LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081758.D
Acq On : 23 Sep 2015 6:29
Operator : UM/IZ
Sample : G3748-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP202-38-40

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-BF090115.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	1.247	11	14	16	rVB	1114891	1210346	31.71%	5.757%
2	1.430	29	30	36	rBV	216823	576502	15.10%	2.742%
3	1.521	36	38	79	rVB	1034281	3816768	100.00%	18.154%
4	4.436	288	293	319	rBV	267447	848745	22.24%	4.037%
5	5.316	366	370	394	rBV	697664	1525332	39.96%	7.255%
6	6.619	480	484	498	rBV3	18542	108713	2.85%	0.517%
7	7.579	565	568	572	rBV	419581	1132880	29.68%	5.388%
8	7.659	572	575	588	rVV	905938	2193398	57.47%	10.433%
9	7.990	603	604	609	rBV	110465	196993	5.16%	0.937%
10	8.128	613	616	619	rVV	164308	272812	7.15%	1.298%
11	8.459	641	645	648	rVB	676347	1147378	30.06%	5.457%
12	9.442	726	731	734	rBV	527945	995675	26.09%	4.736%
13	11.031	866	870	883	rBB	197611	343542	9.00%	1.634%
14	12.894	1031	1033	1047	rBB	140313	269417	7.06%	1.281%
15	13.682	1096	1102	1105	rBV	925941	1736081	45.49%	8.257%
16	14.734	1191	1194	1202	rBB	126684	210053	5.50%	0.999%
17	15.157	1227	1231	1236	rBV2	207236	358106	9.38%	1.703%
18	17.066	1394	1398	1410	rBB	521300	1039789	27.24%	4.946%
19	17.889	1466	1470	1481	rBB	18663	49500	1.30%	0.235%
20	18.666	1534	1538	1545	rBV	215502	372643	9.76%	1.772%
21	20.437	1690	1693	1704	rBV	19834	48137	1.26%	0.229%
22	22.049	1831	1834	1837	rBV	1126999	1648536	43.19%	7.841%
23	23.295	1940	1943	1944	rBV	123671	144856	3.80%	0.689%
24	23.329	1944	1946	1953	rVV	304583	328998	8.62%	1.565%
25	24.255	2025	2027	2030	rBV	177860	222017	5.82%	1.056%
26	24.769	2069	2072	2076	rBV	210609	227277	5.95%	1.081%

Sum of corrected areas: 21024494

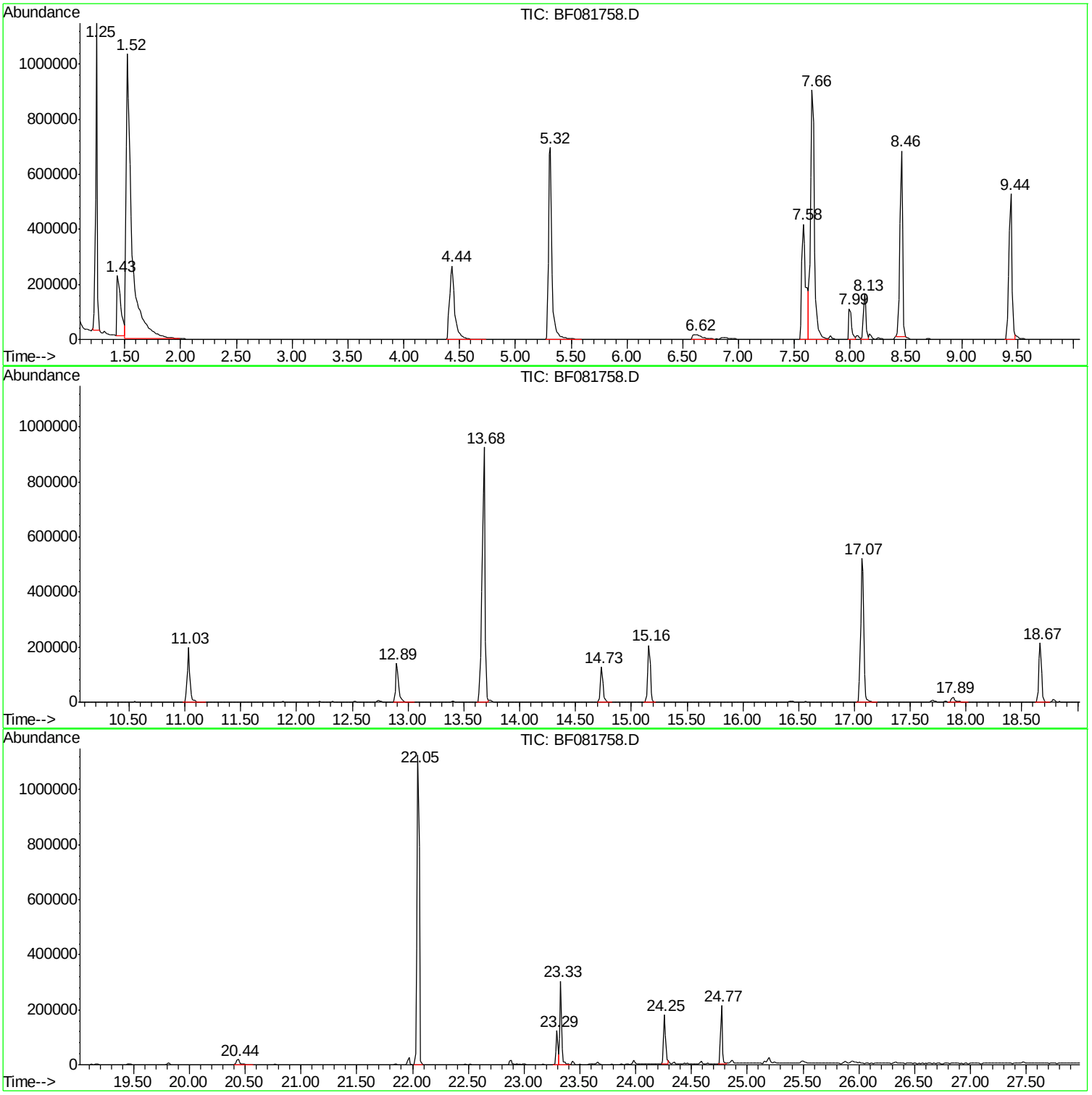
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081758.D
Acq On : 23 Sep 2015 6:29
Operator : UM/IZ
Sample : G3748-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP202-38-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF092215\
Data File : BF081758.D
Acq On : 23 Sep 2015 6:29
Operator : UM/IZ
Sample : G3748-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP202-38-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

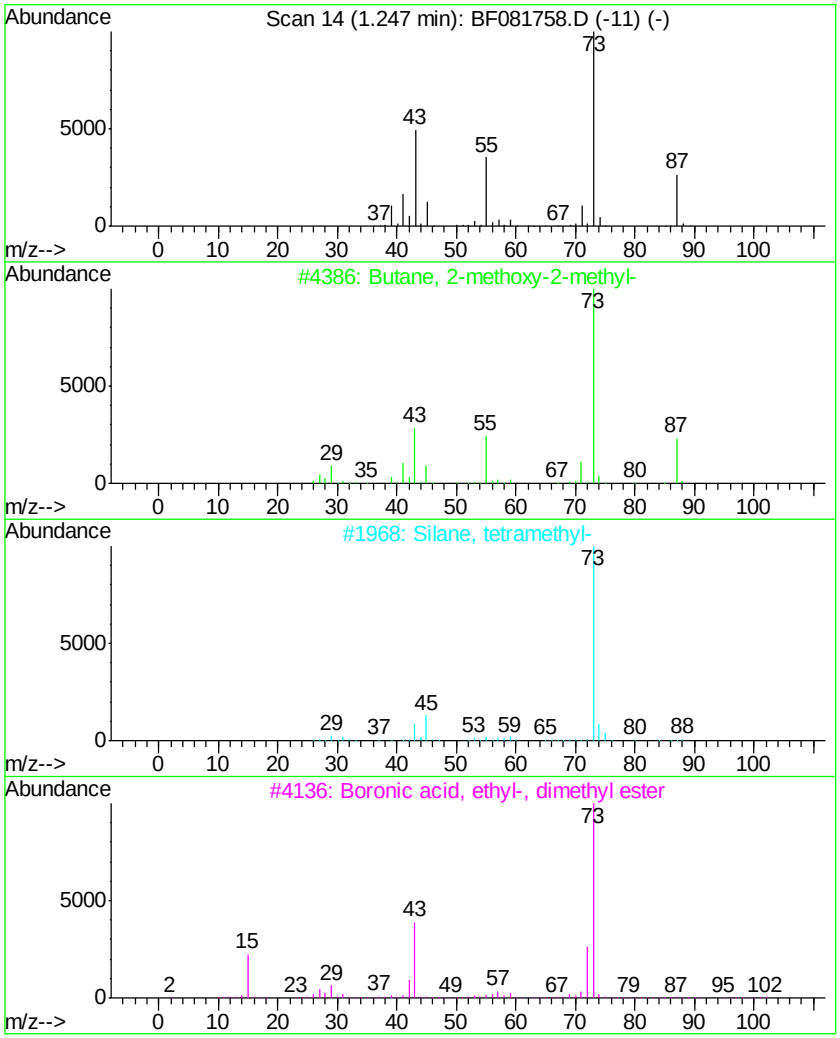
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

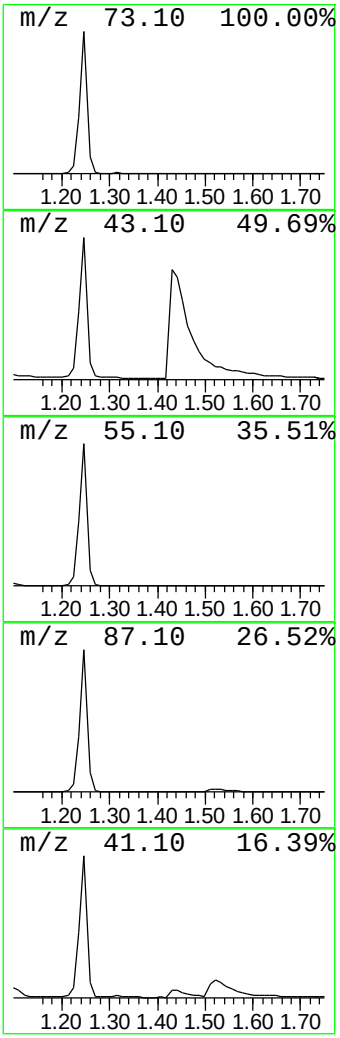
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.25	88.73 ng	1210350	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
3	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081758.D
Acq On : 23 Sep 2015 6:29
Operator : UM/IZ
Sample : G3748-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP202-38-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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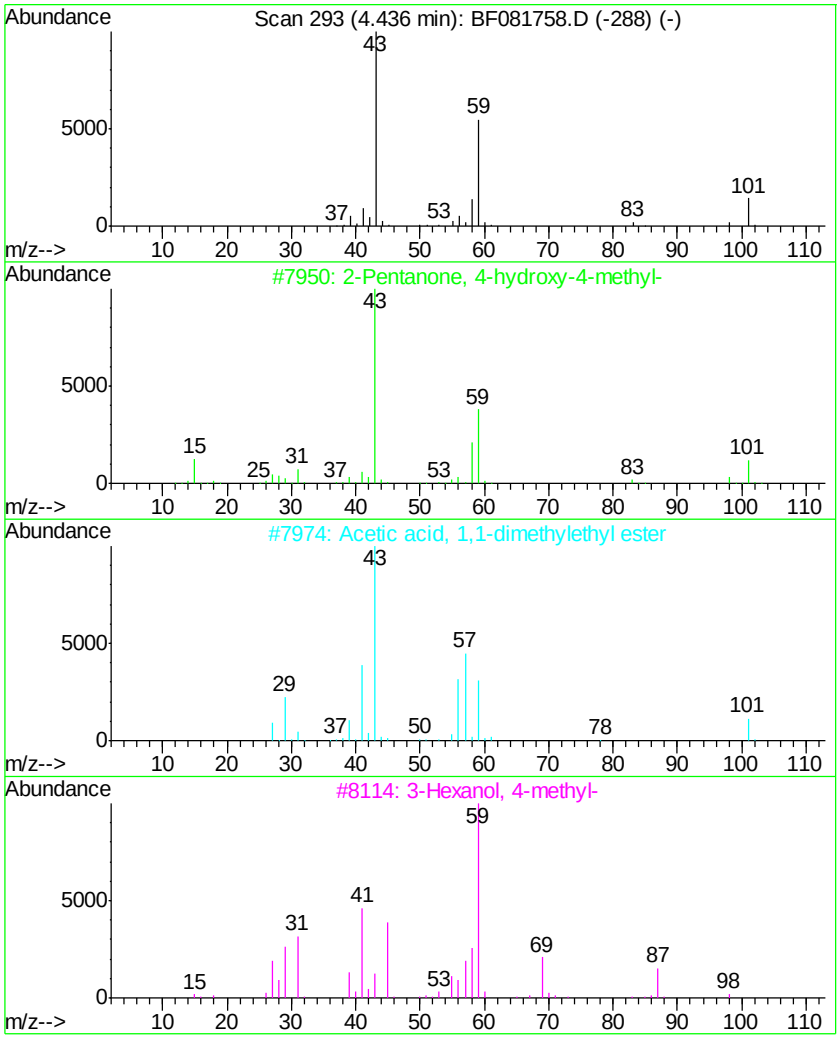
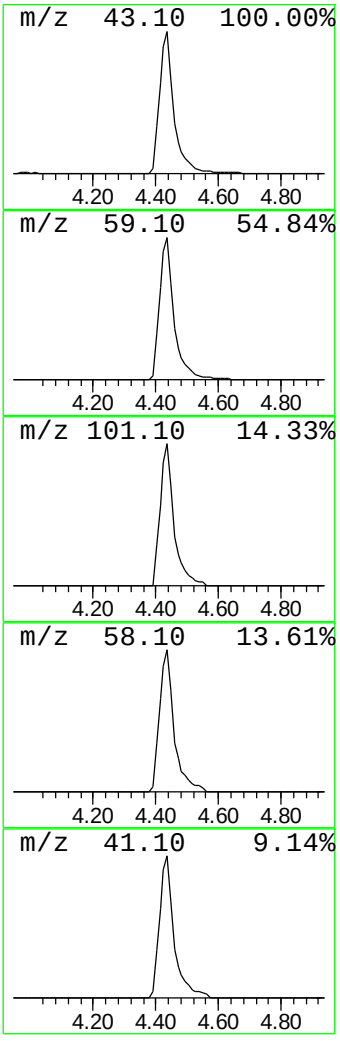
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	62.22 ng	848745	1,4-Dichlorobenzene-d4	8.13

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081758.D
Acq On : 23 Sep 2015 6:29
Operator : UM/IZ
Sample : G3748-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP202-38-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

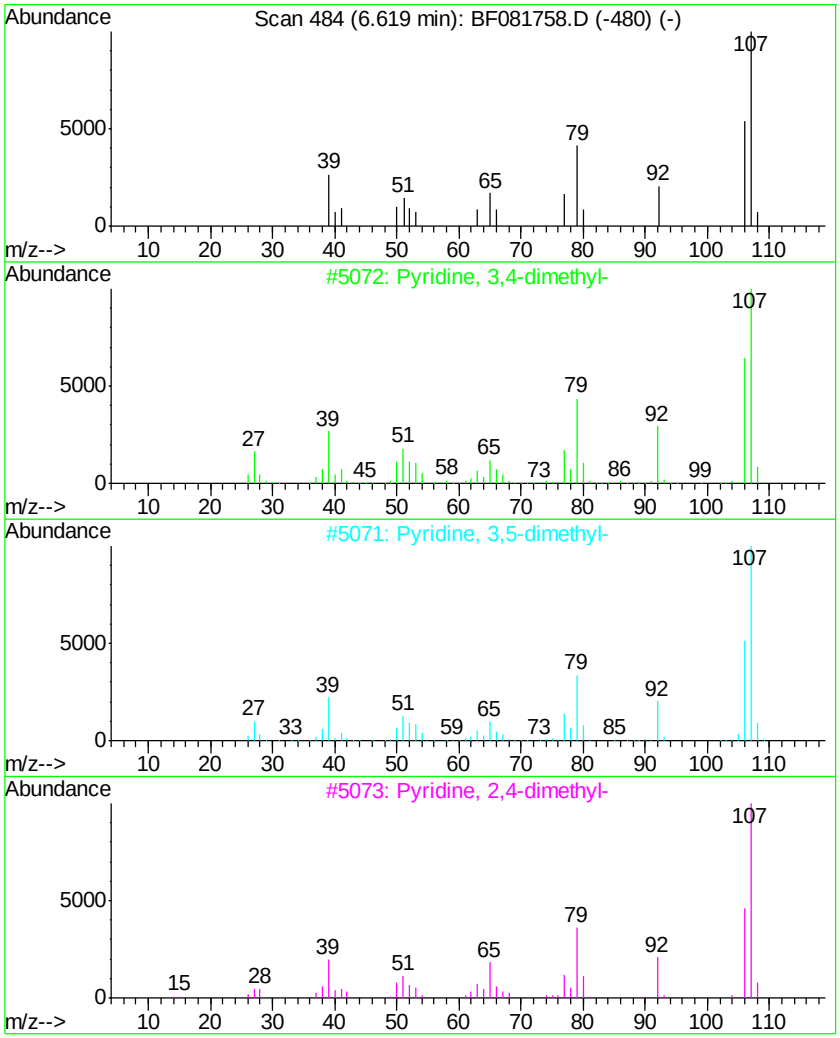
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

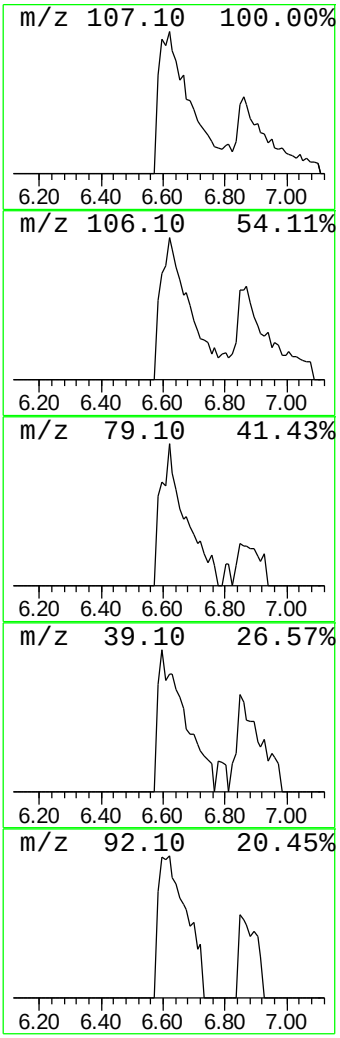
****

Peak Number 5 Pyridine, 3,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	7.97 ng	108713	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 3,4-dimethyl-	107	C7H9N	000583-58-4	96
2	Pyridine, 3,5-dimethyl-	107	C7H9N	000591-22-0	91
3	Pyridine, 2,4-dimethyl-	107	C7H9N	000108-47-4	91
4	Pyridine, 2,5-dimethyl-	107	C7H9N	000589-93-5	90
5	Pyridine, 2,3-dimethyl-	107	C7H9N	000583-61-9	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081758.D
Acq On : 23 Sep 2015 6:29
Operator : UM/IZ
Sample : G3748-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP202-38-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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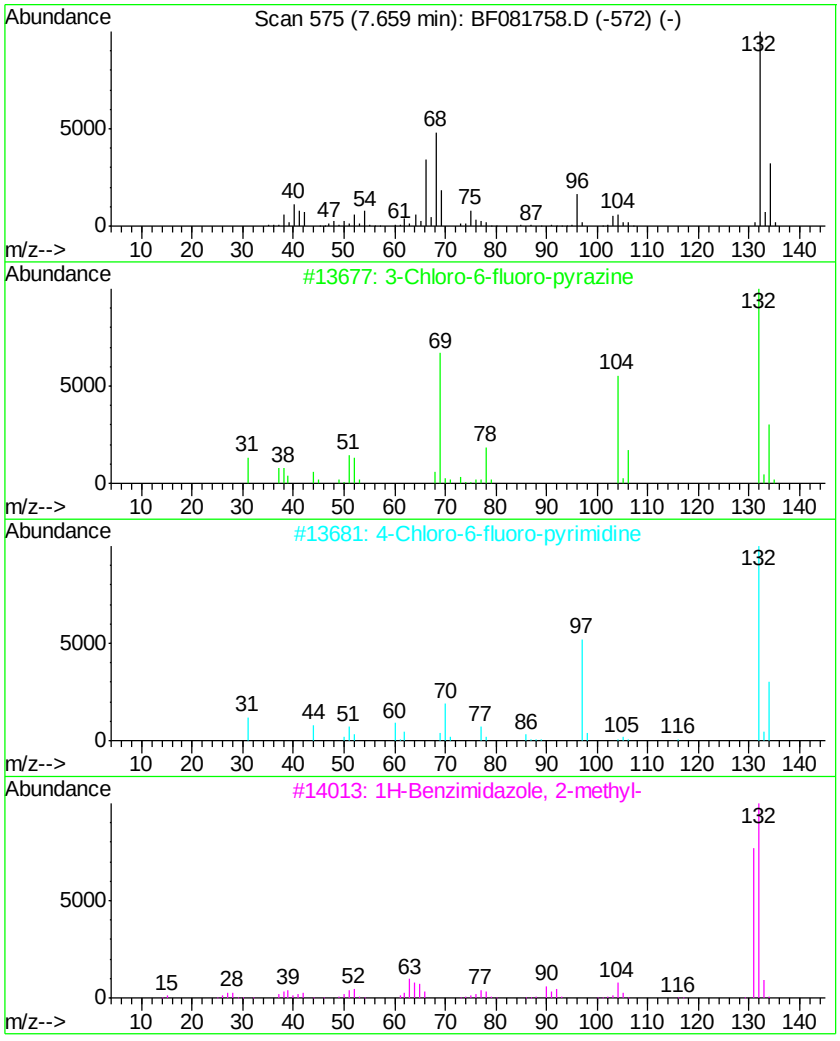
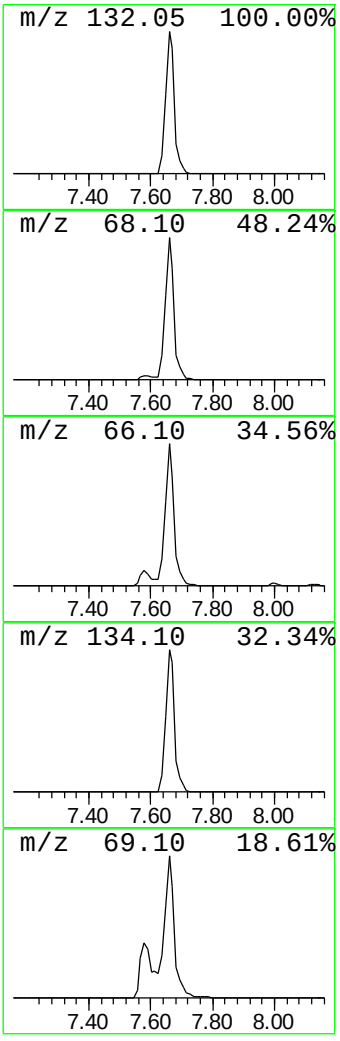
Peak Number 6 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	160.80 ng	2193400	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081758.D
Acq On : 23 Sep 2015 6:29
Operator : UM/IZ
Sample : G3748-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP202-38-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

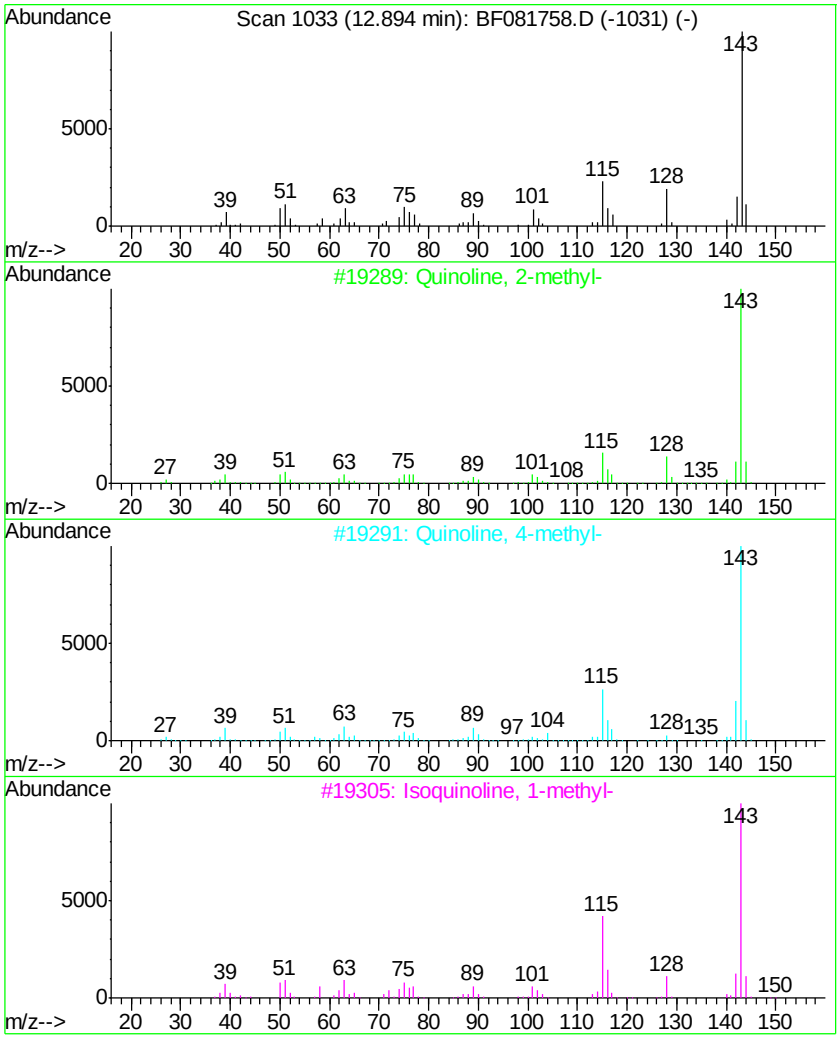
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

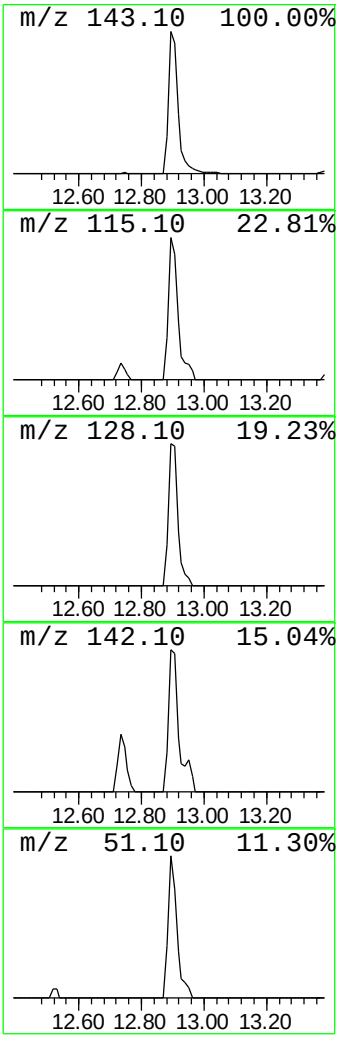
****

Peak Number 9 Quinoline, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	15.68 ng	269417	Naphthalene-d8	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline, 2-methyl-	143	C10H9N	000091-63-4	97
2	Quinoline, 4-methyl-	143	C10H9N	000491-35-0	87
3	Isoquinoline, 1-methyl-	143	C10H9N	001721-93-3	87
4	Quinoline, 3-methyl-	143	C10H9N	000612-58-8	76
5	2-Naphthalenamine	143	C10H9N	000091-59-8	76





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Operator : UM/IZ
Sample : G3748-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP202-38-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

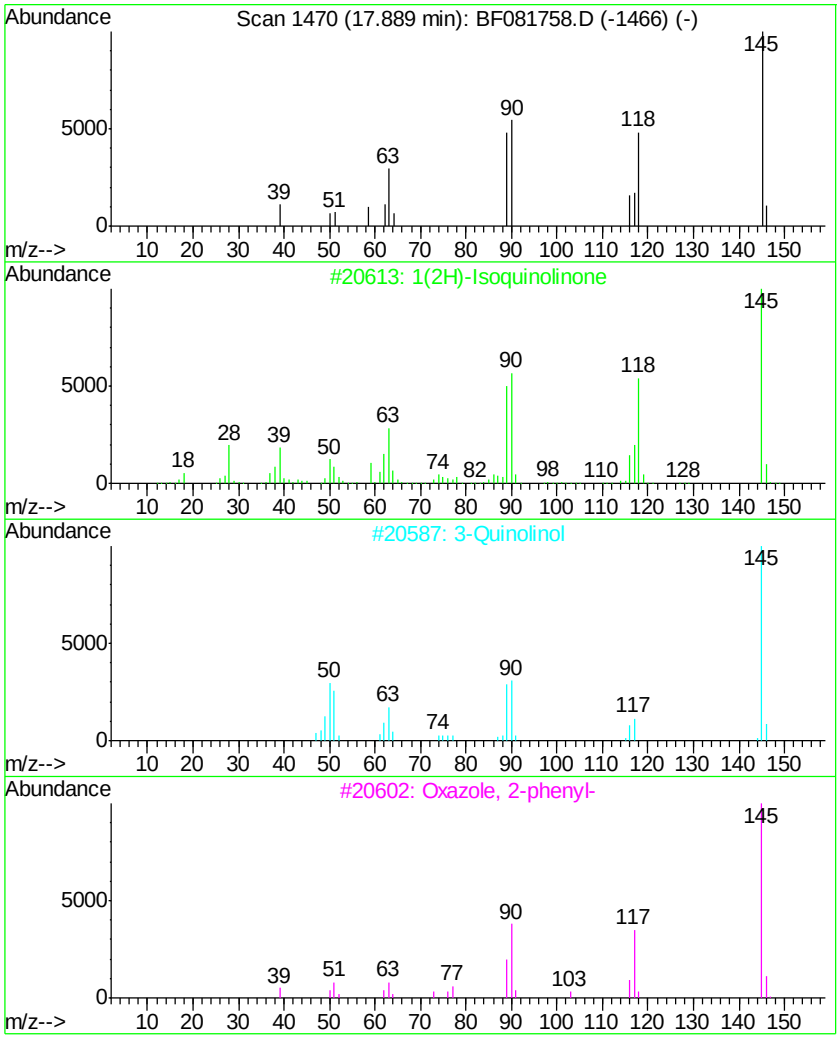
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

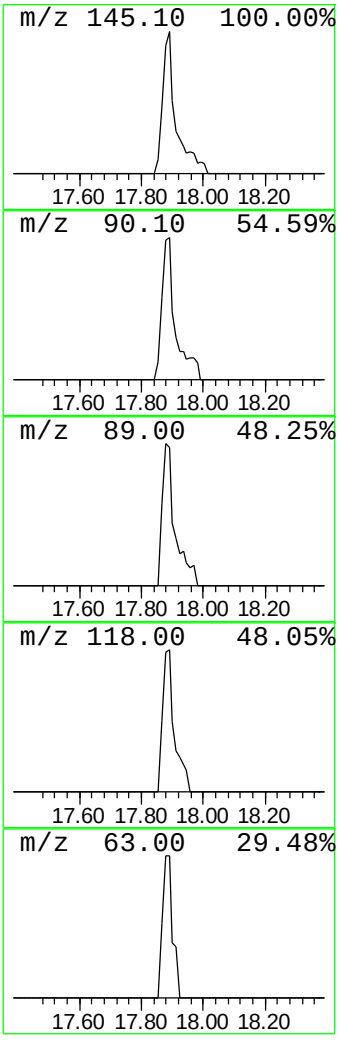
****

Peak Number 10 1(2H)-Isoquinolinone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	2.66 ng	49500	Phenanthrene-d10	18.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Isoquinolinone	145	C9H7NO	000491-30-5	91
2	3-Quinolinol	145	C9H7NO	000580-18-7	81
3	Oxazole, 2-phenyl-	145	C9H7NO	020662-88-8	64
4	1-Phthalazinamine	145	C8H7N3	019064-69-8	64
5	Isoquinoline, 2-oxide	145	C9H7NO	001532-72-5	64





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Misc :
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ClientSampleId : MGP202-38-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

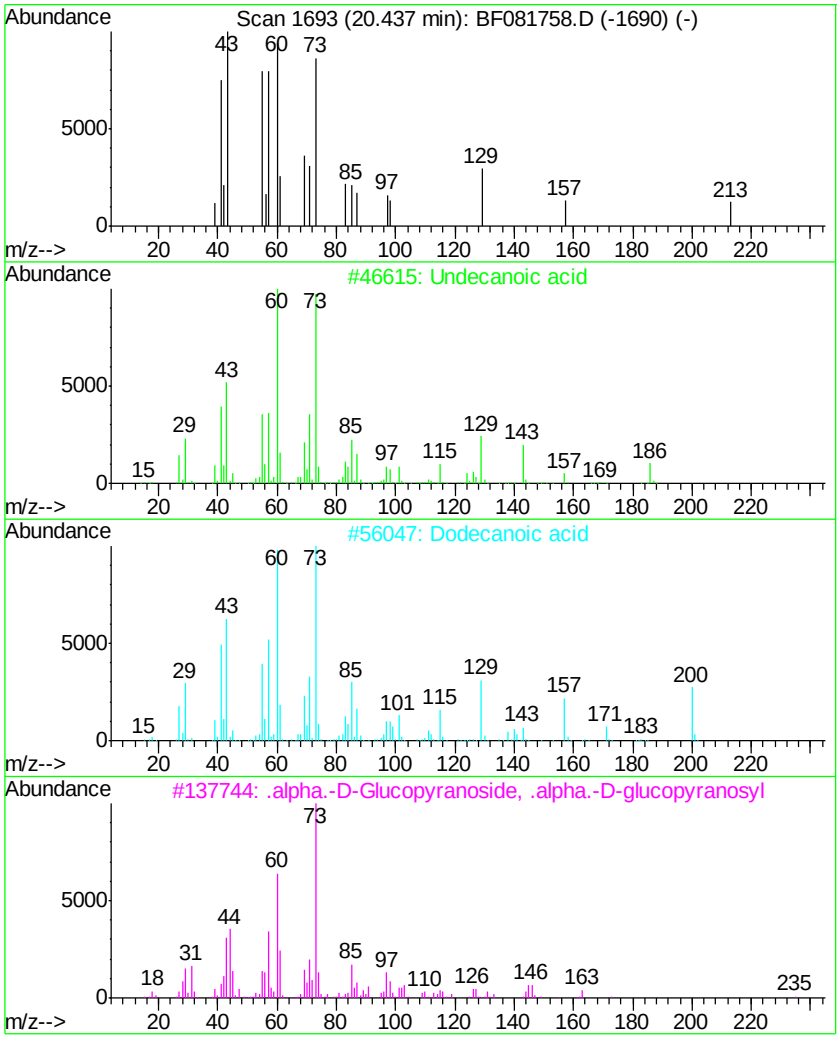
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

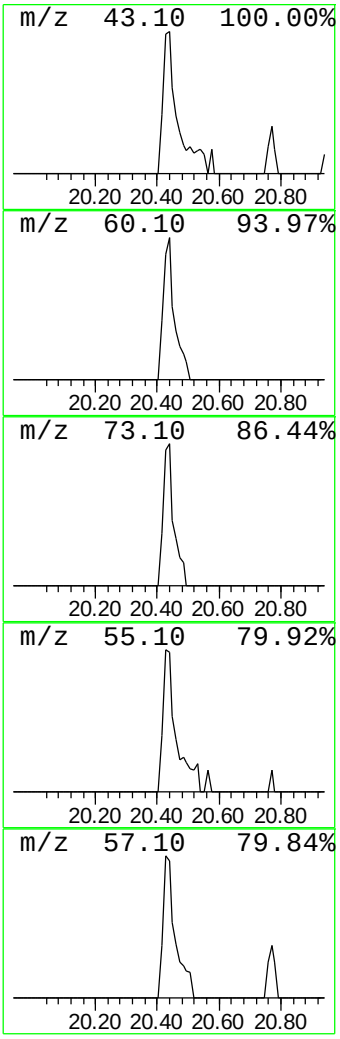
****

Peak Number 11 Undecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.44	2.58 ng	48137	Phenanthrene-d10	18.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	(1R,3R,4R,5R)-(-)-Quinic acid	192	C7H12O6	000077-95-2	53





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Integration Parameters: LSCINT.P

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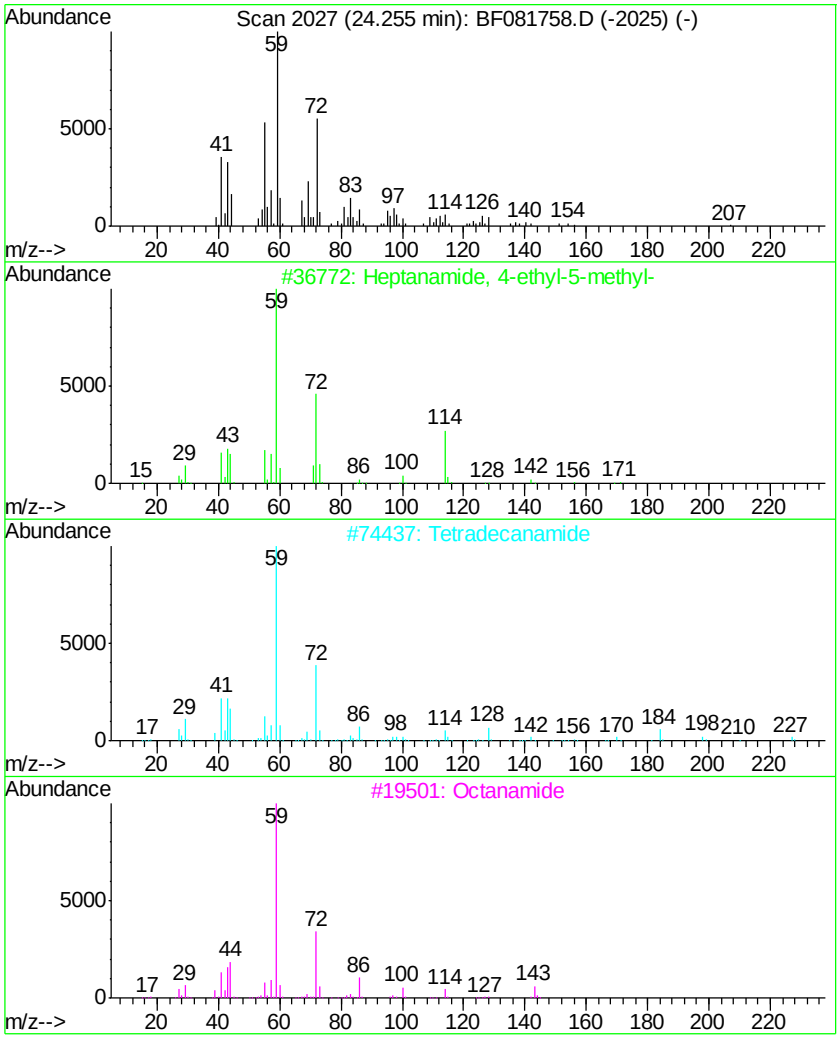
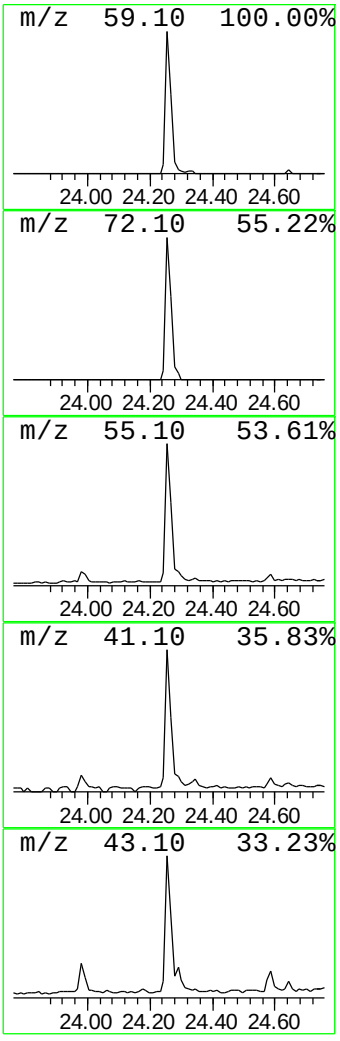
Peak Number 12 Heptanamide, 4-ethyl-5-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.26	19.54 ng	222017	Perylene-d12	24.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
2	Tetradecanamide	227	C14H29NO	000638-58-4	53
3	Octanamide	143	C8H17NO	000629-01-6	50
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50
5	Hexanamide	115	C6H13NO	000628-02-4	47





Tentatively Identified Compound (LSC) summary

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Operator : UM/IZ
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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
Butane, 2-methoxy...	1.25	88.7	ng	1210350	1	8.13	272812	20.0
2-Pentanone, 4-hy...	4.44	62.2	ng	848745	1	8.13	272812	20.0
Pyridine, 3,4-dim...	6.62	8.0	ng	108713	1	8.13	272812	20.0
unknown7.66	7.66	160.8	ng	2193400	1	8.13	272812	20.0
Quinoline, 2-methyl-	12.89	15.7	ng	269417	2	11.03	343542	20.0
1(2H)-Isoquinolinone	17.89	2.7	ng	49500	4	18.67	372643	20.0
Undecanoic acid	20.44	2.6	ng	48137	4	18.67	372643	20.0
Heptanamide, 4-et...	24.26	19.5	ng	222017	6	24.77	227277	20.0