LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121315\
Data File : BG020141.D
Acq On : 13 Dec 2015 12:44
Operator : UM/SJ
Sample : G4772-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALE-FILL-SOURCE-6A

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	2.979	18	24	43	rVV	1504048	2123147	100.00%	22.663%
2	5.171	391	397	407	rVB	70424	104134	4.90%	1.112%
3	5.647	471	478	489	rVB	295630	461700	21.75%	4.928%
4	7.251	743	751	761	rBV	310859	529526	24.94%	5.652%
5	7.627	808	815	821	rBV	307001	508812	23.96%	5.431%
6	8.097	889	895	901	rBV	66320	109492	5.16%	1.169%
7	8.426	943	951	957	rBV	215709	368520	17.36%	3.934%
8	9.266	1086	1094	1102	rVB	192521	327450	15.42%	3.495%
9	10.917	1368	1375	1381	rBV	94649	161733	7.62%	1.726%
10	13.350	1780	1789	1796	rBV	513744	792457	37.32%	8.459%
11	14.172	1921	1929	1935	rBV	70109	101608	4.79%	1.085%
12	14.730	2017	2024	2031	rVB2	163593	265856	12.52%	2.838%
13	16.211	2265	2276	2291	rBV	553539	823643	38.79%	8.792%
14	16.417	2306	2311	2321	rBV	13996	24138	1.14%	0.258%
15	17.468	2483	2490	2497	rBV	253564	373724	17.60%	3.989%
16	18.338	2632	2638	2643	rBV	31675	40348	1.90%	0.431%
17	19.190	2778	2783	2792	rBV3	17460	28010	1.32%	0.299%
18	20.071	2927	2933	2940	rBV	974173	1312928	61.84%	14.014%
19	21.364	3149	3153	3164	rVB	38513	60348	2.84%	0.644%
20	21.740	3209	3217	3223	rBV	267647	446270	21.02%	4.764%
21	25.001	3762	3772	3786	rVB	144728	404625	19.06%	4.319%

Sum of corrected areas: 9368469

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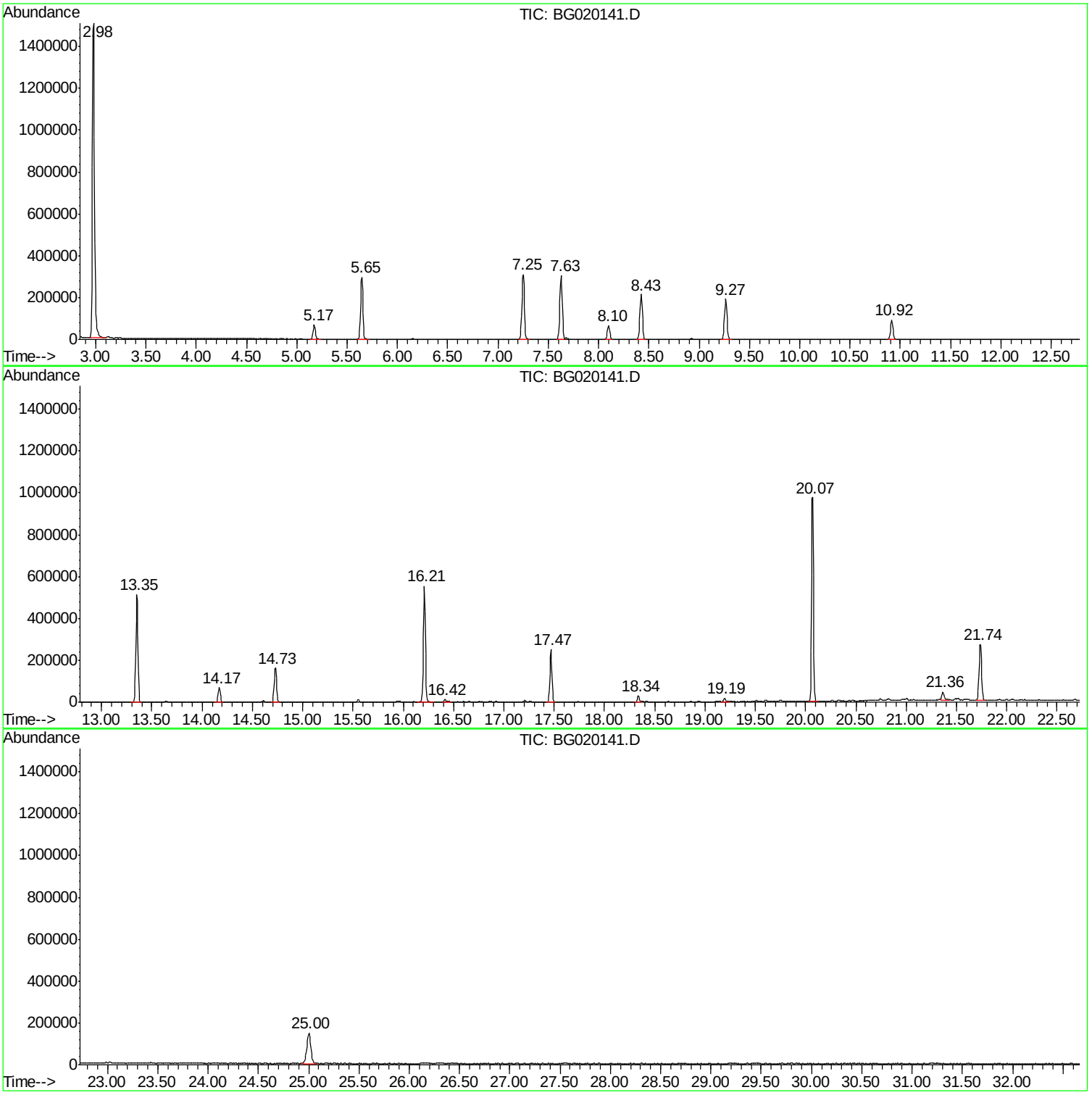
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VITALE-FILL-SOURCE-6A

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



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Data File : BG020141.D
Acq On : 13 Dec 2015 12:44
Operator : UM/SJ
Sample : G4772-05
Misc :
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Instrument : BNA_G
ClientSampleId : VITALE-FILL-SOURCE-6A

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

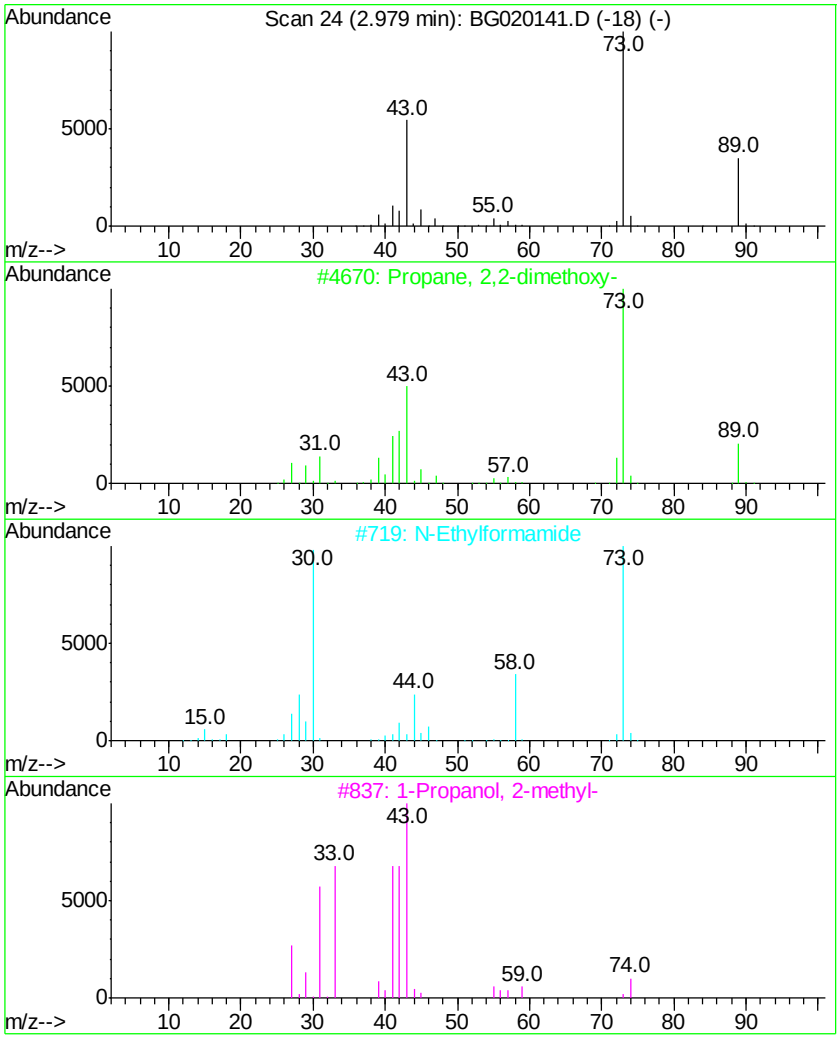
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

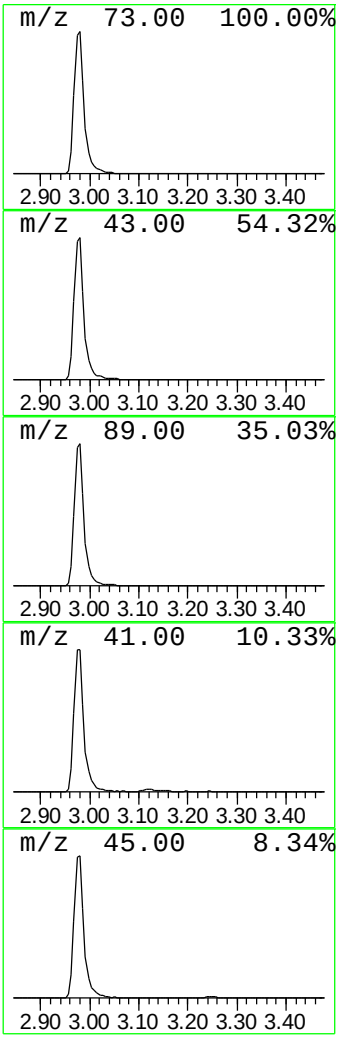
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	387.82 ng	2123150	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121315\
Data File : BG020141.D
Acq On : 13 Dec 2015 12:44
Operator : UM/SJ
Sample : G4772-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VITALE-FILL-SOURCE-6A

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

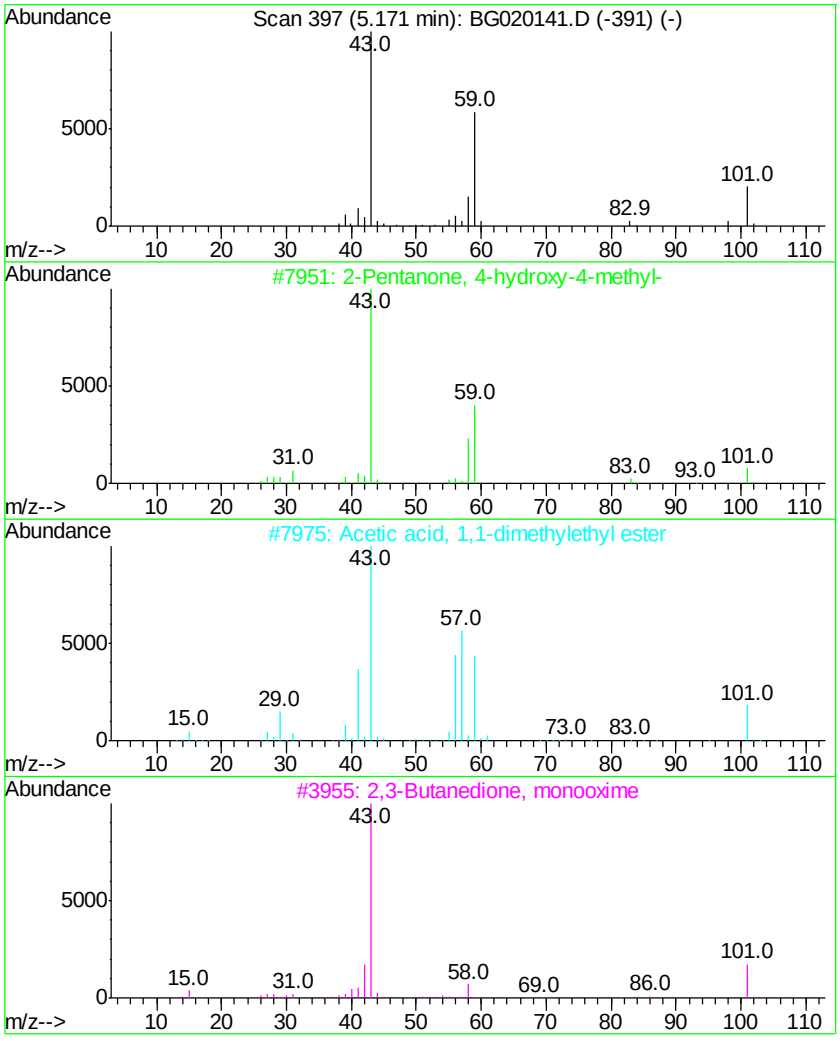
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

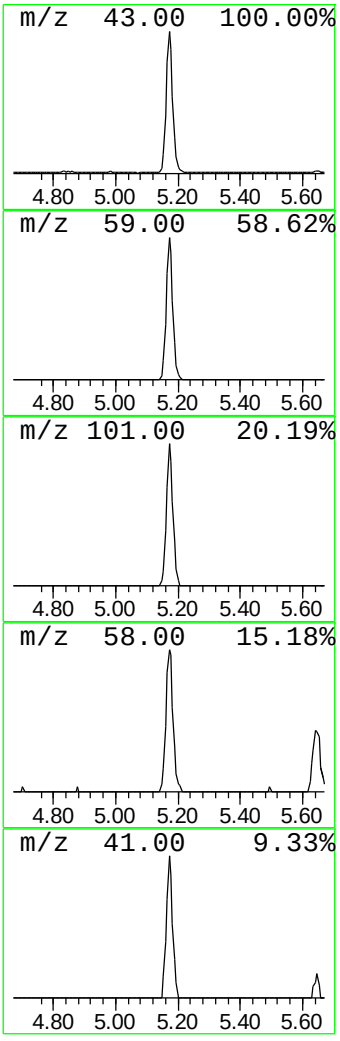
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	19.02 ng	104134	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	t-Butyl ethyl ether	102	C6H14O	1000118-18-4	17
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121315\
Data File : BG020141.D
Acq On : 13 Dec 2015 12:44
Operator : UM/SJ
Sample : G4772-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALE-FILL-SOURCE-6A

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

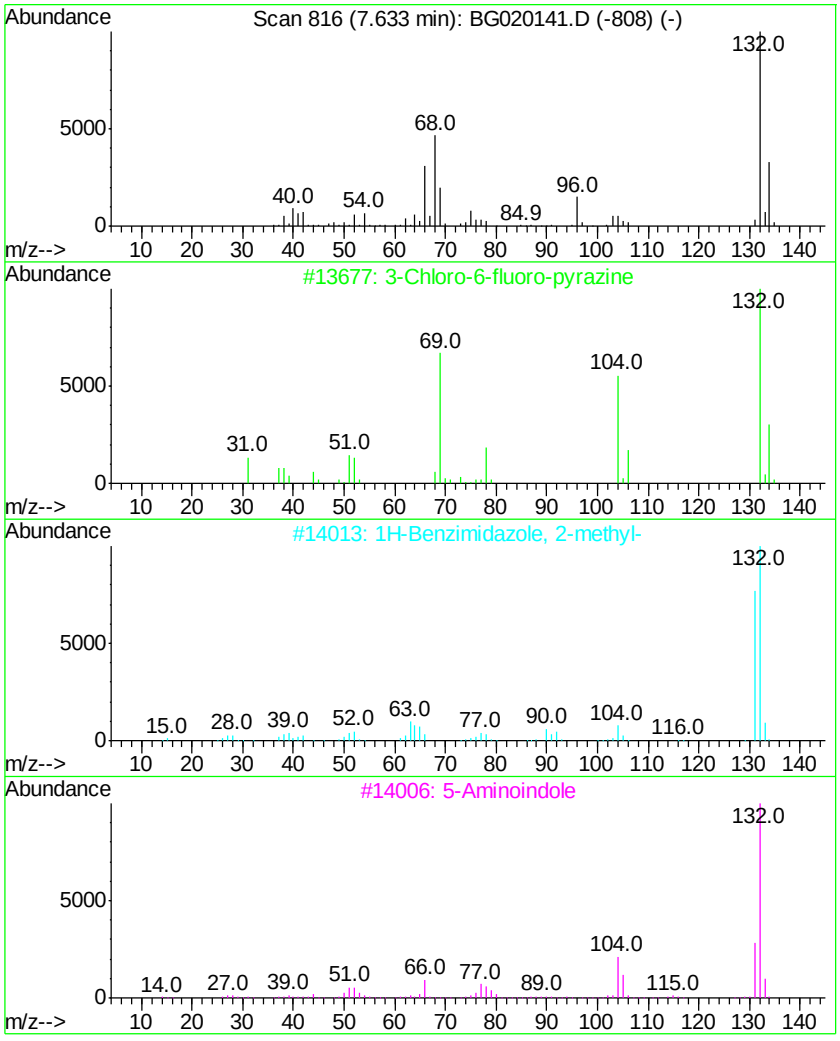
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

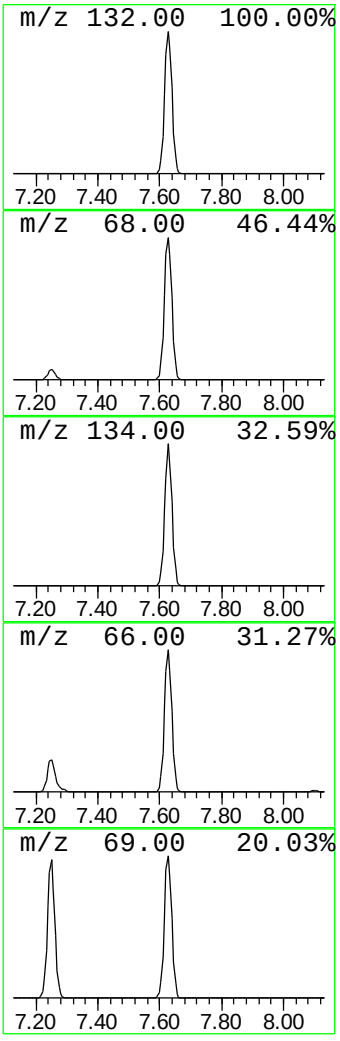
****

Peak Number 3 unknown7.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	92.94 ng	508812	1,4-Dichlorobenzene-d4	8.10

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-Aminoindole	132	C8H8N2	005192-03-0	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG121315\
Data File : BG020141.D
Acq On : 13 Dec 2015 12:44
Operator : UM/SJ
Sample : G4772-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALE-FILL-SOURCE-6A

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
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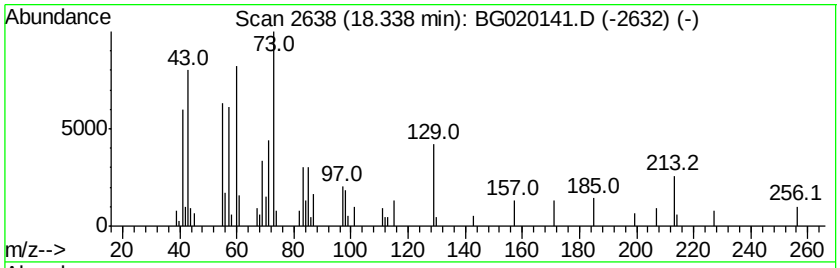
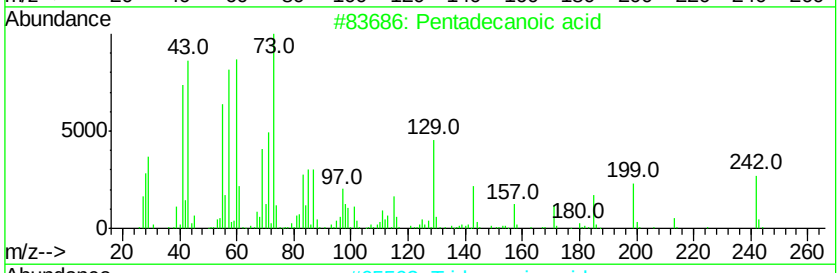
****

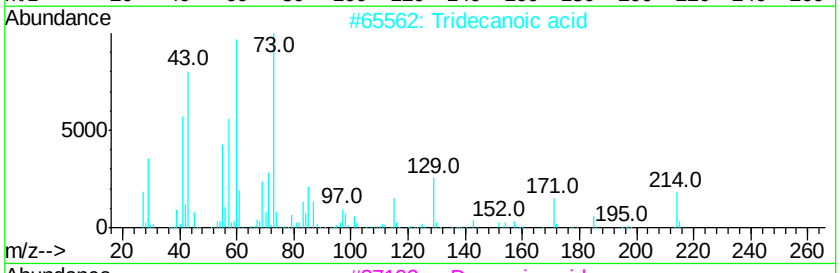
Peak Number 5 Pentadecanoic acid Concentration Rank 6

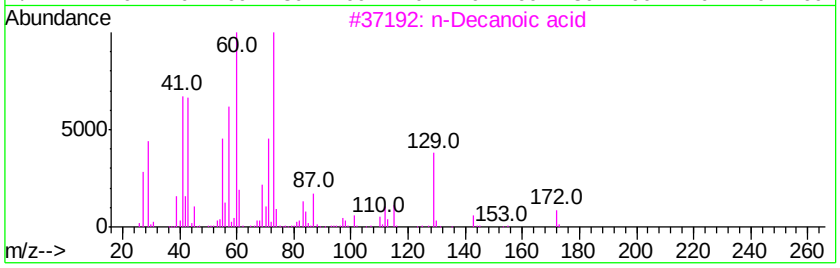
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	2.16 ng	40348	Phenanthrene-d10	17.47

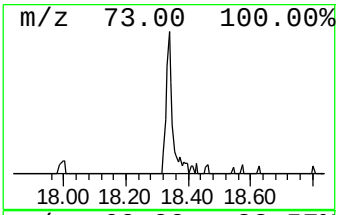
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
2	Tridecanoic acid	214	C13H26O2	000638-53-9	62
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35
5	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	10

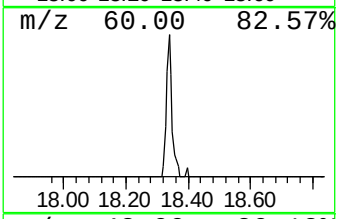


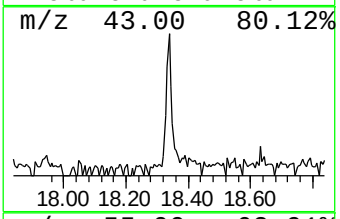


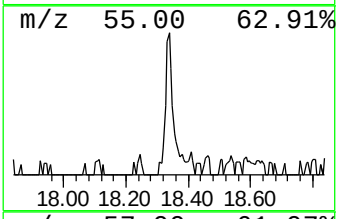


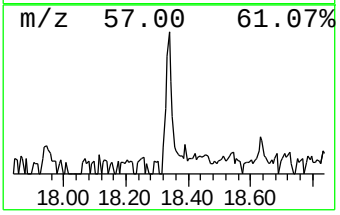












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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

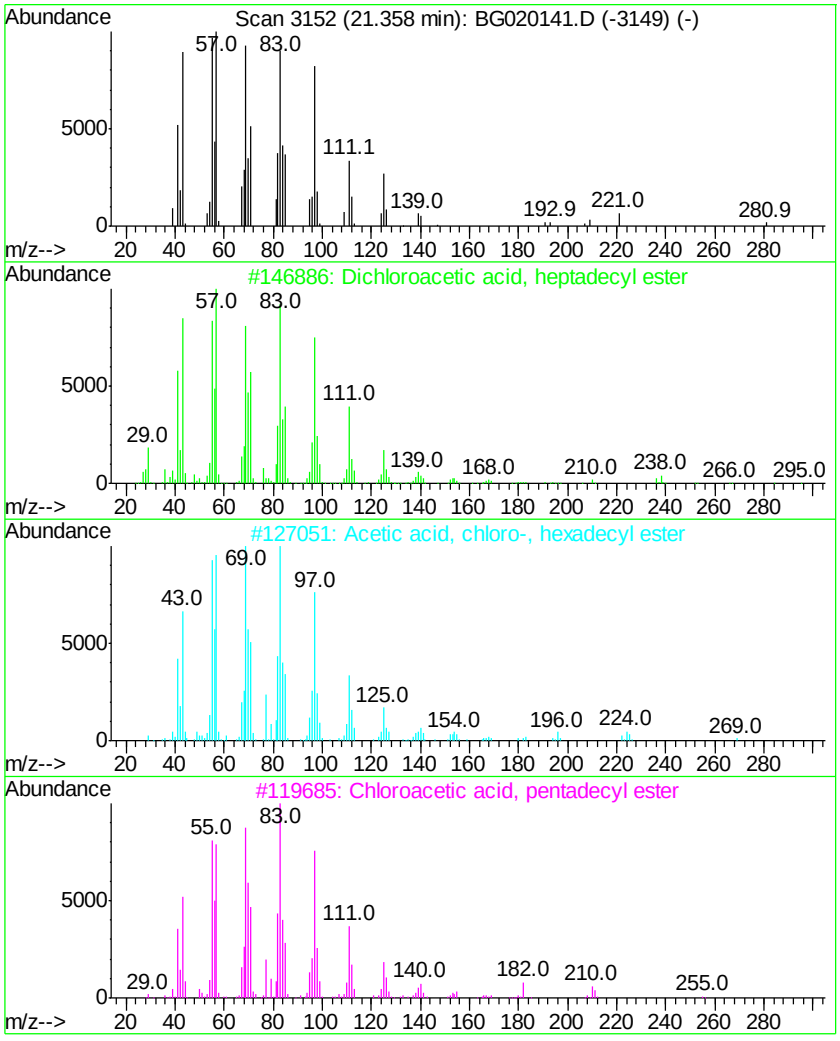
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

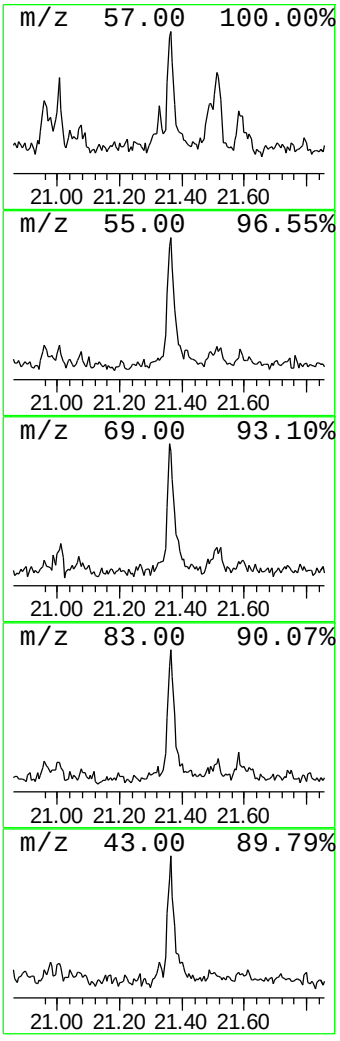
****

Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.36	2.70 ng	60348	Chrysene-d12	21.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
3	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	91
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	90





Tentatively Identified Compound (LSC) summary

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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
Propane, 2,2-dime...	2.98	387.8	ng	2123150	1	8.10	109492	20.0
2-Pentanone, 4-hy...	5.17	19.0	ng	104134	1	8.10	109492	20.0
unknown7.63	7.63	92.9	ng	508812	1	8.10	109492	20.0
Pentadecanoic acid	18.34	2.2	ng	40348	4	17.47	373724	20.0
Dichloroacetic ac...	21.36	2.7	ng	60348	5	21.74	446270	20.0