

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
 Data File : BM020118.D
 Acq On : 03 May 2019 18:52
 Operator : JU/SJ
 Sample : K2668-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-3

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_M\METHODS\8270-BM043019.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	3.010	3	4	12	rVB	112389	115242	1.50%	0.227%
2	5.363	397	404	416	rBV	3129288	4346275	56.58%	8.557%
3	6.951	666	674	685	rBV	2840016	4870456	63.40%	9.589%
4	7.316	728	736	745	rBV	3120457	4828953	62.86%	9.507%
5	7.786	808	816	822	rVB	482892	736293	9.58%	1.450%
6	8.104	863	870	877	rBV	2287057	3569035	46.46%	7.027%
7	8.951	1006	1014	1025	rBV	1806941	2918914	38.00%	5.747%
8	10.580	1284	1291	1298	rVB	532411	897103	11.68%	1.766%
9	13.045	1703	1710	1717	rVB	4016264	5729573	74.58%	11.280%
10	13.880	1846	1852	1859	rBV	441391	630969	8.21%	1.242%
11	14.310	1920	1925	1932	rBV	78355	101080	1.32%	0.199%
12	14.427	1939	1945	1953	rVB2	765695	1169773	15.23%	2.303%
13	15.262	2081	2087	2092	rVB	93966	126728	1.65%	0.249%
14	15.915	2188	2198	2207	rBV	3530608	4956861	64.53%	9.759%
15	16.127	2229	2234	2242	rBV	111074	211416	2.75%	0.416%
16	16.921	2365	2369	2372	rBV	89588	102968	1.34%	0.203%
17	17.174	2403	2412	2418	rBV2	988180	1431738	18.64%	2.819%
18	17.656	2490	2494	2500	rBV	81495	101985	1.33%	0.201%
19	18.056	2556	2562	2574	rBV	253277	405003	5.27%	0.797%
20	18.351	2608	2612	2616	rBV	68513	82819	1.08%	0.163%
21	19.339	2775	2780	2788	rBV	118974	194774	2.54%	0.383%
22	19.797	2853	2858	2864	rVB	6341797	7681950	100.00%	15.124%
23	21.056	3068	3072	3081	rBV	365716	468275	6.10%	0.922%
24	21.356	3118	3123	3129	rBV	1314875	1626865	21.18%	3.203%
25	21.497	3144	3147	3151	rVB2	100506	103114	1.34%	0.203%
26	21.939	3218	3222	3228	rBV4	158059	295192	3.84%	0.581%
27	22.409	3298	3302	3307	rBV	182630	224773	2.93%	0.443%
28	22.927	3386	3390	3396	rBV	247306	366682	4.77%	0.722%
29	23.509	3485	3489	3497	rVB2	160240	274172	3.57%	0.540%
30	23.638	3505	3511	3525	rVB2	880477	1761753	22.93%	3.468%
31	24.174	3597	3602	3609	rVB2	161130	305439	3.98%	0.601%
32	24.262	3614	3617	3627	rVB8	76131	157558	2.05%	0.310%

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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 >
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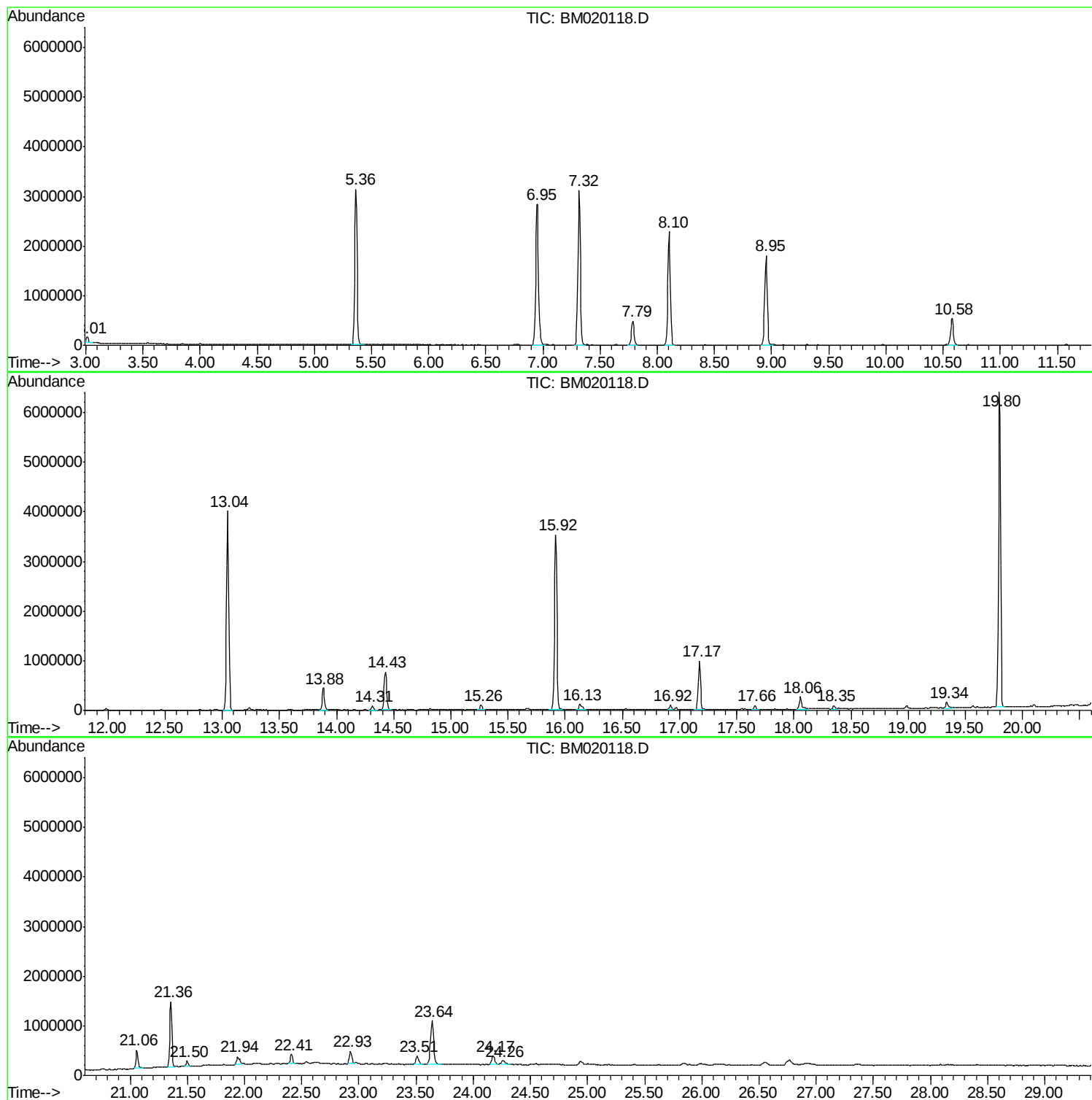
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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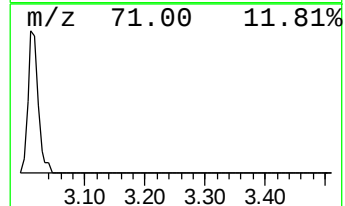
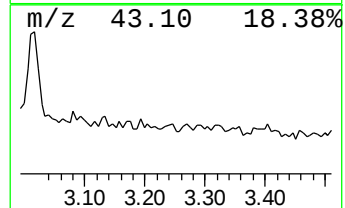
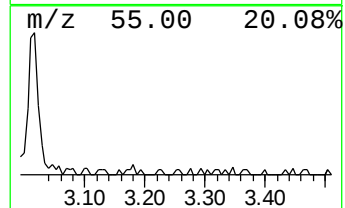
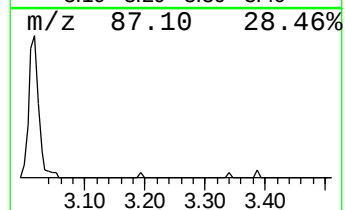
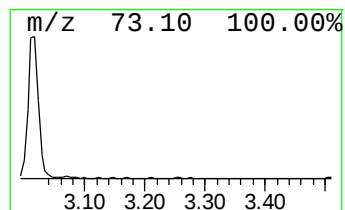
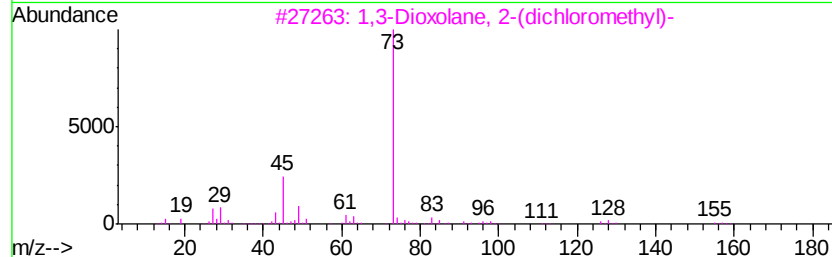
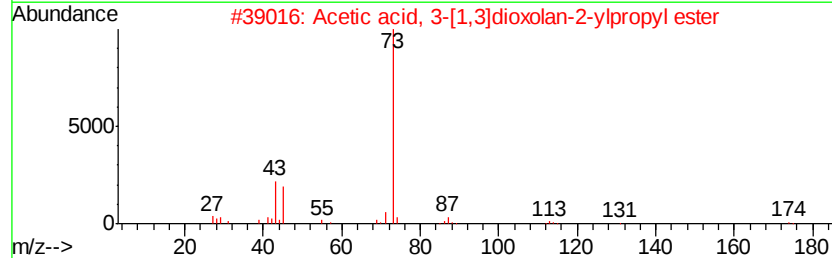
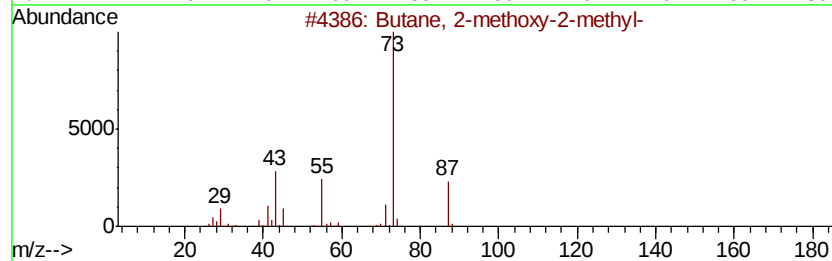
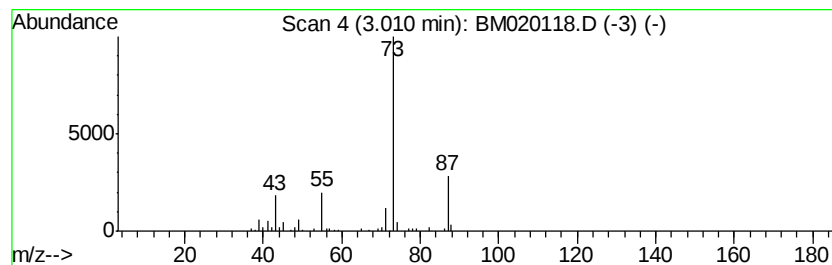
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.01	3.13 ng	115242	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2		Acetic acid, 3-[1,3]dioxolan-2-ylpropyl ester	174	C8H14O4	1000186-02-3	23
3		1,3-Dioxolane, 2-(dichloromethyl)-	156	C4H6Cl2O2	002612-35-3	9
4		1,3-Dioxolane, 2-(3-bromo-5,5,5-trifluoroethyl)-	352	C10H16BrCl3O2	1000115-31-4	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	7



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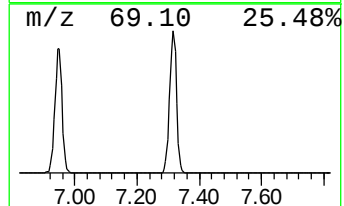
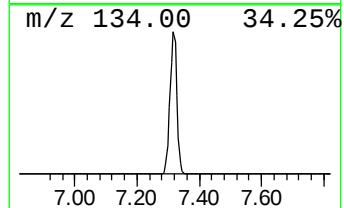
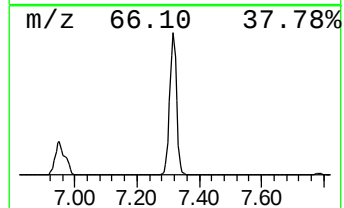
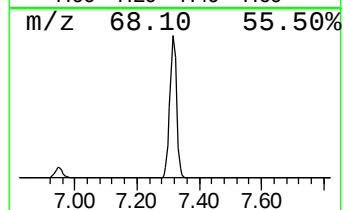
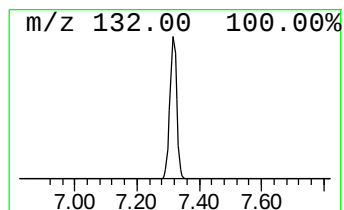
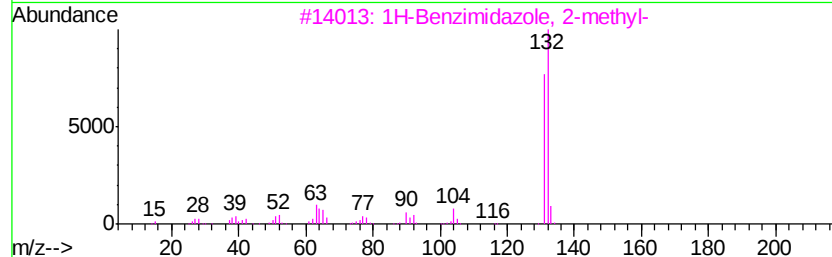
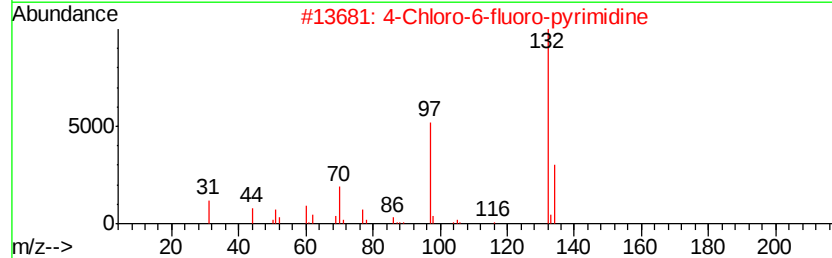
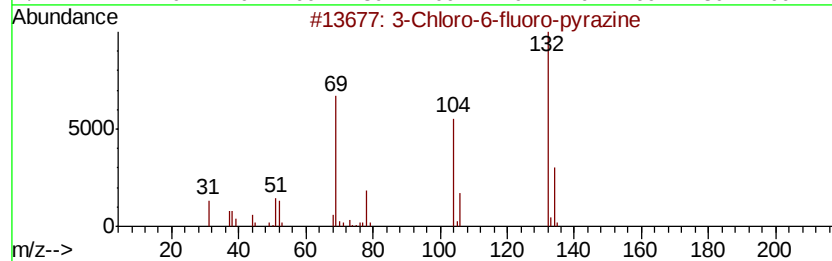
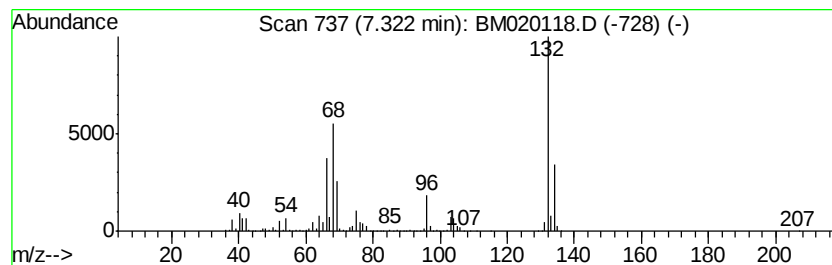
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Peak Number 2 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	131.17 ng	4828950	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		2H-Cyclopentadipyridazine, 2-me...	132	C8H8N2	022291-85-6	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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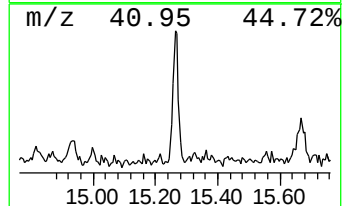
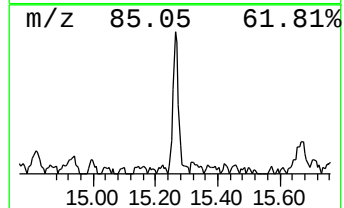
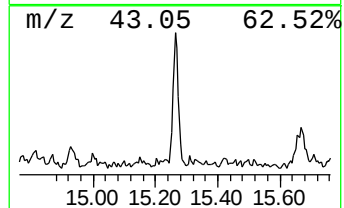
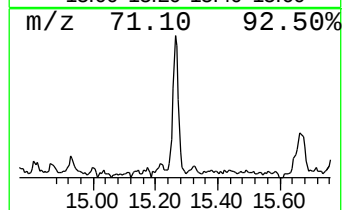
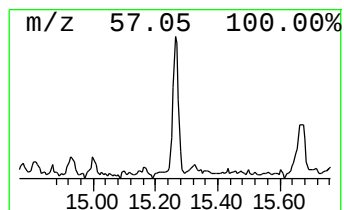
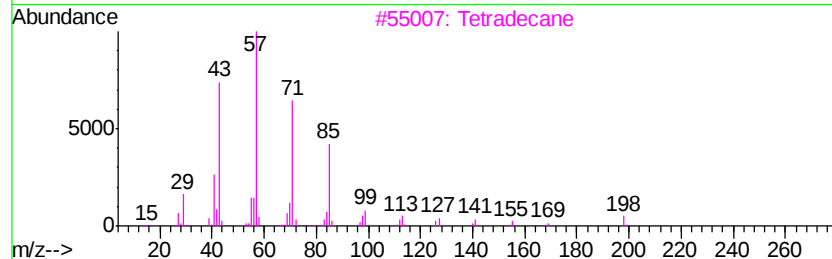
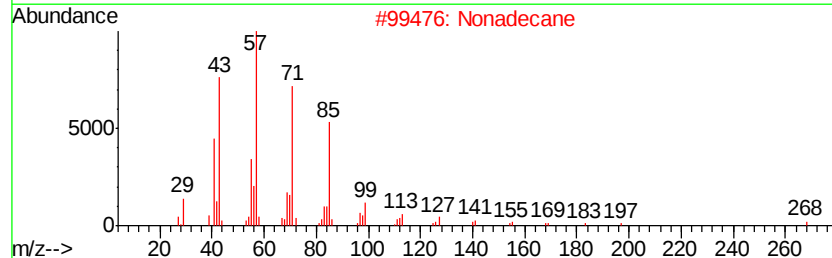
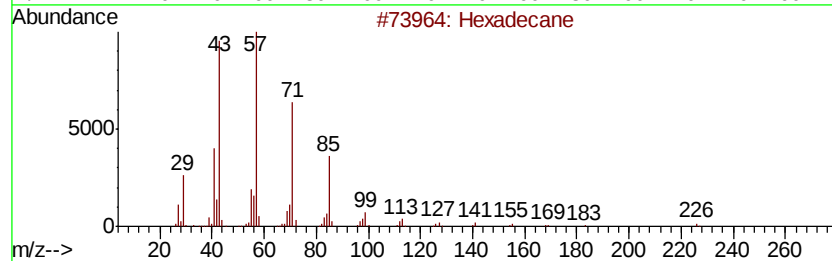
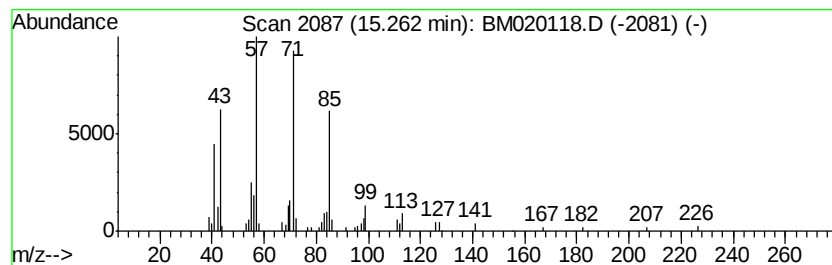
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	2.17 ng	126728	Acenaphthene-d10	14.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Nonadecane	268	C19H40	000629-92-5	90
3		Tetradecane	198	C14H30	000629-59-4	90
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
5		Tridecane	184	C13H28	000629-50-5	86



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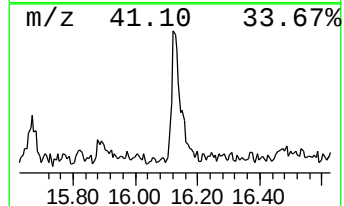
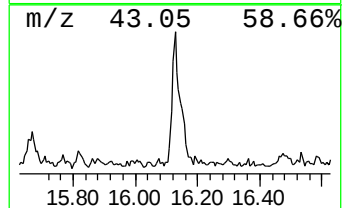
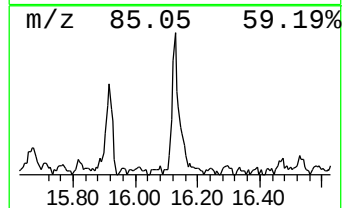
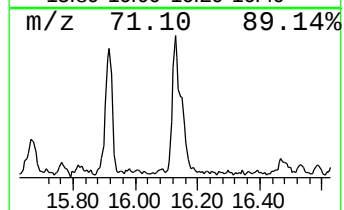
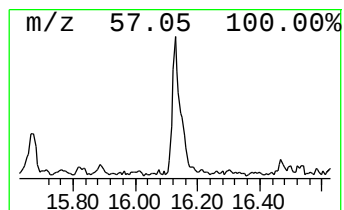
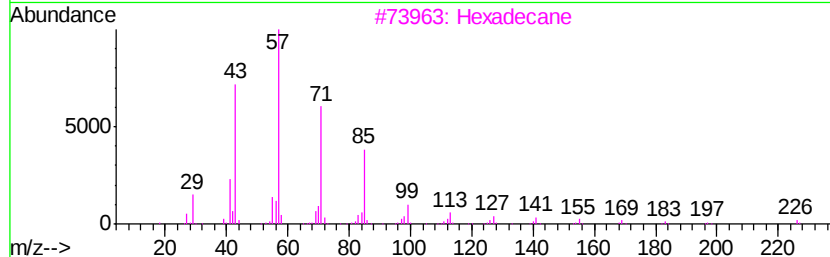
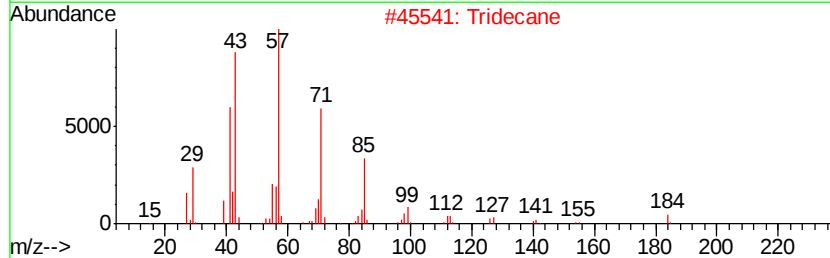
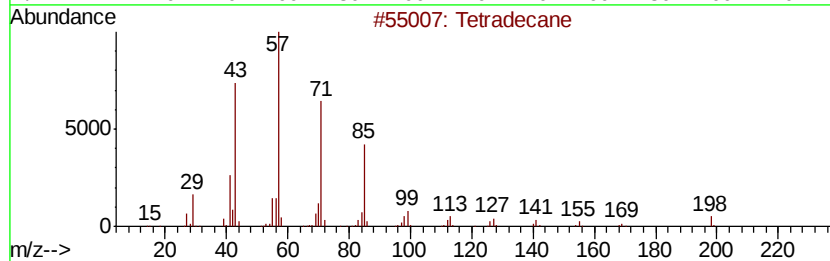
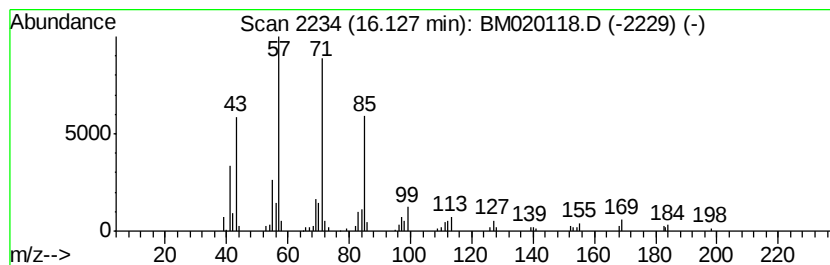
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.95 ng	211416	Phenanthrene-d10	17.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	94
2		Tridecane	184	C13H28	000629-50-5	90
3		Hexadecane	226	C16H34	000544-76-3	90
4		Tetracosane	338	C24H50	000646-31-1	86
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83



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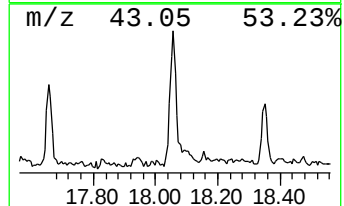
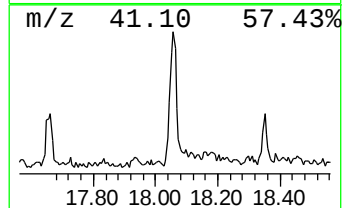
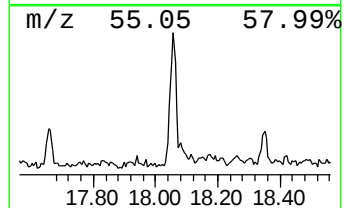
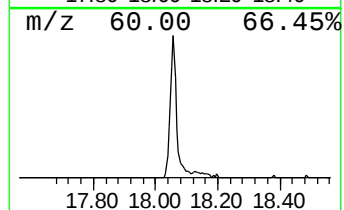
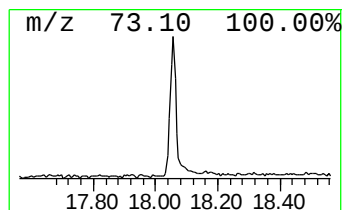
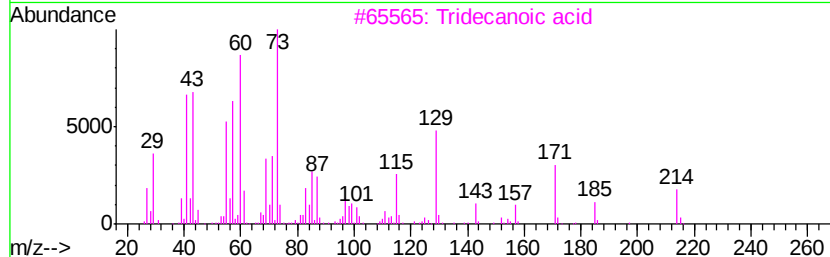
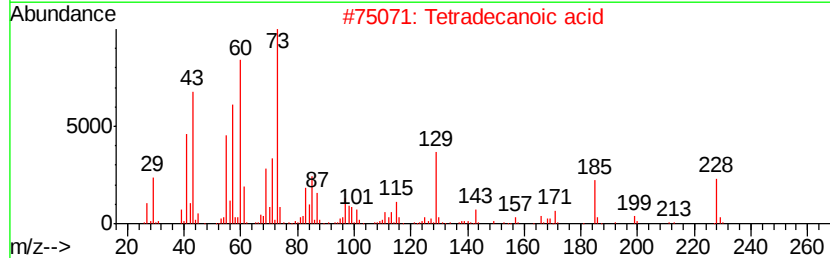
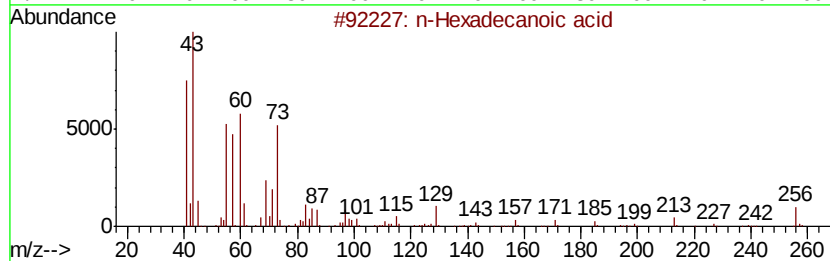
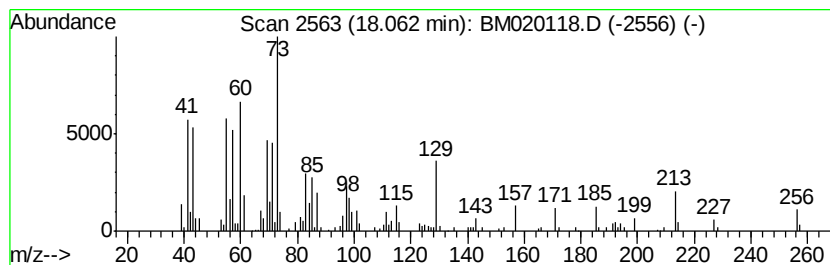
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	5.66 ng	405003	Phenanthrene-d10	17.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Tridecanoic acid	214	C13H26O2	000638-53-9	64
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5		Dodecanoic acid	200	C12H24O2	000143-07-7	43



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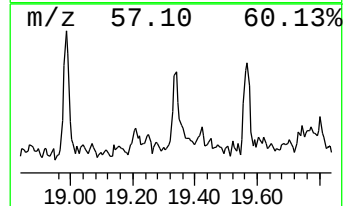
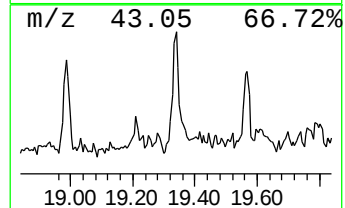
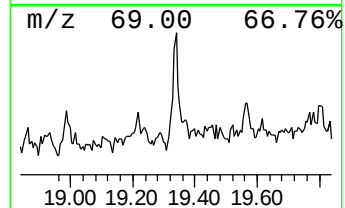
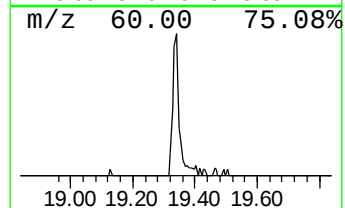
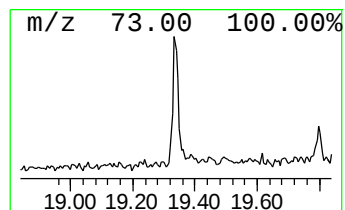
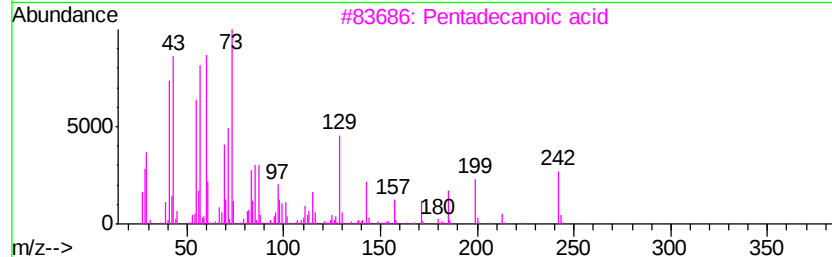
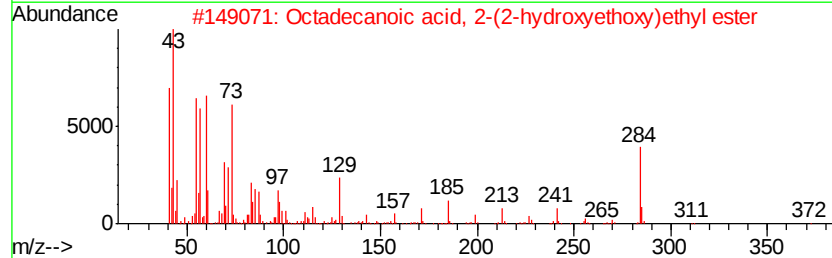
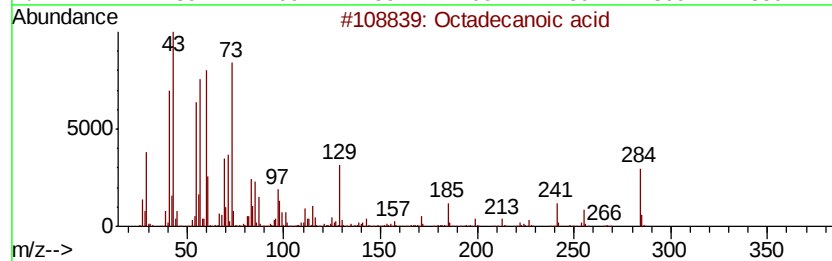
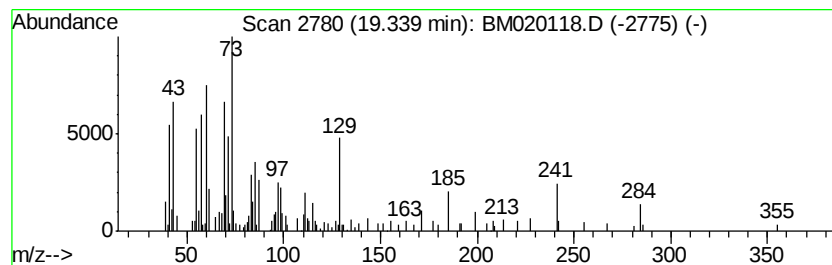
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	2.39 ng	194774	Chrysene-d12	21.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	80
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020118.D
Acq On : 03 May 2019 18:52
Operator : JU/SJ
Sample : K2668-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

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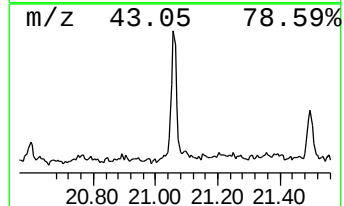
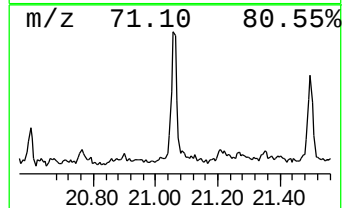
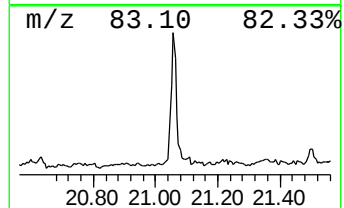
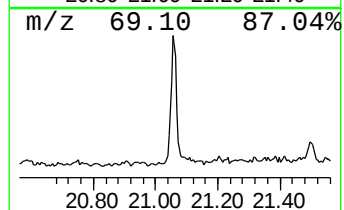
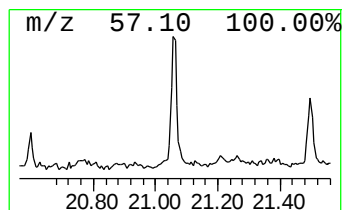
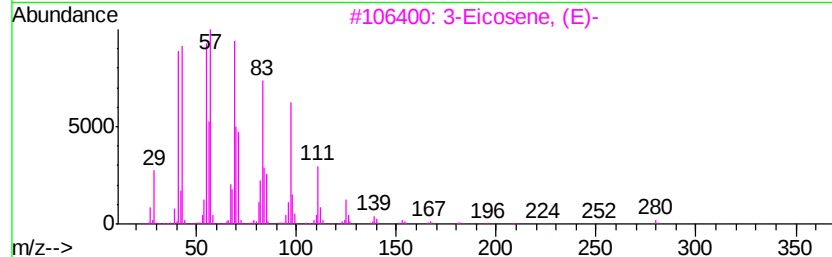
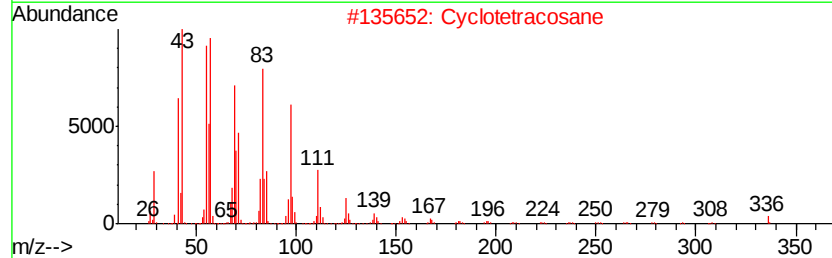
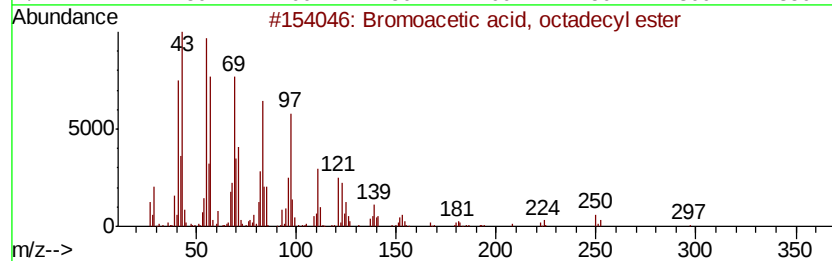
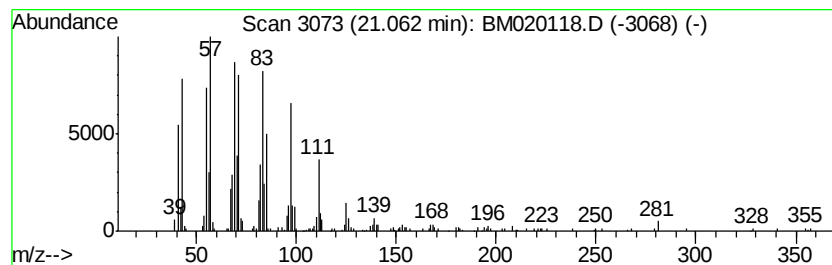
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Bromoacetic acid, octadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	5.76 ng	468275	Chrysene-d12	21.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
2		Cyclotetracosane	336	C24H48	000297-03-0	74
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	74
4		1-Heptadecanol	256	C17H36O	001454-85-9	72
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
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Sample : K2668-05
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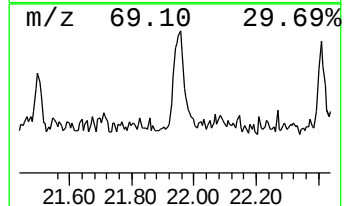
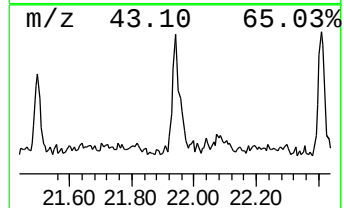
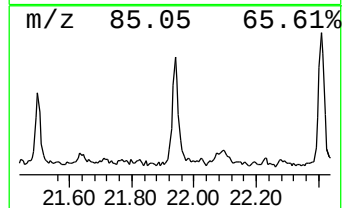
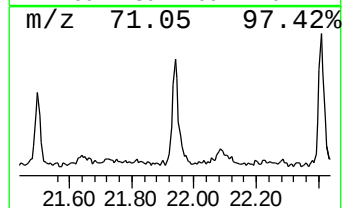
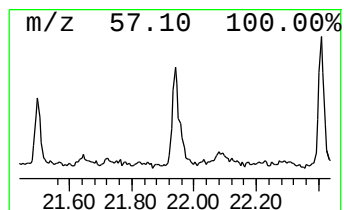
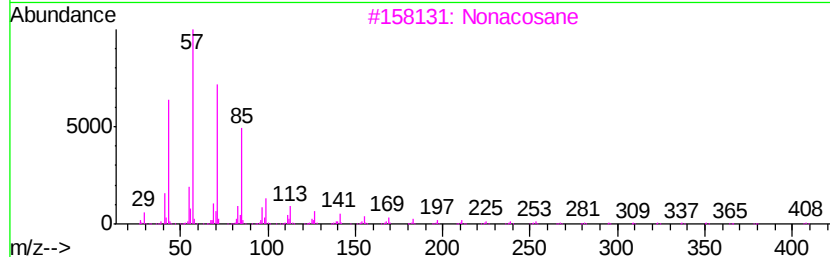
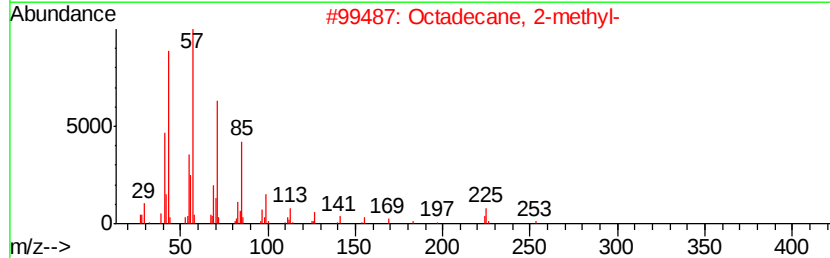
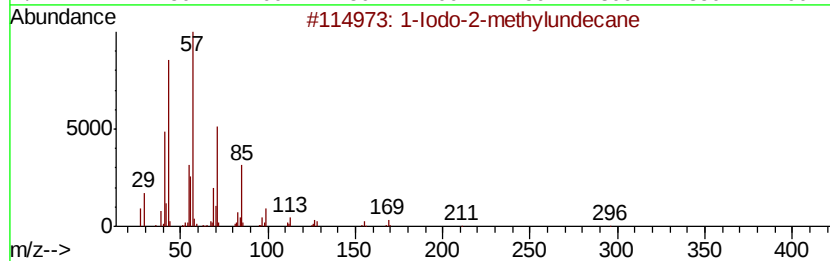
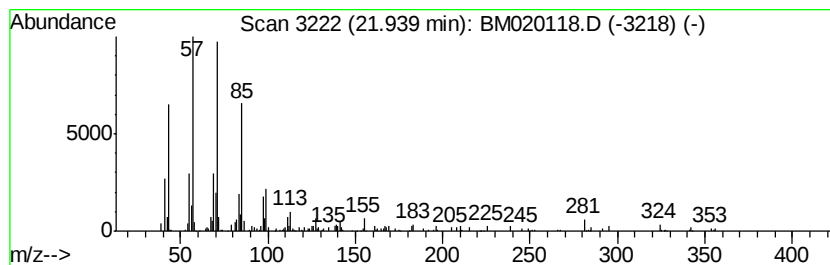
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Iodo-2-methylundecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
21.94	3.63 ng	295192	Chrysene-d12		21.36		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80
2			Octadecane, 2-methyl-	268	C19H40	001560-88-9	80
3			Nonacosane	408	C29H60	000630-03-5	64
4			Eicosane	282	C20H42	000112-95-8	59
5			Heptacosane	380	C27H56	000593-49-7	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020118.D
Acq On : 03 May 2019 18:52
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Sample : K2668-05
Misc :
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Instrument :
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ClientSampleId :
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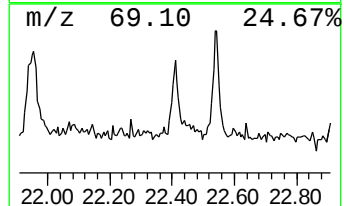
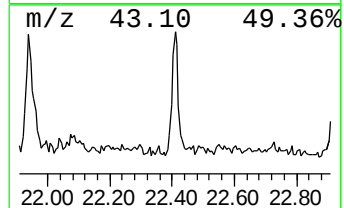
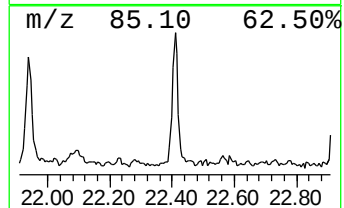
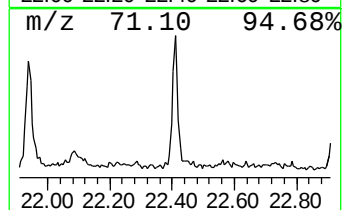
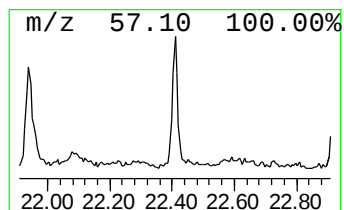
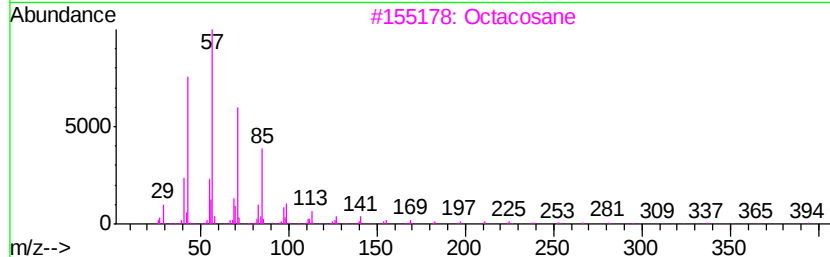
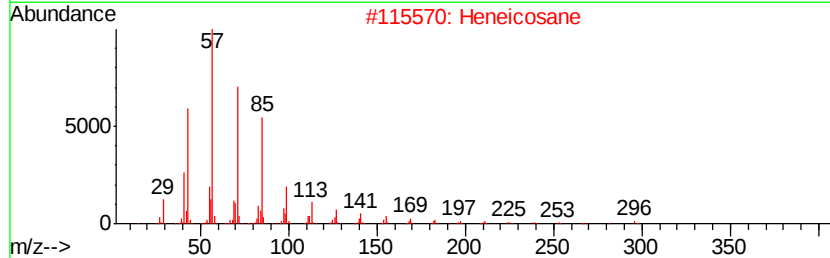
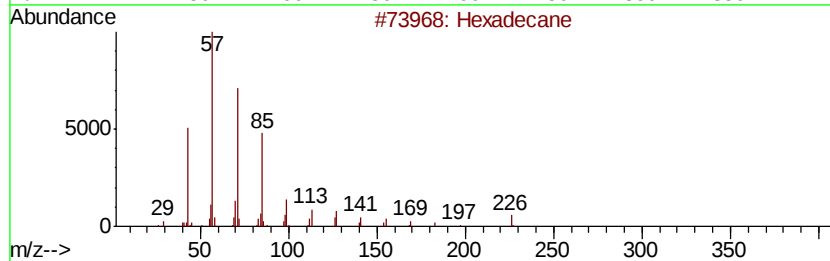
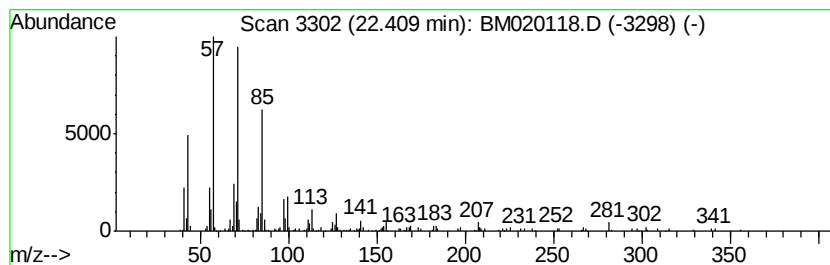
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Nonacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	2.76 ng	224773	Chrysene-d12	21.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Heneicosane	296	C21H44	000629-94-7	87
3		Octacosane	394	C28H58	000630-02-4	83
4		Nonacosane	408	C29H60	000630-03-5	80
5		Tetracosane	338	C24H50	000646-31-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
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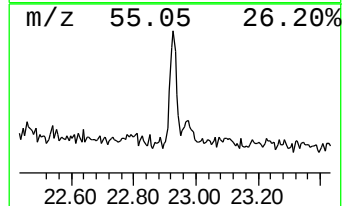
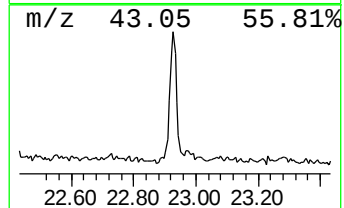
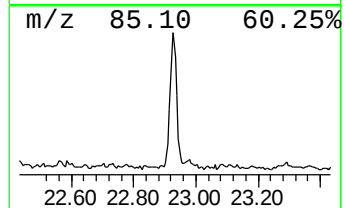
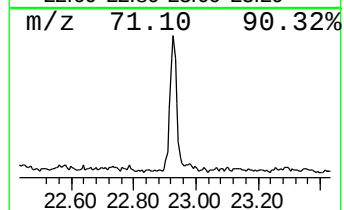
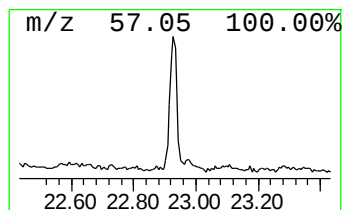
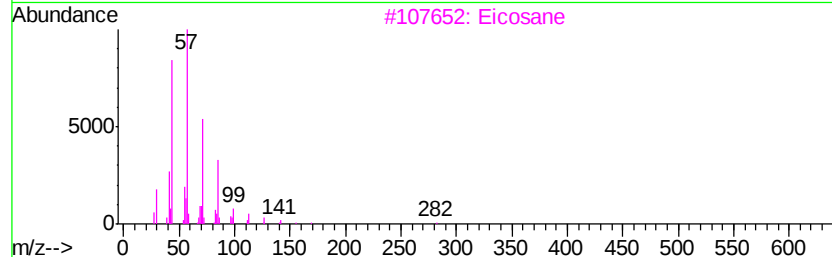
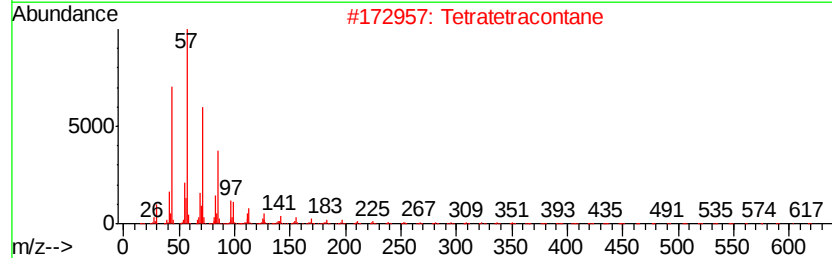
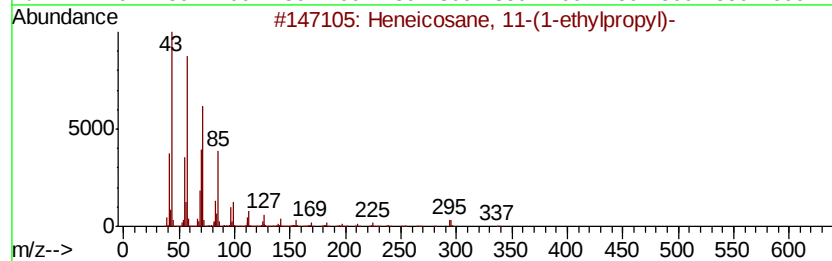
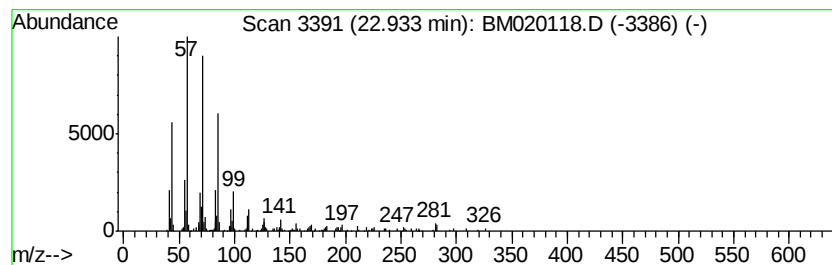
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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 11 Heneicosane, 11-(1-ethylpro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.93	4.16 ng	366682	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Eicosane	282	C20H42	000112-95-8	81
4		Heptadecane	240	C17H36	000629-78-7	80
5		Nonacosane	408	C29H60	000630-03-5	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
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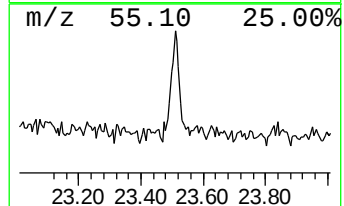
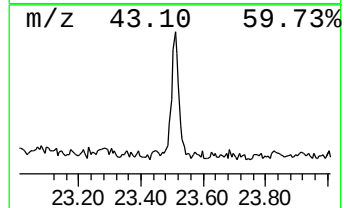
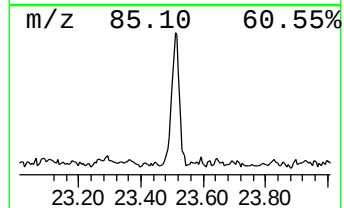
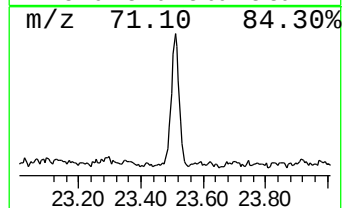
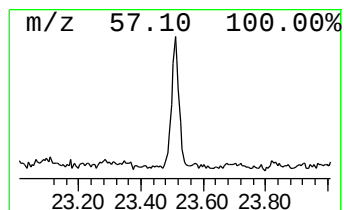
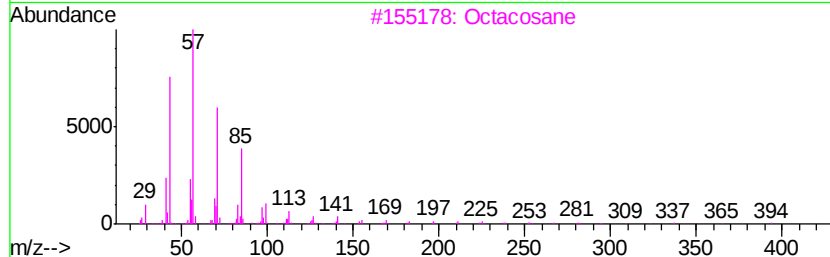
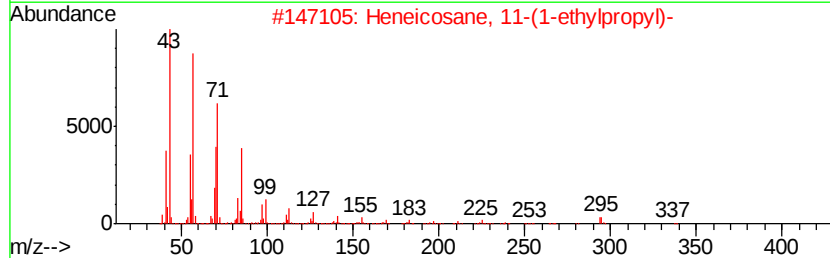
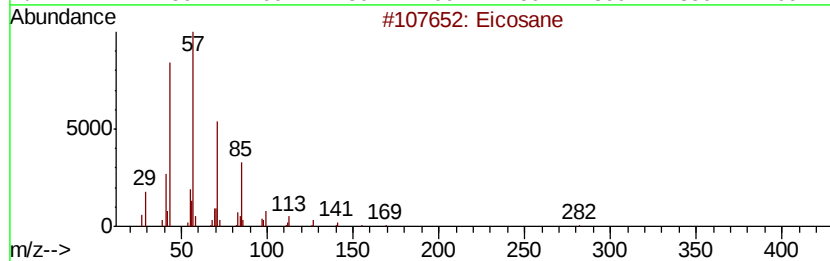
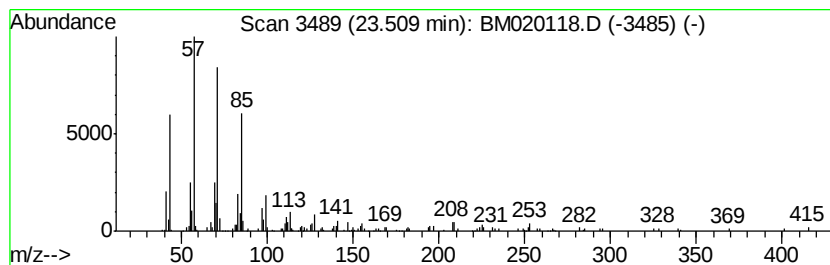
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.51	3.11 ng	274172	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexatriacontane	507	C36H74	000630-06-8	90
5		Tetratetracontane	619	C44H90	007098-22-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
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Sample : K2668-05
Misc :
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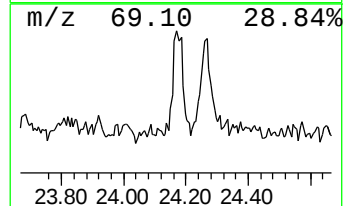
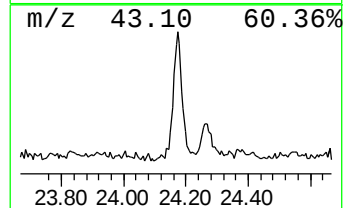
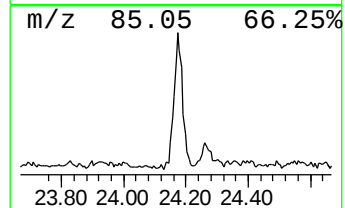
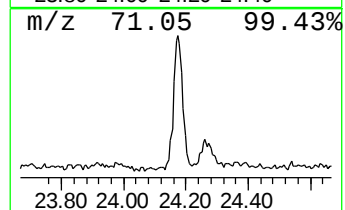
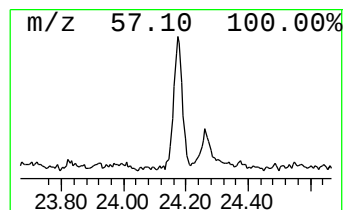
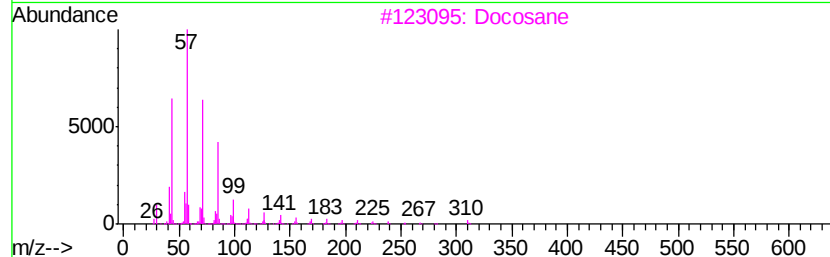
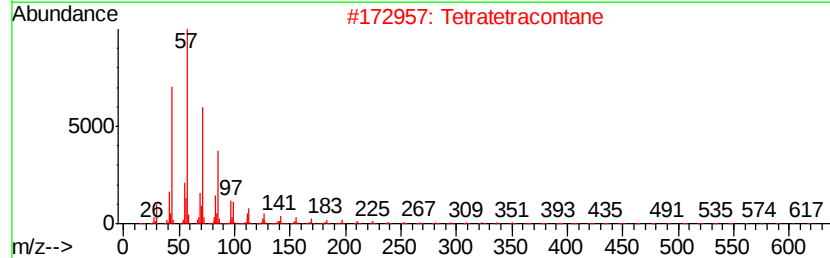
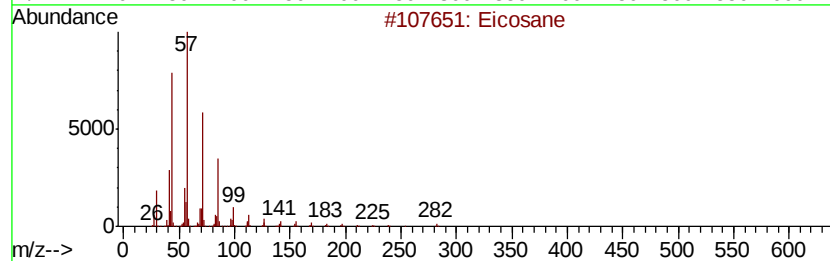
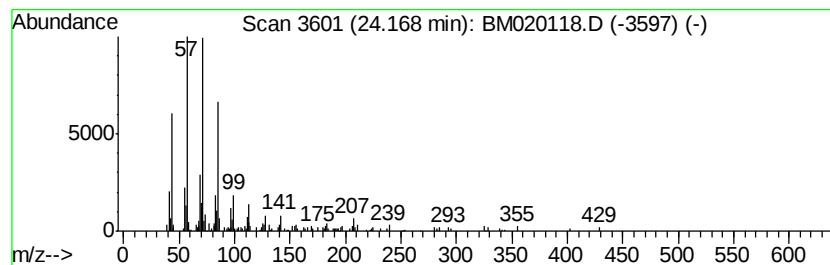
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.17	3.47 ng	305439	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	90
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Docosane	310	C22H46	000629-97-0	87
4		Methoxyacetic acid, 4-hexadecyl ...	314	C19H38O3	1000282-99-0	86
5		Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM050319\
Data File : BM020118.D
Acq On : 03 May 2019 18:52
Operator : JU/SJ
Sample : K2668-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.01	3.1 ng		115242	1	7.79	736293	20.0
unknown7.32	7.32	131.2 ng		4828950	1	7.79	736293	20.0
Hexadecane	15.26	2.2 ng		126728	3	14.43	1169770	20.0
Tetradecane	16.13	3.0 ng		211416	4	17.17	1431740	20.0
n-Hexadecanoic acid	18.06	5.7 ng		405003	4	17.17	1431740	20.0
Octadecanoic acid	19.34	2.4 ng		194774	5	21.36	1626870	20.0
Bromoacetic acid,...	21.06	5.8 ng		468275	5	21.36	1626870	20.0
1-Iodo-2-methylun...	21.94	3.6 ng		295192	5	21.36	1626870	20.0
Nonacosane	22.41	2.8 ng		224773	5	21.36	1626870	20.0
Heneicosane, 11-(...	22.93	4.2 ng		366682	6	23.64	1761750	20.0
Eicosane	23.51	3.1 ng		274172	6	23.64	1761750	20.0
Tetratetracontane	24.17	3.5 ng		305439	6	23.64	1761750	20.0