LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098802.D
Acq On : 26 Sep 2017 00:24
Operator : SJ/JU
Sample : I5361-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-A-B-COMP

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-BF092317.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	2.222	19	23	38	rVB	305285	431212	2.18%	0.847%
2	5.222	514	533	536	rBV	5135872	19821753	100.00%	38.948%
3	5.540	582	587	590	rBV	1922257	1751708	8.84%	3.442%
4	6.528	751	755	758	rBV	994641	752179	3.79%	1.478%
5	6.681	777	781	785	rBV	3209782	3189623	16.09%	6.267%
6	6.916	817	821	824	rBV	937933	846505	4.27%	1.663%
7	7.075	843	848	851	rBV	3611006	3538663	17.85%	6.953%
8	7.475	911	916	919	rBV	2566049	2931051	14.79%	5.759%
9	8.192	1034	1038	1042	rBV	1326662	1191522	6.01%	2.341%
10	9.186	1203	1207	1216	rVB	280253	251626	1.27%	0.494%
11	9.275	1216	1222	1225	rBV	4988675	5202771	26.25%	10.223%
12	9.951	1333	1337	1341	rVB	1544764	1301927	6.57%	2.558%
13	10.563	1435	1441	1443	rBV	307612	277858	1.40%	0.546%
14	10.592	1443	1446	1449	rVB	683503	516020	2.60%	1.014%
15	10.733	1467	1470	1477	rVB	566158	462340	2.33%	0.908%
16	11.416	1583	1586	1588	rVV	681058	666319	3.36%	1.309%
17	11.439	1588	1590	1593	rVB	1494427	1131012	5.71%	2.222%
18	13.027	1854	1860	1863	rBV	4357429	4629049	23.35%	9.096%
19	13.716	1973	1977	1981	rBV	403375	351212	1.77%	0.690%
20	14.074	2034	2038	2042	rVB	1043163	869572	4.39%	1.709%
21	15.562	2286	2291	2300	rBV2	594624	778661	3.93%	1.530%

Sum of corrected areas: 50892583

LSC Report - Integrated Chromatogram

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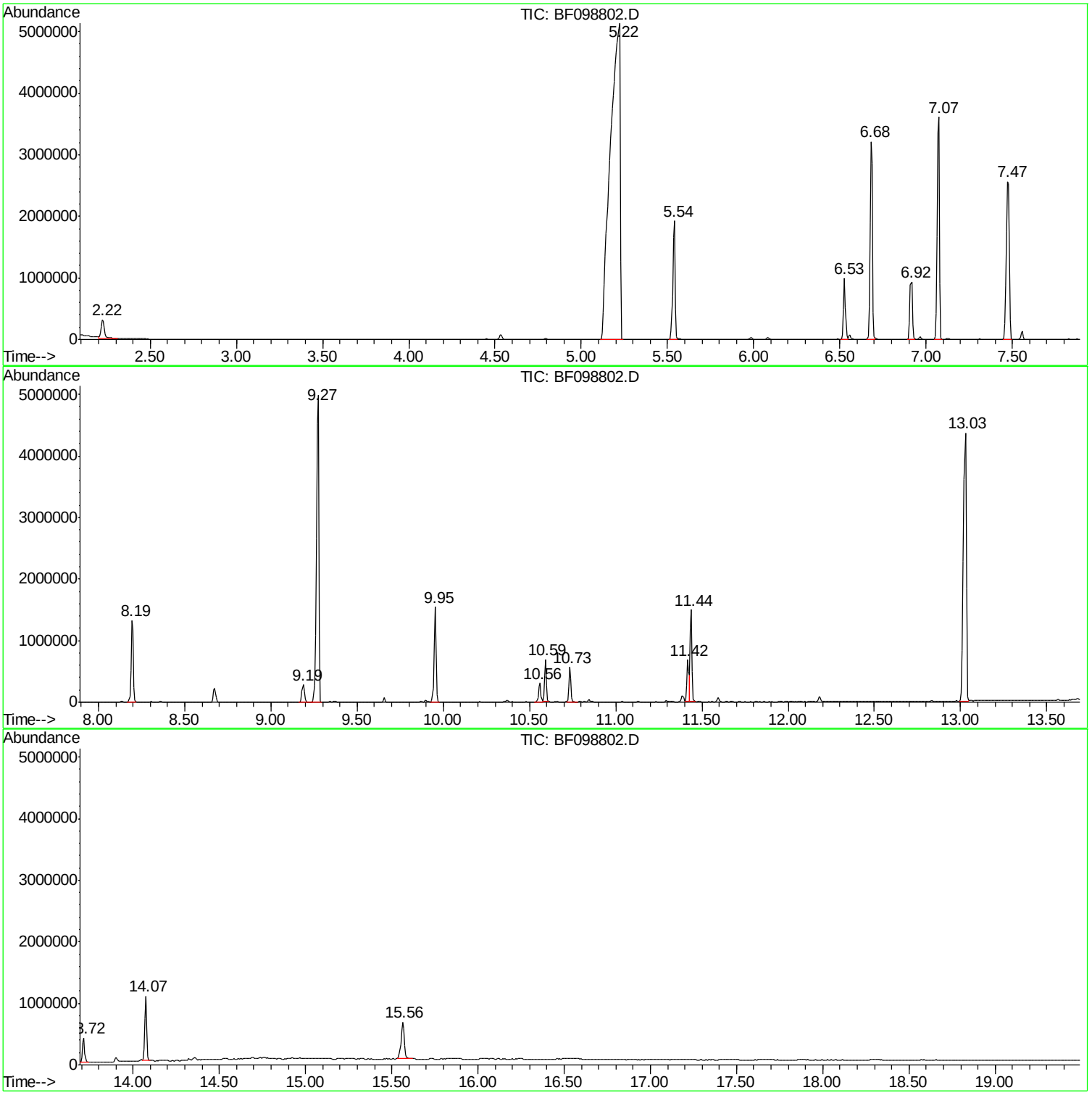
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-A-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BF098802.D
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Operator : SJ/JU
Sample : I5361-02
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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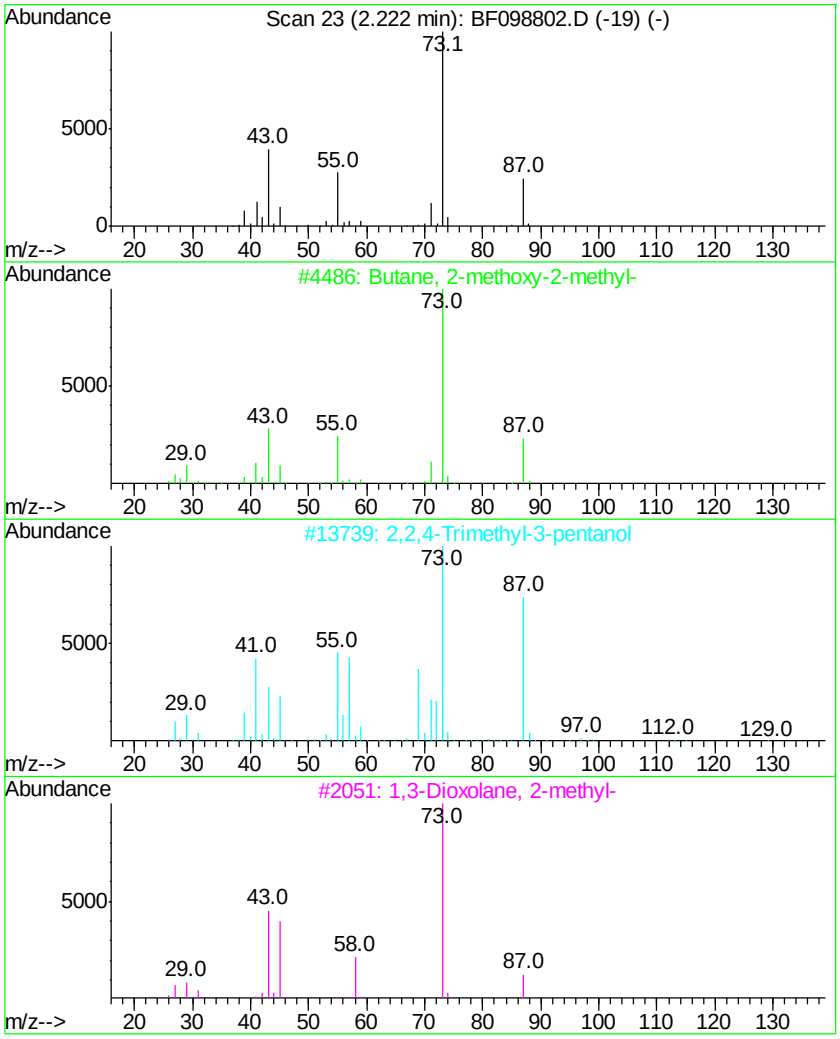
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

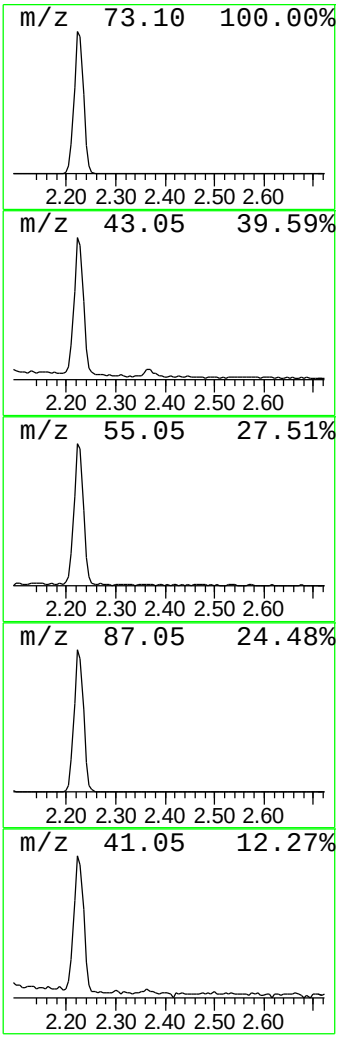
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	10.19 ng	431212	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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Sample : I5361-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-A-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

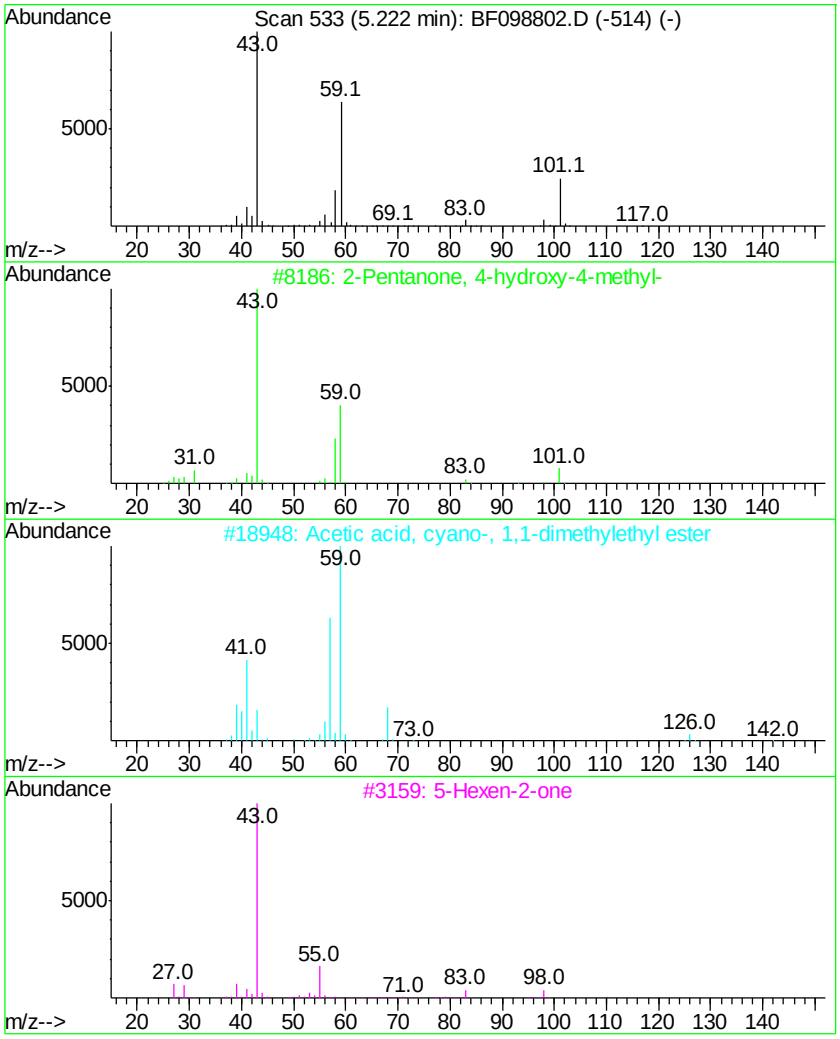
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

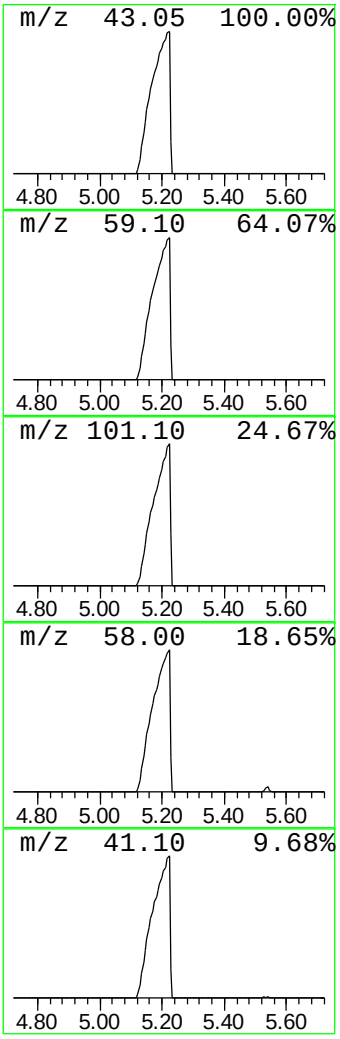
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	468.32 ng	19821800	1,4-Dichlorobenzene-d4	6.92

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Operator : SJ/JU
Sample : I5361-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-A-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

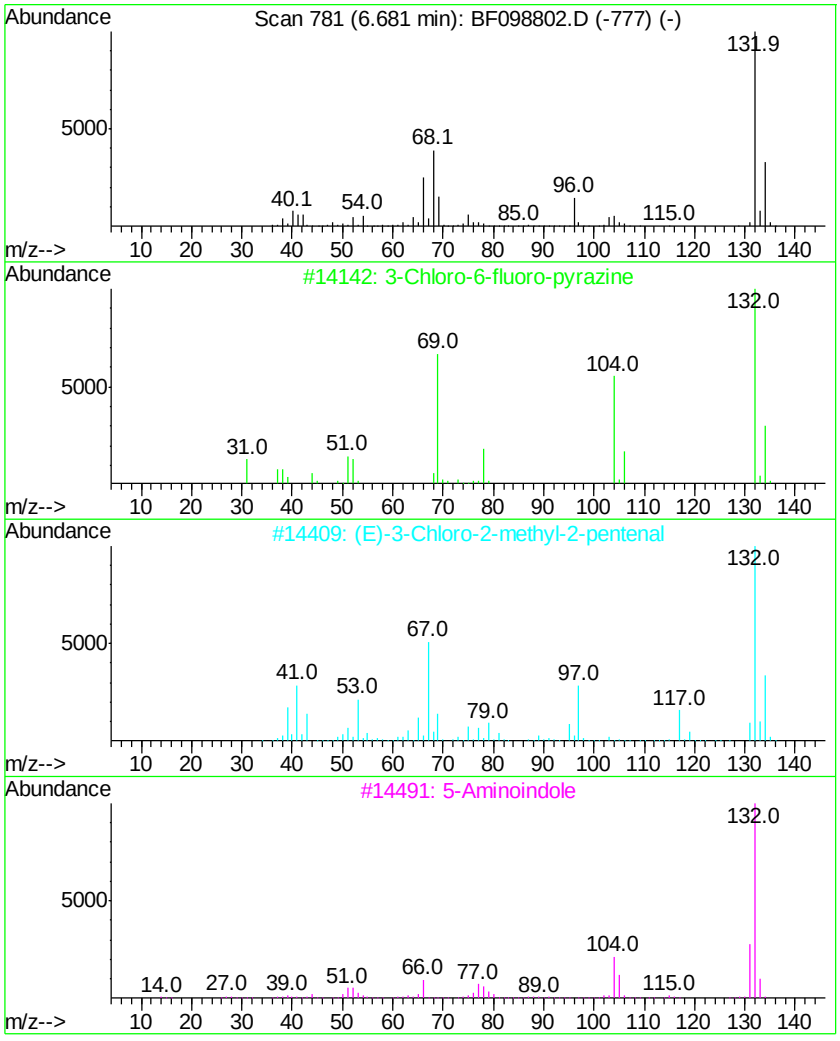
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

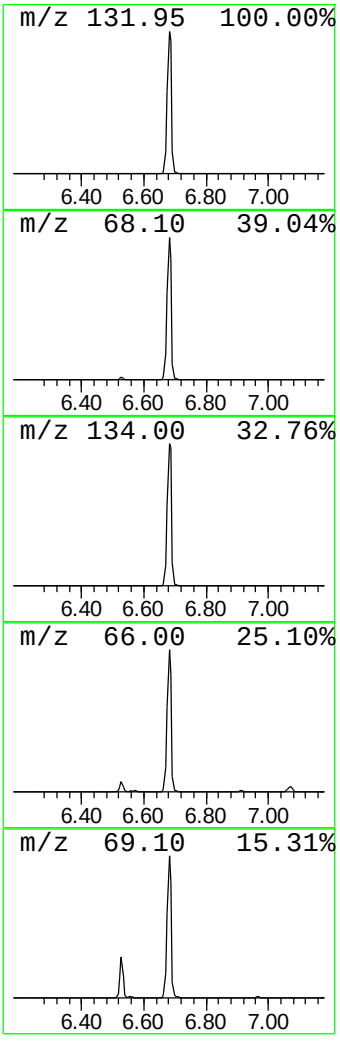
****

Peak Number 3 unknown6.68 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	75.36 ng	3189620	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Sample : I5361-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-A-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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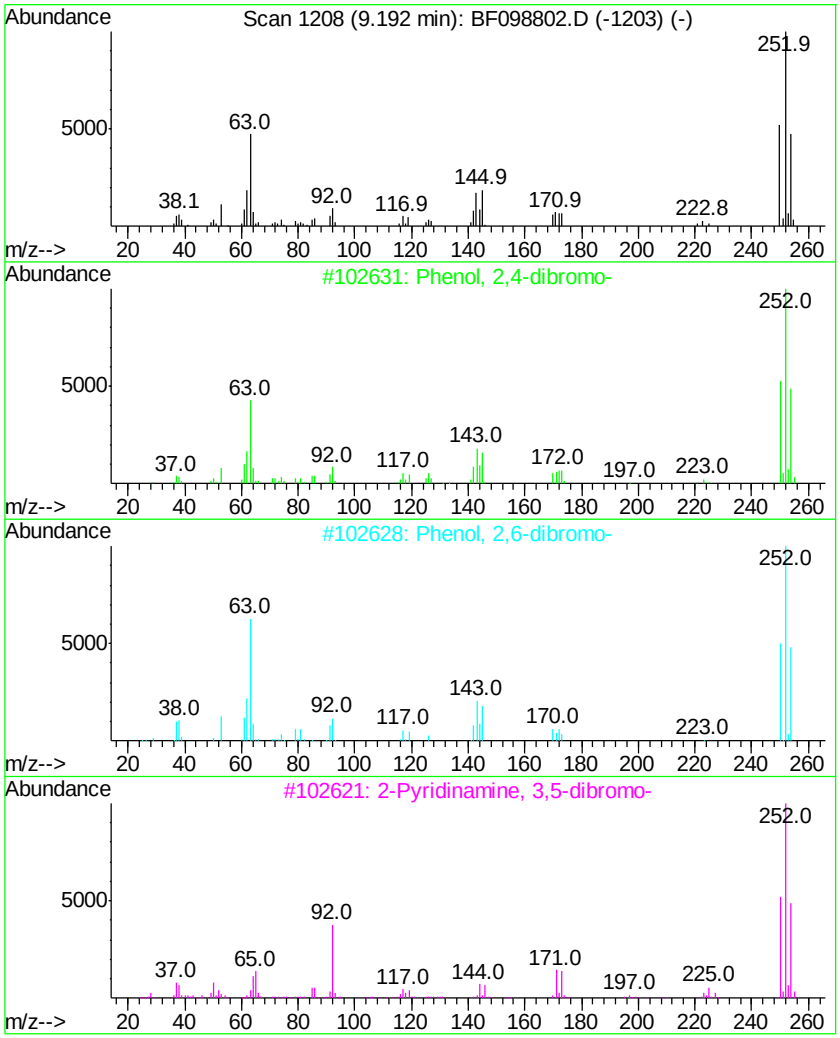
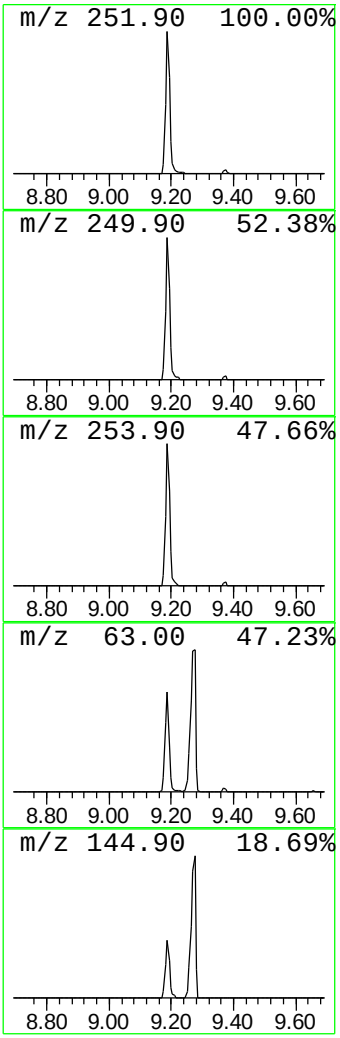
Peak Number 5 Phenol, 2,4-dibromo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.19	3.87 ng	251626	Acenaphthene-d10	9.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	99
2	Phenol, 2,6-dibromo-	250	C6H4Br2O	000608-33-3	98
3	2-Pyridinamine, 3,5-dibromo-	250	C5H4Br2N2	035486-42-1	47
4	1H-Benzotriazole, 5-nitro-	164	C6H4N4O2	002338-12-7	32
5	2-Chloroethyl carbonate	186	C5H8Cl2O3	000623-97-2	32





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Sample : I5361-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-A-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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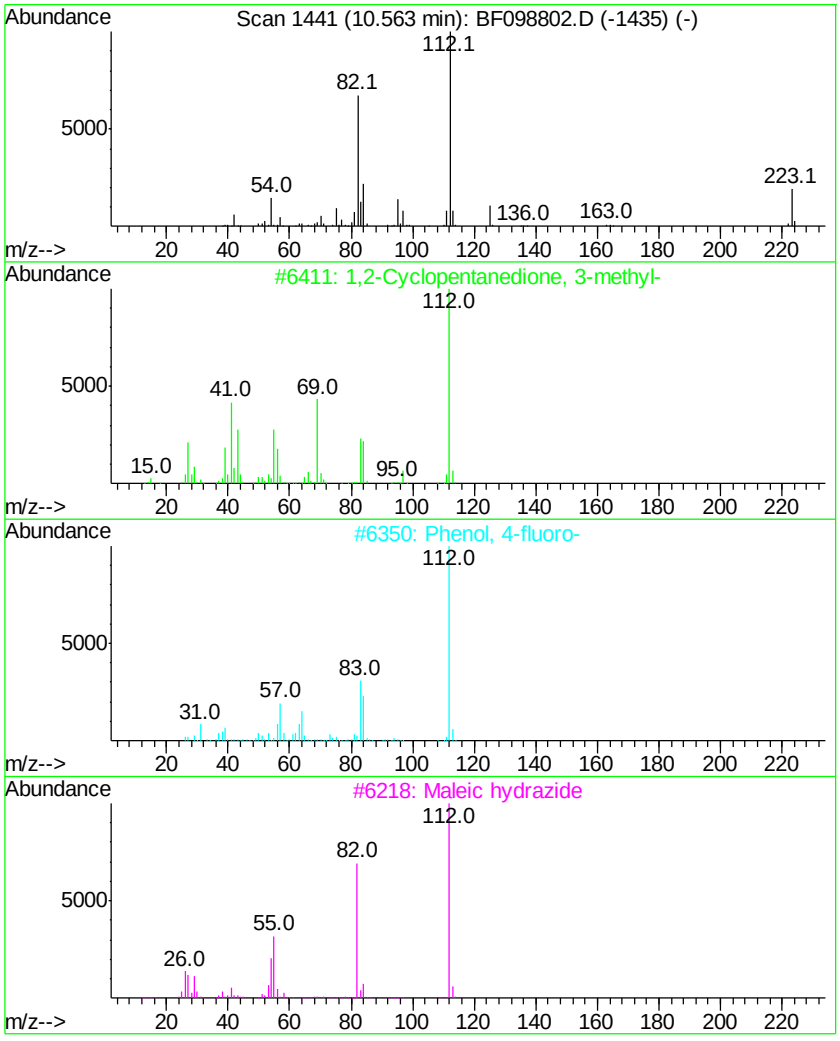
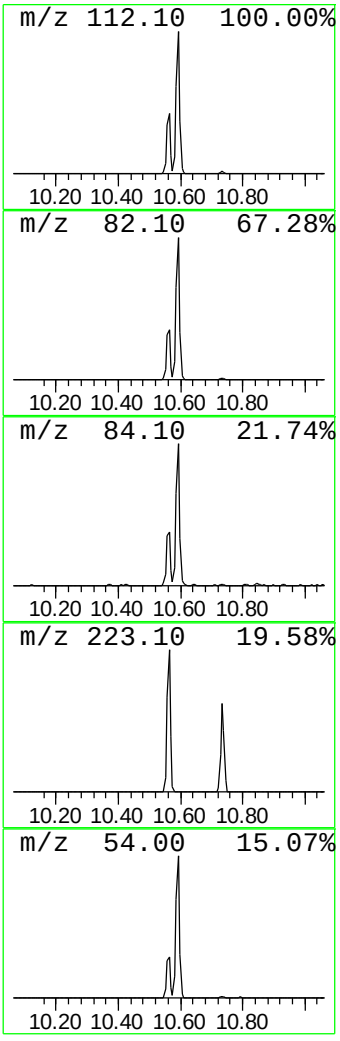
****

Peak Number 6 unknown10.56 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	4.27 ng	277858	Acenaphthene-d10	9.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclopentanedione, 3-methyl-	112	C6H8O2	000765-70-8	46
2	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	43
3	Maleic hydrazide	112	C4H4N2O2	000123-33-1	40
4	Phenol, 3-fluoro-	112	C6H5FO	000372-20-3	37
5	1,4-Cyclohexanedione	112	C6H8O2	000637-88-7	35





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-A-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

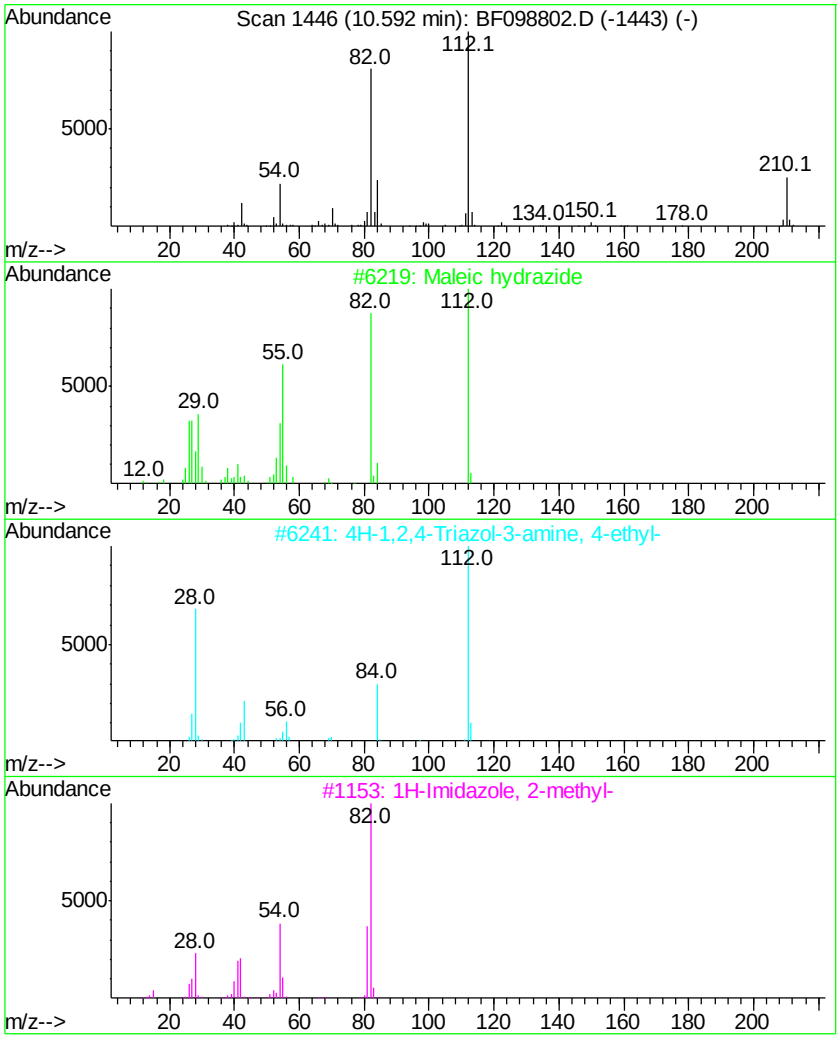
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

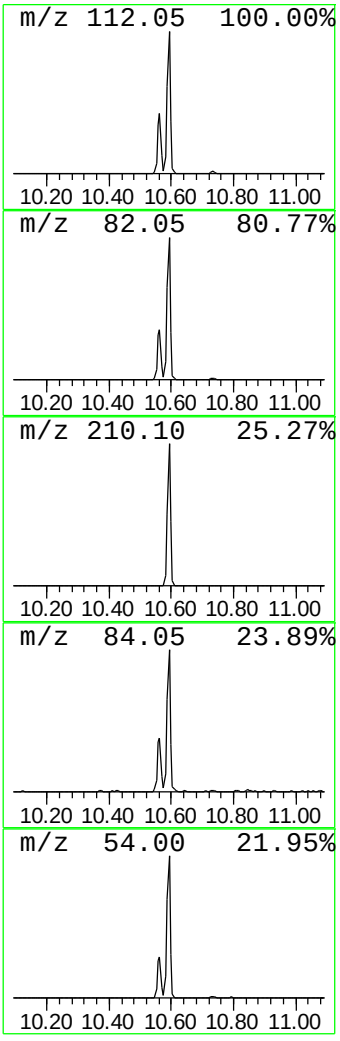
****

Peak Number 7 Maleic hydrazide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	7.93 ng	516020	Acenaphthene-d10	9.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Maleic hydrazide	112	C4H4N2O2	000123-33-1	59
2	4H-1,2,4-Triazol-3-amine, 4-ethyl-	112	C4H8N4	042786-06-1	35
3	1H-Imidazole, 2-methyl-	82	C4H6N2	000693-98-1	30
4	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	27
5	5-Azacytosine	112	C3H4N4O	000931-86-2	27





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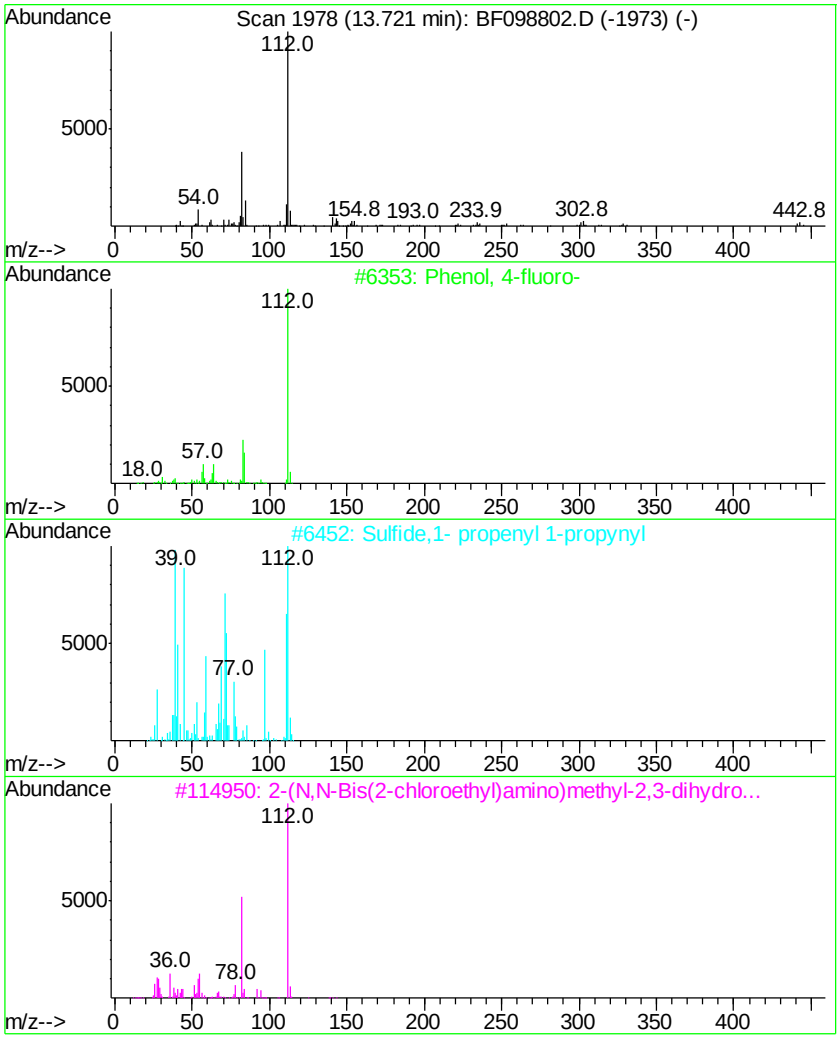
TIC Integration Parameters: LSCINT.P

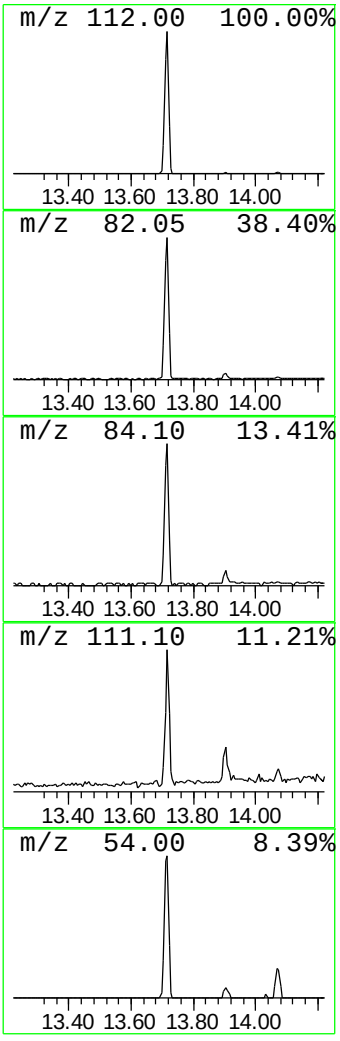
****

Peak Number 8 unknown13.72 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	8.08 ng	351212	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	47
2	Sulfide,1- propenyl 1-propynyl	112	C6H8S	089533-93-7	43
3	2-(N,N-Bis(2-chloroethyl)amino)m...	265	C9H13Cl2N3O2	014628-36-5	40
4	5-Azacytosine	112	C3H4N4O	000931-86-2	37
5	6-[2-Hexahydroazepino-1-hydroxye...	374	C25H30N2O	035871-87-5	37





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	10.2	ng	431212	1	6.92	846505	20.0
2-Pentanone, 4-hy...	5.22	468.3	ng	19821800	1	6.92	846505	20.0
unknown6.68	6.68	75.4	ng	3189620	1	6.92	846505	20.0
Phenol, 2,4-dibromo-	9.19	3.9	ng	251626	3	9.95	1301930	20.0
unknown10.56	10.56	4.3	ng	277858	3	9.95	1301930	20.0
Maleic hydrazide	10.59	7.9	ng	516020	3	9.95	1301930	20.0
unknown13.72	13.72	8.1	ng	351212	5	14.07	869572	20.0