

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
 Data File : BM017909.D
 Acq On : 04 Dec 2018 19:10
 Operator : JU/SJ
 Sample : J5761-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 AU-06-112918

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-BM111218.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	4.769	296	303	311	rBV	146382	218752	2.98%	0.281%
2	5.210	371	378	390	rBV	3654545	5310036	72.39%	6.822%
3	6.775	636	644	658	rBV	3256799	5592008	76.24%	7.184%
4	7.122	696	703	714	rBV	3849912	5844630	79.68%	7.509%
5	7.581	772	781	789	rBV	1099780	1744358	23.78%	2.241%
6	7.893	827	834	843	rVB	2738529	4474021	60.99%	5.748%
7	8.740	969	978	995	rBV	1952963	3476209	47.39%	4.466%
8	10.351	1241	1252	1259	rBV	1260485	2223139	30.31%	2.856%
9	12.839	1668	1675	1684	rBV	4183523	6144760	83.77%	7.894%
10	13.692	1815	1820	1828	rBV	256384	435085	5.93%	0.559%
11	14.227	1902	1911	1919	rVV2	1559361	2422122	33.02%	3.112%
12	14.363	1930	1934	1942	rVB	50673	77348	1.05%	0.099%
13	15.727	2160	2166	2175	rBV	2997770	4429649	60.39%	5.691%
14	15.980	2201	2209	2217	rBV	97007	224387	3.06%	0.288%
15	16.804	2346	2349	2359	rVB2	66417	111471	1.52%	0.143%
16	16.986	2374	2380	2384	rBV	1730630	2386769	32.54%	3.066%
17	17.027	2384	2387	2393	rVB	217634	302808	4.13%	0.389%
18	17.539	2471	2474	2481	rVB7	58766	80681	1.10%	0.104%
19	17.668	2491	2496	2501	rBV	1703775	2042735	27.85%	2.624%
20	17.898	2530	2535	2544	rBV	841459	1206284	16.45%	1.550%
21	18.821	2687	2692	2694	rBV	4111669	5055714	68.92%	6.495%
22	18.851	2694	2697	2708	rVB2	5118228	7335210	100.00%	9.424%
23	18.986	2716	2720	2726	rBV	849580	966458	13.18%	1.242%
24	19.057	2727	2732	2737	rVV	577094	921082	12.56%	1.183%
25	19.109	2738	2741	2747	rVB	453479	568959	7.76%	0.731%
26	19.186	2750	2754	2767	rVV2	342345	499976	6.82%	0.642%
27	19.415	2790	2793	2798	rVB	408195	527250	7.19%	0.677%
28	19.633	2825	2830	2836	rVB	4790188	5964500	81.31%	7.663%
29	20.915	3044	3048	3055	rBV	800401	1036363	14.13%	1.331%
30	21.192	3090	3095	3099	rBV	2165761	2980262	40.63%	3.829%
31	22.721	3352	3355	3361	rBV3	372435	570495	7.78%	0.733%
32	23.380	3461	3467	3473	rBV2	1471758	2662687	36.30%	3.421%

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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

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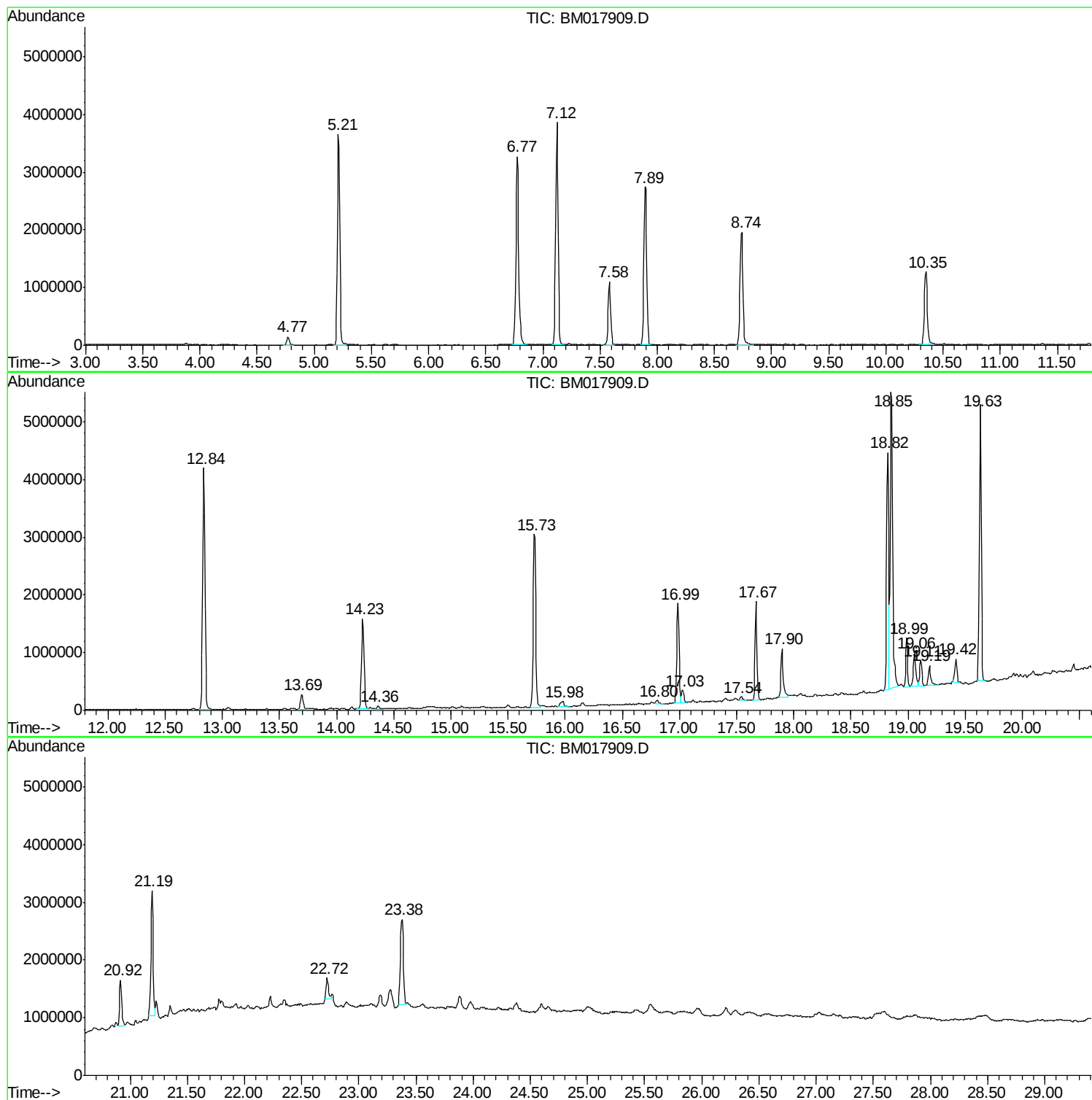
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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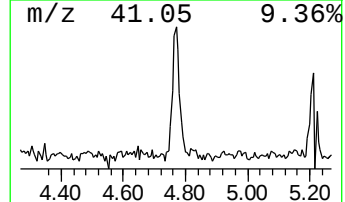
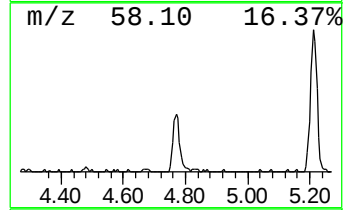
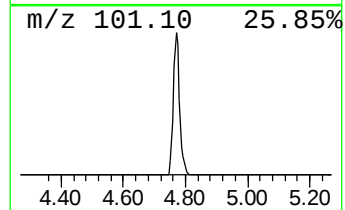
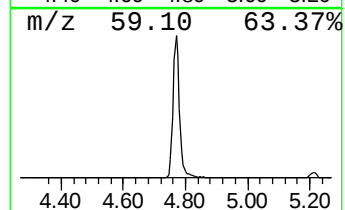
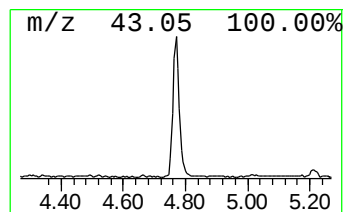
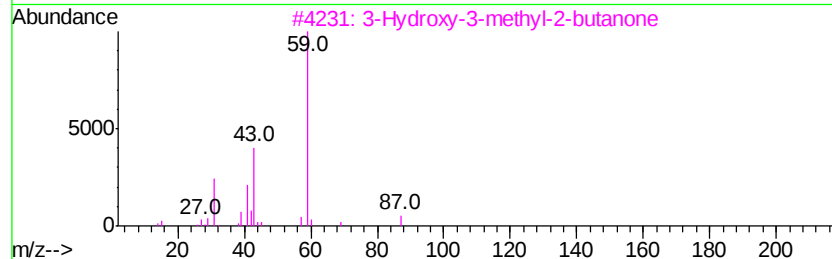
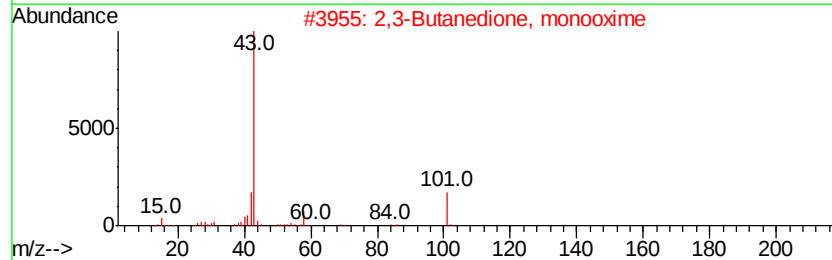
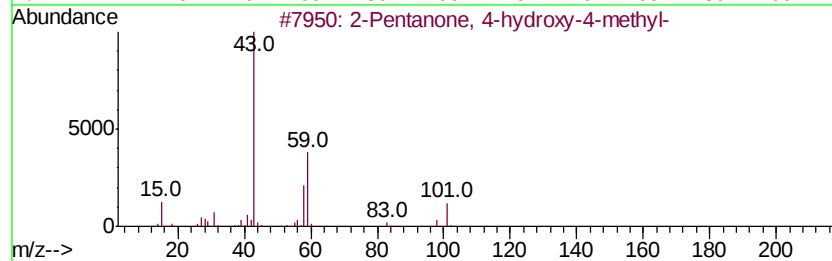
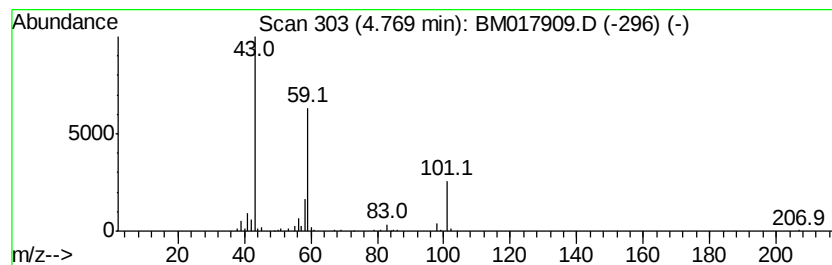
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	2.51 ng	218752	1,4-Dichlorobenzene-d4	7.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4			4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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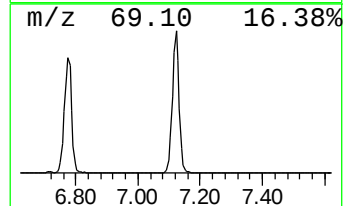
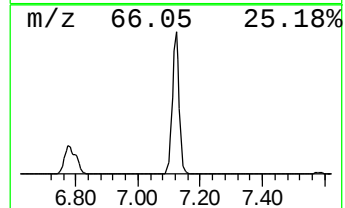
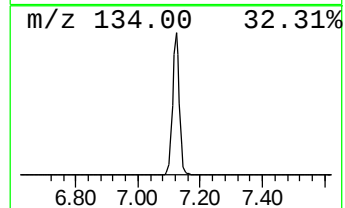
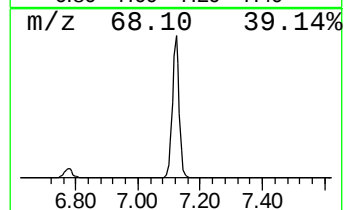
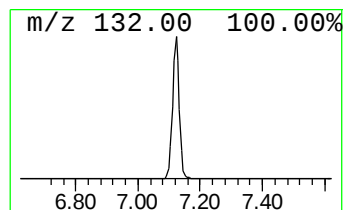
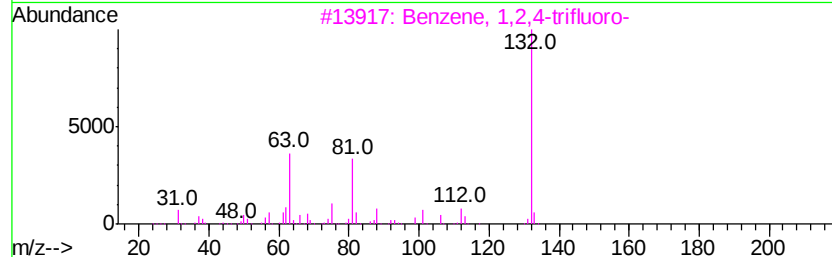
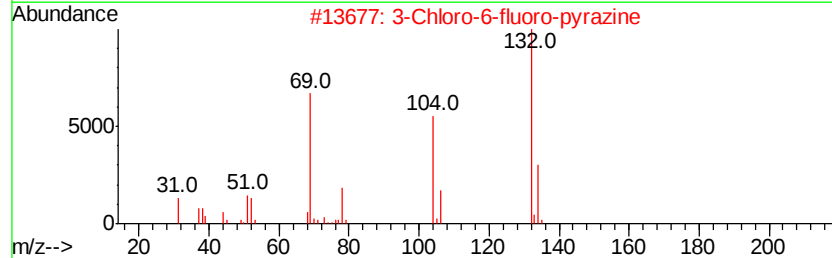
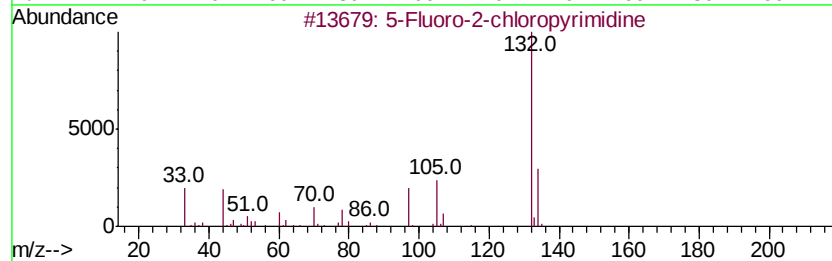
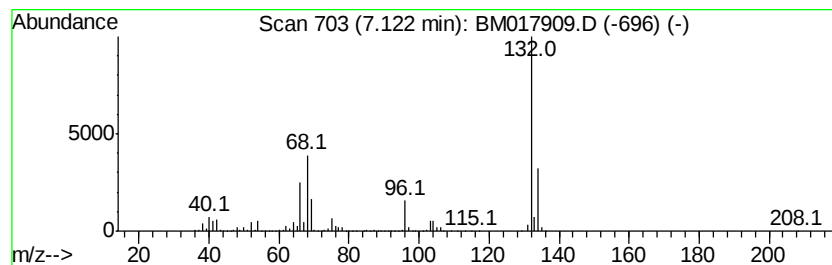
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	67.01 ng	5844630	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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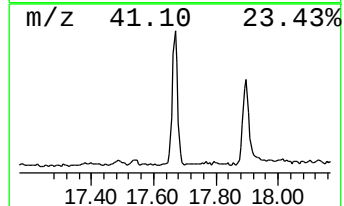
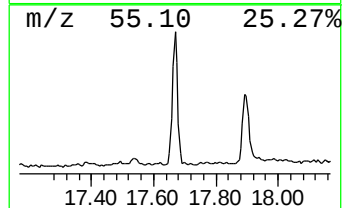
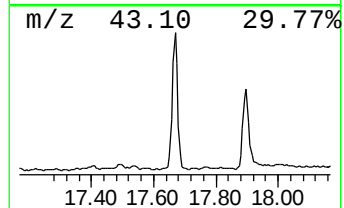
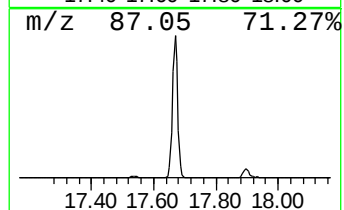
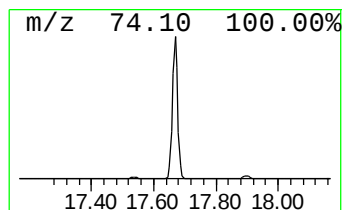
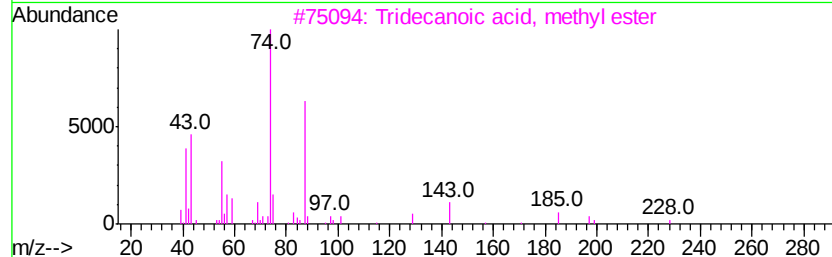
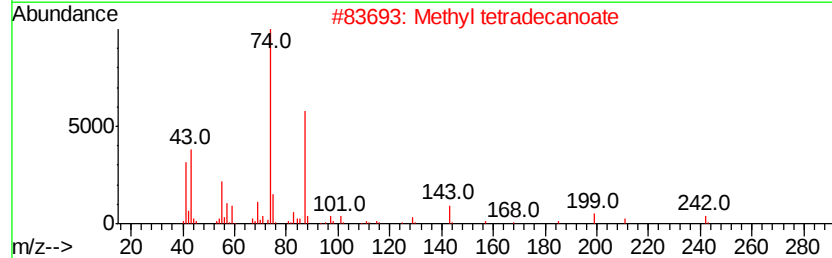
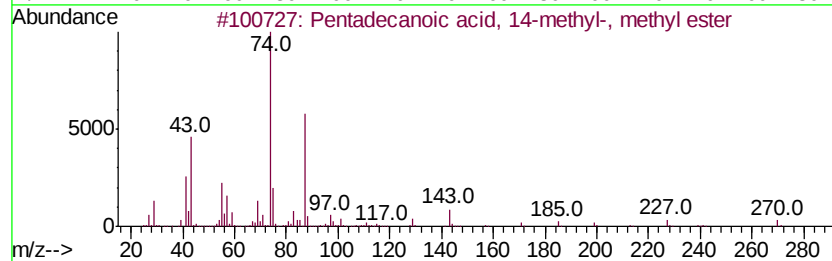
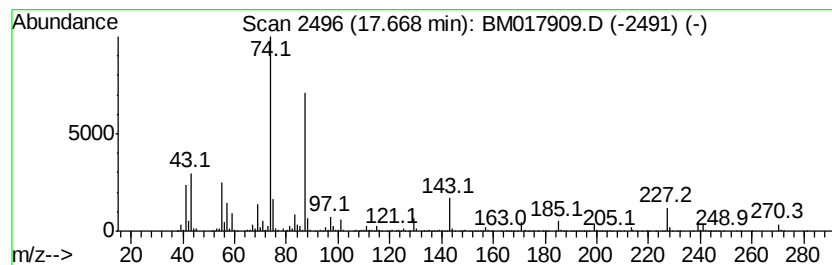
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Pentadecanoic acid, 14-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.67	17.12 ng	2042740	Phenanthrene-d10	16.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
2		Methyl tetradecanoate	242	C15H30O2	000124-10-7	95
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4		9-Octadecenoic acid, 12-(acetylo...	354	C21H38O4	000140-03-4	91
5		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90



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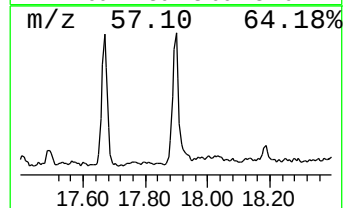
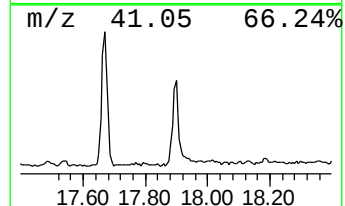
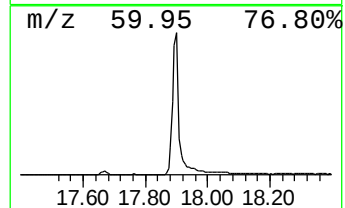
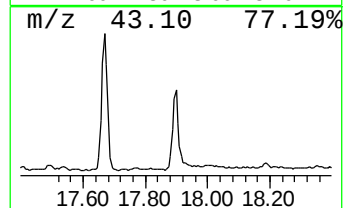
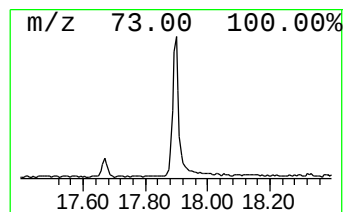
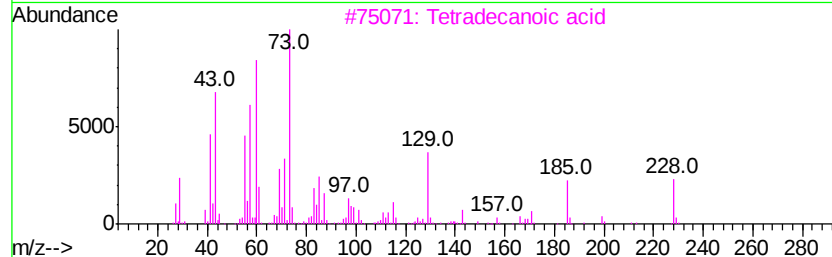
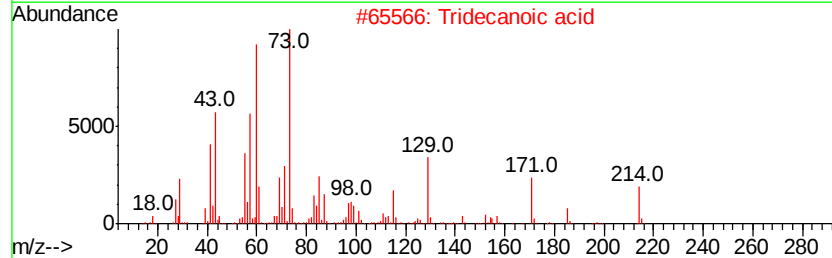
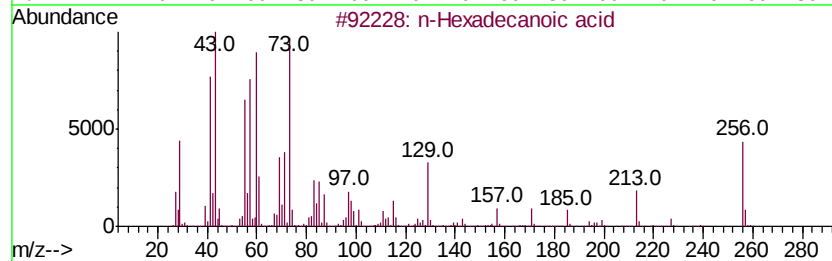
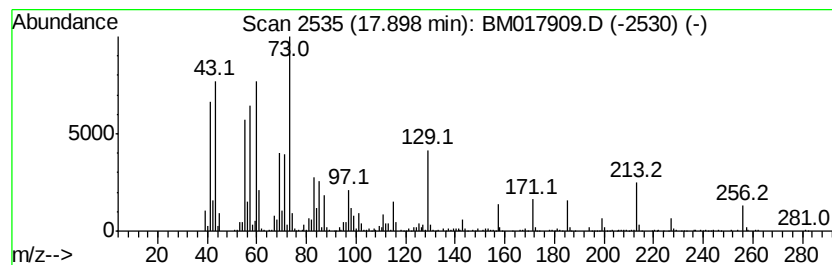
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	10.11 ng	1206280	Phenanthrene-d10	16.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	70
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	70
4		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	25



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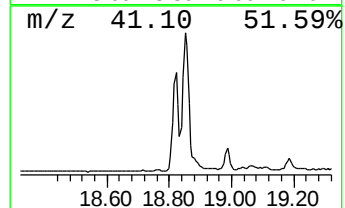
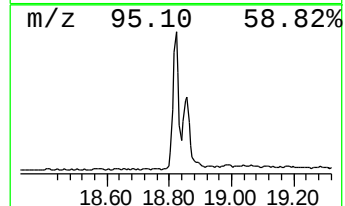
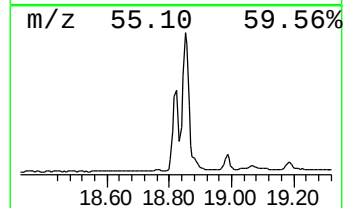
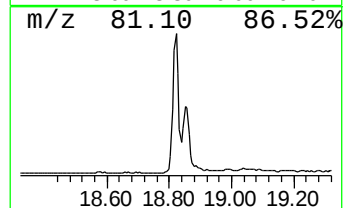
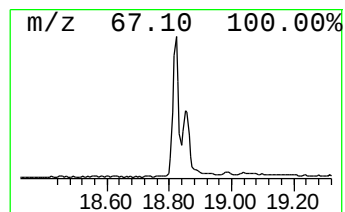
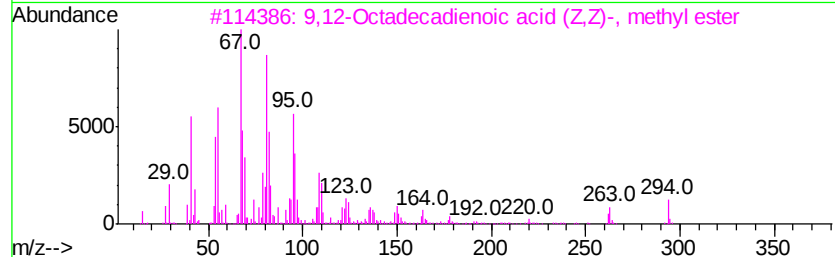
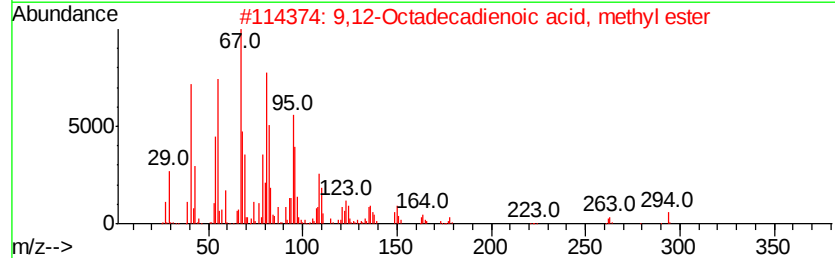
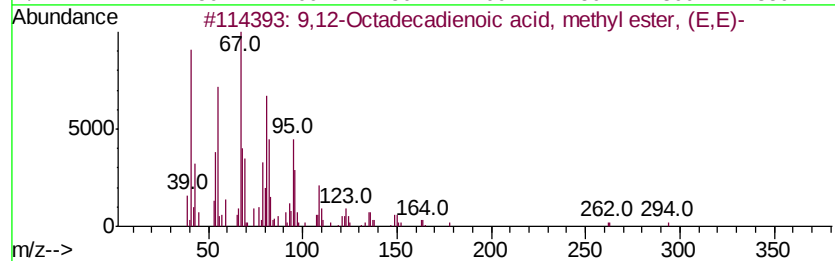
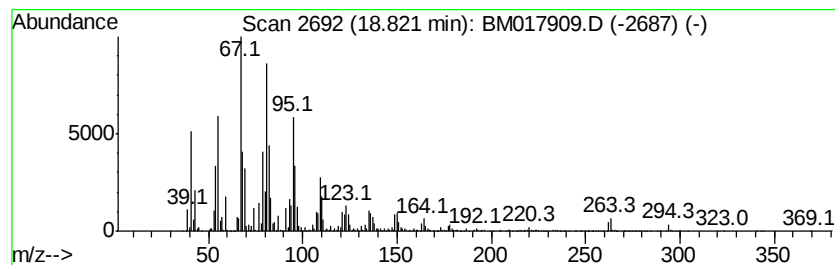
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.82	42.36 ng	5055710	Phenanthrene-d10	16.99

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, methy...	294	C19H34O2	002462-85-3	99
3		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5		11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
Data File : BM017909.D
Acq On : 04 Dec 2018 19:10
Operator : JU/SJ
Sample : J5761-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-06-112918

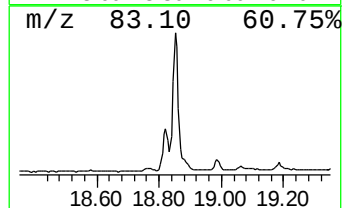
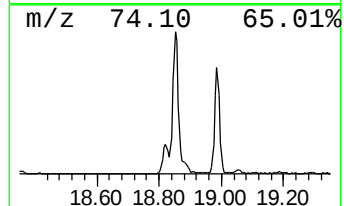
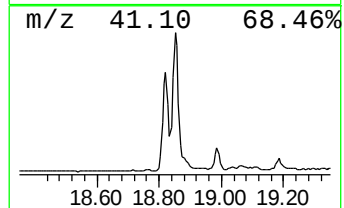
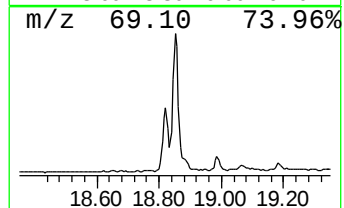
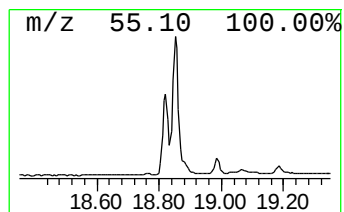
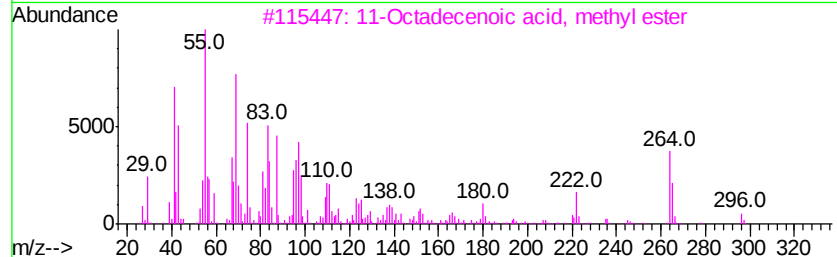
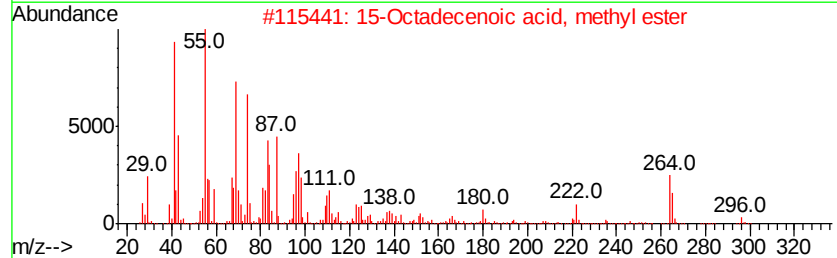
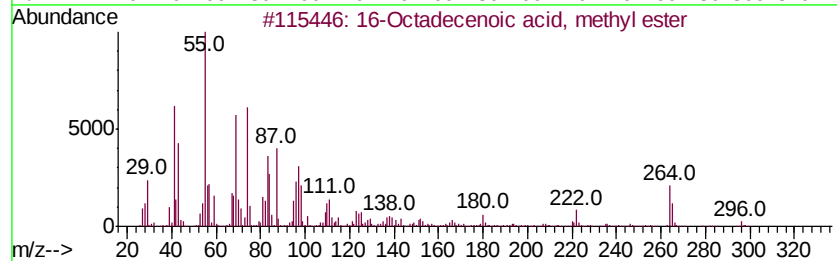
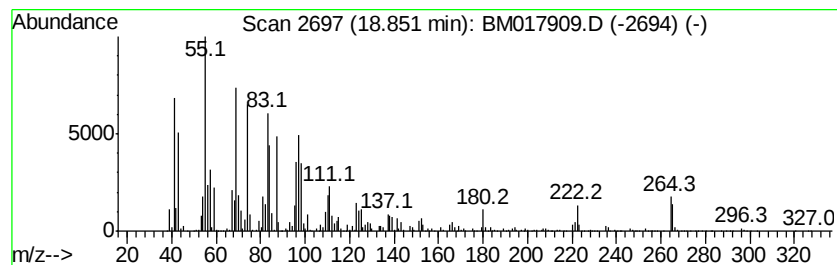
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 16-Octadecenoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.85	61.47 ng	7335210	Phenanthrene-d10	16.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	95
2		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	95
3		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	94
4		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	92
5		6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	92



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
Data File : BM017909.D
Acq On : 04 Dec 2018 19:10
Operator : JU/SJ
Sample : J5761-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

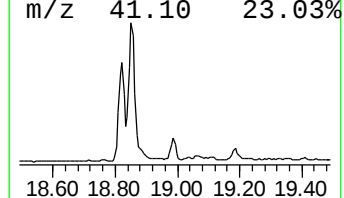
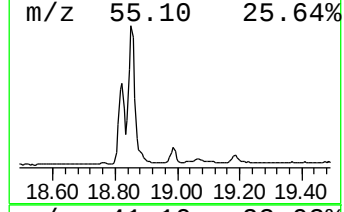
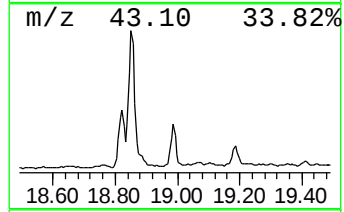
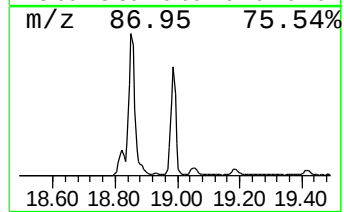
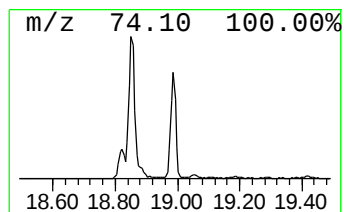
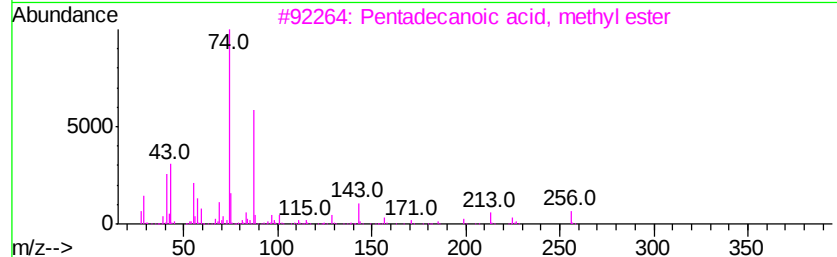
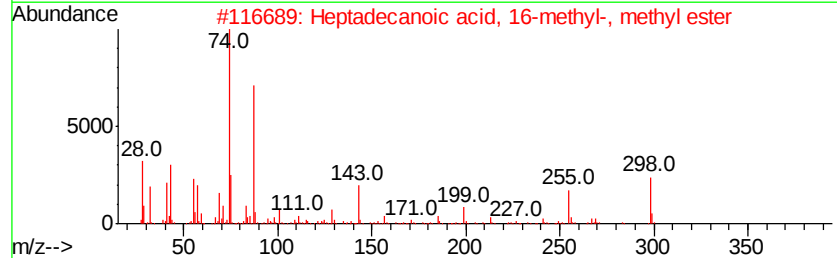
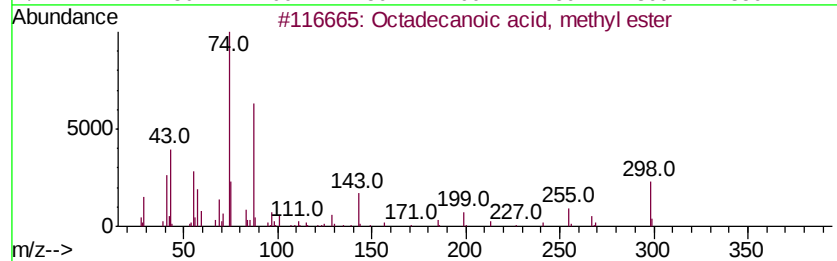
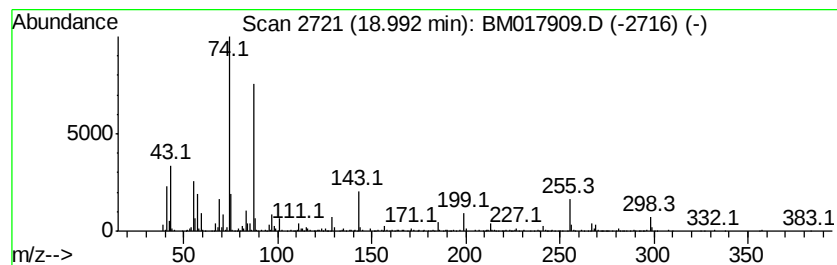
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ClientSampleId :
AU-06-112918

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM111218.M
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 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.99	8.10 ng	966458	Phenanthrene-d10		16.99	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, methyl ester	298	C19H38O2	000112-61-8	95
2		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
4		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
Data File : BM017909.D
Acq On : 04 Dec 2018 19:10
Operator : JU/SJ
Sample : J5761-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

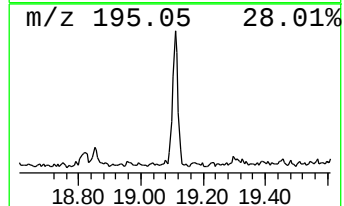
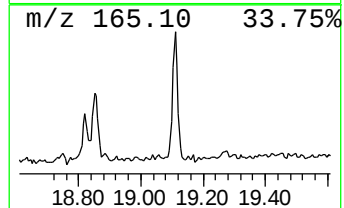
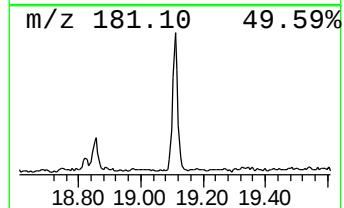
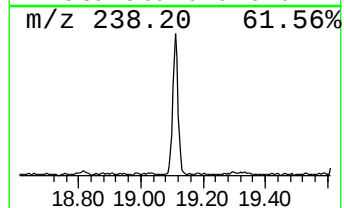
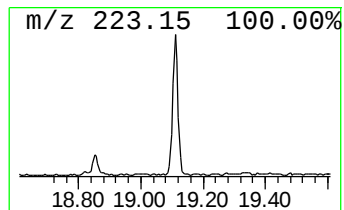
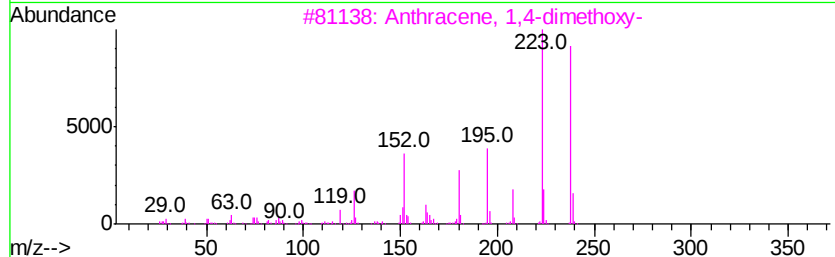
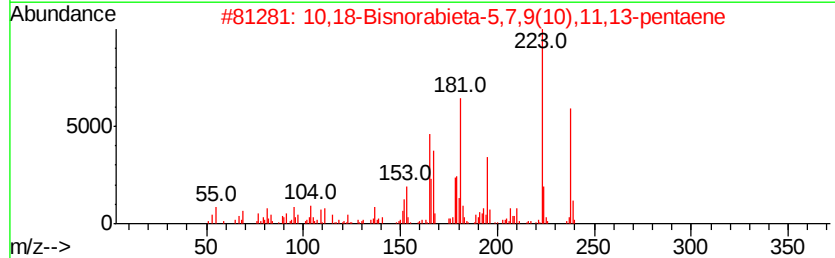
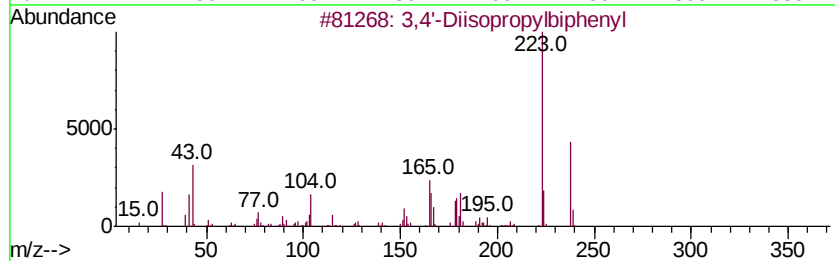
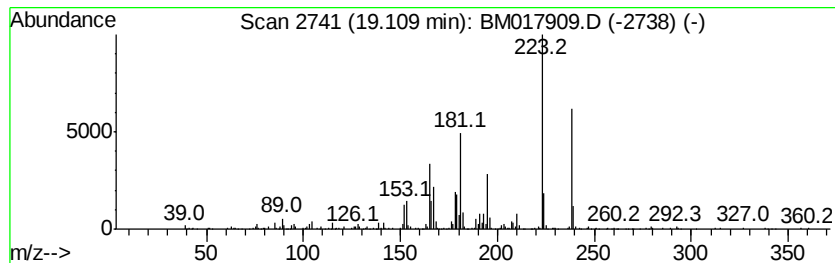
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3,4'-Diisopropylbiphenyl Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.11	3.82 ng	568959	Chrysene-d12	21.19	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	86
2	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	70
3	Anthracene, 1,4-dimethoxy-	238	C16H14O2	013076-29-4	64
4	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	60
5	3,3'-Diacetylbiphenyl	238	C16H14O2	094113-07-2	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
Data File : BM017909.D
Acq On : 04 Dec 2018 19:10
Operator : JU/SJ
Sample : J5761-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-06-112918

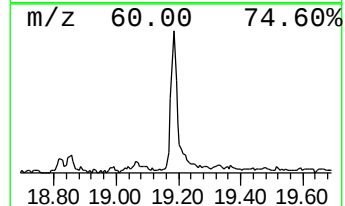
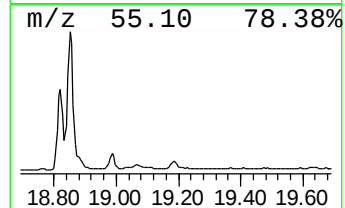
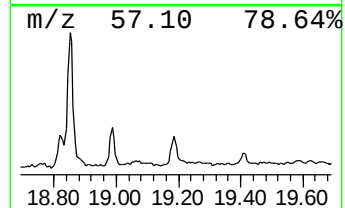
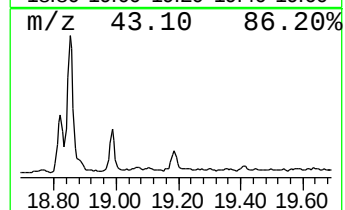
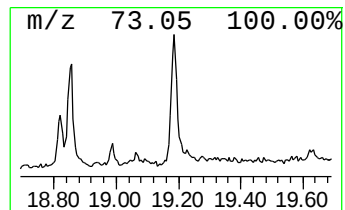
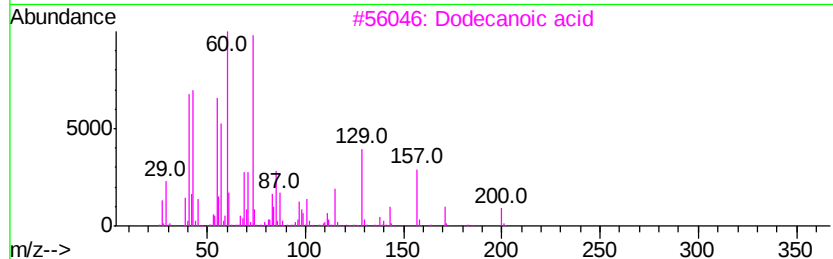
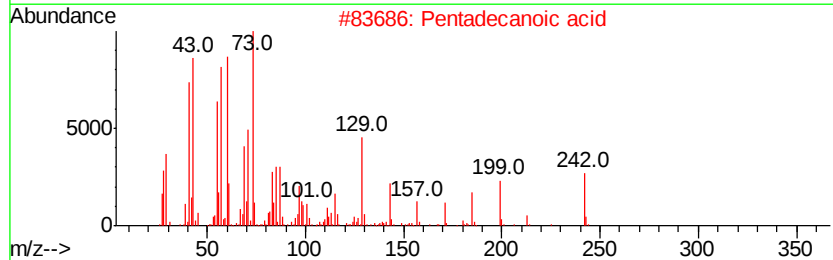
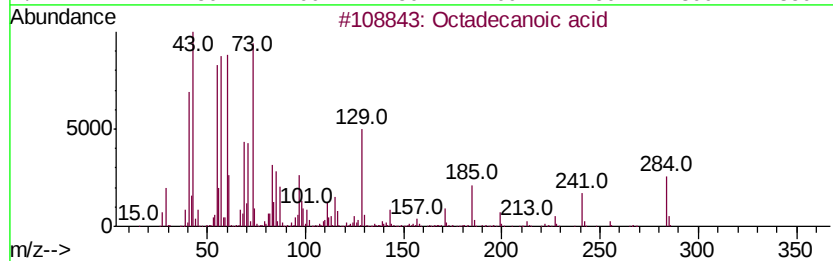
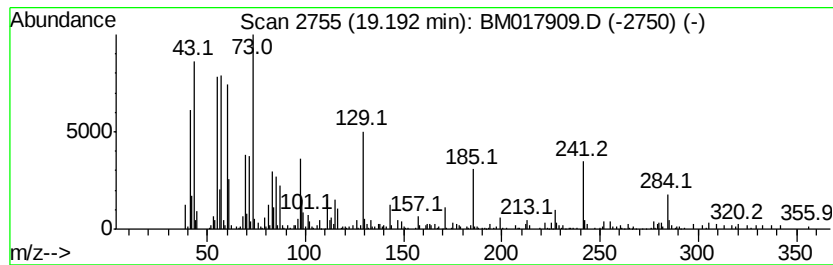
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.19	3.36 ng	499976	Chrysene-d12	21.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
3			Dodecanoic acid	200	C12H24O2	000143-07-7	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	55
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
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Operator : JU/SJ
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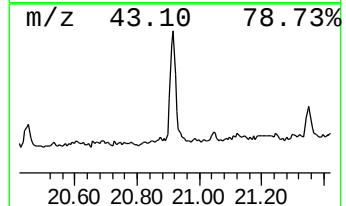
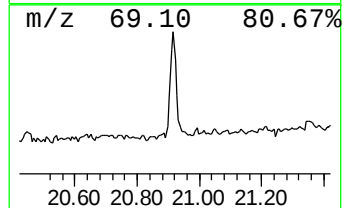
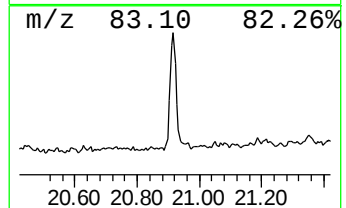
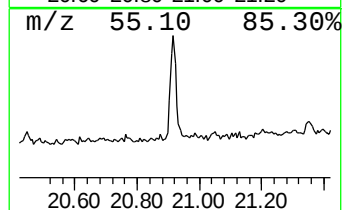
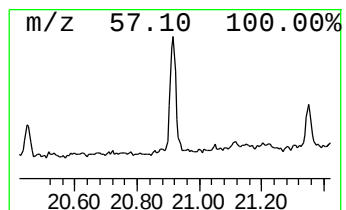
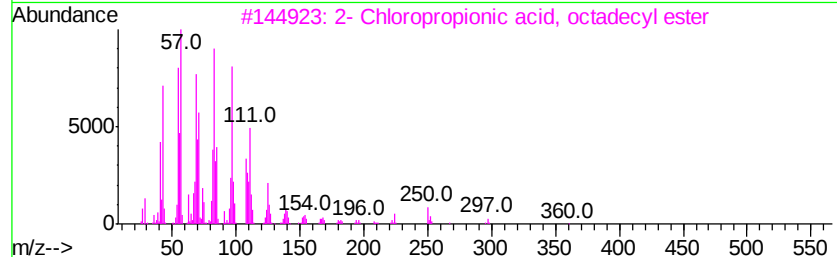
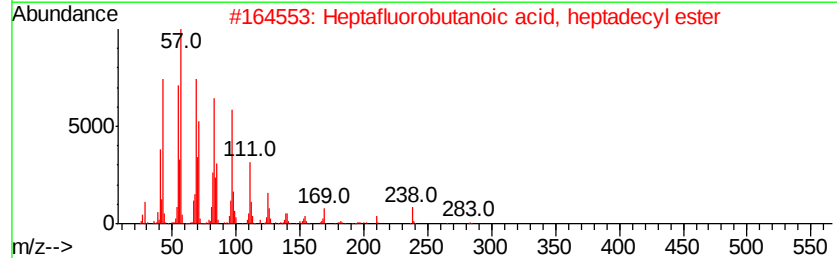
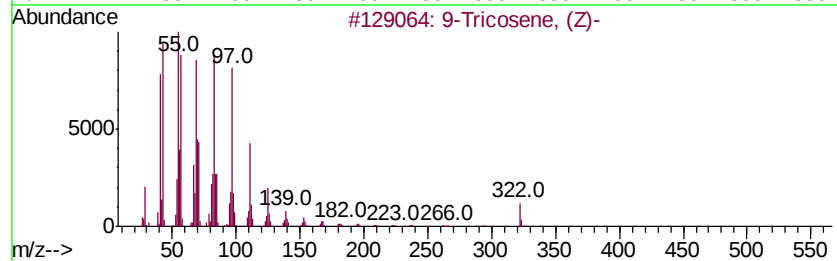
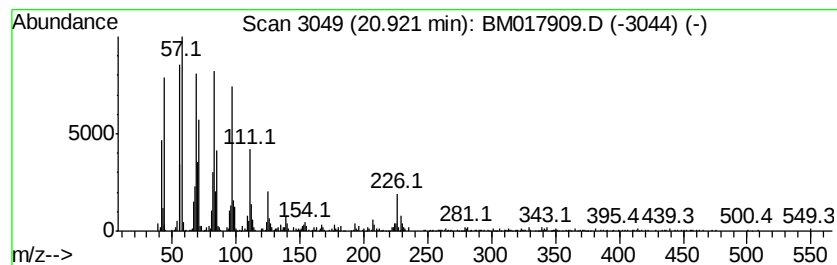
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Tricosene, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.92	6.95 ng	1036360	Chrysene-d12	21.19	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
2	Heptafluorobutanoic acid, heptadecyl ester	452	C21H35F7O2	1000282-97-3	93
3	2-Chloropropionic acid, octadecyl ester	360	C21H41ClO2	088104-31-8	91
4	Cyclohexadecane	224	C16H32	000295-65-8	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM120518\
Data File : BM017909.D
Acq On : 04 Dec 2018 19:10
Operator : JU/SJ
Sample : J5761-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown7.12	7.12	67.0	ng	5844630	1	7.58	1744360	20.0
Pentadecanoic aci...	17.67	17.1	ng	2042740	4	16.99	2386770	20.0
n-Hexadecanoic acid	17.90	10.1	ng	1206280	4	16.99	2386770	20.0
9,12-Octadecadien...	18.82	42.4	ng	5055710	4	16.99	2386770	20.0
16-Octadecenoic a...	18.85	61.5	ng	7335210	4	16.99	2386770	20.0
Octadecanoic acid...	18.99	8.1	ng	966458	4	16.99	2386770	20.0
3,4'-Diisopropylb...	19.11	3.8	ng	568959	5	21.19	2980260	20.0
Octadecanoic acid	19.19	3.4	ng	499976	5	21.19	2980260	20.0
9-Tricosene, (Z)-	20.92	7.0	ng	1036360	5	21.19	2980260	20.0