LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116743.D
Acq On : 1 Sep 2019 15:32
Operator : HP/JU
Sample : K4527-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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	5.451	568	572	576	rBV	1837962	1712625	71.31%	7.678%
2	6.469	740	745	748	rBV	2127236	1915710	79.77%	8.589%
3	6.610	765	769	773	rBV	2207478	1960778	81.65%	8.791%
4	6.845	805	809	812	rBV	722297	599496	24.96%	2.688%
5	7.004	832	836	839	rVB	1614502	1442400	60.06%	6.467%
6	7.398	895	903	906	rBV	1417748	1241708	51.70%	5.567%
7	8.127	1023	1027	1030	rBV	967399	850118	35.40%	3.811%
8	8.880	1152	1155	1162	rBV	108646	123830	5.16%	0.555%
9	9.198	1204	1209	1212	rBV	2807422	2401533	100.00%	10.767%
10	9.286	1220	1224	1227	rBV2	120679	136975	5.70%	0.614%
11	9.316	1227	1229	1233	rVB	101488	100297	4.18%	0.450%
12	9.592	1273	1276	1280	rBV2	607767	515000	21.44%	2.309%
13	9.651	1284	1286	1290	rVV2	116811	112516	4.69%	0.504%
14	9.751	1300	1303	1306	rBV3	259921	268838	11.19%	1.205%
15	9.798	1309	1311	1314	rVB	479467	352476	14.68%	1.580%
16	9.880	1319	1325	1328	rVV	1231704	1306755	54.41%	5.859%
17	9.927	1330	1333	1338	rVB2	149587	181685	7.57%	0.815%
18	10.080	1356	1359	1362	rVB3	117145	109725	4.57%	0.492%
19	10.221	1378	1383	1386	rBV	310497	375997	15.66%	1.686%
20	10.257	1386	1389	1392	rBV3	242123	278292	11.59%	1.248%
21	10.292	1392	1395	1398	rVV	572526	497442	20.71%	2.230%
22	10.345	1401	1404	1410	rVB5	242093	372445	15.51%	1.670%
23	10.510	1430	1432	1435	rBV2	142427	129364	5.39%	0.580%
24	10.663	1454	1458	1461	rBV	1550438	1389863	57.87%	6.231%
25	10.704	1463	1465	1468	rVB	256056	247313	10.30%	1.109%
26	10.892	1495	1497	1502	rBV	157639	165316	6.88%	0.741%
27	10.939	1503	1505	1513	rVV3	189316	293100	12.20%	1.314%
28	11.363	1574	1577	1579	rBV	1010128	946615	39.42%	4.244%
29	11.386	1579	1581	1583	rVB	557332	442250	18.42%	1.983%
30	11.892	1665	1667	1668	rBV	709921	590294	24.58%	2.646%
31	12.957	1845	1848	1852	rBV	1353213	1244109	51.80%	5.578%

Sum of corrected areas: 22304865

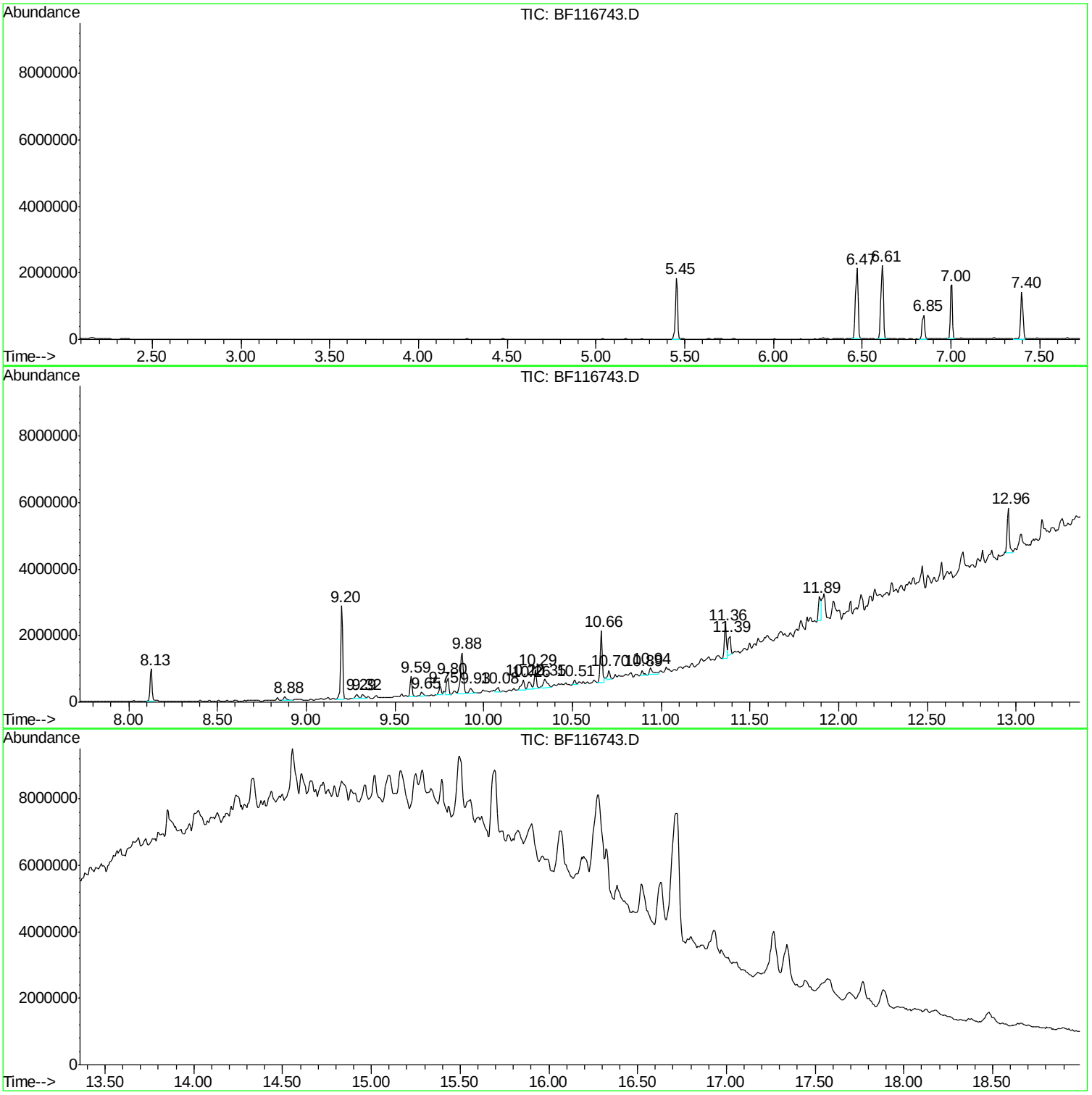
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116743.D
Acq On : 1 Sep 2019 15:32
Operator : HP/JU
Sample : K4527-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116743.D
Acq On : 1 Sep 2019 15:32
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

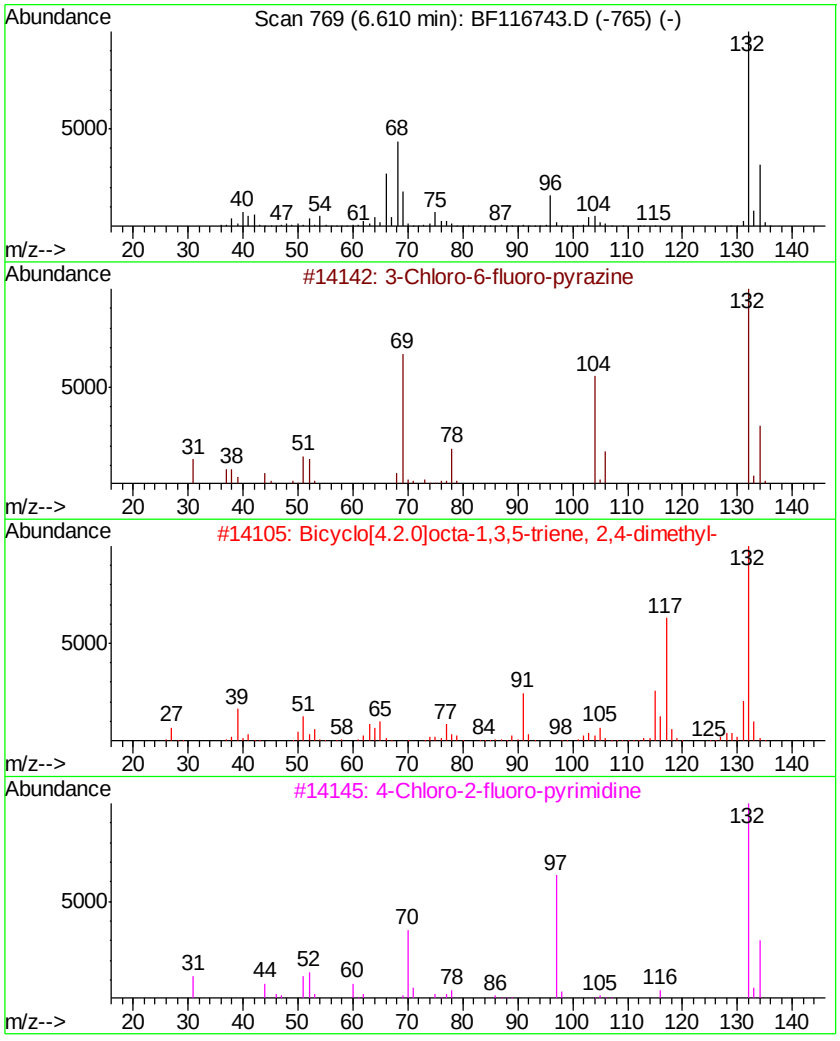
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

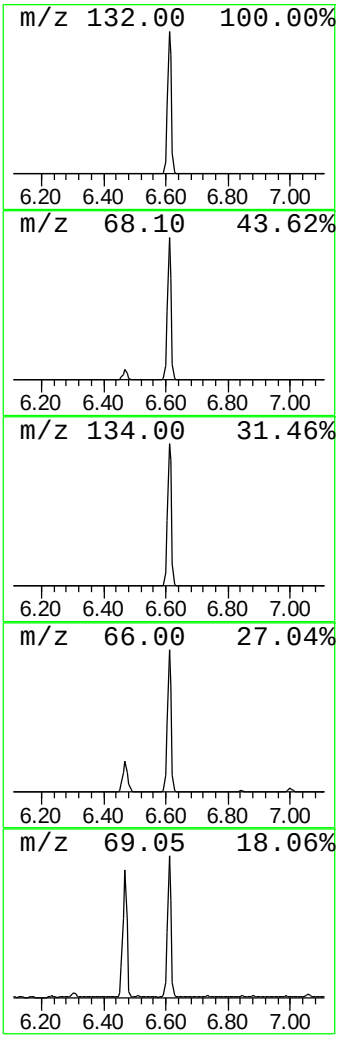
****

Peak Number 1 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	65.41 ng	1960780	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Data File : BF116743.D
Acq On : 1 Sep 2019 15:32
Operator : HP/JU
Sample : K4527-14
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Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

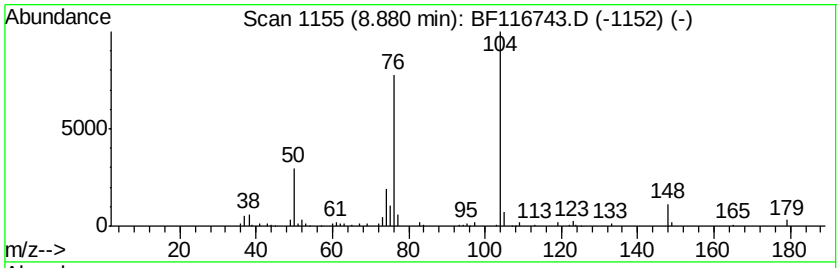
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

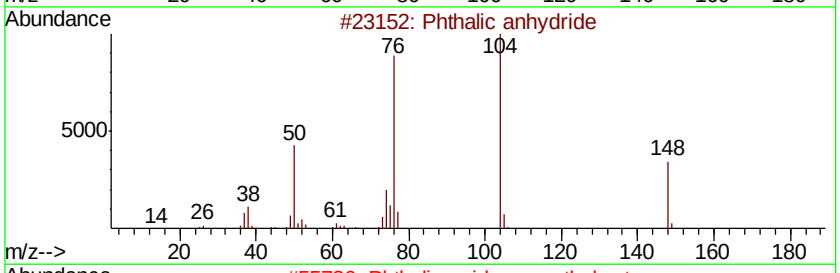
****

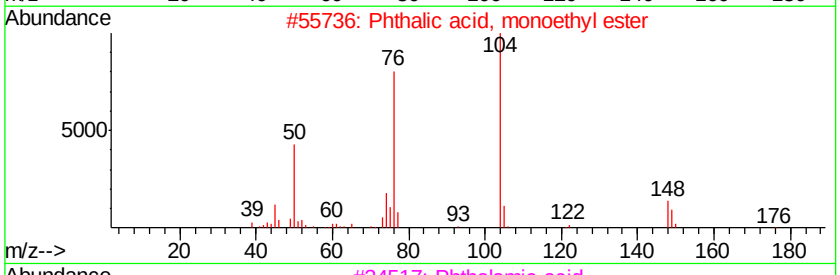
Peak Number 3 Phthalic anhydride Concentration Rank 11

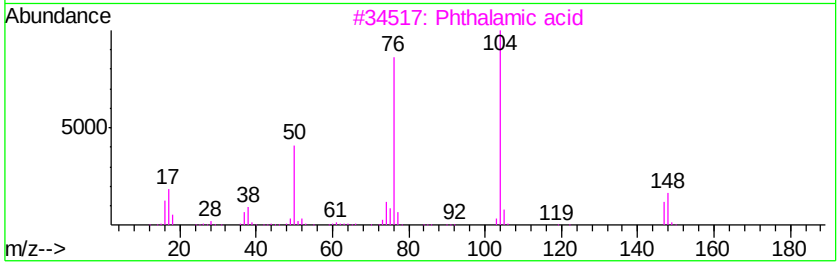
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	2.91 ng	123830	Naphthalene-d8	8.13

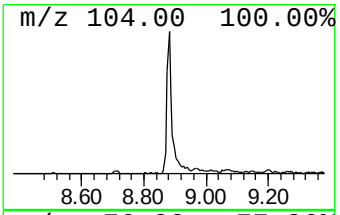
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	94
2	Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	83
3	Phthalamic acid	165	C8H7NO3	000088-97-1	78
4	Indan-1,2,3-trione	160	C9H4O3	000938-24-9	74
5	Ninhydrin	178	C9H6O4	000485-47-2	64

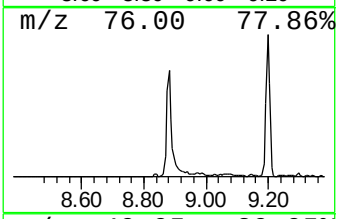


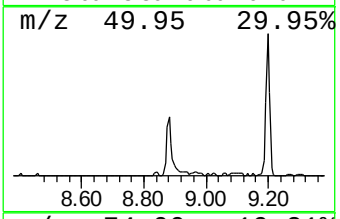


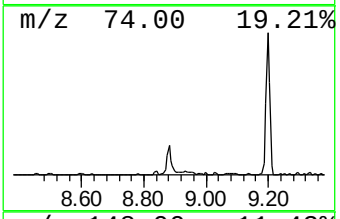


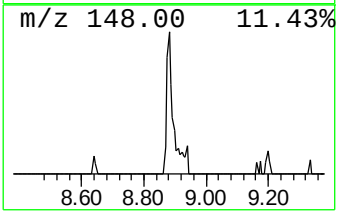












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116743.D
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

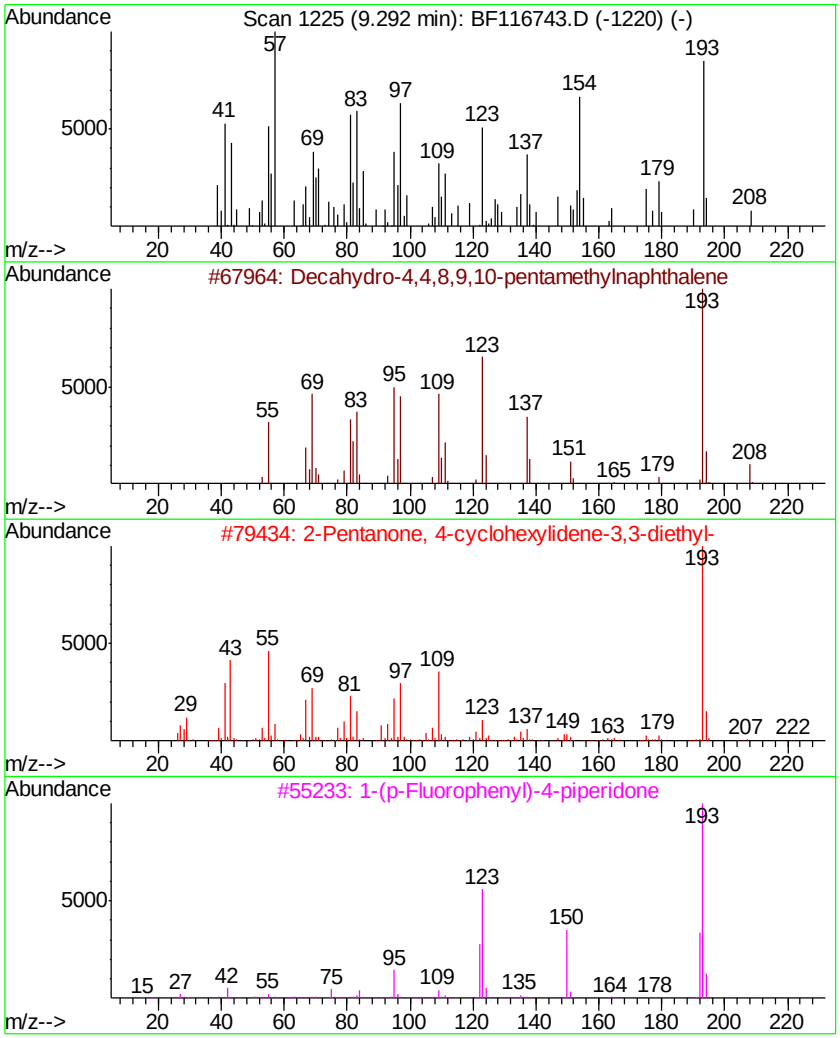
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

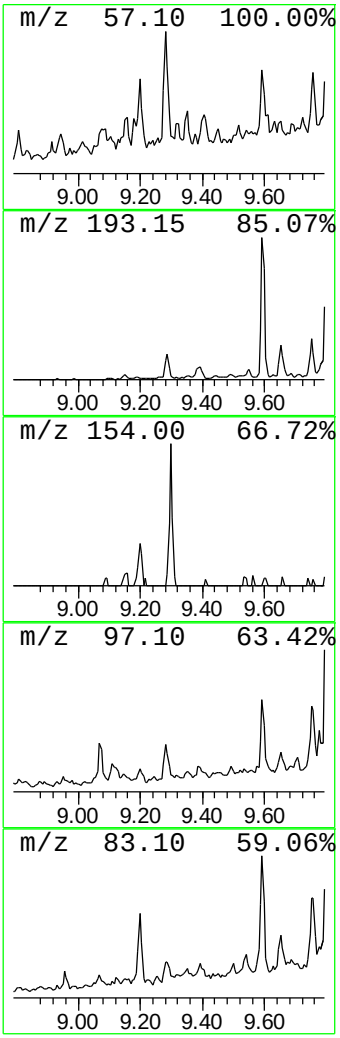
****

Peak Number 4 Decahydro-4,4,8,9,10-pentam... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.29	2.10 ng	136975	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	93
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	35
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
4	Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	25
5	1H-Pyrrole-2,5-dione, dihydro-1-...	193	C10H11NO3	1000351-31-4	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
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Misc :
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Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

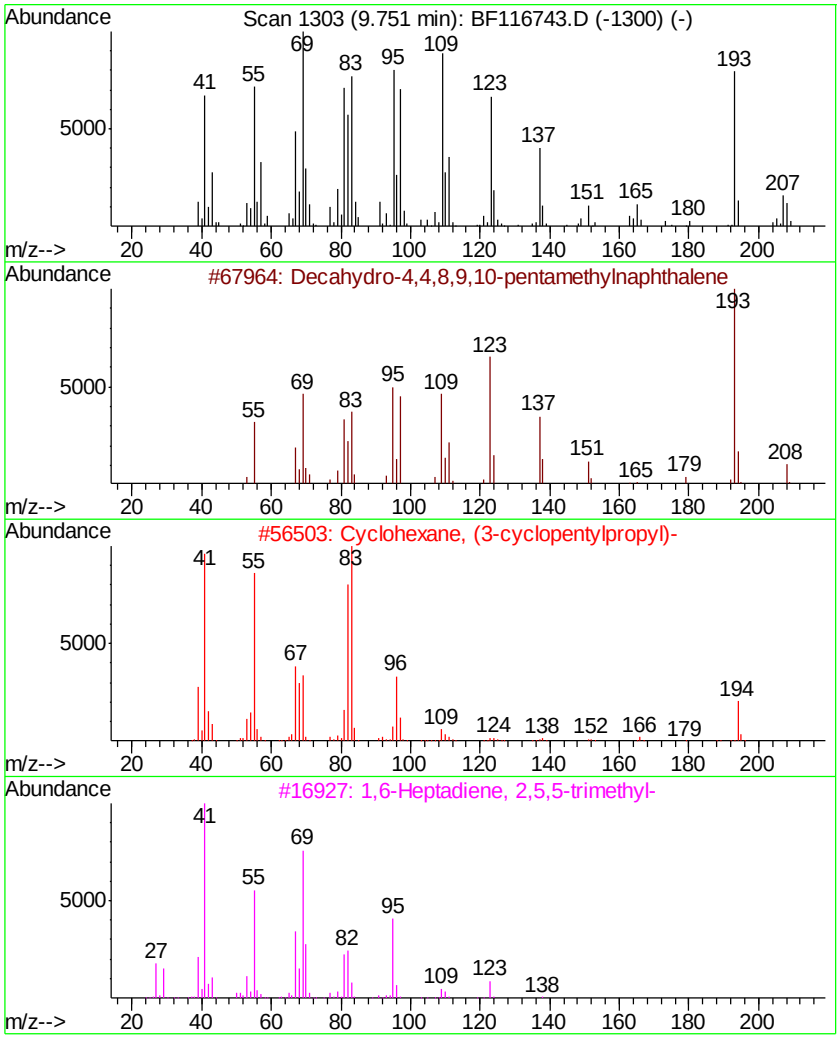
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

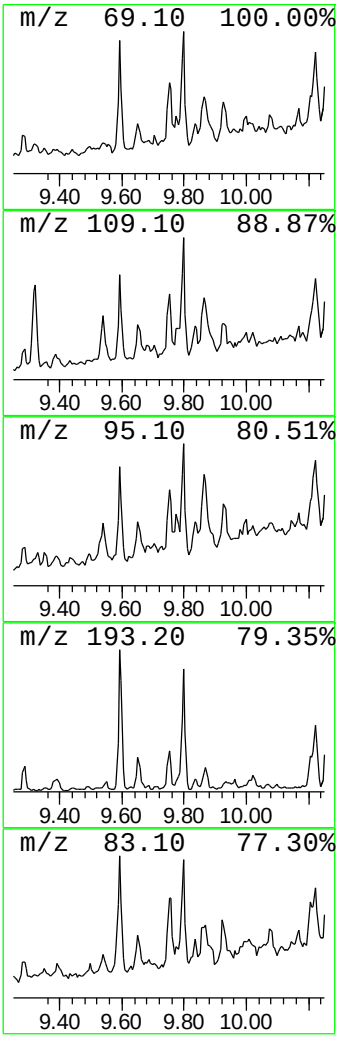
****

Peak Number 5 Cyclohexane, (3-cyclopentyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	4.11 ng	268838	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	94
2	Cyclohexane, (3-cyclopentylpropyl)-	194	C14H26	002883-07-0	53
3	1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	22
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	22
5	(2Z,4E)-3,7,11-Trimethyl-2,4-dod...	208	C15H28	1000374-08-6	15





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Operator : HP/JU
Sample : K4527-14
Misc :
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Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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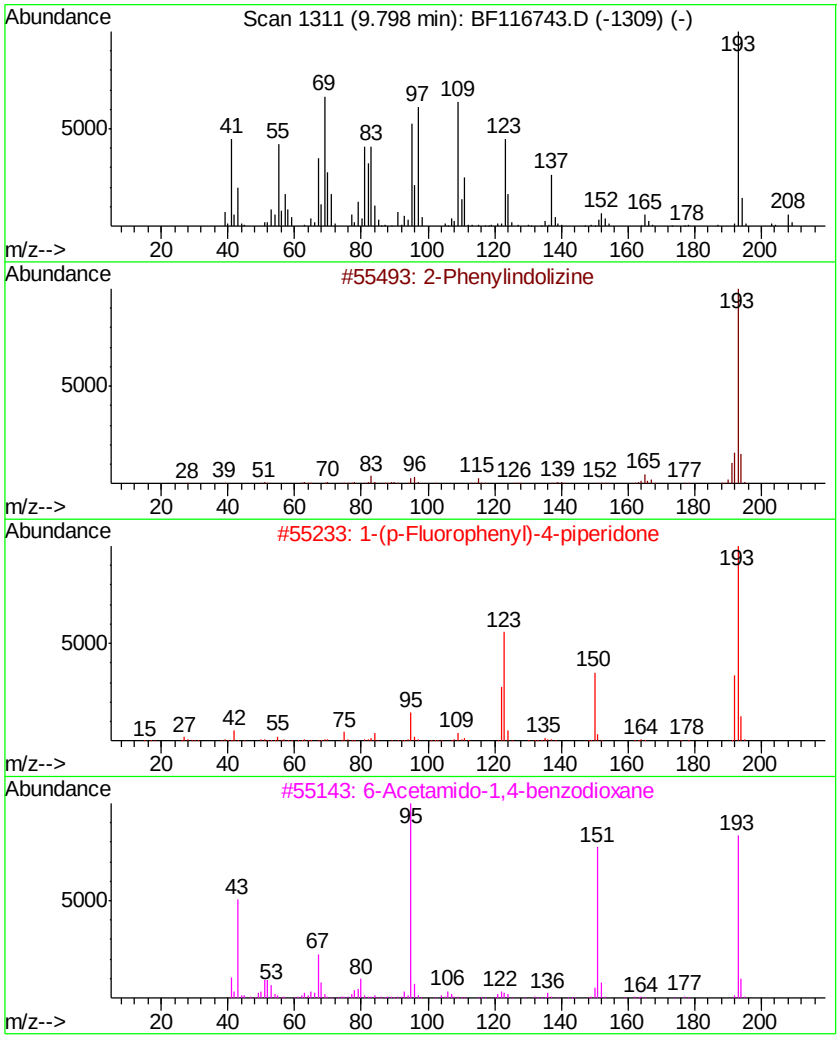
TIC Integration Parameters: LSCINT.P

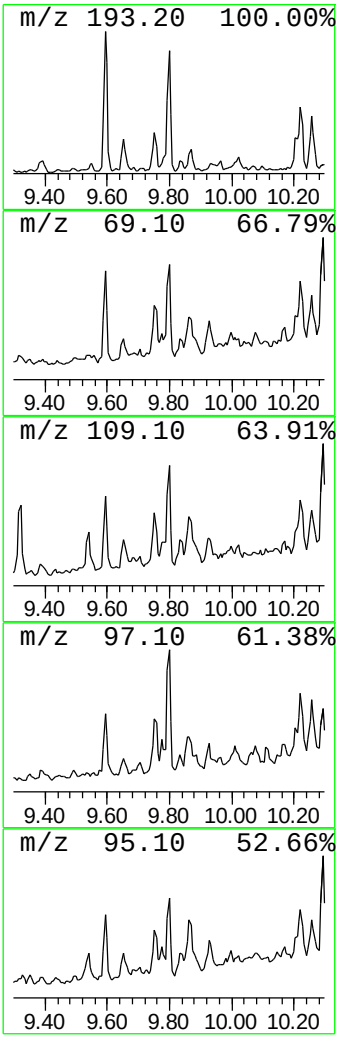
****

Peak Number 6 unknown9.80 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.80	5.39 ng	352476	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenylindolizine	193	C14H11N	025379-20-8	35
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	30
3	6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	22
4	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	18
5	[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	14





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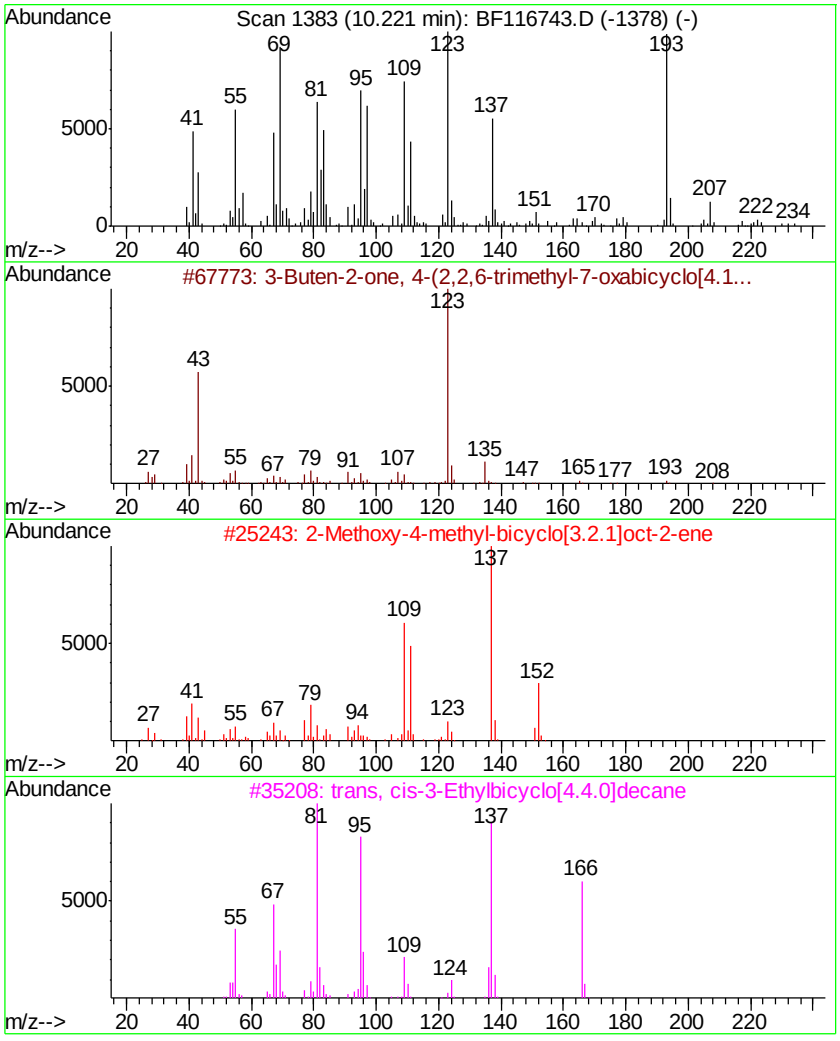
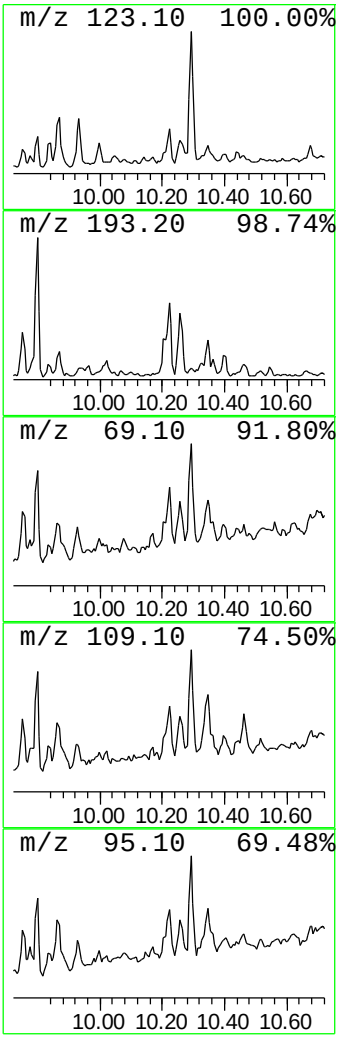
****

Peak Number 7 unknown10.22 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.22	5.75 ng	375997	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 4-(2,2,6-trimethy...	208	C13H20O2	023267-57-4	35
2	2-Methoxy-4-methyl-bicyclo[3.2.1...	152	C10H16O	1000188-09-4	20
3	trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	15
4	1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	11
5	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	11





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TIC Library : C:\DATABASE\NIST11.L
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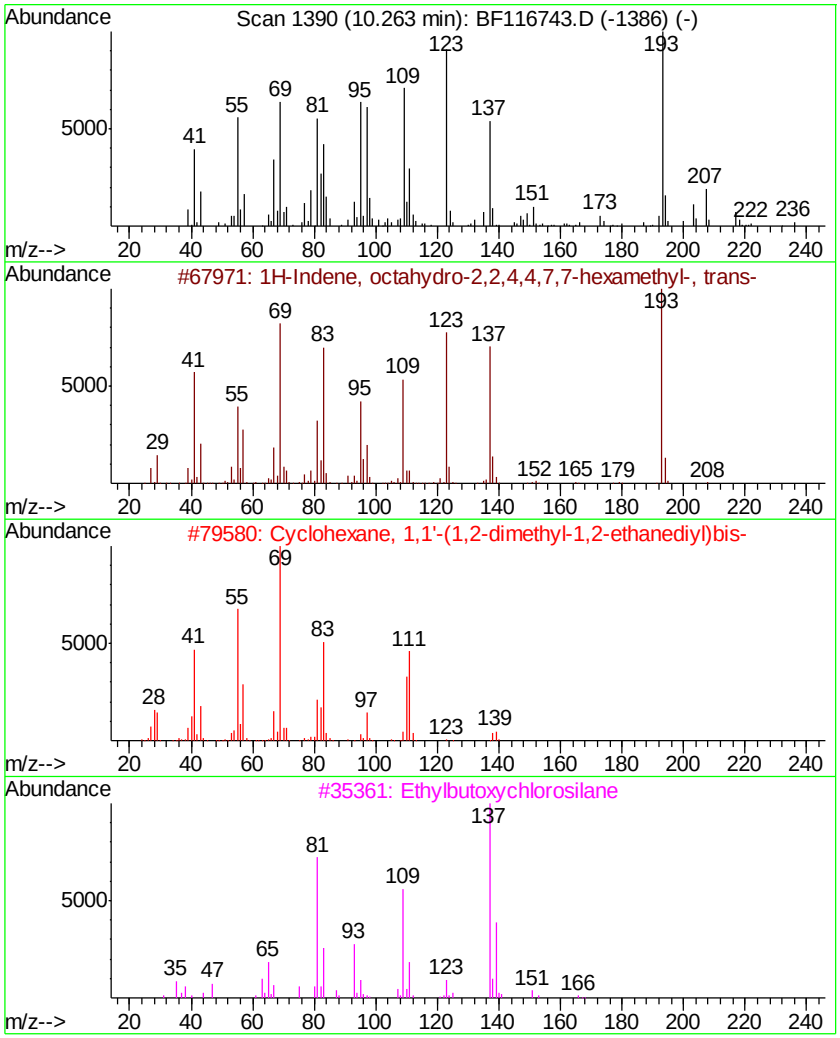
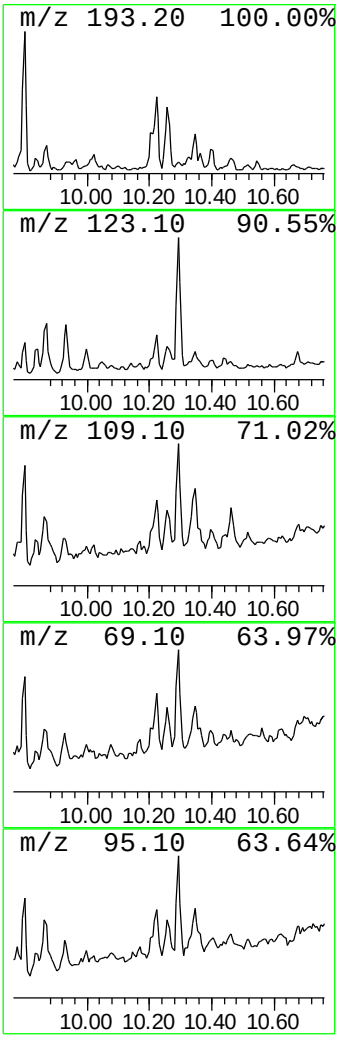
****

Peak Number 8 1H-Indene, octahydro-2,2,4,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	4.26 ng	278292	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	58
2	Cyclohexane, 1,1'-(1,2-dimethyl-...	222	C16H30	074663-71-1	22
3	Ethylbutoxychlorosilane	166	C6H15ClOSi	018171-08-9	14
4	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	14
5	Phorone	138	C9H14O	000504-20-1	11





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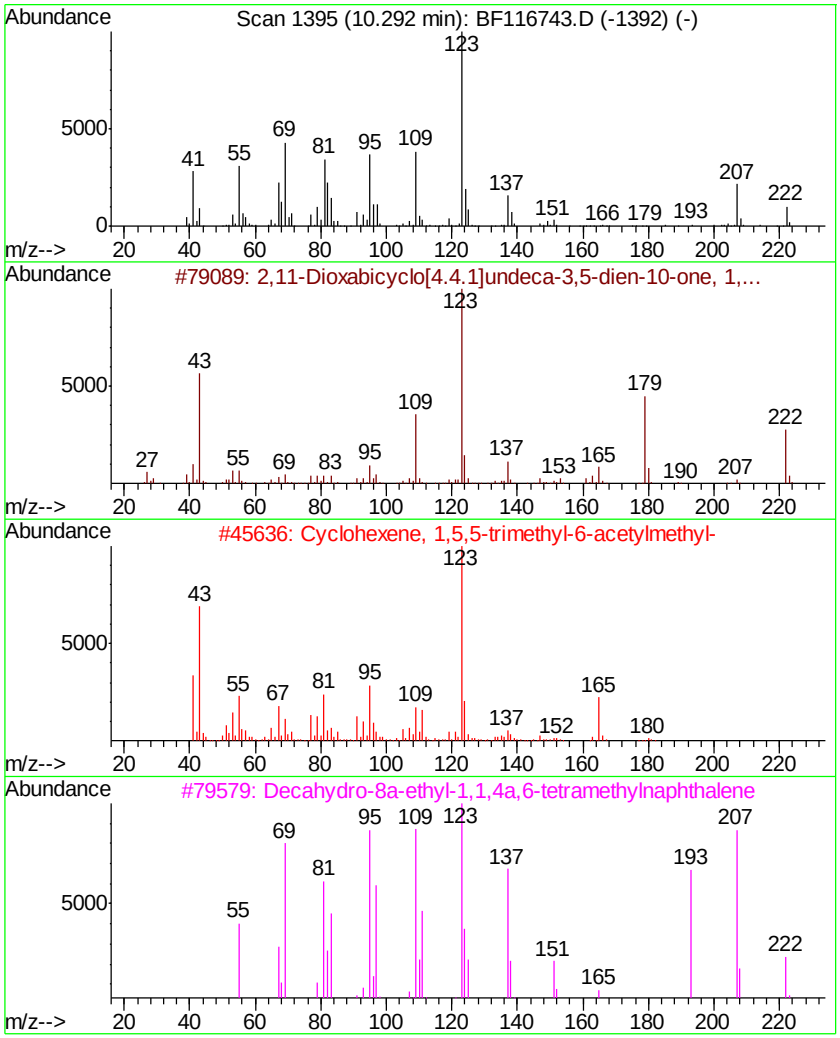
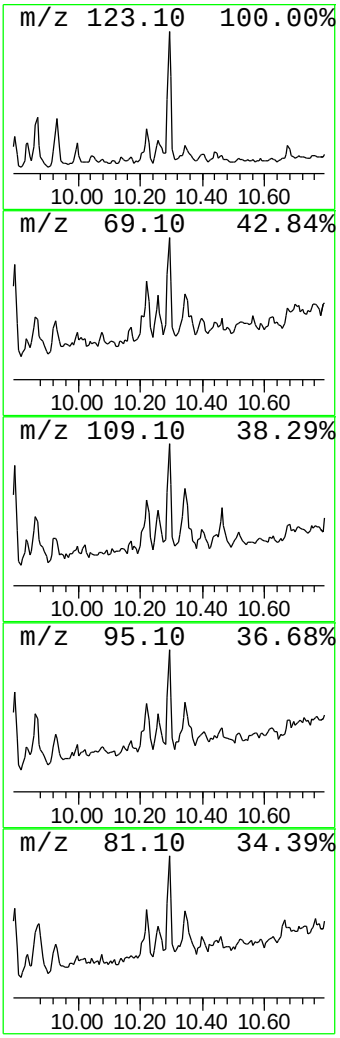
****

Peak Number 9 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.29	7.61 ng	497442	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	53
2	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	40
3	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	38
4	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	38
5	4-Fluorobenzoic acid, 3-tetradec...	336	C21H33FO2	1000280-68-1	38





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Acq On : 1 Sep 2019 15:32
Operator : HP/JU
Sample : K4527-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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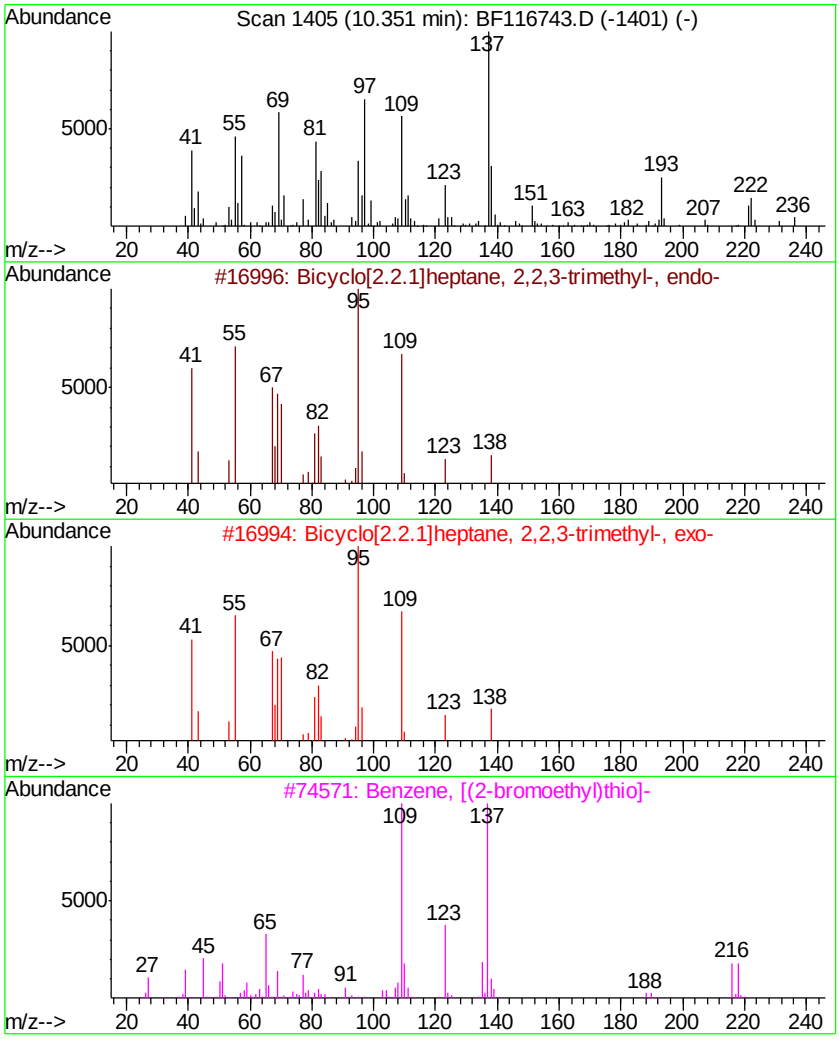
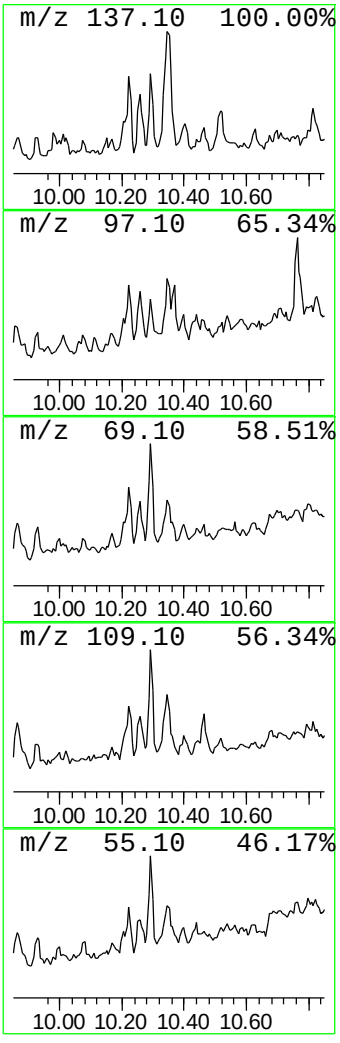
Peak Number 10 unknown10.35 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	5.70 ng	372445	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	42
2	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	42
3	Benzene, [(2-bromoethyl)thio]-	216	C8H9BrS	004837-01-8	27
4	Benzenamine, 3-ethoxy-	137	C8H11NO	000621-33-0	22
5	2(1H)-Pyridone, 1-ethyl-4-methyl-	137	C8H11NO	019006-62-3	22





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Data File : BF116743.D
Acq On : 1 Sep 2019 15:32
Operator : HP/JU
Sample : K4527-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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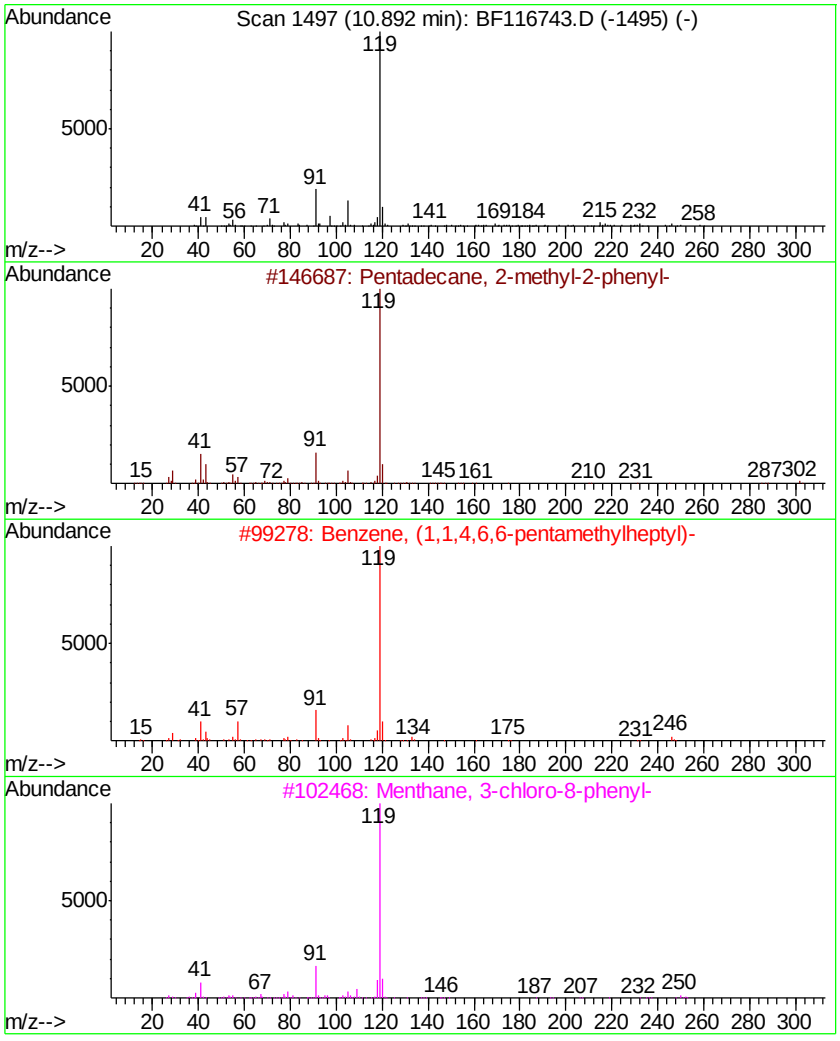
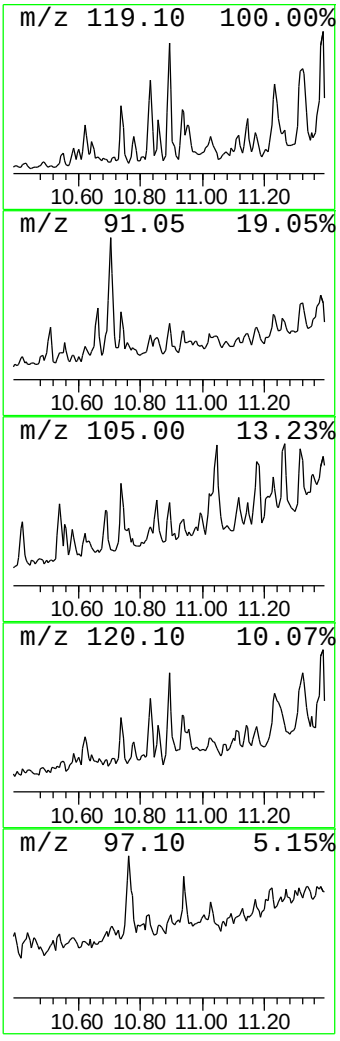
Peak Number 11 Pentadecane, 2-methyl-2-phe... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.89	3.49 ng	165316	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	72
2	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	72
3	Menthane, 3-chloro-8-phenyl-	250	C16H23Cl	184007-21-4	64
4	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	64
5	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	64





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Data File : BF116743.D
Acq On : 1 Sep 2019 15:32
Operator : HP/JU
Sample : K4527-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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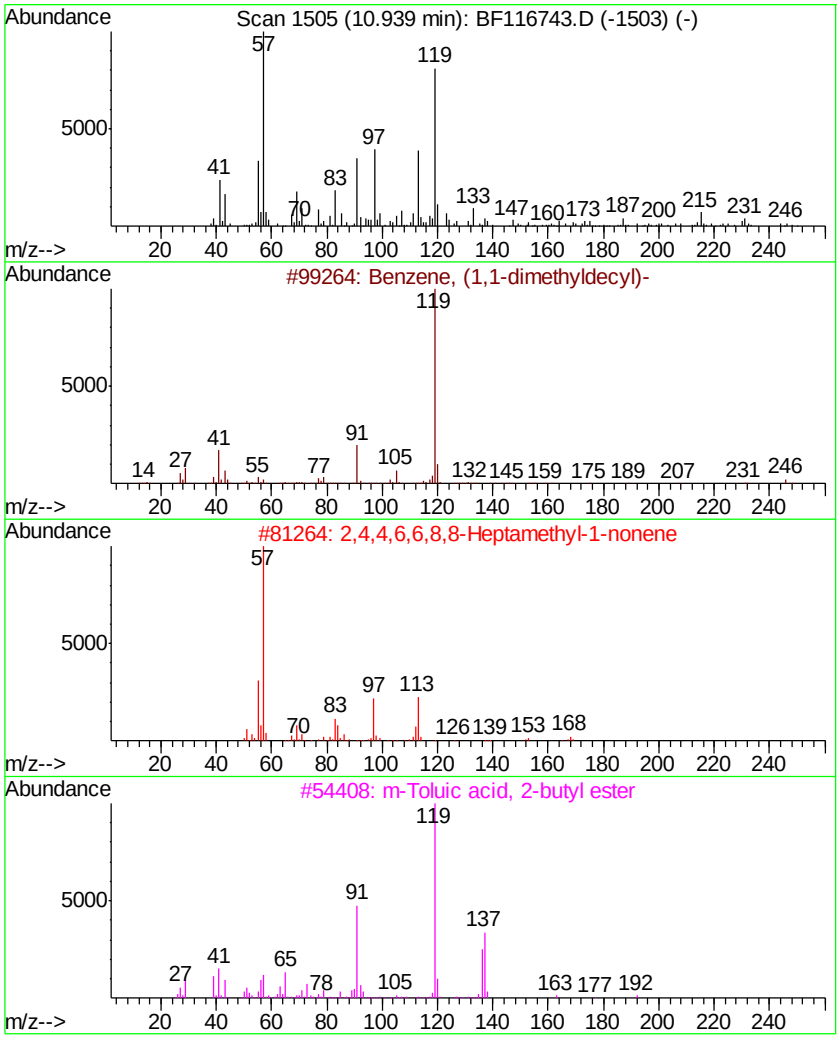
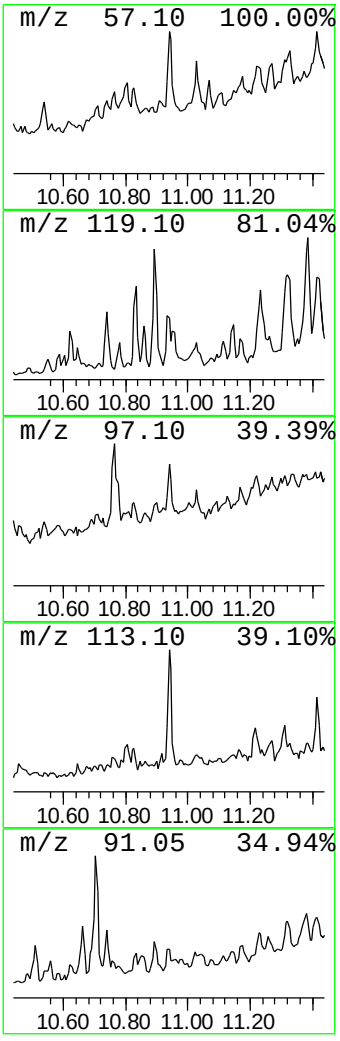
Peak Number 12 unknown10.94 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.94	6.19 ng	293100	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	38
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38
3	m-Toluic acid, 2-butyl ester	192	C12H16O2	005448-57-7	38
4	o-Toluic acid, oct-3-en-2-yl ester	246	C16H22O2	1000292-51-3	38
5	2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090119\
Data File : BF116743.D
Acq On : 1 Sep 2019 15:32
Operator : HP/JU
Sample : K4527-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T9-12-13-O-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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
unknown6.61	6.61	65.4	ng	1960780	1	6.85	599496	20.0
Phthalic anhydride	8.88	2.9	ng	123830	2	8.13	850118	20.0
Decahydro-4,4,8,9...	9.29	2.1	ng	136975	3	9.88	1306760	20.0
Cyclohexane, (3-c...	9.75	4.1	ng	268838	3	9.88	1306760	20.0
unknown9.80	9.80	5.4	ng	352476	3	9.88	1306760	20.0
unknown10.22	10.22	5.8	ng	375997	3	9.88	1306760	20.0
1H-Indene, octahy...	10.26	4.3	ng	278292	3	9.88	1306760	20.0
2,11-Dioxabicyclo...	10.29	7.6	ng	497442	3	9.88	1306760	20.0
unknown10.35	10.35	5.7	ng	372445	3	9.88	1306760	20.0
Pentadecane, 2-me...	10.89	3.5	ng	165316	4	11.36	946615	20.0
unknown10.94	10.94	6.2	ng	293100	4	11.36	946615	20.0