

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
 Data File : BF093823.D
 Acq On : 22 Mar 2017 8:13
 Operator : SJ/MA
 Sample : I2329-02
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 031617-PRRT-F-D-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:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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	4.984	270	271	277	rBV	147067	200108	3.62%	0.543%
2	5.419	307	309	311	rBV	1856905	1642940	29.71%	4.459%
3	6.447	397	399	402	rBV2	1200963	1264319	22.86%	3.432%
4	6.585	409	411	414	rBV	2285406	2978580	53.87%	8.085%
5	6.825	430	432	434	rBV	1517669	1265895	22.89%	3.436%
6	6.985	443	446	448	rBV	4263405	4037692	73.02%	10.960%
7	7.053	448	452	455	rVB	27528	62537	1.13%	0.170%
8	7.385	478	481	484	rBV	2726535	3362786	60.82%	9.128%
9	8.105	542	544	547	rBV	1178086	1646559	29.78%	4.469%
10	9.191	636	639	641	rBV	5547914	5529506	100.00%	15.009%
11	9.579	671	673	675	rBV	198638	165146	2.99%	0.448%
12	9.865	695	698	700	rBV	1868366	1845775	33.38%	5.010%
13	10.642	763	766	769	rBV	1921604	1975166	35.72%	5.361%
14	10.779	776	778	783	rVB	80751	89093	1.61%	0.242%
15	11.225	815	817	819	rBV	60532	57584	1.04%	0.156%
16	11.339	824	827	829	rVB	1903110	1629900	29.48%	4.424%
17	12.139	894	897	899	rVB	70393	82053	1.48%	0.223%
18	12.757	948	951	953	rBV	44610	57132	1.03%	0.155%
19	12.837	955	958	960	rVB	433740	362613	6.56%	0.984%
20	12.928	963	966	968	rBV	4199769	4305641	77.87%	11.687%
21	13.362	1002	1004	1005	rBV	122727	132986	2.41%	0.361%
22	13.397	1005	1007	1011	rVV2	104136	203505	3.68%	0.552%
23	13.488	1012	1015	1016	rVV	56904	78390	1.42%	0.213%
24	13.534	1017	1019	1021	rVB	140009	121685	2.20%	0.330%
25	13.831	1043	1045	1052	rBV	89931	134635	2.43%	0.365%
26	13.968	1054	1057	1059	rBV	1051542	1151324	20.82%	3.125%
27	14.825	1129	1132	1134	rBV	165574	162622	2.94%	0.441%
28	15.374	1177	1180	1183	rBV	748165	998237	18.05%	2.710%
29	16.277	1256	1259	1269	rBV2	156293	306716	5.55%	0.833%
30	16.711	1294	1297	1300	rBV	36858	67060	1.21%	0.182%
31	16.917	1312	1315	1322	rVB3	25168	57685	1.04%	0.157%
32	17.294	1344	1348	1353	rBV	177438	429242	7.76%	1.165%
33	17.397	1353	1357	1363	rVB4	61952	162858	2.95%	0.442%
34	17.774	1386	1390	1395	rVB3	48963	115088	2.08%	0.312%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.346	1437	1440	1451	rVB5	23365	74676	1.35%	0.203%
36	19.500	1536	1541	1545	rBV2	29351	83910	1.52%	0.228%

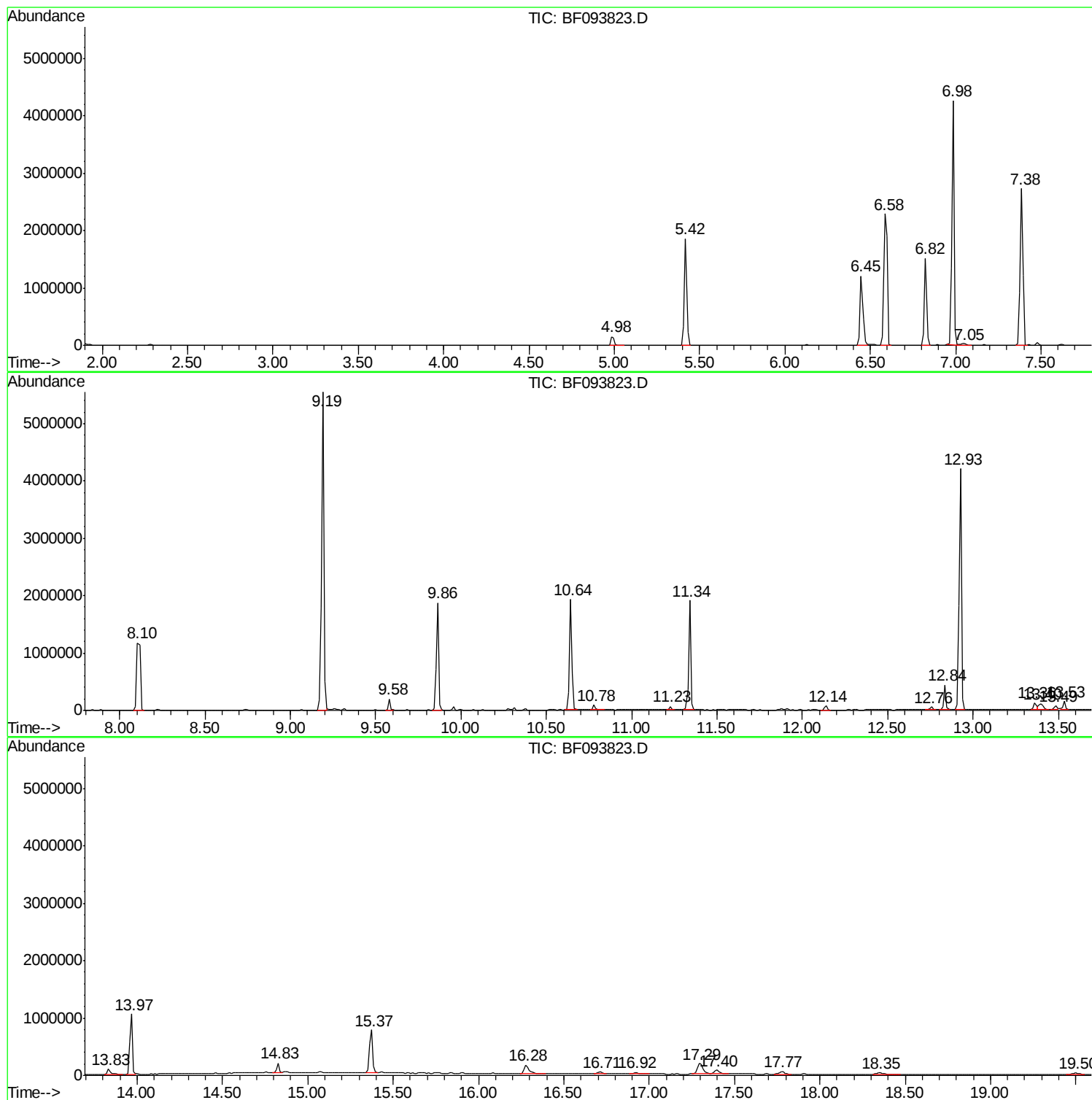
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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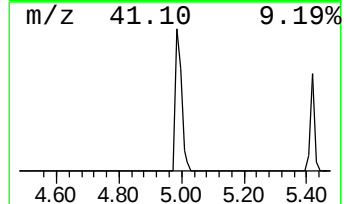
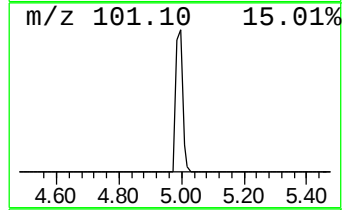
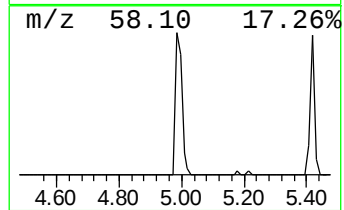
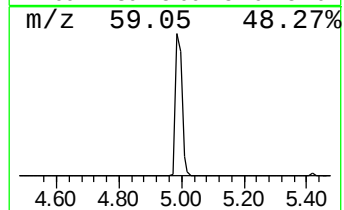
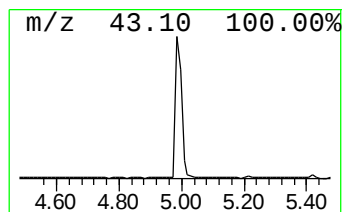
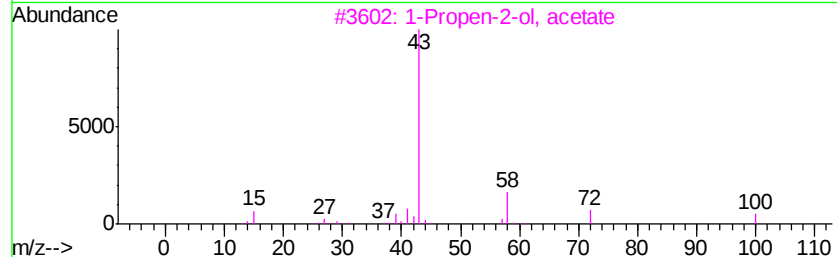
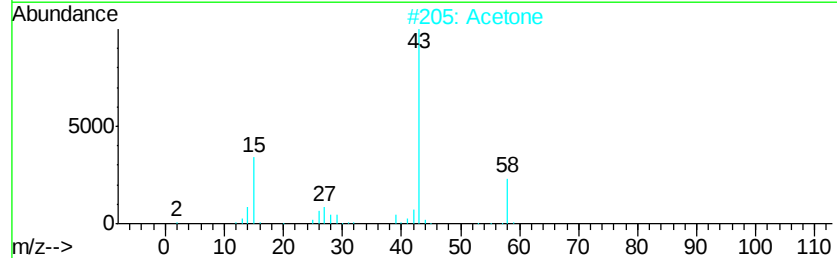
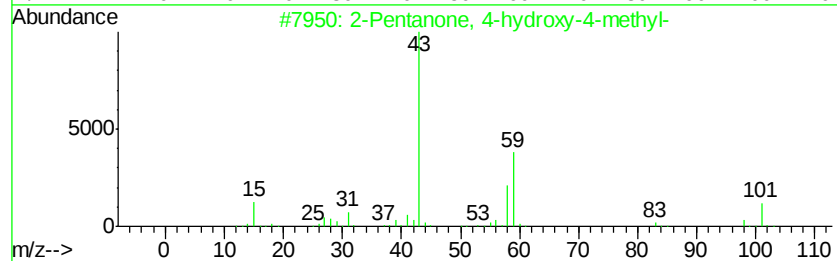
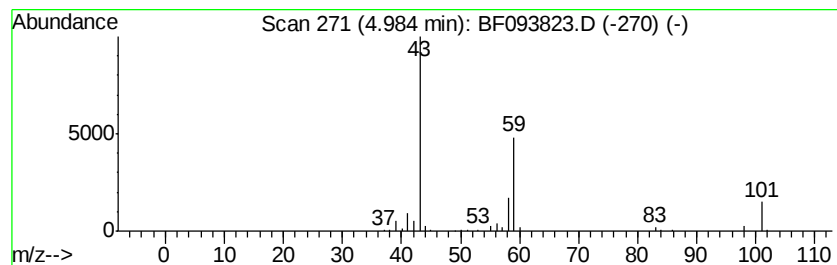
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	3.16 ng	200108	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetone	58	C3H6O	000067-64-1	12
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5			Butane	58	C4H10	000106-97-8	9



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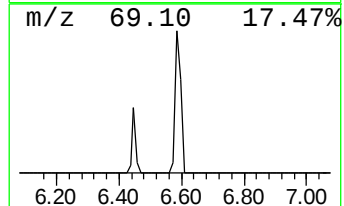
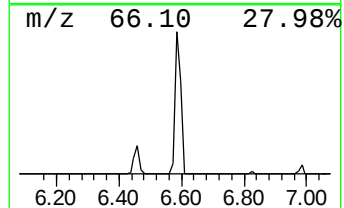
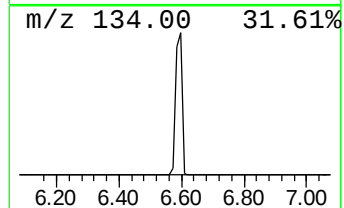
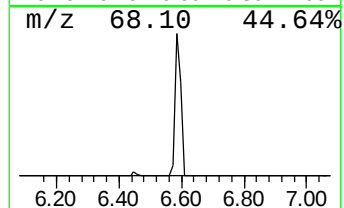
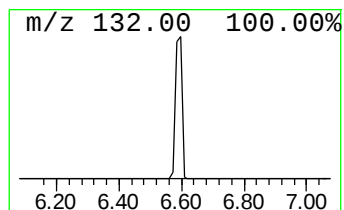
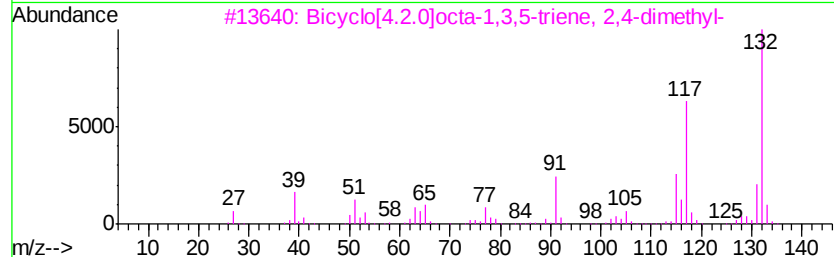
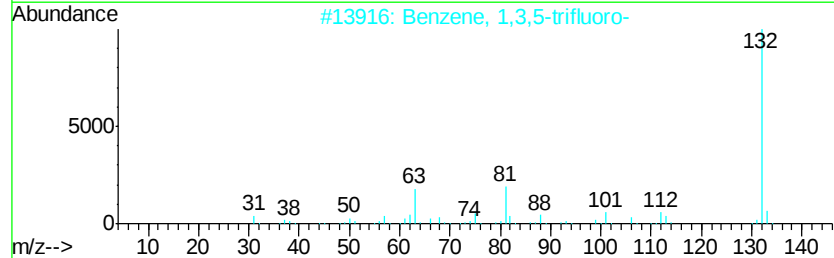
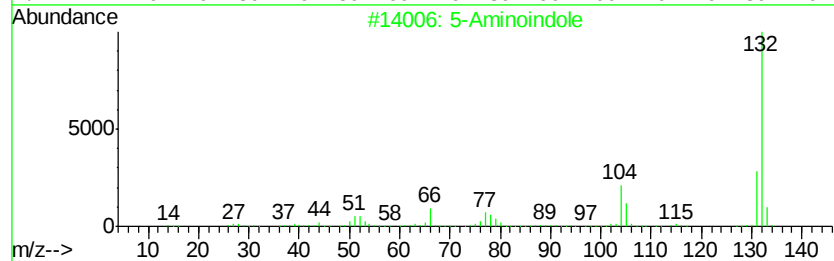
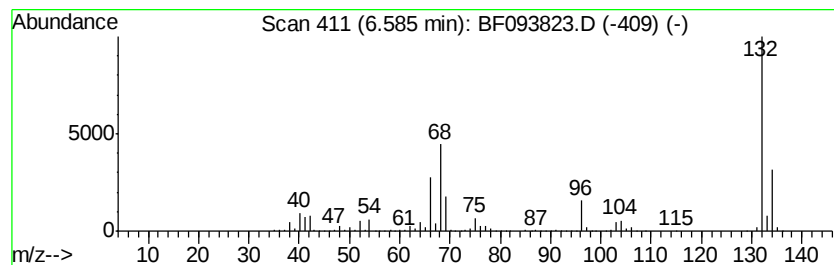
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	47.06 ng	2978580	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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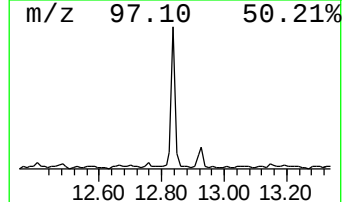
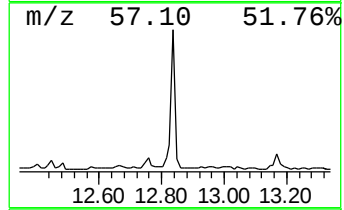
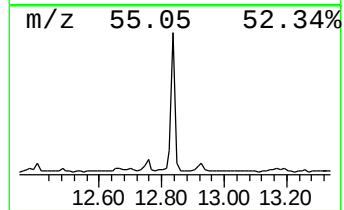
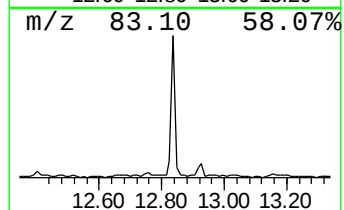
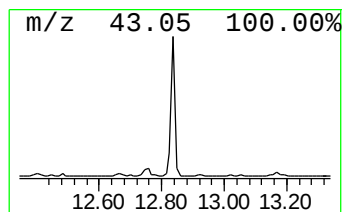
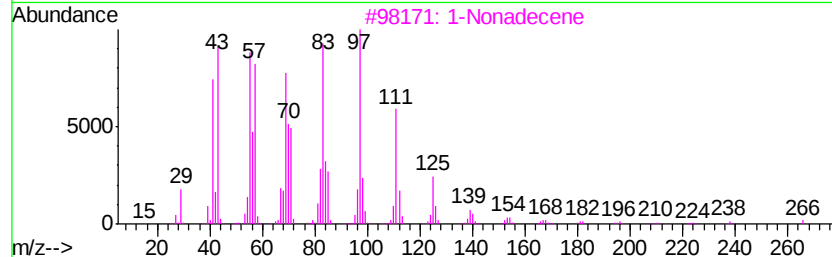
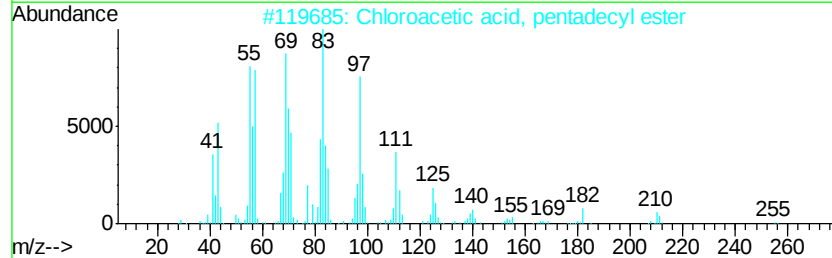
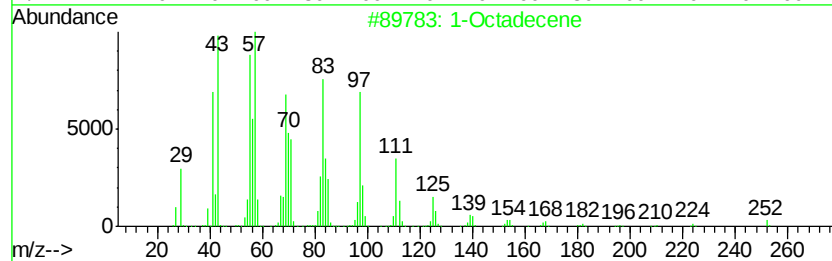
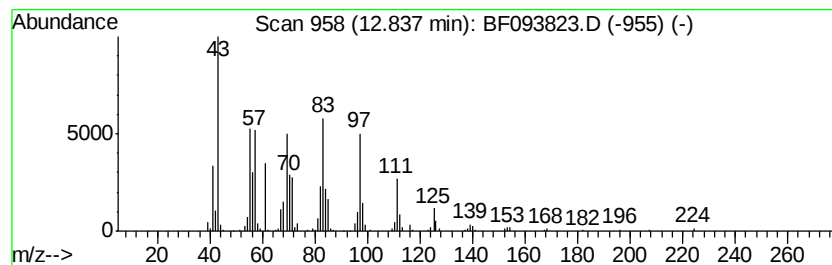
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	6.30 ng	362613	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecene	252	C18H36	000112-88-9	93
2		Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	90
3		1-Nonadecene	266	C19H38	018435-45-5	87
4		Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	83
5		1-Octadecanol	270	C18H38O	000112-92-5	83



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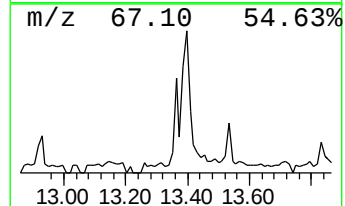
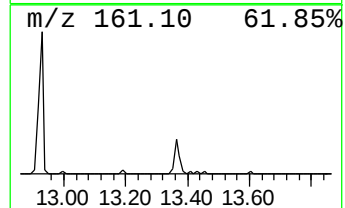
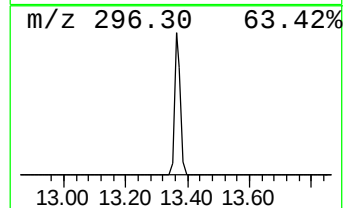
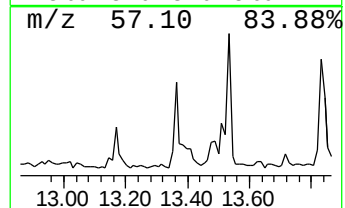
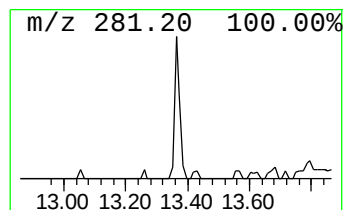
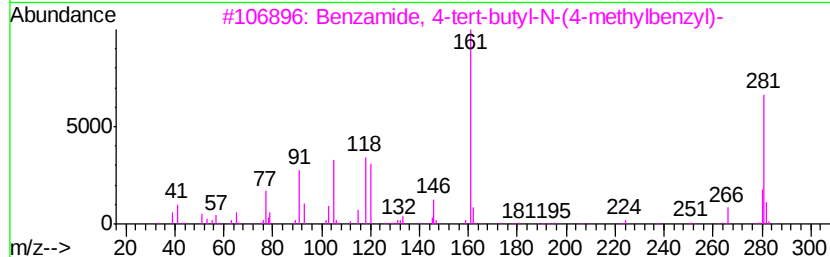
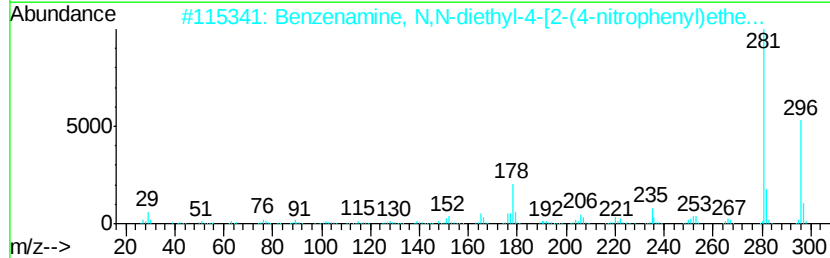
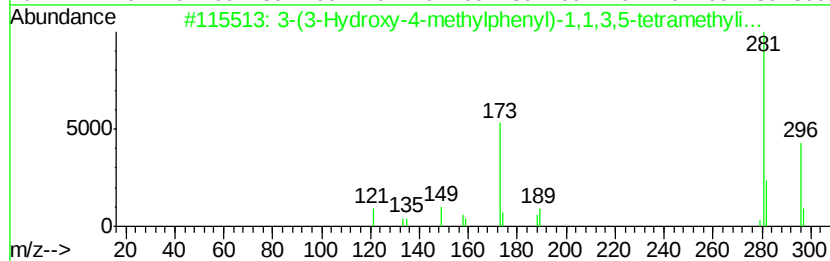
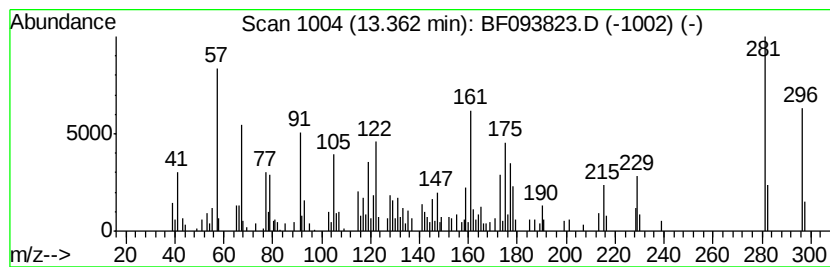
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.36 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.36	2.31 ng	132986	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(3-Hydroxy-4-methylphenyl)-1,1...	296	C20H24O2	1000105-90-6	46
2	Benzenamine, N,N-diethyl-4-[2-(4...	296	C18H20N2O2	017951-64-3	43
3	Benzamide, 4-tert-butyl-N-(4-met...	281	C19H23NO	328283-57-4	27
4	9H-Imidazo[1,2-a]benzimidazole, ...	281	C16H12ClN3	1000274-13-7	18
5	1,2-Dihydroanthra[1,2-d]thiazole...	281	C15H7N03S	1000110-33-6	14



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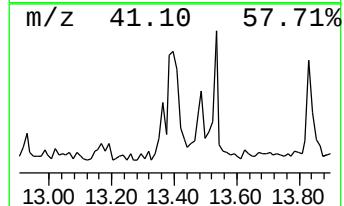
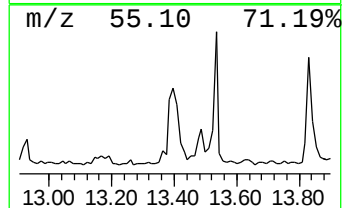
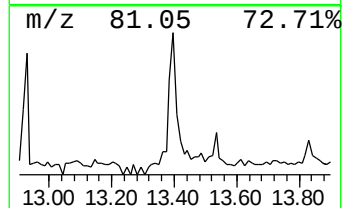
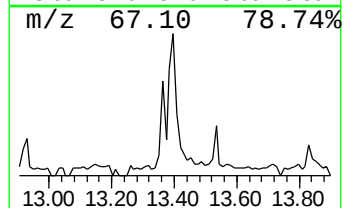
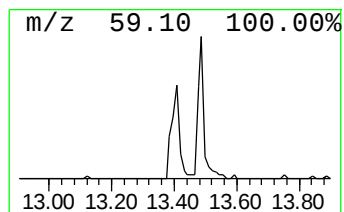
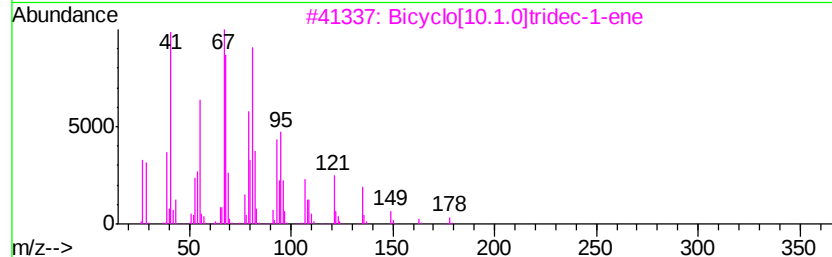
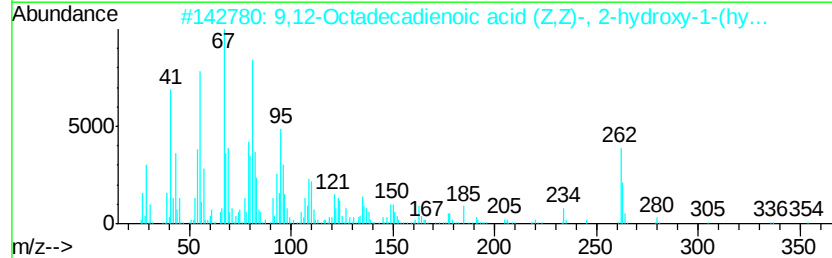
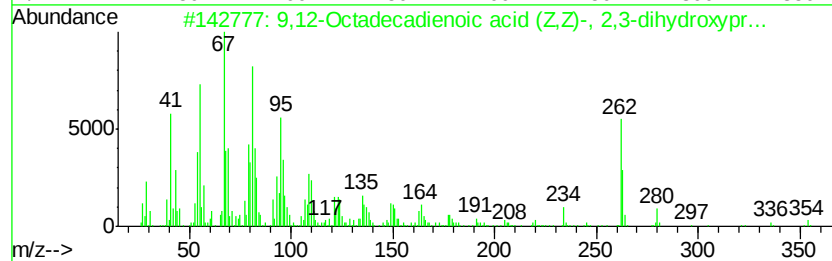
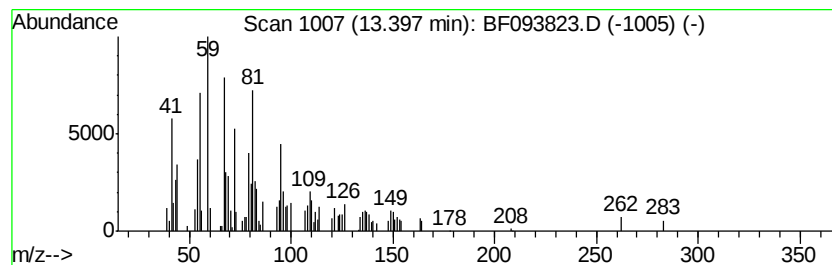
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	3.54 ng	203505	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid (Z,Z)-...	354	C21H38O4	002277-28-3	55
2		9,12-Octadecadienoic acid (Z,Z)-...	354	C21H38O4	003443-82-1	55
3		Bicyclo[10.1.0]tridec-1-ene	178	C13H22	054766-91-5	46
4		9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	45
5		Cyclododecyne	164	C12H20	001129-90-4	42



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Acq On : 22 Mar 2017 8:13
Operator : SJ/MA
Sample : I2329-02
Misc :
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ClientSampleId :
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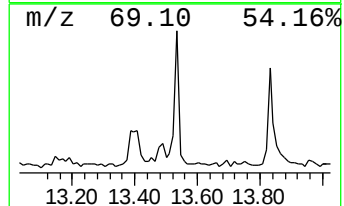
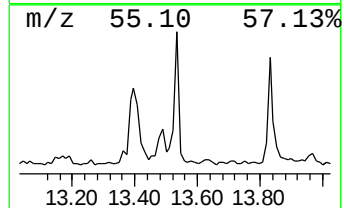
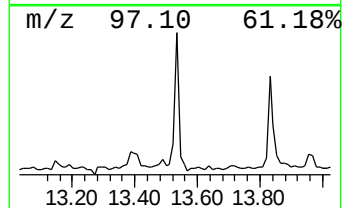
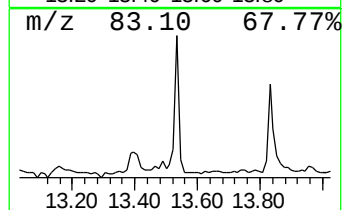
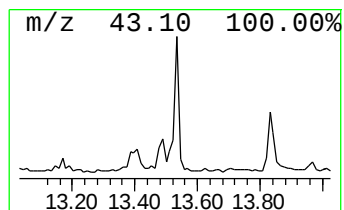
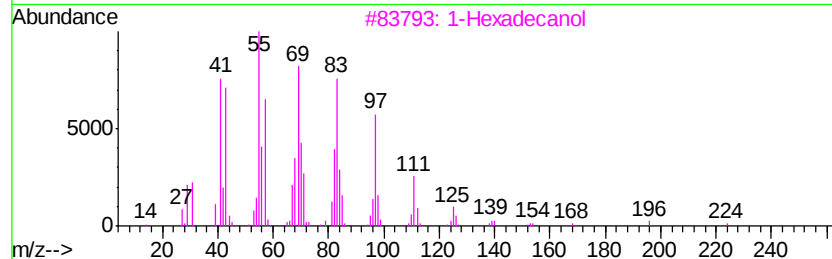
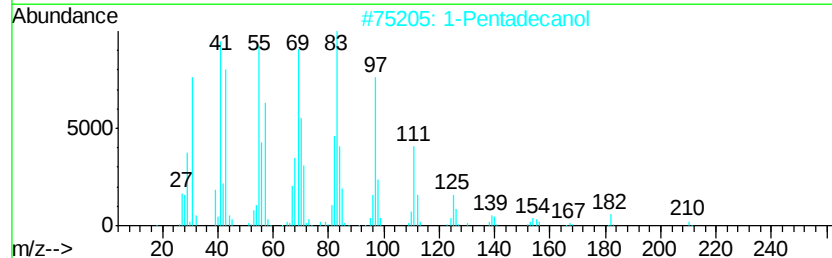
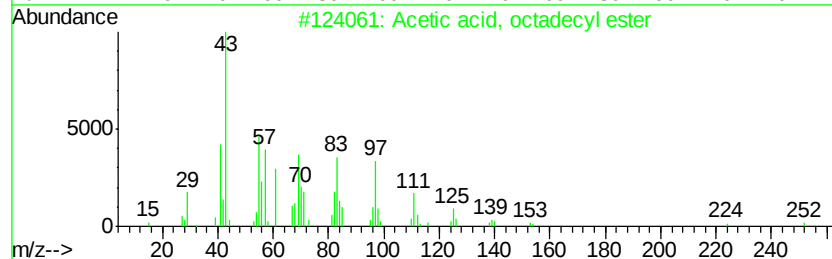
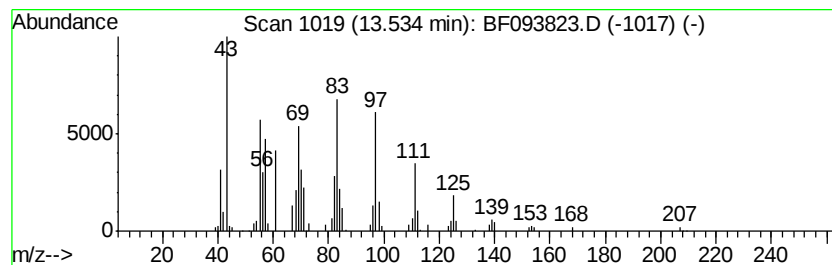
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Acetic acid, octadecyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.11 ng	121685	Chrysene-d12	13.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	91
2			1-Pentadecanol	228	C15H32O	000629-76-5	81
3			1-Hexadecanol	242	C16H34O	036653-82-4	81
4			Cyclotetradecane	196	C14H28	000295-17-0	72
5			1-Tetradecanol, acetate	256	C16H32O2	000638-59-5	72



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Operator : SJ/MA
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ClientSampleId :
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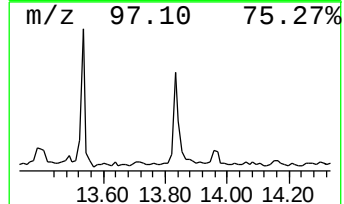
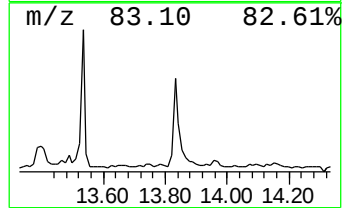
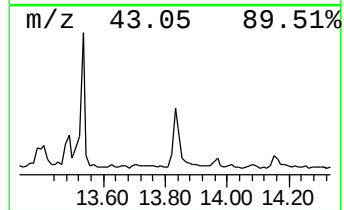
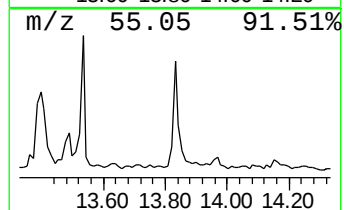
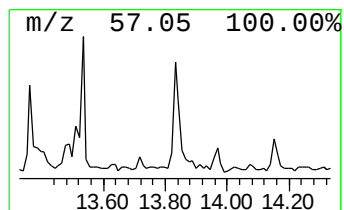
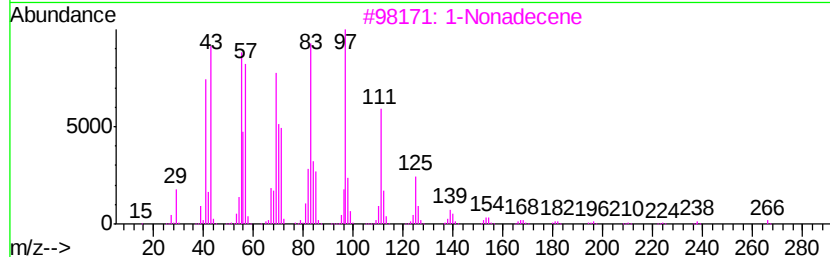
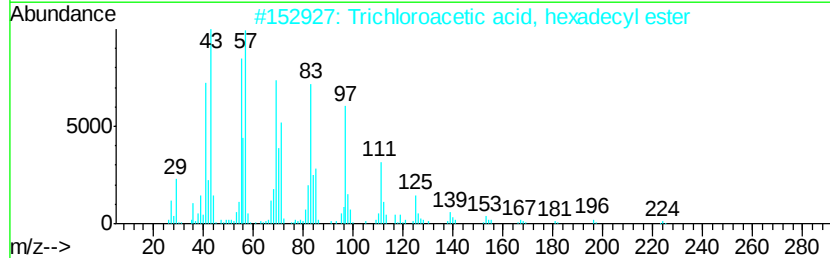
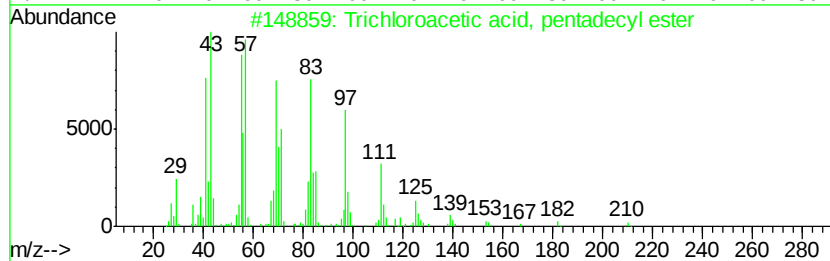
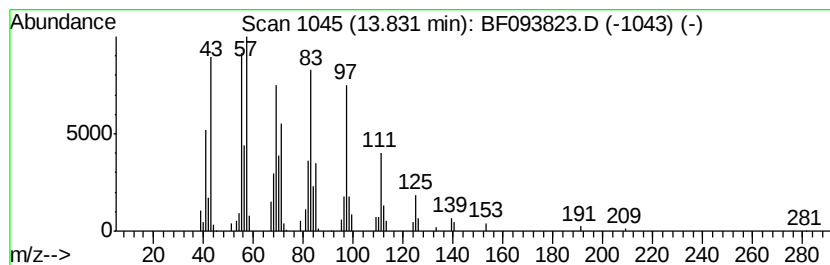
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, penta... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.34 ng	134635	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		1-Nonadecene	266	C19H38	018435-45-5	90
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5		1-Hexacosanol	382	C26H54O	000506-52-5	90



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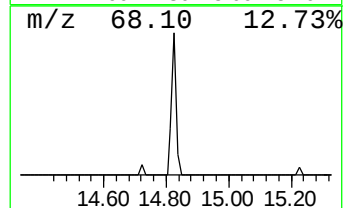
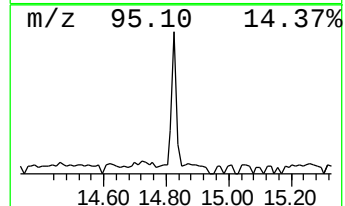
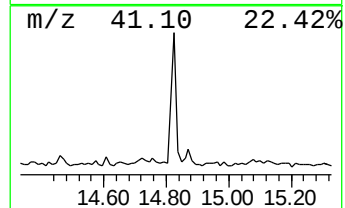
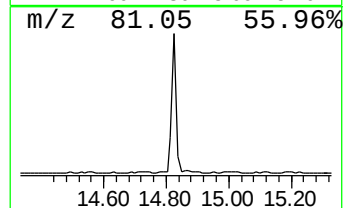
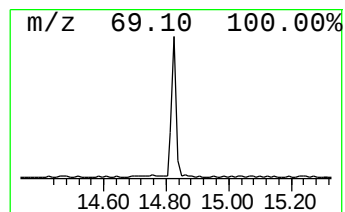
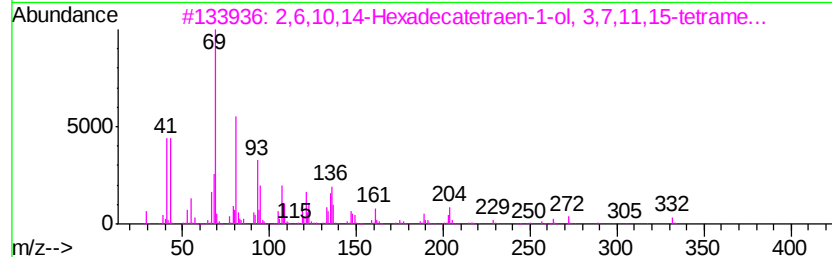
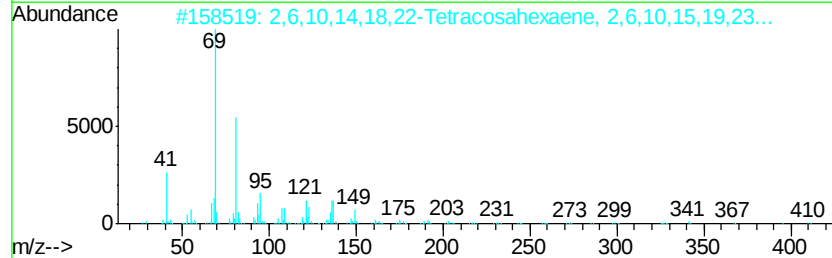
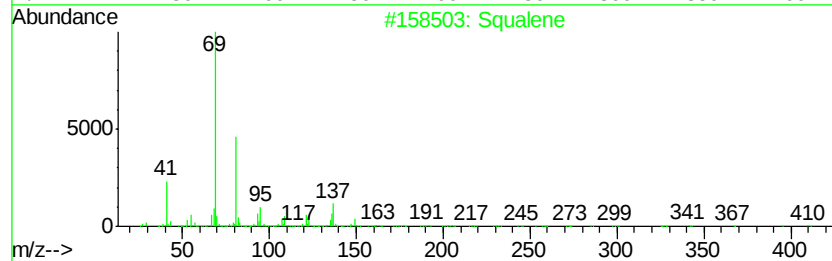
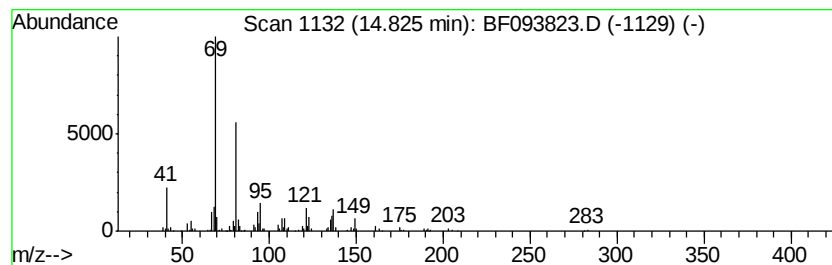
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.26 ng	162622	Perylene-d12	15.37
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	91
3	2,6,10,14-Hexadecatetraen-1-ol, ...	332 C22H36O2	061691-98-3	78
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	000106-28-5	64
5	1,3-Dioxolan-2-one, 3-methyl-3-(...	264 C16H24O3	336879-76-6	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093823.D
Acq On : 22 Mar 2017 8:13
Operator : SJ/MA
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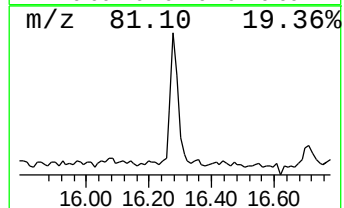
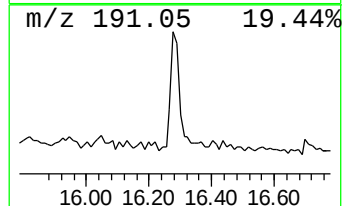
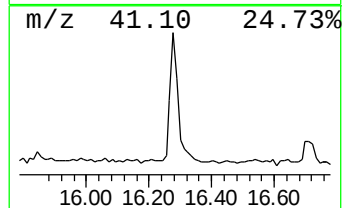
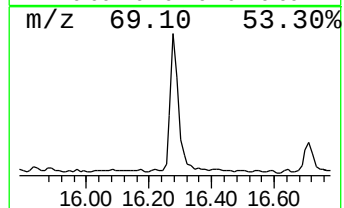
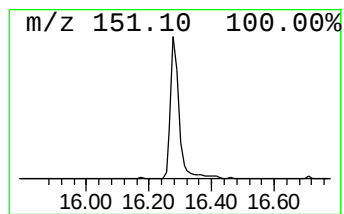
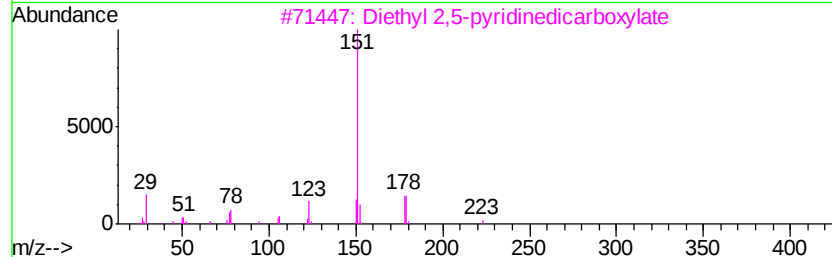
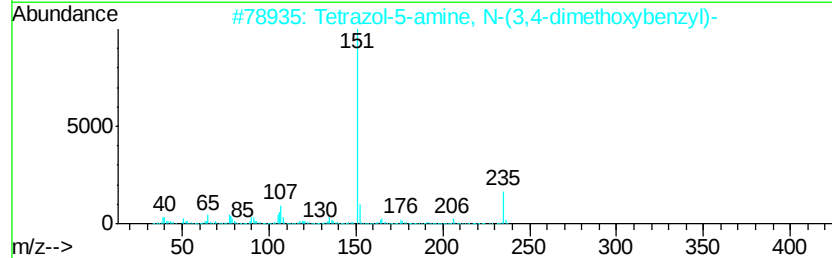
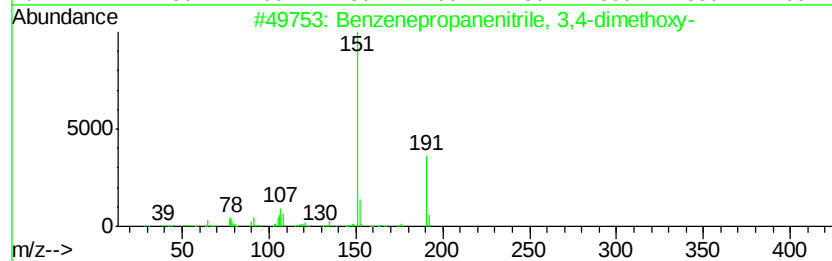
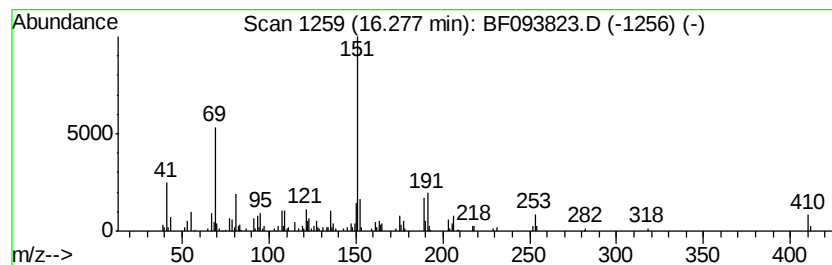
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzenepropanenitrile, 3,4-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.28	6.15 ng	306716	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenepropanenitrile, 3,4-dimet...	191	C11H13N02	049621-56-9	53
2		Tetrazol-5-amine, N-(3,4-dimetho...	235	C10H13N5O2	1000272-73-1	47
3		Diethyl 2,5-pyridinedicarboxylate	223	C11H13N04	005552-44-3	47
4		4H-1,3,2-Dioxaborin, 6-ethenyl-2...	208	C12H21B02	074630-05-0	43
5		Thiazolo[5,4-d]pyrimidine, 7-met...	151	C6H5N3S	013316-06-8	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093823.D
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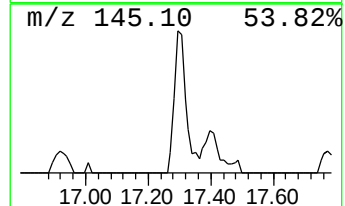
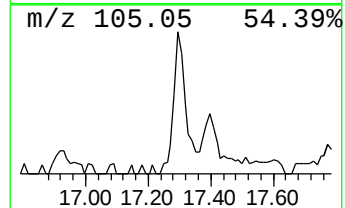
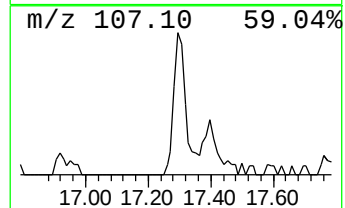
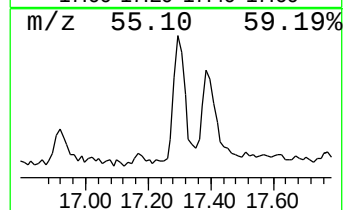
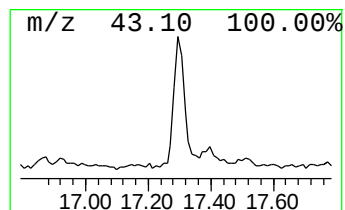
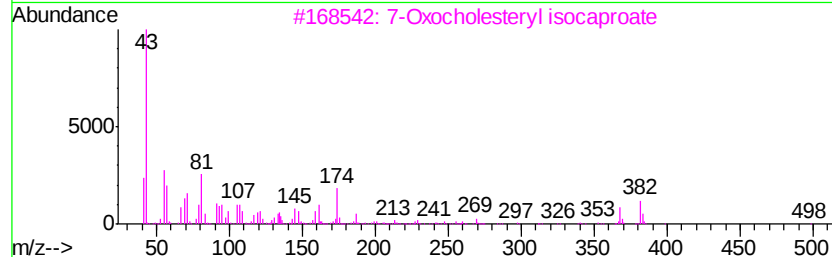
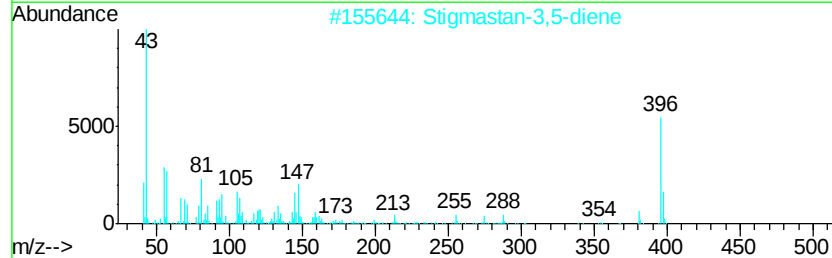
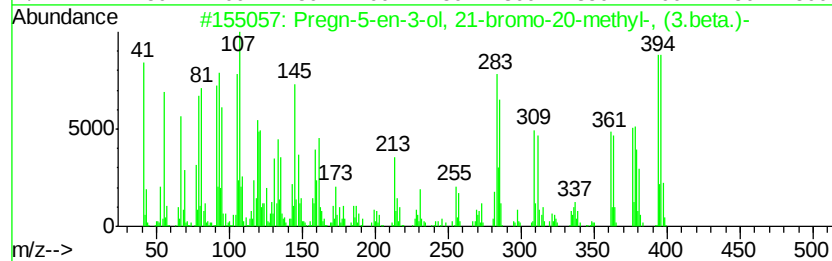
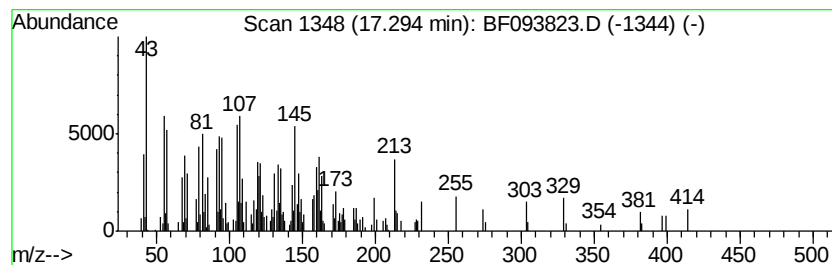
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.29 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.29	8.60 ng	429242	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	49
2		Stigmastan-3,5-diene	396	C29H48	1000214-16-4	43
3		7-Oxocholesteryl isocaproate	498	C33H54O3	1000251-06-0	28
4		9,19-Cyclochoolan-24-al, 3-(acety...	442	C29H46O3	025089-90-1	25
5		Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
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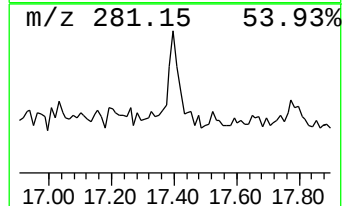
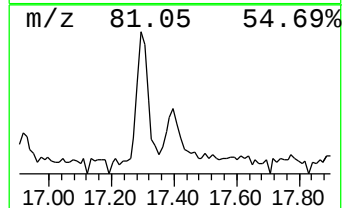
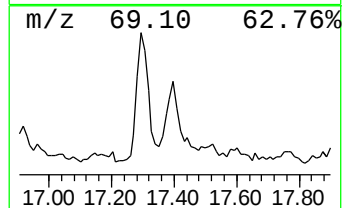
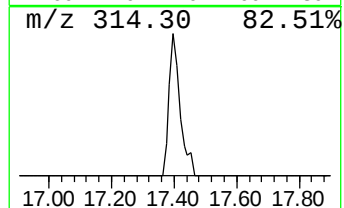
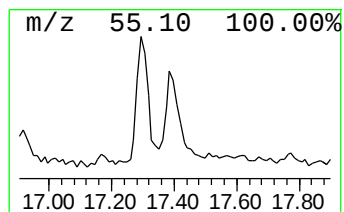
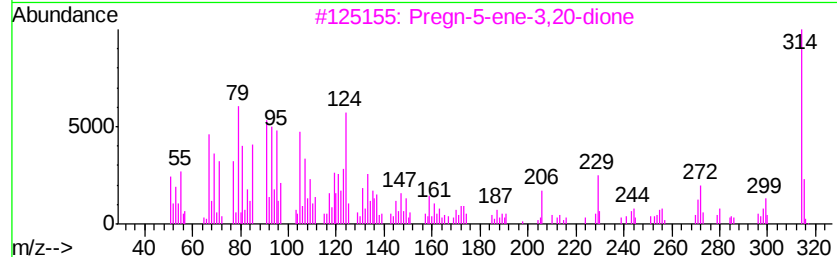
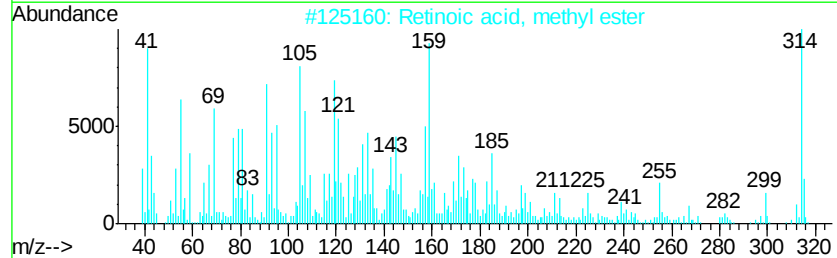
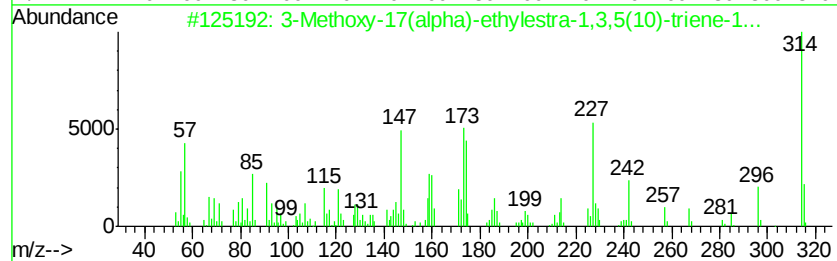
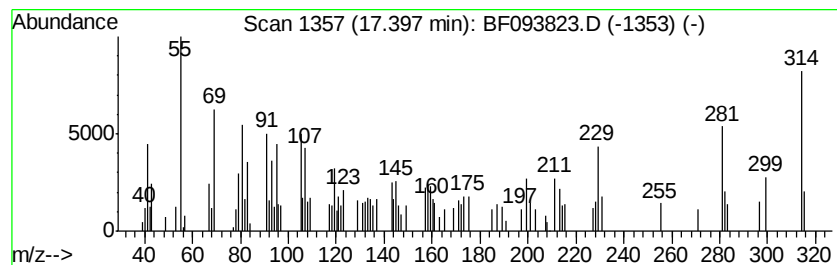
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 3-Methoxy-17(alpha)-ethyles... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.40	3.26 ng	162858	Perylene-d12	15.37		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methoxy-17(alpha)-ethylestra-1...	314	C21H30O2	1000215-58-4	55
2		Retinoic acid, methyl ester	314	C21H30O2	000339-16-2	55
3		Pregn-5-ene-3,20-dione	314	C21H30O2	001236-09-5	41
4		Pregnane-3,20-dione, 11-hydroxy-...	332	C21H32O3	000565-95-7	32
5		19-Norpregna-1,3,5(10)-trien-17-...	314	C21H30O2	017550-02-6	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
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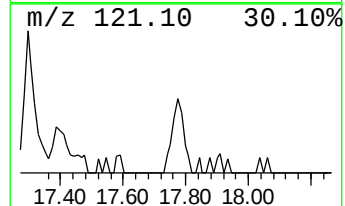
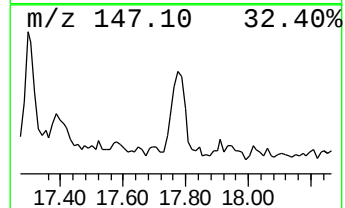
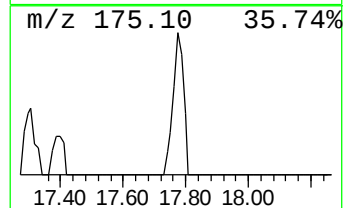
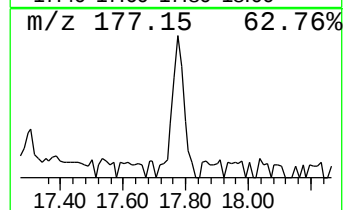
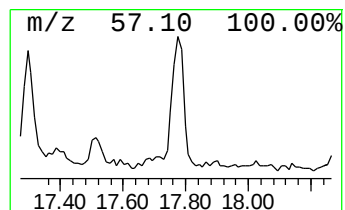
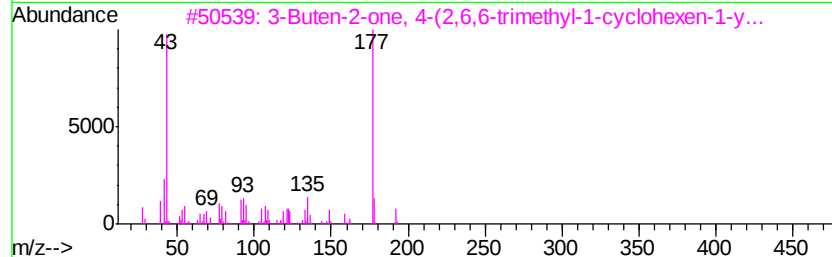
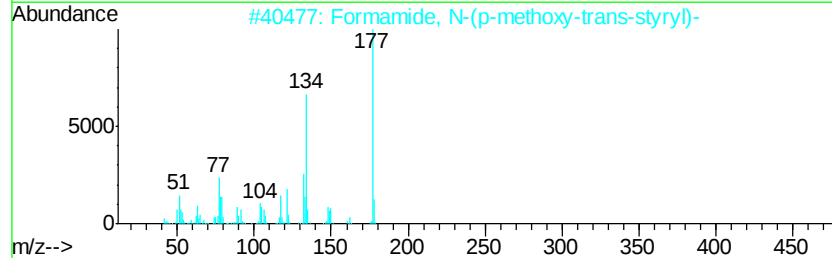
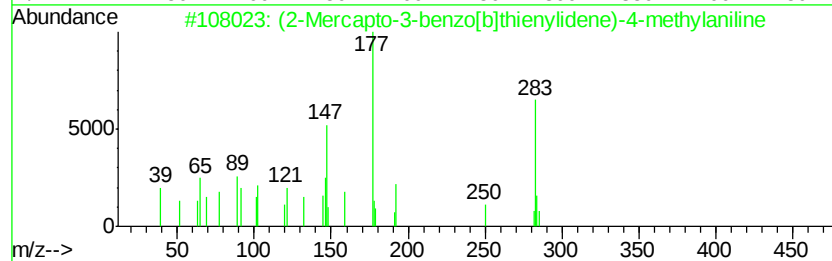
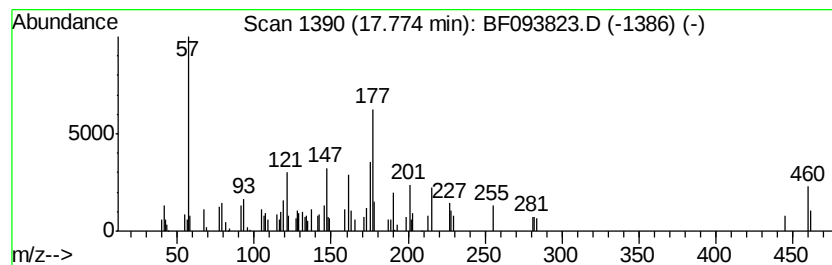
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.77 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.77	2.31 ng	115088	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(2-Mercapto-3-benzo[b]thienylidene...	283	C16H13NS2	092886-26-5	14
2		Formamide, N-(p-methoxy-trans-st...	177	C10H11NO2	002501-37-3	11
3		3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	000079-77-6	10
4		7-Methoxy-2-methyl-1,2,3,4-tetra...	177	C11H15NO	054893-23-1	10
5		Ethane, 1,2-dibromo-1,2-dichloro-	254	C2H2Br2Cl2	000683-68-1	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
 Data File : BF093823.D
 Acq On : 22 Mar 2017 8:13
 Operator : SJ/MA
 Sample : I2329-02
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 031617-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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...	4.98	3.2	ng	200108	1	6.82	1265900	20.0
unknown6.58	6.58	47.1	ng	2978580	1	6.82	1265900	20.0
1-Octadecene	12.84	6.3	ng	362613	5	13.97	1151320	20.0
unknown13.36	13.36	2.3	ng	132986	5	13.97	1151320	20.0
9,12-Octadecadien...	13.40	3.5	ng	203505	5	13.97	1151320	20.0
Acetic acid, octa...	13.53	2.1	ng	121685	5	13.97	1151320	20.0
Trichloroacetic a...	13.83	2.3	ng	134635	5	13.97	1151320	20.0
Squalene	14.83	3.3	ng	162622	6	15.37	998237	20.0
Benzenepropanenit...	16.28	6.2	ng	306716	6	15.37	998237	20.0
unknown17.29	17.29	8.6	ng	429242	6	15.37	998237	20.0
3-Methoxy-17(alph...	17.40	3.3	ng	162858	6	15.37	998237	20.0
unknown17.77	17.77	2.3	ng	115088	6	15.37	998237	20.0