LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015920.D
Acq On : 12 Jul 2018 18:17
Operator : SJ/JU
Sample : J3931-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 070918-DBRI-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-BM070518.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	5.793	421	426	443	rBV	465972	757417	12.84%	3.164%
2	7.440	700	706	727	rBV	308148	553727	9.39%	2.313%
3	7.810	763	769	787	rBV	993467	1636320	27.75%	6.836%
4	8.287	844	850	861	rBV	289653	481123	8.16%	2.010%
5	8.610	898	905	917	rBV	1309982	2129814	36.12%	8.898%
6	9.475	1045	1052	1065	rBV	1156365	1918410	32.53%	8.015%
7	11.116	1324	1331	1340	rBV	339937	587257	9.96%	2.453%
8	13.533	1735	1742	1756	rBV	2685357	3709811	62.91%	15.499%
9	13.775	1777	1783	1790	rBV	231094	352473	5.98%	1.473%
10	14.357	1877	1882	1892	rBV	107149	151943	2.58%	0.635%
11	14.910	1965	1976	1984	rBV2	456428	724340	12.28%	3.026%
12	16.163	2185	2189	2194	rBV	87177	106775	1.81%	0.446%
13	16.386	2221	2227	2240	rBV	1415496	1970399	33.41%	8.232%
14	17.633	2433	2439	2448	rBV	570416	814424	13.81%	3.403%
15	18.468	2576	2581	2588	rBV	103811	143561	2.43%	0.600%
16	19.721	2790	2794	2802	rBV2	51087	72433	1.23%	0.303%
17	20.198	2869	2875	2883	rBV	5093304	5897158	100.00%	24.637%
18	21.409	3077	3081	3092	rBV2	89646	191150	3.24%	0.799%
19	21.745	3133	3138	3147	rBV	680313	908334	15.40%	3.795%
20	24.139	3539	3545	3552	rBV	436997	829109	14.06%	3.464%

Sum of corrected areas: 23935978

LSC Report - Integrated Chromatogram

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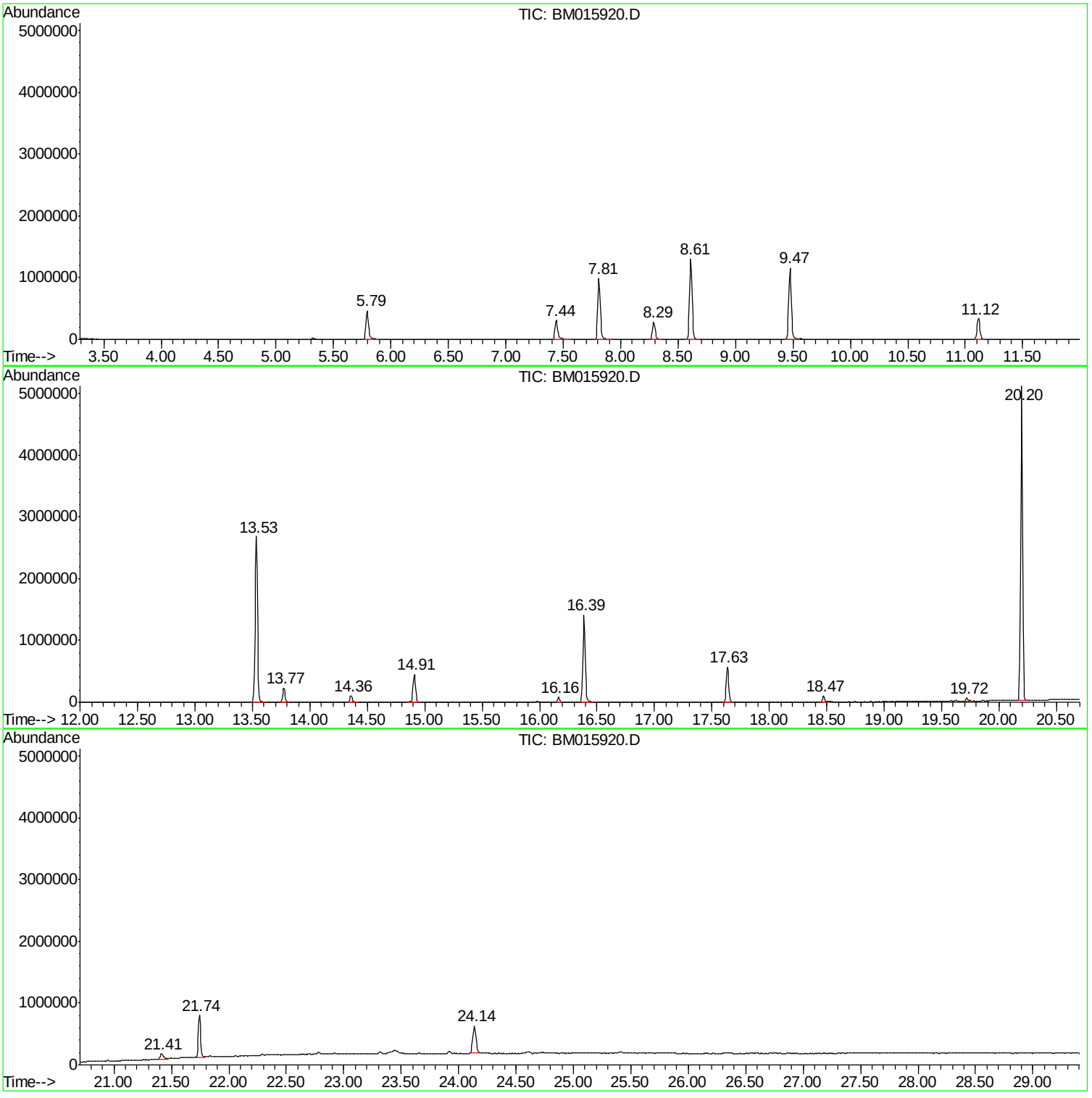
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 070918-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.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

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Data File : BM015920.D
Acq On : 12 Jul 2018 18:17
Operator : SJ/JU
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 070918-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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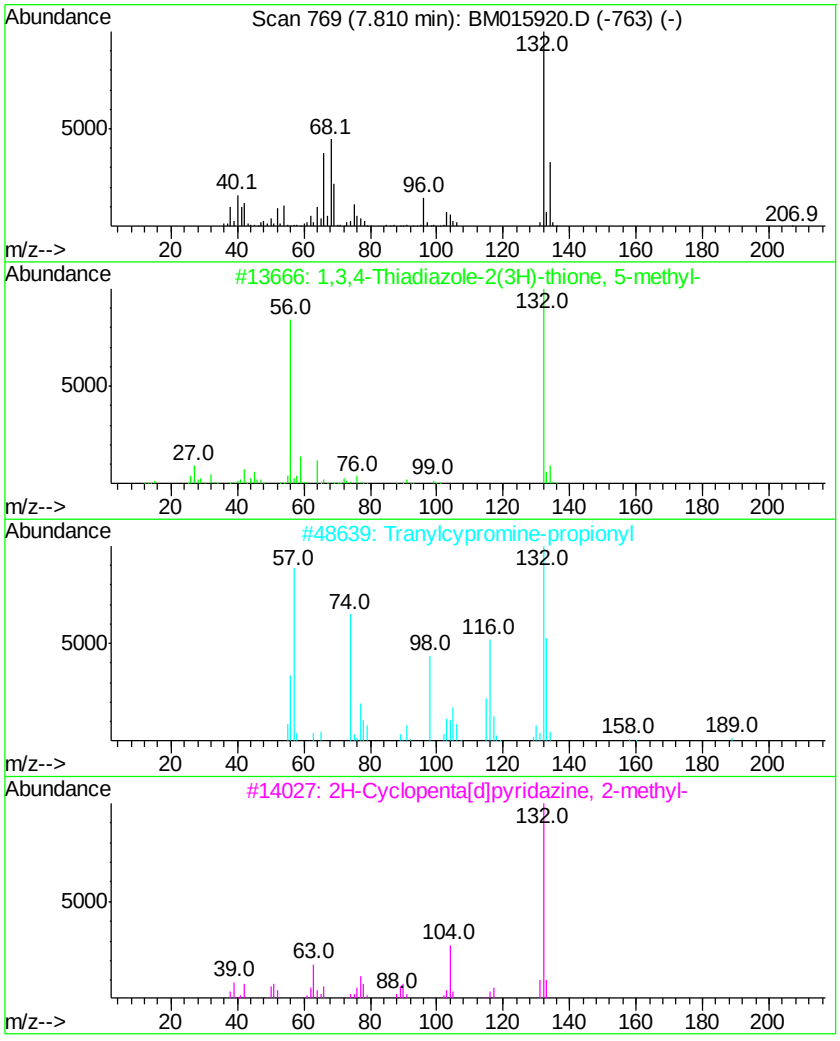
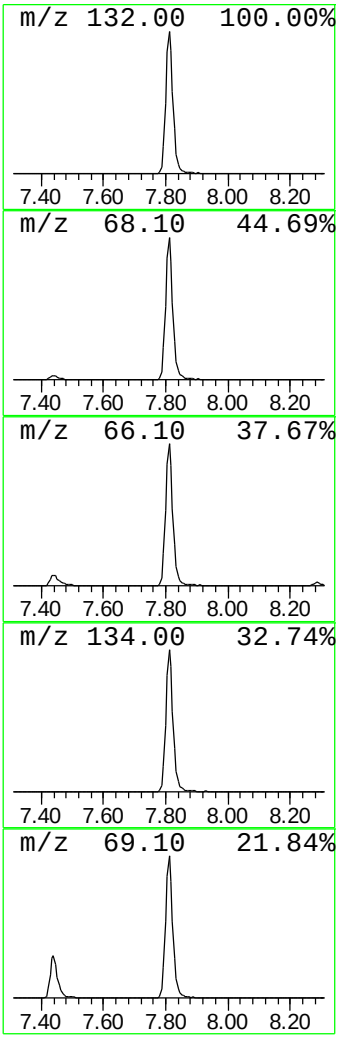
Peak Number 1 unknown7.81 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	68.02 ng	1636320	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12





Library Search Compound Report

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Operator : SJ/JU
Sample : J3931-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 070918-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
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TIC Library : C:\DATABASE\NIST02.L
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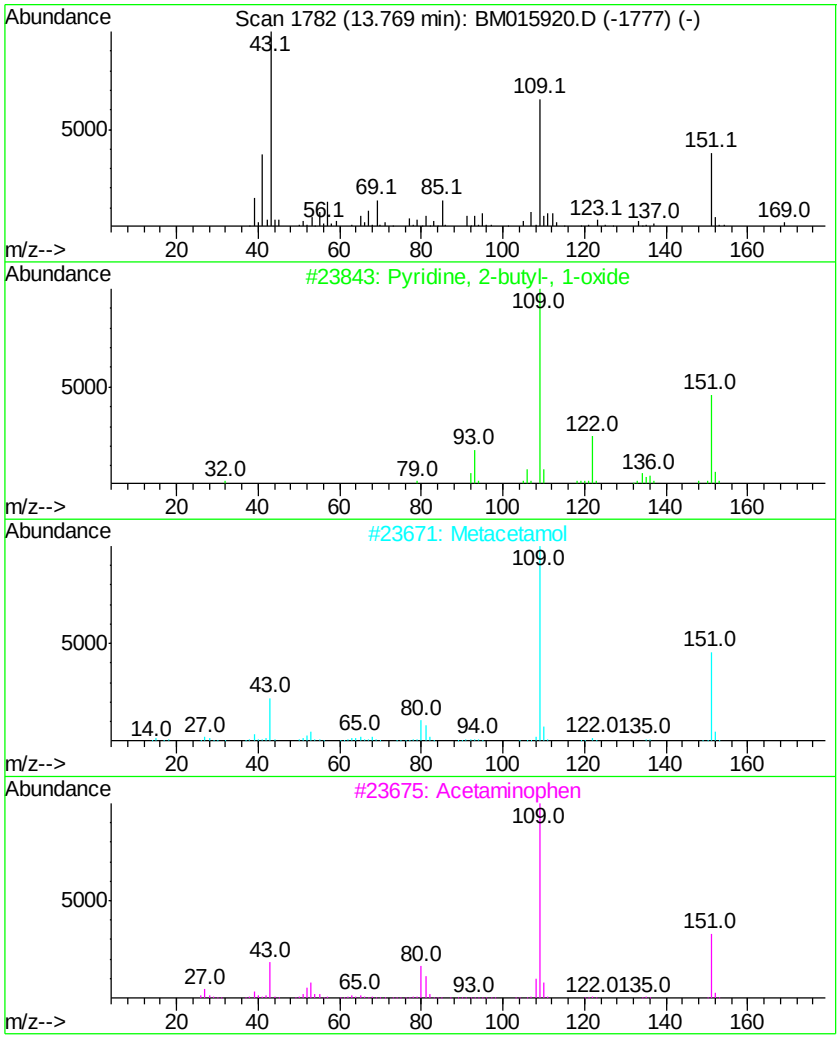
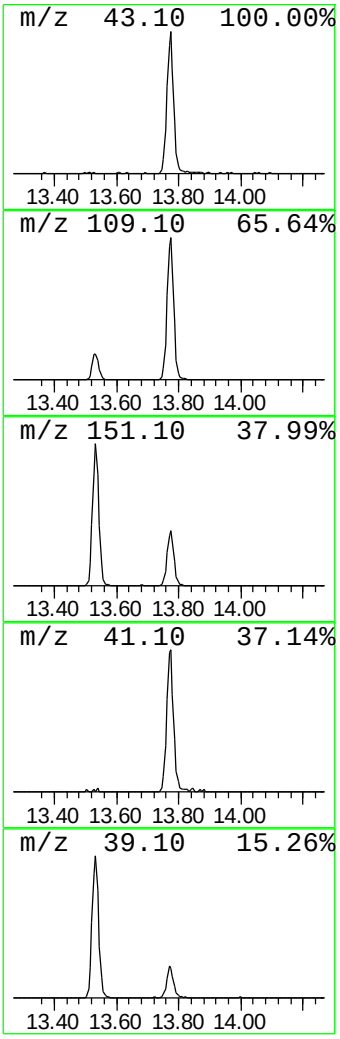
Peak Number 3 Pyridine, 2-butyl-, 1-oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	9.73 ng	352473	Acenaphthene-d10	14.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
2	Metacetamol	151	C8H9NO2	000621-42-1	49
3	Acetaminophen	151	C8H9NO2	000103-90-2	47
4	Cyclohexanol, 3,3,5-trimethyl-, ...	142	C9H18O	000767-54-4	38
5	2-Amino-4-methylpyrimidine	109	C5H7N3	000108-52-1	38





Library Search Compound Report

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Sample : J3931-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 070918-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
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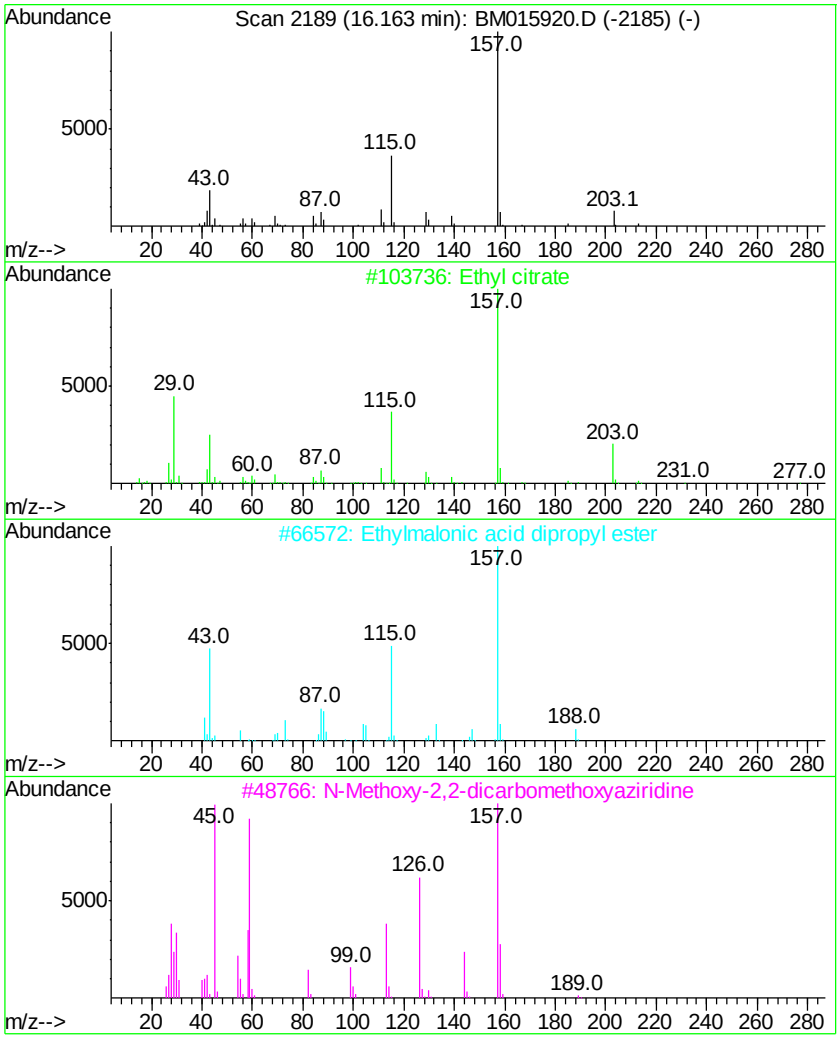
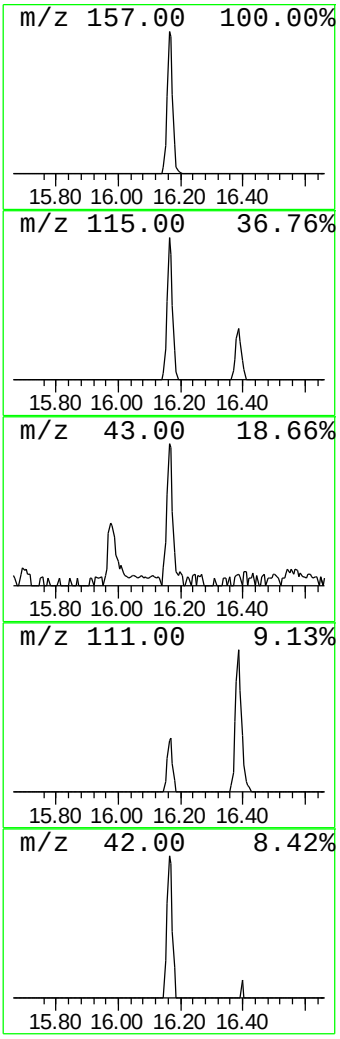
Peak Number 4 Ethyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	2.95 ng	106775	Acenaphthene-d10	14.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl citrate	276	C12H20O7	000077-93-0	90
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	72
3	N-Methoxy-2,2-dicarbomethoxyazir...	189	C7H11NO5	053084-34-7	38
4	2-Fluoro-6-nitrophenol	157	C6H4FNO3	001526-17-6	33
5	2-Chlorobenzoic acid, pentadecyl...	366	C22H35ClO2	1000292-43-0	28





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Data File : BM015920.D
Acq On : 12 Jul 2018 18:17
Operator : SJ/JU
Sample : J3931-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 070918-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
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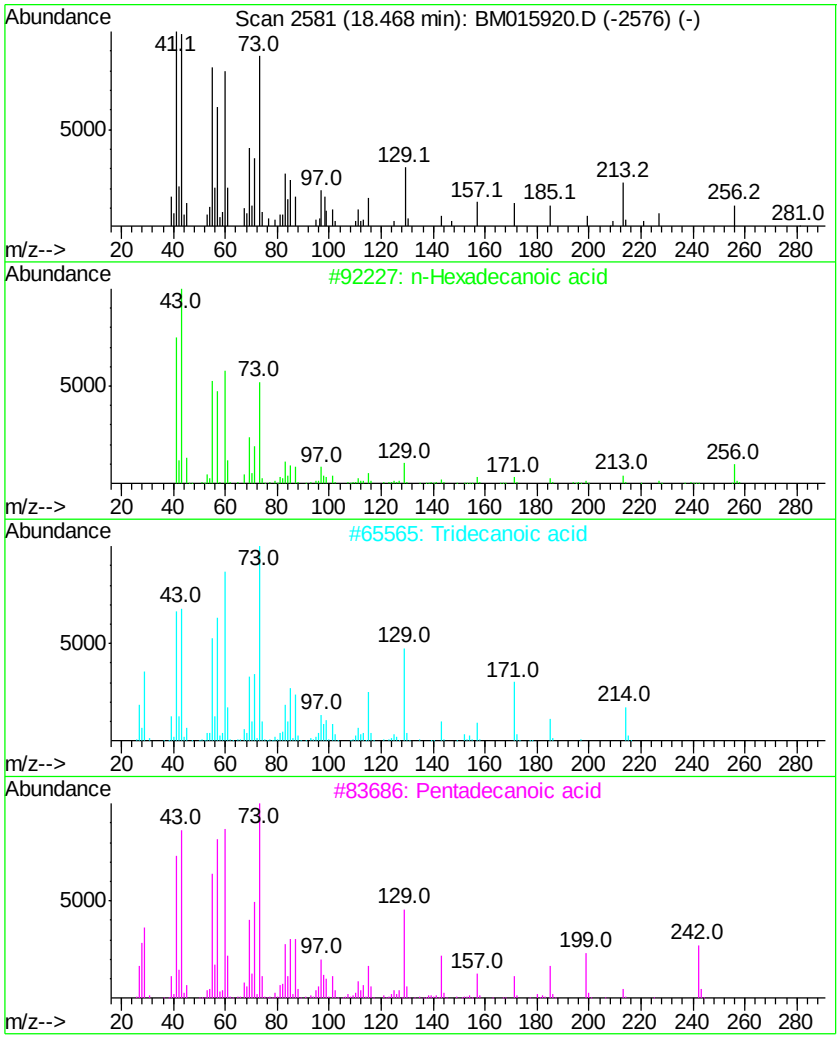
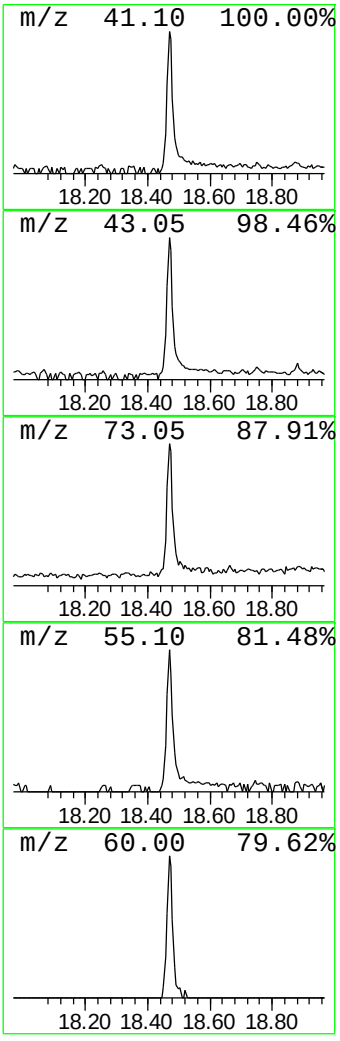
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	3.53 ng	143561	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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Sample : J3931-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 070918-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

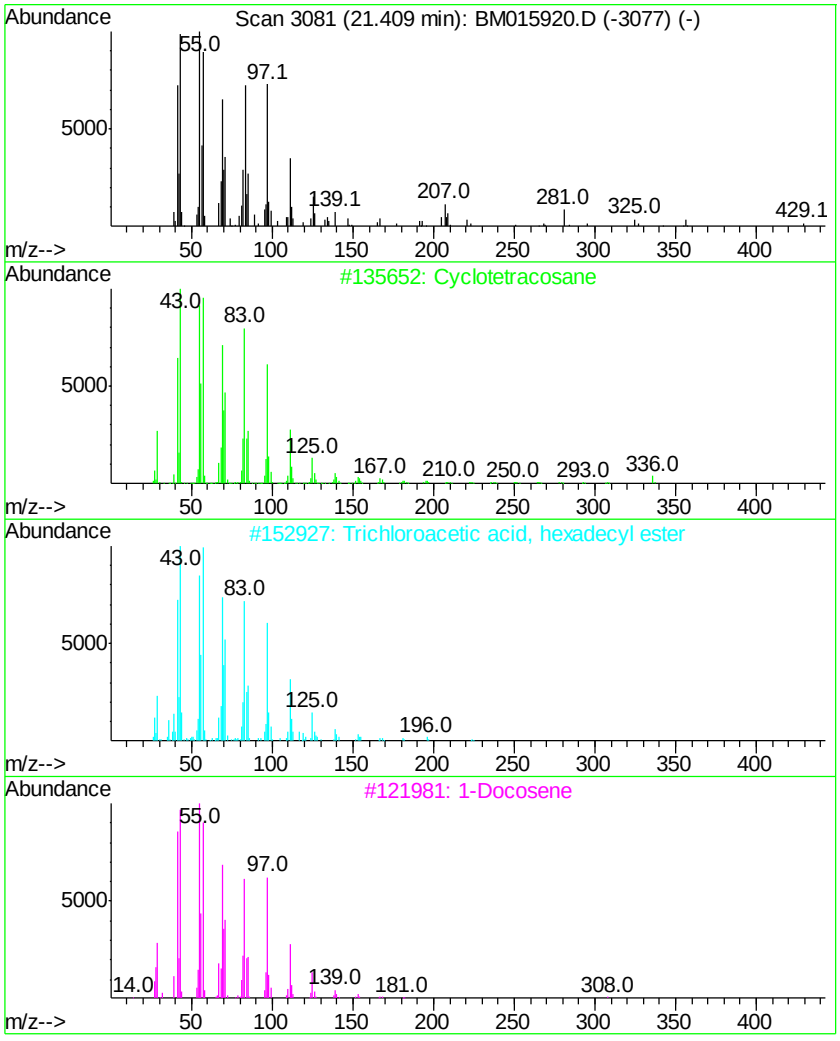
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

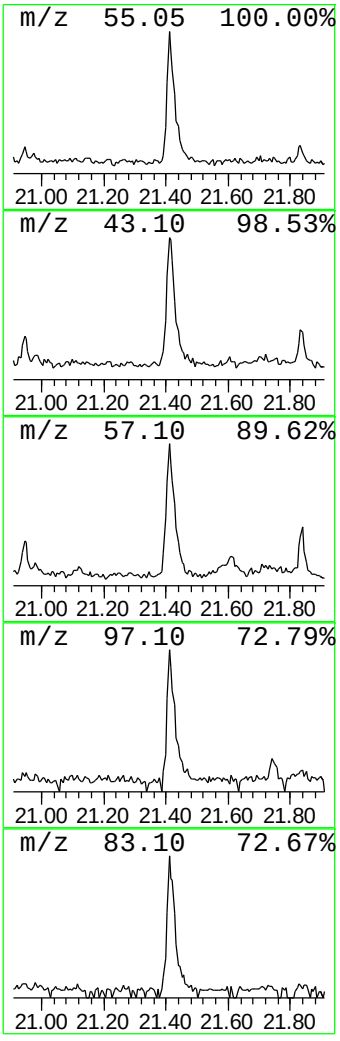
****

Peak Number 6 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	4.21 ng	191150	Chrysene-d12	21.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	87
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
3	1-Docosene	308	C22H44	001599-67-3	81
4	1-Tetracosanol	354	C24H50O	000506-51-4	70
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	68





Tentatively Identified Compound (LSC) summary

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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
unknown7.81	7.81	68.0	ng	1636320	1	8.29	481123	20.0
Pyridine, 2-butyl...	13.77	9.7	ng	352473	3	14.91	724340	20.0
Ethyl citrate	16.16	3.0	ng	106775	3	14.91	724340	20.0
n-Hexadecanoic acid	18.47	3.5	ng	143561	4	17.63	814424	20.0
Cyclotetracosane	21.41	4.2	ng	191150	5	21.74	908334	20.0