LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081518\
Data File : BM016375.D
Acq On : 15 Aug 2018 11:53
Operator : SJ/JU
Sample : PB112017BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB112017BL

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	5.163	314	319	328	rBV	118502	170547	6.35%	1.263%
2	5.646	395	401	418	rBV	835270	1240874	46.21%	9.191%
3	7.287	673	680	696	rBV	780044	1231292	45.86%	9.120%
4	7.640	734	740	752	rBV	887957	1411150	52.55%	10.452%
5	8.110	815	820	829	rBB	137454	208205	7.75%	1.542%
6	8.434	868	875	885	rBB	686816	1075690	40.06%	7.967%
7	9.298	1015	1022	1036	rBV	459657	766840	28.56%	5.680%
8	10.922	1292	1298	1308	rBV	136227	231788	8.63%	1.717%
9	13.369	1707	1714	1724	rBV	1171204	1599702	59.58%	11.848%
10	14.627	1920	1928	1939	rBV5	9580	31057	1.16%	0.230%
11	14.745	1943	1948	1959	rVB2	170620	270311	10.07%	2.002%
12	16.239	2196	2202	2213	rBV	1018756	1415088	52.70%	10.481%
13	17.486	2409	2414	2424	rBB2	219908	305178	11.37%	2.260%
14	18.333	2552	2558	2566	rBV2	26286	44469	1.66%	0.329%
15	19.592	2766	2772	2779	rBV5	22586	39797	1.48%	0.295%
16	20.068	2847	2853	2858	rBV	2407726	2685092	100.00%	19.887%
17	21.615	3112	3116	3123	rBV	307994	390863	14.56%	2.895%
18	23.950	3507	3513	3520	rVB	194013	383735	14.29%	2.842%

Sum of corrected areas: 13501678

LSC Report - Integrated Chromatogram

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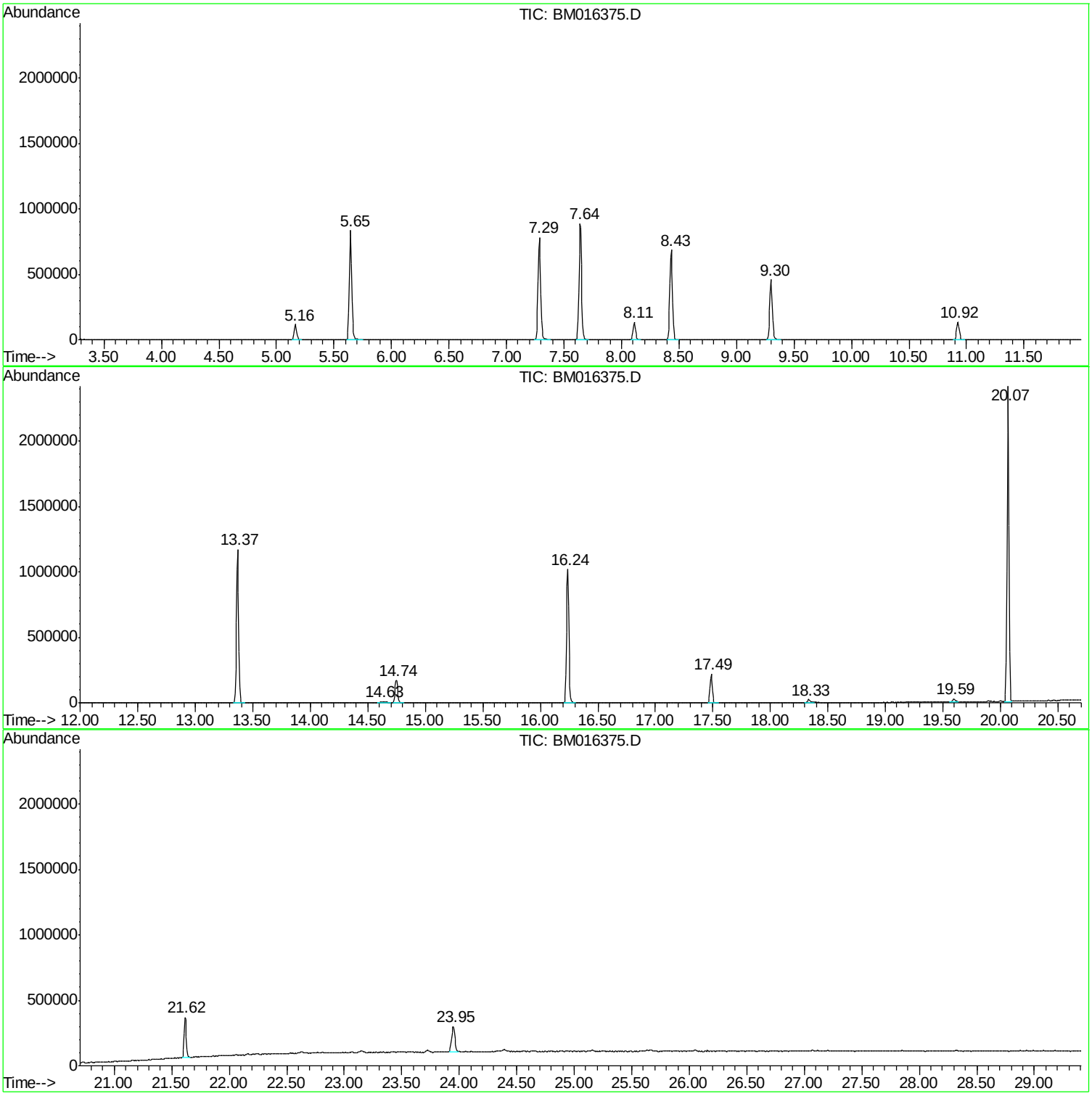
Sample : PB112017BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB112017BL

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\BM081518\
Data File : BM016375.D
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Operator : SJ/JU
Sample : PB112017BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB112017BL

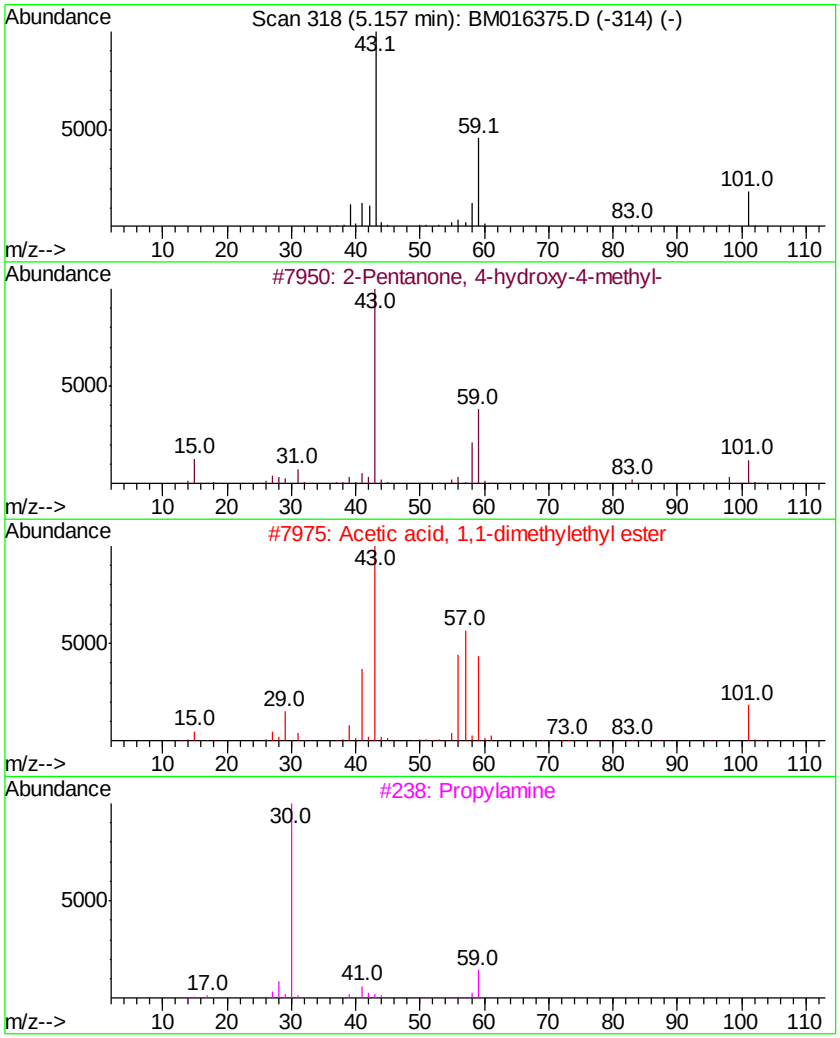
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

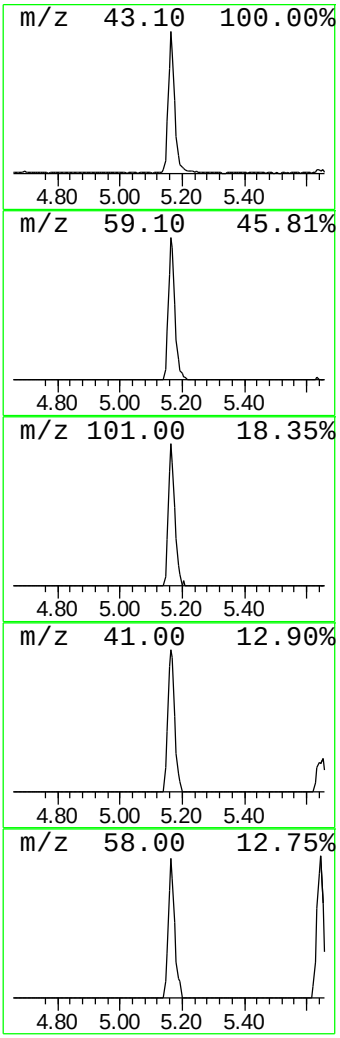
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	16.38 ng	170547	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	42
3	Propylamine	59	C3H9N	000107-10-8	42
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	Butane	58	C4H10	000106-97-8	22





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BNA_M
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

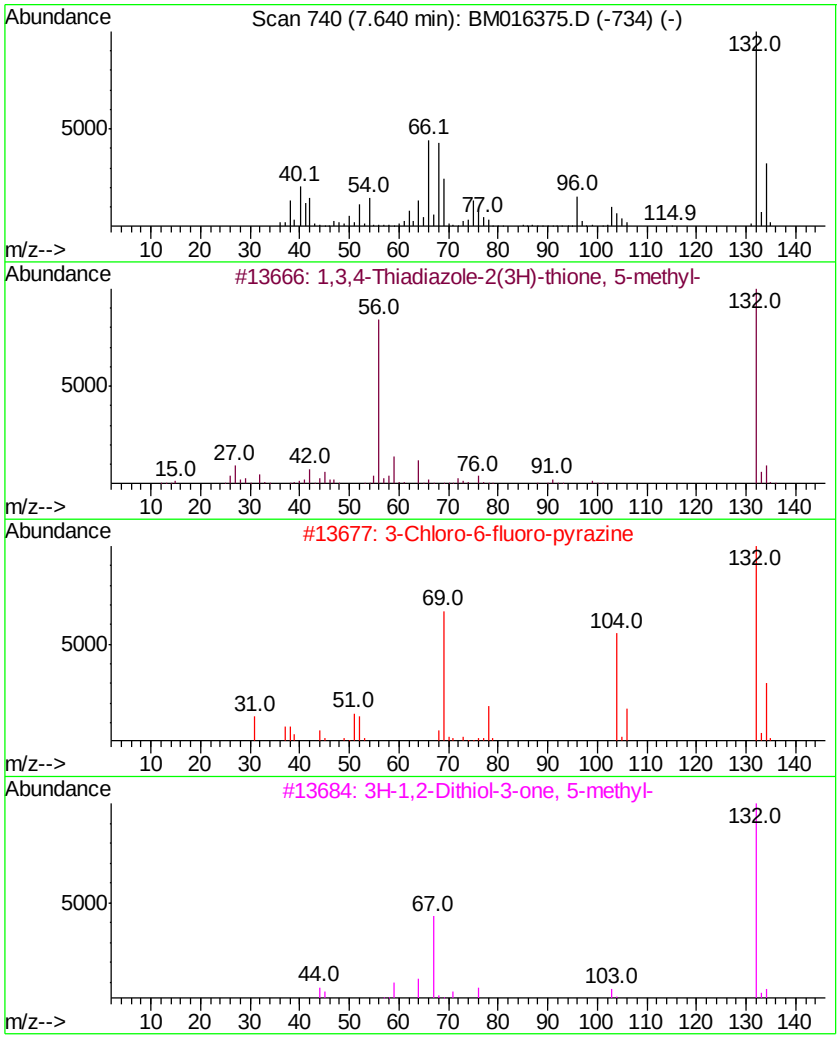
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

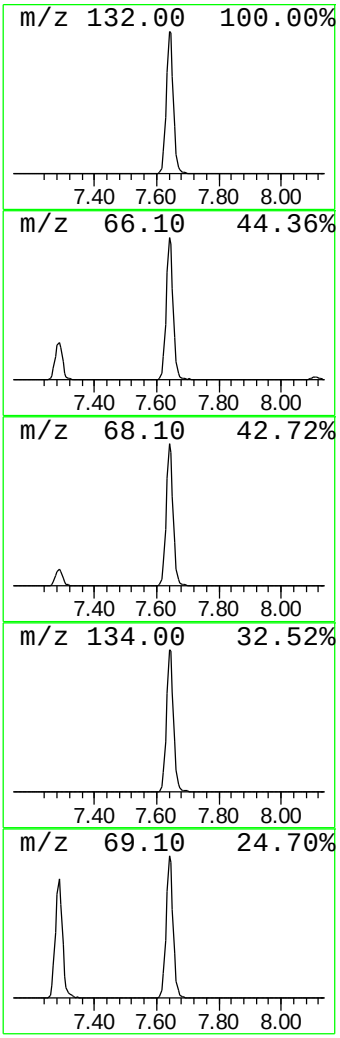
****

Peak Number 2 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	135.55 ng	1411150	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





Library Search Compound Report

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ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB112017BL

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

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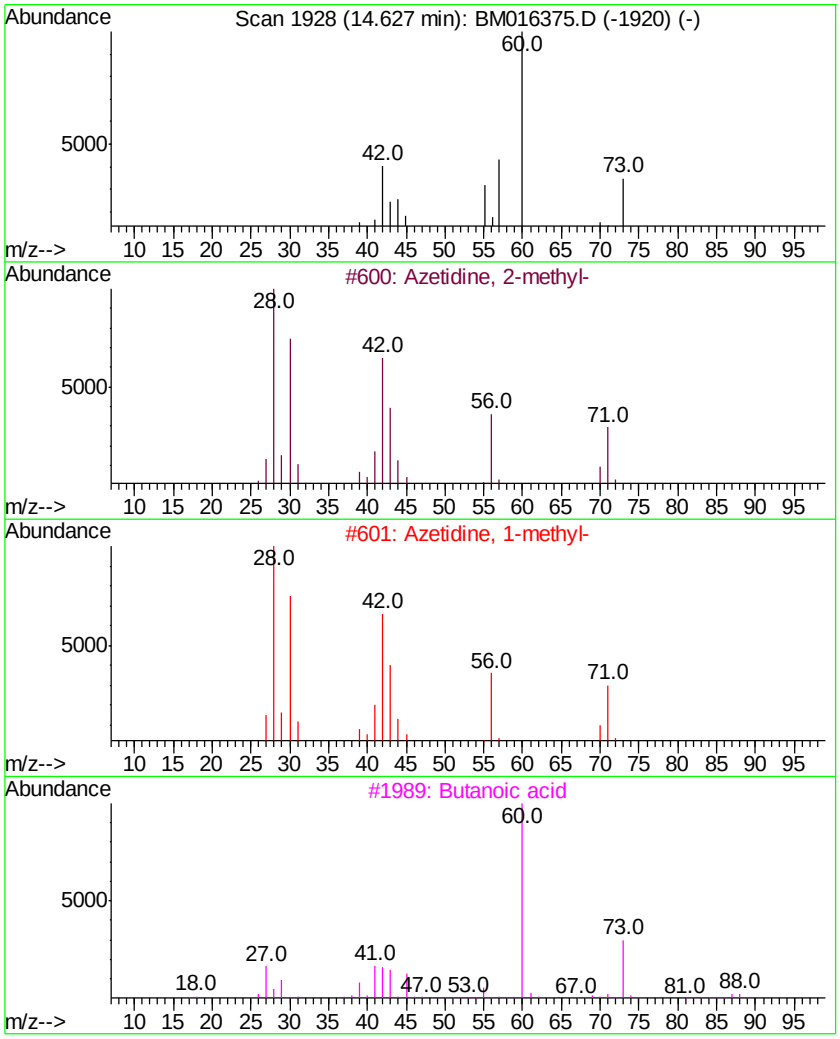
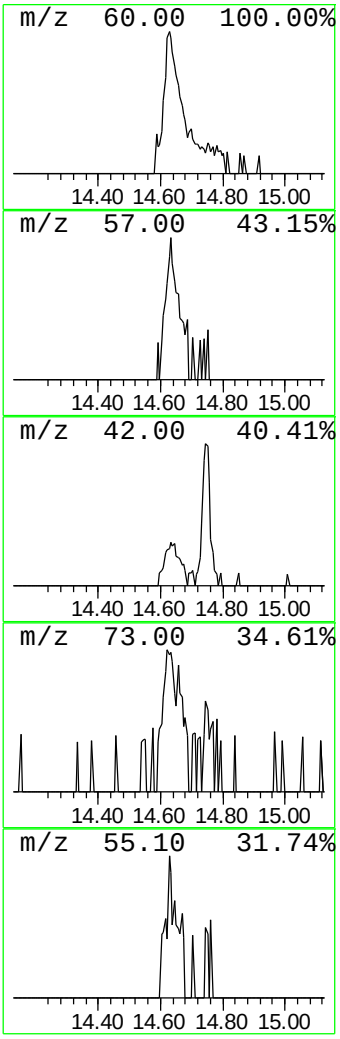
Peak Number 4 unknown14.63 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.30 ng	31057	Acenaphthene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	12
2	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	9
3	Butanoic acid	88	C4H8O2	000107-92-6	9
4	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	5
5	Formic acid hydrazide	60	CH4N2O	000624-84-0	4





Library Search Compound Report

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Instrument :
BNA_M
ClientSampleId :
PB112017BL

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

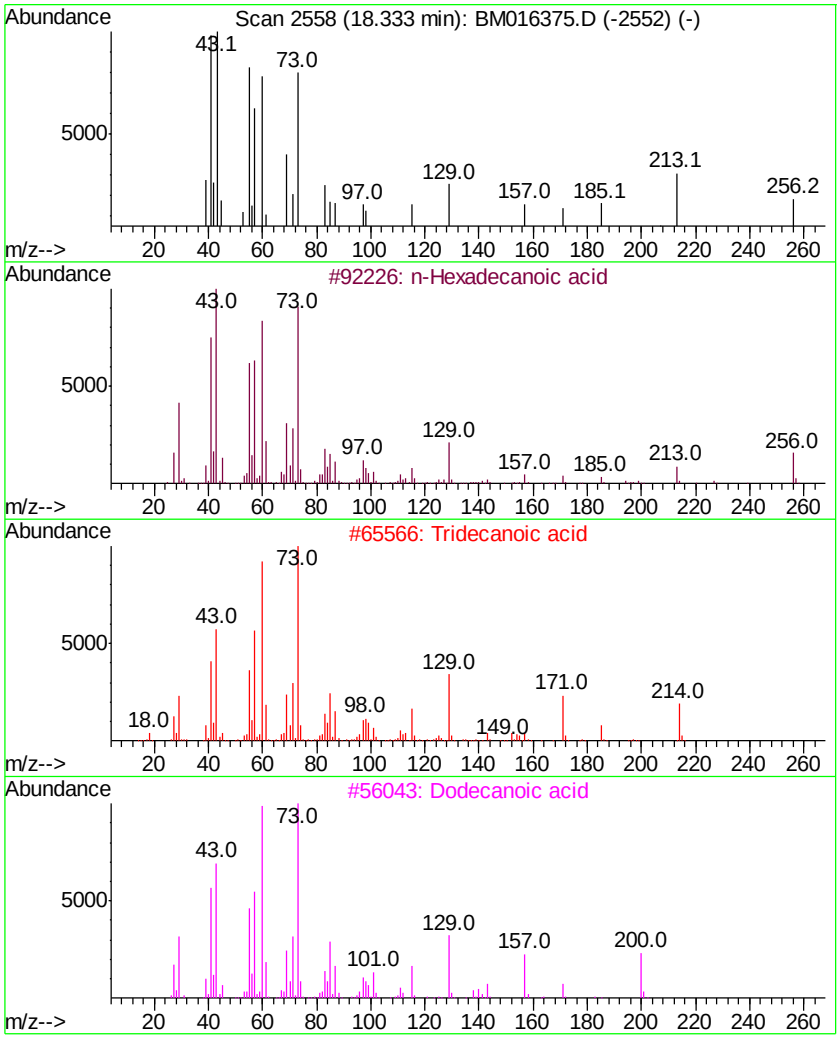
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

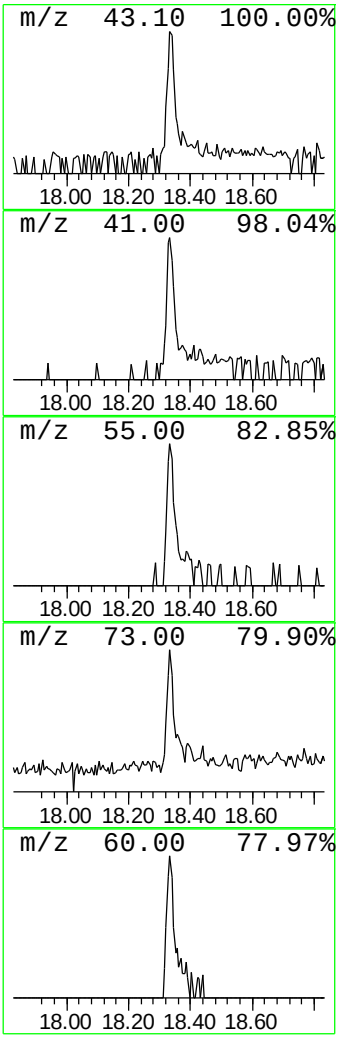
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	2.91 ng	44469	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	53
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	50





Library Search Compound Report

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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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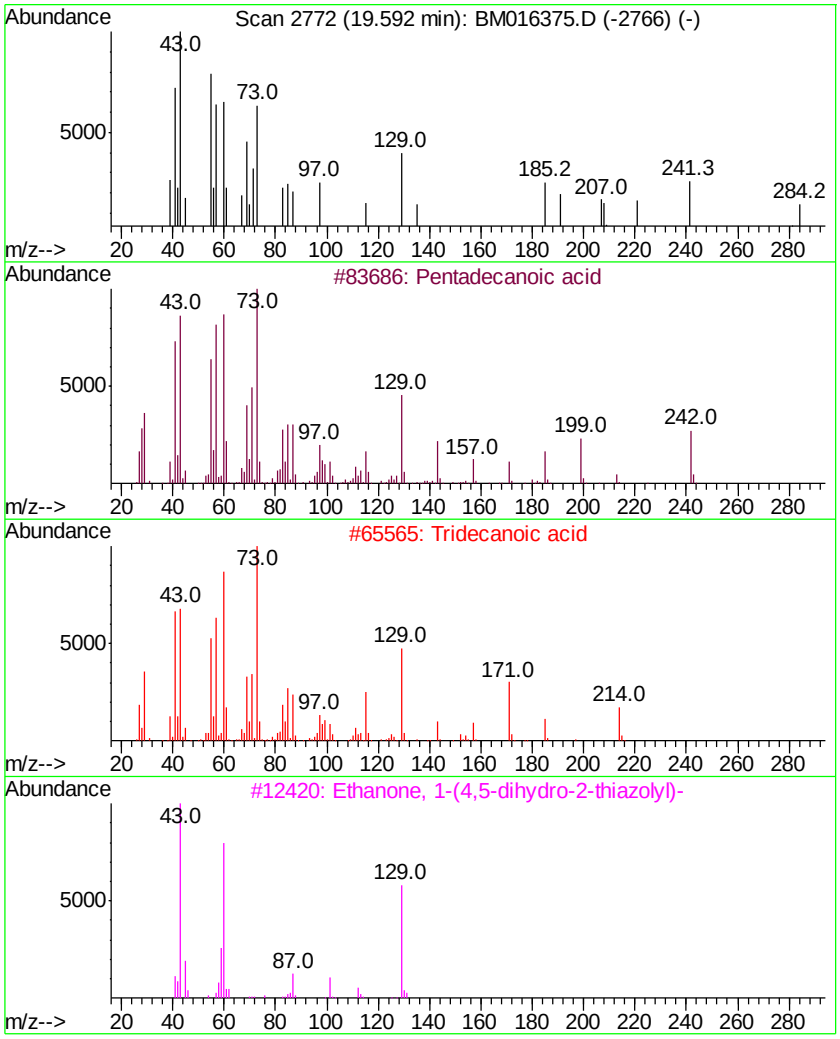
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

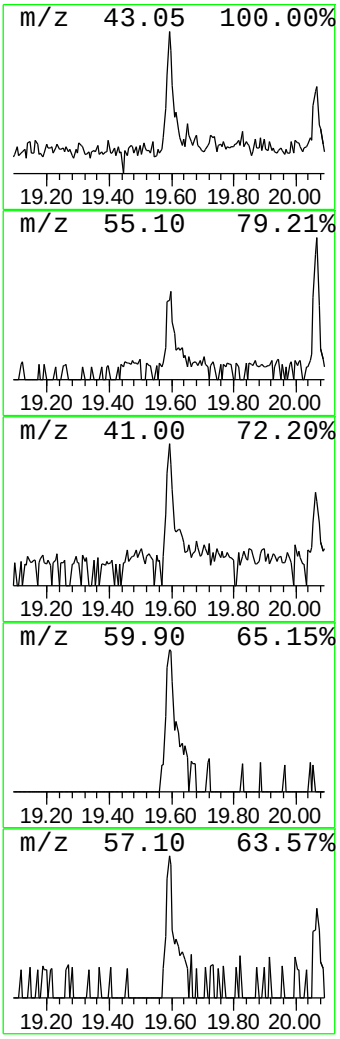
****

Peak Number 6 unknown19.59 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	2.04 ng	39797	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
2	Tridecanoic acid	214	C13H26O2	000638-53-9	35
3	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	22
4	n-Decanoic acid	172	C10H20O2	000334-48-5	16
5	Undecanoic acid	186	C11H22O2	000112-37-8	16





Tentatively Identified Compound (LSC) summary

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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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.16	16.4	ng	170547	1	8.11	208205	20.0
unknown7.64	7.64	135.6	ng	1411150	1	8.11	208205	20.0
unknown14.63	14.63	2.3	ng	31057	3	14.74	270311	20.0
n-Hexadecanoic acid	18.33	2.9	ng	44469	4	17.49	305178	20.0
unknown19.59	19.59	2.0	ng	39797	5	21.62	390863	20.0