

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031320\
 Data File : BG044776.D
 Acq On : 13 Mar 2020 20:55
 Operator : CG/JU
 Sample : L1913-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MK-031220-2-5-COMP-B3

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-BG031020.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.155	5	11	20	rVV2	86453	207096	3.44%	0.567%
2	3.231	20	24	33	rVB3	53764	98846	1.64%	0.271%
3	5.622	423	431	441	rBV	1681124	2790703	46.38%	7.647%
4	7.209	692	701	711	rBV	1736024	3065081	50.95%	8.399%
5	7.650	769	776	781	rBV2	33619	62631	1.04%	0.172%
6	8.055	838	845	854	rBV	399991	708590	11.78%	1.942%
7	8.378	892	900	910	rVB	1336818	2361505	39.25%	6.471%
8	9.207	1032	1041	1053	rBV	1064357	2013740	33.47%	5.518%
9	10.863	1314	1323	1330	rBV	547344	1033781	17.18%	2.833%
10	13.313	1732	1740	1747	rBV	2716927	4440218	73.80%	12.167%
11	14.130	1873	1879	1891	rVB	372132	573444	9.53%	1.571%
12	14.682	1965	1973	1982	rBV	885285	1458819	24.25%	3.998%
13	16.169	2219	2226	2235	rBV	2200934	3503329	58.23%	9.600%
14	17.432	2434	2441	2449	rBV	1115537	1752983	29.14%	4.804%
15	18.331	2589	2594	2605	rBV2	128027	208904	3.47%	0.572%
16	19.600	2805	2810	2815	rBV7	36682	70341	1.17%	0.193%
17	20.047	2879	2886	2891	rBV	4283331	6016411	100.00%	16.486%
18	21.363	3105	3110	3118	rBV2	276207	485357	8.07%	1.330%
19	21.704	3161	3168	3175	rBV2	926199	1650336	27.43%	4.522%
20	21.933	3203	3207	3214	rVB	104362	163538	2.72%	0.448%
21	22.550	3307	3312	3316	rBV2	167240	282906	4.70%	0.775%
22	23.255	3426	3432	3437	rBV2	217615	408038	6.78%	1.118%
23	24.071	3565	3571	3580	rVB2	237476	533031	8.86%	1.461%
24	24.918	3706	3715	3727	rVB3	567080	1656403	27.53%	4.539%
25	25.035	3727	3735	3746	rBV2	215885	550752	9.15%	1.509%
26	26.187	3925	3931	3942	rVB3	128998	396393	6.59%	1.086%

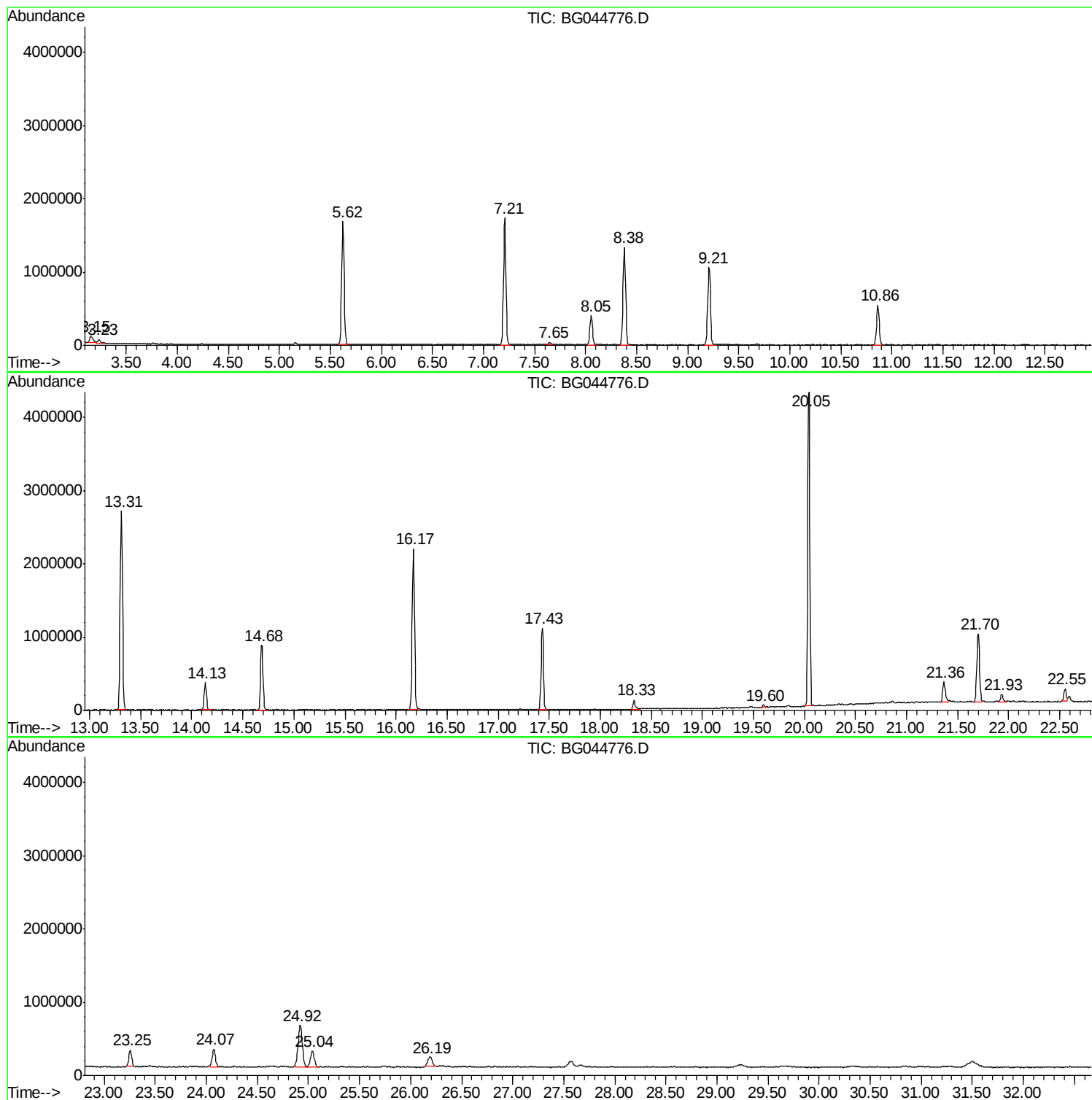
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG031020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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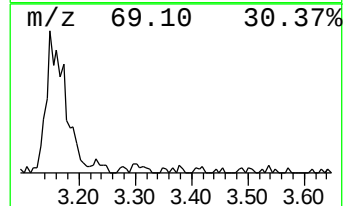
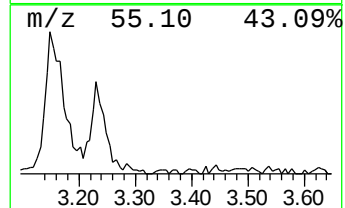
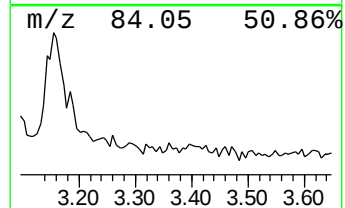
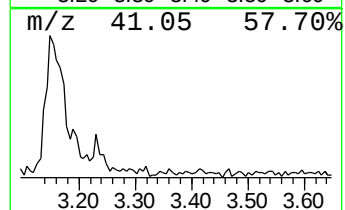
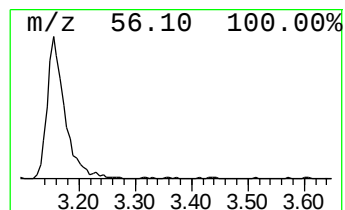
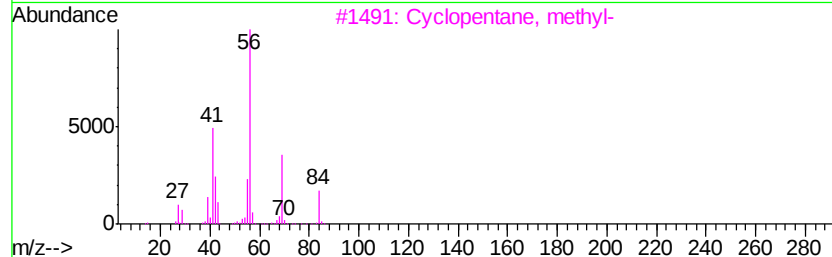
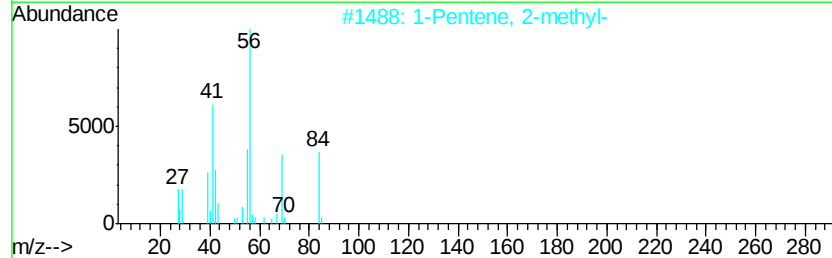
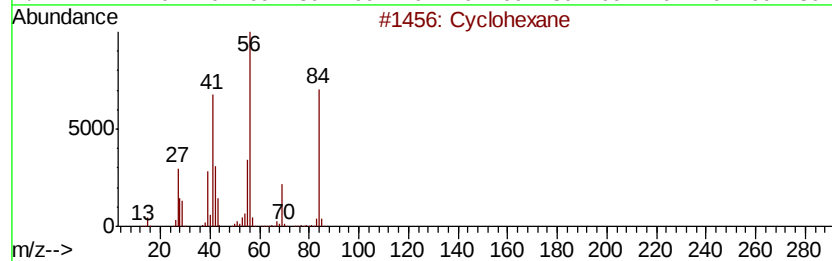
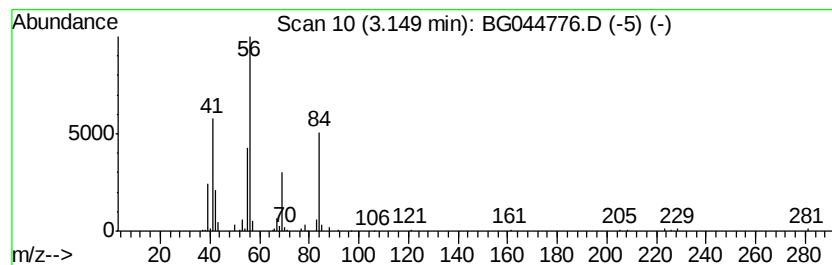
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	5.85 ng	207096	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane	84	C6H12	000110-82-7	86
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	64
4		Cyclobutanone, 2-methyl-	84	C5H8O	001517-15-3	56
5		Iron pentacarbonyl	196	C5FeO5	013463-40-6	40



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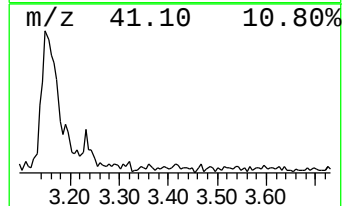
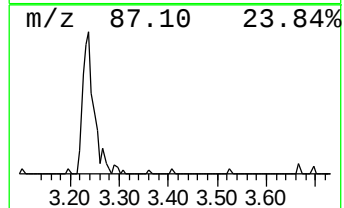
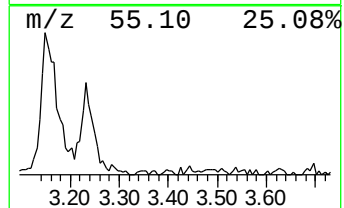
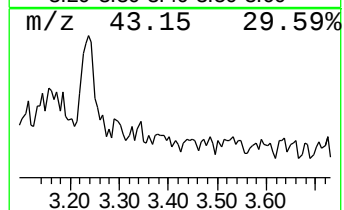
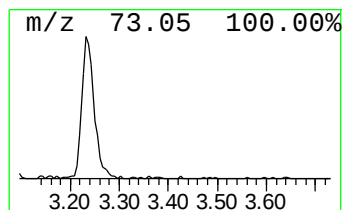
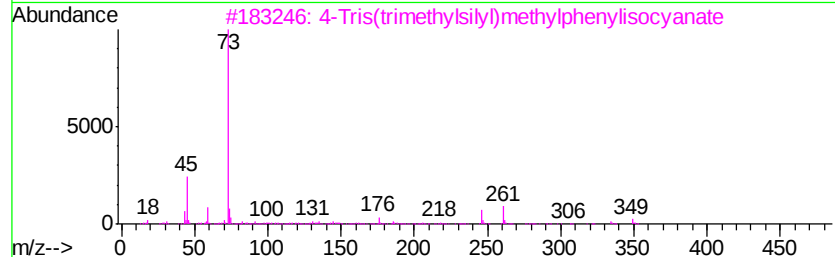
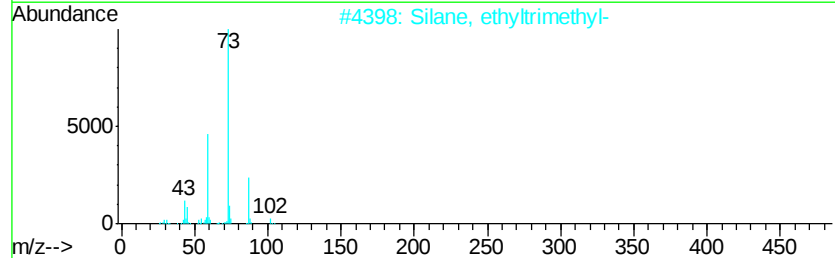
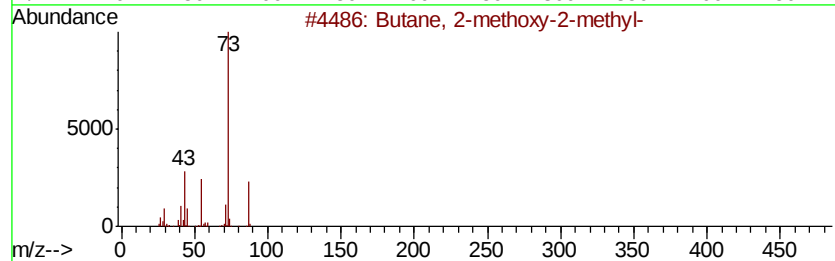
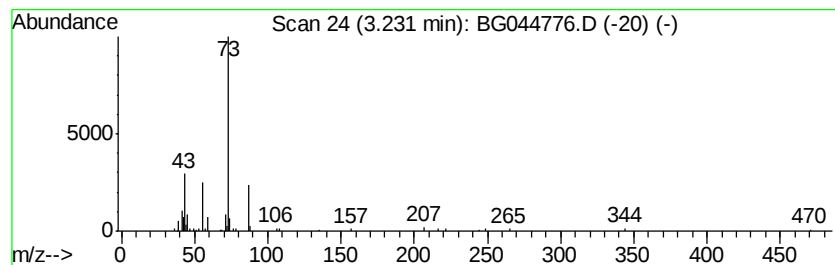
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	2.79 ng	98846	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	28
3		4-Tris(trimethylsilyl)methylphen...	349	C17H31NOSi3	1000286-59-7	17
4		3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	12
5		3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	10



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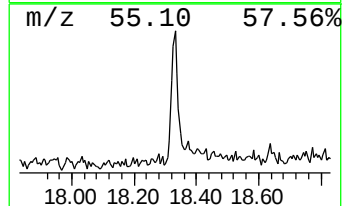
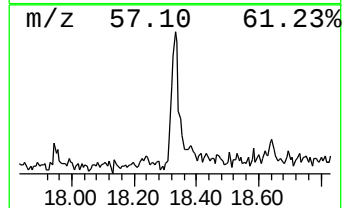
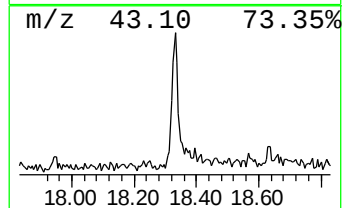
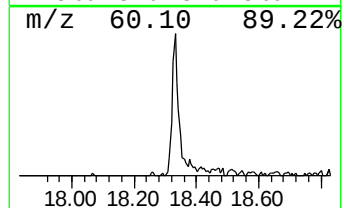
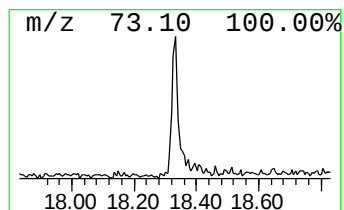
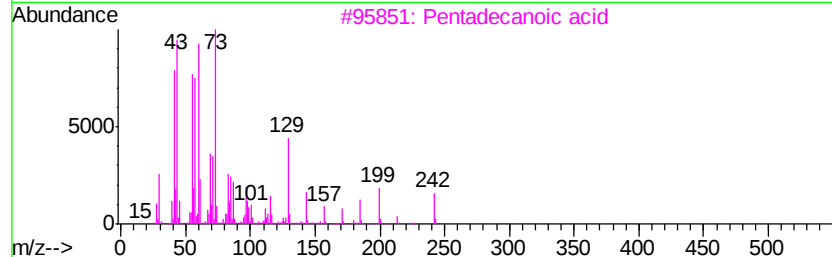
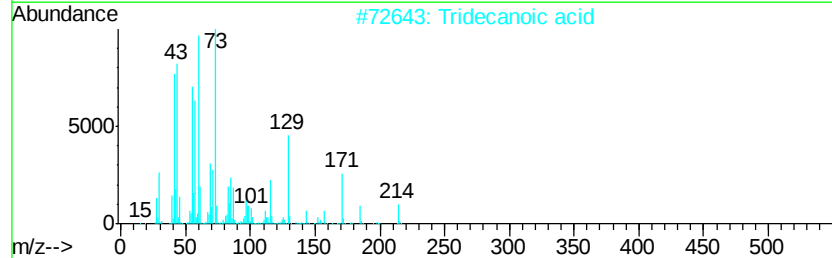
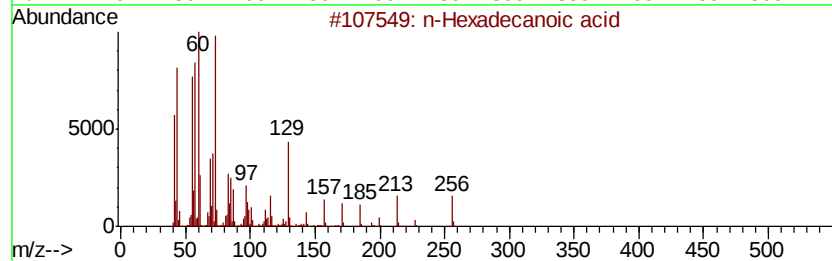
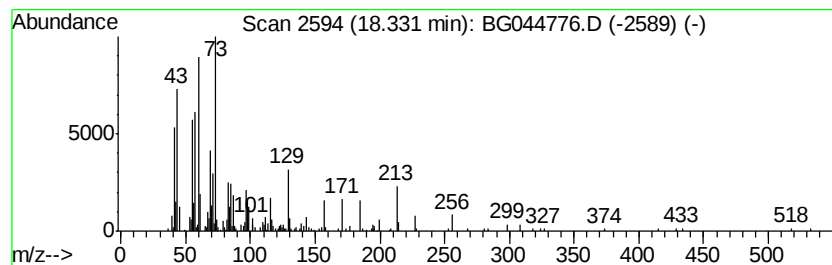
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	2.38 ng	208904	Phenanthrene-d10	17.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Octadecanoic acid	284	C18H36O2	000057-11-4	60



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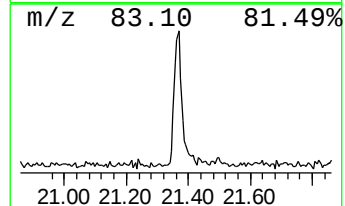
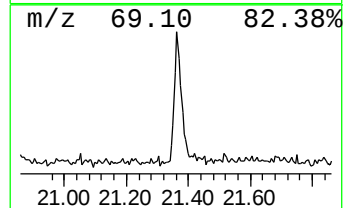
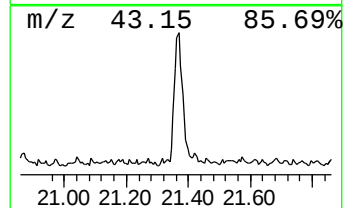
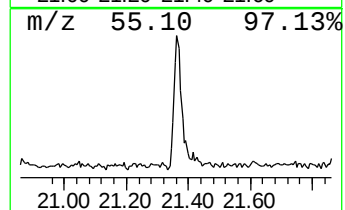
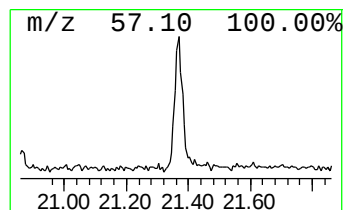
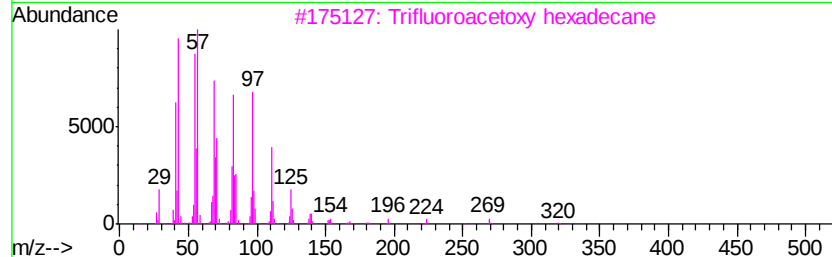
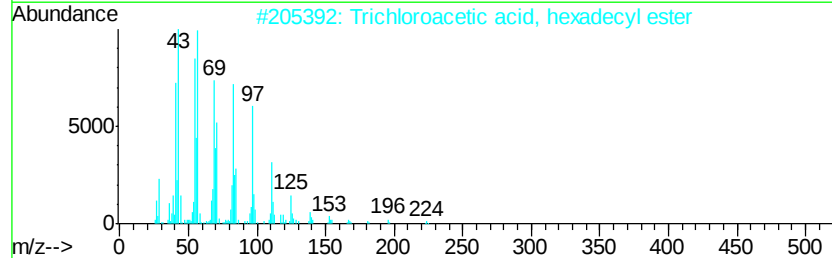
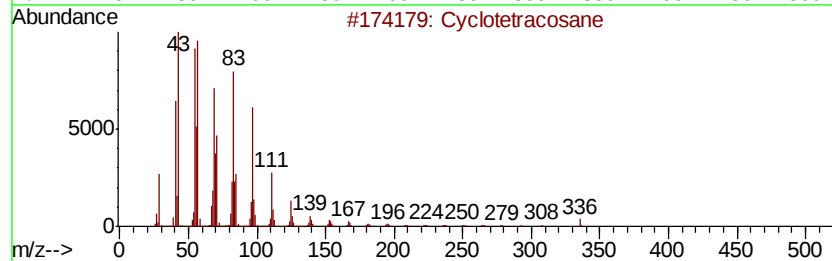
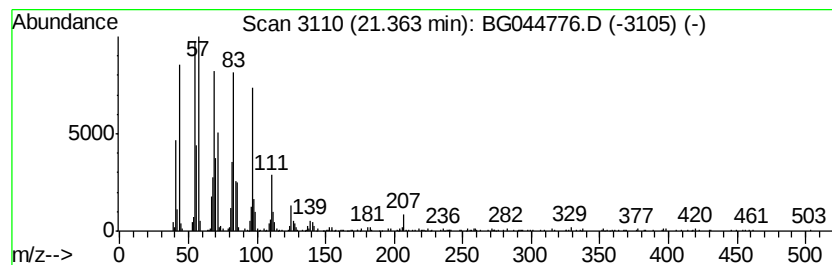
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Peak Number 5 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.36	5.88 ng	485357	Chrysene-d12	21.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	99
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5		Behenic alcohol	326	C22H46O	000661-19-8	91



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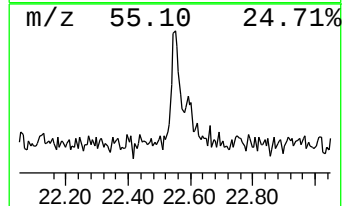
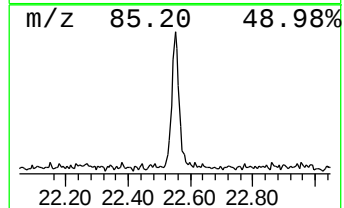
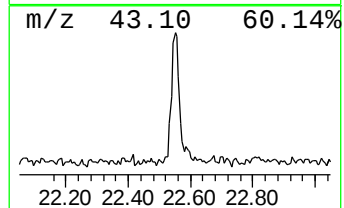
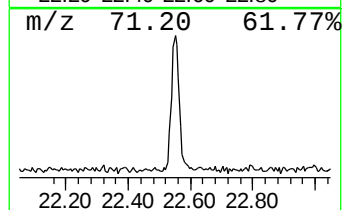
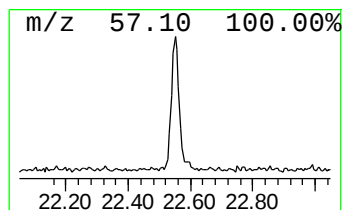
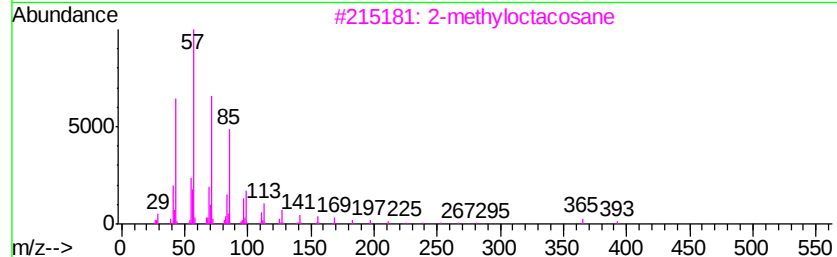
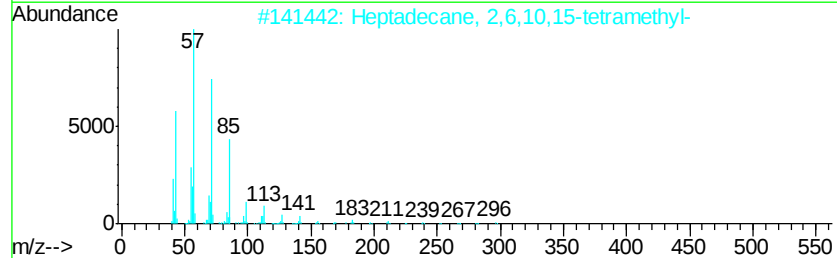
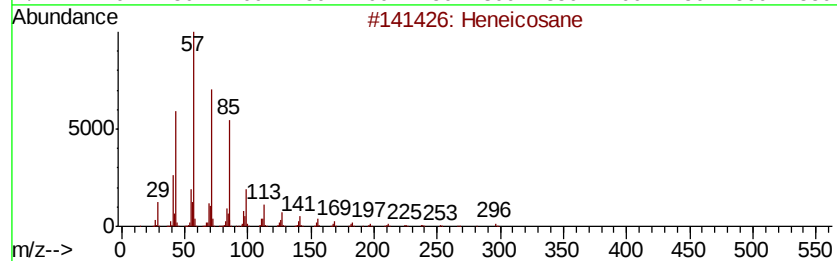
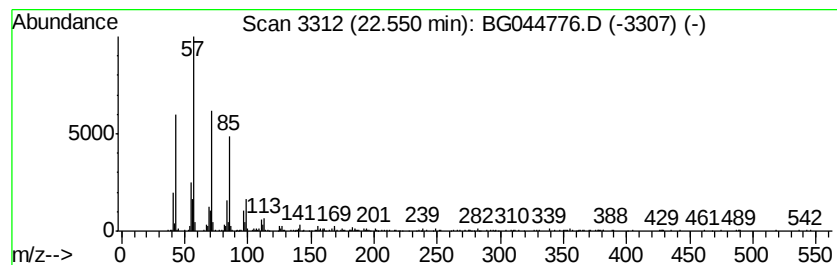
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.55	3.43 ng	282906	Chrysene-d12	21.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	93
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	87
3	2-methyloctacosane		408	C29H60	1000376-72-8	86
4	Hexacosane		366	C26H54	000630-01-3	86
5	Octacosane		394	C28H58	000630-02-4	68



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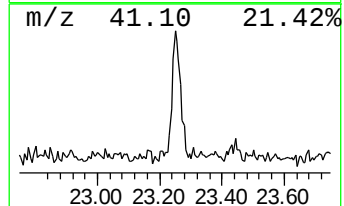
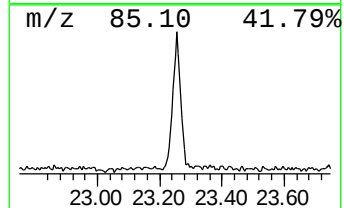
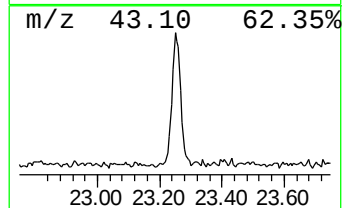
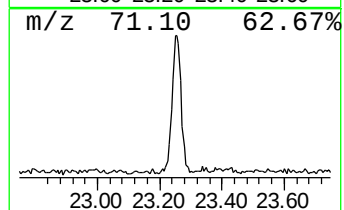
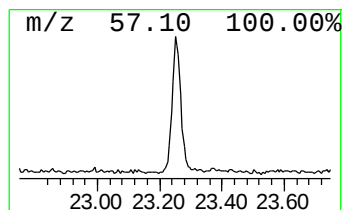
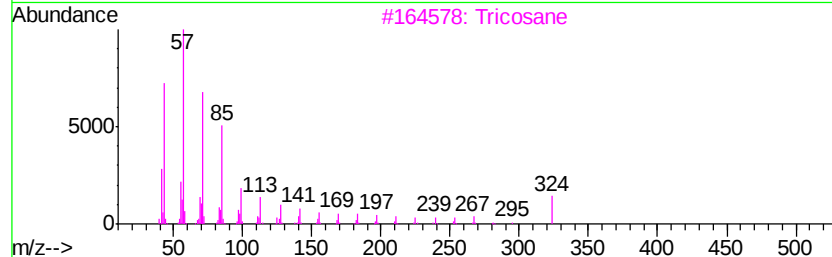
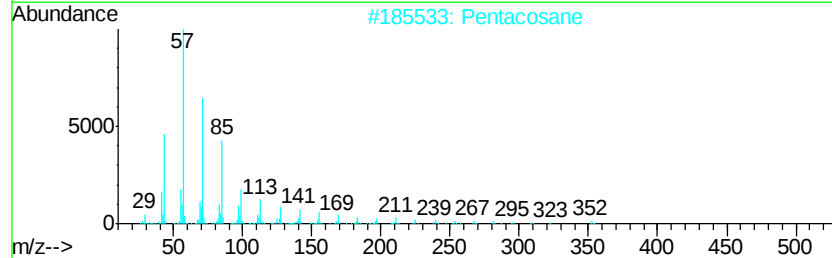
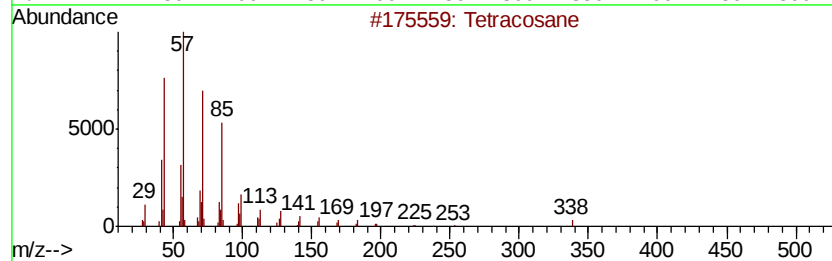
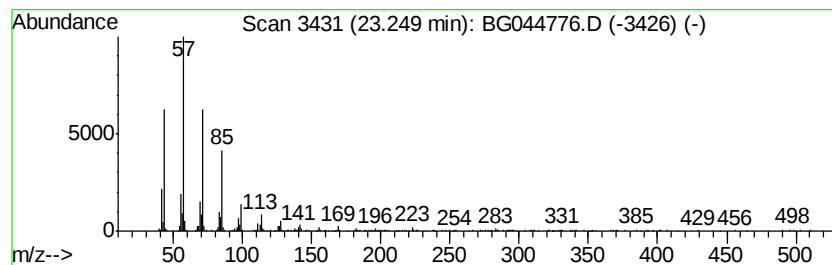
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.25	4.94 ng	408038	Chrysene-d12	21.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	89
2		Pentacosane	352	C25H52	000629-99-2	72
3		Tricosane	324	C23H48	000638-67-5	72
4		Eicosane	282	C20H42	000112-95-8	62
5		Nonadecane	268	C19H40	000629-92-5	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031320\
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Acq On : 13 Mar 2020 20:55
Operator : CG/JU
Sample : L1913-07
Misc :
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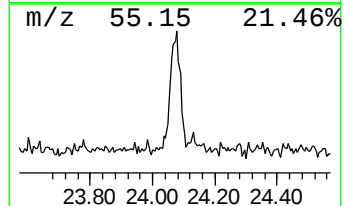
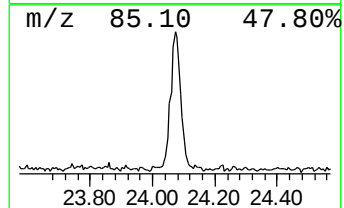
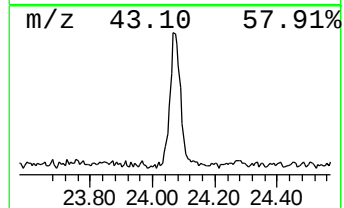
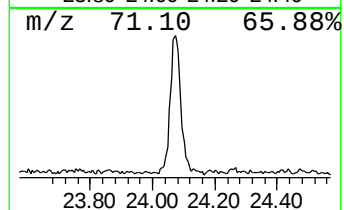
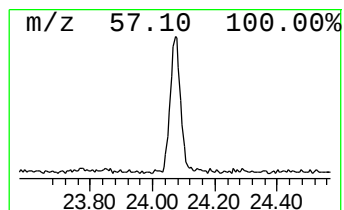
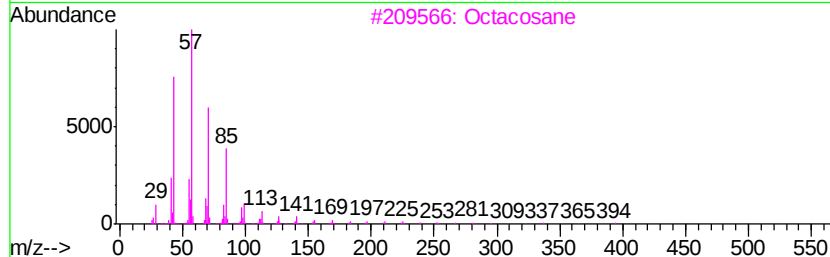
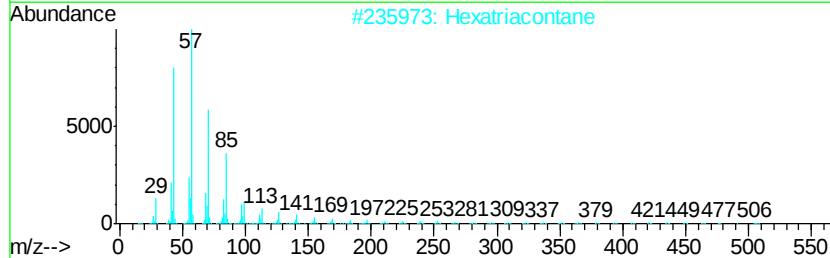
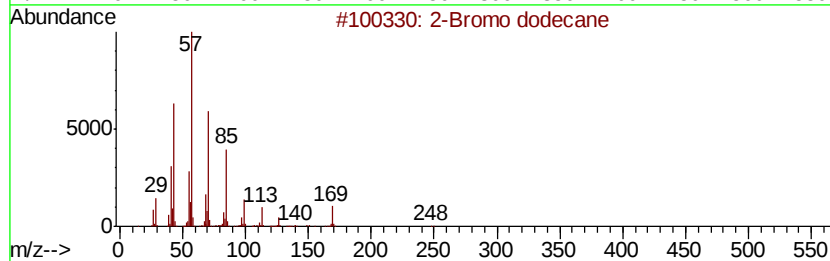
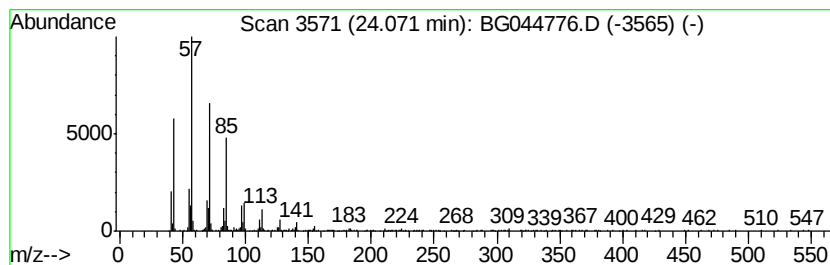
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MK-031220-2-5-COMP-B3

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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 2-Bromo dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
24.07	6.44 ng	533031	Perylene-d12	24.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane		248	C12H25Br	013187-99-0	91
2	Hexatriacontane		507	C36H74	000630-06-8	90
3	Octacosane		394	C28H58	000630-02-4	90
4	2-methyloctacosane		408	C29H60	1000376-72-8	87
5	Hexacosane		366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031320\
Data File : BG044776.D
Acq On : 13 Mar 2020 20:55
Operator : CG/JU
Sample : L1913-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

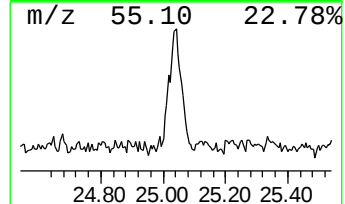
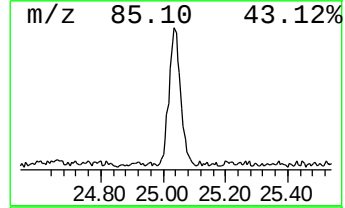
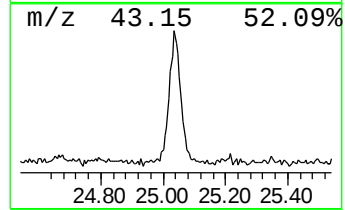
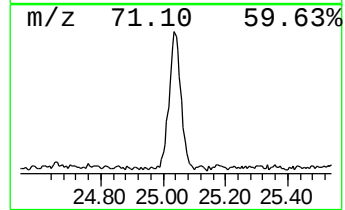
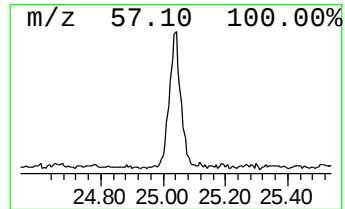
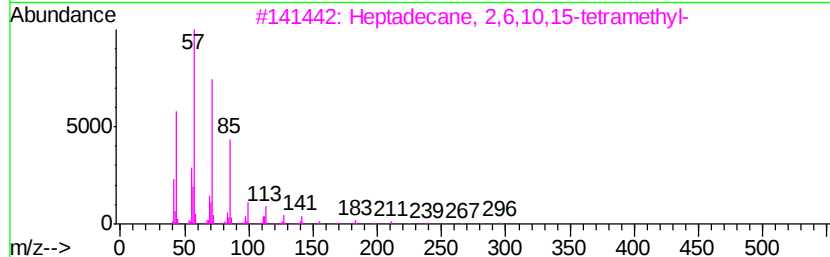
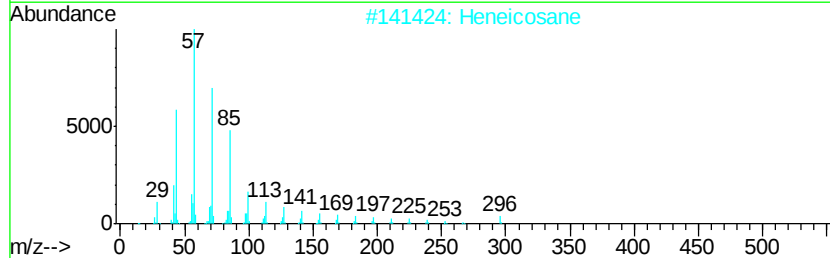
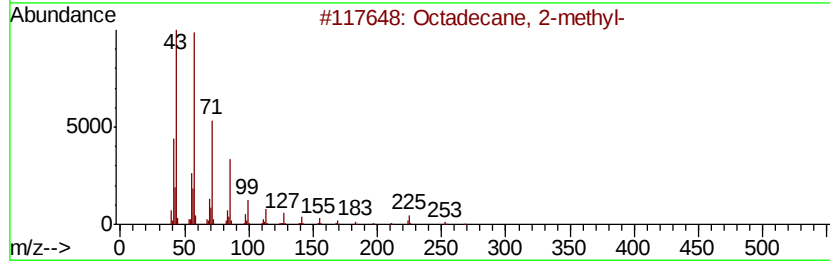
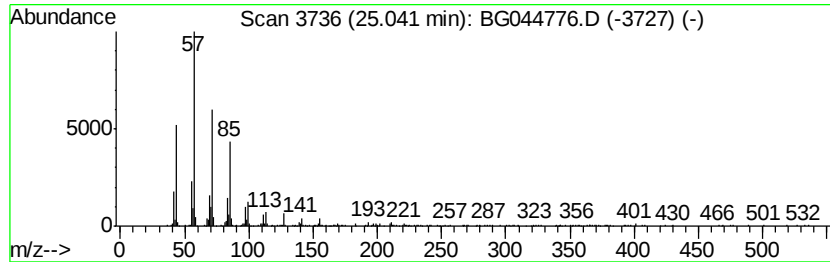
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.04	6.65 ng	550752	Perylene-d12	24.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4	Tetratetracontane	619	C44H90	007098-22-8	86
5	Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031320\
Data File : BG044776.D
Acq On : 13 Mar 2020 20:55
Operator : CG/JU
Sample : L1913-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MK-031220-2-5-COMP-B3

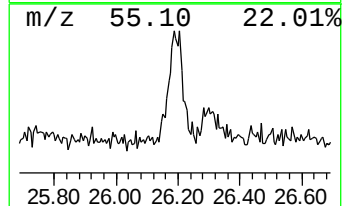
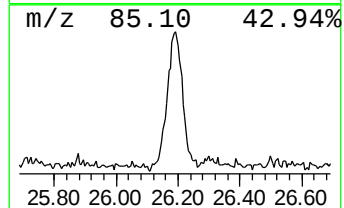
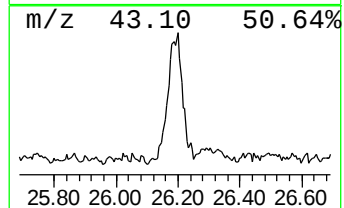
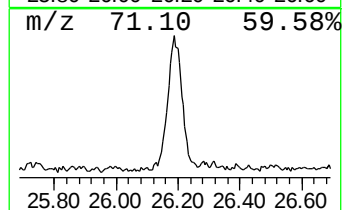
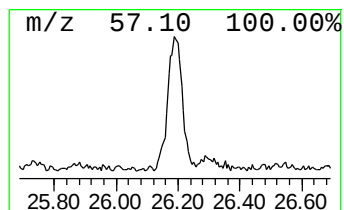
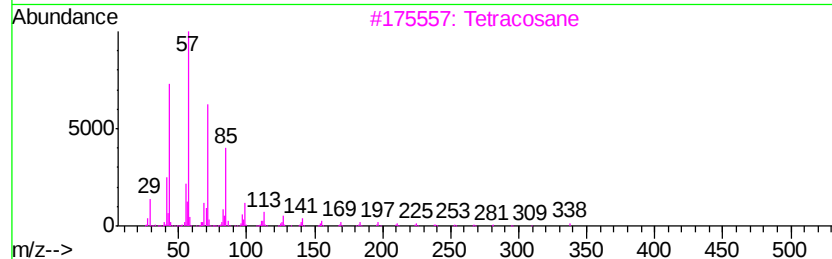
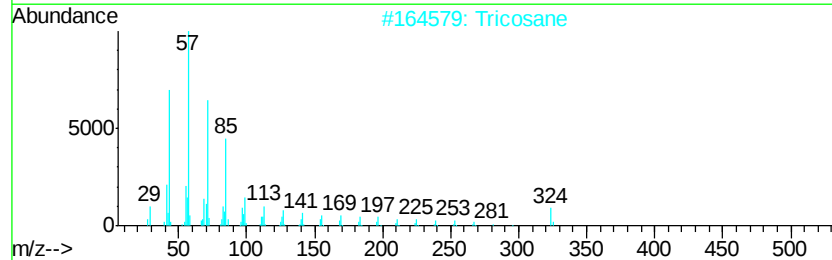
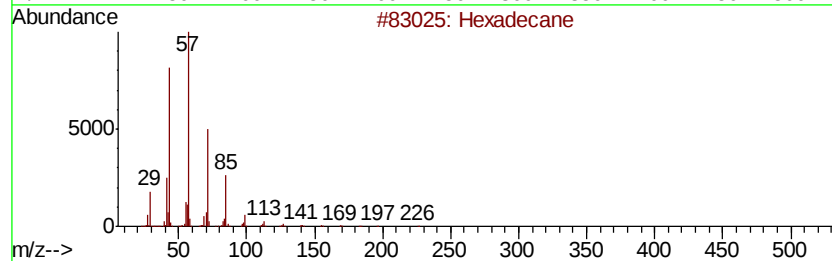
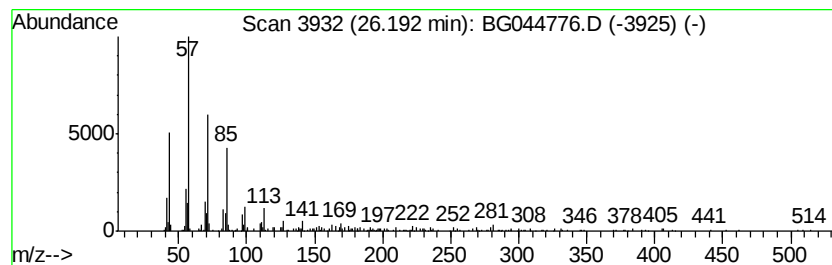
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.19	4.79 ng	396393	Perylene-d12	24.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane			226	C16H34	000544-76-3	91
2	Tricosane			324	C23H48	000638-67-5	90
3	Tetracosane			338	C24H50	000646-31-1	87
4	Heptadecane			240	C17H36	000629-78-7	87
5	Octacosane			394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG031320\
Data File : BG044776.D
Acq On : 13 Mar 2020 20:55
Operator : CG/JU
Sample : L1913-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MK-031220-2-5-COMP-B3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031020.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
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Butane, 2-methoxy...	3.23	2.8	ng	98846	1	8.05	708590	20.0
n-Hexadecanoic acid	18.33	2.4	ng	208904	4	17.43	1752980	20.0
Cyclotetracosane	21.36	5.9	ng	485357	5	21.70	1650340	20.0
Heneicosane	22.55	3.4	ng	282906	5	21.70	1650340	20.0
Tetracosane	23.25	4.9	ng	408038	5	21.70	1650340	20.0
2-Bromo dodecane	24.07	6.4	ng	533031	6	24.92	1656400	20.0
Octadecane, 2-met...	25.04	6.7	ng	550752	6	24.92	1656400	20.0
Hexadecane	26.19	4.8	ng	396393	6	24.92	1656400	20.0