

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
 Data File : BM016289.D
 Acq On : 09 Aug 2018 19:44
 Operator : SJ/JU
 Sample : J4380-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-37

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	318	323	333	rBV2	42357	68812	2.40%	0.431%
2	5.663	399	404	420	rBV	400984	646748	22.52%	4.054%
3	7.310	678	684	704	rBB	226159	406408	14.15%	2.548%
4	7.663	737	744	756	rBV	898274	1454412	50.65%	9.118%
5	8.128	818	823	835	rBB	188496	308817	10.76%	1.936%
6	8.451	871	878	893	rBB	828603	1308383	45.57%	8.202%
7	9.322	1019	1026	1038	rBV	640842	1102966	38.41%	6.914%
8	10.945	1295	1302	1312	rVB	208644	352585	12.28%	2.210%
9	13.386	1707	1717	1724	rBV	1499834	2048740	71.35%	12.843%
10	13.633	1750	1759	1763	rBV5	15462	31671	1.10%	0.199%
11	14.222	1854	1859	1864	rBV	64355	88640	3.09%	0.556%
12	14.769	1946	1952	1956	rBV2	245621	385062	13.41%	2.414%
13	14.827	1959	1962	1970	rVB2	45942	73294	2.55%	0.459%
14	14.957	1980	1984	1989	rBV2	22676	33125	1.15%	0.208%
15	15.045	1992	1999	2009	rVB5	23738	41763	1.45%	0.262%
16	15.745	2113	2118	2122	rBV2	51324	67778	2.36%	0.425%
17	15.816	2122	2130	2134	rVB3	22458	47022	1.64%	0.295%
18	15.951	2150	2153	2161	rVB	48124	68046	2.37%	0.427%
19	16.257	2199	2205	2216	rBV	1237390	1671625	58.22%	10.479%
20	17.504	2411	2417	2422	rBV	281262	413191	14.39%	2.590%
21	18.233	2537	2541	2549	rBV6	23730	40751	1.42%	0.255%
22	18.357	2557	2562	2572	rBV	295217	415189	14.46%	2.603%
23	18.574	2594	2599	2609	rBV	166940	252221	8.78%	1.581%
24	19.609	2771	2775	2788	rBV	153213	244818	8.53%	1.535%
25	20.080	2850	2855	2861	rBV	2429443	2871324	100.00%	18.000%
26	20.839	2980	2984	2989	rBV	261874	284437	9.91%	1.783%
27	21.298	3059	3062	3069	rBV	125558	151610	5.28%	0.950%
28	21.633	3114	3119	3124	rVB	350849	460187	16.03%	2.885%
29	22.780	3311	3314	3321	rVB	111266	159577	5.56%	1.000%
30	23.968	3511	3516	3523	rVB	244319	452488	15.76%	2.837%

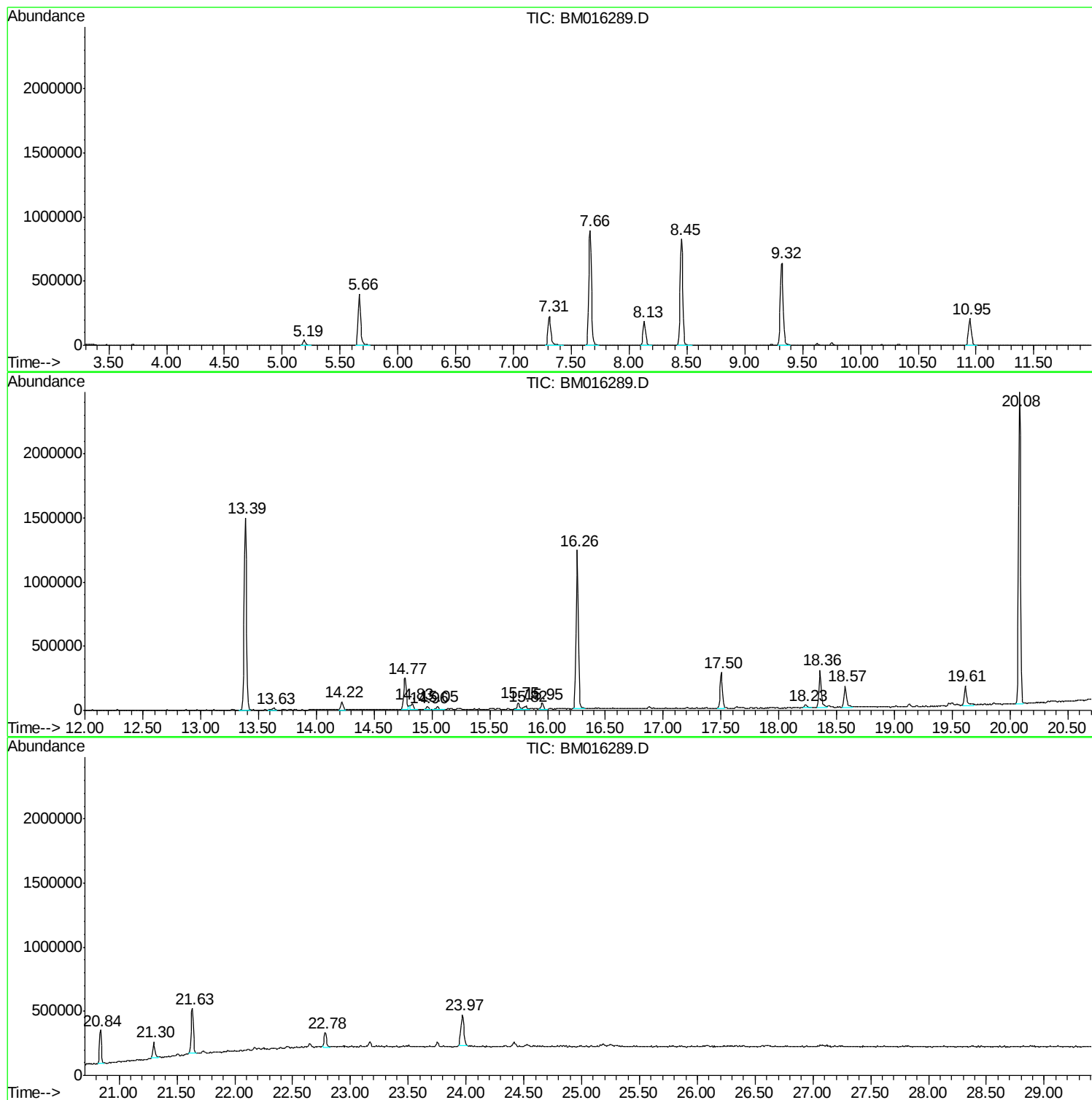
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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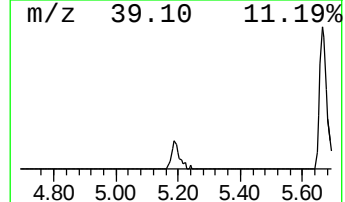
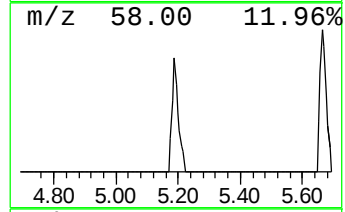
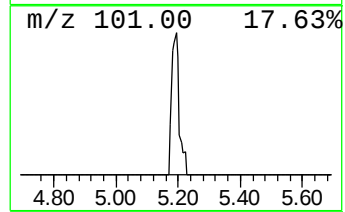
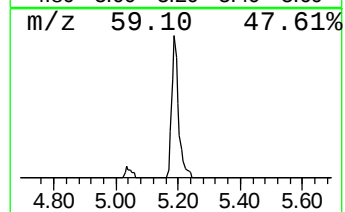
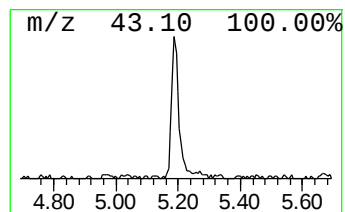
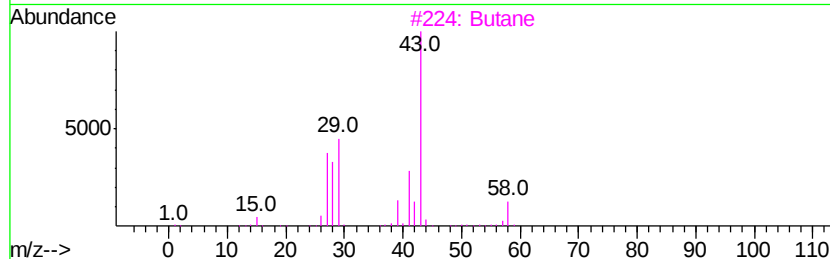
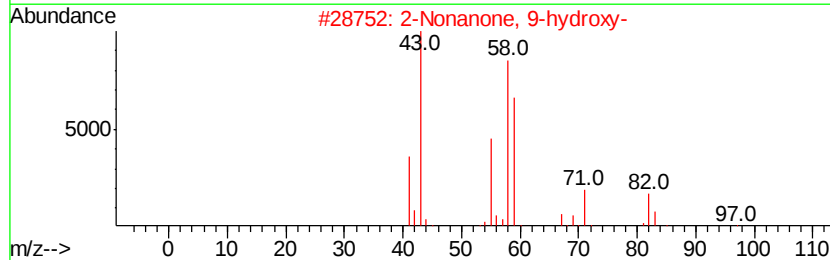
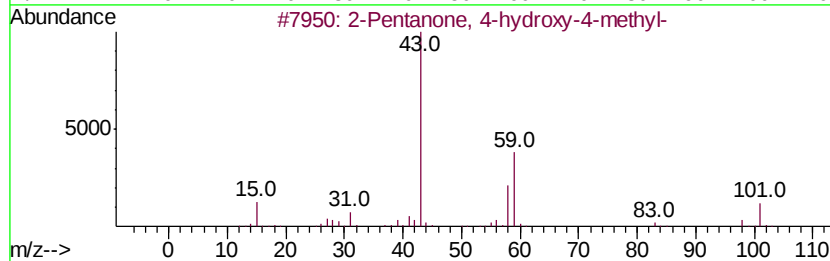
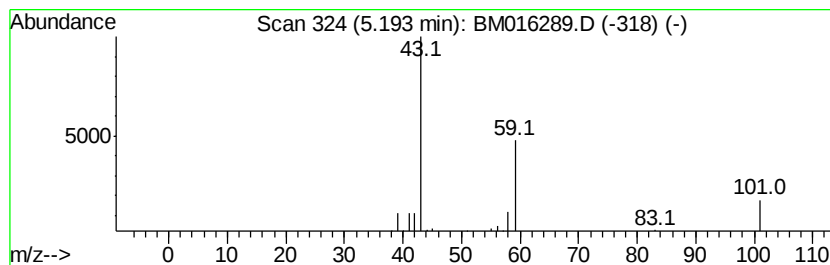
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	4.46 ng	68812	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	56
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
3	Butane	58	C4H10	000106-97-8	12
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9



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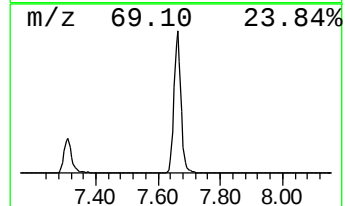
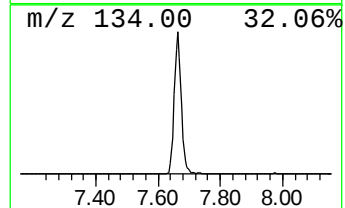
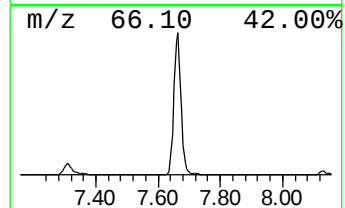
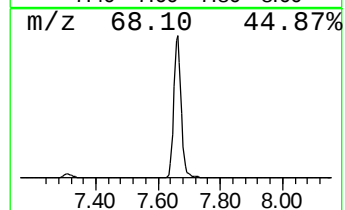
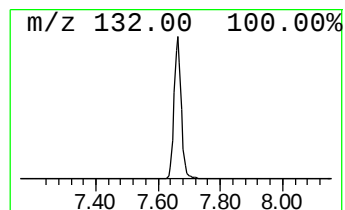
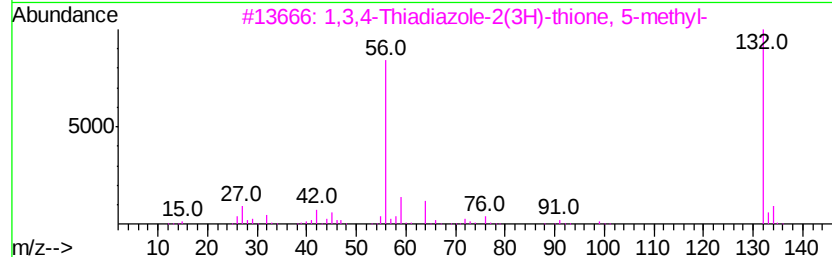
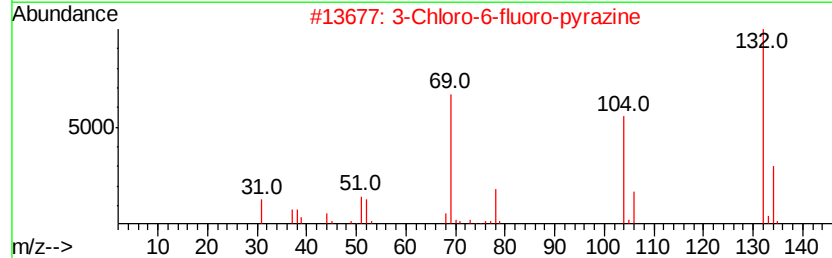
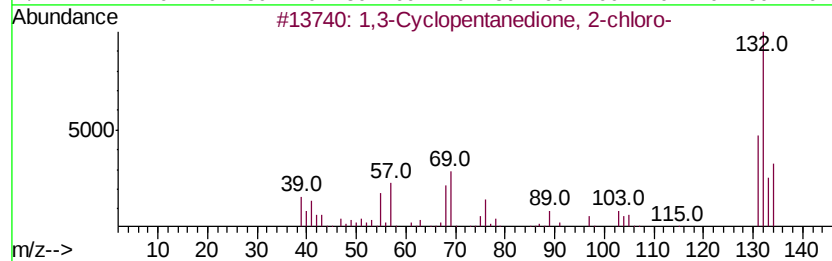
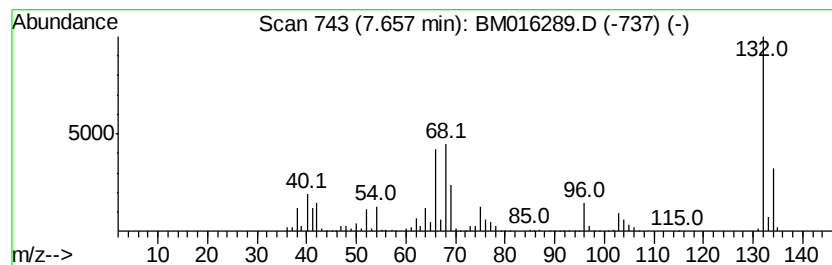
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Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	94.19 ng	1454410	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	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10



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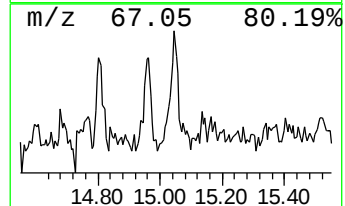
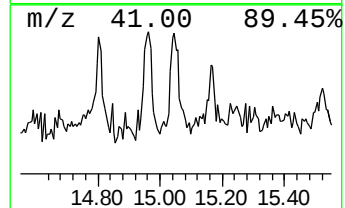
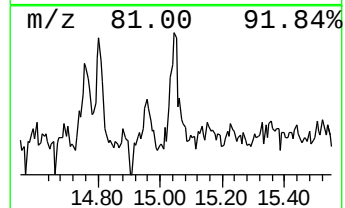
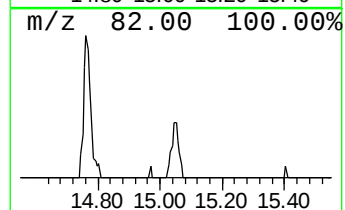
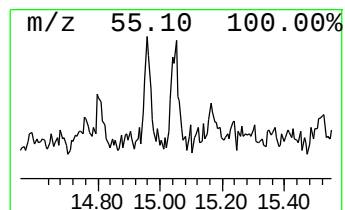
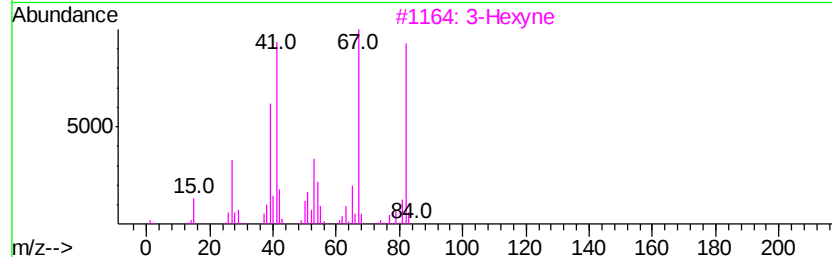
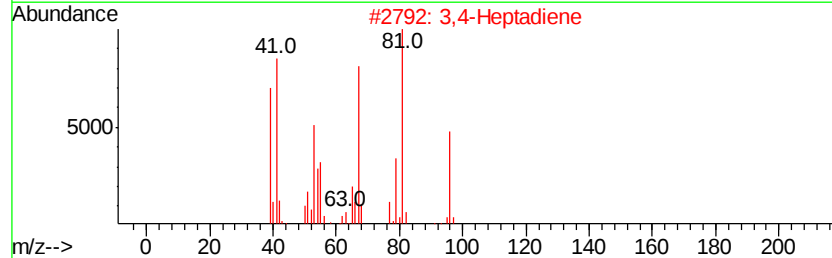
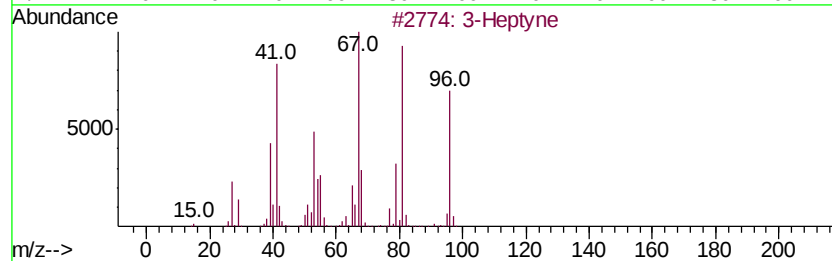
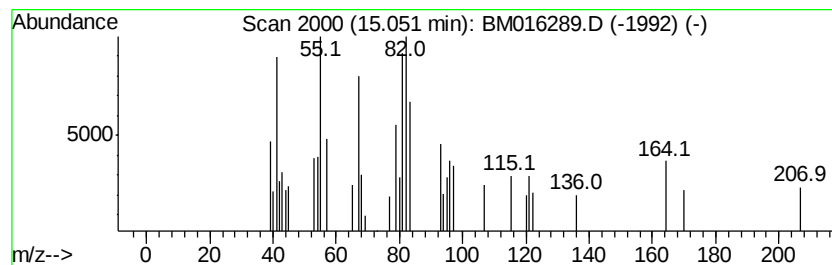
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 3-Heptyne Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	2.17 ng	41763	Acenaphthene-d10	14.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Heptyne	96	C7H12	002586-89-2	64
2		3,4-Heptadiene	96	C7H12	002454-31-1	50
3		3-Hexyne	82	C6H10	000928-49-4	49
4		2,3-Hexadiene, 2-methyl-	96	C7H12	029212-09-7	46
5		1,3-Pentadiene, 2,4-dimethyl-	96	C7H12	001000-86-8	43



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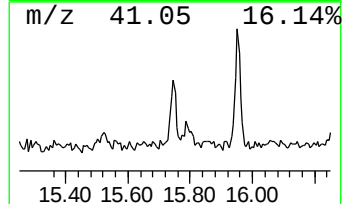
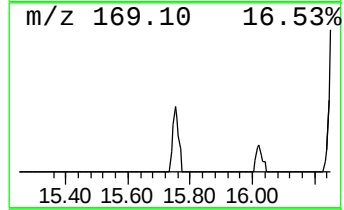
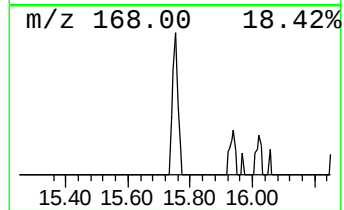
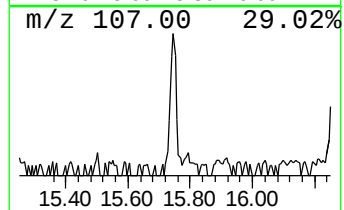
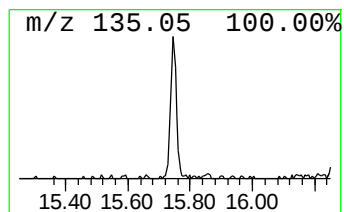
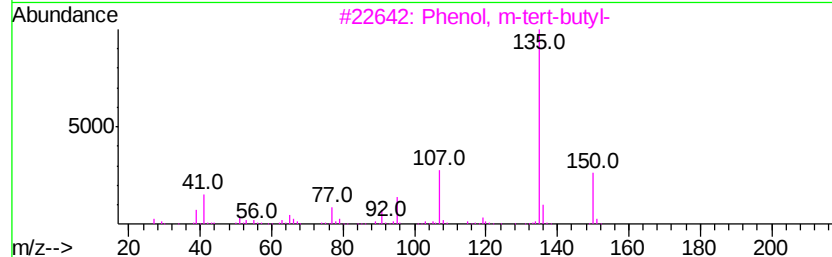
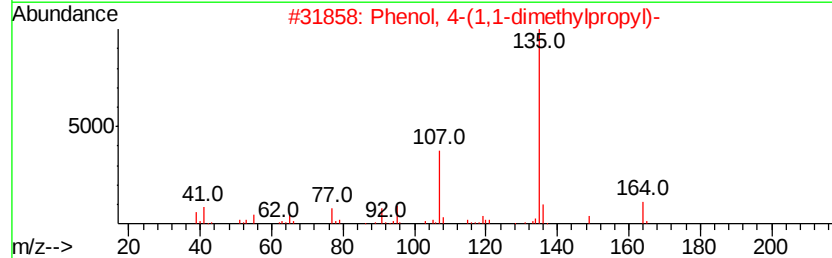
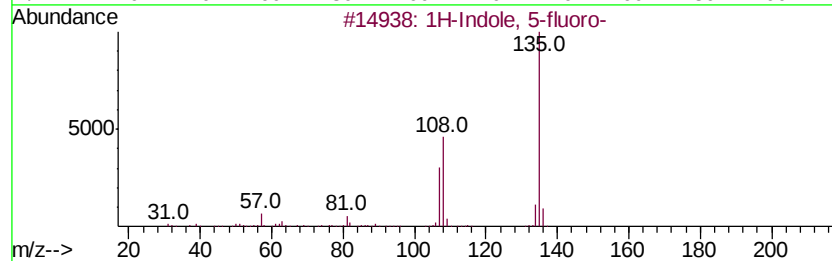
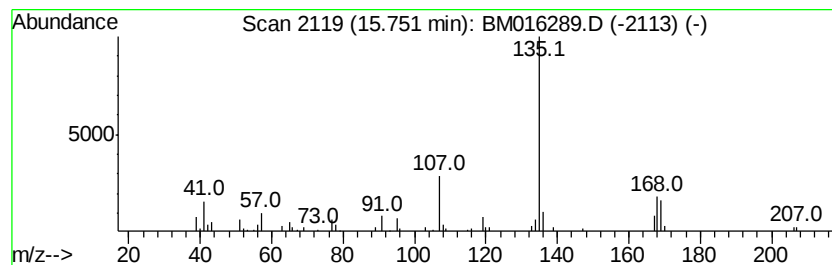
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Peak Number 5 1H-Indole, 5-fluoro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	3.52 ng	67778	Acenaphthene-d10	14.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	64
2		Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	64
3		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
4		((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	59
5		Hexestrol	270	C18H22O2	005635-50-7	53



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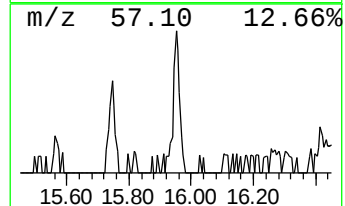
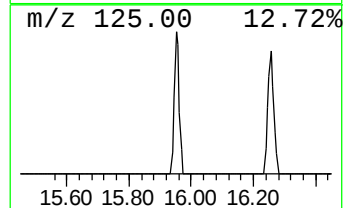
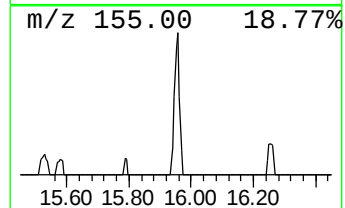
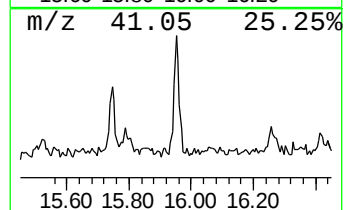
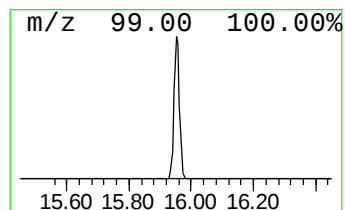
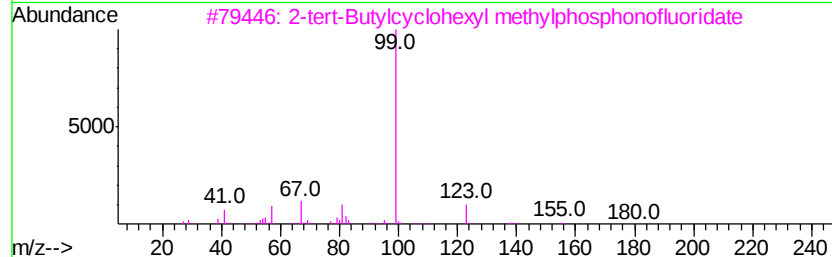
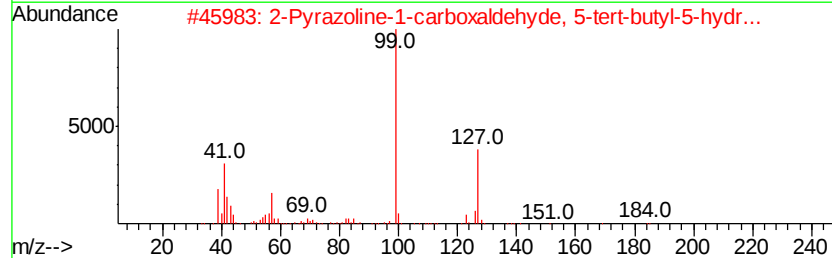
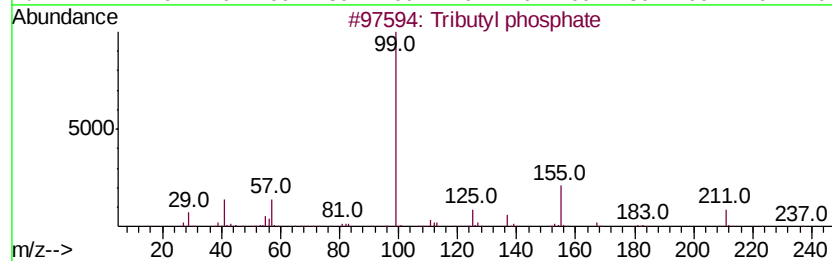
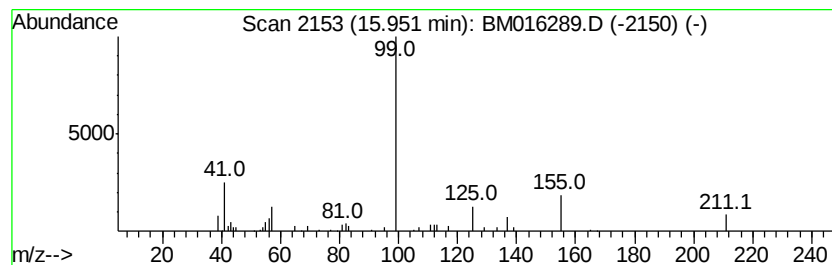
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Peak Number 7 Tributyl phosphate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	3.53 ng	68046	Acenaphthene-d10	14.77
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tributyl phosphate	266 C12H27O4P	000126-73-8 83
2		2-Pyrazoline-1-carboxaldehyde, 5...	184 C9H16N2O2	103214-44-4 42
3		2-tert-Butylcyclohexyl methylpho...	236 C11H22F02P	1000298-39-6 36
4		1,4-Dioxaspiro[4.6]undec-7-ene	154 C9H14O2	007140-60-5 36
5		Spiro(1,3-dioxolane)-2,3'-(pregn...	476 C27H40O7	1000194-70-1 36



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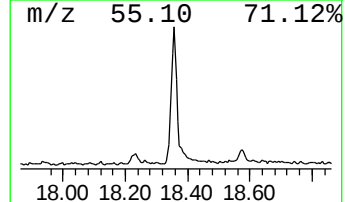
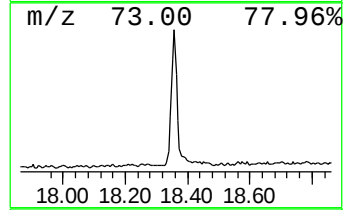
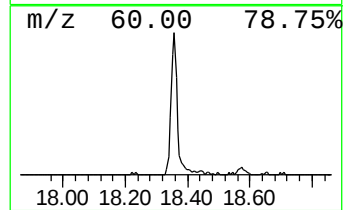
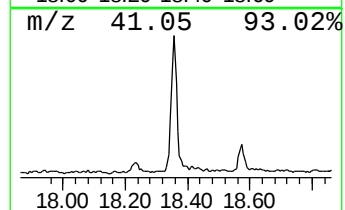
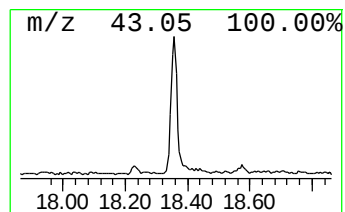
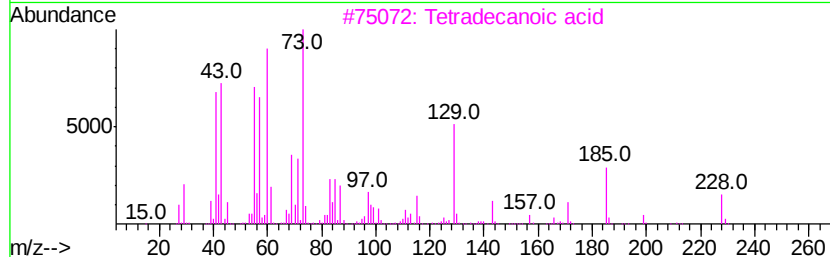
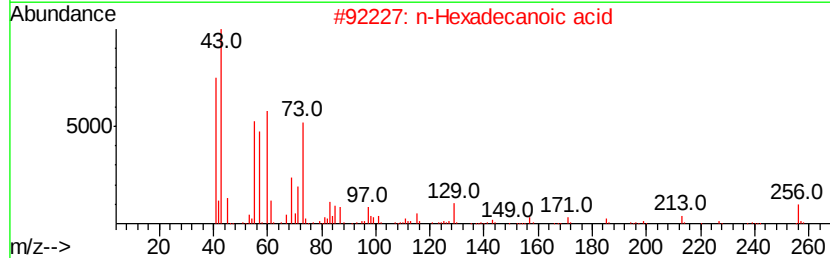
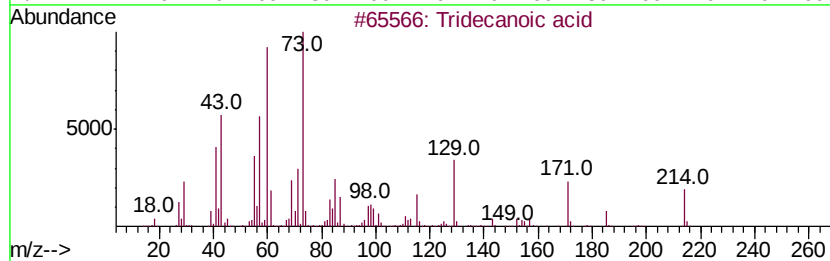
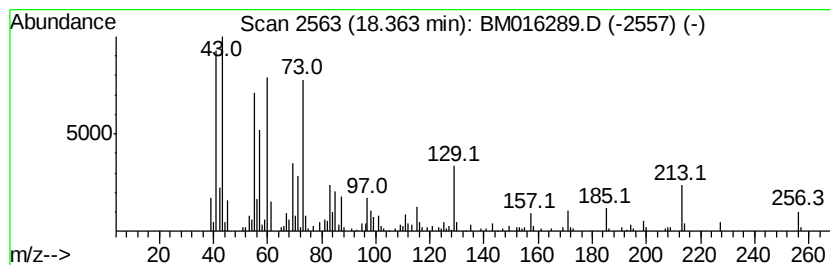
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	20.10 ng	415189	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
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Acq On : 09 Aug 2018 19:44
Operator : SJ/JU
Sample : J4380-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-37

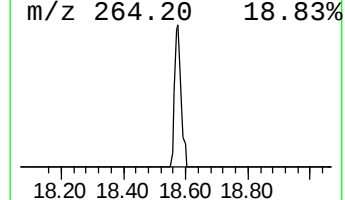
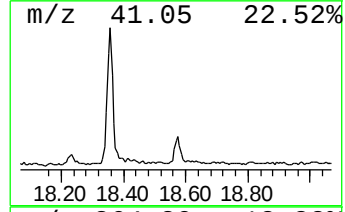
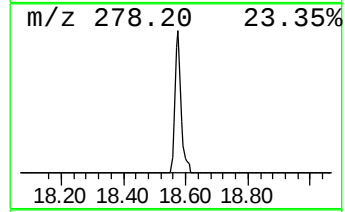
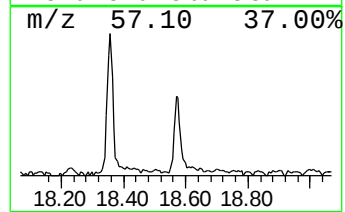
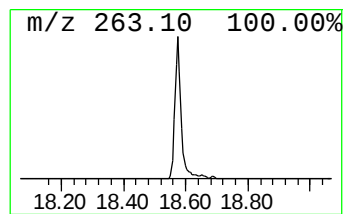
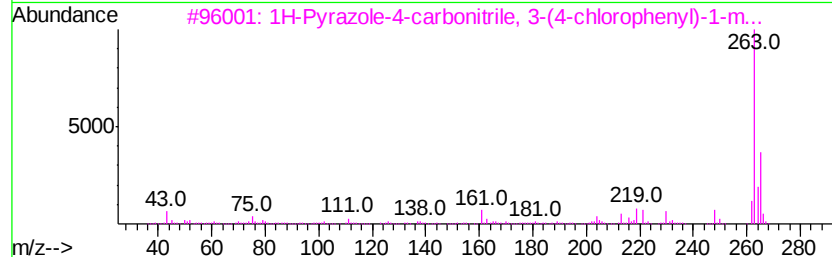
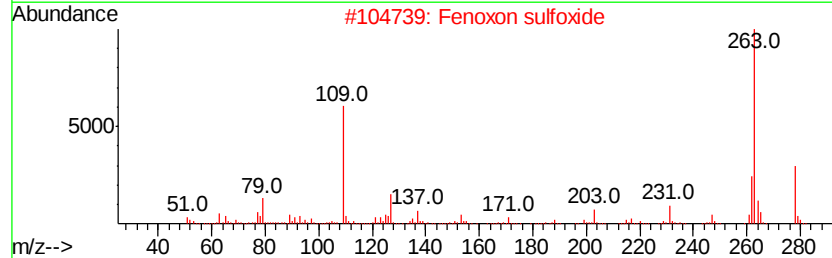
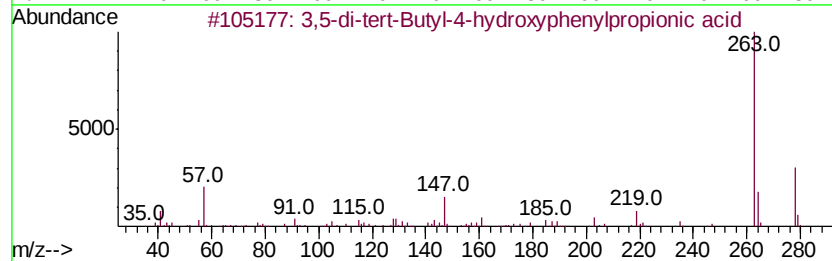
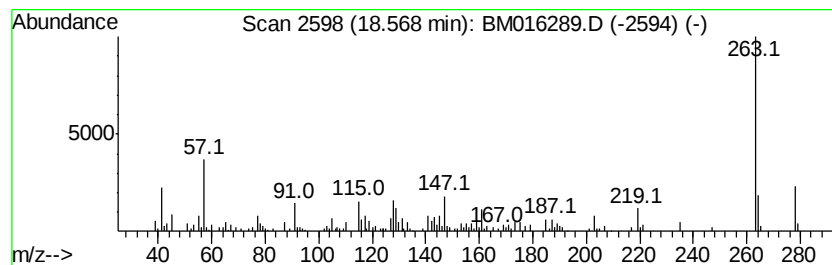
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	12.21 ng	252221	Phenanthrene-d10	17.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-di-tert-Butyl-4-hydroxyphenyl...	278	C17H26O3	020170-32-5	95
2		Fenoxon sulfoxide	278	C10H15O5PS	006552-13-2	58
3		1H-Pyrazole-4-carbonitrile, 3-(4...	263	C12H10ClN3S	068364-67-0	49
4		Pentan-2-one, 4-(2-fluorenylimino)-	263	C18H17NO	050651-58-6	38
5		2-Trifluoromethylbenzo[h]quinoli...	263	C14H8F3NO	001700-94-3	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016289.D
Acq On : 09 Aug 2018 19:44
Operator : SJ/JU
Sample : J4380-01
Misc :
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Instrument :
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ClientSampleId :
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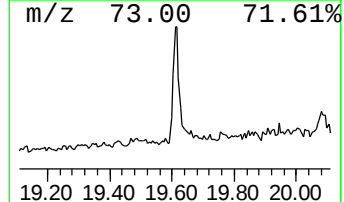
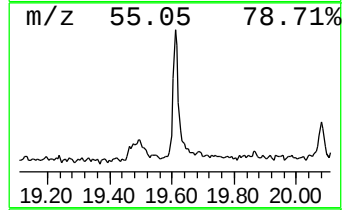
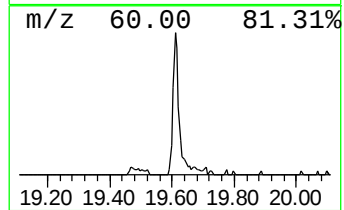
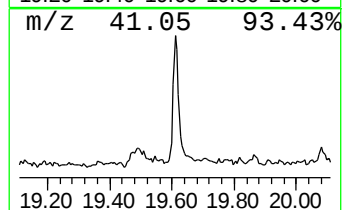
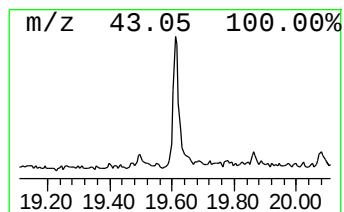
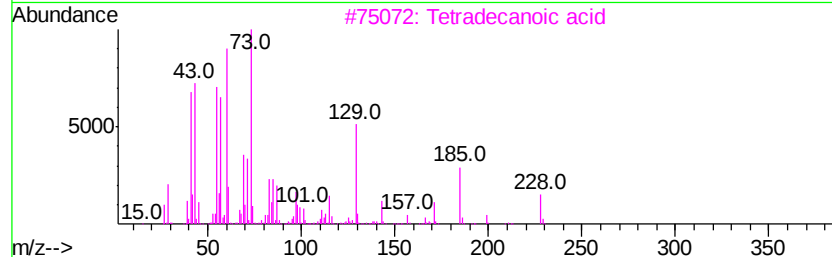
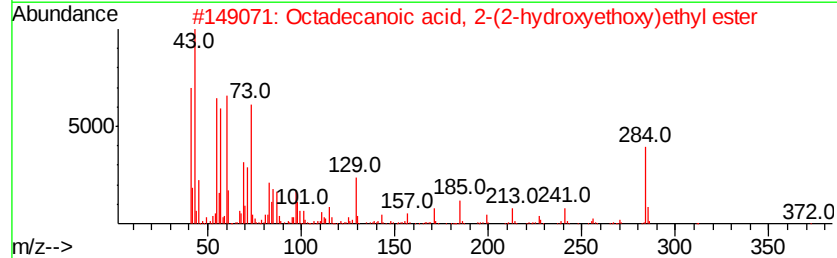
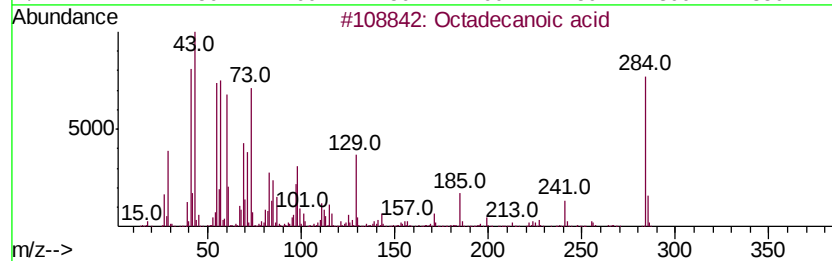
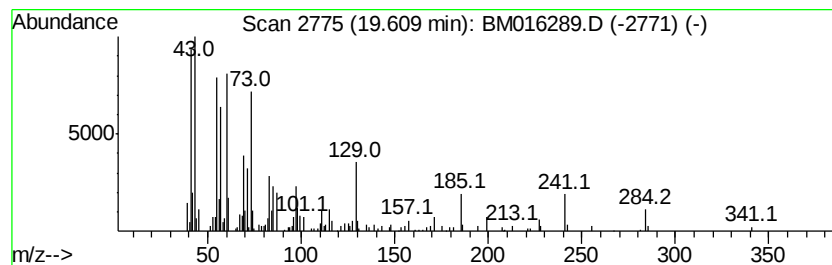
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	10.64 ng	244818	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		Undecanoic acid	186	C11H22O2	000112-37-8	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016289.D
Acq On : 09 Aug 2018 19:44
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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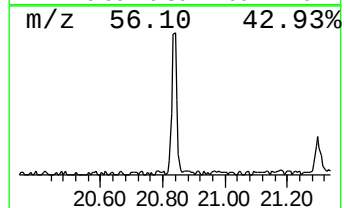
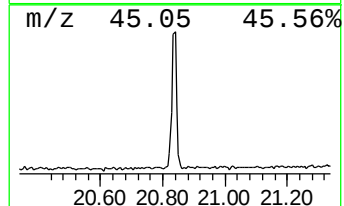
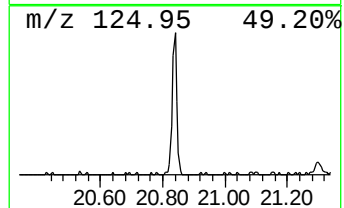
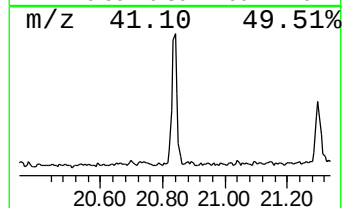
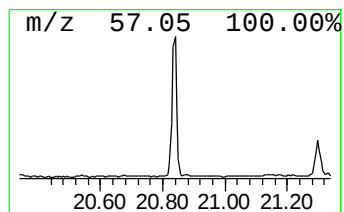
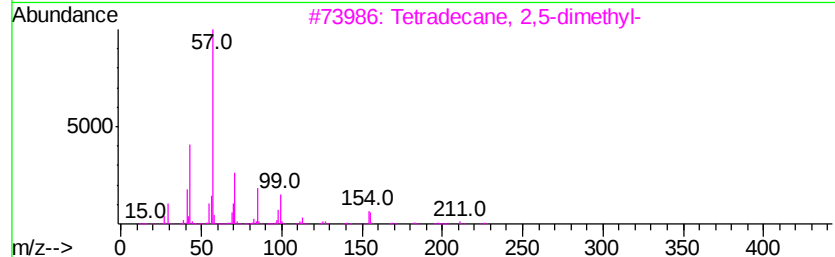
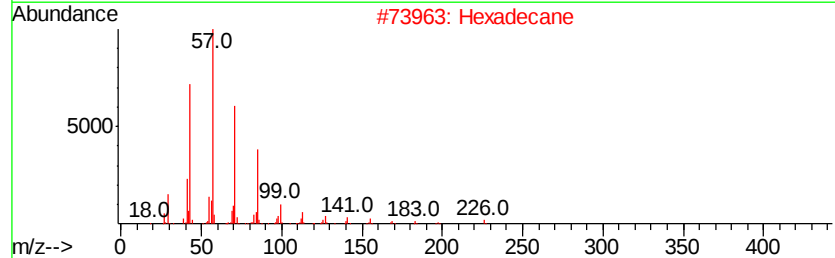
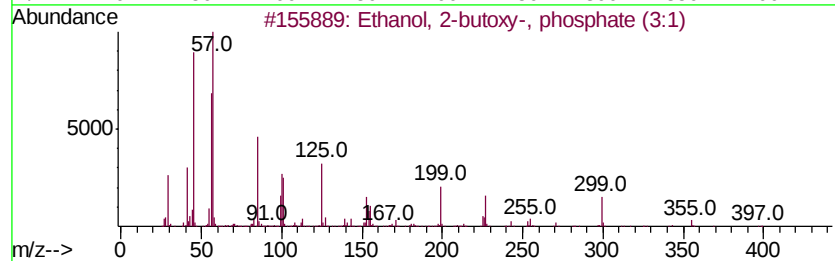
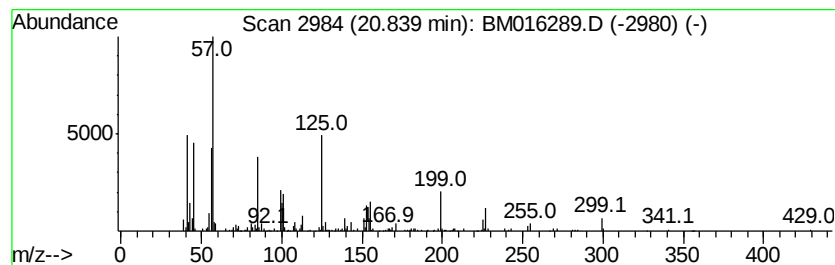
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Ethanol, 2-butoxy-, phospho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.84	12.36 ng	284437	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	50
2		Hexadecane	226	C16H34	000544-76-3	25
3		Tetradecane, 2,5-dimethyl-	226	C16H34	056292-69-4	22
4		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	14
5		Ether, heptyl hexyl	200	C13H28O	007289-40-9	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016289.D
Acq On : 09 Aug 2018 19:44
Operator : SJ/JU
Sample : J4380-01
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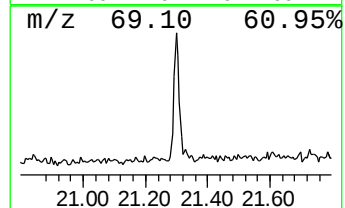
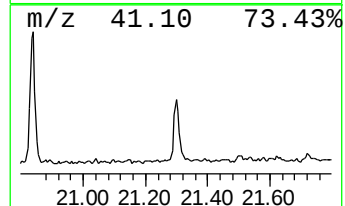
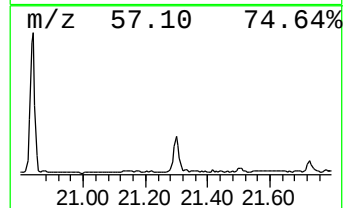
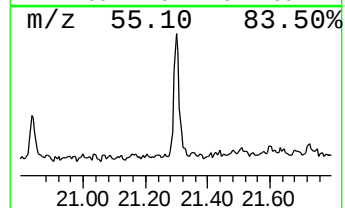
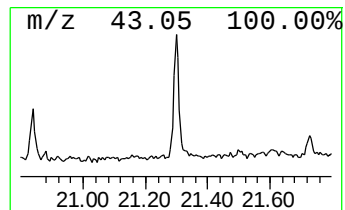
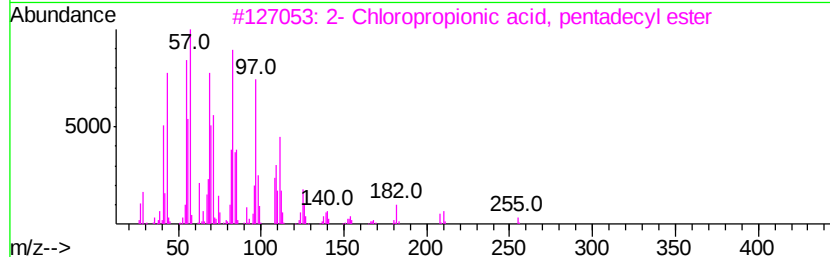
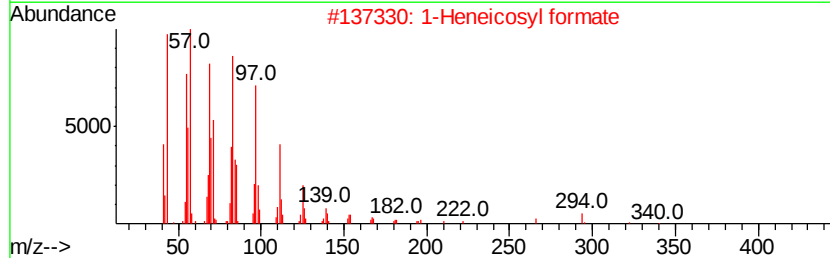
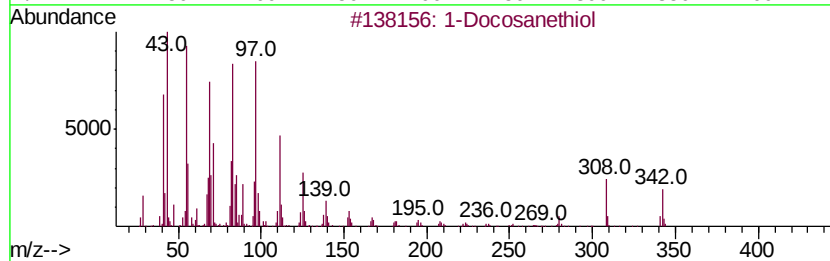
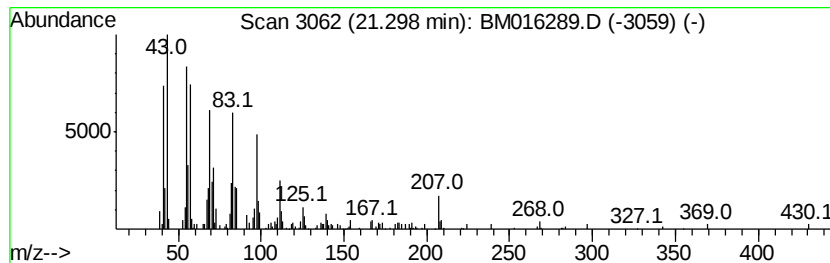
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Docosanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.30	6.59 ng	151610	Chrysene-d12	21.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1	Docosanethiol	342	C22H46S	007773-83-3	93
2	1	Heneicosyl formate	340	C22H44O2	077899-03-7	91
3	2	Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	90
4	1	Tricosanol	340	C23H48O	003133-01-5	87
5	11	Tricosene	322	C23H46	052078-56-5	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016289.D
Acq On : 09 Aug 2018 19:44
Operator : SJ/JU
Sample : J4380-01
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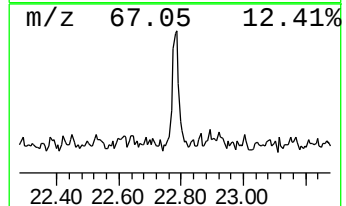
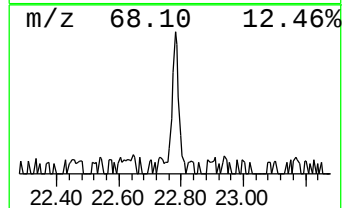
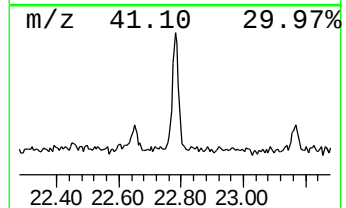
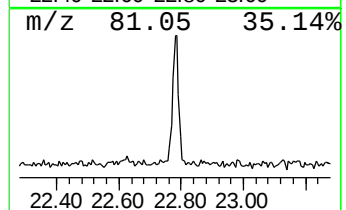
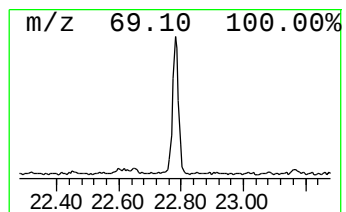
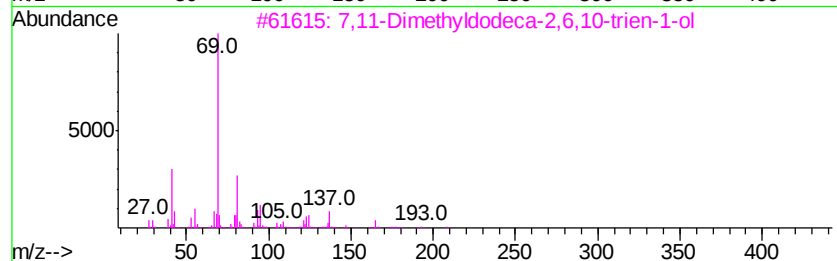
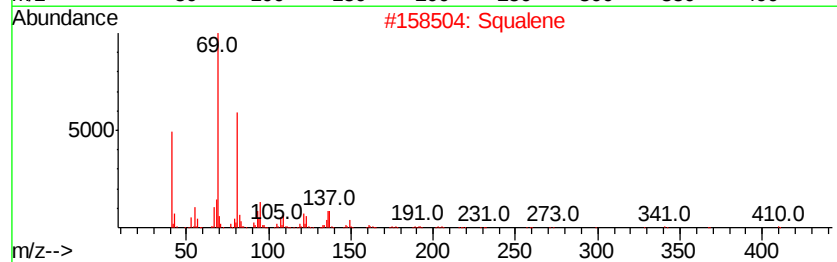
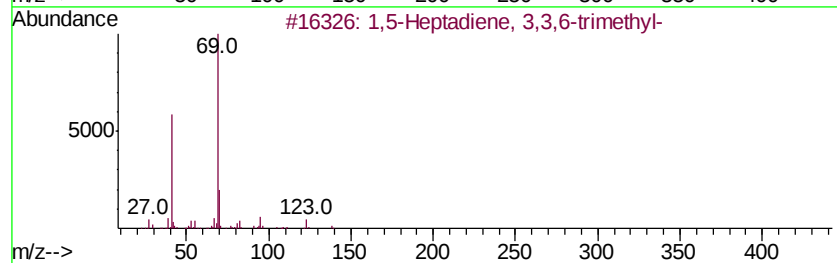
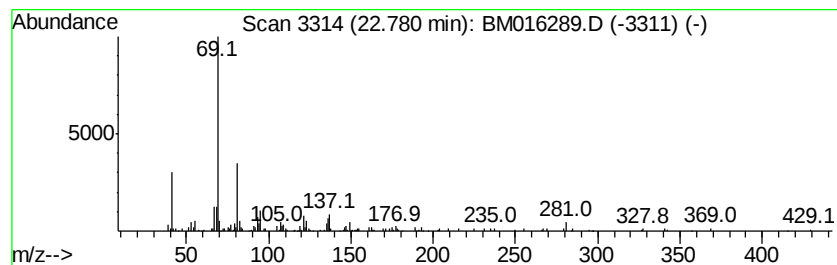
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1,5-Heptadiene, 3,3,6-trime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.78	6.94 ng	159577	Chrysene-d12	21.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	72
2	Squalene	410	C30H50	007683-64-9	72
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	64
5	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080918\
Data File : BM016289.D
Acq On : 09 Aug 2018 19:44
Operator : SJ/JU
Sample : J4380-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	4.5	ng	68812	1	8.13	308817	20.0
unknown7.66	7.66	94.2	ng	1454410	1	8.13	308817	20.0
3-Heptyne	15.05	2.2	ng	41763	3	14.77	385062	20.0
1H-Indole, 5-fluoro-	15.75	3.5	ng	67778	3	14.77	385062	20.0
Tributyl phosphate	15.95	3.5	ng	68046	3	14.77	385062	20.0
Tridecanoic acid	18.36	20.1	ng	415189	4	17.50	413191	20.0
3,5-di-tert-Butyl...	18.57	12.2	ng	252221	4	17.50	413191	20.0
Octadecanoic acid	19.61	10.6	ng	244818	5	21.63	460187	20.0
Ethanol, 2-butoxy...	20.84	12.4	ng	284437	5	21.63	460187	20.0
1-Docosanethiol	21.30	6.6	ng	151610	5	21.63	460187	20.0
1,5-Heptadiene, 3...	22.78	6.9	ng	159577	5	21.63	460187	20.0