

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050720\
 Data File : BG045283.D
 Acq On : 7 May 2020 23:59
 Operator : CG/JU
 Sample : L2529-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 72-11936

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-BG041520.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	5.552	411	419	430	rBV	1096987	1851218	27.75%	5.663%
2	7.144	683	690	704	rBV	1172382	2167858	32.49%	6.631%
3	7.978	825	832	841	rBV	185286	334529	5.01%	1.023%
4	8.307	880	888	898	rBV	989121	1785659	26.76%	5.462%
5	9.141	1021	1030	1040	rBV	795105	1495419	22.41%	4.574%
6	10.786	1303	1310	1325	rBV	243456	464549	6.96%	1.421%
7	13.248	1721	1729	1743	rBV	2407037	3911129	58.62%	11.963%
8	13.518	1770	1775	1783	rVB	73269	117297	1.76%	0.359%
9	14.070	1863	1869	1876	rBV	176077	274213	4.11%	0.839%
10	14.622	1953	1963	1977	rBV2	426598	710851	10.65%	2.174%
11	16.114	2210	2217	2231	rBV	2267971	3528119	52.88%	10.792%
12	17.371	2422	2431	2443	rBV	598971	948317	14.21%	2.901%
13	19.986	2869	2876	2889	rBV	4701183	6672256	100.00%	20.409%
14	20.749	3002	3006	3009	rBV	103856	113347	1.70%	0.347%
15	21.296	3093	3099	3114	rBV2	232568	475519	7.13%	1.455%
16	21.636	3150	3157	3173	rVB	598477	1051616	15.76%	3.217%
17	21.842	3185	3192	3198	rBV4	64048	107473	1.61%	0.329%
18	22.083	3227	3233	3239	rVB2	79038	122213	1.83%	0.374%
19	22.453	3289	3296	3308	rBV3	291715	853327	12.79%	2.610%
20	23.128	3404	3411	3417	rVB4	122882	263539	3.95%	0.806%
21	23.469	3463	3469	3476	rVB3	176506	357070	5.35%	1.092%
22	23.933	3539	3548	3555	rBV	838905	1755504	26.31%	5.370%
23	24.803	3686	3696	3704	rBV2	359093	1091640	16.36%	3.339%
24	25.372	3782	3793	3804	rBV3	188772	532415	7.98%	1.629%
25	25.983	3885	3897	3908	rBV2	345211	1057161	15.84%	3.234%
26	26.101	3911	3917	3925	rBV2	30964	96930	1.45%	0.296%
27	27.323	4115	4125	4132	rBV5	34123	105722	1.58%	0.323%
28	28.092	4242	4256	4270	rBV6	90352	369970	5.54%	1.132%
29	31.499	4825	4836	4837	rBV9	29923	77359	1.16%	0.237%

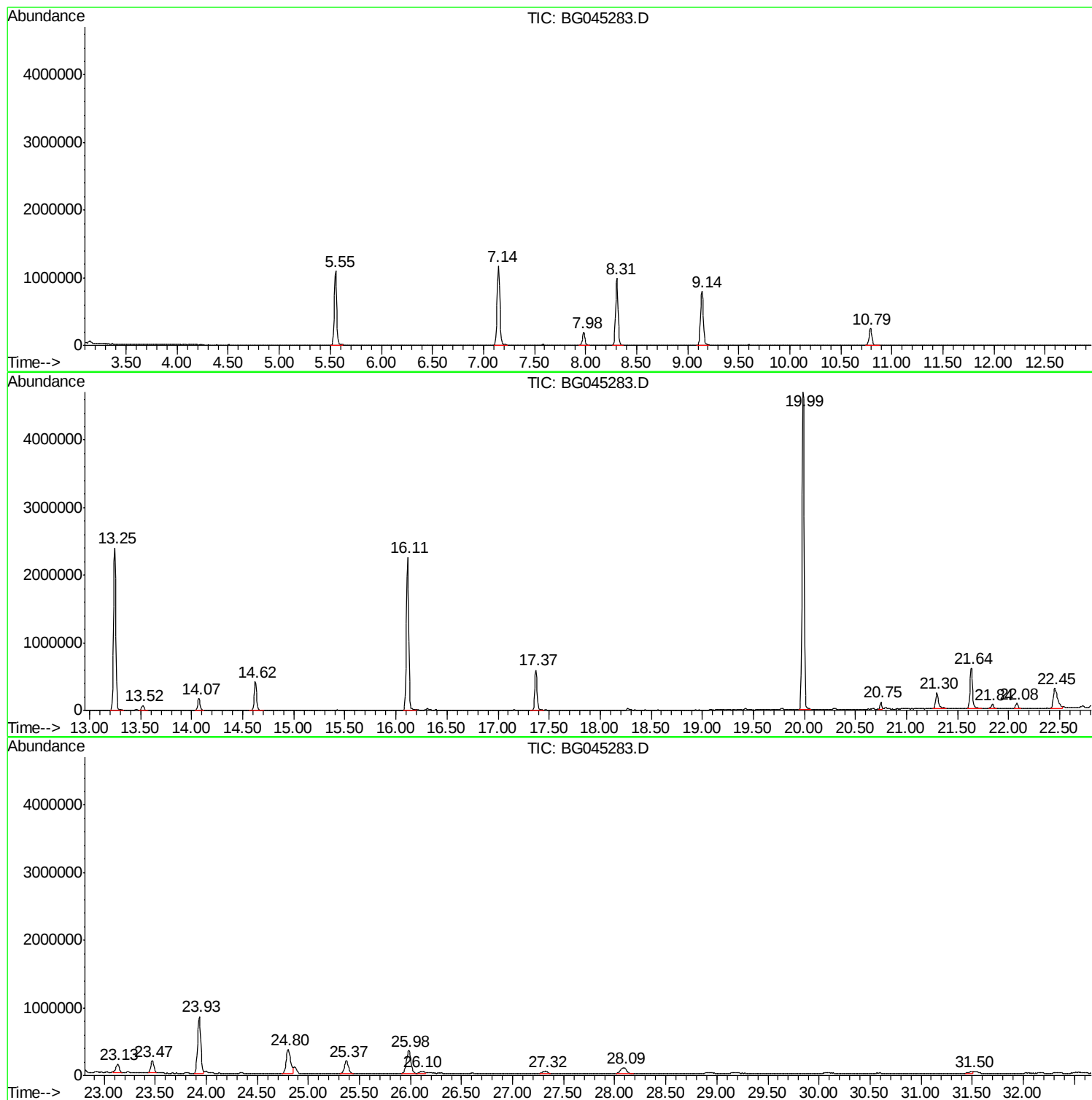
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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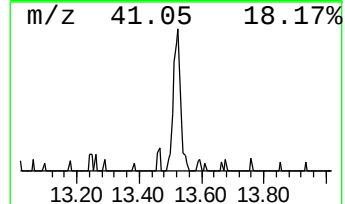
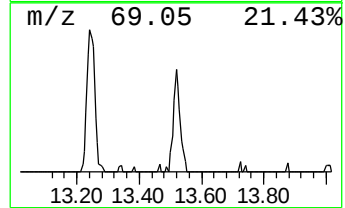
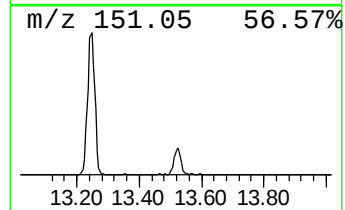
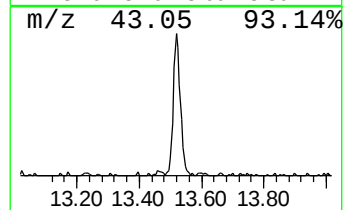
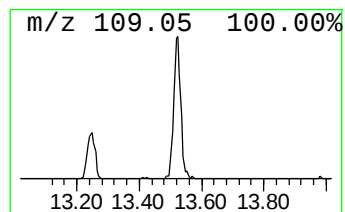
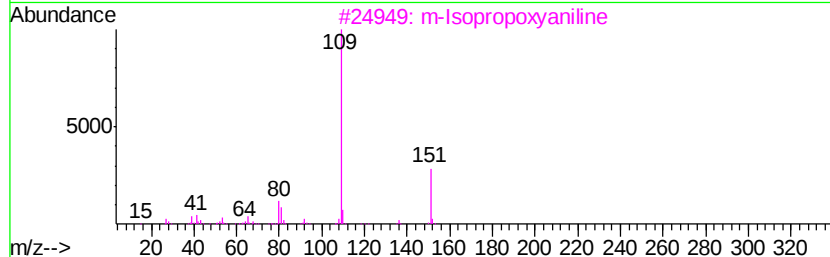
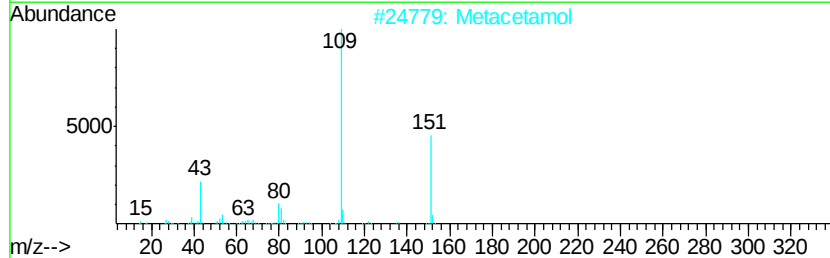
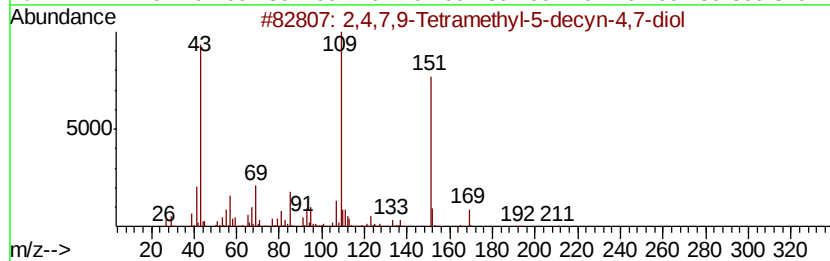
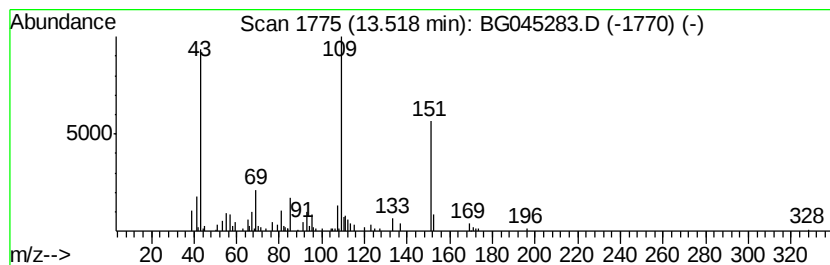
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.52	3.30 ng	117297	Acenaphthene-d10	14.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	78
2	Metacetamol	151	C8H9NO2	000621-42-1	59
3	m-Isopropoxvaniline	151	C9H13NO	041406-00-2	59
4	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	50
5	Ethanone, 1-(1,3-dimethyl-3-cycl...	152	C10H16O	051733-68-7	43



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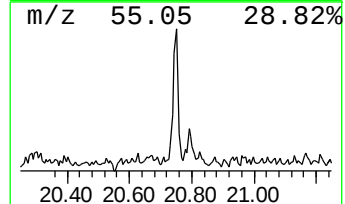
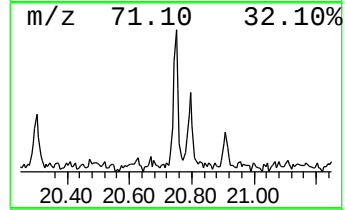
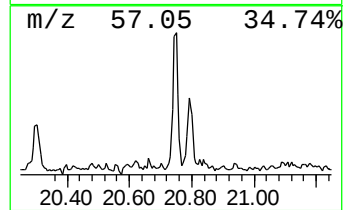
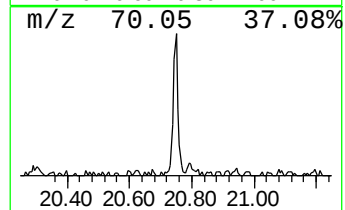
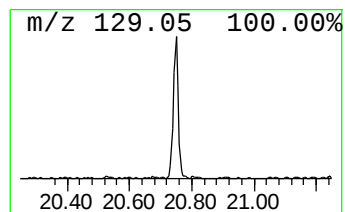
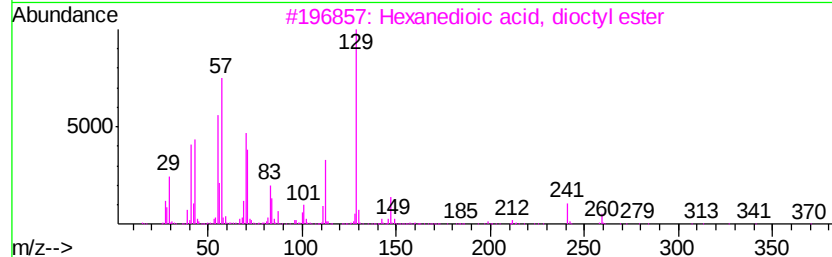
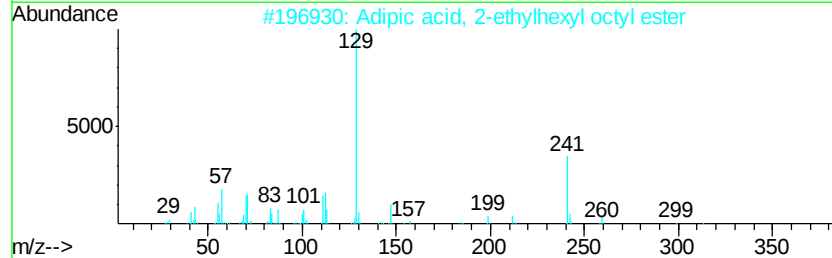
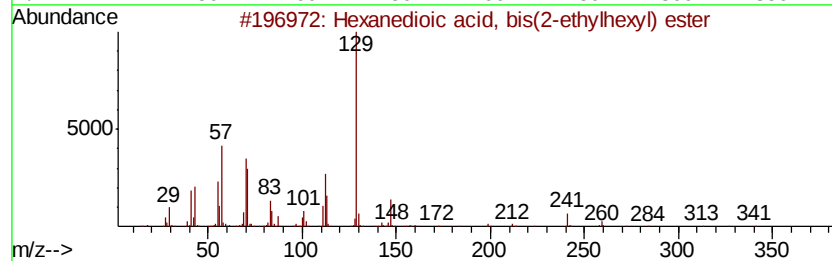
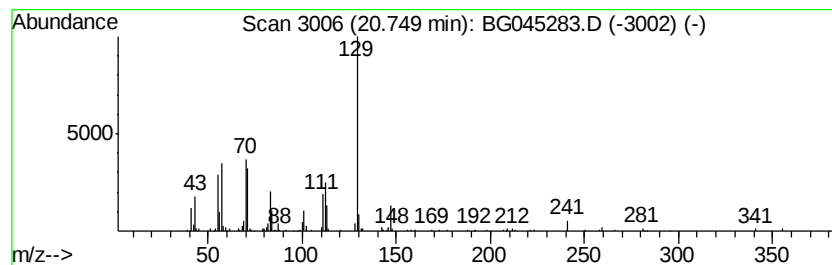
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Peak Number 3 Hexanedioic acid, bis(2-eth... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.75	2.16 ng	113347	Chrysene-d12	21.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2		Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	83
3		Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	72
4		Adipic acid, cyclopentylmethyl o...	340	C20H36O4	1000324-77-8	53
5		Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	53



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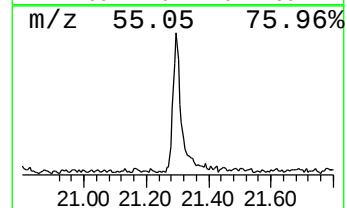
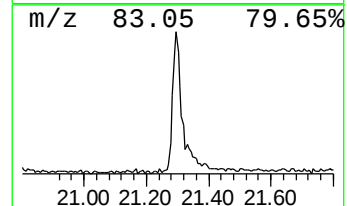
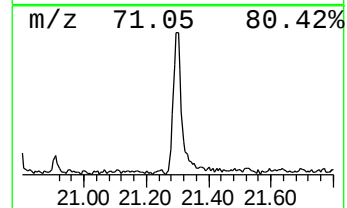
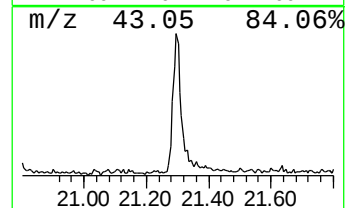
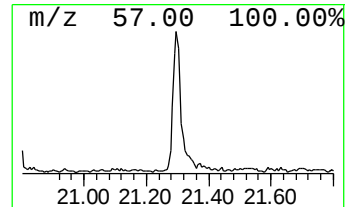
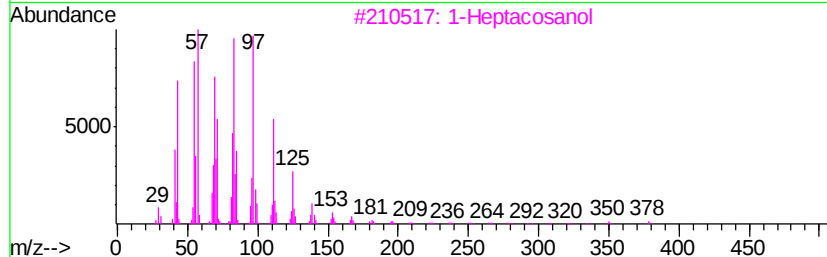
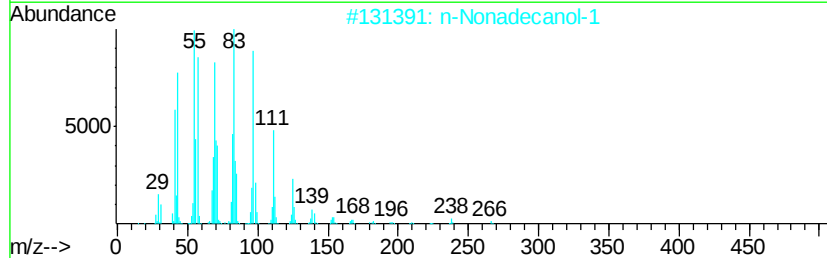
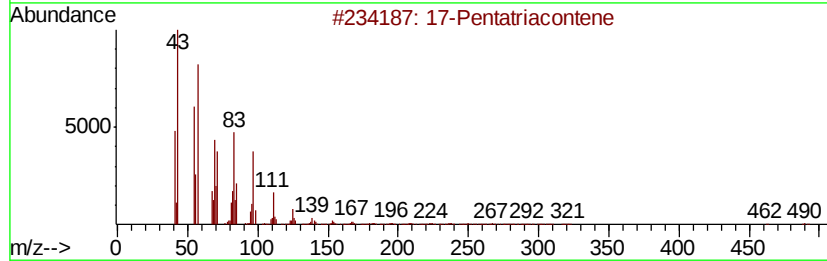
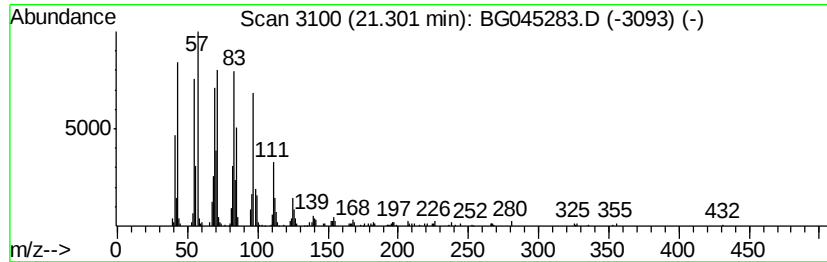
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Peak Number 4 17-Pentatriacontene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	9.04 ng	475519	Chrysene-d12	21.64
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		17-Pentatriacontene	491 C35H70	006971-40-0 91
2		n-Nonadecanol-1	284 C19H40O	001454-84-8 87
3		1-Heptacosanol	396 C27H56O	002004-39-9 87
4		Oxalic acid, isobutyl hexadecyl ...	370 C22H42O4	1000309-38-1 83
5		Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3 83



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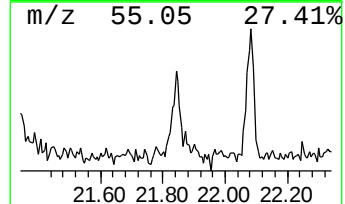
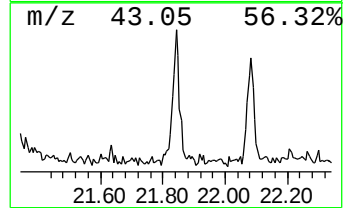
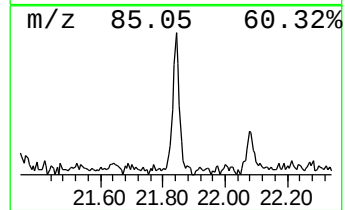
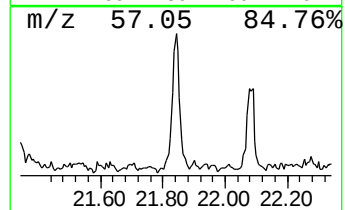
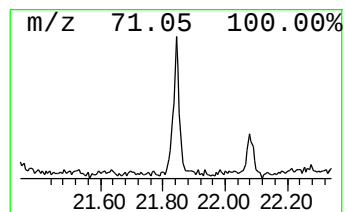
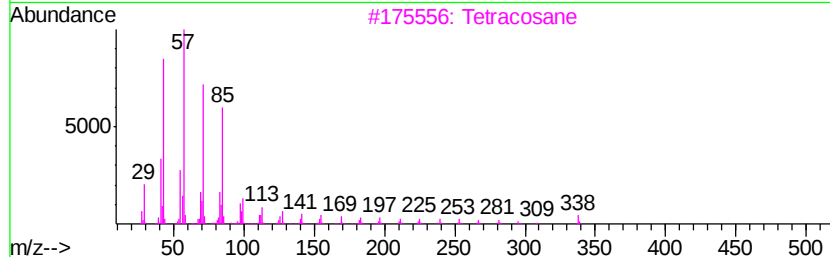
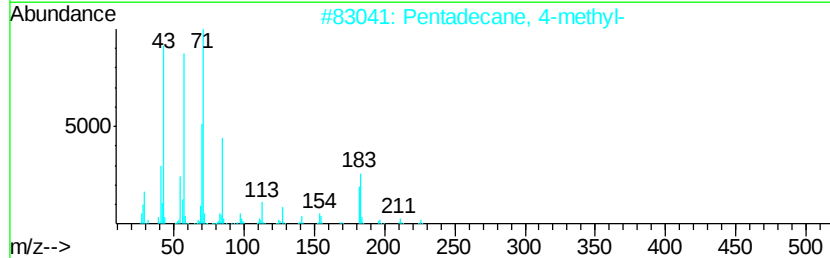
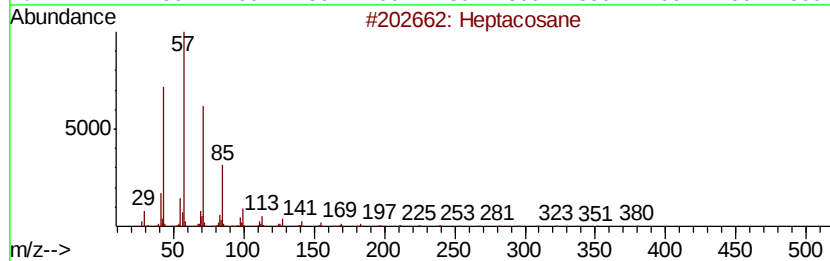
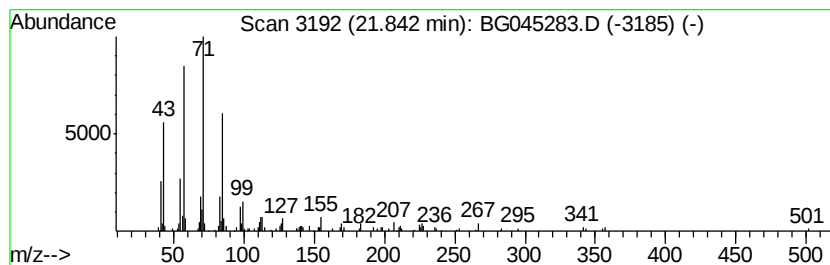
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Peak Number 5 Heptacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.84	2.04 ng	107473	Chrysene-d12	21.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	72
2	Pentadecane, 4-methyl-		226	C16H34	002801-87-8	58
3	Tetracosane		338	C24H50	000646-31-1	58
4	Dodecane, 2,6,10-trimethyl-		212	C15H32	003891-98-3	55
5	Hexadecane, 2,6,10,14-tetramethyl-		282	C20H42	000638-36-8	46



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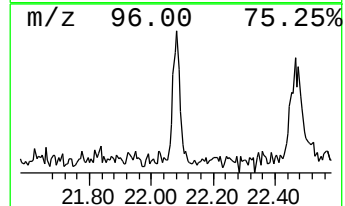
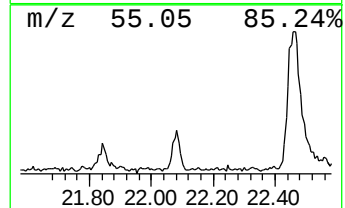
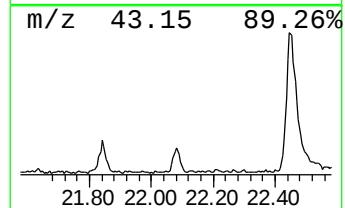
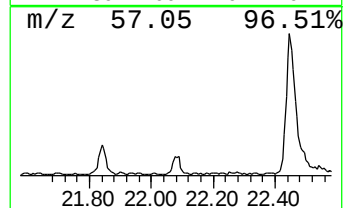
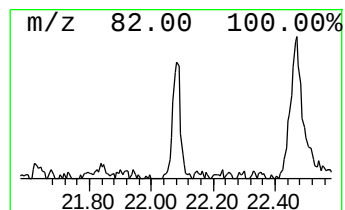
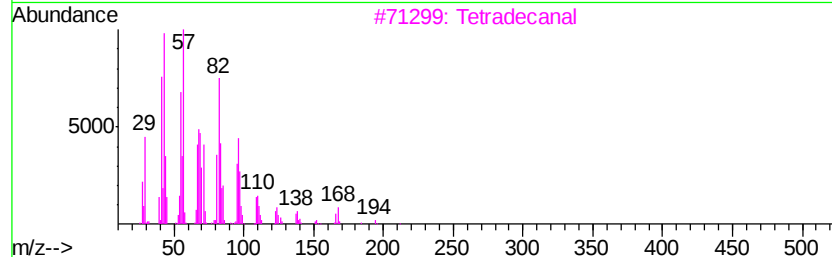
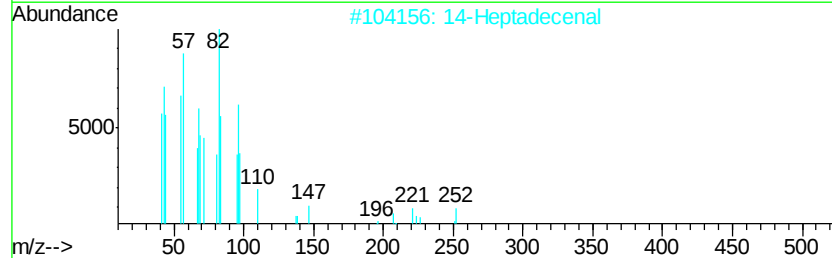
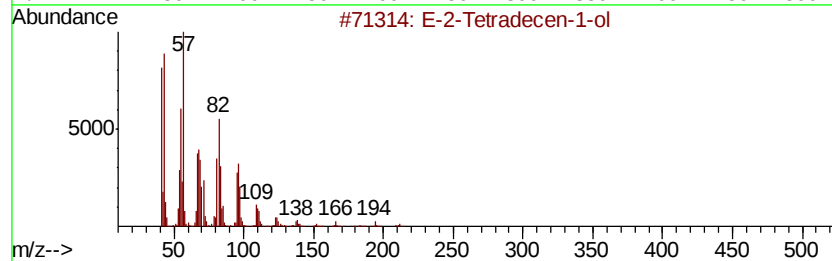
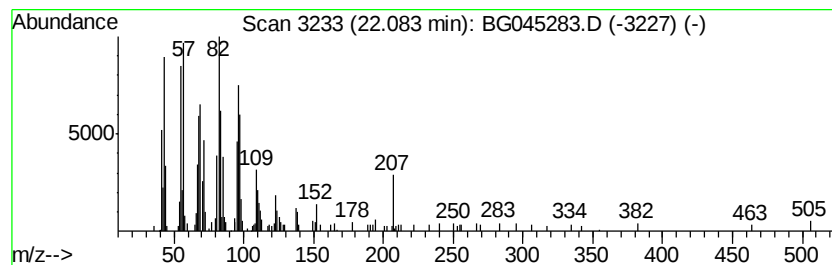
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Peak Number 6 E-2-Tetradecen-1-ol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.08	2.32 ng	122213	Chrysene-d12	21.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	90
2		14-Heptadecenal	252	C17H32O	1000144-58-0	89
3		Tetradecanal	212	C14H28O	000124-25-4	89
4		Tetracosanal	352	C24H48O	057866-08-7	87
5		Oxirane, tetradecyl-	240	C16H32O	007320-37-8	87



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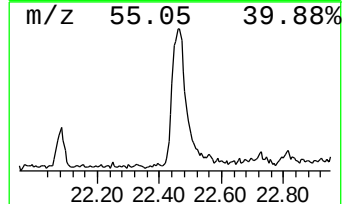
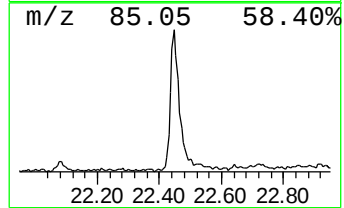
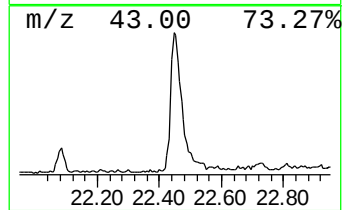
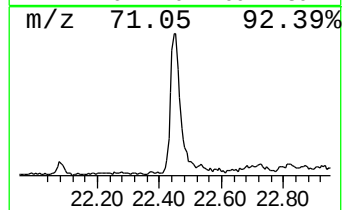
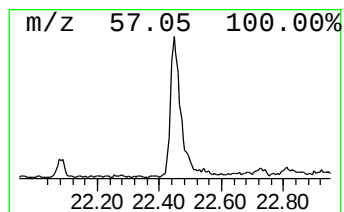
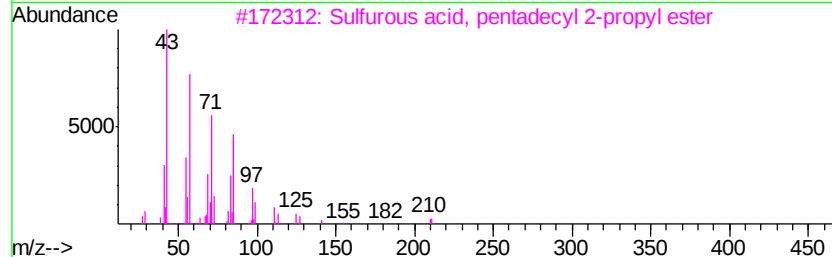
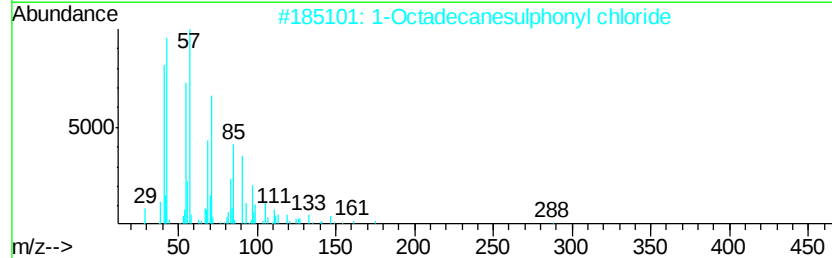
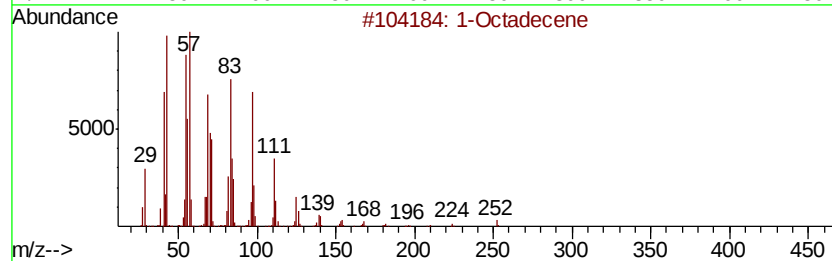
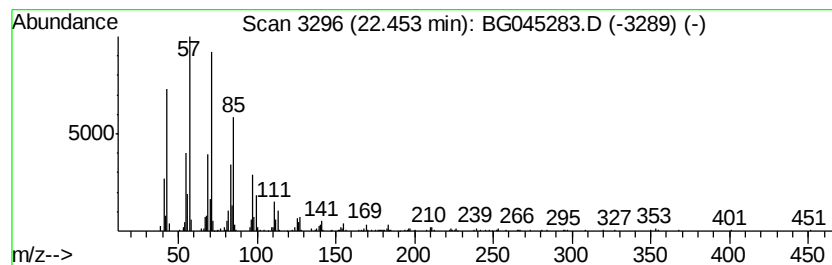
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.45	16.23 ng	853327	Chrysene-d12	21.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecene	252	C18H36	000112-88-9	93
2		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
3		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91
4		Tetracosane	338	C24H50	000646-31-1	83
5		1-Heptadecene	238	C17H34	006765-39-5	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050720\
Data File : BG045283.D
Acq On : 7 May 2020 23:59
Operator : CG/JU
Sample : L2529-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11936

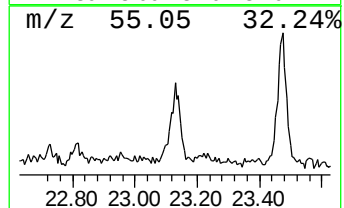
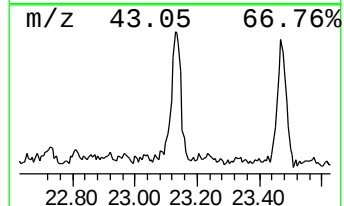
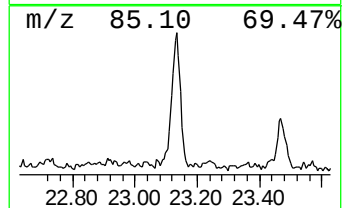
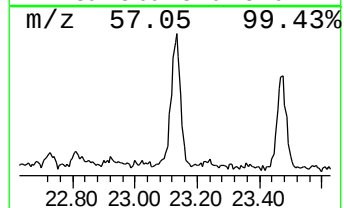
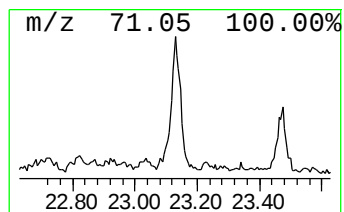
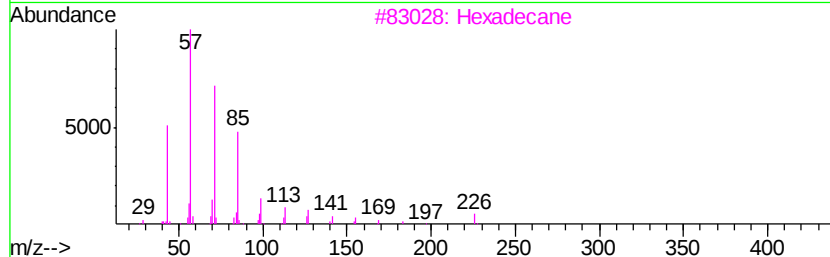
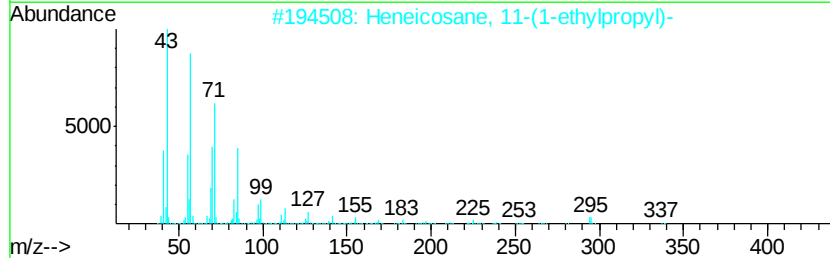
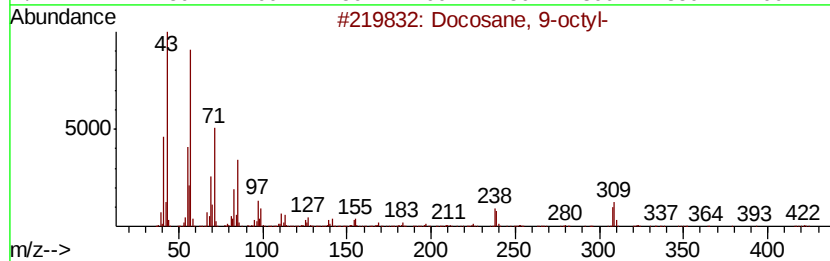
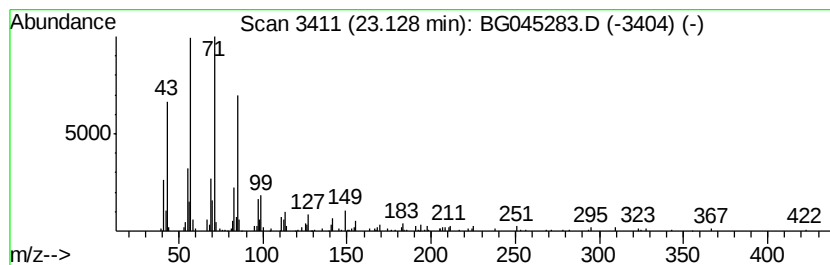
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	5.01 ng	263539	Chrysene-d12	21.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 9-octyl-	422	C30H62	055319-83-0	83
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
3		Hexadecane	226	C16H34	000544-76-3	76
4		Tetratetracontane	619	C44H90	007098-22-8	74
5		Octacosane	394	C28H58	000630-02-4	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050720\
Data File : BG045283.D
Acq On : 7 May 2020 23:59
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Sample : L2529-03
Misc :
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Instrument :
BNA_G
ClientSampleId :
72-11936

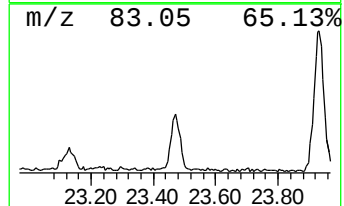
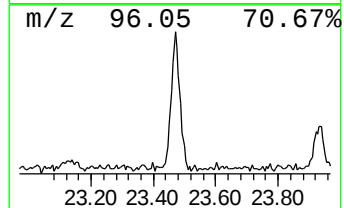
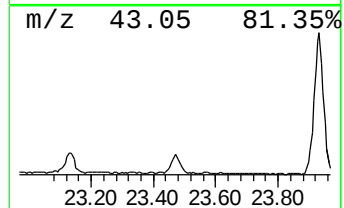
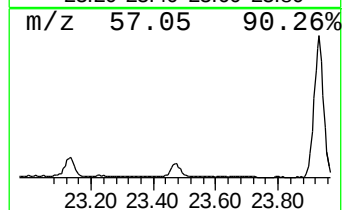
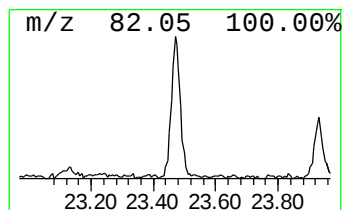
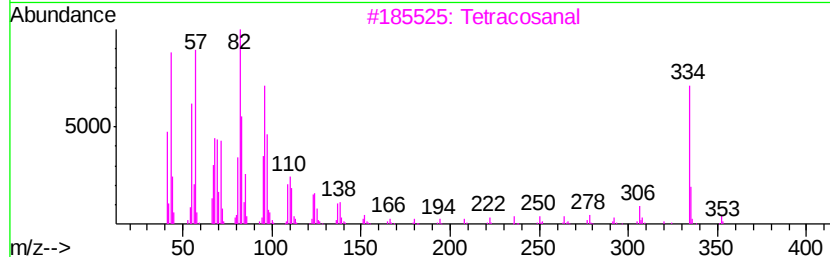
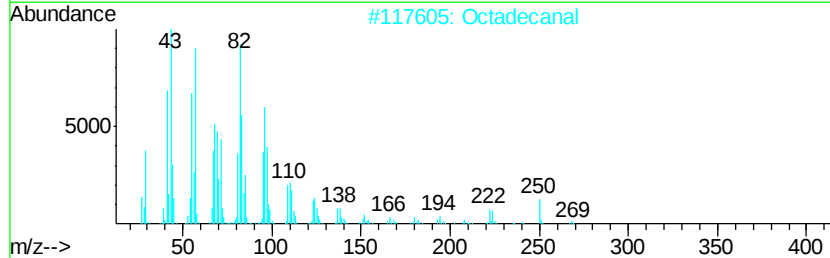
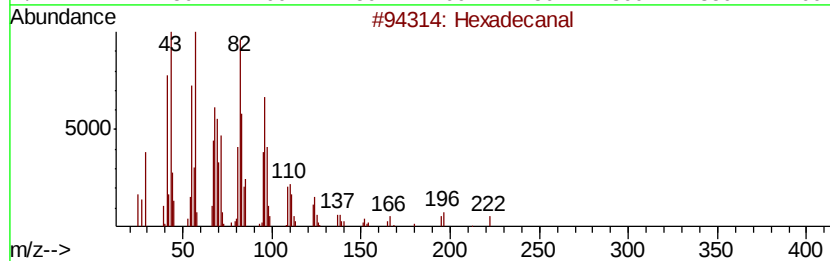
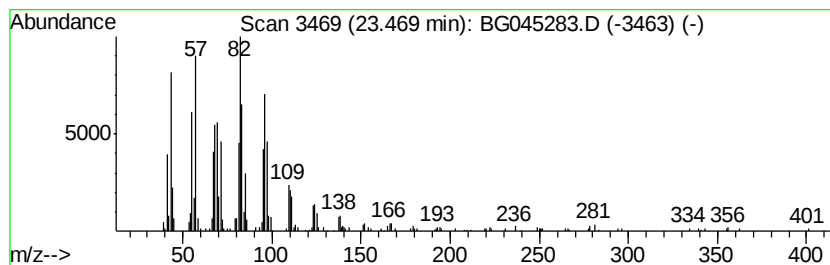
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.47	6.54 ng	357070	Perylene-d12	24.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal		240	C16H32O	000629-80-1	91
2	Octadecanal		268	C18H36O	000638-66-4	91
3	Tetracosanal		352	C24H48O	057866-08-7	91
4	17-Octadecenal		266	C18H34O	056554-86-0	91
5	16-Heptadecenal		252	C17H32O	1000144-57-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050720\
Data File : BG045283.D
Acq On : 7 May 2020 23:59
Operator : CG/JU
Sample : L2529-03
Misc :
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ClientSampleId :
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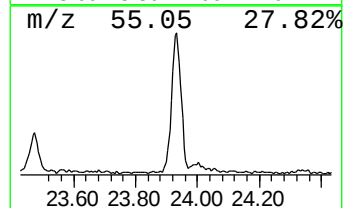
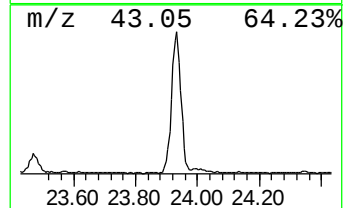
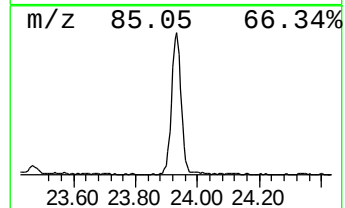
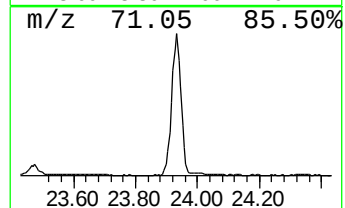
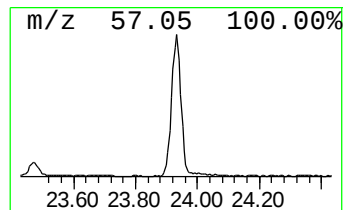
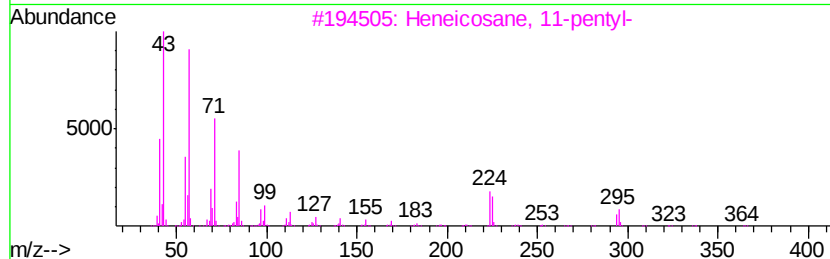
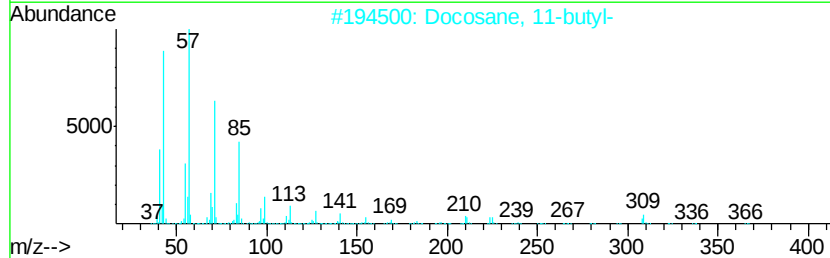
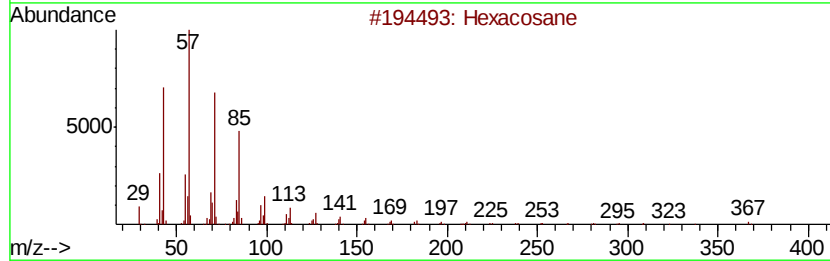
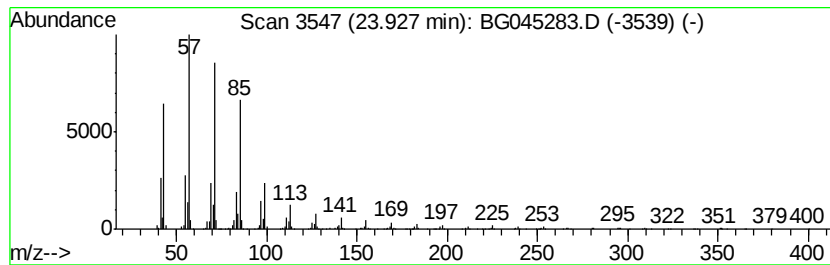
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	32.16 ng	1755500	Perylene-d12	24.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	94
3		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
4		Tridecane, 7-hexyl-	268	C19H40	007225-66-3	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050720\
Data File : BG045283.D
Acq On : 7 May 2020 23:59
Operator : CG/JU
Sample : L2529-03
Misc :
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ClientSampleId :
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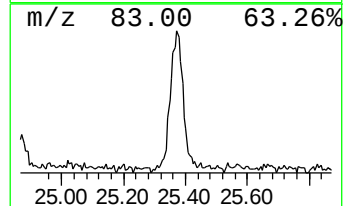
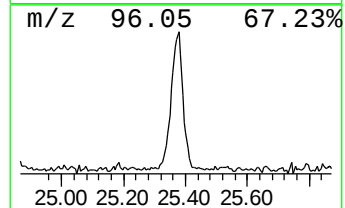
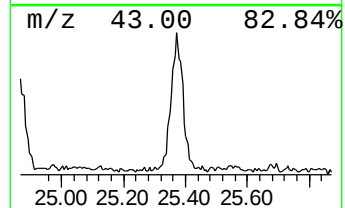
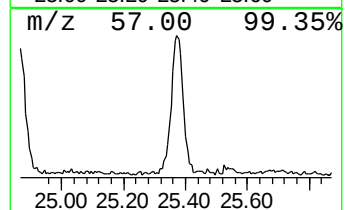
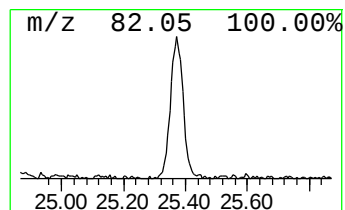
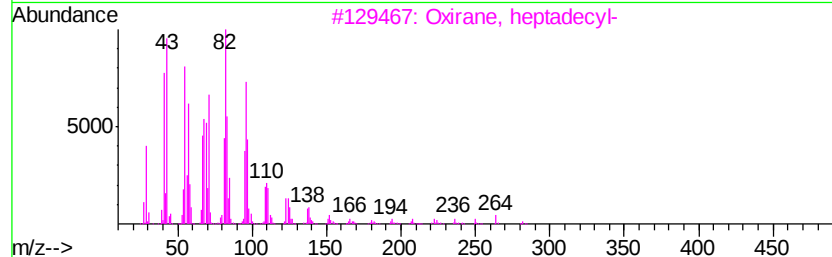
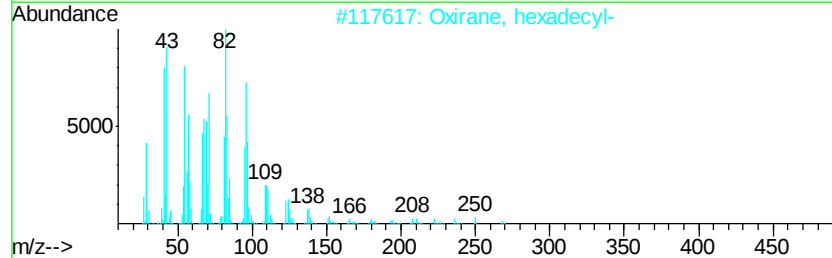
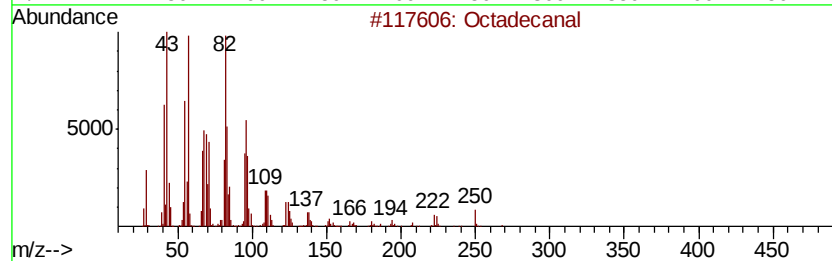
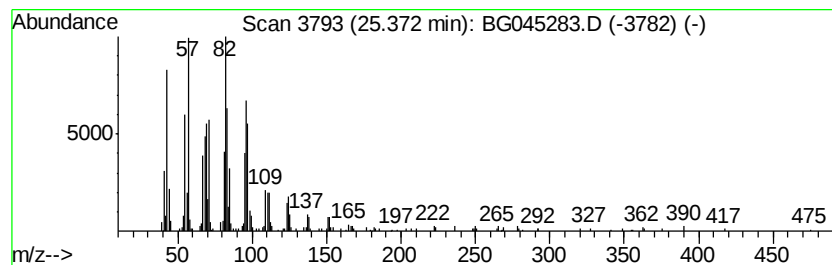
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octadecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.37	9.75 ng	532415	Perylene-d12	24.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	95
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
3		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
4		Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	90
5		Hexadecanal	240	C16H32O	000629-80-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050720\
Data File : BG045283.D
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Operator : CG/JU
Sample : L2529-03
Misc :
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Instrument :
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ClientSampleId :
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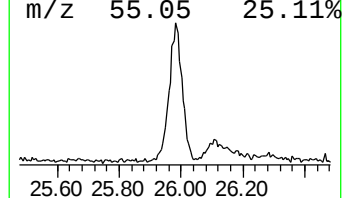
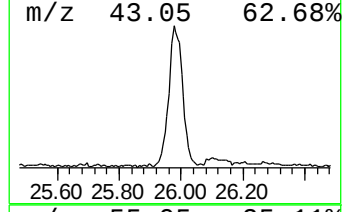
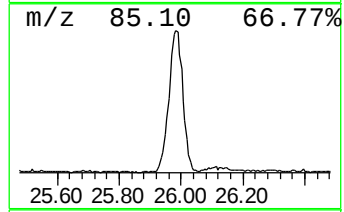
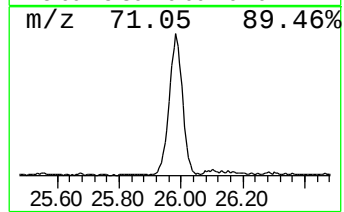
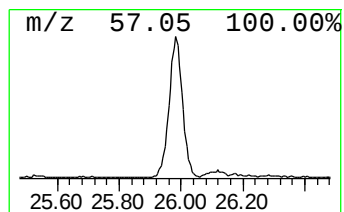
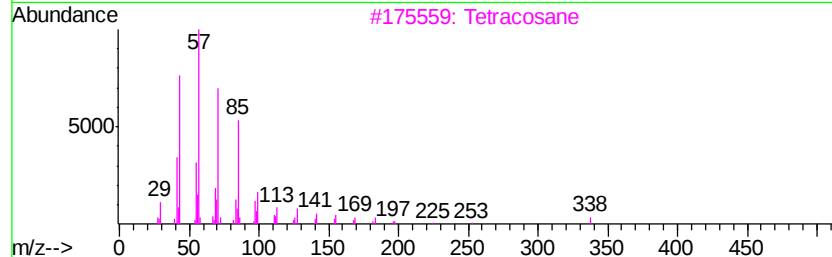
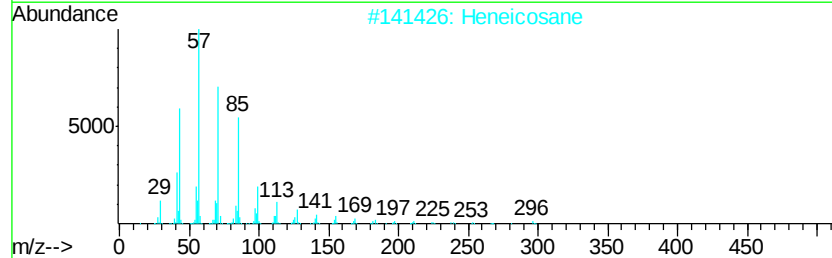
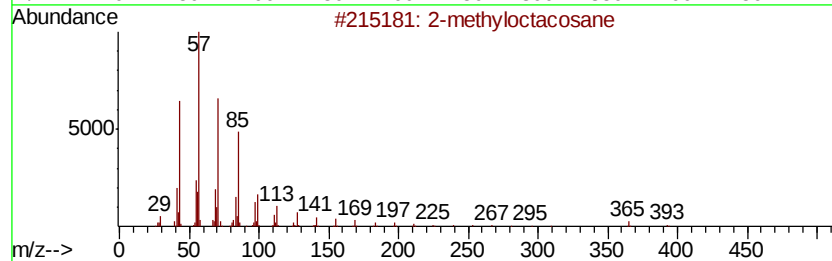
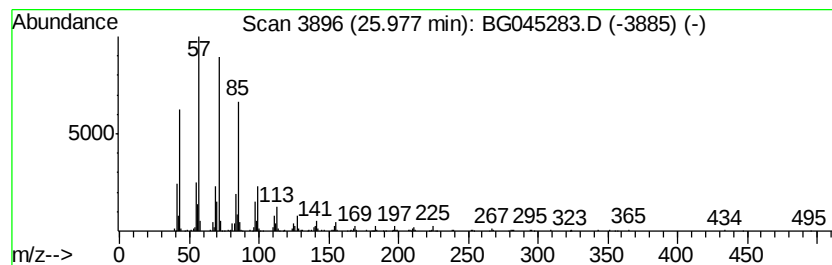
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.98	19.37 ng	1057160	Perylene-d12	24.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		triacontane	422	C30H62	000638-68-6	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050720\
Data File : BG045283.D
Acq On : 7 May 2020 23:59
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Misc :
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ClientSampleId :
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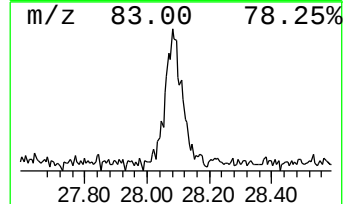
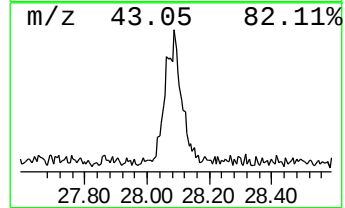
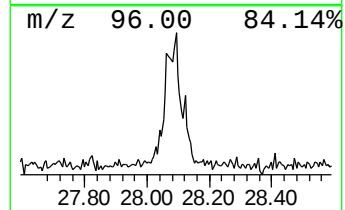
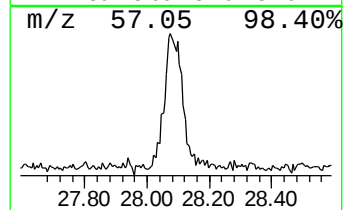
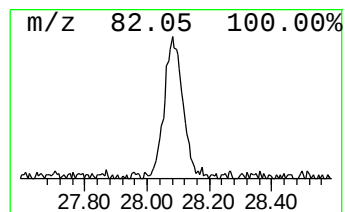
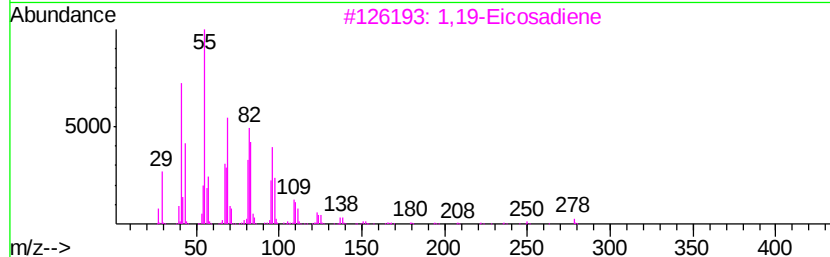
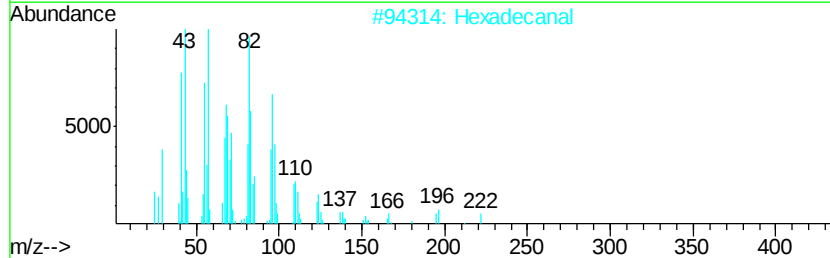
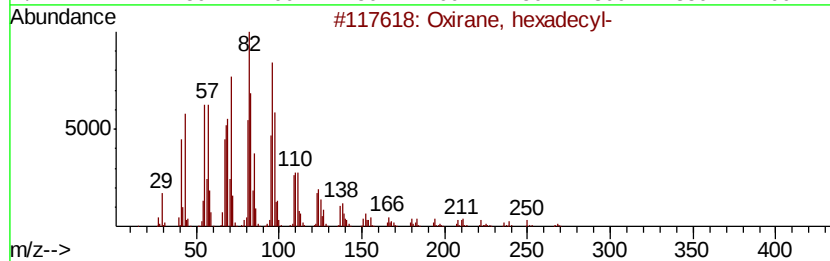
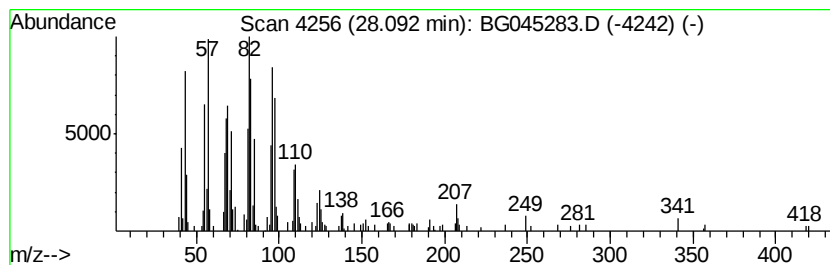
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.09	6.78 ng	369970	Perylene-d12	24.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
2			Hexadecanal	240	C16H32O	000629-80-1	86
3			1,19-Eicosadiene	278	C20H38	014811-95-1	74
4			(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	72
5			16-Heptadecenal	252	C17H32O	1000144-57-9	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG050720\
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 Misc :
 ALS Vial : 18 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrameth...	13.52	3.3	ng	117297	3	14.62	710851	20.0
Hexanedioic acid,...	20.75	2.2	ng	113347	5	21.64	1051620	20.0
17-Pentatriacontene	21.30	9.0	ng	475519	5	21.64	1051620	20.0
Heptacosane	21.84	2.0	ng	107473	5	21.64	1051620	20.0
E-2-Tetradecen-1-ol	22.08	2.3	ng	122213	5	21.64	1051620	20.0
1-Octadecene	22.45	16.2	ng	853327	5	21.64	1051620	20.0
Docosane, 9-octyl-	23.13	5.0	ng	263539	5	21.64	1051620	20.0
Hexadecanal	23.47	6.5	ng	357070	6	24.80	1091640	20.0
Hexacosane	23.93	32.2	ng	1755500	6	24.80	1091640	20.0
Octadecanal	25.37	9.8	ng	532415	6	24.80	1091640	20.0
2-methyloctacosane	25.98	19.4	ng	1057160	6	24.80	1091640	20.0
Oxirane, hexadecyl-	28.09	6.8	ng	369970	6	24.80	1091640	20.0