LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

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-BG120215.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	2.993	20	26	38	rVB	89447	132557	7.31%	1.169%
2	5.190	391	400	407	rBV	85222	131180	7.23%	1.157%
3	5.660	472	480	488	rBV	405049	657413	36.24%	5.797%
4	7.258	744	752	767	rBV	452748	781678	43.09%	6.892%
5	7.640	810	817	825	rBV	440442	728989	40.19%	6.428%
6	8.116	891	898	905	rBV	111252	190533	10.50%	1.680%
7	8.439	944	953	960	rBV	288388	489134	26.97%	4.313%
8	9.280	1088	1096	1105	rBV	282764	491504	27.10%	4.334%
9	10.931	1370	1377	1384	rVB	165031	285711	15.75%	2.519%
10	13.369	1783	1792	1800	rBV	768109	1184537	65.30%	10.444%
11	14.186	1926	1931	1939	rBV	147137	211985	11.69%	1.869%
12	14.626	2001	2006	2012	rVB2	20873	26979	1.49%	0.238%
13	14.744	2019	2026	2034	rVB2	275471	442254	24.38%	3.899%
14	15.572	2163	2167	2173	rVB2	30651	38360	2.11%	0.338%
15	15.983	2229	2237	2240	rBV3	9164	18884	1.04%	0.167%
16	16.224	2270	2278	2288	rBV	640448	943064	51.99%	8.315%
17	16.436	2309	2314	2317	rBV	30936	43998	2.43%	0.388%
18	17.229	2443	2449	2453	rBV	17736	24474	1.35%	0.216%
19	17.482	2486	2492	2500	rBV	384688	574151	31.65%	5.062%
20	18.357	2636	2641	2647	rBV	72160	101385	5.59%	0.894%
21	18.880	2724	2730	2733	rBV2	11963	21518	1.19%	0.190%
22	19.215	2782	2787	2794	rBV2	24499	35773	1.97%	0.315%
23	19.620	2851	2856	2860	rBV4	27500	35066	1.93%	0.309%
24	19.773	2875	2882	2887	rBV3	75539	107327	5.92%	0.946%
25	19.885	2898	2901	2906	rVB2	26705	30322	1.67%	0.267%
26	20.085	2929	2935	2940	rBV	1424378	1813889	100.00%	15.993%
27	20.813	3055	3059	3067	rVV	59409	75749	4.18%	0.668%
28	20.878	3067	3070	3073	rVV	16362	18854	1.04%	0.166%
29	21.383	3152	3156	3164	rVB2	104392	152637	8.41%	1.346%
30	21.753	3212	3219	3226	rBV	455831	753606	41.55%	6.645%
31	21.947	3248	3252	3257	rVB3	21730	34658	1.91%	0.306%
32	22.570	3354	3358	3365	rBV4	17015	30580	1.69%	0.270%
33	23.275	3475	3478	3485	rVB4	13028	21314	1.18%	0.188%
34	24.109	3614	3620	3623	rBV7	11917	21998	1.21%	0.194%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

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-BG120215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	25.038	3767	3778	3792	rBV2	244681	689429	38.01%	6.079%

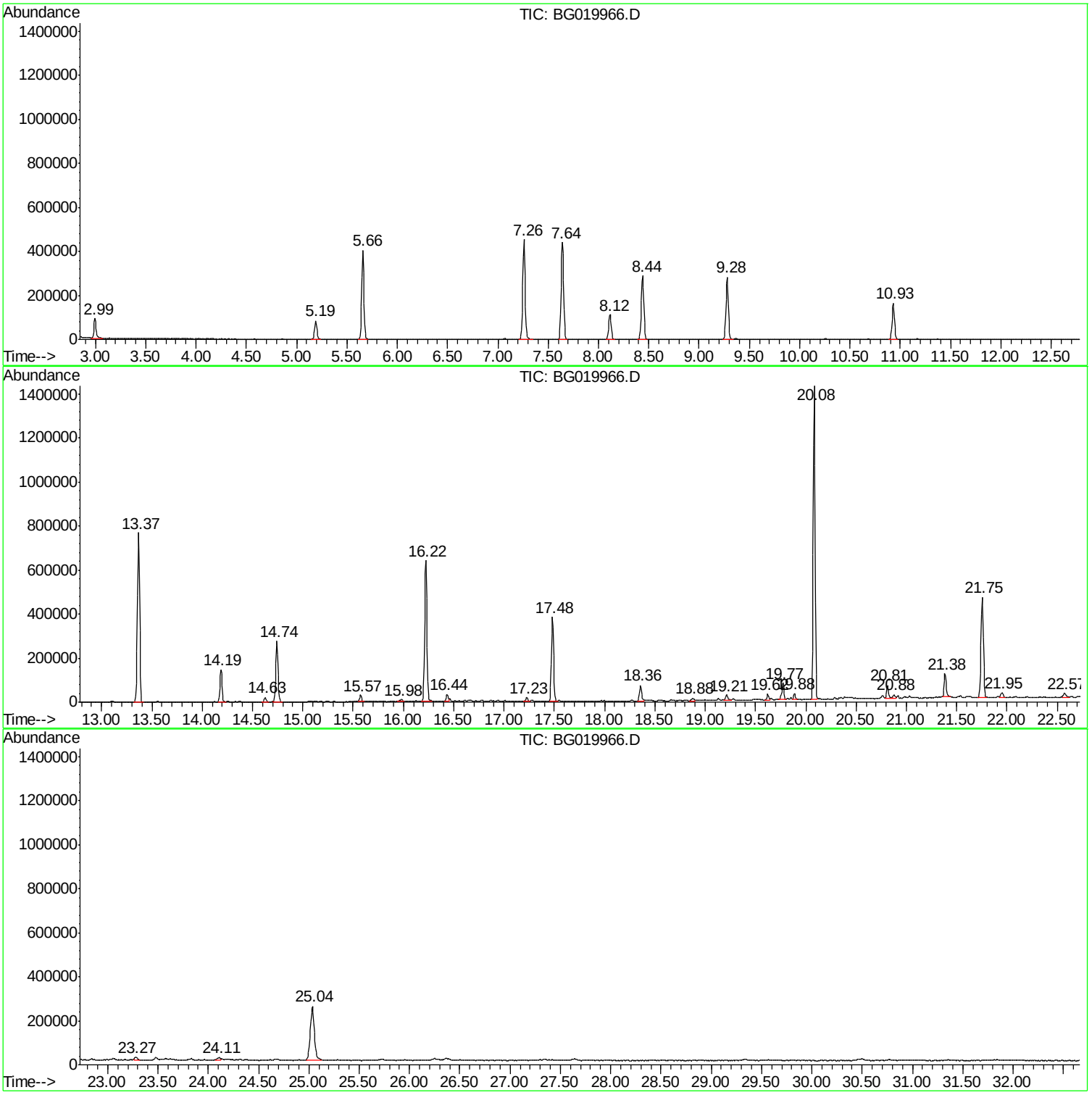
Sum of corrected areas: 11341490

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

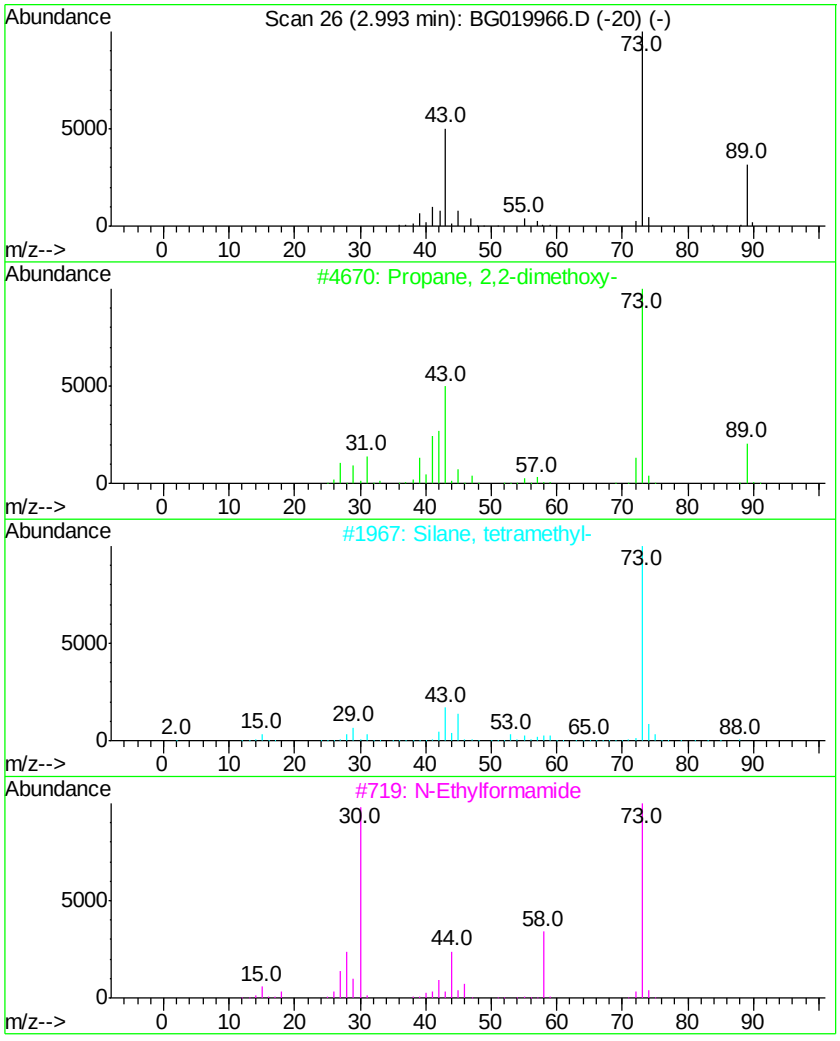
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

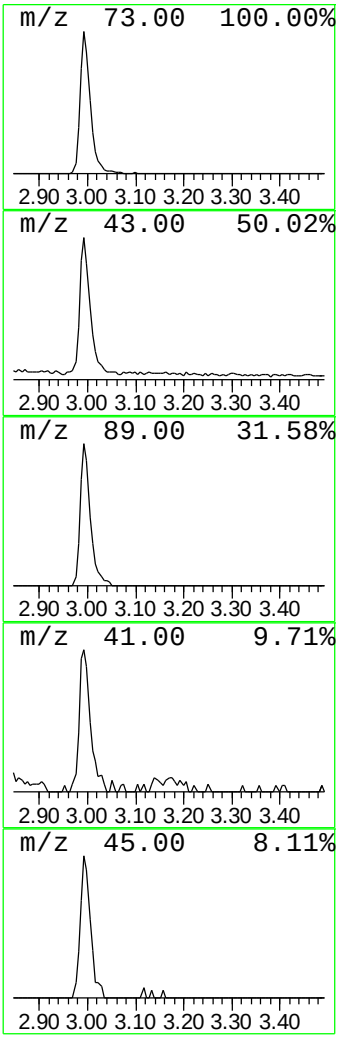
****

Peak Number 1 unknown2.99 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	13.91 ng	132557	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

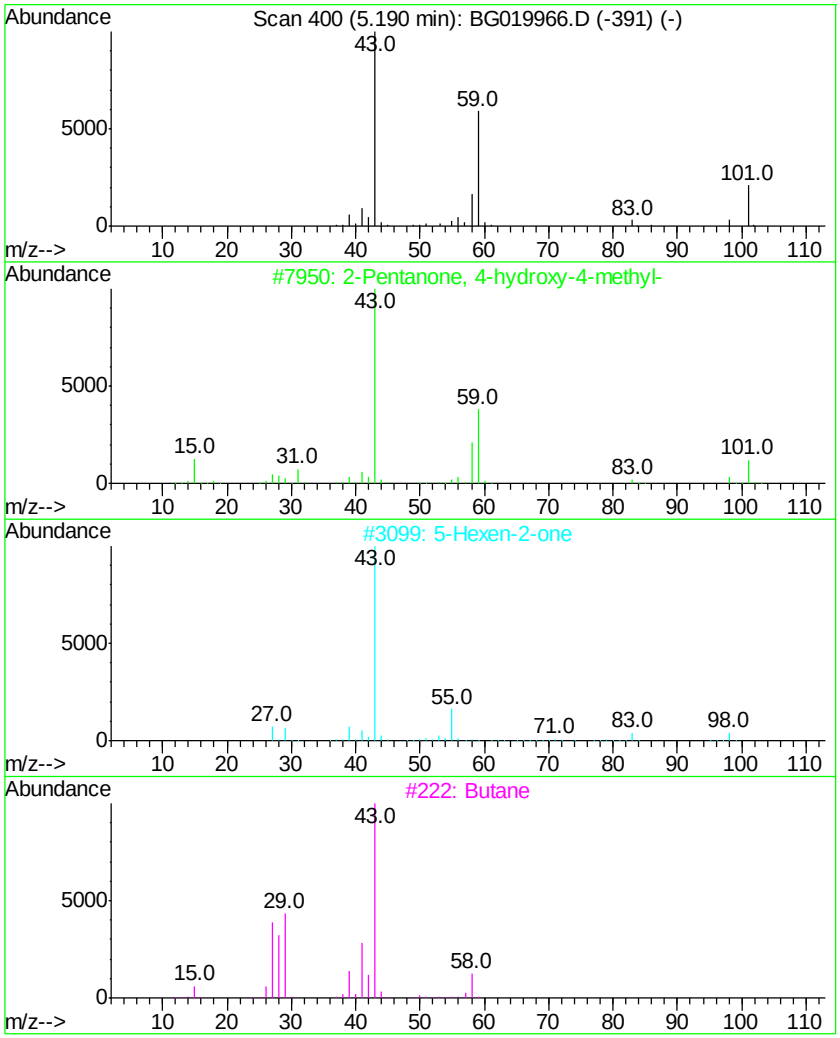
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

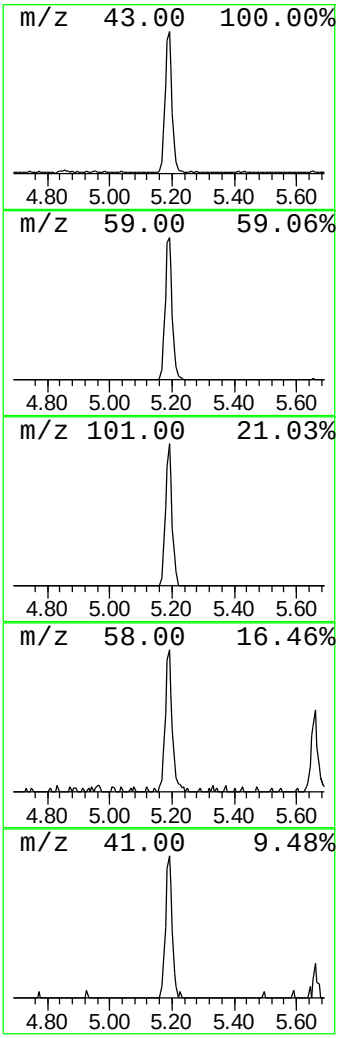
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	13.77 ng	131180	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Butane	58	C4H10	000106-97-8	9
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5	2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

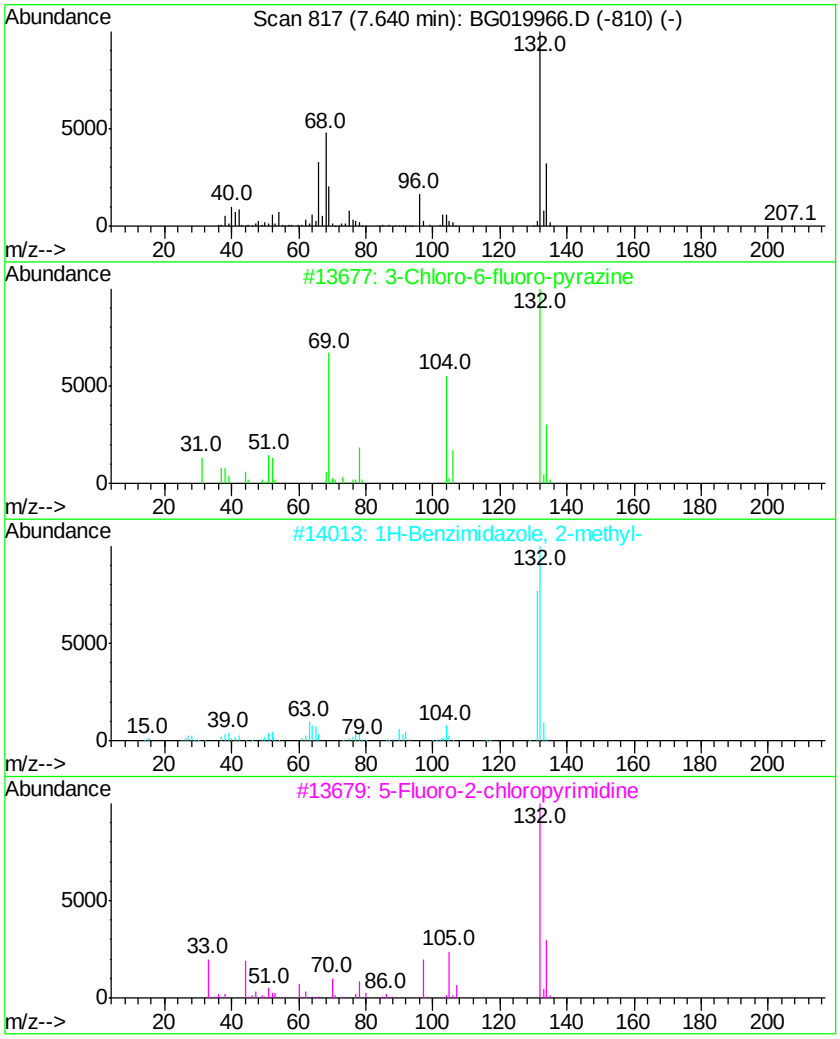
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

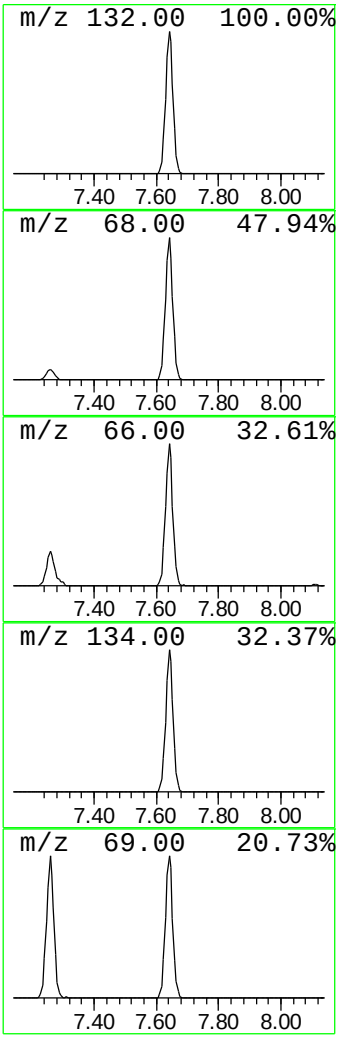
****

Peak Number 3 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	76.52 ng	728989	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

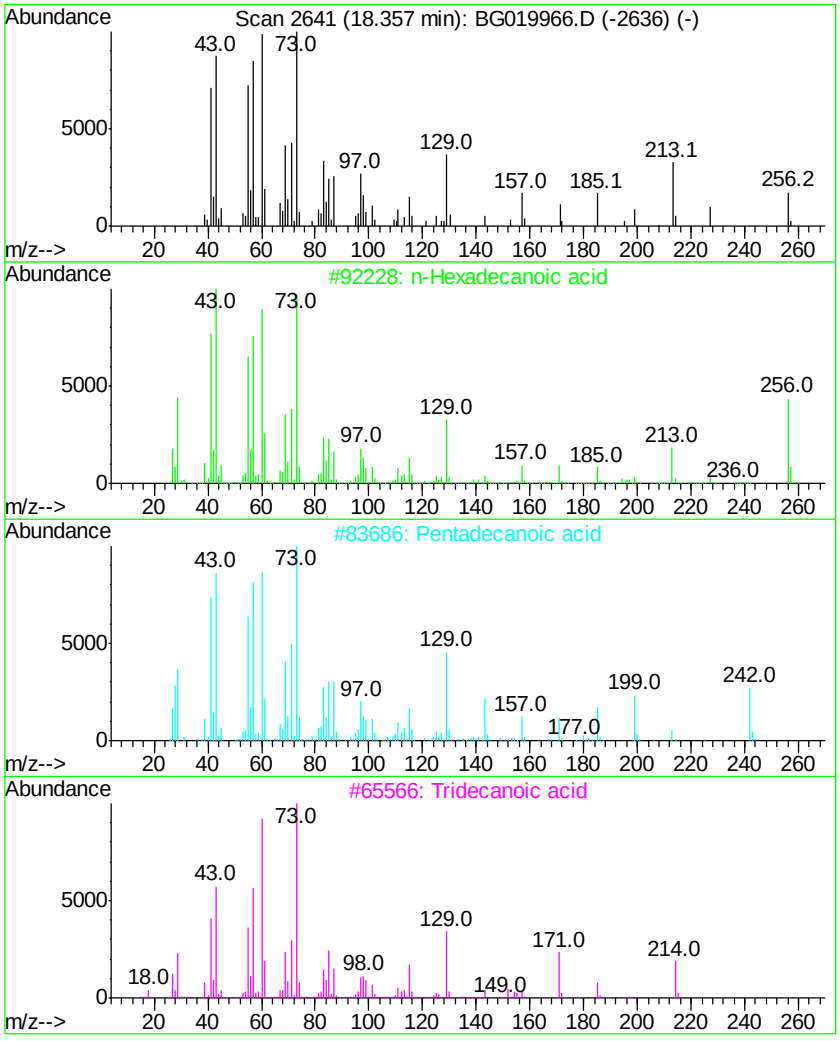
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

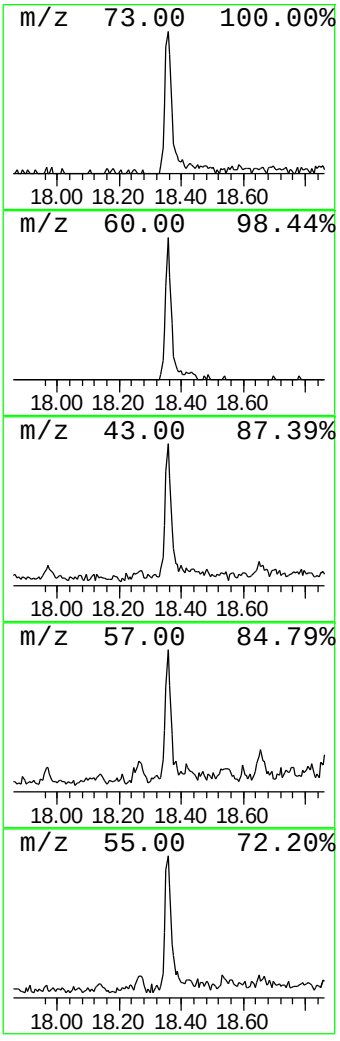
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	3.53 ng	101385	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

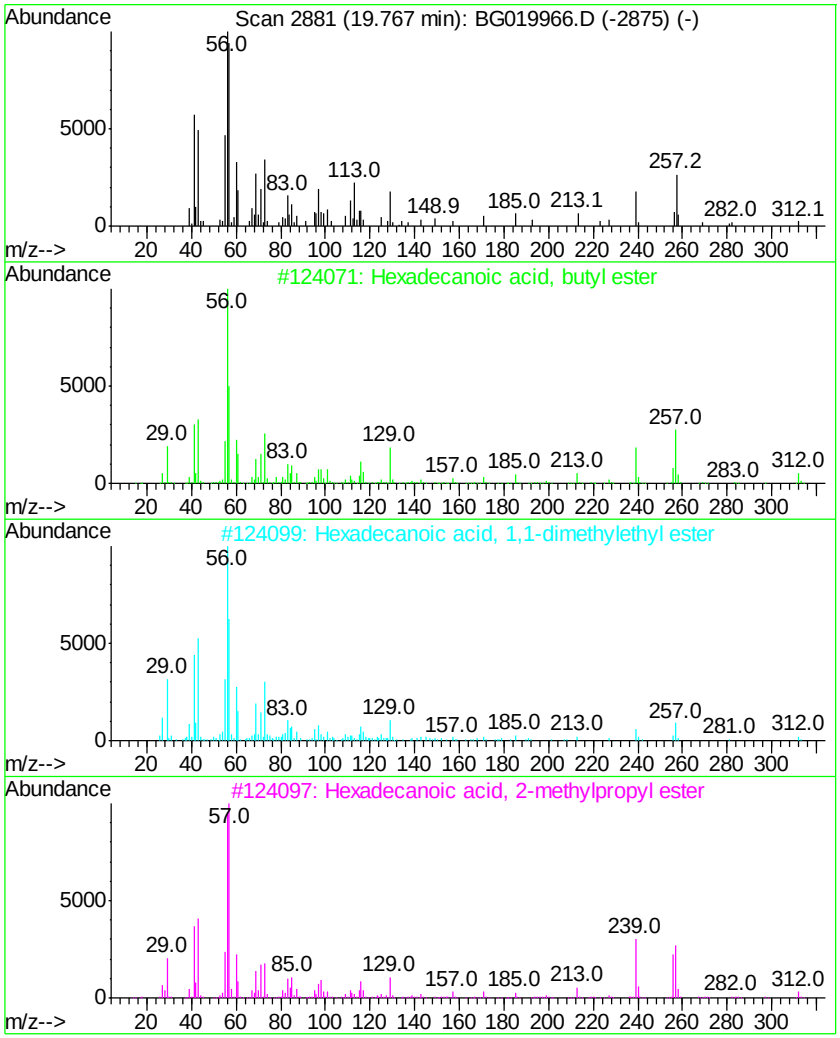
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

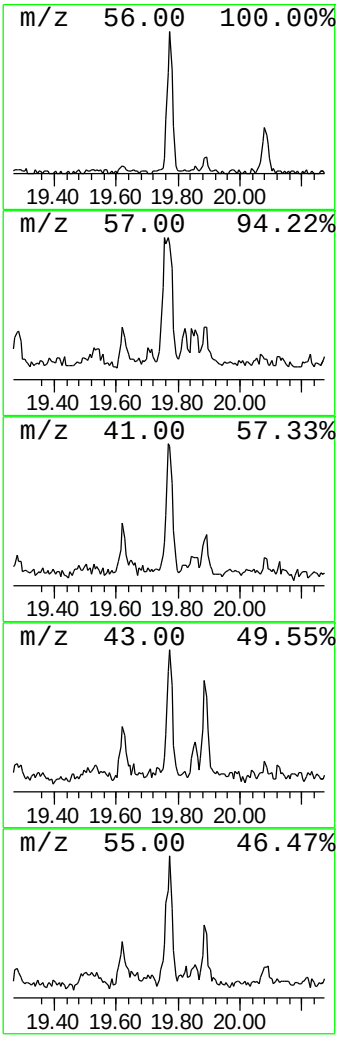
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	2.85 ng	107327	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	35
4	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	35
5	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	25





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

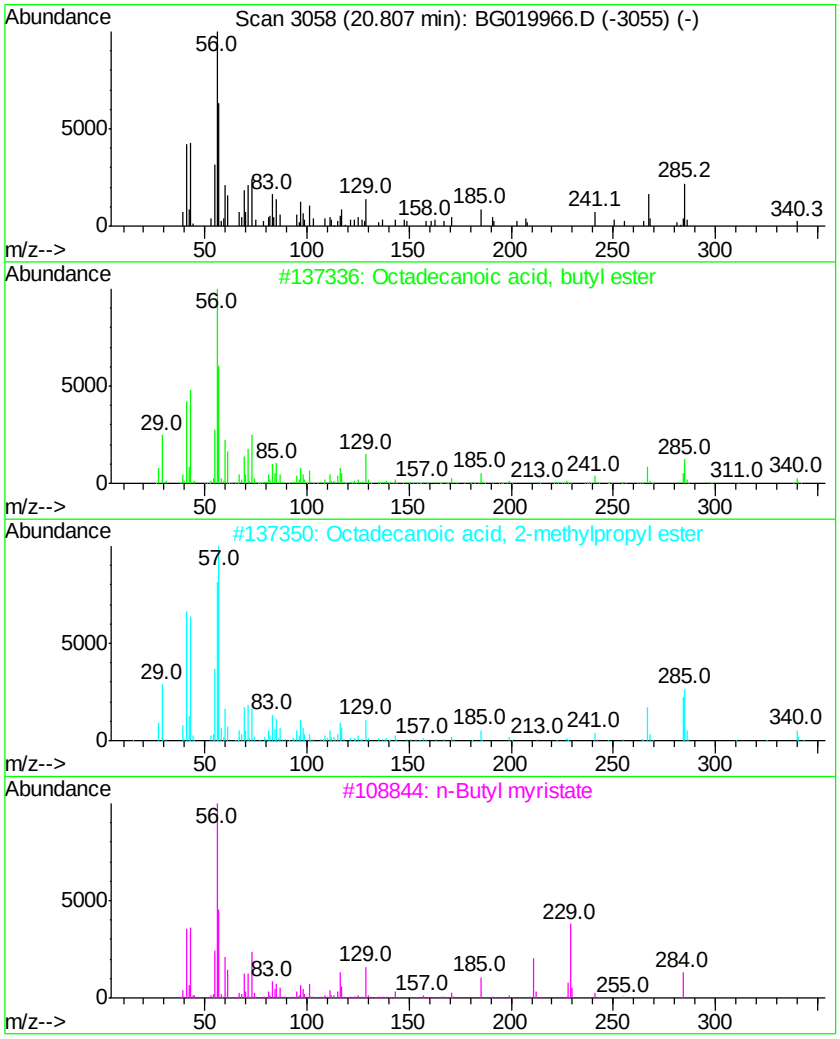
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

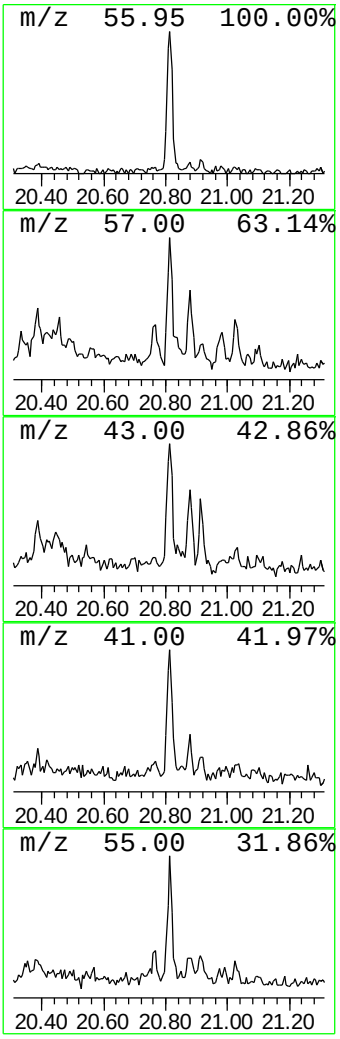
****

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.81	2.01 ng	75749	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	68
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	59
3	n-Butyl myristate	284	C18H36O2	000110-36-1	43
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	30
5	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	27





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

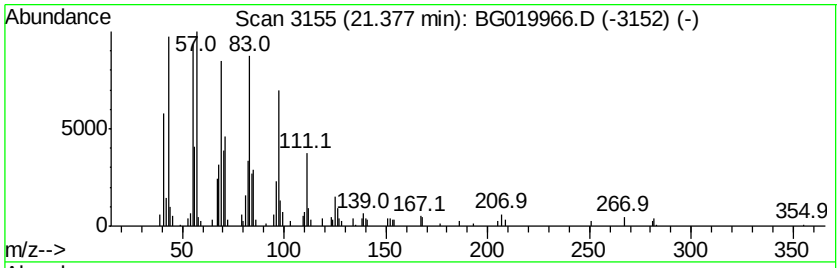
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

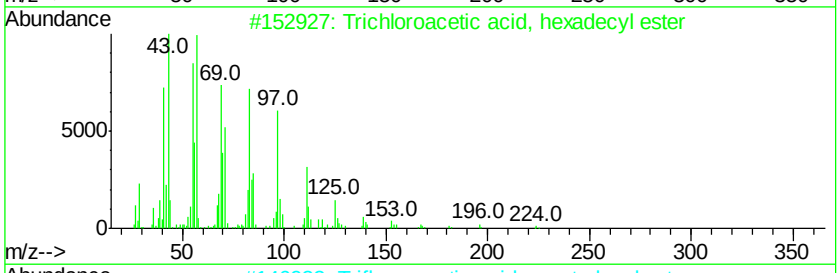
****

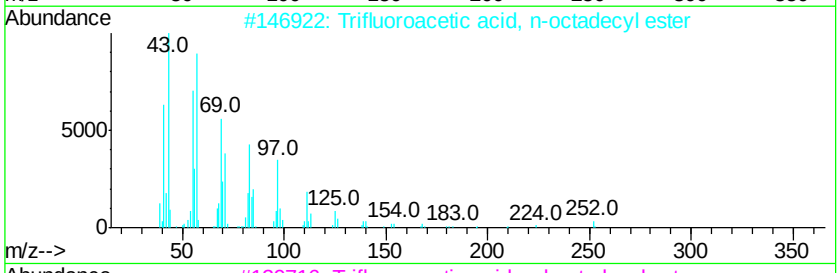
Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 5

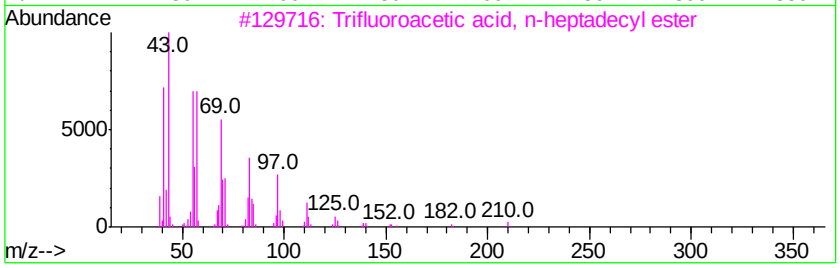
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	4.05 ng	152637	Chrysene-d12	21.75

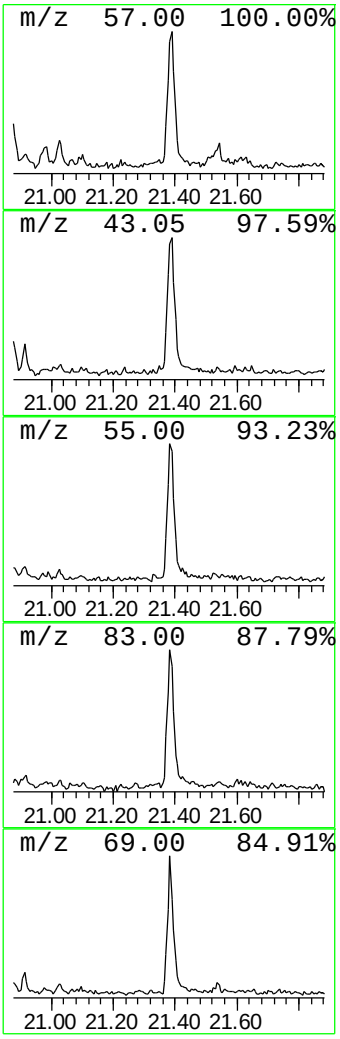
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
4	Cyclotetradecane	196	C14H28	000295-17-0	87
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	87











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120615\
Data File : BG019966.D
Acq On : 6 Dec 2015 14:28
Operator : UM/NP
Sample : G4650-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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
unknown2.99	2.99	13.9	ng	132557	1	8.12	190533	20.0
2-Pentanone, 4-hy...	5.19	13.8	ng	131180	1	8.12	190533	20.0
unknown7.64	7.64	76.5	ng	728989	1	8.12	190533	20.0
n-Hexadecanoic acid	18.36	3.5	ng	101385	4	17.48	574151	20.0
Hexadecanoic acid...	19.77	2.9	ng	107327	5	21.75	753606	20.0
Octadecanoic acid...	20.81	2.0	ng	75749	5	21.75	753606	20.0
Trichloroacetic a...	21.38	4.0	ng	152637	5	21.75	753606	20.0