LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024682.D
Acq On : 4 Nov 2016 14:39
Operator : UM/SJ
Sample : H5509-16
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-4.5-5.0

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	3.126	44	49	66	rVB	4425825	7082472	94.51%	14.706%
2	5.329	418	424	432	rBV2	352611	557515	7.44%	1.158%
3	5.794	496	503	514	rBV	1512282	2620208	34.96%	5.441%
4	6.716	654	660	666	rBV3	47268	84637	1.13%	0.176%
5	7.403	768	777	786	rBV	1724235	3053027	40.74%	6.339%
6	7.791	835	843	852	rBV	1555307	2785288	37.17%	5.783%
7	8.267	917	924	933	rBV	383634	701599	9.36%	1.457%
8	8.520	957	967	972	rBV4	49895	117529	1.57%	0.244%
9	8.590	972	979	992	rVB	1136723	2058778	27.47%	4.275%
10	9.442	1115	1124	1132	rBV	1007945	1897260	25.32%	3.939%
11	11.093	1397	1405	1413	rBV	516761	948502	12.66%	1.969%
12	13.508	1805	1816	1823	rBV	2538332	4038601	53.89%	8.386%
13	14.319	1948	1954	1960	rBV	819302	1212110	16.17%	2.517%
14	14.883	2043	2050	2057	rBV	885142	1365553	18.22%	2.835%
15	16.363	2295	2302	2314	rBV	2606242	4099671	54.71%	8.512%
16	16.534	2326	2331	2336	rBV	58933	100917	1.35%	0.210%
17	17.621	2510	2516	2529	rVB2	1166582	1952349	26.05%	4.054%
18	18.467	2655	2660	2666	rBV2	127676	206289	2.75%	0.428%
19	19.660	2857	2863	2866	rBV	59862	85311	1.14%	0.177%
20	20.206	2949	2956	2963	rBV	5450194	7493990	100.00%	15.560%
21	21.499	3171	3176	3184	rBV3	164068	276476	3.69%	0.574%
22	21.922	3240	3248	3255	rBV	1479690	2666707	35.58%	5.537%
23	25.347	3816	3831	3845	rBV2	877915	2755858	36.77%	5.722%

Sum of corrected areas: 48160647

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024682.D
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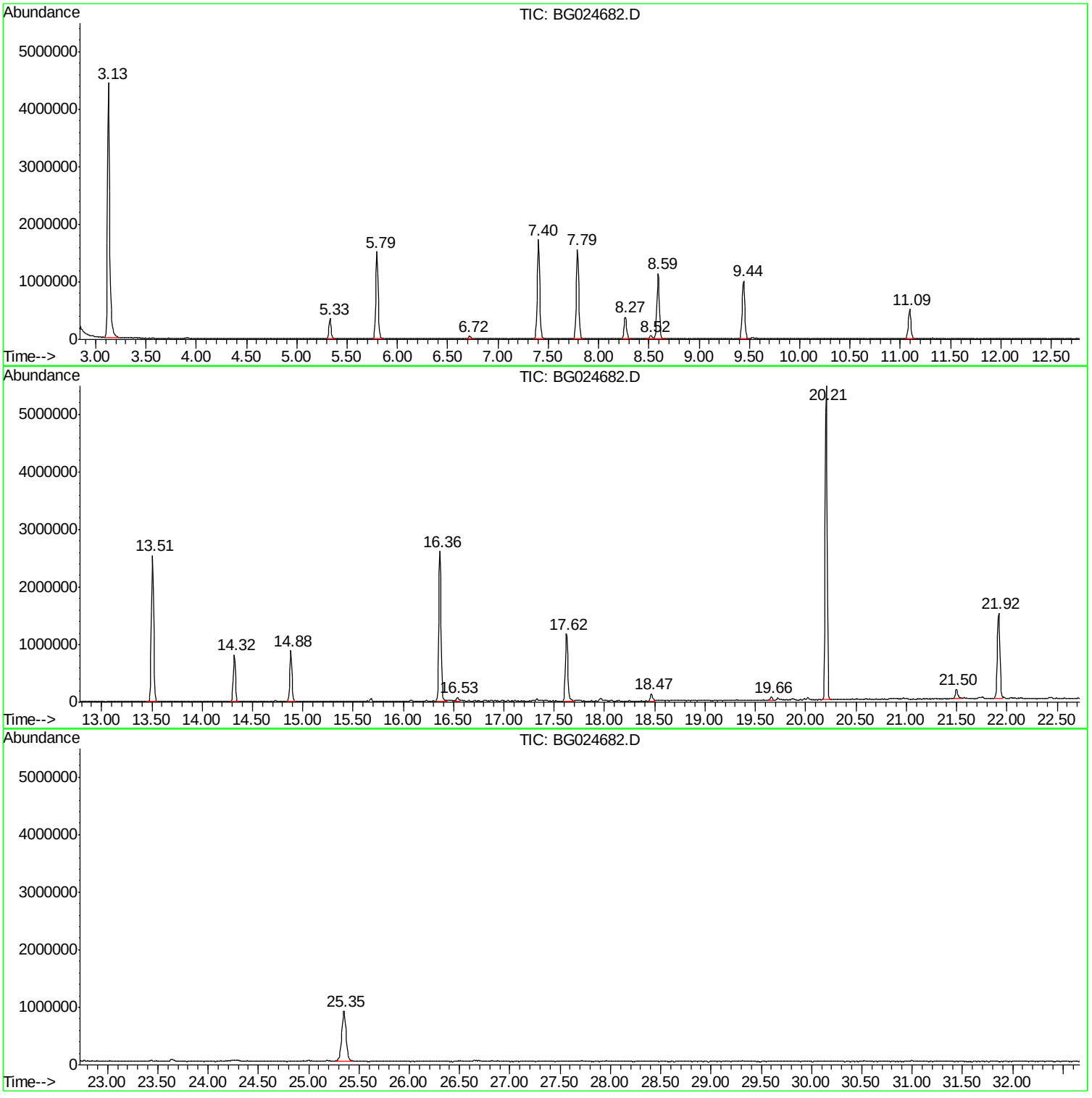
Operator : UM/SJ
Sample : H5509-16
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-4.5-5.0

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024682.D
Acq On : 4 Nov 2016 14:39
Operator : UM/SJ
Sample : H5509-16
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-4.5-5.0

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

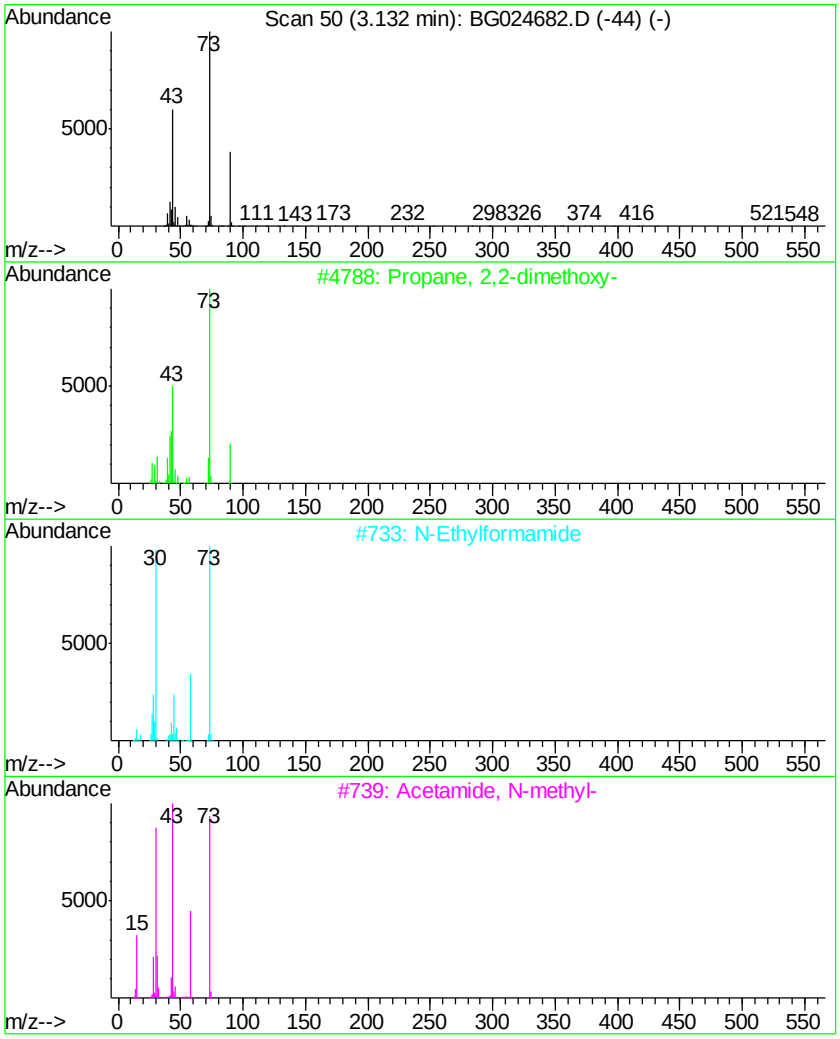
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

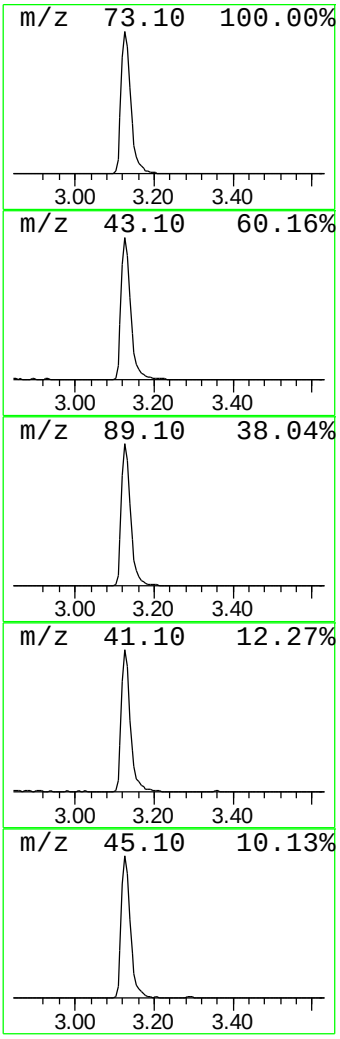
****

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	201.90 ng	7082470	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	33
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024682.D
Acq On : 4 Nov 2016 14:39
Operator : UM/SJ
Sample : H5509-16
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-4.5-5.0

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

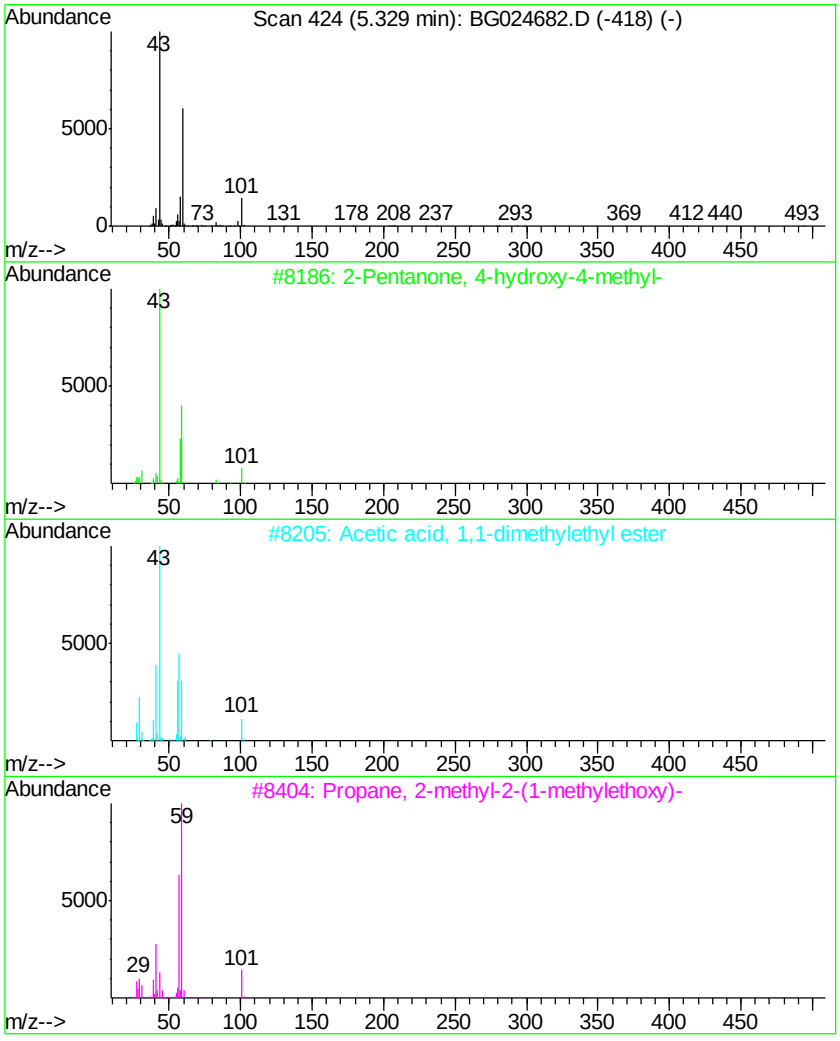
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

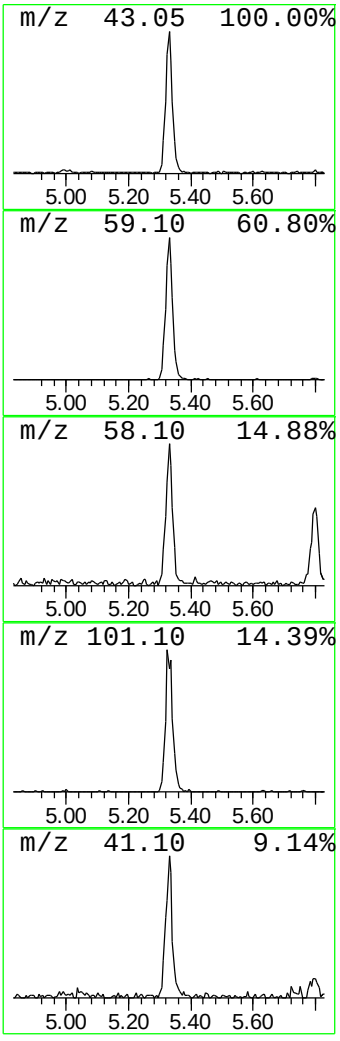
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	15.89 ng	557515	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	32
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024682.D
Acq On : 4 Nov 2016 14:39
Operator : UM/SJ
Sample : H5509-16
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-4.5-5.0

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

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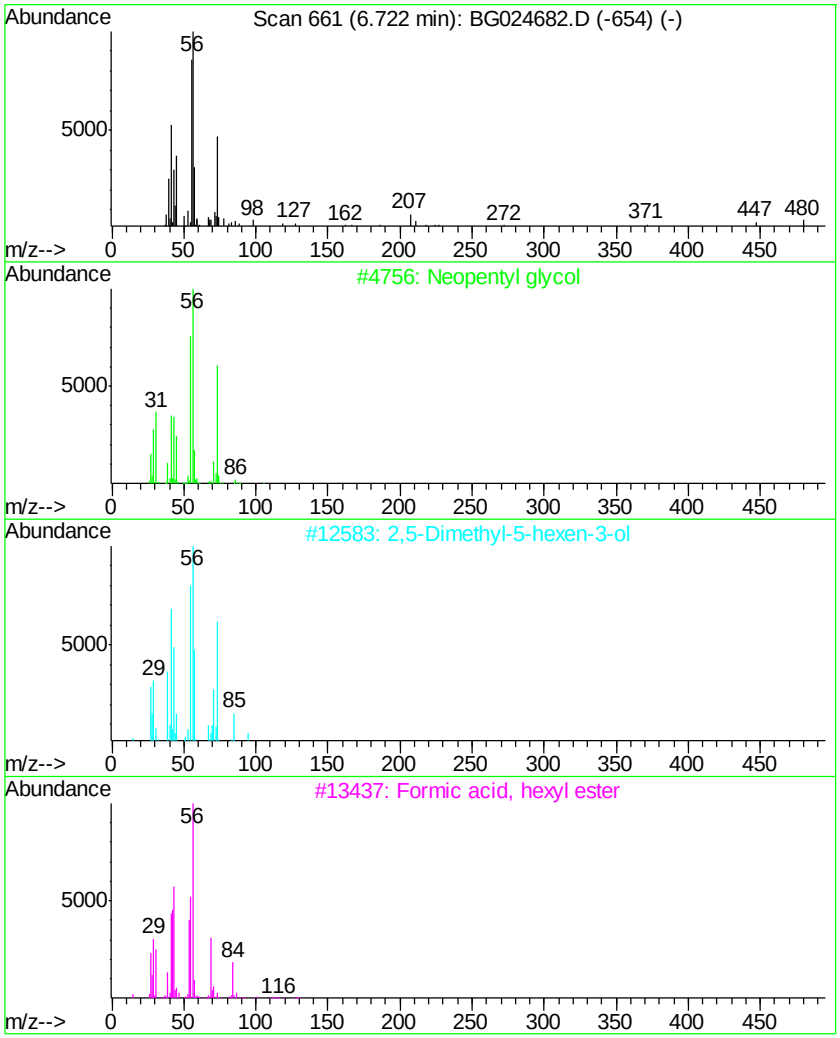
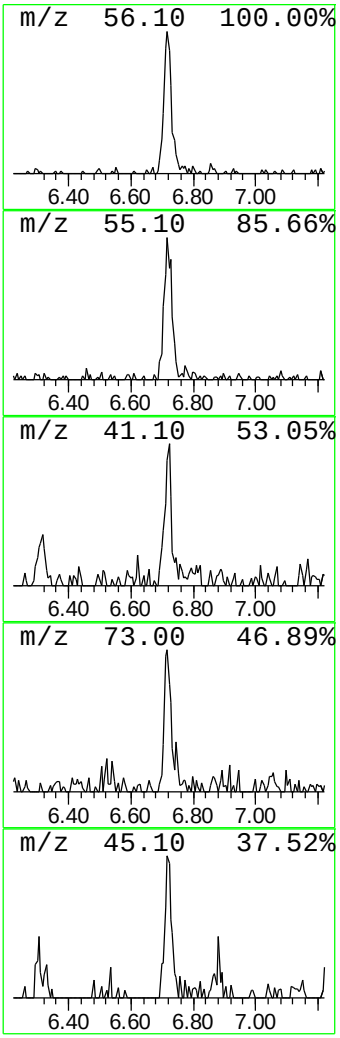
Peak Number 3 Neopentyl glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	2.41 ng	84637	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentyl glycol	104	C5H12O2	000126-30-7	50
2	2,5-Dimethyl-5-hexen-3-ol	128	C8H16O	067760-91-2	39
3	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	36
4	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	33
5	(S)-(+)-3-Methyl-1-pentanol	102	C6H14O	042072-39-9	33





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024682.D
Acq On : 4 Nov 2016 14:39
Operator : UM/SJ
Sample : H5509-16
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-4.5-5.0

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

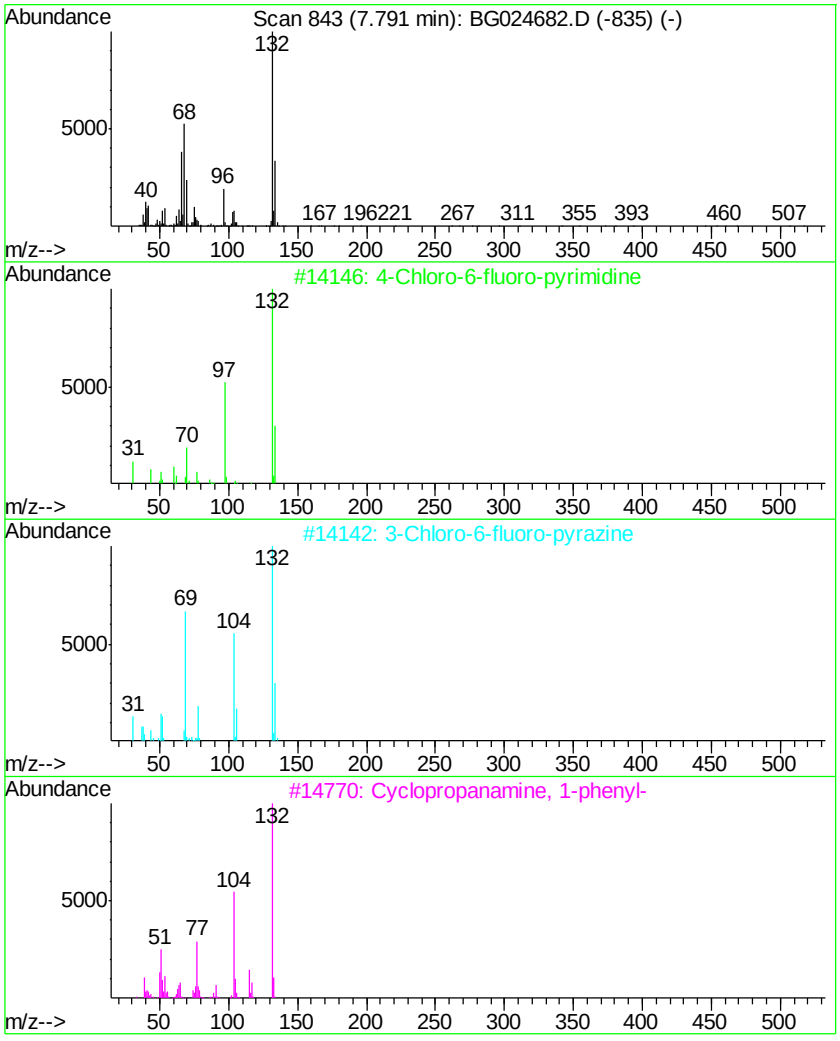
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

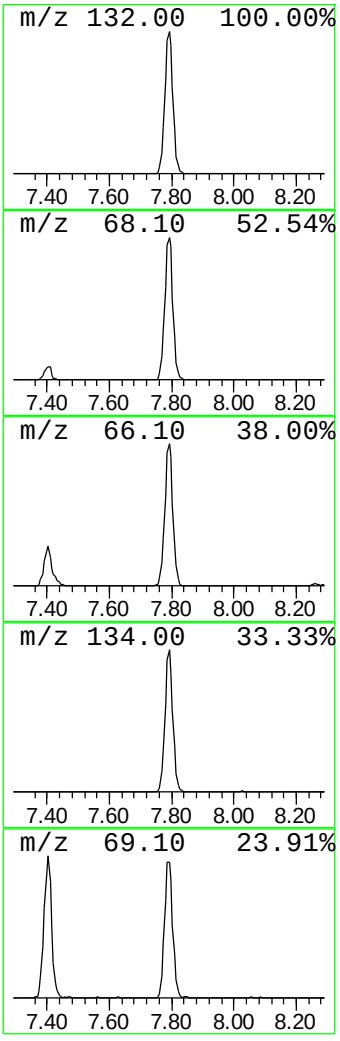
****

Peak Number 4 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	79.40 ng	2785290	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
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Acq On : 4 Nov 2016 14:39
Operator : UM/SJ
Sample : H5509-16
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-4.5-5.0

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

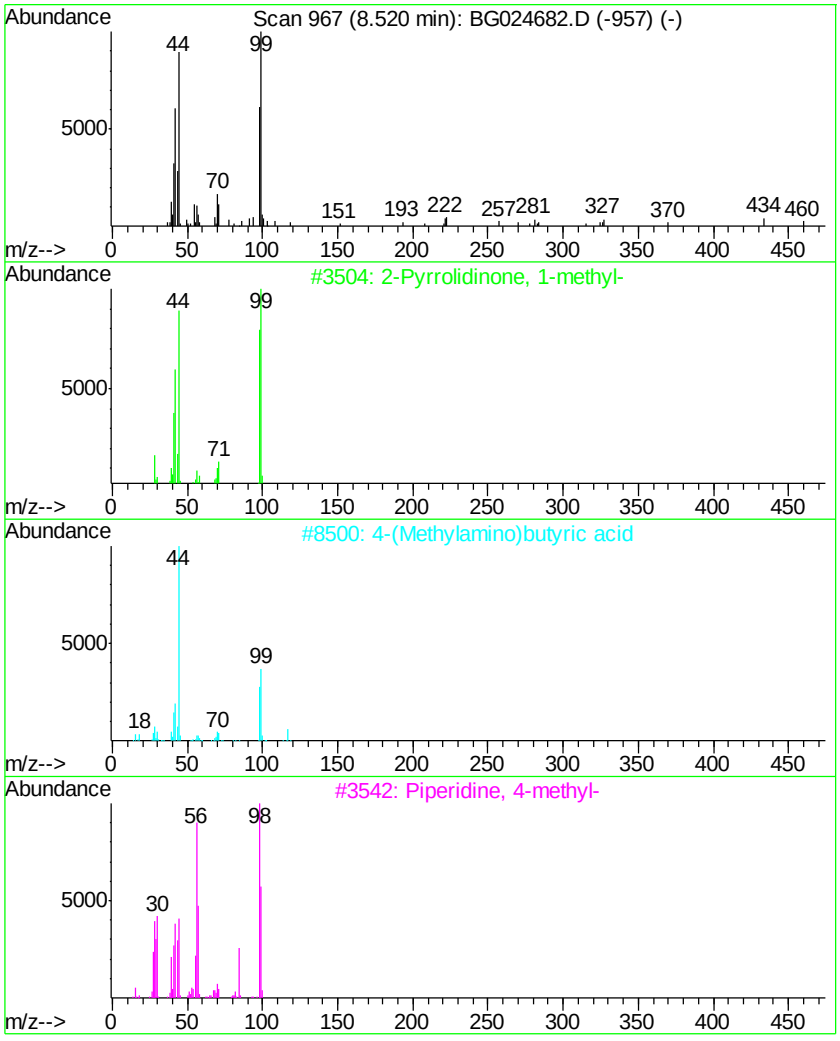
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

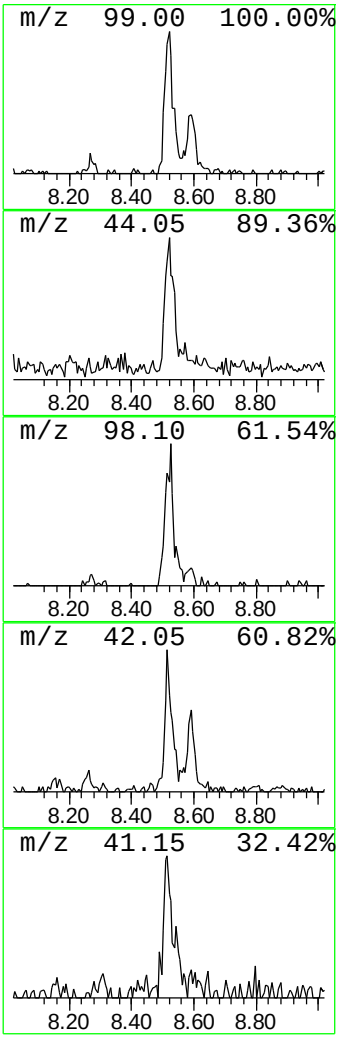
****

Peak Number 5 2-Pyrrolidinone, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	3.35 ng	117529	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	90
2	4-(Methylamino)butyric acid	117	C5H11NO2	001119-48-8	59
3	Piperidine, 4-methyl-	99	C6H13N	000626-58-4	45
4	Imidosulfurous difluoride, methyl-	99	CH3F2NS	000758-20-3	38
5	Propanal, (1-methylethyl)hydrazone	114	C6H14N2	016713-38-5	38





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Sample : H5509-16
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-4.5-5.0

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

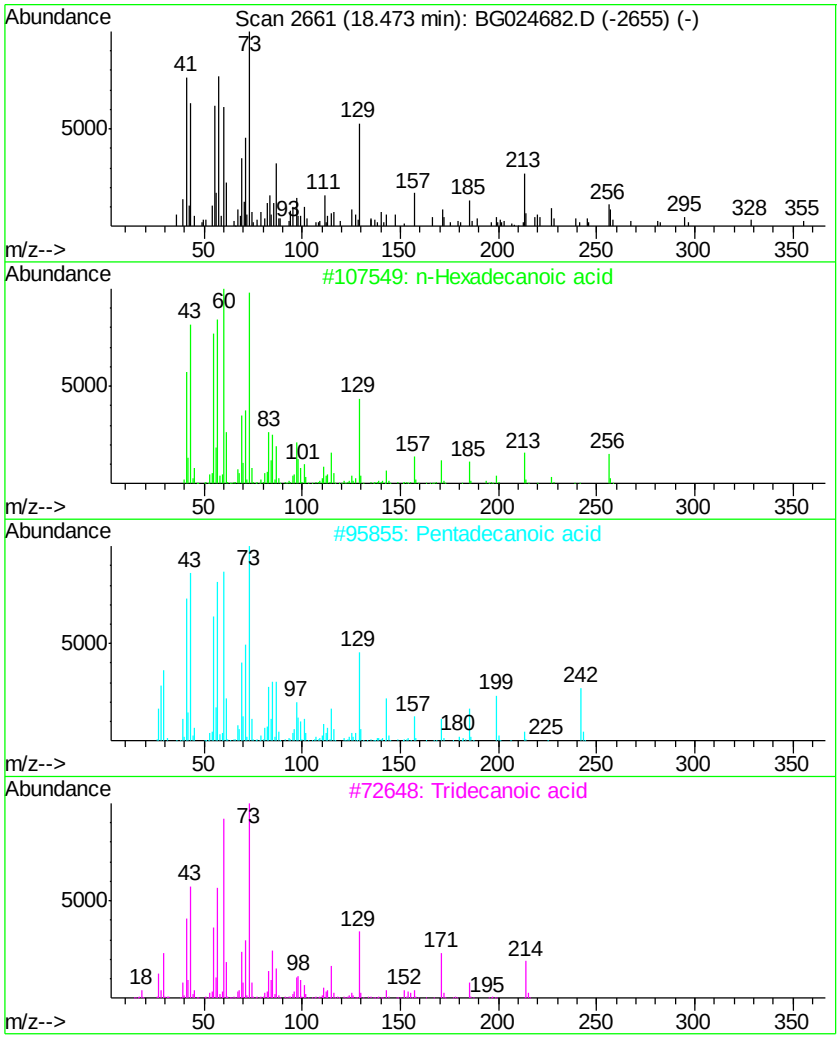
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

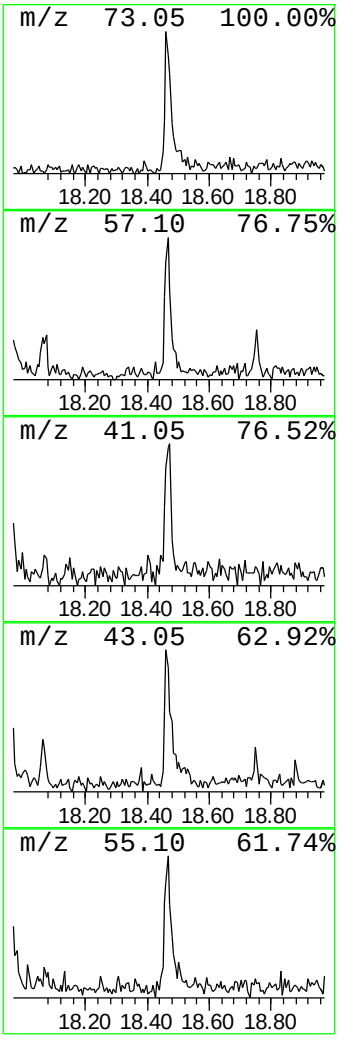
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.11 ng	206289	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Misc :
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Instrument : BNA_G
ClientSampleId : S-1-4.5-5.0

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

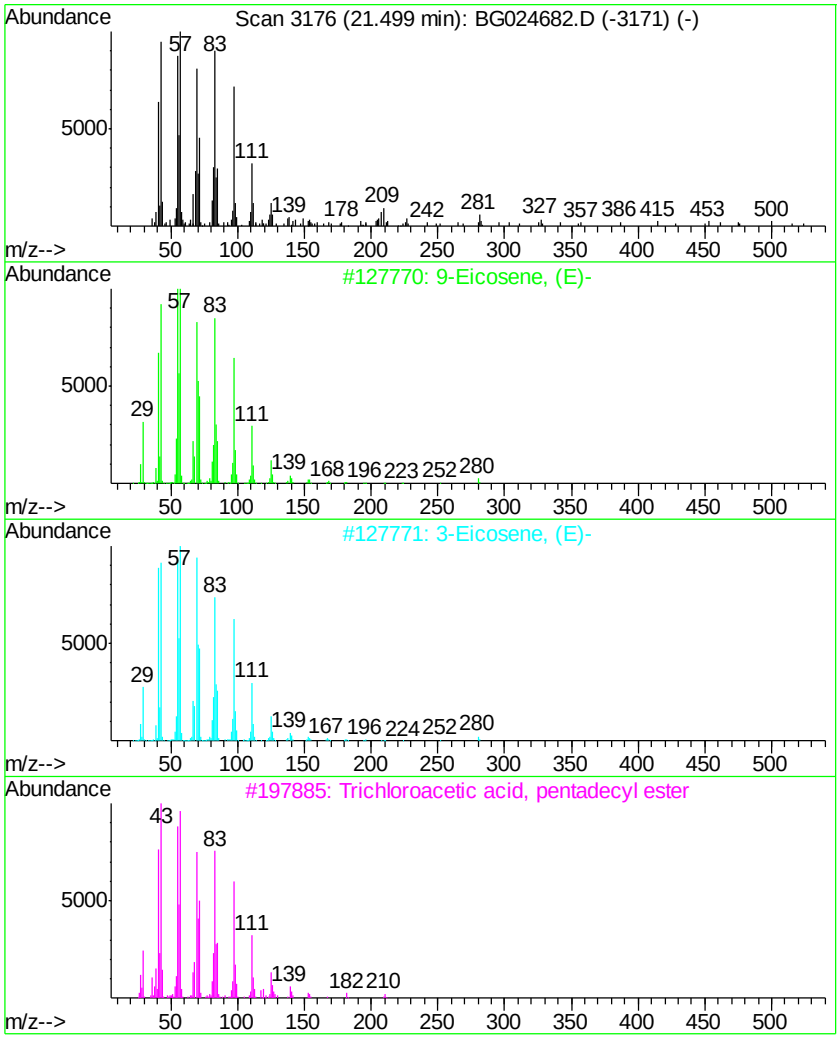
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

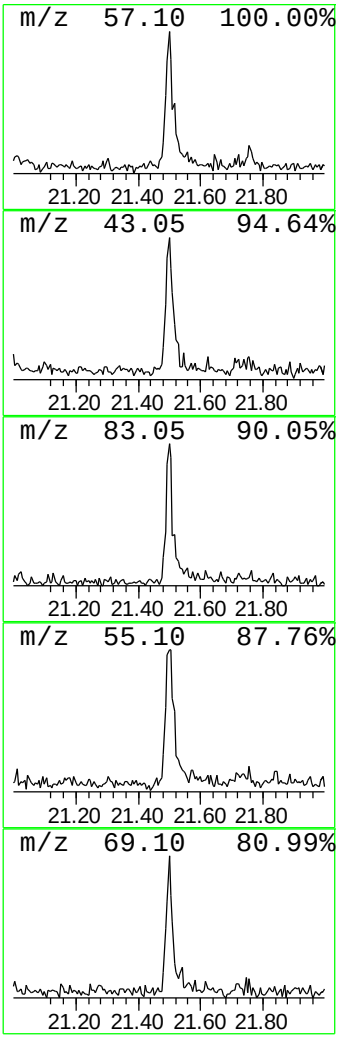
****

Peak Number 8 9-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	2.07 ng	276476	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	94
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
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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	201.9	ng	7082470	1	8.27	701599	20.0
2-Pentanone, 4-hy...	5.33	15.9	ng	557515	1	8.27	701599	20.0
Neopentyl glycol	6.72	2.4	ng	84637	1	8.27	701599	20.0
unknown7.79	7.79	79.4	ng	2785290	1	8.27	701599	20.0
2-Pyrrolidinone, ...	8.52	3.4	ng	117529	1	8.27	701599	20.0
n-Hexadecanoic acid	18.47	2.1	ng	206289	4	17.62	1952350	20.0
9-Eicosene, (E)-	21.50	2.1	ng	276476	5	21.92	2666710	20.0