LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016214.D
Acq On : 07 Aug 2018 05:38
Operator : SJ/JU
Sample : J4331-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 073118-TIPC-E-U-M

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_M\METHODS\8270-BM072318.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	5.693	404	409	424	rBV	242865	406779	14.65%	3.450%
2	7.328	682	687	701	rBV	143617	272489	9.81%	2.311%
3	7.692	743	749	764	rBV	538638	875632	31.53%	7.426%
4	8.169	825	830	838	rBV	155242	246588	8.88%	2.091%
5	8.487	878	884	899	rBB	693362	1137346	40.96%	9.645%
6	9.357	1025	1032	1047	rBV	565446	967709	34.85%	8.207%
7	10.986	1303	1309	1319	rBV	169403	288143	10.38%	2.444%
8	13.422	1716	1723	1735	rBV	1310552	1831406	65.95%	15.531%
9	14.798	1949	1957	1964	rBB2	230902	340125	12.25%	2.884%
10	16.068	2168	2173	2178	rBB	43994	49666	1.79%	0.421%
11	16.286	2204	2210	2220	rVB	736757	1029958	37.09%	8.735%
12	17.533	2416	2422	2431	rVB	281870	388795	14.00%	3.297%
13	18.380	2562	2566	2574	rBV	37667	49647	1.79%	0.421%
14	20.109	2855	2860	2865	rBV	2595337	2777010	100.00%	23.550%
15	21.339	3065	3069	3079	rBV7	31359	67637	2.44%	0.574%
16	21.656	3118	3123	3129	rBV	365892	486957	17.54%	4.130%
17	22.662	3291	3294	3304	rVB5	47469	94273	3.39%	0.799%
18	24.009	3517	3523	3532	rVB	243252	481603	17.34%	4.084%

Sum of corrected areas: 11791763

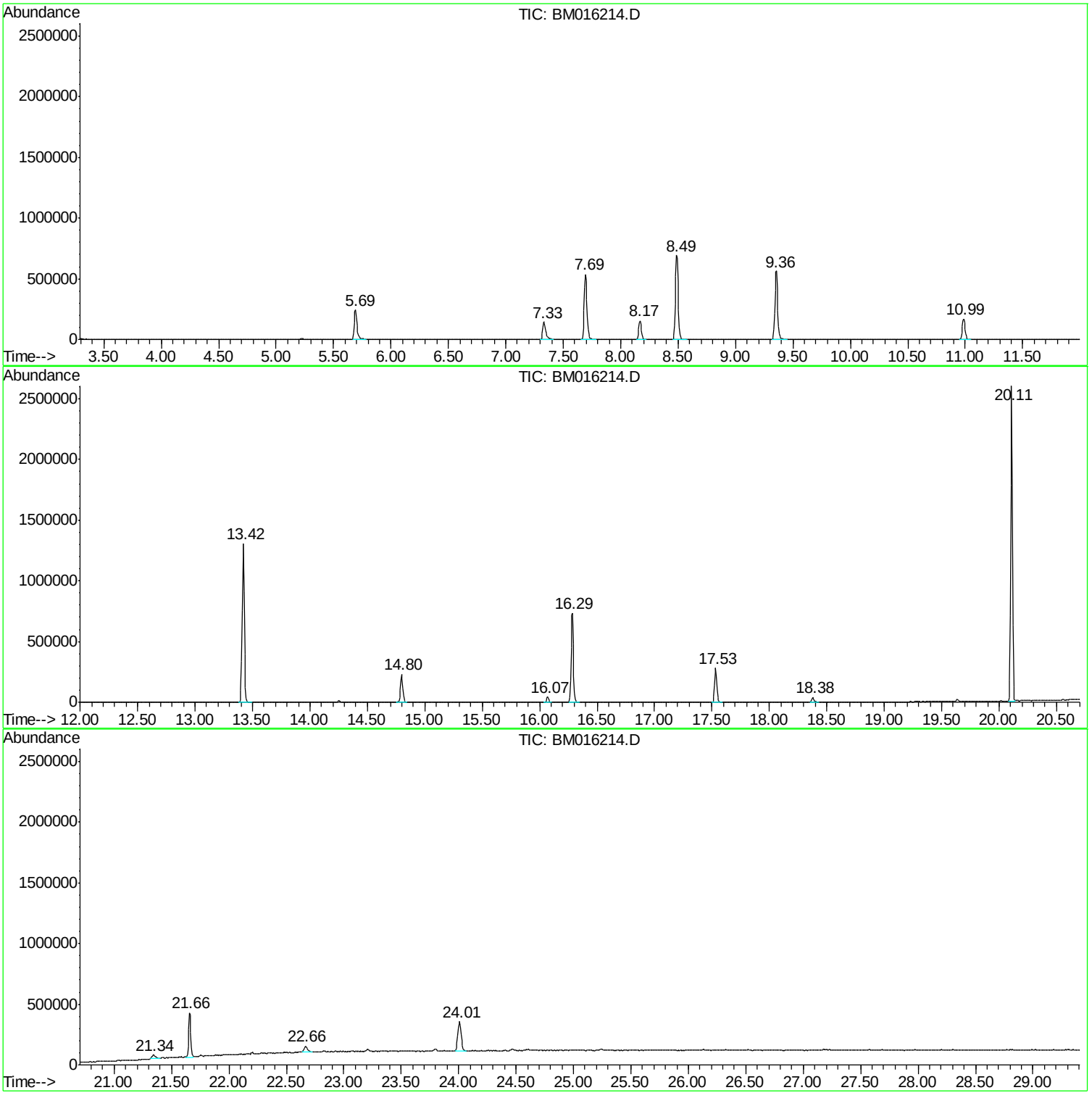
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016214.D
Acq On : 07 Aug 2018 05:38
Operator : SJ/JU
Sample : J4331-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
073118-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016214.D
Acq On : 07 Aug 2018 05:38
Operator : SJ/JU
Sample : J4331-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 073118-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

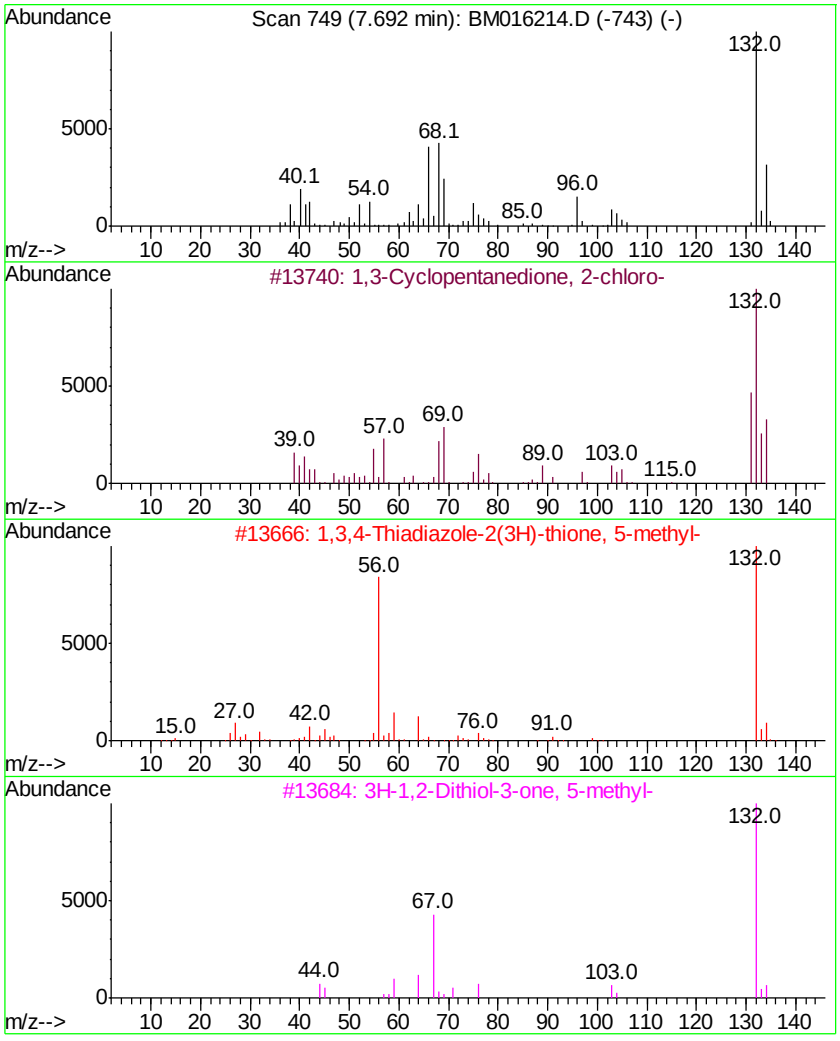
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

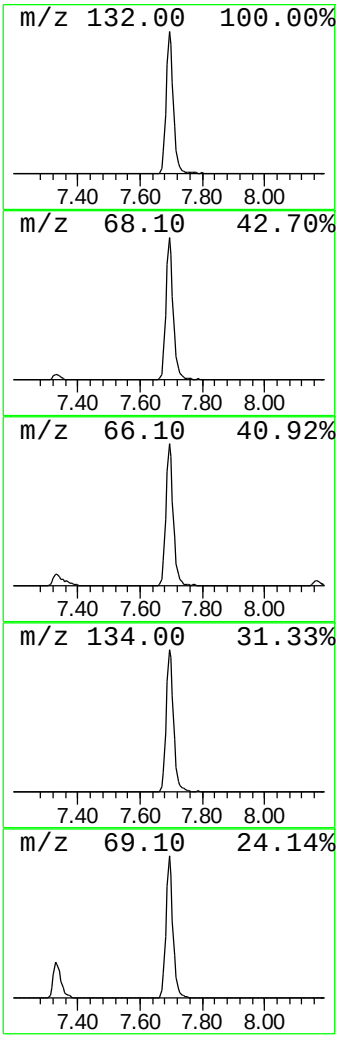
****

Peak Number 1 unknown7.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	71.02 ng	875632	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016214.D
Acq On : 07 Aug 2018 05:38
Operator : SJ/JU
Sample : J4331-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 073118-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

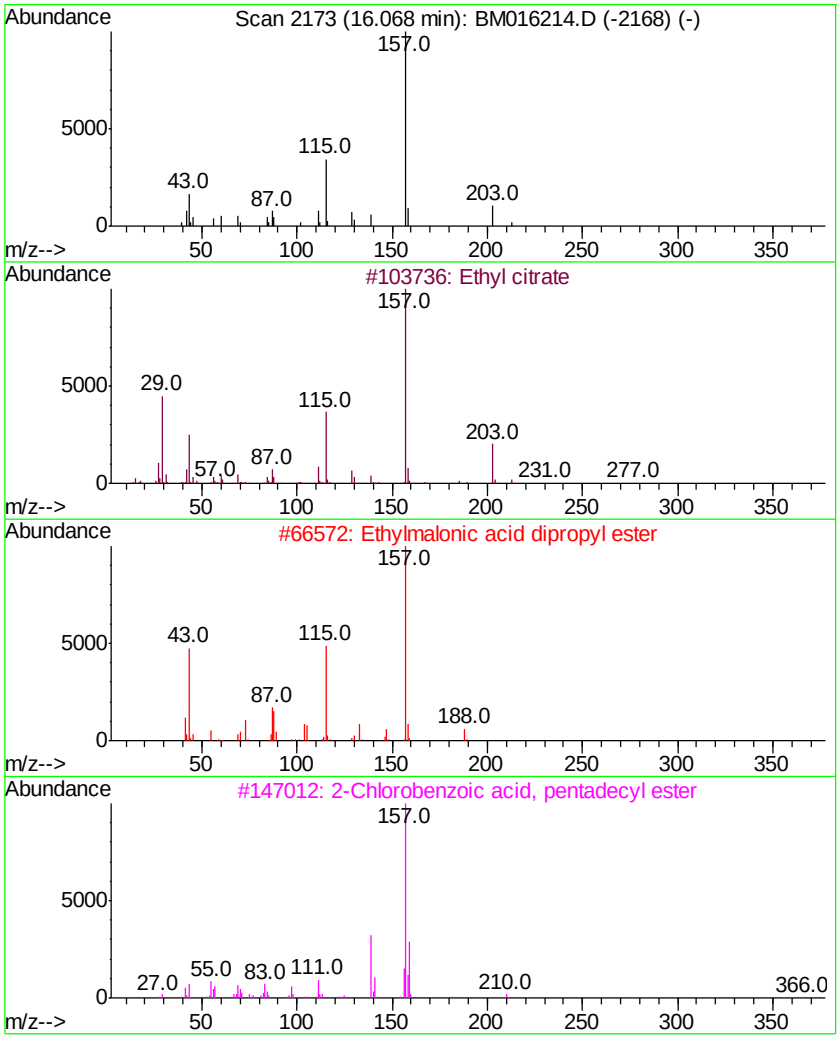
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

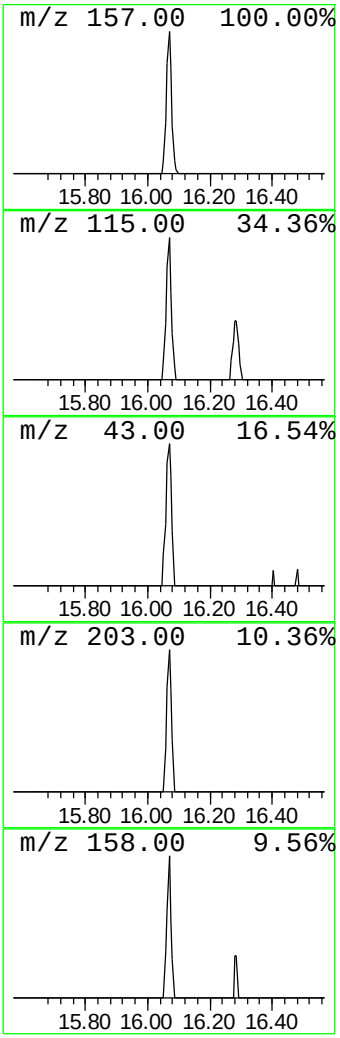
****

Peak Number 3 Ethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.92 ng	49666	Acenaphthene-d10	14.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl citrate	276	C12H20O7	000077-93-0	86
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	50
3	2-Chlorobenzoic acid, pentadecyl...	366	C22H35ClO2	1000292-43-0	50
4	2-Chlorobenzoic acid, hexadecyl ...	380	C23H37ClO2	070152-86-2	50
5	2-Chlorobenzoic acid, undecyl ester	310	C18H27ClO2	097221-96-0	40





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016214.D
Acq On : 07 Aug 2018 05:38
Operator : SJ/JU
Sample : J4331-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 073118-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

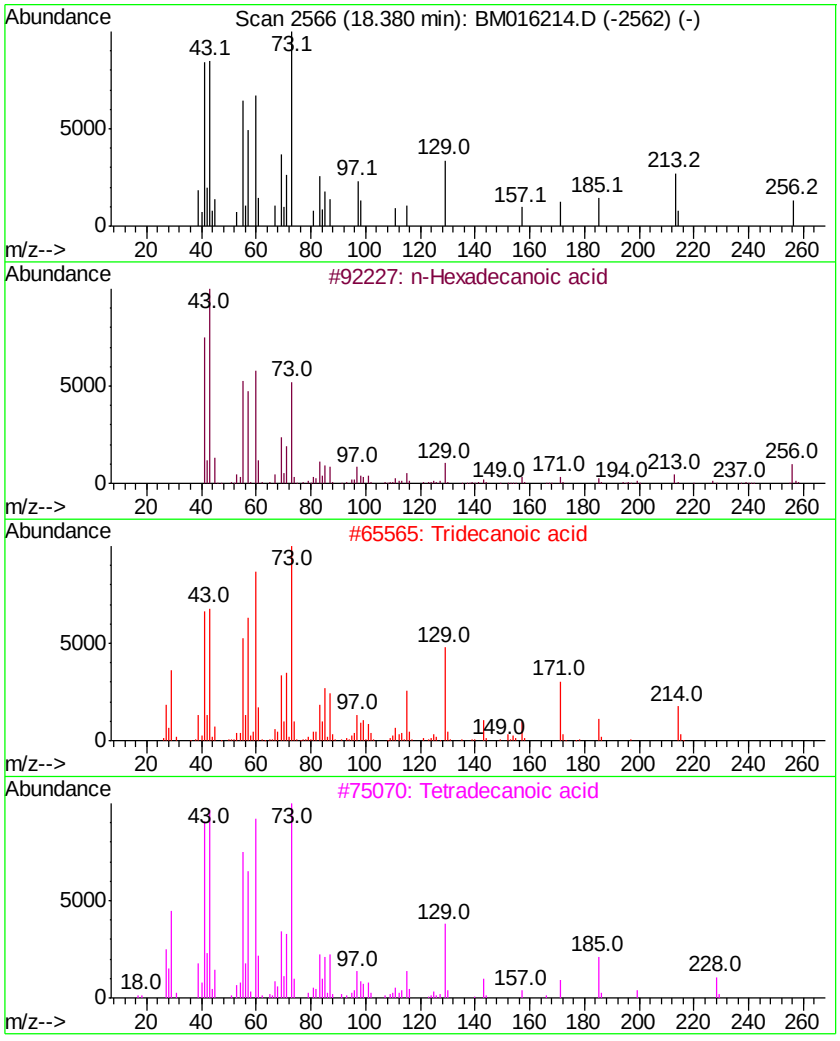
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

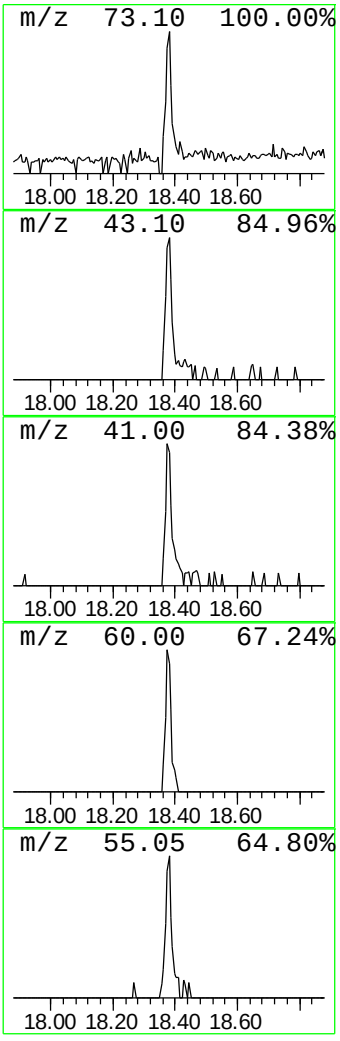
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	2.55 ng	49647	Phenanthrene-d10	17.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
2	Tridecanoic acid	214	C13H26O2	000638-53-9	50
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	Dodecanoic acid	200	C12H24O2	000143-07-7	38
5	n-Decanoic acid	172	C10H20O2	000334-48-5	35





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016214.D
Acq On : 07 Aug 2018 05:38
Operator : SJ/JU
Sample : J4331-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 073118-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

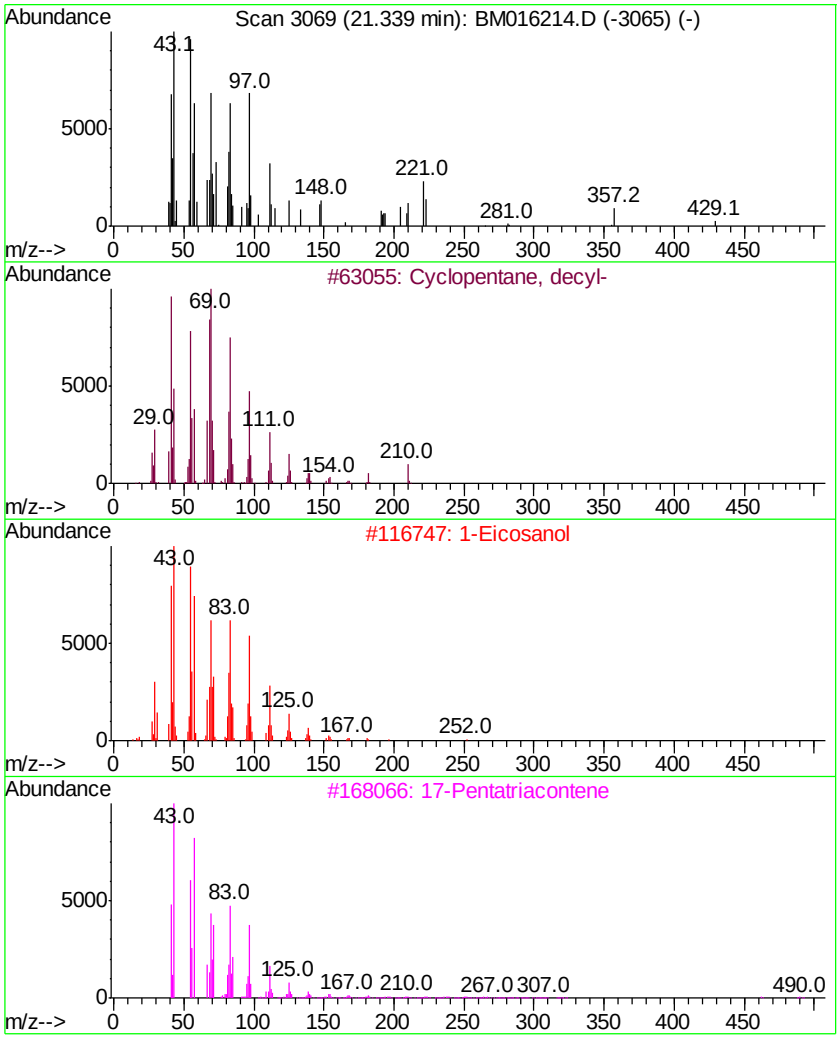
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

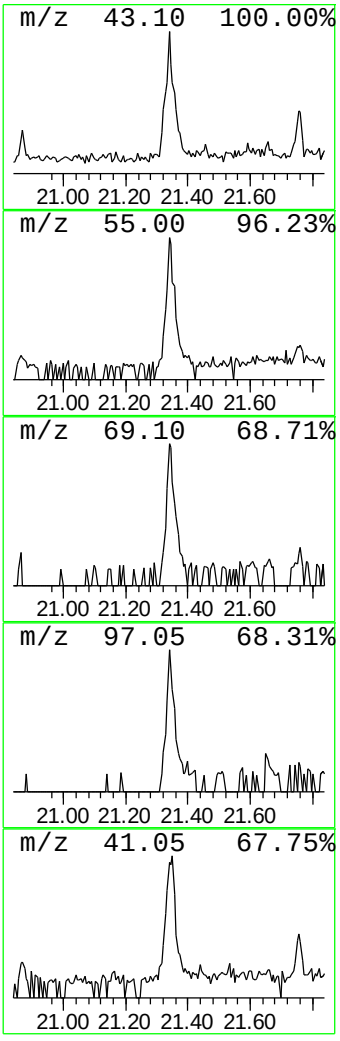
****

Peak Number 5 Cyclopentane, decyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.34	2.78 ng	67637	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, decyl-	210	C15H30	001795-21-7	70
2	1-Eicosanol	298	C20H42O	000629-96-9	52
3	17-Pentatriacontene	491	C35H70	006971-40-0	49
4	1-Docosanol	326	C22H46O	000661-19-8	49
5	Dodecane, 1-cyclopentyl-4-(3-cyc...	348	C25H48	007225-68-5	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016214.D
Acq On : 07 Aug 2018 05:38
Operator : SJ/JU
Sample : J4331-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 073118-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

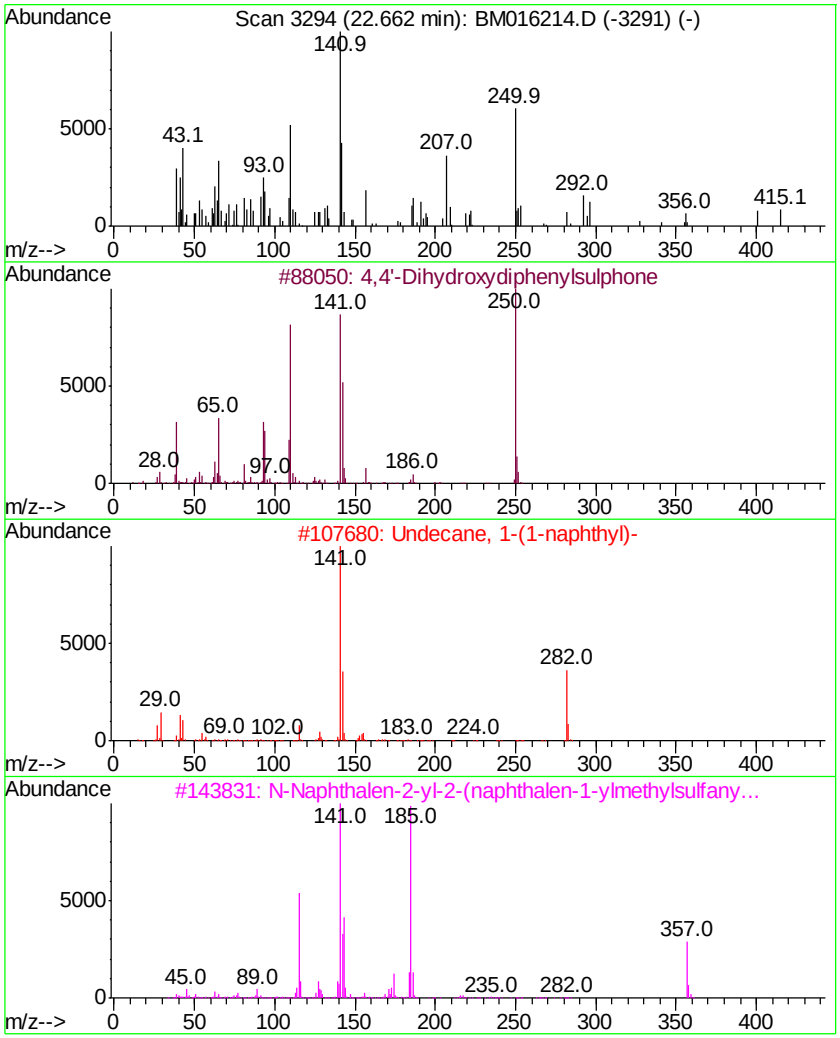
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

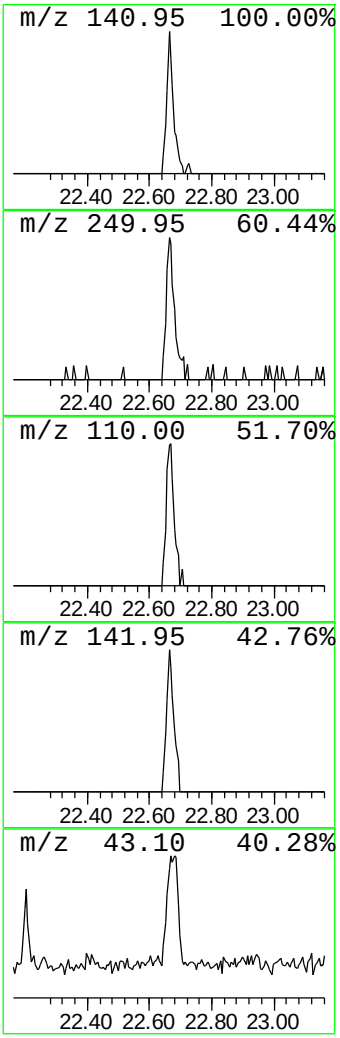
****

Peak Number 6 4,4'-Dihydroxydiphenylsulphone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.66	3.87 ng	94273	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	60
2	Undecane, 1-(1-naphthyl)-	282	C21H30	007225-71-0	35
3	N-Naphthalen-2-yl-2-(naphthalen-...	357	C23H19NOS	302567-99-3	23
4	Imidazole, 1-methyl-2-[2-(4-meth...	296	C13H16N2O2S2	1000263-81-5	22
5	2-Thiophenecarboxylic acid, 5-no...	254	C14H22O2S	059782-34-2	17





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080618\
Data File : BM016214.D
Acq On : 07 Aug 2018 05:38
Operator : SJ/JU
Sample : J4331-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 073118-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.69	7.69	71.0	ng	875632	1	8.17	246588	20.0
Ethyl citrate	16.07	2.9	ng	49666	3	14.80	340125	20.0
n-Hexadecanoic acid	18.38	2.5	ng	49647	4	17.53	388795	20.0
Cyclopentane, decyl-	21.34	2.8	ng	67637	5	21.66	486957	20.0
4,4'-Dihydroxydip...	22.66	3.9	ng	94273	5	21.66	486957	20.0