

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100115\
 Data File : BF081976.D
 Acq On : 2 Oct 2015 9:52
 Operator : UM/IZ
 Sample : G3875-06
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A6-COMP

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-BF092815.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	5.040	252	254	255	rBV	25293	25082	1.02%	0.117%
2	5.074	255	257	260	rVV	683922	920085	37.40%	4.286%
3	5.486	290	293	296	rBV	1532947	1518722	61.74%	7.075%
4	6.514	381	383	386	rBV	1258903	1603594	65.19%	7.470%
5	6.663	393	396	398	rBV	1651031	1900761	77.27%	8.855%
6	6.892	414	416	428	rBV	446785	612165	24.88%	2.852%
7	7.052	428	430	432	rBV	1630976	1480457	60.18%	6.897%
8	7.463	463	466	468	rBV	959440	1018749	41.41%	4.746%
9	8.183	526	529	531	rBV	767773	760671	30.92%	3.544%
10	9.258	620	623	625	rBV	2464934	2338906	95.08%	10.896%
11	9.646	655	657	660	rBV	380328	413654	16.81%	1.927%
12	9.932	680	682	685	rBV	1050375	987628	40.15%	4.601%
13	10.721	748	751	759	rBV	1421171	1524326	61.96%	7.101%
14	10.835	759	761	768	rVB	43205	71055	2.89%	0.331%
15	11.281	798	800	801	rBV	34211	31267	1.27%	0.146%
16	11.418	810	812	825	rBV	972195	1074225	43.67%	5.004%
17	11.703	835	837	844	rBV	25501	33401	1.36%	0.156%
18	11.944	856	858	871	rBV	149305	211320	8.59%	0.984%
19	12.721	924	926	932	rVB3	74383	74647	3.03%	0.348%
20	12.824	932	935	938	rBV	159264	177103	7.20%	0.825%
21	13.006	948	951	953	rBV	2329701	2460044	100.00%	11.460%
22	13.521	994	996	999	rBV2	56633	75387	3.06%	0.351%
23	14.058	1040	1043	1053	rBV	832158	993410	40.38%	4.628%
24	14.812	1106	1109	1114	rBV2	122076	206112	8.38%	0.960%
25	14.892	1114	1116	1119	rVB	194863	209351	8.51%	0.975%
26	15.498	1167	1169	1178	rBV	427491	743707	30.23%	3.465%

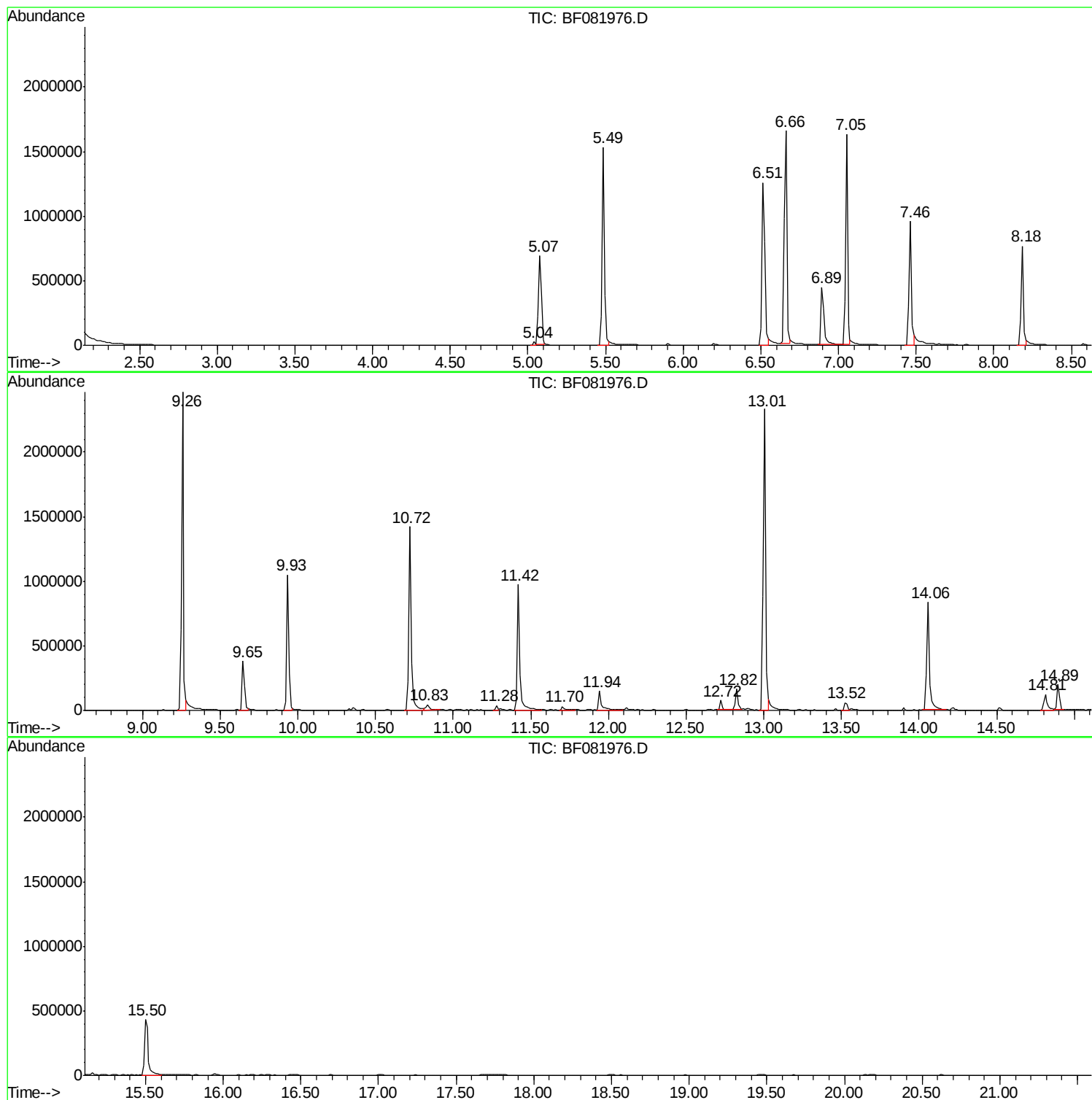
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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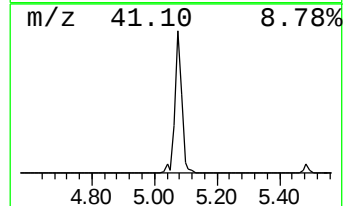
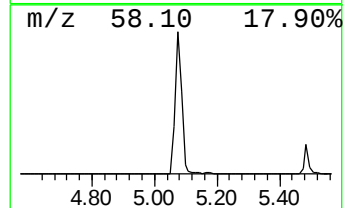
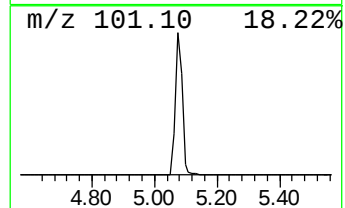
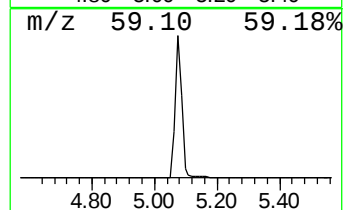
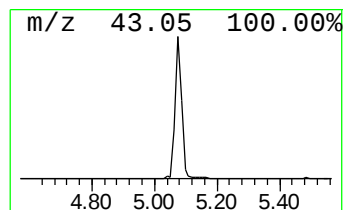
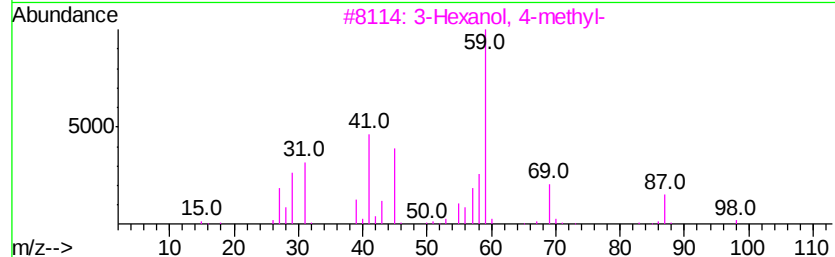
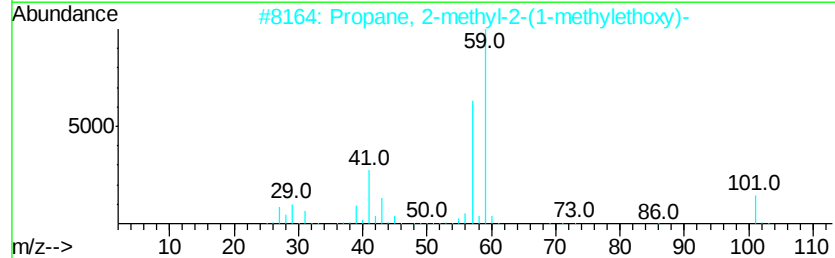
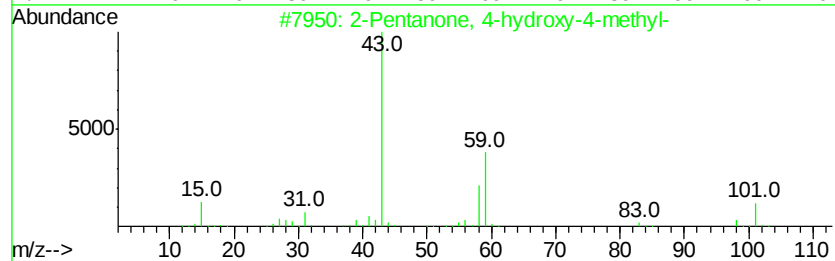
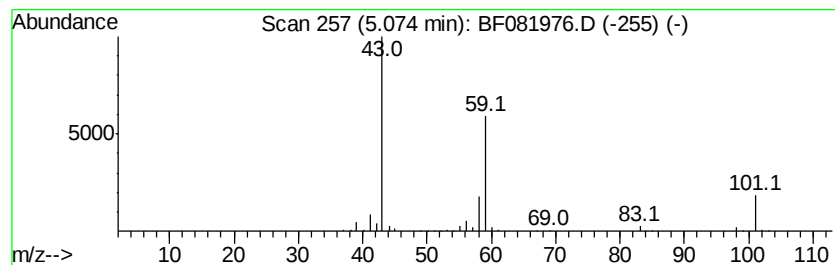
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	30.06 ng	920085	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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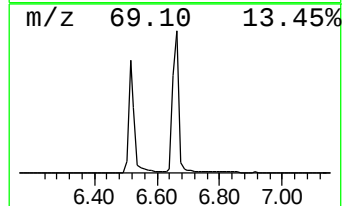
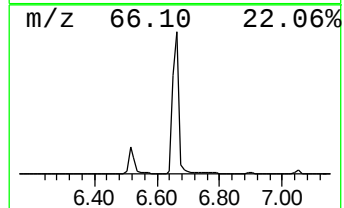
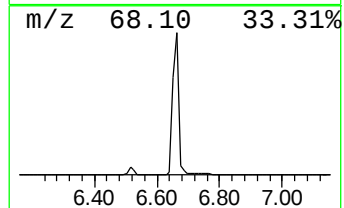
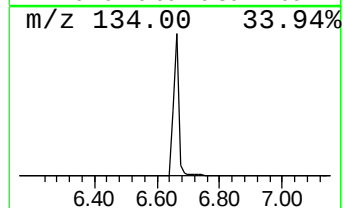
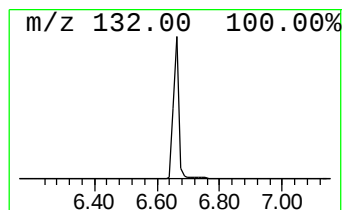
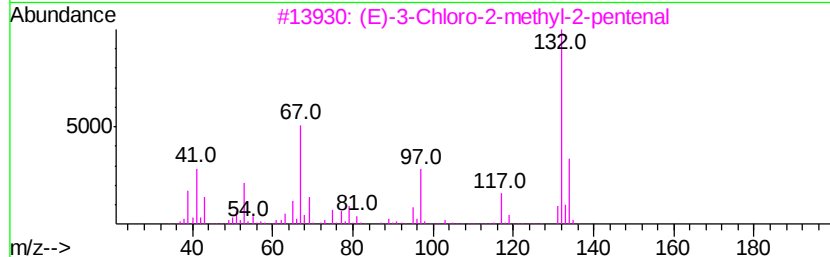
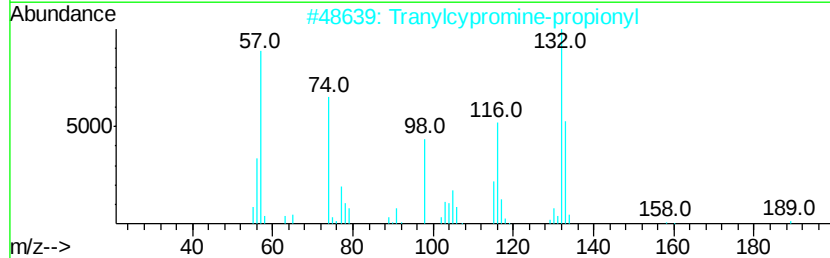
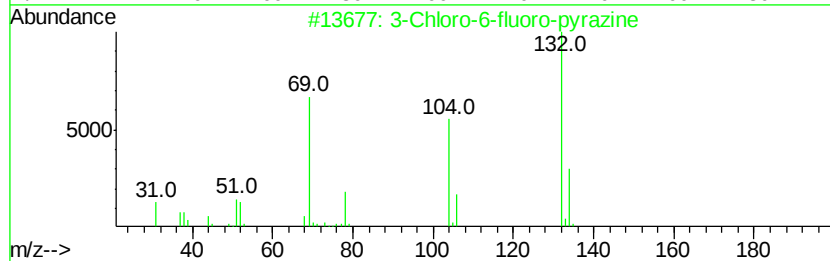
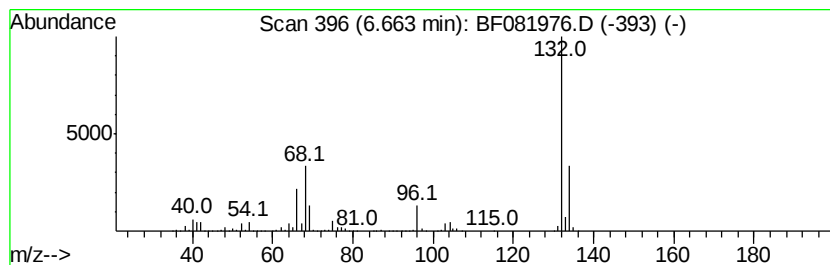
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	62.10 ng	1900760	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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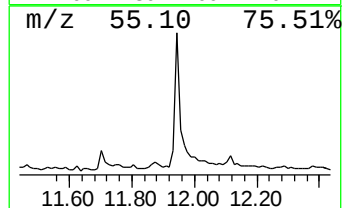
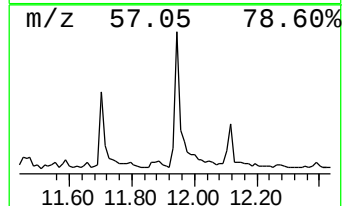
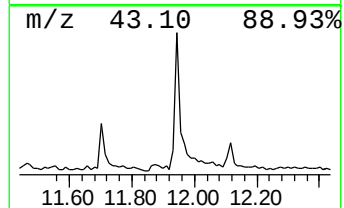
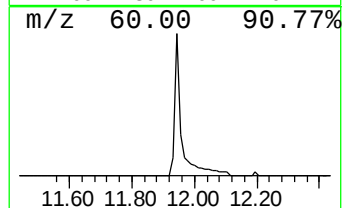
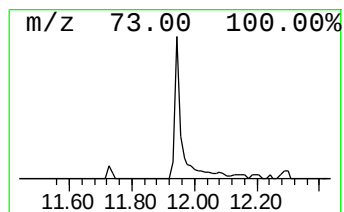
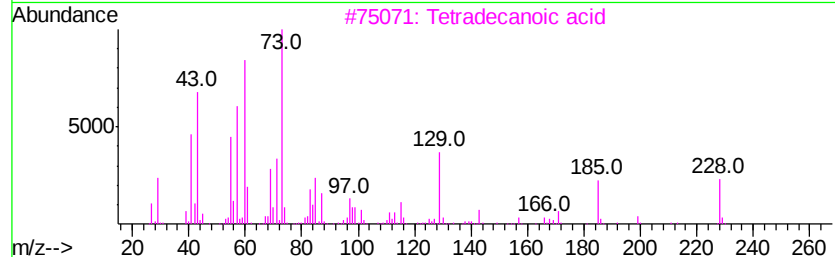
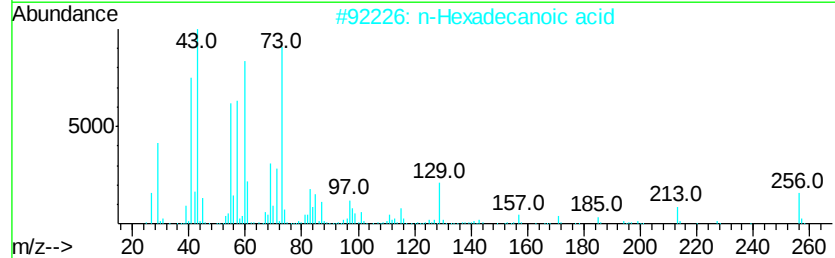
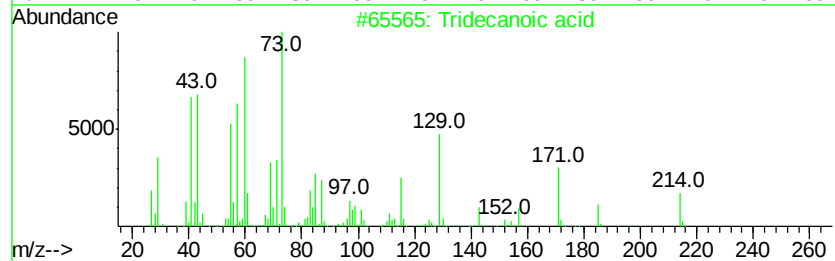
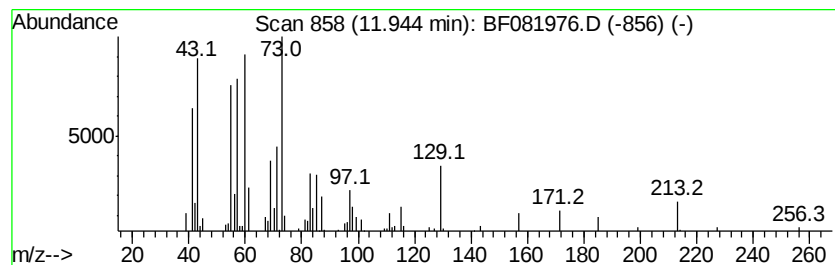
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	3.93 ng	211320	Phenanthrene-d10	11.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	91
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		n-Dodecyl acetate	228	C14H28O2	000112-66-3	11
5		Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	11



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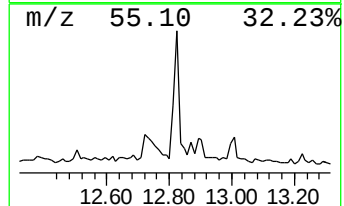
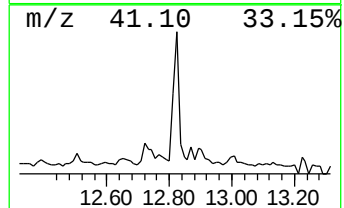
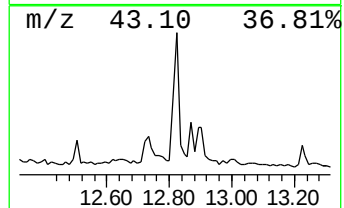
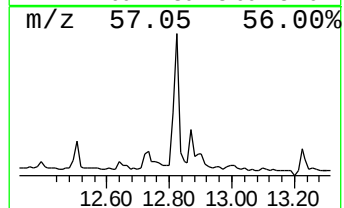
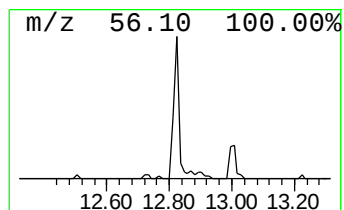
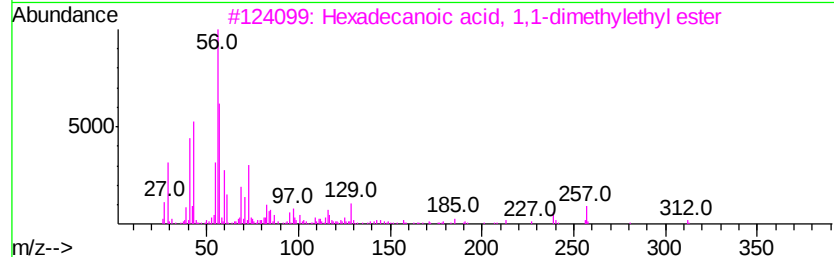
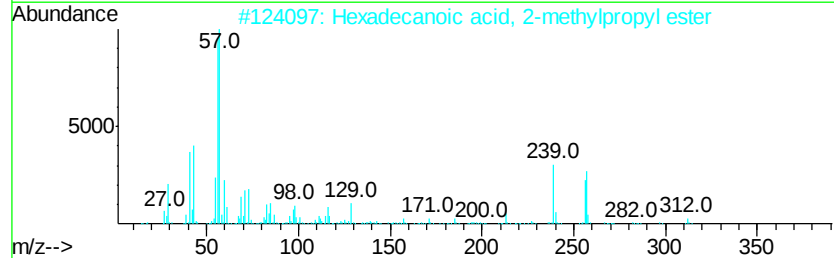
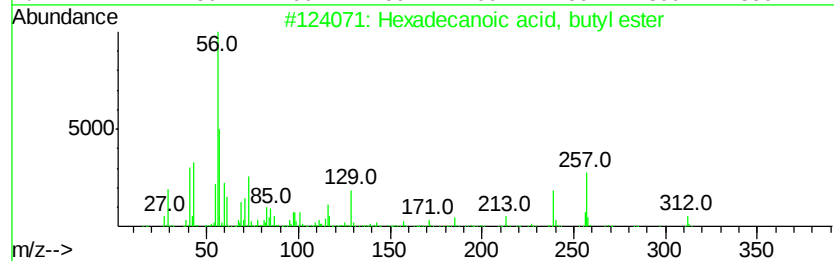
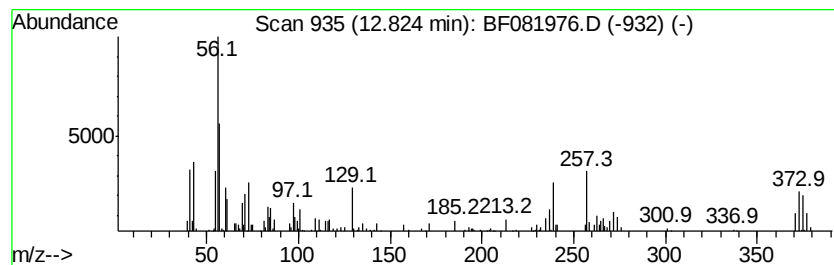
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	3.57 ng	177103	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	50
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	30
4		3-Amino-2,2-dimethyl-1-propanol	103	C5H13NO	026734-09-8	16
5		3-(antipyrin-4-yl)-5-(5-nitrosal...	468	C21H16N4O5S2	314275-32-6	12



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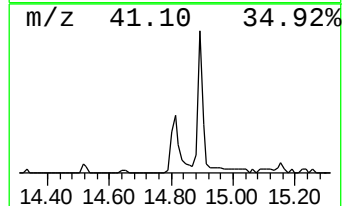
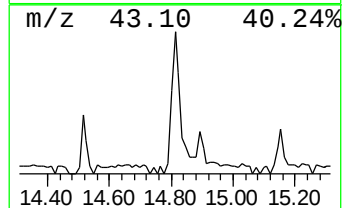
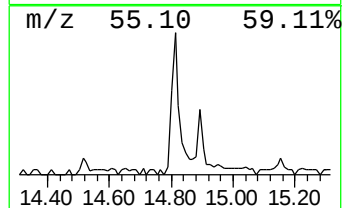
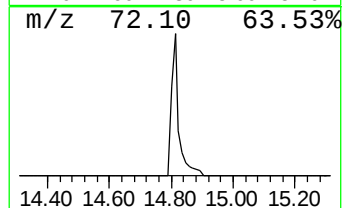
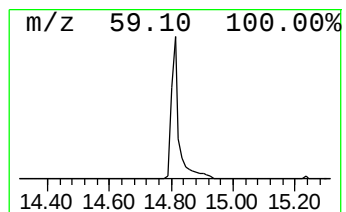
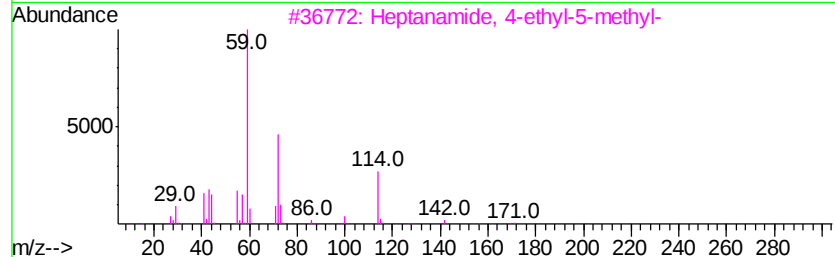
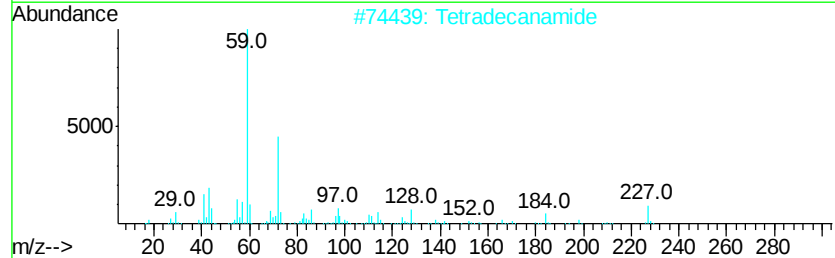
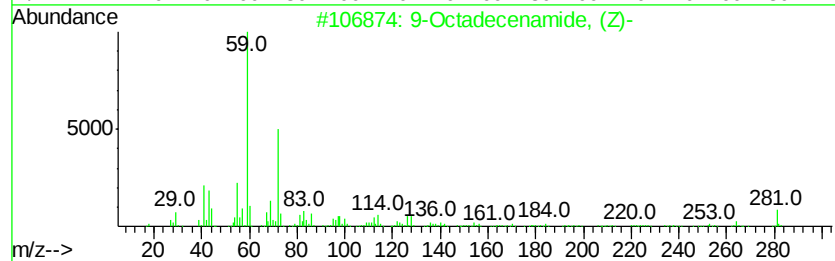
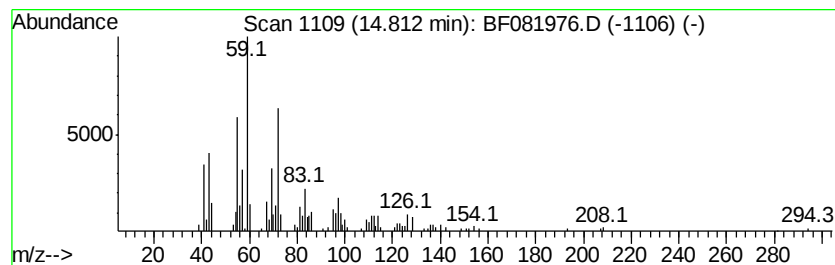
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	5.54 ng	206112	Perylene-d12	15.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2		Tetradecanamide	227	C14H29NO	000638-58-4	59
3		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	47
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	43
5		Octadecanamide	283	C18H37NO	000124-26-5	43



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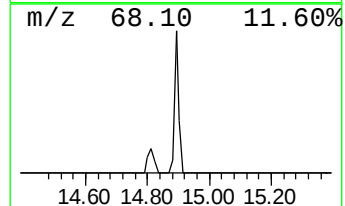
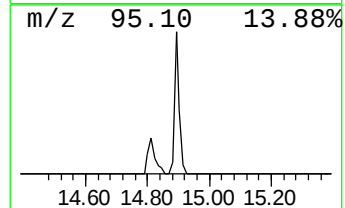
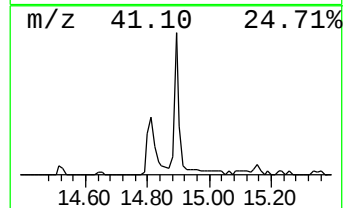
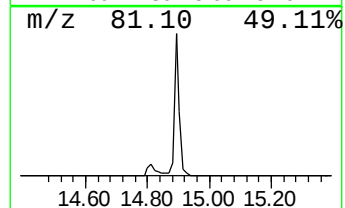
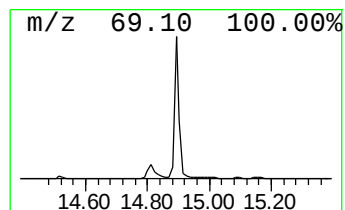
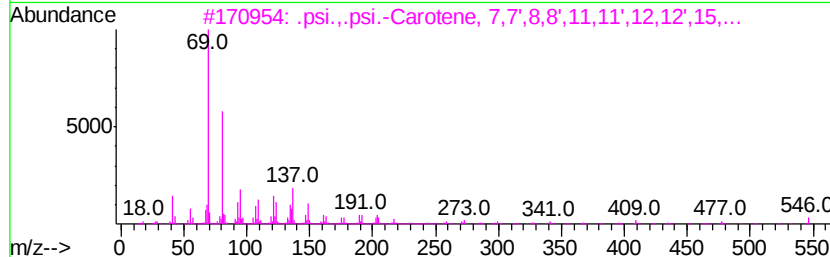
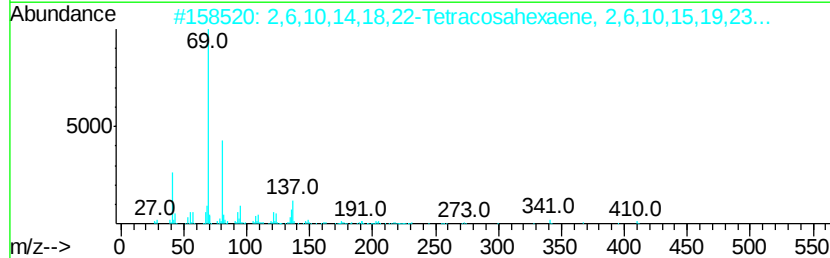
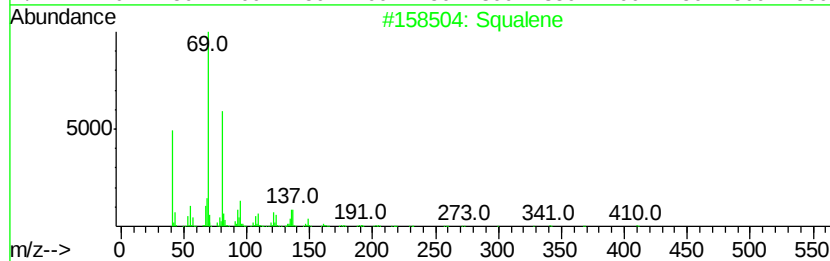
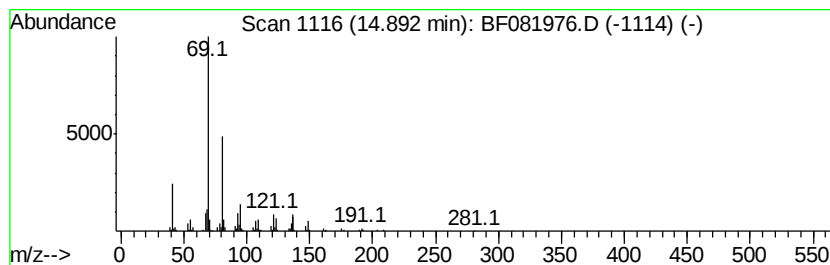
Instrument :
BNA_F
ClientSampleId :
A6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	5.63 ng	209351	Perylene-d12	15.50
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	.psi.,.psi.-Carotene, 7,7',8,8',...		547 C40H66	000502-62-5 83
4	1,5-Heptadiene, 3,3,6-trimethyl-		138 C10H18	035387-63-4 53
5	Trideca-1,7,11-triene-1,1-dicarb...		270 C18H26N2	1000161-46-0 53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100115\
Data File : BF081976.D
Acq On : 2 Oct 2015 9:52
Operator : UM/IZ
Sample : G3875-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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...	5.07	30.1	ng	920085	1	6.89	612165	20.0
unknown6.66	6.66	62.1	ng	1900760	1	6.89	612165	20.0
Tridecanoic acid	11.94	3.9	ng	211320	4	11.42	1074230	20.0
Hexadecanoic acid...	12.82	3.6	ng	177103	5	14.06	993410	20.0
9-Octadecenamide,...	14.81	5.5	ng	206112	6	15.50	743707	20.0
Squalene	14.89	5.6	ng	209351	6	15.50	743707	20.0