LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030216\
Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

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-BF030116.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	2.344	3	5	13	rVB	64076	102489	1.73%	0.200%
2	5.201	252	255	265	rVB	857102	1127158	18.99%	2.195%
3	5.601	286	290	292	rBV	4372889	5303903	89.38%	10.327%
4	6.436	360	363	369	rBV2	79776	139602	2.35%	0.272%
5	6.607	375	378	381	rBV	4024015	4748700	80.02%	9.246%
6	6.756	388	391	393	rVB	4992885	5045230	85.02%	9.823%
7	6.984	409	411	414	rBV	999492	979583	16.51%	1.907%
8	7.144	422	425	428	rBV	4299225	3862745	65.09%	7.521%
9	7.544	456	460	463	rBV	2638471	3630228	61.17%	7.068%
10	7.910	491	492	494	rBV	83112	62765	1.06%	0.122%
11	7.967	494	497	500	rVV	82648	182298	3.07%	0.355%
12	8.013	500	501	504	rVB	492905	433353	7.30%	0.844%
13	8.276	521	524	526	rBV	1193761	1427563	24.06%	2.780%
14	9.350	615	618	620	rBV	6151433	5934399	100.00%	11.555%
15	9.739	650	652	654	rBV	1006680	837931	14.12%	1.632%
16	9.956	669	671	673	rBV	161854	128163	2.16%	0.250%
17	10.025	675	677	679	rVB	1520873	1510975	25.46%	2.942%
18	10.459	711	715	716	rBV	200332	204645	3.45%	0.398%
19	10.676	731	734	737	rBV	66957	110341	1.86%	0.215%
20	10.813	743	746	749	rBV	3535724	3872912	65.26%	7.541%
21	10.928	754	756	763	rVB	219255	260556	4.39%	0.507%
22	11.373	793	795	797	rBV	78881	76954	1.30%	0.150%
23	11.511	805	807	810	rBV	1948899	1712371	28.86%	3.334%
24	11.579	810	813	815	rVB4	83370	109435	1.84%	0.213%
25	12.036	849	853	855	rBV	92407	148342	2.50%	0.289%
26	12.722	910	913	915	rBV	199541	179269	3.02%	0.349%
27	12.813	919	921	925	rBV2	49890	60716	1.02%	0.118%
28	12.951	929	933	935	rBV	238995	230429	3.88%	0.449%
29	13.099	943	946	948	rBV	5966007	5934346	100.00%	11.555%
30	13.991	1022	1024	1029	rBV	111800	186271	3.14%	0.363%
31	14.151	1033	1038	1040	rBV2	1039960	1729461	29.14%	3.367%
32	15.191	1126	1129	1133	rBV	58102	139485	2.35%	0.272%
33	15.625	1163	1167	1169	rBV	601629	946295	15.95%	1.843%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030216\
Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

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-BF030116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

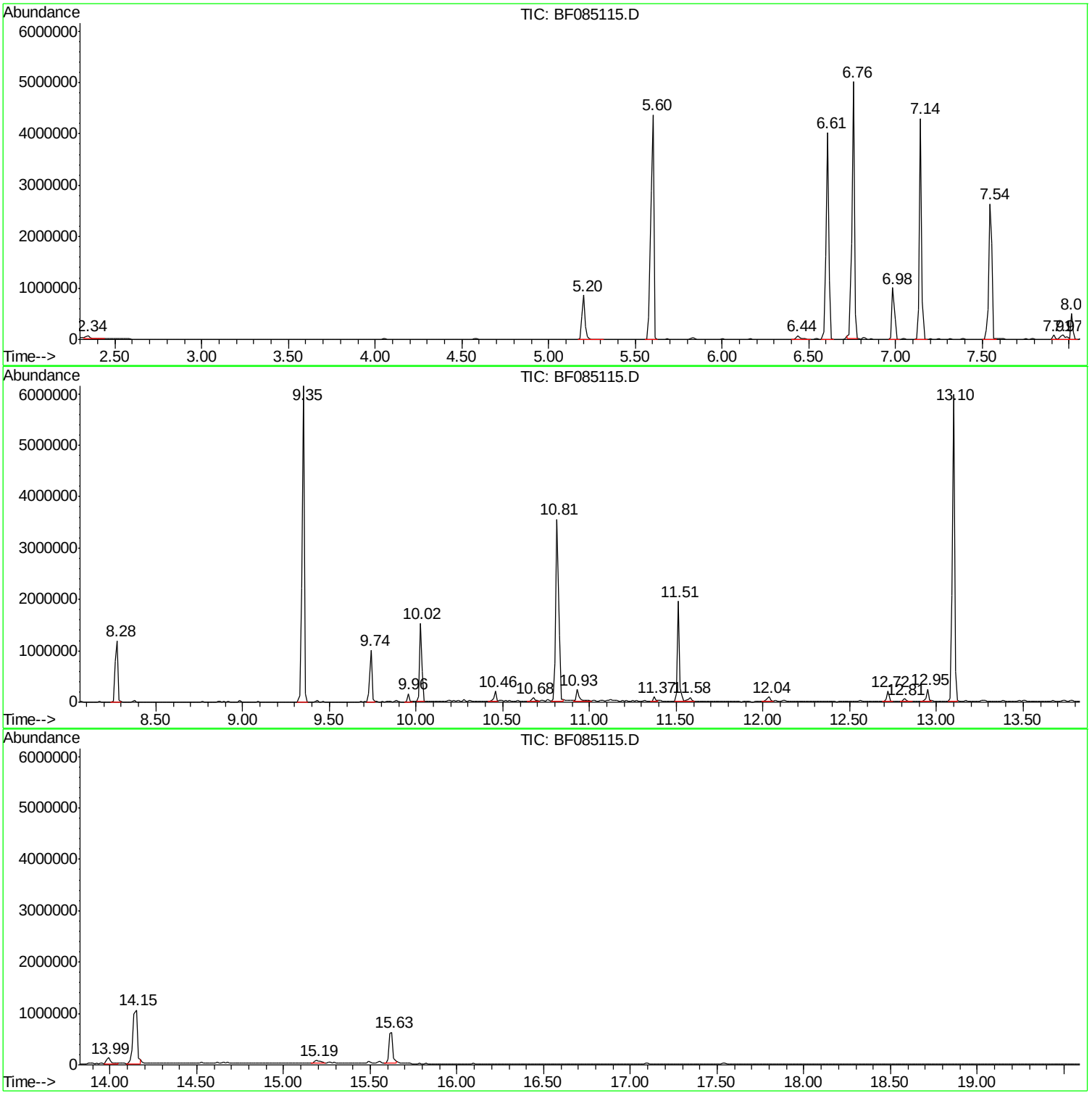
Sum of corrected areas: 51358913

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030216\
Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.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\BF030216\
Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
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Instrument : BNA_F
ClientSampleId : 20160225-WC-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

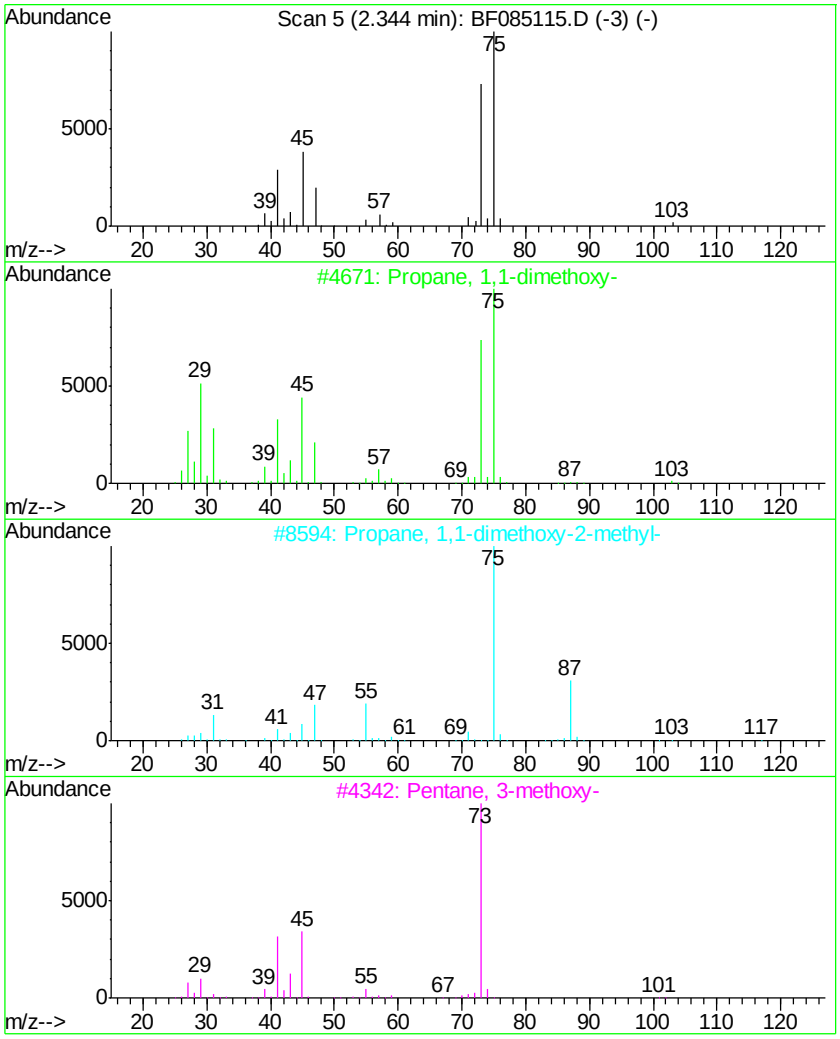
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

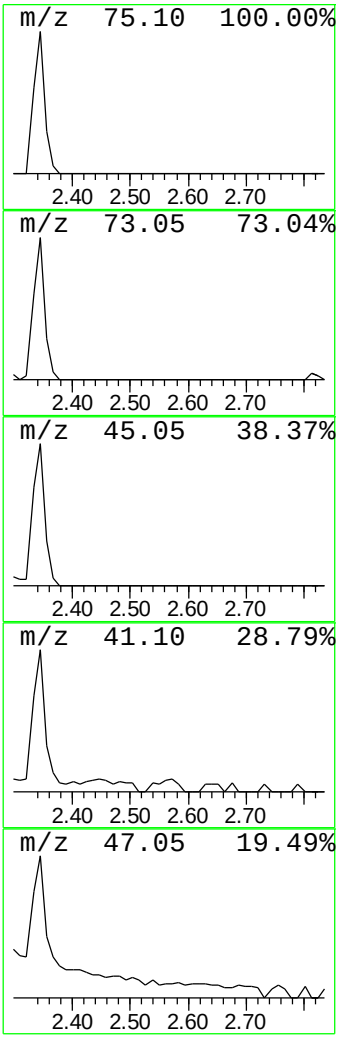
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	2.09 ng	102489	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	33
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
5	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030216\
Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

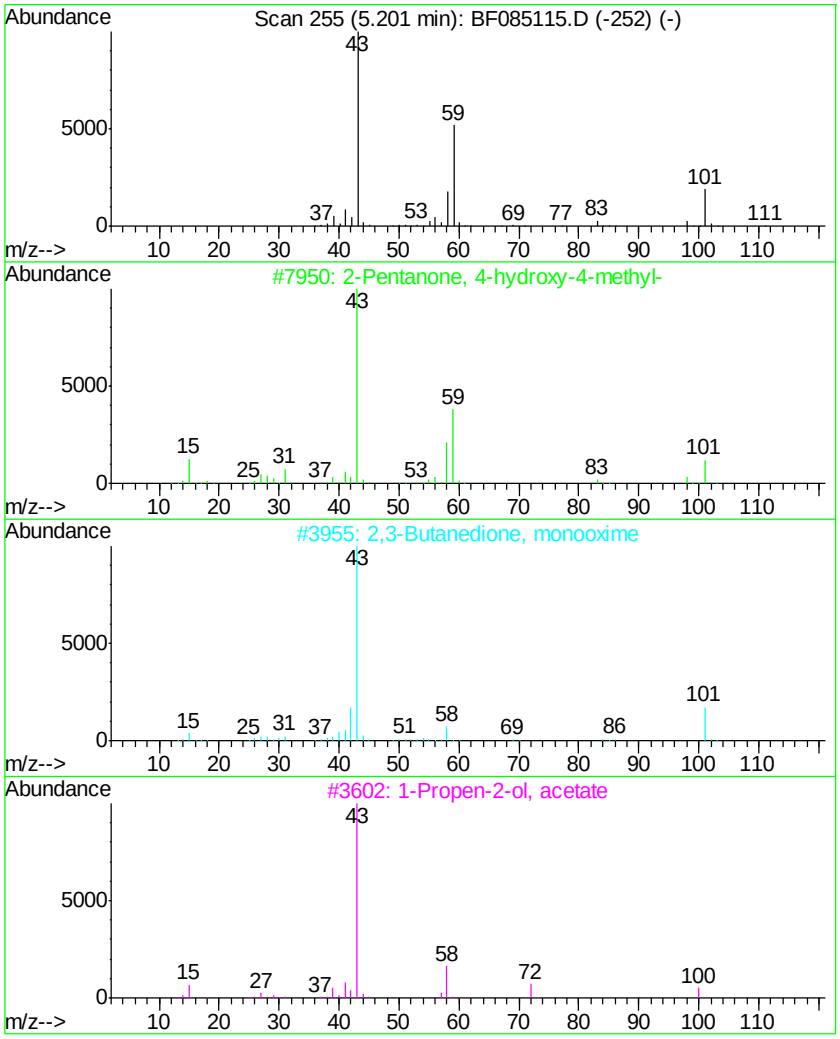
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

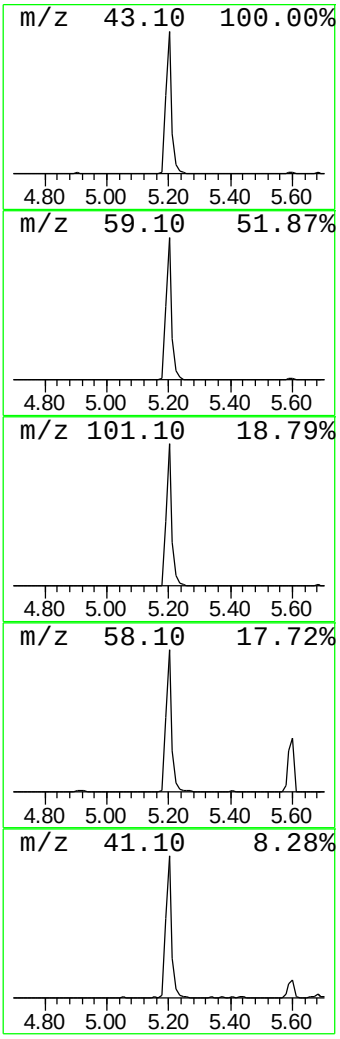
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	23.01 ng	1127160	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030216\
Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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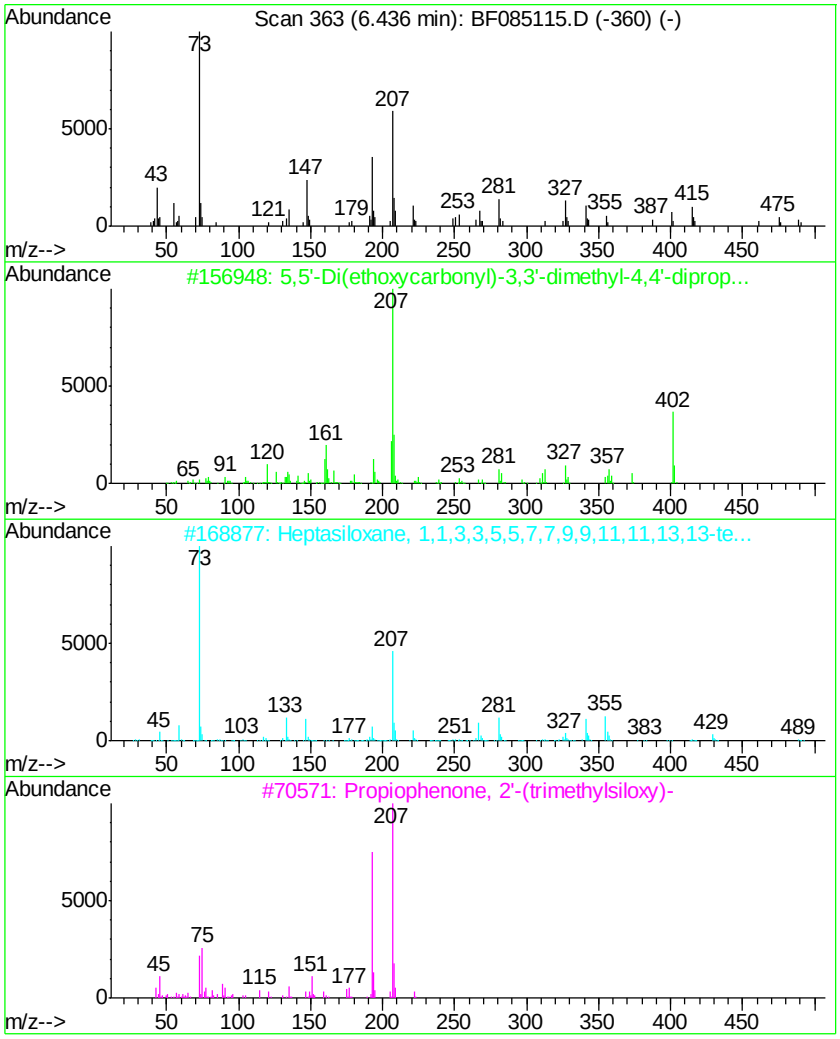
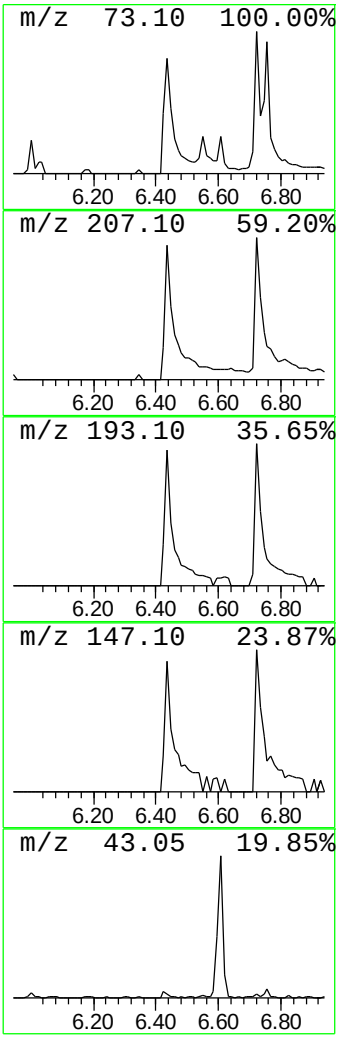
Peak Number 3 unknown6.44 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	2.85 ng	139602	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5'-Di(ethoxycarbonyl)-3,3'-dim...	402	C23H34N2O4	102586-97-0	47
2	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	38
3	Propiophenone, 2'-(trimethylsilo...	222	C12H18O2Si	033342-87-9	35
4	4-Hydroxyphenyl pyrrolidinyl thione	207	C11H13NOS	084783-02-8	35
5	Indole-2-one, 2,3-dihydro-N-hydr...	207	C11H13NO3	1000129-52-1	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030216\
Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

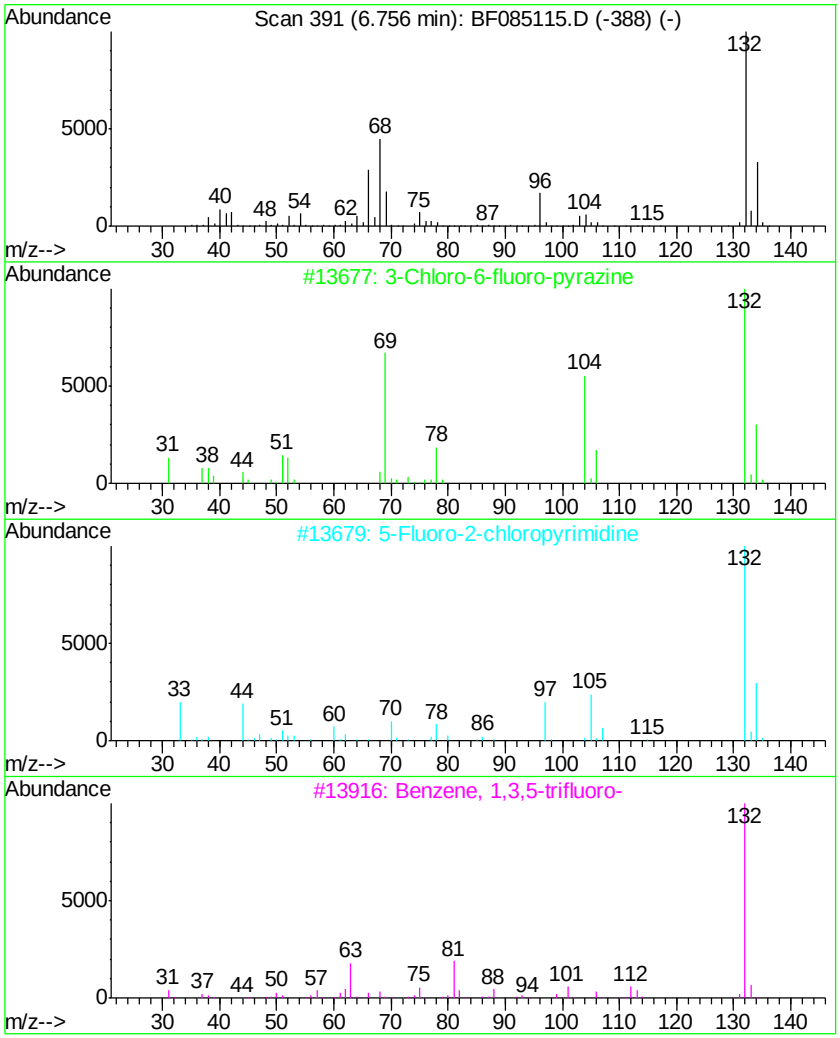
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

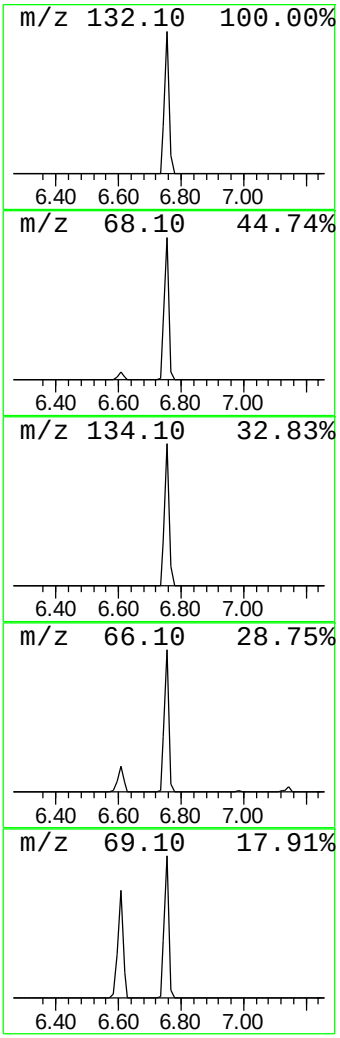
****

Peak Number 4 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	103.01 ng	5045230	1,4-Dichlorobenzene-d4	6.98

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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

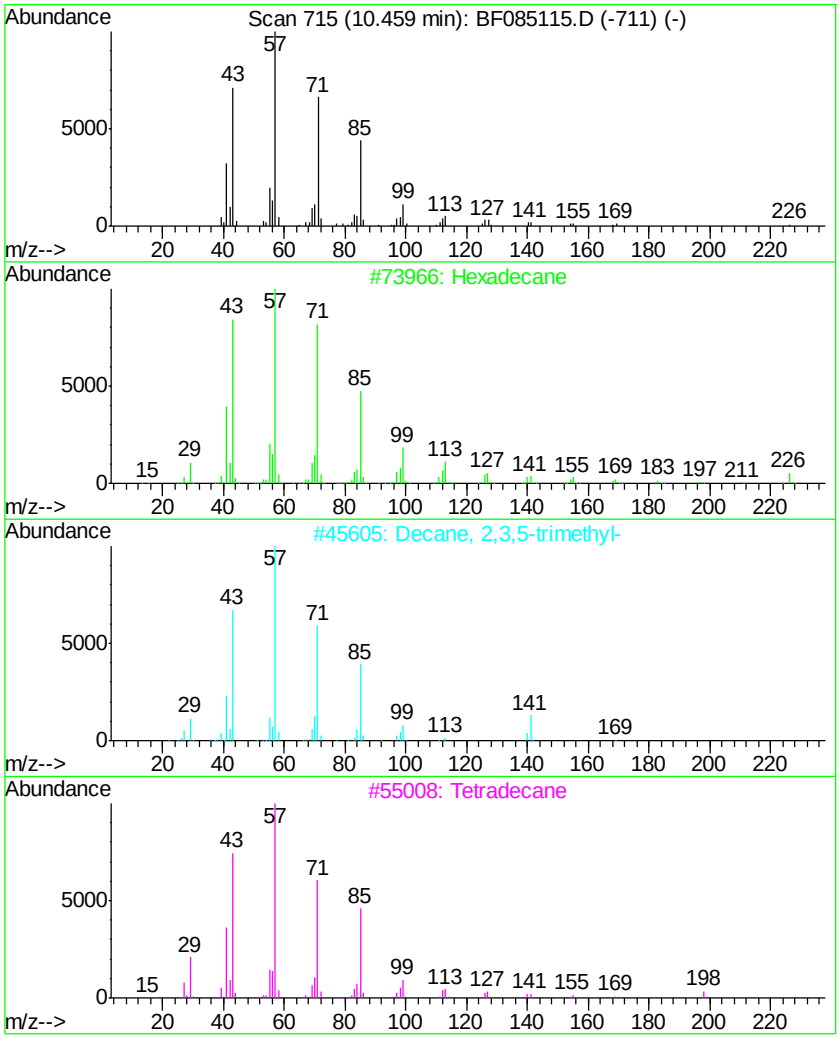
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

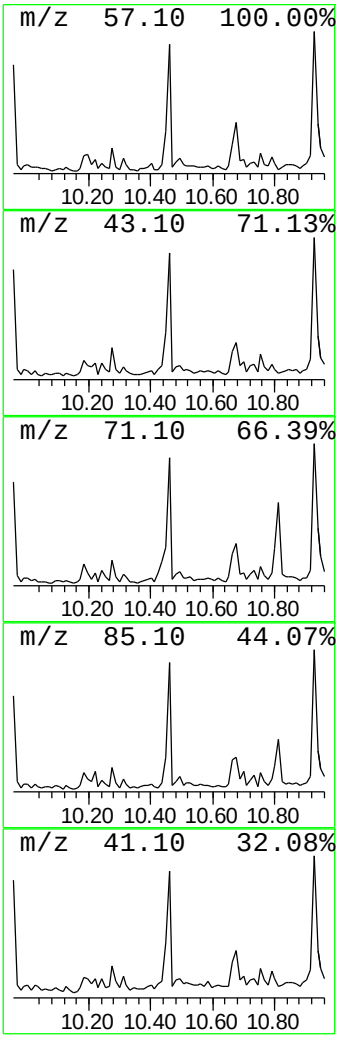
****

Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.46	2.71 ng	204645	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
3	Tetradecane	198	C14H30	000629-59-4	87
4	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86
5	Pentadecane	212	C15H32	000629-62-9	86





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Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

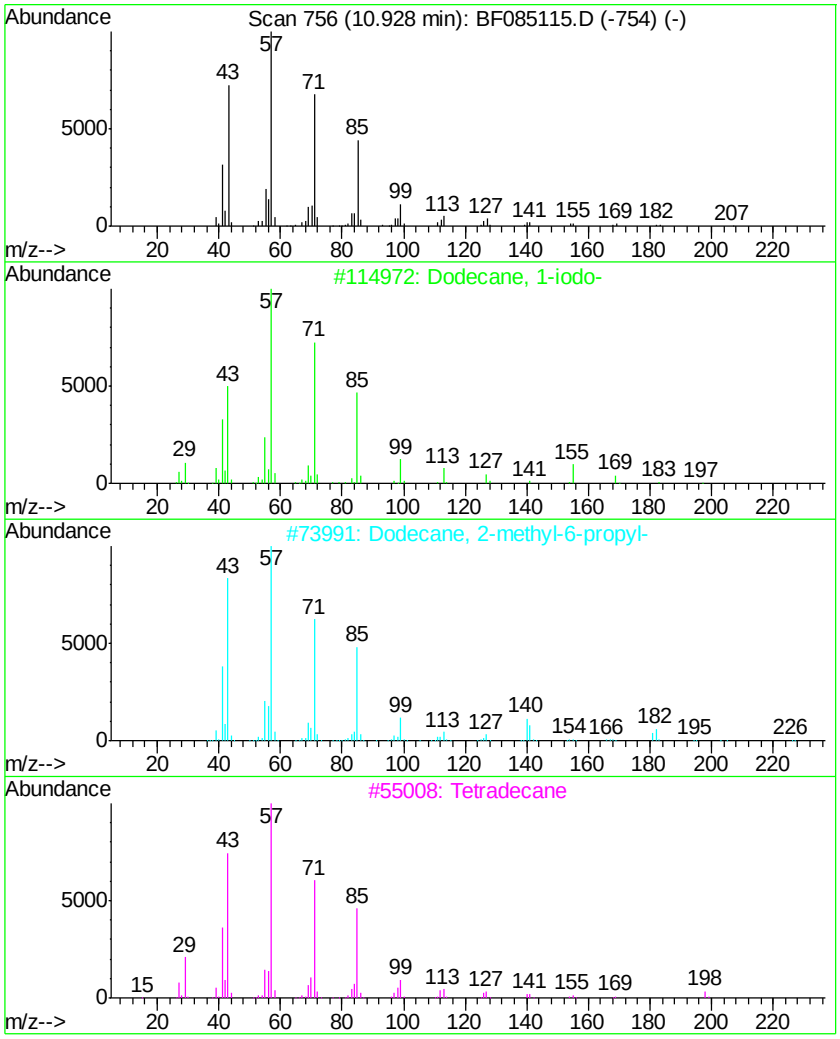
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

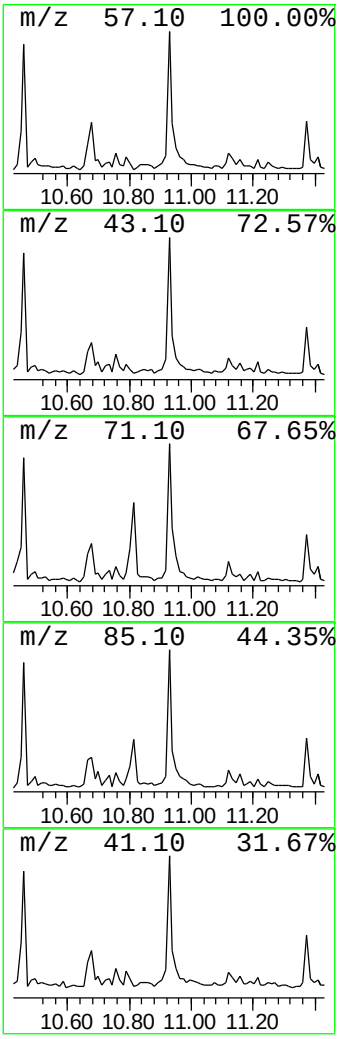
****

Peak Number 7 Dodecane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	3.04 ng	260556	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Tritetracontane	605	C43H88	007098-21-7	86
5	Eicosane	282	C20H42	000112-95-8	83





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Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

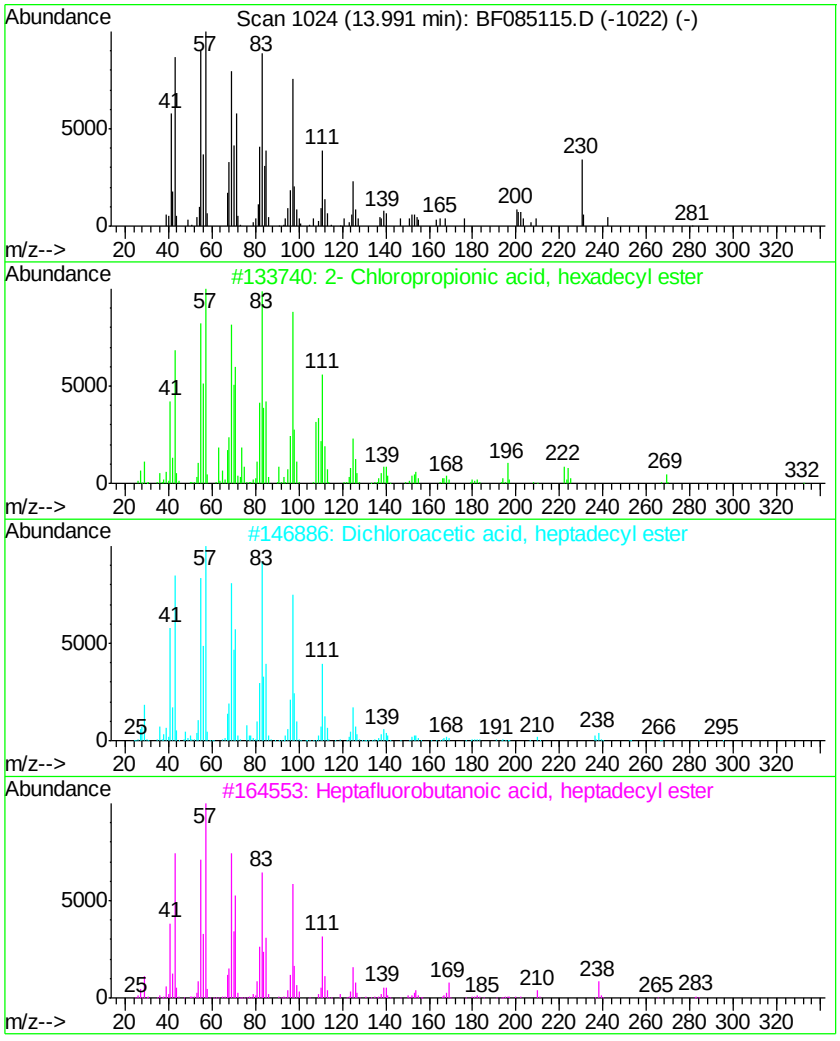
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

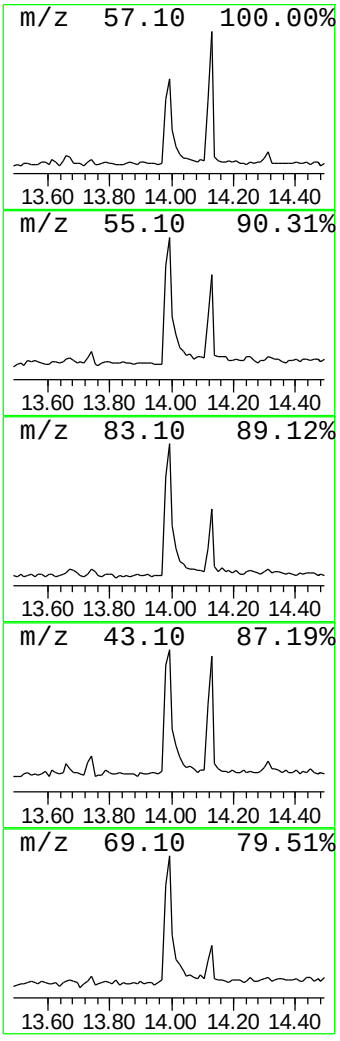
****

Peak Number 8 2- Chloropropionic acid, he... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	2.15 ng	186271	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
4	1-Octadecanol	270	C18H38O	000112-92-5	93
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030216\
Data File : BF085115.D
Acq On : 2 Mar 2016 13:15
Operator : SJ/IZ
Sample : H1617-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20160225-WC-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.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
Propane, 1,1-dime...	2.34	2.1	ng	102489	1	6.98	979583	20.0
2-Pentanone, 4-hy...	5.20	23.0	ng	1127160	1	6.98	979583	20.0
unknown6.44	6.44	2.9	ng	139602	1	6.98	979583	20.0
unknown6.76	6.76	103.0	ng	5045230	1	6.98	979583	20.0
Hexadecane	10.46	2.7	ng	204645	3	10.02	1510980	20.0
Dodecane, 1-iodo-	10.93	3.0	ng	260556	4	11.51	1712370	20.0
2- Chloropropioni...	13.99	2.1	ng	186271	5	14.15	1729460	20.0