

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031519\
 Data File : BM019183.D
 Acq On : 15 Mar 2019 13:10
 Operator : JU/SJ
 Sample : K1817-15
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PST-027-B111-030619

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-BM031119.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	5.252	379	385	399	rBV	3273390	4878541	43.42%	5.646%
2	6.840	647	655	676	rBV	3629716	6095767	54.26%	7.054%
3	7.187	707	714	733	rBV	3616505	5821702	51.82%	6.737%
4	7.651	787	793	801	rBV	957401	1531417	13.63%	1.772%
5	7.969	839	847	855	rBV	2400760	3778190	33.63%	4.372%
6	8.822	985	992	1009	rBV	1989333	3502578	31.18%	4.053%
7	10.440	1259	1267	1284	rBV	1368976	2421531	21.55%	2.802%
8	12.922	1682	1689	1704	rBV	5734190	8423588	74.98%	9.748%
9	13.775	1827	1834	1845	rBV	365823	596505	5.31%	0.690%
10	14.310	1918	1925	1942	rBV2	2302699	3491180	31.08%	4.040%
11	15.810	2173	2180	2196	rBV	4777244	6884080	61.28%	7.966%
12	17.063	2387	2393	2398	rBV2	2779887	4022607	35.81%	4.655%
13	17.104	2398	2400	2404	rVB	163212	197761	1.76%	0.229%
14	17.957	2538	2545	2560	rBV2	801175	1373377	12.22%	1.589%
15	18.133	2570	2575	2579	rBV3	74436	123228	1.10%	0.143%
16	19.127	2736	2744	2749	rBV	444887	730664	6.50%	0.846%
17	19.174	2749	2752	2759	rVV2	88793	132502	1.18%	0.153%
18	19.239	2759	2763	2777	rVV2	272888	503487	4.48%	0.583%
19	19.498	2803	2807	2814	rVB	324726	474349	4.22%	0.549%
20	19.704	2836	2842	2857	rBV	9117091	11234679	100.00%	13.001%
21	19.974	2883	2888	2890	rBV2	167394	243414	2.17%	0.282%
22	20.492	2973	2976	2981	rVB3	92619	120516	1.07%	0.139%
23	20.962	3051	3056	3065	rBV	1313572	1749581	15.57%	2.025%
24	21.262	3101	3107	3111	rBV	3300377	4355631	38.77%	5.040%
25	21.398	3127	3130	3139	rVB2	211948	311678	2.77%	0.361%
26	21.827	3199	3203	3204	rBV2	392016	420005	3.74%	0.486%
27	21.851	3204	3207	3216	rVV	1517656	2082098	18.53%	2.409%
28	21.927	3216	3220	3223	rVB	212592	250453	2.23%	0.290%
29	22.180	3260	3263	3267	rVB	218549	271524	2.42%	0.314%
30	22.286	3277	3281	3284	rBV	360338	460480	4.10%	0.533%
31	22.786	3362	3366	3370	rBV	472755	640449	5.70%	0.741%
32	22.839	3370	3375	3385	rVV2	1944531	3330905	29.65%	3.855%
33	22.927	3386	3390	3399	rVB	304703	524603	4.67%	0.607%
34	23.139	3423	3426	3434	rVB	214936	353550	3.15%	0.409%

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ClientSampleId :
PST-027-B111-030619

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

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35	23.345	3458	3461	3466	rVB	323854	450383	4.01%	0.521%
36	23.497	3480	3487	3499	rBV	1839454	3518097	31.31%	4.071%
37	23.992	3566	3571	3578	rVB	394828	724079	6.45%	0.838%
38	24.186	3601	3604	3611	rVB	221289	388741	3.46%	0.450%

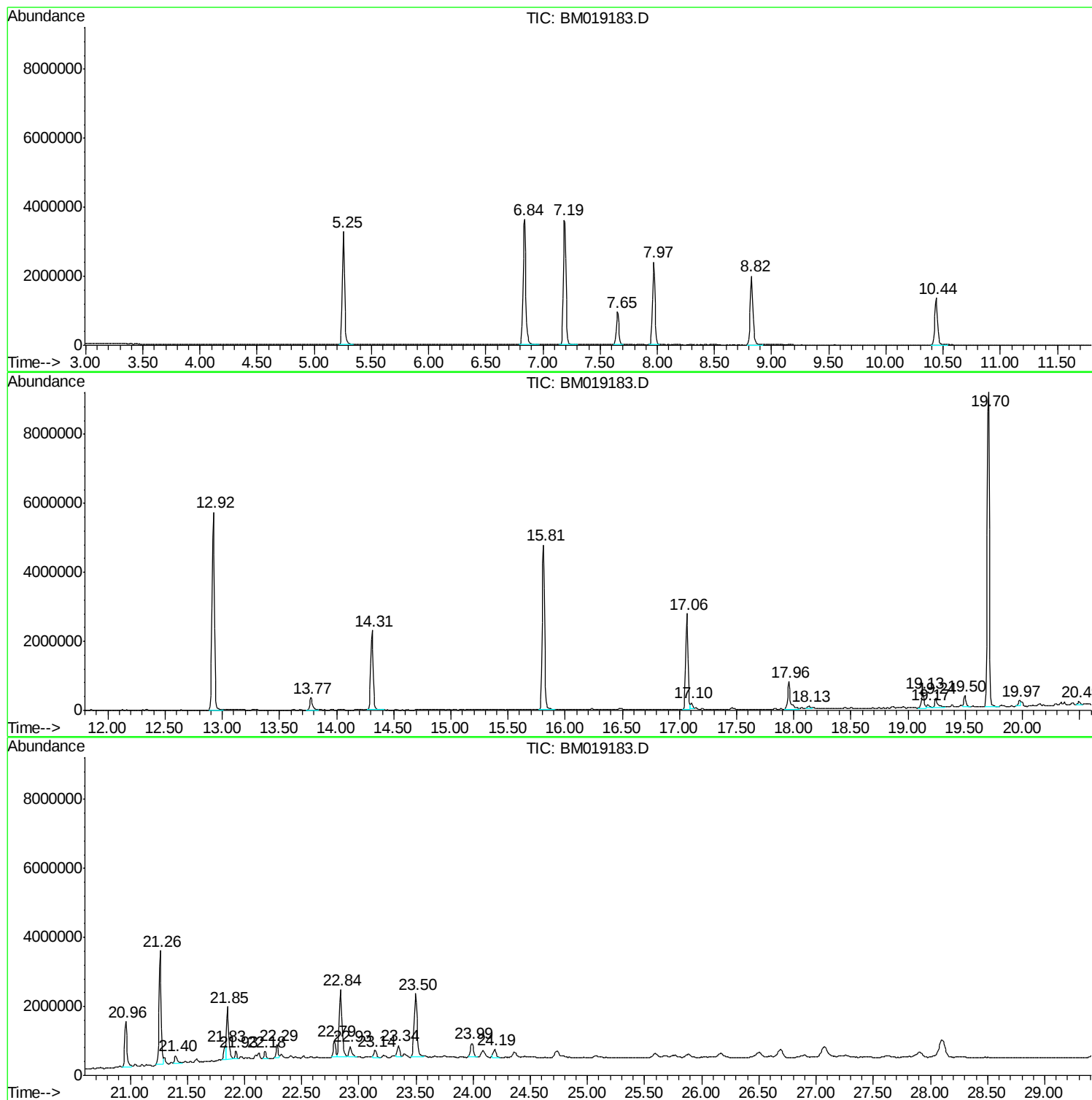
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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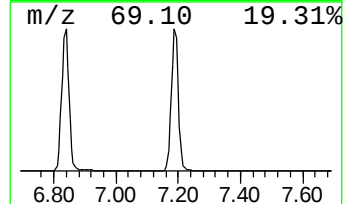
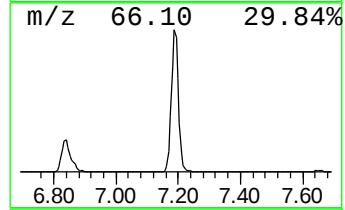
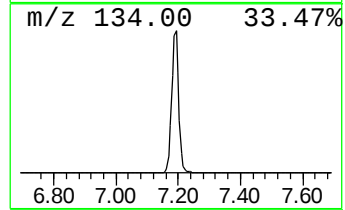
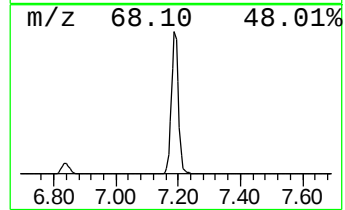
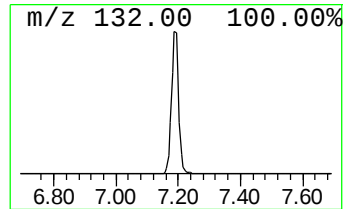
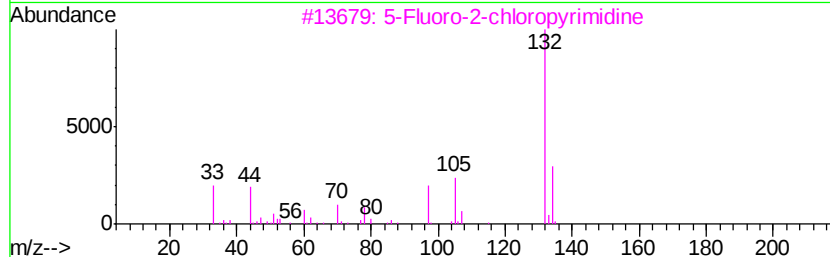
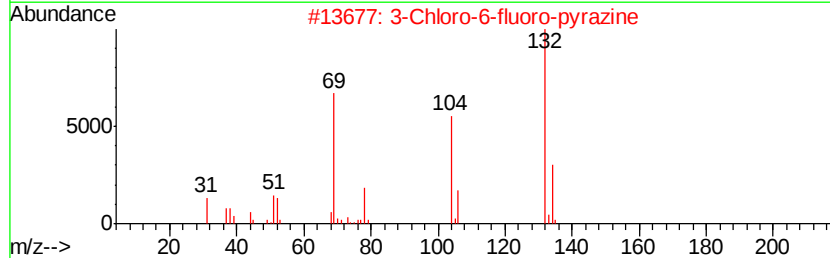
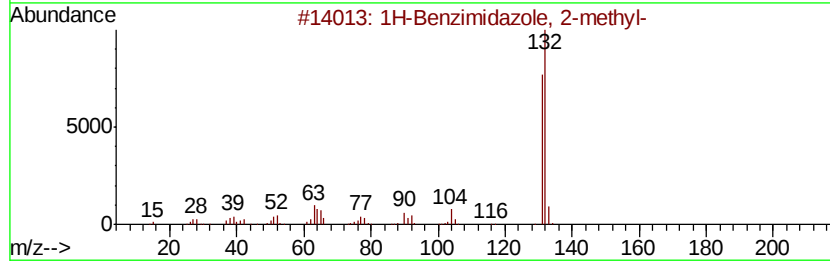
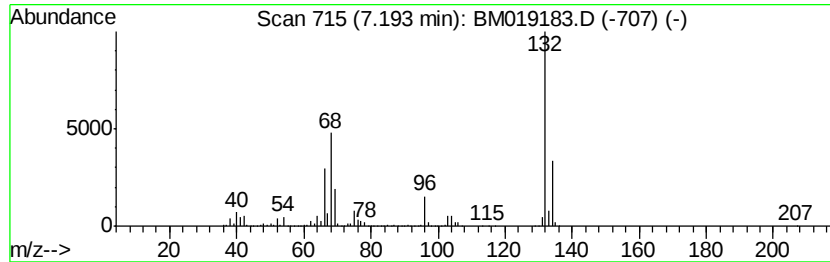
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	76.03 ng	5821700	1,4-Dichlorobenzene-d4	7.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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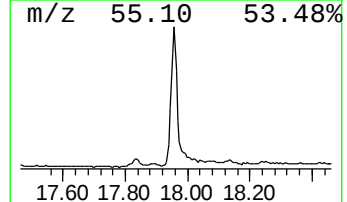
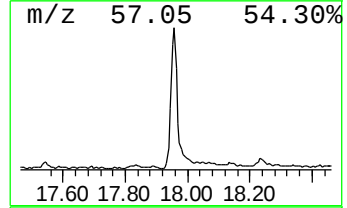
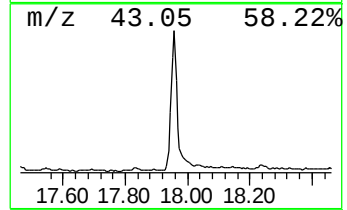
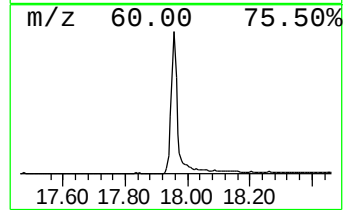
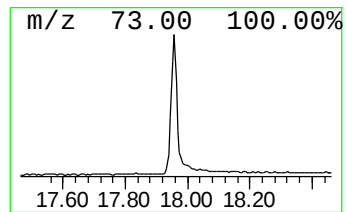
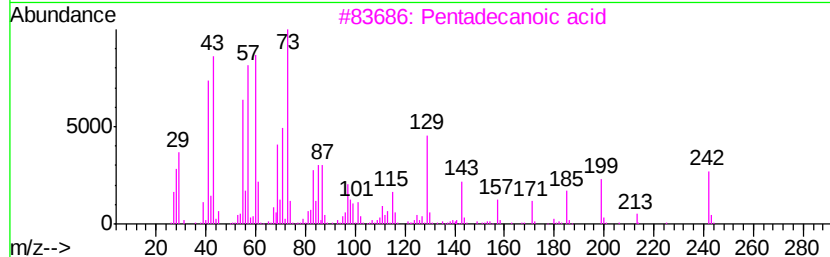
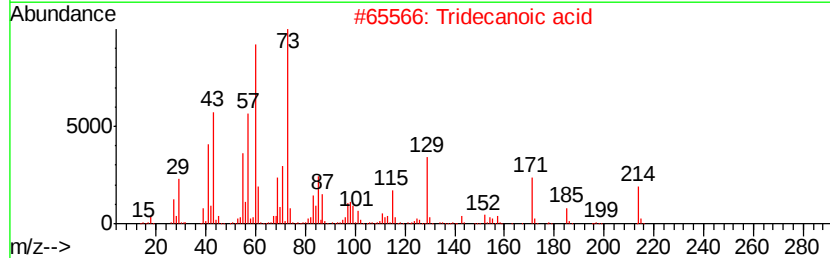
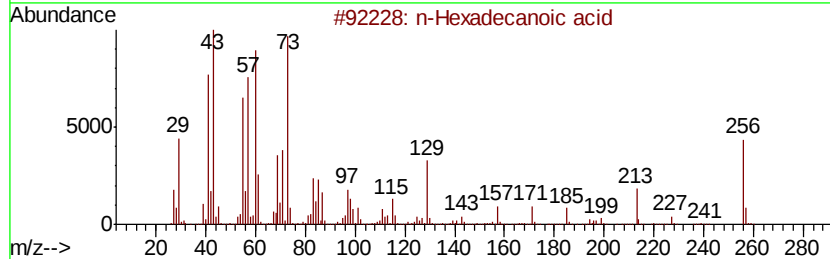
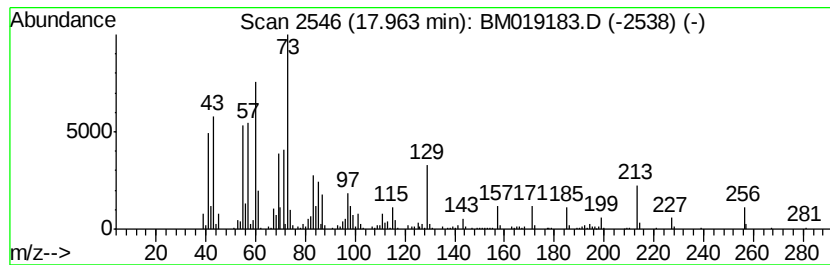
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.96	6.83 ng	1373380	Phenanthrene-d10	17.06	
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	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Sedoheptulosan	192	C7H12O6	000469-90-9	35
5	Eicosane	282	C20H42	000112-95-8	25



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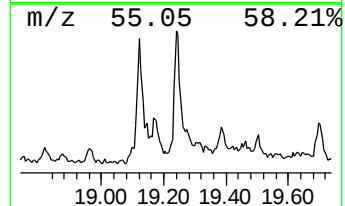
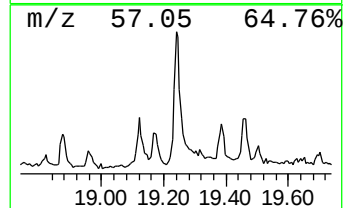
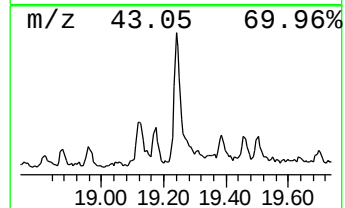
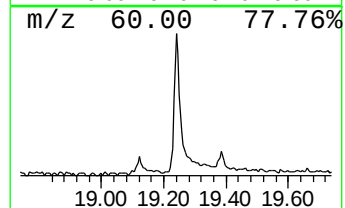
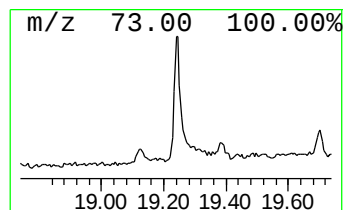
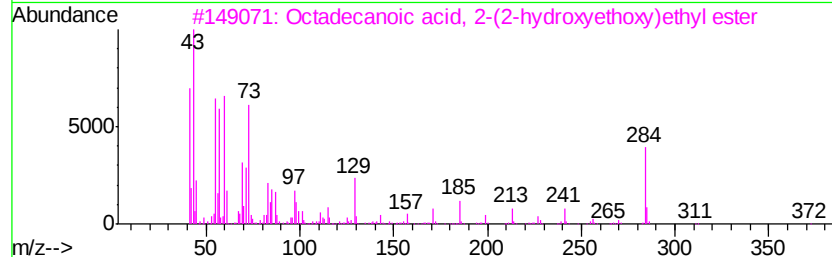
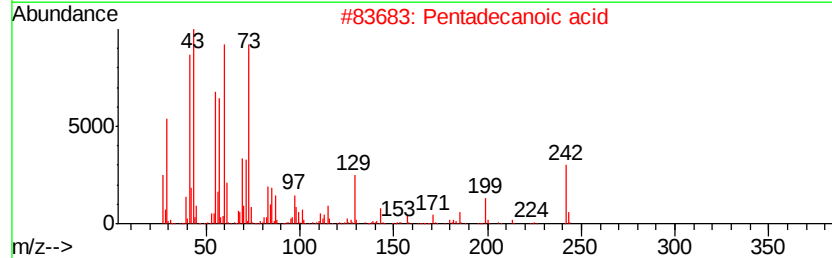
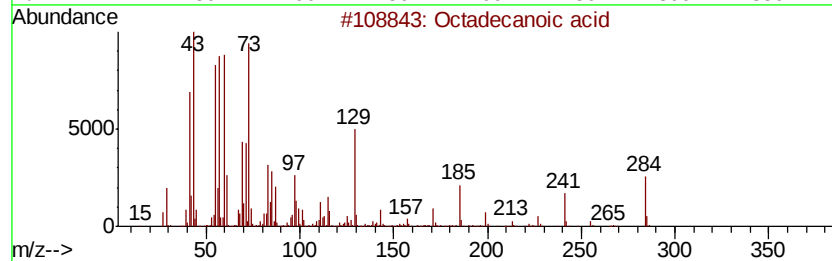
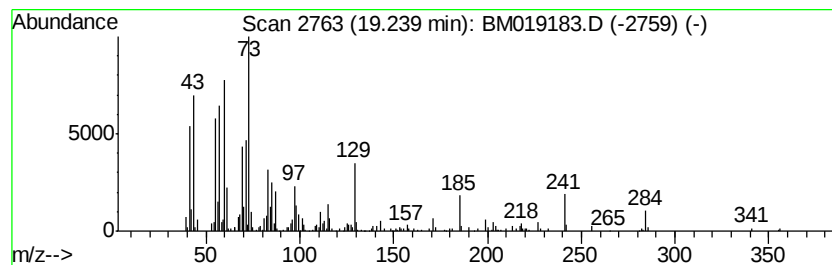
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.24	2.31 ng	503487	Chrysene-d12	21.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	18



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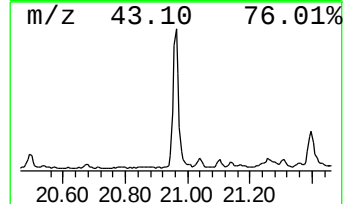
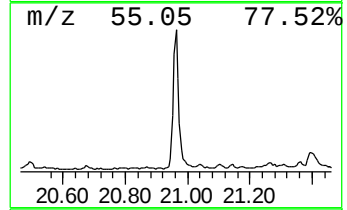
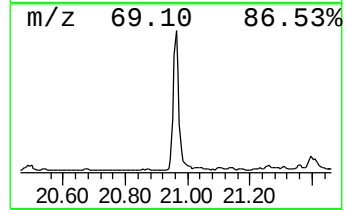
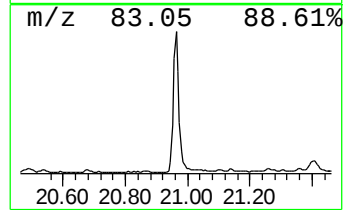
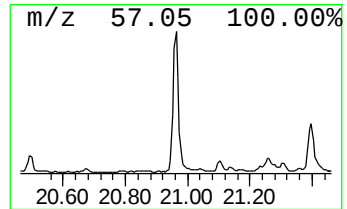
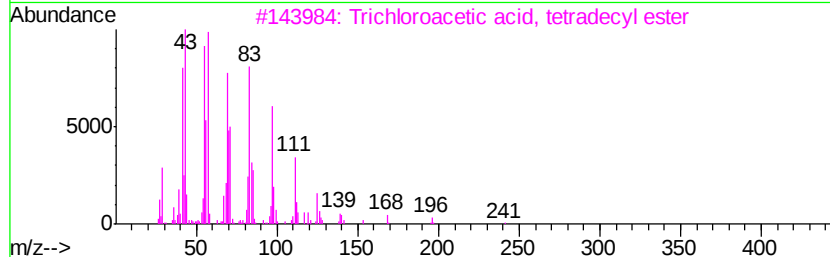
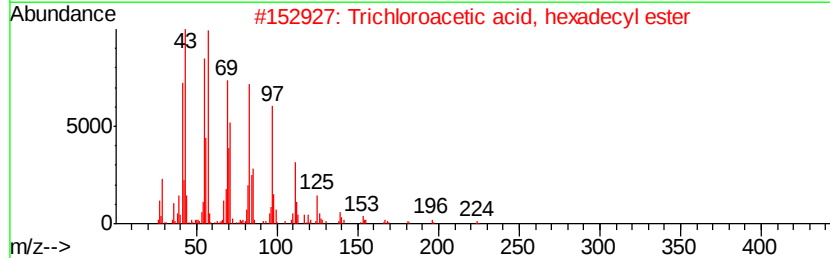
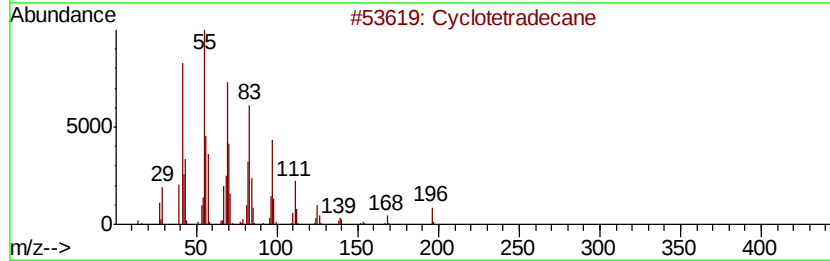
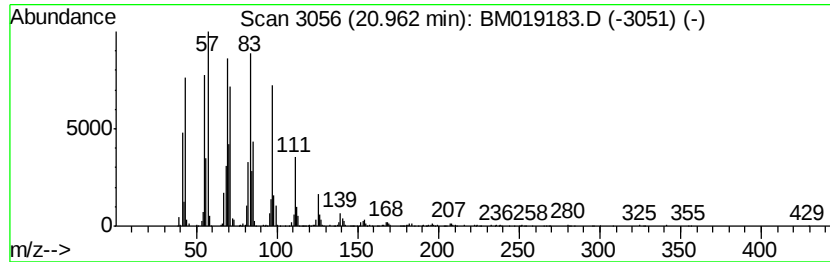
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
20.96	8.03 ng	1749580	Chrysene-d12		21.26
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvcclotetradecane	196	C14H28	000295-17-0	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	90



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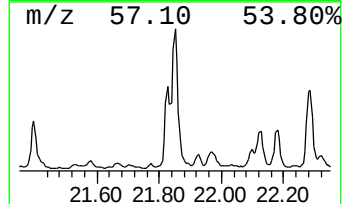
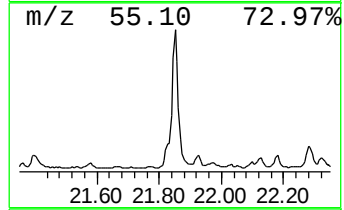
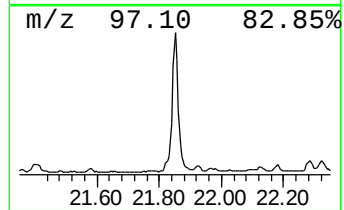
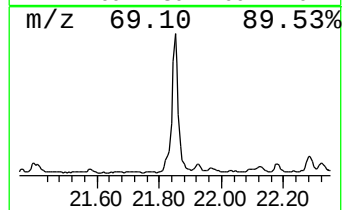
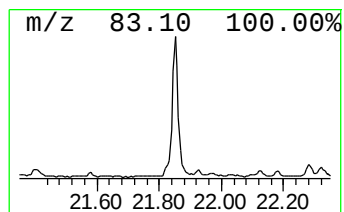
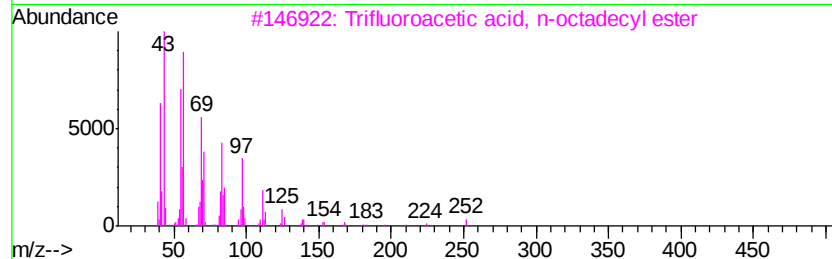
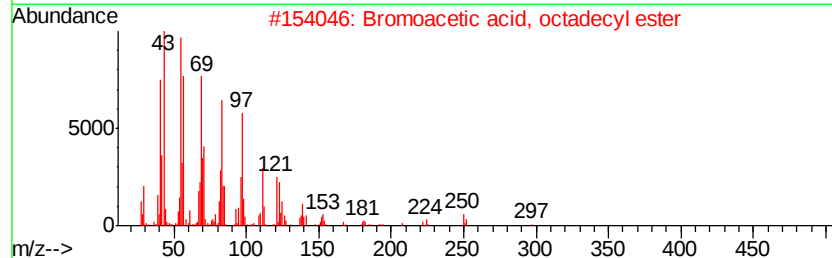
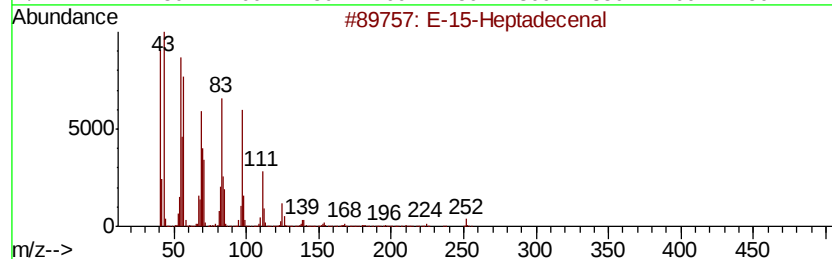
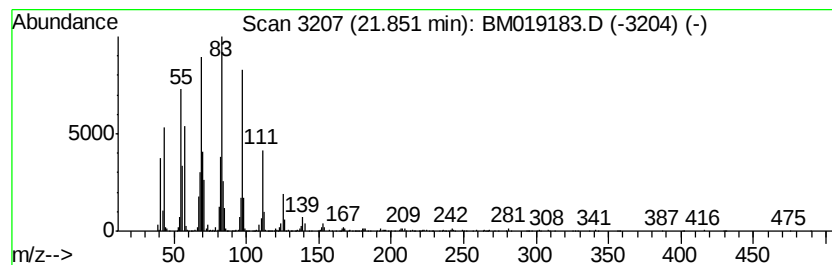
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.85	9.56 ng	2082100	Chrysene-d12	21.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
3		Trifluoroacetic acid, n-octadecyl ester	366	C20H37F3O2	079392-43-1	90
4		Cyclopentane, decyl-	210	C15H30	001795-21-7	80
5		1-Hexadecanol	242	C16H34O	036653-82-4	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031519\
Data File : BM019183.D
Acq On : 15 Mar 2019 13:10
Operator : JU/SJ
Sample : K1817-15
Misc :
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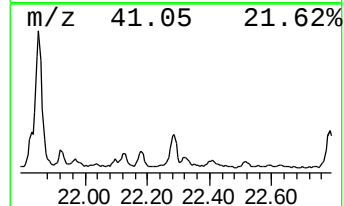
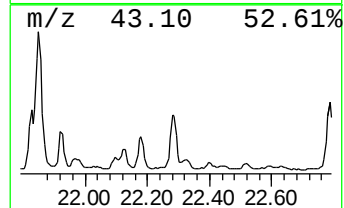
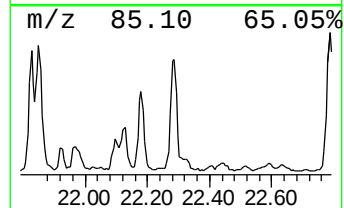
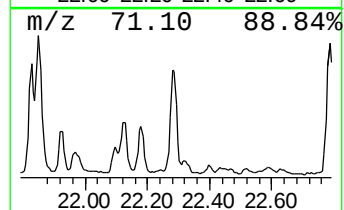
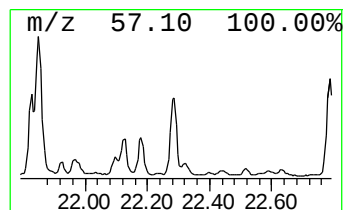
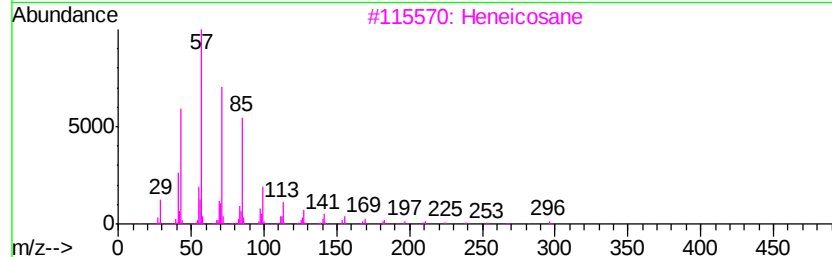
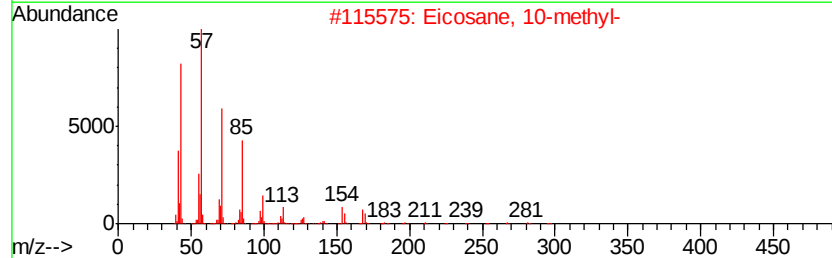
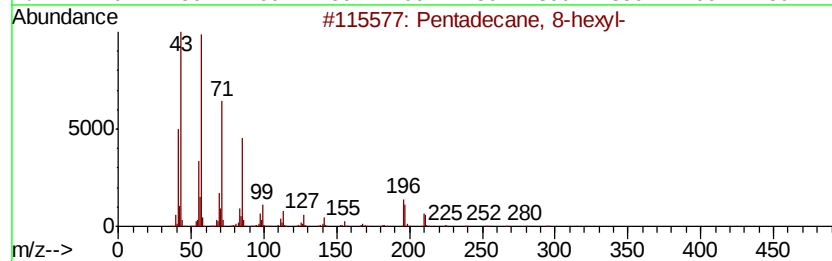
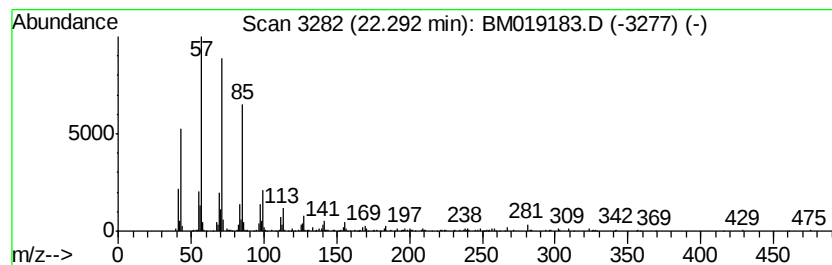
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ClientSampleId :
PST-027-B111-030619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.		
22.29	2.11 ng	460480	Chrysene-d12	21.26		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94	
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91	
3	Heneicosane	296	C21H44	000629-94-7	91	
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91	
5	Heptacosane	380	C27H56	000593-49-7	91	



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031519\
 Data File : BM019183.D
 Acq On : 15 Mar 2019 13:10
 Operator : JU/SJ
 Sample : K1817-15
 Misc :
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Instrument :
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 ClientSampleId :
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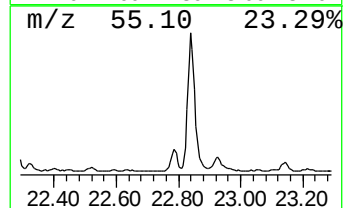
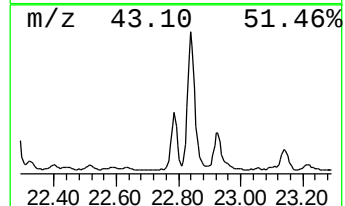
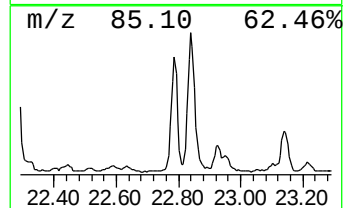
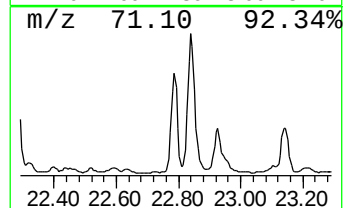
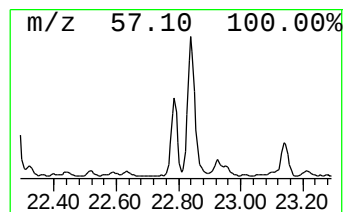
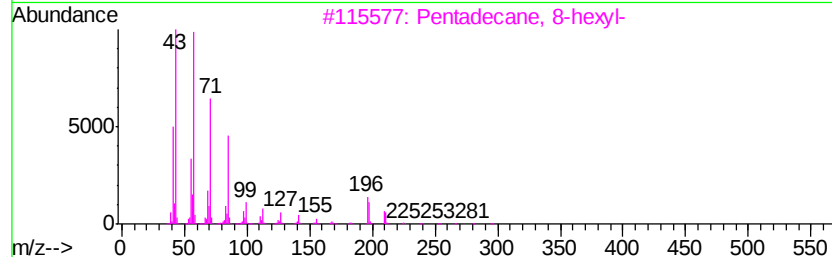
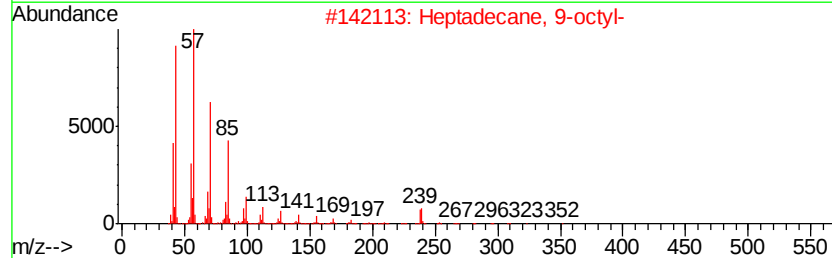
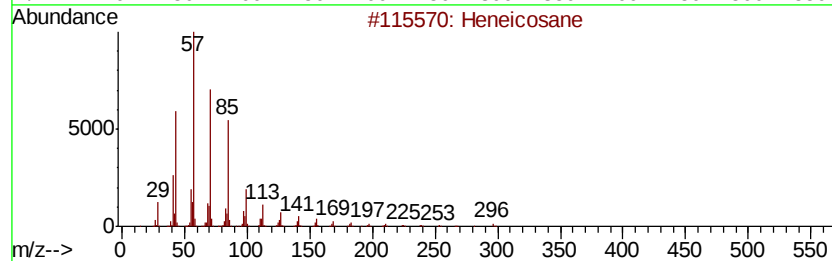
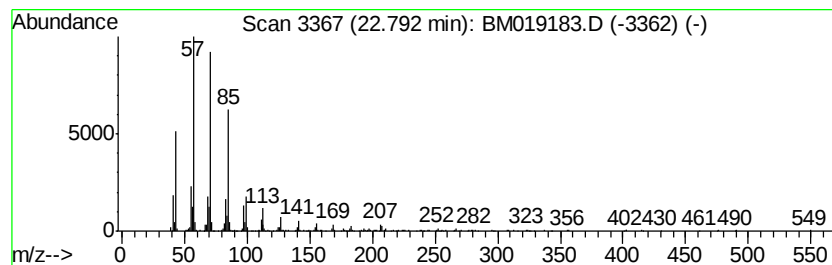
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.79	3.64 ng	640449	Perylene-d12	23.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	Pentadecane, 8-hexyl-		296	C21H44	013475-75-7	91
4	Pentacosane		352	C25H52	000629-99-2	90
5	Tridecane, 7-hexyl-		268	C19H40	007225-66-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031519\
Data File : BM019183.D
Acq On : 15 Mar 2019 13:10
Operator : JU/SJ
Sample : K1817-15
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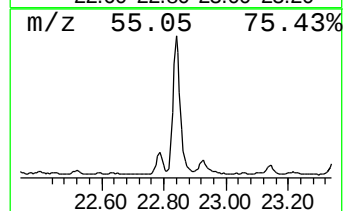
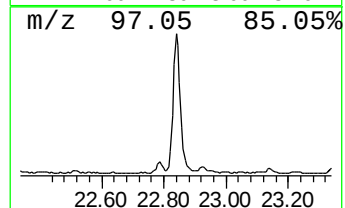
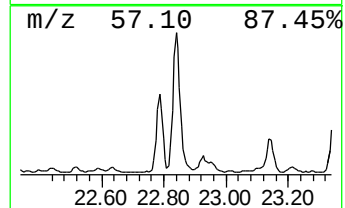
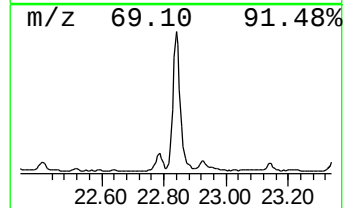
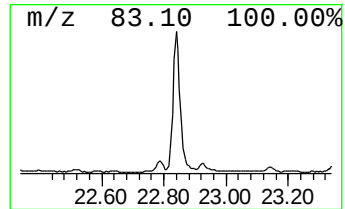
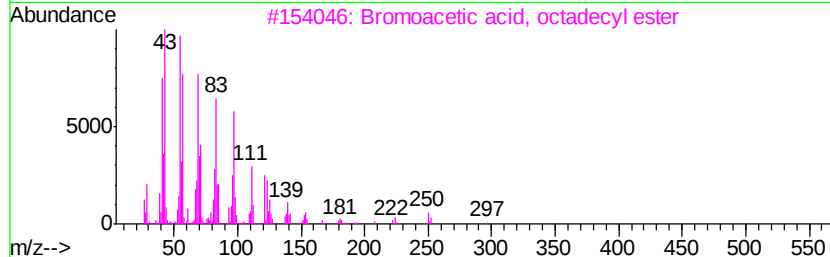
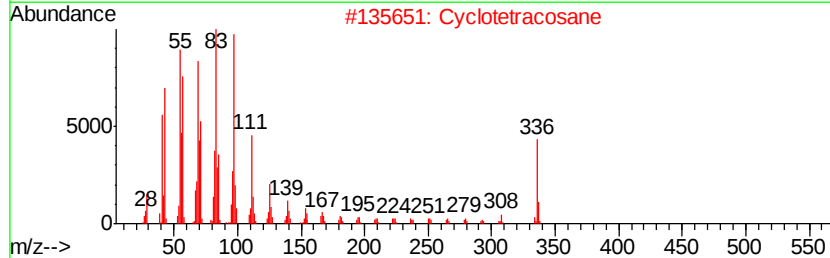
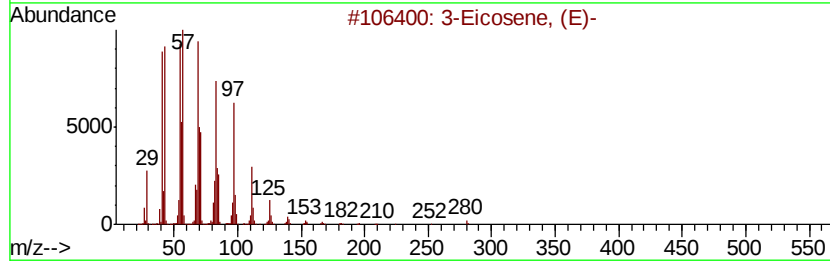
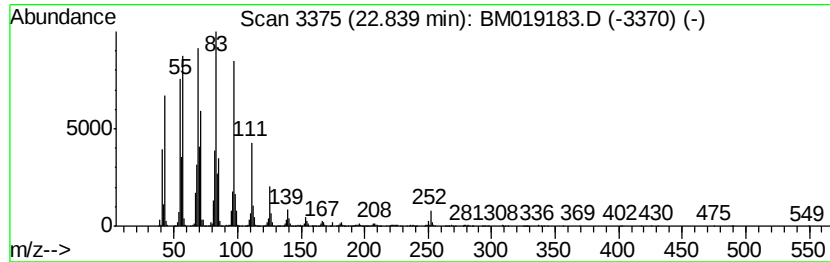
Instrument :
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ClientSampleId :
PST-027-B111-030619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.84	18.94 ng	3330910	Perylene-d12	23.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Eicosene, (E)-	280 C20H40	074685-33-9	96
2	Cyclotetracosane	336 C24H48	000297-03-0	93
3	Bromoacetic acid, octadecyl ester	390 C20H39BrO2	018992-03-5	91
4	1-Heneicosyl formate	340 C22H44O2	077899-03-7	91
5	1-Heptadecanol	256 C17H36O	001454-85-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031519\
Data File : BM019183.D
Acq On : 15 Mar 2019 13:10
Operator : JU/SJ
Sample : K1817-15
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Instrument :
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ClientSampleId :
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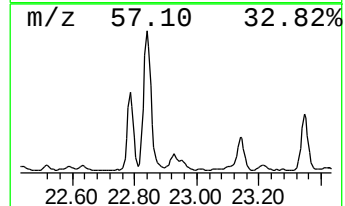
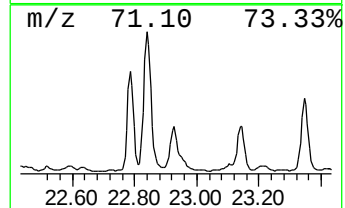
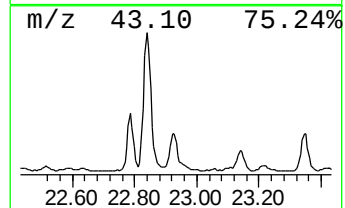
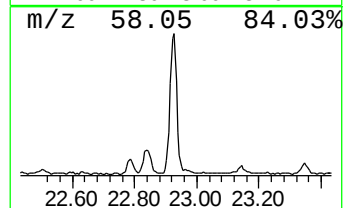
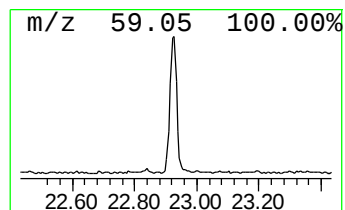
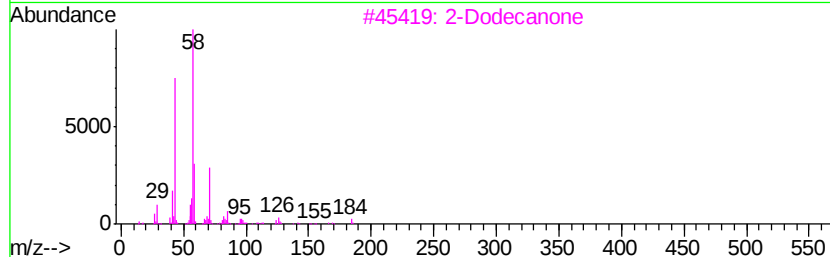
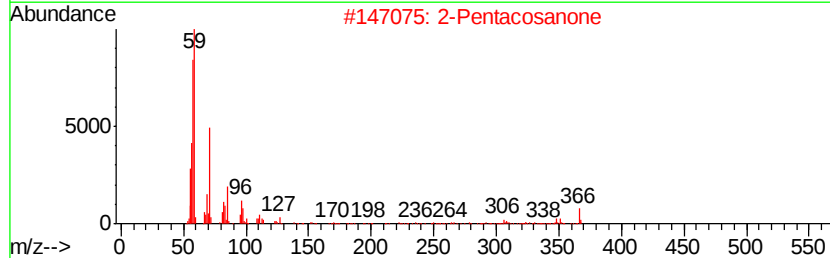
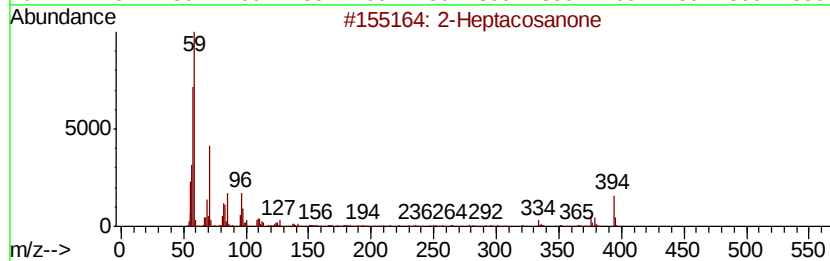
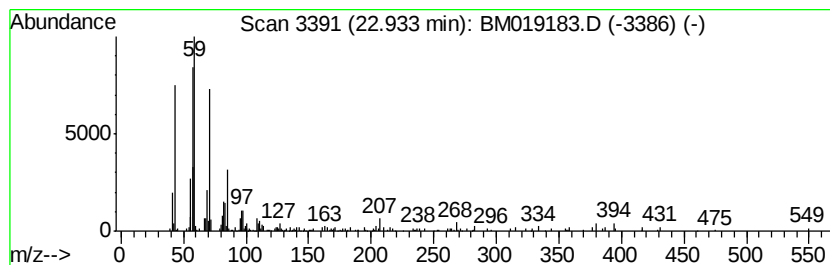
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Heptacosanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.93	2.98 ng	524603	Perylene-d12	23.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptacosanone	394	C27H54O	007796-19-2	92
2			2-Pentacosanone	366	C25H50O	075207-54-4	86
3			2-Dodecanone	184	C12H24O	006175-49-1	47
4			2-Undecanone, 6,10-dimethyl-	198	C13H26O	001604-34-8	40
5			2-Tridecanone	198	C13H26O	000593-08-8	40



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031519\
Data File : BM019183.D
Acq On : 15 Mar 2019 13:10
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Instrument :
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ClientSampleId :
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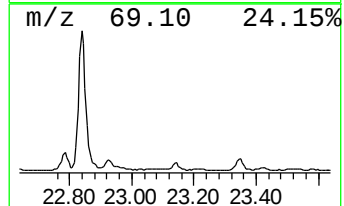
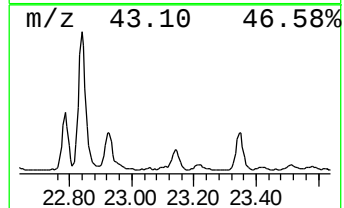
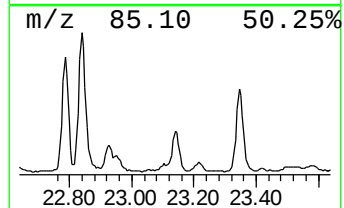
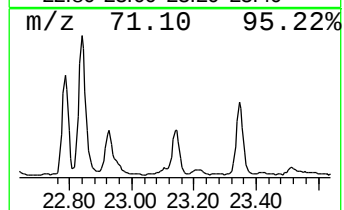
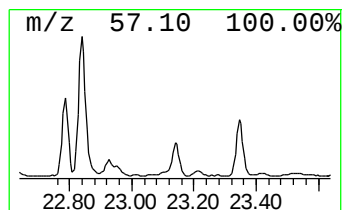
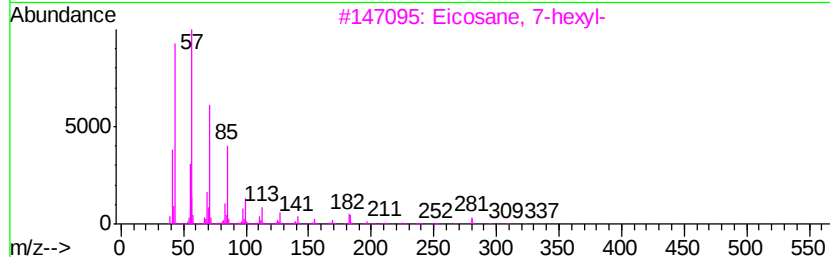
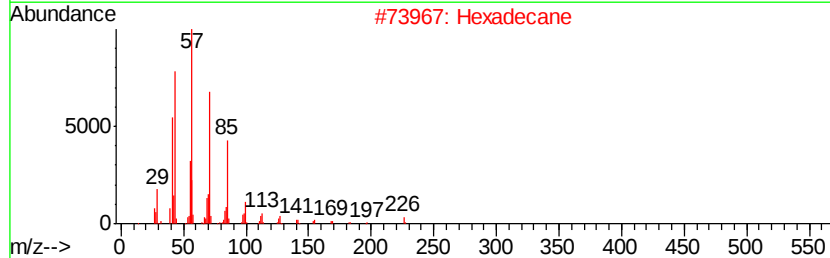
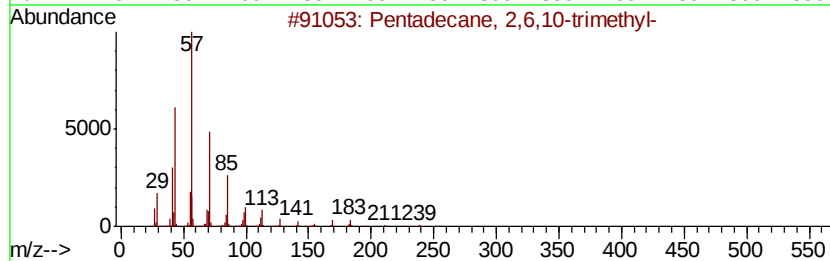
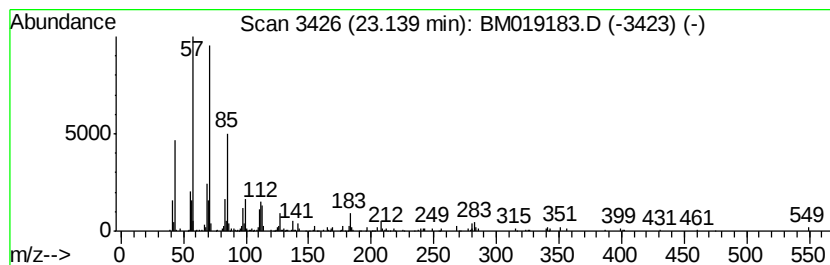
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentadecane, 2,6,10-trimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	2.01 ng	353550	Perylene-d12	23.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	87
2		Hexadecane	226	C16H34	000544-76-3	83
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
4		Heptacosane	380	C27H56	000593-49-7	80
5		Pentadecane, 7-methyl-	226	C16H34	006165-40-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031519\
Data File : BM019183.D
Acq On : 15 Mar 2019 13:10
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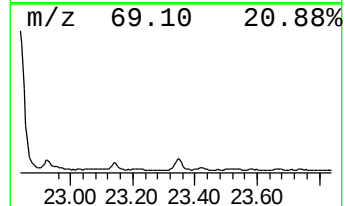
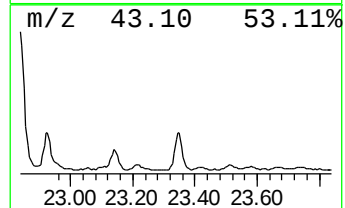
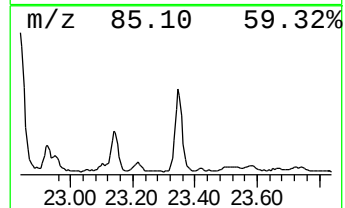
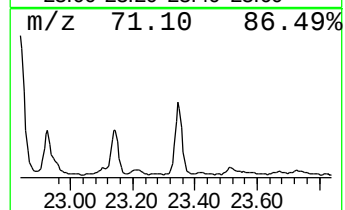
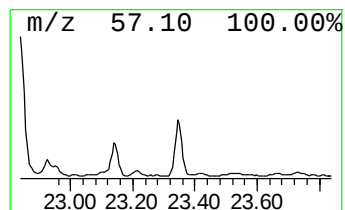
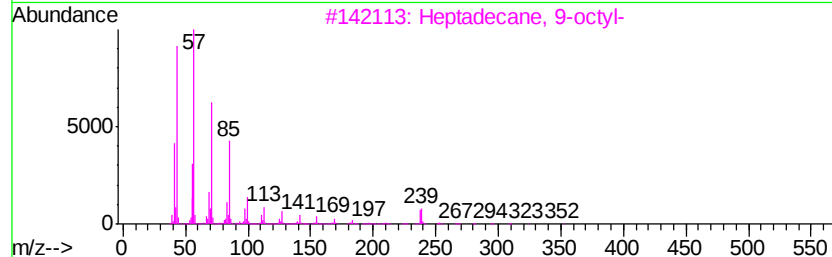
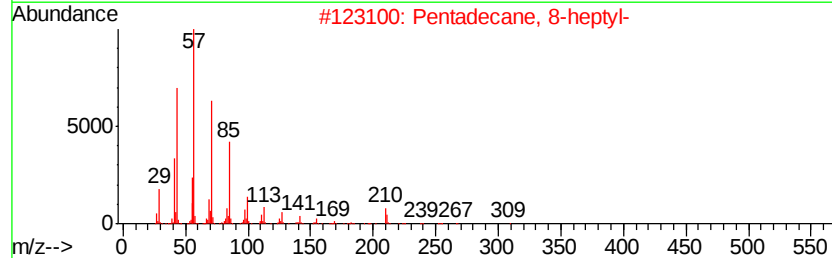
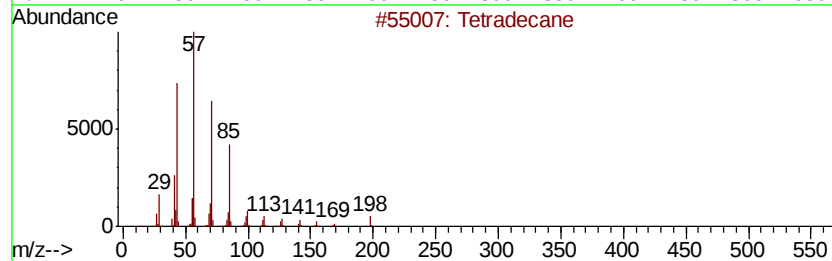
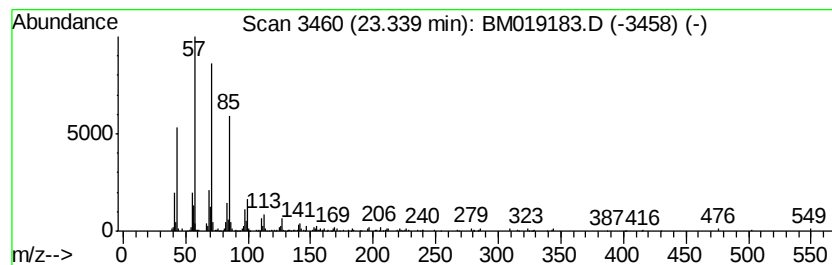
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetradecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.34	2.56 ng	450383	Perylene-d12	23.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	87
2			Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4			Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
5			Heptacosane	380	C27H56	000593-49-7	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031519\
 Data File : BM019183.D
 Acq On : 15 Mar 2019 13:10
 Operator : JU/SJ
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 Misc :
 ALS Vial : 4 Sample Multiplier: 1

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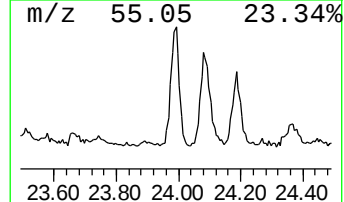
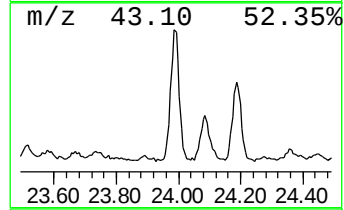
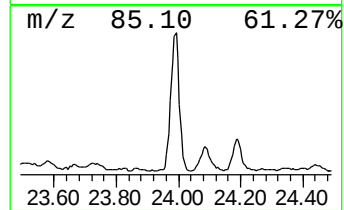
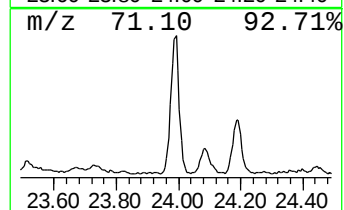
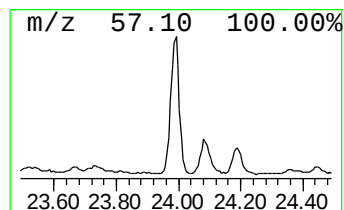
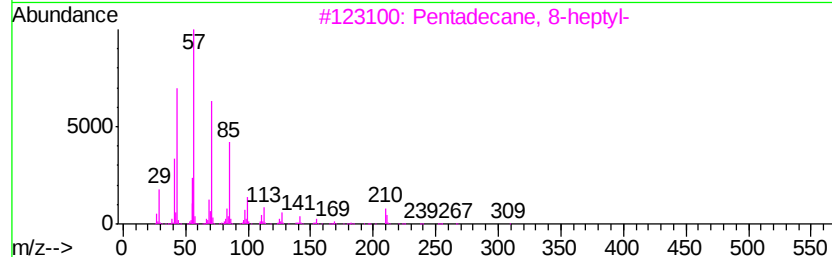
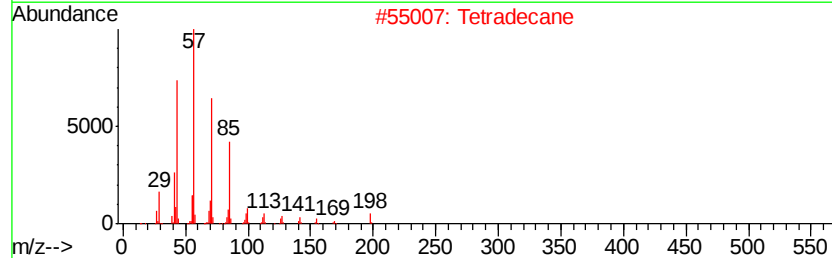
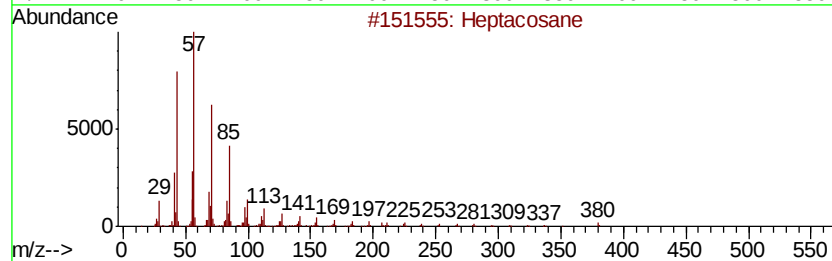
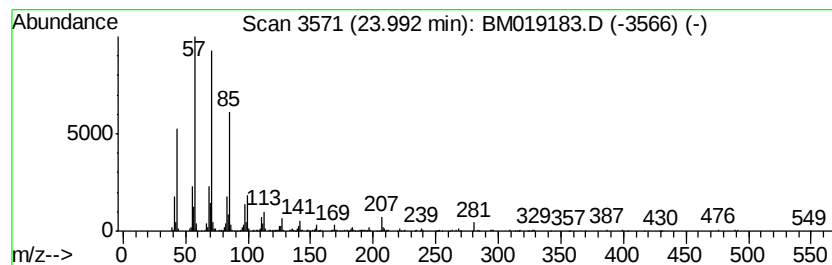
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 14 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	4.12 ng	724079	Perylene-d12	23.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	90
2		Tetradecane	198	C14H30	000629-59-4	87
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
4		Docosane, 5-butyl-	366	C26H54	055282-16-1	86
5		Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031519\
Data File : BM019183.D
Acq On : 15 Mar 2019 13:10
Operator : JU/SJ
Sample : K1817-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PST-027-B111-030619

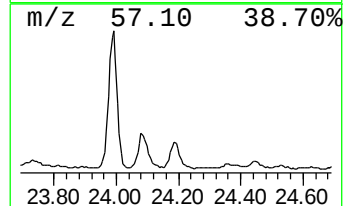
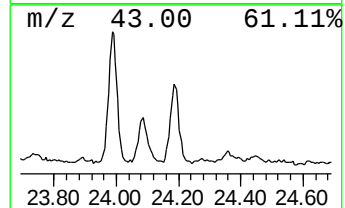
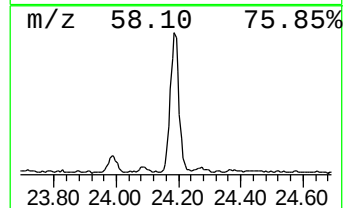
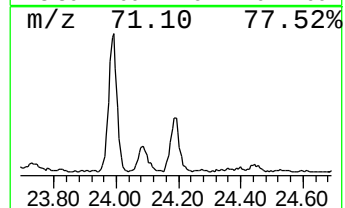
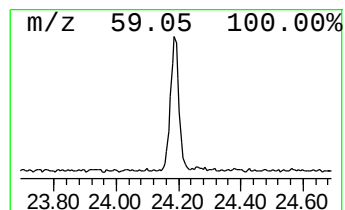
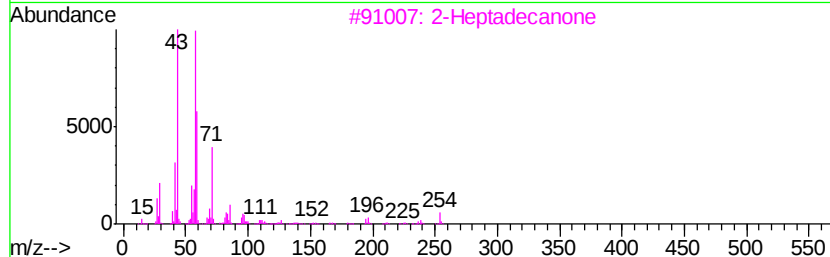
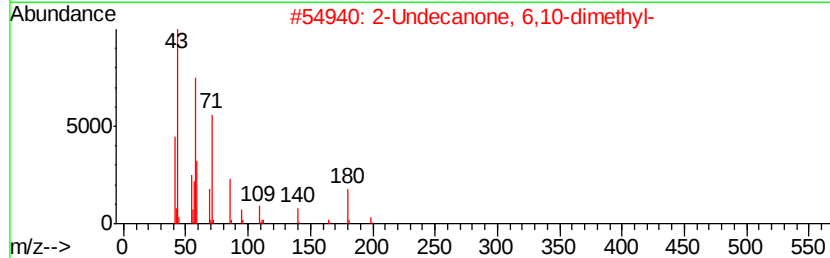
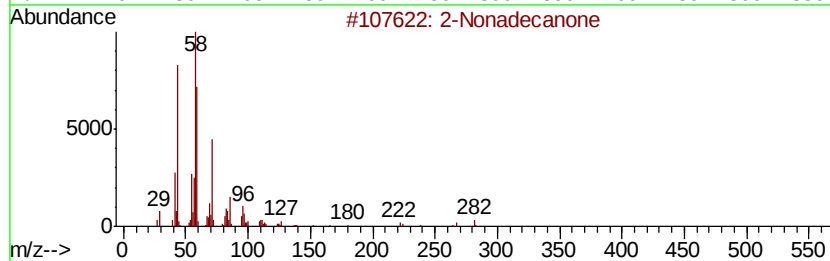
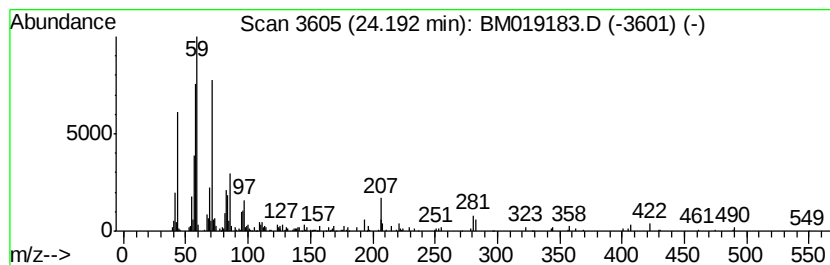
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2-Nonadecanone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.19	2.21 ng	388741	Perylene-d12	23.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonadecanone	282	C19H38O	000629-66-3	78
2			2-Undecanone, 6,10-dimethyl-	198	C13H26O	001604-34-8	50
3			2-Heptadecanone	254	C17H34O	002922-51-2	43
4			2-Dodecanone	184	C12H24O	006175-49-1	43
5			2-Tridecanone	198	C13H26O	000593-08-8	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM031519\
 Data File : BM019183.D
 Acq On : 15 Mar 2019 13:10
 Operator : JU/SJ
 Sample : K1817-15
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PST-027-B111-030619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.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
unknown7.19	7.19	76.0	ng	5821700	1	7.65	1531420	20.0
n-Hexadecanoic acid	17.96	6.8	ng	1373380	4	17.06	4022610	20.0
Octadecanoic acid	19.24	2.3	ng	503487	5	21.26	4355630	20.0
Cyclotetradecane	20.96	8.0	ng	1749580	5	21.26	4355630	20.0
E-15-Heptadecenal	21.85	9.6	ng	2082100	5	21.26	4355630	20.0
Pentadecane, 8-he...	22.29	2.1	ng	460480	5	21.26	4355630	20.0
Heneicosane	22.79	3.6	ng	640449	6	23.50	3518100	20.0
3-Eicosene, (E)-	22.84	18.9	ng	3330910	6	23.50	3518100	20.0
2-Heptacosanone	22.93	3.0	ng	524603	6	23.50	3518100	20.0
Pentadecane, 2,6,...	23.14	2.0	ng	353550	6	23.50	3518100	20.0
Tetradecane	23.34	2.6	ng	450383	6	23.50	3518100	20.0
Heptacosane	23.99	4.1	ng	724079	6	23.50	3518100	20.0
2-Nonadecanone	24.19	2.2	ng	388741	6	23.50	3518100	20.0