LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG062817\
Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
Sample : I3657-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105D

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-BG062817.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	5.604	285	292	299	rBV	37607	62688	1.57%	0.357%
2	5.927	339	347	355	rBV2	32050	57071	1.43%	0.325%
3	6.051	361	368	378	rVB	323471	566333	14.20%	3.224%
4	7.614	626	634	647	rBV	226635	429925	10.78%	2.447%
5	8.007	693	701	709	rBV	610774	1105289	27.71%	6.291%
6	8.471	774	780	791	rBV	134859	257544	6.46%	1.466%
7	8.800	829	836	846	rVB	489450	885855	22.21%	5.042%
8	9.641	970	979	988	rBV	488552	909690	22.81%	5.178%
9	10.792	1172	1175	1186	rVB4	15260	41434	1.04%	0.236%
10	11.292	1253	1260	1278	rBV	259822	524378	13.15%	2.985%
11	11.938	1363	1370	1376	rBV3	30774	61110	1.53%	0.348%
12	12.214	1411	1417	1423	rBV3	21315	43671	1.09%	0.249%
13	13.683	1656	1667	1677	rBV	1415942	2263908	56.76%	12.886%
14	14.494	1799	1805	1812	rBV	361632	545851	13.69%	3.107%
15	14.564	1812	1817	1826	rVV2	97549	151185	3.79%	0.861%
16	15.058	1887	1901	1913	rBV2	358305	619988	15.55%	3.529%
17	15.698	2004	2010	2017	rVB3	21868	41779	1.05%	0.238%
18	15.775	2017	2023	2028	rBV2	72540	106840	2.68%	0.608%
19	16.544	2147	2154	2161	rBV	1194922	1924111	48.24%	10.952%
20	16.726	2179	2185	2191	rBV4	30000	61947	1.55%	0.353%
21	17.584	2324	2331	2338	rVB3	31824	61955	1.55%	0.353%
22	17.807	2363	2369	2379	rVB	471176	771192	19.34%	4.390%
23	18.648	2507	2512	2520	rBV3	29085	51462	1.29%	0.293%
24	20.387	2802	2808	2819	rBV	2934103	3988328	100.00%	22.701%
25	22.167	3104	3111	3121	rBV	476787	896194	22.47%	5.101%
26	22.355	3134	3143	3155	rBV	131883	264731	6.64%	1.507%
27	25.775	3713	3725	3740	rVB2	272068	874338	21.92%	4.977%

Sum of corrected areas: 17568797

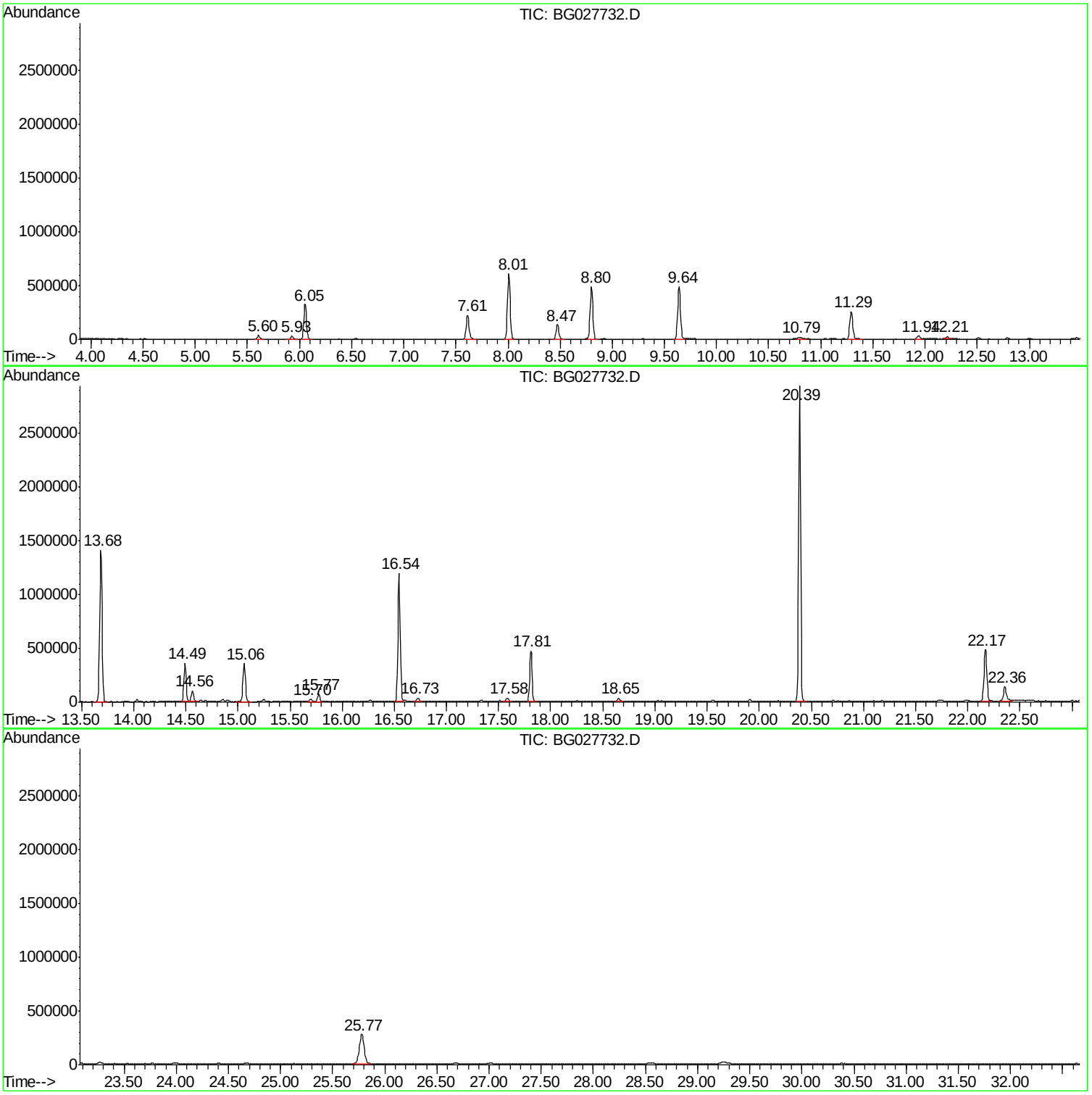
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG062817\
Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
Sample : I3657-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-105D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.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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Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
Sample : I3657-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

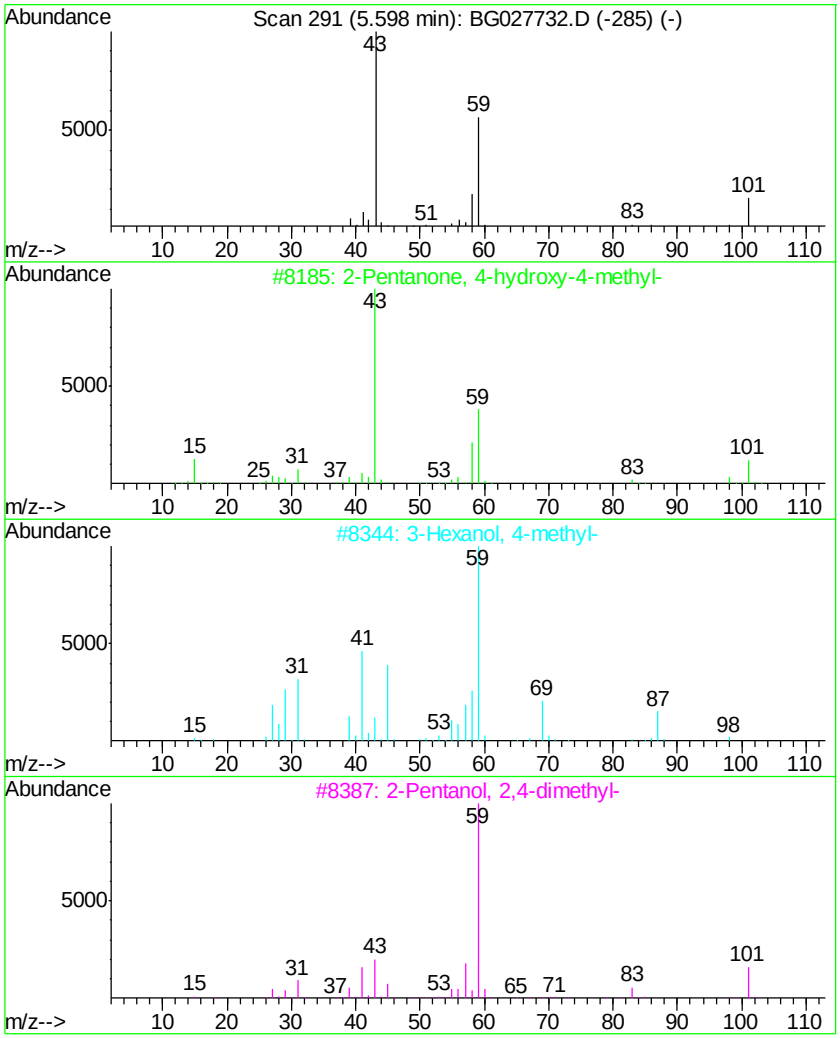
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

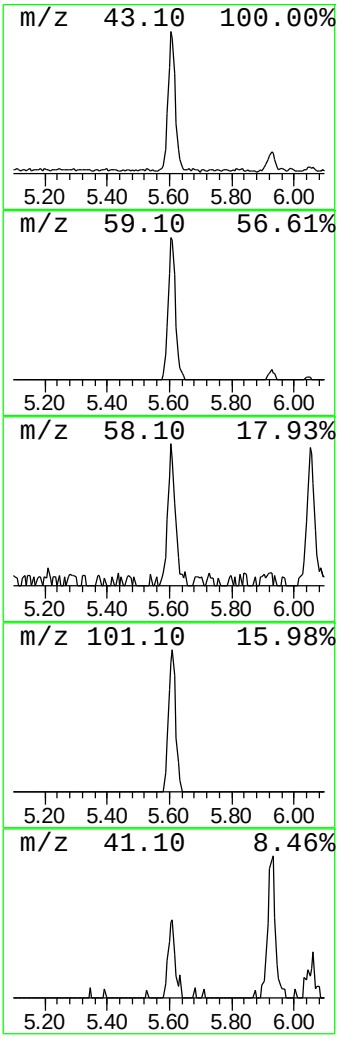
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	4.87 ng	62688	1,4-Dichlorobenzene-d4	8.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	23





Library Search Compound Report

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Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
Sample : I3657-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

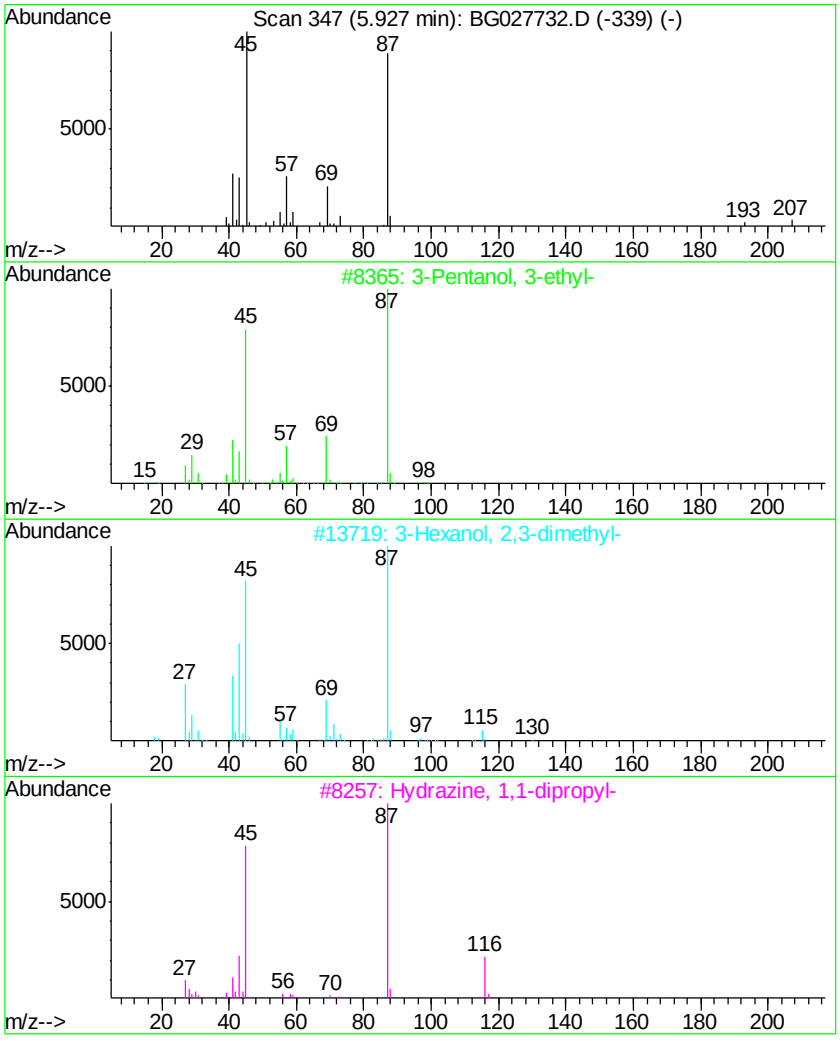
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

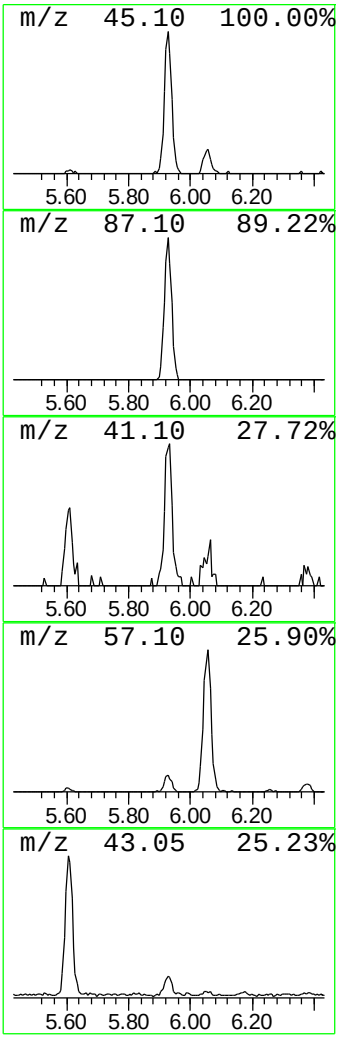
****

Peak Number 2 3-Pentanol, 3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	4.43 ng	57071	1,4-Dichlorobenzene-d4	8.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-ethyl-	116	C7H16O	000597-49-9	78
2	3-Hexanol, 2,3-dimethyl-	130	C8H18O	004166-46-5	74
3	Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	72
4	4-Octanol, 4-methyl-	144	C9H20O	023418-37-3	64
5	4-Heptanol, 4-methyl-	130	C8H18O	000598-01-6	64





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Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
Sample : I3657-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

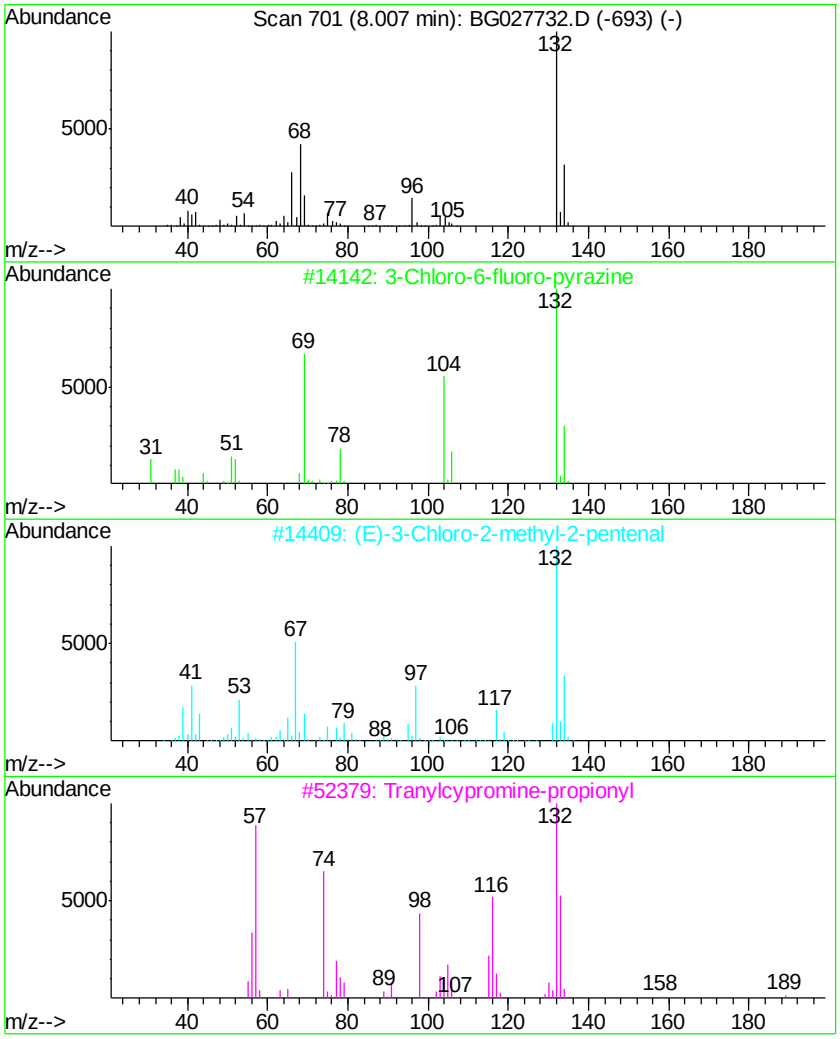
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

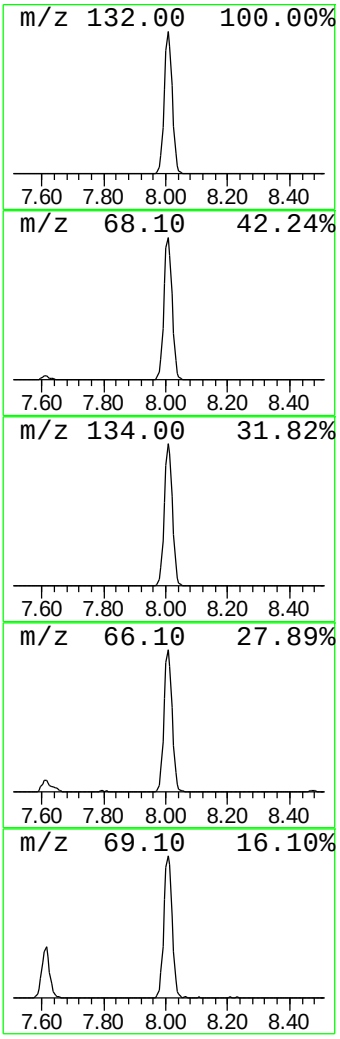
****

Peak Number 3 unknown8.01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	85.83 ng	1105290	1,4-Dichlorobenzene-d4	8.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
Sample : I3657-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

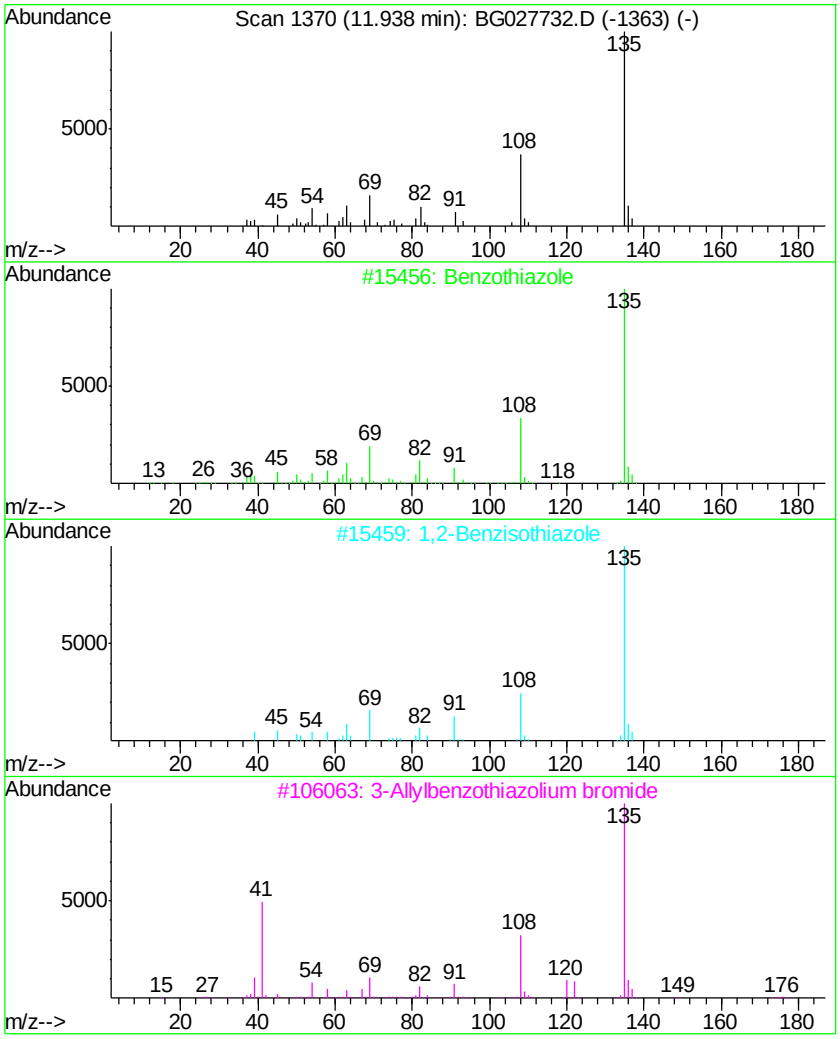
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

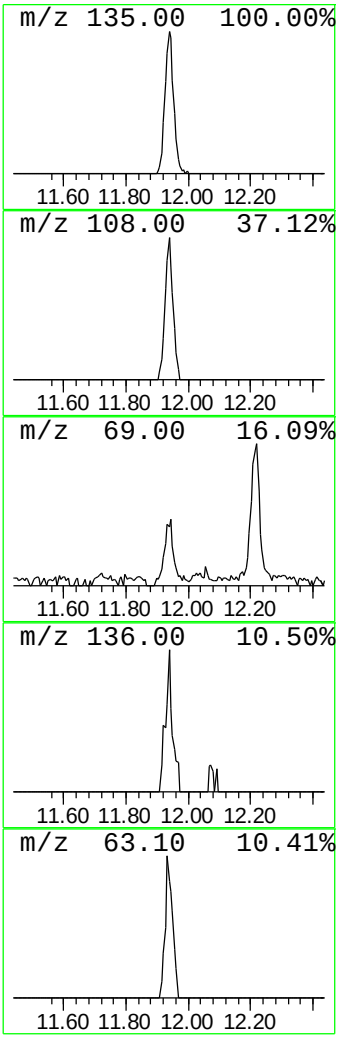
****

Peak Number 5 Benzothiazole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.33 ng	61110	Naphthalene-d8	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	93
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	86
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	78
4	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
5	Adenine	135	C5H5N5	000073-24-5	59





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Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
Sample : I3657-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

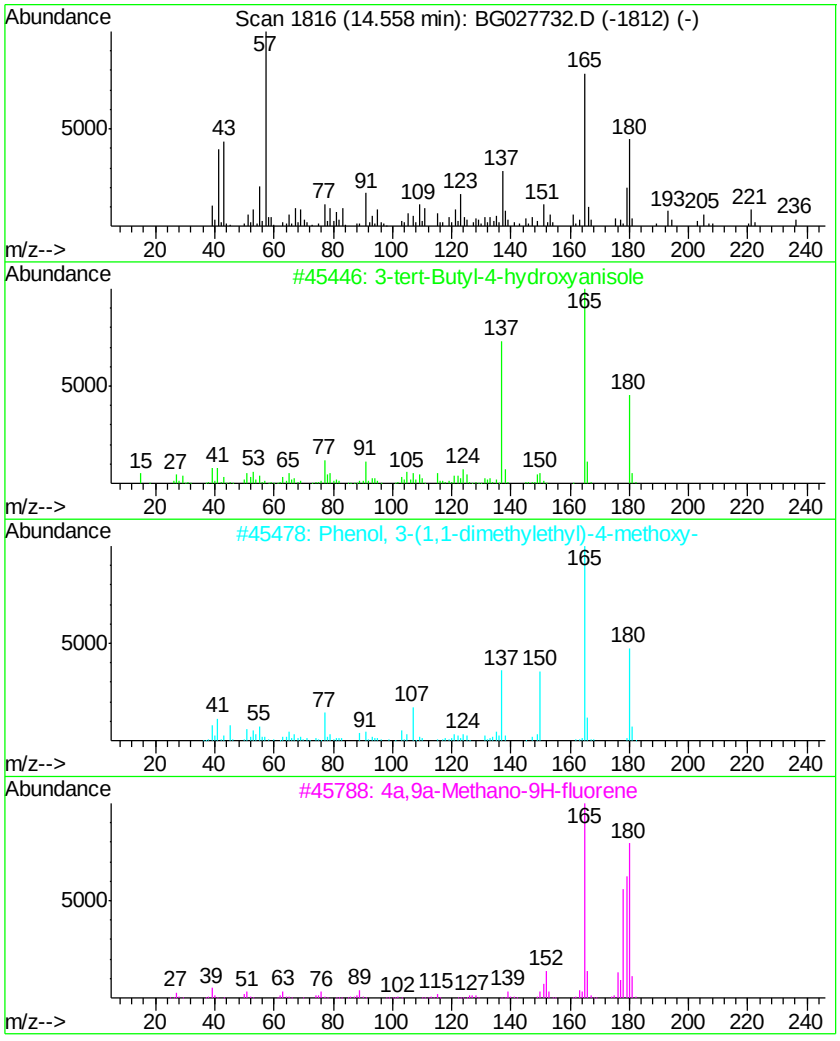
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

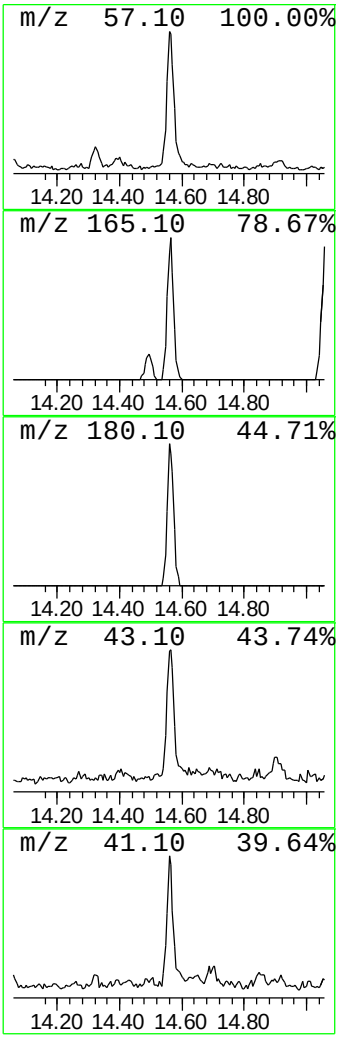
****

Peak Number 6 3-tert-Butyl-4-hydroxyanisole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	4.88 ng	151185	Acenaphthene-d10	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	78
2	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	62
3	4a,9a-Methano-9H-fluorene	180	C14H12	019540-84-2	58
4	Furan, 2,5-dihydro-2,2-dimethyl-...	180	C12H20O	077822-53-8	58
5	Benzenamine, N-ethyl-N-methyl-4-...	180	C9H12N2O2	056269-48-8	53





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG062817\
Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
Sample : I3657-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

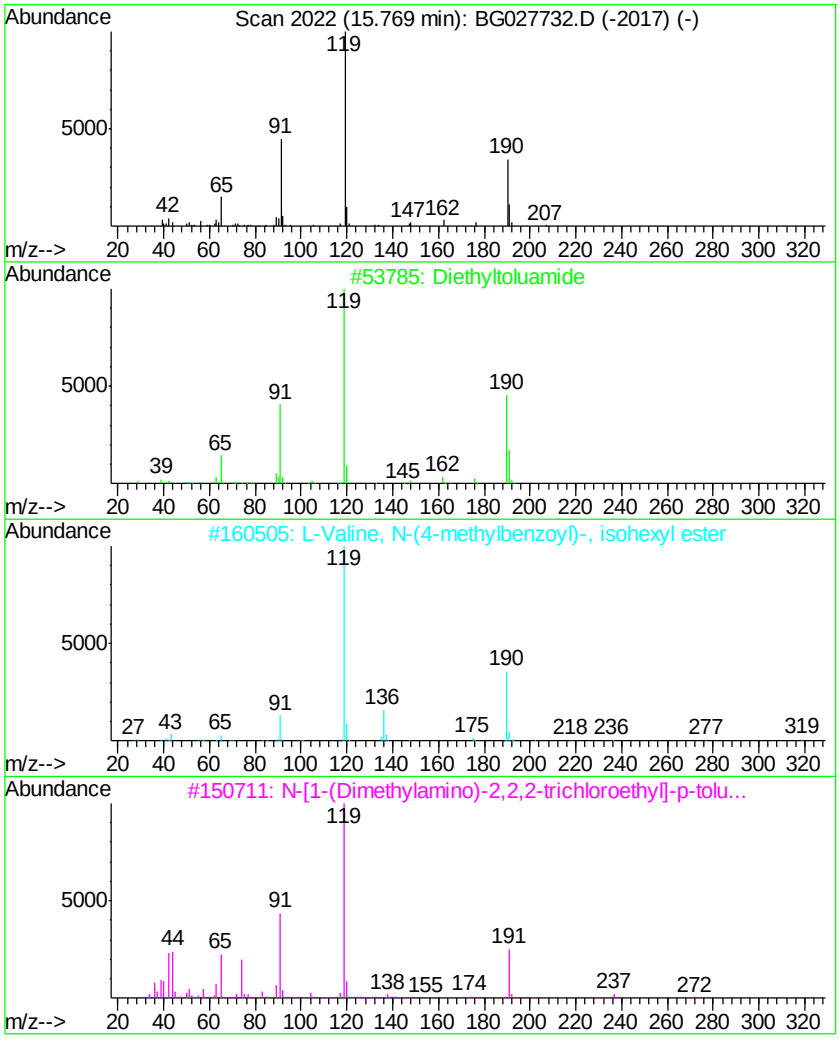
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

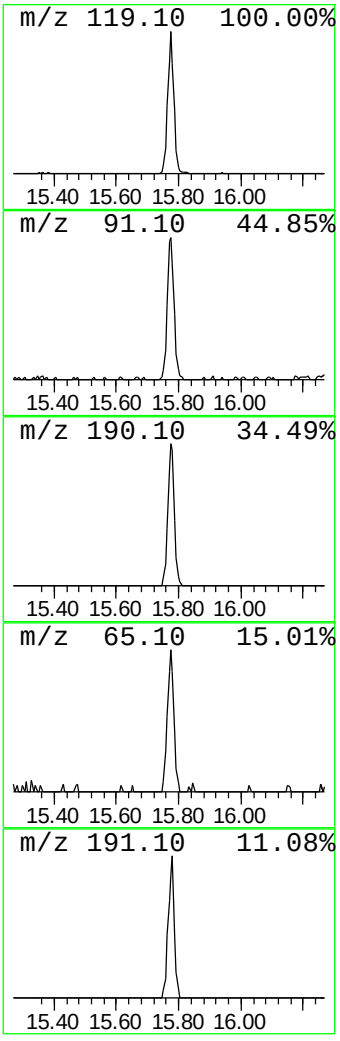
****

Peak Number 7 Diethyltoluamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	3.45 ng	106840	Acenaphthene-d10	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	92
2	L-Valine, N-(4-methylbenzoyl)-, ...	319	C19H29NO3	1000346-64-2	78
3	N-[1-(Dimethylamino)-2,2,2-trich...	308	C12H15Cl3N2O	300814-41-9	64
4	Benzamide, 3-methyl-N-[5-trifluo...	409	C18H14F7NO2	339240-75-4	64
5	3-Methyl-benzoic acid 3-oxo-2-ph...	340	C23H16O3	097586-13-5	59





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG062817\
Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
Sample : I3657-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

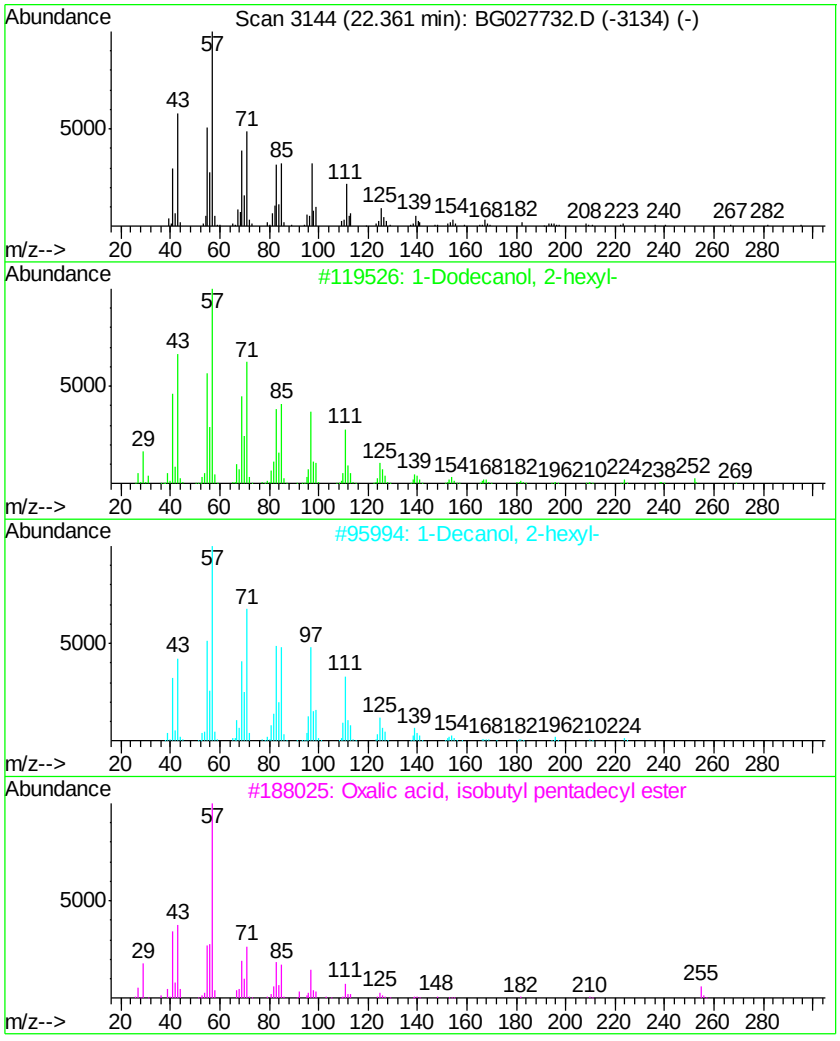
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

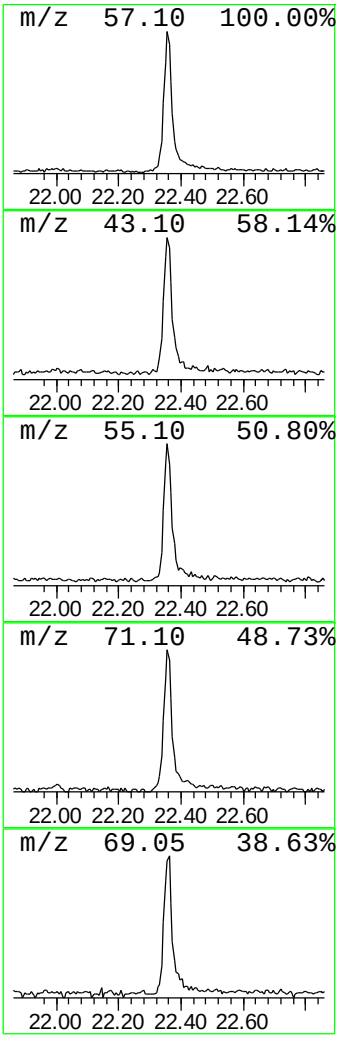
****

Peak Number 8 1-Dodecanol, 2-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.36	5.91 ng	264731	Chrysene-d12	22.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	91
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
3	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90
5	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	86





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG062817\
Data File : BG027732.D
Acq On : 29 Jun 2017 8:38
Operator : SJ/JU
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Misc :
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.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...	5.60	4.9	ng	62688	1	8.48	257544	20.0
3-Pentanol, 3-ethyl-	5.93	4.4	ng	57071	1	8.48	257544	20.0
unknown8.01	8.01	85.8	ng	1105290	1	8.48	257544	20.0
Benzothiazole	11.94	2.3	ng	61110	2	11.29	524378	20.0
3-tert-Butyl-4-hy...	14.56	4.9	ng	151185	3	15.06	619988	20.0
Diethyltoluamide	15.77	3.5	ng	106840	3	15.06	619988	20.0
1-Dodecanol, 2-he...	22.36	5.9	ng	264731	5	22.17	896194	20.0