LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-7

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	3.179	11	15	26	rVB	66115	105754	5.03%	1.048%
2	3.731	106	109	121	rVB	15722	28038	1.33%	0.278%
3	5.141	344	349	358	rVB	22931	37952	1.81%	0.376%
4	5.605	421	428	440	rBV	425378	708389	33.69%	7.023%
5	7.209	694	701	712	rBV	456126	840725	39.99%	8.335%
6	7.585	758	765	779	rVB	418511	739461	35.17%	7.331%
7	8.061	839	846	851	rBV	70449	121653	5.79%	1.206%
8	8.379	892	900	908	rBV	314278	561050	26.69%	5.562%
9	9.236	1038	1046	1056	rBV	273852	506245	24.08%	5.019%
10	10.876	1318	1325	1337	rBV	89154	167742	7.98%	1.663%
11	13.314	1733	1740	1753	rBV	744924	1181303	56.19%	11.711%
12	14.142	1875	1881	1893	rVB	57090	90001	4.28%	0.892%
13	14.695	1969	1975	1985	rVB3	155177	256441	12.20%	2.542%
14	16.187	2222	2229	2244	rBV2	652228	1015047	48.28%	10.063%
15	17.444	2436	2443	2449	rBV2	218886	356545	16.96%	3.535%
16	18.302	2582	2589	2597	rBV2	68631	113928	5.42%	1.129%
17	19.466	2783	2787	2791	rBV	52476	71853	3.42%	0.712%
18	19.571	2800	2805	2811	rBV3	32228	52036	2.48%	0.516%
19	20.041	2879	2885	2891	rBV	1543413	2102388	100.00%	20.842%
20	21.322	3093	3103	3107	rBV3	58739	119185	5.67%	1.182%
21	21.358	3107	3109	3114	rVV2	22684	36096	1.72%	0.358%
22	21.428	3117	3121	3128	rVB	14231	23798	1.13%	0.236%
23	21.722	3163	3171	3178	rBV2	249028	431815	20.54%	4.281%
24	25.018	3722	3732	3744	rVB2	140005	419740	19.96%	4.161%

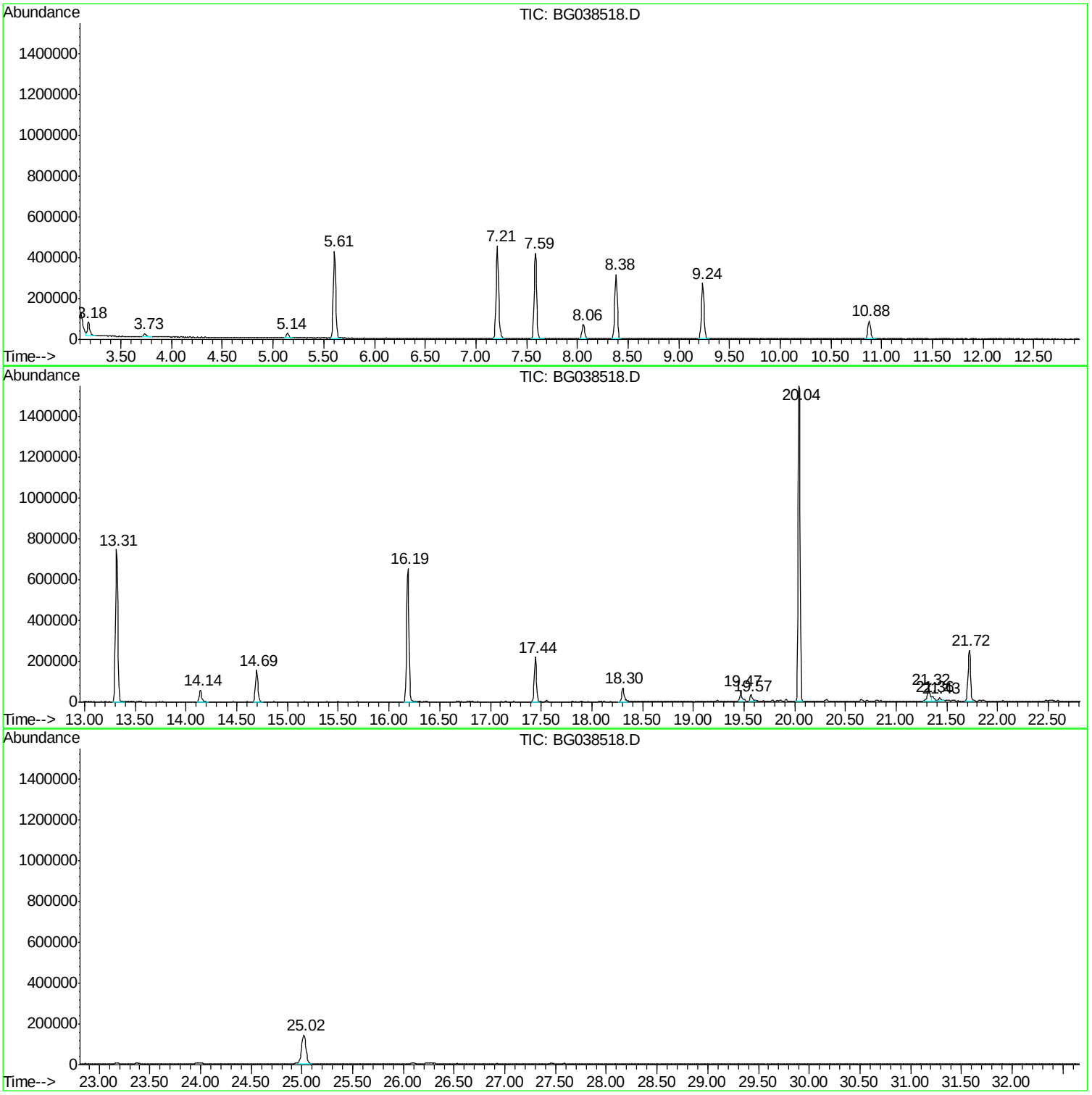
Sum of corrected areas: 10087185

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

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\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-7

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

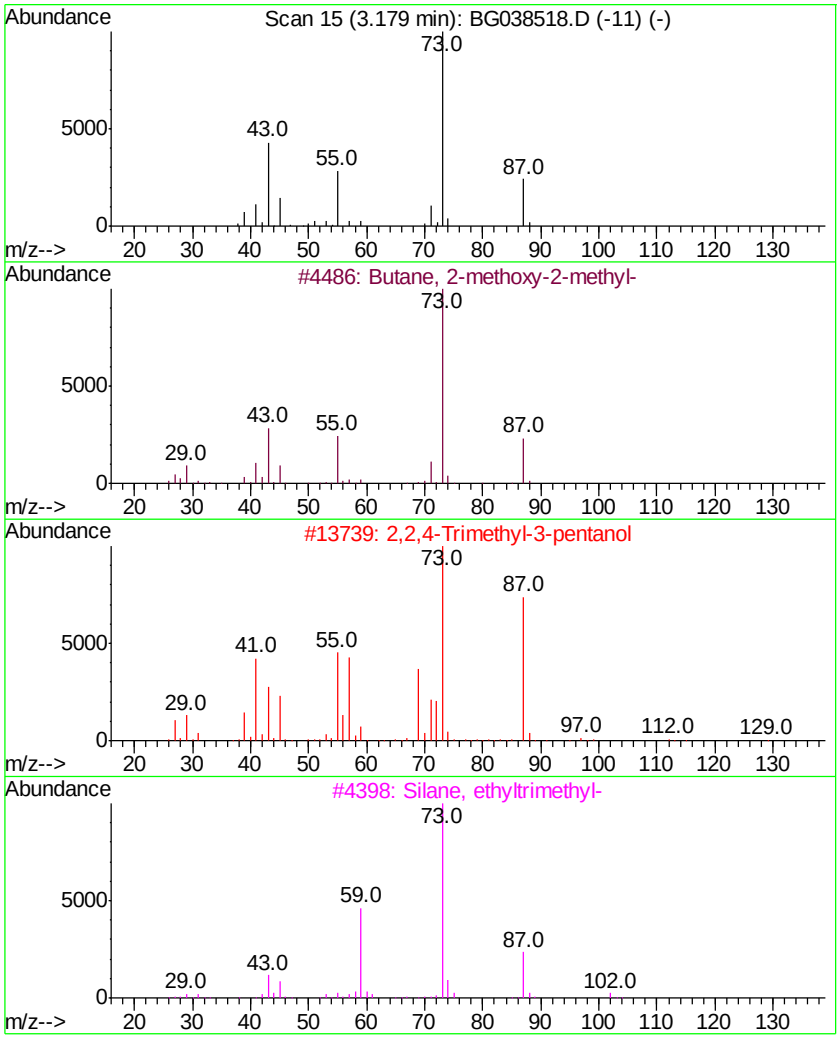
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

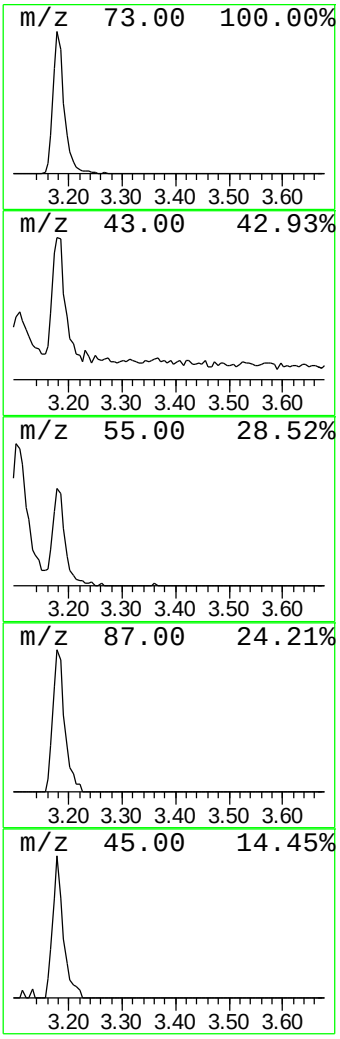
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	17.39 ng	105754	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-7

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

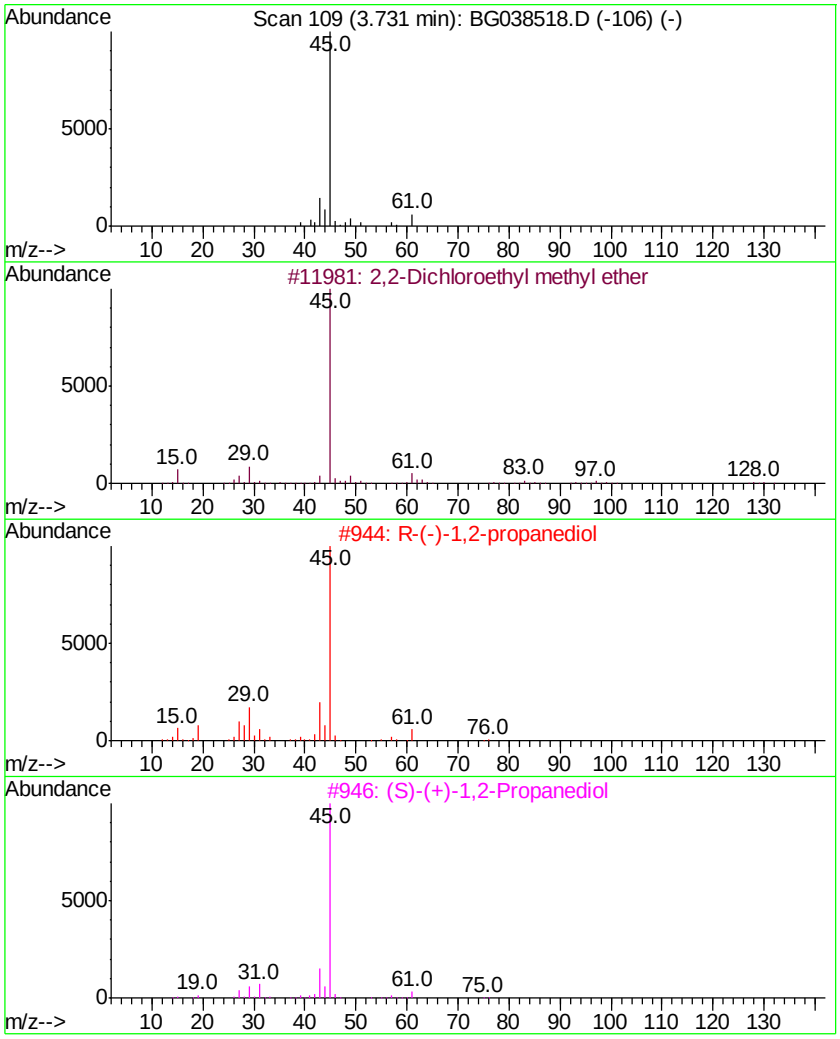
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

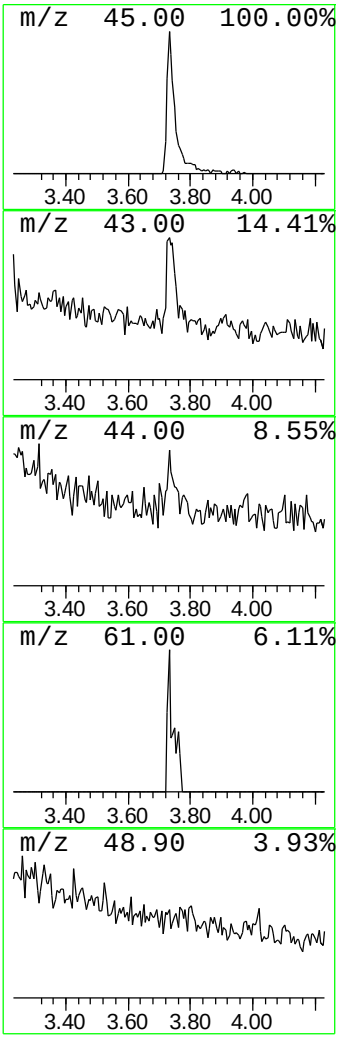
****

Peak Number 2 2,2-Dichloroethyl methyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.73	4.61 ng	28038	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dichloroethyl methyl ether	128	C3H6Cl2O	034862-07-2	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	Methane, nitroso-	45	CH3NO	000865-40-7	7





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-7

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

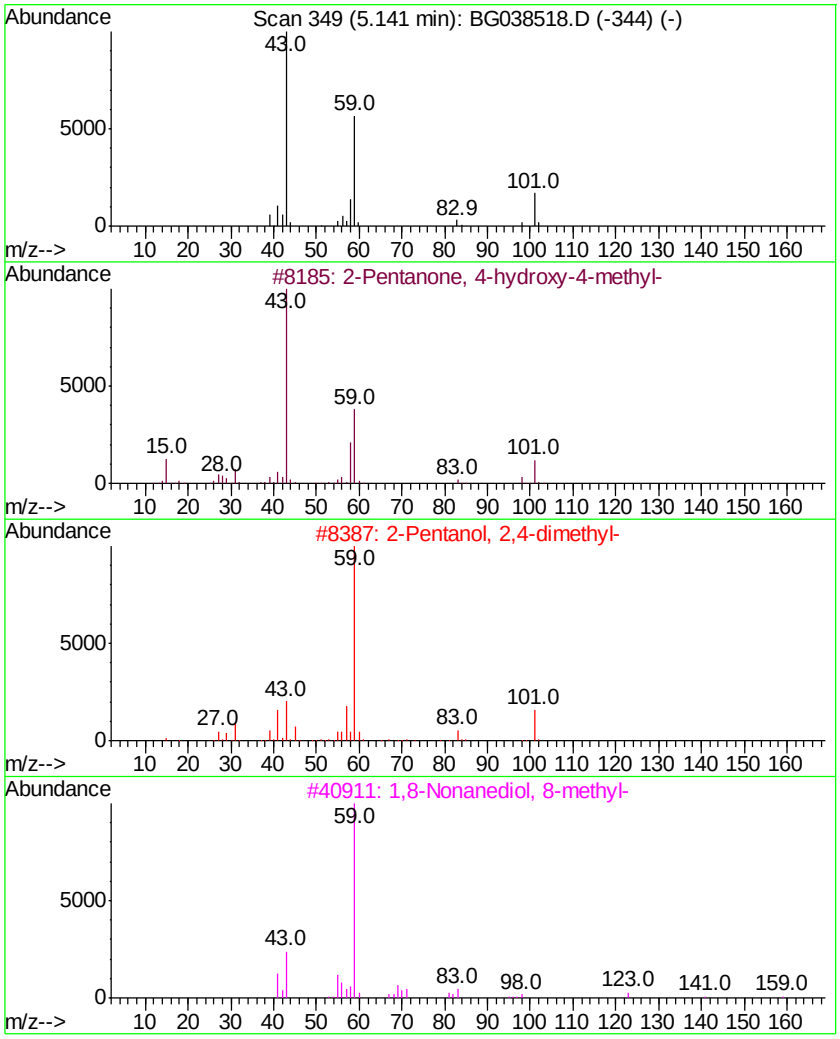
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

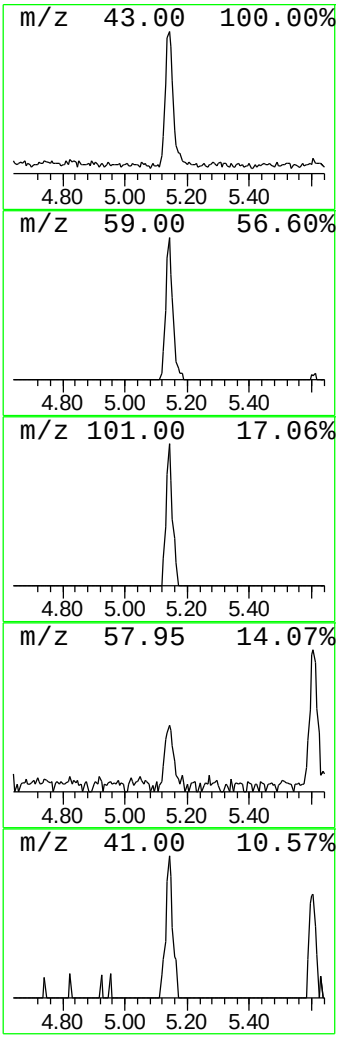
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	6.24 ng	37952	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	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-7

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

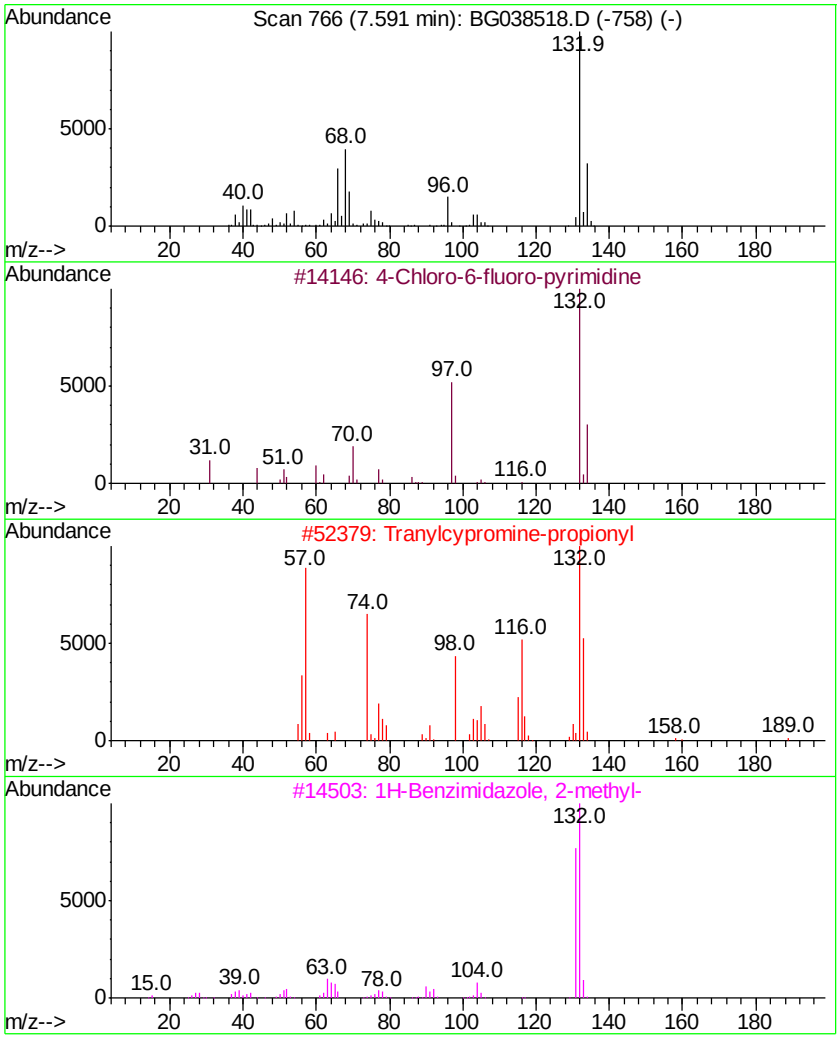
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

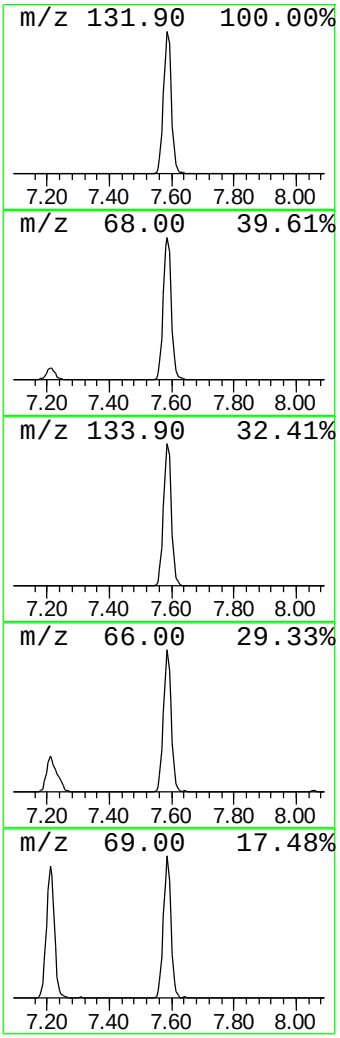
****

Peak Number 4 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	121.57 ng	739461	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-7

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

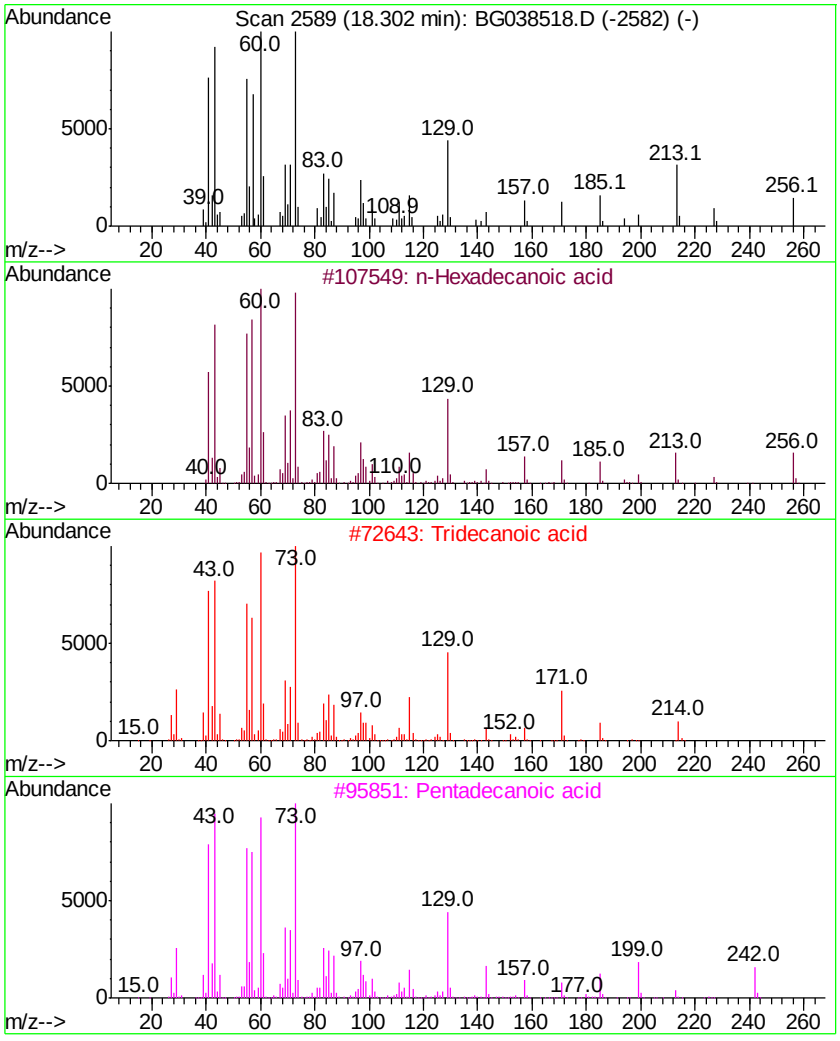
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

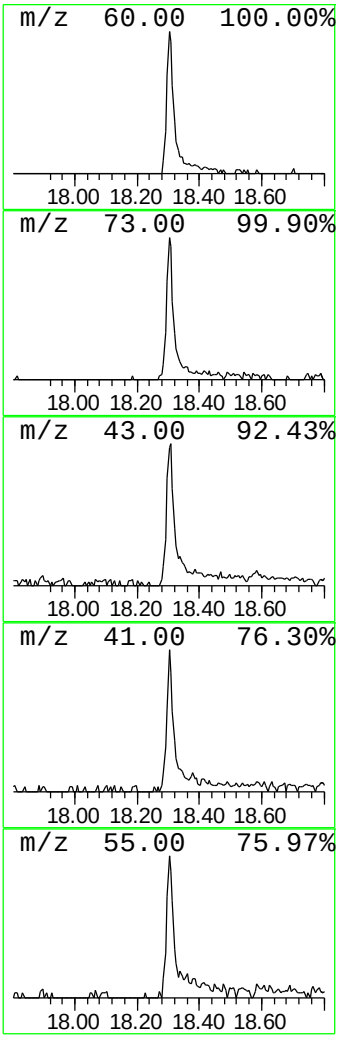
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	6.39 ng	113928	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-7

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

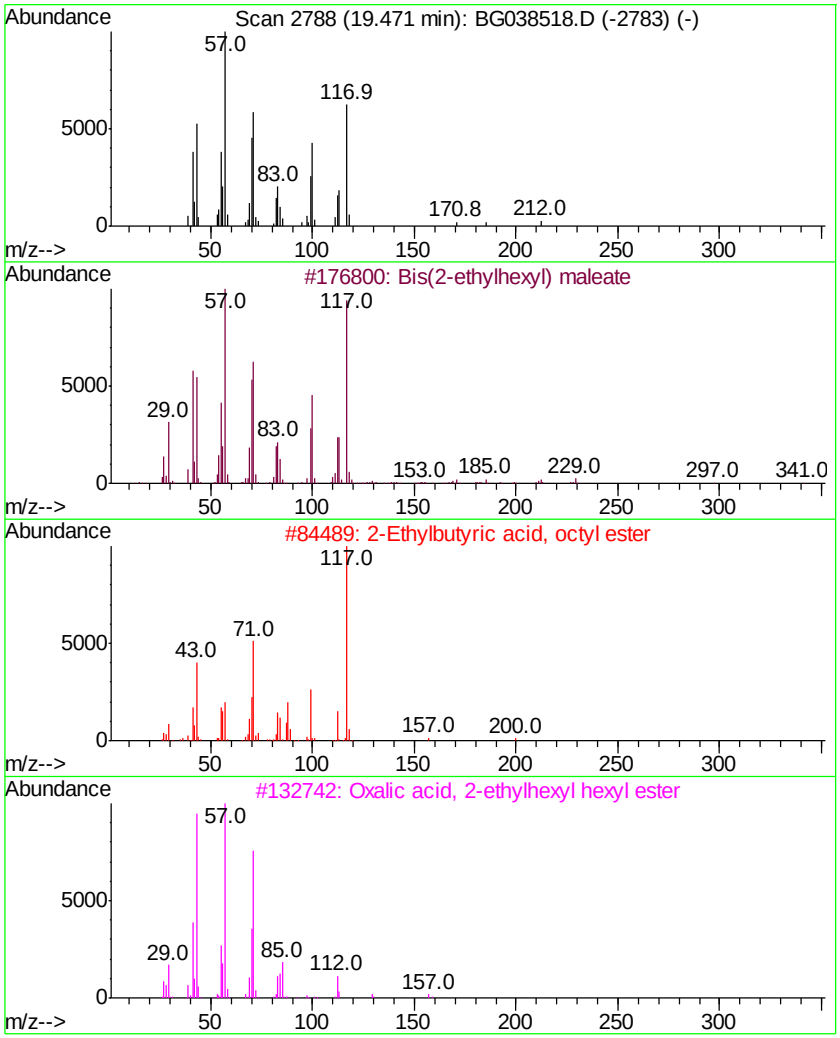
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

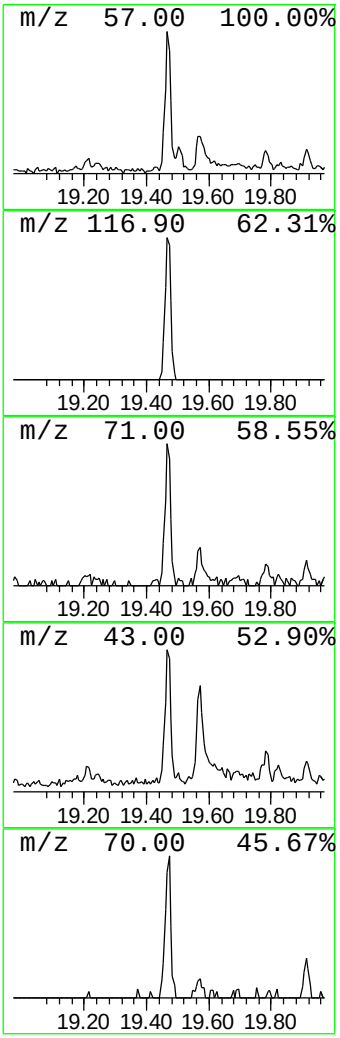
****

Peak Number 7 Bis(2-ethylhexyl) maleate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.47	4.03 ng	71853	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	76
2	2-Ethylbutyric acid, octyl ester	228	C14H28O2	1000340-24-3	38
3	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	38
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	35
5	Isobutyl octyl carbonate	230	C13H26O3	1000372-74-6	35





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-7

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

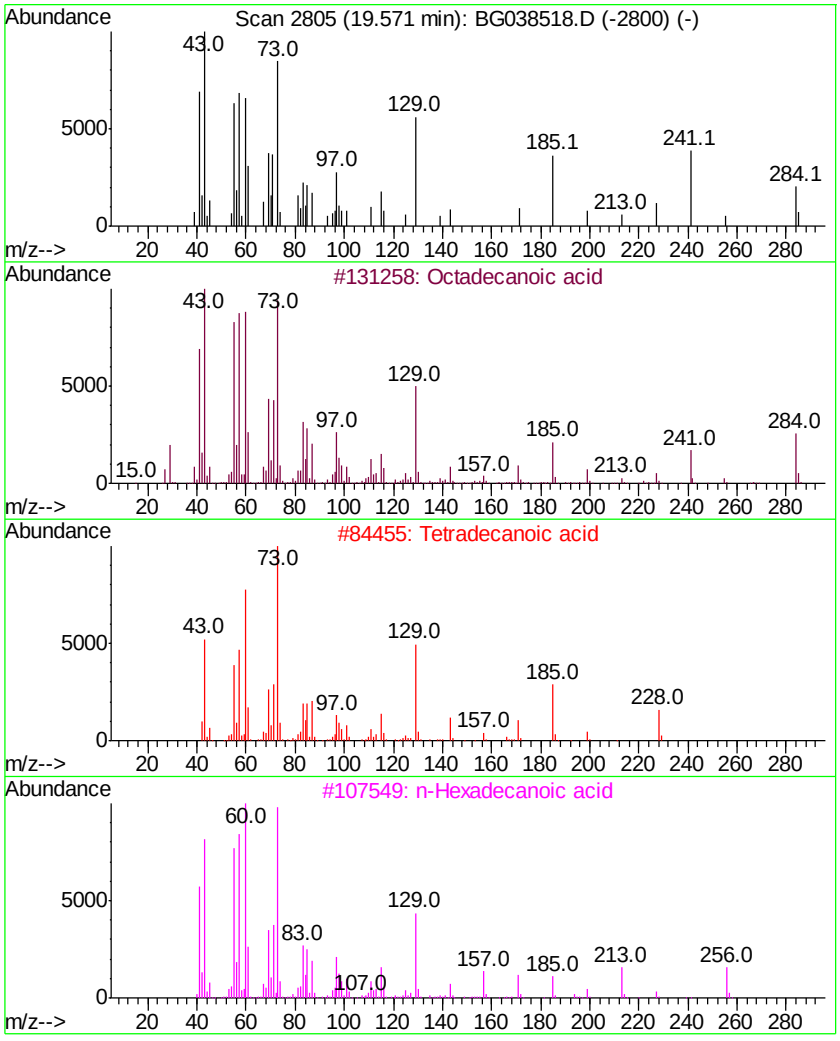
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

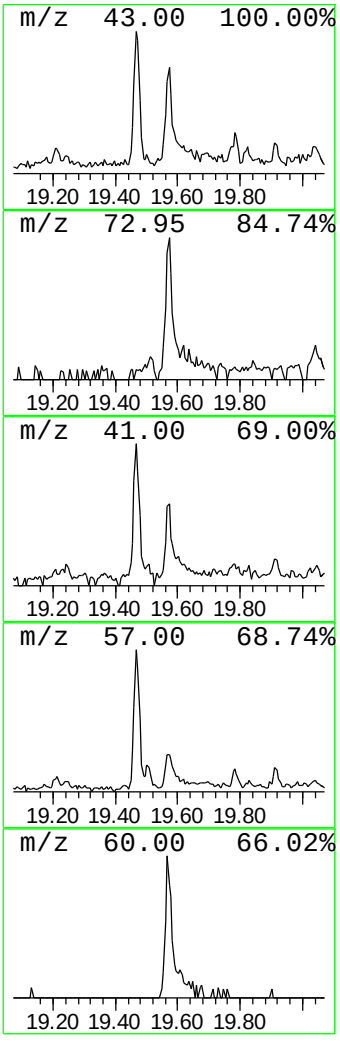
****

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.57	2.92 ng	52036	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5	Maltose	342	C12H22O11	000069-79-4	35





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Sample : J6331-37
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-7

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

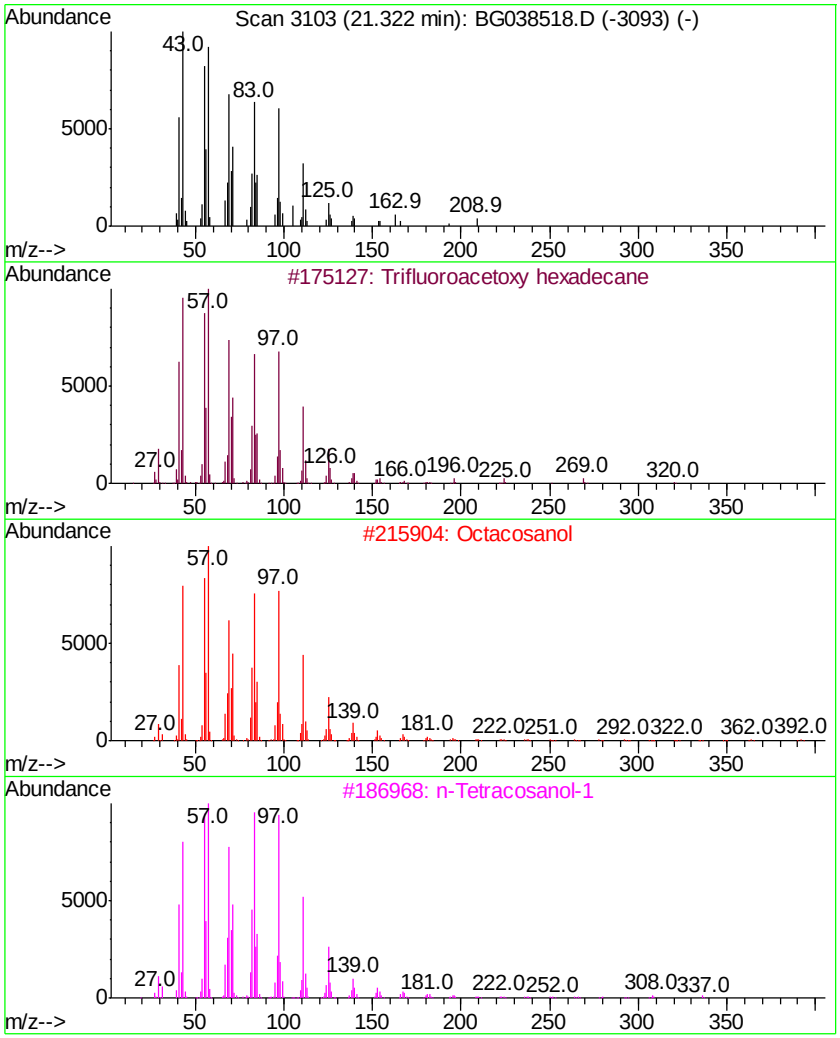
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

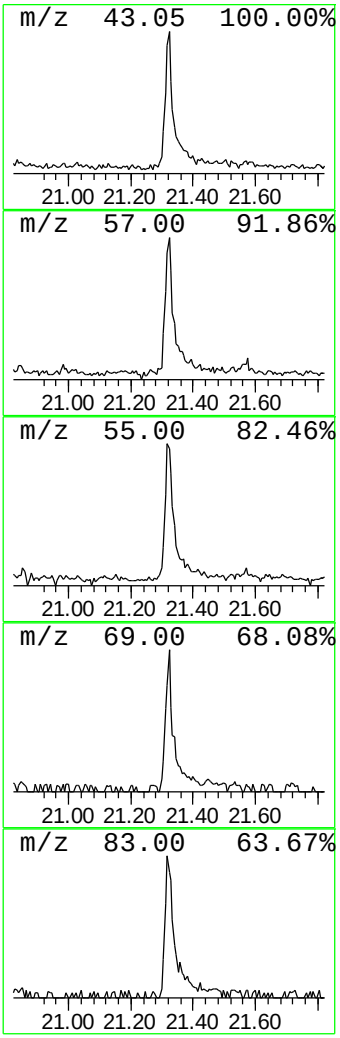
****

Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	5.52 ng	119185	Chrysene-d12	21.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Octacosanol	410	C28H58O	000557-61-9	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121218\
Data File : BG038518.D
Acq On : 13 Dec 2018 3:57
Operator : JU/SJ
Sample : J6331-37
Misc :
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Instrument : BNA_G
ClientSampleId : TP-7

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
Butane, 2-methoxy...	3.18	17.4	ng	105754	1	8.06	121653	20.0
2,2-Dichloroethyl...	3.73	4.6	ng	28038	1	8.06	121653	20.0
2-Pentanone, 4-hy...	5.14	6.2	ng	37952	1	8.06	121653	20.0
unknown7.59	7.59	121.6	ng	739461	1	8.06	121653	20.0
n-Hexadecanoic acid	18.30	6.4	ng	113928	4	17.44	356545	20.0
Bis(2-ethylhexyl)...	19.47	4.0	ng	71853	4	17.44	356545	20.0
Octadecanoic acid	19.57	2.9	ng	52036	4	17.44	356545	20.0
Trifluoroacetoxy ...	21.32	5.5	ng	119185	5	21.72	431815	20.0