LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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	175773	306814	8.31%	1.477%
2	1.758	14	15	70	rVB	1595423	3691387	100.00%	17.776%
3	2.730	97	100	107	rVB	172594	294050	7.97%	1.416%
4	3.370	153	156	164	rVB	28381	58244	1.58%	0.280%
5	4.787	277	280	286	rBV	79683	104543	2.83%	0.503%
6	5.244	318	320	329	rVB	591123	800331	21.68%	3.854%
7	6.307	411	413	418	rBV	328561	528976	14.33%	2.547%
8	6.422	420	423	425	rBV	1615422	1489298	40.35%	7.172%
9	6.650	441	443	446	rBV	515809	432727	11.72%	2.084%
10	6.730	448	450	454	rVV	36623	42134	1.14%	0.203%
11	6.810	454	457	459	rVV	1371061	1570946	42.56%	7.565%
12	7.062	476	479	485	rBV	33092	75609	2.05%	0.364%
13	7.222	490	493	495	rBV	1270182	1247082	33.78%	6.005%
14	7.359	503	505	510	rBV	34824	58989	1.60%	0.284%
15	7.725	533	537	543	rBV2	62275	122161	3.31%	0.588%
16	7.930	554	555	558	rVB	447458	568197	15.39%	2.736%
17	8.170	574	576	577	rBV	46430	43440	1.18%	0.209%
18	8.193	577	578	583	rVB	49431	63771	1.73%	0.307%
19	8.330	584	590	594	rBV	94745	172045	4.66%	0.828%
20	8.468	598	602	605	rBV	25885	73223	1.98%	0.353%
21	8.570	608	611	617	rVB3	19372	44528	1.21%	0.214%
22	8.719	623	624	633	rVB3	26216	43714	1.18%	0.211%
23	8.890	635	639	642	rBV	53594	89385	2.42%	0.430%
24	9.016	647	650	652	rVB	2415206	2416815	65.47%	11.638%
25	9.416	683	685	687	rBV	43465	37995	1.03%	0.183%
26	9.462	687	689	692	rVV	33738	48406	1.31%	0.233%
27	9.519	692	694	702	rVB4	14053	37336	1.01%	0.180%
28	9.679	706	708	711	rVB	482092	660569	17.89%	3.181%
29	10.079	741	743	744	rBV	52719	48607	1.32%	0.234%
30	10.102	744	745	749	rVB2	52559	62183	1.68%	0.299%
31	10.479	775	778	780	rBV	1100705	1287503	34.88%	6.200%
32	11.165	836	838	840	rBV	791079	682194	18.48%	3.285%
33	11.736	886	888	890	rVB	166439	137001	3.71%	0.660%
34	12.754	974	977	979	rBV	1899468	2263924	61.33%	10.902%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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

35	13.668	1053	1057	1061	rBV2	20719	44299	1.20%	0.213%
36	13.794	1065	1068	1072	rVB	669902	688513	18.65%	3.316%
37	15.165	1185	1188	1193	rBV	345463	428968	11.62%	2.066%

Sum of corrected areas: 20765907

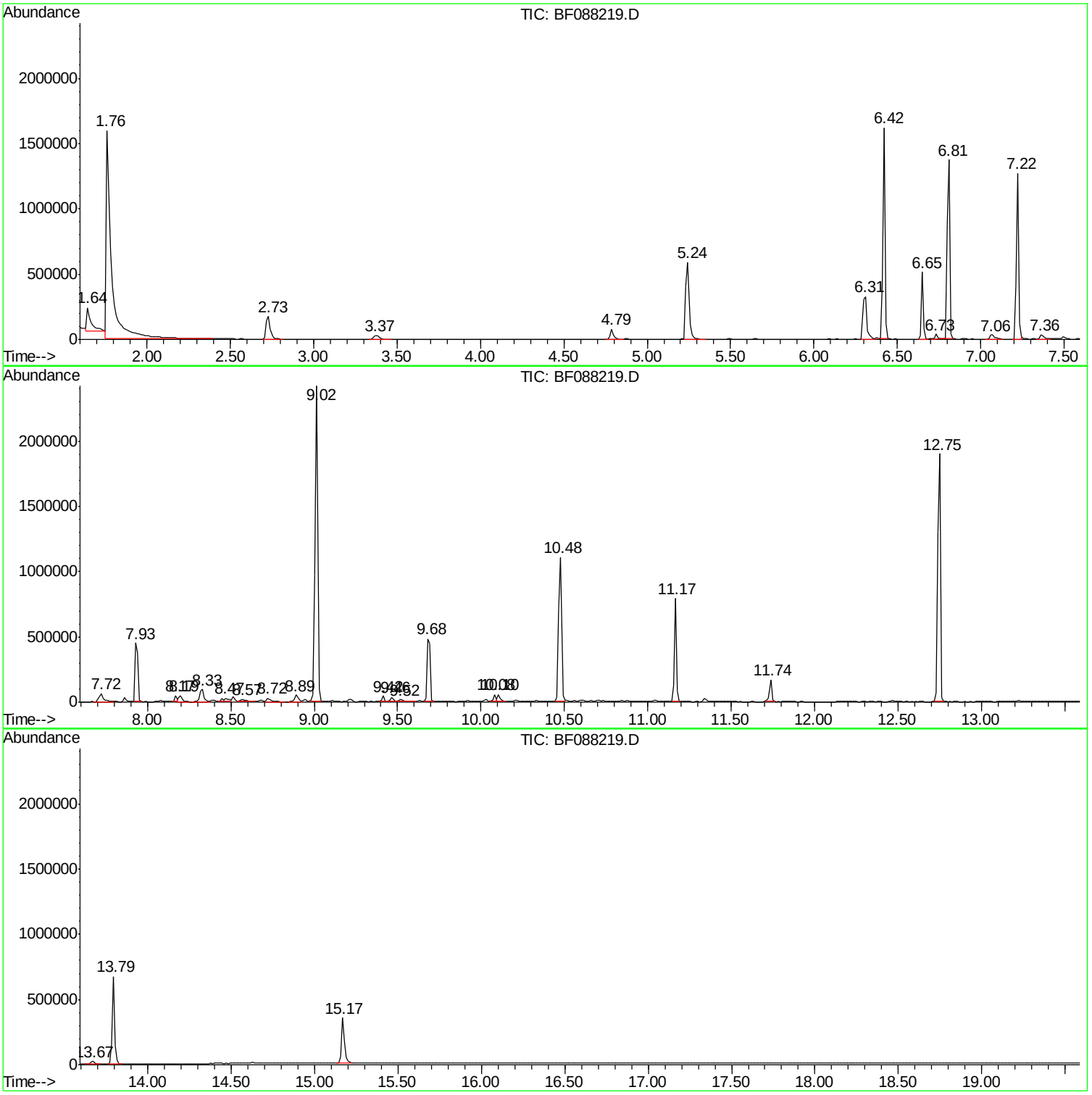
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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 : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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

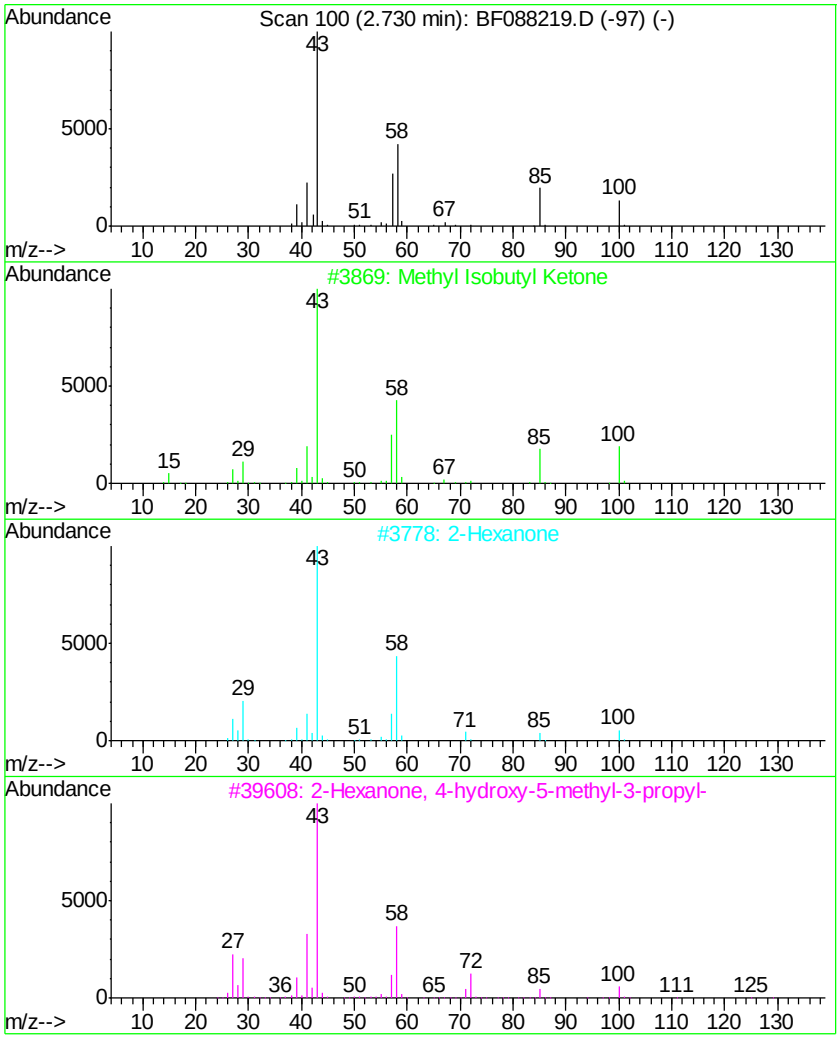
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

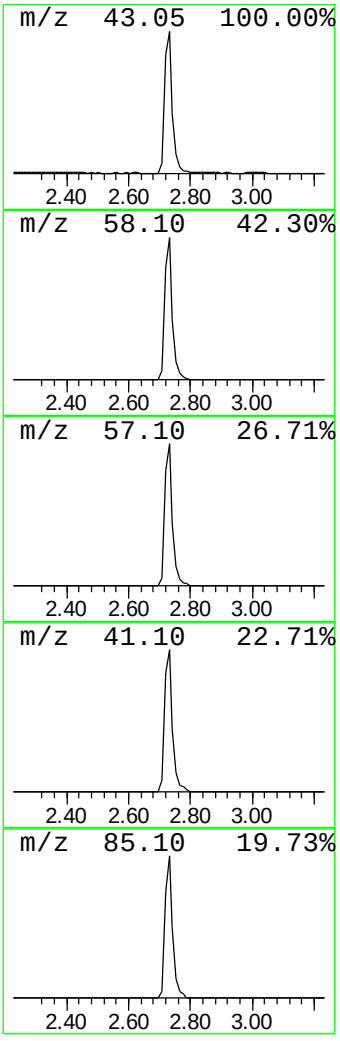
****

Peak Number 3 Methyl Isobutyl Ketone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.73	13.59 ng	294050	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	86
2	2-Hexanone	100	C6H12O	000591-78-6	80
3	2-Hexanone, 4-hydroxy-5-methyl-3...	172	C10H20O2	061141-74-0	40
4	Acetylacetone	100	C5H8O2	000123-54-6	35
5	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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

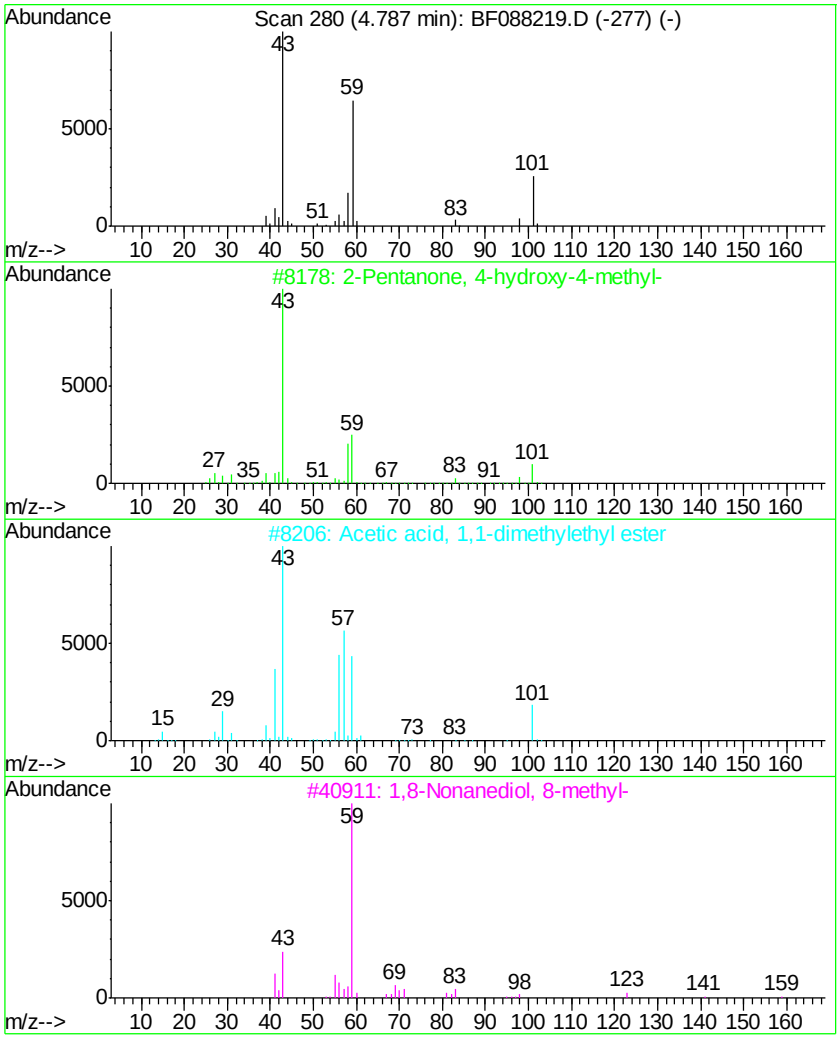
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

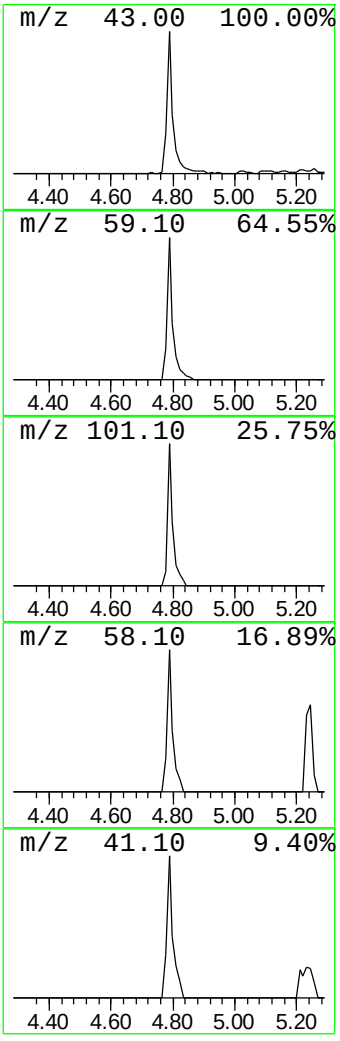
****

Peak Number 5 unknown4.79 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	4.83 ng	104543	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	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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

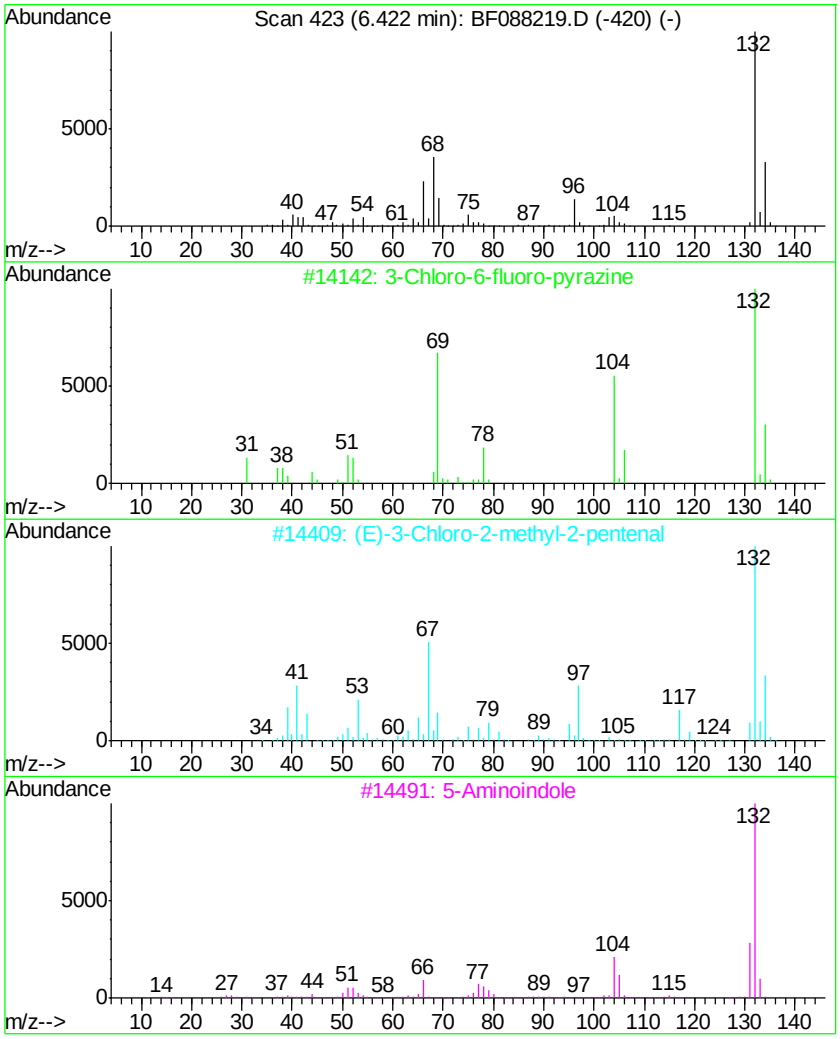
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

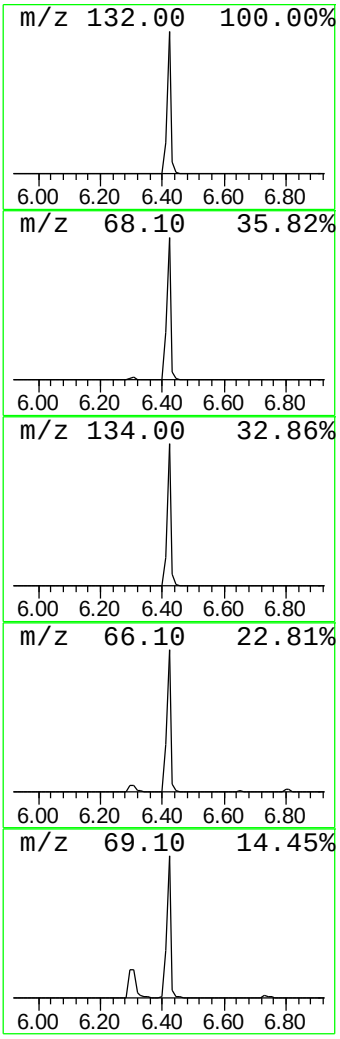
****

Peak Number 6 unknown6.42 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	68.83 ng	1489300	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	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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

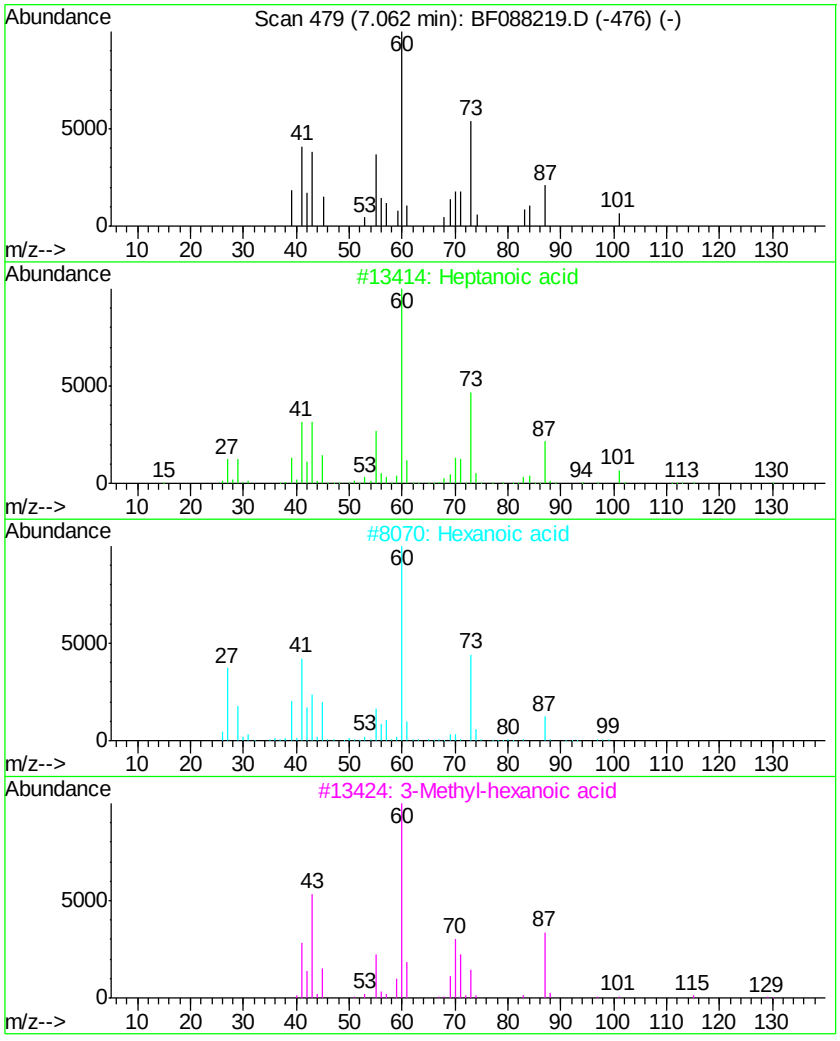
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

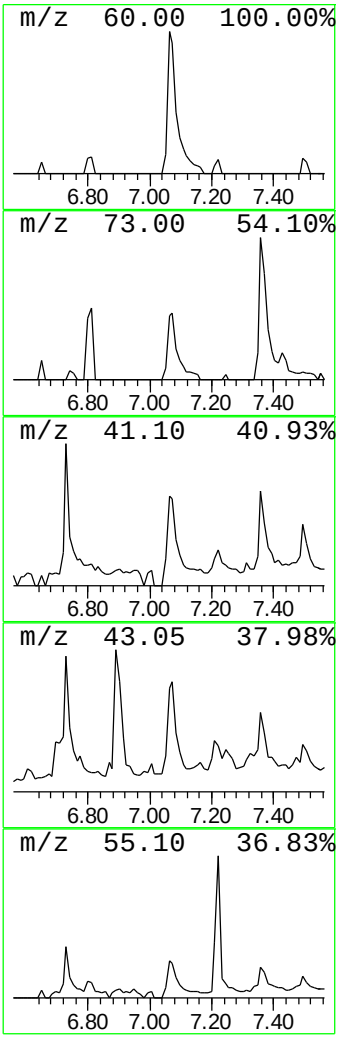
****

Peak Number 8 Heptanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	3.49 ng	75609	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	78
2	Hexanoic acid	116	C6H12O2	000142-62-1	53
3	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	50
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	42
5	3,4-Altrosan	162	C6H10O5	1000129-76-4	42





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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

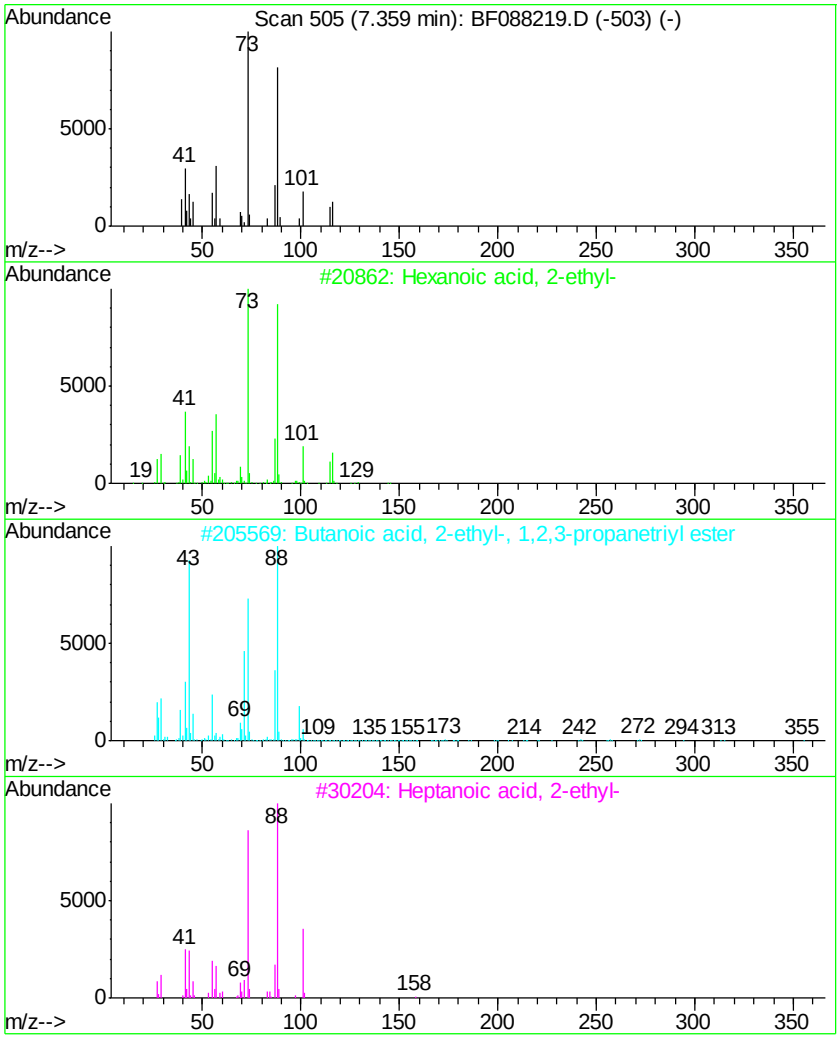
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

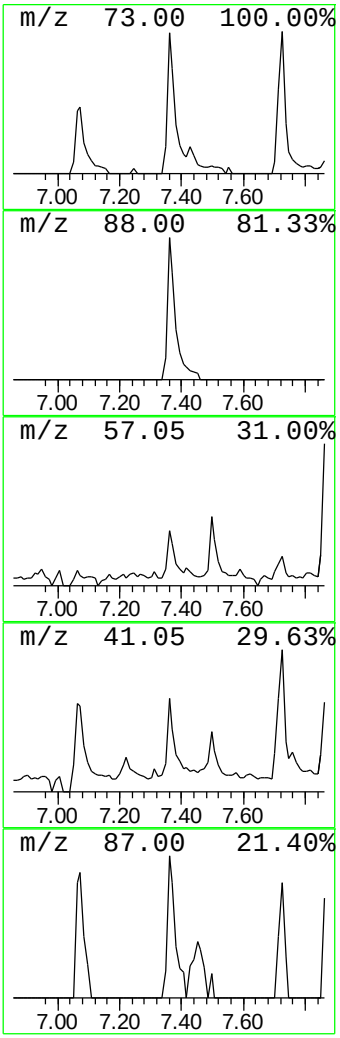
****

Peak Number 9 Hexanoic acid, 2-ethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	2.08 ng	58989	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
4	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	40
5	1,4-Dioxane	88	C4H8O2	000123-91-1	37





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Acq On : 21 Jun 2016 18:18
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Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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

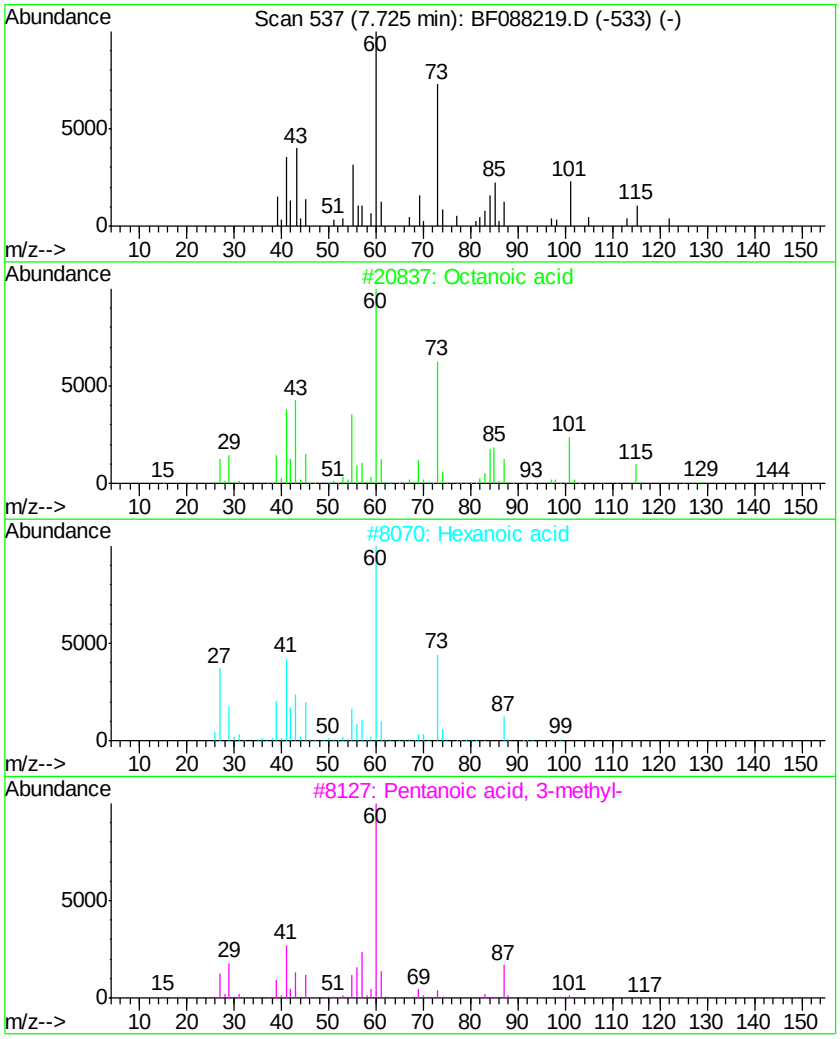
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

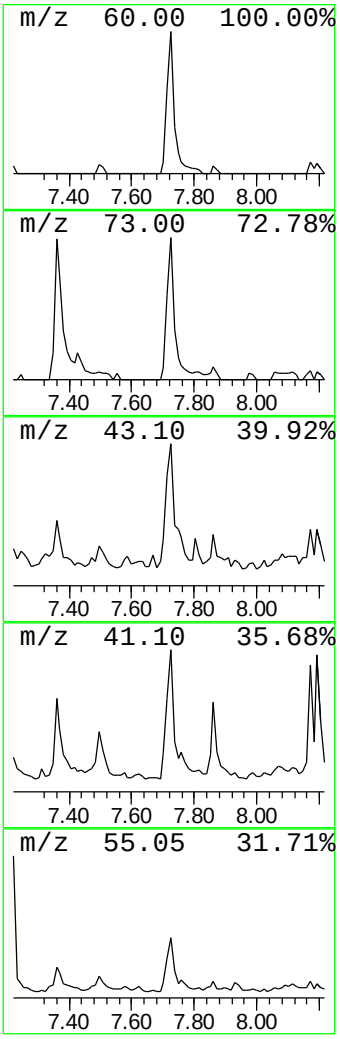
****

Peak Number 10 Octanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	4.30 ng	122161	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	91
2	Hexanoic acid	116	C6H12O2	000142-62-1	50
3	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43
4	Heptanoic acid	130	C7H14O2	000111-14-8	38
5	Pentanoic acid	102	C5H10O2	000109-52-4	38





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Acq On : 21 Jun 2016 18:18
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Sample : H3697-04
Misc :
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Instrument : BNA_F
ClientSampleId : EB-GW-02

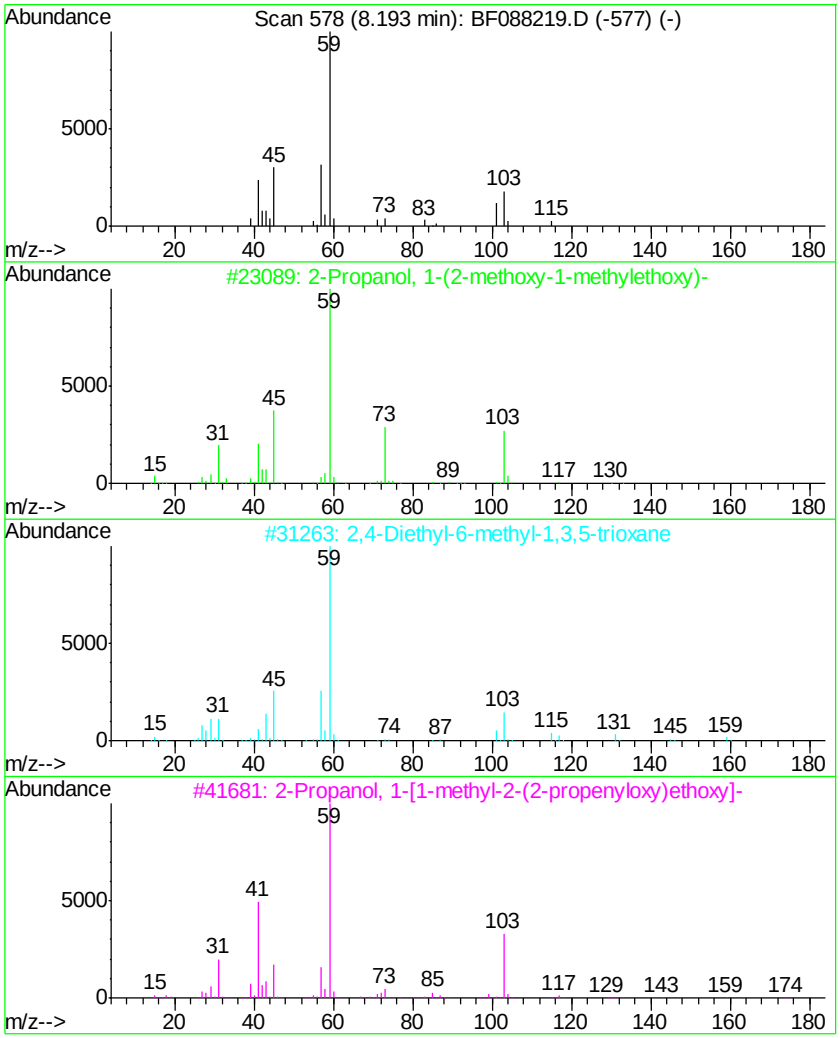
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

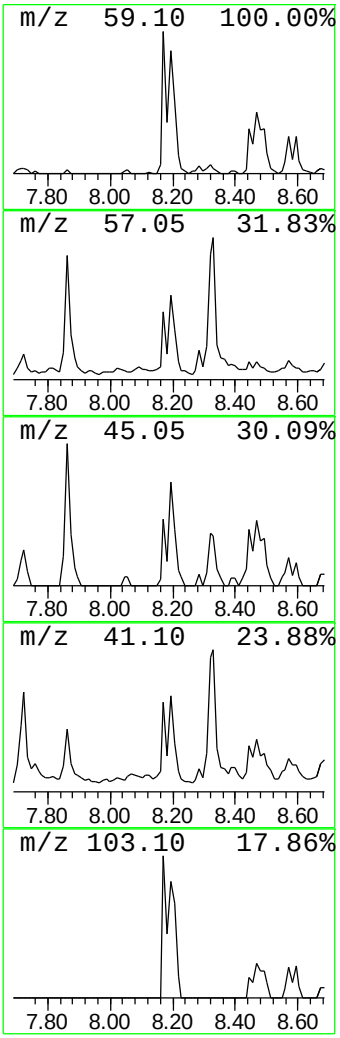
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.19	2.24 ng	63771	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	56
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	50
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	45
5	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	43





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Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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

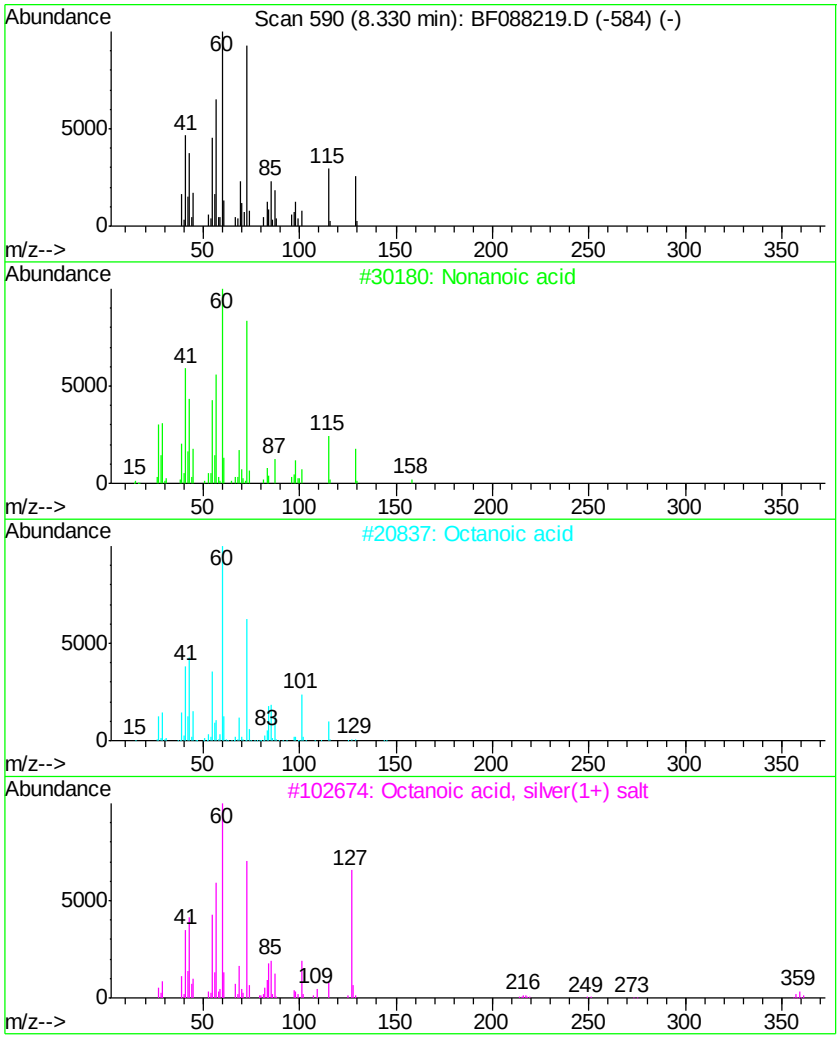
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

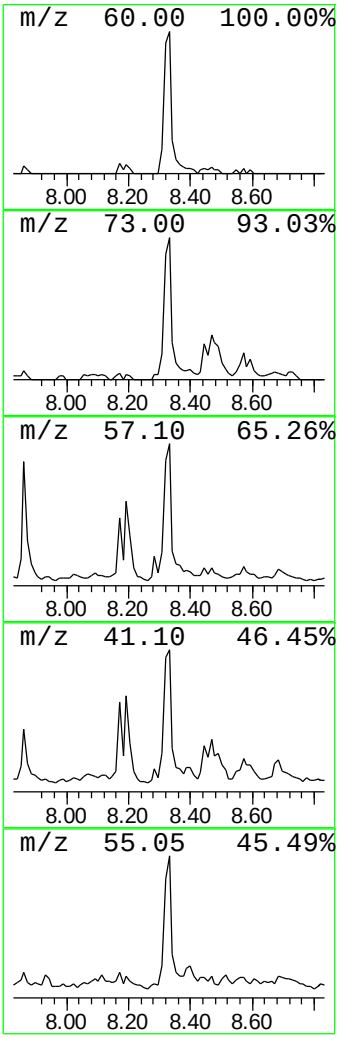
****

Peak Number 12 Nonanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.33	6.06 ng	172045	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	83
2	Octanoic acid	144	C8H16O2	000124-07-2	59
3	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	53
4	Heptanoic acid	130	C7H14O2	000111-14-8	43
5	Hexanoic acid	116	C6H12O2	000142-62-1	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062116\
Data File : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

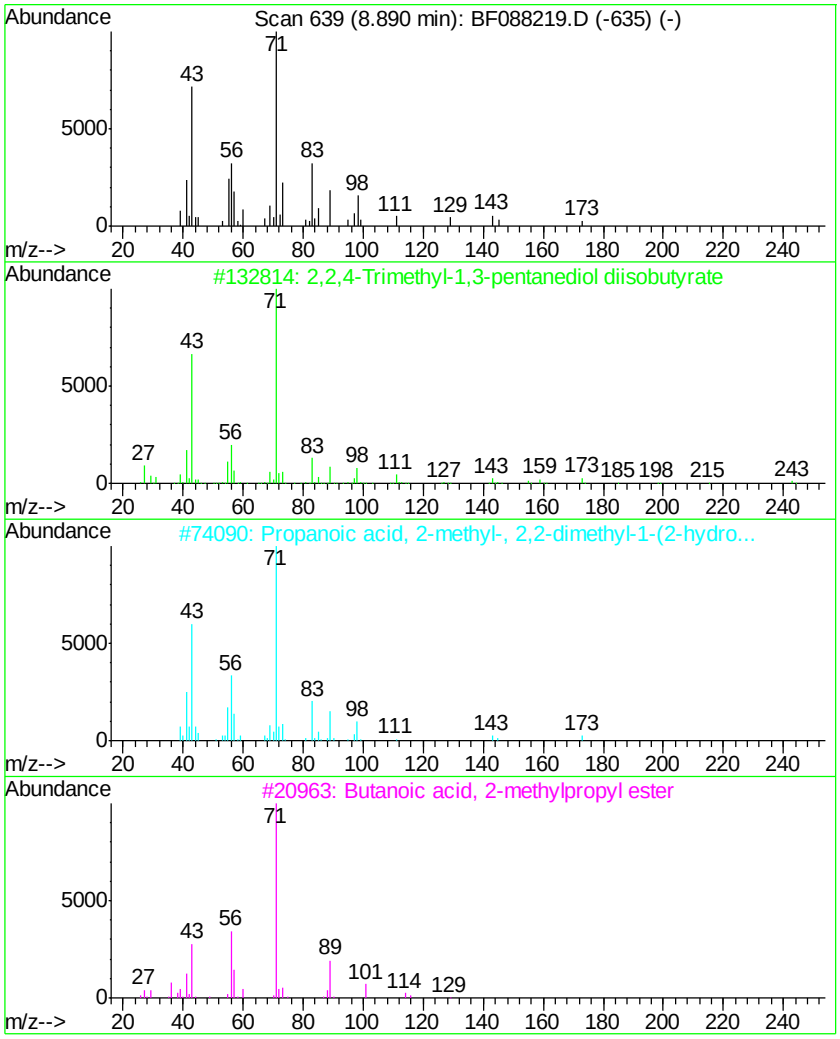
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

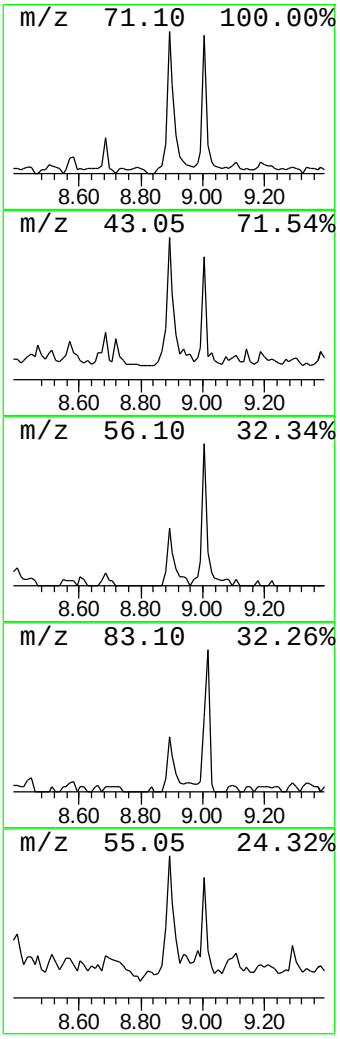
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	2.71 ng	89385	Acenaphthene-d10	9.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	59
2	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	56
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	47
4	Butanoic acid, decyl ester	228	C14H28O2	005454-09-1	45
5	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062116\
Data File : BF088219.D
Acq On : 21 Jun 2016 18:18
Operator : UM/SJ
Sample : H3697-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-GW-02

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...	2.73	13.6	ng	294050	1	6.65	432727	20.0
unknown4.79	4.79	4.8	ng	104543	1	6.65	432727	20.0
unknown6.42	6.42	68.8	ng	1489300	1	6.65	432727	20.0
Heptanoic acid	7.06	3.5	ng	75609	1	6.65	432727	20.0
Hexanoic acid, 2-...	7.36	2.1	ng	58989	2	7.93	568197	20.0
Octanoic acid	7.72	4.3	ng	122161	2	7.93	568197	20.0
2-Propanol, 1-(2-...	8.19	2.2	ng	63771	2	7.93	568197	20.0
Nonanoic acid	8.33	6.1	ng	172045	2	7.93	568197	20.0
2,2,4-Trimethyl-1...	8.89	2.7	ng	89385	3	9.68	660569	20.0