LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120516\
Data File : BF091435.D
Acq On : 5 Dec 2016 23:13
Operator : UM/SJ
Sample : H5802-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-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-BF112916.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	2.367	4	7	10	rVB	332004	460346	7.32%	1.085%
2	2.493	15	18	24	rVB	106439	176844	2.81%	0.417%
3	4.070	153	156	159	rVB	86636	110260	1.75%	0.260%
4	5.030	238	240	246	rBV	481077	774263	12.32%	1.825%
5	5.453	274	277	279	rBV	3537855	3545482	56.41%	8.357%
6	6.482	364	367	369	rBV	2610973	2779846	44.23%	6.552%
7	6.619	376	379	381	rBV	4751865	4793241	76.27%	11.298%
8	6.847	397	399	401	rVB	1137357	940058	14.96%	2.216%
9	7.007	410	413	415	rBV	4135916	3748102	59.64%	8.834%
10	7.419	445	449	451	rBV	1911880	2987673	47.54%	7.042%
11	7.499	454	456	462	rVB2	44550	84845	1.35%	0.200%
12	8.127	509	511	514	rBV	847695	1057025	16.82%	2.491%
13	9.213	603	606	608	rBV	5381003	5175853	82.36%	12.200%
14	9.888	662	665	667	rBV	1537555	1365363	21.73%	3.218%
15	10.676	731	734	736	rBV	3906911	4113437	65.45%	9.696%
16	11.362	792	794	797	rBV	1198724	1443463	22.97%	3.402%
17	11.899	839	841	849	rBV2	240538	278814	4.44%	0.657%
18	12.688	908	910	917	rBV	211326	249764	3.97%	0.589%
19	12.962	931	934	936	rBV	5277316	6284694	100.00%	14.813%
20	13.854	1009	1012	1018	rBV	60229	65722	1.05%	0.155%
21	14.002	1022	1025	1027	rBV	961192	1105752	17.59%	2.606%
22	15.431	1146	1150	1152	rBV	584395	885002	14.08%	2.086%

Sum of corrected areas: 42425849

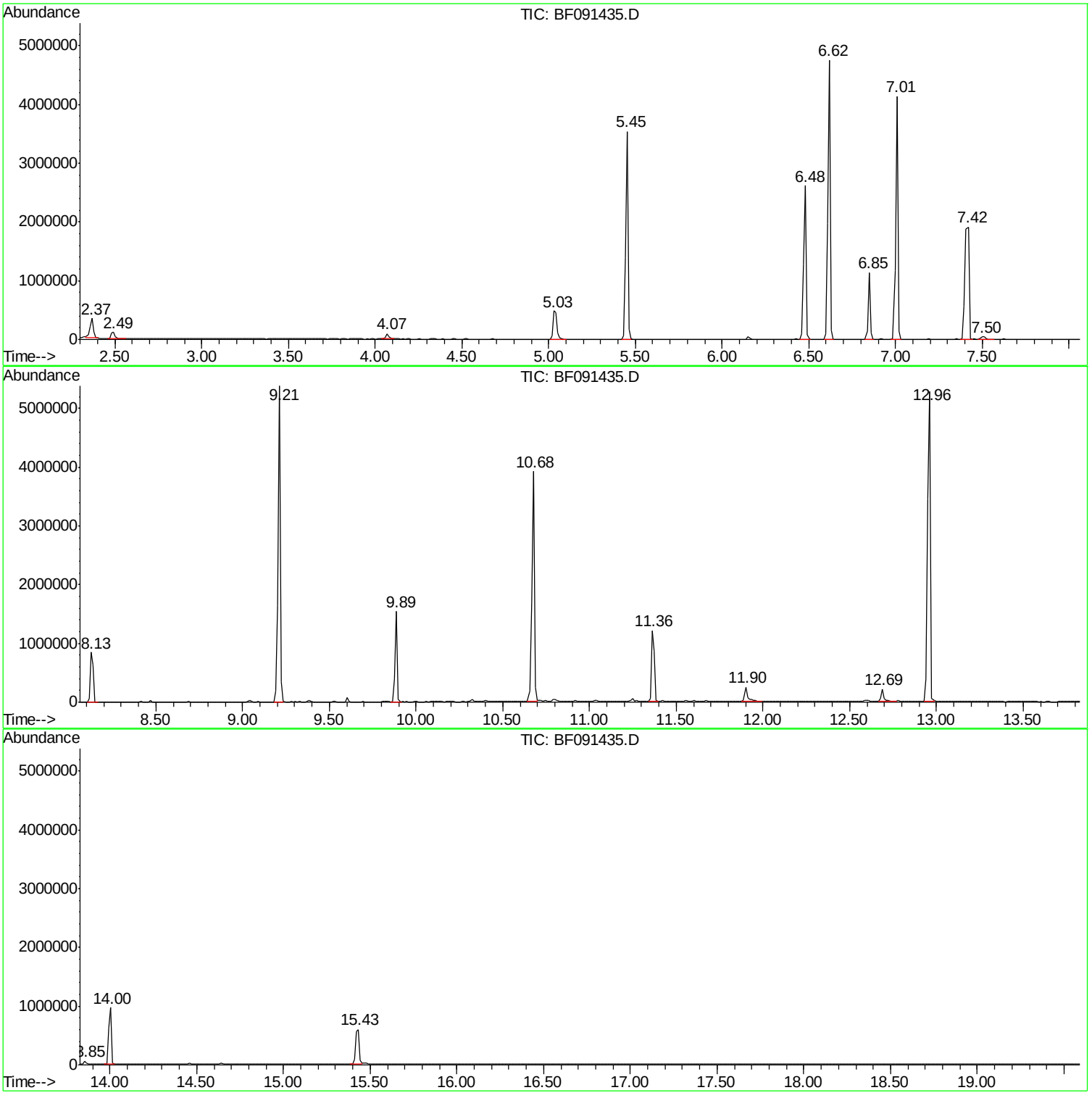
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120516\
Data File : BF091435.D
Acq On : 5 Dec 2016 23:13
Operator : UM/SJ
Sample : H5802-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120516\
Data File : BF091435.D
Acq On : 5 Dec 2016 23:13
Operator : UM/SJ
Sample : H5802-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

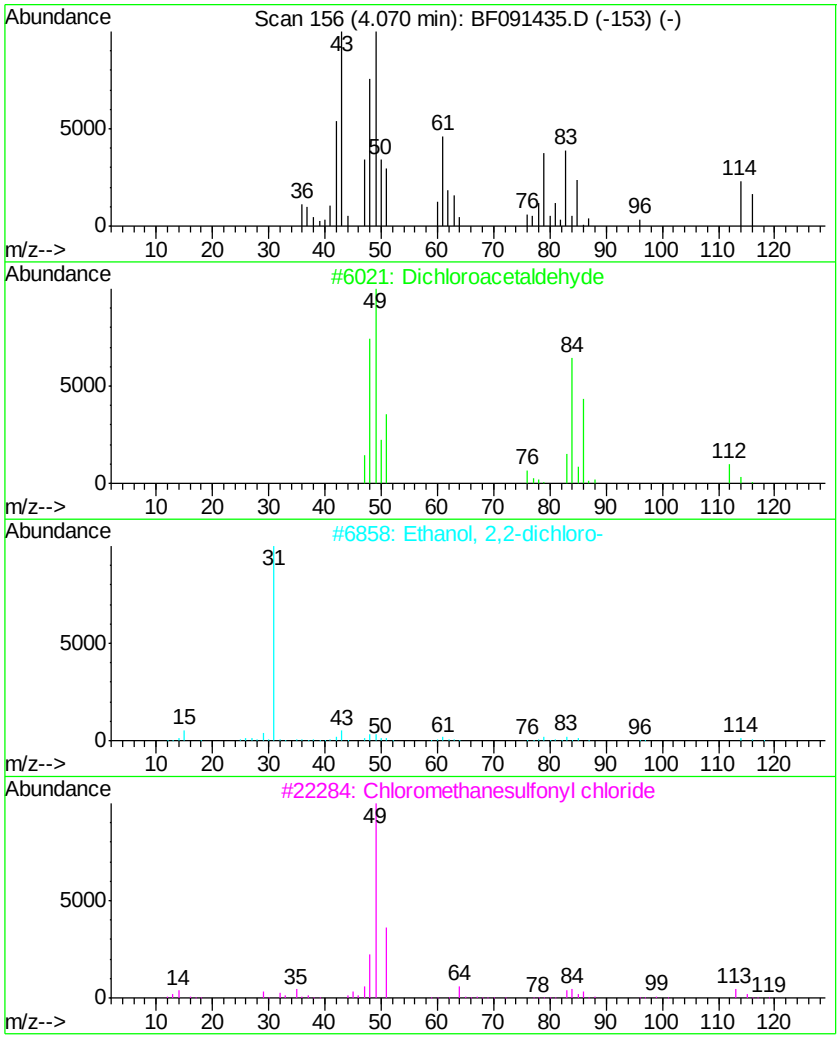
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

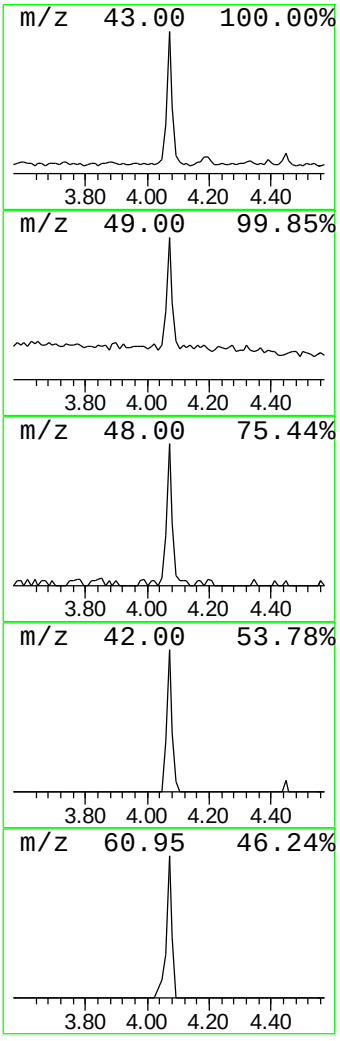
****

Peak Number 2 unknown4.07 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.07	2.35 ng	110260	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetaldehyde	112	C2H2Cl2O	000079-02-7	42
2	Ethanol, 2,2-dichloro-	114	C2H4Cl2O	000598-38-9	18
3	Chloromethanesulfonyl chloride	148	CH2Cl2O2S	003518-65-8	9
4	Ethyl Chloride	64	C2H5Cl	000075-00-3	9
5	Acetic acid, dichloro-	128	C2H2Cl2O2	000079-43-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120516\
Data File : BF091435.D
Acq On : 5 Dec 2016 23:13
Operator : UM/SJ
Sample : H5802-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

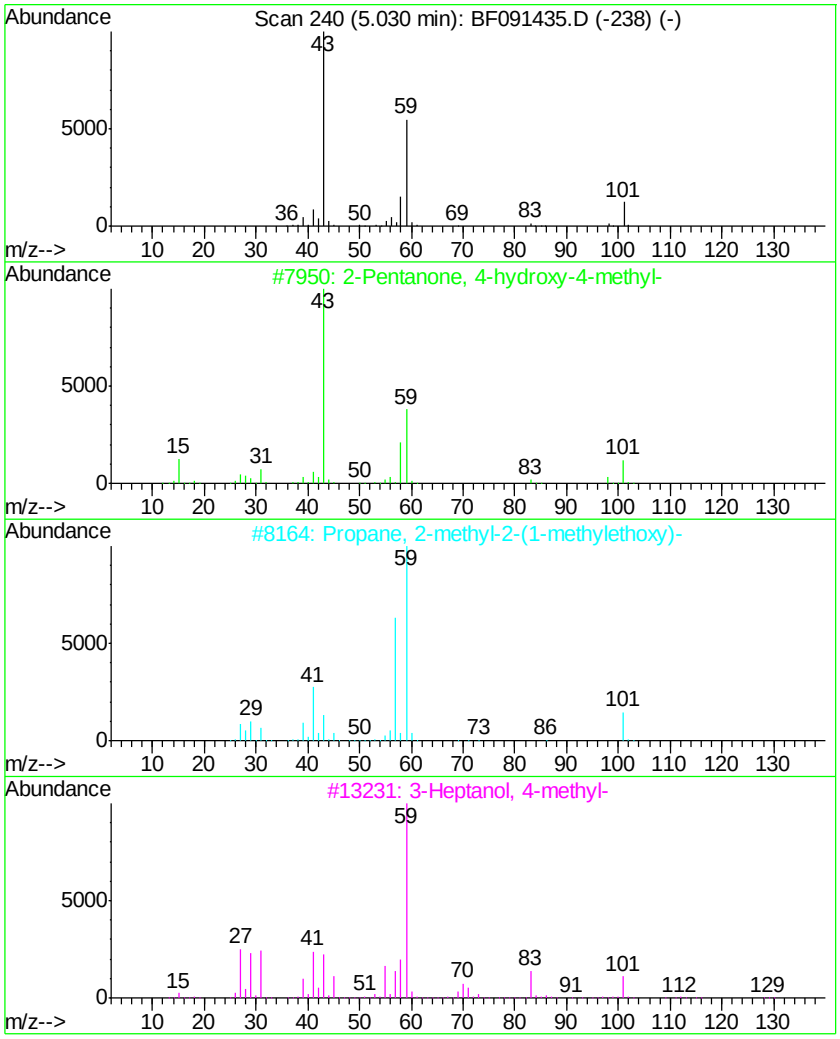
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

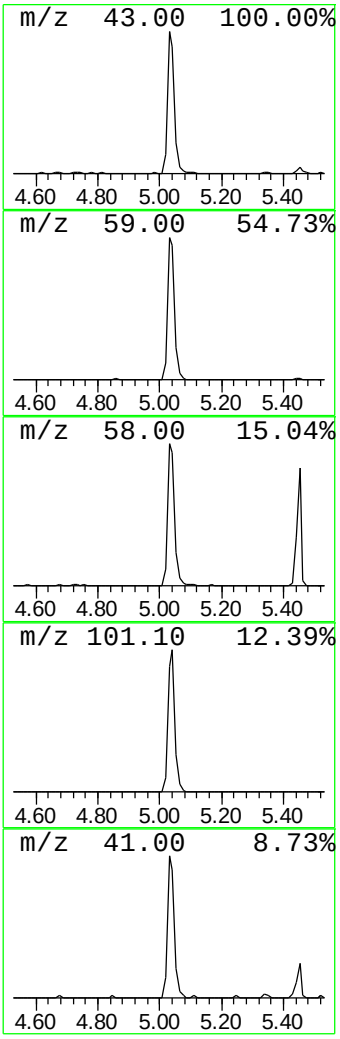
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	16.47 ng	774263	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120516\
Data File : BF091435.D
Acq On : 5 Dec 2016 23:13
Operator : UM/SJ
Sample : H5802-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

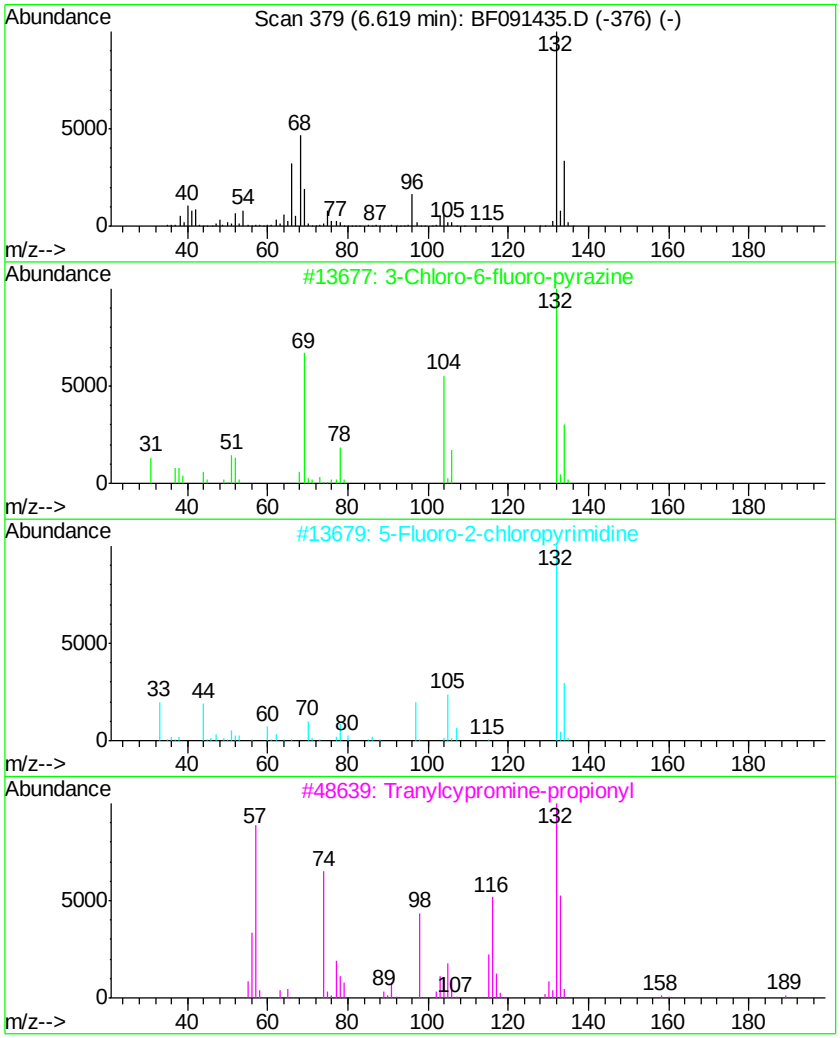
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

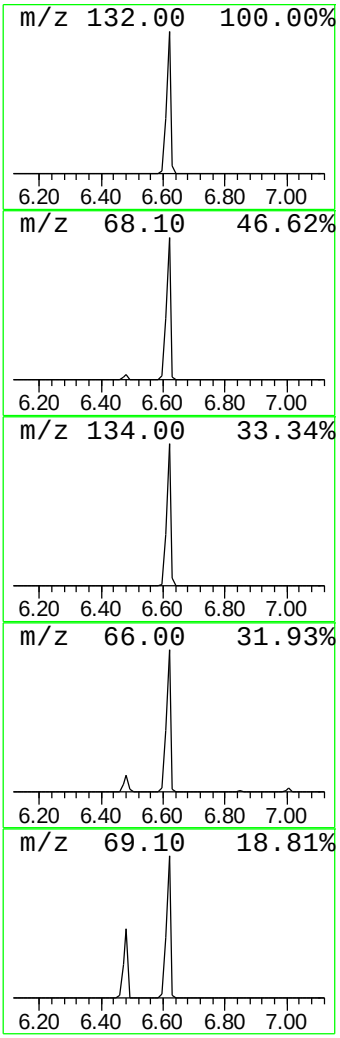
****

Peak Number 4 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	101.98 ng	4793240	1,4-Dichlorobenzene-d4	6.85

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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120516\
Data File : BF091435.D
Acq On : 5 Dec 2016 23:13
Operator : UM/SJ
Sample : H5802-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

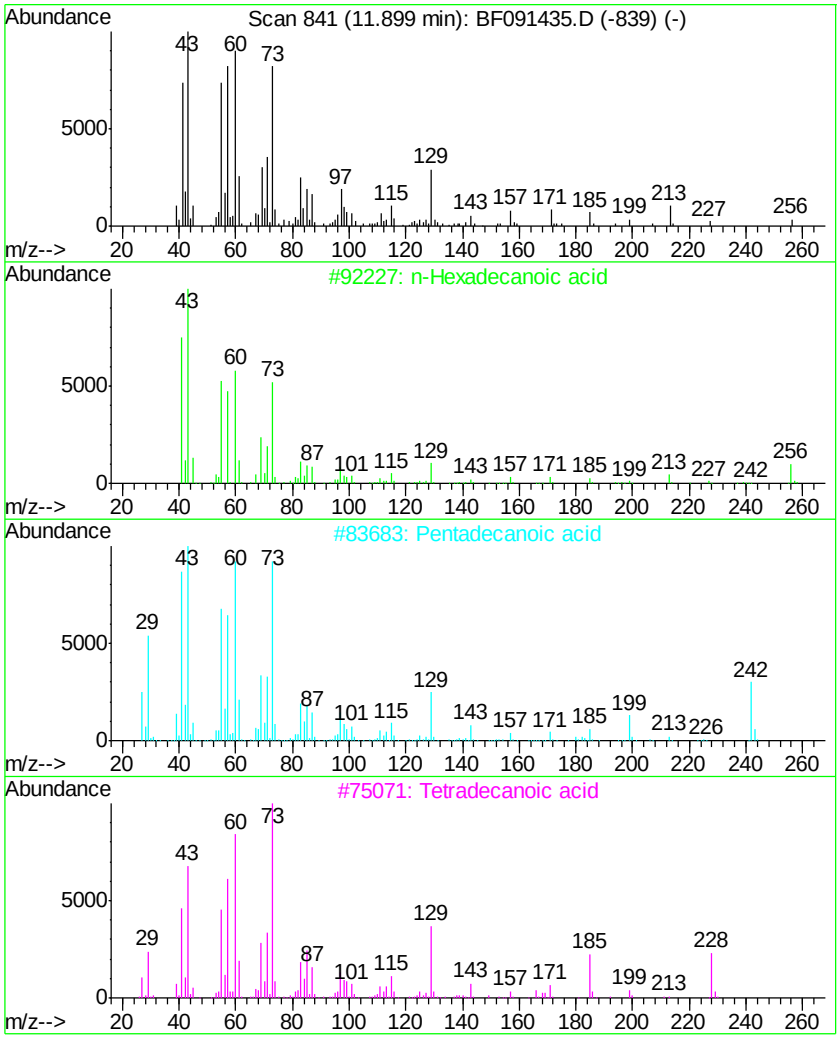
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

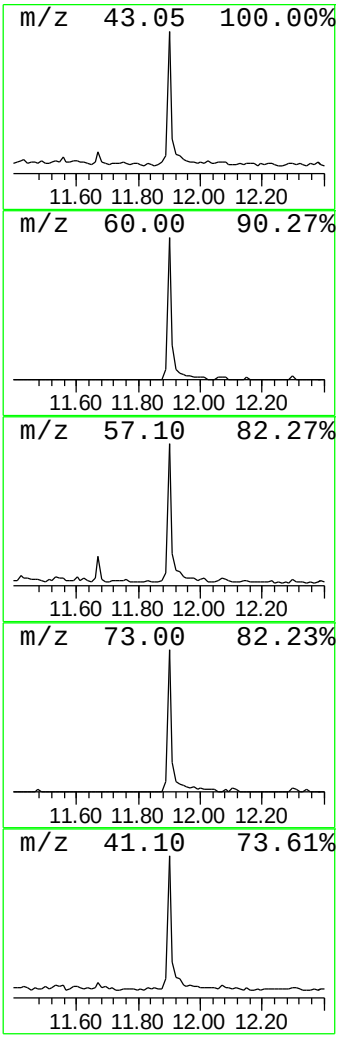
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.86 ng	278814	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120516\
Data File : BF091435.D
Acq On : 5 Dec 2016 23:13
Operator : UM/SJ
Sample : H5802-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

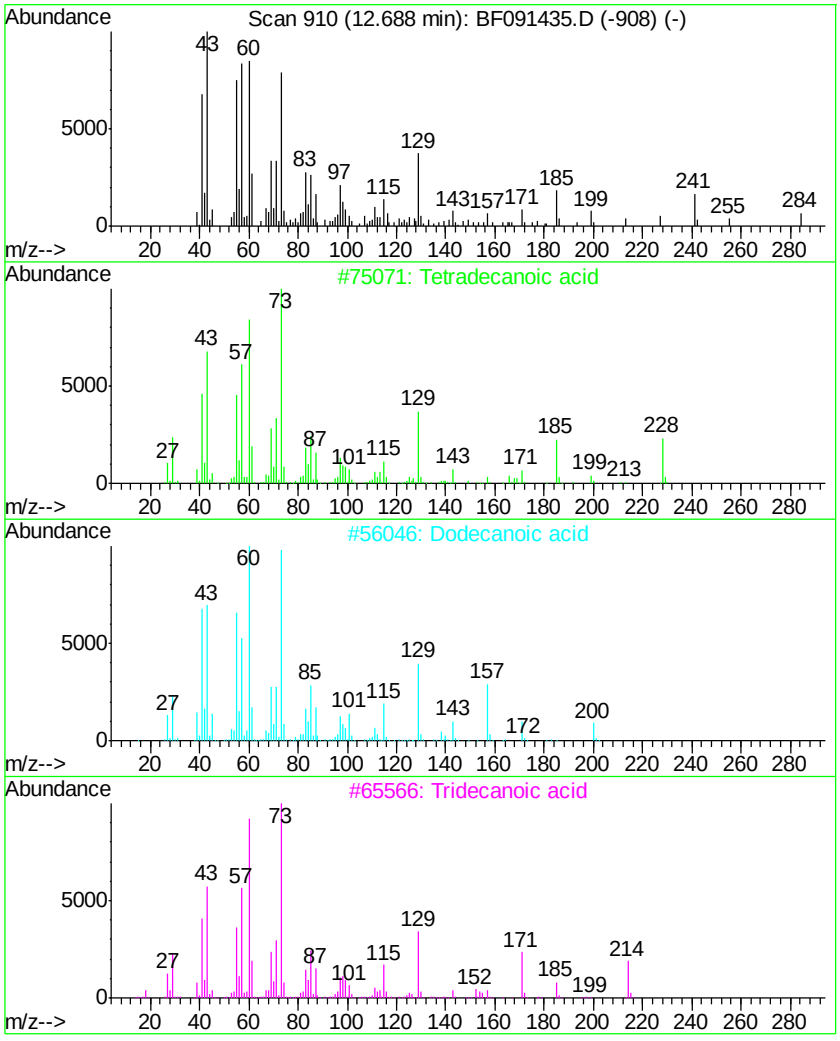
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

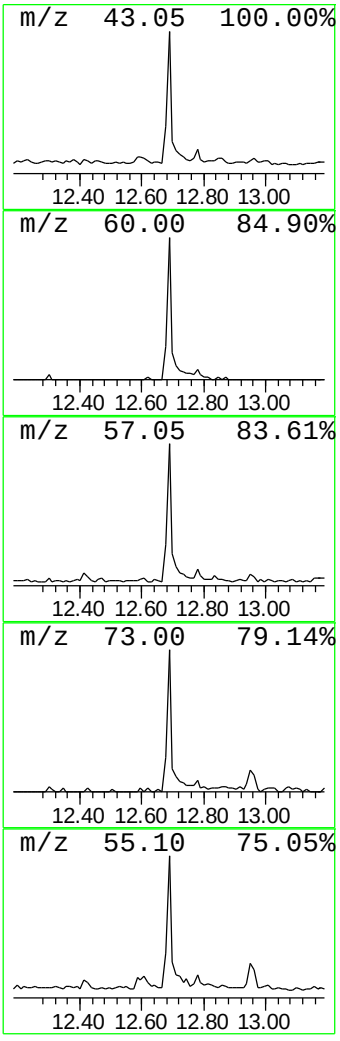
****

Peak Number 7 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	4.52 ng	249764	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120516\
Data File : BF091435.D
Acq On : 5 Dec 2016 23:13
Operator : UM/SJ
Sample : H5802-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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
unknown4.07	4.07	2.4	ng	110260	1	6.85	940058	20.0
2-Pentanone, 4-hy...	5.03	16.5	ng	774263	1	6.85	940058	20.0
unknown6.62	6.62	102.0	ng	4793240	1	6.85	940058	20.0
n-Hexadecanoic acid	11.90	3.9	ng	278814	4	11.36	1443460	20.0
Tetradecanoic acid	12.69	4.5	ng	249764	5	14.00	1105750	20.0