

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
 Data File : BM015930.D
 Acq On : 13 Jul 2018 00:24
 Operator : SJ/JU
 Sample : J3951-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 071018-DBRI-E-U-M

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-BM070518.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	5.316	340	345	357	rVB	34709	59380	1.02%	0.233%
2	5.792	420	426	443	rBV	499493	815257	14.02%	3.196%
3	7.439	700	706	724	rBV	347820	616675	10.60%	2.417%
4	7.810	763	769	784	rBV	1041682	1708419	29.38%	6.697%
5	8.286	842	850	863	rBV	317306	521239	8.96%	2.043%
6	8.610	898	905	916	rBV	1390962	2291207	39.40%	8.982%
7	9.475	1045	1052	1064	rBV	1193330	2006091	34.50%	7.864%
8	11.110	1324	1330	1340	rBV	361337	640296	11.01%	2.510%
9	13.533	1735	1742	1752	rBV	2694409	3842812	66.08%	15.064%
10	14.357	1877	1882	1896	rVB	79188	117053	2.01%	0.459%
11	14.904	1964	1975	1988	rVB2	503762	810312	13.93%	3.176%
12	16.162	2184	2189	2197	rBV	150308	179787	3.09%	0.705%
13	16.386	2221	2227	2241	rBV	1372778	1971162	33.90%	7.727%
14	17.633	2433	2439	2450	rBV2	600411	884807	15.22%	3.468%
15	18.468	2577	2581	2586	rBV2	137089	178063	3.06%	0.698%
16	19.721	2790	2794	2804	rVB2	64569	93337	1.61%	0.366%
17	20.197	2869	2875	2881	rBV	5065959	5815358	100.00%	22.796%
18	20.944	2999	3002	3006	rBV2	76130	84905	1.46%	0.333%
19	21.403	3076	3080	3088	rBV2	164253	312667	5.38%	1.226%
20	21.744	3133	3138	3146	rBV	716514	953071	16.39%	3.736%
21	21.833	3150	3153	3159	rVB	112818	131434	2.26%	0.515%
22	22.286	3227	3230	3235	rBV	108649	133423	2.29%	0.523%
23	22.774	3310	3313	3319	rVB	108259	134093	2.31%	0.526%
24	22.915	3334	3337	3343	rVB	126505	167359	2.88%	0.656%
25	23.309	3401	3404	3410	rVB	98302	141848	2.44%	0.556%
26	24.132	3538	3544	3552	rVB2	456877	900141	15.48%	3.529%

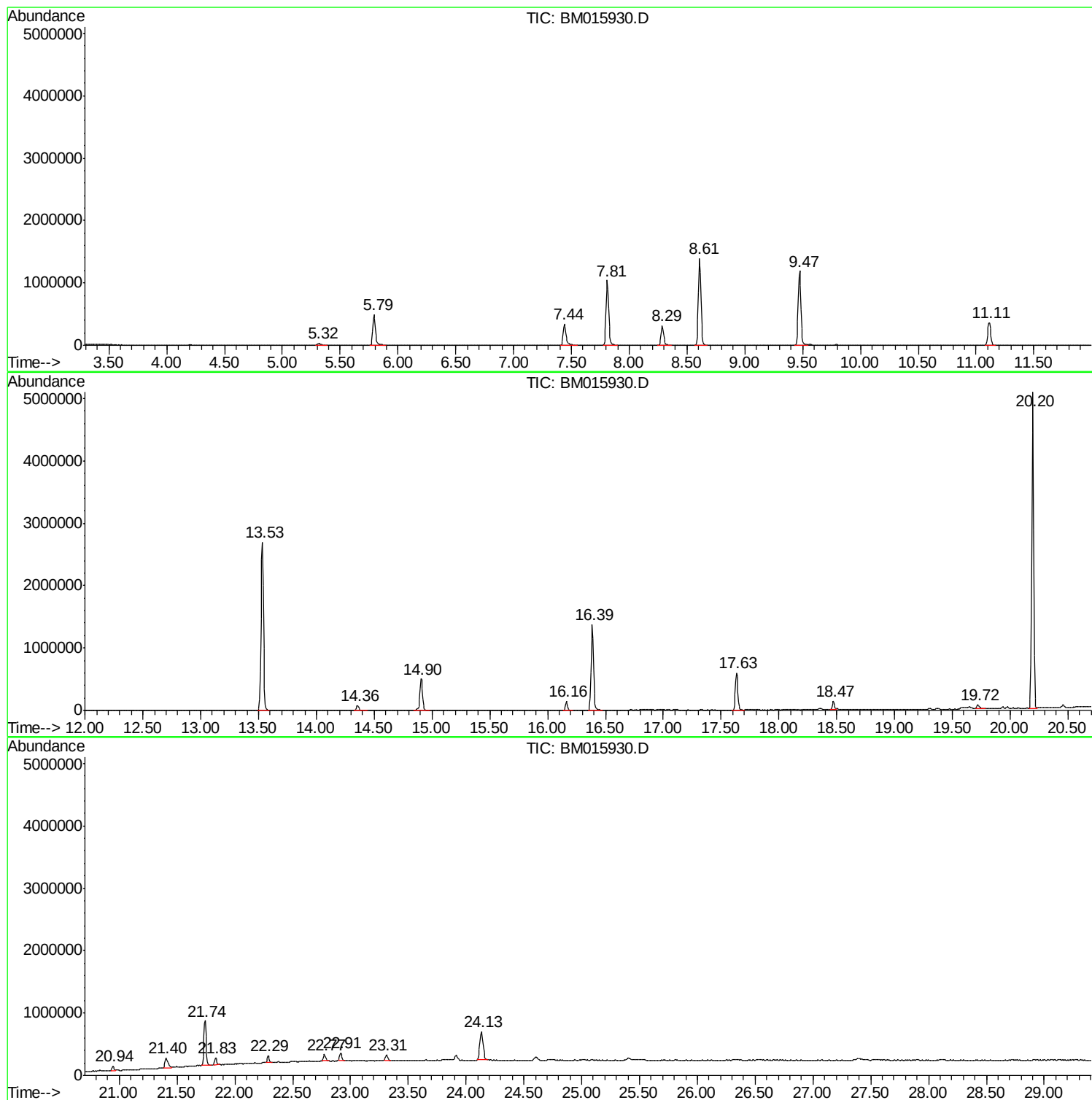
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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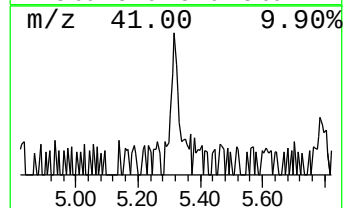
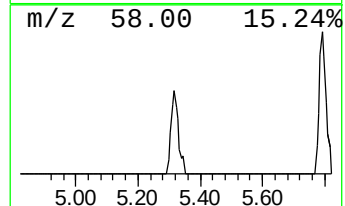
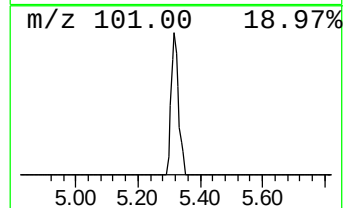
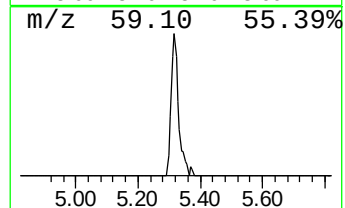
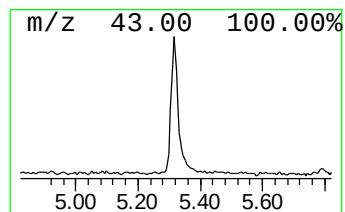
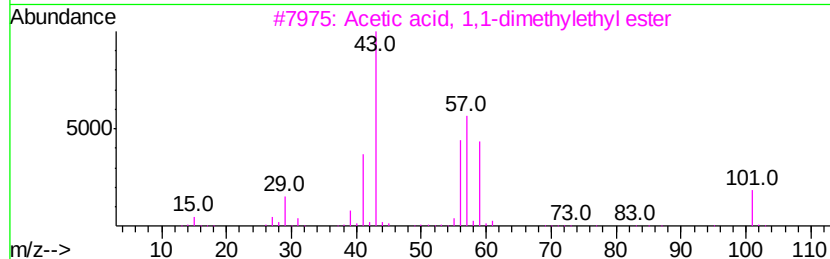
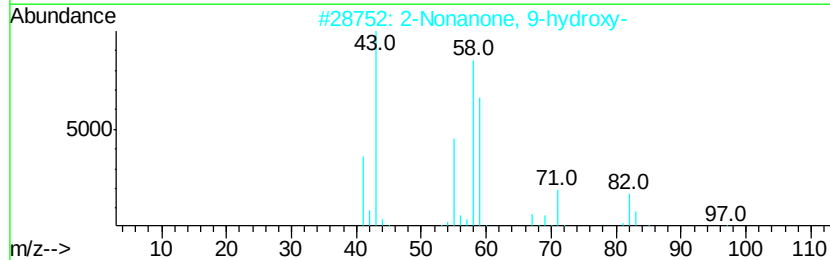
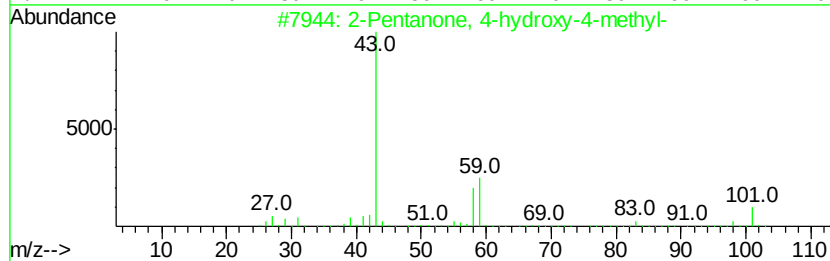
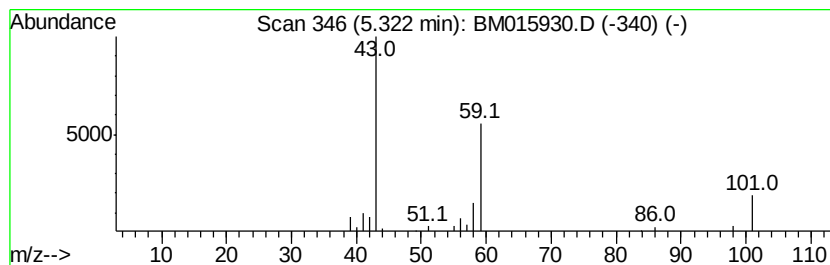
Instrument :
BNA_M
ClientSampleId :
071018-DBRI-E-U-M

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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 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.32	2.28 ng	59380	1,4-Dichlorobenzene-d4	8.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	9
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4	Diacetamide	101	C4H7NO2	000625-77-4	7
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7



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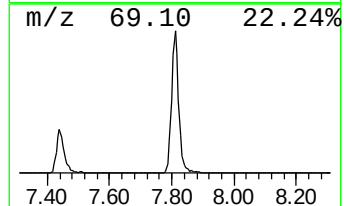
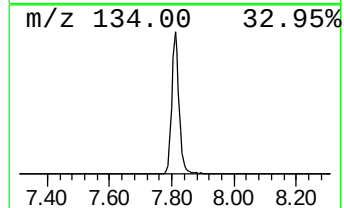
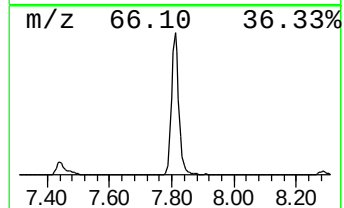
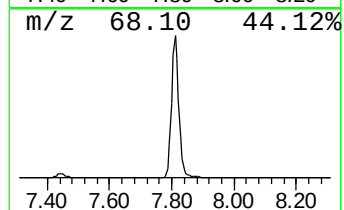
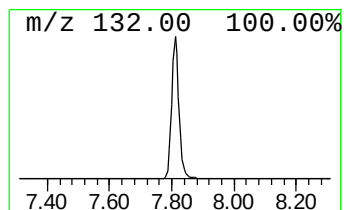
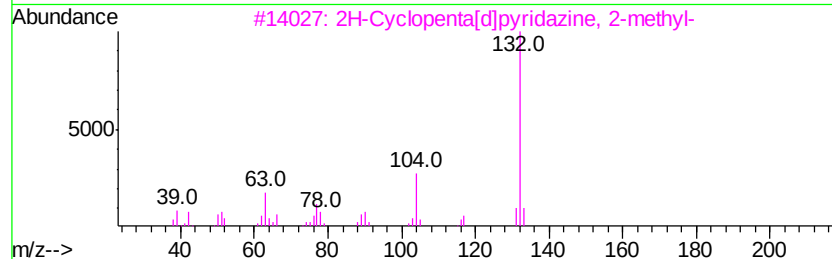
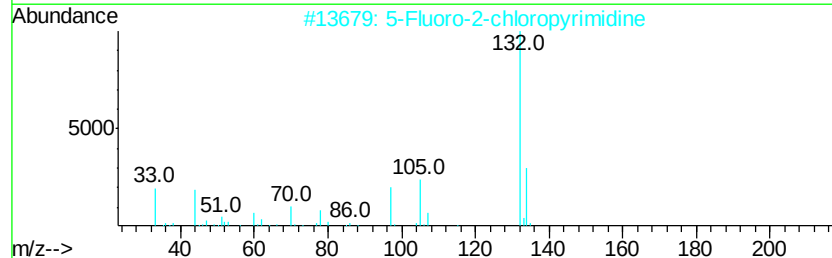
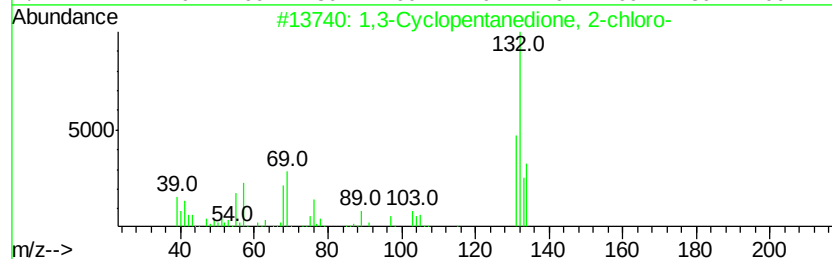
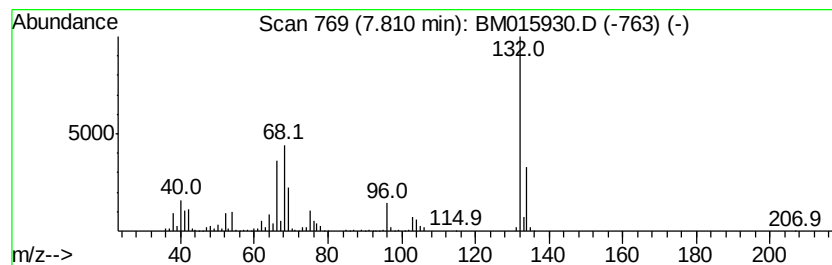
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Peak Number 2 unknown7.81 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	65.55 ng	1708420	1,4-Dichlorobenzene-d4	8.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	27
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	27
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	22



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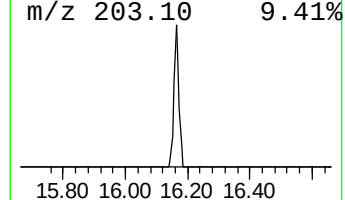
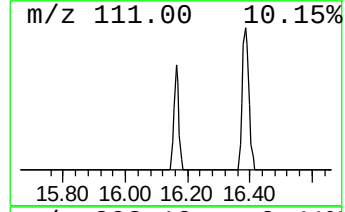
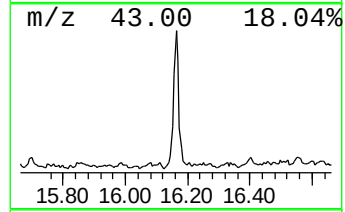
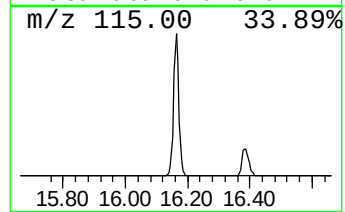
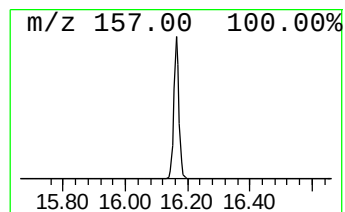
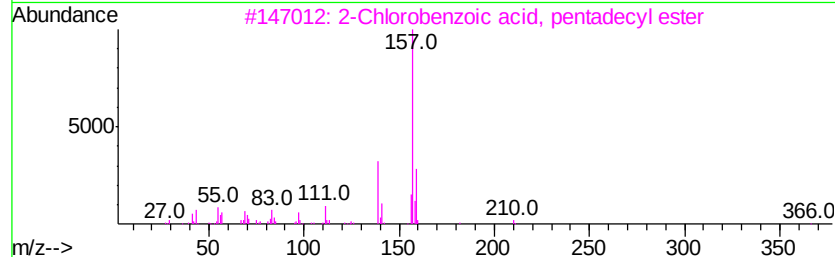
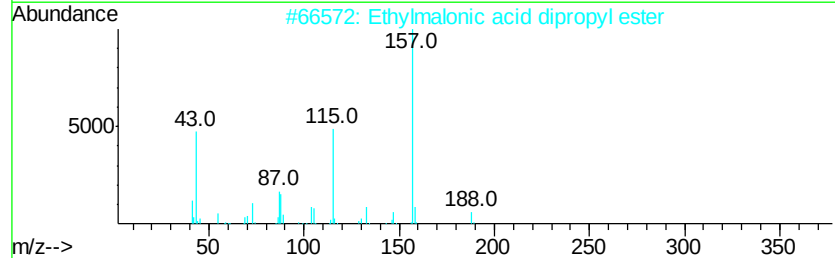
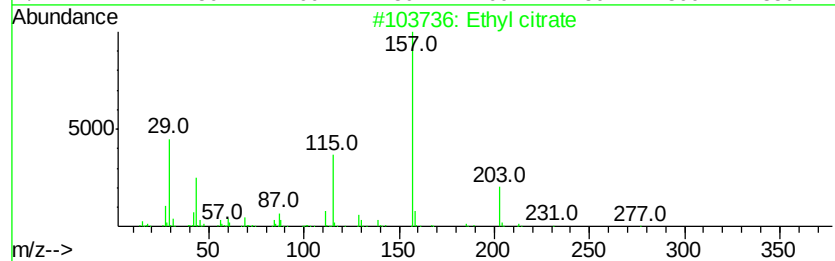
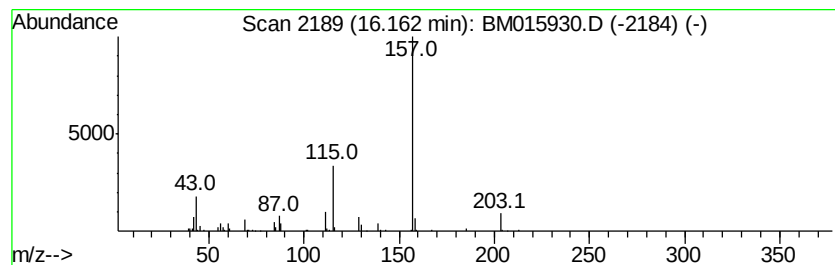
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Peak Number 4 Ethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	4.44 ng	179787	Acenaphthene-d10	14.90
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Ethyl citrate	276 C12H20O7	000077-93-0 83
2		Ethylmalonic acid dipropyl ester	216 C11H20O4	001113-91-3 64
3		2-Chlorobenzoic acid, pentadecyl...	366 C22H35ClO2	1000292-43-0 28
4		2-Chlorobenzoic acid, heptadecyl...	394 C24H39ClO2	1000292-28-3 10
5		4-Quinolinecarboxylic acid, 3-hy...	203 C11H9NO3	000117-57-7 9



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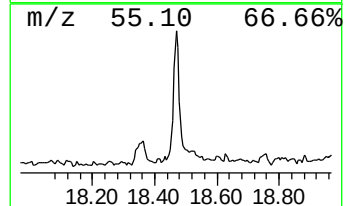
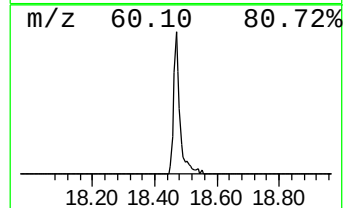
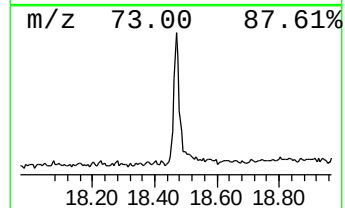
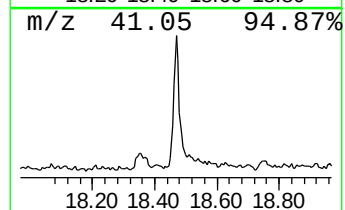
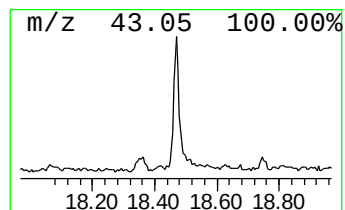
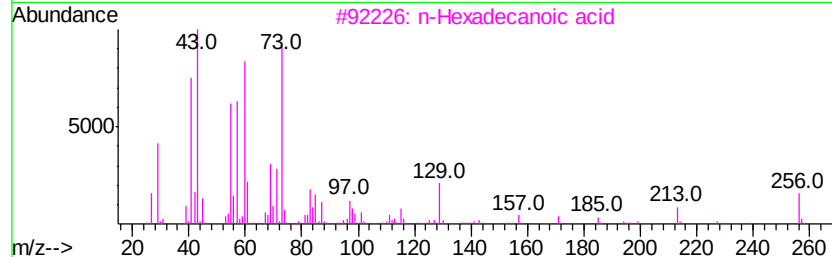
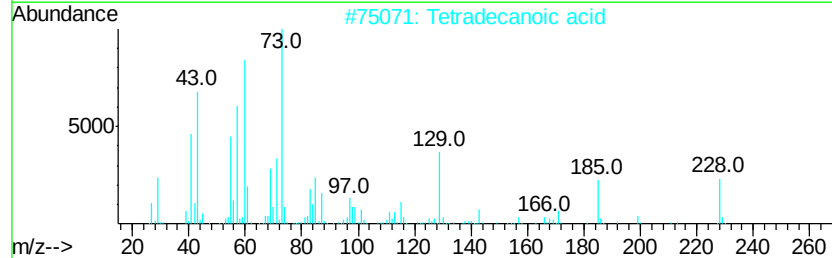
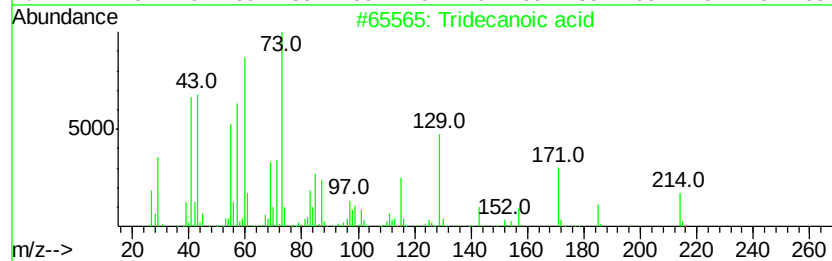
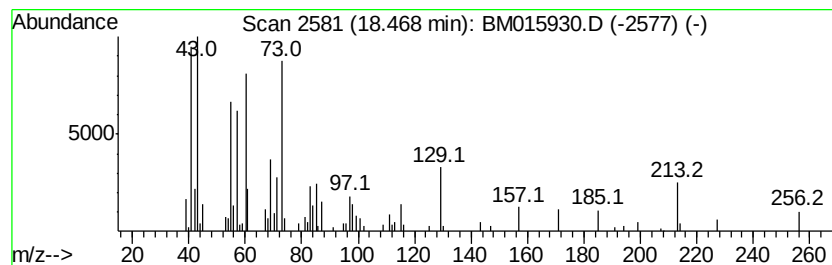
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Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	4.02 ng	178063	Phenanthrene-d10	17.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecanoic acid	214	C13H26O2	000638-53-9	94
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4		Undecanoic acid	186	C11H22O2	000112-37-8	53
5		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	47



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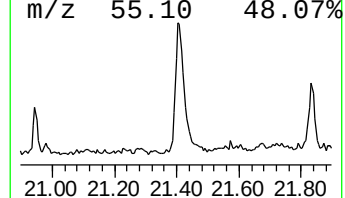
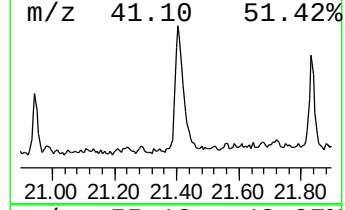
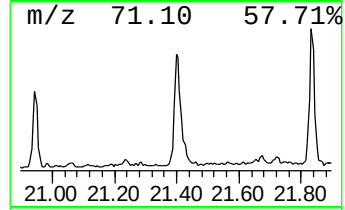
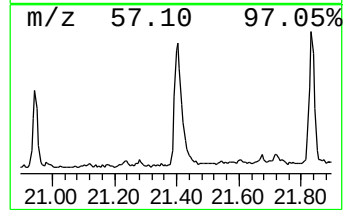
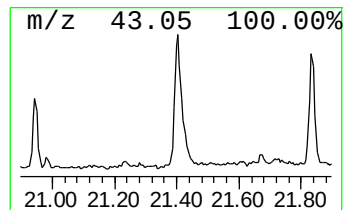
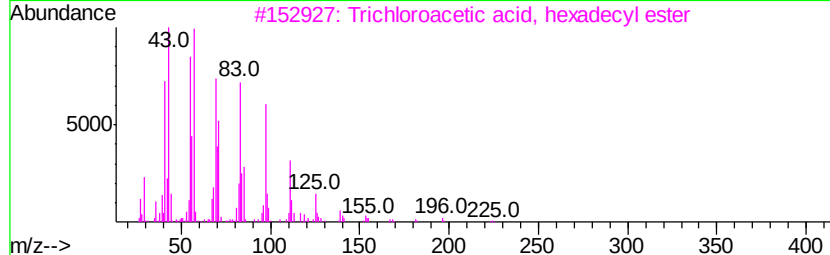
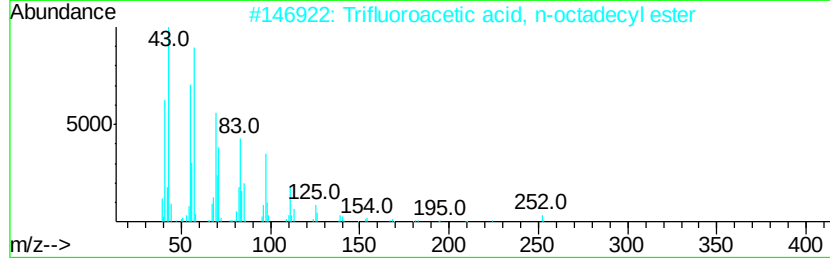
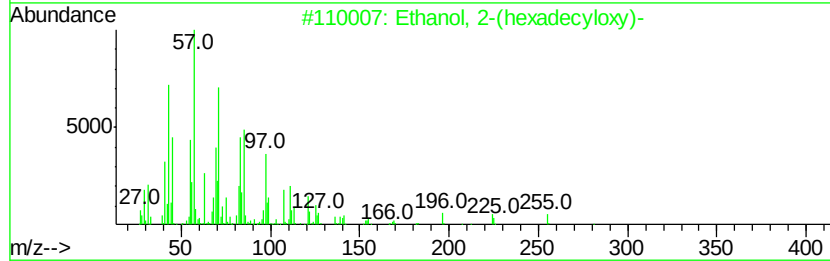
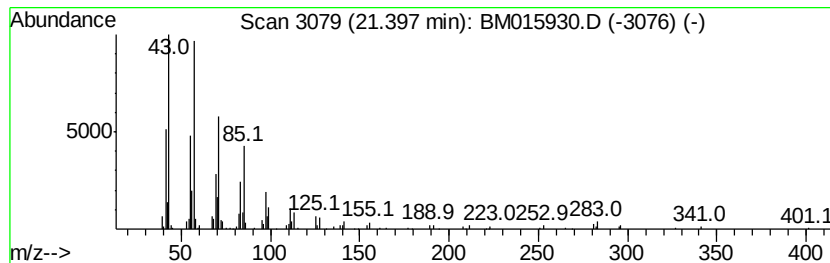
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethanol, 2-(hexadecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.		
21.40	6.56 ng	312667	Chrysene-d12		21.74		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87
2			Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	70
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	62
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	62
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	62



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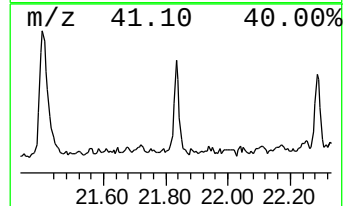
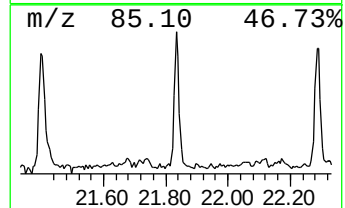
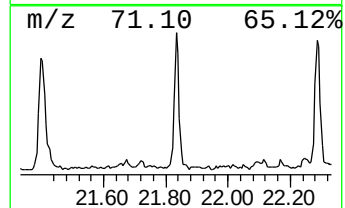
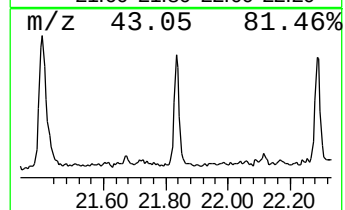
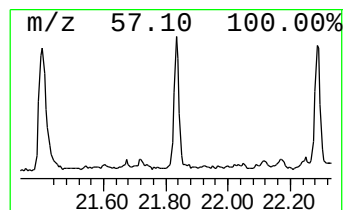
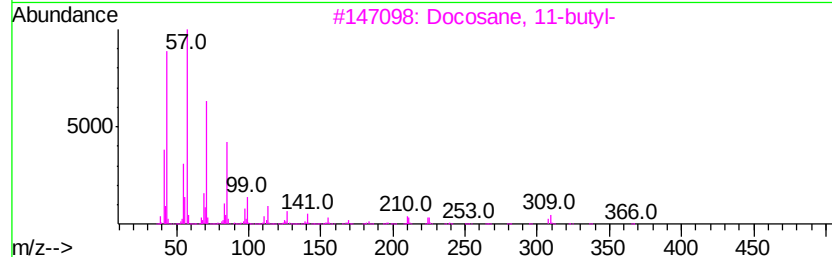
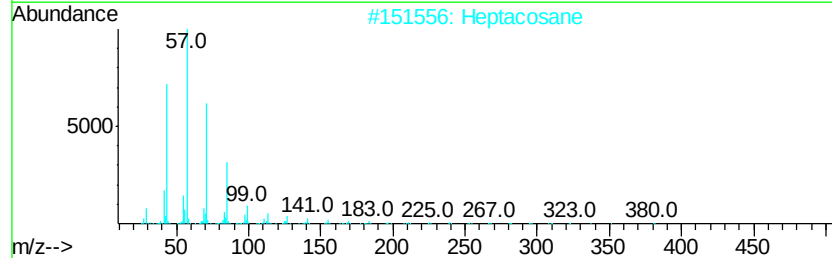
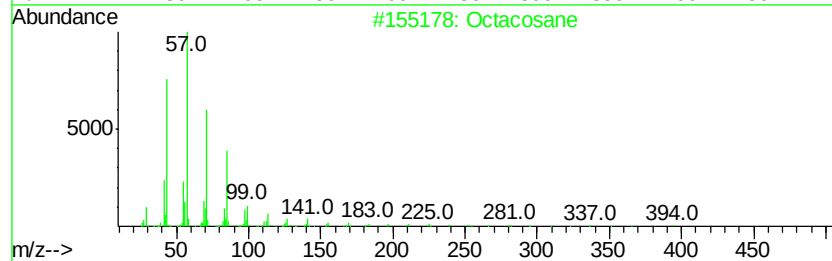
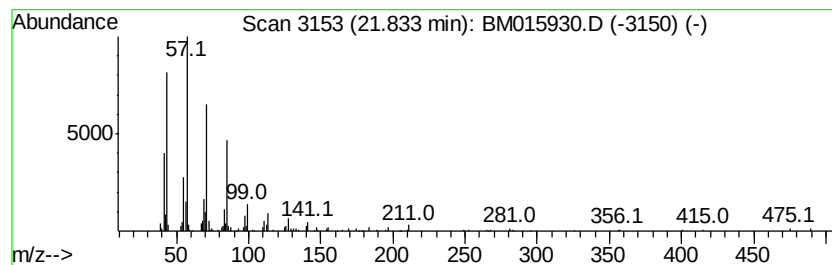
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.83	2.76 ng	131434	Chrysene-d12	21.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Heptacosane	380	C27H56	000593-49-7	90
3		Docosane, 11-butyl-	366	C26H54	013475-76-8	90
4		Docosane, 9-butyl-	366	C26H54	055282-14-9	90
5		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015930.D
Acq On : 13 Jul 2018 00:24
Operator : SJ/JU
Sample : J3951-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
071018-DBRI-E-U-M

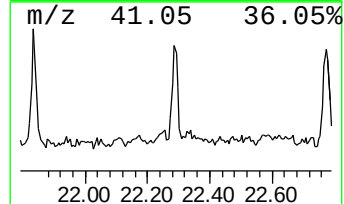
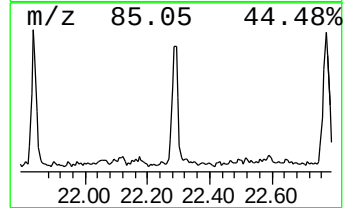
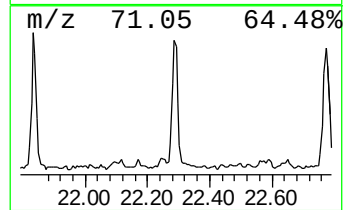
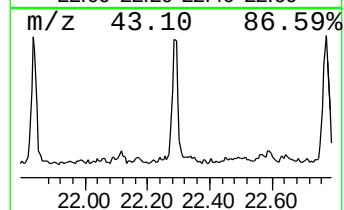
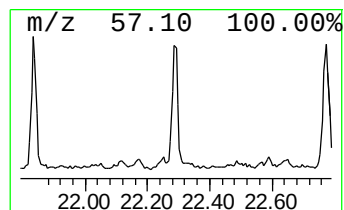
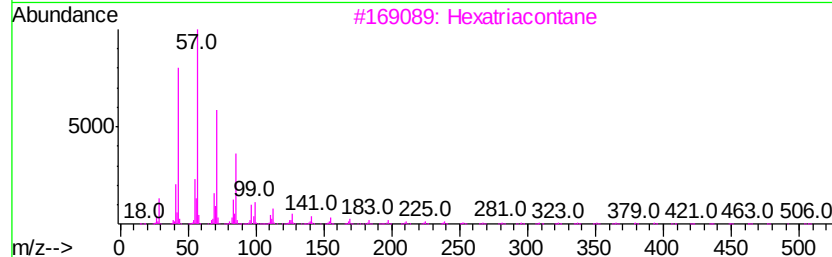
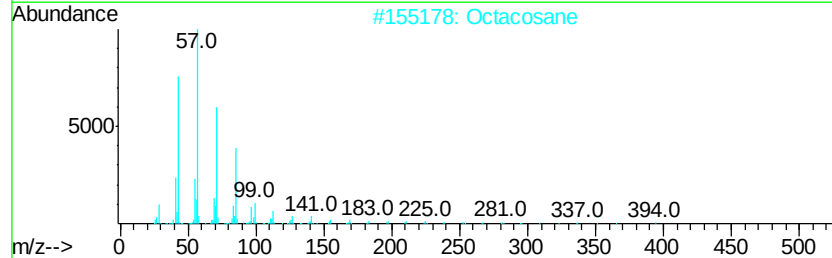
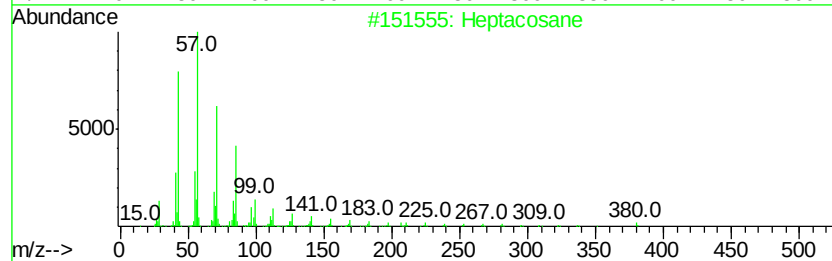
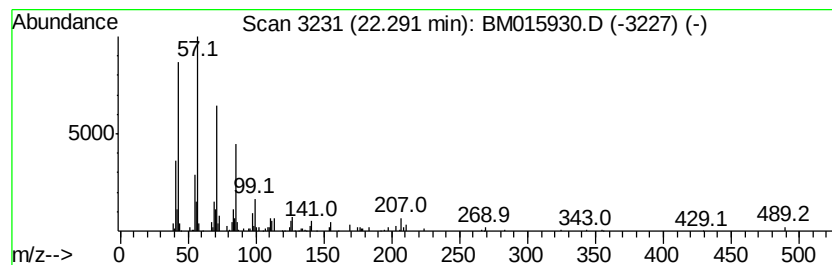
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.29	2.80 ng	133423	Chrysene-d12	21.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	87
2		Octacosane	394	C28H58	000630-02-4	87
3		Hexatriacontane	507	C36H74	000630-06-8	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015930.D
Acq On : 13 Jul 2018 00:24
Operator : SJ/JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
071018-DBRI-E-U-M

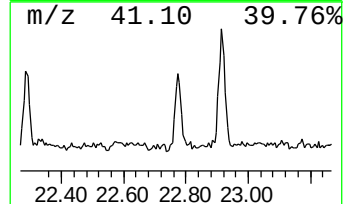
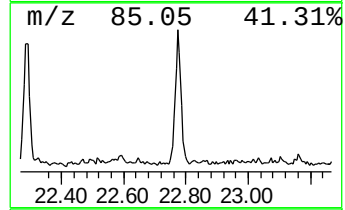
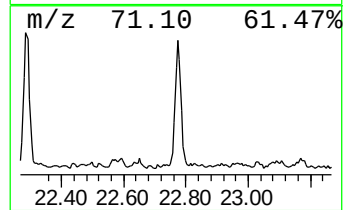
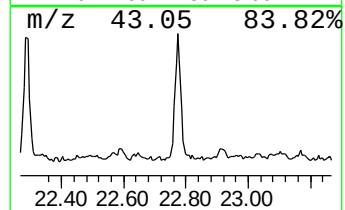
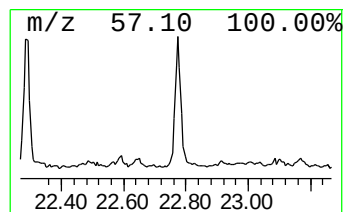
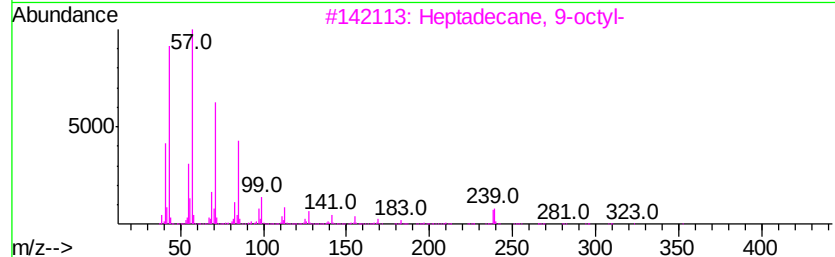
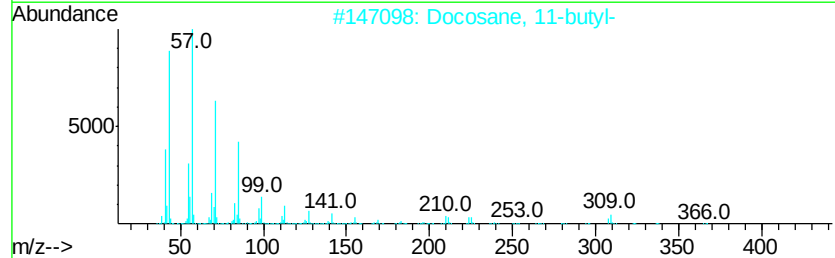
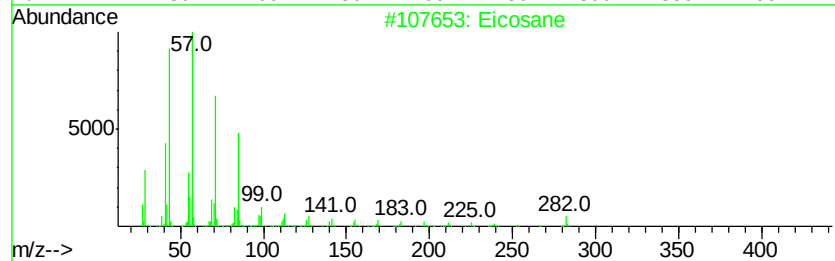
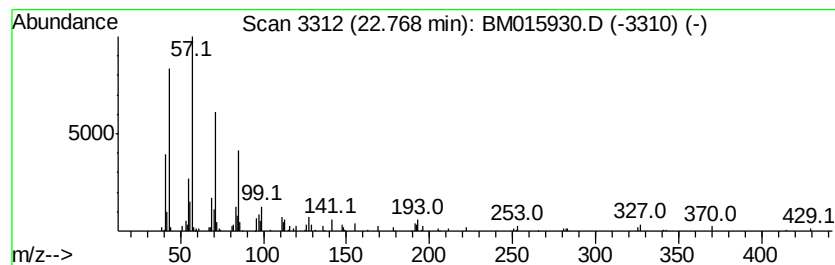
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	2.81 ng	134093	Chrysene-d12	21.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	98
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	87
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Hentriacontane	437	C31H64	000630-04-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015930.D
Acq On : 13 Jul 2018 00:24
Operator : SJ/JU
Sample : J3951-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

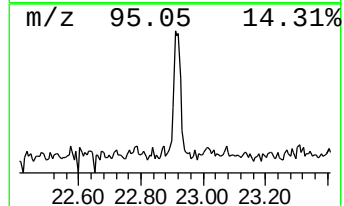
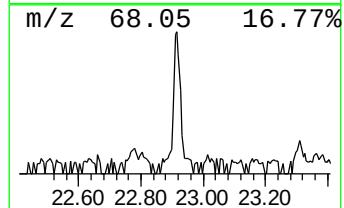
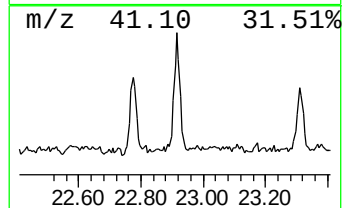
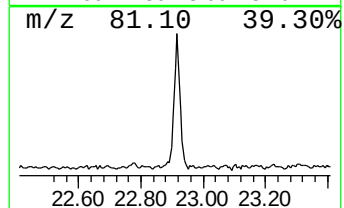
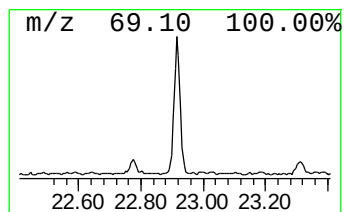
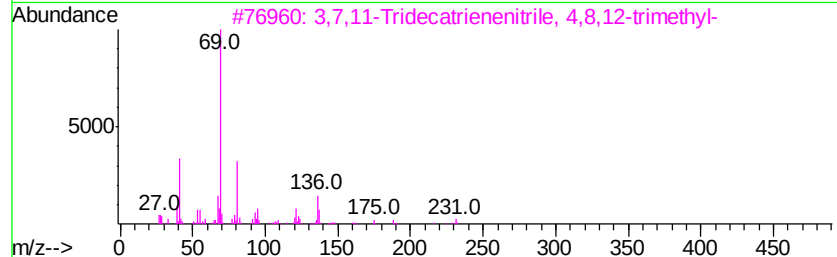
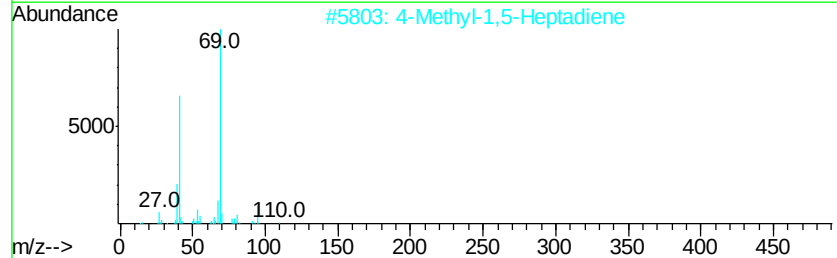
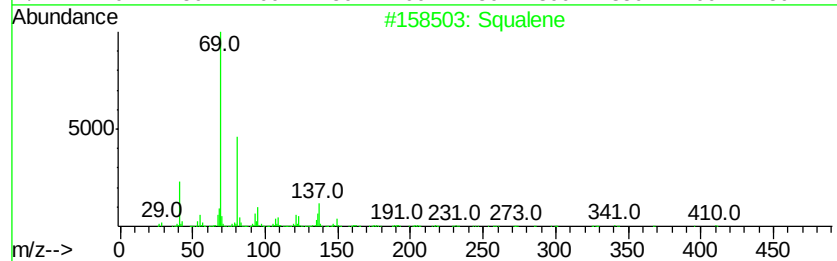
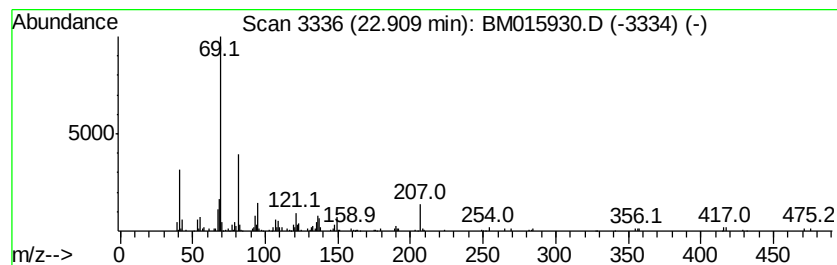
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.91	3.51 ng	167359	Chrysene-d12	21.74	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	72
2	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	64
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64
4	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015930.D
Acq On : 13 Jul 2018 00:24
Operator : SJ/JU
Sample : J3951-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
071018-DBRI-E-U-M

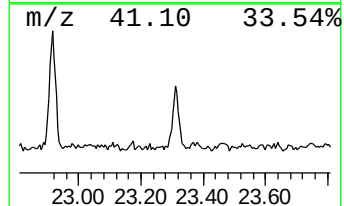
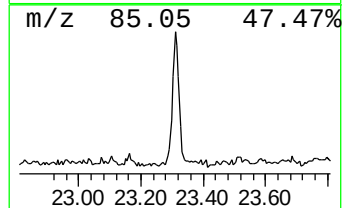
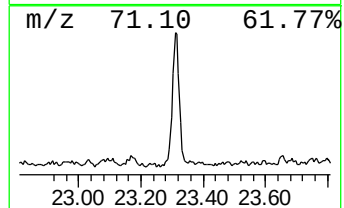
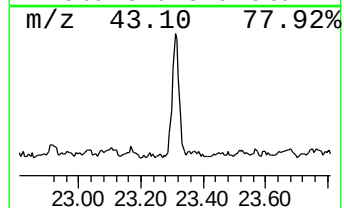
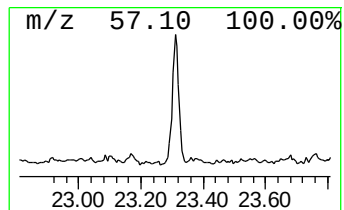
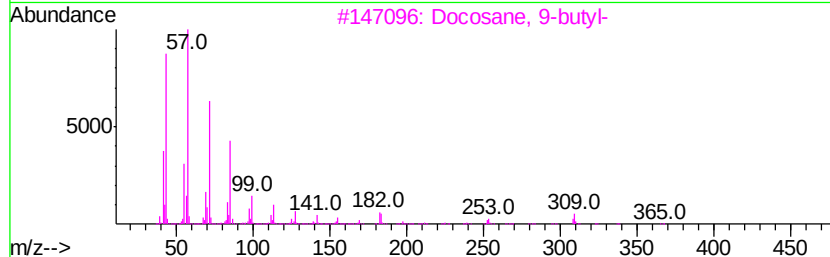
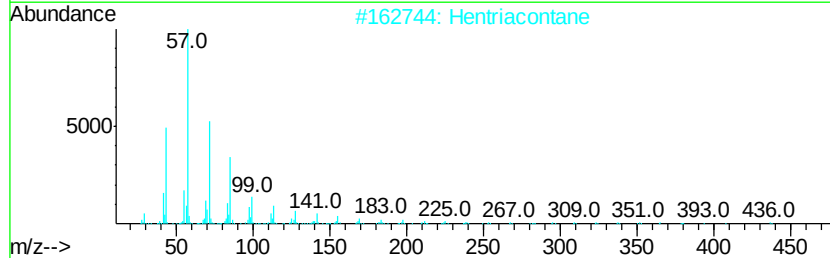
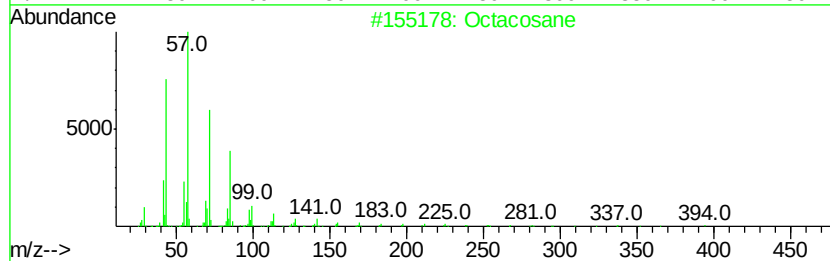
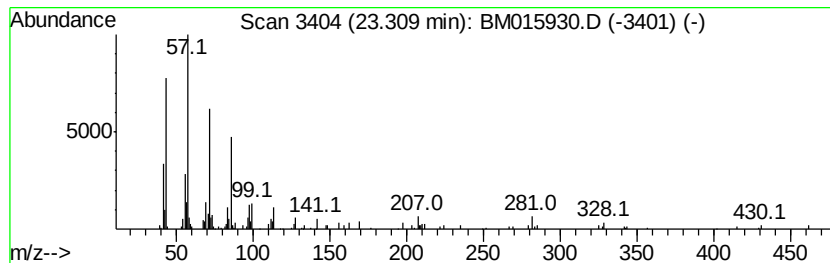
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	3.15 ng	141848	Perylene-d12	24.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Docosane, 9-butyl-	366	C26H54	055282-14-9	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM071218\
Data File : BM015930.D
Acq On : 13 Jul 2018 00:24
Operator : SJ/JU
Sample : J3951-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.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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unknown7.81	7.81	65.5	ng	1708420	1	8.29	521239	20.0
Ethyl citrate	16.16	4.4	ng	179787	3	14.90	810312	20.0
Tridecanoic acid	18.47	4.0	ng	178063	4	17.63	884807	20.0
Ethanol, 2-(hexad...	21.40	6.6	ng	312667	5	21.74	953071	20.0
Octacosane	21.83	2.8	ng	131434	5	21.74	953071	20.0
Heptacosane	22.29	2.8	ng	133423	5	21.74	953071	20.0
Eicosane	22.77	2.8	ng	134093	5	21.74	953071	20.0
Squalene	22.91	3.5	ng	167359	5	21.74	953071	20.0
Hentriacontane	23.31	3.1	ng	141848	6	24.13	900141	20.0