

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
 Data File : BF085572.D
 Acq On : 19 Mar 2016 14:55
 Operator : UM/SJ
 Sample : H1816-02
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TRACK-D-GRID-9B

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-BF031816.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	5.064	241	243	253	rVB	47368	80957	1.95%	0.211%
2	5.464	274	278	280	rBV	2447388	3758081	90.55%	9.812%
3	6.493	364	368	370	rBV	2789079	3903424	94.05%	10.192%
4	6.619	376	379	382	rBV	3025620	3526327	84.96%	9.207%
5	6.847	397	399	402	rBV	689584	736401	17.74%	1.923%
6	7.007	410	413	416	rBV	2831330	2818677	67.91%	7.360%
7	7.224	431	432	438	rBV	426473	647294	15.60%	1.690%
8	7.339	439	442	446	rVV	88790	254314	6.13%	0.664%
9	7.419	446	449	451	rVV	2228705	2466487	59.43%	6.440%
10	7.510	455	457	467	rVB	33949	59239	1.43%	0.155%
11	7.876	480	489	501	rBV4	32674	91850	2.21%	0.240%
12	8.139	509	512	514	rBV	1072320	1044837	25.17%	2.728%
13	9.213	603	606	609	rBV	3748497	3858596	92.97%	10.075%
14	9.602	638	640	642	rBV	278036	278061	6.70%	0.726%
15	9.887	663	665	668	rVB	1208490	1076665	25.94%	2.811%
16	10.322	699	703	705	rBV	48606	56203	1.35%	0.147%
17	10.539	719	722	725	rBV	33117	50512	1.22%	0.132%
18	10.676	731	734	737	rBV2	2010341	2609335	62.87%	6.813%
19	10.733	737	739	743	rVV	58885	89217	2.15%	0.233%
20	10.790	743	744	749	rVB	45679	63916	1.54%	0.167%
21	11.373	792	795	797	rBV	1190759	1115949	26.89%	2.914%
22	11.911	839	842	850	rBV2	301991	489586	11.80%	1.278%
23	12.608	899	903	907	rBV2	21206	44240	1.07%	0.116%
24	12.688	907	910	916	rVV	116135	141459	3.41%	0.369%
25	12.779	916	918	920	rBV	94600	80617	1.94%	0.210%
26	12.962	931	934	936	rBV	3967880	4150475	100.00%	10.837%
27	13.191	951	954	960	rVB	46394	55495	1.34%	0.145%
28	13.431	973	975	978	rBV	66463	133771	3.22%	0.349%
29	13.488	978	980	982	rVV2	50247	81198	1.96%	0.212%
30	13.534	982	984	985	rVB	76125	80857	1.95%	0.211%
31	13.808	1005	1008	1009	rBV	40232	47343	1.14%	0.124%
32	13.865	1009	1013	1021	rBV3	278373	647509	15.60%	1.691%
33	14.002	1021	1025	1028	rBV2	1030488	1130818	27.25%	2.953%
34	14.174	1038	1040	1042	rBV	270045	246120	5.93%	0.643%

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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

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35	14.368	1055	1057	1060	rBV4	46478	81651	1.97%	0.213%
36	14.482	1064	1067	1068	rBV	234710	281962	6.79%	0.736%
37	14.779	1090	1093	1095	rBV	198464	243517	5.87%	0.636%
38	14.848	1097	1099	1101	rBV	70428	76125	1.83%	0.199%
39	15.099	1119	1121	1124	rVB	151809	173526	4.18%	0.453%
40	15.237	1130	1133	1134	rBV2	36564	54389	1.31%	0.142%
41	15.305	1137	1139	1143	rVV4	30931	60588	1.46%	0.158%
42	15.431	1147	1150	1156	rBV	561862	782119	18.84%	2.042%
43	15.579	1159	1163	1166	rVB4	40455	63565	1.53%	0.166%
44	15.877	1186	1189	1191	rBV	38623	66501	1.60%	0.174%
45	16.014	1194	1201	1212	rVV4	51909	402903	9.71%	1.052%
46	16.151	1212	1213	1218	rVB4	30785	46762	1.13%	0.122%
47	16.357	1228	1231	1237	rVB2	21761	49628	1.20%	0.130%

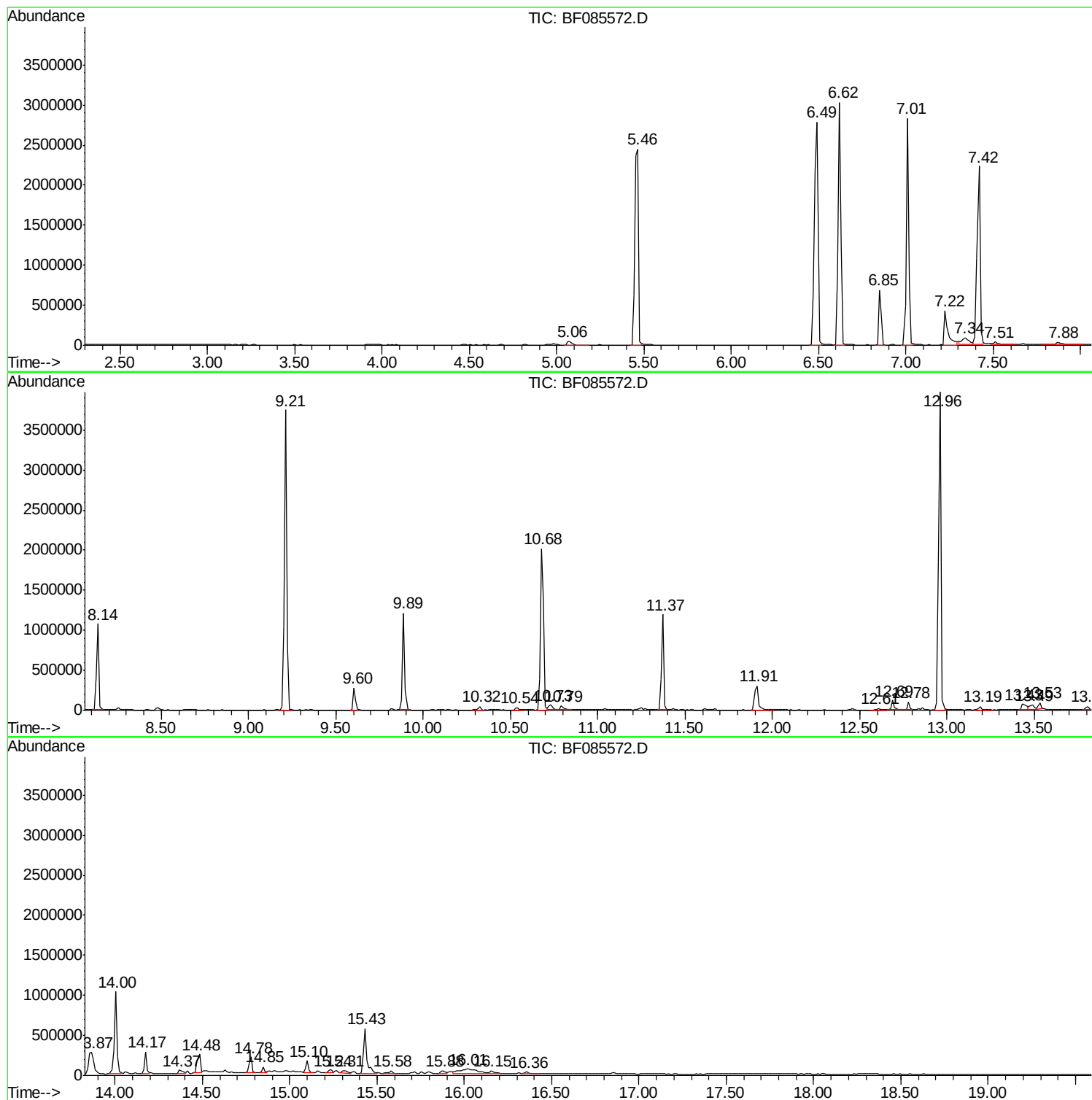
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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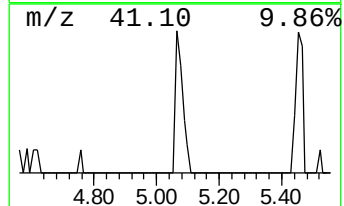
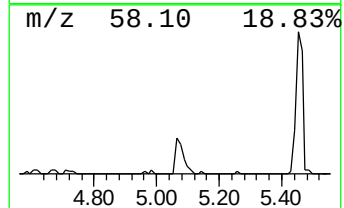
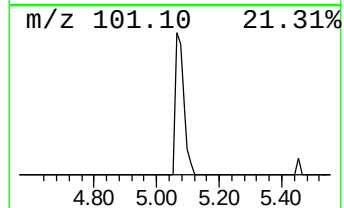
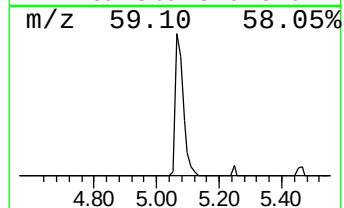
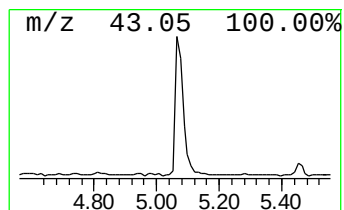
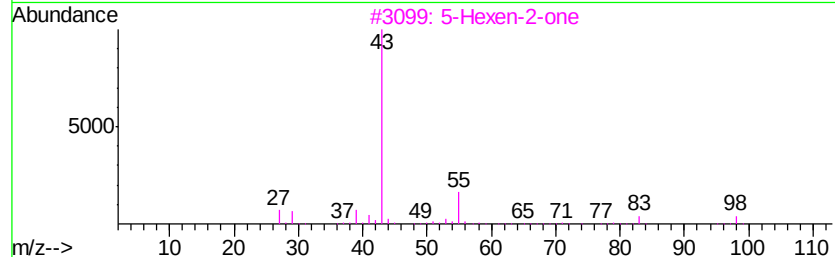
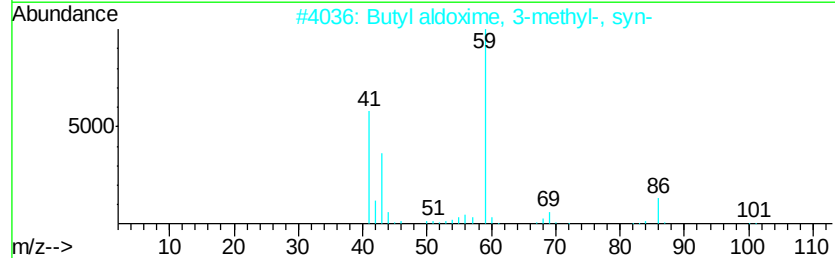
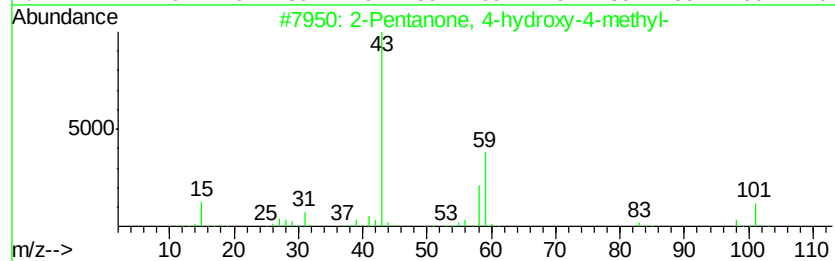
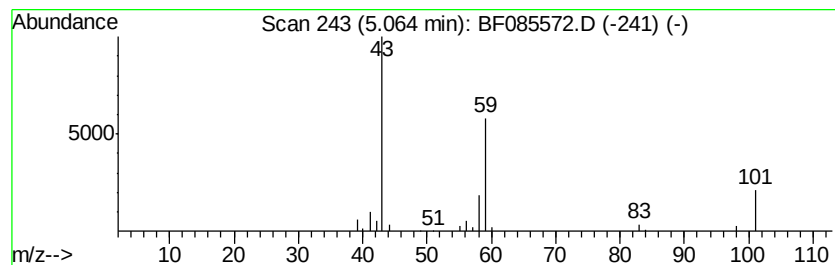
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	2.20 ng	80957	1,4-Dichlorobenzene-d4	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetone	58	C3H6O	000067-64-1	9



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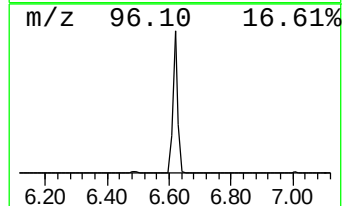
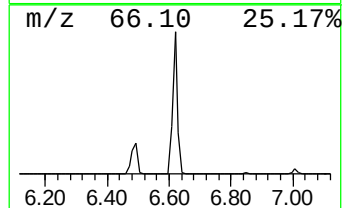
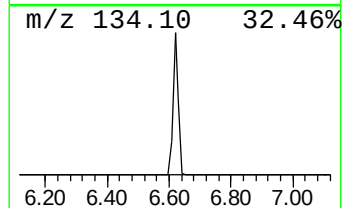
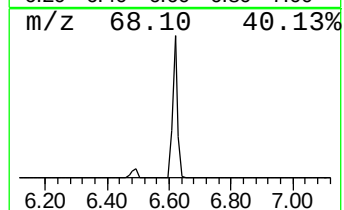
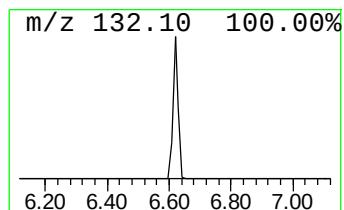
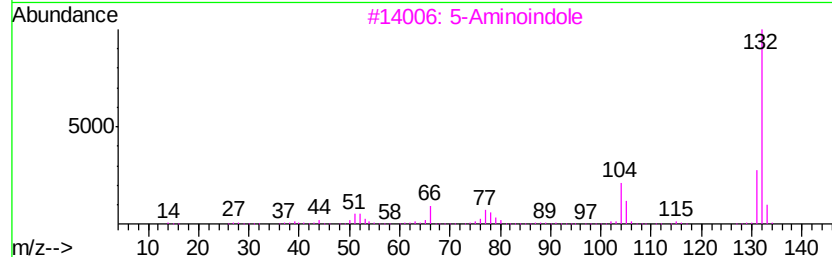
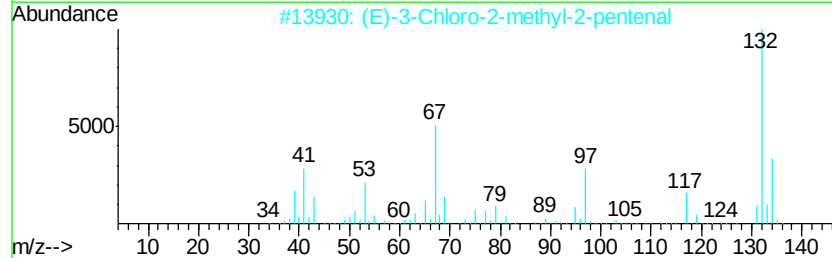
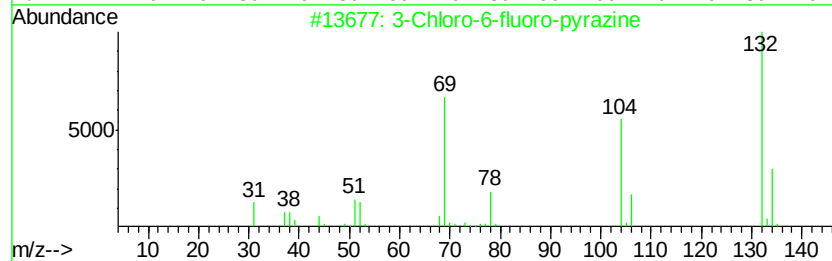
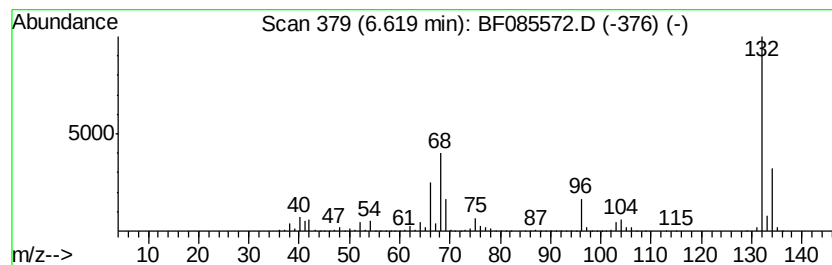
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	95.77 ng	3526330	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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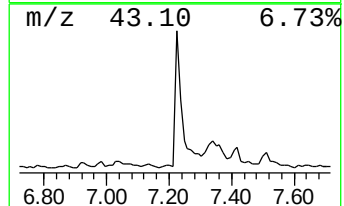
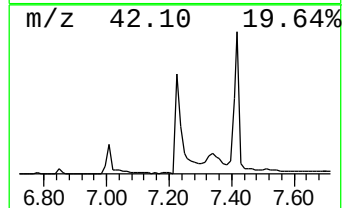
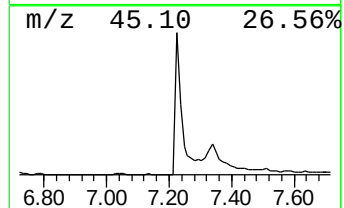
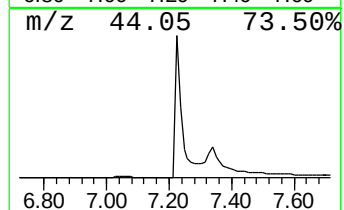
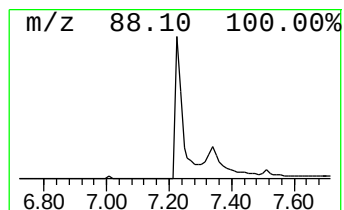
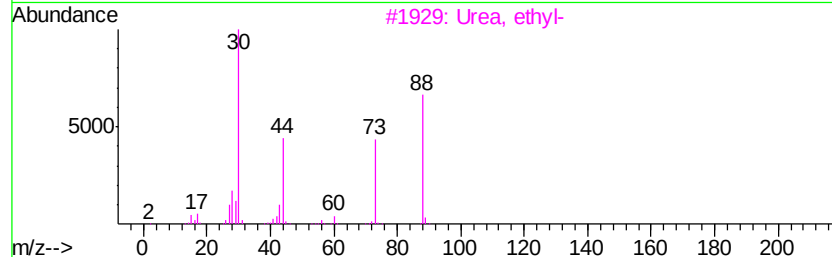
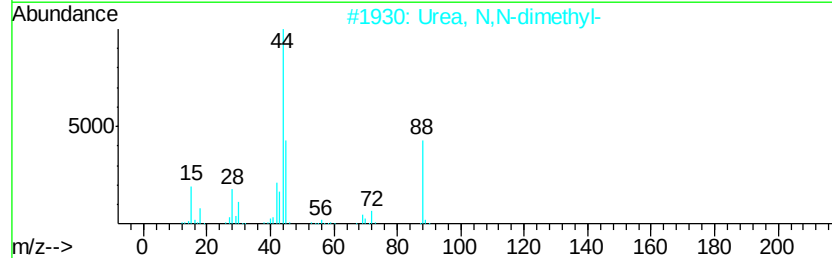
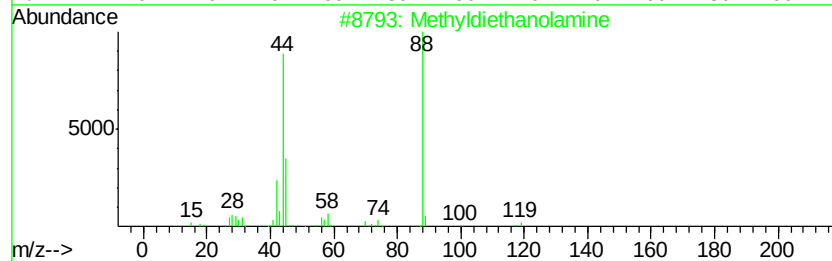
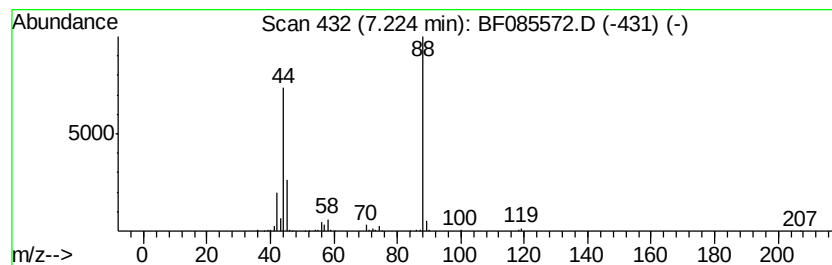
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Methyldiethanolamine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	17.58 ng	647294	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyldiethanolamine	119	C5H13NO2	000105-59-9	91
2		Urea, N,N-dimethyl-	88	C3H8N2O	000598-94-7	64
3		Urea, ethyl-	88	C3H8N2O	000625-52-5	50
4		Methanamine, 1,1-dimethoxy-N,N-d...	119	C5H13NO2	004637-24-5	43
5		3-Hydroxy-azetidine-1-carboxylic...	131	C5H9NO3	118972-97-7	40



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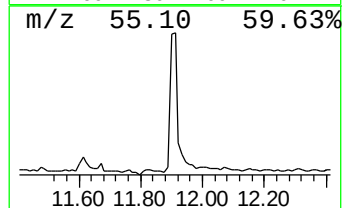
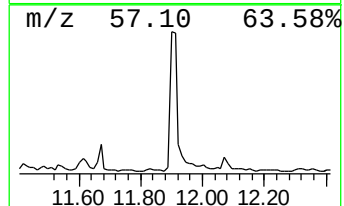
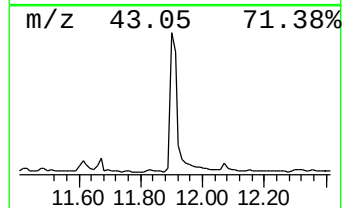
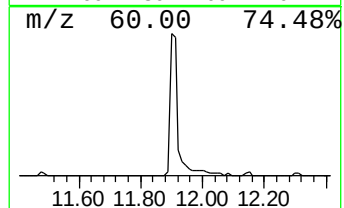
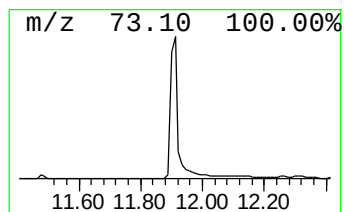
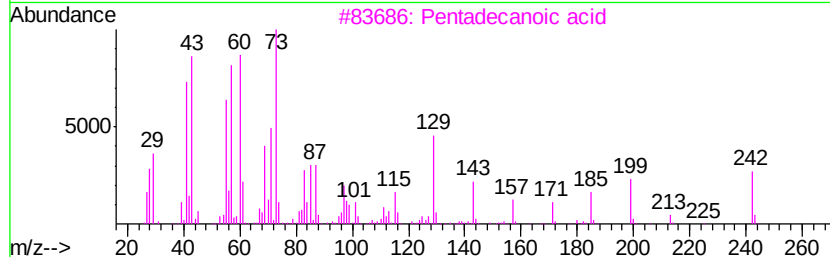
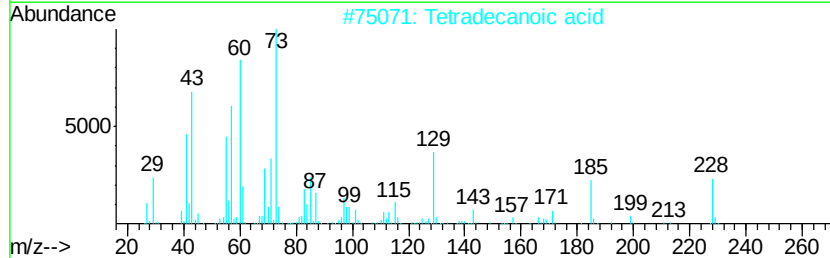
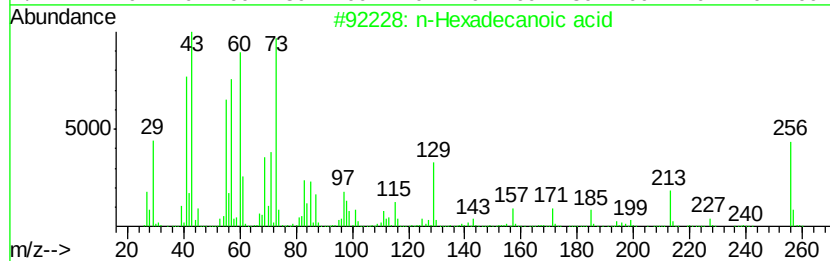
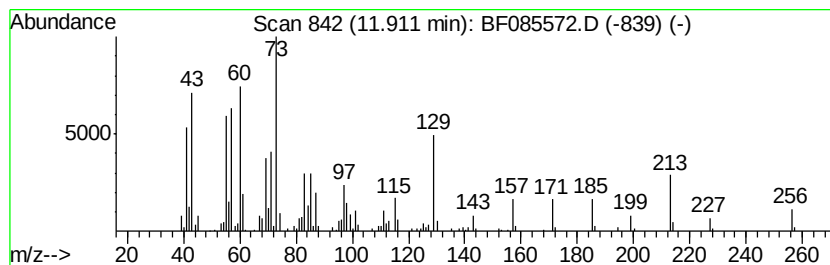
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.91	8.77 ng	489586	Phenanthrene-d10	11.37	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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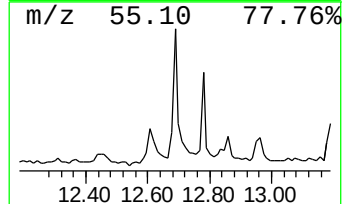
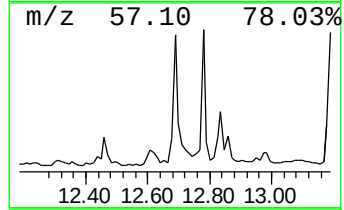
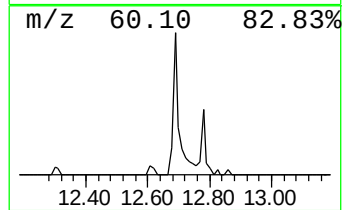
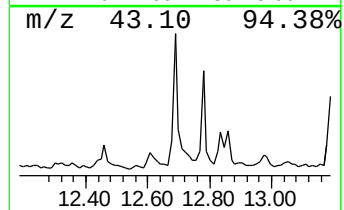
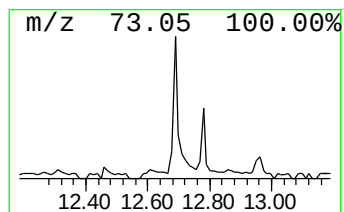
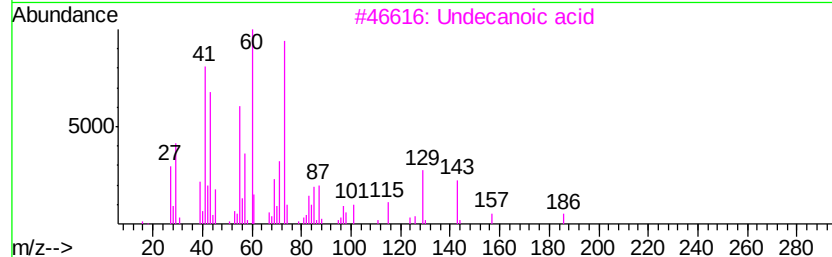
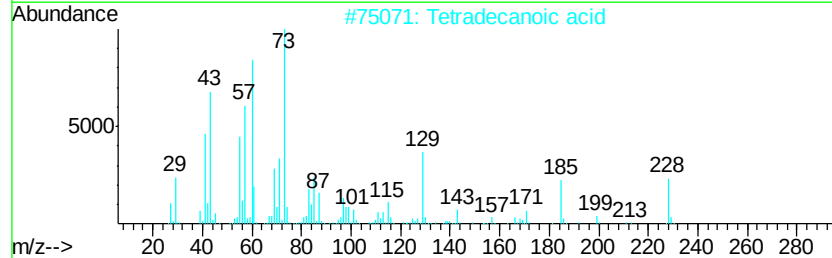
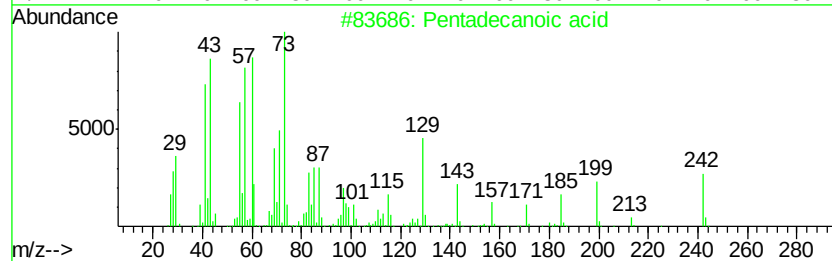
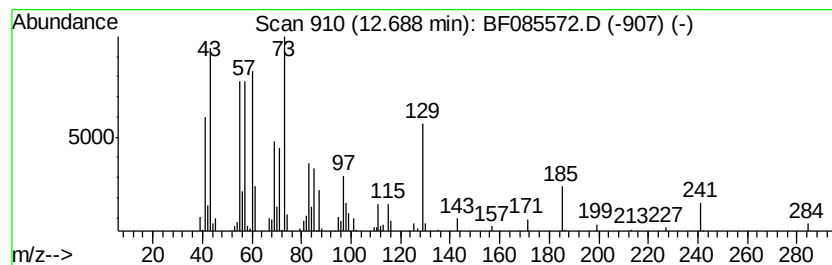
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ClientSampleId :
TRACK-D-GRID-9B

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TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.69	2.54 ng	141459	Phenanthrene-d10		11.37
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	58
4	Dodecane, 1,2-dibromo-	326	C12H24Br2	055334-42-4	11
5	5-Acetoxypentadecane	270	C17H34O2	1000245-62-3	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085572.D
Acq On : 19 Mar 2016 14:55
Operator : UM/SJ
Sample : H1816-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

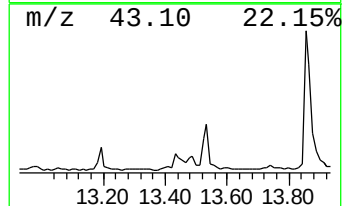
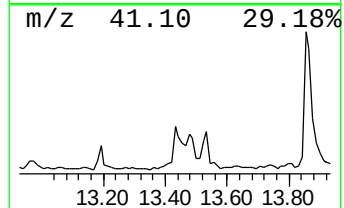
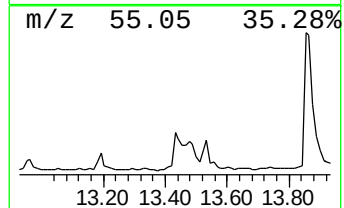
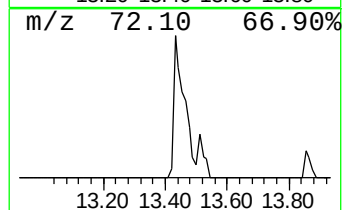
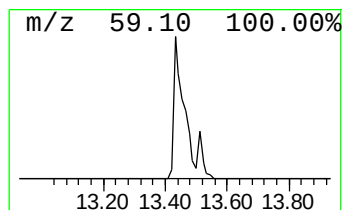
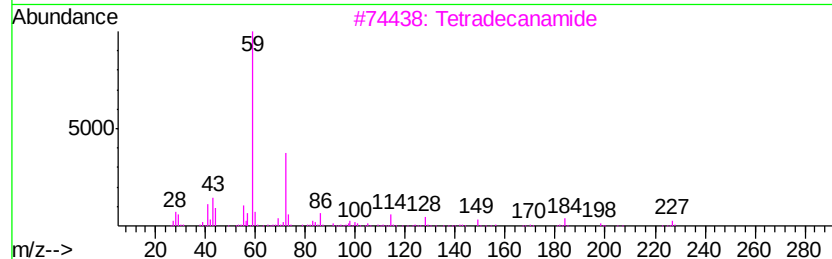
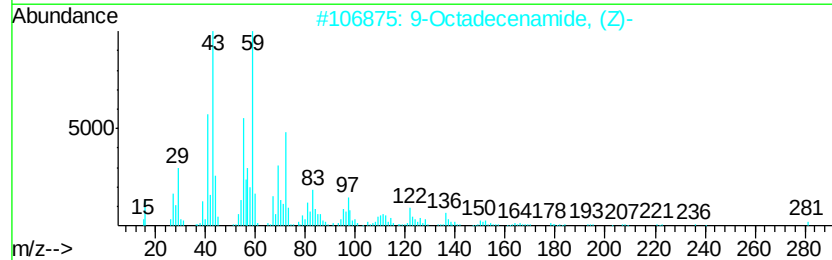
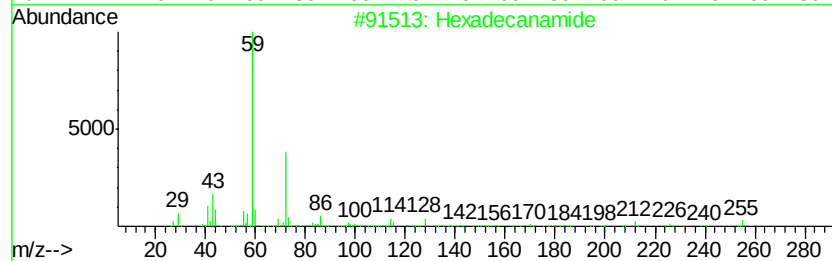
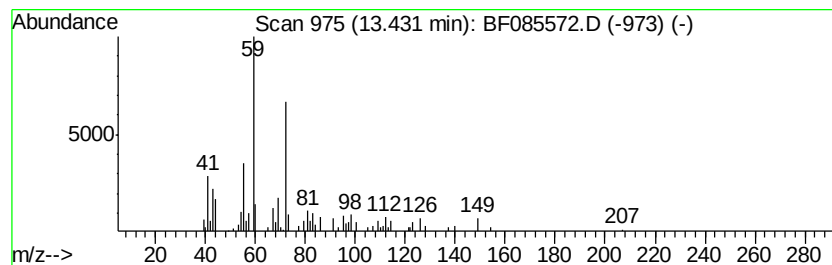
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanamide Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	2.37 ng	133771	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecanamide	255 C16H33NO	000629-54-9	59
2	9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0	56
3	Tetradecanamide	227 C14H29NO	000638-58-4	56
4	Dodecanamide	199 C12H25NO	001120-16-7	53
5	d-Glucosamine	179 C6H13NO5	000090-77-7	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085572.D
Acq On : 19 Mar 2016 14:55
Operator : UM/SJ
Sample : H1816-02
Misc :
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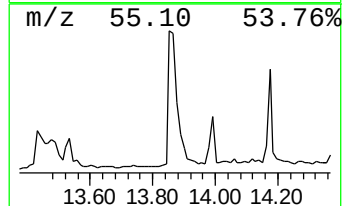
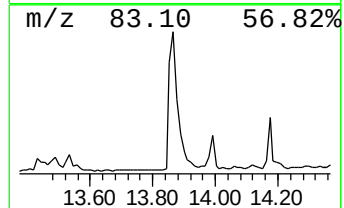
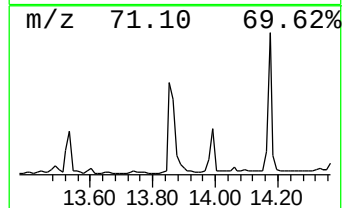
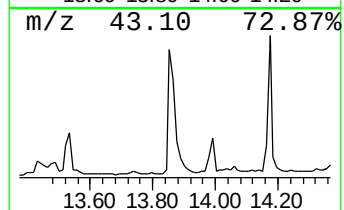
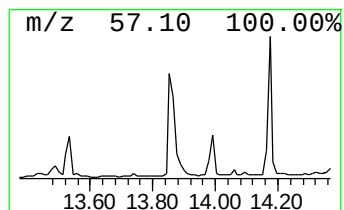
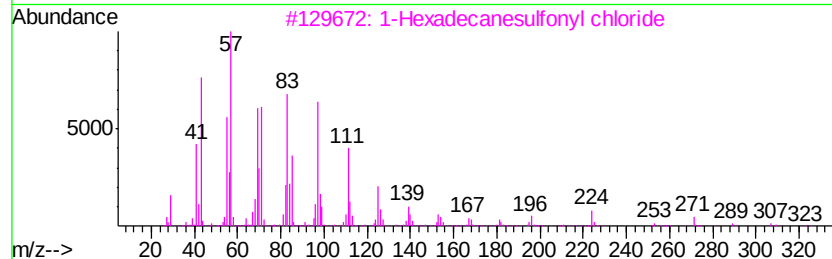
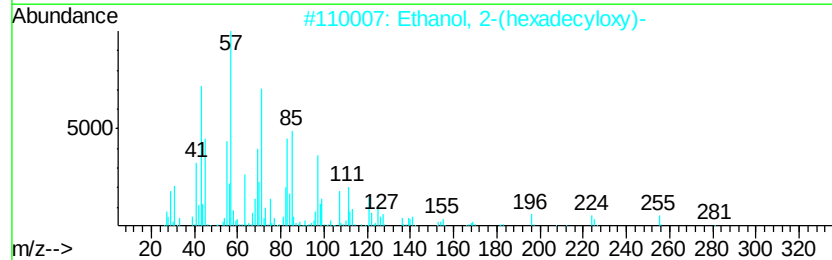
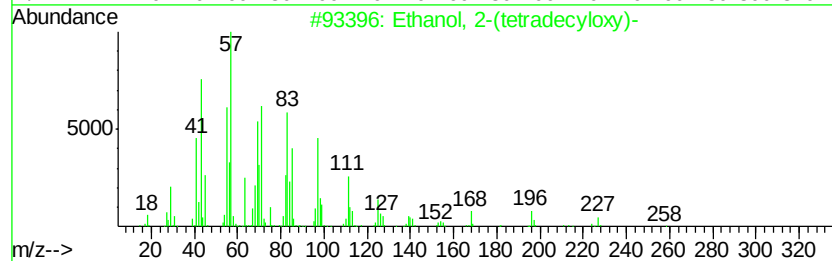
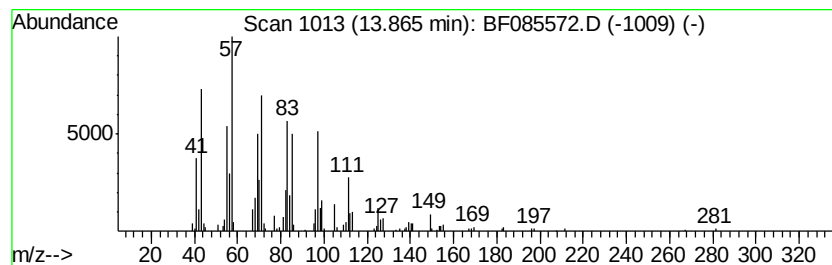
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.87	11.45 ng	647509	Chrysene-d12	14.00		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87
3		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	83
4		Heptafluorobutanoic acid, heptadecyl ester	452	C21H35F7O2	1000282-97-3	76
5		Dichloroacetic acid, heptadecyl ester	366	C19H36Cl2O2	1000282-98-2	76



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Operator : UM/SJ
Sample : H1816-02
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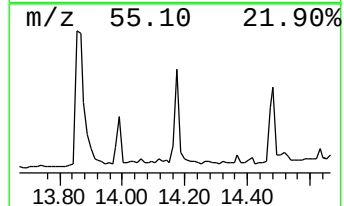
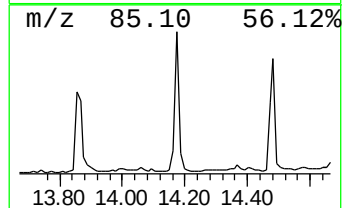
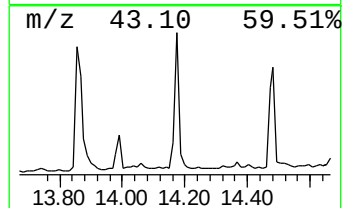
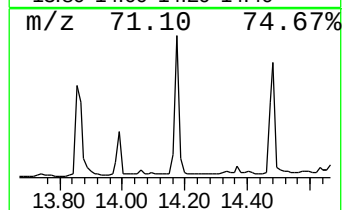
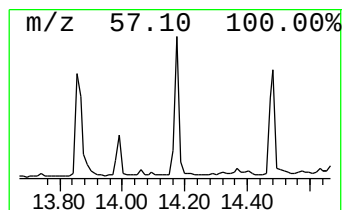
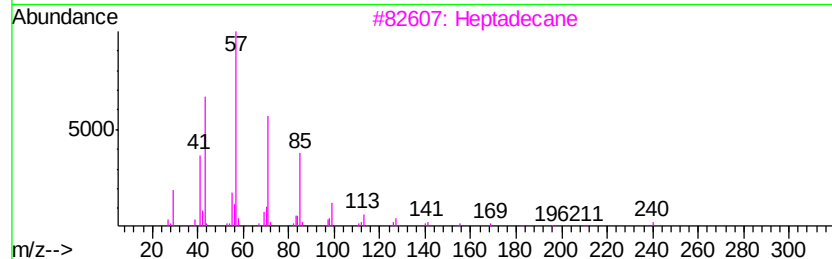
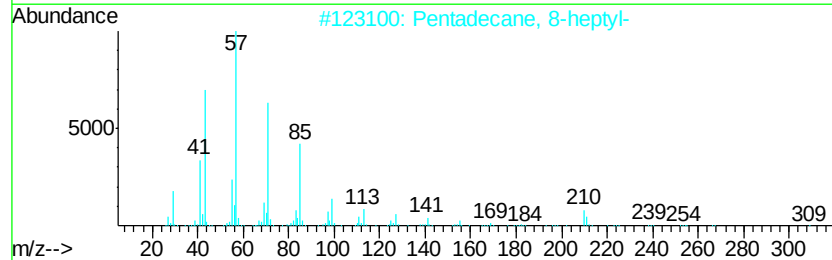
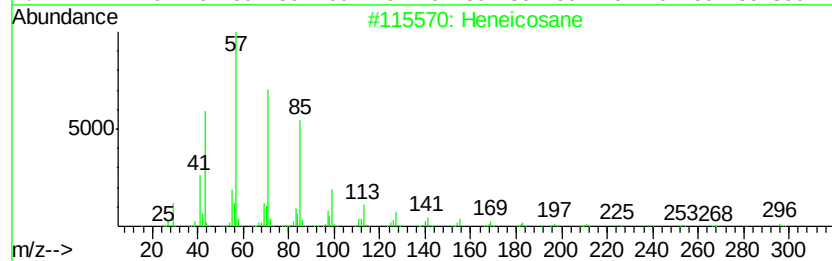
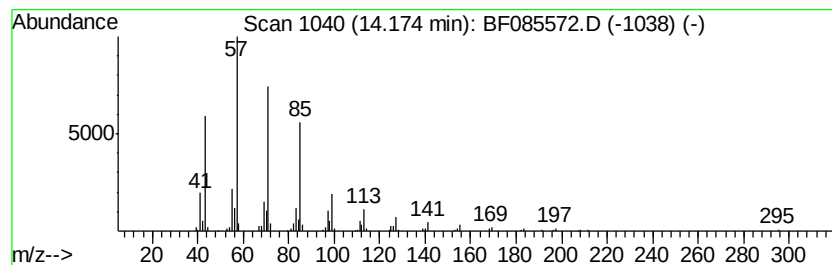
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	4.35 ng	246120	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	91
3	Heptadecane	240 C17H36	000629-78-7	90
4	Eicosane, 7-hexyl-	366 C26H54	055333-99-8	90
5	Octadecane	254 C18H38	000593-45-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085572.D
Acq On : 19 Mar 2016 14:55
Operator : UM/SJ
Sample : H1816-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

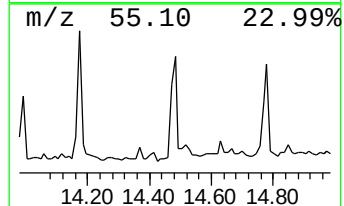
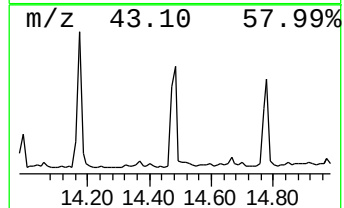
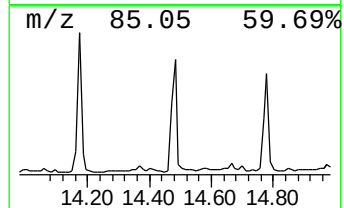
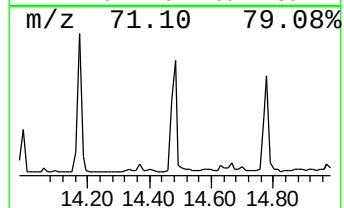
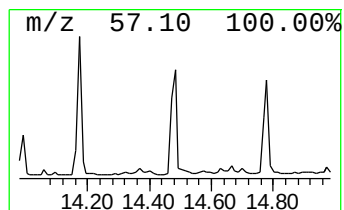
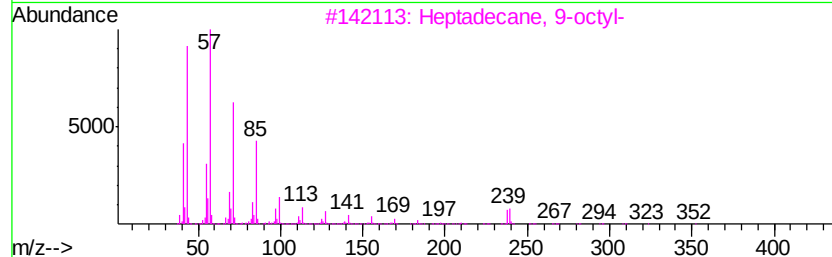
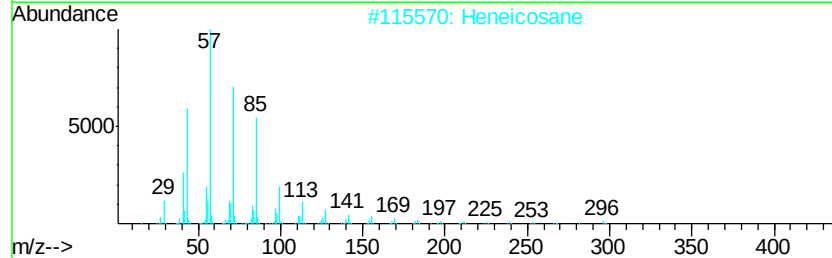
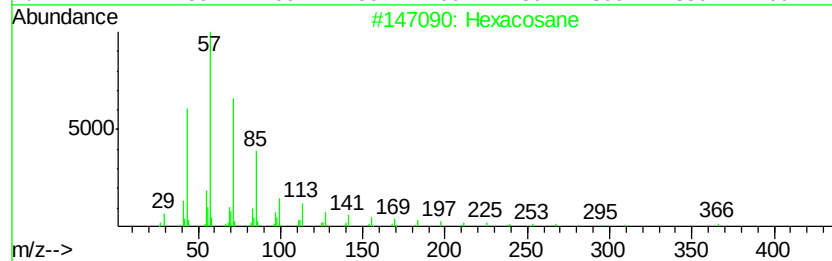
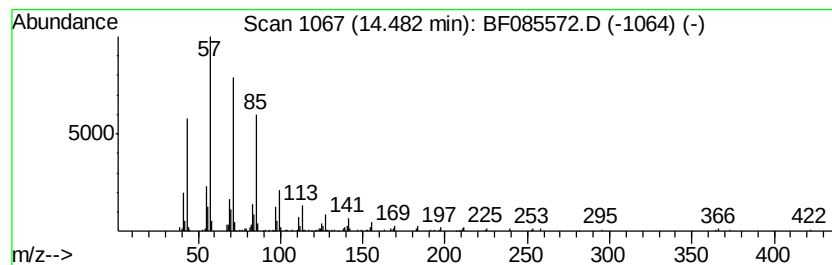
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	4.99 ng	281962	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	94
2	Heneicosane	296 C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
4	Triacontane	422 C30H62	000638-68-6	91
5	Pentadecane, 8-hexyl-	296 C21H44	013475-75-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085572.D
Acq On : 19 Mar 2016 14:55
Operator : UM/SJ
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ALS Vial : 33 Sample Multiplier: 1

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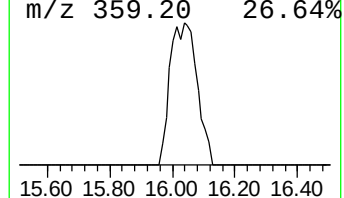
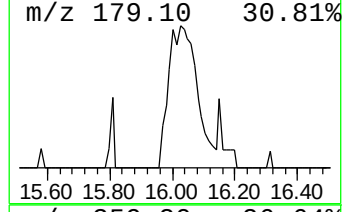
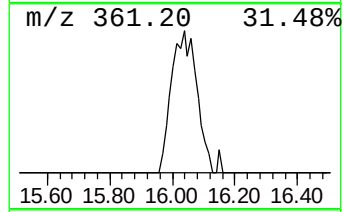
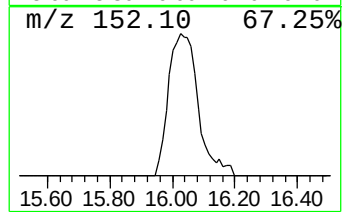
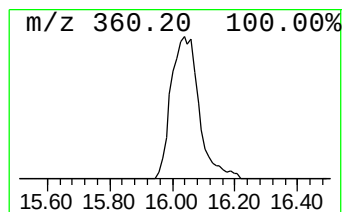
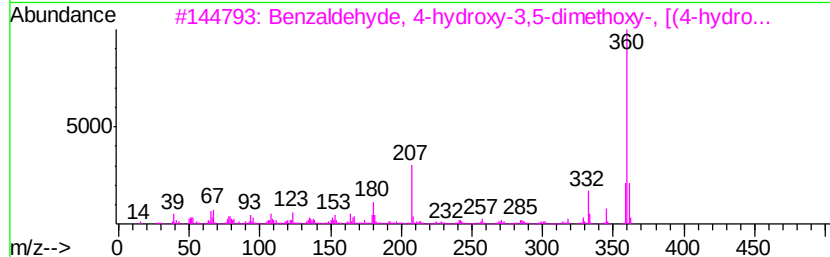
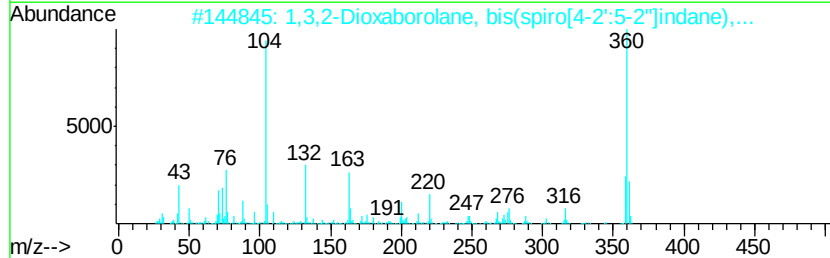
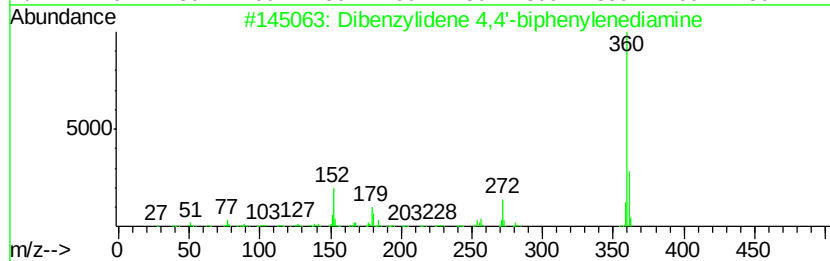
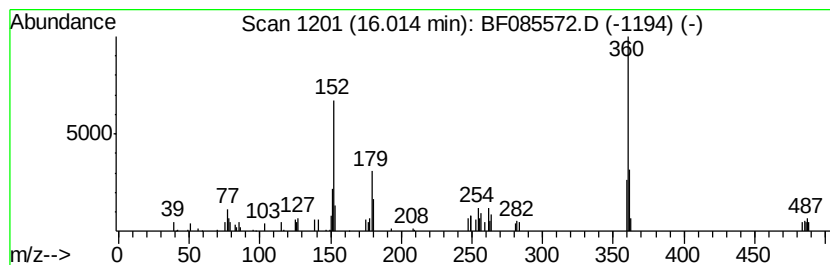
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	10.30 ng	402903	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	90
2		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	52
3		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	50
4		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
5		2-Cyclohexylamino-3-methyl(pheny...	360	C23H24N2O2	134614-17-8	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
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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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unknown6.62	6.62	95.8	ng	3526330	1	6.85	736401	20.0
Methyldiethanolamine	7.22	17.6	ng	647294	1	6.85	736401	20.0
n-Hexadecanoic acid	11.91	8.8	ng	489586	4	11.37	1115950	20.0
Pentadecanoic acid	12.69	2.5	ng	141459	4	11.37	1115950	20.0
Hexadecanamide	13.43	2.4	ng	133771	5	14.00	1130820	20.0
Ethanol, 2-(tetra...	13.87	11.4	ng	647509	5	14.00	1130820	20.0
Heneicosane	14.17	4.3	ng	246120	5	14.00	1130820	20.0
Hexacosane	14.48	5.0	ng	281962	5	14.00	1130820	20.0
Dibenzylidene 4,4...	16.01	10.3	ng	402903	6	15.43	782119	20.0