LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101817\
Data File : BG029363.D
Acq On : 19 Oct 2017 12:38
Operator : SJ/JU
Sample : I5901-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-20170688

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-BG101617.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	5.238	326	332	342	rBV	209405	326092	7.05%	1.227%
2	5.714	404	413	423	rBV	1146621	1862075	40.28%	7.005%
3	7.318	678	686	697	rBV	1164588	2076239	44.91%	7.811%
4	7.694	742	750	760	rBV	1139276	1977084	42.76%	7.438%
5	8.164	823	830	837	rVB	216075	360928	7.81%	1.358%
6	8.493	877	886	895	rVB	805834	1409529	30.49%	5.303%
7	9.328	1020	1028	1037	rBV	673022	1206538	26.10%	4.539%
8	10.984	1302	1310	1318	rBV	305795	547463	11.84%	2.060%
9	13.411	1716	1723	1733	rBV	1745187	2713516	58.69%	10.209%
10	14.228	1856	1862	1868	rBV	61711	92046	1.99%	0.346%
11	14.786	1950	1957	1967	rVB2	509468	845940	18.30%	3.183%
12	16.267	2201	2209	2220	rBV	1780634	2757349	59.64%	10.374%
13	17.524	2412	2423	2431	rBV2	782345	1198508	25.92%	4.509%
14	18.388	2565	2570	2578	rBV	126855	186340	4.03%	0.701%
15	19.651	2780	2785	2795	rBV3	40181	62273	1.35%	0.234%
16	20.115	2857	2864	2872	rBV	3428223	4623296	100.00%	17.394%
17	21.413	3080	3085	3094	rBV	143137	247044	5.34%	0.929%
18	21.789	3142	3149	3157	rBV2	897285	1537353	33.25%	5.784%
19	22.224	3218	3223	3232	rBV	195060	296418	6.41%	1.115%
20	22.612	3283	3289	3294	rBV10	19448	51537	1.11%	0.194%
21	23.670	3462	3469	3478	rBV2	194792	375504	8.12%	1.413%
22	24.146	3544	3550	3556	rBV3	24569	52232	1.13%	0.197%
23	25.097	3698	3712	3725	rBV2	512320	1532754	33.15%	5.766%
24	25.661	3800	3808	3816	rVB4	57124	147779	3.20%	0.556%
25	31.455	4786	4794	4796	rBV8	40300	94560	2.05%	0.356%

Sum of corrected areas: 26580397

LSC Report - Integrated Chromatogram

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Misc :
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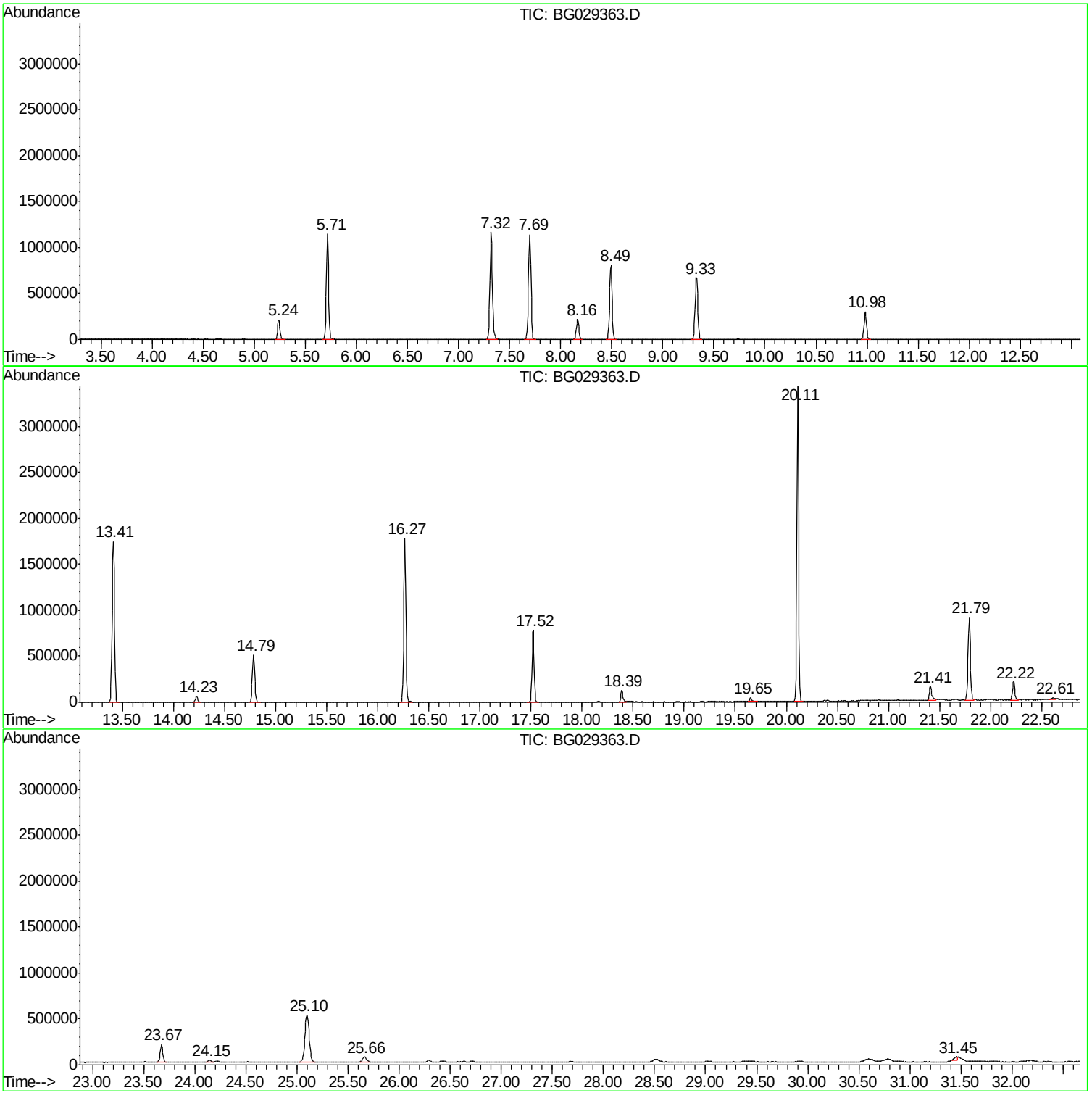
Instrument : BNA_G
ClientSampleId : S-1-20170688

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.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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Acq On : 19 Oct 2017 12:38
Operator : SJ/JU
Sample : I5901-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-20170688

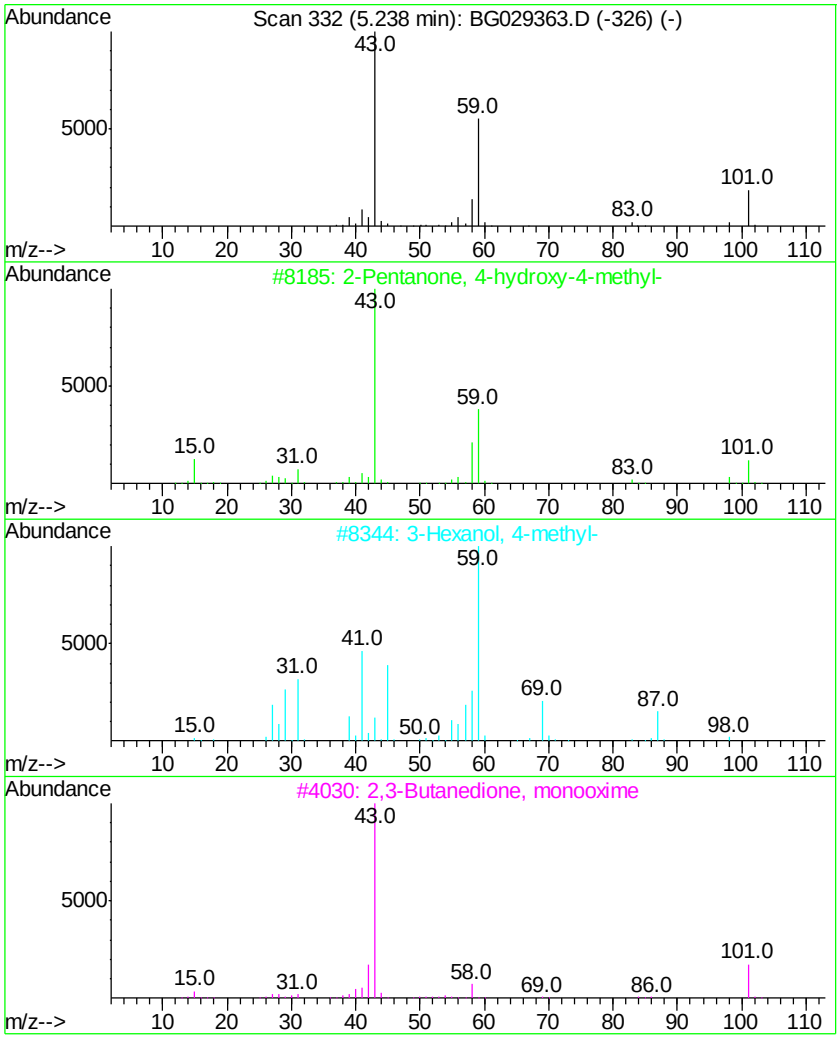
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

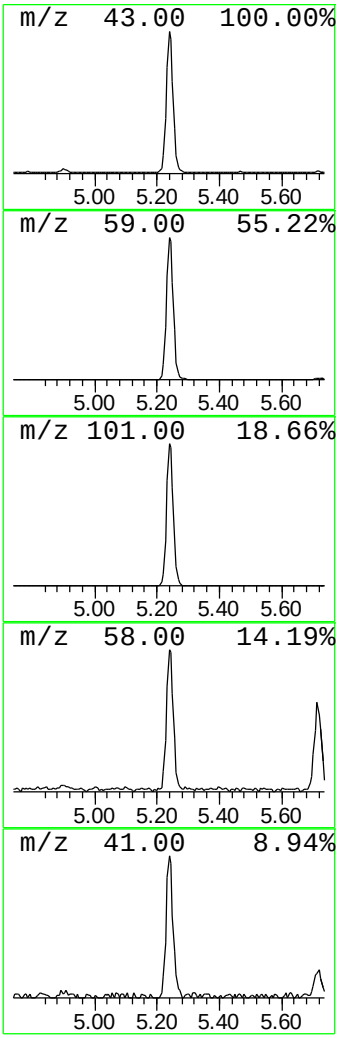
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	18.07 ng	326092	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101817\
Data File : BG029363.D
Acq On : 19 Oct 2017 12:38
Operator : SJ/JU
Sample : I5901-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-20170688

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

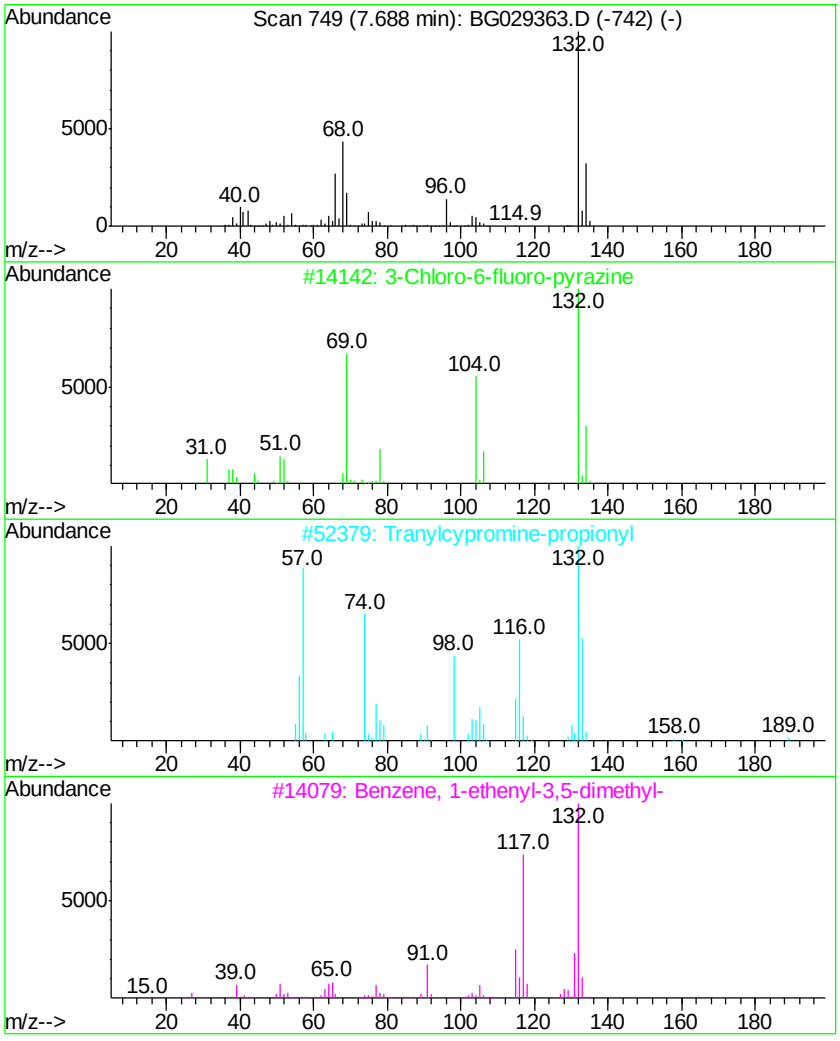
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

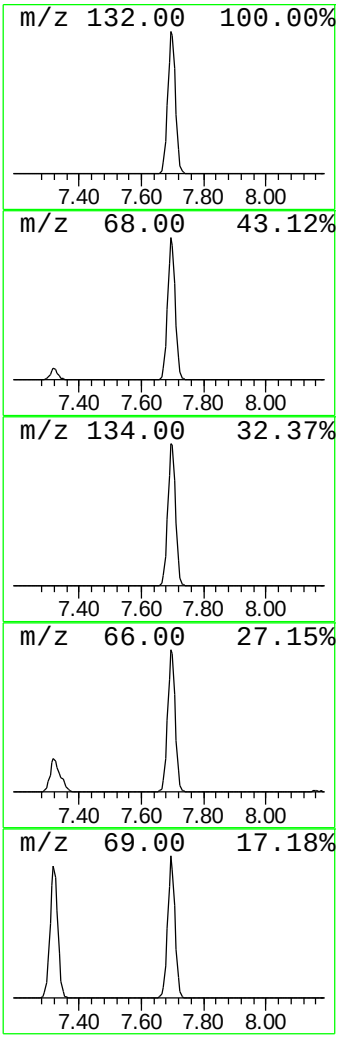
****

Peak Number 2 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	109.56 ng	1977080	1,4-Dichlorobenzene-d4	8.16

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	10
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Operator : SJ/JU
Sample : I5901-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-20170688

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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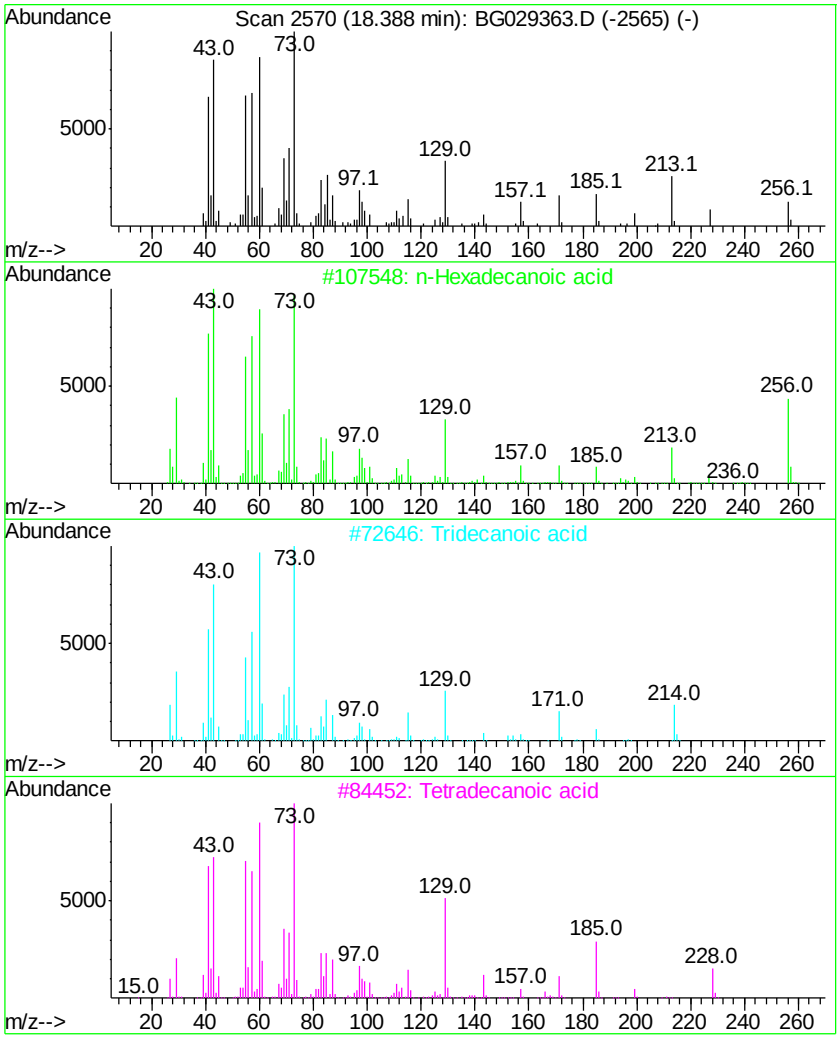
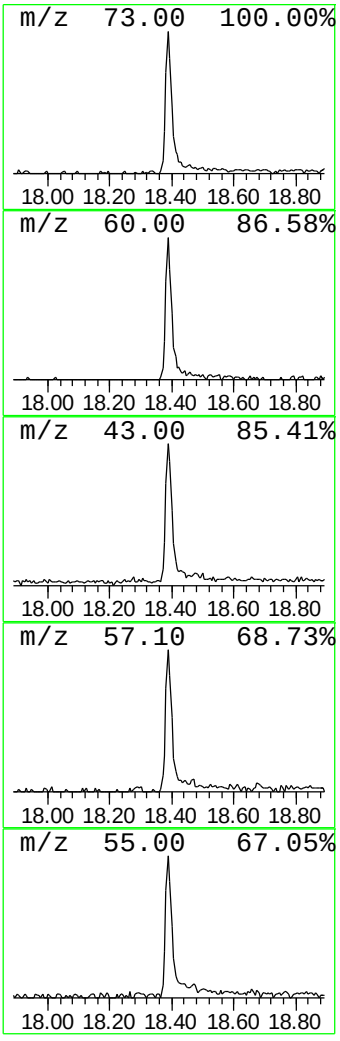
Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	3.11 ng	186340	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Nonanoic acid	158	C9H18O2	000112-05-0	30
5	3,7-Dimethyl-8-oxo-1,5-dioxa-spi...	256	C13H20O5	1000193-79-8	25





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Sample : I5901-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-20170688

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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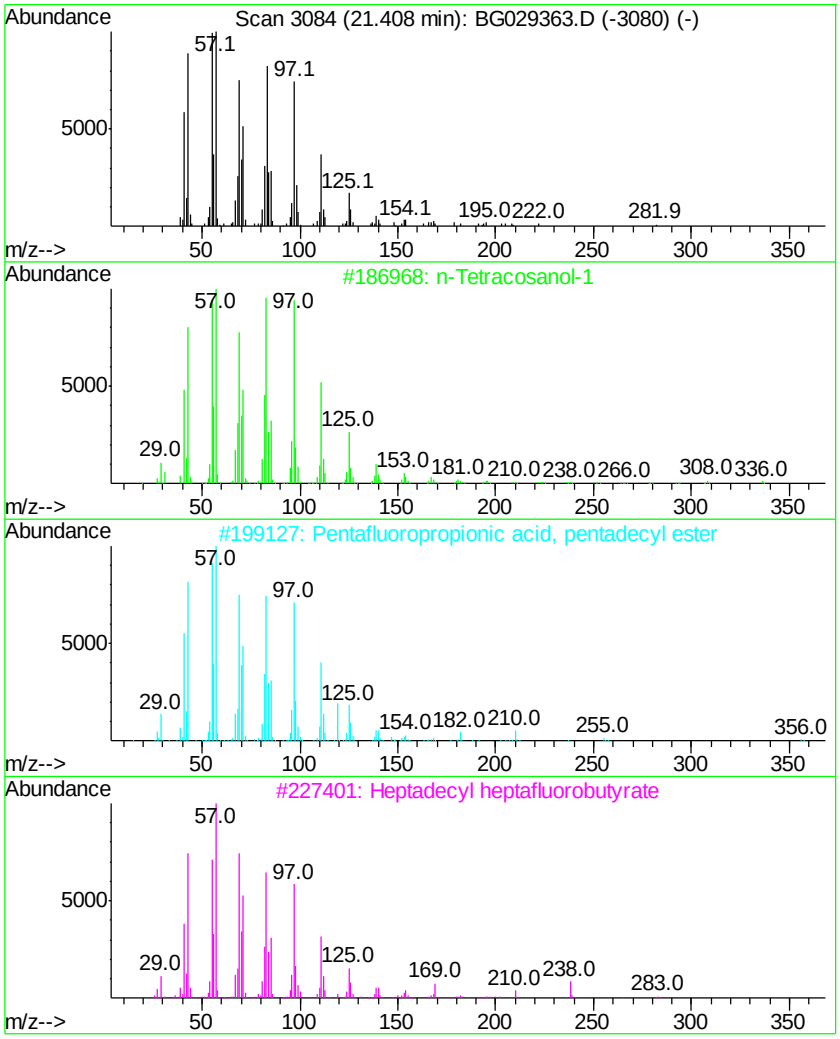
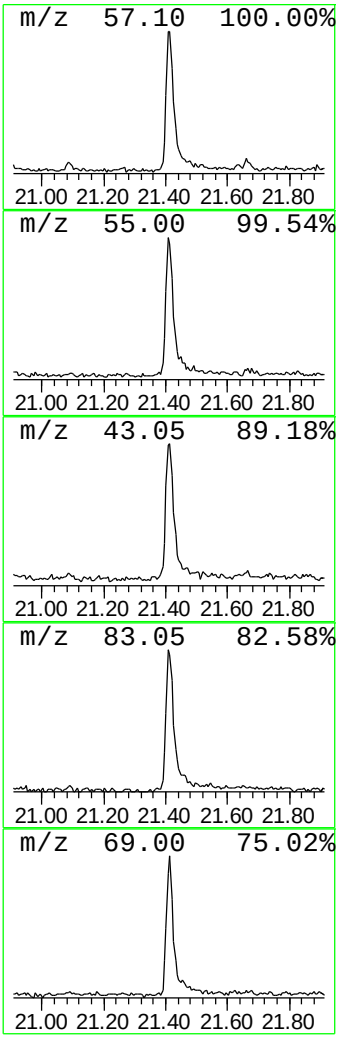
Peak Number 5 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	3.21 ng	247044	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94





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Instrument : BNA_G
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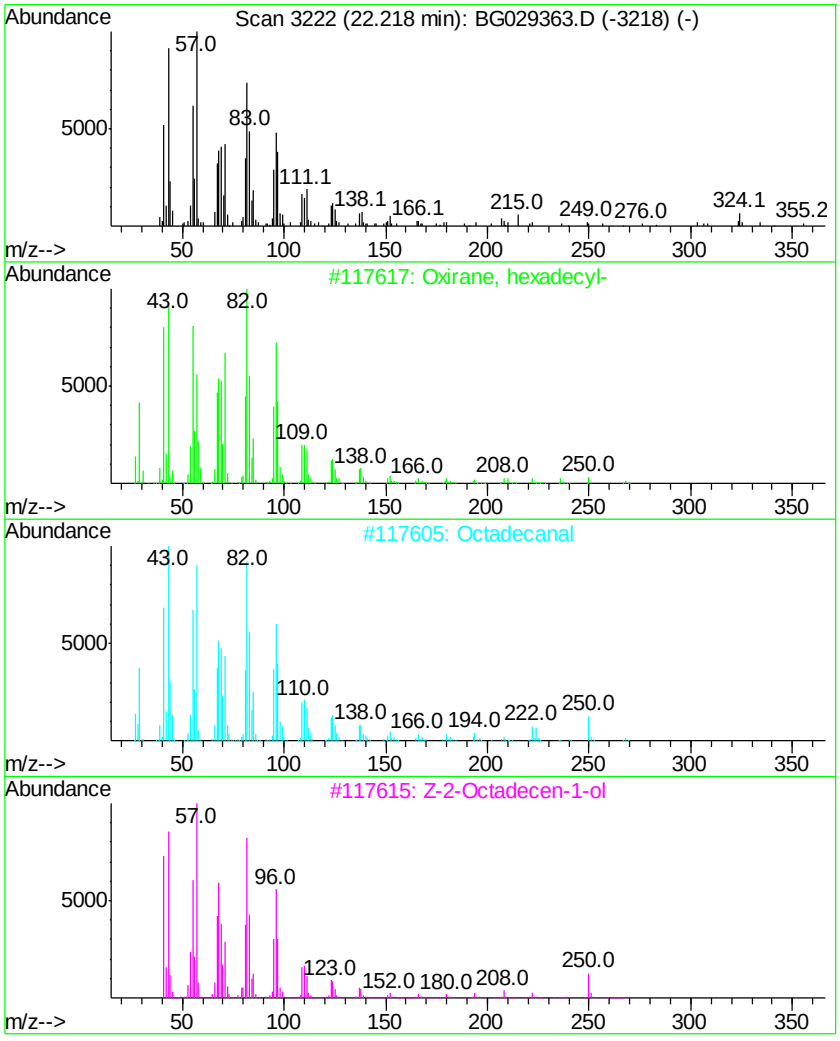
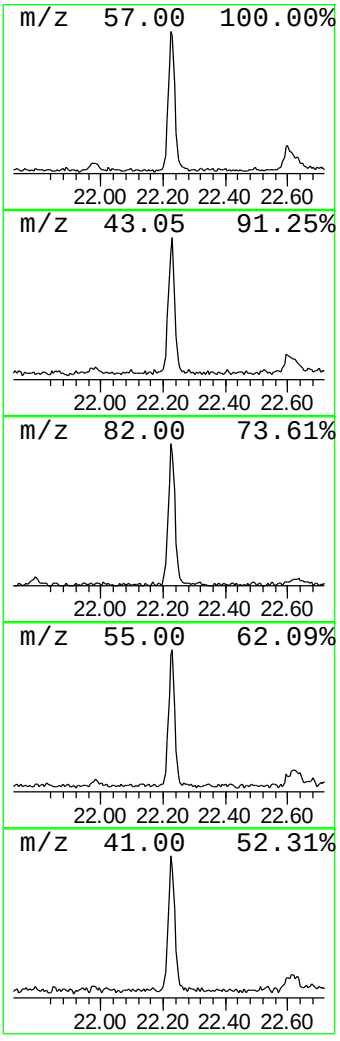
****

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.22	3.86 ng	296418	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
2	Octadecanal	268	C18H36O	000638-66-4	95
3	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	92
4	Hexadecanal	240	C16H32O	000629-80-1	91
5	Tetradecanal	212	C14H28O	000124-25-4	87





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Instrument : BNA_G
ClientSampleId : S-1-20170688

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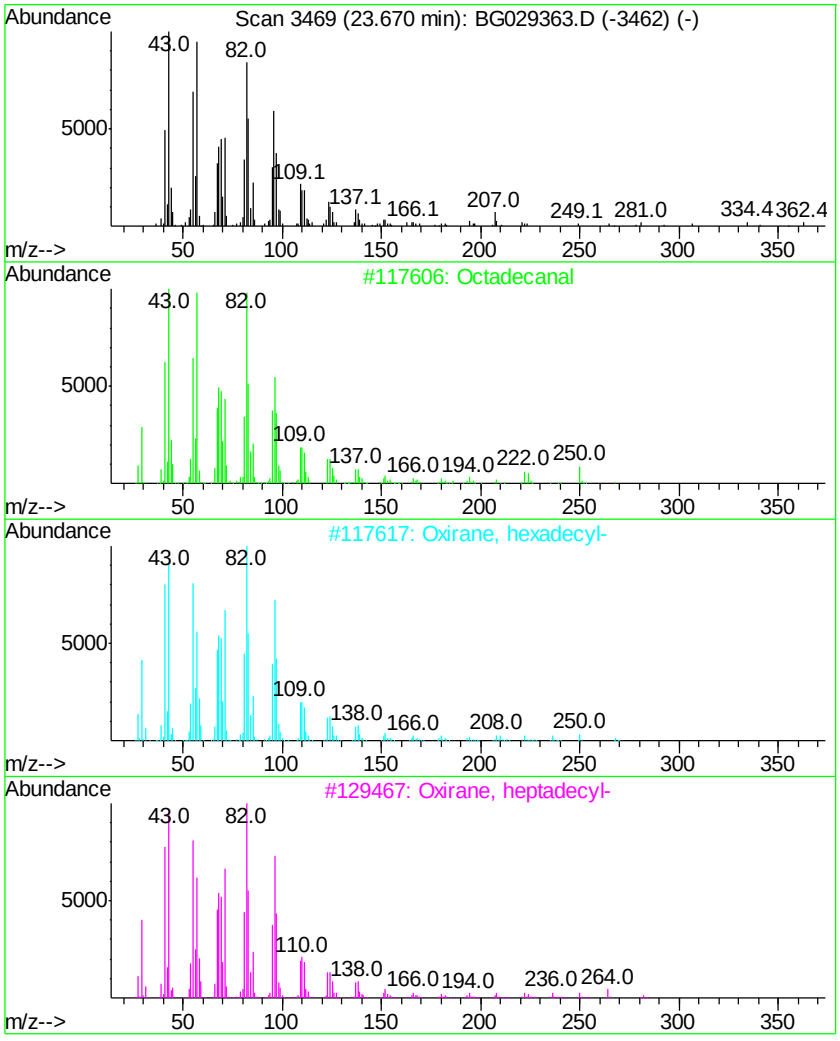
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

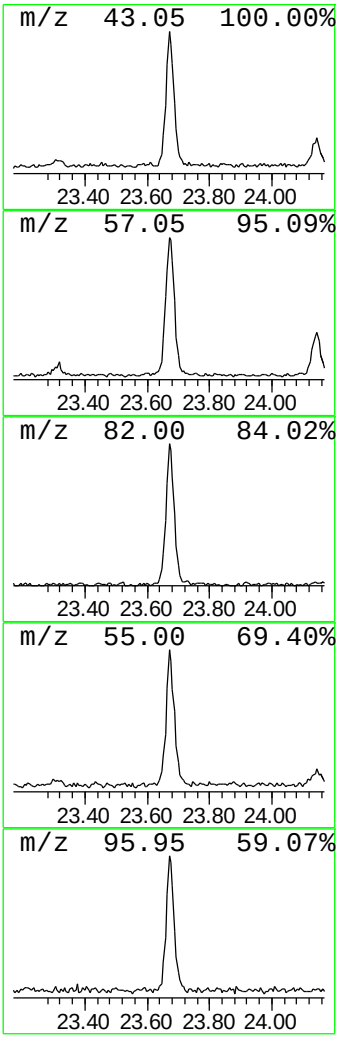
****

Peak Number 7 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.67	4.90 ng	375504	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
4	1,19-Eicosadiene	278	C20H38	014811-95-1	90
5	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	86





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.24	18.1	ng	326092	1	8.16	360928	20.0
unknown7.69	7.69	109.6	ng	1977080	1	8.16	360928	20.0
n-Hexadecanoic acid	18.39	3.1	ng	186340	4	17.52	1198510	20.0
n-Tetracosanol-1	21.41	3.2	ng	247044	5	21.79	1537350	20.0
Oxirane, hexadecyl-	22.22	3.9	ng	296418	5	21.79	1537350	20.0
Octadecanal	23.67	4.9	ng	375504	6	25.10	1532750	20.0