LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024612.D
Acq On : 2 Nov 2016 4:26
Operator : UM/SJ
Sample : H5489-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-76-17.5-18.0

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-BG102516.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	3.132	43	50	71	rVB	8043410	18303648	100.00%	22.618%
2	5.335	418	425	436	rBV	604207	1032046	5.64%	1.275%
3	5.799	496	504	515	rBV	2856946	4900971	26.78%	6.056%
4	7.403	767	777	790	rBV	2987412	5522902	30.17%	6.825%
5	7.797	835	844	854	rBV	2893763	5166150	28.22%	6.384%
6	8.267	917	924	936	rBV2	486225	943861	5.16%	1.166%
7	8.596	970	980	989	rBV	1924000	3437391	18.78%	4.248%
8	9.442	1115	1124	1135	rBV	1826162	3388553	18.51%	4.187%
9	11.093	1398	1405	1413	rBV	673853	1218382	6.66%	1.506%
10	13.508	1806	1816	1826	rBV	4233658	6611384	36.12%	8.170%
11	14.319	1947	1954	1961	rBV	964641	1450347	7.92%	1.792%
12	14.883	2041	2050	2058	rBV	1122778	1763214	9.63%	2.179%
13	16.363	2295	2302	2318	rBV	4242514	6863817	37.50%	8.482%
14	16.534	2327	2331	2342	rBV	104712	198429	1.08%	0.245%
15	17.621	2510	2516	2526	rBV2	1328553	2204337	12.04%	2.724%
16	18.467	2656	2660	2670	rBV3	149125	261255	1.43%	0.323%
17	20.206	2949	2956	2962	rBV	8432200	11282444	61.64%	13.942%
18	21.499	3165	3176	3187	rBV2	291186	626005	3.42%	0.774%
19	21.916	3240	3247	3255	rBV	1633233	2872793	15.70%	3.550%
20	25.347	3818	3831	3842	rBV	907717	2876286	15.71%	3.554%

Sum of corrected areas: 80924215

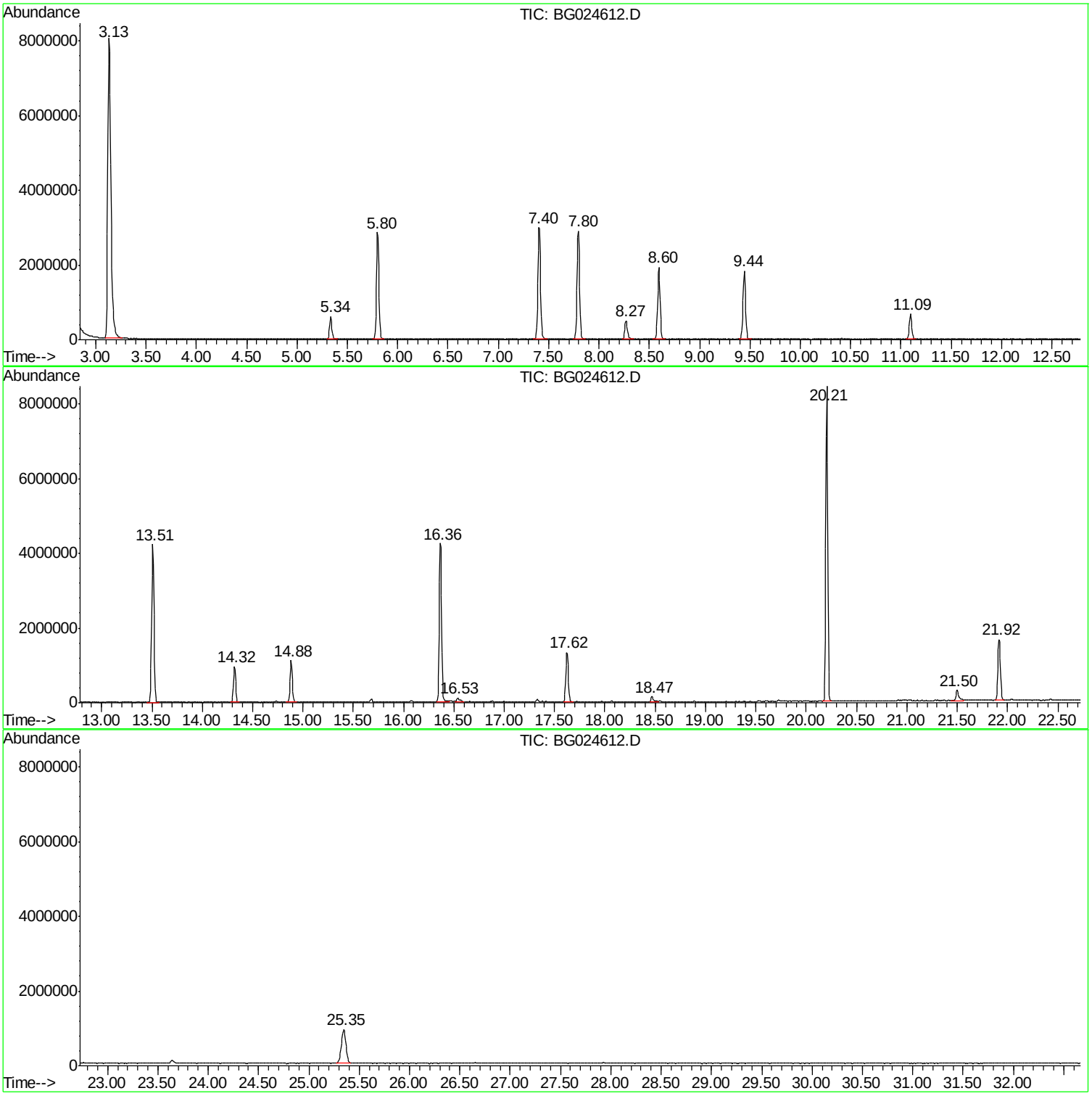
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024612.D
Acq On : 2 Nov 2016 4:26
Operator : UM/SJ
Sample : H5489-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-76-17.5-18.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024612.D
Acq On : 2 Nov 2016 4:26
Operator : UM/SJ
Sample : H5489-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-76-17.5-18.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

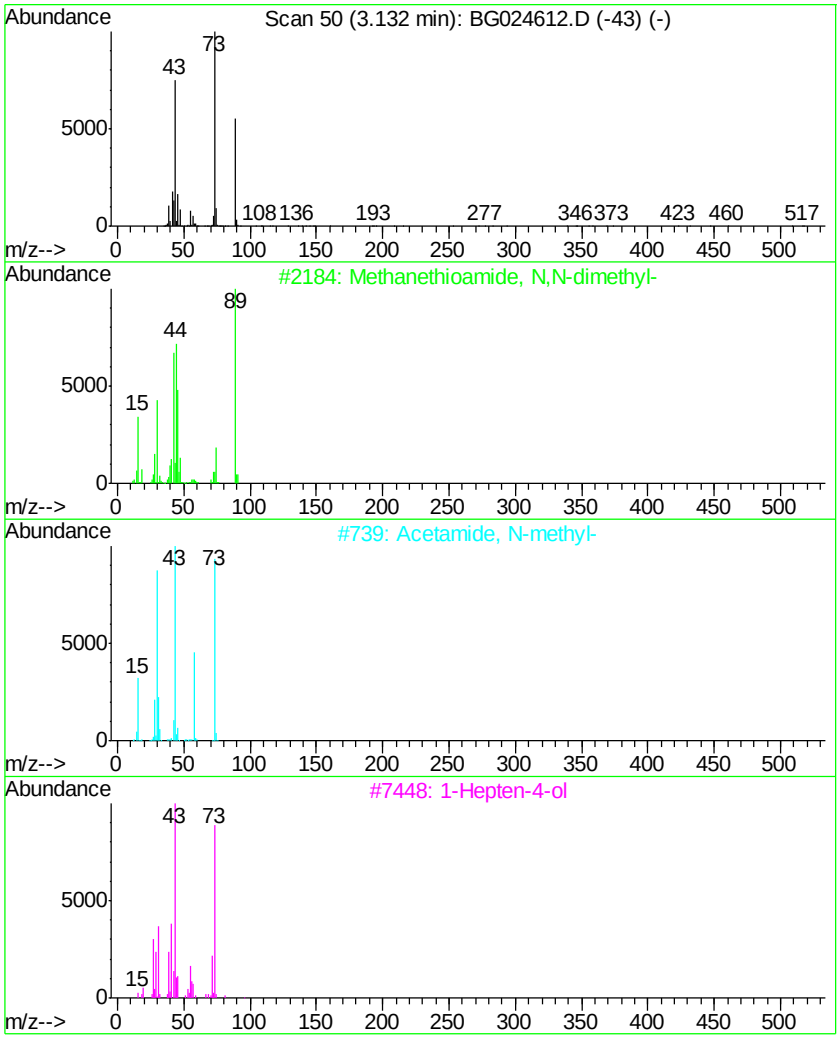
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

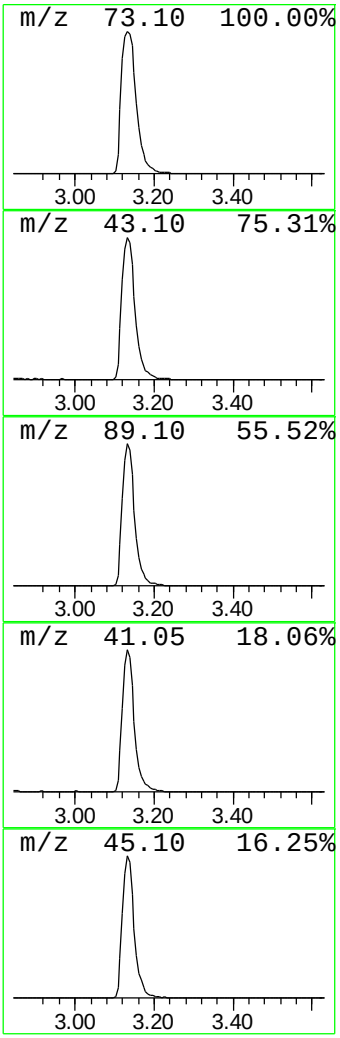
****

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	387.85 ng	18303600	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	38
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3	1-Hepten-4-ol	114	C7H14O	003521-91-3	23
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024612.D
Acq On : 2 Nov 2016 4:26
Operator : UM/SJ
Sample : H5489-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-76-17.5-18.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

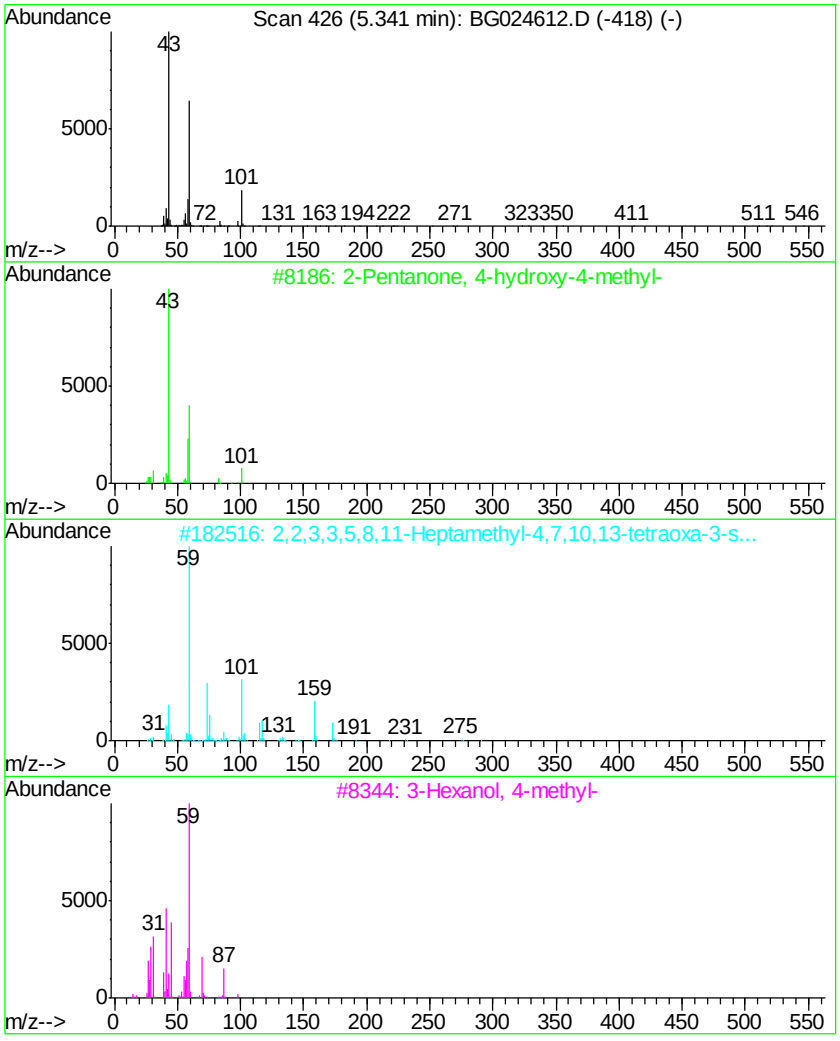
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

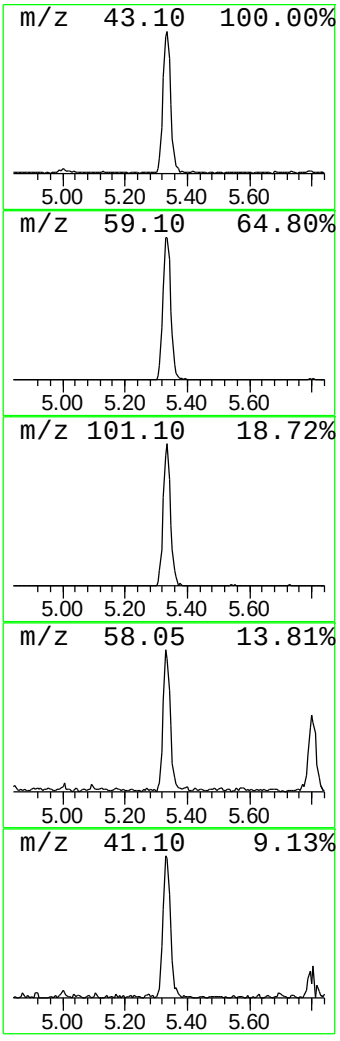
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	21.87 ng	1032050	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,2,3,3,5,8,11-Heptamethyl-4,7,1...	348	C18H40O4Si	1000367-07-2	28
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Propanoic acid, 3-nitro-, methyl...	133	C4H7NO4	020497-95-4	23





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024612.D
Acq On : 2 Nov 2016 4:26
Operator : UM/SJ
Sample : H5489-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-76-17.5-18.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

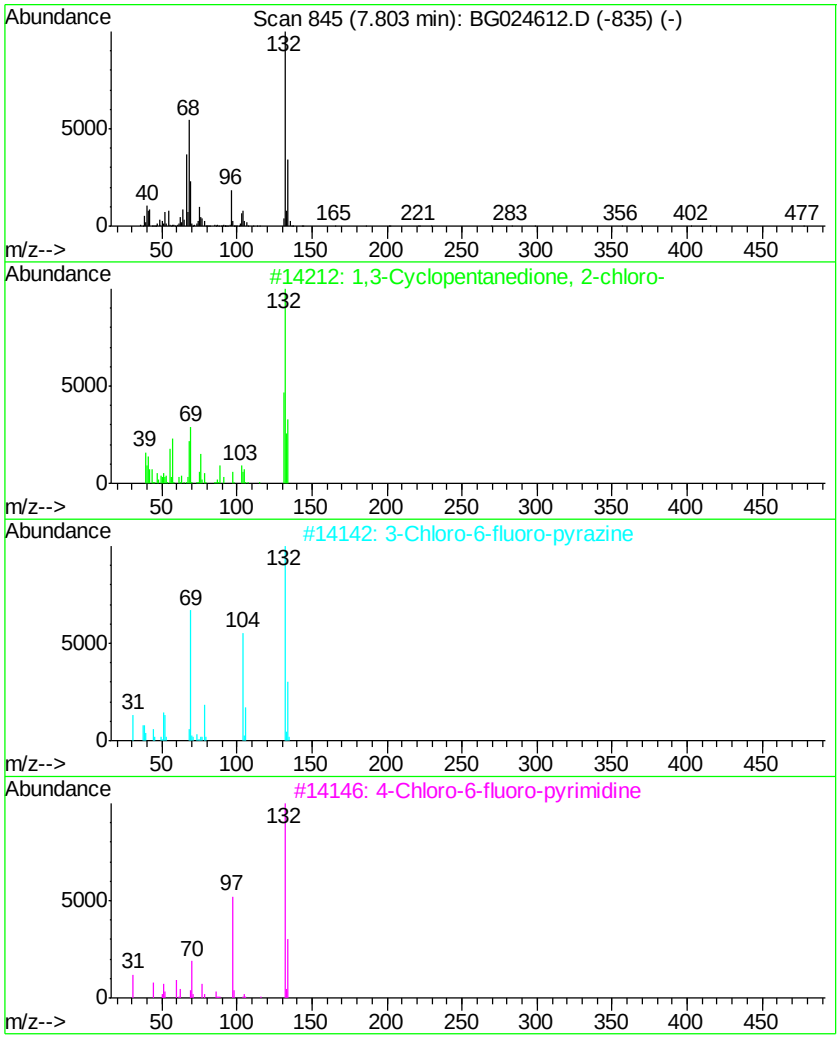
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

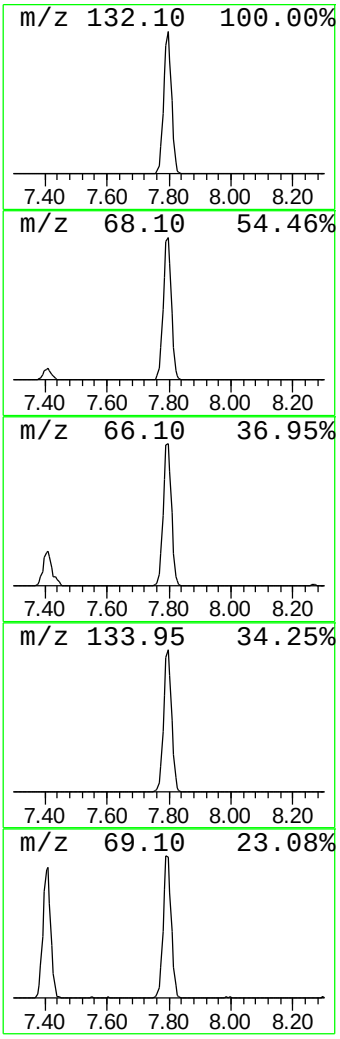
****

Peak Number 3 unknown7.80 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	109.47 ng	5166150	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024612.D
Acq On : 2 Nov 2016 4:26
Operator : UM/SJ
Sample : H5489-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-76-17.5-18.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

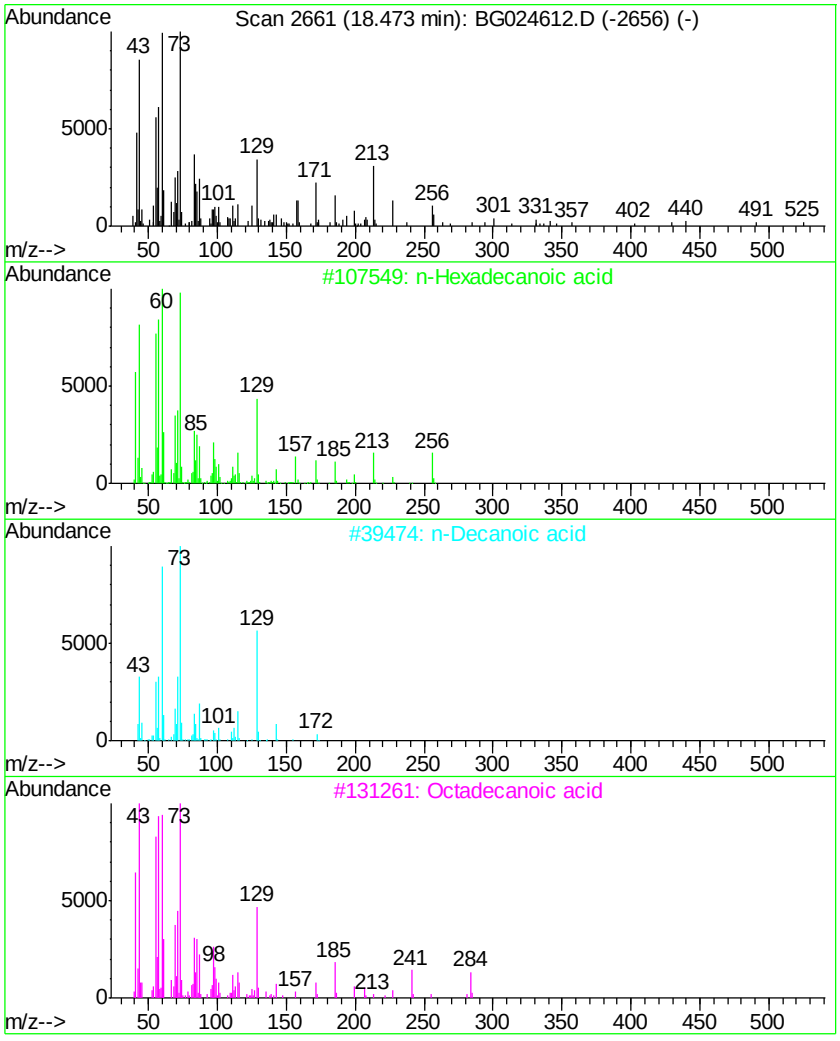
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

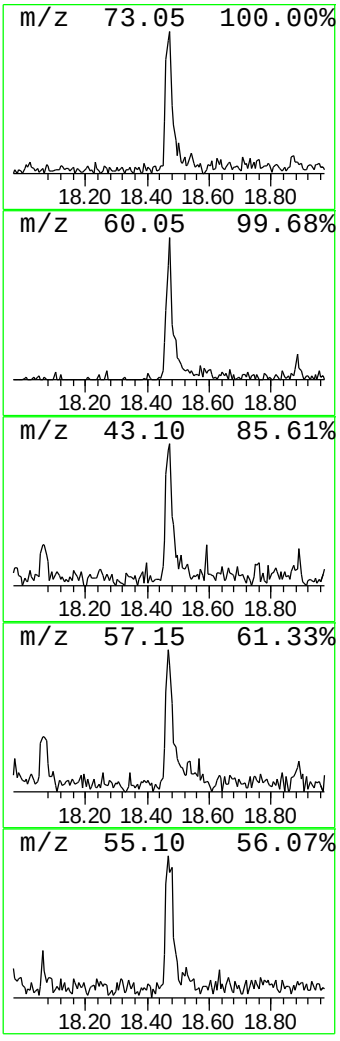
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.37 ng	261255	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	n-Decanoic acid	172	C10H20O2	000334-48-5	90
3	Octadecanoic acid	284	C18H36O2	000057-11-4	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	52





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024612.D
Acq On : 2 Nov 2016 4:26
Operator : UM/SJ
Sample : H5489-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-76-17.5-18.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

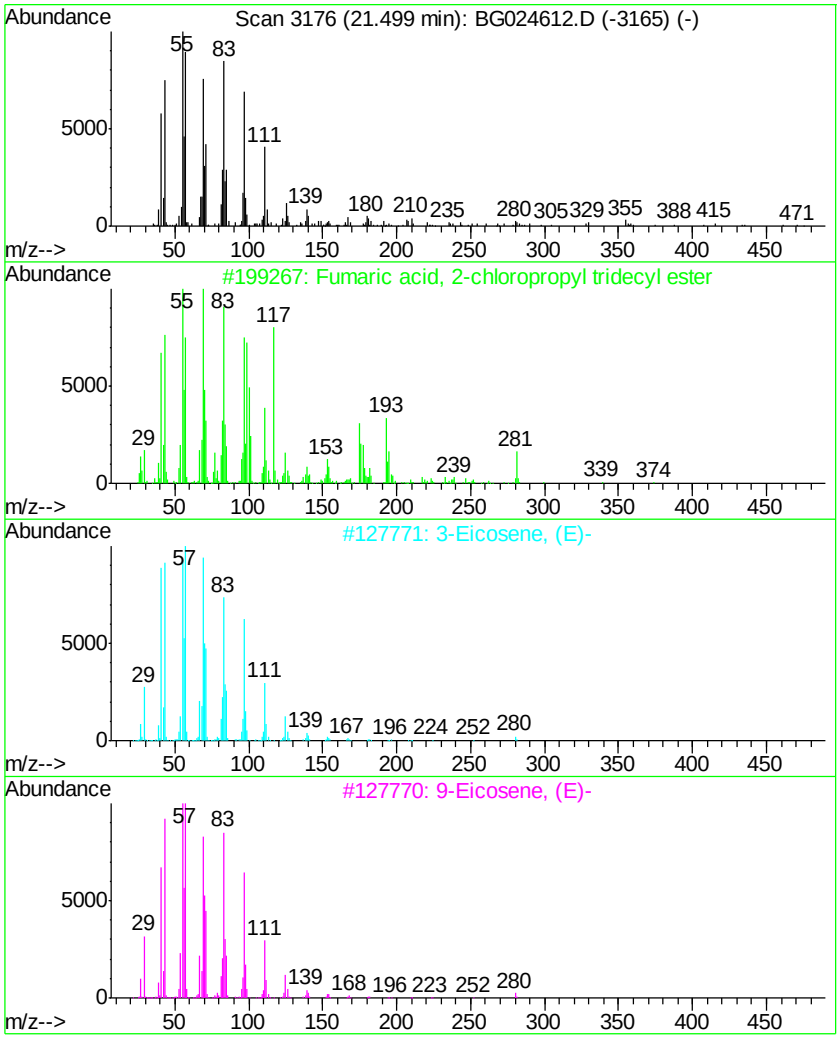
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

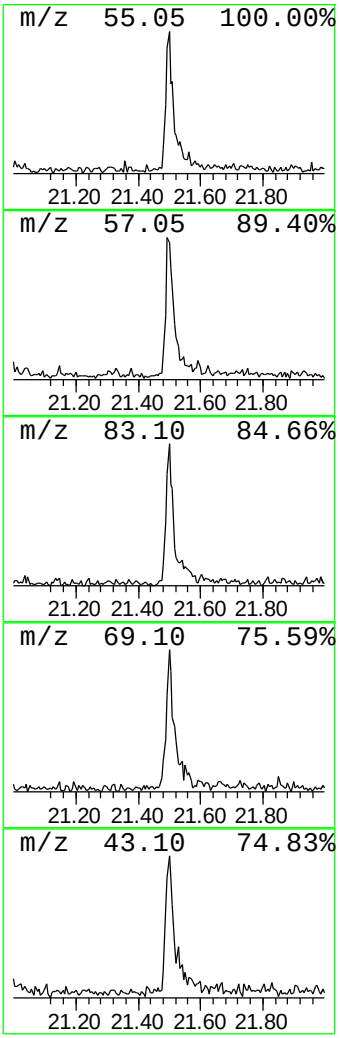
****

Peak Number 6 Fumaric acid, 2-chloropropy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	4.36 ng	626005	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	96
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110116\
Data File : BG024612.D
Acq On : 2 Nov 2016 4:26
Operator : UM/SJ
Sample : H5489-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-76-17.5-18.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.13	3.13	387.9	ng	18303600	1	8.27	943861	20.0
2-Pentanone, 4-hy...	5.34	21.9	ng	1032050	1	8.27	943861	20.0
unknown7.80	7.80	109.5	ng	5166150	1	8.27	943861	20.0
n-Hexadecanoic acid	18.47	2.4	ng	261255	4	17.62	2204340	20.0
Fumaric acid, 2-c...	21.50	4.4	ng	626005	5	21.92	2872790	20.0