LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022974.D
Acq On : 9 Jul 2016 20:49
Operator : UM/SJ
Sample : H3934-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C2.3-03

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_G\METHODS\8270-BG070816.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	3.037	30	34	48	rVB	2374053	3382320	41.31%	6.210%
2	5.223	396	406	413	rBV	218014	353629	4.32%	0.649%
3	5.699	480	487	497	rVB	1835538	3001287	36.66%	5.510%
4	7.309	753	761	771	rBV	2133395	3791773	46.31%	6.962%
5	7.679	815	824	838	rBV	1891037	3368727	41.15%	6.185%
6	8.149	898	904	913	rVB	335750	598129	7.31%	1.098%
7	8.478	951	960	968	rBV	1333091	2278605	27.83%	4.183%
8	9.324	1095	1104	1113	rBV	1338024	2367078	28.91%	4.346%
9	10.382	1277	1284	1291	rVB4	70301	125419	1.53%	0.230%
10	10.981	1378	1386	1392	rBV	537737	949658	11.60%	1.744%
11	12.420	1624	1631	1639	rBV	1789816	2904997	35.48%	5.333%
12	13.413	1791	1800	1811	rBV	3514032	5666085	69.21%	10.403%
13	14.236	1934	1940	1945	rBV	588585	877751	10.72%	1.612%
14	14.794	2026	2035	2043	rBV2	1008451	1661249	20.29%	3.050%
15	16.286	2282	2289	2302	rBV	3720471	5801066	70.86%	10.651%
16	17.273	2452	2457	2461	rBV	143545	189784	2.32%	0.348%
17	17.550	2497	2504	2514	rBV2	1357413	2164747	26.44%	3.974%
18	17.908	2558	2565	2574	rBV2	112491	221510	2.71%	0.407%
19	18.020	2580	2584	2591	rVB2	91166	107480	1.31%	0.197%
20	18.419	2647	2652	2663	rBV2	263196	380619	4.65%	0.699%
21	19.271	2792	2797	2806	rBV	345301	567954	6.94%	1.043%
22	19.682	2862	2867	2872	rBV4	82097	120652	1.47%	0.222%
23	20.152	2941	2947	2954	rBV	6443272	8187006	100.00%	15.031%
24	20.769	3048	3052	3056	rBV2	72326	101031	1.23%	0.185%
25	21.034	3092	3097	3100	rBV4	57296	90341	1.10%	0.166%
26	21.451	3164	3168	3182	rBV4	181064	371477	4.54%	0.682%
27	21.845	3228	3235	3242	rBV2	1396062	2425844	29.63%	4.454%
28	23.560	3523	3527	3533	rVB6	47296	97177	1.19%	0.178%
29	25.194	3796	3805	3822	rVB2	777403	2313946	28.26%	4.248%

Sum of corrected areas: 54467341

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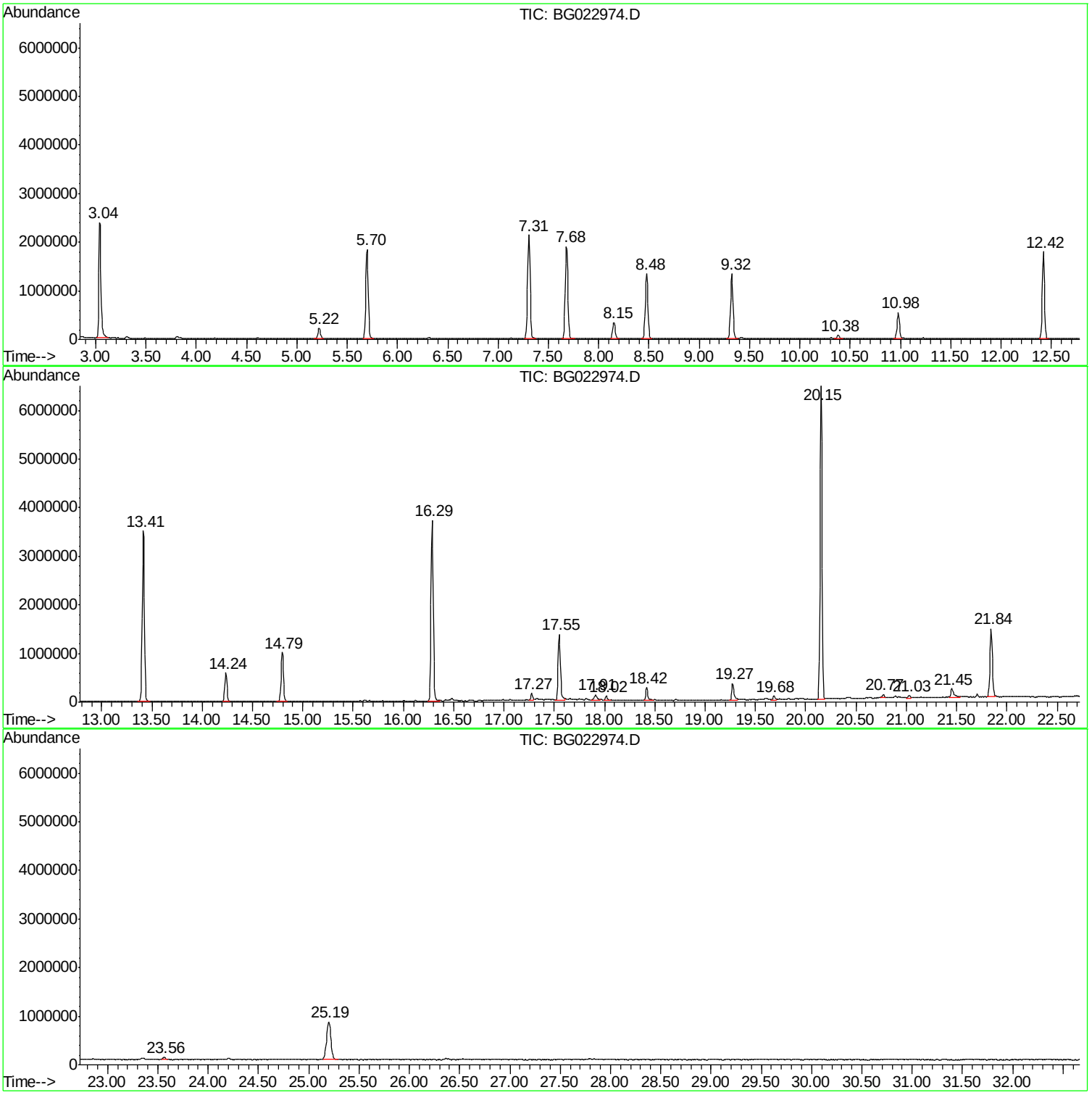
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C2.3-03

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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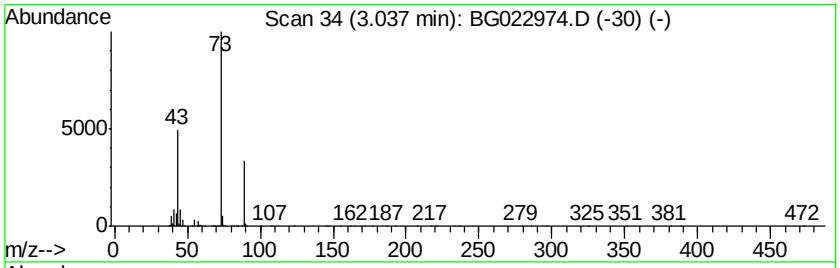
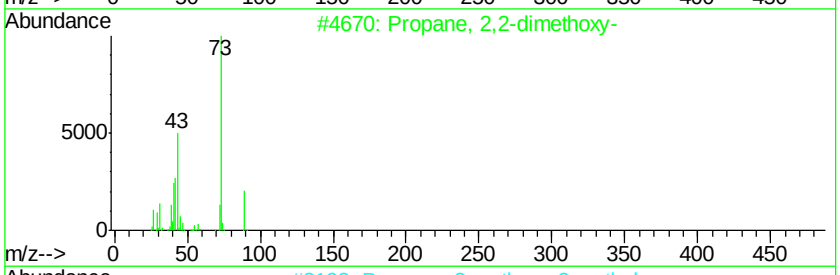
****

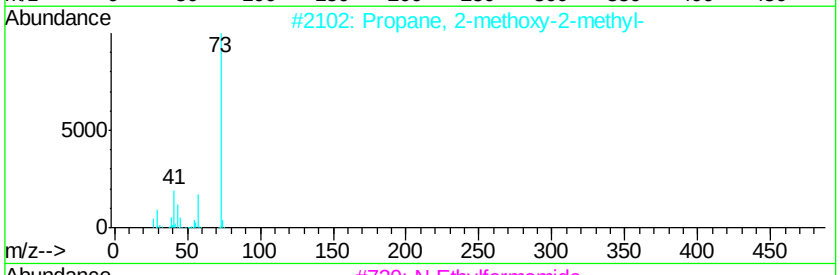
Peak Number 1 unknown3.04 Concentration Rank 1

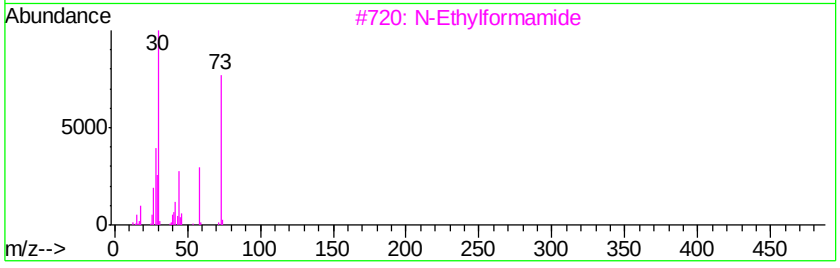
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	113.10 ng	3382320	1,4-Dichlorobenzene-d4	8.15

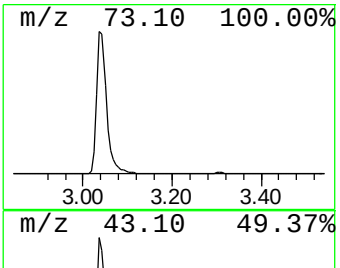
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	5
4	Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	5
5	Formic acid, ethyl ester	74	C3H6O2	000109-94-4	5

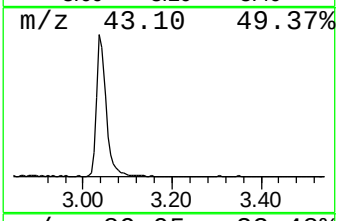


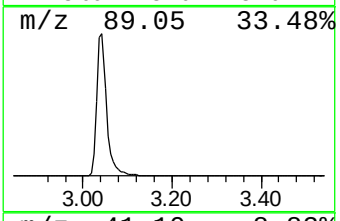


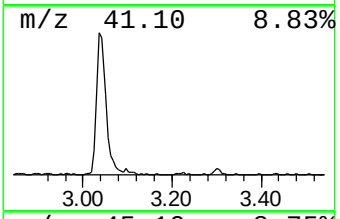


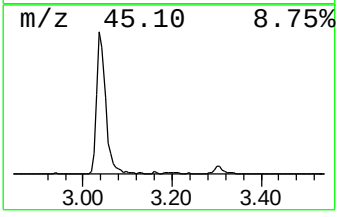












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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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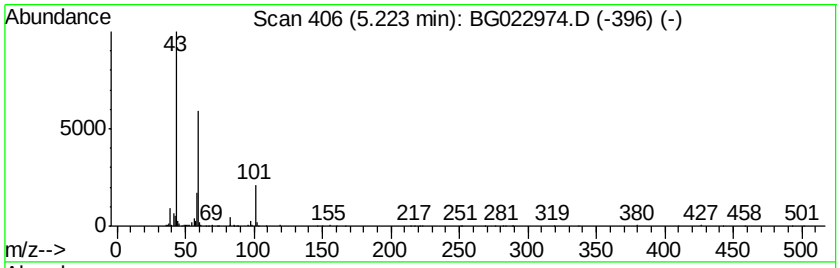
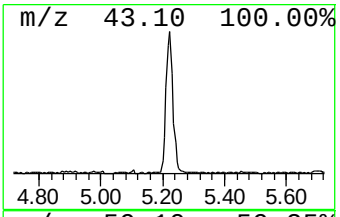
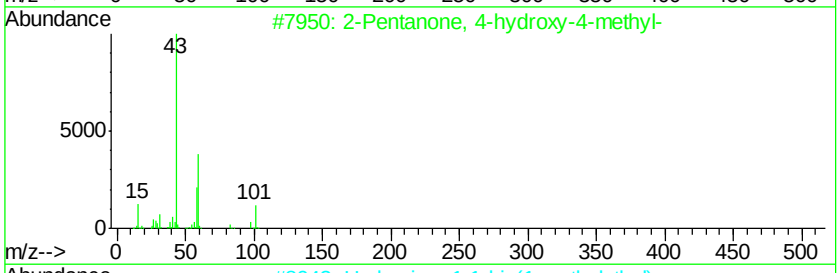
Peak Number 2 unknown5.22 Concentration Rank 5

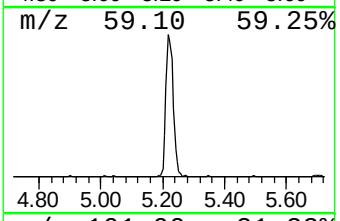
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	11.82 ng	353629	1,4-Dichlorobenzene-d4	8.15

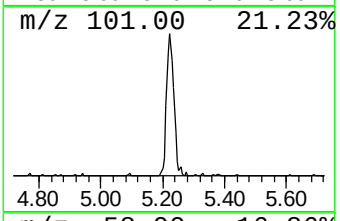
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	10
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	10
5	Guanidine	59	CH5N3	000113-00-8	9

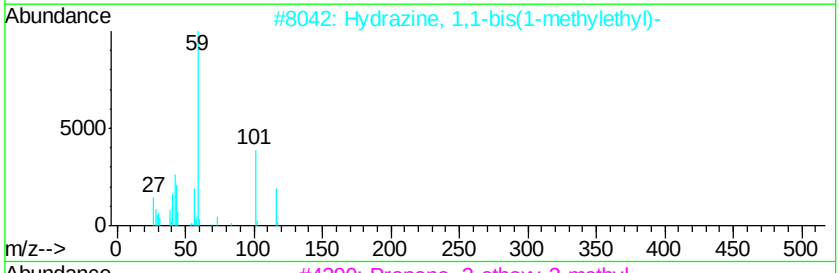


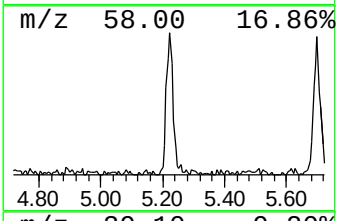


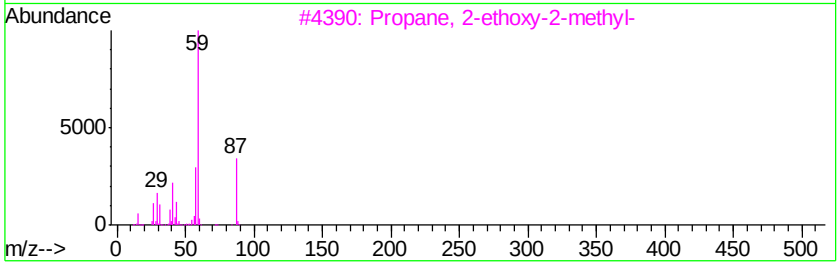


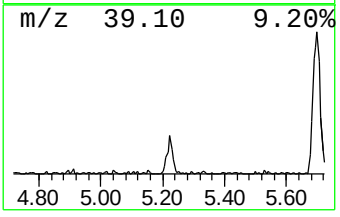












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Instrument : BNA_G
ClientSampleId : C2.3-03

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

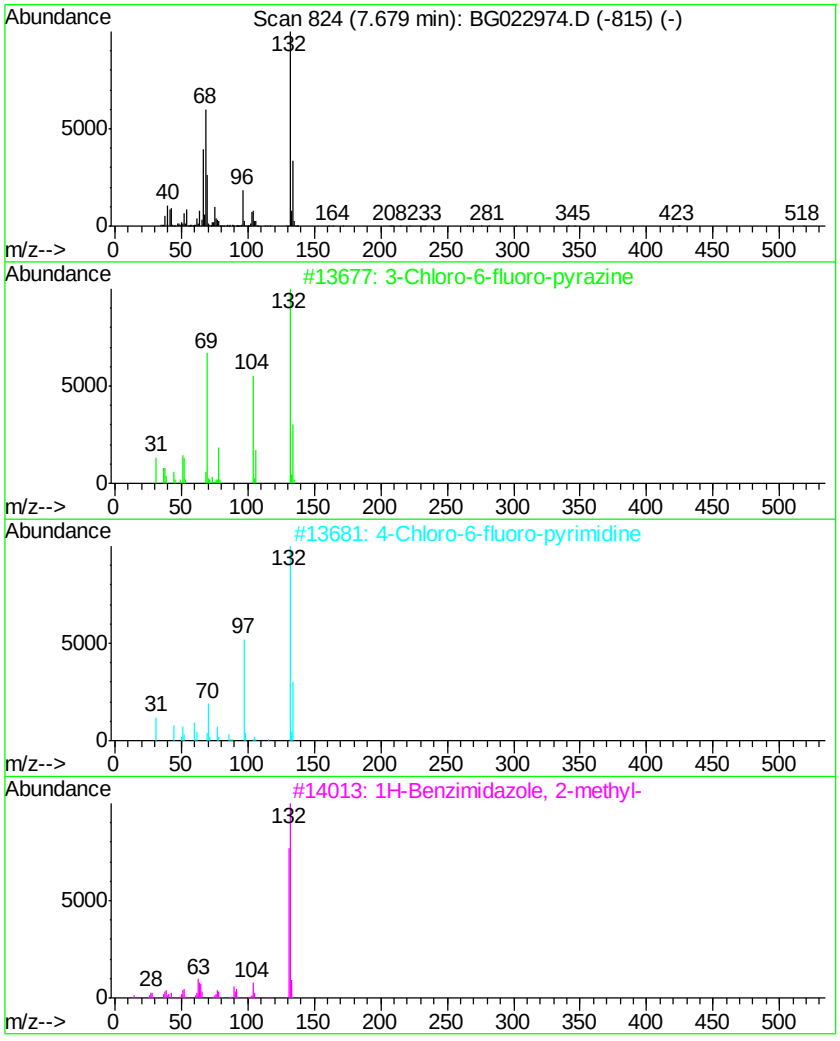
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

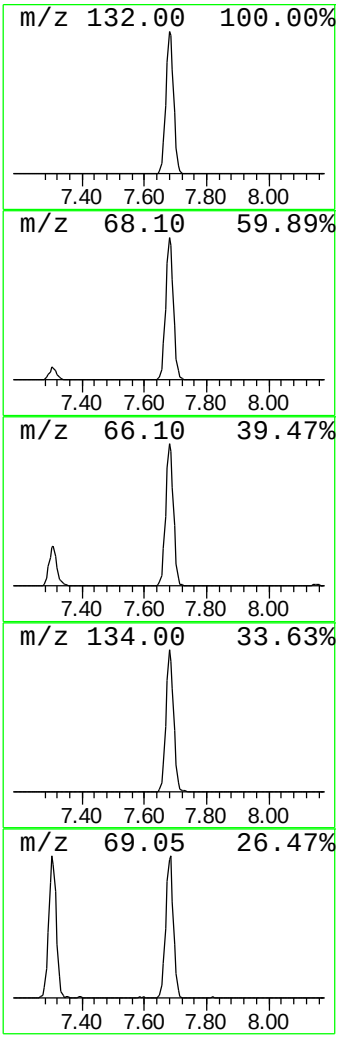
****

Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	112.64 ng	3368730	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	18
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5	Xenon	132	Xe	007440-63-3	9





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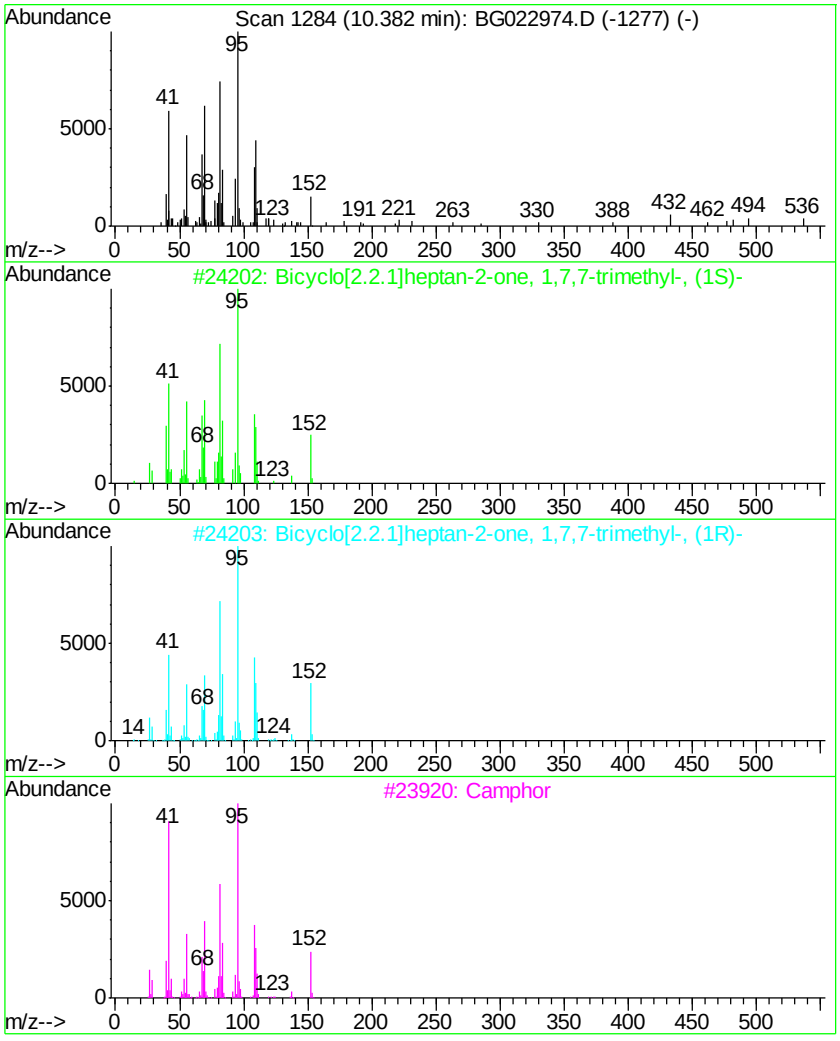
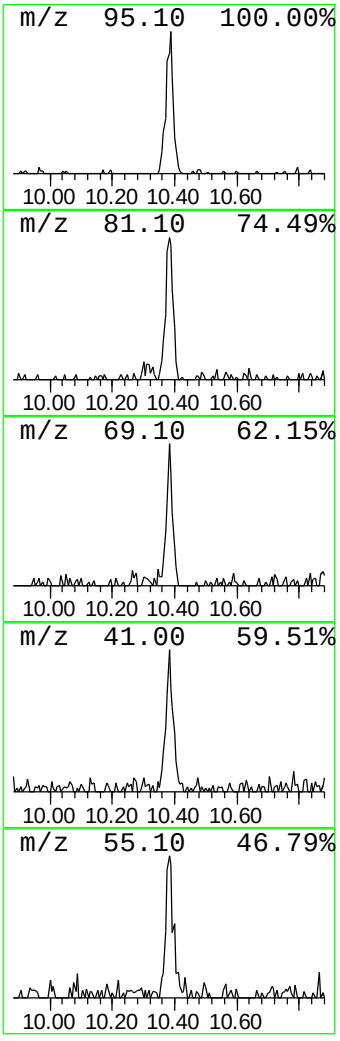
Peak Number 5 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.64 ng	125419	Naphthalene-d8	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	93
2	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-49-3	93
3	Camphor	152	C10H16O	000076-22-2	89
4	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	021368-68-3	76
5	Limonene-1,2-epoxide(fr.2)	152	C10H16O	1000292-83-8	43





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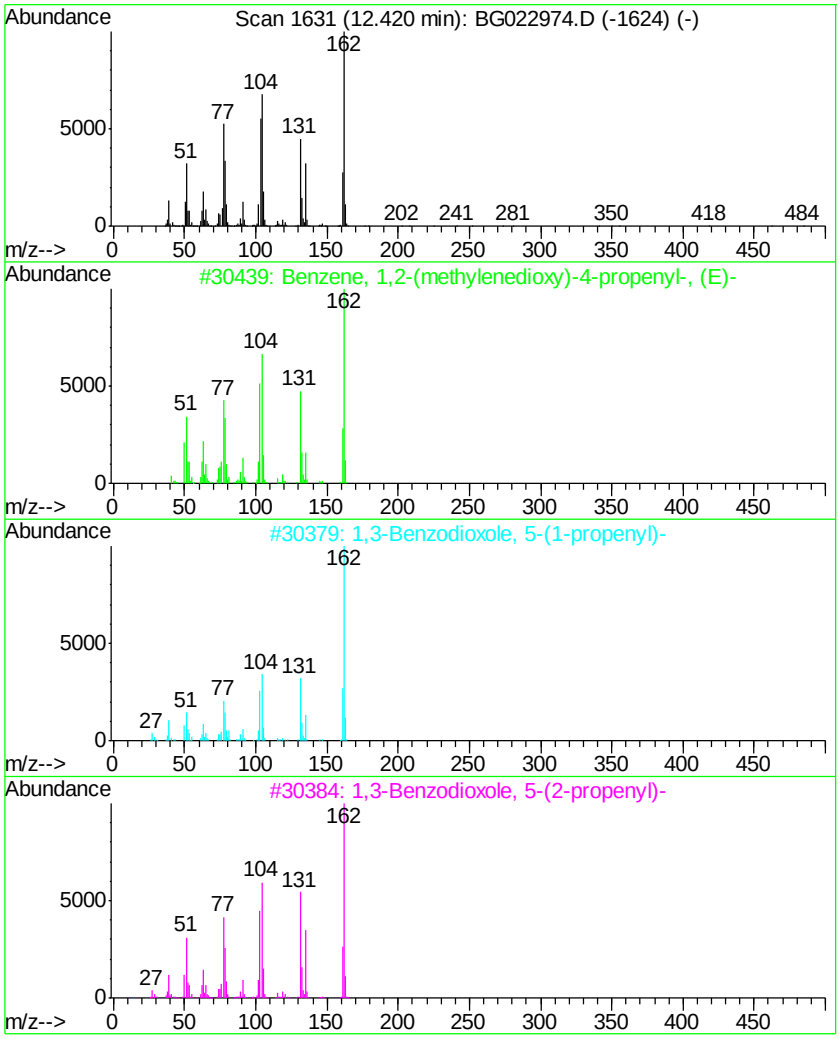
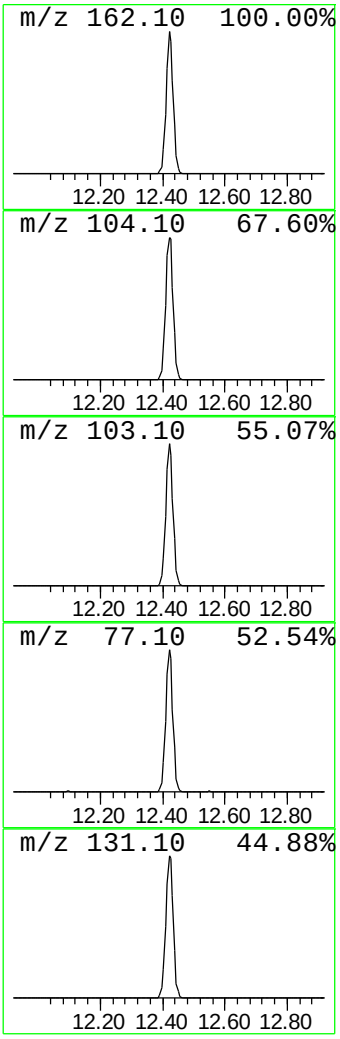
Peak Number 6 Benzene, 1,2-(methylenediox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	61.18 ng	2905000	Naphthalene-d8	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	98
2	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3	1,3-Benzodioxole, 5-(2-propenyl)-	162	C10H10O2	000094-59-7	97
4	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	95
5	Sydnone, 3-phenyl-	162	C8H6N2O2	000120-06-9	49





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TIC Library : C:\DATABASE\NIST02.L
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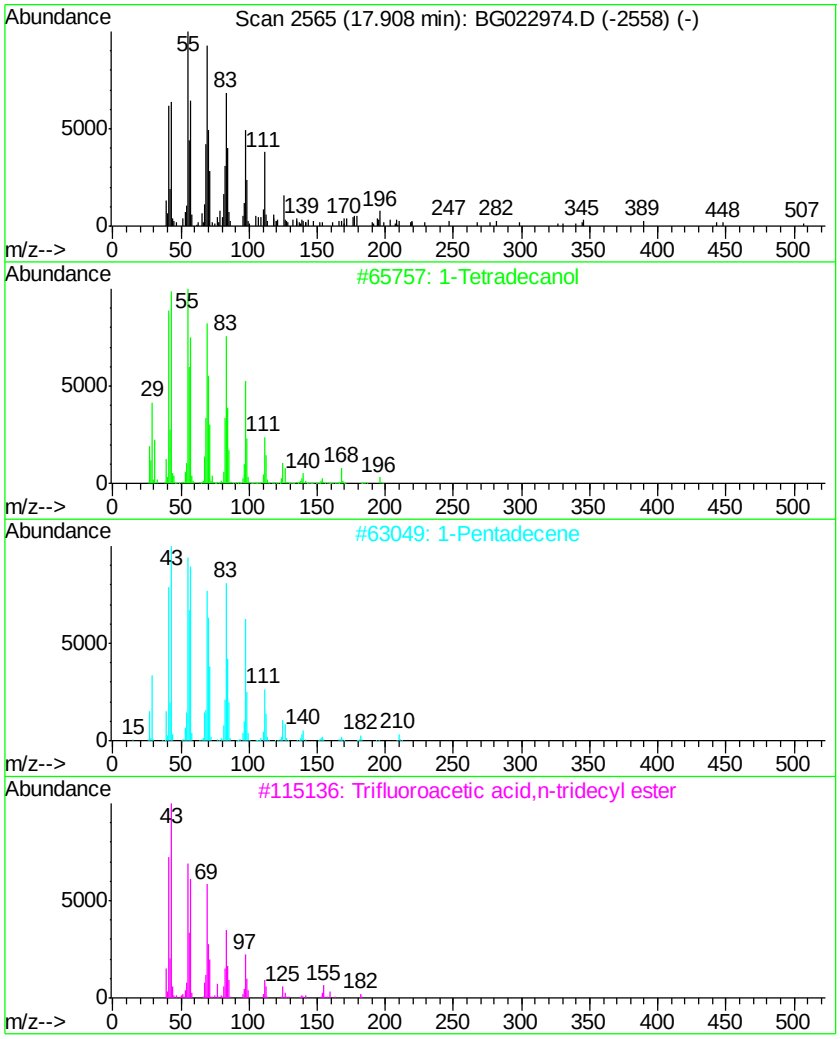
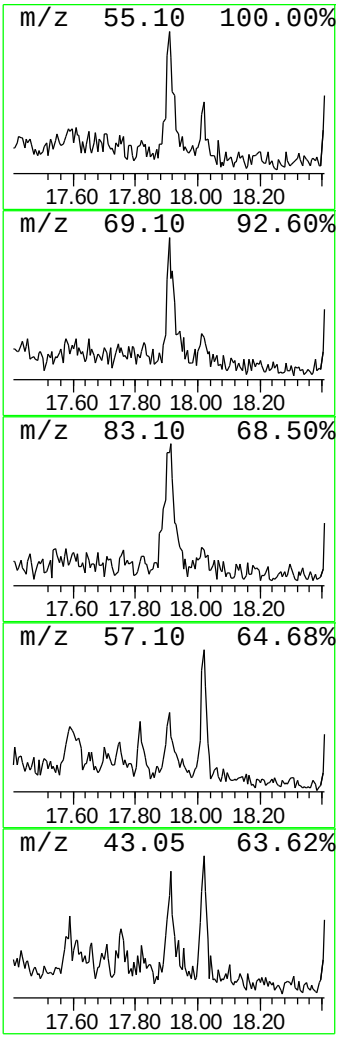
Peak Number 7 1-Tetradecanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	2.05 ng	221510	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecanol	214	C14H30O	000112-72-1	83
2	1-Pentadecene	210	C15H30	013360-61-7	78
3	Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	72
4	1-Tetradecene	196	C14H28	001120-36-1	64
5	1-Tridecanol	200	C13H28O	000112-70-9	64





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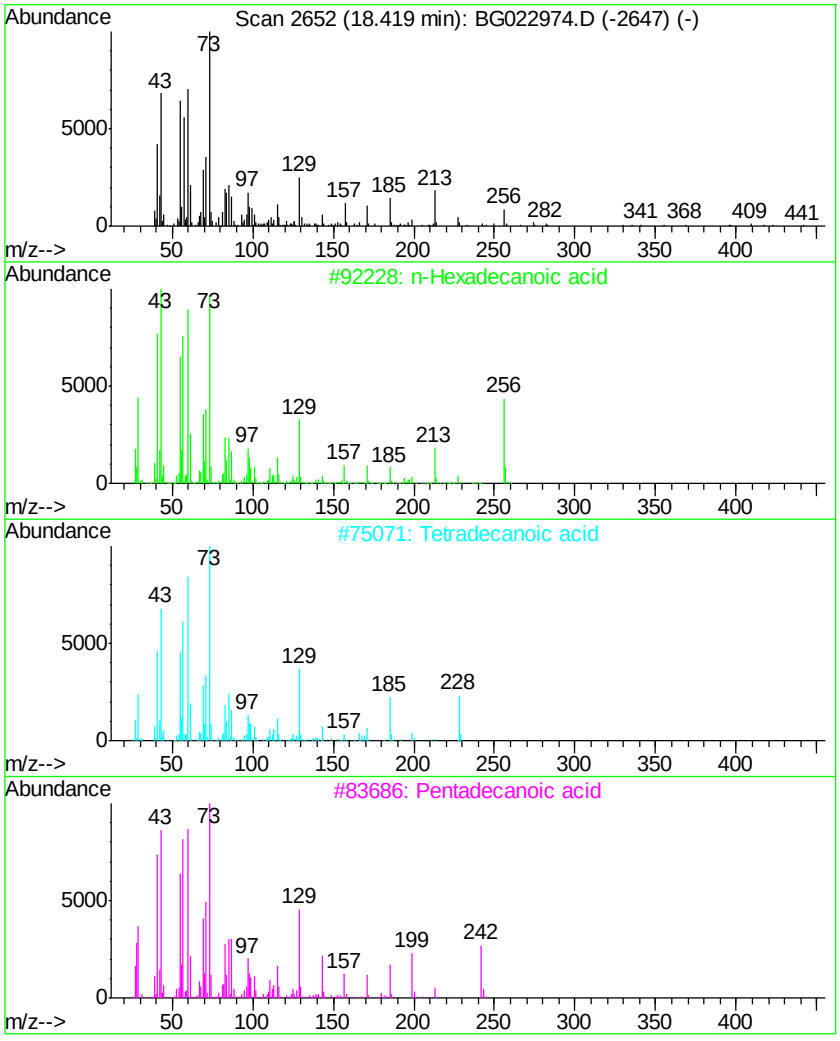
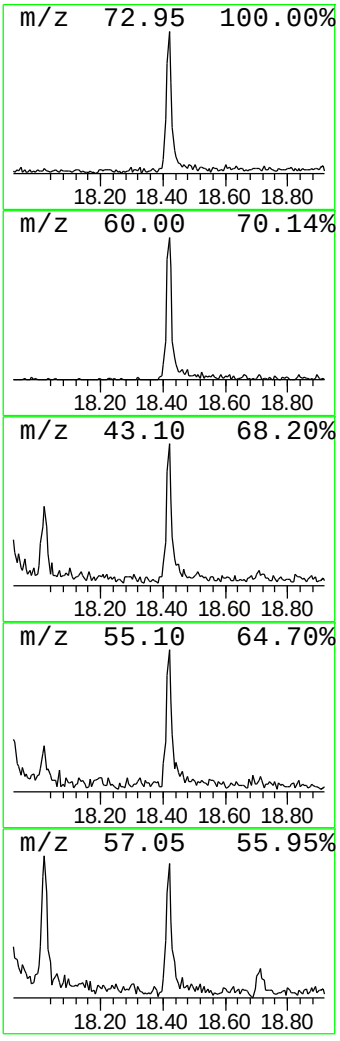
Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	3.52 ng	380619	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022974.D
Acq On : 9 Jul 2016 20:49
Operator : UM/SJ
Sample : H3934-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C2.3-03

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

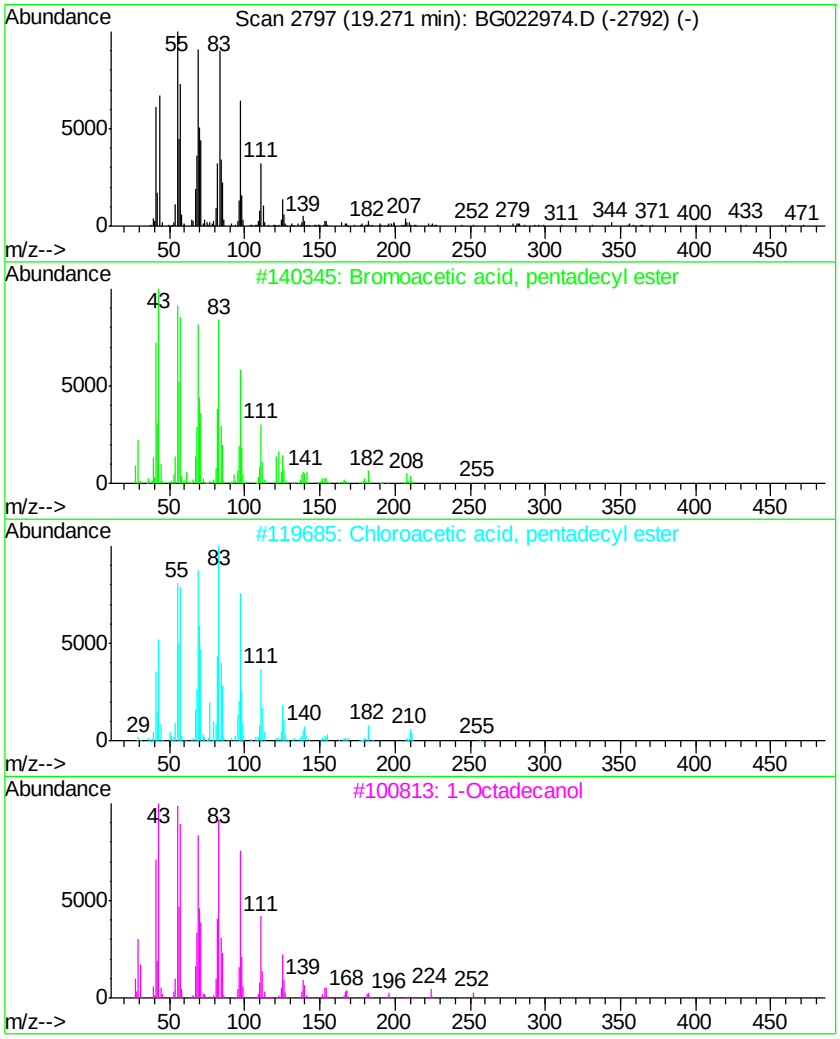
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

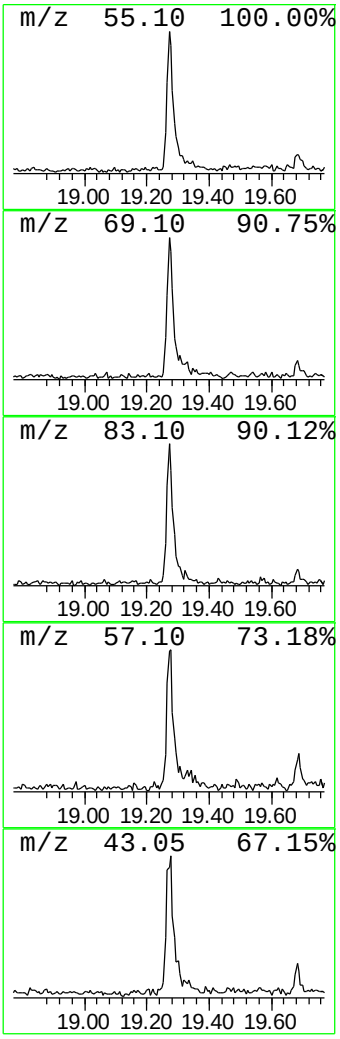
****

Peak Number 9 Bromoacetic acid, pentadecy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	5.25 ng	567954	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
2	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	91
3	1-Octadecanol	270	C18H38O	000112-92-5	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022974.D
Acq On : 9 Jul 2016 20:49
Operator : UM/SJ
Sample : H3934-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C2.3-03

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

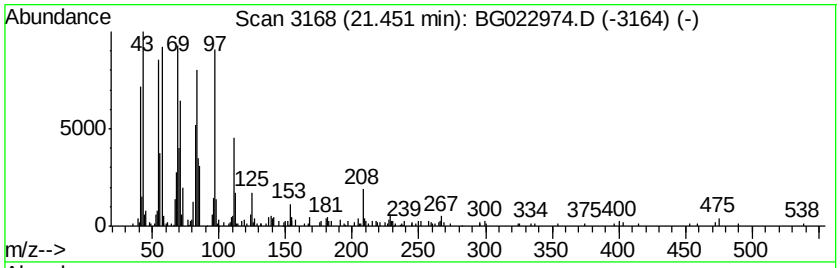
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

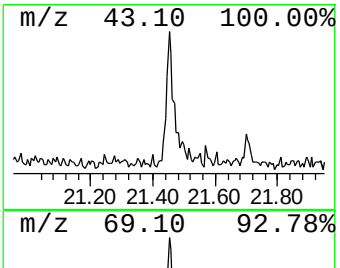
****

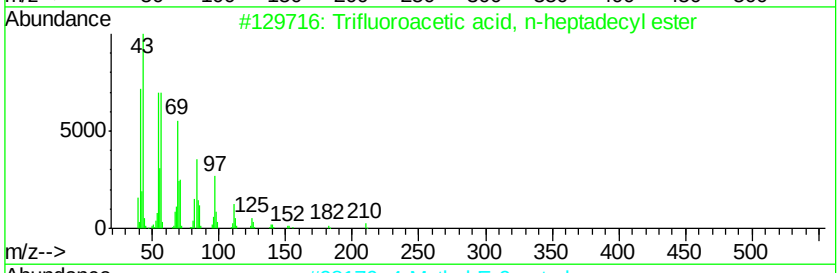
Peak Number 10 Trifluoroacetic acid, n-hep... Concentration Rank 8

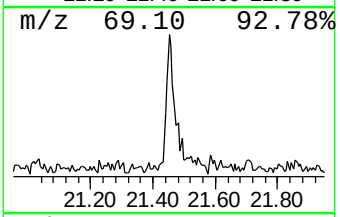
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.45	3.06 ng	371477	Chrysene-d12	21.84

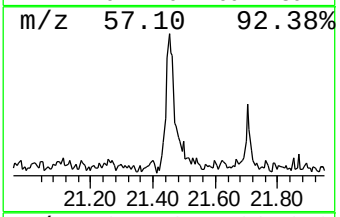
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	87
2	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	78
3	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	74
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	72
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	62

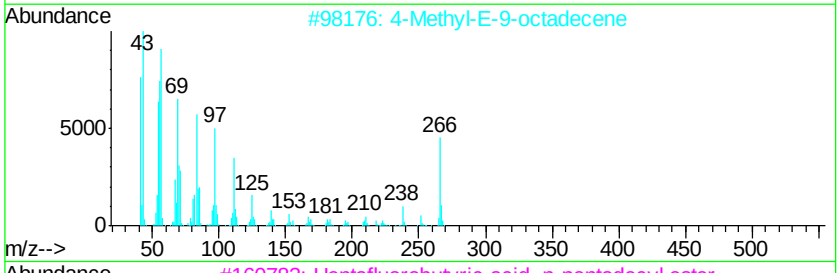


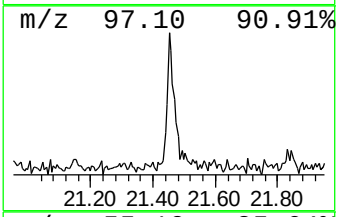


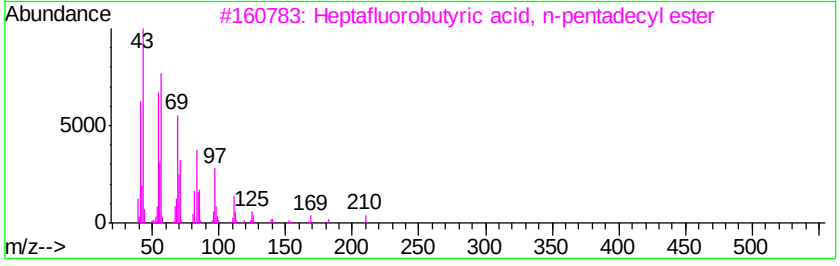


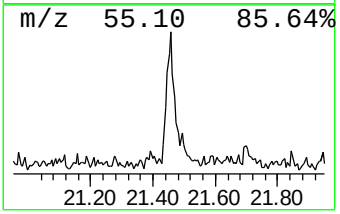












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022974.D
Acq On : 9 Jul 2016 20:49
Operator : UM/SJ
Sample : H3934-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C2.3-03

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.04	3.04	113.1	ng	3382320	1	8.15	598129	20.0
unknown5.22	5.22	11.8	ng	353629	1	8.15	598129	20.0
unknown7.68	7.68	112.6	ng	3368730	1	8.15	598129	20.0
Bicyclo[2.2.1]hep...	10.38	2.6	ng	125419	2	10.98	949658	20.0
Benzene, 1,2-(met...	12.42	61.2	ng	2905000	2	10.98	949658	20.0
1-Tetradecanol	17.91	2.0	ng	221510	4	17.55	2164750	20.0
n-Hexadecanoic acid	18.42	3.5	ng	380619	4	17.55	2164750	20.0
Bromoacetic acid,...	19.27	5.3	ng	567954	4	17.55	2164750	20.0
Trifluoroacetic a...	21.45	3.1	ng	371477	5	21.84	2425840	20.0