LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

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-BF103015.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	5.230	269	275	278	rVB	20619275	55179108	100.00%	37.358%
2	5.504	293	299	301	rBV	2076944	2208716	4.00%	1.495%
3	5.767	317	322	324	rVB2	1537606	2495436	4.52%	1.690%
4	6.133	352	354	357	rBV	925625	856841	1.55%	0.580%
5	6.522	386	388	390	rBV	921709	1637909	2.97%	1.109%
6	6.567	390	392	394	rBV	1593294	3909904	7.09%	2.647%
7	6.670	399	401	405	rVB	3938061	3741789	6.78%	2.533%
8	6.899	419	421	425	rBV2	1373050	2393305	4.34%	1.620%
9	7.059	432	435	439	rBV2	3938494	7179019	13.01%	4.860%
10	7.470	467	471	474	rVV2	4285730	5991592	10.86%	4.057%
11	7.596	478	482	484	rBV	4556612	5705869	10.34%	3.863%
12	7.756	488	496	498	rBV2	488180	589217	1.07%	0.399%
13	8.190	528	534	536	rBV	2382405	2680375	4.86%	1.815%
14	8.236	536	538	540	rVV	1004211	916721	1.66%	0.621%
15	8.762	583	584	586	rVB	760368	773787	1.40%	0.524%
16	8.819	586	589	592	rBV3	267515	610957	1.11%	0.414%
17	8.956	598	601	602	rBV2	535223	636412	1.15%	0.431%
18	8.990	602	604	605	rVB	1225857	1059160	1.92%	0.717%
19	9.162	617	619	622	rVV	1367421	1894328	3.43%	1.283%
20	9.276	625	629	631	rVB	9275690	9185843	16.65%	6.219%
21	9.402	636	640	642	rBV	620180	707766	1.28%	0.479%
22	9.493	645	648	651	rVV	6510590	6514607	11.81%	4.411%
23	9.950	685	688	690	rVB	2431998	2328483	4.22%	1.576%
24	10.739	754	757	758	rVV	3529599	4193654	7.60%	2.839%
25	10.831	762	765	767	rBV	4708629	4304492	7.80%	2.914%
26	11.436	815	818	820	rBV	2005797	2188050	3.97%	1.481%
27	11.973	863	865	867	rBV	1101223	1045490	1.89%	0.708%
28	12.145	877	880	883	rBV	1544535	1925723	3.49%	1.304%
29	12.716	928	930	932	rVV	2917464	2482506	4.50%	1.681%
30	12.762	932	934	936	rVV	849404	845932	1.53%	0.573%
31	13.025	954	957	960	rVB	6589423	7192260	13.03%	4.869%
32	13.814	1022	1026	1030	rBV2	300042	760434	1.38%	0.515%
33	13.928	1034	1036	1039	rVB	513398	584306	1.06%	0.396%
34	14.077	1046	1049	1051	rBV	1810184	1817535	3.29%	1.231%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

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-BF103015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.540	1174	1177	1180	rBV	962067	1164451	2.11%	0.788%

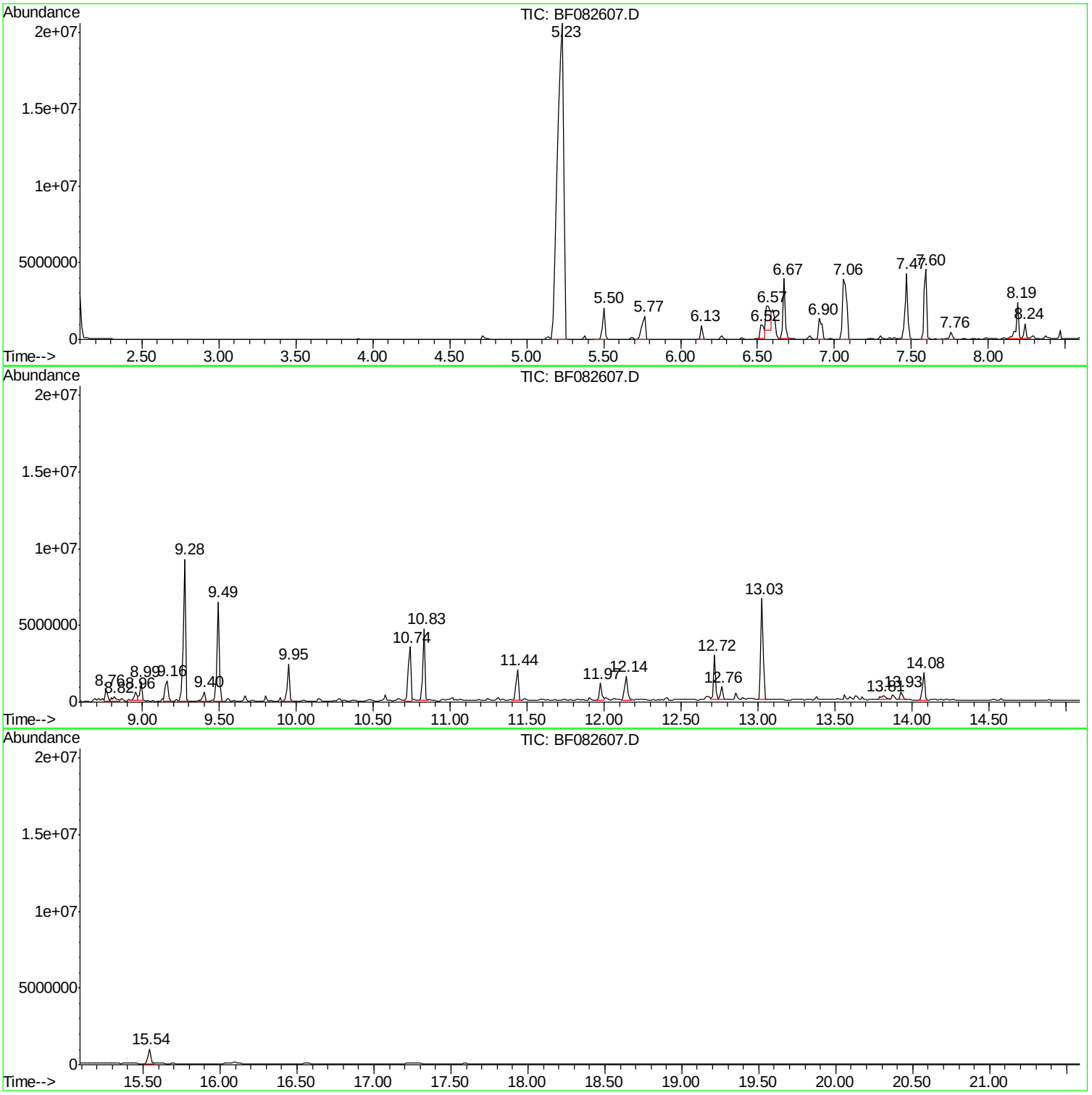
Sum of corrected areas: 147701977

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

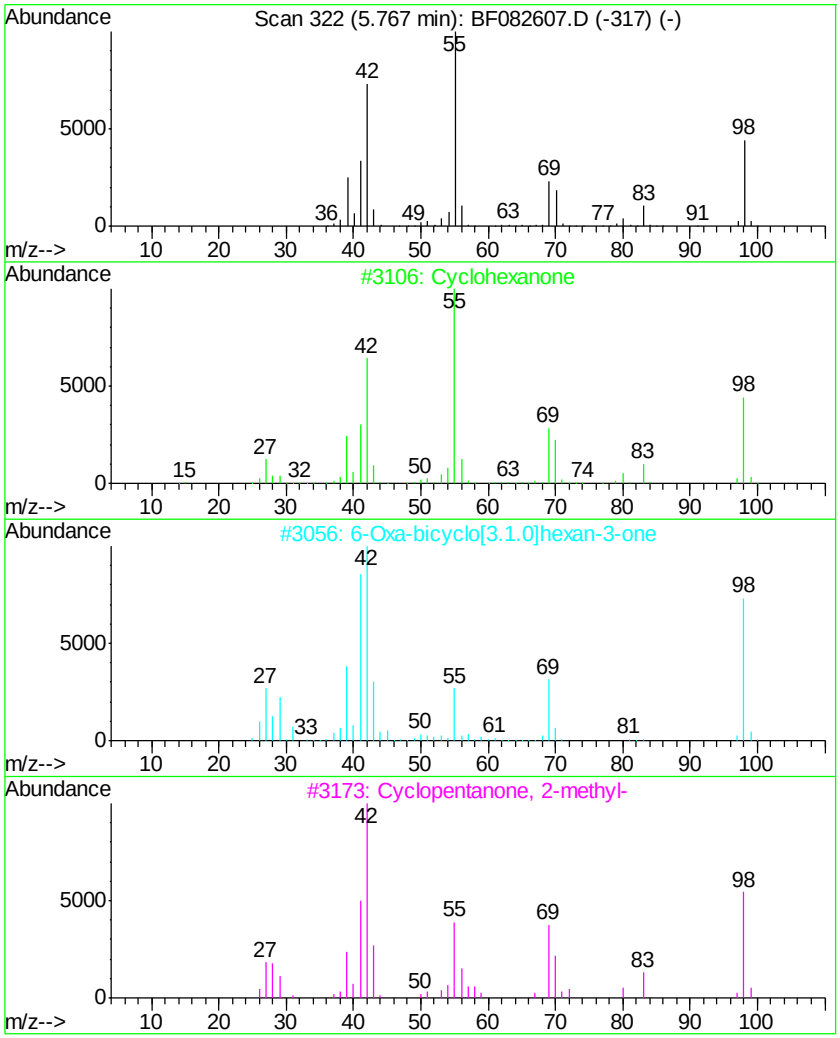
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

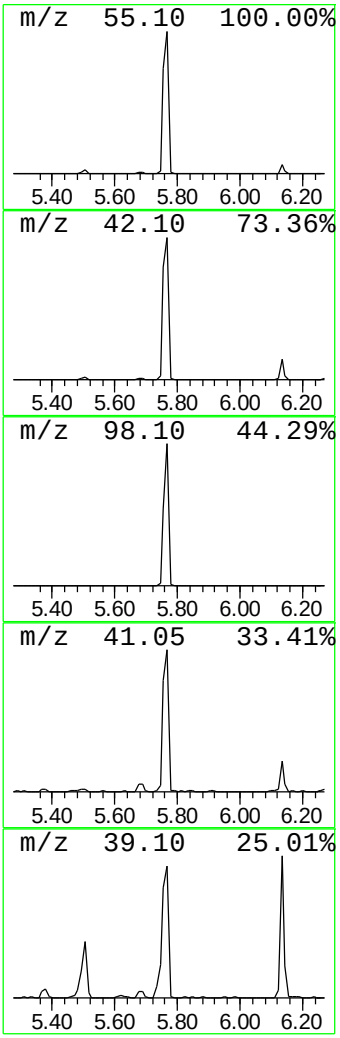
****

Peak Number 2 Cyclohexanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	20.85 ng	2495440	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	94
2	6-Oxa-bicyclo[3.1.0]hexan-3-one	98	C5H6O2	074017-10-0	53
3	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	50
4	1-Pentene	70	C5H10	000109-67-1	43
5	Cyclohexane, methyl-	98	C7H14	000108-87-2	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

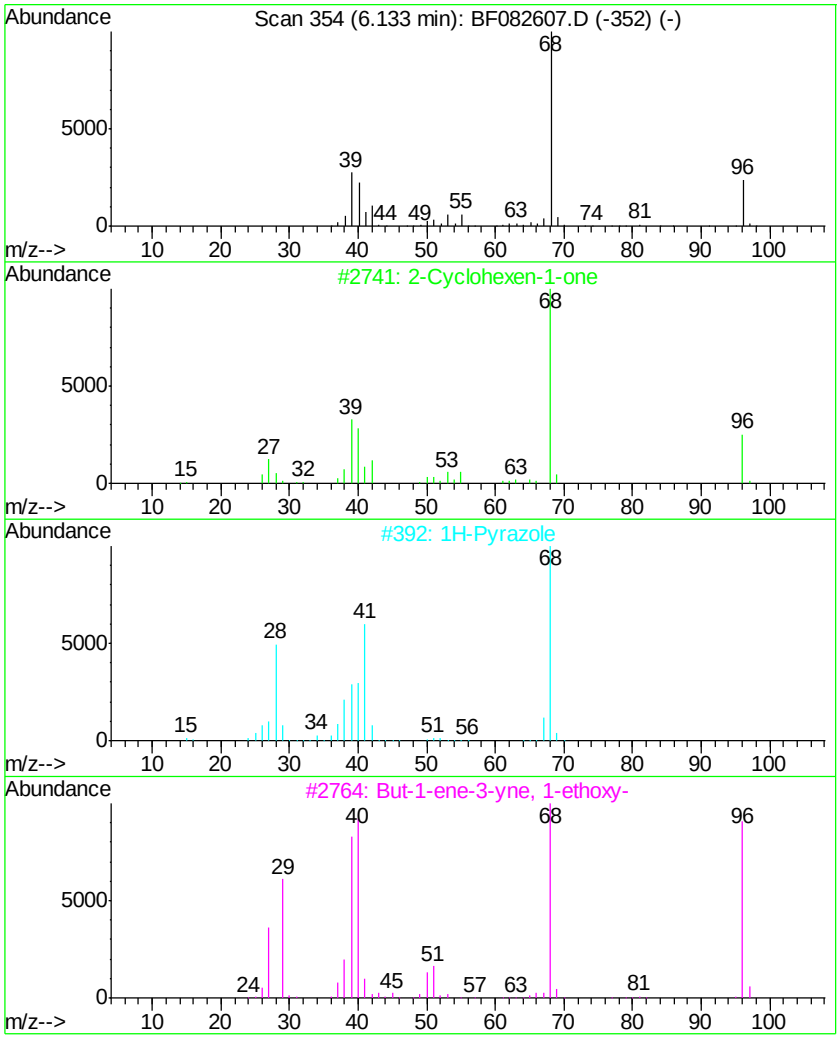
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

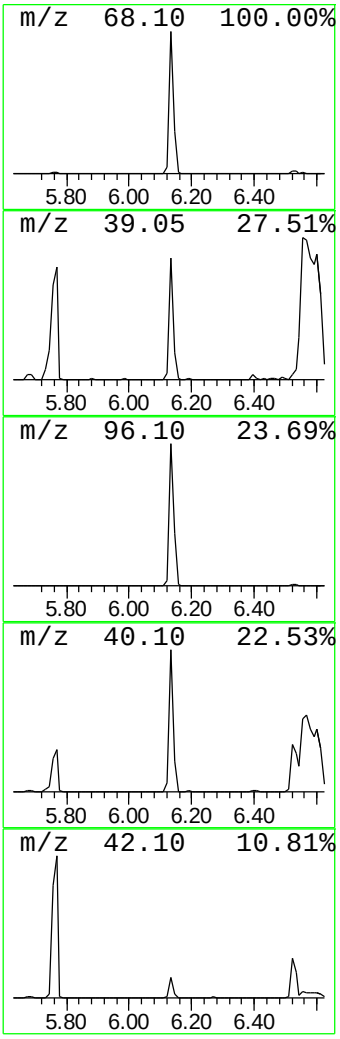
****

Peak Number 3 2-Cyclohexen-1-one Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.13	7.16 ng	856841	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	94
2	1H-Pyrazole	68	C3H4N2	000288-13-1	36
3	But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	14
4	7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	12
5	1,5-Cyclooctadien-4-one	122	C8H10O	001460-21-5	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

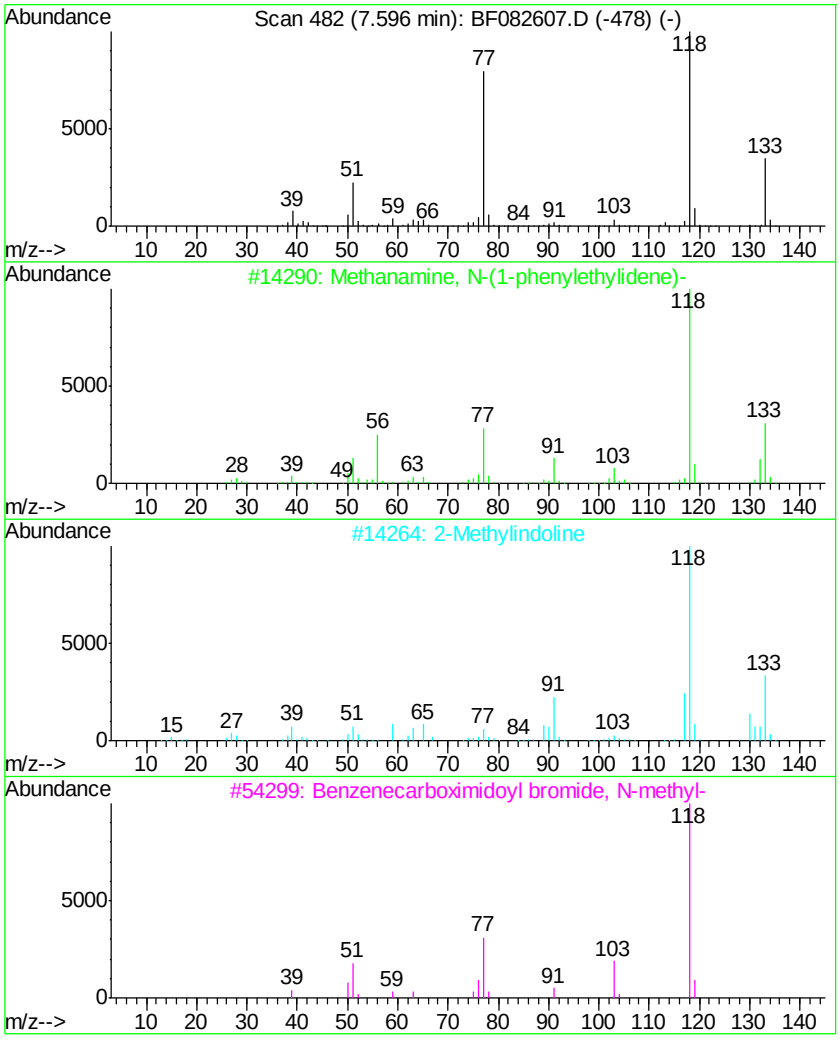
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

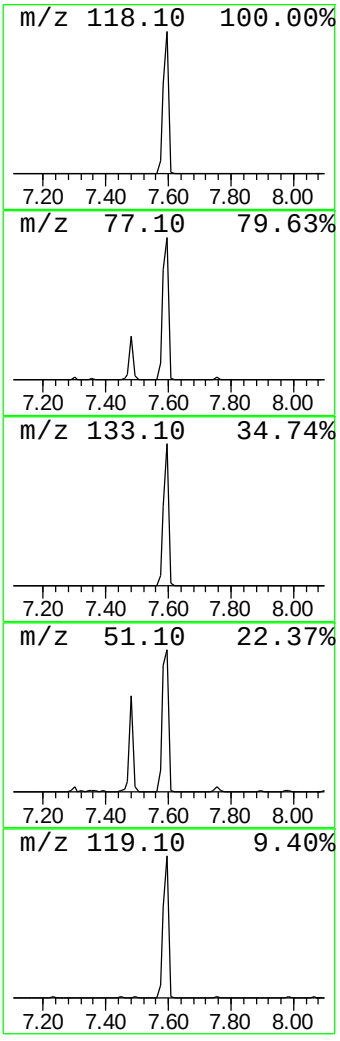
****

Peak Number 4 unknown7.60 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	42.58 ng	5705870	Naphthalene-d8	8.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanamine, N-(1-phenylethylide...	133	C9H11N	006907-71-7	40
2	2-Methylindoline	133	C9H11N	006872-06-6	38
3	Benzenecarboximidoyl bromide, N-...	197	C8H8BrN	041182-85-8	37
4	1H-Indazole	118	C7H6N2	000271-44-3	27
5	Ethanone, 1-phenyl-, o-(4-coumar...	279	C17H13NO3	034605-11-3	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

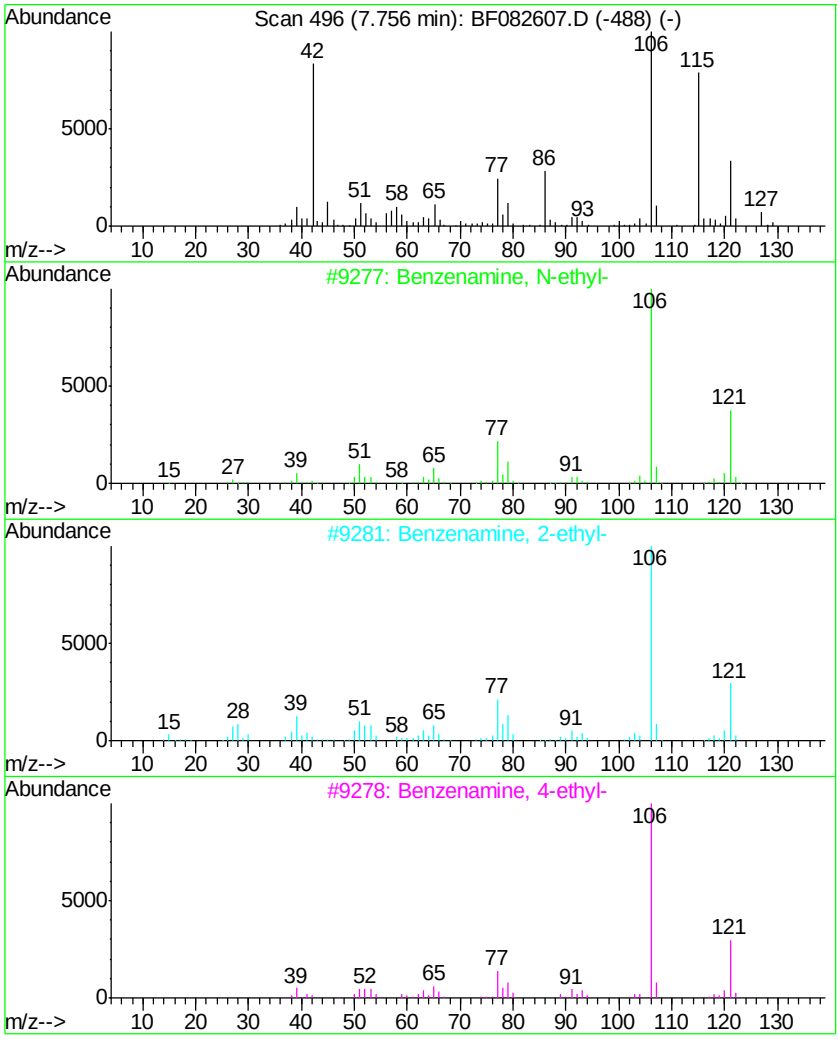
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

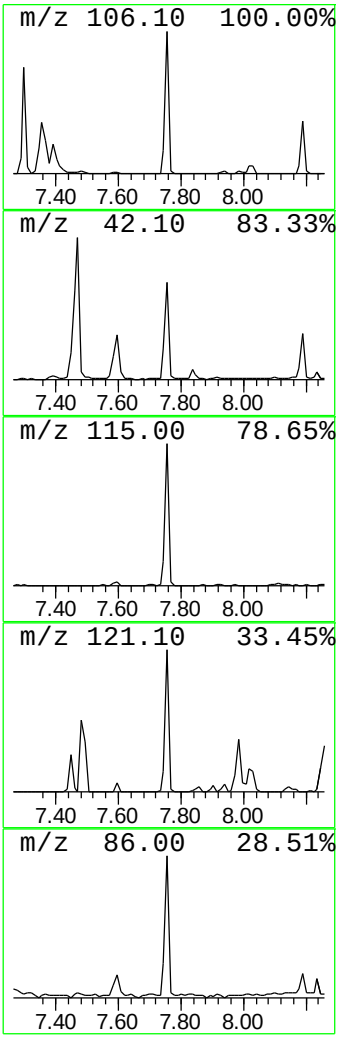
****

Peak Number 5 Benzenamine, N-ethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.76	4.40 ng	589217	Naphthalene-d8	8.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, N-ethyl-	121	C8H11N	000103-69-5	86
2	Benzenamine, 2-ethyl-	121	C8H11N	000578-54-1	42
3	Benzenamine, 4-ethyl-	121	C8H11N	000589-16-2	38
4	3-Methyl-2,5-oxazolidine-dione	115	C4H5NO3	005840-76-6	38
5	Pyridine, 3-ethyl-4-methyl-	121	C8H11N	000529-21-5	22





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

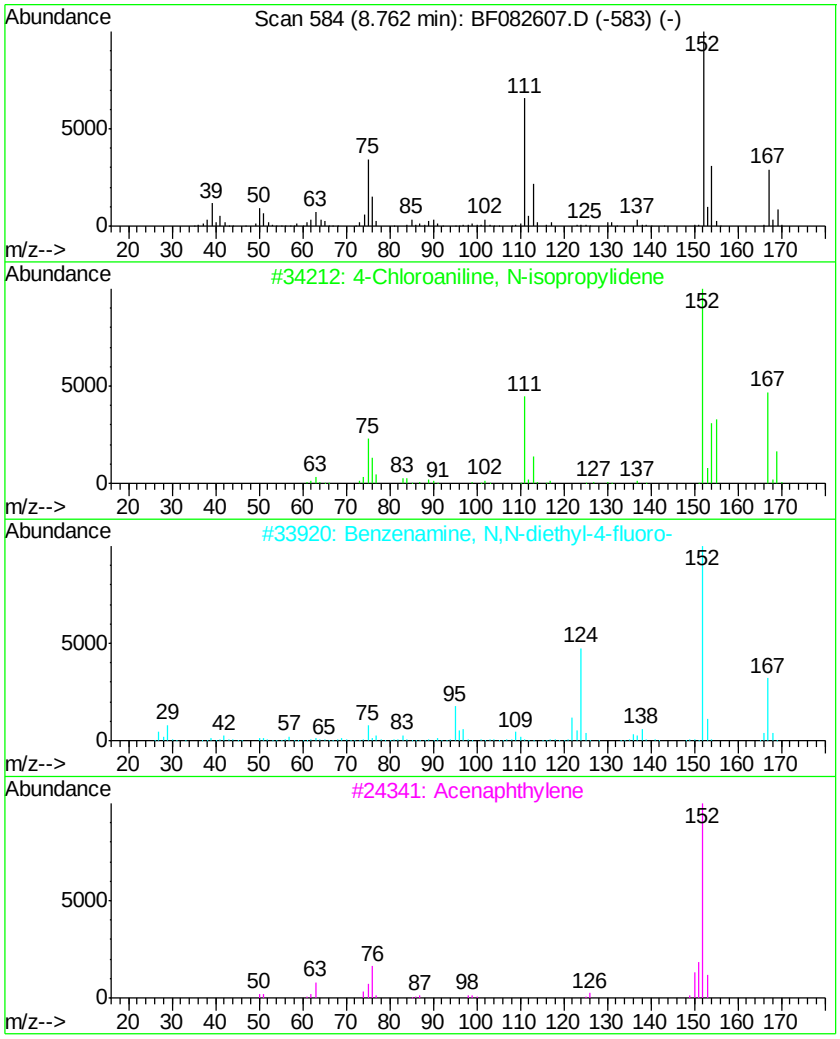
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

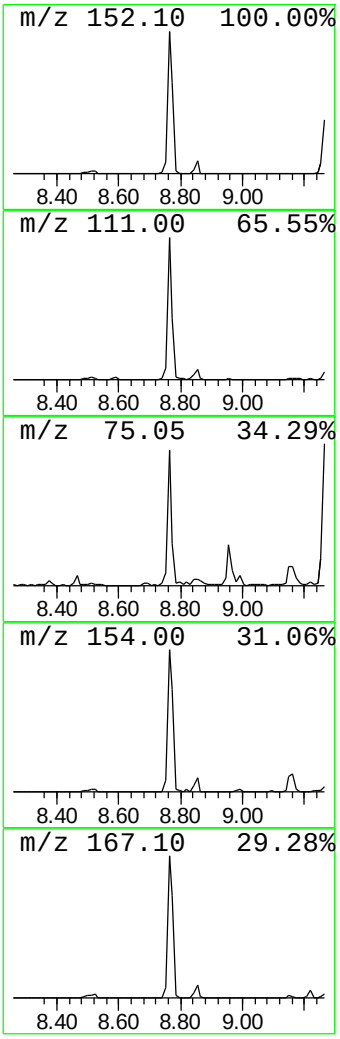
****

Peak Number 6 4-Chloroaniline, N-isopropy... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	5.77 ng	773787	Naphthalene-d8	8.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloroaniline, N-isopropylidene	167	C9H10ClN	040938-43-0	95
2	Benzenamine, N,N-diethyl-4-fluoro-	167	C10H14FN	000347-39-7	38
3	Acenaphthylene	152	C12H8	000208-96-8	38
4	6-Chloroanthranilonitrile	152	C7H5ClN2	006575-11-7	38
5	Pyridine, 3-trimethylsiloxy-	167	C8H13NOSi	041571-88-4	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

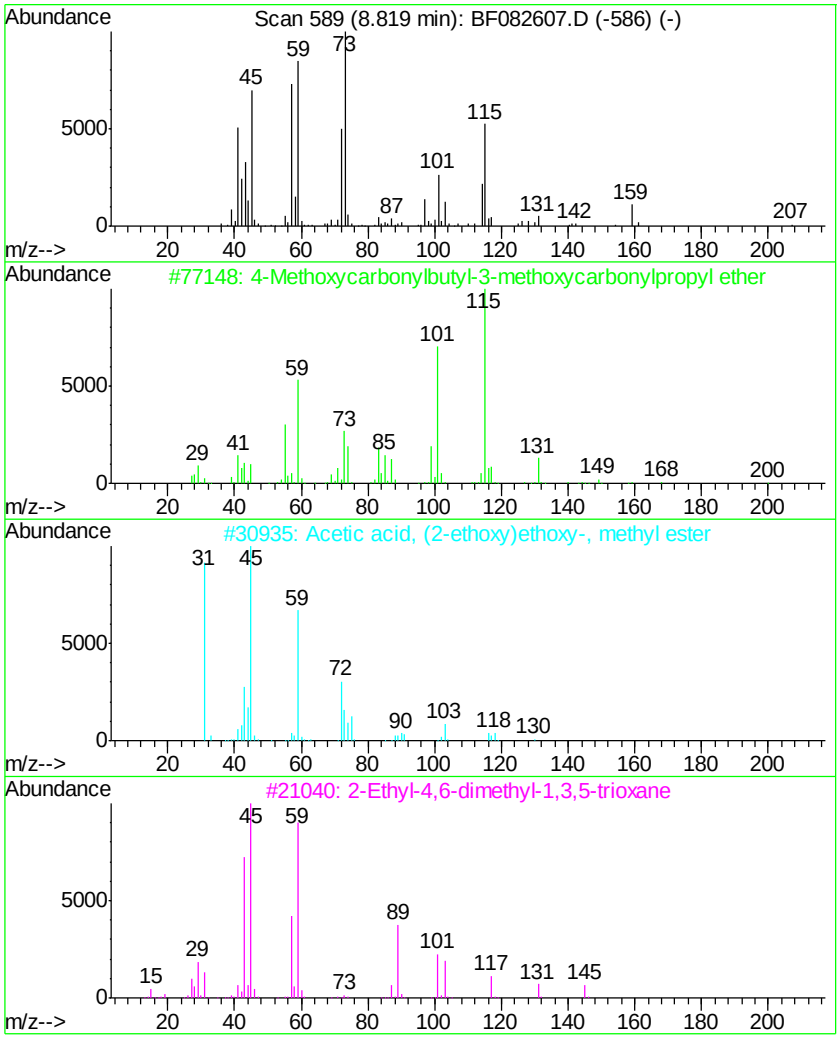
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

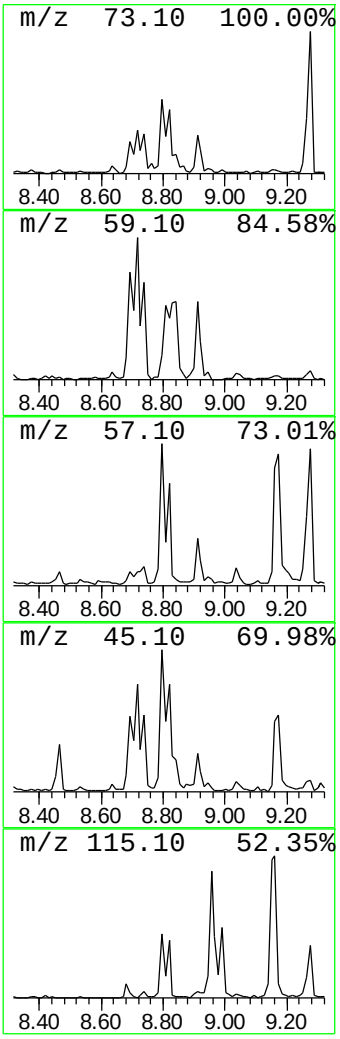
****

Peak Number 7 unknown8.82 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.82	4.56 ng	610957	Naphthalene-d8	8.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methoxycarbonylbutyl-3-methoxy...	232	C11H20O5	017361-53-4	38
2	Acetic acid, (2-ethoxy)ethoxy-, ...	162	C7H14O4	016326-34-4	38
3	2-Ethyl-4,6-dimethyl-1,3,5-trioxane	146	C7H14O3	024261-86-7	35
4	.alpha.-D-Galactopyranoside, met...	235	C9H17NO6	006082-22-0	32
5	Propanedioic acid, methyl-, dime...	146	C6H10O4	000609-02-9	32





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

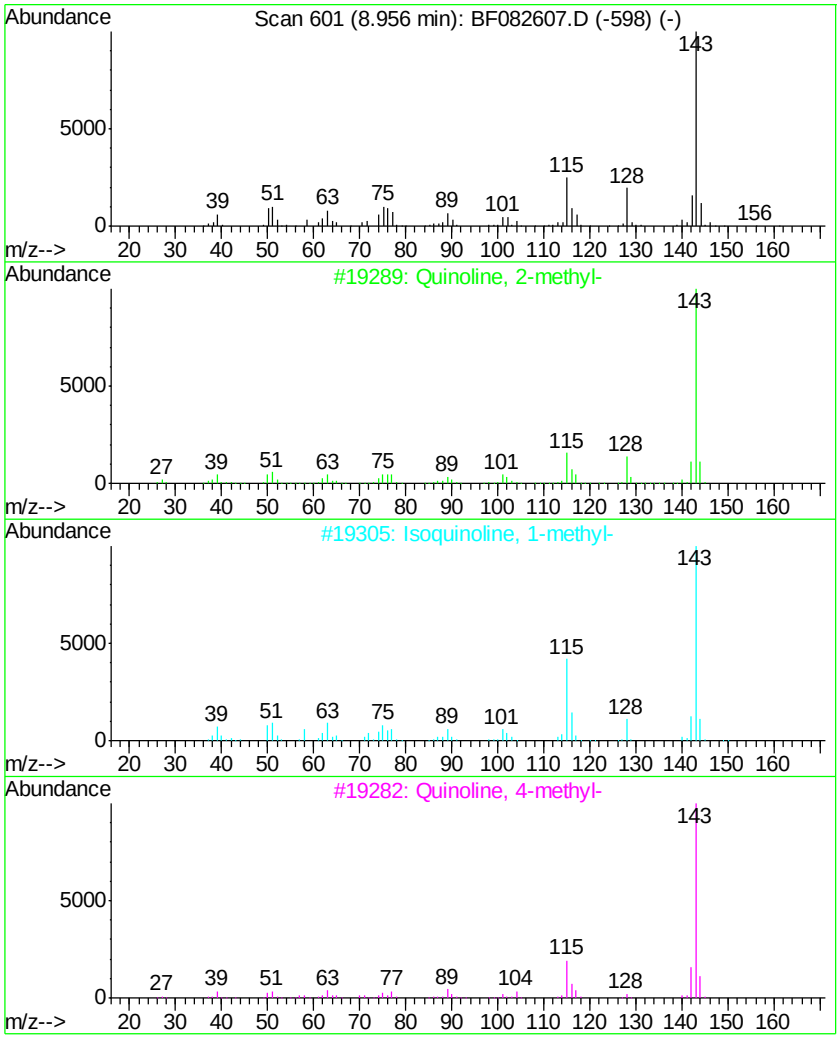
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

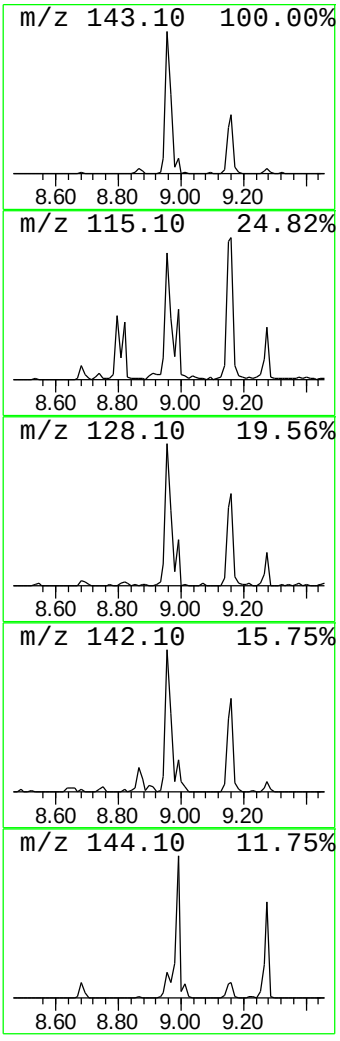
****

Peak Number 8 Quinoline, 2-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	4.75 ng	636412	Naphthalene-d8	8.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline, 2-methyl-	143	C10H9N	000091-63-4	94
2	Isoquinoline, 1-methyl-	143	C10H9N	001721-93-3	87
3	Quinoline, 4-methyl-	143	C10H9N	000491-35-0	81
4	Isoquinoline, 3-methyl-	143	C10H9N	001125-80-0	81
5	Quinoline, 3-methyl-	143	C10H9N	000612-58-8	76





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

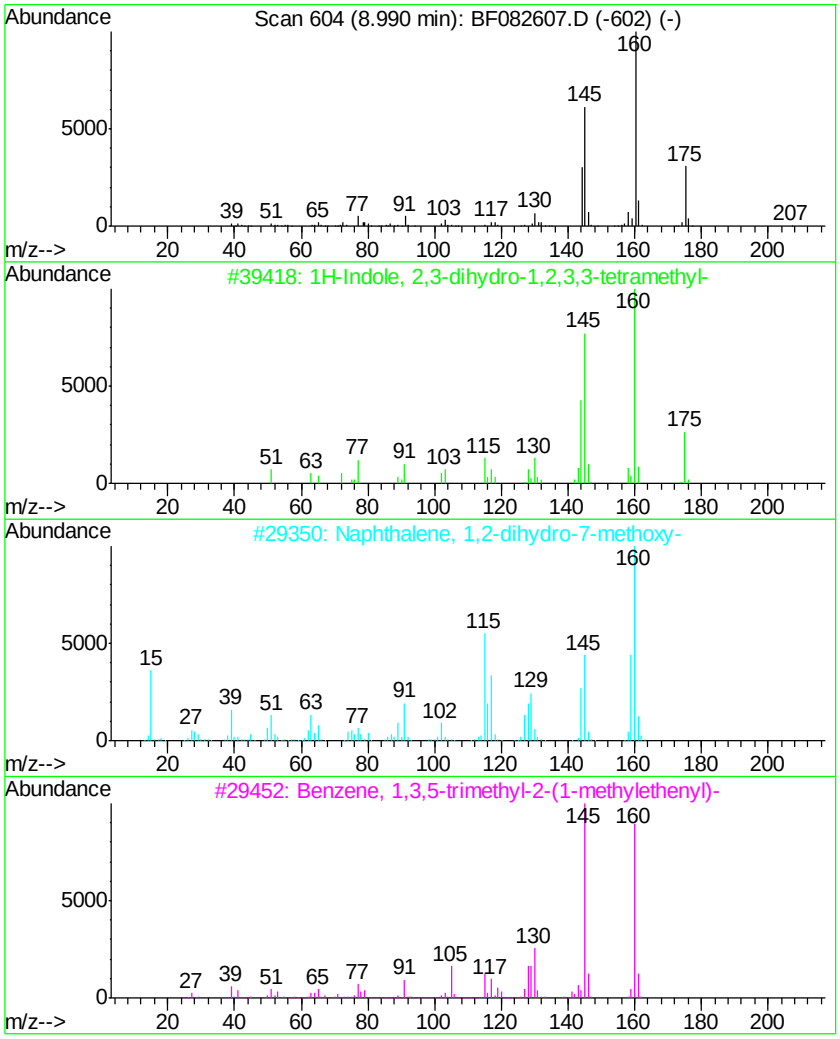
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

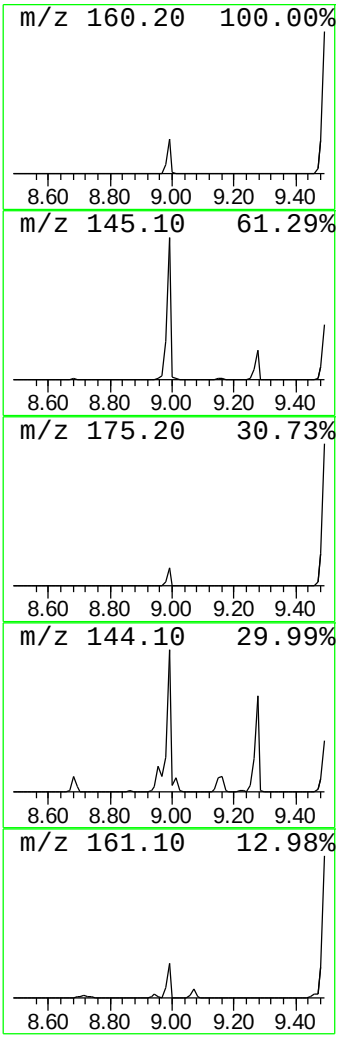
****

Peak Number 9 1H-Indole, 2,3-dihydro-1,2,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.99	7.90 ng	1059160	Naphthalene-d8	8.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2,3-dihydro-1,2,3,3-t...	175	C12H17N	013034-76-9	91
2	Naphthalene, 1,2-dihydro-7-methoxy-	160	C11H12O	052178-91-3	72
3	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	64
4	2,3-Dimethyl-1-phenylpyrrolidine	175	C12H17N	003783-58-2	53
5	Benzene, 4-chloro-2-fluoro-1-met...	160	C7H6ClFO	000452-09-5	53





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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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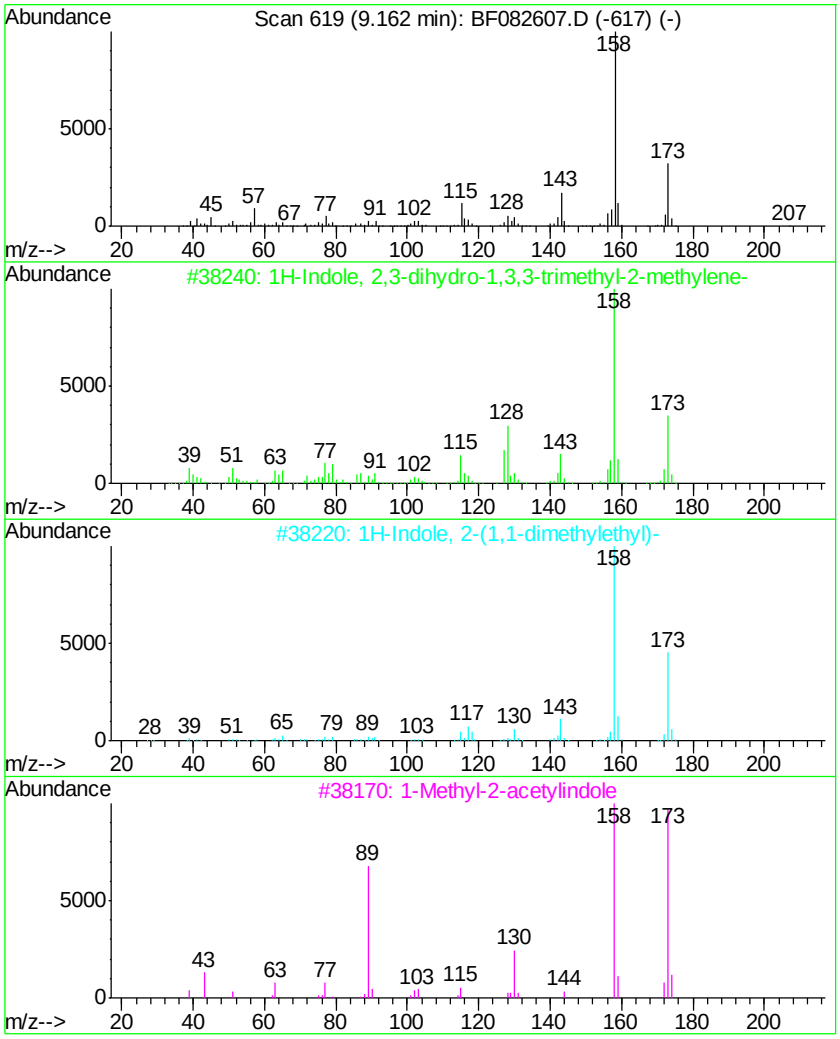
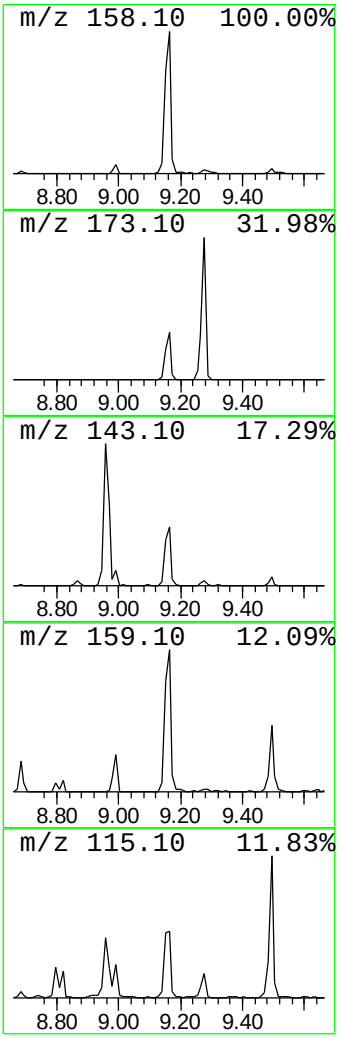
Peak Number 10 1H-Indole, 2,3-dihydro-1,3,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.16	16.27 ng	1894330	Acenaphthene-d10	9.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2,3-dihydro-1,3,3-tri...	173	C12H15N	000118-12-7	94
2	1H-Indole, 2-(1,1-dimethylethyl)-	173	C12H15N	001805-65-8	91
3	1-Methyl-2-acetylindole	173	C11H11NO	016498-68-3	72
4	4H-Pyrrolo[3,2,1-ij]quinoline, 1...	173	C12H15N	040135-93-1	64
5	2,4,4-Trimethyl-3,4-dihydroquino...	173	C12H15N	063177-93-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082607.D
Acq On : 31 Oct 2015 8:19
Operator : UM/IZ
Sample : G4192-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SYSDIS10282015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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
Cyclohexanone	5.77	20.9	ng	2495440	1	6.90	2393310	20.0
2-Cyclohexen-1-one	6.13	7.2	ng	856841	1	6.90	2393310	20.0
unknown7.60	7.60	42.6	ng	5705870	2	8.19	2680380	20.0
Benzenamine, N-et...	7.76	4.4	ng	589217	2	8.19	2680380	20.0
4-Chloroaniline, ...	8.76	5.8	ng	773787	2	8.19	2680380	20.0
unknown8.82	8.82	4.6	ng	610957	2	8.19	2680380	20.0
Quinoline, 2-methyl-	8.96	4.8	ng	636412	2	8.19	2680380	20.0
1H-Indole, 2,3-di...	8.99	7.9	ng	1059160	2	8.19	2680380	20.0
1H-Indole, 2,3-di...	9.16	16.3	ng	1894330	3	9.95	2328480	20.0