LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051115\
Data File : BF079154.D
Acq On : 12 May 2015 11:25
Operator : TP/IZ
Sample : G2176-21
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-26(5-10)

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	1.450	20	23	25	rBV	4417094	5607109	100.00%	21.774%
2	1.575	31	34	47	rVB	171396	342420	6.11%	1.330%
3	1.758	47	50	57	rVV2	190841	421223	7.51%	1.636%
4	1.861	57	59	86	rVB	976371	1683360	30.02%	6.537%
5	5.096	340	342	348	rVB	75830	100401	1.79%	0.390%
6	5.599	384	386	389	rBV	1417574	1635421	29.17%	6.351%
7	6.867	494	497	499	rBV	1974206	1783245	31.80%	6.925%
8	7.016	507	510	512	rBV	1851429	1839881	32.81%	7.145%
9	7.302	533	535	537	rBV	334734	327029	5.83%	1.270%
10	7.485	549	551	554	rVB	1477124	1334814	23.81%	5.183%
11	7.988	593	595	598	rBV	1002778	1041430	18.57%	4.044%
12	8.879	670	673	675	rBV	435019	449908	8.02%	1.747%
13	10.228	788	791	793	rBV	1667231	2131168	38.01%	8.276%
14	10.731	833	835	837	rBV	52860	60760	1.08%	0.236%
15	11.051	861	863	866	rBV	534103	510673	9.11%	1.983%
16	12.034	946	949	952	rBV	1417089	1470089	26.22%	5.709%
17	12.902	1022	1025	1027	rBV	554724	561432	10.01%	2.180%
18	14.720	1177	1184	1185	rBV5	29899	110837	1.98%	0.430%
19	14.903	1197	1200	1202	rVB	2262942	2588517	46.16%	10.052%
20	16.080	1301	1303	1310	rVB	141968	204919	3.65%	0.796%
21	16.217	1312	1315	1317	rBV	510723	743449	13.26%	2.887%
22	16.251	1317	1318	1320	rVV	83807	80936	1.44%	0.314%
23	18.023	1470	1473	1475	rBV	536266	722805	12.89%	2.807%

Sum of corrected areas: 25751826

LSC Report - Integrated Chromatogram

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Operator : TP/IZ
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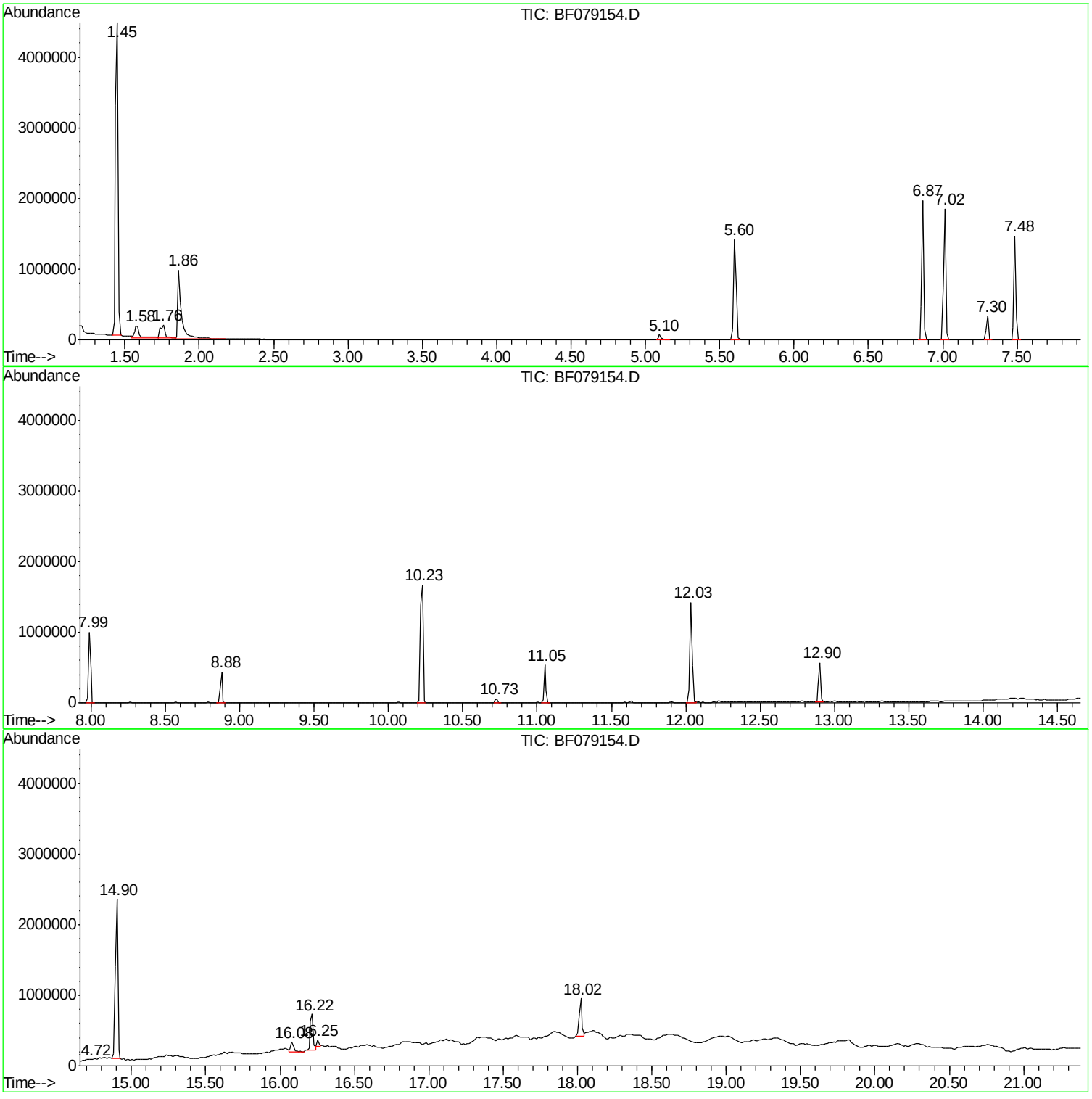
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-26(5-10)

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\BF051115\
Data File : BF079154.D
Acq On : 12 May 2015 11:25
Operator : TP/IZ
Sample : G2176-21
Misc :
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Instrument : BNA_F
ClientSampleId : PS-26(5-10)

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

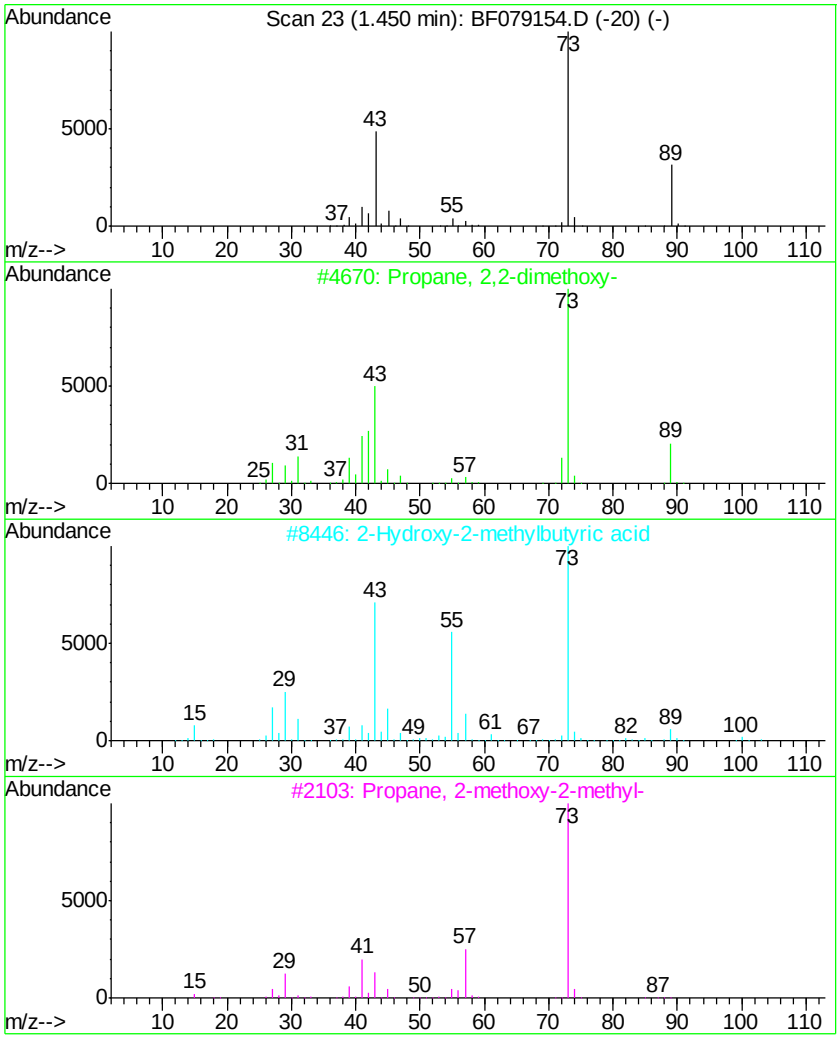
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

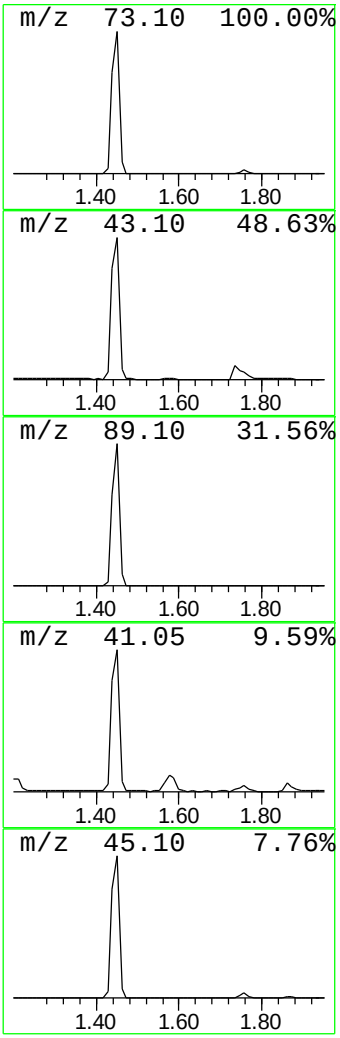
****

Peak Number 1 unknown1.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.45	342.91 ng	5607110	1,4-Dichlorobenzene-d4	7.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	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	N-Ethylformamide	73	C3H7NO	000627-45-2	5





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Data File : BF079154.D
Acq On : 12 May 2015 11:25
Operator : TP/IZ
Sample : G2176-21
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-26(5-10)

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

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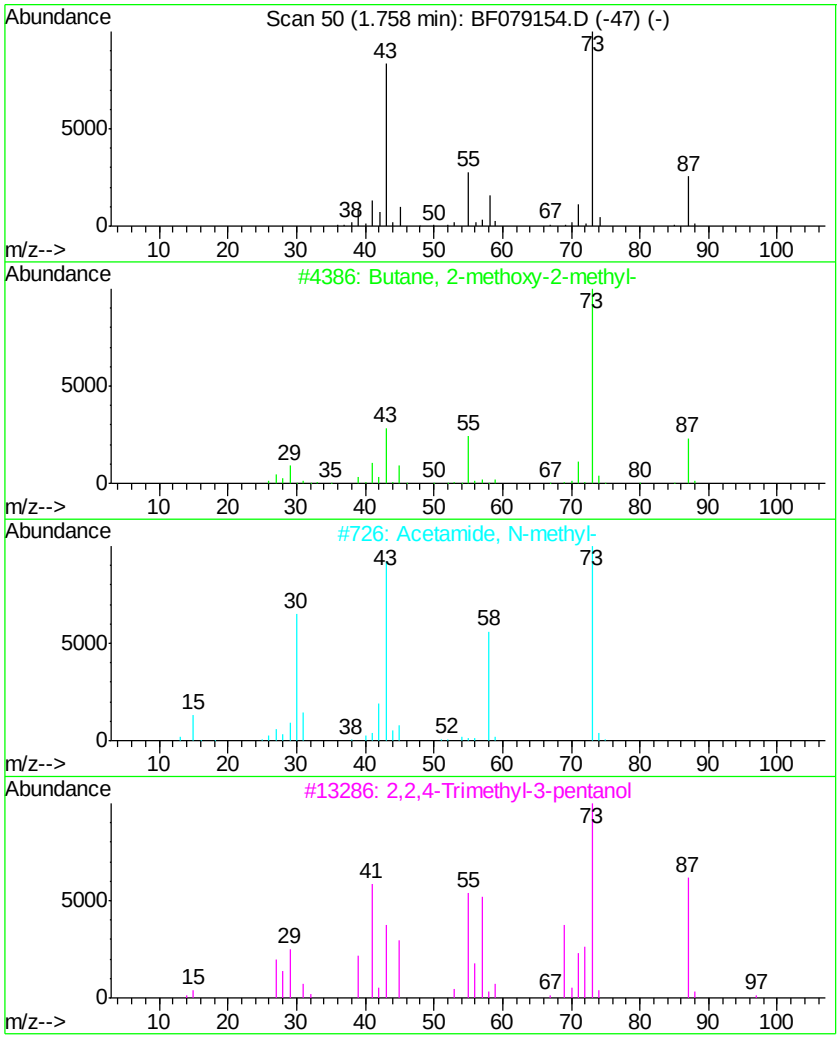
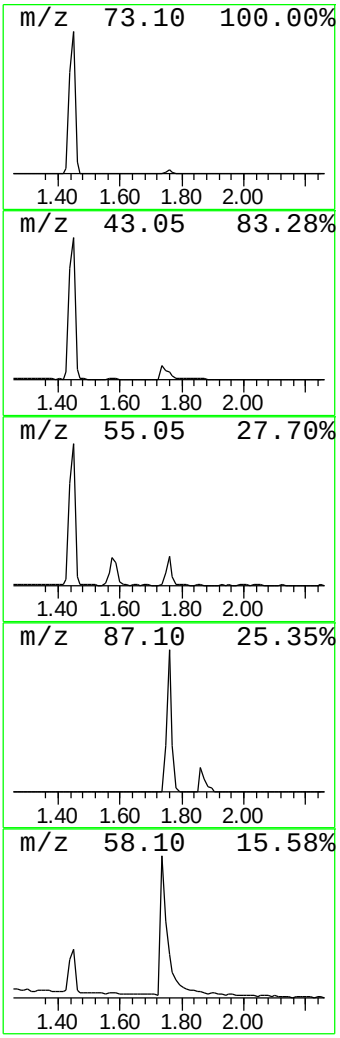
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	25.76 ng	421223	1,4-Dichlorobenzene-d4	7.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	37
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	25
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051115\
Data File : BF079154.D
Acq On : 12 May 2015 11:25
Operator : TP/IZ
Sample : G2176-21
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-26(5-10)

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

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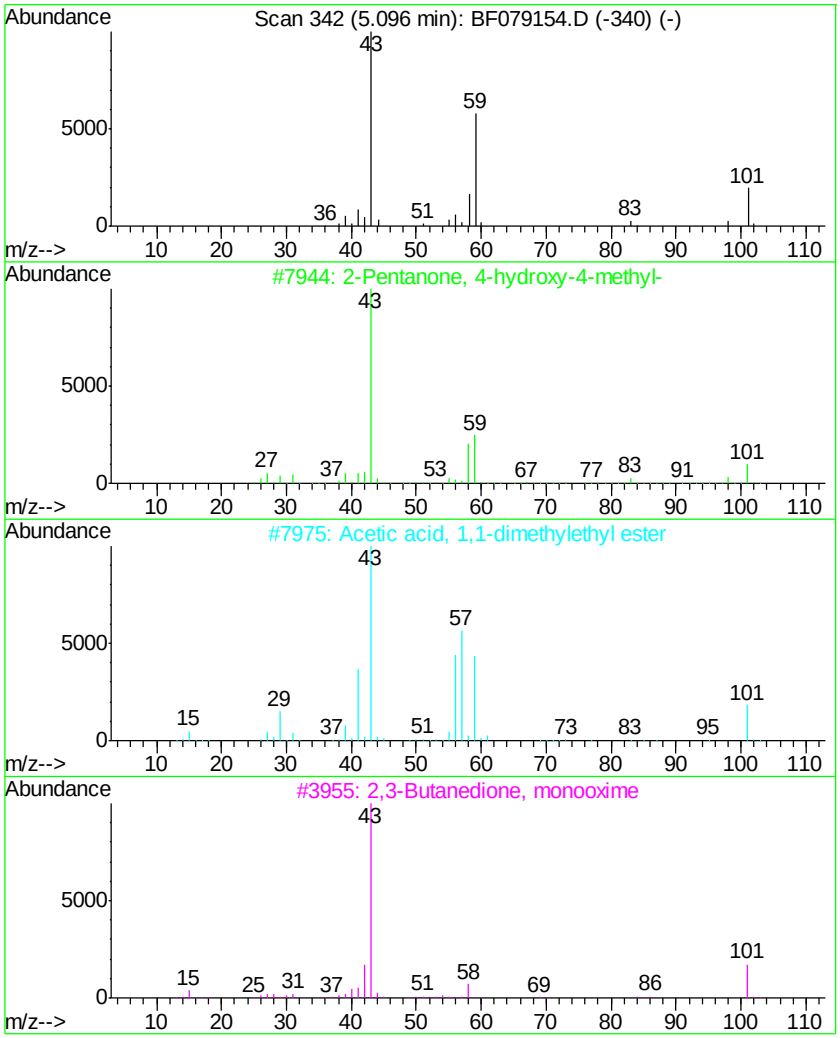
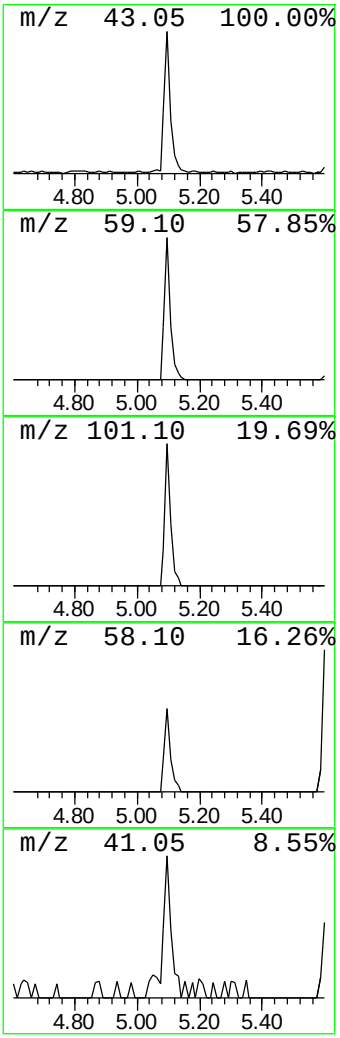
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.14 ng	100401	1,4-Dichlorobenzene-d4	7.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Acq On : 12 May 2015 11:25
Operator : TP/IZ
Sample : G2176-21
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-26(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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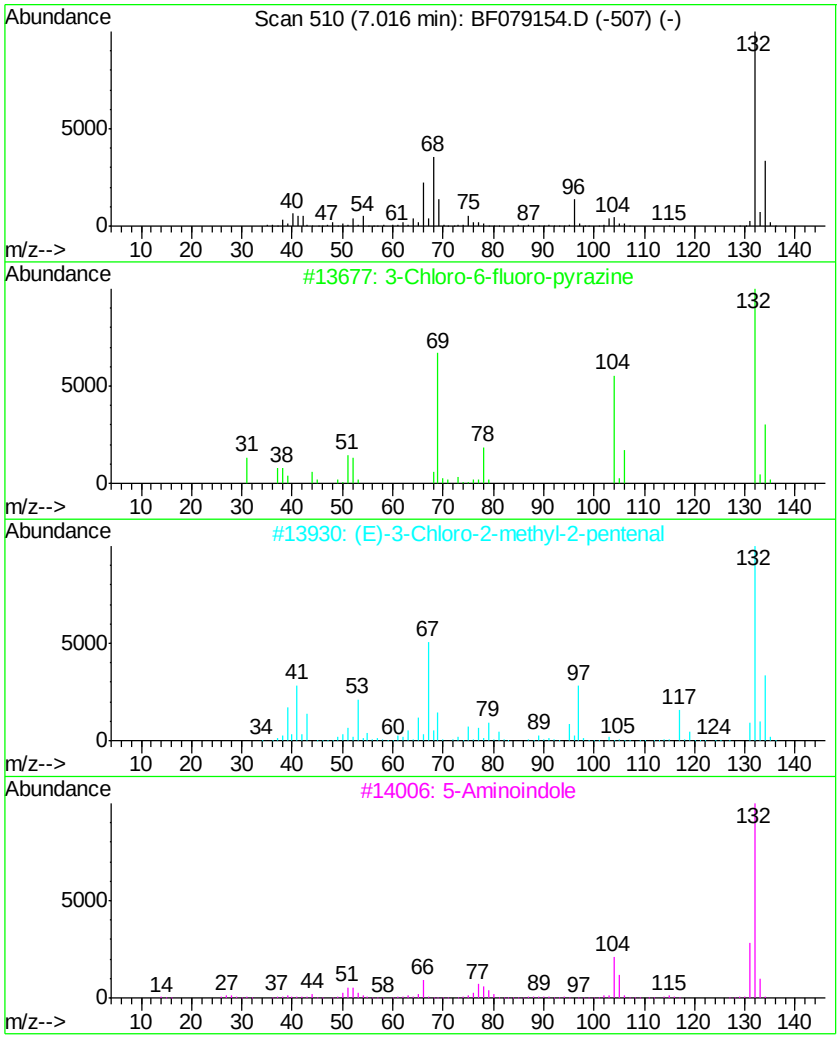
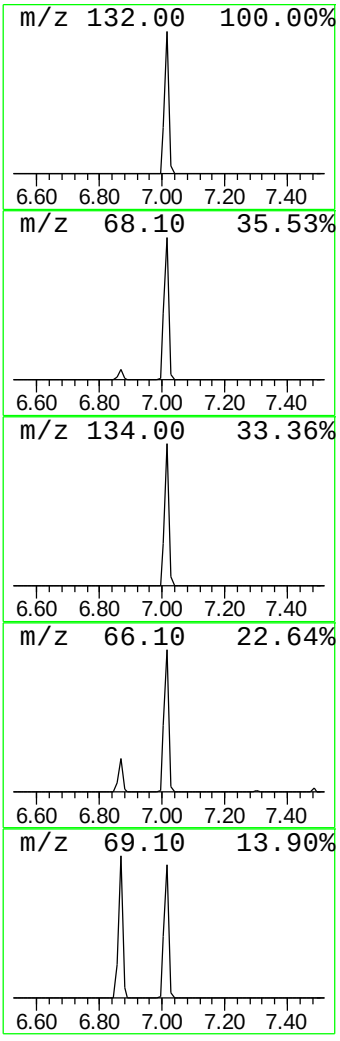
Peak Number 6 unknown7.02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	112.52 ng	1839880	1,4-Dichlorobenzene-d4	7.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051115\
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Acq On : 12 May 2015 11:25
Operator : TP/IZ
Sample : G2176-21
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-26(5-10)

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

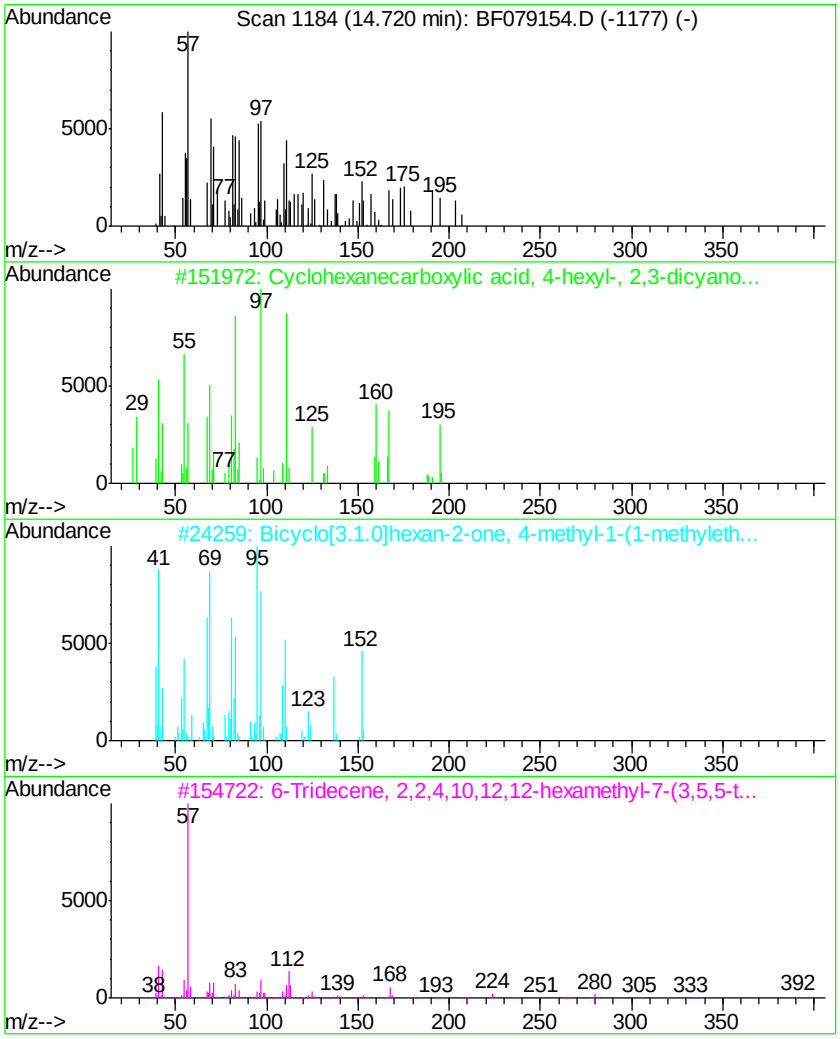
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

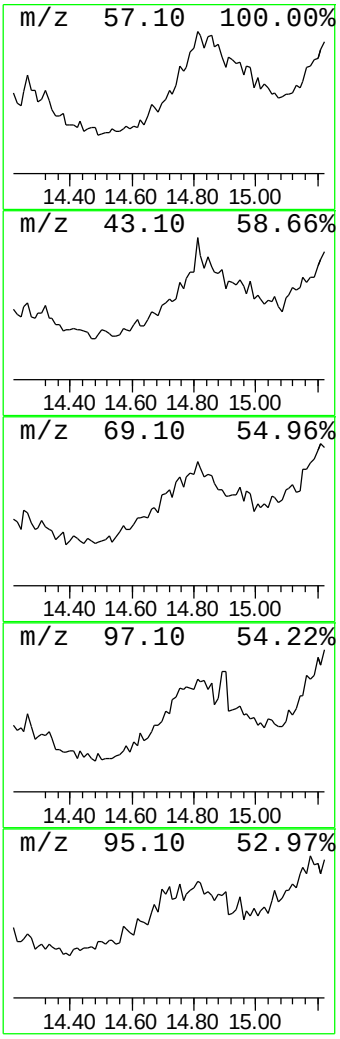
****

Peak Number 8 unknown14.72 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.98 ng	110837	Chrysene-d12	16.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 4-he...	382	C23H30N2O3	133856-88-9	27
2	Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	18
3	6-Tridecene, 2,2,4,10,12,12-hexa...	392	C28H56	055255-73-7	16
4	3-Methyl-2-(2-oxopropyl)furan	138	C8H10O2	087773-62-4	15
5	Cyclohexanecarboxylic acid, 4-he...	424	C26H36N2O3	075941-53-6	14





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ALS Vial : 43 Sample Multiplier: 1

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ClientSampleId : PS-26(5-10)

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

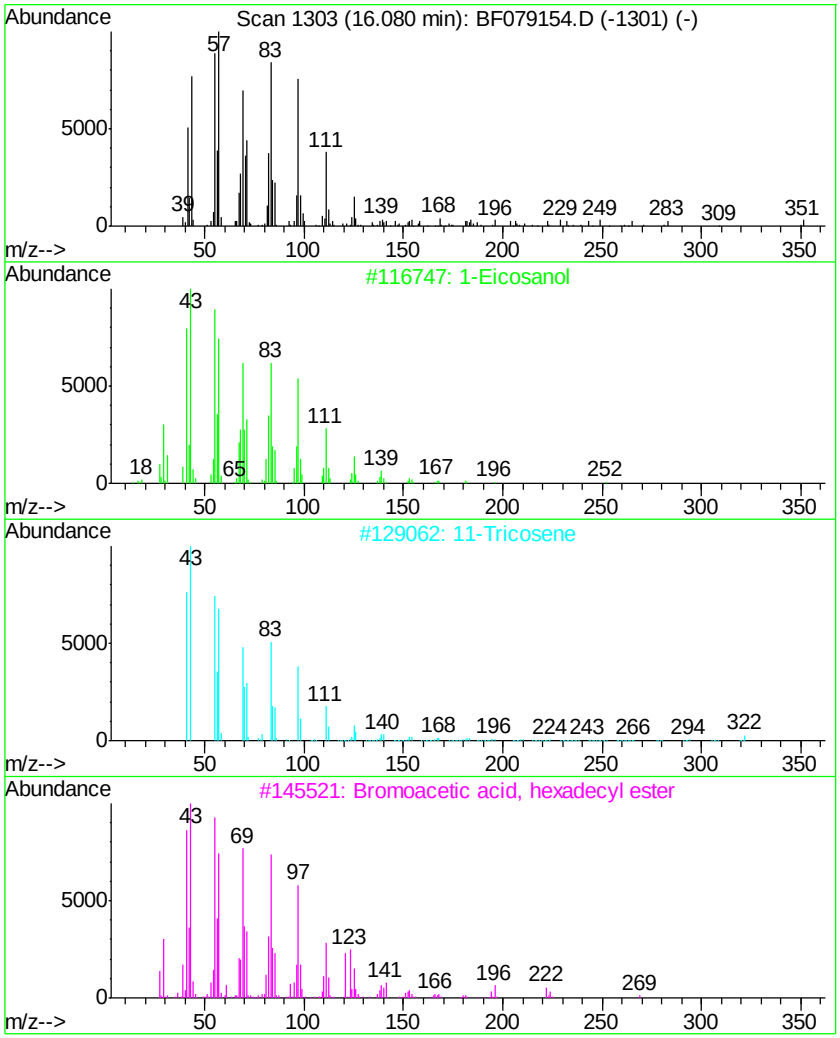
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

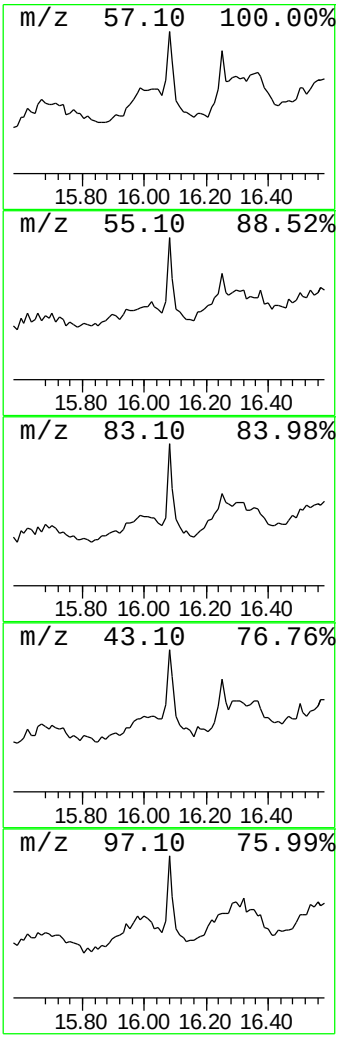
****

Peak Number 9 1-Eicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	5.51 ng	204919	Chrysene-d12	16.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	91
2	11-Tricosene	322	C23H46	052078-56-5	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4	1-Nonadecanol	284	C19H40O	001454-84-8	87
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87





Tentatively Identified Compound (LSC) summary

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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
unknown1.45	1.45	342.9	ng	5607110	1	7.30	327029	20.0
Butane, 2-methoxy...	1.76	25.8	ng	421223	1	7.30	327029	20.0
2-Pentanone, 4-hy...	5.10	6.1	ng	100401	1	7.30	327029	20.0
unknown7.02	7.02	112.5	ng	1839880	1	7.30	327029	20.0
unknown14.72	14.72	3.0	ng	110837	5	16.22	743449	20.0
1-Eicosanol	16.08	5.5	ng	204919	5	16.22	743449	20.0