LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116496.D
Acq On : 23 Aug 2019 23:57
Operator : HP/JU
Sample : K4385-16
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

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-BF082319.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	2.146	4	10	18	rVB	1692742	2315158	100.00%	12.348%
2	5.498	575	580	583	rBV	1806671	1627165	70.28%	8.679%
3	6.504	741	751	754	rBV	1854067	1633597	70.56%	8.713%
4	6.651	771	776	779	rBV	1994197	1690215	73.01%	9.015%
5	6.886	812	816	819	rBV	573619	521226	22.51%	2.780%
6	7.039	837	842	846	rBV	1579444	1349980	58.31%	7.200%
7	7.439	903	910	913	rBV	1159601	977091	42.20%	5.211%
8	8.163	1030	1033	1036	rBV	723525	565552	24.43%	3.016%
9	8.910	1157	1160	1164	rBV	135954	128236	5.54%	0.684%
10	9.233	1211	1215	1219	rBV	1989068	1688890	72.95%	9.008%
11	9.322	1227	1230	1236	rBV3	189069	208034	8.99%	1.110%
12	9.386	1236	1241	1244	rVV6	97130	126834	5.48%	0.676%
13	9.427	1245	1248	1251	rVB2	130527	135334	5.85%	0.722%
14	9.633	1279	1283	1287	rVB2	522022	502727	21.71%	2.681%
15	9.692	1290	1293	1296	rBV2	133027	141347	6.11%	0.754%
16	9.792	1307	1310	1312	rBV2	337661	337746	14.59%	1.801%
17	9.833	1315	1317	1320	rVB	701868	572648	24.73%	3.054%
18	9.874	1321	1324	1326	rBV2	175921	165817	7.16%	0.884%
19	9.916	1326	1331	1335	rVB2	816586	987232	42.64%	5.265%
20	9.969	1337	1340	1344	rBV2	178548	230509	9.96%	1.229%
21	10.180	1374	1376	1378	rBV2	94772	101216	4.37%	0.540%
22	10.263	1388	1390	1392	rVB	252681	185952	8.03%	0.992%
23	10.292	1392	1395	1398	rBV4	238037	272081	11.75%	1.451%
24	10.333	1399	1402	1405	rVB	624290	517097	22.34%	2.758%
25	10.386	1408	1411	1413	rBV	206259	223798	9.67%	1.194%
26	10.698	1461	1464	1467	rBV	1098905	993908	42.93%	5.301%
27	11.404	1581	1584	1586	rBV	550462	549726	23.74%	2.932%

Sum of corrected areas: 18749116

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
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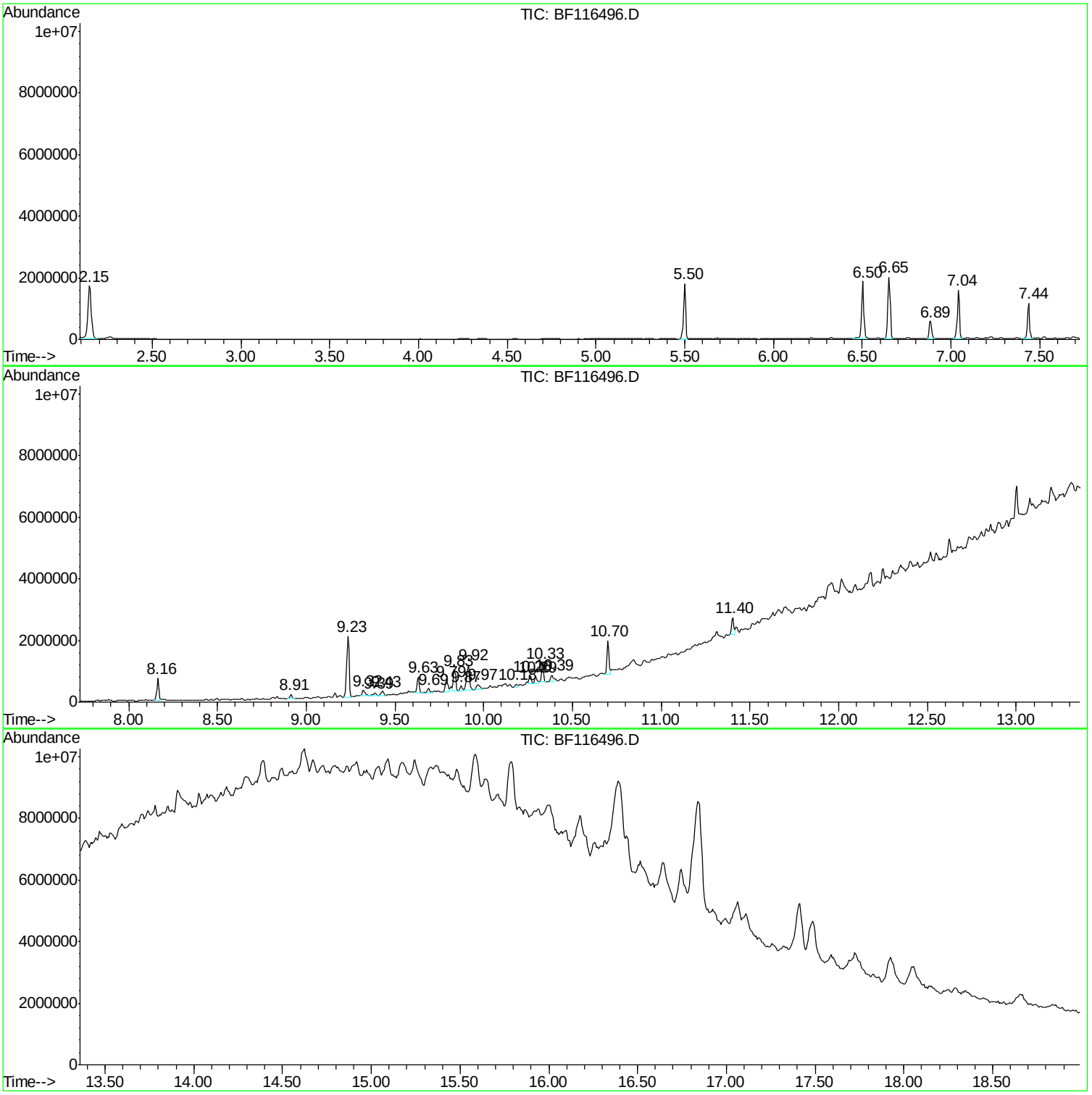
Operator : HP/JU
Sample : K4385-16
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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

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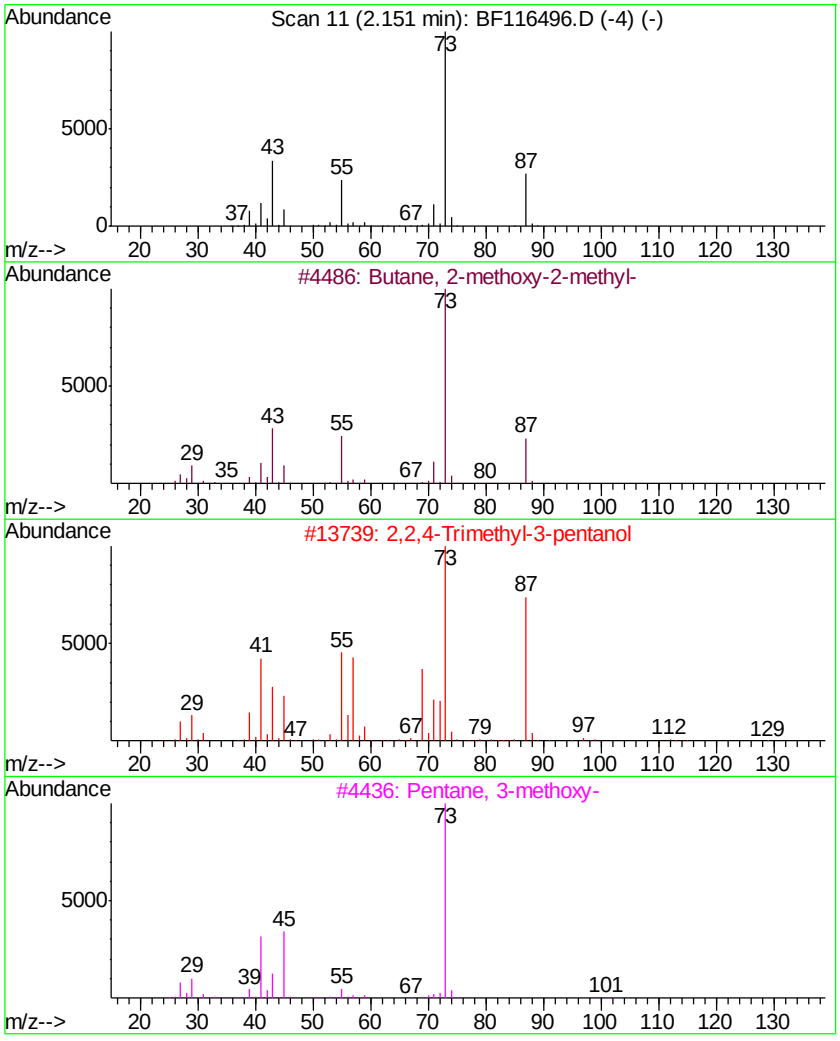
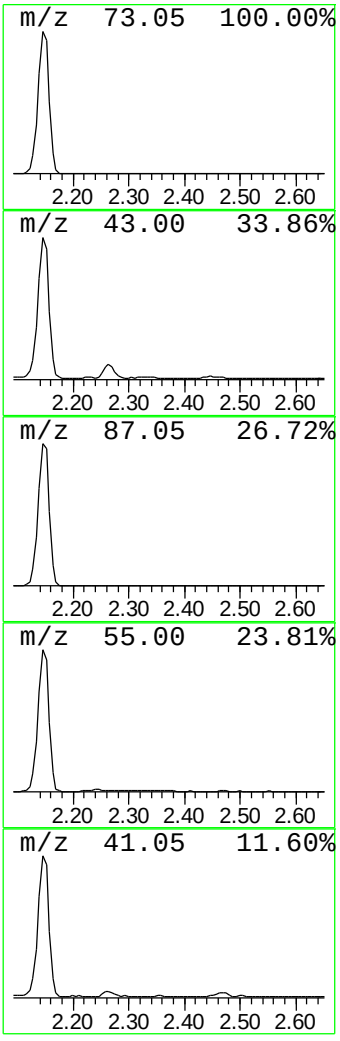
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	88.84 ng	2315160	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Operator : HP/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

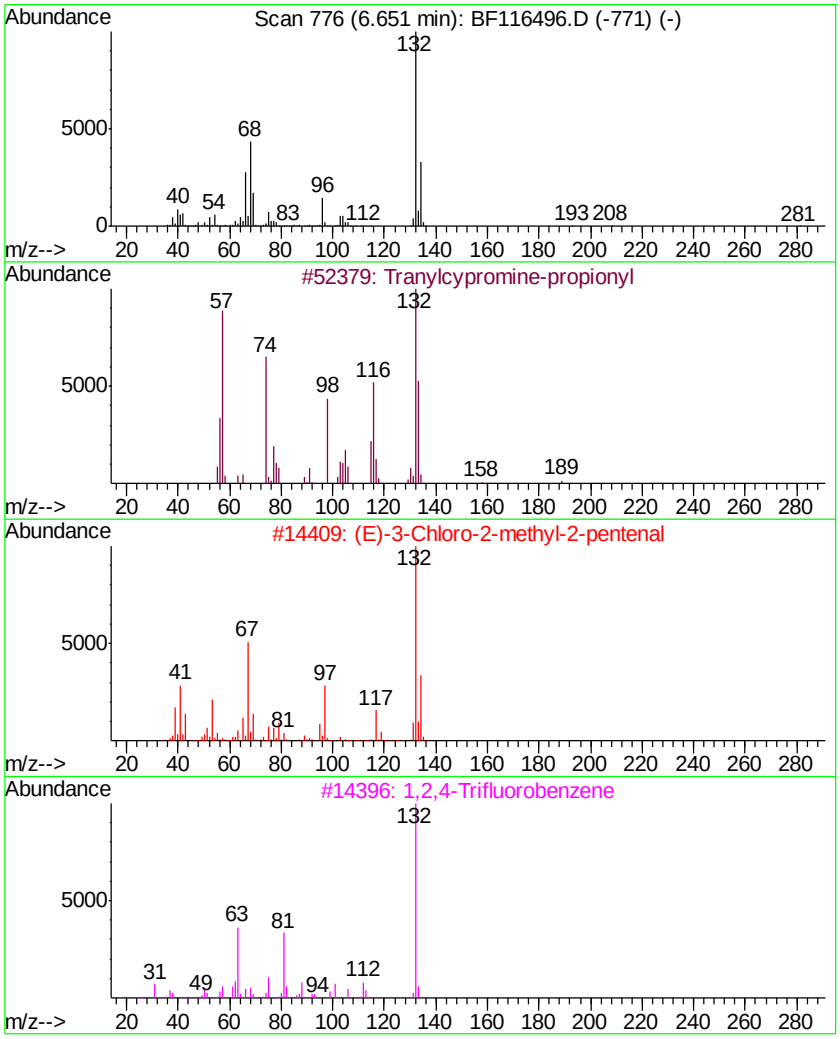
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

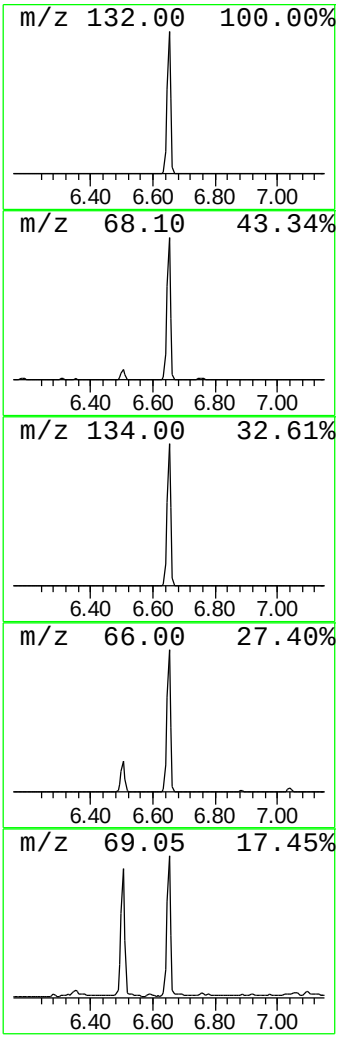
****

Peak Number 2 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	64.86 ng	1690220	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Data File : BF116496.D
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Operator : HP/JU
Sample : K4385-16
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
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TIC Library : C:\DATABASE\NIST11.L
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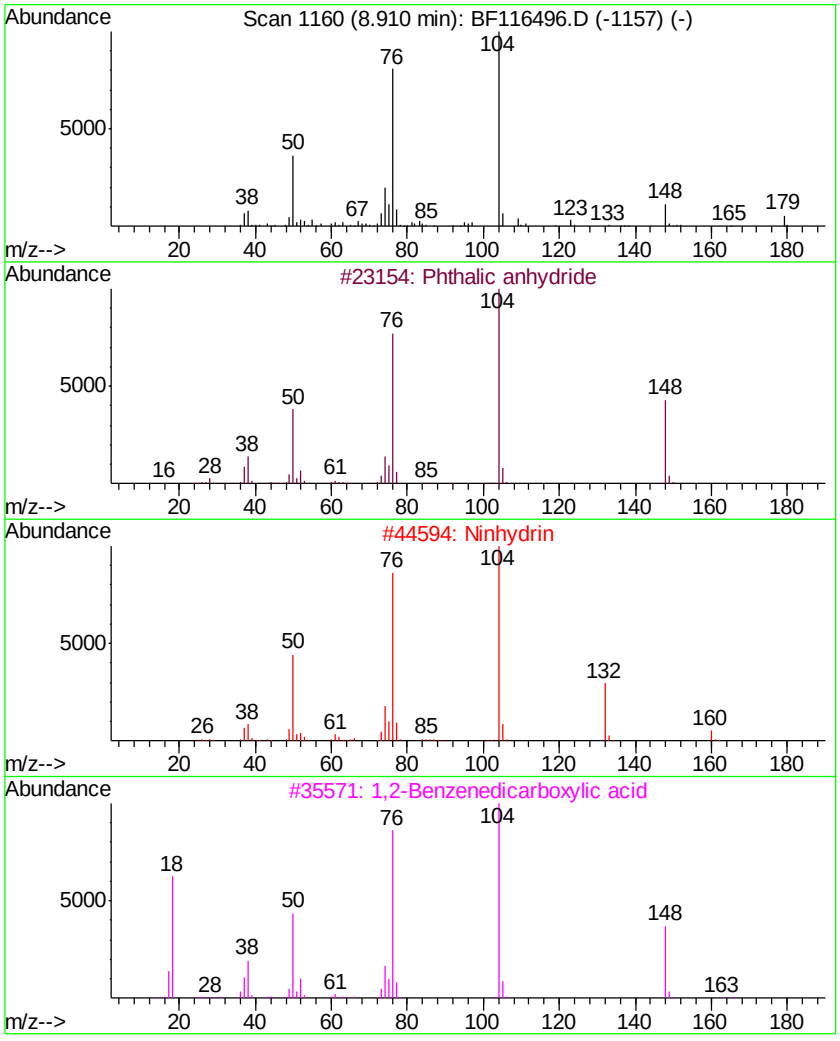
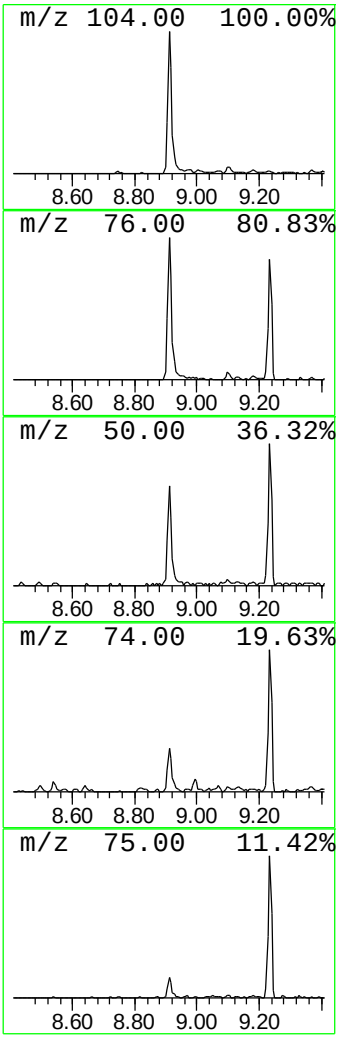
****

Peak Number 4 Phthalic anhydride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.91	4.53 ng	128236	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	95
2	Ninhydrin	178	C9H6O4	000485-47-2	90
3	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	83
4	Phthalamic acid	165	C8H7NO3	000088-97-1	78
5	Indan-1,2,3-trione	160	C9H4O3	000938-24-9	78





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Sample : K4385-16
Misc :
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Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

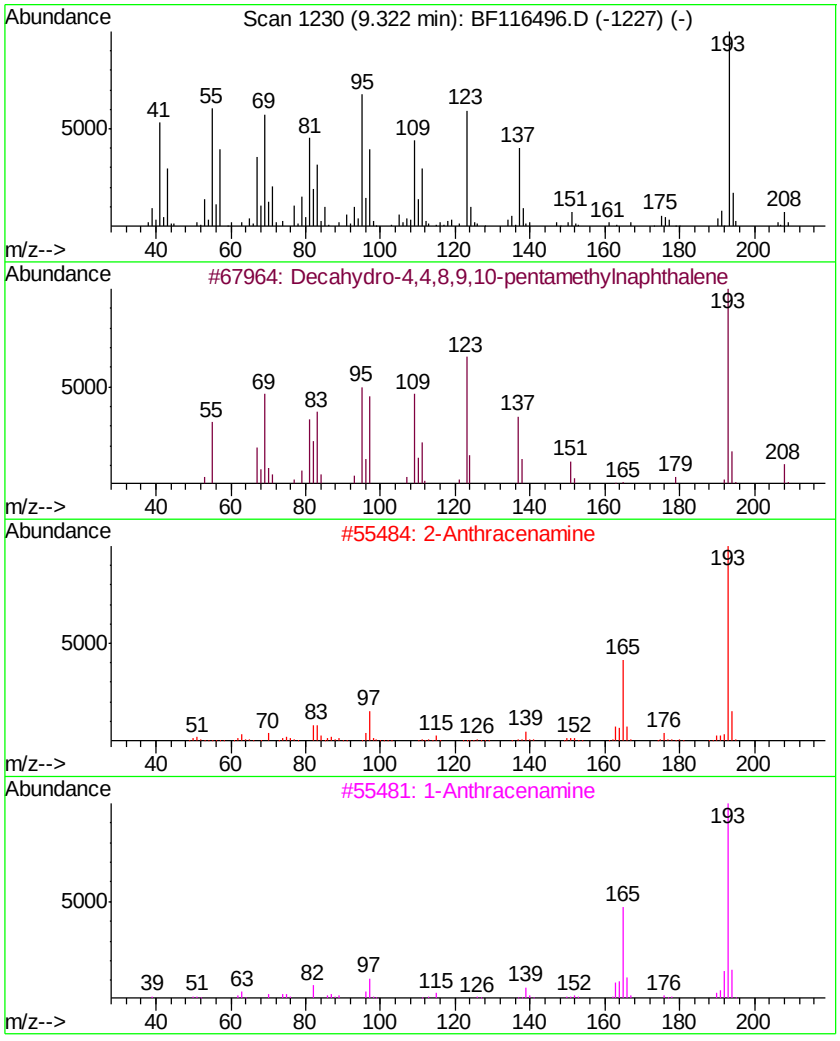
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

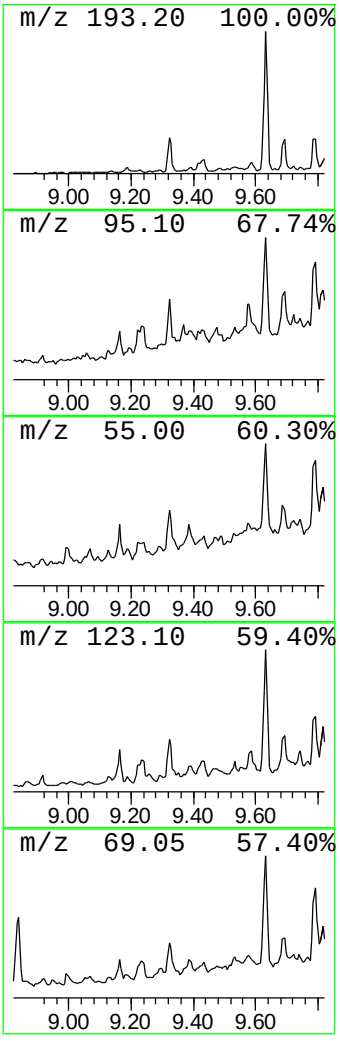
****

Peak Number 5 Decahydro-4,4,8,9,10-pentam... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.32	4.21 ng	208034	Acenaphthene-d10	9.92

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-Anthracenamine	193	C14H11N	000613-13-8	27
3	1-Anthracenamine	193	C14H11N	000610-49-1	27
4	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	20
5	3-Aminophenanthrene	193	C14H11N	001892-54-2	18





Library Search Compound Report

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

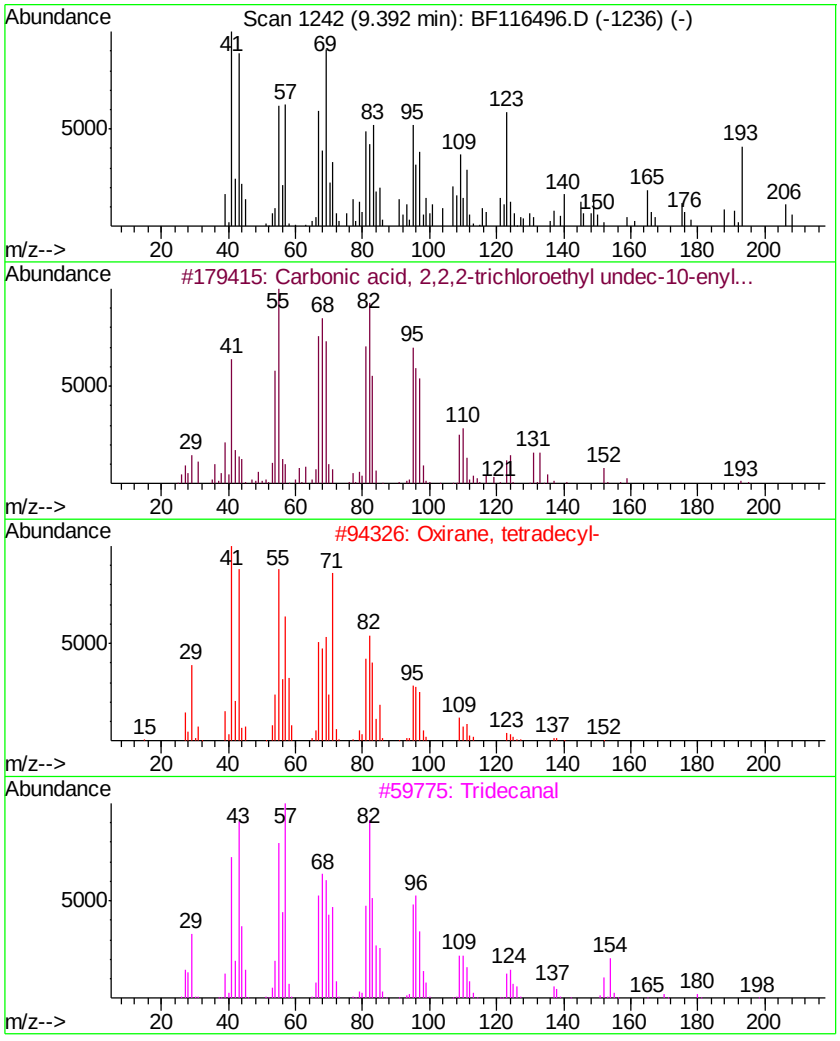
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

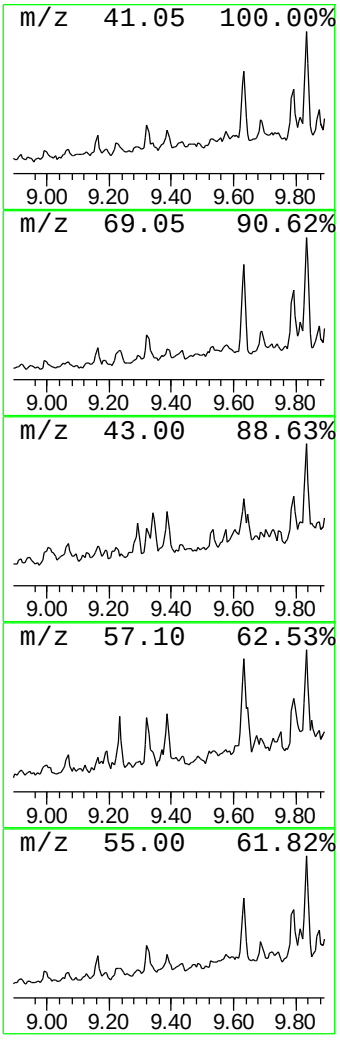
****

Peak Number 6 Carbonic acid, 2,2,2-trichl... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.39	2.57 ng	126834	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, 2,2,2-trichloroet...	344	C14H23Cl3O3	1000314-55-7	64
2	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	64
3	Tridecanal	198	C13H26O	010486-19-8	62
4	Tetradecanal	212	C14H28O	000124-25-4	58
5	Pentadecanal-	226	C15H30O	002765-11-9	58





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Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
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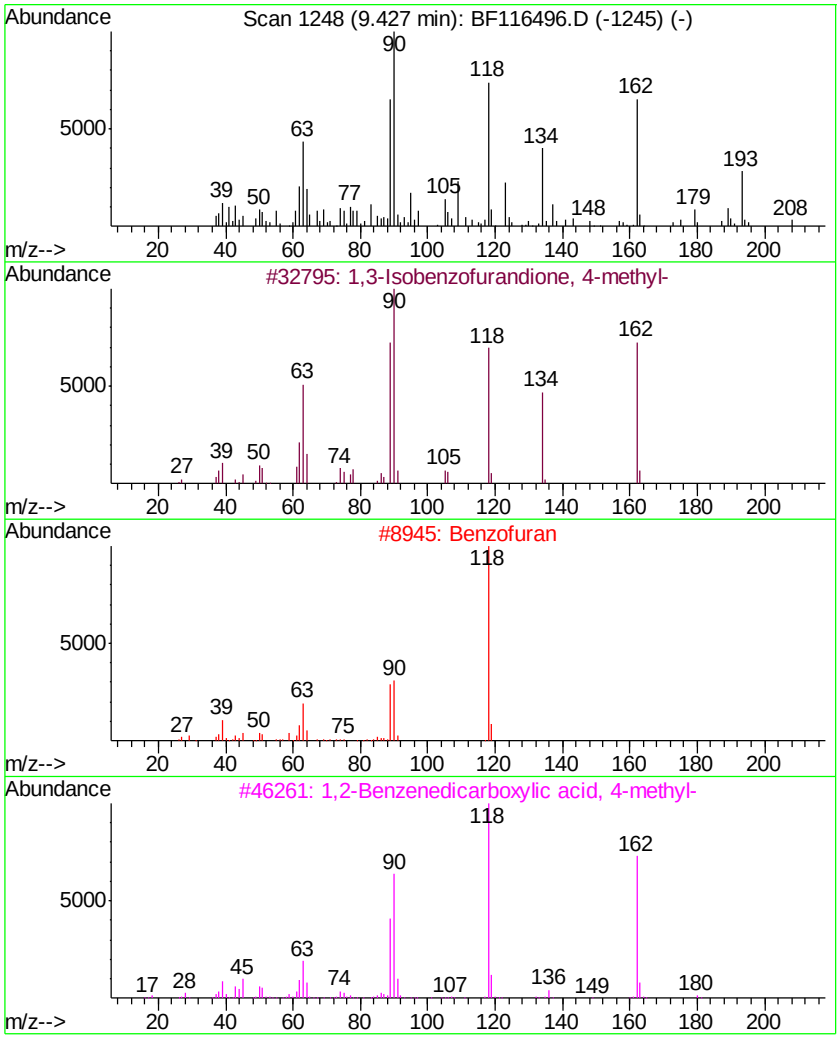
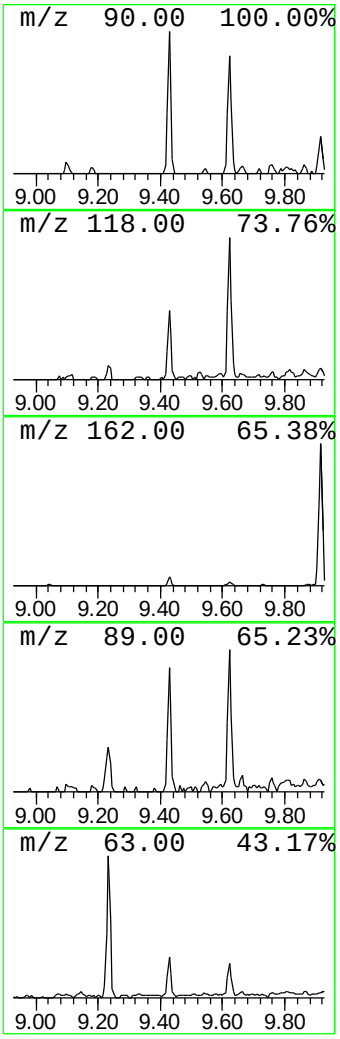
****

Peak Number 7 1,3-Isobenzofurandione, 4-m... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.43	2.74 ng	135334	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Isobenzofurandione, 4-methyl-	162	C9H6O3	004792-30-7	98
2	Benzofuran	118	C8H6O	000271-89-6	95
3	1,2-Benzenedicarboxylic acid, 4-...	180	C9H8O4	004316-23-8	93
4	Benzocyclobuten-1(2H)-one	118	C8H6O	003469-06-5	90
5	4-Methylphthalic anhydride	162	C9H6O3	019438-61-0	89





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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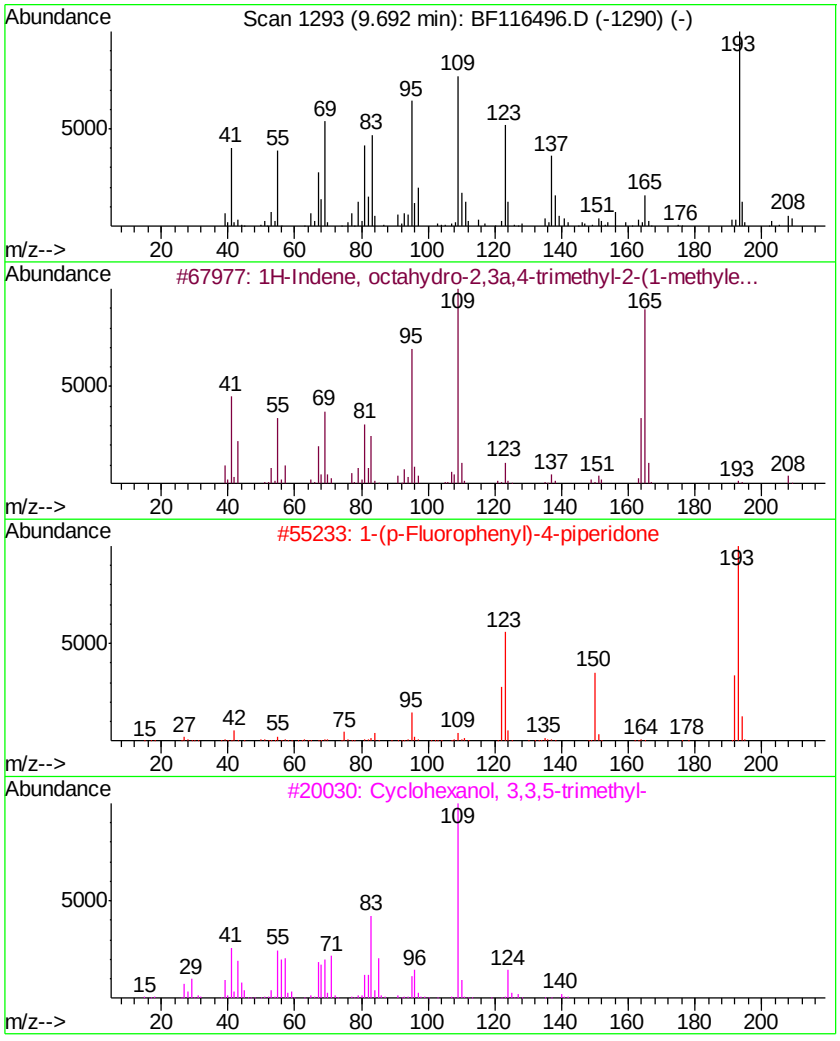
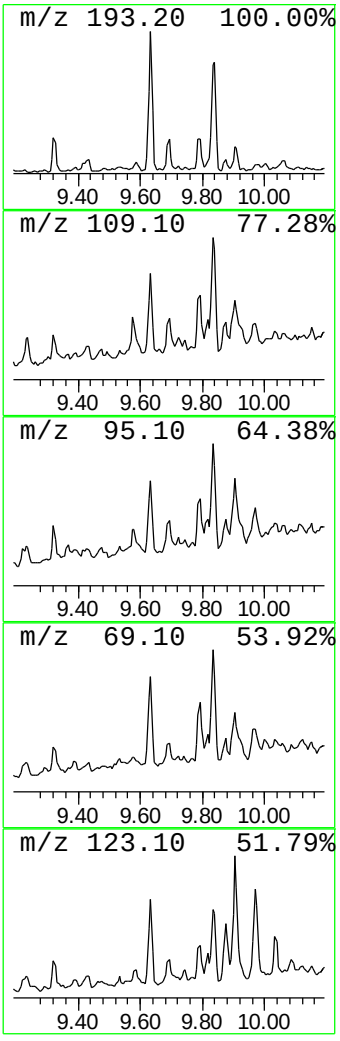
****

Peak Number 8 unknown9.69 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.86 ng	141347	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,3a,4-trim...	208	C15H28	031230-13-4	38
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
3	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	22
4	Cyclohexanol, 3,3,5-trimethyl-, ...	142	C9H18O	000933-48-2	22
5	6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	22





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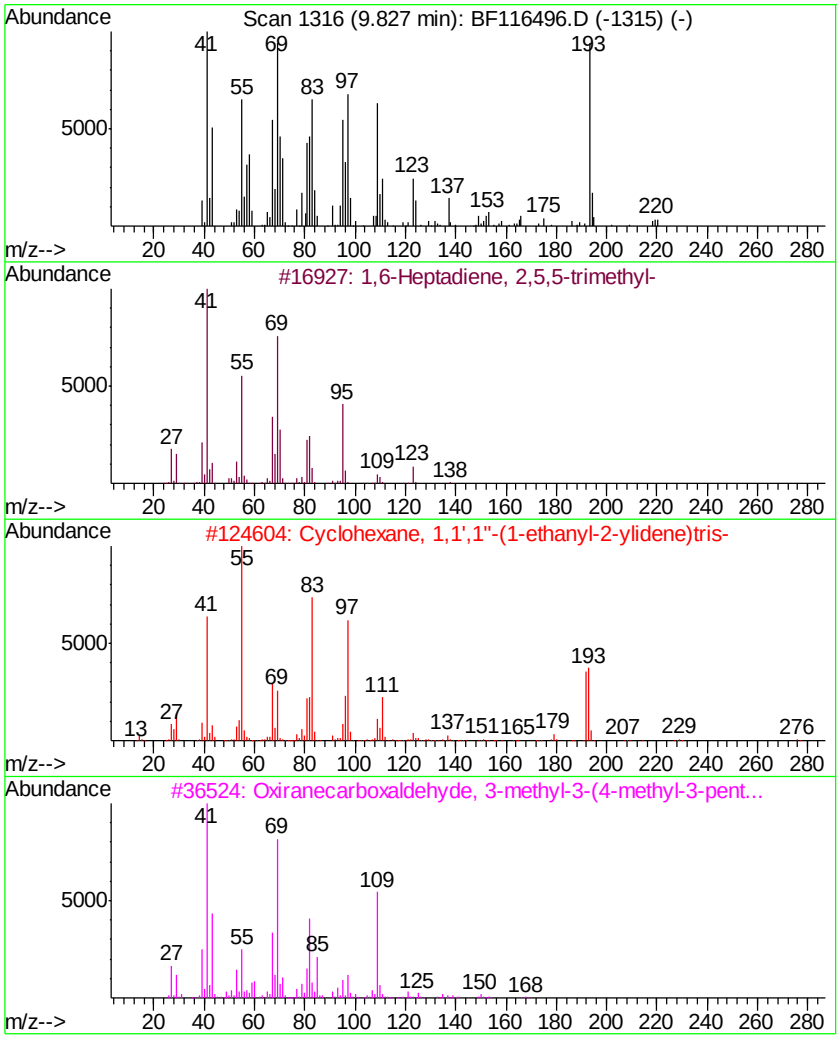
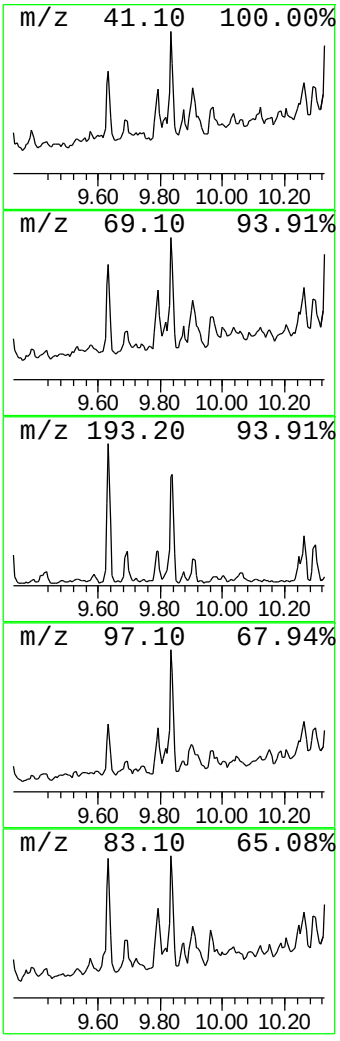
****

Peak Number 10 unknown9.83 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	11.60 ng	572648	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	27
2	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	22
3	Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2	016996-12-6	22
4	Disparlure	282	C19H38O	029804-22-6	22
5	1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	18





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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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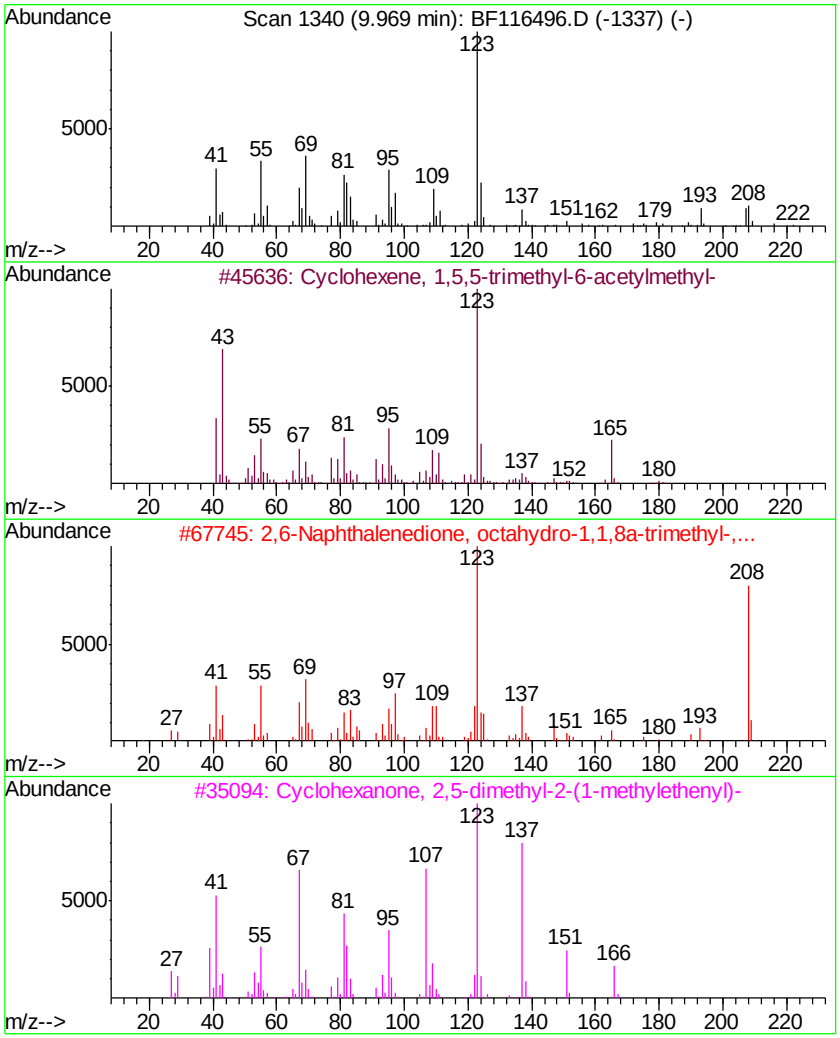
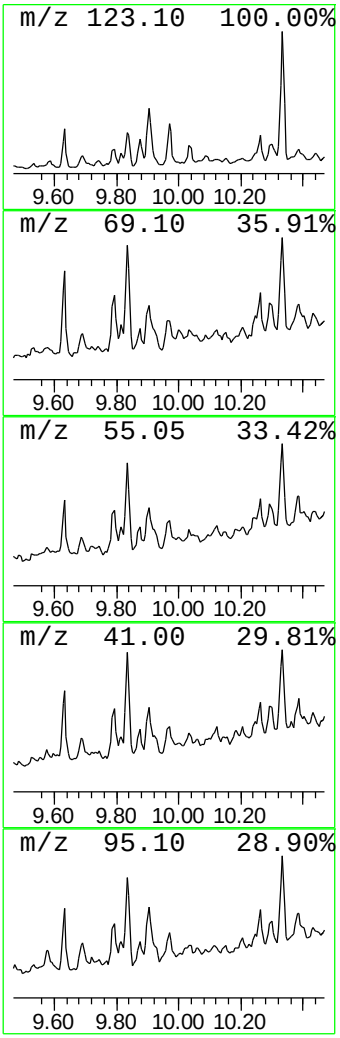
Peak Number 11 unknown9.97 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	4.67 ng	230509	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	42
2	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	42
3	Cyclohexanone, 2,5-dimethyl-2-(1...	166	C11H18O	006711-26-8	42
4	4-Fluorobenzoic acid, morpholide	209	C11H12FNO2	1000307-09-9	38
5	4,4-Dimethoxy-2,5-cyclohexadien-...	154	C8H10O3	000935-50-2	38





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Sample : K4385-16
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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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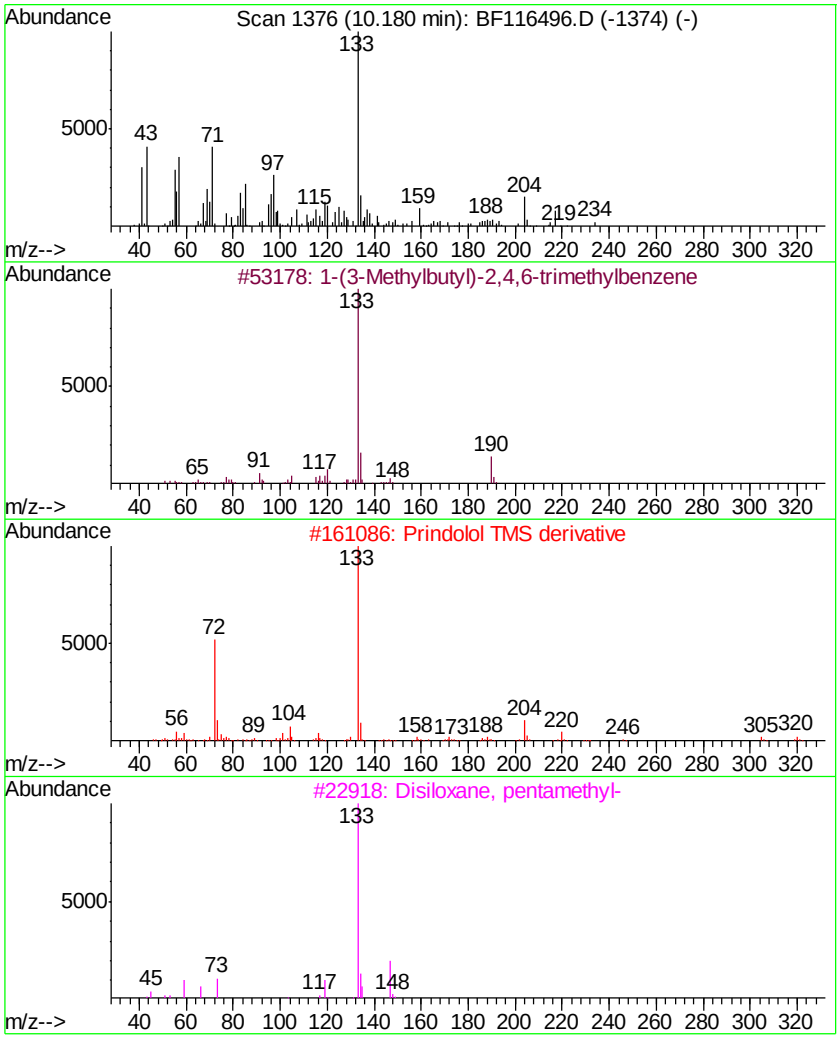
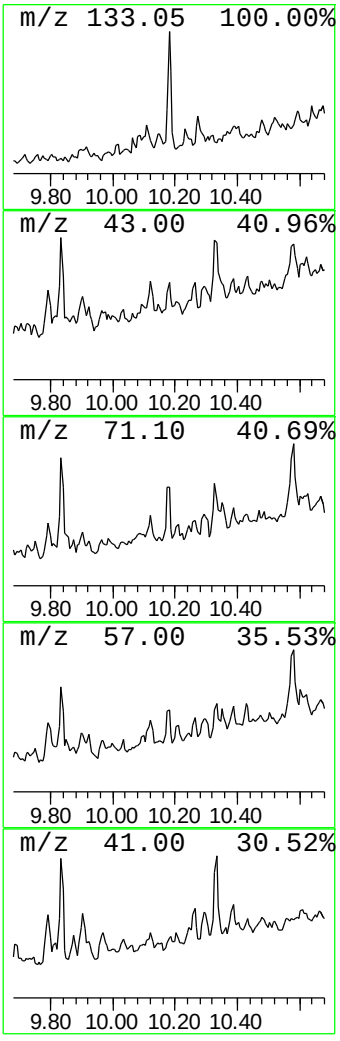
Peak Number 12 unknown10.18 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	2.05 ng	101216	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(3-Methylbutyl)-2,4,6-trimethy...	190	C14H22	016204-65-2	38
2	Prindolol TMS derivative	320	C17H28N2O2Si	1000137-17-9	35
3	Disiloxane, pentamethyl-	148	C5H16OSi2	001438-82-0	27
4	Benzene, 2-(chloromethyl)-1,3,5-...	168	C10H13Cl	001585-16-6	27
5	Benzenepropanol, 2,4,6-trimethyl-	178	C12H18O	027645-07-4	25





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Data File : BF116496.D
Acq On : 23 Aug 2019 23:57
Operator : HP/JU
Sample : K4385-16
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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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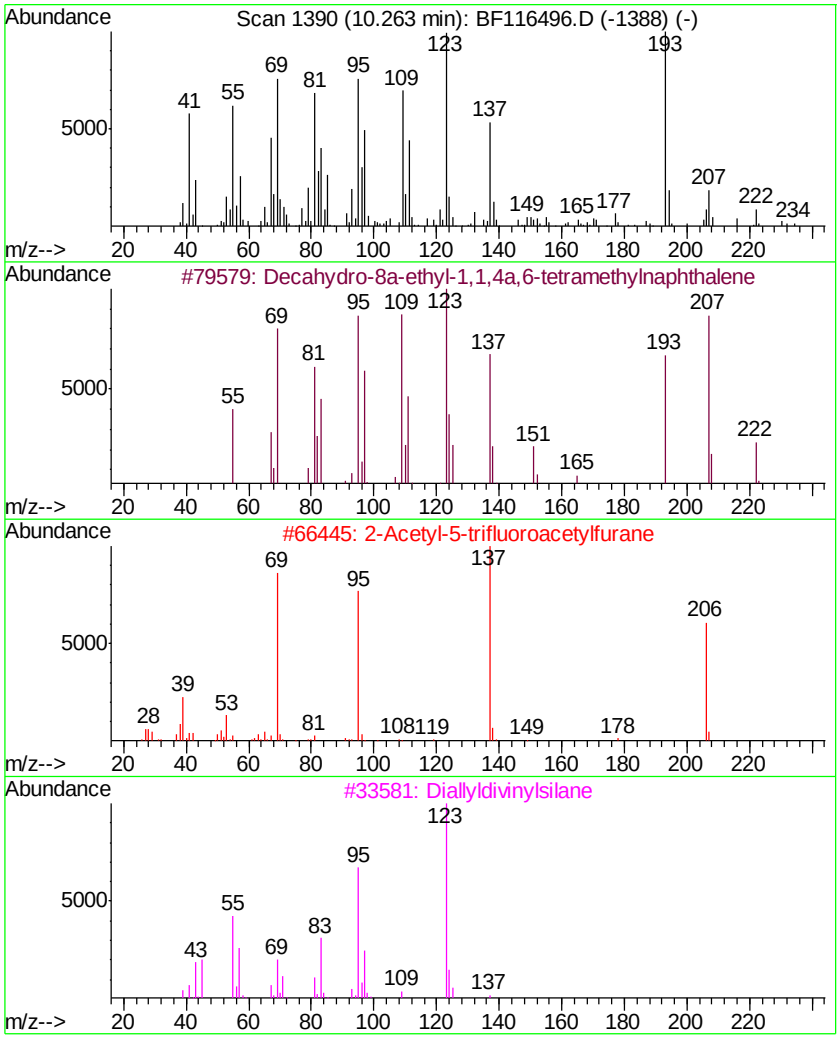
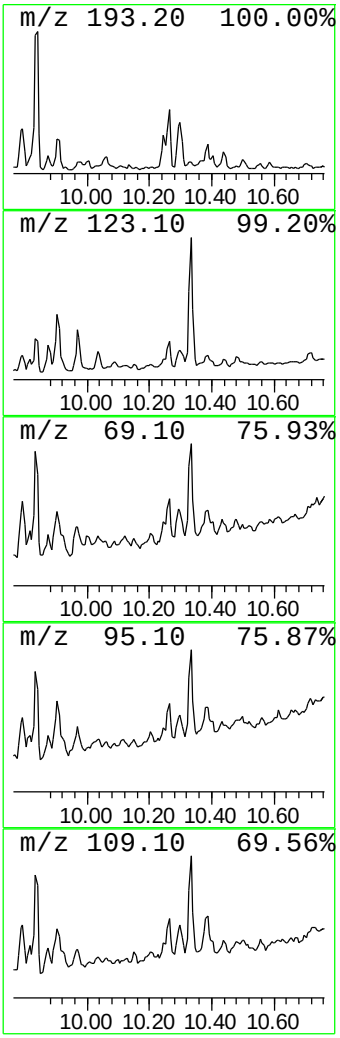
Peak Number 13 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	3.77 ng	185952	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	72
2	2-Acetyl-5-trifluoroacetylfurane	206	C8H5F3O3	1000222-23-5	30
3	Diallyldivinylsilane	164	C10H16Si	119901-88-1	22
4	Ethanone, 1-(3-fluorophenyl)-	138	C8H7FO	000455-36-7	18
5	Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	18





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Data File : BF116496.D
Acq On : 23 Aug 2019 23:57
Operator : HP/JU
Sample : K4385-16
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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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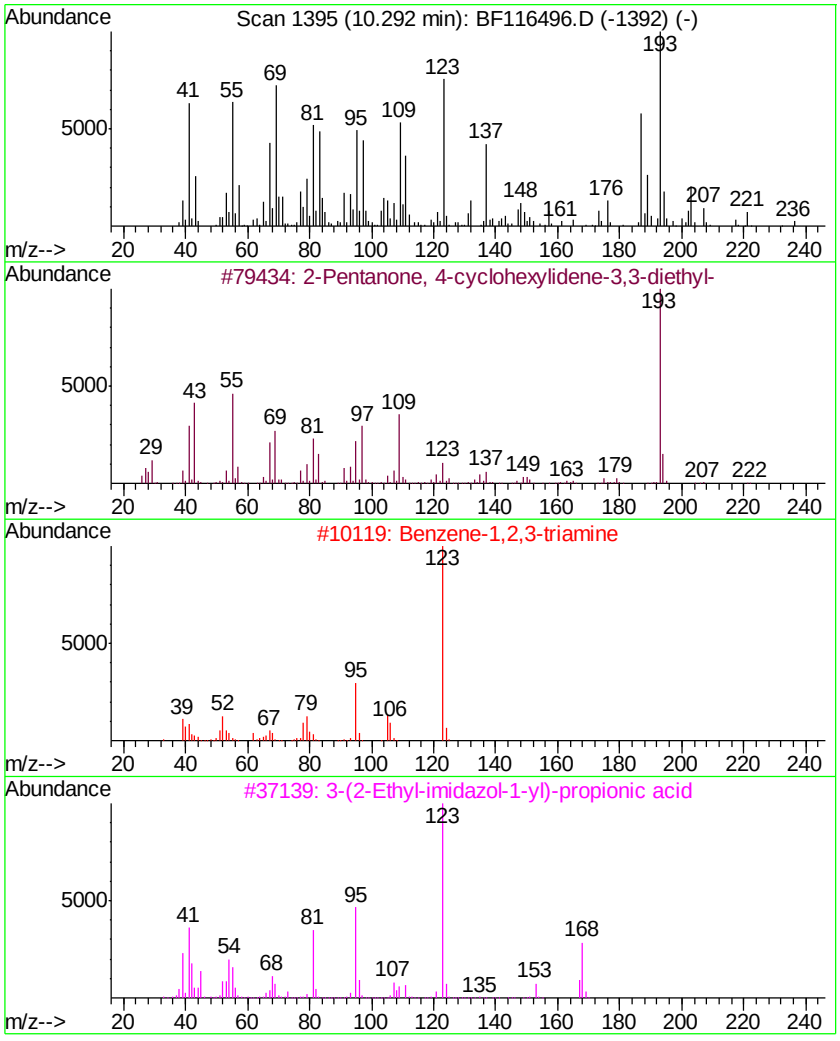
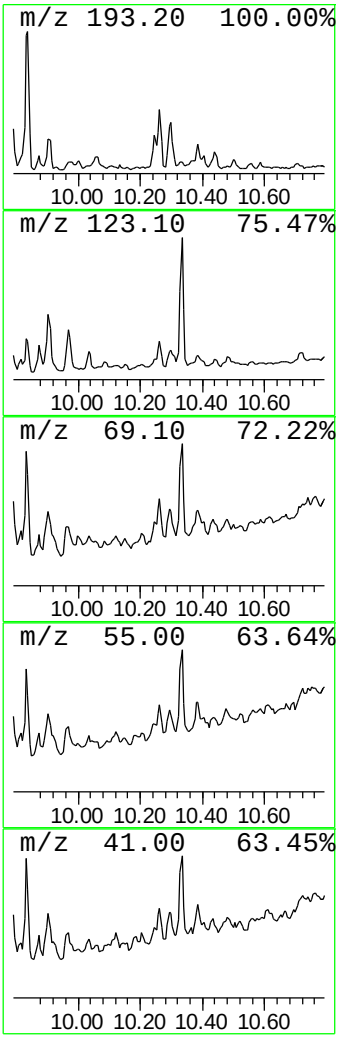
Peak Number 14 unknown10.29 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.29	5.51 ng	272081	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	35
2	Benzene-1,2,3-triamine	123	C6H9N3	1000316-45-3	18
3	3-(2-Ethyl-imidazol-1-yl)-propio...	168	C8H12N2O2	1000277-78-0	14
4	[2-(4-Fluorophenyl)oxazol-4-yl]a...	221	C11H8FNO3	1000316-47-5	14
5	Benzene, 1,3-bis(2-fluorobenzoyl...	354	C20H12F2O4	294874-06-9	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116496.D
Acq On : 23 Aug 2019 23:57
Operator : HP/JU
Sample : K4385-16
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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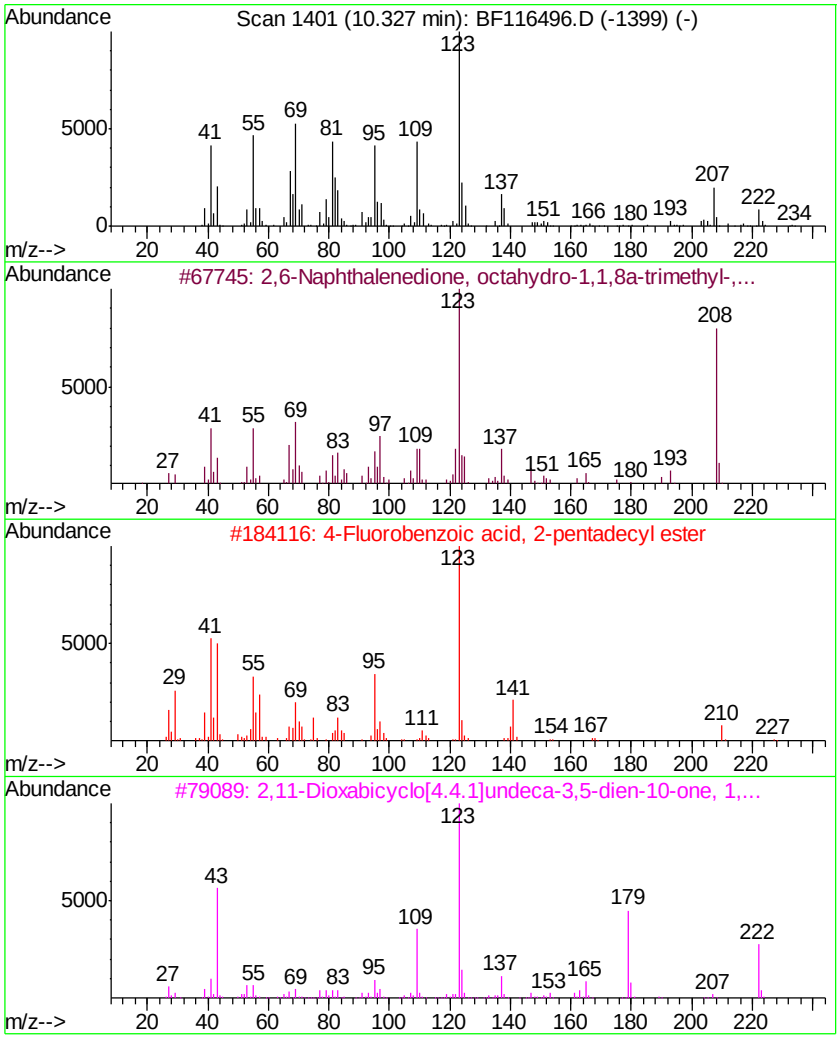
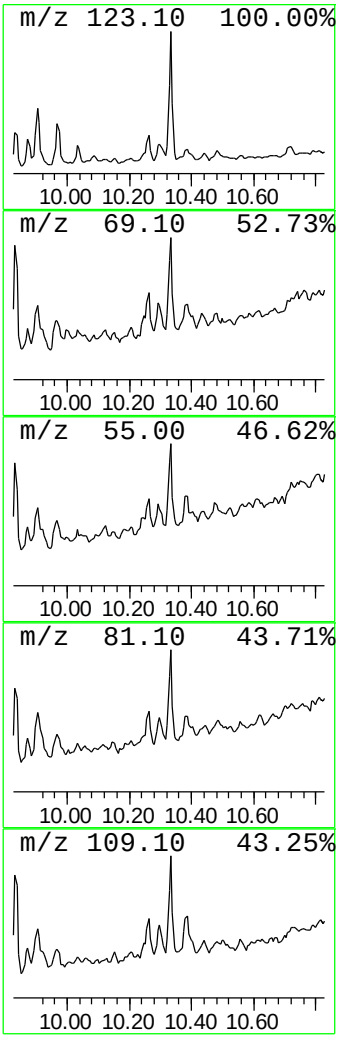
Peak Number 15 unknown10.33 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	10.48 ng	517097	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	47
2	4-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-68-3	47
3	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	47
4	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	46
5	Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	38





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Data File : BF116496.D
Acq On : 23 Aug 2019 23:57
Operator : HP/JU
Sample : K4385-16
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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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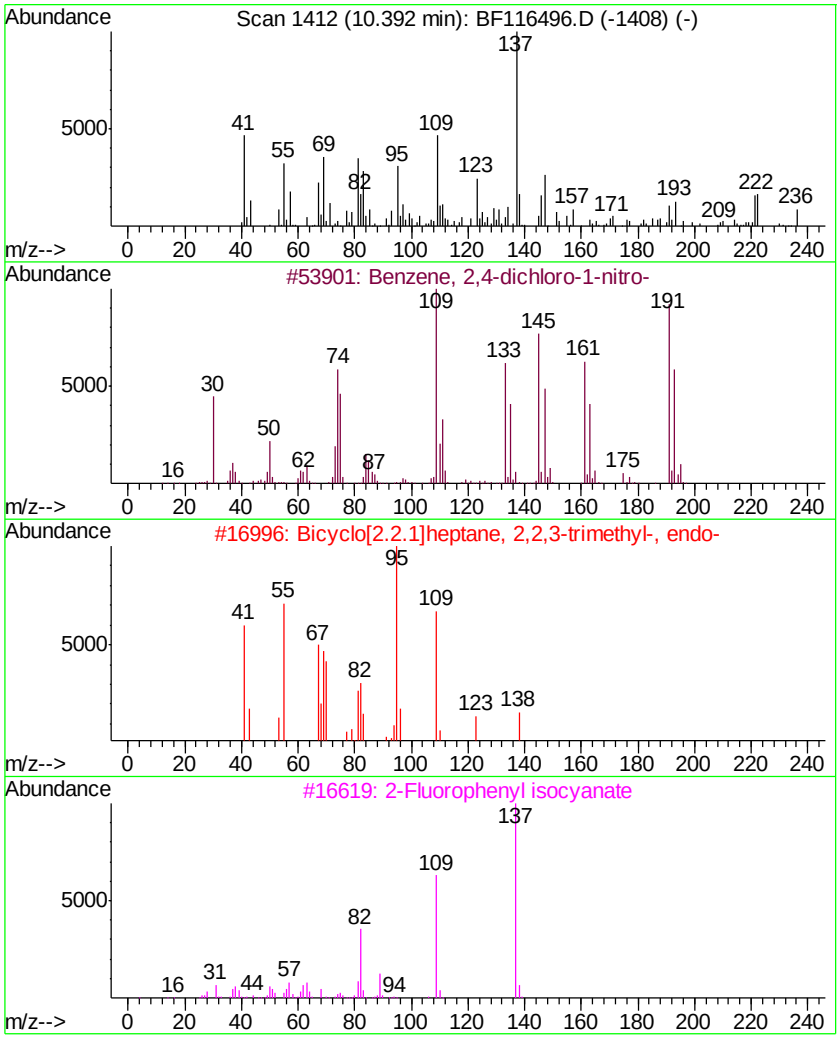
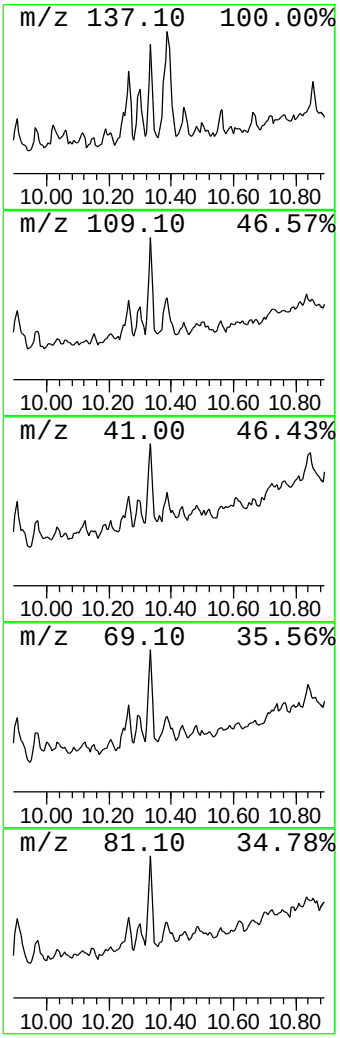
Peak Number 16 Benzene, 2,4-dichloro-1-nitro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.39	4.53 ng	223798	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2,4-dichloro-1-nitro-	191	C6H3Cl2NO2	000611-06-3	53
2	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	38
3	2-Fluorophenyl isocyanate	137	C7H4FNO	016744-98-2	30
4	4-Fluorophenyl isocyanate	137	C7H4FNO	001195-45-5	30
5	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082319\
Data File : BF116496.D
Acq On : 23 Aug 2019 23:57
Operator : HP/JU
Sample : K4385-16
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-D-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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
Butane, 2-methoxy...	2.15	88.8	ng	2315160	1	6.89	521226	20.0
unknown6.65	6.65	64.9	ng	1690220	1	6.89	521226	20.0
Phthalic anhydride	8.91	4.5	ng	128236	2	8.16	565552	20.0
Decahydro-4,4,8,9...	9.32	4.2	ng	208034	3	9.92	987232	20.0
Carbonic acid, 2,...	9.39	2.6	ng	126834	3	9.92	987232	20.0
1,3-Isobenzofuran...	9.43	2.7	ng	135334	3	9.92	987232	20.0
unknown9.69	9.69	2.9	ng	141347	3	9.92	987232	20.0
unknown9.83	9.83	11.6	ng	572648	3	9.92	987232	20.0
unknown9.97	9.97	4.7	ng	230509	3	9.92	987232	20.0
unknown10.18	10.18	2.0	ng	101216	3	9.92	987232	20.0
Decahydro-8a-ethy...	10.26	3.8	ng	185952	3	9.92	987232	20.0
unknown10.29	10.29	5.5	ng	272081	3	9.92	987232	20.0
unknown10.33	10.33	10.5	ng	517097	3	9.92	987232	20.0
Benzene, 2,4-dich...	10.39	4.5	ng	223798	3	9.92	987232	20.0