LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079070.D
Acq On : 9 May 2015 8:33
Operator : TP/IZ
Sample : G2151-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-3.5

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-BF043015.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	1.484	23	26	28	rVB	2599934	3533128	21.38%	7.280%
2	1.621	35	38	48	rVB	286542	541273	3.28%	1.115%
3	1.747	48	49	52	rVV	293475	406369	2.46%	0.837%
4	1.793	52	53	58	rVB	190774	244796	1.48%	0.504%
5	1.873	58	60	85	rVB	3167147	5940444	35.95%	12.240%
6	3.336	157	188	191	rBV	1229771	16523958	100.00%	34.046%
7	5.622	386	388	391	rBV	1407908	2035701	12.32%	4.194%
8	6.890	496	499	501	rBV	1837990	2337556	14.15%	4.816%
9	7.027	509	511	514	rBV	1662555	2219247	13.43%	4.573%
10	7.325	534	537	543	rBV	291337	455954	2.76%	0.939%
11	7.508	550	553	555	rBV	1772227	1640805	9.93%	3.381%
12	8.010	594	597	599	rBV	1559115	1358454	8.22%	2.799%
13	8.891	672	674	677	rBV	476054	557463	3.37%	1.149%
14	10.239	790	792	795	rBV	2808361	2665351	16.13%	5.492%
15	11.074	863	865	867	rBV	637973	625629	3.79%	1.289%
16	11.737	921	923	926	rVB	234618	204014	1.23%	0.420%
17	12.057	948	951	953	rBV	1764006	1914365	11.59%	3.944%
18	12.914	1024	1026	1029	rVB	612531	654922	3.96%	1.349%
19	14.914	1198	1201	1204	rBV	2845130	3123957	18.91%	6.437%
20	16.114	1303	1306	1314	rBV	139822	247923	1.50%	0.511%
21	16.240	1314	1317	1320	rBV	638283	667647	4.04%	1.376%
22	18.091	1476	1479	1482	rBV	448548	635477	3.85%	1.309%

Sum of corrected areas: 48534433

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
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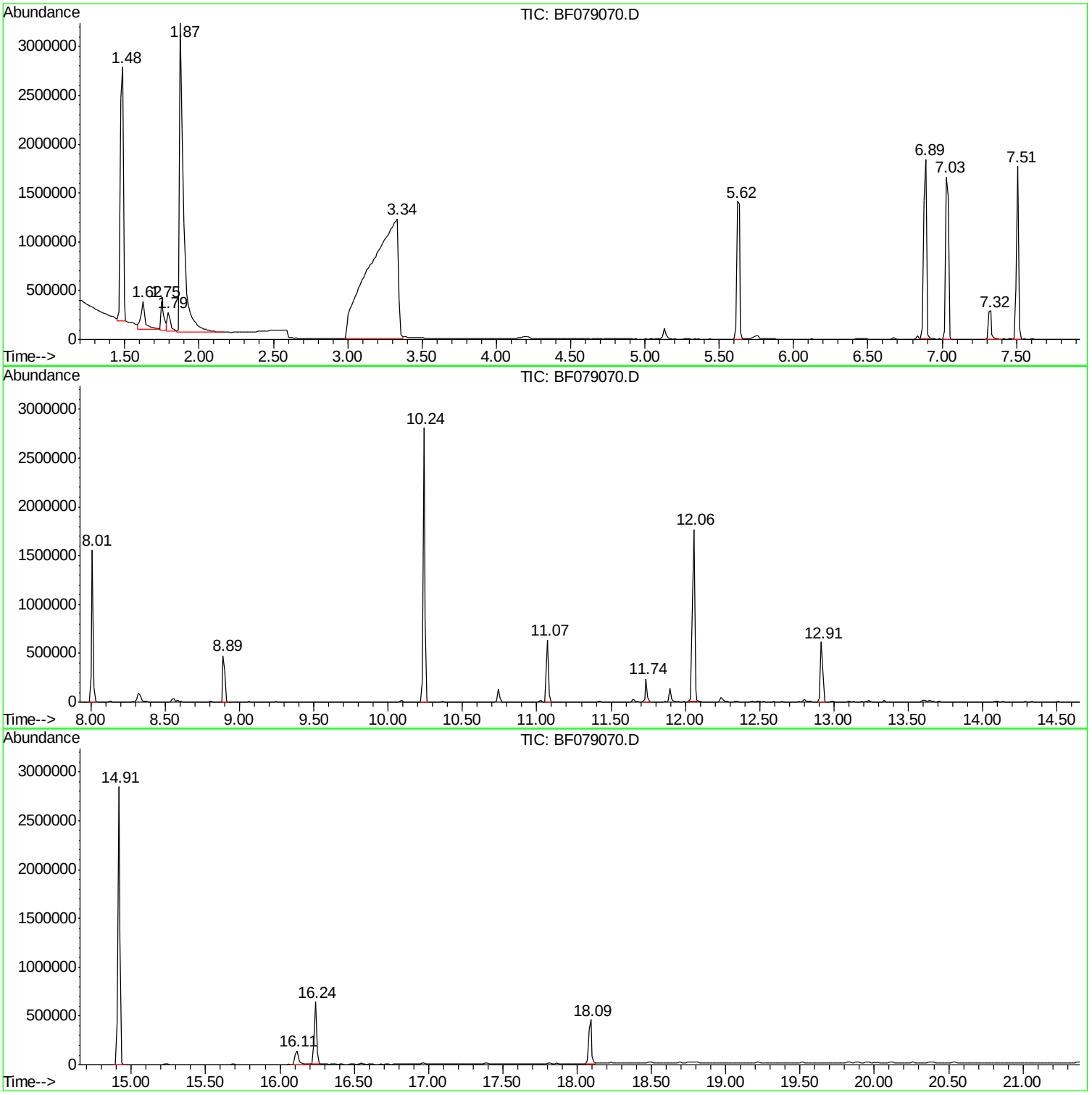
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TU012-SB-16-3.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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\BF050815\
Data File : BF079070.D
Acq On : 9 May 2015 8:33
Operator : TP/IZ
Sample : G2151-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-3.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

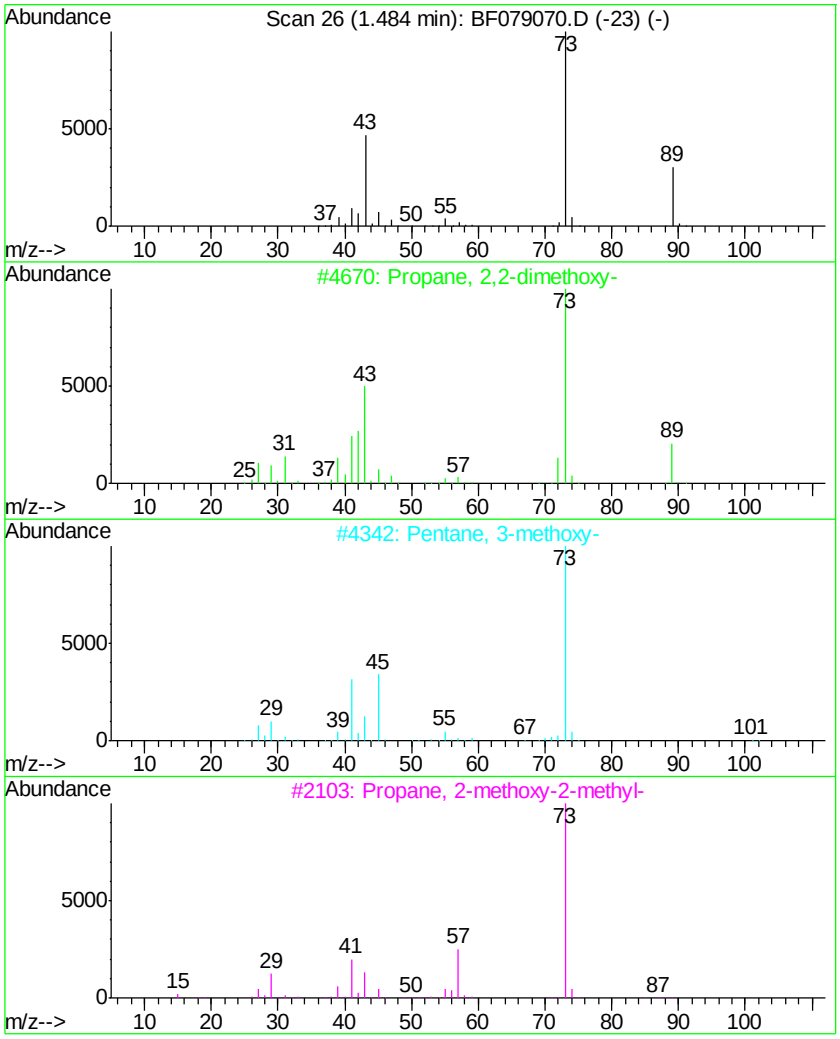
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

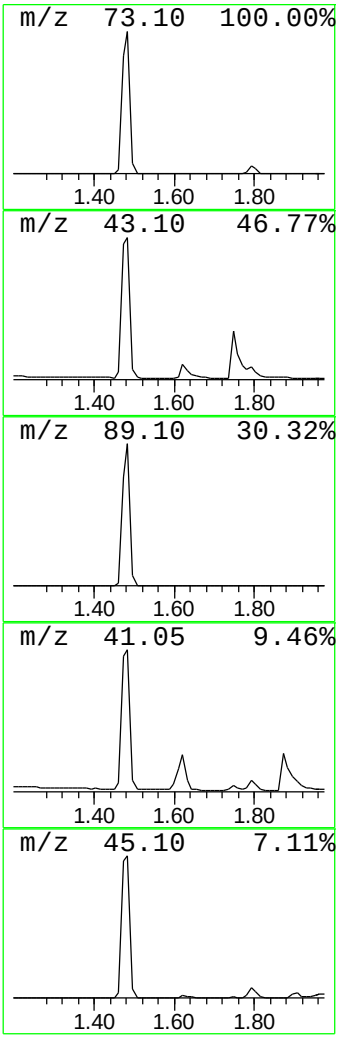
****

Peak Number 1 unknown1.48 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	154.98 ng	3533130	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	40
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	5





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079070.D
Acq On : 9 May 2015 8:33
Operator : TP/IZ
Sample : G2151-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-3.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

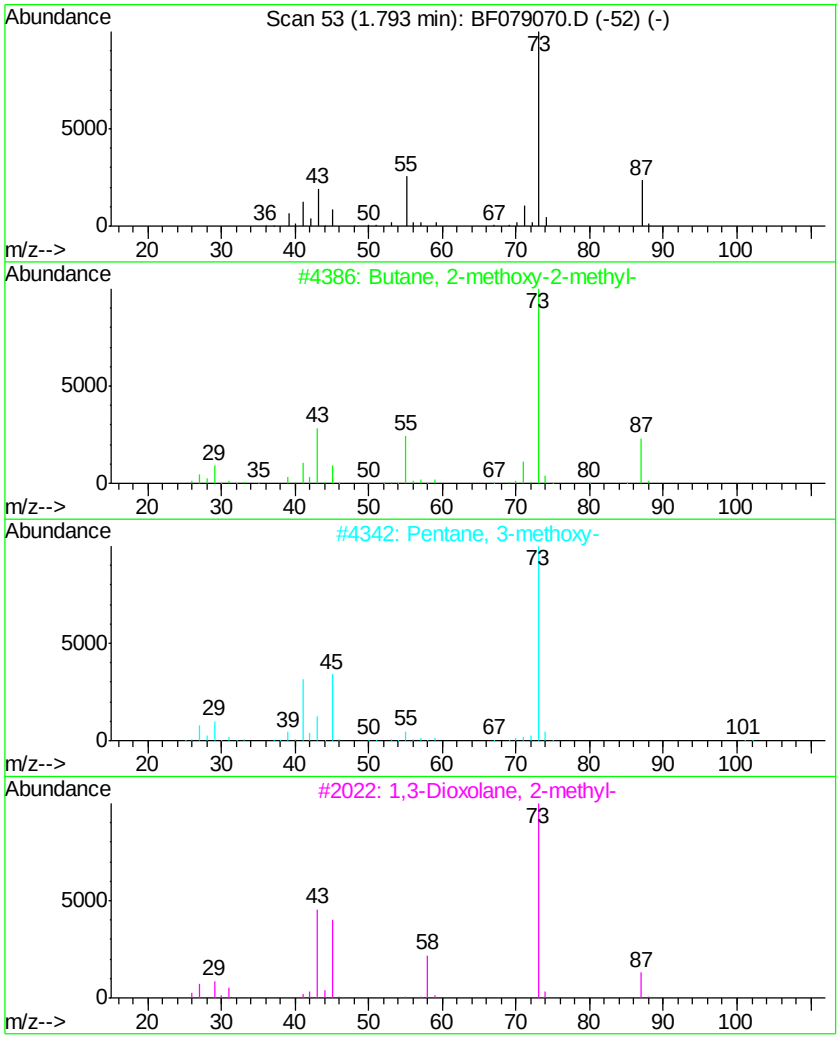
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

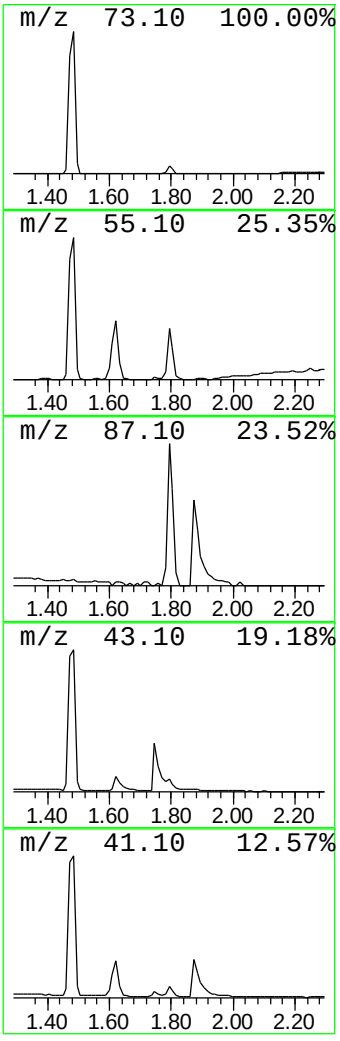
****

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	10.74 ng	244796	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079070.D
Acq On : 9 May 2015 8:33
Operator : TP/IZ
Sample : G2151-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-3.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

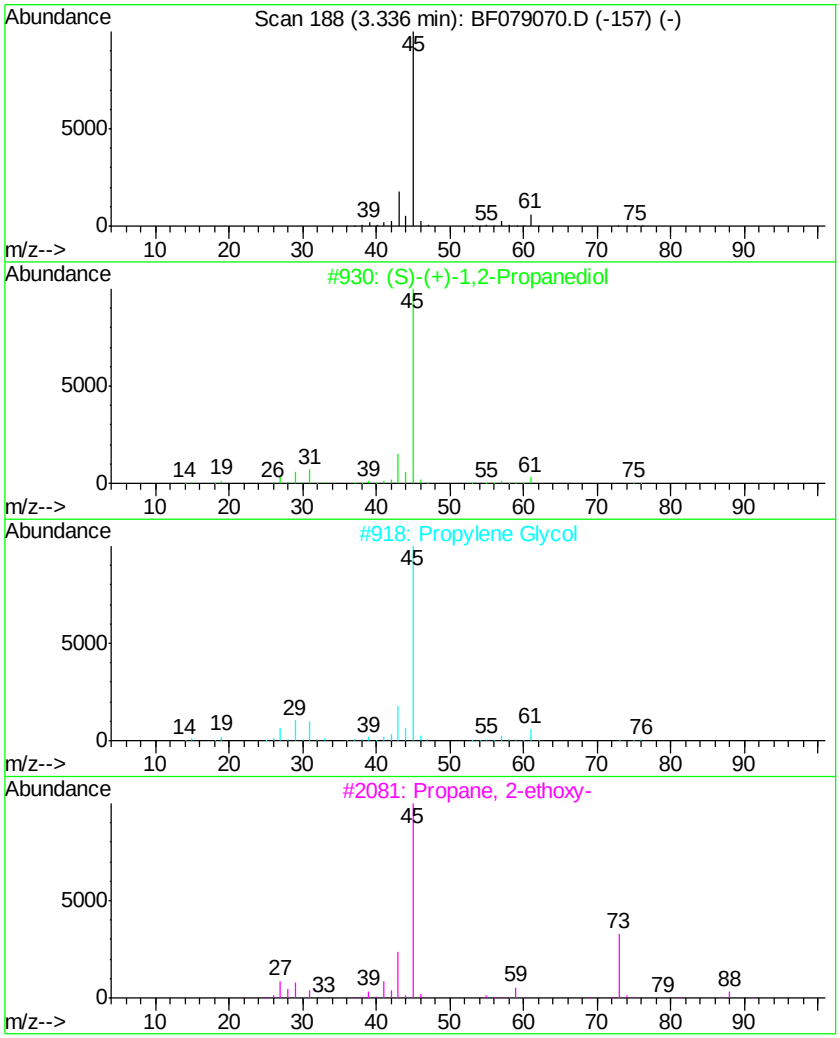
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

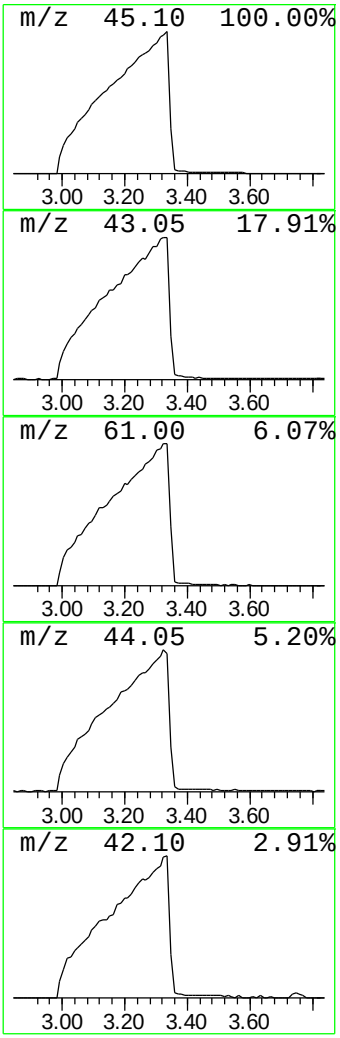
****

Peak Number 6 (S)-(+)-1,2-Propanediol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.34	724.81 ng	16524000	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	49
3	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079070.D
Acq On : 9 May 2015 8:33
Operator : TP/IZ
Sample : G2151-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-3.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

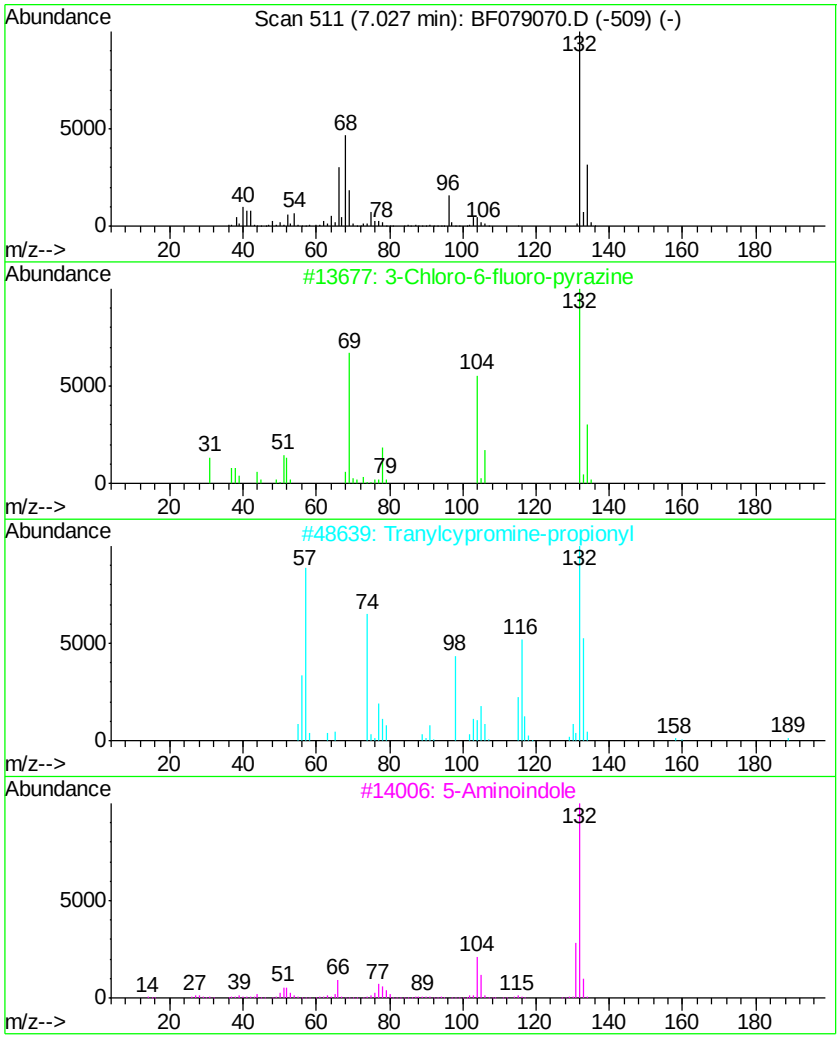
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

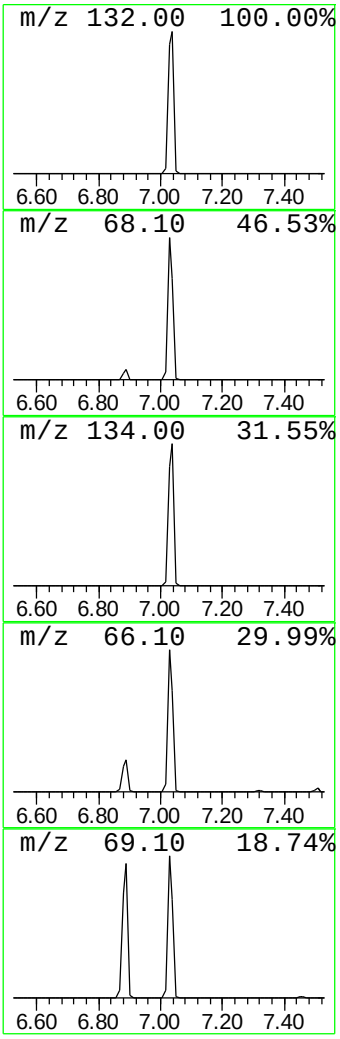
****

Peak Number 7 unknown7.03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	97.35 ng	2219250	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079070.D
Acq On : 9 May 2015 8:33
Operator : TP/IZ
Sample : G2151-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-3.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

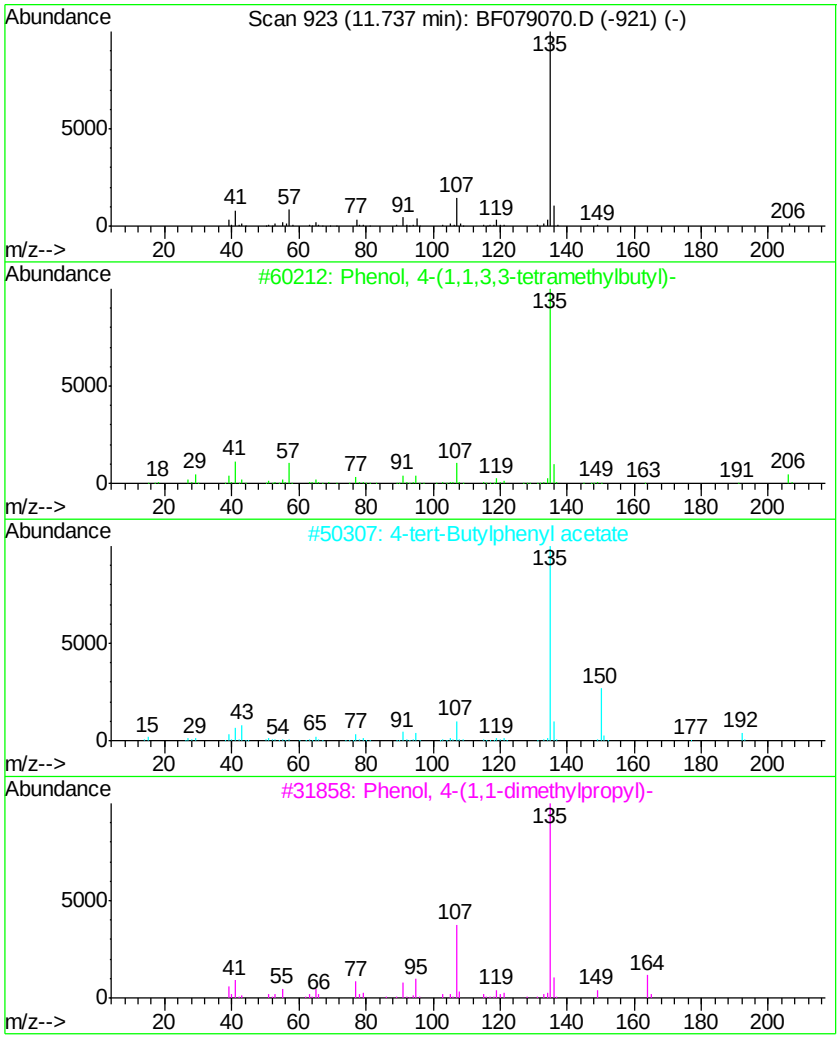
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

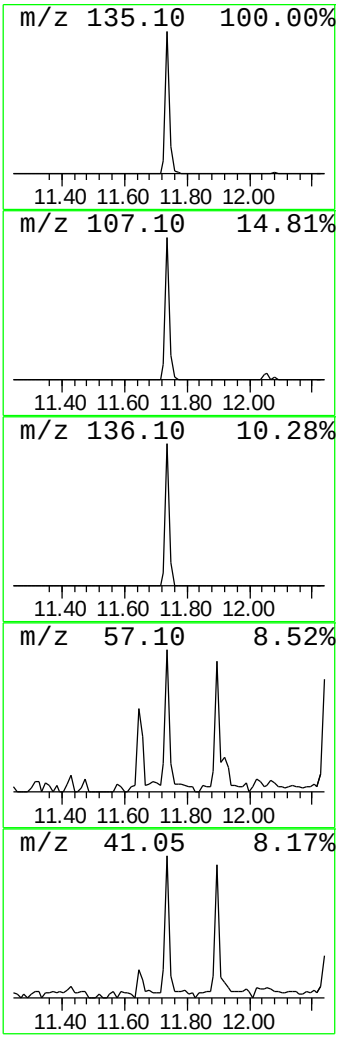
****

Peak Number 9 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	6.52 ng	204014	Acenaphthene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
2	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	78
3	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	72
4	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	64
5	2-Methyl-2-(4'-hydroxyphenyl)pen...	192	C12H16O2	070205-18-4	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
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Acq On : 9 May 2015 8:33
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Sample : G2151-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-3.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

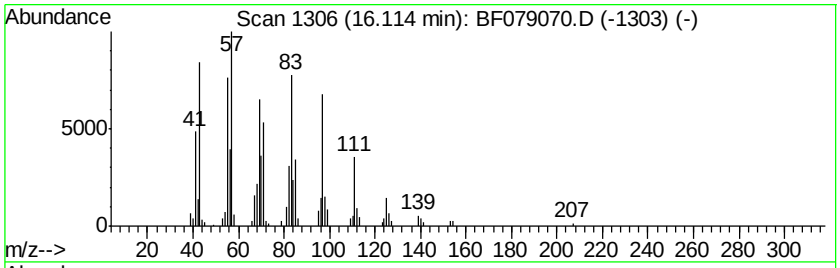
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

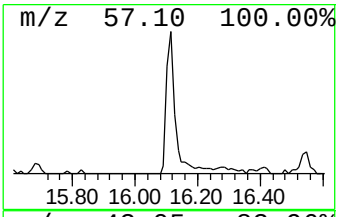
****

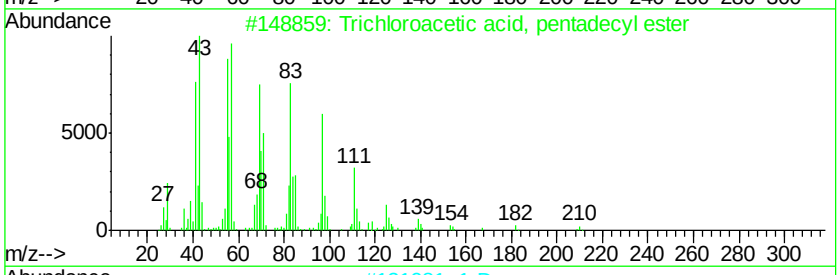
Peak Number 10 Trichloroacetic acid, penta... Concentration Rank 9

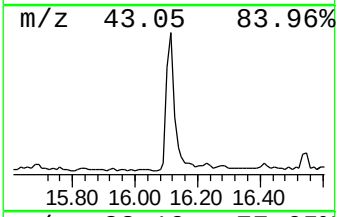
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	7.43 ng	247923	Chrysene-d12	16.24

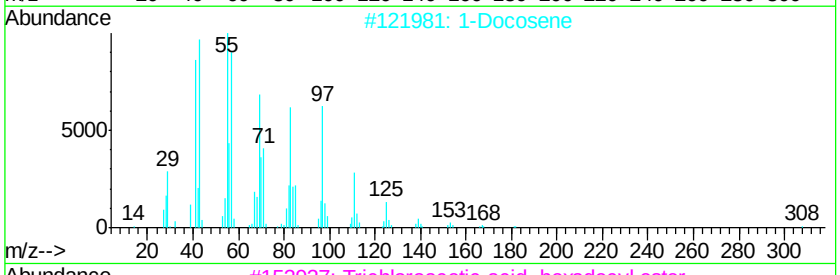
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	1-Heptadecanol	256	C17H36O	001454-85-9	90
5	17-Pentatriacontene	491	C35H70	006971-40-0	90

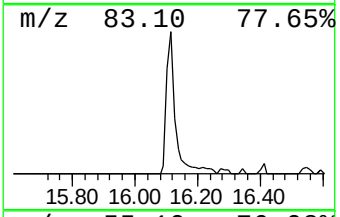


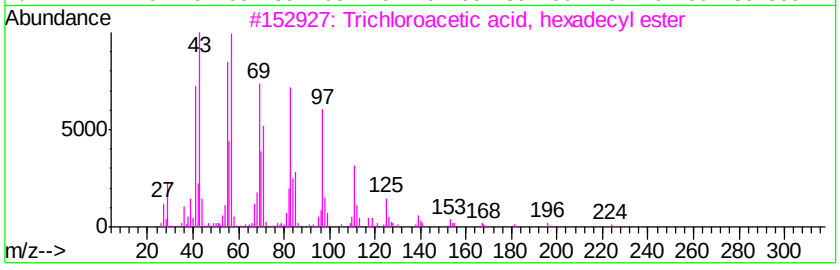


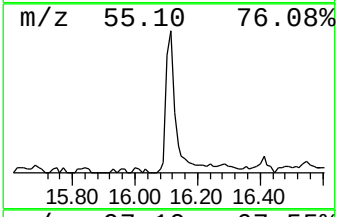


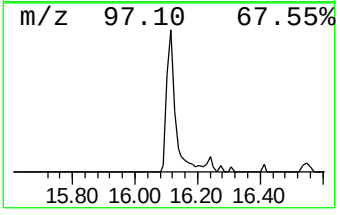












Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.48	1.48	155.0	ng	3533130	1	7.32	455954	20.0
Butane, 2-methoxy...	1.79	10.7	ng	244796	1	7.32	455954	20.0
(S)-(+)-1,2-Propa...	3.34	724.8	ng	16524000	1	7.32	455954	20.0
unknown7.03	7.03	97.3	ng	2219250	1	7.32	455954	20.0
Phenol, 4-(1,1,3,...	11.74	6.5	ng	204014	3	11.07	625629	20.0
Trichloroacetic a...	16.11	7.4	ng	247923	5	16.24	667647	20.0