

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
 Data File : BF093616.D
 Acq On : 13 Mar 2017 19:17
 Operator : SJ/MA
 Sample : I2174-26
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-81

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-BF030717.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	2.413	44	46	57	rVB	47173	147983	2.98%	0.345%
2	4.150	196	198	204	rVB	43019	70182	1.41%	0.164%
3	4.859	258	260	283	rBV	1101989	2020097	40.63%	4.714%
4	5.316	298	300	330	rBV	2902930	4972502	100.00%	11.603%
5	5.716	332	335	343	rVB	46999	86367	1.74%	0.202%
6	6.367	390	392	400	rBV	3461505	4532478	91.15%	10.576%
7	6.482	400	402	405	rVB	4540152	4444679	89.39%	10.371%
8	6.710	419	422	431	rVB	924939	989867	19.91%	2.310%
9	6.859	433	435	438	rBV	3416008	3521126	70.81%	8.216%
10	7.282	470	472	487	rBV	2763920	3177891	63.91%	7.415%
11	8.002	532	535	546	rBV	1211221	1364518	27.44%	3.184%
12	9.076	627	629	632	rBV	3660492	4825937	97.05%	11.261%
13	9.762	686	689	691	rBV	935222	1363166	27.41%	3.181%
14	10.550	756	758	761	rBV	2250492	2516028	50.60%	5.871%
15	11.248	817	819	824	rBV	1446356	1377600	27.70%	3.214%
16	12.596	935	937	951	rBV	577507	746026	15.00%	1.741%
17	12.836	955	958	960	rBV	4233493	4310732	86.69%	10.059%
18	13.019	972	974	981	rBV	42779	68738	1.38%	0.160%
19	13.899	1049	1051	1059	rVB	698793	1017954	20.47%	2.375%
20	15.305	1170	1174	1184	rBV	558876	860902	17.31%	2.009%
21	15.682	1204	1207	1211	rBV	73369	106932	2.15%	0.250%
22	16.128	1243	1246	1250	rBV	70962	119890	2.41%	0.280%
23	16.654	1288	1292	1296	rBV	48462	105419	2.12%	0.246%
24	17.260	1341	1345	1355	rVB	38108	109183	2.20%	0.255%

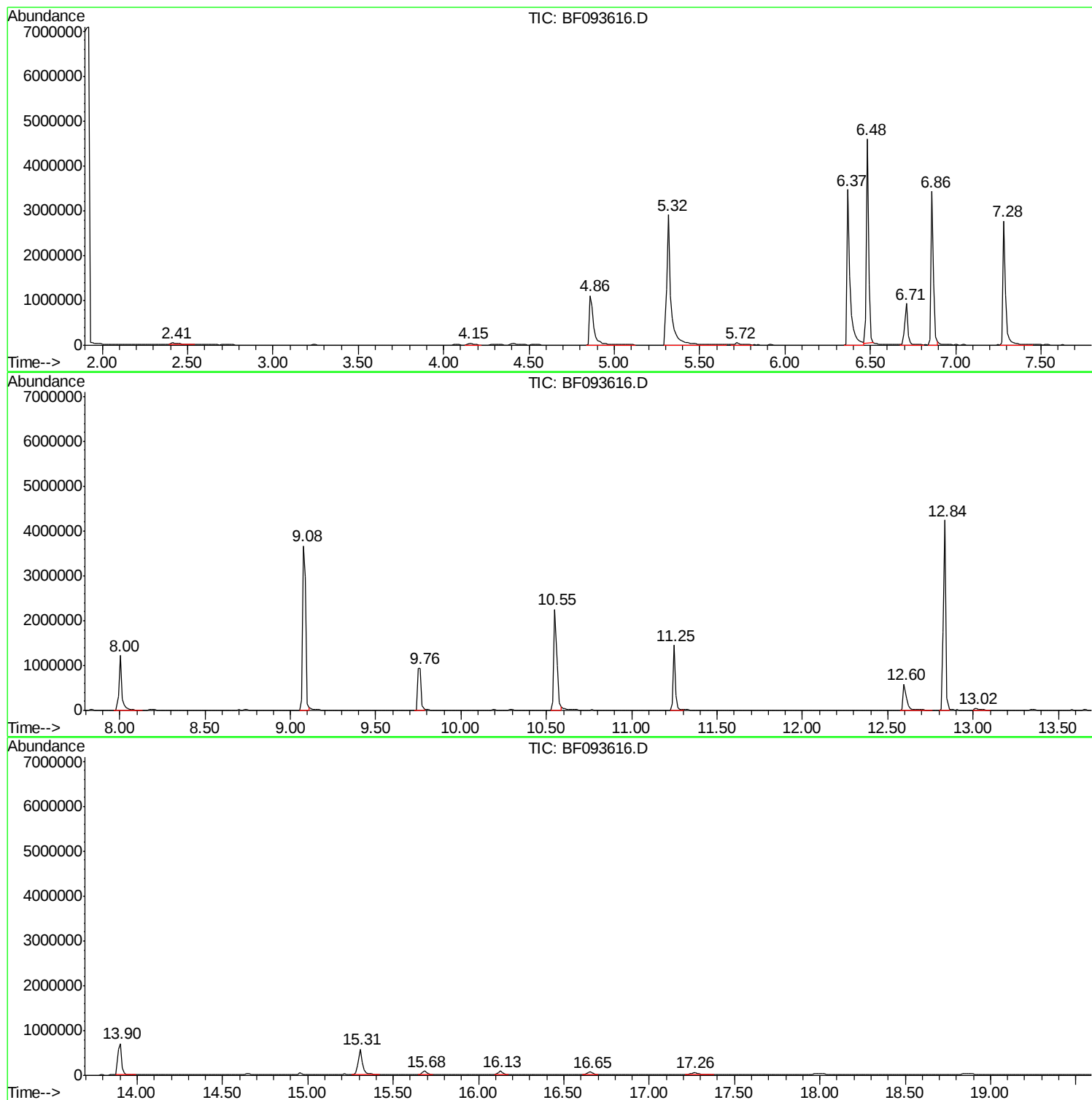
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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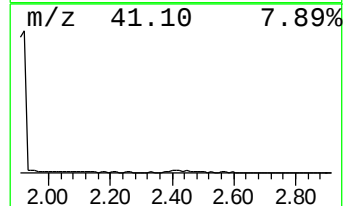
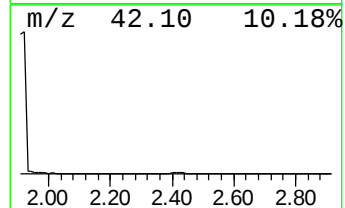
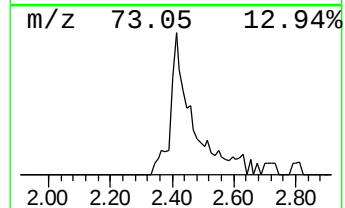
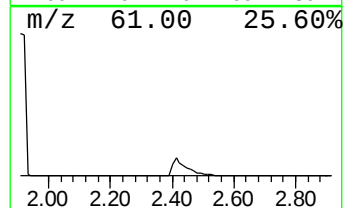
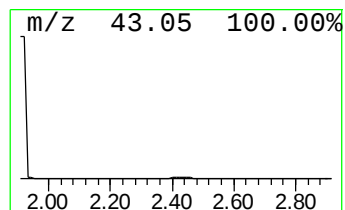
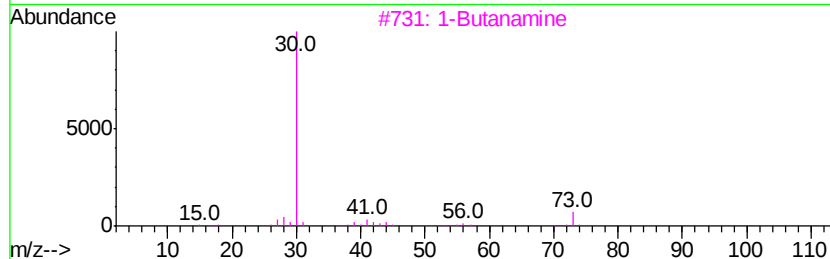
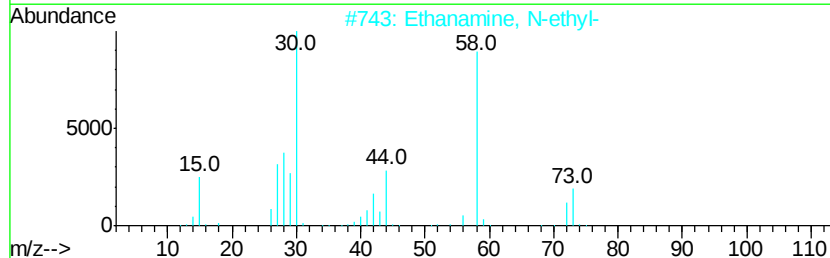
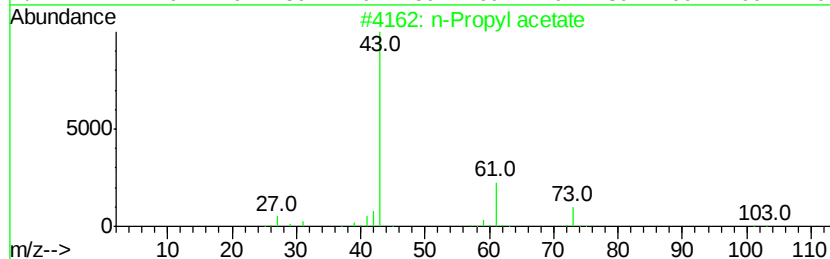
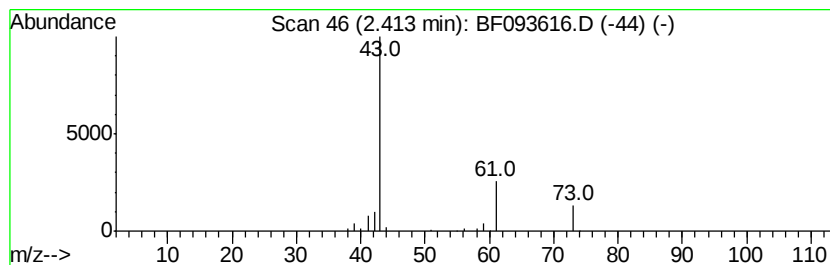
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.41	2.99 ng	147983	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	56
2		Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	7
3		1-Butanamine	73	C4H11N	000109-73-9	5
4		Isobutylamine	73	C4H11N	000078-81-9	4
5		Hydrogen azide	43	HN3	007782-79-8	4



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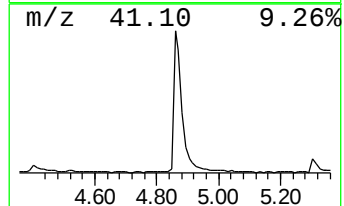
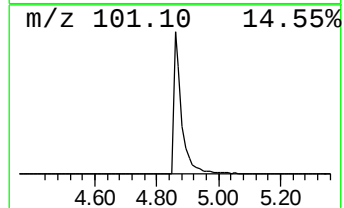
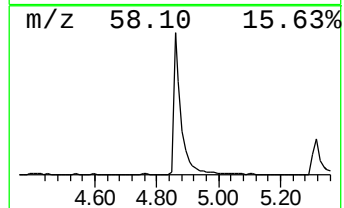
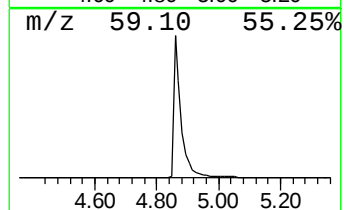
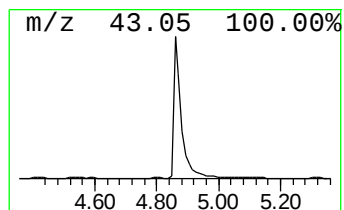
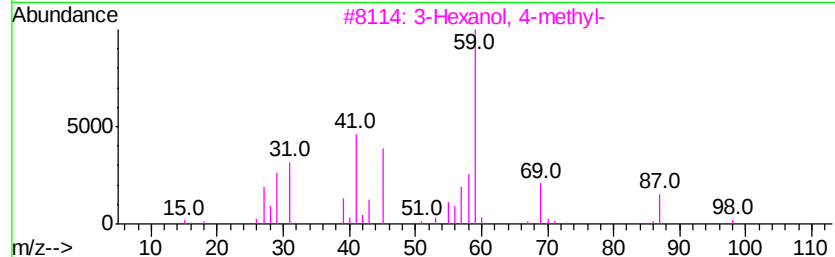
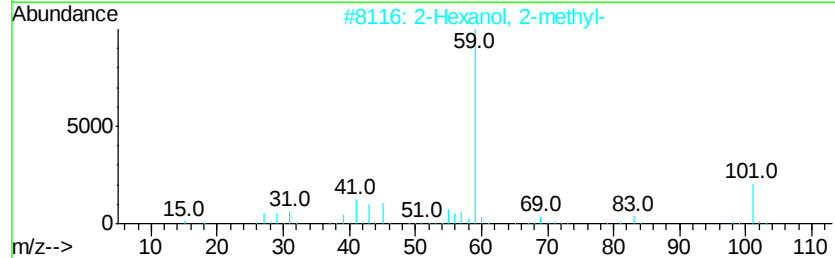
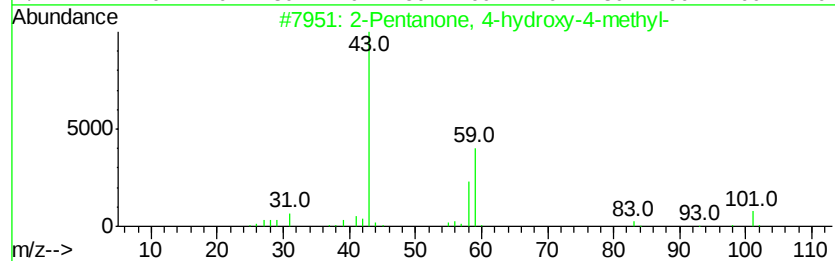
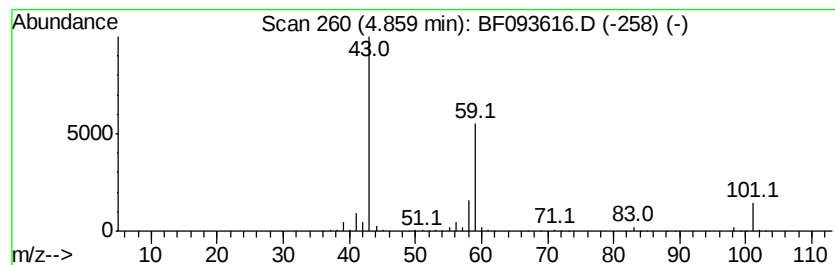
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	40.82 ng	2020100	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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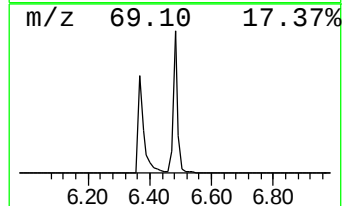
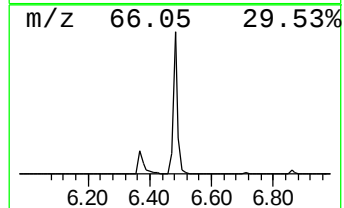
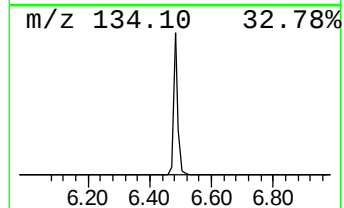
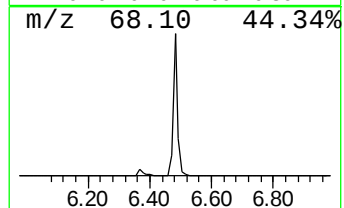
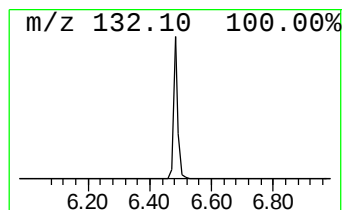
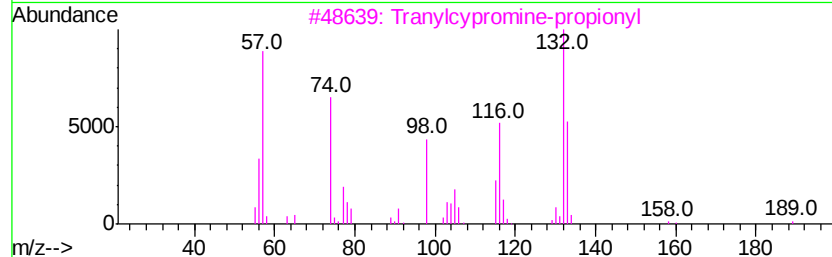
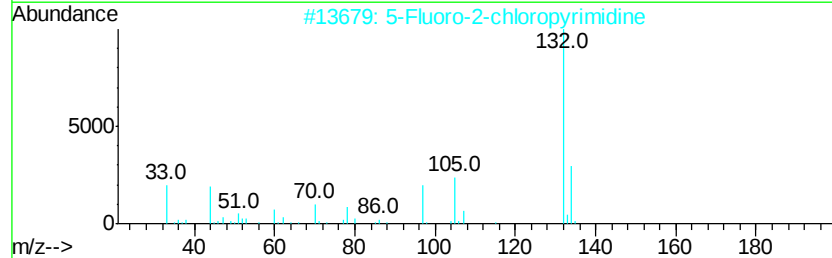
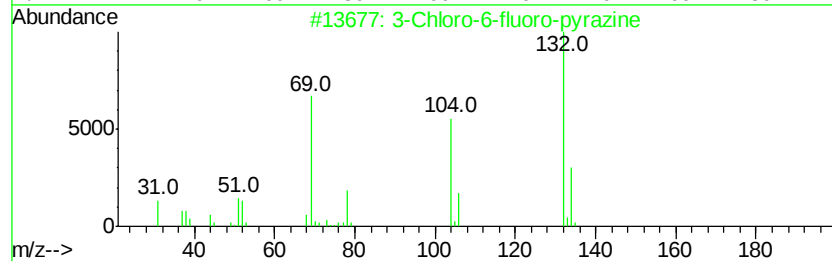
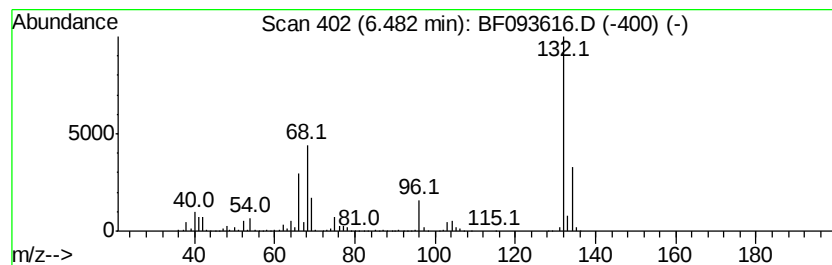
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Peak Number 3 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	89.80 ng	4444680	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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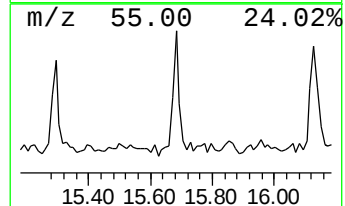
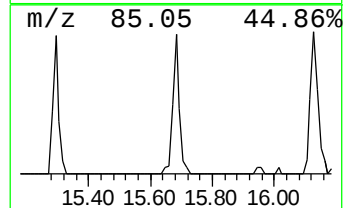
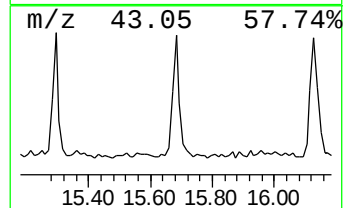
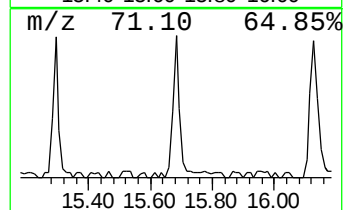
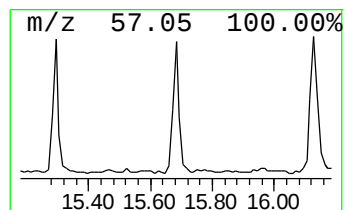
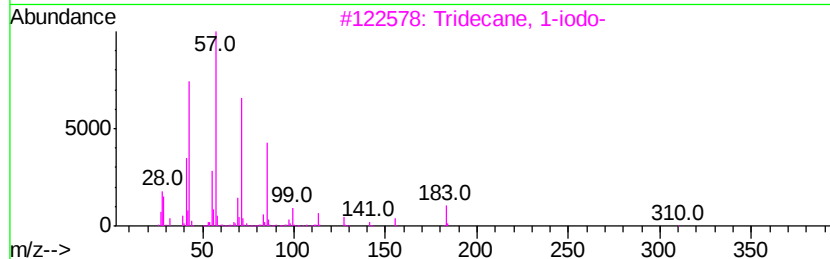
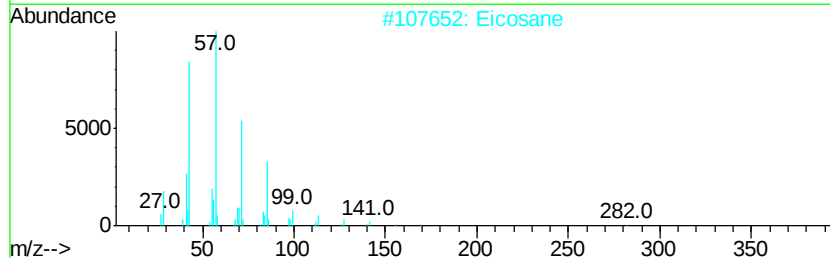
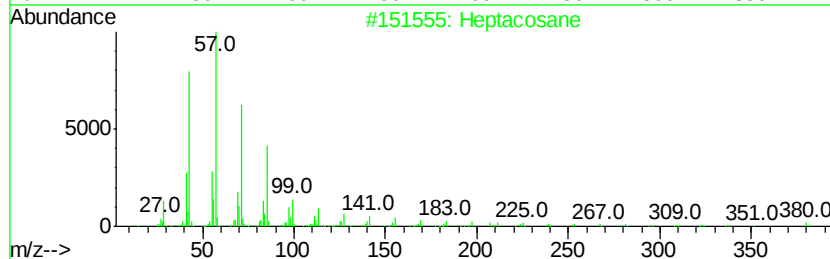
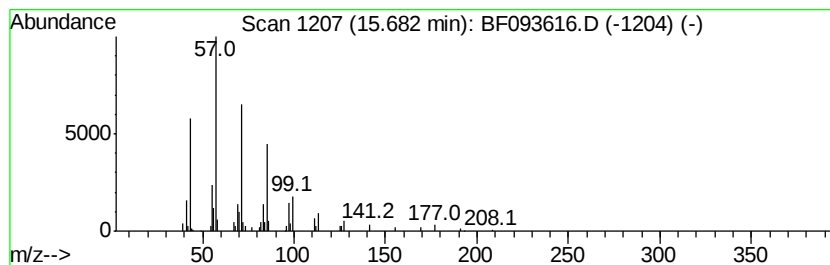
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	2.48 ng	106932	Perylene-d12	15.31
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	91
2	Eicosane	282 C20H42	000112-95-8	86
3	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	86
4	Tetracosane	338 C24H50	000646-31-1	86
5	Hexatriacontane	507 C36H74	000630-06-8	80



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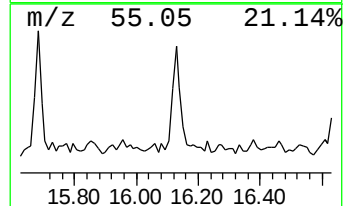
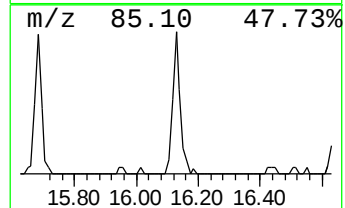
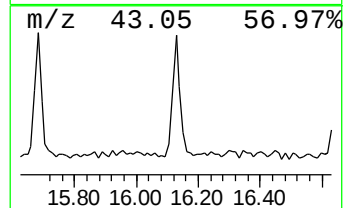
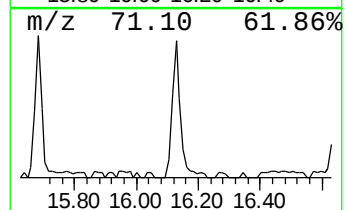
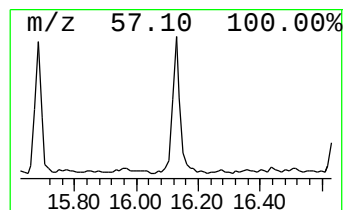
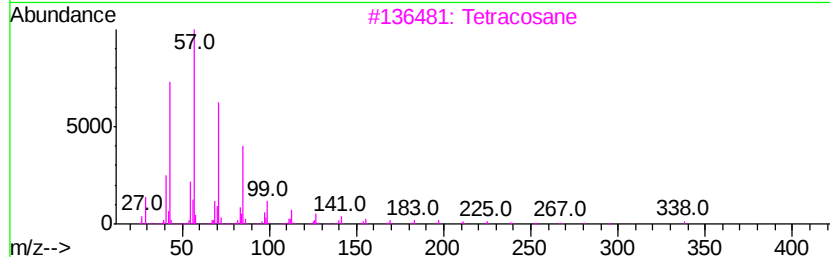
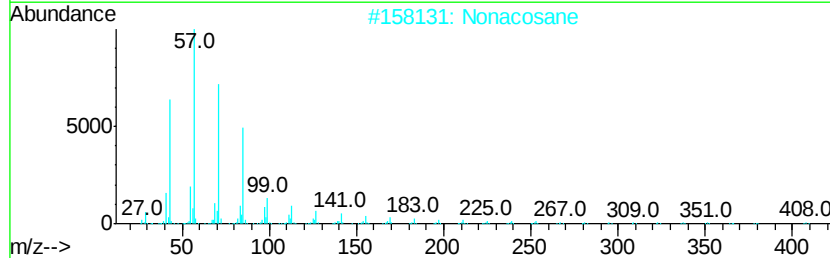
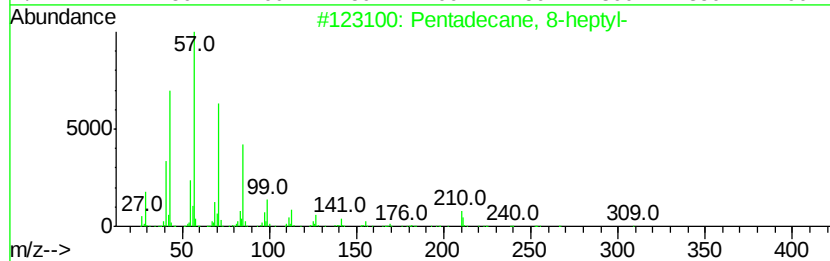
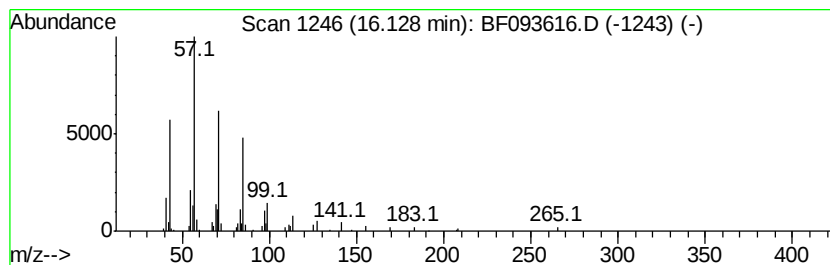
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Pentadecane, 8-heptyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.79 ng	119890	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2		Nonacosane	408	C29H60	000630-03-5	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86



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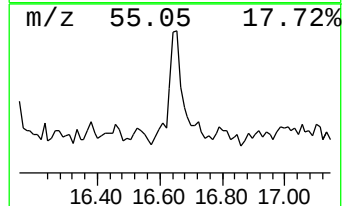
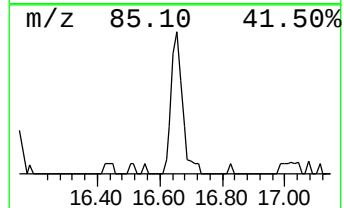
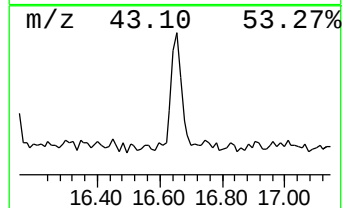
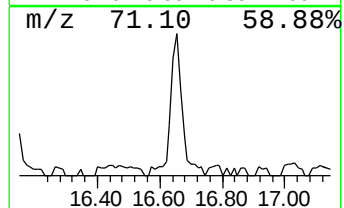
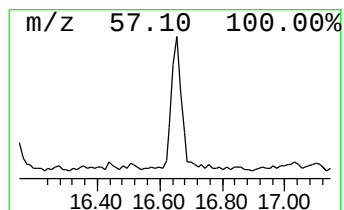
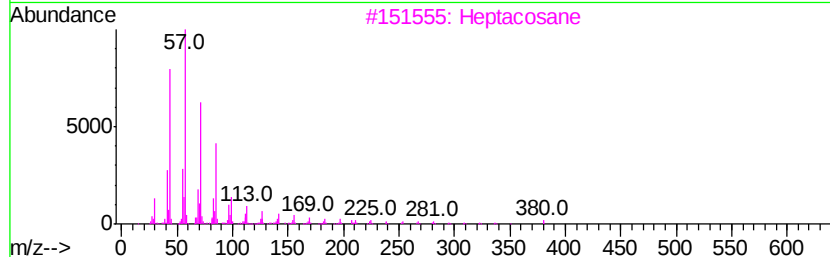
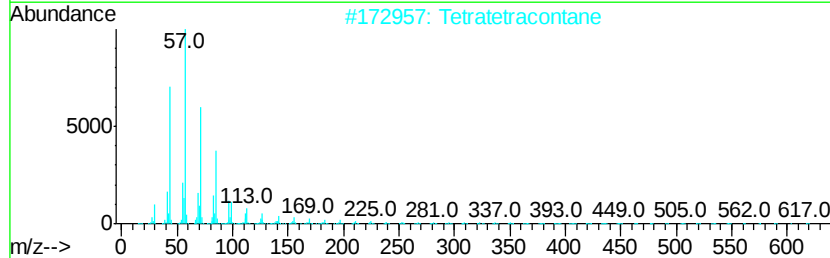
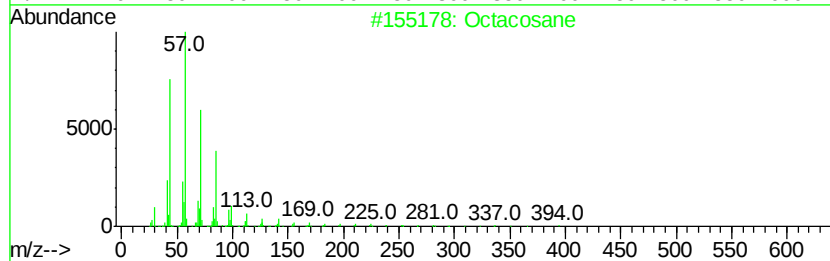
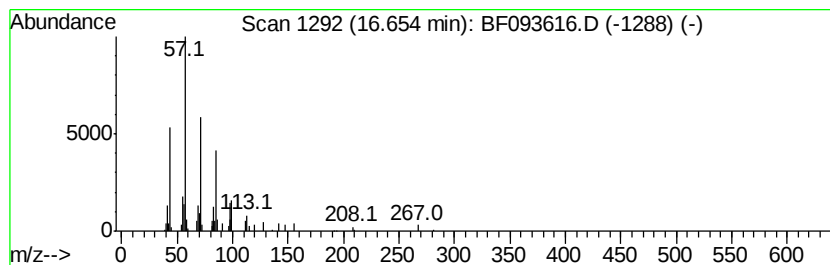
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BNA_F
ClientSampleId :
D-81

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.65	2.45 ng	105419	Perylene-d12	15.31
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394 C28H58	000630-02-4	91
2	Tetratetracontane	619 C44H90	007098-22-8	91
3	Heptacosane	380 C27H56	000593-49-7	90
4	Eicosane, 9-octyl-	394 C28H58	013475-77-9	90
5	Hexatriacontane	507 C36H74	000630-06-8	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093616.D
Acq On : 13 Mar 2017 19:17
Operator : SJ/MA
Sample : I2174-26
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-81

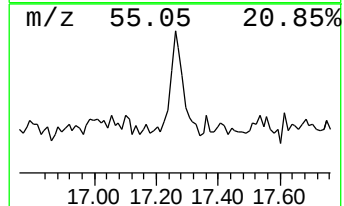
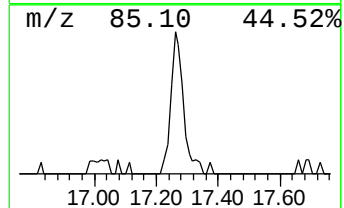
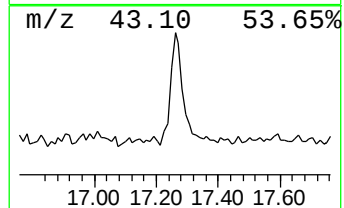
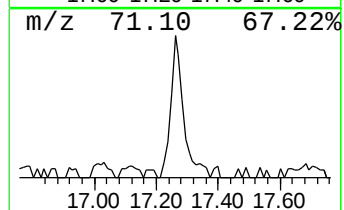
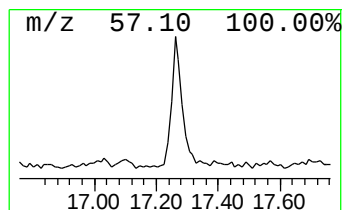
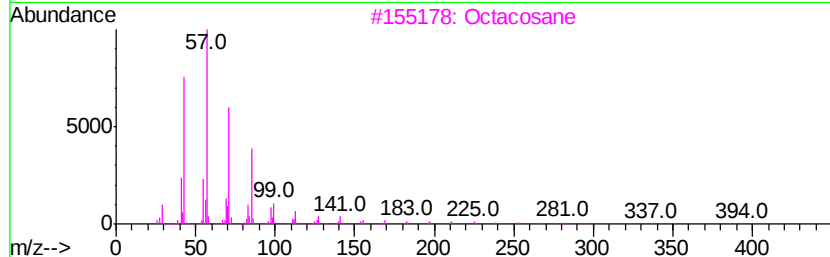
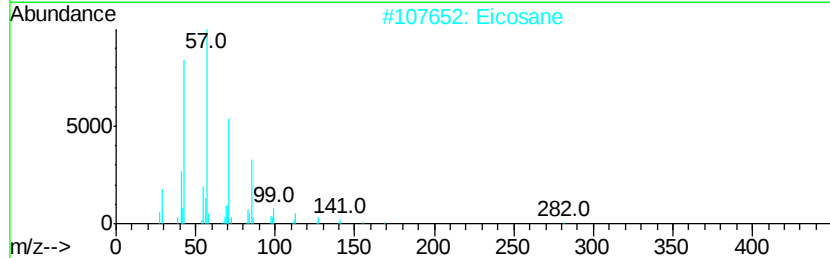
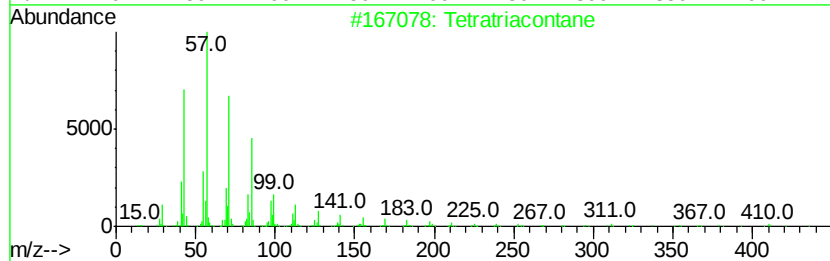
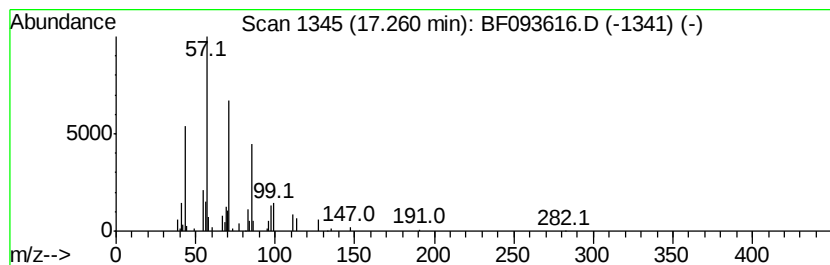
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.26	2.54 ng	109183	Perylene-d12	15.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratriacontane	479	C34H70	014167-59-0	86
2		Eicosane	282	C20H42	000112-95-8	86
3		Octacosane	394	C28H58	000630-02-4	86
4		Hexatriacontane	507	C36H74	000630-06-8	86
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093616.D
Acq On : 13 Mar 2017 19:17
Operator : SJ/MA
Sample : I2174-26
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-81

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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
n-Propyl acetate	2.41	3.0	ng	147983	1	6.71	989867	20.0
2-Pentanone, 4-hy...	4.86	40.8	ng	2020100	1	6.71	989867	20.0
unknown6.48	6.48	89.8	ng	4444680	1	6.71	989867	20.0
Heptacosane	15.68	2.5	ng	106932	6	15.31	860902	20.0
Pentadecane, 8-he...	16.13	2.8	ng	119890	6	15.31	860902	20.0
Octacosane	16.65	2.5	ng	105419	6	15.31	860902	20.0
Tetratriacontane	17.26	2.5	ng	109183	6	15.31	860902	20.0