

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
 Data File : BM018856.D
 Acq On : 19 Feb 2019 14:45
 Operator : JU/SJ
 Sample : K1515-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TS-2

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-BM021119.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	4.857	296	301	317	rVB	241098	366344	2.07%	0.338%
2	5.298	369	376	388	rBV	6246400	8938014	50.58%	8.241%
3	6.881	637	645	663	rBV	6141509	9810254	55.51%	9.046%
4	7.240	698	706	721	rBV	6409049	9932648	56.20%	9.159%
5	7.704	778	785	793	rBV	1067741	1670482	9.45%	1.540%
6	8.022	831	839	848	rBV	4394614	6936977	39.25%	6.396%
7	8.875	975	984	1001	rBV	3475111	5839199	33.04%	5.384%
8	10.492	1251	1259	1272	rBV	1302809	2244957	12.70%	2.070%
9	12.969	1673	1680	1700	rBV	8440513	12271673	69.44%	11.315%
10	13.821	1816	1825	1837	rBV	301144	508098	2.88%	0.469%
11	14.351	1905	1915	1928	rBV2	1806620	2900691	16.41%	2.675%
12	15.851	2163	2170	2195	rBV	6965532	10176928	57.59%	9.384%
13	17.104	2377	2383	2399	rBV	2374702	3495309	19.78%	3.223%
14	17.998	2529	2535	2546	rBV	1135305	1663264	9.41%	1.534%
15	19.280	2748	2753	2768	rBV	470352	780540	4.42%	0.720%
16	19.739	2825	2831	2839	rBV	15440830	17672634	100.00%	16.295%
17	20.533	2962	2966	2971	rBV	153386	183691	1.04%	0.169%
18	20.997	3041	3045	3059	rBV	1674665	2305149	13.04%	2.126%
19	21.297	3090	3096	3106	rBV	3064205	3954544	22.38%	3.646%
20	21.433	3116	3119	3127	rBV	333896	377987	2.14%	0.349%
21	21.868	3189	3193	3196	rBV	426090	516360	2.92%	0.476%
22	22.333	3268	3272	3276	rVB	403308	518319	2.93%	0.478%
23	22.839	3354	3358	3362	rVB	419036	567561	3.21%	0.523%
24	23.403	3450	3454	3462	rVB	329485	504333	2.85%	0.465%
25	23.550	3473	3479	3488	rVB	1722416	3212511	18.18%	2.962%
26	24.056	3561	3565	3571	rVB	285877	500373	2.83%	0.461%
27	24.156	3578	3582	3594	rVB2	273537	602761	3.41%	0.556%

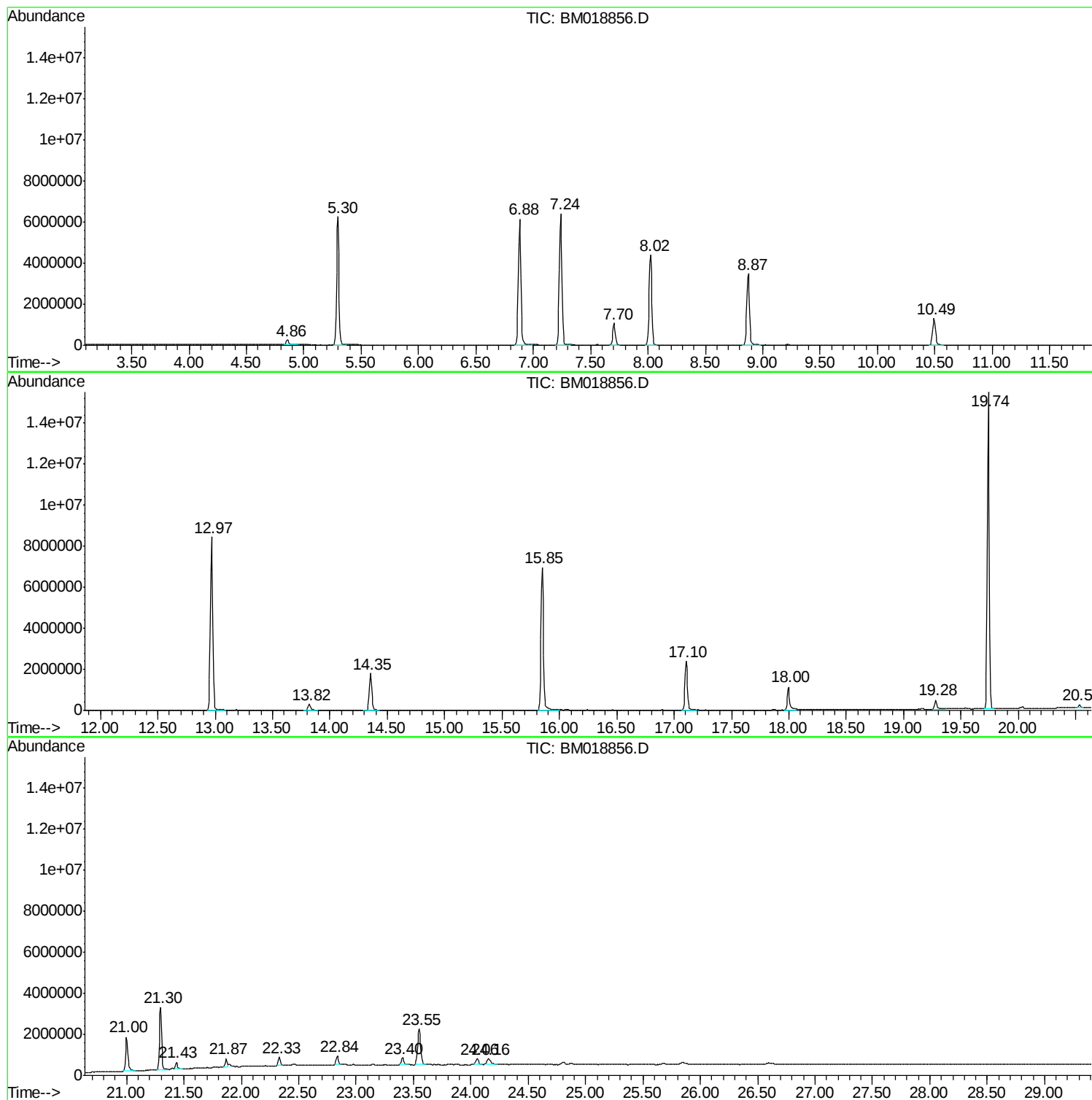
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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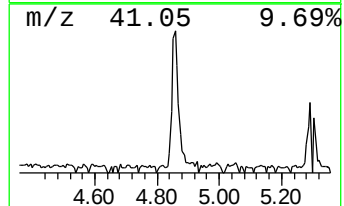
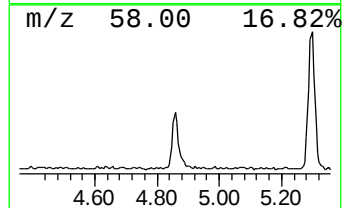
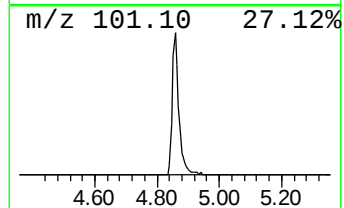
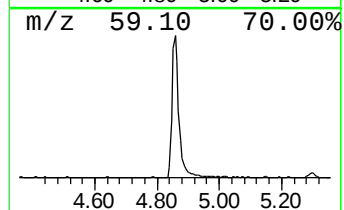
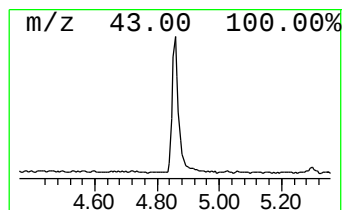
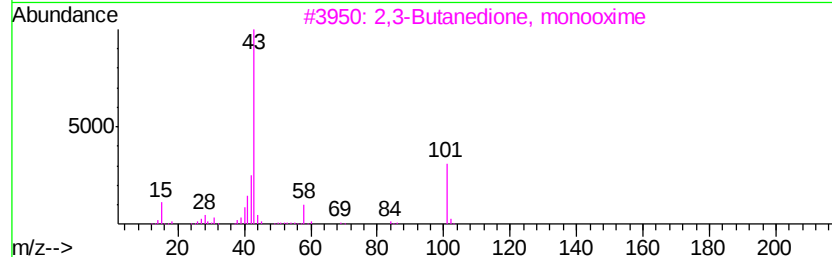
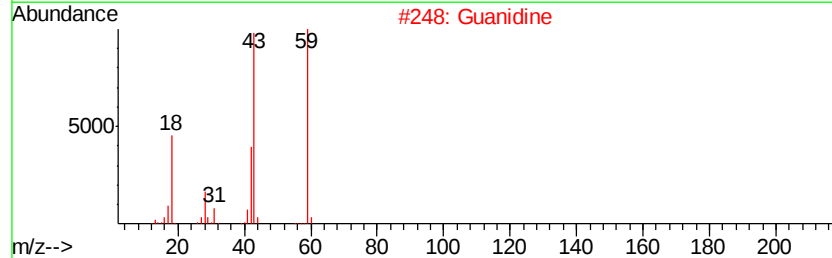
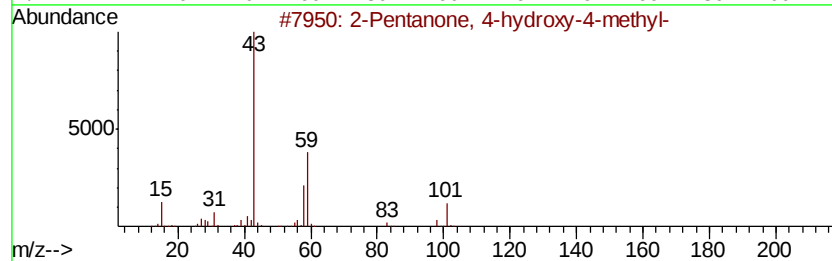
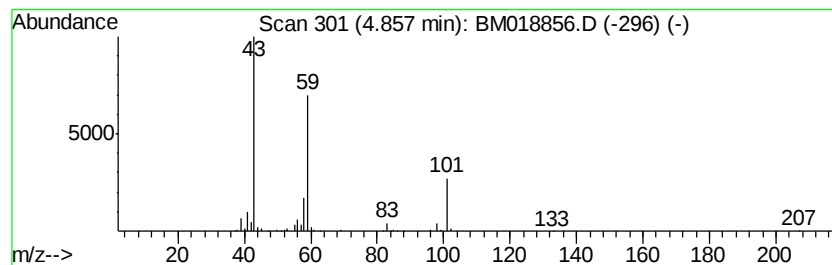
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	4.39 ng	366344	1,4-Dichlorobenzene-d4	7.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Guanidine	59	CH5N3	000113-00-8	43
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	23
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23



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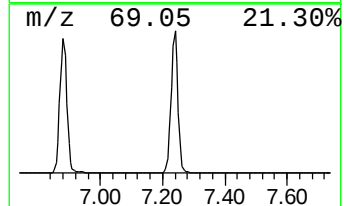
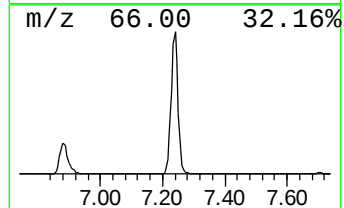
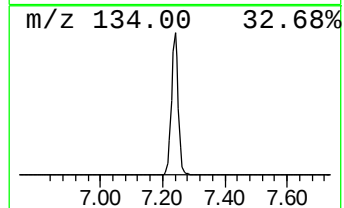
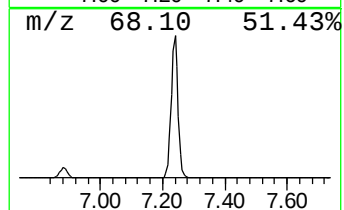
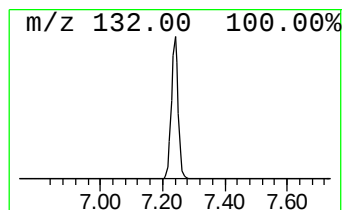
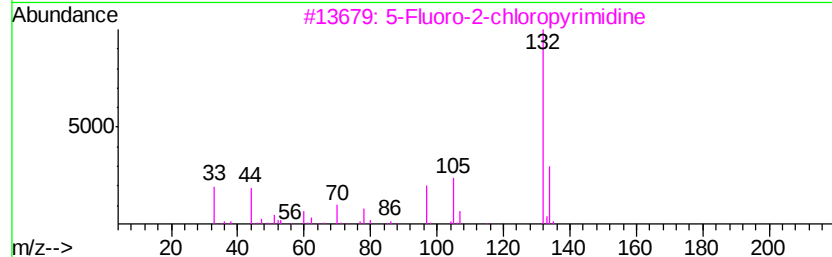
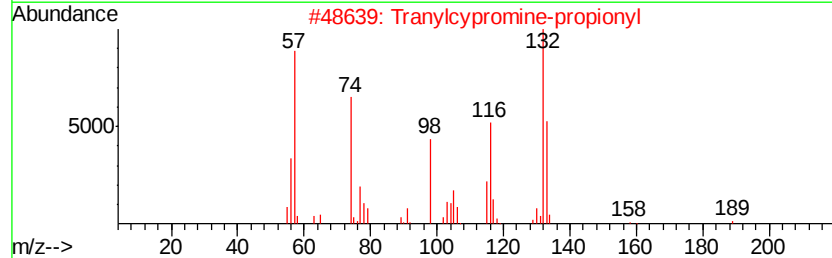
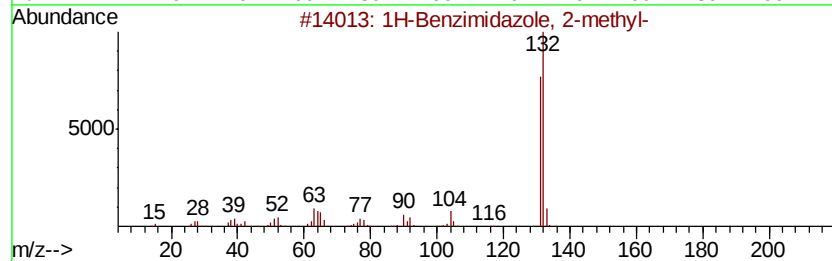
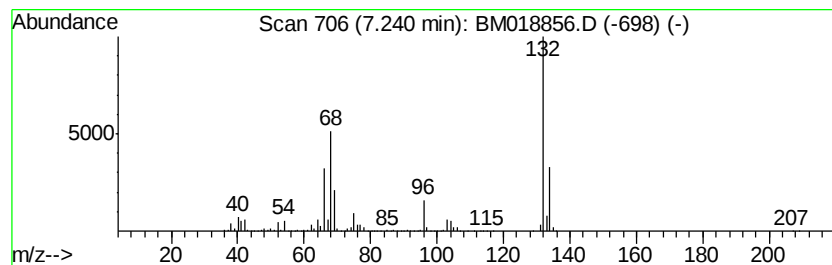
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Peak Number 2 unknown7.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.24	118.92 ng	9932650	1,4-Dichlorobenzene-d4	7.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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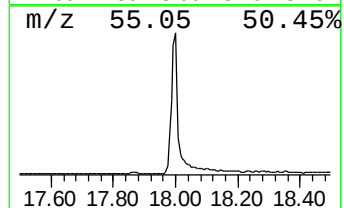
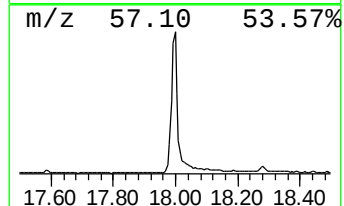
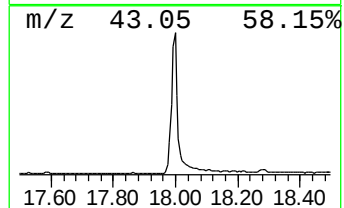
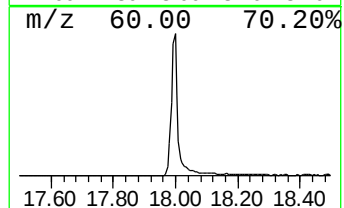
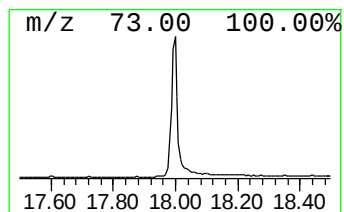
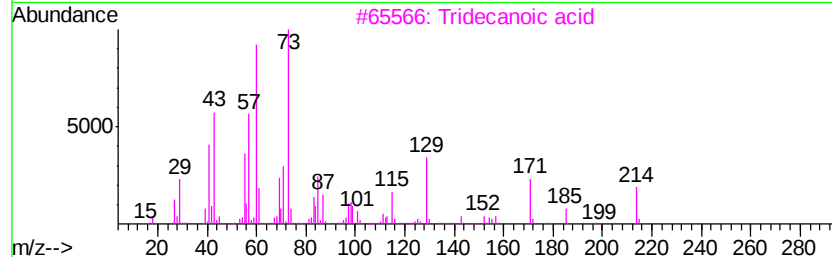
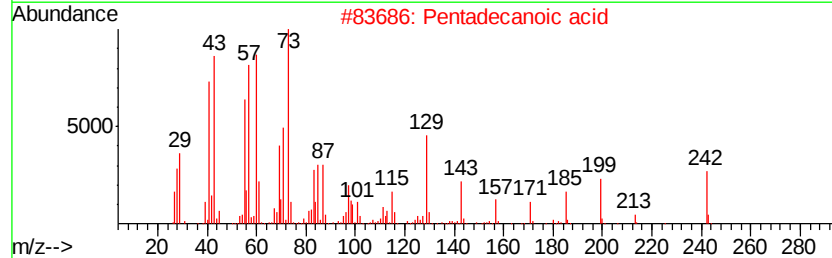
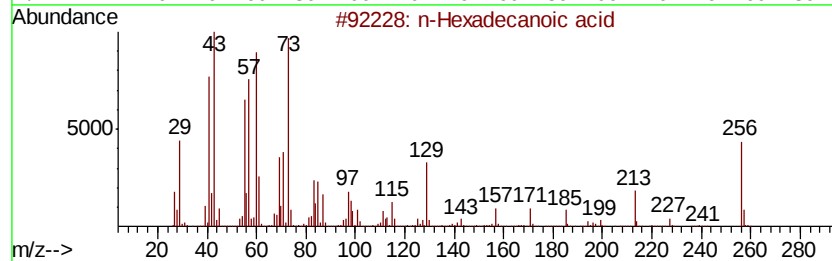
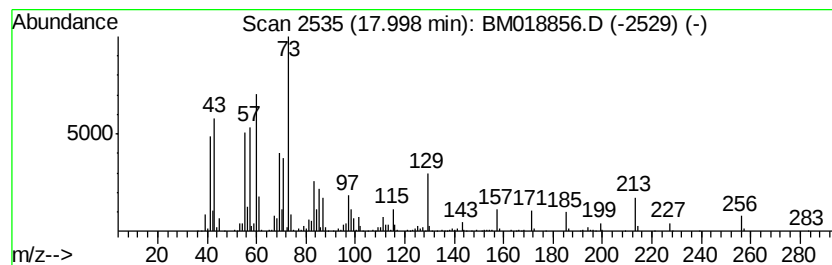
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.00	9.52 ng	1663260	Phenanthrene-d10	17.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Dodecanoic acid	200	C12H24O2	000143-07-7	42



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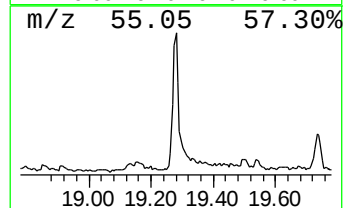
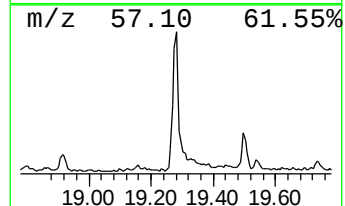
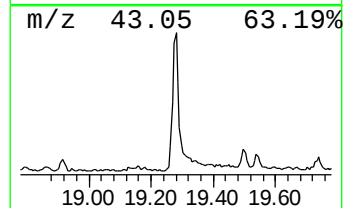
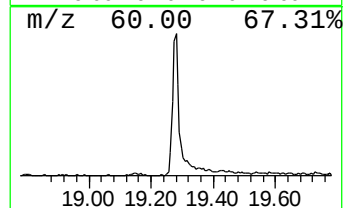
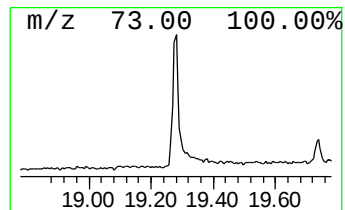
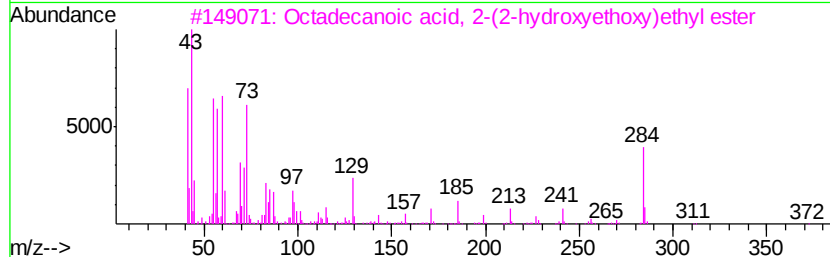
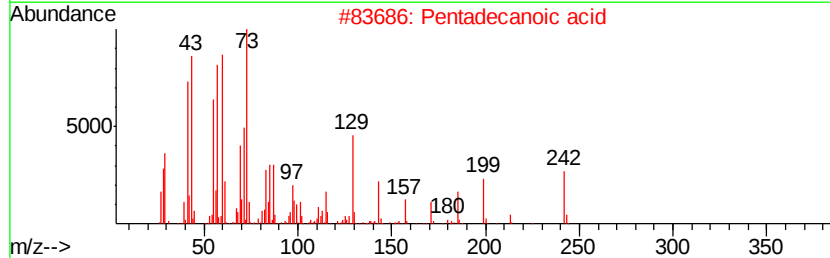
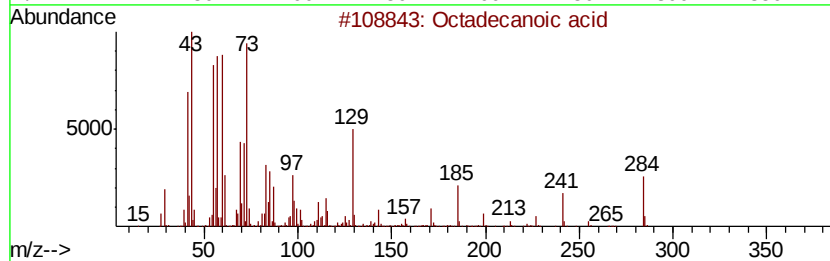
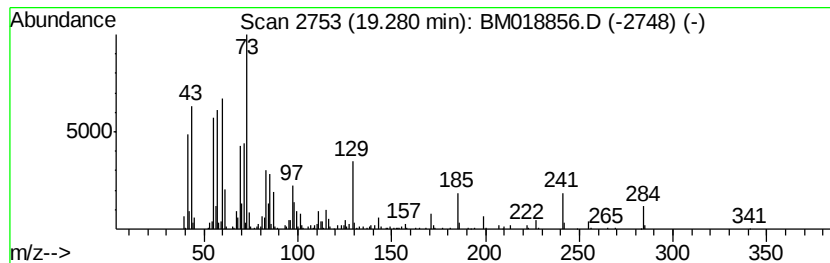
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.28	3.95 ng	780540	Chrysene-d12	21.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	30



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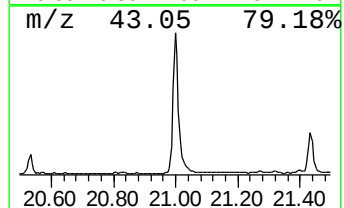
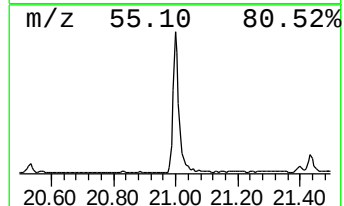
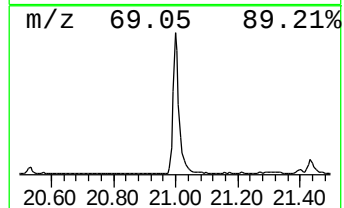
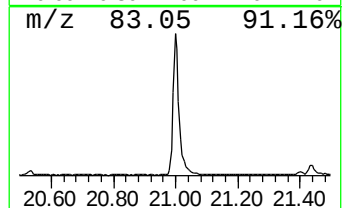
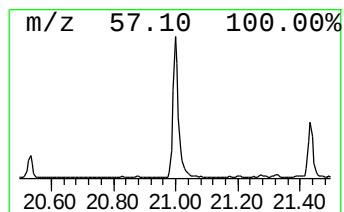
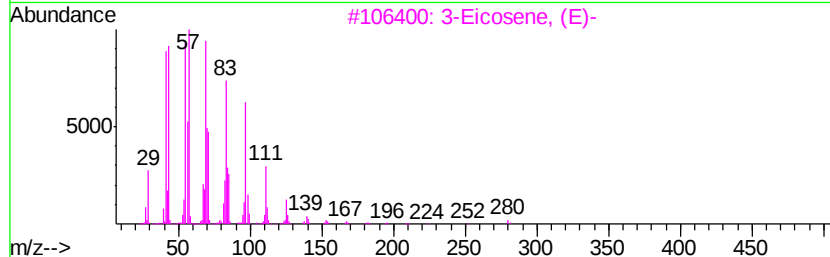
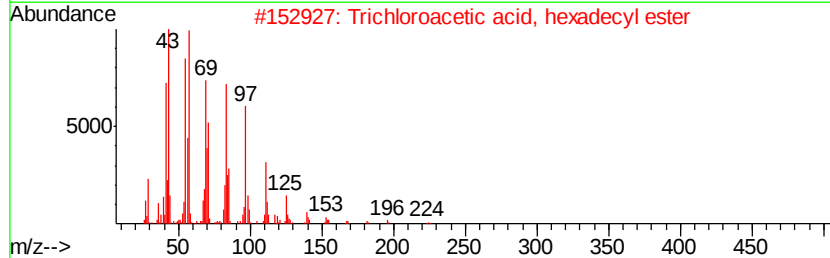
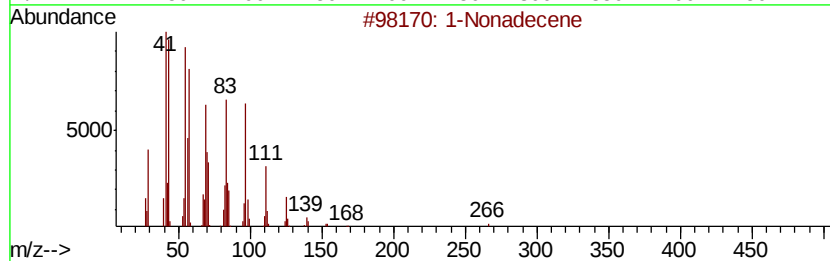
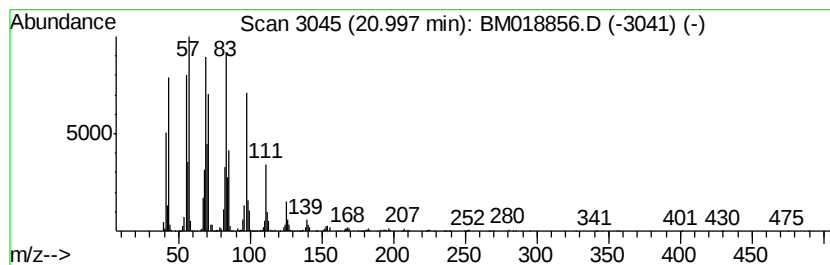
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	11.66 ng	2305150	Chrysene-d12	21.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	97
2	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	91
3	3-Eicosene, (E)-		280	C20H40	074685-33-9	91
4	Trichloroacetic acid, pentadecyl...		372	C17H31Cl3O2	074339-53-0	91
5	Trichloroacetic acid, tetradecyl...		358	C16H29Cl3O2	074339-52-9	91



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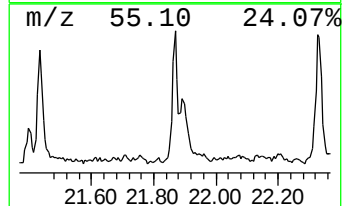
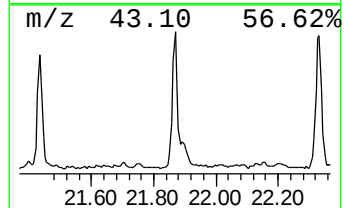
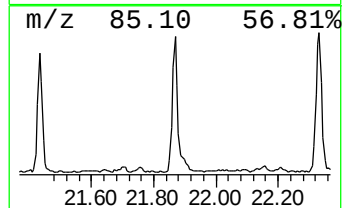
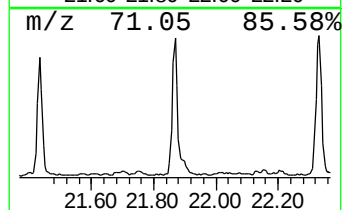
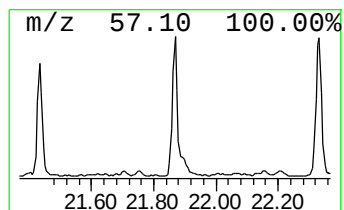
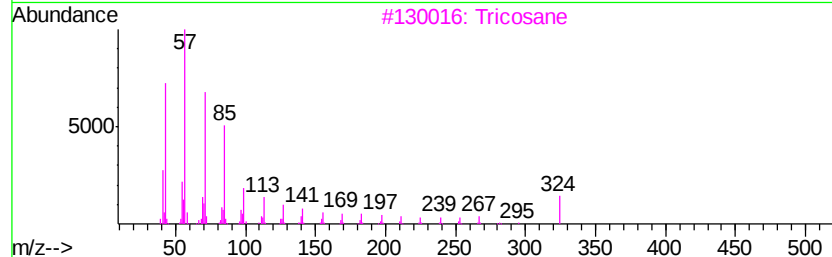
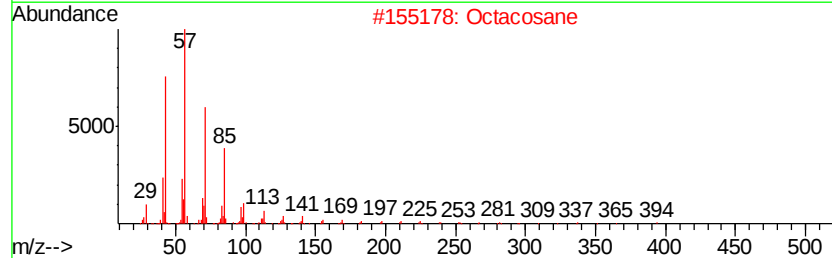
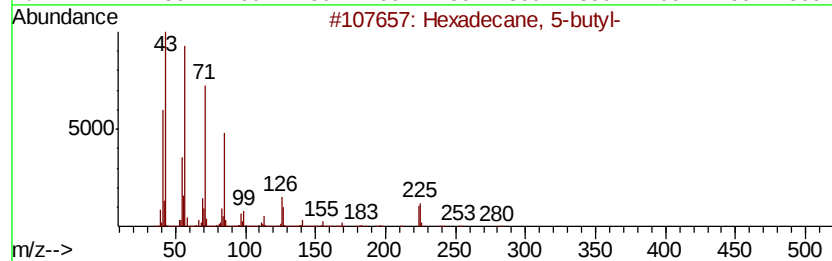
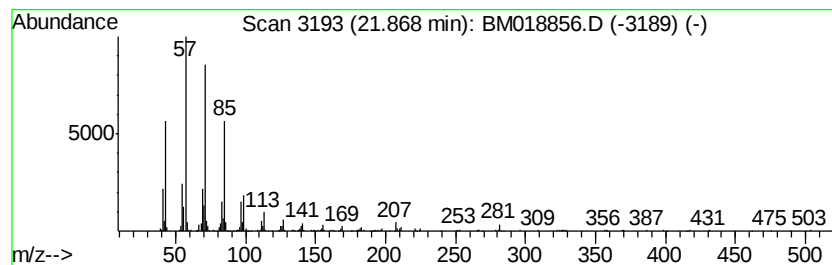
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane, 5-butyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.87	2.61 ng	516360	Chrysene-d12	21.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	90
2		Octacosane	394	C28H58	000630-02-4	87
3		Tricosane	324	C23H48	000638-67-5	87
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5		Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
Data File : BM018856.D
Acq On : 19 Feb 2019 14:45
Operator : JU/SJ
Sample : K1515-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

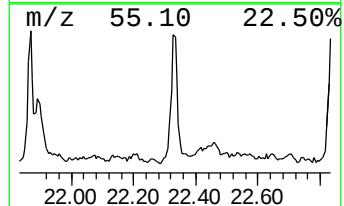
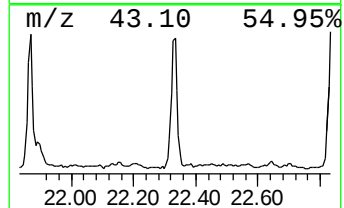
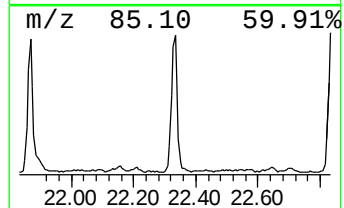
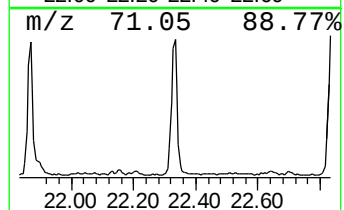
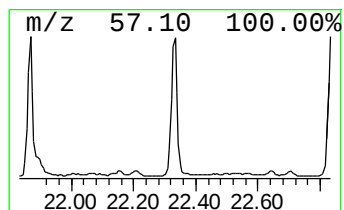
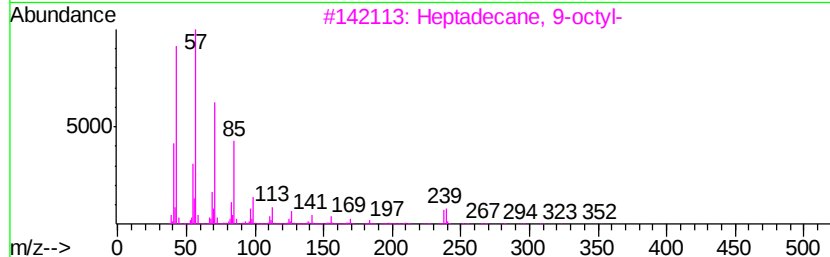
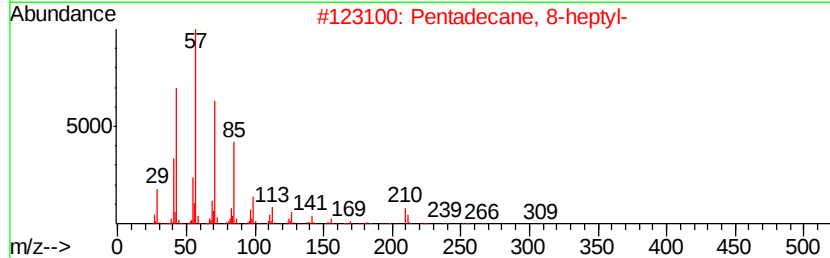
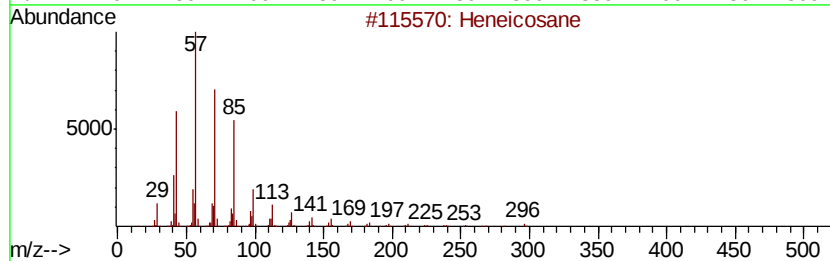
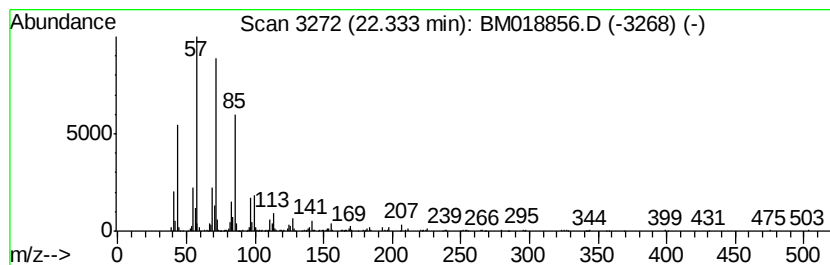
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.33	2.62 ng	518319	Chrysene-d12	21.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	90
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	90
4	Octadecane	254 C18H38	000593-45-3	87
5	Octadecane, 1-iodo-	380 C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
Data File : BM018856.D
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TS-2

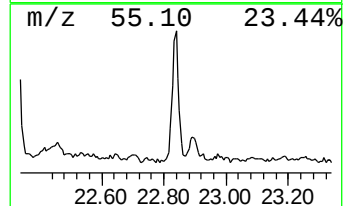
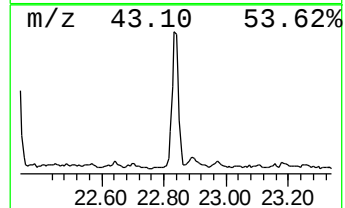
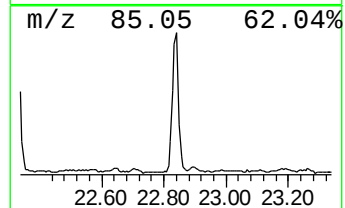
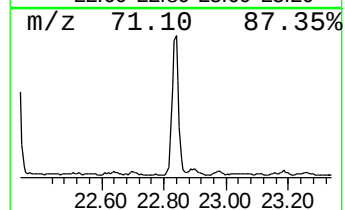
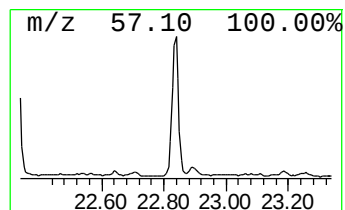
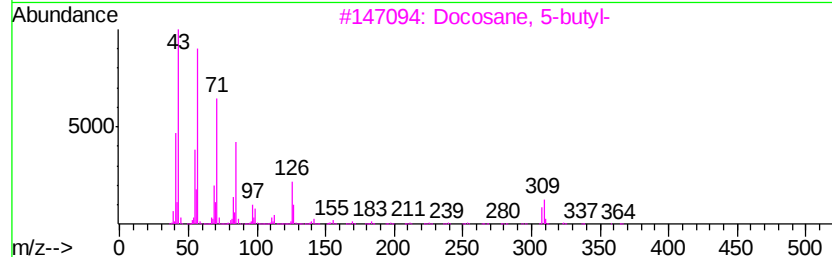
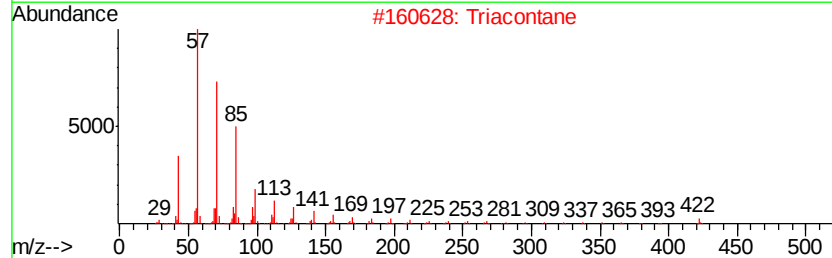
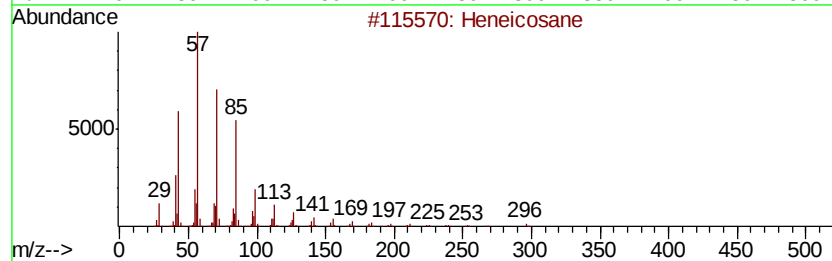
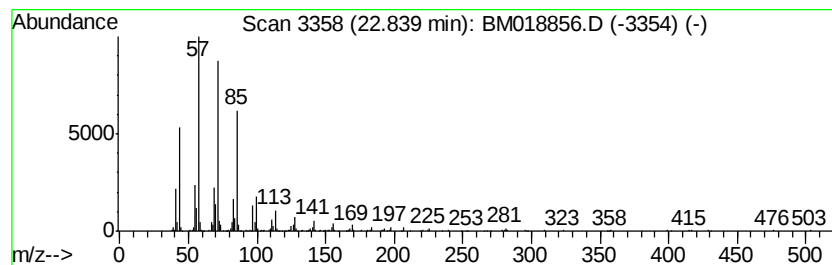
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.84	3.53 ng	567561	Perylene-d12	23.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Docosane, 5-butyl-	366	C26H54	055282-16-1	90
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90
5		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
Data File : BM018856.D
Acq On : 19 Feb 2019 14:45
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Sample : K1515-02
Misc :
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Instrument :
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ClientSampleId :
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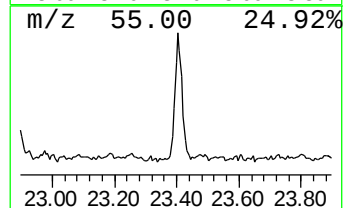
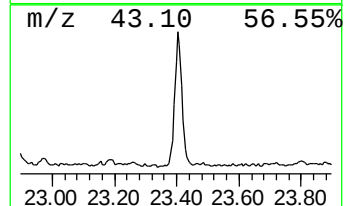
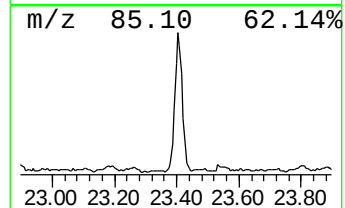
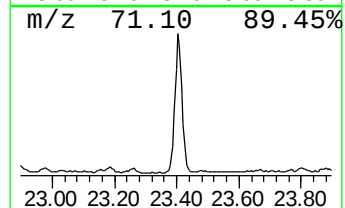
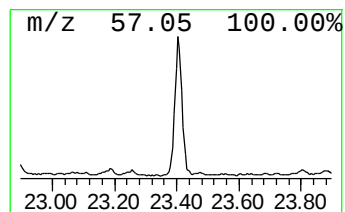
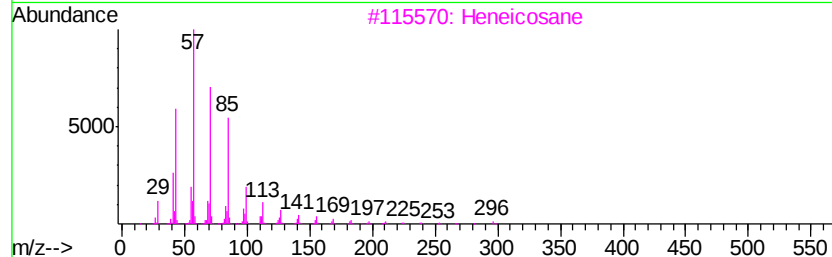
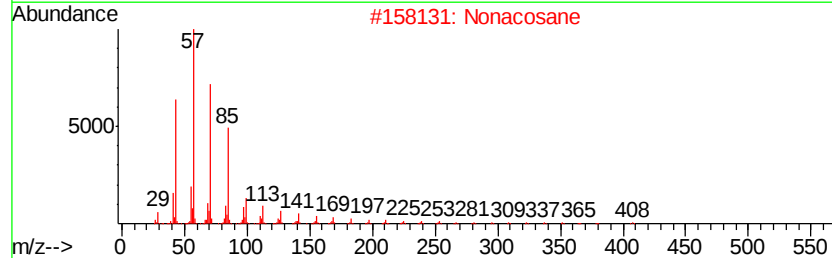
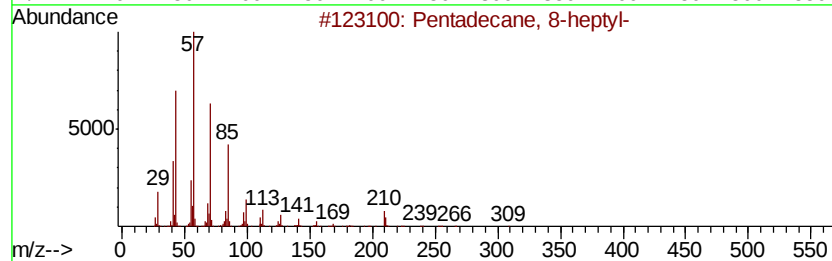
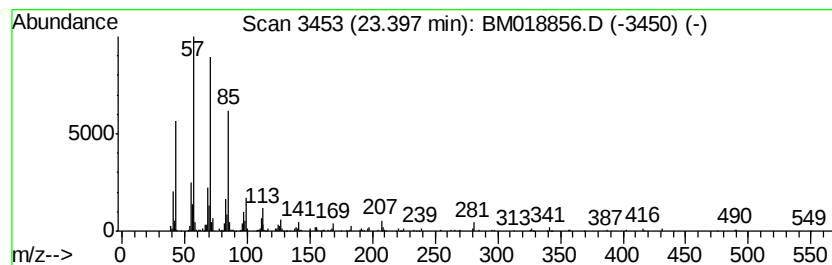
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Pentadecane, 8-heptyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.40	3.14 ng	504333	Perylene-d12	23.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
2		Nonacosane	408	C29H60	000630-03-5	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5		Docosane, 9-butyl-	366	C26H54	055282-14-9	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
Data File : BM018856.D
Acq On : 19 Feb 2019 14:45
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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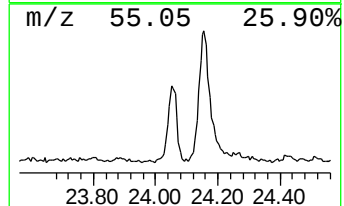
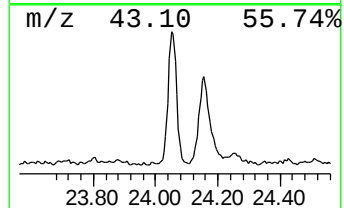
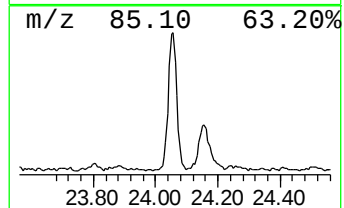
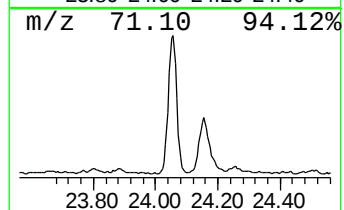
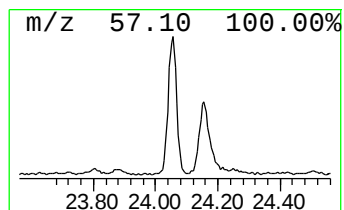
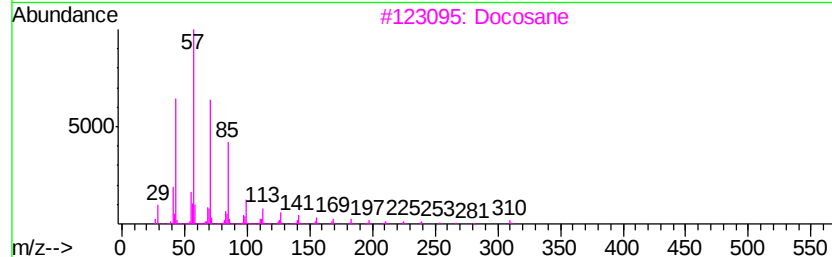
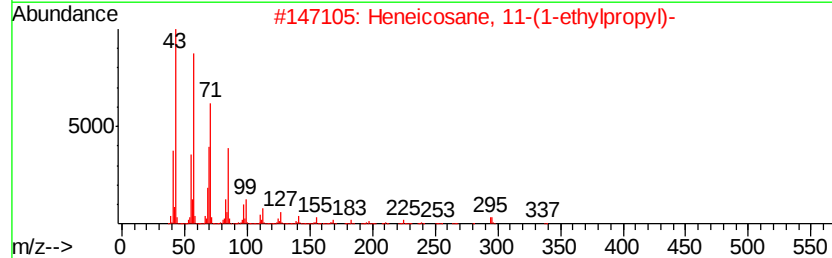
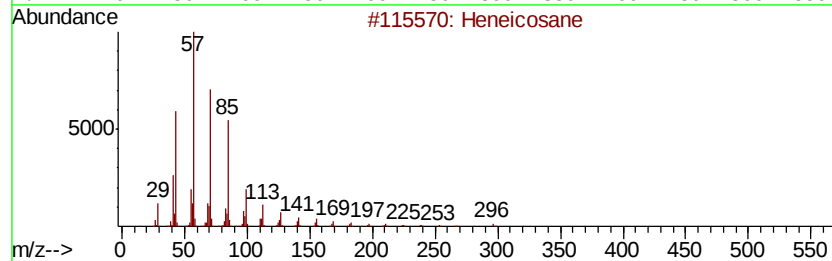
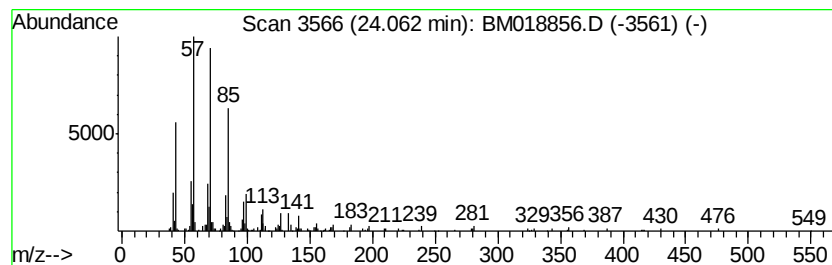
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane, 11-(1-ethylpro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.06	3.12 ng	500373	Perylene-d12	23.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3		Docosane	310	C22H46	000629-97-0	87
4		2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	80
5		Octacosane	394	C28H58	000630-02-4	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
Data File : BM018856.D
Acq On : 19 Feb 2019 14:45
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ALS Vial : 5 Sample Multiplier: 1

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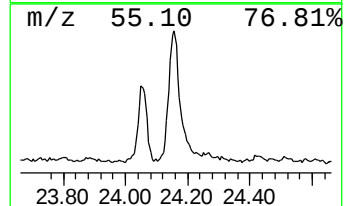
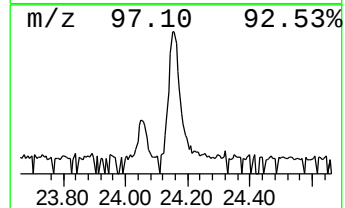
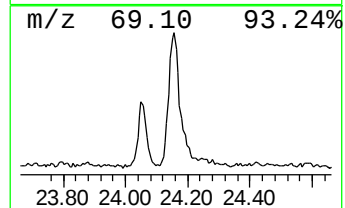
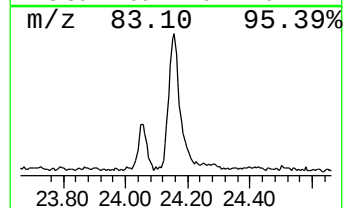
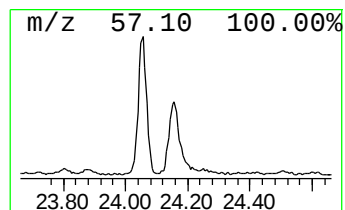
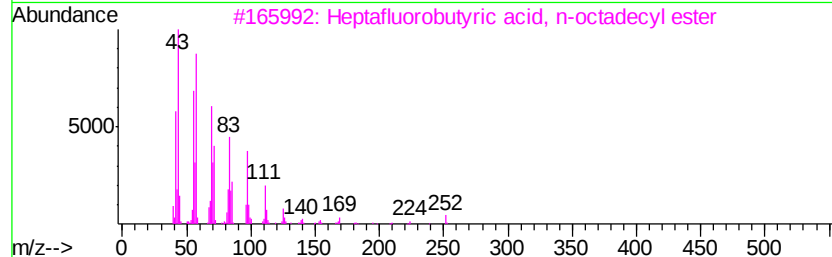
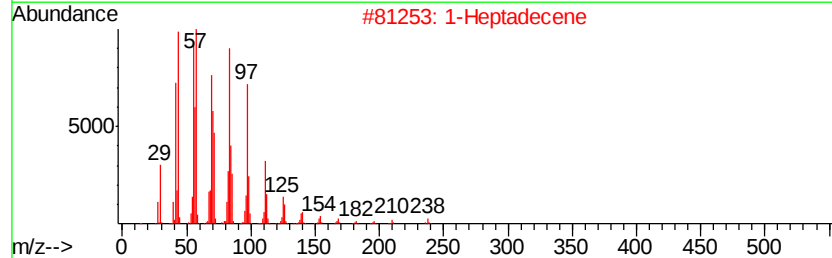
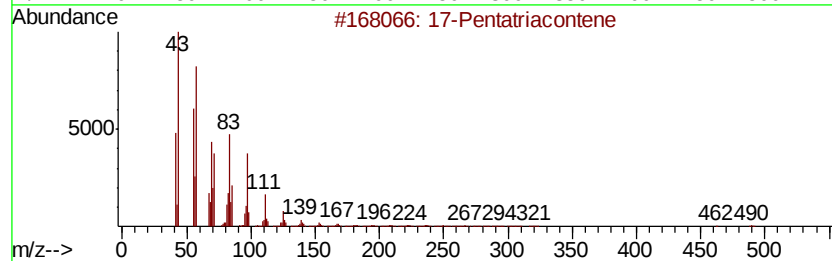
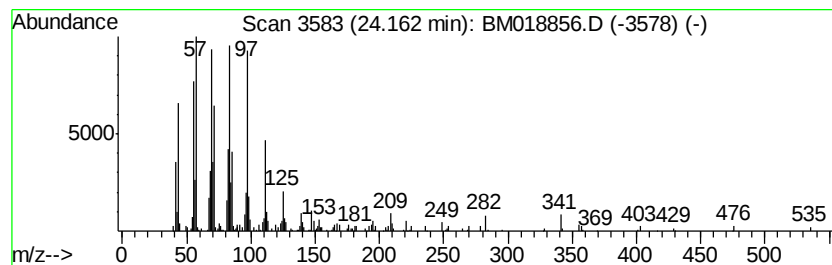
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.16	3.75 ng	602761	Perylene-d12	23.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	94
2		1-Heptadecene	238	C17H34	006765-39-5	86
3		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	83
4		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	80
5		10-Heneicosene (c,t)	294	C21H42	095008-11-0	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM021919\
Data File : BM018856.D
Acq On : 19 Feb 2019 14:45
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Sample : K1515-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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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unknown7.24	7.24	118.9	ng	9932650	1	7.70	1670480	20.0
n-Hexadecanoic acid	18.00	9.5	ng	1663260	4	17.10	3495310	20.0
Octadecanoic acid	19.28	4.0	ng	780540	5	21.30	3954540	20.0
1-Nonadecene	21.00	11.7	ng	2305150	5	21.30	3954540	20.0
Hexadecane, 5-butyl-	21.87	2.6	ng	516360	5	21.30	3954540	20.0
Heneicosane	22.33	2.6	ng	518319	5	21.30	3954540	20.0
Triacontane	22.84	3.5	ng	567561	6	23.55	3212510	20.0
Pentadecane, 8-he...	23.40	3.1	ng	504333	6	23.55	3212510	20.0
Heneicosane, 11-(...	24.06	3.1	ng	500373	6	23.55	3212510	20.0
17-Pentatriacontene	24.16	3.8	ng	602761	6	23.55	3212510	20.0