

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
 Data File : BF104368.D
 Acq On : 9 Apr 2018 13:31
 Operator : JU/SJ
 Sample : J2184-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3-2(9-11)

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-BF040618.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	5.016	493	498	506	rVB	188885	248374	7.76%	0.881%
2	5.416	560	566	569	rBV	3006736	3057510	95.49%	10.851%
3	6.434	733	739	742	rBV	2849390	3029160	94.61%	10.750%
4	6.575	758	763	766	rVB	3080769	3120570	97.46%	11.075%
5	6.804	798	802	805	rBV	1017673	792444	24.75%	2.812%
6	6.963	824	829	832	rVB	2681473	2383986	74.46%	8.461%
7	7.369	893	898	901	rBV	2048551	1910921	59.68%	6.782%
8	8.086	1016	1020	1023	rBV	1344482	1052418	32.87%	3.735%
9	9.163	1198	1203	1206	rBV	3505045	3201823	100.00%	11.363%
10	9.557	1266	1270	1273	rBV	338503	274310	8.57%	0.974%
11	9.775	1304	1307	1310	rVB	70567	59328	1.85%	0.211%
12	9.839	1314	1318	1322	rVB	1259095	1110778	34.69%	3.942%
13	10.145	1365	1370	1385	rBV2	62818	229138	7.16%	0.813%
14	10.274	1389	1392	1395	rVB	84362	70927	2.22%	0.252%
15	10.633	1447	1453	1456	rBV	1841408	1912290	59.73%	6.787%
16	10.745	1469	1472	1480	rVB	77128	76734	2.40%	0.272%
17	11.192	1541	1548	1551	rBV2	43465	44835	1.40%	0.159%
18	11.327	1567	1571	1574	rBV	1155876	946561	29.56%	3.359%
19	11.857	1658	1661	1665	rBV	228337	196124	6.13%	0.696%
20	12.433	1753	1759	1761	rBV2	28325	41793	1.31%	0.148%
21	12.915	1837	1841	1845	rBV	2293930	2202311	68.78%	7.816%
22	13.810	1990	1993	1997	rBV	378343	336902	10.52%	1.196%
23	13.968	2015	2020	2023	rBV	829087	753814	23.54%	2.675%
24	14.586	2121	2125	2128	rBV2	31277	59610	1.86%	0.212%
25	14.757	2152	2154	2163	rVB7	33117	73944	2.31%	0.262%
26	15.433	2263	2269	2273	rBV	674182	848571	26.50%	3.012%
27	15.898	2344	2348	2352	rBV2	33692	49316	1.54%	0.175%
28	15.945	2352	2356	2363	rVV3	56351	92931	2.90%	0.330%

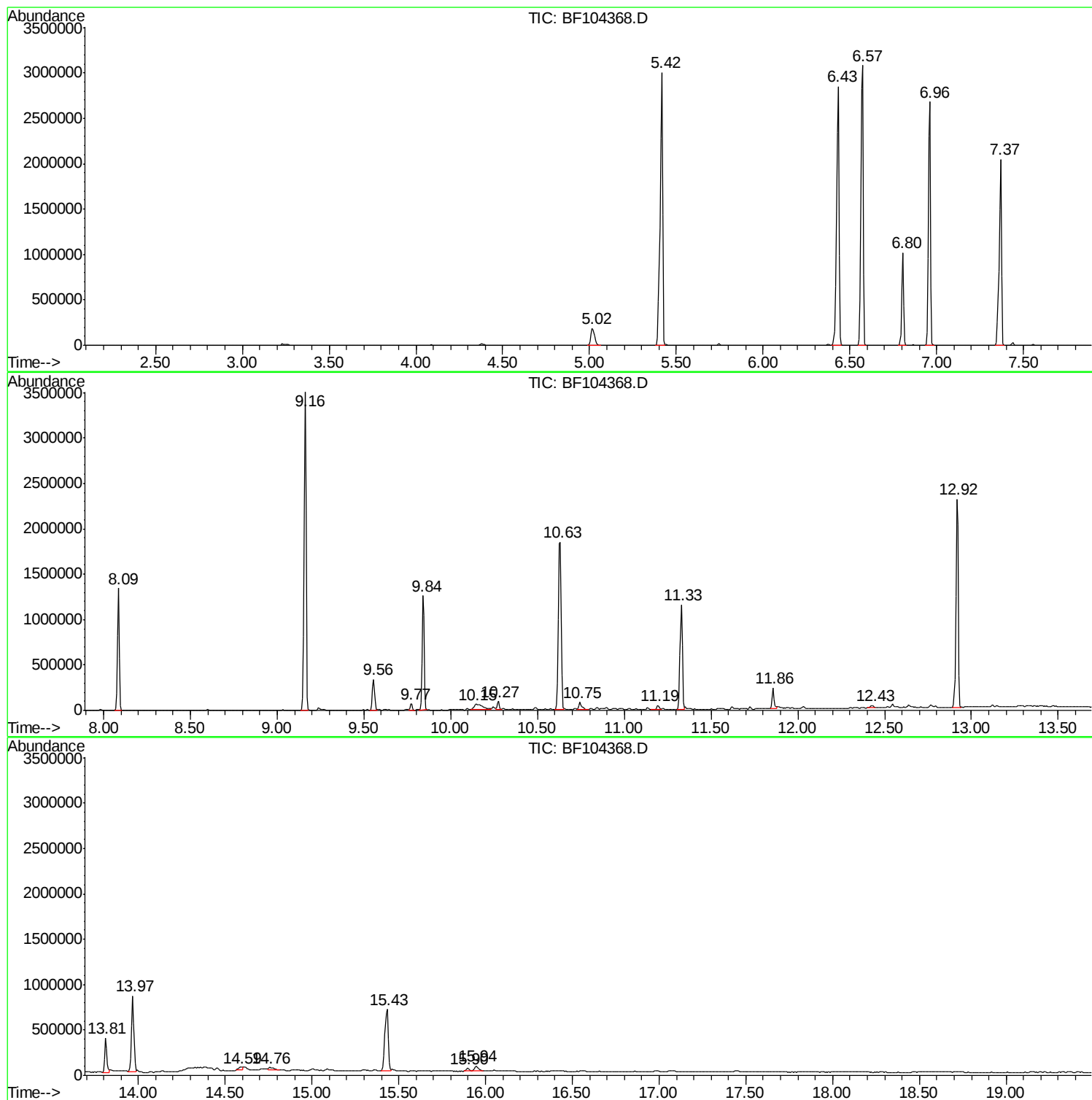
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3-2(9-11)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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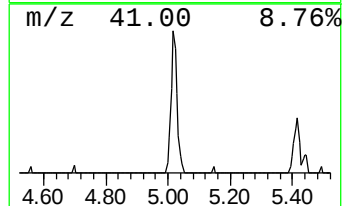
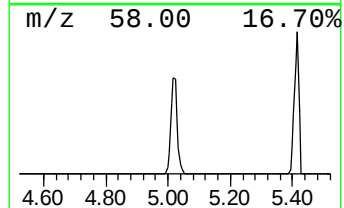
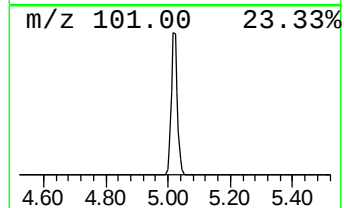
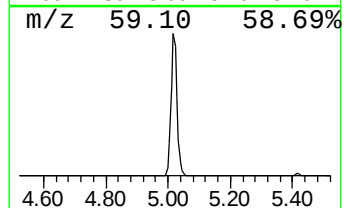
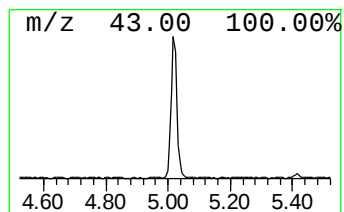
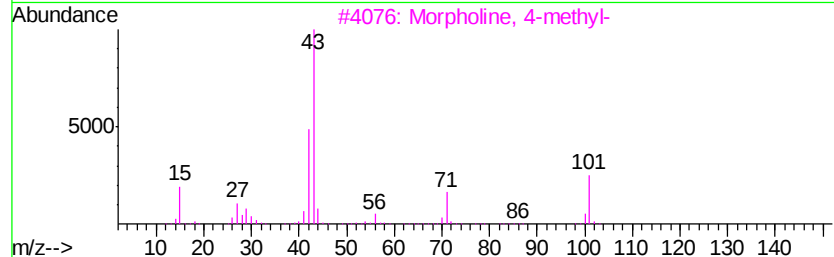
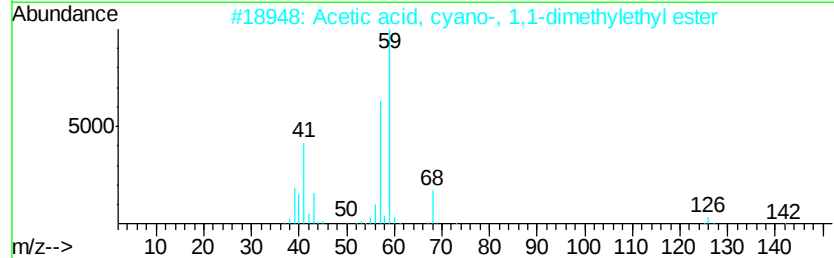
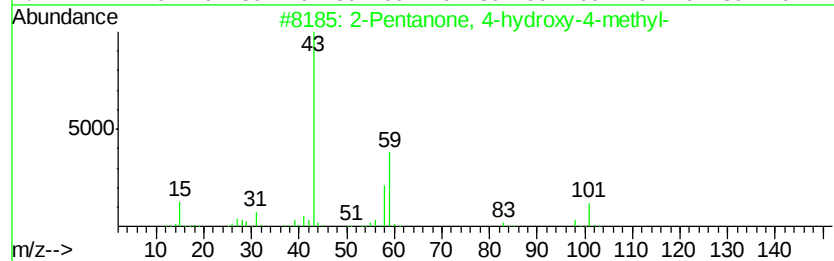
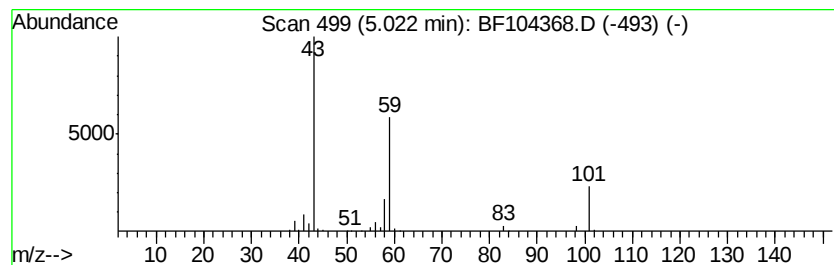
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	6.27 ng	248374	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9



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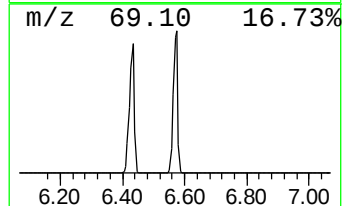
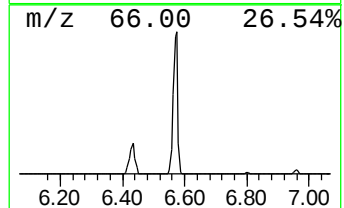
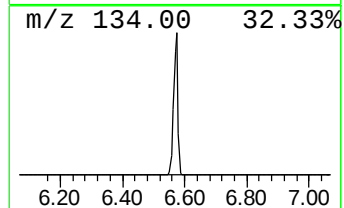
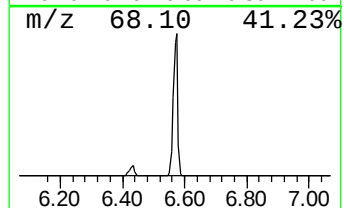
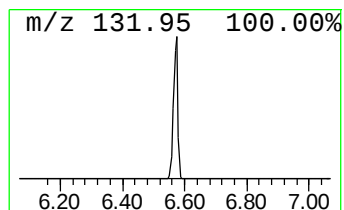
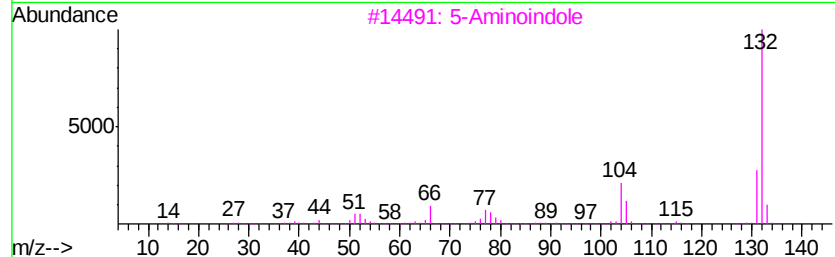
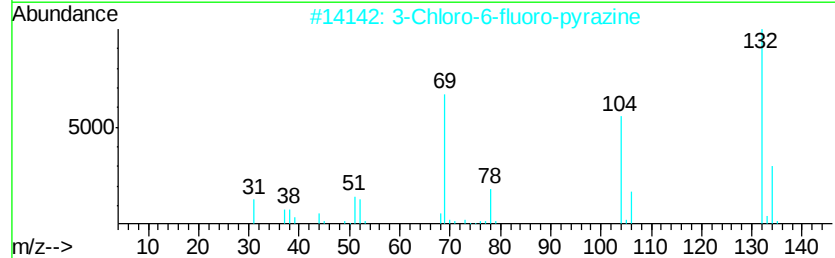
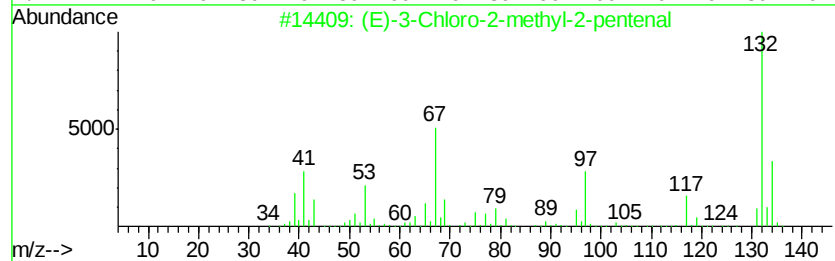
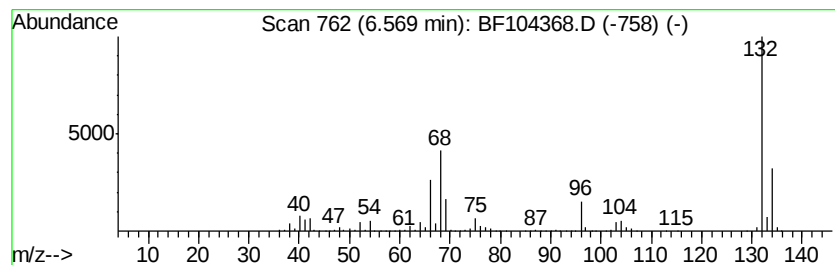
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	78.76 ng	3120570	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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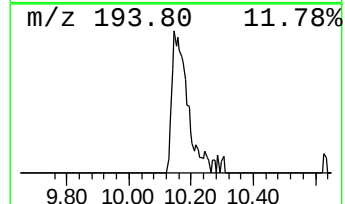
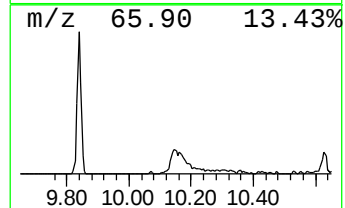
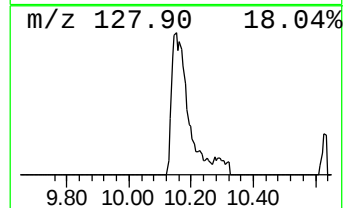
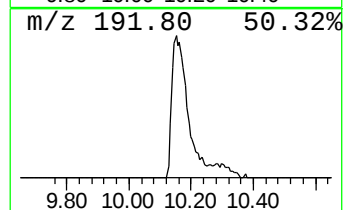
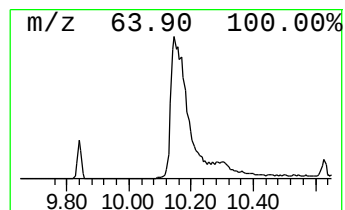
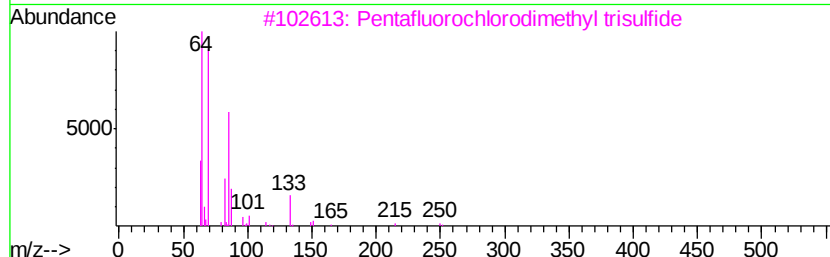
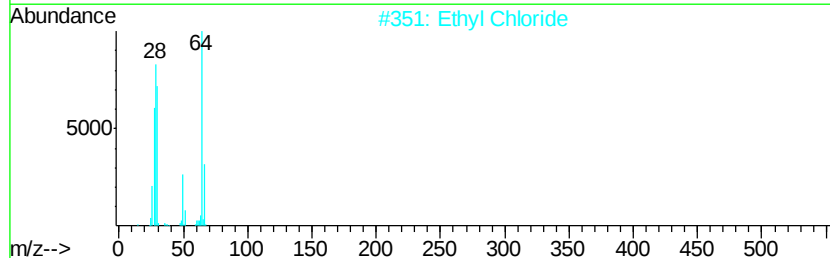
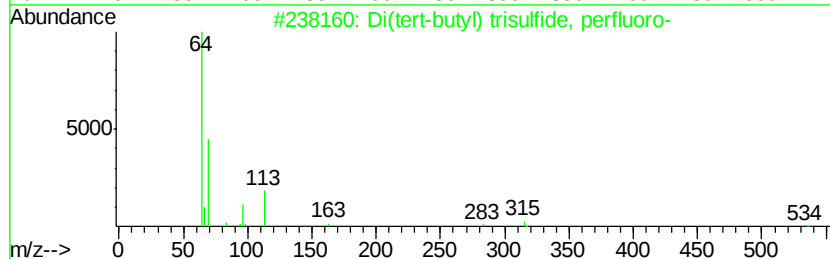
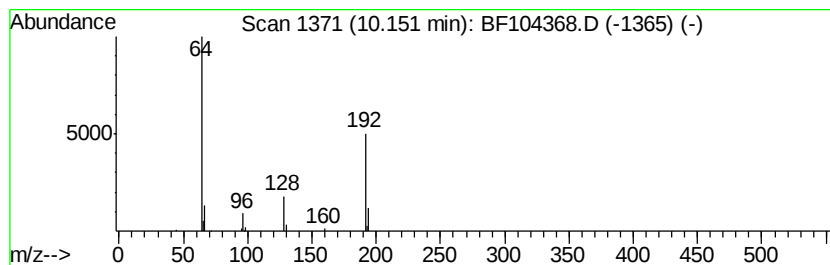
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Peak Number 4 unknown10.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.15	4.13 ng	229138	Acenaphthene-d10	9.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	4
3	Pentafluorochlorodimethyl trisul...	250	C2ClF5S3	1000226-65-9	4
4	Sulfur dioxide	64	O2S	007446-09-5	3
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3



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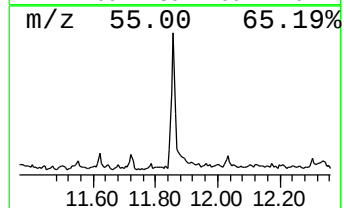
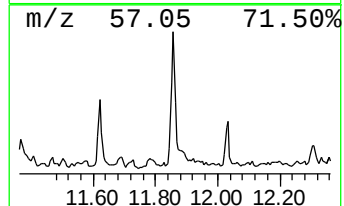
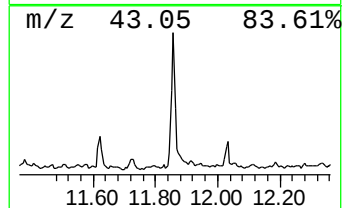
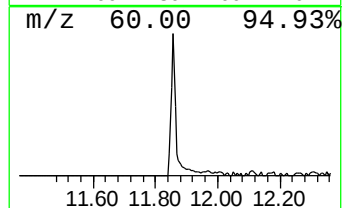
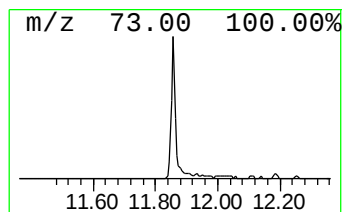
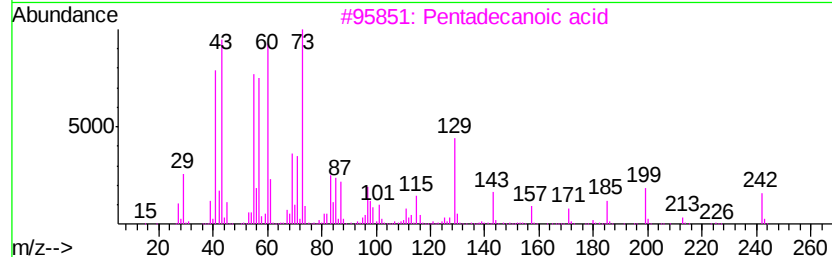
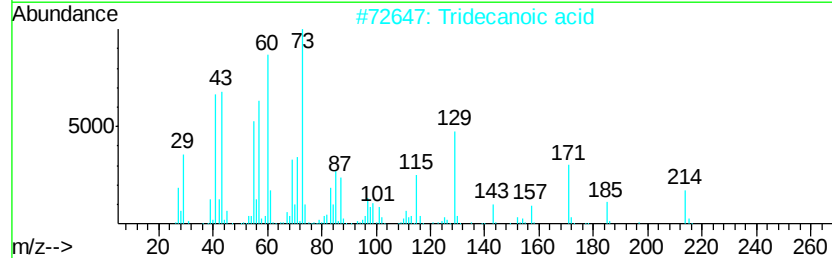
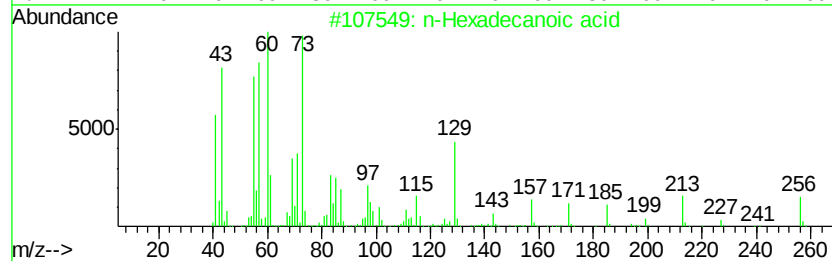
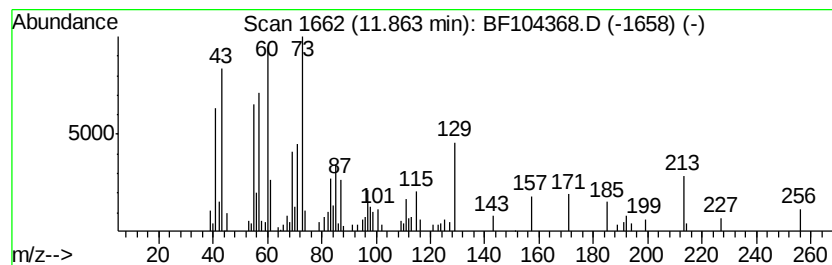
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	4.14 ng	196124	Phenanthrene-d10	11.33	
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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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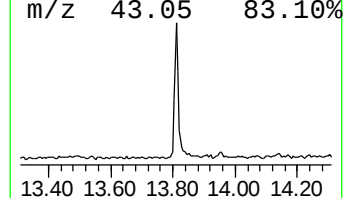
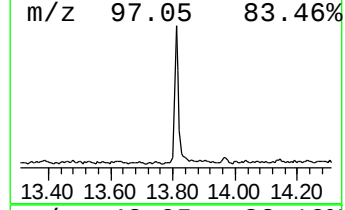
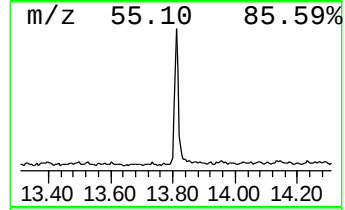
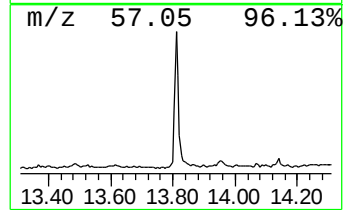
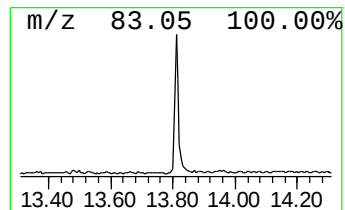
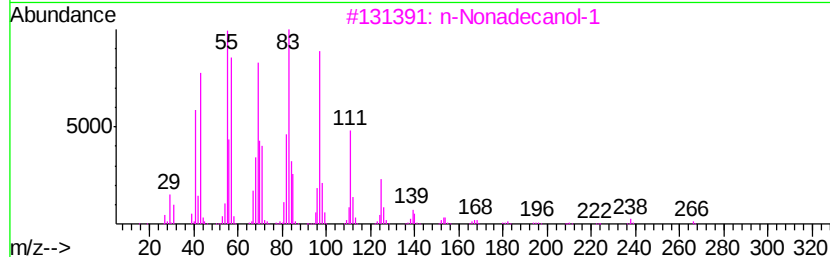
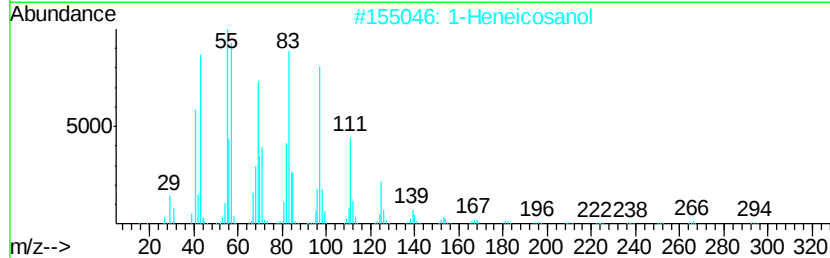
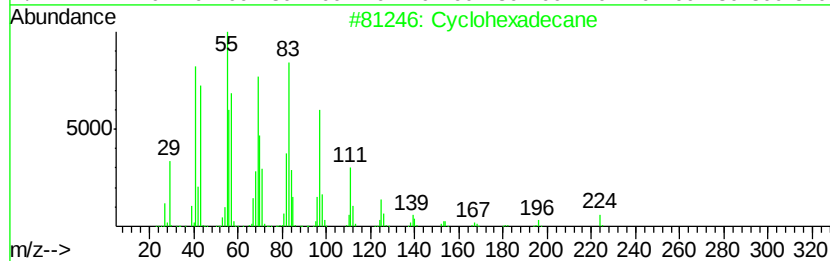
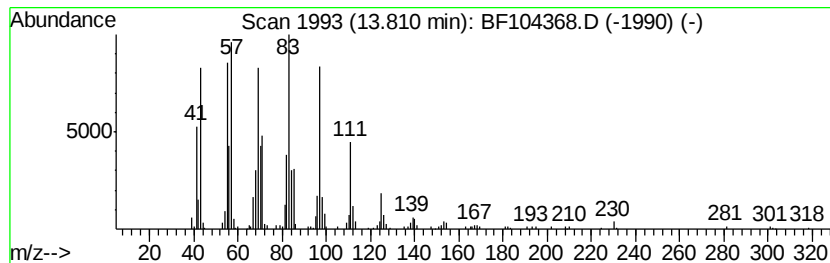
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Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	8.94 ng	336902	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93



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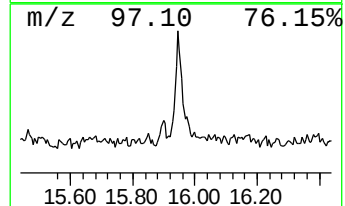
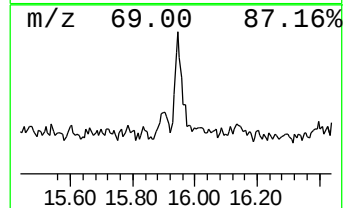
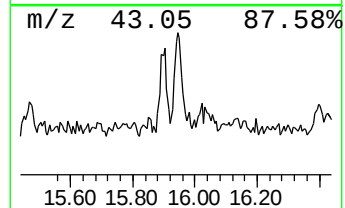
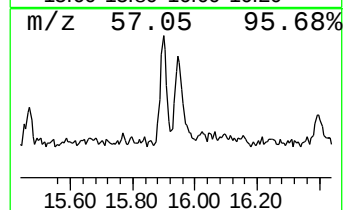
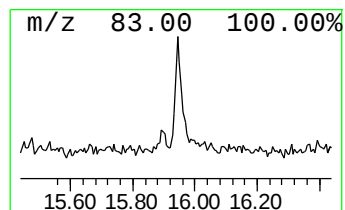
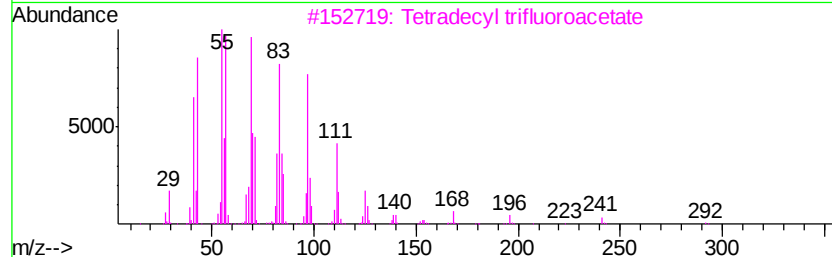
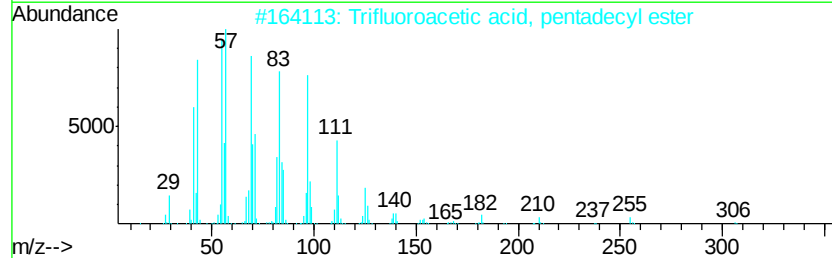
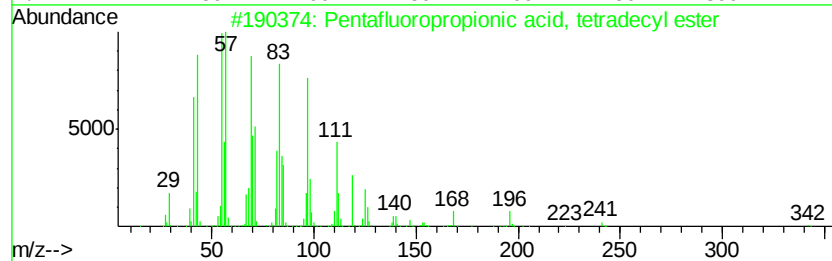
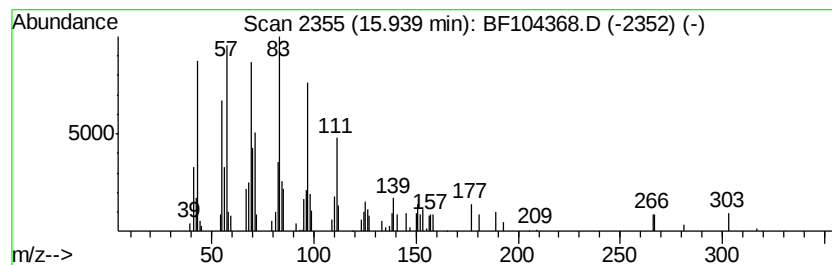
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.19 ng	92931	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	87
4		Isoheptadecanol	256	C17H36O	057289-07-3	83
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104368.D
Acq On : 9 Apr 2018 13:31
Operator : JU/SJ
Sample : J2184-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3-2(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	6.3	ng	248374	1	6.80	792444	20.0
unknown6.57	6.57	78.8	ng	3120570	1	6.80	792444	20.0
unknown10.15	10.15	4.1	ng	229138	3	9.84	1110780	20.0
n-Hexadecanoic acid	11.86	4.1	ng	196124	4	11.33	946561	20.0
Cyclohexadecane	13.81	8.9	ng	336902	5	13.97	753814	20.0
Pentafluoropropio...	15.94	2.2	ng	92931	6	15.43	848571	20.0