LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

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-BF070117.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	3.028	157	160	177	rBV	28876	87141	3.21%	0.353%
2	4.875	469	474	485	rVB	382458	529540	19.50%	2.143%
3	5.298	541	546	549	rBV	2573438	2541805	93.60%	10.284%
4	6.322	715	720	723	rBV	2407582	2598841	95.70%	10.515%
5	6.451	737	742	745	rBV	2586630	2517296	92.70%	10.185%
6	6.681	777	781	785	rBV	822352	670756	24.70%	2.714%
7	6.840	804	808	811	rBV	2146982	1918144	70.64%	7.761%
8	7.240	871	876	880	rBV	1497573	1604814	59.10%	6.493%
9	7.963	994	999	1002	rBV	1046651	920222	33.89%	3.723%
10	9.039	1177	1182	1186	rBV	2614515	2715537	100.00%	10.987%
11	9.434	1245	1249	1252	rBV	471657	361199	13.30%	1.461%
12	9.710	1291	1296	1300	rBV	1019542	1019889	37.56%	4.127%
13	10.163	1369	1373	1376	rVB	46438	41330	1.52%	0.167%
14	10.498	1425	1430	1433	rBV	1638821	1579475	58.16%	6.391%
15	10.633	1450	1453	1461	rBV	70449	84761	3.12%	0.343%
16	11.080	1525	1529	1531	rBV2	53280	47513	1.75%	0.192%
17	11.192	1543	1548	1551	rBV	1075477	952485	35.08%	3.854%
18	11.598	1613	1617	1621	rVB	161468	140076	5.16%	0.567%
19	12.280	1730	1733	1735	rBV	620705	524928	19.33%	2.124%
20	12.304	1735	1737	1740	rVB	406493	328431	12.09%	1.329%
21	12.392	1749	1752	1755	rBV	81064	64853	2.39%	0.262%
22	12.774	1812	1817	1821	rBV	2056363	2208369	81.32%	8.935%
23	13.680	1967	1971	1978	rBV	121677	135397	4.99%	0.548%
24	13.816	1990	1994	1998	rBV	695972	639846	23.56%	2.589%
25	15.210	2227	2231	2238	rVB	404480	482563	17.77%	1.952%

Sum of corrected areas: 24715211

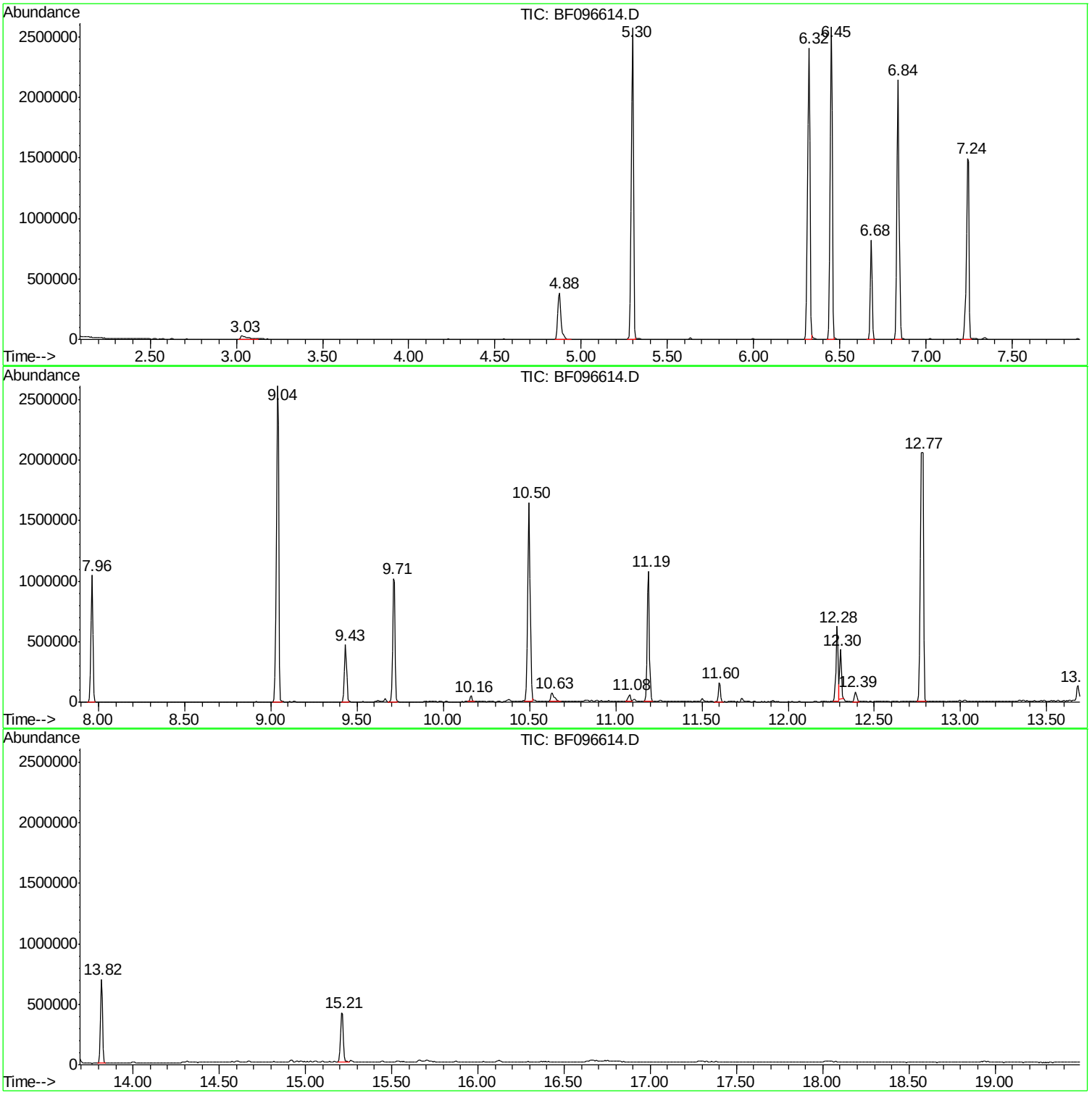
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

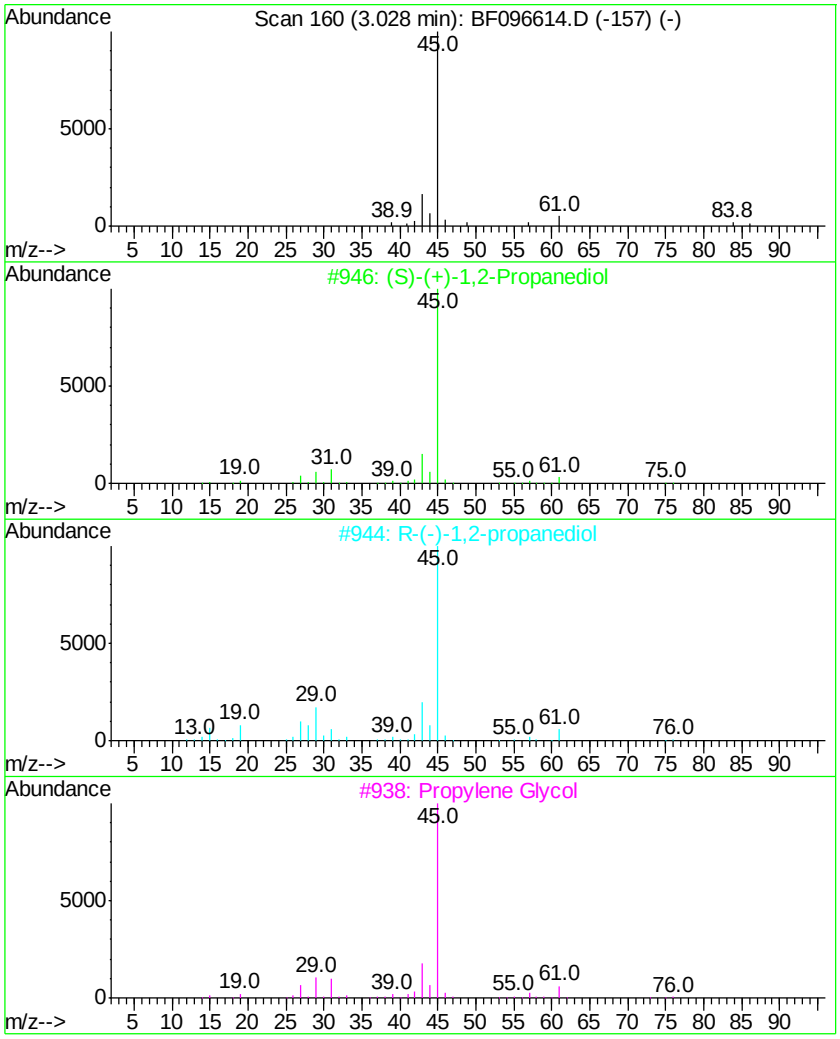
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

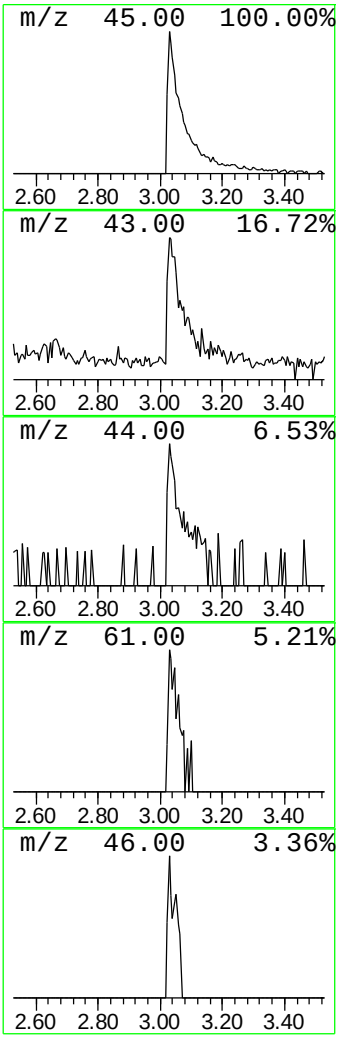
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.03	2.60 ng	87141	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Nitrobenzene, 2-bromo-4-methoxy-...	291	C9H10BrNO5	1000255-48-9	9
5	2-Butanol, (R)-	74	C4H10O	014898-79-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

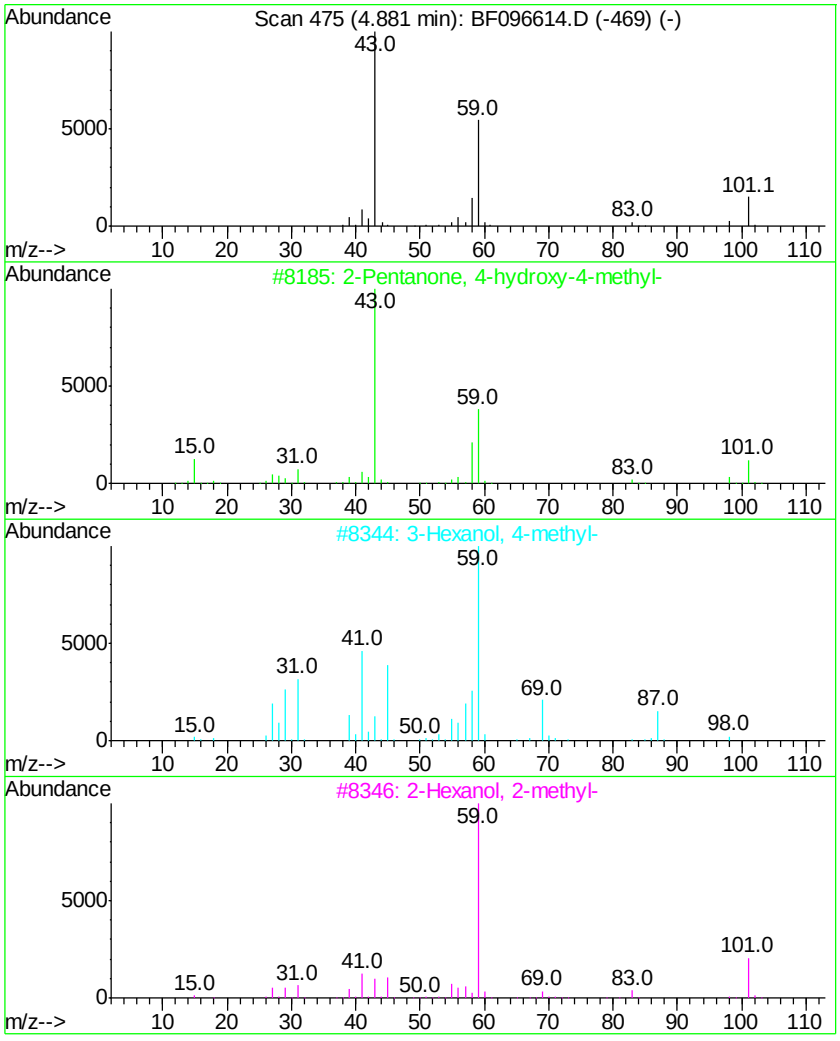
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

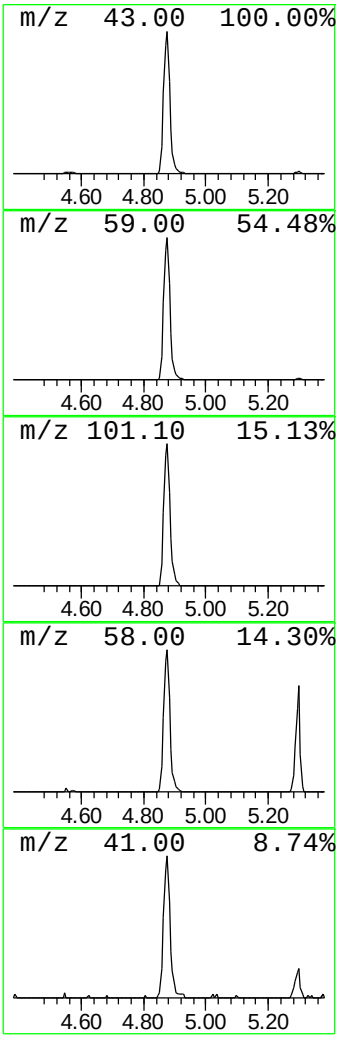
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	15.79 ng	529540	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

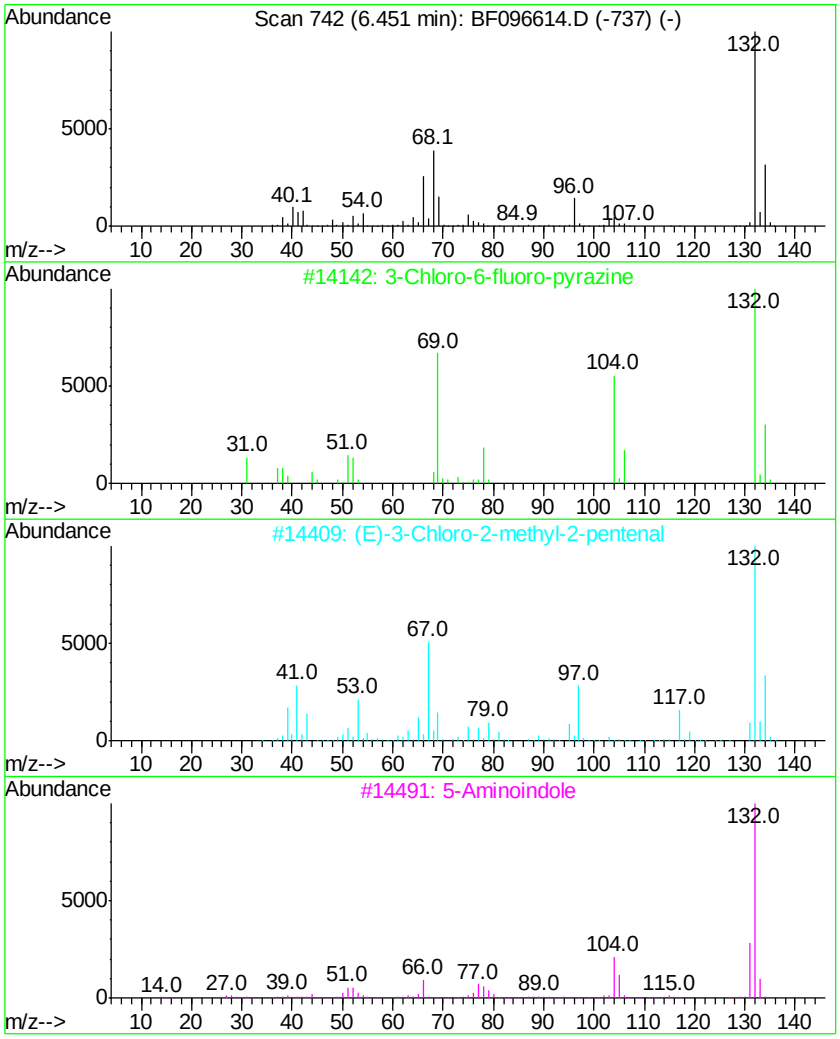
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

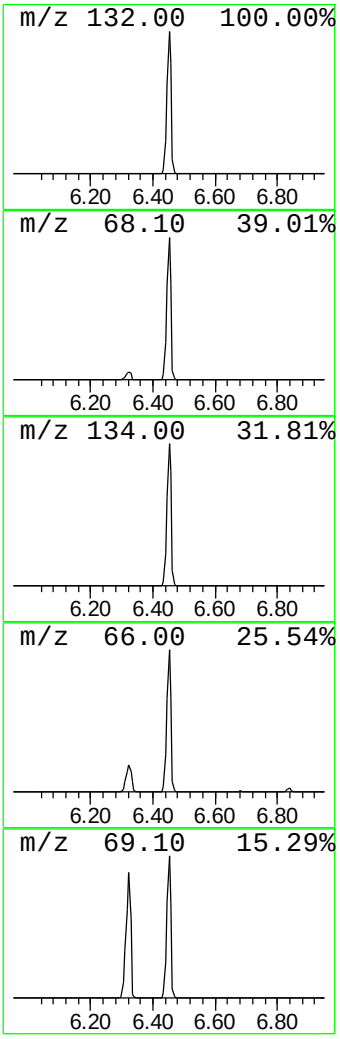
****

Peak Number 3 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	75.06 ng	2517300	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

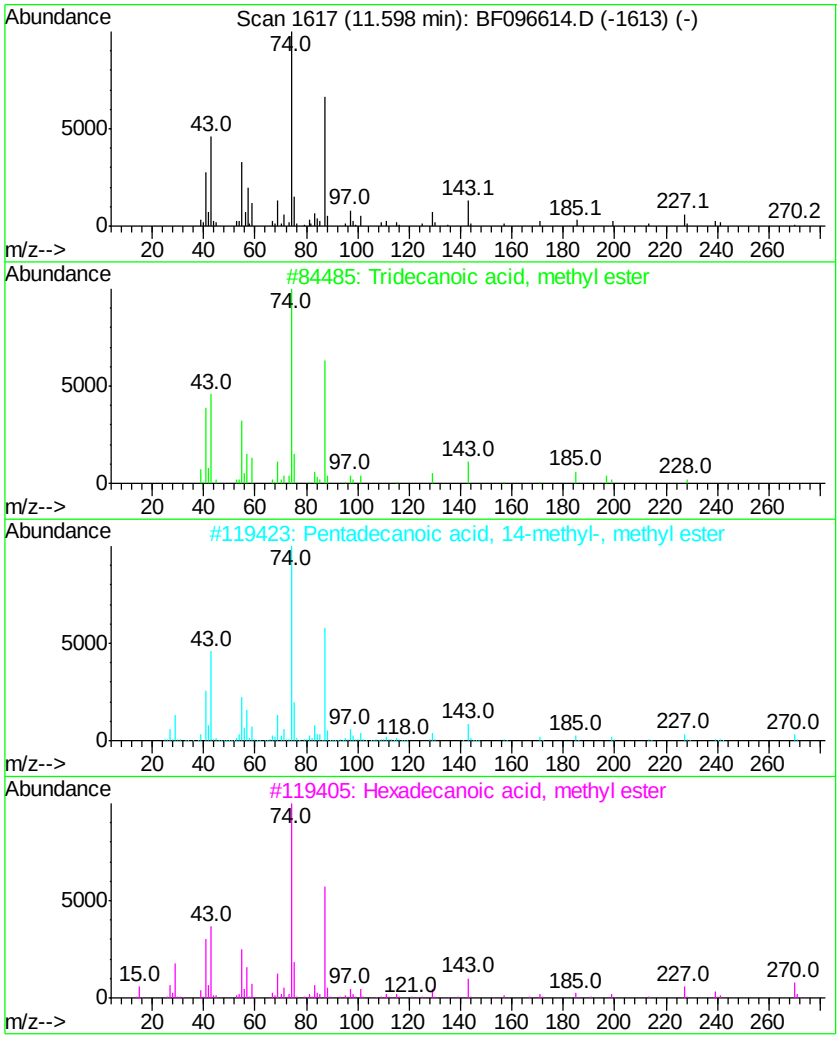
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

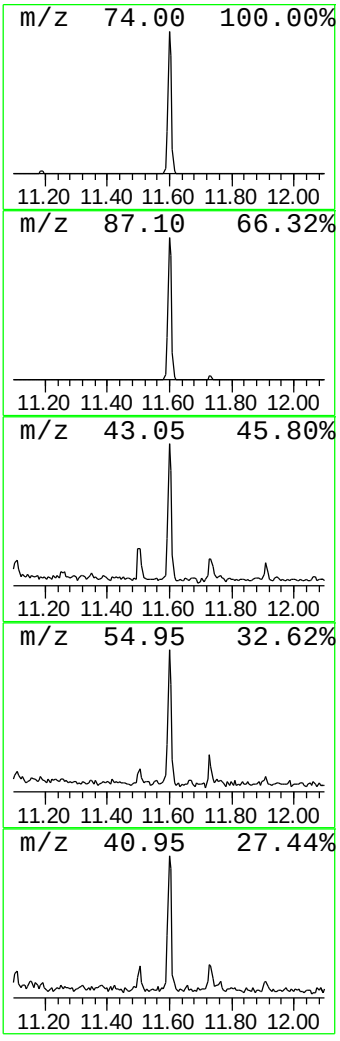
****

Peak Number 5 Tridecanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	2.94 ng	140076	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	94
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

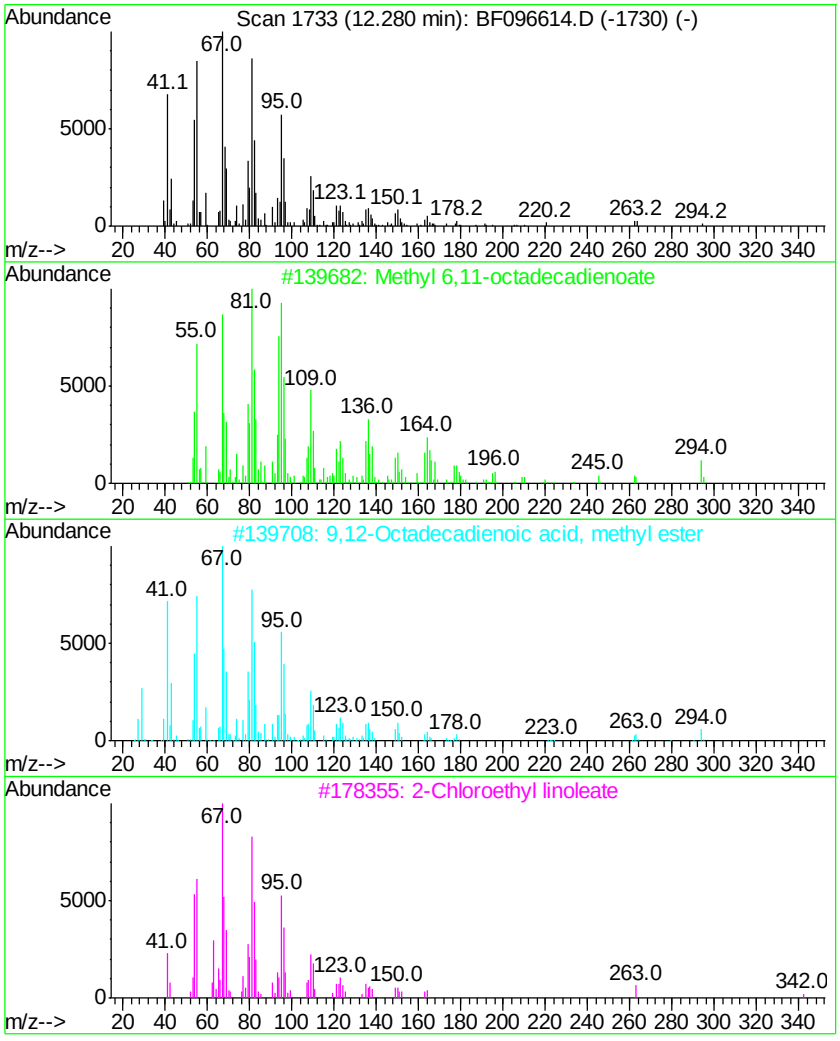
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

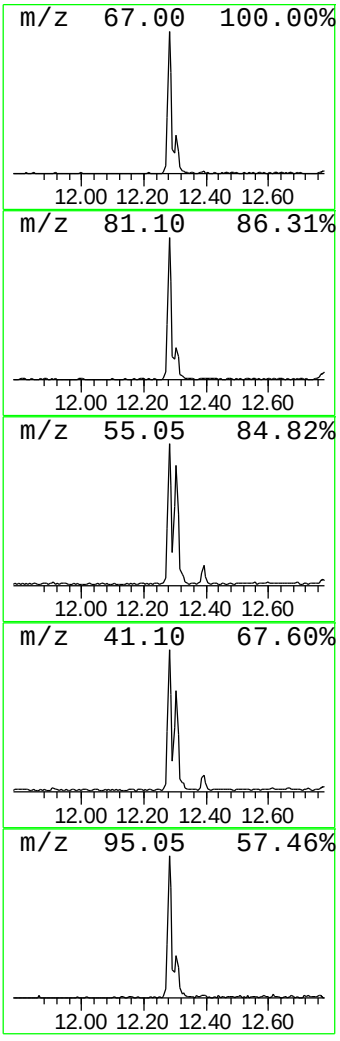
****

Peak Number 6 Methyl 6,11-octadecadienoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	11.02 ng	524928	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 6,11-octadecadienoate	294	C19H34O2	1000336-43-2	95
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	94
3	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	94
4	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	93
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	93





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

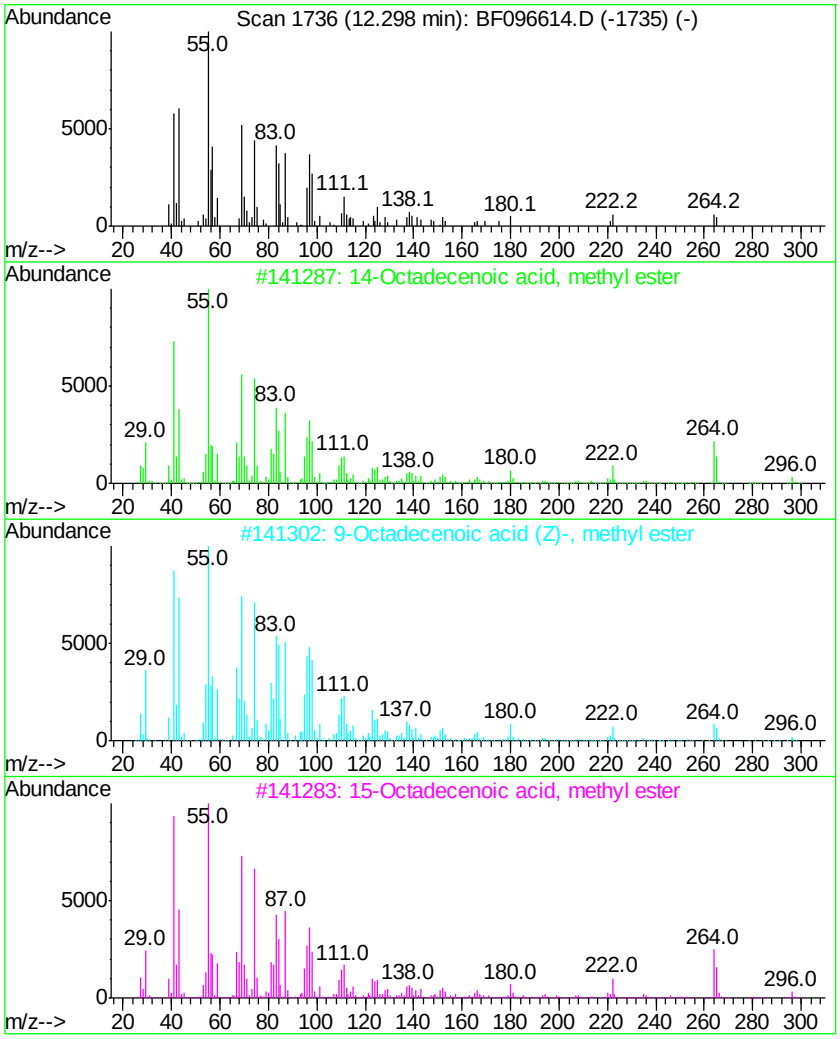
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

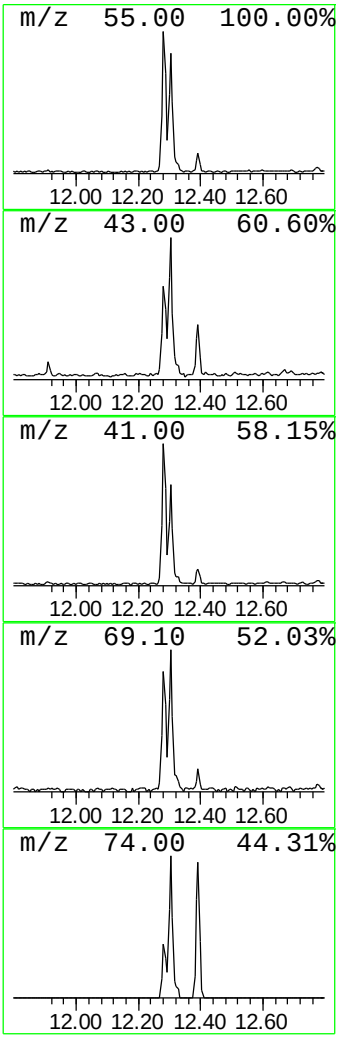
****

Peak Number 7 14-Octadecenoic acid, methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	6.90 ng	328431	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	80
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	68
5	Palmitoleic acid	254	C16H30O2	000373-49-9	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

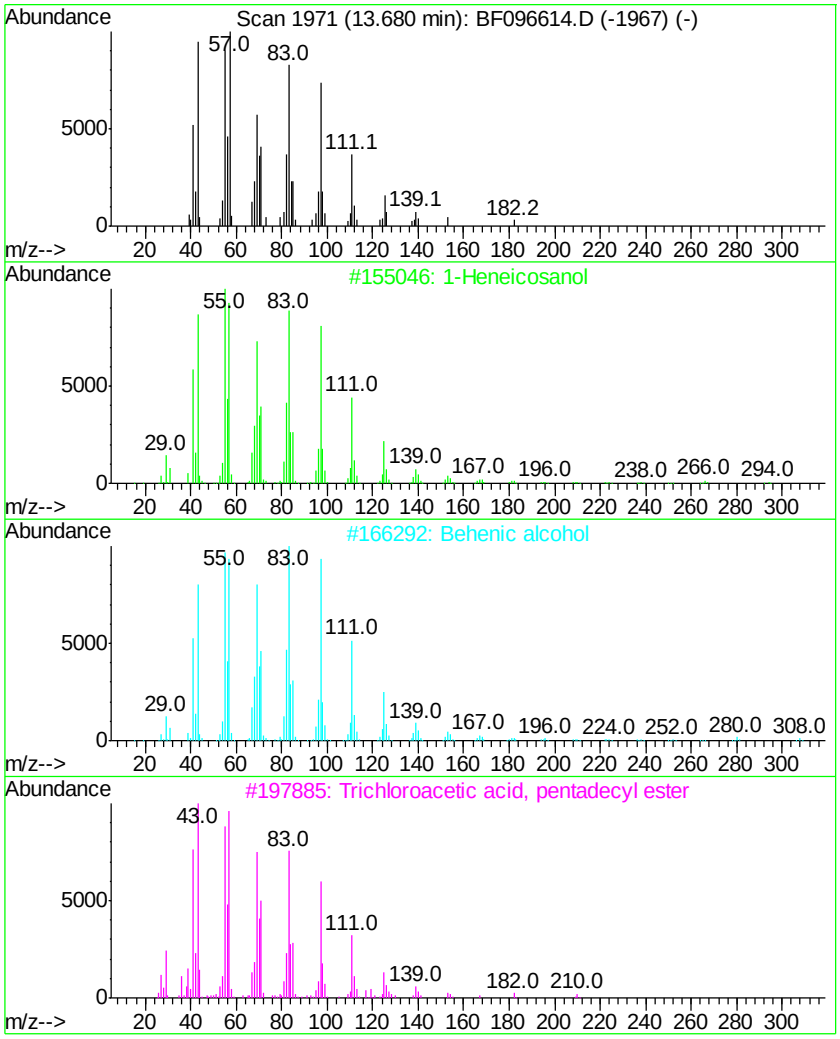
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

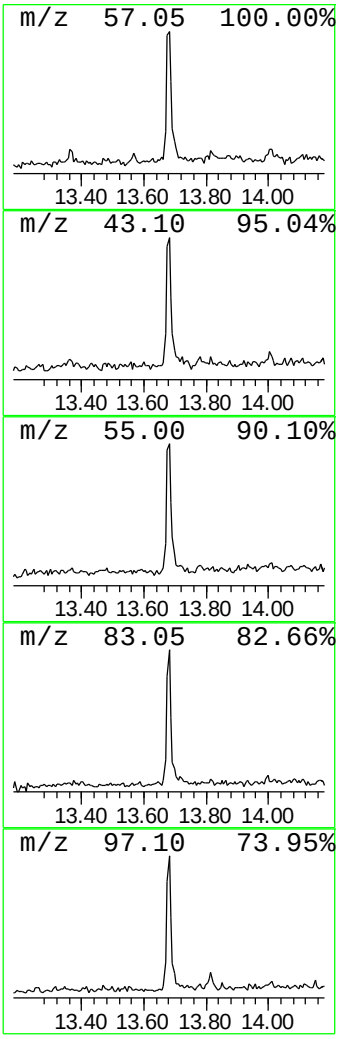
****

Peak Number 8 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	4.23 ng	135397	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
Data File : BF096614.D
Acq On : 10 Jul 2017 21:21
Operator : SJ/JU
Sample : I4071-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-06-070617-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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
(S)-(+)-1,2-Propa...	3.03	2.6	ng	87141	1	6.68	670756	20.0
2-Pentanone, 4-hy...	4.88	15.8	ng	529540	1	6.68	670756	20.0
unknown6.45	6.45	75.1	ng	2517300	1	6.68	670756	20.0
Tridecanoic acid,...	11.60	2.9	ng	140076	4	11.19	952485	20.0
Methyl 6,11-octad...	12.28	11.0	ng	524928	4	11.19	952485	20.0
14-Octadecenoic a...	12.30	6.9	ng	328431	4	11.19	952485	20.0
1-Heneicosanol	13.68	4.2	ng	135397	5	13.82	639846	20.0