LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088218.D
Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-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_F\METHODS\8270-BF060716.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	1.644	4	5	14	rVB	255409	432297	8.83%	1.928%
2	1.758	14	15	68	rVB	1983348	4896859	100.00%	21.842%
3	2.718	96	99	107	rBV	137877	233732	4.77%	1.043%
4	4.787	278	280	286	rBV	73942	97238	1.99%	0.434%
5	5.244	317	320	331	rVB	816467	1015145	20.73%	4.528%
6	6.307	410	413	415	rBV	469593	634177	12.95%	2.829%
7	6.422	420	423	425	rBV	1836352	1663538	33.97%	7.420%
8	6.650	441	443	446	rBV	551782	454089	9.27%	2.025%
9	6.810	454	457	459	rBV	1549848	1687690	34.46%	7.528%
10	7.062	477	479	487	rBV	29313	60771	1.24%	0.271%
11	7.222	490	493	496	rBV	1267598	1254203	25.61%	5.594%
12	7.359	503	505	514	rBV	30546	51728	1.06%	0.231%
13	7.725	533	537	543	rBV2	47383	98336	2.01%	0.439%
14	7.930	553	555	558	rBV	461070	592319	12.10%	2.642%
15	8.319	584	589	594	rBV2	69231	119645	2.44%	0.534%
16	8.467	598	602	605	rVV	21882	63292	1.29%	0.282%
17	8.890	635	639	642	rBV	33692	64130	1.31%	0.286%
18	9.016	647	650	652	rVV	2509354	2467418	50.39%	11.006%
19	9.690	706	709	711	rVB	520114	682906	13.95%	3.046%
20	10.102	741	745	750	rVB3	46566	83373	1.70%	0.372%
21	10.479	775	778	780	rBV	1269272	1463275	29.88%	6.527%
22	11.165	836	838	841	rBV	800364	693000	14.15%	3.091%
23	11.736	886	888	890	rVB	141573	116010	2.37%	0.517%
24	12.754	974	977	979	rBV	2102870	2364090	48.28%	10.545%
25	13.794	1065	1068	1072	rBV	689859	692283	14.14%	3.088%
26	15.165	1186	1188	1194	rBV	349090	438270	8.95%	1.955%

Sum of corrected areas: 22419814

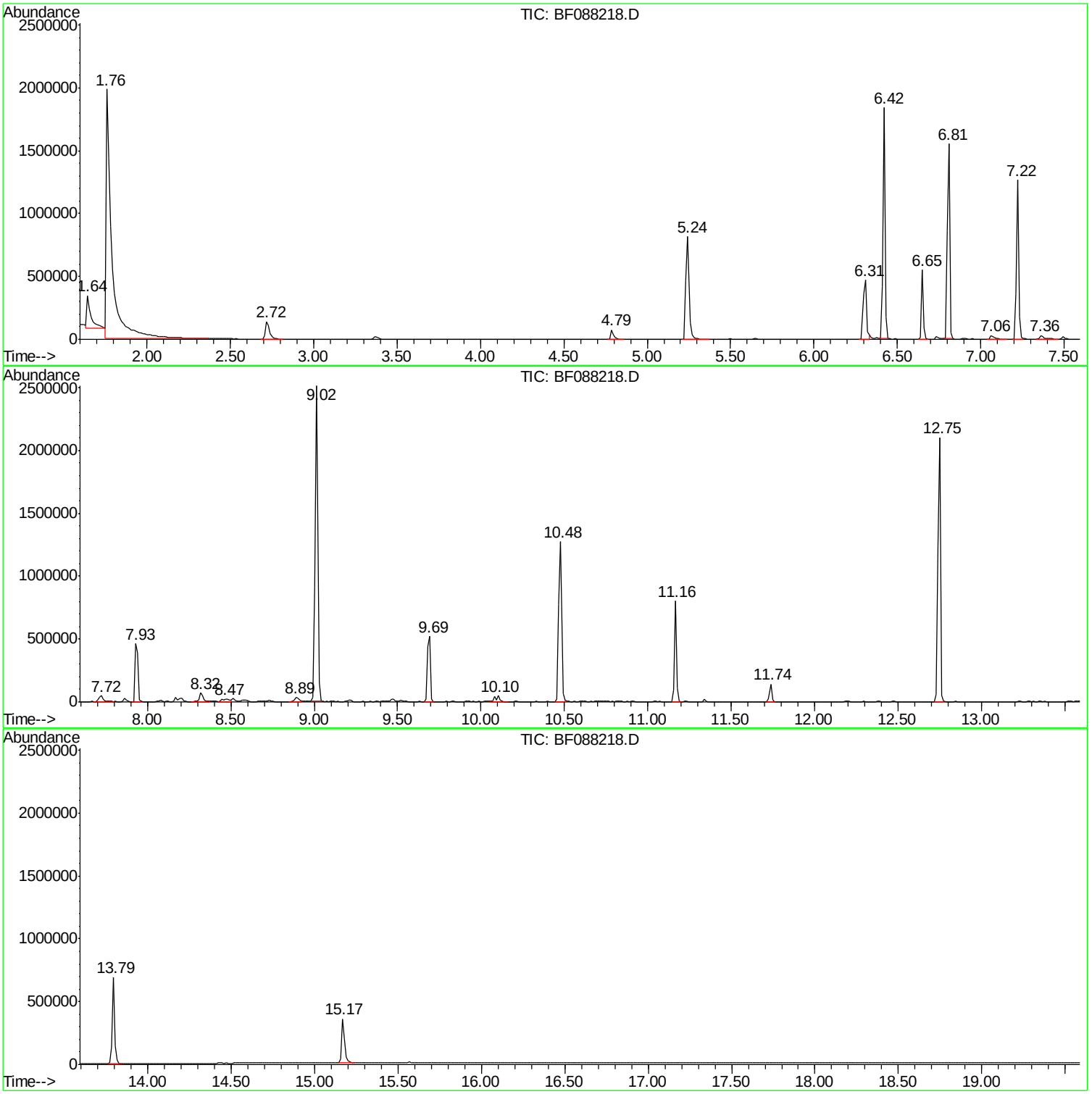
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088218.D
Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088218.D
Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

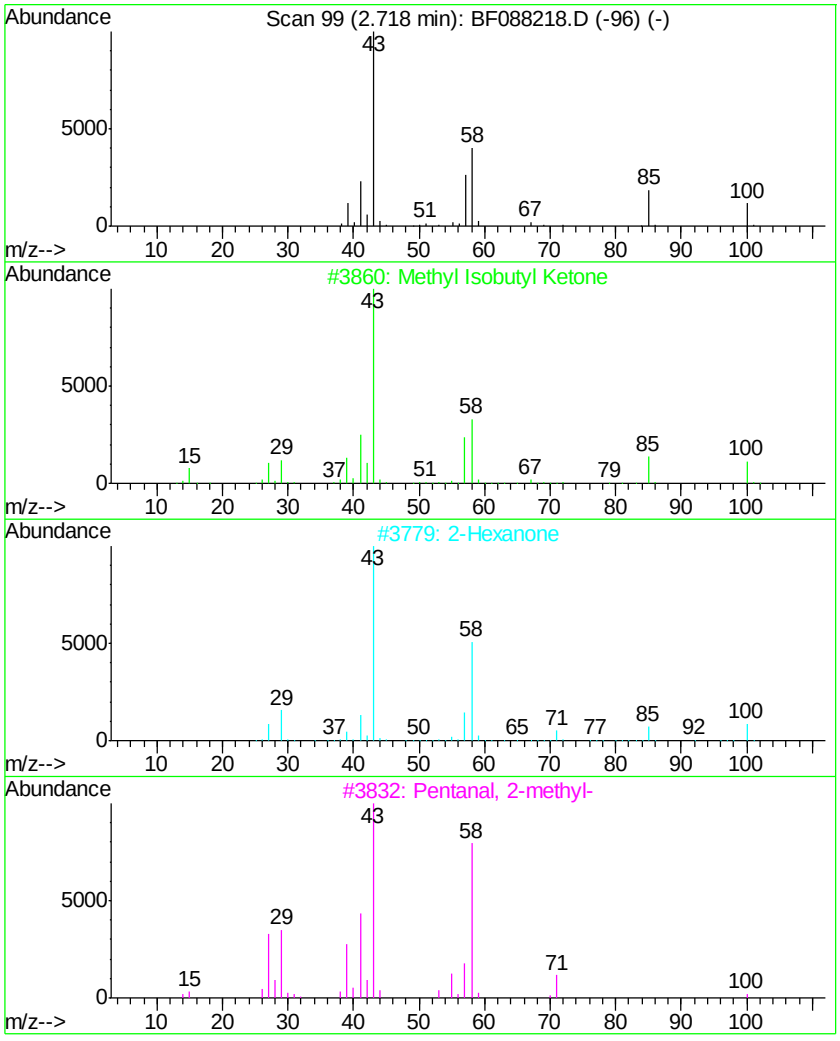
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

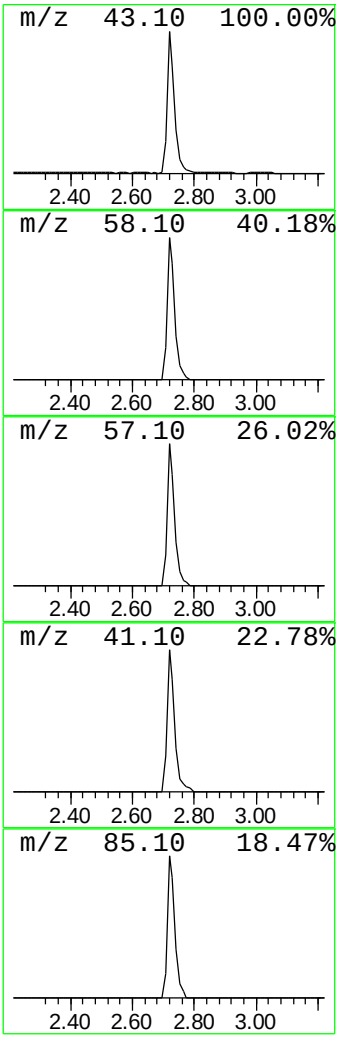
****

Peak Number 3 Methyl Isobutyl Ketone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.72	10.29 ng	233732	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	80
2	2-Hexanone	100	C6H12O	000591-78-6	78
3	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	36
4	2-Heptanone, 7,7,7-trichloro-	216	C7H11Cl3O	154264-40-1	33
5	Acetylacetone	100	C5H8O2	000123-54-6	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088218.D
Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

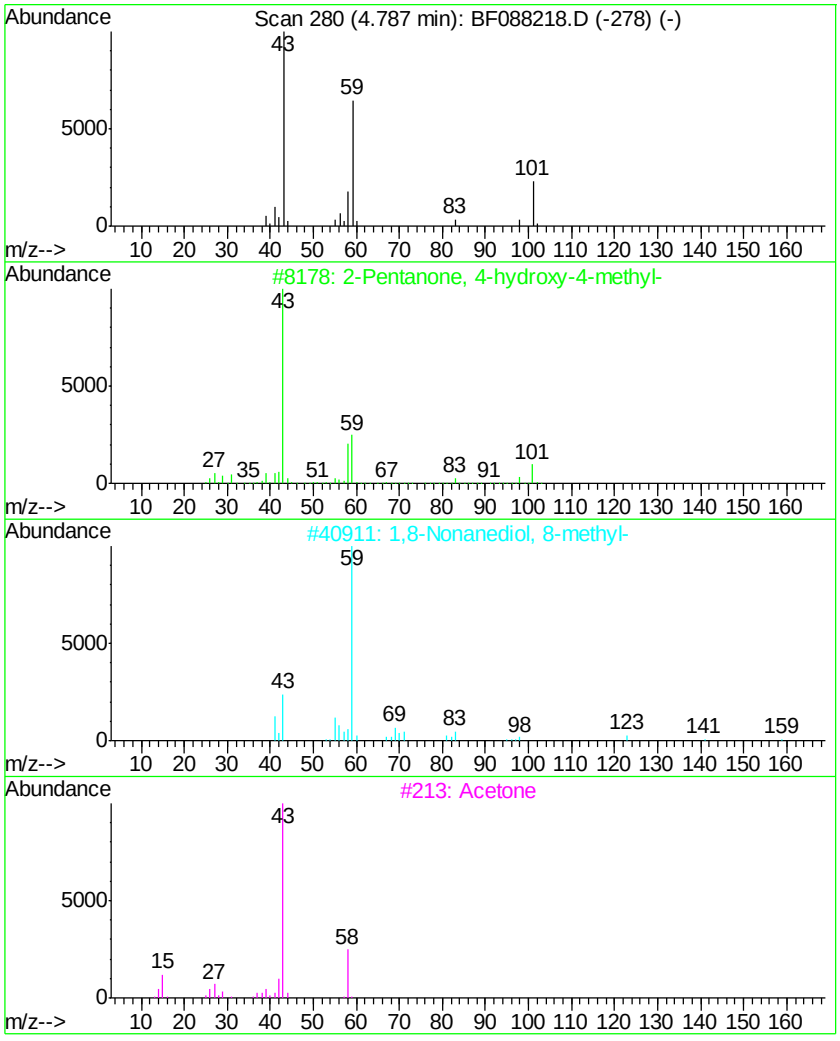
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

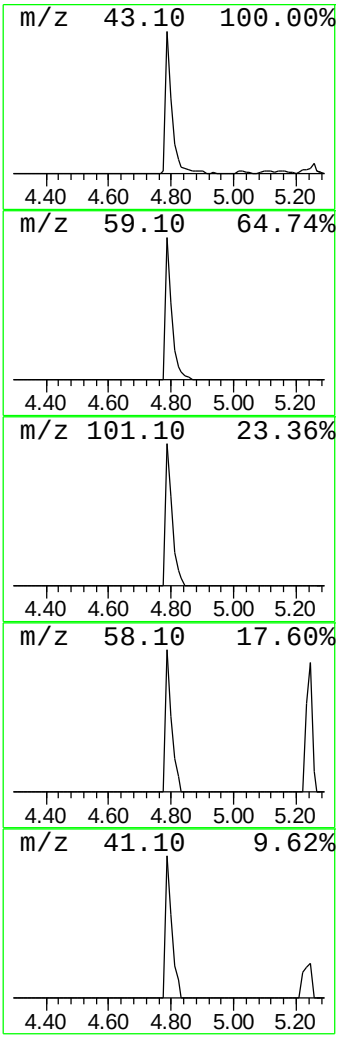
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	4.28 ng	97238	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
3	Acetone	58	C3H6O	000067-64-1	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088218.D
Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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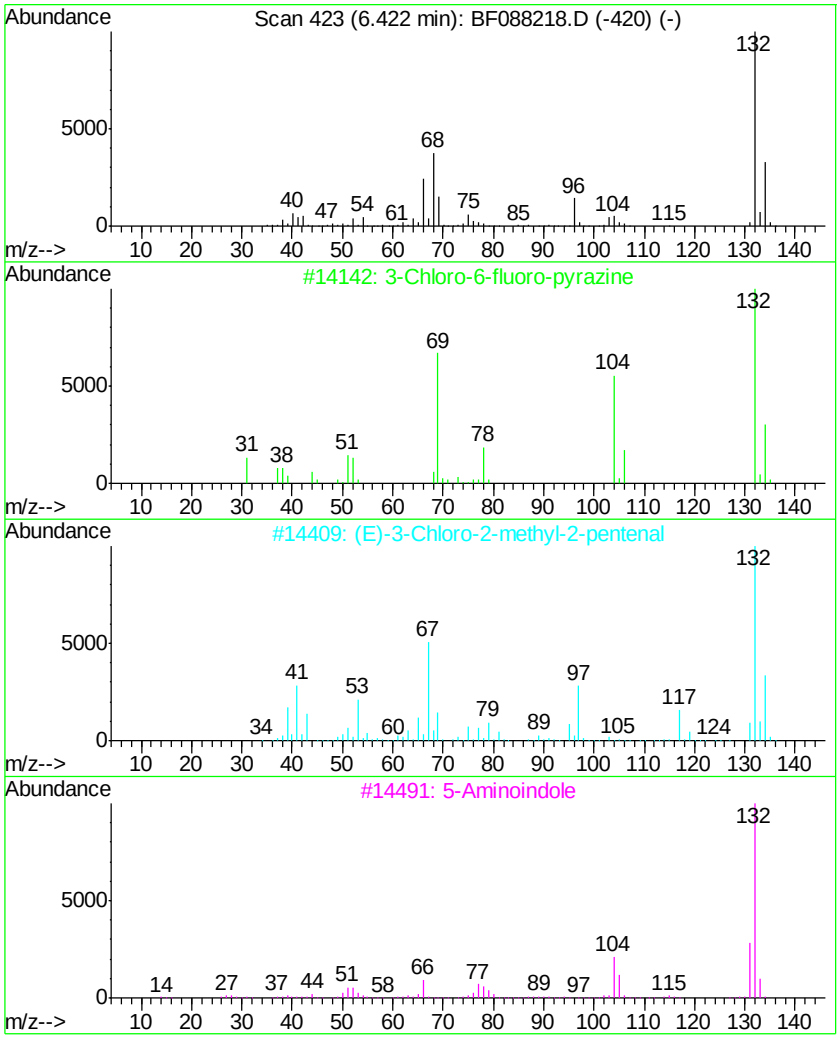
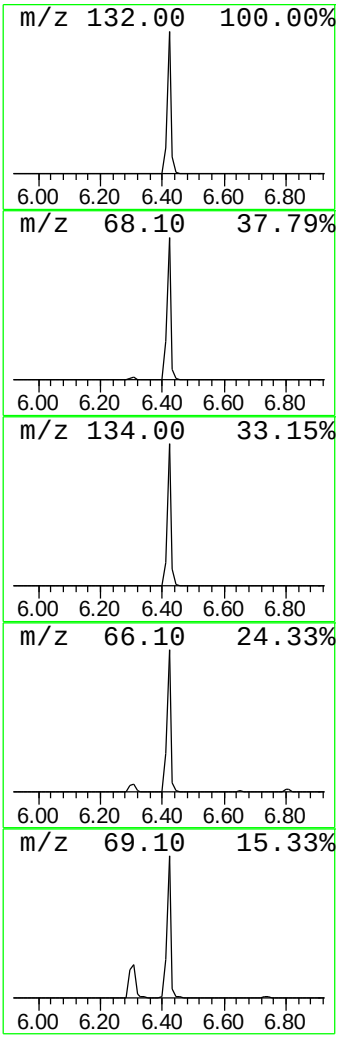
Peak Number 5 unknown6.42 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	73.27 ng	1663540	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
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Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

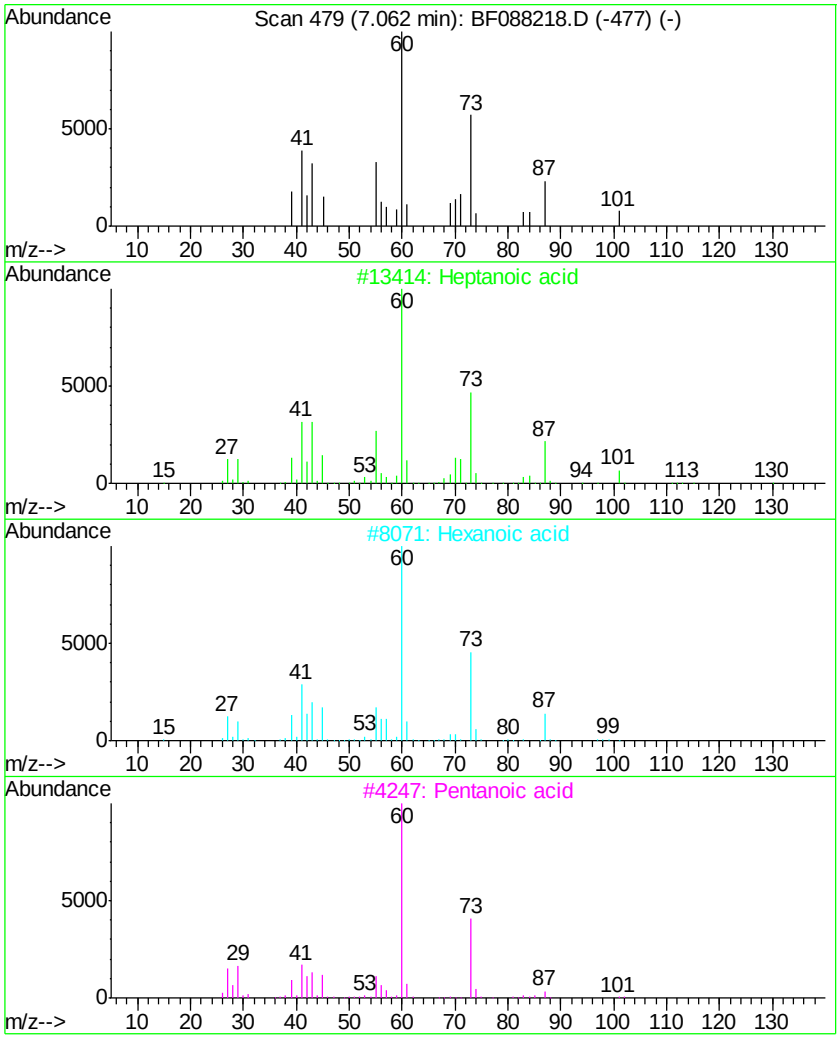
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

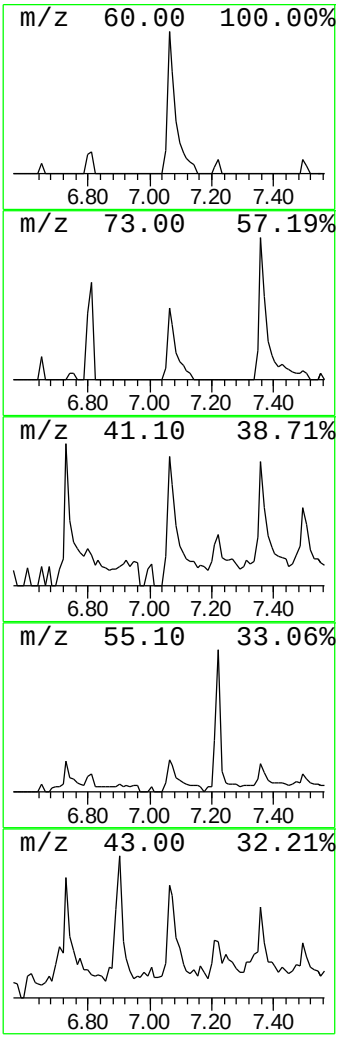
****

Peak Number 7 Heptanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	2.68 ng	60771	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	86
2	Hexanoic acid	116	C6H12O2	000142-62-1	53
3	Pentanoic acid	102	C5H10O2	000109-52-4	50
4	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	39
5	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088218.D
Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

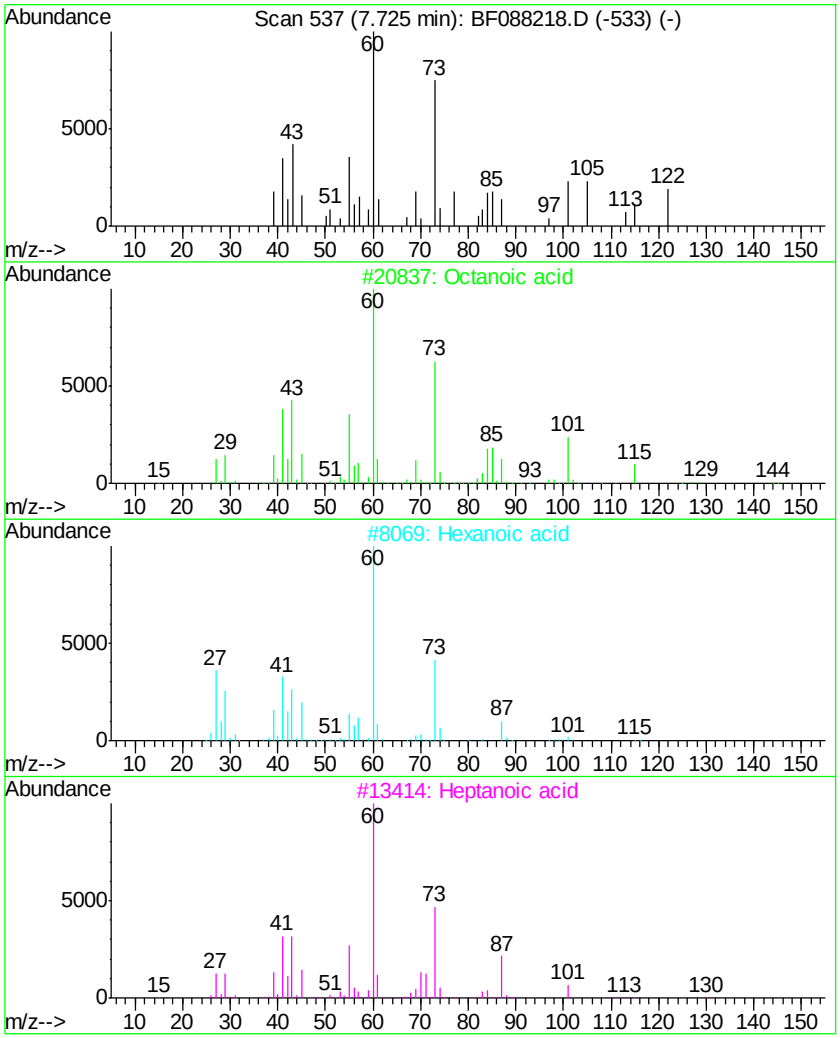
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

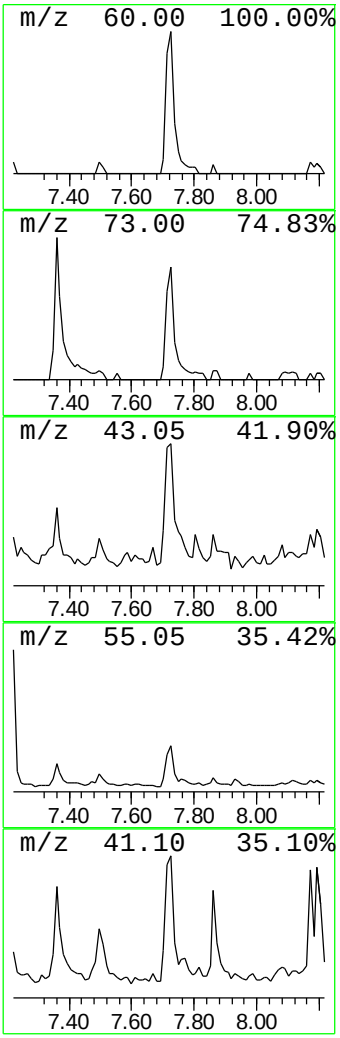
****

Peak Number 8 Octanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	3.32 ng	98336	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	72
2	Hexanoic acid	116	C6H12O2	000142-62-1	43
3	Heptanoic acid	130	C7H14O2	000111-14-8	38
4	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	38
5	Pentanoic acid	102	C5H10O2	000109-52-4	38





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Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

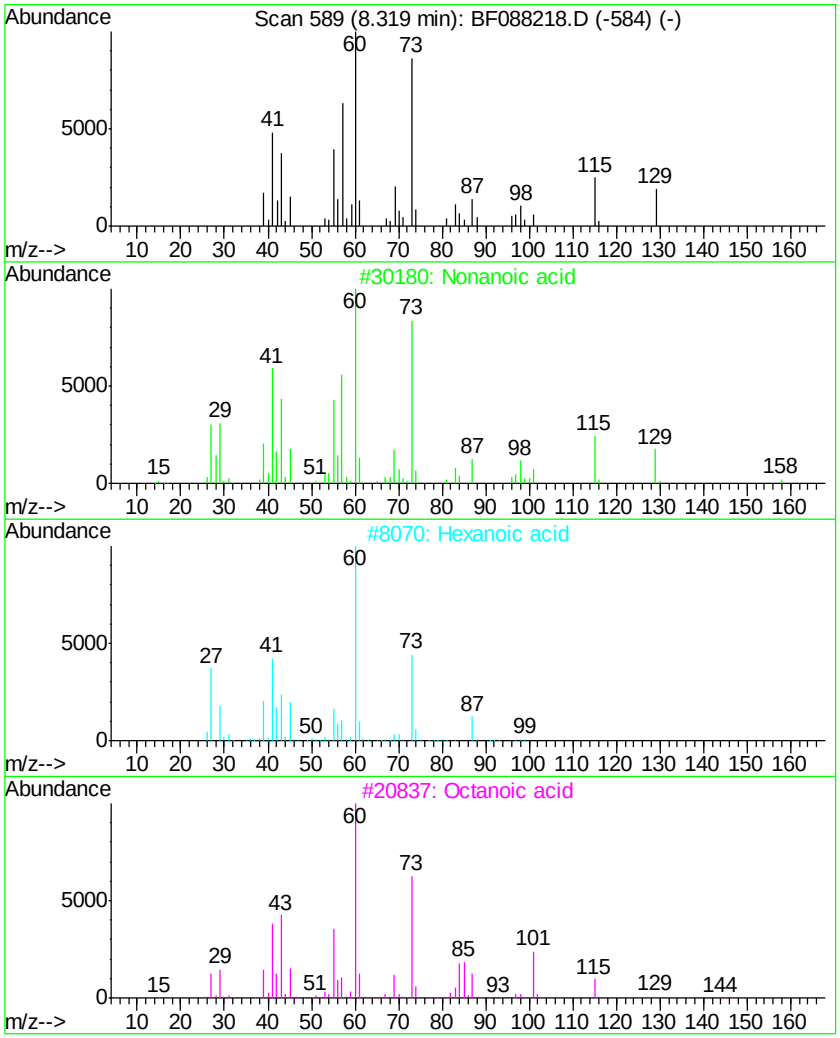
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

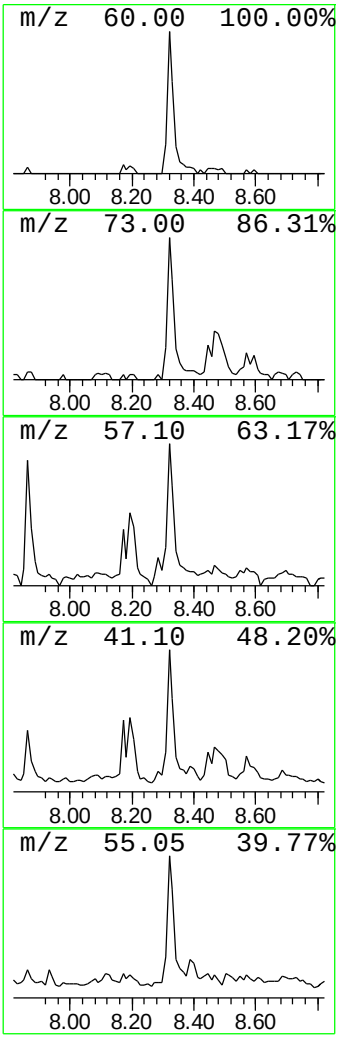
****

Peak Number 9 Nonanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.32	4.04 ng	119645	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	91
2	Hexanoic acid	116	C6H12O2	000142-62-1	50
3	Octanoic acid	144	C8H16O2	000124-07-2	42
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	40
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	37





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : EB-GW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

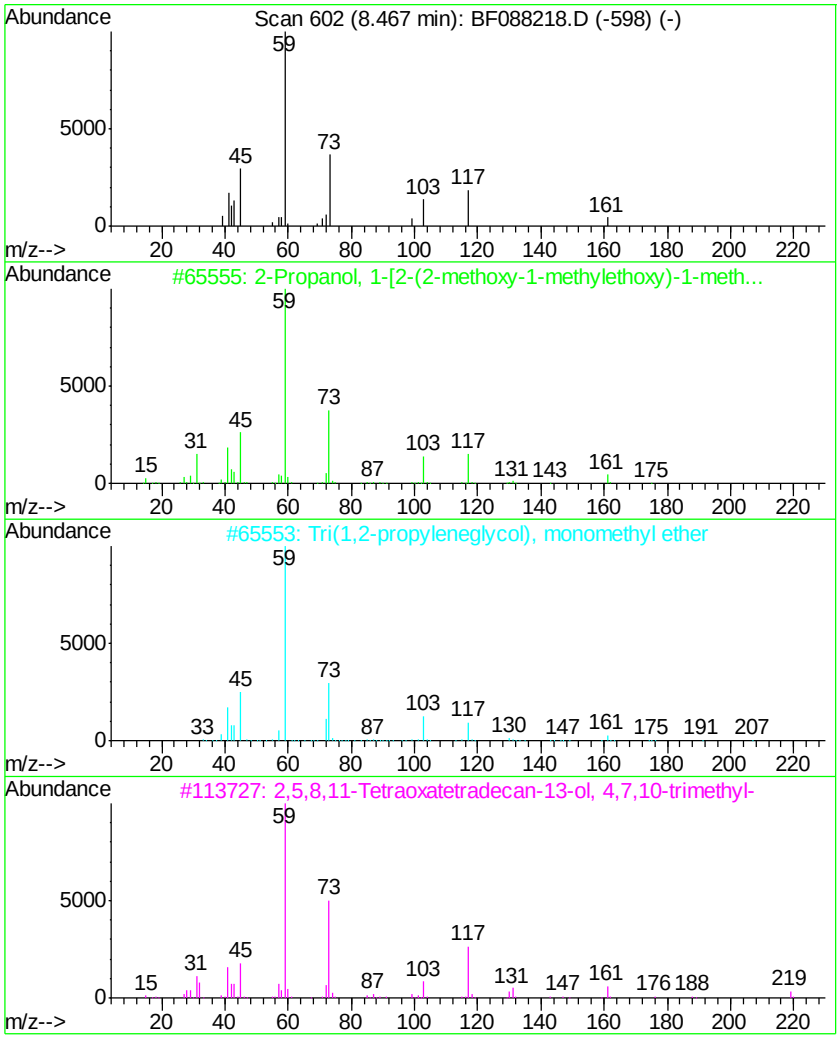
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

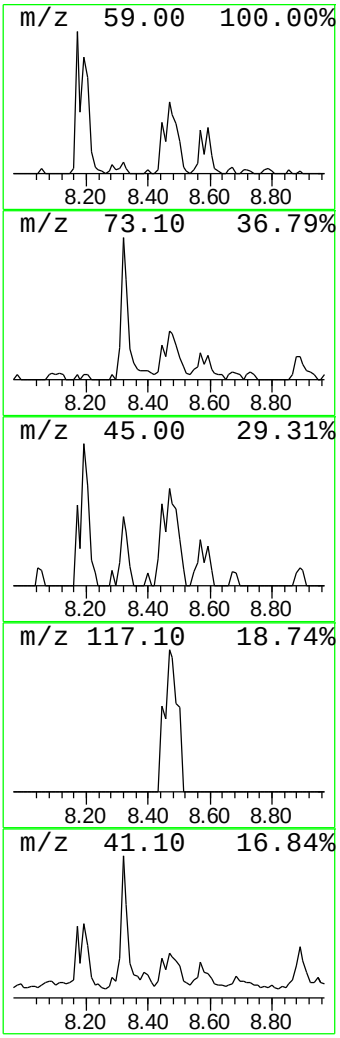
****

Peak Number 10 2-Propanol, 1-[2-(2-methoxy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	2.14 ng	63292	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	83
2	Tri(1,2-propyleneglycol), monome...	206	C10H22O4	1000262-26-6	56
3	2,5,8,11-Tetraoxatetradecan-13-o...	264	C13H28O5	020324-34-9	50
4	N,N-Dimethylformamide-di-t-butyl...	203	C11H25NO2	036805-97-7	36
5	1-Propanol, 2-(2-methoxypropoxy)-	148	C7H16O3	013588-28-8	36





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088218.D
Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

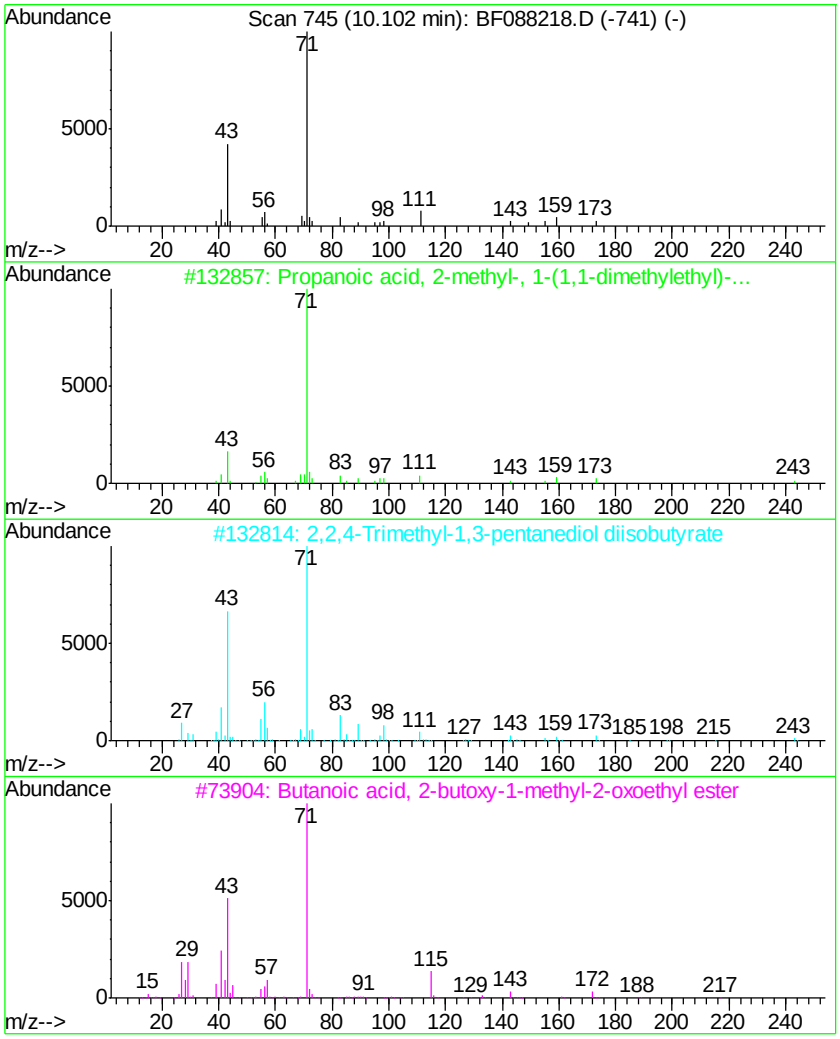
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

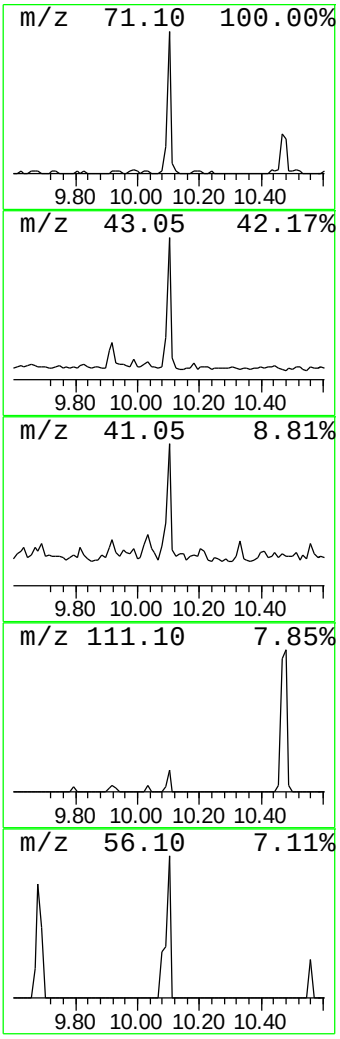
****

Peak Number 11 Propanoic acid, 2-methyl-, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	2.44 ng	83373	Acenaphthene-d10	9.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	83
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
3	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	64
4	diethyl 2-hydroxy-3-(tetrahydrof...	260	C12H20O6	1000365-67-1	50
5	Oxalic acid, neopentyl nonyl ester	286	C16H30O4	1000309-73-3	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062116\
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Acq On : 21 Jun 2016 17:49
Operator : UM/SJ
Sample : H3697-01
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
Methyl Isobutyl K...	2.72	10.3	ng	233732	1	6.65	454089	20.0
2-Pentanone, 4-hy...	4.79	4.3	ng	97238	1	6.65	454089	20.0
unknown6.42	6.42	73.3	ng	1663540	1	6.65	454089	20.0
Heptanoic acid	7.06	2.7	ng	60771	1	6.65	454089	20.0
Octanoic acid	7.72	3.3	ng	98336	2	7.93	592319	20.0
Nonanoic acid	8.32	4.0	ng	119645	2	7.93	592319	20.0
2-Propanol, 1-[2-...	8.47	2.1	ng	63292	2	7.93	592319	20.0
Propanoic acid, 2...	10.10	2.4	ng	83373	3	9.69	682906	20.0