

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
 Data File : BF104345.D
 Acq On : 7 Apr 2018 8:58
 Operator : JU/SJ
 Sample : J2225-20
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040218-JETT-F-U-B

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-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	4.998	492	495	502	rVB	181632	193001	4.66%	0.784%
2	5.404	560	564	567	rBV	1442664	1263518	30.51%	5.130%
3	6.416	732	736	746	rVB	906500	815572	19.69%	3.311%
4	6.569	757	762	765	rBV	2494655	2249158	54.30%	9.132%
5	6.622	768	771	776	rBV	120898	101716	2.46%	0.413%
6	6.804	798	802	805	rBV	915374	775997	18.74%	3.151%
7	6.963	824	829	832	rVB	2990566	2863116	69.13%	11.625%
8	7.369	892	898	901	rBV	2398078	2450838	59.17%	9.951%
9	8.086	1016	1020	1023	rVB	1294231	1034913	24.99%	4.202%
10	9.163	1198	1203	1206	rBV	4008701	4141808	100.00%	16.816%
11	9.551	1266	1269	1273	rBV	87831	84738	2.05%	0.344%
12	9.769	1303	1306	1309	rBV	81744	67610	1.63%	0.275%
13	9.839	1313	1318	1322	rVB	1325392	1123401	27.12%	4.561%
14	10.275	1389	1392	1394	rVB	99535	85162	2.06%	0.346%
15	10.628	1447	1452	1455	rBV	1784601	1566911	37.83%	6.362%
16	10.745	1469	1472	1482	rVB	94580	90367	2.18%	0.367%
17	11.327	1567	1571	1574	rBV	1103468	873641	21.09%	3.547%
18	11.851	1657	1660	1669	rBV2	60828	74520	1.80%	0.303%
19	12.739	1808	1811	1814	rBV	111875	82369	1.99%	0.334%
20	12.921	1837	1842	1845	rBV	3168509	3049699	73.63%	12.382%
21	13.445	1928	1931	1934	rBV	64318	50390	1.22%	0.205%
22	13.810	1990	1993	2001	rBV	179248	185901	4.49%	0.755%
23	13.968	2016	2020	2024	rVB	875955	732365	17.68%	2.973%
24	15.427	2263	2268	2272	rBV	550148	673074	16.25%	2.733%

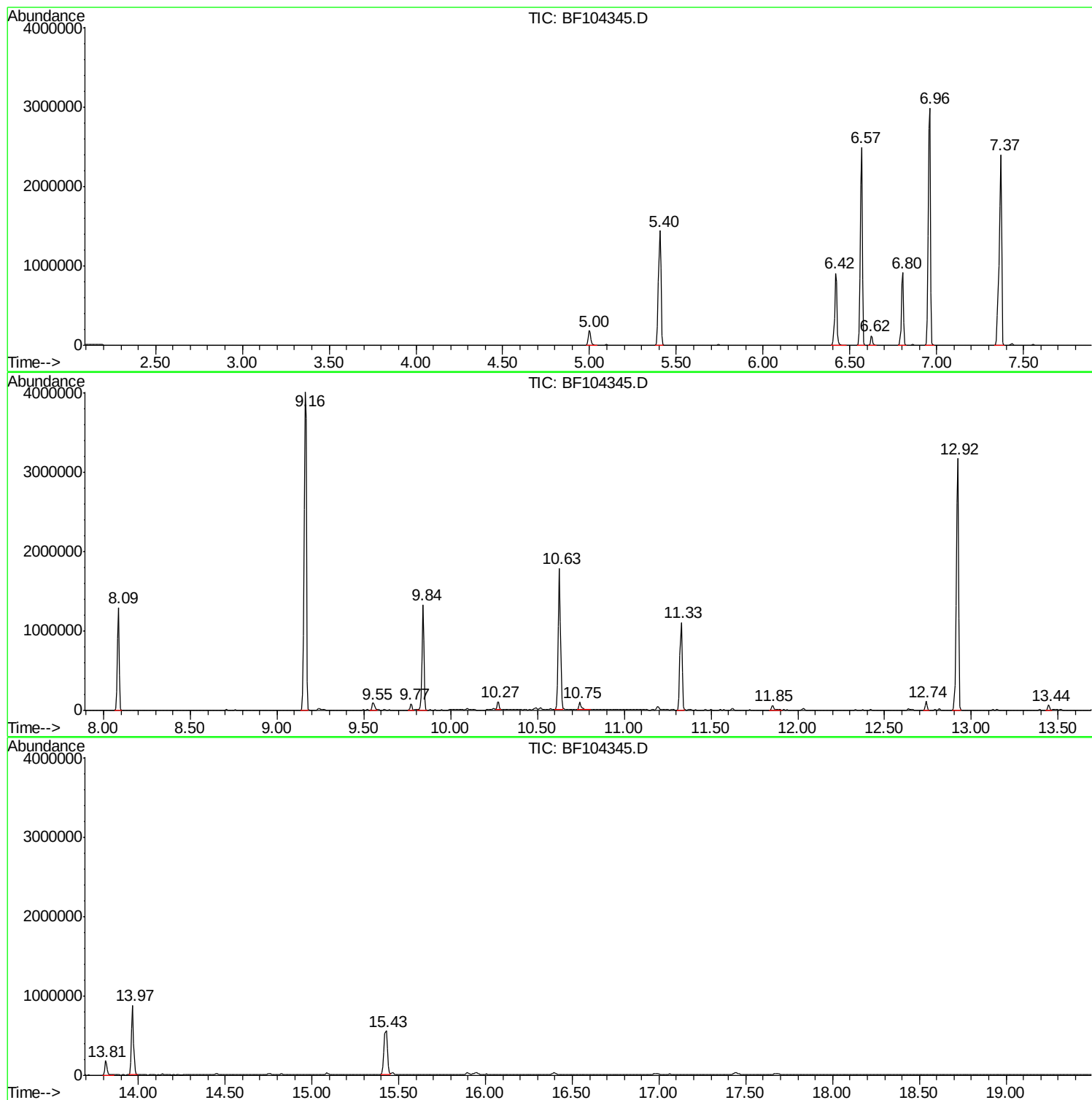
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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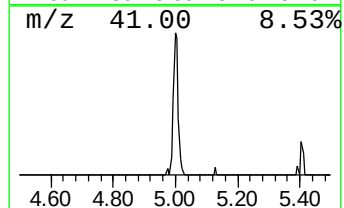
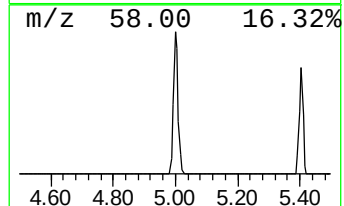
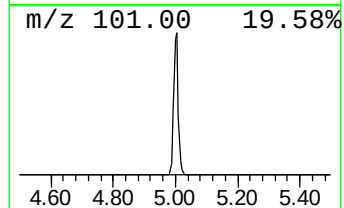
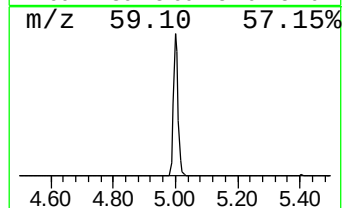
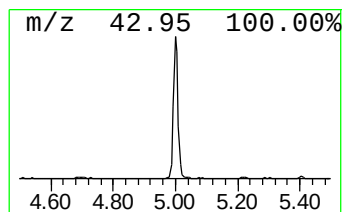
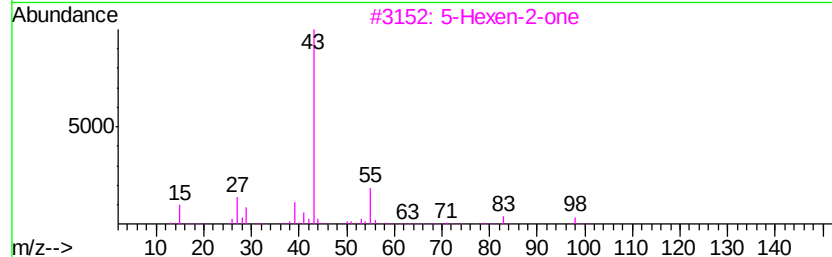
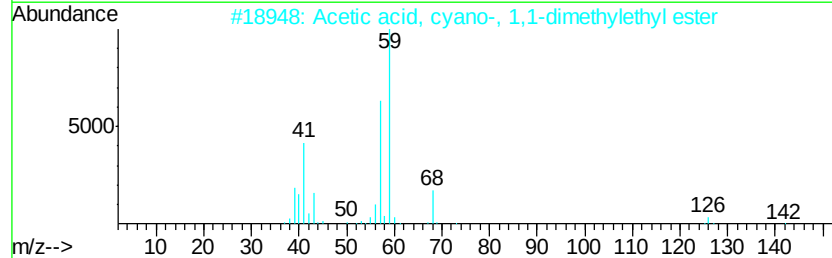
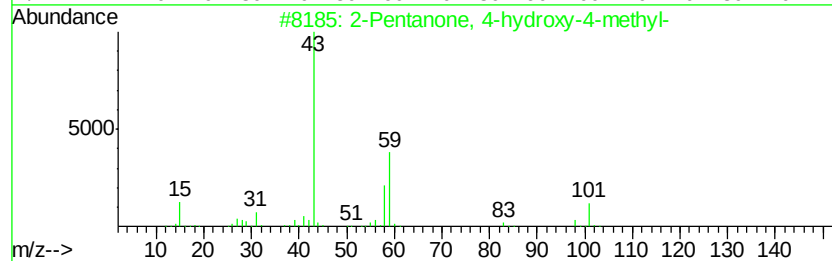
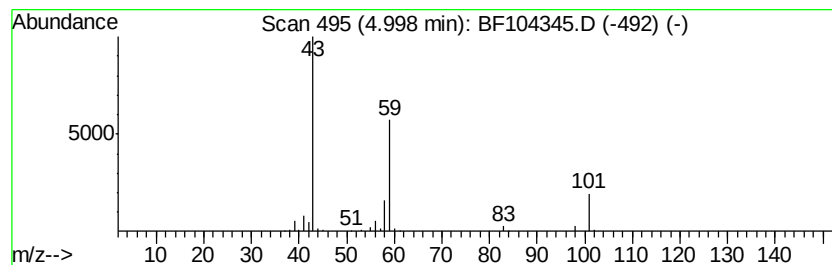
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.97 ng	193001	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	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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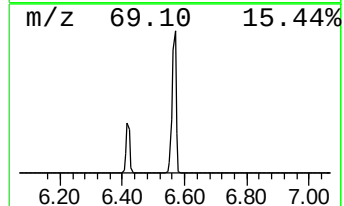
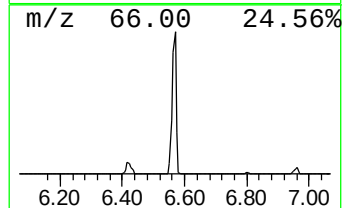
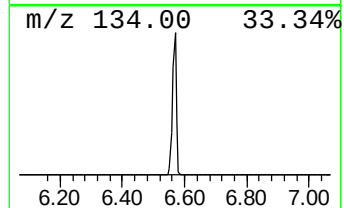
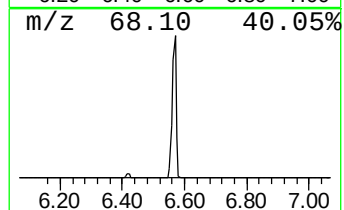
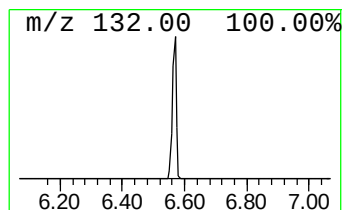
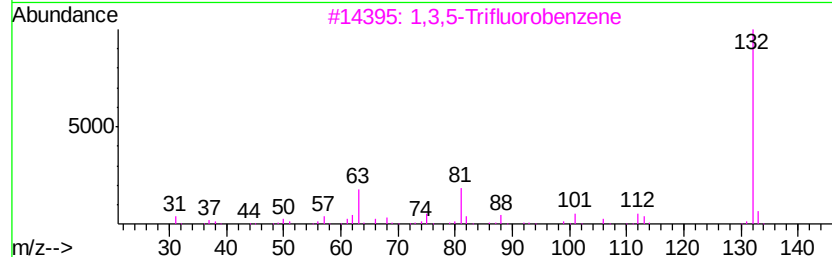
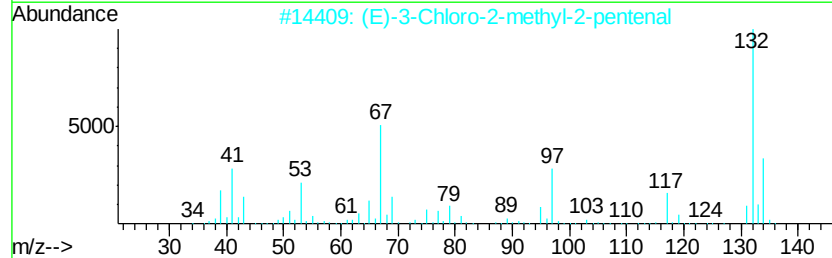
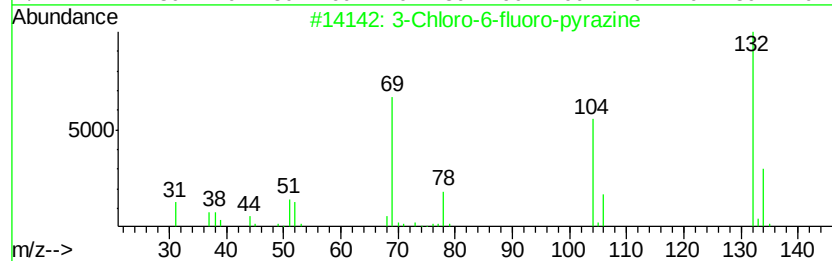
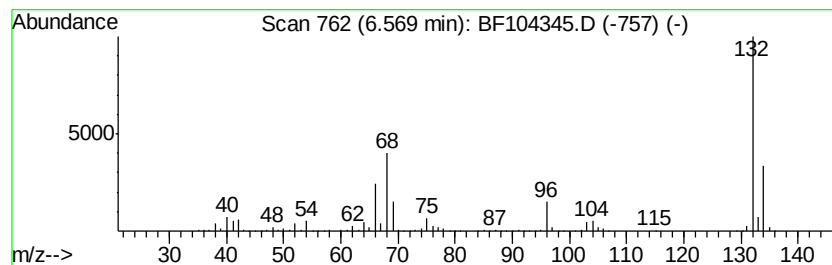
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	57.97 ng	2249160	1,4-Dichlorobenzene-d4	6.80

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	16
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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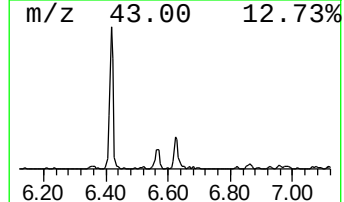
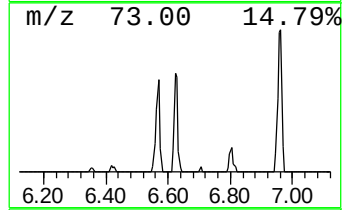
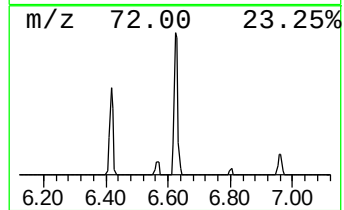
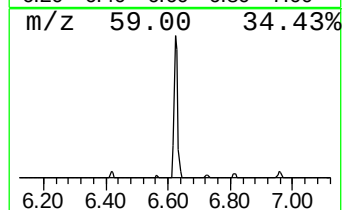
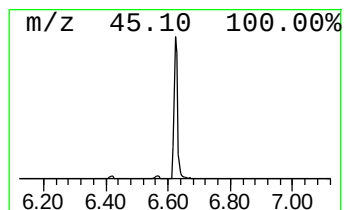
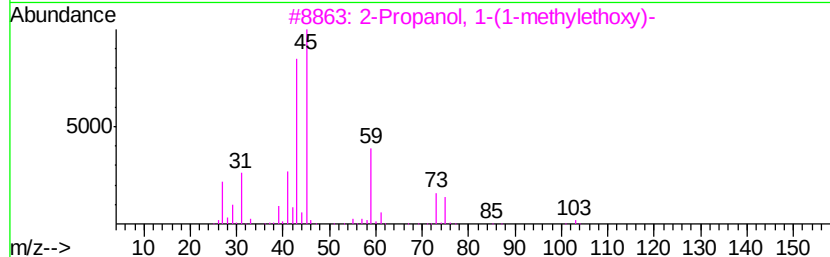
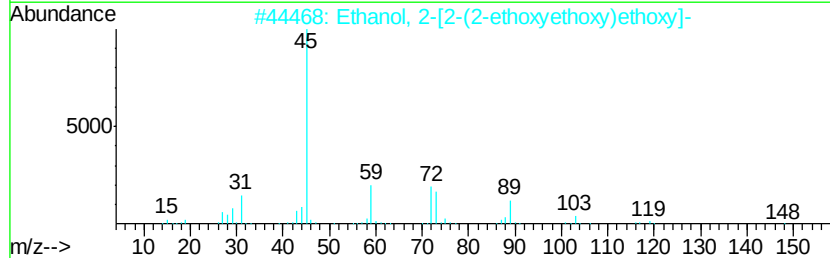
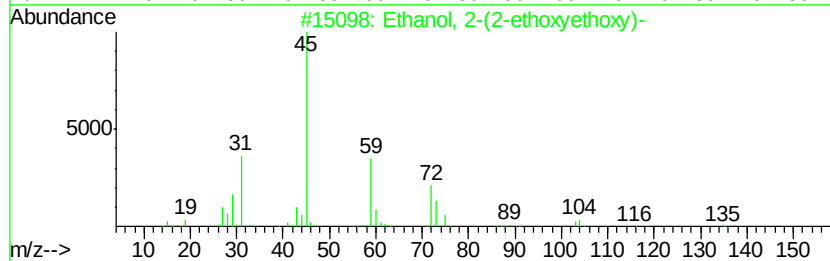
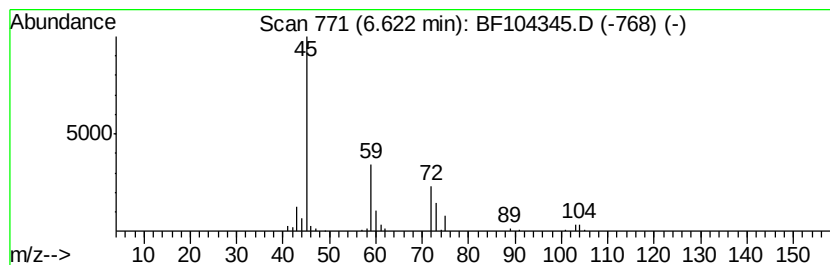
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Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	2.62 ng	101716	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2		Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	40
3		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
4		.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	36
5		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	33



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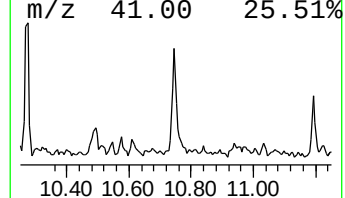
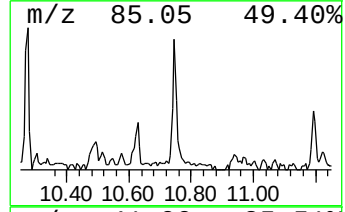
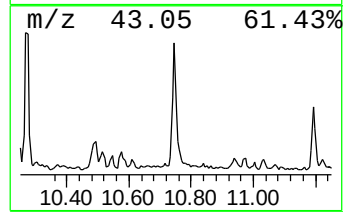
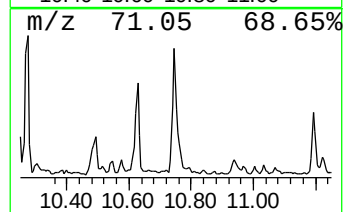
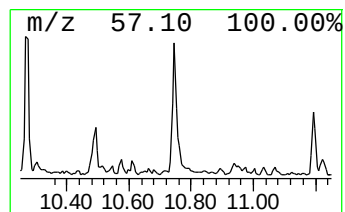
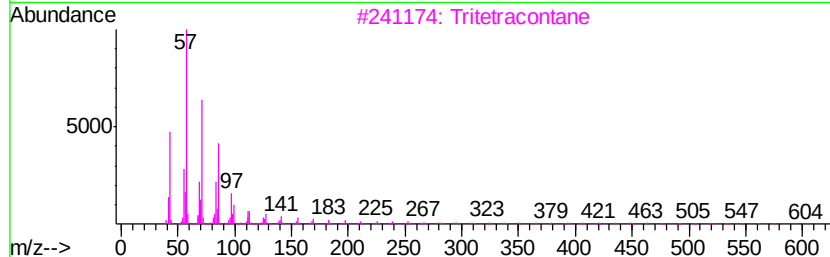
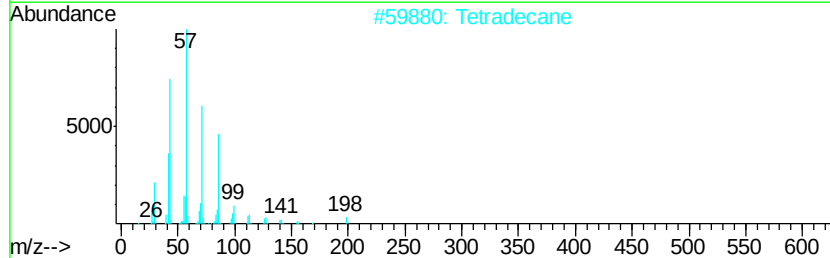
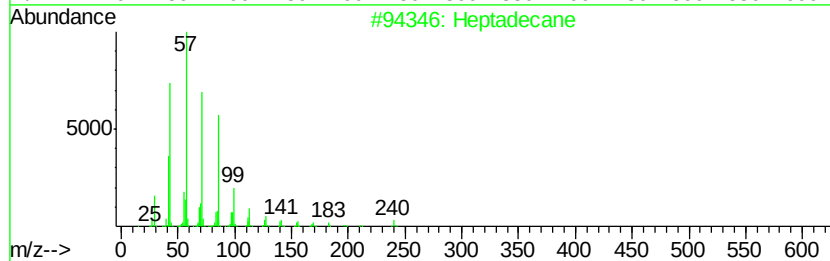
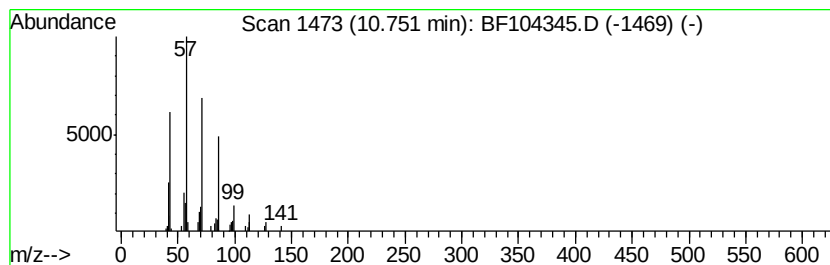
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Peak Number 5 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.07 ng	90367	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Tetradecane		198	C14H30	000629-59-4	91
3	Tritetracontane		605	C43H88	007098-21-7	90
4	Hexadecane		226	C16H34	000544-76-3	90
5	Octacosane		394	C28H58	000630-02-4	86



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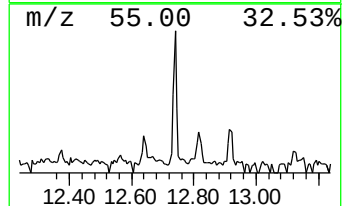
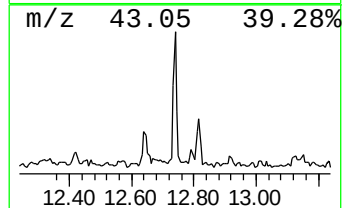
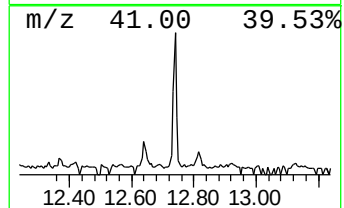
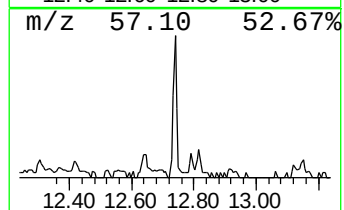
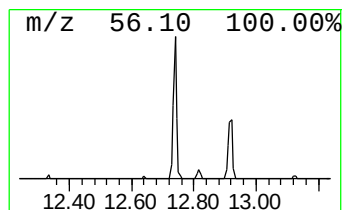
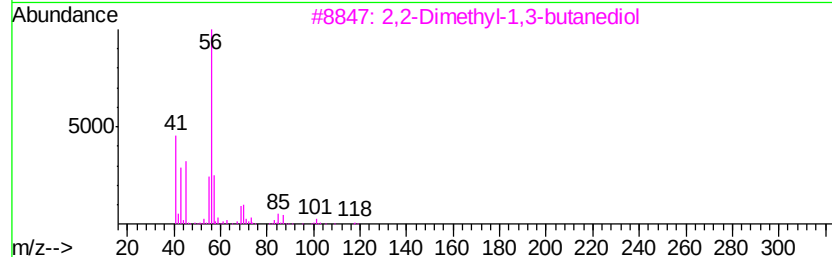
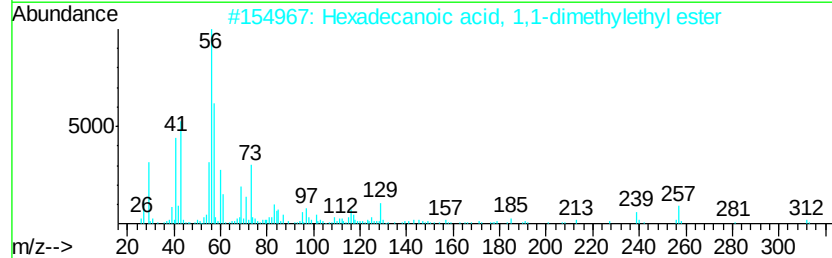
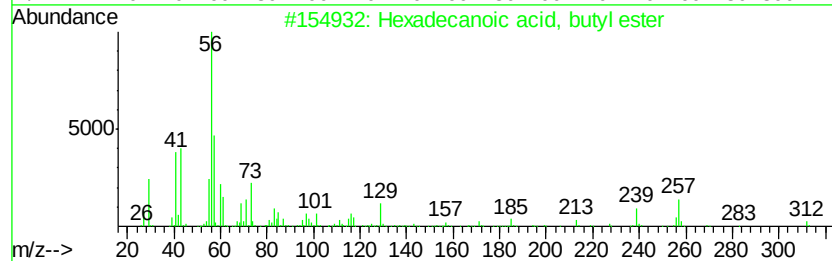
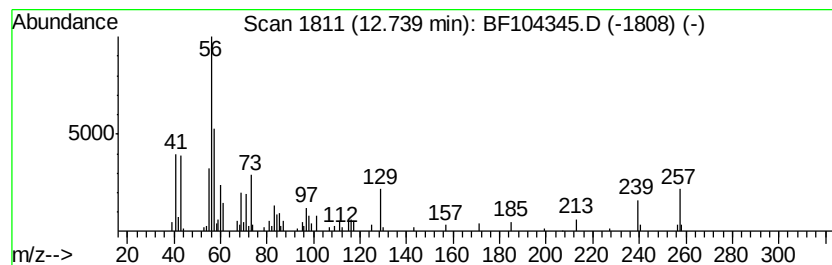
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.25 ng	82369	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	35
4		2-Methyl-1-tetradecene	210	C15H30	052254-38-3	35
5		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35



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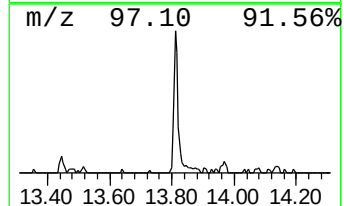
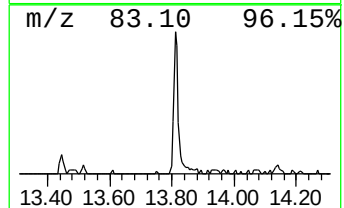
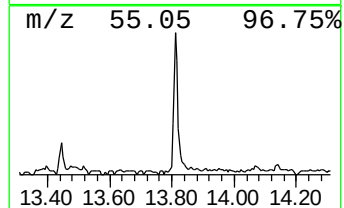
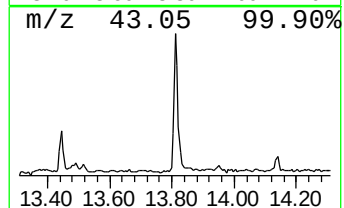
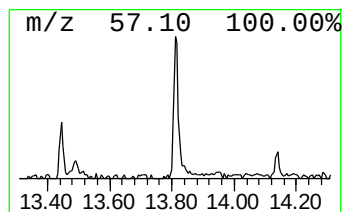
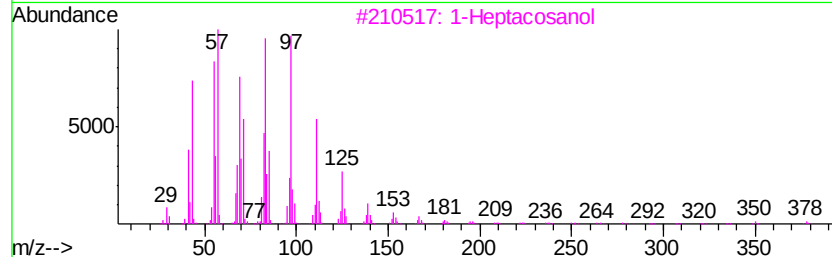
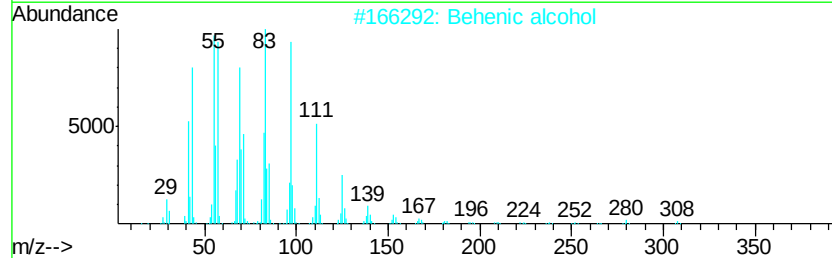
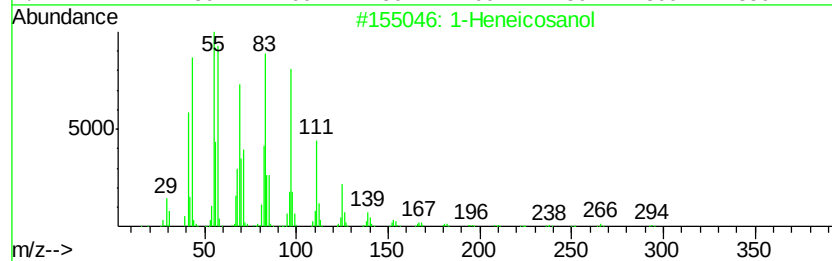
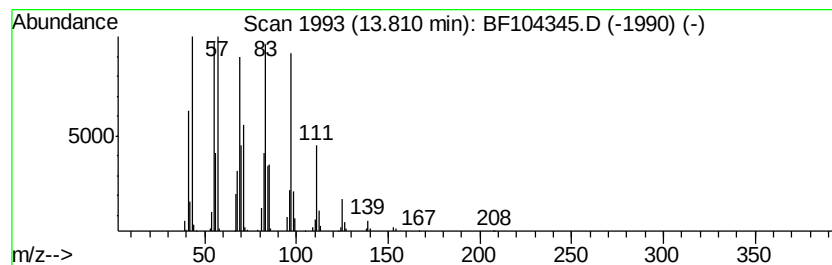
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	5.08 ng	185901	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
Data File : BF104345.D
Acq On : 7 Apr 2018 8:58
Operator : JU/SJ
Sample : J2225-20
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040218-JETT-F-U-B

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...	5.00	5.0	ng	193001	1	6.80	775997	20.0
unknown6.57	6.57	58.0	ng	2249160	1	6.80	775997	20.0
Ethanol, 2-(2-eth...	6.62	2.6	ng	101716	1	6.80	775997	20.0
Heptadecane	10.75	2.1	ng	90367	4	11.33	873641	20.0
Hexadecanoic acid...	12.74	2.3	ng	82369	5	13.97	732365	20.0
1-Heneicosanol	13.81	5.1	ng	185901	5	13.97	732365	20.0