LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031715\
Data File : BF077784.D
Acq On : 17 Mar 2015 21:11
Operator : TP/IZ
Sample : G1544-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

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-BF031115.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	1.093	14	18	21	rVB	26828	45731	2.63%	0.393%
2	1.435	45	48	51	rVB	179217	302890	17.44%	2.604%
3	1.607	60	63	66	rVB	431364	489572	28.19%	4.208%
4	1.790	77	79	88	rBV	45324	70153	4.04%	0.603%
5	4.922	351	353	358	rVB	59186	80495	4.64%	0.692%
6	5.447	396	399	401	rBV	517351	655521	37.75%	5.635%
7	6.727	509	511	513	rBV	426573	452006	26.03%	3.885%
8	6.865	521	523	526	rBV	943960	1062851	61.20%	9.136%
9	7.162	546	549	551	rBV	227128	233594	13.45%	2.008%
10	7.345	562	565	568	rBV	1104772	996118	57.36%	8.562%
11	7.848	607	609	612	rBV	557728	728560	41.95%	6.263%
12	8.008	617	623	627	rVB	10785	19496	1.12%	0.168%
13	8.179	636	638	643	rBV	16652	24006	1.38%	0.206%
14	8.453	658	662	668	rBV2	35491	55011	3.17%	0.473%
15	8.739	684	687	689	rBV	288004	315332	18.16%	2.711%
16	9.448	747	749	751	rBV	30829	28580	1.65%	0.246%
17	10.088	802	805	807	rBV	1298395	1614650	92.98%	13.879%
18	10.591	846	849	851	rVB	27384	22814	1.31%	0.196%
19	10.899	874	876	879	rVB	262286	363018	20.90%	3.120%
20	11.436	922	923	927	rBV	11212	23478	1.35%	0.202%
21	11.814	953	956	958	rVB	88463	112367	6.47%	0.966%
22	11.882	959	962	965	rBV	953016	921467	53.06%	7.921%
23	12.739	1035	1037	1040	rBV	337882	379071	21.83%	3.258%
24	12.991	1057	1059	1062	rBV	11396	18096	1.04%	0.156%
25	14.740	1210	1212	1215	rBV	1646112	1736596	100.00%	14.927%
26	15.940	1314	1317	1323	rBV2	14695	31856	1.83%	0.274%
27	16.043	1323	1326	1328	rBV	307018	430086	24.77%	3.697%
28	17.826	1479	1482	1485	rBV	310770	420236	24.20%	3.612%

Sum of corrected areas: 11633651

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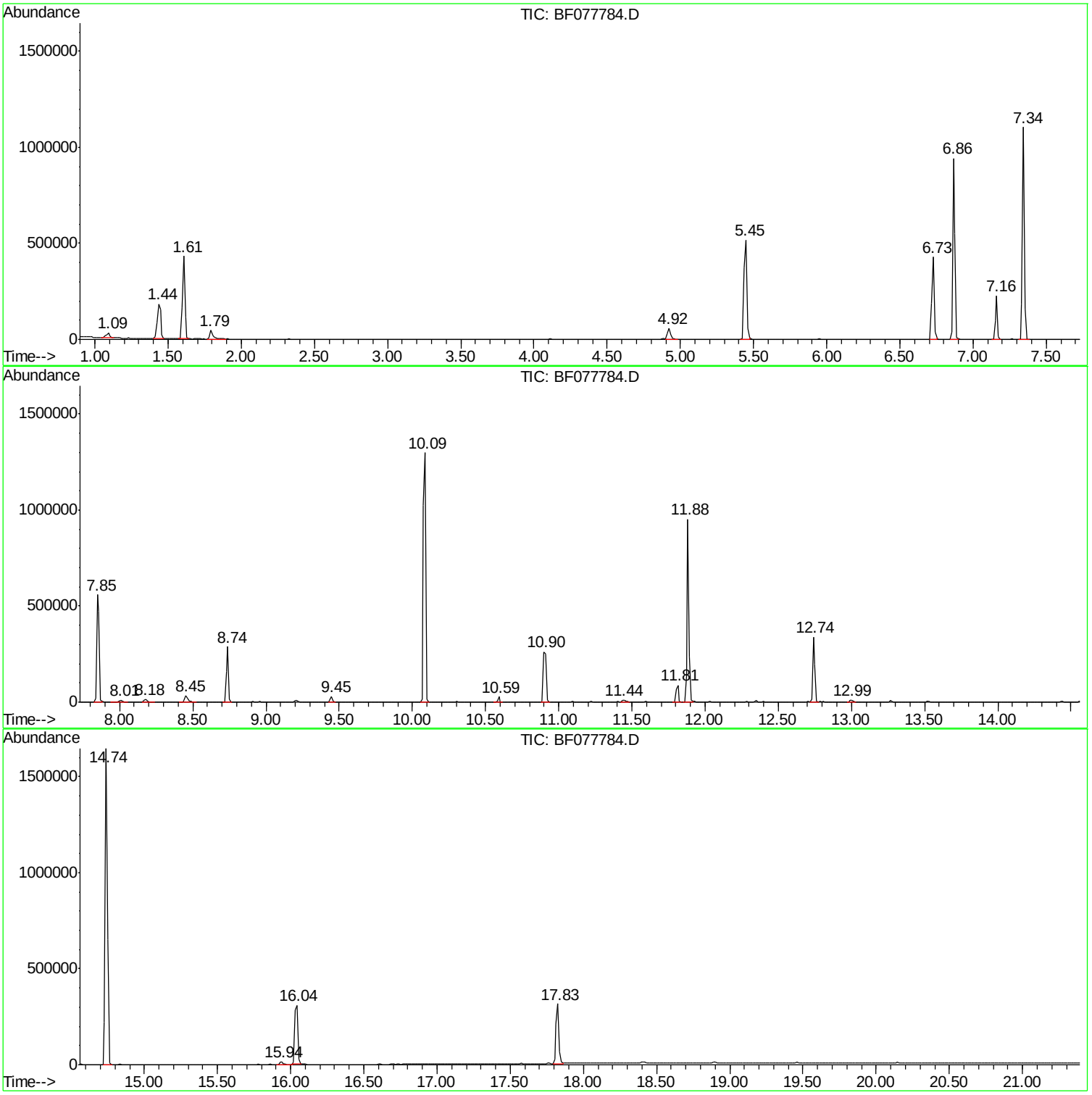
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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\BF031715\
Data File : BF077784.D
Acq On : 17 Mar 2015 21:11
Operator : TP/IZ
Sample : G1544-10
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ClientSampleId : TW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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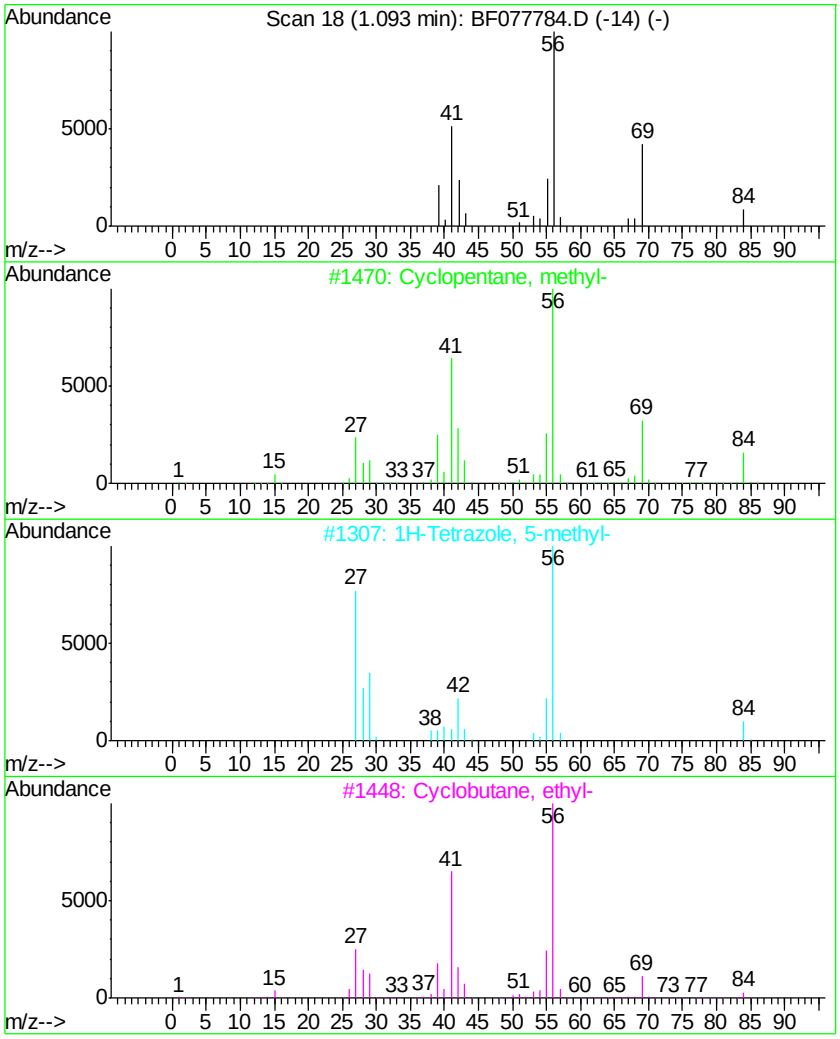
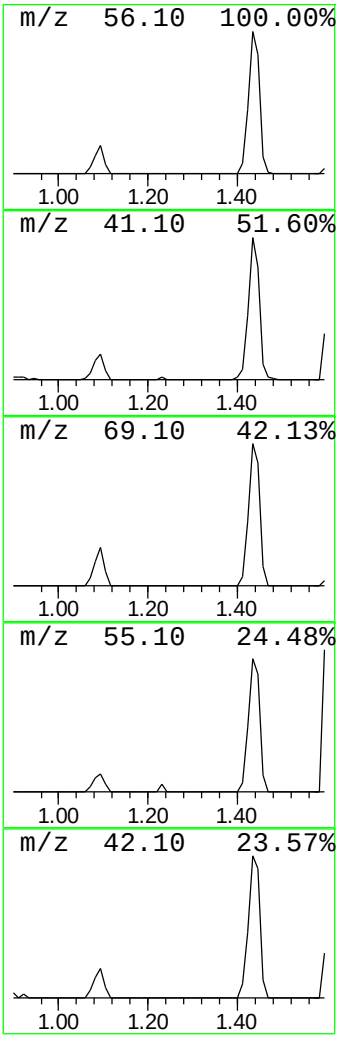
Peak Number 1 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.09	3.92 ng	45731	1,4-Dichlorobenzene-d4	7.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
5	Cyclobutane	56	C4H8	000287-23-0	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031715\
Data File : BF077784.D
Acq On : 17 Mar 2015 21:11
Operator : TP/IZ
Sample : G1544-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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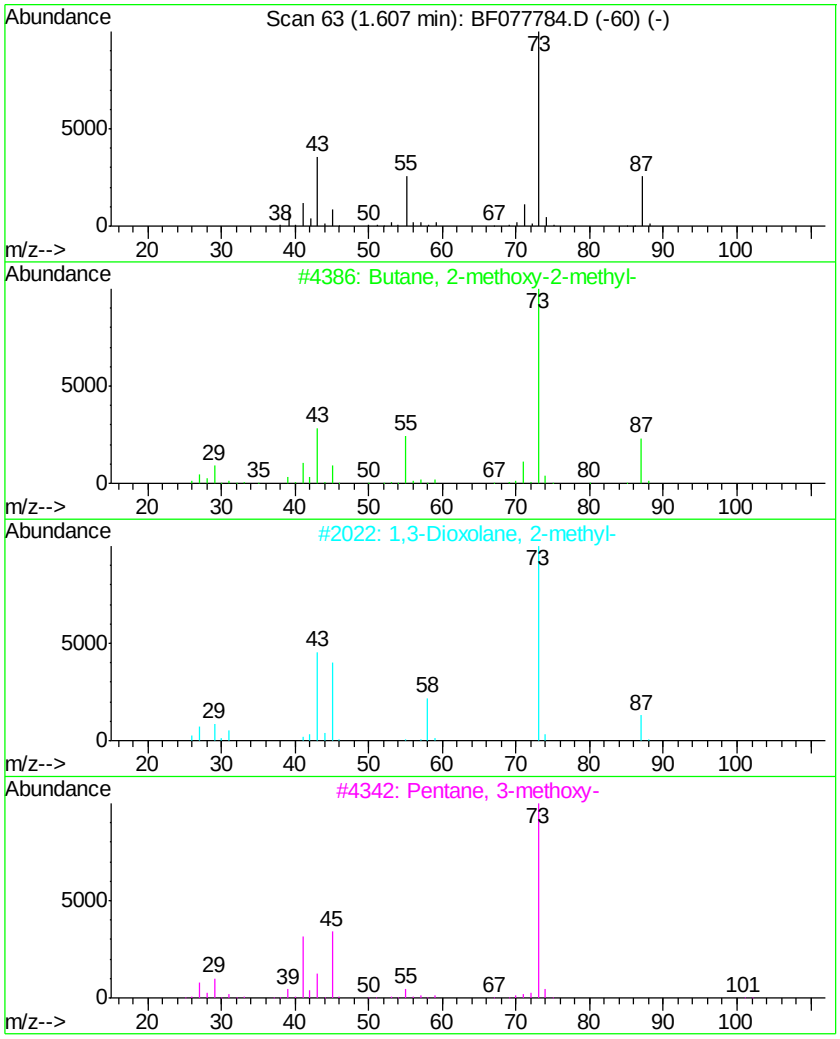
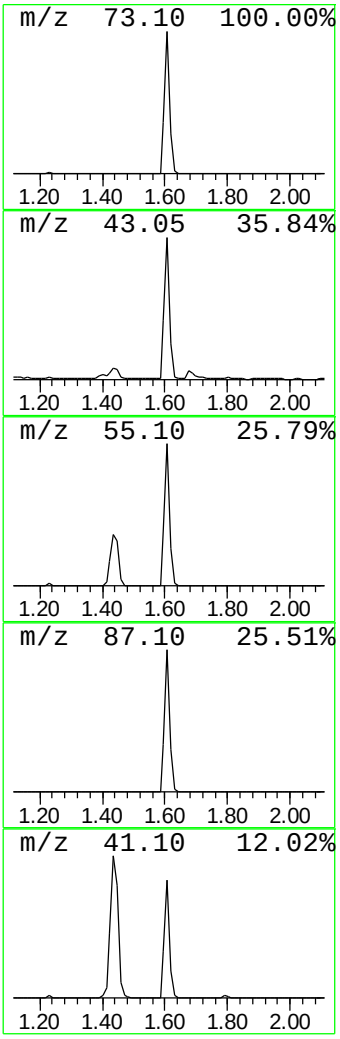
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.61	41.92 ng	489572	1,4-Dichlorobenzene-d4	7.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031715\
Data File : BF077784.D
Acq On : 17 Mar 2015 21:11
Operator : TP/IZ
Sample : G1544-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

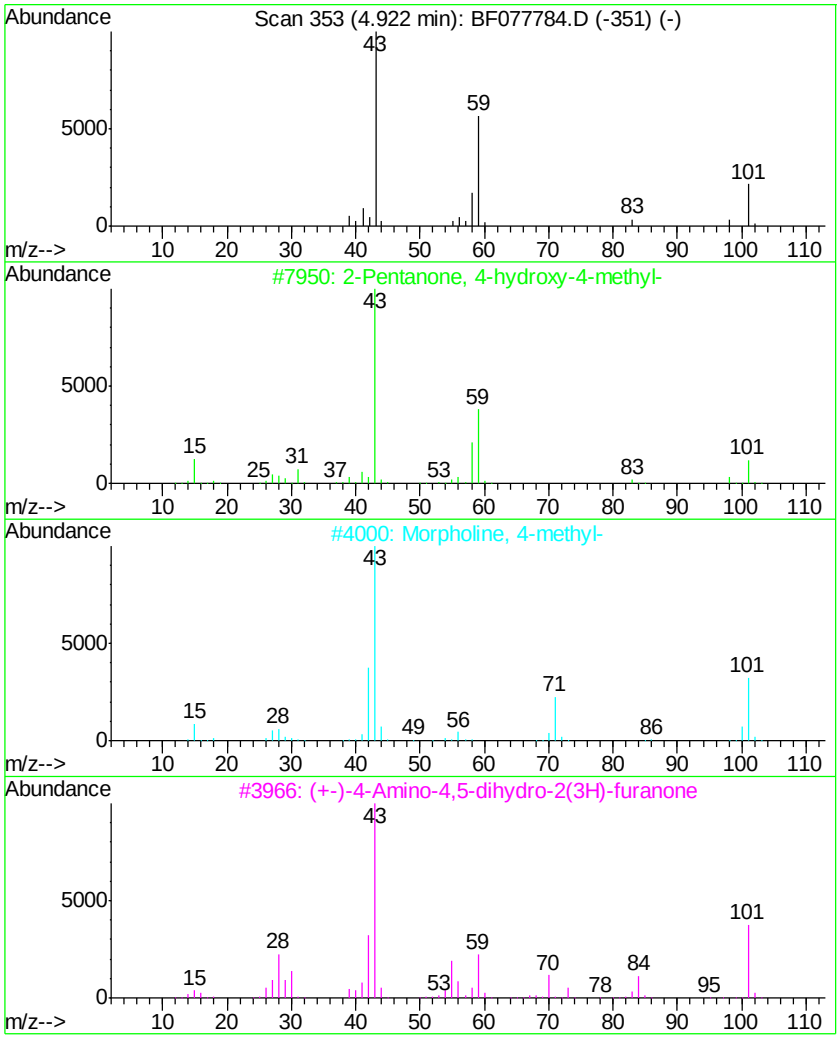
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

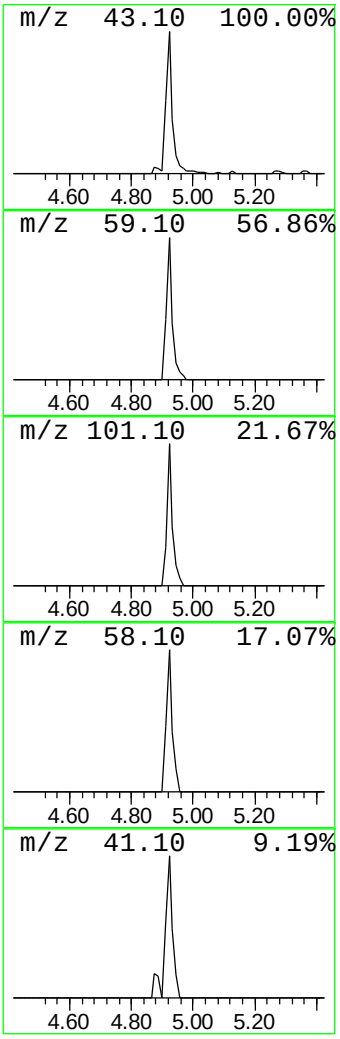
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	6.89 ng	80495	1,4-Dichlorobenzene-d4	7.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Operator : TP/IZ
Sample : G1544-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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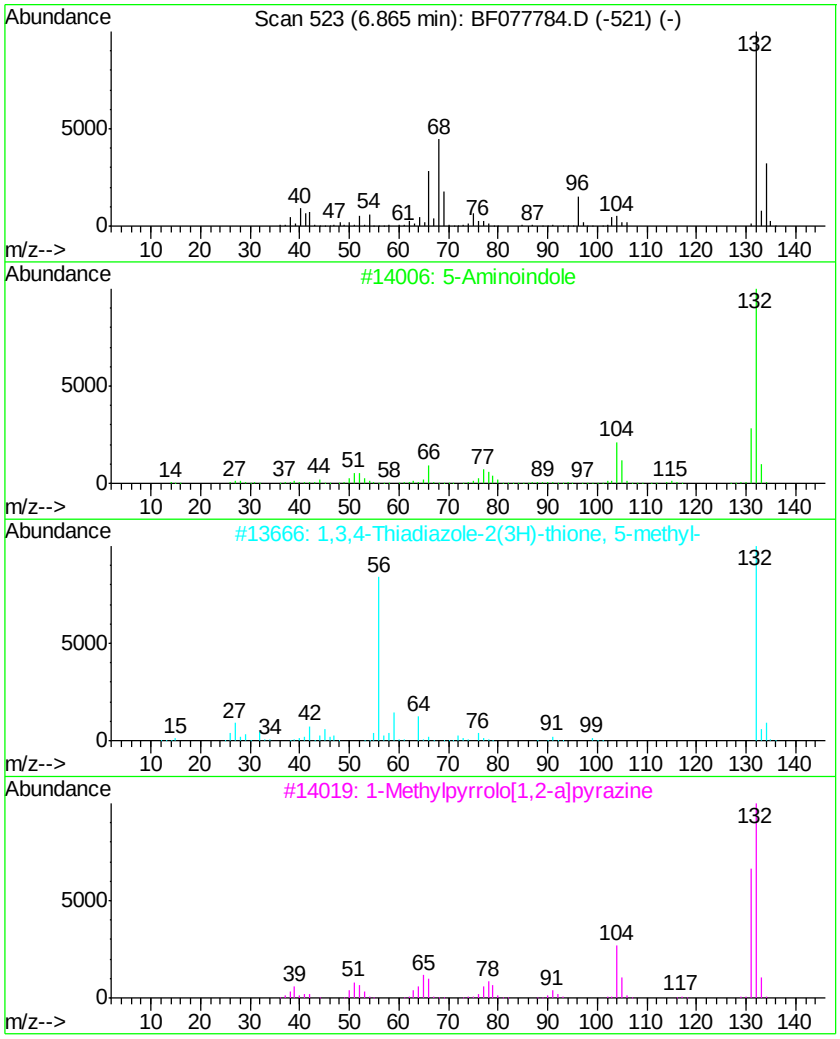
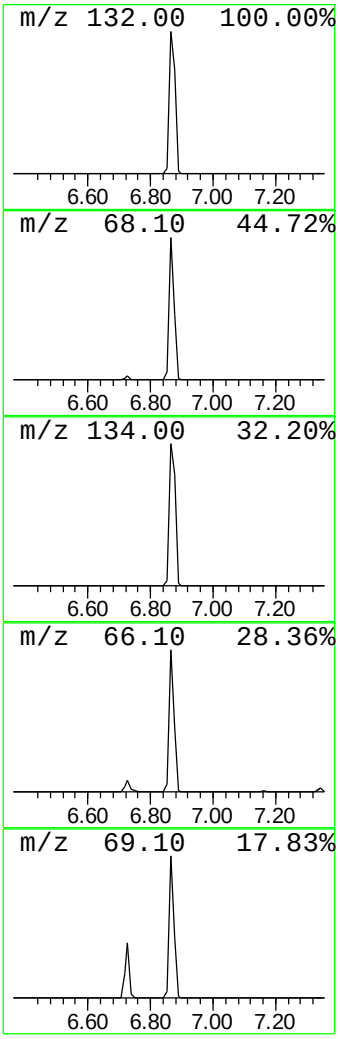
Peak Number 6 unknown6.86 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.86	91.00 ng	1062850	1,4-Dichlorobenzene-d4	7.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031715\
Data File : BF077784.D
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Operator : TP/IZ
Sample : G1544-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

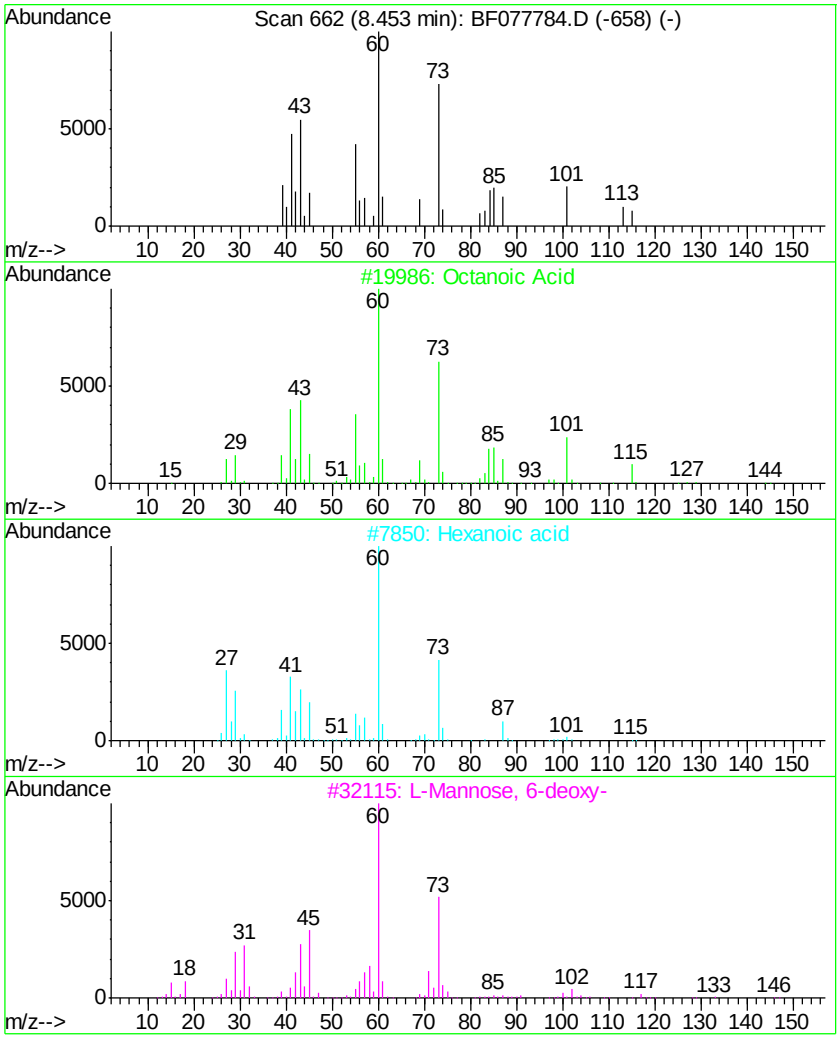
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

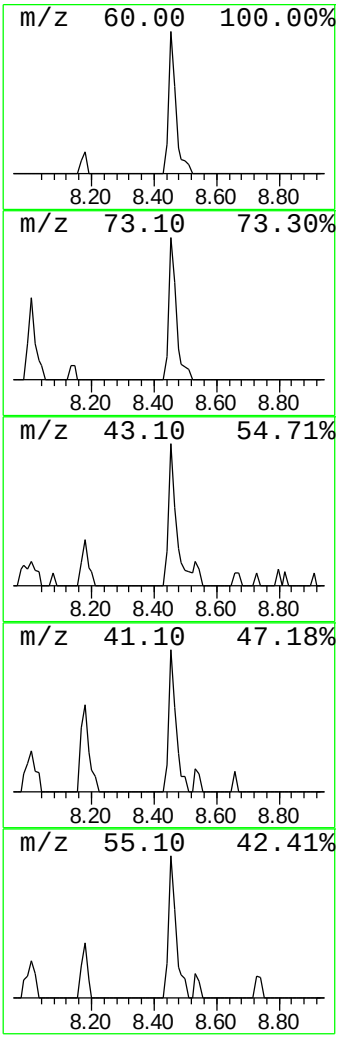
****

Peak Number 8 Octanoic Acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	3.49 ng	55011	Naphthalene-d8	8.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic Acid	144	C8H16O2	000124-07-2	90
2	Hexanoic acid	116	C6H12O2	000142-62-1	50
3	L-Mannose, 6-deoxy-	164	C6H12O5	003615-41-6	37
4	D-Galactose, 6-deoxy-	164	C6H12O5	003615-37-0	25
5	4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	25





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Operator : TP/IZ
Sample : G1544-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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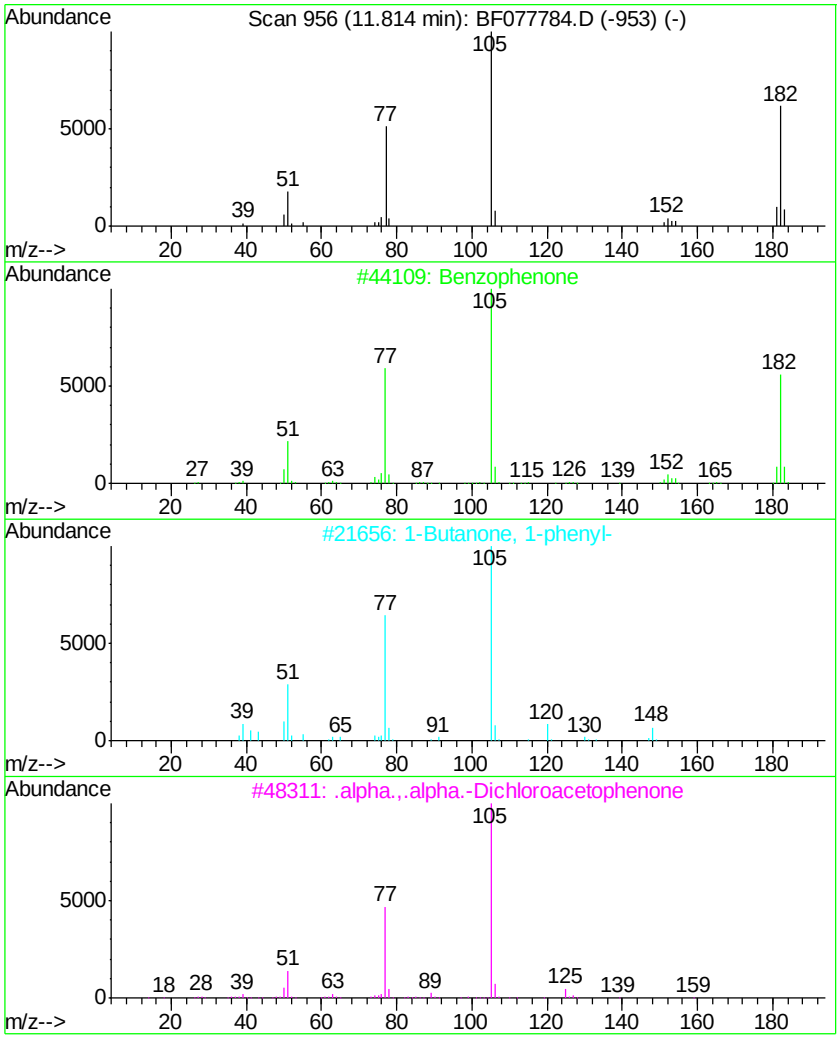
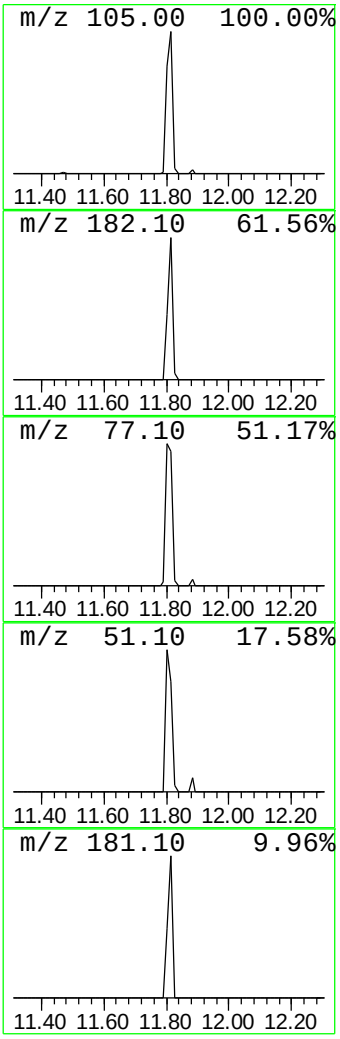
Peak Number 9 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	6.19 ng	112367	Acenaphthene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	43
3	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	43
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
5	Methanone, (4-chlorophenyl)(3-be...	311	C17H10ClNO3	1000276-36-3	43





Tentatively Identified Compound (LSC) summary

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Acq On : 17 Mar 2015 21:11
Operator : TP/IZ
Sample : G1544-10
Misc :
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Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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
Cyclopentane, met...	1.09	3.9	ng	45731	1	7.16	233594	20.0
Butane, 2-methoxy...	1.61	41.9	ng	489572	1	7.16	233594	20.0
2-Pentanone, 4-hy...	4.92	6.9	ng	80495	1	7.16	233594	20.0
unknown6.86	6.86	91.0	ng	1062850	1	7.16	233594	20.0
Octanoic Acid	8.45	3.5	ng	55011	2	8.74	315332	20.0
Benzophenone	11.81	6.2	ng	112367	3	10.90	363018	20.0