LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087848.D
Acq On : 9 Jun 2016 13:10
Operator : UM/SJ
Sample : H3477-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-05-CB-06072016

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	1.667	4	7	10	rVB	3633538	6265505	100.00%	17.033%
2	1.747	13	14	24	rVB	437709	672256	10.73%	1.828%
3	1.873	24	25	40	rVB	1732780	3334261	53.22%	9.064%
4	2.067	40	42	78	rVB	100604	433283	6.92%	1.178%
5	5.004	296	299	306	rVB	137228	222242	3.55%	0.604%
6	5.416	332	335	337	rBV	2304127	2399752	38.30%	6.524%
7	6.456	423	426	428	rBV	2329194	2608526	41.63%	7.091%
8	6.582	435	437	440	rBV	1986265	2667301	42.57%	7.251%
9	6.822	455	458	460	rBV	726640	736669	11.76%	2.003%
10	6.970	469	471	474	rVB	1592783	2146345	34.26%	5.835%
11	7.382	504	507	510	rBV	1563397	1564683	24.97%	4.254%
12	8.102	568	570	573	rBV	1142917	981238	15.66%	2.668%
13	9.176	661	664	667	rBV	2670138	2989891	47.72%	8.128%
14	9.576	696	699	700	rBV	286109	360345	5.75%	0.980%
15	9.851	721	723	726	rVB	1340450	1165422	18.60%	3.168%
16	10.285	760	761	763	rVB	68483	69045	1.10%	0.188%
17	10.639	789	792	794	rBV	1885120	1876566	29.95%	5.102%
18	10.765	801	803	807	rBV	66808	106199	1.69%	0.289%
19	11.325	850	852	855	rVB2	918904	1093645	17.46%	2.973%
20	12.742	973	976	978	rBV	233174	192753	3.08%	0.524%
21	12.914	988	991	993	rBV	2810265	2720631	43.42%	7.396%
22	13.440	1035	1037	1039	rBV	136014	144272	2.30%	0.392%
23	13.805	1067	1069	1079	rBV	213204	330725	5.28%	0.899%
24	13.954	1079	1082	1084	rBV	1108162	1002048	15.99%	2.724%
25	15.360	1202	1205	1208	rBV	596503	700605	11.18%	1.905%

Sum of corrected areas: 36784208

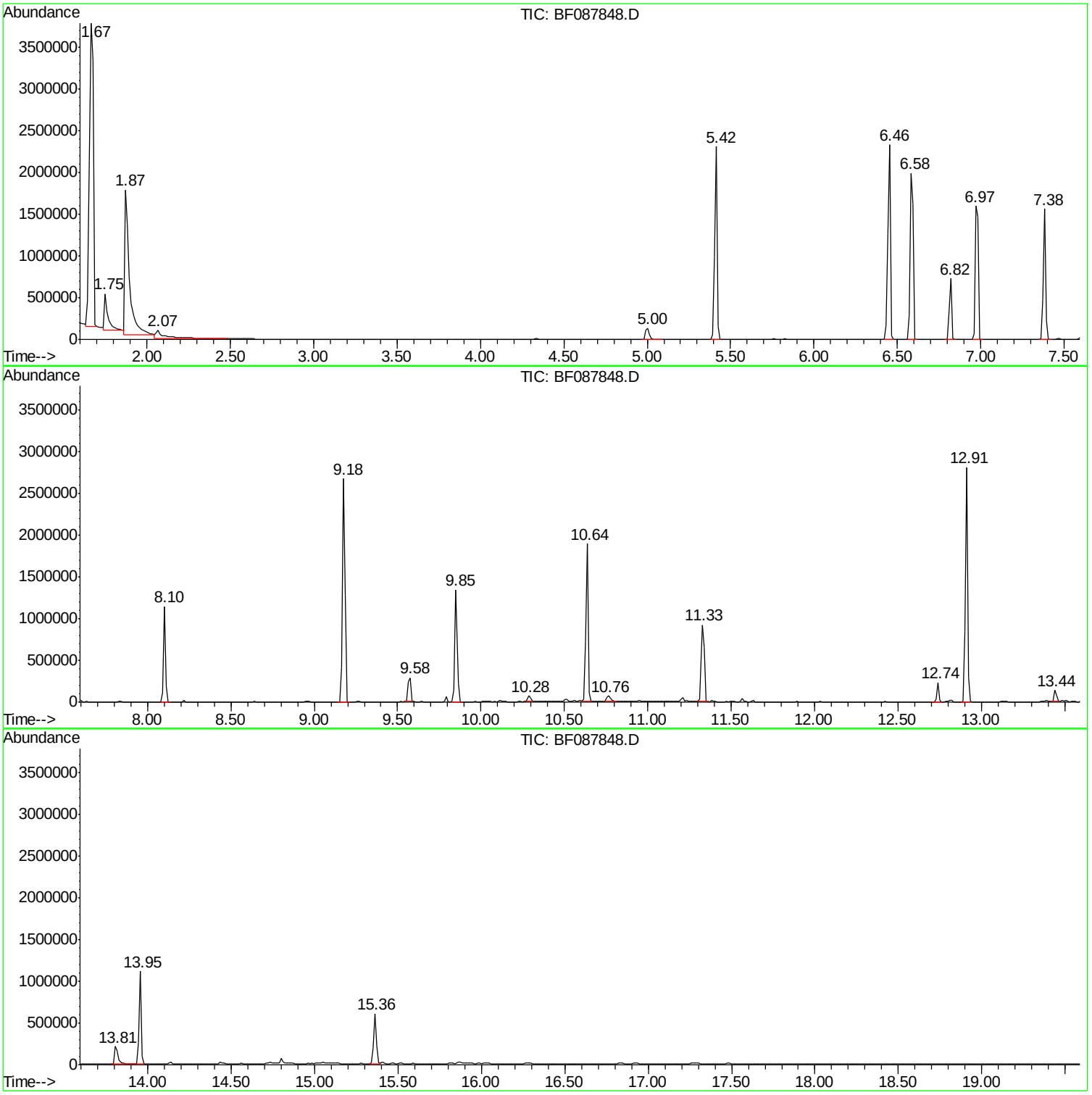
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087848.D
Acq On : 9 Jun 2016 13:10
Operator : UM/SJ
Sample : H3477-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1300-05-CB-06072016

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\BF060916\
Data File : BF087848.D
Acq On : 9 Jun 2016 13:10
Operator : UM/SJ
Sample : H3477-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-05-CB-06072016

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

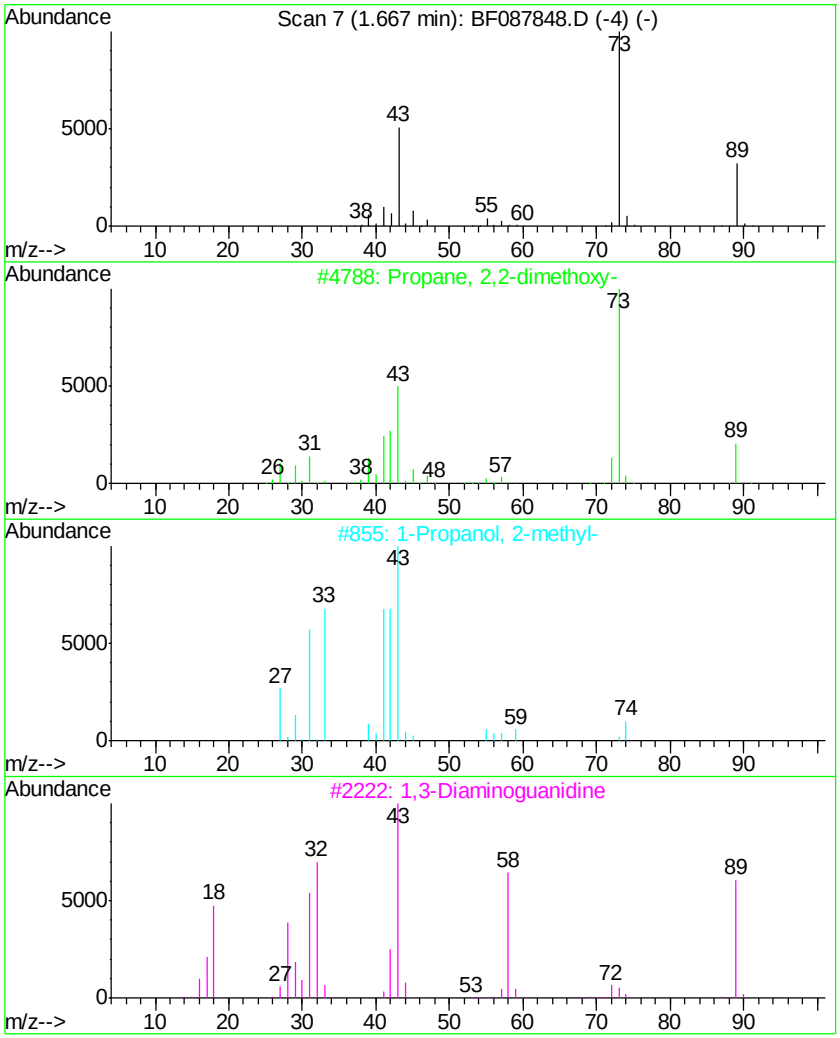
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

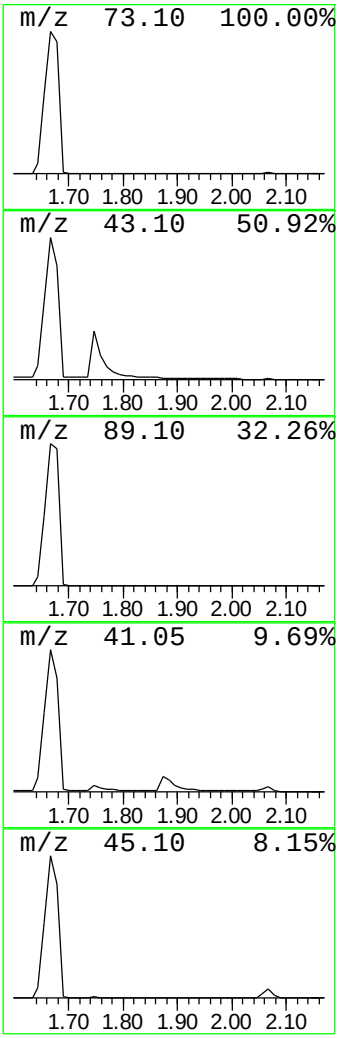
****

Peak Number 1 unknown1.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	170.10 ng	6265510	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087848.D
Acq On : 9 Jun 2016 13:10
Operator : UM/SJ
Sample : H3477-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-05-CB-06072016

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

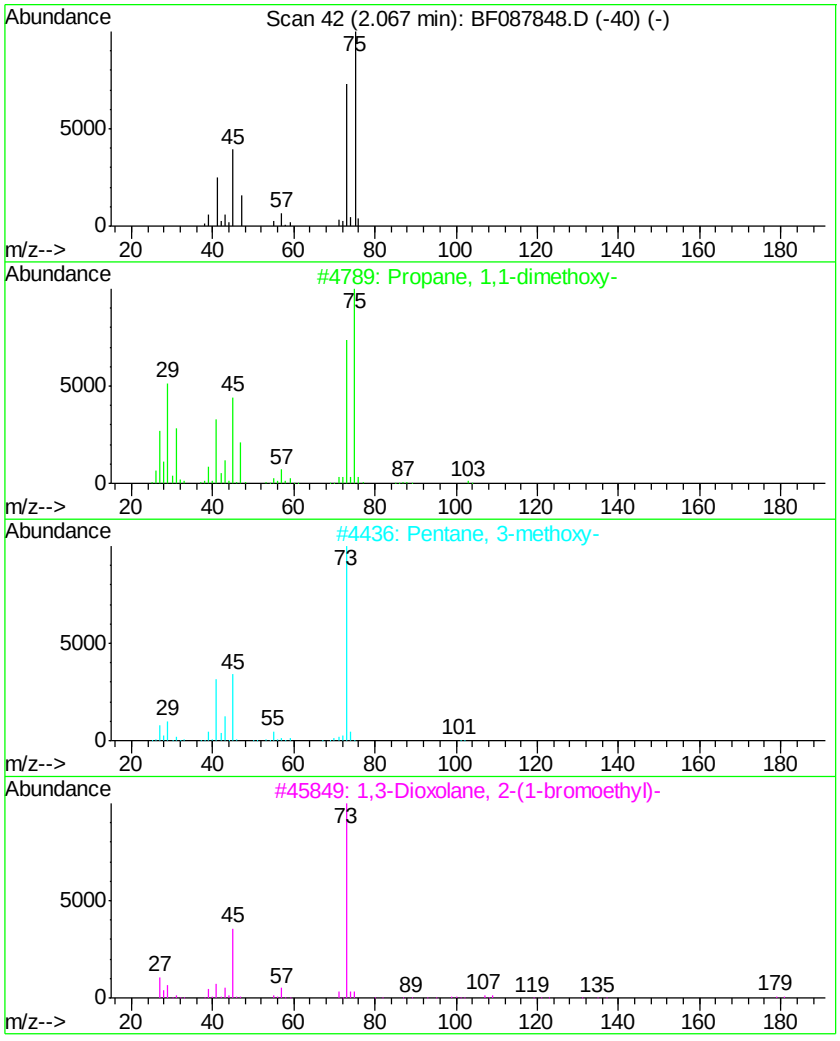
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

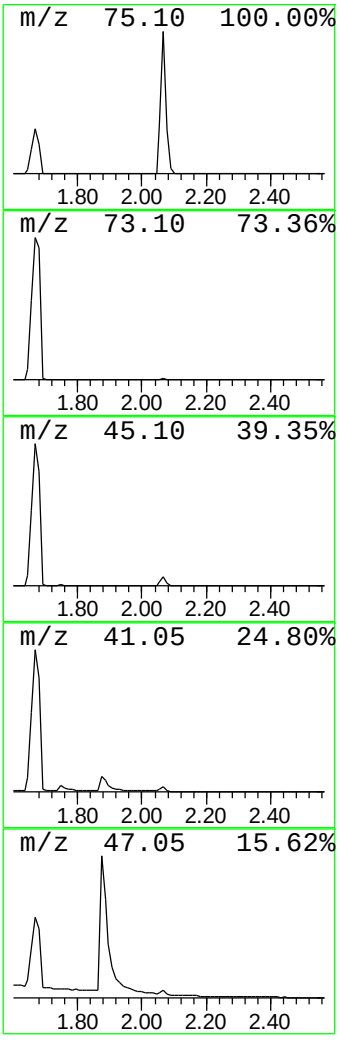
****

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	11.76 ng	433283	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	25
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5	Glycine	75	C2H5NO2	000056-40-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087848.D
Acq On : 9 Jun 2016 13:10
Operator : UM/SJ
Sample : H3477-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-05-CB-06072016

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

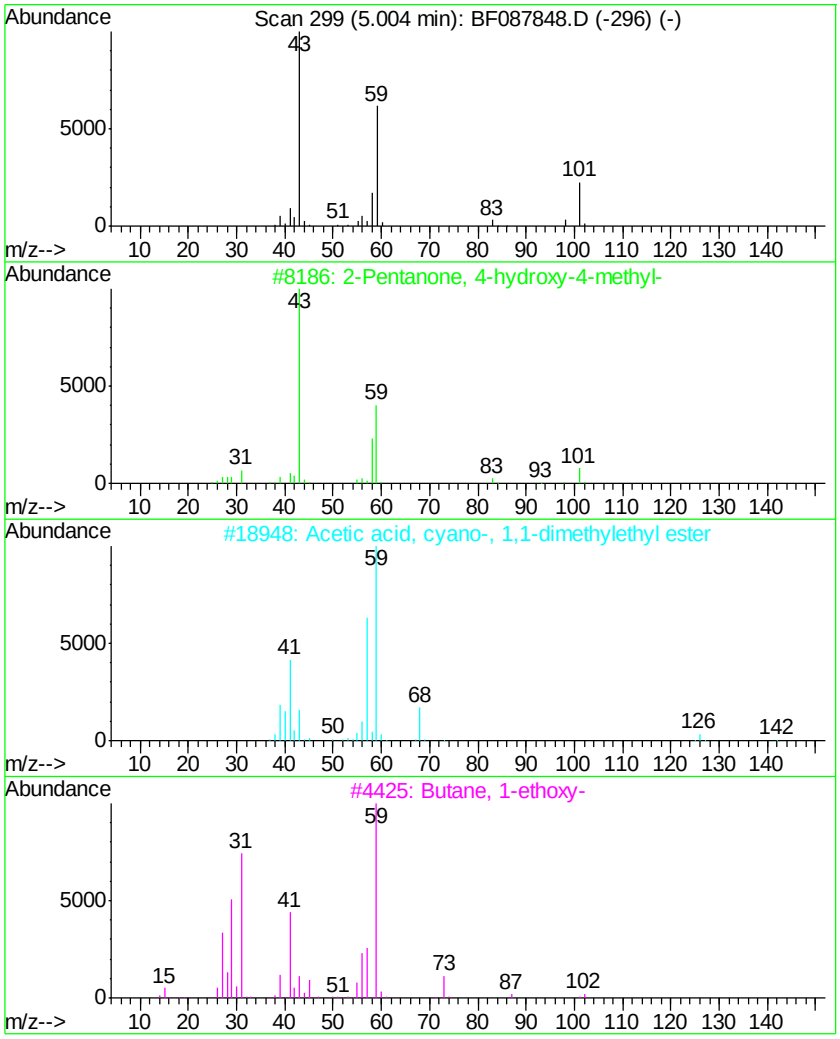
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

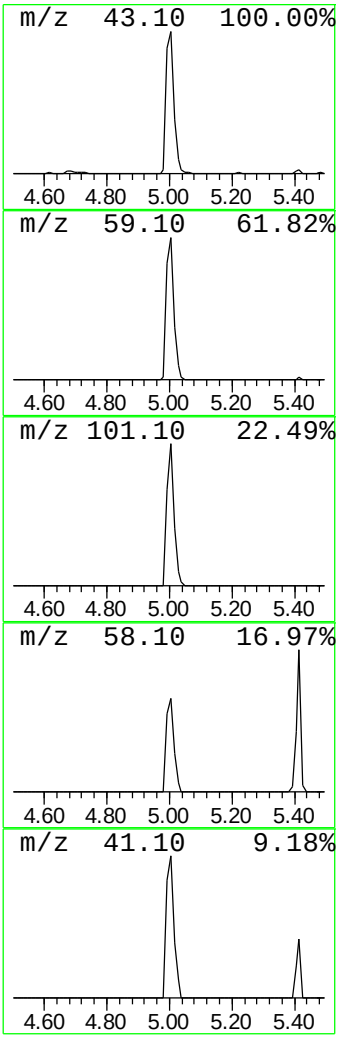
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	6.03 ng	222242	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087848.D
Acq On : 9 Jun 2016 13:10
Operator : UM/SJ
Sample : H3477-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1300-05-CB-06072016

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

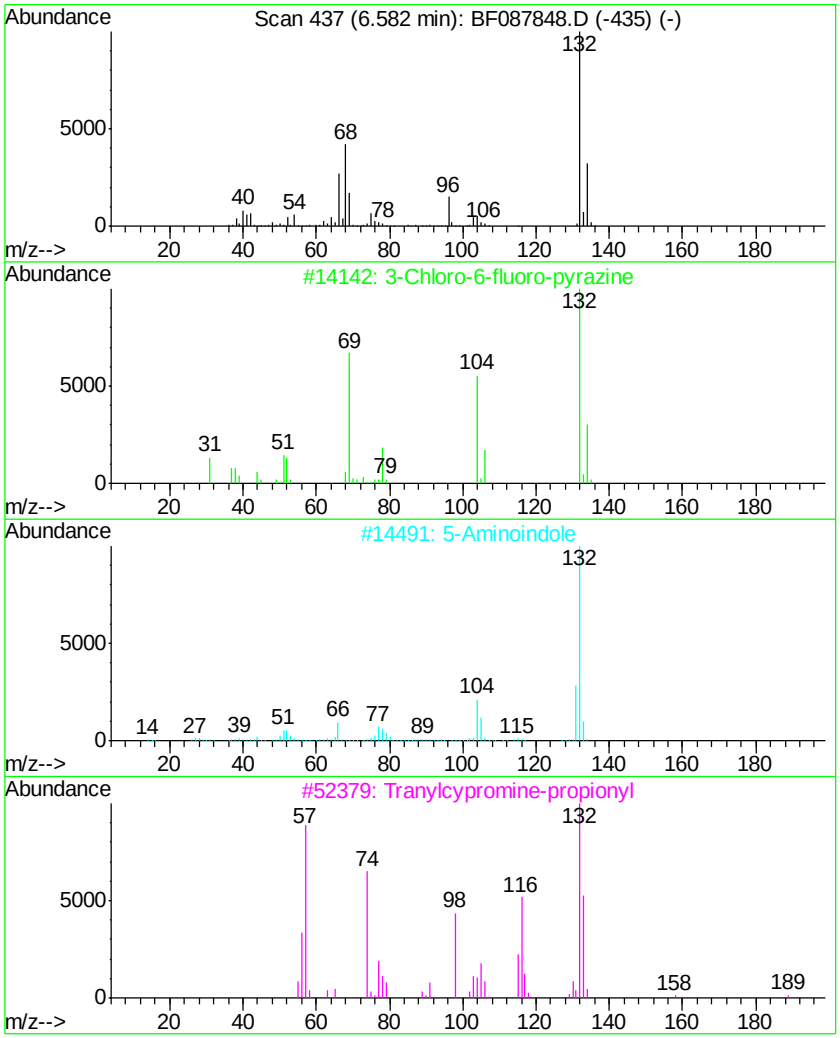
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

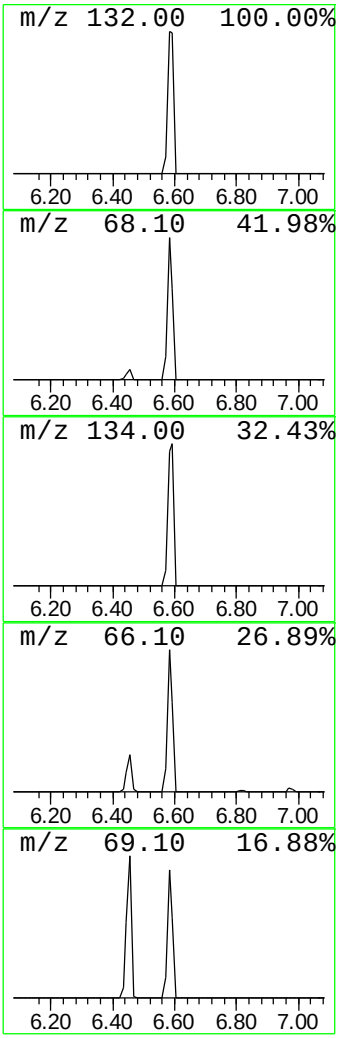
****

Peak Number 6 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	72.42 ng	2667300	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
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Acq On : 9 Jun 2016 13:10
Operator : UM/SJ
Sample : H3477-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-05-CB-06072016

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

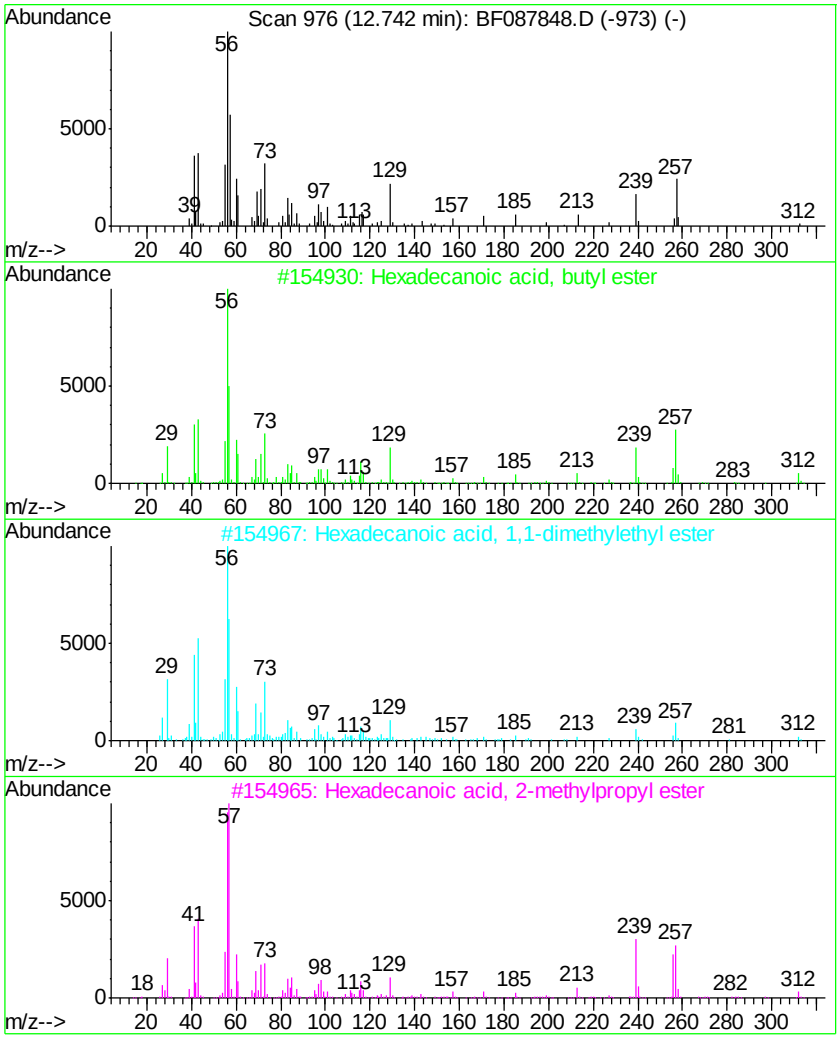
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

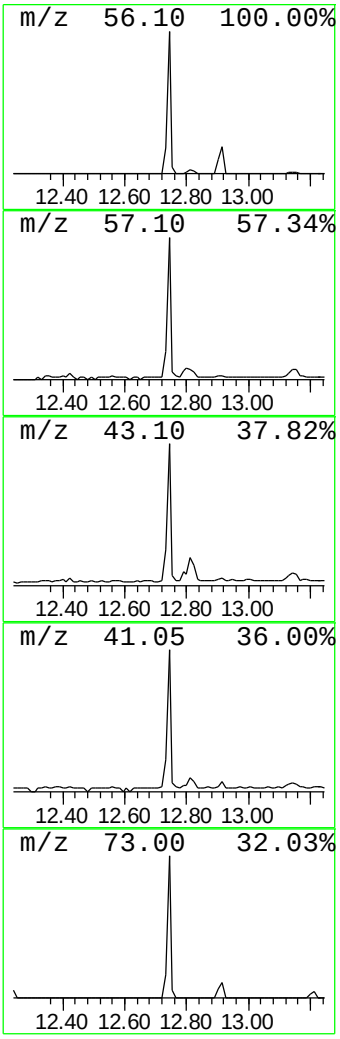
****

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	3.85 ng	192753	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	72
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	59
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	45





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Sample : H3477-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-05-CB-06072016

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

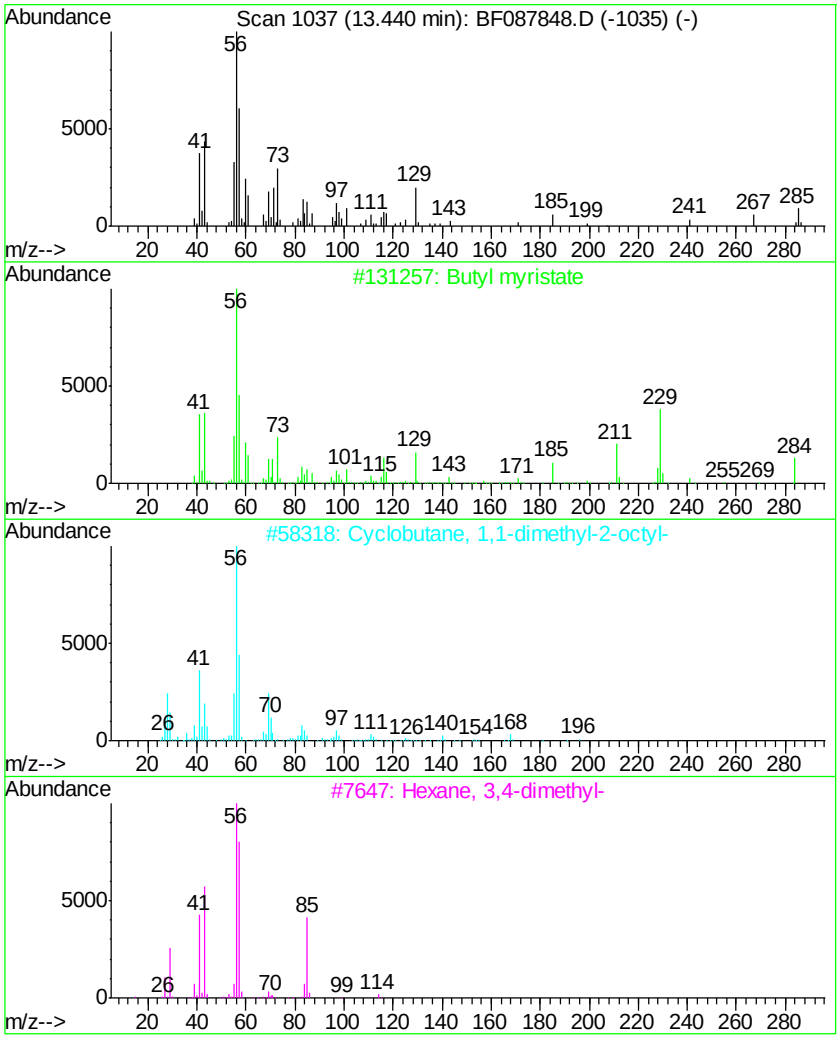
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

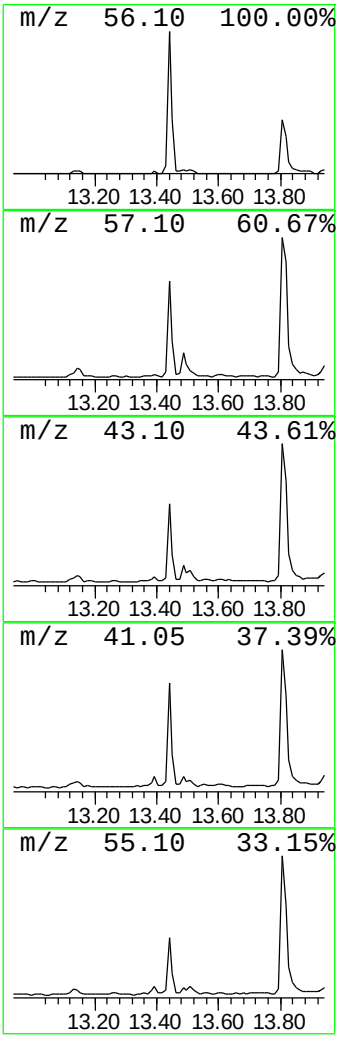
****

Peak Number 9 Butyl myristate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	2.88 ng	144272	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	72
2	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
3	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	35
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27





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Instrument : BNA_F
ClientSampleId : 1300-05-CB-06072016

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

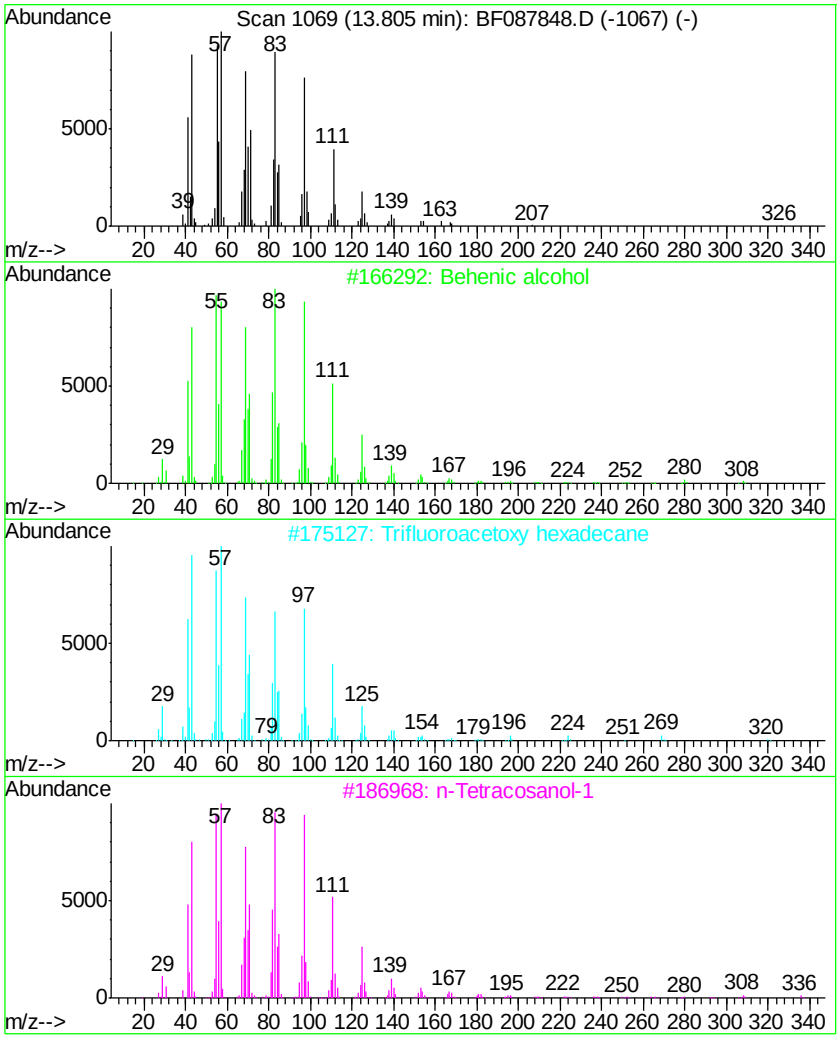
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

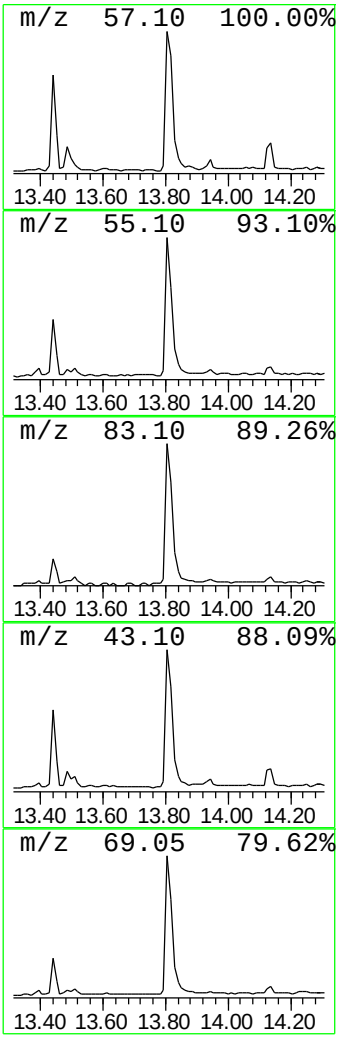
****

Peak Number 10 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	6.60 ng	330725	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060916\
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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
unknown1.67	1.67	170.1	ng	6265510	1	6.82	736669	20.0
Propane, 1,1-dime...	2.07	11.8	ng	433283	1	6.82	736669	20.0
2-Pentanone, 4-hy...	5.00	6.0	ng	222242	1	6.82	736669	20.0
unknown6.58	6.58	72.4	ng	2667300	1	6.82	736669	20.0
Hexadecanoic acid...	12.74	3.9	ng	192753	5	13.95	1002050	20.0
Butyl myristate	13.44	2.9	ng	144272	5	13.95	1002050	20.0
Behenic alcohol	13.81	6.6	ng	330725	5	13.95	1002050	20.0