

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF031618\
 Data File : BF103730.D
 Acq On : 17 Mar 2018 9:00
 Operator : JU/SJ
 Sample : J1947-03
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-GF-02-013-B

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-BF031518.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.334	36	42	50	rVB	181043	250268	4.97%	0.589%
2	5.228	530	534	543	rVB	187527	272461	5.41%	0.641%
3	5.604	591	598	601	rBV	3987703	4889566	97.03%	11.501%
4	5.916	648	651	658	rVB	177924	167387	3.32%	0.394%
5	6.598	760	767	770	rBV	3839217	5038977	100.00%	11.852%
6	6.745	786	792	795	rBV	4365829	4783959	94.94%	11.252%
7	6.969	827	830	834	rBV	1277074	1101646	21.86%	2.591%
8	7.134	853	858	861	rBV	3599368	3725480	73.93%	8.763%
9	7.539	920	927	930	rBV	2862371	3129615	62.11%	7.361%
10	8.251	1044	1048	1052	rBV	1690623	1451378	28.80%	3.414%
11	9.328	1225	1231	1234	rBV	4580425	4730185	93.87%	11.126%
12	9.716	1293	1297	1300	rBV	581307	432044	8.57%	1.016%
13	9.928	1330	1333	1336	rVB	134074	102623	2.04%	0.241%
14	10.010	1343	1347	1351	rBV	1669772	1441509	28.61%	3.391%
15	10.428	1415	1418	1421	rVB	182645	130659	2.59%	0.307%
16	10.645	1450	1455	1458	rBV	43981	60755	1.21%	0.143%
17	10.804	1477	1482	1485	rBV	2580398	2480931	49.23%	5.835%
18	10.898	1496	1498	1509	rVB	122618	146884	2.91%	0.345%
19	11.351	1572	1575	1578	rBV	76043	61938	1.23%	0.146%
20	11.504	1597	1601	1604	rBV	1415710	1198848	23.79%	2.820%
21	11.527	1604	1605	1609	rVB2	116508	70306	1.40%	0.165%
22	12.016	1683	1688	1697	rBV2	202495	260959	5.18%	0.614%
23	12.121	1702	1706	1713	rVB3	33871	55497	1.10%	0.131%
24	12.721	1804	1808	1813	rBV	189302	170632	3.39%	0.401%
25	12.898	1835	1838	1841	rVB	146548	112192	2.23%	0.264%
26	12.951	1844	1847	1850	rVB	171905	133630	2.65%	0.314%
27	13.092	1866	1871	1874	rBV	3354318	3281401	65.12%	7.718%
28	13.604	1955	1958	1961	rVB	84626	66957	1.33%	0.157%
29	13.804	1989	1992	1996	rVB	92232	89910	1.78%	0.211%
30	13.974	2018	2021	2029	rVB	466743	443035	8.79%	1.042%
31	14.157	2047	2052	2055	rBV	1085823	1063525	21.11%	2.502%
32	14.621	2128	2131	2138	rBV4	88333	124560	2.47%	0.293%
33	15.233	2232	2235	2239	rBV	61895	96760	1.92%	0.228%
34	15.298	2243	2246	2249	rBV	50067	53672	1.07%	0.126%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.698	2309	2314	2324	rVB	573125	795052	15.78%	1.870%
36	16.227	2401	2404	2411	rVB6	49634	99886	1.98%	0.235%

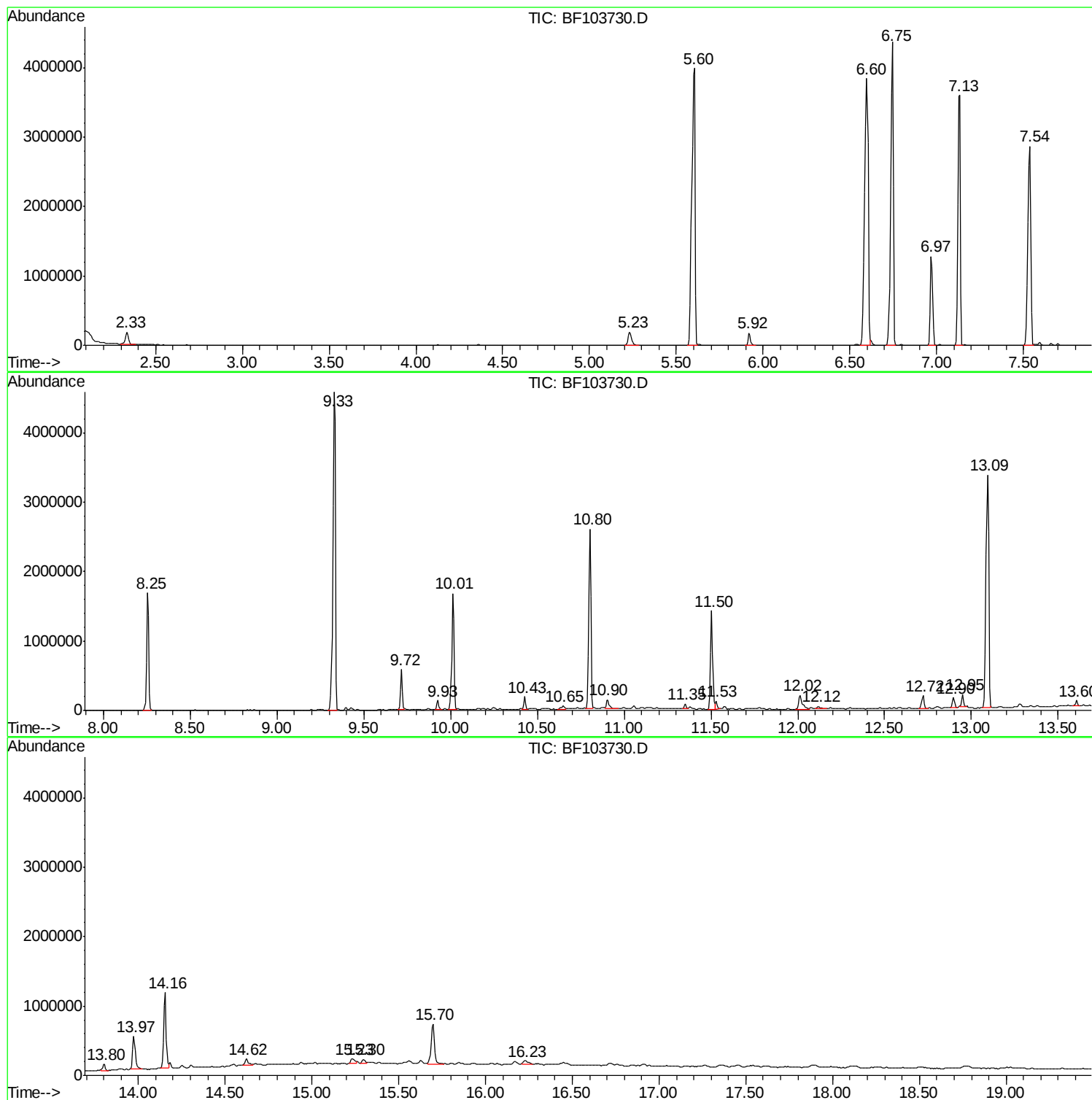
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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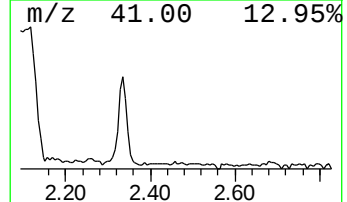
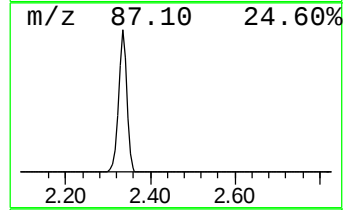
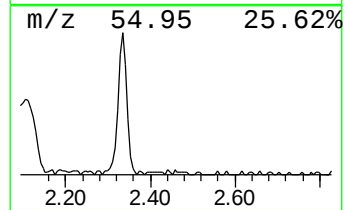
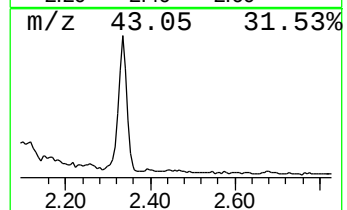
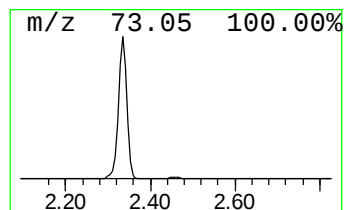
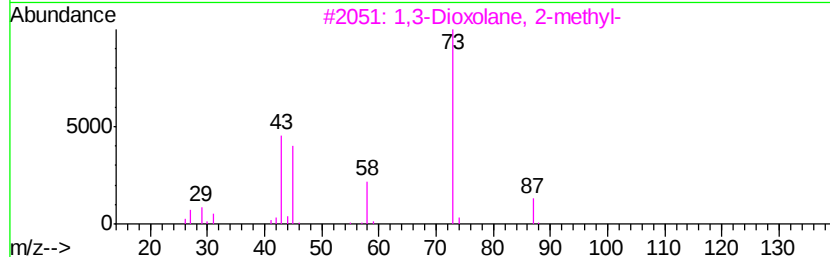
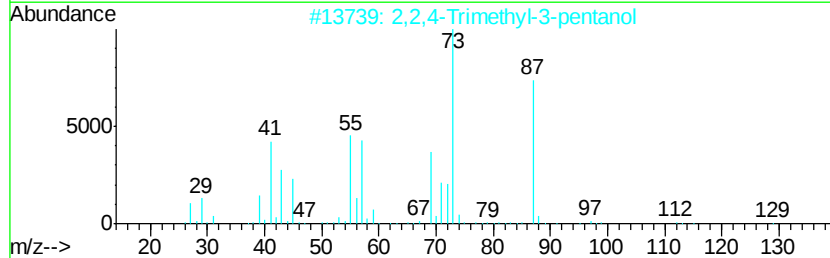
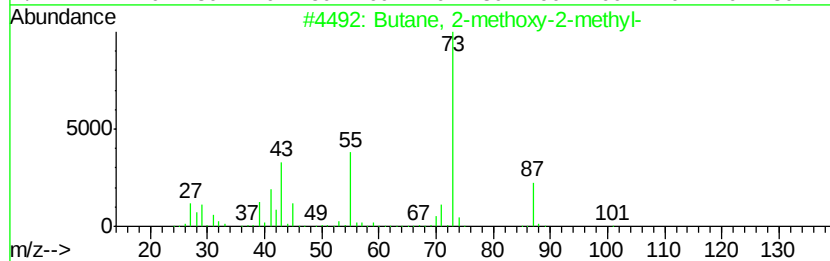
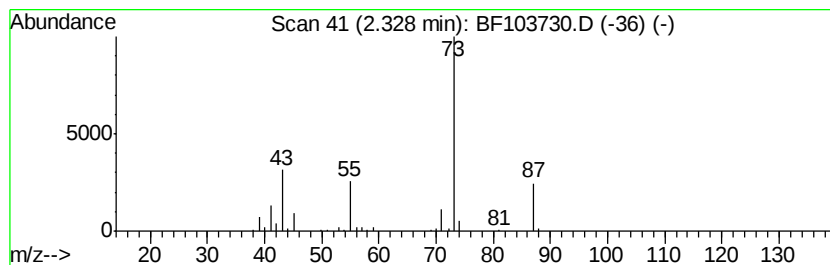
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	4.54 ng	250268	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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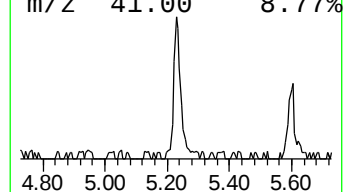
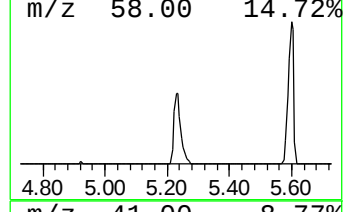
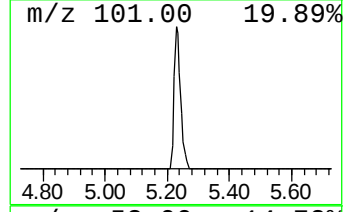
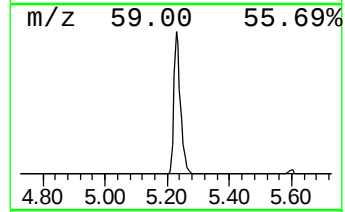
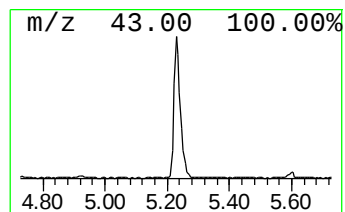
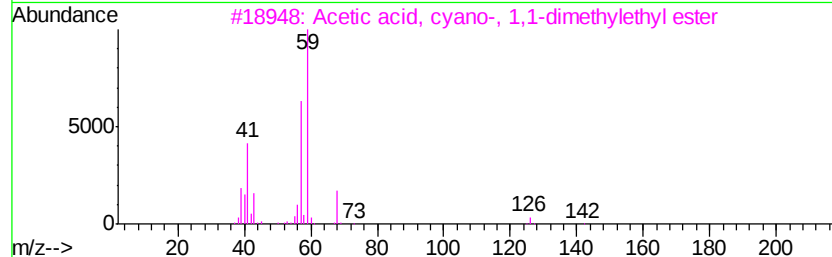
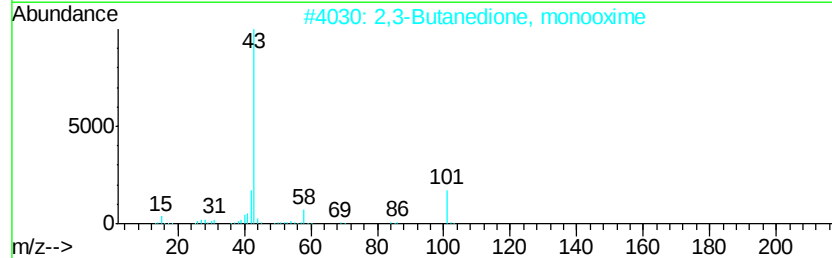
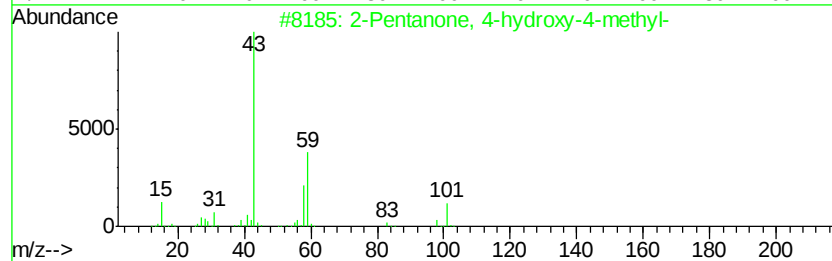
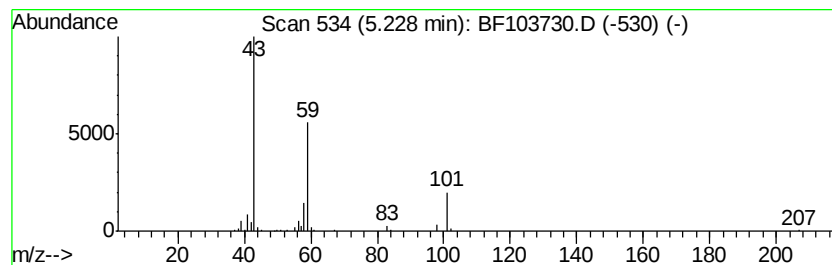
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	4.95 ng	272461	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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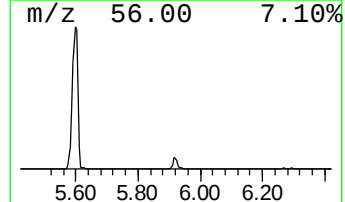
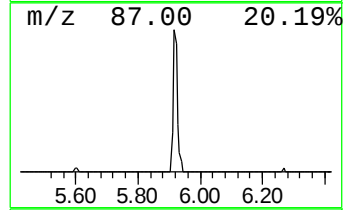
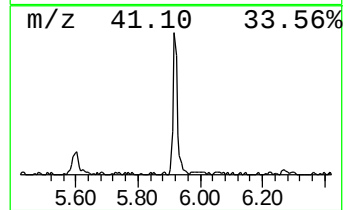
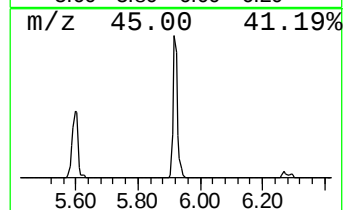
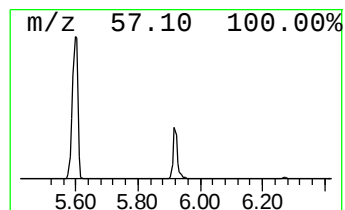
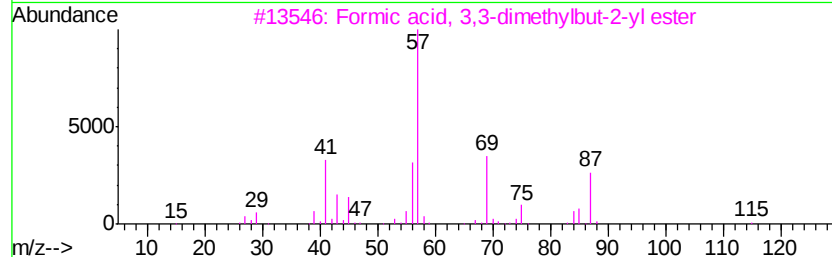
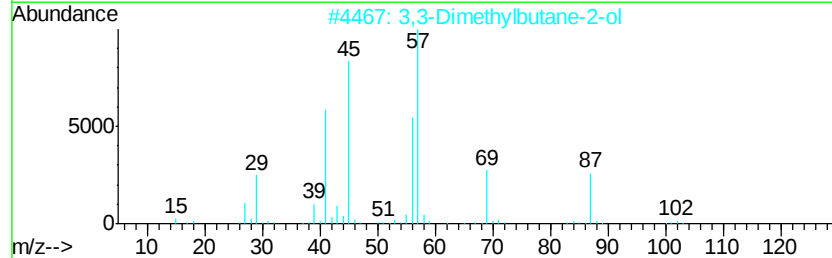
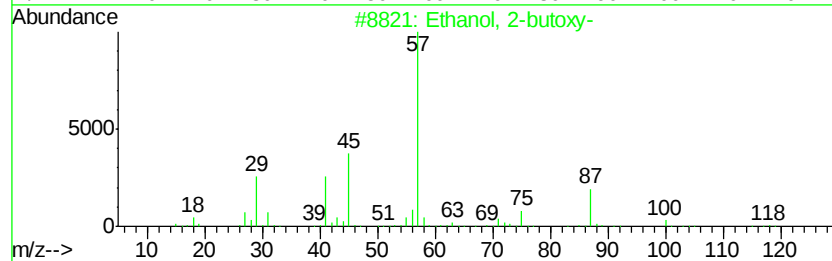
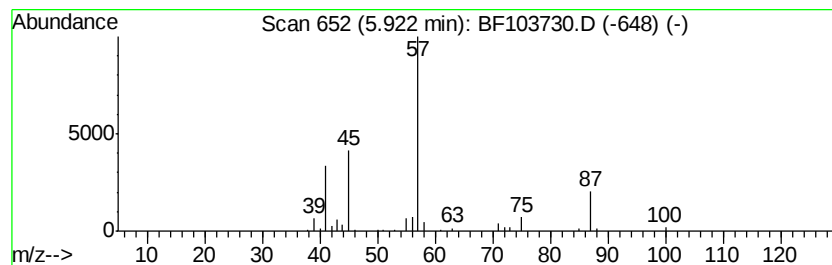
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.92	3.04 ng	167387	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	36
3			Formic acid, 3,3-dimethylbut-2-yl...	130	C7H14O2	1000368-20-5	23
4			n-Butyl ether	130	C8H18O	000142-96-1	16
5			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	12



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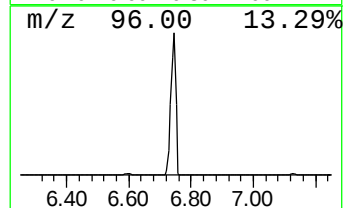
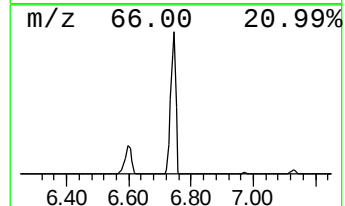
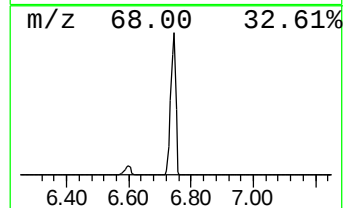
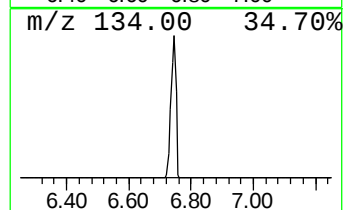
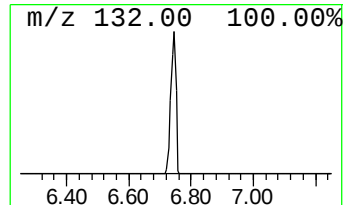
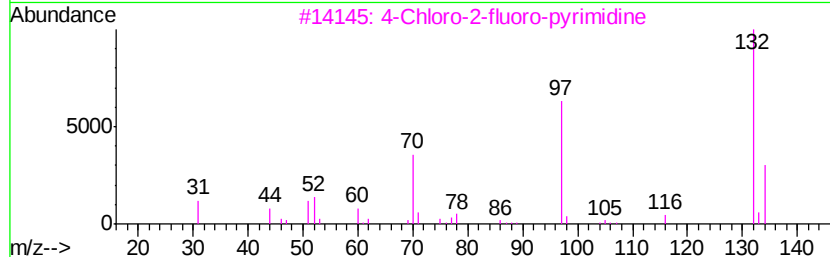
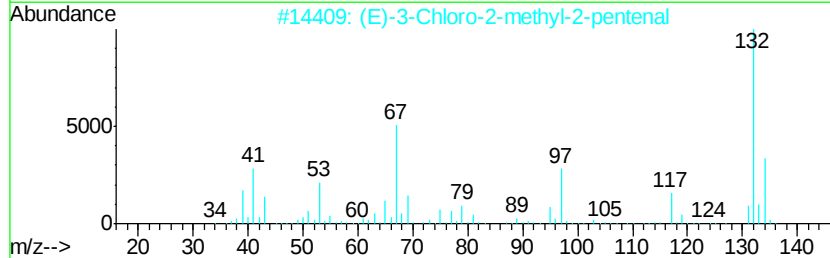
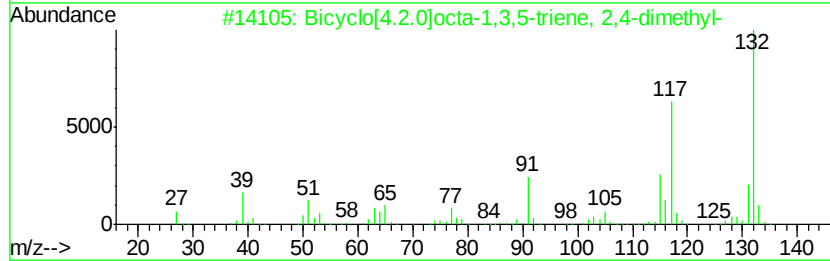
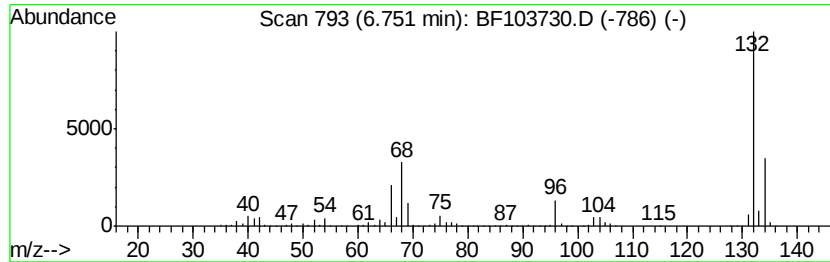
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	86.85 ng	4783960	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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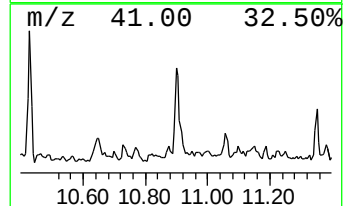
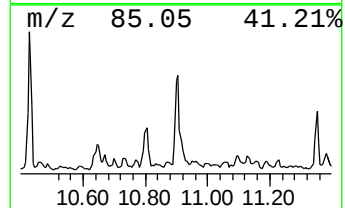
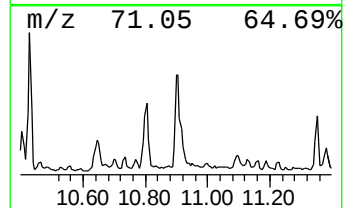
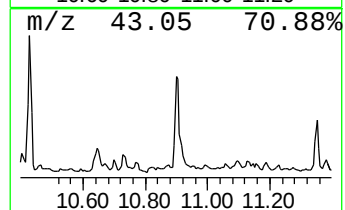
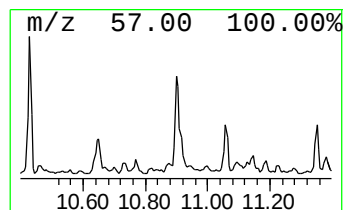
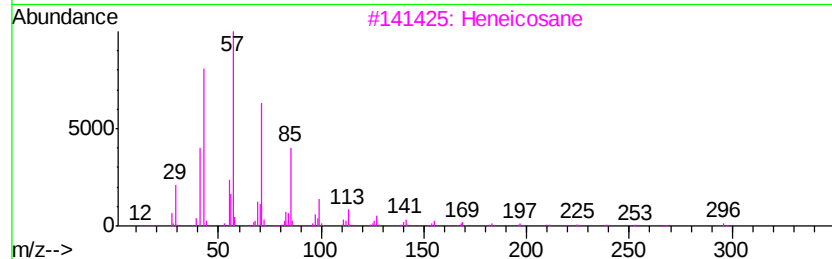
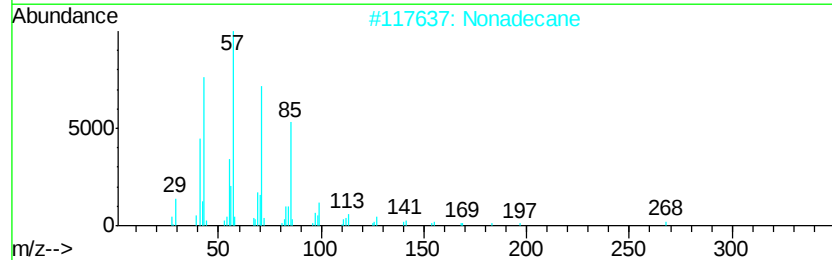
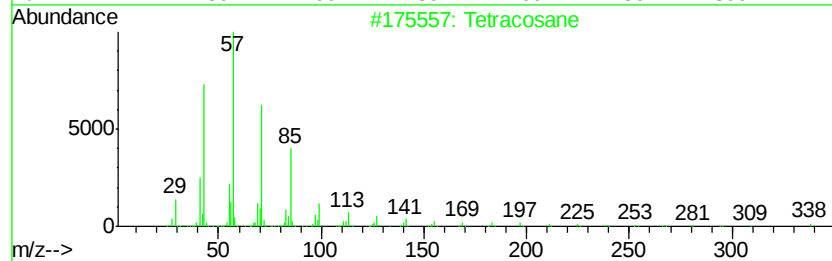
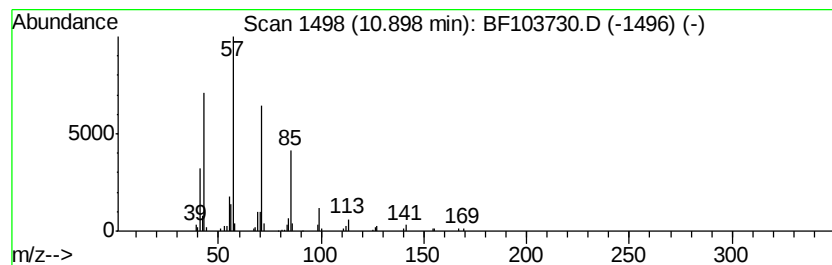
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.45 ng	146884	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	90
2		Nonadecane	268	C19H40	000629-92-5	86
3		Heneicosane	296	C21H44	000629-94-7	86
4		Hexadecane	226	C16H34	000544-76-3	86
5		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83



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Data File : BF103730.D
Acq On : 17 Mar 2018 9:00
Operator : JU/SJ
Sample : J1947-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-013-B

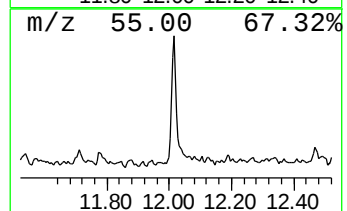
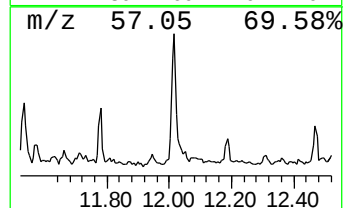
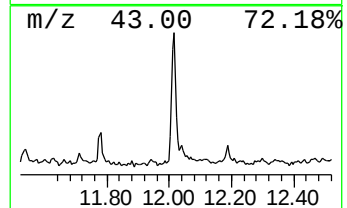
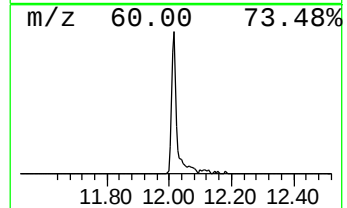
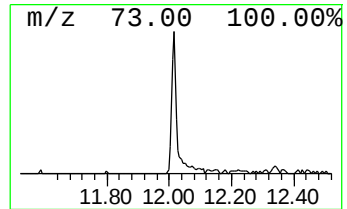
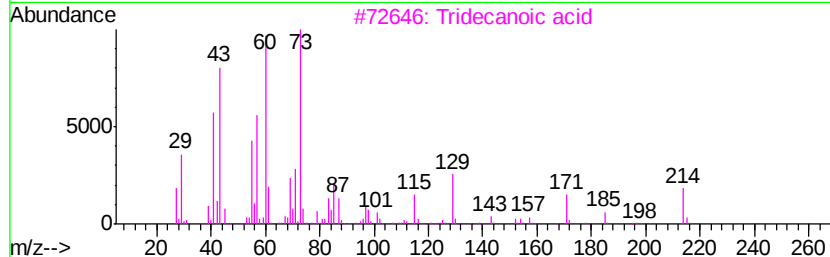
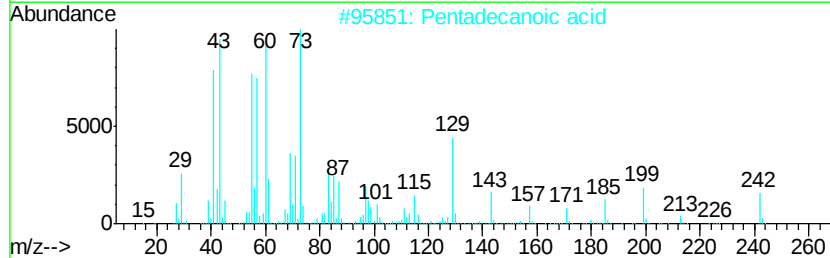
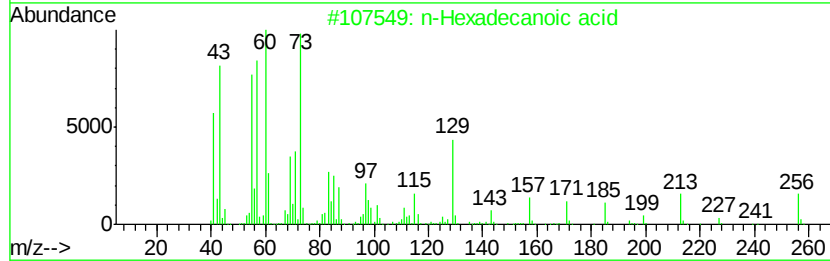
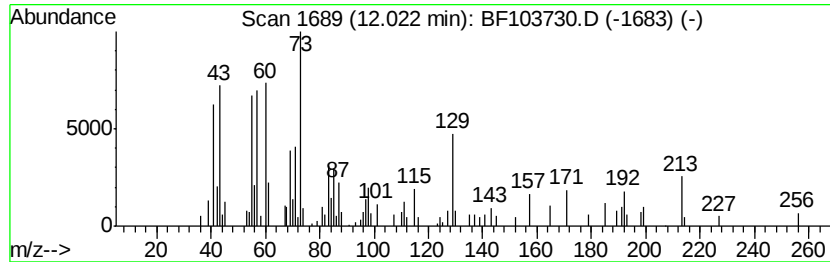
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	4.35 ng	260959	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	n-Decanoic acid	172	C10H20O2	000334-48-5	89
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF031618\
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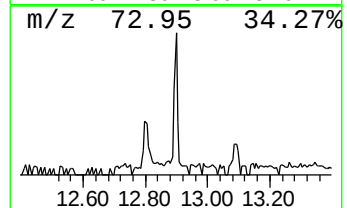
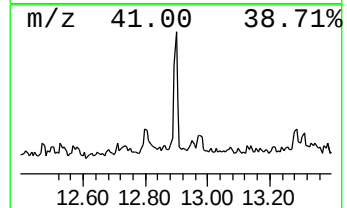
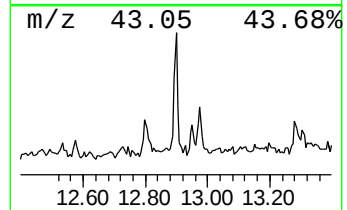
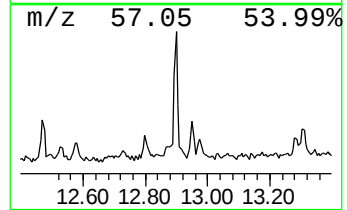
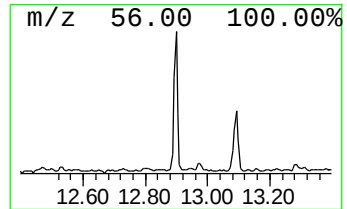
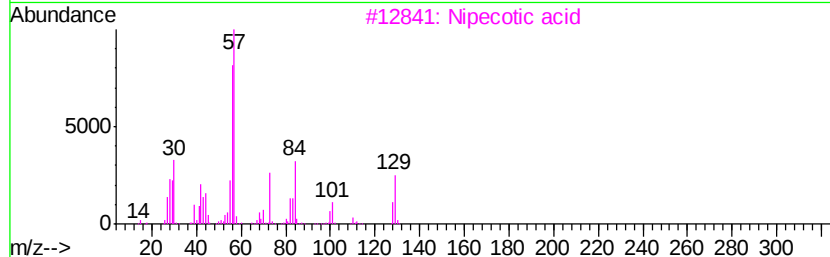
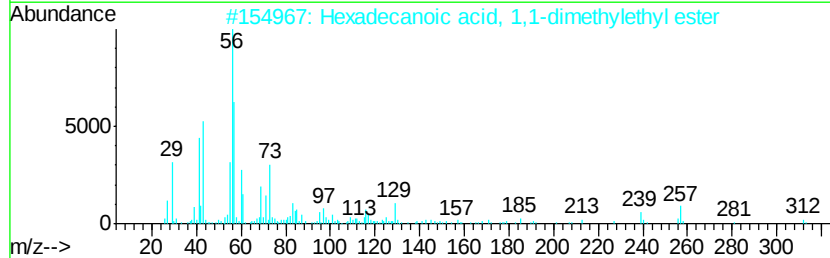
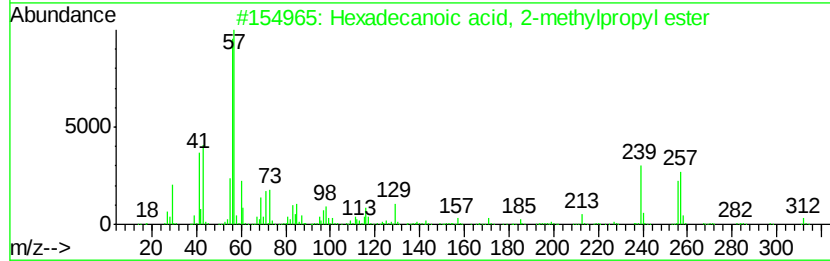
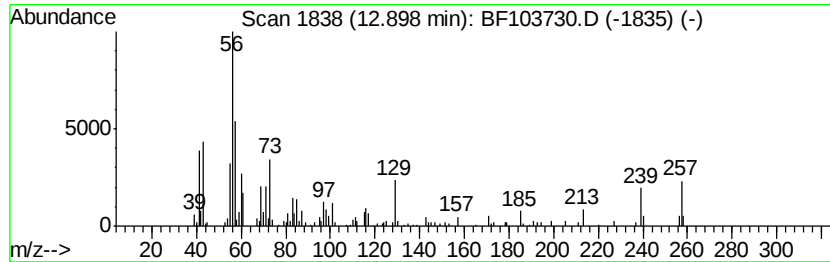
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, 2-methyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.90	2.11 ng	112192	Chrysene-d12		14.16	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2-methylpropyl ester	312	C20H40O2	000110-34-9	64	
2	Hexadecanoic acid, 1,1-dimethyl-2-propyl ester	312	C20H40O2	031158-91-5	58	
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47	
4	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	41	
5	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	25	



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF031618\
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Acq On : 17 Mar 2018 9:00
Operator : JU/SJ
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ClientSampleId :
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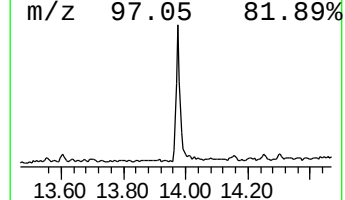
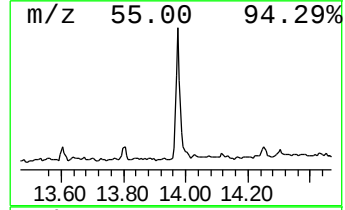
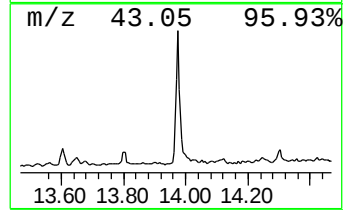
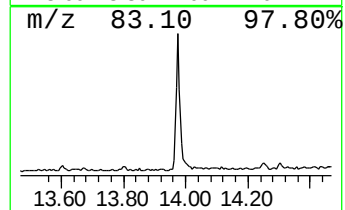
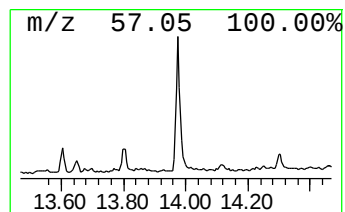
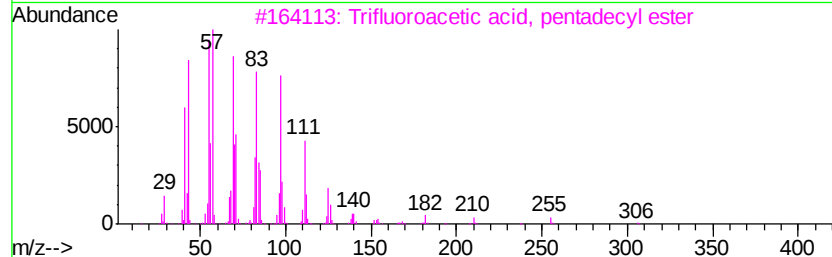
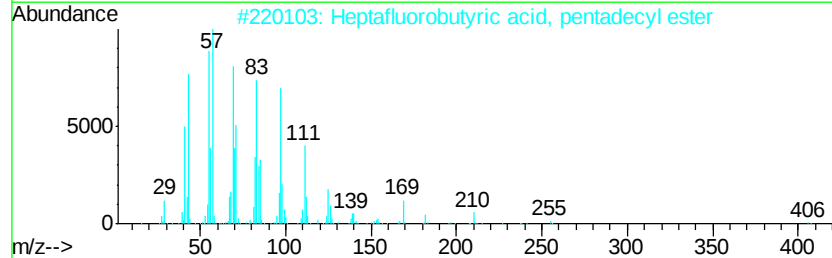
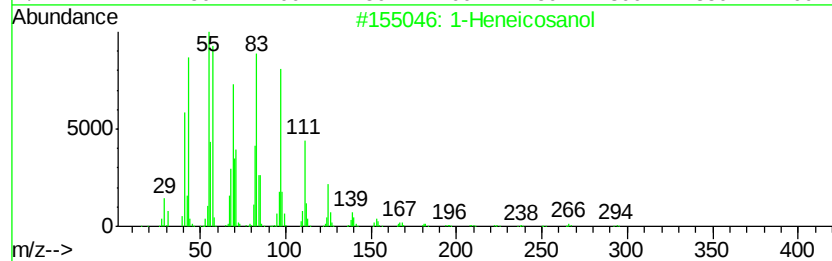
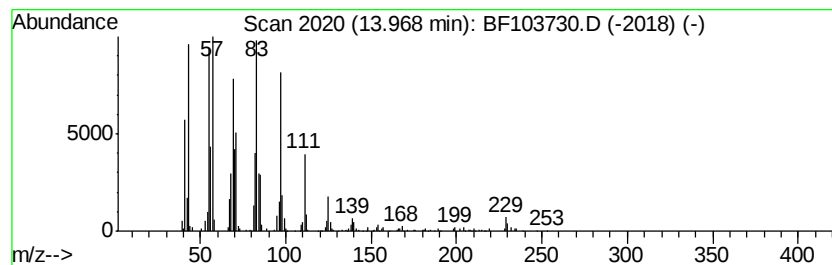
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	8.33 ng	443035	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5		Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF031618\
Data File : BF103730.D
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Operator : JU/SJ
Sample : J1947-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

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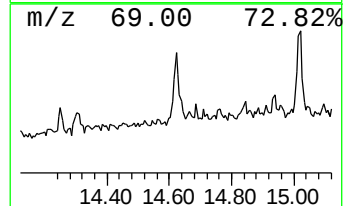
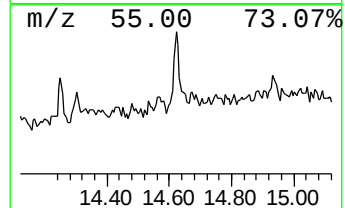
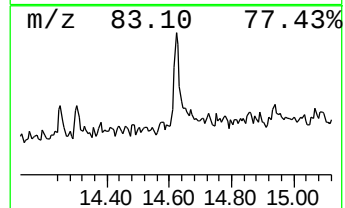
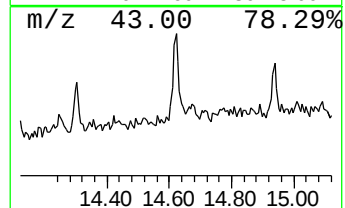
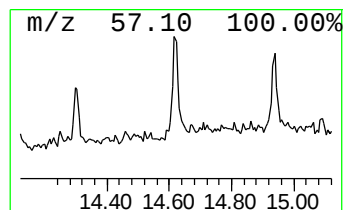
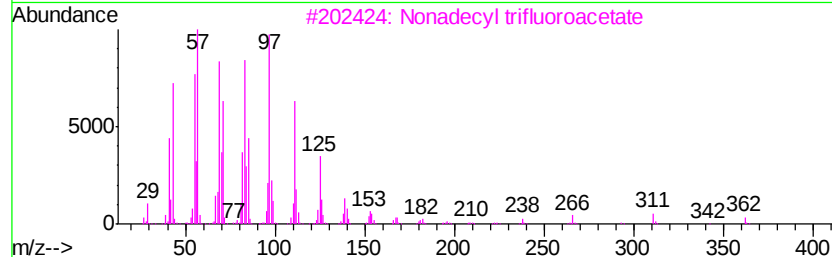
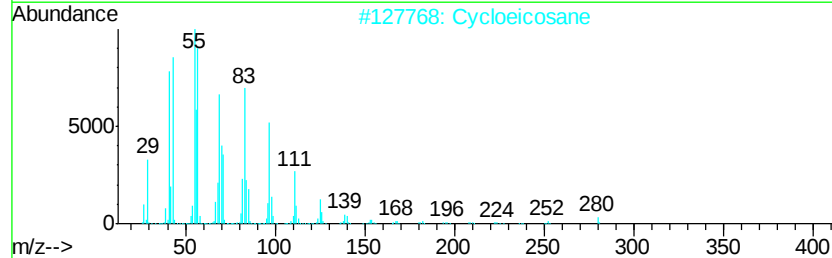
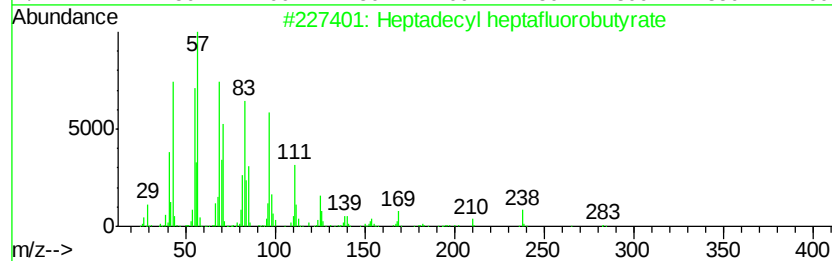
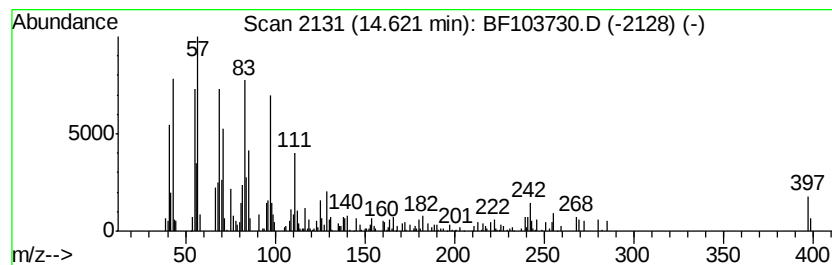
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.34 ng	124560	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	91
2		Cycloeicosane	280	C20H40	000296-56-0	89
3		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	83
5		1-Eicosene	280	C20H40	003452-07-1	81



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF031618\
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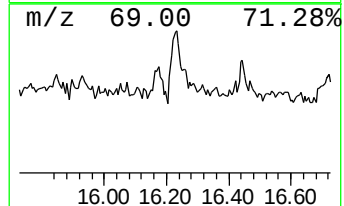
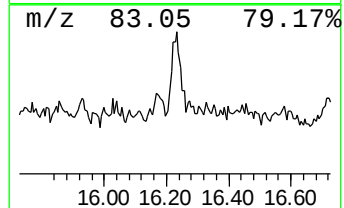
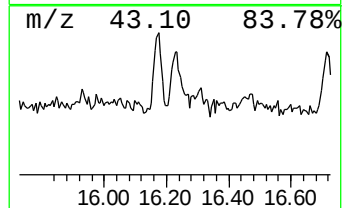
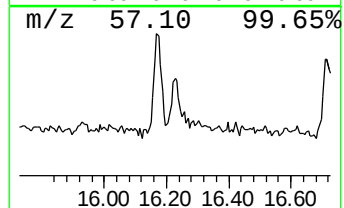
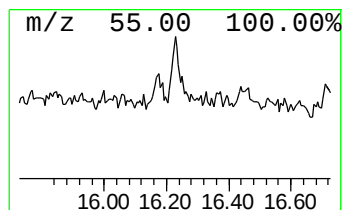
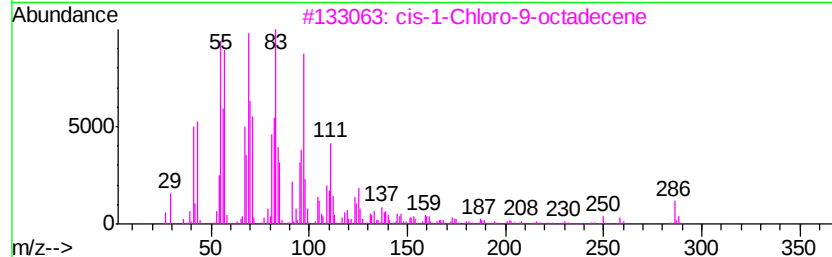
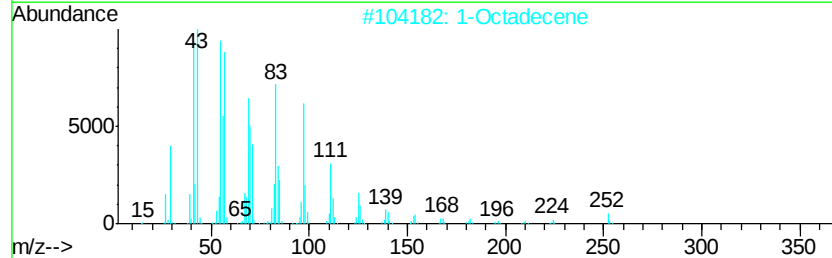
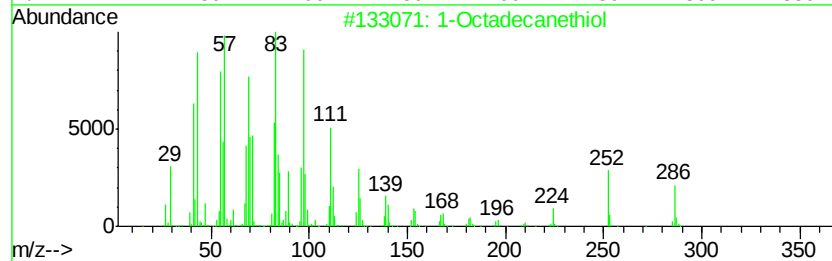
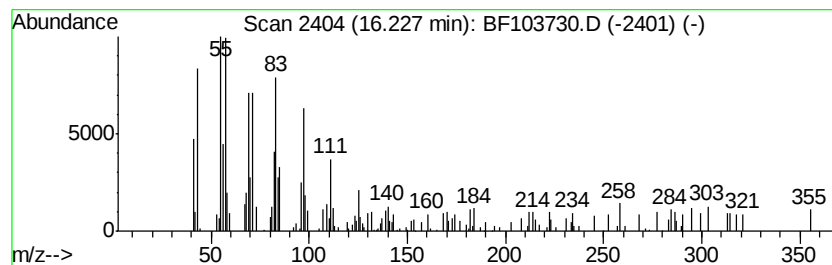
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Octadecanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.23	2.51 ng	99886	Perylene-d12	15.70	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanethiol	286	C18H38S	002885-00-9	83
2	1-Octadecene	252	C18H36	000112-88-9	78
3	cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	64
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	60
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	60



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF031618\
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Misc :
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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
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2-Pentanone, 4-hy...	5.23	5.0	ng	272461	1	6.97	1101650	20.0
Ethanol, 2-butoxy-	5.92	3.0	ng	167387	1	6.97	1101650	20.0
unknown6.75	6.75	86.8	ng	4783960	1	6.97	1101650	20.0
Tetracosane	10.90	2.5	ng	146884	4	11.50	1198850	20.0
n-Hexadecanoic acid	12.02	4.3	ng	260959	4	11.50	1198850	20.0
Hexadecanoic acid...	12.90	2.1	ng	112192	5	14.16	1063530	20.0
1-Heneicosanol	13.97	8.3	ng	443035	5	14.16	1063530	20.0
Heptadecyl heptaf...	14.62	2.3	ng	124560	5	14.16	1063530	20.0
1-Octadecanethiol	16.23	2.5	ng	99886	6	15.70	795052	20.0