

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
 Data File : BF102240.D
 Acq On : 20 Jan 2018 1:59
 Operator : SJ/JU
 Sample : J1113-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-12-3.5-4.0

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-BF010918.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	4.928	478	483	492	rVB	186456	277202	7.47%	0.907%
2	5.334	547	552	555	rBV	3325698	3710607	100.00%	12.142%
3	6.363	722	727	730	rBV	3199754	3686628	99.35%	12.063%
4	6.492	744	749	752	rBV	3777580	3691768	99.49%	12.080%
5	6.716	784	787	791	rBV	918870	791223	21.32%	2.589%
6	6.875	810	814	817	rBV	3230275	2854871	76.94%	9.342%
7	7.286	878	884	887	rBV	2363554	2347806	63.27%	7.682%
8	7.381	894	900	907	rBV	59384	67736	1.83%	0.222%
9	7.998	1001	1005	1009	rBV	1125089	1005583	27.10%	3.290%
10	9.080	1183	1189	1192	rBV	3612747	3434986	92.57%	11.240%
11	9.469	1251	1255	1259	rBV	325002	293114	7.90%	0.959%
12	9.686	1288	1292	1295	rVB	94575	77024	2.08%	0.252%
13	9.751	1299	1303	1307	rVB	1089667	978955	26.38%	3.203%
14	10.157	1369	1372	1374	rBV	62515	52893	1.43%	0.173%
15	10.186	1374	1377	1379	rVB	124050	102040	2.75%	0.334%
16	10.404	1408	1414	1416	rBV	35348	41638	1.12%	0.136%
17	10.545	1431	1438	1441	rBV	1976237	1895077	51.07%	6.201%
18	10.657	1454	1457	1462	rBV	121122	123294	3.32%	0.403%
19	11.104	1530	1533	1536	rBV	78095	64589	1.74%	0.211%
20	11.233	1552	1555	1559	rBV	930193	806540	21.74%	2.639%
21	11.527	1603	1605	1611	rVB	47863	45338	1.22%	0.148%
22	12.645	1791	1795	1798	rBV	219579	174906	4.71%	0.572%
23	12.821	1821	1825	1828	rBV	2373510	2151195	57.97%	7.039%
24	13.351	1911	1915	1918	rBV	135980	109078	2.94%	0.357%
25	13.715	1973	1977	1989	rBV2	124735	143244	3.86%	0.469%
26	13.868	1997	2003	2007	rBV	754930	716983	19.32%	2.346%
27	14.345	2080	2084	2089	rBV2	40634	46347	1.25%	0.152%
28	15.292	2240	2245	2249	rBV	661071	777806	20.96%	2.545%
29	15.727	2315	2319	2324	rBV	35174	43143	1.16%	0.141%
30	17.203	2568	2570	2579	rVB8	27741	49126	1.32%	0.161%

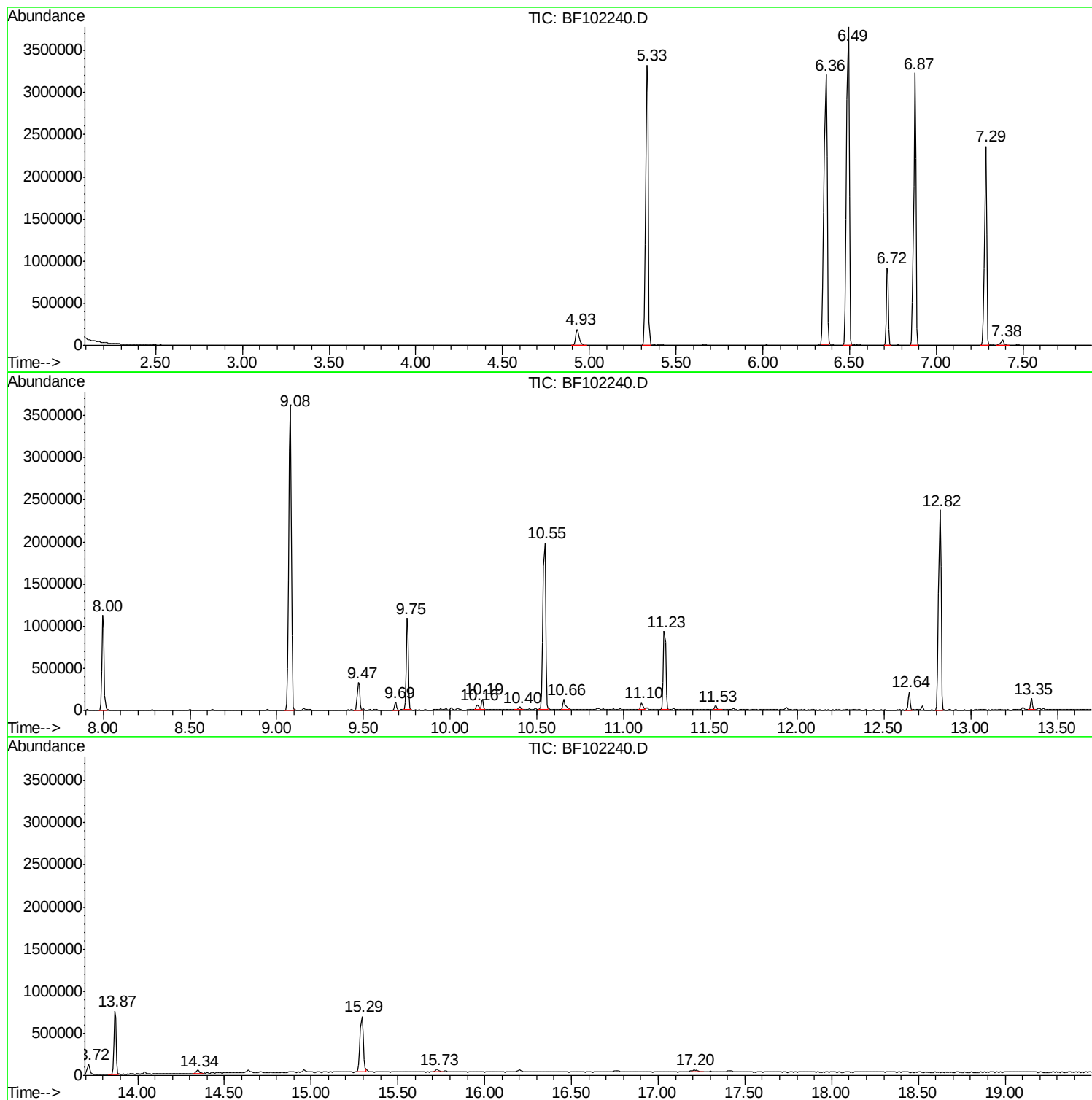
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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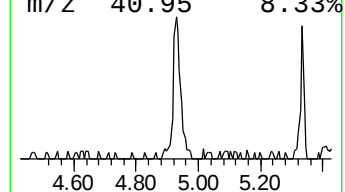
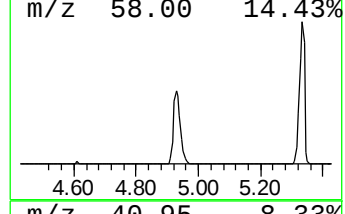
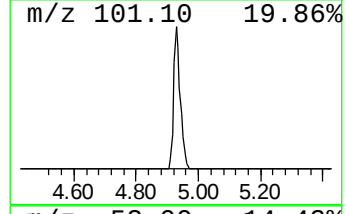
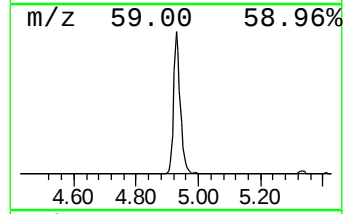
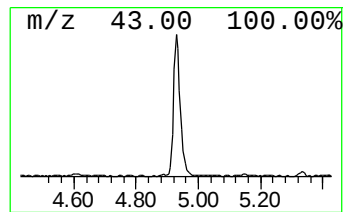
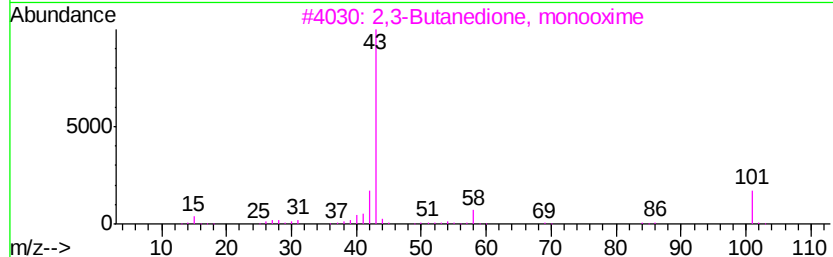
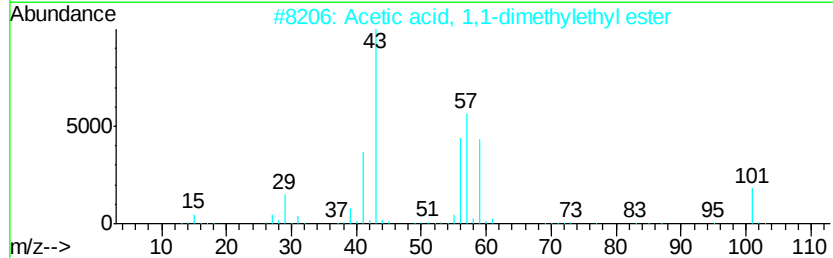
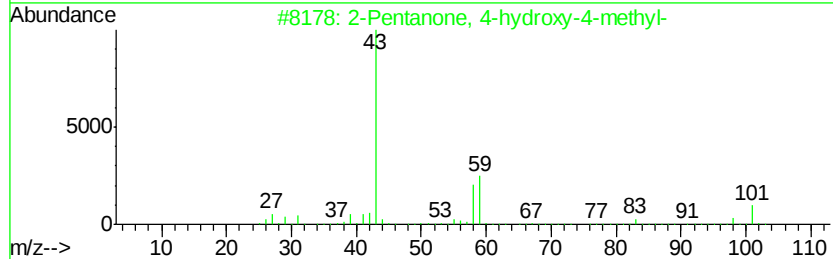
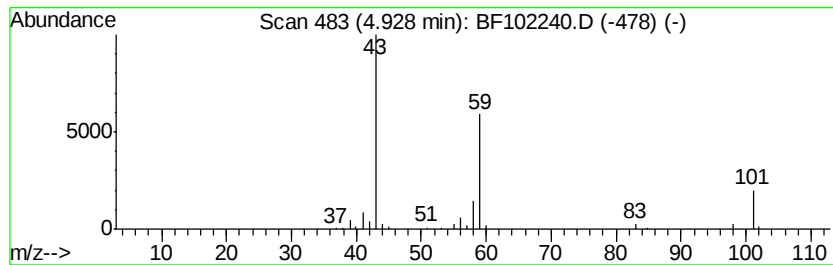
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	7.01 ng	277202	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4			3-Hexanol	102	C6H14O	000623-37-0	28
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28



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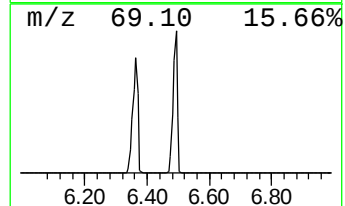
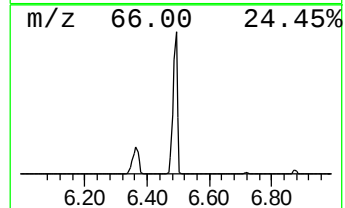
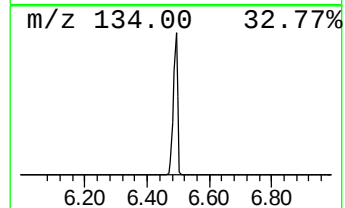
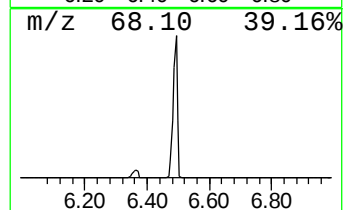
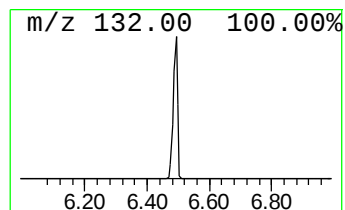
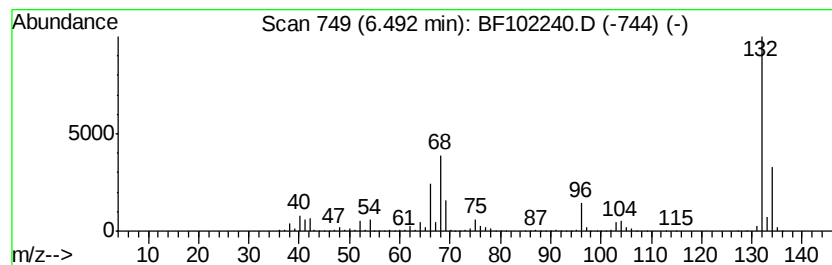
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	93.32 ng	3691770	1,4-Dichlorobenzene-d4	6.72

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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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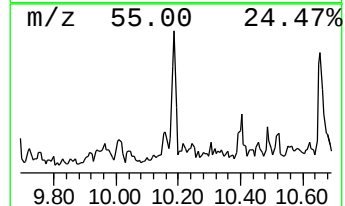
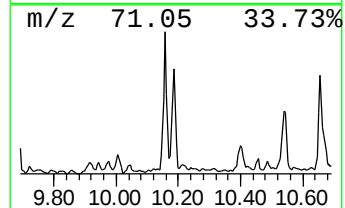
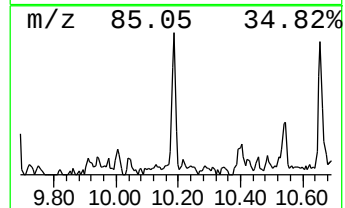
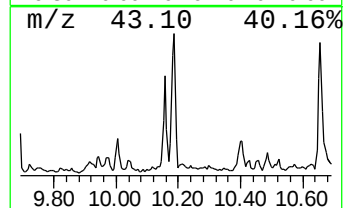
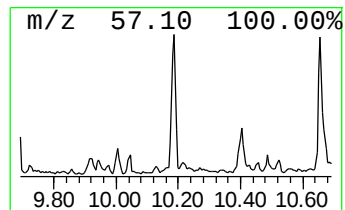
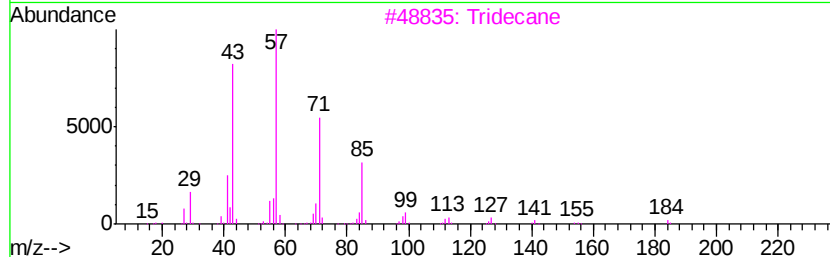
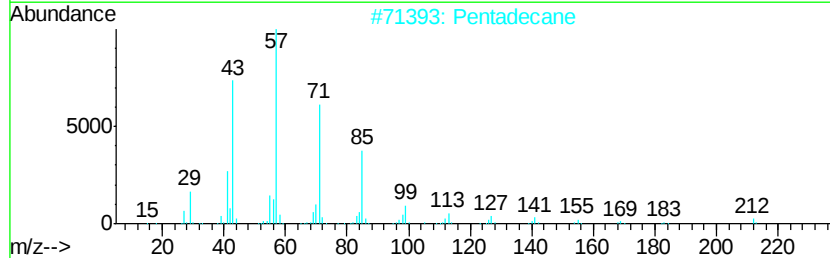
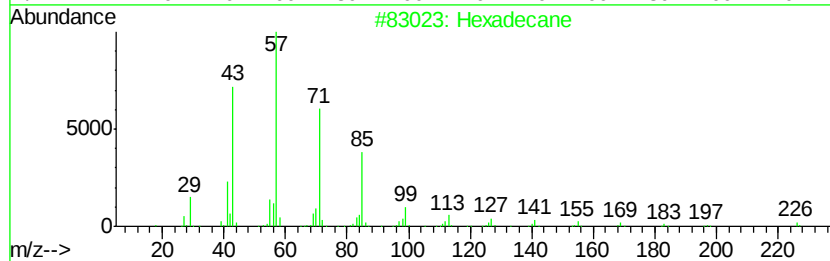
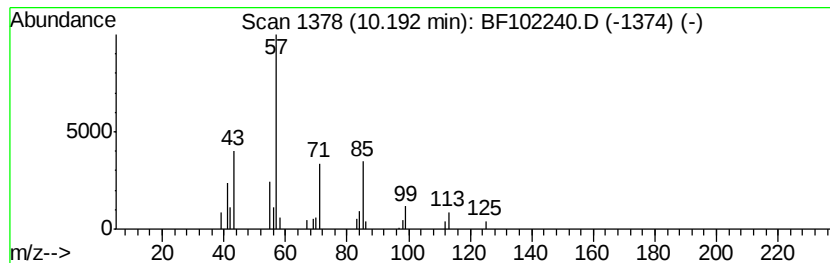
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Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.19	2.08 ng	102040	Acenaphthene-d10	9.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Pentadecane	212	C15H32	000629-62-9	83
3	Tridecane	184	C13H28	000629-50-5	78
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64
5	Decane, 3-bromo-	220	C10H21Br	030571-71-2	64



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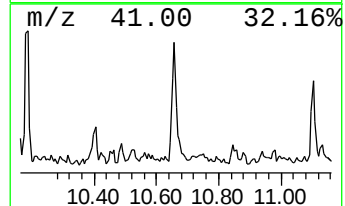
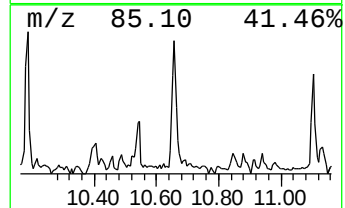
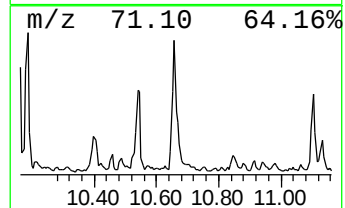
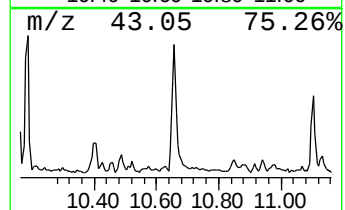
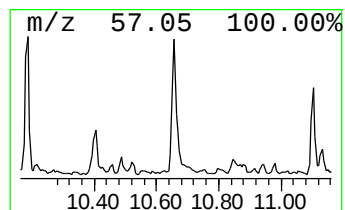
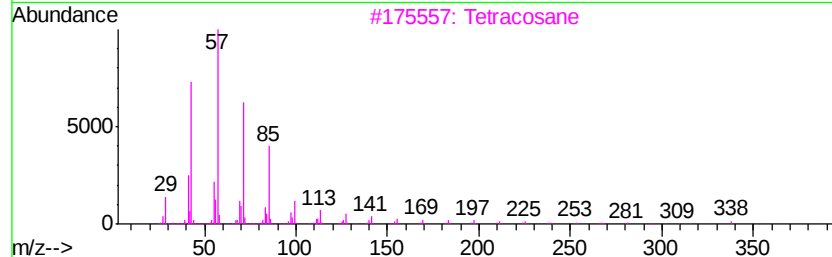
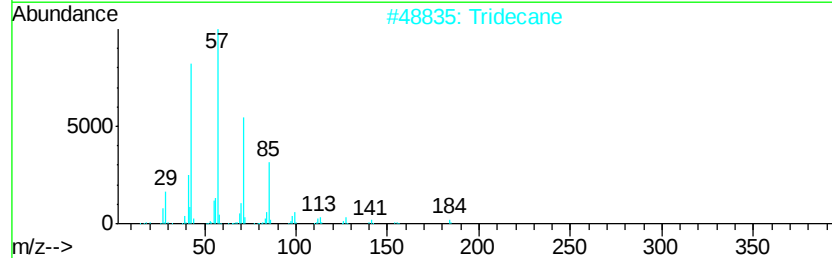
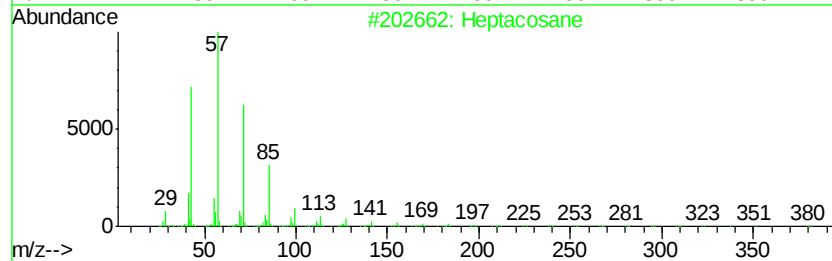
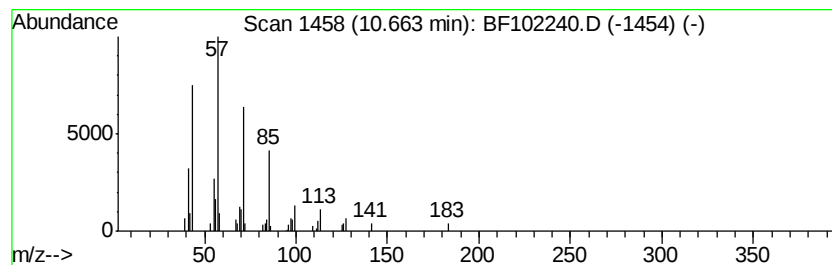
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Peak Number 5 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.06 ng	123294	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Tridecane		184	C13H28	000629-50-5	90
3	Tetracosane		338	C24H50	000646-31-1	90
4	Docosane		310	C22H46	000629-97-0	90
5	Tetradecane		198	C14H30	000629-59-4	90



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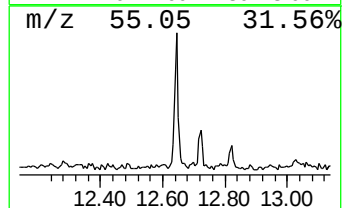
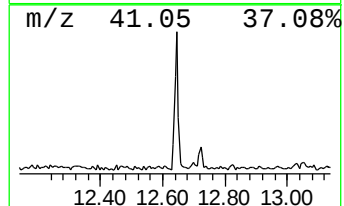
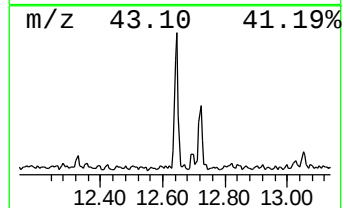
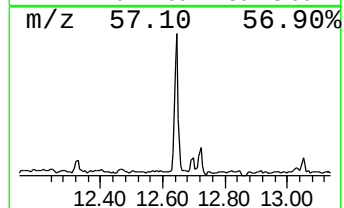
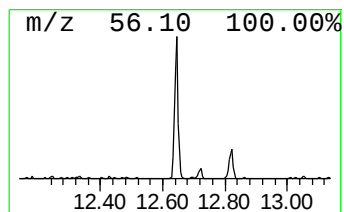
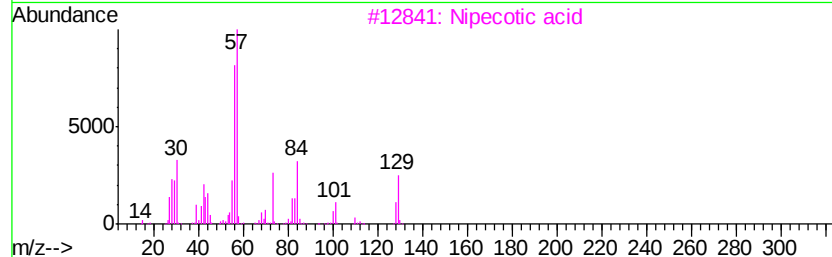
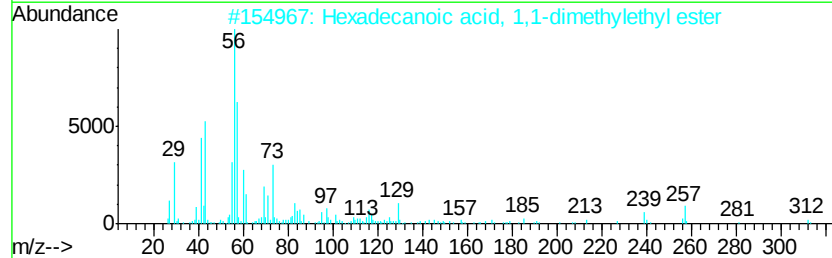
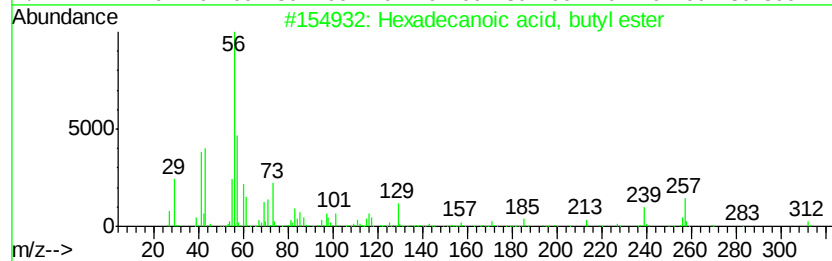
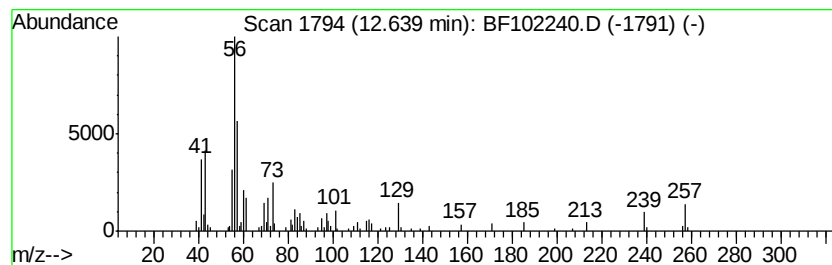
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	4.88 ng	174906	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	72
3			Nipecotic acid	129	C6H11NO2	000498-95-3	47
4			Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	37
5			Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35



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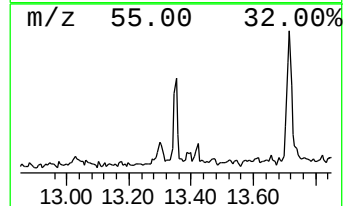
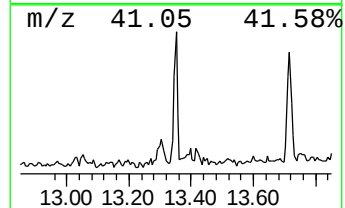
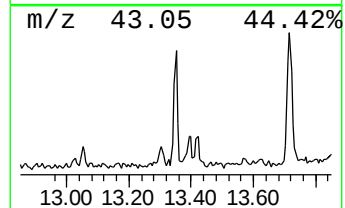
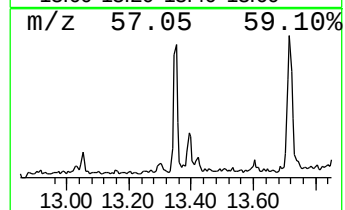
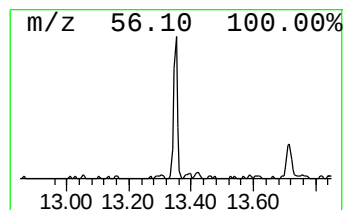
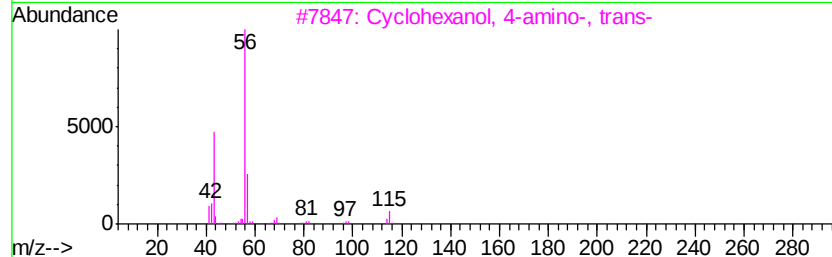
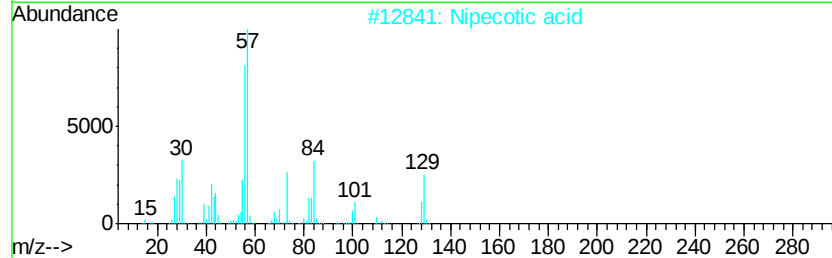
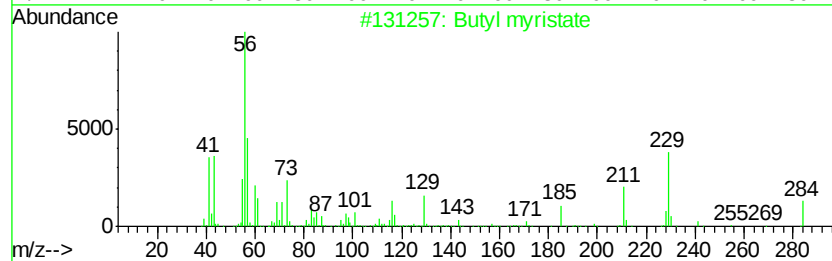
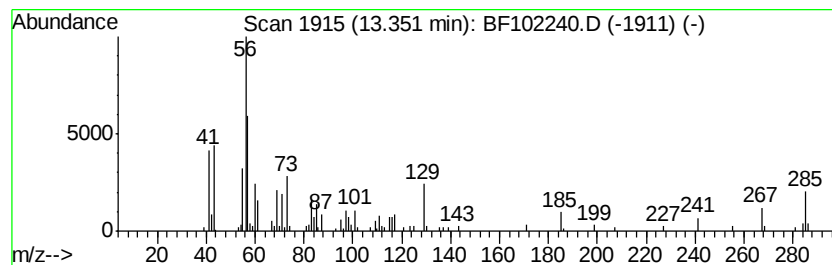
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BNA_F
ClientSampleId :
SB-12-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Butyl myristate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.35	3.04 ng	109078	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	64
2	Nipecotic acid	129	C6H11NO2	000498-95-3	50
3	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102240.D
Acq On : 20 Jan 2018 1:59
Operator : SJ/JU
Sample : J1113-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

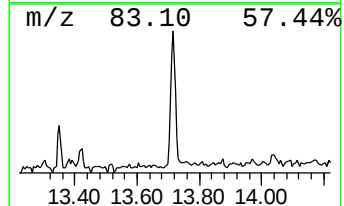
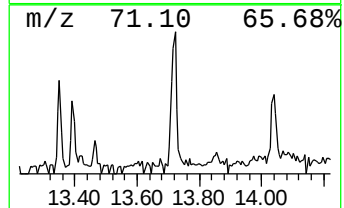
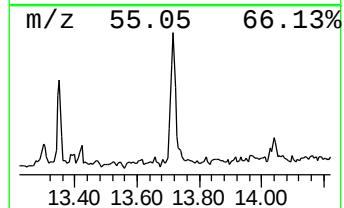
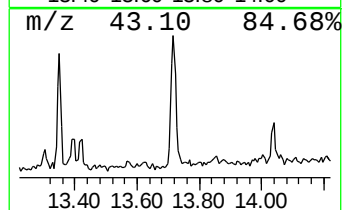
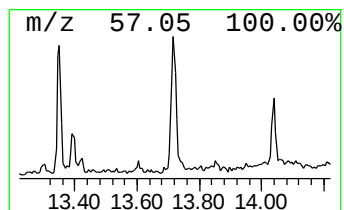
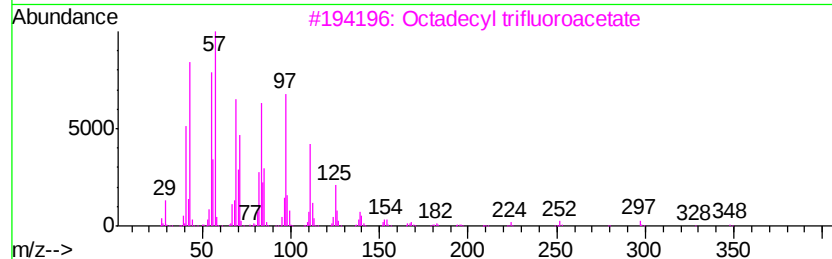
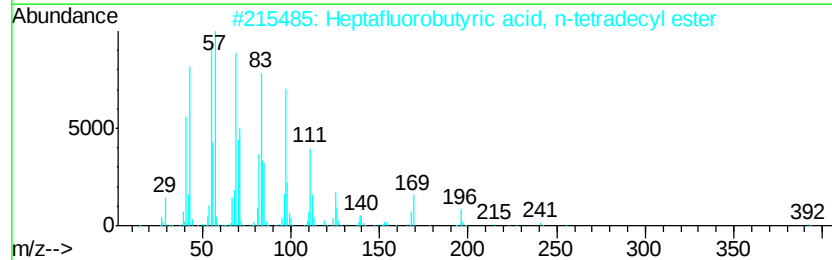
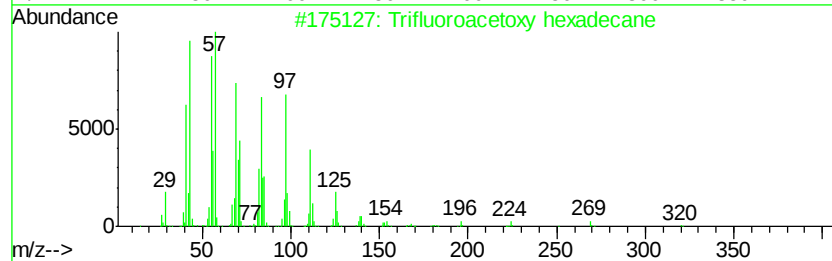
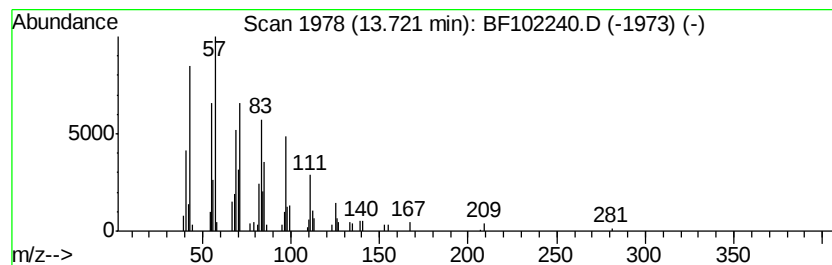
Instrument :
BNA_F
ClientSampleId :
SB-12-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.72	4.00 ng	143244	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3	Octadecvyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102240.D
Acq On : 20 Jan 2018 1:59
Operator : SJ/JU
Sample : J1113-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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
2-Pentanone, 4-hy...	4.93	7.0	ng	277202	1	6.72	791223	20.0
unknown6.49	6.49	93.3	ng	3691770	1	6.72	791223	20.0
Hexadecane	10.19	2.1	ng	102040	3	9.75	978955	20.0
Heptacosane	10.66	3.1	ng	123294	4	11.23	806540	20.0
Hexadecanoic acid...	12.64	4.9	ng	174906	5	13.87	716983	20.0
Butyl myristate	13.35	3.0	ng	109078	5	13.87	716983	20.0
Trifluoroacetoxy ...	13.72	4.0	ng	143244	5	13.87	716983	20.0