LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104024.D
Acq On : 28 Mar 2018 21:36
Operator : JU/SJ
Sample : J2088-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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-BF032818.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	5.610	594	599	616	rBV2	49561	217070	9.85%	2.587%
2	6.604	764	768	785	rBV	77325	271449	12.32%	3.235%
3	6.739	787	791	797	rBV	176282	268403	12.18%	3.199%
4	6.963	826	829	851	rBV	501534	712335	32.32%	8.489%
5	7.116	852	855	868	rVB	208999	287748	13.06%	3.429%
6	7.533	922	926	935	rBV	97488	207254	9.40%	2.470%
7	8.245	1042	1047	1057	rBV	770705	926117	42.03%	11.037%
8	8.963	1162	1169	1174	rBV2	152352	262836	11.93%	3.132%
9	9.027	1177	1180	1183	rBV	40435	62293	2.83%	0.742%
10	9.227	1210	1214	1216	rBV3	52079	64301	2.92%	0.766%
11	9.316	1226	1229	1234	rVB	366689	339866	15.42%	4.050%
12	9.698	1291	1294	1297	rBV4	182900	169579	7.70%	2.021%
13	9.733	1298	1300	1303	rBV3	59562	57356	2.60%	0.684%
14	9.857	1319	1321	1324	rBV2	148483	152773	6.93%	1.821%
15	9.904	1326	1329	1332	rVB2	261732	241646	10.97%	2.880%
16	9.980	1339	1342	1343	rBV	157778	148311	6.73%	1.768%
17	10.004	1343	1346	1349	rVV	664418	585126	26.55%	6.973%
18	10.239	1384	1386	1390	rBV3	159379	236561	10.73%	2.819%
19	10.410	1412	1415	1417	rBV	559993	516574	23.44%	6.156%
20	15.280	2239	2243	2257	rVB	986256	2203686	100.00%	26.263%
21	15.733	2317	2320	2325	rVB	377423	459681	20.86%	5.478%

Sum of corrected areas: 8390965

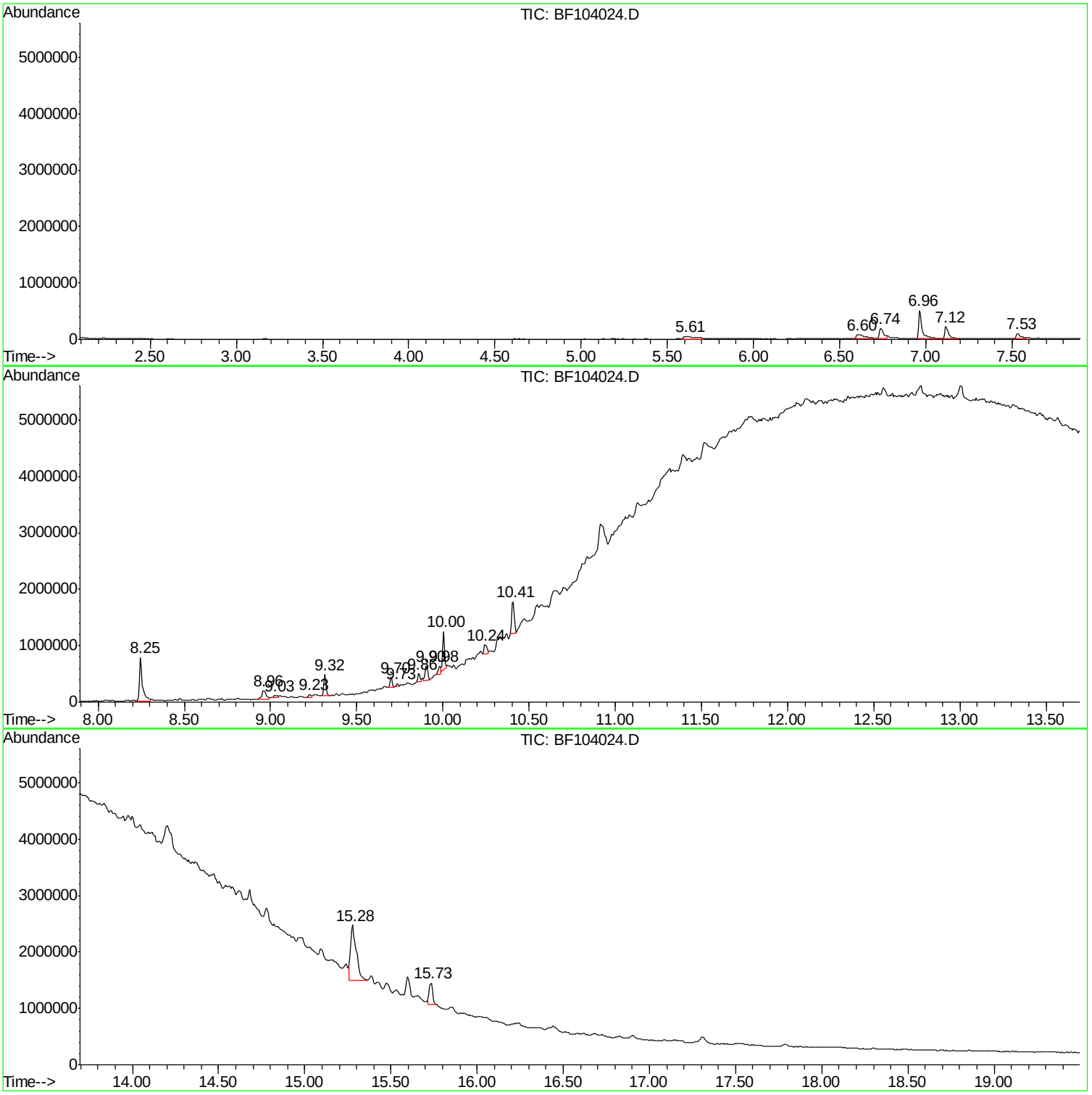
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104024.D
Acq On : 28 Mar 2018 21:36
Operator : JU/SJ
Sample : J2088-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104024.D
Acq On : 28 Mar 2018 21:36
Operator : JU/SJ
Sample : J2088-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

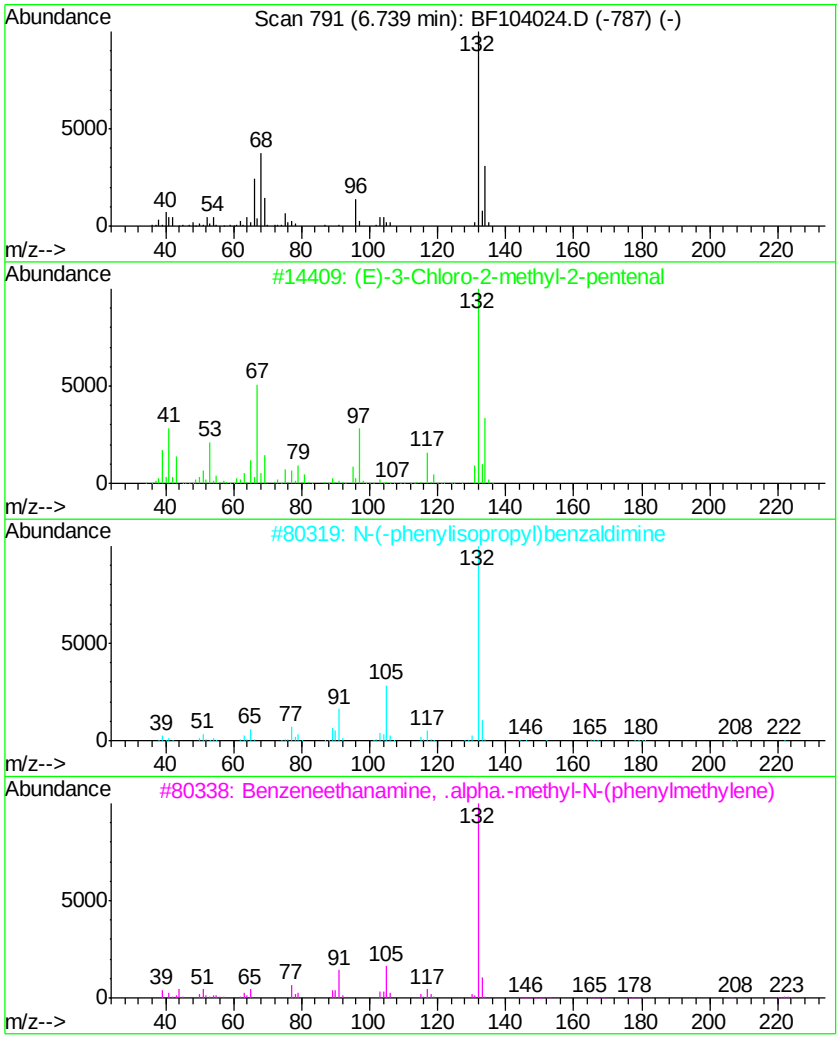
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

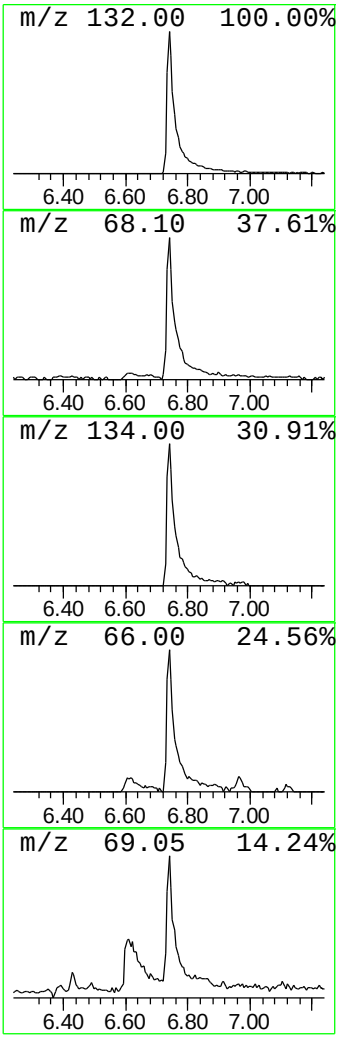
****

Peak Number 1 unknown6.74 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	7.54 ng	268403	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	12
3	Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Data File : BF104024.D
Acq On : 28 Mar 2018 21:36
Operator : JU/SJ
Sample : J2088-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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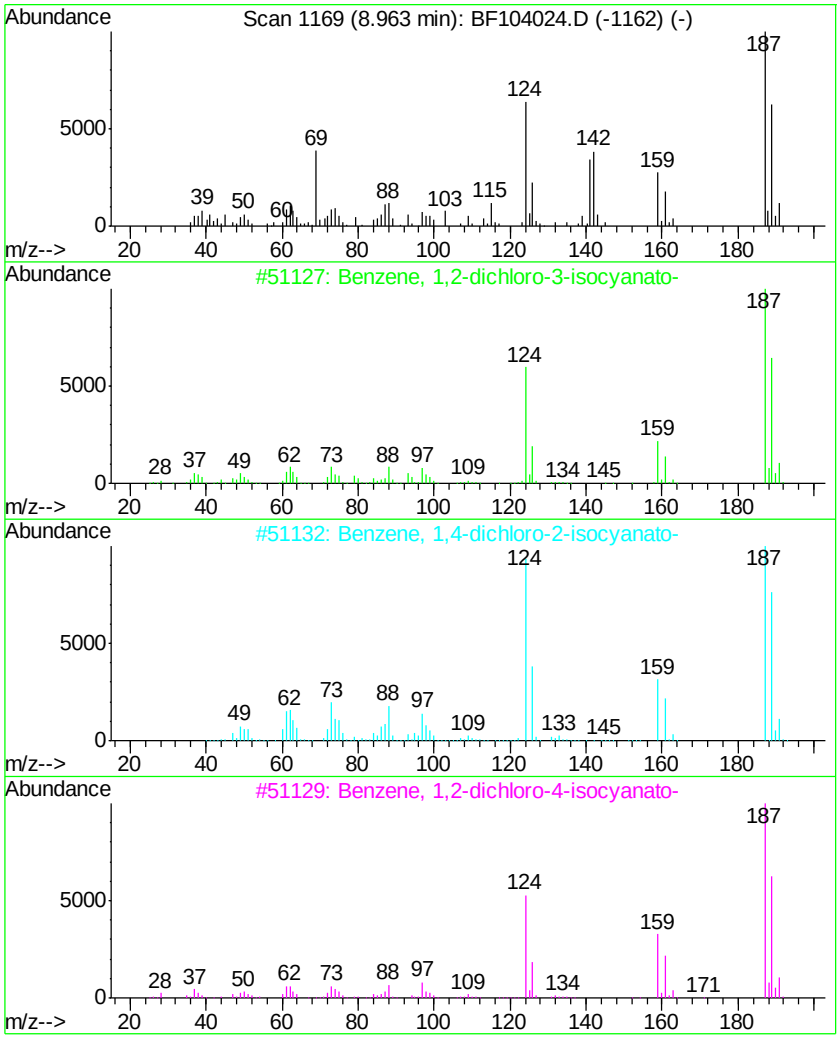
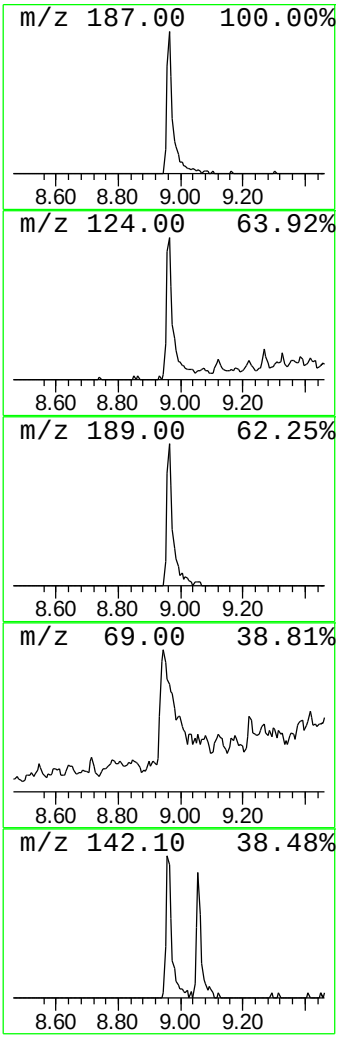
Peak Number 3 Benzene, 1,2-dichloro-3-iso... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	5.68 ng	262836	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-dichloro-3-isocyanato-	187	C7H3Cl2NO	041195-90-8	99
2	Benzene, 1,4-dichloro-2-isocyanato-	187	C7H3Cl2NO	005392-82-5	98
3	Benzene, 1,2-dichloro-4-isocyanato-	187	C7H3Cl2NO	000102-36-3	98
4	Benzene, 1,3-dichloro-2-isocyanato-	187	C7H3Cl2NO	039920-37-1	97
5	3,5-Dichlorophenyl isocyanate	187	C7H3Cl2NO	034893-92-0	97





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Data File : BF104024.D
Acq On : 28 Mar 2018 21:36
Operator : JU/SJ
Sample : J2088-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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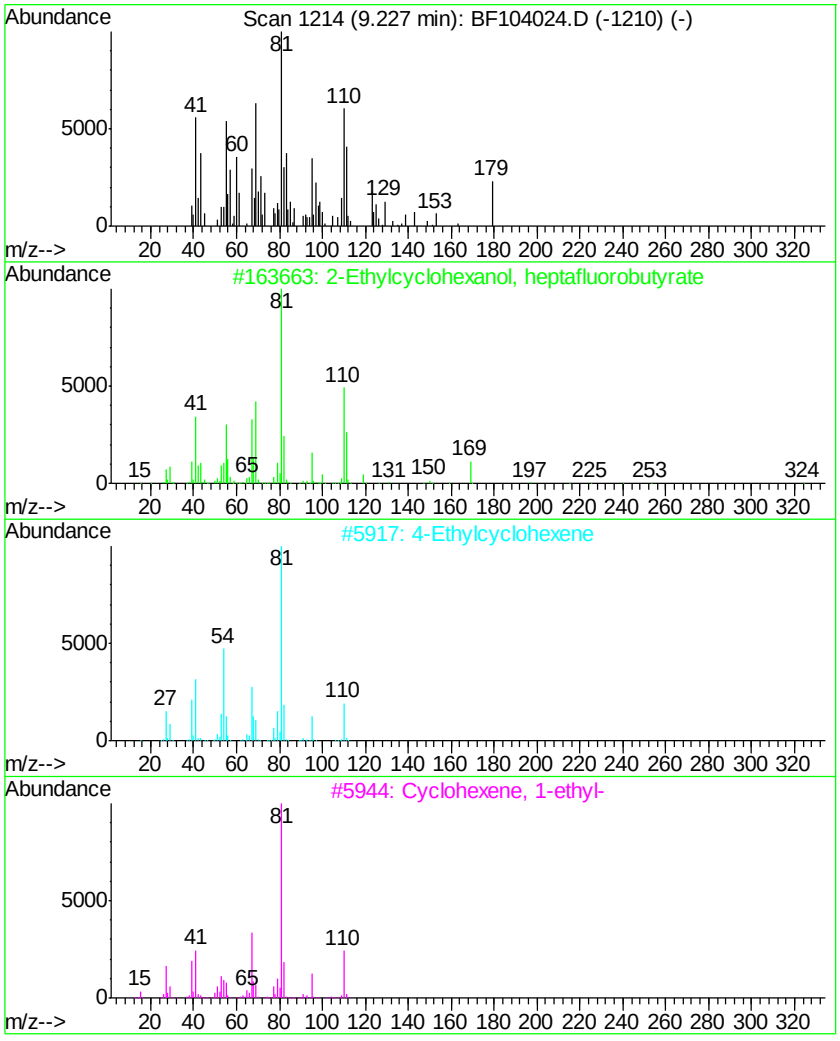
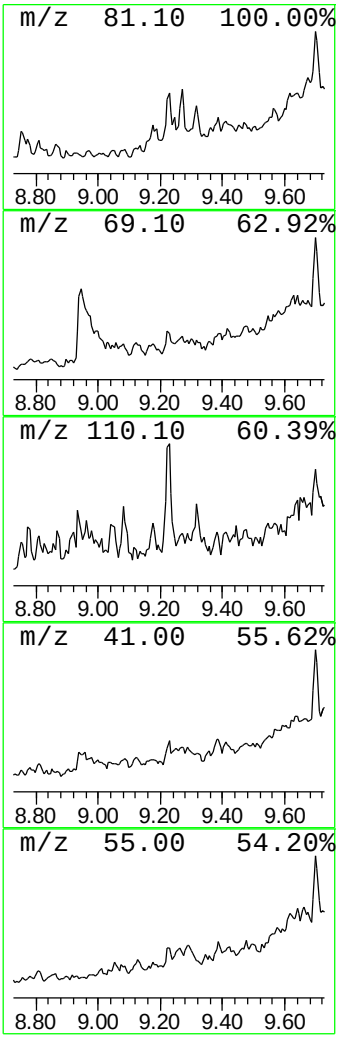
Peak Number 4 unknown9.23 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.23	2.20 ng	64301	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylcyclohexanol, heptafluoro...	324	C12H15F7O2	959079-92-6	46
2	4-Ethylcyclohexene	110	C8H14	003742-42-5	43
3	Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	38
4	Bromoacetic acid, 2-ethylcyclohe...	248	C10H17BrO2	1000282-66-9	38
5	1-Ethyl-2-trifluoroacetoxycycloh...	224	C10H15F3O2	1000216-64-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104024.D
Acq On : 28 Mar 2018 21:36
Operator : JU/SJ
Sample : J2088-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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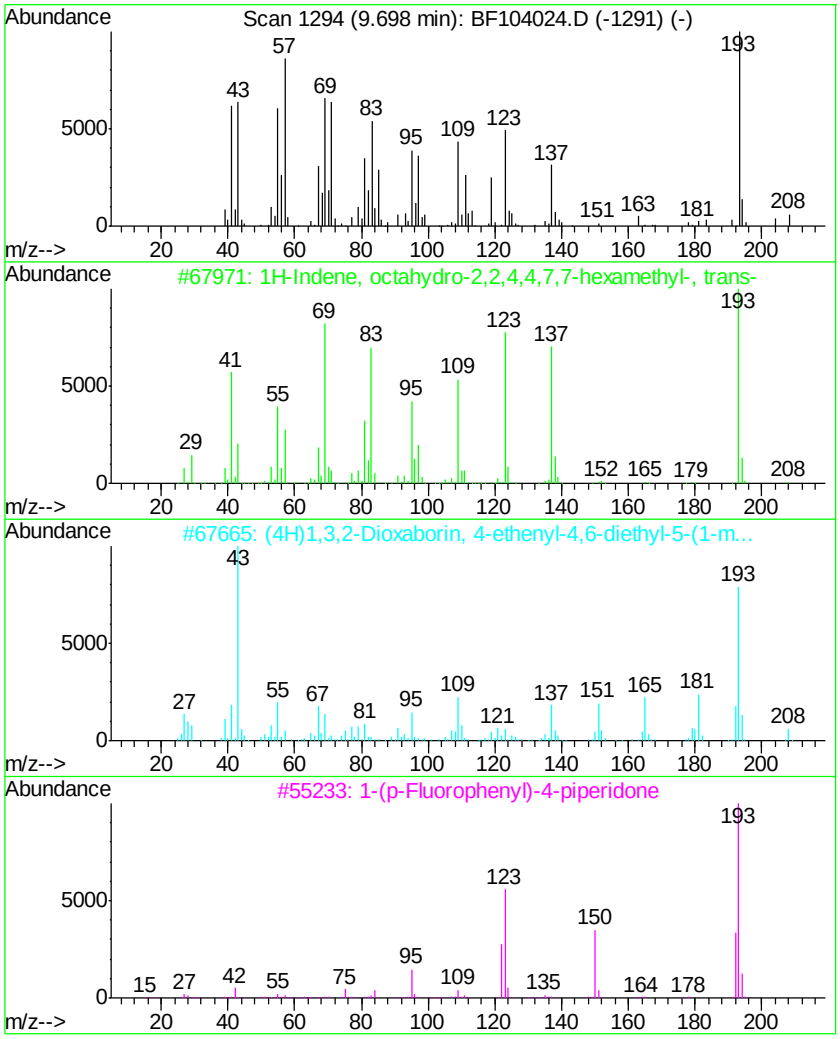
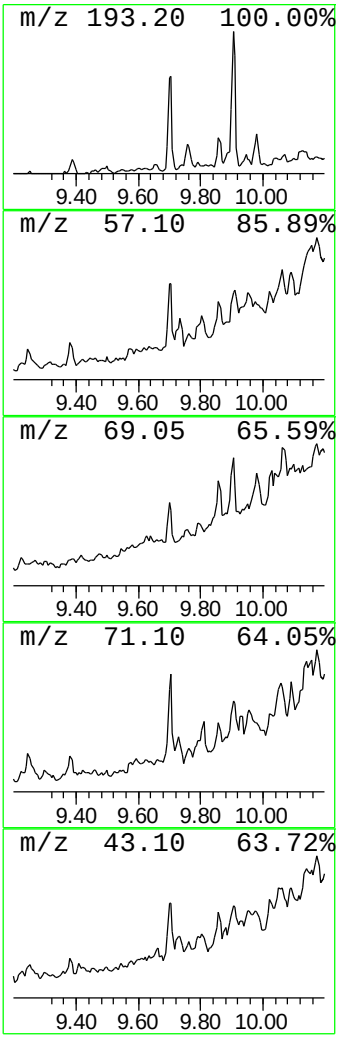
Peak Number 5 1H-Indene, octahydro-2,2,4,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.70	5.80 ng	169579	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	50
2	(4H)1,3,2-Dioxaborin, 4-ethenyl-...	208	C12H21BO2	1000062-14-4	38
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
4	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	35
5	Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104024.D
Acq On : 28 Mar 2018 21:36
Operator : JU/SJ
Sample : J2088-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

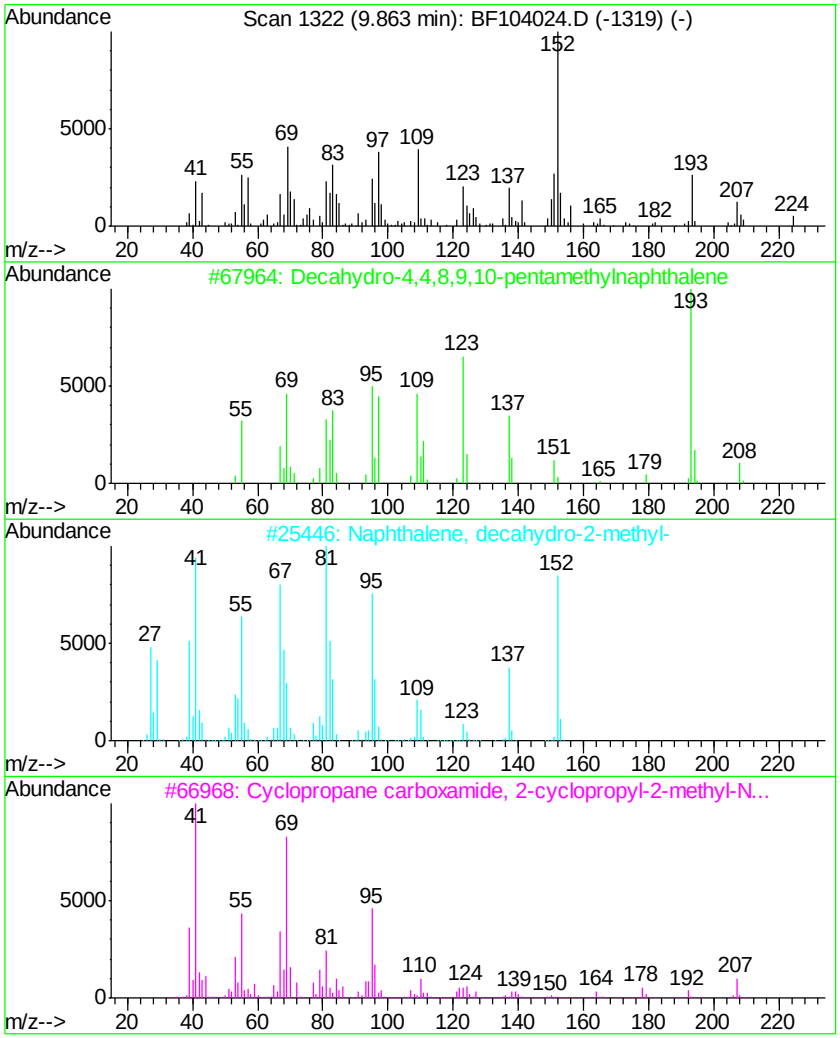
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

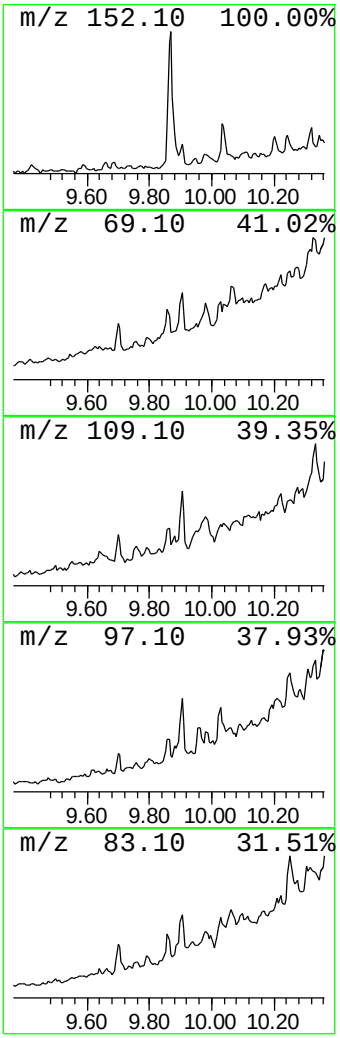
****

Peak Number 6 unknown9.86 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	5.22 ng	152773	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	49
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	40
3	Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	30
4	2-(2-Methyl-propenyl)-cyclohexanone	152	C10H16O	065737-44-2	30
5	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	25





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

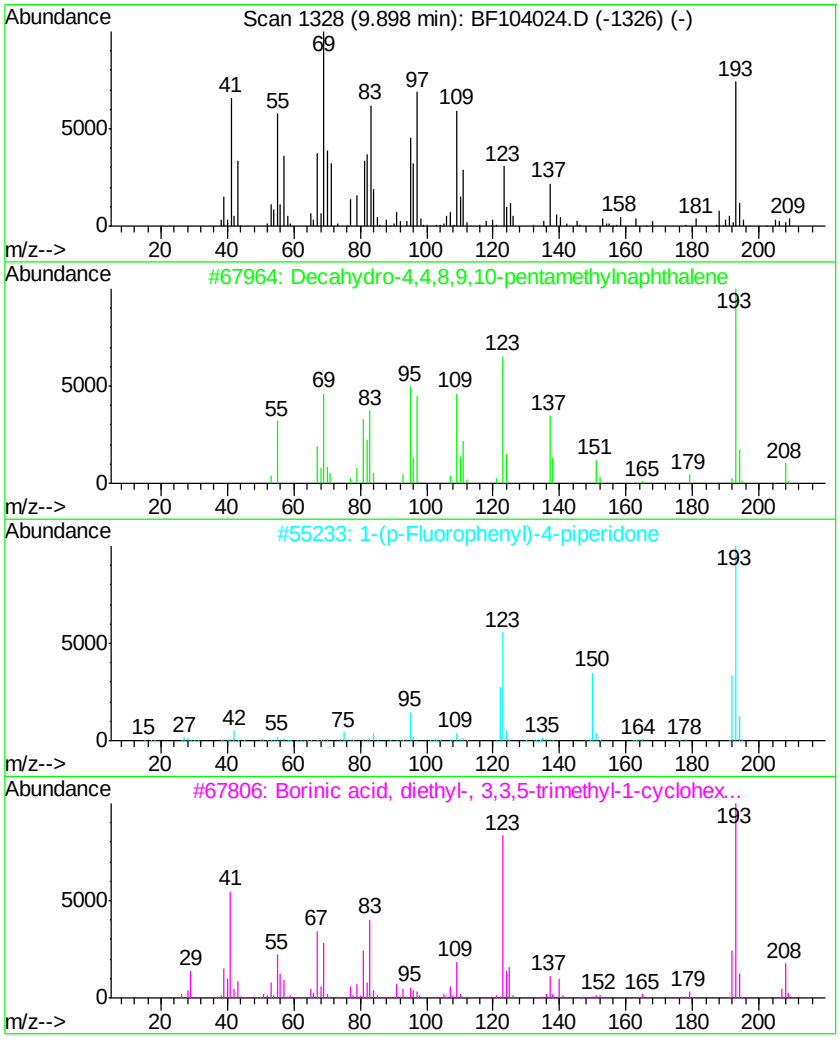
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

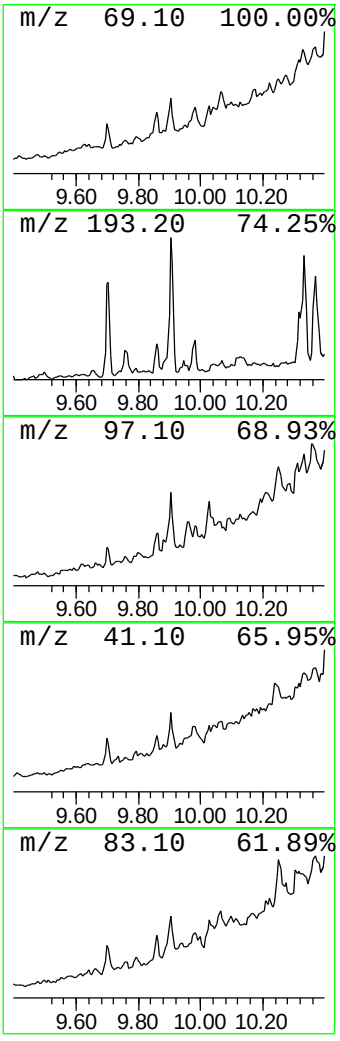
****

Peak Number 7 unknown9.90 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.90	8.26 ng	241646	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
3	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	35
4	2-Isobutylideneamino-3-methylbut...	152	C9H16N2	125213-17-4	25
5	Cyclopentanemethanol, .alpha.-cy...	227	C12H21NO3	103077-58-3	22





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

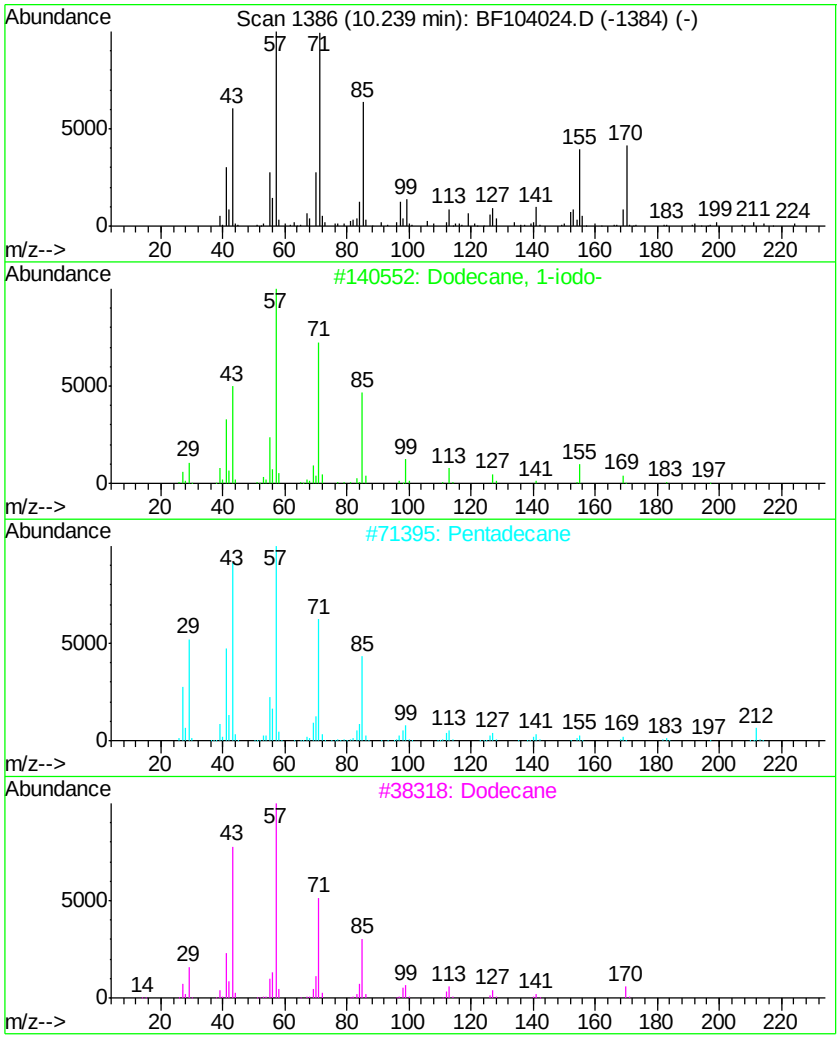
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

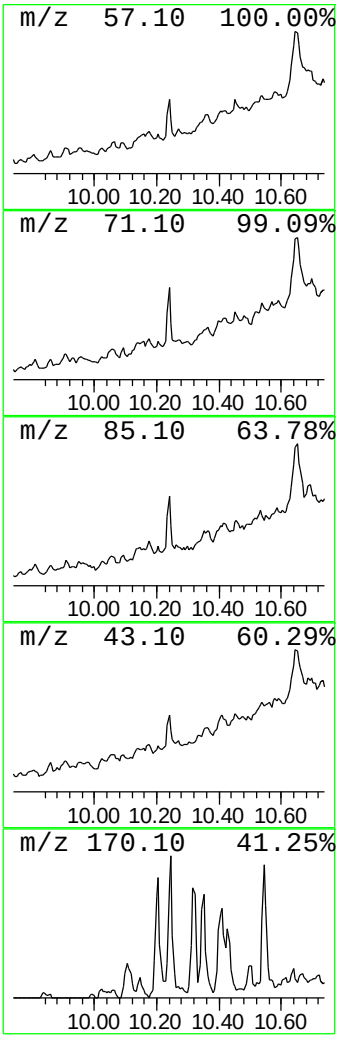
****

Peak Number 8 unknown10.24 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	8.09 ng	236561	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	49
2	Pentadecane	212	C15H32	000629-62-9	47
3	Dodecane	170	C12H26	000112-40-3	46
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	43
5	1-Undecene, 4-methyl-	168	C12H24	074630-39-0	43





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
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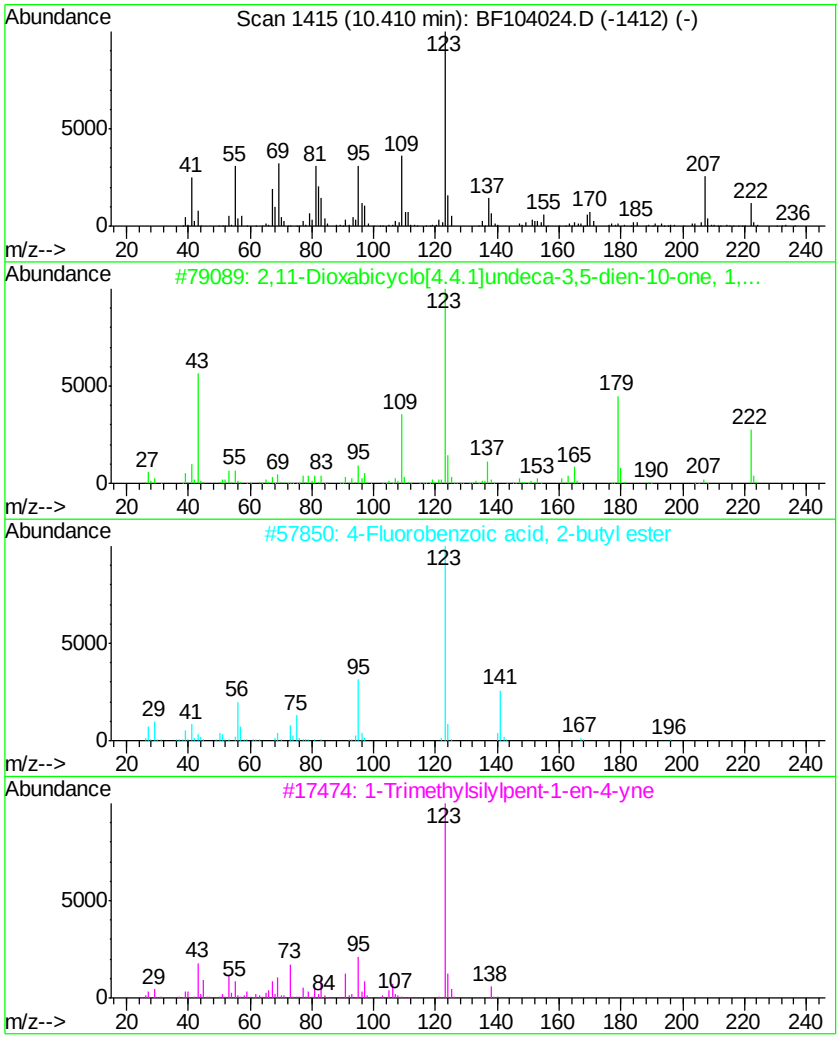
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

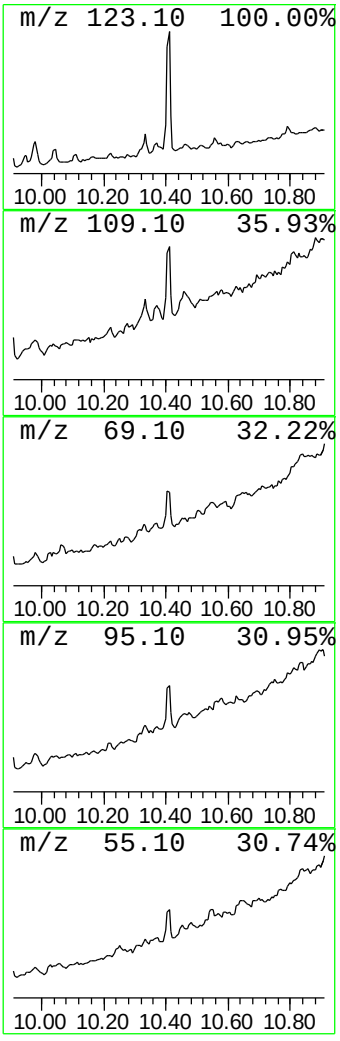
****

Peak Number 9 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	17.66 ng	516574	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	59
2	4-Fluorobenzoic acid, 2-butyl ester	196	C11H13FO2	090172-12-6	49
3	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	49
4	(Phenylthio)acetic acid, cyclobu...	222	C12H14O2S	1000299-95-5	49
5	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032818\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.74	6.74	7.5	ng	268403	1	6.96	712335	20.0
Benzene, 1,2-dich...	8.96	5.7	ng	262836	2	8.25	926117	20.0
unknown9.23	9.23	2.2	ng	64301	3	10.00	585126	20.0
1H-Indene, octahy...	9.70	5.8	ng	169579	3	10.00	585126	20.0
unknown9.86	9.86	5.2	ng	152773	3	10.00	585126	20.0
unknown9.90	9.90	8.3	ng	241646	3	10.00	585126	20.0
unknown10.24	10.24	8.1	ng	236561	3	10.00	585126	20.0
2,11-Dioxabicyclo...	10.41	17.7	ng	516574	3	10.00	585126	20.0