

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022119\
 Data File : BM018901.D
 Acq On : 21 Feb 2019 18:20
 Operator : JU/SJ
 Sample : K1546-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RT-3422

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	4.852	295	300	314	rVB	233966	367560	2.15%	0.295%
2	5.293	368	375	390	rBV	6561165	9338299	54.50%	7.504%
3	6.875	636	644	665	rBV	6424799	10241579	59.77%	8.230%
4	7.234	697	705	718	rBV	6620528	10430475	60.87%	8.382%
5	7.699	777	784	791	rBV	1108285	1747608	10.20%	1.404%
6	8.010	829	837	851	rBV	4410795	7159683	41.78%	5.754%
7	8.863	974	982	1003	rBV	3564332	6075292	35.45%	4.882%
8	10.481	1248	1257	1271	rBV	1402884	2450454	14.30%	1.969%
9	12.963	1672	1679	1693	rBV	8246769	12193882	71.16%	9.799%
10	13.810	1817	1823	1834	rBV	356832	550459	3.21%	0.442%
11	14.345	1908	1914	1920	rBV2	2053225	3158875	18.43%	2.538%
12	14.410	1920	1925	1933	rVB	473610	673145	3.93%	0.541%
13	14.751	1978	1983	1991	rVB	194169	322047	1.88%	0.259%
14	15.398	2087	2093	2105	rBV	456972	738525	4.31%	0.593%
15	15.845	2163	2169	2181	rBV	7409293	10832696	63.22%	8.705%
16	16.080	2203	2209	2219	rVB3	272198	659602	3.85%	0.530%
17	17.098	2376	2382	2386	rBV	2794982	3932510	22.95%	3.160%
18	17.139	2386	2389	2396	rVB	1258374	1790771	10.45%	1.439%
19	17.233	2402	2405	2409	rVB	162200	198347	1.16%	0.159%
20	17.992	2528	2534	2537	rBV2	1119146	1591508	9.29%	1.279%
21	18.168	2560	2564	2568	rBV2	383450	547145	3.19%	0.440%
22	19.162	2728	2733	2739	rVB	2445578	3133085	18.28%	2.518%
23	19.274	2748	2752	2763	rVB2	367296	507013	2.96%	0.407%
24	19.498	2786	2790	2792	rBV2	340968	507256	2.96%	0.408%
25	19.527	2792	2795	2804	rVB	1592026	2116772	12.35%	1.701%
26	19.733	2825	2830	2840	rVB	13769125	17135611	100.00%	13.770%
27	20.027	2877	2880	2885	rVB2	269544	370917	2.16%	0.298%
28	20.127	2893	2897	2899	rBV2	228463	292425	1.71%	0.235%
29	20.998	3040	3045	3054	rBV2	1807637	2531676	14.77%	2.034%
30	21.204	3076	3080	3084	rVB	295047	345197	2.01%	0.277%
31	21.298	3089	3096	3100	rVV	3295429	4913897	28.68%	3.949%
32	21.333	3100	3102	3109	rVB	331265	372901	2.18%	0.300%
33	21.433	3116	3119	3129	rVB3	326388	424423	2.48%	0.341%
34	21.868	3189	3193	3196	rBV	346571	407988	2.38%	0.328%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.327	3267	3271	3278	rVB	410749	552478	3.22%	0.444%
36	22.833	3353	3357	3361	rBV	429304	647509	3.78%	0.520%
37	23.403	3450	3454	3458	rBV	287474	422321	2.46%	0.339%
38	23.545	3472	3478	3491	rVB	1819458	3689542	21.53%	2.965%
39	24.050	3561	3564	3570	rVB	270798	430858	2.51%	0.346%
40	24.150	3577	3581	3594	rVB2	279998	638003	3.72%	0.513%

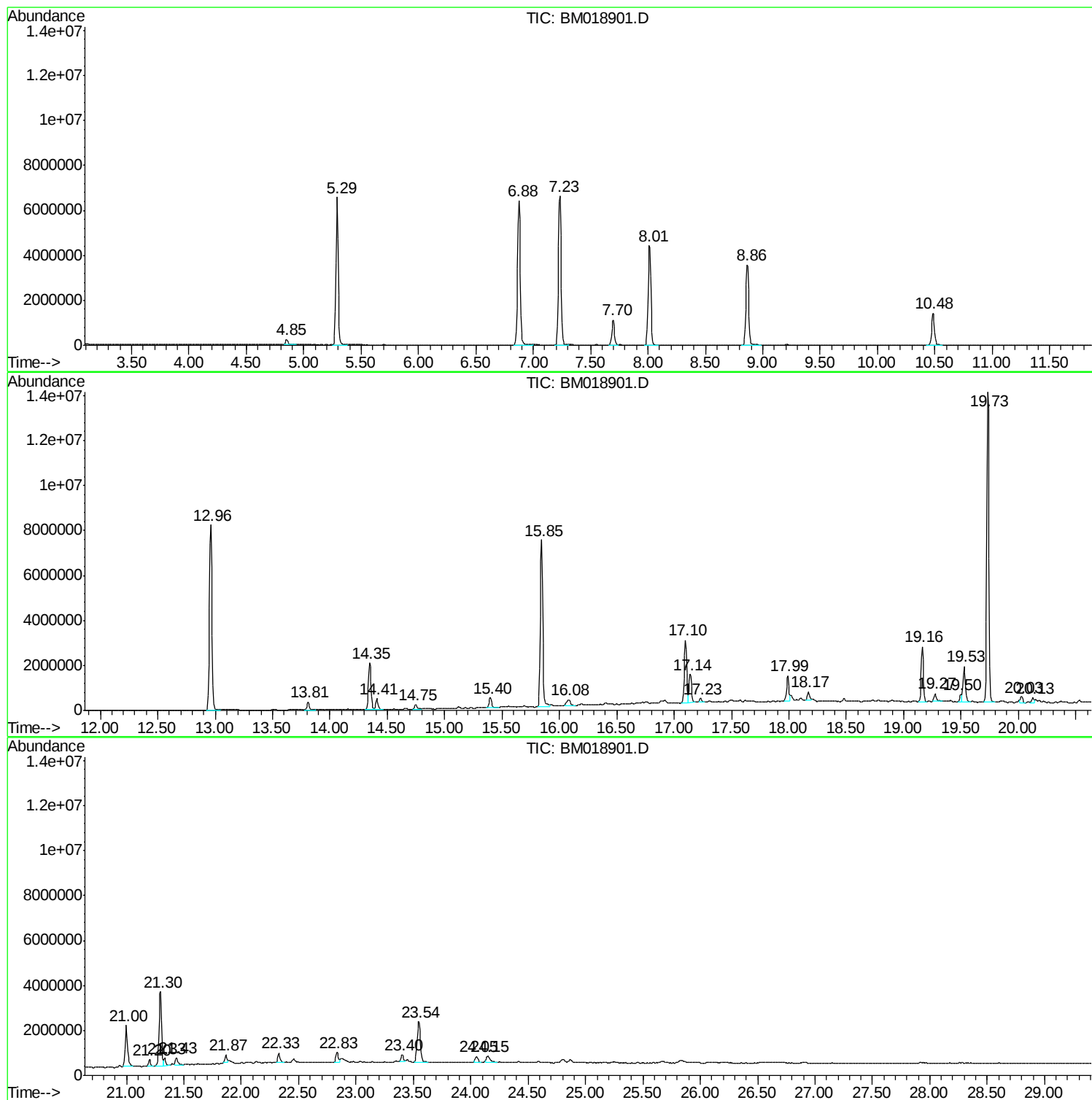
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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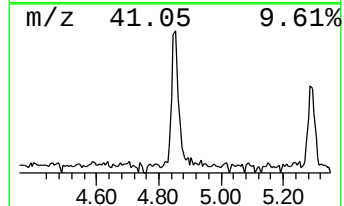
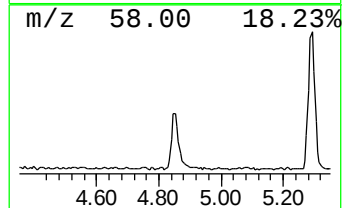
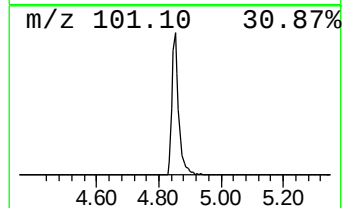
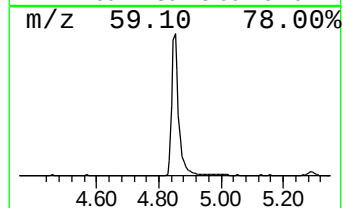
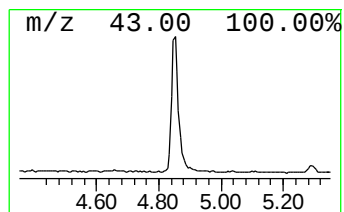
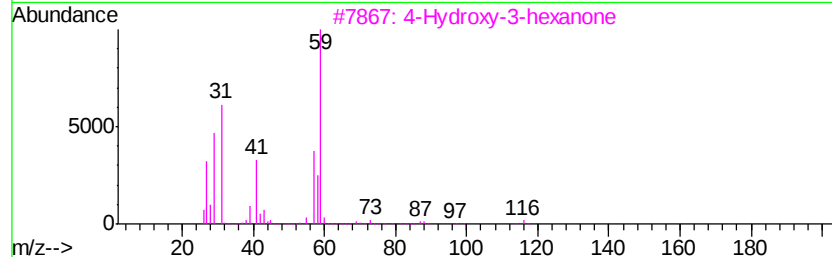
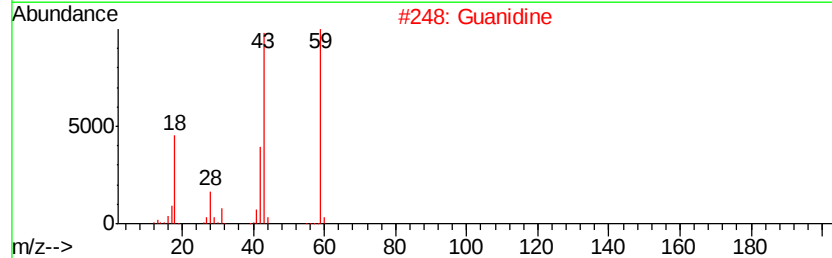
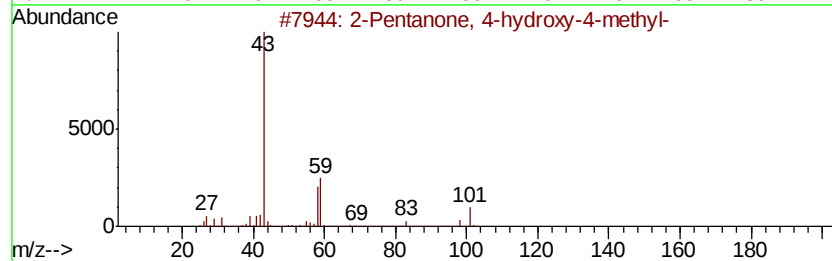
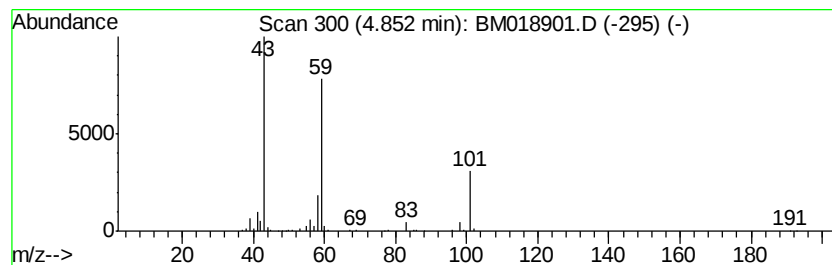
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	4.21 ng	367560	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	50
3		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	28
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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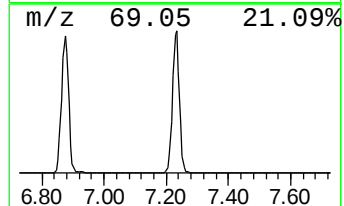
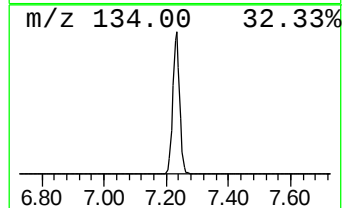
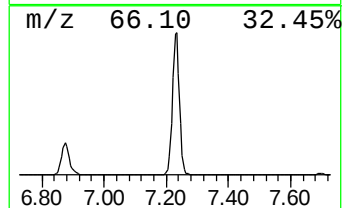
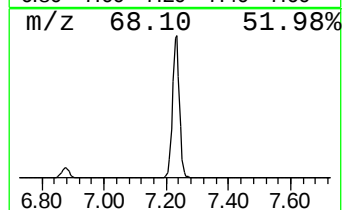
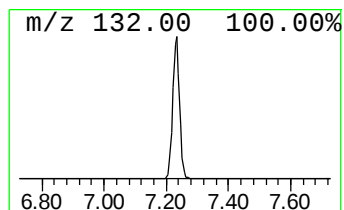
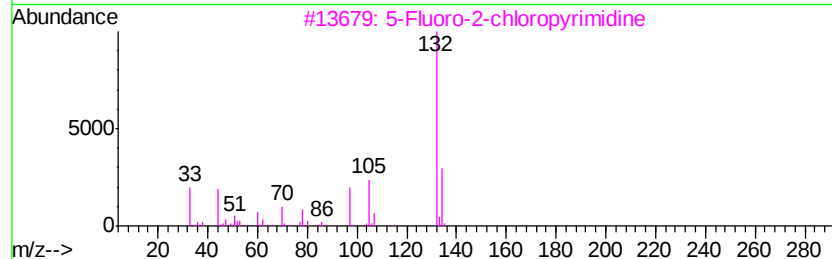
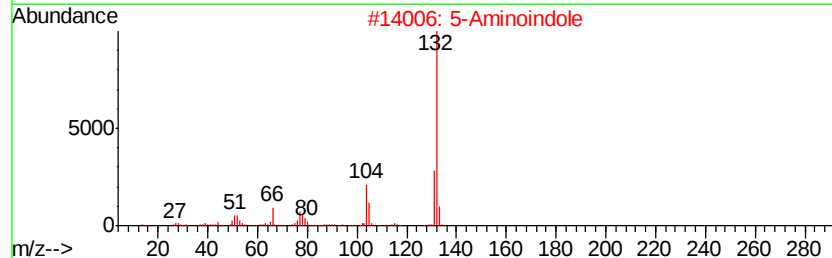
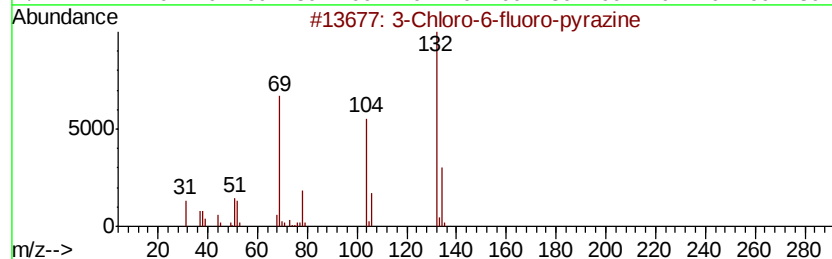
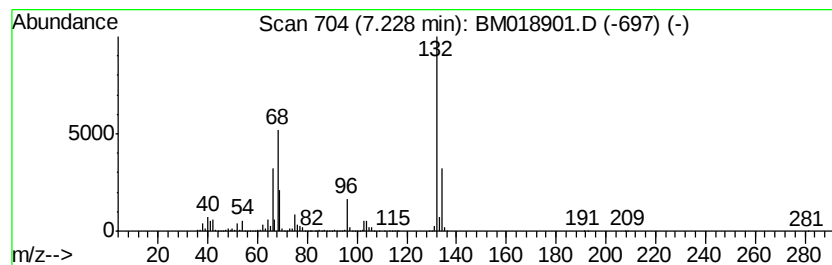
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown7.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	119.37 ng	10430500	1,4-Dichlorobenzene-d4	7.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	9



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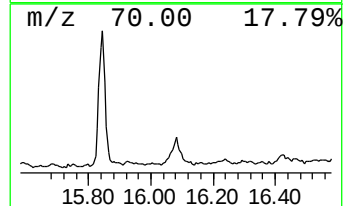
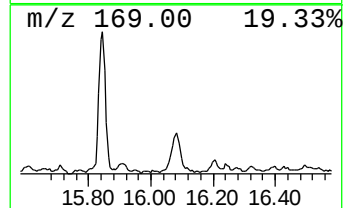
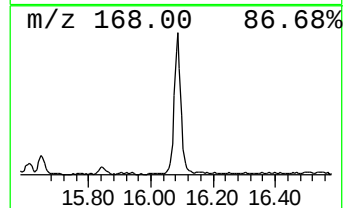
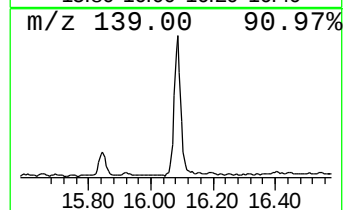
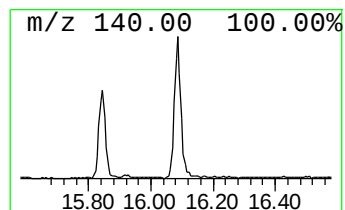
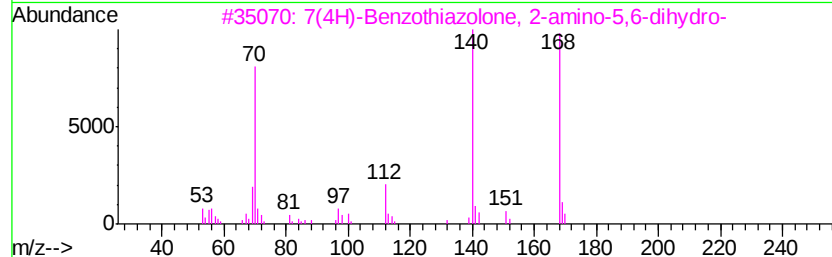
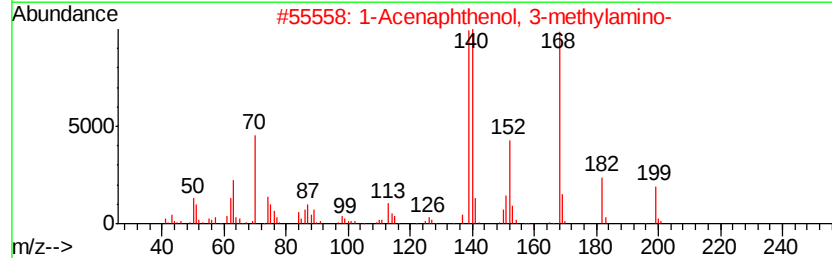
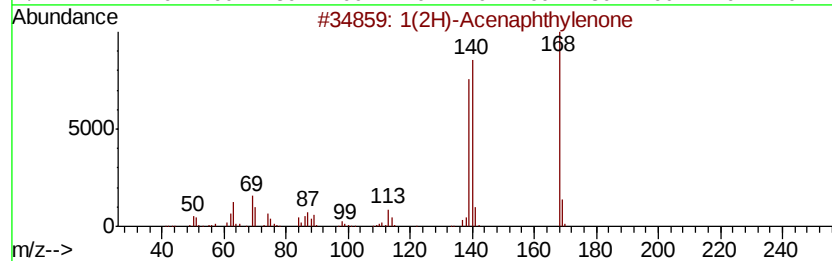
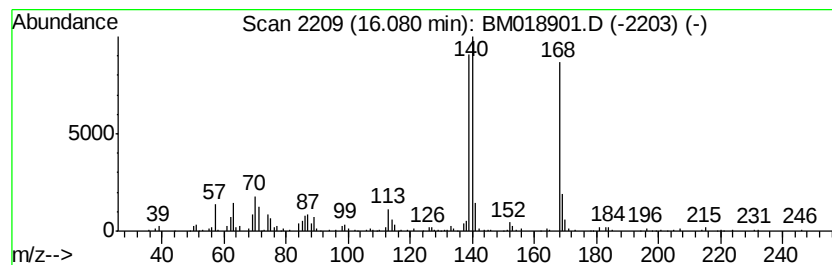
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1(2H)-Acenaphthylenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.35 ng	659602	Phenanthrene-d10	17.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	95
2		1-Acenaphthenol, 3-methylamino-	199	C13H13NO	1000129-22-6	78
3		7(4H)-Benzothiazolone, 2-amino-5...	168	C7H8N2OS	017583-10-7	50
4		Dibenzofuran	168	C12H8O	000132-64-9	49
5		Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	47



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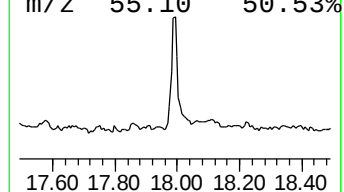
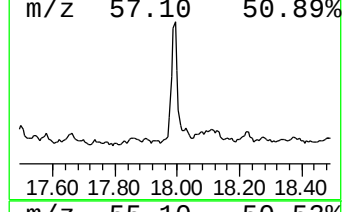
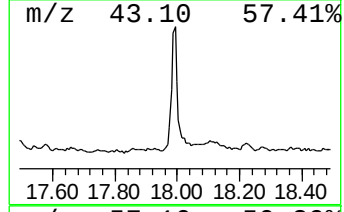
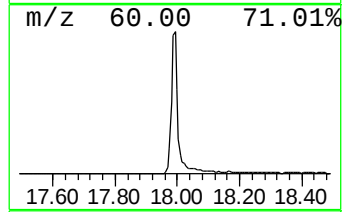
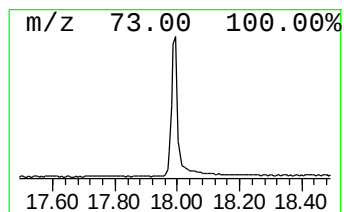
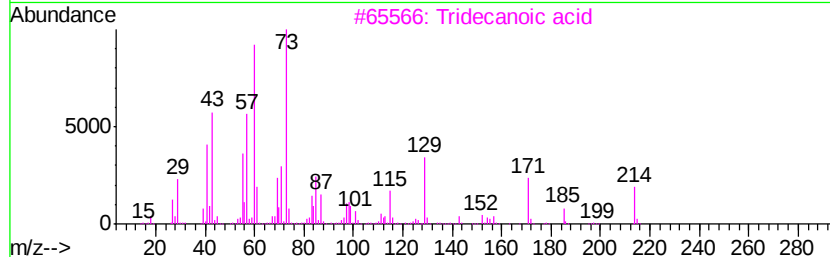
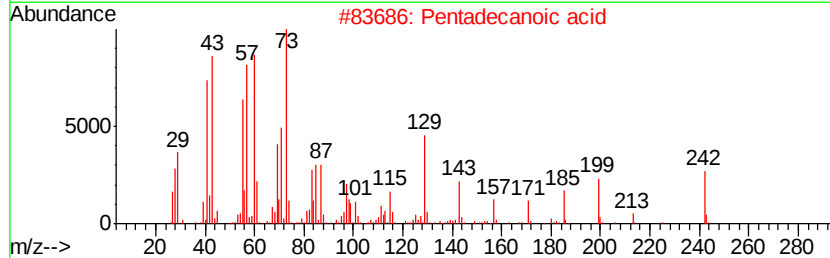
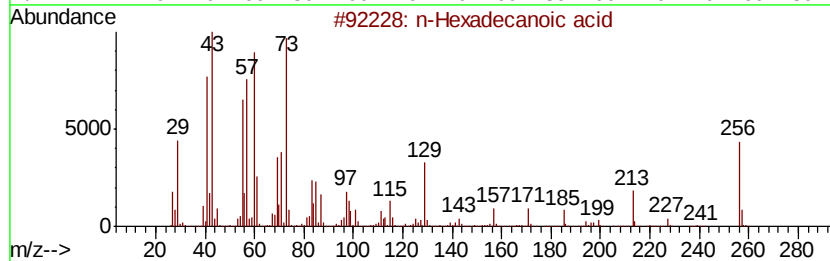
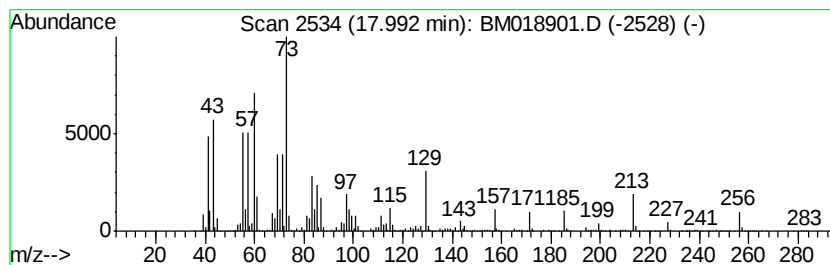
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.99	8.09 ng	1591510	Phenanthrene-d10	17.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	52
4	Hexadecane	226	C16H34	000544-76-3	18
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	18



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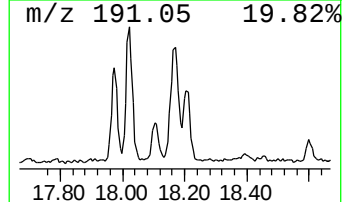
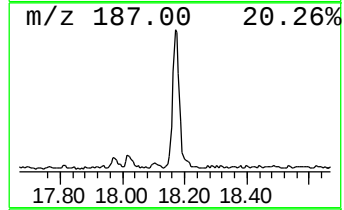
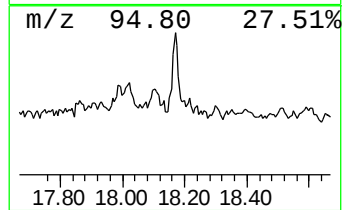
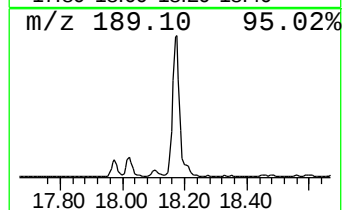
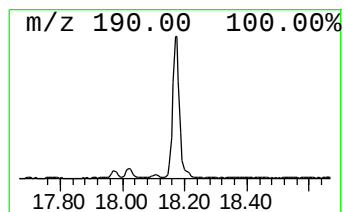
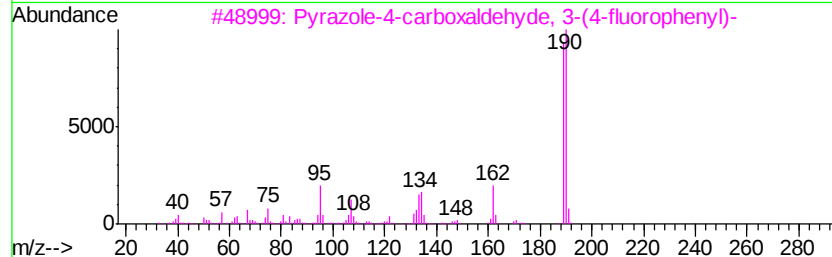
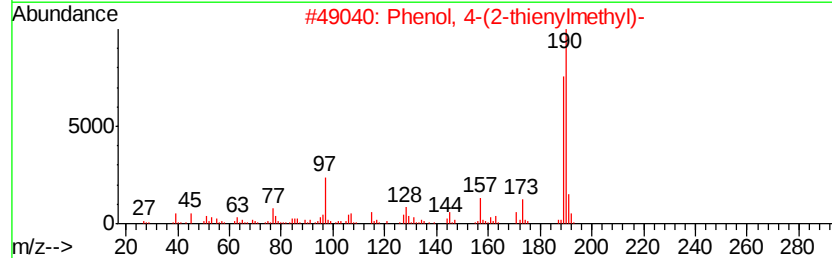
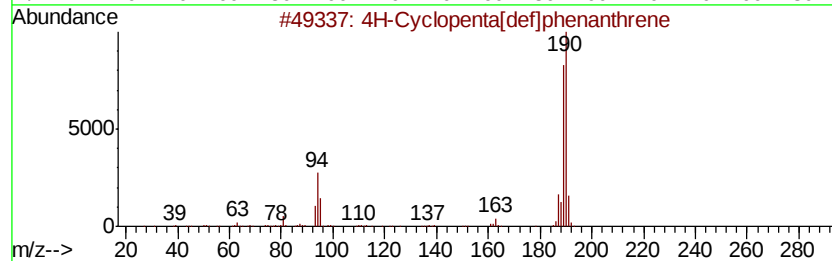
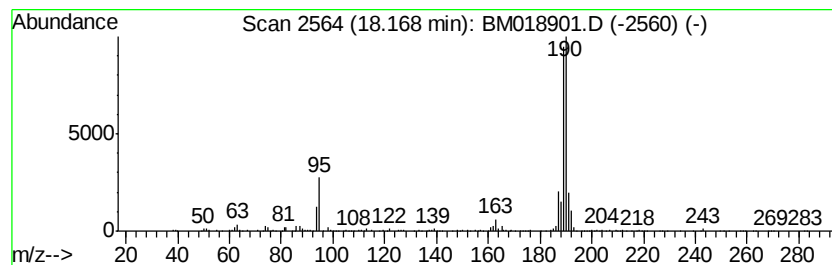
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	2.78 ng	547145	Phenanthrene-d10	17.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2		Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	59
3		Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	53
4		6H-Cyclobuta[fl]phenanthrene	190	C15H10	083469-43-6	50
5		2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022119\
Data File : BM018901.D
Acq On : 21 Feb 2019 18:20
Operator : JU/SJ
Sample : K1546-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

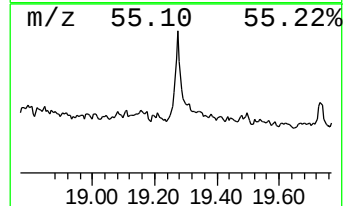
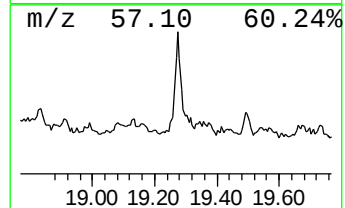
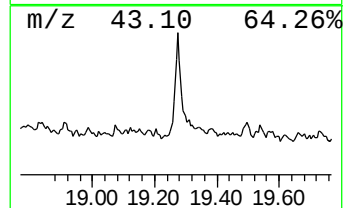
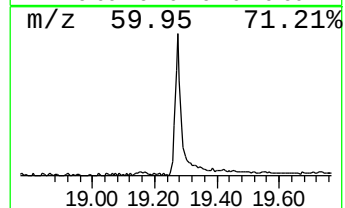
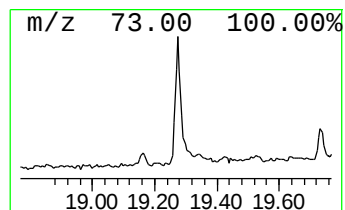
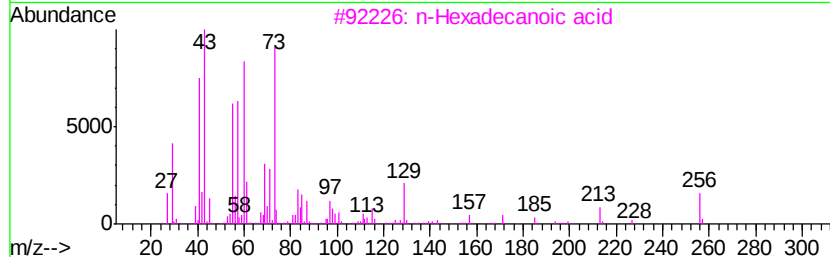
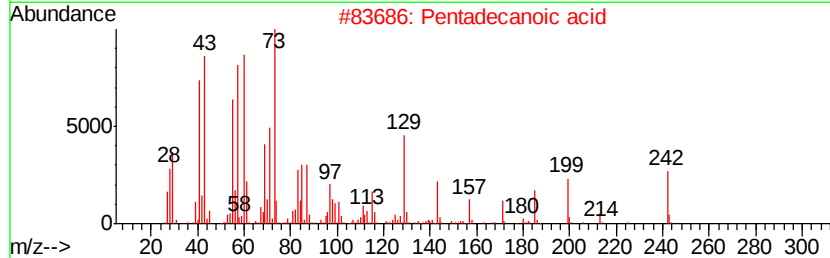
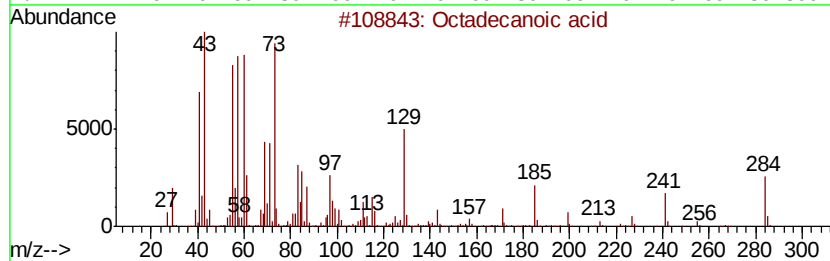
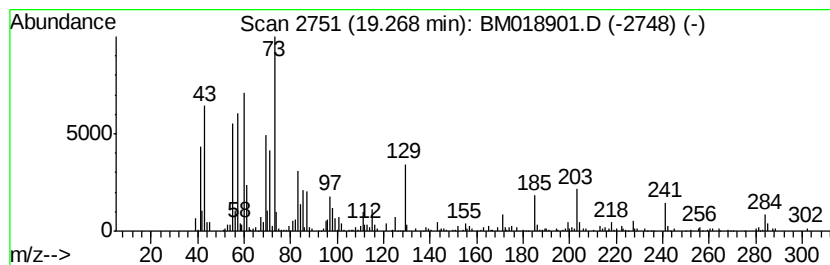
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	2.06 ng	507013	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 93
3		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 91
4		Tetradecanoic acid	228 C14H28O2	000544-63-8 86
5		.beta.-d-Lyxofuranoside, thio-de...	306 C15H30O4S	1000154-40-2 35



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022119\
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Sample : K1546-04
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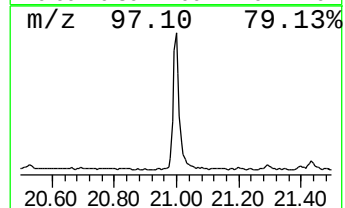
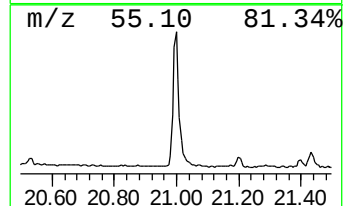
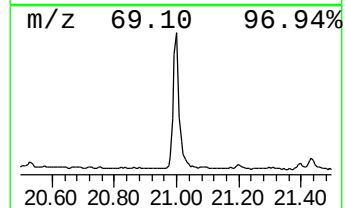
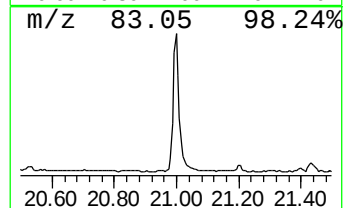
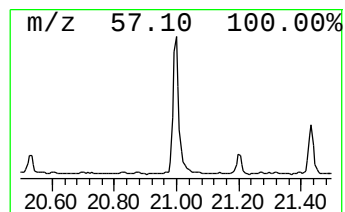
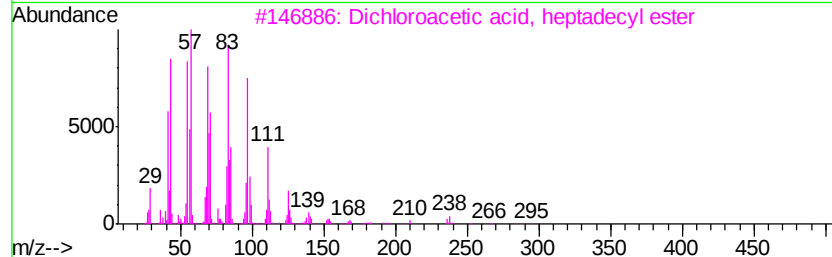
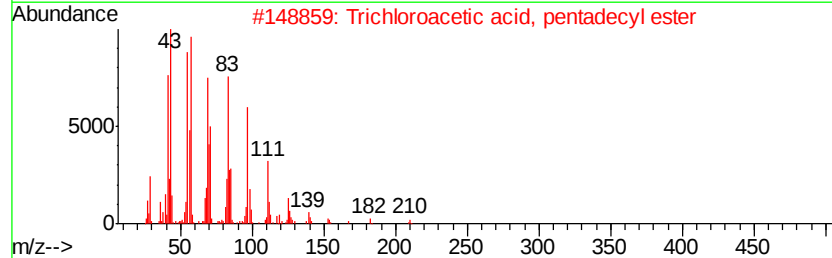
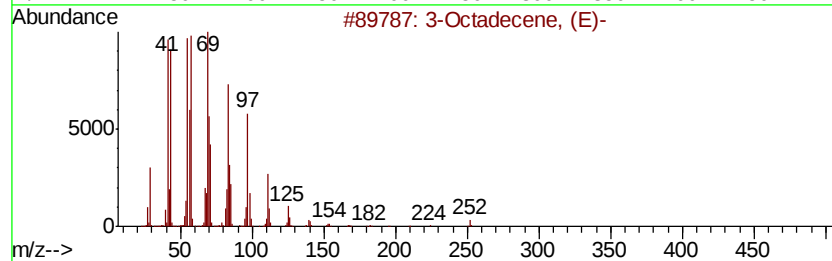
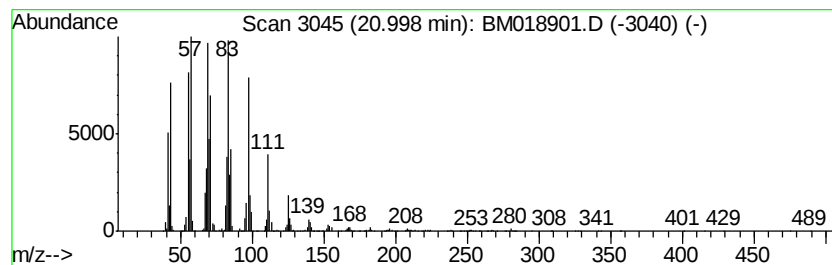
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	10.30 ng	2531680	Chrysene-d12	21.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Octadecene, (E)-	252 C18H36	007206-19-1	94
2	Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0	91
3	Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2	91
4	Bromoacetic acid, octadecyl ester	390 C20H39BrO2	018992-03-5	91
5	3-Eicosene, (E)-	280 C20H40	074685-33-9	90



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Sample : K1546-04
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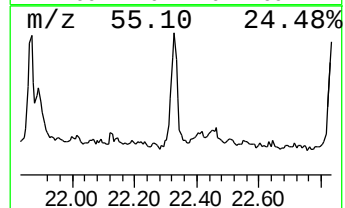
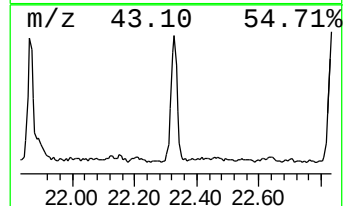
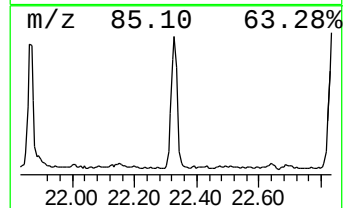
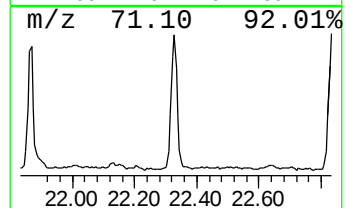
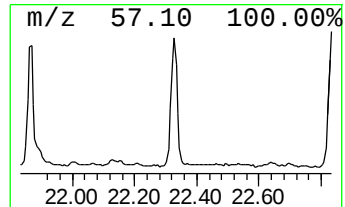
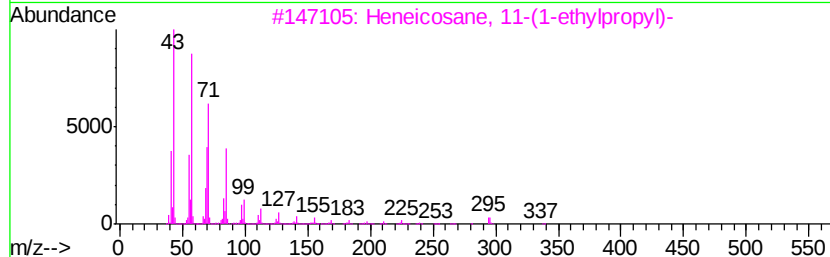
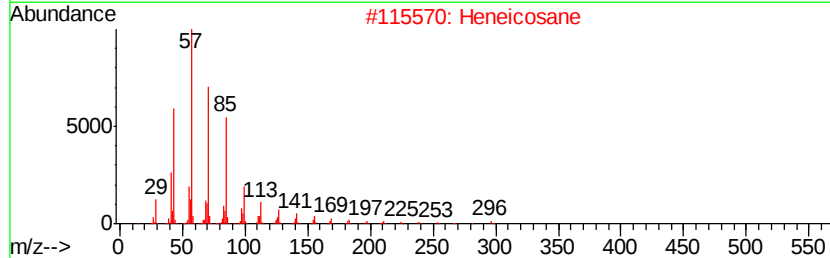
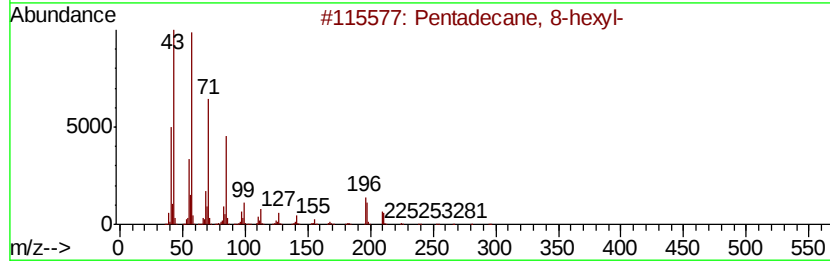
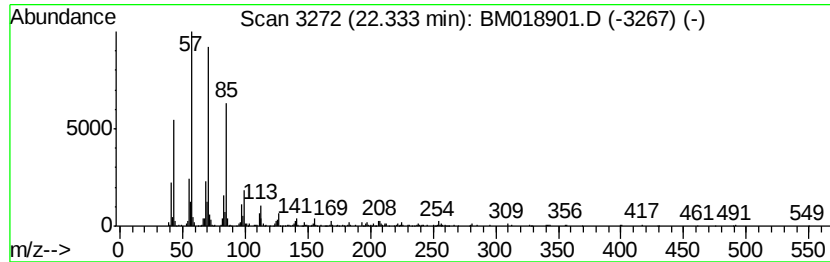
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecane, 8-hexyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.33	2.25 ng	552478	Chrysene-d12	21.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pentadecane, 8-hexyl-	296 C21H44	013475-75-7 91
2		Heneicosane	296 C21H44	000629-94-7 91
3		Heneicosane, 11-(1-ethylpropyl)-	366 C26H54	055282-11-6 90
4		Tetradecane	198 C14H30	000629-59-4 87
5		Docosane, 5-butyl-	366 C26H54	055282-16-1 86



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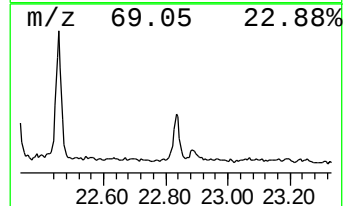
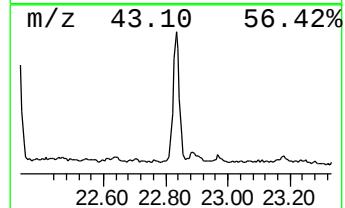
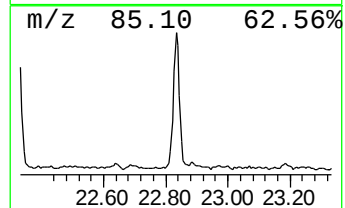
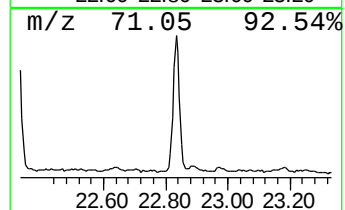
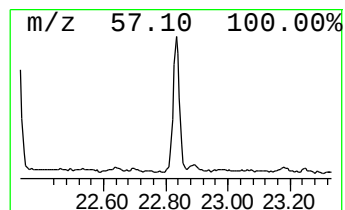
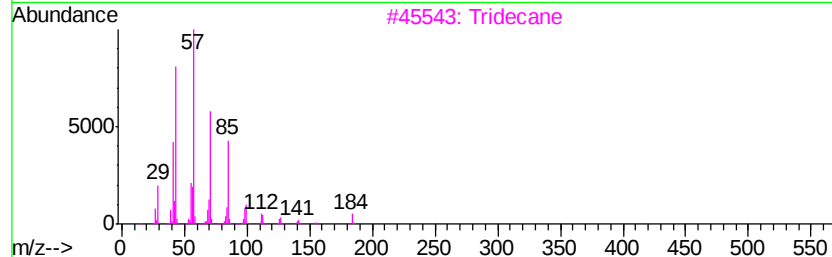
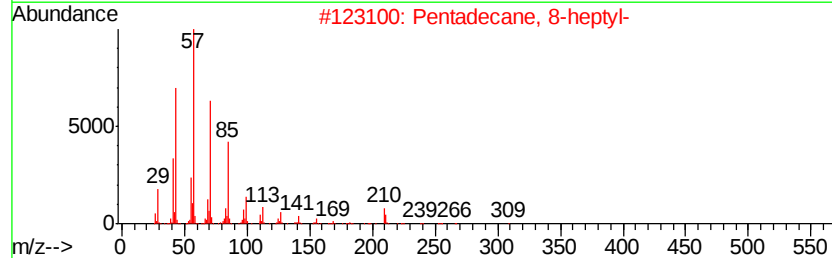
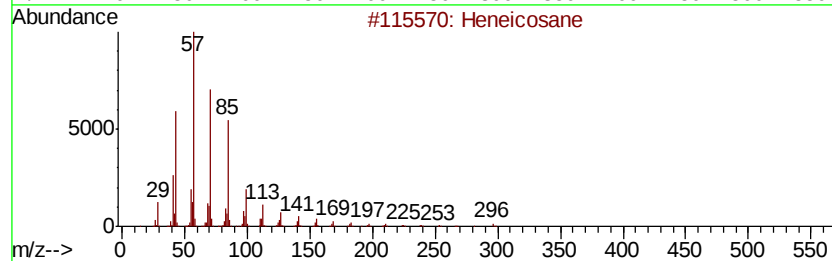
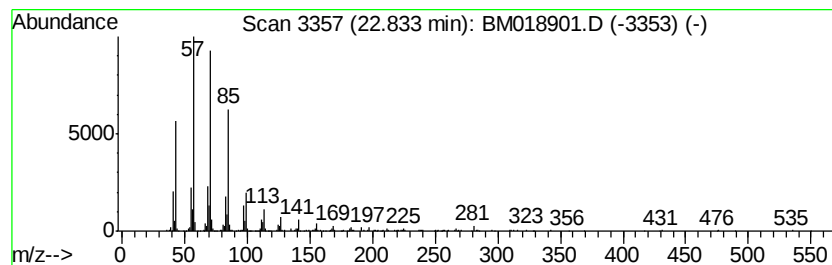
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.83	3.51 ng	647509	Perylene-d12	23.54

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			Tridecane	184	C13H28	000629-50-5	87
4			Octadecane, 2-methyl-	268	C19H40	001560-88-9	87
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022119\
Data File : BM018901.D
Acq On : 21 Feb 2019 18:20
Operator : JU/SJ
Sample : K1546-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RT-3422

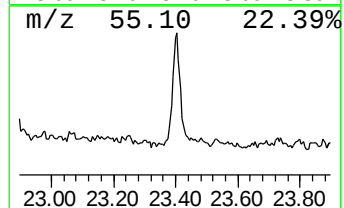
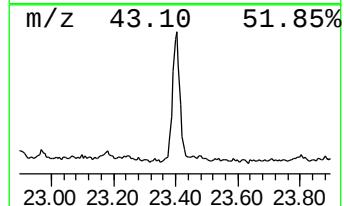
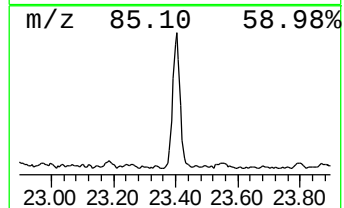
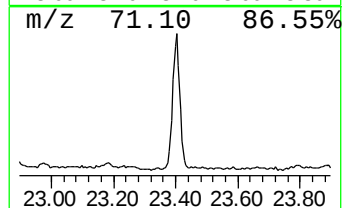
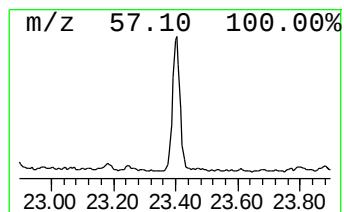
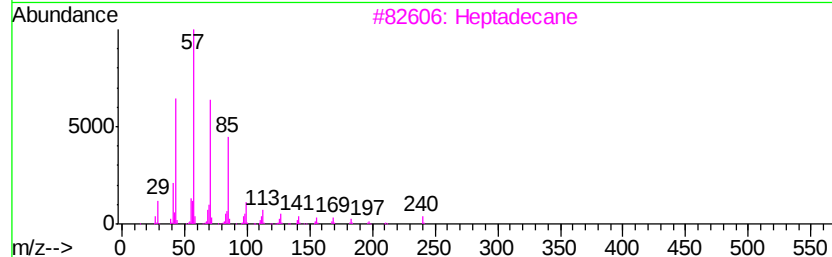
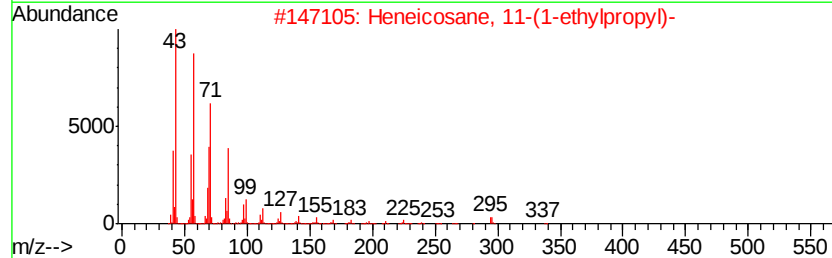
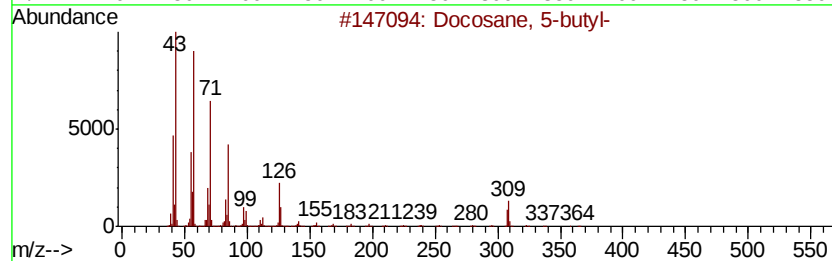
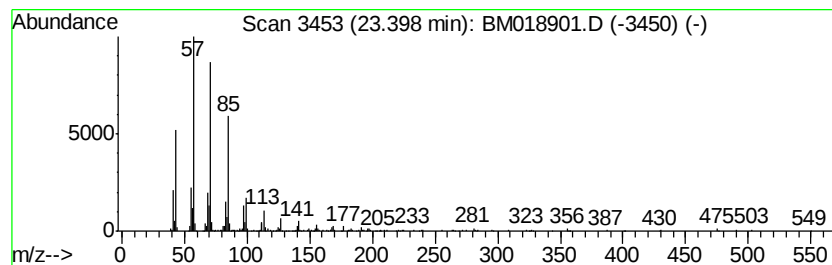
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Docosane, 5-butyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.40	2.29 ng	422321	Perylene-d12	23.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 5-butyl-	366	C26H54	055282-16-1	90
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3		Heptadecane	240	C17H36	000629-78-7	86
4		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
5		Hexadecane, 3-methyl-	240	C17H36	006418-43-5	81



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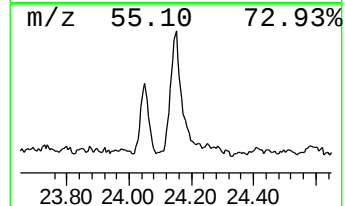
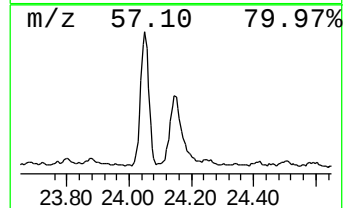
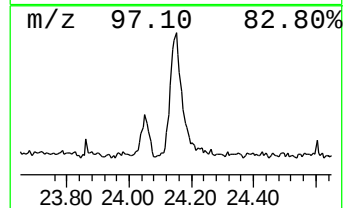
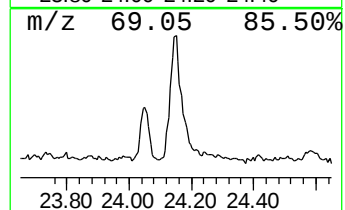
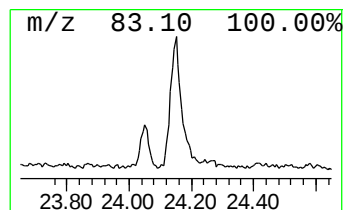
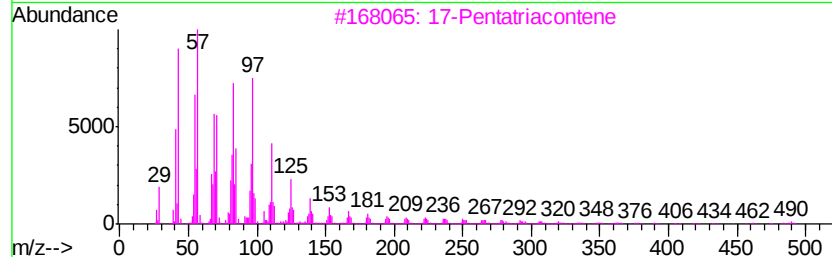
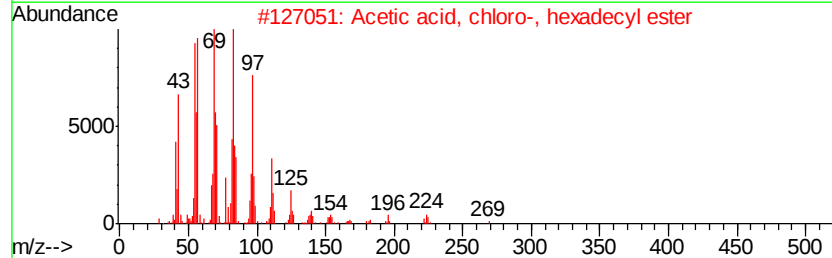
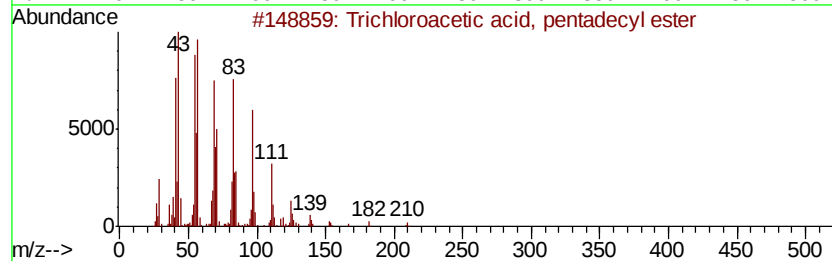
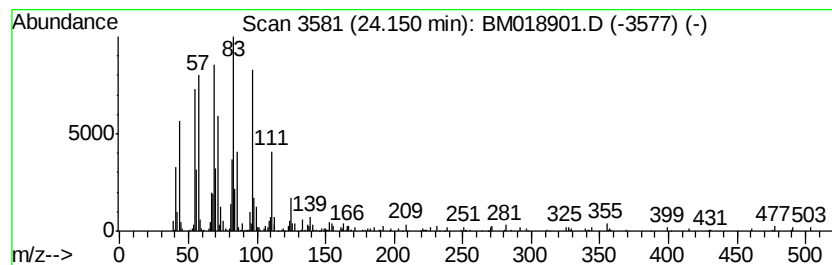
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Trichloroacetic acid, penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.15	3.46 ng	638003	Perylene-d12	23.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	86
2			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	86
3			17-Pentatriacontene	491	C35H70	006971-40-0	68
4			Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	64
5			1-Hexacosanol	382	C26H54O	000506-52-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM022119\
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 Operator : JU/SJ
 Sample : K1546-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RT-3422

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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
2-Pentanone, 4-hy...	4.85	4.2 ng		367560	1	7.70	1747610	20.0
unknown7.23	7.23	119.4 ng		10430500	1	7.70	1747610	20.0
1(2H)-Acenaphthyl...	16.08	3.4 ng		659602	4	17.10	3932510	20.0
n-Hexadecanoic acid	17.99	8.1 ng		1591510	4	17.10	3932510	20.0
4H-Cyclopenta[def...	18.17	2.8 ng		547145	4	17.10	3932510	20.0
Octadecanoic acid	19.27	2.1 ng		507013	5	21.30	4913900	20.0
3-Octadecene, (E)-	21.00	10.3 ng		2531680	5	21.30	4913900	20.0
Pentadecane, 8-he...	22.33	2.3 ng		552478	5	21.30	4913900	20.0
Heneicosane	22.83	3.5 ng		647509	6	23.54	3689540	20.0
Docosane, 5-butyl-	23.40	2.3 ng		422321	6	23.54	3689540	20.0
Trichloroacetic a...	24.15	3.5 ng		638003	6	23.54	3689540	20.0