LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038857.D
Acq On : 27 Dec 2018 23:51
Operator : JU/SJ
Sample : J6549-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-9

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	3.178	11	15	21	rVB2	27515	40879	1.73%	0.396%
2	5.141	342	349	355	rBV	15062	24077	1.02%	0.233%
3	5.611	422	429	439	rBV	218367	363871	15.39%	3.524%
4	7.215	695	702	715	rBV	153986	291544	12.33%	2.824%
5	7.585	757	765	779	rVB	416240	748081	31.63%	7.246%
6	8.055	838	845	855	rBV	77463	130344	5.51%	1.262%
7	8.378	892	900	908	rBV	357176	629973	26.64%	6.102%
8	9.236	1037	1046	1057	rBV	314477	576701	24.38%	5.586%
9	10.875	1316	1325	1335	rBV	108005	203168	8.59%	1.968%
10	13.313	1733	1740	1753	rVB	1040454	1609823	68.07%	15.592%
11	14.694	1968	1975	1984	rBV2	197153	333111	14.08%	3.226%
12	16.186	2222	2229	2244	rBV	880246	1377521	58.25%	13.342%
13	17.438	2436	2442	2449	rBV2	257438	411737	17.41%	3.988%
14	20.041	2879	2885	2895	rVB	1751387	2365038	100.00%	22.907%
15	20.799	3012	3014	3021	rVB2	24365	32082	1.36%	0.311%
16	21.310	3097	3101	3110	rVB	46109	79942	3.38%	0.774%
17	21.721	3164	3171	3179	rBV2	250336	448857	18.98%	4.347%
18	21.856	3190	3194	3200	rVB	31794	51077	2.16%	0.495%
19	22.461	3294	3297	3304	rBV2	25167	37341	1.58%	0.362%
20	23.161	3412	3416	3422	rVB2	31611	55349	2.34%	0.536%
21	23.971	3549	3554	3561	rBV3	28326	64000	2.71%	0.620%
22	25.017	3723	3732	3743	rVB2	148632	450066	19.03%	4.359%

Sum of corrected areas: 10324582

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
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Sample : J6549-05
Misc :
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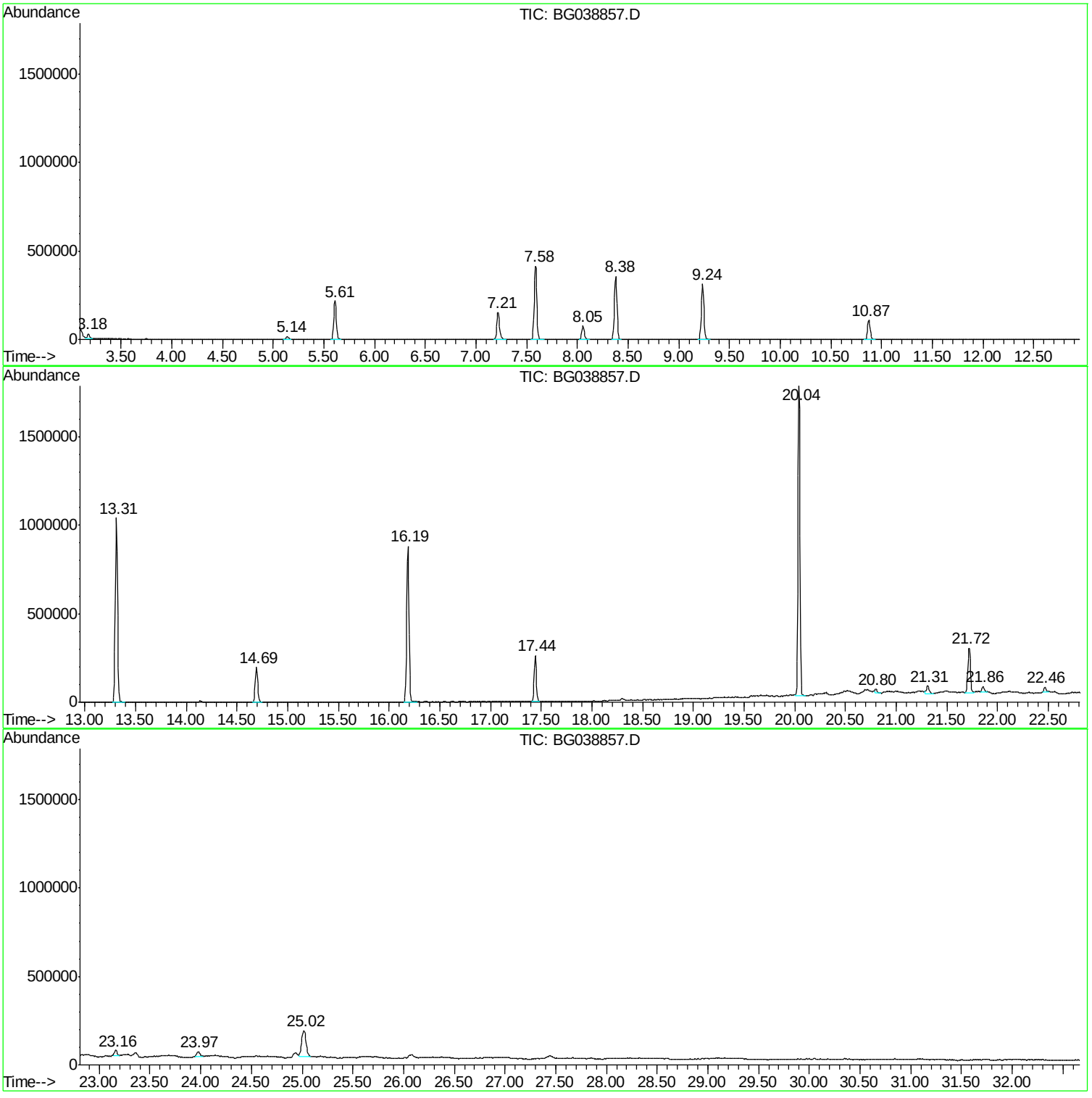
Instrument : BNA_G
ClientSampleId : MW-9

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038857.D
Acq On : 27 Dec 2018 23:51
Operator : JU/SJ
Sample : J6549-05
Misc :
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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

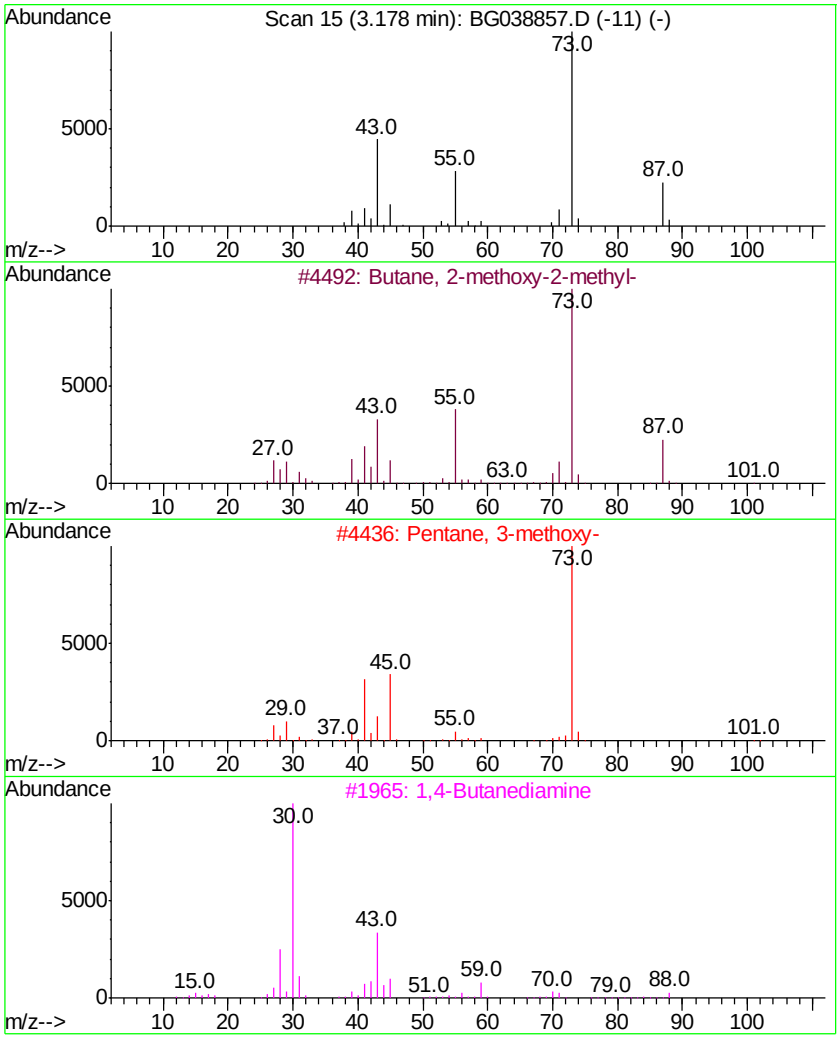
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

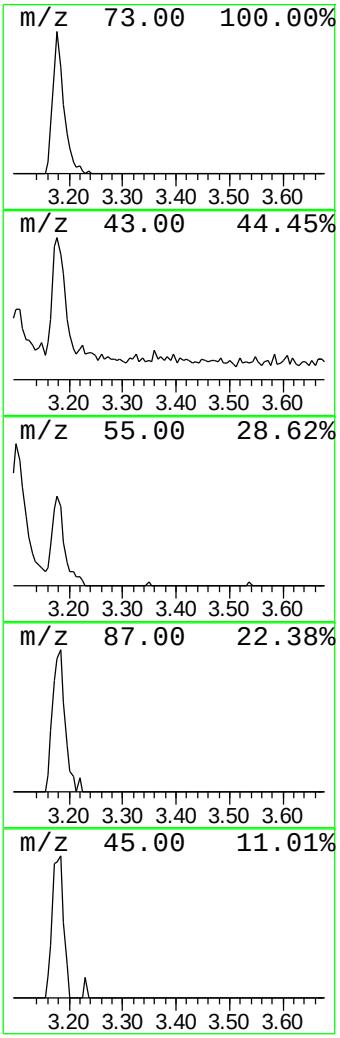
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	6.27 ng	40879	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	9
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
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Acq On : 27 Dec 2018 23:51
Operator : JU/SJ
Sample : J6549-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-9

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

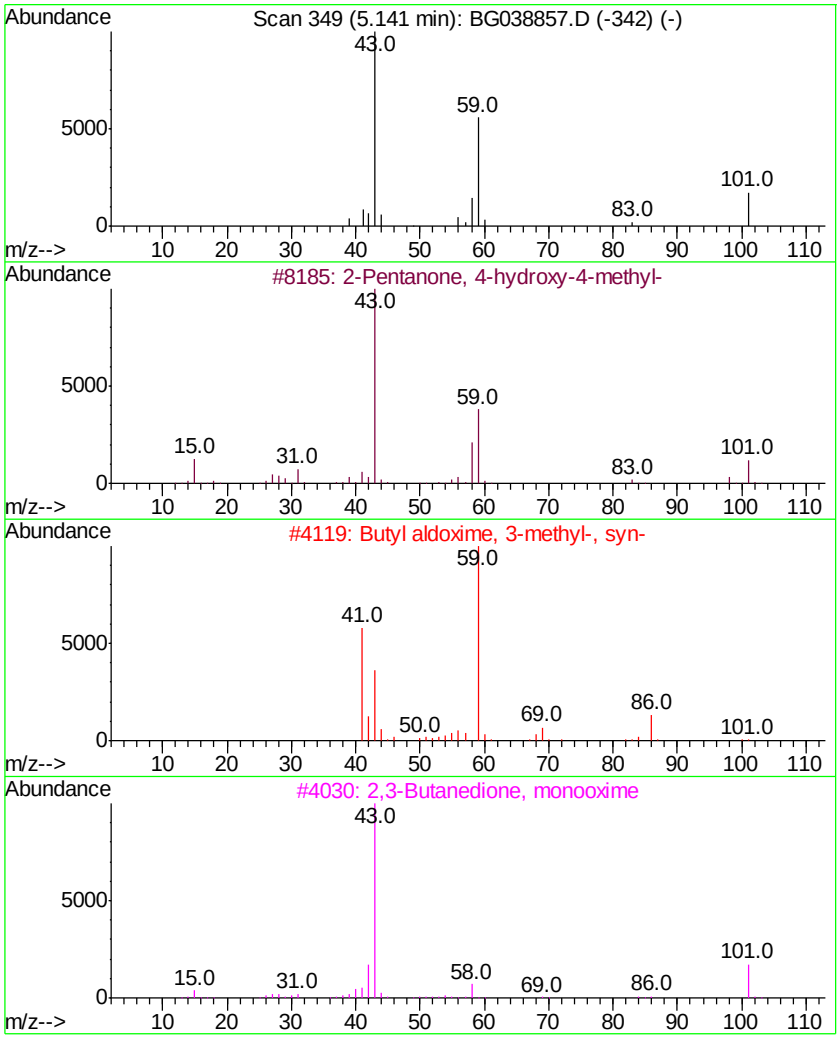
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

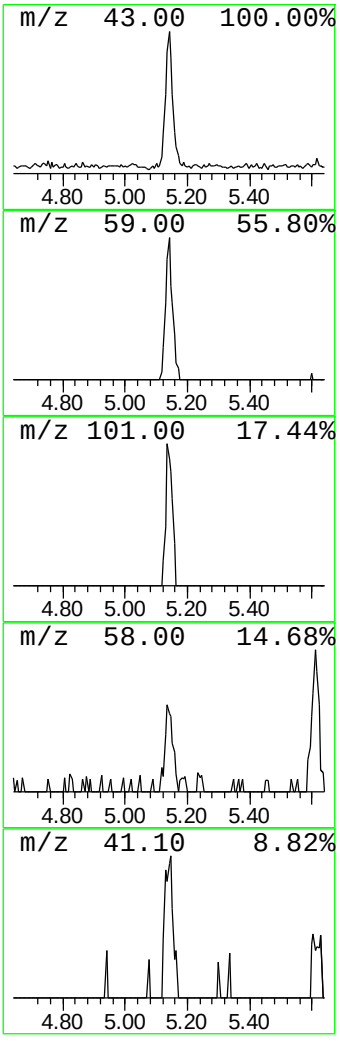
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	3.69 ng	24077	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Tetramethylammonium acetate	133	C6H15NO2	010581-12-1	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038857.D
Acq On : 27 Dec 2018 23:51
Operator : JU/SJ
Sample : J6549-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-9

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

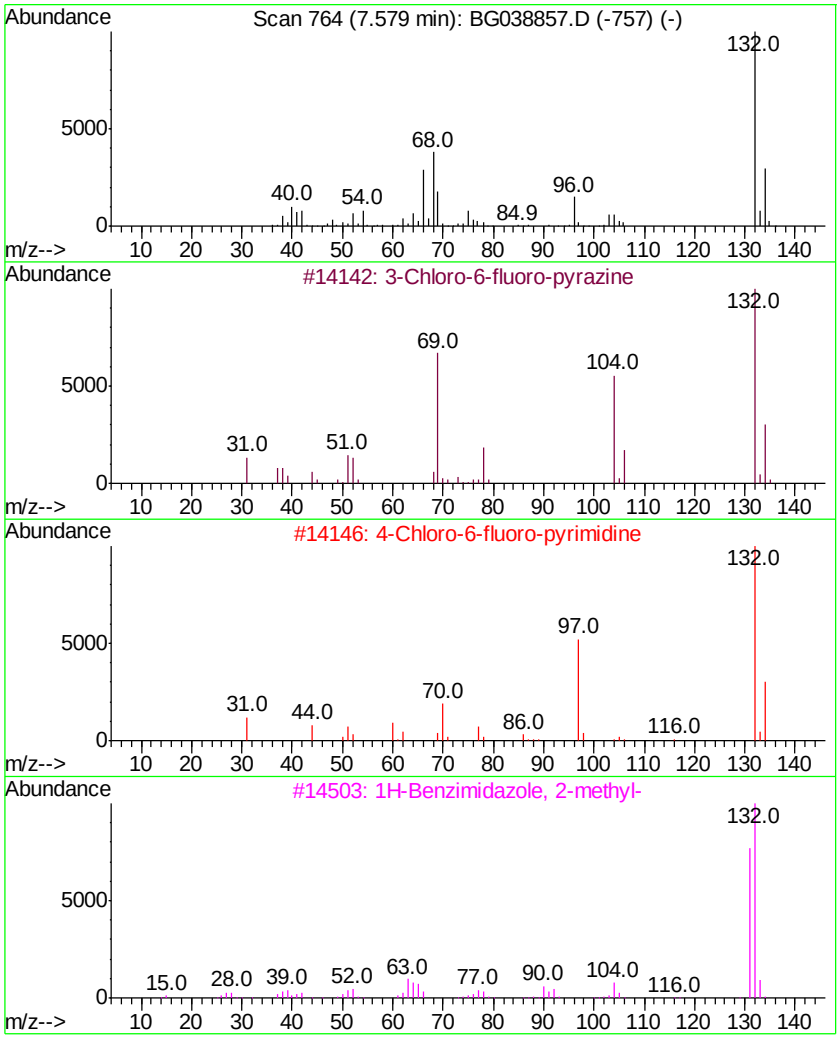
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

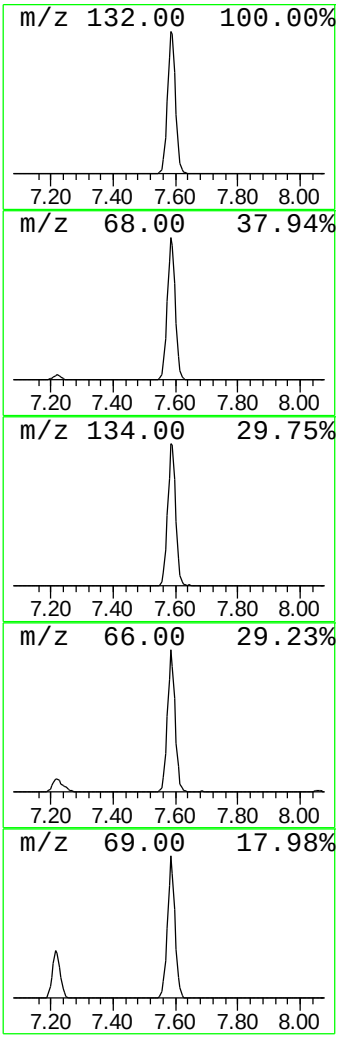
****

Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	114.79 ng	748081	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	35
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
4	5-Aminoindole	132	C8H8N2	005192-03-0	27
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
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Operator : JU/SJ
Sample : J6549-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-9

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

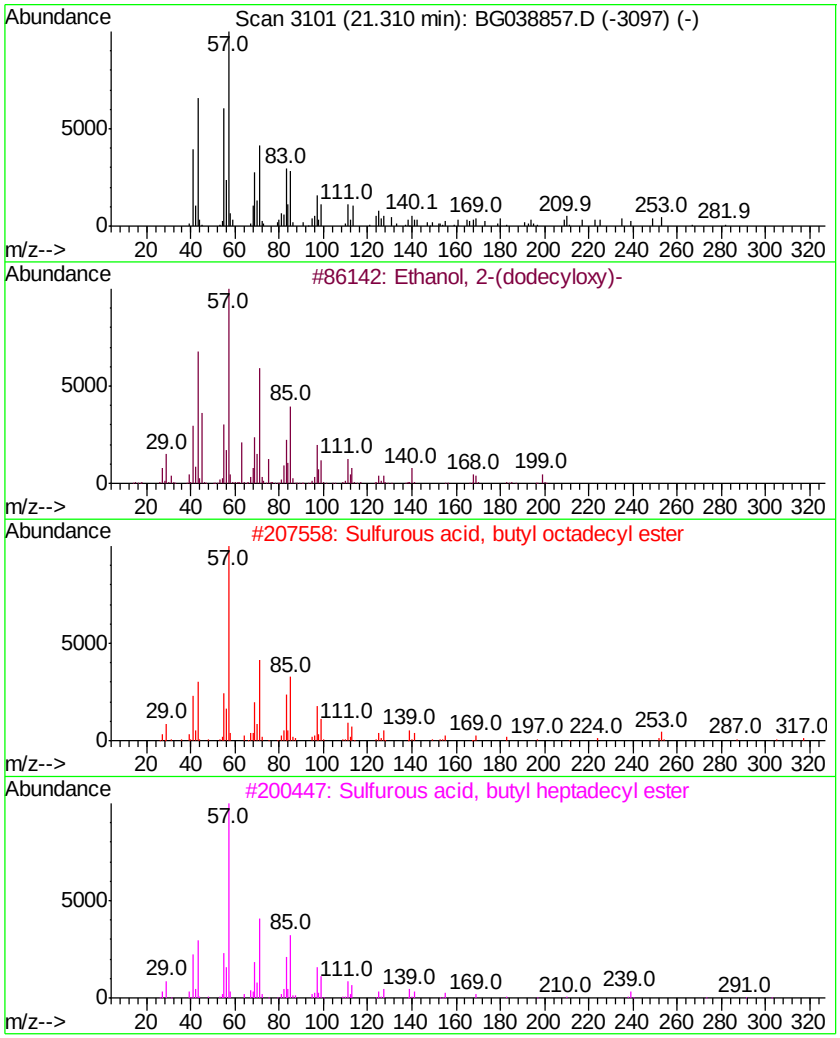
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

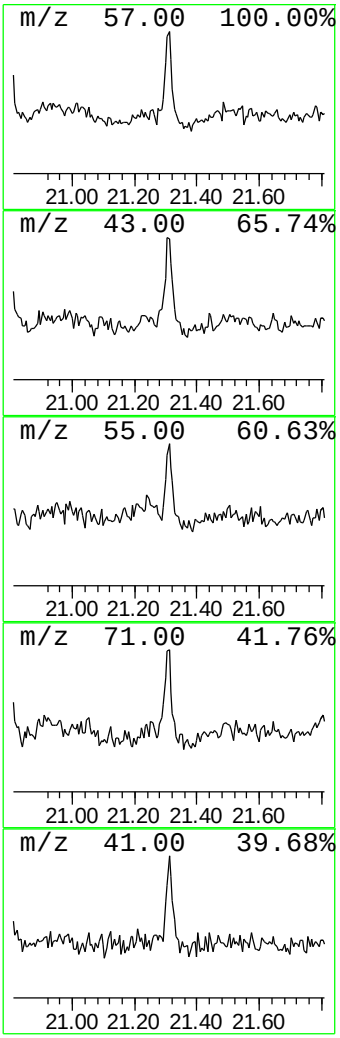
****

Peak Number 5 Ethanol, 2-(dodecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	3.56 ng	79942	Chrysene-d12	21.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	80
2	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	72
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	72
4	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	64
5	Hexatriacontane	507	C36H74	000630-06-8	64





Library Search Compound Report

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Sample : J6549-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-9

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
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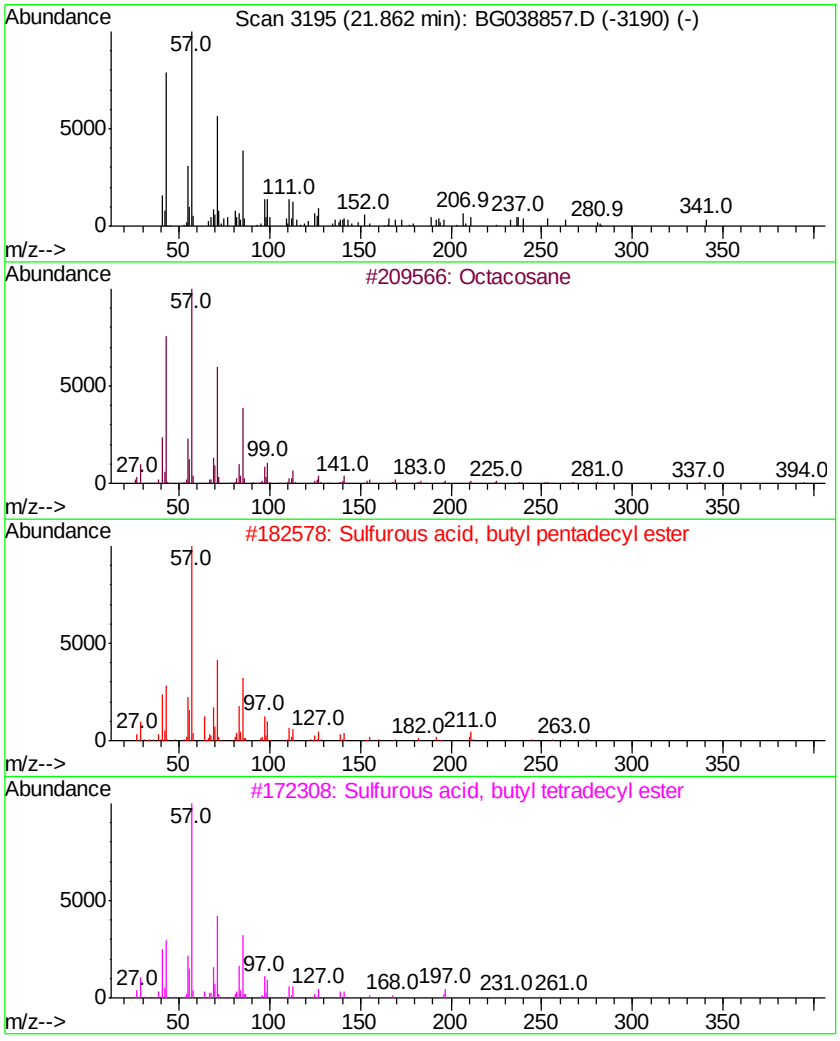
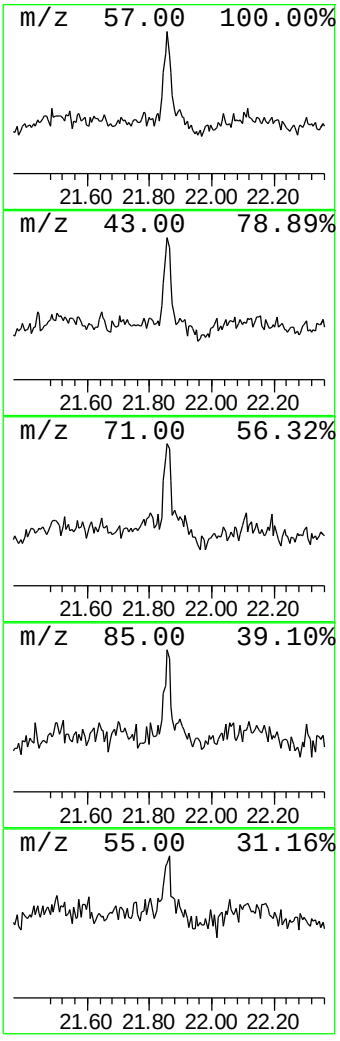
****

Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	2.28 ng	51077	Chrysene-d12	21.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	80
3	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80





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Misc :
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Instrument : BNA_G
ClientSampleId : MW-9

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

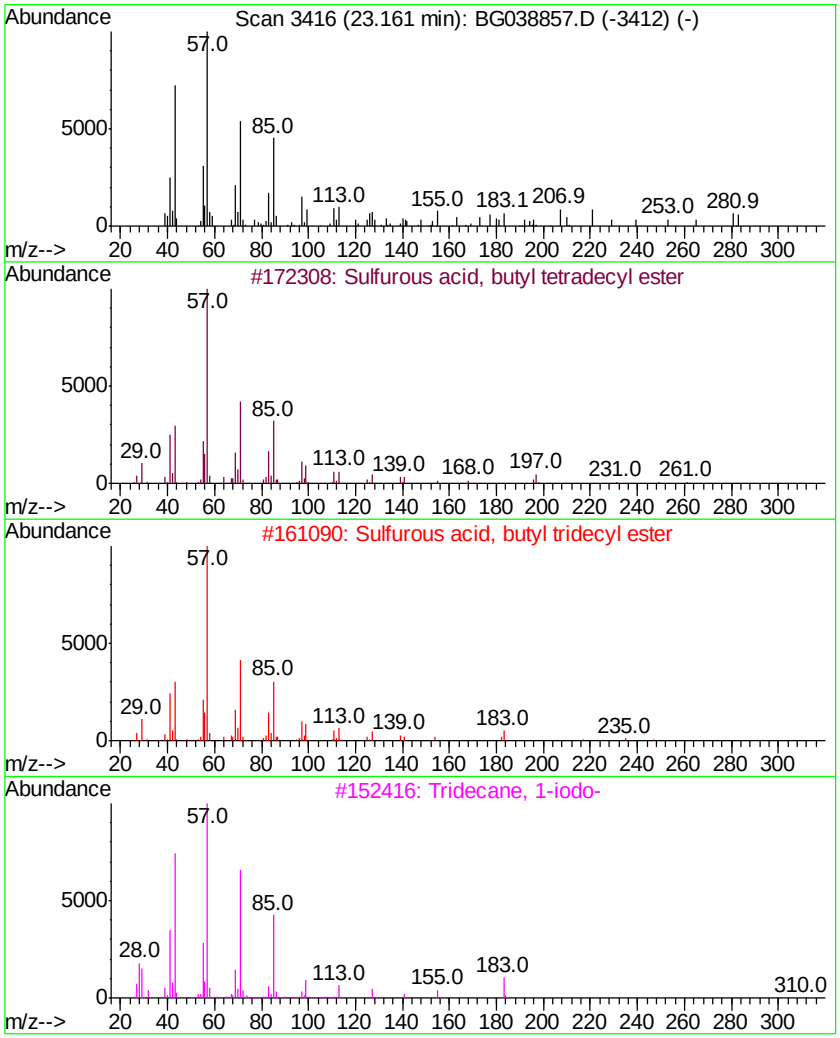
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

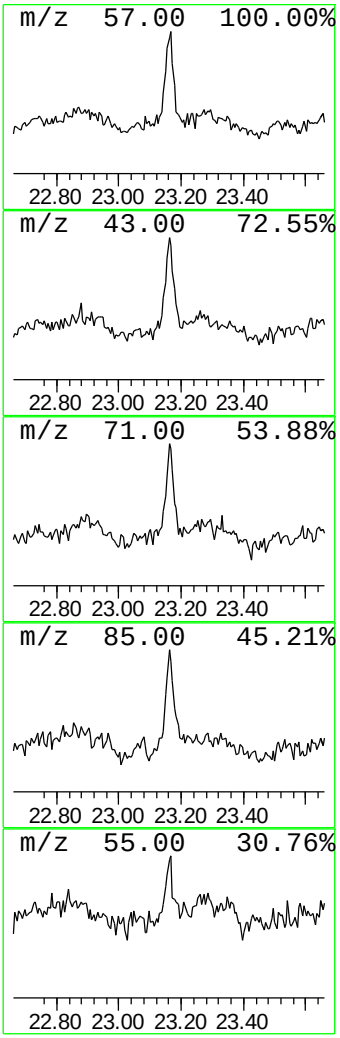
****

Peak Number 7 Sulfurous acid, butyl tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.16	2.47 ng	55349	Chrysene-d12	21.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
2	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	72
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
4	Nonadecane	268	C19H40	000629-92-5	59
5	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	59





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

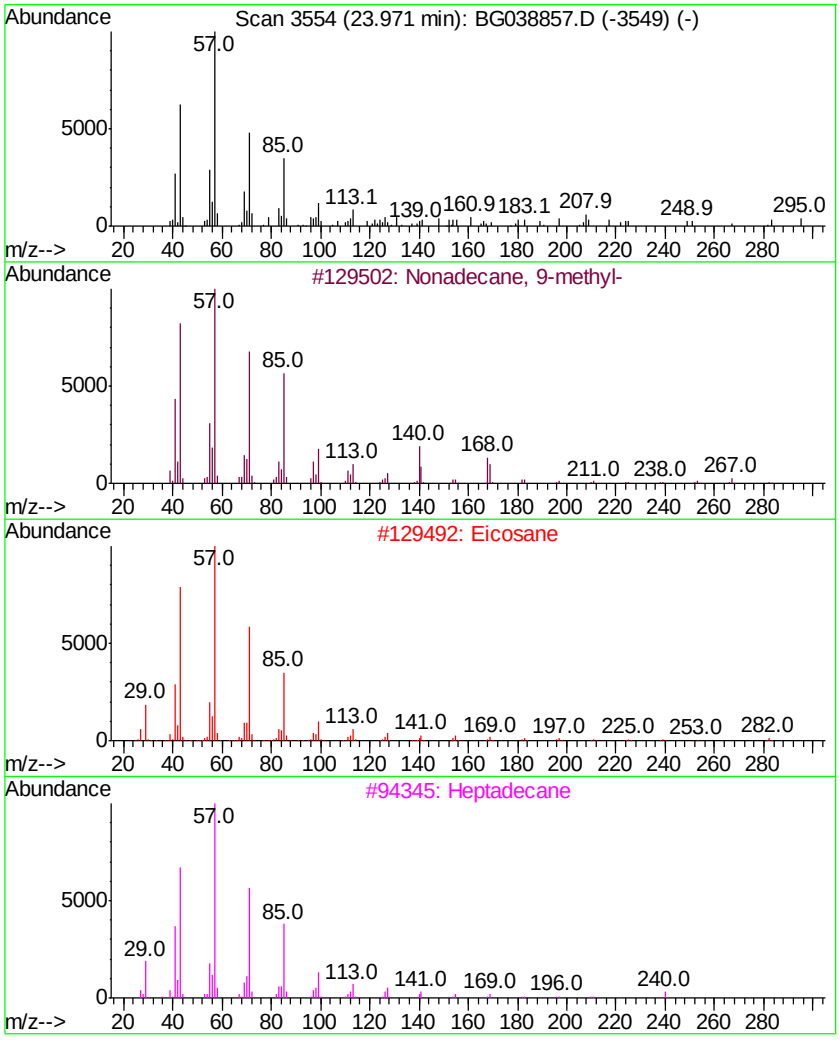
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

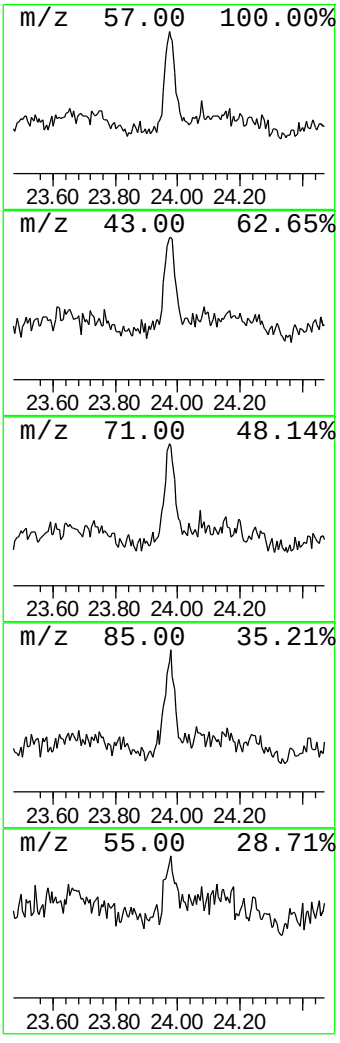
****

Peak Number 8 Nonadecane, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.97	2.84 ng	64000	Perylene-d12	25.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	81
2	Eicosane	282	C20H42	000112-95-8	81
3	Heptadecane	240	C17H36	000629-78-7	74
4	Heneicosane	296	C21H44	000629-94-7	74
5	Docosane	310	C22H46	000629-97-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG122718\
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.18	6.3	ng	40879	1	8.05	130344	20.0
2-Pentanone, 4-hy...	5.14	3.7	ng	24077	1	8.05	130344	20.0
unknown7.58	7.58	114.8	ng	748081	1	8.05	130344	20.0
Ethanol, 2-(dodec...	21.31	3.6	ng	79942	5	21.72	448857	20.0
Octacosane	21.86	2.3	ng	51077	5	21.72	448857	20.0
Sulfurous acid, b...	23.16	2.5	ng	55349	5	21.72	448857	20.0
Nonadecane, 9-met...	23.97	2.8	ng	64000	6	25.02	450066	20.0