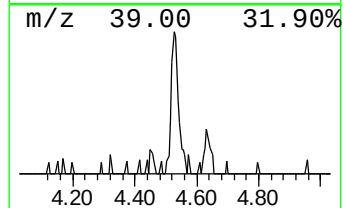
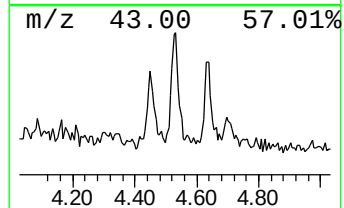
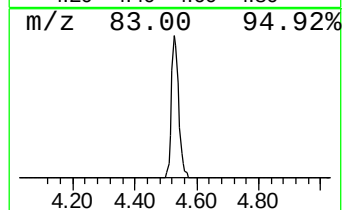
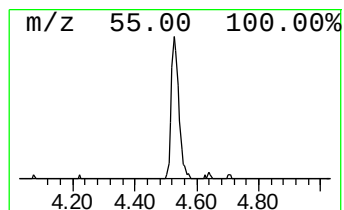
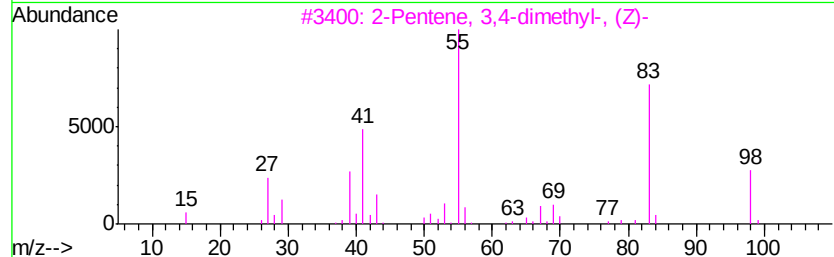
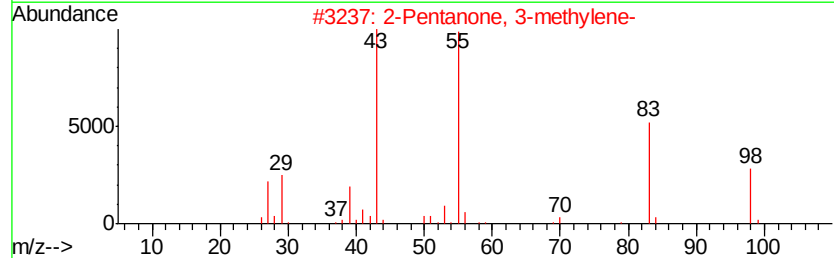
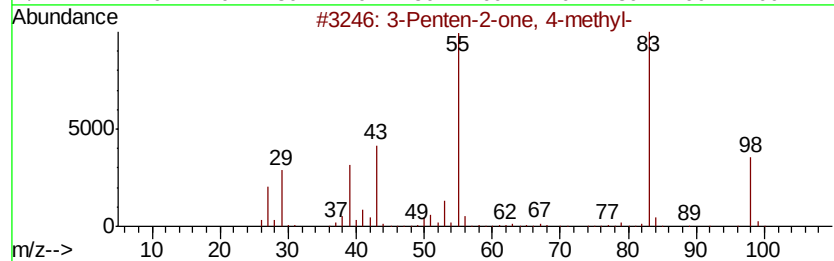
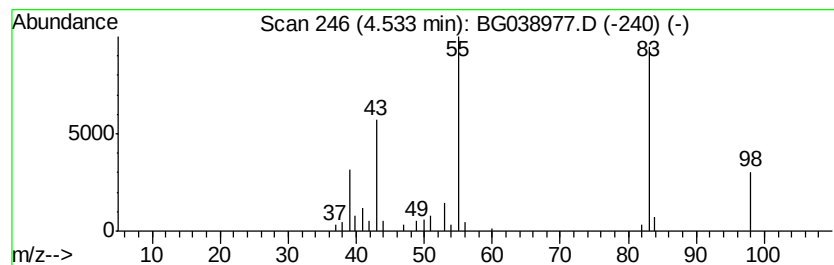
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TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	4.99 ng	42387	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	83
2		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	64
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	64
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	59
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	59



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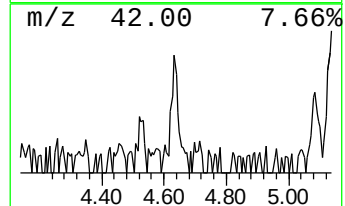
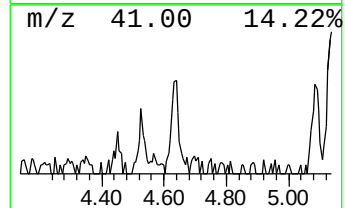
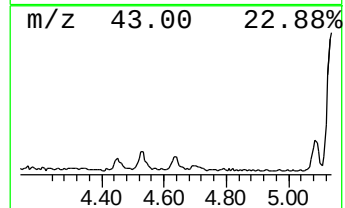
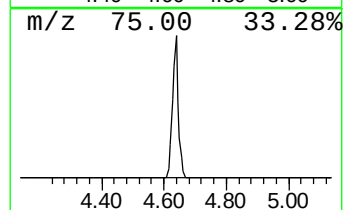
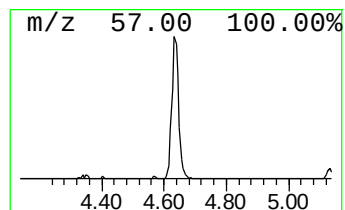
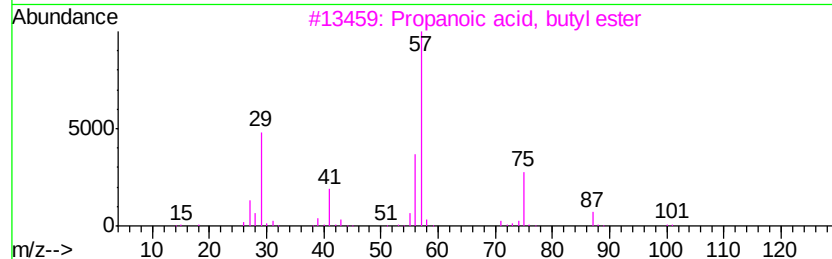
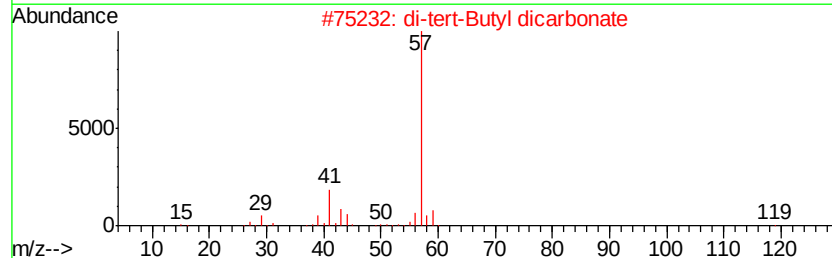
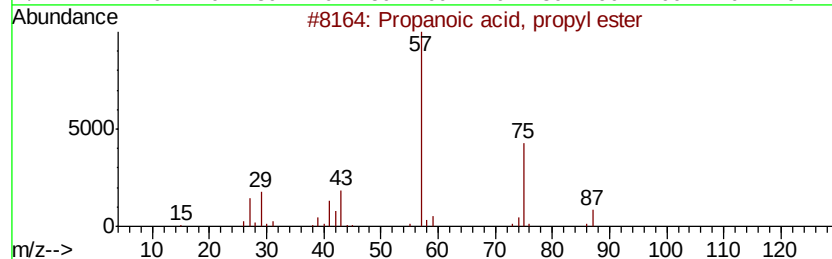
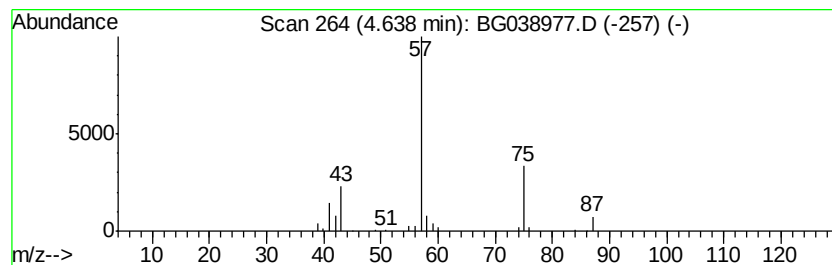
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Peak Number 5 Propanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	4.26 ng	36192	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
2		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
3		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9
4		Azetidine	57	C3H7N	000503-29-7	5
5		Isobutyl ether	130	C8H18O	000628-55-7	4



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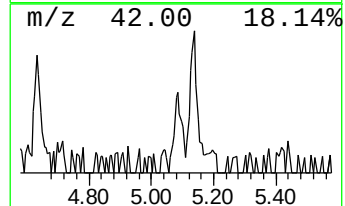
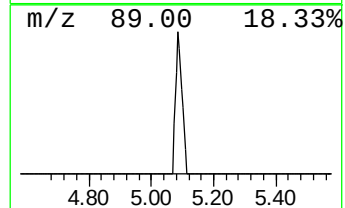
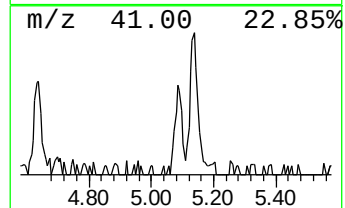
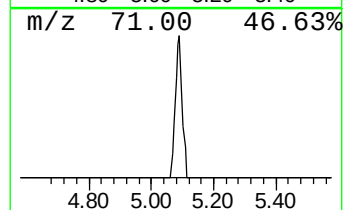
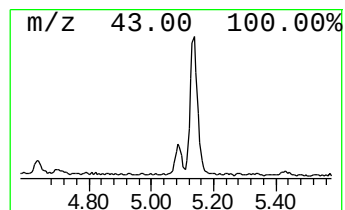
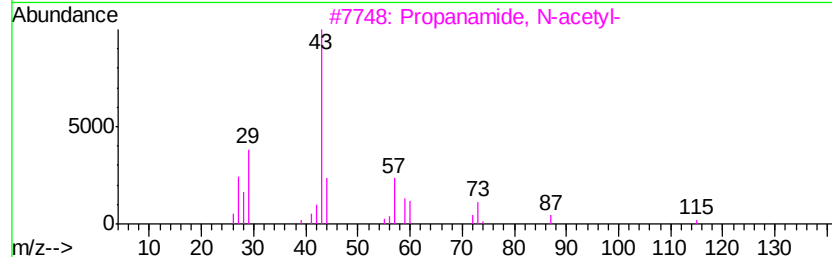
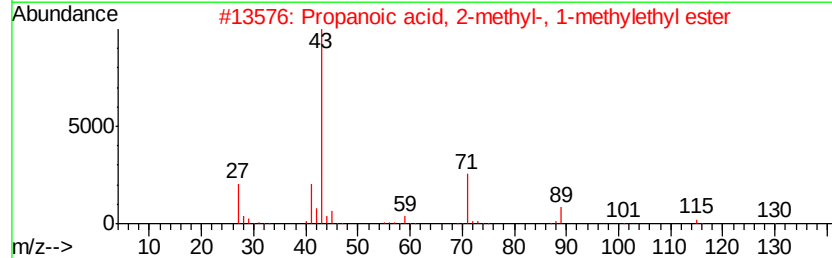
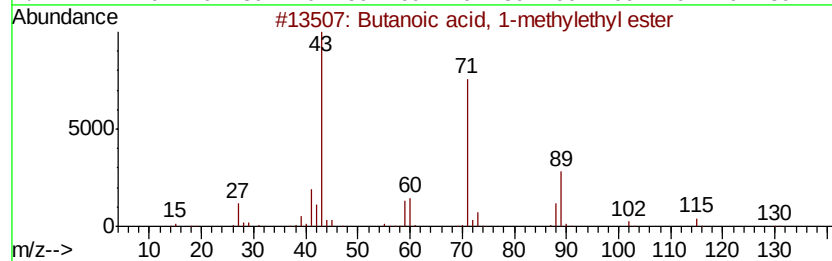
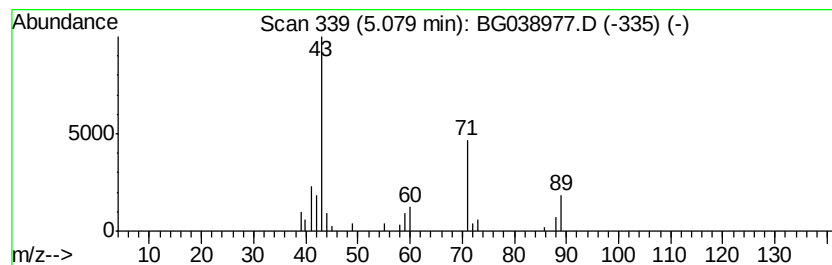
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	2.98 ng	25267	1,4-Dichlorobenzene-d4	8.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	74
2		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56
3		Propanamide, N-acetyl-	115	C5H9NO2	019264-34-7	9
4		N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	9
5		Propyl nitrite	89	C3H7NO2	000543-67-9	9



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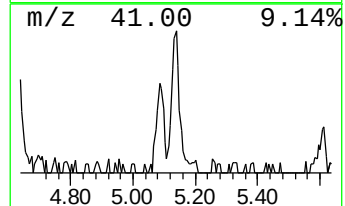
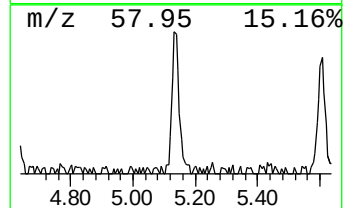
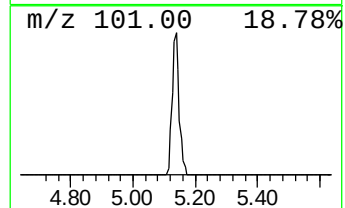
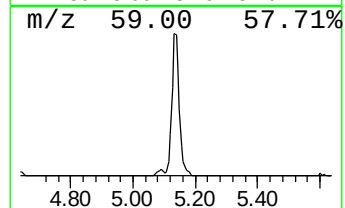
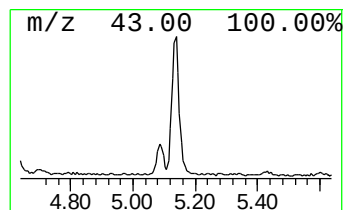
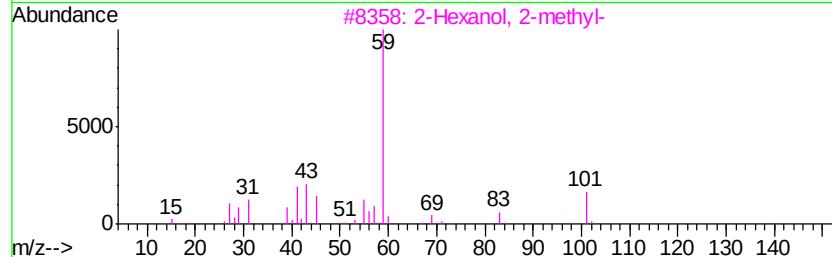
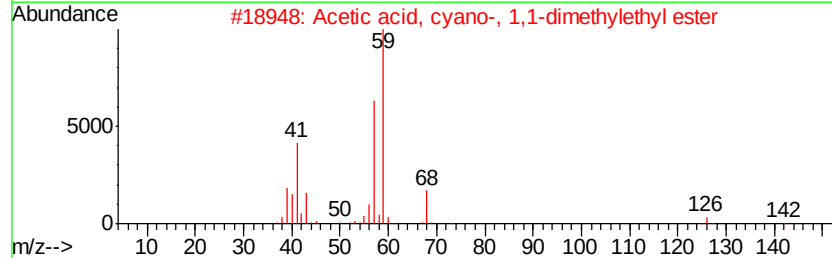
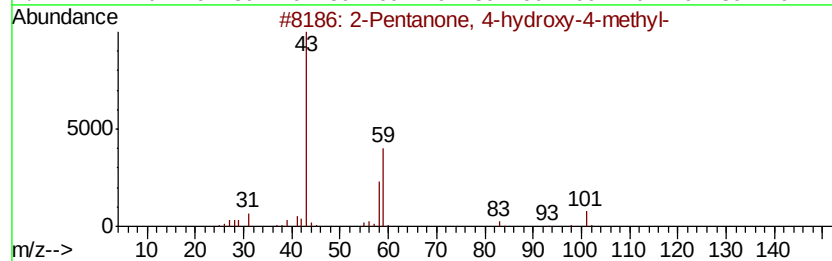
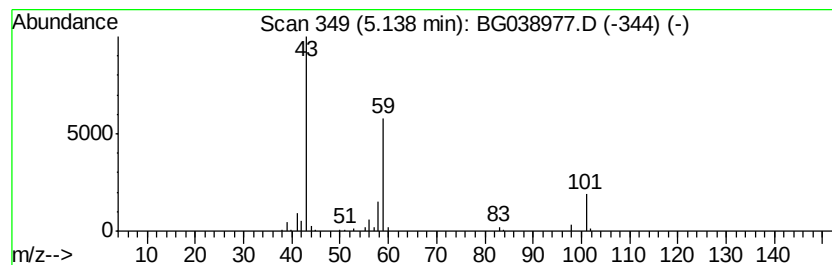
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	12.65 ng	107349	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010719\
Data File : BG038977.D
Acq On : 7 Jan 2019 21:48
Operator : JU/SJ
Sample : K1012-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-02-010419-A

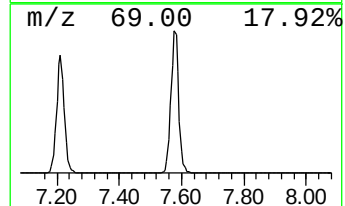
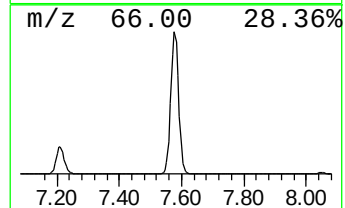
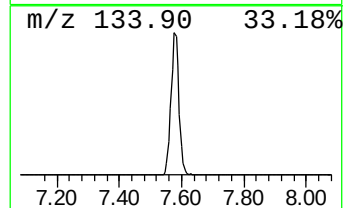
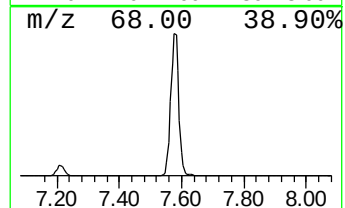
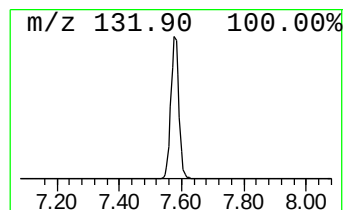
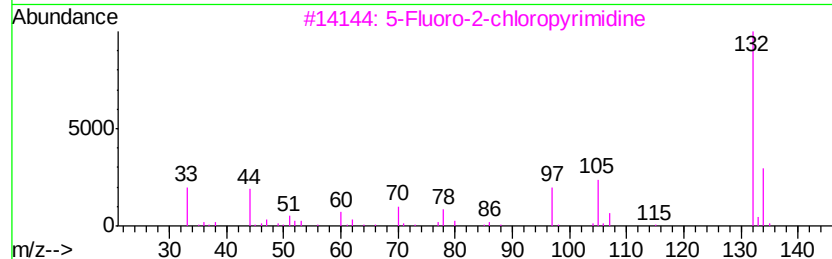
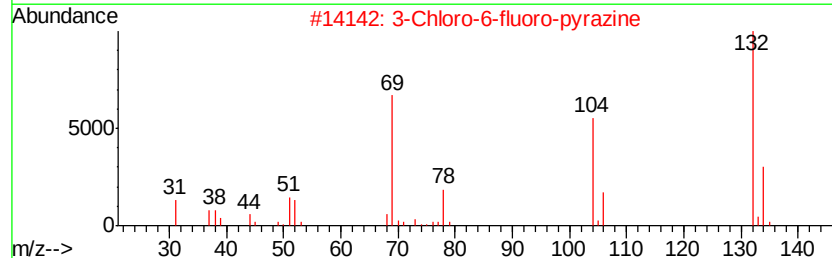
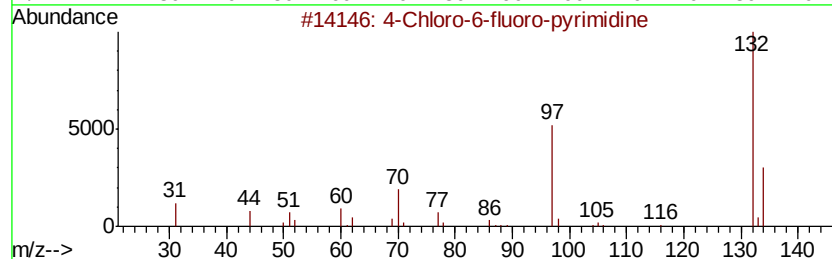
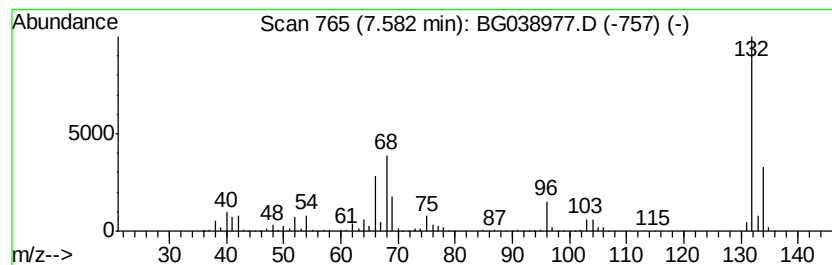
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	95.21 ng	808185	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010719\
Data File : BG038977.D
Acq On : 7 Jan 2019 21:48
Operator : JU/SJ
Sample : K1012-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

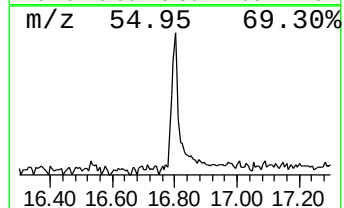
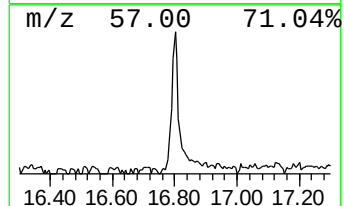
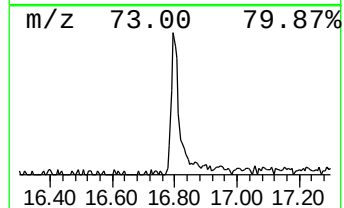
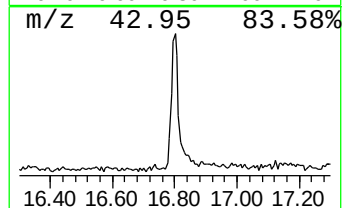
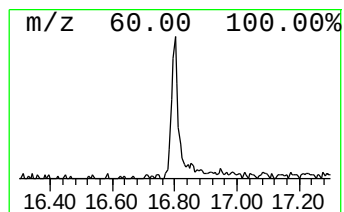
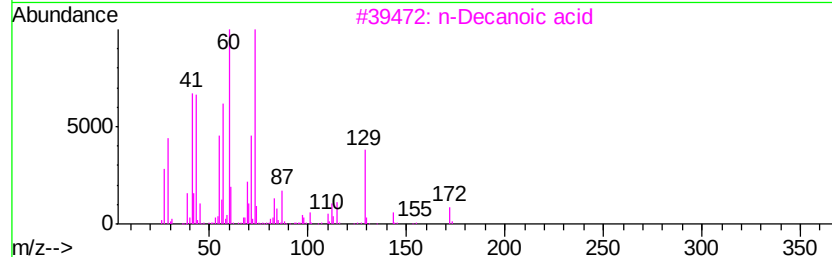
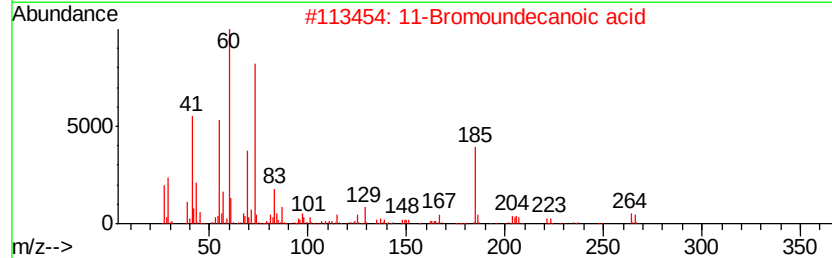
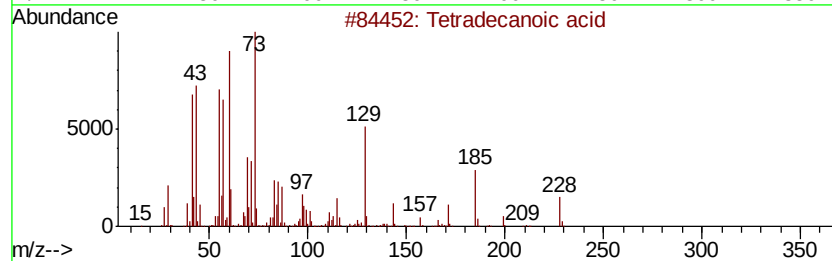
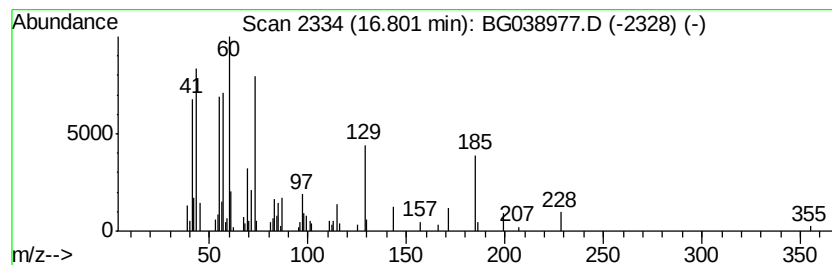
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BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.80	5.60 ng	117759	Phenanthrene-d10	17.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	96
2	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	1,3,4-Thiadiazol-2-amine, 5-ethyl-	129	C4H7N3S	014068-53-2	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010719\
Data File : BG038977.D
Acq On : 7 Jan 2019 21:48
Operator : JU/SJ
Sample : K1012-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-02-010419-A

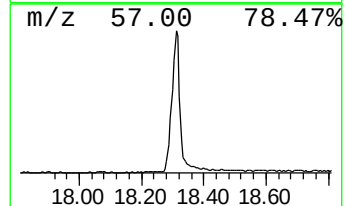
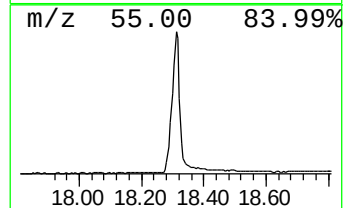
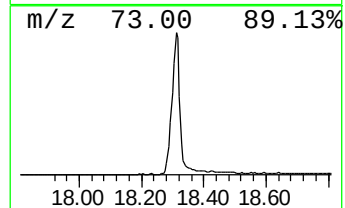
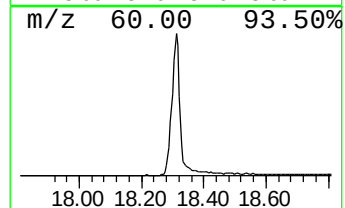
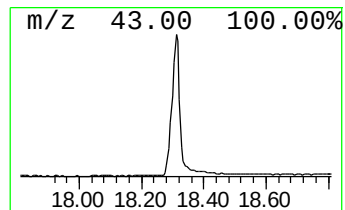
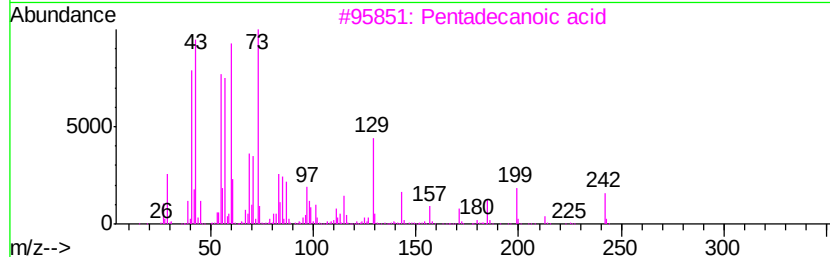
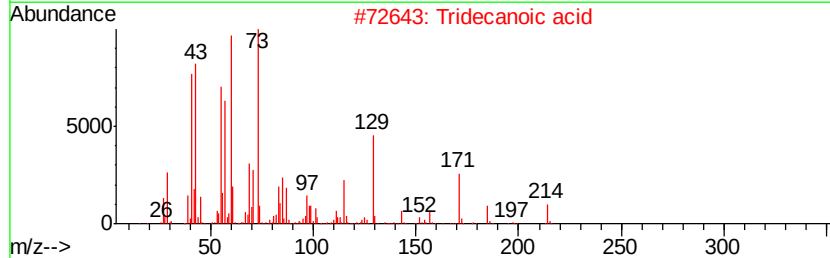
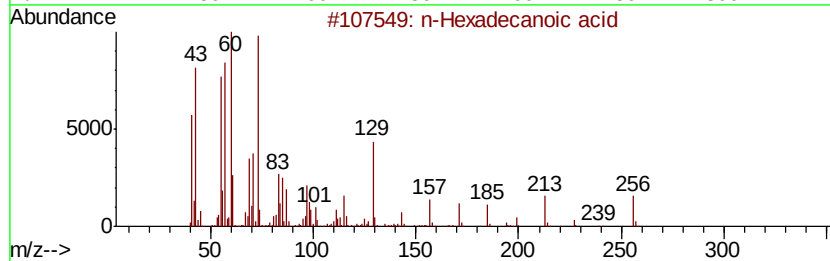
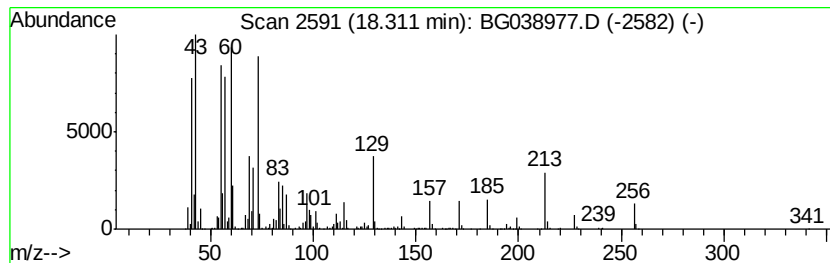
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	103.00 ng	2165180	Phenanthrene-d10	17.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010719\
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Operator : JU/SJ
Sample : K1012-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EO-02-010419-A

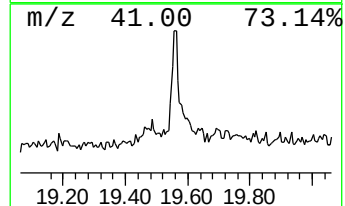
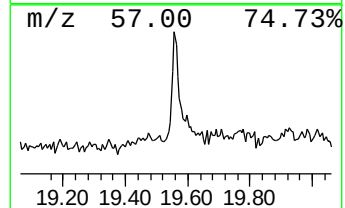
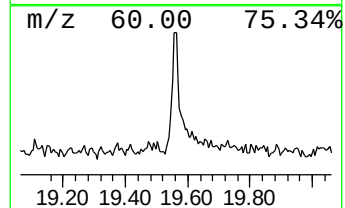
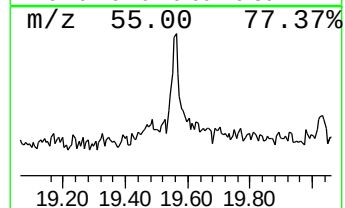
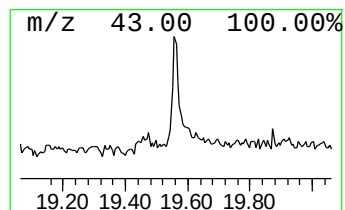
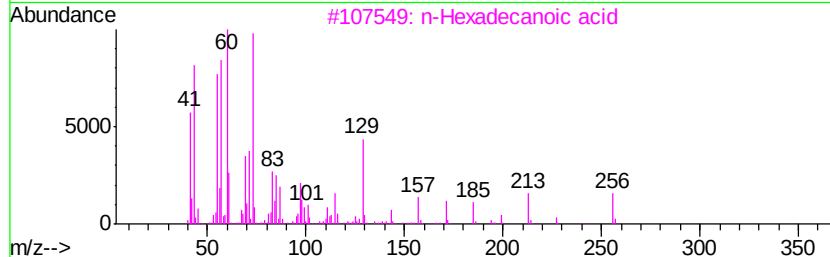
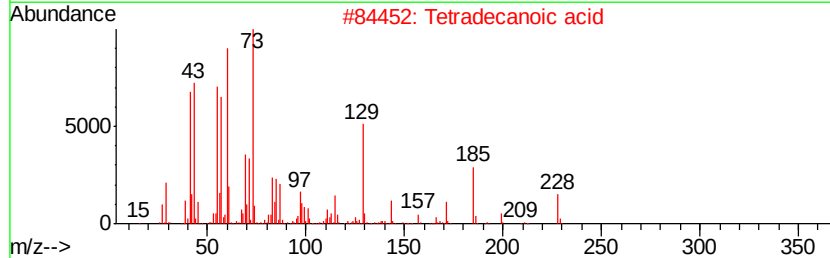
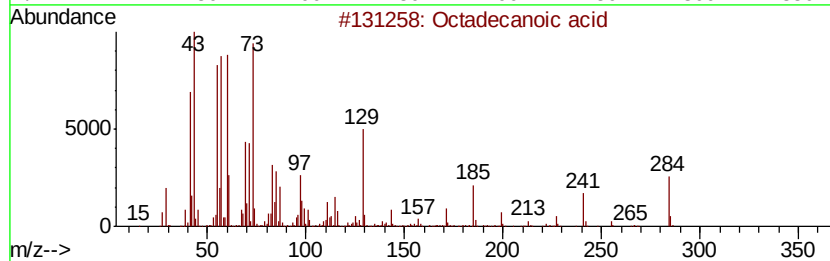
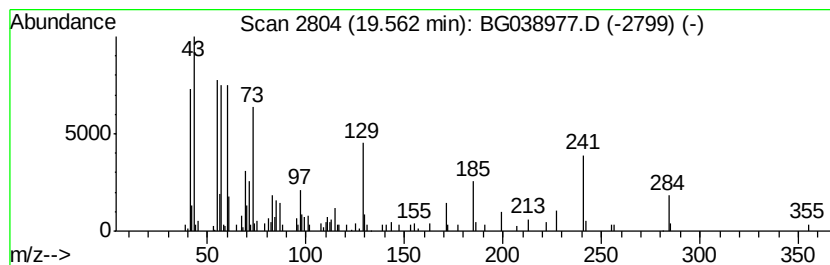
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.56	3.91 ng	82265	Phenanthrene-d10	17.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
4		Undecanoic acid	186	C11H22O2	000112-37-8	42
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG010719\
Data File : BG038977.D
Acq On : 7 Jan 2019 21:48
Operator : JU/SJ
Sample : K1012-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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...	3.20	9.4	ng	80237	1	8.05	169762	20.0
n-Propyl acetate	3.49	6.8	ng	58128	1	8.05	169762	20.0
3-Penten-2-one, 4...	4.53	5.0	ng	42387	1	8.05	169762	20.0
Propanoic acid, p...	4.64	4.3	ng	36192	1	8.05	169762	20.0
Butanoic acid, 1-...	5.08	3.0	ng	25267	1	8.05	169762	20.0
2-Pentanone, 4-hy...	5.14	12.7	ng	107349	1	8.05	169762	20.0
unknown7.58	7.58	95.2	ng	808185	1	8.05	169762	20.0
Tetradecanoic acid	16.80	5.6	ng	117759	4	17.43	420445	20.0
n-Hexadecanoic acid	18.31	103.0	ng	2165180	4	17.43	420445	20.0
Octadecanoic acid	19.56	3.9	ng	82265	4	17.43	420445	20.0