LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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	3.595	121	129	146	rBV	6164498	11840568	100.00%	21.017%
2	5.322	417	423	429	rBV2	209042	329100	2.78%	0.584%
3	5.792	496	503	511	rBV	1029837	1687262	14.25%	2.995%
4	7.396	769	776	785	rBV	666277	1189841	10.05%	2.112%
5	7.784	834	842	851	rBV	1717331	3111928	26.28%	5.524%
6	8.260	915	923	936	rVB2	384675	703399	5.94%	1.249%
7	8.589	971	979	988	rVB	1553879	2862124	24.17%	5.080%
8	9.435	1115	1123	1132	rVB	1366869	2493170	21.06%	4.425%
9	9.564	1141	1145	1152	rVB3	82254	134956	1.14%	0.240%
10	11.086	1394	1404	1411	rBV	496371	962561	8.13%	1.709%
11	11.832	1524	1531	1538	rBV4	96538	195741	1.65%	0.347%
12	13.501	1807	1815	1824	rVB	3638716	5717000	48.28%	10.148%
13	14.312	1948	1953	1959	rVB	299887	446650	3.77%	0.793%
14	14.876	2043	2049	2056	rVB	847846	1326335	11.20%	2.354%
15	15.246	2108	2112	2119	rBV3	110147	157749	1.33%	0.280%
16	15.675	2180	2185	2194	rVB3	87803	143891	1.22%	0.255%
17	16.362	2295	2302	2309	rBV	3536853	5523042	46.65%	9.803%
18	16.527	2327	2330	2337	rBV2	107427	214117	1.81%	0.380%
19	16.973	2402	2406	2411	rBV6	85340	153678	1.30%	0.273%
20	17.620	2510	2516	2522	rBV2	1174380	1749453	14.78%	3.105%
21	18.466	2656	2660	2667	rBV2	299595	409978	3.46%	0.728%
22	19.723	2871	2874	2879	rBV6	103859	162721	1.37%	0.289%
23	20.205	2950	2956	2961	rVB	6488977	9017946	76.16%	16.007%
24	21.492	3171	3175	3186	rVB2	258638	462015	3.90%	0.820%
25	21.915	3241	3247	3259	rVB	1459685	2561325	21.63%	4.546%
26	23.425	3498	3504	3511	rVB5	98804	212749	1.80%	0.378%
27	25.340	3820	3830	3842	rVB2	862319	2569614	21.70%	4.561%

Sum of corrected areas: 56338913

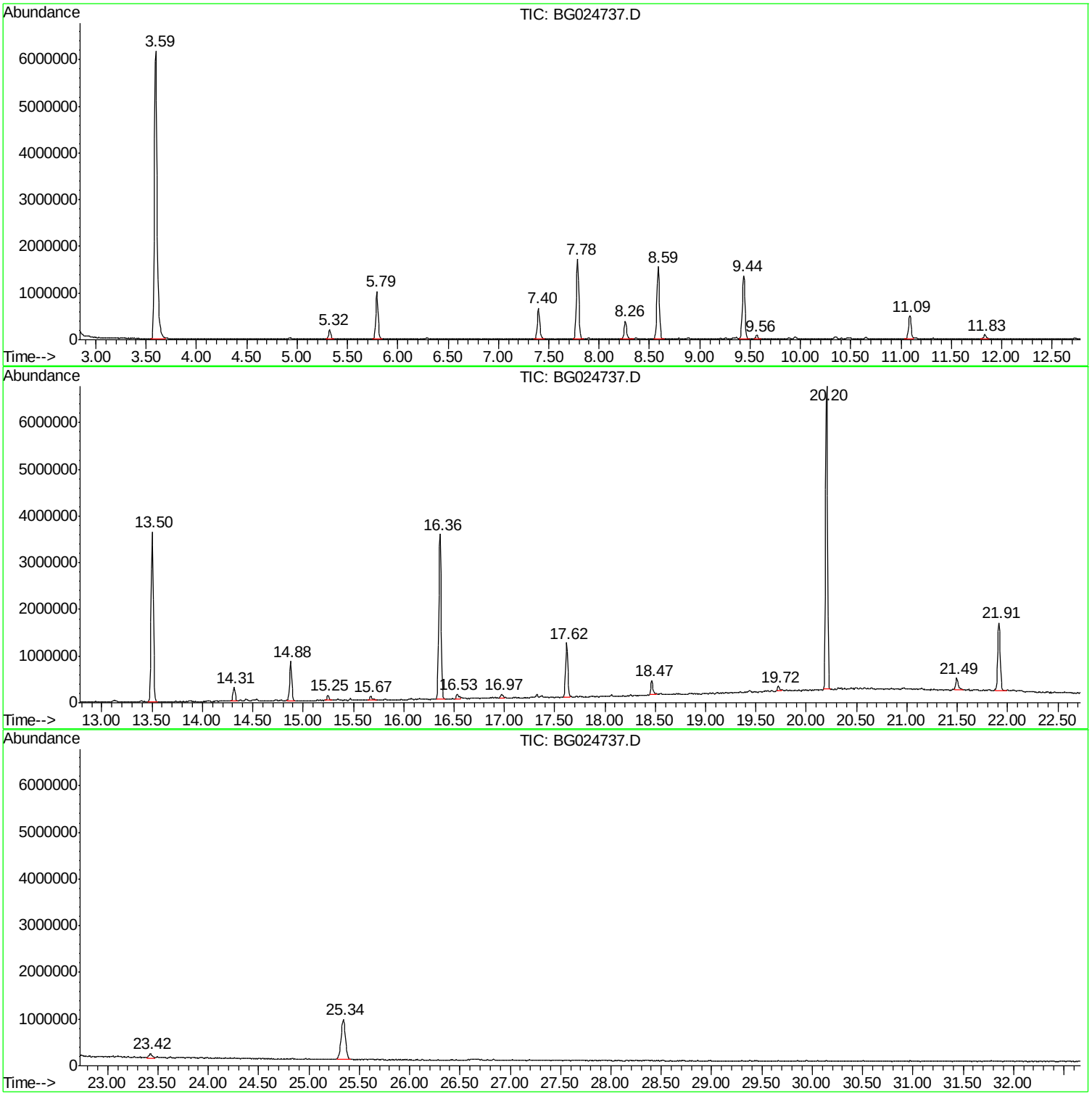
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-111-10.5-21.0

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\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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

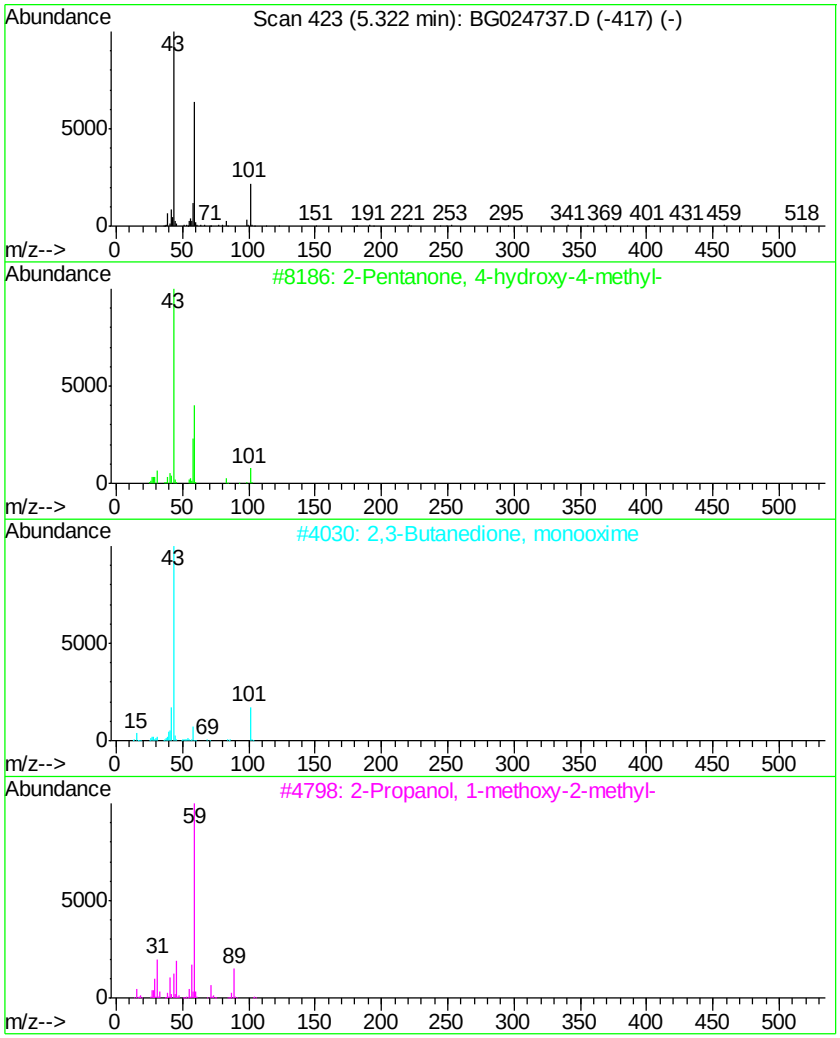
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

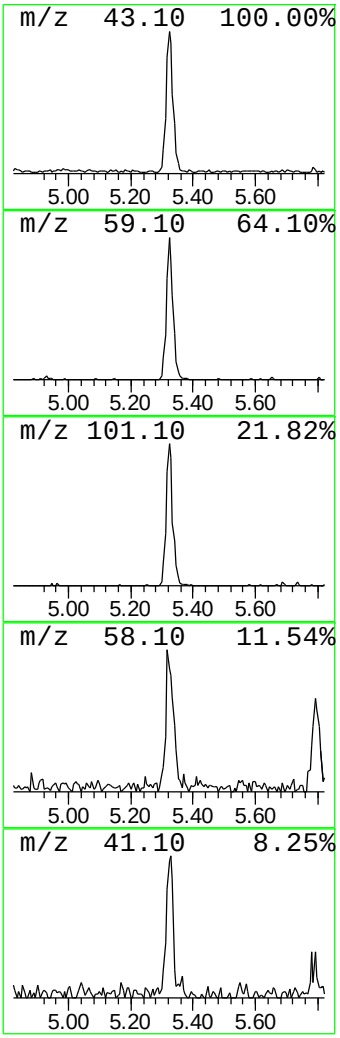
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	9.36 ng	329100	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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	3-Hexanol	102	C6H14O	000623-37-0	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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

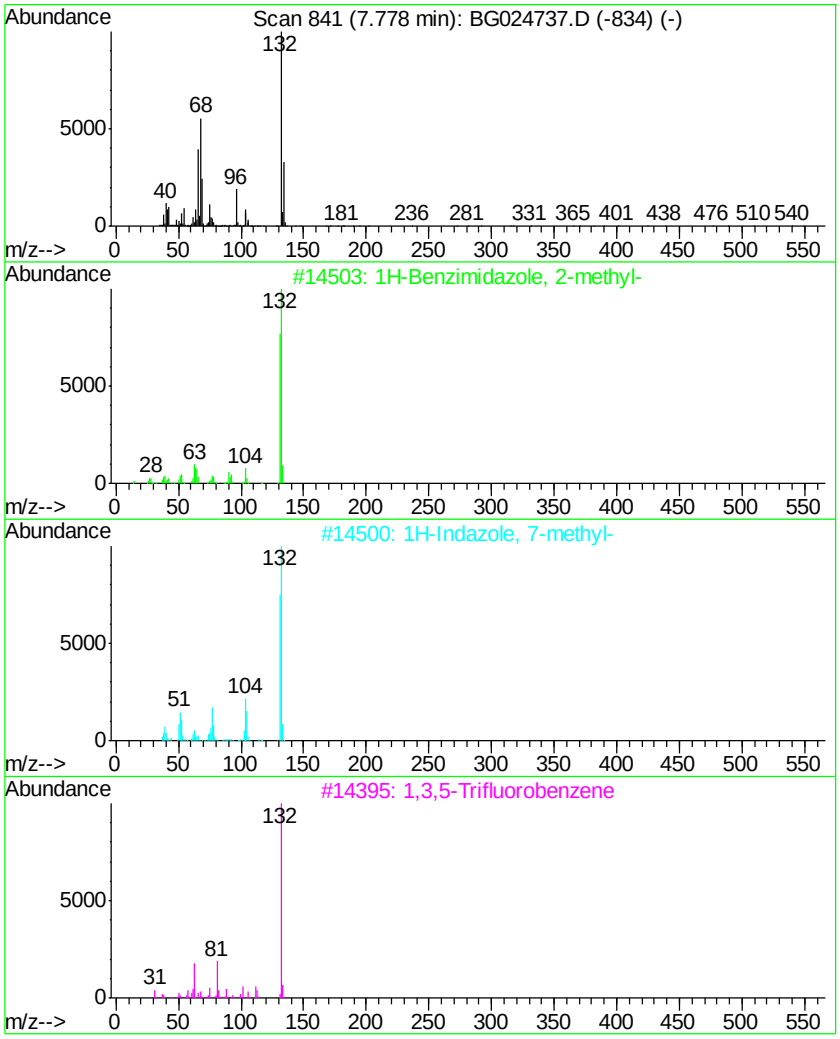
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

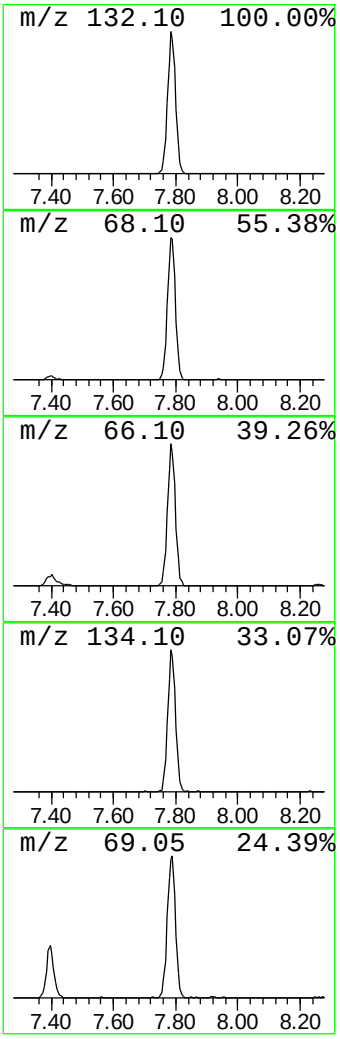
****

Peak Number 3 unknown7.78 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	88.48 ng	3111930	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	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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

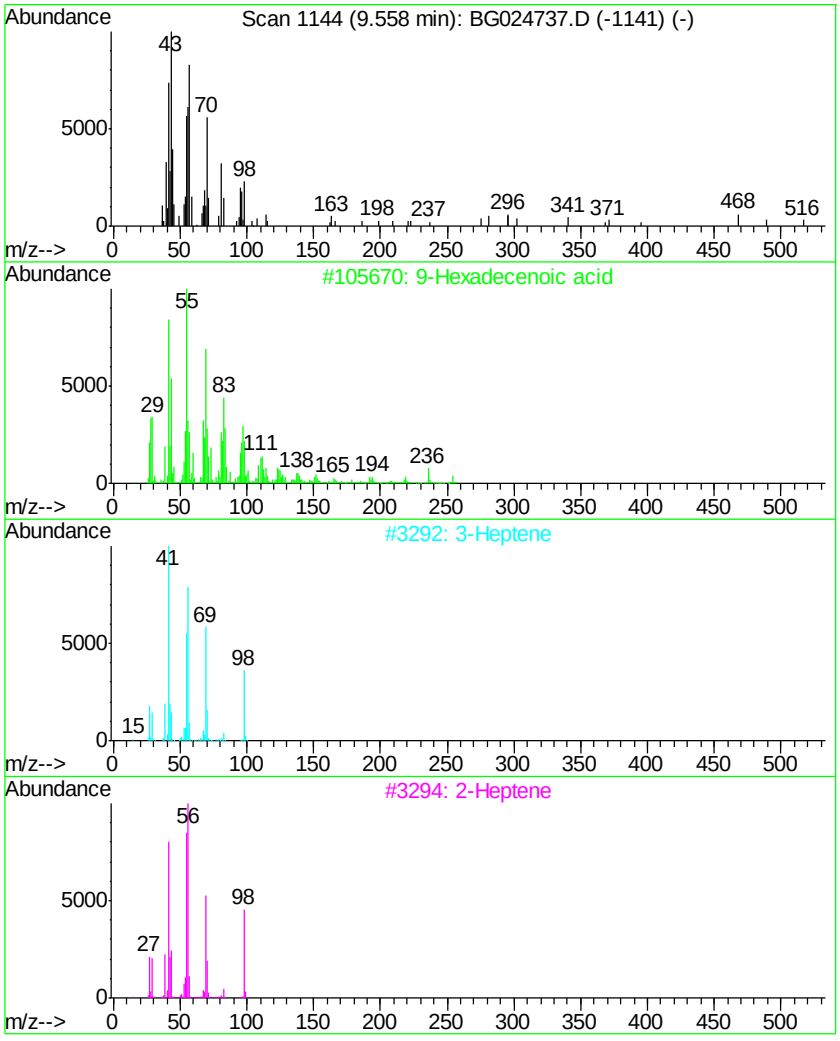
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

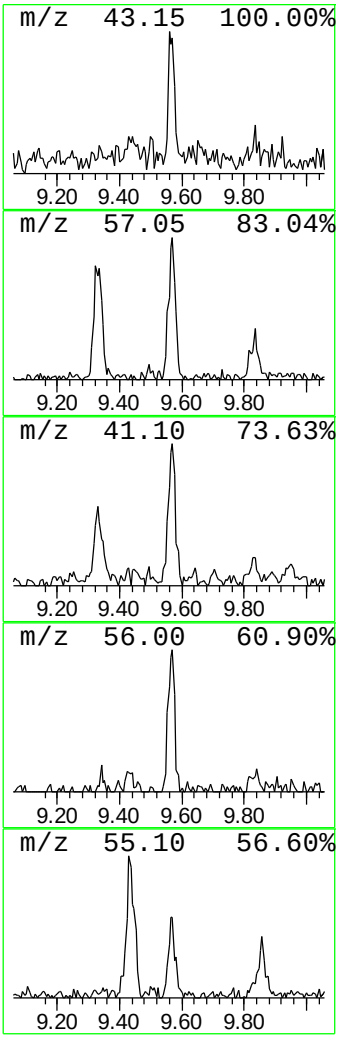
****

Peak Number 5 unknown9.56 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.56	3.84 ng	134956	1,4-Dichlorobenzene-d4	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	27
2	3-Heptene	98	C7H14	000592-78-9	25
3	2-Heptene	98	C7H14	000592-77-8	25
4	2-Heptene, (E)-	98	C7H14	014686-13-6	25
5	(Z)-2-Heptene	98	C7H14	006443-92-1	25





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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

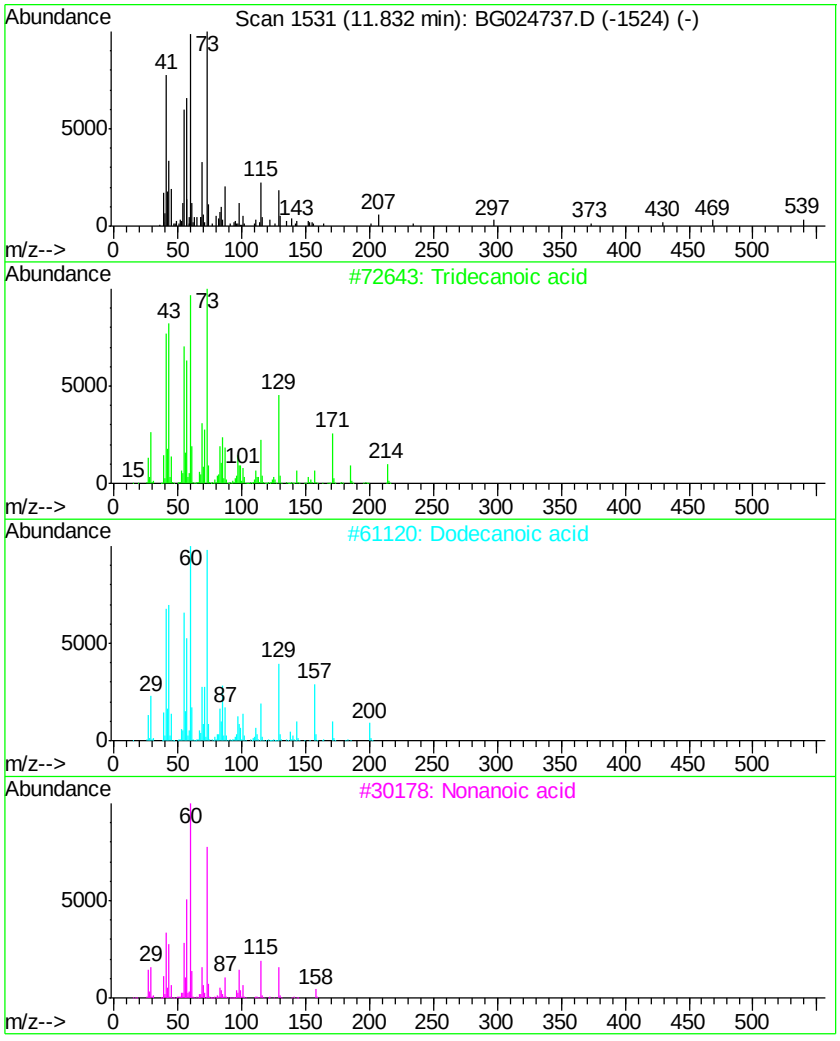
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

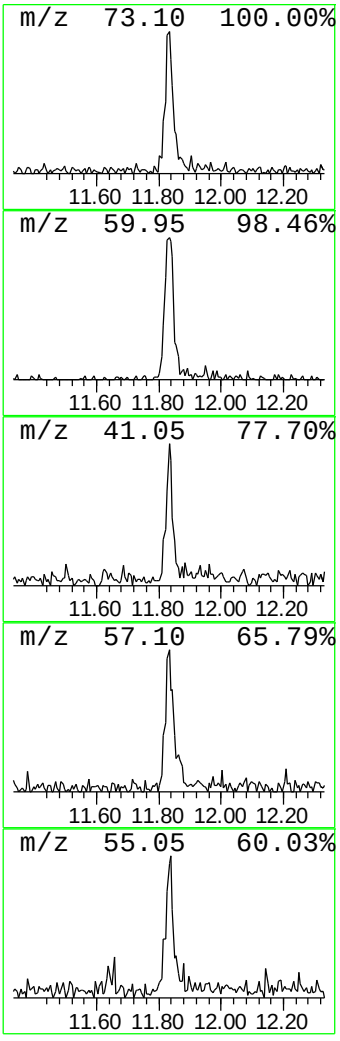
****

Peak Number 6 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	4.07 ng	195741	Naphthalene-d8	11.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	64
2	Dodecanoic acid	200	C12H24O2	000143-07-7	56
3	Nonanoic acid	158	C9H18O2	000112-05-0	50
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	Hexanoic acid	116	C6H12O2	000142-62-1	47





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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

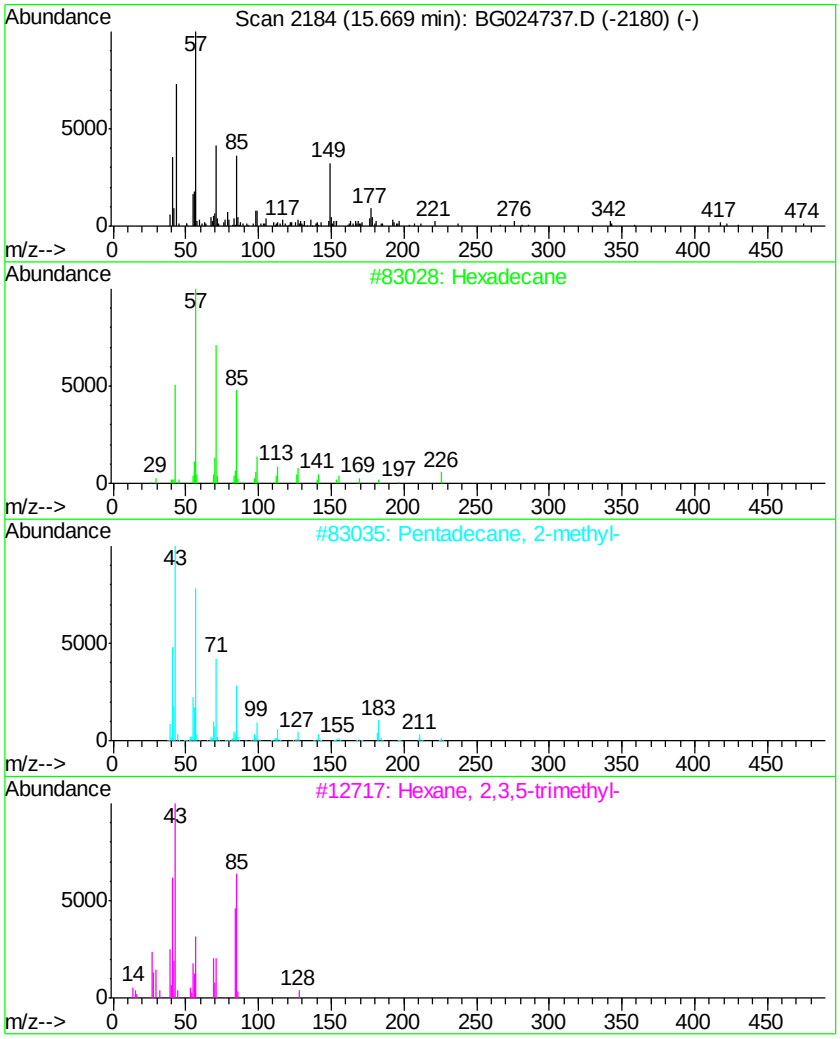
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

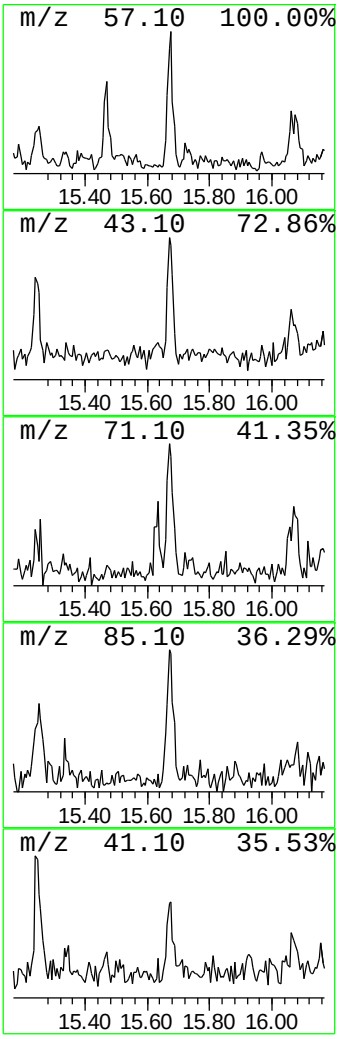
****

Peak Number 8 unknown15.67 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	2.17 ng	143891	Acenaphthene-d10	14.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	38
2	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	38
3	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	35
4	5-Undecanone	170	C11H22O	033083-83-9	35
5	2-Butanone, 1-chloro-3,3-dimethyl-	134	C6H11ClO	013547-70-1	35





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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

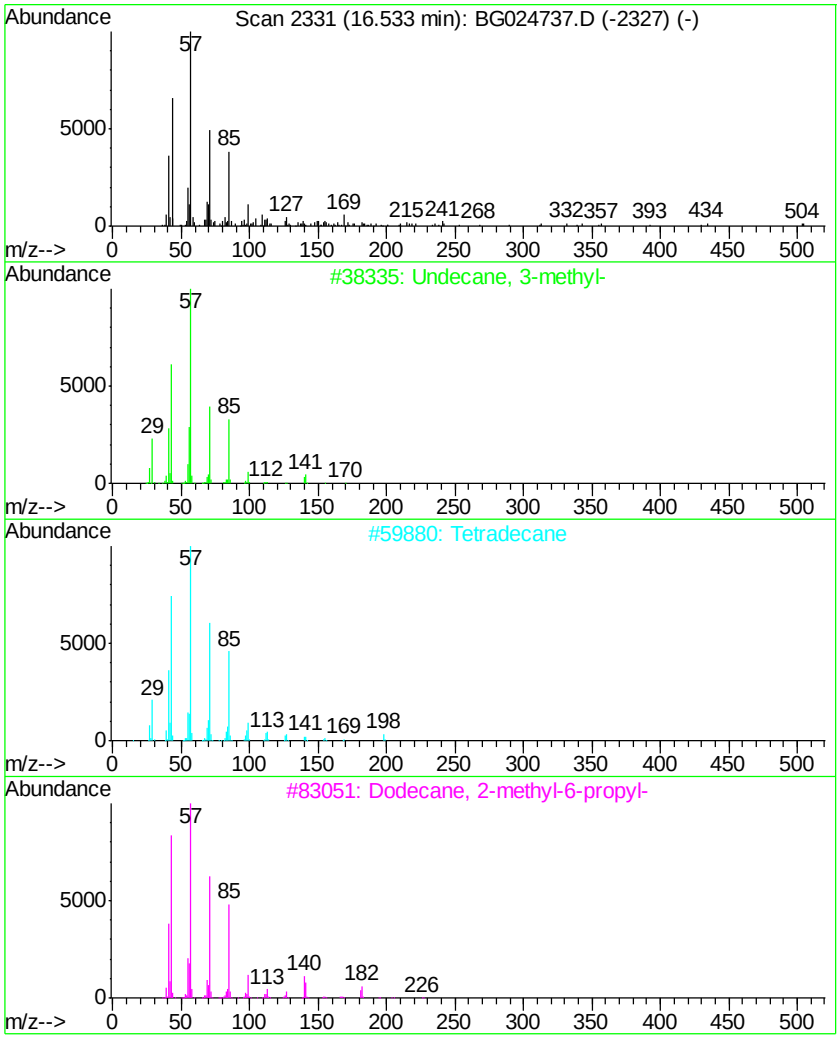
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

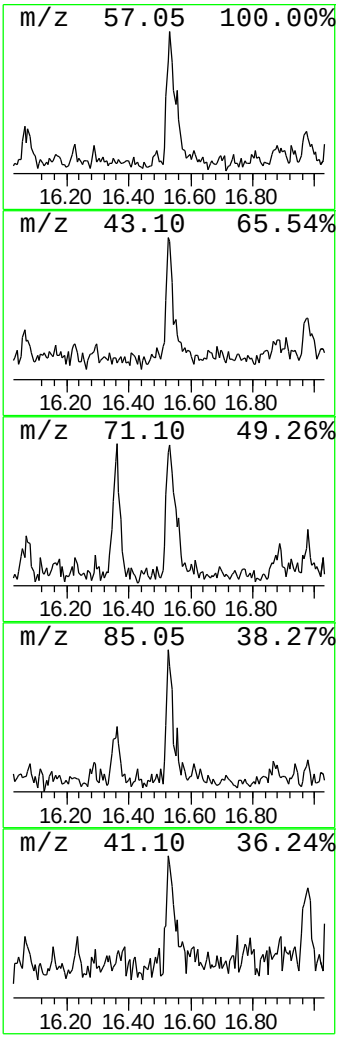
****

Peak Number 9 Undecane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.45 ng	214117	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3-methyl-	170	C12H26	001002-43-3	72
2	Tetradecane	198	C14H30	000629-59-4	64
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	64
4	Heptadecane	240	C17H36	000629-78-7	64
5	Octacosane	394	C28H58	000630-02-4	59





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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

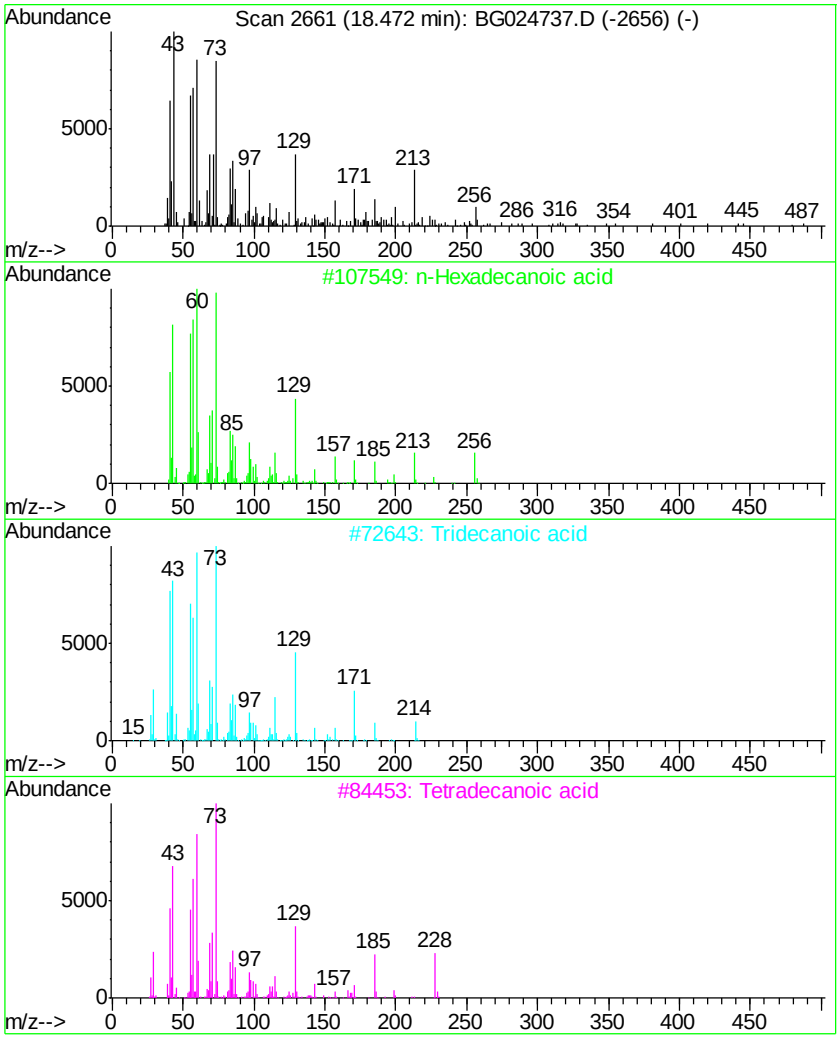
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

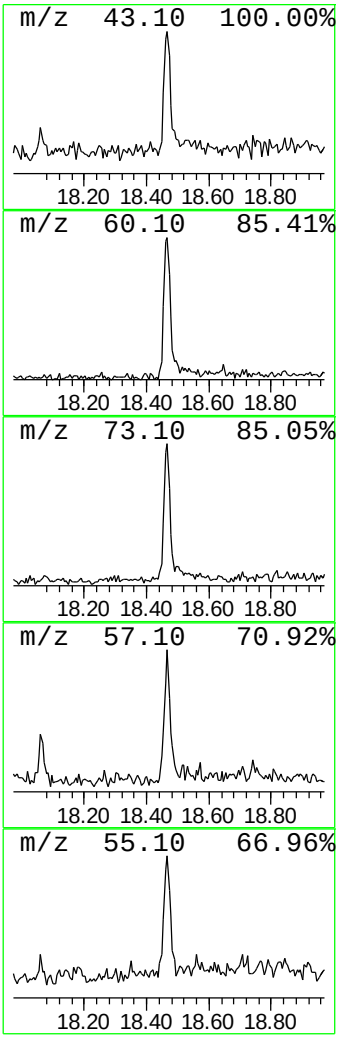
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	4.69 ng	409978	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Dodecanoic acid	200	C12H24O2	000143-07-7	80
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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

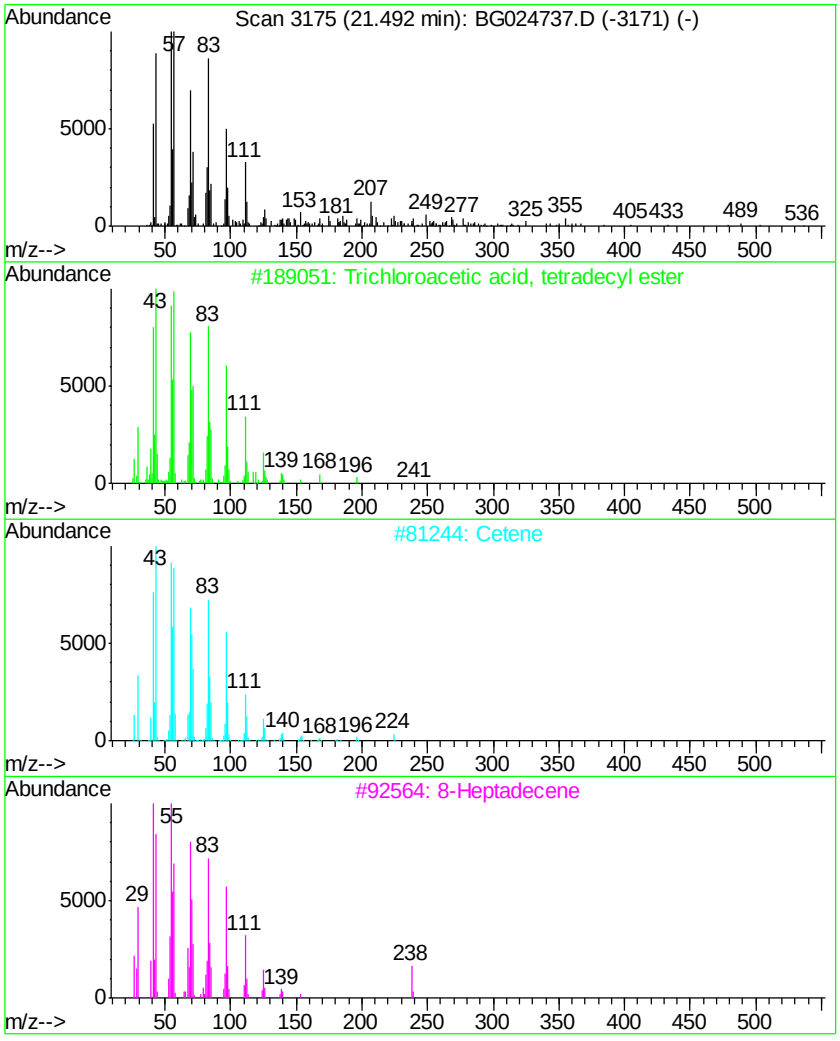
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

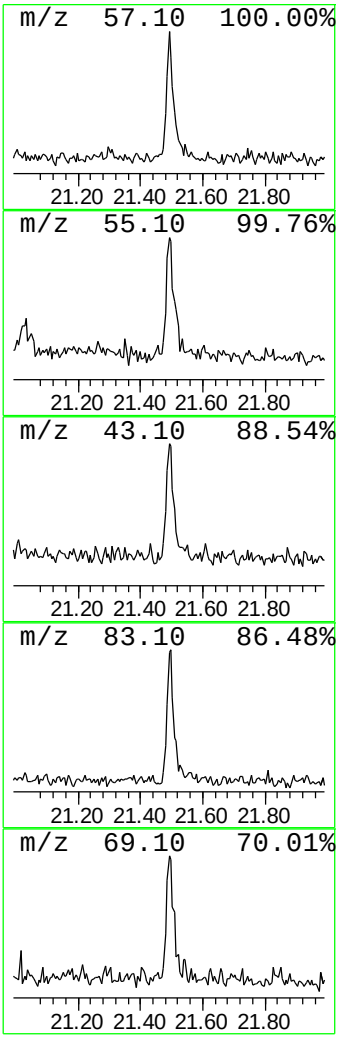
****

Peak Number 11 Trichloroacetic acid, tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.49	3.61 ng	462015	Chrysene-d12	21.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
2	Cetene	224	C16H32	000629-73-2	90
3	8-Heptadecene	238	C17H34	002579-04-6	83
4	1-Heptadecene	238	C17H34	006765-39-5	83
5	1-Tetradecene	196	C14H28	001120-36-1	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110716\
Data File : BG024737.D
Acq On : 7 Nov 2016 20:24
Operator : UM/SJ
Sample : H5544-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-111-10.5-21.0

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
2-Pentanone, 4-hy...	5.32	9.4	ng	329100	1	8.26	703399	20.0
unknown7.78	7.78	88.5	ng	3111930	1	8.26	703399	20.0
unknown9.56	9.56	3.8	ng	134956	1	8.26	703399	20.0
Tridecanoic acid	11.83	4.1	ng	195741	2	11.09	962561	20.0
unknown15.67	15.67	2.2	ng	143891	3	14.88	1326340	20.0
Undecane, 3-methyl-	16.53	2.5	ng	214117	4	17.62	1749450	20.0
n-Hexadecanoic acid	18.47	4.7	ng	409978	4	17.62	1749450	20.0
Trichloroacetic a...	21.49	3.6	ng	462015	5	21.91	2561330	20.0