LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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	3.179	11	15	43	rVB	415553	721809	43.12%	8.093%
2	3.608	84	88	94	rVB2	24811	33722	2.01%	0.378%
3	3.925	137	142	149	rVB	22461	34263	2.05%	0.384%
4	4.531	239	245	259	rBV	403954	664762	39.71%	7.454%
5	5.142	345	349	355	rVB2	11620	19508	1.17%	0.219%
6	5.606	422	428	440	rBV	110224	192945	11.53%	2.163%
7	7.210	694	701	704	rBV	72049	140291	8.38%	1.573%
8	7.586	757	765	774	rBV	197624	356104	21.27%	3.993%
9	8.056	839	845	852	rBV	93435	163501	9.77%	1.833%
10	8.379	893	900	911	rVB	262624	489977	29.27%	5.494%
11	9.237	1038	1046	1059	rBV	234706	446180	26.65%	5.003%
12	10.153	1195	1202	1207	rBV5	9492	20519	1.23%	0.230%
13	10.876	1317	1325	1334	rBV	121287	226569	13.53%	2.540%
14	13.314	1732	1740	1750	rBV	625317	1005213	60.05%	11.271%
15	14.137	1874	1880	1893	rBV	101215	162633	9.72%	1.824%
16	14.695	1968	1975	1984	rBV2	186455	307886	18.39%	3.452%
17	15.494	2106	2111	2117	rVB	46045	64142	3.83%	0.719%
18	16.182	2222	2228	2240	rBV3	335334	563878	33.68%	6.322%
19	17.445	2436	2443	2452	rBV2	288903	460144	27.49%	5.159%
20	18.303	2584	2589	2599	rBV	90794	162827	9.73%	1.826%
21	19.572	2800	2805	2821	rVB	53154	89597	5.35%	1.005%
22	20.042	2879	2885	2898	rBV	1247619	1674034	100.00%	18.770%
23	21.722	3164	3171	3181	rVB	313062	536550	32.05%	6.016%
24	23.173	3409	3418	3425	rBV6	12564	28870	1.72%	0.324%
25	23.990	3550	3557	3563	rBV3	13216	28058	1.68%	0.315%
26	24.948	3712	3720	3723	rBV7	10412	25983	1.55%	0.291%
27	25.018	3723	3732	3745	rVB2	91462	298670	17.84%	3.349%

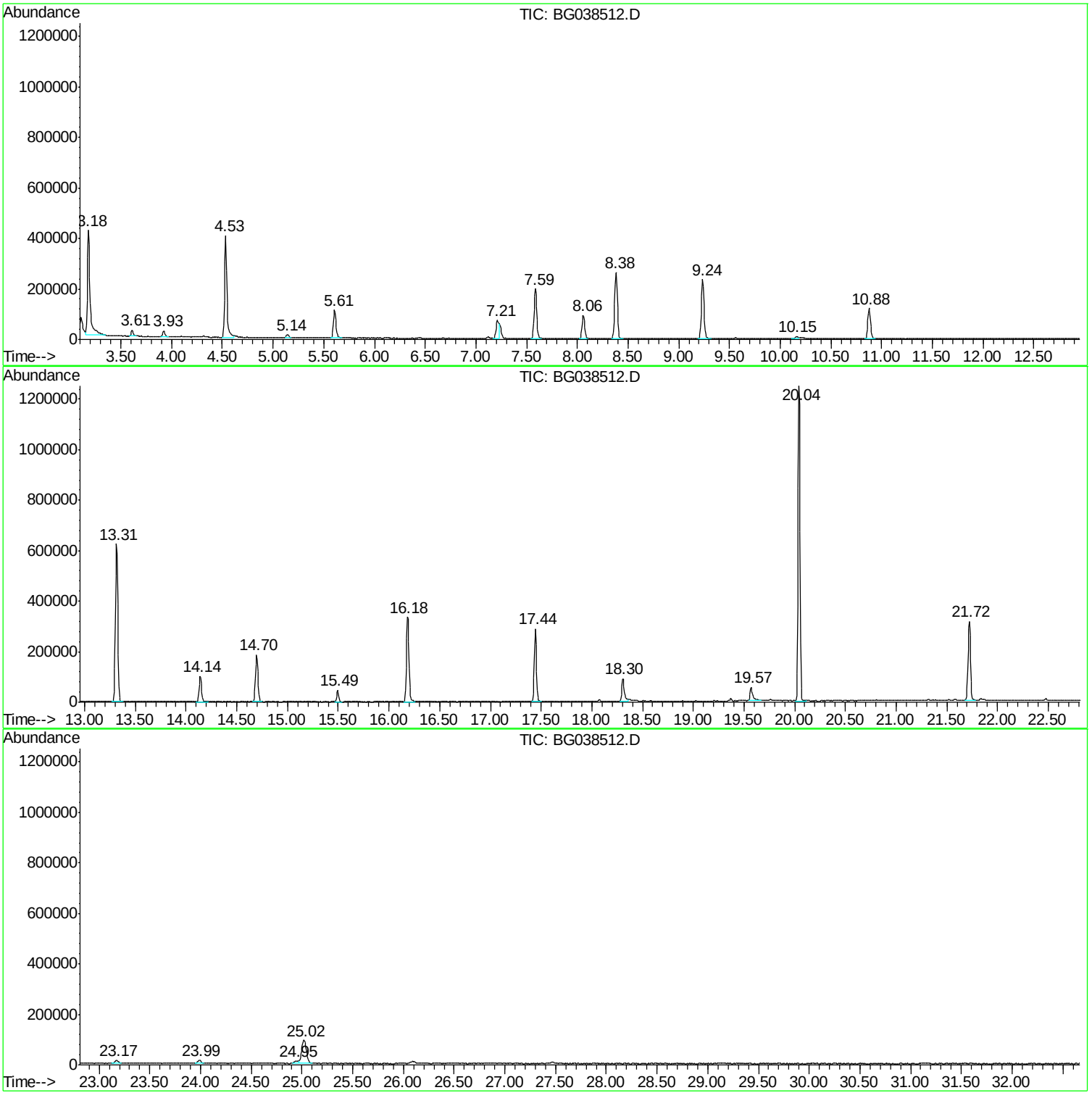
Sum of corrected areas: 8918635

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

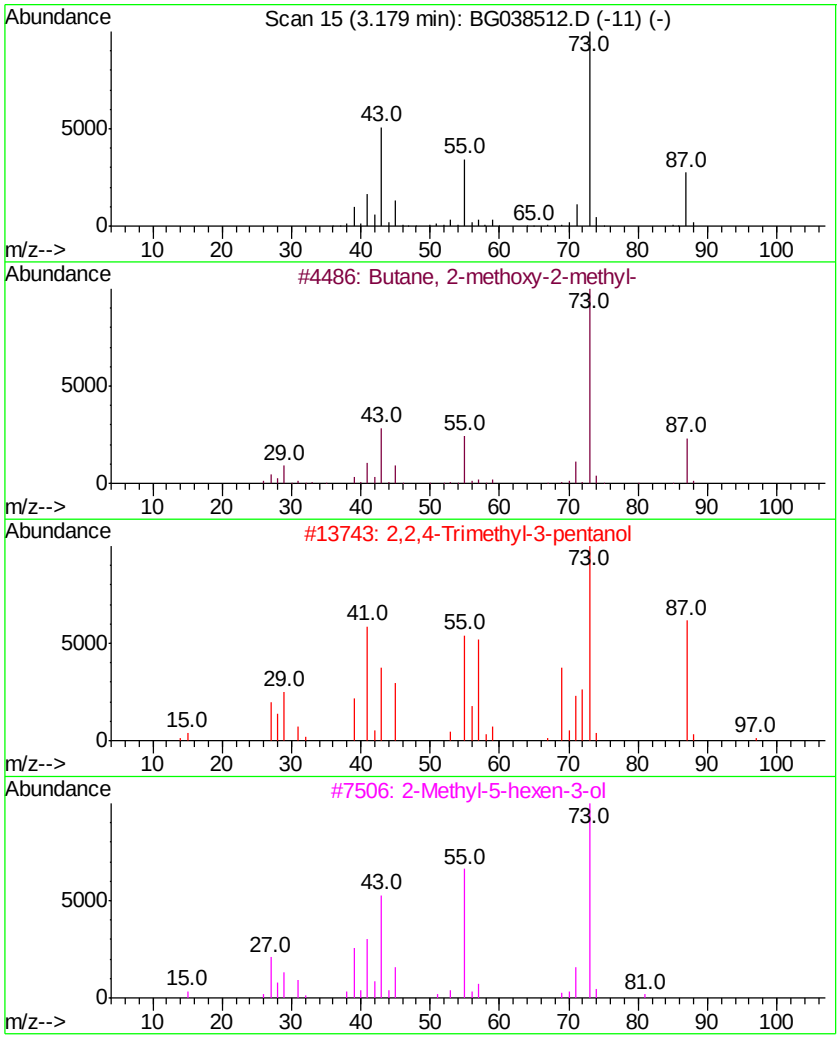
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

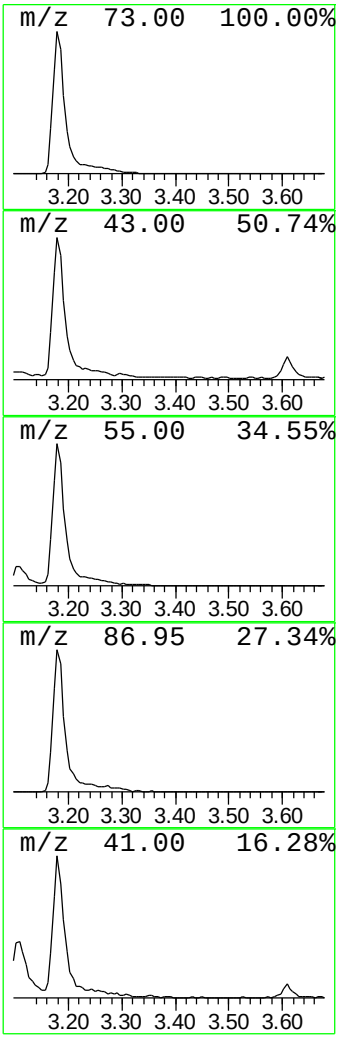
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	88.29 ng	721809	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
4	Propanoic acid, 2-oxo-	88	C3H4O3	000127-17-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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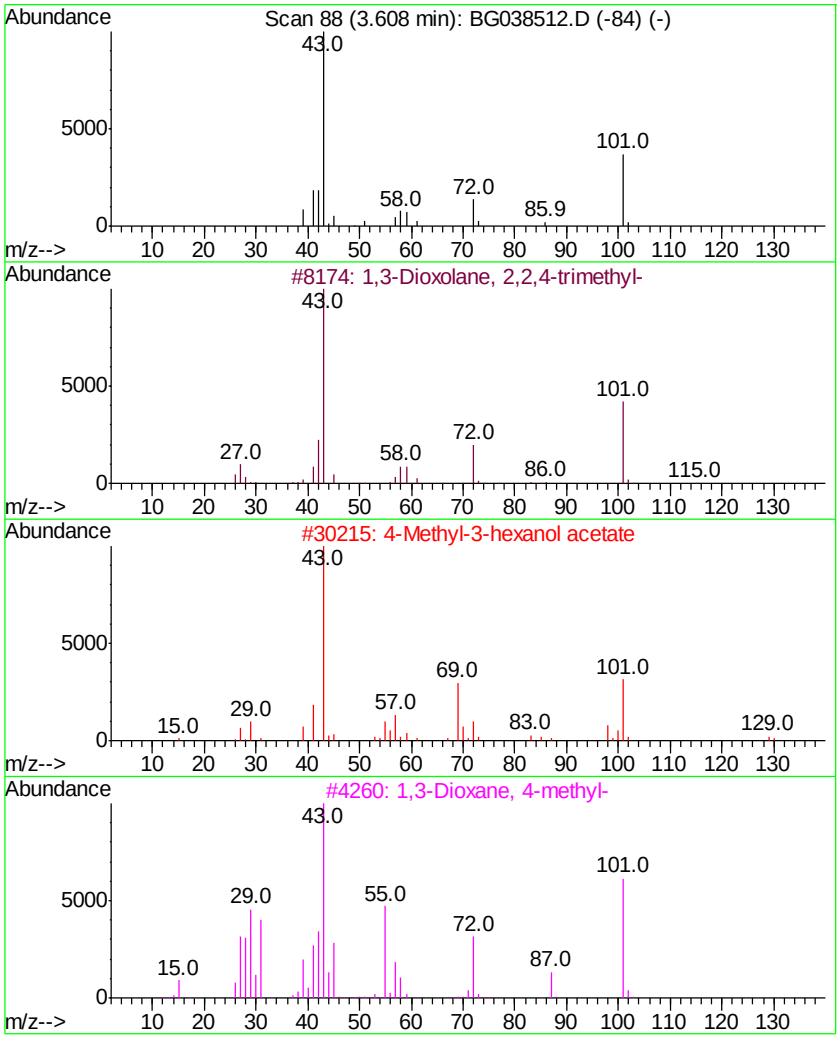
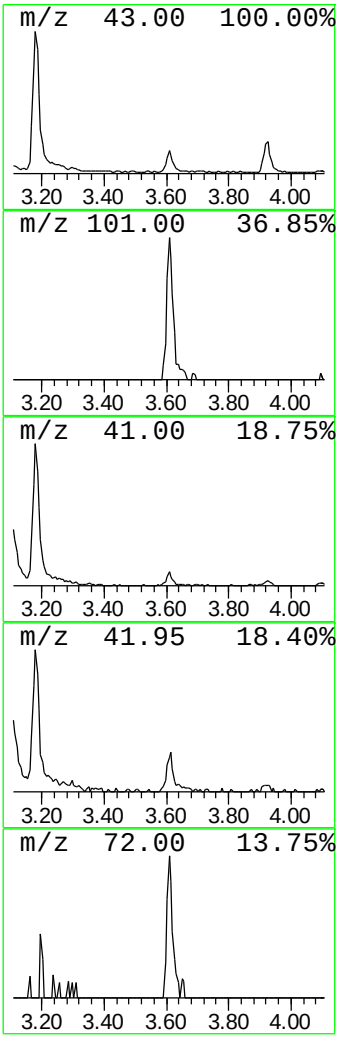
Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	4.12 ng	33722	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2	4-Methyl-3-hexanol acetate	158	C9H18O2	084612-71-5	38
3	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	36
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Furazan-3-ol, 4-amino-	101	C2H3N3O2	159013-90-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

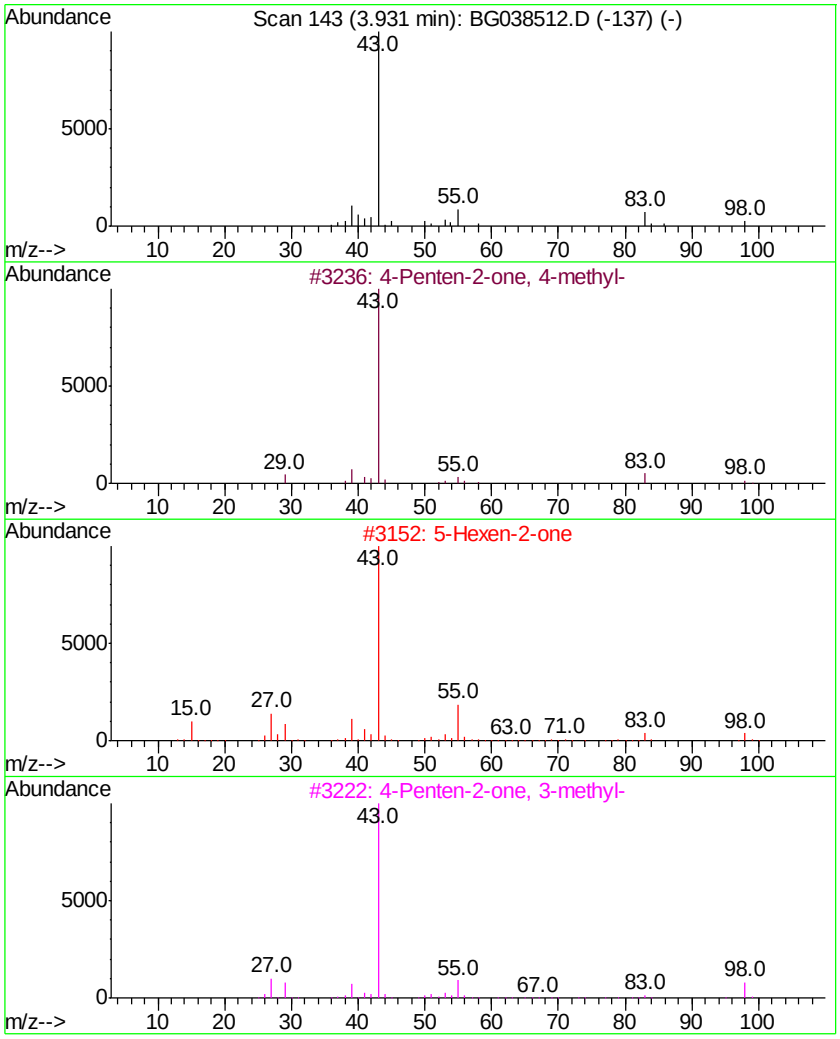
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

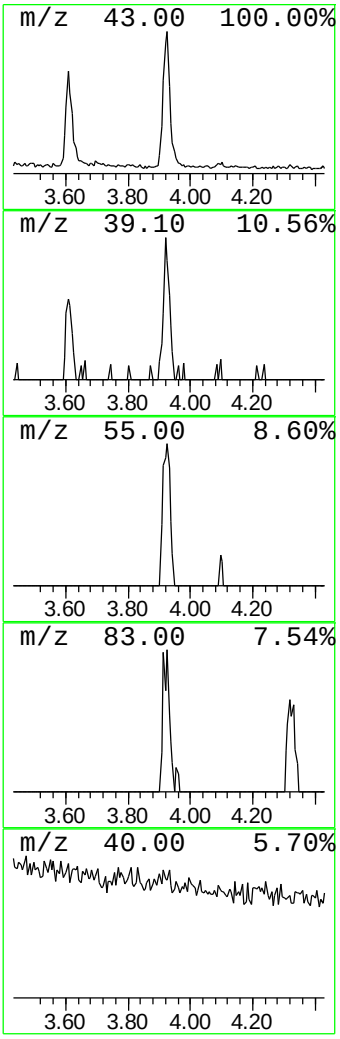
****

Peak Number 3 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.93	4.19 ng	34263	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
4	3,5-Hexadien-2-ol	98	C6H10O	003280-51-1	5
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	5





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

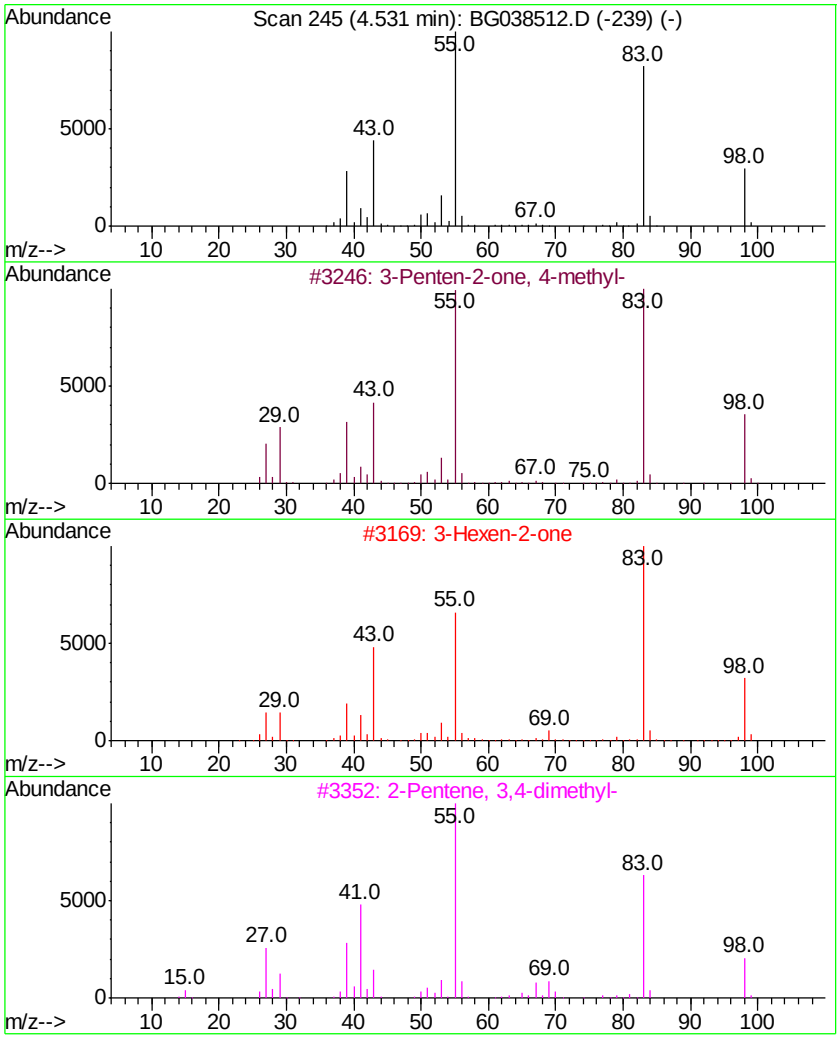
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

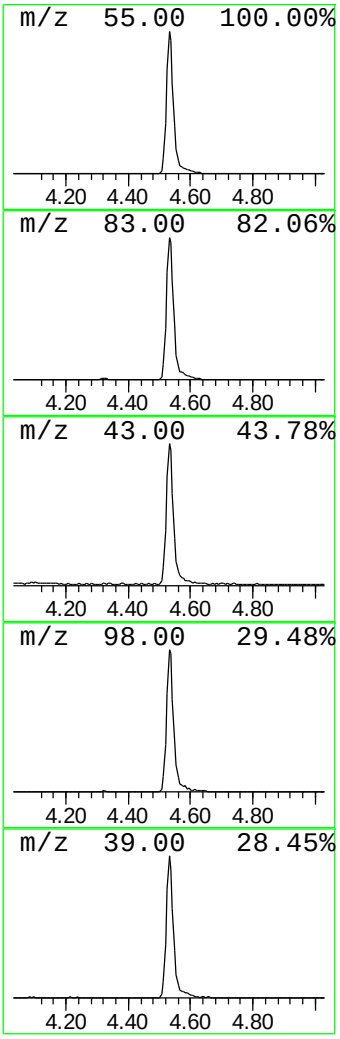
****

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	81.32 ng	664762	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	87
3	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

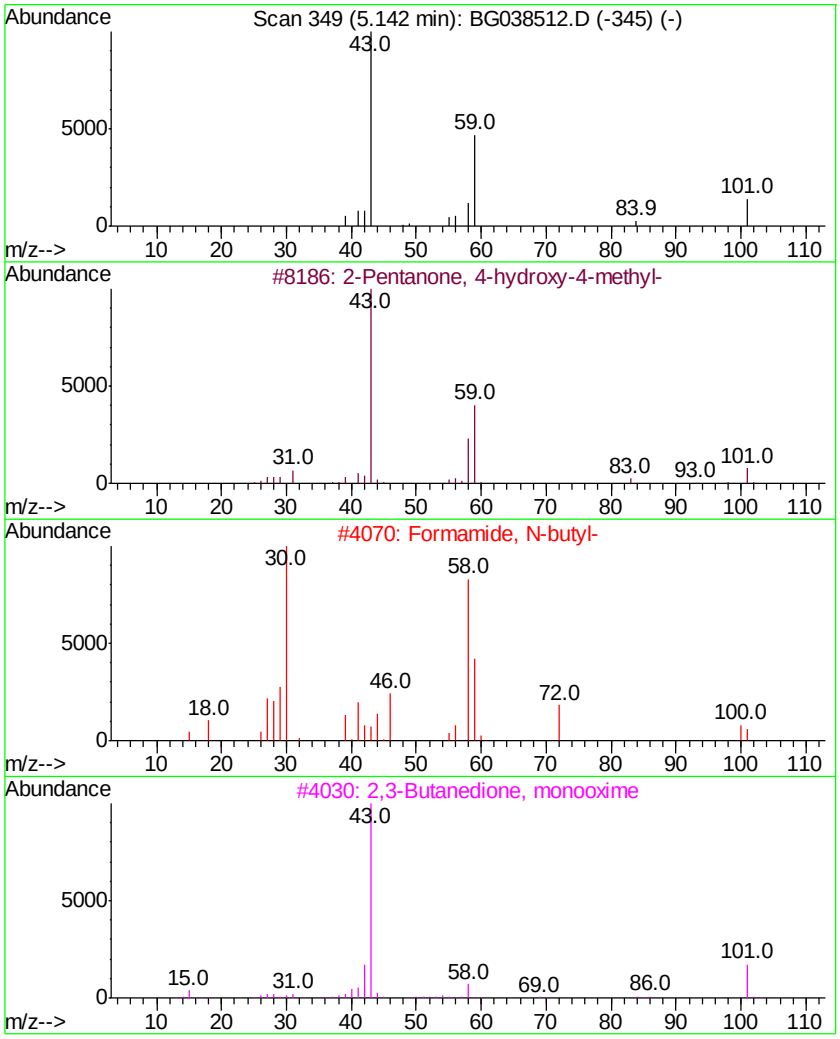
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

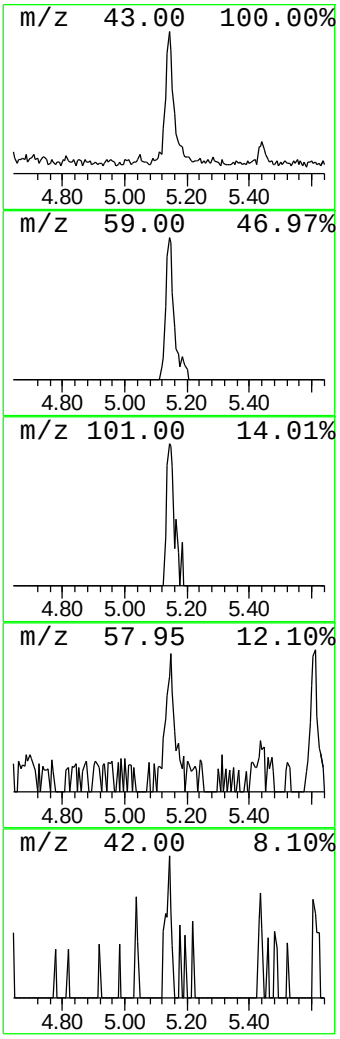
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	2.39 ng	19508	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
4	Diacetamide	101	C4H7NO2	000625-77-4	7
5	Propylamine	59	C3H9N	000107-10-8	5





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

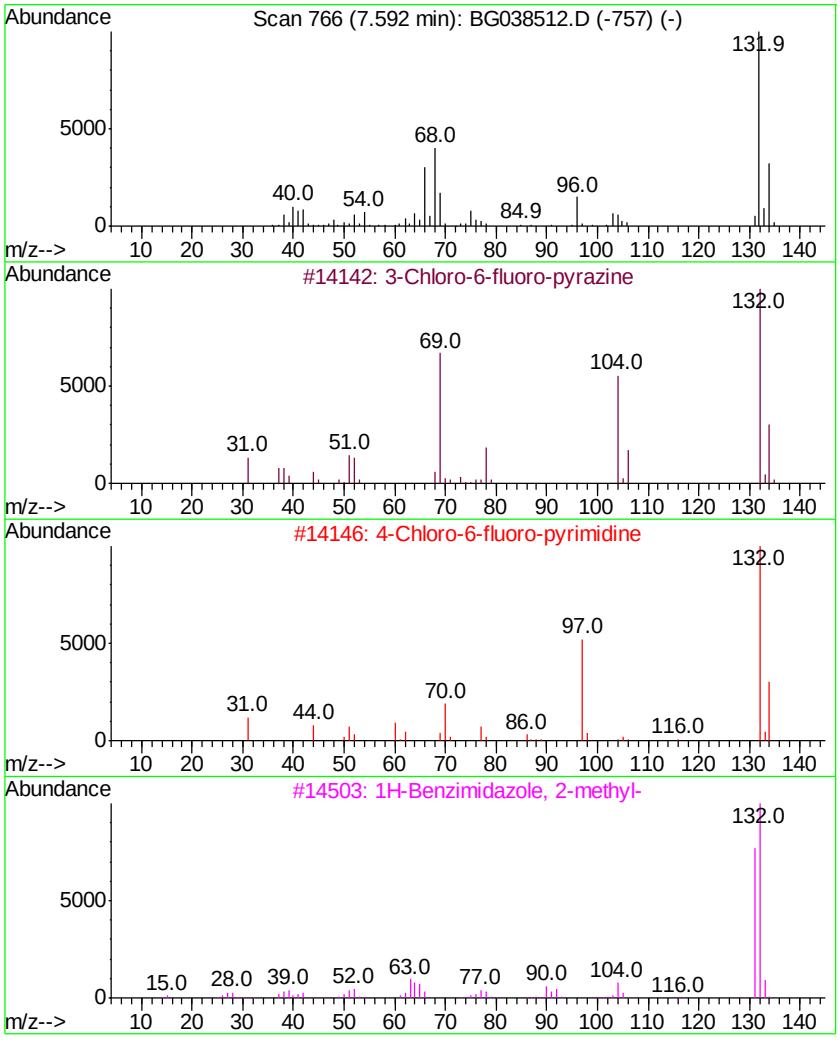
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

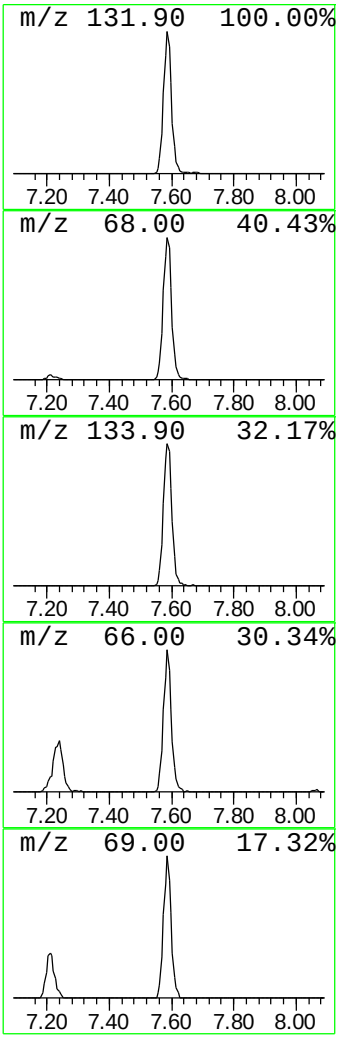
****

Peak Number 6 unknown7.59 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	43.56 ng	356104	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

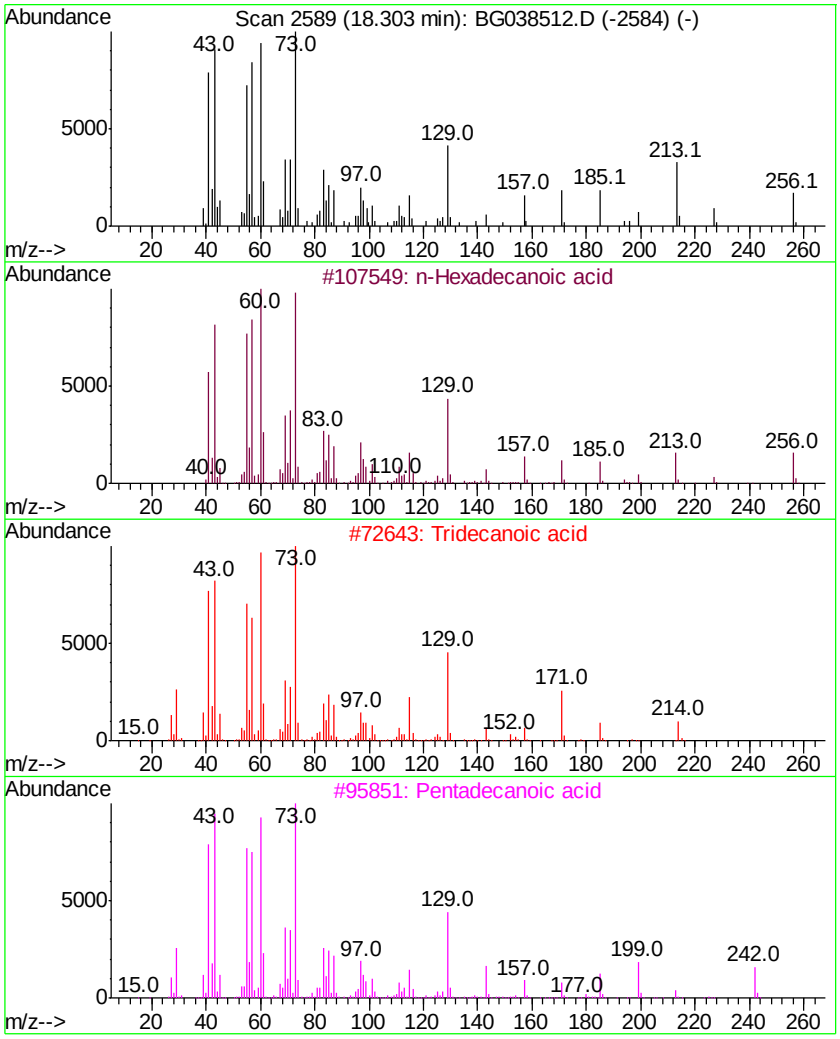
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

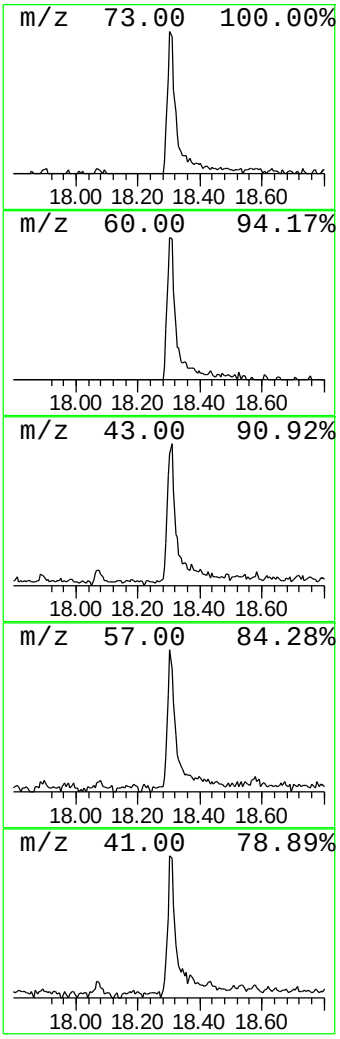
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	7.08 ng	162827	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	78
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

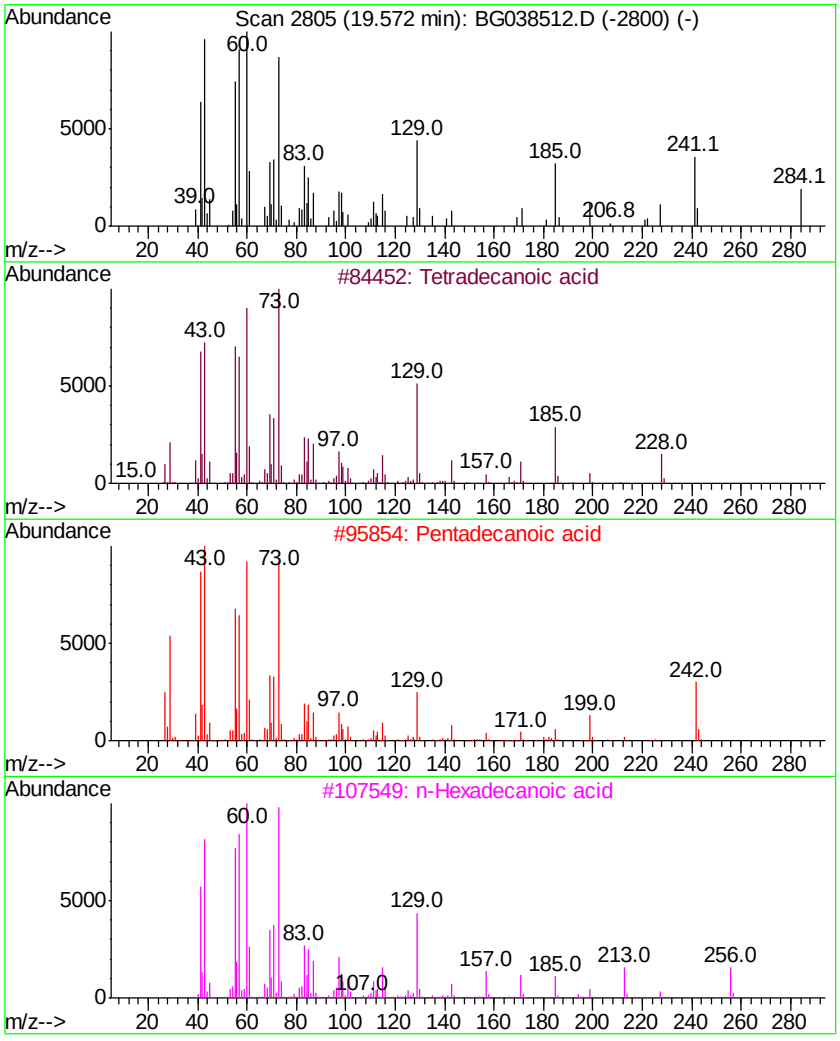
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

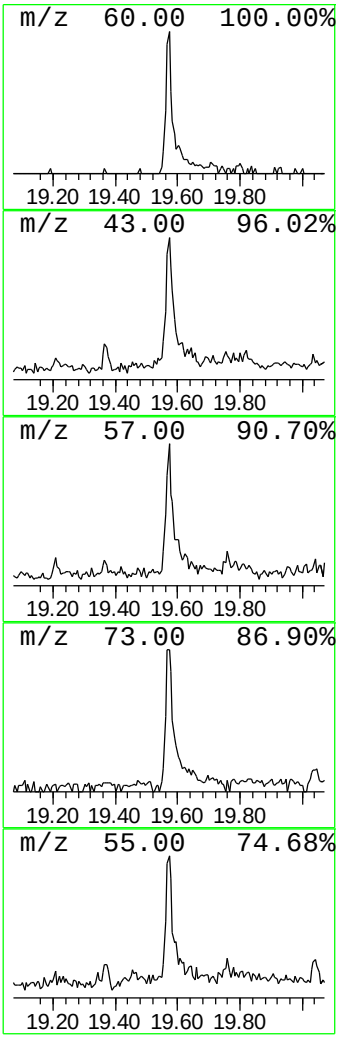
****

Peak Number 9 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.57	3.89 ng	89597	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	n-Decanoic acid	172	C10H20O2	000334-48-5	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121218\
Data File : BG038512.D
Acq On : 13 Dec 2018 00:02
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMPOSITE-6-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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
Butane, 2-methoxy...	3.18	88.3	ng	721809	1	8.06	163501	20.0
1,3-Dioxolane, 2,...	3.61	4.1	ng	33722	1	8.06	163501	20.0
4-Penten-2-one, 4...	3.93	4.2	ng	34263	1	8.06	163501	20.0
3-Penten-2-one, 4...	4.53	81.3	ng	664762	1	8.06	163501	20.0
2-Pentanone, 4-hy...	5.14	2.4	ng	19508	1	8.06	163501	20.0
unknown7.59	7.59	43.6	ng	356104	1	8.06	163501	20.0
n-Hexadecanoic acid	18.30	7.1	ng	162827	4	17.44	460144	20.0
Tetradecanoic acid	19.57	3.9	ng	89597	4	17.44	460144	20.0