LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051315\
Data File : BF079201.D
Acq On : 13 May 2015 18:49
Operator : TP/IZ
Sample : G2194-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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	1.370	14	16	19	rVB	587802	601711	10.09%	2.484%
2	1.507	25	28	40	rVB2	121622	370219	6.21%	1.528%
3	1.678	40	43	44	rVV	221795	314484	5.27%	1.298%
4	1.701	44	45	54	rVV	448464	751321	12.59%	3.101%
5	1.827	54	56	100	rVB	2279871	5965501	100.00%	24.623%
6	5.016	333	335	343	rVB	78560	120879	2.03%	0.499%
7	5.530	377	380	382	rBV	1141478	1466585	24.58%	6.054%
8	6.799	489	491	494	rBV	1642465	1570616	26.33%	6.483%
9	6.947	501	504	506	rBV	1682972	1752772	29.38%	7.235%
10	7.233	526	529	531	rBV	332090	295282	4.95%	1.219%
11	7.416	543	545	548	rBV	1236703	1242810	20.83%	5.130%
12	7.930	587	590	592	rBV	944934	1061676	17.80%	4.382%
13	8.810	664	667	669	rVV	440013	379082	6.35%	1.565%
14	10.159	782	785	787	rBV	2168432	1898362	31.82%	7.836%
15	10.662	827	829	832	rBV	381928	337595	5.66%	1.393%
16	10.982	855	857	860	rBV2	404633	421507	7.07%	1.740%
17	11.965	940	943	946	rVB	1228680	1251841	20.98%	5.167%
18	12.834	1016	1019	1021	rBV	475790	497907	8.35%	2.055%
19	14.880	1195	1198	1200	rBV	2076493	2223676	37.28%	9.179%
20	15.440	1244	1247	1251	rVB2	37351	69204	1.16%	0.286%
21	16.217	1312	1315	1323	rBV	112450	203924	3.42%	0.842%
22	16.343	1323	1326	1328	rVV	427615	551715	9.25%	2.277%
23	16.423	1330	1333	1335	rVB	44084	64079	1.07%	0.264%
24	17.188	1391	1400	1402	rBV6	37466	157680	2.64%	0.651%
25	18.503	1512	1515	1519	rBV	380503	554897	9.30%	2.290%
26	20.777	1711	1714	1720	rVB4	44028	101632	1.70%	0.419%

Sum of corrected areas: 24226957

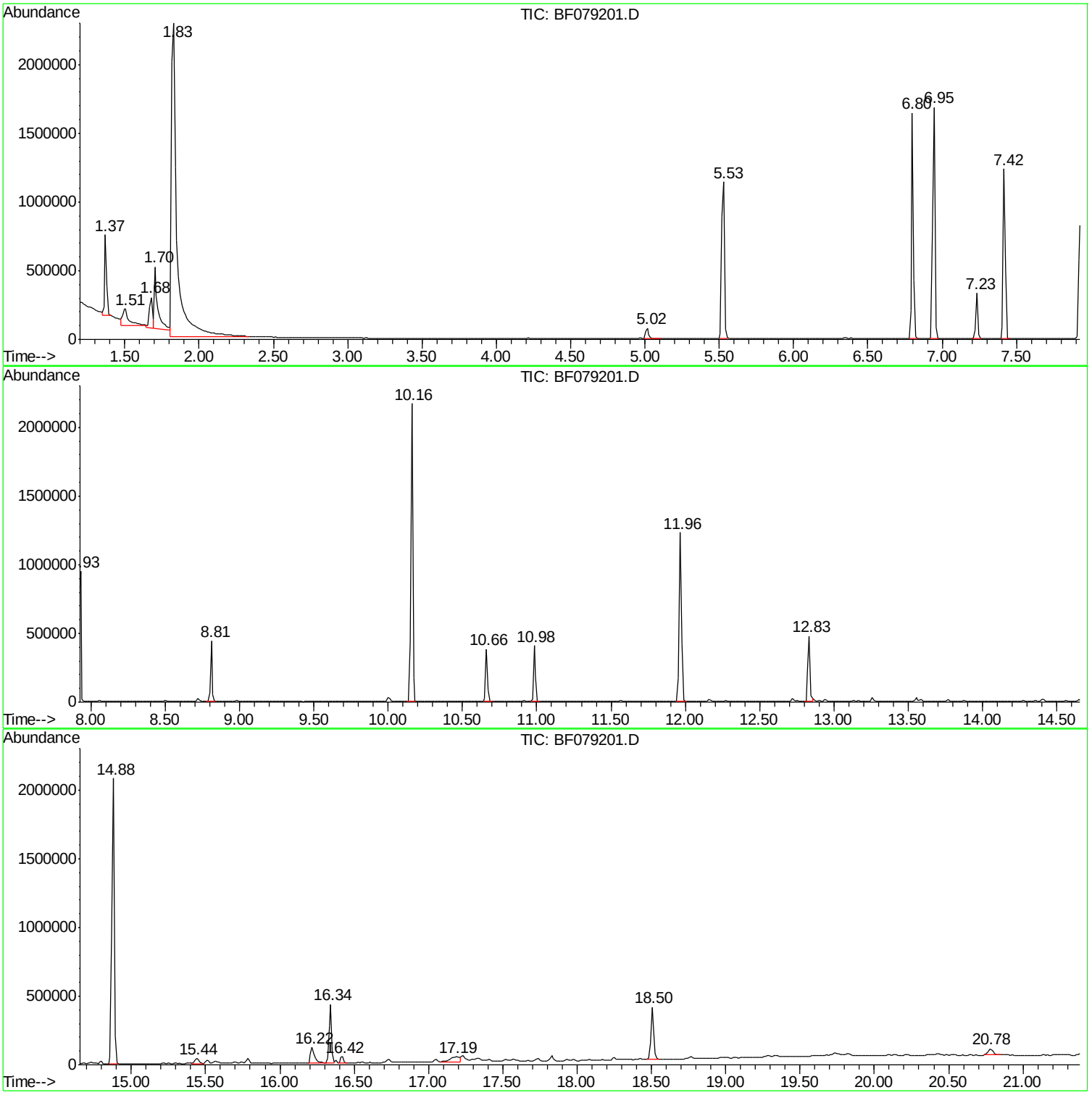
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051315\
Data File : BF079201.D
Acq On : 13 May 2015 18:49
Operator : TP/IZ
Sample : G2194-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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\BF051315\
Data File : BF079201.D
Acq On : 13 May 2015 18:49
Operator : TP/IZ
Sample : G2194-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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

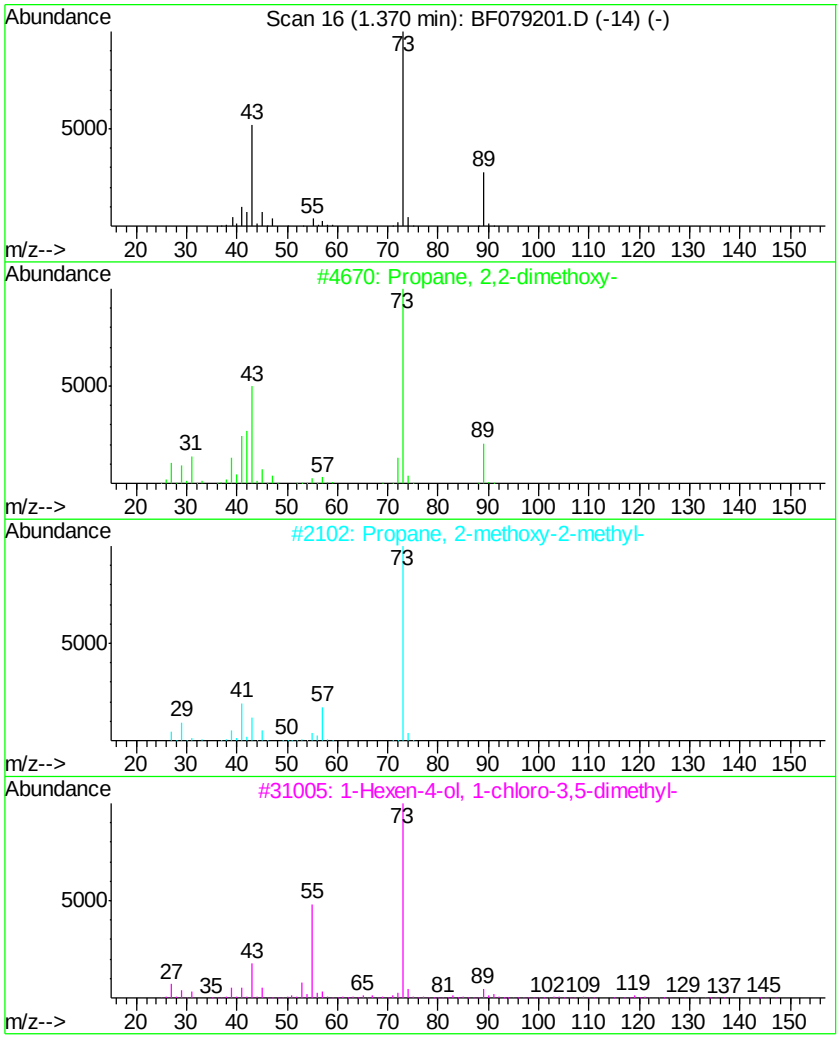
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

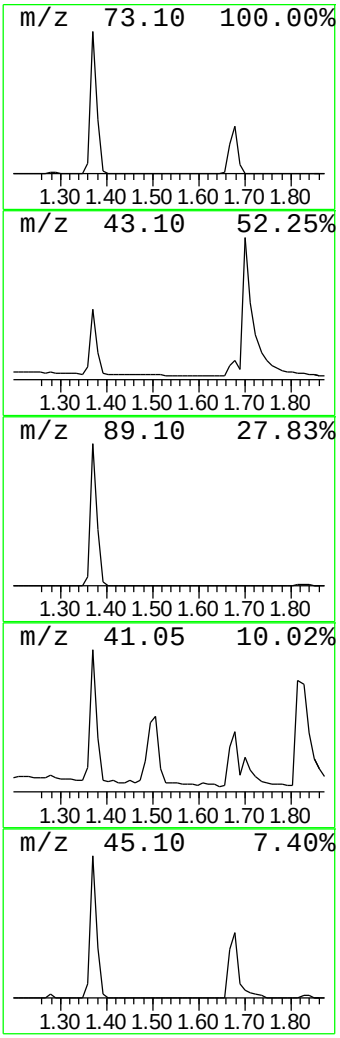
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	40.76 ng	601711	1,4-Dichlorobenzene-d4	7.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	7
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	7





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051315\
Data File : BF079201.D
Acq On : 13 May 2015 18:49
Operator : TP/IZ
Sample : G2194-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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

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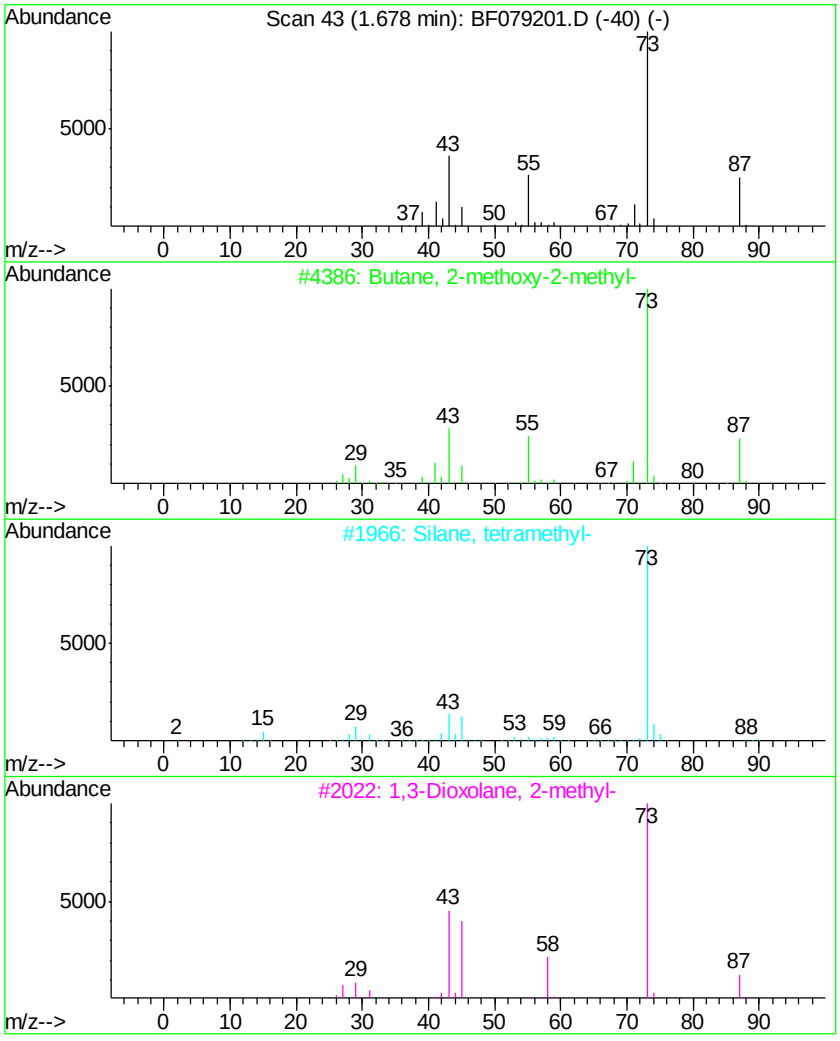
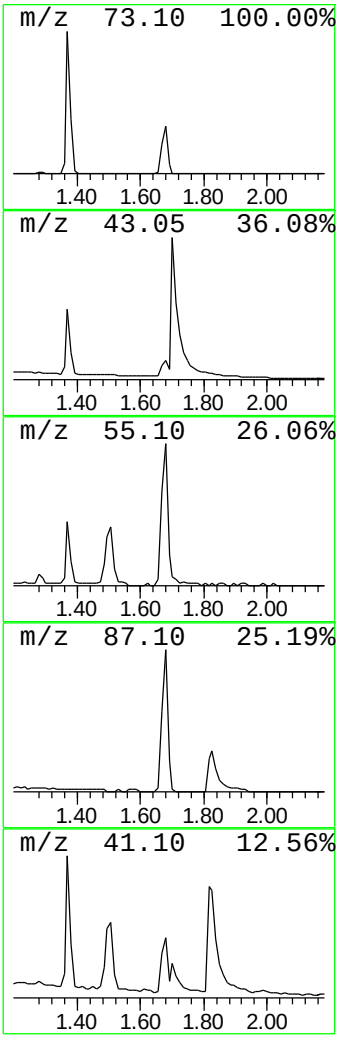
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.68	21.30 ng	314484	1,4-Dichlorobenzene-d4	7.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051315\
Data File : BF079201.D
Acq On : 13 May 2015 18:49
Operator : TP/IZ
Sample : G2194-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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

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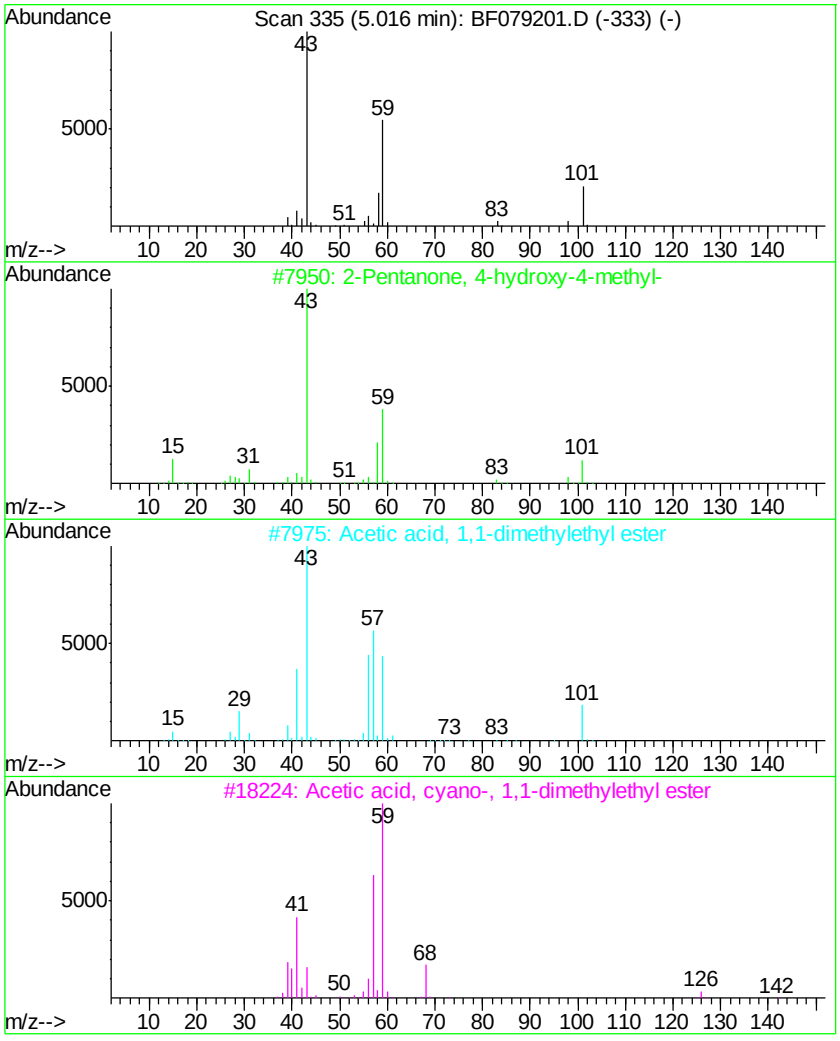
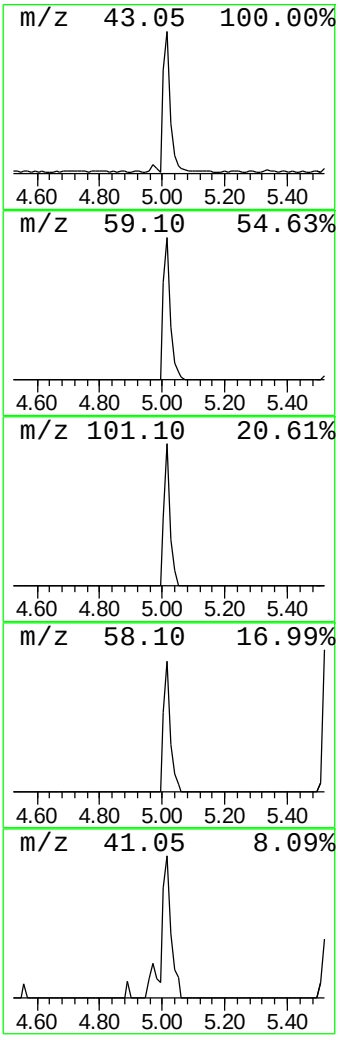
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	8.19 ng	120879	1,4-Dichlorobenzene-d4	7.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051315\
Data File : BF079201.D
Acq On : 13 May 2015 18:49
Operator : TP/IZ
Sample : G2194-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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

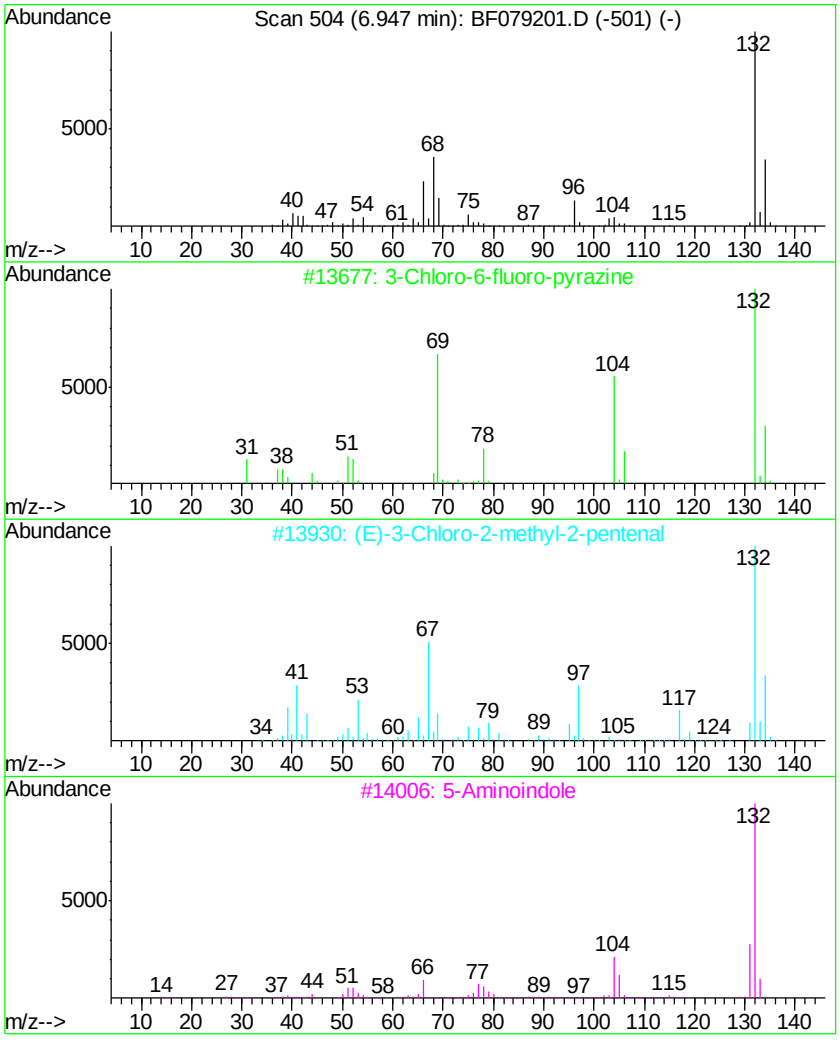
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

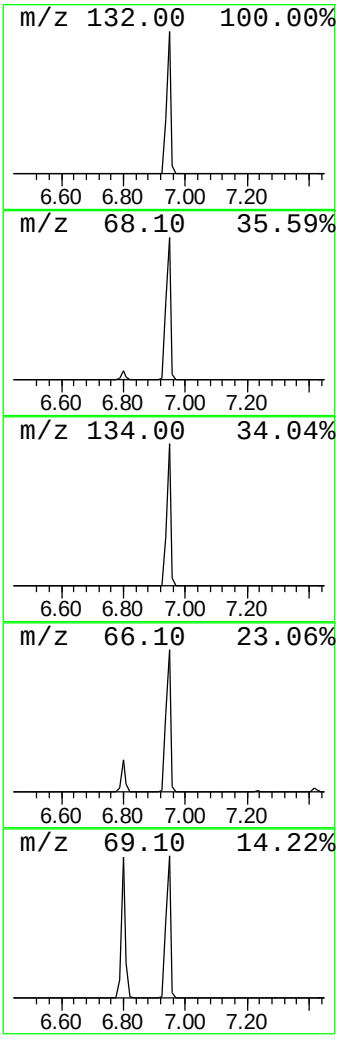
****

Peak Number 7 unknown6.95 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	118.72 ng	1752770	1,4-Dichlorobenzene-d4	7.23

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	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051315\
Data File : BF079201.D
Acq On : 13 May 2015 18:49
Operator : TP/IZ
Sample : G2194-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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

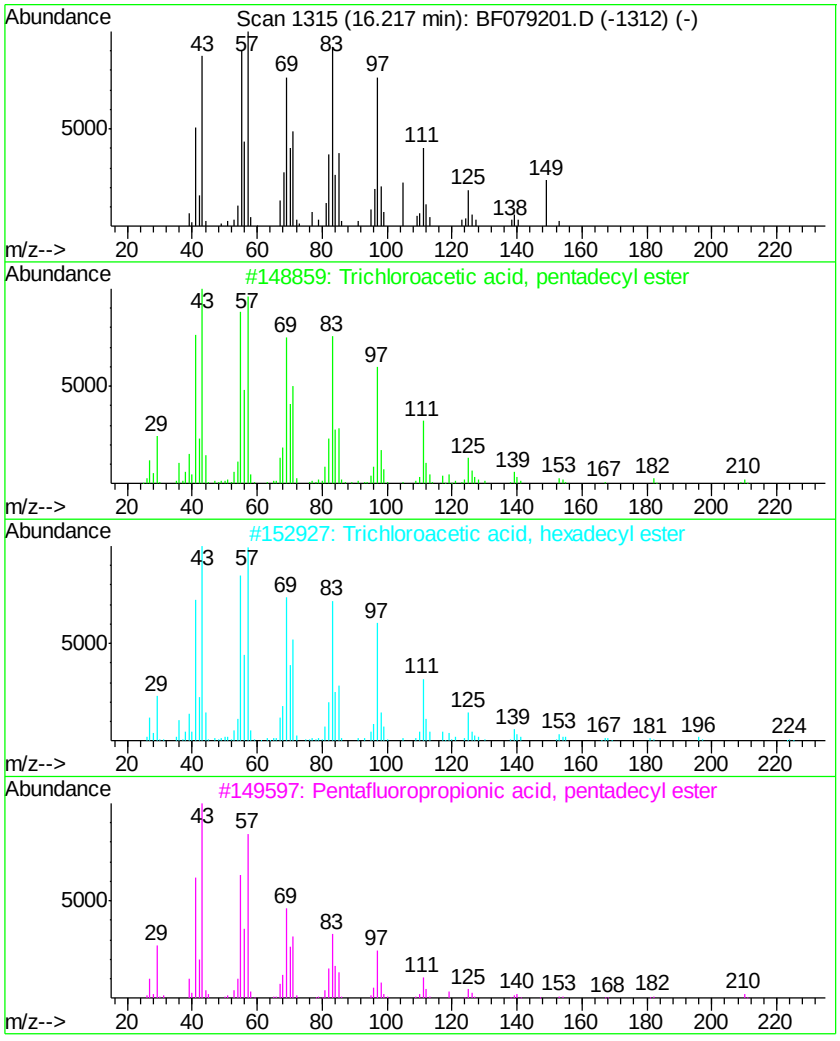
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

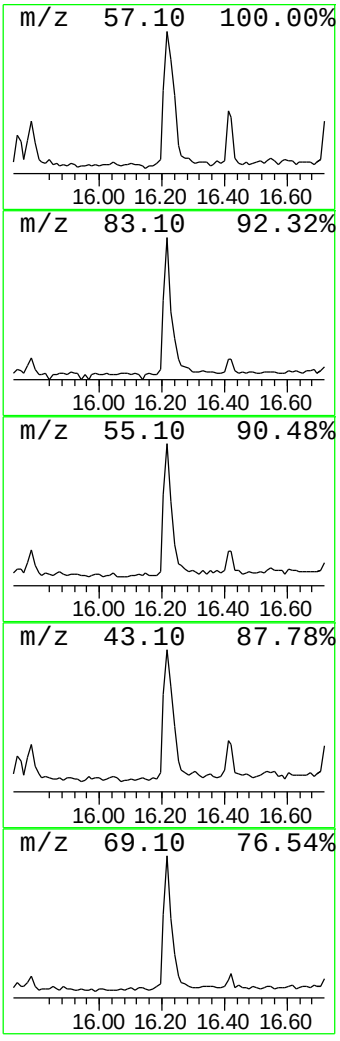
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	7.39 ng	203924	Chrysene-d12	16.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	86
4	1-Docosene	308	C22H44	001599-67-3	76
5	1-Nonadecene	266	C19H38	018435-45-5	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051315\
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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

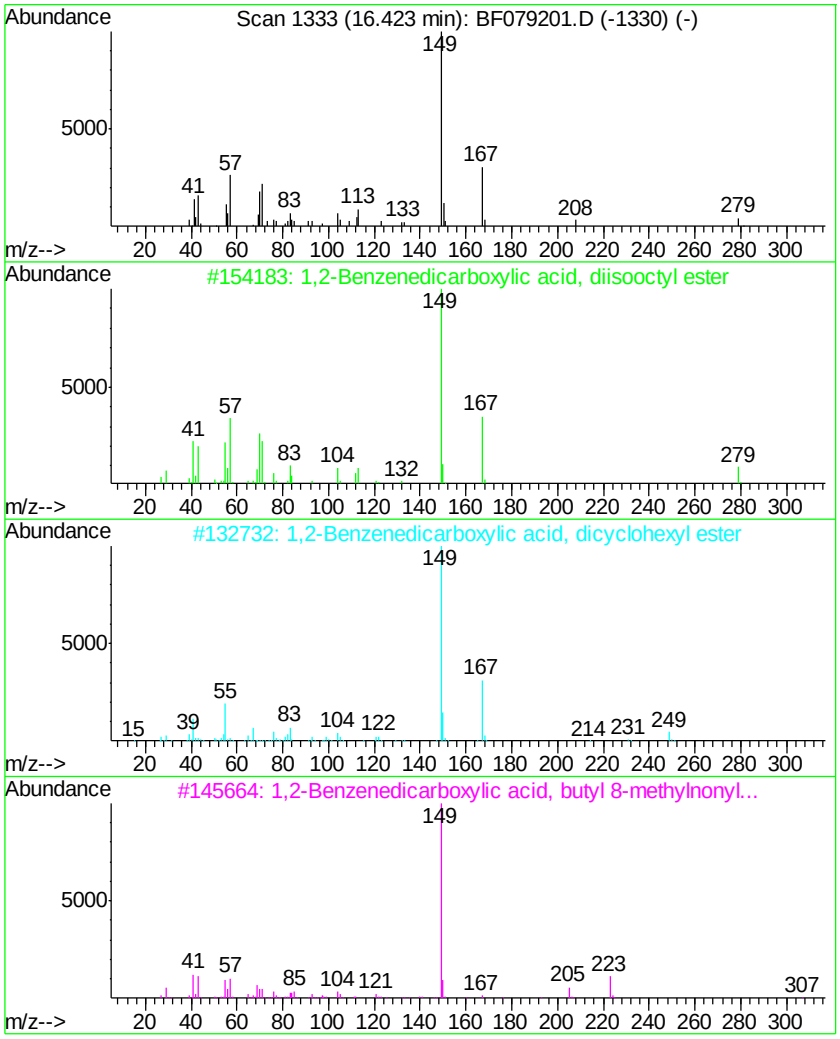
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

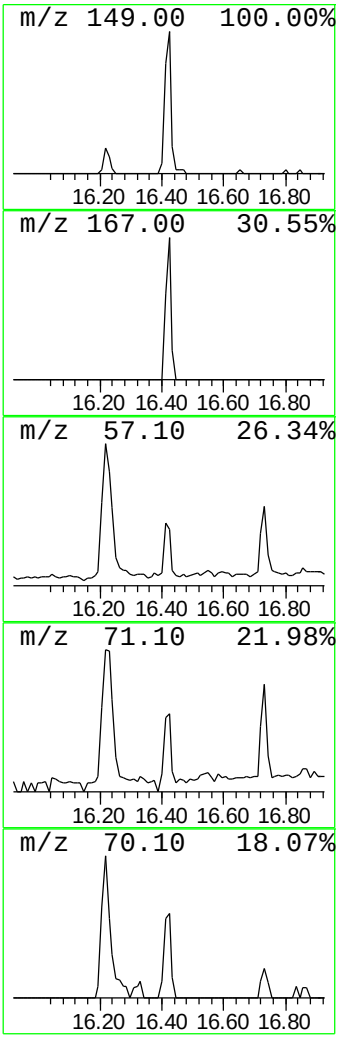
****

Peak Number 11 1,2-Benzenedicarboxylic aci... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.42	2.32 ng	64079	Chrysene-d12	16.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	90
2	1,2-Benzenedicarboxylic acid, di...	330	C20H26O4	000084-61-7	53
3	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	50
4	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	47
5	1,2-Benzenedicarboxylic acid, di...	334	C20H30O4	000084-75-3	47





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Operator : TP/IZ
Sample : G2194-03
Misc :
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Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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

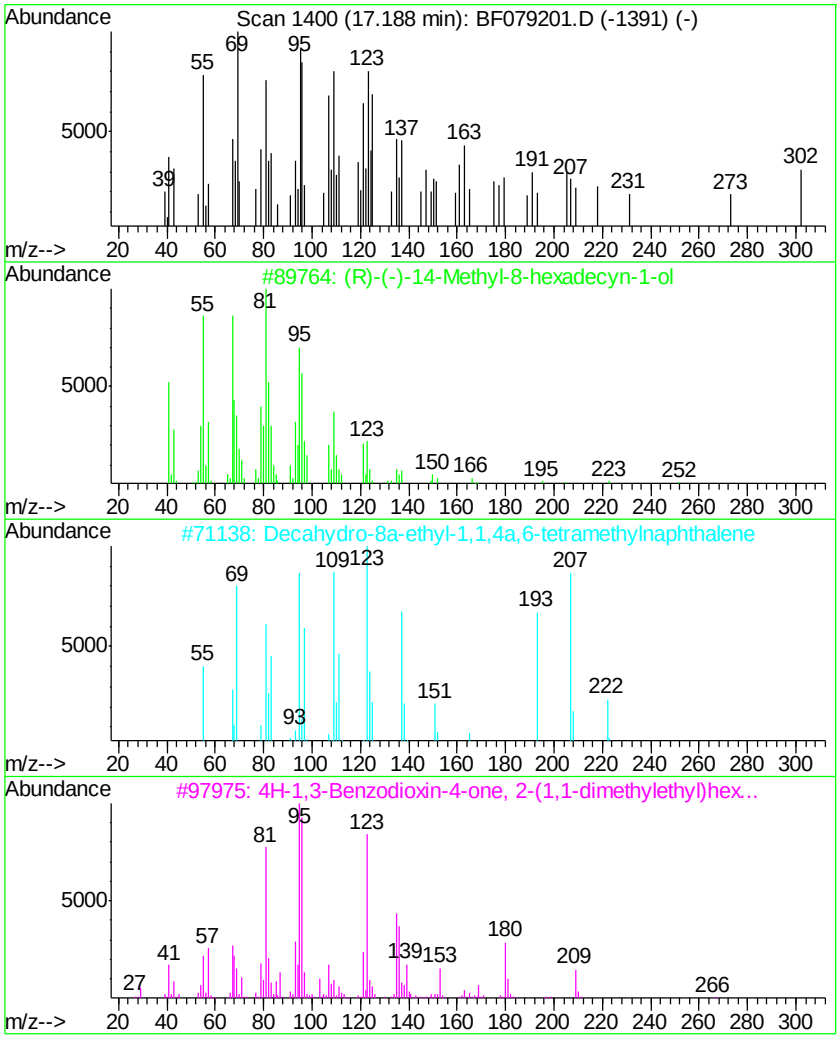
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

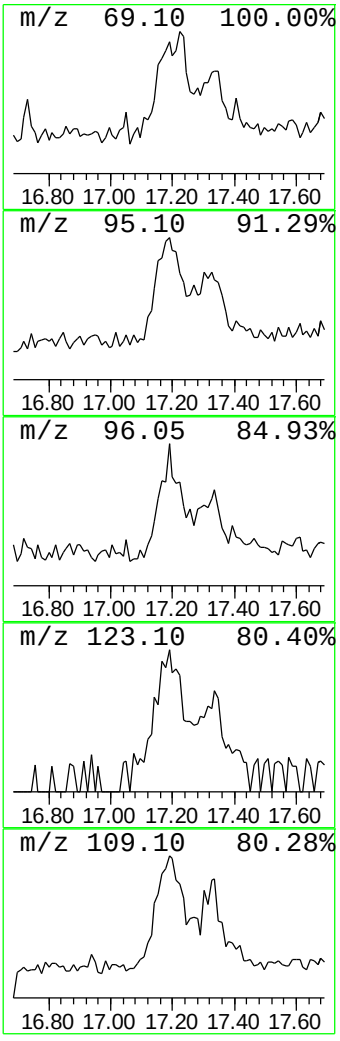
****

Peak Number 12 unknown17.19 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.19	5.72 ng	157680	Chrysene-d12	16.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	064566-18-3	49
2	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	47
3	4H-1,3-Benzodioxin-4-one, 2-(1,1...	266	C16H26O3	124899-18-9	38
4	2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	35
5	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	27





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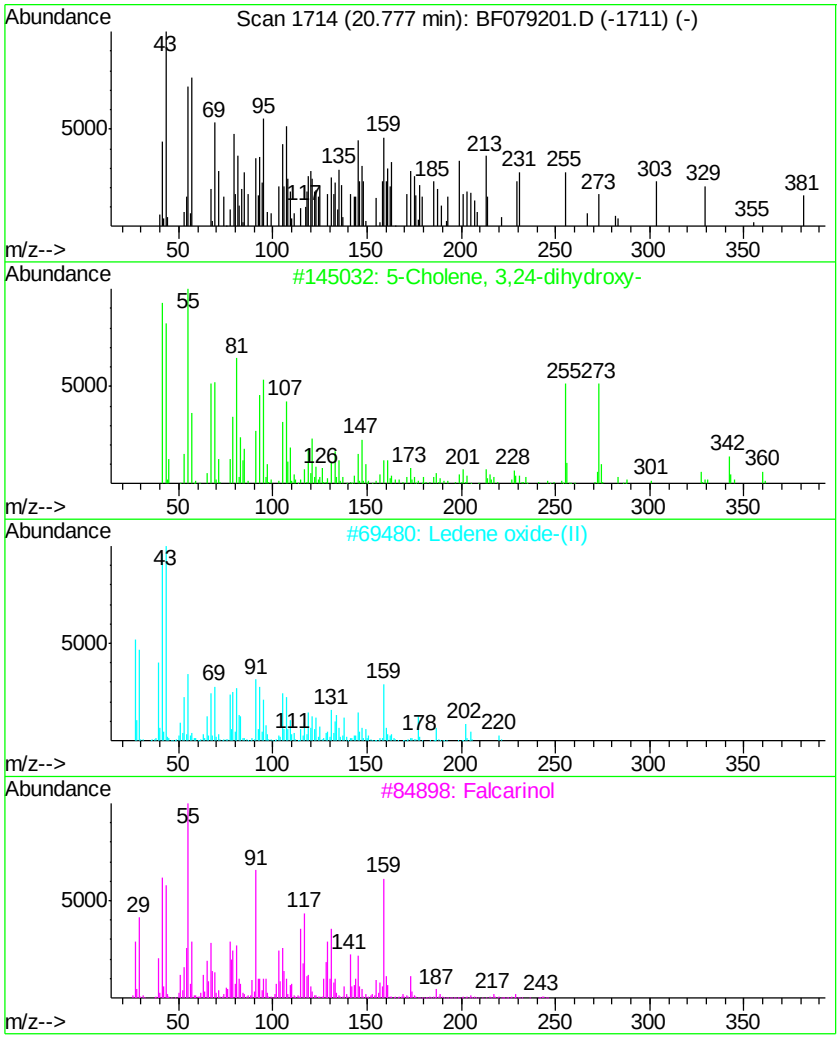
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

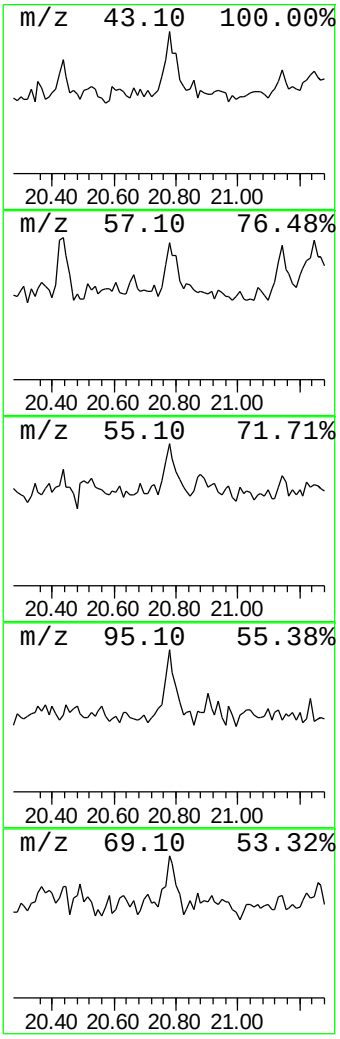
****

Peak Number 13 unknown20.78 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	3.66 ng	101632	Perylene-d12	18.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Cholene, 3,24-dihydroxy-	360	C24H40O2	1000251-69-2	32
2	Ledene oxide-(II)	220	C15H24O	1000159-36-7	22
3	Falcarinol	244	C17H24O	081203-57-8	10
4	6-Methyl-2-nitro-3-pyridinyl 4-f...	312	C12H9FN2O5S	1000298-19-9	9
5	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051315\
Data File : BF079201.D
Acq On : 13 May 2015 18:49
Operator : TP/IZ
Sample : G2194-03
Misc :
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Instrument : BNA_F
ClientSampleId : TU021-SB-15-6.5

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
Propane, 2,2-dime...	1.37	40.8	ng	601711	1	7.23	295282	20.0
Butane, 2-methoxy...	1.68	21.3	ng	314484	1	7.23	295282	20.0
2-Pentanone, 4-hy...	5.02	8.2	ng	120879	1	7.23	295282	20.0
unknown6.95	6.95	118.7	ng	1752770	1	7.23	295282	20.0
Trichloroacetic a...	16.22	7.4	ng	203924	5	16.34	551715	20.0
1,2-Benzenedicarb...	16.42	2.3	ng	64079	5	16.34	551715	20.0
unknown17.19	17.19	5.7	ng	157680	5	16.34	551715	20.0
unknown20.78	20.78	3.7	ng	101632	6	18.50	554897	20.0