LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
Data File : BM010880.D
Acq On : 18 Jul 2017 20:53
Operator : SJ/JU
Sample : I4224-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DEC-01

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_M\METHODS\8270-BM071217.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	3.316	69	73	85	rBV	154656	202059	1.22%	0.188%
2	4.640	293	298	306	rBV	448378	593973	3.58%	0.553%
3	5.081	364	373	384	rBV	7082043	9454359	56.91%	8.804%
4	6.640	630	638	649	rBV	6650896	10147023	61.08%	9.449%
5	6.981	687	696	709	rBV	6476459	10106626	60.84%	9.411%
6	7.440	768	774	783	rVB	1127980	1688669	10.17%	1.572%
7	7.757	819	828	837	rBV	5091787	7924639	47.70%	7.379%
8	8.587	962	969	977	rBV	4158511	6570553	39.55%	6.118%
9	8.722	982	992	1000	rVB4	88348	167071	1.01%	0.156%
10	10.198	1236	1243	1250	rBV	1317996	2173577	13.08%	2.024%
11	12.704	1661	1669	1676	rBV	10472991	14597123	87.87%	13.593%
12	13.563	1807	1815	1822	rBV	1494217	2084386	12.55%	1.941%
13	14.092	1898	1905	1914	rBV2	1827128	2742492	16.51%	2.554%
14	15.592	2153	2160	2171	rBV	8030422	10924725	65.76%	10.173%
15	16.845	2367	2373	2381	rBV2	2144487	3024296	18.21%	2.816%
16	17.768	2525	2530	2539	rBV2	452248	619675	3.73%	0.577%
17	19.068	2745	2751	2759	rBV2	271516	406375	2.45%	0.378%
18	19.504	2820	2825	2832	rVB	13462343	16611905	100.00%	15.469%
19	20.215	2940	2946	2953	rBV	1040336	1299635	7.82%	1.210%
20	20.803	3042	3046	3054	rBV6	148705	249487	1.50%	0.232%
21	21.062	3084	3090	3095	rBV	2395757	3048645	18.35%	2.839%
22	23.186	3446	3451	3459	rVB2	1537615	2751289	16.56%	2.562%

Sum of corrected areas: 107388582

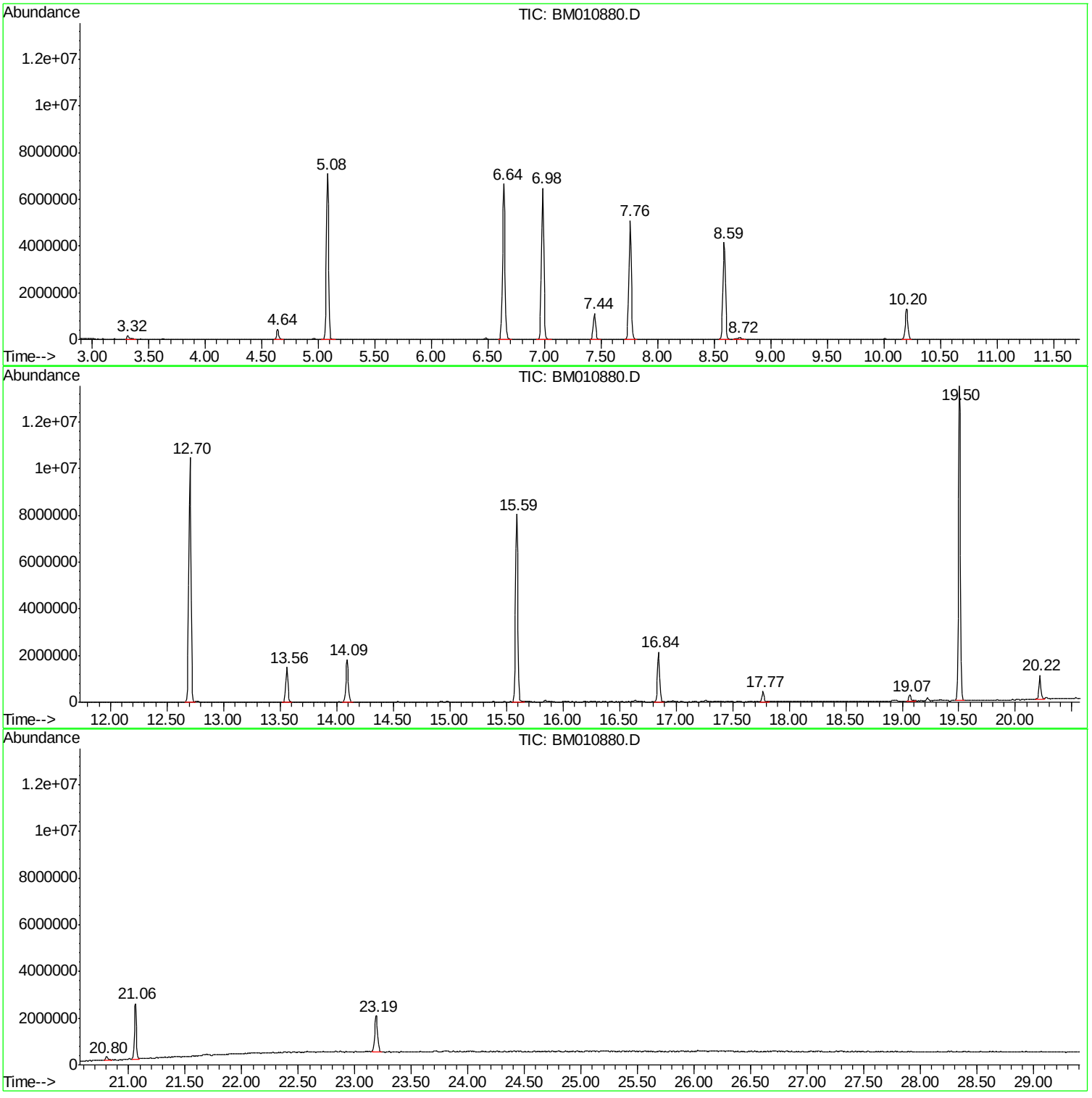
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
Data File : BM010880.D
Acq On : 18 Jul 2017 20:53
Operator : SJ/JU
Sample : I4224-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DEC-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
Data File : BM010880.D
Acq On : 18 Jul 2017 20:53
Operator : SJ/JU
Sample : I4224-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DEC-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

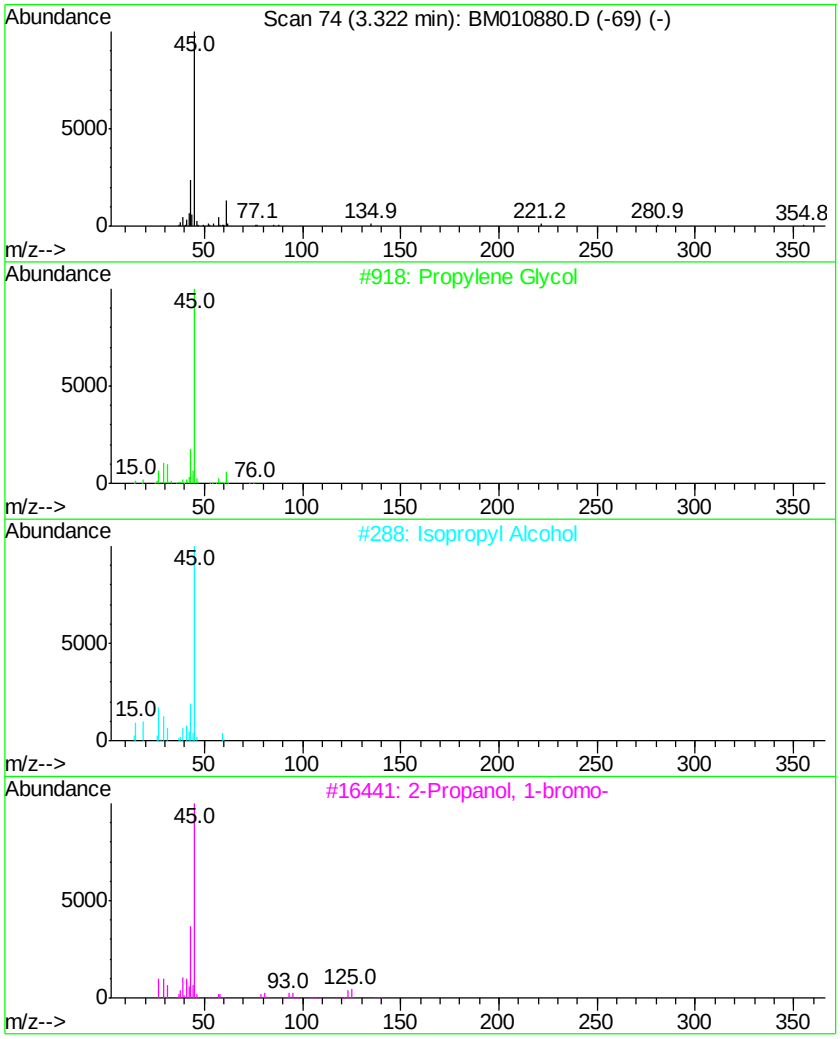
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

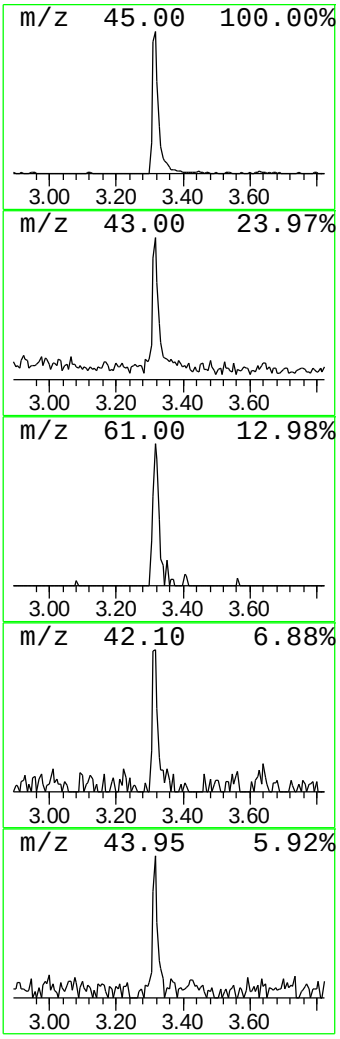
****

Peak Number 1 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.32	2.39 ng	202059	1,4-Dichlorobenzene-d4	7.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	56
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	45
3	2-Propanol, 1-bromo-	138	C3H7BrO	019686-73-8	38
4	2-Butanol, (.+/-.)-	74	C4H10O	015892-23-6	9
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	9





Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
Data File : BM010880.D
Acq On : 18 Jul 2017 20:53
Operator : SJ/JU
Sample : I4224-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DEC-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

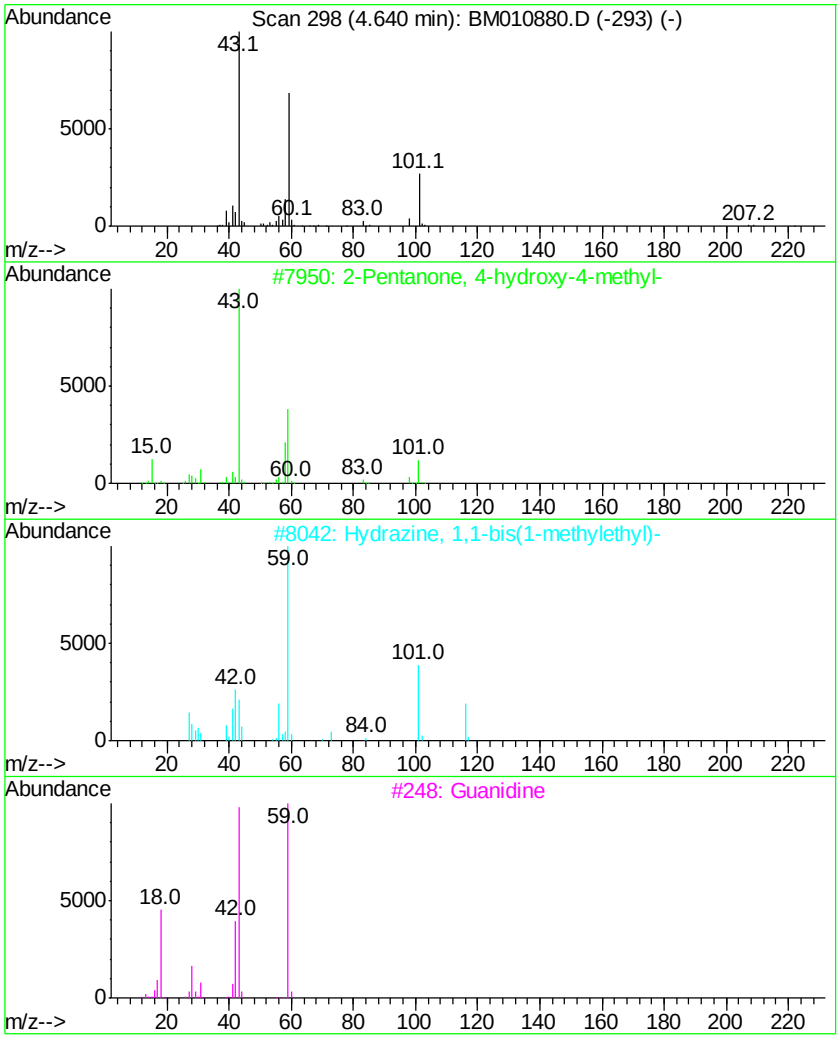
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

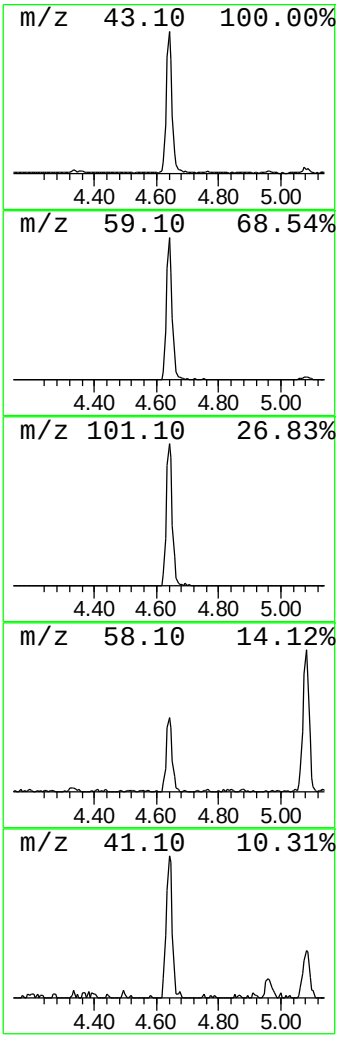
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	7.03 ng	593973	1,4-Dichlorobenzene-d4	7.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	50
3	Guanidine	59	CH5N3	000113-00-8	43
4	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	23
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17





Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
Data File : BM010880.D
Acq On : 18 Jul 2017 20:53
Operator : SJ/JU
Sample : I4224-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DEC-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

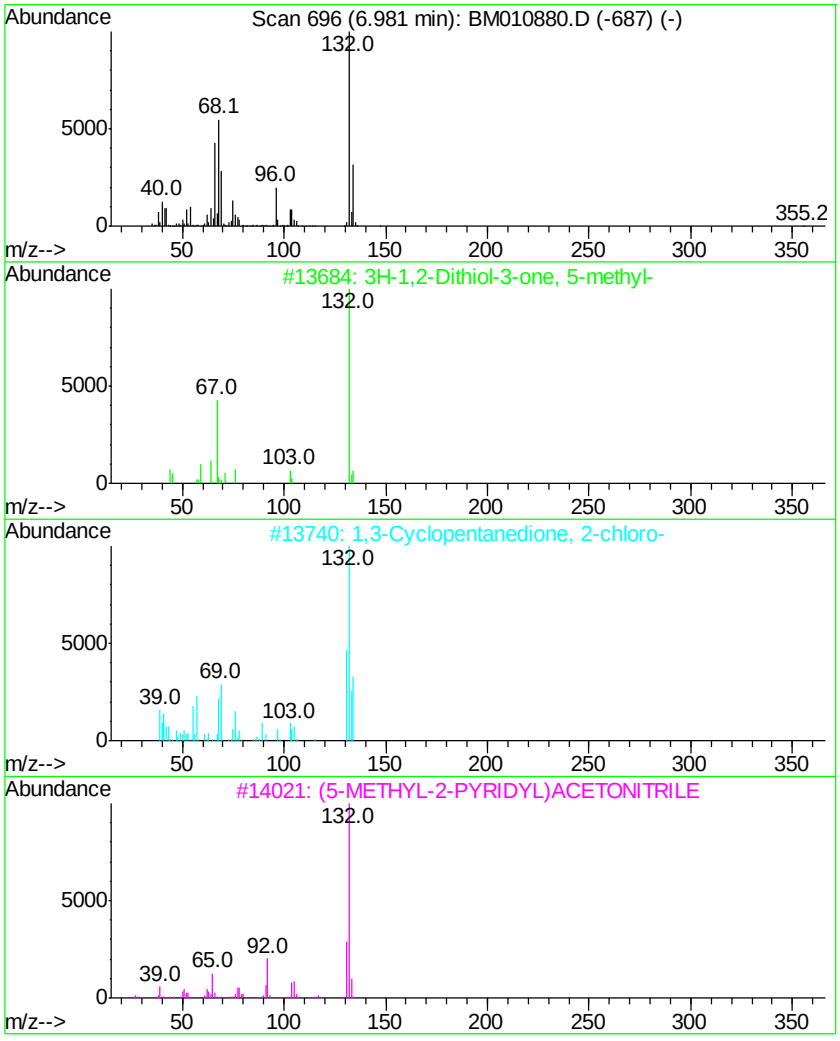
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

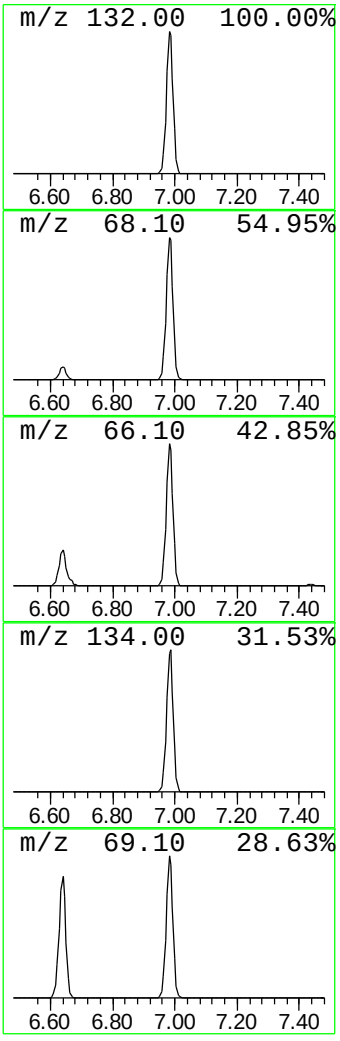
****

Peak Number 3 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	119.70 ng	10106600	1,4-Dichlorobenzene-d4	7.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10





Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
Data File : BM010880.D
Acq On : 18 Jul 2017 20:53
Operator : SJ/JU
Sample : I4224-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DEC-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

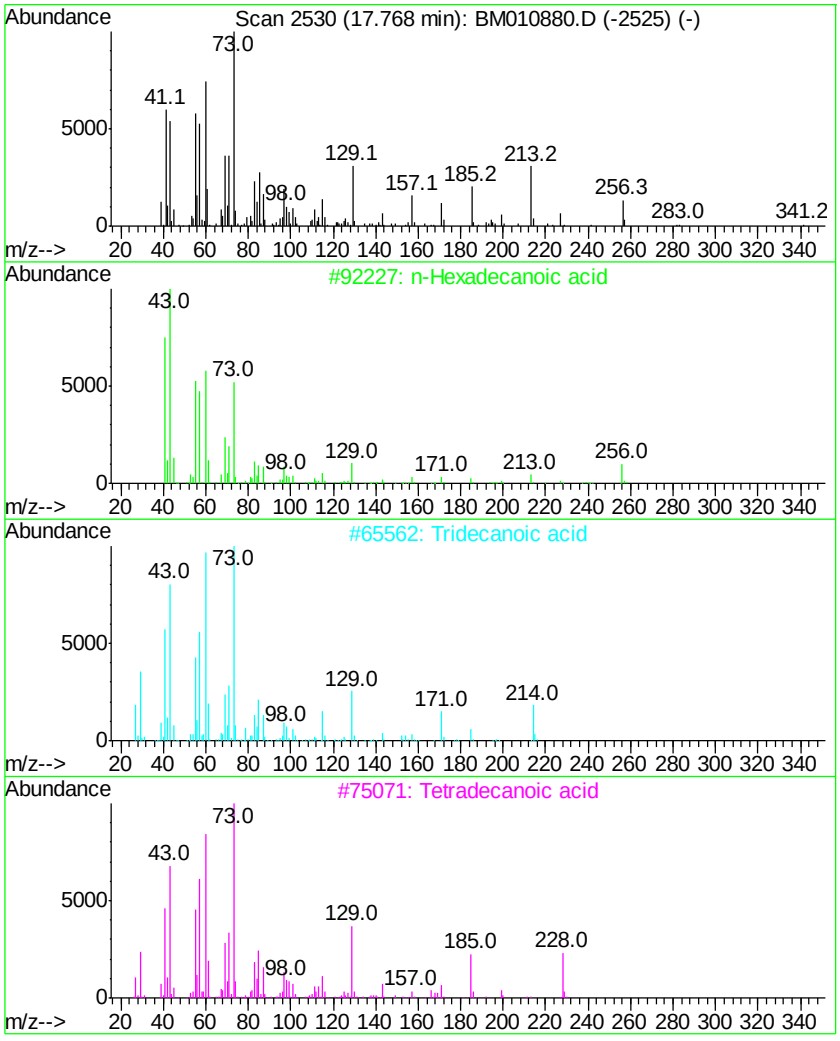
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

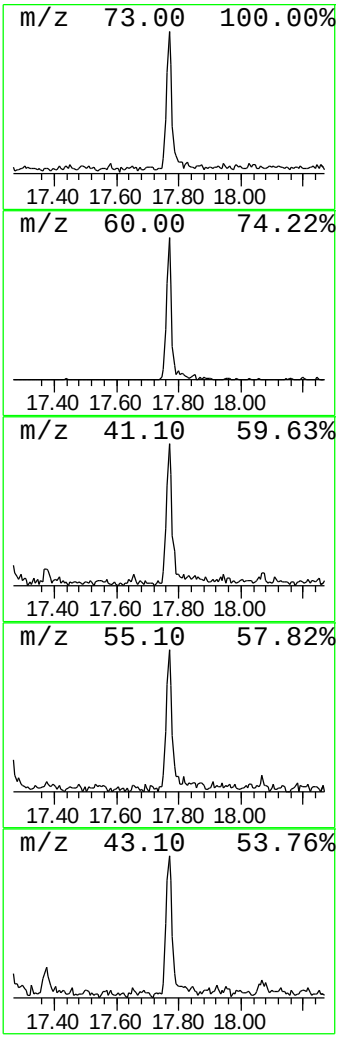
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.77	4.10 ng	619675	Phenanthrene-d10	16.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Dodecanoic acid	200	C12H24O2	000143-07-7	52
5	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
Data File : BM010880.D
Acq On : 18 Jul 2017 20:53
Operator : SJ/JU
Sample : I4224-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DEC-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

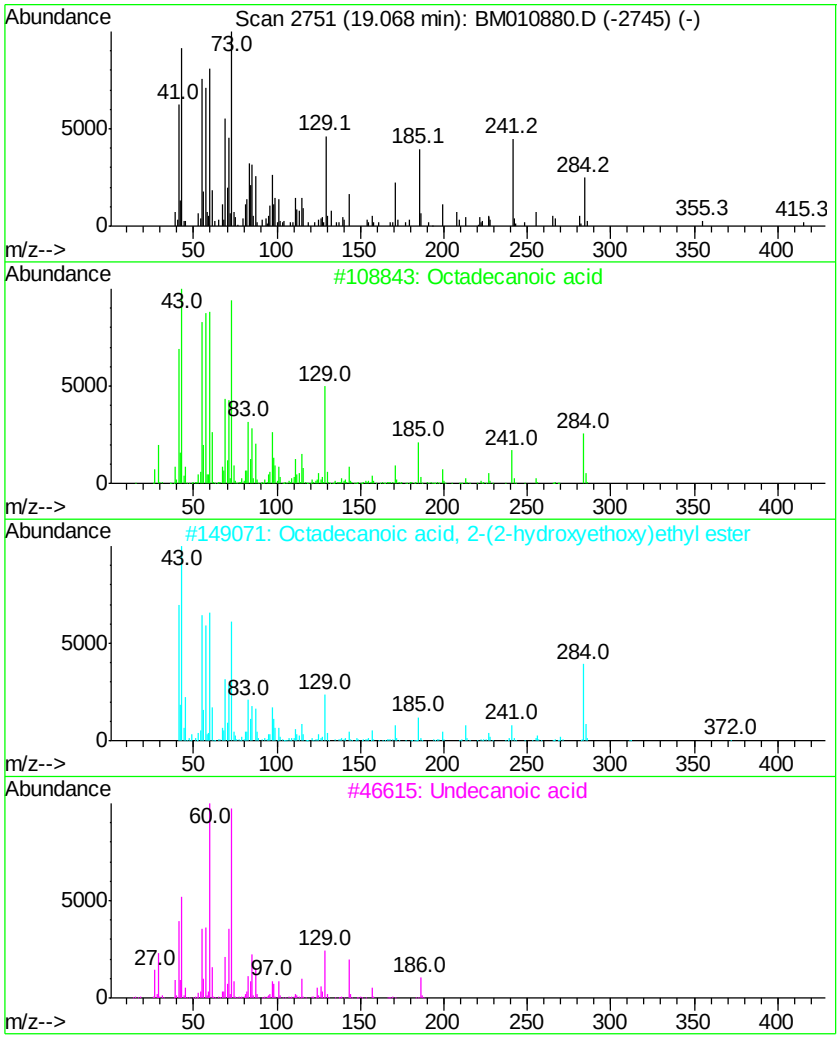
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

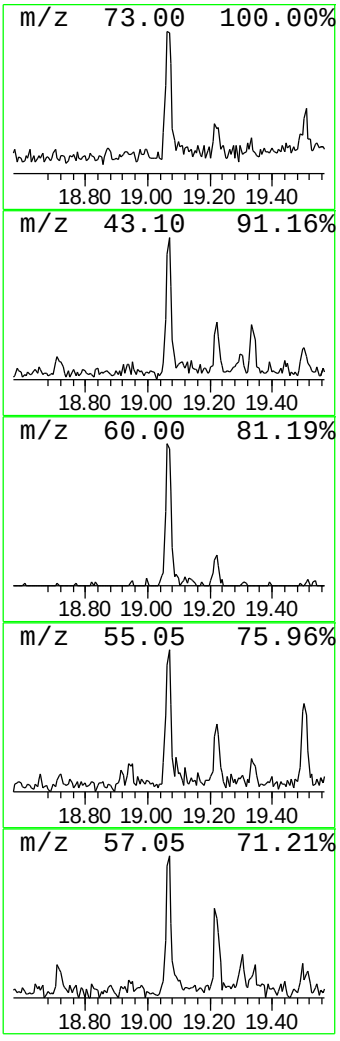
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.07	2.67 ng	406375	Chrysene-d12	21.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	55
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5	n-Decanoic acid	172	C10H20O2	000334-48-5	46





Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
Data File : BM010880.D
Acq On : 18 Jul 2017 20:53
Operator : SJ/JU
Sample : I4224-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DEC-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

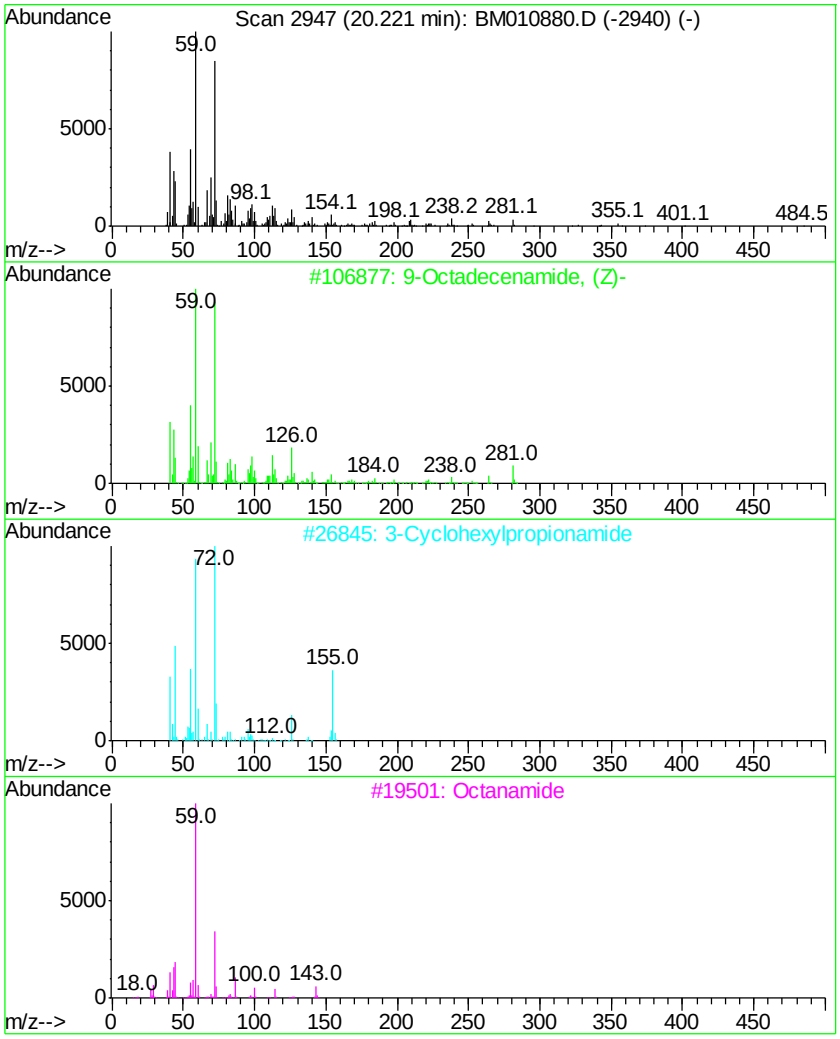
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

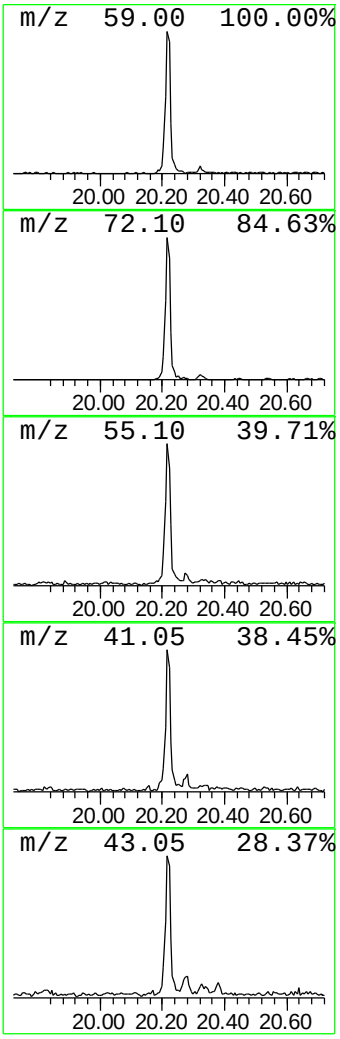
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.22	8.53 ng	1299640	Chrysene-d12	21.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	3-Cyclohexylpropionamide	155	C9H17NO	004361-29-9	50
3	Octanamide	143	C8H17NO	000629-01-6	43
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	38
5	Tetradecanamide	227	C14H29NO	000638-58-4	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM071817\
Data File : BM010880.D
Acq On : 18 Jul 2017 20:53
Operator : SJ/JU
Sample : I4224-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DEC-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM071217.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
Propylene Glycol	3.32	2.4	ng	202059	1	7.44	1688670	20.0
2-Pentanone, 4-hy...	4.64	7.0	ng	593973	1	7.44	1688670	20.0
unknown6.98	6.98	119.7	ng	10106600	1	7.44	1688670	20.0
n-Hexadecanoic acid	17.77	4.1	ng	619675	4	16.84	3024300	20.0
Octadecanoic acid	19.07	2.7	ng	406375	5	21.06	3048650	20.0
9-Octadecenamide,...	20.22	8.5	ng	1299640	5	21.06	3048650	20.0