Quantitation Report (Not Reviewed)

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN102920\
Data File : BN012451.D
Acq On : 30 Oct 2020 00:12
Operator : CG/JU
Sample : PB132717BS
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : PB132717BS

Quant Time: Oct 30 03:06:17 2020
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN102620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION
QLast Update : Wed Oct 28 10:32:42 2020
Response via : Initial Calibration

Compound	R.T.	QIon	Response	Conc	Units		Dev(Min)
Internal Standards							
1) 1,4-Dichlorobenzene-d4	7.578	152	961	0.40	ng		0.00
7) Naphthalene-d8	10.339	136	4000	0.40	ng		-0.01
13) Acenaphthene-d10	14.217	164	2176	0.40	ng		0.00
19) Phenanthrene-d10	16.968	188	4432	0.40	ng		0.00
29) Chrysene-d12	21.174	240	4269	0.40	ng		# 0.00
36) Perylene-d12	23.340	264	5065	0.40	ng		-0.01
System Monitoring Compounds							
4) 2-Fluorophenol	5.186	112	1191	0.35	ng		0.00
5) Phenol-d6	6.757	99	1480	0.37	ng		0.00
8) Nitrobenzene-d5	8.729	82	1576	0.36	ng		0.00
11) 2-Methylnaphthalene-d10	11.940	152	2330	0.36	ng		-0.01
14) 2,4,6-Tribromophenol	15.714	330	538	0.35	ng		-0.01
15) 2-Fluorobiphenyl	12.834	172	3037	0.38	ng		-0.01
27) Fluoranthene-d10	19.008	212	4757	0.35	ng		0.00
31) Terphenyl-d14	19.618	244	3699	0.37	ng		0.00
Target Compounds							Qvalue
2) 1,4-Dioxane	3.173	88	515	0.33	ng	#	78
3) n-Nitrosodimethylamine	3.487	42	1350	0.36	ng	#	70
6) bis(2-Chloroethyl)ether	7.014	93	943	0.35	ng	#	82
9) Naphthalene	10.390	128	4068	0.36	ng		99
10) Hexachlorobutadiene	10.681	225	868	0.37	ng	#	98
12) 2-Methylnaphthalene	12.015	142	2681	0.37	ng	#	87
16) Acenaphthylene	13.925	152	3962	0.37	ng		99
17) Acenaphthene	14.281	154	2505	0.37	ng		90
18) Fluorene	15.270	166	3110	0.36	ng		98
20) 4,6-Dinitro-2-methylph...	15.372	198	205	0.20	ng	#	1
21) 4-Bromophenyl-phenylether	16.165	248	968	0.36	ng	#	87
22) Hexachlorobenzene	16.274	284	1223	0.38	ng	#	83
23) Atrazine	16.445	200	913	0.35	ng		94
24) Pentachlorophenol	16.627	266	537	0.36	ng		95
25) Phenanthrene	17.005	178	4743	0.37	ng		98
26) Anthracene	17.102	178	4274	0.36	ng		98
28) Fluoranthene	19.037	202	5361	0.35	ng		99
30) Pyrene	19.400	202	5459	0.38	ng		99
32) Benzo(a)anthracene	21.152	228	4861	0.37	ng		97
33) Chrysene	21.205	228	5225	0.36	ng		98
34) Bis(2-ethylhexyl)phtha...	21.099	149	3115	0.37	ng		93
35) Indeno(1,2,3-cd)pyrene	25.500	276	8141	0.39	ng		97
37) Benzo(b)fluoranthene	22.738	252	6119	0.38	ng		93
38) Benzo(k)fluoranthene	22.738	252	6119	0.35	ng		93
39) Benzo(a)pyrene	23.244	252	5754	0.37	ng	#	84
40) Dibenzo(a,h)anthracene	25.517	278	6586	0.38	ng		94
41) Benzo(g,h,i)perylene	26.160	276	6825	0.37	ng		97

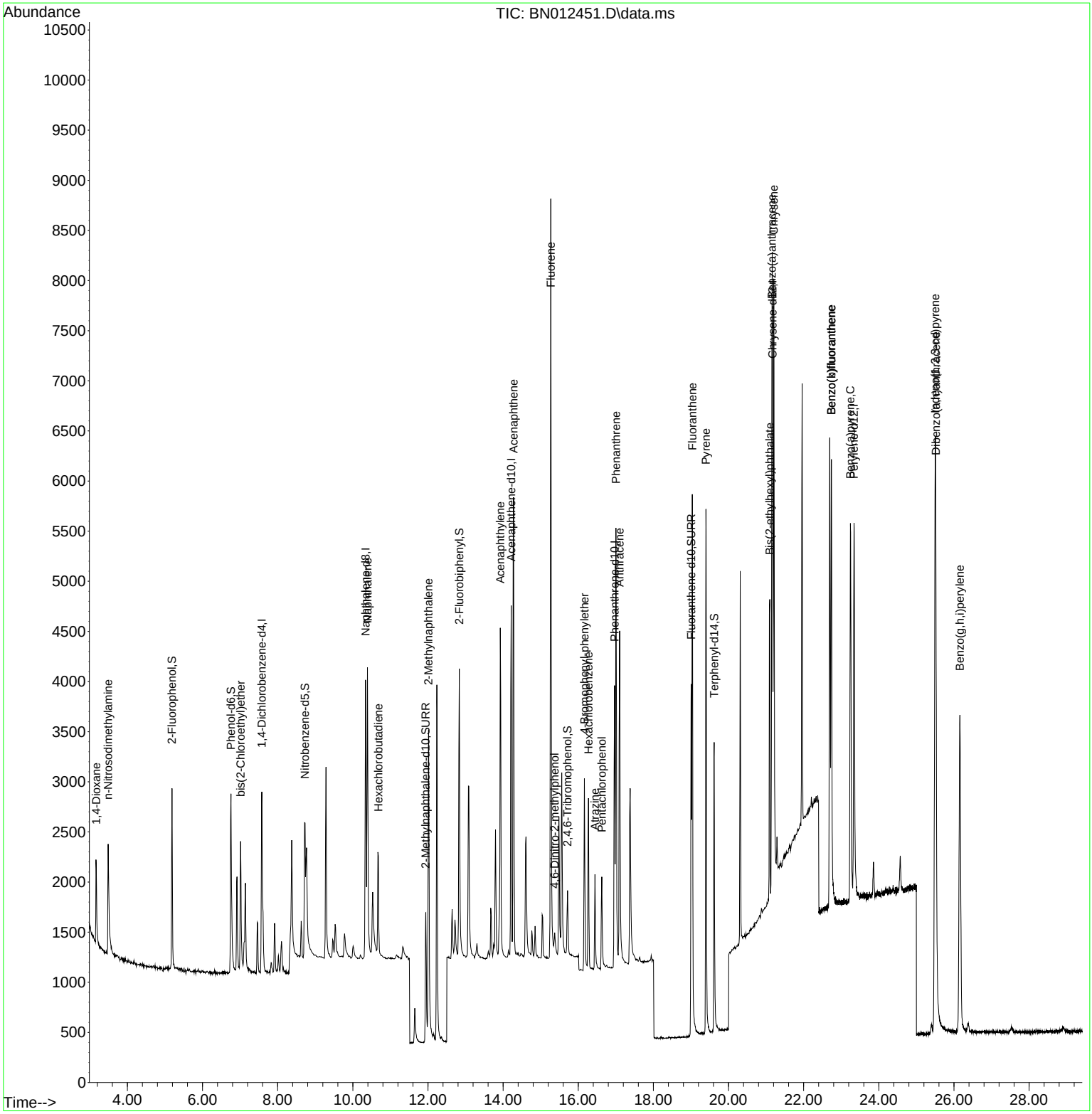
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (Not Reviewed)

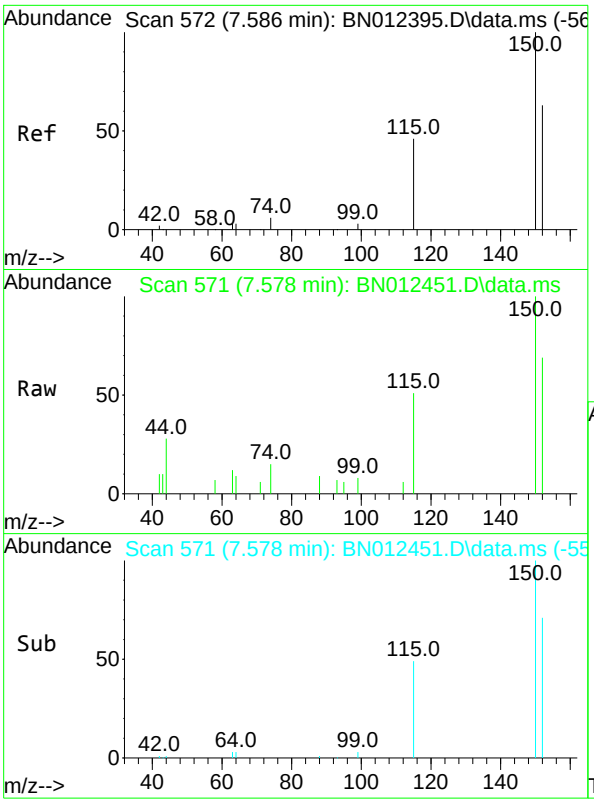
Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN102920\
Data File : BN012451.D
Acq On : 30 Oct 2020 00:12
Operator : CG/JU
Sample : PB132717BS
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB132717BS

Quant Time: Oct 30 03:06:17 2020
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN102620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION
QLast Update : Wed Oct 28 10:32:42 2020
Response via : Initial Calibration



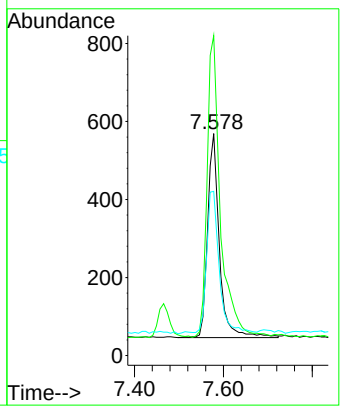
Instrument :
BNA_N
ClientSampleId :
PB132717BS

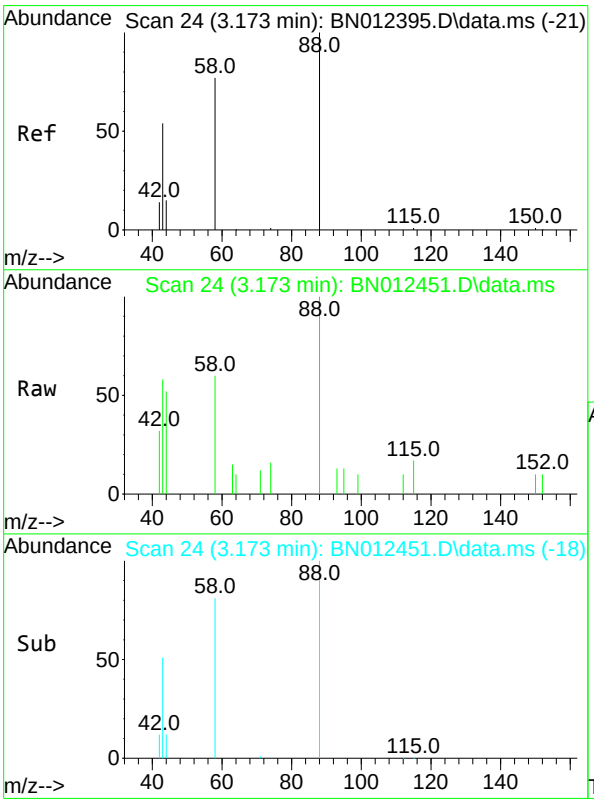


#1
1,4-Dichlorobenzene-d4
Concen: 0.40 ng
RT: 7.578 min Scan# 571
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:152 Resp: 961

Ion	Ratio	Lower	Upper
152	100		
150	144.1	116.6	174.8
115	74.0	52.9	79.3

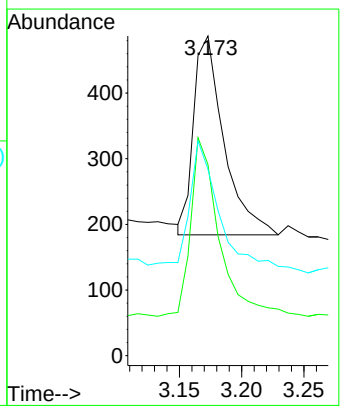




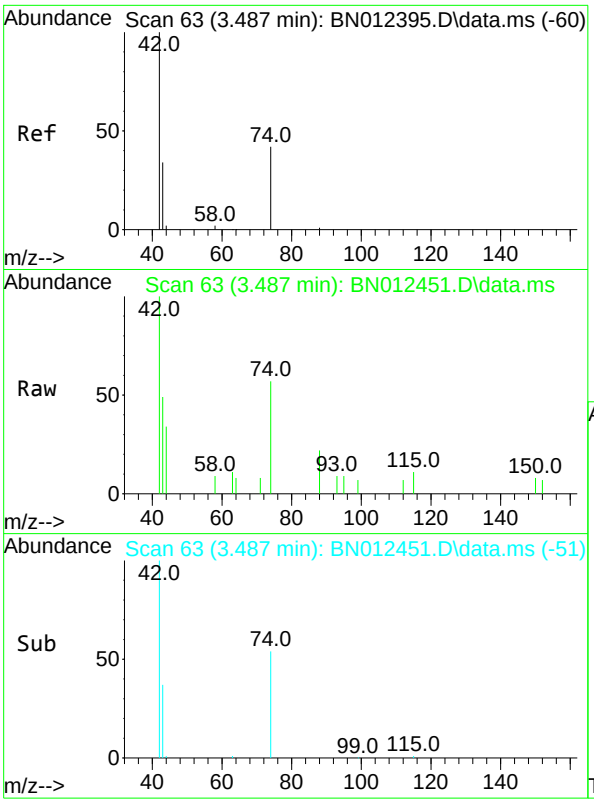
#2
1,4-Dioxane
Concen: 0.33 ng
RT: 3.173 min Scan# 24
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion: 88 Resp: 515

Ion	Ratio	Lower	Upper
88	100		
58	83.7	59.4	89.2
43	66.2	32.3	48.5#



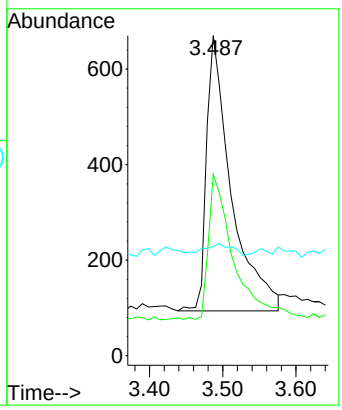
Instrument :
BNA_N
ClientSampleId :
PB132717BS

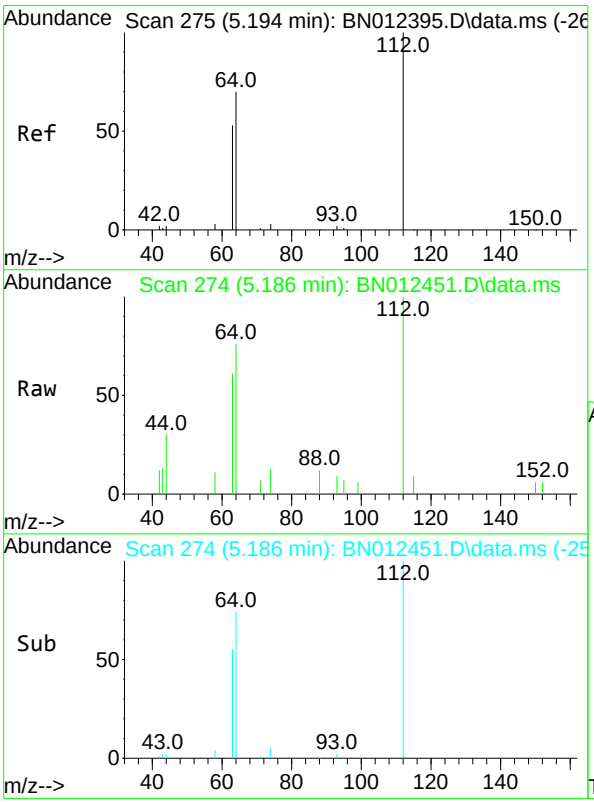


#3
n-Nitrosodimethylamine
Concen: 0.36 ng
RT: 3.487 min Scan# 63
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion: 42 Resp: 1350

Ion	Ratio	Lower	Upper
42	100		
74	53.0	64.4	96.6#
44	4.4	2.8	4.2#

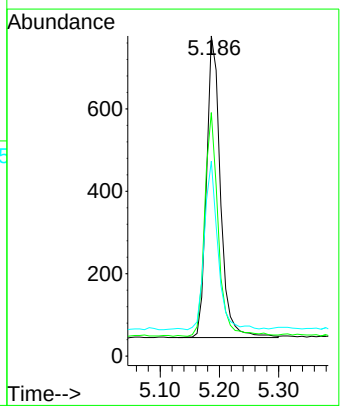




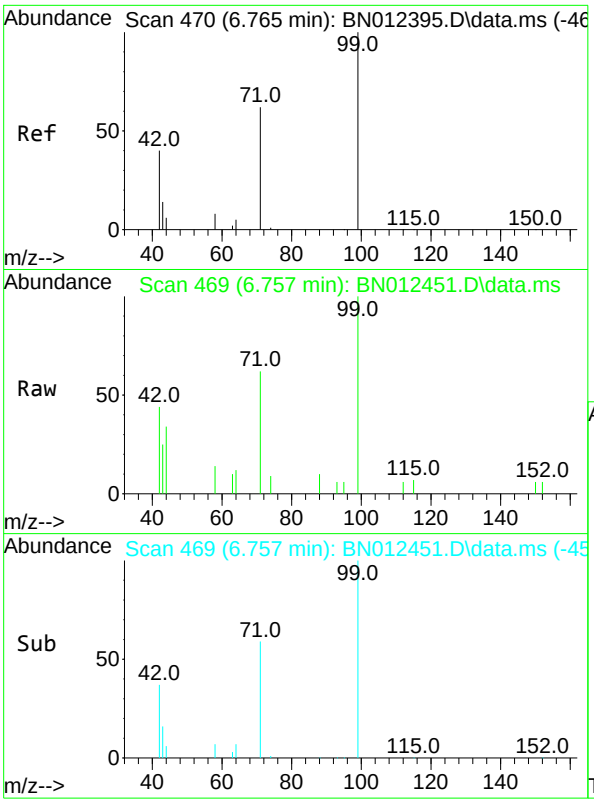
#4
2-Fluorophenol
Concen: 0.35 ng
RT: 5.186 min Scan# 274
Delta R.T. -0.008 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:112 Resp: 1191

Ion	Ratio	Lower	Upper
112	100		
64	71.5	49.5	74.3
63	54.1	32.0	48.0#



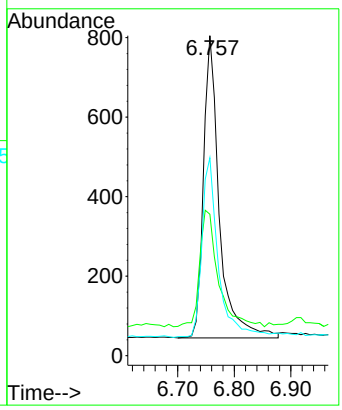
Instrument :
BNA_N
ClientSampleId :
PB132717BS

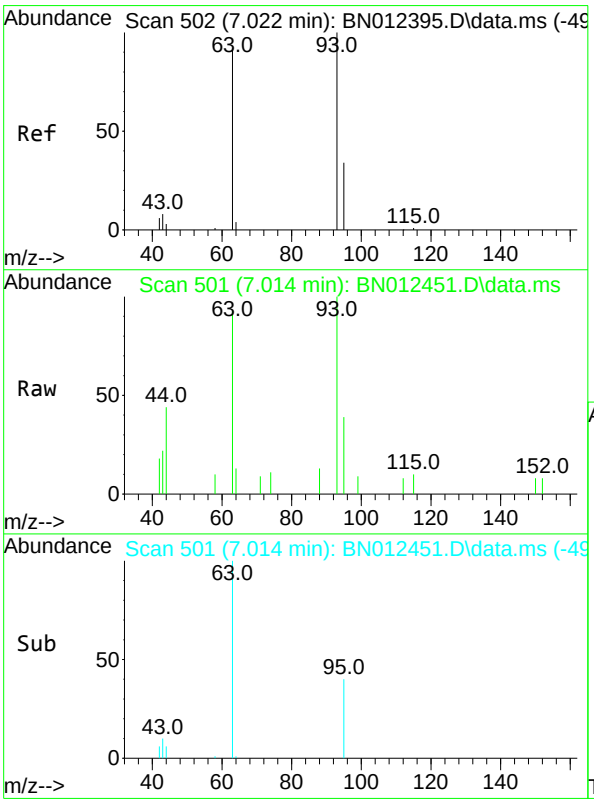


#5
Phenol-d6
Concen: 0.37 ng
RT: 6.757 min Scan# 469
Delta R.T. -0.008 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion: 99 Resp: 1480

Ion	Ratio	Lower	Upper
99	100		
42	44.7	22.4	33.6#
71	61.8	37.8	56.6#

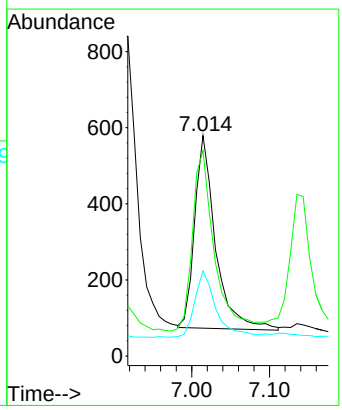




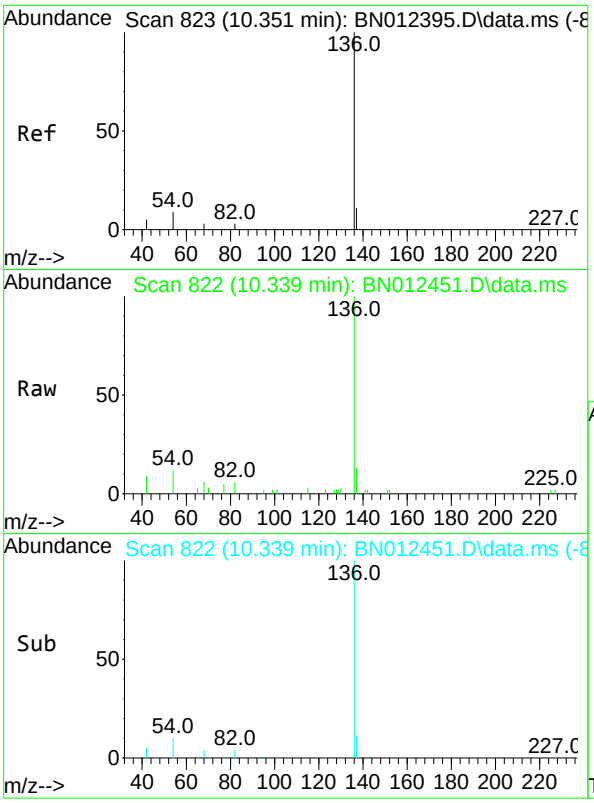
#6
bis(2-Chloroethyl)ether
Concen: 0.35 ng
RT: 7.014 min Scan# 501
Delta R.T. -0.008 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion: 93 Resp: 943

Ion	Ratio	Lower	Upper
93	100		
63	98.6	63.1	94.7#
95	35.7	26.1	39.1



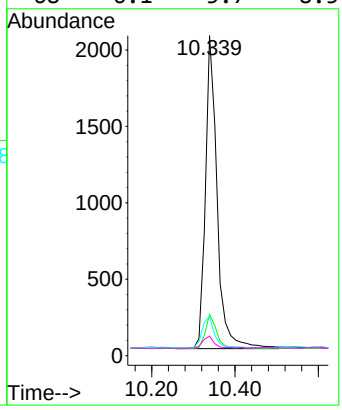
Instrument :
BNA_N
ClientSampleId :
PB132717BS

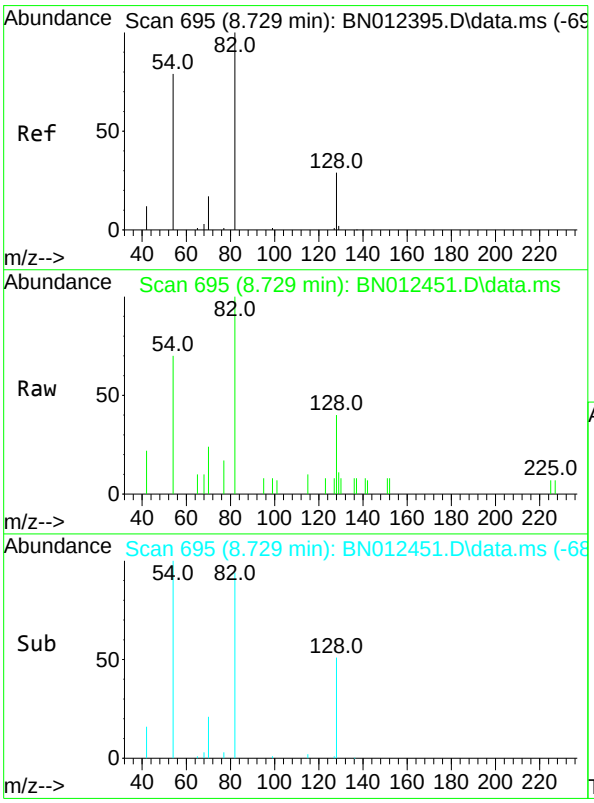


#7
Naphthalene-d8
Concen: 0.40 ng
RT: 10.339 min Scan# 822
Delta R.T. -0.013 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:136 Resp: 4000

Ion	Ratio	Lower	Upper
136	100		
137	12.9	10.6	15.8
54	12.2	8.6	12.8
68	6.1	5.7	8.5

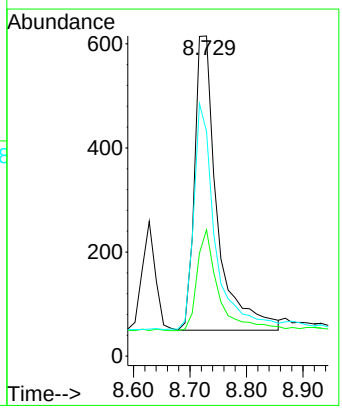




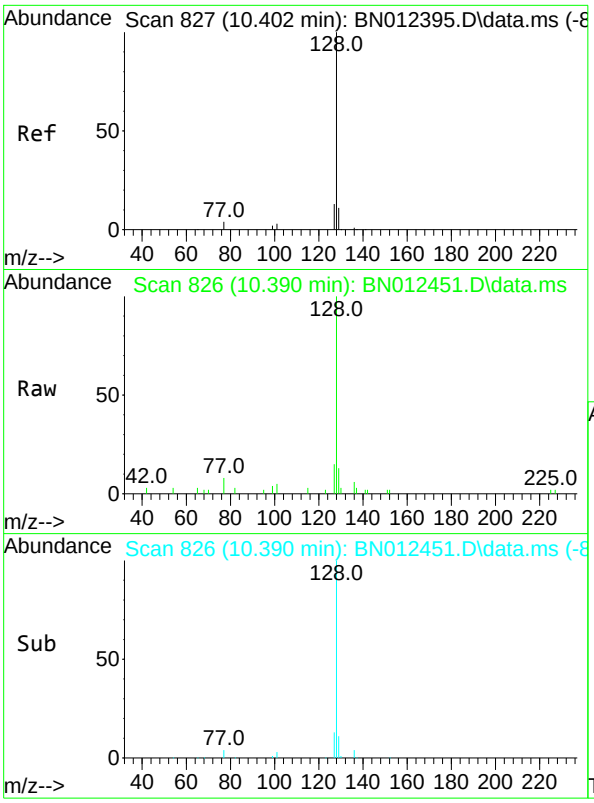
#8
Nitrobenzene-d5
Concen: 0.36 ng
RT: 8.729 min Scan# 695
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion: 82 Resp: 1576

Ion	Ratio	Lower	Upper
82	100		
128	39.5	30.6	46.0
54	70.2	48.3	72.5



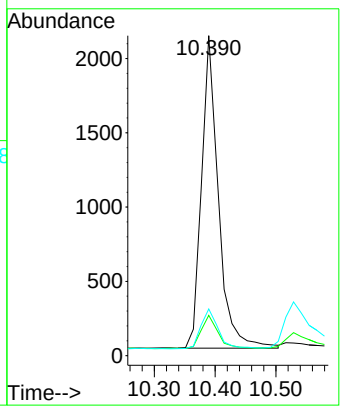
Instrument :
BNA_N
ClientSampleId :
PB132717BS

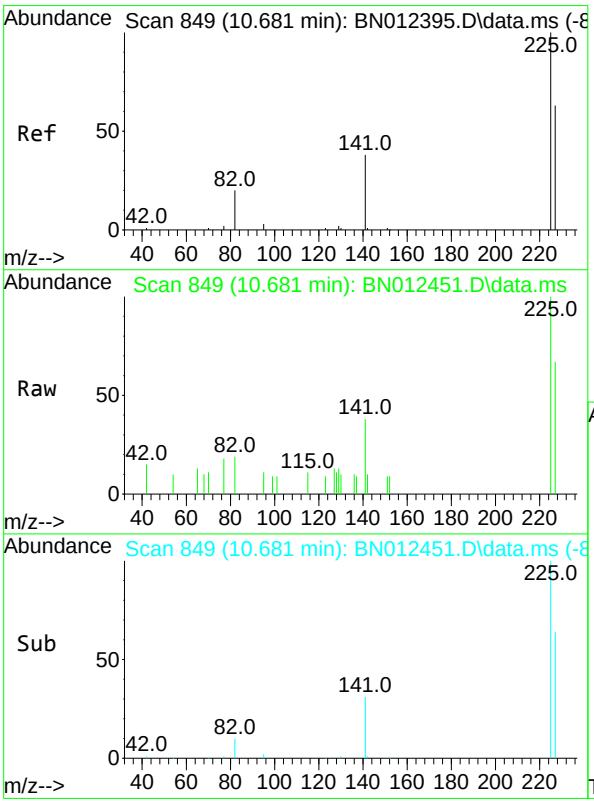


#9
Naphthalene
Concen: 0.36 ng
RT: 10.390 min Scan# 826
Delta R.T. -0.013 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:128 Resp: 4068

Ion	Ratio	Lower	Upper
128	100		
129	12.6	9.8	14.8
127	14.6	12.2	18.4

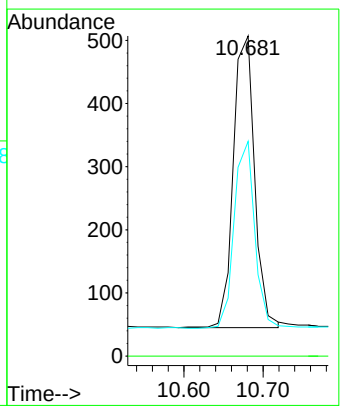




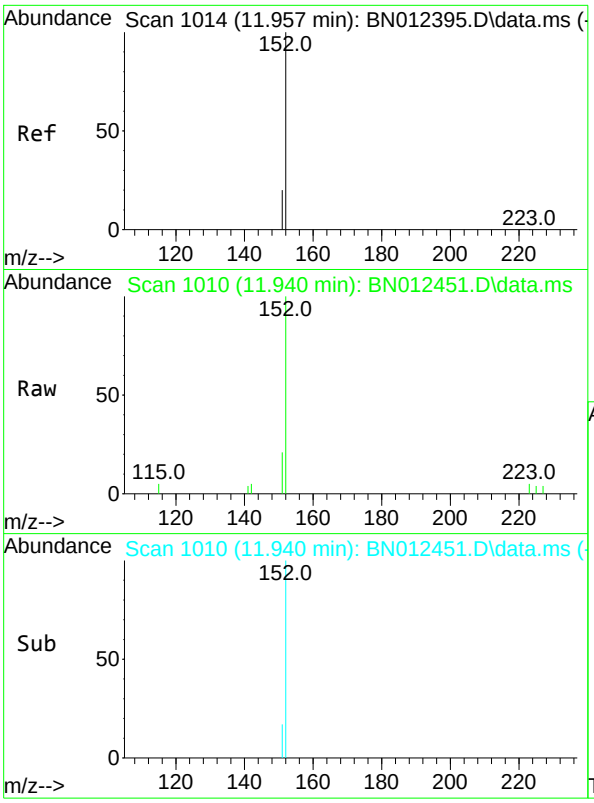
#10
Hexachlorobutadiene
Concen: 0.37 ng
RT: 10.681 min Scan# 849
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:225 Resp: 868

Ion	Ratio	Lower	Upper
225	100		
223	0.0	0.0	0.0
227	61.9	51.0	76.6



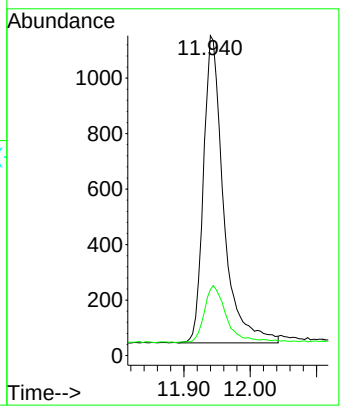
Instrument :
BNA_N
ClientSampleId :
PB132717BS

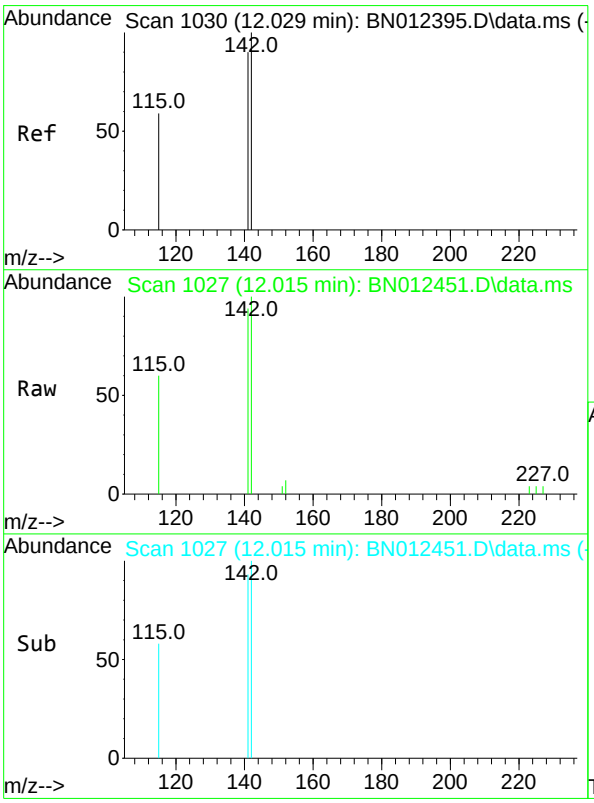


#11
2-Methylnaphthalene-d10
Concen: 0.36 ng
RT: 11.940 min Scan# 1010
Delta R.T. -0.013 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:152 Resp: 2330

Ion	Ratio	Lower	Upper
152	100		
151	20.6	16.7	25.1

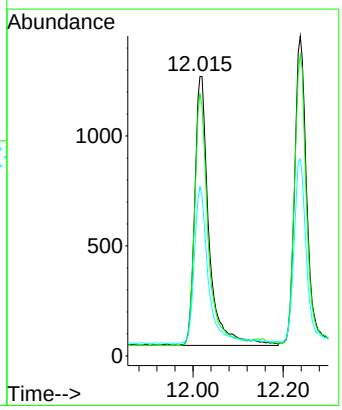




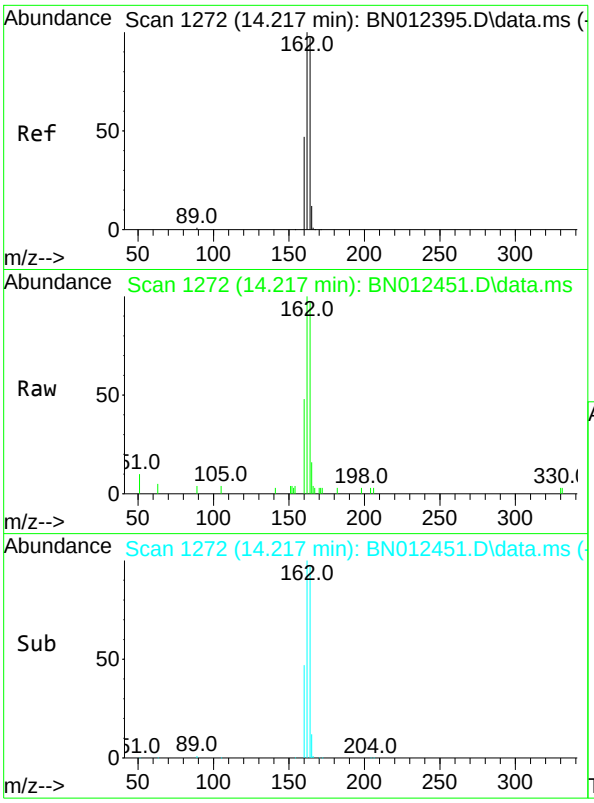
#12
2-Methylnaphthalene
Concen: 0.37 ng
RT: 12.015 min Scan# 1027
Delta R.T. -0.013 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:142 Resp: 2681

Ion	Ratio	Lower	Upper
142	100		
141	93.6	69.4	104.2
115	60.4	35.7	53.5#



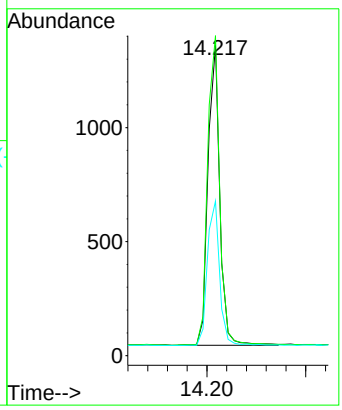
Instrument :
BNA_N
ClientSampleId :
PB132717BS

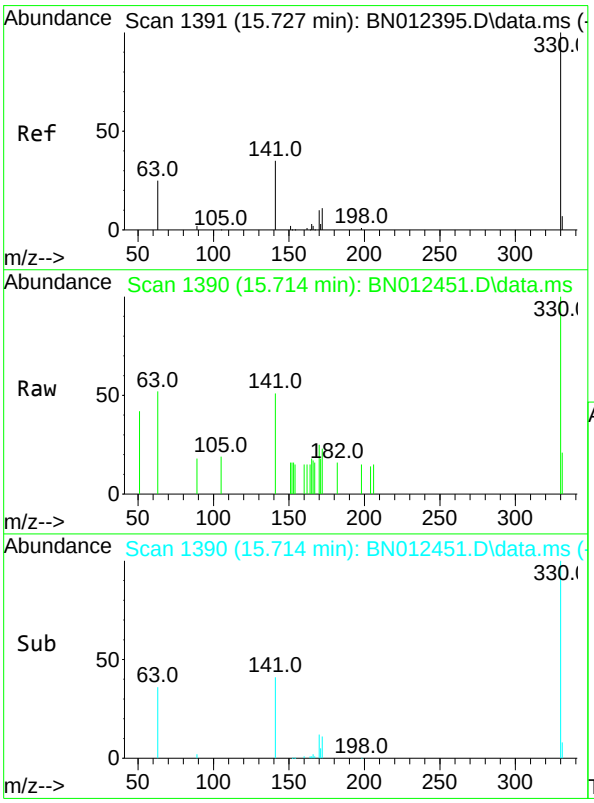


#13
Acenaphthene-d10
Concen: 0.40 ng
RT: 14.217 min Scan# 1272
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:164 Resp: 2176

Ion	Ratio	Lower	Upper
164	100		
162	103.2	80.6	120.8
160	49.9	39.5	59.3

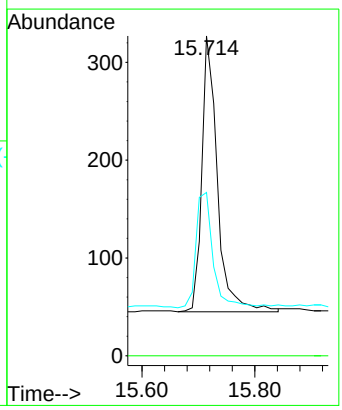




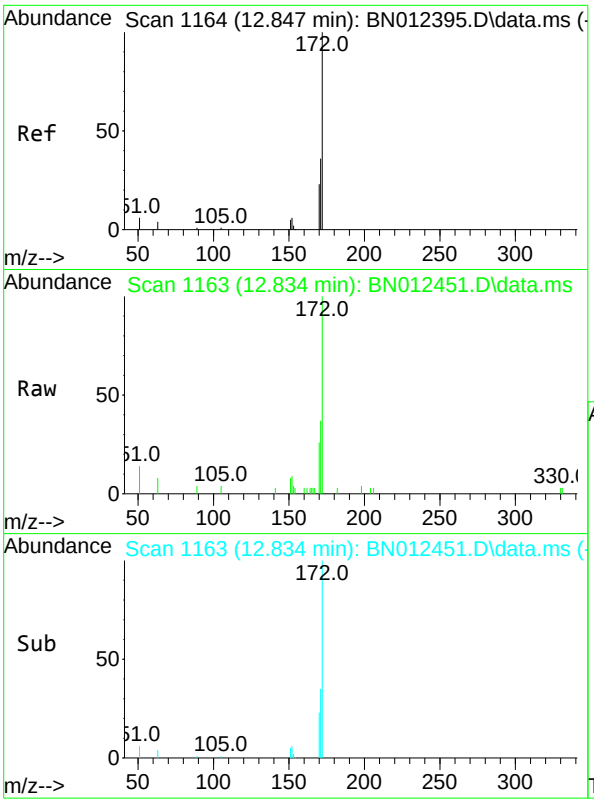
#14
2,4,6-Tribromophenol
Concen: 0.35 ng
RT: 15.714 min Scan# 1390
Delta R.T. -0.013 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:330 Resp: 538

Ion	Ratio	Lower	Upper
330	100		
332	0.0	0.0	0.0
141	45.9	34.4	51.6



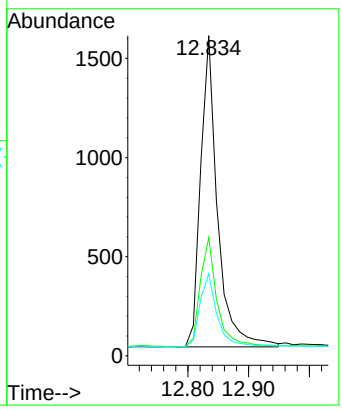
Instrument :
BNA_N
ClientSampleId :
PB132717BS

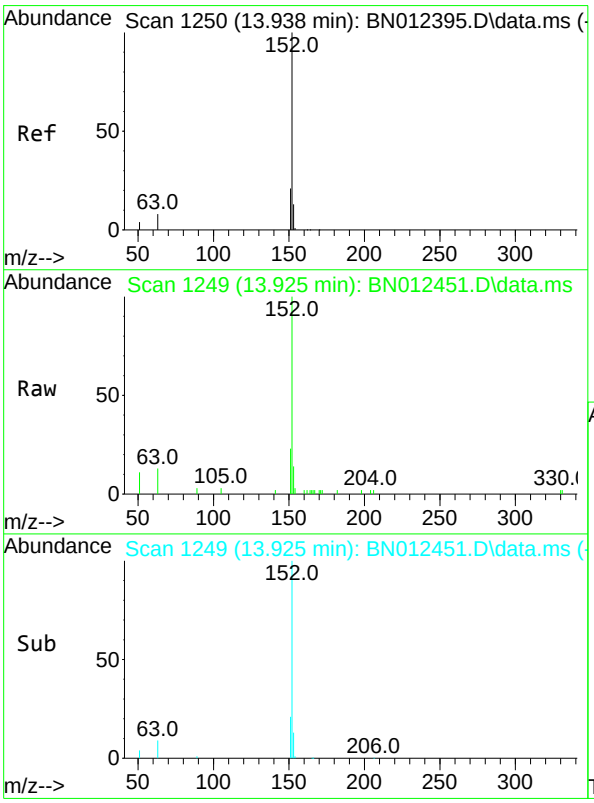


#15
2-Fluorobiphenyl
Concen: 0.38 ng
RT: 12.834 min Scan# 1163
Delta R.T. -0.013 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:172 Resp: 3037

Ion	Ratio	Lower	Upper
172	100		
171	37.0	28.2	42.4
170	25.6	20.0	30.0

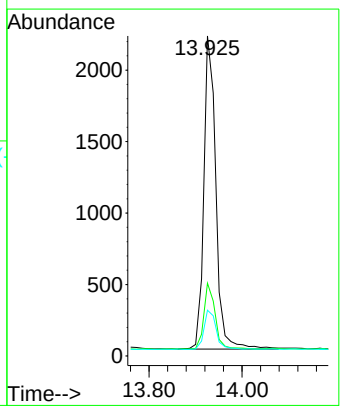




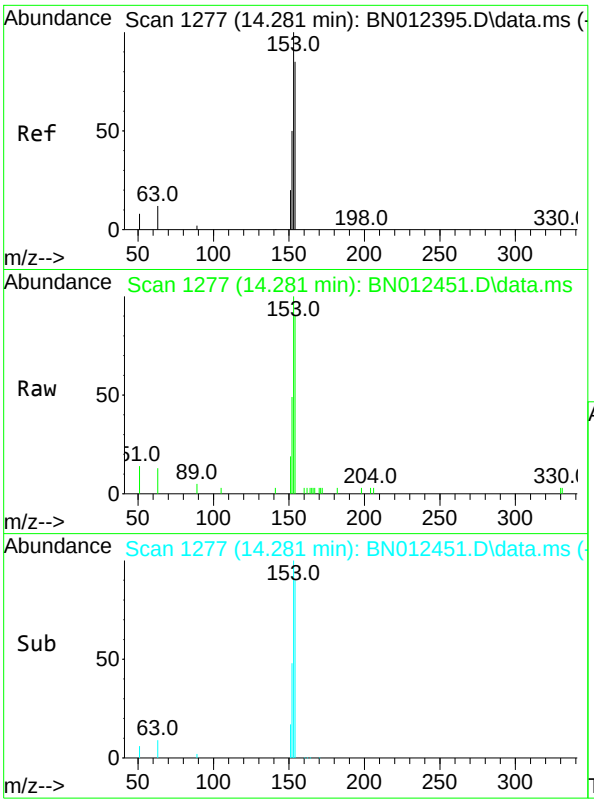
#16
Acenaphthylene
Concen: 0.37 ng
RT: 13.925 min Scan# 1249
Delta R.T. -0.013 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:152 Resp: 3962

Ion	Ratio	Lower	Upper
152	100		
151	19.5	15.8	23.8
153	12.8	10.6	16.0



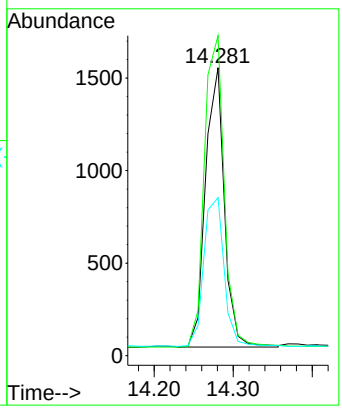
Instrument :
BNA_N
ClientSampleId :
PB132717BS

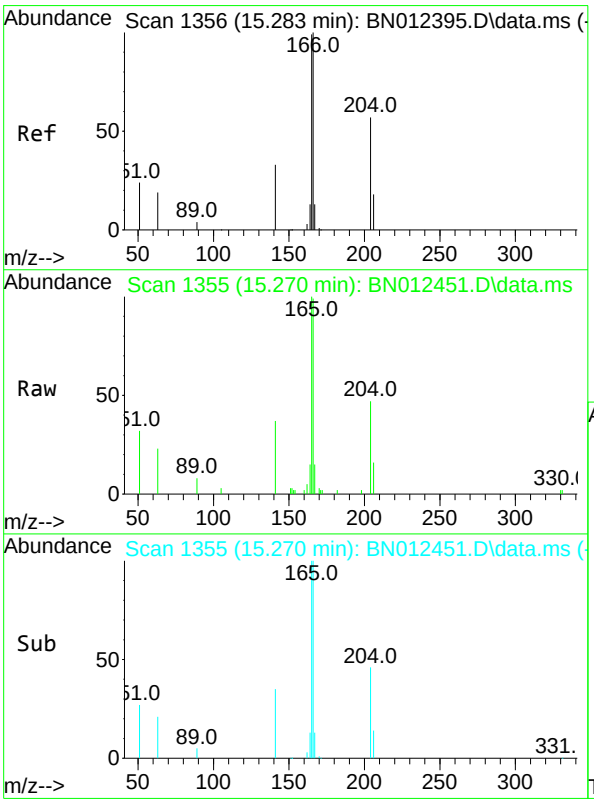


#17
Acenaphthene
Concen: 0.37 ng
RT: 14.281 min Scan# 1277
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:154 Resp: 2505

Ion	Ratio	Lower	Upper
154	100		
153	118.2	83.6	125.4
152	57.5	43.9	65.9

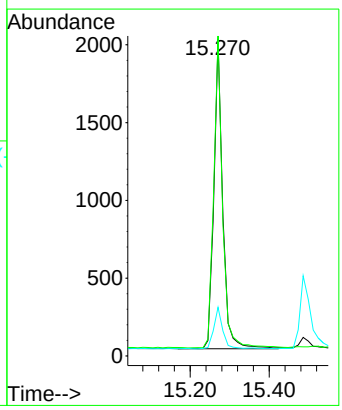




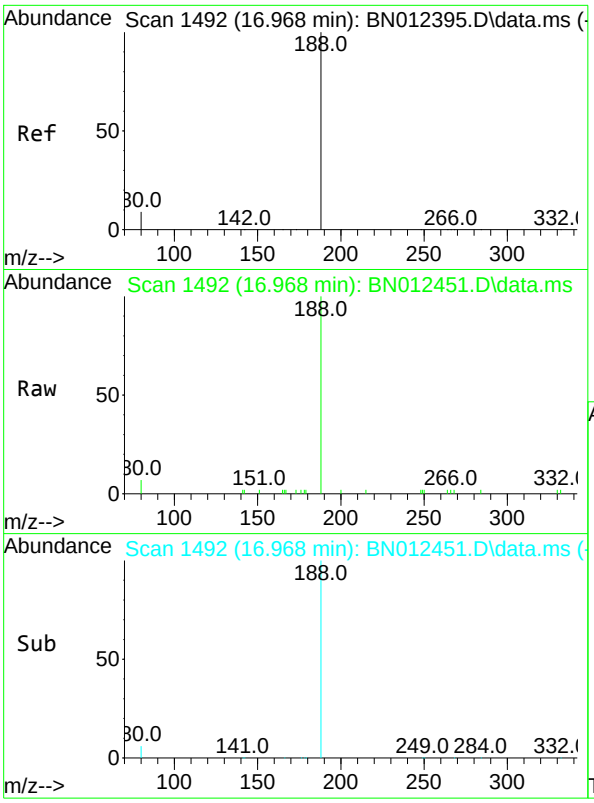
#18
Fluorene
Concen: 0.36 ng
RT: 15.270 min Scan# 1355
Delta R.T. -0.013 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:166 Resp: 3110

Ion	Ratio	Lower	Upper
166	100		
165	100.8	78.6	118.0
167	13.7	10.7	16.1



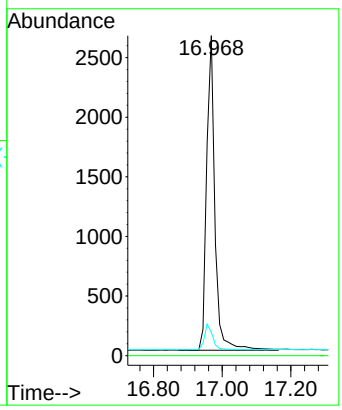
Instrument :
BNA_N
ClientSampleId :
PB132717BS

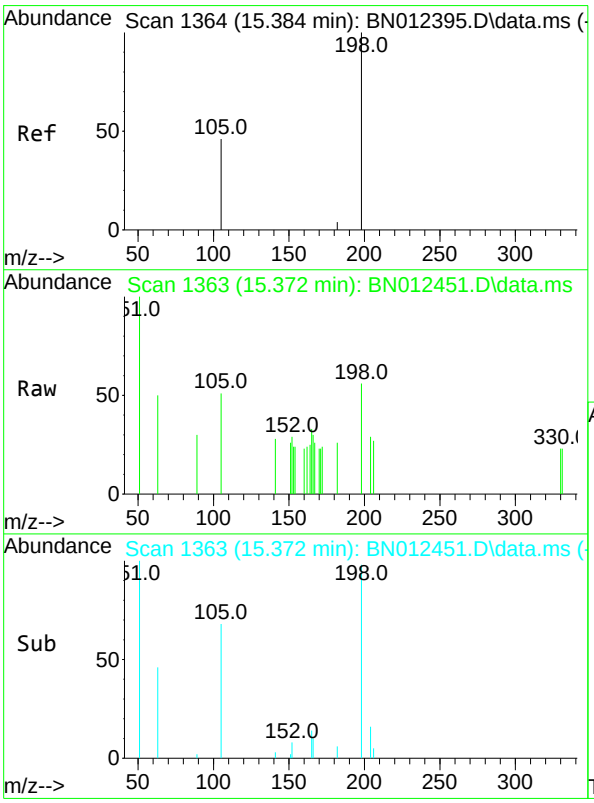


#19
Phenanthrene-d10
Concen: 0.40 ng
RT: 16.968 min Scan# 1492
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:188 Resp: 4432

Ion	Ratio	Lower	Upper
188	100		
94	0.0	0.0	0.0
80	7.3	5.0	7.4

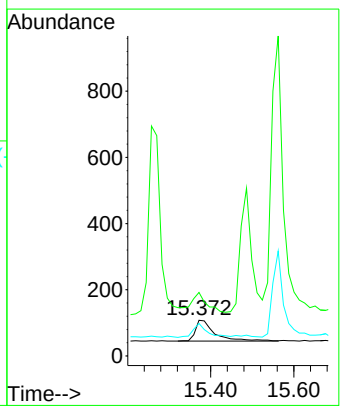


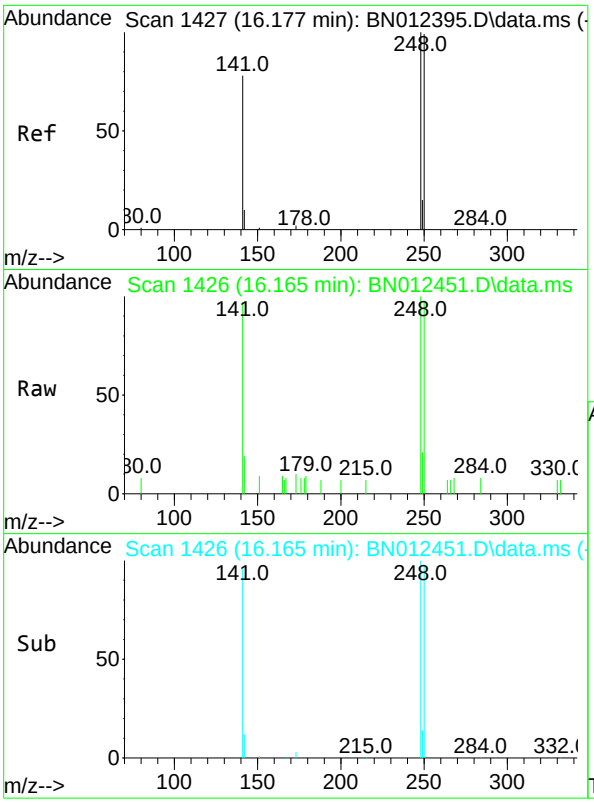


#20
4,6-Dinitro-2-methylphenol
Concen: 0.20 ng
RT: 15.372 min Scan# 1363
Delta R.T. -0.025 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:198 Resp: 205

Ion	Ratio	Lower	Upper
198	100		
51	177.8	43.5	65.3#
105	90.7	27.2	40.8#

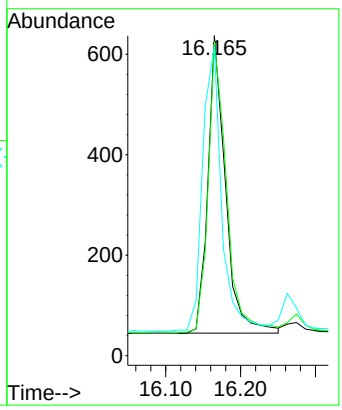




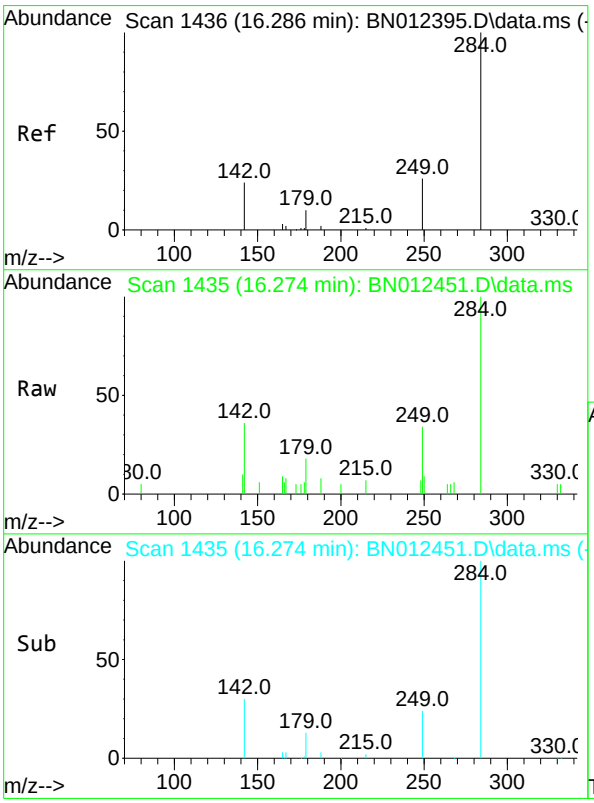
#21
4-Bromophenyl-phenylether
Concen: 0.36 ng
RT: 16.165 min Scan# 1426
Delta R.T. -0.012 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:248 Resp: 968

Ion	Ratio	Lower	Upper
248	100		
250	98.3	77.3	115.9
141	96.7	57.8	86.8#



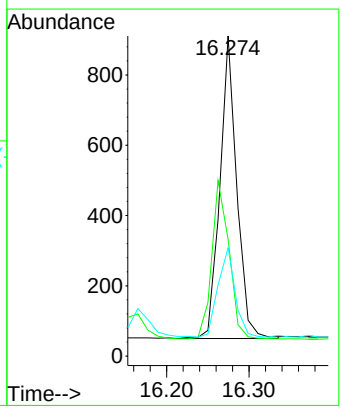
Instrument :
BNA_N
ClientSampleId :
PB132717BS



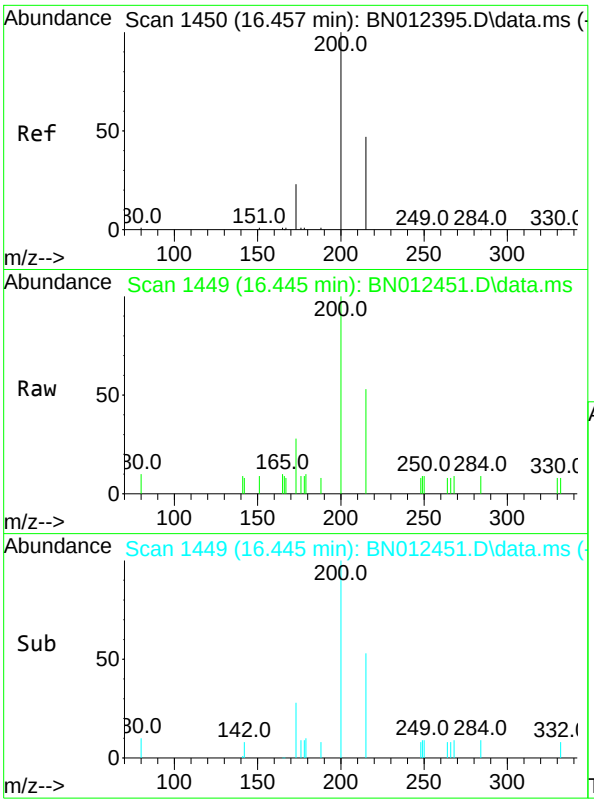
#22
Hexachlorobenzene
Concen: 0.38 ng
RT: 16.274 min Scan# 1435
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:284 Resp: 1223

Ion	Ratio	Lower	Upper
284	100		
142	55.7	32.0	48.0#
249	29.8	27.0	40.6



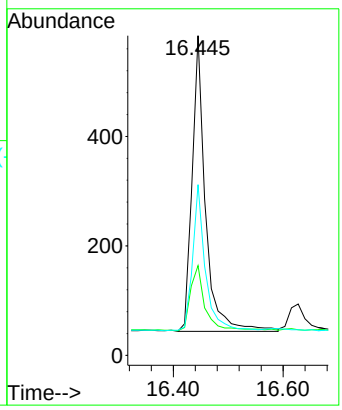
Instrument :
BNA_N
ClientSampleId :
PB132717BS

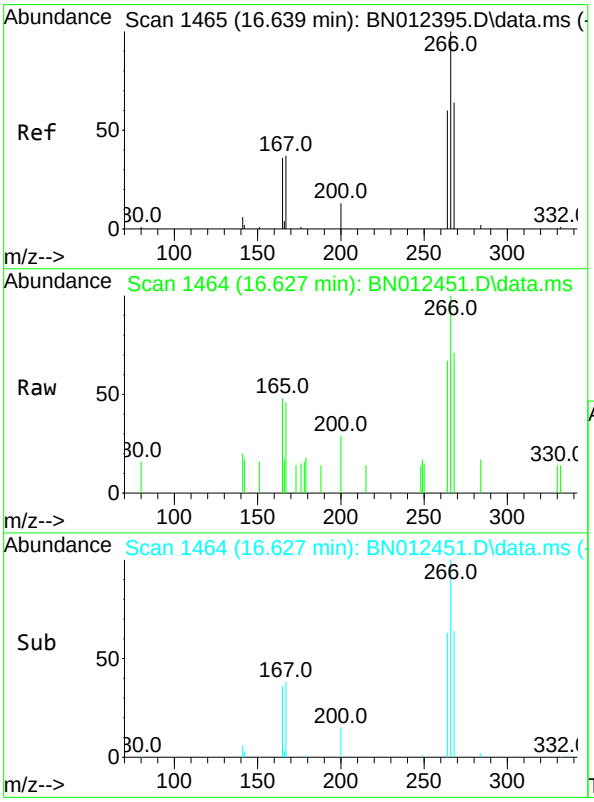


#23
Atrazine
Concen: 0.35 ng
RT: 16.445 min Scan# 1449
Delta R.T. -0.012 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:200 Resp: 913

Ion	Ratio	Lower	Upper
200	100		
173	28.1	22.8	34.2
215	53.4	38.1	57.1

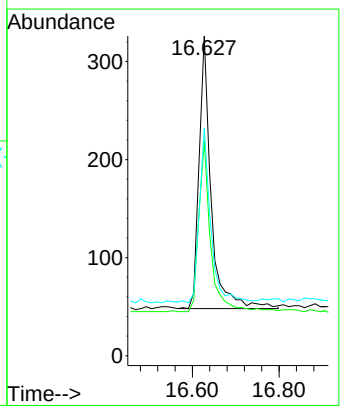




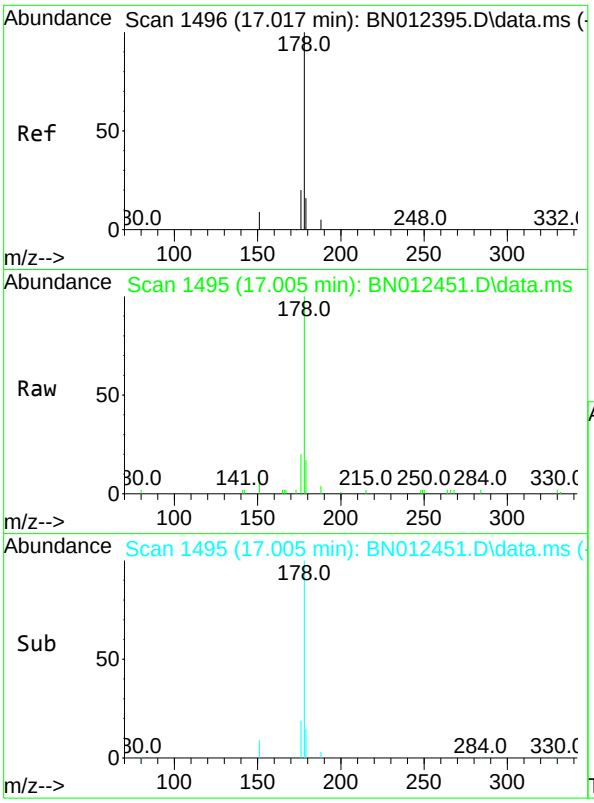
#24
Pentachlorophenol
Concen: 0.36 ng
RT: 16.627 min Scan# 1464
Delta R.T. -0.012 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:266 Resp: 537

Ion	Ratio	Lower	Upper
266	100		
264	61.3	50.9	76.3
268	59.0	51.5	77.3



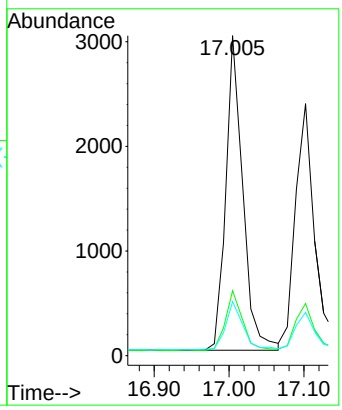
Instrument :
BNA_N
ClientSampleId :
PB132717BS

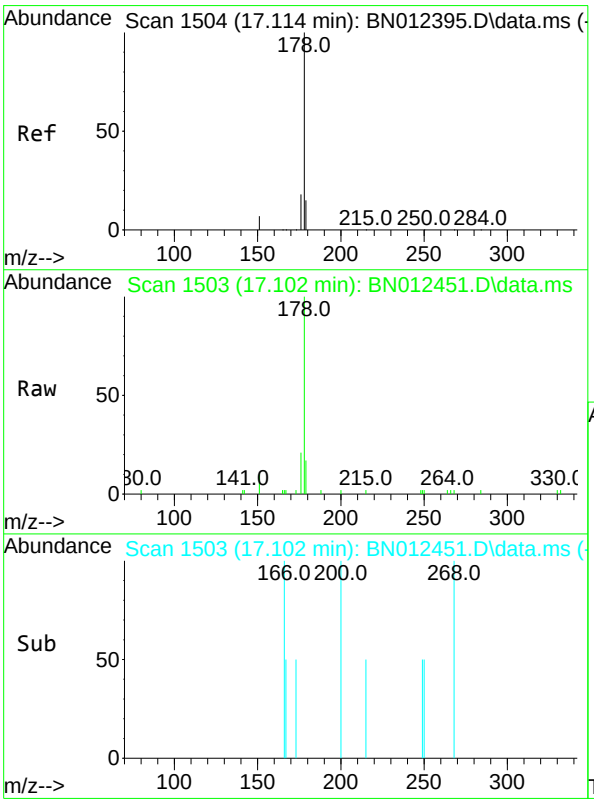


#25
Phenanthrene
Concen: 0.37 ng
RT: 17.005 min Scan# 1495
Delta R.T. -0.012 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:178 Resp: 4743

Ion	Ratio	Lower	Upper
178	100		
176	19.4	14.8	22.2
179	15.8	12.4	18.6

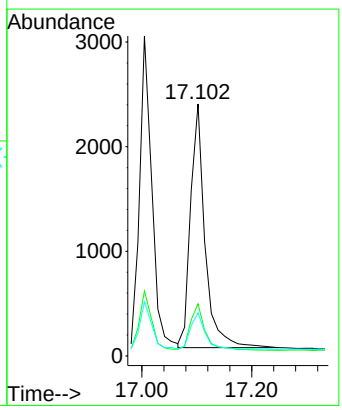


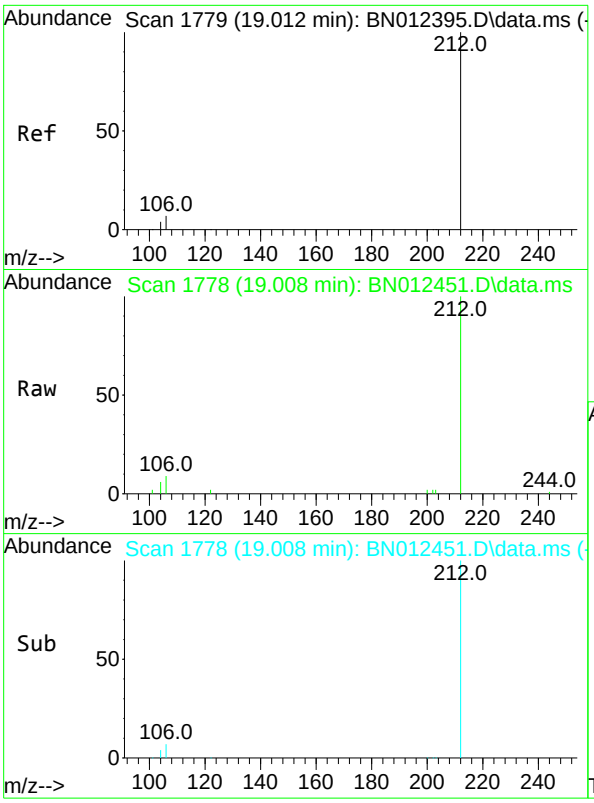


#26
Anthracene
Concen: 0.36 ng
RT: 17.102 min Scan# 1503
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:178 Resp: 4274

Ion	Ratio	Lower	Upper
178	100		
176	19.5	14.8	22.2
179	14.7	12.5	18.7

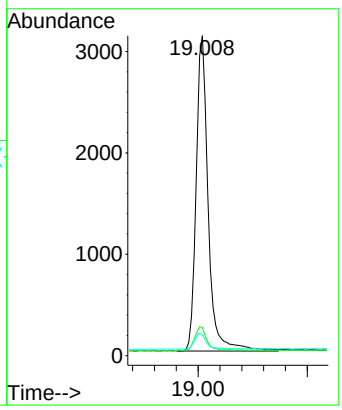




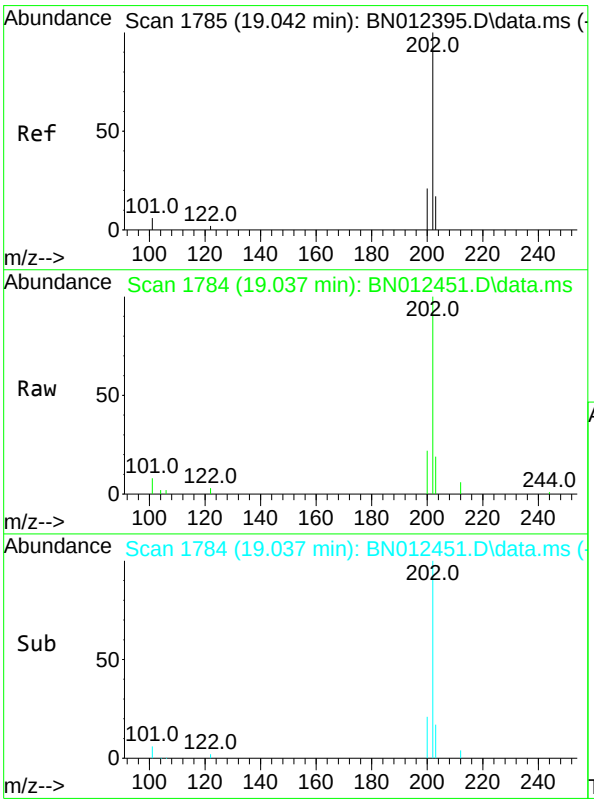
#27
Fluoranthene-d10
Concen: 0.35 ng
RT: 19.008 min Scan# 1778
Delta R.T. -0.005 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:212 Resp: 4757

Ion	Ratio	Lower	Upper
212	100		
106	7.5	6.8	10.2
104	4.8	4.1	6.1



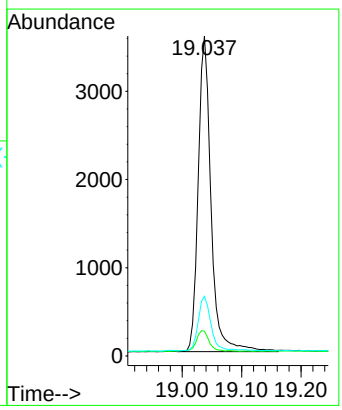
Instrument :
BNA_N
ClientSampleId :
PB132717BS



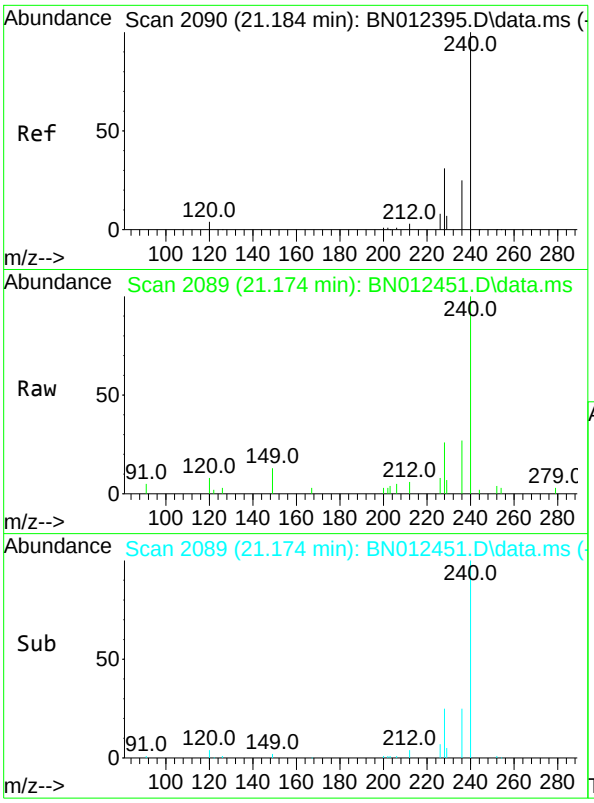
#28
Fluoranthene
Concen: 0.35 ng
RT: 19.037 min Scan# 1784
Delta R.T. -0.005 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:202 Resp: 5361

Ion	Ratio	Lower	Upper
202	100		
101	7.0	5.8	8.6
203	17.7	13.7	20.5



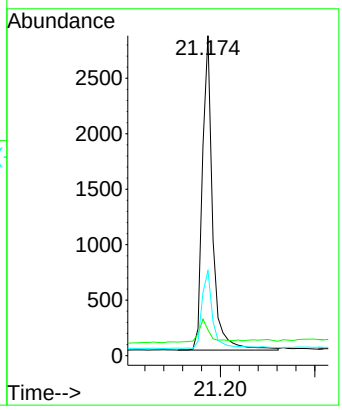
Instrument :
BNA_N
ClientSampleId :
PB132717BS

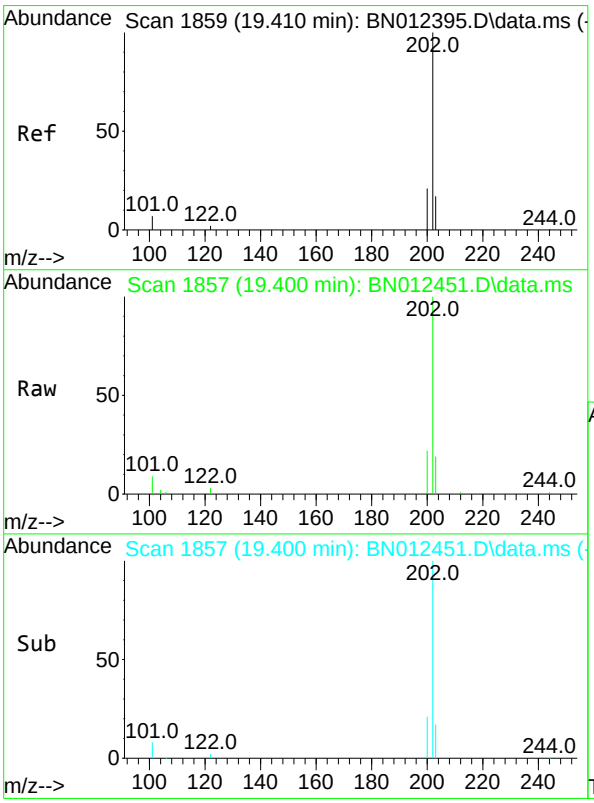


#29
Chrysene-d12
Concen: 0.40 ng
RT: 21.174 min Scan# 2089
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:240 Resp: 4269

Ion	Ratio	Lower	Upper
240	100		
120	8.0	5.3	7.9#
236	26.5	21.8	32.8

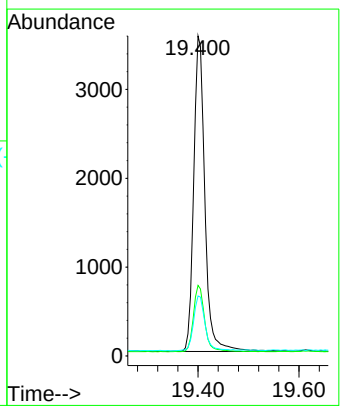




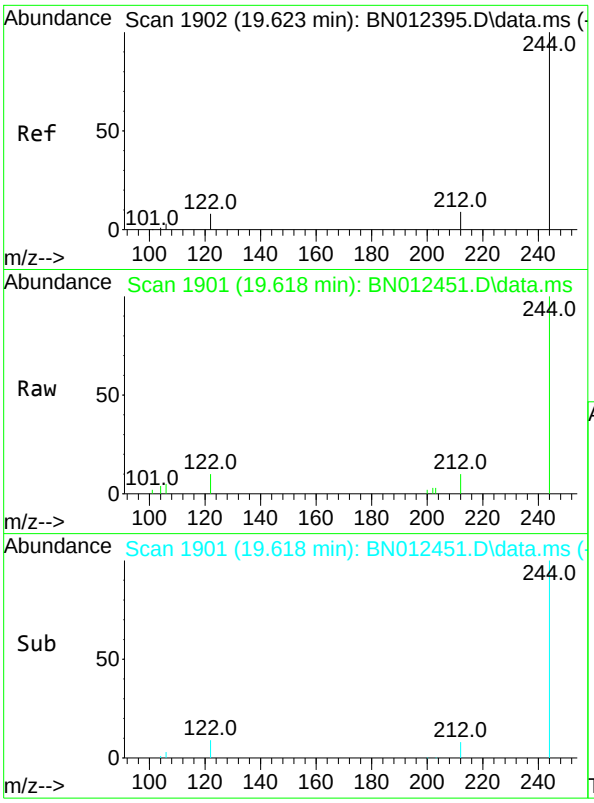
#30
Pyrene
Concen: 0.38 ng
RT: 19.400 min Scan# 1857
Delta R.T. -0.010 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:202 Resp: 5459

Ion	Ratio	Lower	Upper
202	100		
200	21.0	16.6	24.8
203	18.1	13.8	20.8



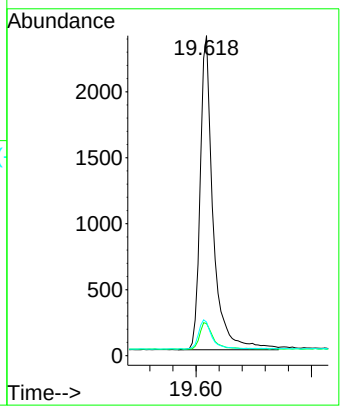
Instrument :
BNA_N
ClientSampleId :
PB132717BS

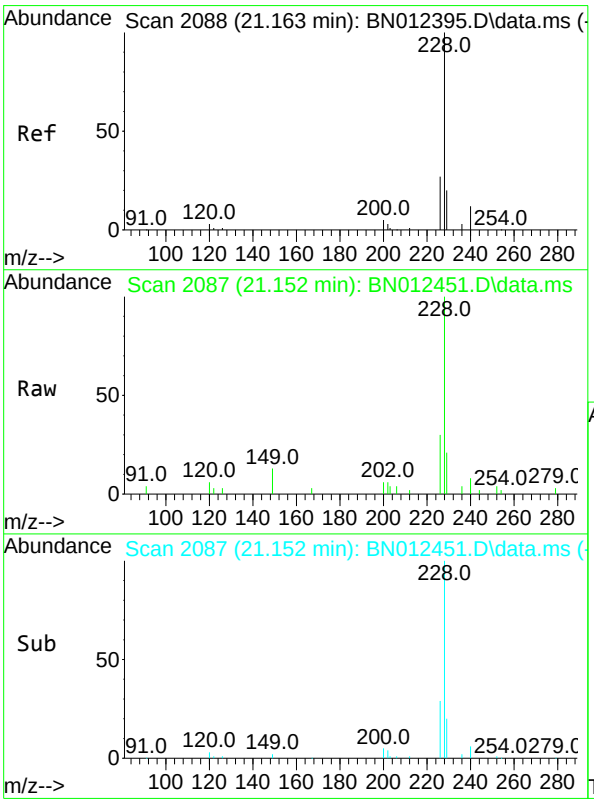


#31
Terphenyl-d14
Concen: 0.37 ng
RT: 19.618 min Scan# 1901
Delta R.T. -0.005 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:244 Resp: 3699

Ion	Ratio	Lower	Upper
244	100		
212	10.1	7.3	10.9
122	10.5	7.3	10.9

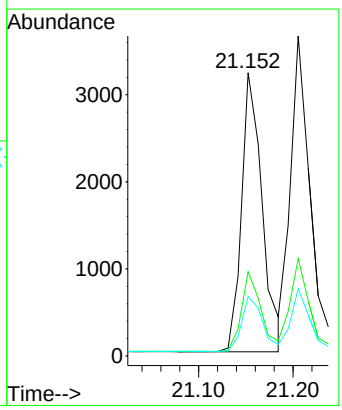




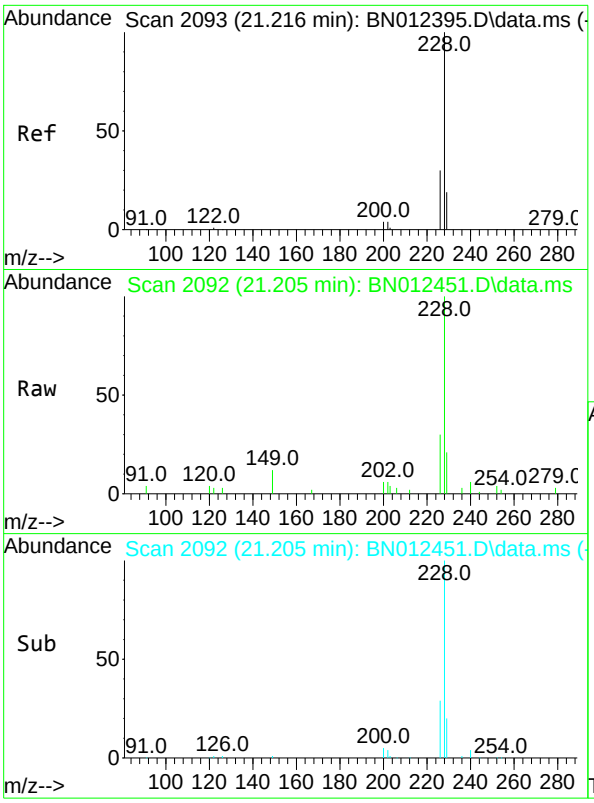
#32
Benzo(a)anthracene
Concen: 0.37 ng
RT: 21.152 min Scan# 2087
Delta R.T. -0.011 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:228 Resp: 4861

Ion	Ratio	Lower	Upper
228	100		
226	29.8	22.3	33.5
229	21.0	15.7	23.5



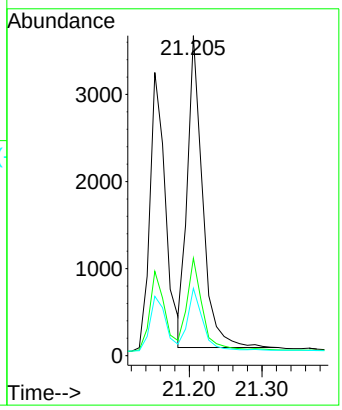
Instrument :
BNA_N
ClientSampleId :
PB132717BS

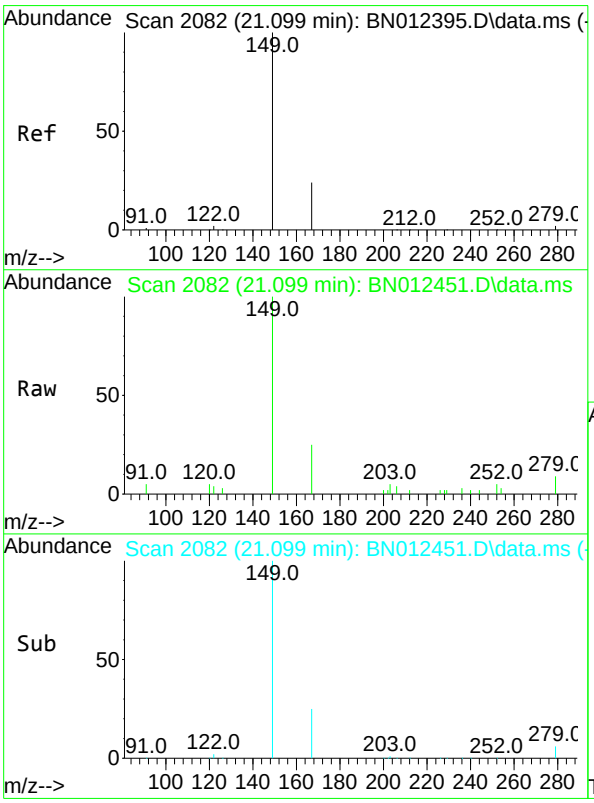


#33
Chrysene
Concen: 0.36 ng
RT: 21.205 min Scan# 2092
Delta R.T. -0.011 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:228 Resp: 5225

Ion	Ratio	Lower	Upper
228	100		
226	30.5	24.2	36.2
229	21.0	15.7	23.5

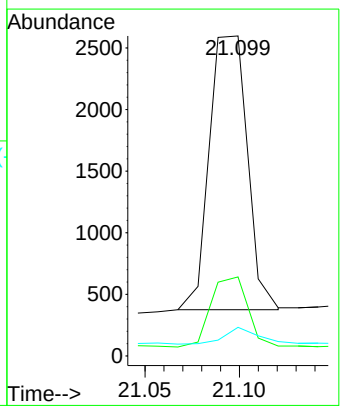




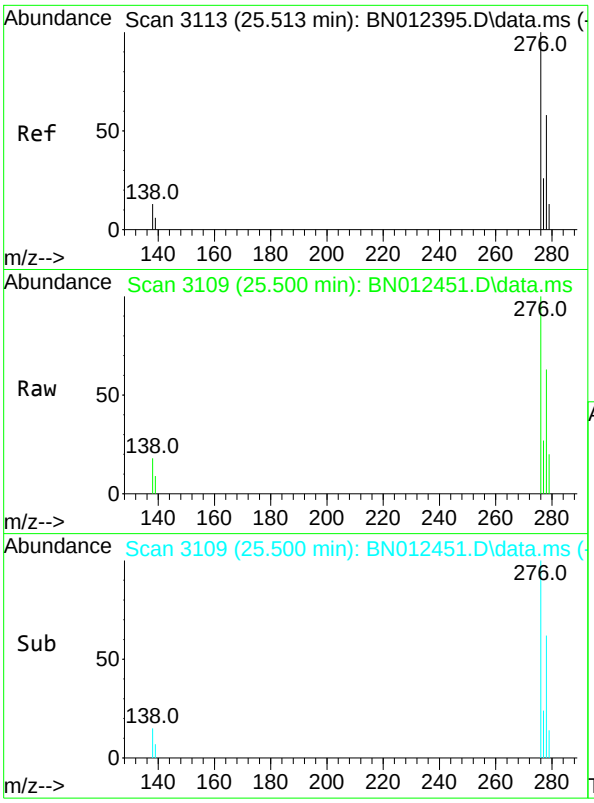
#34
Bis(2-ethylhexyl)phthalate
Concen: 0.37 ng
RT: 21.099 min Scan# 2082
Delta R.T. 0.000 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:149 Resp: 3115

Ion	Ratio	Lower	Upper
149	100		
167	25.0	23.2	34.8
279	5.5	3.9	5.9



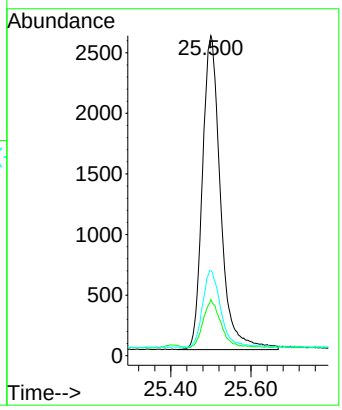
Instrument :
BNA_N
ClientSampleId :
PB132717BS

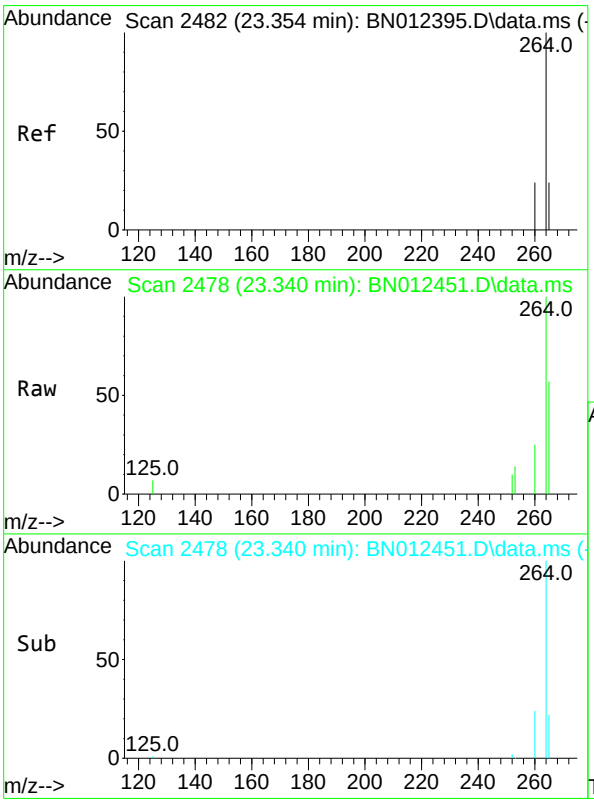


#35
Indeno(1,2,3-cd)pyrene
Concen: 0.39 ng
RT: 25.500 min Scan# 3109
Delta R.T. -0.010 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:276 Resp: 8141

Ion	Ratio	Lower	Upper
276	100		
138	14.6	13.3	19.9
277	24.2	20.2	30.4

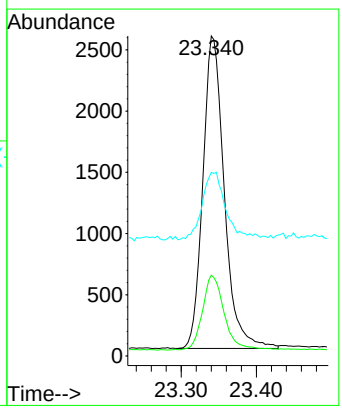




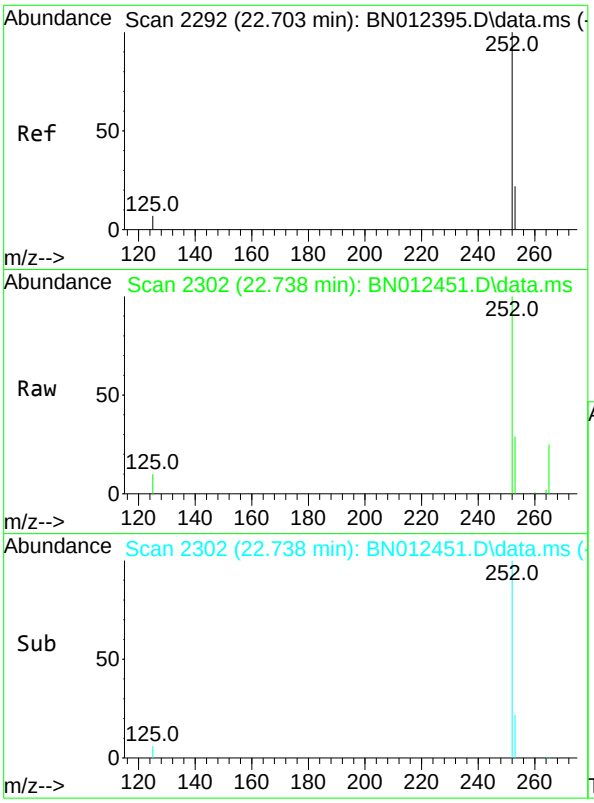
#36
Perylene-d12
Concen: 0.40 ng
RT: 23.340 min Scan# 2478
Delta R.T. -0.014 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:264 Resp: 5065

Ion	Ratio	Lower	Upper
264	100		
260	25.2	19.8	29.6
265	57.3	51.4	77.0



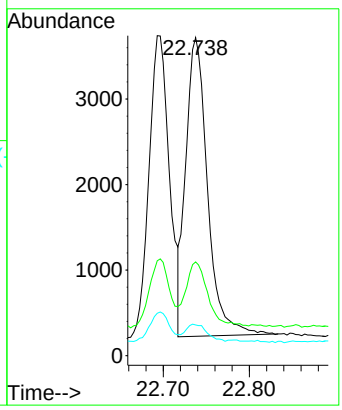
Instrument :
BNA_N
ClientSampleId :
PB132717BS

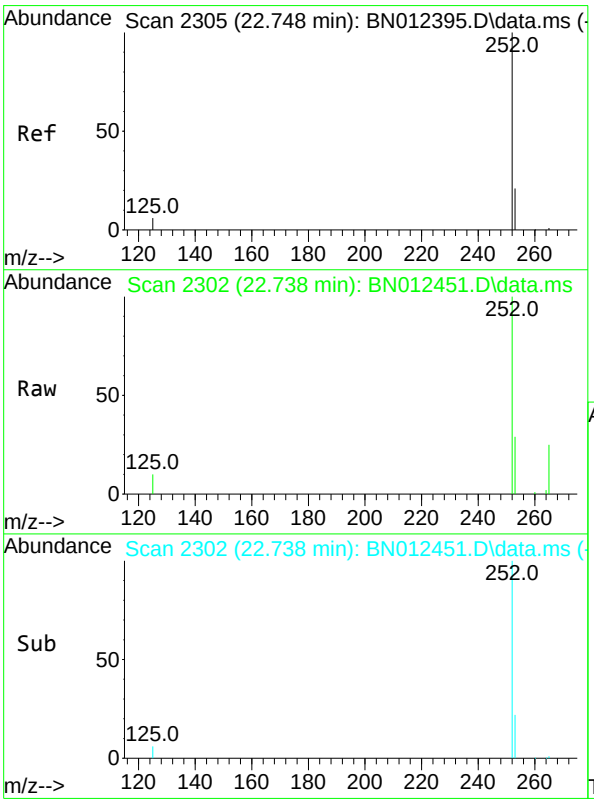


#37
Benzo(b)fluoranthene
Concen: 0.38 ng
RT: 22.738 min Scan# 2302
Delta R.T. 0.034 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:252 Resp: 6119

Ion	Ratio	Lower	Upper
252	100		
253	29.5	20.1	30.1
125	9.7	7.2	10.8

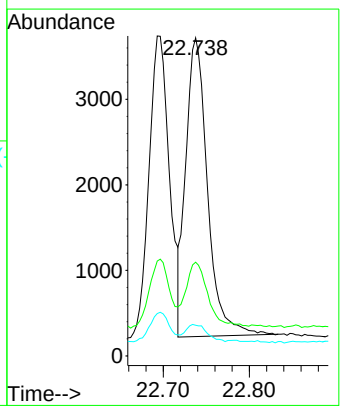




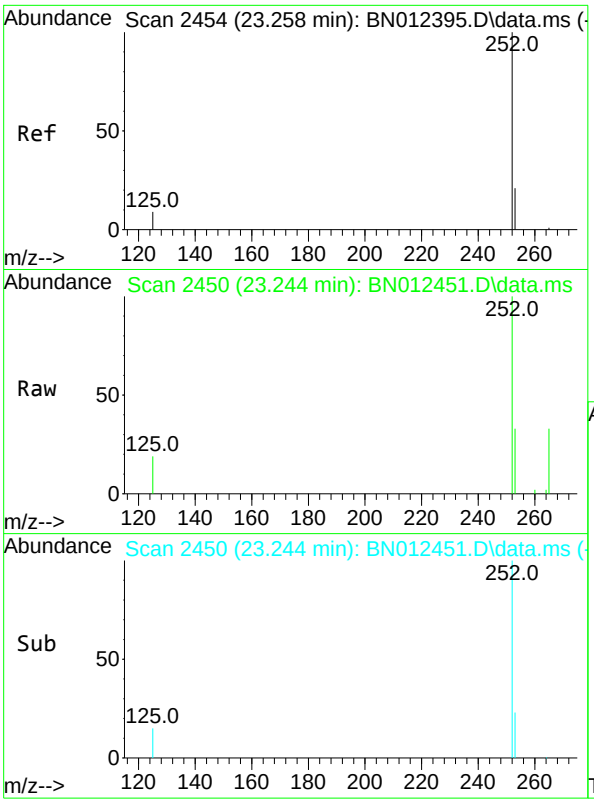
#38
Benzo(k)fluoranthene
Concen: 0.35 ng
RT: 22.738 min Scan# 2302
Delta R.T. -0.010 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:252 Resp: 6119

Ion	Ratio	Lower	Upper
252	100		
253	29.5	19.8	29.8
125	9.7	7.1	10.7



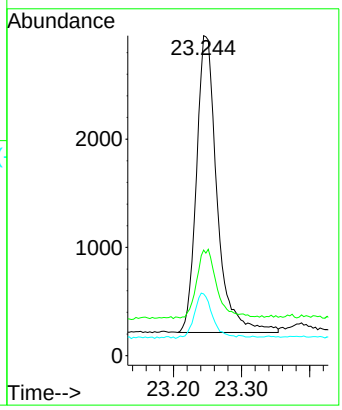
Instrument :
BNA_N
ClientSampleId :
PB132717BS

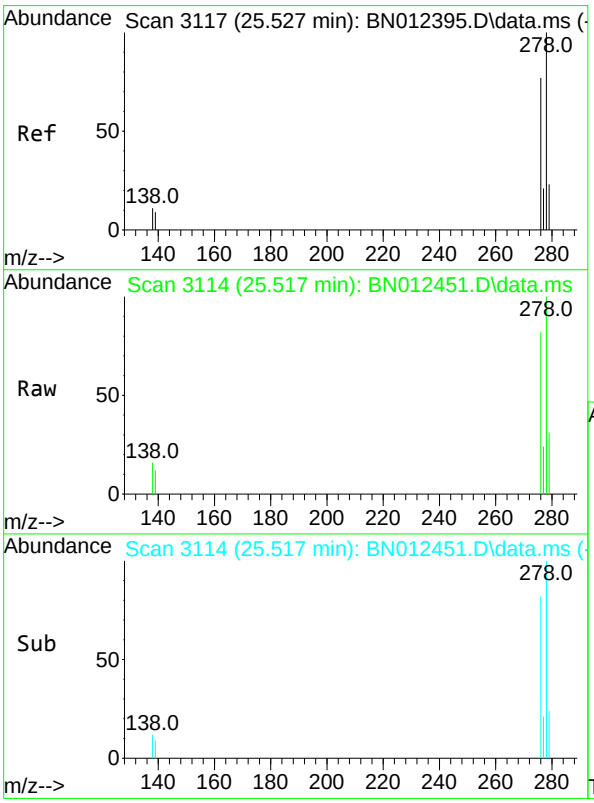


#39
Benzo(a)pyrene
Concen: 0.37 ng
RT: 23.244 min Scan# 2450
Delta R.T. -0.017 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:252 Resp: 5754

Ion	Ratio	Lower	Upper
252	100		
253	33.0	21.3	31.9#
125	19.3	8.3	12.5#

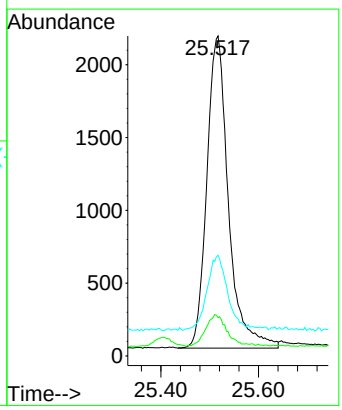


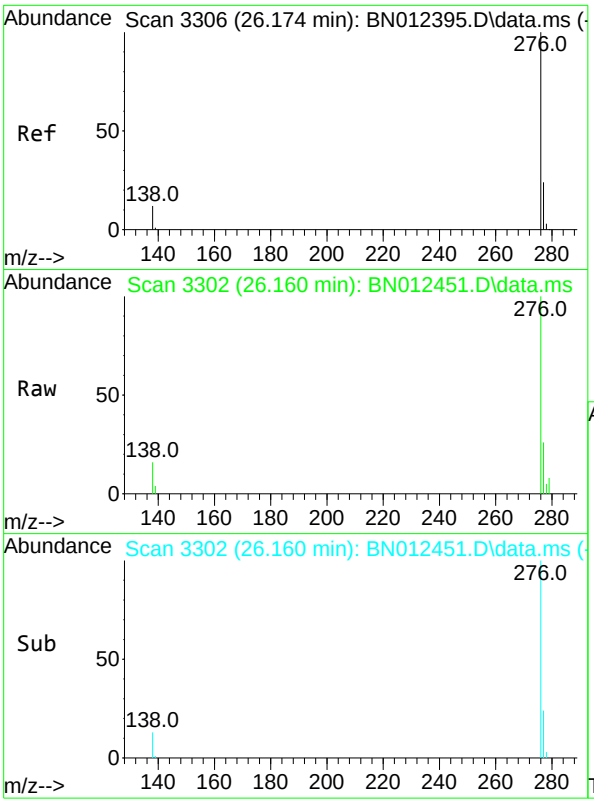


#40
Dibenzo(a,h)anthracene
Concen: 0.38 ng
RT: 25.517 min Scan# 3114
Delta R.T. -0.010 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:278 Resp: 6586

Ion	Ratio	Lower	Upper
278	100		
139	12.0	9.3	13.9
279	31.4	21.6	32.4

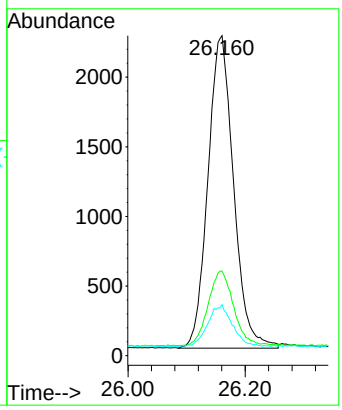




#41
Benzo(g,h,i)perylene
Concen: 0.37 ng
RT: 26.160 min Scan# 3302
Delta R.T. -0.010 min
Lab File: BN012451.D
Acq: 30 Oct 2020 00:12

Tgt Ion:276 Resp: 6825

Ion	Ratio	Lower	Upper
276	100		
277	26.5	19.8	29.8
138	15.9	11.7	17.5



Instrument :
BNA_N
ClientSampleId :
PB132717BS