LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051415\
Data File : BF079253.D
Acq On : 15 May 2015 1:55
Operator : TP/IZ
Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(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	1.267	6	7	13	rVB	108087	145506	4.79%	0.760%
2	1.358	13	15	18	rVB	2516774	2645412	87.16%	13.824%
3	1.495	23	27	29	rVB	763311	1211541	39.92%	6.331%
4	1.655	39	41	43	rBV	558685	696073	22.93%	3.637%
5	1.690	43	44	53	rVV	330628	524196	17.27%	2.739%
6	1.815	53	55	77	rVB	1686597	3035062	100.00%	15.860%
7	2.078	77	78	95	rVB5	28871	108343	3.57%	0.566%
8	4.947	326	329	332	rBV	56122	67022	2.21%	0.350%
9	4.993	332	333	341	rVB	38705	56493	1.86%	0.295%
10	5.507	376	378	381	rBV	862372	889928	29.32%	4.650%
11	6.787	487	490	492	rBV	815852	979438	32.27%	5.118%
12	6.924	500	502	505	rBV	972021	1003140	33.05%	5.242%
13	7.222	525	528	530	rBV	234905	295447	9.73%	1.544%
14	7.405	542	544	546	rBV	836809	779550	25.68%	4.074%
15	7.907	586	588	591	rBV	683275	598297	19.71%	3.126%
16	8.787	663	665	667	rBV	321412	443679	14.62%	2.318%
17	10.136	781	783	786	rBV	1207609	1252775	41.28%	6.547%
18	10.651	826	828	830	rBV	28198	36564	1.20%	0.191%
19	10.971	854	856	858	rBV	420326	457927	15.09%	2.393%
20	11.942	939	941	944	rBV2	543740	693232	22.84%	3.623%
21	12.811	1014	1017	1019	rBV	493587	465218	15.33%	2.431%
22	14.811	1189	1192	1194	rBV	1172944	1385188	45.64%	7.238%
23	15.977	1291	1294	1300	rBV2	90008	150063	4.94%	0.784%
24	16.091	1302	1304	1307	rBV	411557	566150	18.65%	2.958%
25	17.245	1402	1405	1408	rBV	39351	44869	1.48%	0.234%
26	17.817	1452	1455	1458	rBV	490395	605389	19.95%	3.164%

Sum of corrected areas: 19136502

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051415\
Data File : BF079253.D
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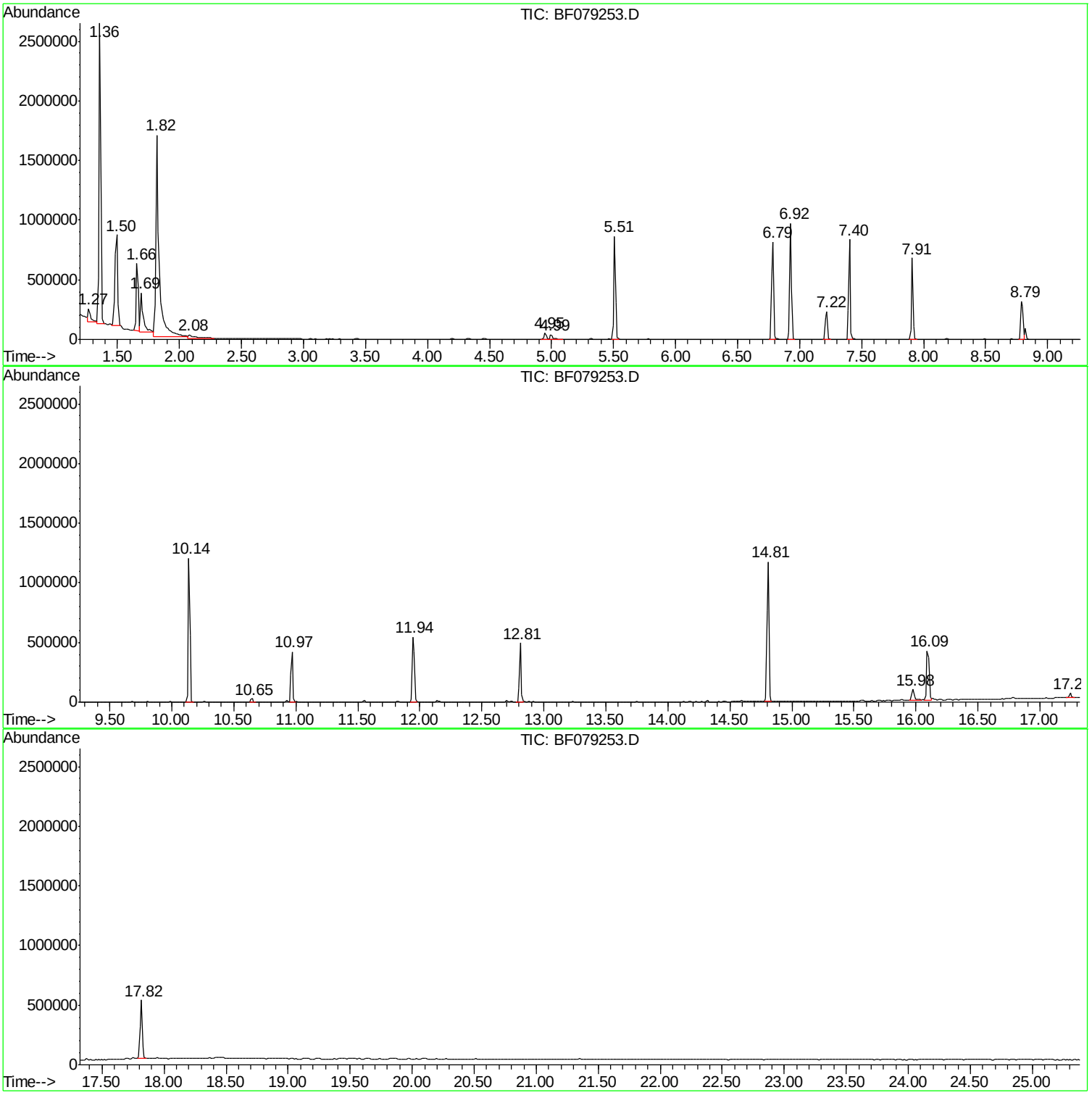
Operator : TP/IZ
Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051415\
Data File : BF079253.D
Acq On : 15 May 2015 1:55
Operator : TP/IZ
Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(3-5)

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

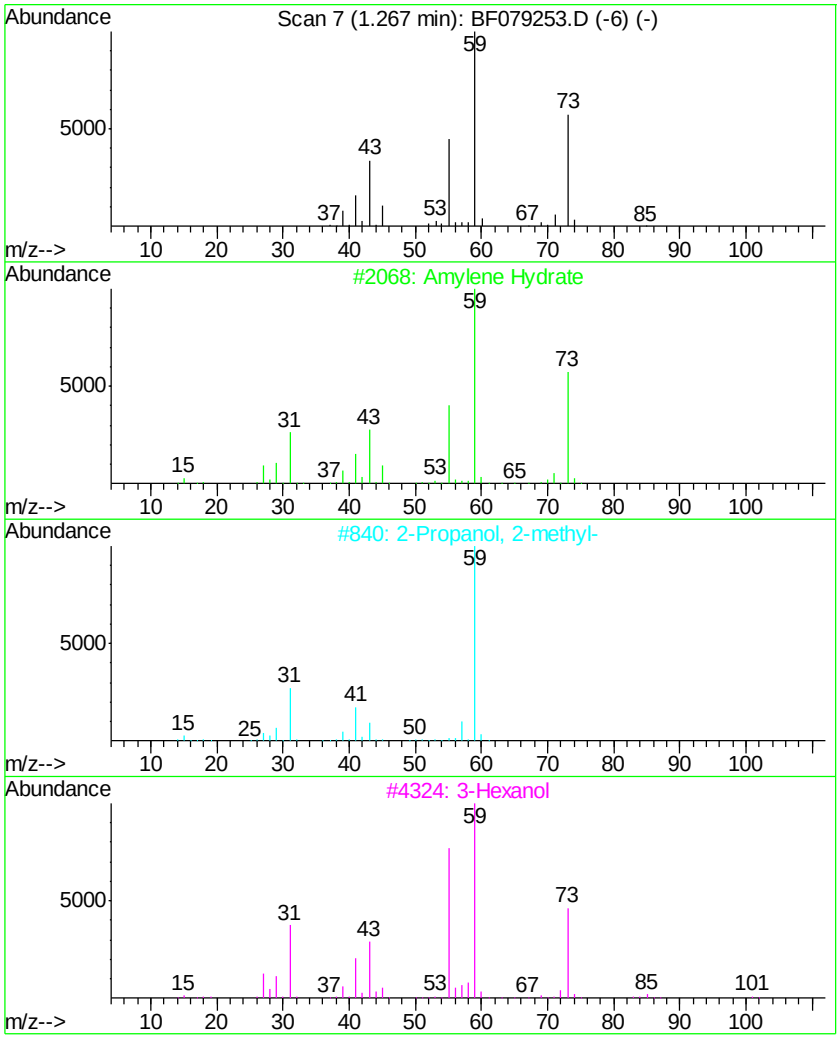
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

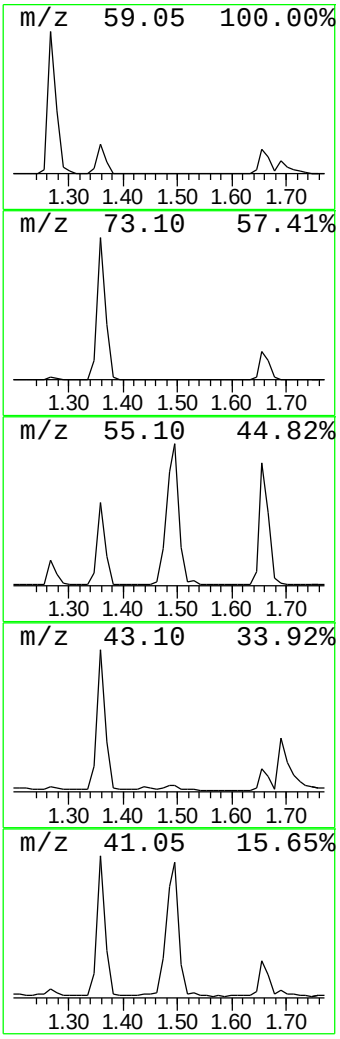
****

Peak Number 1 Amylene Hydrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.27	9.85 ng	145506	1,4-Dichlorobenzene-d4	7.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene Hydrate	88	C5H12O	000075-85-4	83
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	40
3	3-Hexanol	102	C6H14O	000623-37-0	40
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	40
5	Silane, trimethyl-	74	C3H10Si	000993-07-7	39





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Data File : BF079253.D
Acq On : 15 May 2015 1:55
Operator : TP/IZ
Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(3-5)

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

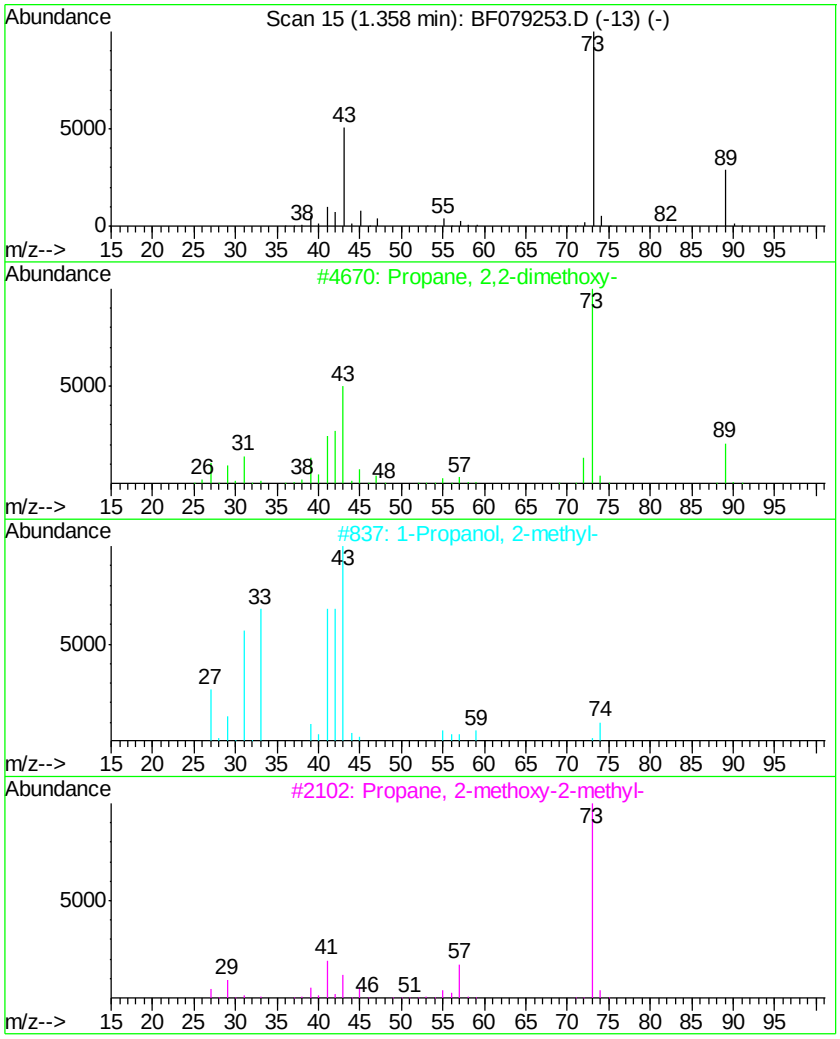
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

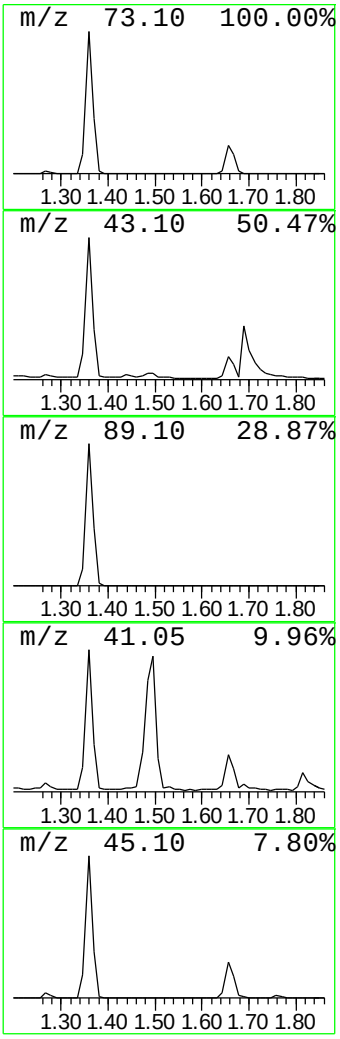
****

Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.36	179.08 ng	2645410	1,4-Dichlorobenzene-d4	7.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051415\
Data File : BF079253.D
Acq On : 15 May 2015 1:55
Operator : TP/IZ
Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(3-5)

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

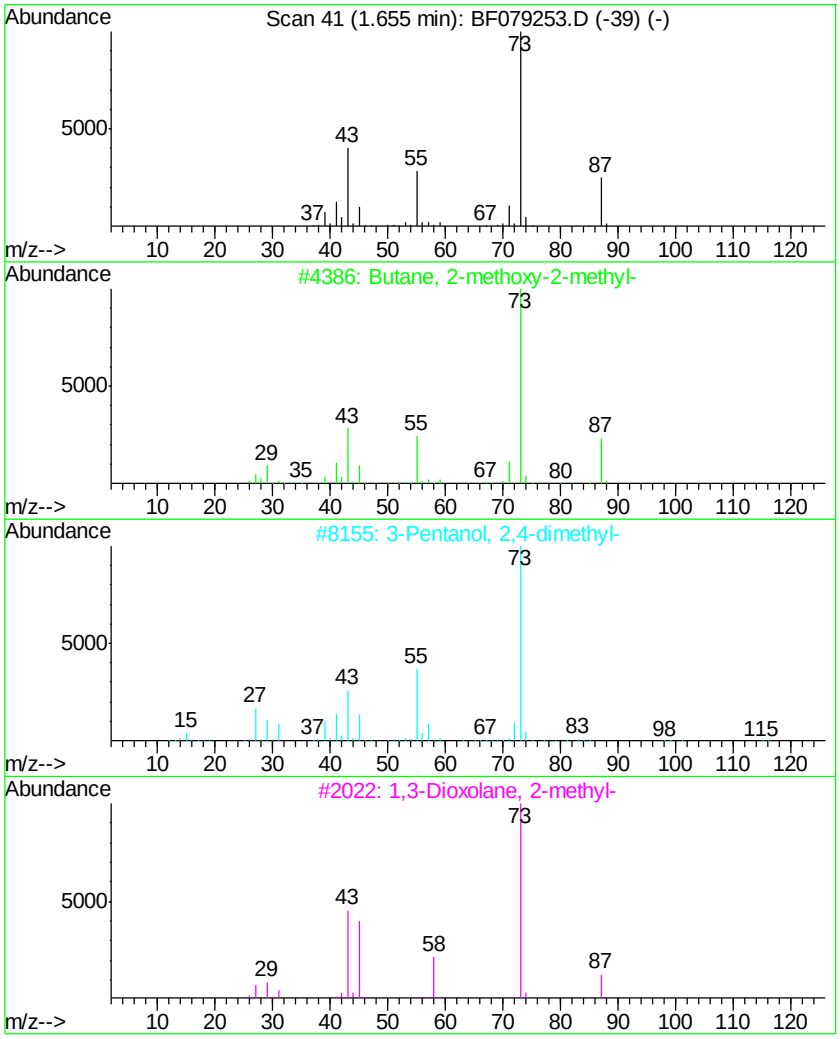
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

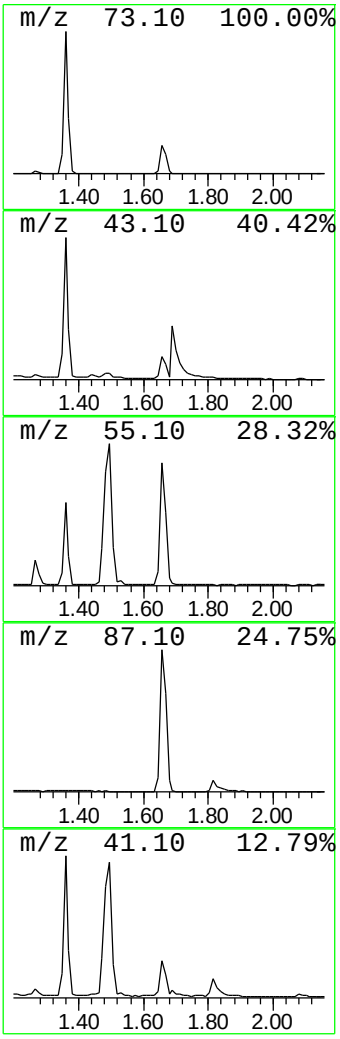
****

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.66	47.12 ng	696073	1,4-Dichlorobenzene-d4	7.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051415\
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Acq On : 15 May 2015 1:55
Operator : TP/IZ
Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(3-5)

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

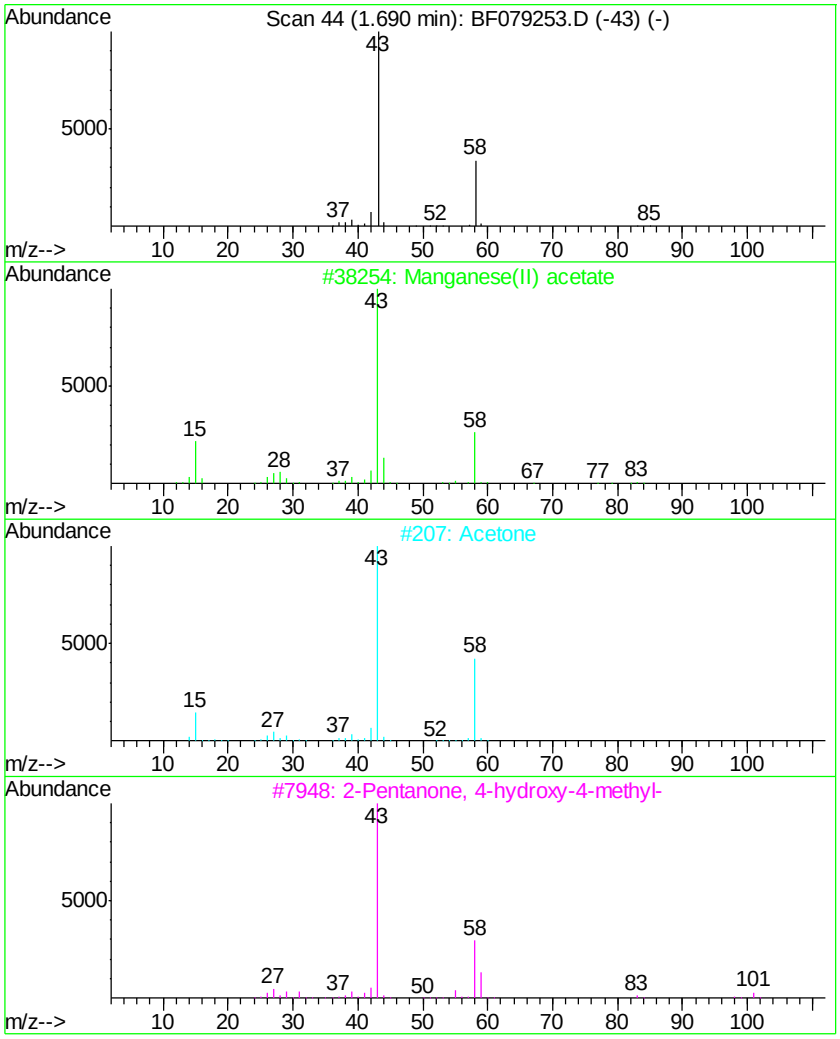
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

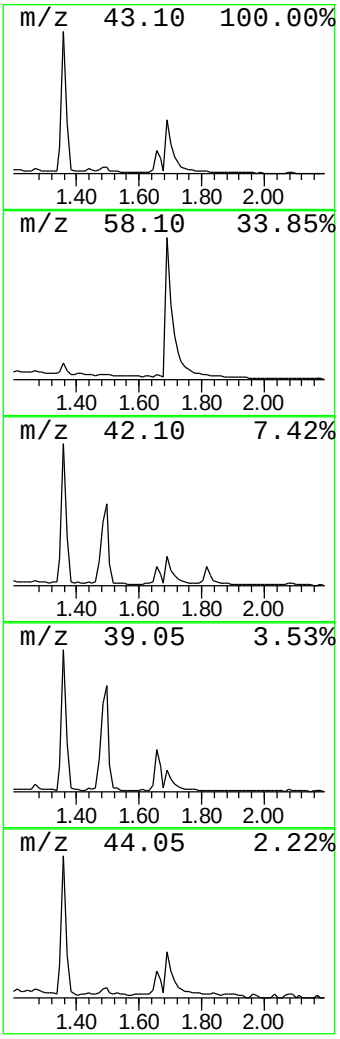
****

Peak Number 5 unknown1.69 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.69	35.48 ng	524196	1,4-Dichlorobenzene-d4	7.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Manganese(II) acetate	173	C4H6MnO4	006156-78-1	40
2	Acetone	58	C3H6O	000067-64-1	39
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
4	Ethene, methoxy-	58	C3H6O	000107-25-5	4
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051415\
Data File : BF079253.D
Acq On : 15 May 2015 1:55
Operator : TP/IZ
Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(3-5)

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

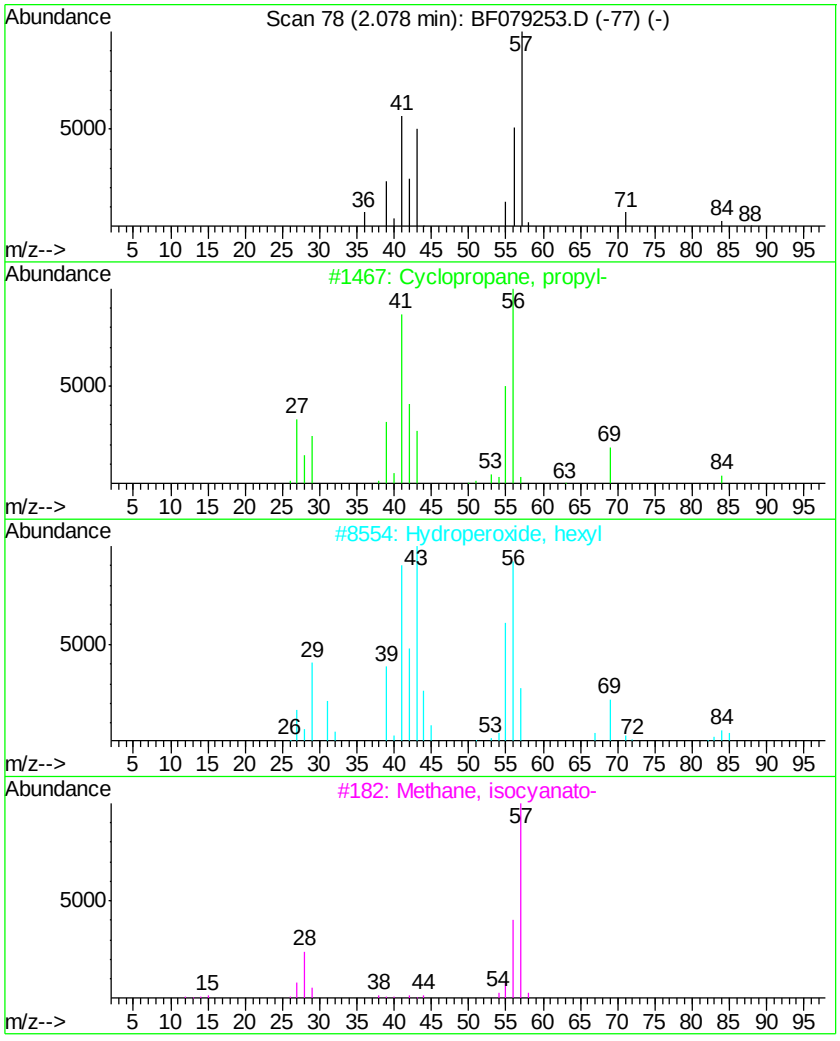
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

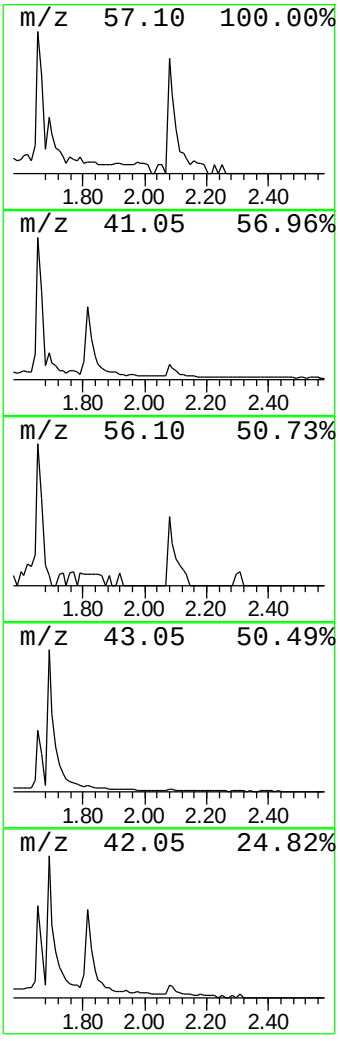
****

Peak Number 7 Cyclopropane, propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.08	7.33 ng	108343	1,4-Dichlorobenzene-d4	7.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, propyl-	84	C6H12	002415-72-7	50
2	Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	36
3	Methane, isocyanato-	57	C2H3NO	000624-83-9	9
4	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	9
5	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	9





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Data File : BF079253.D
Acq On : 15 May 2015 1:55
Operator : TP/IZ
Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(3-5)

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

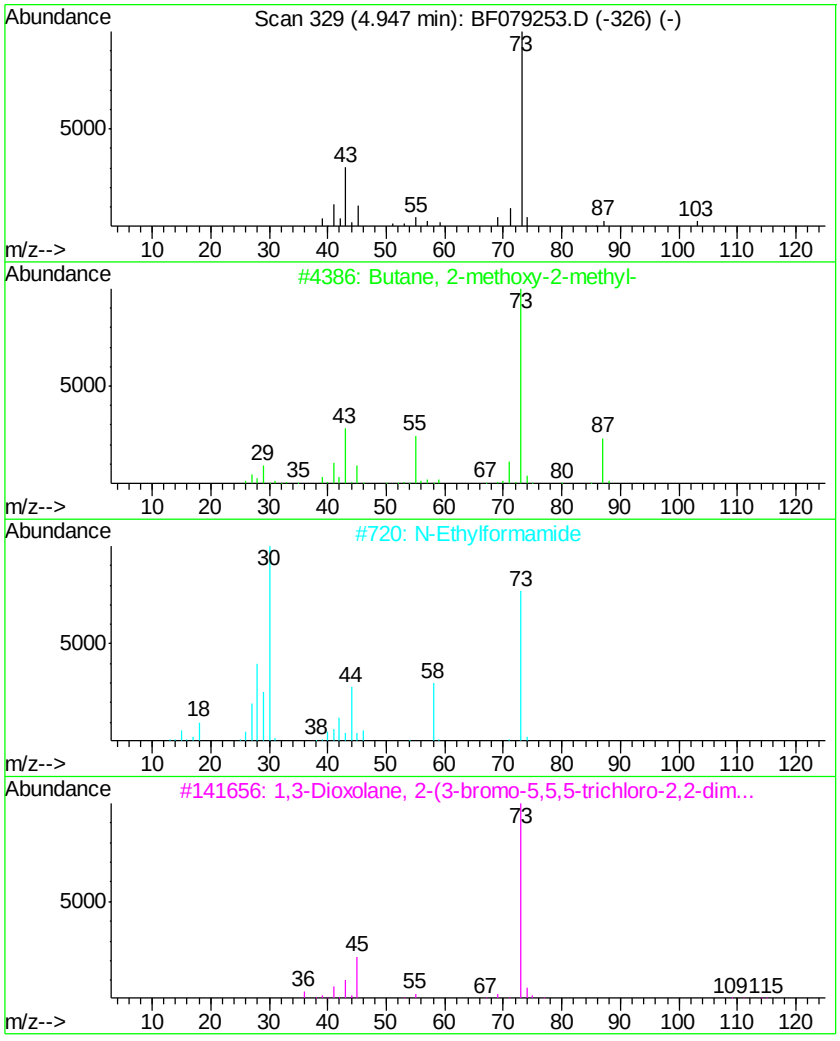
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

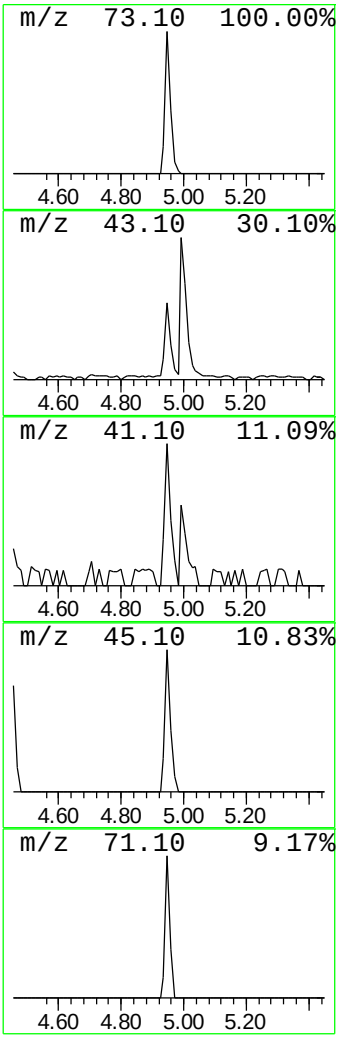
****

Peak Number 8 unknown4.95 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	4.54 ng	67022	1,4-Dichlorobenzene-d4	7.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	36
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





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Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(3-5)

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

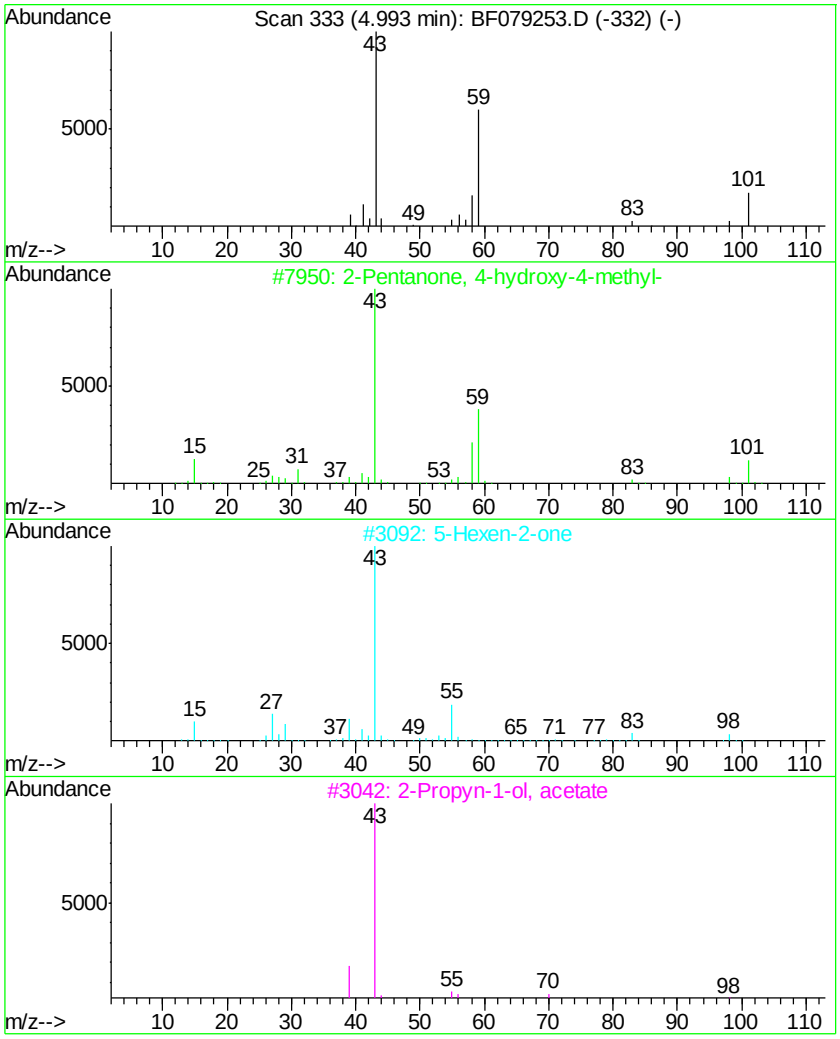
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

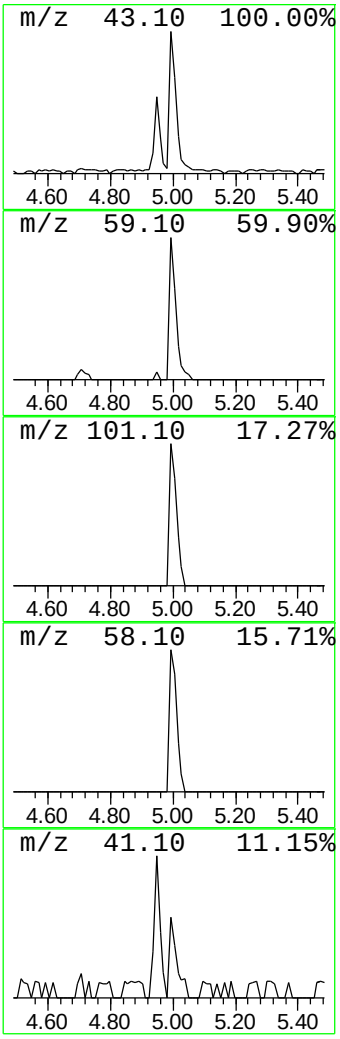
****

Peak Number 9 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	3.82 ng	56493	1,4-Dichlorobenzene-d4	7.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





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Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(3-5)

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

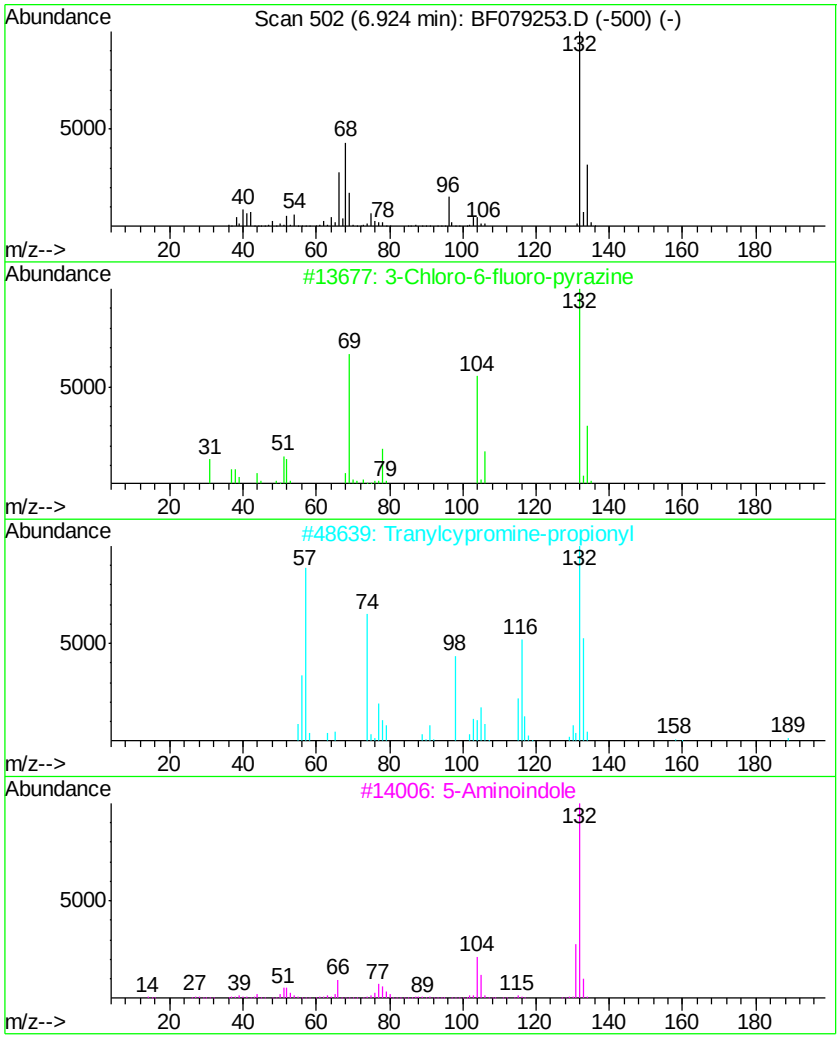
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

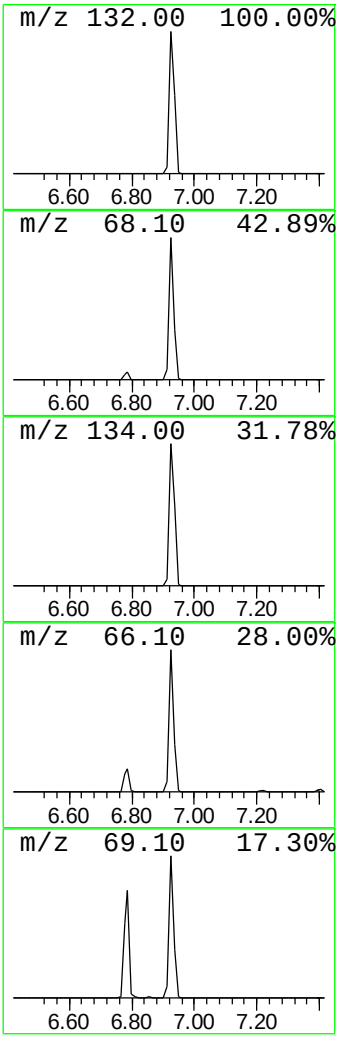
****

Peak Number 10 unknown6.92 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	67.91 ng	1003140	1,4-Dichlorobenzene-d4	7.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Aminoindole	132	C8H8N2	005192-03-0	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





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(3-5)

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

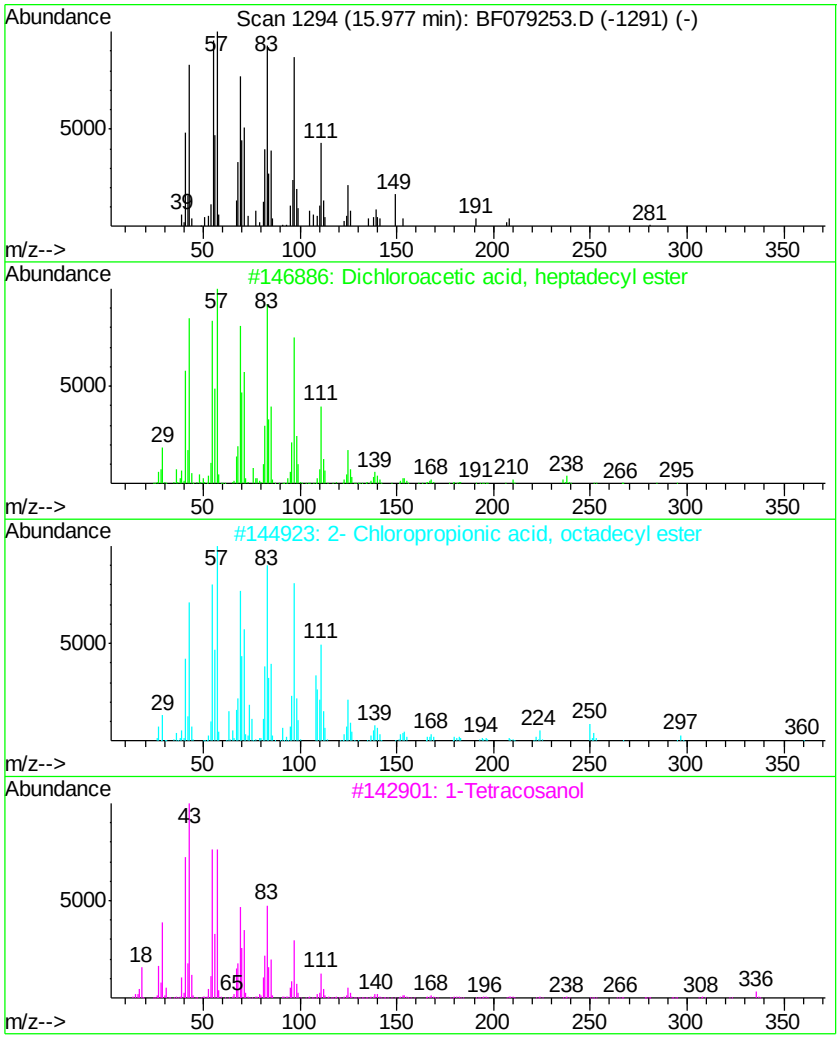
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

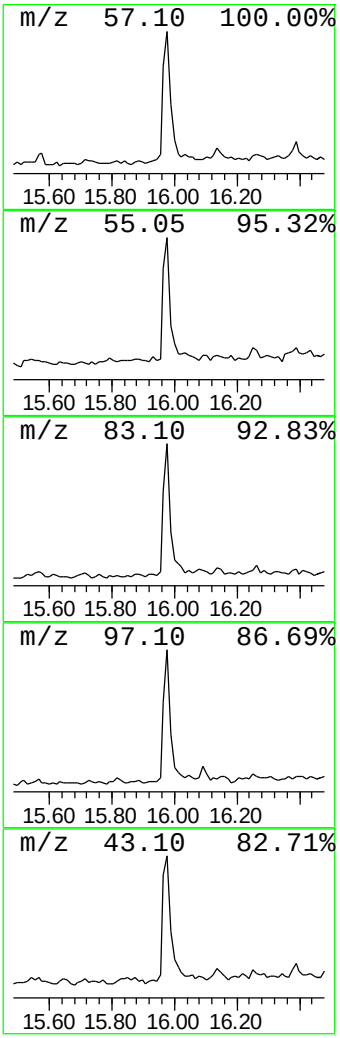
****

Peak Number 12 Dichloroacetic acid, heptad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	5.30 ng	150063	Chrysene-d12	16.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
3	1-Tetracosanol	354	C24H50O	000506-51-4	90
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051415\
Data File : BF079253.D
Acq On : 15 May 2015 1:55
Operator : TP/IZ
Sample : G2177-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-19(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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Amylene Hydrate	1.27	9.8	ng	145506	1	7.22	295447	20.0
Propane, 2,2-dime...	1.36	179.1	ng	2645410	1	7.22	295447	20.0
Butane, 2-methoxy...	1.66	47.1	ng	696073	1	7.22	295447	20.0
unknown1.69	1.69	35.5	ng	524196	1	7.22	295447	20.0
Cyclopropane, pro...	2.08	7.3	ng	108343	1	7.22	295447	20.0
unknown4.95	4.95	4.5	ng	67022	1	7.22	295447	20.0
2-Pentanone, 4-hy...	4.99	3.8	ng	56493	1	7.22	295447	20.0
unknown6.92	6.92	67.9	ng	1003140	1	7.22	295447	20.0
Dichloroacetic ac...	15.98	5.3	ng	150063	5	16.10	566150	20.0