

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120718\
 Data File : BG038425.D
 Acq On : 8 Dec 2018 6:37
 Operator : JU/SJ
 Sample : PB115307BL
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB115307BL

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-BG120418.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	5.147	311	316	325	rBV	23275	38837	1.91%	0.372%
2	5.611	388	395	406	rBV	399989	683413	33.53%	6.549%
3	7.215	660	668	681	rBV	442054	807747	39.63%	7.741%
4	7.597	725	733	742	rBV	405624	750172	36.81%	7.189%
5	8.067	806	813	819	rBV2	82804	140970	6.92%	1.351%
6	8.390	860	868	877	rVB	308069	552377	27.10%	5.294%
7	9.242	1005	1013	1024	rBV	252894	484930	23.79%	4.647%
8	10.887	1284	1293	1303	rBV	105425	200020	9.81%	1.917%
9	13.326	1701	1708	1717	rBV	710905	1154221	56.63%	11.061%
10	14.706	1936	1943	1952	rBV2	176207	305643	15.00%	2.929%
11	16.193	2189	2196	2212	rBV	831757	1320210	64.78%	12.652%
12	17.450	2403	2410	2423	rBV2	277222	437540	21.47%	4.193%
13	19.718	2791	2796	2801	rVB	138825	163207	8.01%	1.564%
14	19.830	2811	2815	2822	rVB	30180	36645	1.80%	0.351%
15	20.053	2847	2853	2864	rBV	1515995	2038096	100.00%	19.532%
16	20.752	2968	2972	2978	rVB	107963	126059	6.19%	1.208%
17	21.728	3131	3138	3146	rBV	274979	480472	23.57%	4.605%
18	21.875	3157	3163	3169	rBV	19092	28709	1.41%	0.275%
19	22.486	3260	3267	3273	rBV4	19070	33396	1.64%	0.320%
20	23.185	3380	3386	3394	rVB3	23631	47931	2.35%	0.459%
21	24.001	3518	3525	3535	rVB3	22037	48409	2.38%	0.464%
22	24.965	3681	3689	3692	rBV3	20511	50522	2.48%	0.484%
23	25.036	3692	3701	3712	rVB3	141188	429934	21.09%	4.120%
24	26.105	3872	3883	3884	rBV5	15447	27600	1.35%	0.264%
25	27.491	4107	4119	4131	rBV6	12984	47745	2.34%	0.458%

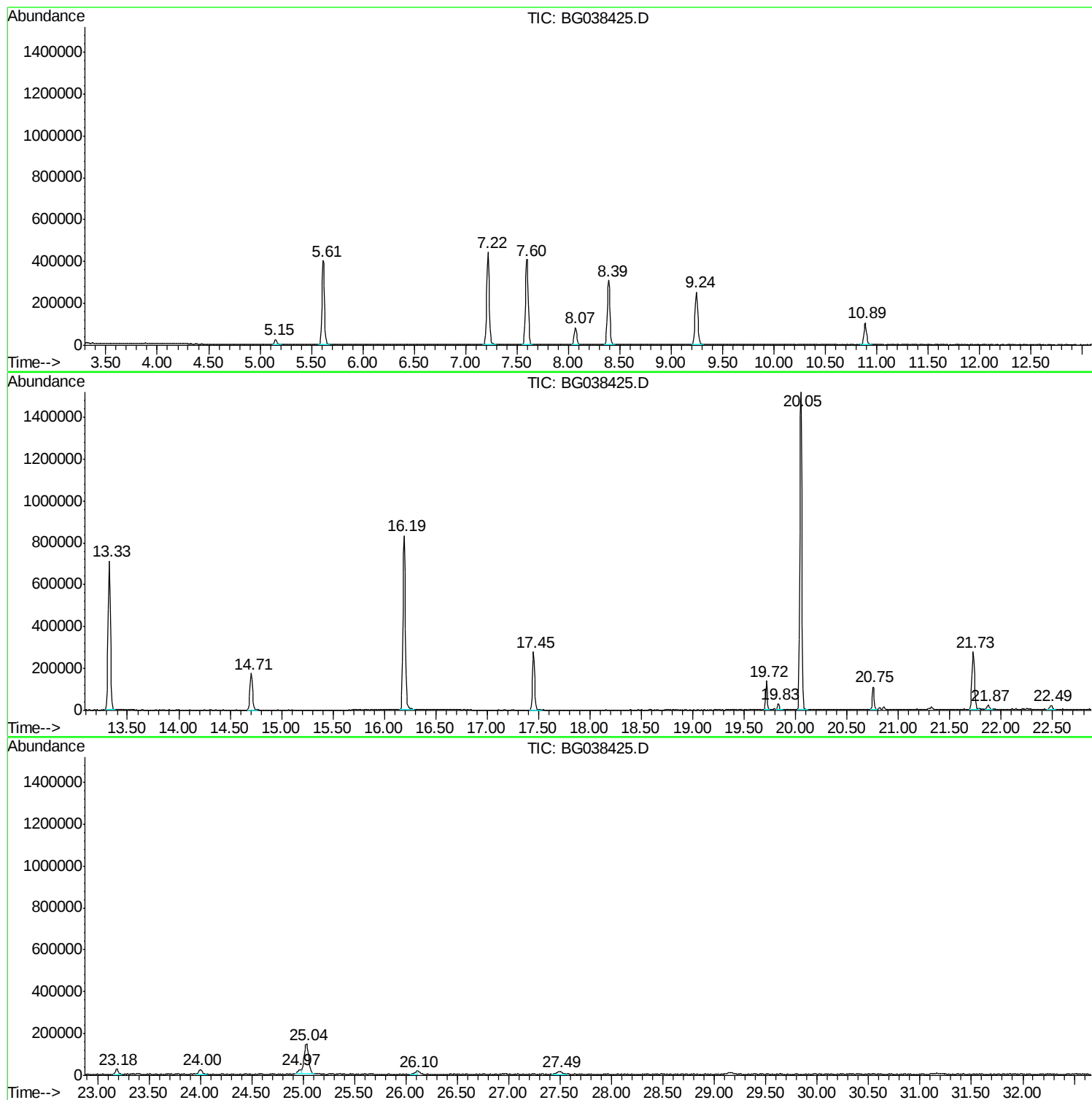
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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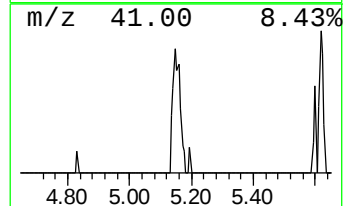
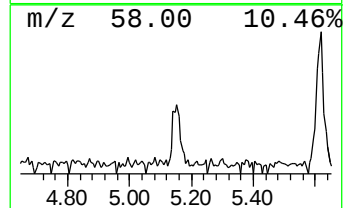
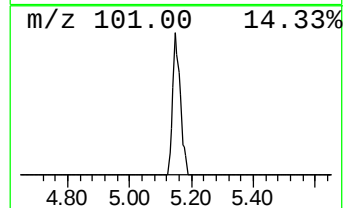
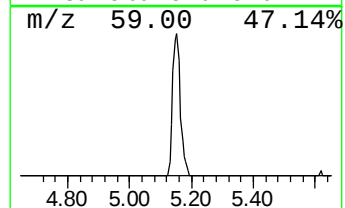
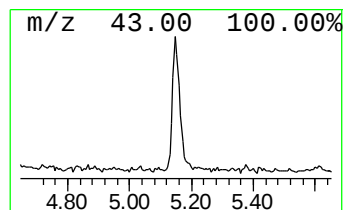
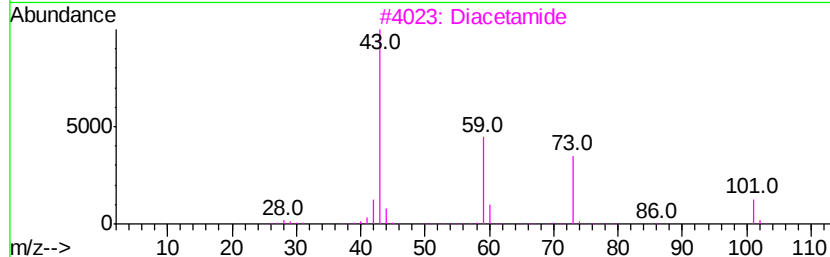
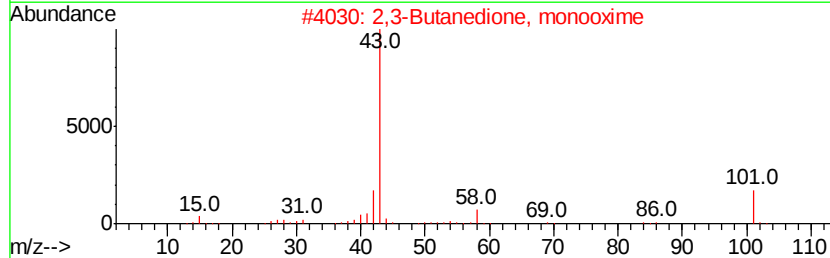
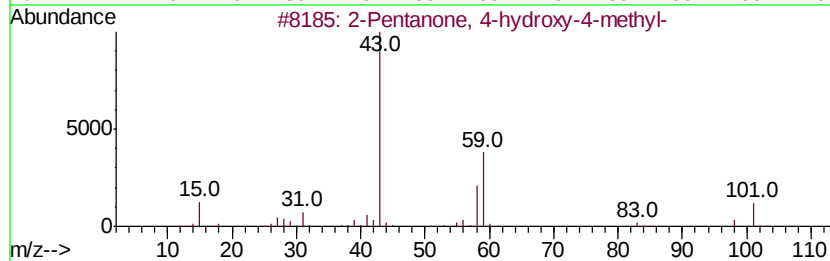
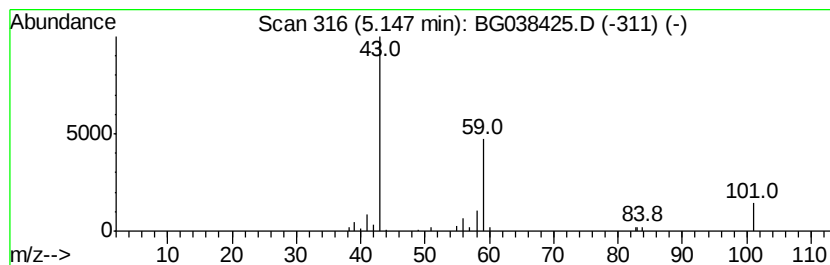
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	5.51 ng	38837	1,4-Dichlorobenzene-d4	8.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			Diacetamide	101	C4H7NO2	000625-77-4	9
4			1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9
5			2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9



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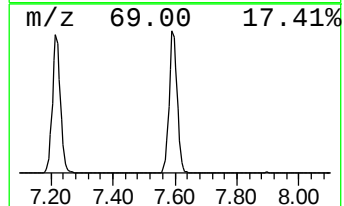
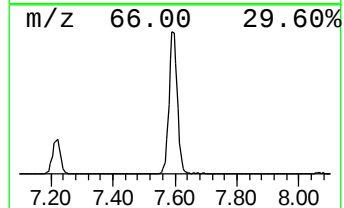
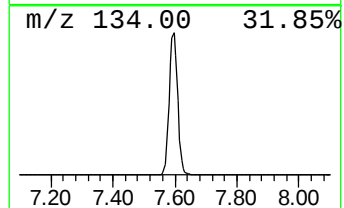
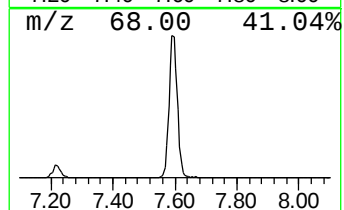
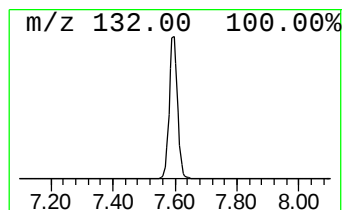
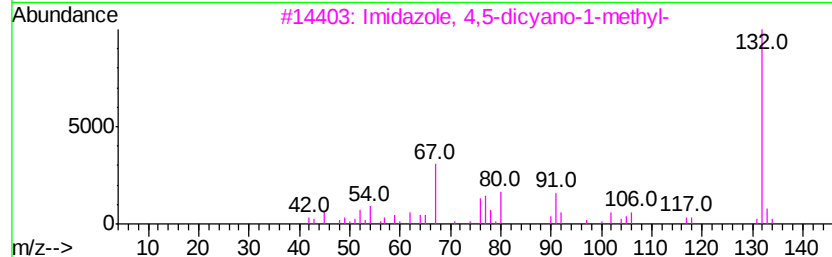
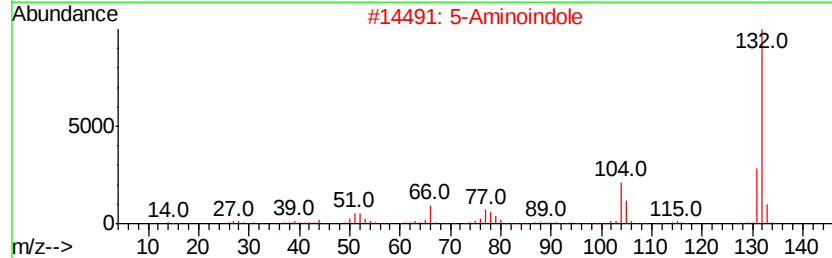
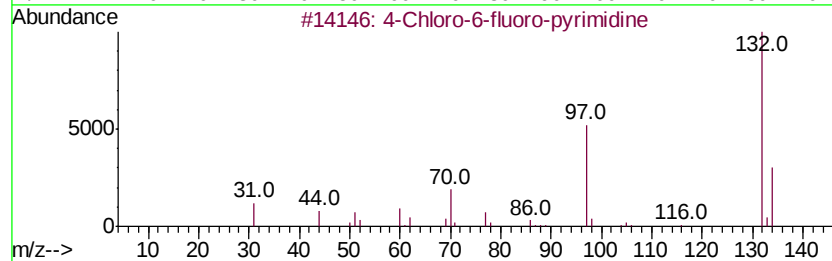
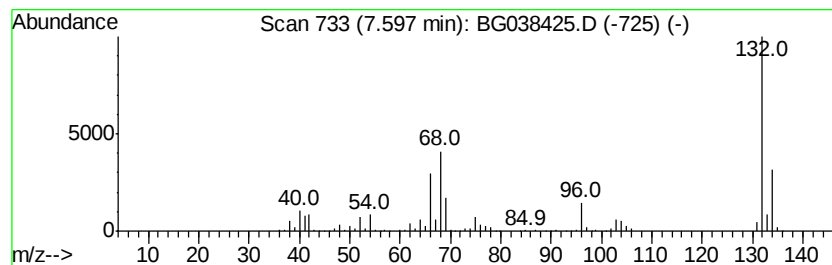
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Peak Number 2 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	106.43 ng	750172	1,4-Dichlorobenzene-d4	8.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	22
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12



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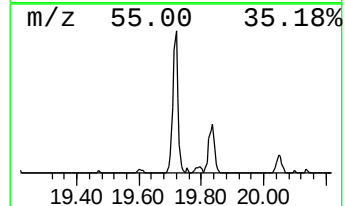
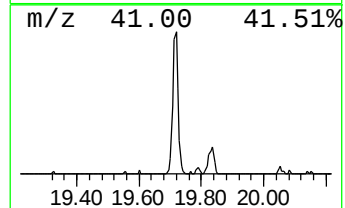
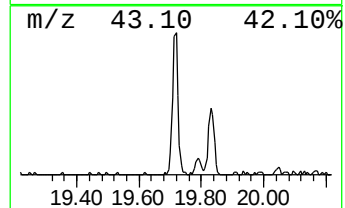
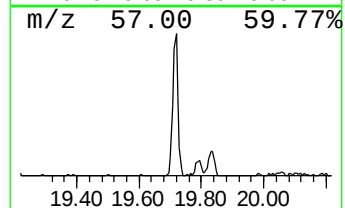
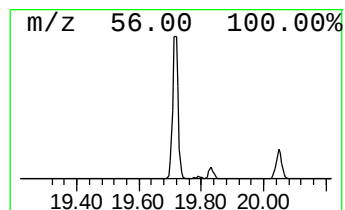
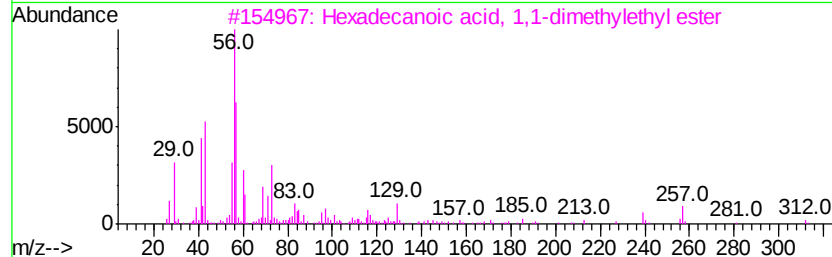
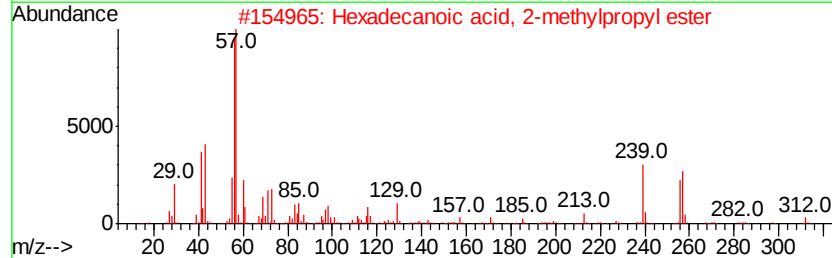
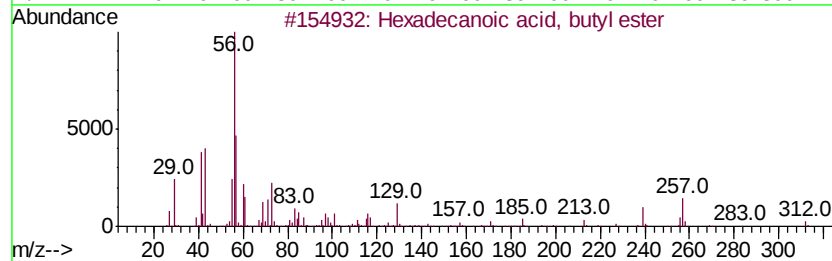
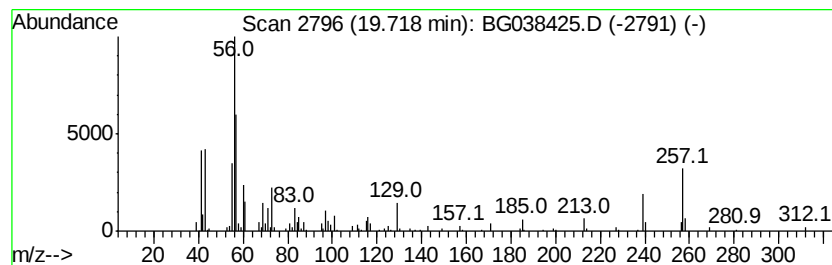
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.72	6.79 ng	163207	Chrysene-d12	21.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	98
2		Hexadecanoic acid, 2-methylpropyl ester	312	C20H40O2	000110-34-9	64
3		Hexadecanoic acid, 1,1-dimethylethyl ester	312	C20H40O2	031158-91-5	60
4		Methanimidamide, N'-(2,3-dihydro-1H-imidazo[4,5-b]pyridin-2-yl)-	258	C14H18N4O	105949-64-2	35
5		Cyclopentanecarboxylic acid, 2-allyl ester	129	C6H11NO2	037910-65-9	35



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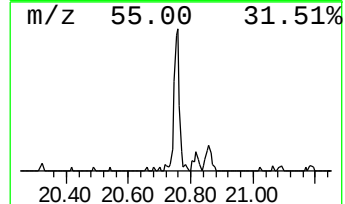
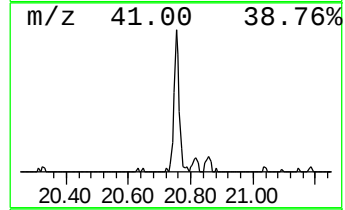
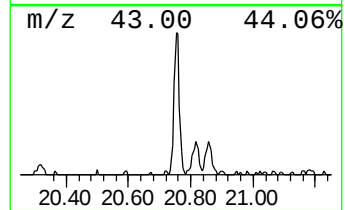
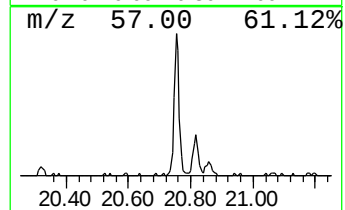
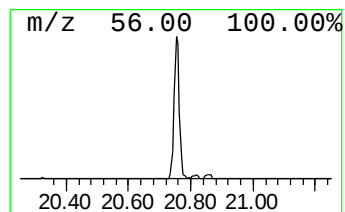
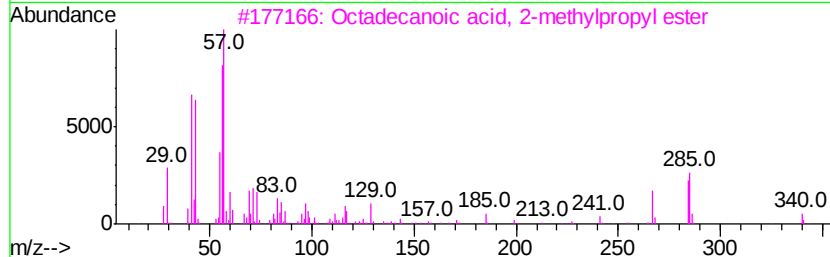
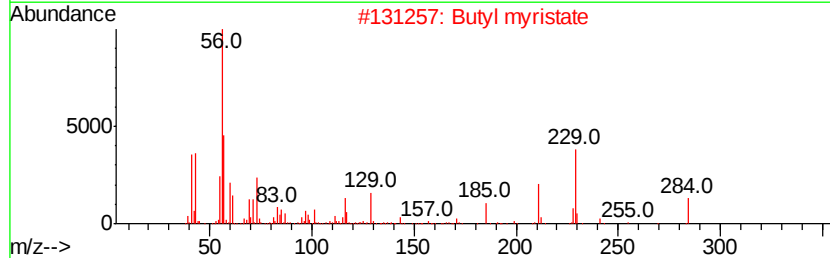
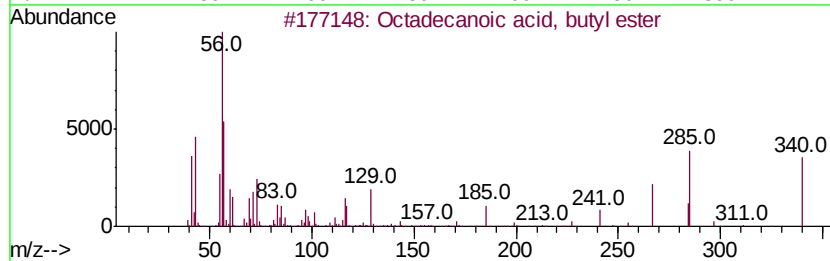
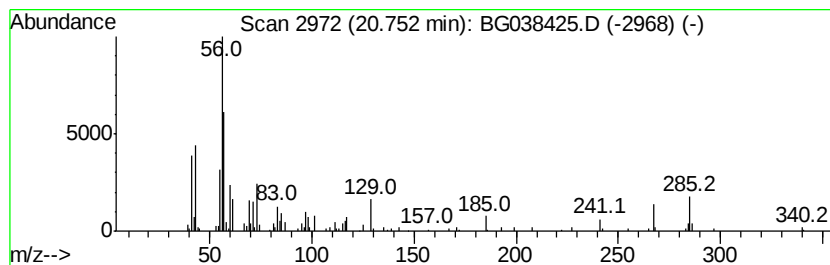
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Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.75	5.25 ng	126059	Chrysene-d12	21.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2		Butyl myristate	284	C18H36O2	000110-36-1	72
3		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	43
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35



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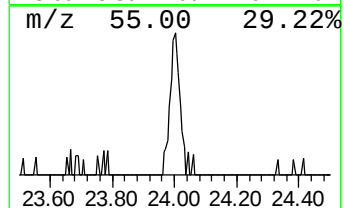
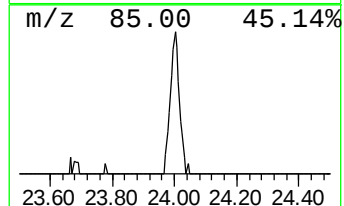
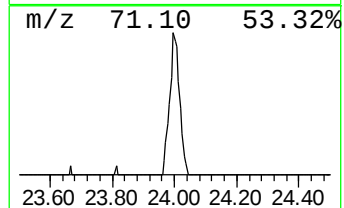
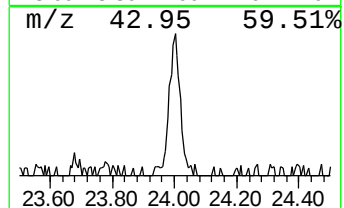
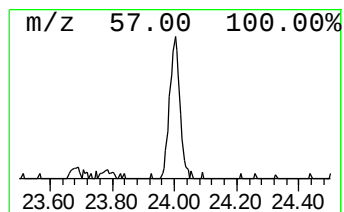
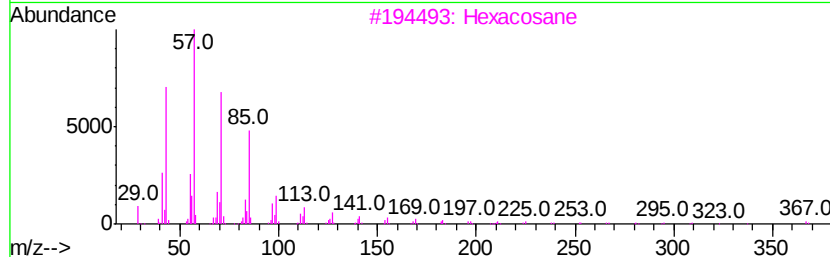
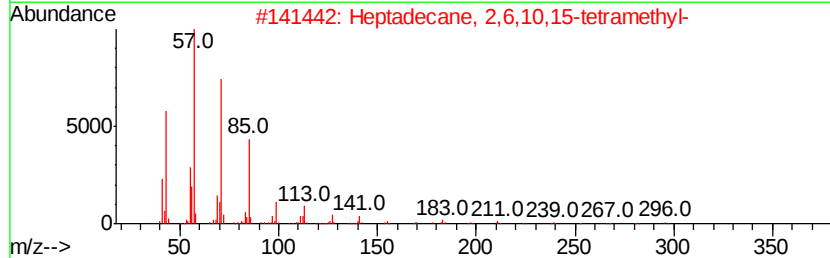
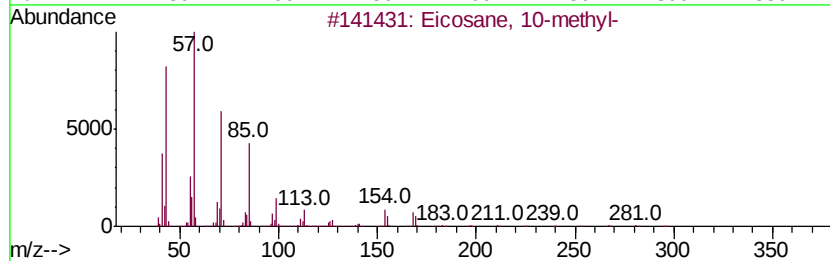
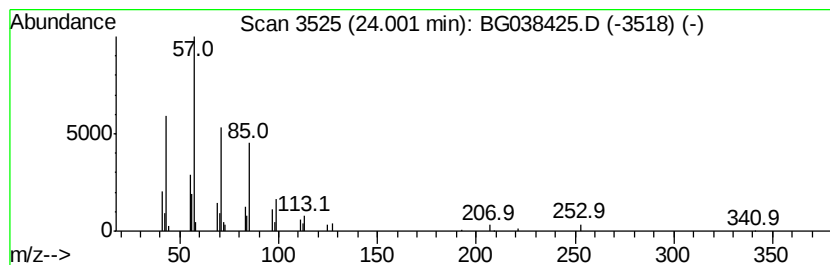
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Peak Number 6 Eicosane, 10-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	2.25 ng	48409	Perylene-d12	25.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3		Hexacosane	366	C26H54	000630-01-3	86
4		Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	86
5		Tetradecane	198	C14H30	000629-59-4	80



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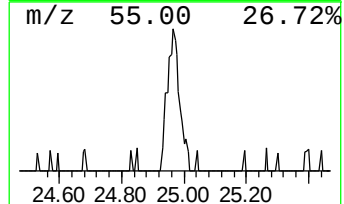
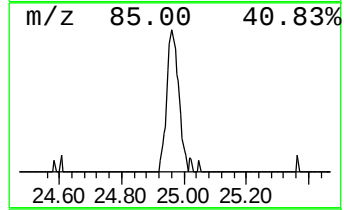
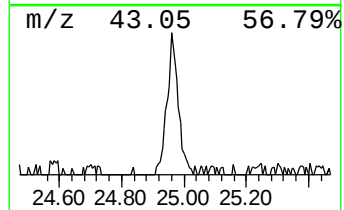
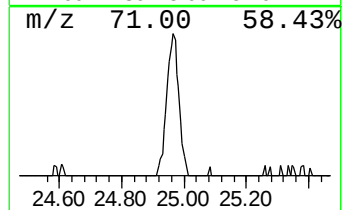
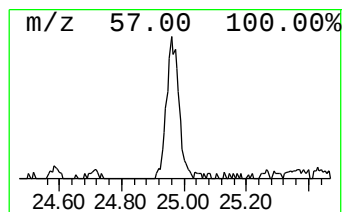
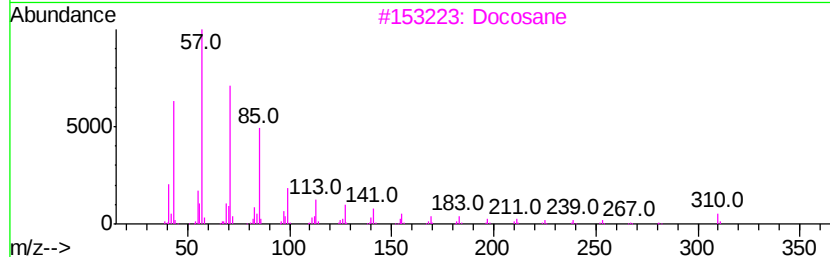
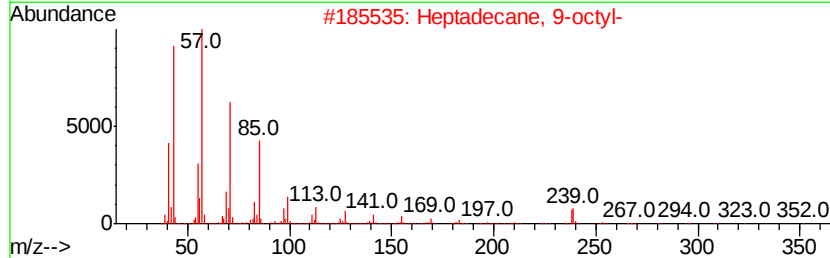
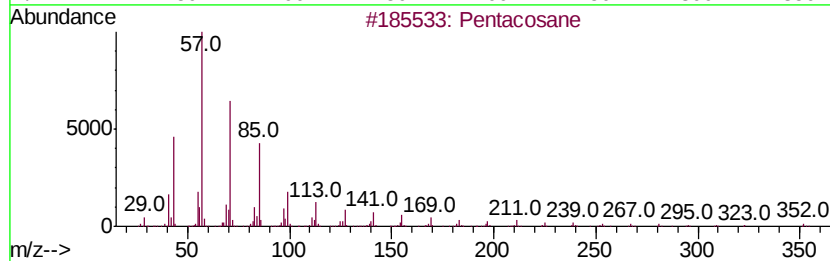
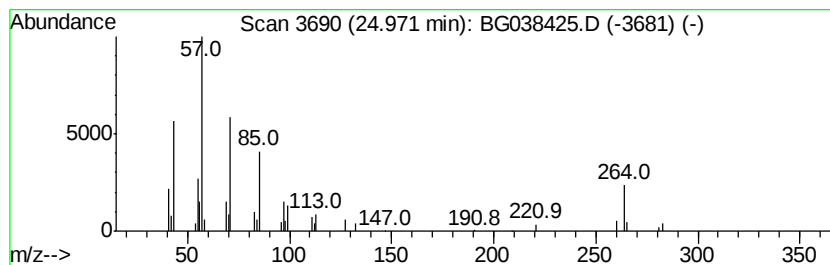
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.97	2.35 ng	50522	Perylene-d12	25.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	83
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	80
3	Docosane		310	C22H46	000629-97-0	80
4	Docosane, 11-decyl-		451	C32H66	055401-55-3	80
5	Tetracosane, 11-decyl-		479	C34H70	055429-84-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120718\
 Data File : BG038425.D
 Acq On : 8 Dec 2018 6:37
 Operator : JU/SJ
 Sample : PB115307BL
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

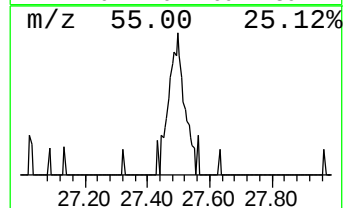
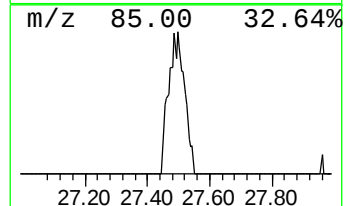
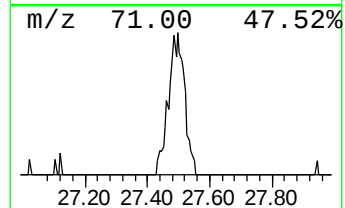
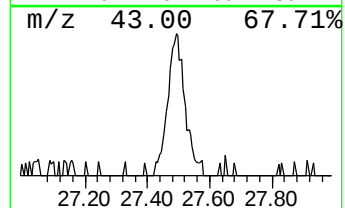
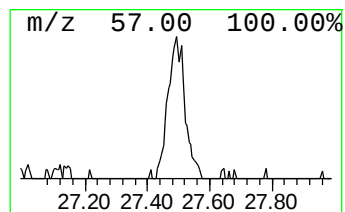
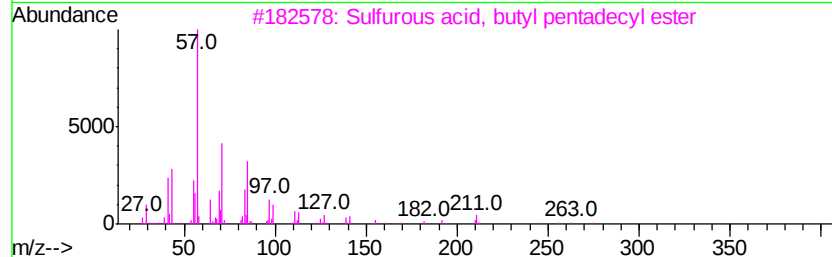
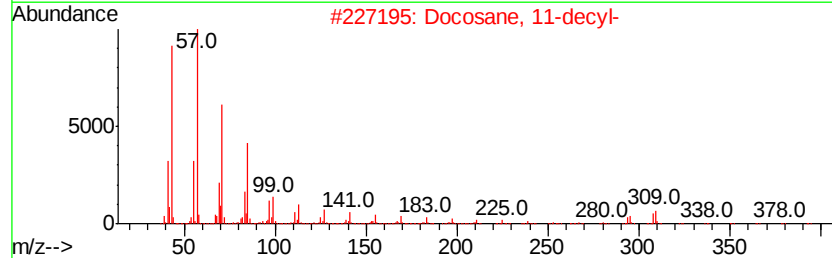
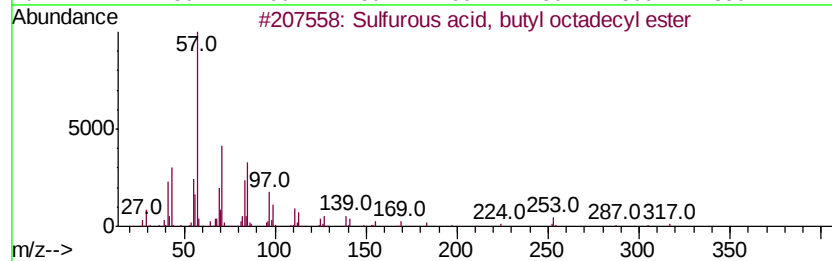
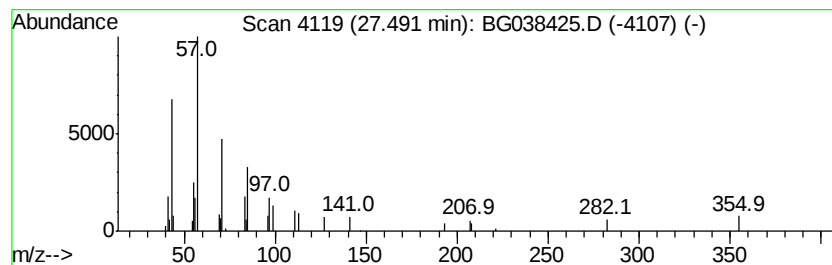
Instrument :
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 ClientSampleId :
 PB115307BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG120418.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Sulfurous acid, butyl octadecyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.49	2.22 ng	47745	Perylene-d12	25.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Sulfurous acid, butyl octadecyl ...	390 C22H46O3S	1000309-18-5 80
2		Docosane, 11-decyl-	451 C32H66	055401-55-3 80
3		Sulfurous acid, butyl pentadecyl...	348 C19H40O3S	1000309-18-2 80
4		Sulfurous acid, butyl hexadecyl ...	362 C20H42O3S	1000309-18-3 80
5		Tetracosane, 11-decyl-	479 C34H70	055429-84-0 80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG120718\
Data File : BG038425.D
Acq On : 8 Dec 2018 6:37
Operator : JU/SJ
Sample : PB115307BL
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB115307BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120418.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
2-Pentanone, 4-hy...	5.15	5.5	ng	38837	1	8.07	140970	20.0
unknown7.60	7.60	106.4	ng	750172	1	8.07	140970	20.0
Hexadecanoic acid...	19.72	6.8	ng	163207	5	21.73	480472	20.0
Octadecanoic acid...	20.75	5.3	ng	126059	5	21.73	480472	20.0
Eicosane, 10-methyl-	24.00	2.3	ng	48409	6	25.04	429934	20.0
Pentacosane	24.97	2.4	ng	50522	6	25.04	429934	20.0
Sulfurous acid, b...	27.49	2.2	ng	47745	6	25.04	429934	20.0