

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
 Data File : BG039235.D
 Acq On : 21 Jan 2019 16:01
 Operator : JU/SJ
 Sample : K1205-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C-6

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-BG010919.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	5.093	333	341	350	rBV	17048	26930	2.21%	0.418%
2	5.563	414	421	432	rBV	226988	387318	31.73%	6.008%
3	7.173	687	695	708	rBV	236808	455168	37.28%	7.060%
4	7.537	750	757	765	rBV	230626	396894	32.51%	6.157%
5	8.007	831	837	846	rBB	56947	96166	7.88%	1.492%
6	8.330	885	892	900	rBB	171148	293041	24.00%	4.546%
7	9.188	1030	1038	1046	rBV	140107	262794	21.53%	4.076%
8	10.822	1308	1316	1325	rBV	72162	138125	11.31%	2.143%
9	13.266	1724	1732	1743	rBV	482905	732964	60.04%	11.370%
10	14.094	1868	1873	1882	rBV	28378	41422	3.39%	0.643%
11	14.647	1960	1967	1978	rVB2	145679	233795	19.15%	3.627%
12	16.139	2215	2221	2237	rBV2	428705	666634	54.60%	10.341%
13	17.396	2429	2435	2444	rBV	197176	309009	25.31%	4.793%
14	18.260	2577	2582	2589	rBV3	12729	18523	1.52%	0.287%
15	19.999	2873	2878	2885	rBV	908362	1220835	100.00%	18.937%
16	20.763	3001	3008	3012	rVB2	15902	18678	1.53%	0.290%
17	21.268	3087	3094	3106	rBV2	44705	76110	6.23%	1.181%
18	21.668	3156	3162	3172	rVB	218977	359760	29.47%	5.581%
19	21.809	3181	3186	3192	rVB	26406	37304	3.06%	0.579%
20	22.408	3283	3288	3298	rBV2	29611	47494	3.89%	0.737%
21	23.101	3396	3406	3416	rBV3	56745	115712	9.48%	1.795%
22	23.895	3532	3541	3550	rBV2	27942	61663	5.05%	0.957%
23	24.840	3693	3702	3708	rBV4	22093	57419	4.70%	0.891%
24	24.929	3708	3717	3731	rVB2	115472	339513	27.81%	5.266%
25	25.974	3882	3895	3904	rVB3	15939	53435	4.38%	0.829%

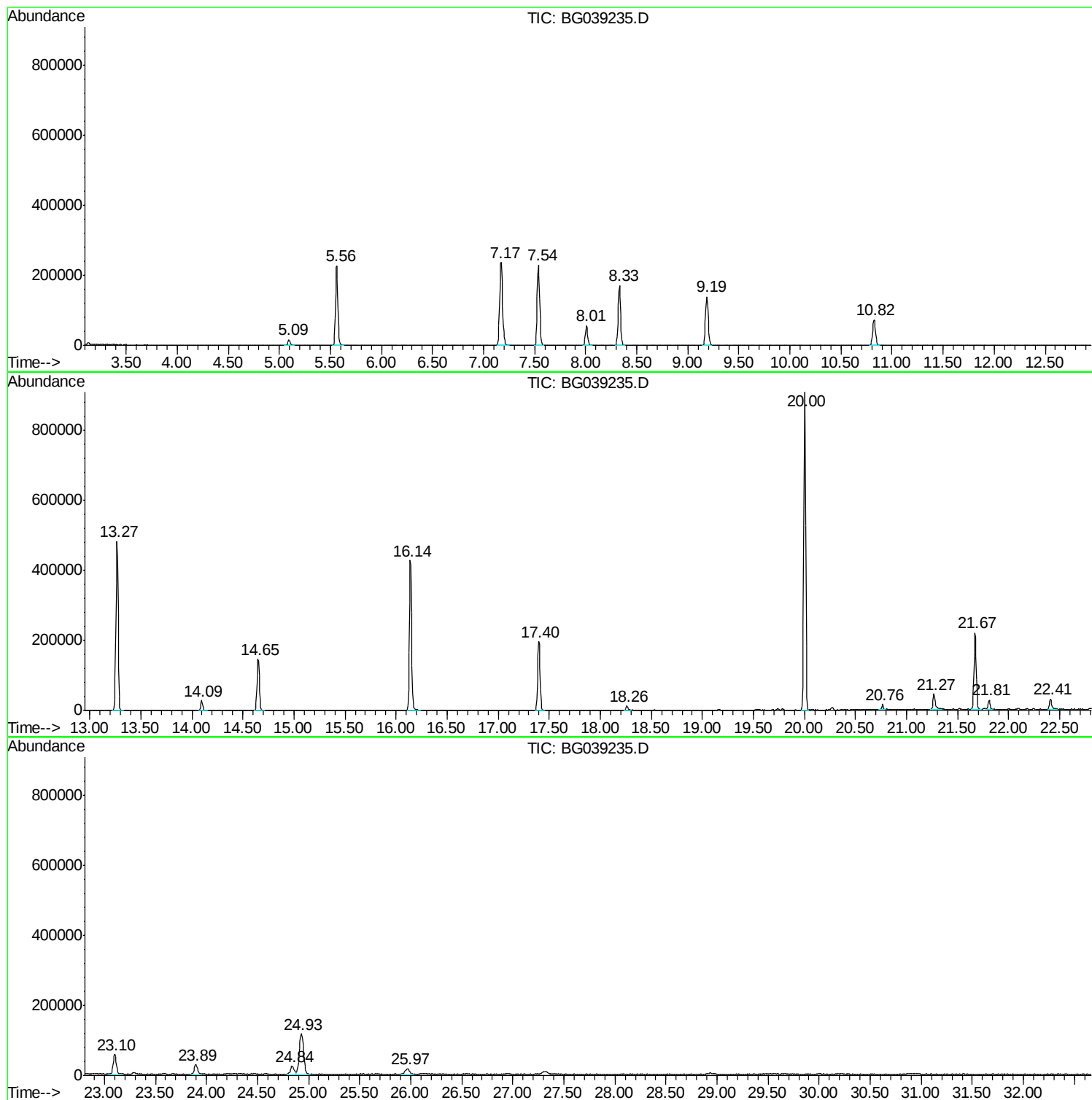
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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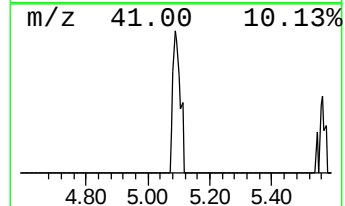
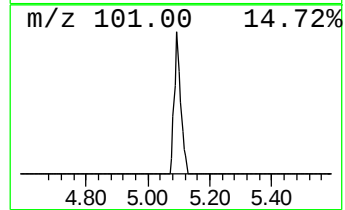
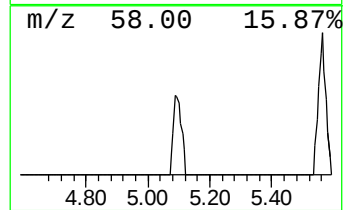
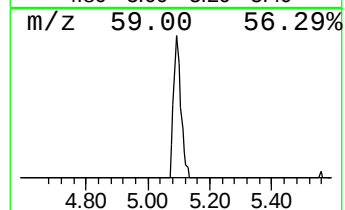
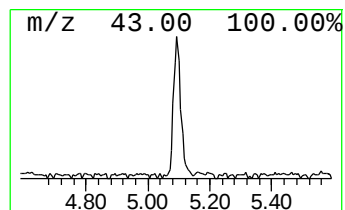
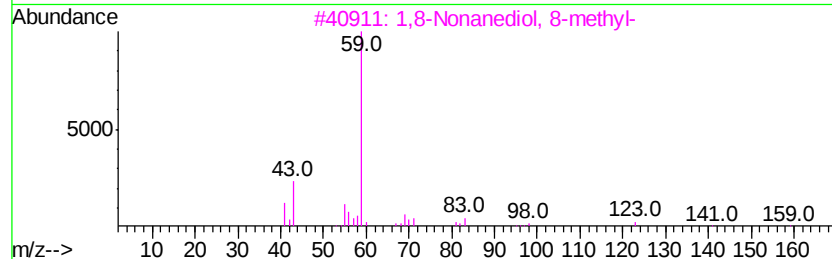
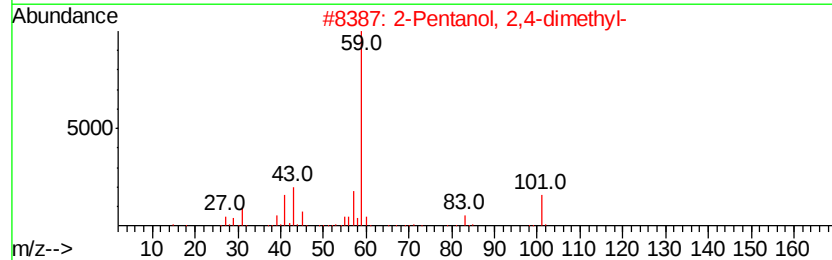
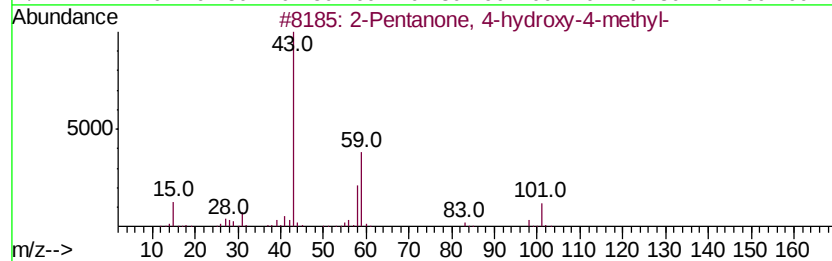
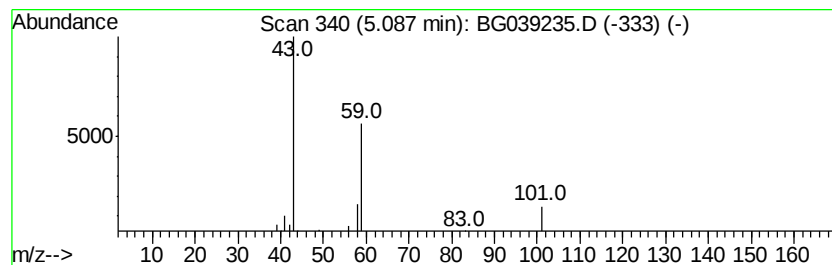
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.09	5.60 ng	26930	1,4-Dichlorobenzene-d4	8.01

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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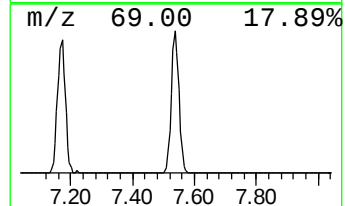
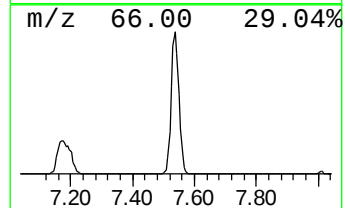
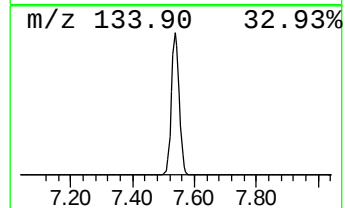
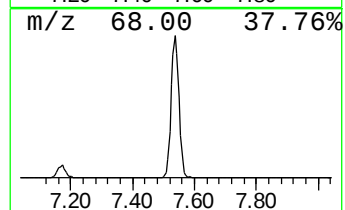
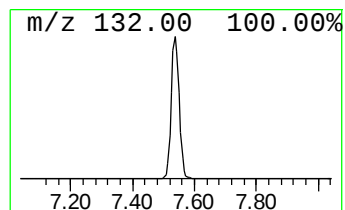
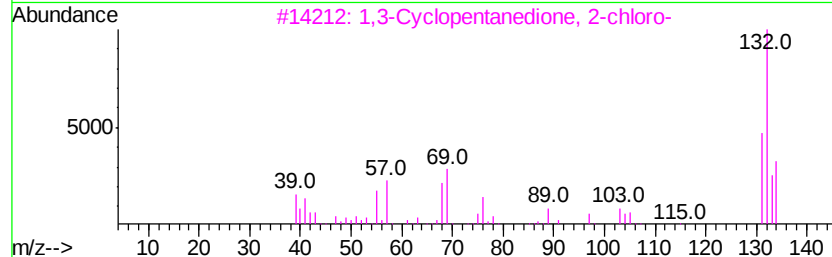
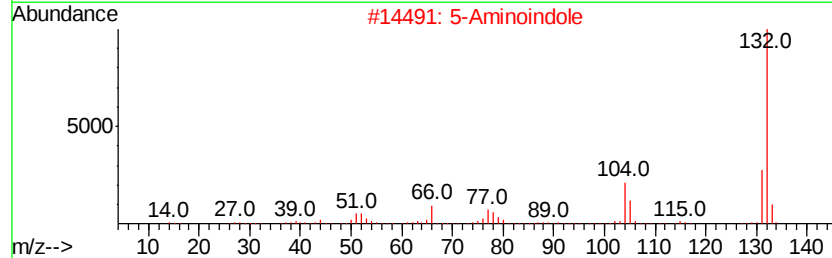
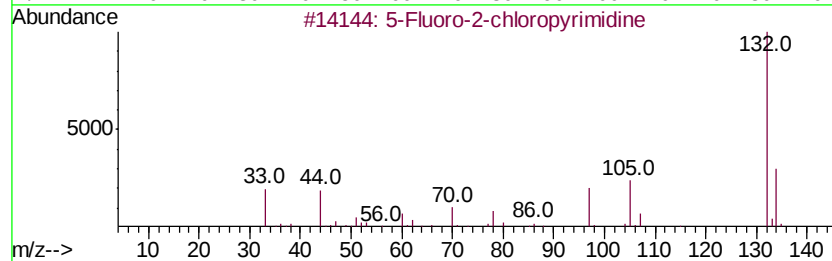
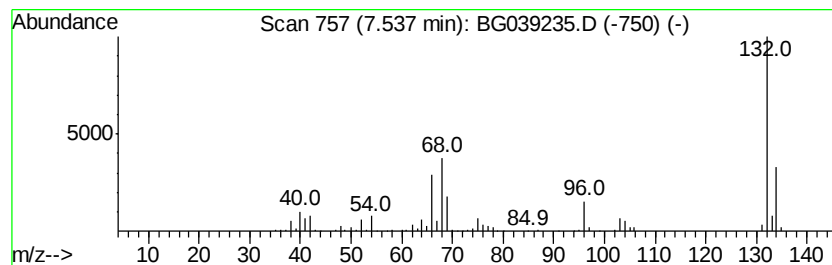
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Peak Number 2 unknown7.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	82.54 ng	396894	1,4-Dichlorobenzene-d4	8.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	35
2			5-Aminoindole	132	C8H8N2	005192-03-0	27
3			1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
5			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10



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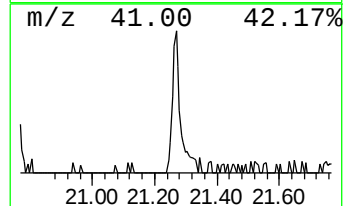
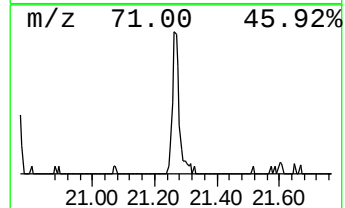
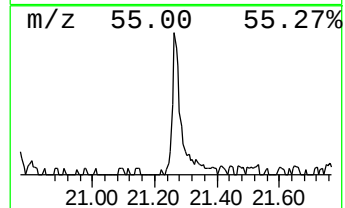
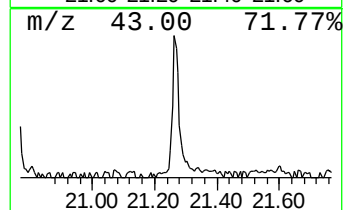
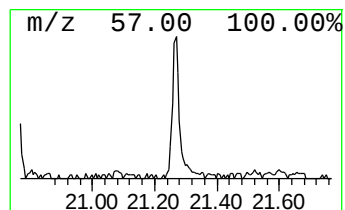
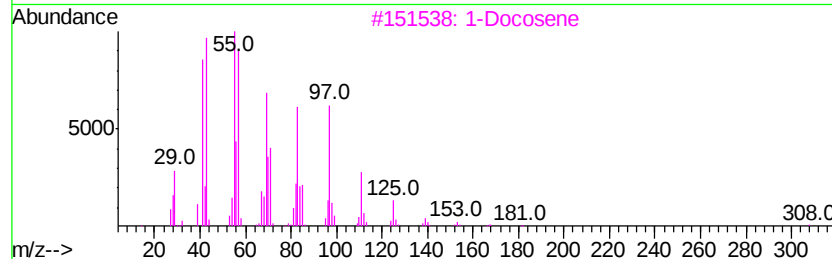
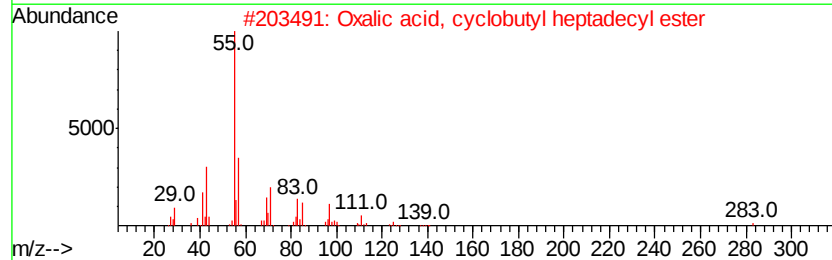
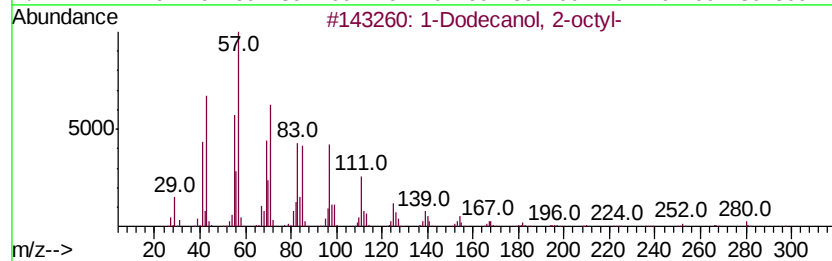
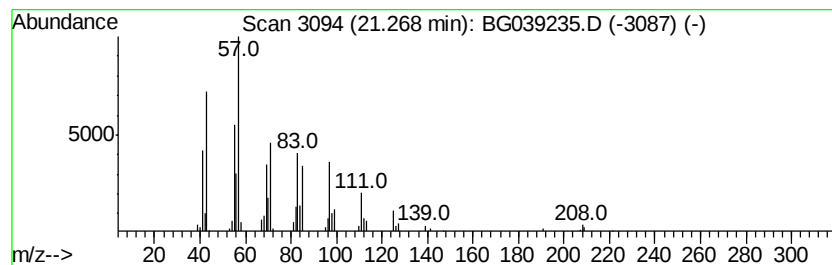
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 Peak Number 4 1-Dodecanol, 2-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	4.23 ng	76110	Chrysene-d12	21.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2		Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	86
3		1-Docosene	308	C22H44	001599-67-3	76
4		Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	72
5		Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	72



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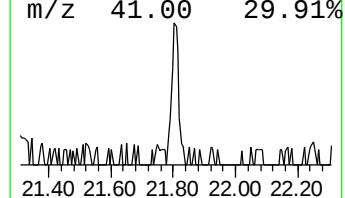
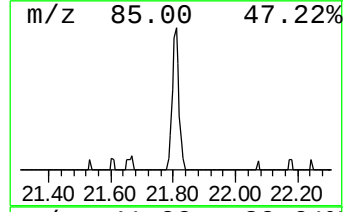
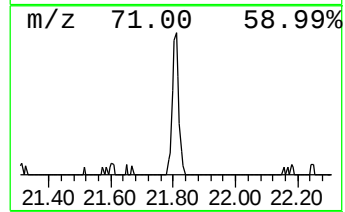
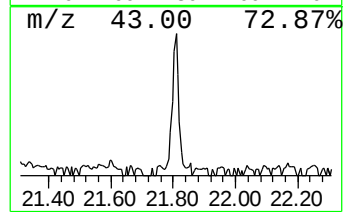
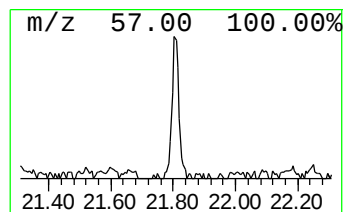
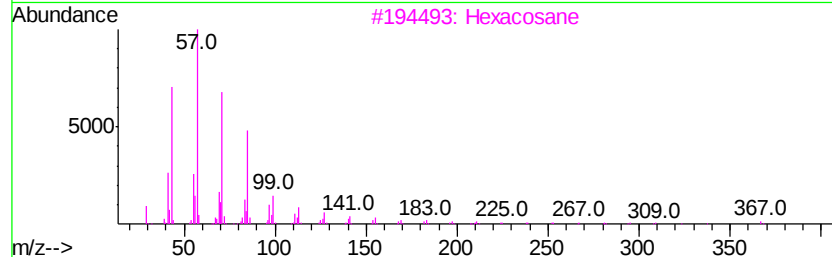
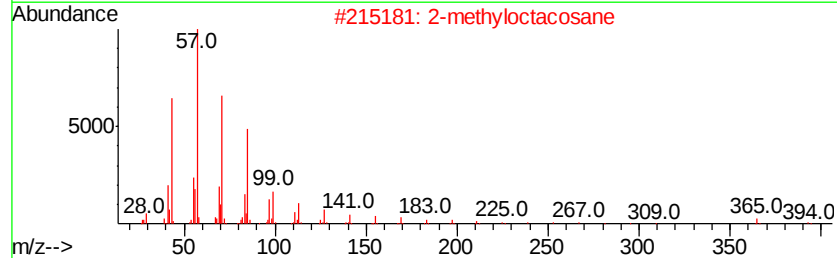
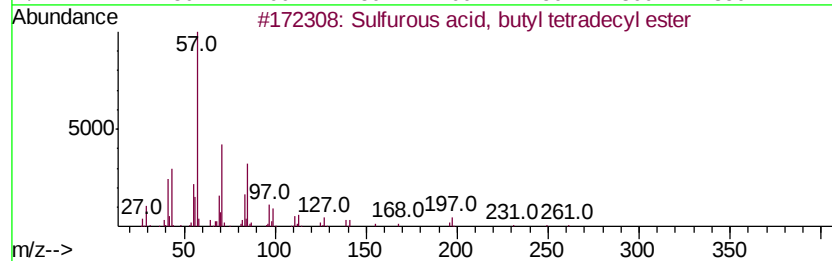
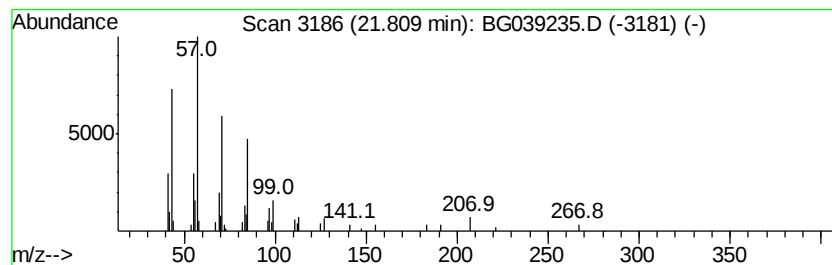
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Peak Number 5 Sulfurous acid, butyl tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.81	2.07 ng	37304	Chrysene-d12	21.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	86
2		2-methyloctacosane	408	C29H60	1000376-72-8	86
3		Hexacosane	366	C26H54	000630-01-3	83
4		Octacosane	394	C28H58	000630-02-4	80
5		Tetracosane	338	C24H50	000646-31-1	80



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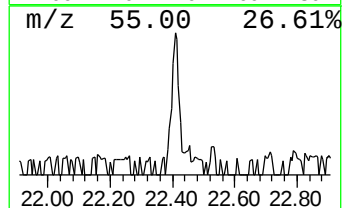
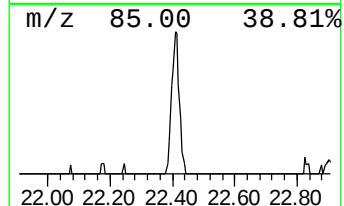
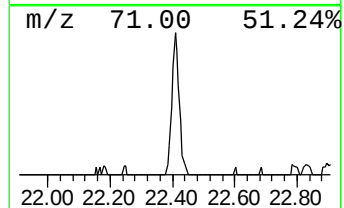
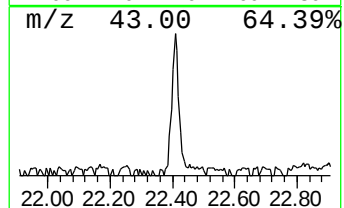
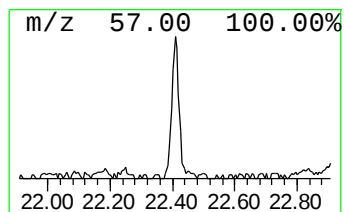
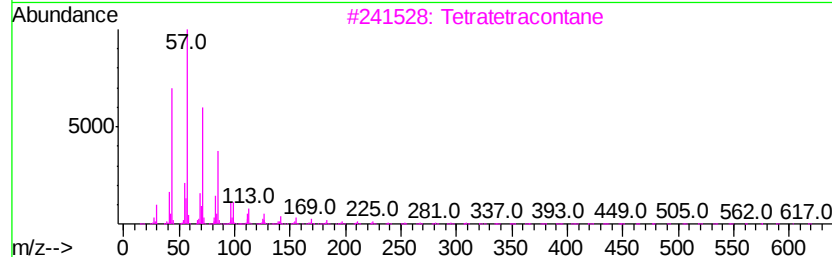
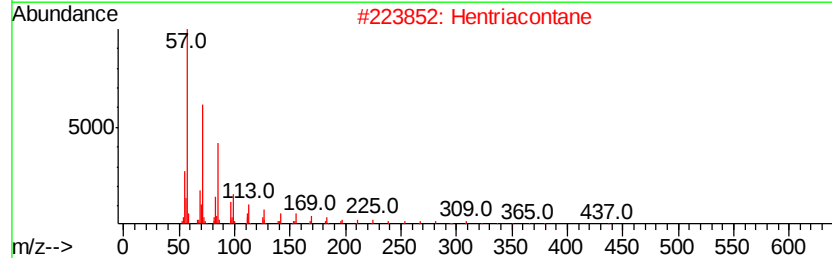
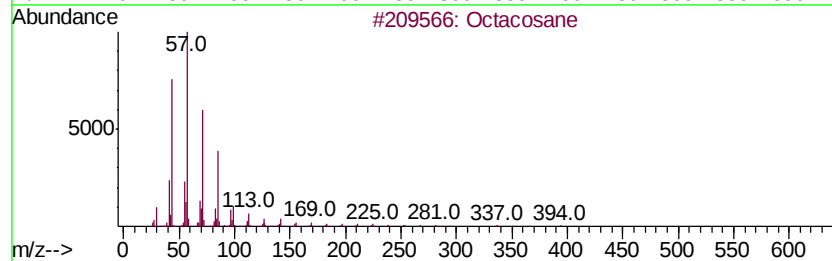
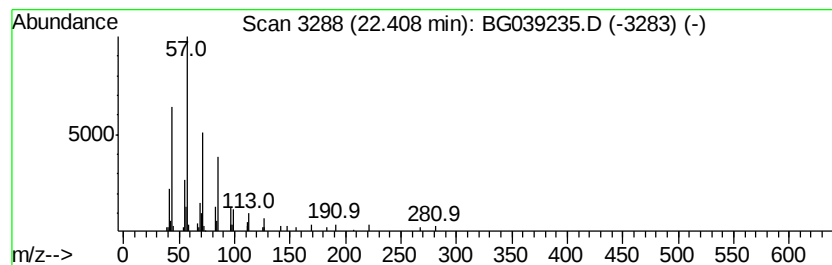
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Peak Number 6 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	2.64 ng	47494	Chrysene-d12	21.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Tetratetracontane	619	C44H90	007098-22-8	90
4		Hexacosane	366	C26H54	000630-01-3	87
5		Pentacosane	352	C25H52	000629-99-2	87



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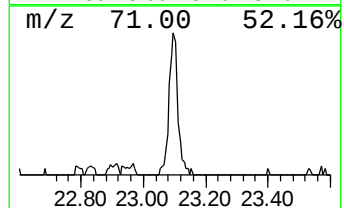
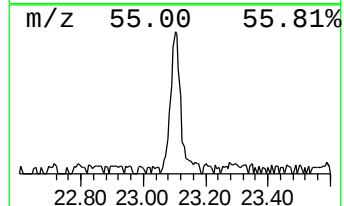
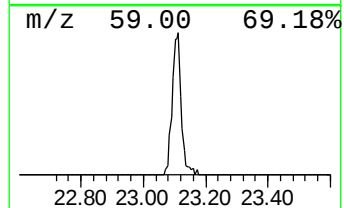
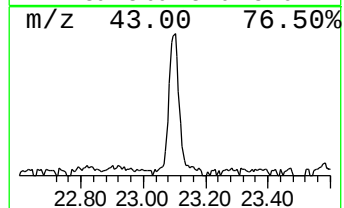
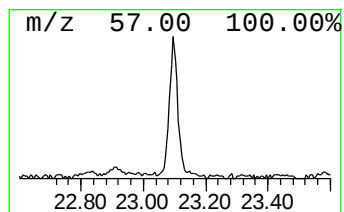
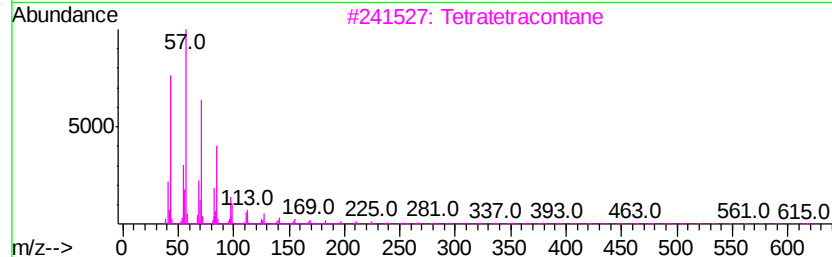
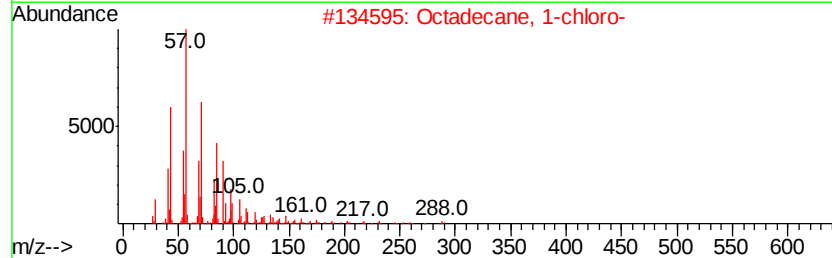
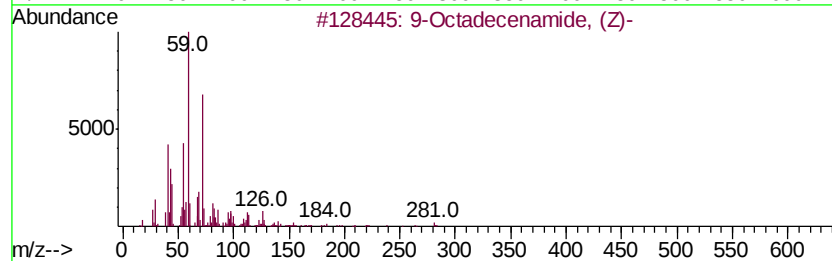
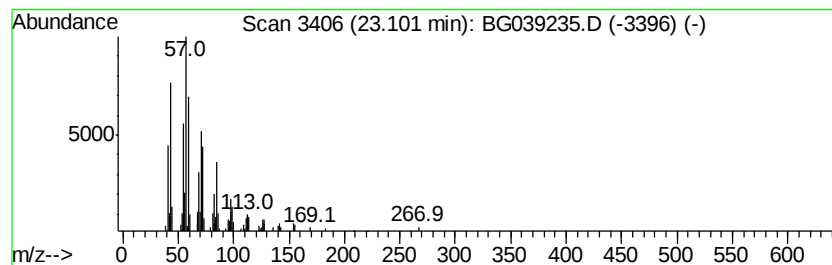
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown23.10 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.10	6.43 ng	115712	Chrysene-d12	21.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	46	
2	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	43	
3	Tetratetracontane	619	C44H90	007098-22-8	43	
4	Tritetracontane	605	C43H88	007098-21-7	43	
5	Heptacosane	380	C27H56	000593-49-7	43	



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
Data File : BG039235.D
Acq On : 21 Jan 2019 16:01
Operator : JU/SJ
Sample : K1205-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-6

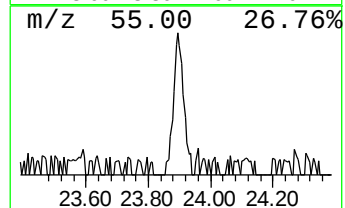
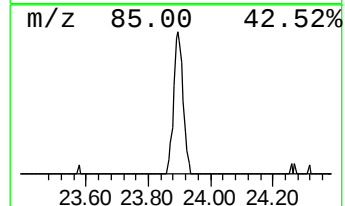
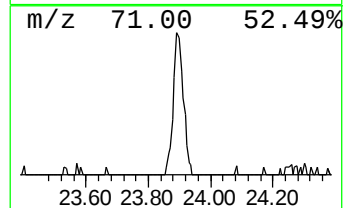
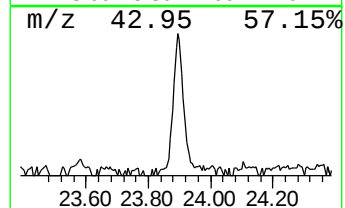
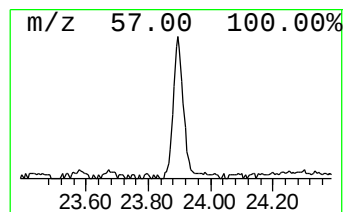
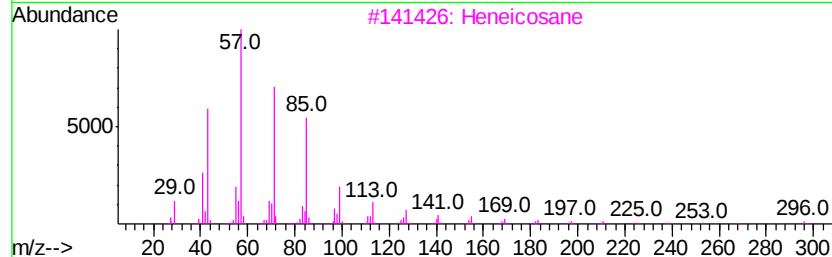
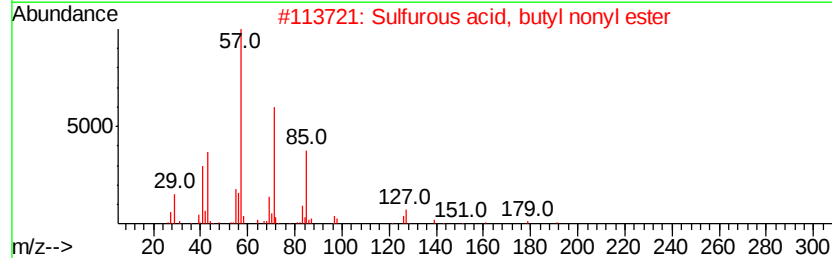
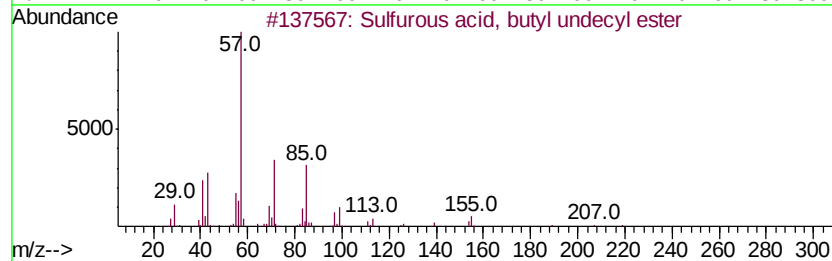
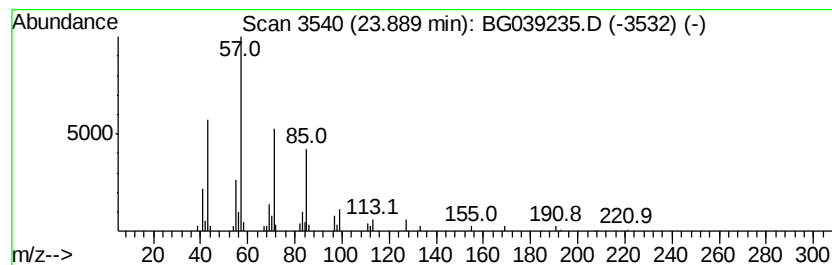
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Sulfurous acid, butyl undec... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.89	3.63 ng	61663	Perylene-d12	24.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	90
2		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	80
3		Heneicosane	296	C21H44	000629-94-7	80
4		Heptacosane	380	C27H56	000593-49-7	74
5		Octadecane	254	C18H38	000593-45-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
Data File : BG039235.D
Acq On : 21 Jan 2019 16:01
Operator : JU/SJ
Sample : K1205-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-6

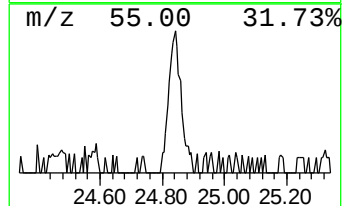
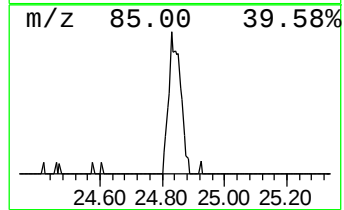
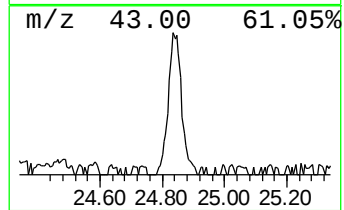
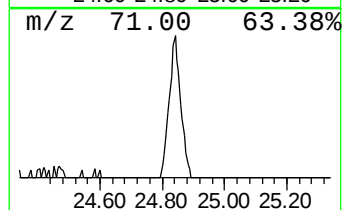
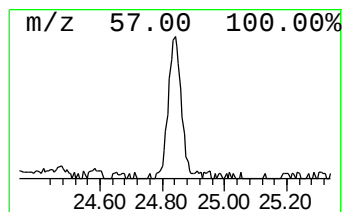
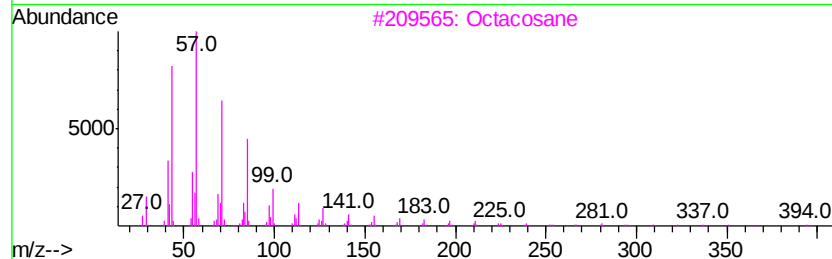
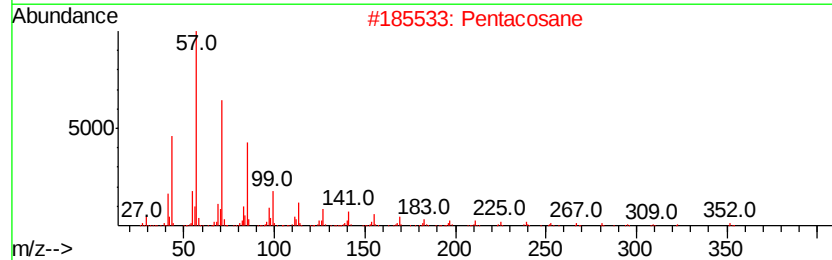
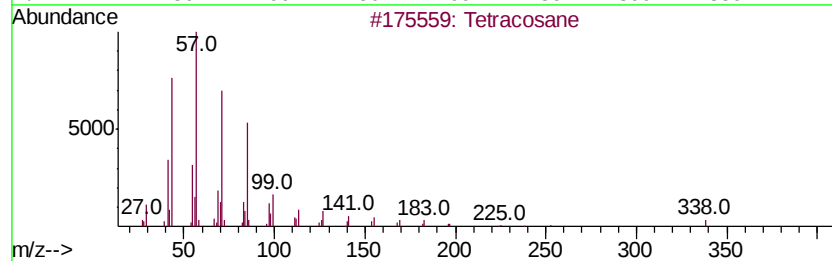
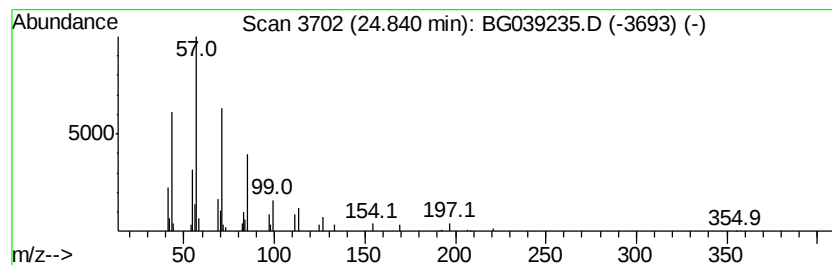
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.84	3.38 ng	57419	Perylene-d12	24.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	87
2		Pentacosane	352	C25H52	000629-99-2	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5		Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
 Data File : BG039235.D
 Acq On : 21 Jan 2019 16:01
 Operator : JU/SJ
 Sample : K1205-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C-6

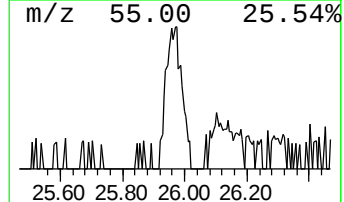
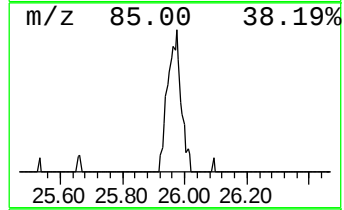
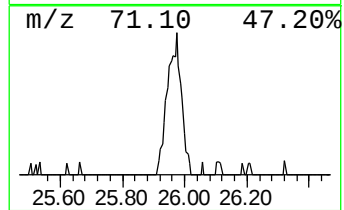
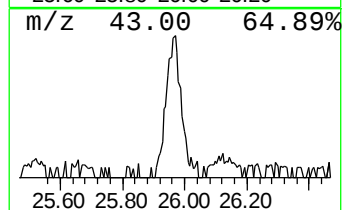
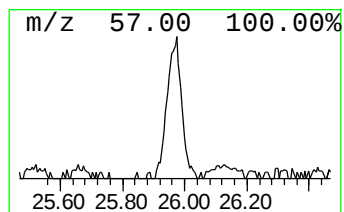
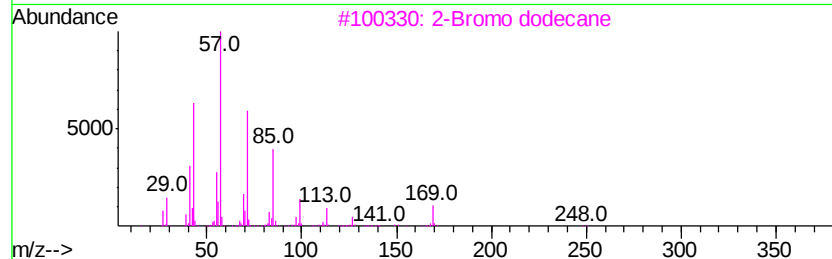
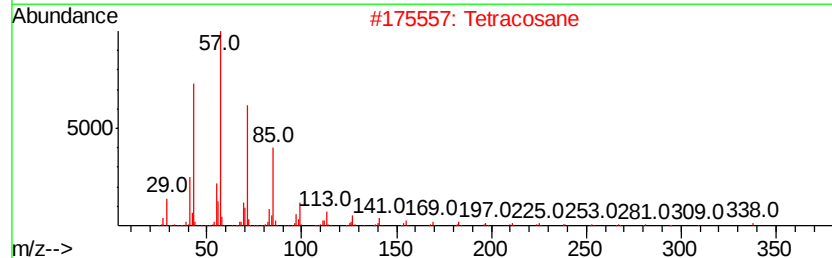
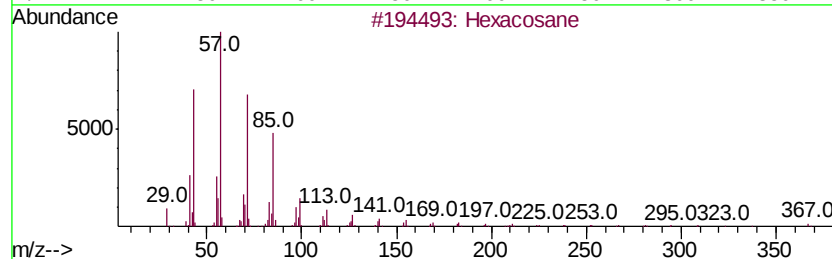
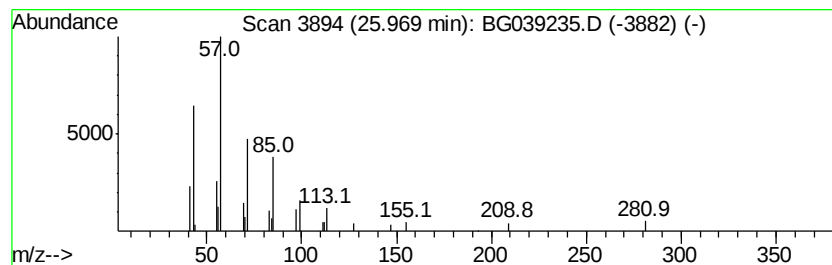
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.97	3.15 ng	53435	Perylene-d12	24.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	80
2		Tetracosane	338	C24H50	000646-31-1	80
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	72
4		Octadecane	254	C18H38	000593-45-3	72
5		Hexatriacontane	507	C36H74	000630-06-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG012119\
Data File : BG039235.D
Acq On : 21 Jan 2019 16:01
Operator : JU/SJ
Sample : K1205-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.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...	5.09	5.6	ng	26930	1	8.01	96166	20.0
unknown7.54	7.54	82.5	ng	396894	1	8.01	96166	20.0
1-Dodecanol, 2-oc...	21.27	4.2	ng	76110	5	21.67	359760	20.0
Sulfurous acid, b...	21.81	2.1	ng	37304	5	21.67	359760	20.0
Octacosane	22.41	2.6	ng	47494	5	21.67	359760	20.0
unknown23.10	23.10	6.4	ng	115712	5	21.67	359760	20.0
Sulfurous acid, b...	23.89	3.6	ng	61663	6	24.93	339513	20.0
Tetracosane	24.84	3.4	ng	57419	6	24.93	339513	20.0
Hexacosane	25.97	3.1	ng	53435	6	24.93	339513	20.0