

Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
 Data File : BF102073.D
 Acq On : 15 Jan 2018 20:00
 Operator : SJ/JU
 Sample : J1117-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1

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-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	4.934	475	484	495	rVB	311104	456857	8.99%	1.094%
2	5.340	547	553	556	rBV	4471183	5079017	100.00%	12.165%
3	6.363	721	727	730	rBV	4379858	5032475	99.08%	12.053%
4	6.492	744	749	752	rBV	4895545	5013325	98.71%	12.007%
5	6.722	784	788	791	rBV	1511138	1171841	23.07%	2.807%
6	6.881	810	815	818	rBV	3673145	3521447	69.33%	8.434%
7	7.287	878	884	887	rBV	2982845	3261048	64.21%	7.811%
8	7.375	894	899	902	rBV	93341	107210	2.11%	0.257%
9	8.004	1001	1006	1009	rBV	1790744	1525529	30.04%	3.654%
10	9.081	1183	1189	1192	rBV	4756081	4270746	84.09%	10.229%
11	9.475	1252	1256	1259	rBV	613777	484108	9.53%	1.159%
12	9.686	1290	1292	1297	rVB	144281	123790	2.44%	0.296%
13	9.757	1297	1304	1307	rBV	1621586	1421870	27.99%	3.406%
14	10.163	1370	1373	1375	rBV	61154	61851	1.22%	0.148%
15	10.186	1375	1377	1380	rVB	192471	151479	2.98%	0.363%
16	10.404	1410	1414	1417	rBV	48301	59031	1.16%	0.141%
17	10.539	1432	1437	1441	rBV	2291253	2263440	44.56%	5.421%
18	10.657	1454	1457	1463	rBV	169572	186524	3.67%	0.447%
19	11.110	1530	1534	1536	rBV	109041	98697	1.94%	0.236%
20	11.233	1551	1555	1559	rBV	1270446	1111424	21.88%	2.662%
21	11.533	1603	1606	1609	rBV	76992	62662	1.23%	0.150%
22	11.763	1642	1645	1650	rBV	114335	125338	2.47%	0.300%
23	12.821	1820	1825	1828	rBV	3299462	2963673	58.35%	7.098%
24	13.716	1973	1977	1986	rBV2	177534	256394	5.05%	0.614%
25	13.868	1999	2003	2006	rBV	1001062	977741	19.25%	2.342%
26	14.039	2029	2032	2035	rBV	70953	60933	1.20%	0.146%
27	14.345	2081	2084	2086	rBV	65351	60477	1.19%	0.145%
28	14.621	2128	2131	2133	rBV	154327	155929	3.07%	0.373%
29	14.957	2186	2188	2196	rVB	109519	135280	2.66%	0.324%
30	15.280	2239	2243	2247	rBV2	765249	911380	17.94%	2.183%
31	15.315	2247	2249	2253	rVB	129062	147539	2.90%	0.353%
32	15.727	2316	2319	2323	rVB2	120575	159173	3.13%	0.381%
33	16.198	2395	2399	2404	rVB2	117158	180526	3.55%	0.432%
34	16.756	2489	2494	2501	rVB2	74693	153025	3.01%	0.367%

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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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

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

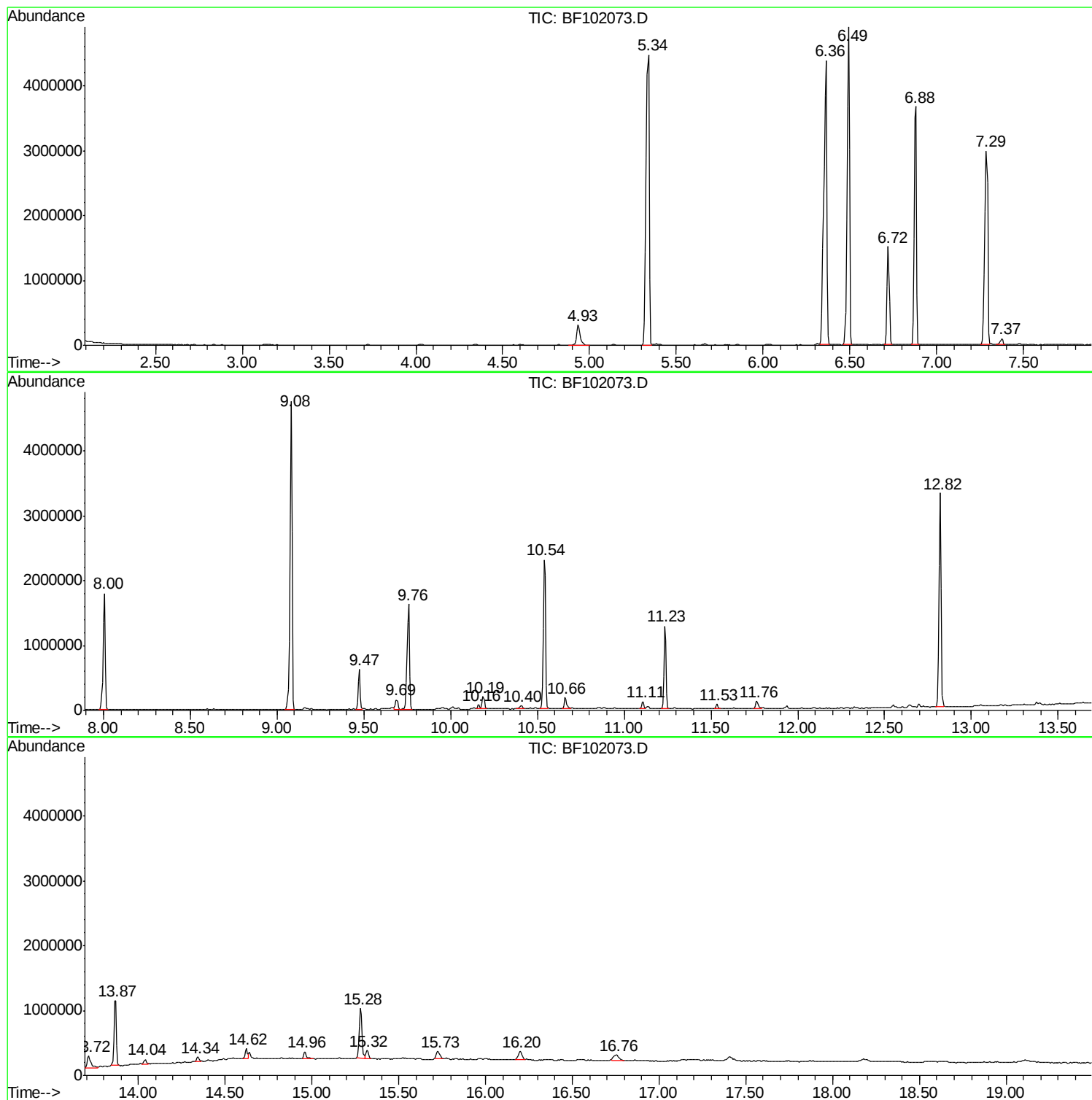
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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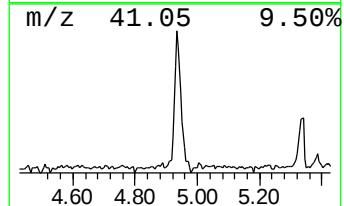
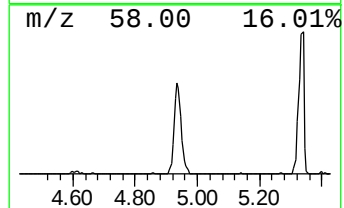
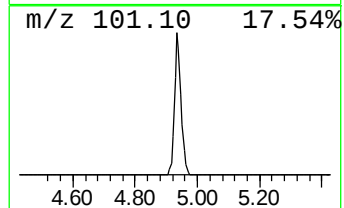
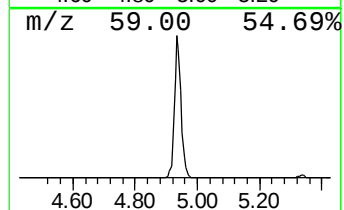
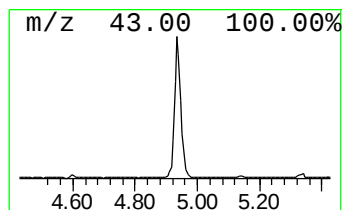
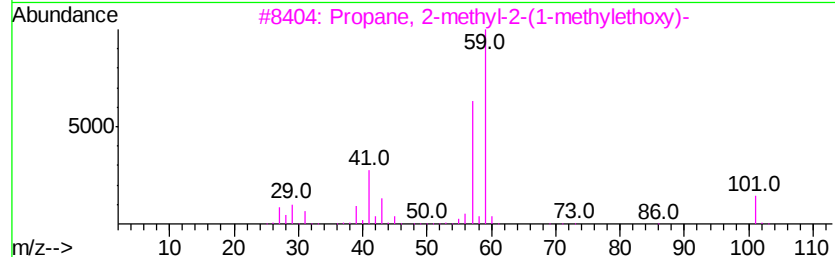
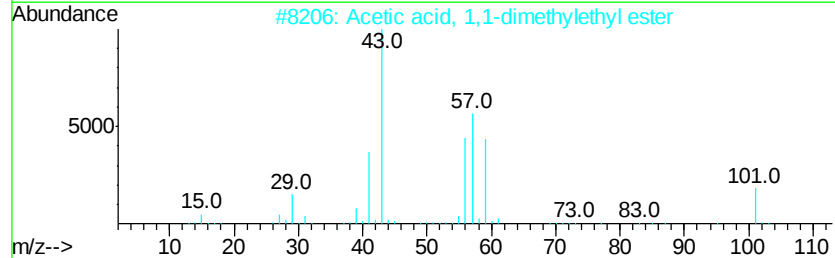
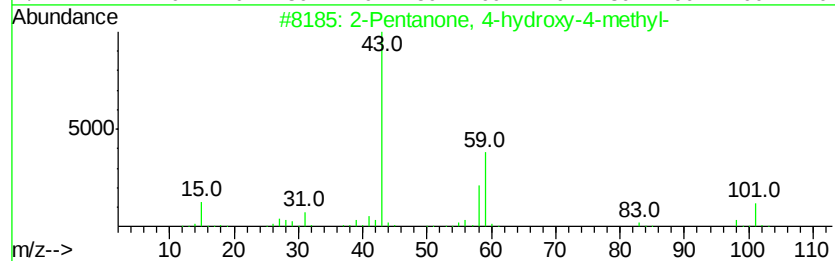
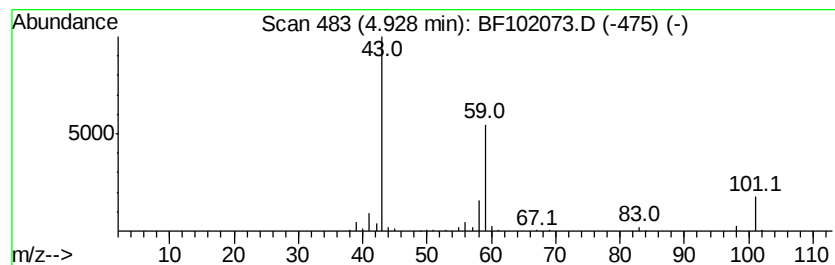
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	7.80 ng	456857	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	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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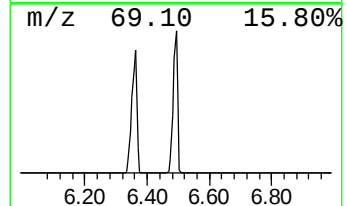
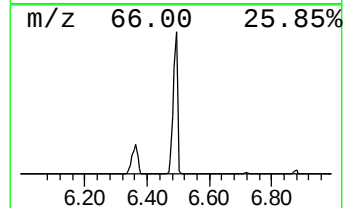
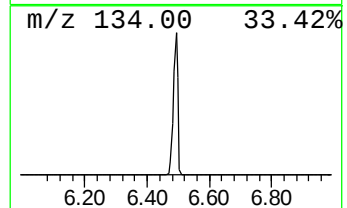
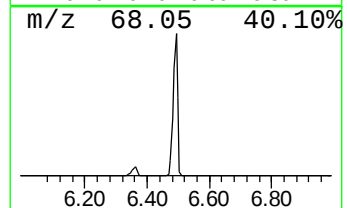
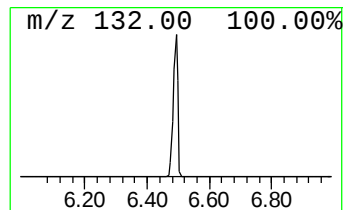
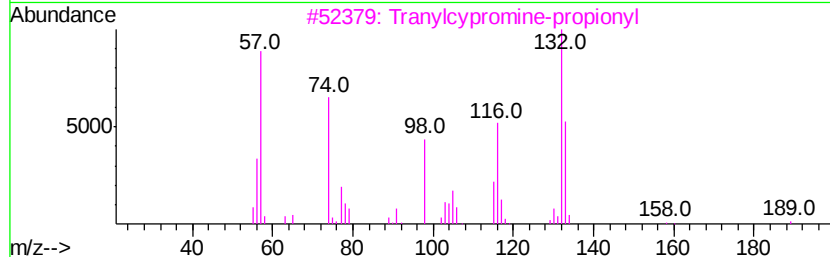
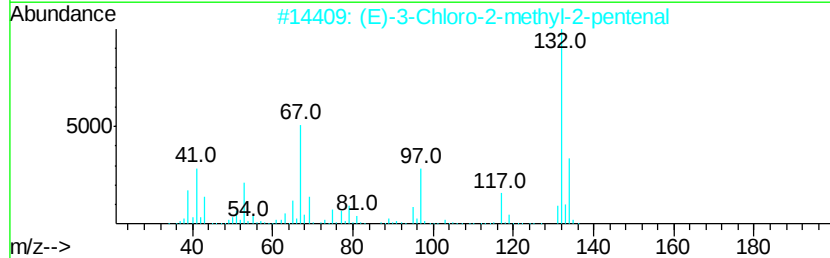
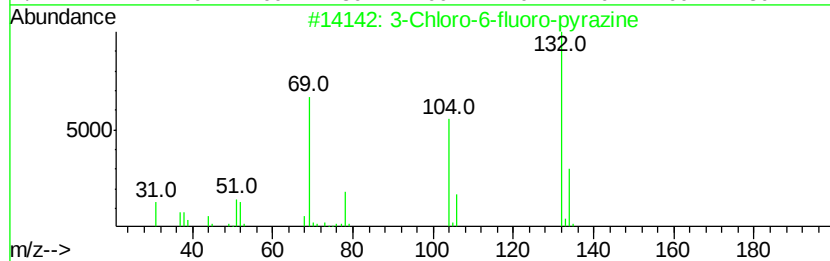
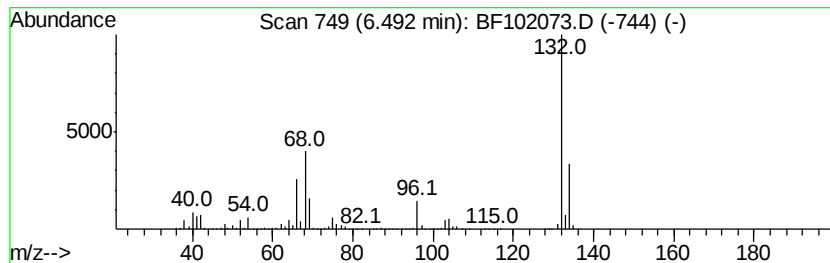
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	85.56 ng	5013330	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		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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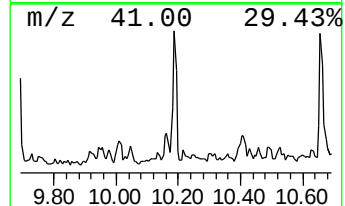
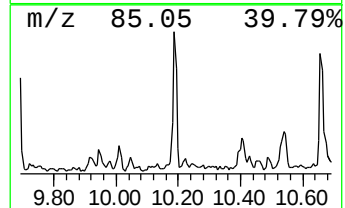
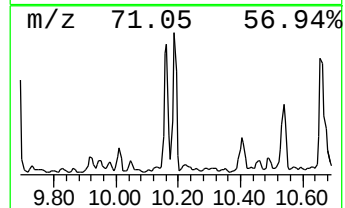
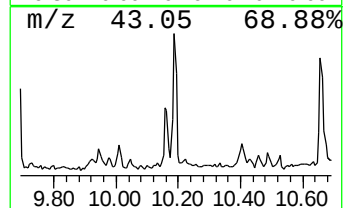
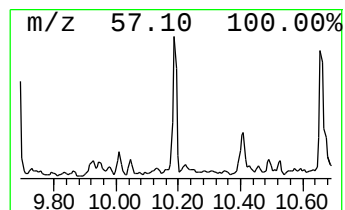
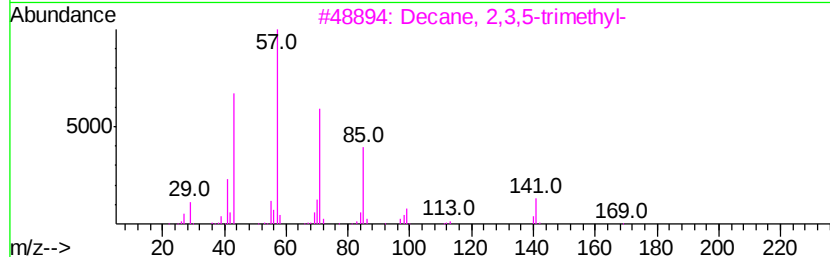
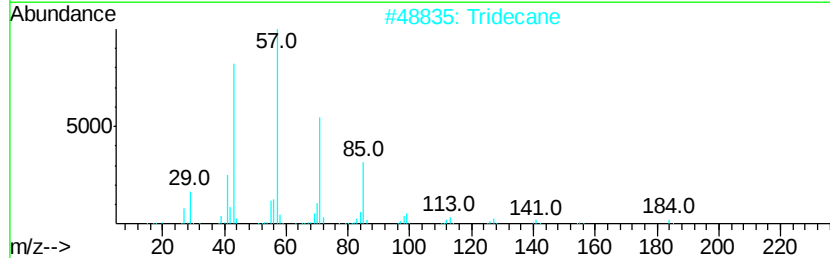
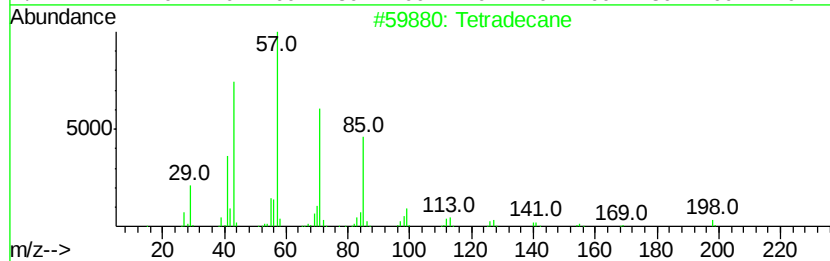
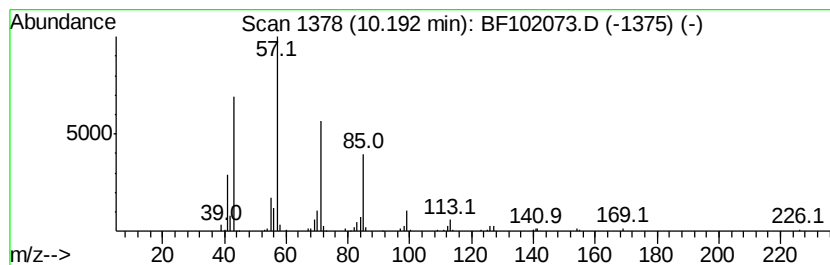
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.19	2.13 ng	151479	Acenaphthene-d10	9.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
4	Hexadecane	226	C16H34	000544-76-3	72
5	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	72



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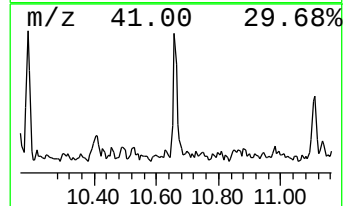
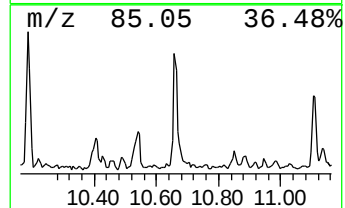
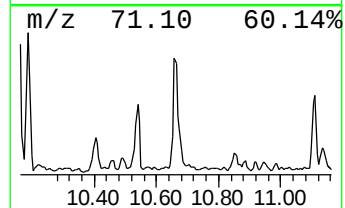
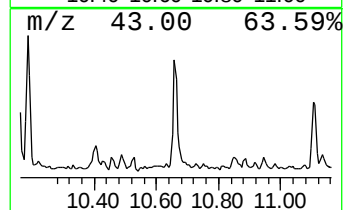
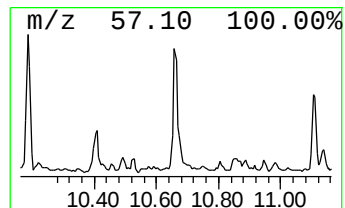
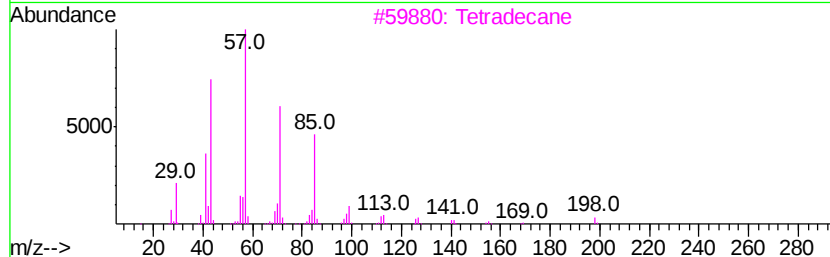
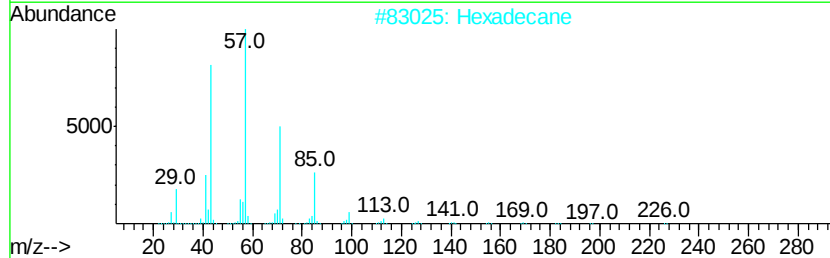
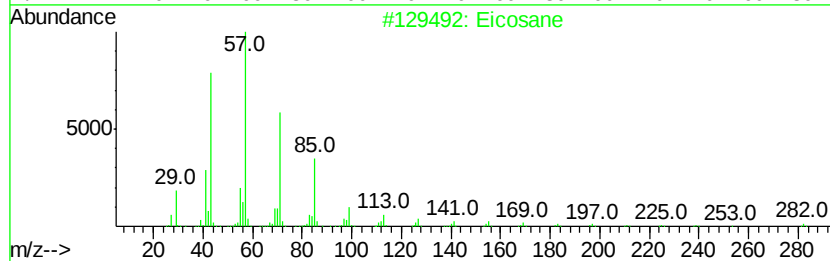
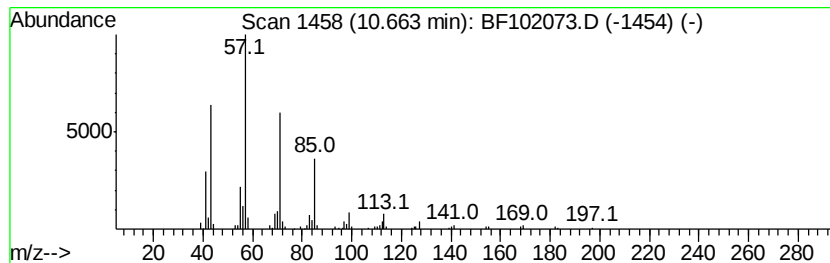
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.36 ng	186524	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Tetradecane		198	C14H30	000629-59-4	87
4	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	86
5	Octadecane		254	C18H38	000593-45-3	86



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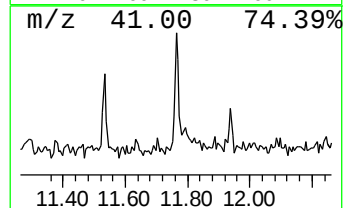
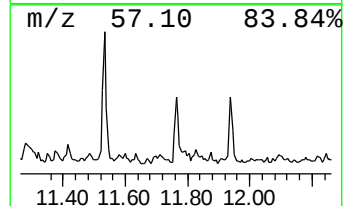
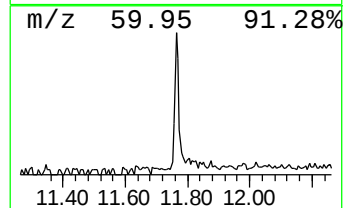
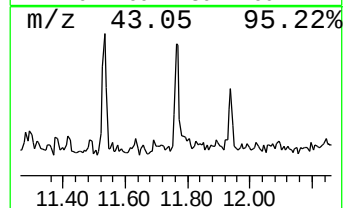
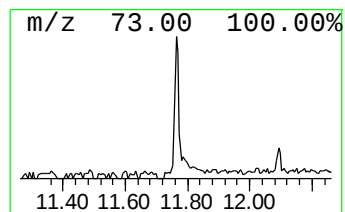
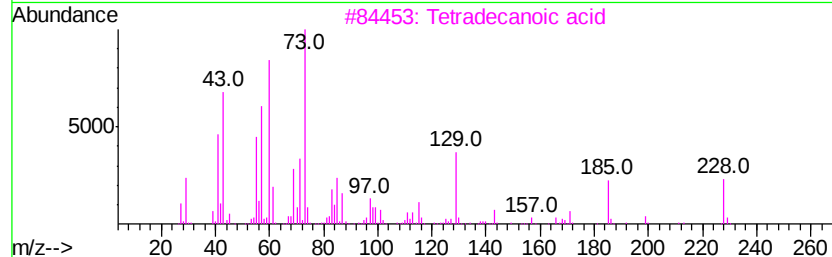
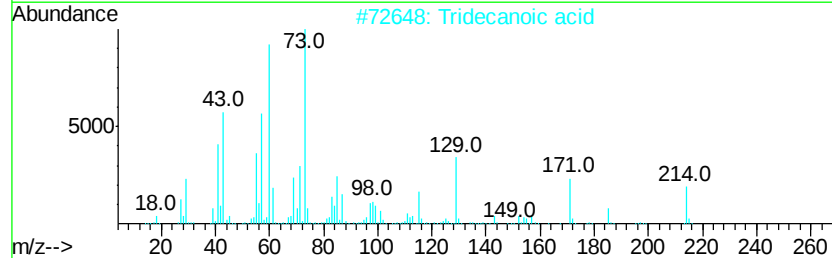
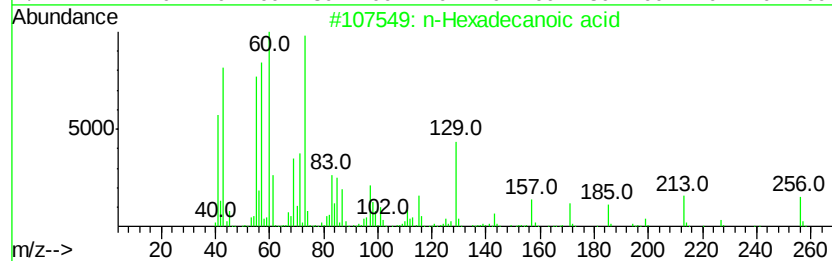
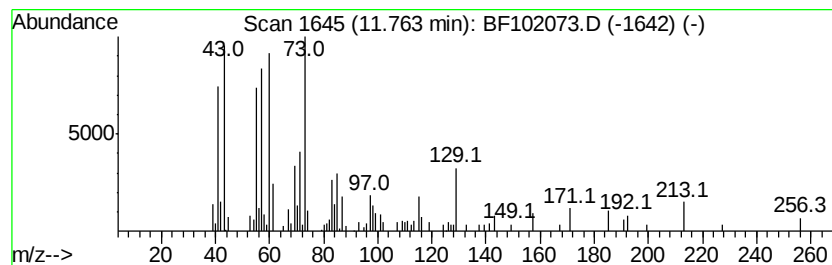
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.76	2.26 ng	125338	Phenanthrene-d10		11.23	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	86
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Dodecanoic acid	200	C12H24O2	000143-07-7	86
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	80



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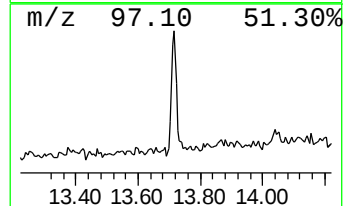
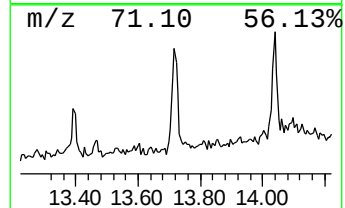
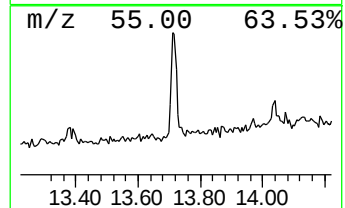
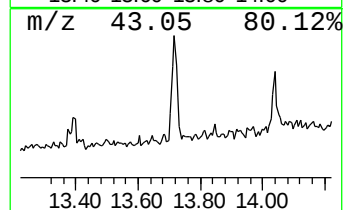
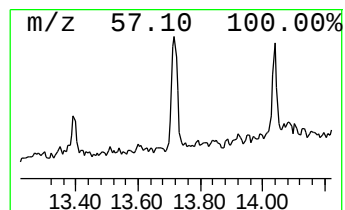
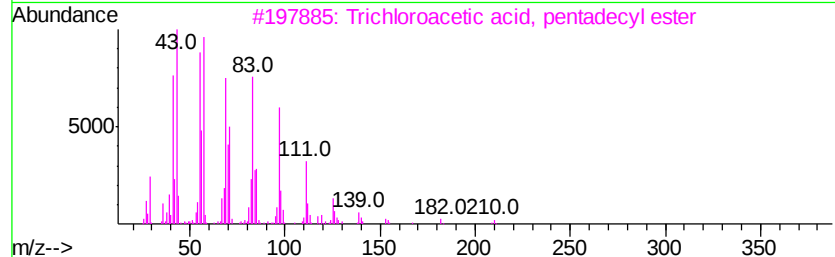
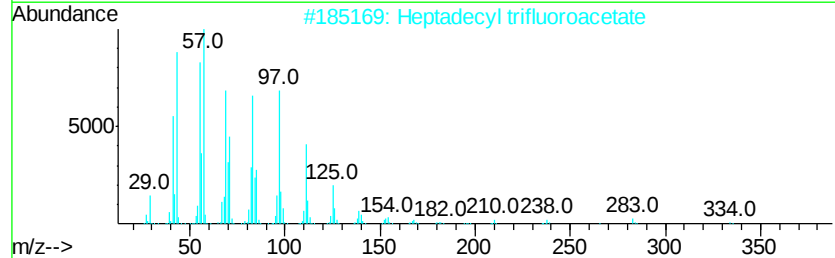
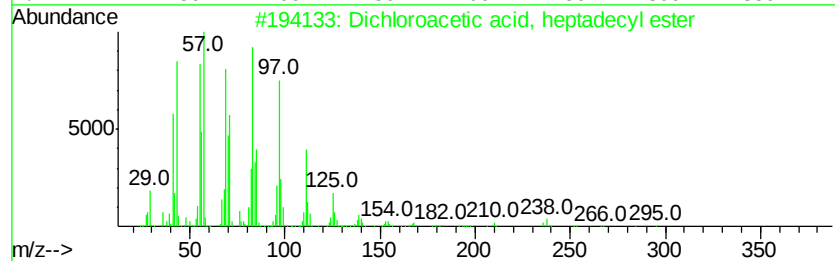
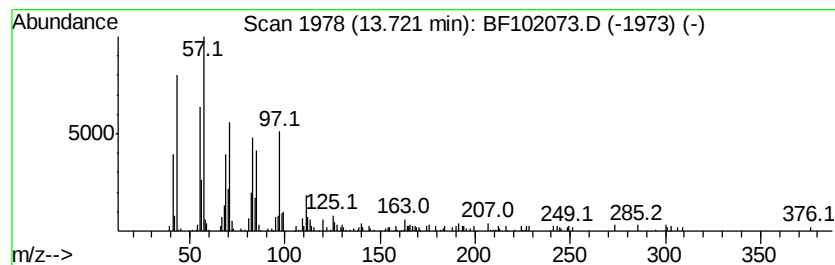
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.24 ng	256394	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011518\
Data File : BF102073.D
Acq On : 15 Jan 2018 20:00
Operator : SJ/JU
Sample : J1117-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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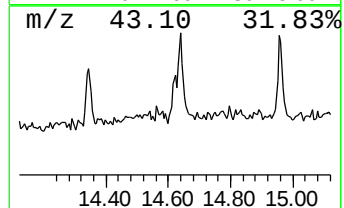
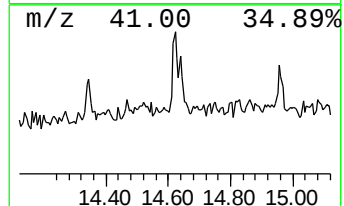
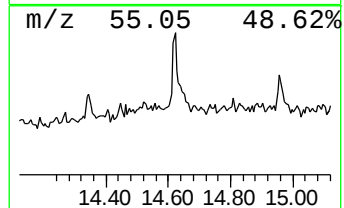
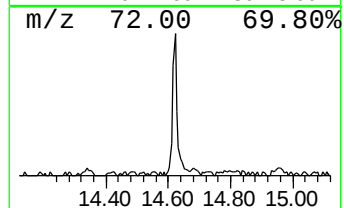
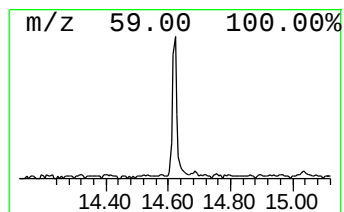
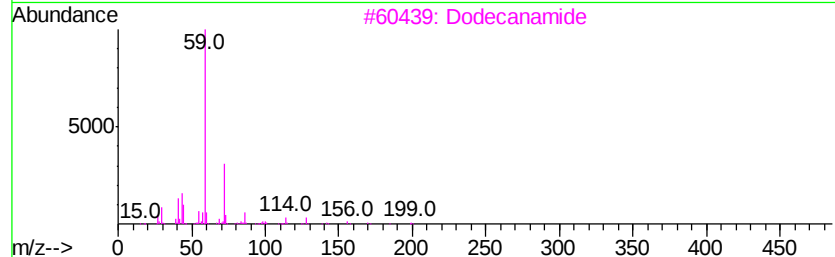
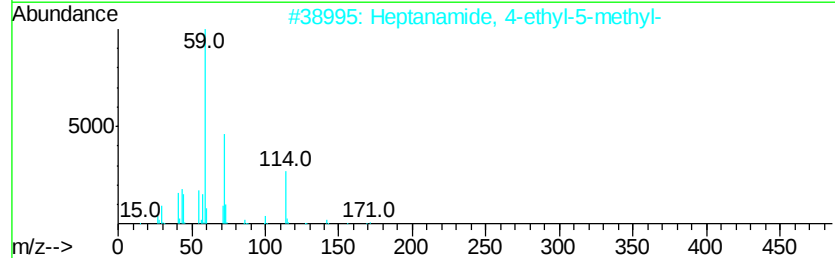
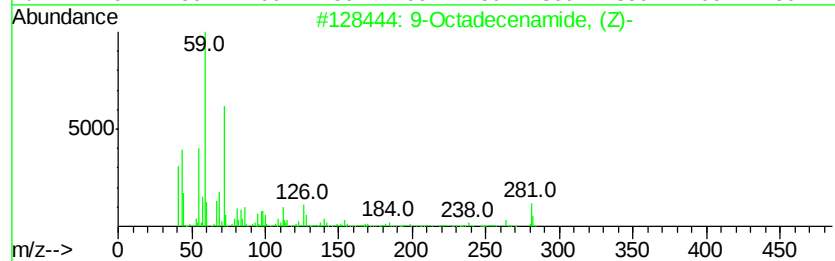
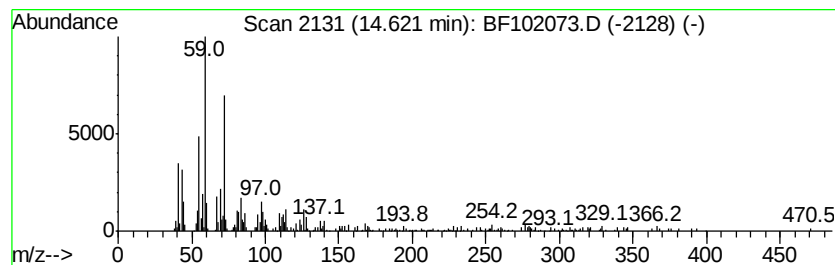
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.42 ng	155929	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	76
2		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50
3		Dodecanamide	199	C12H25NO	001120-16-7	50
4		Decanamide-	171	C10H21NO	002319-29-1	47
5		1-Phenyl-9-thioureido-3,6-diazah...	302	C16H22N4S	153464-71-2	38



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011518\
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Misc :
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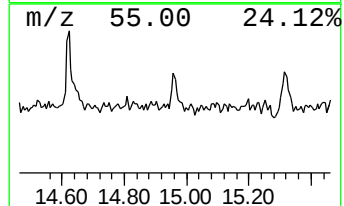
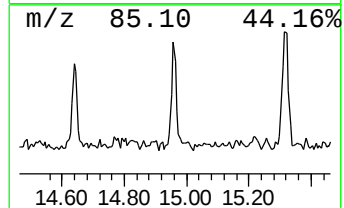
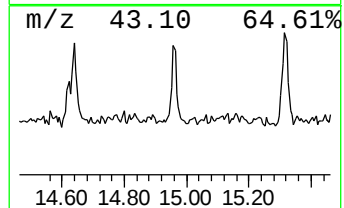
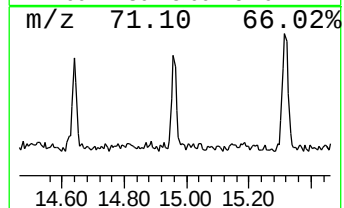
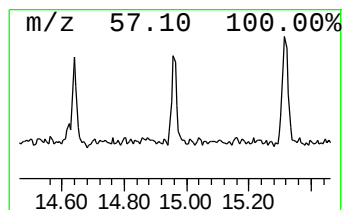
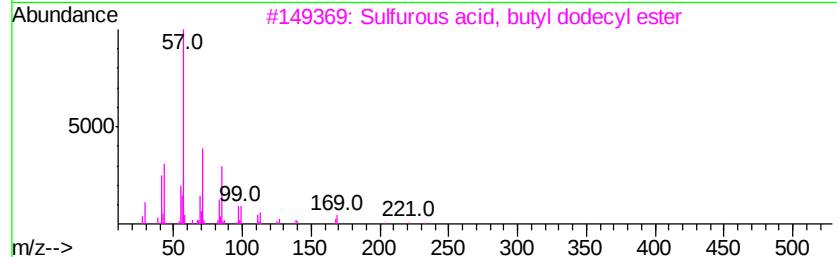
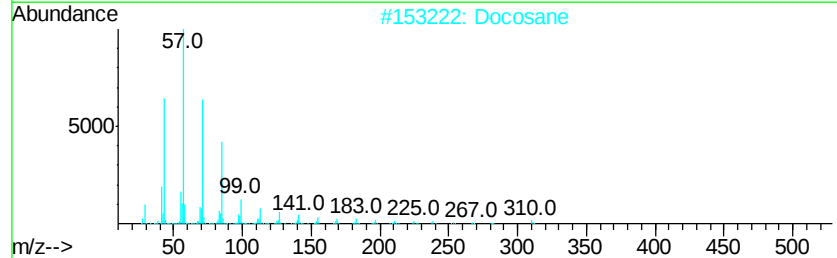
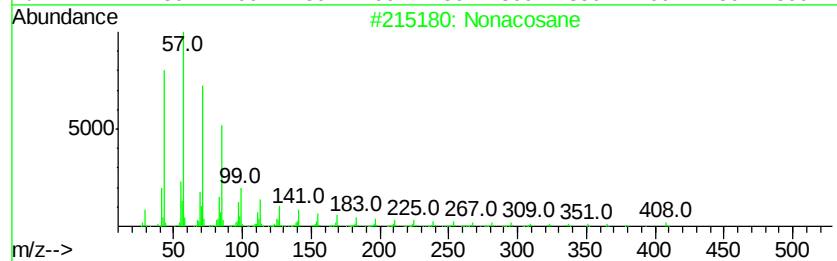
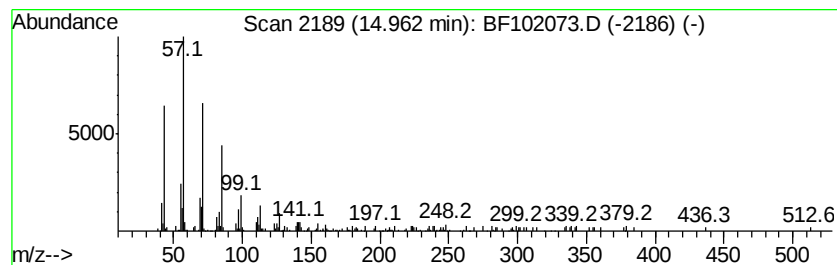
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.97 ng	135280	Perylene-d12	15.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonacosane	408 C29H60	000630-03-5	83
2	Docosane	310 C22H46	000629-97-0	81
3	Sulfurous acid, butyl dodecyl ester	306 C16H34O3S	1000309-17-9	80
4	2-methyloctacosane	408 C29H60	1000376-72-8	80
5	Octadecane, 5,14-dibutyl-	366 C26H54	055282-13-8	80



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011518\
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Acq On : 15 Jan 2018 20:00
Operator : SJ/JU
Sample : J1117-07
Misc :
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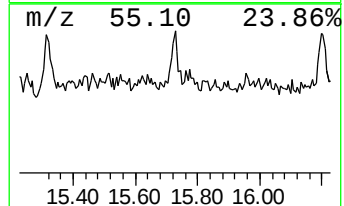
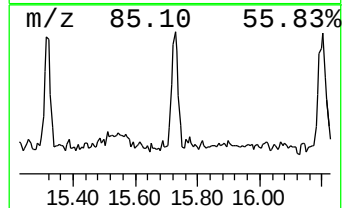
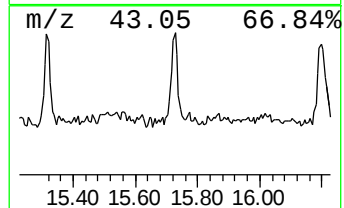
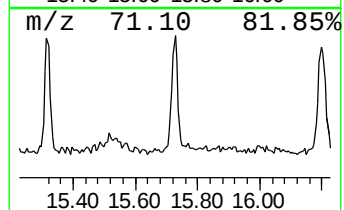
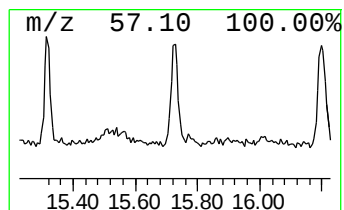
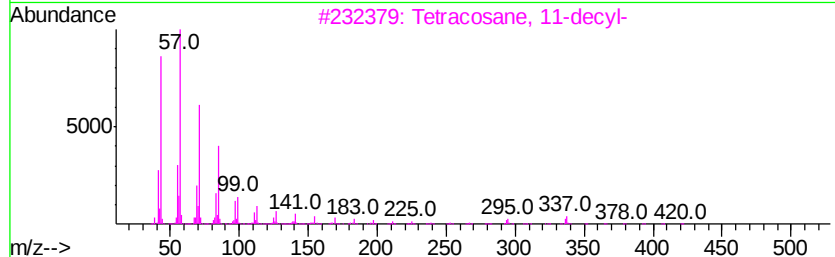
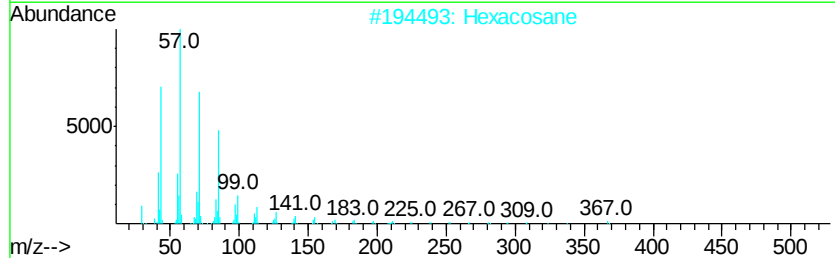
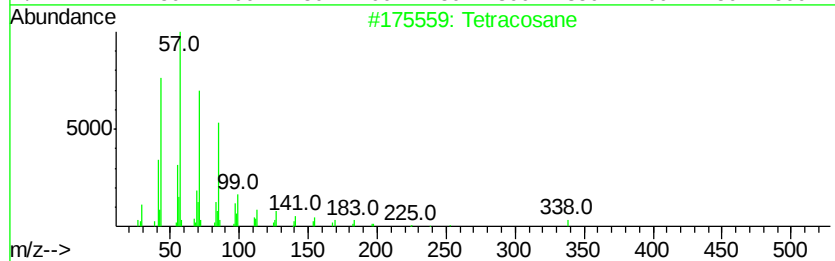
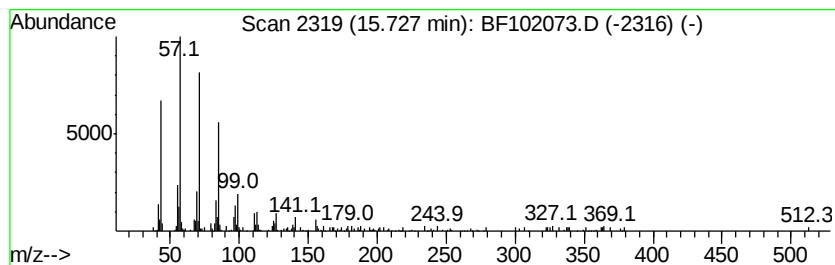
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.73	3.49 ng	159173	Perylene-d12	15.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
4	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	90
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87



Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
Data File : BF102073.D
Acq On : 15 Jan 2018 20:00
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Misc :
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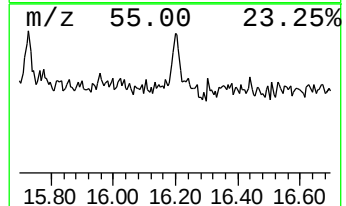
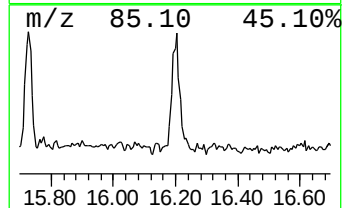
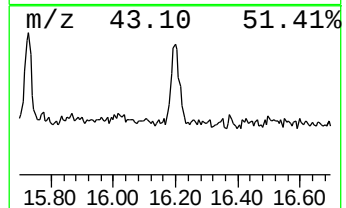
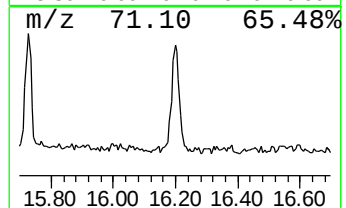
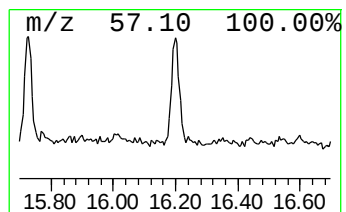
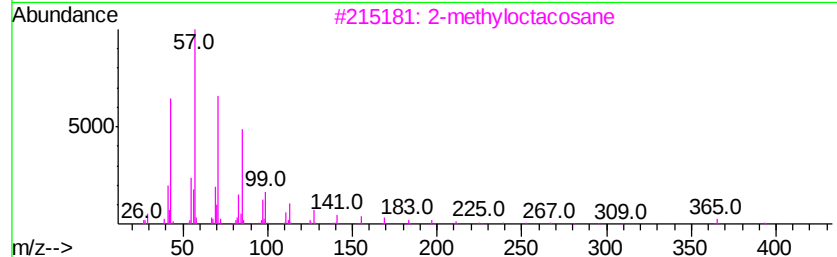
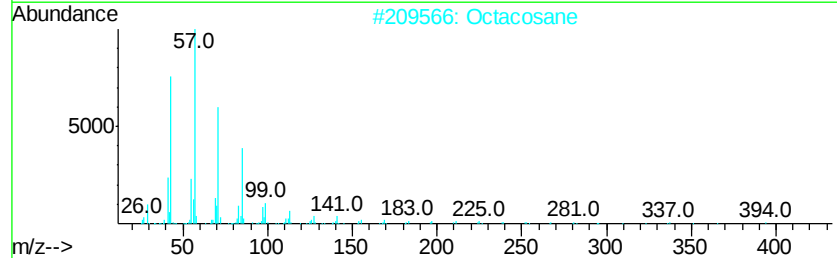
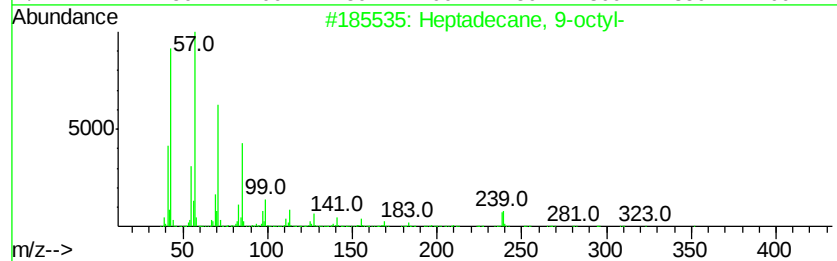
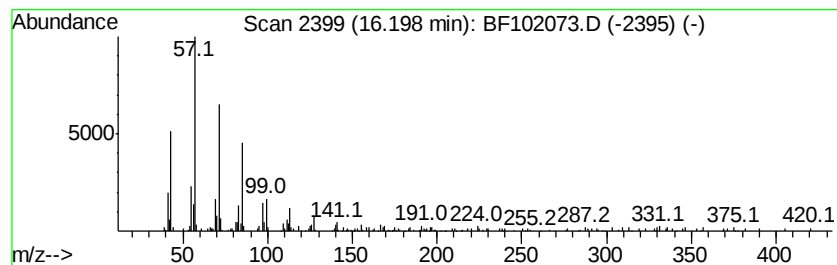
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	3.96 ng	180526	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2		Octacosane	394	C28H58	000630-02-4	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011518\
Data File : BF102073.D
Acq On : 15 Jan 2018 20:00
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Sample : J1117-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

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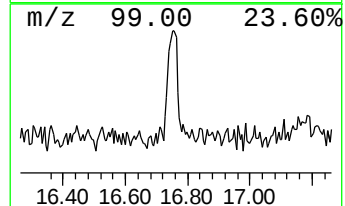
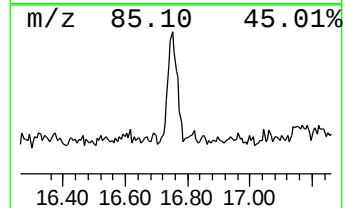
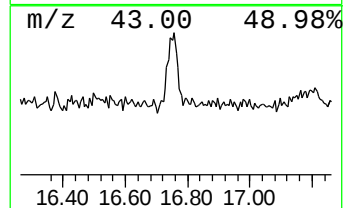
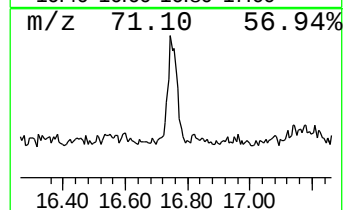
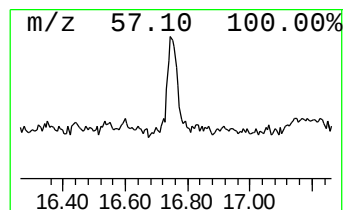
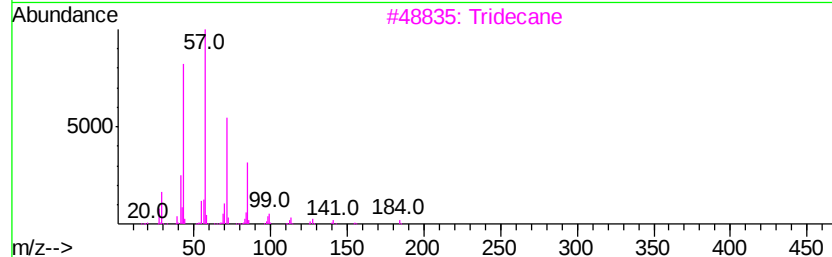
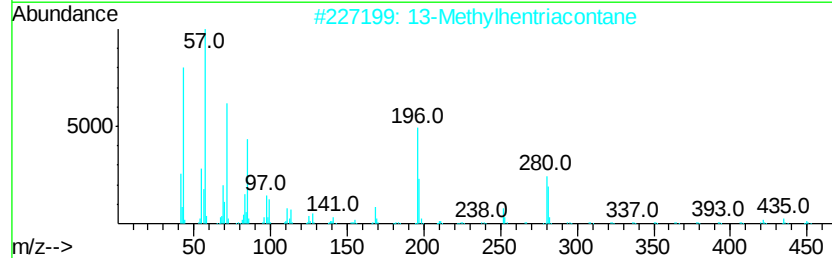
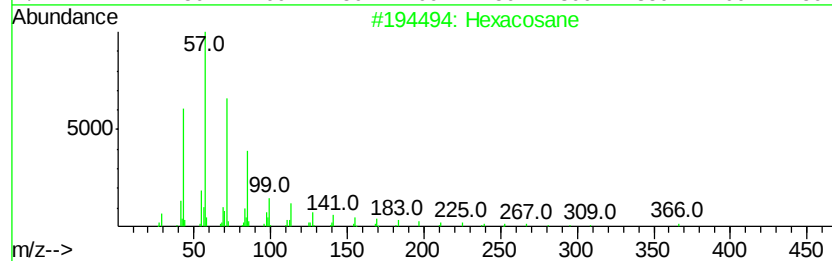
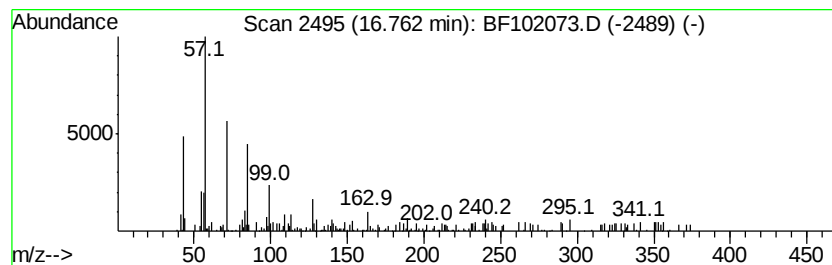
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.76	3.36 ng	153025	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	86
2		13-Methylhentriacontane	451	C32H66	1000131-19-4	70
3		Tridecane	184	C13H28	000629-50-5	58
4		11-Methylhentriacontane	451	C32H66	035799-05-4	58
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	53



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011518\
Data File : BF102073.D
Acq On : 15 Jan 2018 20:00
Operator : SJ/JU
Sample : J1117-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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	7.8 ng		456857	1	6.72	1171840	20.0
unknown6.49	6.49	85.6 ng		5013330	1	6.72	1171840	20.0
Tetradecane	10.19	2.1 ng		151479	3	9.76	1421870	20.0
Eicosane	10.66	3.4 ng		186524	4	11.23	1111420	20.0
n-Hexadecanoic acid	11.76	2.3 ng		125338	4	11.23	1111420	20.0
Dichloroacetic ac...	13.72	5.2 ng		256394	5	13.87	977741	20.0
9-Octadecenamide,...	14.62	3.4 ng		155929	6	15.28	911380	20.0
Nonacosane	14.96	3.0 ng		135280	6	15.28	911380	20.0
Tetracosane	15.73	3.5 ng		159173	6	15.28	911380	20.0
Heptadecane, 9-oc...	16.20	4.0 ng		180526	6	15.28	911380	20.0
Hexacosane	16.76	3.4 ng		153025	6	15.28	911380	20.0