LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024667.D
Acq On : 4 Nov 2016 4:11
Operator : UM/SJ
Sample : H5509-13
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-97-0.5-1.0

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	3.128	43	49	71	rVB	7096387	12273871	100.00%	19.387%
2	5.325	416	423	433	rBV	477926	797901	6.50%	1.260%
3	5.795	495	503	515	rBV	2213505	3707050	30.20%	5.856%
4	7.405	768	777	788	rBV	2320458	4257369	34.69%	6.725%
5	7.793	832	843	853	rVB	2192290	3893686	31.72%	6.150%
6	8.269	913	924	932	rBV	398094	725357	5.91%	1.146%
7	8.592	969	979	990	rBV	1556886	2758569	22.48%	4.357%
8	9.444	1115	1124	1135	rBV	1390792	2599217	21.18%	4.106%
9	11.095	1395	1405	1413	rBV	522673	966850	7.88%	1.527%
10	13.510	1807	1816	1824	rBV	3183418	5130704	41.80%	8.104%
11	14.321	1947	1954	1960	rBV	875409	1279926	10.43%	2.022%
12	14.885	2041	2050	2059	rBV	898592	1406866	11.46%	2.222%
13	16.365	2294	2302	2313	rBV	3552210	5548052	45.20%	8.764%
14	16.536	2326	2331	2340	rVB2	75582	148288	1.21%	0.234%
15	17.623	2509	2516	2528	rBV2	1233636	1960494	15.97%	3.097%
16	18.469	2655	2660	2669	rBV2	162547	273001	2.22%	0.431%
17	20.208	2948	2956	2963	rBV	6682721	9269373	75.52%	14.642%
18	21.500	3171	3176	3191	rBV3	169248	344158	2.80%	0.544%
19	21.918	3241	3247	3261	rVB	1516102	2647400	21.57%	4.182%
20	25.349	3819	3831	3843	rVB	863055	2566373	20.91%	4.054%
21	29.785	4576	4586	4602	rVB	165643	753954	6.14%	1.191%

Sum of corrected areas: 63308459

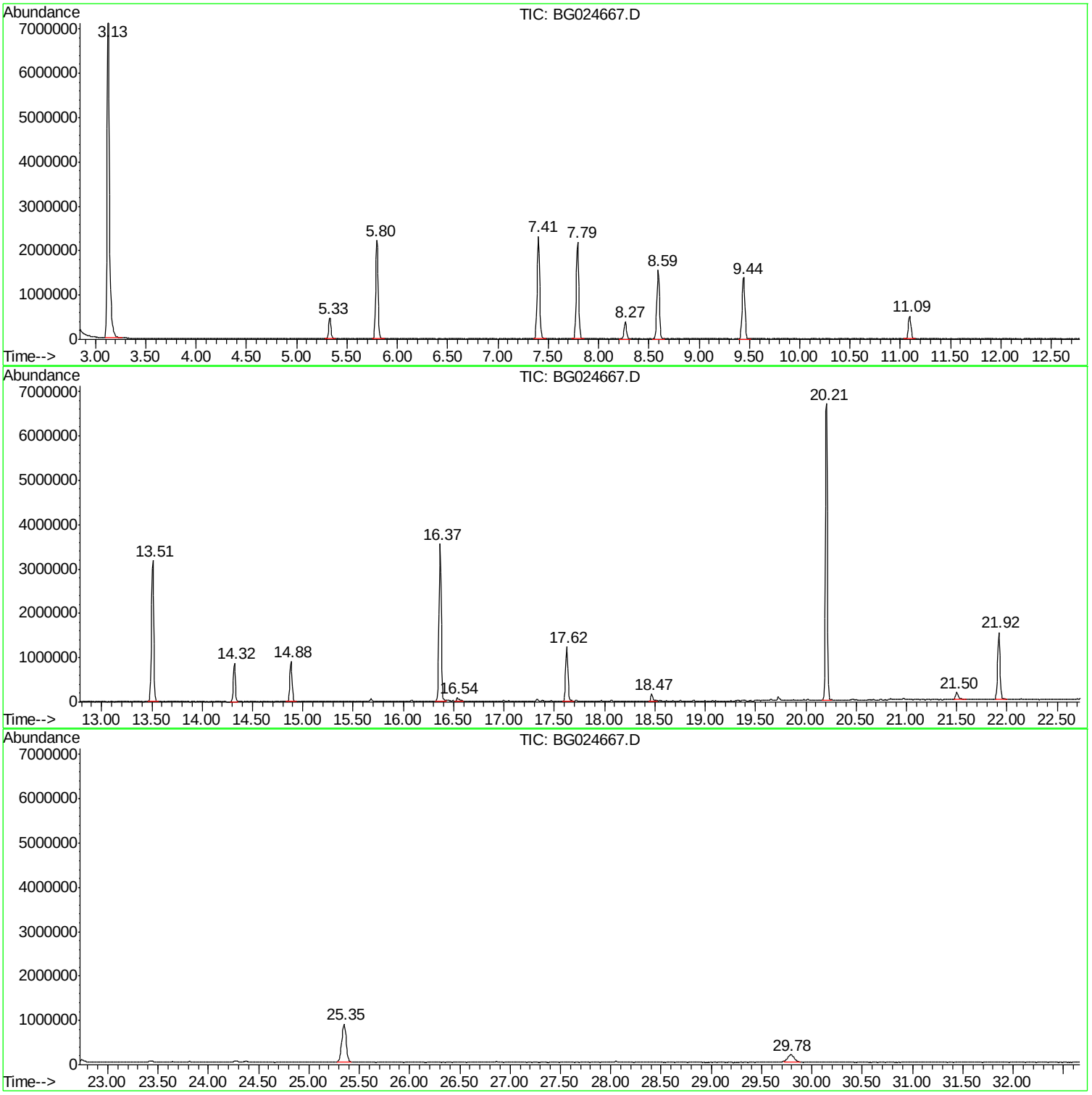
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024667.D
Acq On : 4 Nov 2016 4:11
Operator : UM/SJ
Sample : H5509-13
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-97-0.5-1.0

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\BG110316\
Data File : BG024667.D
Acq On : 4 Nov 2016 4:11
Operator : UM/SJ
Sample : H5509-13
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-97-0.5-1.0

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

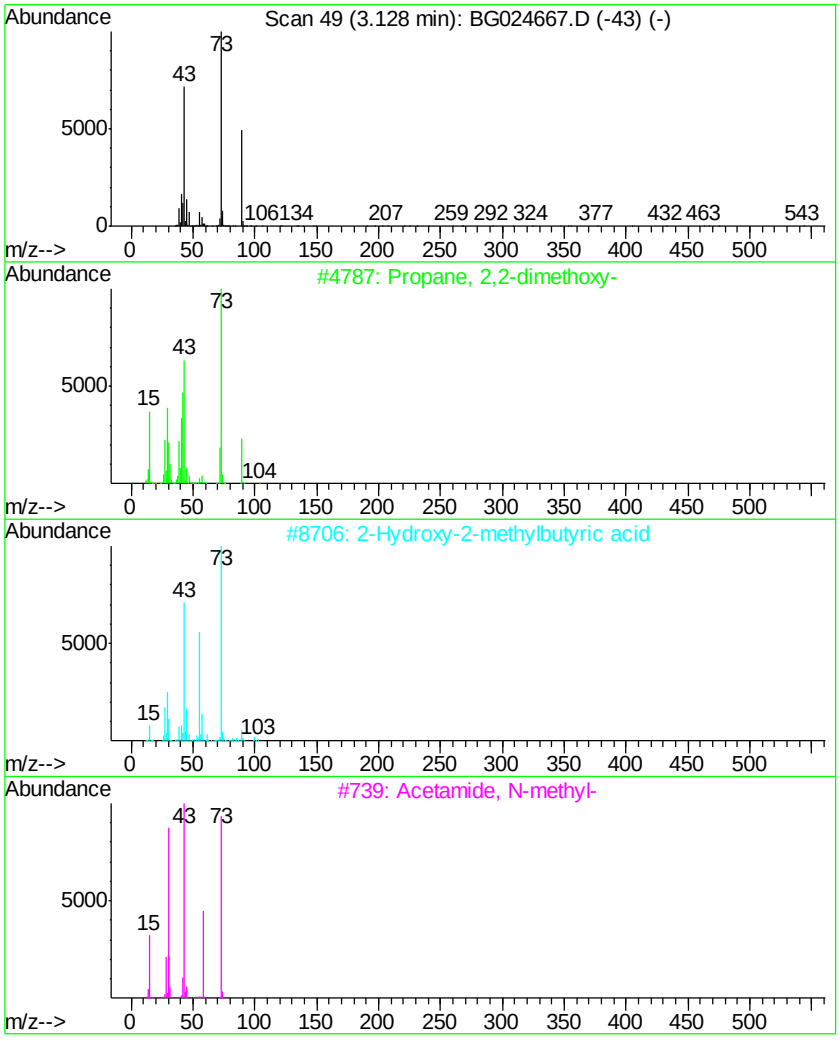
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

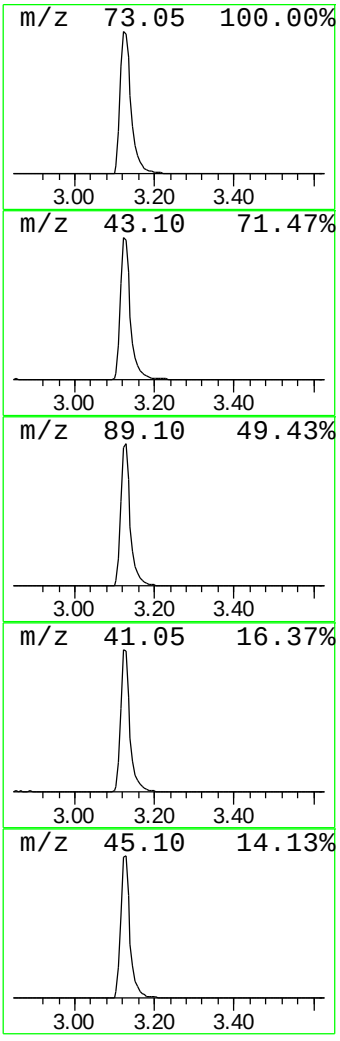
****

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	338.42 ng	12273900	1,4-Dichlorobenzene-d4	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	1-Hepten-4-ol	114	C7H14O	003521-91-3	9
5	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024667.D
Acq On : 4 Nov 2016 4:11
Operator : UM/SJ
Sample : H5509-13
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-97-0.5-1.0

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

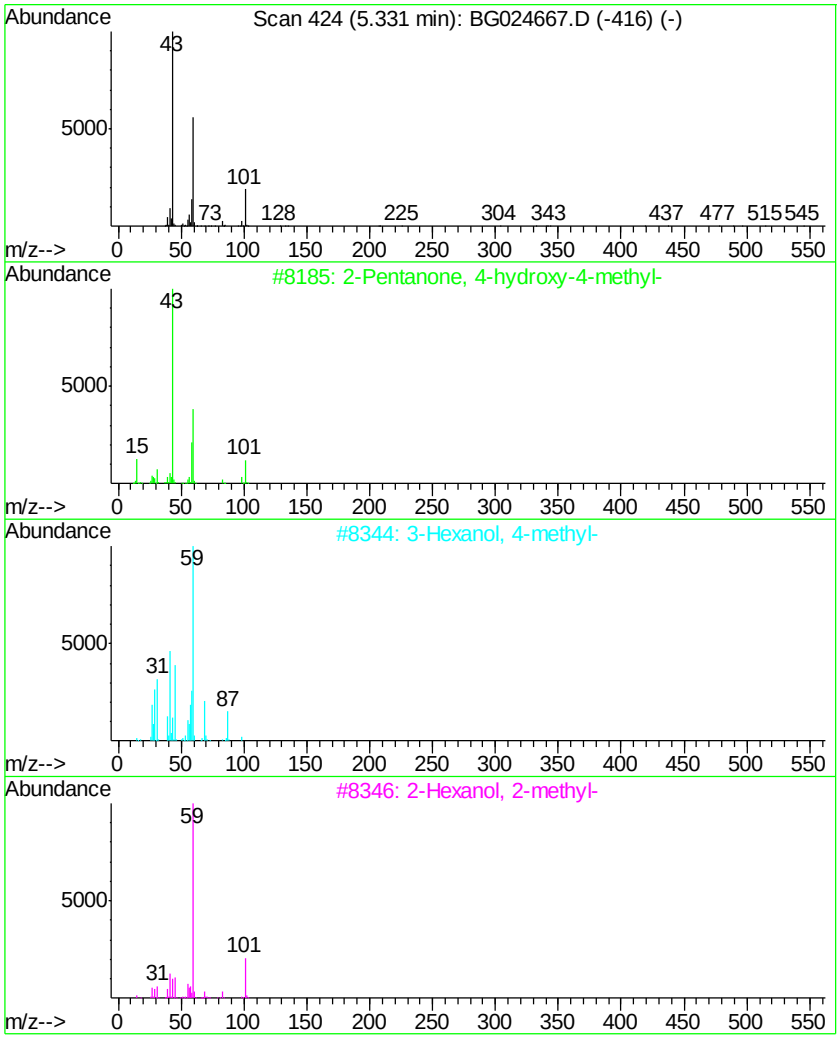
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

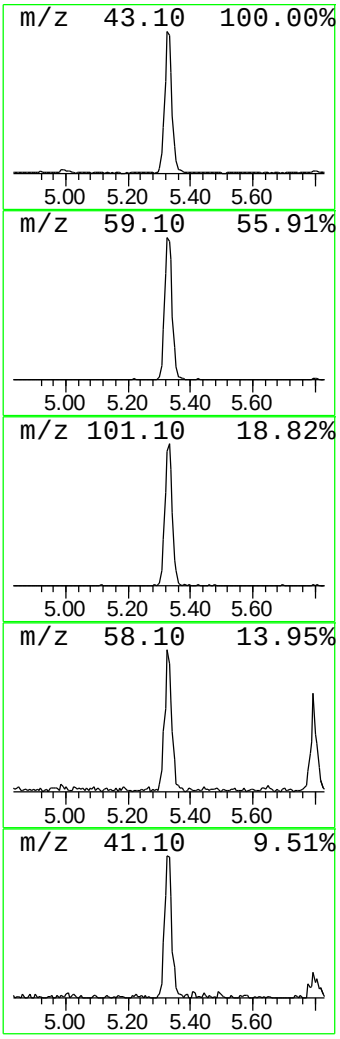
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	22.00 ng	797901	1,4-Dichlorobenzene-d4	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024667.D
Acq On : 4 Nov 2016 4:11
Operator : UM/SJ
Sample : H5509-13
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-97-0.5-1.0

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

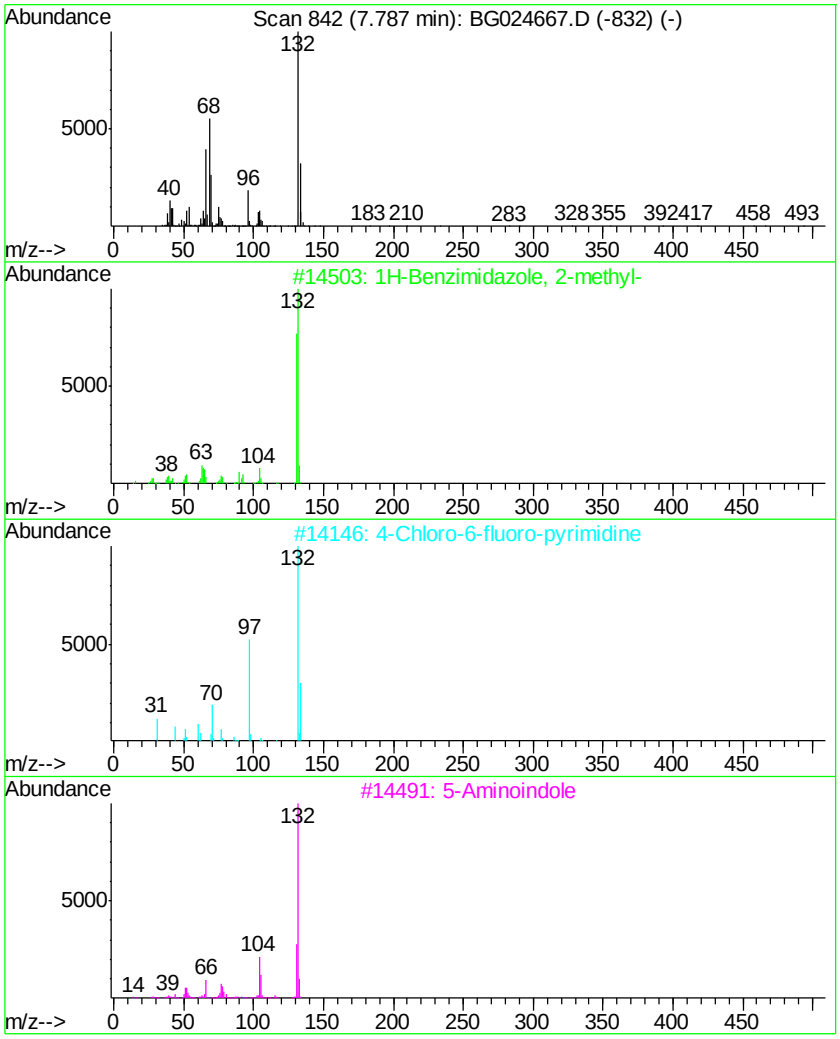
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

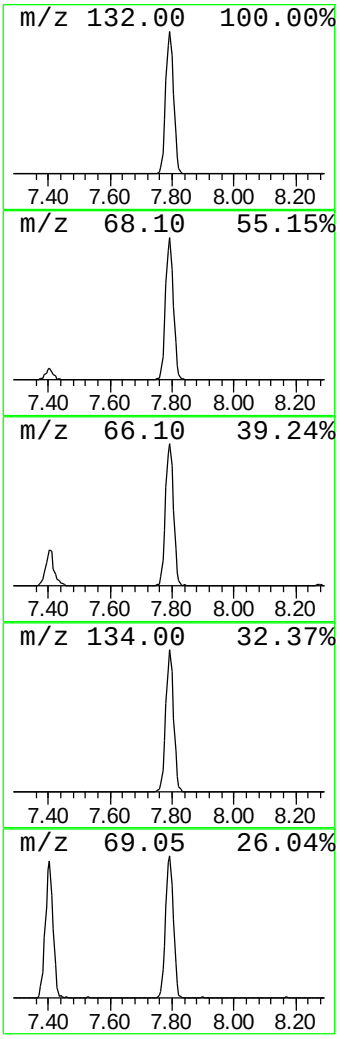
****

Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	107.36 ng	3893690	1,4-Dichlorobenzene-d4	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024667.D
Acq On : 4 Nov 2016 4:11
Operator : UM/SJ
Sample : H5509-13
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-97-0.5-1.0

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

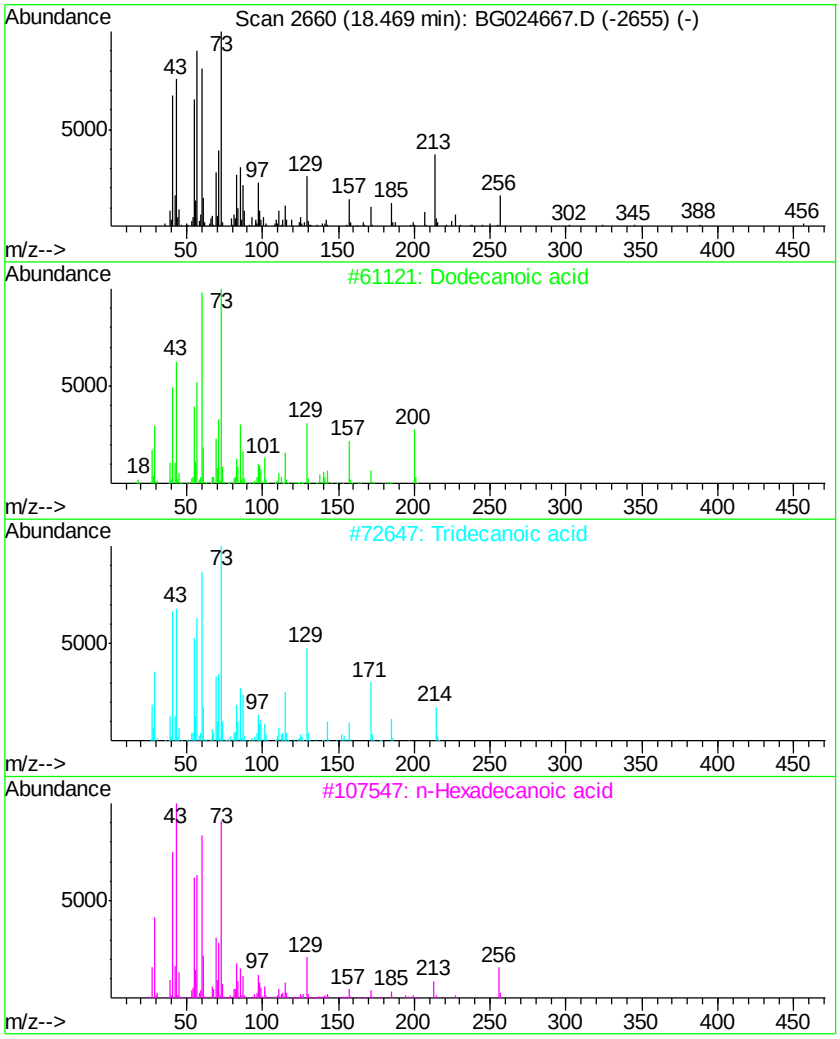
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

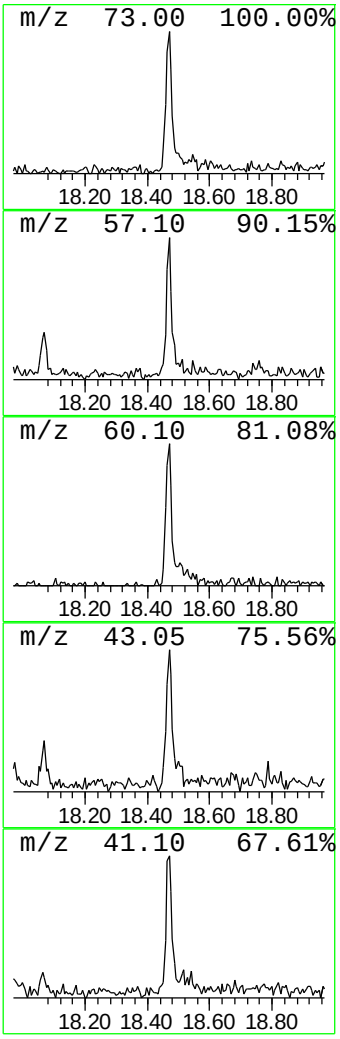
****

Peak Number 5 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.79 ng	273001	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	81
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5	Nonanoic acid	158	C9H18O2	000112-05-0	30





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024667.D
Acq On : 4 Nov 2016 4:11
Operator : UM/SJ
Sample : H5509-13
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-97-0.5-1.0

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

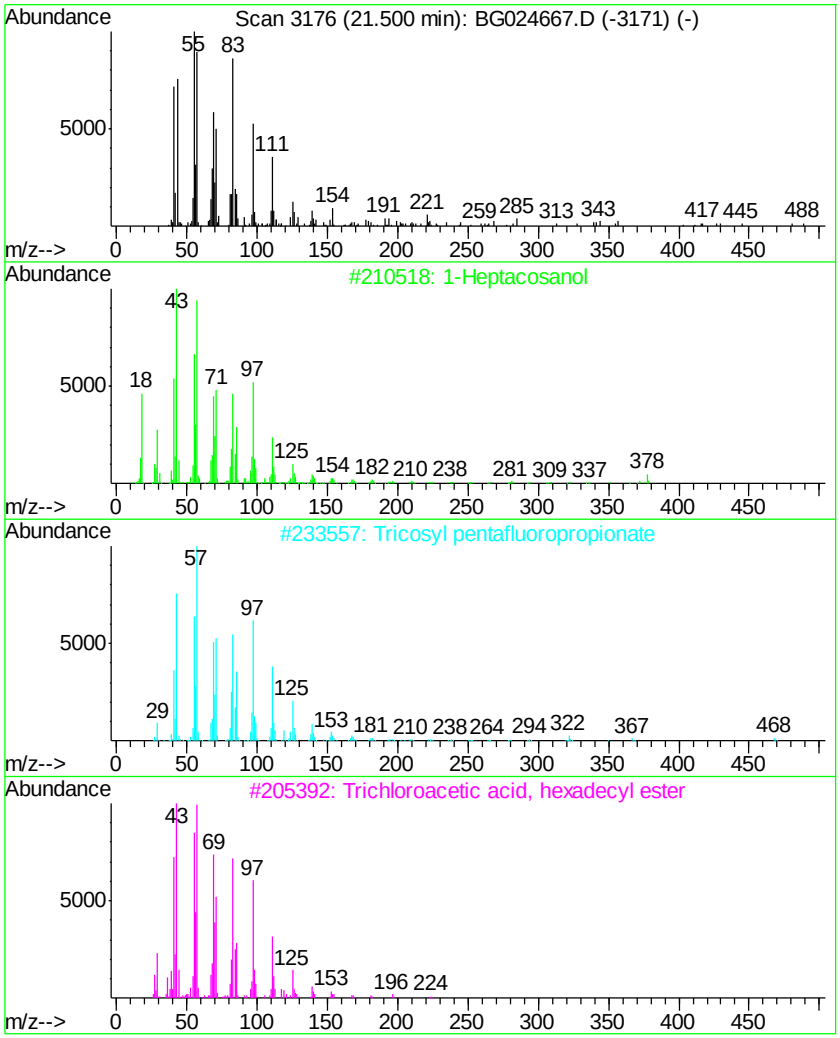
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

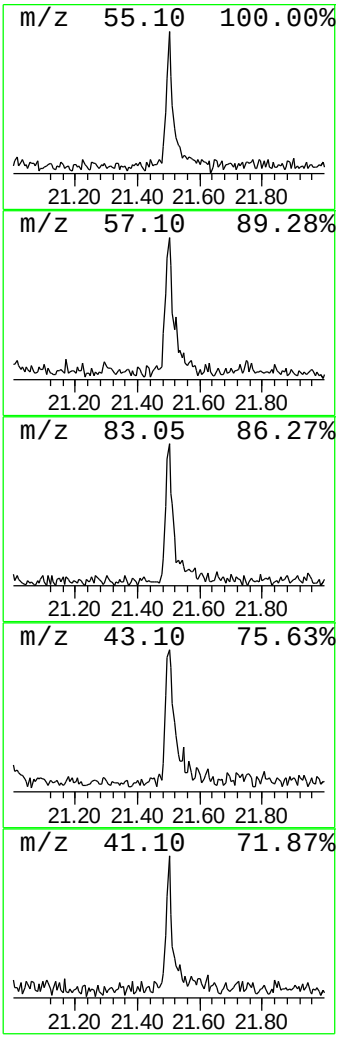
****

Peak Number 6 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	2.60 ng	344158	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	64
2	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	64
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	43
4	Cyclohexanecarboxylic acid, 3-tr...	310	C20H38O2	1000280-59-4	43
5	(2-Bromo-1,1,2,2-tetrafluoroethy...	262	C8H11BrF4	1000283-89-5	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024667.D
Acq On : 4 Nov 2016 4:11
Operator : UM/SJ
Sample : H5509-13
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-97-0.5-1.0

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

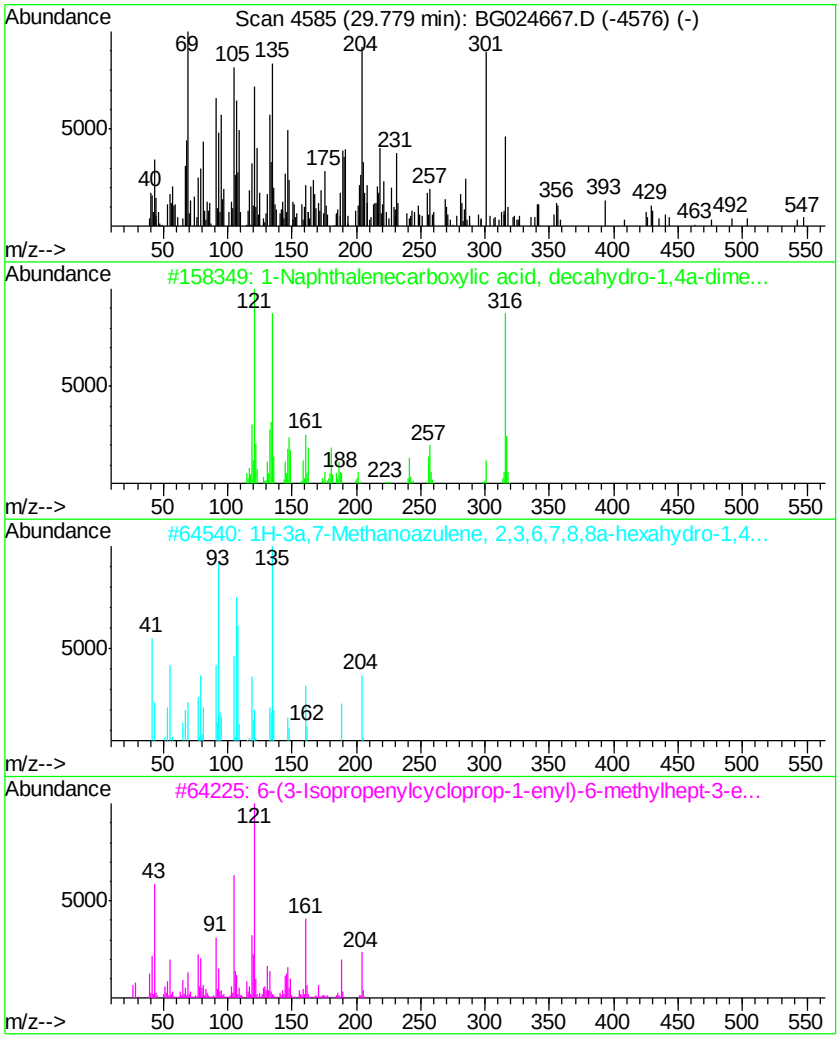
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

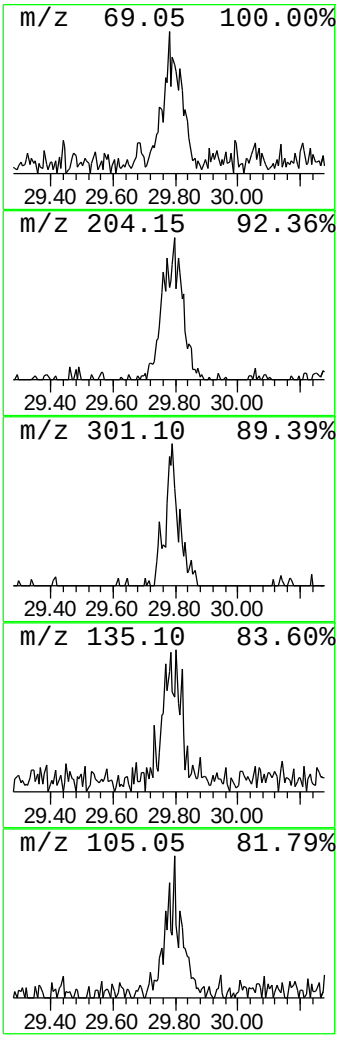
****

Peak Number 7 unknown29.78 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.78	5.88 ng	753954	Perylene-d12	25.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenecarboxylic acid, de...	316	C21H32O2	001235-39-8	38
2	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	30
3	6-(3-Isopropenylcycloprop-1-enyl...	204	C14H20O	1000195-43-0	30
4	(2S,4aS,5R,8aS)-2,5-Di(penta-3,4...	271	C19H29N	220024-80-6	25
5	4-Butoxy-N-(2-fluoro-benzyl)-ben...	301	C18H20FNO2	302569-92-2	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024667.D
Acq On : 4 Nov 2016 4:11
Operator : UM/SJ
Sample : H5509-13
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-97-0.5-1.0

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	338.4	ng	12273900	1	8.26	725357	20.0
2-Pentanone, 4-hy...	5.33	22.0	ng	797901	1	8.26	725357	20.0
unknown7.79	7.79	107.4	ng	3893690	1	8.26	725357	20.0
Dodecanoic acid	18.47	2.8	ng	273001	4	17.62	1960490	20.0
1-Heptacosanol	21.50	2.6	ng	344158	5	21.92	2647400	20.0
unknown29.78	29.78	5.9	ng	753954	6	25.35	2566370	20.0