LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062918\
Data File : BG035530.D
Acq On : 30 Jun 2018 7:04
Operator : JU/SJ
Sample : J3757-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 062618-DBRI-F-D-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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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	5.637	395	400	409	rBV	158003	263295	8.42%	2.315%
2	7.223	664	670	680	rVB	100406	185093	5.92%	1.628%
3	7.593	726	733	745	rBV	302641	517766	16.56%	4.553%
4	8.063	807	813	819	rBV	101191	165109	5.28%	1.452%
5	8.386	860	868	876	rBV	423187	733403	23.45%	6.449%
6	9.226	1002	1011	1023	rBV	368040	677936	21.68%	5.962%
7	10.865	1282	1290	1300	rBV	130731	237842	7.61%	2.092%
8	13.309	1698	1706	1712	rBV	1154191	1782184	56.99%	15.672%
9	14.131	1840	1846	1852	rBV	44767	67938	2.17%	0.597%
10	14.683	1931	1940	1948	rVB2	255074	411883	13.17%	3.622%
11	15.964	2153	2158	2165	rBV	48665	60921	1.95%	0.536%
12	16.170	2184	2193	2205	rBV	658829	1024877	32.78%	9.012%
13	17.427	2400	2407	2416	rBV	371285	581601	18.60%	5.114%
14	18.302	2552	2556	2564	rBV3	41167	60237	1.93%	0.530%
15	20.029	2844	2850	2857	rBV	2484820	3126915	100.00%	27.497%
16	21.327	3066	3071	3081	rBV6	29032	65030	2.08%	0.572%
17	21.691	3126	3133	3140	rBV	403929	674515	21.57%	5.931%
18	23.366	3413	3418	3426	rVB	37847	74846	2.39%	0.658%
19	24.917	3671	3682	3695	rBV2	234864	660395	21.12%	5.807%

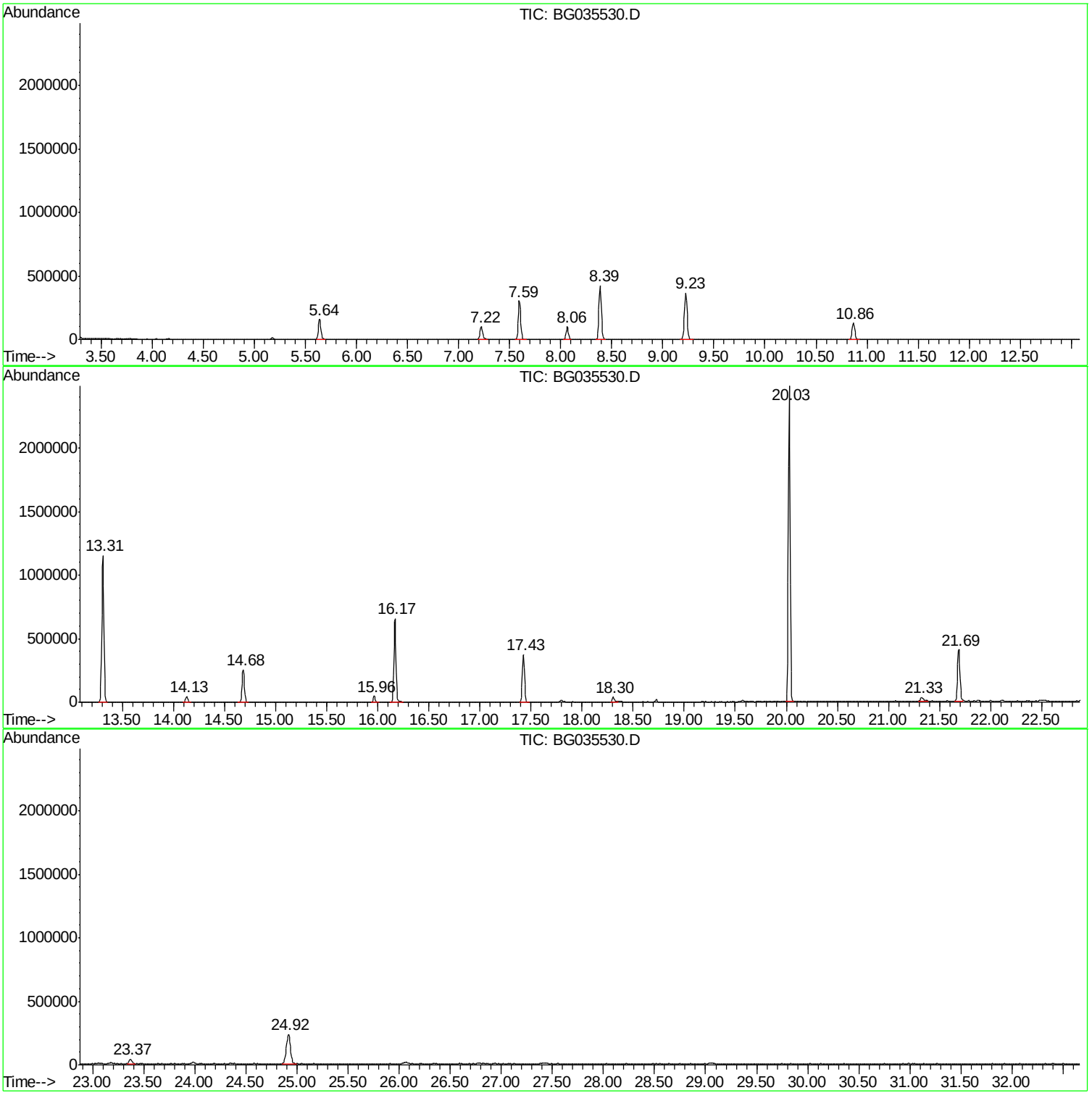
Sum of corrected areas: 11371786

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062918\
Data File : BG035530.D
Acq On : 30 Jun 2018 7:04
Operator : JU/SJ
Sample : J3757-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
062618-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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\BG062918\
Data File : BG035530.D
Acq On : 30 Jun 2018 7:04
Operator : JU/SJ
Sample : J3757-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 062618-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

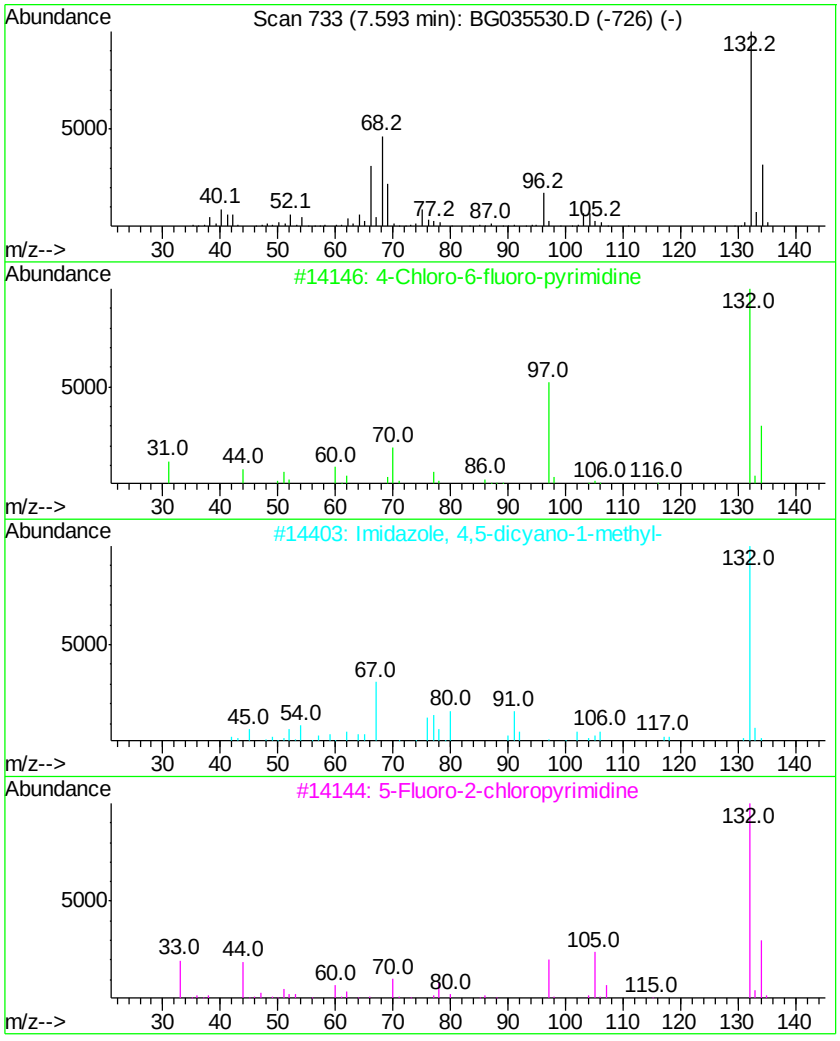
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

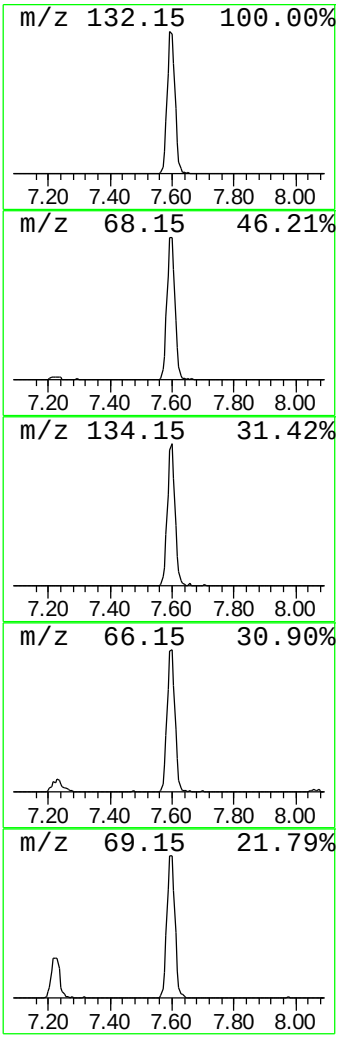
****

Peak Number 1 unknown7.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	62.72 ng	517766	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	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062918\
Data File : BG035530.D
Acq On : 30 Jun 2018 7:04
Operator : JU/SJ
Sample : J3757-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 062618-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

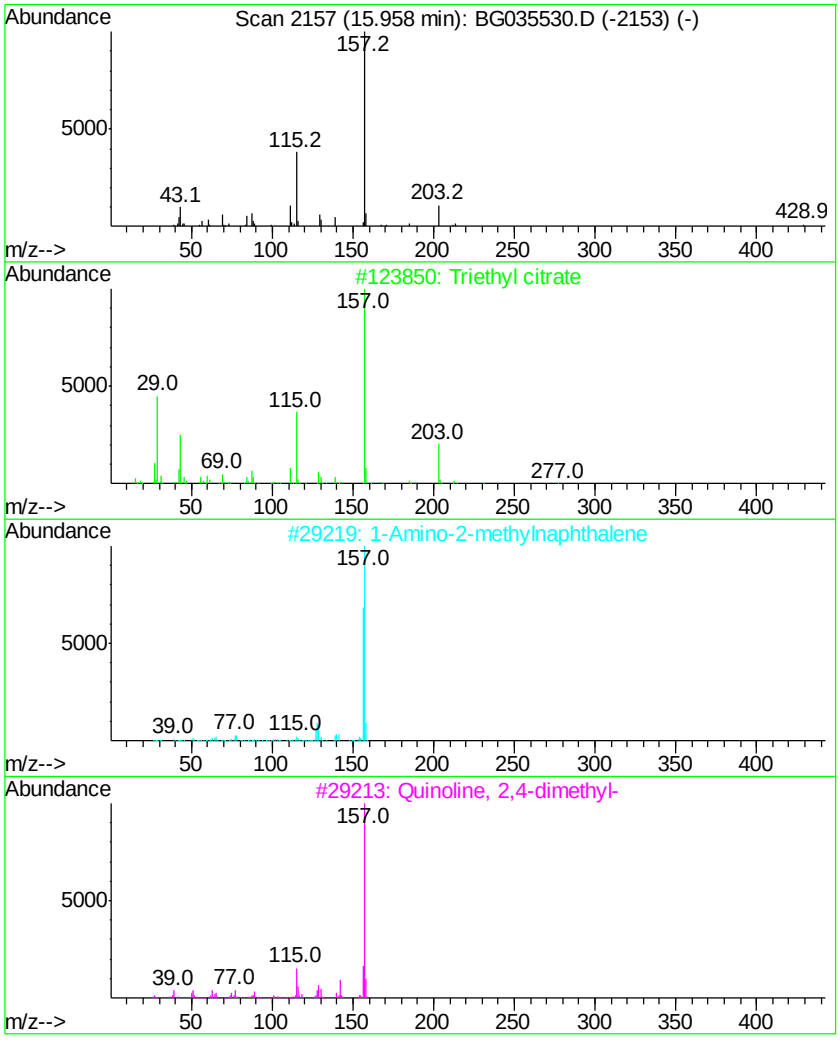
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

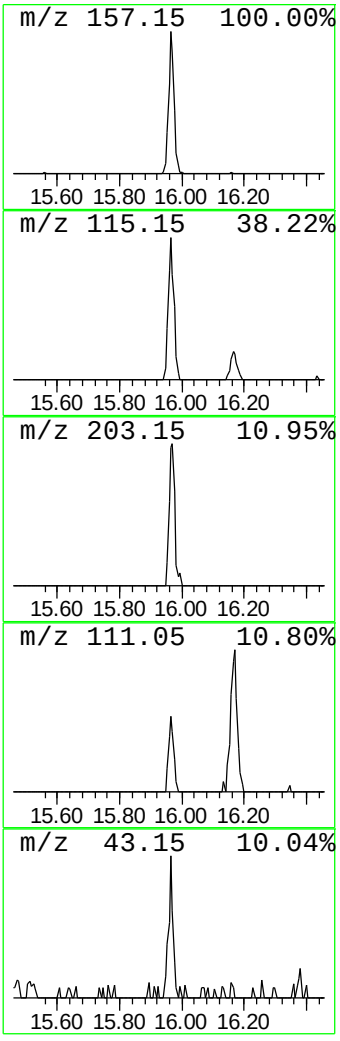
****

Peak Number 3 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	2.96 ng	60921	Acenaphthene-d10	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	78
2	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	50
3	Quinoline, 2,4-dimethyl-	157	C11H11N	001198-37-4	45
4	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	42
5	O-Acetylcitric acid triethyl ester	318	C14H22O8	000077-89-4	39





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062918\
Data File : BG035530.D
Acq On : 30 Jun 2018 7:04
Operator : JU/SJ
Sample : J3757-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 062618-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

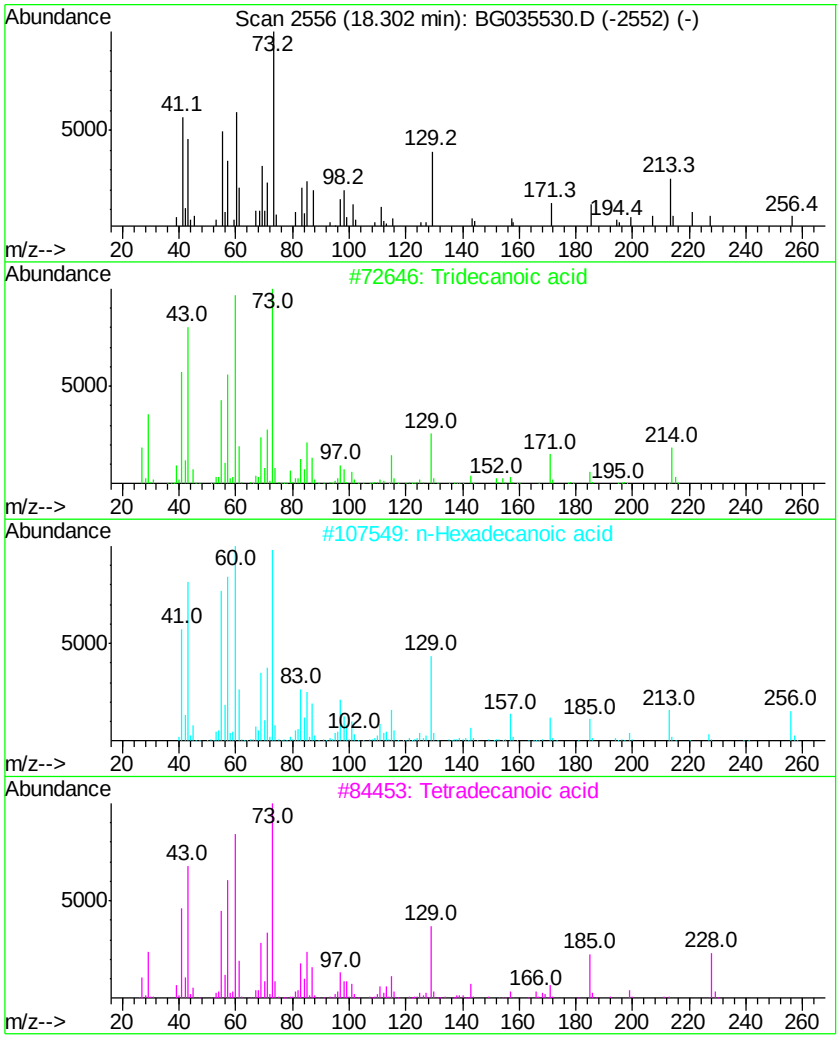
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

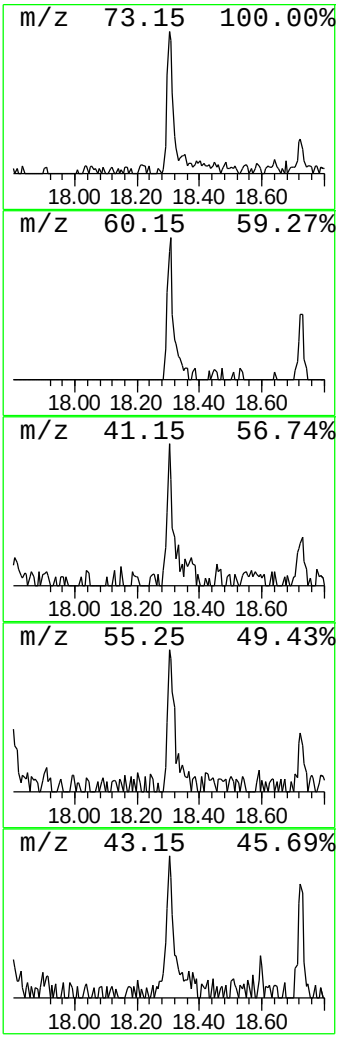
****

Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	2.07 ng	60237	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	76
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4	Dodecanoic acid	200	C12H24O2	000143-07-7	42
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	40





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062918\
Data File : BG035530.D
Acq On : 30 Jun 2018 7:04
Operator : JU/SJ
Sample : J3757-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 062618-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

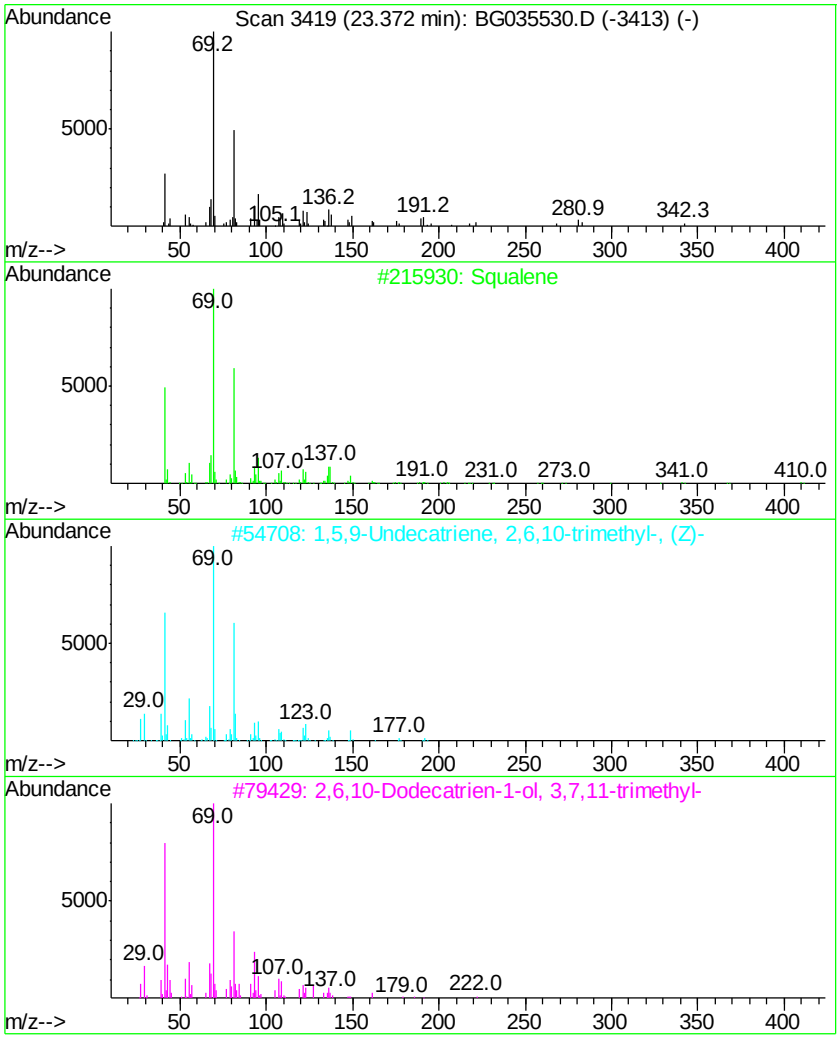
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

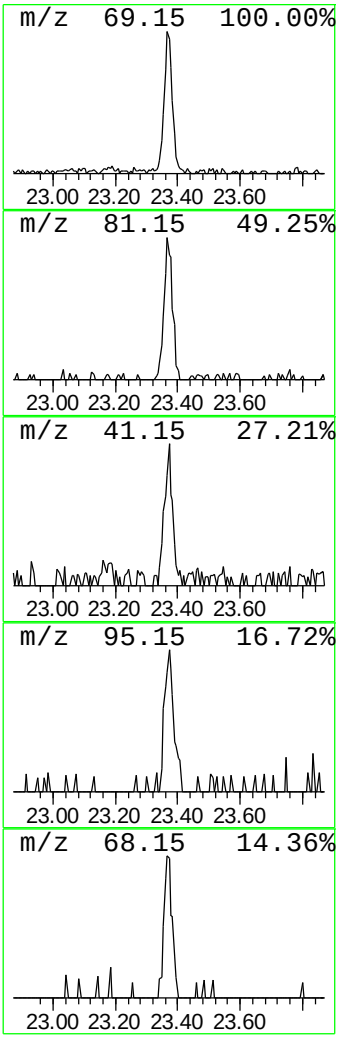
****

Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.37	2.27 ng	74846	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	72
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
4	Supraene	410	C30H50	007683-64-9	64
5	1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG062918\
Data File : BG035530.D
Acq On : 30 Jun 2018 7:04
Operator : JU/SJ
Sample : J3757-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 062618-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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
unknown7.59	7.59	62.7	ng	517766	1	8.06	165109	20.0
Triethyl citrate	15.96	3.0	ng	60921	3	14.68	411883	20.0
Tridecanoic acid	18.30	2.1	ng	60237	4	17.42	581601	20.0
Squalene	23.37	2.3	ng	74846	6	24.92	660395	20.0