LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122592.D
Acq On : 8 Dec 2020 17:13
Operator : JU/CG
Sample : L4971-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 5S2-A-D-COMP

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-BF120520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.416	392	396	404	rBV	612764	722773	19.51%	2.367%
2	5.046	498	503	516	rBV	800331	1025640	27.69%	3.359%
3	5.457	568	573	576	rBV	3204850	3103249	83.77%	10.162%
4	5.851	636	640	645	rBV	128017	110290	2.98%	0.361%
5	6.469	740	745	765	rBV	3213413	3352831	90.51%	10.979%
6	6.840	804	808	811	rBV	1129259	937172	25.30%	3.069%
7	7.398	898	903	906	rBV	2149966	2050278	55.35%	6.714%
8	8.122	1022	1026	1033	rBV	1504467	1258695	33.98%	4.122%
9	9.198	1205	1209	1212	rBV	4205971	3704329	100.00%	12.130%
10	9.281	1219	1223	1226	rBV3	107471	117061	3.16%	0.383%
11	9.592	1272	1276	1280	rBV	517893	551473	14.89%	1.806%
12	9.645	1283	1285	1288	rVV3	60043	70044	1.89%	0.229%
13	9.745	1299	1302	1305	rBV3	223277	277494	7.49%	0.909%
14	9.792	1308	1310	1312	rVB	290775	221570	5.98%	0.726%
15	9.881	1318	1325	1329	rBV	1701871	1738543	46.93%	5.693%
16	9.922	1329	1332	1337	rBV3	150149	268720	7.25%	0.880%
17	9.992	1342	1344	1346	rBV2	92266	72597	1.96%	0.238%
18	10.251	1386	1388	1392	rBV2	182454	213201	5.76%	0.698%
19	10.292	1392	1395	1398	rBV	408138	414855	11.20%	1.358%
20	10.339	1401	1403	1406	rBV3	236048	281831	7.61%	0.923%
21	10.669	1455	1459	1462	rBV	2317854	2322363	62.69%	7.605%
22	11.369	1576	1578	1583	rVB	1133392	1061124	28.65%	3.475%
23	12.957	1845	1848	1853	rVB	2981373	3003281	81.07%	9.834%
24	14.010	2023	2027	2029	rBV	1056737	1054533	28.47%	3.453%
25	14.527	2112	2115	2120	rVB	927199	864669	23.34%	2.831%
26	15.039	2199	2202	2213	rVB	261491	534549	14.43%	1.750%
27	15.468	2270	2275	2286	rBV	894923	1205071	32.53%	3.946%

Sum of corrected areas: 30538236

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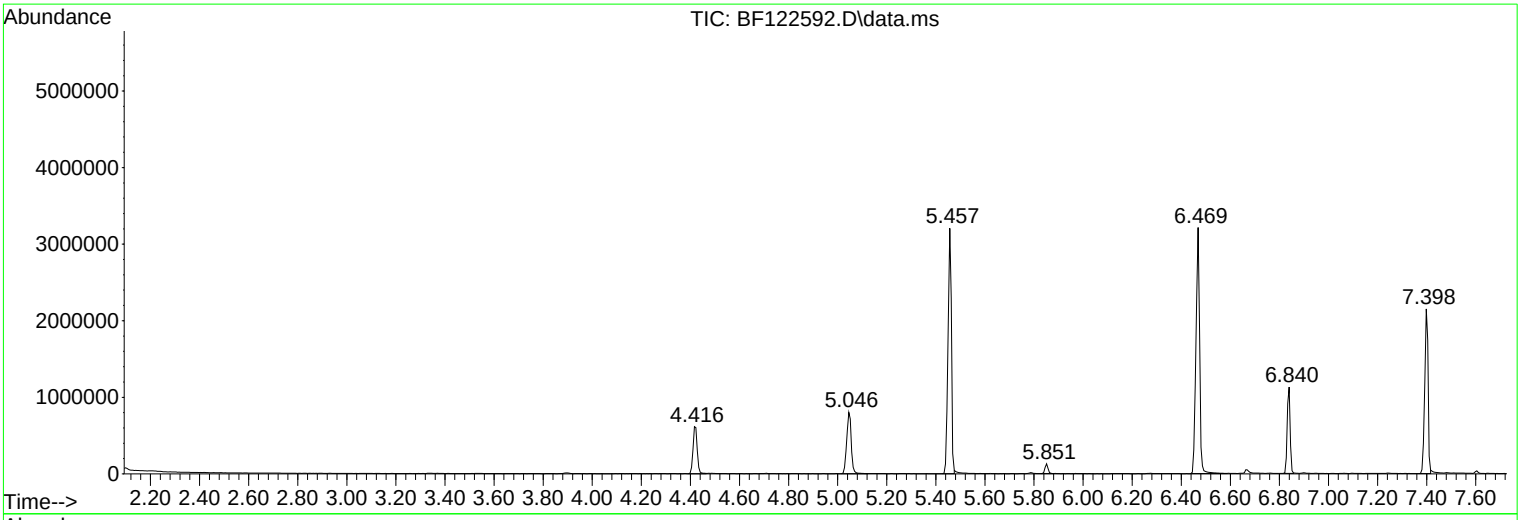
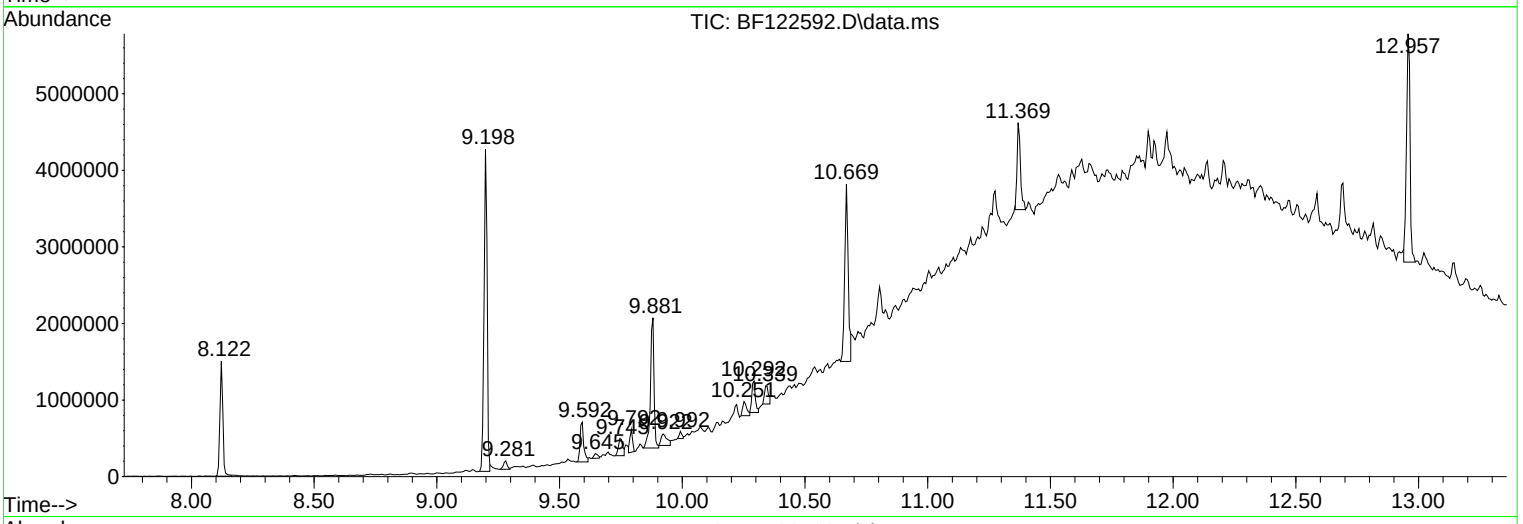
Misc :
ALS Vial : 9 Sample Multiplier: 1

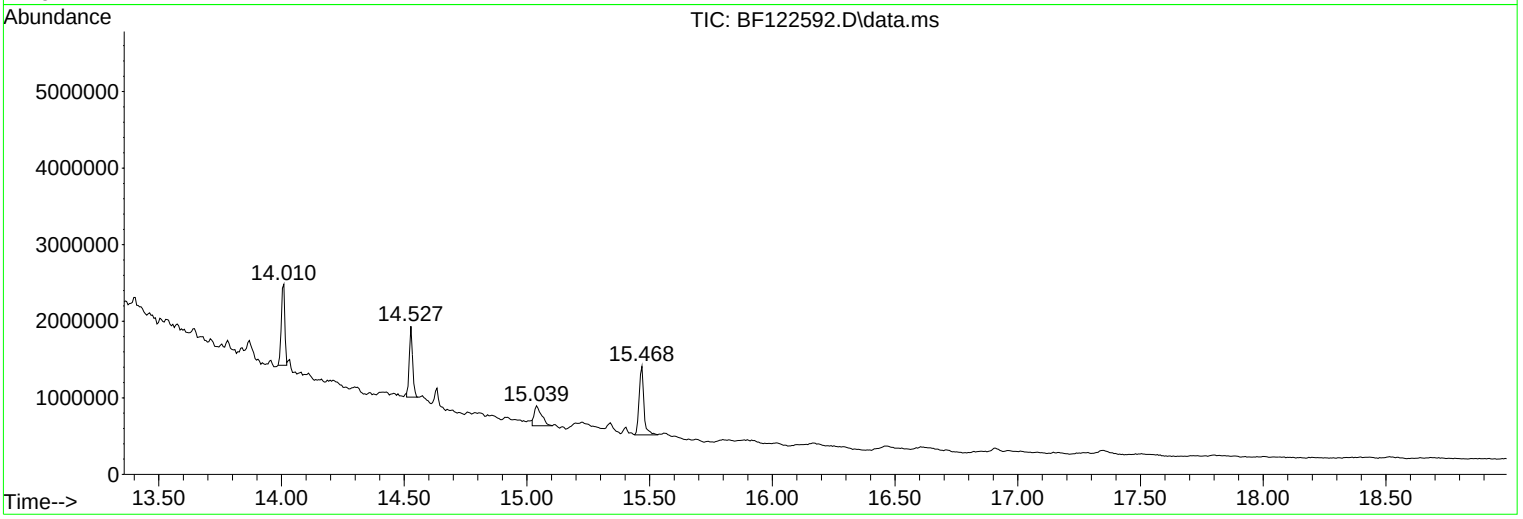
Instrument :
BNA_F
ClientSampleId :
5S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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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Instrument :
BNA_F
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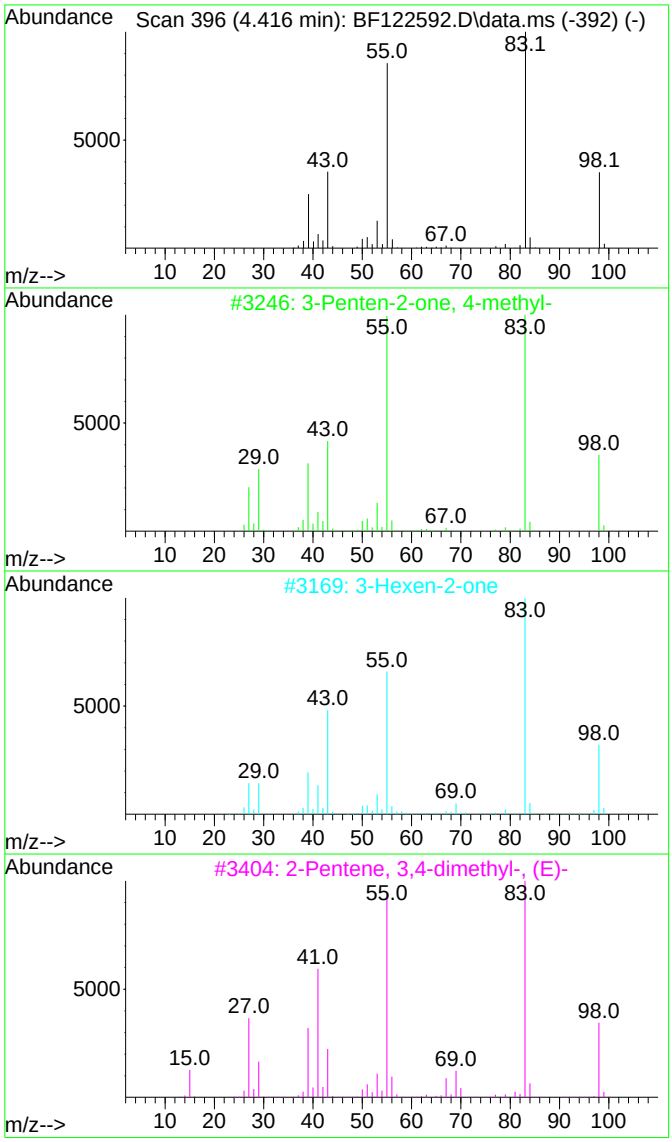
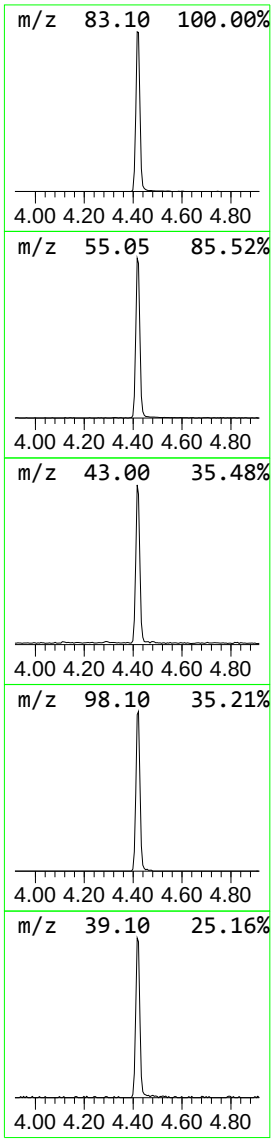
****
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	15.42 ng	722773	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Acq On : 8 Dec 2020 17:13
Operator : JU/CG
Sample : L4971-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 5S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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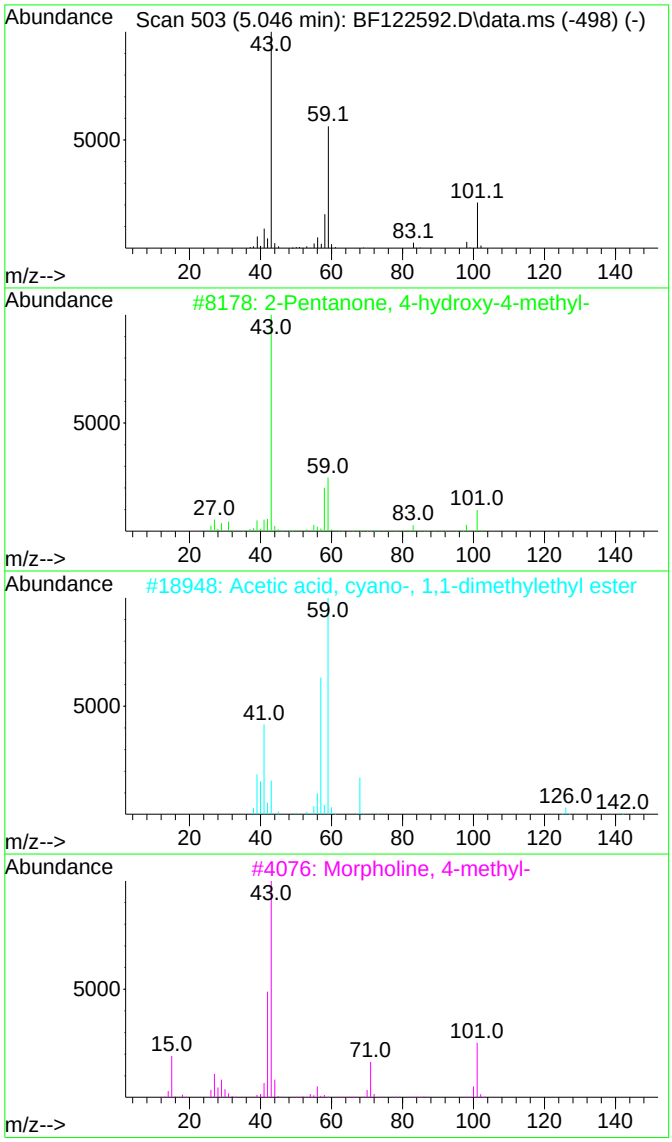
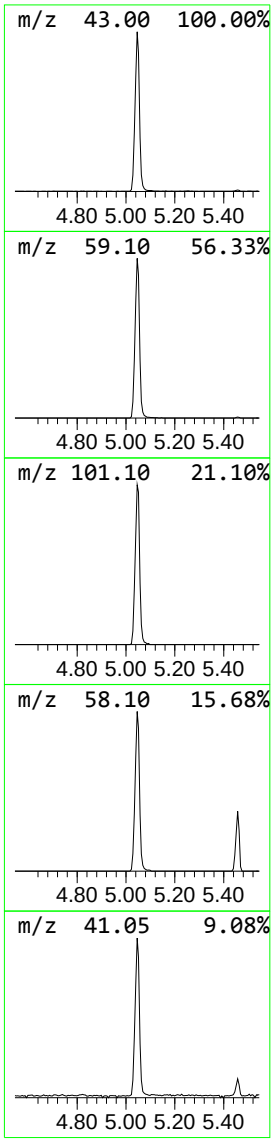
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	21.89 ng	1025640	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	9





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Data File : BF122592.D
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Operator : JU/CG
Sample : L4971-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 5S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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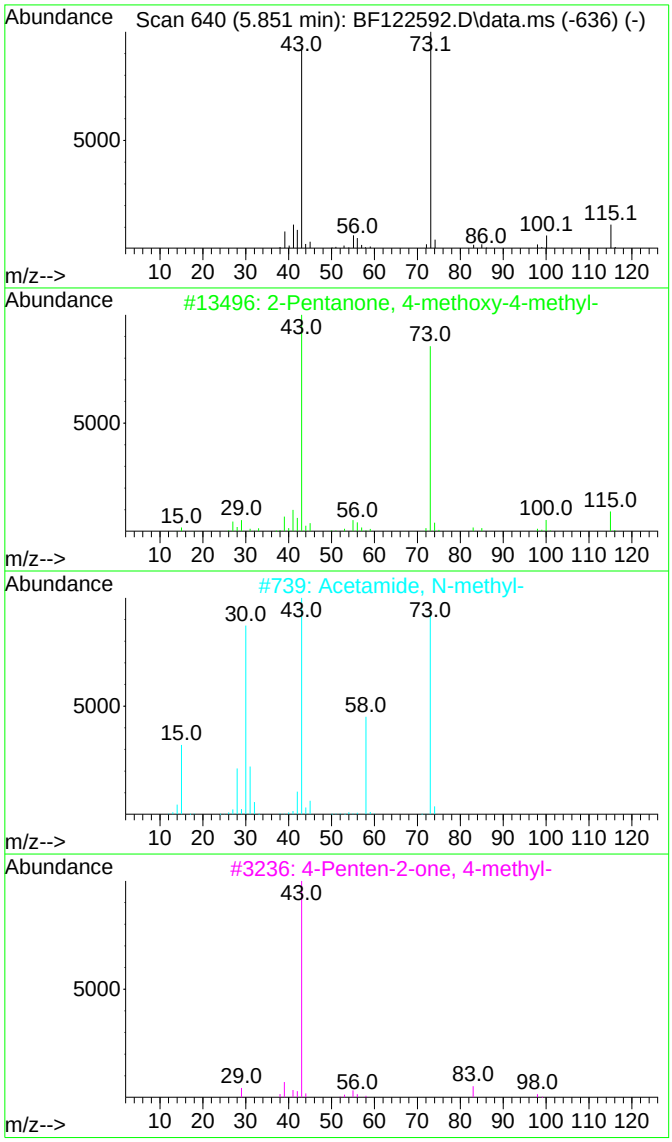
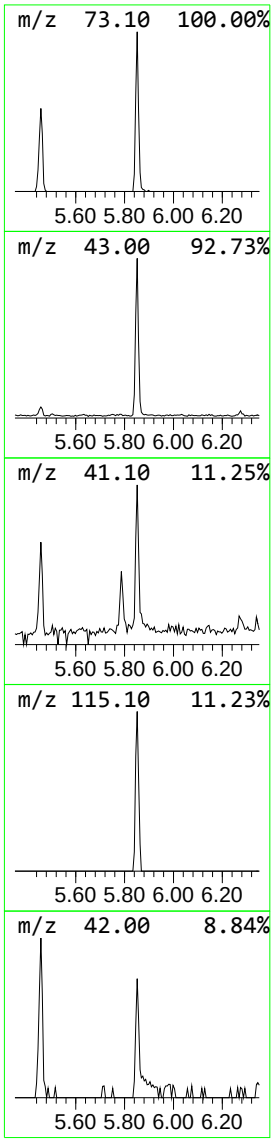
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	2.35 ng	110290	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	38
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122592.D
Acq On : 8 Dec 2020 17:13
Operator : JU/CG
Sample : L4971-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 5S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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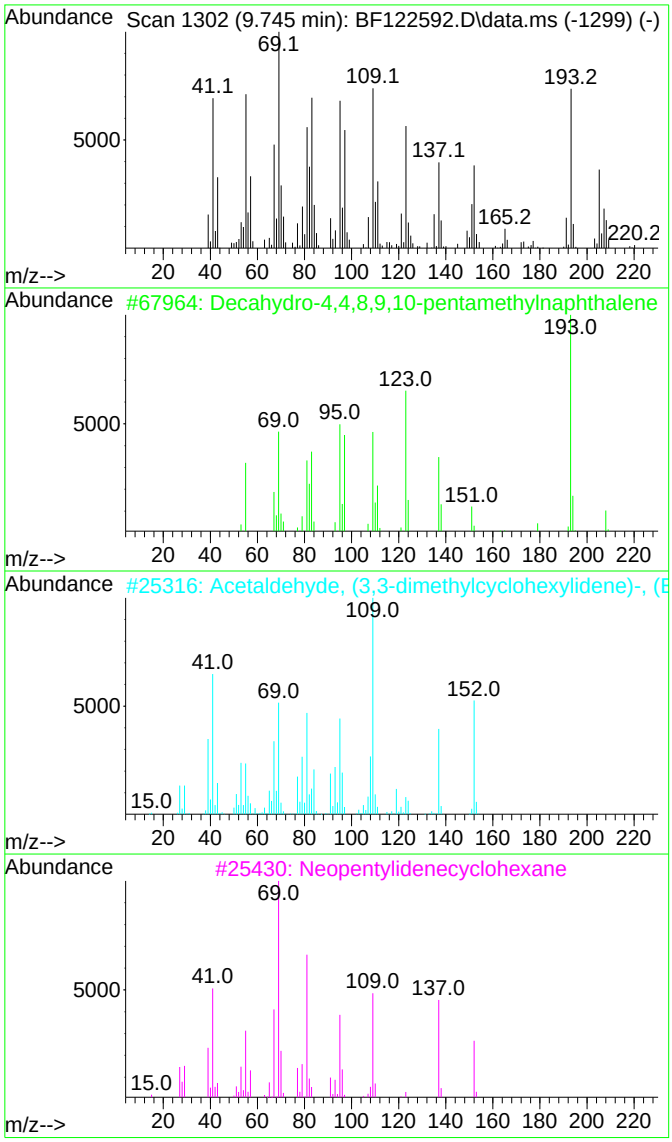
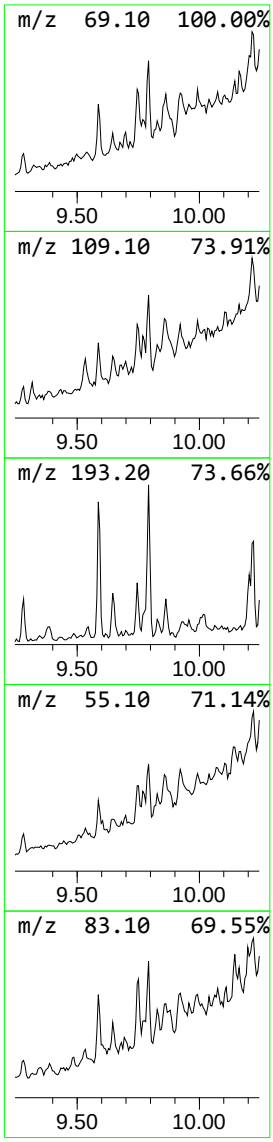
****
Peak Number 4 Decahydro-4,4,8,9,10-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.745	3.19 ng	277494	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	91
2	Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	30
3	Neopentylidenecyclohexane	152	C11H20	039546-80-0	25
4	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	22
5	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122592.D
Acq On : 8 Dec 2020 17:13
Operator : JU/CG
Sample : L4971-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 5S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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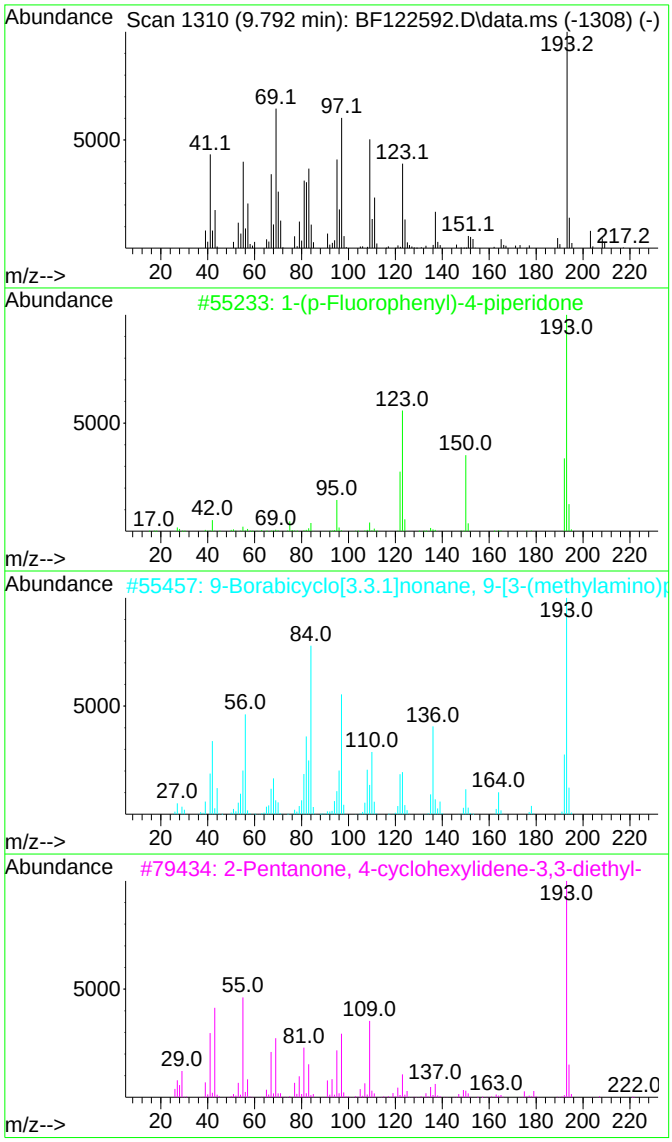
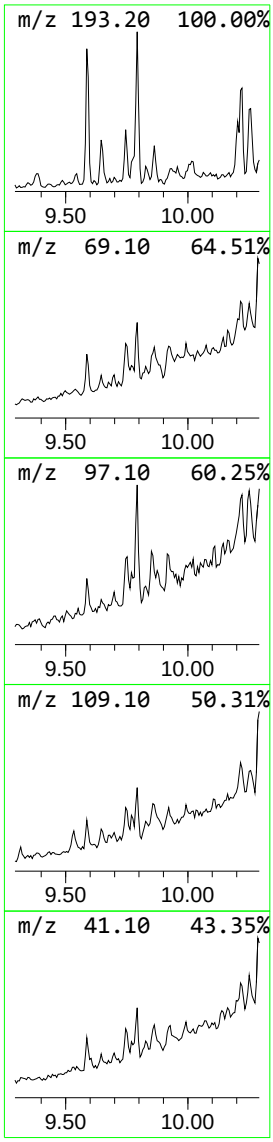
****

Peak Number 5 unknown9.792 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.792	2.55 ng	221570	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
2	9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1000162-56-0	38
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	25
4	Benzo[f]quinoline, 2-methyl-	193	C14H11N	039258-30-5	18
5	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122592.D
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Sample : L4971-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 5S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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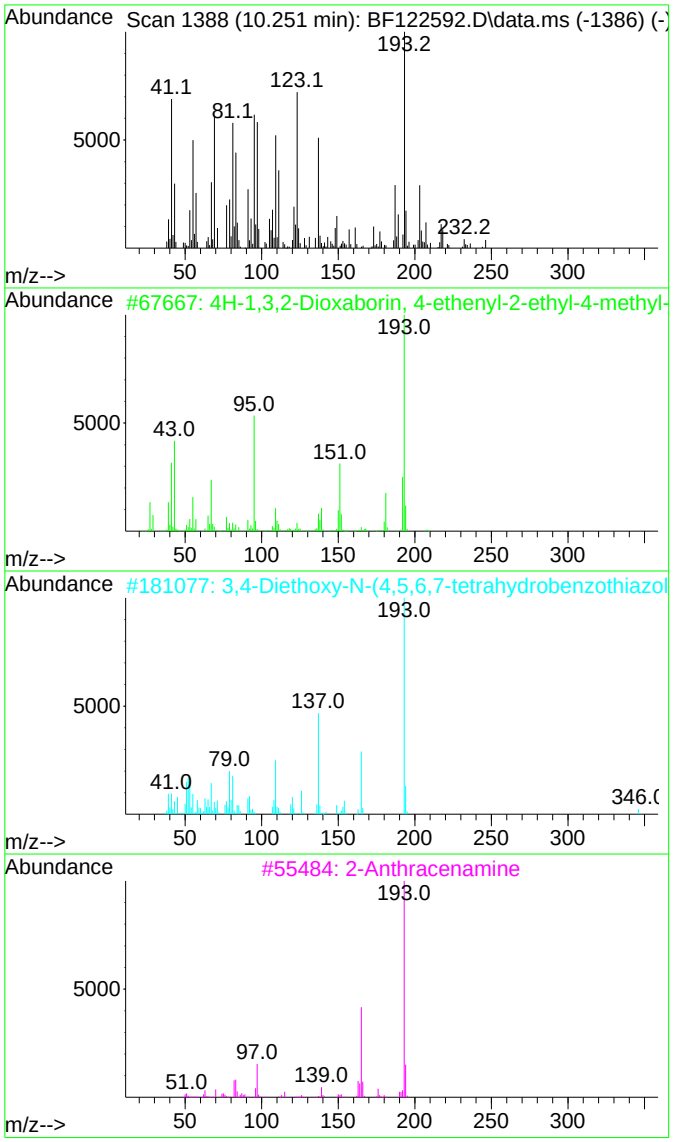
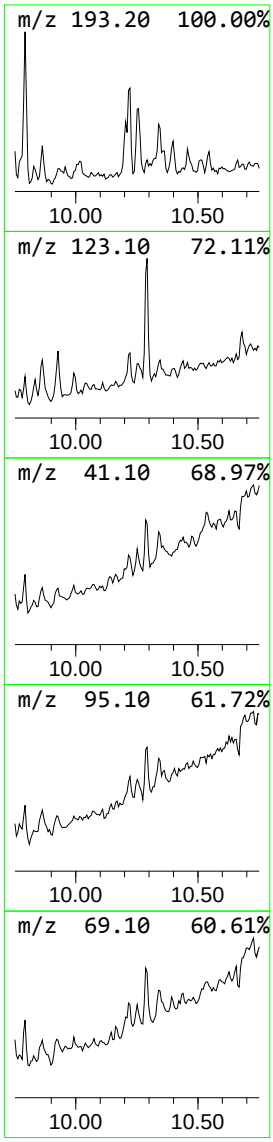
****

Peak Number 6 unknown10.251 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.251	2.45 ng	213201	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	30
2	3,4-Diethoxy-N-(4,5,6,7-tetrahyd...	346	C18H22N2O3S	1000311-37-1	27
3	2-Anthracenamine	193	C14H11N	000613-13-8	22
4	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22
5	Hexahydroindole	123	C8H13N	018159-32-5	11





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 5S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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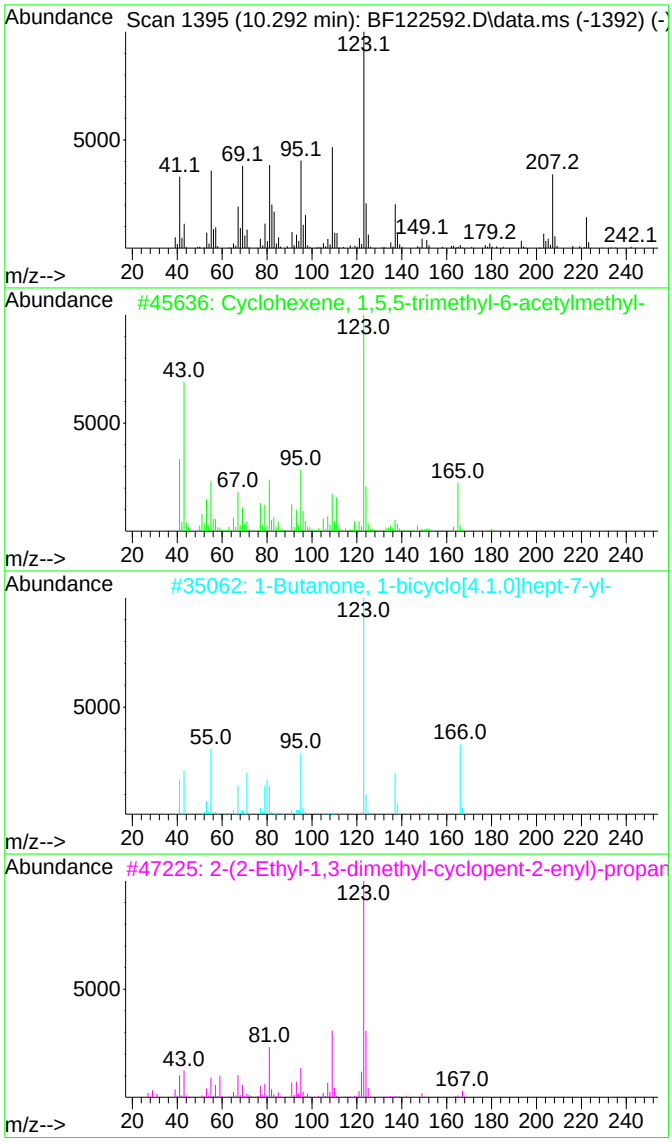
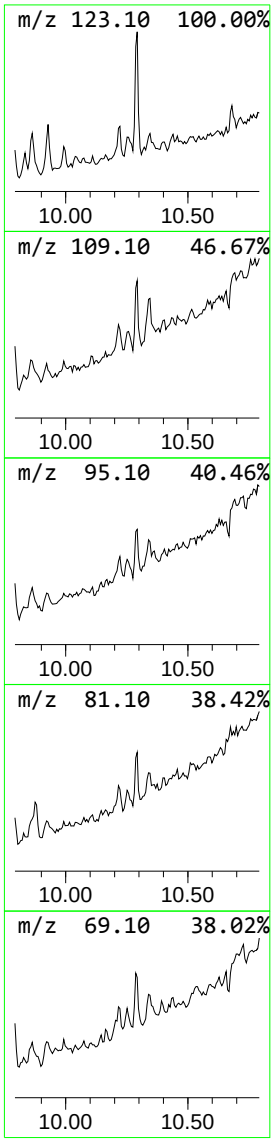
****

Peak Number 7 Cyclohexene, 1,5,5-trimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.292	4.77 ng	414855	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	50
2	1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	47
3	2-(2-Ethyl-1,3-dimethyl-cyclopen...	182	C12H22O	1000186-82-4	43
4	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	43
5	3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-04-9	38





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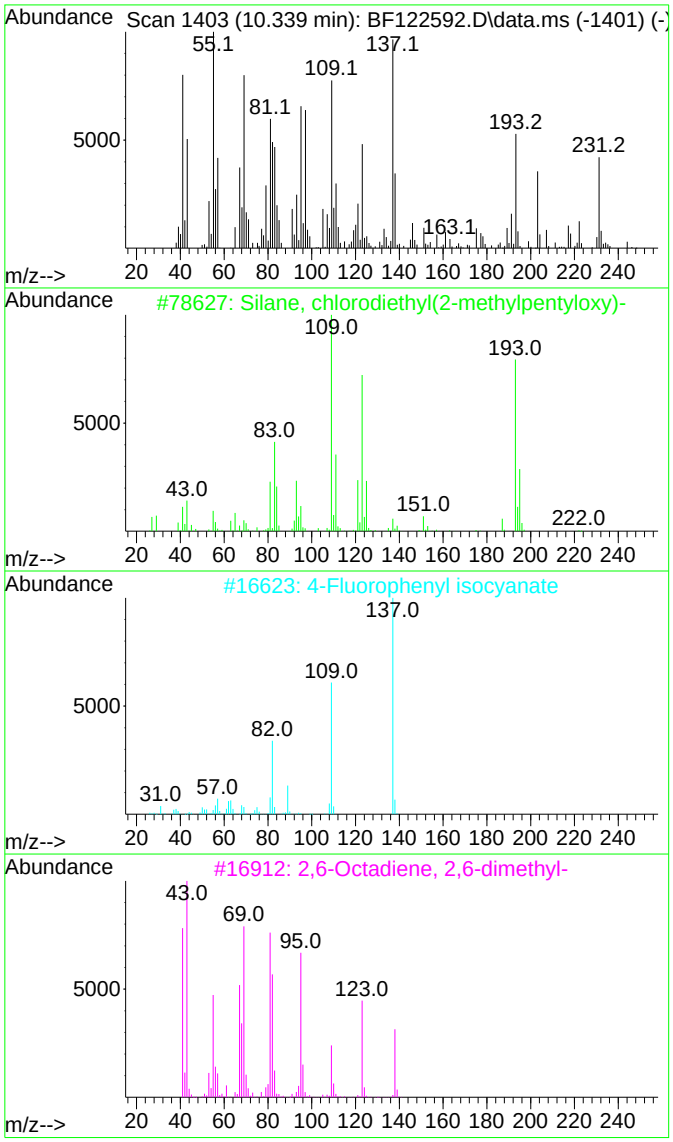
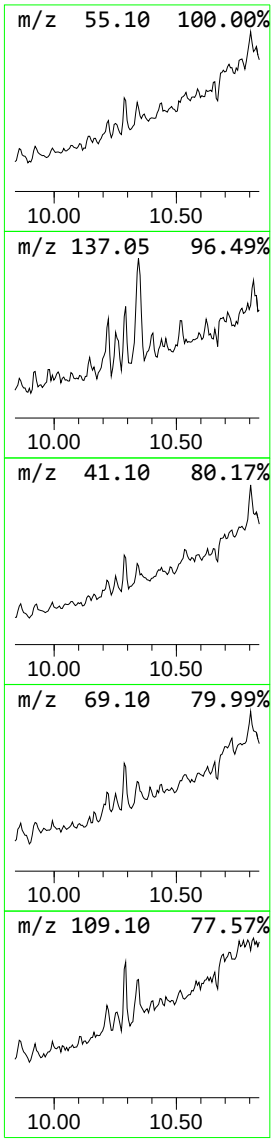
****

Peak Number 8 unknown10.339 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.339	3.24 ng	281831	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	25
2	4-Fluorophenyl isocyanate	137	C7H4FNO	001195-45-5	25
3	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	25
4	6-Octen-1-ol, 3,7-dimethyl-, ace...	198	C12H22O2	000150-84-5	22
5	Benzenamine, 3-ethoxy-	137	C8H11NO	000621-33-0	22





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Data File : BF122592.D
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Operator : JU/CG
Sample : L4971-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 5S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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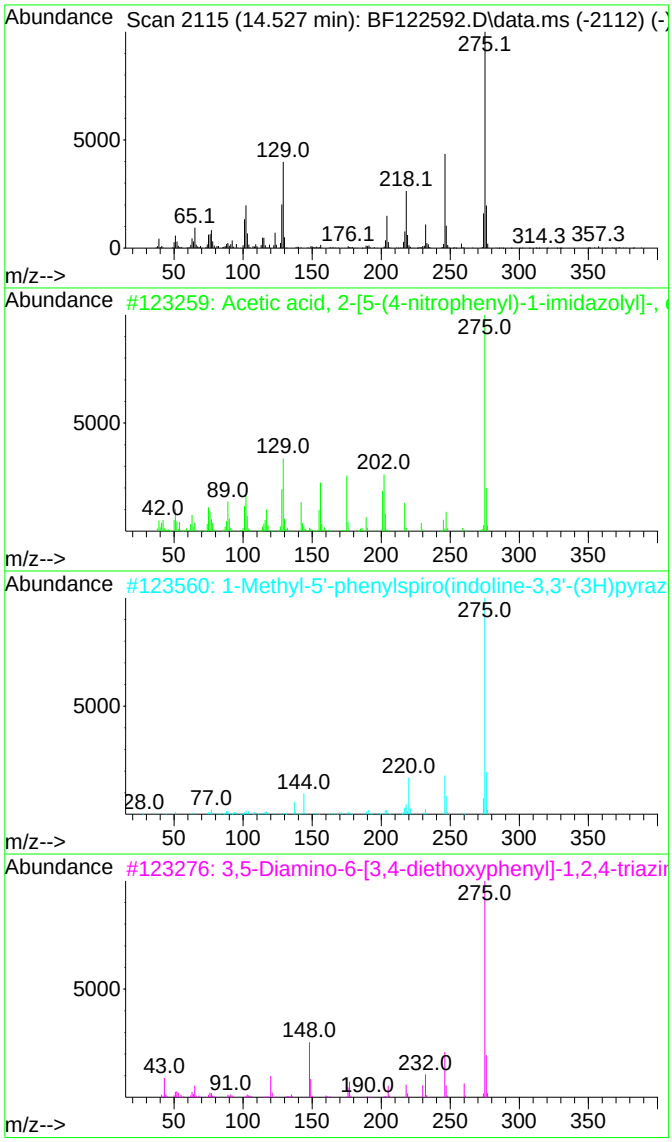
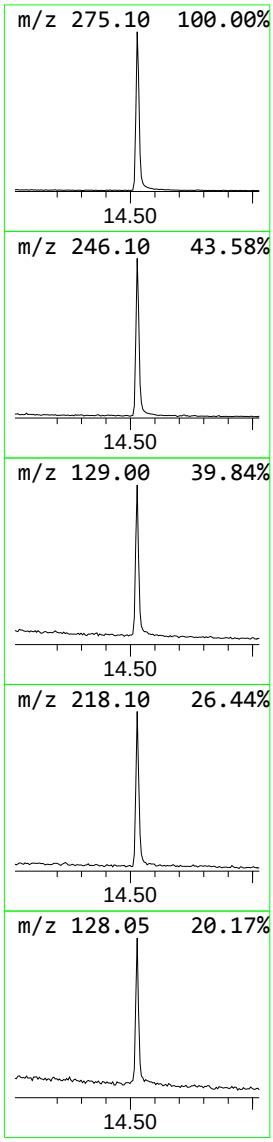
****
Peak Number 9 Acetic acid, 2-[5-(4-nitrop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	16.40 ng	864669	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-[5-(4-nitrophenyl...	275	C13H13N3O4	351064-45-4	58
2	1-Methyl-5'-phenylspiro(indoline...	275	C17H13N3O	015970-21-5	43
3	3,5-Diamino-6-[3,4-diethoxypheny...	275	C13H17N5O2	058848-69-4	43
4	5H-[1]Benzopyrano[4,3-d]pyrimidi...	275	C16H9N3O2	1000337-49-1	42
5	8H-Benzo[g]-1,3-benzodioxolo[6,5...	275	C17H9NO3	000475-75-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122592.D
Acq On : 8 Dec 2020 17:13
Operator : JU/CG
Sample : L4971-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 5S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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
3-Penten-2-one,...	4.416	15.4	ng	722773	1	6.840	937172	20.0
2-Pentanone, 4-...	5.046	21.9	ng	1025640	1	6.840	937172	20.0
2-Pentanone, 4-...	5.851	2.4	ng	110290	1	6.840	937172	20.0
Decahydro-4,4,8...	9.745	3.2	ng	277494	3	9.881	1738540	20.0
unknown9.792	9.792	2.5	ng	221570	3	9.881	1738540	20.0
unknown10.251	10.251	2.5	ng	213201	3	9.881	1738540	20.0
Cyclohexene, 1,...	10.292	4.8	ng	414855	3	9.881	1738540	20.0
unknown10.339	10.339	3.2	ng	281831	3	9.881	1738540	20.0
Acetic acid, 2-...	14.527	16.4	ng	864669	5	14.010	1054530	20.0