LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033252.D
Acq On : 19 Mar 2018 22:51
Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

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-BG031918.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	3.500	30	36	46	rBV	149714	299897	8.51%	1.974%
2	3.588	46	51	60	rVB	81426	134042	3.80%	0.882%
3	6.308	509	514	528	rBV	116911	276487	7.84%	1.820%
4	6.843	599	605	622	rBV	146983	320996	9.11%	2.113%
5	8.000	792	802	826	rBV	67388	234429	6.65%	1.543%
6	8.400	863	870	888	rBV	280740	648508	18.40%	4.269%
7	8.894	946	954	973	rBV	91027	223748	6.35%	1.473%
8	9.228	1003	1011	1029	rBV	435134	929253	26.36%	6.117%
9	10.092	1150	1158	1176	rBV	362034	852093	24.17%	5.609%
10	11.778	1437	1445	1460	rBV2	134388	315282	8.94%	2.075%
11	14.134	1835	1846	1866	rBV	1207885	2138854	60.67%	14.079%
12	14.928	1973	1981	1986	rBV	43431	74057	2.10%	0.487%
13	15.339	2045	2051	2057	rBV	29536	44827	1.27%	0.295%
14	15.509	2074	2080	2089	rVB2	289594	494886	14.04%	3.258%
15	16.273	2205	2210	2215	rVB	57573	76485	2.17%	0.503%
16	16.673	2269	2278	2282	rBV3	16930	35447	1.01%	0.233%
17	16.726	2282	2287	2292	rVV	31637	43253	1.23%	0.285%
18	16.978	2324	2330	2342	rBV	739217	1300372	36.89%	8.560%
19	17.131	2351	2356	2369	rVB2	55865	106479	3.02%	0.701%
20	17.918	2485	2490	2496	rBV2	33101	44498	1.26%	0.293%
21	18.241	2538	2545	2556	rBV	418527	742735	21.07%	4.889%
22	19.035	2675	2680	2689	rBV	136395	222823	6.32%	1.467%
23	20.268	2887	2890	2898	rBV6	30645	43645	1.24%	0.287%
24	20.762	2968	2974	2985	rBV	2510625	3525240	100.00%	23.205%
25	22.107	3198	3203	3218	rBV2	164173	333215	9.45%	2.193%
26	22.595	3279	3286	3295	rBV2	426066	827566	23.48%	5.448%
27	24.481	3602	3607	3615	rVB2	55849	116870	3.32%	0.769%
28	26.397	3920	3933	3948	rBV2	222195	785638	22.29%	5.172%

Sum of corrected areas: 15191625

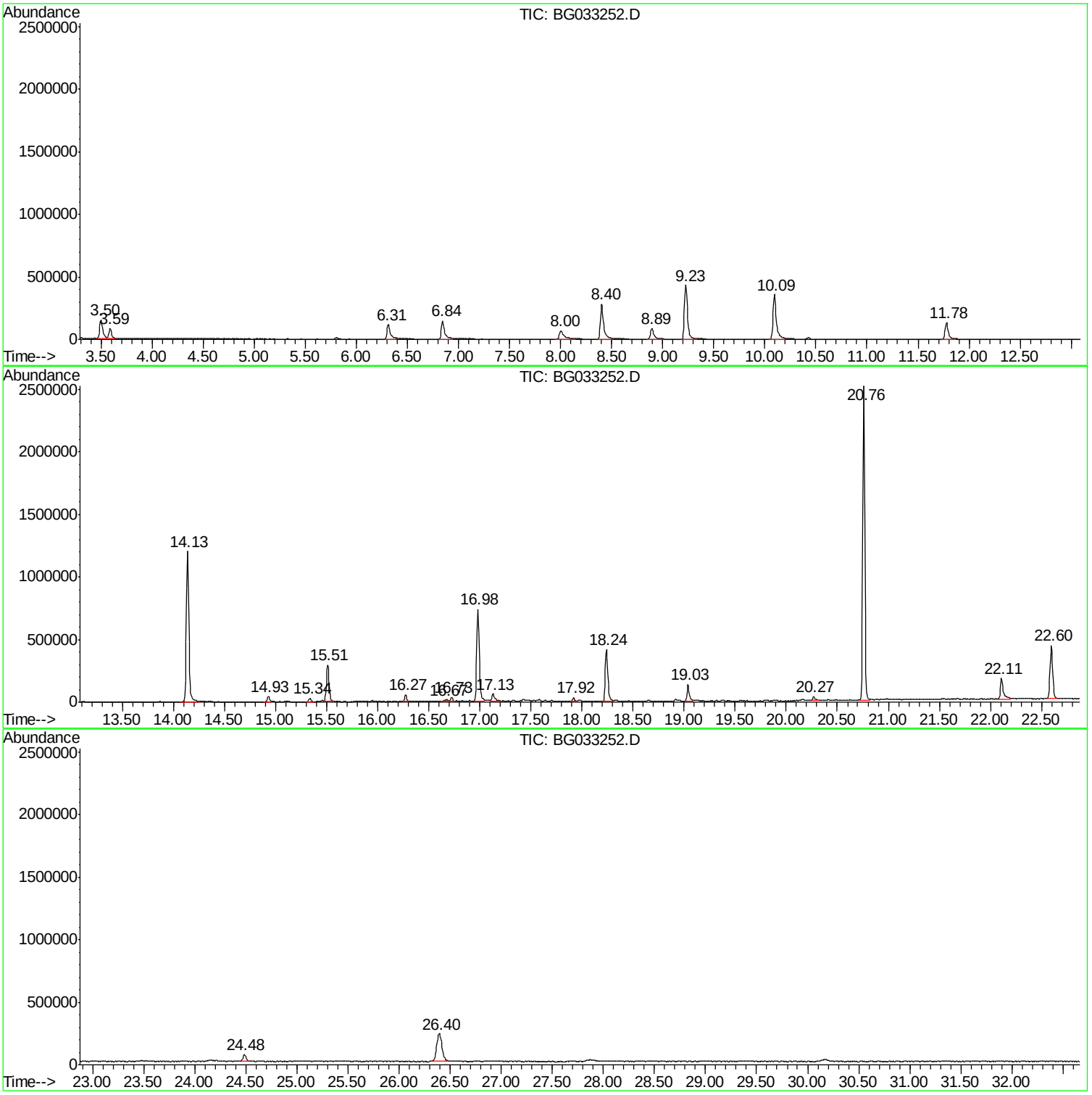
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033252.D
Acq On : 19 Mar 2018 22:51
Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033252.D
Acq On : 19 Mar 2018 22:51
Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

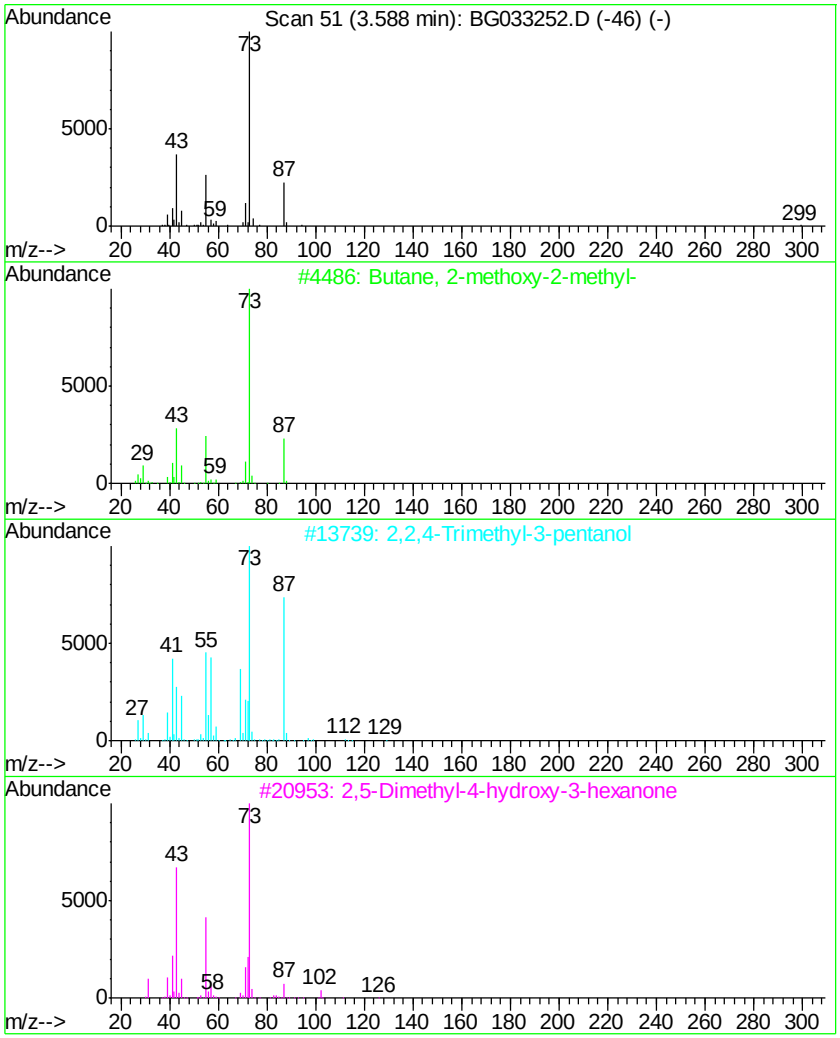
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

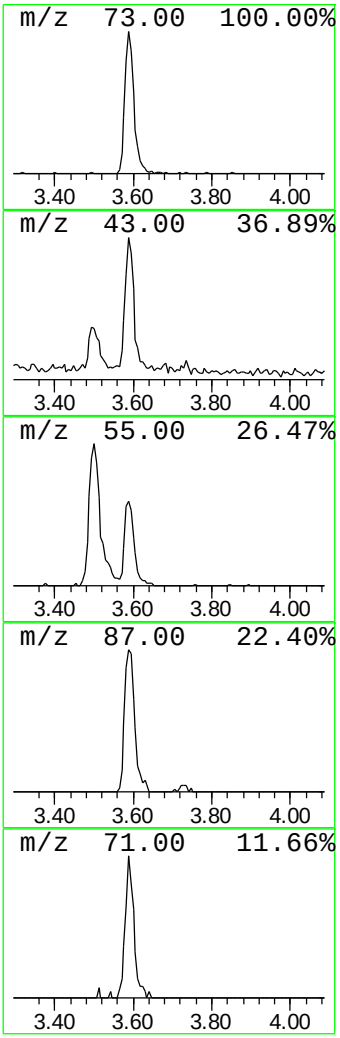
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	11.98 ng	134042	1,4-Dichlorobenzene-d4	8.89

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	39
3	2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	33
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17





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Data File : BG033252.D
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Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

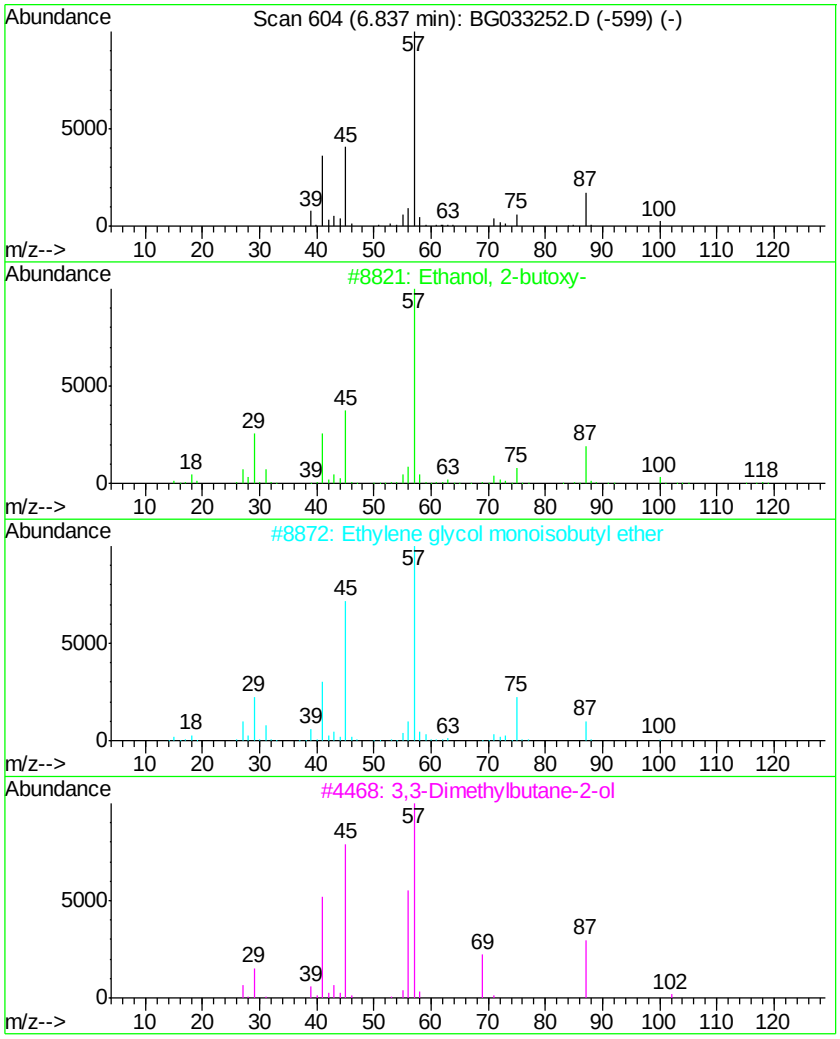
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

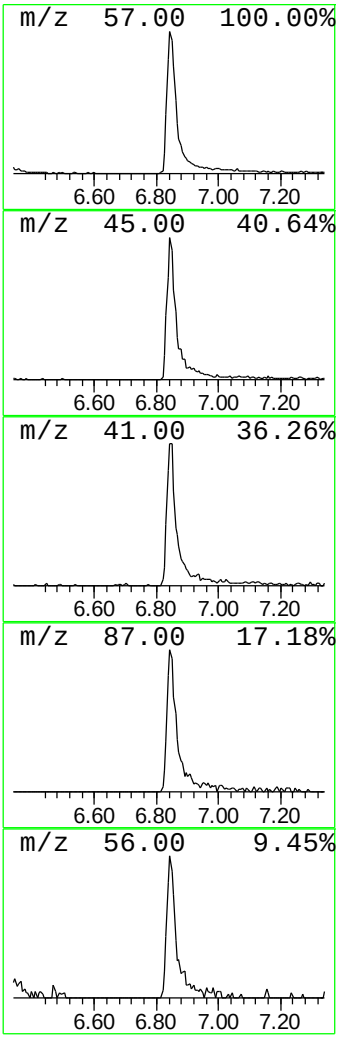
****

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.84	28.69 ng	320996	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	74
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	59
4	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	25
5	Isobutyl ether	130	C8H18O	000628-55-7	17





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033252.D
Acq On : 19 Mar 2018 22:51
Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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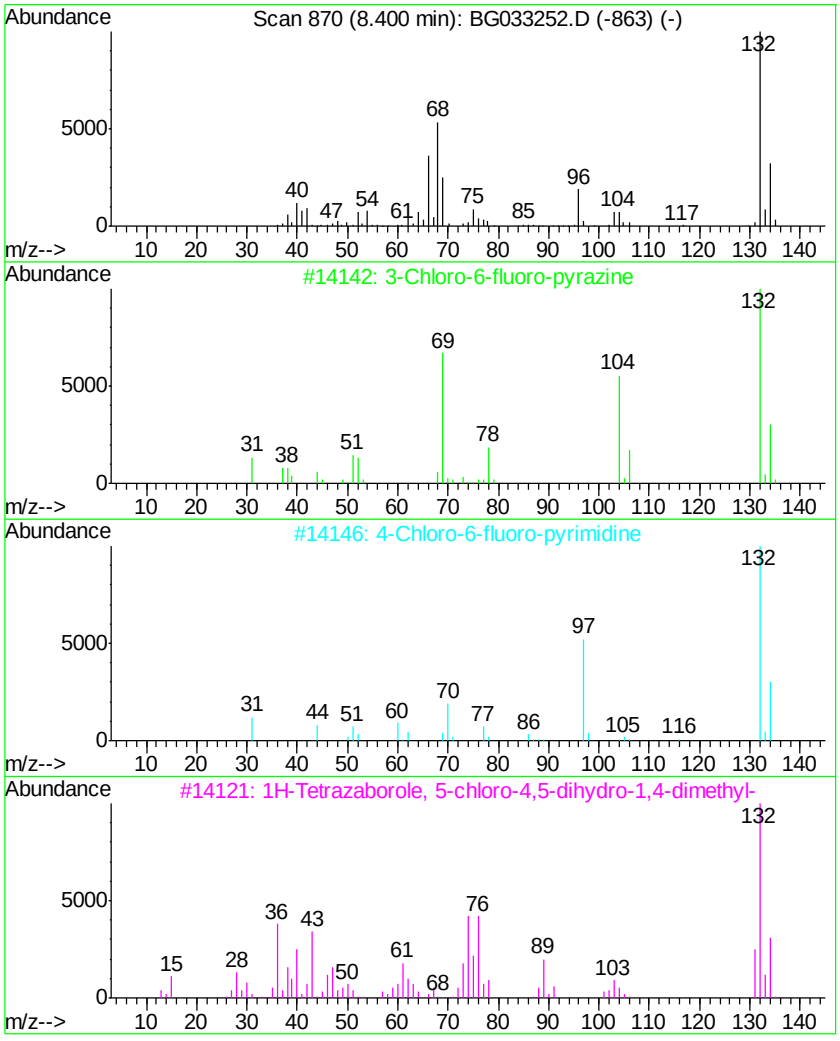
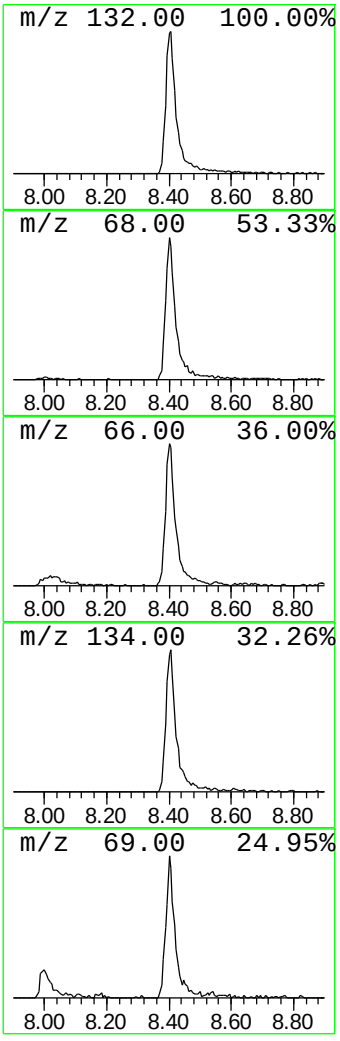
Peak Number 4 unknown8.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	57.97 ng	648508	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	16
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033252.D
Acq On : 19 Mar 2018 22:51
Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

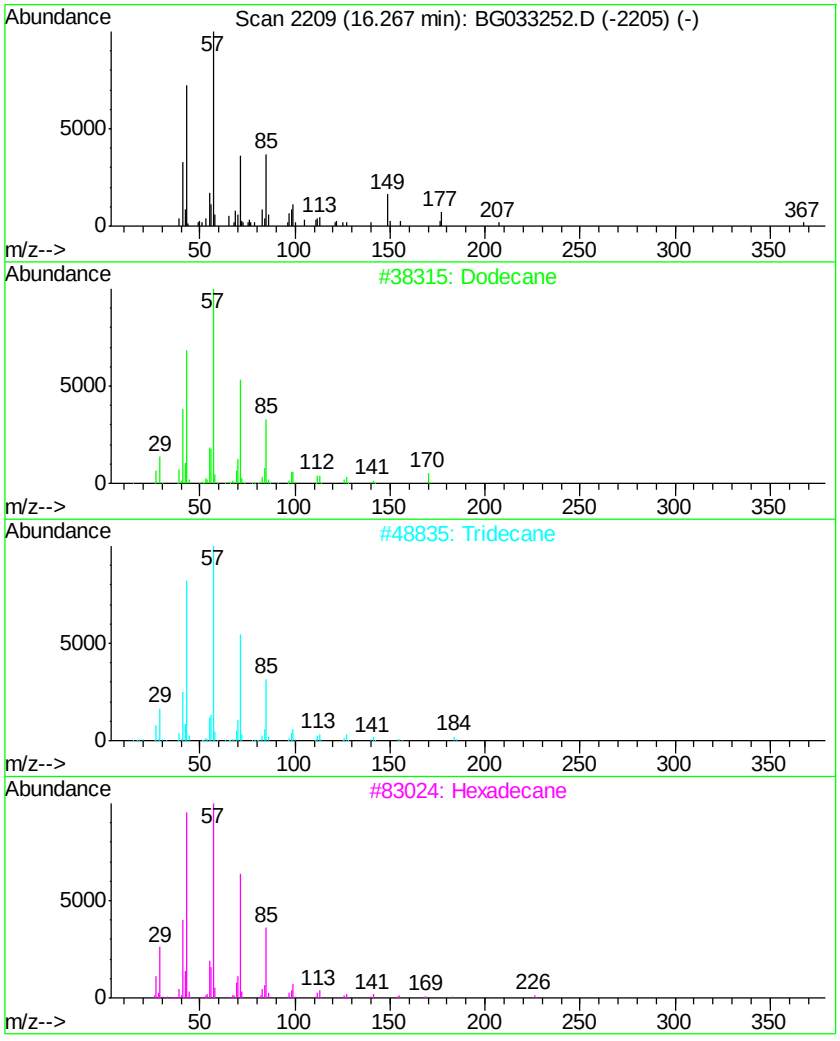
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

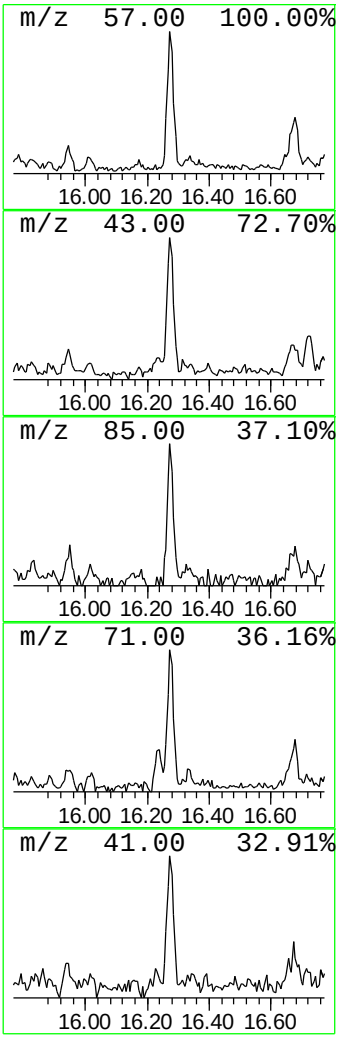
****

Peak Number 6 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	3.09 ng	76485	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	72
2	Tridecane	184	C13H28	000629-50-5	72
3	Hexadecane	226	C16H34	000544-76-3	70
4	Eicosane	282	C20H42	000112-95-8	64
5	Undecane	156	C11H24	001120-21-4	59





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033252.D
Acq On : 19 Mar 2018 22:51
Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

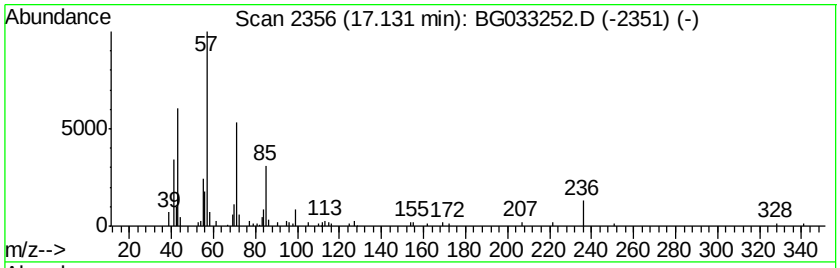
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

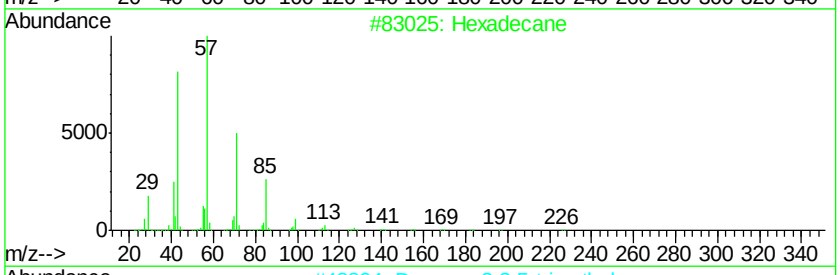
****

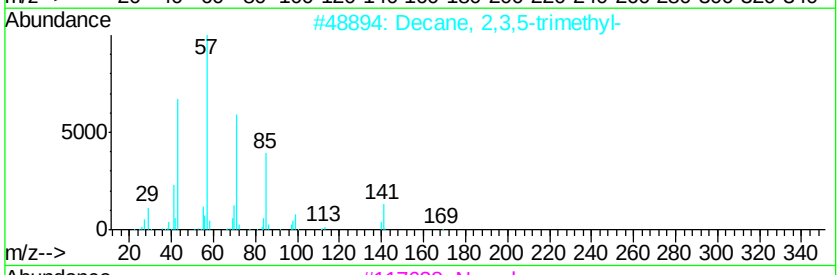
Peak Number 7 Hexadecane Concentration Rank 9

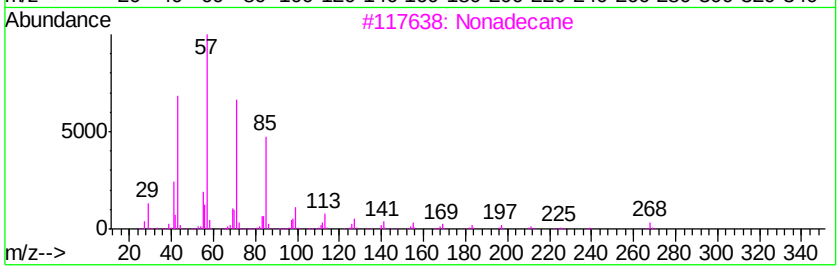
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	2.87 ng	106479	Phenanthrene-d10	18.24

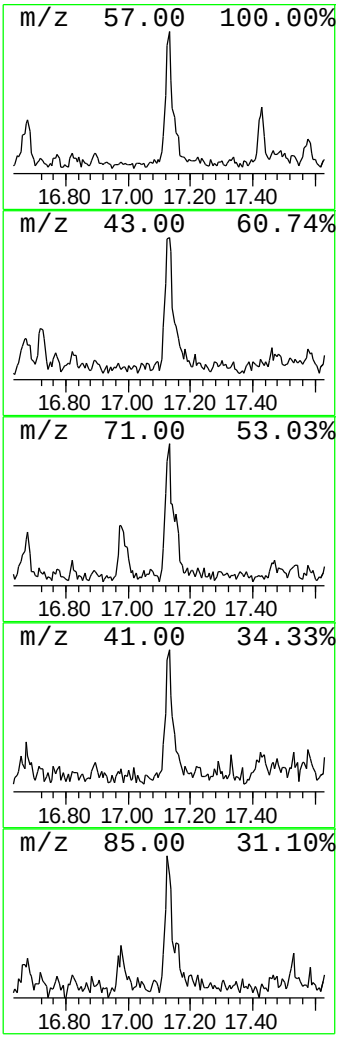
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	64
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	64
3	Nonadecane	268	C19H40	000629-92-5	64
4	Tridecane	184	C13H28	000629-50-5	64
5	Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64











Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033252.D
Acq On : 19 Mar 2018 22:51
Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

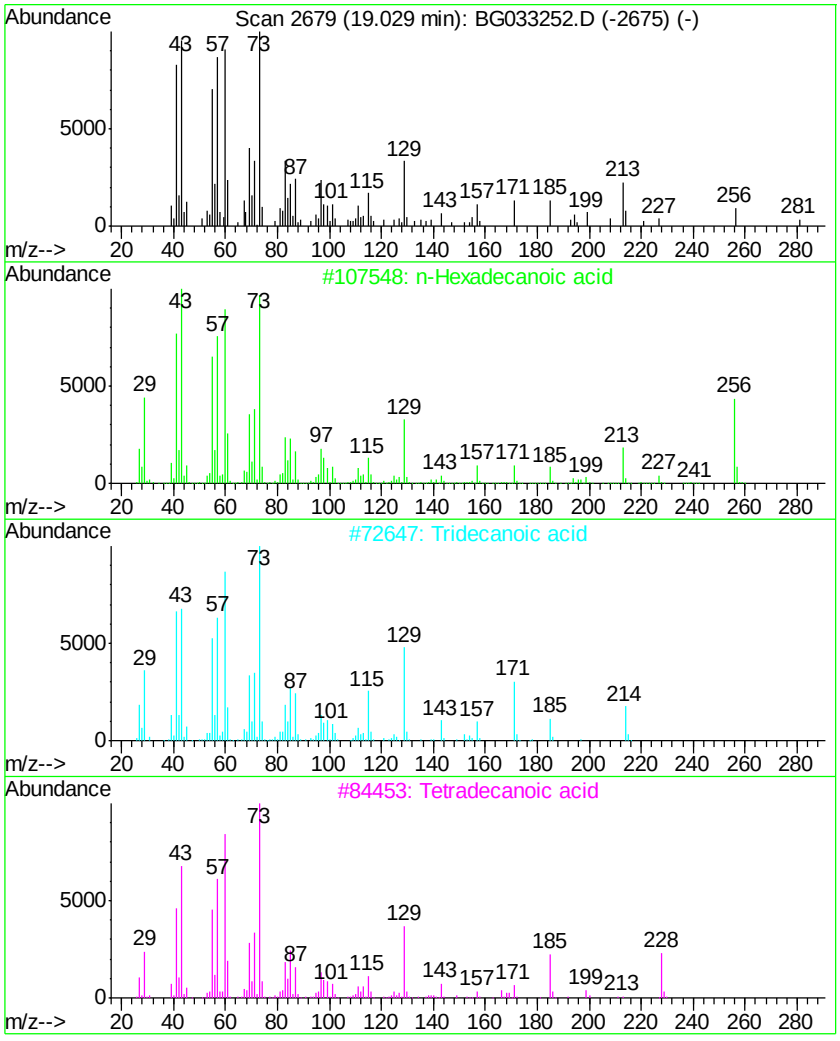
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

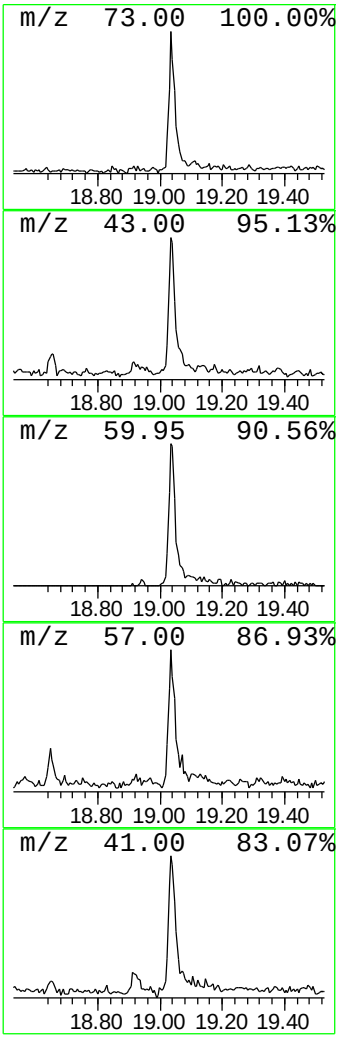
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	6.00 ng	222823	Phenanthrene-d10	18.24

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	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	68





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Data File : BG033252.D
Acq On : 19 Mar 2018 22:51
Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

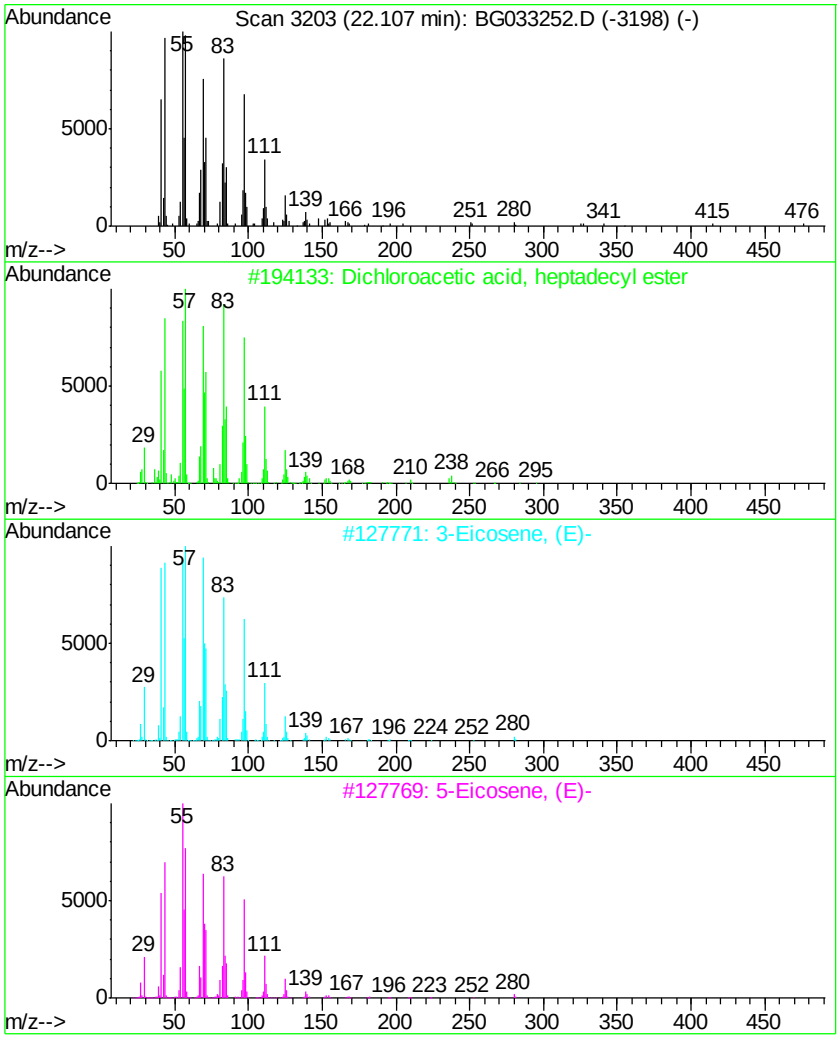
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

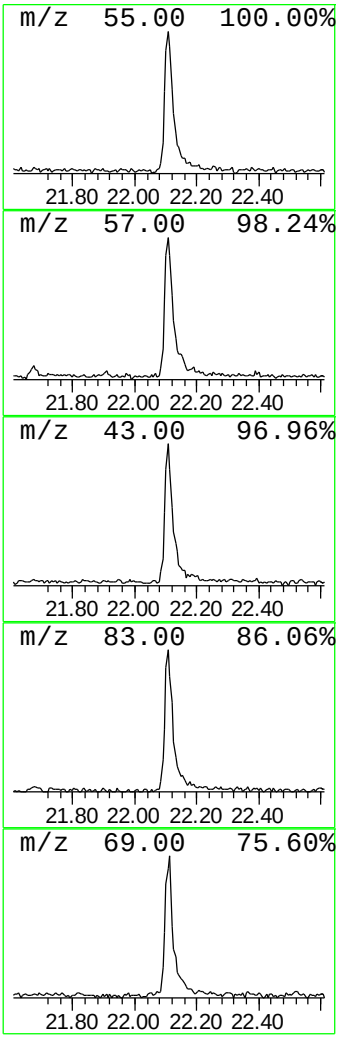
****

Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	8.05 ng	333215	Chrysene-d12	22.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Cyclotetracosane	336	C24H48	000297-03-0	93





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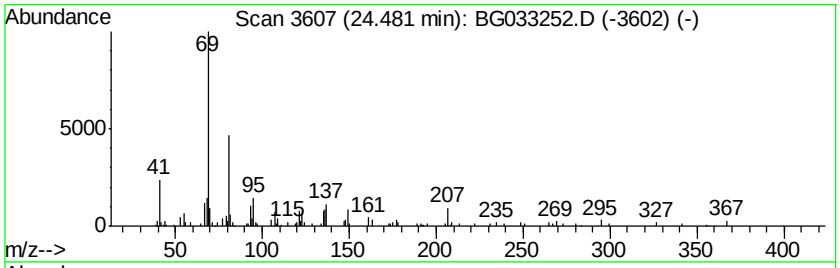
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

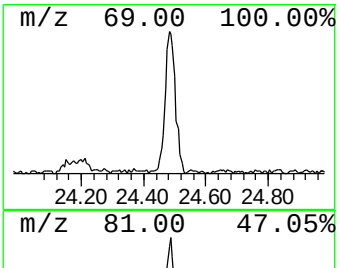
****

Peak Number 10 Docosa-2,6,10,14,18-pentaen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.48	2.82 ng	116870	Chrysene-d12	22.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	74
2	Supraene	410	C30H50	007683-64-9	72
3	Squalene	410	C30H50	000111-02-4	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG031918\
Data File : BG033252.D
Acq On : 19 Mar 2018 22:51
Operator : SJ/JU
Sample : J1953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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...	3.59	12.0	ng	134042	1	8.89	223748	20.0
Ethanol, 2-butoxy-	6.84	28.7	ng	320996	1	8.89	223748	20.0
unknown8.40	8.40	58.0	ng	648508	1	8.89	223748	20.0
Dodecane	16.27	3.1	ng	76485	3	15.51	494886	20.0
Hexadecane	17.13	2.9	ng	106479	4	18.24	742735	20.0
n-Hexadecanoic acid	19.03	6.0	ng	222823	4	18.24	742735	20.0
Dichloroacetic ac...	22.11	8.1	ng	333215	5	22.60	827566	20.0
Docosa-2,6,10,14,...	24.48	2.8	ng	116870	5	22.60	827566	20.0