LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
Data File : BF077465.D
Acq On : 26 Feb 2015 15:14
Operator : TP/IZ
Sample : G1384-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-WW-022515

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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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	1.424	45	47	50	rVB	3685666	4141057	100.00%	20.807%
2	1.561	56	59	62	rVB	125438	200160	4.83%	1.006%
3	1.733	72	74	82	rVV	104500	170918	4.13%	0.859%
4	1.847	82	84	105	rVB	500424	1123660	27.13%	5.646%
5	5.047	362	364	370	rVB	214493	241261	5.83%	1.212%
6	5.562	406	409	411	rBV	973855	1184541	28.60%	5.952%
7	6.819	517	519	522	rBV	1110265	1189907	28.73%	5.979%
8	6.979	530	533	535	rBV	1416120	1336755	32.28%	6.716%
9	7.265	556	558	560	rVB	353713	338135	8.17%	1.699%
10	7.459	572	575	577	rVB	774044	1022519	24.69%	5.138%
11	7.962	616	619	621	rBV	566728	759989	18.35%	3.819%
12	8.842	694	696	699	rBV	542678	462663	11.17%	2.325%
13	10.191	811	814	816	rBV	2036518	1742931	42.09%	8.757%
14	11.014	884	886	889	rVB	464386	538923	13.01%	2.708%
15	11.916	963	965	967	rBV	69043	67295	1.63%	0.338%
16	11.996	969	972	975	rBV	1067167	1035863	25.01%	5.205%
17	12.865	1045	1048	1050	rBV	524657	576230	13.92%	2.895%
18	14.865	1220	1223	1225	rBV	1577966	2170516	52.41%	10.906%
19	15.494	1274	1278	1283	rBV2	23912	44264	1.07%	0.222%
20	16.031	1323	1325	1331	rBV	88222	147754	3.57%	0.742%
21	16.157	1334	1336	1339	rBV	592042	702778	16.97%	3.531%
22	17.951	1490	1493	1496	rBV	532380	704555	17.01%	3.540%

Sum of corrected areas: 19902674

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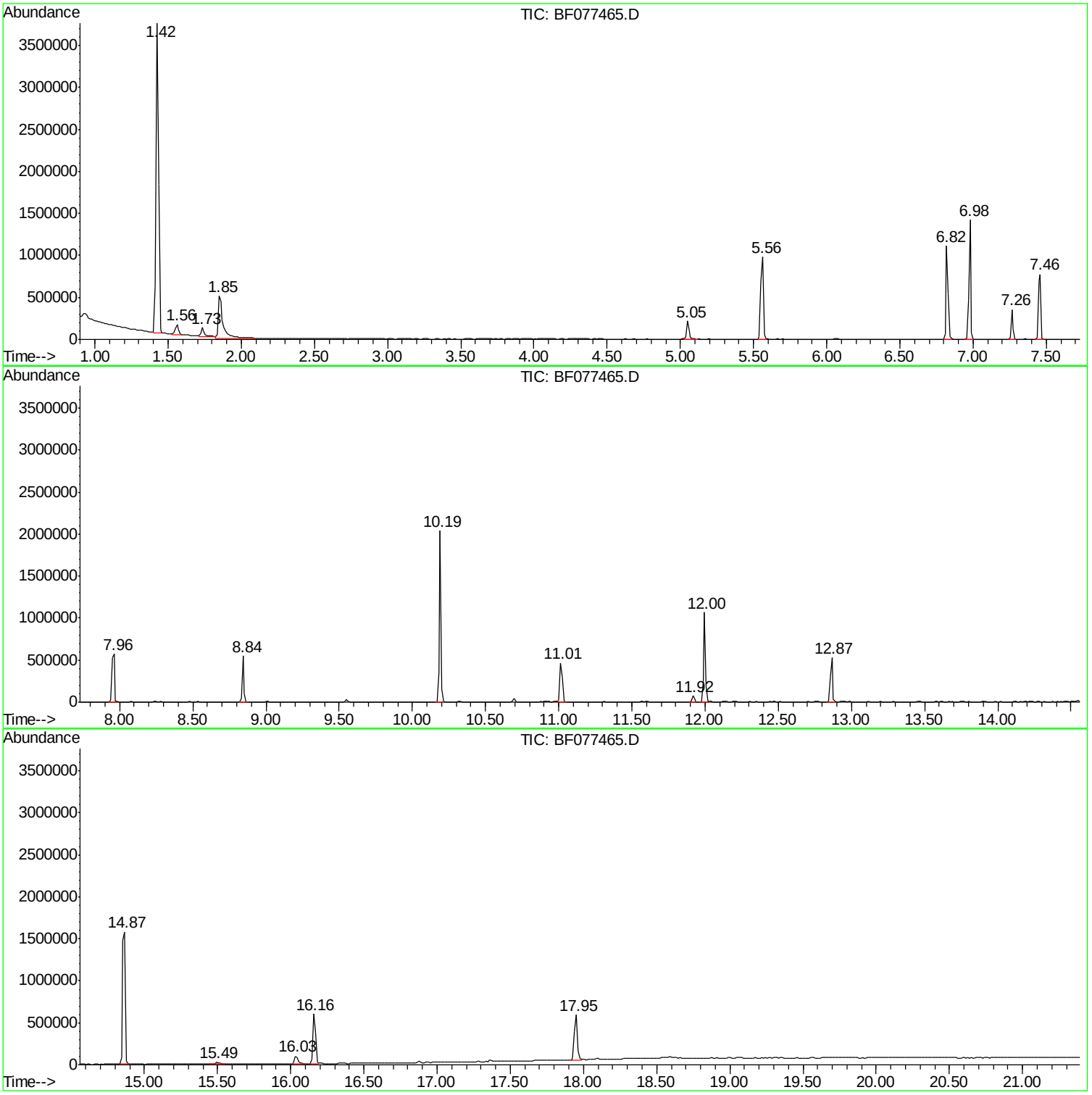
Instrument :
BNA_F
ClientSampleId :
41A-WW-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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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Acq On : 26 Feb 2015 15:14
Operator : TP/IZ
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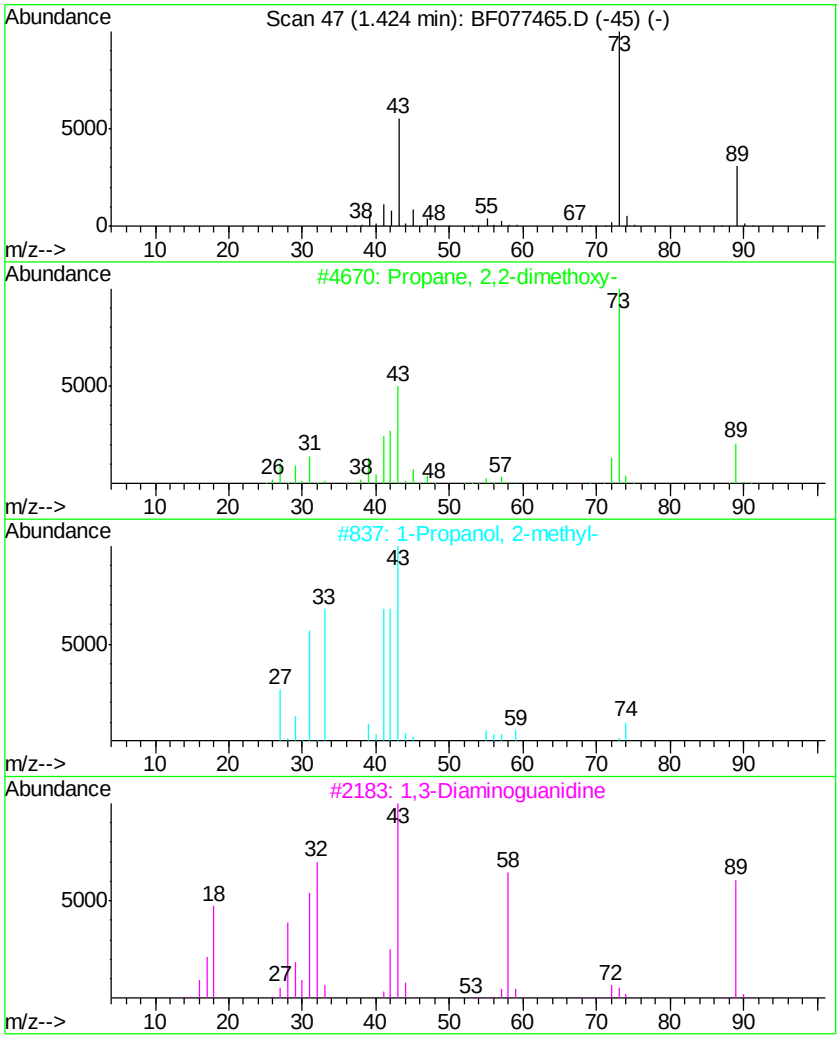
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

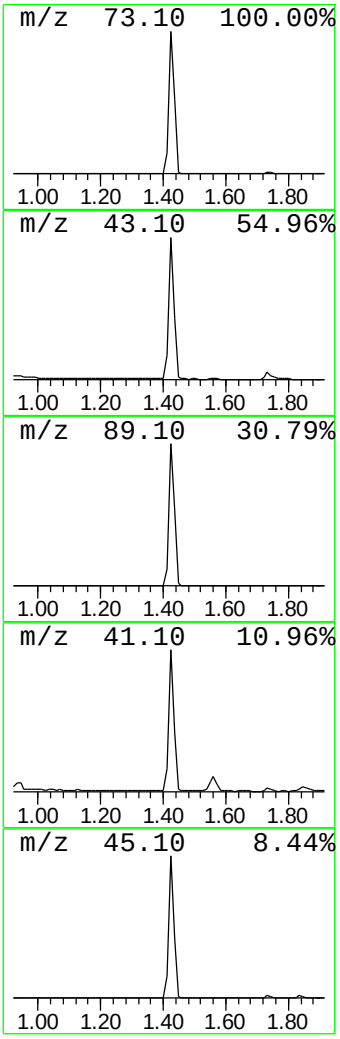
****

Peak Number 1 unknown1.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.42	244.94 ng	4141060	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9





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Data File : BF077465.D
Acq On : 26 Feb 2015 15:14
Operator : TP/IZ
Sample : G1384-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-WW-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

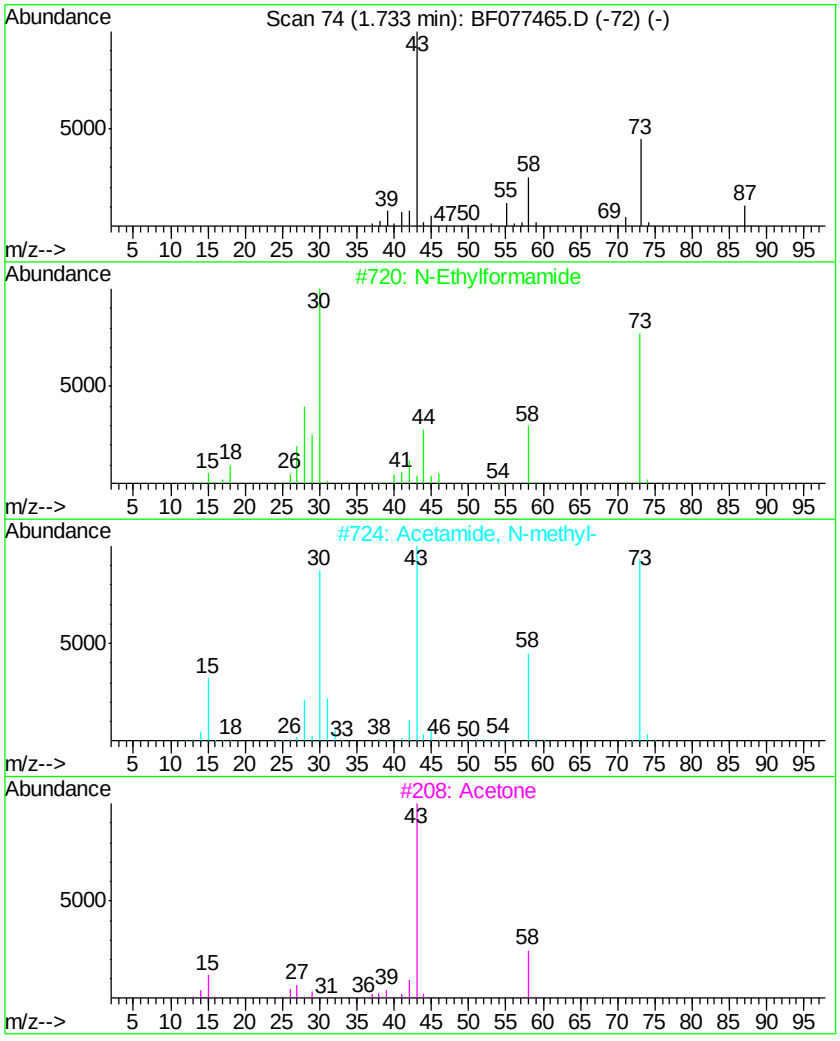
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

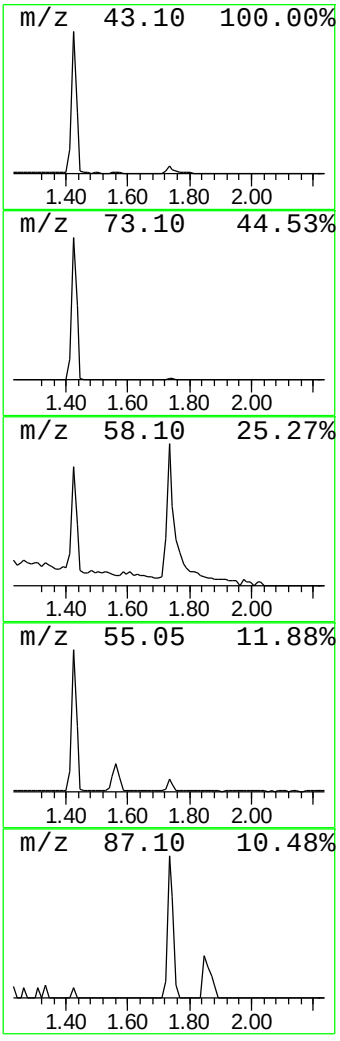
****

Peak Number 3 unknown1.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.73	10.11 ng	170918	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Ethylformamide	73	C3H7NO	000627-45-2	43
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	38
3	Acetone	58	C3H6O	000067-64-1	37
4	2-Butanol, 3-methyl-, acetate	130	C7H14O2	005343-96-4	37
5	Manganese(II) acetate	173	C4H6MnO4	006156-78-1	28





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
Data File : BF077465.D
Acq On : 26 Feb 2015 15:14
Operator : TP/IZ
Sample : G1384-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-WW-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

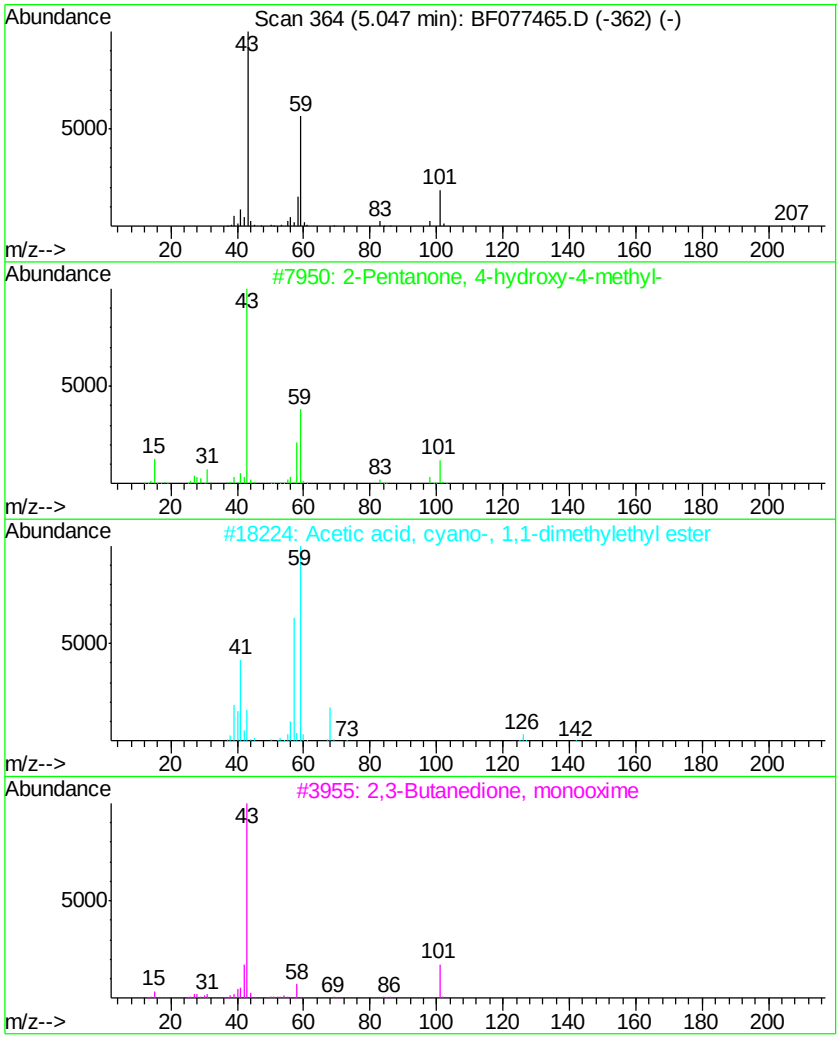
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

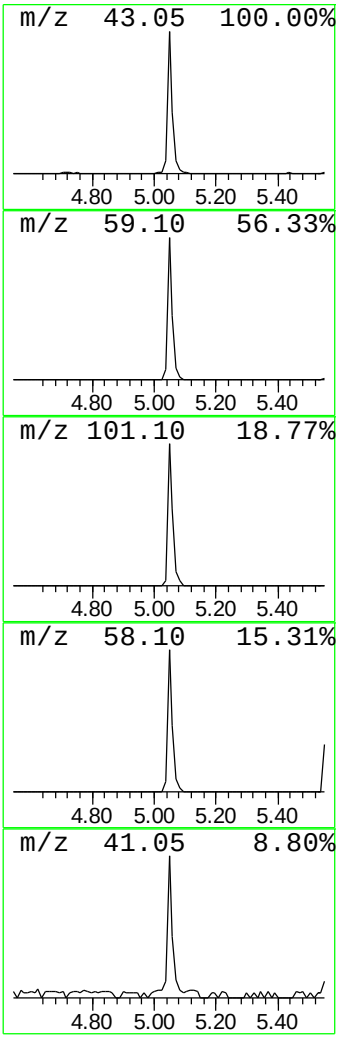
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	14.27 ng	241261	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF077465.D
Acq On : 26 Feb 2015 15:14
Operator : TP/IZ
Sample : G1384-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-WW-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

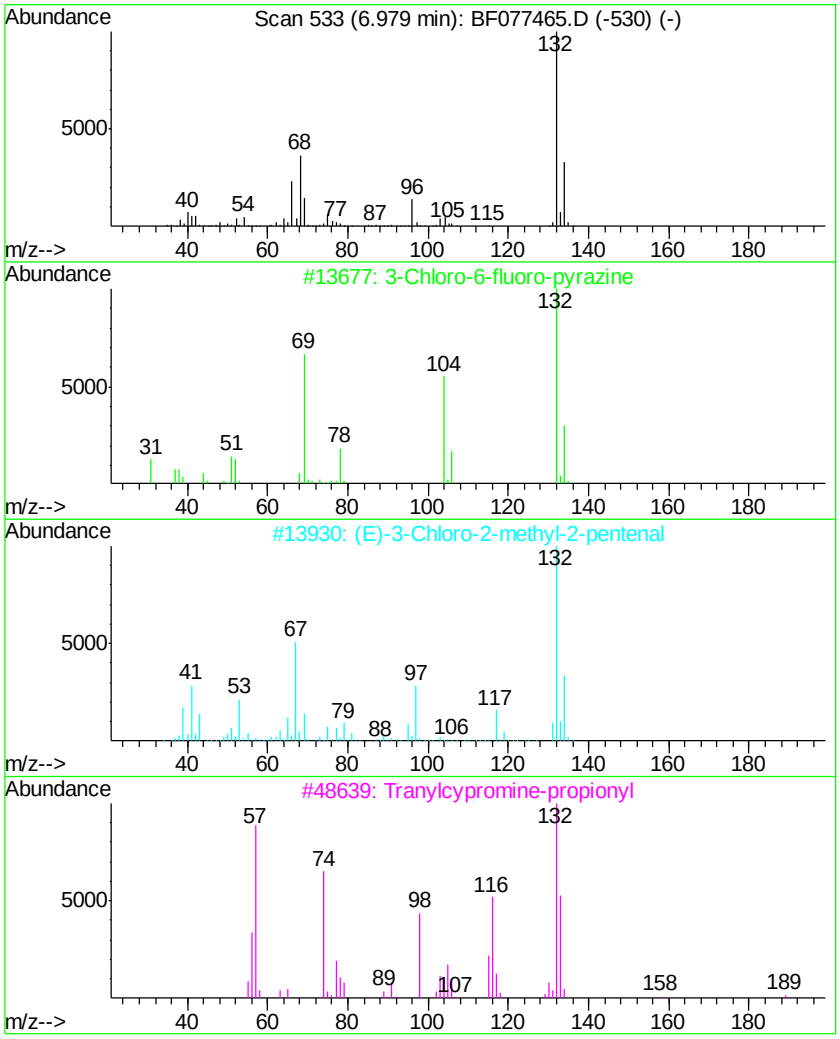
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

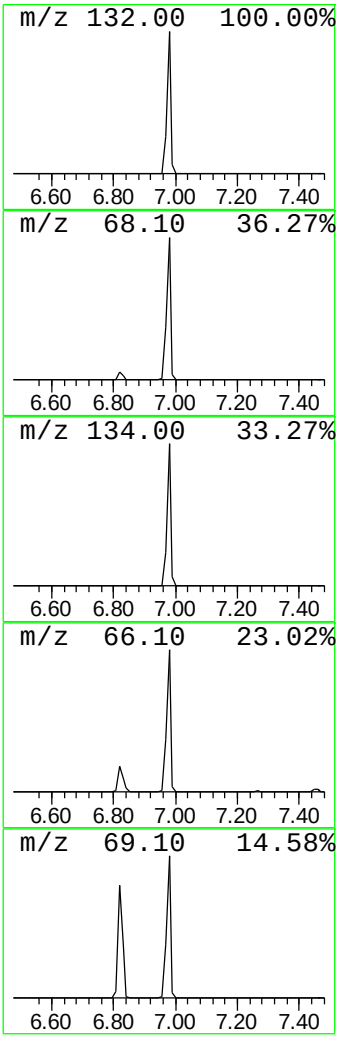
****

Peak Number 6 unknown6.98 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	79.07 ng	1336760	1,4-Dichlorobenzene-d4	7.26

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
Data File : BF077465.D
Acq On : 26 Feb 2015 15:14
Operator : TP/IZ
Sample : G1384-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-WW-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

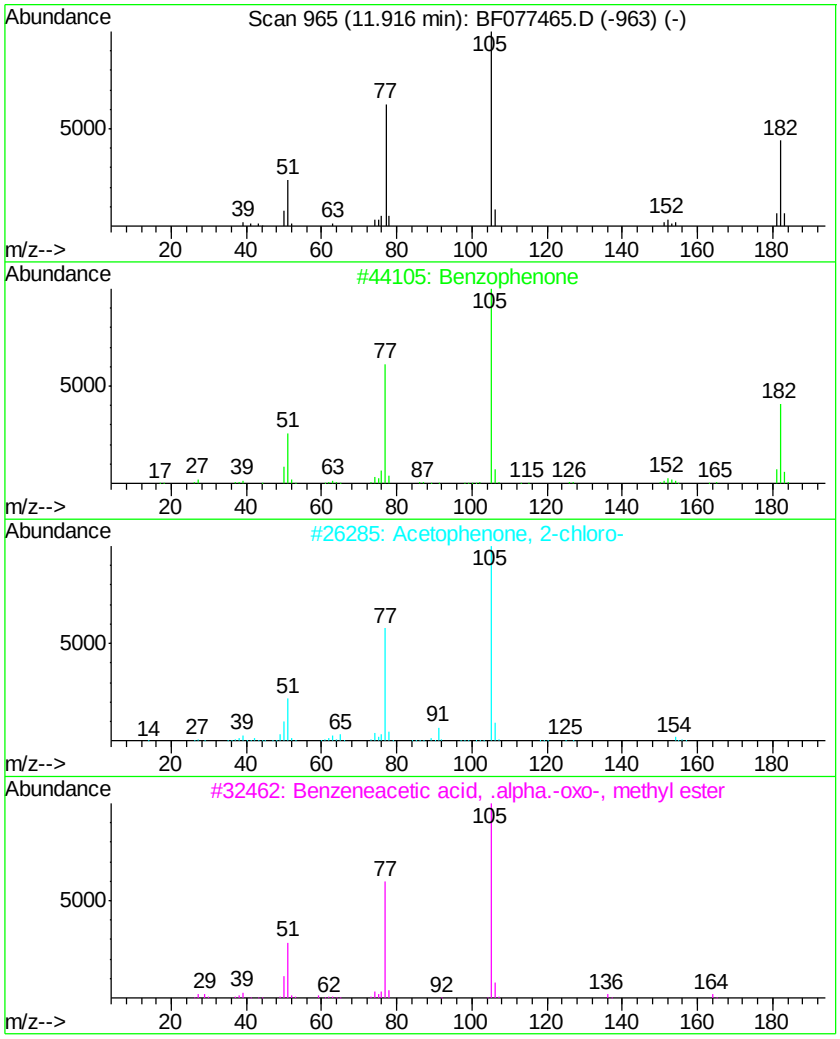
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

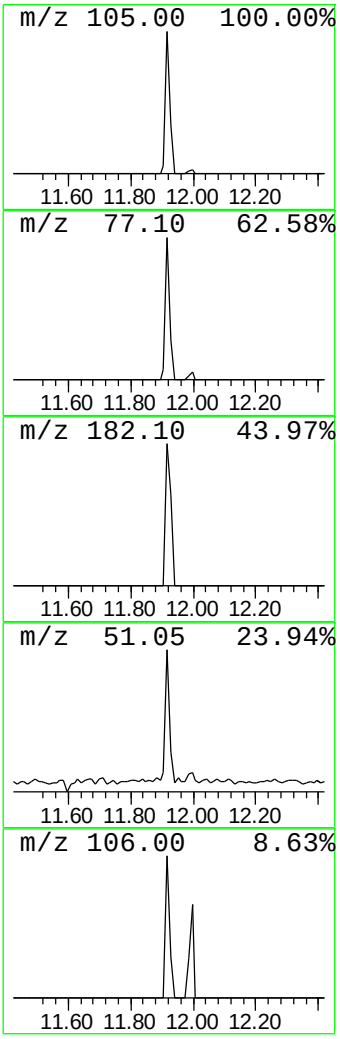
****

Peak Number 8 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.50 ng	67295	Acenaphthene-d10	11.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
4	Phenylglyoxal	134	C8H6O2	001074-12-0	47
5	Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47





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Instrument : BNA_F
ClientSampleId : 41A-WW-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

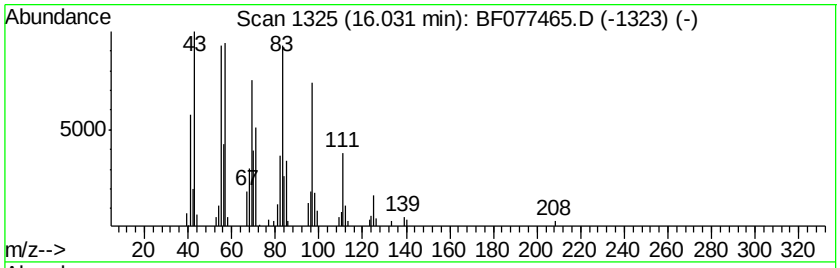
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

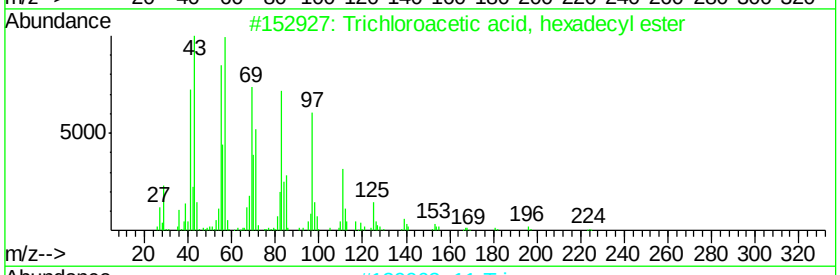
****

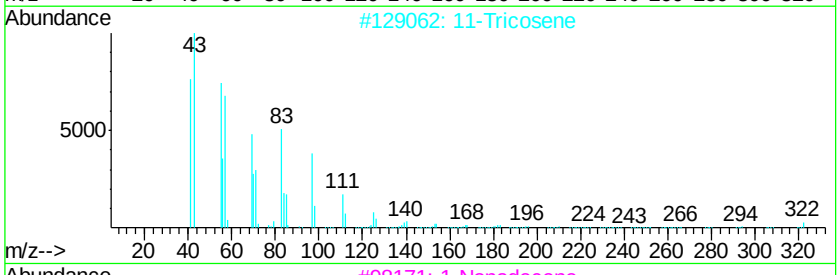
Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 8

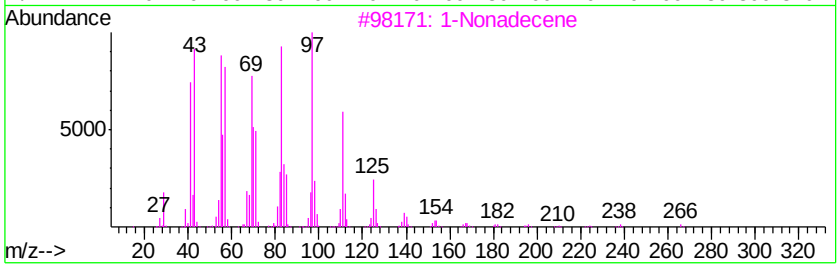
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	4.20 ng	147754	Chrysene-d12	16.16

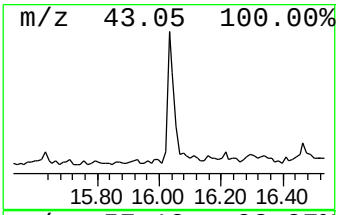
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2	11-Tricosene	322	C23H46	052078-56-5	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91

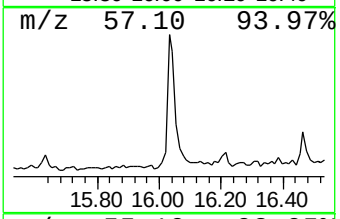


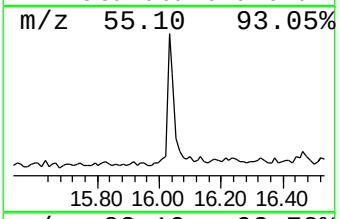


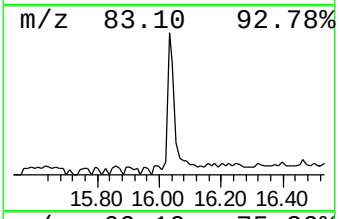


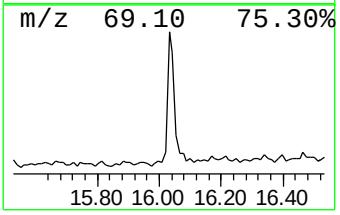












Tentatively Identified Compound (LSC) summary

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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
unknown1.42	1.42	244.9	ng	4141060	1	7.26	338135	20.0
unknown1.73	1.73	10.1	ng	170918	1	7.26	338135	20.0
2-Pentanone, 4-hy...	5.05	14.3	ng	241261	1	7.26	338135	20.0
unknown6.98	6.98	79.1	ng	1336760	1	7.26	338135	20.0
Benzophenone	11.92	2.5	ng	67295	3	11.01	538923	20.0
Trichloroacetic a...	16.03	4.2	ng	147754	5	16.16	702778	20.0