

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA M\DATA\BM030718\
 Data File : BM014514.D
 Acq On : 07 Mar 2018 00:48
 Operator : SJ/JU
 Sample : J1699-77
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B24

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:\HPCHEM1\BNA_M\METHODS\8270-BM020718.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	4.687	286	289	298	rVB2	61212	95047	1.77%	0.219%
2	5.134	359	365	385	rVB	2398313	3568336	66.58%	8.205%
3	6.710	626	633	651	rBV	2095804	3607032	67.30%	8.294%
4	7.045	683	690	703	rBV	2561261	3935628	73.43%	9.049%
5	7.498	761	767	775	rBV	467655	777337	14.50%	1.787%
6	7.816	814	821	832	rBV	1911769	3084279	57.55%	7.092%
7	8.669	958	966	982	rBV	1261264	2432293	45.38%	5.593%
8	10.275	1232	1239	1253	rBV	443071	902361	16.84%	2.075%
9	12.769	1656	1663	1681	rBV	2847904	4586707	85.58%	10.546%
10	13.651	1807	1813	1824	rVB	68737	149731	2.79%	0.344%
11	14.063	1877	1883	1887	rBV3	40603	61542	1.15%	0.142%
12	14.168	1892	1901	1914	rVV3	584323	998875	18.64%	2.297%
13	15.021	2041	2046	2051	rBV3	58381	73639	1.37%	0.169%
14	15.680	2149	2158	2174	rBV	1818633	3125865	58.32%	7.187%
15	15.892	2189	2194	2203	rBV3	54760	96600	1.80%	0.222%
16	16.933	2365	2371	2382	rBV2	635122	1055927	19.70%	2.428%
17	17.604	2480	2485	2493	rBV	837339	977395	18.24%	2.247%
18	17.833	2519	2524	2532	rBV2	119167	223183	4.16%	0.513%
19	18.756	2675	2681	2683	rBV	1871927	2153226	40.17%	4.951%
20	18.786	2683	2686	2690	rVV2	2255552	2773966	51.76%	6.378%
21	18.821	2690	2692	2699	rVB2	180602	216194	4.03%	0.497%
22	18.921	2705	2709	2716	rVB	405900	472516	8.82%	1.086%
23	19.009	2721	2724	2735	rVB	41785	97875	1.83%	0.225%
24	19.392	2785	2789	2792	rBV	60660	68384	1.28%	0.157%
25	19.580	2815	2821	2830	rBV	4435303	5359691	100.00%	12.323%
26	20.850	3034	3037	3042	rBV3	153763	192338	3.59%	0.442%
27	21.150	3083	3088	3100	rBV2	913480	1311909	24.48%	3.016%
28	23.327	3452	3458	3466	rBV	568936	1094067	20.41%	2.516%

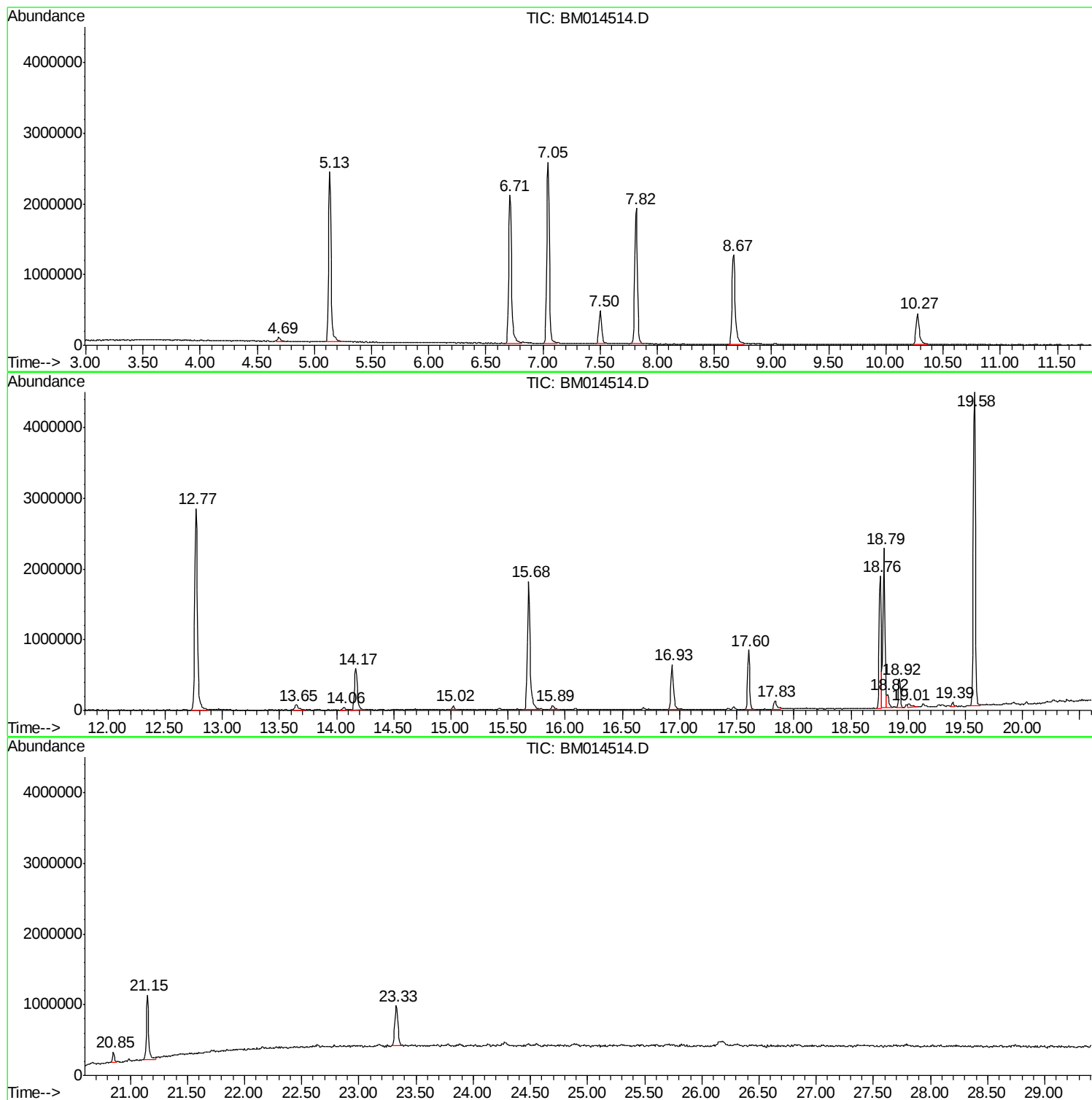
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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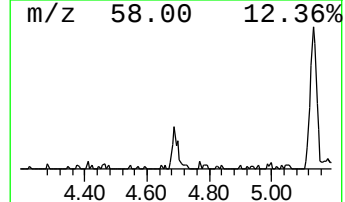
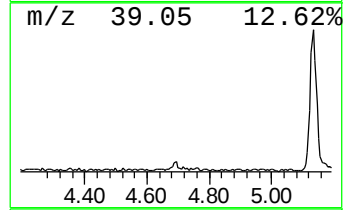
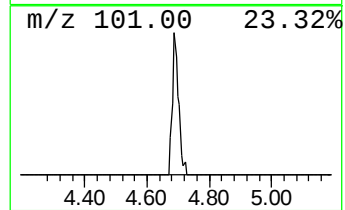
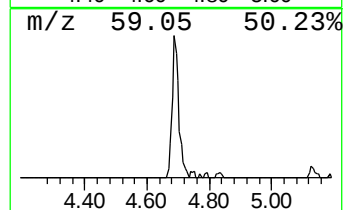
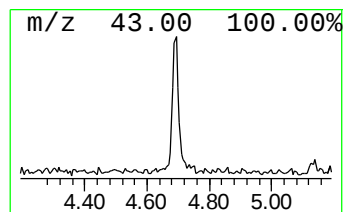
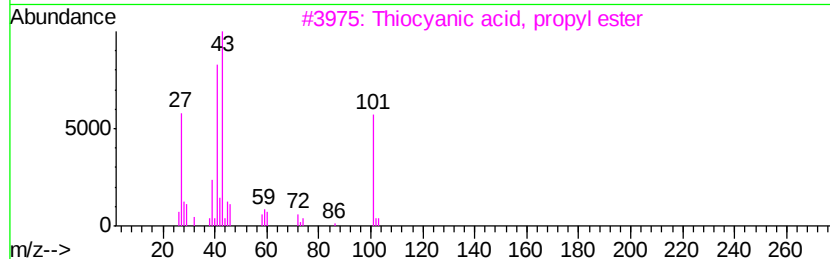
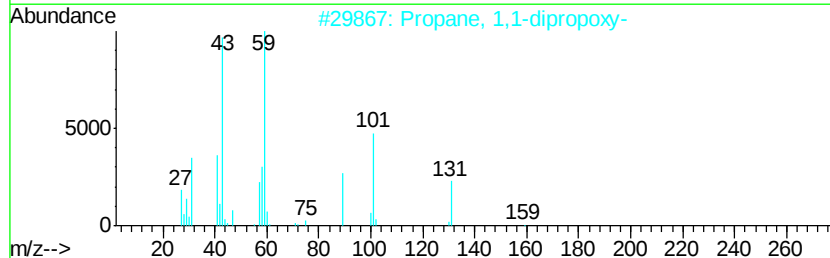
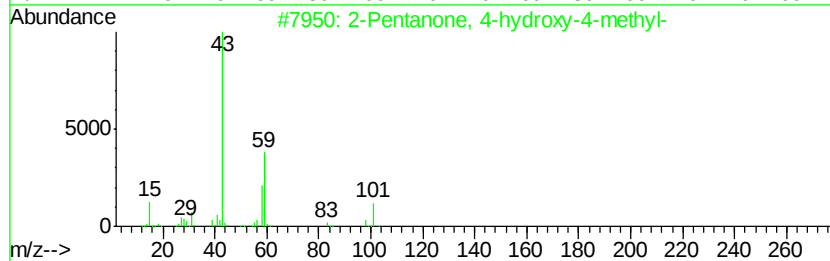
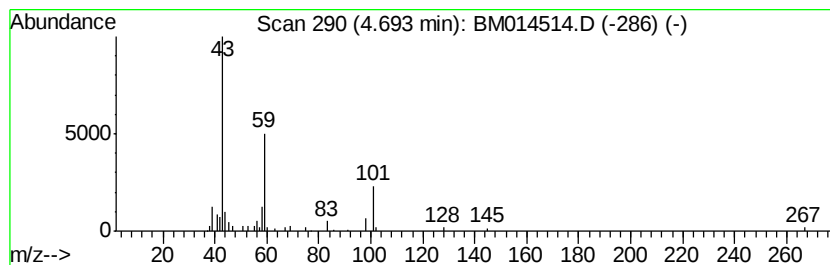
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.69	2.45 ng	95047	1,4-Dichlorobenzene-d4	7.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	39
3			Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
4			Guanidine	59	CH5N3	000113-00-8	9
5			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



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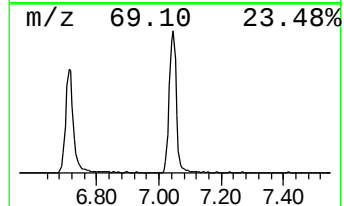
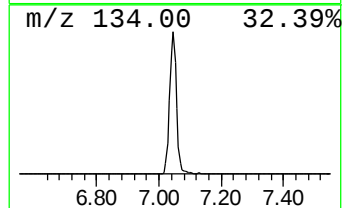
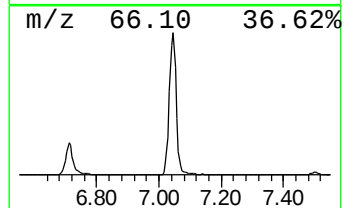
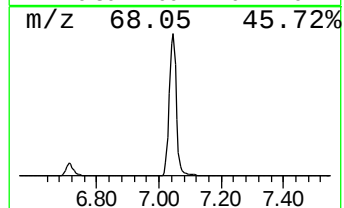
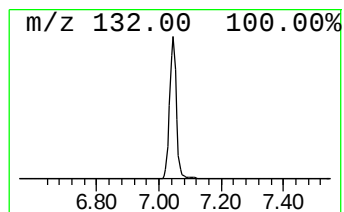
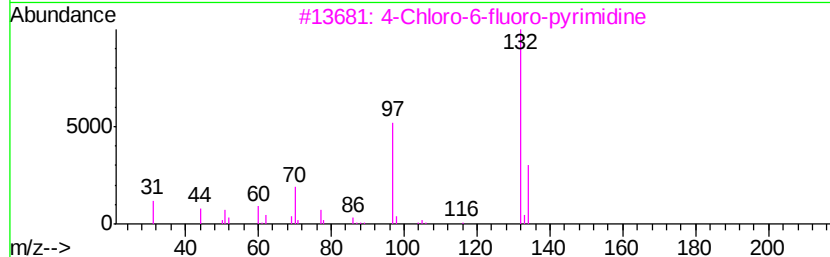
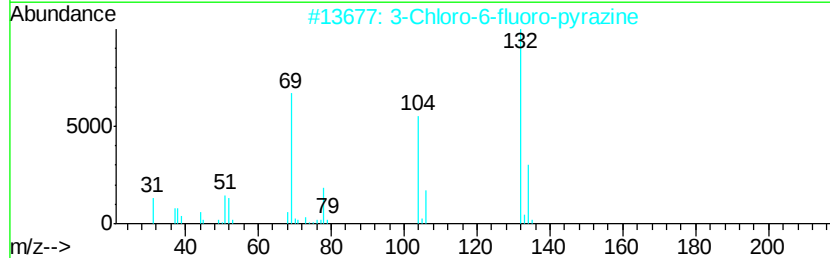
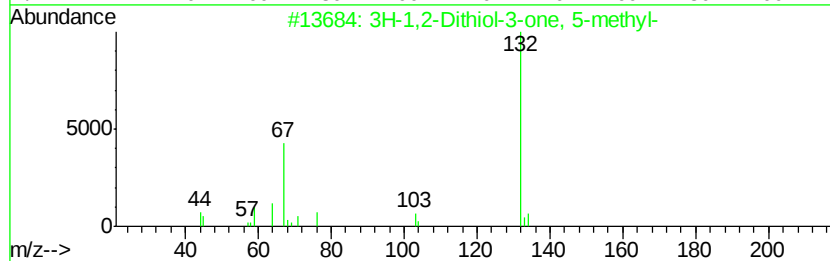
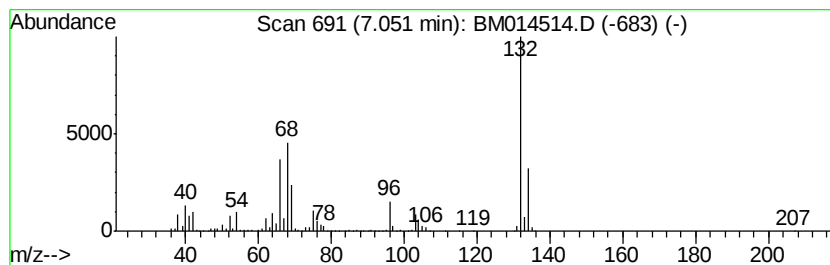
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Peak Number 2 unknown7.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	101.26 ng	3935630	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25



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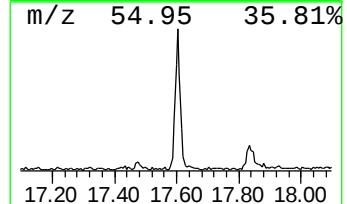
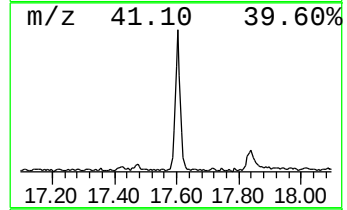
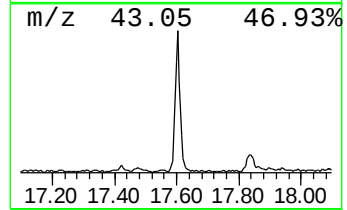
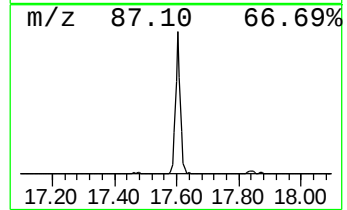
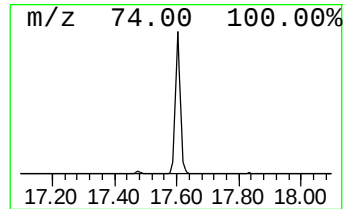
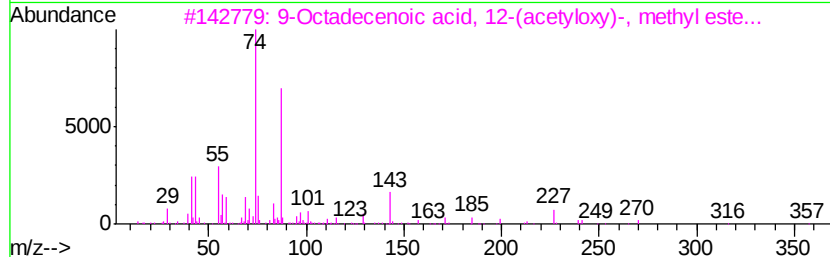
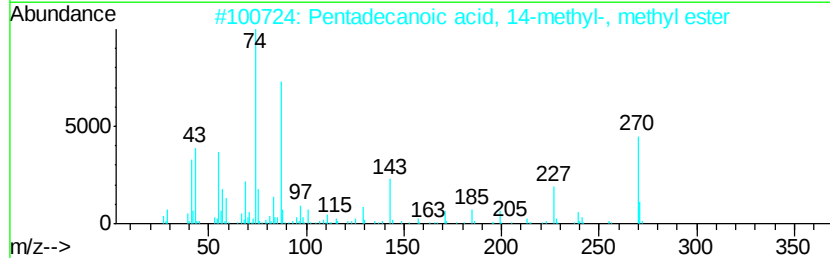
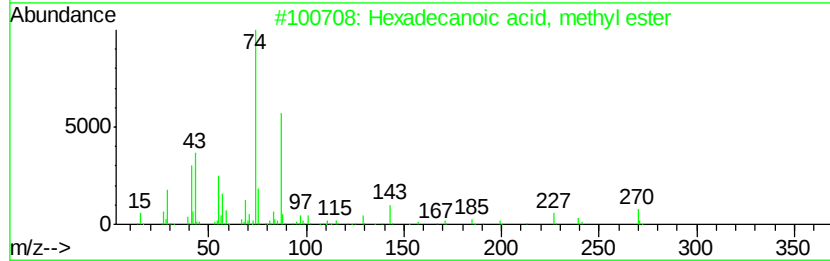
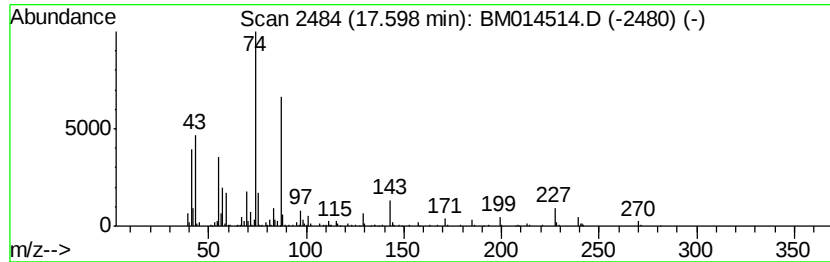
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.60	18.51 ng	977395	Phenanthrene-d10	16.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3		9-Octadecenoic acid, 12-(acetylo...	354	C21H38O4	000140-03-4	90
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	80
5		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80



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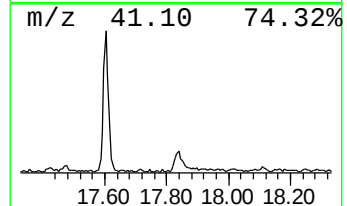
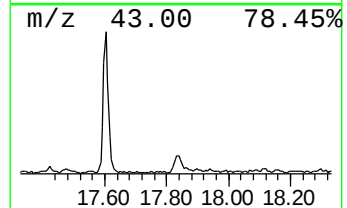
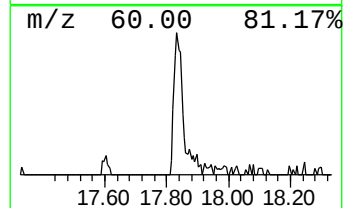
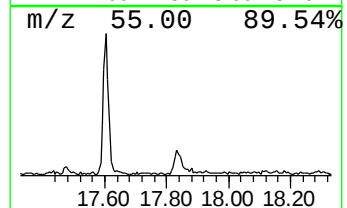
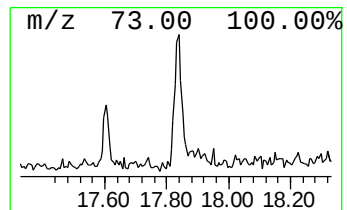
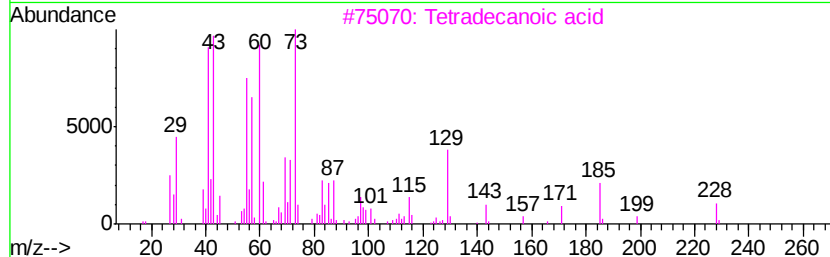
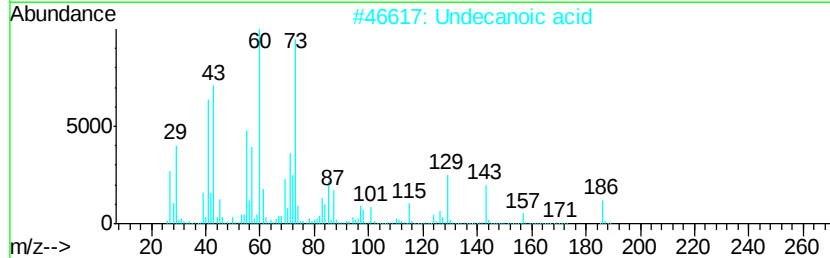
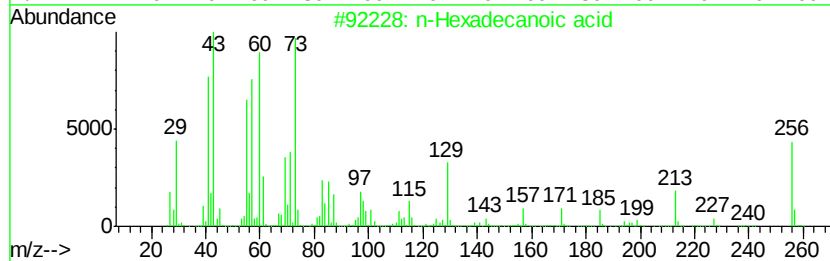
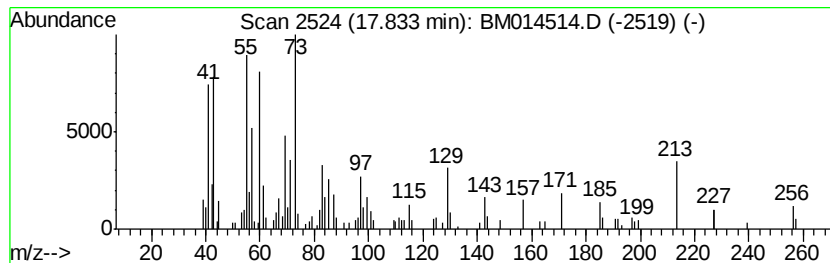
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.83	4.23 ng	223183	Phenanthrene-d10	16.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



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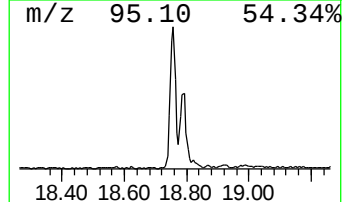
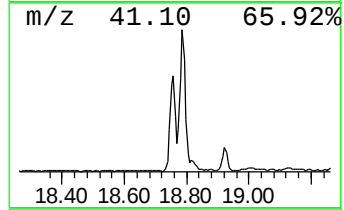
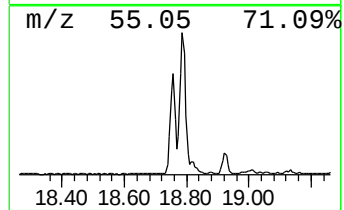
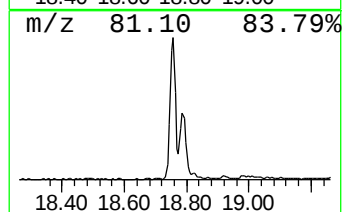
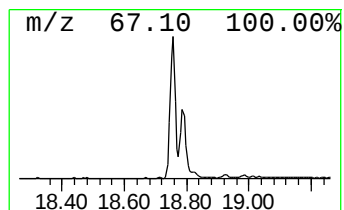
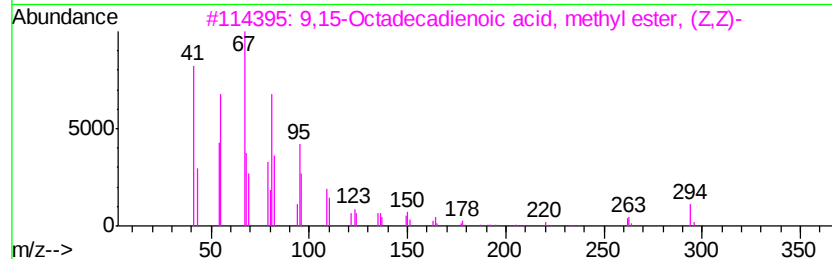
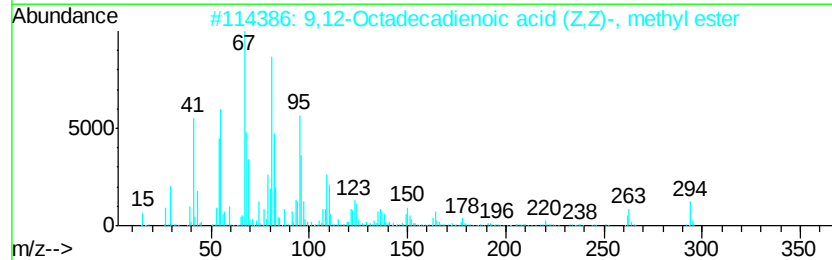
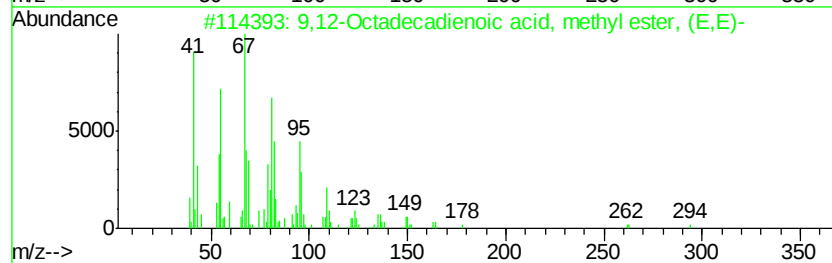
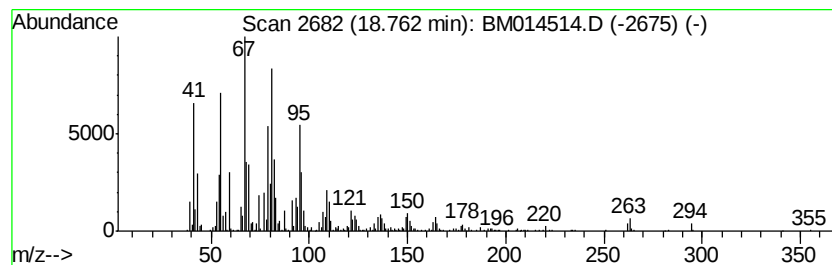
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Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.76	40.78 ng	2153230	Phenanthrene-d10	16.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	97
3		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	95
4		8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	95
5		9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	83



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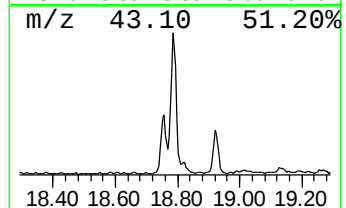
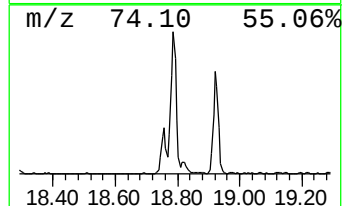
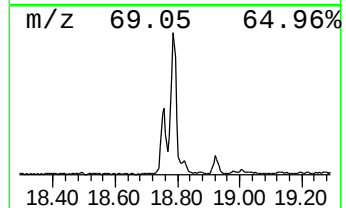
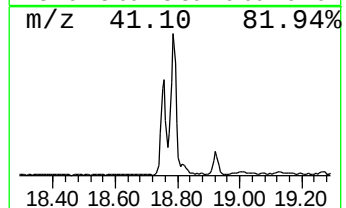
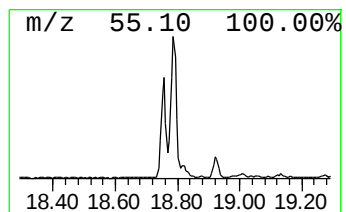
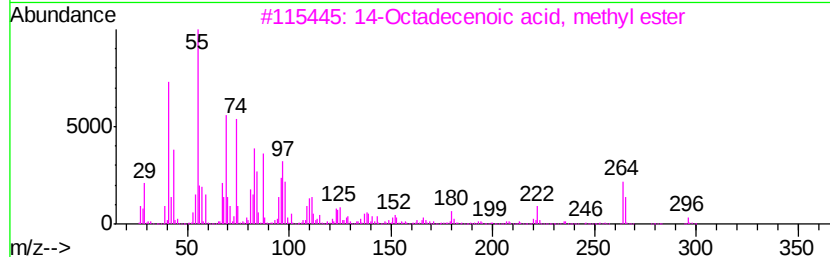
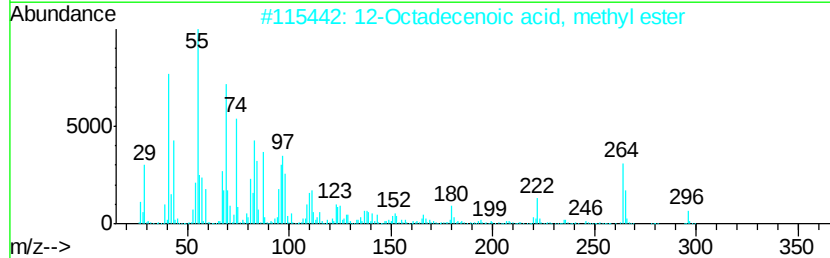
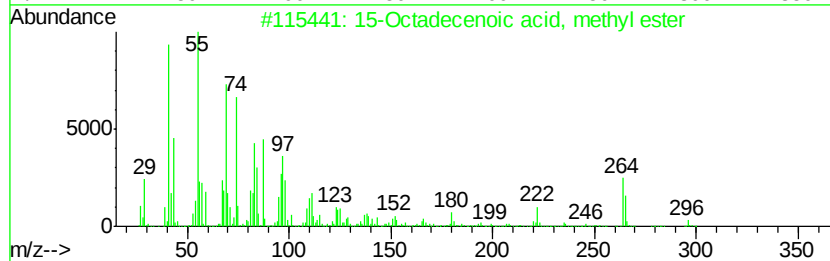
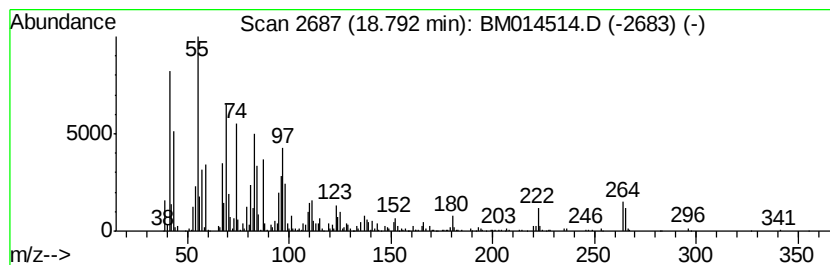
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 15-Octadecenoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.79	52.54 ng	2773970	Phenanthrene-d10	16.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
2		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	98
3		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	97
4		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	96
5		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	95



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA M\DATA\BM030718\
Data File : BM014514.D
Acq On : 07 Mar 2018 00:48
Operator : SJ/JU
Sample : J1699-77
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B24

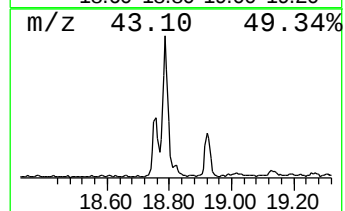
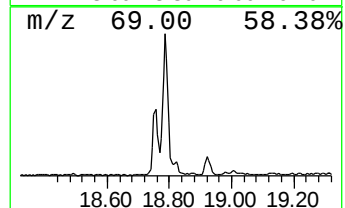
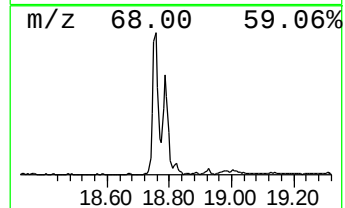
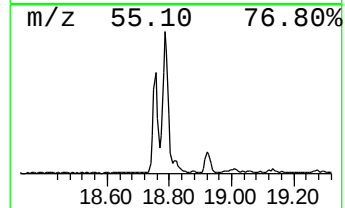
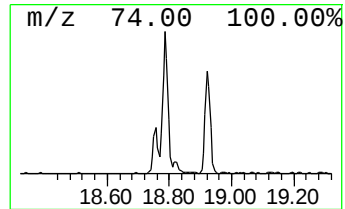
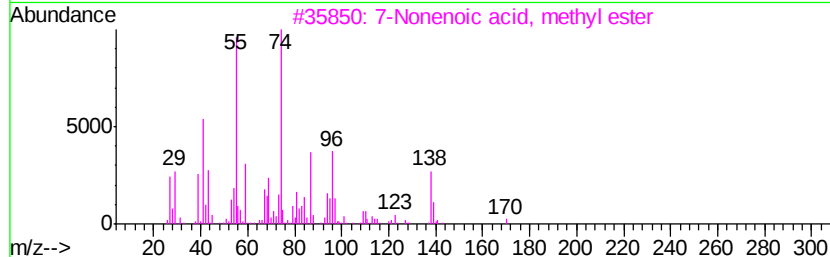
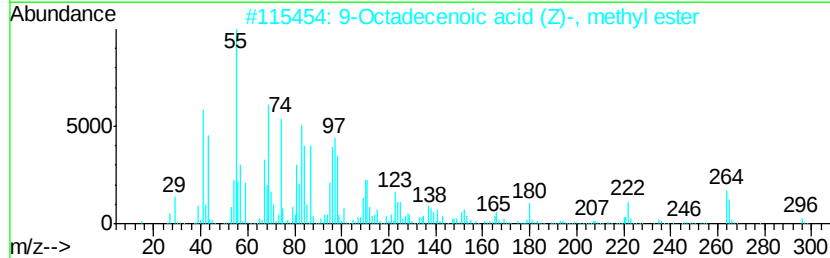
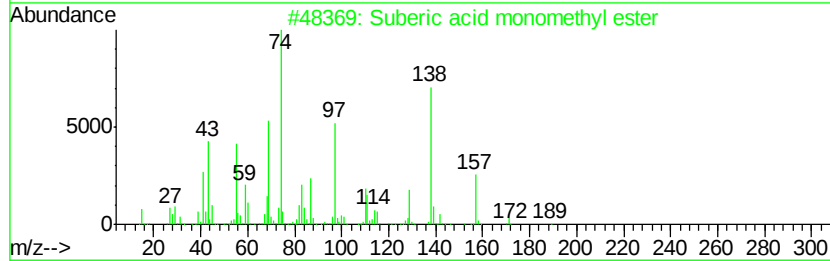
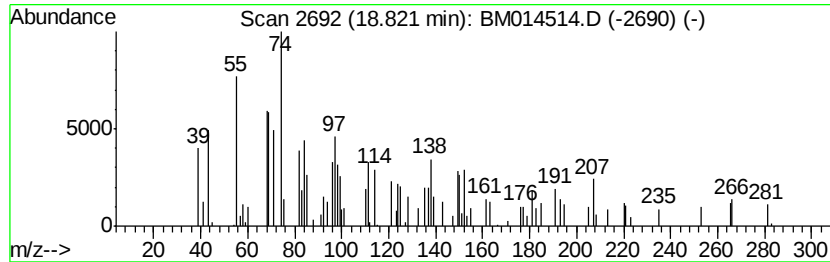
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.82 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.82	4.09 ng	216194	Phenanthrene-d10	16.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Suberic acid monomethyl ester	188	C9H16O4	003946-32-5	35
2		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	25
3		7-Nonenoic acid, methyl ester	170	C10H18O2	020731-22-0	22
4		7-Octynoic acid, methyl ester	154	C9H14O2	018458-50-9	14
5		Ricinoleic acid	298	C18H34O3	000141-22-0	12



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA M\DATA\BM030718\
Data File : BM014514.D
Acq On : 07 Mar 2018 00:48
Operator : SJ/JU
Sample : J1699-77
Misc :
ALS Vial : 16 Sample Multiplier: 1

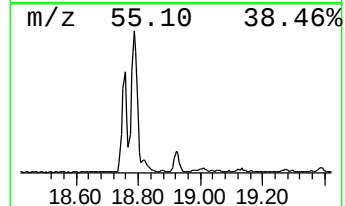
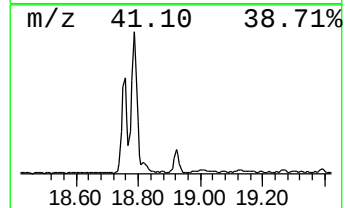
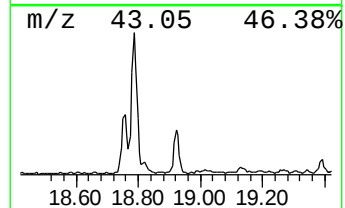
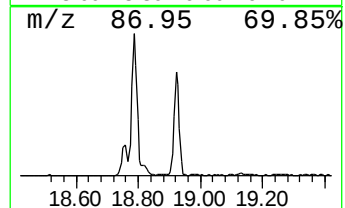
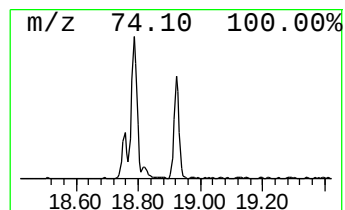
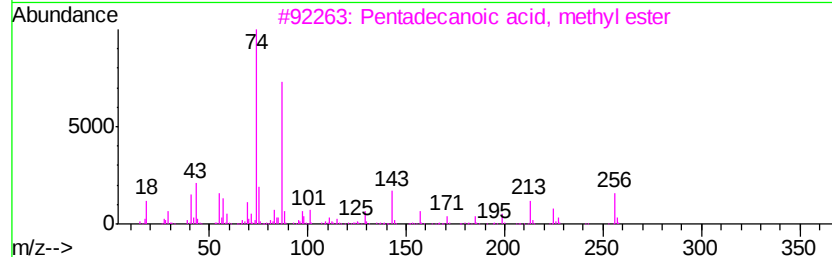
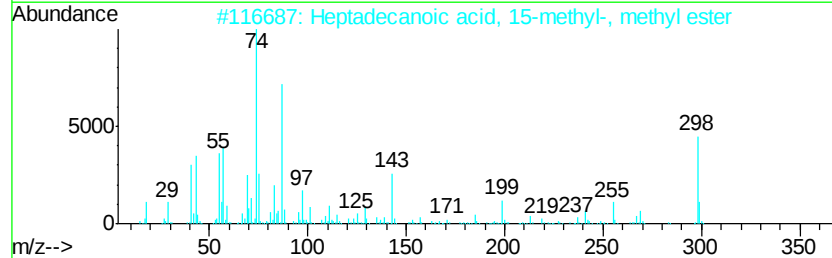
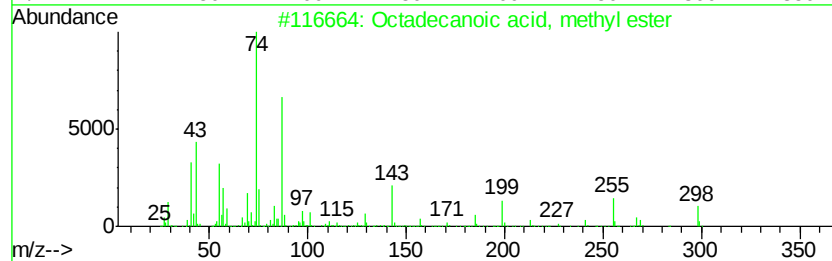
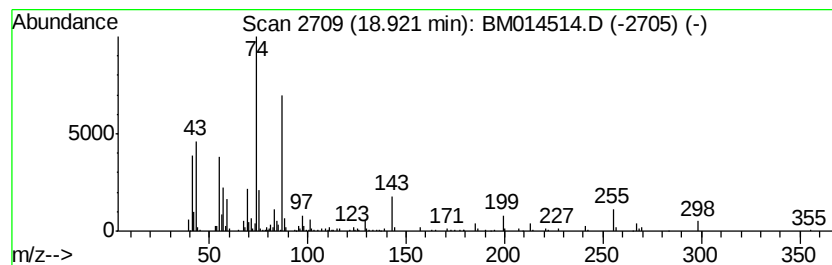
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.92	8.95 ng	472516	Phenanthrene-d10	16.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, methyl ester	298	C19H38O2	000112-61-8	94
2	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	90
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	86
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA M\DATA\BM030718\
Data File : BM014514.D
Acq On : 07 Mar 2018 00:48
Operator : SJ/JU
Sample : J1699-77
Misc :
ALS Vial : 16 Sample Multiplier: 1

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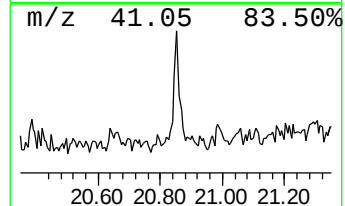
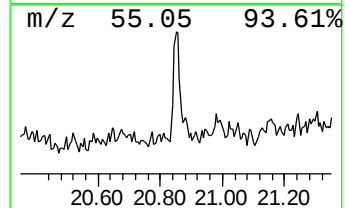
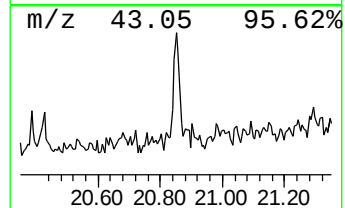
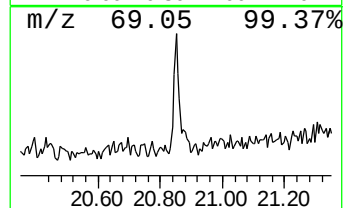
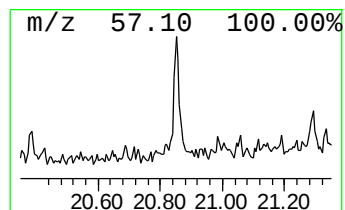
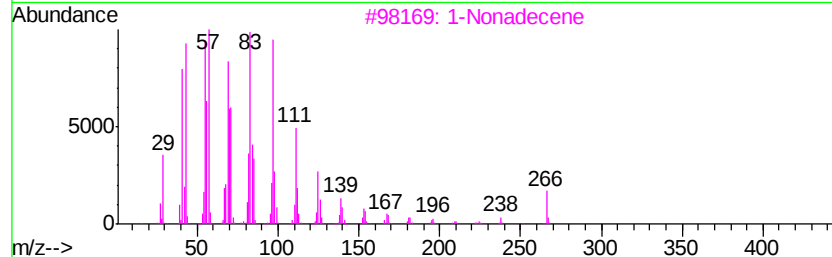
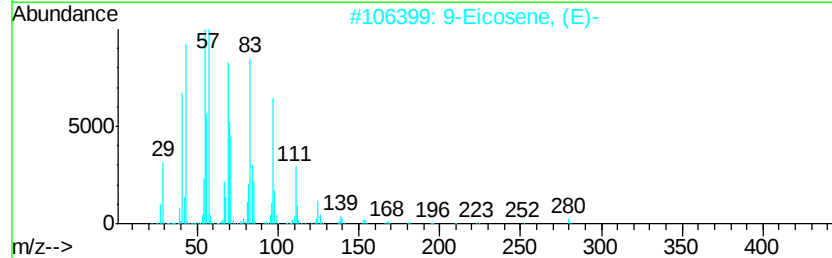
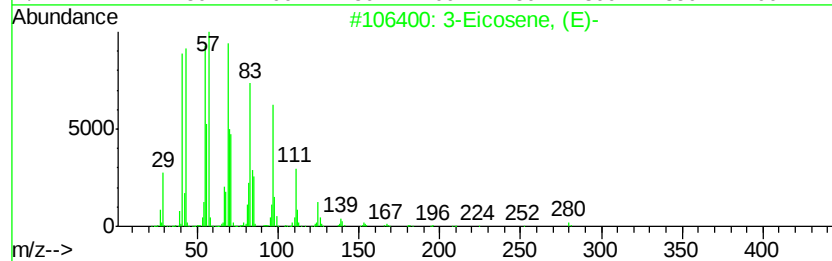
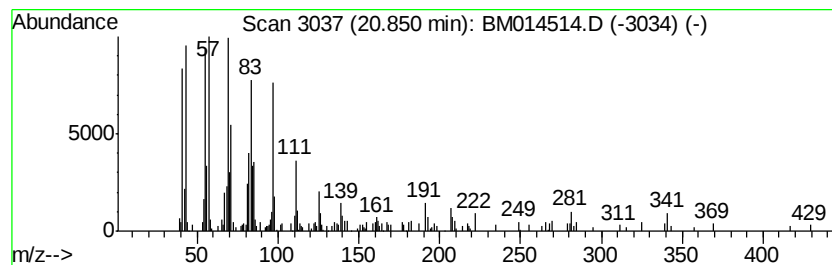
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 3-Eicosene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	2.93 ng	192338	Chrysene-d12	21.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3		1-Nonadecene	266	C19H38	018435-45-5	87
4		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87
5		1-Eicosene	280	C20H40	003452-07-1	83



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_M\DATA\BM030718\
Data File : BM014514.D
Acq On : 07 Mar 2018 00:48
Operator : SJ/JU
Sample : J1699-77
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.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...	4.69	2.5	ng	95047	1	7.50	777337	20.0
unknown7.05	7.05	101.3	ng	3935630	1	7.50	777337	20.0
Hexadecanoic acid...	17.60	18.5	ng	977395	4	16.93	1055930	20.0
n-Hexadecanoic acid	17.83	4.2	ng	223183	4	16.93	1055930	20.0
9,12-Octadecadien...	18.76	40.8	ng	2153230	4	16.93	1055930	20.0
15-Octadecenoic a...	18.79	52.5	ng	2773970	4	16.93	1055930	20.0
unknown18.82	18.82	4.1	ng	216194	4	16.93	1055930	20.0
Octadecanoic acid...	18.92	8.9	ng	472516	4	16.93	1055930	20.0
3-Eicosene, (E)-	20.85	2.9	ng	192338	5	21.15	1311910	20.0