

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
 Data File : BF088943.D
 Acq On : 13 Jul 2016 4:23
 Operator : UM/SJ
 Sample : H3987-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-WALL-E-070816

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-BF063016.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	1.667	6	7	13	rVV	85112	121956	6.21%	0.807%
2	1.792	16	18	26	rVV	398882	558781	28.47%	3.698%
3	1.907	26	28	31	rVB	39377	47551	2.42%	0.315%
4	4.856	283	286	293	rBB	225988	339691	17.31%	2.248%
5	5.301	322	325	328	rBV	1379382	1463511	74.58%	9.685%
6	5.701	357	360	362	rBB	27928	23444	1.19%	0.155%
7	6.353	414	417	419	rBV	1422601	1476129	75.22%	9.769%
8	6.479	425	428	430	rBV	1432570	1798755	91.66%	11.904%
9	6.707	445	448	450	rBV	280040	359198	18.30%	2.377%
10	6.856	459	461	464	rVB	1150064	1265485	64.49%	8.375%
11	7.267	494	497	500	rBV	894533	964159	49.13%	6.380%
12	7.987	557	560	562	rBV	580522	481106	24.52%	3.184%
13	9.073	652	655	657	rBV	1693577	1962418	100.00%	12.987%
14	9.462	687	689	691	rBV	366478	288289	14.69%	1.908%
15	9.736	711	713	715	rBB	539231	457032	23.29%	3.024%
16	10.525	779	782	784	rBV	935745	870773	44.37%	5.762%
17	10.650	792	793	798	rBV	22614	28703	1.46%	0.190%
18	10.971	819	821	824	rVB	29734	43712	2.23%	0.289%
19	11.096	830	832	834	rBV	22267	24551	1.25%	0.162%
20	11.211	840	842	844	rVB	428158	363716	18.53%	2.407%
21	12.799	978	981	983	rBV	1466426	1314260	66.97%	8.697%
22	13.702	1058	1060	1069	rBV	123167	130958	6.67%	0.867%
23	13.839	1069	1072	1074	rBV	361614	375607	19.14%	2.486%
24	14.331	1113	1115	1121	rBV	41798	60989	3.11%	0.404%
25	15.211	1189	1192	1194	rBV	246868	290293	14.79%	1.921%

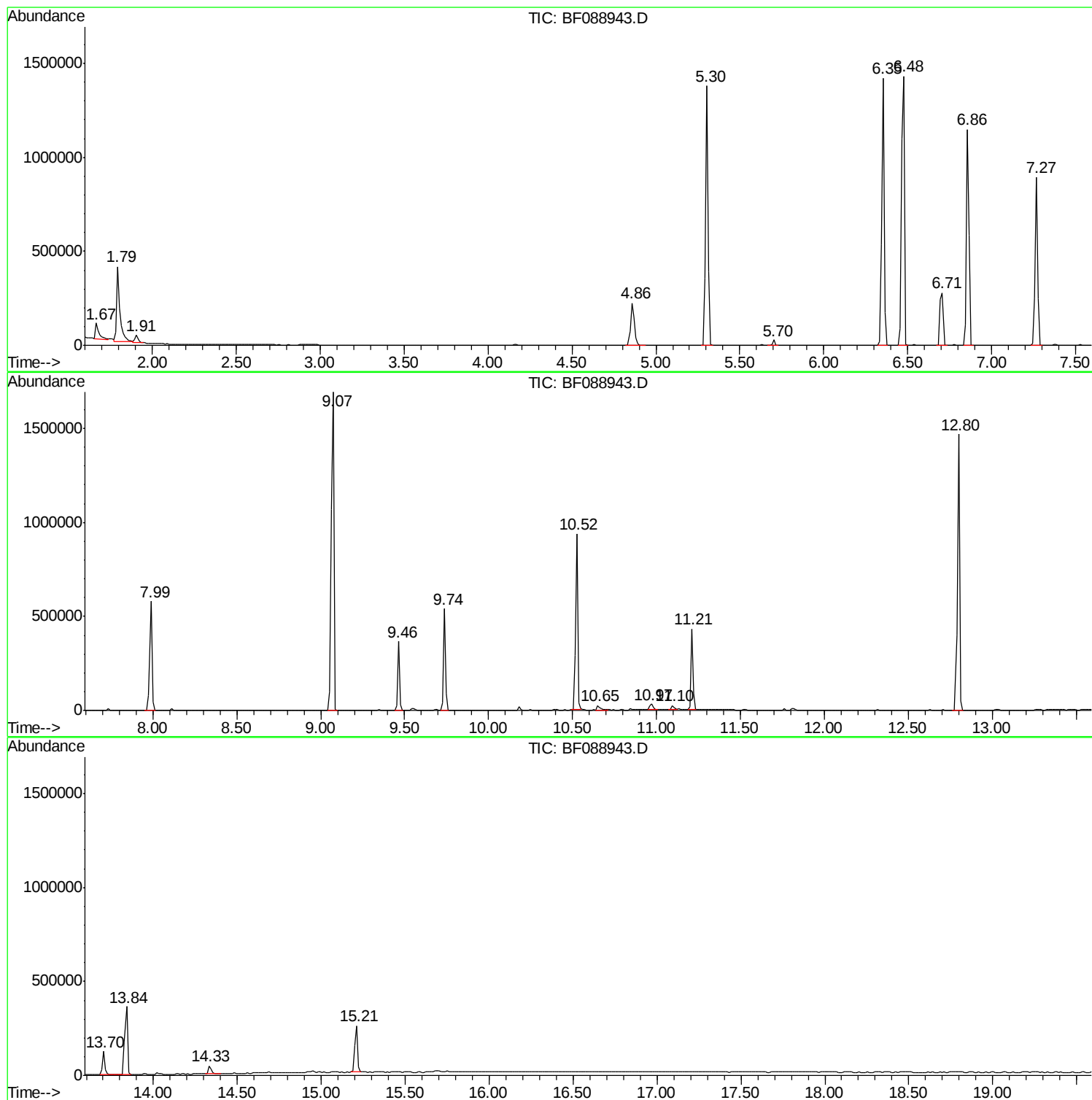
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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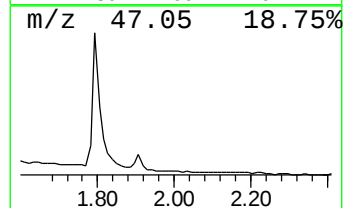
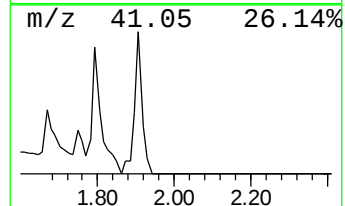
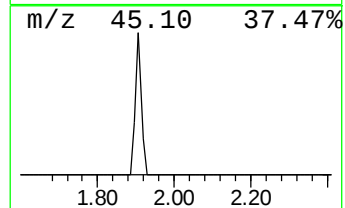
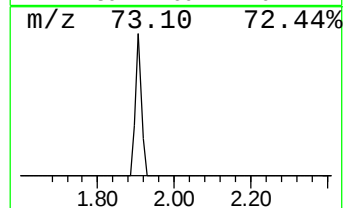
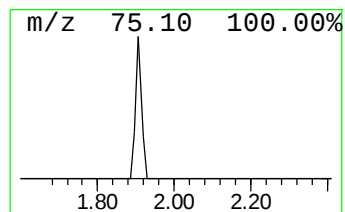
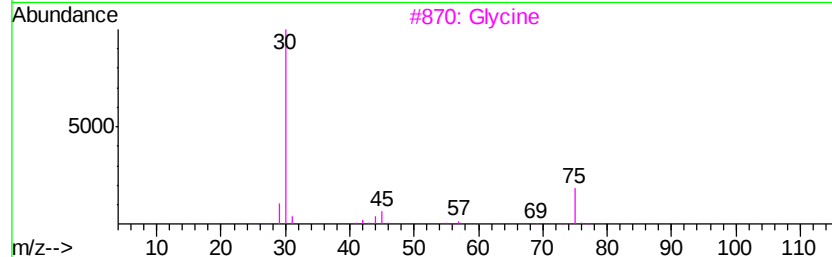
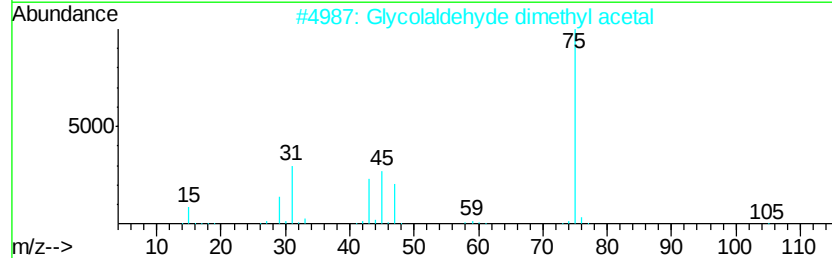
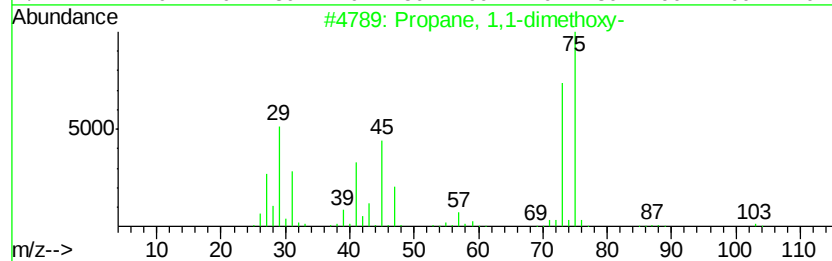
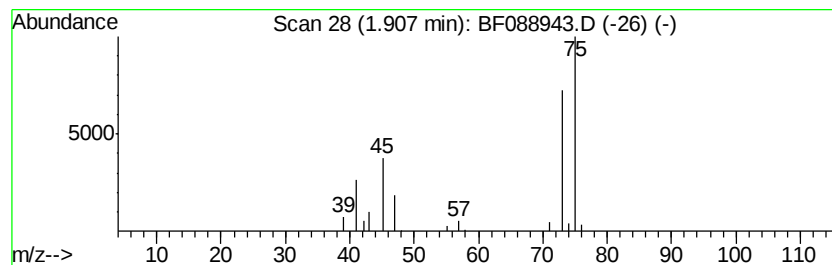
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.91	2.65 ng	47551	1,4-Dichlorobenzene-d4	6.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
3		Glycine	75	C2H5NO2	000056-40-6	7
4		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	4
5		2-Bromomethyl-1,3-dioxolane	166	C4H7BrO2	004360-63-8	4



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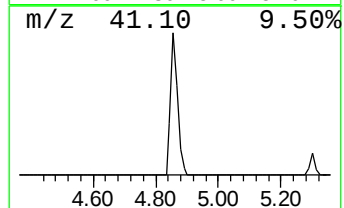
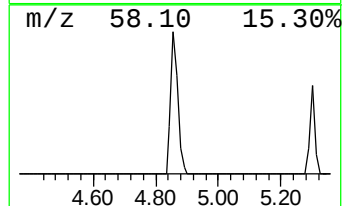
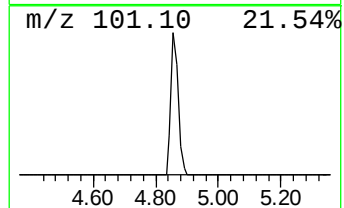
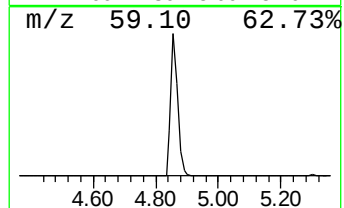
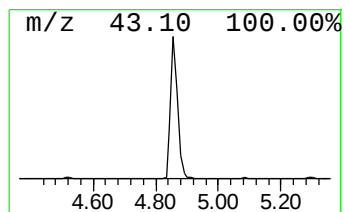
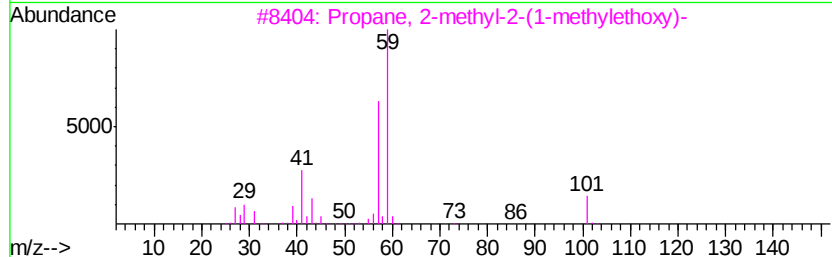
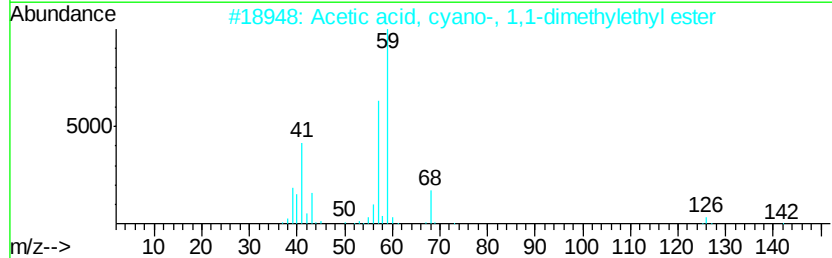
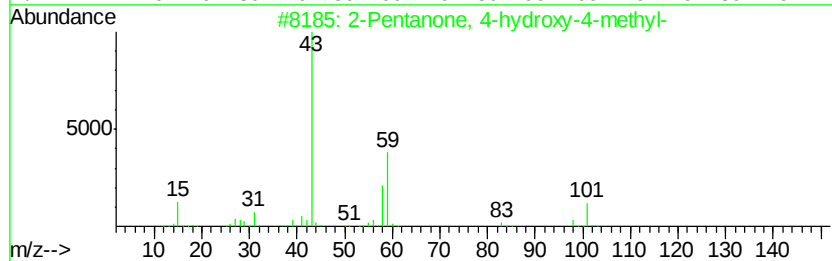
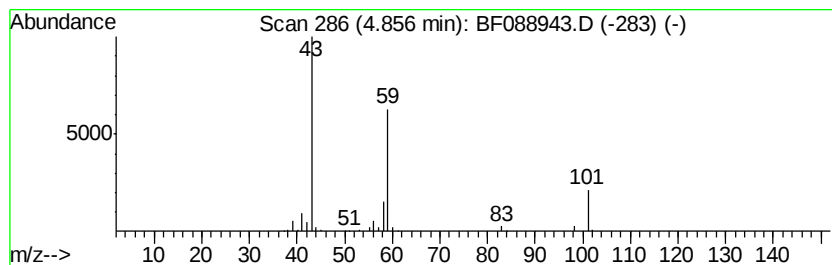
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	18.91 ng	339691	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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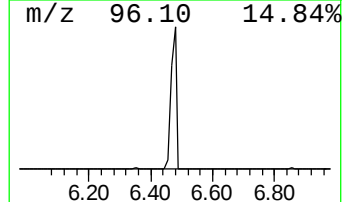
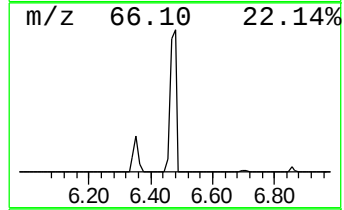
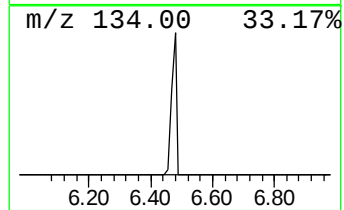
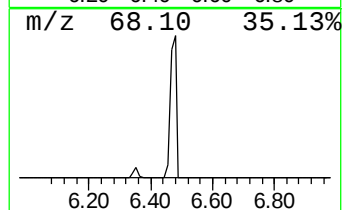
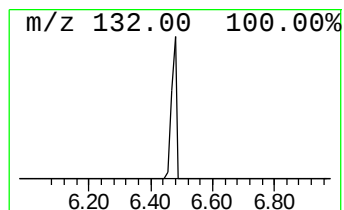
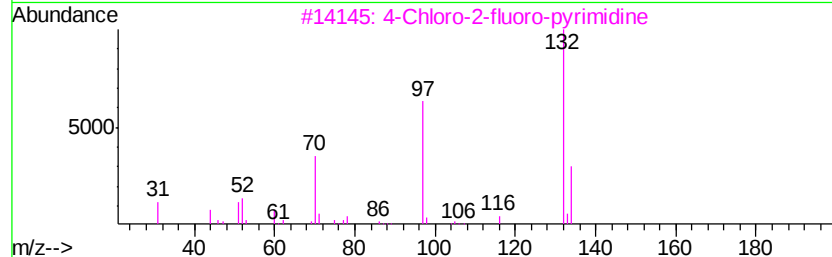
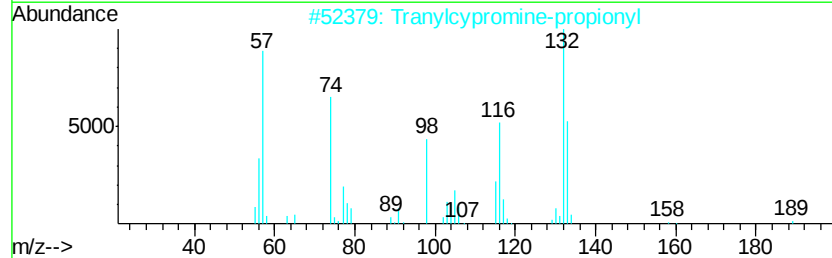
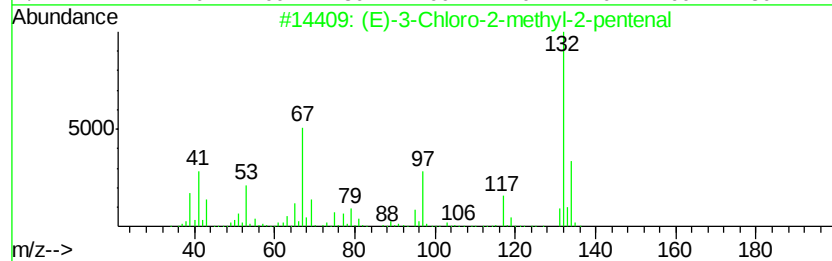
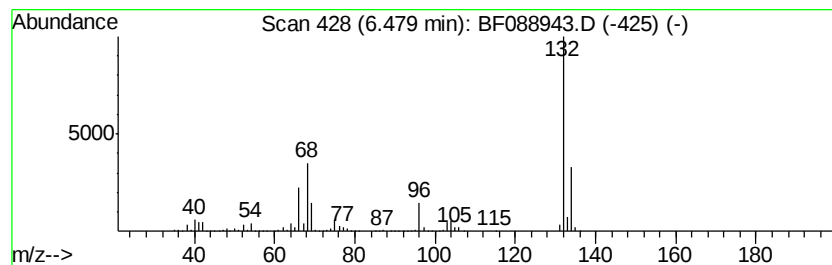
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Peak Number 5 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	100.15 ng	1798760	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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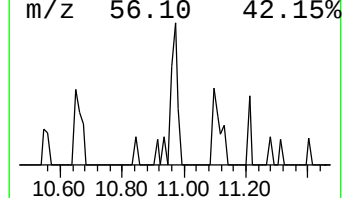
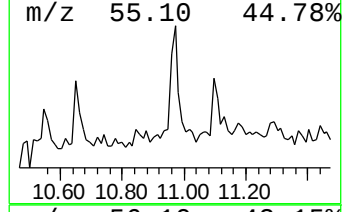
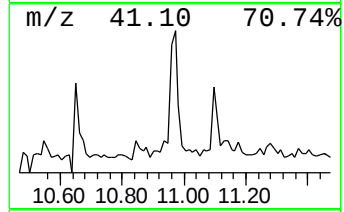
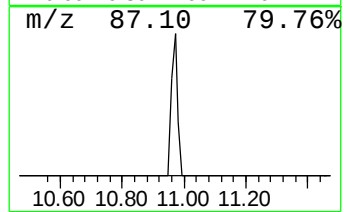
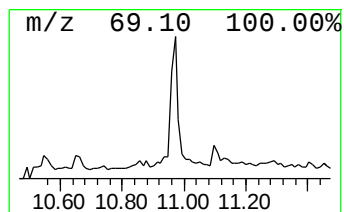
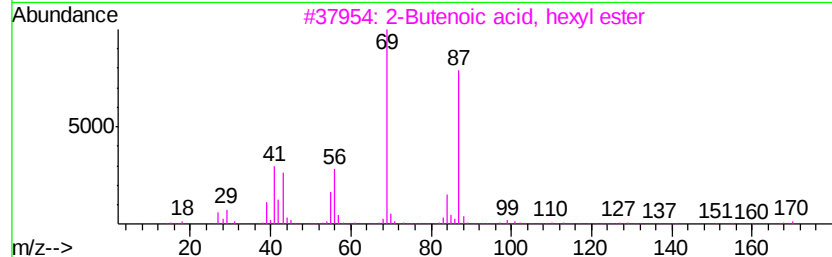
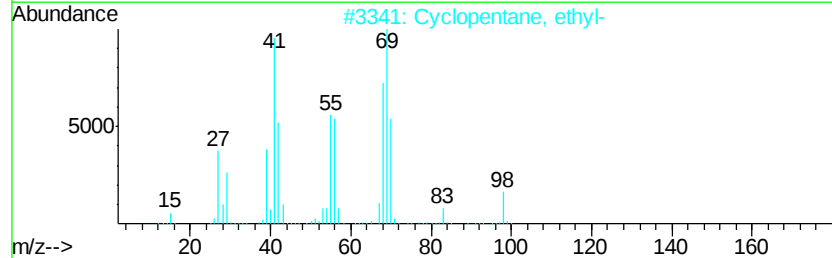
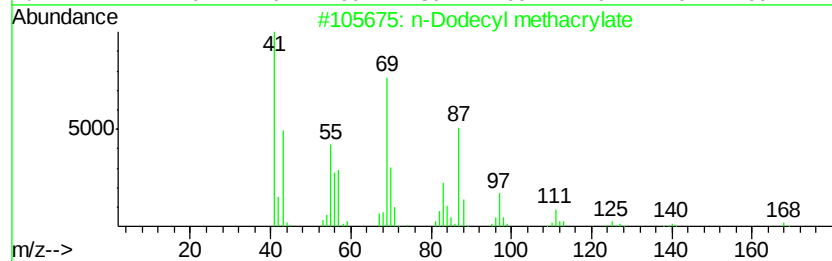
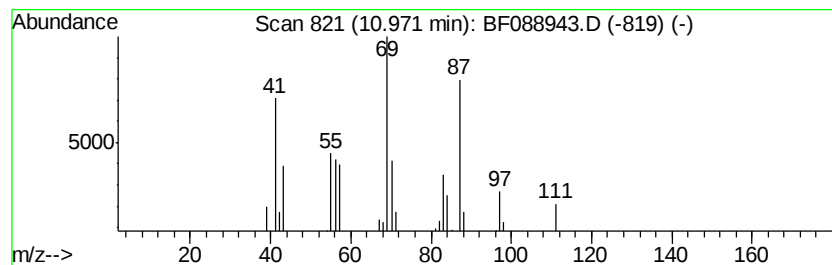
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Peak Number 7 n-Dodecyl methacrylate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	2.40 ng	43712	Phenanthrene-d10	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	86
2		Cyclopentane, ethyl-	98	C7H14	001640-89-7	45
3		2-Butenoic acid, hexyl ester	170	C10H18O2	019089-92-0	40
4		1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	38
5		Cyclopropane, 1,1-diethyl-	98	C7H14	001003-19-6	35



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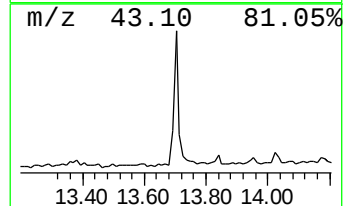
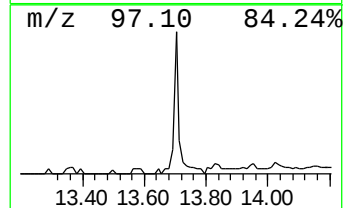
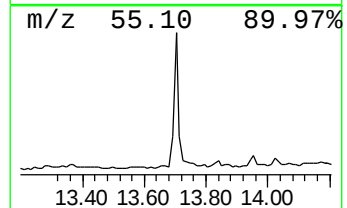
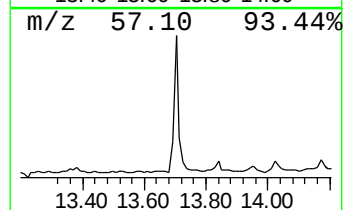
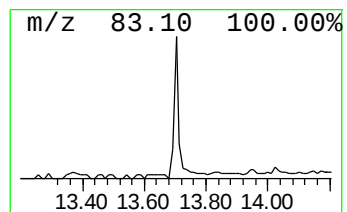
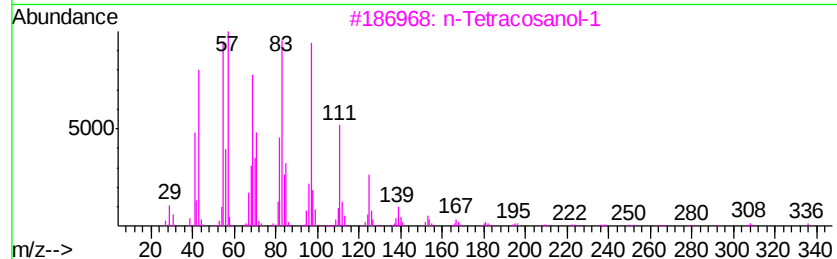
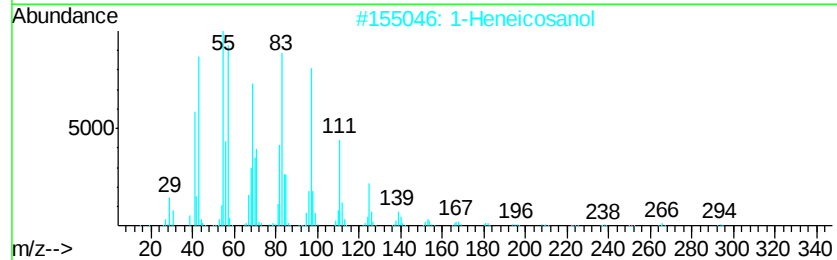
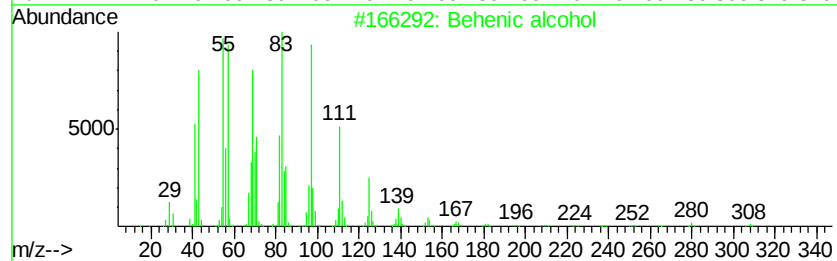
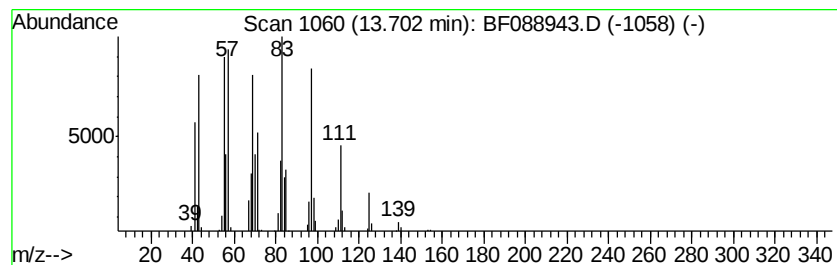
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Peak Number 8 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.70	6.97 ng	130958	Chrysene-d12		13.84
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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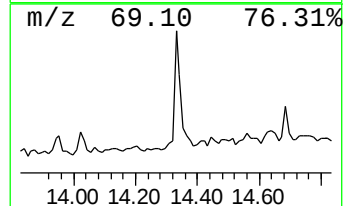
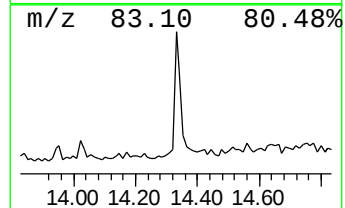
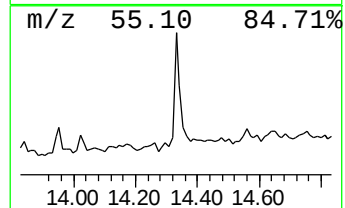
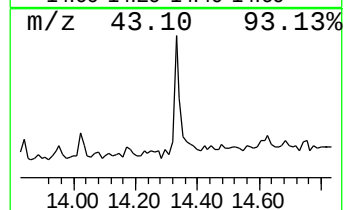
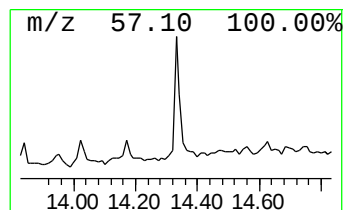
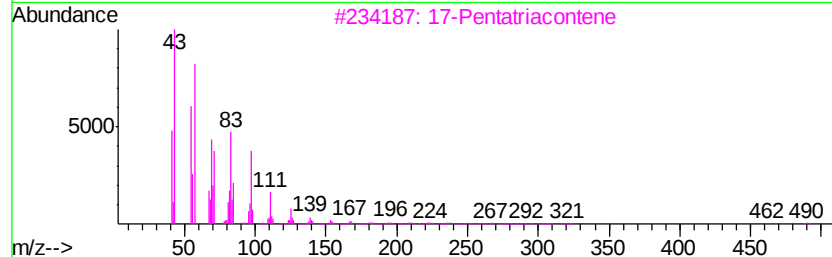
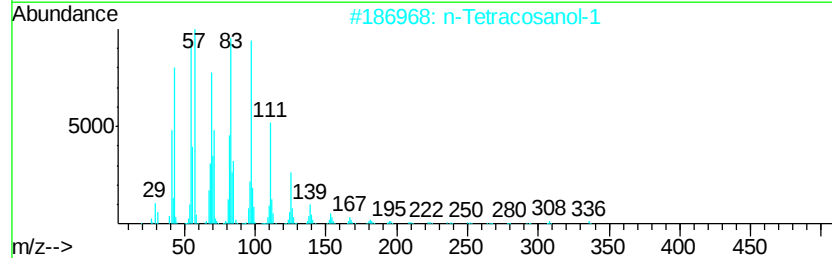
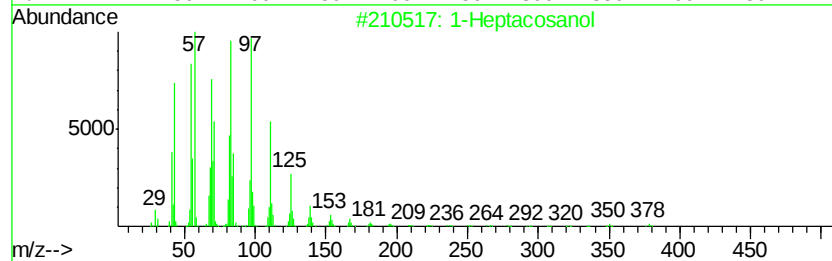
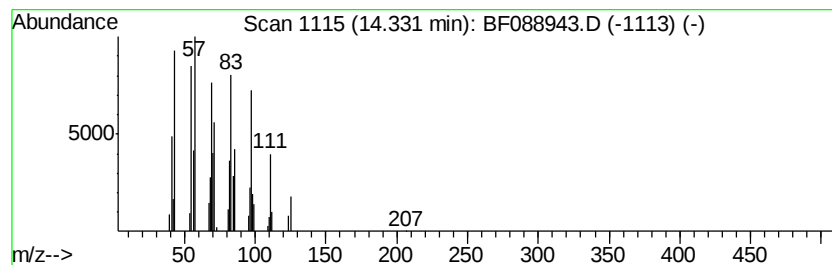
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	3.25 ng	60989	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		Behenic alcohol	326	C22H46O	000661-19-8	90
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088943.D
Acq On : 13 Jul 2016 4:23
Operator : UM/SJ
Sample : H3987-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-WALL-E-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.91	2.6	ng	47551	1	6.71	359198	20.0
2-Pentanone, 4-hy...	4.86	18.9	ng	339691	1	6.71	359198	20.0
unknown6.48	6.48	100.2	ng	1798760	1	6.71	359198	20.0
n-Dodecyl methacr...	10.97	2.4	ng	43712	4	11.21	363716	20.0
Behenic alcohol	13.70	7.0	ng	130958	5	13.84	375607	20.0
1-Heptacosanol	14.33	3.3	ng	60989	5	13.84	375607	20.0