LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030315\
Data File : BF077552.D
Acq On : 3 Mar 2015 18:19
Operator : TP/IZ
Sample : G1401-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05-2-27-15

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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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	1.527	52	56	59	rVB	282549	466650	19.17%	2.958%
2	1.698	68	71	74	rBV	309396	359918	14.79%	2.281%
3	1.835	81	83	89	rVB	65310	114010	4.68%	0.723%
4	5.013	359	361	366	rVB	102891	118893	4.88%	0.754%
5	5.527	404	406	409	rBV	725147	729419	29.97%	4.623%
6	6.796	515	517	521	rVB	521394	456470	18.75%	2.893%
7	6.945	528	530	533	rBV	1463739	1388755	57.06%	8.802%
8	7.242	553	556	558	rBV	235568	322787	13.26%	2.046%
9	7.425	569	572	574	rVB	1548182	1446421	59.42%	9.167%
10	7.927	614	616	619	rBV	1258809	1106673	45.47%	7.014%
11	8.808	691	693	696	rVB	324526	382375	15.71%	2.423%
12	9.516	753	755	758	rBV	44580	54088	2.22%	0.343%
13	10.168	809	812	814	rBV	1481455	2051249	84.27%	13.001%
14	10.671	853	856	858	rBV	76462	85790	3.52%	0.544%
15	10.991	882	884	886	rBV	453477	466741	19.18%	2.958%
16	11.516	928	930	936	rVB2	24441	46738	1.92%	0.296%
17	11.894	960	963	965	rBV	136674	152648	6.27%	0.967%
18	11.962	967	969	972	rBV2	1001247	1308229	53.75%	8.292%
19	12.831	1043	1045	1047	rBV	543727	516261	21.21%	3.272%
20	13.551	1106	1108	1110	rBV	49609	62104	2.55%	0.394%
21	14.534	1192	1194	1197	rBV4	21086	31567	1.30%	0.200%
22	14.831	1217	1220	1222	rBV	2255092	2434049	100.00%	15.427%
23	15.997	1320	1322	1325	rBV	107181	136329	5.60%	0.864%
24	16.123	1331	1333	1336	rBV	623553	675665	27.76%	4.282%
25	17.243	1429	1431	1435	rBV5	14666	34098	1.40%	0.216%
26	17.631	1462	1465	1467	rBV3	17893	41785	1.72%	0.265%
27	17.883	1484	1487	1491	rVB	574193	708674	29.12%	4.492%
28	18.134	1506	1509	1515	rBV7	18365	79464	3.26%	0.504%

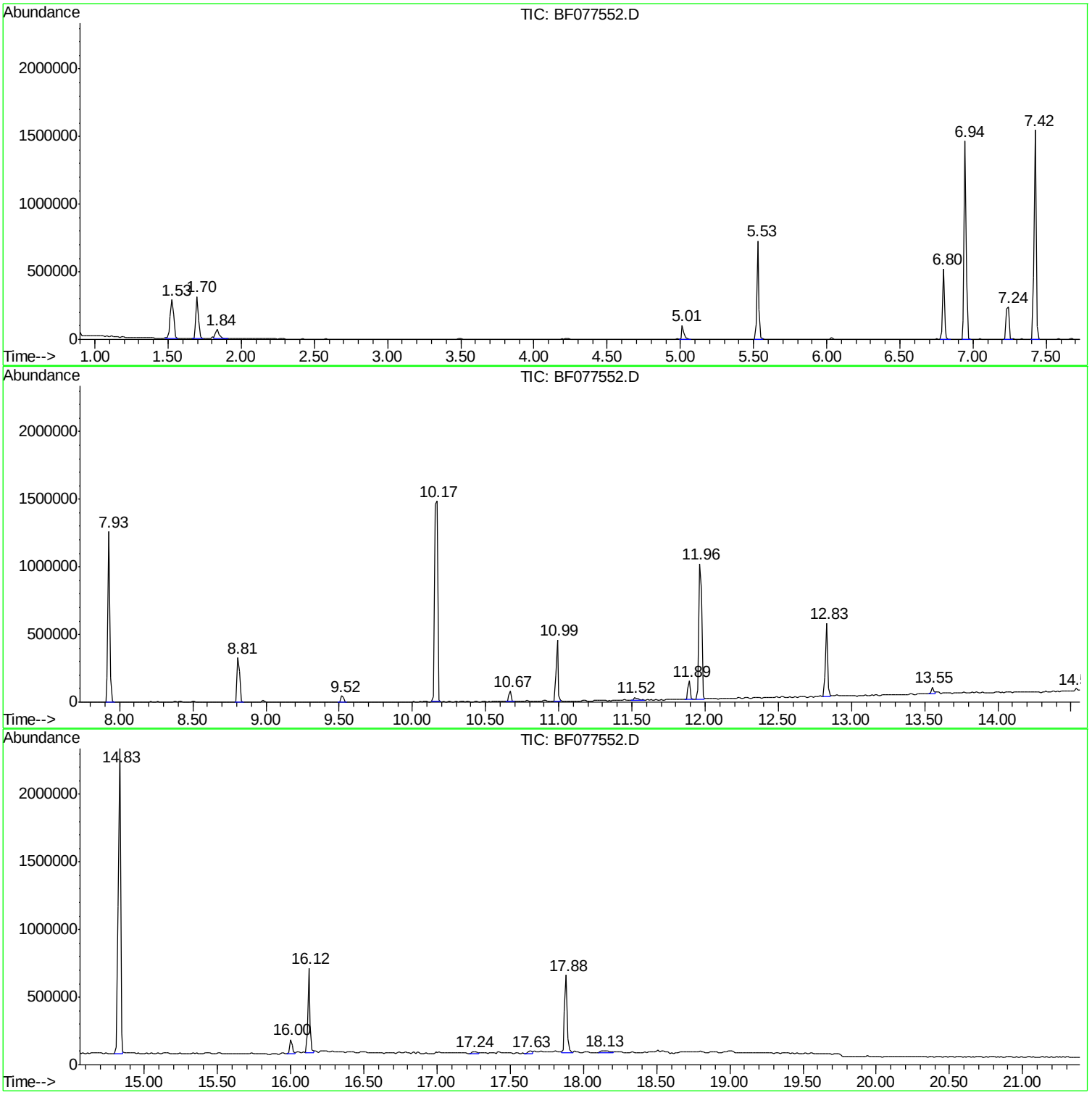
Sum of corrected areas: 15777850

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030315\
Data File : BF077552.D
Acq On : 3 Mar 2015 18:19
Operator : TP/IZ
Sample : G1401-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05-2-27-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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\BF030315\
Data File : BF077552.D
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Operator : TP/IZ
Sample : G1401-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05-2-27-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

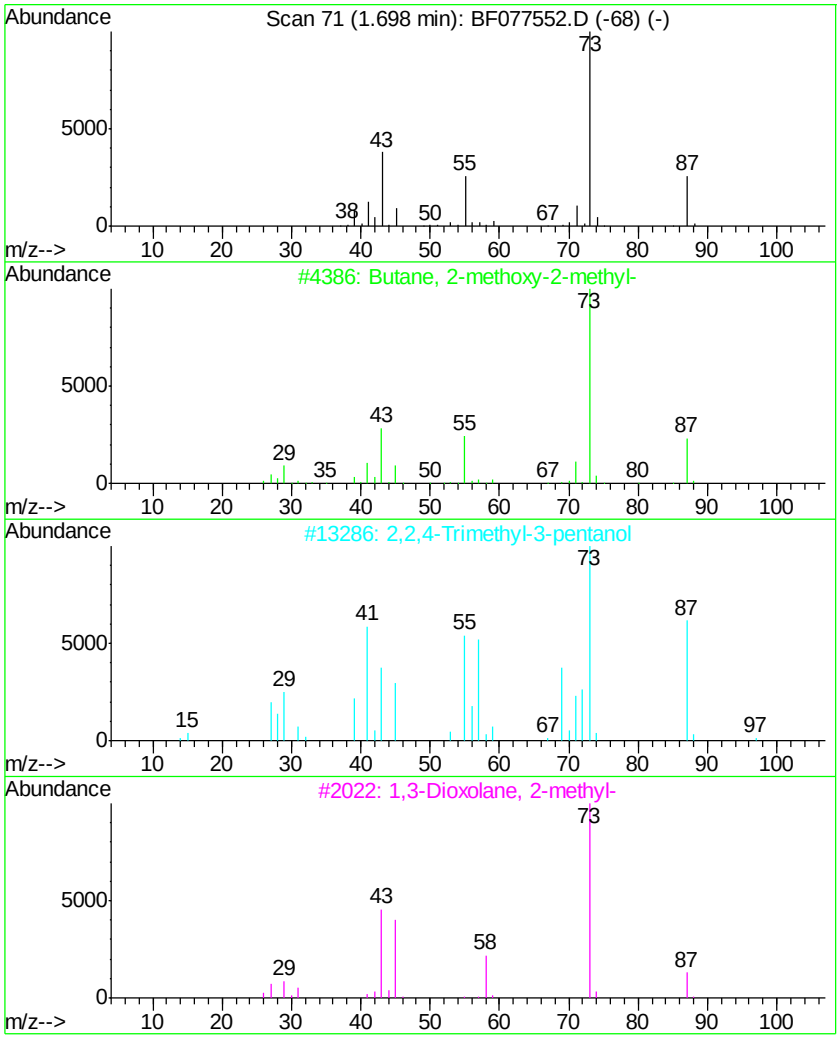
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

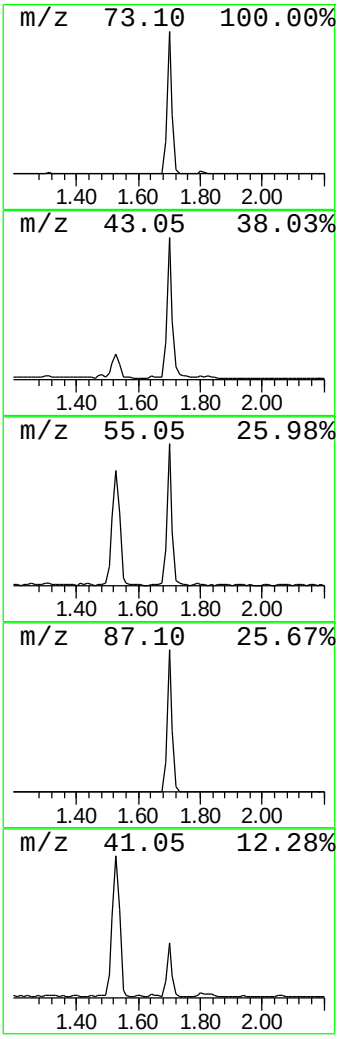
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.70	22.30 ng	359918	1,4-Dichlorobenzene-d4	7.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030315\
Data File : BF077552.D
Acq On : 3 Mar 2015 18:19
Operator : TP/IZ
Sample : G1401-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05-2-27-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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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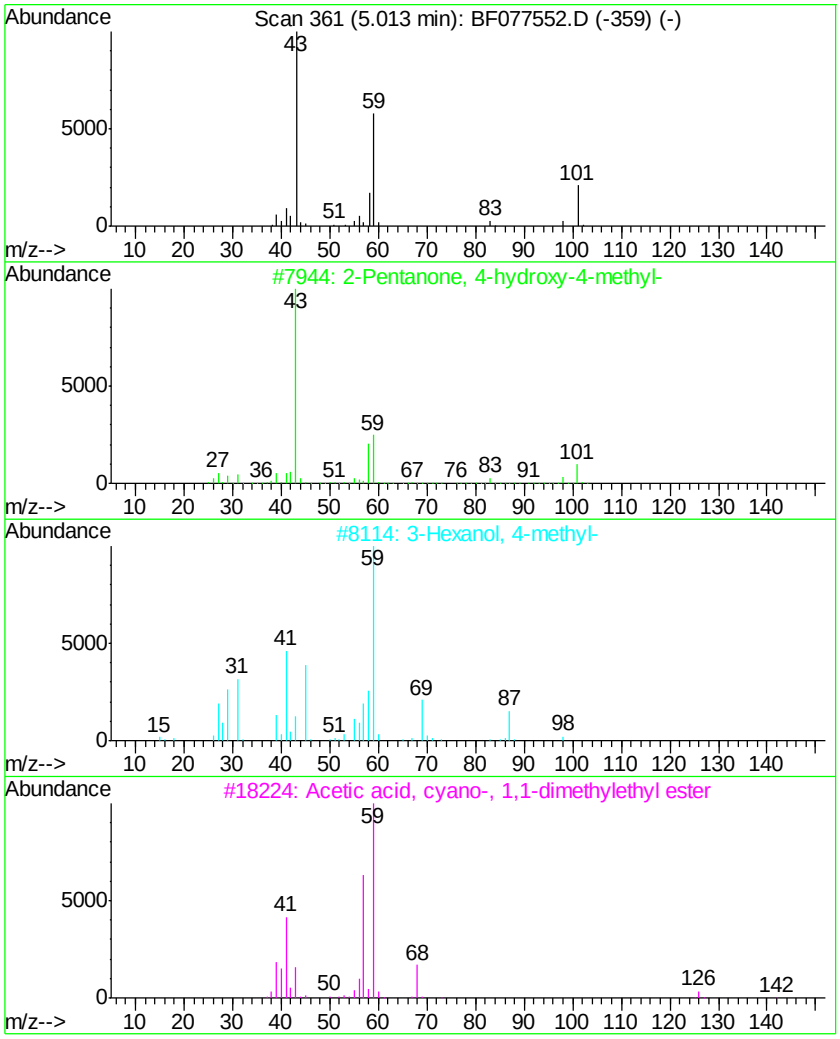
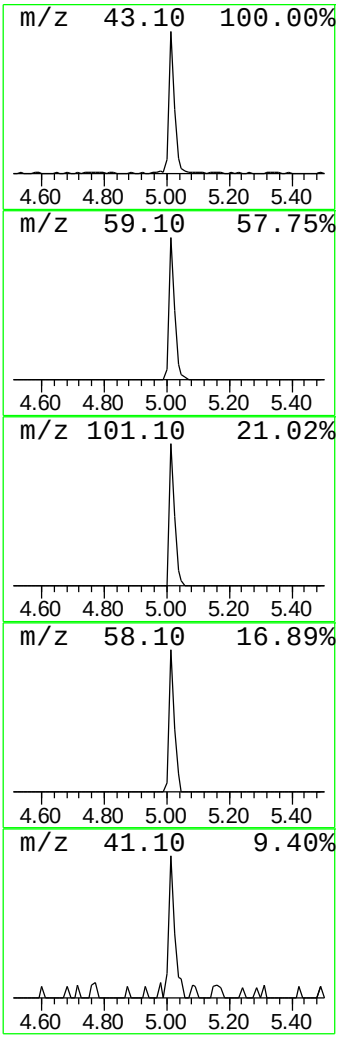
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	7.37 ng	118893	1,4-Dichlorobenzene-d4	7.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	9
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030315\
Data File : BF077552.D
Acq On : 3 Mar 2015 18:19
Operator : TP/IZ
Sample : G1401-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05-2-27-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

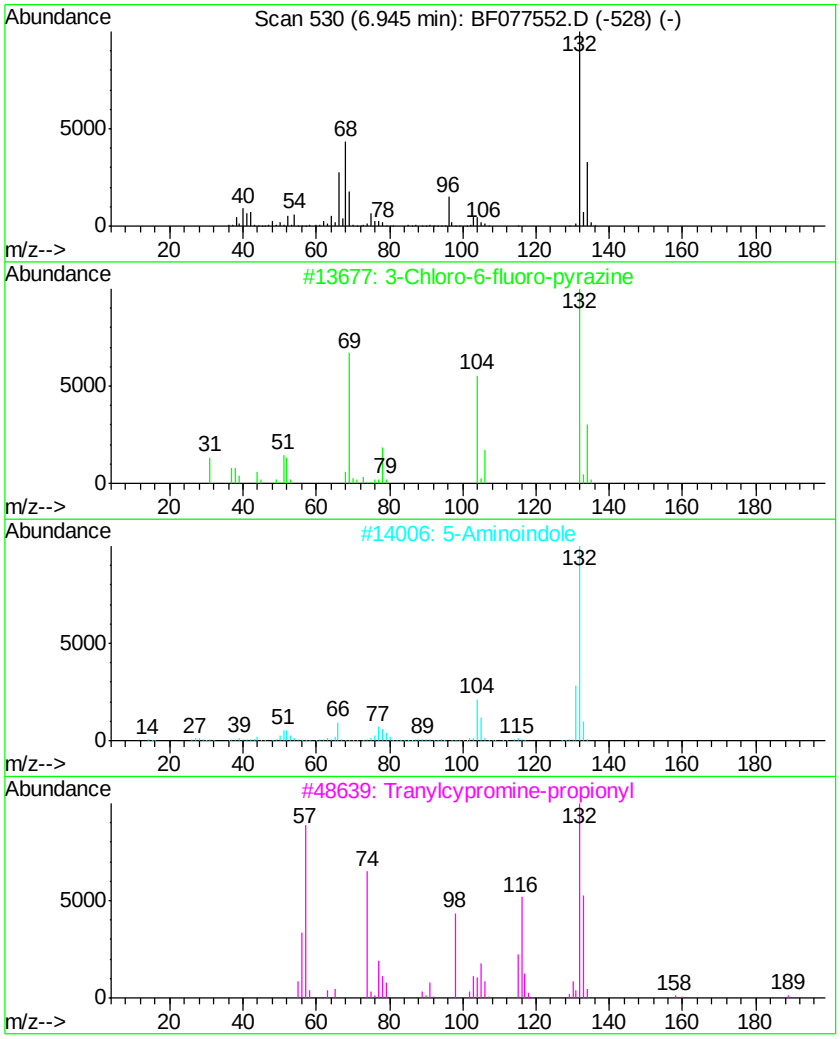
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

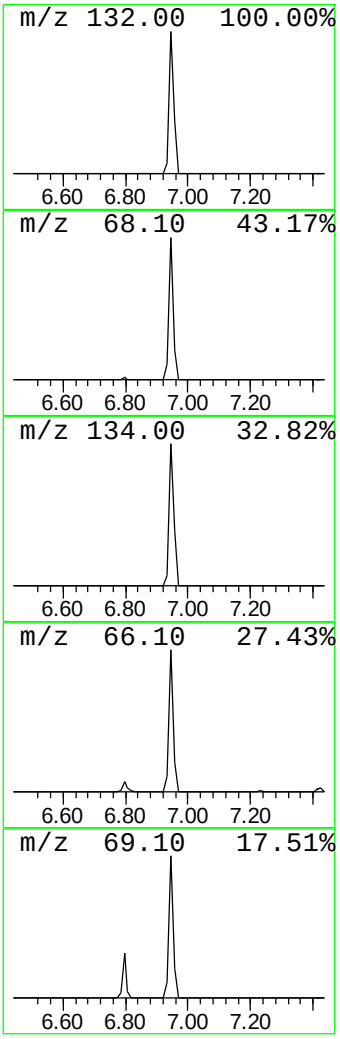
****

Peak Number 5 unknown6.94 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	86.05 ng	1388760	1,4-Dichlorobenzene-d4	7.24

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	10
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030315\
Data File : BF077552.D
Acq On : 3 Mar 2015 18:19
Operator : TP/IZ
Sample : G1401-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05-2-27-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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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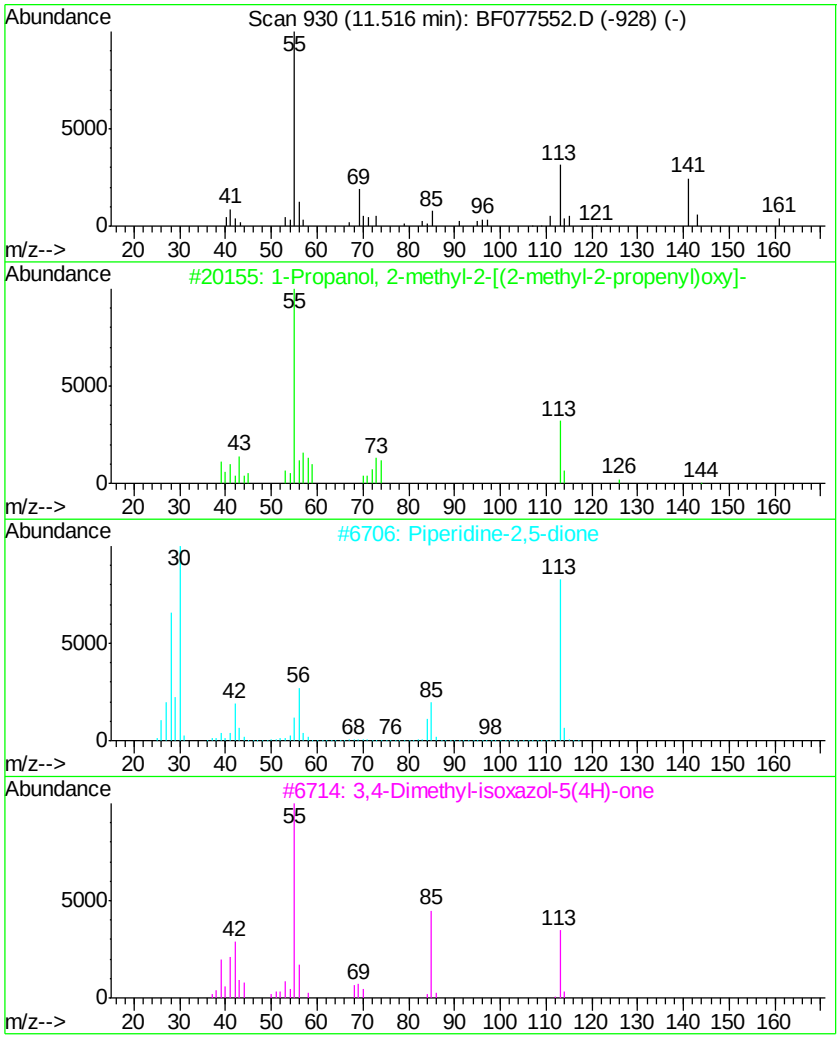
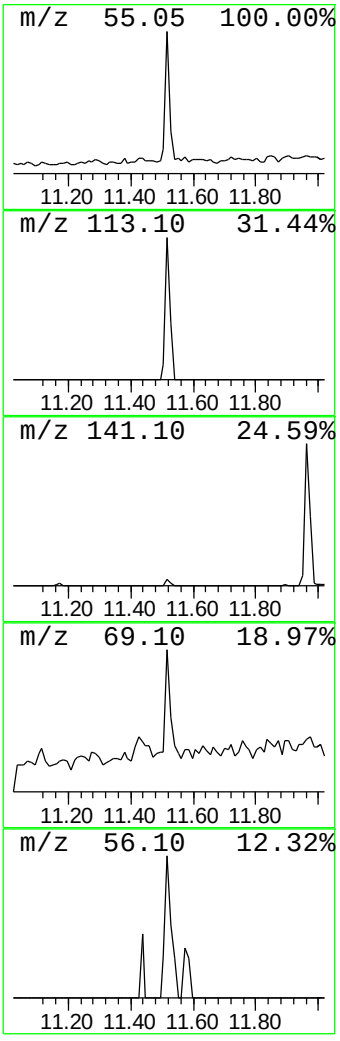
Peak Number 8 unknown11.52 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	2.00 ng	46738	Acenaphthene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-2-[(2-methy...	144	C8H16O2	054004-45-4	12
2	Piperidine-2,5-dione	113	C5H7NO2	052065-78-8	10
3	3,4-Dimethyl-isoxazol-5(4H)-one	113	C5H7NO2	015731-93-8	9
4	3,4-Dimethyl-5-hydroxy-isoxazole	113	C5H7NO2	029279-99-0	9
5	3-Nonanol, 2-methyl-	158	C10H22O	026533-33-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030315\
Data File : BF077552.D
Acq On : 3 Mar 2015 18:19
Operator : TP/IZ
Sample : G1401-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05-2-27-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

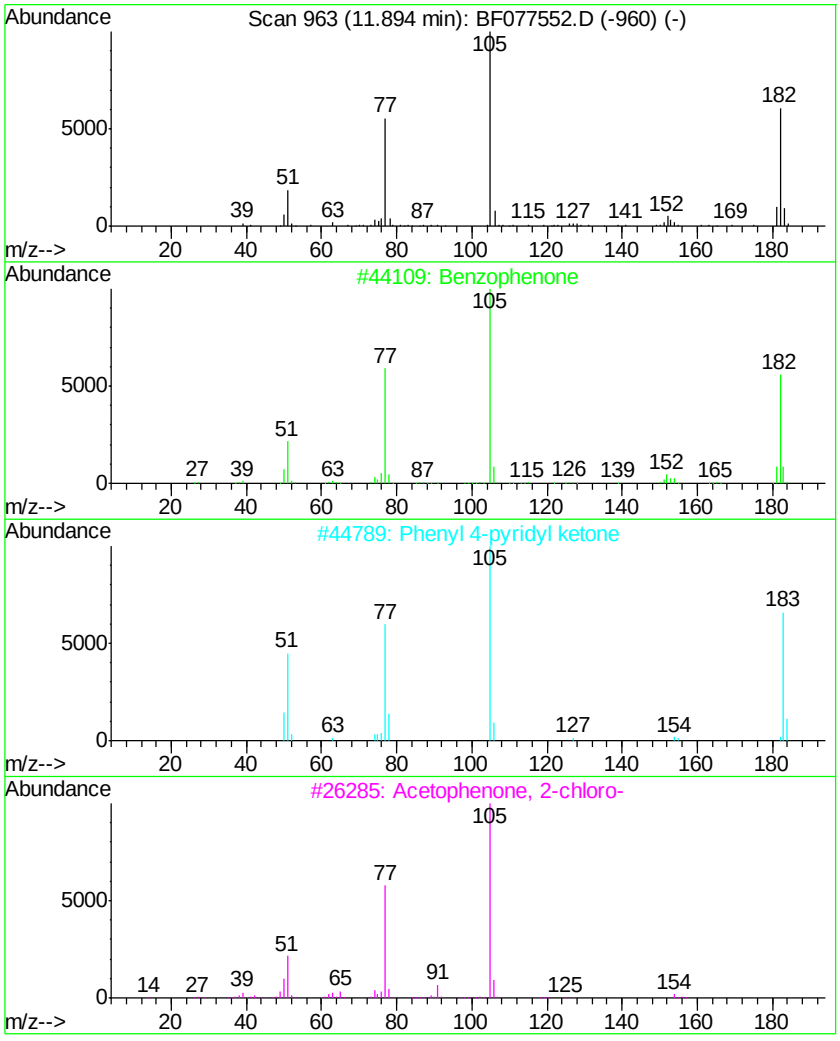
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

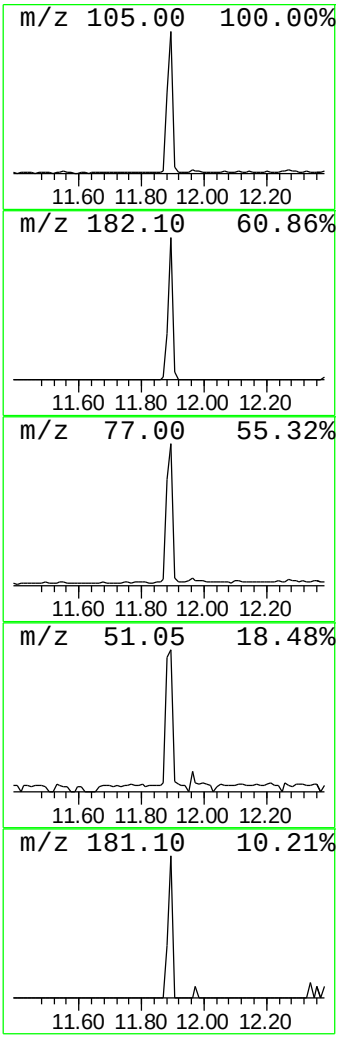
****

Peak Number 9 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	6.54 ng	152648	Acenaphthene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	60
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4	Vinyl benzoate	148	C9H8O2	000769-78-8	43
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030315\
Data File : BF077552.D
Acq On : 3 Mar 2015 18:19
Operator : TP/IZ
Sample : G1401-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05-2-27-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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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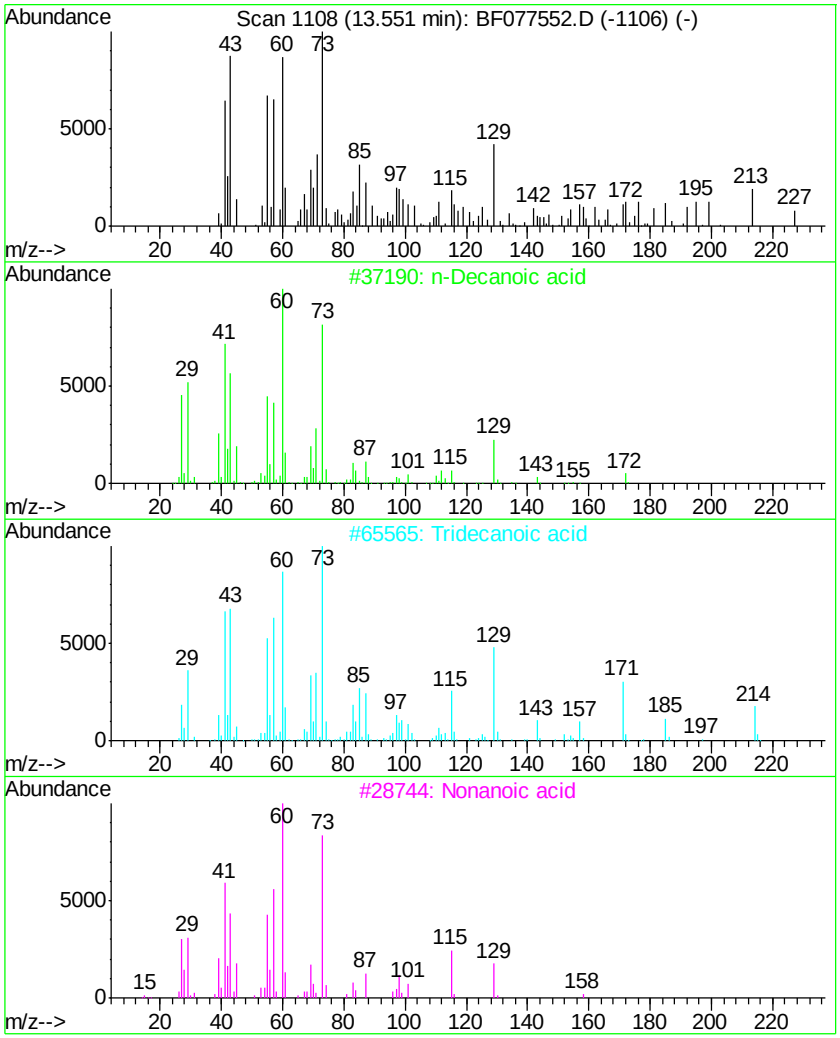
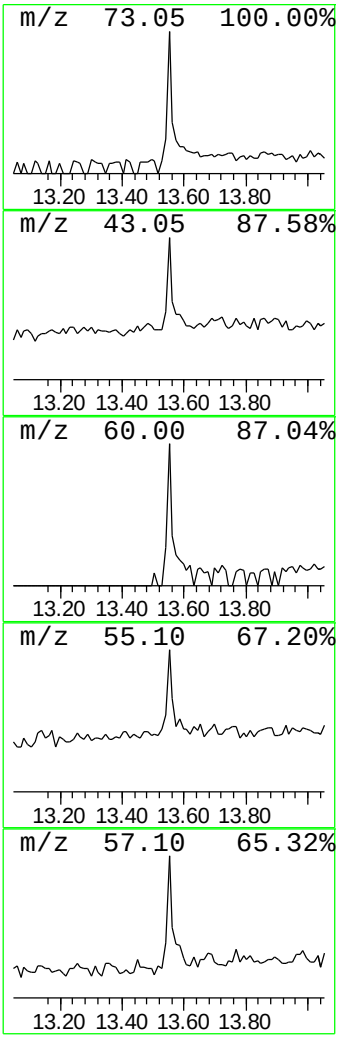
Peak Number 10 n-Decanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	2.41 ng	62104	Phenanthrene-d10	12.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	83
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Nonanoic acid	158	C9H18O2	000112-05-0	47
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030315\
Data File : BF077552.D
Acq On : 3 Mar 2015 18:19
Operator : TP/IZ
Sample : G1401-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05-2-27-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

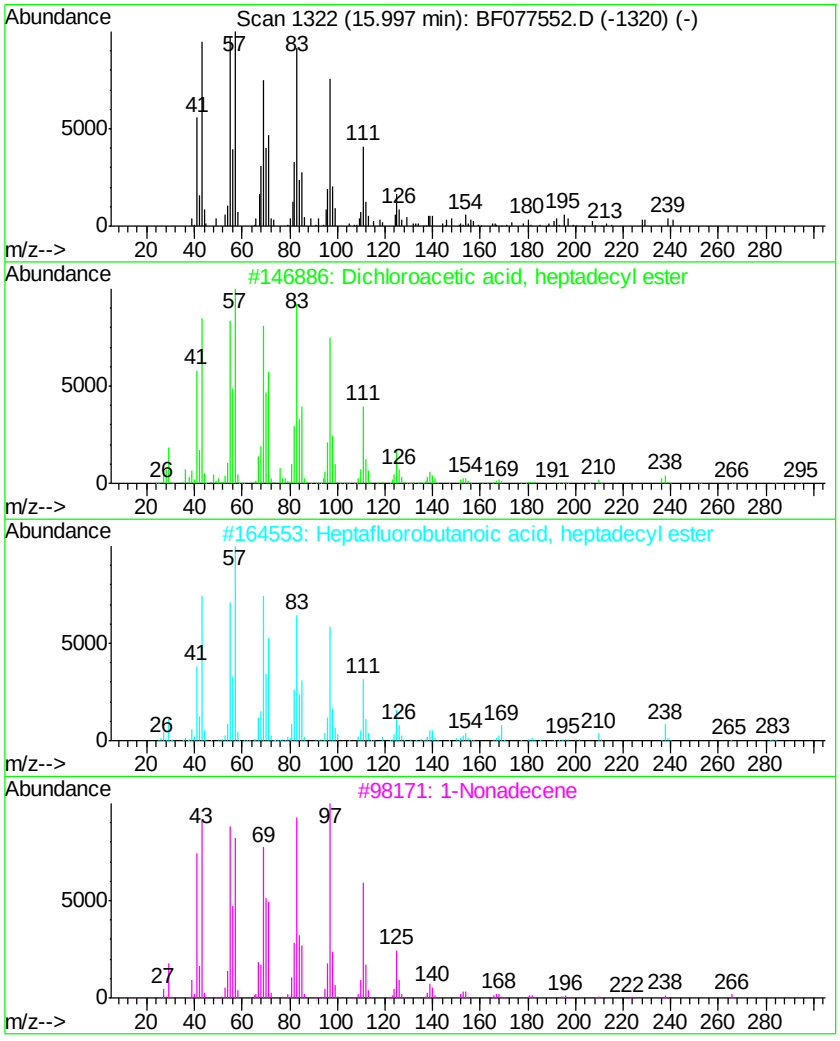
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

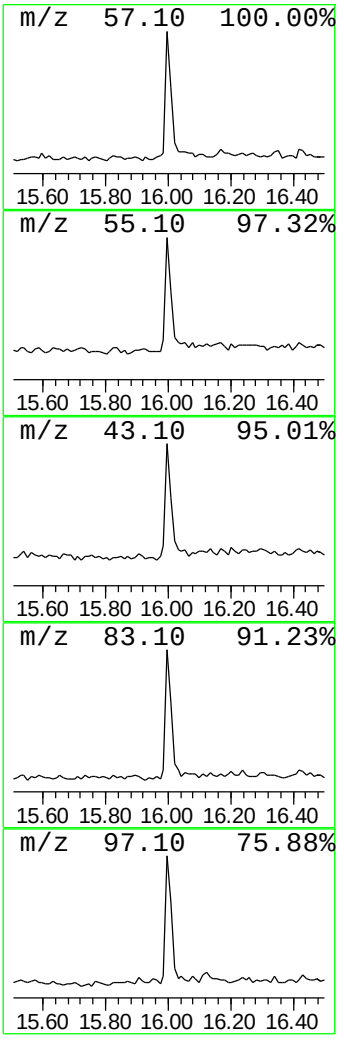
****

Peak Number 11 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	4.04 ng	136329	Chrysene-d12	16.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	11-Tricosene	322	C23H46	052078-56-5	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030315\
Data File : BF077552.D
Acq On : 3 Mar 2015 18:19
Operator : TP/IZ
Sample : G1401-06
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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
Butane, 2-methoxy...	1.70	22.3	ng	359918	1	7.24	322787	20.0
2-Pentanone, 4-hy...	5.01	7.4	ng	118893	1	7.24	322787	20.0
unknown6.94	6.94	86.0	ng	1388760	1	7.24	322787	20.0
unknown11.52	11.52	2.0	ng	46738	3	10.99	466741	20.0
Benzophenone	11.89	6.5	ng	152648	3	10.99	466741	20.0
n-Decanoic acid	13.55	2.4	ng	62104	4	12.83	516261	20.0
Dichloroacetic ac...	16.00	4.0	ng	136329	5	16.13	675665	20.0