

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
 Data File : BG048977.D
 Acq On : 15 Jun 2021 14:35
 Operator : CG/JU
 Sample : M2672-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 17-B6(36-40)

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048977.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.169	16	22	32	rVB	115481	232986	12.05%	1.689%
2	3.293	38	43	49	rVB	42981	67696	3.50%	0.491%
3	4.268	203	209	217	rVB6	10120	20735	1.07%	0.150%
4	5.196	362	367	373	rBV3	15685	26826	1.39%	0.195%
5	5.672	441	448	456	rBV	609517	995577	51.48%	7.219%
6	5.737	456	459	469	rVB5	15375	31844	1.65%	0.231%
7	7.270	711	720	730	rBV	590632	1049351	54.26%	7.609%
8	8.117	858	864	873	rBV	170549	286856	14.83%	2.080%
9	9.286	1055	1063	1071	rBV	362796	666428	34.46%	4.832%
10	10.702	1298	1304	1312	rBV2	18968	35685	1.85%	0.259%
11	10.943	1335	1345	1353	rBV	203679	389262	20.13%	2.823%
12	13.381	1754	1760	1768	rVB	857948	1331059	68.82%	9.652%
13	14.762	1988	1995	2001	rVB	327381	525036	27.15%	3.807%
14	16.160	2227	2233	2239	rBV2	32493	51717	2.67%	0.375%
15	16.248	2241	2248	2256	rBV	746011	1165009	60.24%	8.448%
16	17.511	2456	2463	2470	rBV	432140	654372	33.84%	4.745%
17	17.623	2478	2482	2489	rVB7	25874	40686	2.10%	0.295%
18	18.164	2570	2574	2580	rBV8	13802	21759	1.13%	0.158%
19	18.393	2607	2613	2618	rBV2	101169	146186	7.56%	1.060%
20	18.692	2650	2664	2666	rBV3	128761	374799	19.38%	2.718%
21	19.662	2824	2829	2833	rBV	68766	84313	4.36%	0.611%
22	20.114	2900	2906	2913	rVB	1393133	1934007	100.00%	14.024%
23	20.408	2947	2956	2969	rVB2	209289	601859	31.12%	4.364%
24	21.436	3127	3131	3141	rVB4	52880	93248	4.82%	0.676%
25	21.618	3153	3162	3163	rBV2	143742	281350	14.55%	2.040%
26	21.754	3180	3185	3186	rBV4	21032	33105	1.71%	0.240%
27	21.801	3187	3193	3201	rVB2	412527	714646	36.95%	5.182%
28	22.012	3224	3229	3239	rVB10	44738	129549	6.70%	0.939%
29	23.046	3395	3405	3419	rVB3	142412	513101	26.53%	3.721%
30	24.773	3685	3699	3711	rBV4	84116	372080	19.24%	2.698%
31	25.138	3751	3761	3771	rBV2	232551	720442	37.25%	5.224%
32	29.368	4470	4481	4500	rVB7	35601	199520	10.32%	1.447%

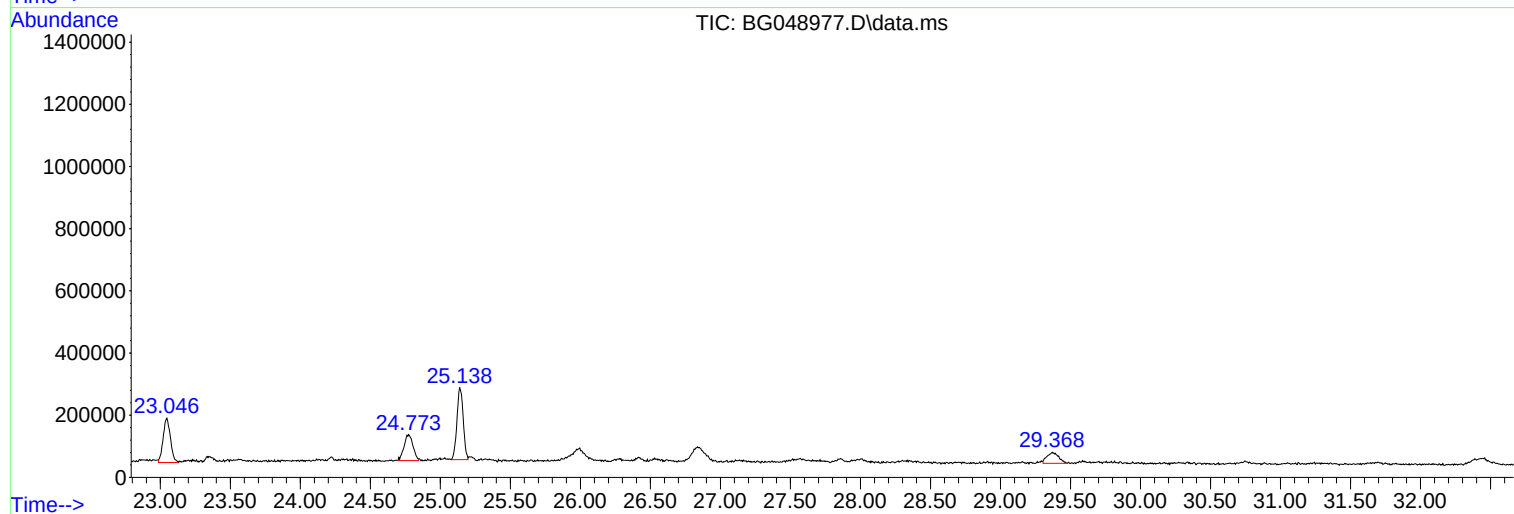
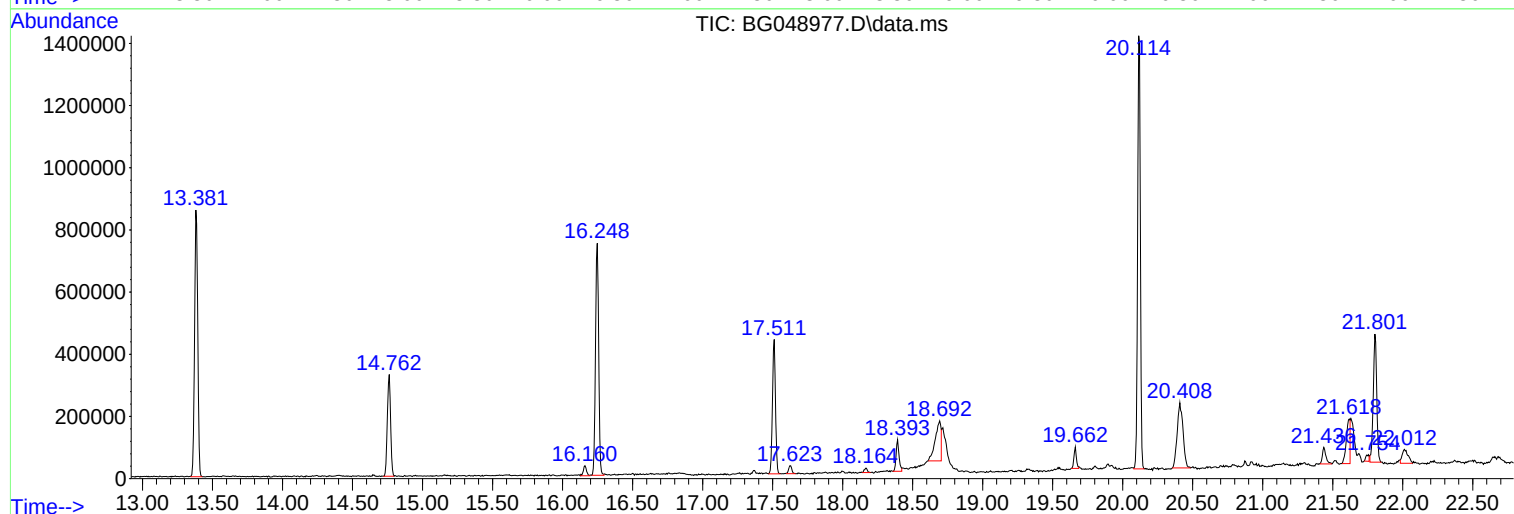
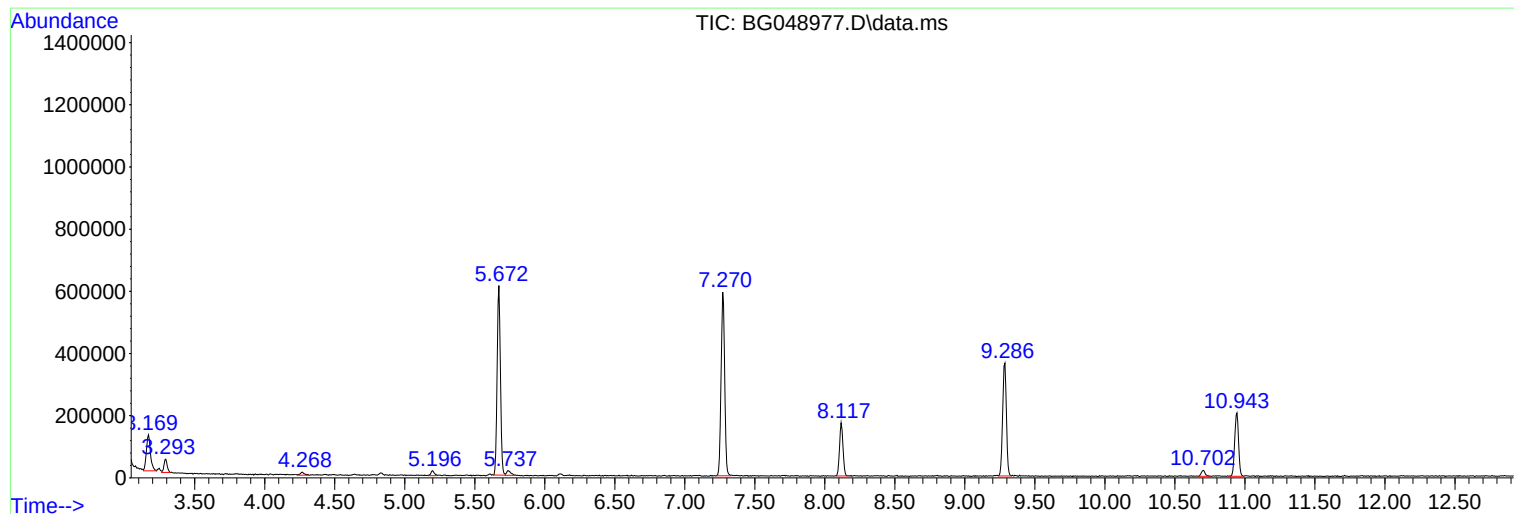
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ClientSampleId :
17-B6(36-40)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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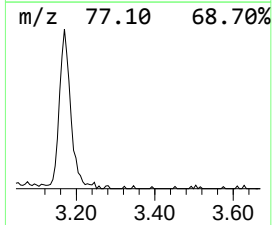
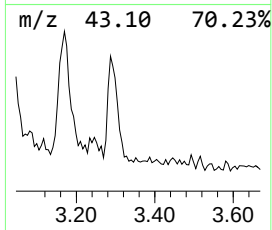
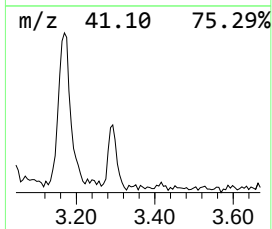
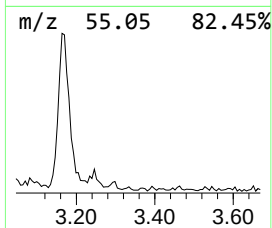
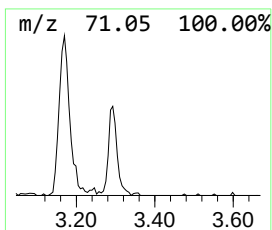
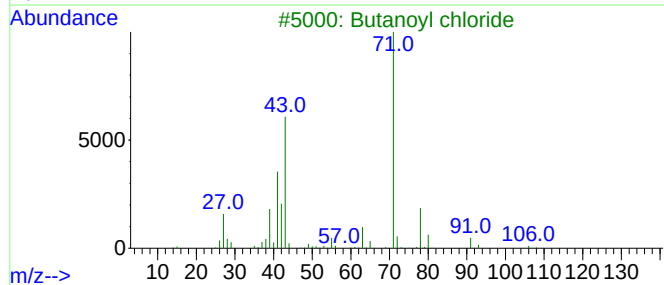
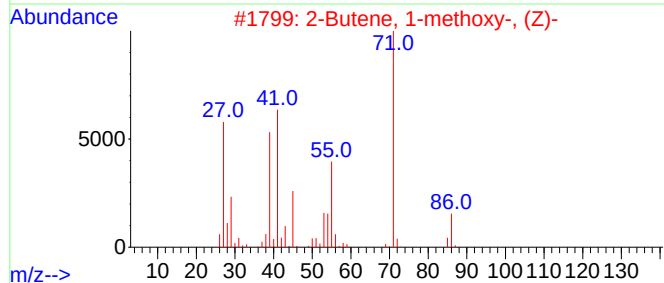
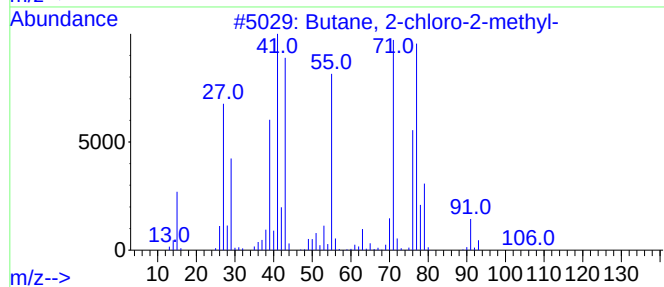
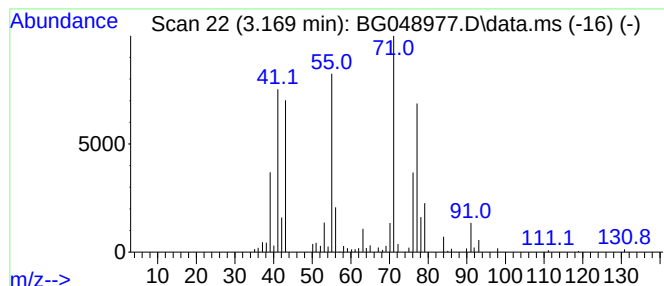
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-chloro-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.169	16.24 ng	232986	1,4-Dichlorobenzene-d4	8.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	80
2			2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	27
3			Butanoyl chloride	106	C4H7ClO	000141-75-3	27
4			Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	25
5			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	22



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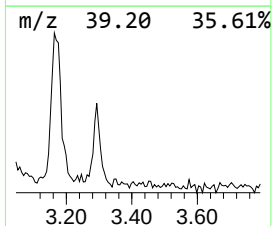
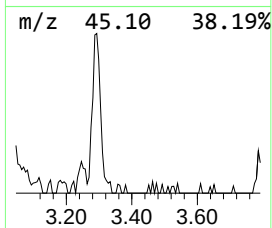
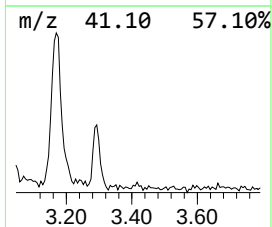
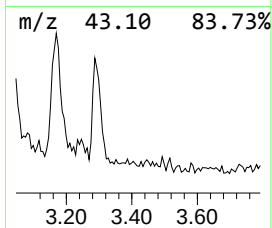
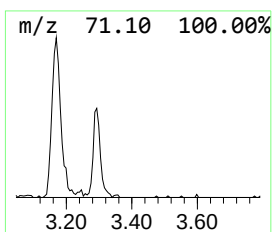
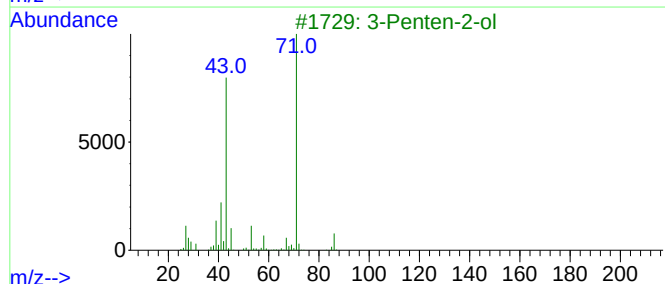
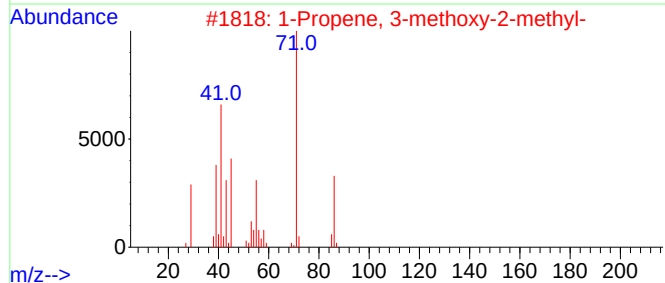
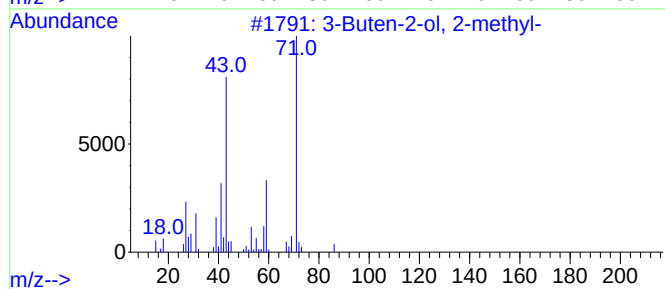
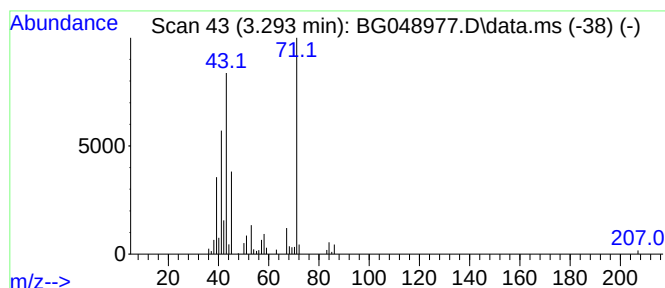
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Buten-2-ol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.293	4.72 ng	67696	1,4-Dichlorobenzene-d4	8.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
2			1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	59
3			3-Penten-2-ol	86	C5H10O	001569-50-2	59
4			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	50
5			Z-1-Methoxy-2-pentene	100	C6H12O	1000279-59-4	45



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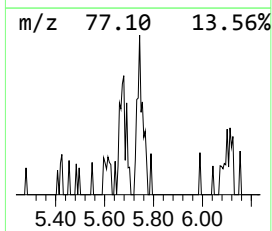
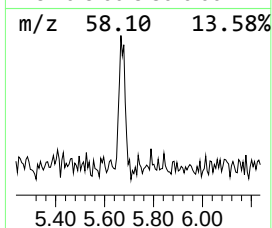
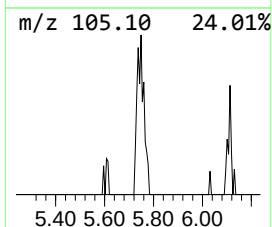
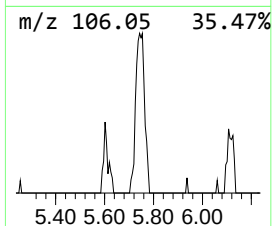
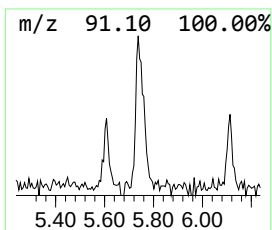
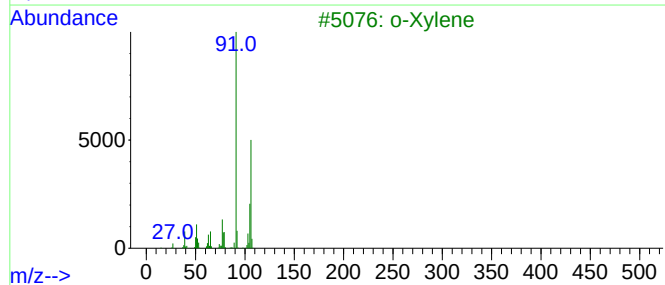
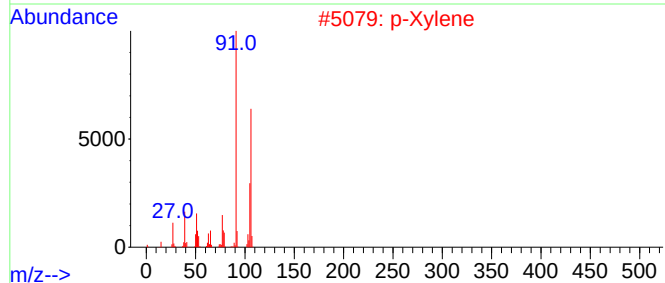
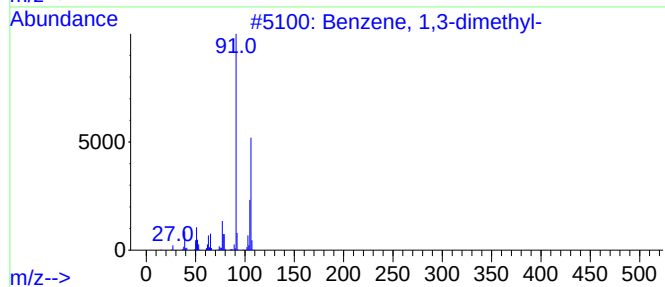
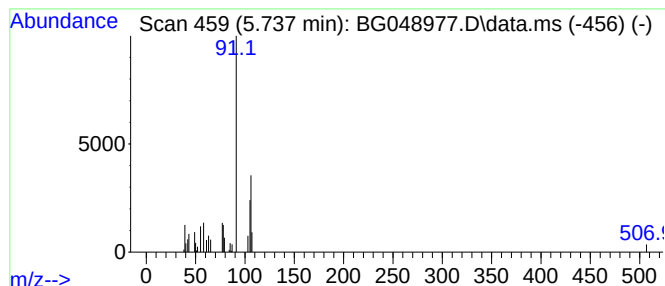
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,3-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.737	2.22 ng	31844	1,4-Dichlorobenzene-d4	8.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	53
2			p-Xylene	106	C8H10	000106-42-3	53
3			o-Xylene	106	C8H10	000095-47-6	47
4			Benzeneethanol, .alpha.,.beta.-d...	150	C10H14O	052089-32-4	45
5			Ethylbenzene	106	C8H10	000100-41-4	43



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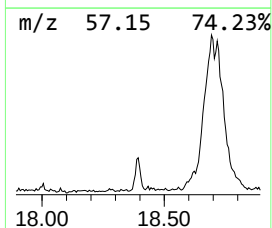
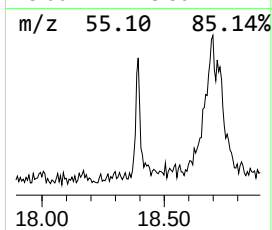
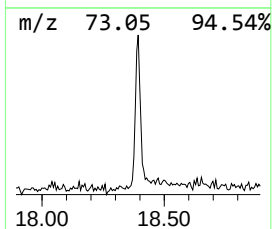
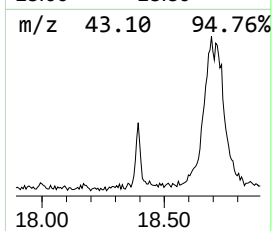
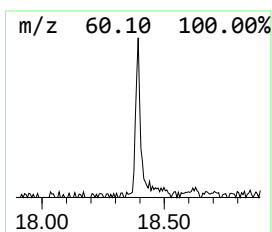
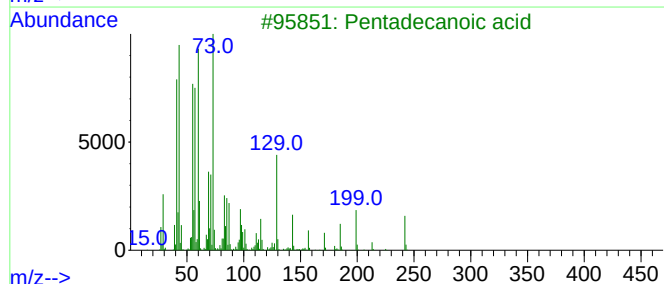
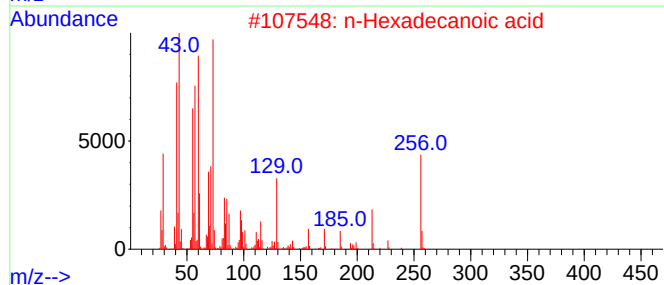
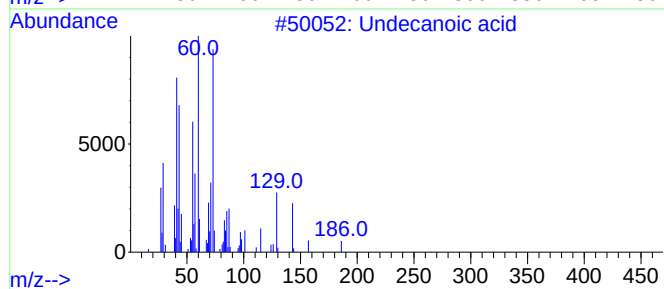
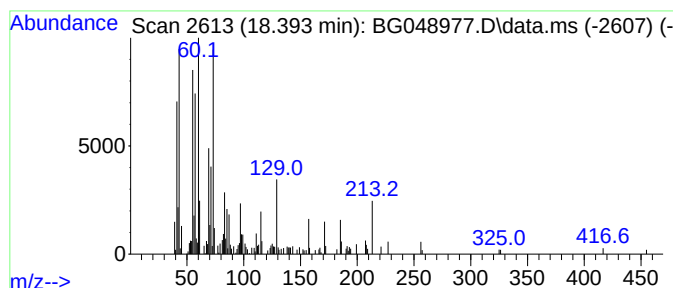
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.393	4.47 ng	146186	Phenanthrene-d10	17.511

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	90
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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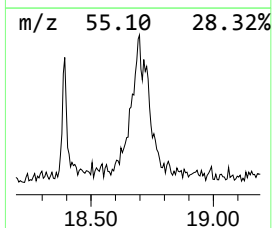
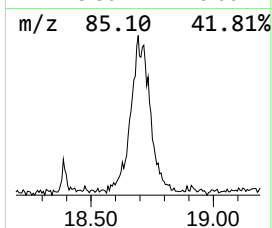
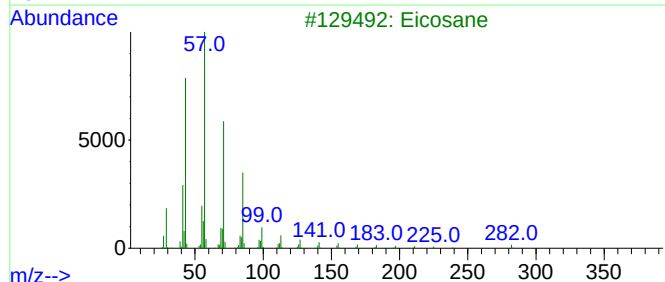
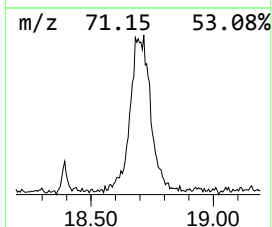
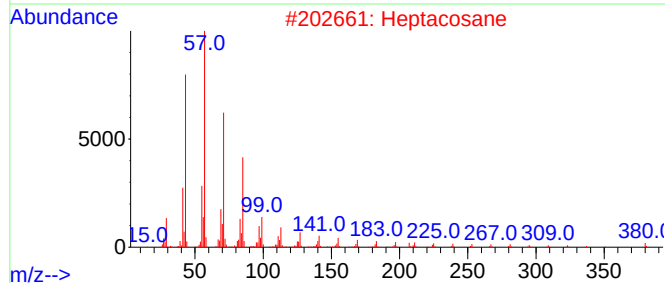
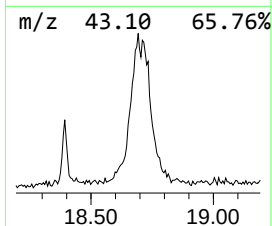
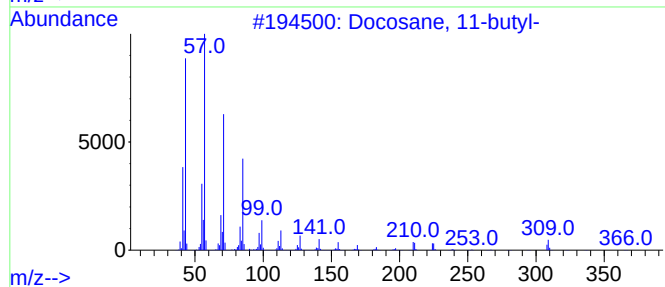
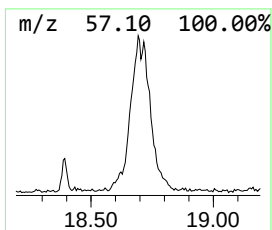
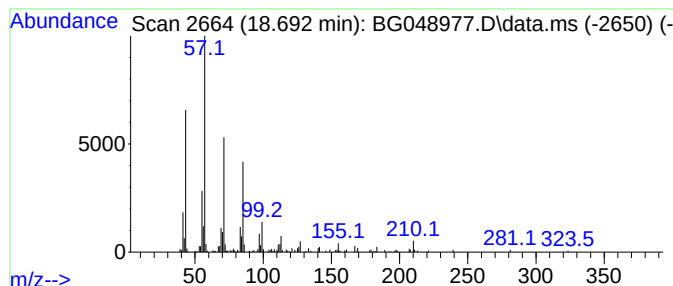
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Docosane, 11-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.692	11.46 ng	374799	Phenanthrene-d10	17.511

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Eicosane	282	C20H42	000112-95-8	90
4			Pentadecane	212	C15H32	000629-62-9	87
5			Tridecane, 2-methyl-	198	C14H30	001560-96-9	87



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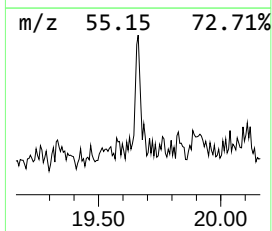
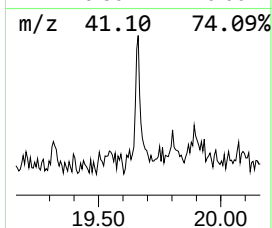
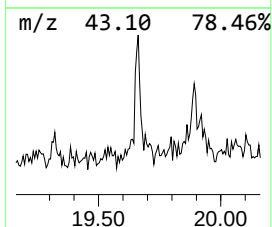
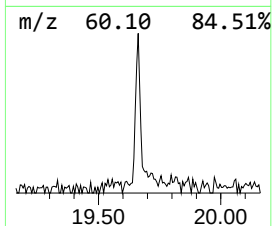
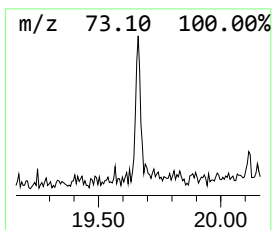
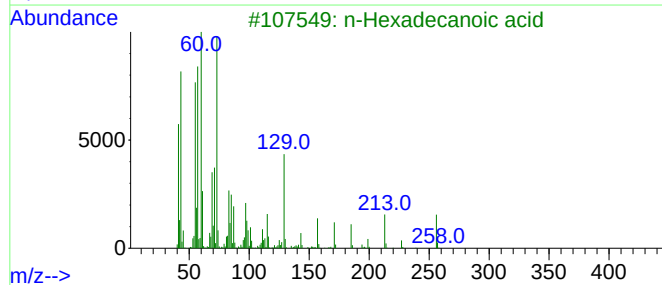
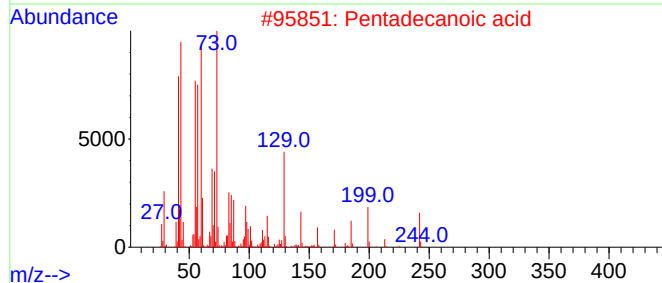
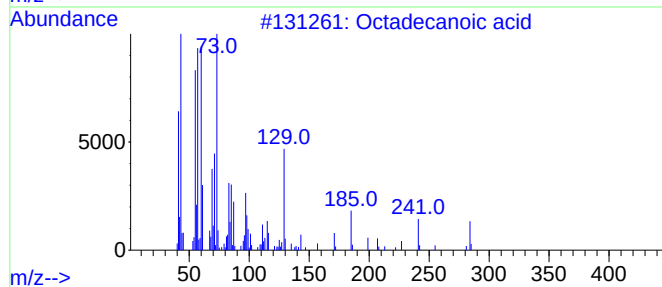
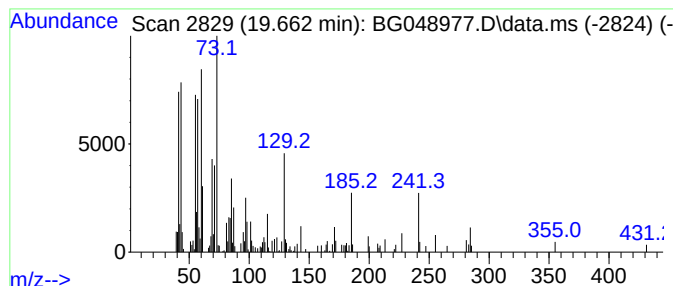
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.662	2.36 ng	84313	Chrysene-d12	21.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
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Acq On : 15 Jun 2021 14:35
Operator : CG/JU
Sample : M2672-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

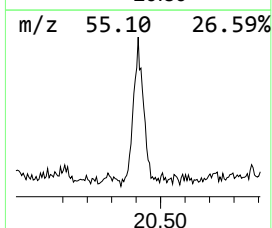
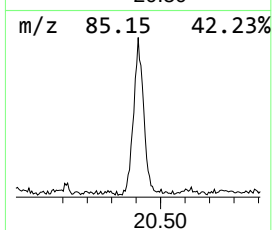
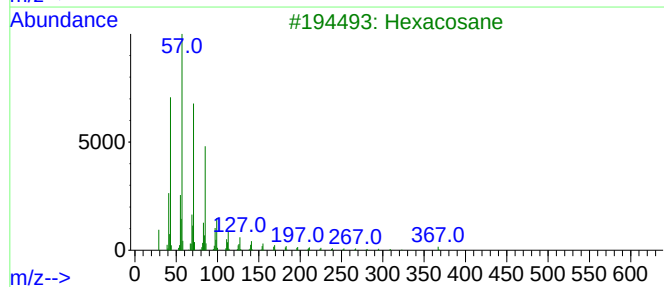
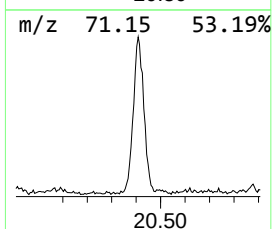
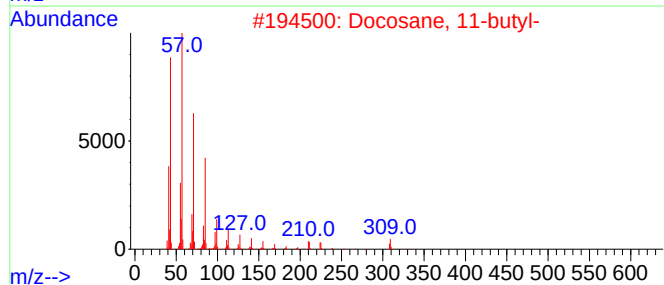
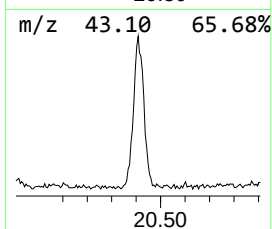
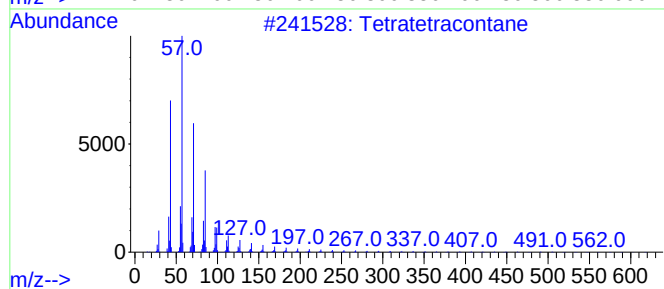
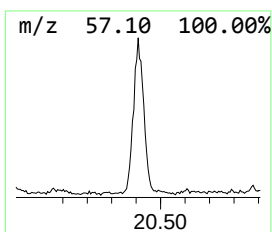
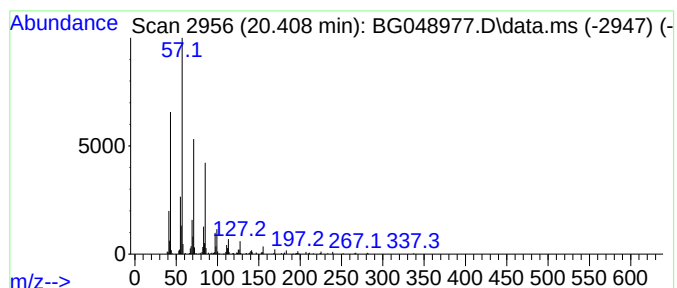
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.408	16.84 ng	601859	Chrysene-d12		21.801	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetratetracontane		619	C44H90	007098-22-8	91
2	Docosane, 11-butyl-		366	C26H54	013475-76-8	91
3	Hexacosane		366	C26H54	000630-01-3	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048977.D
Acq On : 15 Jun 2021 14:35
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
17-B6(36-40)

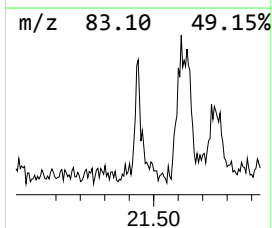
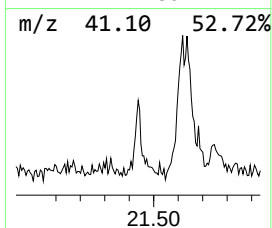
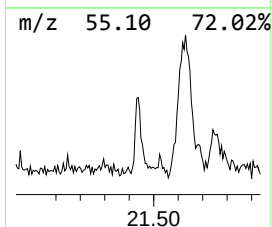
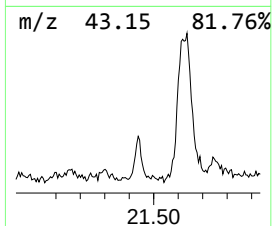
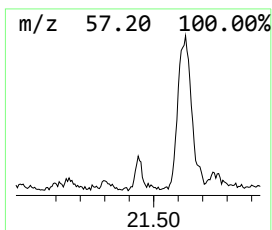
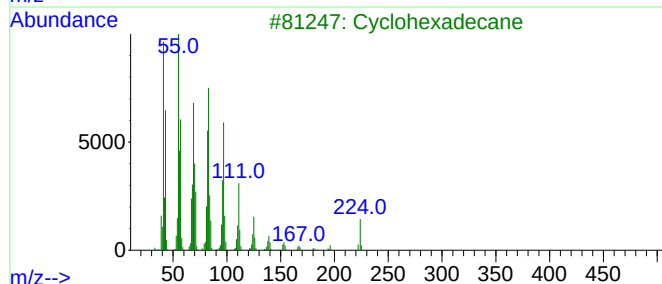
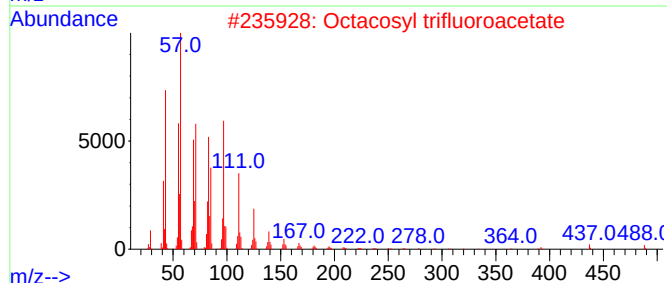
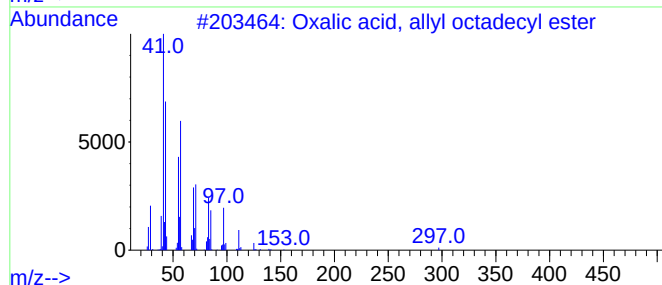
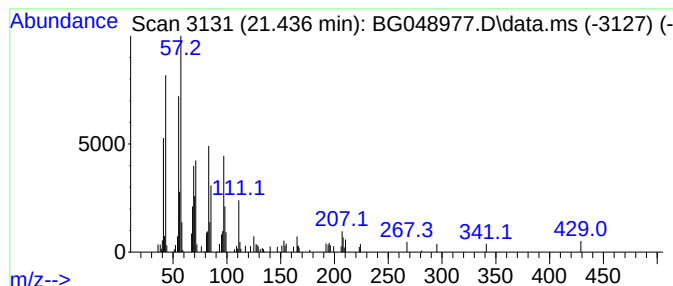
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxalic acid, allyl octadecy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.436	2.61 ng	93248	Chrysene-d12	21.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	72
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	72
3			Cyclohexadecane	224	C16H32	000295-65-8	70
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	64
5			Octacosanol	410	C28H58O	000557-61-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048977.D
Acq On : 15 Jun 2021 14:35
Operator : CG/JU
Sample : M2672-08
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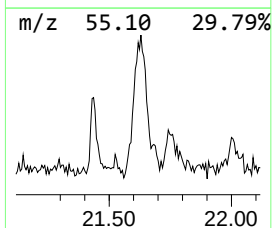
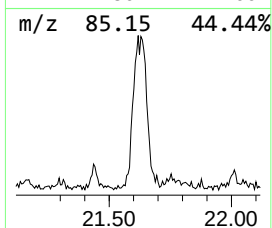
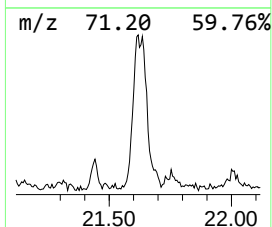
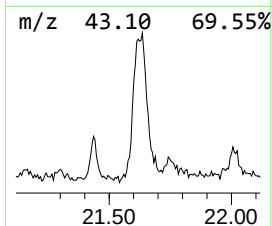
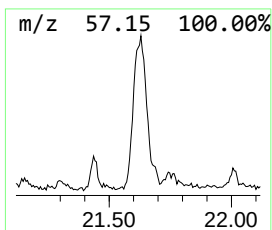
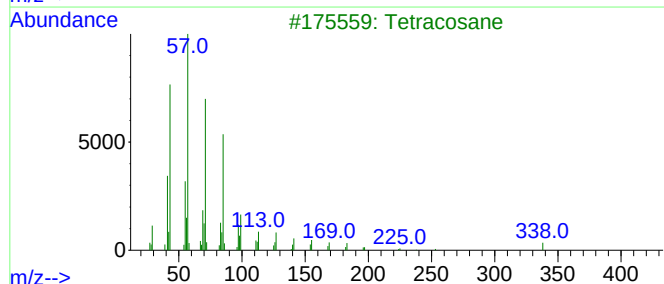
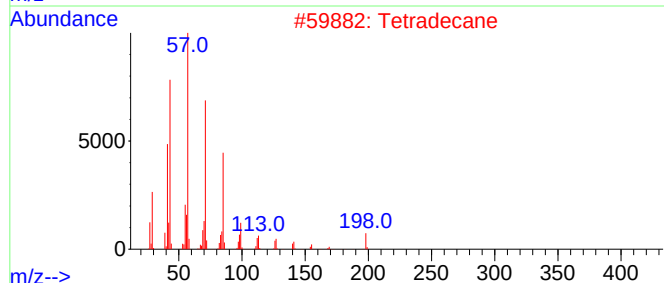
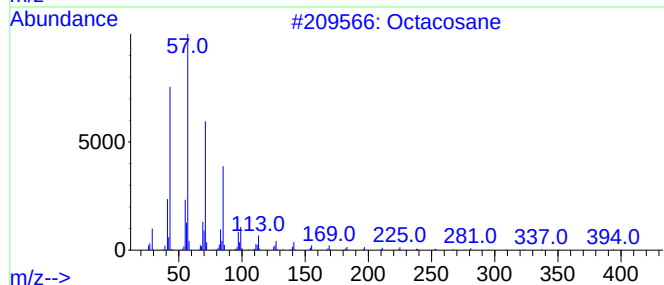
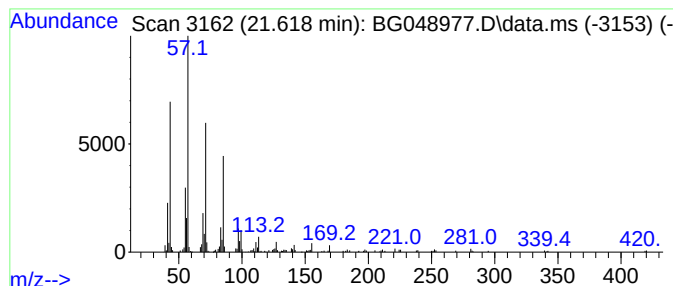
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.618	7.87 ng	281350	Chrysene-d12	21.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Tetradecane	198	C14H30	000629-59-4	87
3			Tetracosane	338	C24H50	000646-31-1	87
4			Eicosane, 9-octyl-	394	C28H58	013475-77-9	87
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048977.D
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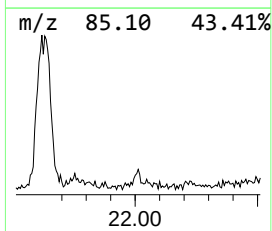
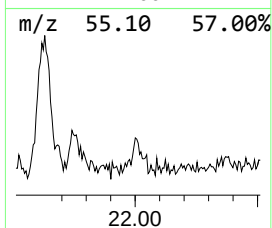
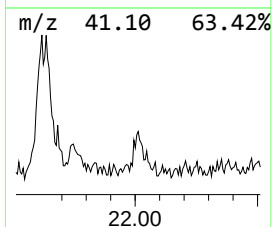
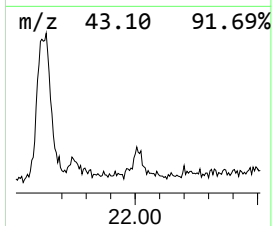
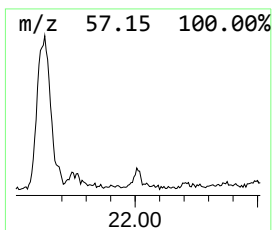
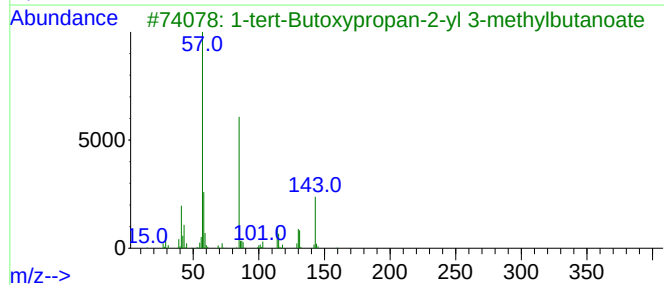
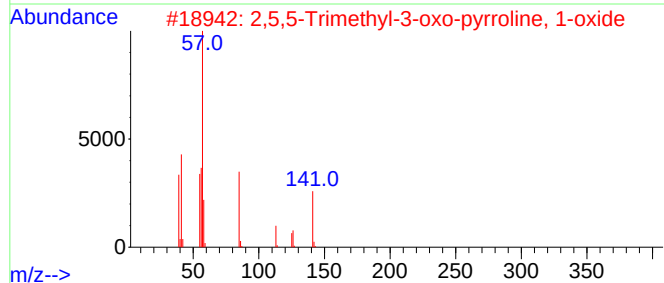
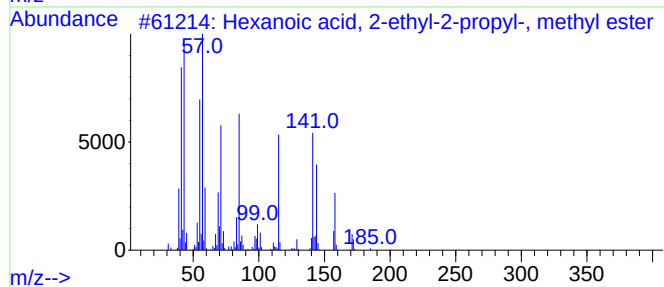
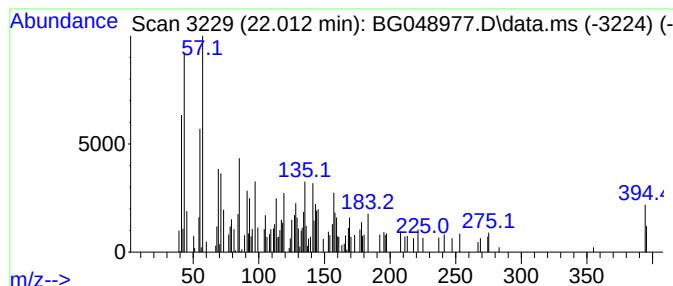
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown22.012 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.012	3.63 ng	129549	Chrysene-d12	21.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-2-propyl-...	200	C12H24O2	054889-60-0	25
2			2,5,5-Trimethyl-3-oxo-pyrroline,...	141	C7H11NO2	1000305-90-5	14
3			1-tert-Butoxypropan-2-yl 3-methy...	216	C12H24O3	1000367-13-3	10
4			2H-Azepin-2-one, 5-(1,1-dimethyl...	169	C10H19NO	032741-89-2	10
5			Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048977.D
Acq On : 15 Jun 2021 14:35
Operator : CG/JU
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ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId :
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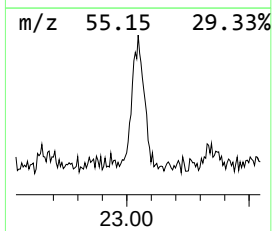
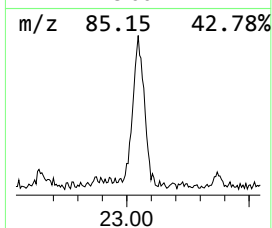
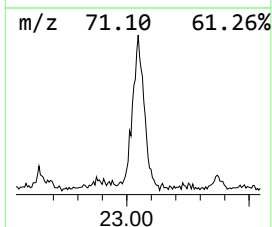
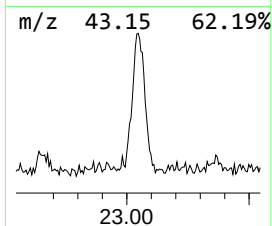
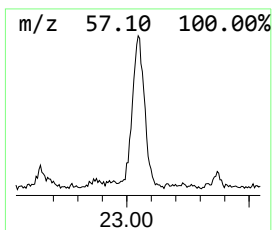
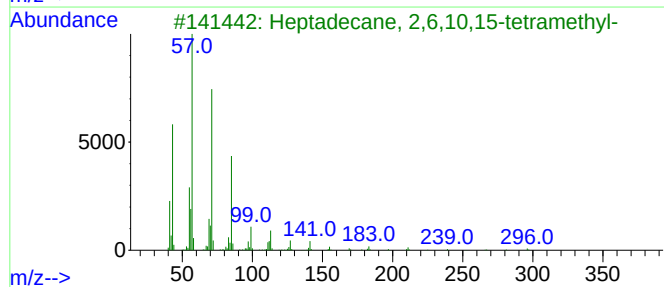
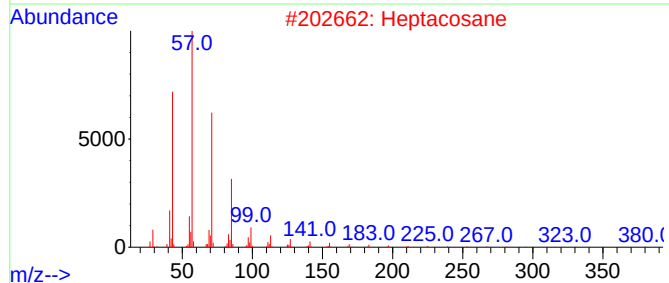
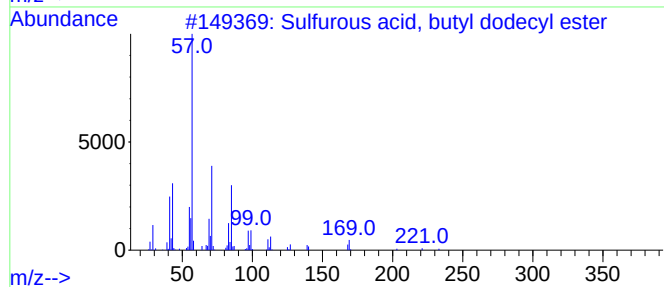
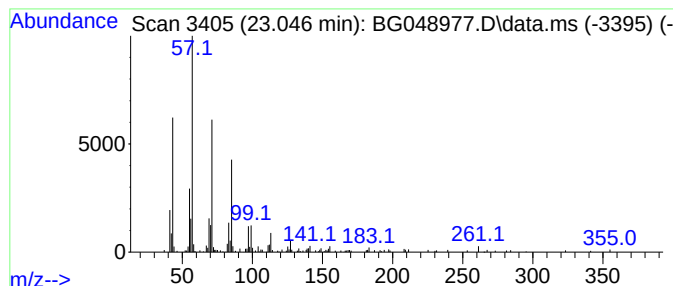
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Sulfurous acid, butyl dodec... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.046	14.36 ng	513101	Chrysene-d12	21.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
2			Heptacosane	380	C27H56	000593-49-7	83
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
4			Heneicosane	296	C21H44	000629-94-7	80
5			Eicosane	282	C20H42	000112-95-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048977.D
Acq On : 15 Jun 2021 14:35
Operator : CG/JU
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
17-B6(36-40)

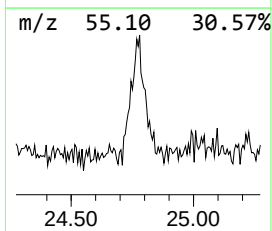
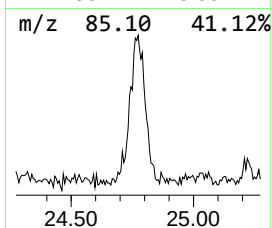
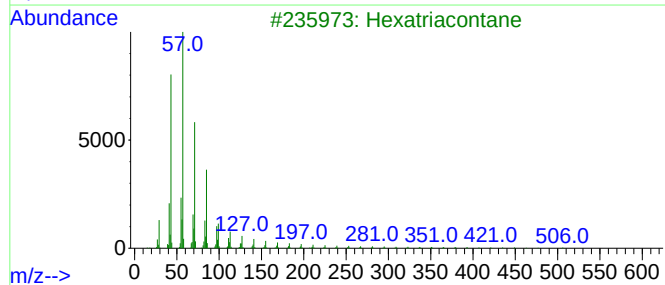
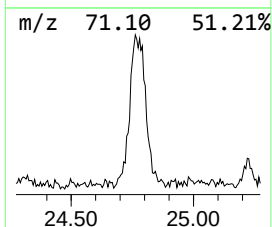
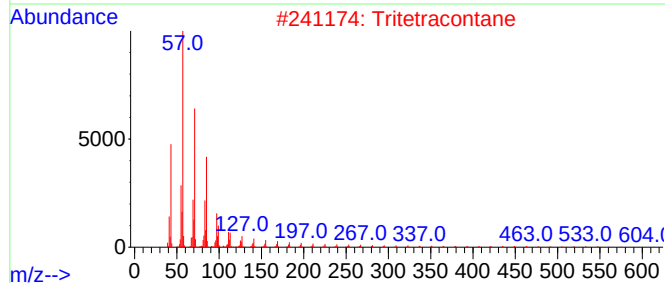
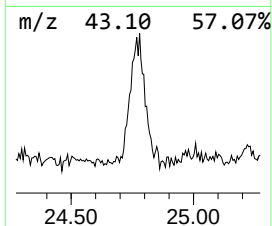
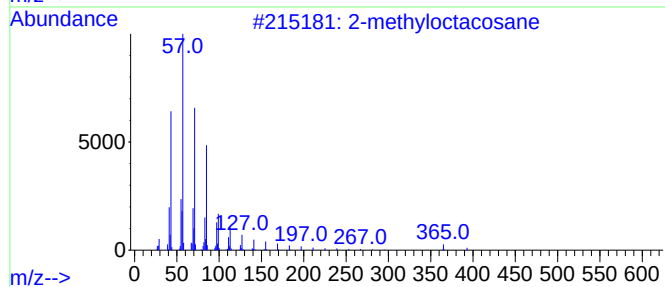
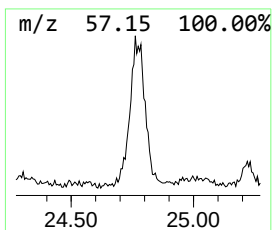
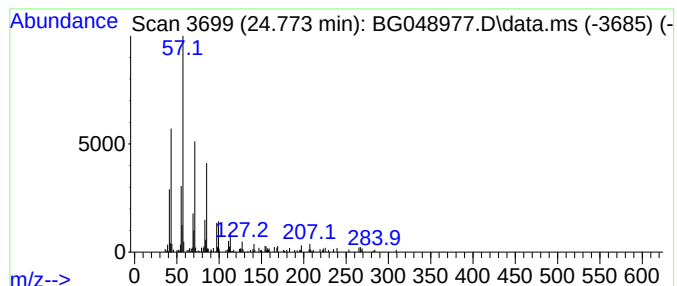
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.773	10.33 ng	372080	Perylene-d12	25.144

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Tritetracontane	605	C43H88	007098-21-7	87
3		Hexatriacontane	507	C36H74	000630-06-8	86
4		Docosane	310	C22H46	000629-97-0	86
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048977.D
Acq On : 15 Jun 2021 14:35
Operator : CG/JU
Sample : M2672-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(36-40)

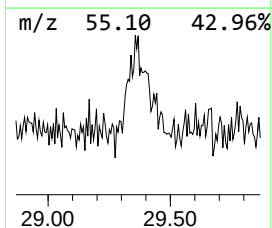
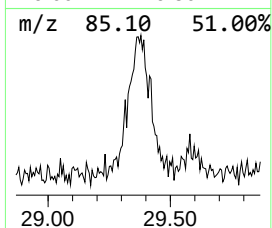
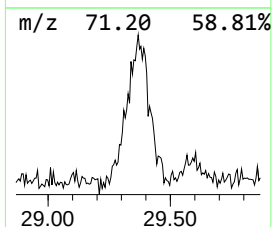
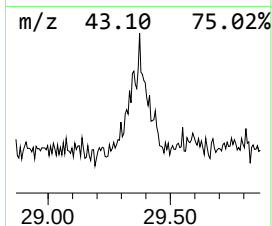
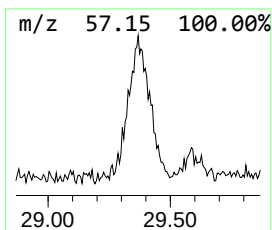
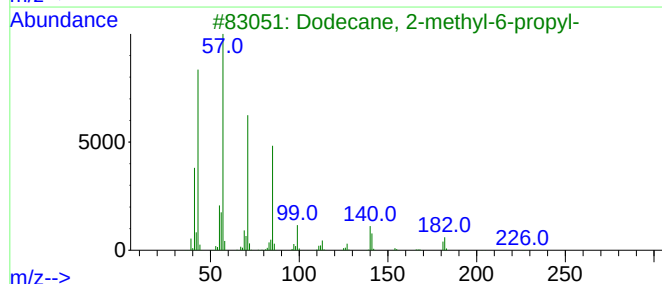
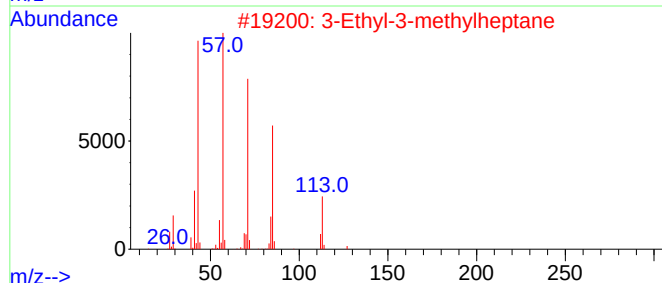
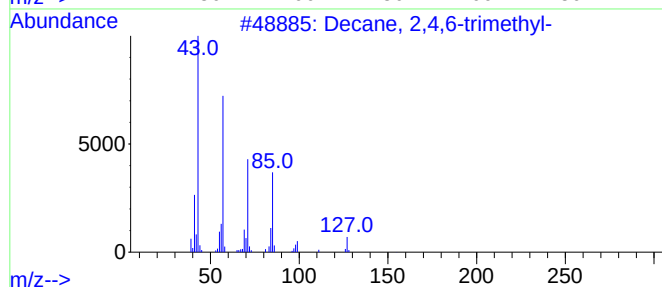
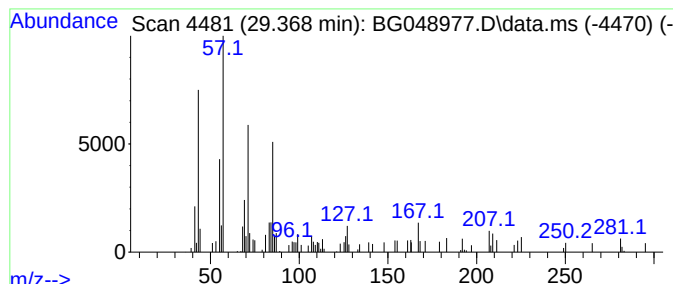
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown29.368 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.368	5.54 ng	199520	Perylene-d12	25.144

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	47
2			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	47
3			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	47
4			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	47
5			Undecane, 4-ethyl-	184	C13H28	017312-59-3	47



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Sample : M2672-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(36-40)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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-chlor...	3.169	16.2	ng	232986	1	8.117	286856	20.0
3-Buten-2-ol, 2...	3.293	4.7	ng	67696	1	8.117	286856	20.0
Benzene, 1,3-di...	5.737	2.2	ng	31844	1	8.117	286856	20.0
Undecanoic acid	18.393	4.5	ng	146186	4	17.511	654372	20.0
Docosane, 11-bu...	18.692	11.5	ng	374799	4	17.511	654372	20.0
Octadecanoic acid	19.662	2.4	ng	84313	5	21.801	714646	20.0
Tetratetracontane	20.408	16.8	ng	601859	5	21.801	714646	20.0
Oxalic acid, al...	21.436	2.6	ng	93248	5	21.801	714646	20.0
Octacosane	21.618	7.9	ng	281350	5	21.801	714646	20.0
unknown22.012	22.012	3.6	ng	129549	5	21.801	714646	20.0
Sulfurous acid,...	23.046	14.4	ng	513101	5	21.801	714646	20.0
2-methyloctacosane	24.773	10.3	ng	372080	6	25.144	720442	20.0
unknown29.368	29.368	5.5	ng	199520	6	25.144	720442	20.0