LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P001-SD008-0006-01

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	5.139	345	349	356	rVB	22129	35189	3.02%	0.398%
2	5.609	422	429	440	rBV	428045	721754	61.96%	8.165%
3	7.213	694	702	714	rBV	455629	843982	72.45%	9.548%
4	7.589	758	766	776	rVB	411884	737044	63.27%	8.338%
5	8.059	838	846	853	rBV	80343	142236	12.21%	1.609%
6	8.382	893	901	908	rBV	275288	499362	42.87%	5.649%
7	9.234	1039	1046	1054	rBV	257548	486489	41.76%	5.503%
8	10.880	1317	1326	1335	rBV	102438	194165	16.67%	2.196%
9	13.312	1733	1740	1751	rBV	517528	848177	72.81%	9.595%
10	14.140	1876	1881	1888	rBV	31295	50452	4.33%	0.571%
11	14.693	1967	1975	1986	rVB2	168229	288495	24.77%	3.264%
12	16.185	2222	2229	2247	rBV	579177	898453	77.13%	10.164%
13	17.442	2437	2443	2449	rBV2	255207	390912	33.56%	4.422%
14	18.306	2584	2590	2601	rBV4	16452	32432	2.78%	0.367%
15	20.045	2876	2886	2893	rBV	857600	1164900	100.00%	13.178%
16	20.316	2928	2932	2939	rVB4	21400	32418	2.78%	0.367%
17	20.598	2976	2980	2983	rBV4	15857	15981	1.37%	0.181%
18	20.680	2986	2994	2995	rBV4	17508	34790	2.99%	0.394%
19	20.815	3013	3017	3019	rBV2	9533	12418	1.07%	0.140%
20	21.314	3099	3102	3112	rVV2	25776	45766	3.93%	0.518%
21	21.726	3164	3172	3180	rBV2	236472	419606	36.02%	4.747%
22	21.867	3191	3196	3202	rBV	12606	21249	1.82%	0.240%
23	22.478	3293	3300	3304	rBV	27584	47990	4.12%	0.543%
24	22.519	3304	3307	3314	rVB8	7206	16949	1.45%	0.192%
25	23.177	3410	3419	3424	rBV4	17518	39188	3.36%	0.443%
26	23.377	3445	3453	3459	rVB5	8747	20259	1.74%	0.229%
27	23.535	3476	3480	3486	rVB7	7637	14142	1.21%	0.160%
28	23.988	3549	3557	3565	rBV2	80364	191261	16.42%	2.164%
29	24.951	3712	3721	3724	rBV4	11062	26640	2.29%	0.301%
30	25.022	3724	3733	3746	rVB2	138771	409503	35.15%	4.633%
31	25.492	3804	3813	3824	rBV8	14070	41889	3.60%	0.474%
32	26.091	3906	3915	3926	rVB3	20829	61775	5.30%	0.699%
33	28.294	4279	4290	4300	rBV9	15421	53899	4.63%	0.610%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P001-SD008-0006-01

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

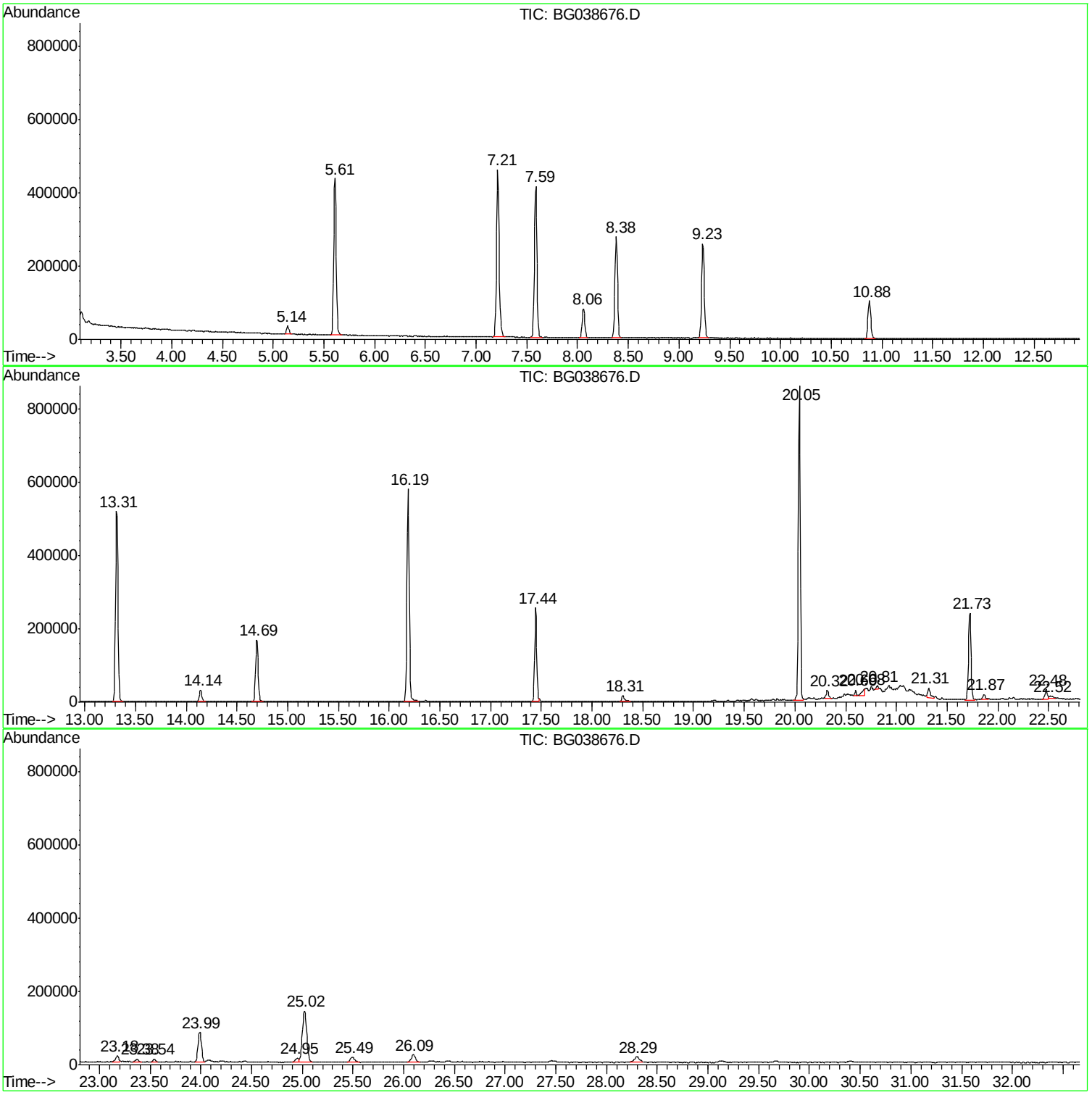
Sum of corrected areas: 8839765

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P001-SD008-0006-01

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\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P001-SD008-0006-01

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

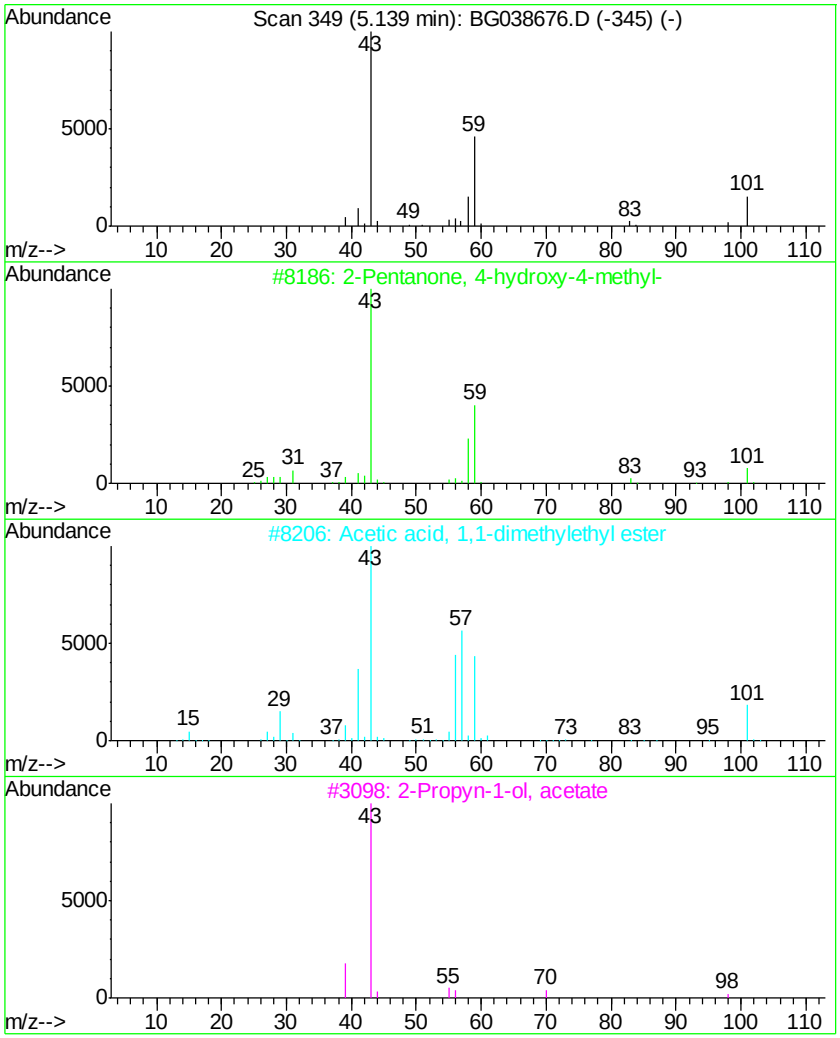
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

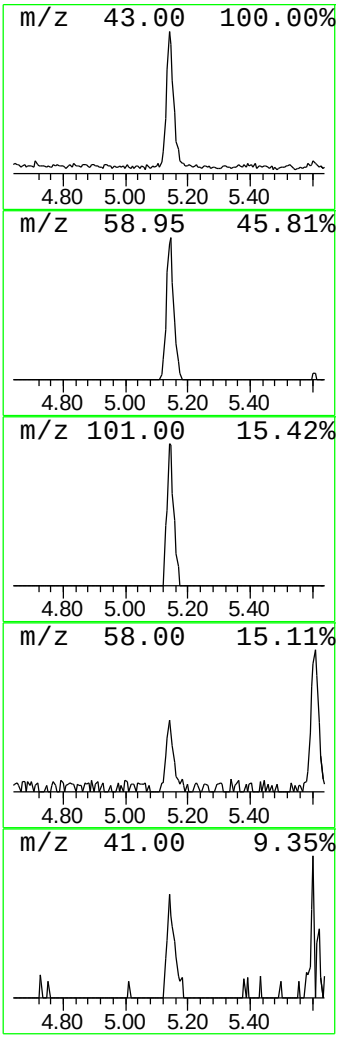
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	4.95 ng	35189	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
5	Diacetamide	101	C4H7NO2	000625-77-4	7





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P001-SD008-0006-01

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

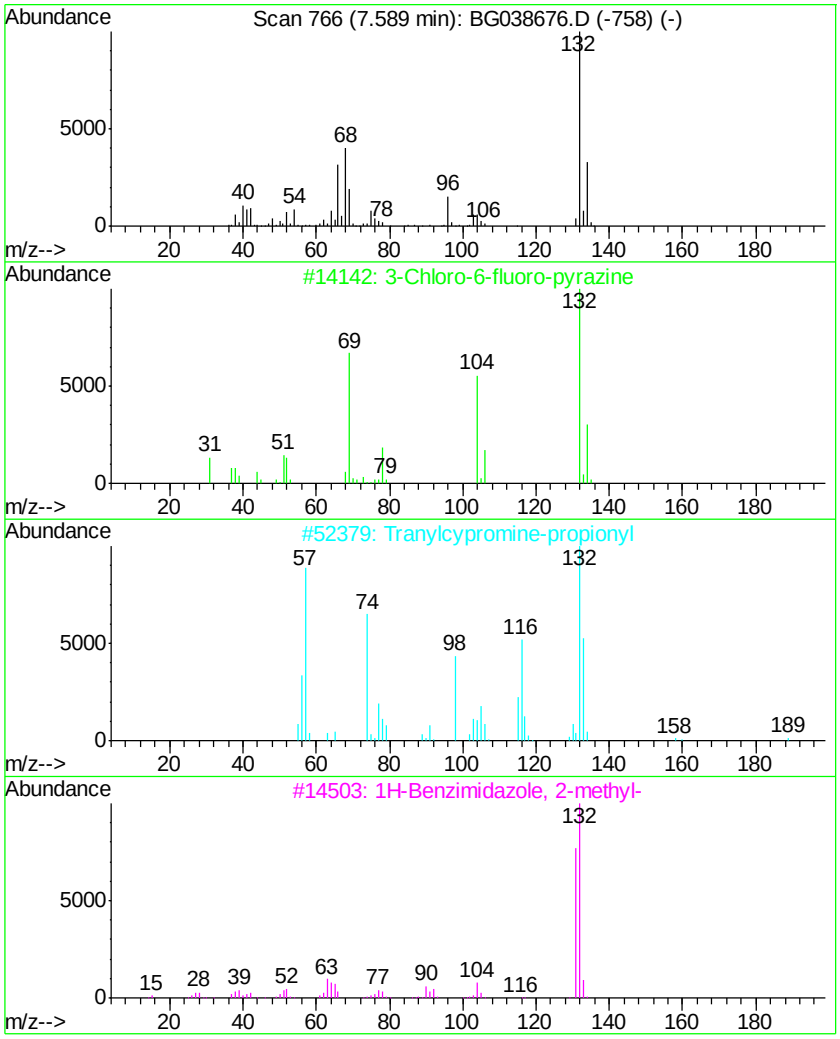
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

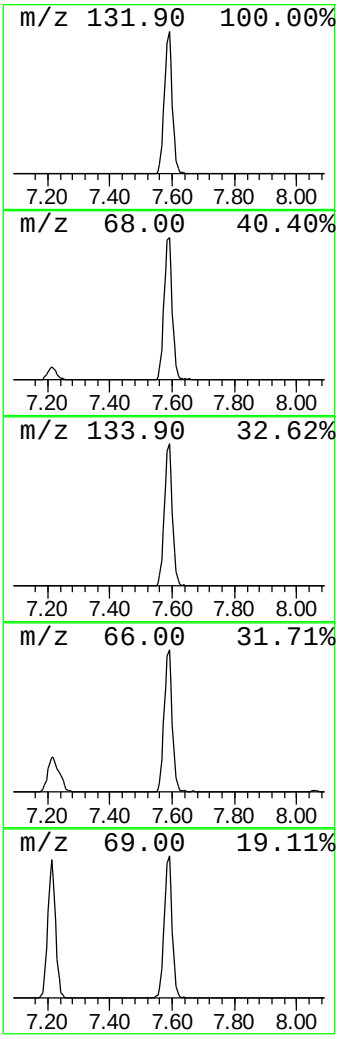
****

Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	103.64 ng	737044	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P001-SD008-0006-01

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

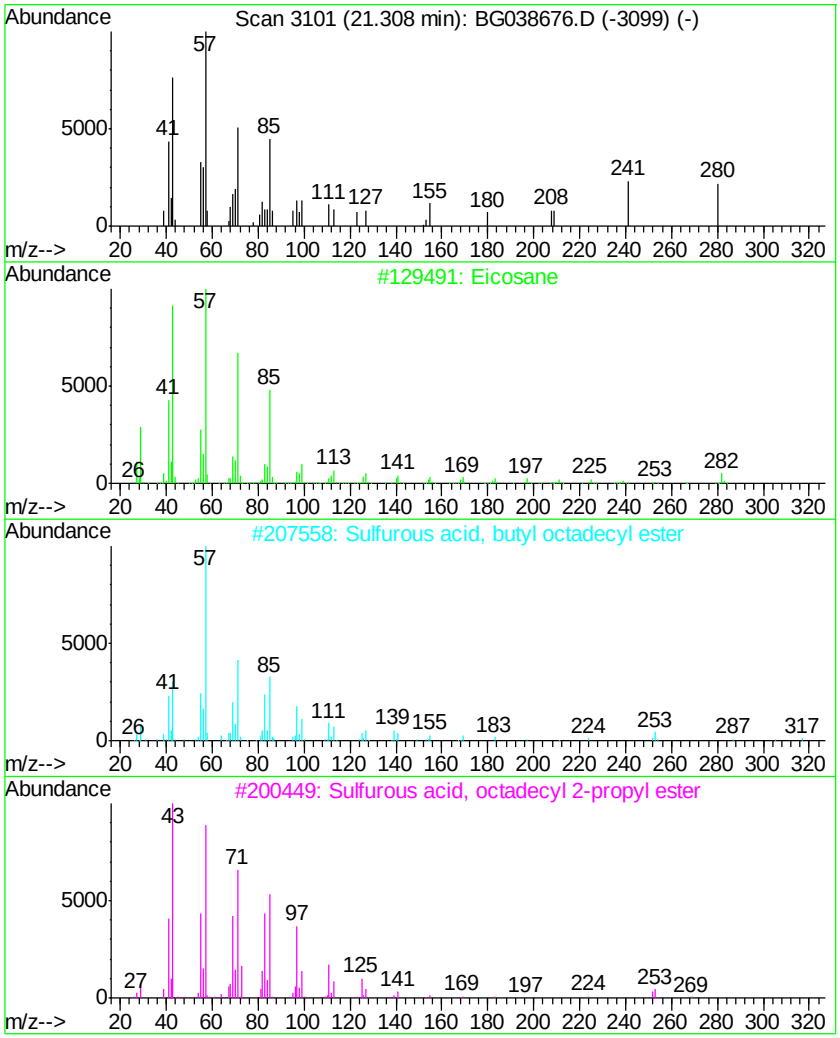
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

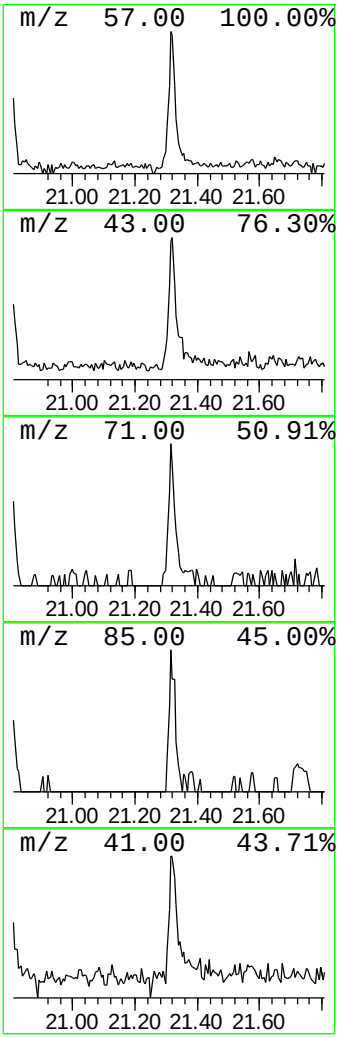
****

Peak Number 4 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	2.18 ng	45766	Chrysene-d12	21.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	58
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	58
4	2-methylhexacosane	380	C27H56	1000376-72-7	52
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P001-SD008-0006-01

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

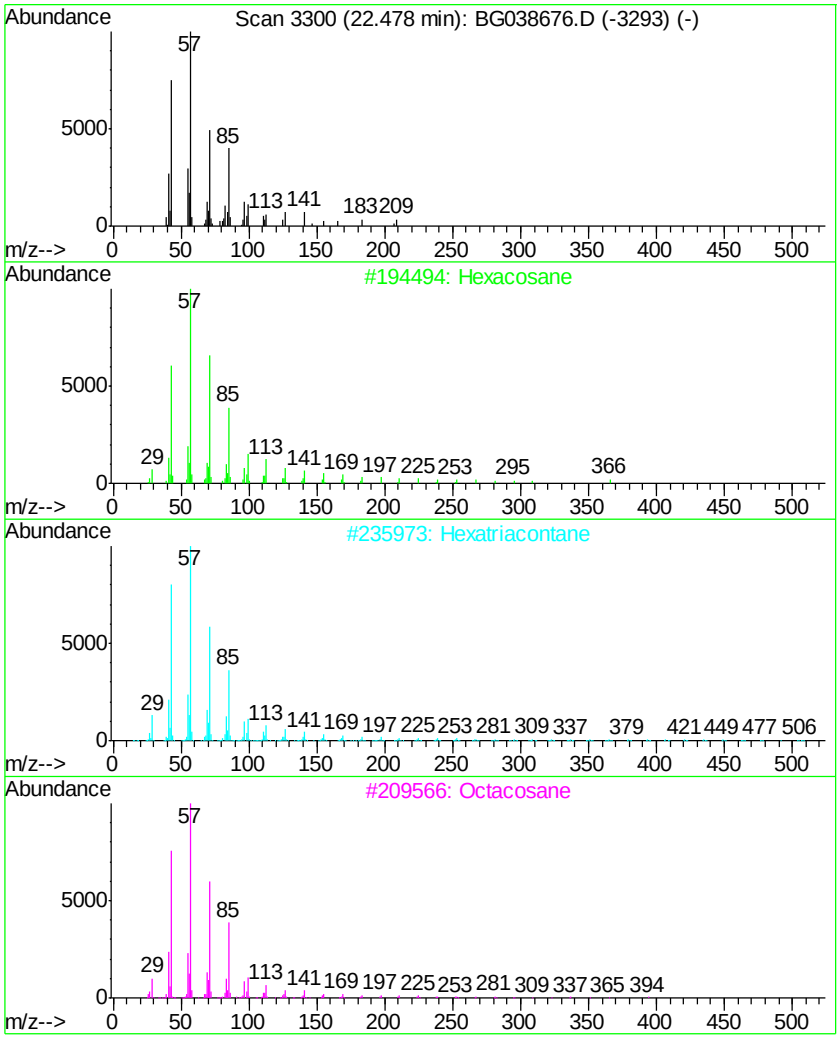
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

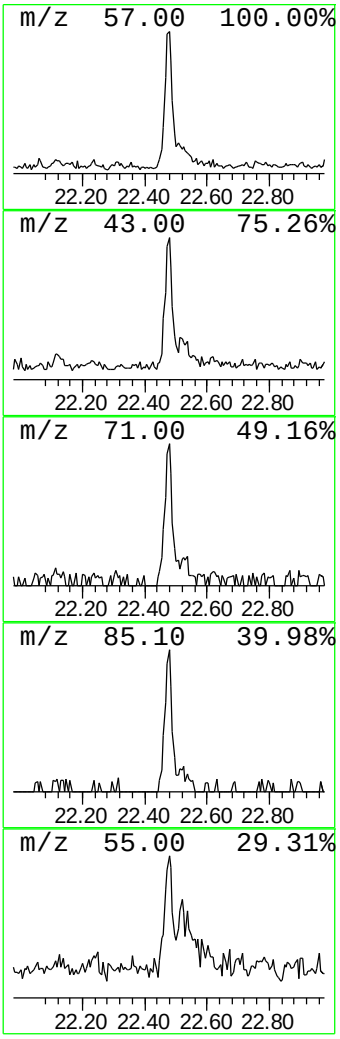
****

Peak Number 5 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.48	2.29 ng	47990	Chrysene-d12	21.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Hexatriacontane	507	C36H74	000630-06-8	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	86
5	Tetracosane	338	C24H50	000646-31-1	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P001-SD008-0006-01

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

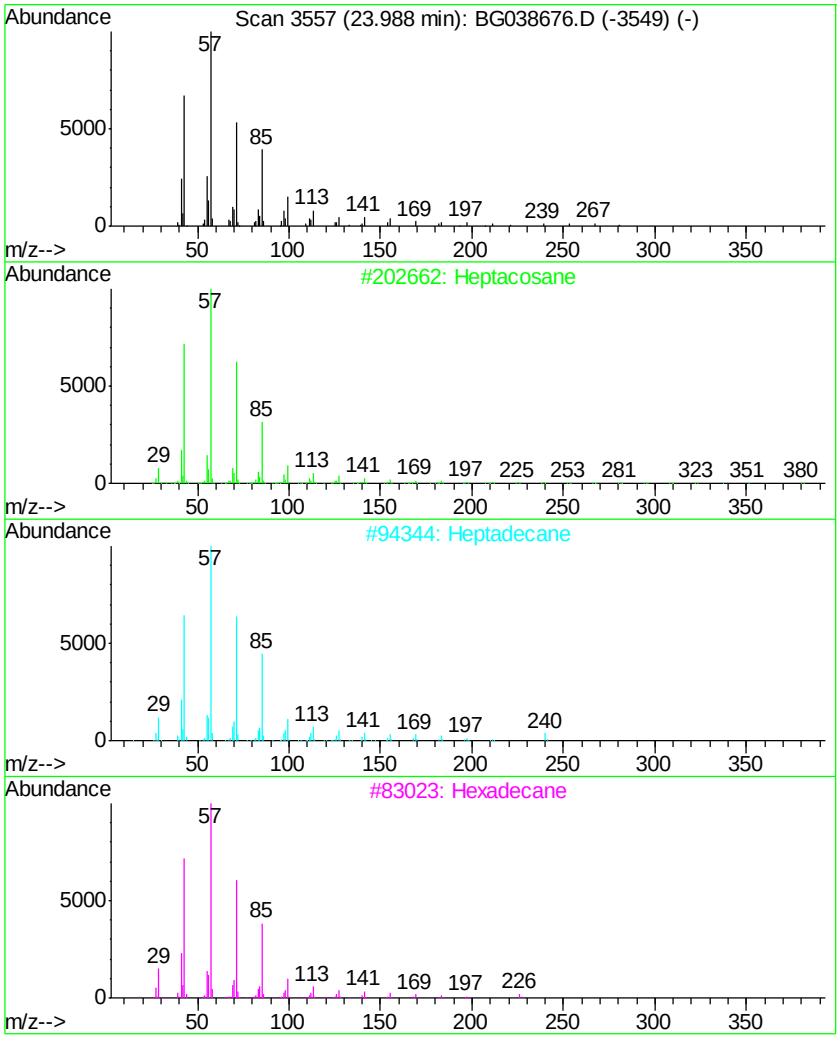
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

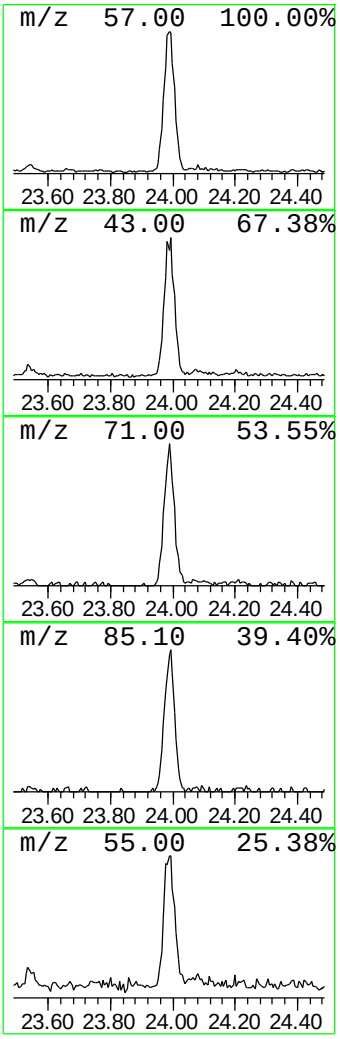
****

Peak Number 6 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	9.34 ng	191261	Perylene-d12	25.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Hexadecane	226	C16H34	000544-76-3	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Docosane	310	C22H46	000629-97-0	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P001-SD008-0006-01

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

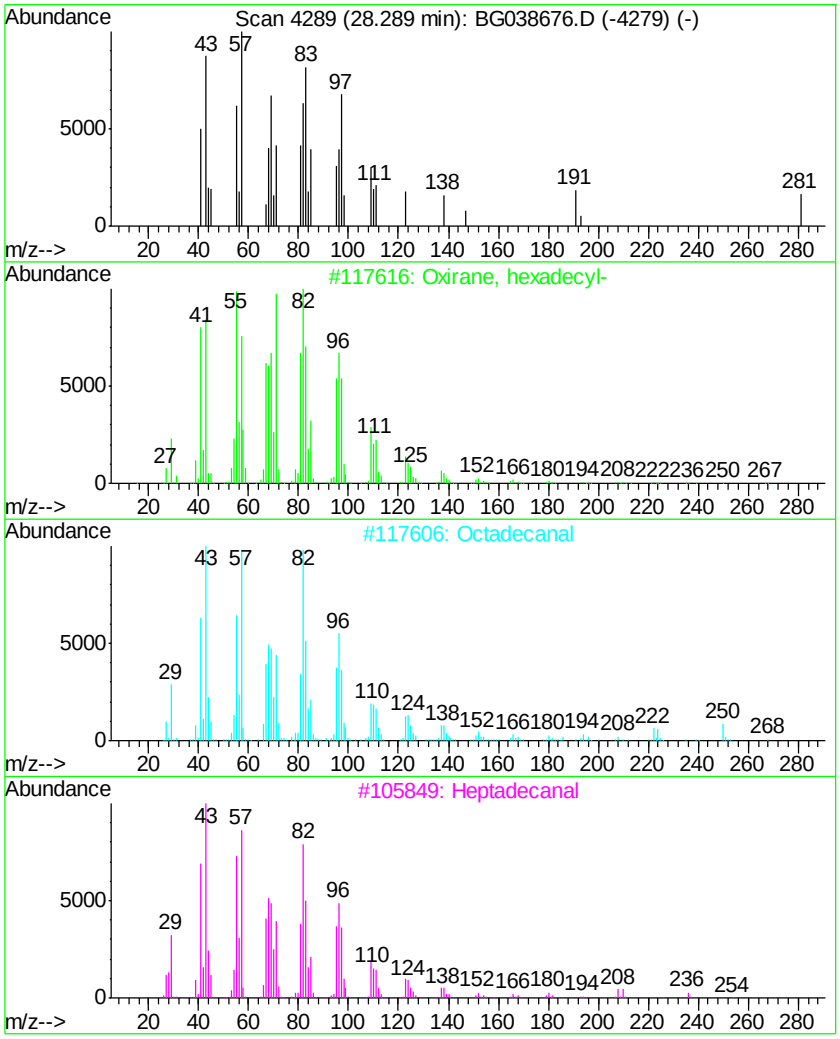
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

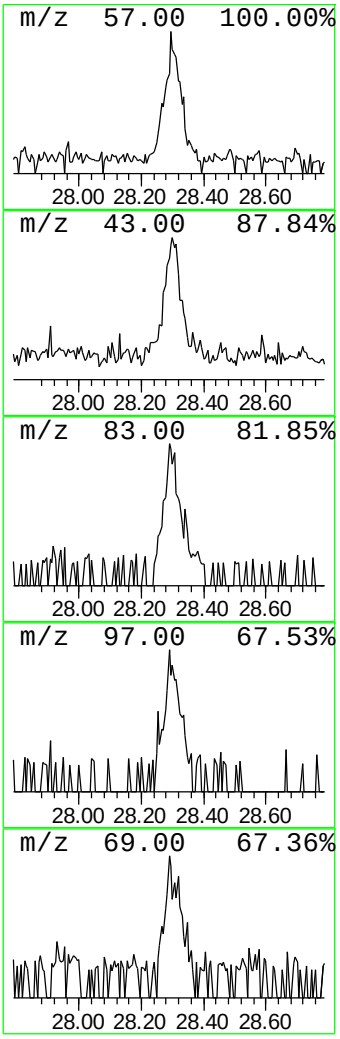
****

Peak Number 9 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.29	2.63 ng	53899	Perylene-d12	25.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72
2	Octadecanal	268	C18H36O	000638-66-4	58
3	Heptadecanal	254	C17H34O	1000376-70-0	52
4	Tetradecanal	212	C14H28O	000124-25-4	49
5	2-Heptadecenal	252	C17H32O	1000143-48-6	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038676.D
Acq On : 18 Dec 2018 00:19
Operator : JU/SJ
Sample : J6378-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P001-SD008-0006-01

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
2-Pentanone, 4-hy...	5.14	5.0	ng	35189	1	8.06	142236	20.0
unknown7.59	7.59	103.6	ng	737044	1	8.06	142236	20.0
Eicosane	21.31	2.2	ng	45766	5	21.73	419606	20.0
Hexacosane	22.48	2.3	ng	47990	5	21.73	419606	20.0
Heptacosane	23.99	9.3	ng	191261	6	25.02	409503	20.0
Oxirane, hexadecyl-	28.29	2.6	ng	53899	6	25.02	409503	20.0