LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121716\
Data File : BF091728.D
Acq On : 18 Dec 2016 3:31
Operator : UM/SJ
Sample : H6099-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB02-121316

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-BF121716.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	2.144	3	5	17	rVB	281180	525913	4.60%	0.650%
2	2.464	30	33	37	rVB	86644	138680	1.21%	0.171%
3	4.259	188	190	194	rBV	89978	144556	1.27%	0.179%
4	4.441	203	206	209	rBV	701804	915313	8.01%	1.131%
5	4.499	209	211	214	rVB	705951	856562	7.50%	1.058%
6	4.933	244	249	255	rBV	1397902	1997783	17.49%	2.468%
7	5.070	259	261	263	rVV	154080	151038	1.32%	0.187%
8	5.150	265	268	270	rBV	333878	374118	3.28%	0.462%
9	5.219	271	274	278	rVB2	188709	268907	2.35%	0.332%
10	5.367	284	287	289	rVB	5044911	4971123	43.52%	6.142%
11	6.407	375	378	380	rBV	1778990	2458131	21.52%	3.037%
12	6.533	386	389	392	rBV	6708898	8426569	73.78%	10.411%
13	6.762	407	409	412	rBV	1841572	1867154	16.35%	2.307%
14	6.922	420	423	426	rBV	6037777	6568766	57.51%	8.116%
15	7.333	456	459	461	rBV	4809818	5799545	50.78%	7.166%
16	8.019	516	519	520	rBV	997855	950600	8.32%	1.174%
17	8.053	520	522	524	rVB	2671029	2621455	22.95%	3.239%
18	9.139	613	617	619	rBV	7531603	11262220	98.60%	13.915%
19	9.528	648	651	653	rBV	514816	510370	4.47%	0.631%
20	9.802	672	675	678	rBV	3017781	2874215	25.16%	3.551%
21	10.591	741	744	747	rBV	4254928	6818532	59.70%	8.425%
22	10.716	753	755	759	rVB	120006	145176	1.27%	0.179%
23	11.288	802	805	807	rBV	3147574	3077483	26.94%	3.802%
24	11.825	850	852	854	rBV	192384	190436	1.67%	0.235%
25	12.877	941	944	947	rBV	6940496	11421597	100.00%	14.112%
26	13.780	1021	1023	1032	rVB2	151111	286574	2.51%	0.354%
27	13.917	1032	1035	1038	rBV	2783020	2821913	24.71%	3.487%
28	15.323	1155	1158	1161	rBV	2003313	2491873	21.82%	3.079%

Sum of corrected areas: 80936602

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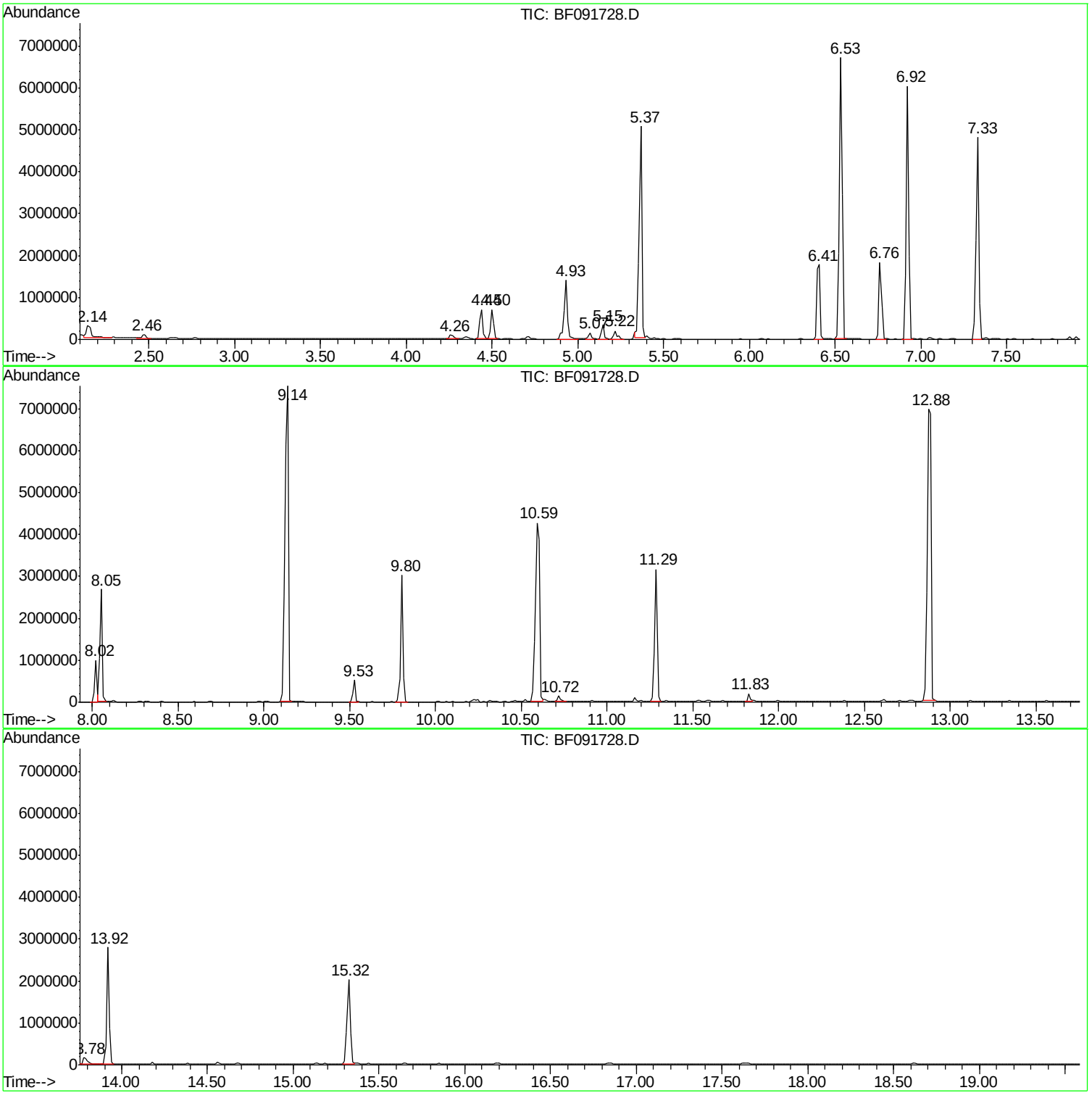
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB02-121316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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\BF121716\
Data File : BF091728.D
Acq On : 18 Dec 2016 3:31
Operator : UM/SJ
Sample : H6099-19
Misc :
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Instrument : BNA_F
ClientSampleId : EB02-121316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

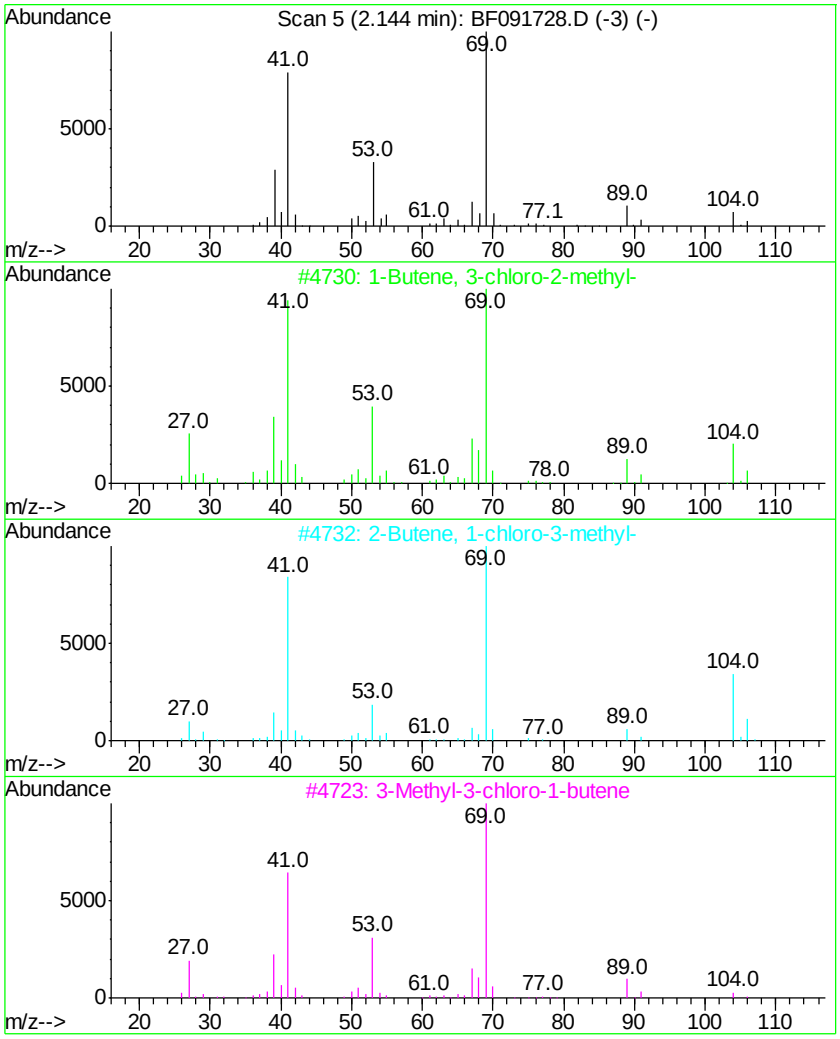
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

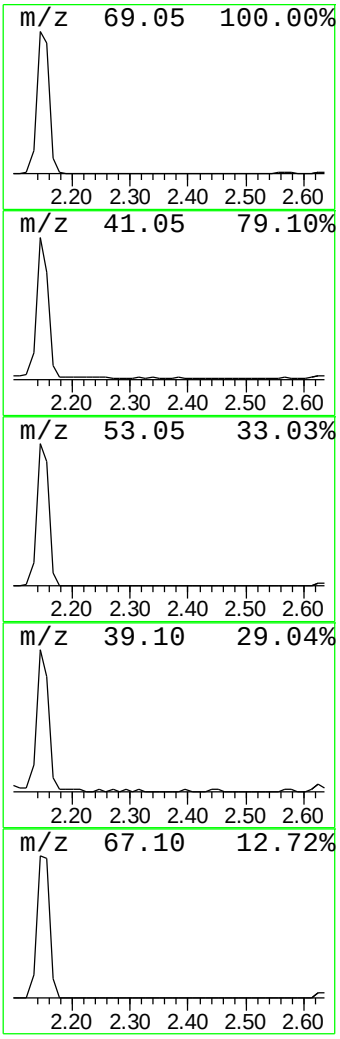
****

Peak Number 1 1-Butene, 3-chloro-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	5.63 ng	525913	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 3-chloro-2-methyl-	104	C5H9Cl	005166-35-8	86
2	2-Butene, 1-chloro-3-methyl-	104	C5H9Cl	000503-60-6	83
3	3-Methyl-3-chloro-1-butene	104	C5H9Cl	002190-48-9	78
4	2-Butene, 1-chloro-2-methyl-	104	C5H9Cl	013417-43-1	64
5	1,5-Heptadiene, 3,6-dimethyl-	124	C9H16	034891-10-6	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121716\
Data File : BF091728.D
Acq On : 18 Dec 2016 3:31
Operator : UM/SJ
Sample : H6099-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB02-121316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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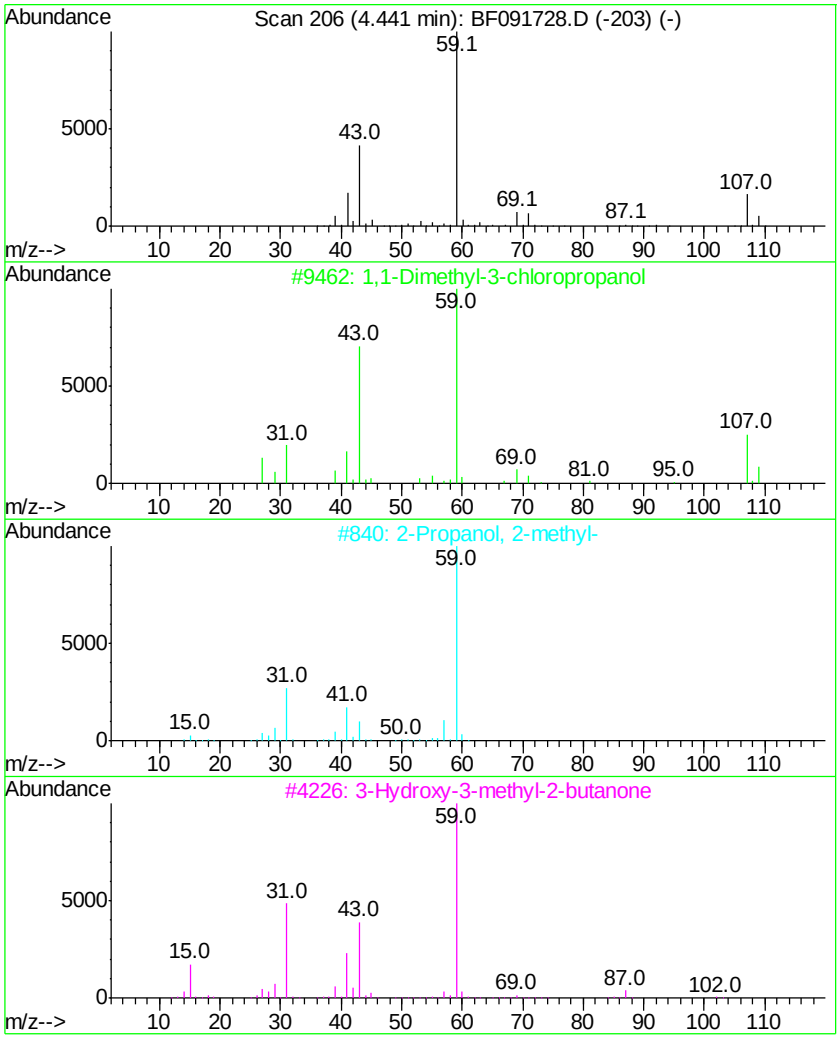
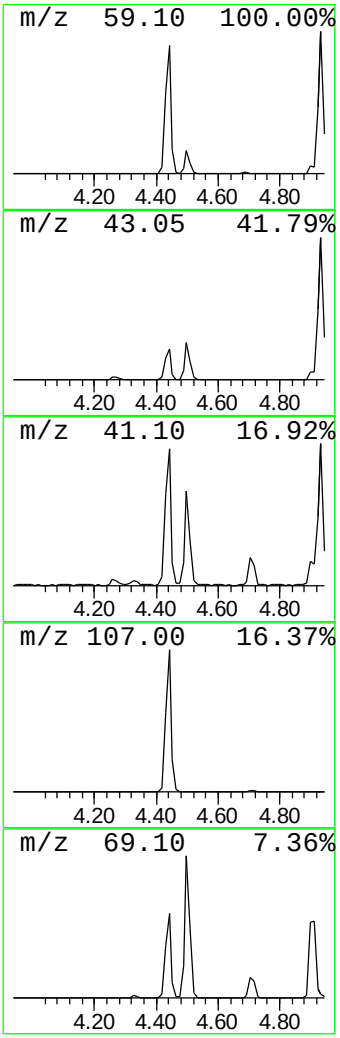
Peak Number 2 1,1-Dimethyl-3-chloropropanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	9.80 ng	915313	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Dimethyl-3-chloropropanol	122	C5H11ClO	001985-88-2	74
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	40
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38
4	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	36
5	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	36





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121716\
Data File : BF091728.D
Acq On : 18 Dec 2016 3:31
Operator : UM/SJ
Sample : H6099-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB02-121316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

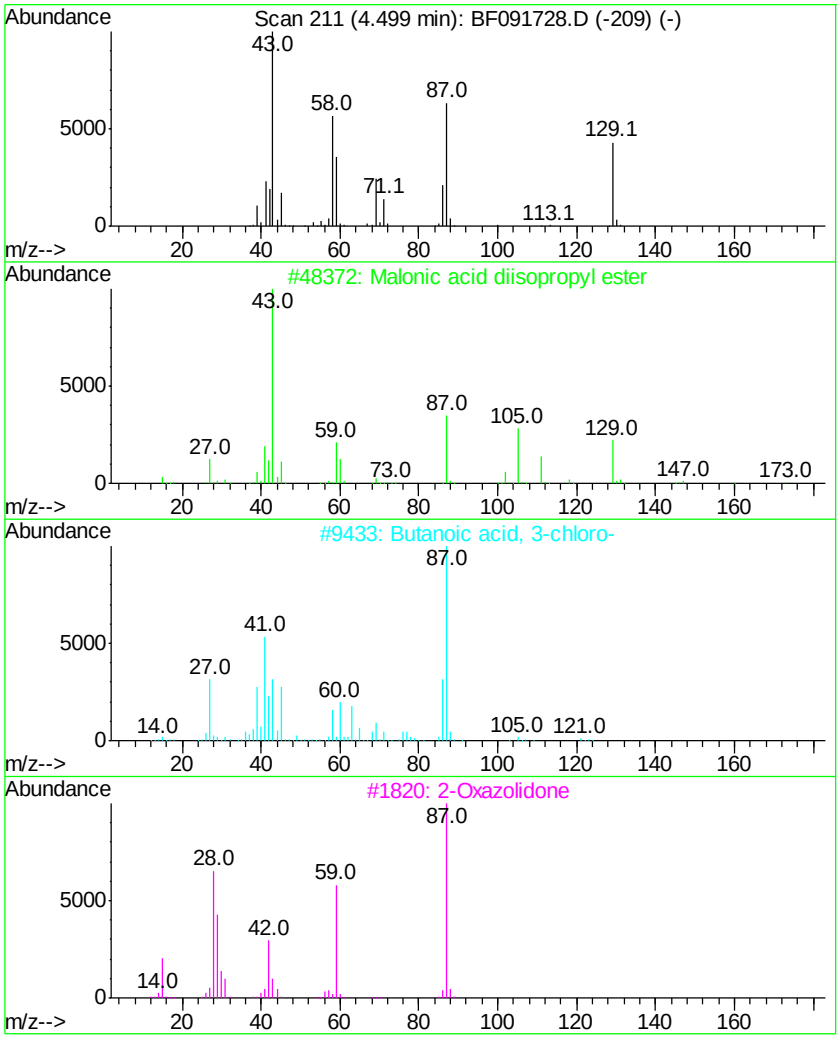
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

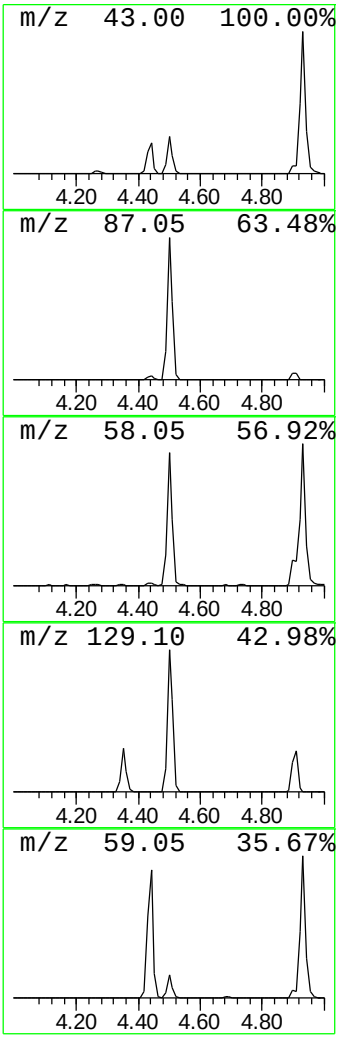
****

Peak Number 3 unknown4.50 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	9.18 ng	856562	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Malonic acid diisopropyl ester	188	C9H16O4	013195-64-7	40
2	Butanoic acid, 3-chloro-	122	C4H7ClO2	001951-12-8	32
3	2-Oxazolidone	87	C3H5NO2	000497-25-6	30
4	2-Propenoic acid, 2-(acetylamino)-	129	C5H7NO3	005429-56-1	25
5	3-Octanol, 3-ethyl-	158	C10H22O	002051-32-3	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121716\
Data File : BF091728.D
Acq On : 18 Dec 2016 3:31
Operator : UM/SJ
Sample : H6099-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB02-121316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

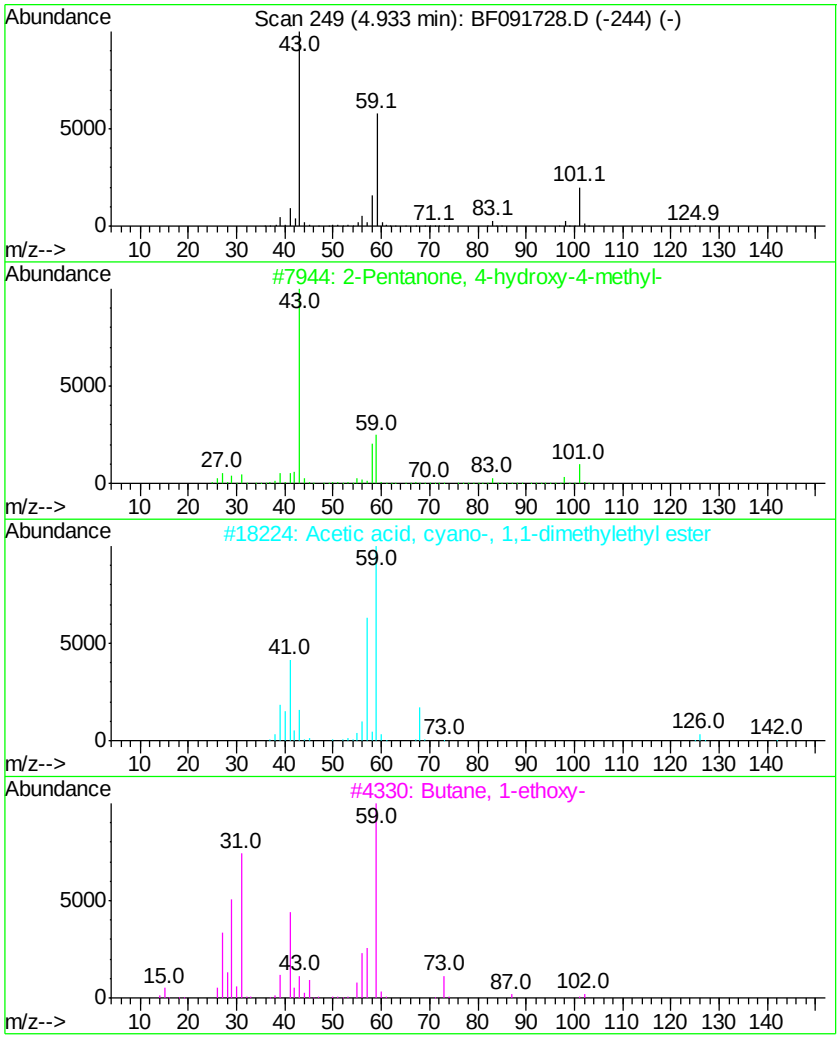
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

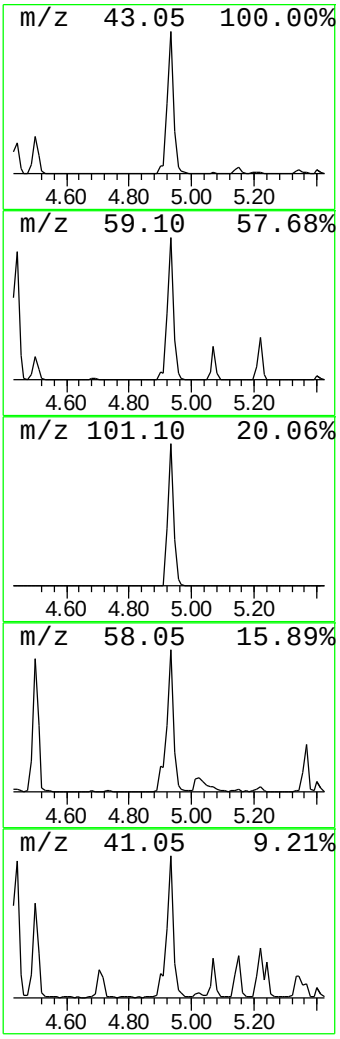
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	21.40 ng	1997780	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121716\
Data File : BF091728.D
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Operator : UM/SJ
Sample : H6099-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB02-121316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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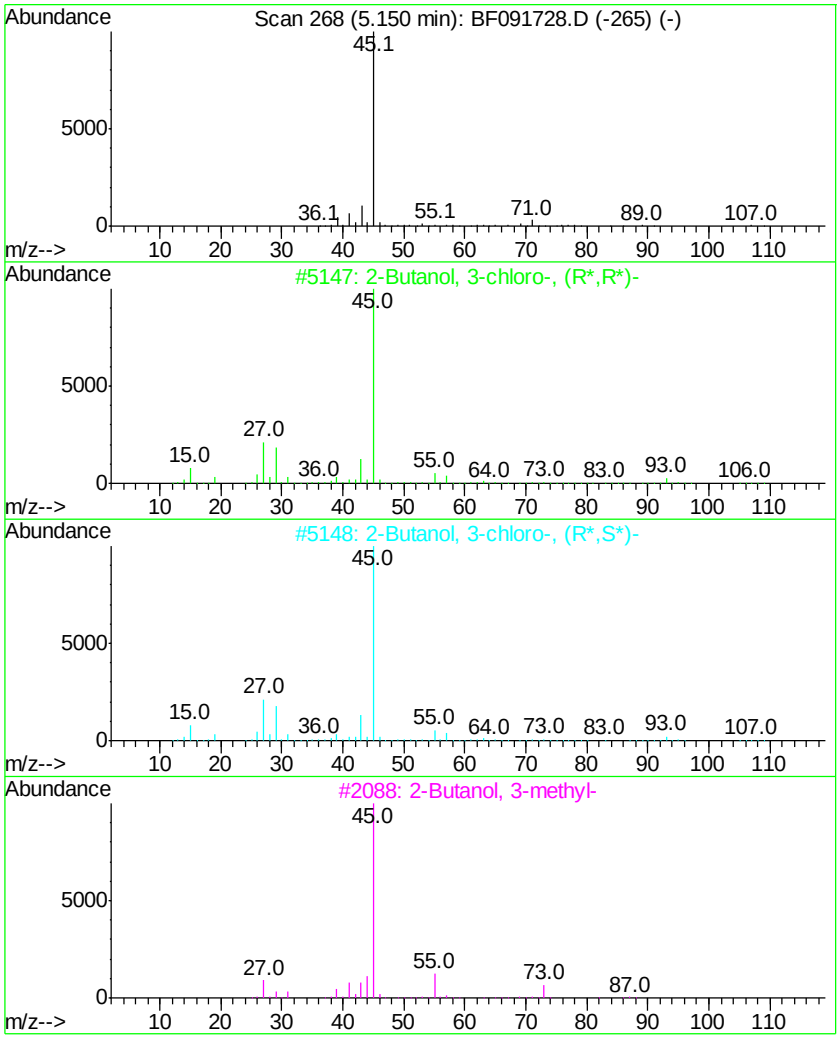
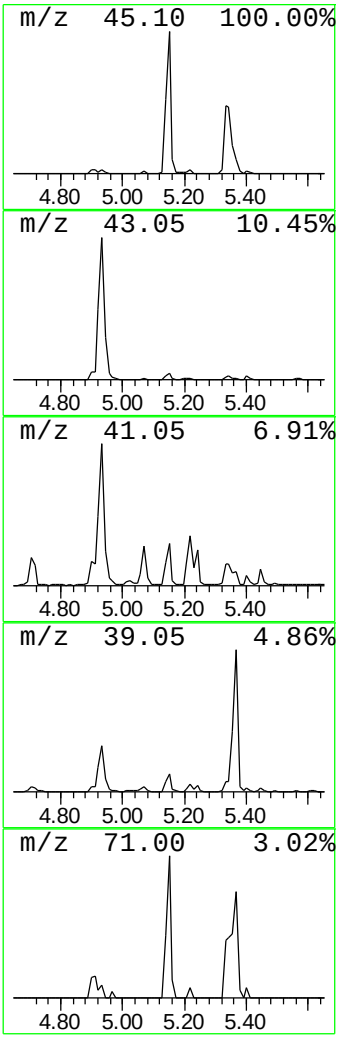
****

Peak Number 5 unknown5.15 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	4.01 ng	374118	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 3-chloro-, (R*,R*)-	108	C4H9ClO	010325-40-3	40
2	2-Butanol, 3-chloro-, (R*,S*)-	108	C4H9ClO	010325-41-4	40
3	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	39
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	4-Pentyn-2-ol	84	C5H8O	002117-11-5	9





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Sample : H6099-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB02-121316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

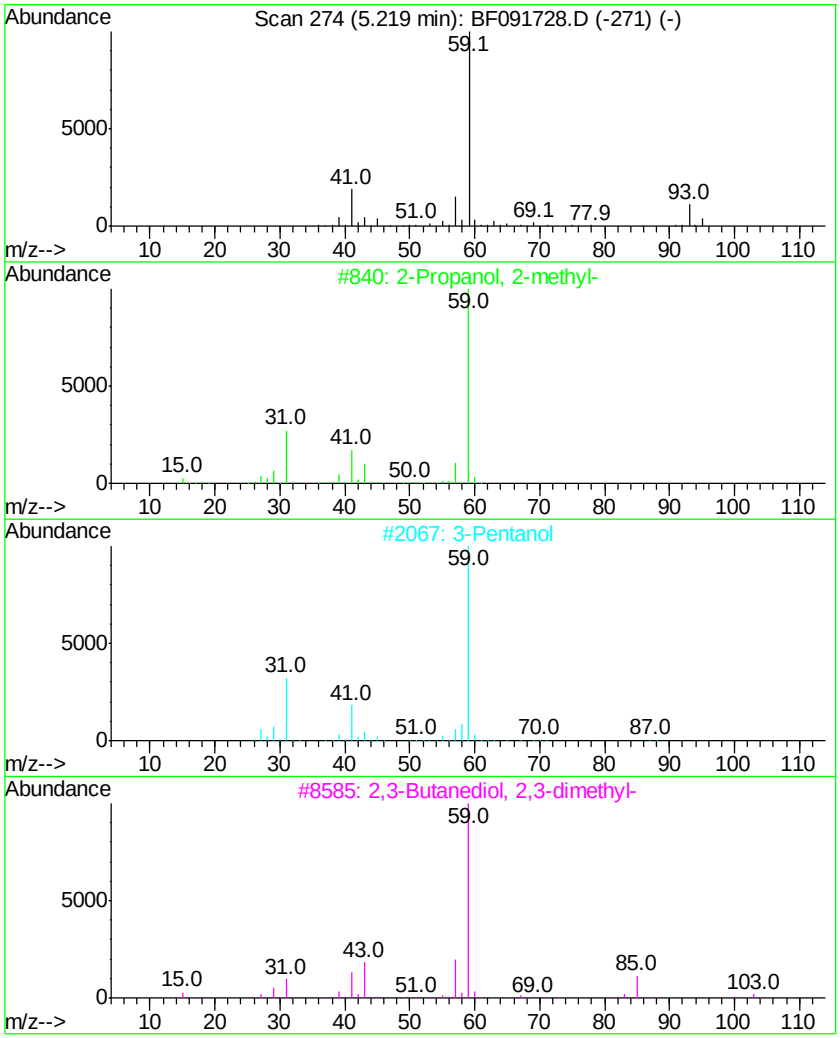
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

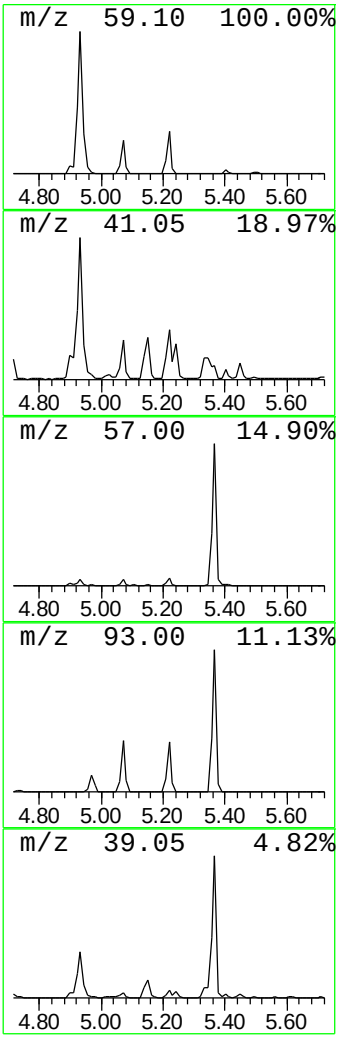
****

Peak Number 6 2-Propanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	2.88 ng	268907	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	59
2	3-Pentanol	88	C5H12O	000584-02-1	45
3	2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	38
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	36
5	Guanidine	59	CH5N3	000113-00-8	7





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Sample : H6099-19
Misc :
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Instrument : BNA_F
ClientSampleId : EB02-121316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

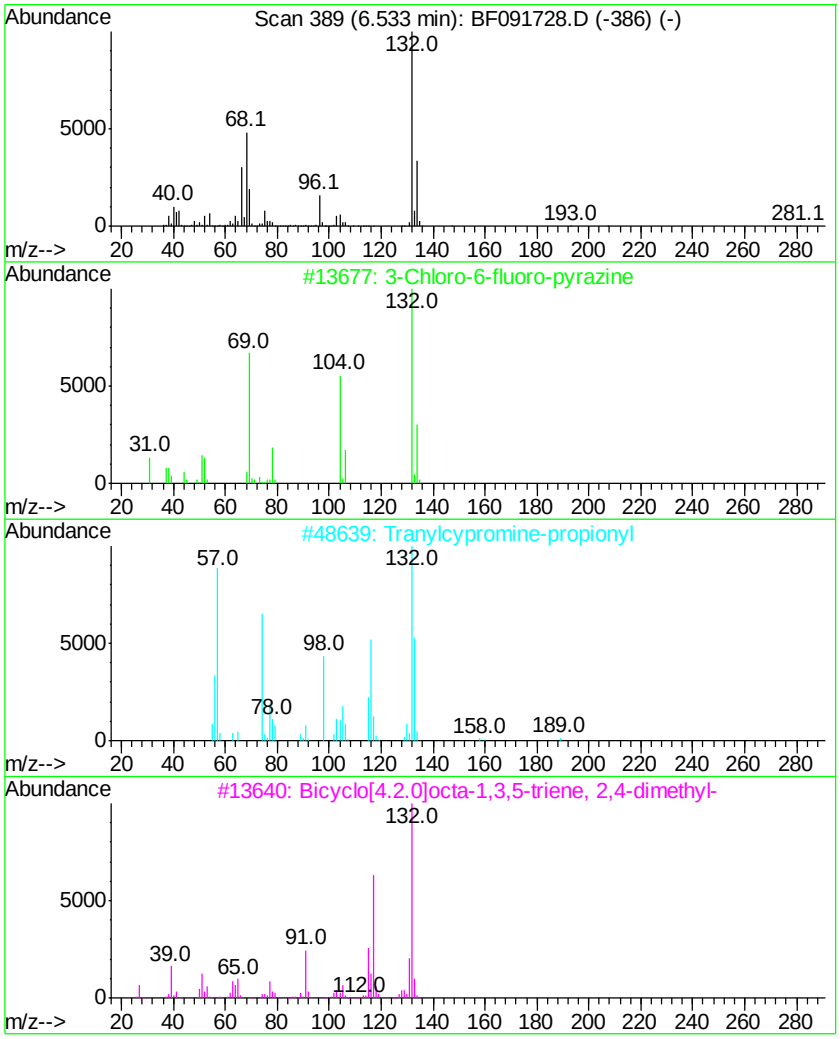
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

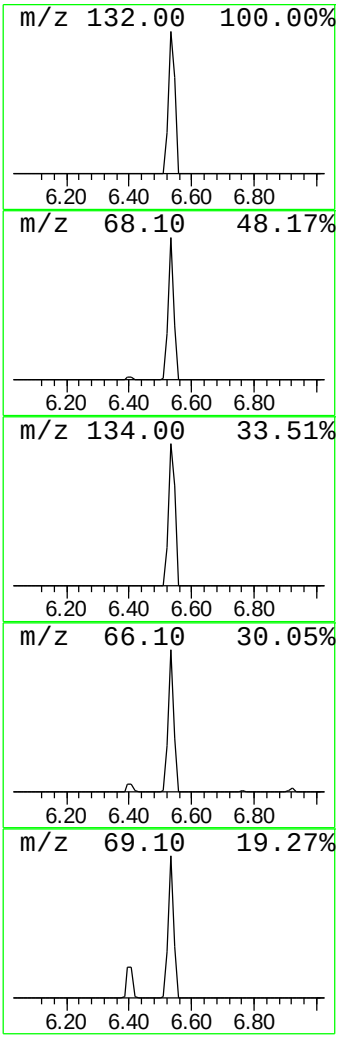
****

Peak Number 7 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	90.26 ng	8426570	1,4-Dichlorobenzene-d4	6.76

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

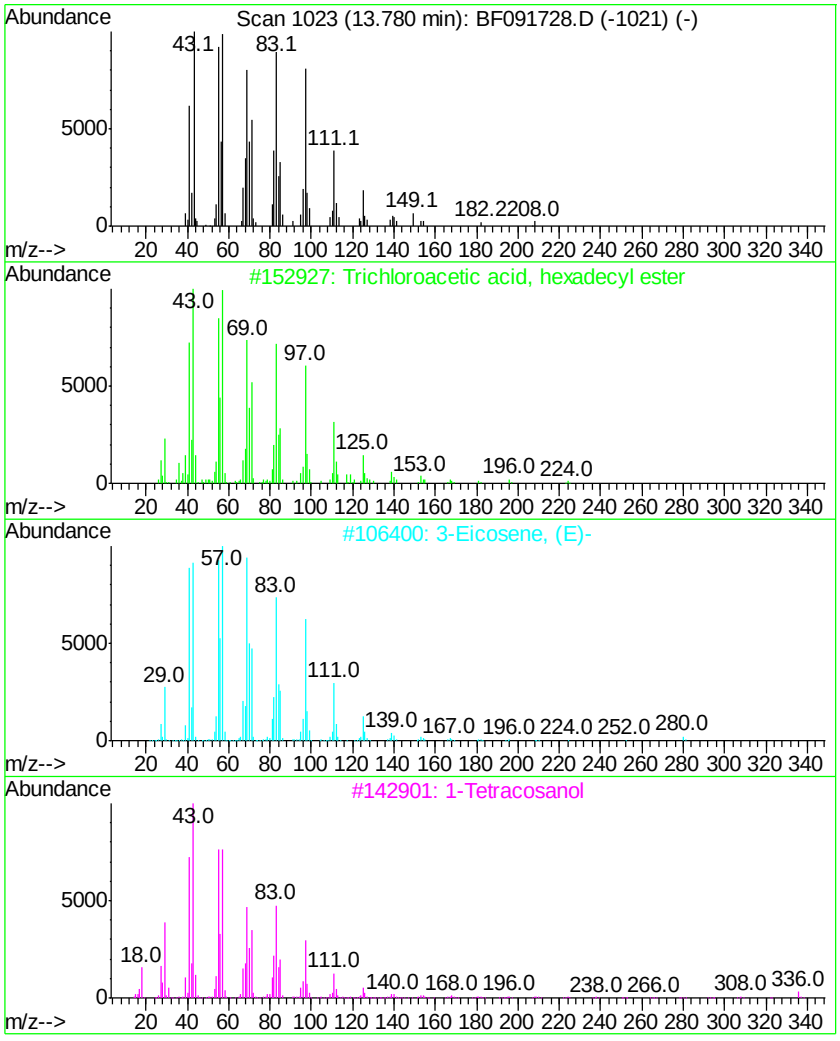
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

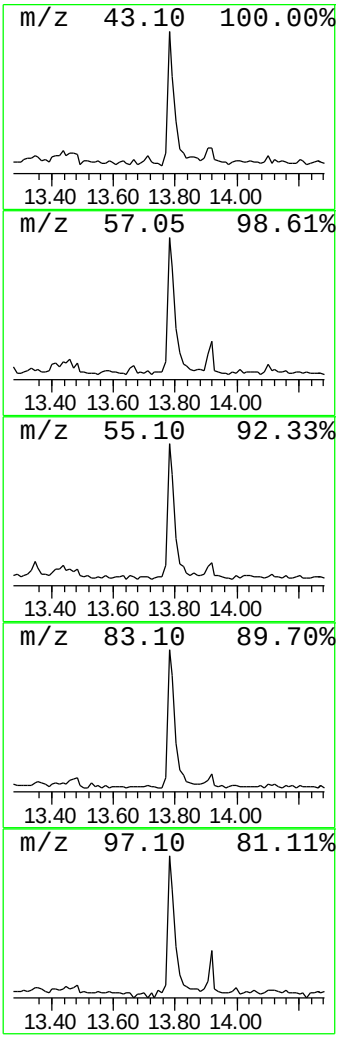
****

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	2.03 ng	286574	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Tetracosanol	354	C24H50O	000506-51-4	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121716\
Data File : BF091728.D
Acq On : 18 Dec 2016 3:31
Operator : UM/SJ
Sample : H6099-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB02-121316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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
1-Butene, 3-chlor...	2.14	5.6	ng	525913	1	6.76	1867150	20.0
1,1-Dimethyl-3-ch...	4.44	9.8	ng	915313	1	6.76	1867150	20.0
unknown4.50	4.50	9.2	ng	856562	1	6.76	1867150	20.0
2-Pentanone, 4-hy...	4.93	21.4	ng	1997780	1	6.76	1867150	20.0
unknown5.15	5.15	4.0	ng	374118	1	6.76	1867150	20.0
2-Propanol, 2-met...	5.22	2.9	ng	268907	1	6.76	1867150	20.0
unknown6.53	6.53	90.3	ng	8426570	1	6.76	1867150	20.0
Trichloroacetic a...	13.78	2.0	ng	286574	5	13.92	2821910	20.0