

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040318\
 Data File : BF104204.D
 Acq On : 4 Apr 2018 2:20
 Operator : JU/SJ
 Sample : J2182-07
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 6-WM-DIP-3-WW@3.5

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-BF032818.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	2.299	30	36	42	rVB	124759	175445	5.17%	0.638%
2	5.210	527	531	545	rBV	79837	133619	3.94%	0.486%
3	5.592	592	596	630	rBV	2026516	2821661	83.22%	10.261%
4	6.598	762	767	786	rBV	1913536	2929910	86.42%	10.655%
5	6.734	786	790	822	rVV	2478825	3215167	94.83%	11.692%
6	6.957	825	828	845	rBV	326950	531889	15.69%	1.934%
7	7.110	851	854	881	rVB	1984807	2369286	69.88%	8.616%
8	7.528	921	925	944	rBV	1142999	1844930	54.42%	6.709%
9	7.669	947	949	958	rVB	30089	45749	1.35%	0.166%
10	8.239	1042	1046	1070	rBV	601914	819001	24.16%	2.978%
11	9.310	1224	1228	1245	rBV	2936188	3390432	100.00%	12.329%
12	9.704	1289	1295	1301	rBV	219678	246240	7.26%	0.895%
13	9.904	1324	1329	1333	rBV	70067	56977	1.68%	0.207%
14	9.998	1341	1345	1361	rBV	879344	948142	27.97%	3.448%
15	10.404	1411	1414	1417	rVB	91522	67635	1.99%	0.246%
16	10.792	1476	1480	1492	rBV	1658255	2089113	61.62%	7.597%
17	10.874	1492	1494	1505	rVB	93532	138771	4.09%	0.505%
18	11.327	1567	1571	1573	rBV	41417	33959	1.00%	0.123%
19	11.492	1596	1599	1615	rBV	715509	927495	27.36%	3.373%
20	13.080	1864	1869	1893	rBV	2715686	3059024	90.23%	11.124%
21	13.951	2014	2017	2024	rBV	90160	103715	3.06%	0.377%
22	14.145	2046	2050	2060	rBV	495287	689438	20.33%	2.507%
23	14.886	2172	2176	2185	rBV	239009	289291	8.53%	1.052%
24	15.686	2307	2312	2329	rVB	308113	571741	16.86%	2.079%

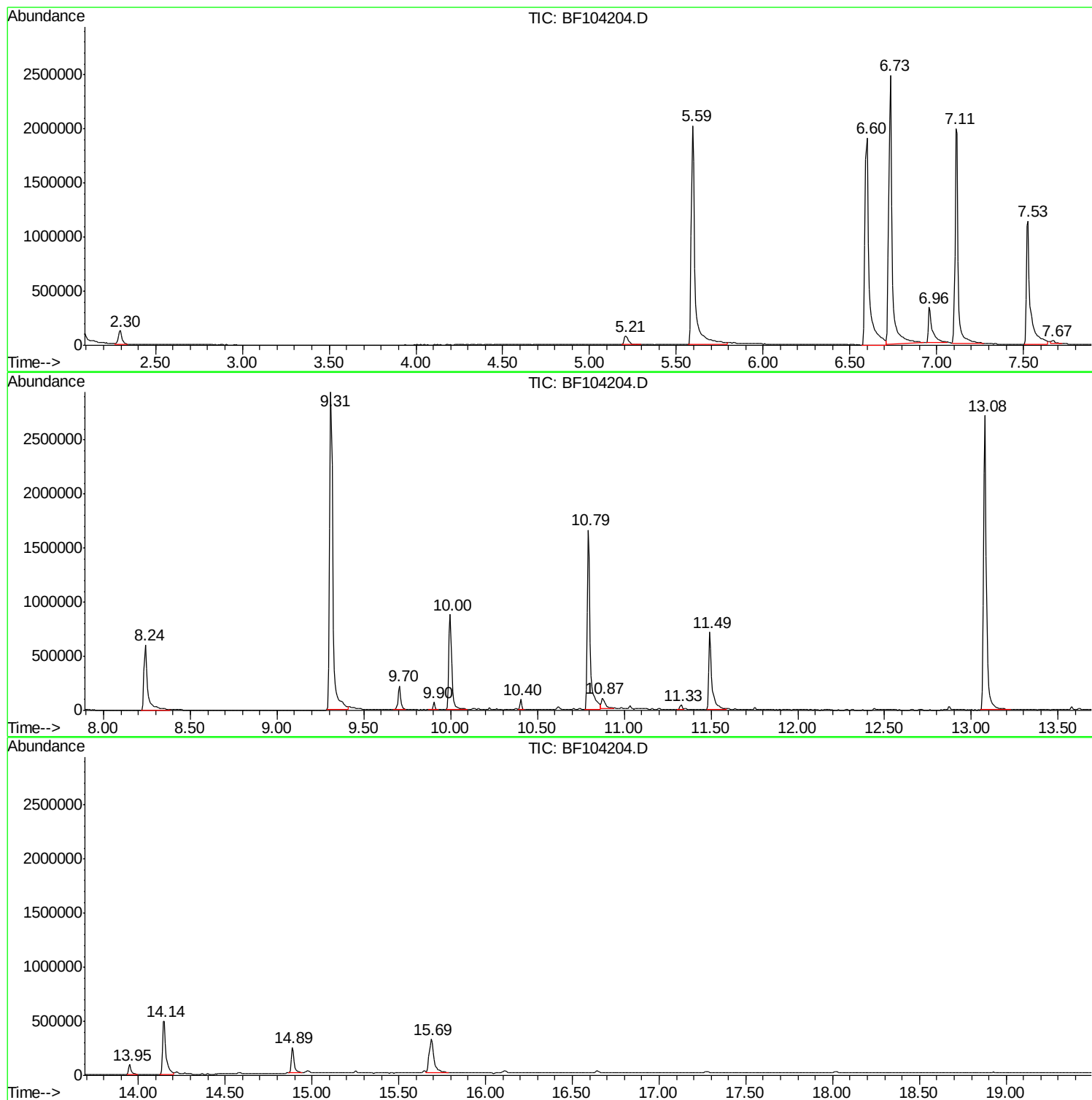
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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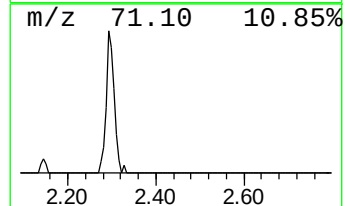
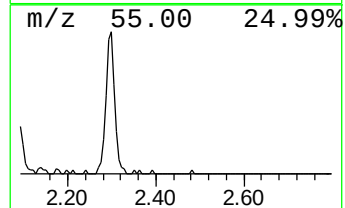
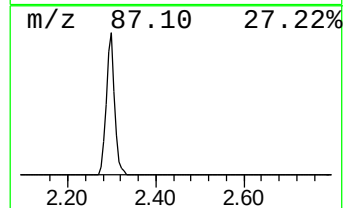
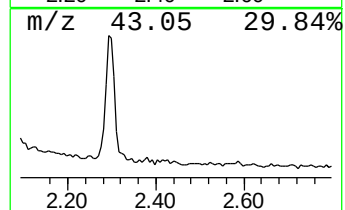
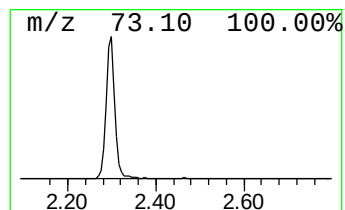
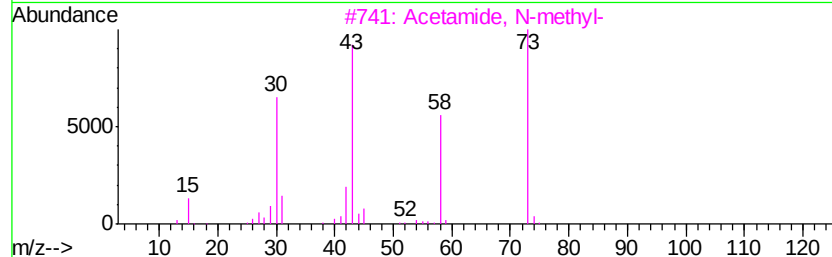
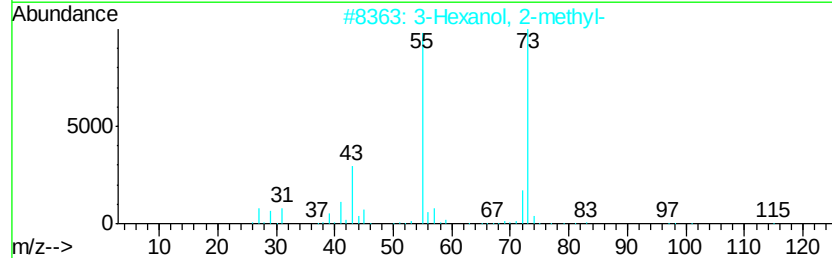
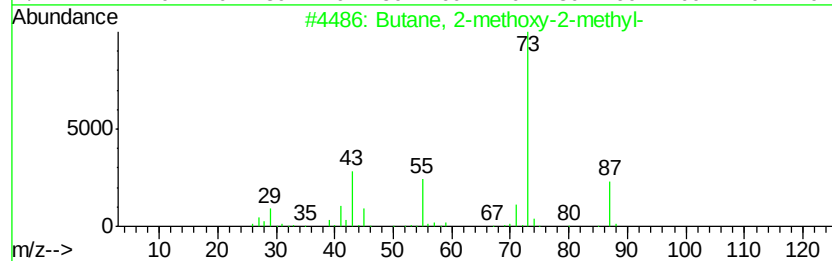
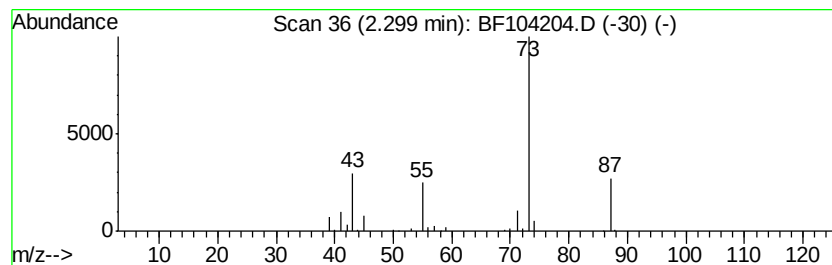
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	6.60 ng	175445	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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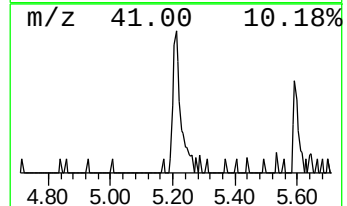
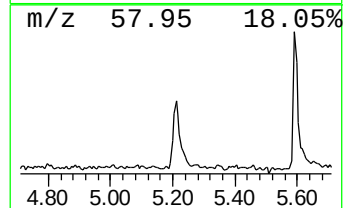
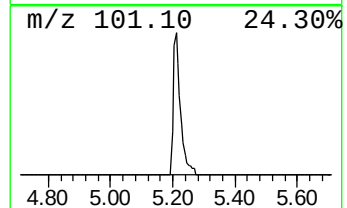
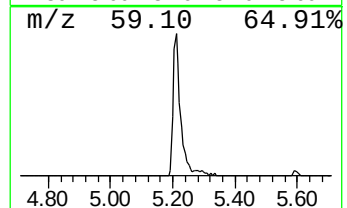
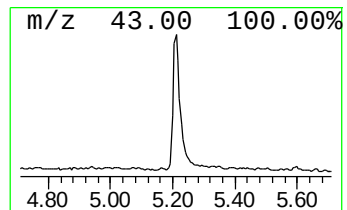
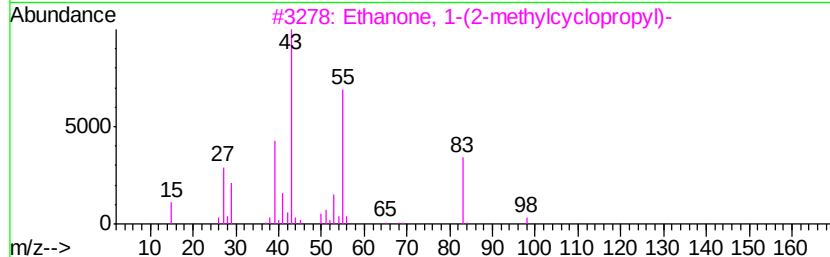
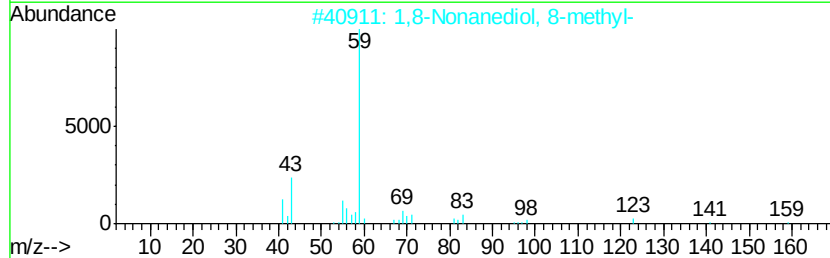
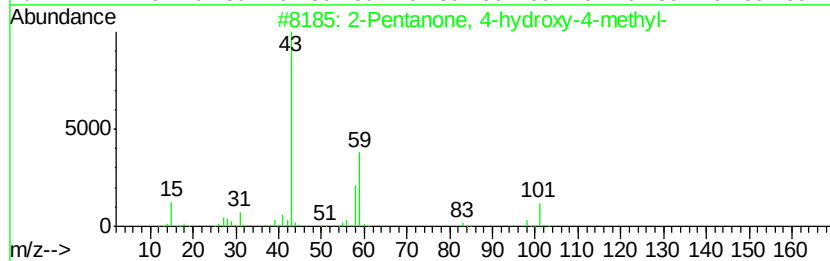
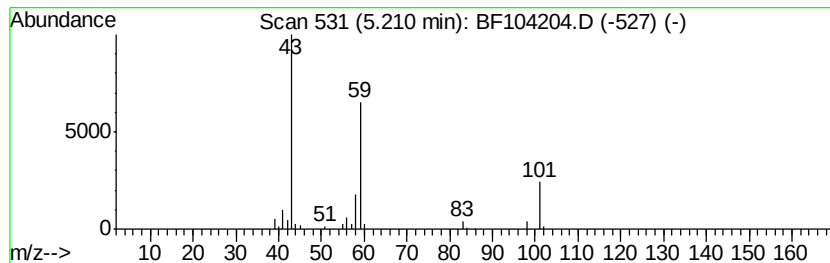
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	5.02 ng	133619	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
3		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4		Guanidine	59	CH5N3	000113-00-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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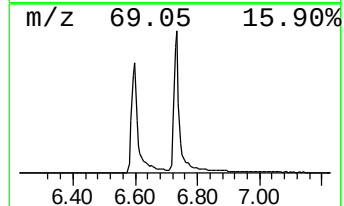
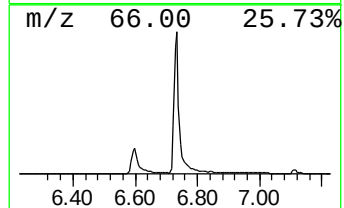
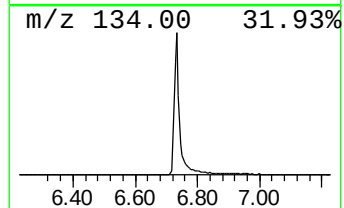
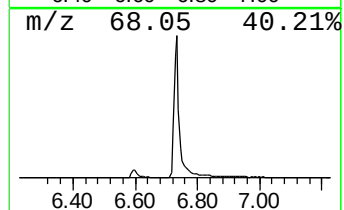
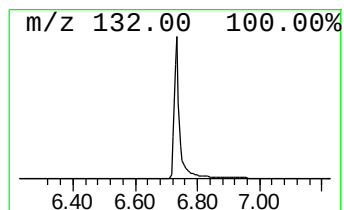
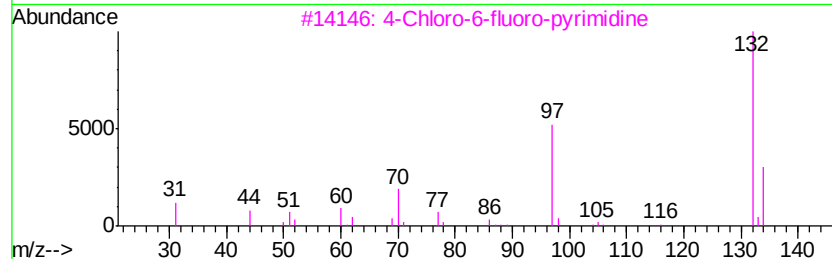
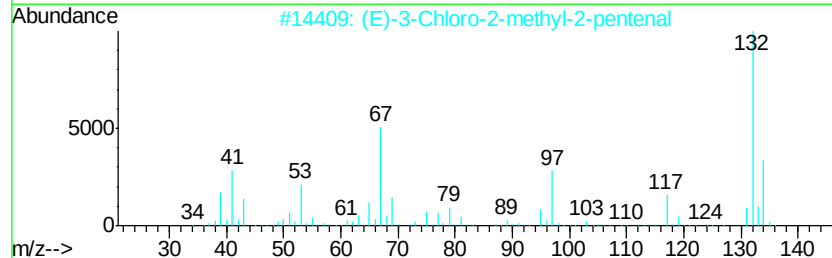
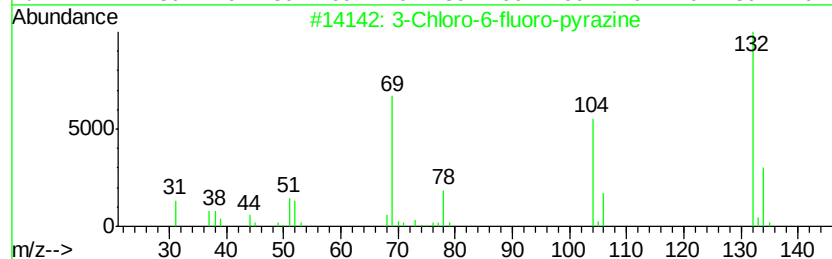
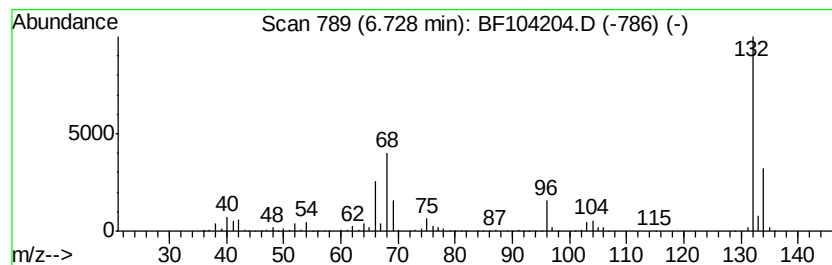
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Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	120.90 ng	3215170	1,4-Dichlorobenzene-d4	6.96

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	17
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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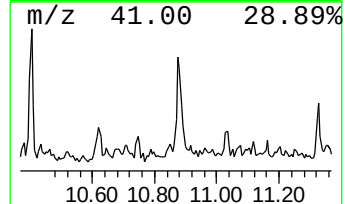
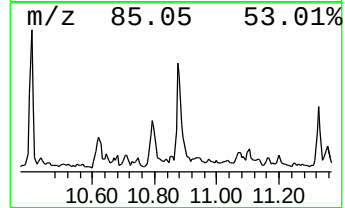
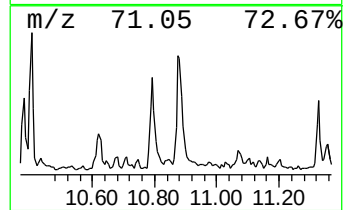
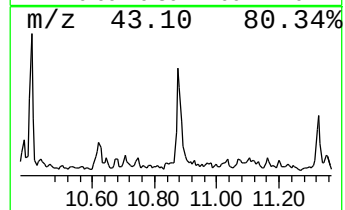
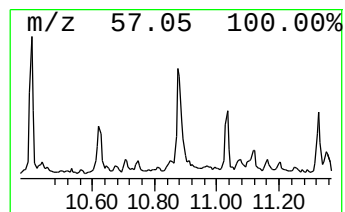
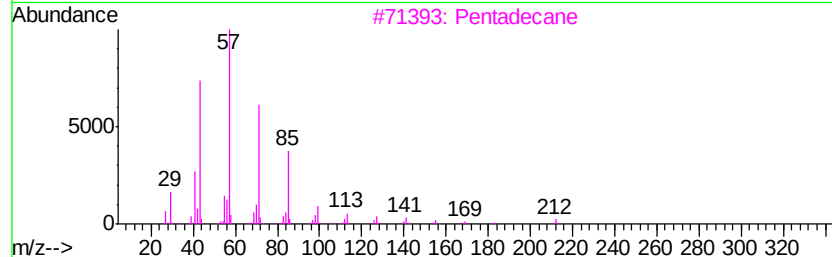
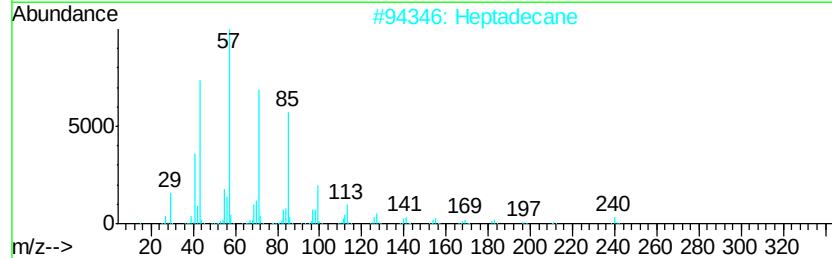
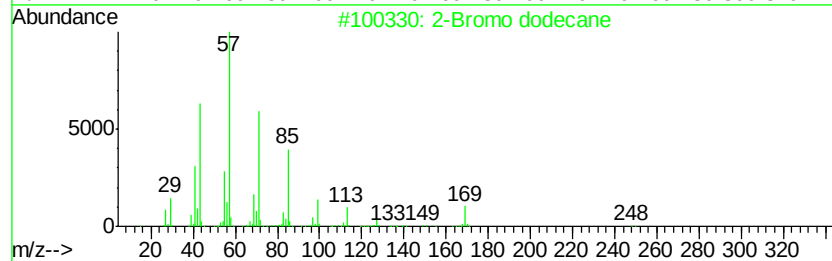
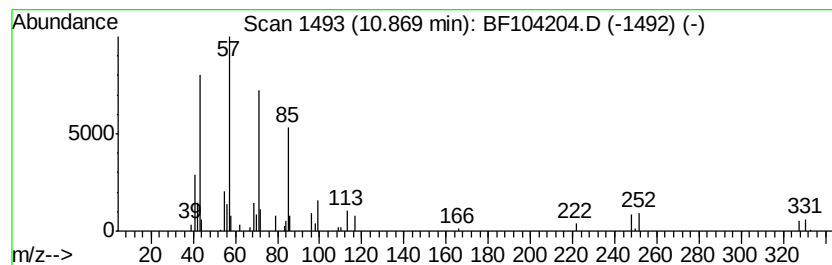
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Peak Number 5 2-Bromo dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	2.99 ng	138771	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane		248	C12H25Br	013187-99-0	90
2	Heptadecane		240	C17H36	000629-78-7	90
3	Pentadecane		212	C15H32	000629-62-9	86
4	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	83
5	Tetradecane		198	C14H30	000629-59-4	78



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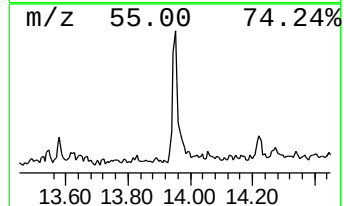
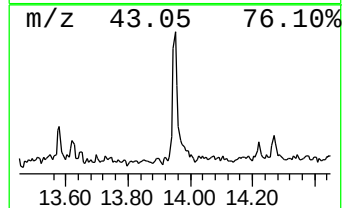
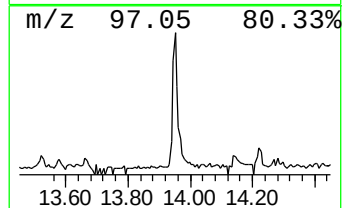
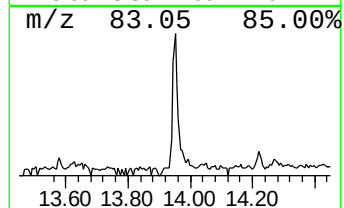
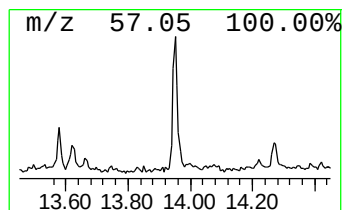
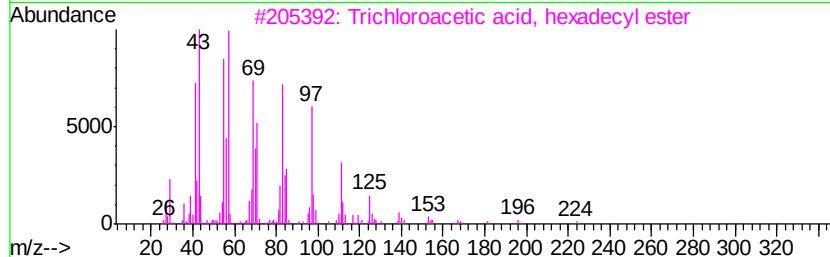
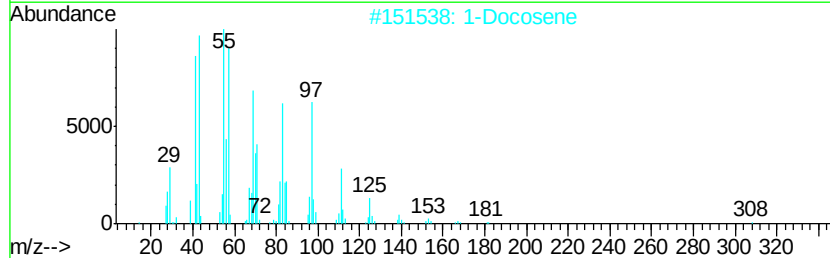
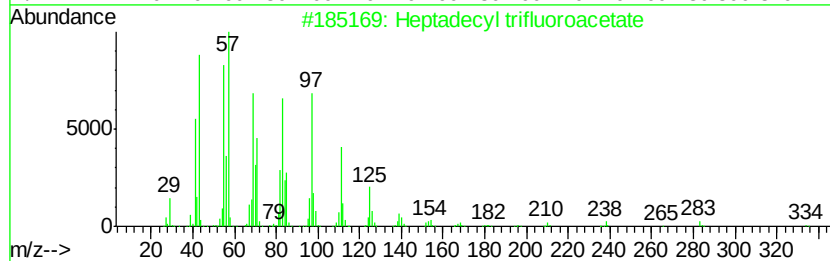
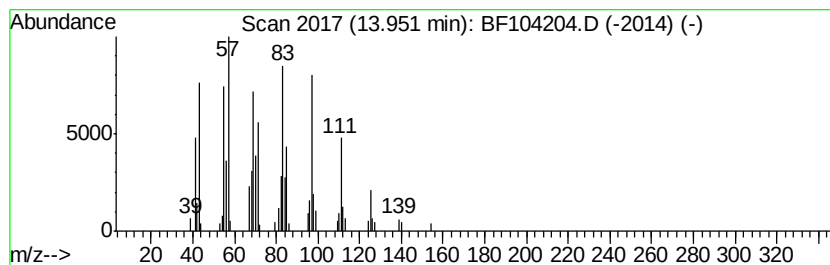
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.01 ng	103715	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
2		1-Docosene	308	C22H44	001599-67-3	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4		1-Nonadecene	266	C19H38	018435-45-5	90
5		1-Octadecanol	270	C18H38O	000112-92-5	87



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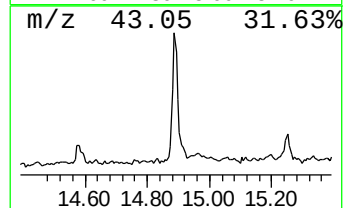
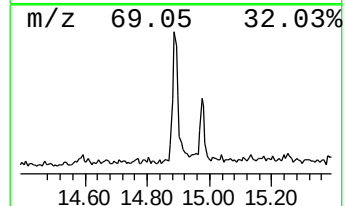
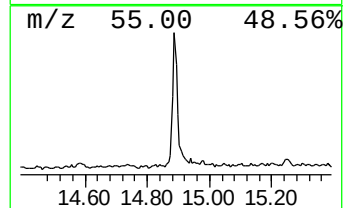
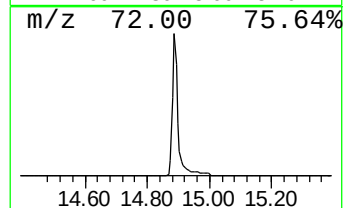
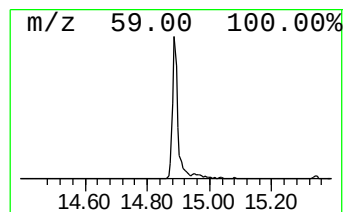
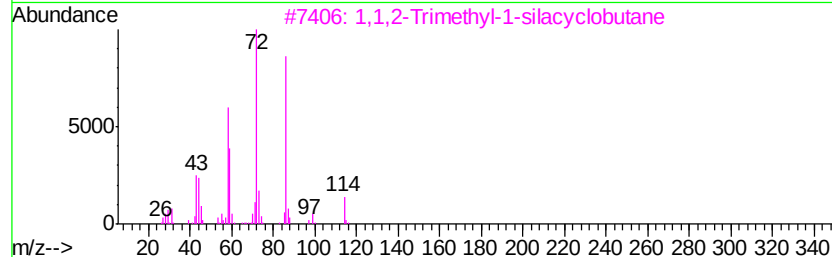
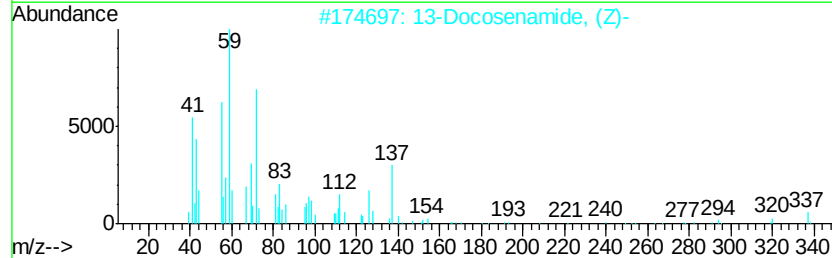
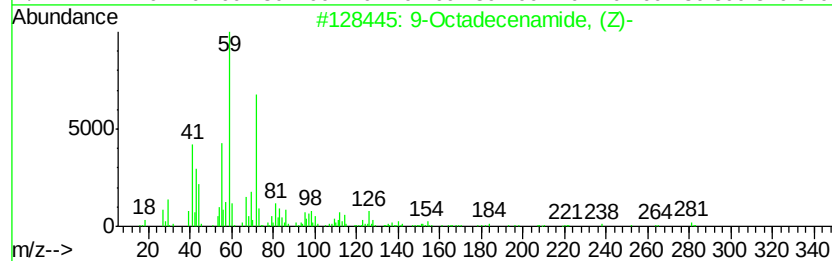
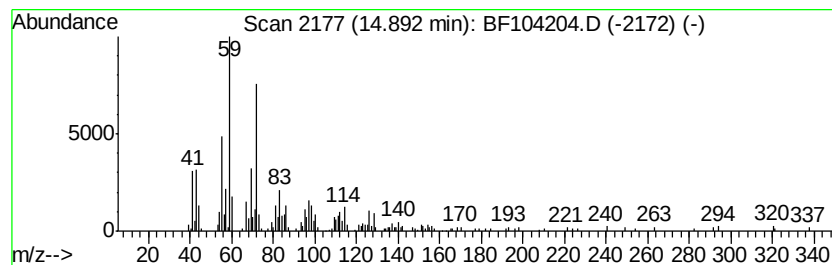
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	8.39 ng	289291	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	50
3		1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	43
4		Dodecanamide	199	C12H25NO	001120-16-7	43
5		Octadecanamide	283	C18H37NO	000124-26-5	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040318\
Data File : BF104204.D
Acq On : 4 Apr 2018 2:20
Operator : JU/SJ
Sample : J2182-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
6-WM-DIP-3-WW@3.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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...	2.30	6.6	ng	175445	1	6.96	531889	20.0
2-Pentanone, 4-hy...	5.21	5.0	ng	133619	1	6.96	531889	20.0
unknown6.73	6.73	120.9	ng	3215170	1	6.96	531889	20.0
2-Bromo dodecane	10.87	3.0	ng	138771	4	11.49	927495	20.0
Heptadecyl triflu...	13.95	3.0	ng	103715	5	14.15	689438	20.0
9-Octadecenamide,...	14.89	8.4	ng	289291	5	14.15	689438	20.0