

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA M\DATA\BM030718\
 Data File : BM014507.D
 Acq On : 06 Mar 2018 20:36
 Operator : SJ/JU
 Sample : J1699-49
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B16

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:\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	5.134	360	365	382	rBV	1156511	1841732	4.37%	1.665%
2	6.710	627	633	648	rBV	979020	1842911	4.38%	1.666%
3	7.045	683	690	697	rBV	1265466	1992063	4.73%	1.801%
4	7.504	762	768	778	rVB	411967	681885	1.62%	0.616%
5	7.816	814	821	834	rVB	989608	1624776	3.86%	1.469%
6	8.669	959	966	981	rBV	620570	1280112	3.04%	1.157%
7	10.275	1232	1239	1251	rBV	441726	850973	2.02%	0.769%
8	12.769	1654	1663	1680	rBV	1562379	2651206	6.30%	2.397%
9	14.168	1895	1901	1911	rBV2	613305	992997	2.36%	0.898%
10	15.680	2152	2158	2177	rBV	1086227	1793836	4.26%	1.622%
11	16.933	2365	2371	2382	rBV2	705661	1071443	2.54%	0.969%
12	17.474	2459	2463	2469	rVB	478399	565827	1.34%	0.511%
13	17.609	2480	2486	2492	rBV	12278966	13392021	31.80%	12.106%
14	17.839	2520	2525	2532	rBV	311326	484908	1.15%	0.438%
15	17.903	2532	2536	2542	rVB	359872	455073	1.08%	0.411%
16	18.762	2676	2682	2685	rBV	20094674	25572163	60.72%	23.116%
17	18.803	2685	2689	2699	rVB	34867352	42112633	100.00%	38.068%
18	18.927	2705	2710	2717	rVB	5069264	5544184	13.17%	5.012%
19	19.580	2816	2821	2827	rVB	2172093	2736356	6.50%	2.474%
20	19.921	2876	2879	2887	rVB2	396083	630928	1.50%	0.570%
21	20.656	2998	3004	3013	rBV8	178167	447342	1.06%	0.404%
22	21.150	3083	3088	3093	rBV	851515	1087919	2.58%	0.983%
23	23.327	3453	3458	3466	rVB	518449	970632	2.30%	0.877%

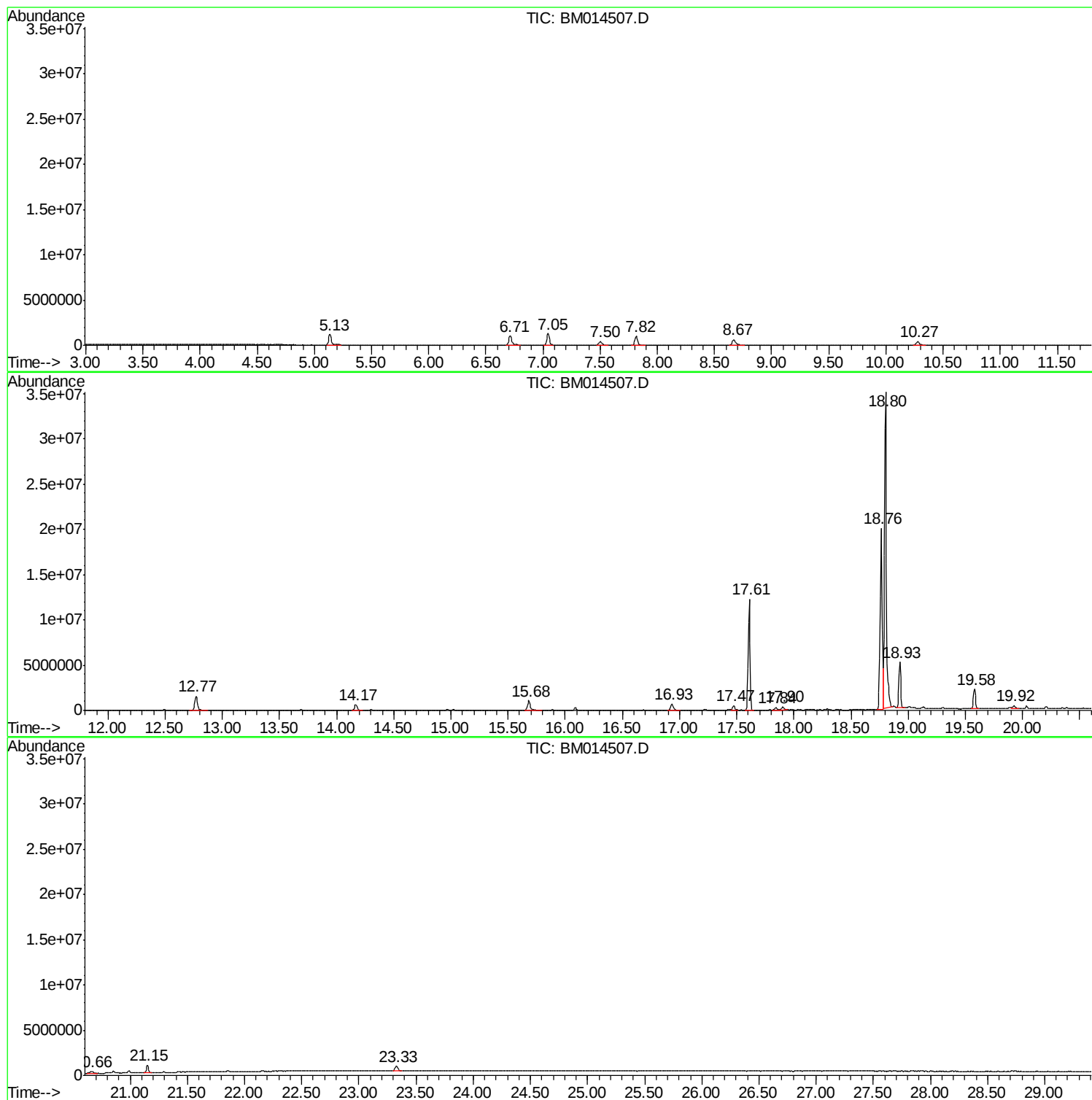
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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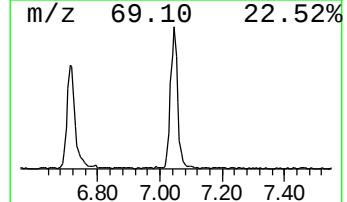
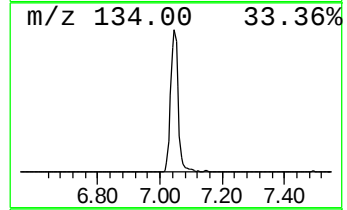
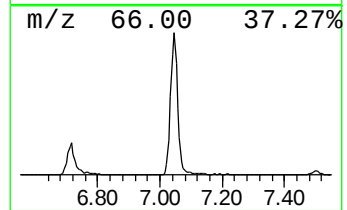
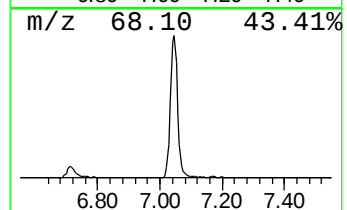
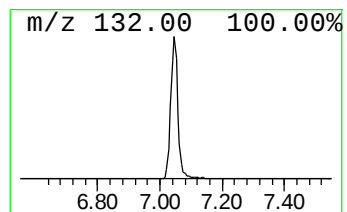
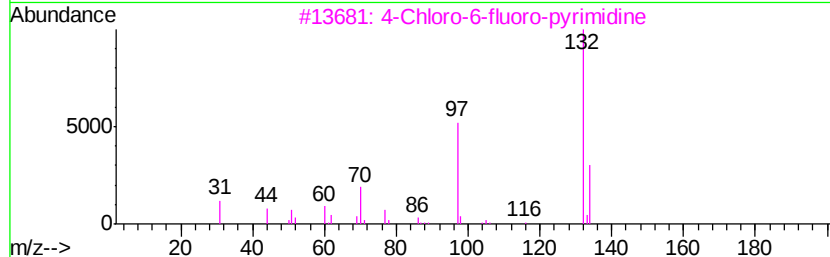
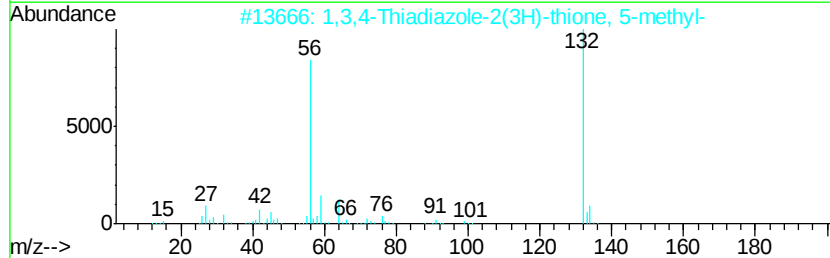
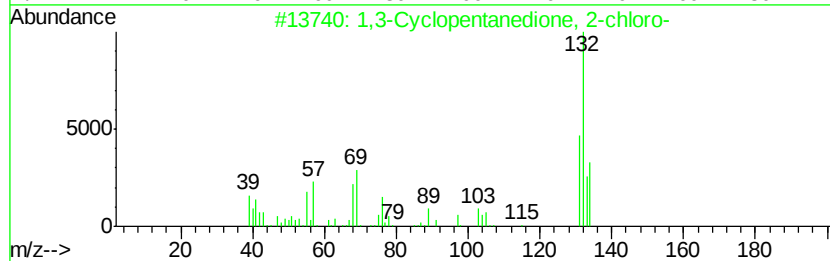
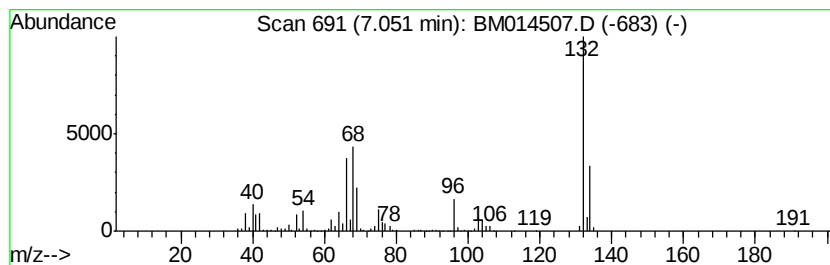
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.05 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	58.43 ng	1992060	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	11
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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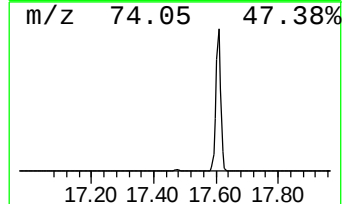
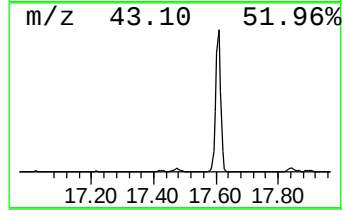
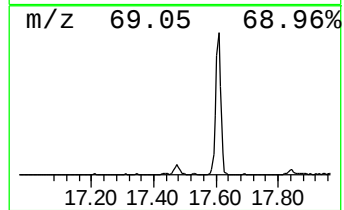
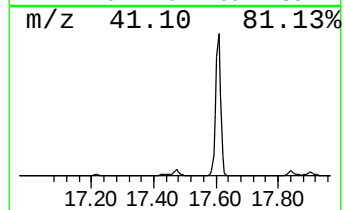
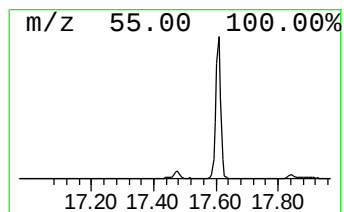
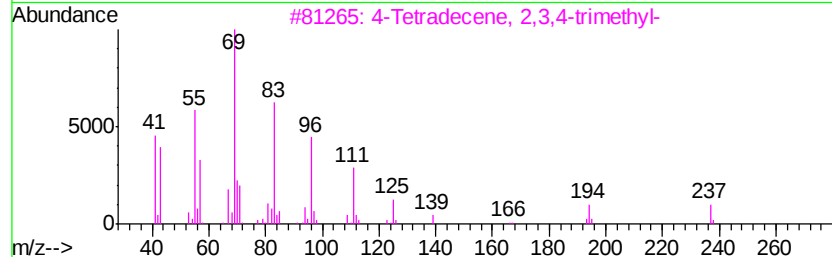
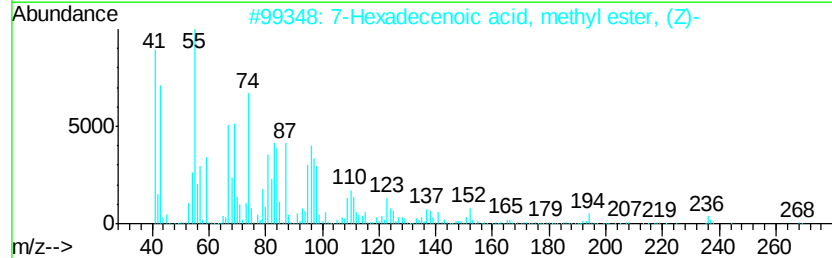
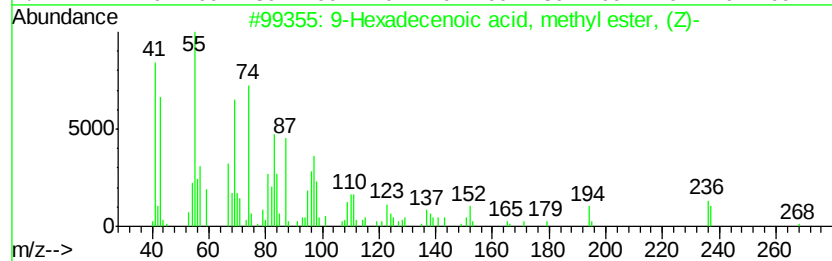
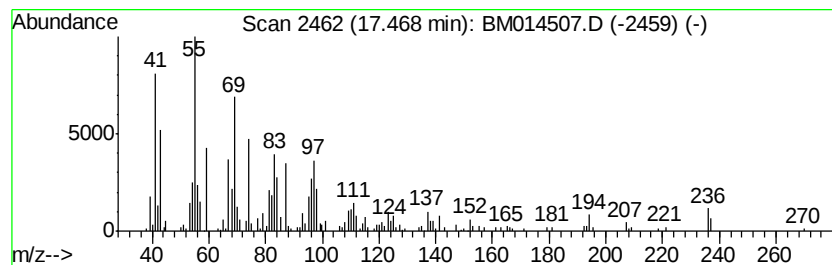
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TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Hexadecenoic acid, methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.47	10.56 ng	565827	Phenanthrene-d10	16.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	91	
2	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	86	
3	4-Tetradecene, 2,3,4-trimethyl-	238	C17H34	055103-81-6	74	
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	52	
5	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	50	



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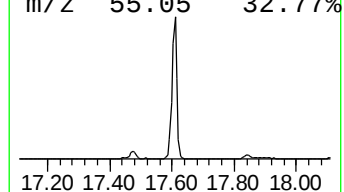
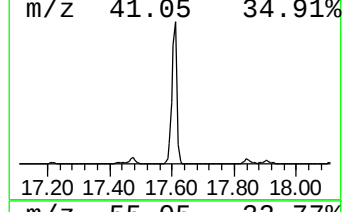
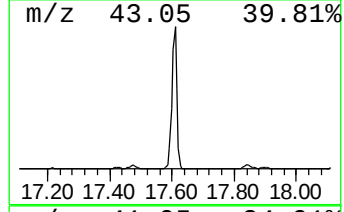
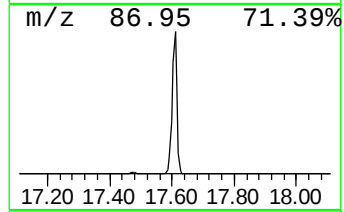
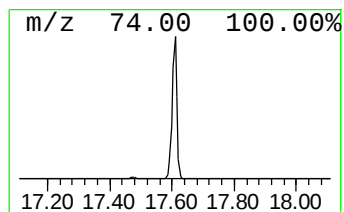
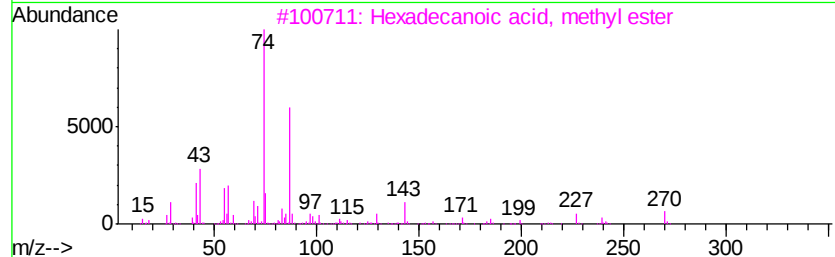
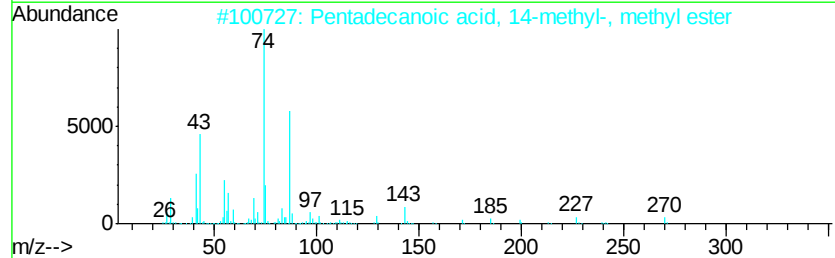
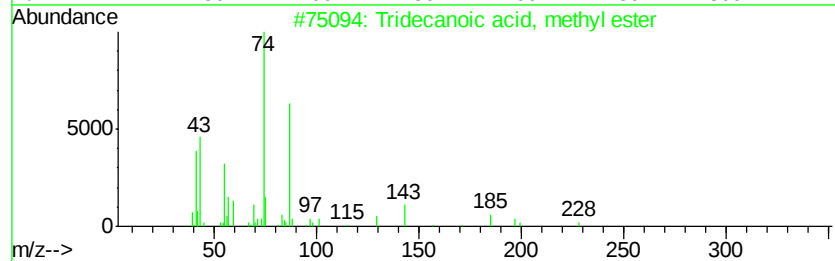
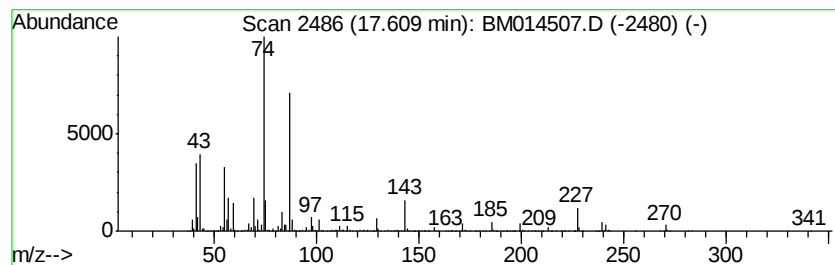
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Peak Number 4 Tridecanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.61	249.98 ng	13392000	Phenanthrene-d10	16.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	96
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
5		9-Octadecenoic acid, 12-(acetylo...	354	C21H38O4	000140-03-4	91



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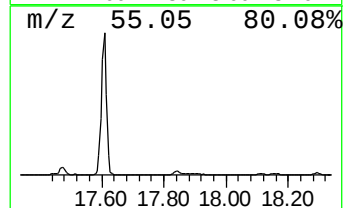
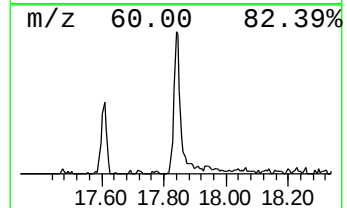
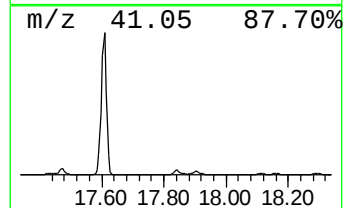
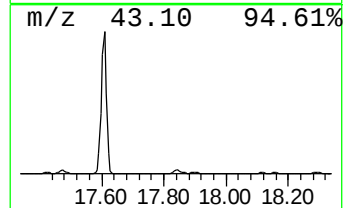
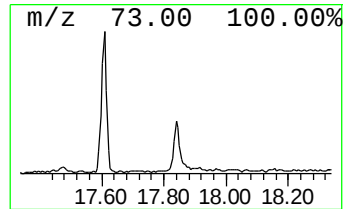
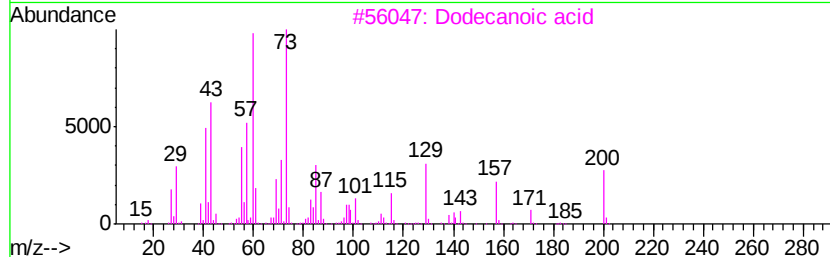
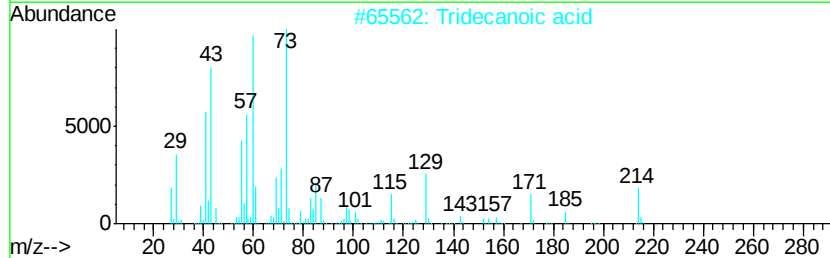
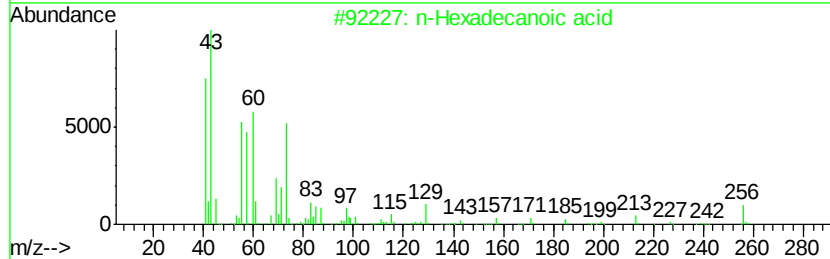
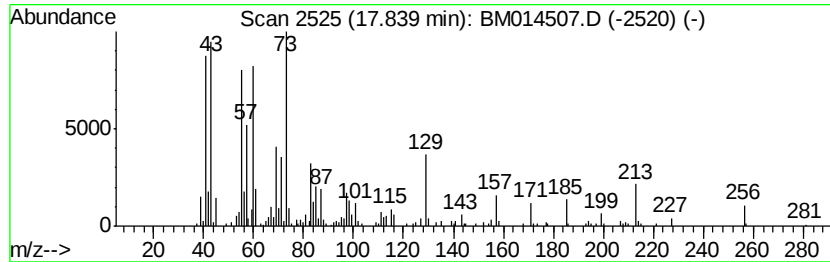
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	9.05 ng	484908	Phenanthrene-d10	16.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Dodecanoic acid	200	C12H24O2	000143-07-7	59
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	53



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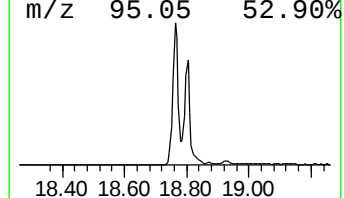
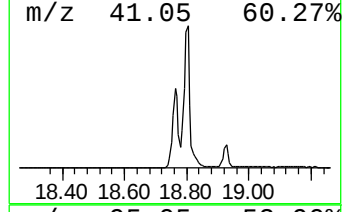
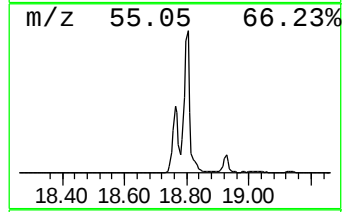
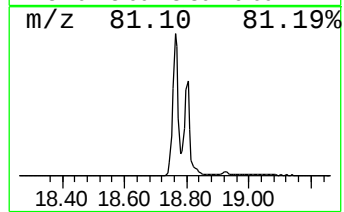
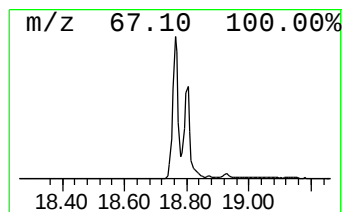
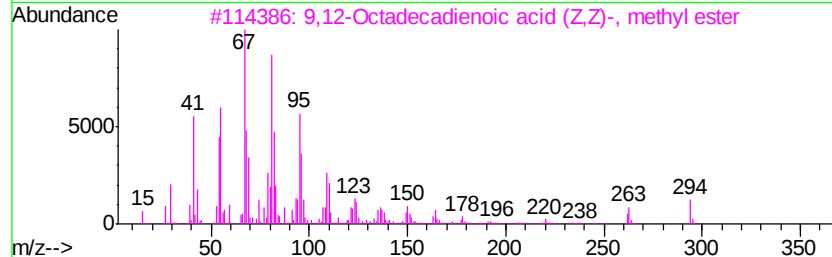
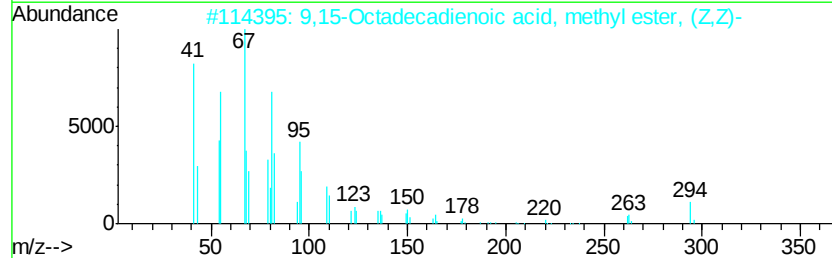
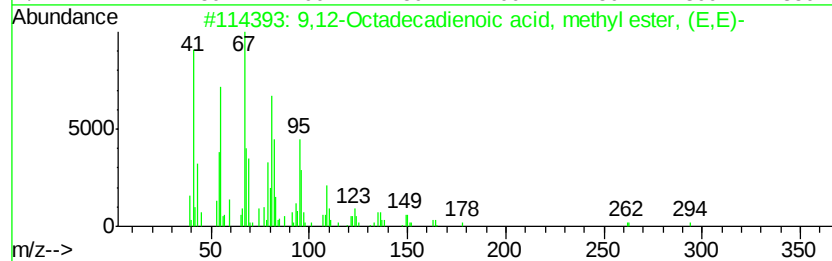
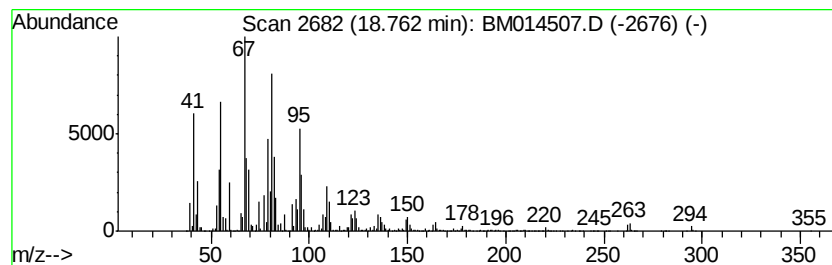
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.76	477.34 ng	25572200	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		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	97
4		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	95
5		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	90



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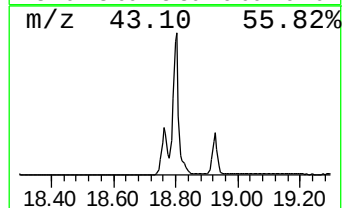
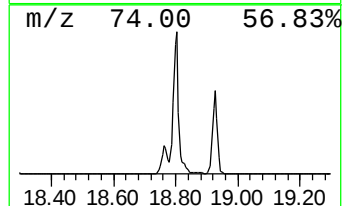
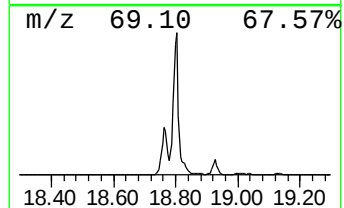
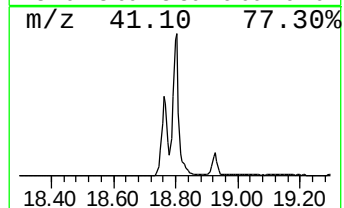
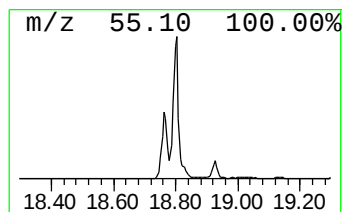
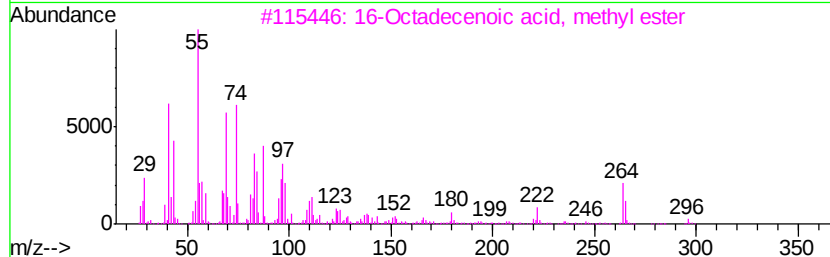
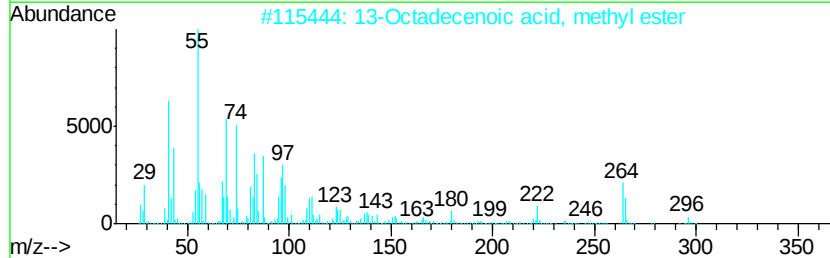
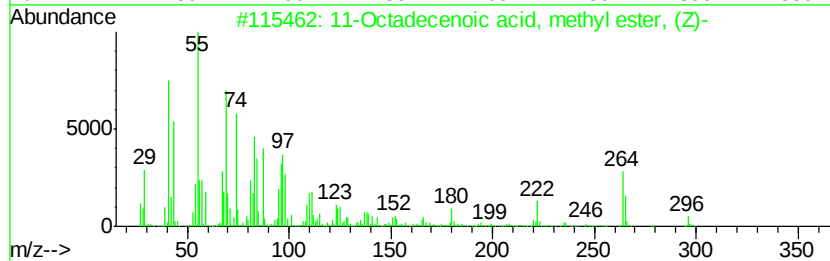
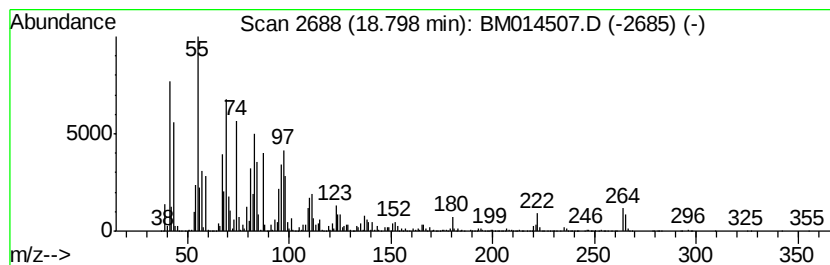
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11-Octadecenoic acid, methyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.80	786.09 ng	42112600	Phenanthrene-d10	16.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	11-Octadecenoic acid, methyl ester	296	C19H36O2	001937-63-9	99
2		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
4		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
5		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA M\DATA\BM030718\
Data File : BM014507.D
Acq On : 06 Mar 2018 20:36
Operator : SJ/JU
Sample : J1699-49
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B16

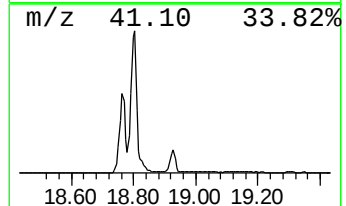
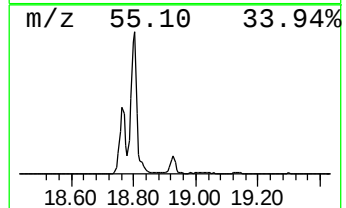
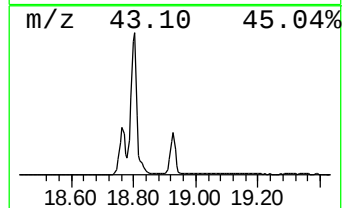
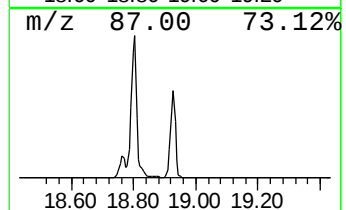
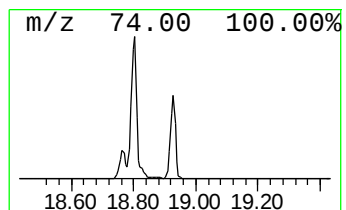
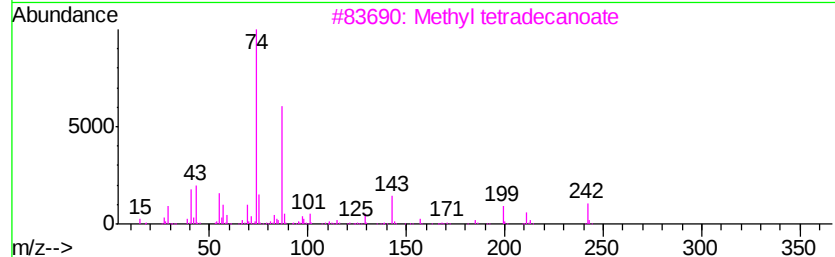
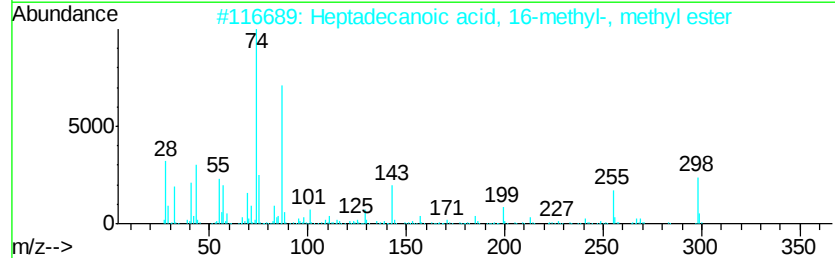
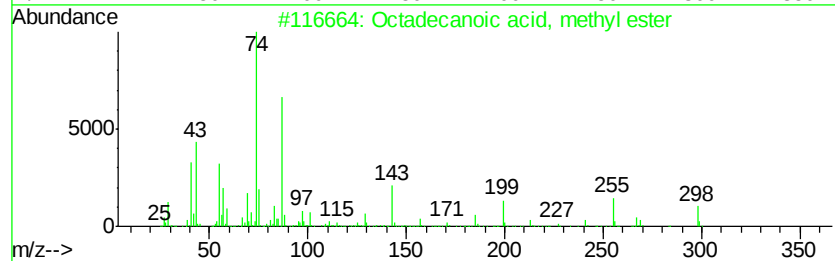
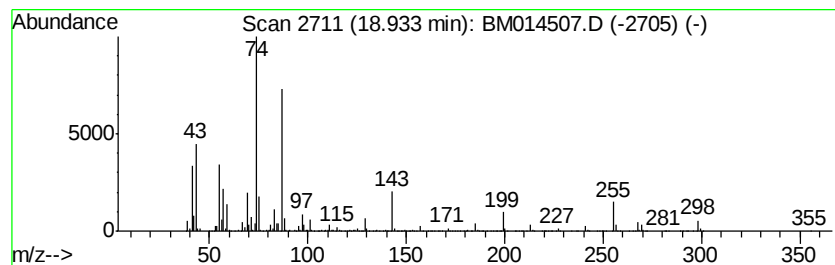
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.93	103.49 ng	5544180	Phenanthrene-d10	16.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, methyl ester	298	C19H38O2	000112-61-8	91
2		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
3		Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4		Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86
5		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA M\DATA\BM030718\
Data File : BM014507.D
Acq On : 06 Mar 2018 20:36
Operator : SJ/JU
Sample : J1699-49
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B16

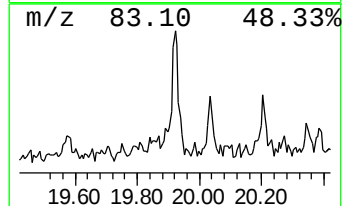
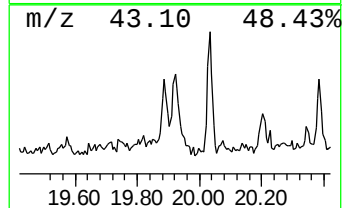
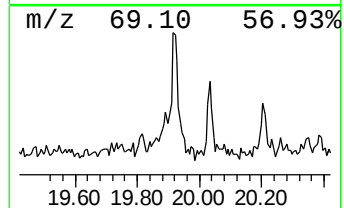
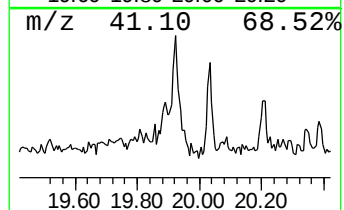
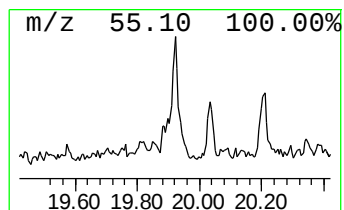
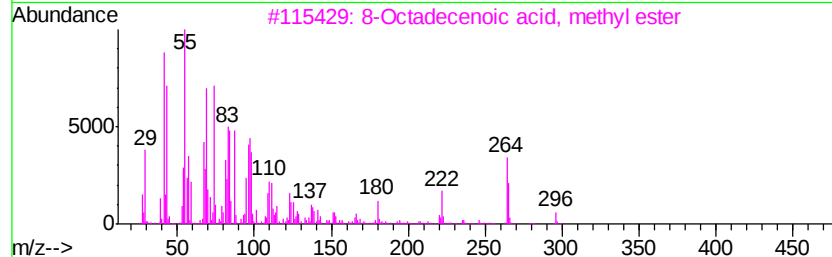
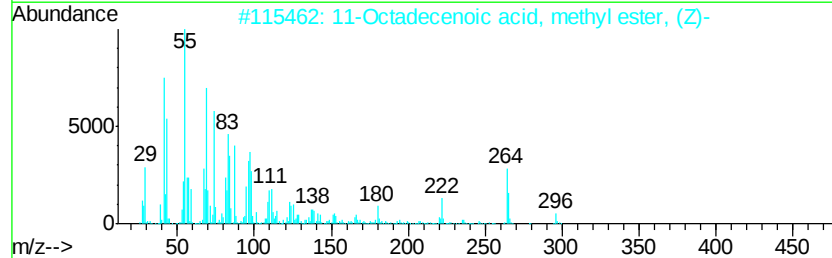
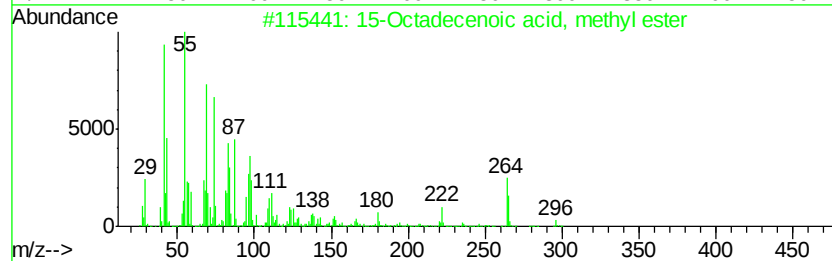
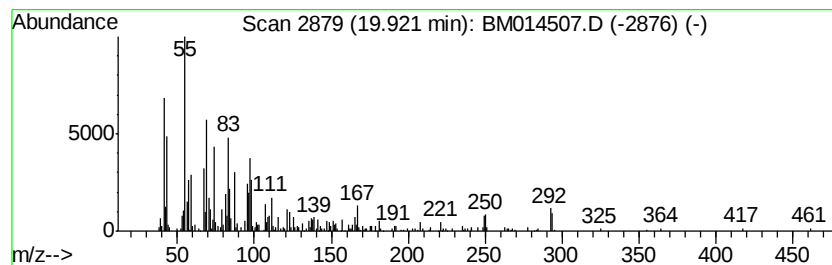
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 15-Octadecenoic acid, methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.92	11.60 ng	630928	Chrysene-d12	21.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	53
2		11-Octadecenoic acid, methyl ester...	296	C19H36O2	001937-63-9	50
3		8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	50
4		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	50
5		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	50



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA M\DATA\BM030718\
Data File : BM014507.D
Acq On : 06 Mar 2018 20:36
Operator : SJ/JU
Sample : J1699-49
Misc :
ALS Vial : 9 Sample Multiplier: 1

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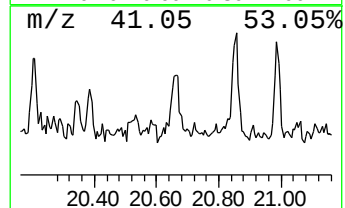
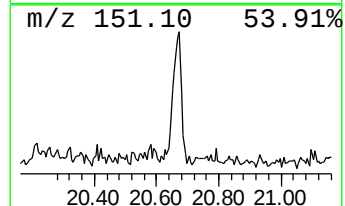
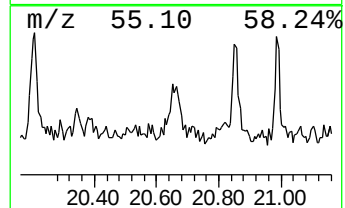
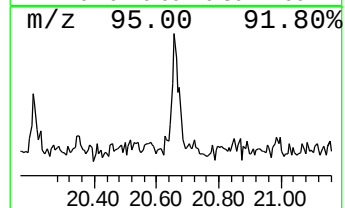
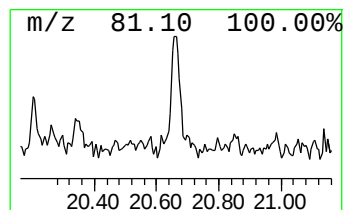
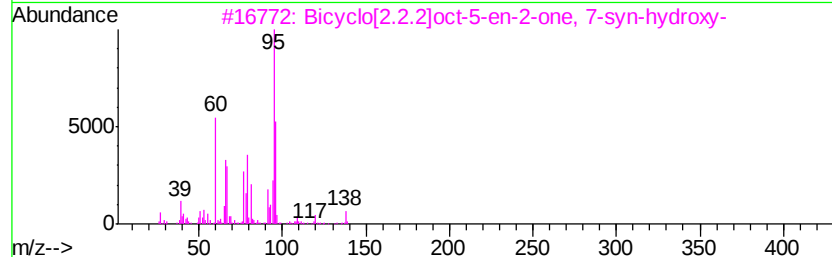
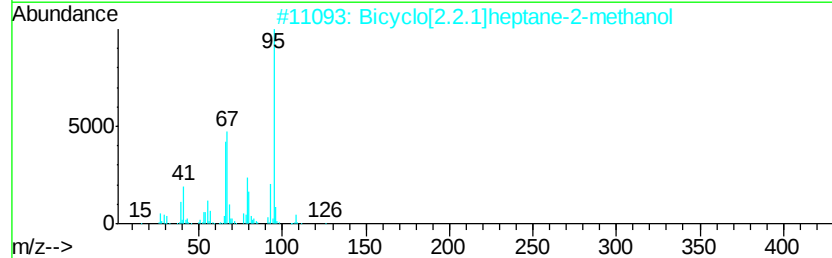
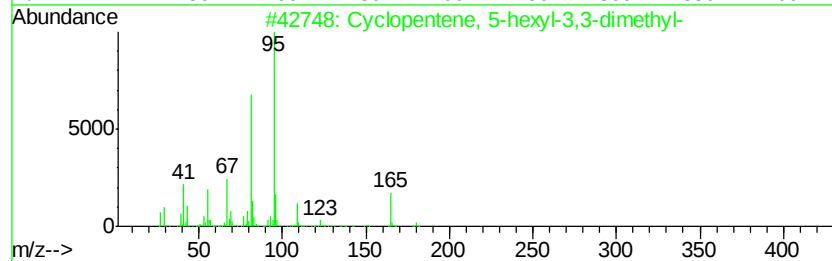
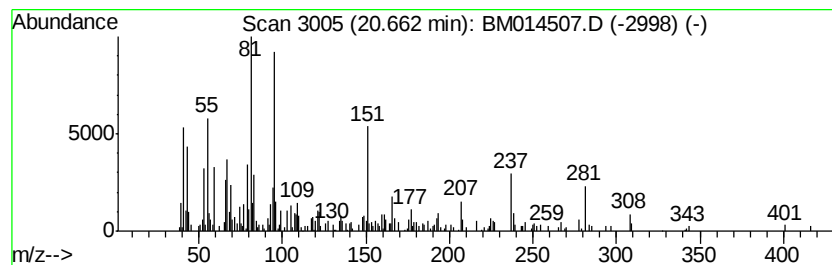
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown20.66 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.66	8.22 ng	447342	Chrysene-d12	21.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentene, 5-hexyl-3,3-dimethyl-	180	C13H24	061142-66-3	38
2		Bicyclo[2.2.1]heptane-2-methanol	126	C8H14O	005240-72-2	35
3		Bicyclo[2.2.2]oct-5-en-2-one, 7-...	138	C8H10O2	1000153-14-9	35
4		Tricyclo[4.3.1.1(3,8)]undecan-3-ol	166	C11H18O	014504-80-4	25
5		3-(2-Hydroxycyclohexyl)-furan	166	C10H14O2	118959-04-9	22



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_M\DATA\BM030718\
Data File : BM014507.D
Acq On : 06 Mar 2018 20:36
Operator : SJ/JU
Sample : J1699-49
Misc :
ALS Vial : 9 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
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9-Hexadecenoic ac...	17.47	10.6	ng	565827	4	16.93	1071440	20.0
Tridecanoic acid,...	17.61	250.0	ng	13392000	4	16.93	1071440	20.0
n-Hexadecanoic acid	17.84	9.1	ng	484908	4	16.93	1071440	20.0
9,12-Octadecadien...	18.76	477.3	ng	25572200	4	16.93	1071440	20.0
11-Octadecenoic a...	18.80	786.1	ng	42112600	4	16.93	1071440	20.0
Octadecanoic acid...	18.93	103.5	ng	5544180	4	16.93	1071440	20.0
15-Octadecenoic a...	19.92	11.6	ng	630928	5	21.15	1087920	20.0
unknown20.66	20.66	8.2	ng	447342	5	21.15	1087920	20.0