LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

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-BF112115.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	4.799	242	246	258	rBV	1769732	2850140	51.70%	5.955%
2	5.256	284	286	301	rBV	4571558	5101572	92.55%	10.659%
3	6.319	376	379	381	rBV	4818658	5512396	100.00%	11.517%
4	6.422	386	388	391	rBV	4715224	4676642	84.84%	9.771%
5	6.650	405	408	410	rBV	1356152	1267904	23.00%	2.649%
6	6.810	419	422	424	rBV	3257720	3706856	67.25%	7.745%
7	7.222	455	458	460	rBV	3328980	3307958	60.01%	6.911%
8	7.942	518	521	523	rBV	1170624	1556811	28.24%	3.253%
9	8.890	602	604	608	rBV2	38755	80686	1.46%	0.169%
10	9.016	612	615	618	rBV	5229392	4980291	90.35%	10.405%
11	9.416	648	650	652	rBV	1190460	1007085	18.27%	2.104%
12	9.633	667	669	671	rBV	64695	56227	1.02%	0.117%
13	9.679	671	673	676	rBV	1160813	1577174	28.61%	3.295%
14	10.136	704	713	714	rBV	103607	129393	2.35%	0.270%
15	10.353	729	732	735	rBV	40833	67871	1.23%	0.142%
16	10.468	740	742	745	rBV	2413094	2571979	46.66%	5.374%
17	10.605	752	754	758	rBV	112539	159159	2.89%	0.333%
18	11.153	800	802	805	rBV	1024348	1373877	24.92%	2.870%
19	11.714	849	851	854	rBV2	235800	264285	4.79%	0.552%
20	12.365	906	908	910	rBV	103517	112031	2.03%	0.234%
21	12.411	910	912	915	rVV4	46814	79366	1.44%	0.166%
22	12.491	917	919	922	rBV	330038	382359	6.94%	0.799%
23	12.594	925	928	931	rVV2	75252	136155	2.47%	0.284%
24	12.742	939	941	944	rBV	3594366	3723188	67.54%	7.779%
25	13.222	981	983	986	rBV3	41670	71281	1.29%	0.149%
26	13.657	1019	1021	1024	rBV	59770	87213	1.58%	0.182%
27	13.782	1030	1032	1035	rBV2	1476870	1608873	29.19%	3.361%
28	14.274	1073	1075	1076	rBV2	46419	62938	1.14%	0.131%
29	14.319	1077	1079	1081	rVB2	76157	102447	1.86%	0.214%
30	14.868	1125	1127	1129	rVB	74912	66686	1.21%	0.139%
31	15.154	1149	1152	1155	rBV	645523	902316	16.37%	1.885%
32	15.577	1186	1189	1191	rBV	59250	96962	1.76%	0.203%
33	16.000	1224	1226	1230	rVB3	59202	112638	2.04%	0.235%
34	16.503	1267	1270	1273	rVB2	37789	69607	1.26%	0.145%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

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-BF112115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 47862366

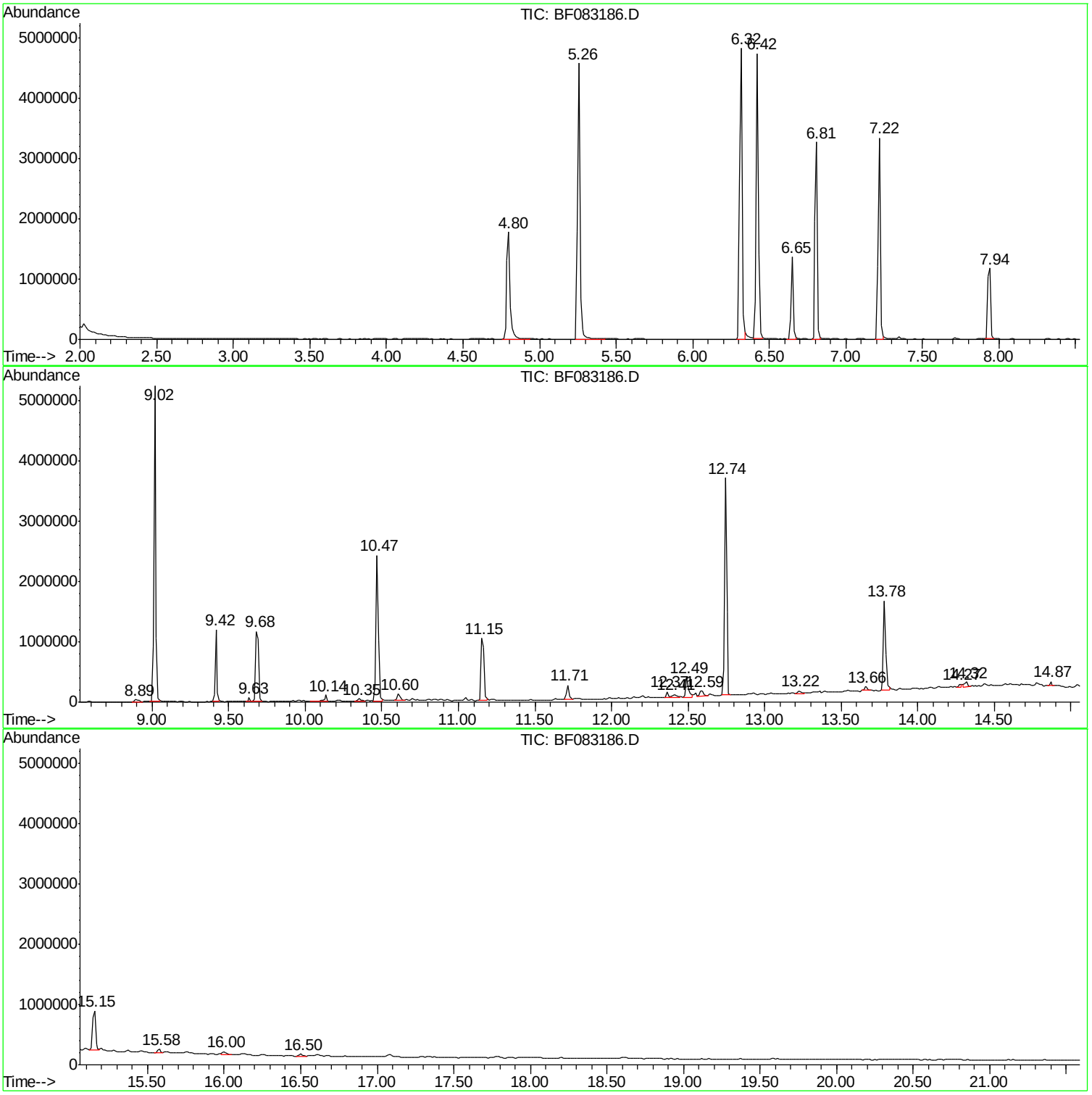
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

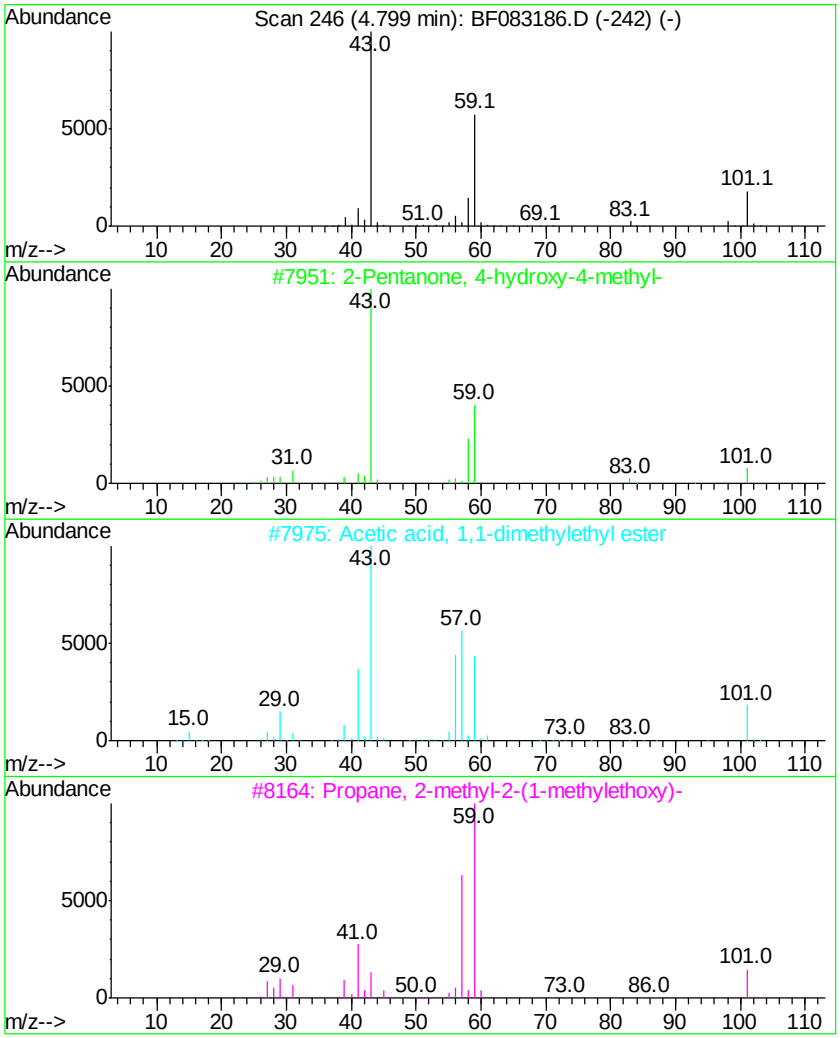
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

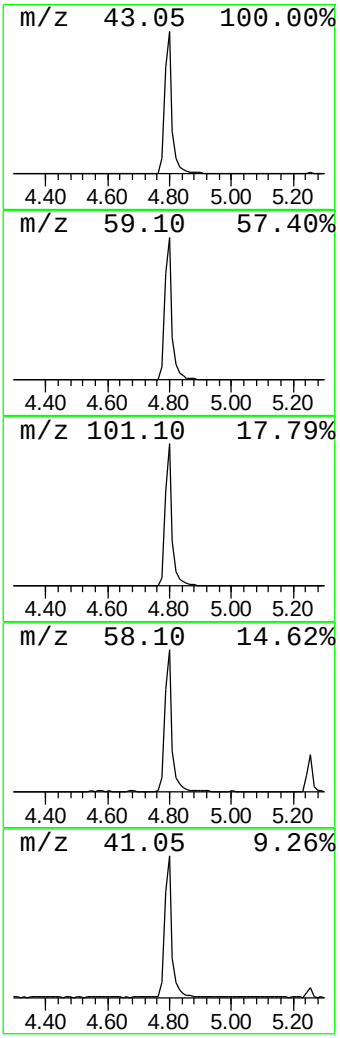
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	44.96 ng	2850140	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

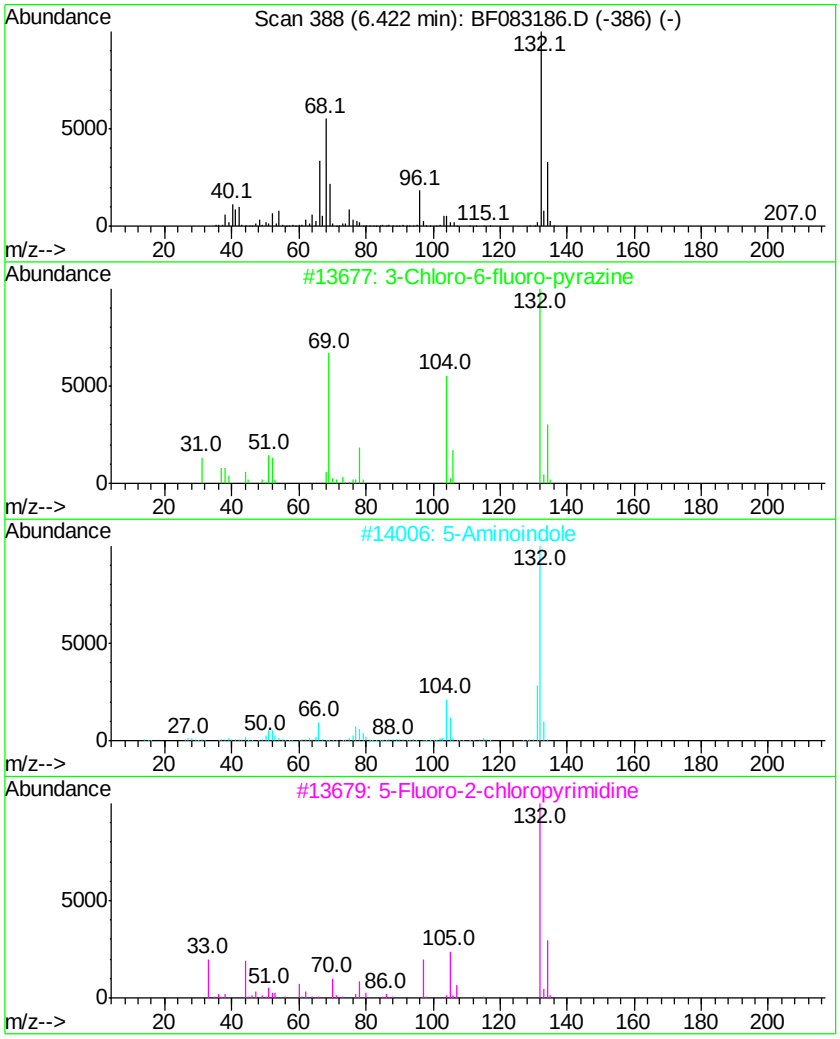
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

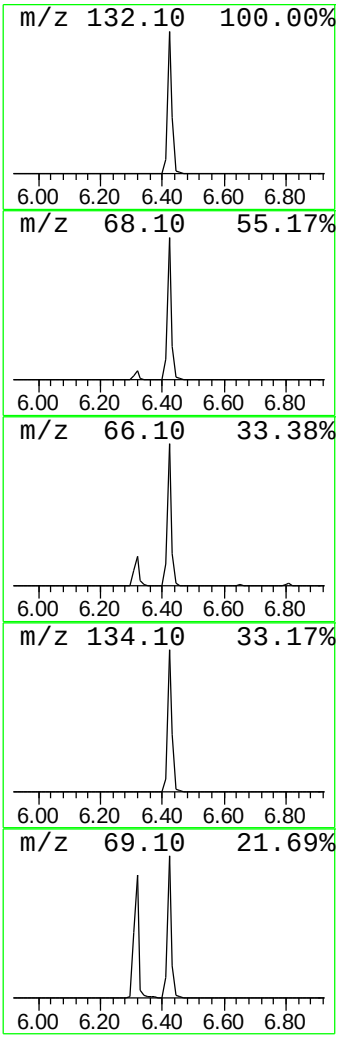
****

Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	73.77 ng	4676640	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	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

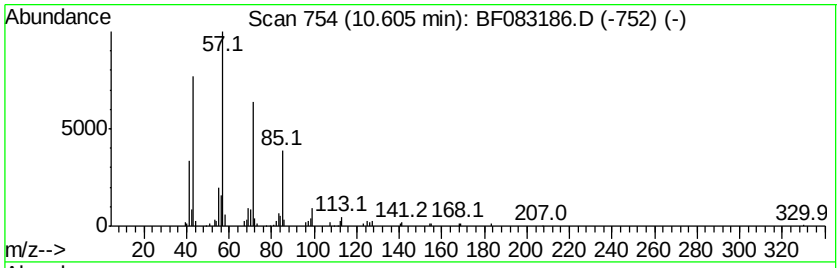
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

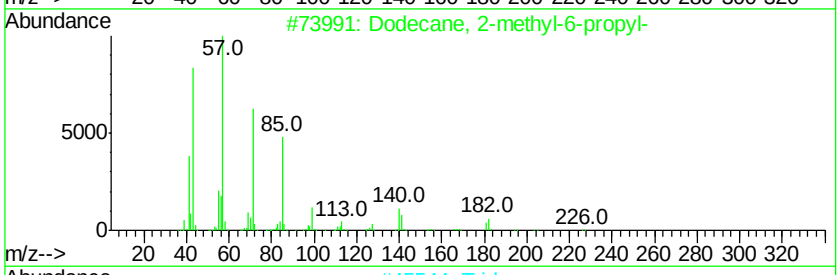
****

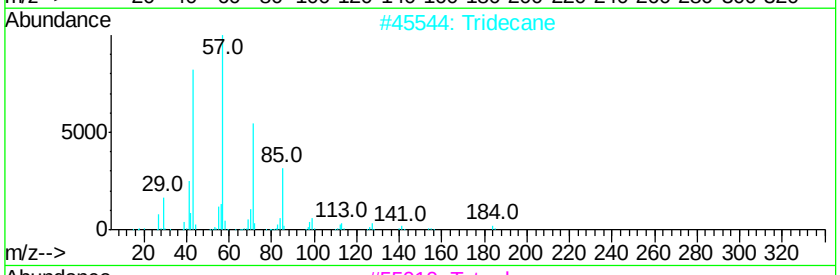
Peak Number 4 Dodecane, 2-methyl-6-propyl- Concentration Rank 7

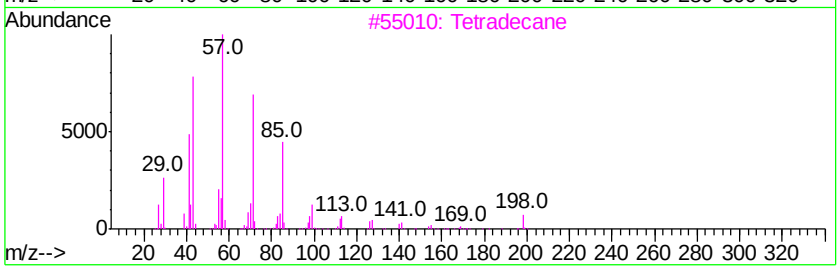
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.32 ng	159159	Phenanthrene-d10	11.16

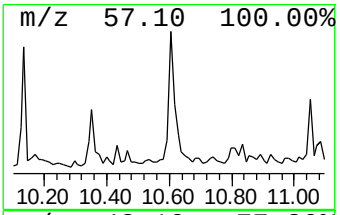
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
2	Tridecane	184	C13H28	000629-50-5	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80

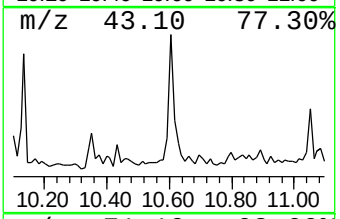


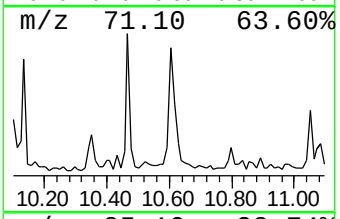


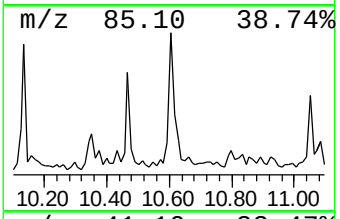


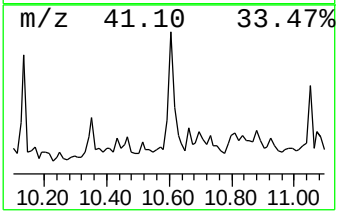












Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

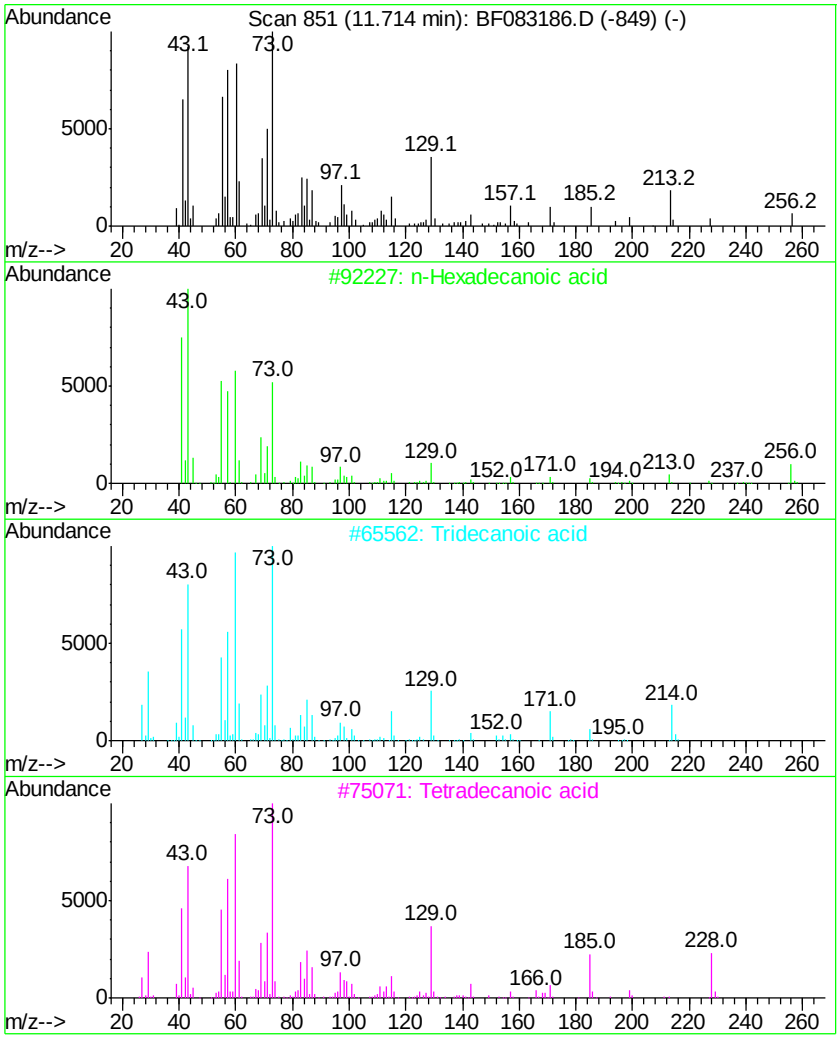
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

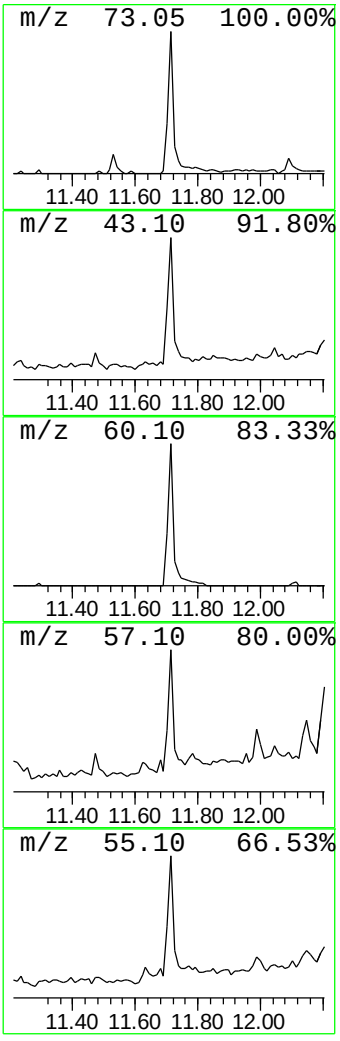
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	3.85 ng	264285	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55
5	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

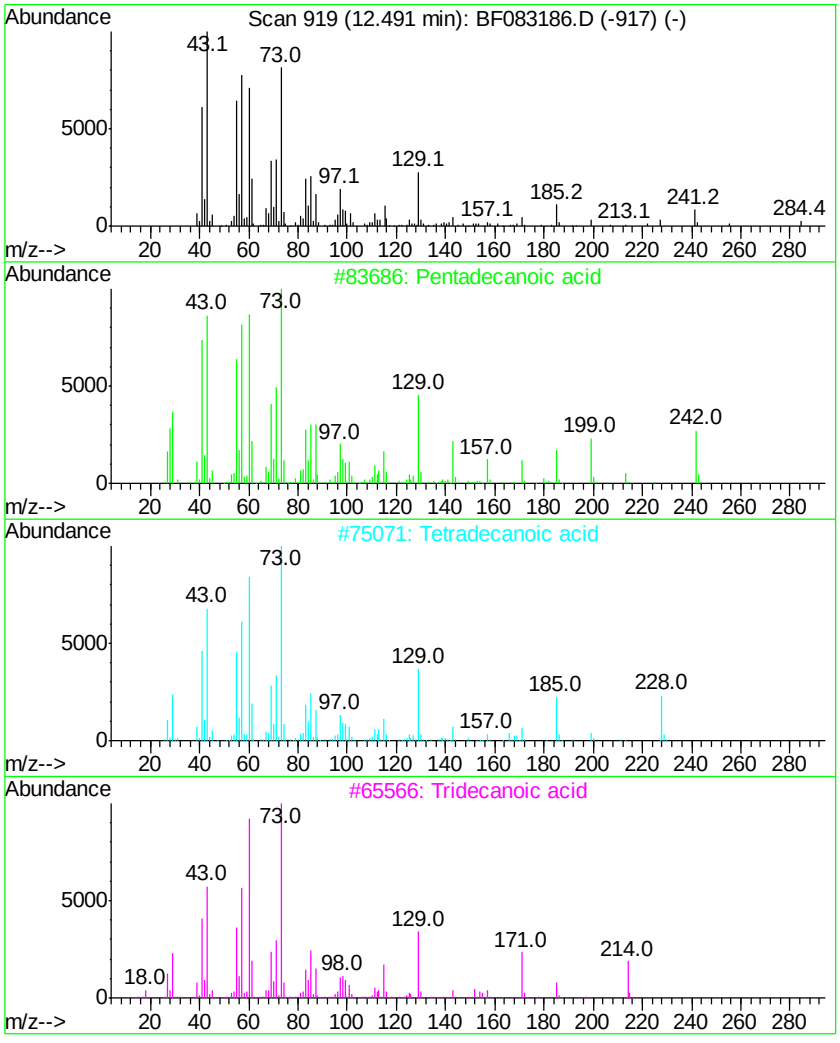
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

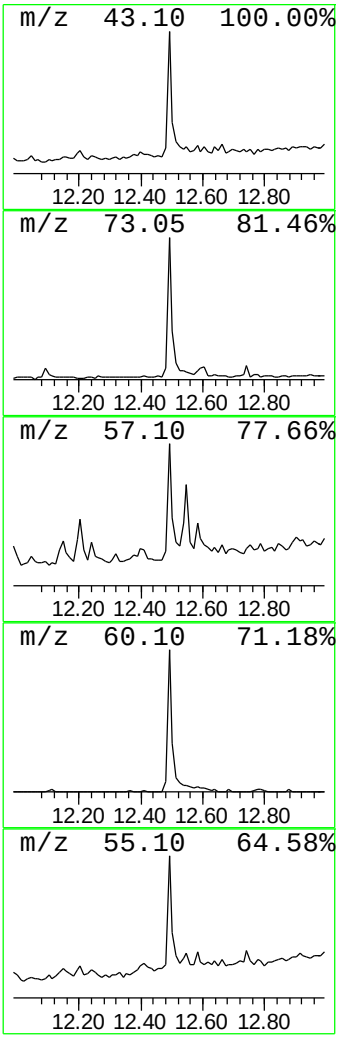
****

Peak Number 6 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	4.75 ng	382359	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
3	Tridecanoic acid	214	C13H26O2	000638-53-9	50
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
5	Lactose	342	C12H22O11	000063-42-3	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

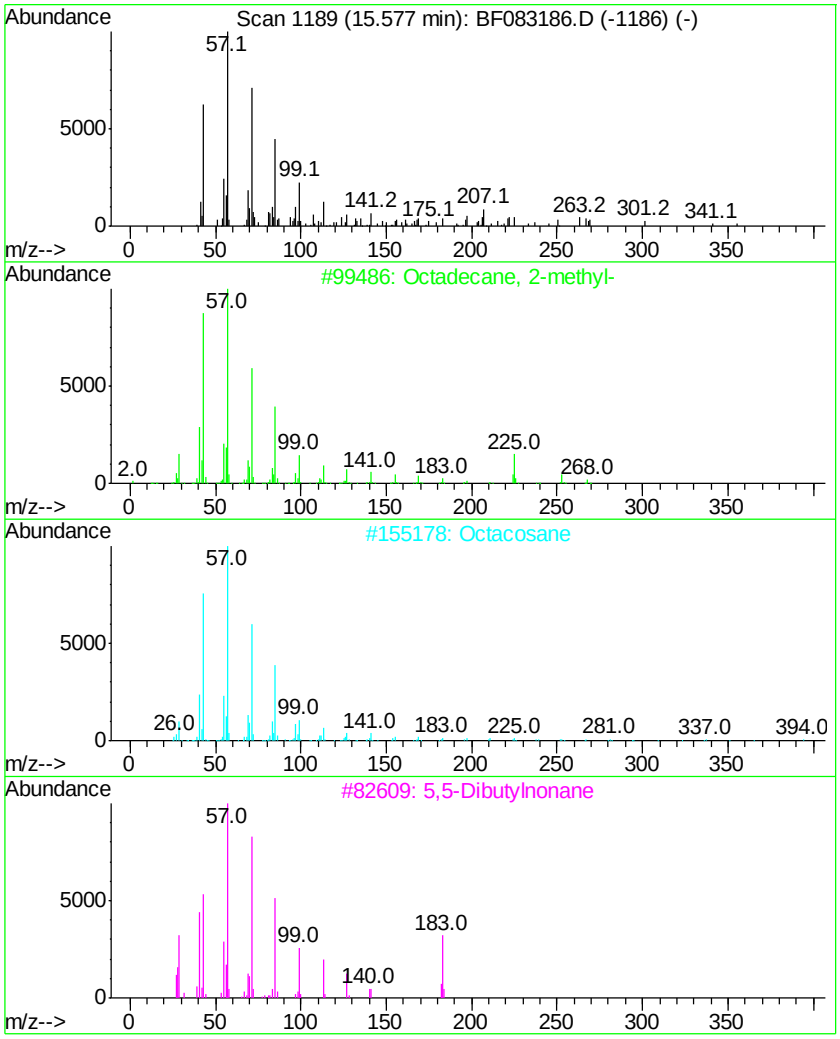
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

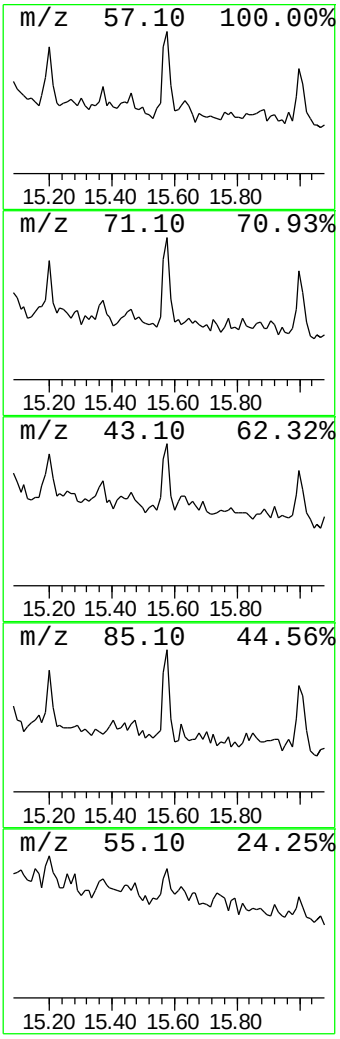
****

Peak Number 7 Octadecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	2.15 ng	96962	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	76
2	Octacosane	394	C28H58	000630-02-4	74
3	5,5-Dibutylnonane	240	C17H36	006008-17-9	64
4	Heptacosane	380	C27H56	000593-49-7	64
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

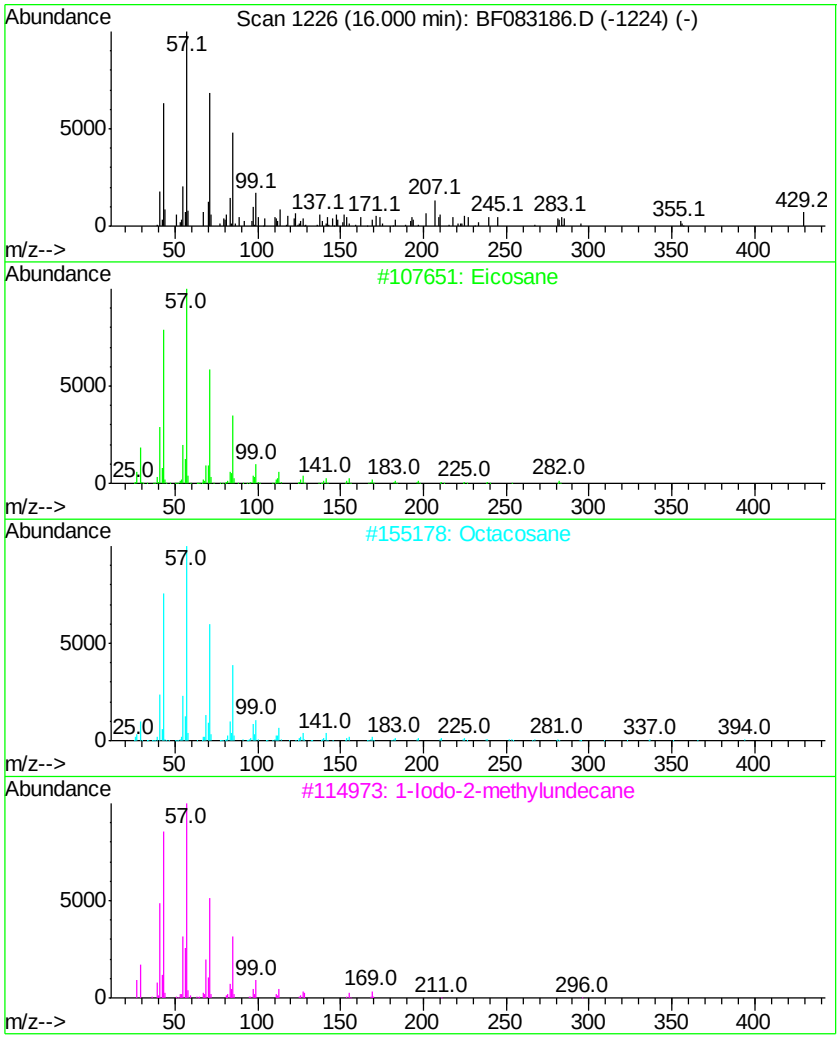
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

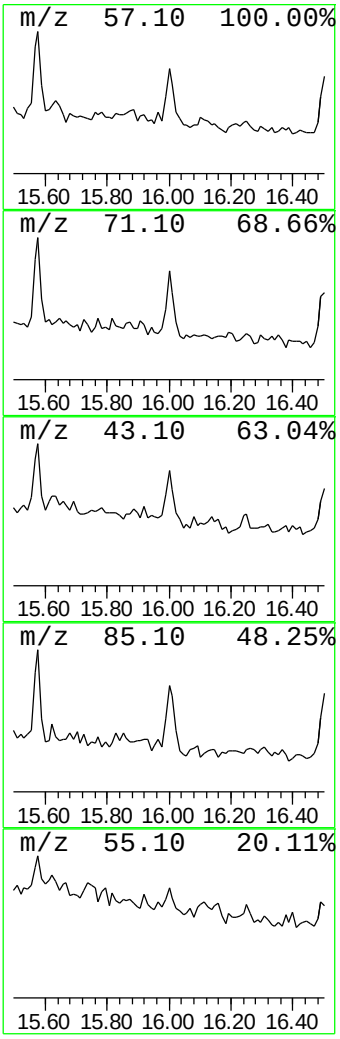
****

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.50 ng	112638	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	64
2	Octacosane	394	C28H58	000630-02-4	59
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	53
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112215\
Data File : BF083186.D
Acq On : 23 Nov 2015 4:31
Operator : UM/IZ
Sample : G4475-04
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	45.0	ng	2850140	1	6.65	1267900	20.0
unknown6.42	6.42	73.8	ng	4676640	1	6.65	1267900	20.0
Dodecane, 2-methy...	10.60	2.3	ng	159159	4	11.16	1373880	20.0
n-Hexadecanoic acid	11.71	3.9	ng	264285	4	11.16	1373880	20.0
Pentadecanoic acid	12.49	4.8	ng	382359	5	13.78	1608870	20.0
Octadecane, 2-met...	15.58	2.1	ng	96962	6	15.15	902316	20.0
Eicosane	16.00	2.5	ng	112638	6	15.15	902316	20.0