LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126319.D
Acq On : 22 Dec 2021 3:00
Operator : JU/CG
Sample : M5182-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	10	rVB	126778	127897	3.16%	0.423%
2	3.881	298	305	311	rBV	107528	142809	3.52%	0.472%
3	5.040	498	502	510	rVB	54310	69973	1.73%	0.231%
4	5.434	560	569	572	rBV	3797123	3976504	98.14%	13.141%
5	6.445	735	741	744	rBV	3481737	4051695	100.00%	13.390%
6	6.816	800	804	807	rBV	1392830	1125865	27.79%	3.721%
7	7.216	869	872	882	rBV3	57766	115970	2.86%	0.383%
8	7.381	894	900	903	rBV	2588879	2638472	65.12%	8.719%
9	7.463	910	914	918	rBV4	48359	68837	1.70%	0.227%
10	8.098	1017	1022	1024	rBV	1707814	1518718	37.48%	5.019%
11	8.122	1024	1026	1029	rVB	286046	250181	6.17%	0.827%
12	8.281	1045	1053	1055	rBV8	33859	67540	1.67%	0.223%
13	8.392	1068	1072	1075	rVB5	46516	70957	1.75%	0.234%
14	8.545	1095	1098	1100	rBV3	78937	75124	1.85%	0.248%
15	8.563	1100	1101	1104	rVB2	88433	71450	1.76%	0.236%
16	8.657	1113	1117	1120	rVB3	71716	101336	2.50%	0.335%
17	8.845	1147	1149	1152	rBV4	85329	88213	2.18%	0.292%
18	8.880	1152	1155	1157	rBV2	60188	78787	1.94%	0.260%
19	8.986	1169	1173	1175	rBV3	87788	113714	2.81%	0.376%
20	9.098	1189	1192	1194	rVB2	189457	168512	4.16%	0.557%
21	9.122	1194	1196	1200	rBV4	72618	92459	2.28%	0.306%
22	9.175	1200	1205	1210	rBV	3384218	3575401	88.24%	11.816%
23	9.257	1216	1219	1223	rBV2	365956	380656	9.39%	1.258%
24	9.404	1242	1244	1246	rBV2	131226	110741	2.73%	0.366%
25	9.522	1260	1264	1269	rBV2	493231	550247	13.58%	1.818%
26	9.569	1269	1272	1276	rBV	937894	904663	22.33%	2.990%
27	9.622	1279	1281	1285	rVB3	249247	259783	6.41%	0.859%
28	9.728	1295	1299	1301	rBV3	648331	795062	19.62%	2.627%
29	9.769	1304	1306	1309	rVB	1373744	1221159	30.14%	4.036%
30	9.810	1310	1313	1315	rBV	324094	308727	7.62%	1.020%
31	9.857	1315	1321	1325	rBV3	2146004	3166285	78.15%	10.464%
32	10.022	1346	1349	1350	rBV	257585	266785	6.58%	0.882%
33	10.122	1364	1366	1368	rBV	260764	274133	6.77%	0.906%
34	10.198	1377	1379	1382	rVB2	489966	379031	9.35%	1.253%
35	10.233	1382	1385	1387	rBV3	438653	488402	12.05%	1.614%
36	10.269	1388	1391	1395	rVV3	1272034	1250215	30.86%	4.132%

LSC Area Percent Report

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Acq On : 22 Dec 2021 3:00
Operator : JU/CG
Sample : M5182-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.645	1452	1455	1458	rBV	1121986	1313719	32.42%	4.341%

Sum of corrected areas: 30260022

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
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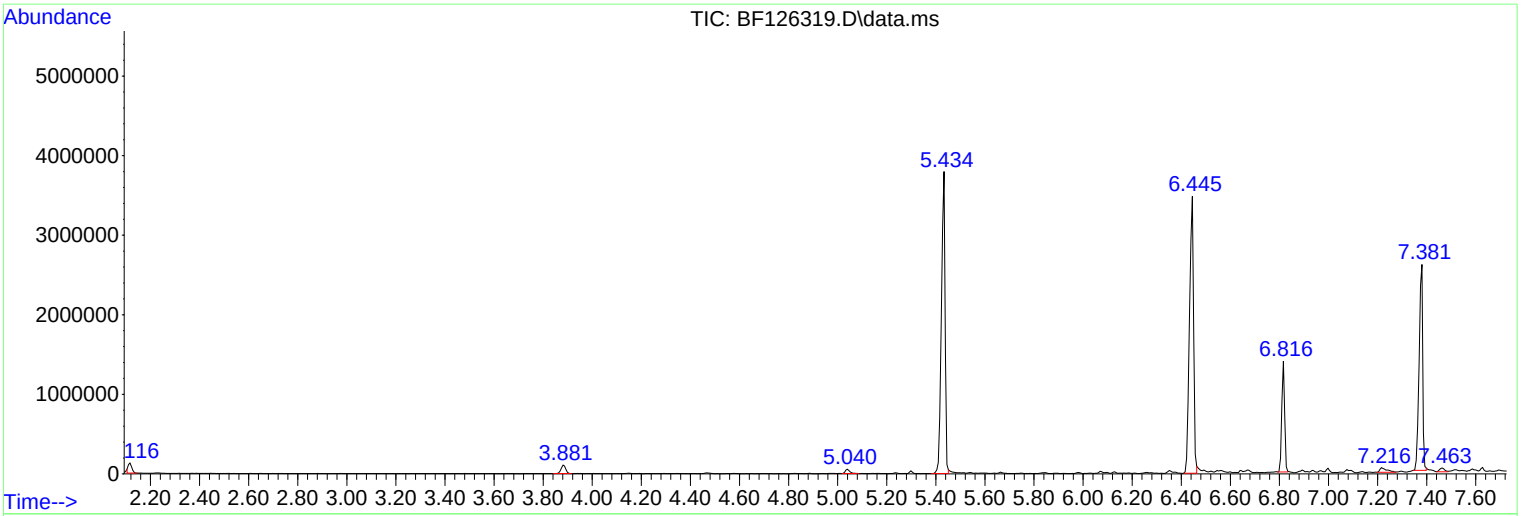
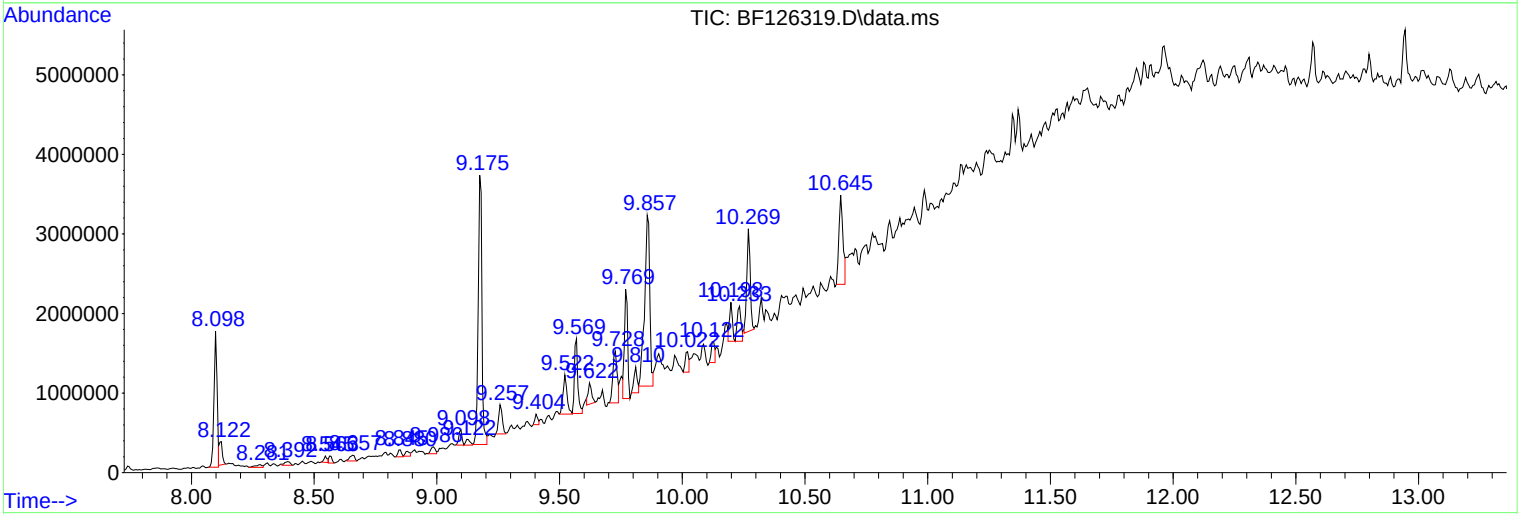
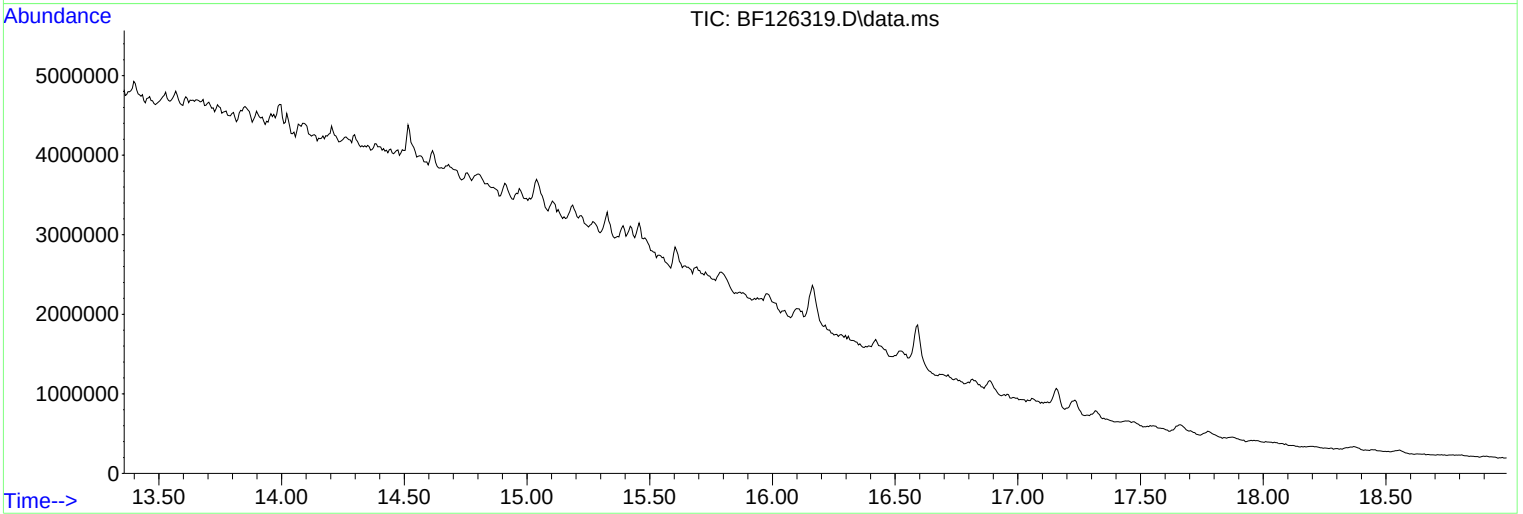
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Acq On : 22 Dec 2021 3:00
Operator : JU/CG
Sample : M5182-04
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Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

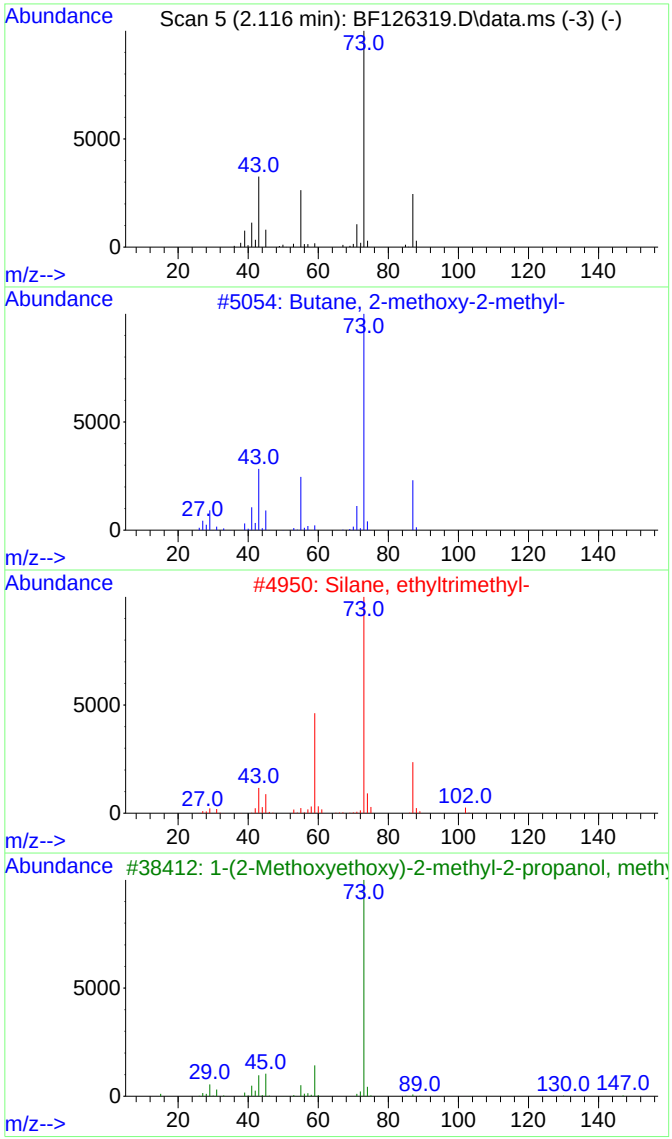
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

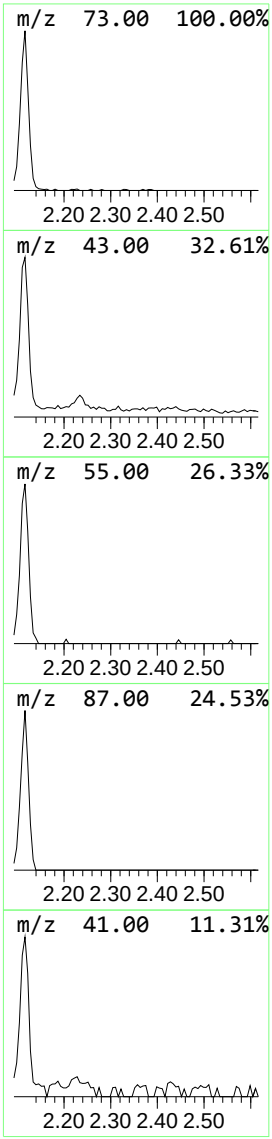
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	2.27 ng	127897	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	17
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126319.D
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Sample : M5182-04
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

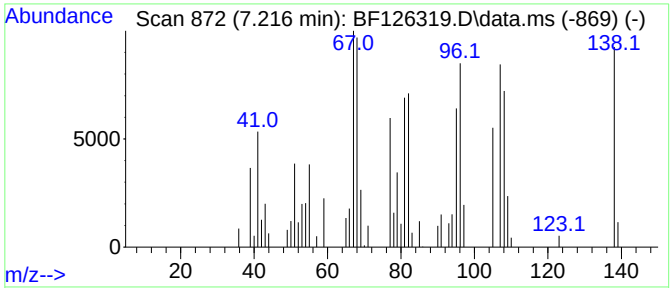
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

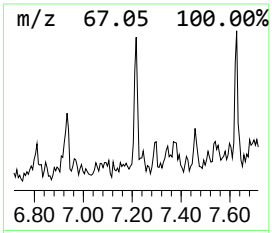
****

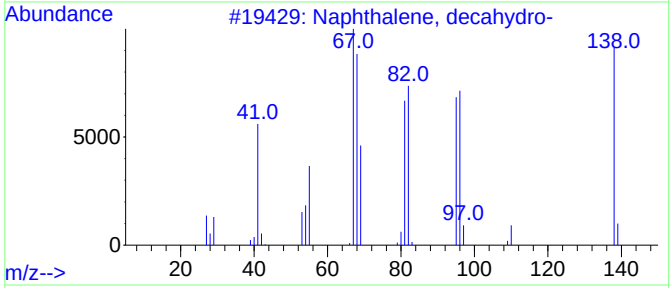
Peak Number 3 Naphthalene, decahydro- Concentration Rank 11

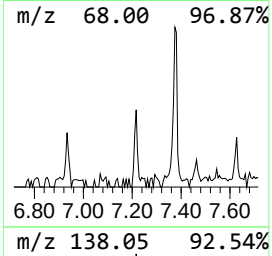
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.216	2.06 ng	115970	1,4-Dichlorobenzene-d4	6.816

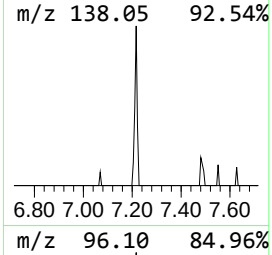
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-	138	C10H18	000091-17-8	92
2	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	89
3	1,1'-Bicyclopentyl	138	C10H18	001636-39-1	62
4	Bicyclo[3.1.0]hexan-2-one, 5-(1-...	138	C9H14O	000513-20-2	60
5	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	60

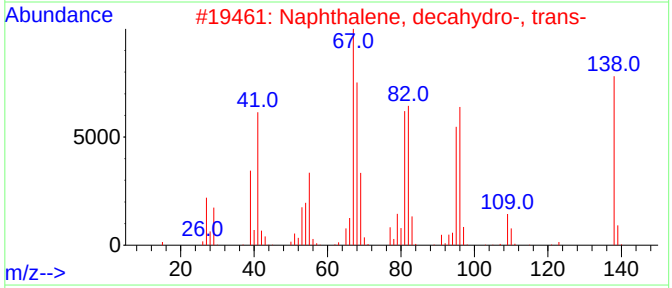


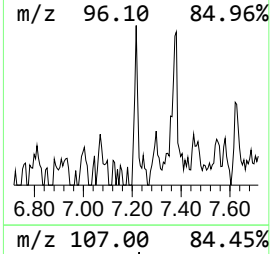


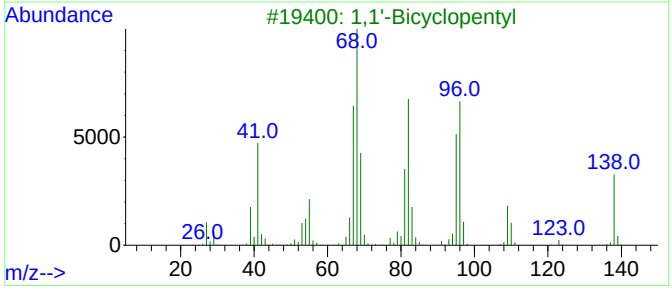


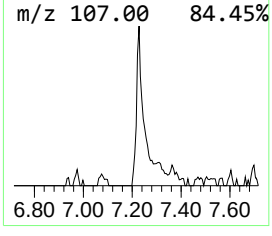












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

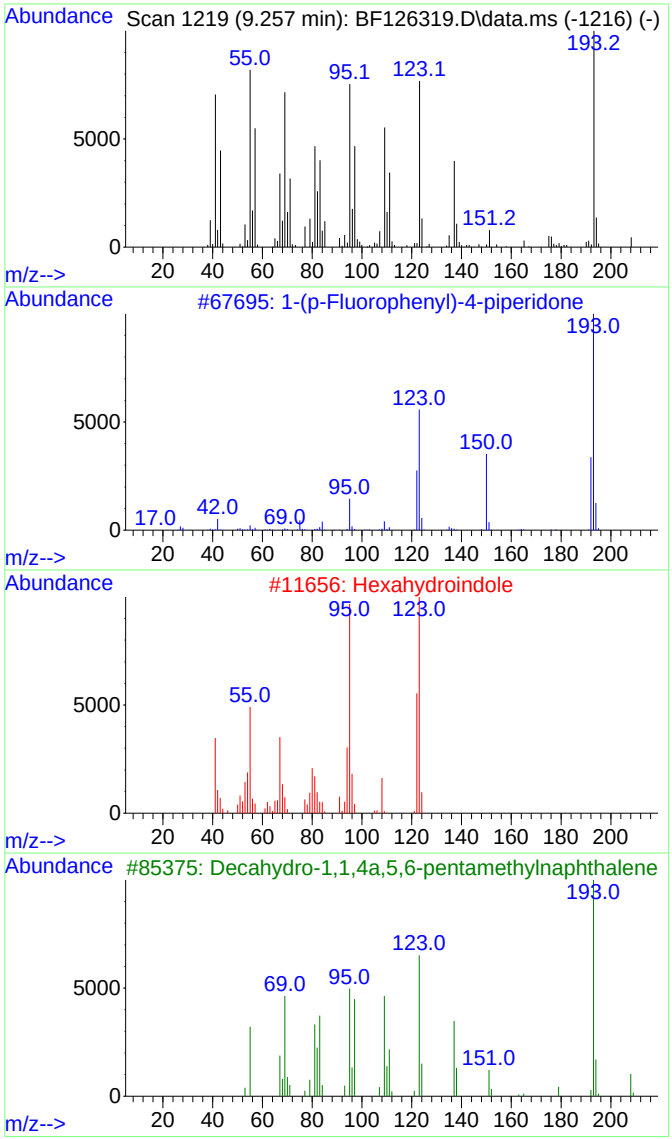
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

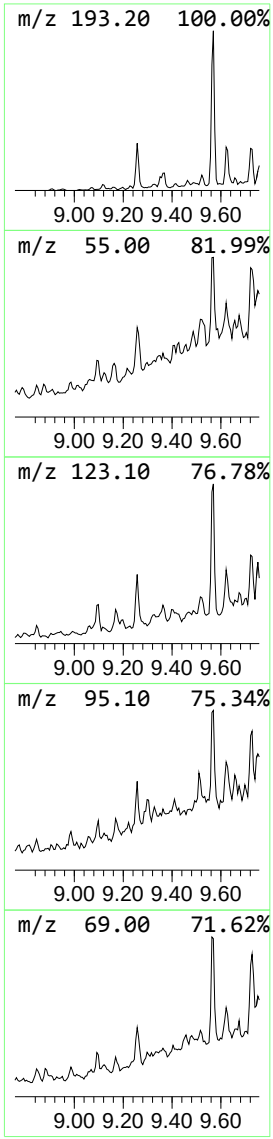
****

Peak Number 4 unknown9.257 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	2.40 ng	380656	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	30
2	Hexahydroindole	123	C8H13N	018159-32-5	30
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30
4	Naphthalene, 2-(1,1-dimethylethy...	208	C15H28	054934-96-2	25
5	Phorone	138	C9H14O	000504-20-1	18





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Instrument :
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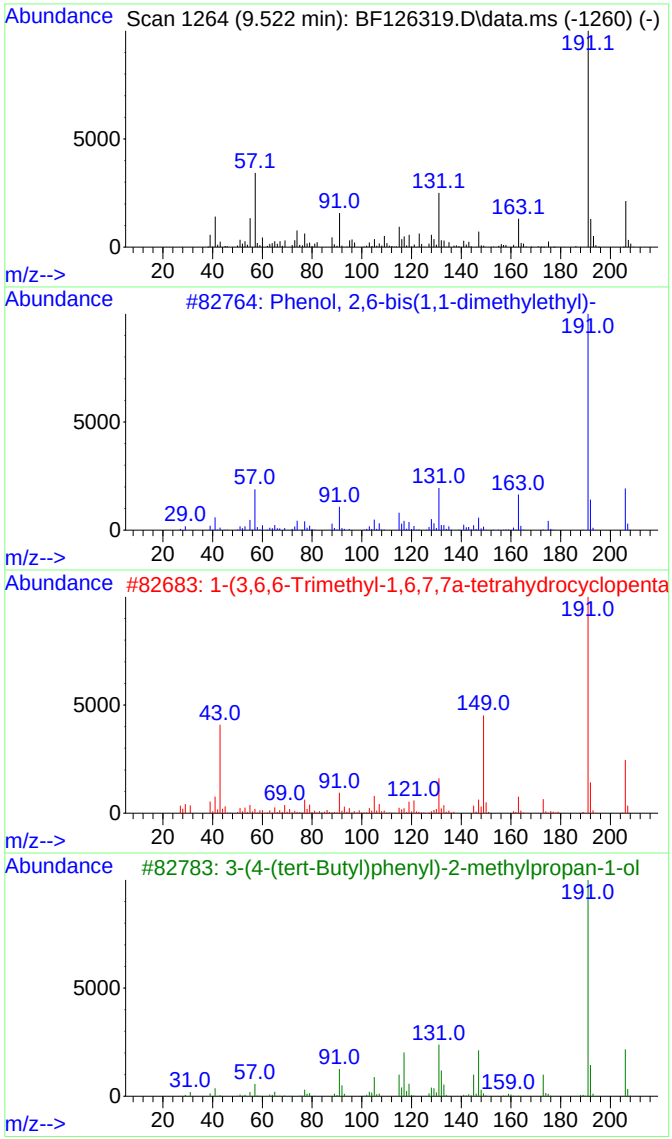
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

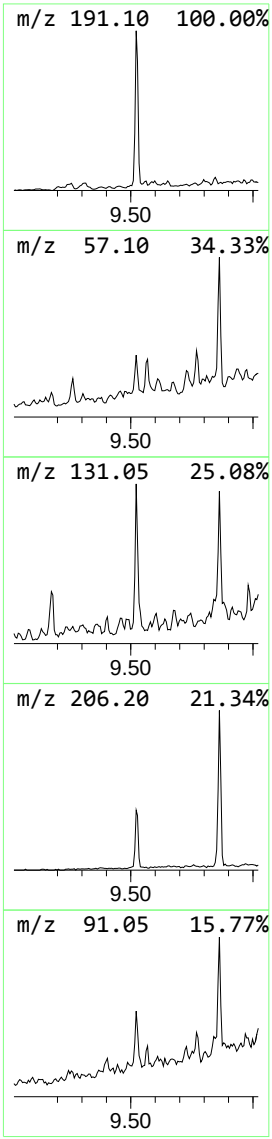
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.522	3.48 ng	550247	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	91
2	1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	87
3	3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	87
4	3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	83
5	Benzeneacetic acid, 4-(1,1-dimet...	206	C13H18O2	003549-23-3	72





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TIC Library : C:\Database\NIST20.L
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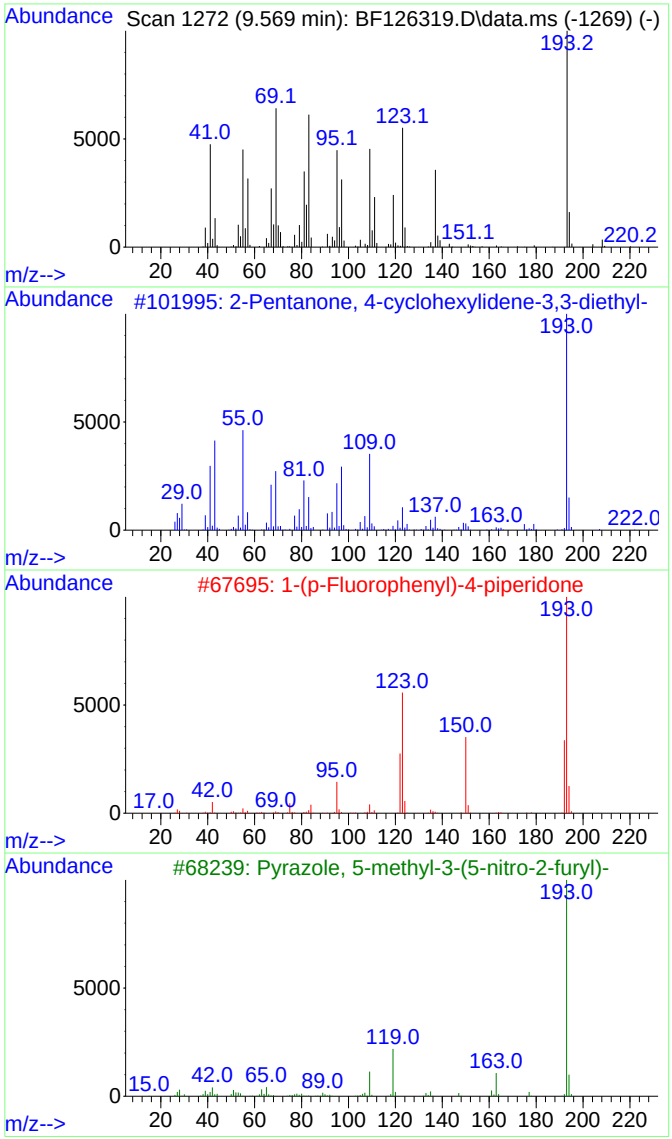
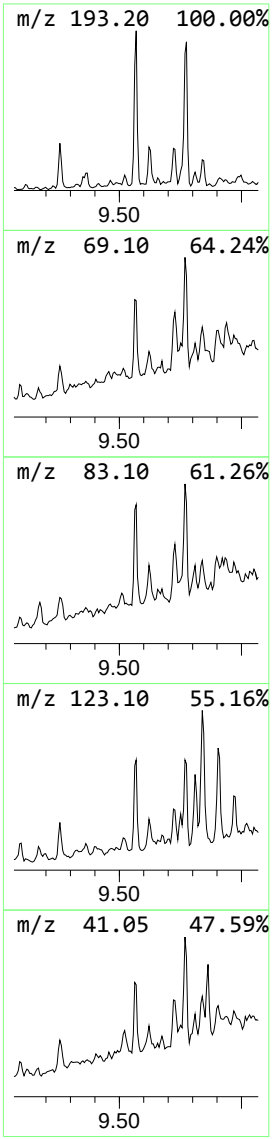
****

Peak Number 6 unknown9.569 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.569	5.71 ng	904663	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	47
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
3	Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	22
4	9-Phenanthrenamine	193	C14H11N	000947-73-9	14
5	2-Anthracenamine	193	C14H11N	000613-13-8	14





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Sample : M5182-04
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

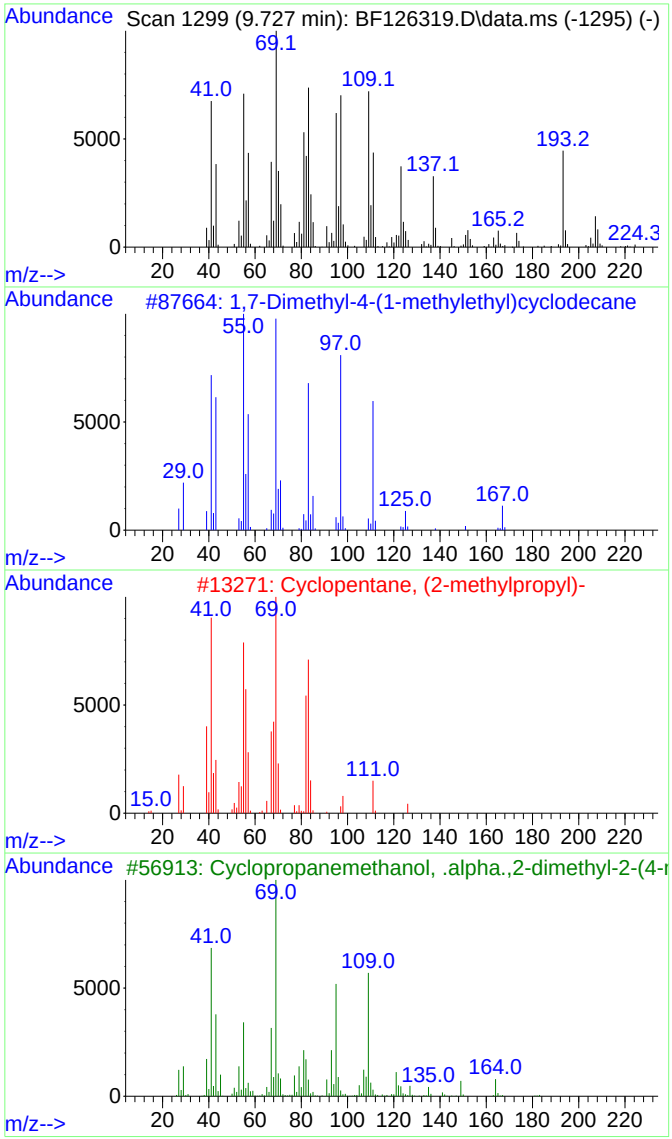
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

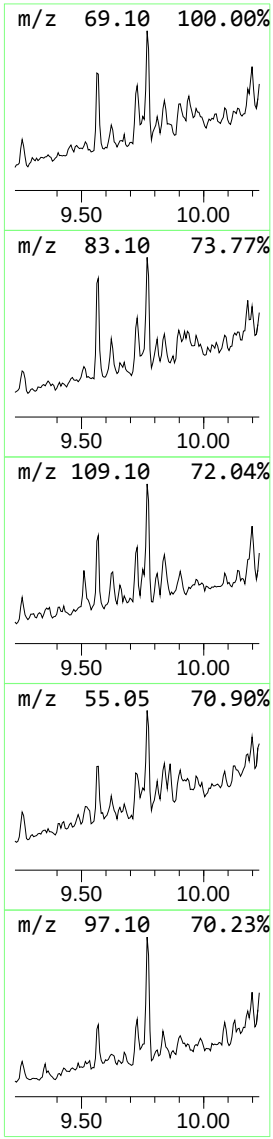
****

Peak Number 7 unknown9.727 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.727	5.02 ng	795062	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	43
2	Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	38
3	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	30
4	Benzene, 1,2-dichloro-3-nitro-	191	C6H3Cl2NO2	003209-22-1	25
5	Benzene, 2,4-dichloro-1-nitro-	191	C6H3Cl2NO2	000611-06-3	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126319.D
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Sample : M5182-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

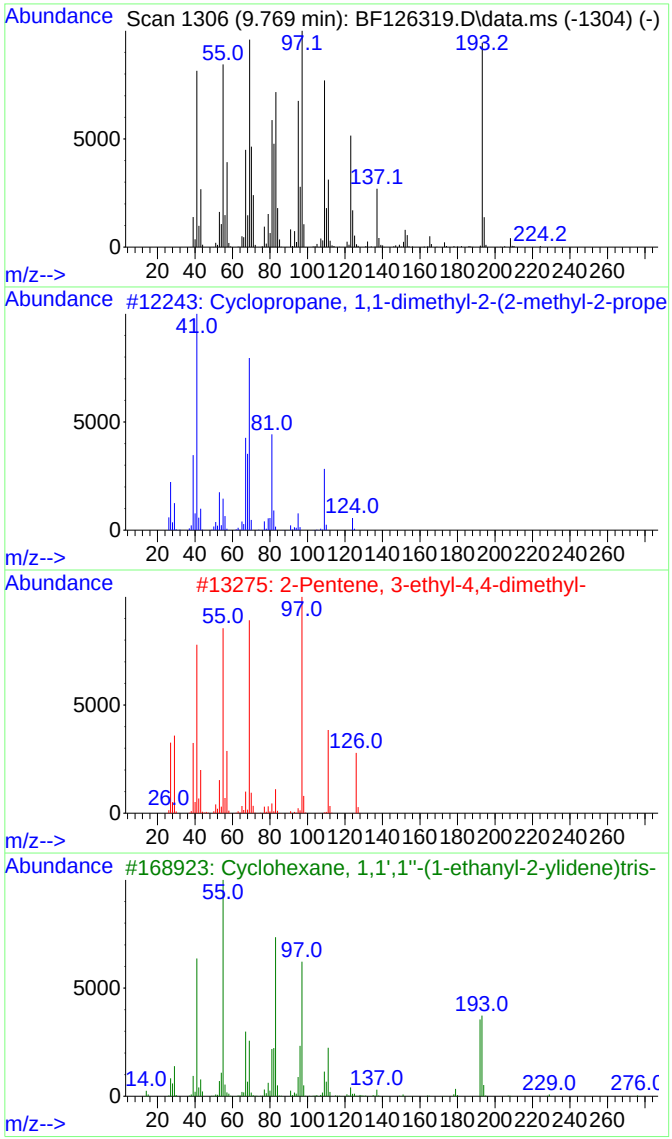
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

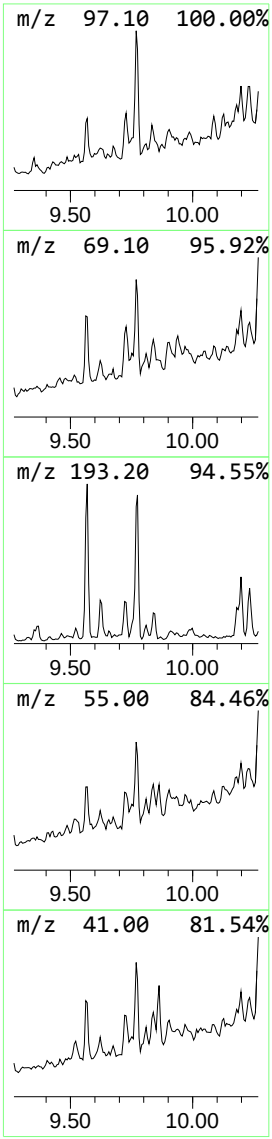
****

Peak Number 8 unknown9.769 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.769	7.71 ng	1221160	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	30
2	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	22
3	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	22
4	7-Ethyl-2-undecen-6-one	196	C13H24O	1000374-14-9	22
5	Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126319.D
Acq On : 22 Dec 2021 3:00
Operator : JU/CG
Sample : M5182-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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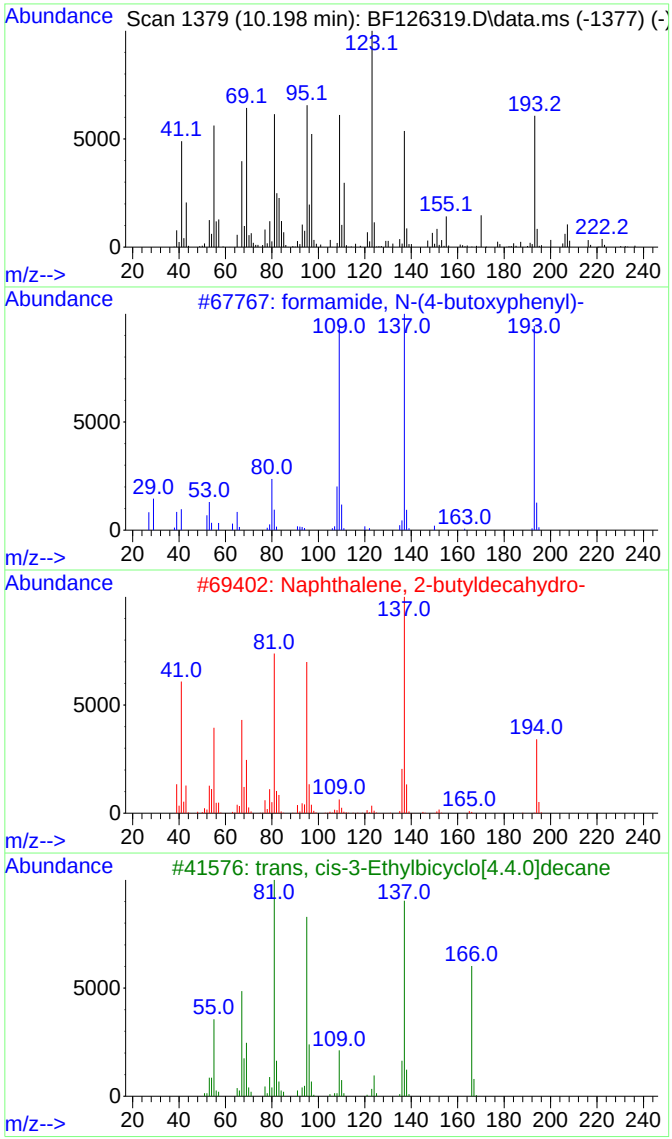
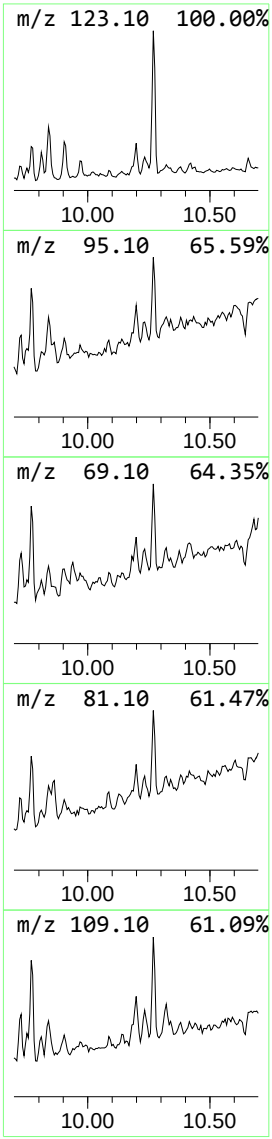
Peak Number 9 unknown10.198 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.198	2.39 ng	379031	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	formamide, N-(4-butoxyphenyl)-	193	C11H15NO2	1000400-28-0	35
2	Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	30
3	trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	27
4	Norbornane, 2-isobutyl-	152	C11H20	018127-14-5	14
5	3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126319.D
Acq On : 22 Dec 2021 3:00
Operator : JU/CG
Sample : M5182-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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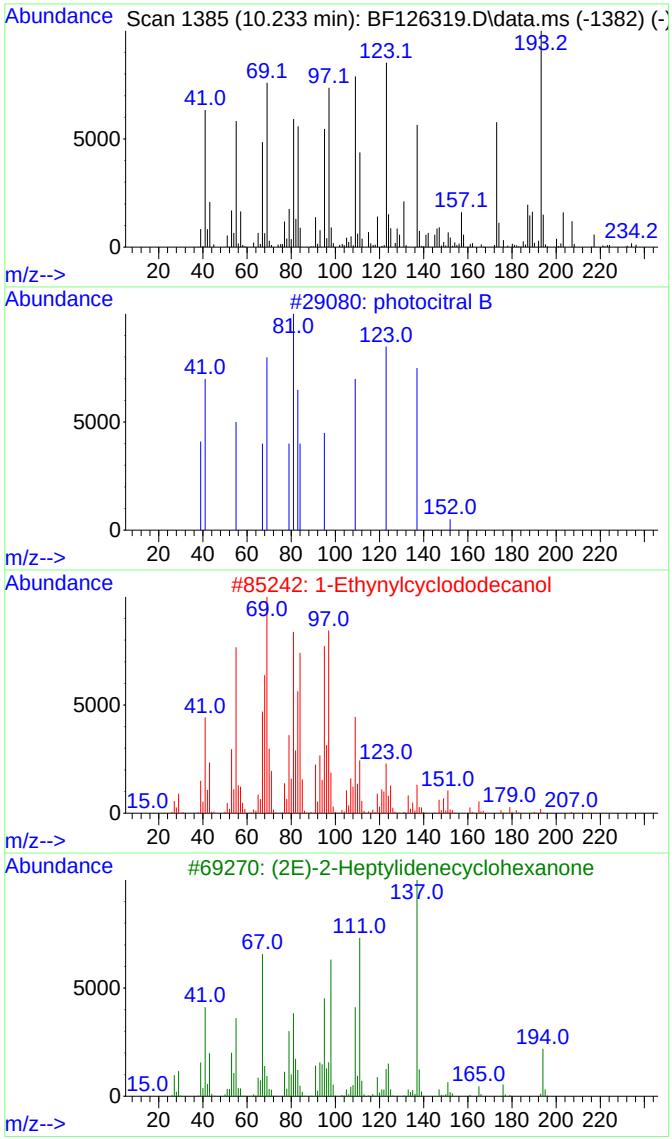
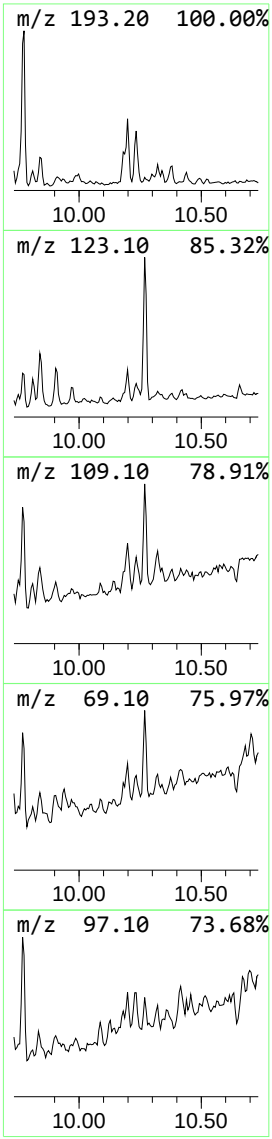
Peak Number 10 unknown10.233 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.233	3.09 ng	488402	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	photocitral B	152	C10H16O	006040-45-5	43
2	1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	38
3	(2E)-2-Heptylidenecyclohexanone	194	C13H22O	173975-69-4	25
4	2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	22
5	2-Butenamide, 2,3-dimethyl-N-phe...	189	C12H15NO	024735-54-4	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126319.D
Acq On : 22 Dec 2021 3:00
Operator : JU/CG
Sample : M5182-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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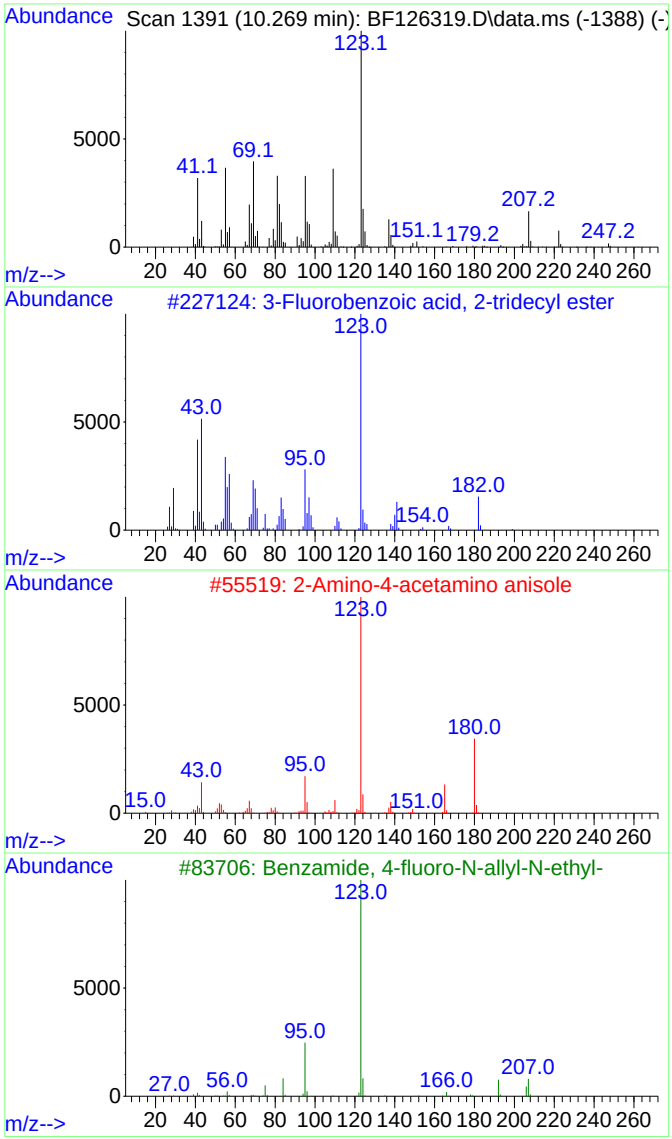
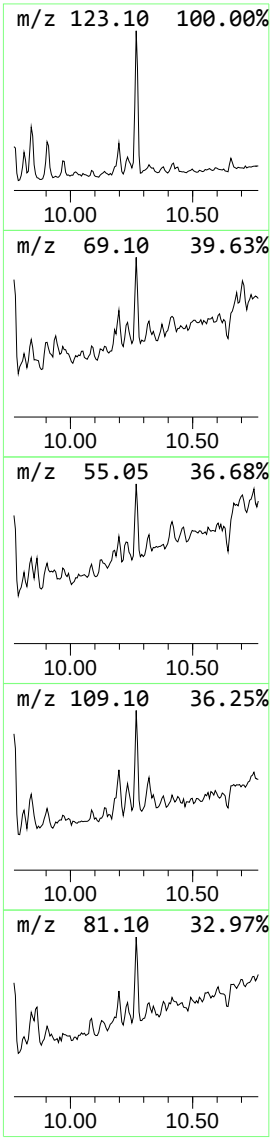
Peak Number 11 3-Fluorobenzoic acid, 2-tri... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.269	7.90 ng	1250220	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Fluorobenzoic acid, 2-tridecyl...	322	C20H31FO2	1000280-60-2	50
2	2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	47
3	Benzamide, 4-fluoro-N-allyl-N-et...	207	C12H14FNO	1000446-42-7	47
4	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	43
5	2-Fluoro-N-(1,3-thiazol-2-yl)ben...	222	C10H7FN2OS	000319-38-0	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126319.D
Acq On : 22 Dec 2021 3:00
Operator : JU/CG
Sample : M5182-04
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BNA_F
ClientSampleId :
HB-3-(10-15)-12-17-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.116	2.3	ng	127897	1	6.816	1125870	20.0
Naphthalene, de...	7.216	2.1	ng	115970	1	6.816	1125870	20.0
unknown9.257	9.257	2.4	ng	380656	3	9.857	3166290	20.0
Phenol, 2,6-bis...	9.522	3.5	ng	550247	3	9.857	3166290	20.0
unknown9.569	9.569	5.7	ng	904663	3	9.857	3166290	20.0
unknown9.727	9.727	5.0	ng	795062	3	9.857	3166290	20.0
unknown9.769	9.769	7.7	ng	1221160	3	9.857	3166290	20.0
unknown10.198	10.198	2.4	ng	379031	3	9.857	3166290	20.0
unknown10.233	10.233	3.1	ng	488402	3	9.857	3166290	20.0
3-Fluorobenzoic...	10.269	7.9	ng	1250220	3	9.857	3166290	20.0