Electronic Supplementary Information

Deep insights to explain the mechanism of carbon dot formation at various reaction times using the hydrothermal technique: FT-IR, ^{13}C-NMR, ^{1}H-NMR, and UV-Visible spectroscopic approaches

Sewara J. Mohammed,[*a,b] Khalid M. Omer, [b] and Farouq E. Hawaiz [c]

a. Department of Chemistry, College of Science, University of Sulaimani, Qlyasan Street, Sulaimani,46002, Kurdistan Regional Government, Iraq.

b. Anesthesia department, College of health sciences, Cihan University Sulaimaniya, Sulaimaniya 46001, Kurdistan Region, Iraq.

c. Department of Chemistry, College of Education, Salahaddin University – Hawler, Erbil-Kurdistan, Iraq

*Corresponding author. E-mail: Sewara.mohammed@univsul.edu.iq

1. **Fig. S1** FT-IR spectra of (a) 4AA, (b) 3h, (c) 6 h, (d) 9h, (e) 12h, (f) 15h, (g) 18h, and (h) 21h NCDs.

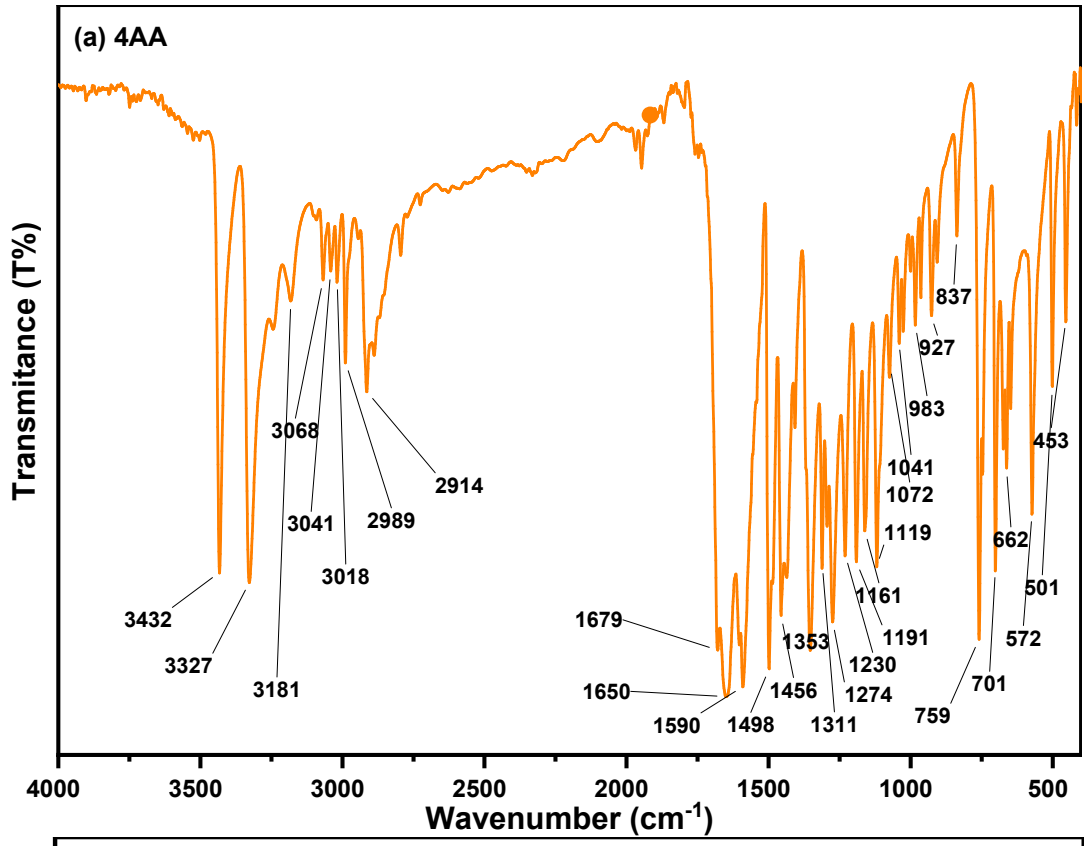
2. **Fig. S2** FT-IR spectra of (a) serine, and (b) d-threonine. We have found both FT-IR spectra from this site. (www.chemicalbook.com)

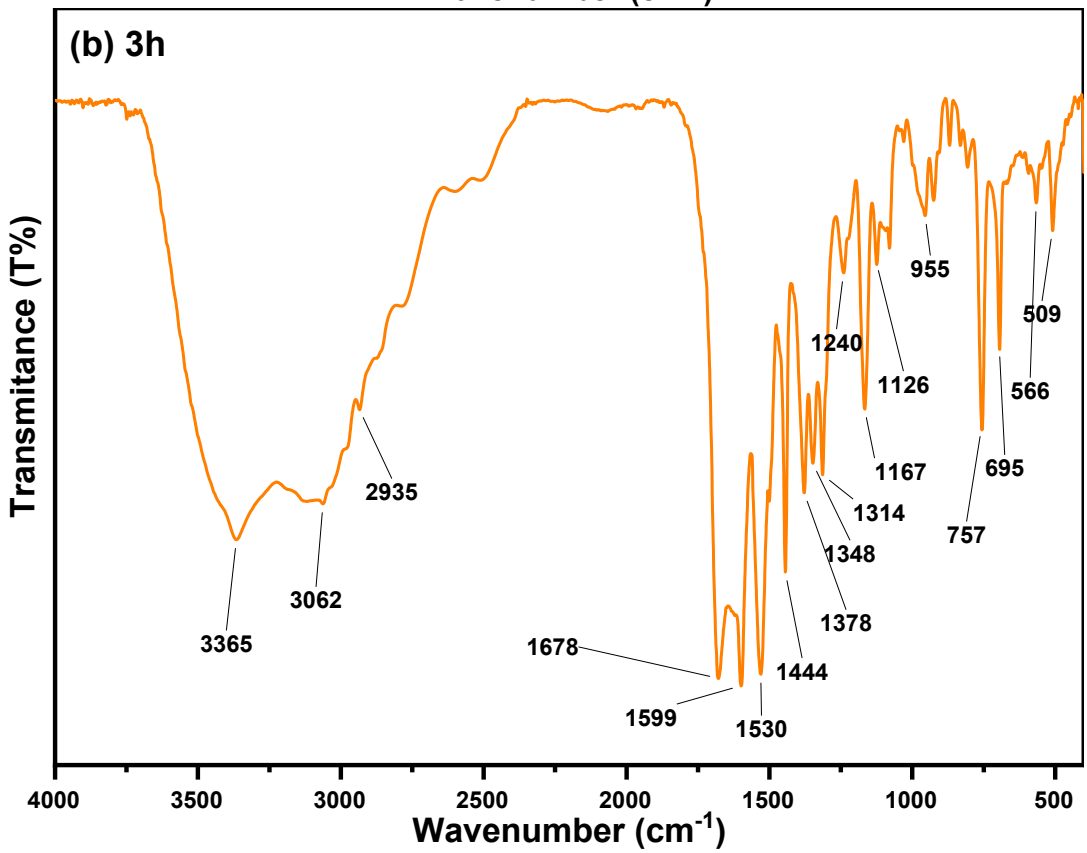
3. **Fig. S3** ^{13}C-NMR spectra of (a) 4AA, (b) 3h, (c) 6 h, (d) 9h, (e) 12h, (f) 15h, (g) 18h, and (h) 21h NCDs.

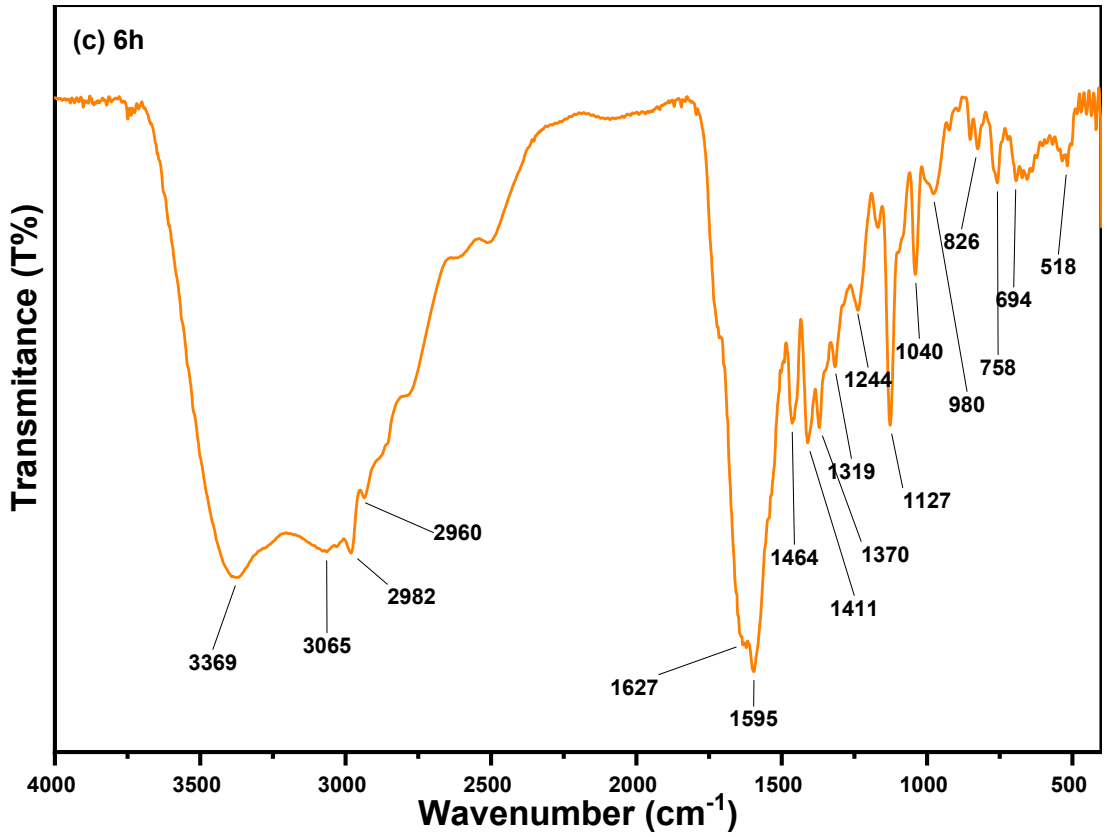
4. **Fig. S4** ^{1}H-NMR spectra of (a) 4AA, (b) 3h, (c) 6 h, (d) 9h, (e) 12h, (f) 15h, (g) 18h, and (h) 21h NCDs.

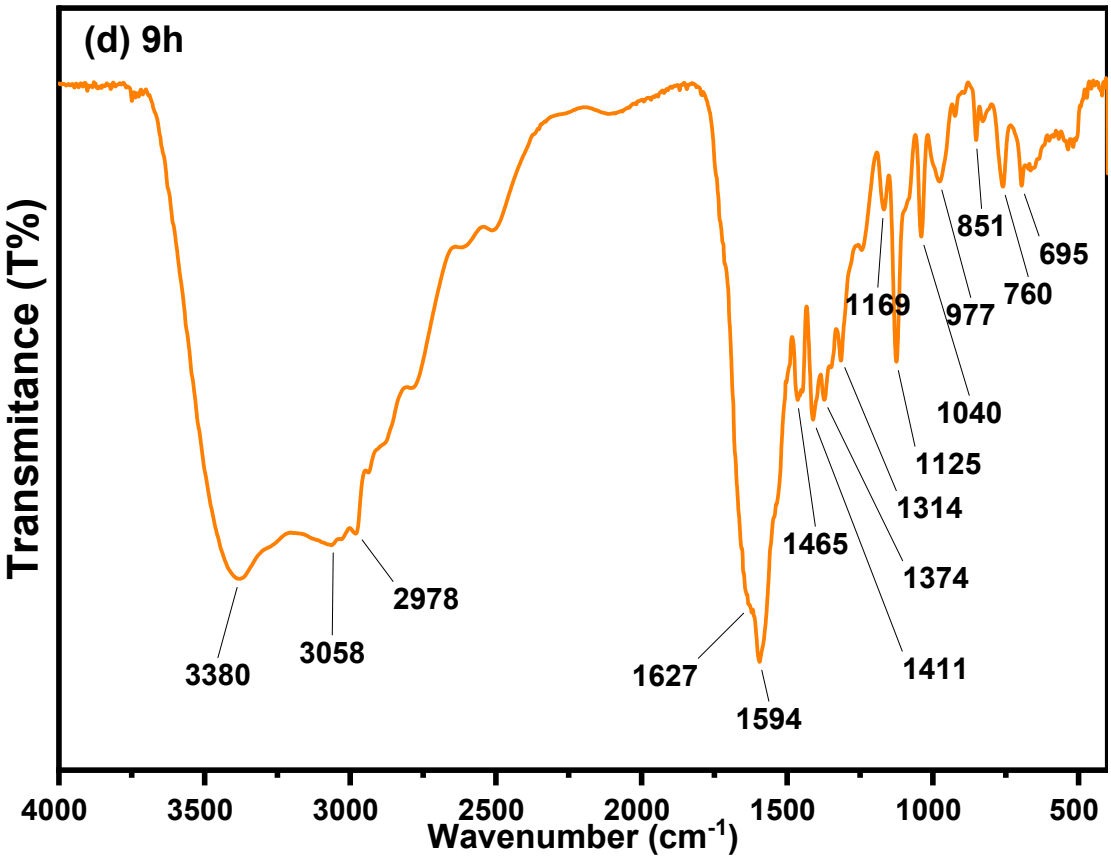
5. **Fig. S5** The UV-vis absorption (black line), PL emission (red line), and Photoluminescence excitation (PLE) (blue line) spectra of the NCDs in deionized water at various times, including (a) 3, (b) 6, (c) 9, (d) 12, (e) 15, (f) 18, and (g) 21 hours. A photo was taken using an iPhone X (2019).

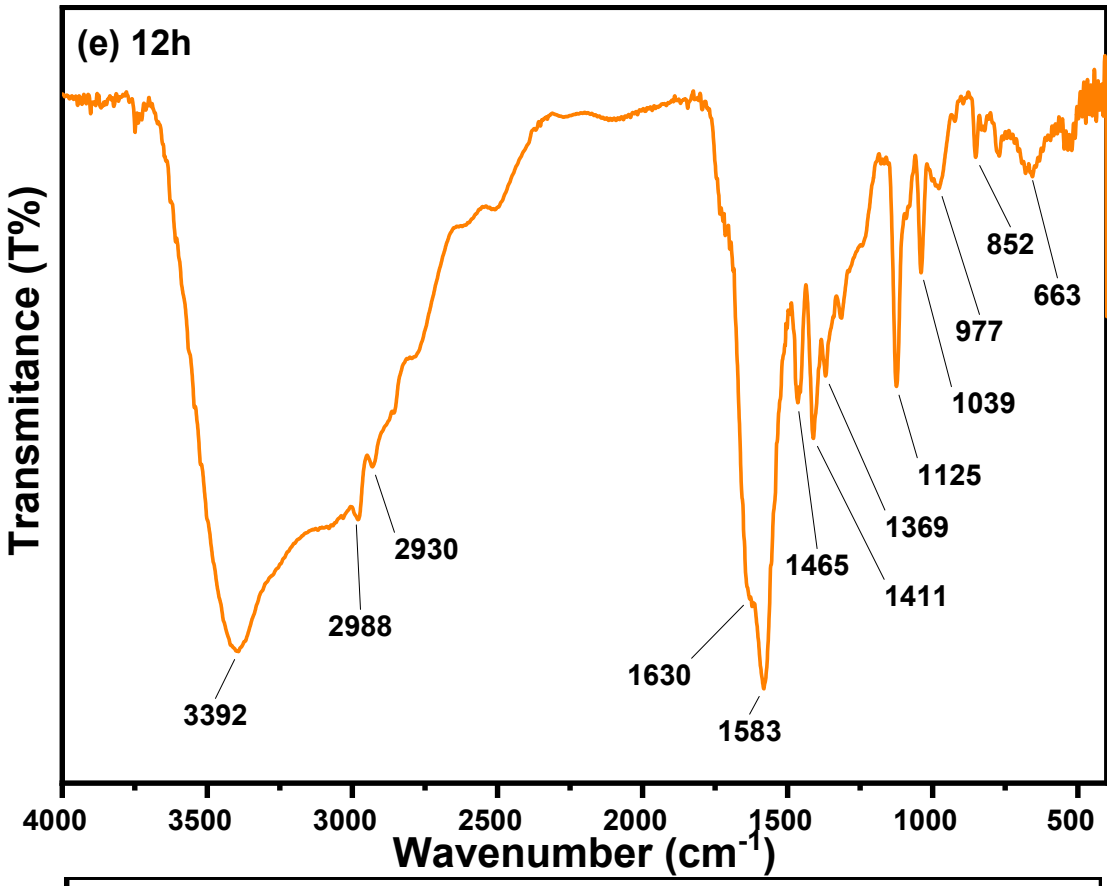
6. **Fig. S6** PL emission spectra of NCDs at different excitation wavelengths changing from 340-400 nm for (a) 3 h, (b) 6 h, (c) 9 h, (d) 12 h, (e) 15 h, (f) 18 h, and (g) 21 h.

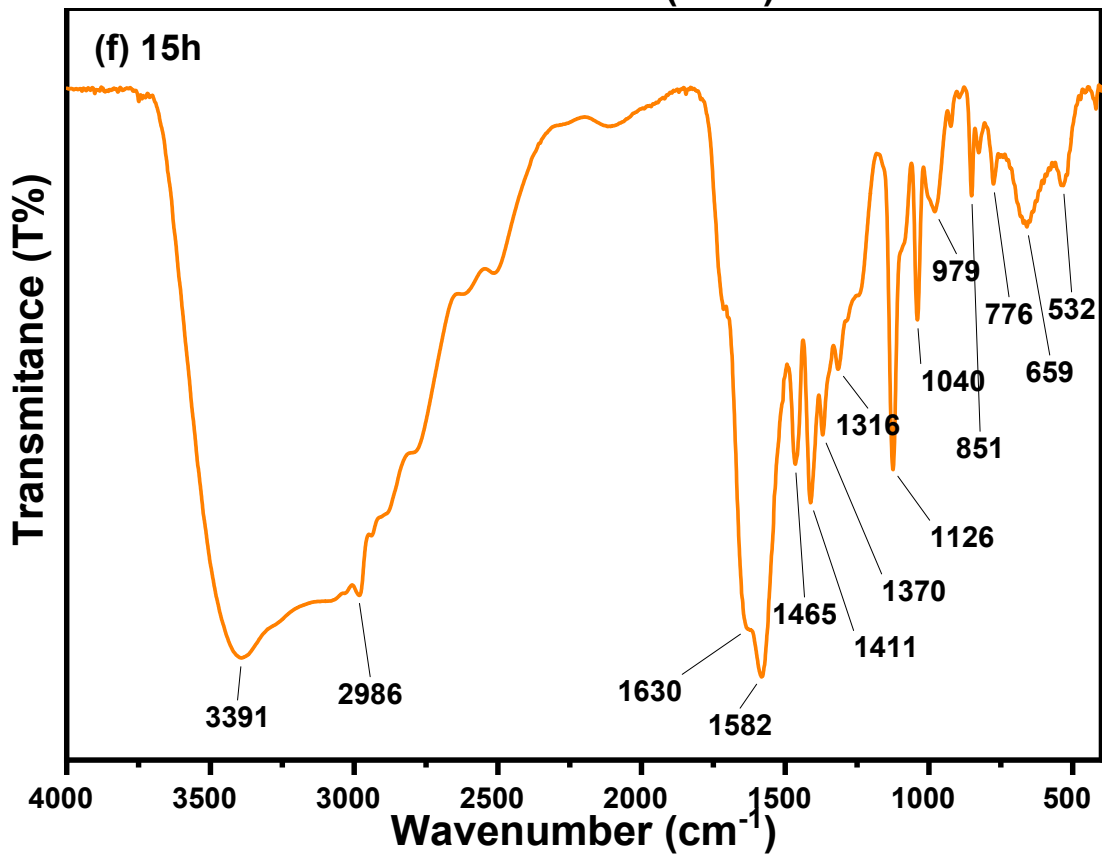

(a) 4AA
Transmitance (T%)
Wavenumber (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
3432
3327
3181
3068
3041
3018
2989
2914
1679
1650
1590
1498
1456
1353
1311
1274
1230
1191
1161
1119
1072
1041
983
927
837
759
701
662
572
501
453


(b) 3h
Transmitance (T%)
Wavenumber (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
3365
3062
2935
1678
1599
1530
1444
1378
1348
1314
1240
1167
1126
955
757
695
566
509


(c) 6h
Transmitance (T%)
Wavenumber (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
3369
3065
2982
2960
1627
1595
1464
1411
1370
1319
1244
1127
1040
980
826
758
694
518


(d) 9h
Transmitance (T%)
Wavenumber (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
3380
3058
2978
1627
1594
1465
1411
1374
1314
1125
1040
977
1169
851
760
695


(e) 12h
Transmitance (T%)
3392
2988
2930
1630
1583
1465
1411
1369
1125
1039
977
852
663
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)


(f) 15h
Transmitance (T%)
3391
2986
1630
1582
1465
1411
1370
1316
1126
1040
979
851
776
659
532
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

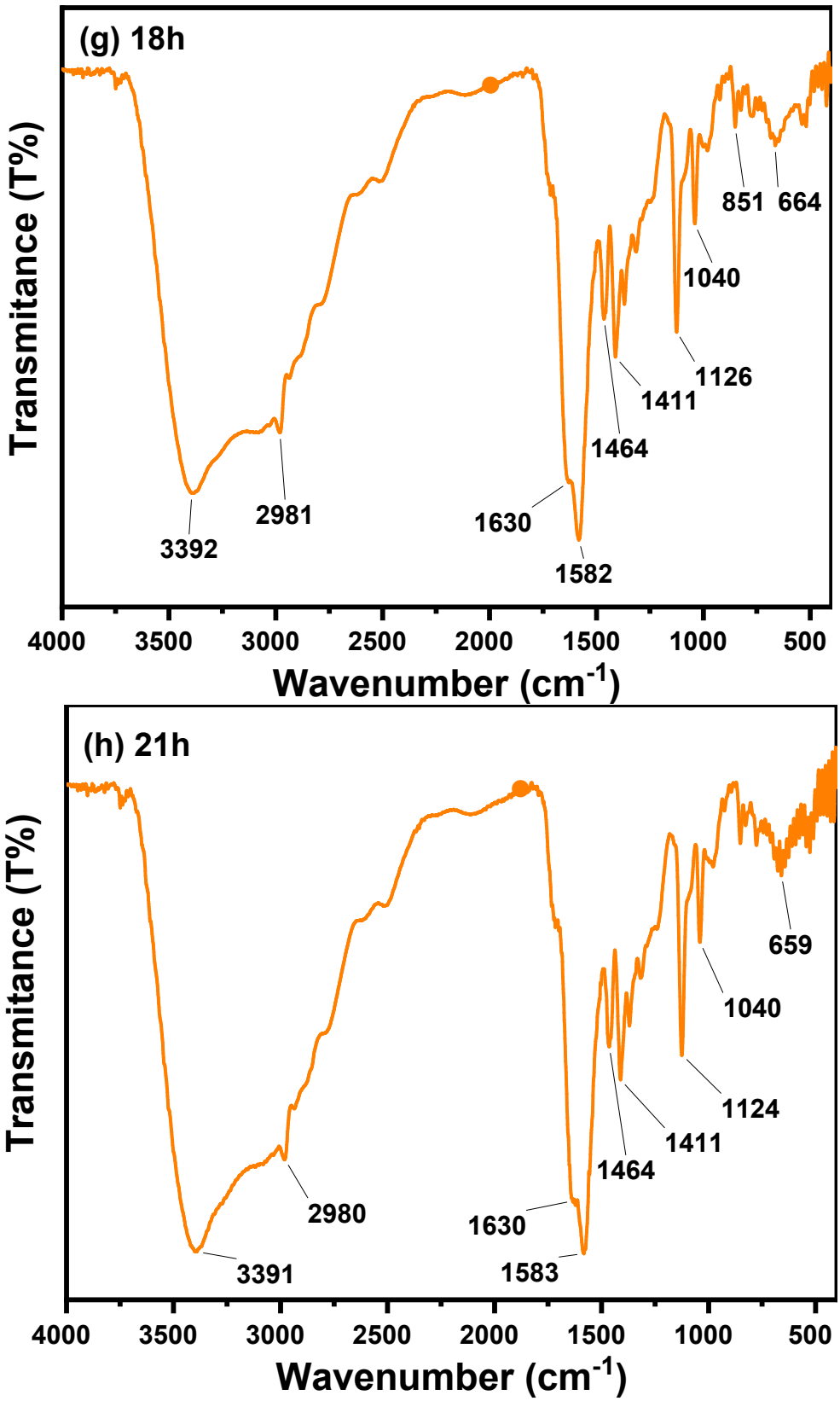
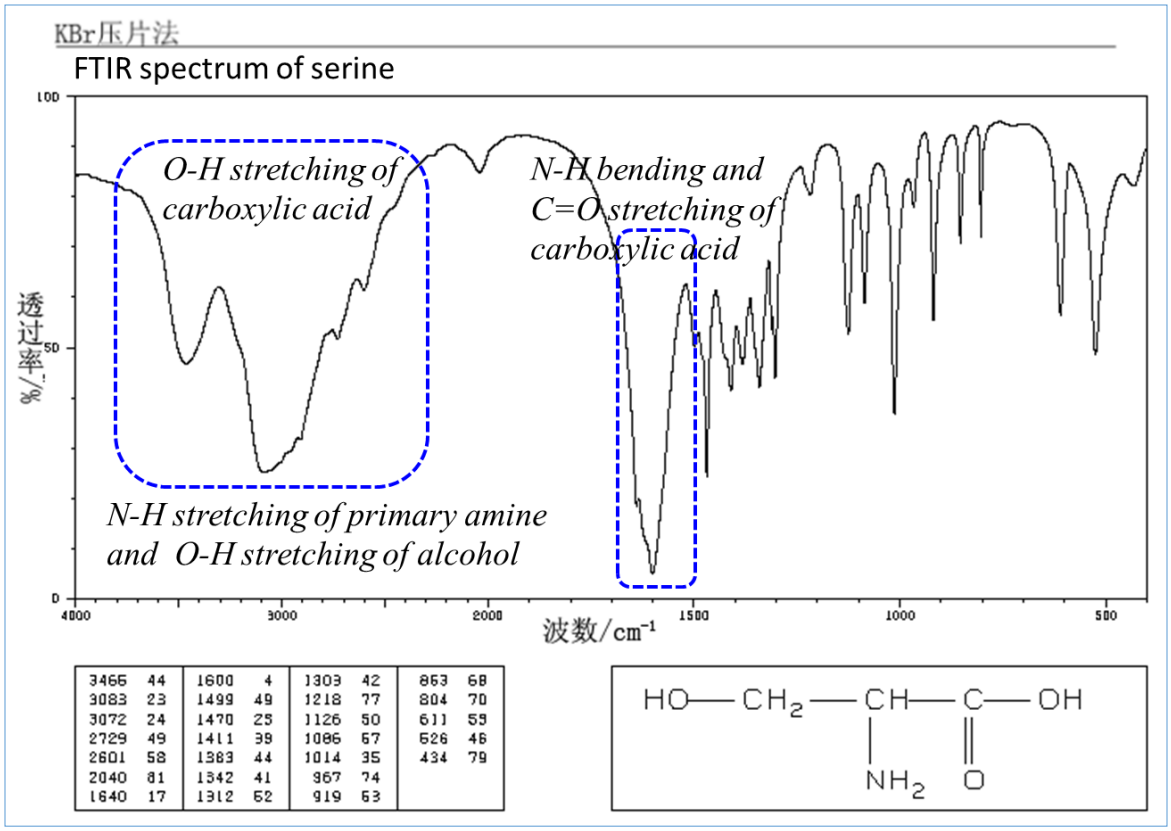


Fig. S1 FT-IR spectra of (a) 4AA, (b) 3h, (c) 6 h, (d) 9h, (e) 12h, (f) 15h, (g) 18h, and (h) 21h NCDs.



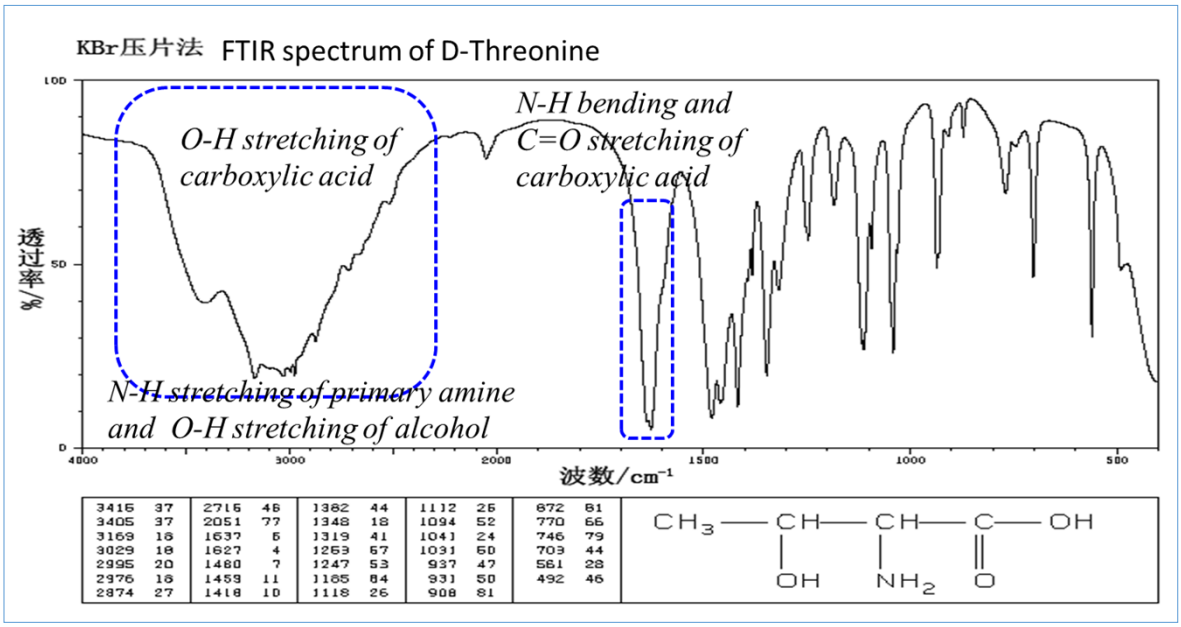
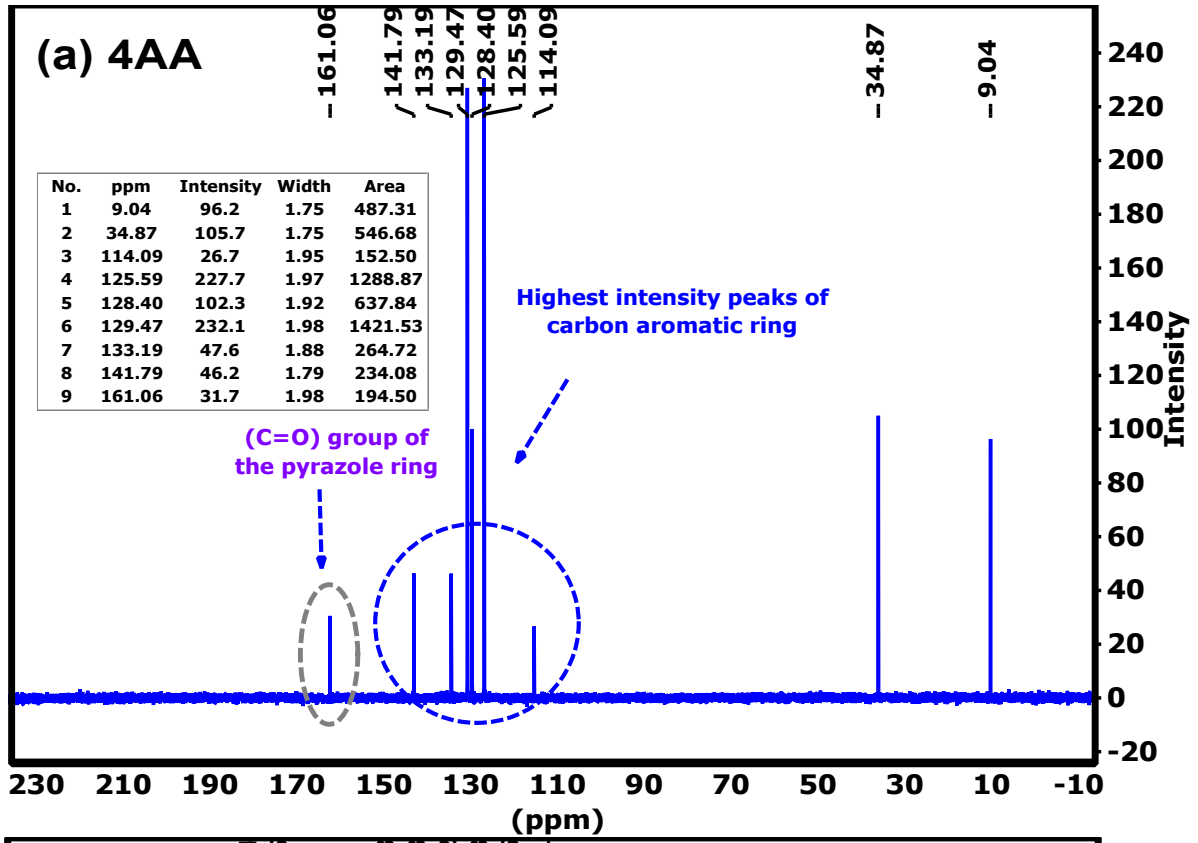
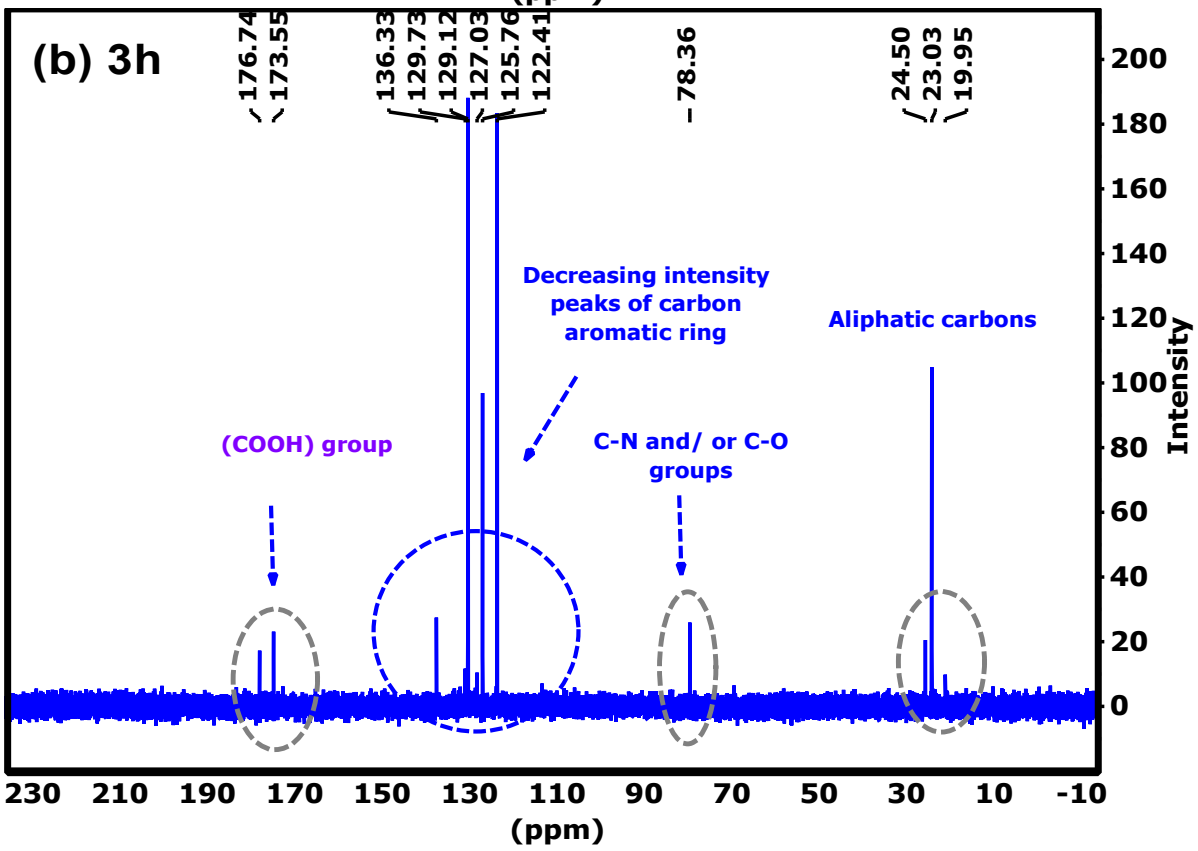
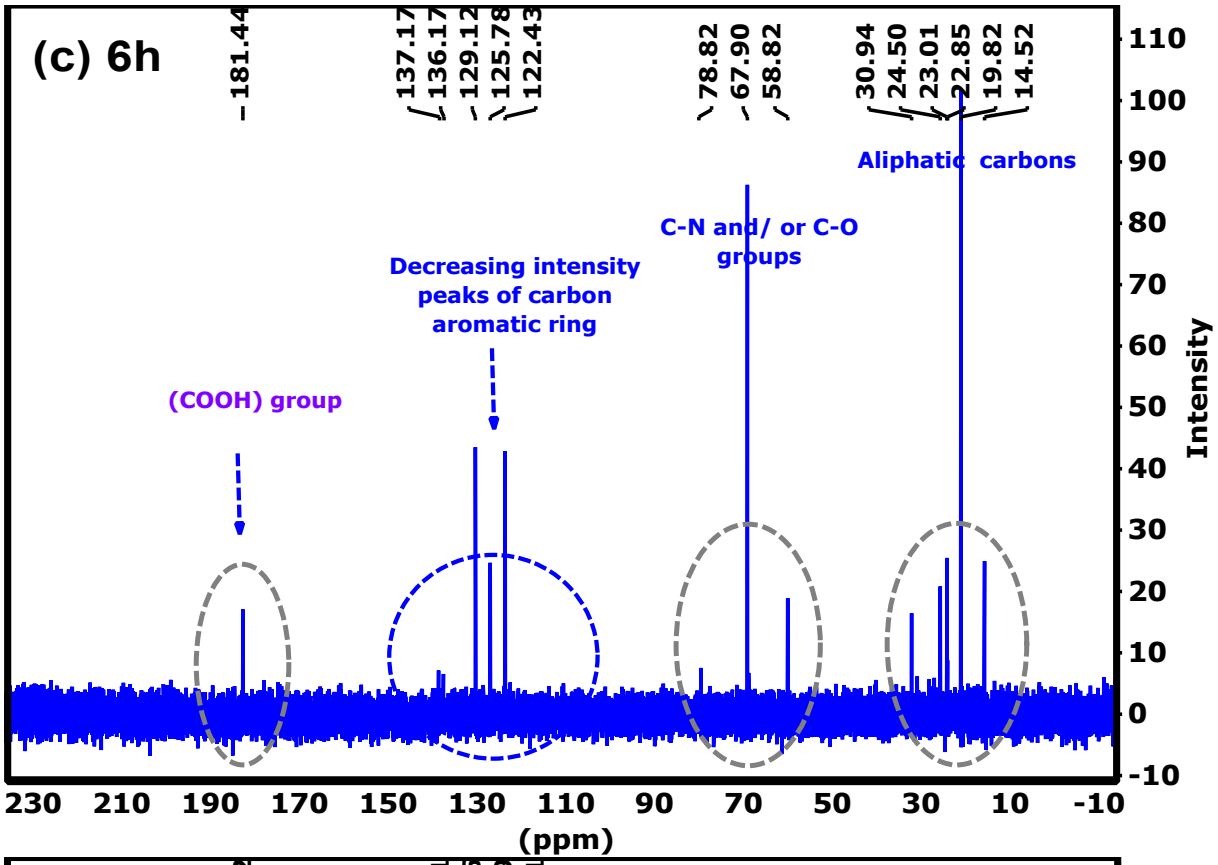
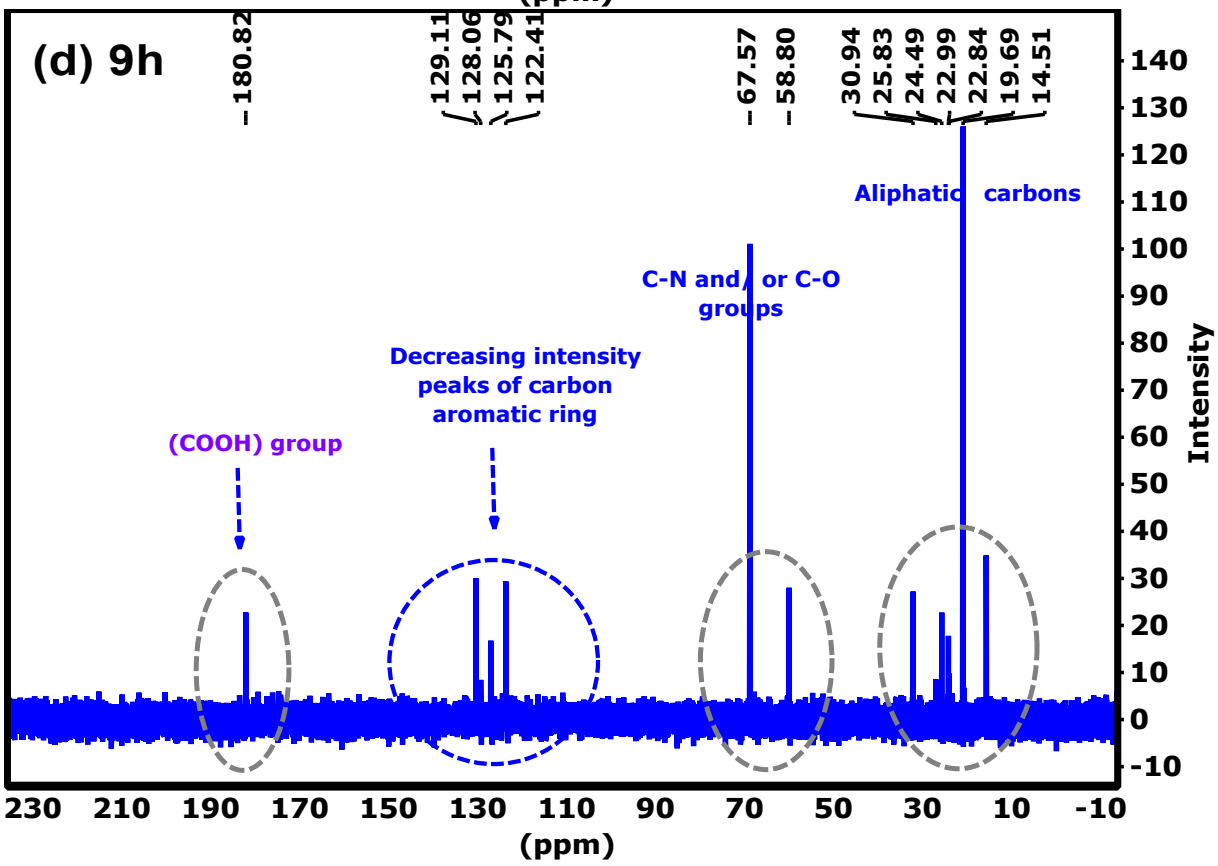


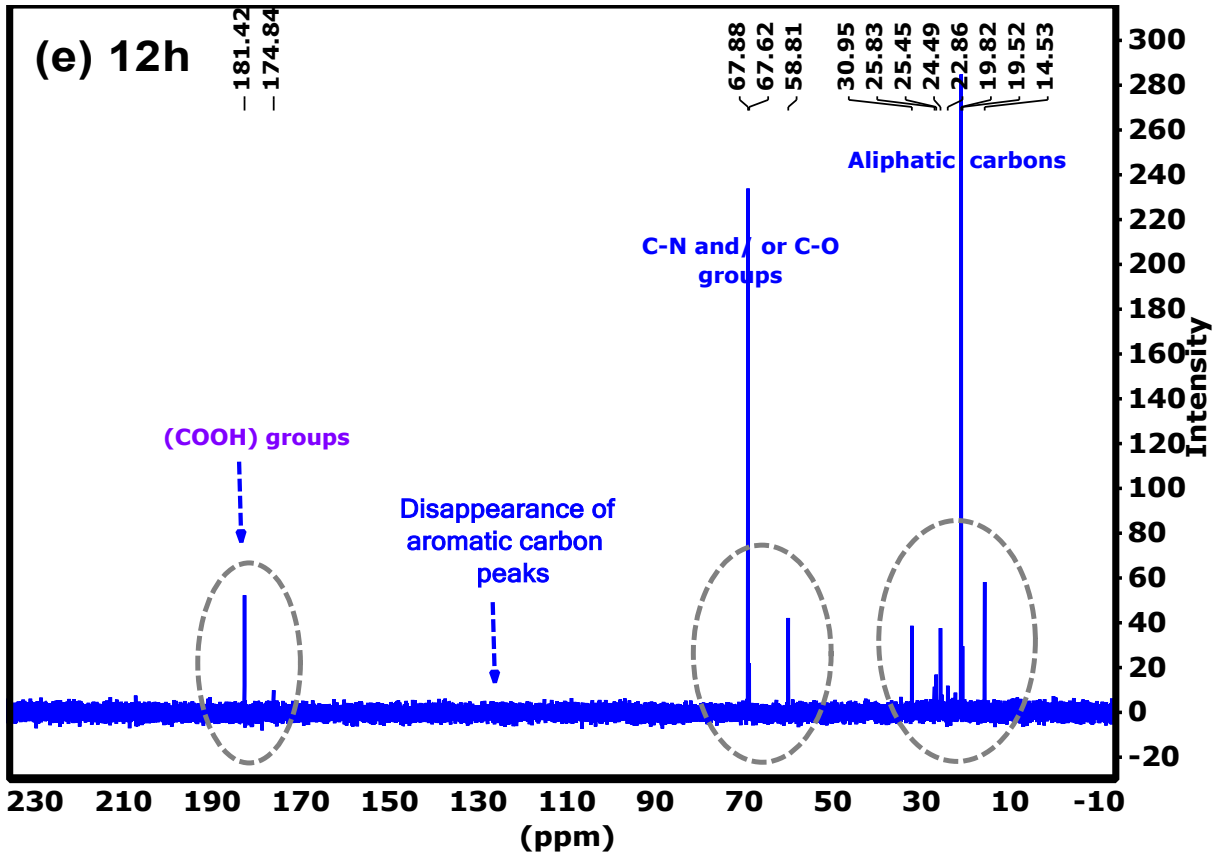
Fig. S2 FT-IR spectra of (a) serine, and (b) d-threonine.

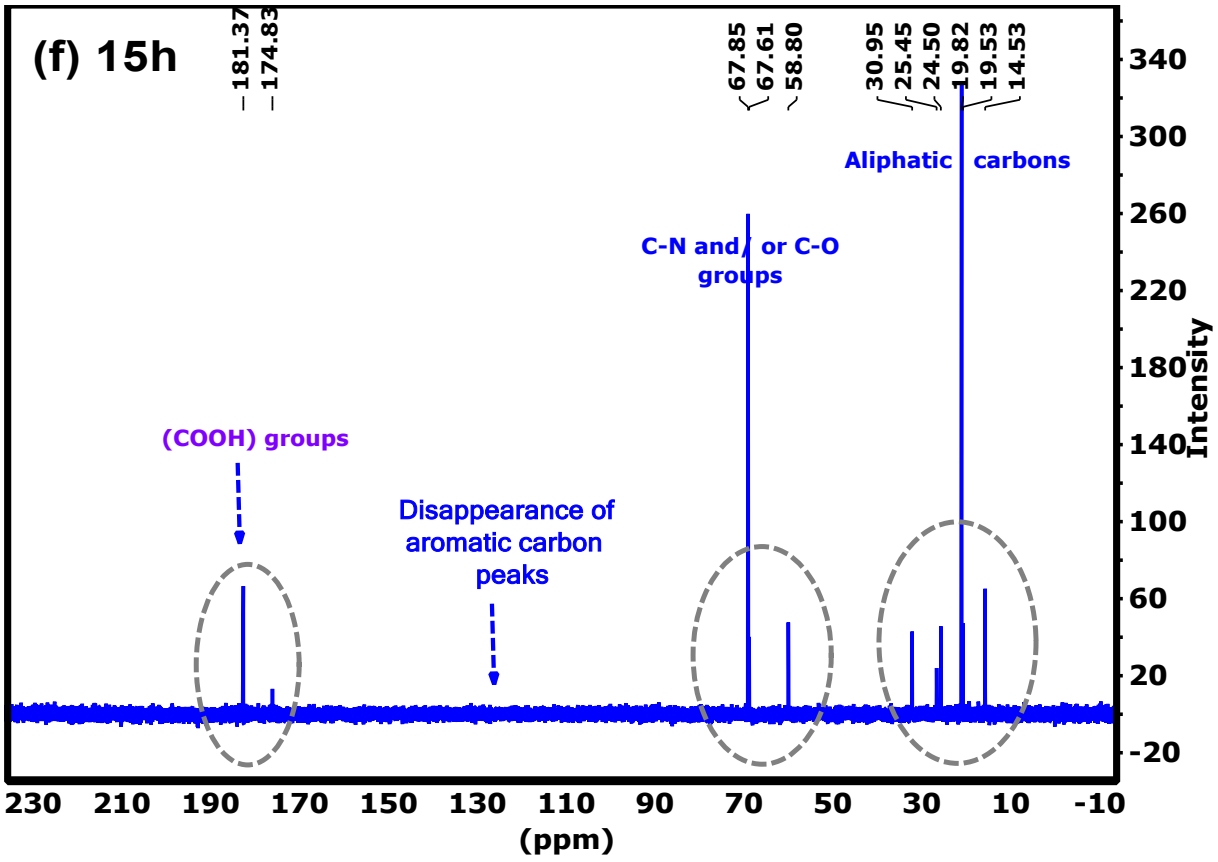

(a) 4AA
161.06
141.79
133.19
129.47
128.40
125.59
114.09
34.87
9.04
No. ppm Intensity Width Area
1 9.04 96.2 1.75 487.31
2 34.87 105.7 1.75 546.68
3 114.09 26.7 1.95 152.50
4 125.59 227.7 1.97 1288.87
5 128.40 102.3 1.92 637.84
6 129.47 232.1 1.98 1421.53
7 133.19 47.6 1.88 264.72
8 141.79 46.2 1.79 234.08
9 161.06 31.7 1.98 194.50
Highest intensity peaks of carbon aromatic ring
(C=O) group of the pyrazole ring
Intensity
(ppm)


(b) 3h
176.74
173.55
136.33
129.73
129.12
127.03
125.76
122.41
78.36
24.50
23.03
19.95
Decreasing intensity peaks of carbon aromatic ring
Aliphatic carbons
(COOH) group
C-N and/ or C-O groups
Intensity
(ppm)


(c) 6h
181.44
137.17
136.17
129.12
125.78
122.43
78.82
67.90
58.82
30.94
24.50
23.01
22.85
19.82
14.52
Aliphatic carbons
C-N and/ or C-O groups
Decreasing intensity peaks of carbon aromatic ring
(COOH) group
Intensity
(ppm)


(d) 9h
180.82
129.11
128.06
125.79
122.41
67.57
58.80
30.94
25.83
24.49
22.99
22.84
19.69
14.51
Aliphatic carbons
C-N and/ or C-O groups
Decreasing intensity peaks of carbon aromatic ring
(COOH) group
Intensity
(ppm)


(e) 12h
181.42
174.84
67.88
67.62
58.81
30.95
25.83
25.45
24.49
22.86
19.82
19.52
14.53
Aliphatic carbons
C-N and/ or C-O groups
(COOH) groups
Disappearance of aromatic carbon peaks
Intensity
(ppm)


(f) 15h
181.37
174.83
67.85
67.61
58.80
30.95
25.45
24.50
19.82
19.53
14.53
Aliphatic carbons
C-N and/ or C-O groups
(COOH) groups
Disappearance of aromatic carbon peaks
Intensity
(ppm)

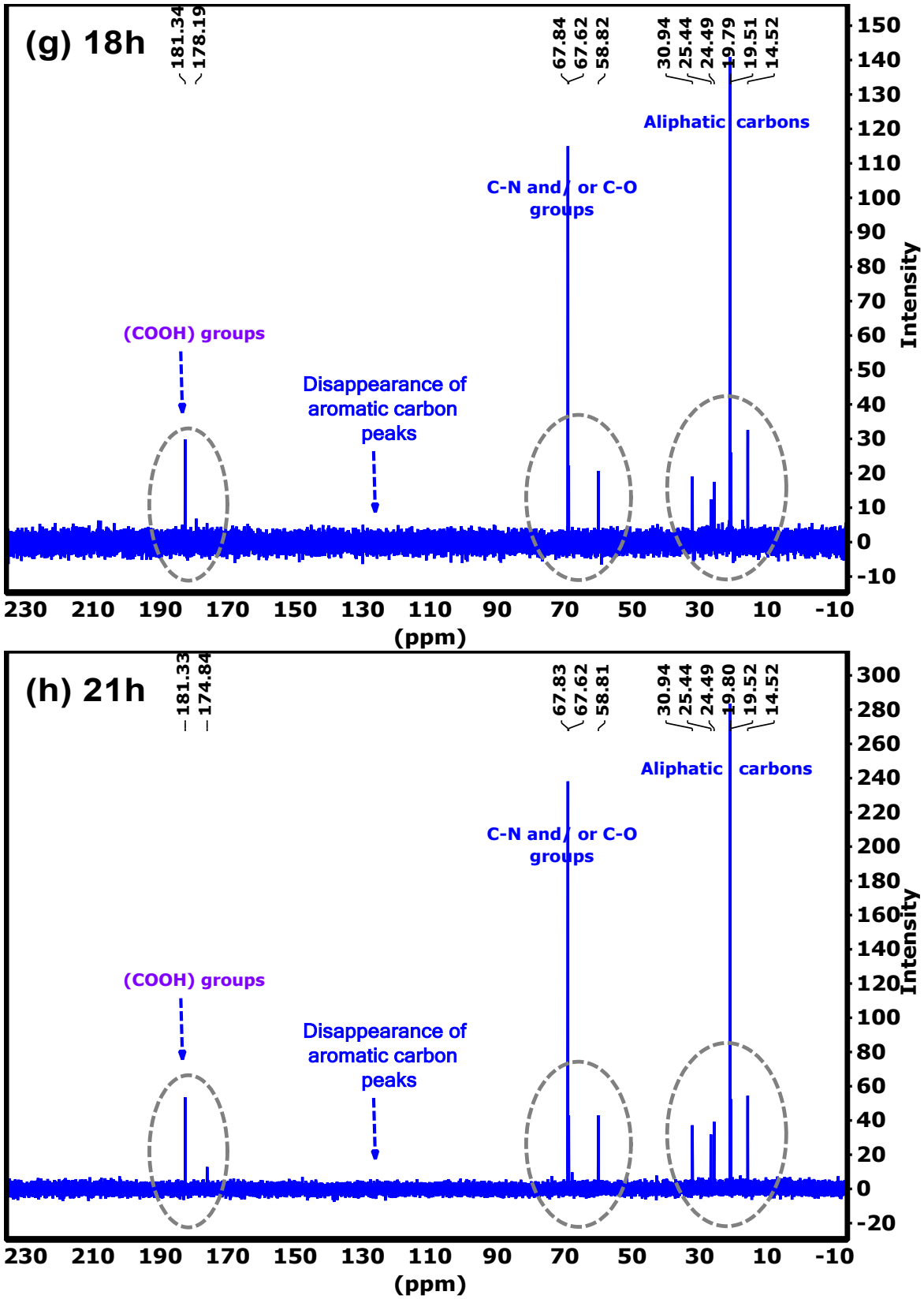
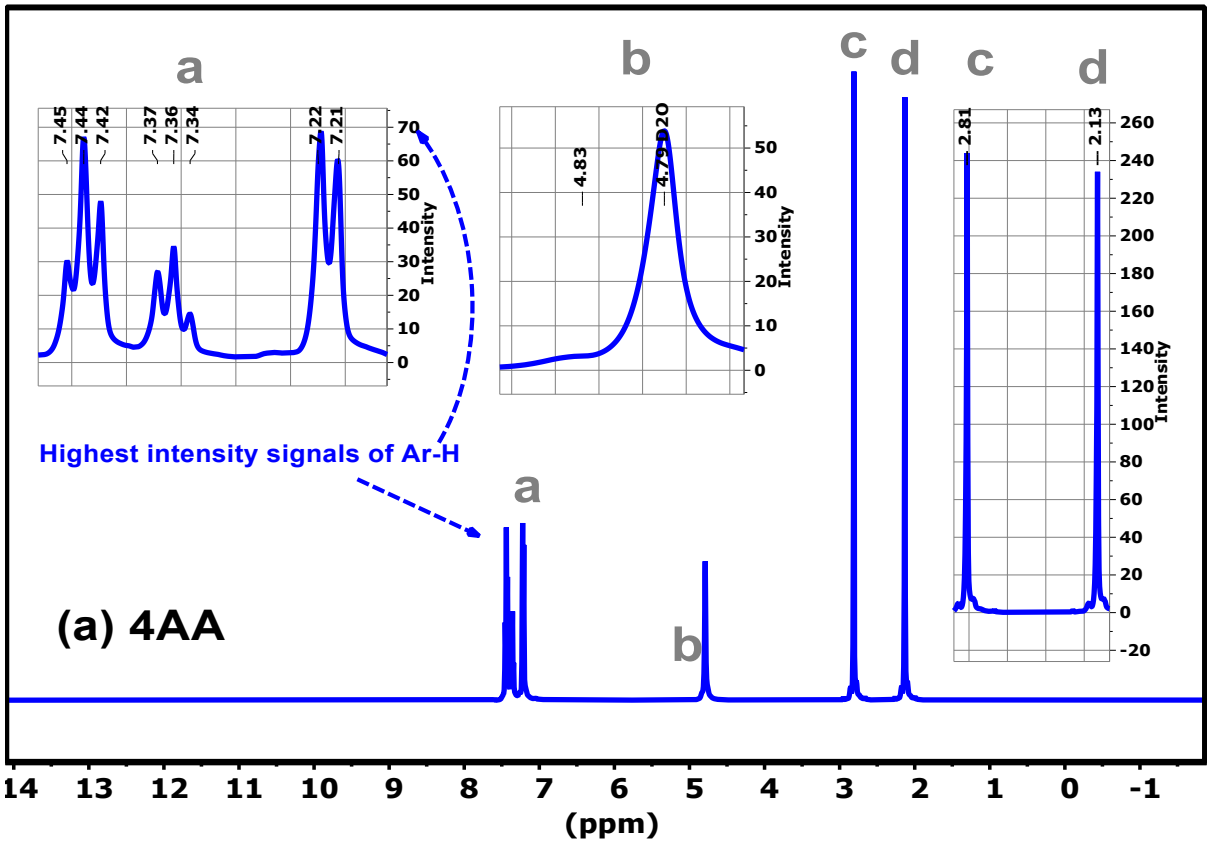
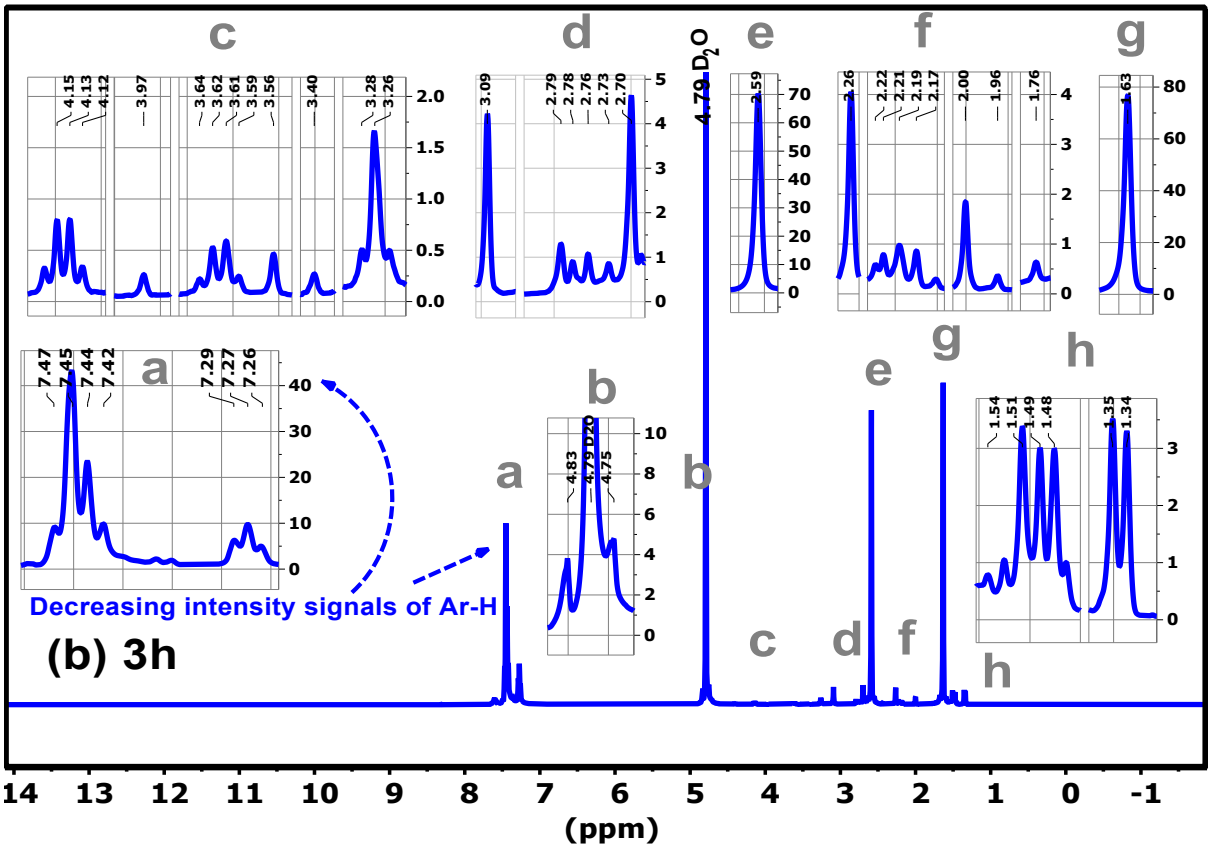
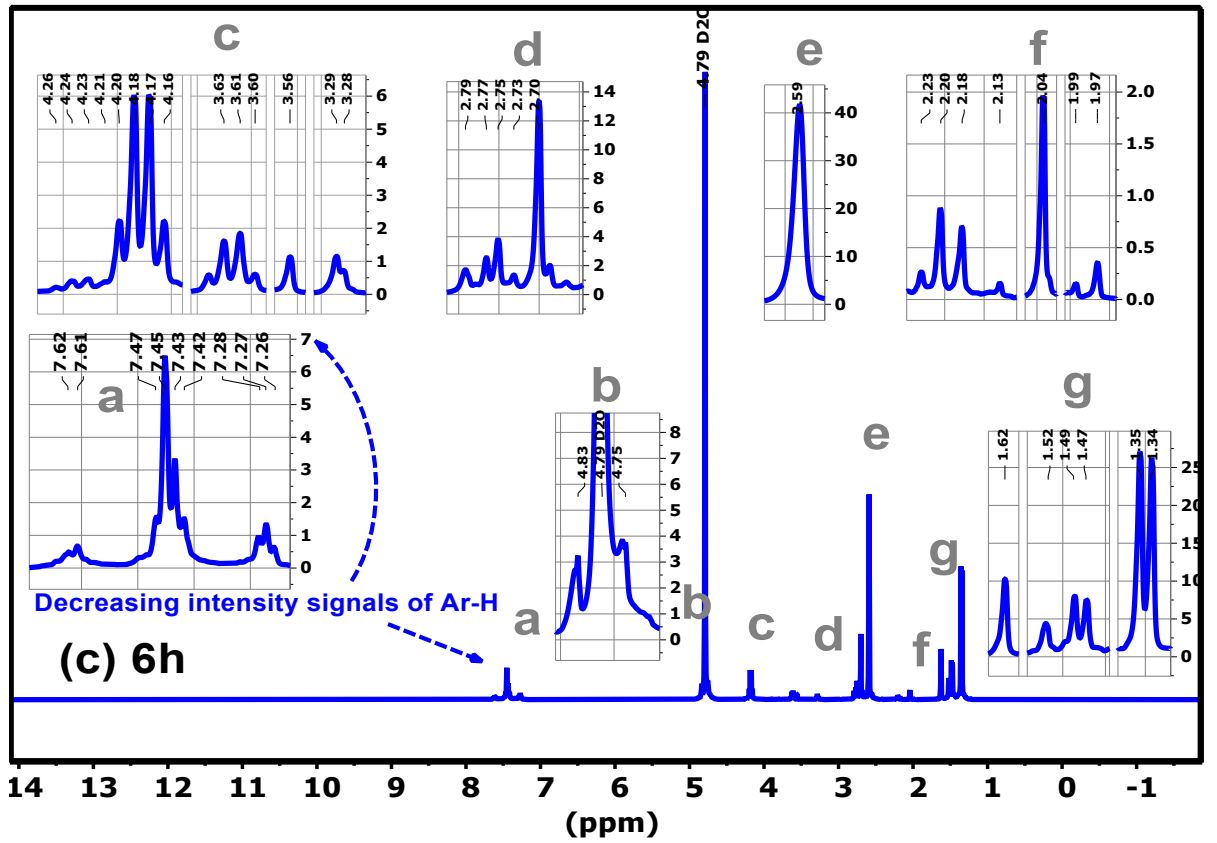
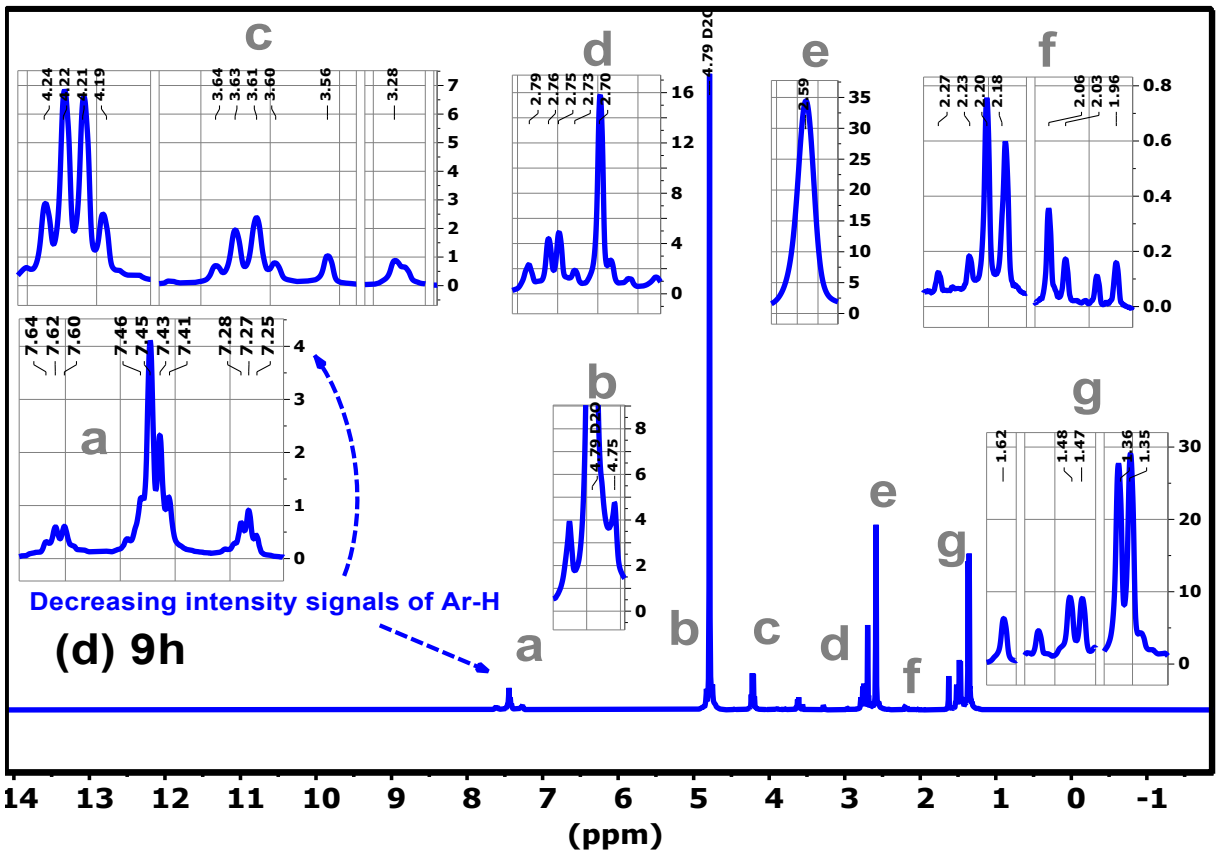


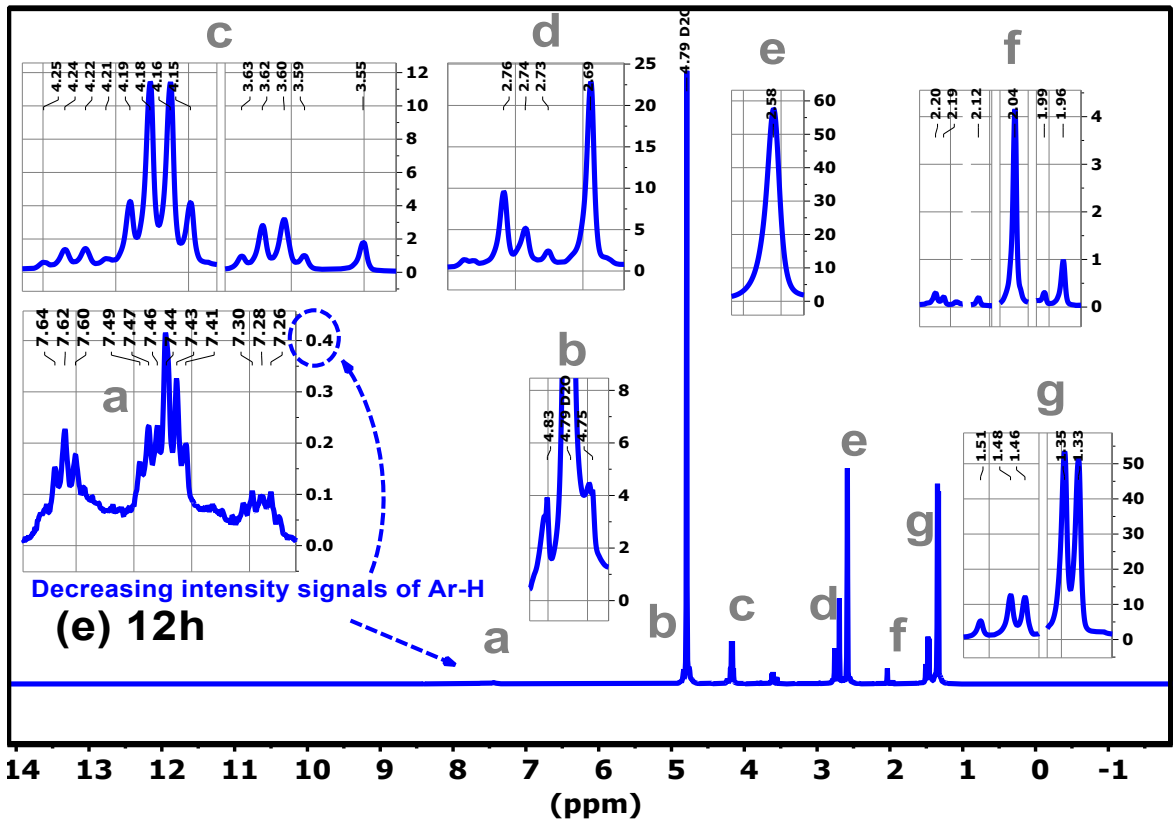
Fig. S3 ^{13}C-NMR spectra of (a) 4AA, (b) 3h, (c) 6 h, (d) 9h, (e) 12h, (f) 15h, (g) 18h, and (h) 21h NCDs.

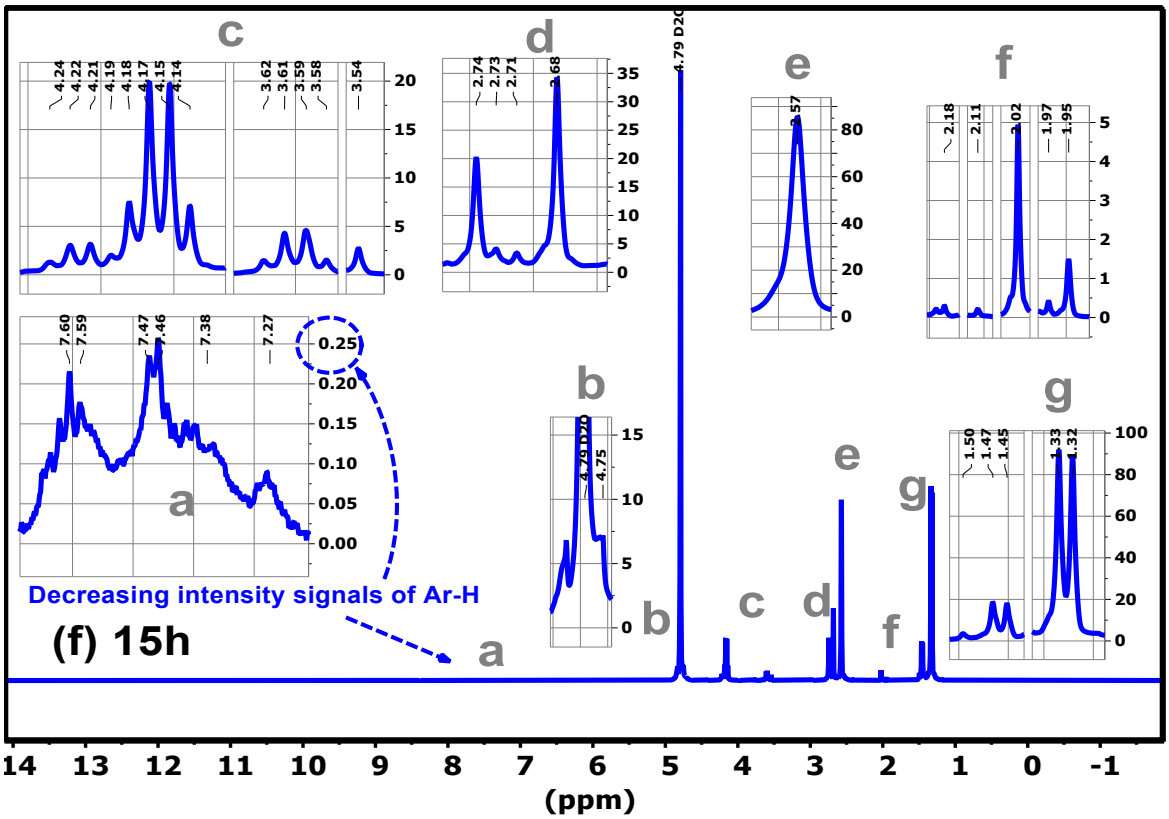

a
b
c
d
c
d
7.45
7.44
7.42
7.37
7.36
7.34
7.22
7.21
4.83
4.79 D2O
2.81
2.13
Intensity
Highest intensity signals of Ar-H
(a) 4AA
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
(ppm)


c
d
e
f
g
h
4.79 D2O
7.47
7.45
7.44
7.42
7.29
7.27
7.26
4.83
4.79 D2O
4.75
Decreasing intensity signals of Ar-H
(b) 3h
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
(ppm)


c
d
e
f
a
b
g
4.79 D2O
Decreasing intensity signals of Ar-H
(c) 6h
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
(ppm)


c
d
e
f
a
b
g
4.79 D2O
Decreasing intensity signals of Ar-H
(d) 9h
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
(ppm)


c
d
e
f
a
b
g
Decreasing intensity signals of Ar-H
(e) 12h
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
(ppm)


c
d
e
f
a
b
g
Decreasing intensity signals of Ar-H
(f) 15h
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
(ppm)

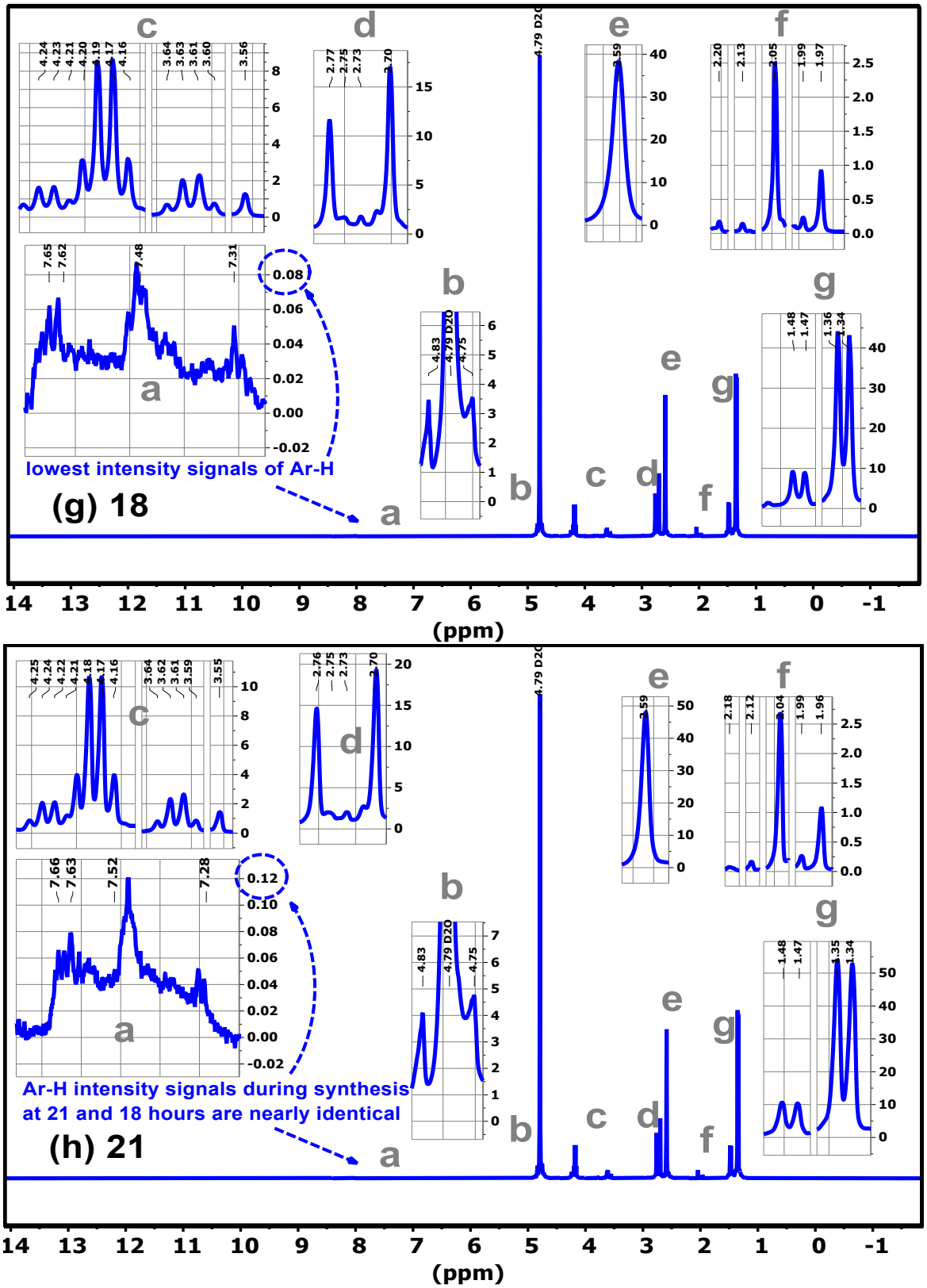


Fig. S4 ^{1}H-NMR spectra of (a) 4AA, (b) 3h, (c) 6 h, (d) 9h, (e) 12h, (f) 15h, (g) 18h, and (h) 21h NCDs.

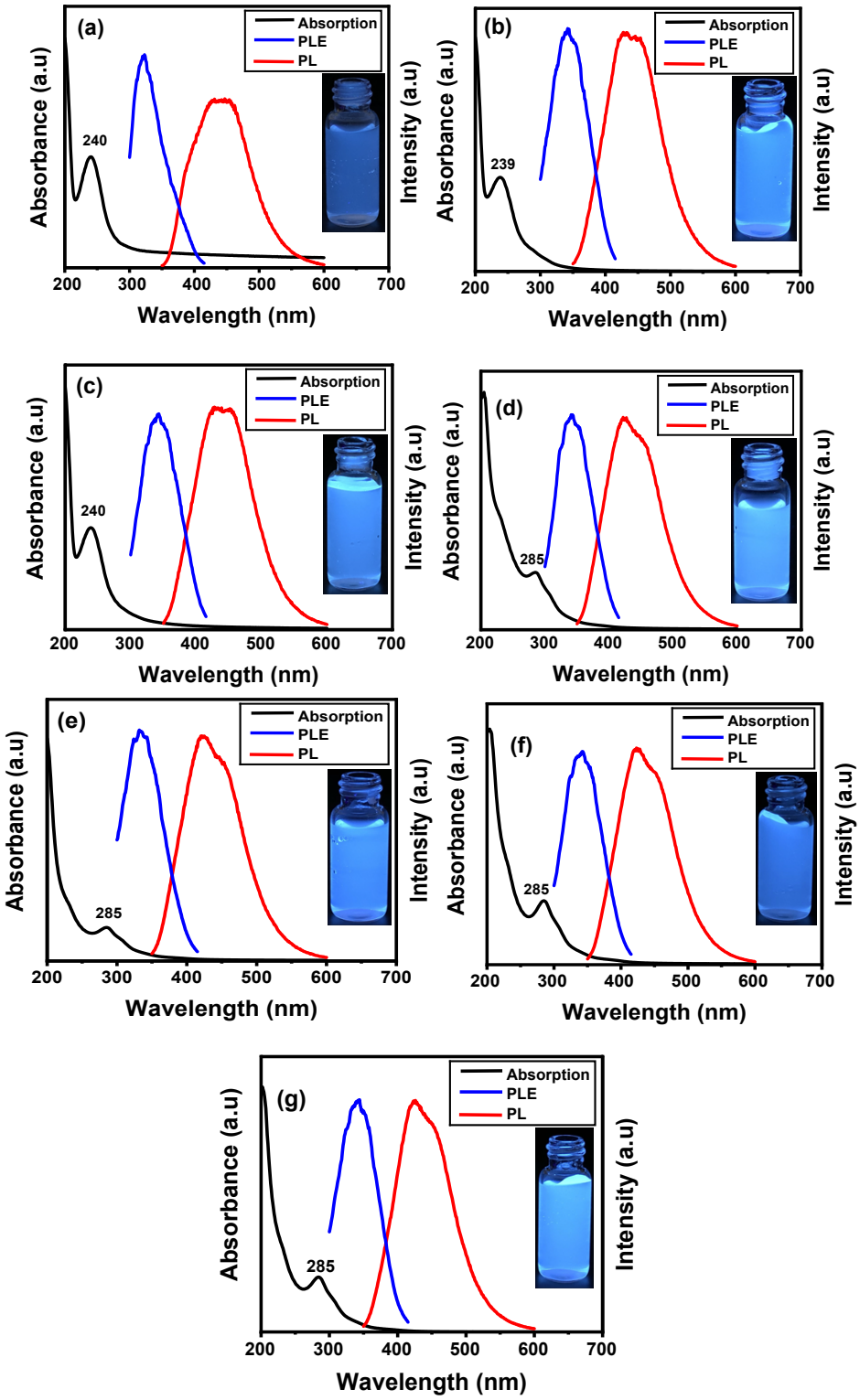


Fig. S5 The UV-vis absorption (black line), PL emission (red line), and Photoluminescence excitation (PLE) (blue line) spectra of the NCDs in deionized water at various times, including (a) 3, (b) 6, (c) 9, (d) 12, (e) 15, (f) 18, and (g) 21 hours. A photo was taken using an iPhone X (2019).

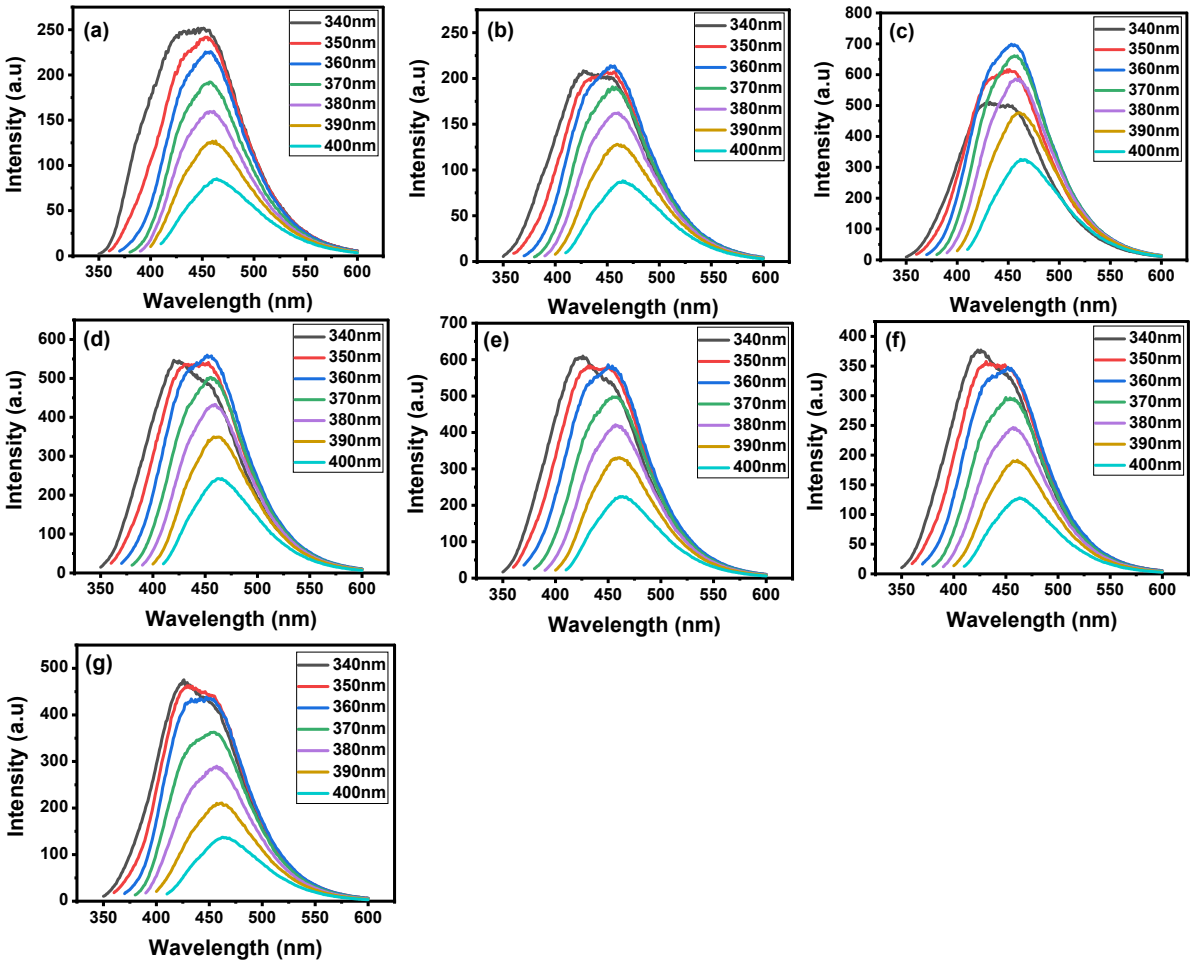


Fig. S6 PL emission spectra of NCDs at different excitation wavelengths changing from 340-400 nm for (a) 3 h, (b) 6 h, (c) 9 h, (d) 12 h, (e) 15 h, (f) 18 h, and (g) 21 h.