

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
 Data File : BM018612.D
 Acq On : 17 Jan 2019 14:00
 Operator : JU/SJ
 Sample : PB116441BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB116441BL

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-BM010919.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	4.887	301	306	314	rVB	215753	318003	2.37%	0.270%
2	5.334	375	382	394	rBV	4897745	6970102	51.95%	5.925%
3	6.916	644	651	665	rBV	4603354	7103609	52.94%	6.038%
4	7.275	704	712	727	rBV	5192011	8034932	59.88%	6.830%
5	7.740	784	791	800	rBV	1102581	1684519	12.55%	1.432%
6	8.057	837	845	853	rBV	4114382	6517961	48.58%	5.541%
7	8.904	981	989	1003	rBV	2774991	4720649	35.18%	4.013%
8	10.528	1258	1265	1276	rVB	1267205	2128064	15.86%	1.809%
9	13.004	1679	1686	1700	rBV	7615525	11015573	82.10%	9.364%
10	14.386	1914	1921	1933	rVB2	1719263	2626455	19.57%	2.233%
11	15.880	2168	2175	2185	rBV	5139079	7361318	54.86%	6.257%
12	17.139	2383	2389	2403	rVB	1933608	2781937	20.73%	2.365%
13	18.027	2533	2540	2550	rBV	690569	1273854	9.49%	1.083%
14	19.309	2753	2758	2775	rBV	801084	1422815	10.60%	1.209%
15	19.774	2831	2837	2851	rBV	10550020	13417817	100.00%	11.406%
16	21.033	3048	3051	3055	rVB	260560	276864	2.06%	0.235%
17	21.333	3096	3102	3106	rBV	2191315	2948274	21.97%	2.506%
18	21.468	3121	3125	3130	rBV	1185825	1272173	9.48%	1.081%
19	21.909	3195	3200	3207	rBV	2806961	3533776	26.34%	3.004%
20	22.380	3274	3280	3290	rBV	4635422	6532024	48.68%	5.552%
21	22.892	3361	3367	3376	rBV	5170420	7931414	59.11%	6.742%
22	23.468	3459	3465	3481	rVB	4266608	7478979	55.74%	6.357%
23	23.603	3482	3488	3497	rVB	1424529	2782551	20.74%	2.365%
24	24.121	3570	3576	3590	rVB	2527085	5083375	37.89%	4.321%
25	24.880	3700	3705	3715	rVB	1110538	2424712	18.07%	2.061%

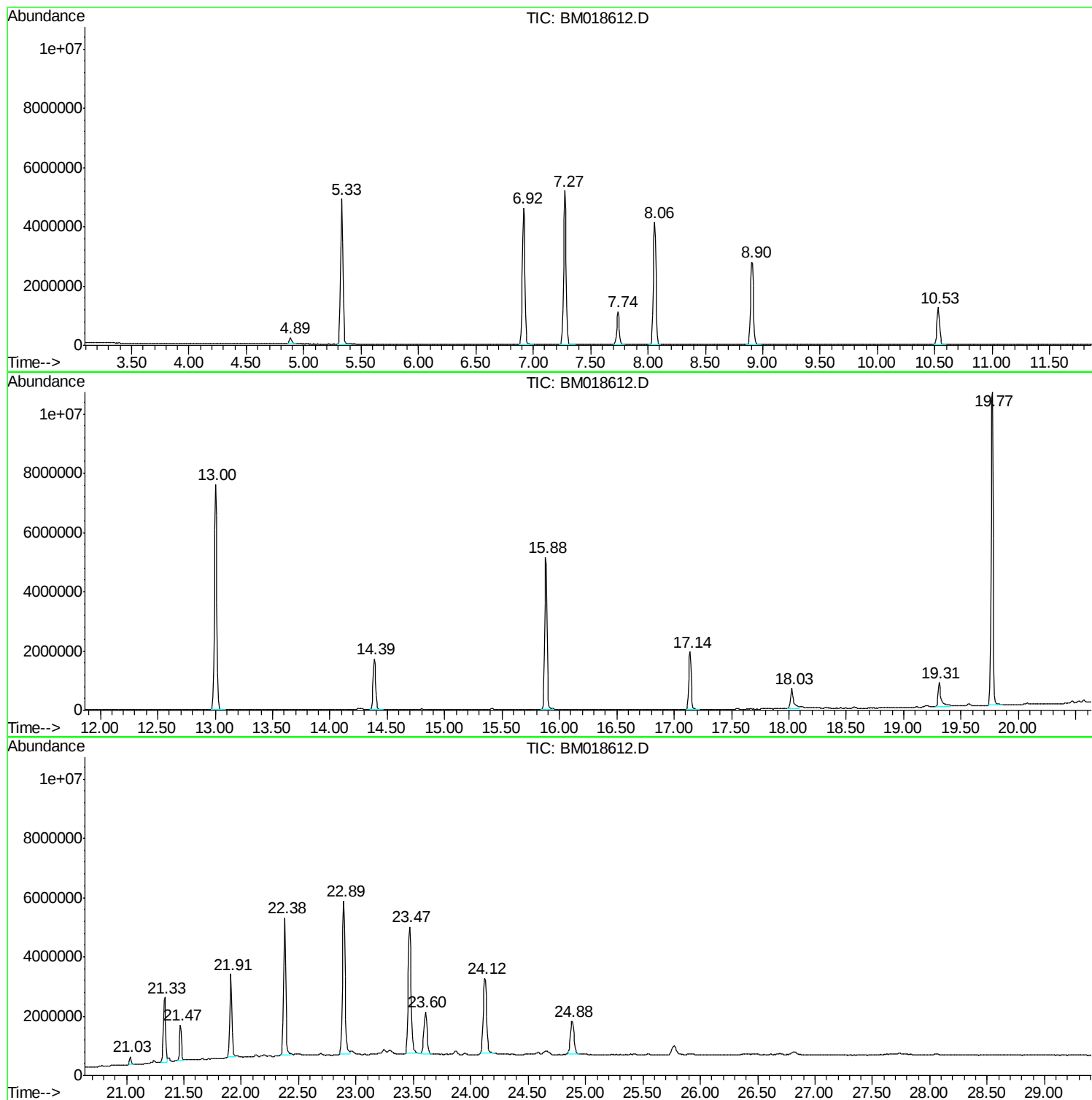
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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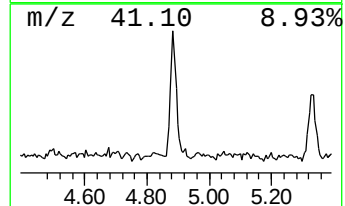
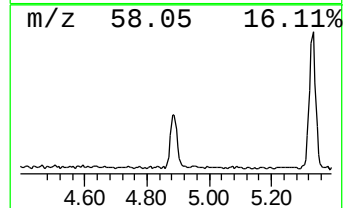
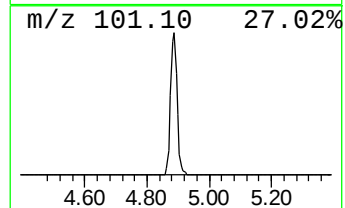
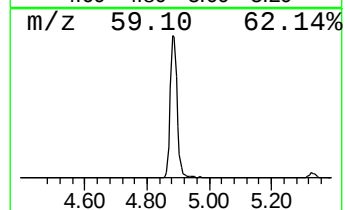
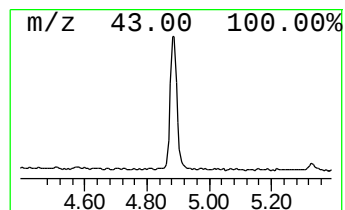
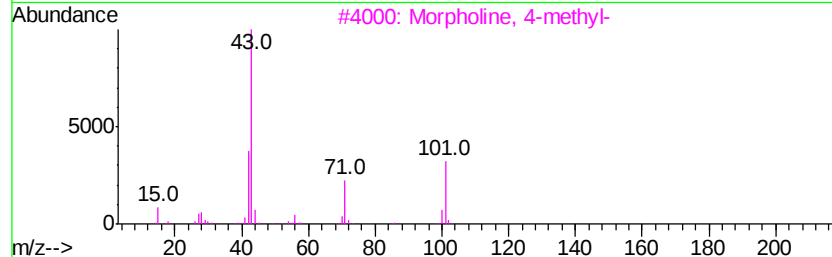
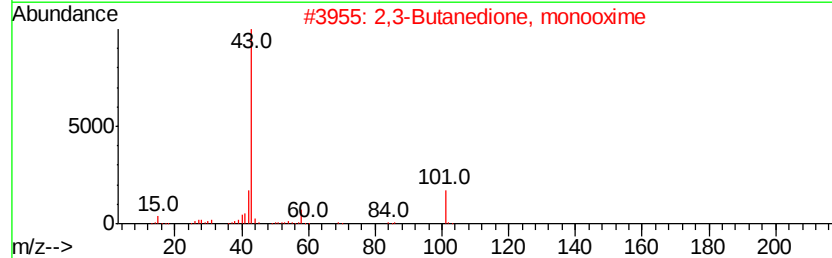
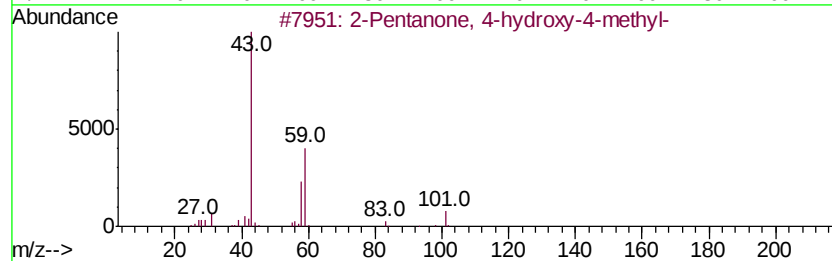
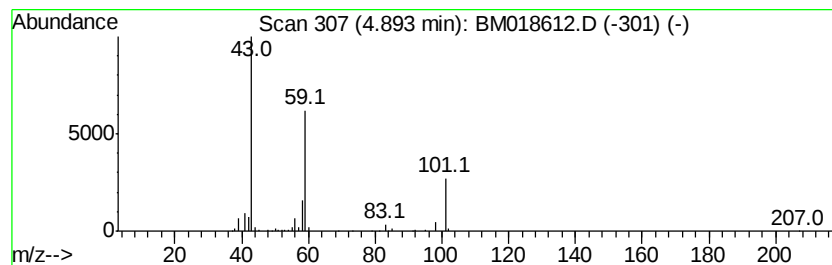
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	3.78 ng	318003	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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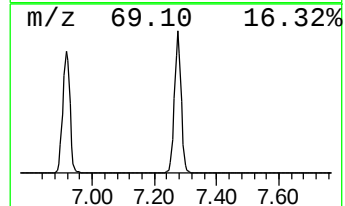
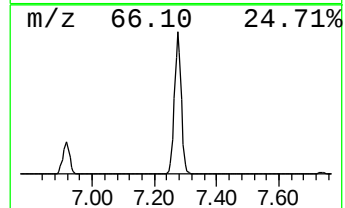
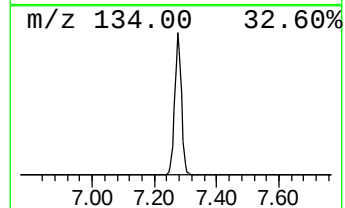
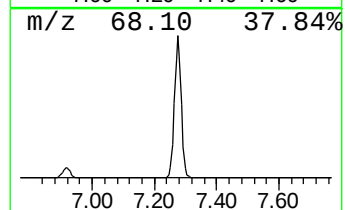
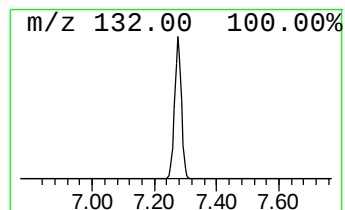
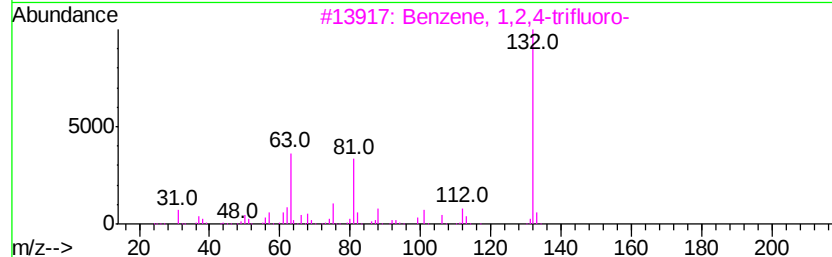
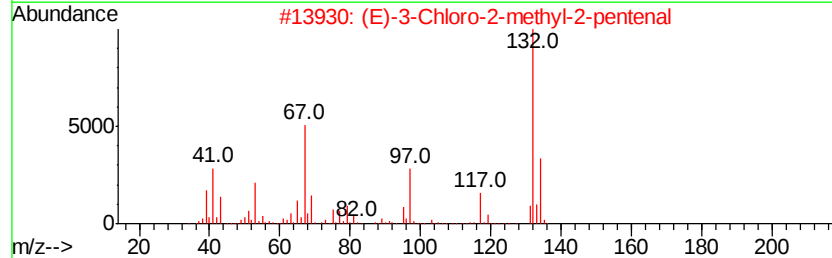
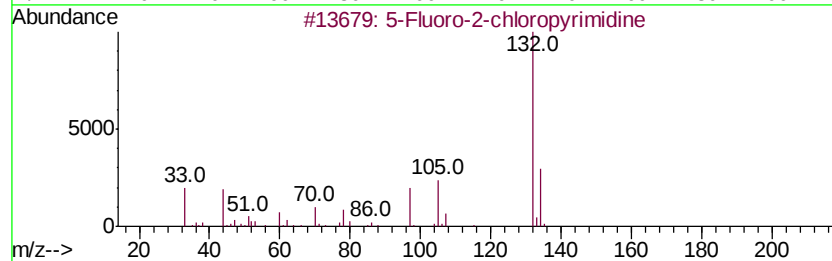
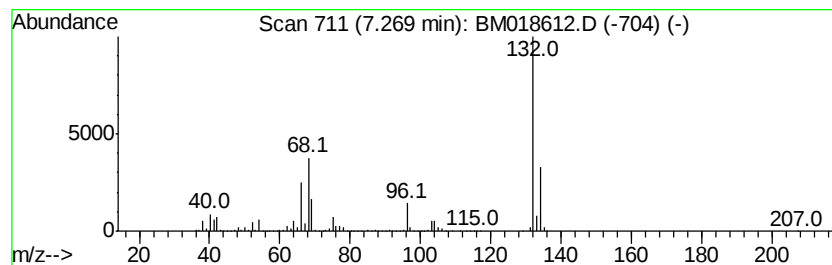
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Peak Number 2 unknown7.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	95.40 ng	8034930	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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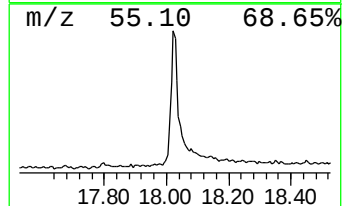
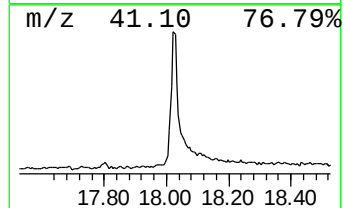
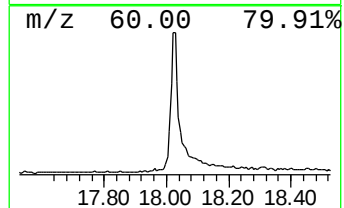
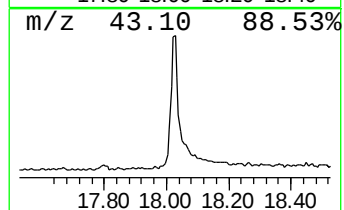
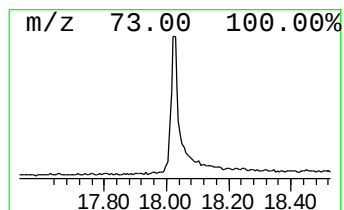
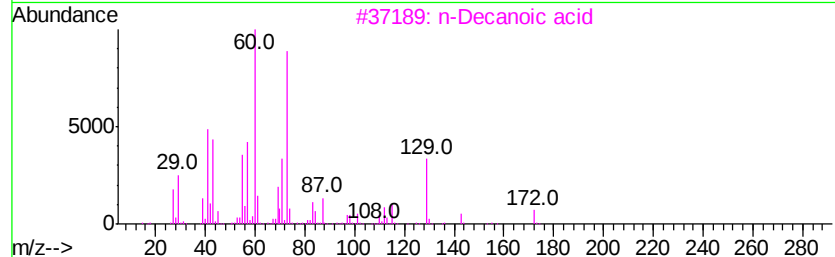
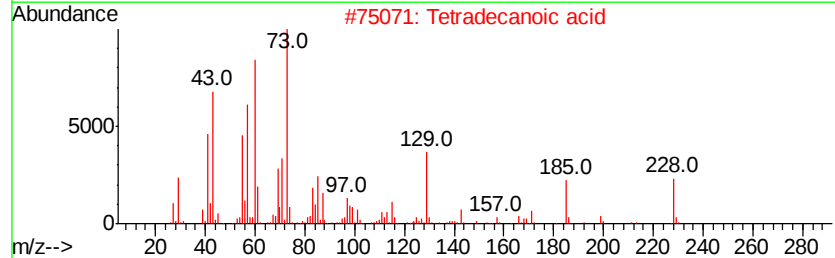
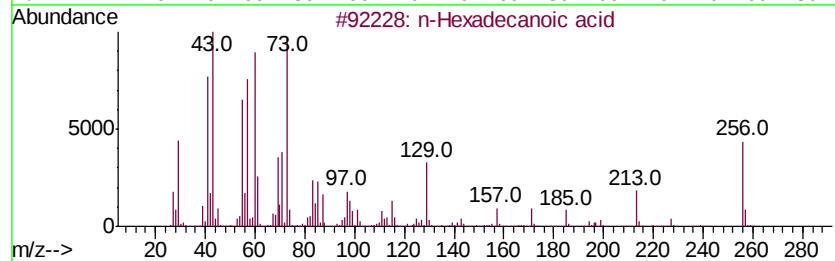
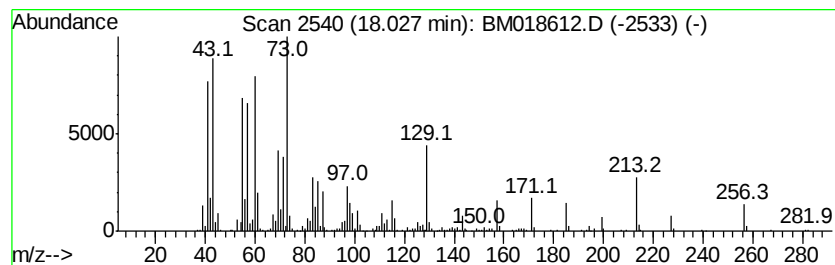
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	9.16 ng	1273850	Phenanthrene-d10	17.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3		n-Decanoic acid	172	C10H20O2	000334-48-5	76
4		Tridecanoic acid	214	C13H26O2	000638-53-9	70
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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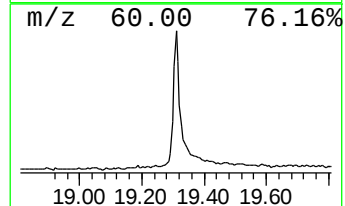
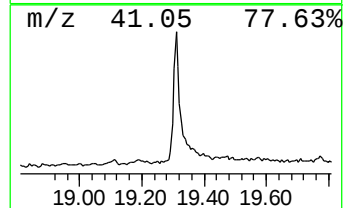
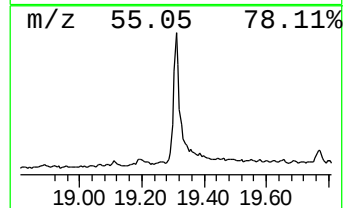
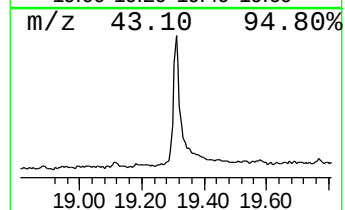
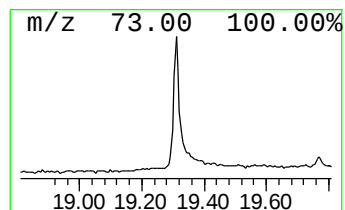
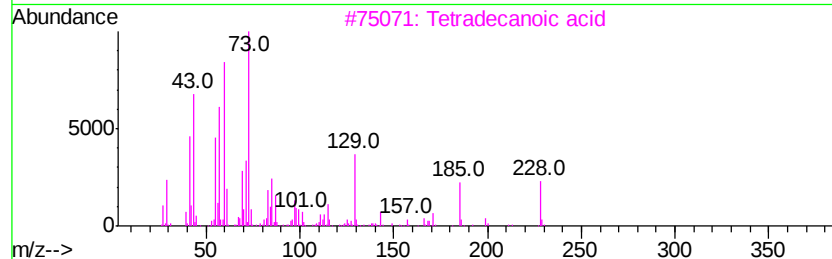
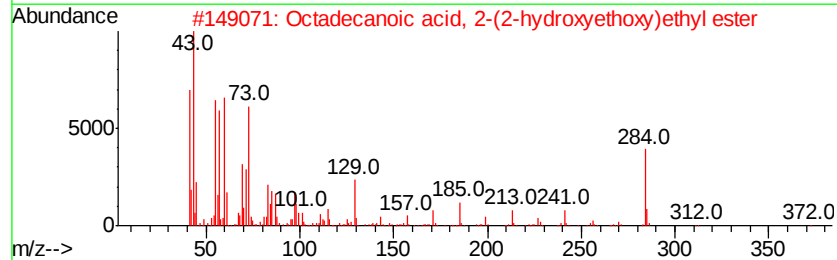
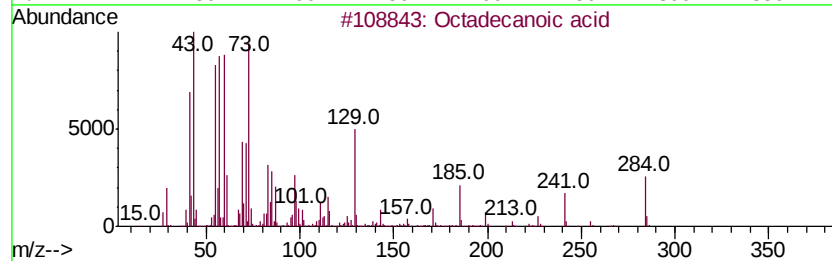
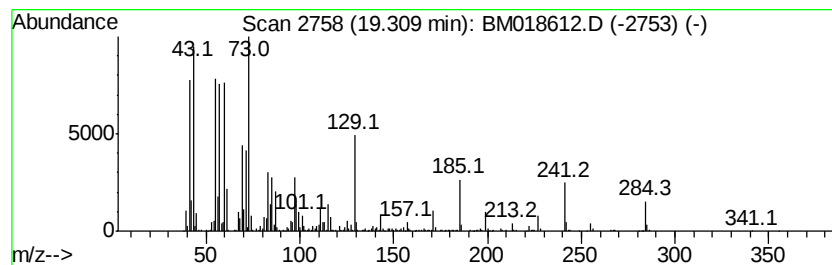
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Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	9.65 ng	1422820	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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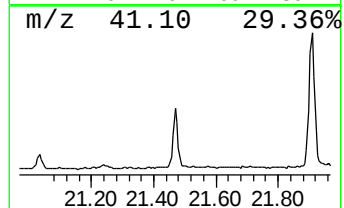
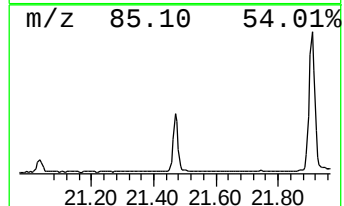
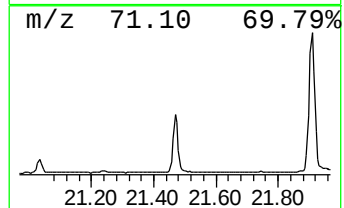
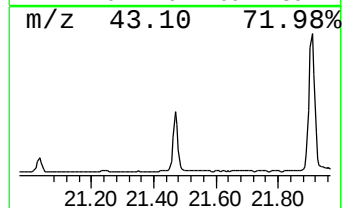
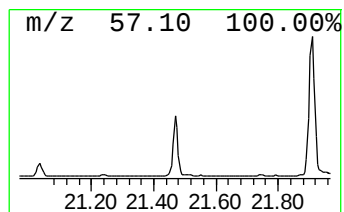
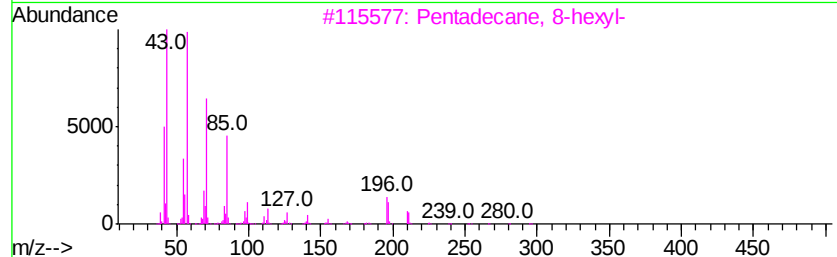
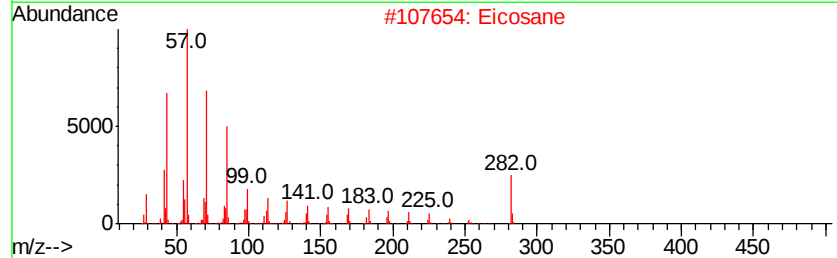
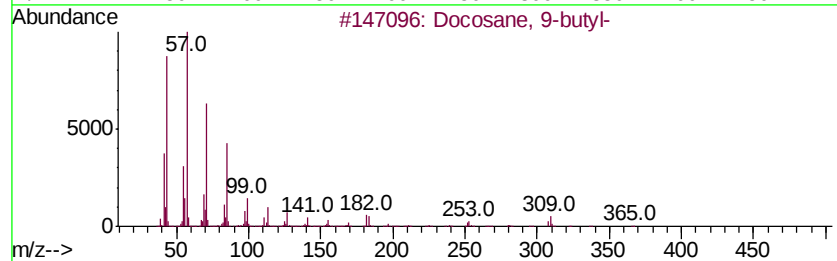
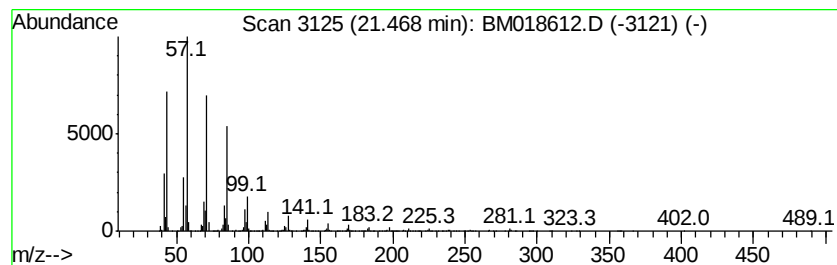
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Docosane, 9-butyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.47	8.63 ng	1272170	Chrysene-d12	21.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Docosane, 9-butyl-	366 C26H54	055282-14-9 95
2		Eicosane	282 C20H42	000112-95-8 94
3		Pentadecane, 8-hexyl-	296 C21H44	013475-75-7 94
4		Heneicosane, 11-pentyl-	366 C26H54	014739-72-1 91
5		Docosane, 11-butyl-	366 C26H54	013475-76-8 91



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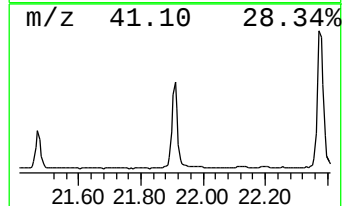
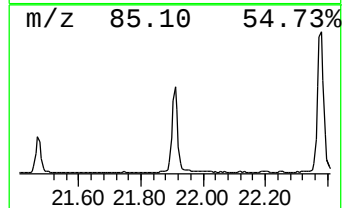
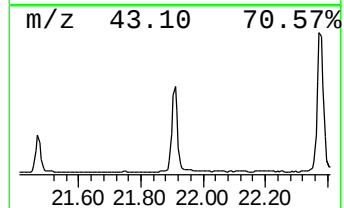
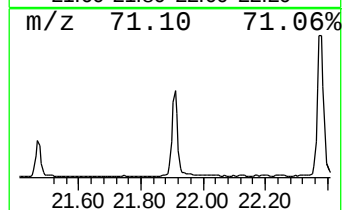
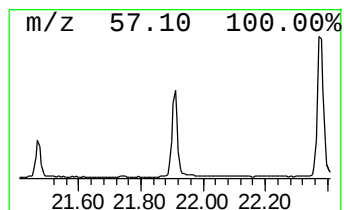
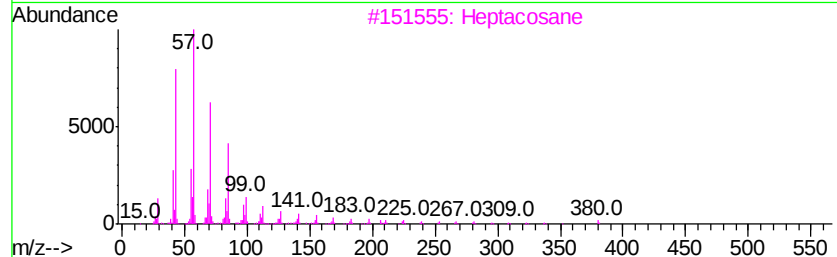
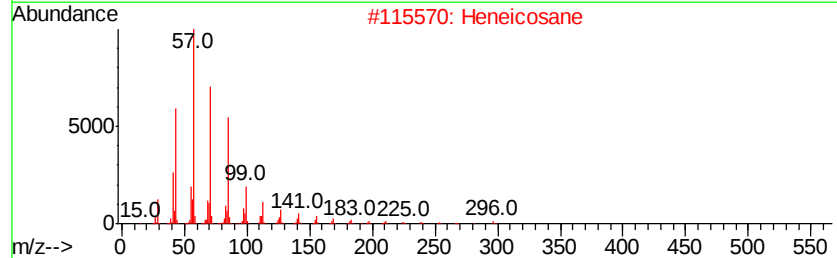
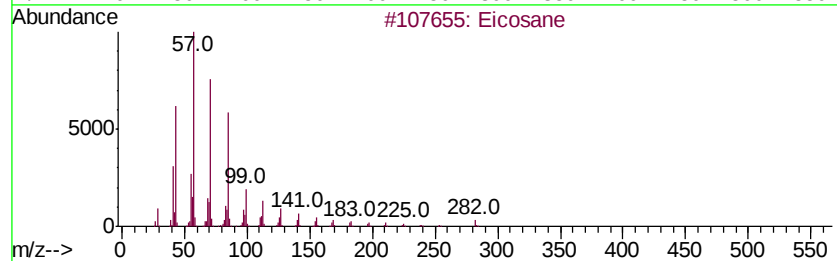
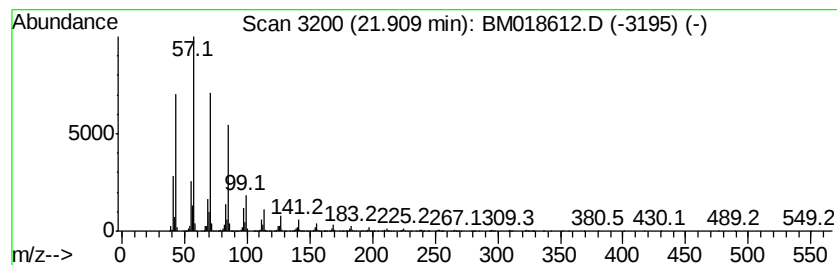
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.91	23.97 ng	3533780	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	97
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Tetratriacontane	479	C34H70	014167-59-0	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018612.D
Acq On : 17 Jan 2019 14:00
Operator : JU/SJ
Sample : PB116441BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB116441BL

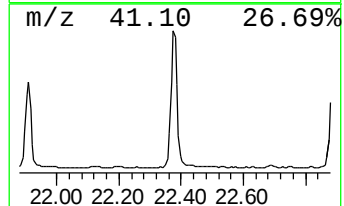
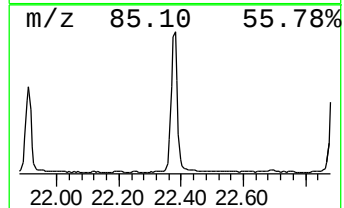
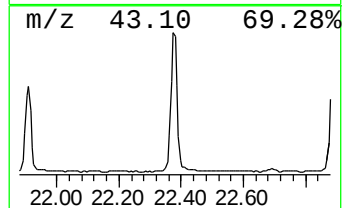
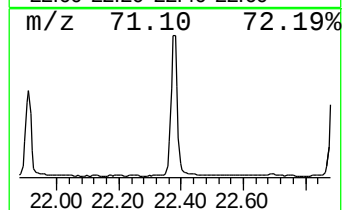
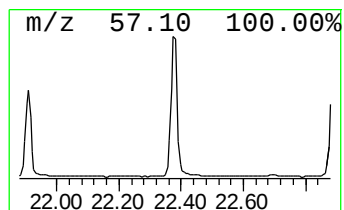
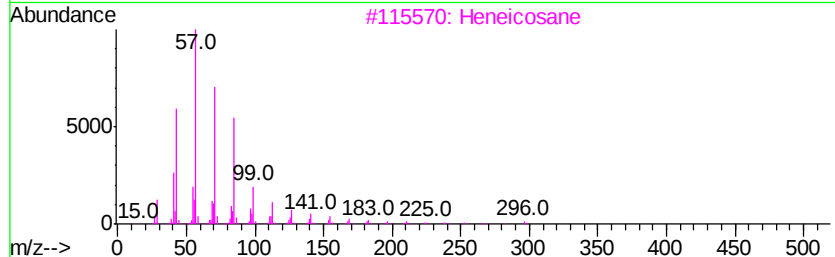
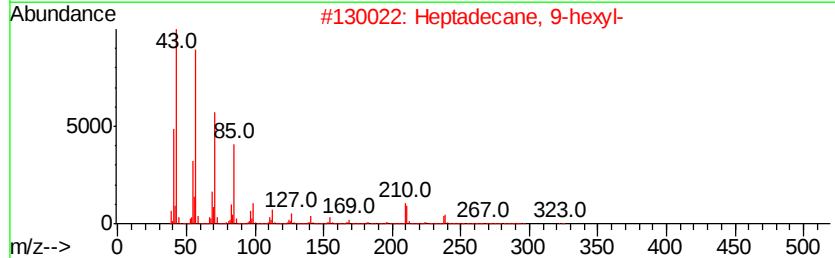
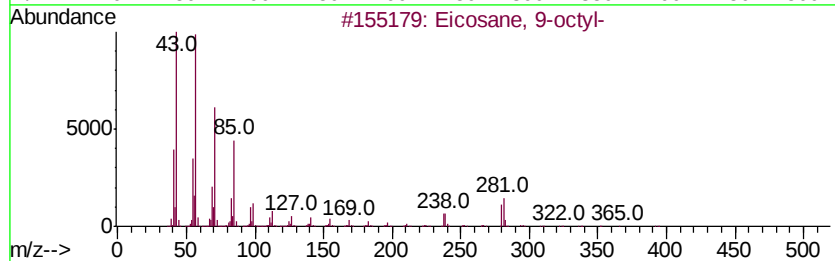
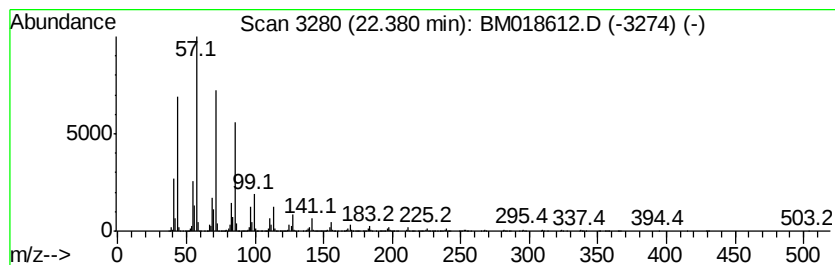
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.38	44.31 ng	6532020	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	94
2		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
3		Heneicosane	296	C21H44	000629-94-7	91
4		Nonacosane	408	C29H60	000630-03-5	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018612.D
Acq On : 17 Jan 2019 14:00
Operator : JU/SJ
Sample : PB116441BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB116441BL

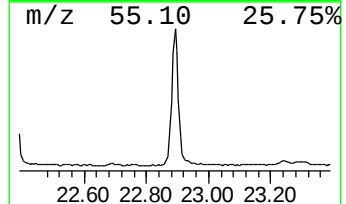
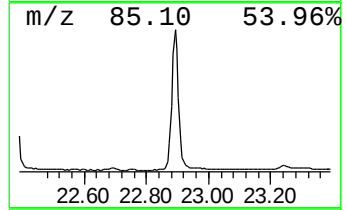
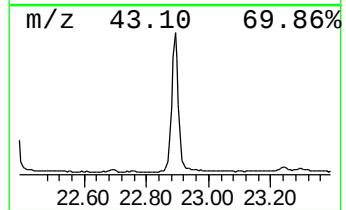
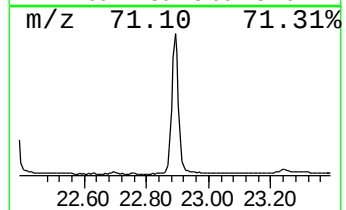
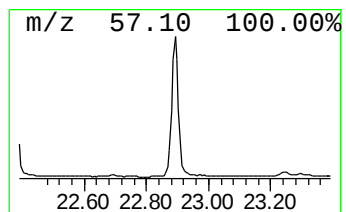
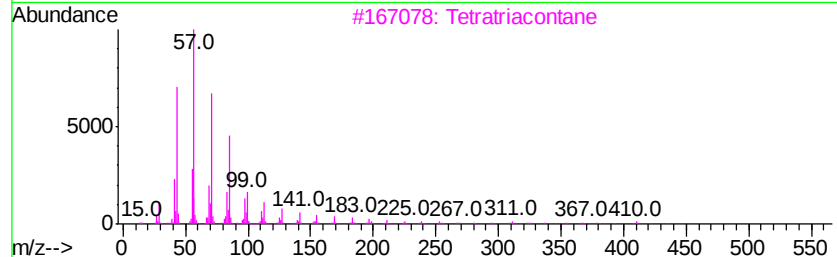
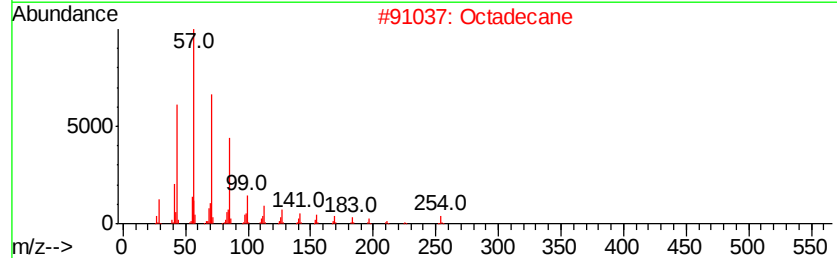
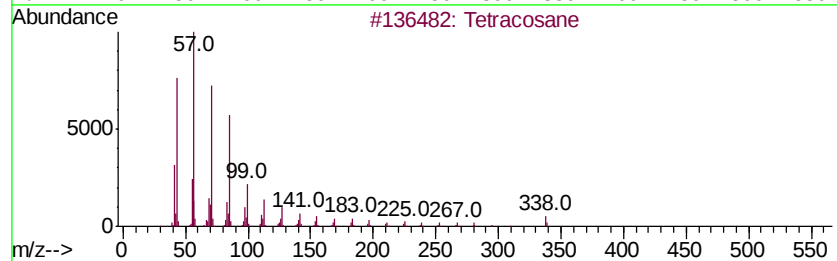
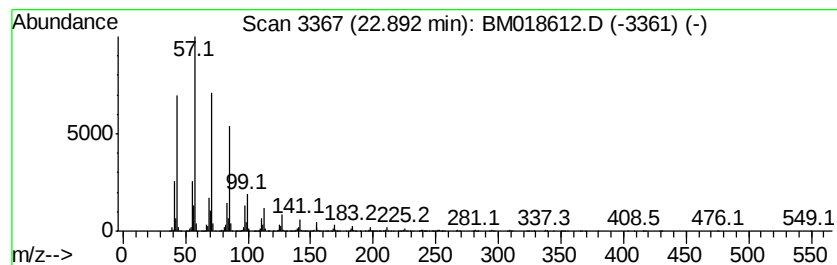
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.89	57.01 ng	7931410	Perylene-d12	23.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	98
2		Octadecane	254	C18H38	000593-45-3	94
3		Tetratriacontane	479	C34H70	014167-59-0	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018612.D
Acq On : 17 Jan 2019 14:00
Operator : JU/SJ
Sample : PB116441BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

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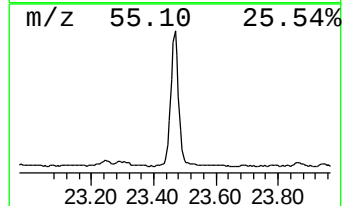
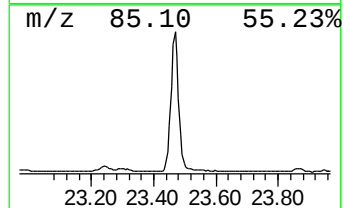
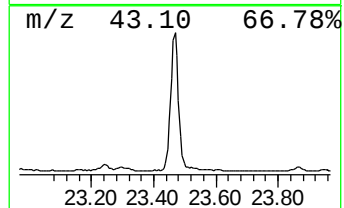
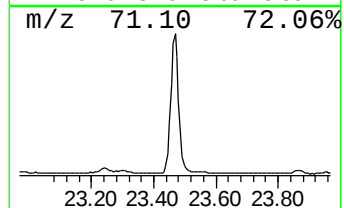
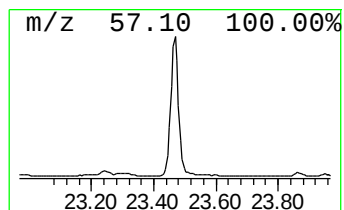
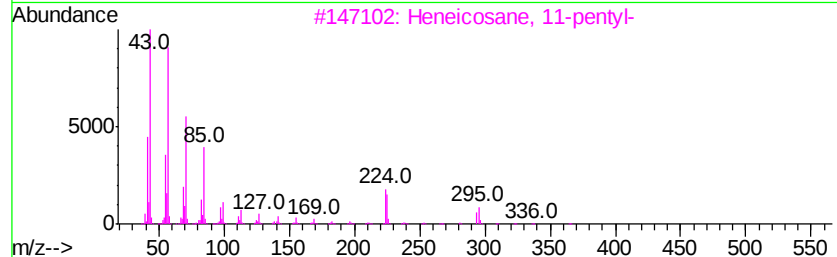
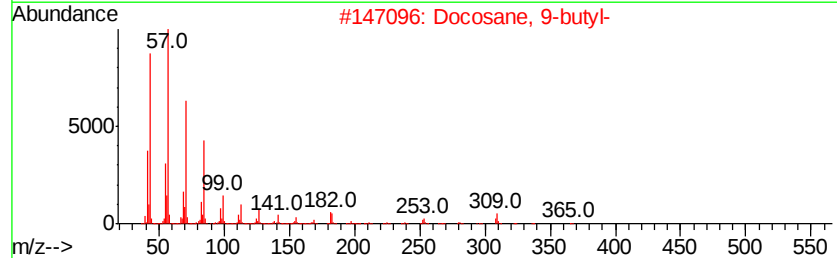
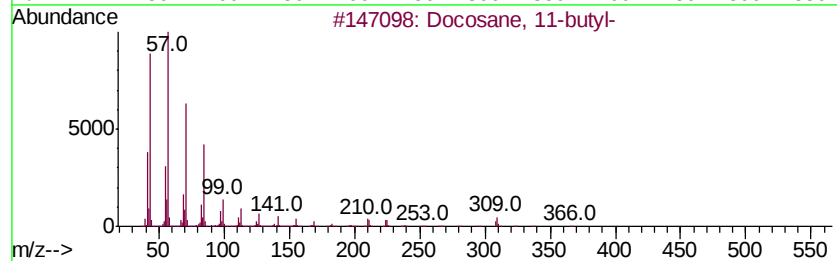
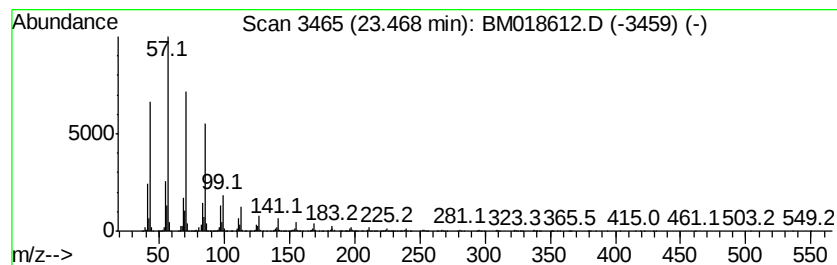
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane, 11-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.47	53.76 ng	7478980	Perylene-d12	23.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 11-butyl-	366	C26H54	013475-76-8	95
2		Docosane, 9-butyl-	366	C26H54	055282-14-9	93
3		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		Nonacosane	408	C29H60	000630-03-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
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Acq On : 17 Jan 2019 14:00
Operator : JU/SJ
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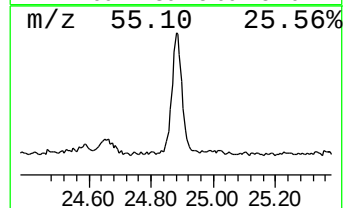
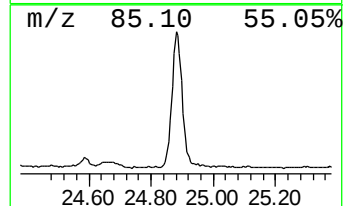
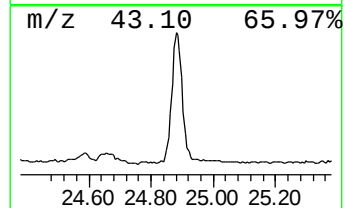
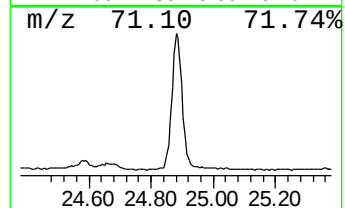
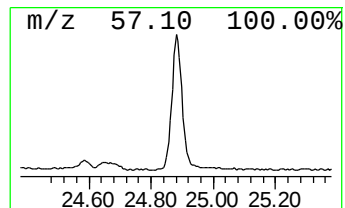
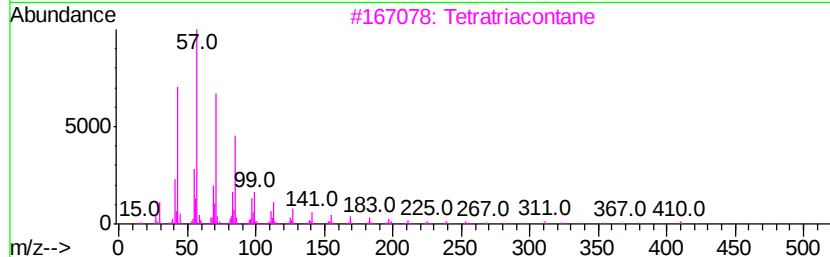
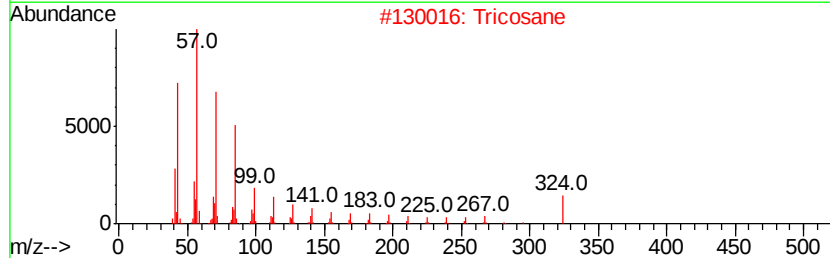
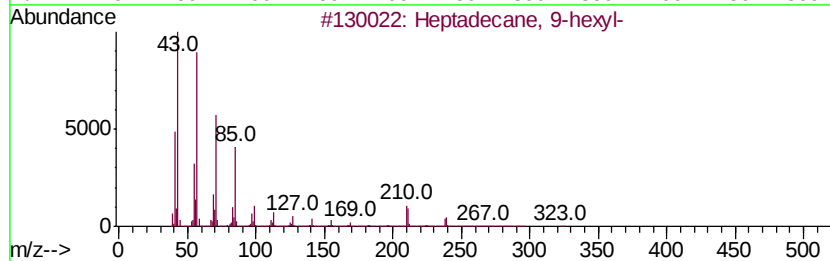
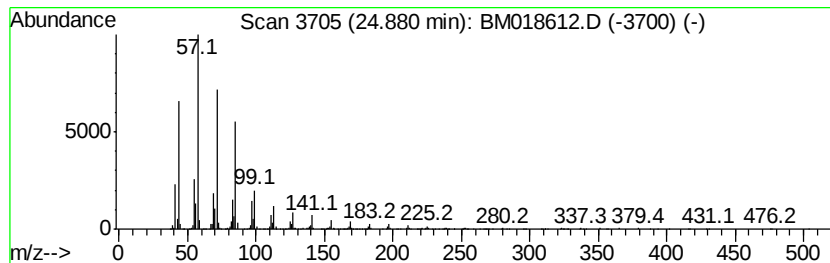
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ClientSampleId :
PB116441BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane, 9-hexyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.88	17.43 ng	2424710	Perylene-d12	23.60
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane, 9-hexyl-	324 C23H48	055124-79-3	93
2	Tricosane	324 C23H48	000638-67-5	93
3	Tetratriacontane	479 C34H70	014167-59-0	91
4	Triacotane	422 C30H62	000638-68-6	91
5	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM011719\
Data File : BM018612.D
Acq On : 17 Jan 2019 14:00
Operator : JU/SJ
Sample : PB116441BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB116441BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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
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unknown7.27	7.27	95.4	ng	8034930	1	7.74	1684520	20.0
n-Hexadecanoic acid	18.03	9.2	ng	1273850	4	17.14	2781940	20.0
Octadecanoic acid	19.31	9.7	ng	1422820	5	21.33	2948270	20.0
Docosane, 9-butyl-	21.47	8.6	ng	1272170	5	21.33	2948270	20.0
Eicosane	21.91	24.0	ng	3533780	5	21.33	2948270	20.0
Eicosane, 9-octyl-	22.38	44.3	ng	6532020	5	21.33	2948270	20.0
Tetracosane	22.89	57.0	ng	7931410	6	23.60	2782550	20.0
Docosane, 11-butyl-	23.47	53.8	ng	7478980	6	23.60	2782550	20.0
Heptadecane, 9-he...	24.88	17.4	ng	2424710	6	23.60	2782550	20.0