

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
 Data File : BF103790.D
 Acq On : 20 Mar 2018 7:43
 Operator : JU/SJ
 Sample : J1954-04
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 031518-JETT-F-U-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	2.287	29	34	45	rVB	322832	436595	10.92%	1.662%
2	5.193	525	528	536	rVB	72162	74062	1.85%	0.282%
3	5.587	591	595	598	rBV	1404936	1203787	30.10%	4.583%
4	5.916	647	651	659	rVB	141975	121244	3.03%	0.462%
5	6.581	760	764	768	rBV	1015456	826553	20.67%	3.147%
6	6.740	786	791	794	rBV	2421638	2203572	55.10%	8.389%
7	6.969	827	830	834	rBV	986657	790359	19.76%	3.009%
8	7.128	853	857	860	rBV	3143804	2823265	70.59%	10.748%
9	7.534	921	926	929	rBV	2363467	2334644	58.38%	8.888%
10	7.592	932	936	945	rVB	40341	45119	1.13%	0.172%
11	7.698	951	954	957	rVB	52399	40017	1.00%	0.152%
12	8.251	1044	1048	1052	rBV	1303349	1051731	26.30%	4.004%
13	9.328	1226	1231	1234	rBV	4160868	3999340	100.00%	15.225%
14	9.716	1293	1297	1299	rBV	294007	222648	5.57%	0.848%
15	9.928	1329	1333	1336	rBV	107802	85157	2.13%	0.324%
16	10.010	1344	1347	1351	rVB	1279230	1117184	27.93%	4.253%
17	10.428	1415	1418	1421	rVB	162784	118659	2.97%	0.452%
18	10.645	1449	1455	1458	rBV2	40112	57182	1.43%	0.218%
19	10.675	1458	1460	1462	rVB	61118	45638	1.14%	0.174%
20	10.804	1478	1482	1485	rBV	1759030	1624995	40.63%	6.186%
21	10.898	1495	1498	1504	rBV	120705	135160	3.38%	0.515%
22	11.351	1572	1575	1577	rBV	82012	61159	1.53%	0.233%
23	11.504	1597	1601	1604	rBV	1246866	1016725	25.42%	3.871%
24	11.780	1644	1648	1650	rBV	45951	41285	1.03%	0.157%
25	12.010	1684	1687	1691	rBV	89041	90141	2.25%	0.343%
26	12.898	1835	1838	1841	rBV	93119	69457	1.74%	0.264%
27	13.092	1866	1871	1874	rBV	3137040	3174966	79.39%	12.087%
28	13.604	1955	1958	1961	rVB	70268	55350	1.38%	0.211%
29	13.974	2017	2021	2030	rBV	455192	434621	10.87%	1.655%
30	14.157	2048	2052	2055	rBV	956058	835400	20.89%	3.180%
31	14.621	2127	2131	2136	rBV2	32750	47819	1.20%	0.182%
32	15.021	2195	2199	2203	rVB	278326	281532	7.04%	1.072%
33	15.698	2309	2314	2320	rBV	579302	736010	18.40%	2.802%
34	16.227	2399	2404	2411	rVB2	39116	66573	1.66%	0.253%

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ClientSampleId :
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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-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

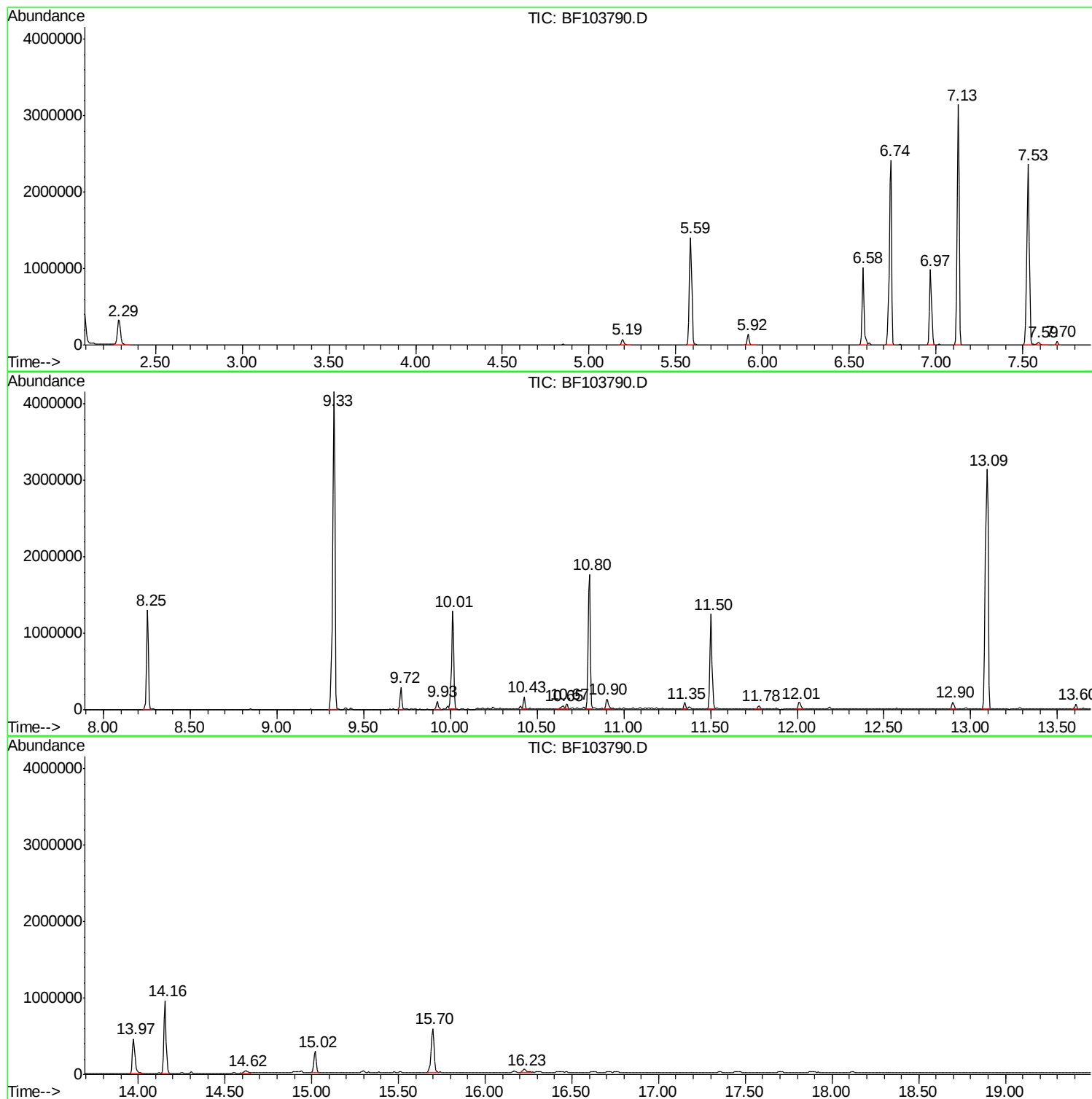
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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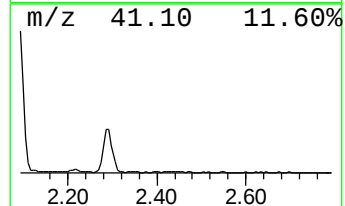
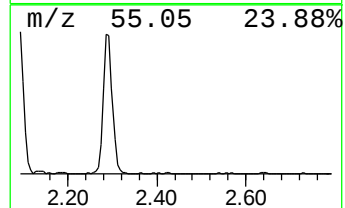
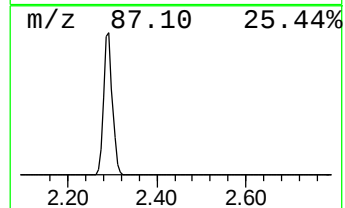
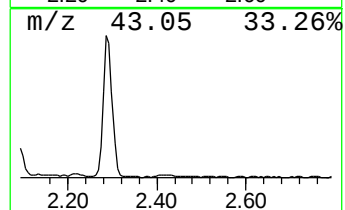
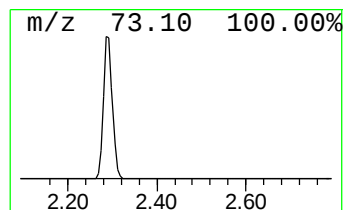
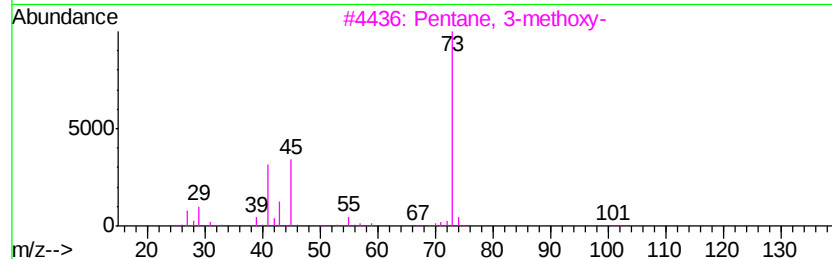
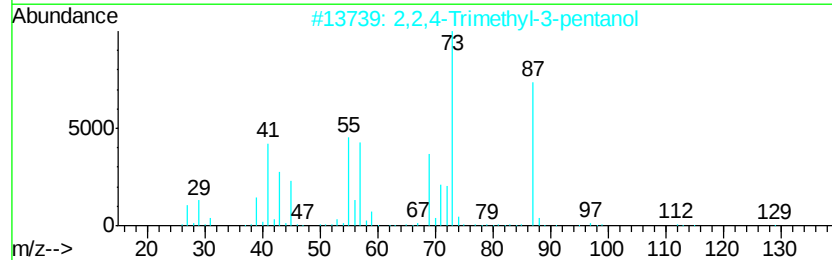
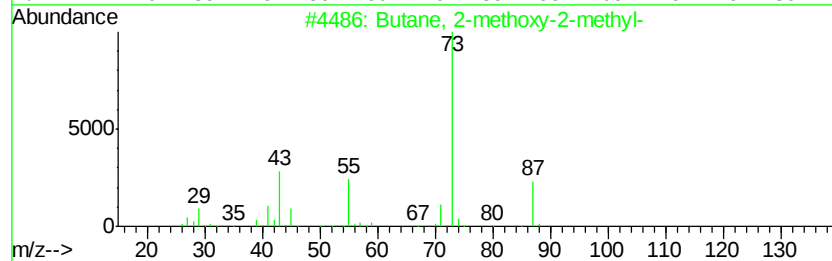
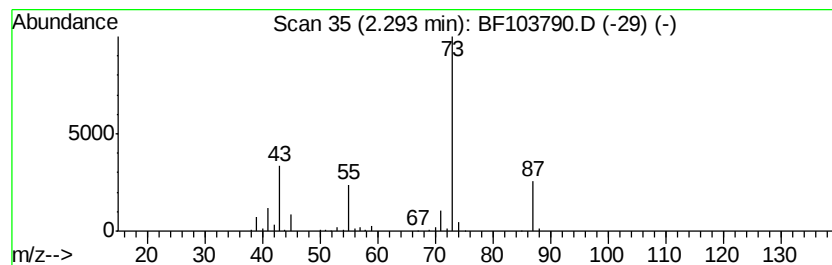
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	11.05 ng	436595	1,4-Dichlorobenzene-d4	6.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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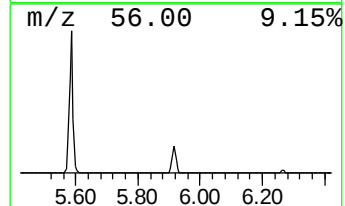
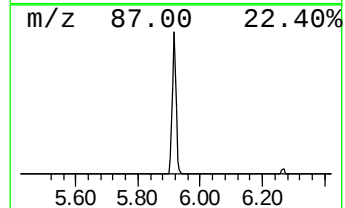
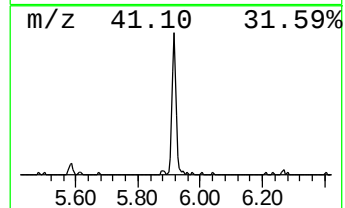
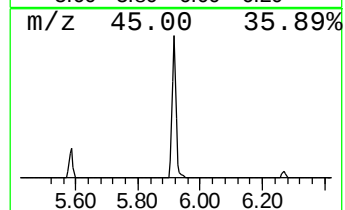
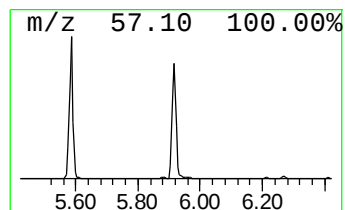
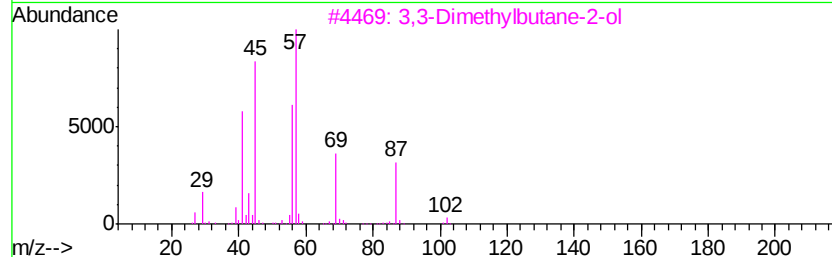
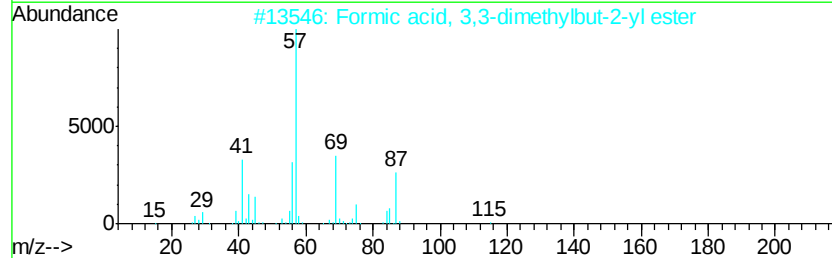
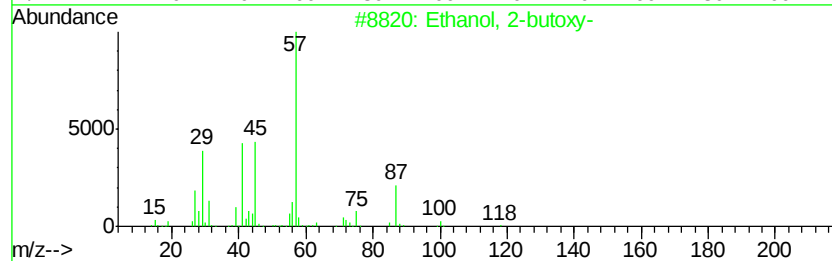
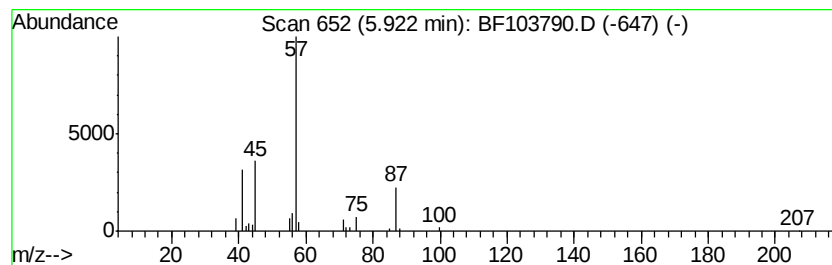
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.92	3.07 ng	121244	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2			Formic acid, 3,3-dimethylbut-2-yl...	130	C7H14O2	1000368-20-5	56
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	38
4			n-Butyl ether	130	C8H18O	000142-96-1	25
5			Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	17



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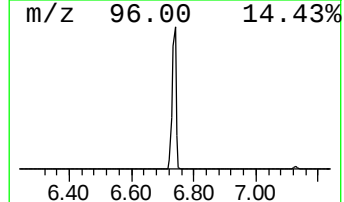
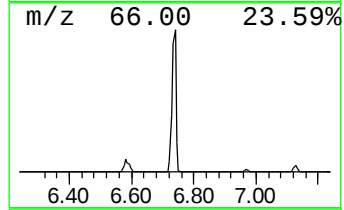
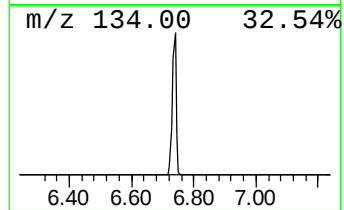
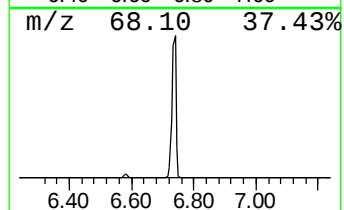
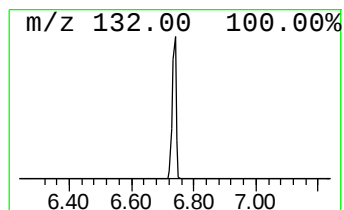
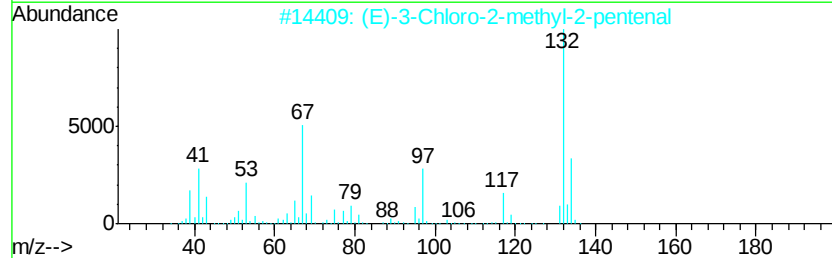
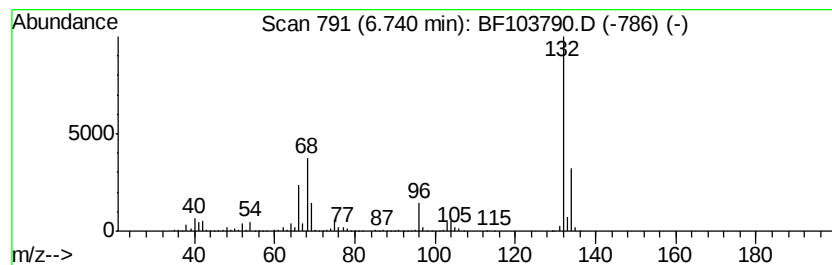
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	55.76 ng	2203570	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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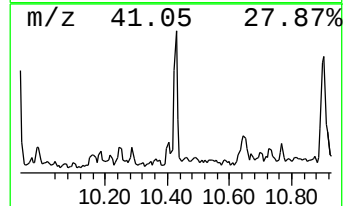
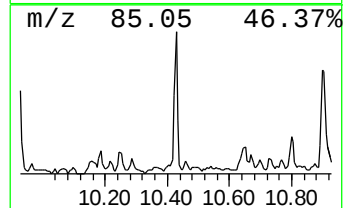
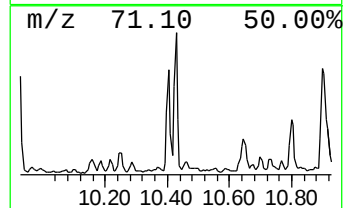
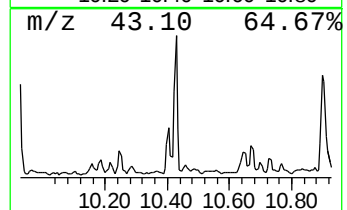
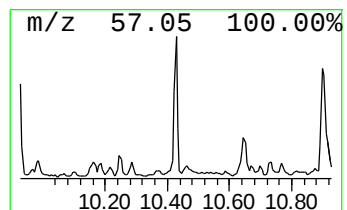
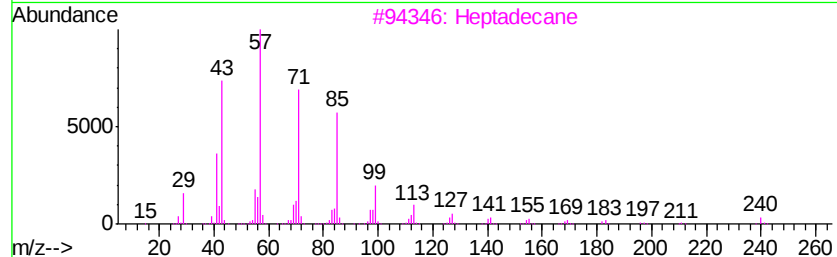
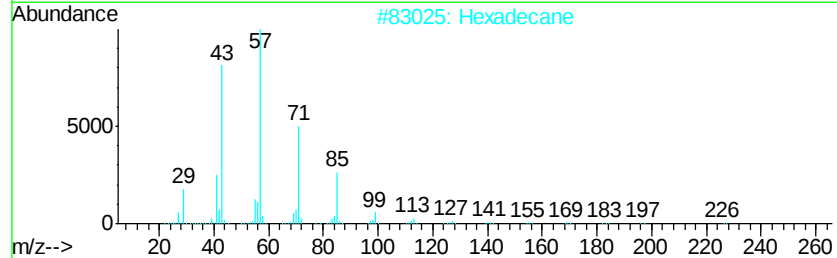
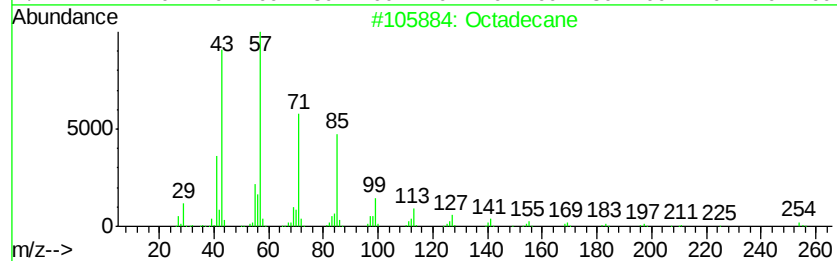
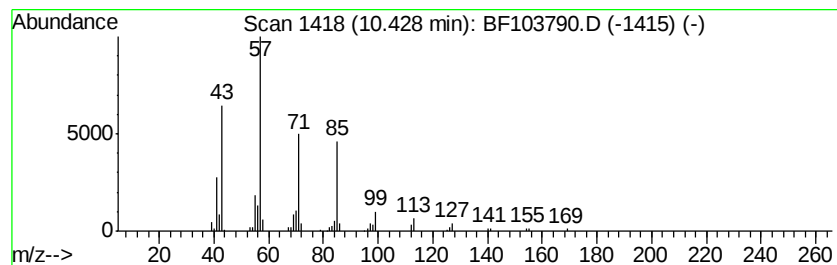
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.12 ng	118659	Acenaphthene-d10	10.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Hexadecane	226	C16H34	000544-76-3	90
3		Heptadecane	240	C17H36	000629-78-7	90
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5		Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	72



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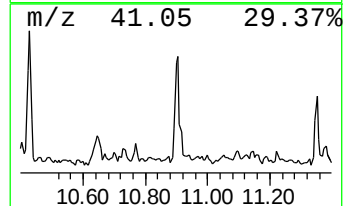
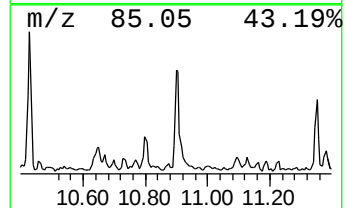
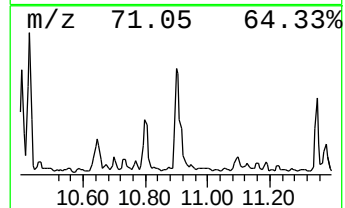
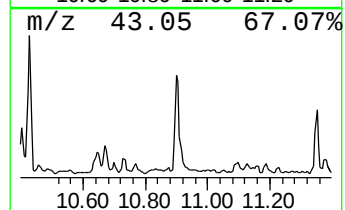
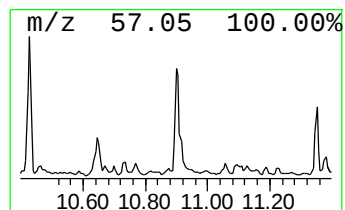
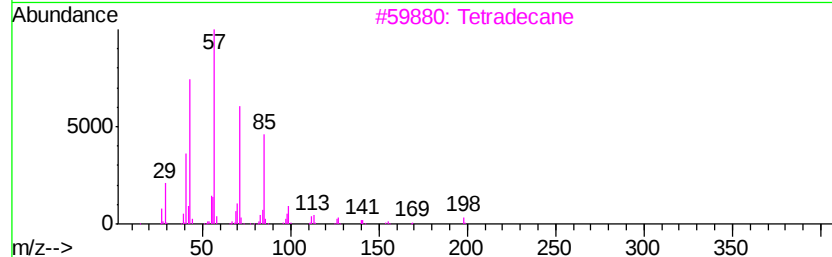
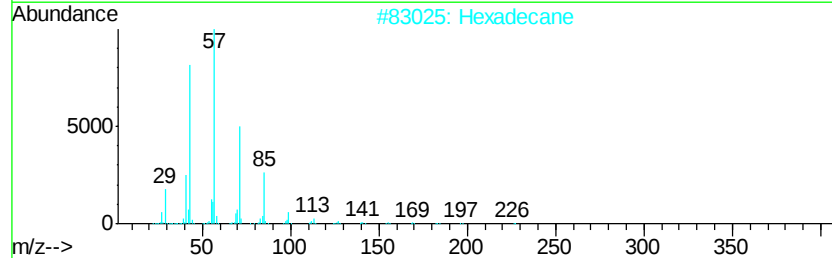
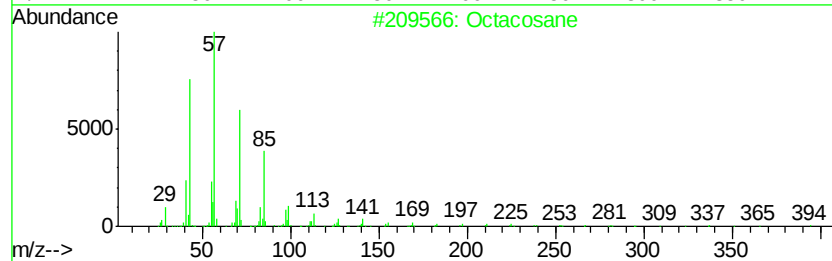
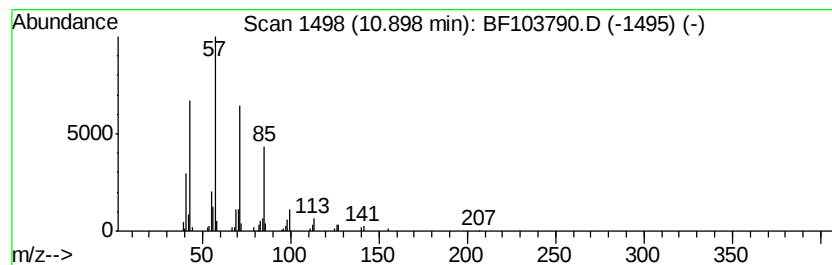
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.66 ng	135160	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Tetradecane		198	C14H30	000629-59-4	87
4	Tridecane		184	C13H28	000629-50-5	86
5	Nonadecane		268	C19H40	000629-92-5	86



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031518-JETT-F-U-B

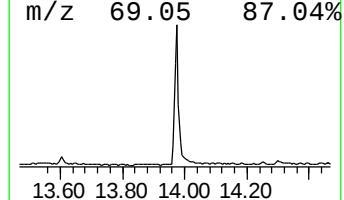
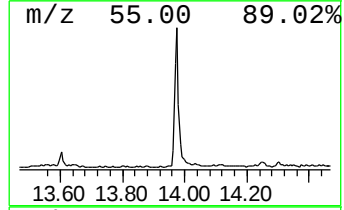
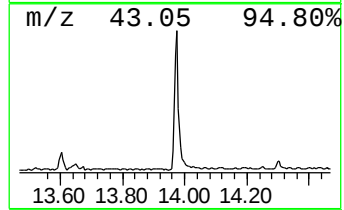
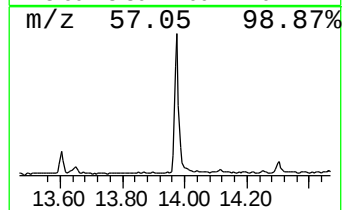
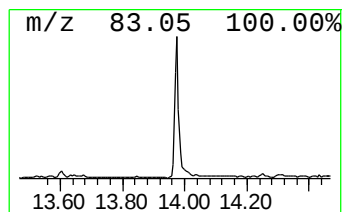
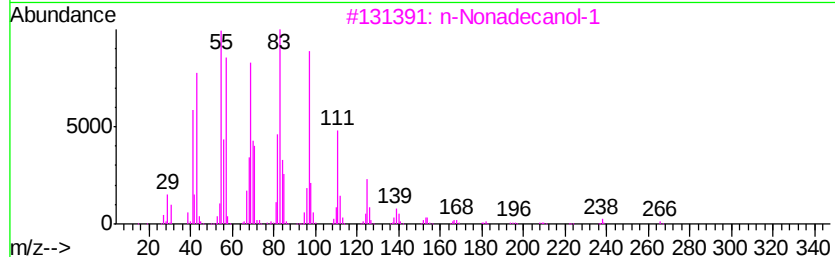
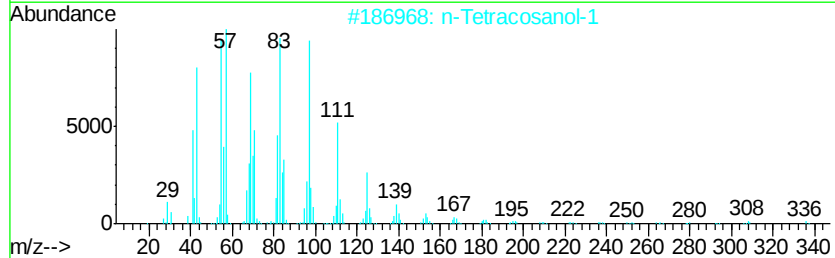
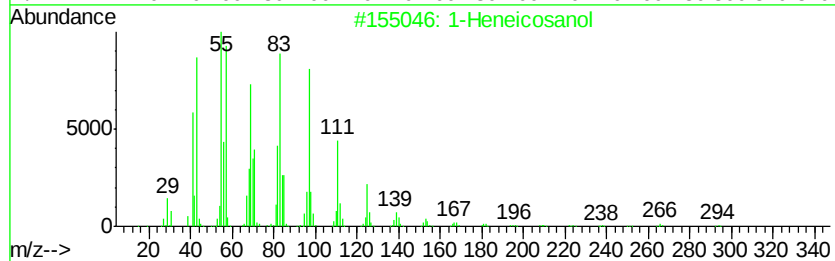
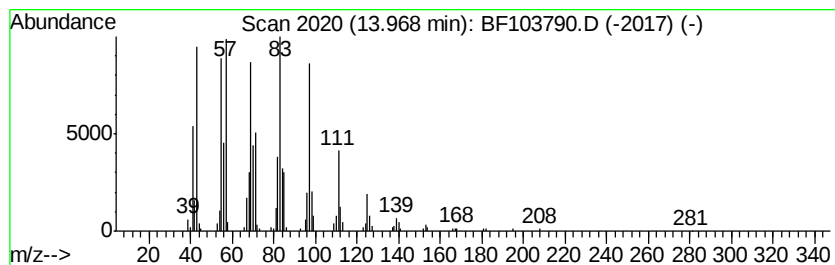
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	10.41 ng	434621	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5		1-Heptacosanol	396	C27H56O	002004-39-9	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103790.D
Acq On : 20 Mar 2018 7:43
Operator : JU/SJ
Sample : J1954-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
031518-JETT-F-U-B

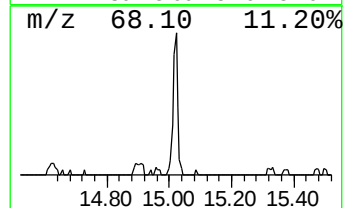
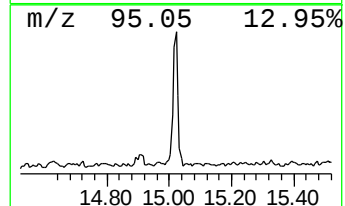
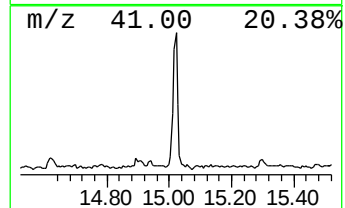
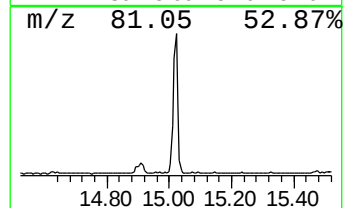
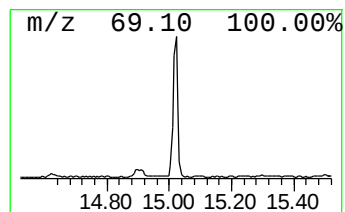
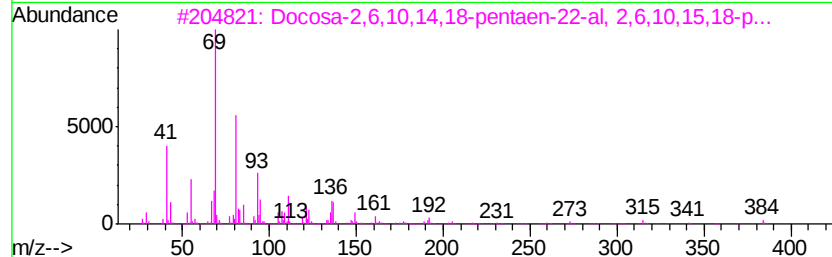
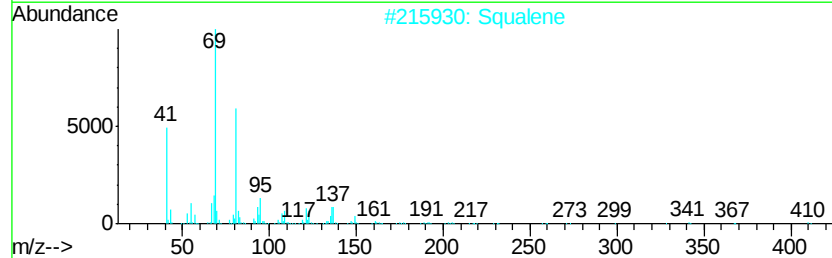
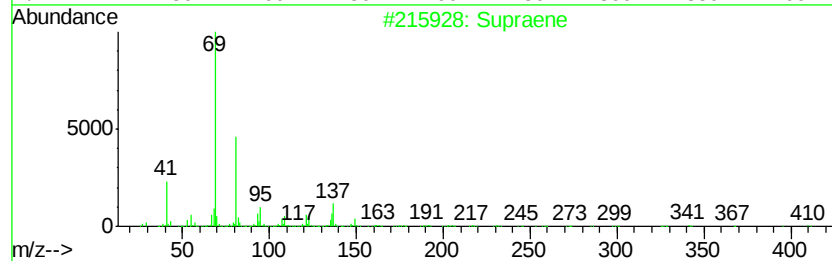
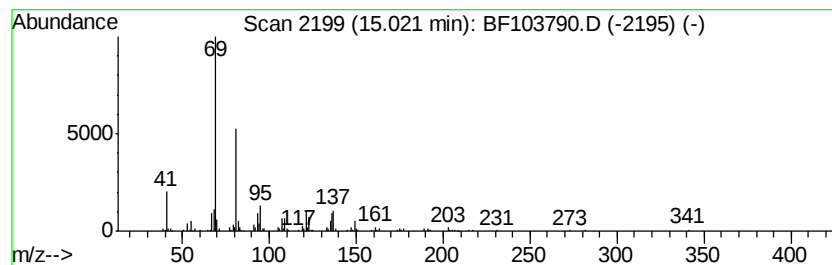
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	7.65 ng	281532	Perylene-d12	15.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	91
2	Squalene		410	C30H50	000111-02-4	91
3	Docosa-2,6,10,14,18-pentaen-22-a...		384	C27H44O	1000163-04-7	83
4	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	64
5	2,6-Octadiene, 4-methyl-		124	C9H16	074498-94-5	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103790.D
Acq On : 20 Mar 2018 7:43
Operator : JU/SJ
Sample : J1954-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
031518-JETT-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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
Butane, 2-methoxy...	2.29	11.1	ng	436595	1	6.97	790359	20.0
Ethanol, 2-butoxy-	5.92	3.1	ng	121244	1	6.97	790359	20.0
unknown6.74	6.74	55.8	ng	2203570	1	6.97	790359	20.0
Octadecane	10.43	2.1	ng	118659	3	10.01	1117180	20.0
Octacosane	10.90	2.7	ng	135160	4	11.50	1016730	20.0
1-Heneicosanol	13.97	10.4	ng	434621	5	14.16	835400	20.0
Supraene	15.02	7.7	ng	281532	6	15.70	736010	20.0