

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
 Data File : BM016292.D
 Acq On : 09 Aug 2018 21:33
 Operator : SJ/JU
 Sample : J4380-05
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-28

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-BM072318.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	5.187	316	323	336	rBV2	29667	49894	1.67%	0.317%
2	5.381	349	356	366	rBV	134557	221824	7.42%	1.408%
3	5.663	399	404	421	rBV	410851	646864	21.63%	4.106%
4	7.304	678	683	698	rBV	215846	382963	12.80%	2.431%
5	7.663	737	744	759	rBV	909037	1458352	48.76%	9.256%
6	8.128	817	823	837	rBB	191710	321445	10.75%	2.040%
7	8.451	871	878	889	rBV	824365	1312589	43.89%	8.331%
8	9.316	1019	1025	1041	rBV	615016	1040371	34.79%	6.603%
9	9.798	1095	1107	1113	rBV2	130703	320728	10.72%	2.036%
10	10.945	1296	1302	1314	rBV	209318	345268	11.54%	2.191%
11	13.386	1710	1717	1724	rBV	1479327	2040317	68.22%	12.949%
12	14.221	1853	1859	1864	rVB	65551	89330	2.99%	0.567%
13	14.763	1946	1951	1958	rBV2	242842	384704	12.86%	2.442%
14	14.957	1980	1984	1989	rVB	23884	33151	1.11%	0.210%
15	15.745	2111	2118	2123	rBV	277256	369216	12.35%	2.343%
16	16.257	2199	2205	2217	rVB	1284845	1797538	60.10%	11.409%
17	16.563	2252	2257	2262	rBV	29741	45592	1.52%	0.289%
18	16.621	2262	2267	2273	rVV2	42907	74324	2.49%	0.472%
19	16.686	2273	2278	2282	rVV2	34869	48958	1.64%	0.311%
20	16.880	2306	2311	2318	rBV5	24570	51060	1.71%	0.324%
21	17.504	2411	2417	2423	rBV	292569	421995	14.11%	2.678%
22	18.351	2557	2561	2569	rBV2	76062	109910	3.67%	0.698%
23	18.568	2594	2598	2605	rBV2	34799	52540	1.76%	0.333%
24	19.609	2772	2775	2779	rBV3	39450	51272	1.71%	0.325%
25	20.080	2850	2855	2861	rBV	2490367	2990786	100.00%	18.982%
26	21.303	3060	3063	3067	rVB3	53338	59470	1.99%	0.377%
27	21.633	3114	3119	3123	rVB	388035	497868	16.65%	3.160%
28	23.968	3511	3516	3526	rVB2	276493	537661	17.98%	3.412%

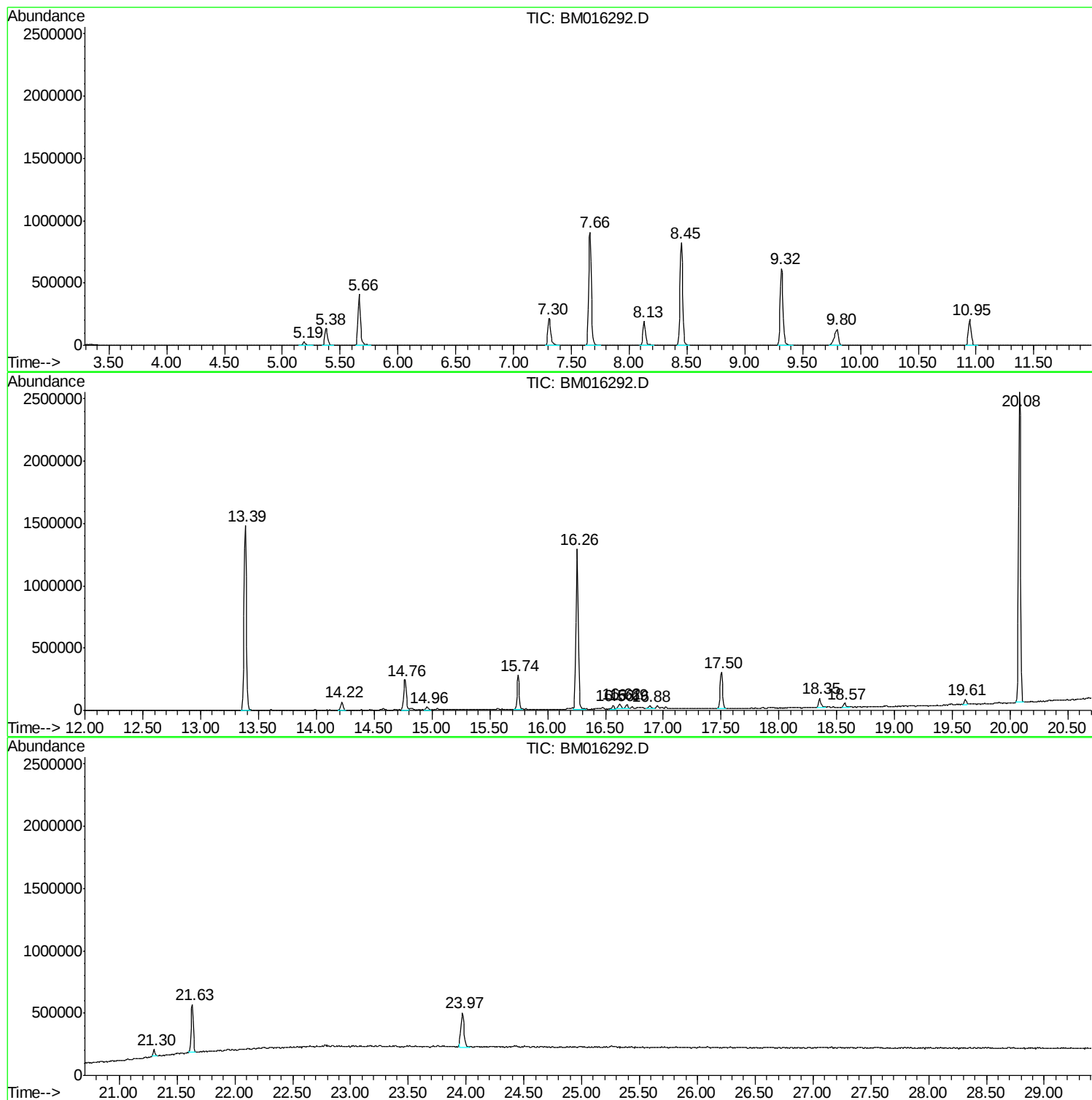
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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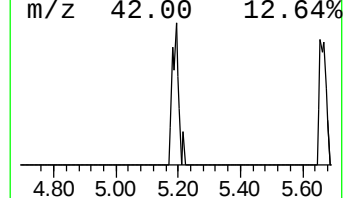
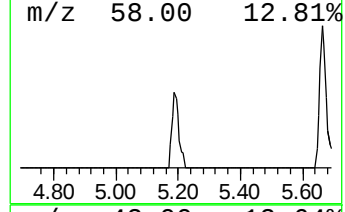
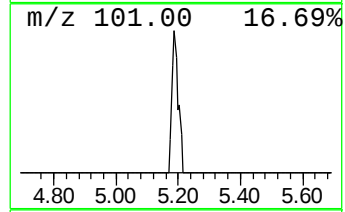
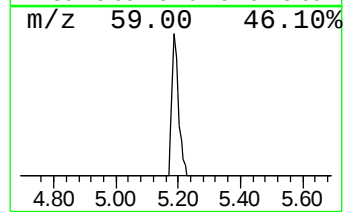
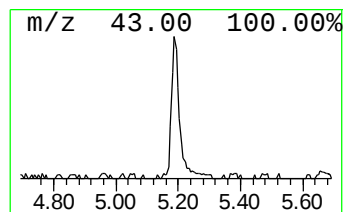
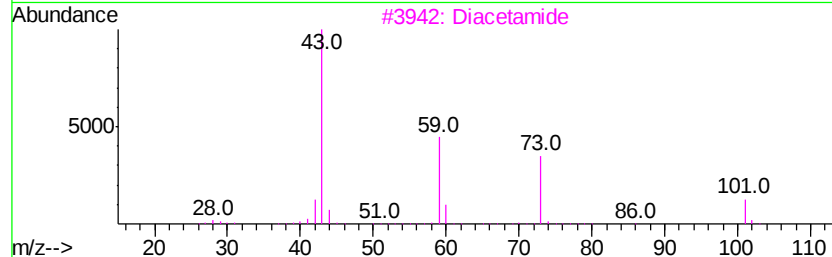
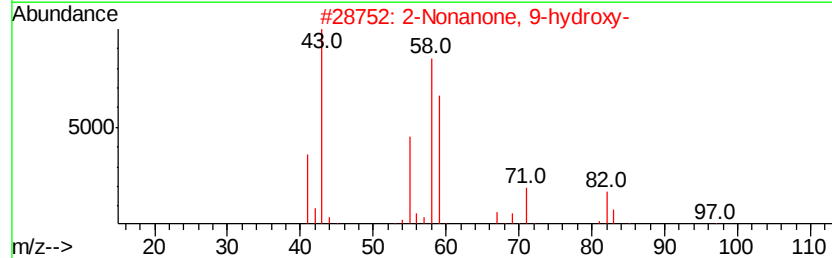
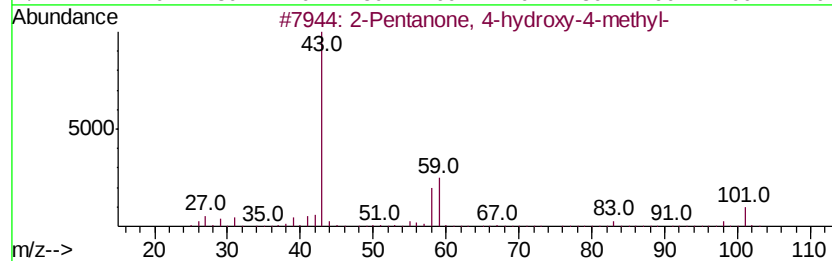
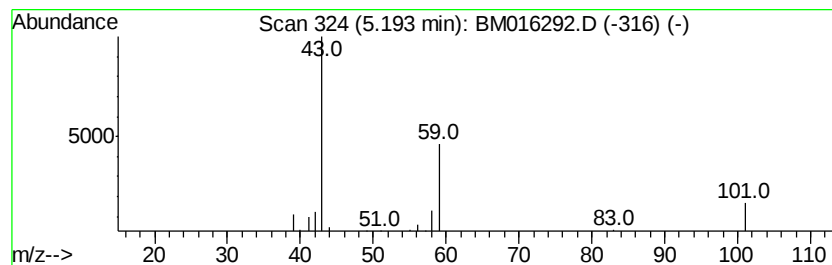
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.10 ng	49894	1,4-Dichlorobenzene-d4	8.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
3			Diacetamide	101	C4H7NO2	000625-77-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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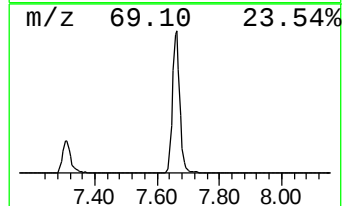
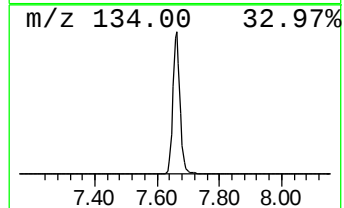
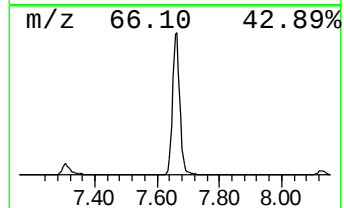
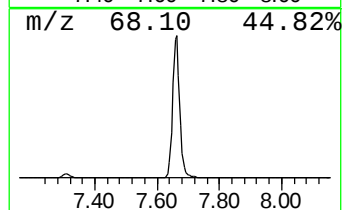
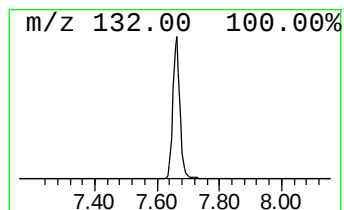
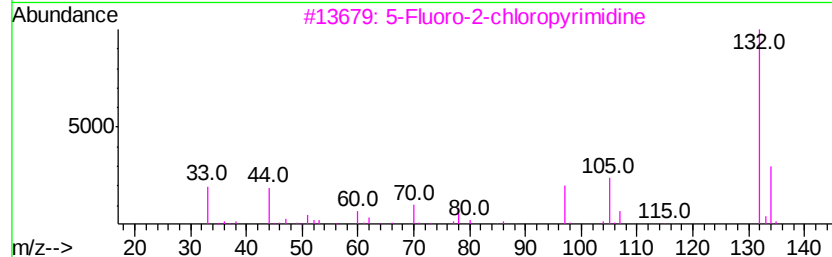
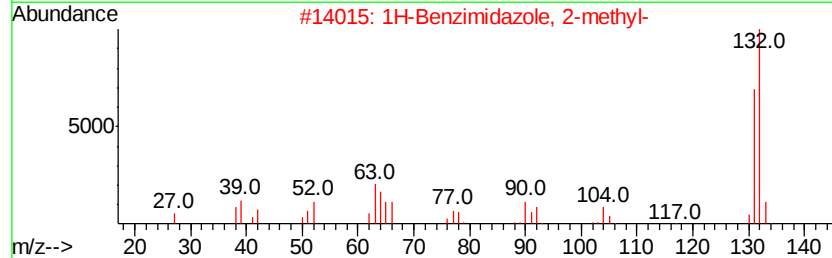
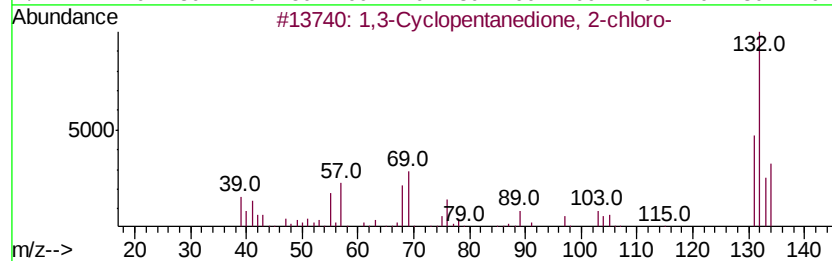
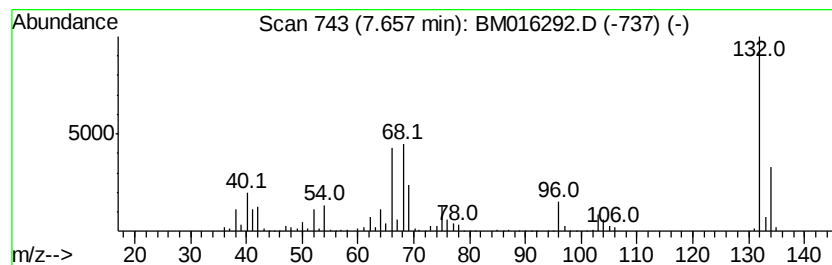
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Peak Number 3 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	90.74 ng	1458350	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	18
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
5		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14



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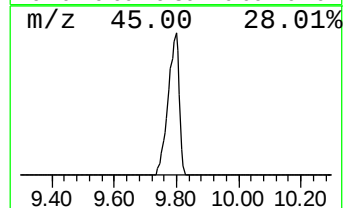
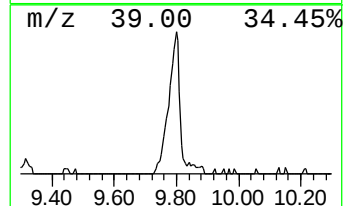
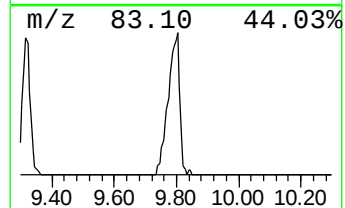
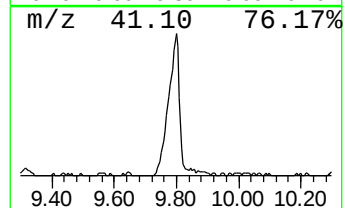
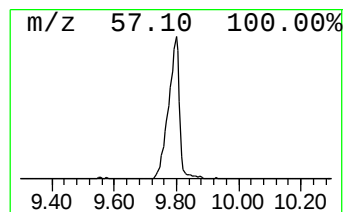
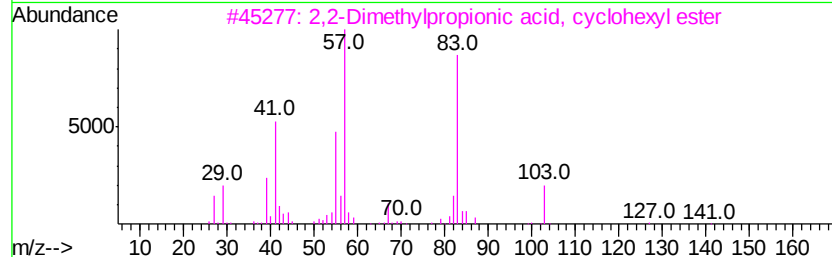
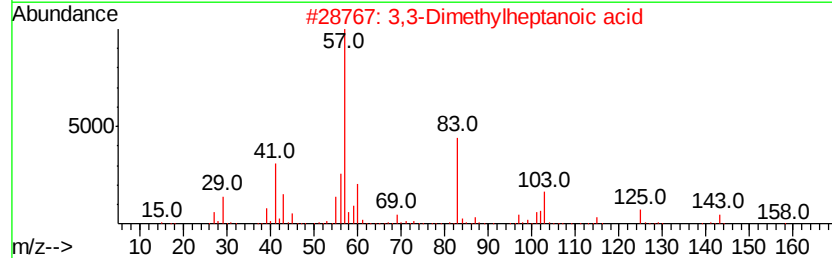
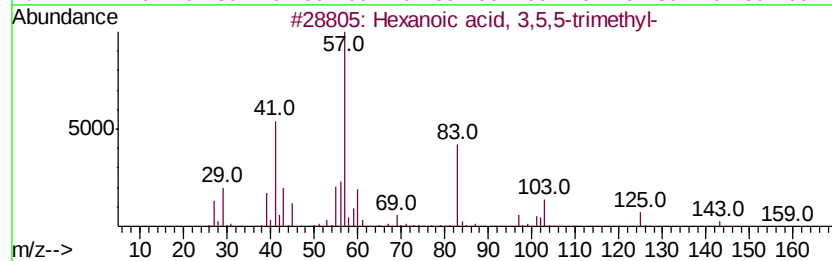
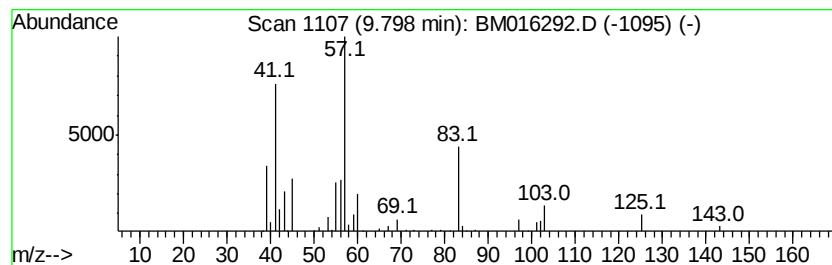
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexanoic acid, 3,5,5-trimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.80	18.58 ng	320728	Naphthalene-d8	10.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	86
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	32
3	2,2-Dimethylpropionic acid, cvcl...	184	C11H20O2	029878-49-7	12
4	Propanoic acid, 2,2-dimethyl-, h...	186	C11H22O2	005434-57-1	10
5	2,2-Dimethylpropionic acid, trid...	284	C18H36O2	105859-93-6	10



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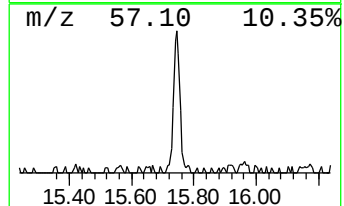
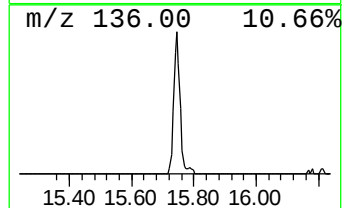
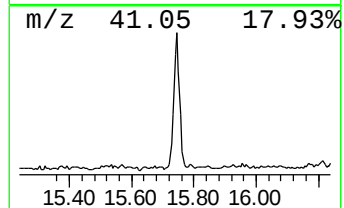
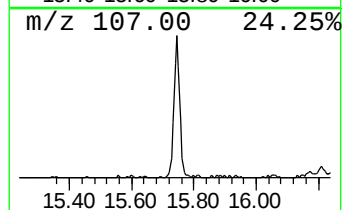
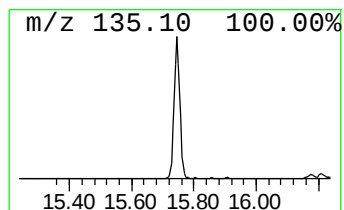
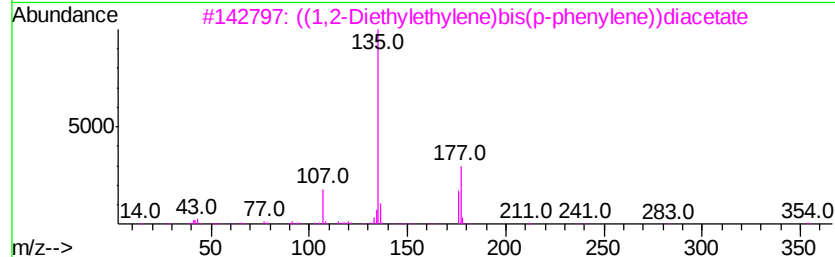
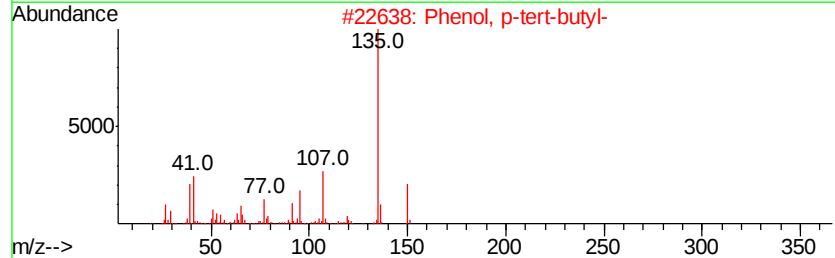
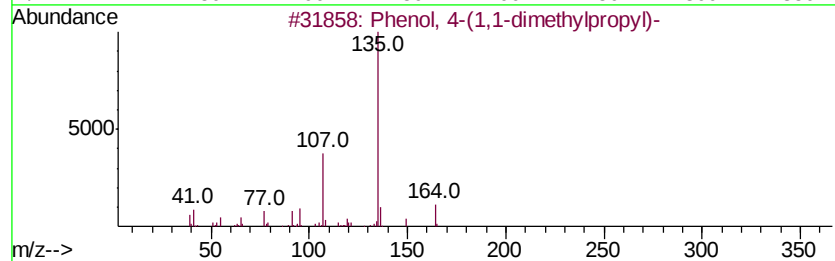
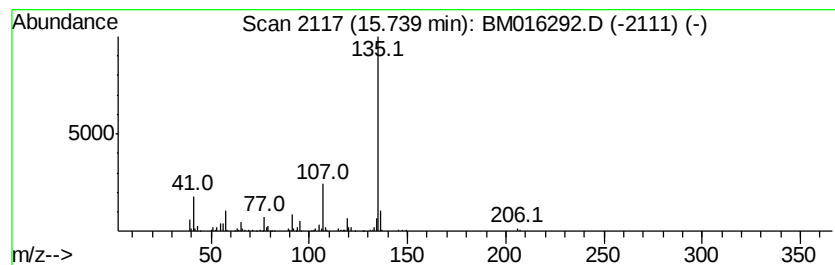
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Peak Number 6 Phenol, 4-(1,1-dimethylprop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	19.19 ng	369216	Acenaphthene-d10	14.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
2		Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72
3		((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	72
4		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
5		Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64



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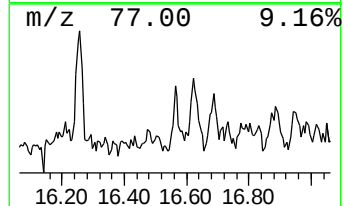
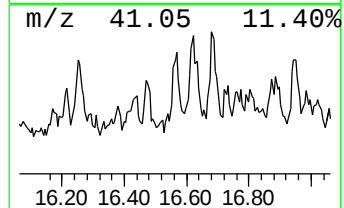
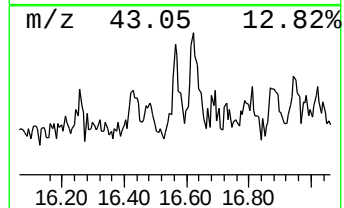
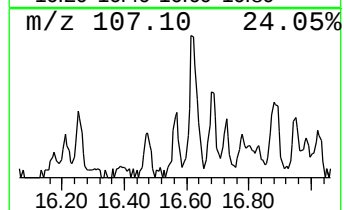
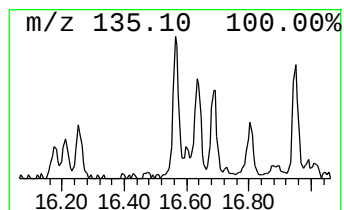
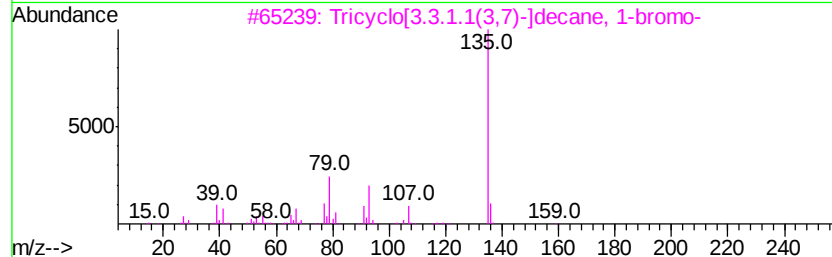
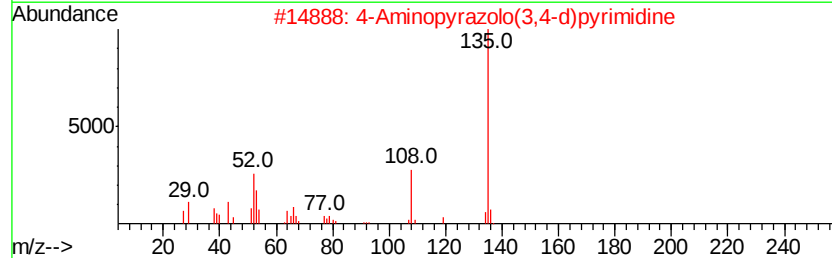
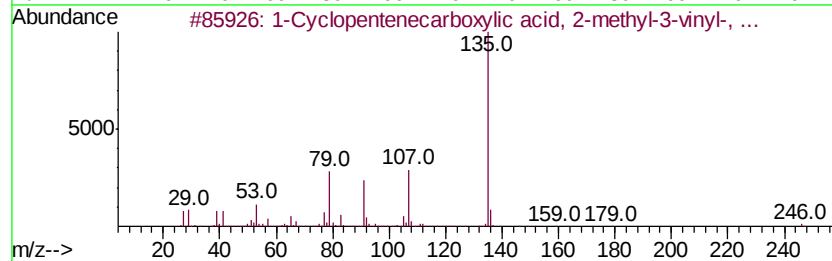
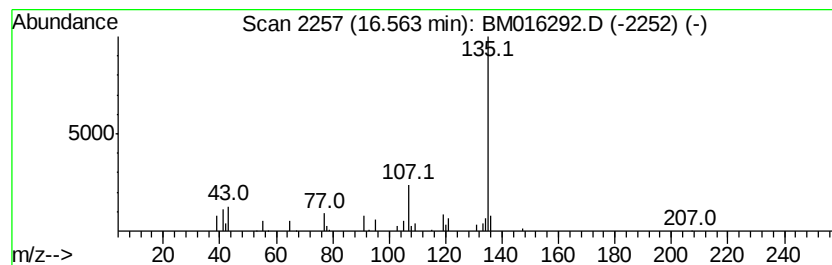
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Peak Number 7 1-Cyclopentenecarboxylic ac... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	2.16 ng	45592	Phenanthrene-d10	17.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Cyclopentenecarboxylic acid, 2...	246	C15H15FO2	1000158-81-1	59
2		4-Aminopyrazolo(3,4-d)pyrimidine	135	C5H5N5	020289-44-5	42
3		Tricyclo[3.3.1.1(3,7)]decane, 1...	214	C10H15Br	000768-90-1	40
4		1-Dodecanone, 2-(imidazol-1-yl)-...	356	C22H32N2O2	1000137-95-7	40
5		2-Iodoadamantane	262	C10H15I	018971-91-0	40



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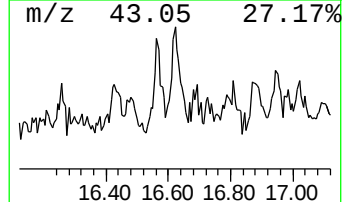
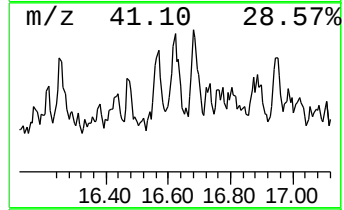
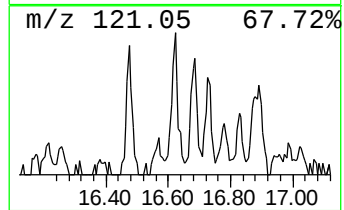
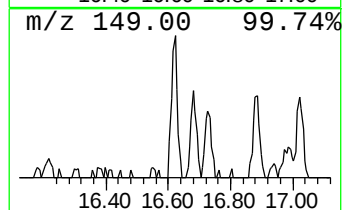
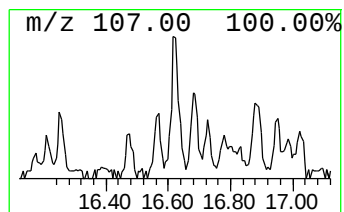
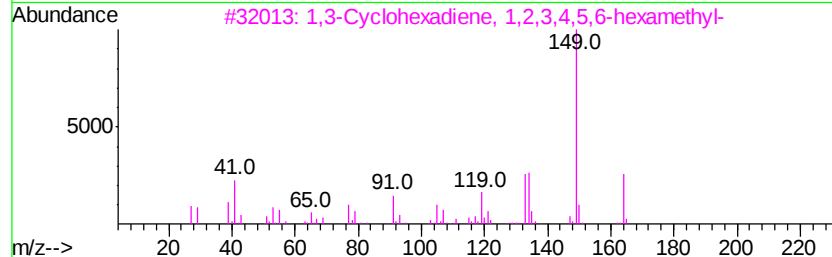
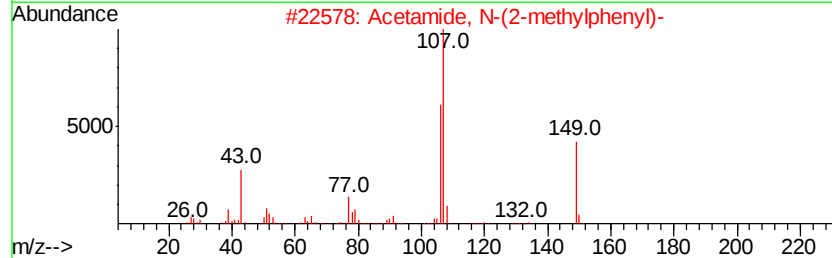
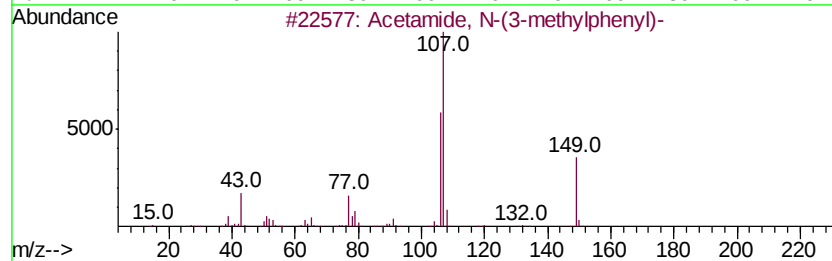
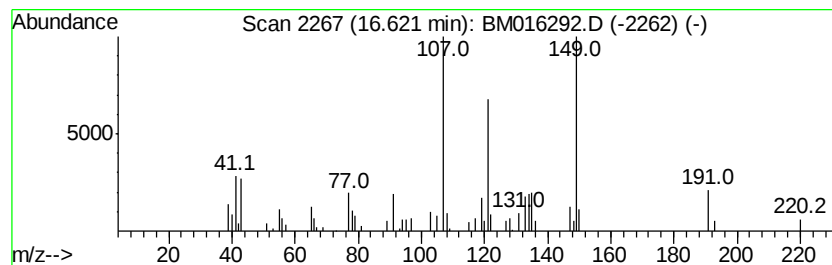
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.62 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	3.52 ng	74324	Phenanthrene-d10	17.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	43
2			Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	43
3			1,3-Cyclohexadiene, 1,2,3,4,5,6-...	164	C12H20	1000152-09-6	38
4			1-(4-Ethoxyphenyl)-2-propanone o...	193	C11H15NO2	319913-93-4	38
5			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016292.D
Acq On : 09 Aug 2018 21:33
Operator : SJ/JU
Sample : J4380-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

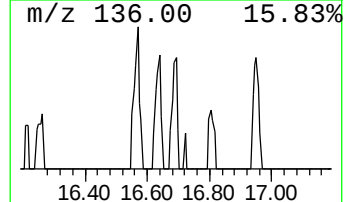
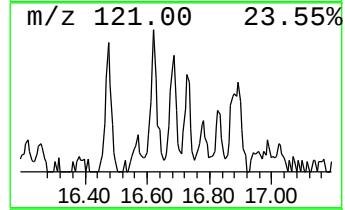
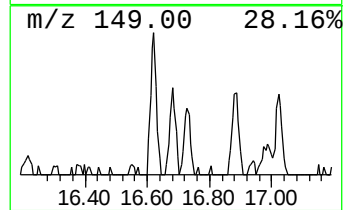
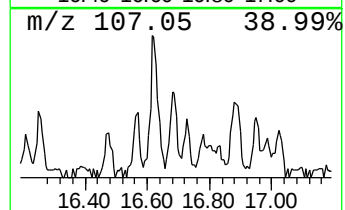
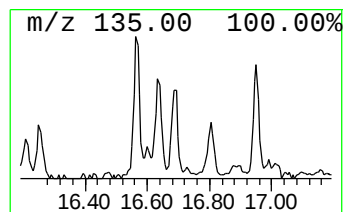
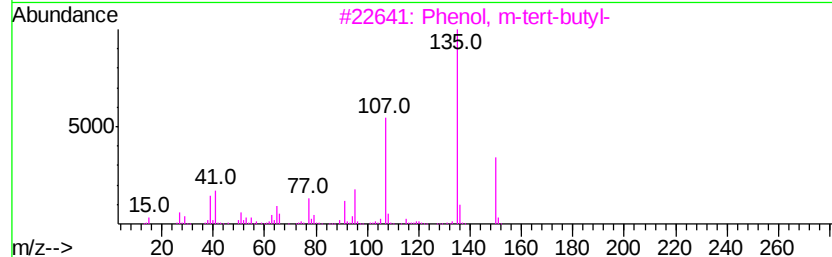
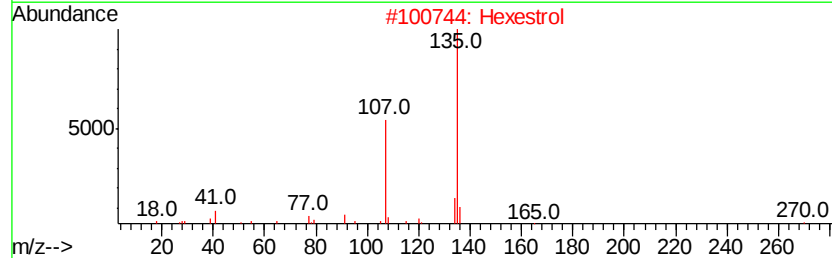
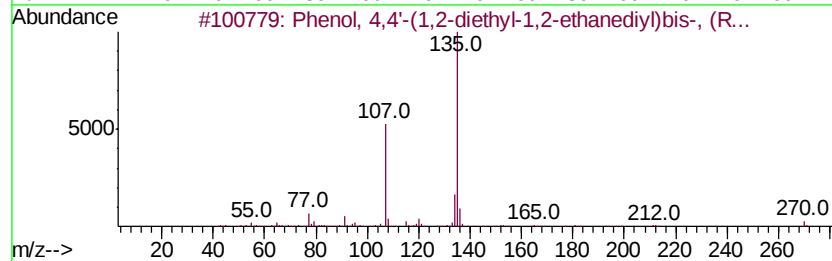
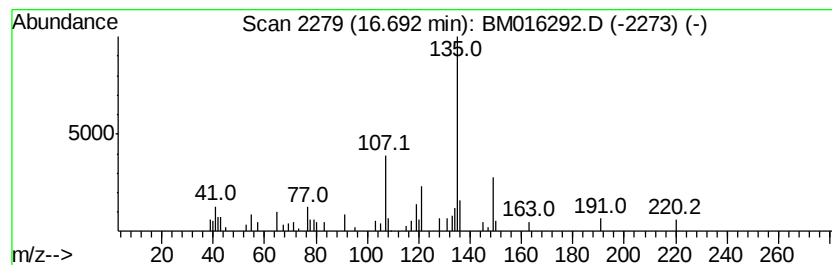
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phenol, 4,4'-(1,2-diethyl-1... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.69	2.32 ng	48958	Phenanthrene-d10	17.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1,2-diethyl-1,2-et...	270	C18H22O2	000084-16-2	50
2	Hexestrol	270	C18H22O2	005635-50-7	47
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	38
4	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	37
5	3,3-Dimethyl-1-phenylazetidine-4...	191	C11H13NS	096594-26-2	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016292.D
Acq On : 09 Aug 2018 21:33
Operator : SJ/JU
Sample : J4380-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

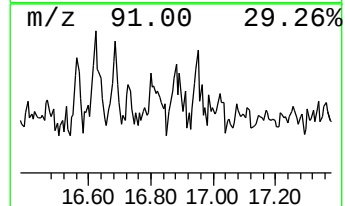
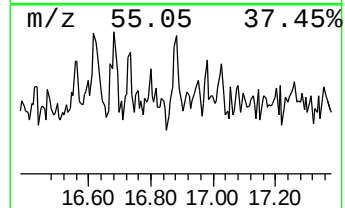
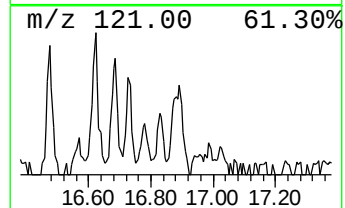
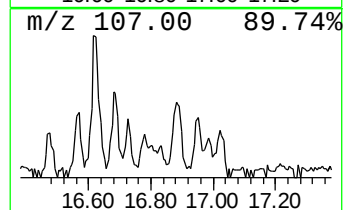
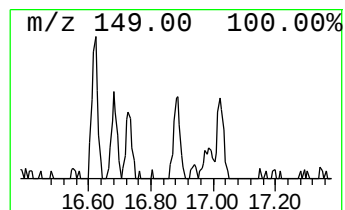
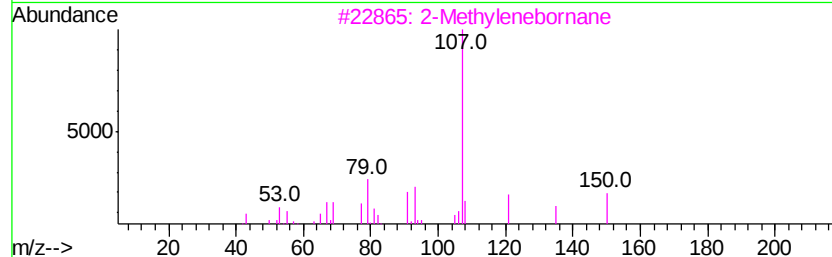
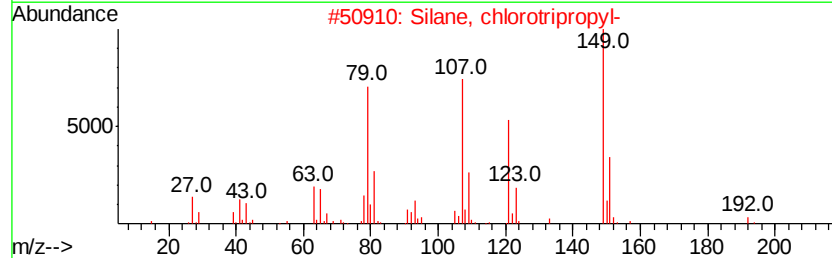
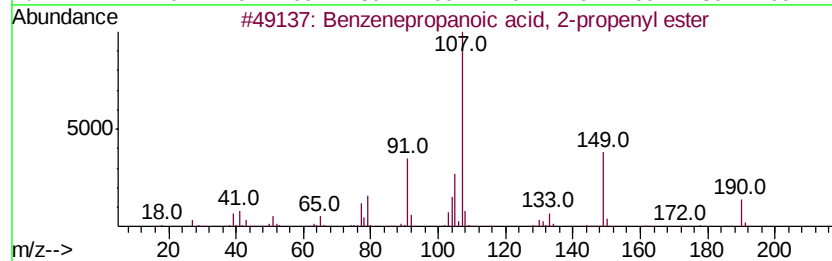
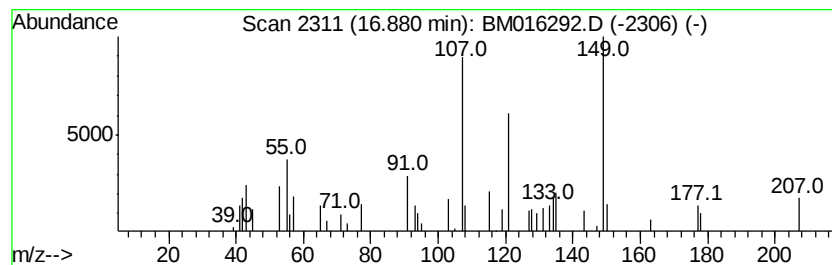
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.88 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.88	2.42 ng	51060	Phenanthrene-d10	17.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, 2-propenyl...	190	C12H14O2	015814-45-6	42
2	Silane, chlorotripropyl-	192	C9H21ClSi	000995-25-5	40
3	2-Methylbornane	150	C11H18	027538-47-2	30
4	Cyclopropane, 1-cyclopropylethyn...	164	C11H16O	1000274-98-5	27
5	3-(p-Hydroxyphenyl)-1-propanol	152	C9H12O2	010210-17-0	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016292.D
Acq On : 09 Aug 2018 21:33
Operator : SJ/JU
Sample : J4380-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

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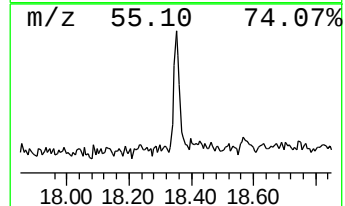
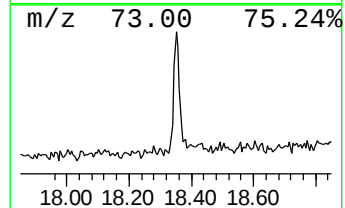
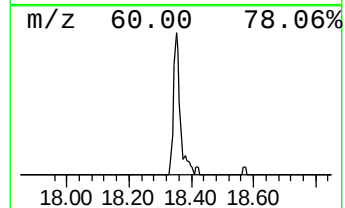
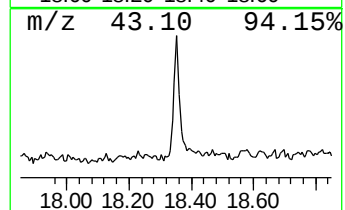
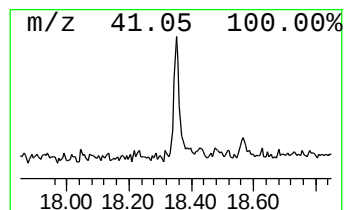
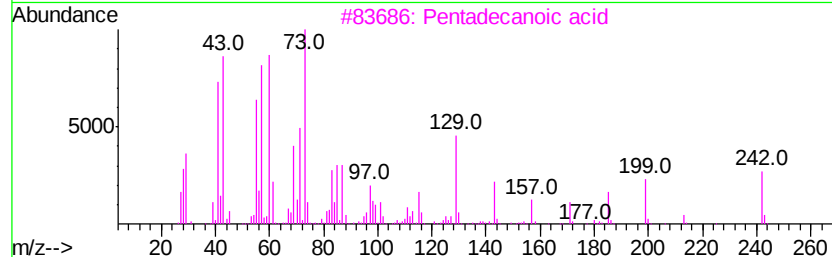
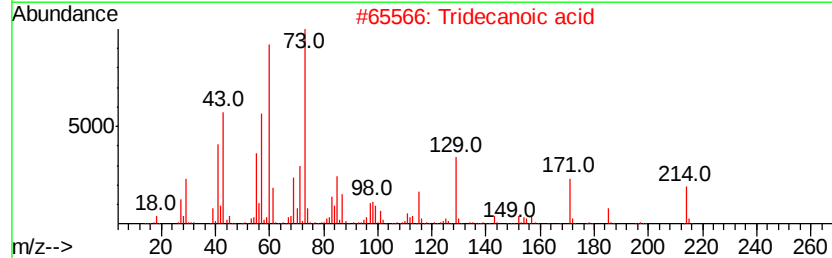
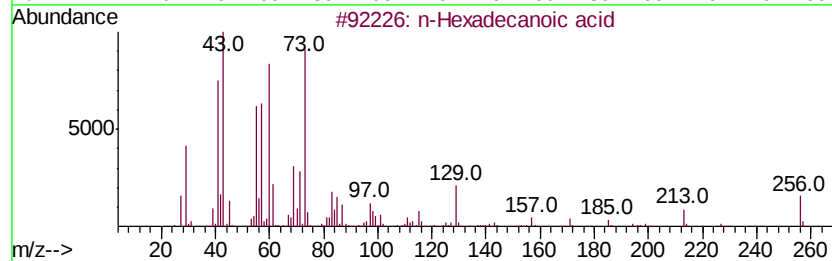
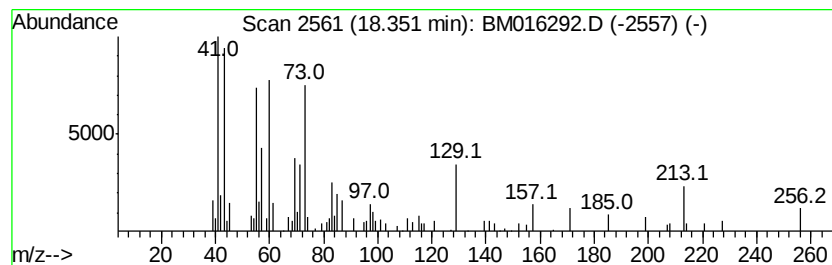
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	5.21 ng	109910	Phenanthrene-d10	17.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2			Tridecanoic acid	214	C13H26O2	000638-53-9	76
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Undecanoic acid	186	C11H22O2	000112-37-8	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016292.D
Acq On : 09 Aug 2018 21:33
Operator : SJ/JU
Sample : J4380-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

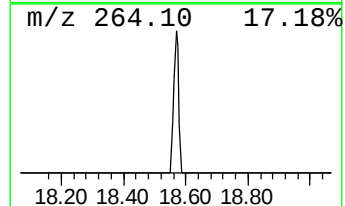
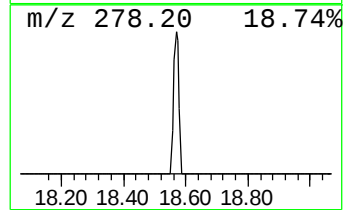
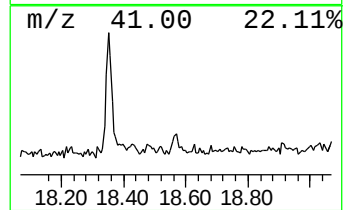
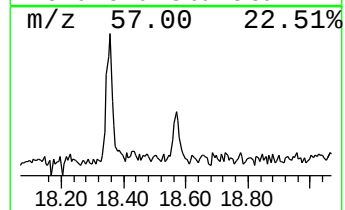
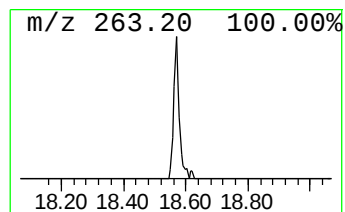
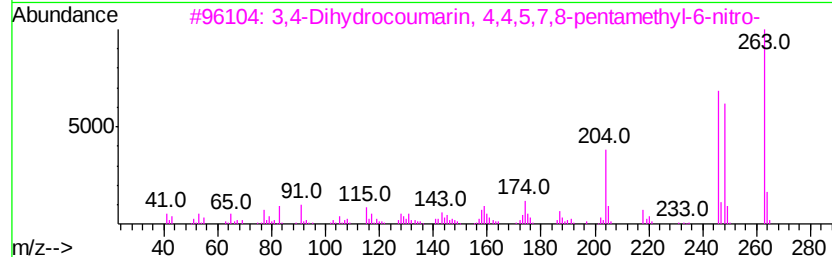
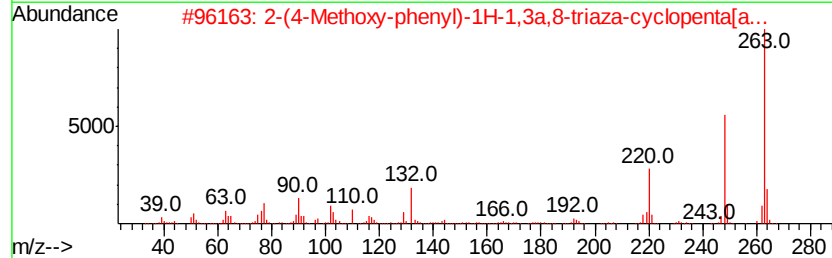
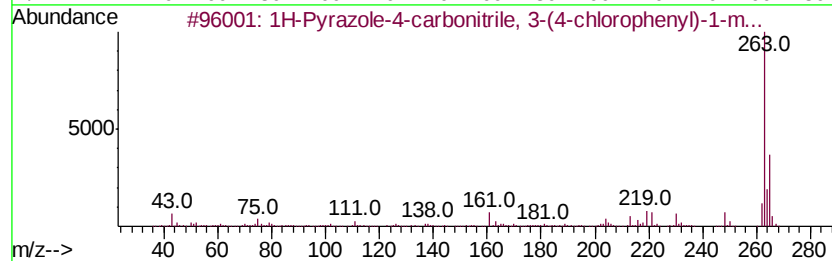
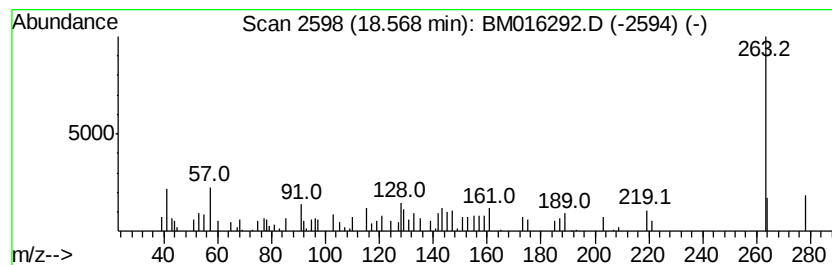
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1H-Pyrazole-4-carbonitrile,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.57	2.49 ng	52540	Phenanthrene-d10	17.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-4-carbonitrile, 3-(4...	263	C12H10ClN3S	068364-67-0	50
2	2-(4-Methoxy-phenyl)-1H-1,3a,8-t...	263	C16H13N3O	036289-23-3	43
3	3,4-Dihydrocoumarin, 4,4,5,7,8-p...	263	C14H17N04	040662-17-7	43
4	Isoquinoline, 5,6,7,8-tetrametho...	263	C14H17N04	093474-27-2	38
5	2-Amino-5-iodobenzoic acid	263	C7H6IN02	005326-47-6	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016292.D
Acq On : 09 Aug 2018 21:33
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Sample : J4380-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

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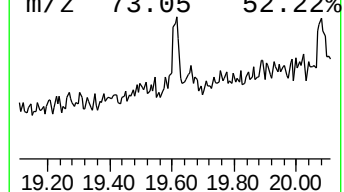
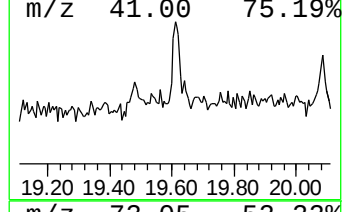
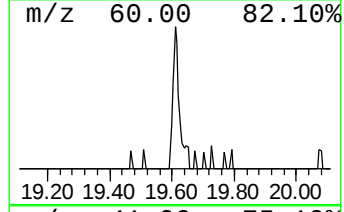
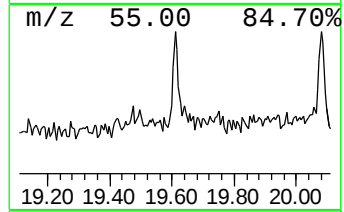
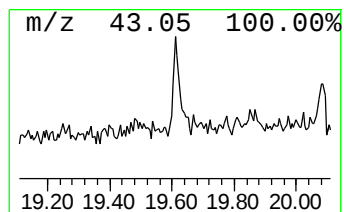
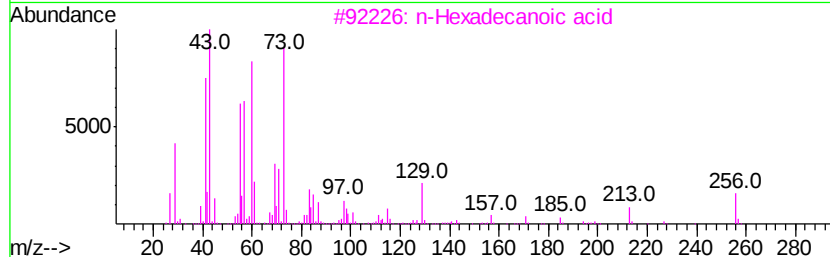
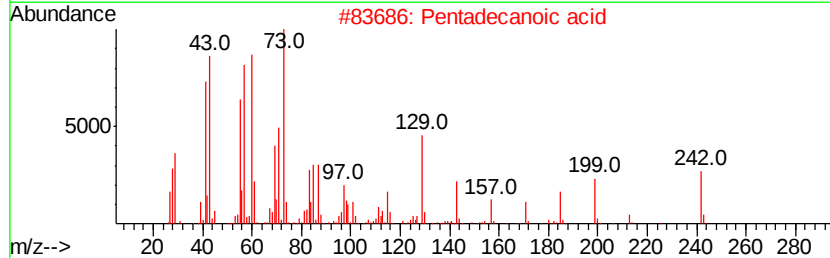
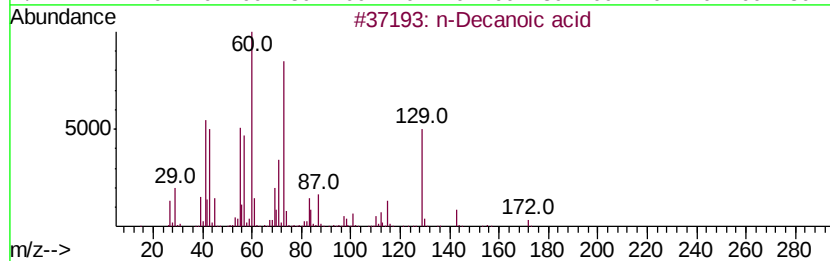
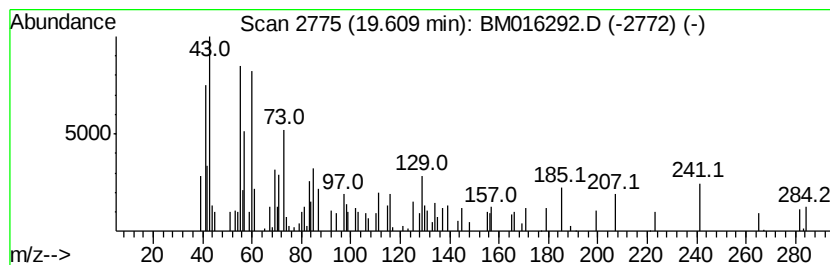
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown19.61 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	2.06 ng	51272	Chrysene-d12	21.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	38
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	38
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	37
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	37
5			3,5-Difluorobenzaldehyde carbamo...	199	C8H7F2N3O	163893-49-0	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016292.D
Acq On : 09 Aug 2018 21:33
Operator : SJ/JU
Sample : J4380-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

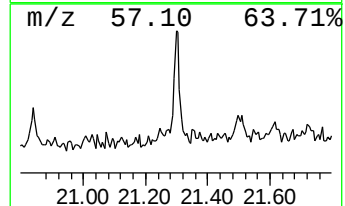
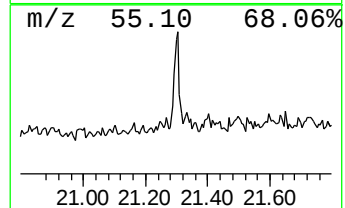
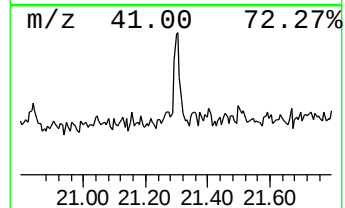
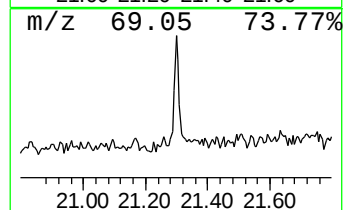
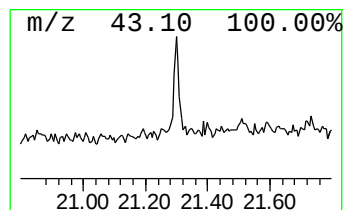
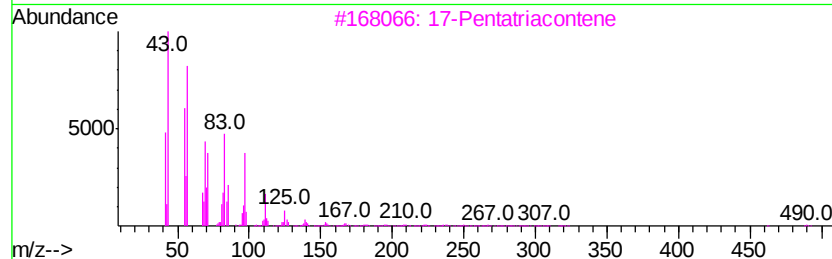
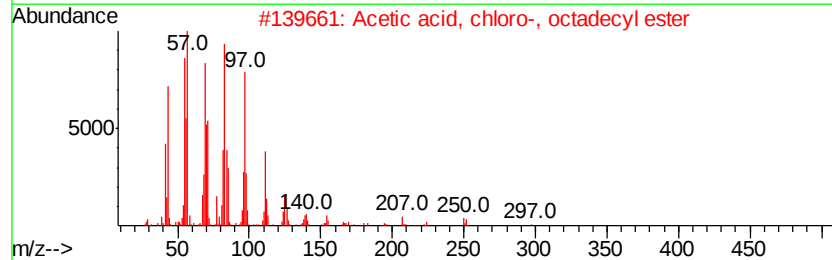
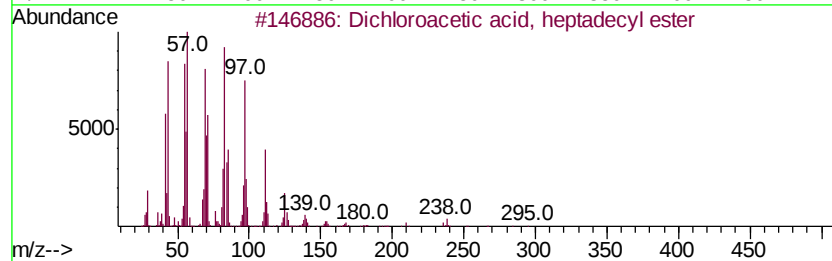
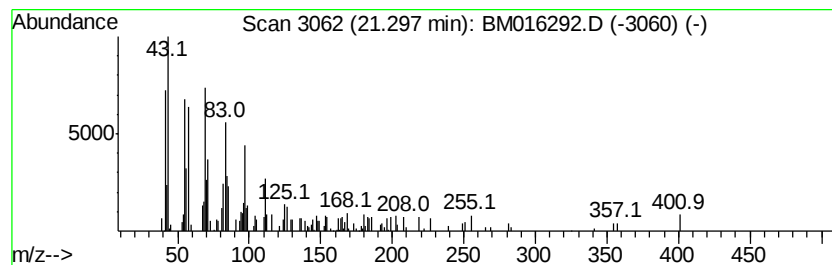
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Dichloroacetic acid, heptad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	2.39 ng	59470	Chrysene-d12	21.63
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2 83
2		Acetic acid, chloro-, octadecyl ...	346 C20H39ClO2	005348-82-3 81
3		17-Pentatriacontene	491 C35H70	006971-40-0 74
4		Heptafluorobutanoic acid, heptad...	452 C21H35F7O2	1000282-97-3 72
5		Chloroacetic acid, pentadecyl ester	304 C17H33ClO2	070301-47-2 64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080918\
 Data File : BM016292.D
 Acq On : 09 Aug 2018 21:33
 Operator : SJ/JU
 Sample : J4380-05
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-28

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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...	5.19	3.1 ng		49894	1	8.13	321445	20.0
unknown7.66	7.66	90.7 ng		1458350	1	8.13	321445	20.0
Hexanoic acid, 3,...	9.80	18.6 ng		320728	2	10.95	345268	20.0
Phenol, 4-(1,1-di...	15.74	19.2 ng		369216	3	14.76	384704	20.0
1-Cyclopentenecar...	16.56	2.2 ng		45592	4	17.50	421995	20.0
unknown16.62	16.62	3.5 ng		74324	4	17.50	421995	20.0
Phenol, 4,4'-(1,2...	16.69	2.3 ng		48958	4	17.50	421995	20.0
unknown16.88	16.88	2.4 ng		51060	4	17.50	421995	20.0
n-Hexadecanoic acid	18.35	5.2 ng		109910	4	17.50	421995	20.0
1H-Pyrazole-4-car...	18.57	2.5 ng		52540	4	17.50	421995	20.0
unknown19.61	19.61	2.1 ng		51272	5	21.63	497868	20.0
Dichloroacetic ac...	21.30	2.4 ng		59470	5	21.63	497868	20.0