LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088944.D
Acq On : 13 Jul 2016 4:52
Operator : UM/SJ
Sample : H3987-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-WALL-W-070816

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-BF063016.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	6	7	16	rVV	49517	82333	5.02%	0.637%
2	1.792	16	18	26	rVV	279496	386586	23.59%	2.991%
3	1.907	26	28	46	rVB2	36067	74909	4.57%	0.580%
4	4.856	283	286	291	rBB	219471	298381	18.21%	2.309%
5	5.301	322	325	327	rBV	1282681	1209963	73.84%	9.362%
6	5.701	358	360	362	rBB	22523	18825	1.15%	0.146%
7	6.353	414	417	419	rBV	1337974	1367037	83.43%	10.577%
8	6.467	425	427	430	rBV	1086485	1306635	79.74%	10.110%
9	6.707	445	448	450	rBV	260798	353902	21.60%	2.738%
10	6.856	459	461	463	rBB	1079305	1052390	64.22%	8.142%
11	7.267	494	497	499	rBV	854831	828625	50.57%	6.411%
12	7.987	557	560	562	rBV	587764	486217	29.67%	3.762%
13	9.073	652	655	657	rBV	1435361	1638600	100.00%	12.678%
14	9.462	687	689	691	rBV	314147	243613	14.87%	1.885%
15	9.736	711	713	715	rBB	544801	455628	27.81%	3.525%
16	10.525	780	782	784	rBV	507016	545987	33.32%	4.224%
17	10.650	792	793	798	rBV	22855	28064	1.71%	0.217%
18	10.970	817	821	824	rBV	27197	45821	2.80%	0.355%
19	11.096	831	832	838	rVB	21669	28051	1.71%	0.217%
20	11.211	840	842	844	rVB	419818	355209	21.68%	2.748%
21	12.799	978	981	983	rBV	1214402	1126859	68.77%	8.719%
22	13.702	1057	1060	1066	rBV	108578	121513	7.42%	0.940%
23	13.839	1069	1072	1074	rBV	307974	346135	21.12%	2.678%
24	14.331	1113	1115	1121	rBV	42542	59796	3.65%	0.463%
25	14.594	1137	1138	1140	rBV	17038	17531	1.07%	0.136%
26	14.925	1164	1167	1171	rBV2	17667	46052	2.81%	0.356%
27	15.211	1189	1192	1194	rBV	252020	292232	17.83%	2.261%
28	15.645	1227	1230	1232	rBV	17560	25928	1.58%	0.201%
29	15.691	1232	1234	1237	rVB	13693	23305	1.42%	0.180%
30	16.800	1328	1331	1335	rVB5	8132	18357	1.12%	0.142%
31	17.017	1346	1350	1355	rVB5	6607	18584	1.13%	0.144%
32	17.908	1423	1428	1433	rBV4	5459	21629	1.32%	0.167%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088944.D
Acq On : 13 Jul 2016 4:52
Operator : UM/SJ
Sample : H3987-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-WALL-W-070816

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 12924697

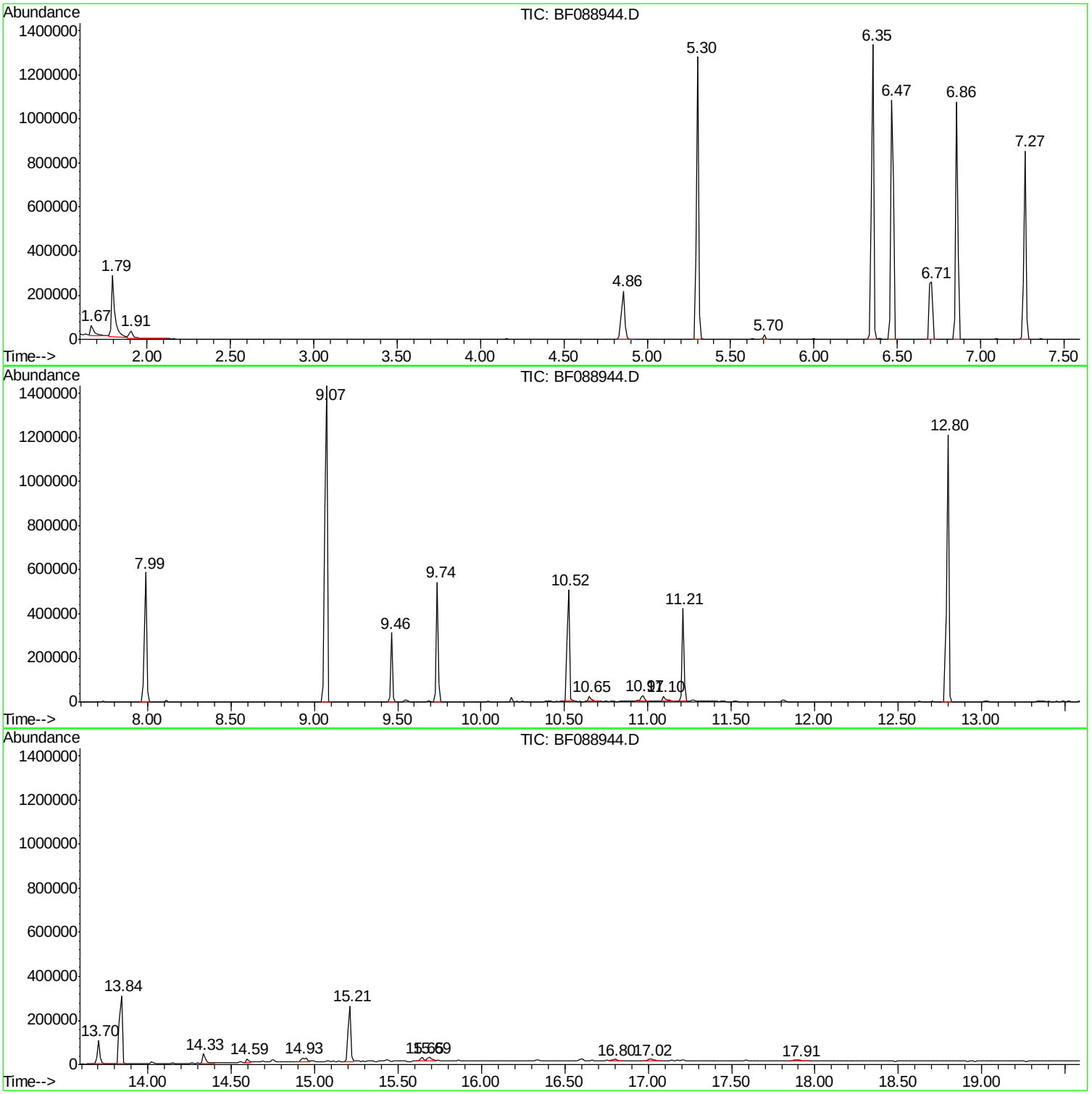
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088944.D
Acq On : 13 Jul 2016 4:52
Operator : UM/SJ
Sample : H3987-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-WALL-W-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088944.D
Acq On : 13 Jul 2016 4:52
Operator : UM/SJ
Sample : H3987-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-WALL-W-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

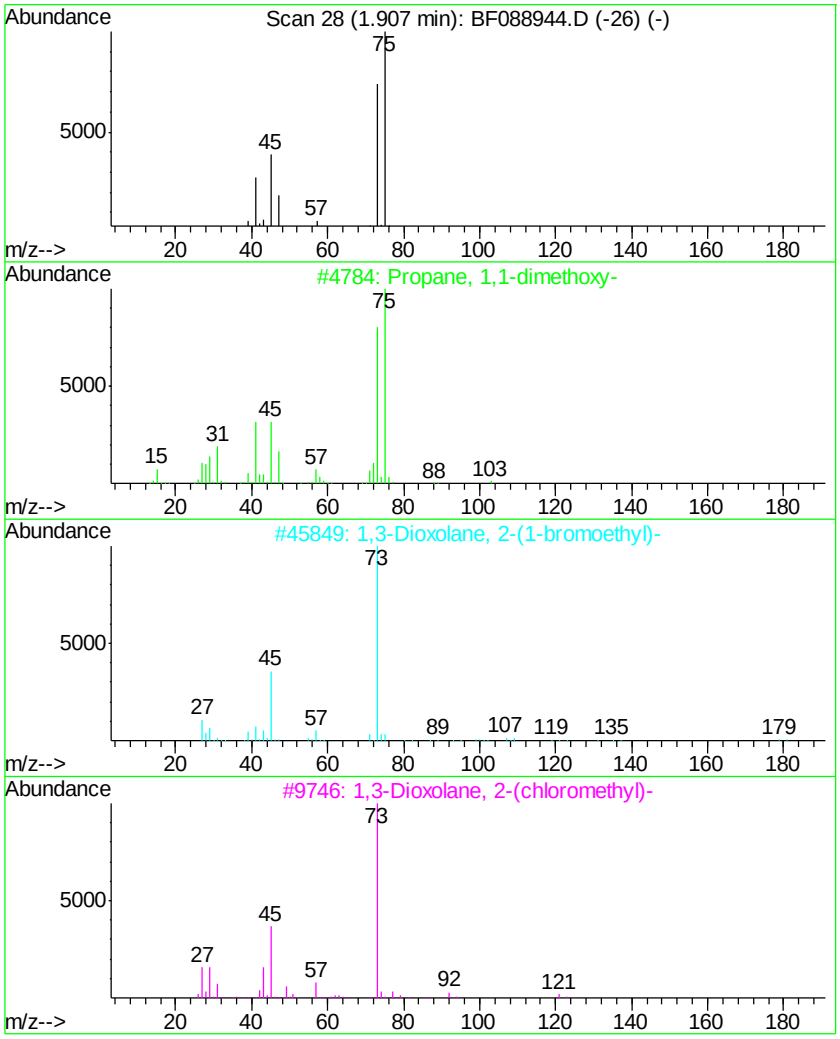
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

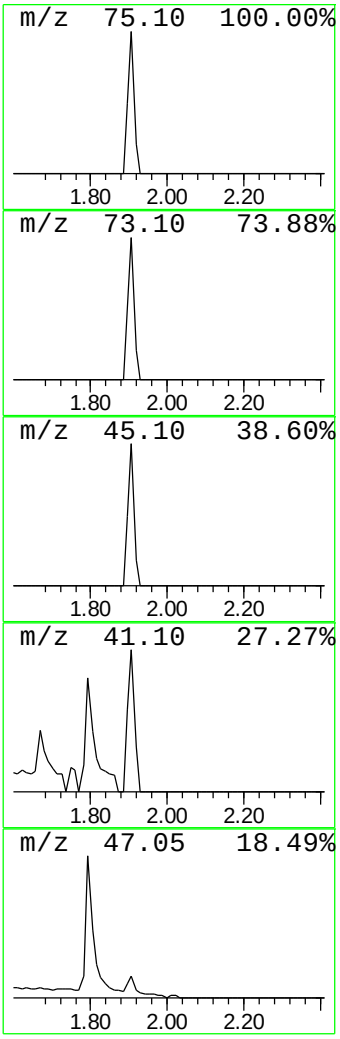
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.91	4.23 ng	74909	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
3	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	Glycine	75	C2H5NO2	000056-40-6	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088944.D
Acq On : 13 Jul 2016 4:52
Operator : UM/SJ
Sample : H3987-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-WALL-W-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

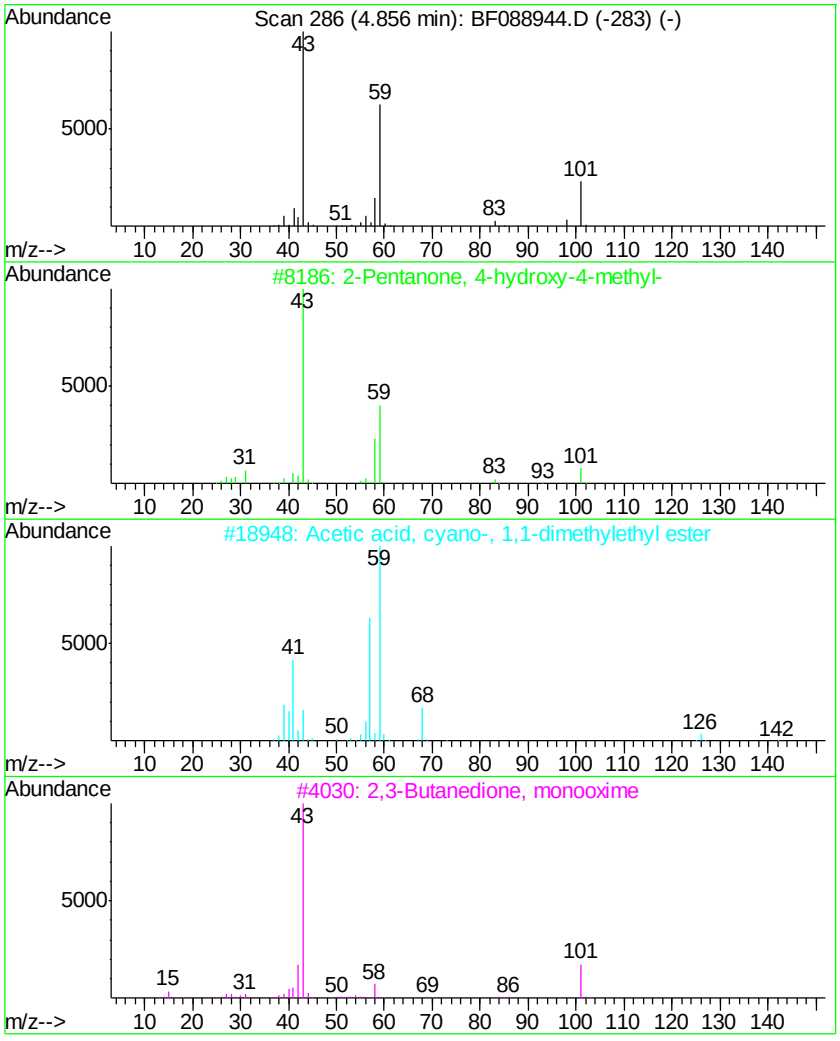
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

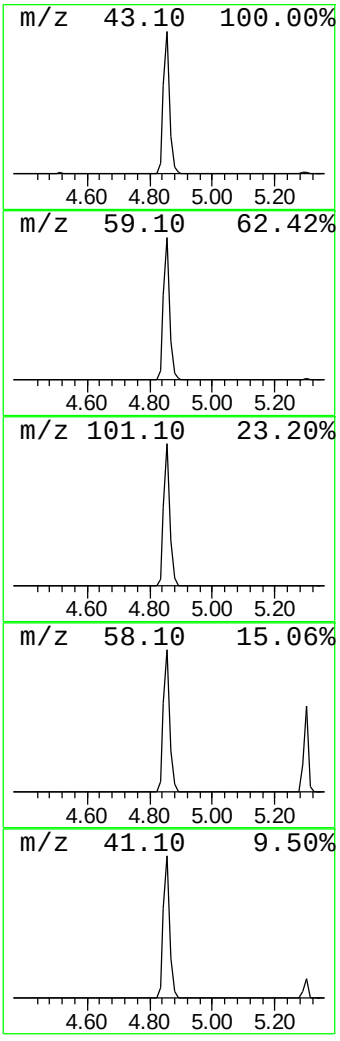
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	16.86 ng	298381	1,4-Dichlorobenzene-d4	6.71

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	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088944.D
Acq On : 13 Jul 2016 4:52
Operator : UM/SJ
Sample : H3987-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-WALL-W-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

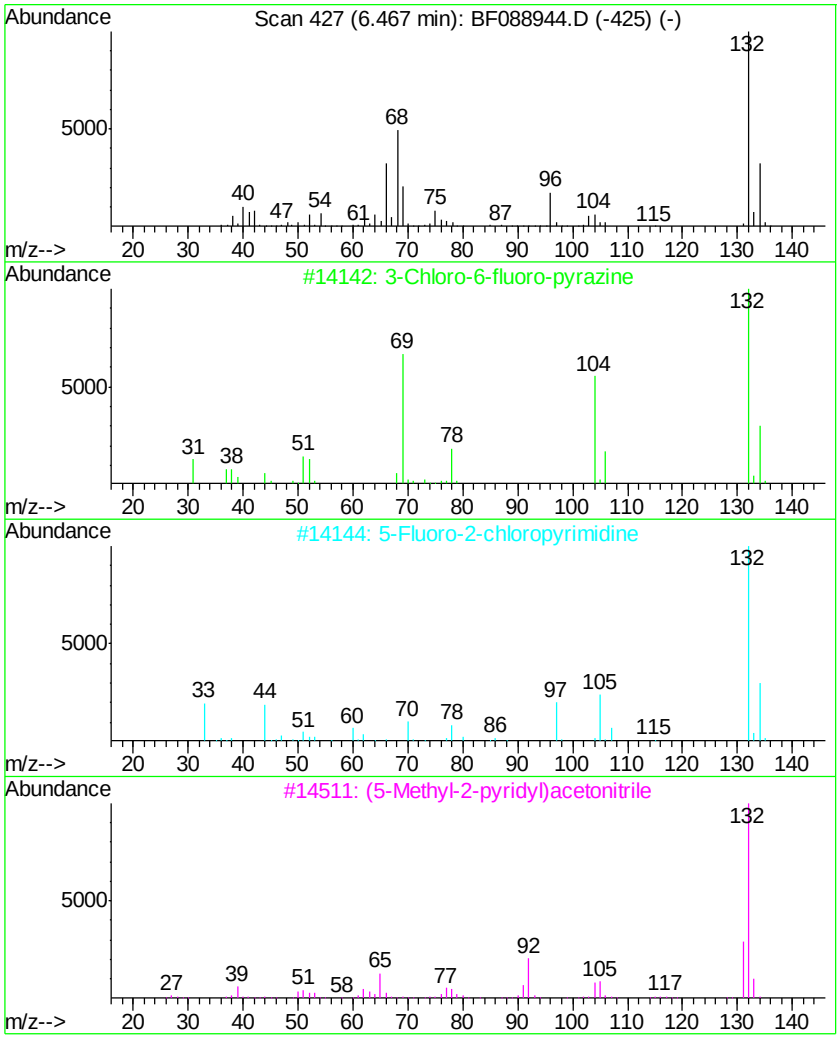
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

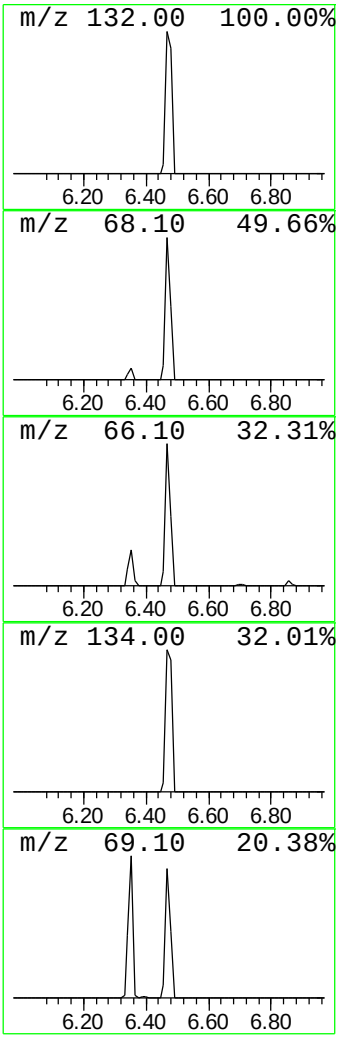
****

Peak Number 5 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	73.84 ng	1306640	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

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Sample : H3987-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-WALL-W-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

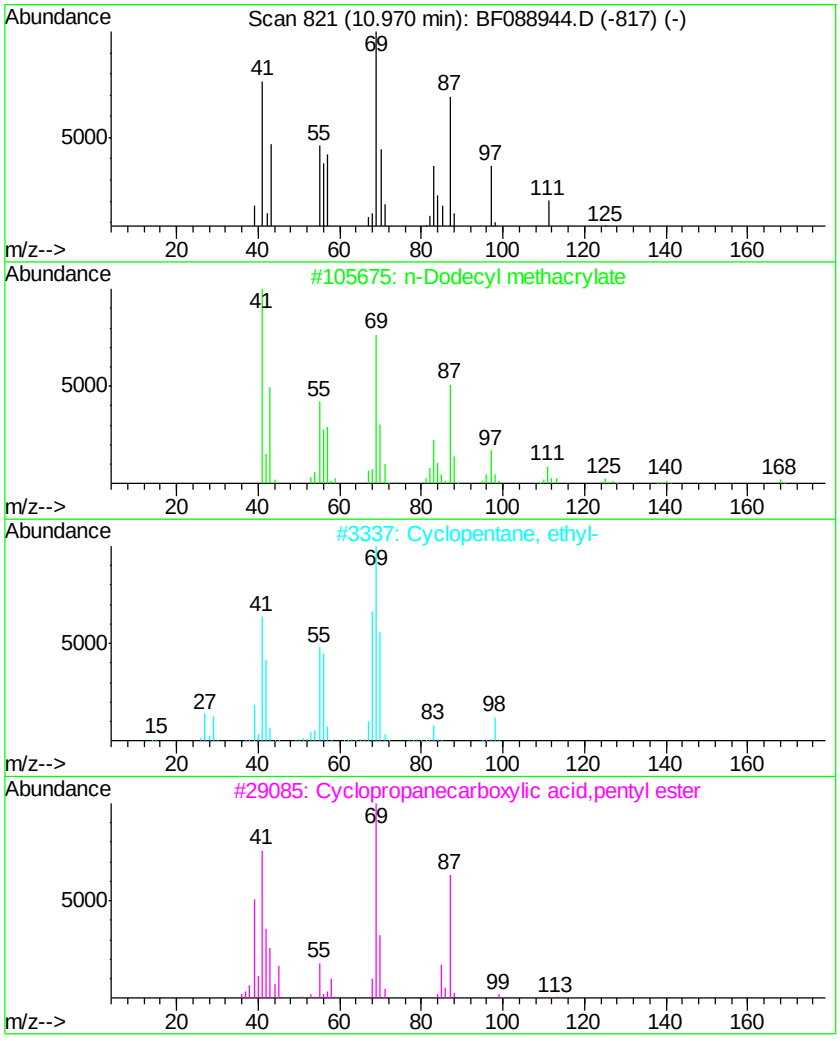
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

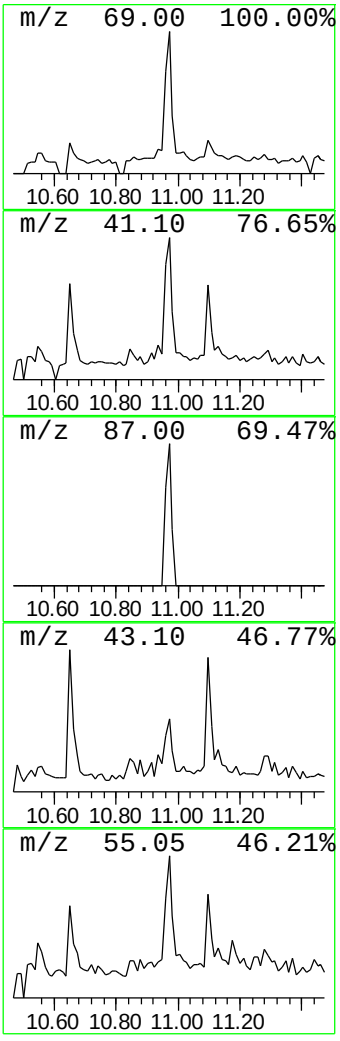
****

Peak Number 7 n-Dodecyl methacrylate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	2.58 ng	45821	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	53
2	Cyclopentane, ethyl-	98	C7H14	001640-89-7	43
3	Cyclopropanecarboxylic acid,pent...	156	C9H16O2	060128-02-1	43
4	1-Dodecene	168	C12H24	000112-41-4	38
5	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	38





Library Search Compound Report

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Sample : H3987-02
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Instrument : BNA_F
ClientSampleId : COMP-WALL-W-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

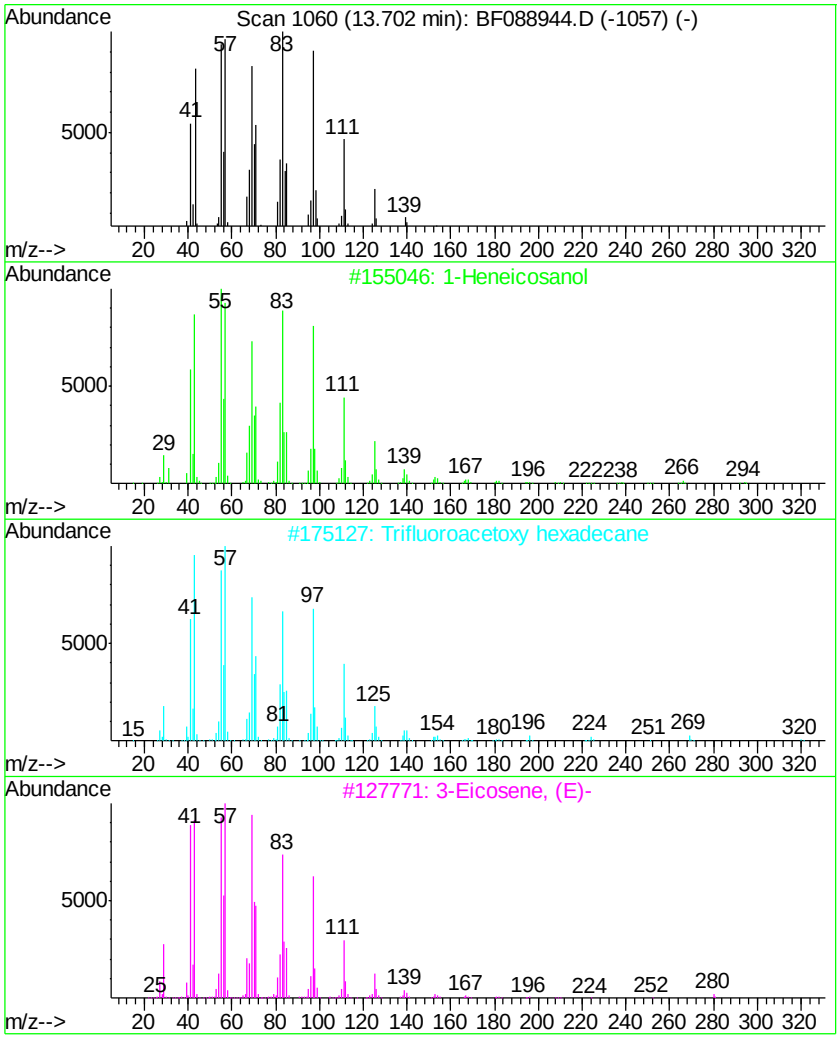
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

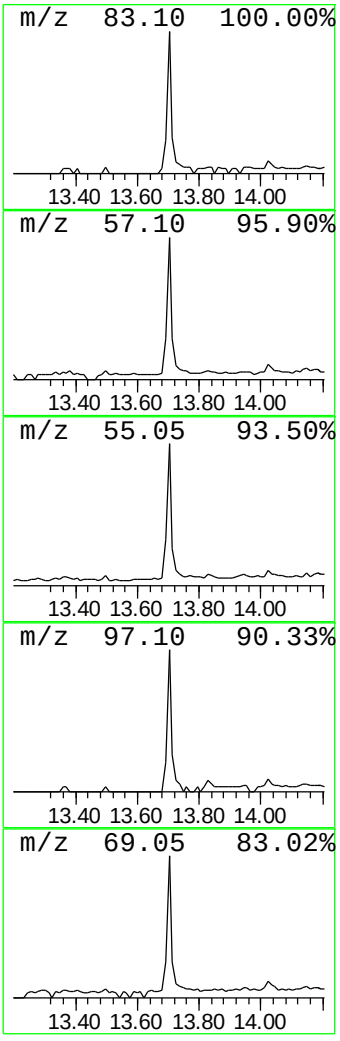
****

Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	7.02 ng	121513	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91





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Sample : H3987-02
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ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-WALL-W-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

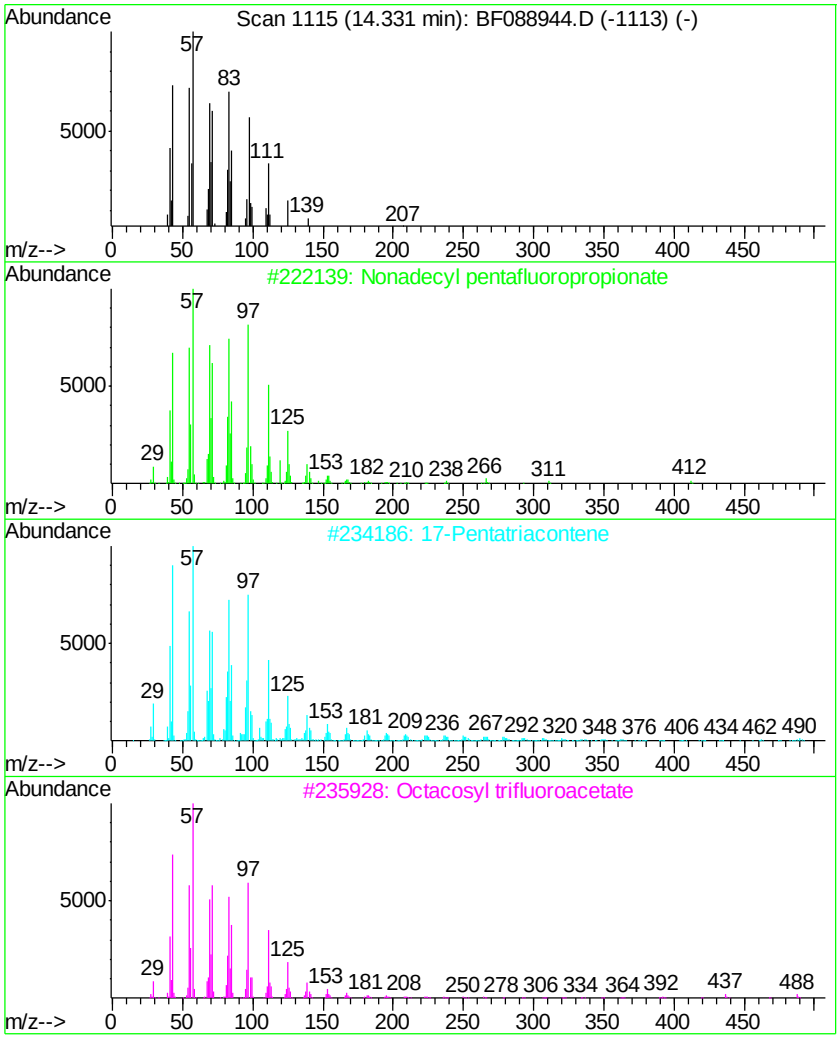
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

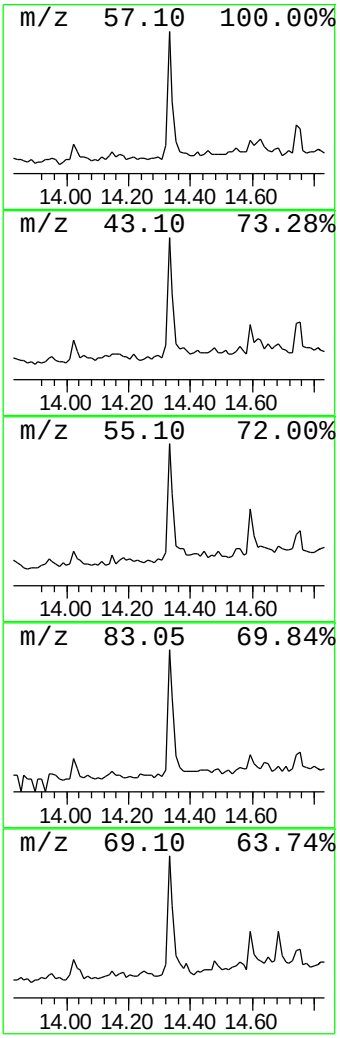
****

Peak Number 9 Nonadecyl pentafluoropropio... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	3.46 ng	59796	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	83
4	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	83
5	1-Heptacosanol	396	C27H56O	002004-39-9	76





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Data File : BF088944.D
Acq On : 13 Jul 2016 4:52
Operator : UM/SJ
Sample : H3987-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-WALL-W-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

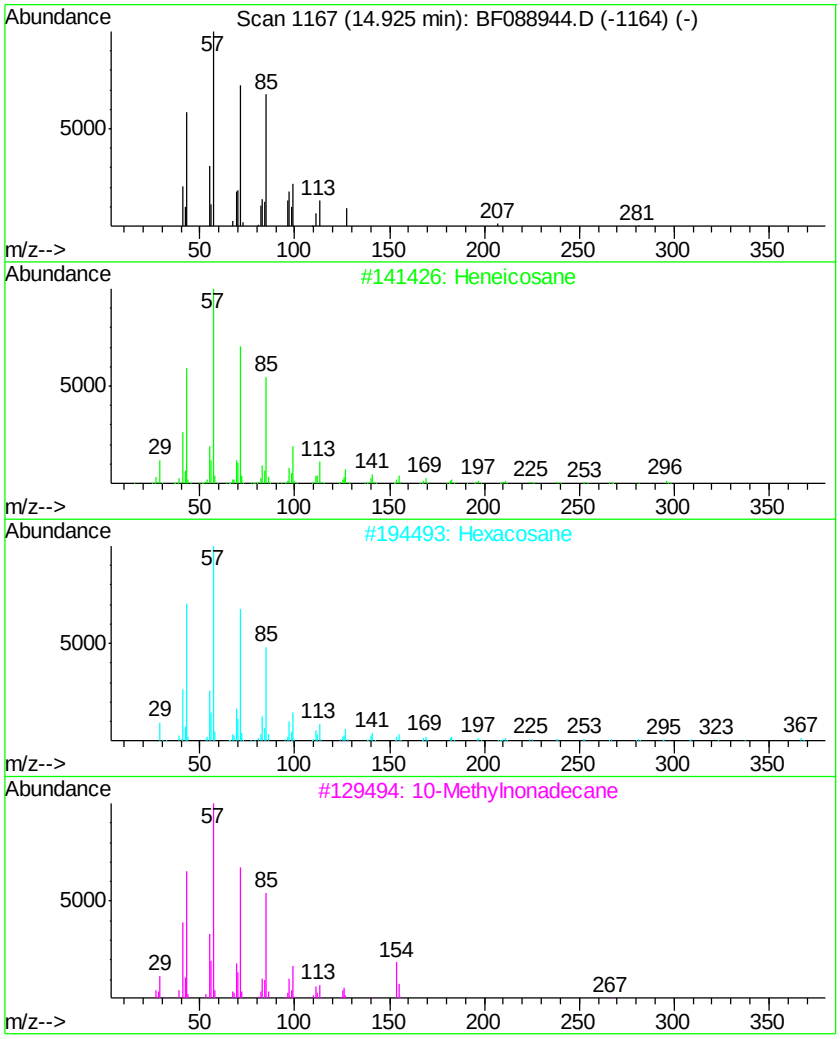
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

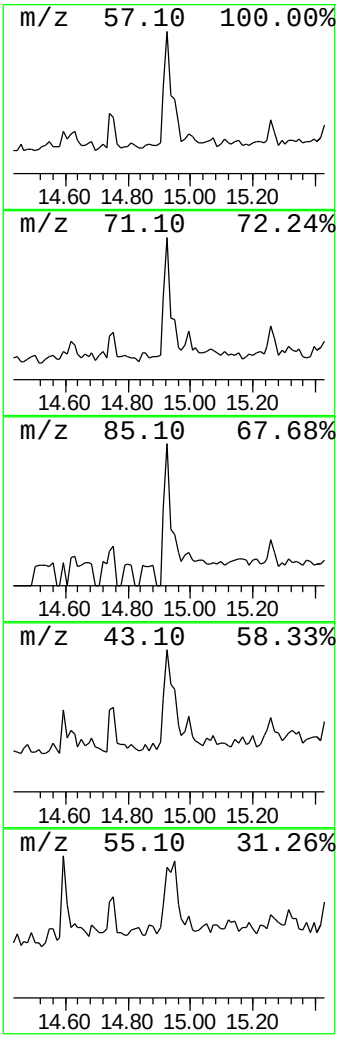
****

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	3.15 ng	46052	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Hexacosane	366	C26H54	000630-01-3	83
3	10-Methylnonadecane	282	C20H42	056862-62-5	80
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	80
5	Hexadecane	226	C16H34	000544-76-3	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088944.D
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Operator : UM/SJ
Sample : H3987-02
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Instrument : BNA_F
ClientSampleId : COMP-WALL-W-070816

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
Propane, 1,1-dime...	1.91	4.2	ng	74909	1	6.71	353902	20.0
2-Pentanone, 4-hy...	4.86	16.9	ng	298381	1	6.71	353902	20.0
unknown6.47	6.47	73.8	ng	1306640	1	6.71	353902	20.0
n-Dodecyl methacr...	10.97	2.6	ng	45821	4	11.21	355209	20.0
1-Heneicosanol	13.70	7.0	ng	121513	5	13.84	346135	20.0
Nonadecyl pentafl...	14.33	3.5	ng	59796	5	13.84	346135	20.0
Heneicosane	14.93	3.1	ng	46052	6	15.21	292232	20.0