Quantitation Report (Not Reviewed)

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN031921\
Data File : BN013988.D
Acq On : 18 Mar 2021 18:43
Operator : CG/JU
Sample : PB135230BS
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : PB135230BS

Quant Time: Mar 19 01:49:47 2021
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN022421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION
QLast Update : Thu Mar 18 15:58:40 2021
Response via : Initial Calibration

Compound	R.T.	QIon	Response	Conc	Units		Dev(Min)
Internal Standards							
1) 1,4-Dichlorobenzene-d4	7.708	152	5792	0.40	ng		0.00
7) Naphthalene-d8	10.492	136	21180	0.40	ng		# 0.00
13) Acenaphthene-d10	14.346	164	11431	0.40	ng		0.00
19) Phenanthrene-d10	17.092	188	24483	0.40	ng		# 0.00
29) Chrysene-d12	21.271	240	24638	0.40	ng		# 0.00
36) Perylene-d12	23.499	264	22376	0.40	ng		# 0.00
System Monitoring Compounds							
4) 2-Fluorophenol	5.300	112	5733	0.37	ng		0.00
5) Phenol-d6	6.871	99	7171	0.35	ng		0.00
8) Nitrobenzene-d5	8.857	82	5429	0.40	ng		0.00
11) 2-Methylnaphthalene-d10	12.080	152	13531	0.40	ng		0.00
14) 2,4,6-Tribromophenol	15.831	330	1349	0.29	ng		0.00
15) 2-Fluorobiphenyl	12.963	172	17822	0.44	ng		0.00
27) Fluoranthene-d10	19.119	212	27347	0.38	ng		0.00
31) Terphenyl-d14	19.719	244	21707	0.40	ng		0.00
Target Compounds							Qvalue
2) 1,4-Dioxane	3.247	88	2993	0.43	ng		99
3) n-Nitrosodimethylamine	3.585	42	1758	0.33	ng	#	99
6) bis(2-Chloroethyl)ether	7.136	93	6263	0.43	ng		96
9) Naphthalene	10.530	128	21802	0.42	ng		99
10) Hexachlorobutadiene	10.822	225	4083	0.41	ng	#	100
12) 2-Methylnaphthalene	12.155	142	14513	0.40	ng		99
16) Acenaphthylene	14.054	152	17321	0.34	ng		99
17) Acenaphthene	14.410	154	12994	0.41	ng		99
18) Fluorene	15.387	166	16062	0.39	ng		99
20) 4,6-Dinitro-2-methylph...	15.463	198	942	0.55	ng	#	52
21) 4-Bromophenyl-phenylether	16.289	248	5182	0.39	ng	#	82
22) Hexachlorobenzene	16.398	284	6109	0.44	ng		100
23) Atrazine	16.556	200	3132	0.25	ng		99
24) Pentachlorophenol	16.739	266	1244	0.27	ng		94
25) Phenanthrene	17.128	178	27419	0.43	ng		100
26) Anthracene	17.214	178	22026	0.35	ng		100
28) Fluoranthene	19.149	202	30041	0.39	ng		99
30) Pyrene	19.511	202	30340	0.40	ng		100
32) Benzo(a)anthracene	21.250	228	26265	0.35	ng		97
33) Chrysene	21.303	228	31303	0.42	ng		100
34) Bis(2-ethylhexyl)phtha...	21.186	149	7518	0.21	ng		99
35) Indeno(1,2,3-cd)pyrene	25.735	276	35629	0.40	ng		98
37) Benzo(b)fluoranthene	22.832	252	32305	0.45	ng		98
38) Benzo(k)fluoranthene	22.832	252	32305	0.47	ng		97
39) Benzo(a)pyrene	23.404	252	29026	0.45	ng		97
40) Dibenzo(a,h)anthracene	25.748	278	29915	0.44	ng		98
41) Benzo(g,h,i)perylene	26.419	276	30982	0.45	ng		98

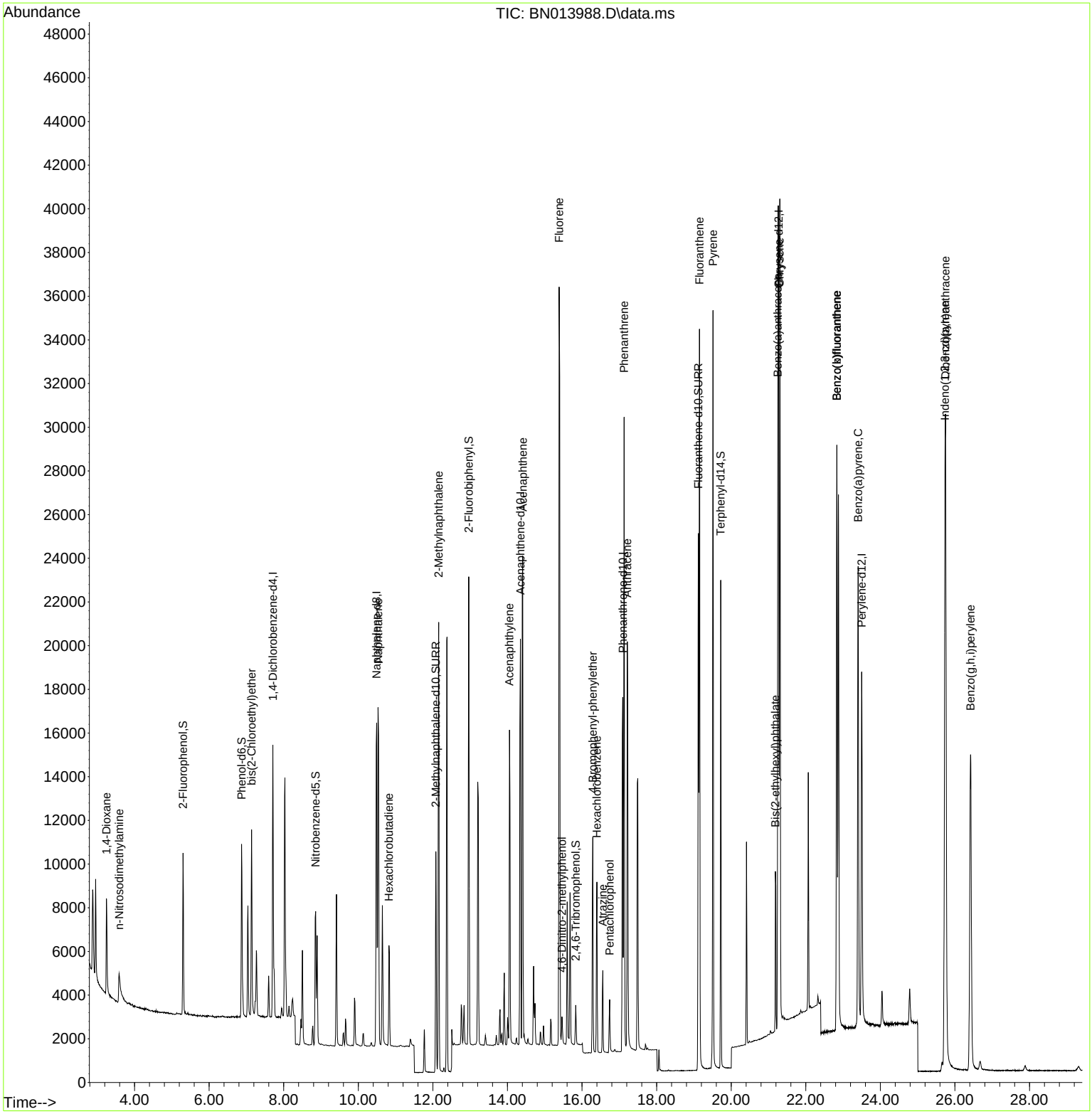
(#) = qualifier out of range (m) = manual integration (+) = signals summed

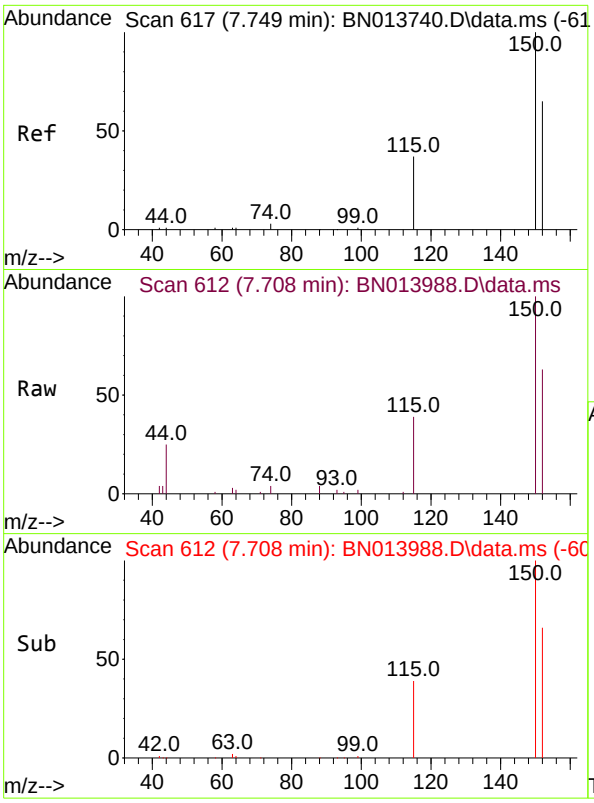
Quantitation Report (Not Reviewed)

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN031921\
Data File : BN013988.D
Acq On : 18 Mar 2021 18:43
Operator : CG/JU
Sample : PB135230BS
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB135230BS

Quant Time: Mar 19 01:49:47 2021
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN022421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION
QLast Update : Thu Mar 18 15:58:40 2021
Response via : Initial Calibration

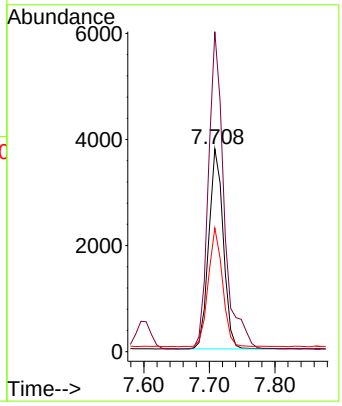




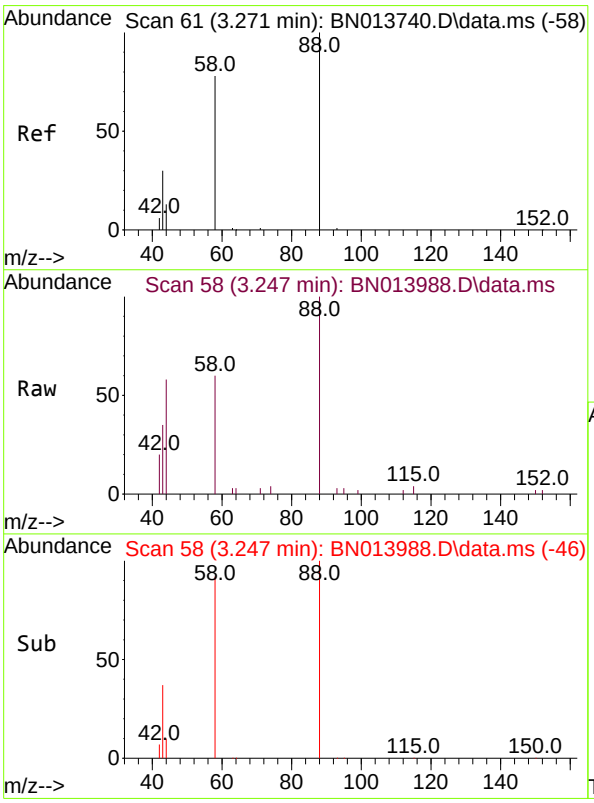
#1
1,4-Dichlorobenzene-d4
Concen: 0.40 ng
RT: 7.708 min Scan# 612
Delta R.T. 0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:152 Resp: 5792

Ion	Ratio	Lower	Upper
152	100		
150	157.7	121.8	182.8
115	60.9	46.6	69.8



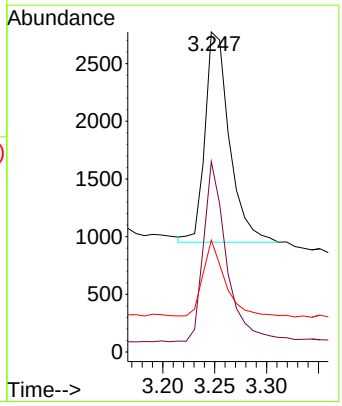
Instrument :
BNA_N
ClientSampleId :
PB135230BS



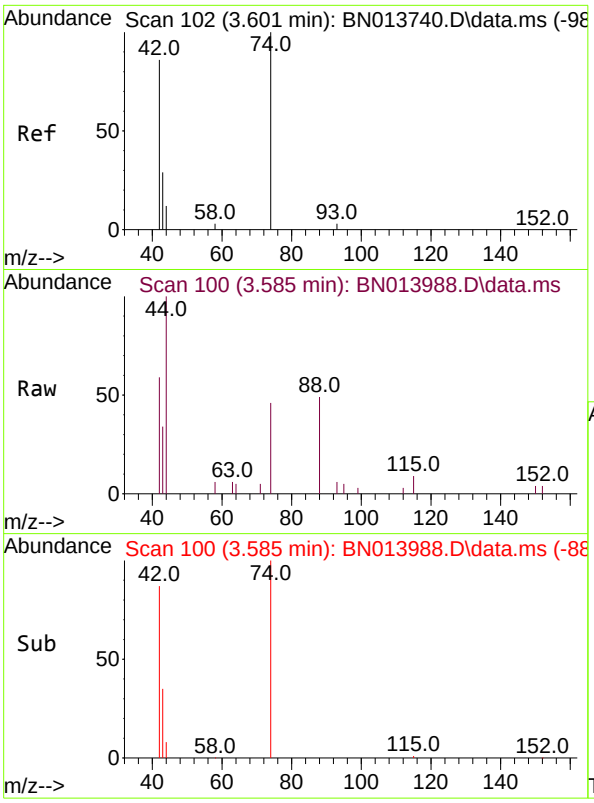
#2
1,4-Dioxane
Concen: 0.43 ng
RT: 3.247 min Scan# 58
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion: 88 Resp: 2993

Ion	Ratio	Lower	Upper
88	100		
58	80.3	64.6	96.8
43	31.7	26.6	40.0



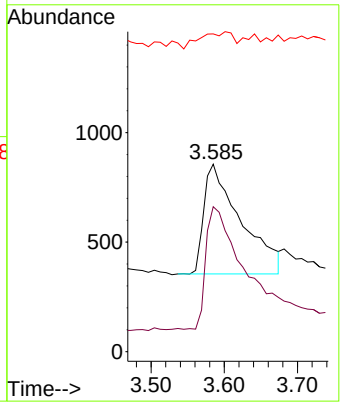
Instrument :
BNA_N
ClientSampleId :
PB135230BS

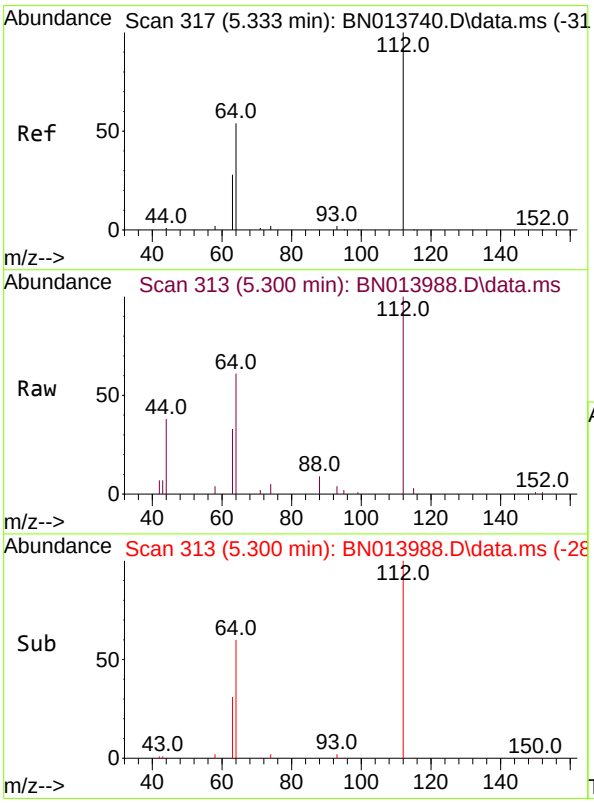


#3
n-Nitrosodimethylamine
Concen: 0.33 ng
RT: 3.585 min Scan# 100
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion: 42 Resp: 1758

Ion	Ratio	Lower	Upper
42	100		
74	120.0	95.0	142.6
44	9.0	5.8	8.8#

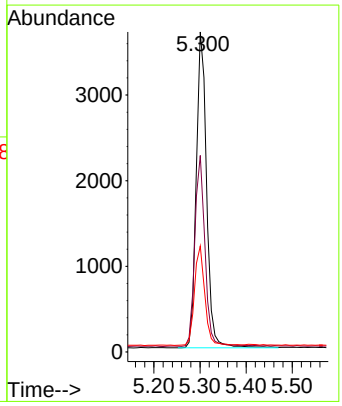




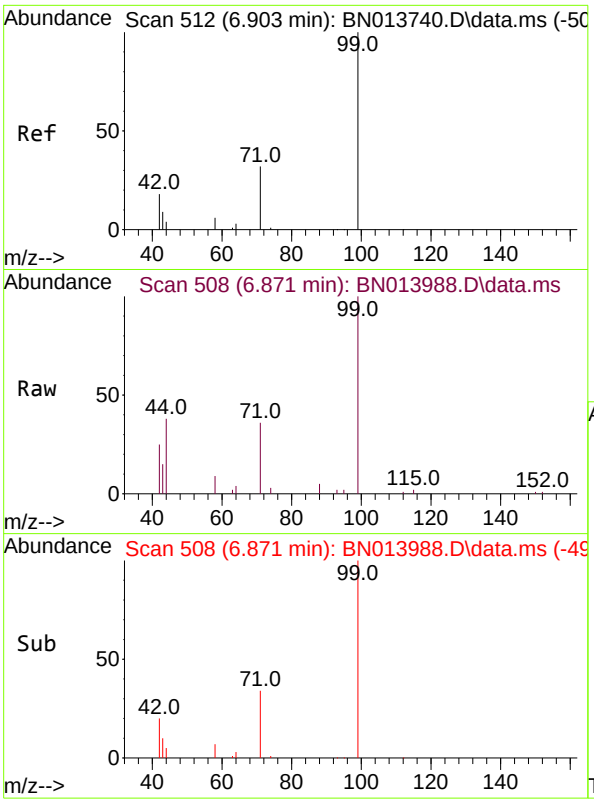
#4
2-Fluorophenol
Concen: 0.37 ng
RT: 5.300 min Scan# 313
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:112 Resp: 5733

Ion	Ratio	Lower	Upper
112	100		
64	59.2	44.3	66.5
63	31.3	23.0	34.6



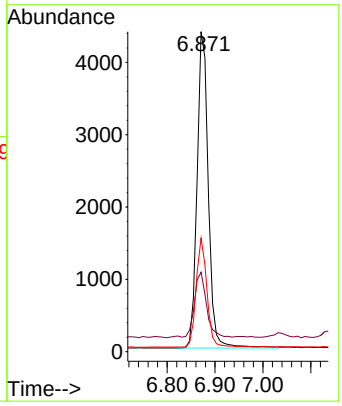
Instrument :
BNA_N
ClientSampleId :
PB135230BS

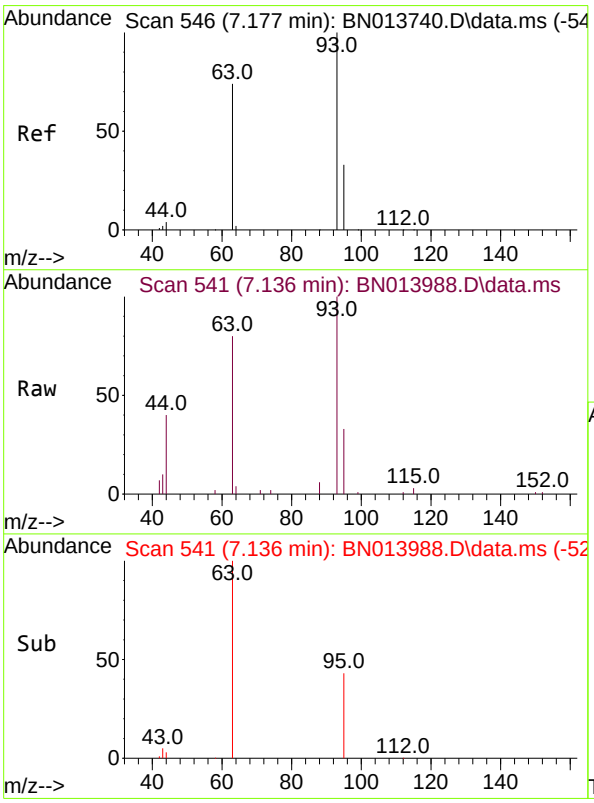


#5
Phenol-d6
Concen: 0.35 ng
RT: 6.871 min Scan# 508
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion: 99 Resp: 7171

Ion	Ratio	Lower	Upper
99	100		
42	22.7	15.2	22.8
71	32.9	26.1	39.1

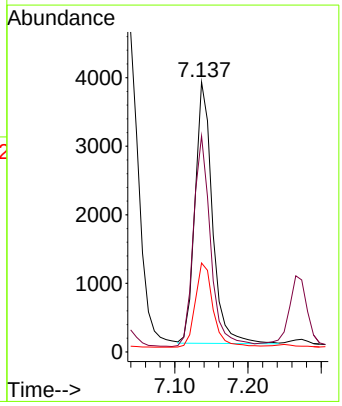




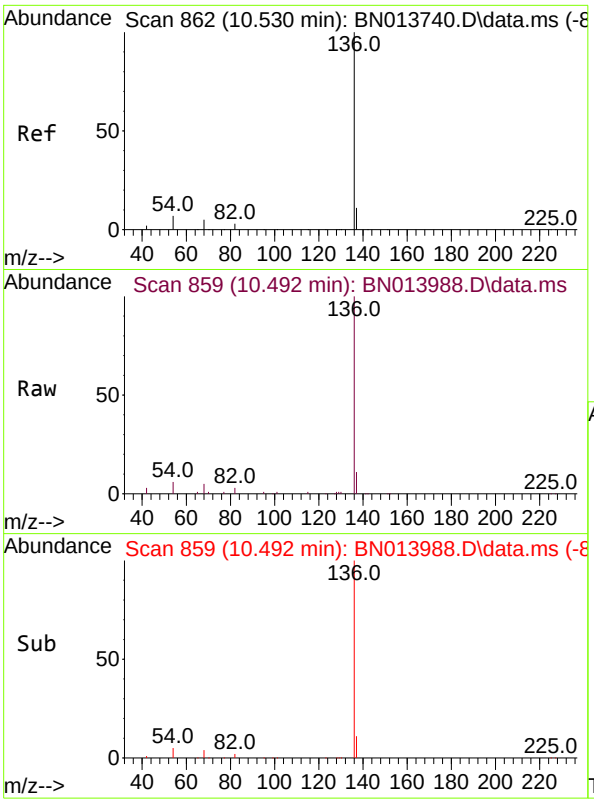
#6
bis(2-Chloroethyl)ether
Concen: 0.43 ng
RT: 7.136 min Scan# 541
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion: 93 Resp: 6263

Ion	Ratio	Lower	Upper
93	100		
63	80.1	60.8	91.2
95	33.1	26.0	39.0



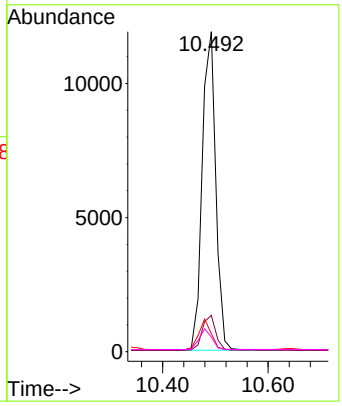
Instrument :
BNA_N
ClientSampleId :
PB135230BS

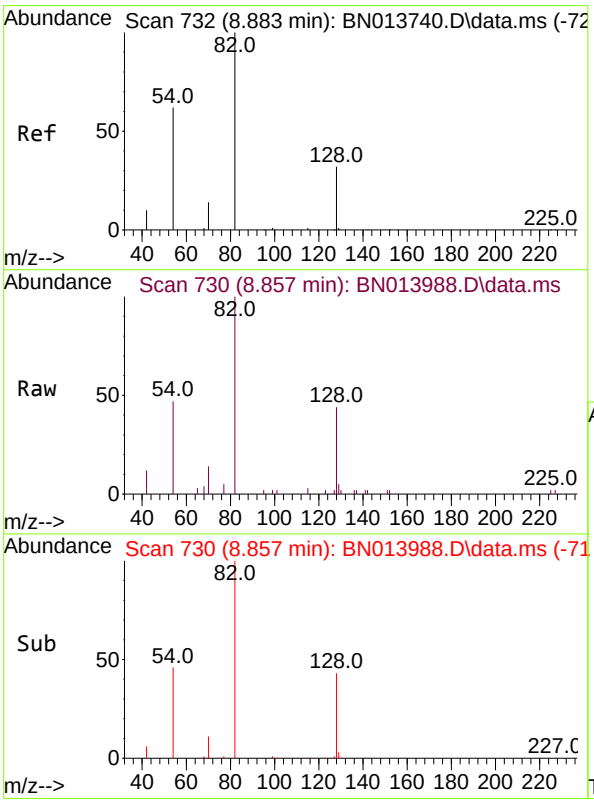


#7
Naphthalene-d8
Concen: 0.40 ng
RT: 10.492 min Scan# 859
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:136 Resp: 21180

Ion	Ratio	Lower	Upper
136	100		
137	11.3	9.0	13.6
54	5.7	6.4	9.6#
68	4.6	4.5	6.7

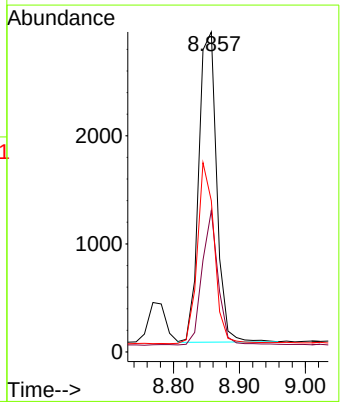




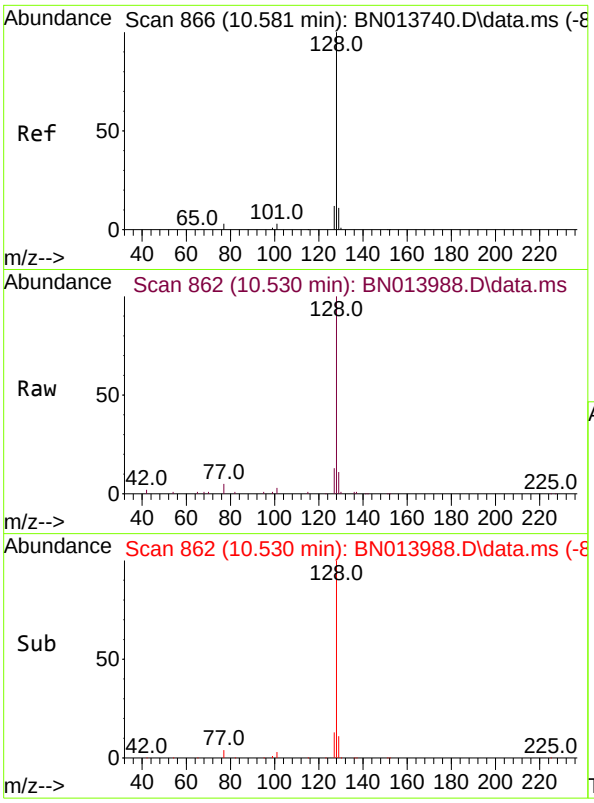
#8
Nitrobenzene-d5
Concen: 0.40 ng
RT: 8.857 min Scan# 730
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion: 82 Resp: 5429

Ion	Ratio	Lower	Upper
82	100		
128	44.2	39.2	58.8
54	47.2	40.1	60.1



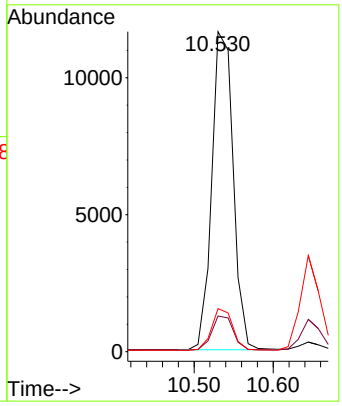
Instrument :
BNA_N
ClientSampleId :
PB135230BS

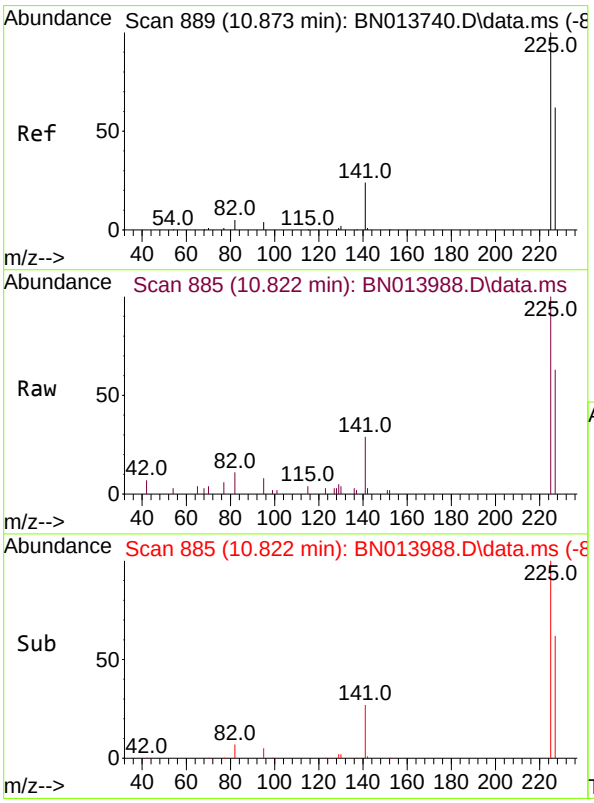


#9
Naphthalene
Concen: 0.42 ng
RT: 10.530 min Scan# 862
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:128 Resp: 21802

Ion	Ratio	Lower	Upper
128	100		
129	11.2	9.0	13.4
127	13.5	10.4	15.6

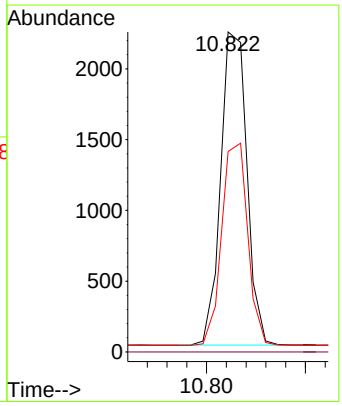




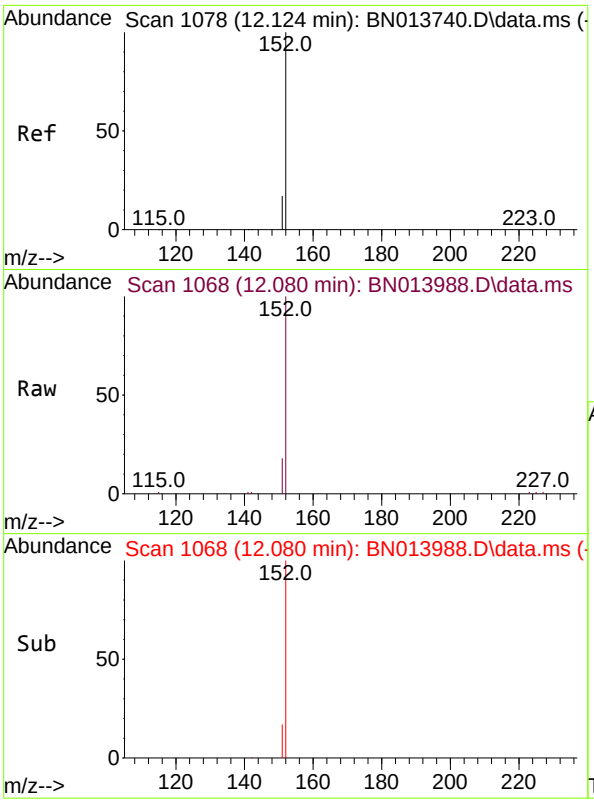
#10
Hexachlorobutadiene
Concen: 0.41 ng
RT: 10.822 min Scan# 885
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:225 Resp: 4083

Ion	Ratio	Lower	Upper
225	100		
223	0.0	0.0	0.0
227	64.1	51.2	76.8



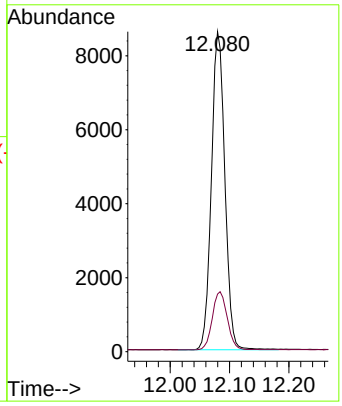
Instrument :
BNA_N
ClientSampleId :
PB135230BS

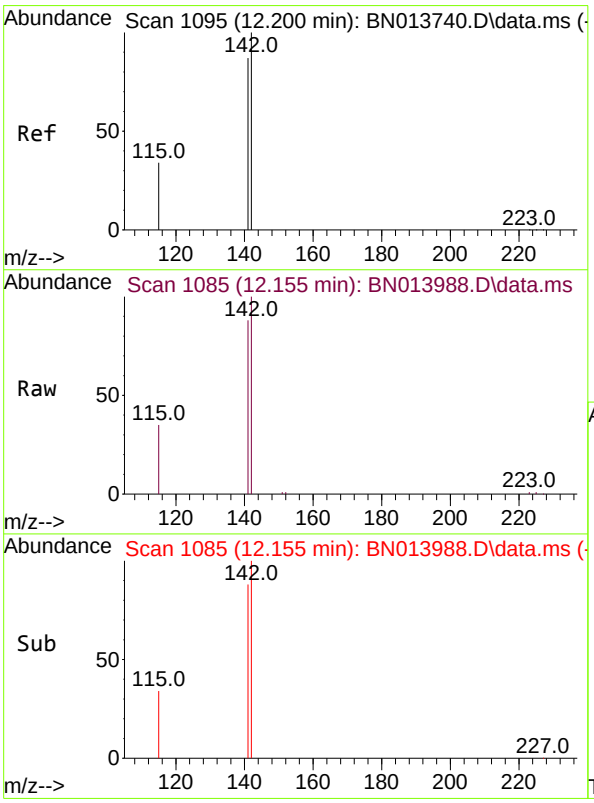


#11
2-Methylnaphthalene-d10
Concen: 0.40 ng
RT: 12.080 min Scan# 1068
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:152 Resp: 13531

Ion	Ratio	Lower	Upper
152	100		
151	20.3	16.2	24.2

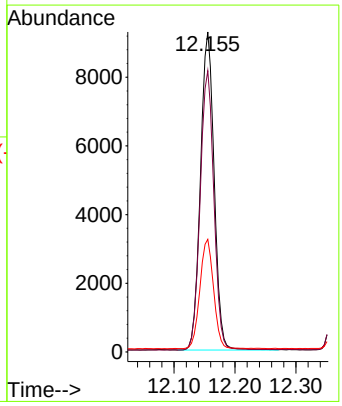




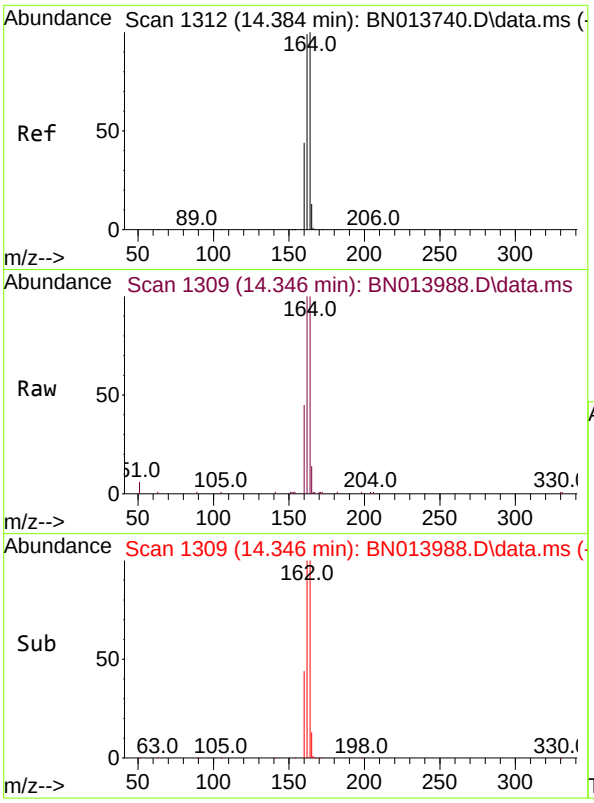
#12
2-Methylnaphthalene
Concen: 0.40 ng
RT: 12.155 min Scan# 1085
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:142 Resp: 14513

Ion	Ratio	Lower	Upper
142	100		
141	87.9	70.5	105.7
115	35.2	27.4	41.0



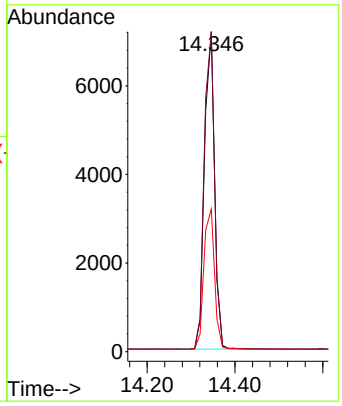
Instrument :
BNA_N
ClientSampleId :
PB135230BS

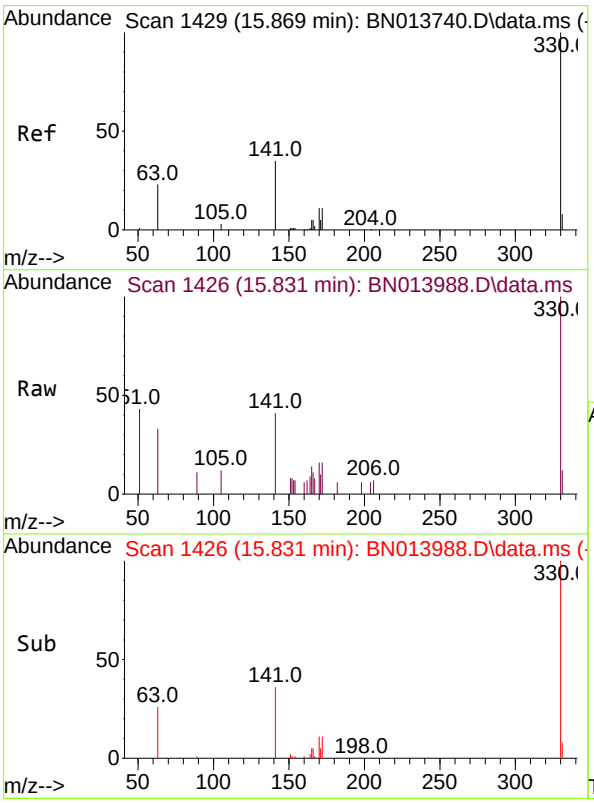


#13
Acenaphthene-d10
Concen: 0.40 ng
RT: 14.346 min Scan# 1309
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:164 Resp: 11431

Ion	Ratio	Lower	Upper
164	100		
162	100.0	79.6	119.4
160	44.6	36.0	54.0

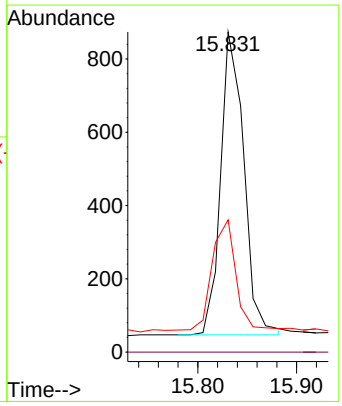




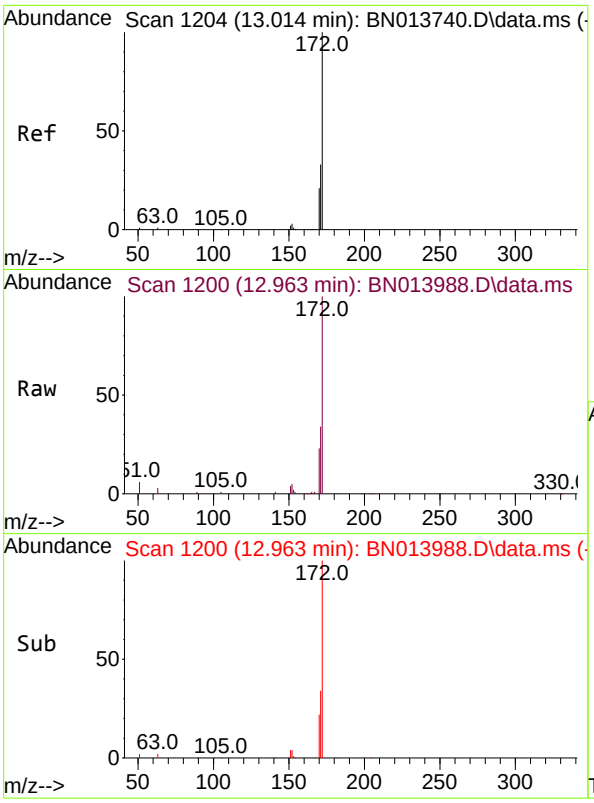
#14
2,4,6-Tribromophenol
Concen: 0.29 ng
RT: 15.831 min Scan# 1426
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:330 Resp: 1349

Ion	Ratio	Lower	Upper
330	100		
332	0.0	0.0	0.0
141	37.2	26.8	40.2



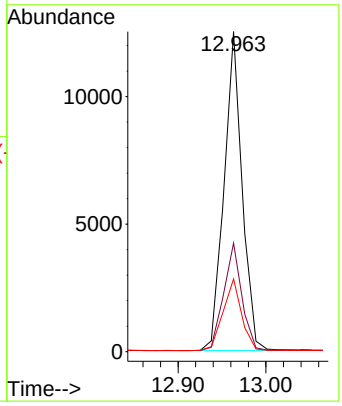
Instrument :
BNA_N
ClientSampleId :
PB135230BS

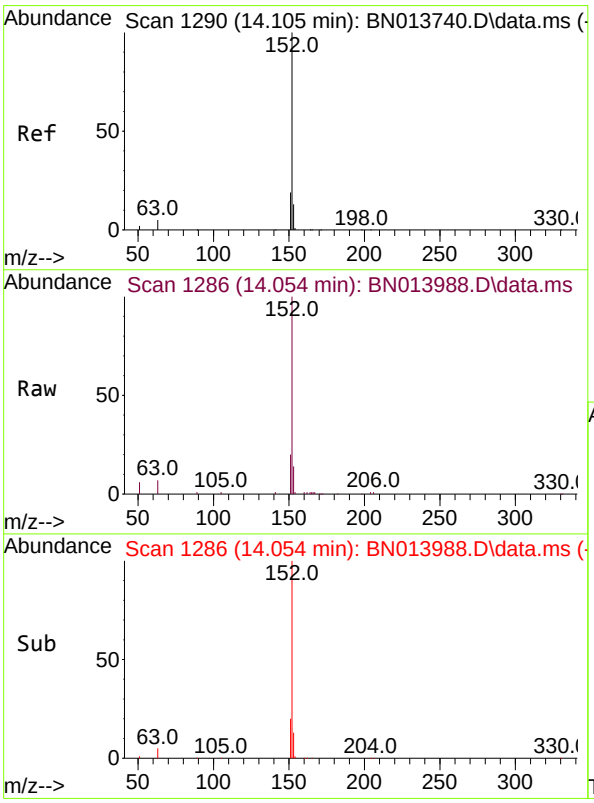


#15
2-Fluorobiphenyl
Concen: 0.44 ng
RT: 12.963 min Scan# 1200
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:172 Resp: 17822

Ion	Ratio	Lower	Upper
172	100		
171	34.0	28.6	42.8
170	22.8	18.9	28.3

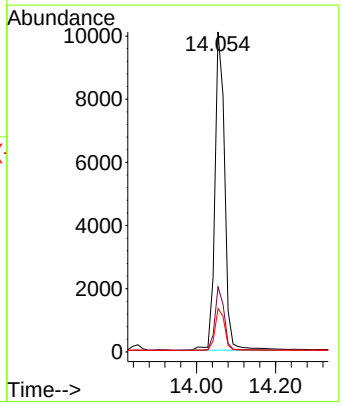




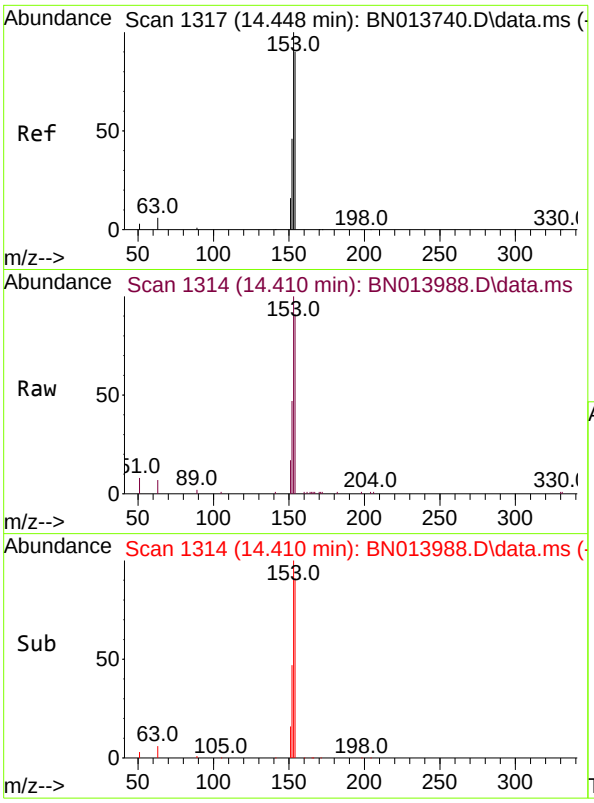
#16
Acenaphthylene
Concen: 0.34 ng
RT: 14.054 min Scan# 1286
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:152 Resp: 17321

Ion	Ratio	Lower	Upper
152	100		
151	19.2	15.7	23.5
153	13.2	10.5	15.7



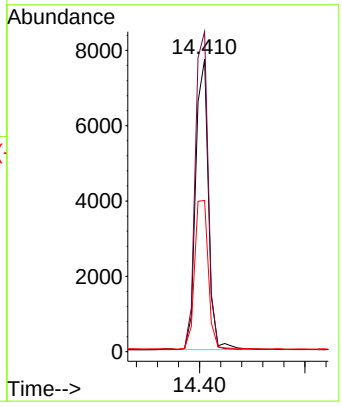
Instrument :
BNA_N
ClientSampleId :
PB135230BS

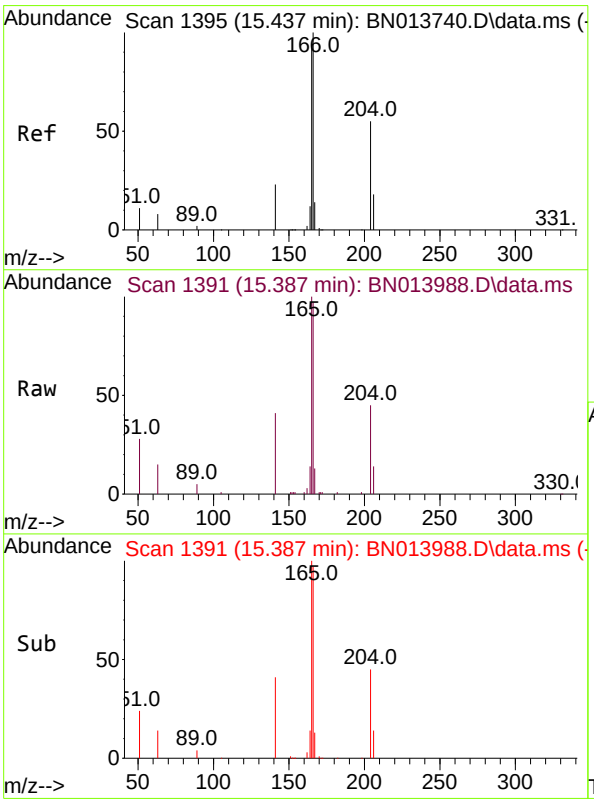


#17
Acenaphthene
Concen: 0.41 ng
RT: 14.410 min Scan# 1314
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:154 Resp: 12994

Ion	Ratio	Lower	Upper
154	100		
153	111.2	88.4	132.6
152	55.0	43.0	64.4

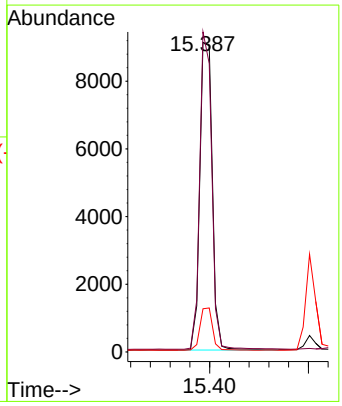




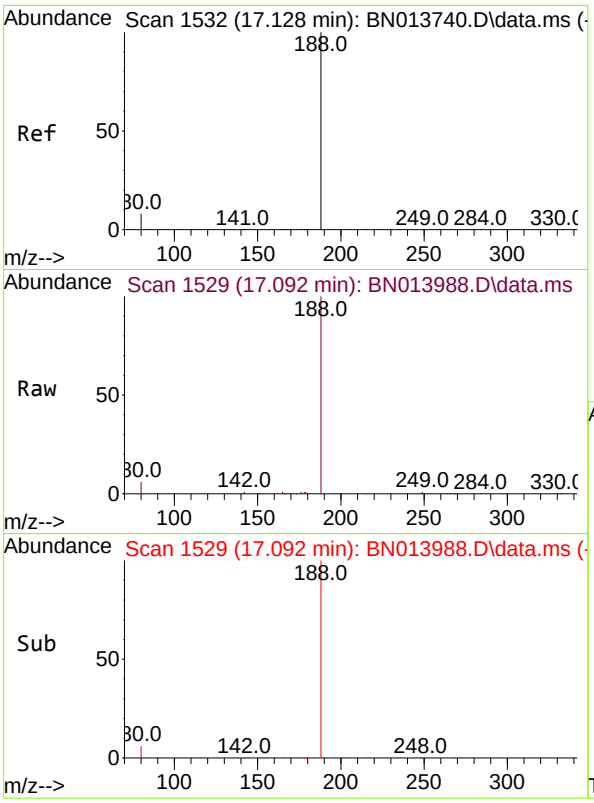
#18
Fluorene
Concen: 0.39 ng
RT: 15.387 min Scan# 1391
Delta R.T. -0.013 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:166 Resp: 16062

Ion	Ratio	Lower	Upper
166	100		
165	98.8	77.8	116.8
167	13.6	10.6	16.0



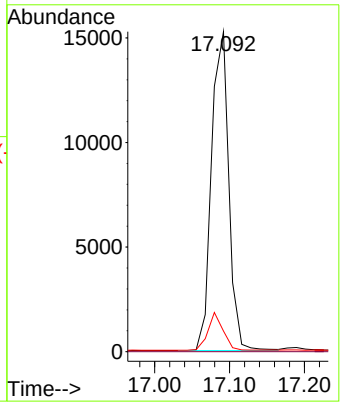
Instrument :
BNA_N
ClientSampleId :
PB135230BS

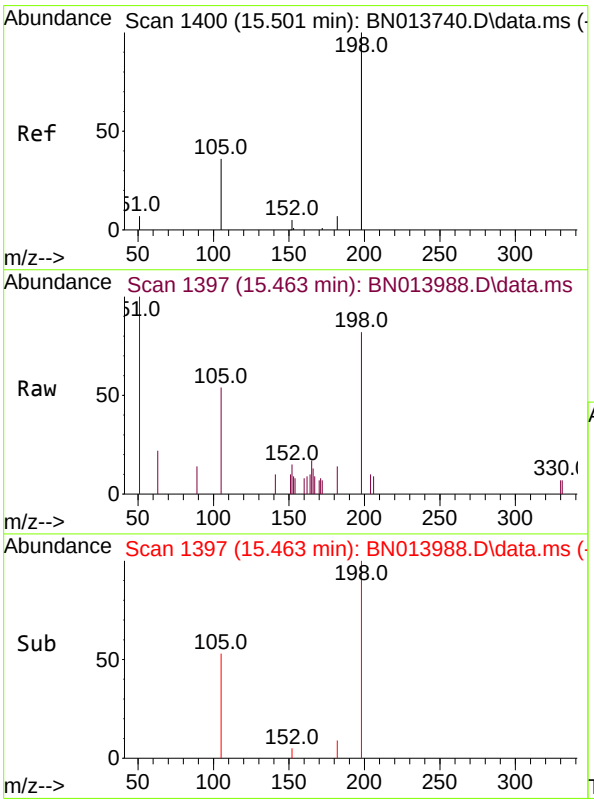


#19
Phenanthrene-d10
Concen: 0.40 ng
RT: 17.092 min Scan# 1529
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:188 Resp: 24483

Ion	Ratio	Lower	Upper
188	100		
94	0.0	0.0	0.0
80	6.5	9.0	13.6#

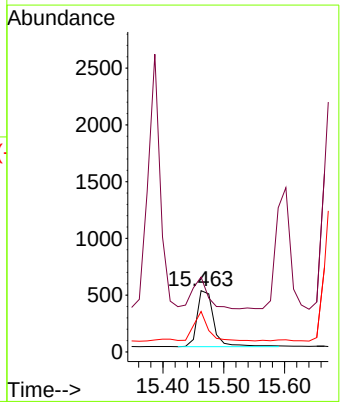




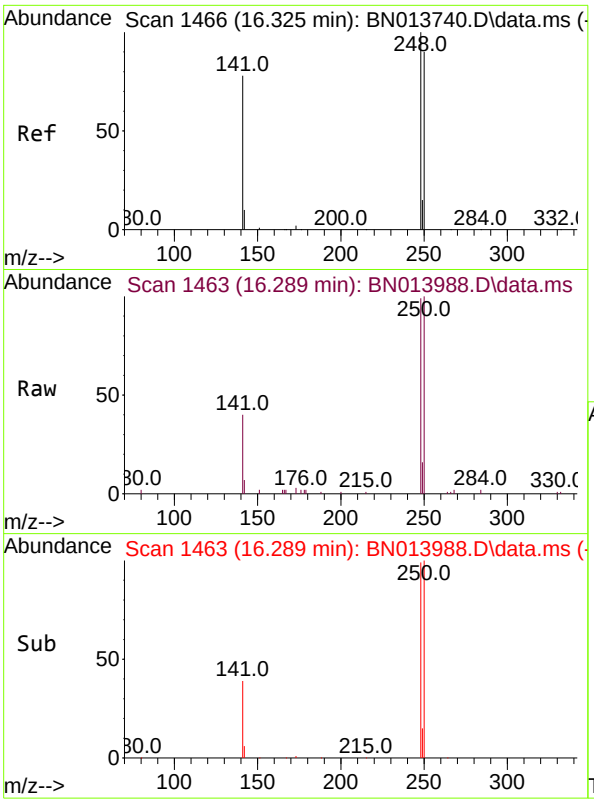
#20
4,6-Dinitro-2-methylphenol
Concen: 0.55 ng
RT: 15.463 min Scan# 1397
Delta R.T. -0.013 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:198 Resp: 942

Ion	Ratio	Lower	Upper
198	100		
51	122.3	61.7	92.5#
105	66.0	33.0	49.6#



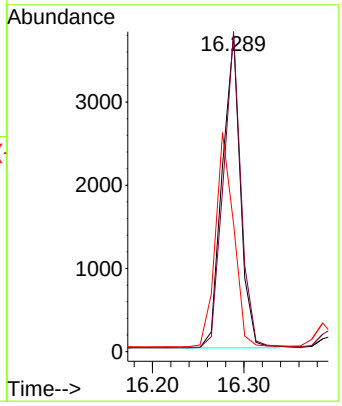
Instrument :
BNA_N
ClientSampleId :
PB135230BS

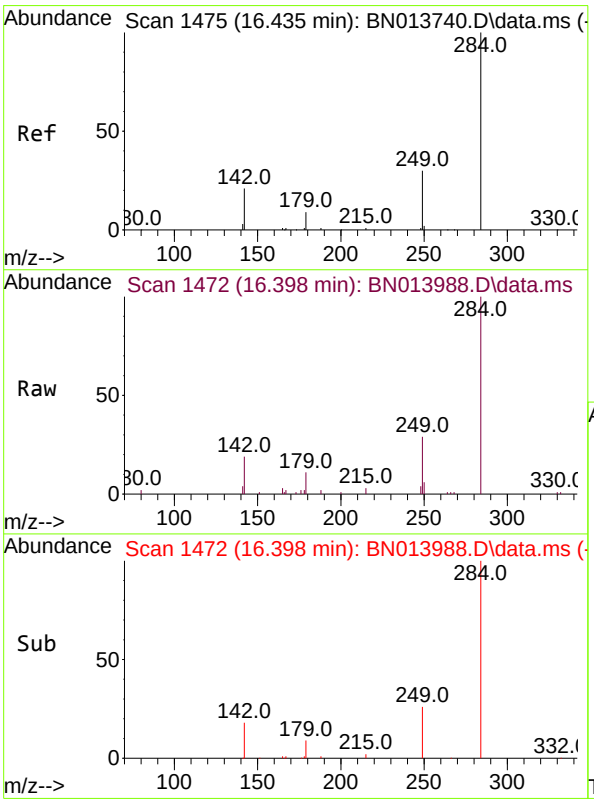


#21
4-Bromophenyl-phenylether
Concen: 0.39 ng
RT: 16.289 min Scan# 1463
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:248 Resp: 5182

Ion	Ratio	Lower	Upper
248	100		
250	101.0	75.5	113.3
141	40.4	53.8	80.8#

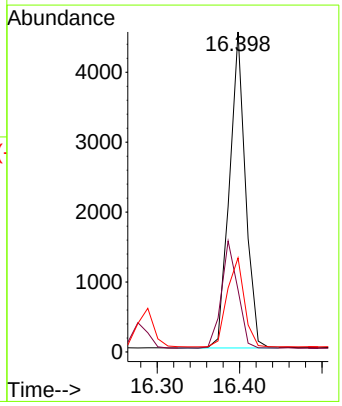




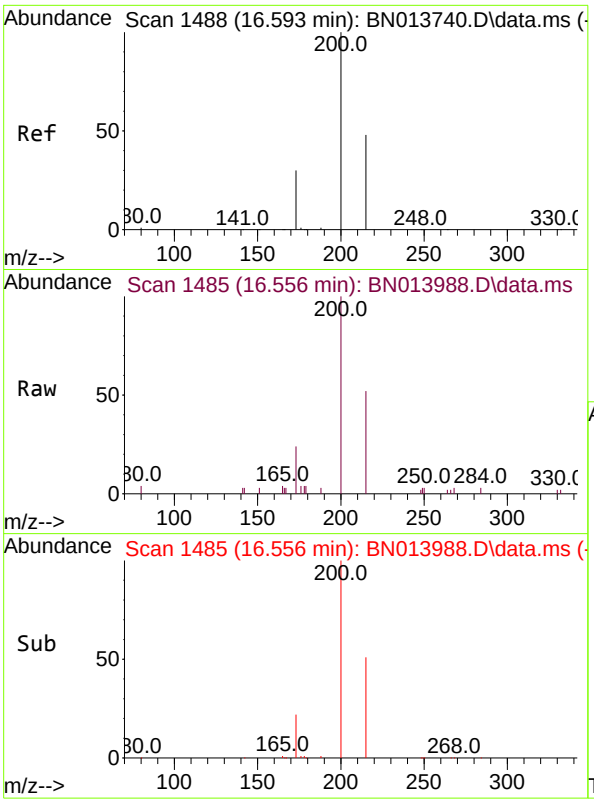
#22
Hexachlorobenzene
Concen: 0.44 ng
RT: 16.398 min Scan# 1472
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:284 Resp: 6109

Ion	Ratio	Lower	Upper
284	100		
142	34.6	27.9	41.9
249	30.3	24.2	36.2



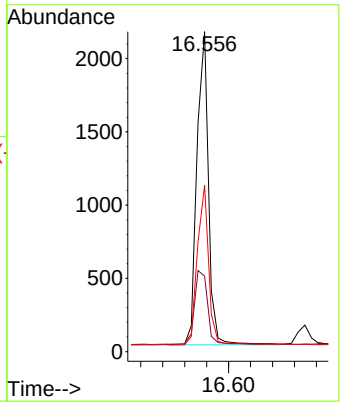
Instrument :
BNA_N
ClientSampleId :
PB135230BS

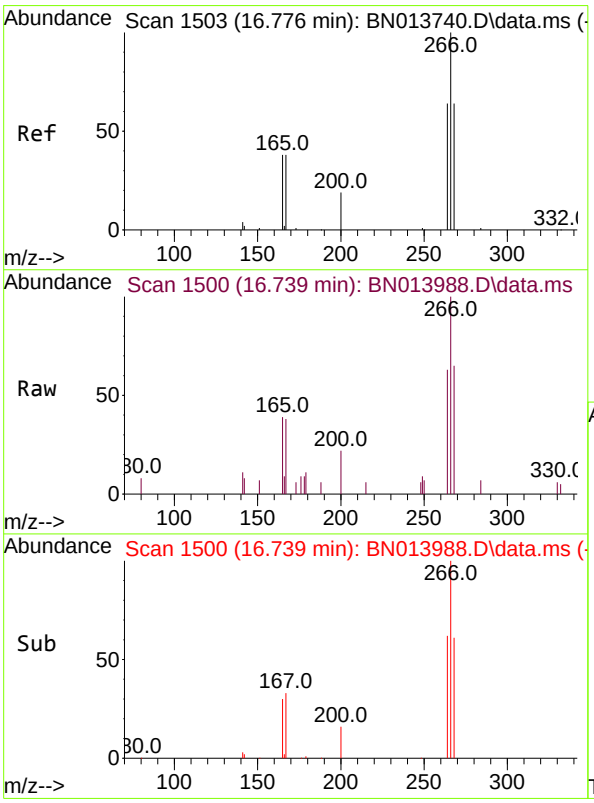


#23
Atrazine
Concen: 0.25 ng
RT: 16.556 min Scan# 1485
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:200 Resp: 3132

Ion	Ratio	Lower	Upper
200	100		
173	23.6	18.6	28.0
215	52.0	41.0	61.6

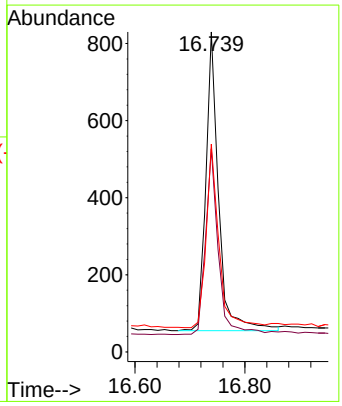




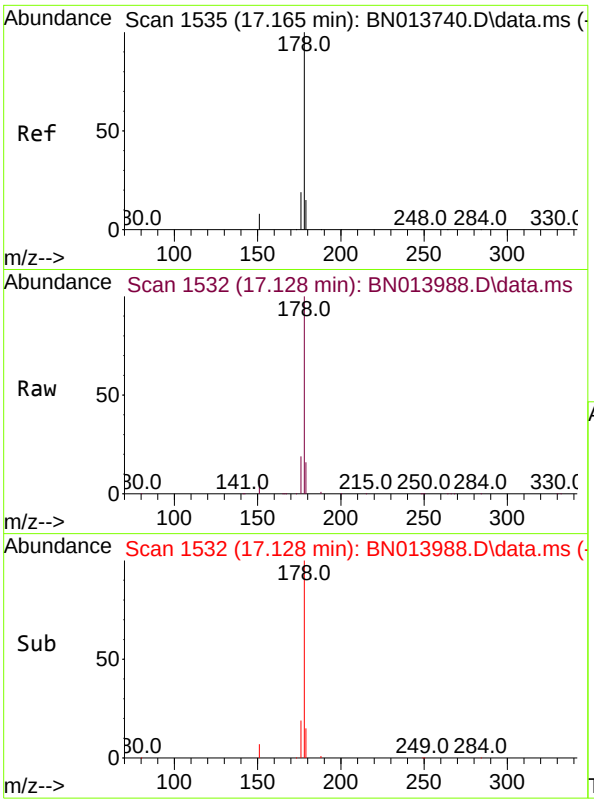
#24
Pentachlorophenol
Concen: 0.27 ng
RT: 16.739 min Scan# 1500
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:266 Resp: 1244

Ion	Ratio	Lower	Upper
266	100		
264	62.3	51.6	77.4
268	61.7	54.6	82.0



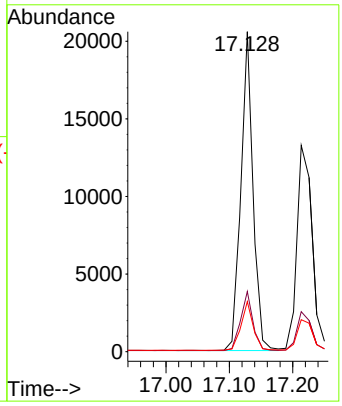
Instrument :
BNA_N
ClientSampleId :
PB135230BS

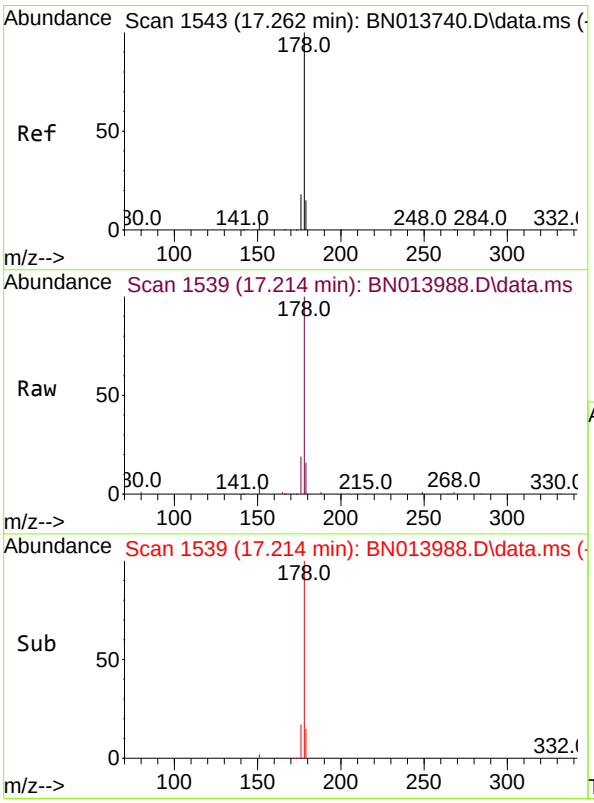


#25
Phenanthrene
Concen: 0.43 ng
RT: 17.128 min Scan# 1532
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:178 Resp: 27419

Ion	Ratio	Lower	Upper
178	100		
176	18.8	15.0	22.4
179	15.4	12.3	18.5

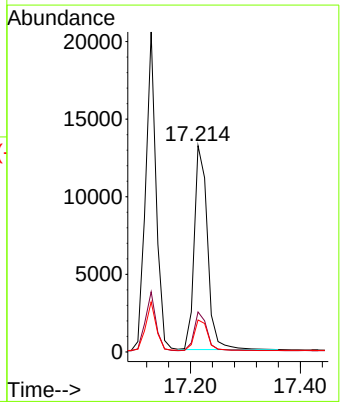




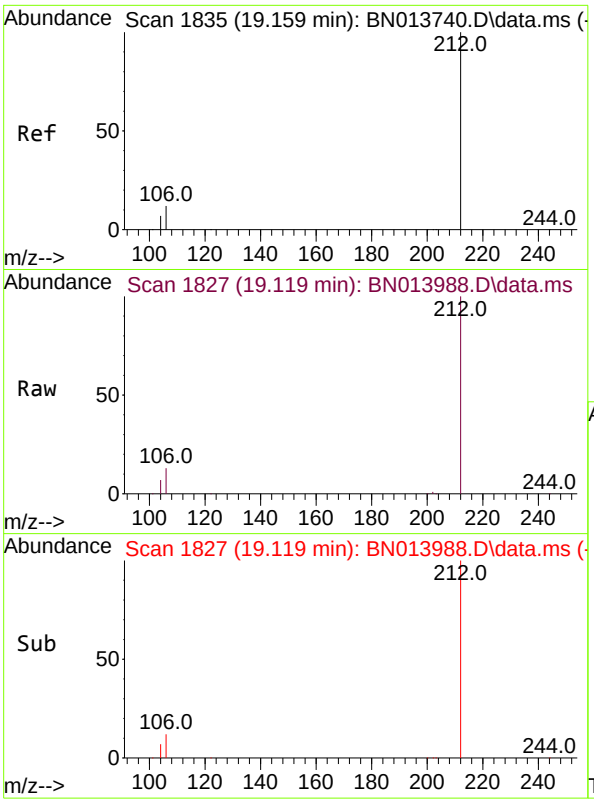
#26
Anthracene
Concen: 0.35 ng
RT: 17.214 min Scan# 1539
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:178 Resp: 22026

Ion	Ratio	Lower	Upper
178	100		
176	18.4	14.6	21.8
179	15.4	12.2	18.2



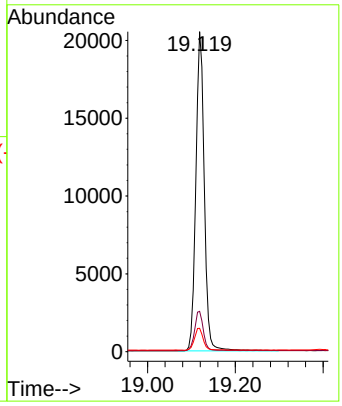
Instrument :
BNA_N
ClientSampleId :
PB135230BS

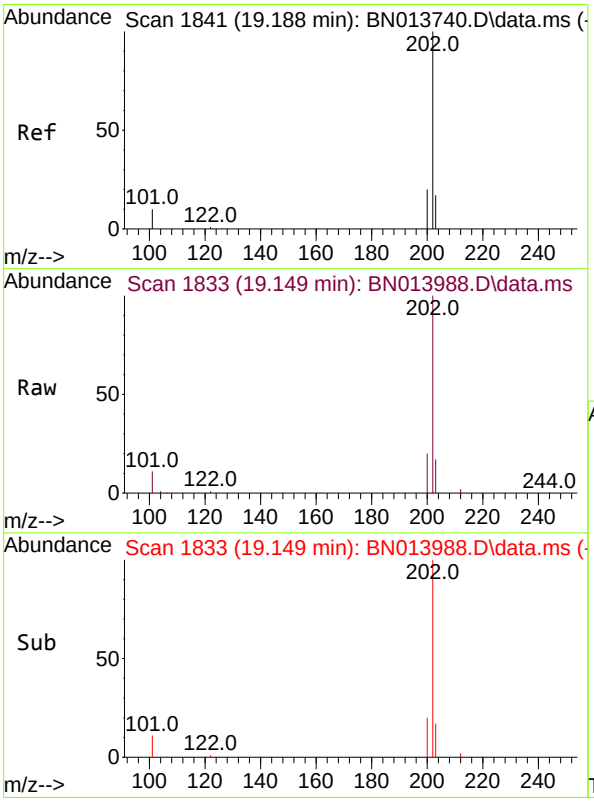


#27
Fluoranthene-d10
Concen: 0.38 ng
RT: 19.119 min Scan# 1827
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:212 Resp: 27347

Ion	Ratio	Lower	Upper
212	100		
106	12.7	9.7	14.5
104	6.9	5.5	8.3

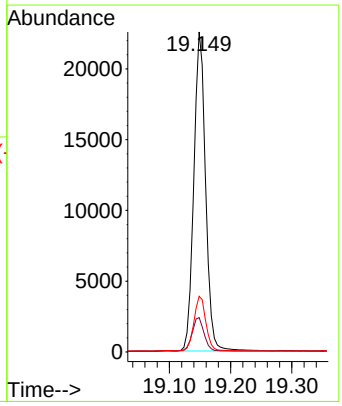




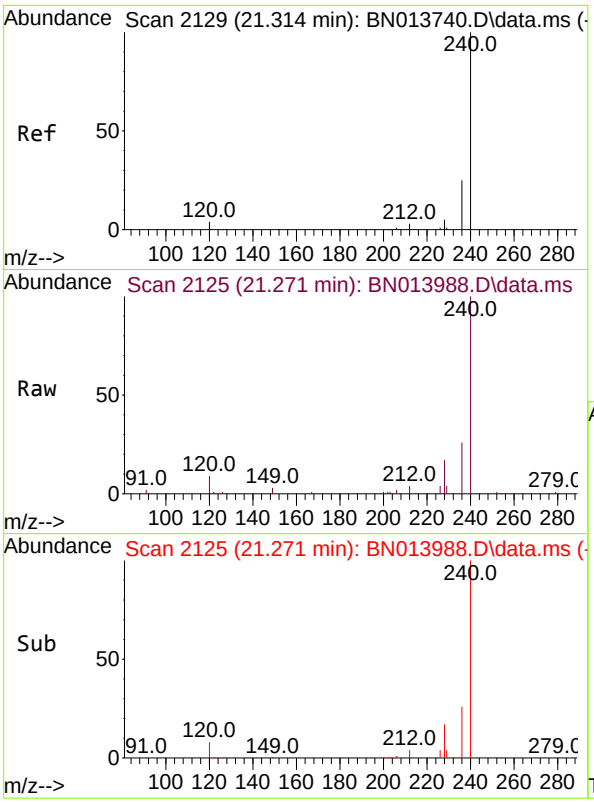
#28
Fluoranthene
Concen: 0.39 ng
RT: 19.149 min Scan# 1833
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:202 Resp: 30041

Ion	Ratio	Lower	Upper
202	100		
101	10.8	8.1	12.1
203	17.4	13.9	20.9



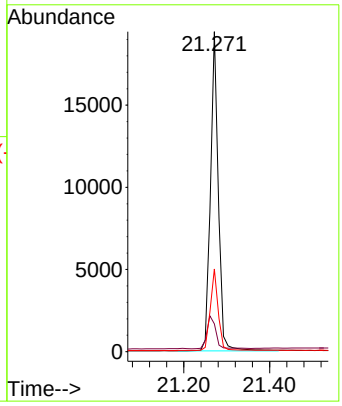
Instrument :
BNA_N
ClientSampleId :
PB135230BS

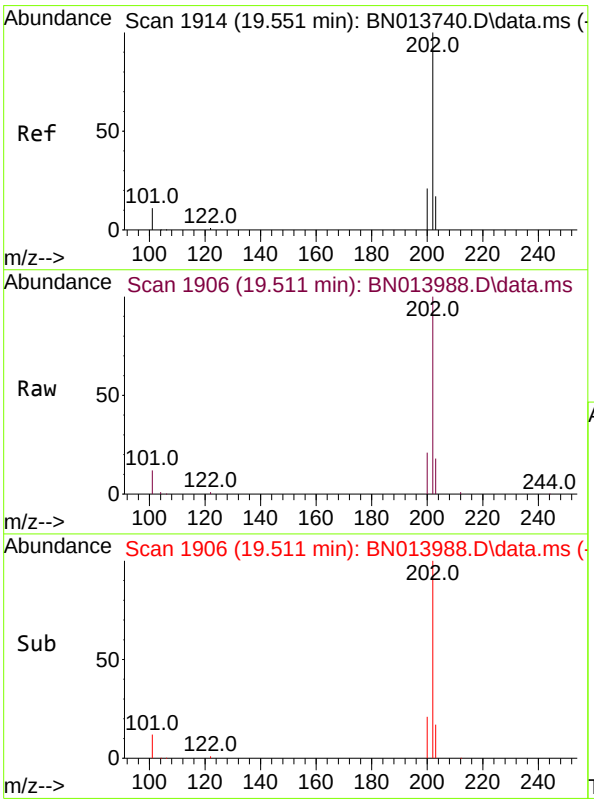


#29
Chrysene-d12
Concen: 0.40 ng
RT: 21.271 min Scan# 2125
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:240 Resp: 24638

Ion	Ratio	Lower	Upper
240	100		
120	8.7	10.2	15.4#
236	25.9	21.3	31.9

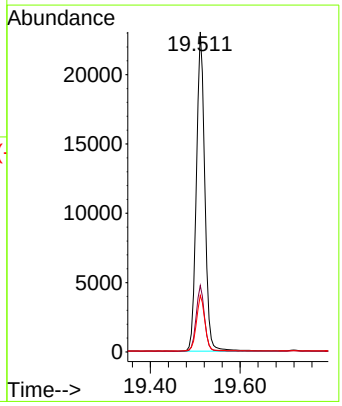




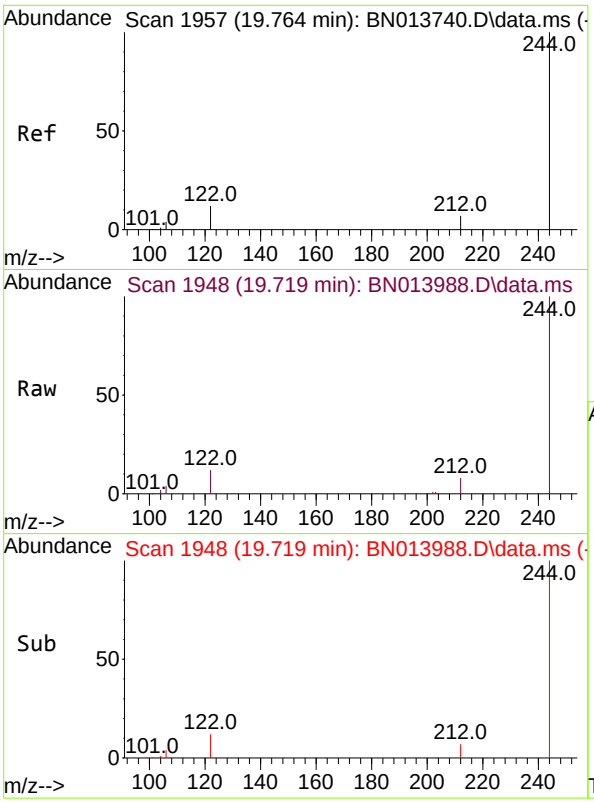
#30
Pyrene
Concen: 0.40 ng
RT: 19.511 min Scan# 1906
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:202 Resp: 30340

Ion	Ratio	Lower	Upper
202	100		
200	20.4	16.3	24.5
203	17.4	14.0	21.0



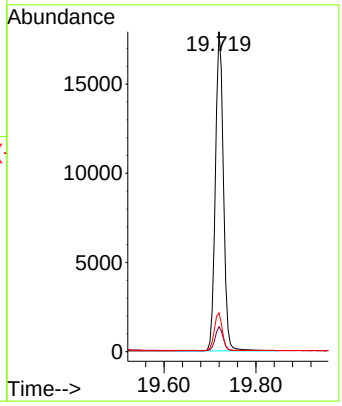
Instrument :
BNA_N
ClientSampleId :
PB135230BS

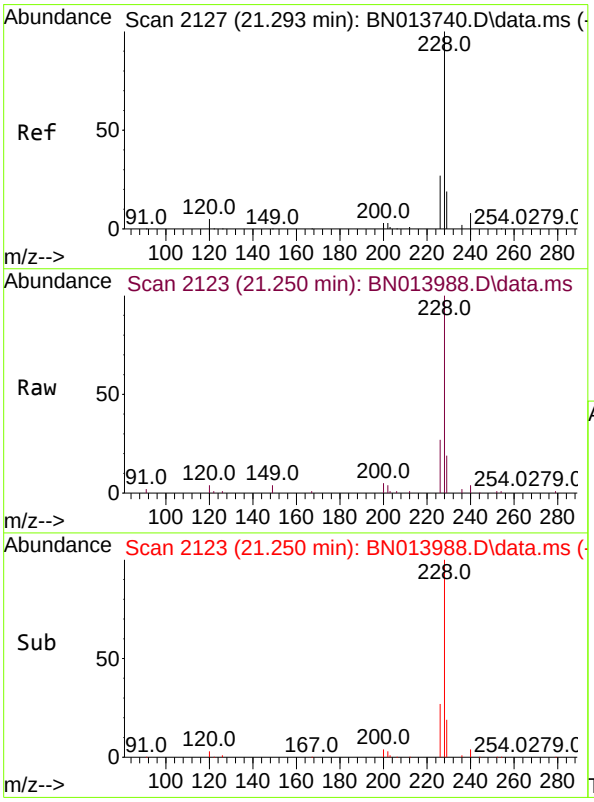


#31
Terphenyl-d14
Concen: 0.40 ng
RT: 19.719 min Scan# 1948
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:244 Resp: 21707

Ion	Ratio	Lower	Upper
244	100		
212	7.8	6.1	9.1
122	12.1	9.8	14.8

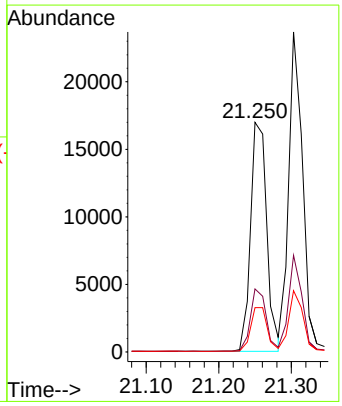




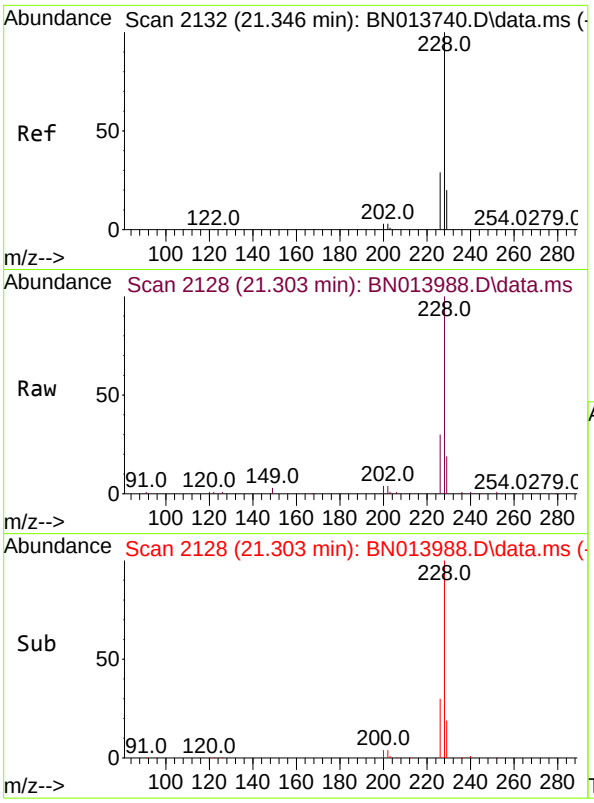
#32
Benzo(a)anthracene
Concen: 0.35 ng
RT: 21.250 min Scan# 2123
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:228 Resp: 26265

Ion	Ratio	Lower	Upper
228	100		
226	27.5	20.5	30.7
229	19.3	16.2	24.4



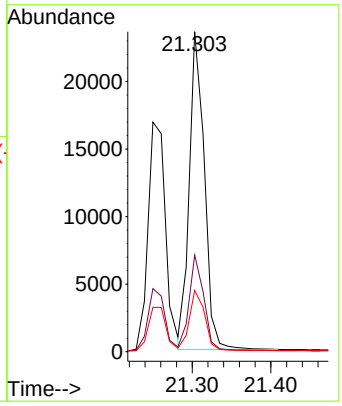
Instrument :
BNA_N
ClientSampleId :
PB135230BS

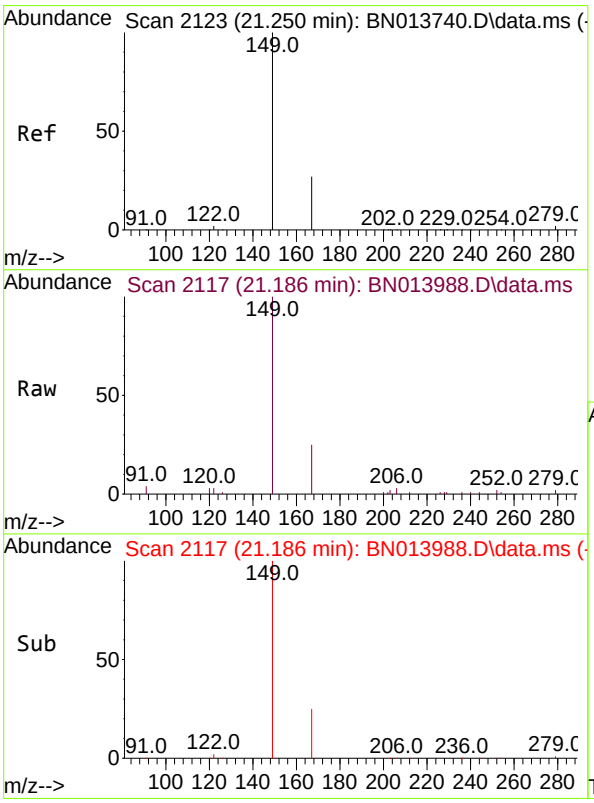


#33
Chrysene
Concen: 0.42 ng
RT: 21.303 min Scan# 2128
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:228 Resp: 31303

Ion	Ratio	Lower	Upper
228	100		
226	30.2	24.3	36.5
229	19.1	15.1	22.7

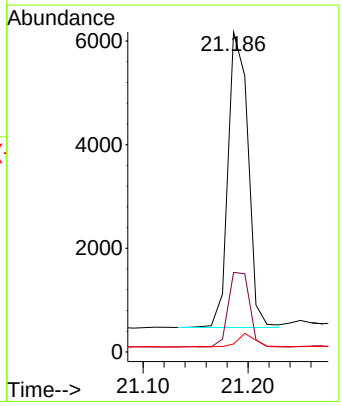




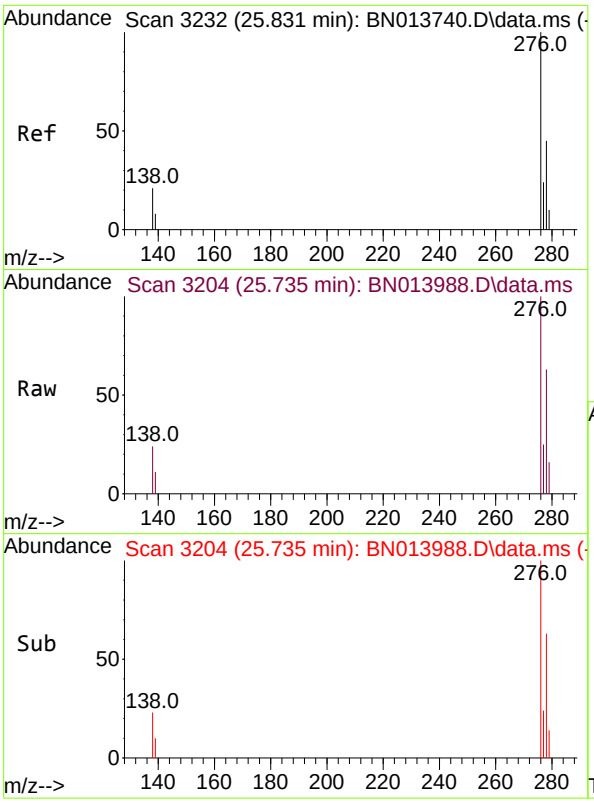
#34
Bis(2-ethylhexyl)phthalate
Concen: 0.21 ng
RT: 21.186 min Scan# 2117
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:149 Resp: 7518

Ion	Ratio	Lower	Upper
149	100		
167	26.8	22.1	33.1
279	4.5	3.5	5.3



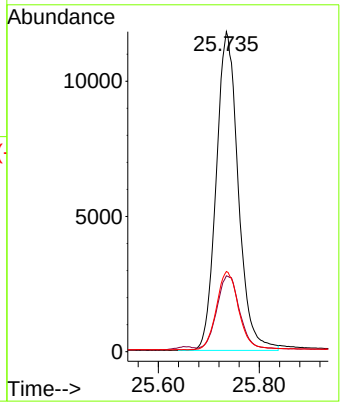
Instrument :
BNA_N
ClientSampleId :
PB135230BS

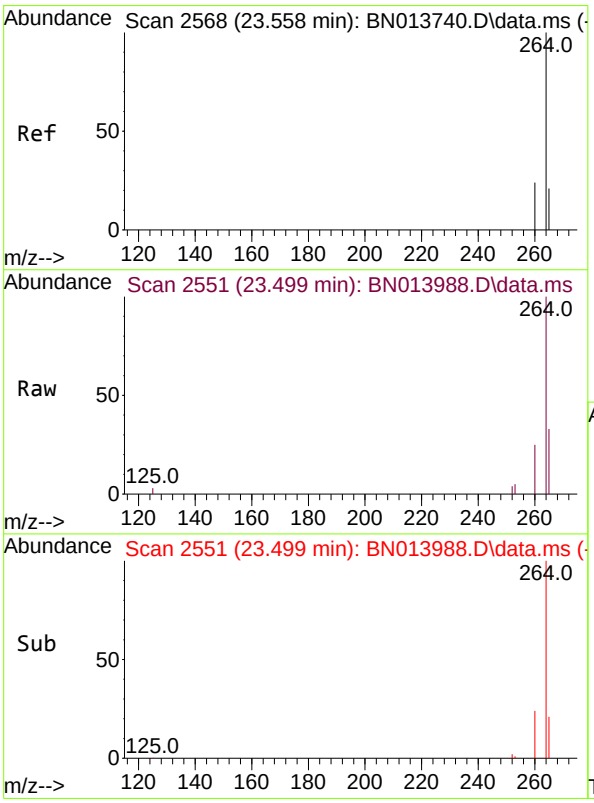


#35
Indeno(1,2,3-cd)pyrene
Concen: 0.40 ng
RT: 25.735 min Scan# 3204
Delta R.T. 0.003 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:276 Resp: 35629

Ion	Ratio	Lower	Upper
276	100		
138	23.0	19.8	29.6
277	24.9	19.9	29.9

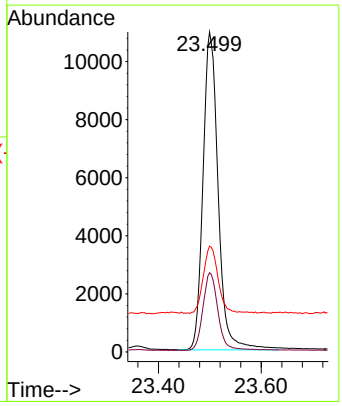




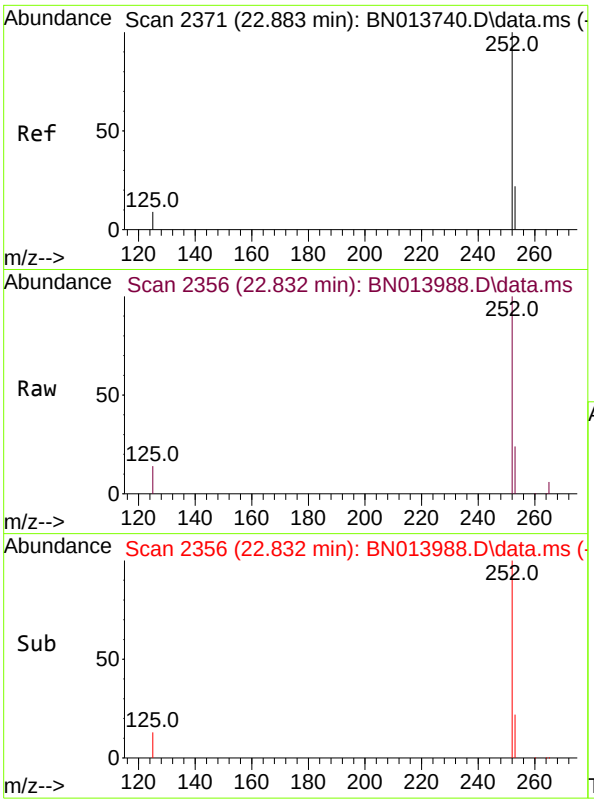
#36
Perylene-d12
Concen: 0.40 ng
RT: 23.499 min Scan# 2551
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:264 Resp: 22376

Ion	Ratio	Lower	Upper
264	100		
260	24.8	19.3	28.9
265	33.0	66.2	99.4#



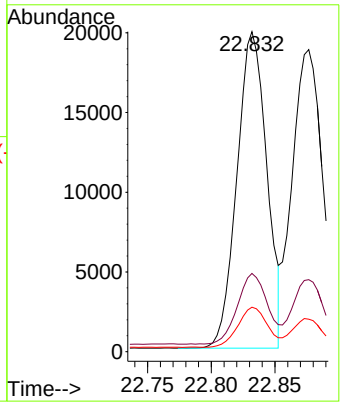
Instrument :
BNA_N
ClientSampleId :
PB135230BS

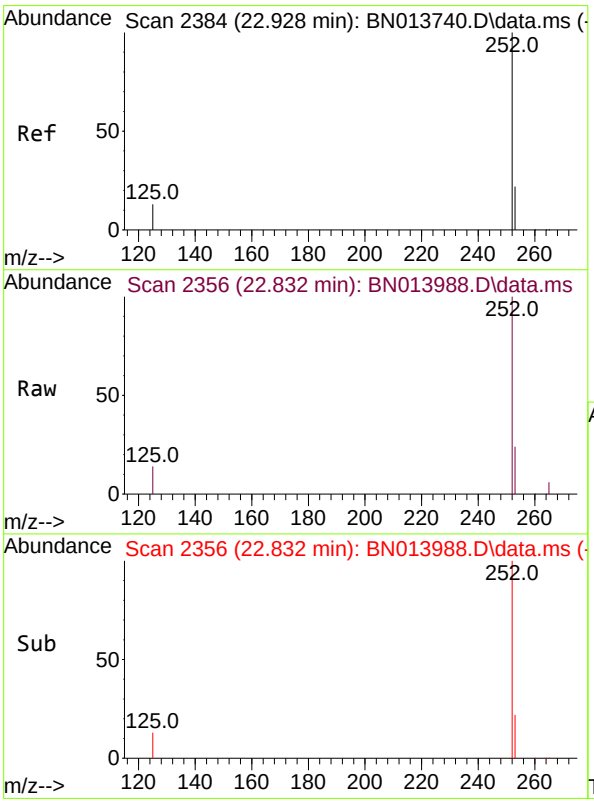


#37
Benzo(b)fluoranthene
Concen: 0.45 ng
RT: 22.832 min Scan# 2356
Delta R.T. 0.003 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:252 Resp: 32305

Ion	Ratio	Lower	Upper
252	100		
253	24.5	20.4	30.6
125	13.9	11.6	17.4

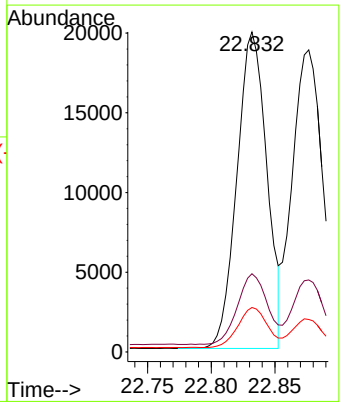




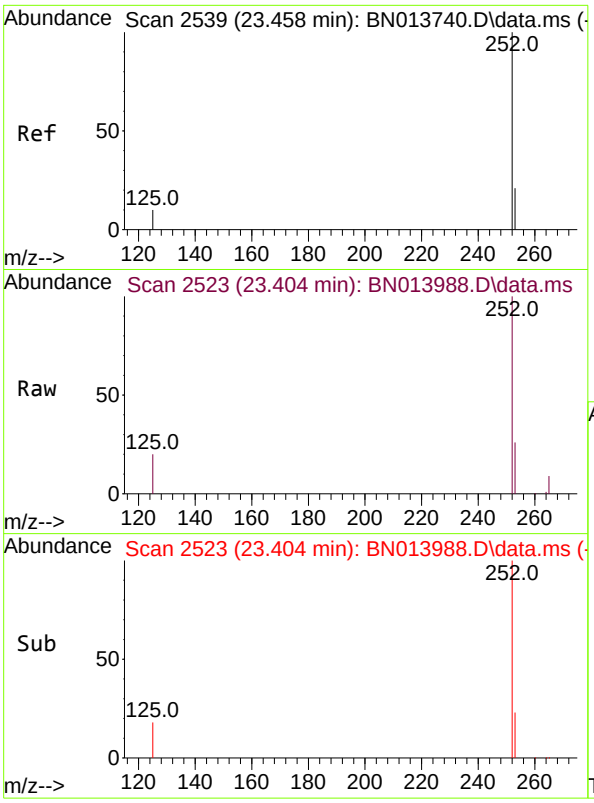
#38
Benzo(k)fluoranthene
Concen: 0.47 ng
RT: 22.832 min Scan# 2356
Delta R.T. -0.041 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:252 Resp: 32305

Ion	Ratio	Lower	Upper
252	100		
253	24.5	20.5	30.7
125	13.9	12.3	18.5



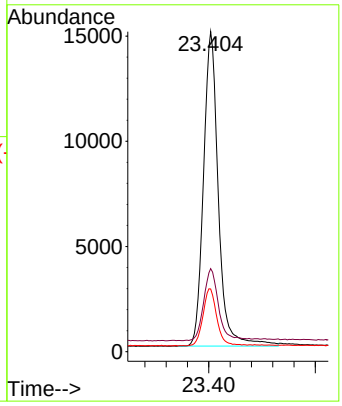
Instrument :
BNA_N
ClientSampleId :
PB135230BS

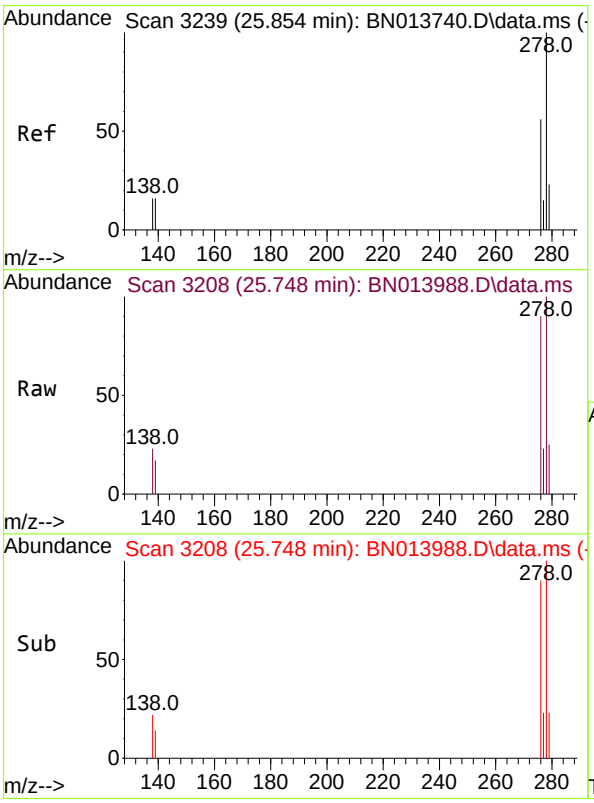


#39
Benzo(a)pyrene
Concen: 0.45 ng
RT: 23.404 min Scan# 2523
Delta R.T. 0.003 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:252 Resp: 29026

Ion	Ratio	Lower	Upper
252	100		
253	26.0	21.8	32.6
125	19.6	14.6	21.8

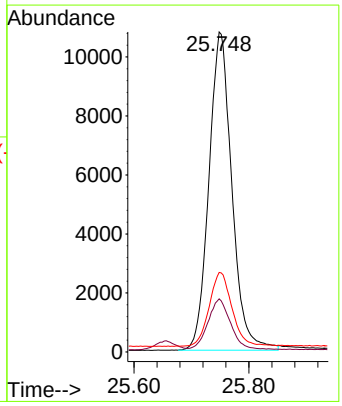


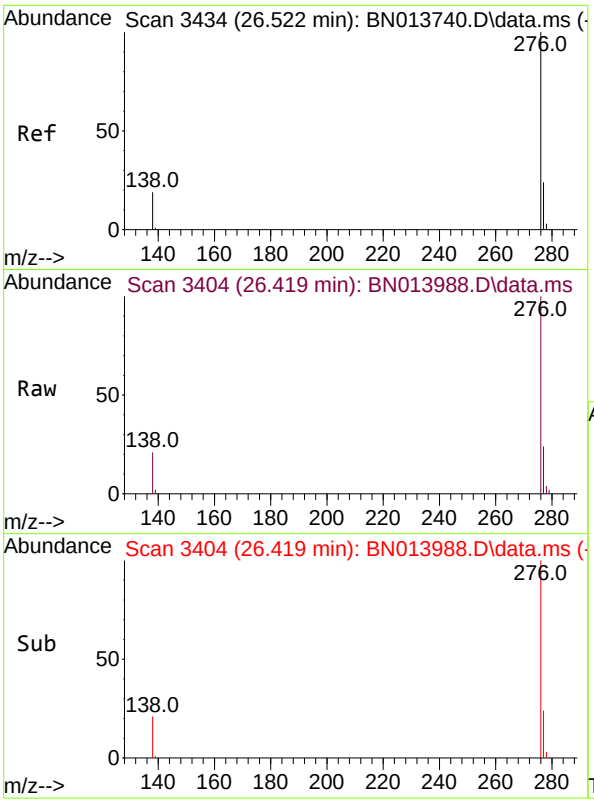


#40
Dibenzo(a,h)anthracene
Concen: 0.44 ng
RT: 25.748 min Scan# 3208
Delta R.T. 0.003 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:278 Resp: 29915

Ion	Ratio	Lower	Upper
278	100		
139	16.6	13.1	19.7
279	24.8	21.4	32.0

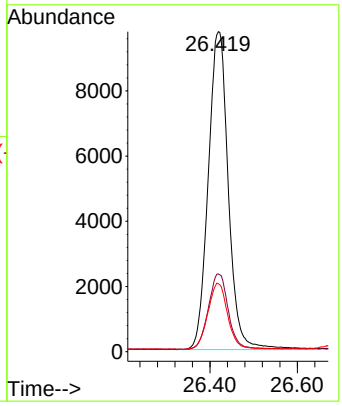




#41
Benzo(g,h,i)perylene
Concen: 0.45 ng
RT: 26.419 min Scan# 3404
Delta R.T. -0.000 min
Lab File: BN013988.D
Acq: 18 Mar 2021 18:43

Tgt Ion:276 Resp: 30982

Ion	Ratio	Lower	Upper
276	100		
277	24.3	20.0	30.0
138	21.3	17.8	26.8



Instrument :
BNA_N
ClientSampleId :
PB135230BS