LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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-BF012417.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	5.562	302	304	307	rBV	1212597	1350246	3.60%	1.119%
2	6.613	393	396	399	rVV2	560476	1004095	2.68%	0.832%
3	6.670	399	401	403	rVB	432606	536787	1.43%	0.445%
4	6.739	404	407	409	rBV	2591727	2464724	6.57%	2.042%
5	6.967	425	427	429	rBV	1226002	1167861	3.12%	0.968%
6	7.127	438	441	443	rBV	2427928	2295977	6.12%	1.902%
7	7.242	450	451	455	rVB3	323823	487447	1.30%	0.404%
8	7.322	455	458	461	rBV4	384172	881680	2.35%	0.731%
9	7.413	464	466	469	rVB	449929	531304	1.42%	0.440%
10	7.505	472	474	475	rBV2	614535	810431	2.16%	0.672%
11	7.539	475	477	478	rBV	1763096	1737324	4.63%	1.440%
12	7.562	478	479	481	rBV2	635283	922074	2.46%	0.764%
13	7.665	486	488	492	rVB4	1279443	1887134	5.03%	1.564%
14	7.733	492	494	497	rVB2	497041	811697	2.17%	0.673%
15	7.802	497	500	501	rBV2	421996	710587	1.90%	0.589%
16	7.836	501	503	507	rVB2	981970	1742161	4.65%	1.444%
17	7.939	510	512	513	rBV	529601	550232	1.47%	0.456%
18	7.985	513	516	517	rBV3	384962	683027	1.82%	0.566%
19	8.099	521	526	528	rVB3	1070872	2151971	5.74%	1.783%
20	8.168	528	532	535	rBV5	824431	2401233	6.40%	1.990%
21	8.270	538	541	542	rBV	1185653	1470051	3.92%	1.218%
22	8.316	543	545	551	rVB5	1134434	2174318	5.80%	1.802%
23	8.408	551	553	557	rVB3	938350	2284469	6.09%	1.893%
24	8.522	557	563	564	rBV4	1420466	4544147	12.12%	3.765%
25	8.613	568	571	572	rBV2	1447628	2717839	7.25%	2.252%
26	8.728	578	581	582	rBV3	1023425	2032708	5.42%	1.684%
27	8.819	587	589	591	rBV	1487517	1771437	4.73%	1.468%
28	8.865	591	593	596	rVB3	1362006	3141594	8.38%	2.603%
29	8.945	596	600	604	rBV5	995832	3172674	8.46%	2.629%
30	9.048	604	609	612	rVB4	1699694	4625275	12.34%	3.832%
31	9.139	612	617	619	rBV5	1736333	6938120	18.51%	5.749%
32	9.333	632	634	635	rBV	1121428	1218210	3.25%	1.009%
33	13.128	964	966	1042	rVB	2298710	37490374	100.00%	31.064%
34	14.191	1057	1059	1123	rVB	1431775	20590003	54.92%	17.061%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.677	1186	1189	1202	rVB	593845	1387576	3.70%	1.150%

Sum of corrected areas: 120686787

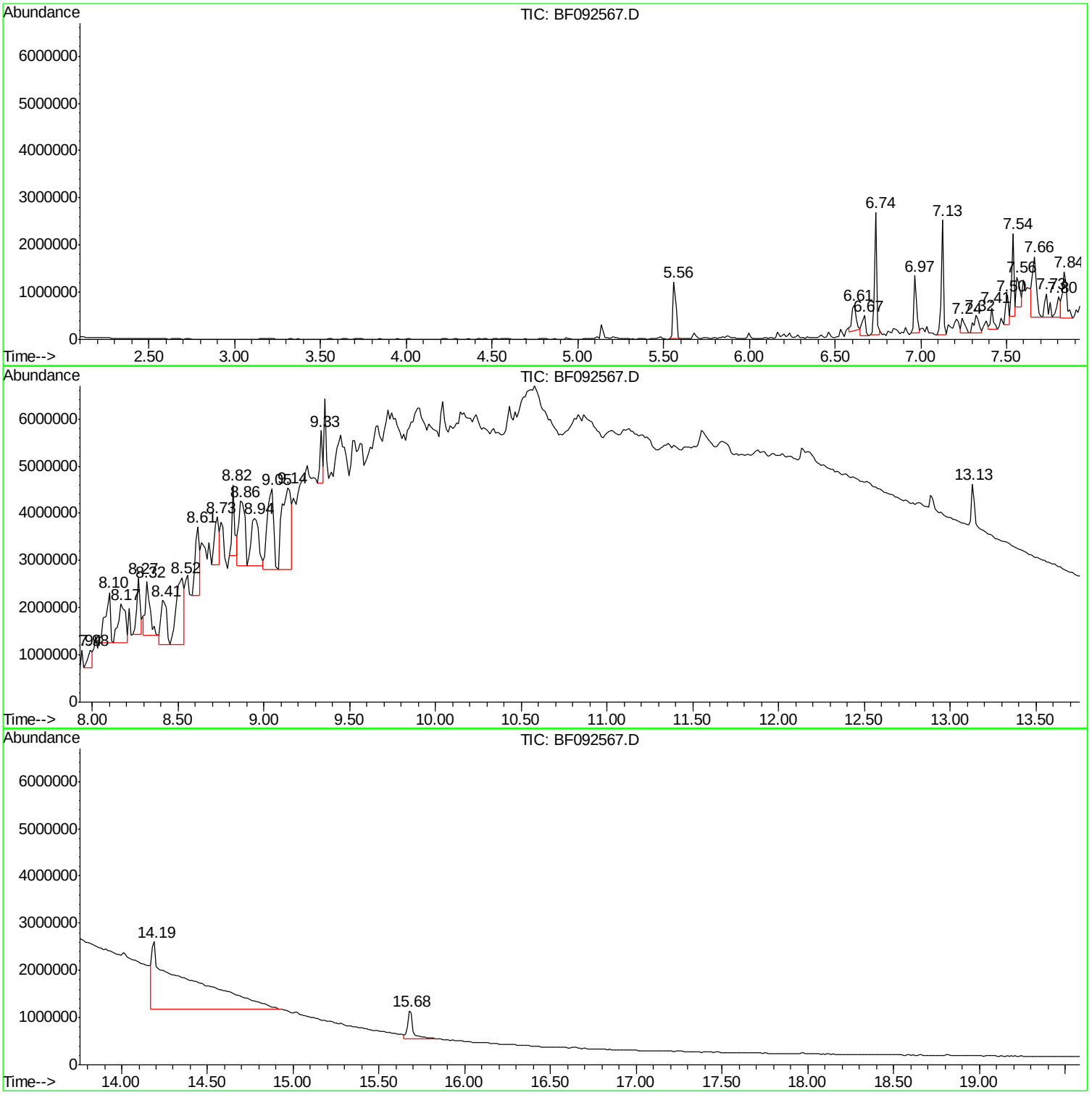
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

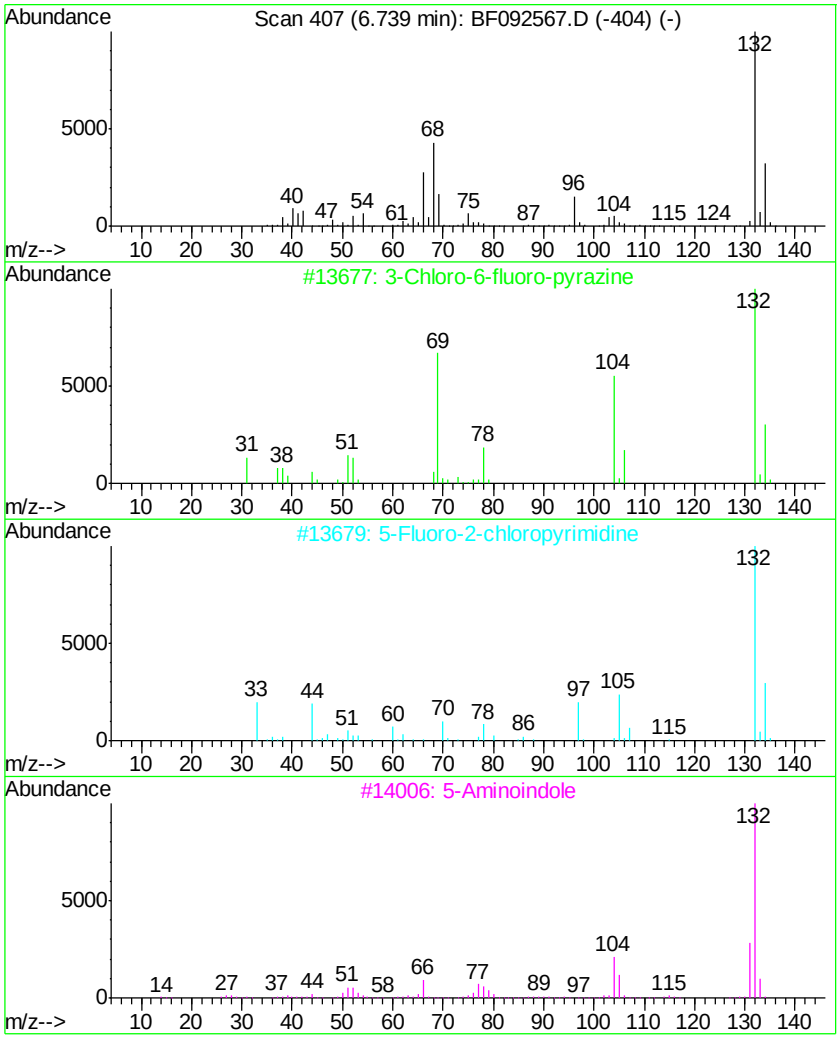
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

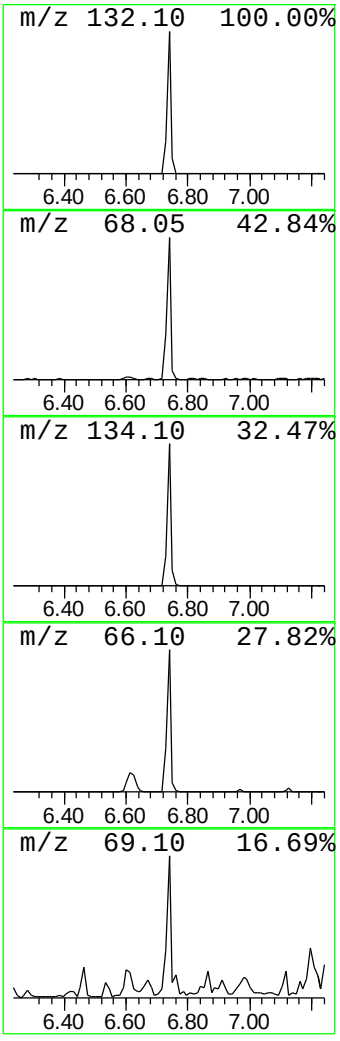
****

Peak Number 1 unknown6.74 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	42.21 ng	2464720	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

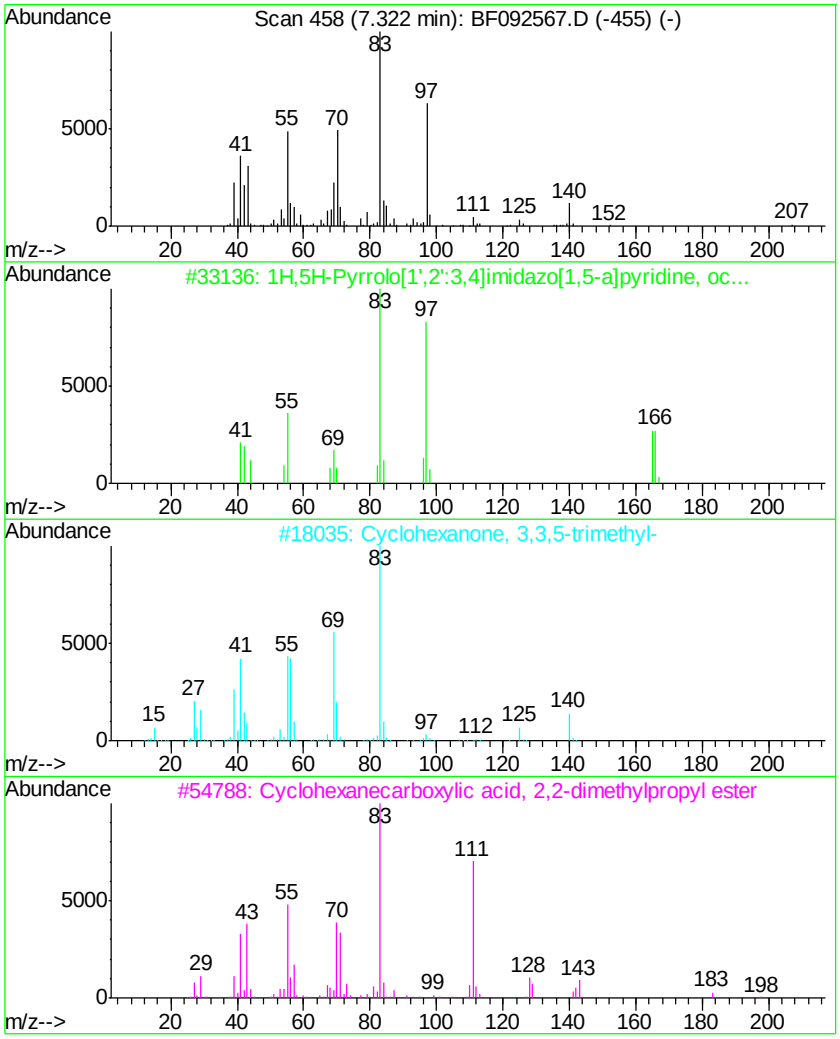
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

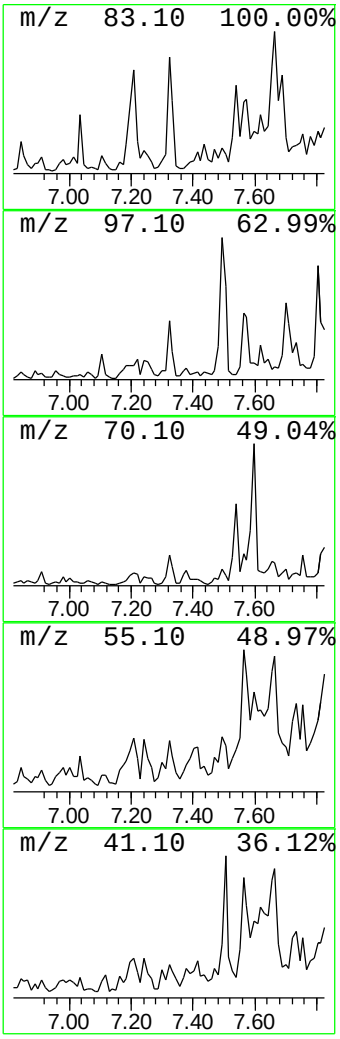
****

Peak Number 3 1H,5H-Pyrrolo[1',2':3,4]imi... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	15.10 ng	881680	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H,5H-Pyrrolo[1',2':3,4]imidazo[...	166	C10H18N2	054966-11-9	53
2	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	43
3	Cyclohexanecarboxylic acid, 2,2-...	198	C12H22O2	1000279-85-6	43
4	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	43
5	2-Butyl-1,2-azaborolidine	125	C7H16BN	005357-10-8	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

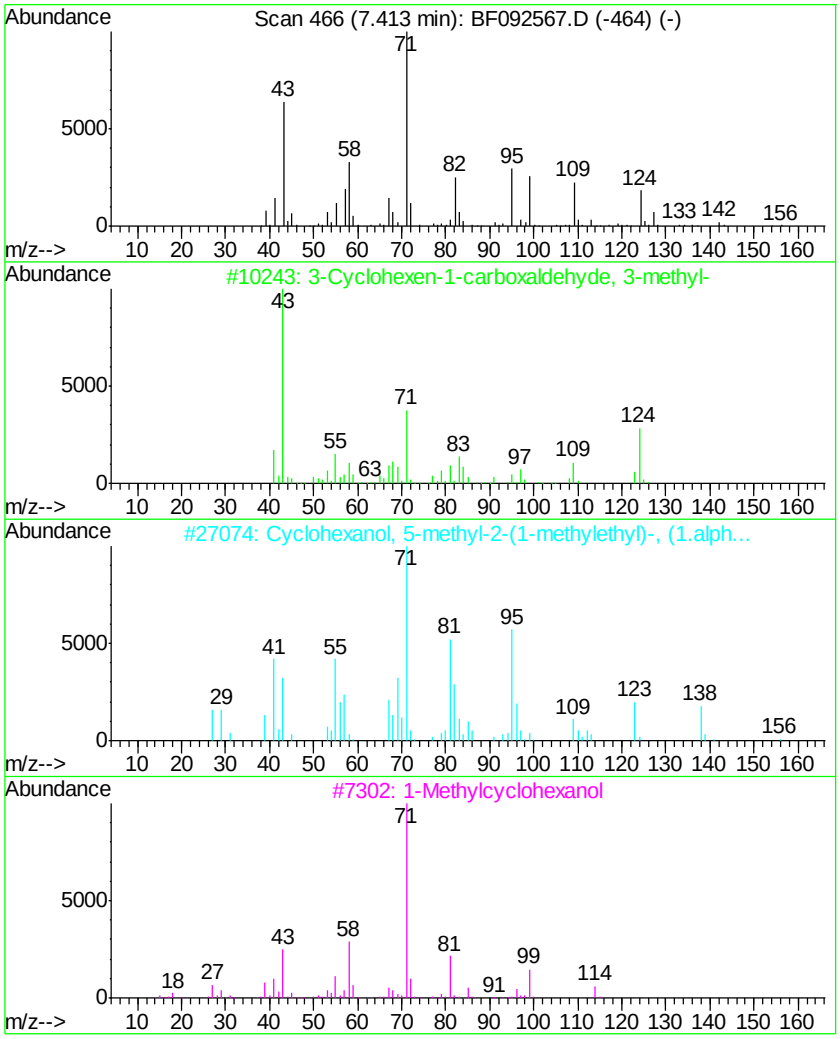
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

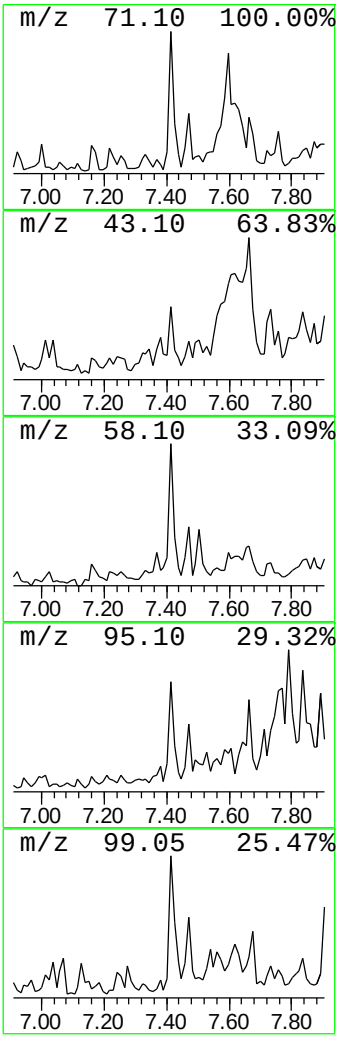
****

Peak Number 4 3-Cyclohexen-1-carboxaldehy... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	9.10 ng	531304	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexen-1-carboxaldehyde, 3...	124	C8H12O	056980-32-6	50
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	000491-02-1	47
3	1-Methylcyclohexanol	114	C7H14O	000590-67-0	37
4	Cyclopentanol, 1-methyl-	100	C6H12O	001462-03-9	35
5	1-Penten-3-ol, 3-methyl-	100	C6H12O	000918-85-4	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

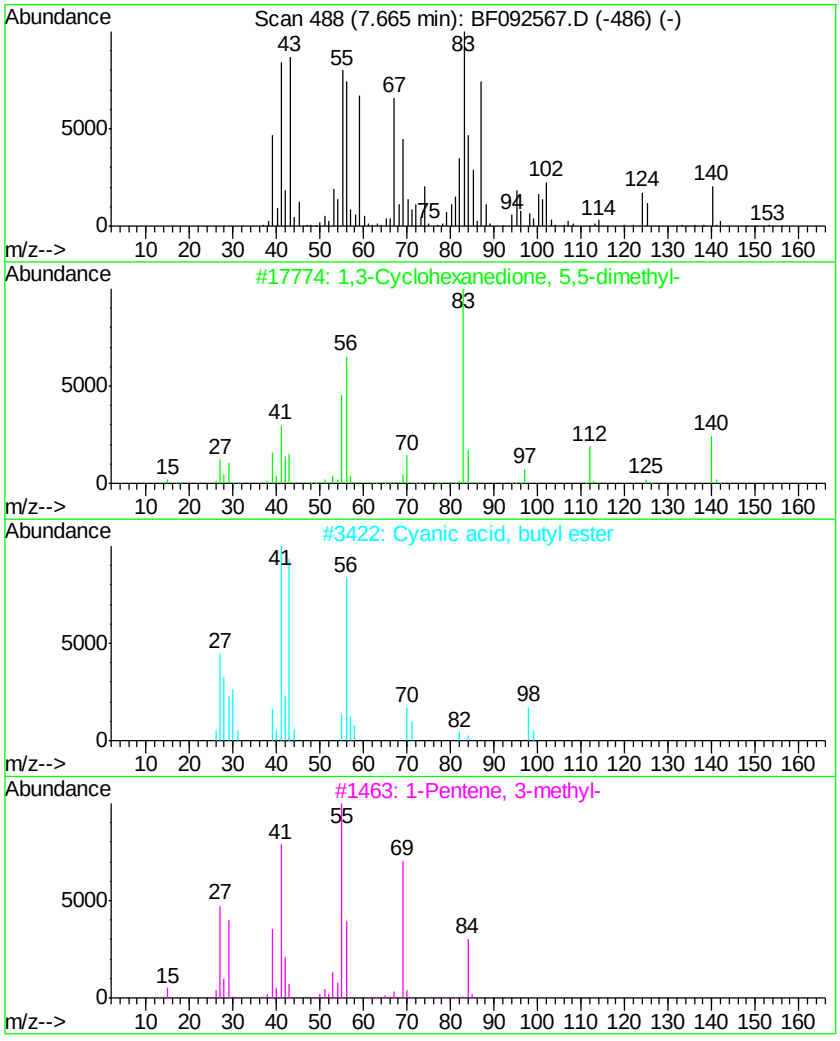
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

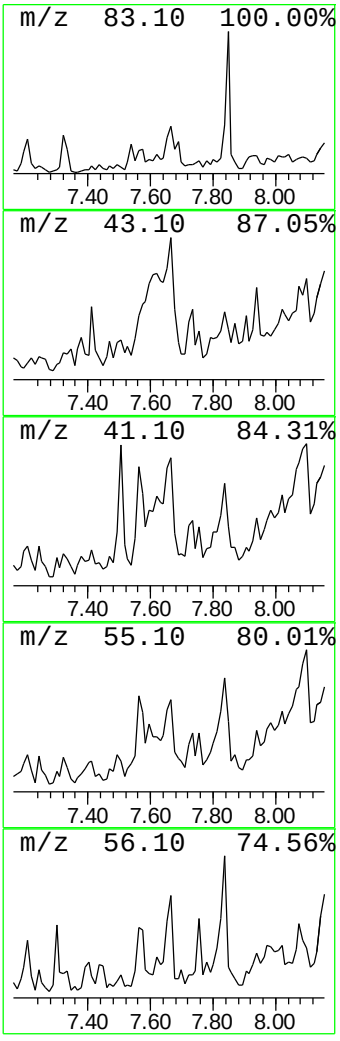
****

Peak Number 5 unknown7.66 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	25.67 ng	1887130	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclohexanedione, 5,5-dimethyl-	140	C8H12O2	000126-81-8	35
2	Cyanic acid, butyl ester	99	C5H9NO	001768-24-7	25
3	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	18
4	2-Heptene	98	C7H14	000592-77-8	15
5	Pentanoic acid, 2-ethyl-, methyl...	144	C8H16O2	000816-16-0	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

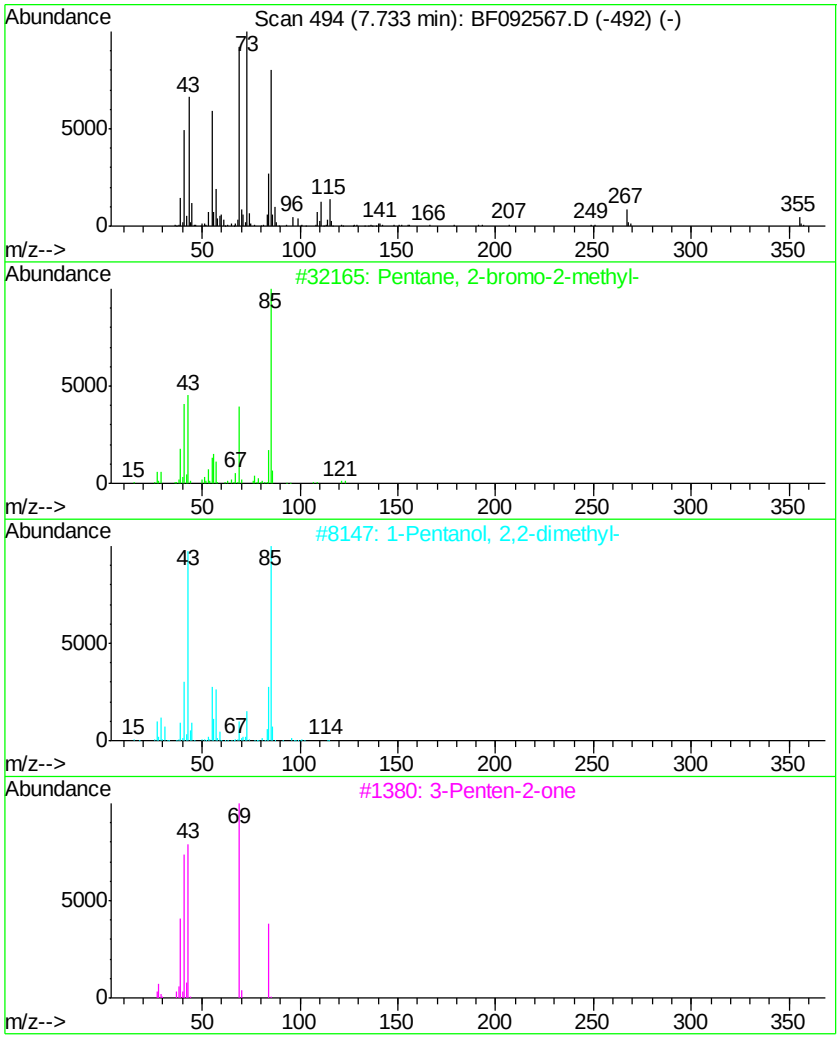
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

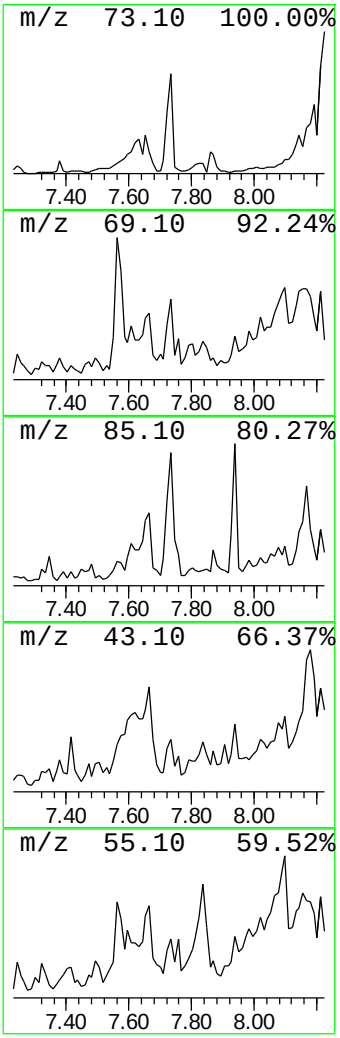
****

Peak Number 6 Pentane, 2-bromo-2-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	11.04 ng	811697	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-bromo-2-methyl-	164	C6H13Br	004283-80-1	53
2	1-Pentanol, 2,2-dimethyl-	116	C7H16O	002370-12-9	35
3	3-Penten-2-one	84	C5H8O	000625-33-2	30
4	1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	27
5	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

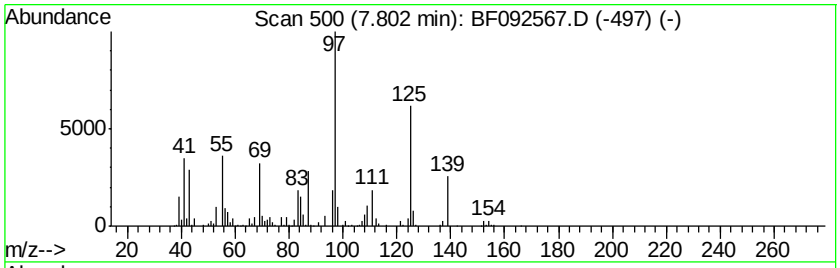
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

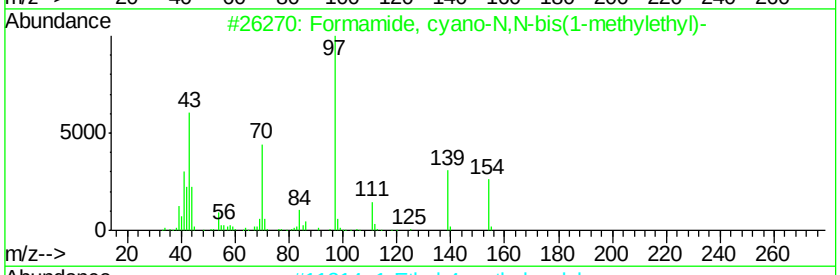
****

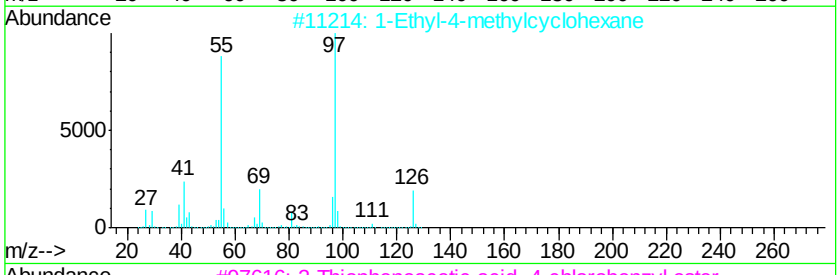
Peak Number 7 unknown7.80 Concentration Rank 18

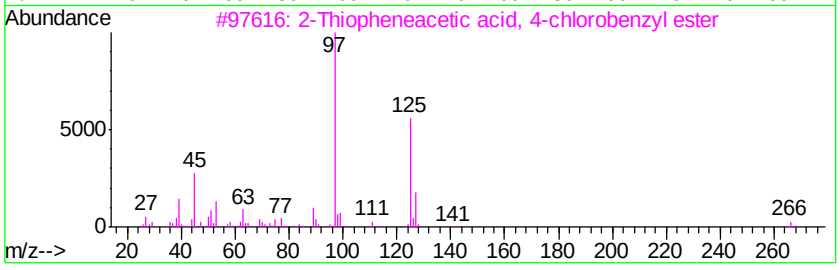
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	9.67 ng	710587	Naphthalene-d8	8.27

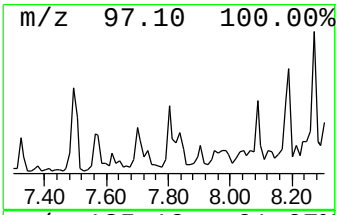
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formamide, cyano-N,N-bis(1-methy...	154	C8H14N2O	034282-81-0	47
2	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	43
3	2-Thiopheneacetic acid, 4-chloro...	266	C13H11ClO2S	1000279-94-4	40
4	Hexahydropyrrolizin-3-one	125	C7H11NO	126424-83-7	40
5	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	38

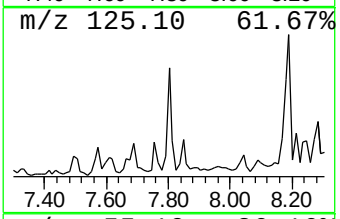


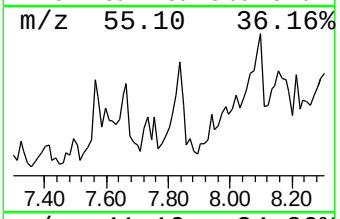


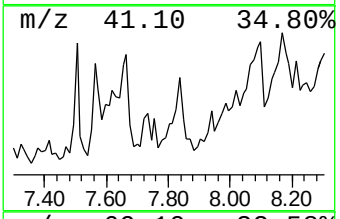


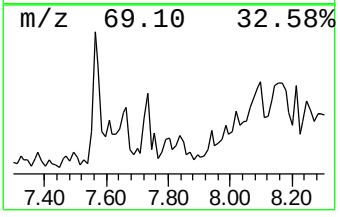












Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

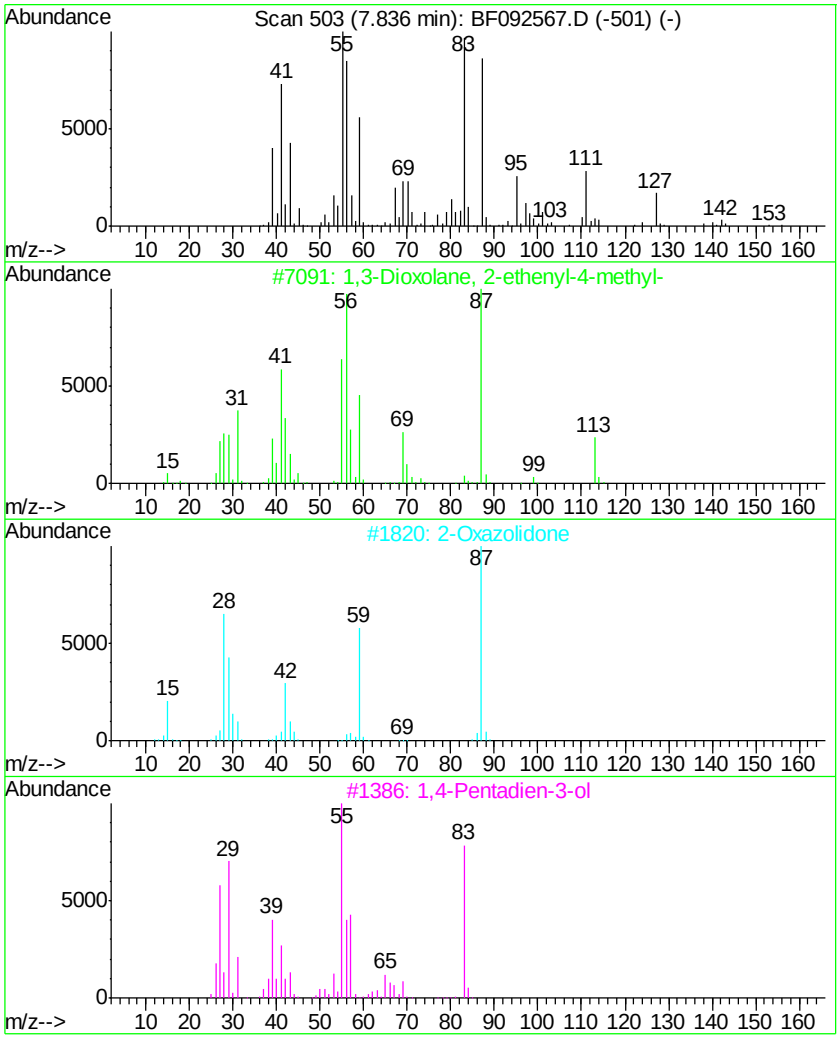
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

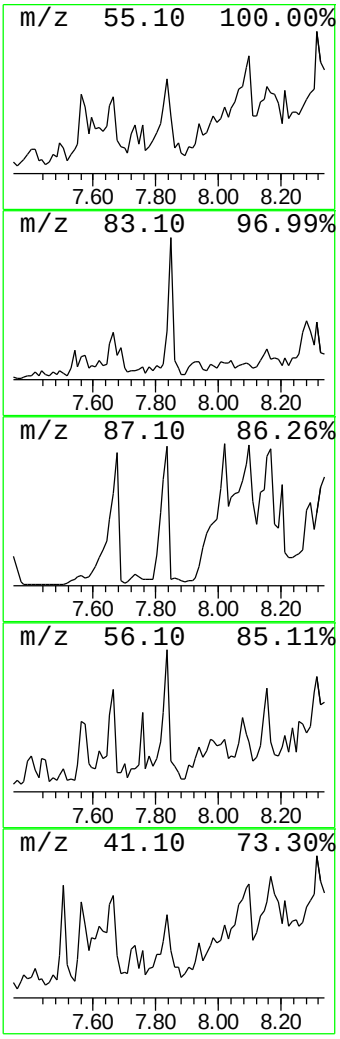
****

Peak Number 8 unknown7.84 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.84	23.70 ng	1742160	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethenyl-4-methyl-	114	C6H10O2	002421-07-0	49
2	2-Oxazolidone	87	C3H5NO2	000497-25-6	22
3	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	22
4	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	18
5	2-Pyrrolidinone, 1-ethenyl-	111	C6H9NO	000088-12-0	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

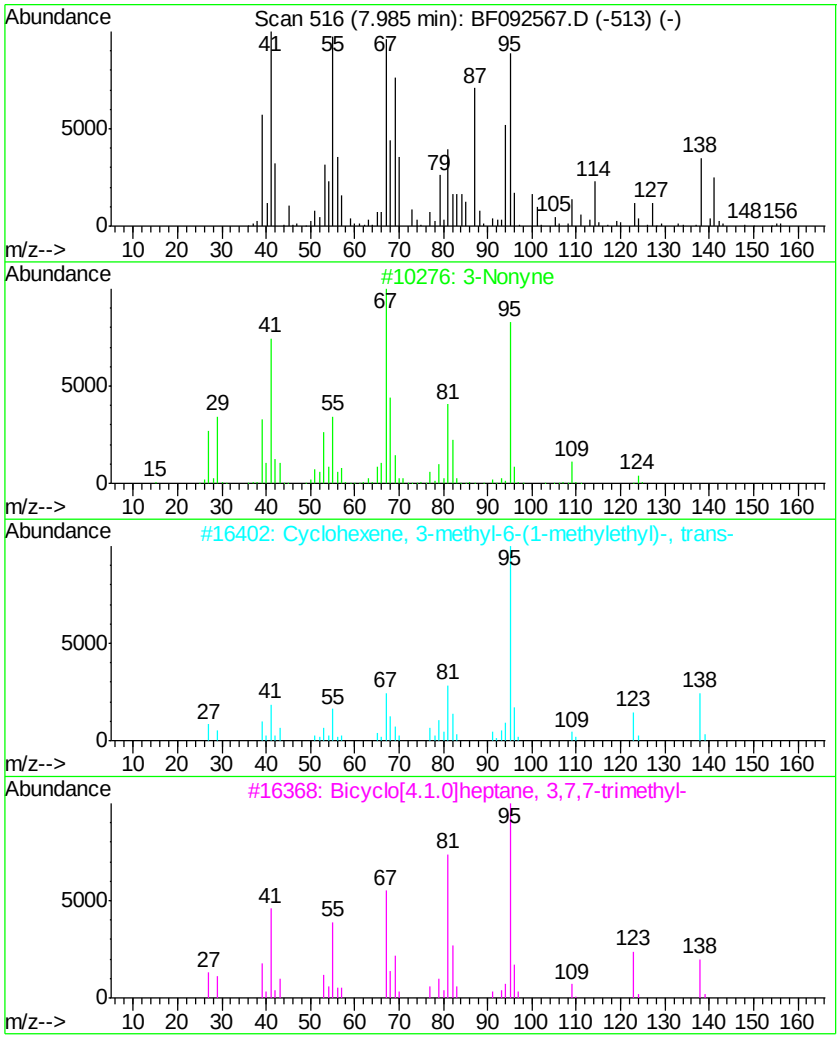
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

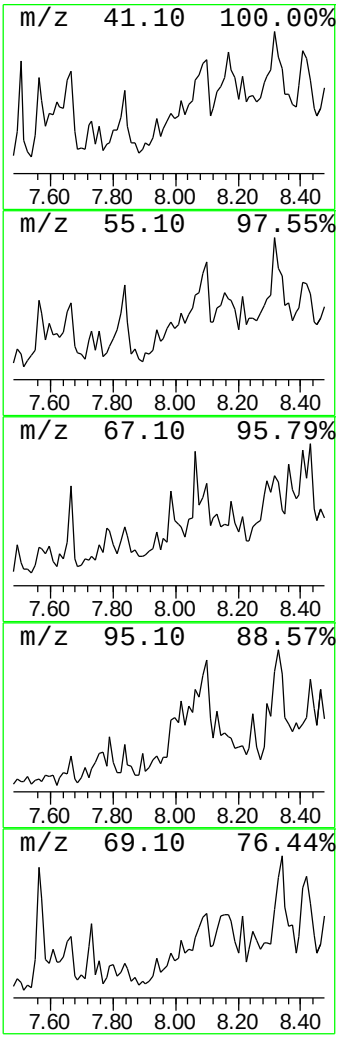
****

Peak Number 9 unknown7.98 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.98	9.29 ng	683027	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Nonyne	124	C9H16	020184-89-8	46
2	Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	001124-26-1	45
3	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	35
4	1H-Inden-1-one, octahydro-, trans-	138	C9H14O	016783-22-5	27
5	Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	005502-88-5	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

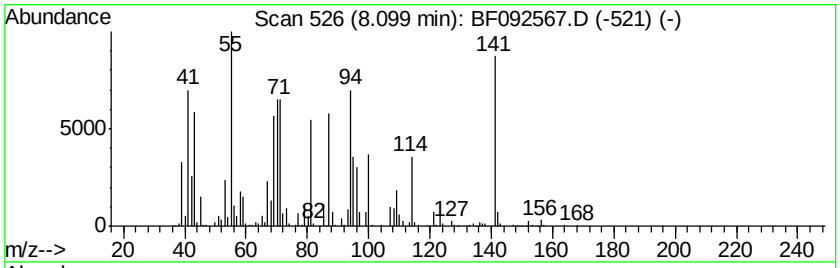
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

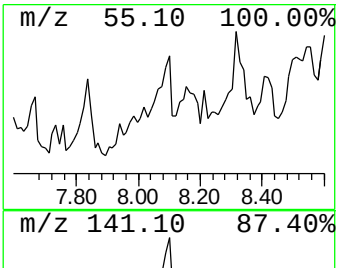
****

Peak Number 10 unknown8.10 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.10	29.28 ng	2151970	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphoramidothioic acid, O,S-di...	141	C2H8NO2PS	010265-92-6	27
2	2,6-Difluorobenzoic acid, 1-(cyc...	254	C14H16F2O2	1000293-30-4	14
3	Thiazole, 2-ethyl-4,5-dimethyl-	141	C7H11NS	000873-64-3	14
4	3-Methyl-2-(2-methylene-cyclohex...	182	C12H22O	1000187-18-4	10
5	Pyrrolidine	71	C4H9N	000123-75-1	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

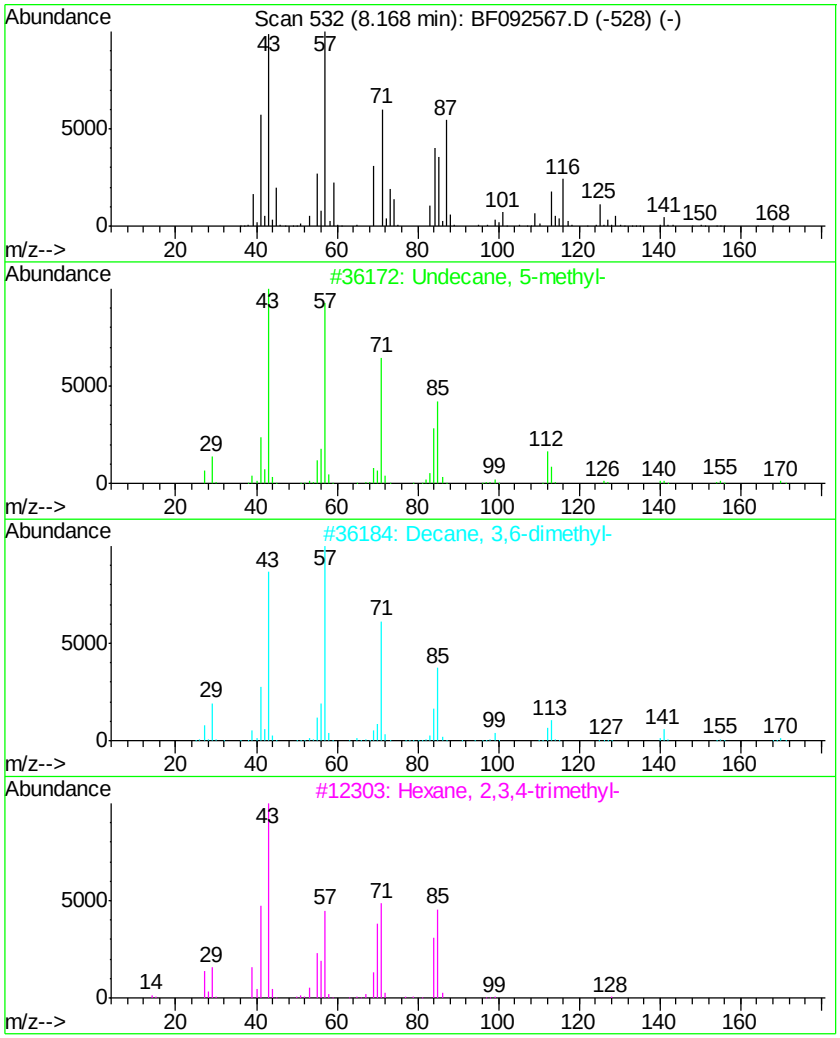
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

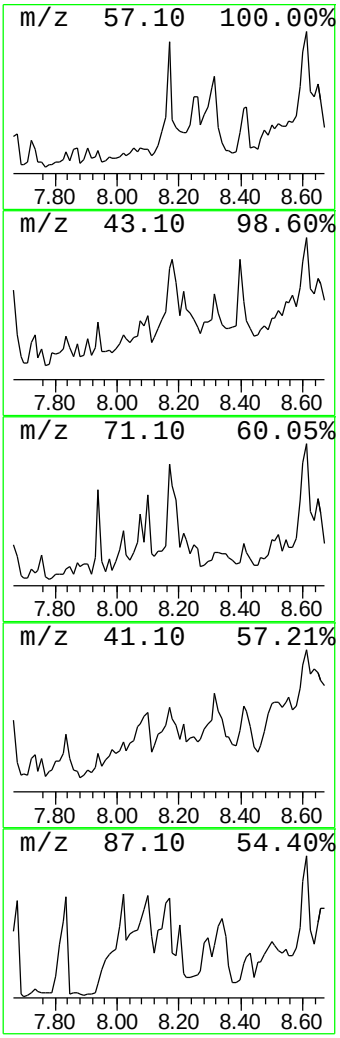
****

Peak Number 11 unknown8.17 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	32.67 ng	2401230	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 5-methyl-	170	C12H26	001632-70-8	22
2	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	22
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	22
4	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	22
5	Hexane, 3-ethyl-	114	C8H18	000619-99-8	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

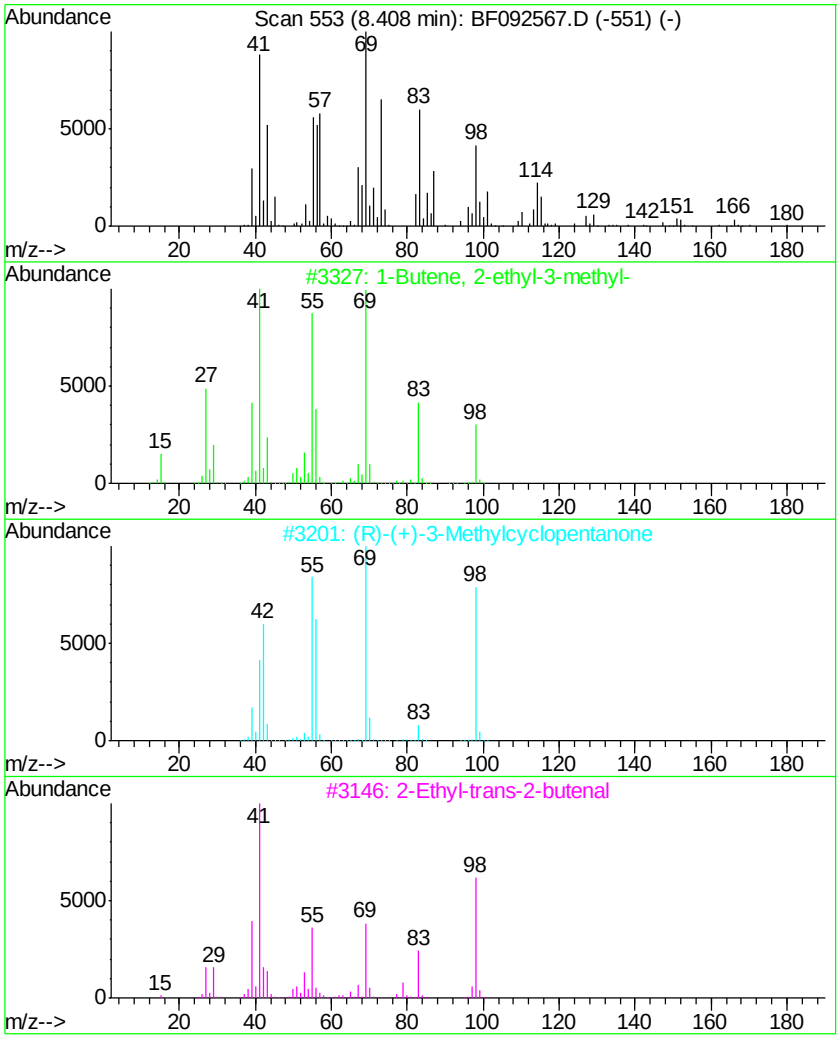
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

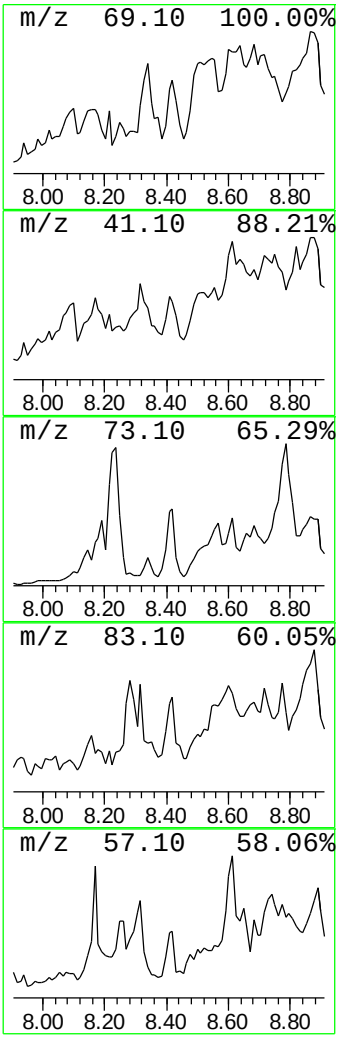
****

Peak Number 12 1-Butene, 2-ethyl-3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	31.08 ng	2284470	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 2-ethyl-3-methyl-	98	C7H14	007357-93-9	50
2	(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	47
3	2-Ethyl-trans-2-butenal	98	C6H10O	063883-69-2	46
4	Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	43
5	2-Pentenoic acid, 2-methyl-, (E)-	114	C6H10O2	016957-70-3	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

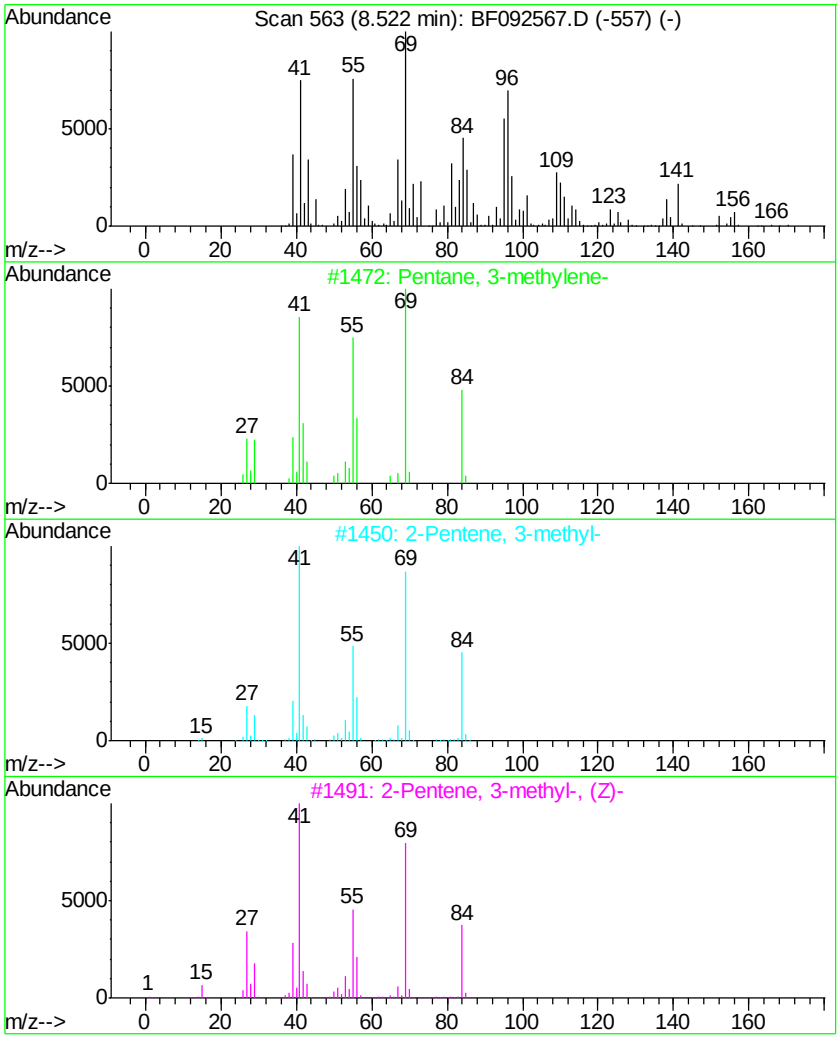
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

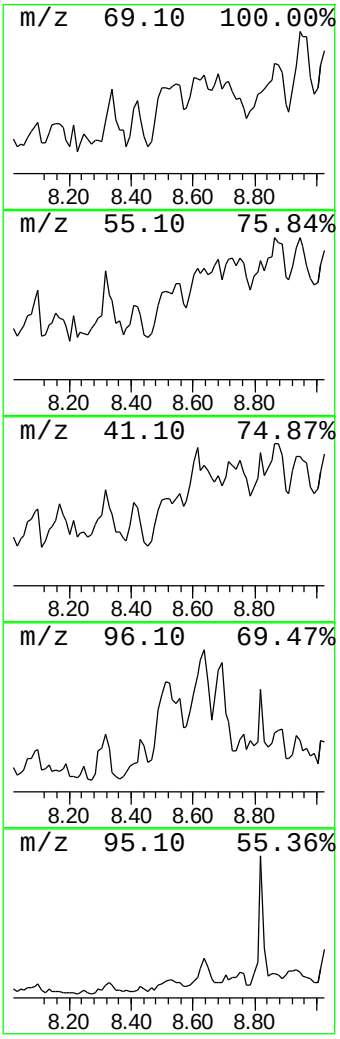
****

Peak Number 13 unknown8.52 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	61.82 ng	4544150	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methylene-	84	C6H12	000760-21-4	38
2	2-Pentene, 3-methyl-	84	C6H12	000922-61-2	30
3	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	30
4	1H-Imidazole-4-ethanamine, 5-met...	125	C6H11N3	036507-31-0	25
5	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

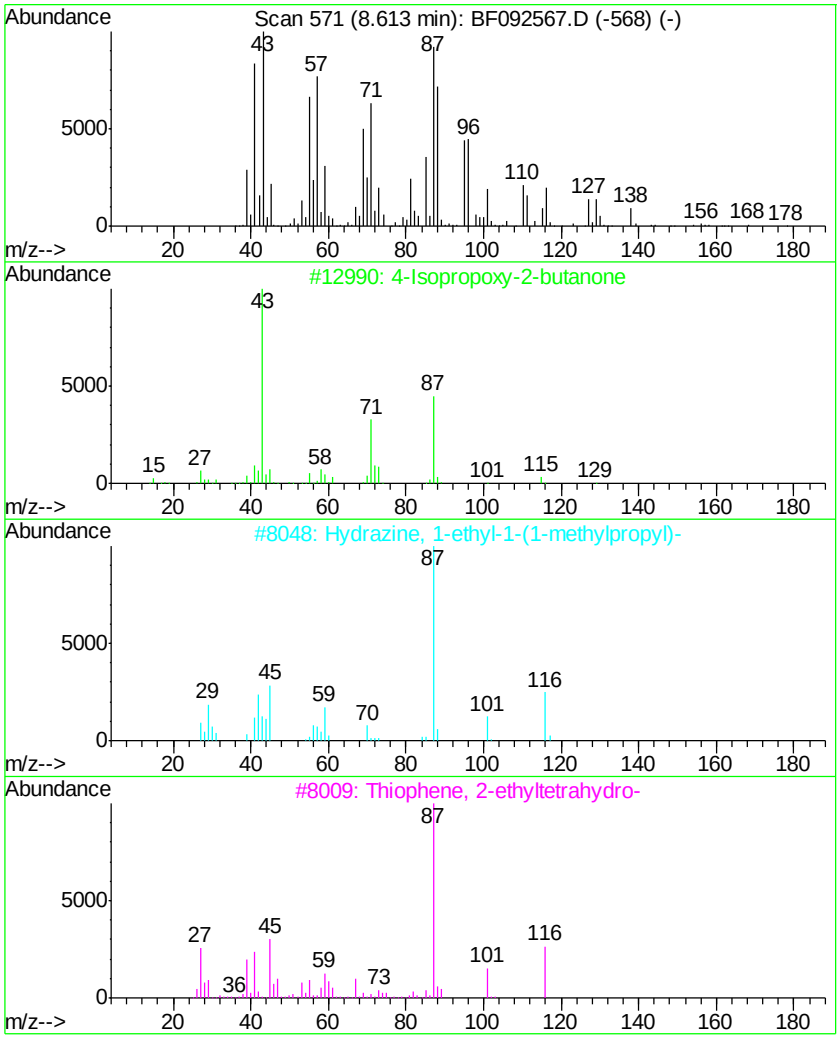
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

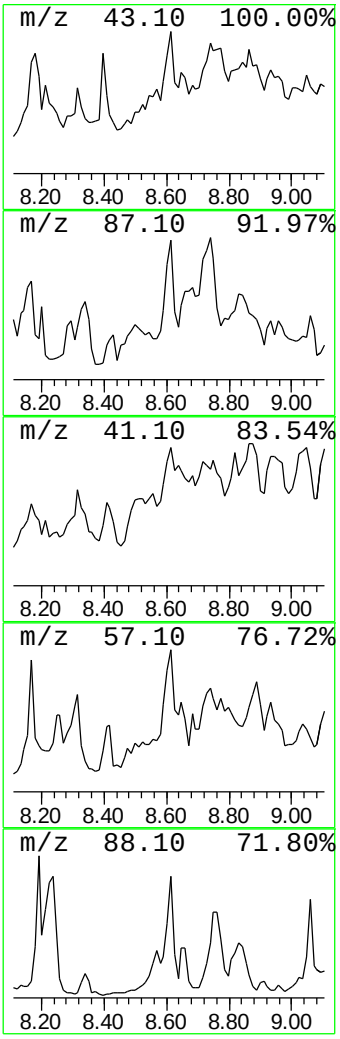
****

Peak Number 14 unknown8.61 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.61	36.98 ng	2717840	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	35
2	Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	25
3	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	25
4	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	18
5	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

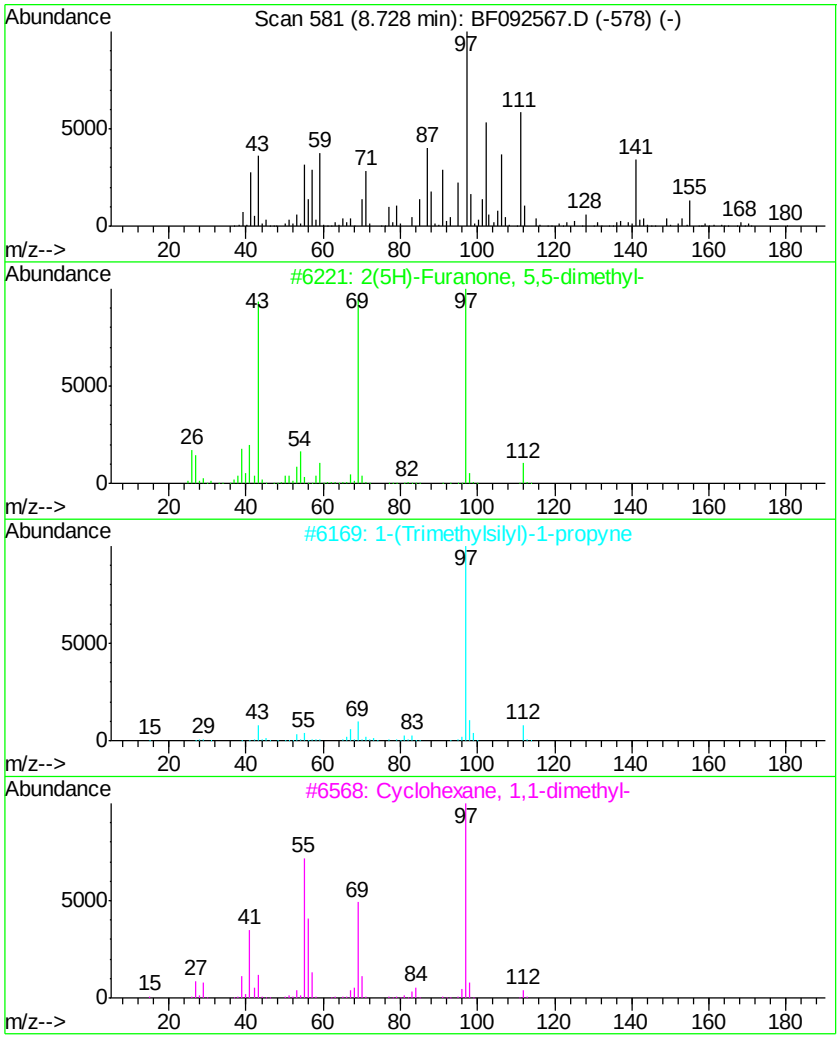
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

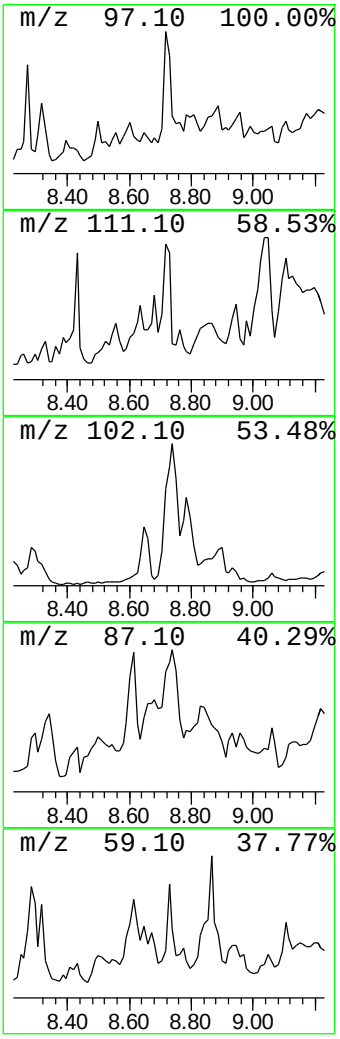
****

Peak Number 15 unknown8.73 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	27.65 ng	2032710	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	14
2	1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	14
3	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	14
4	3-Cyclohexene-1-carboxylic acid,...	273	C17H23NO2	051931-66-9	10
5	Divinyldimethylsilane	112	C6H12Si	010519-87-6	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

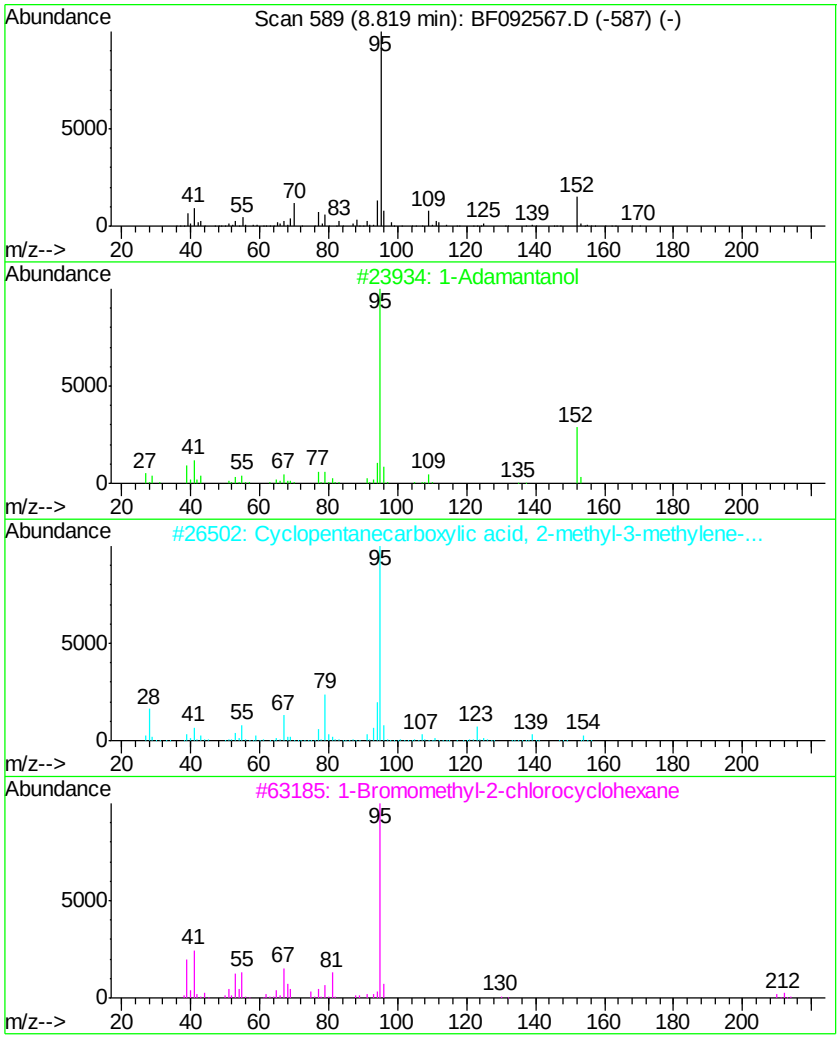
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

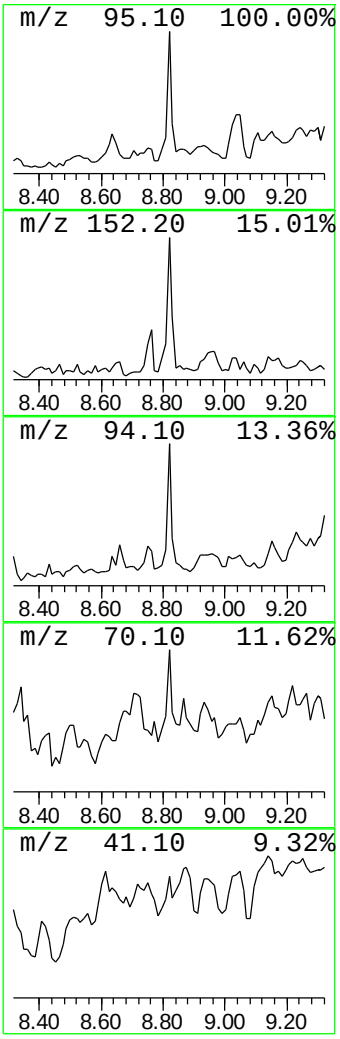
****

Peak Number 16 1-Adamantanol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.82	24.10 ng	1771440	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Adamantanol	152	C10H16O	000768-95-6	83
2	Cyclopentanecarboxylic acid, 2-m...	154	C9H14O2	074764-25-3	38
3	1-Bromomethyl-2-chlorocyclohexane	210	C7H12BrCl	090009-23-7	33
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	33
5	Ethanone, 1-(1H-pyrazol-4-yl)-	110	C5H6N2O	025016-16-4	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

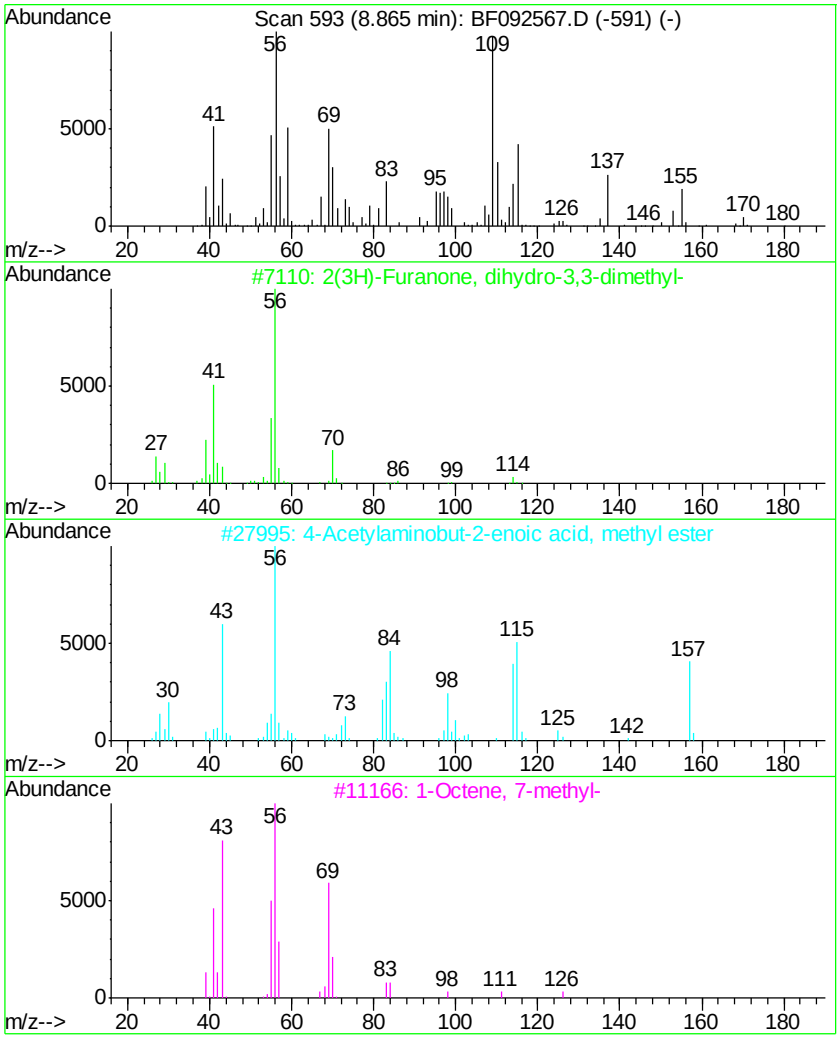
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

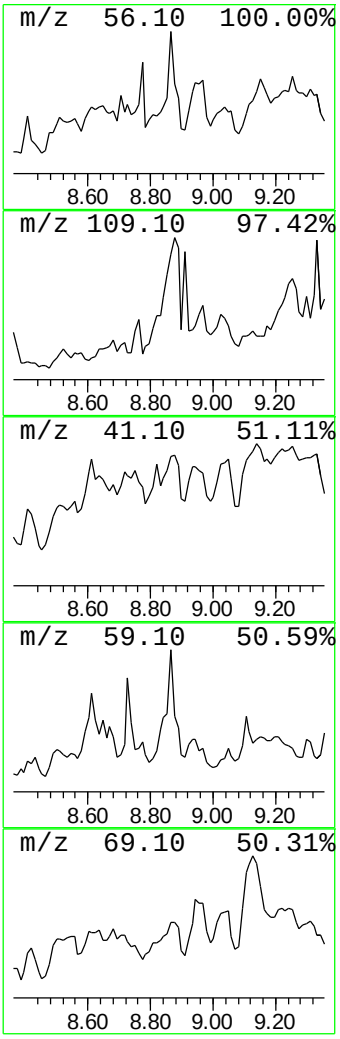
****

Peak Number 17 unknown8.86 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.86	42.74 ng	3141590	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-3,3-dime...	114	C6H10O2	003709-08-8	14
2	4-Acetylaminobut-2-enoic acid, m...	157	C7H11NO3	1000193-45-5	12
3	1-Octene, 7-methyl-	126	C9H18	013151-06-9	11
4	1-Undecene, 10-methyl-	168	C12H24	022370-55-4	11
5	3-Hydroxy-3-methyl-butyric acid,...	132	C5H12N2O2	1000193-80-2	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

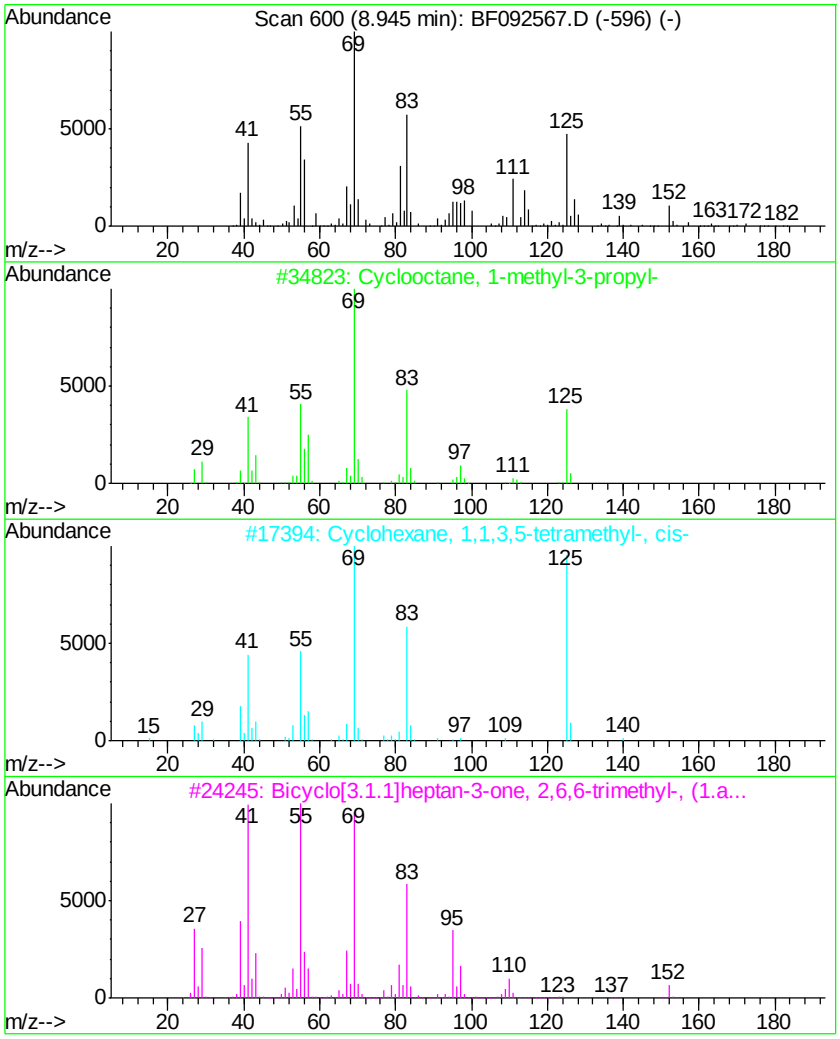
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

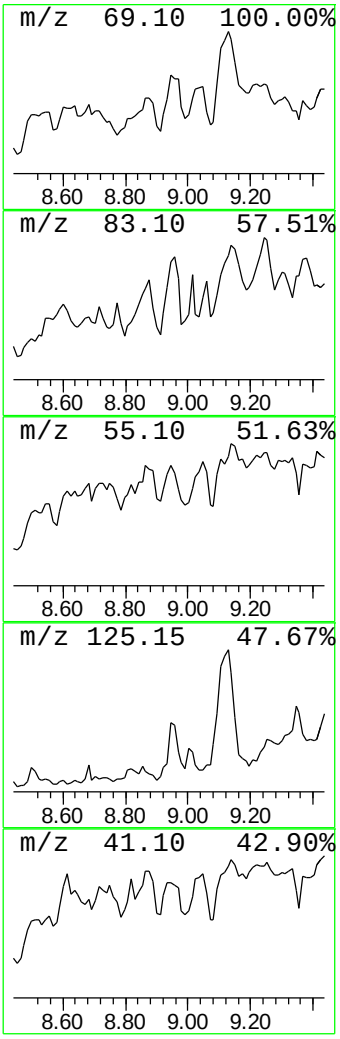
****

Peak Number 18 Cyclooctane, 1-methyl-3-pro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.94	43.16 ng	3172670	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	53
2	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	50
3	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	46
4	Methyl 2-hydroxydecanoate	202	C11H22O3	071271-24-4	43
5	2-Hexene, 2-methyl-	98	C7H14	002738-19-4	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

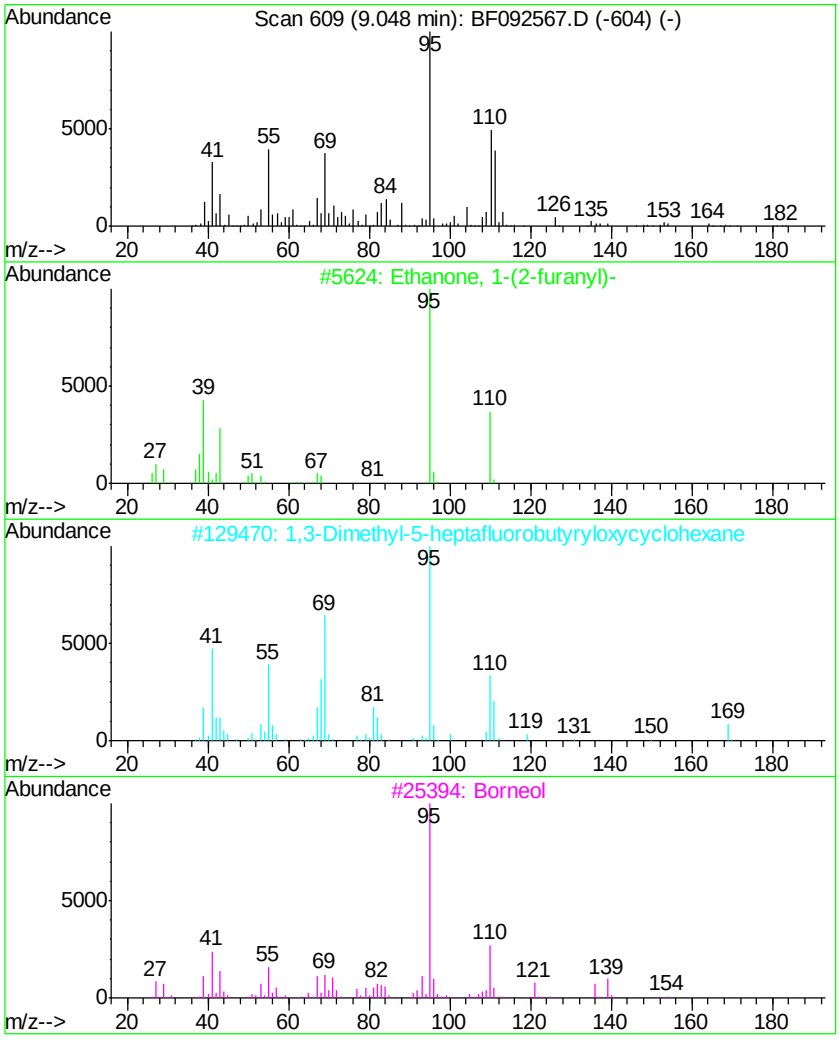
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

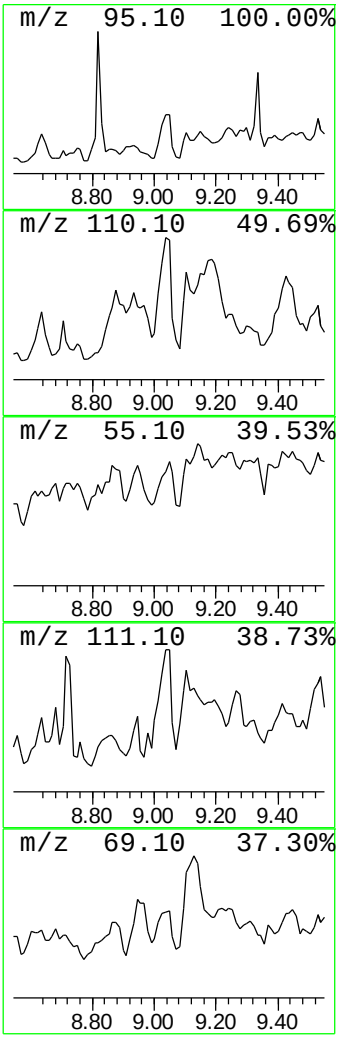
****

Peak Number 19 unknown9.05 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	62.93 ng	4625280	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(2-furanyl)-	110	C6H6O2	001192-62-7	43
2	1,3-Dimethyl-5-heptafluorobutyry...	324	C12H15F7O2	1000216-63-8	42
3	Borneol	154	C10H18O	010385-78-1	37
4	2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	28
5	4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

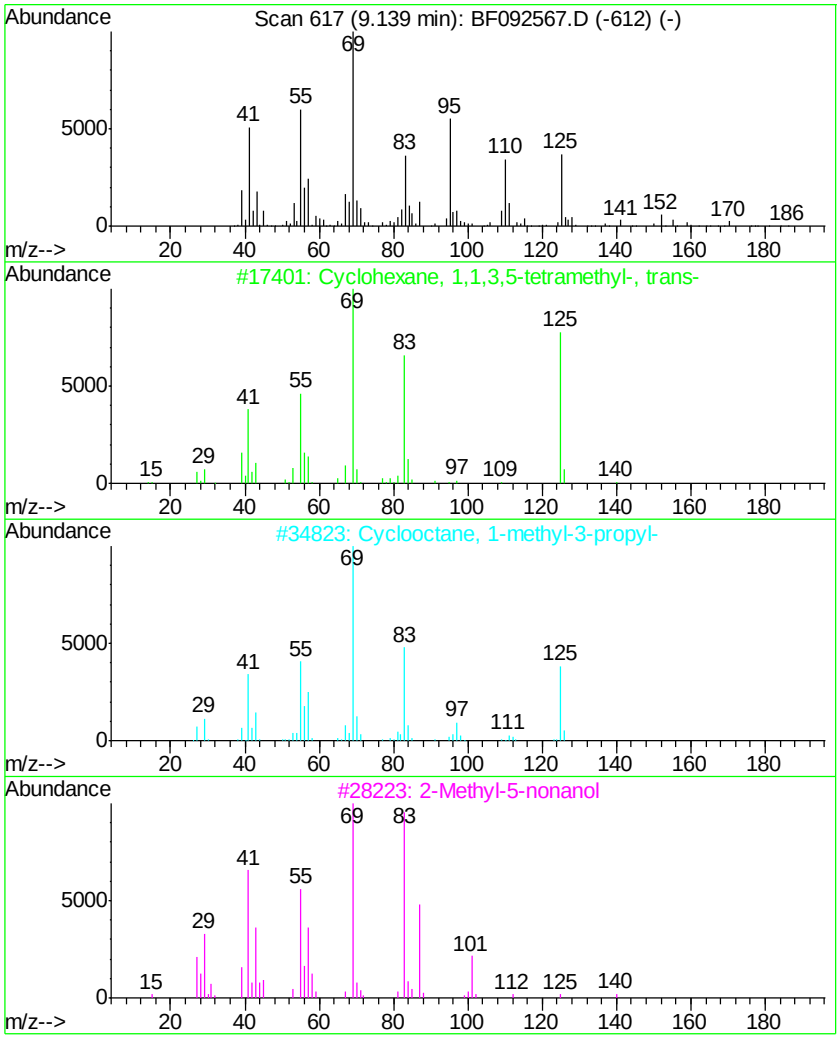
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

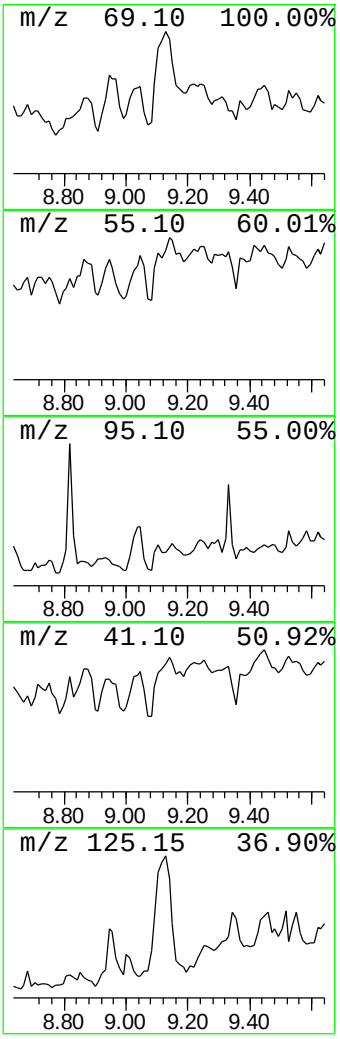
****

Peak Number 20 Cyclohexane, 1,1,3,5-tetram... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.14	94.39 ng	6938120	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	50
2	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	50
3	2-Methyl-5-nonanol	158	C10H22O	029843-62-7	43
4	1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	38
5	2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092567.D
Acq On : 27 Jan 2017 10:38
Operator : SJ/MA
Sample : I1353-03
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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
unknown6.74	6.74	42.2	ng	2464720	1	6.97	1167860	20.0
1H,5H-Pyrrolo[1',...	7.32	15.1	ng	881680	1	6.97	1167860	20.0
3-Cyclohexen-1-ca...	7.41	9.1	ng	531304	1	6.97	1167860	20.0
unknown7.66	7.66	25.7	ng	1887130	2	8.27	1470050	20.0
Pentane, 2-bromo-...	7.73	11.0	ng	811697	2	8.27	1470050	20.0
unknown7.80	7.80	9.7	ng	710587	2	8.27	1470050	20.0
unknown7.84	7.84	23.7	ng	1742160	2	8.27	1470050	20.0
unknown7.98	7.98	9.3	ng	683027	2	8.27	1470050	20.0
unknown8.10	8.10	29.3	ng	2151970	2	8.27	1470050	20.0
unknown8.17	8.17	32.7	ng	2401230	2	8.27	1470050	20.0
1-Butene, 2-ethyl...	8.41	31.1	ng	2284470	2	8.27	1470050	20.0
unknown8.52	8.52	61.8	ng	4544150	2	8.27	1470050	20.0
unknown8.61	8.61	37.0	ng	2717840	2	8.27	1470050	20.0
unknown8.73	8.73	27.6	ng	2032710	2	8.27	1470050	20.0
1-Adamantanol	8.82	24.1	ng	1771440	2	8.27	1470050	20.0
unknown8.86	8.86	42.7	ng	3141590	2	8.27	1470050	20.0
Cyclooctane, 1-me...	8.94	43.2	ng	3172670	2	8.27	1470050	20.0
unknown9.05	9.05	62.9	ng	4625280	2	8.27	1470050	20.0
Cyclohexane, 1,1,...	9.14	94.4	ng	6938120	2	8.27	1470050	20.0