Supporting Information

Comprehensive Profiling of Phytocannabinoids and Semi-Synthetic Cannabinoids in Seized Materials from Northern Italy

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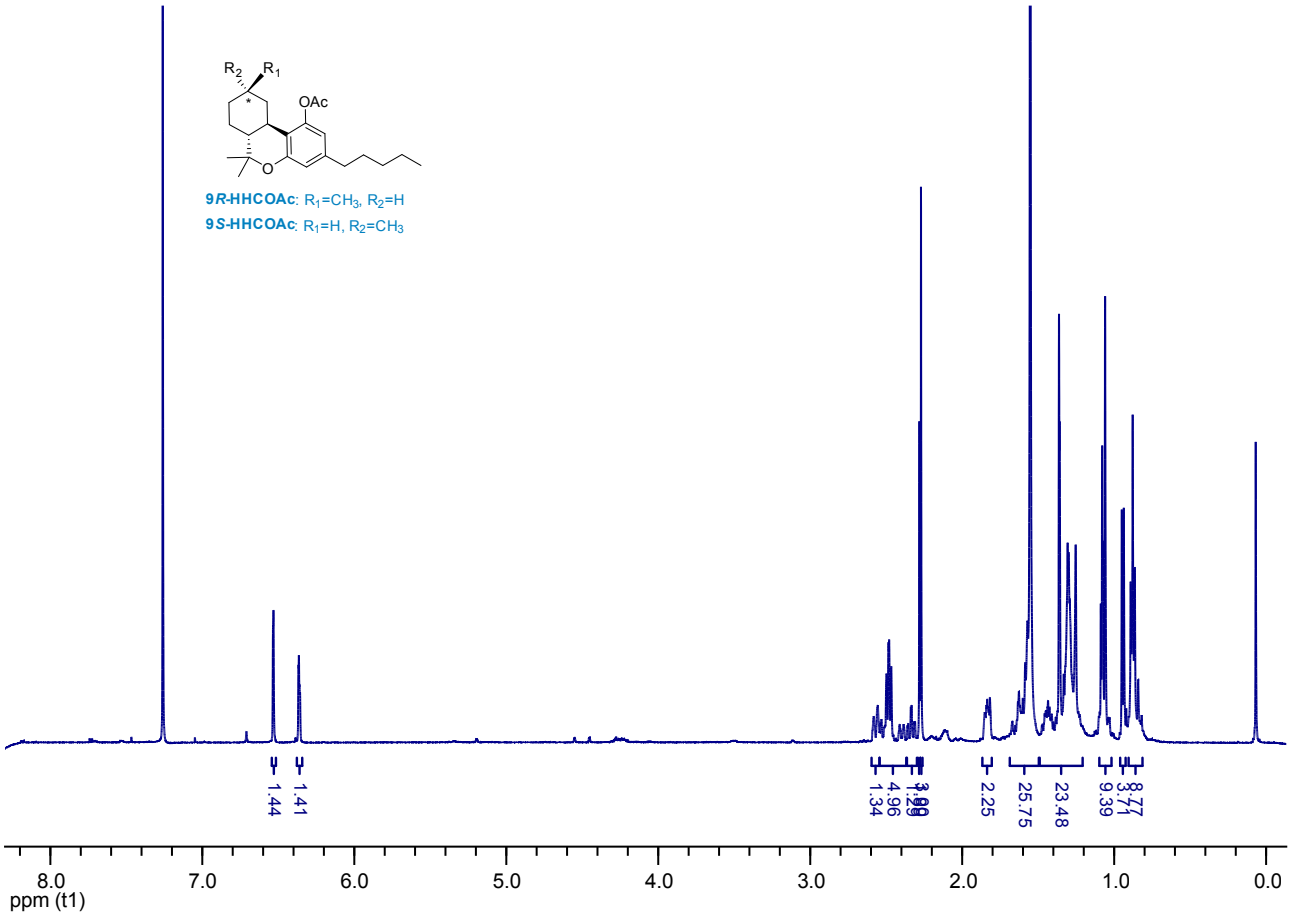
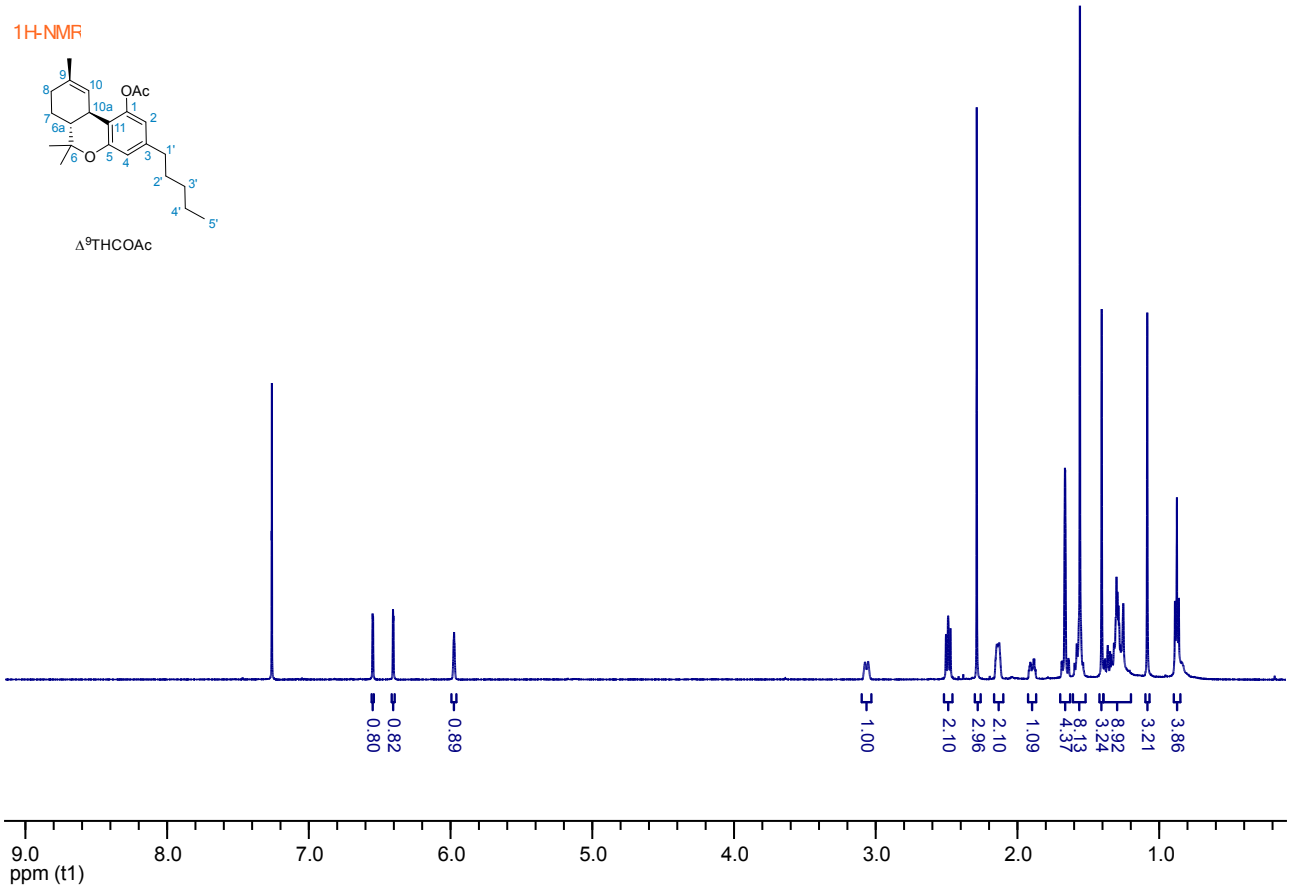
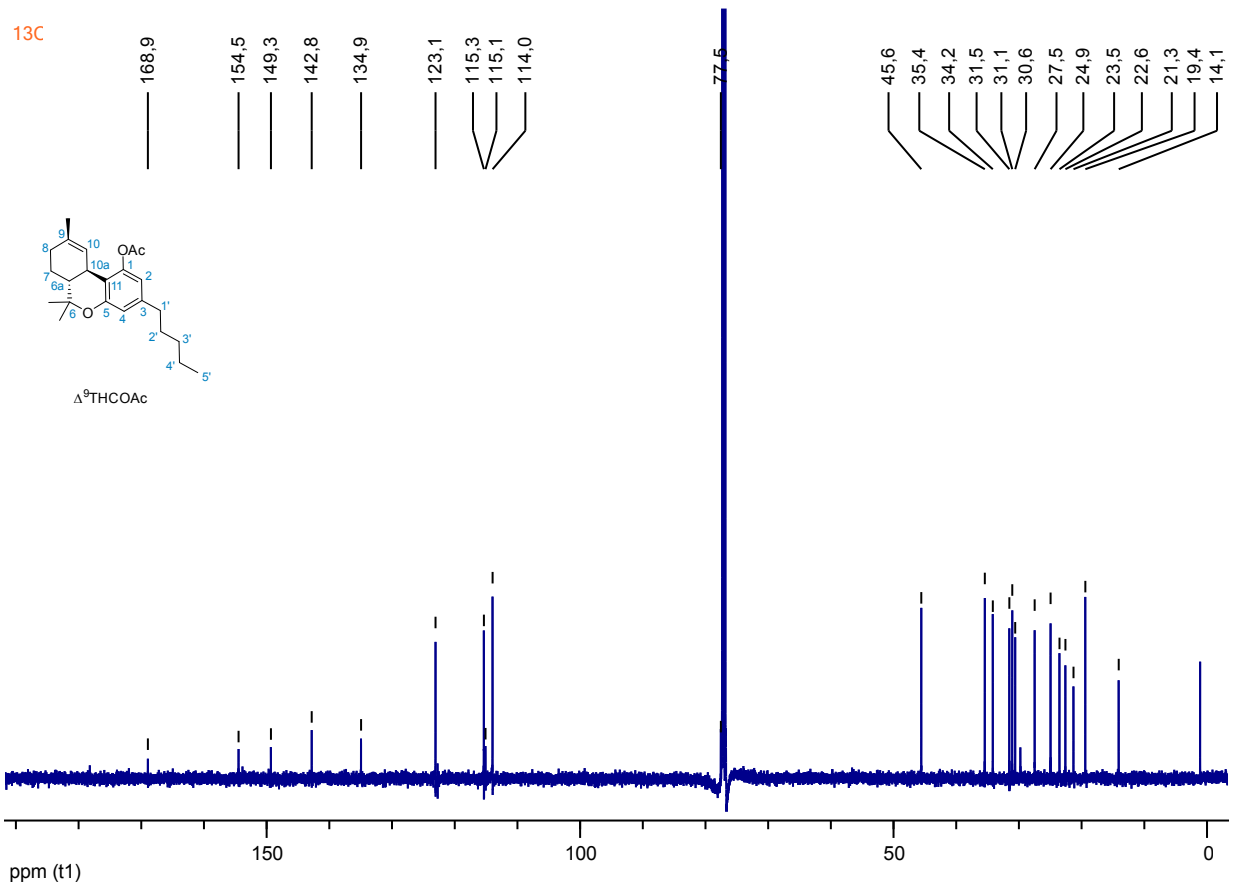
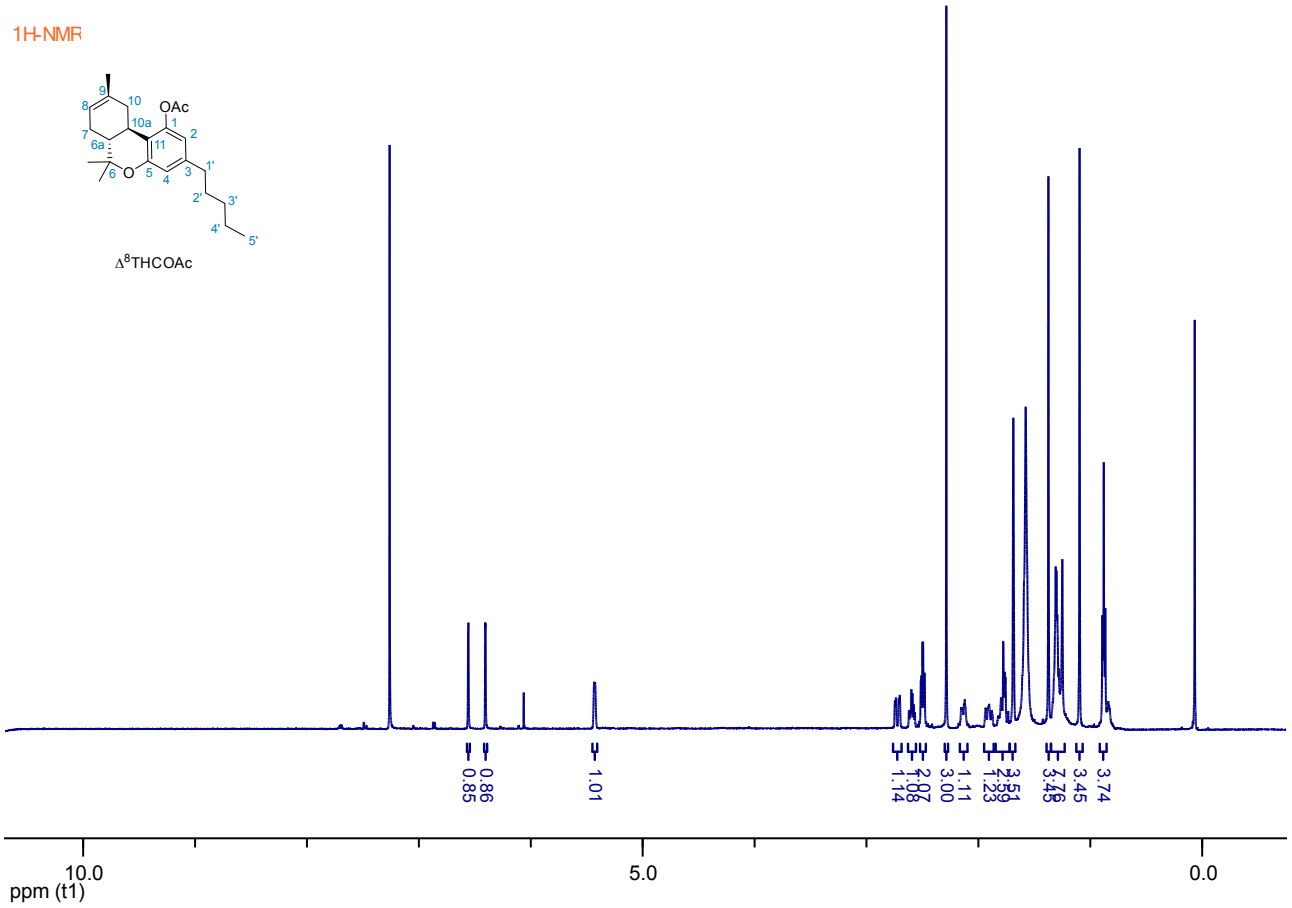
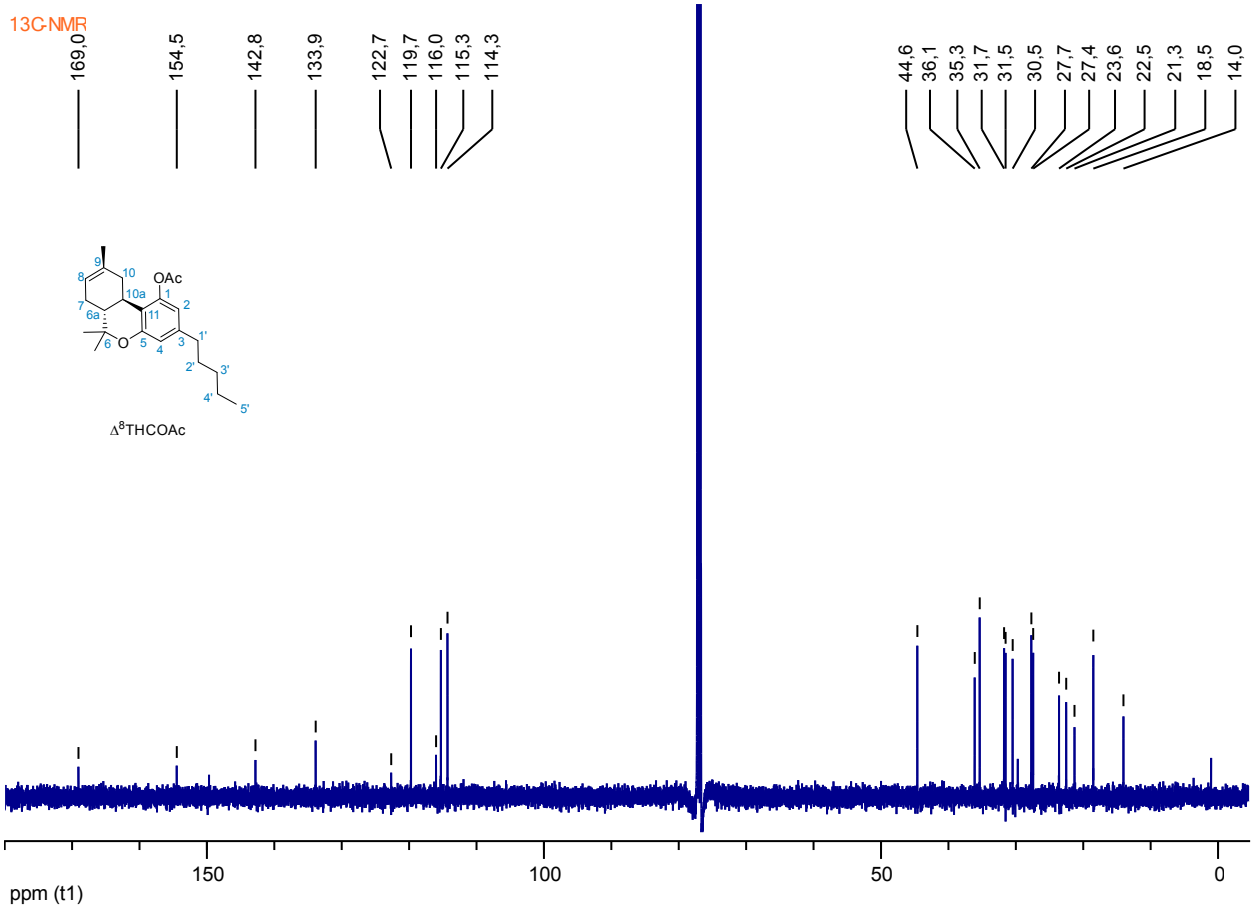
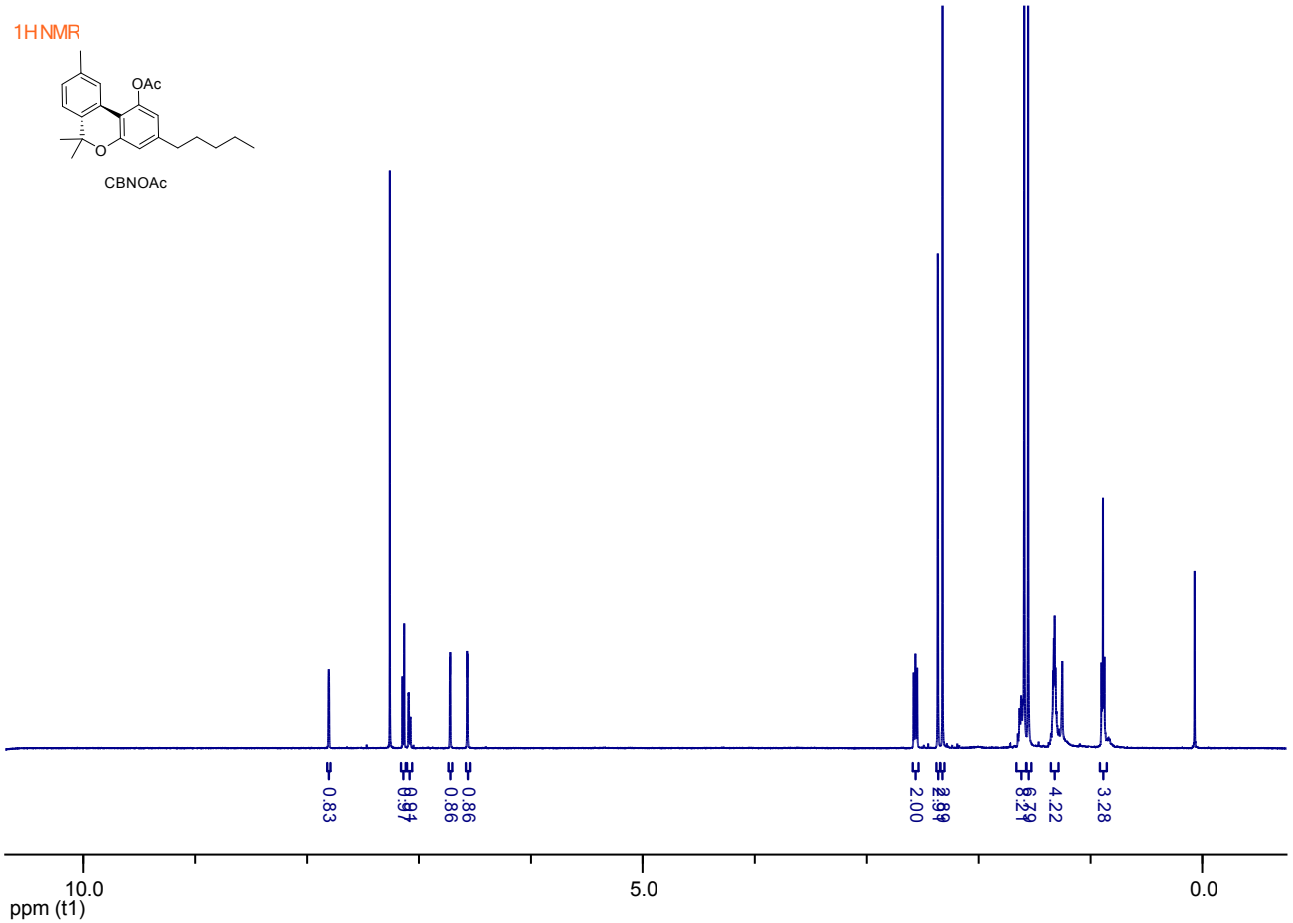

R2
R1
OAc
O
9R-HHCOAc: R1=CH3, R2=H
9S-HHCOAc: R1=H, R2=CH3
1.44
1.41
1.34
4.96
2.25
25.75
23.48
9.39
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

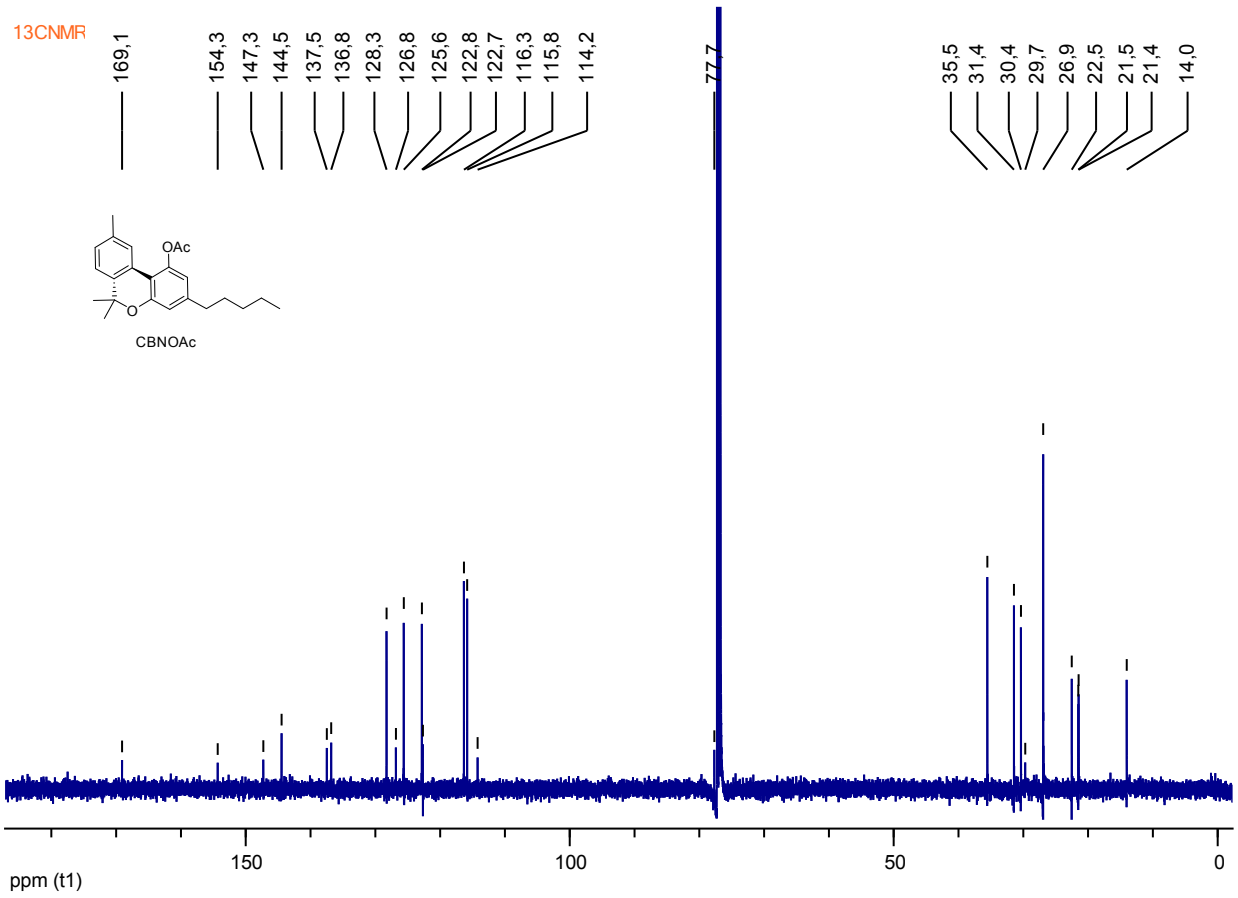

1H-NMR
OAc
Δ9THCOAc
0.80
0.82
0.89
1.00
2.10
2.96
2.10
1.09
4.37
8.13
3.24
8.92
3.21
3.86
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


13C
168,9
154,5
149,3
142,8
134,9
123,1
115,3
115,1
114,0
77,5
45,6
35,4
34,2
31,5
31,1
30,6
27,5
24,9
23,5
22,6
21,3
19,4
14,1
OAc
Δ9THCOAc
150
100
50
0
ppm (t1)

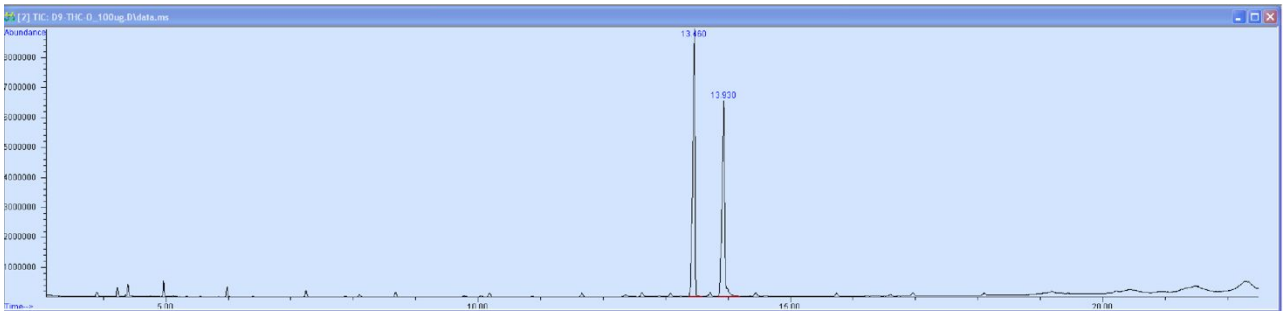

1H-NMR
OAc
Δ8THCOAc
0.85
0.86
1.01
1.14
1.08
1.07
3.00
1.11
1.23
3.51
3.59
3.46
3.76
3.45
3.74
10.0
5.0
0.0
ppm (t1)


13C-NMR
169,0
154,5
142,8
133,9
122,7
119,7
116,0
115,3
114,3
44,6
36,1
35,3
31,7
31,5
30,5
27,7
27,4
23,6
22,5
21,3
18,5
14,0
OAc
Δ8THCOAc
150
100
50
0
ppm (t1)

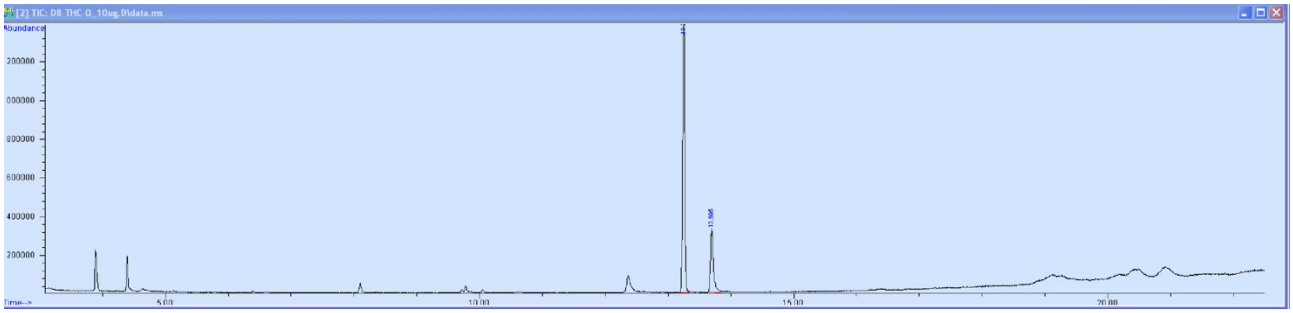

1H NMR
OAc
O
CBNOAc
0.83
0.86
0.86
2.00
4.22
3.28
10.0
5.0
0.0
ppm (t1)


13CNMR
169,1
154,3
147,3
144,5
137,5
136,8
128,3
126,8
125,6
122,8
122,7
116,3
115,8
114,2
77,7
35,5
31,4
30,4
29,7
26,9
22,5
21,5
21,4
14,0
OAc
O
CBNOAc
150
100
50
0
ppm (t1)

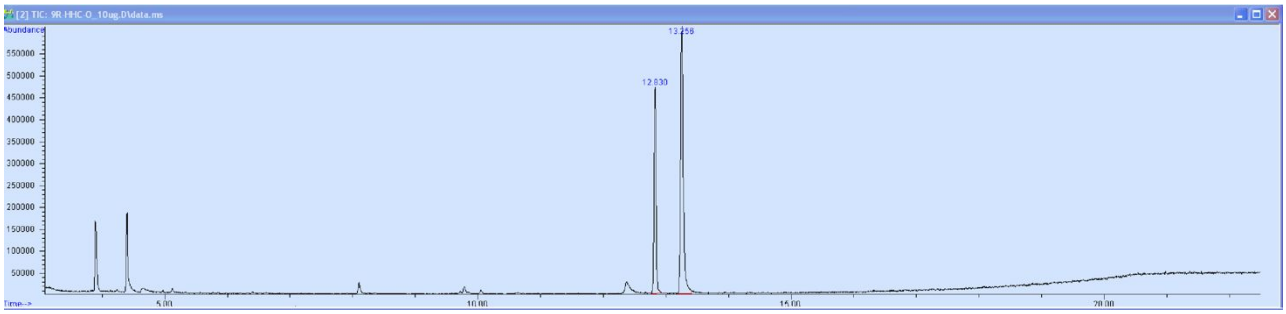
A


[2] TIC: D9-THC-0_100ug.D\data.ms
Abundance
13.460
13.930
Time-->

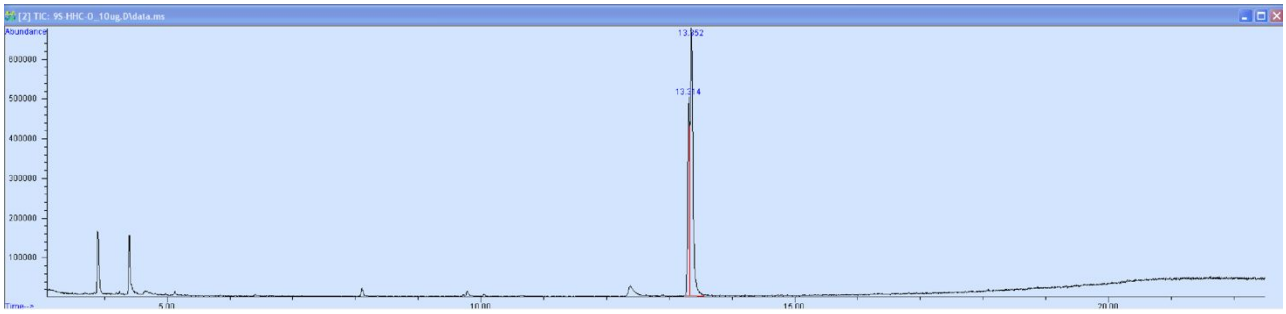
B


[2] TIC: D8-THC-0_10ug.D\data.ms
Abundance
Time-->

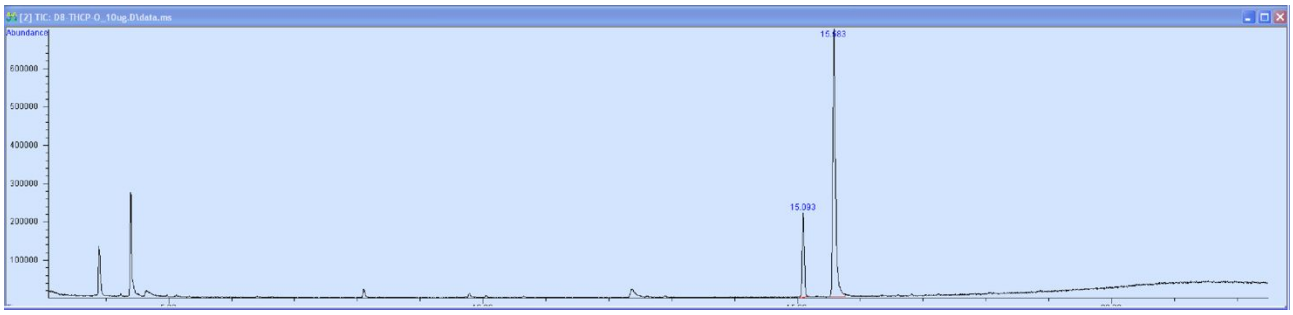
C


[2] TIC: 9R-HHC-0_10ug.D\data.ms
Abundance
13.258
12.930
Time-->

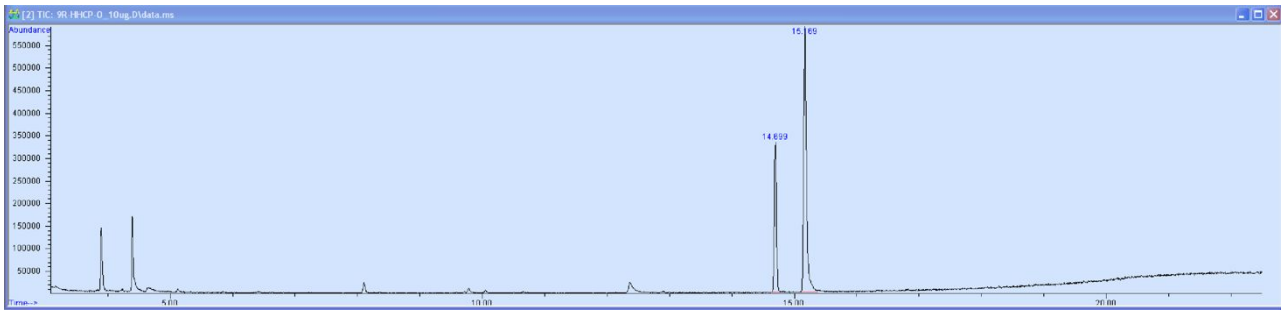
D


[2] TIC: 9S-HHC-0_10ug.D\data.ms
Abundance
13.052
Time-->

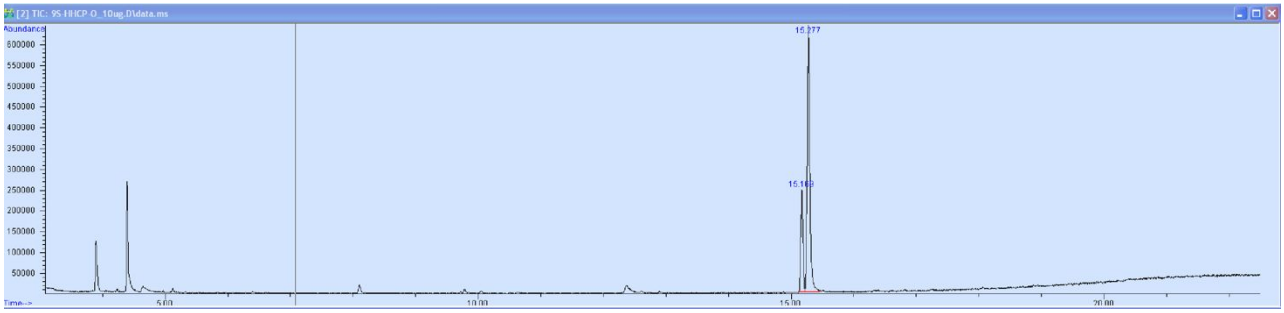
E


[2] TIC: D8-THCP-O_10ug.D\data.ms
Abundance
15.093

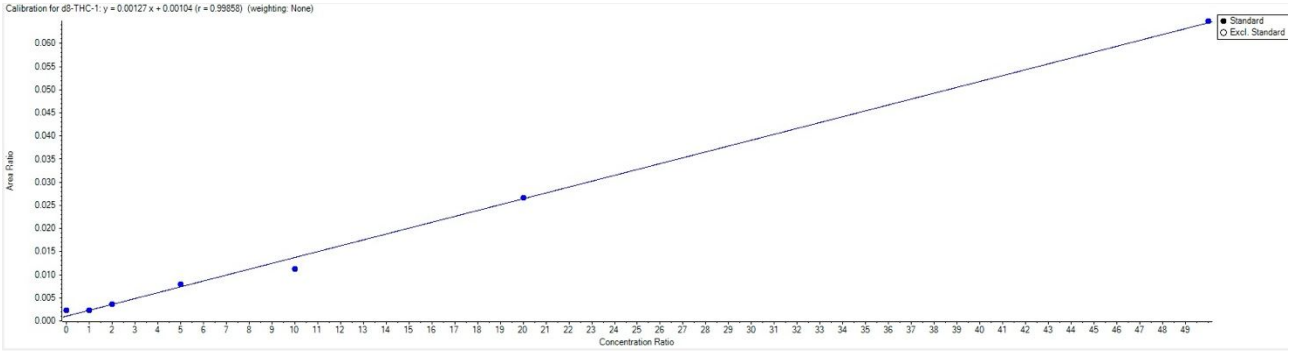
F


[2] TIC: 9R-HHCP-O_10ug.D\data.ms
Abundance
15.169
14.899
Time-->

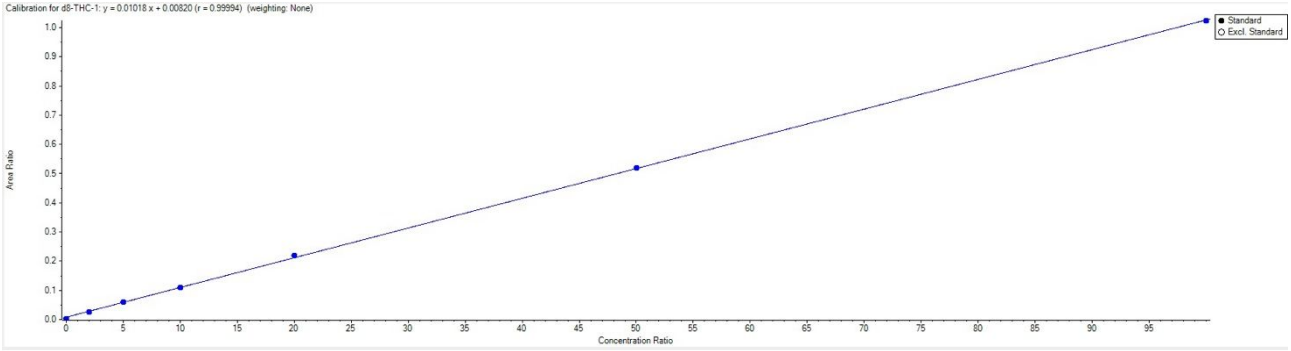
G


[2] TIC: 9S-HHCP-O_10ug.D\data.ms
Abundance
15.277
15.169
Time-->

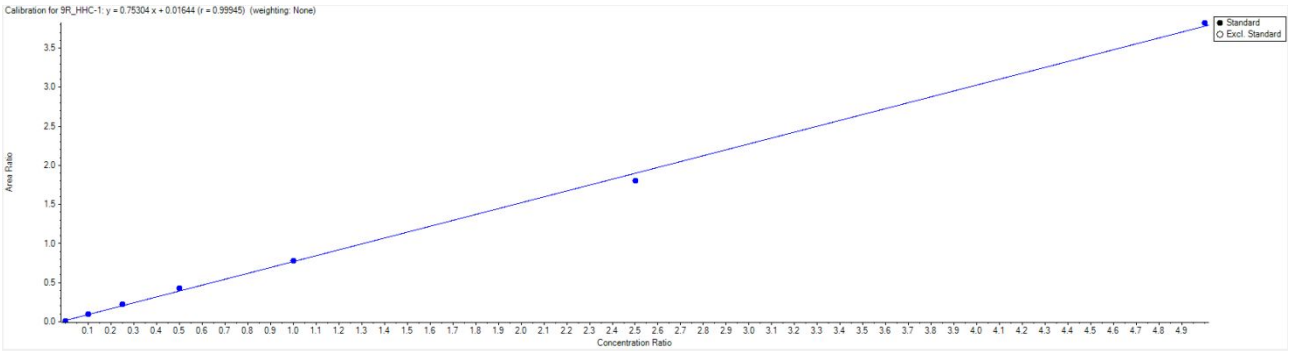
A


Calibration for d8-THC-1: y = 0.00127 x + 0.00104 (r = 0.99858) (weighting: None)
Standard
Excl. Standard
Area Ratio
Concentration Ratio

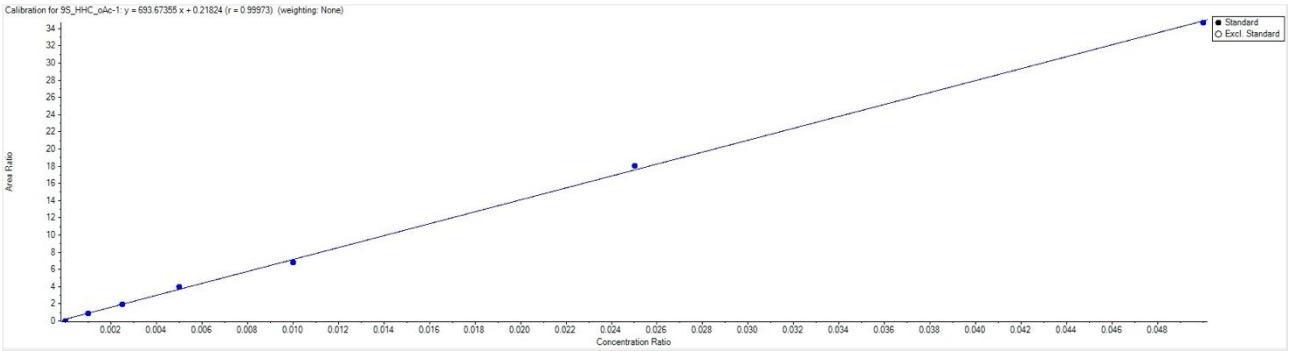
B


Calibration for d8-THC-1: y = 0.01018 x + 0.00820 (r = 0.99994) (weighting: None)
Standard
Excl. Standard
Area Ratio
Concentration Ratio

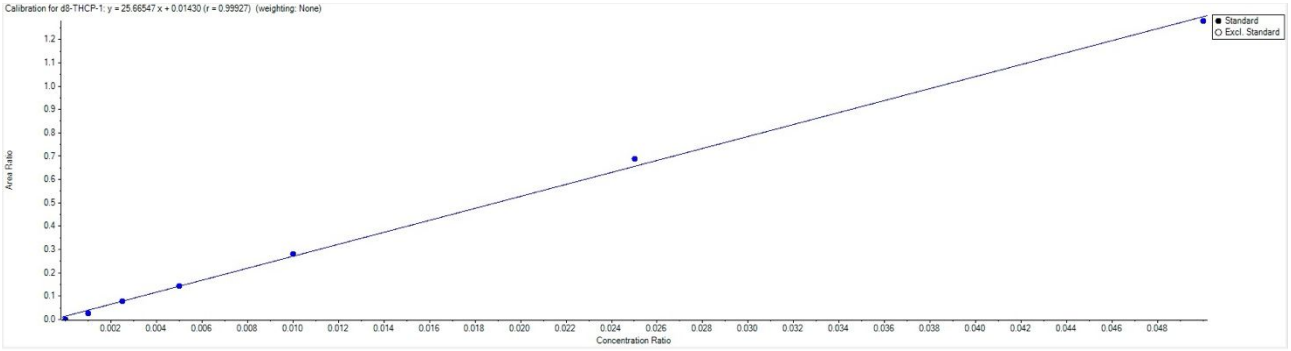
C


Calibration for 9R_HHC-1: y = 0.75304 x + 0.01644 (r = 0.99945) (weighting: None)
Standard
Excl. Standard
Area Ratio
Concentration Ratio

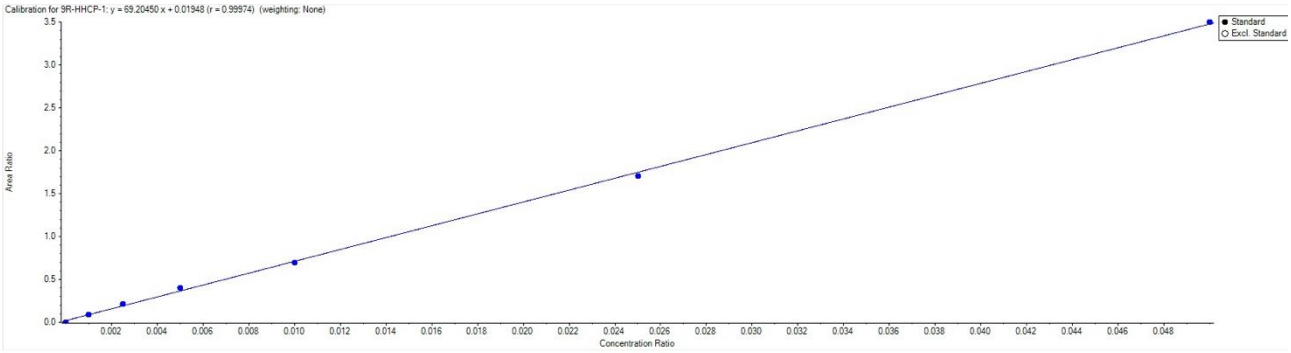
D


Calibration for 9S_HHC_oAc-1: y = 693.67355 x + 0.21824 (r = 0.99973) (weighting: None)
Standard
Excl. Standard
Area Ratio
Concentration Ratio

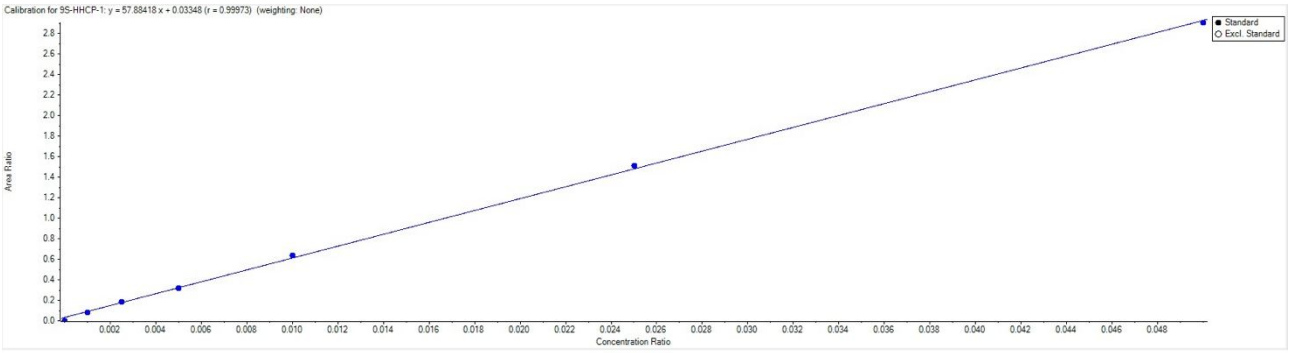
E


Calibration for d8-THCP-1: y = 25.66547 x + 0.01430 (r = 0.99927) (weighting: None)
Standard
Excl. Standard
Area Ratio
Concentration Ratio

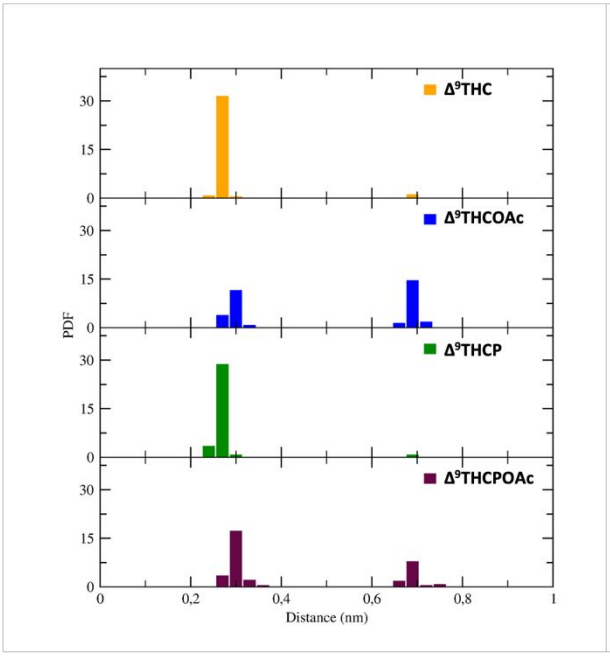
F


Calibration for 9R-HHCP-1: y = 69.20450 x + 0.01948 (r = 0.99974) (weighting: None)
Standard
Excl. Standard
Area Ratio
Concentration Ratio

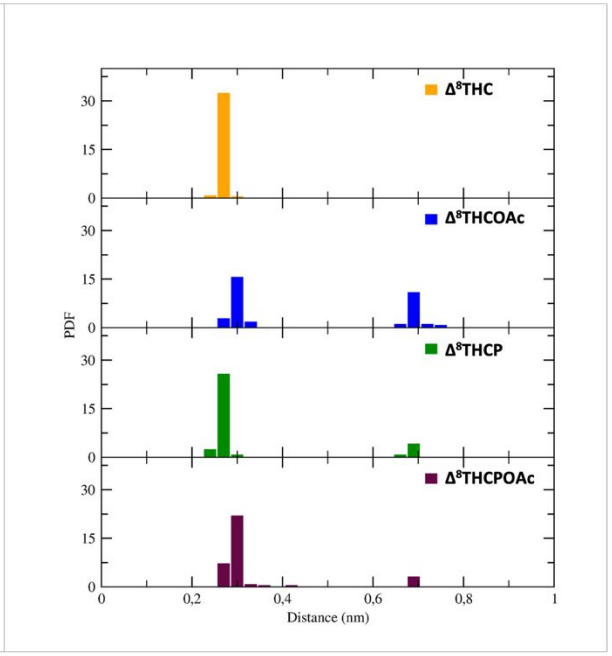
G


Calibration for 9S-HHCP-1: y = 57.88418 x + 0.03348 (r = 0.99973) (weighting: None)
Standard
Excl. Standard
Area Ratio
Concentration Ratio

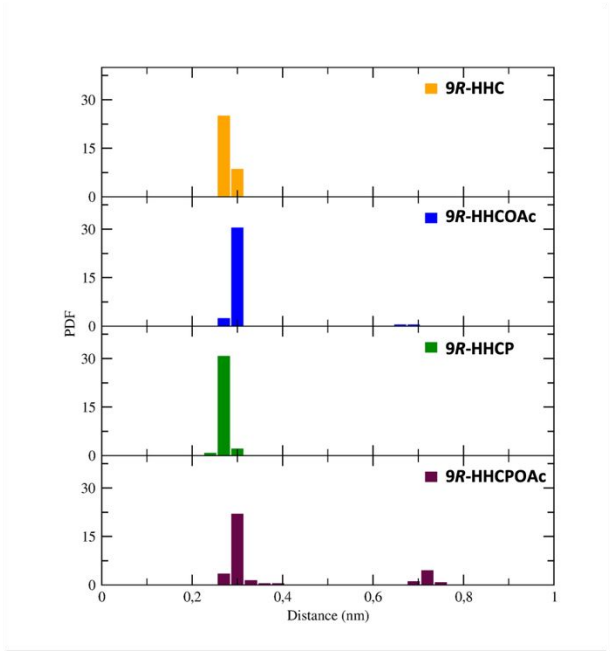
A


Δ9THC
Δ9THCOAc
Δ9THCP
Δ9THCPOAc
PDF
Distance (nm)

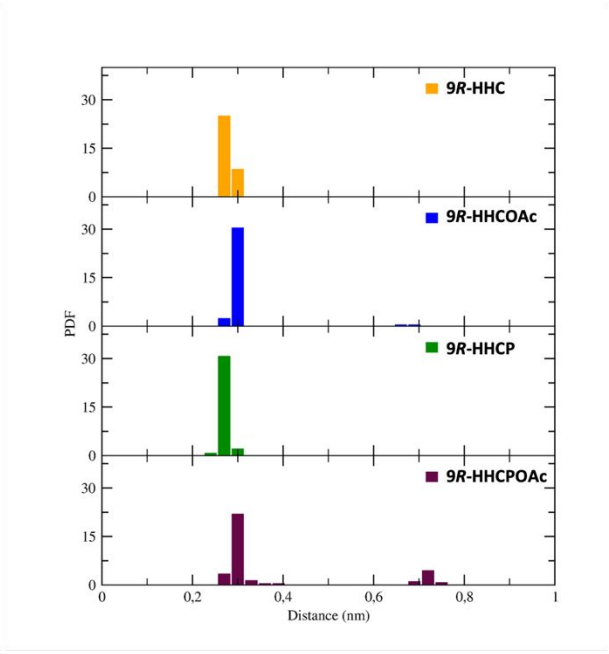
B


Δ8THC
Δ8THCOAc
Δ8THCP
Δ8THCPOAc
PDF
Distance (nm)

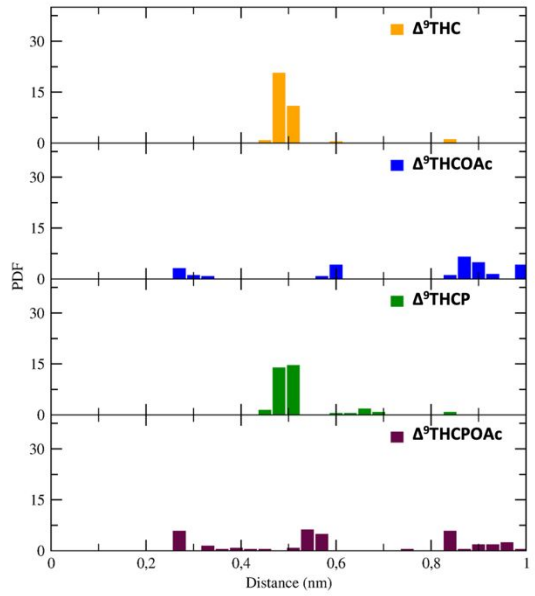
C


9R-HHC
9R-HHCOAc
9R-HHCP
9R-HHCPOAc
PDF
Distance (nm)

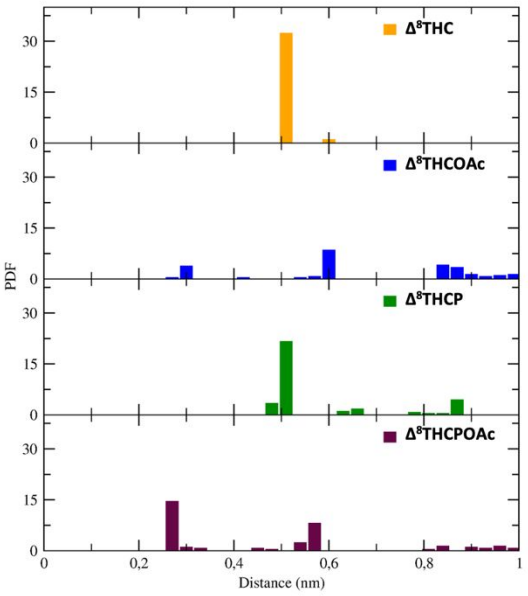
D


9R-HHC
9R-HHCOAc
9R-HHCP
9R-HHCPOAc
PDF
Distance (nm)

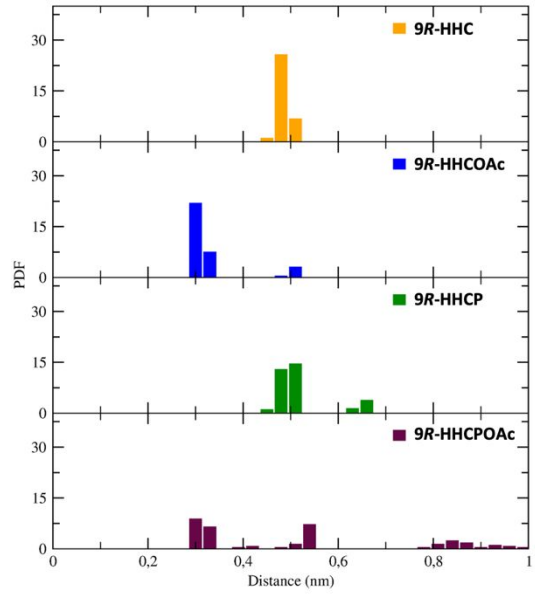
A


Δ9THC
Δ9THCOAc
Δ9THCP
Δ9THCPOAc
PDF
Distance (nm)

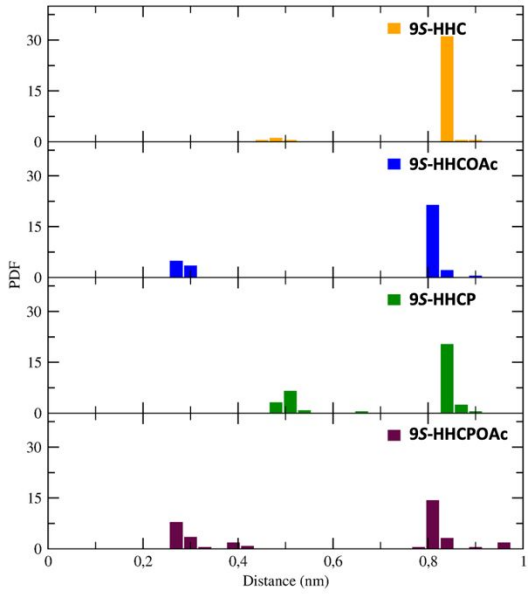
B


Δ8THC
Δ8THCOAc
Δ8THCP
Δ8THCPOAc
PDF
Distance (nm)

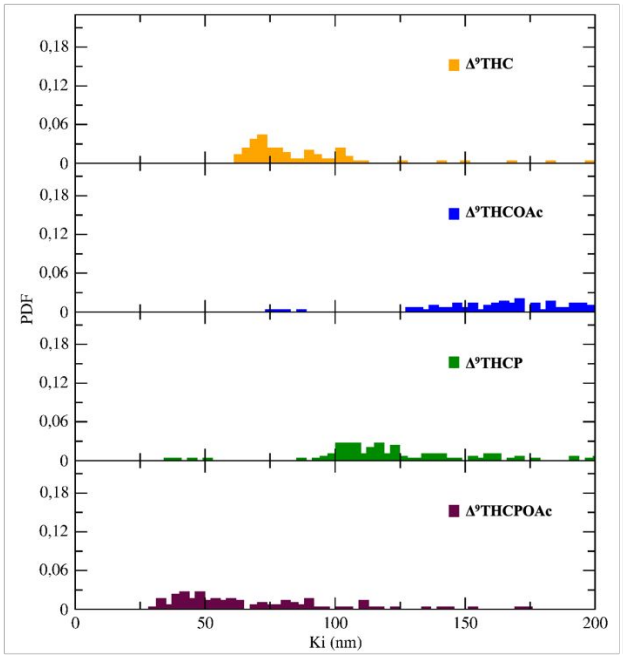
C


9R-HHC
9R-HHCOAc
9R-HHCP
9R-HHCPOAc
PDF
Distance (nm)

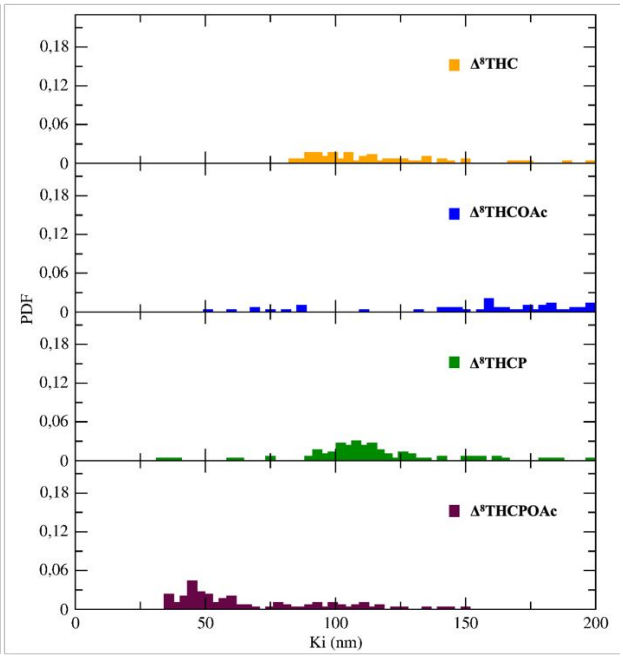
D


9S-HHC
9S-HHCOAc
9S-HHCP
9S-HHCPOAc
PDF
Distance (nm)

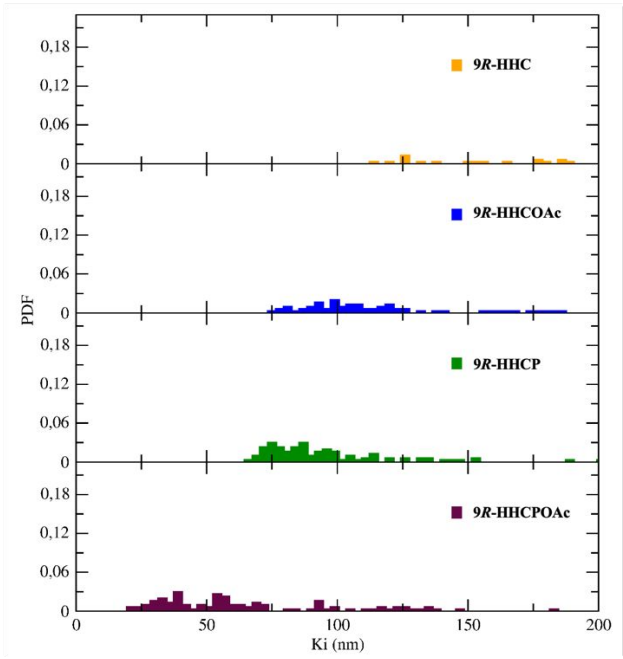
A


Δ⁹THC
Δ⁹THCOAc
Δ⁹THCP
Δ⁹THCPOAc
PDF
Ki (nm)

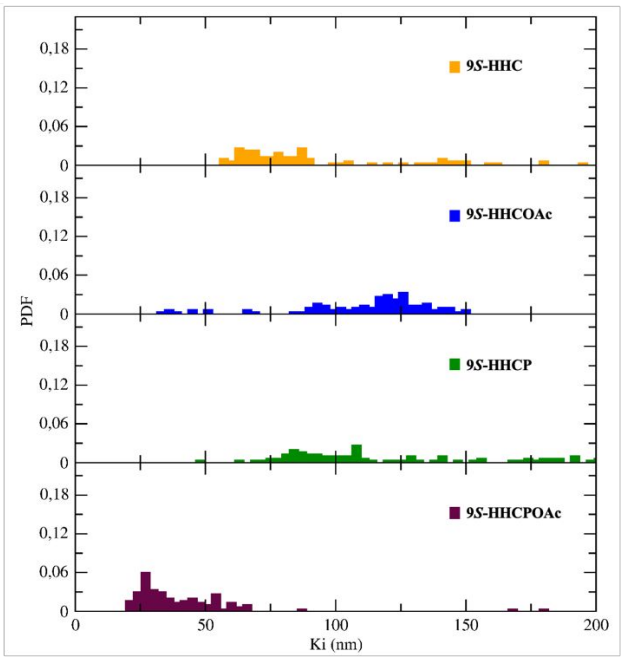
B


Δ⁸THC
Δ⁸THCOAc
Δ⁸THCP
Δ⁸THCPOAc
PDF
Ki (nm)

C


9R-HHC
9R-HHCOAc
9R-HHCP
9R-HHCPOAc
PDF
Ki (nm)

D


9S-HHC
9S-HHCOAc
9S-HHCP
9S-HHCPOAc
PDF
Ki (nm)