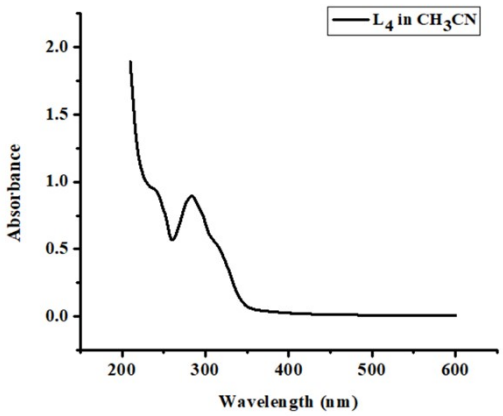
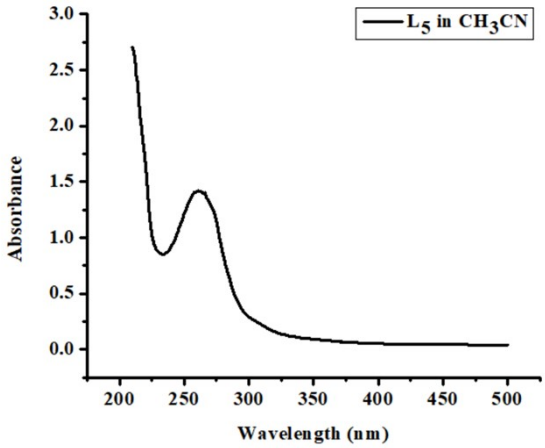
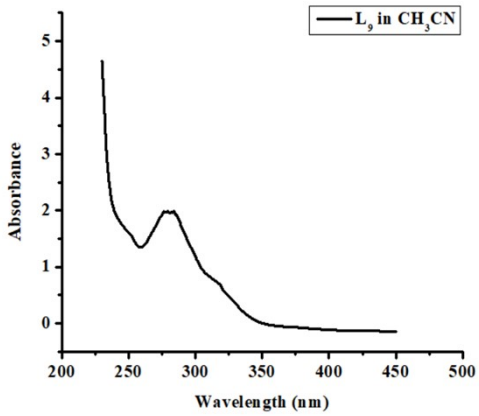
Supplementary Information (SI) for RSC Advances.

Supporting information file for manuscript

Table S1. UV-Vis Spectra of All of the Newly Synthesized Ligands

Compound No.	UV Graphs
L_4	
L_5	
L_9	

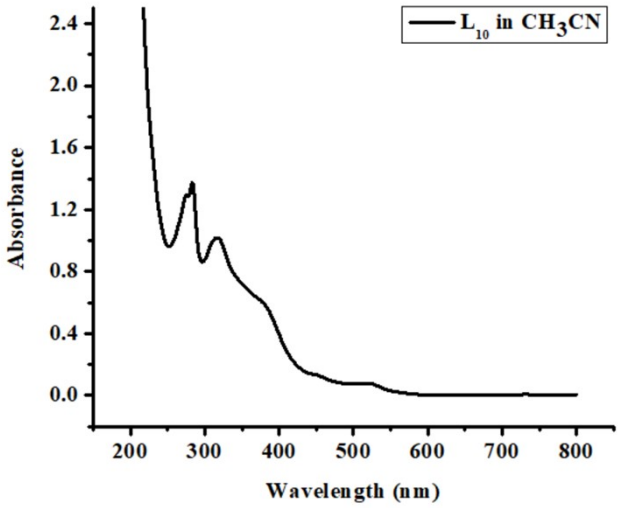
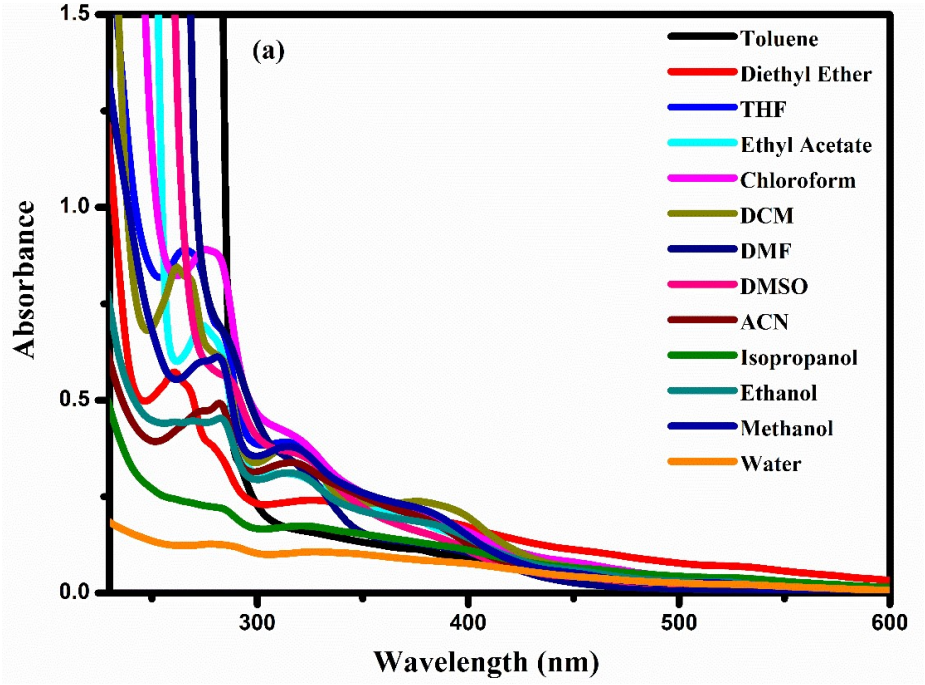
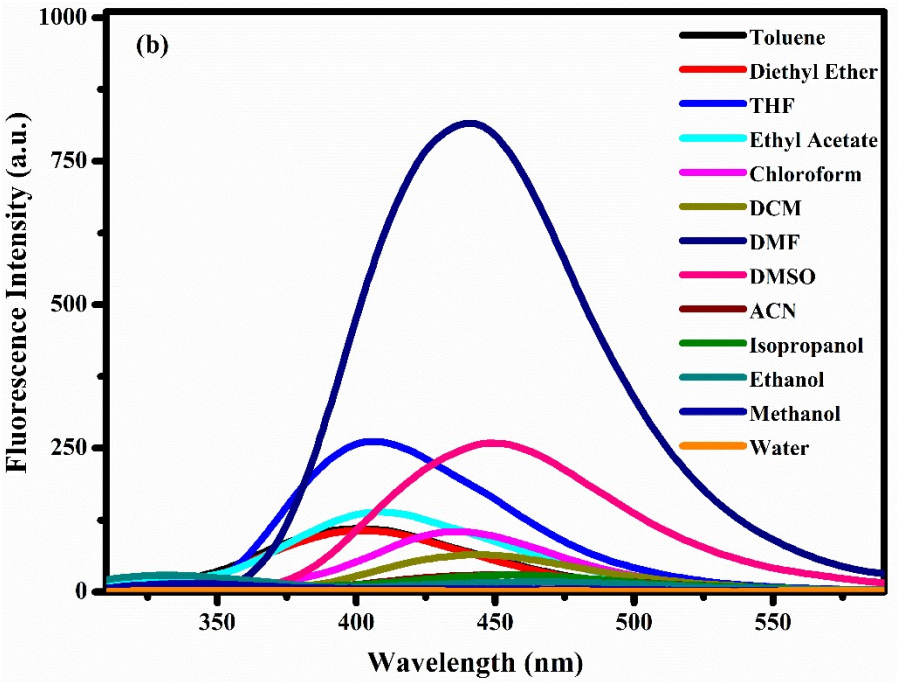
L_{10}	

Figure S1: UV vis. & Fluorescence Spectra of all the Synthesized Terpyridine Complexes (C_1-C_{20})





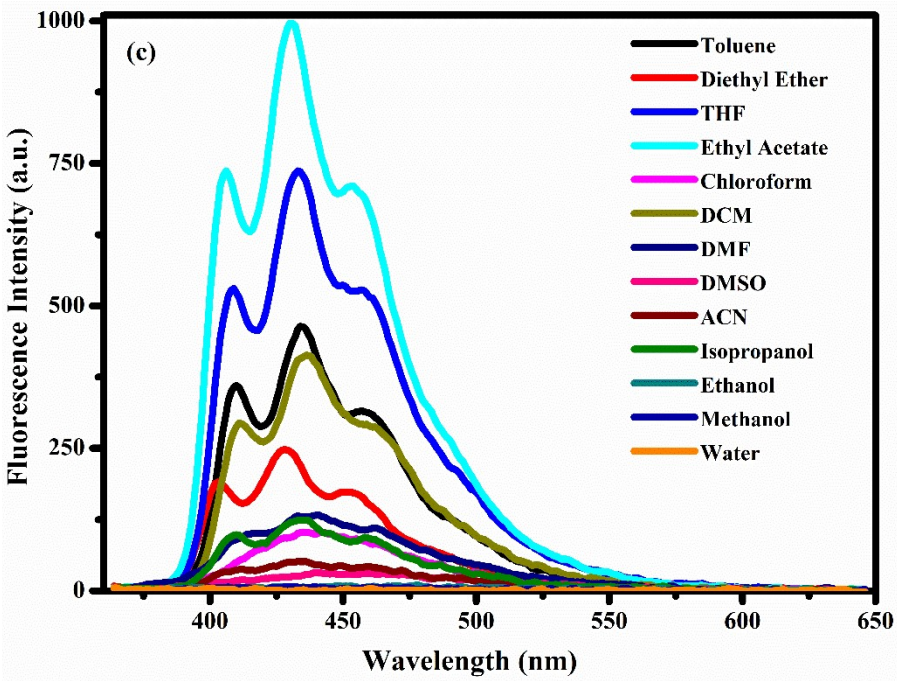
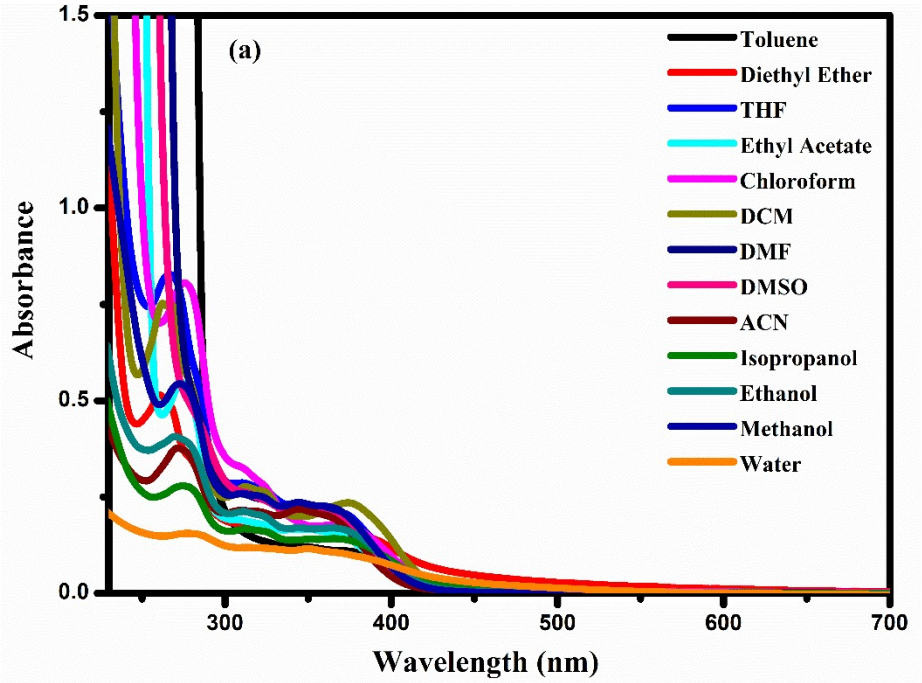
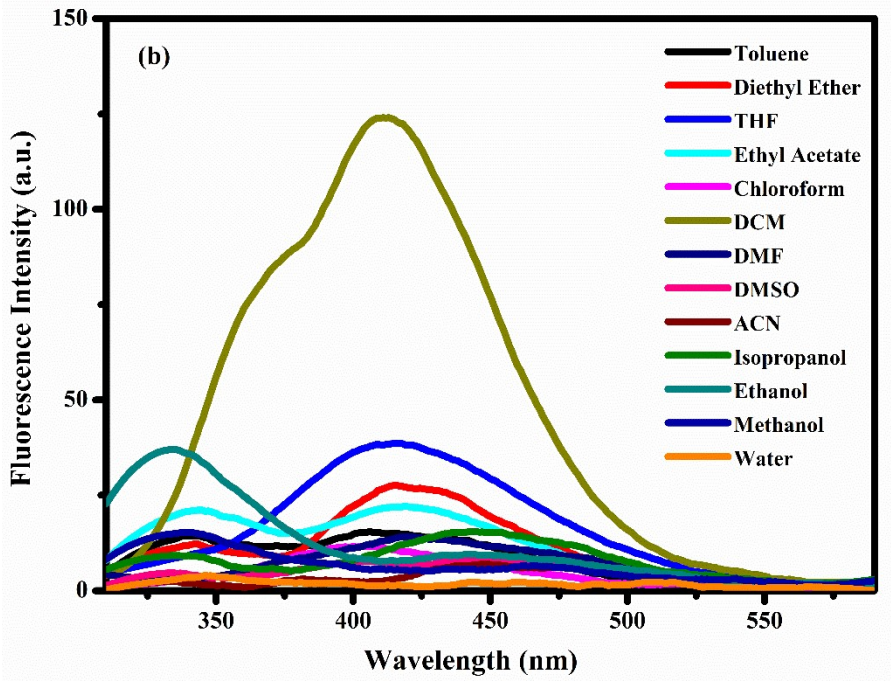


Figure 1. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_1}$ (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
1.5
1.0
0.5
0.0
300
400
500
600
700
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
150
100
50
0
350
400
450
500
550
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

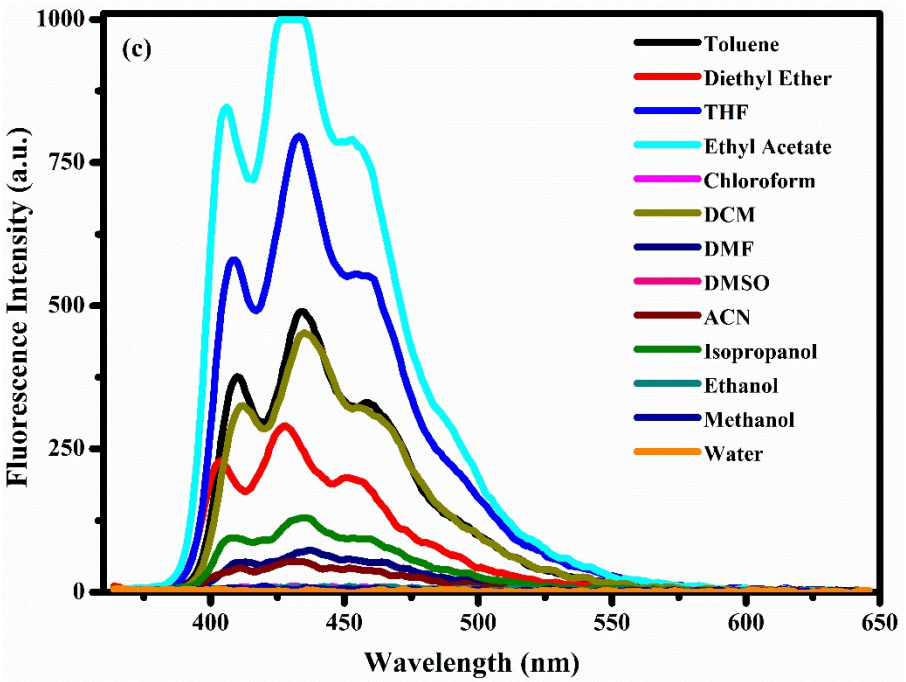
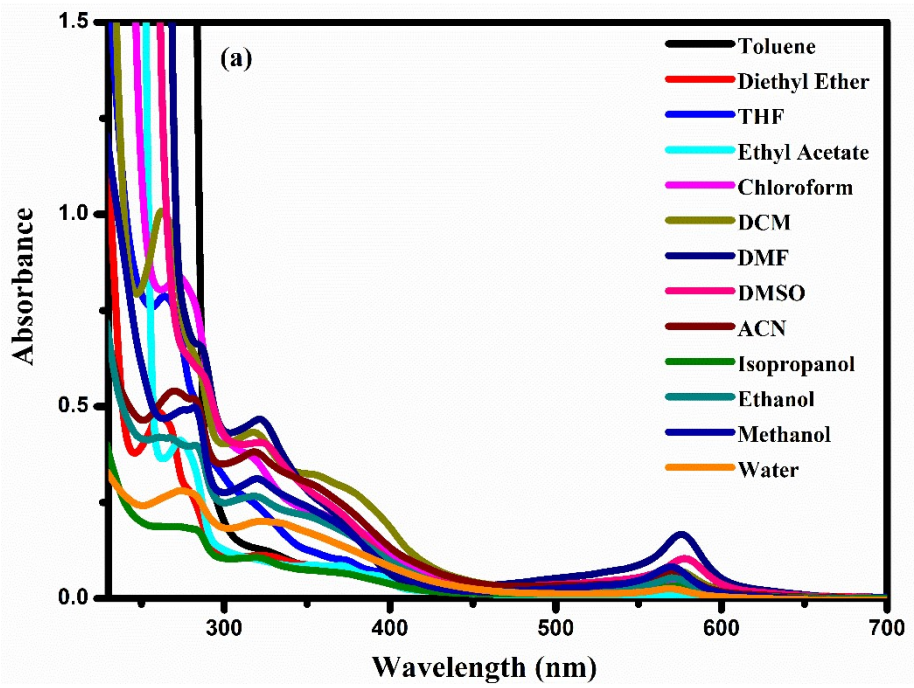
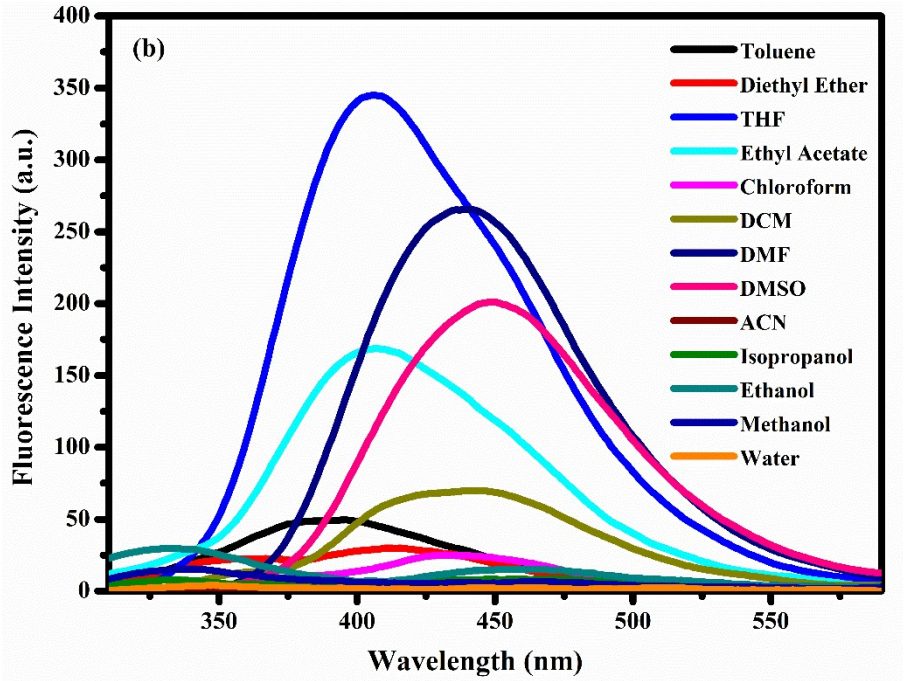


Figure 2. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_2}$ (10 μM) in different solvents





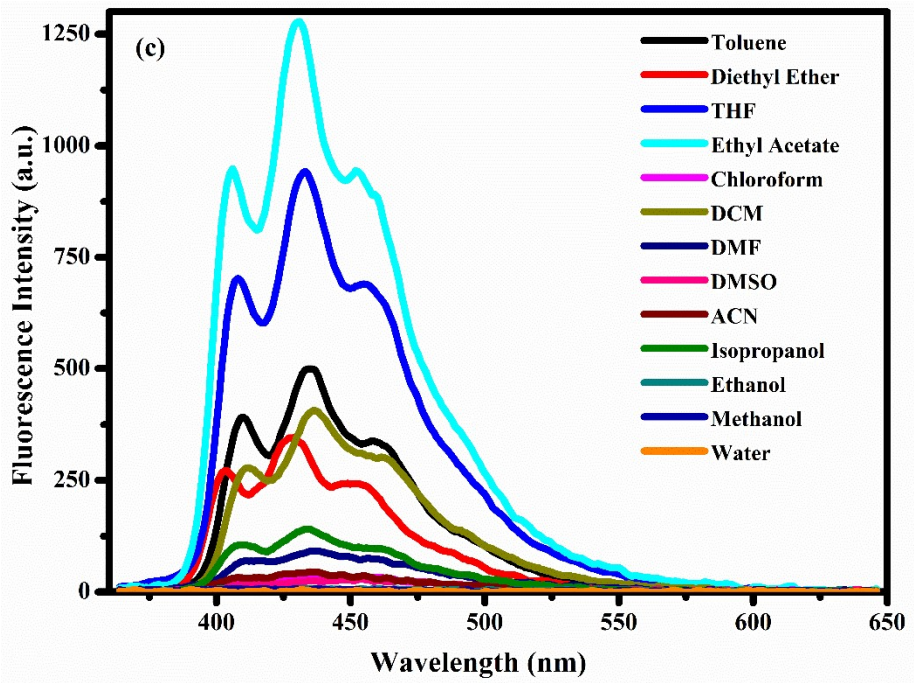
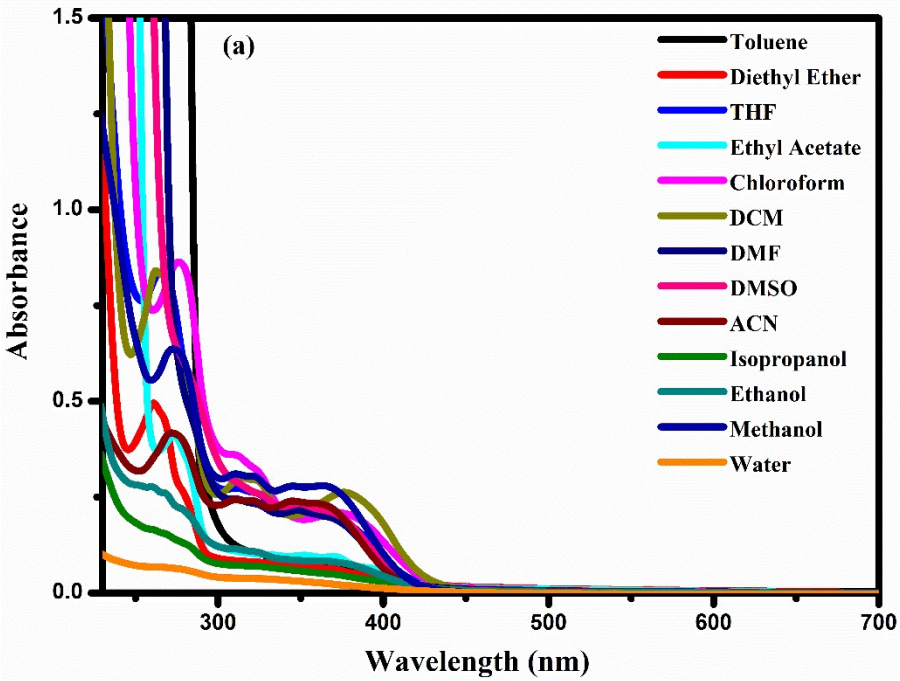
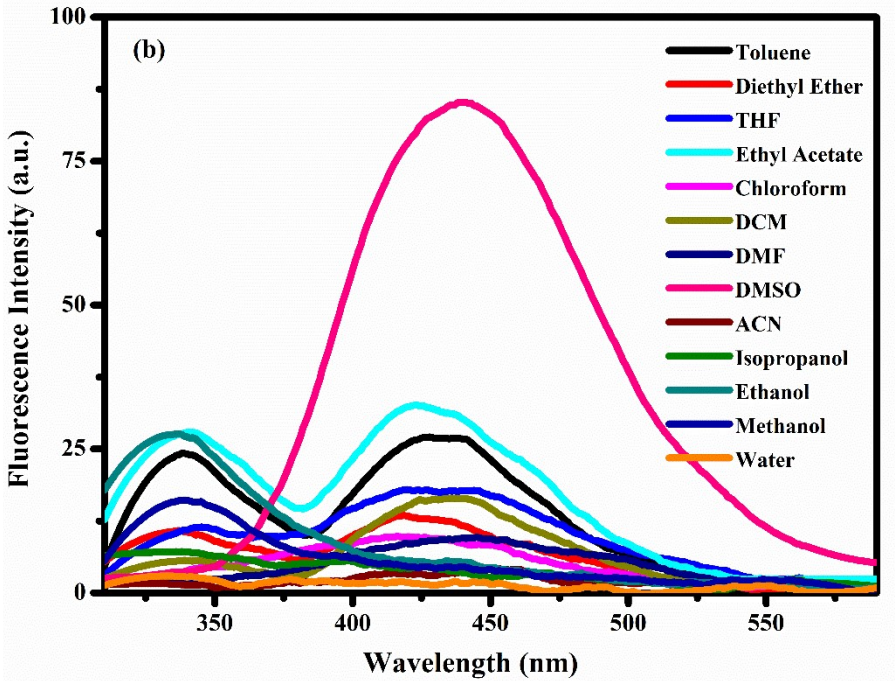


Figure 3. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound **C_3** (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
1.5
1.0
0.5
0.0
300
400
500
600
700
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
100
75
50
25
0
350
400
450
500
550
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

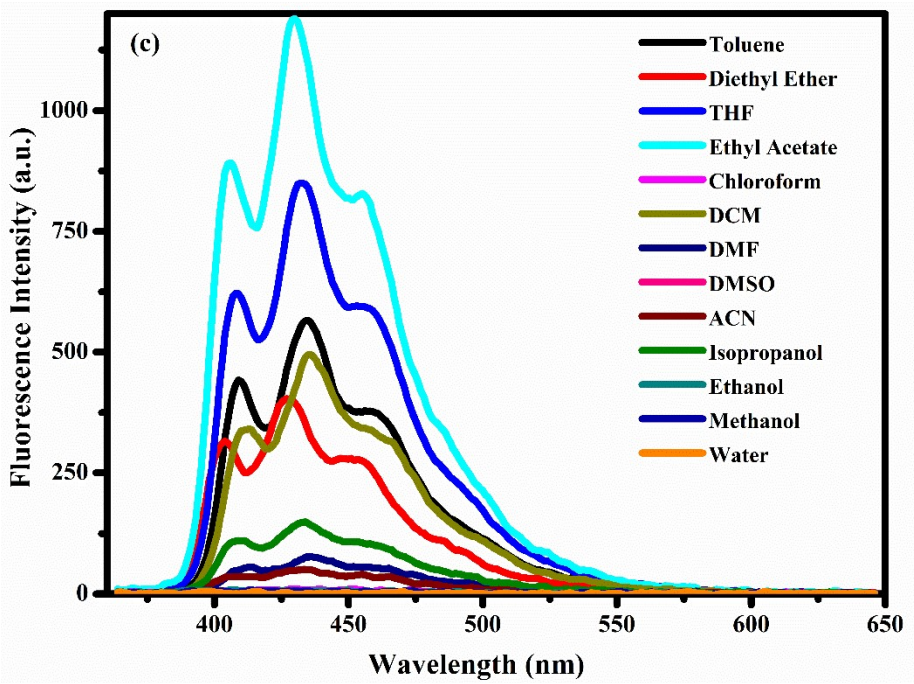
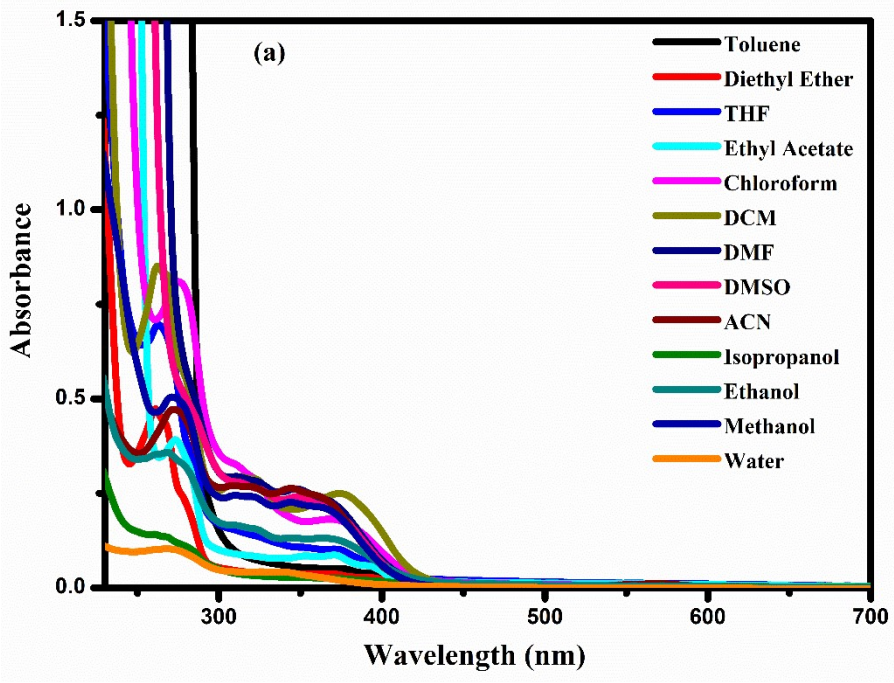
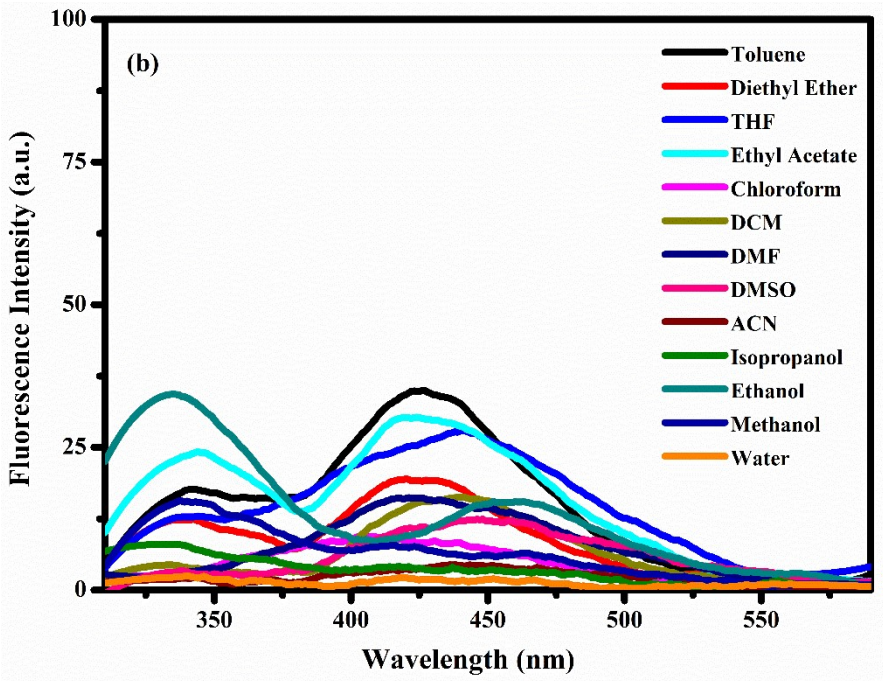


Figure 4. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound **C_4** (10 μM) in different solvents.





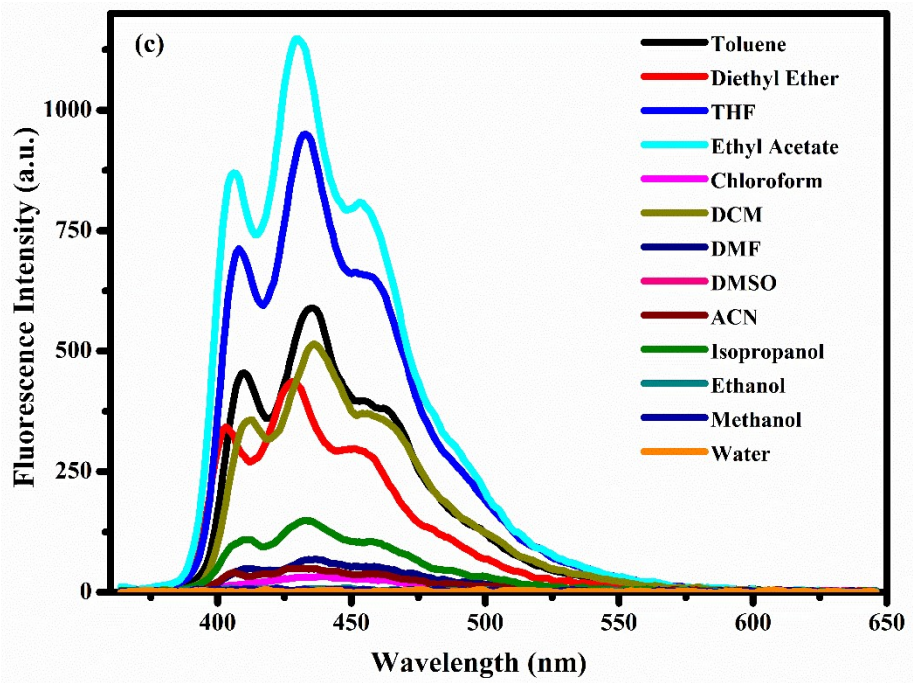
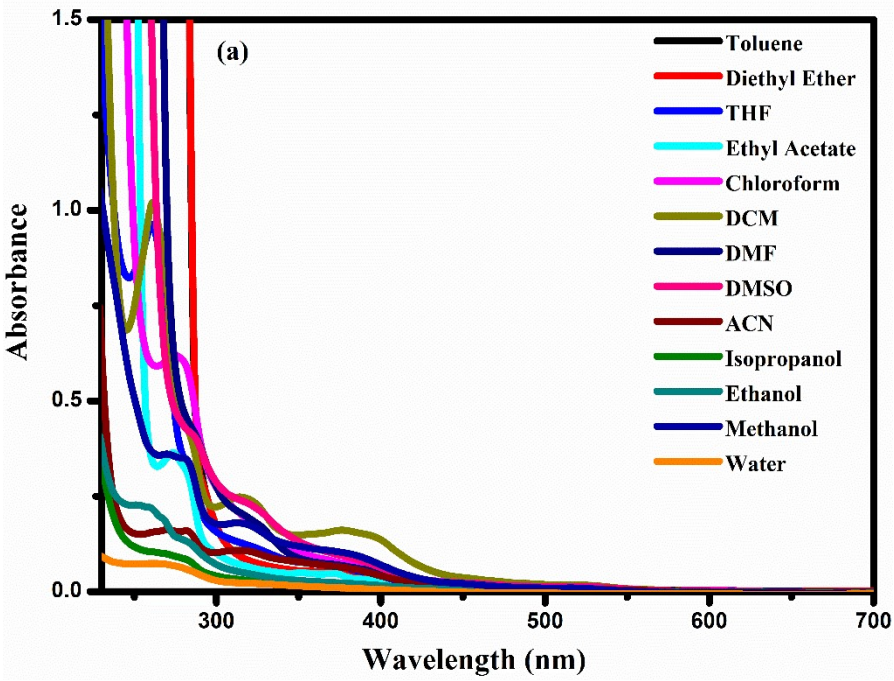
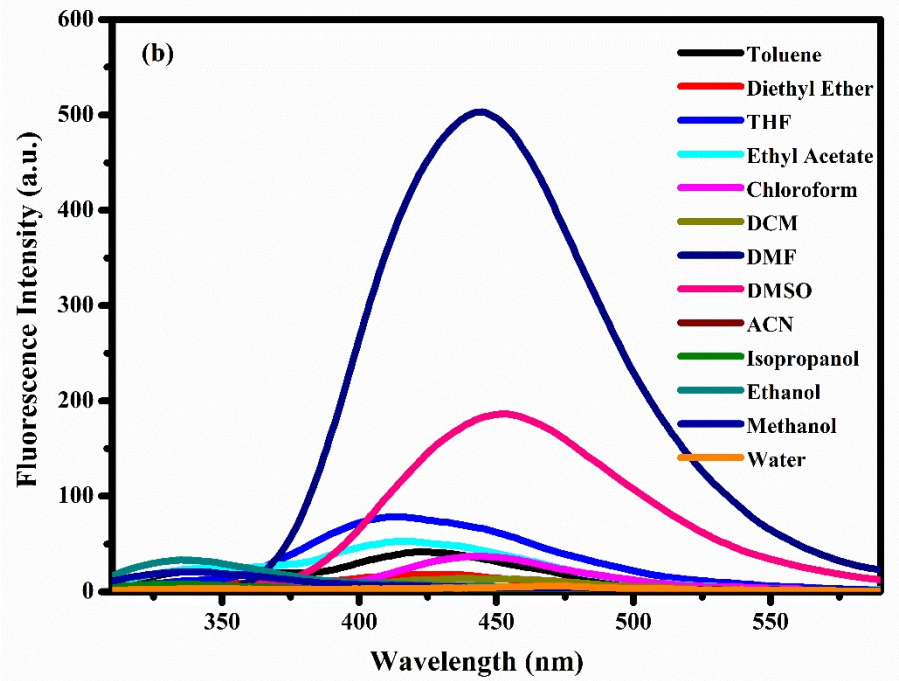


Figure 5. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound **C_5** (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

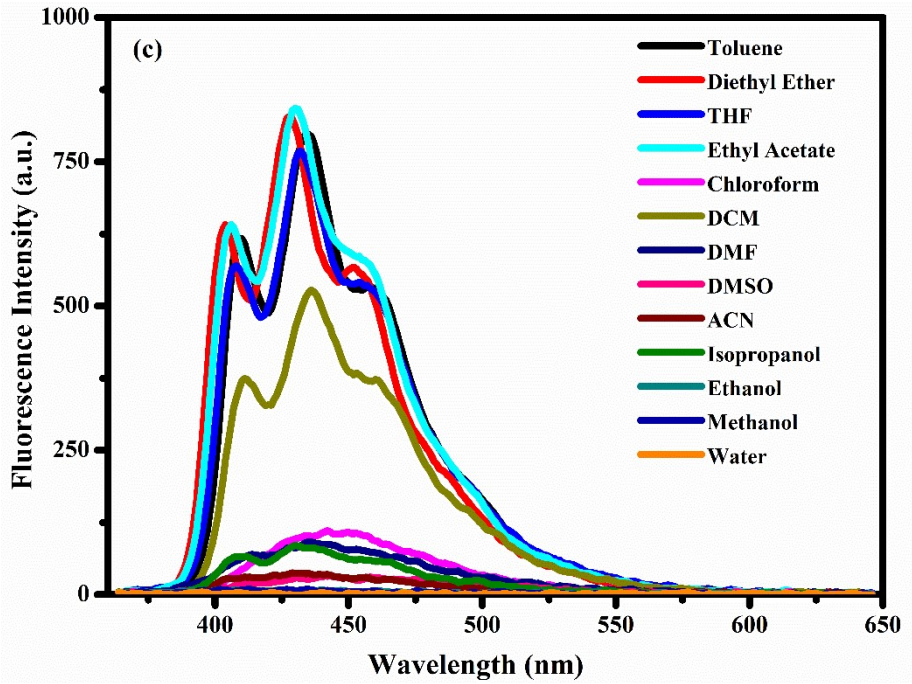
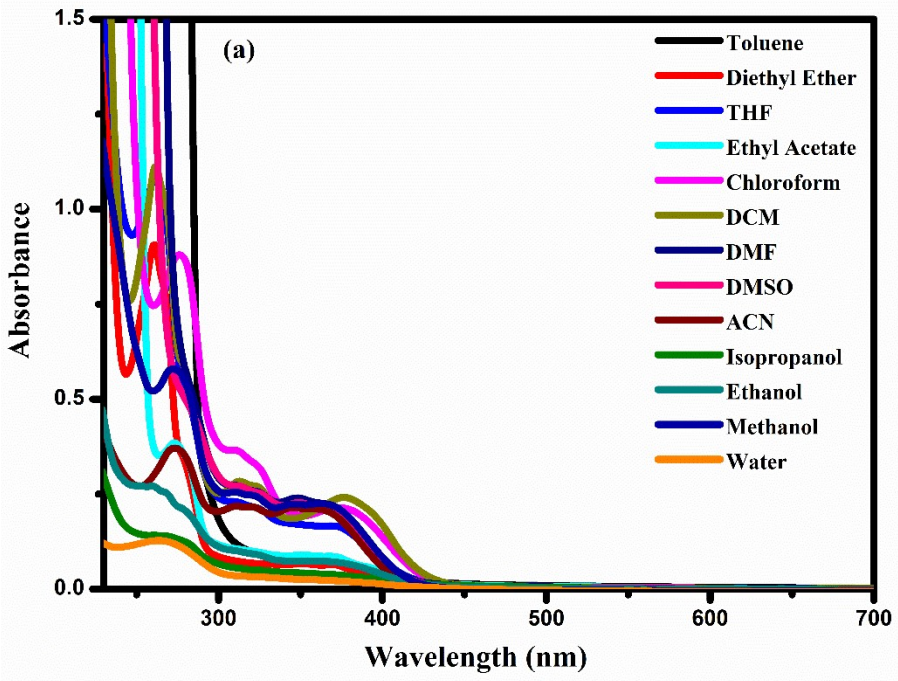
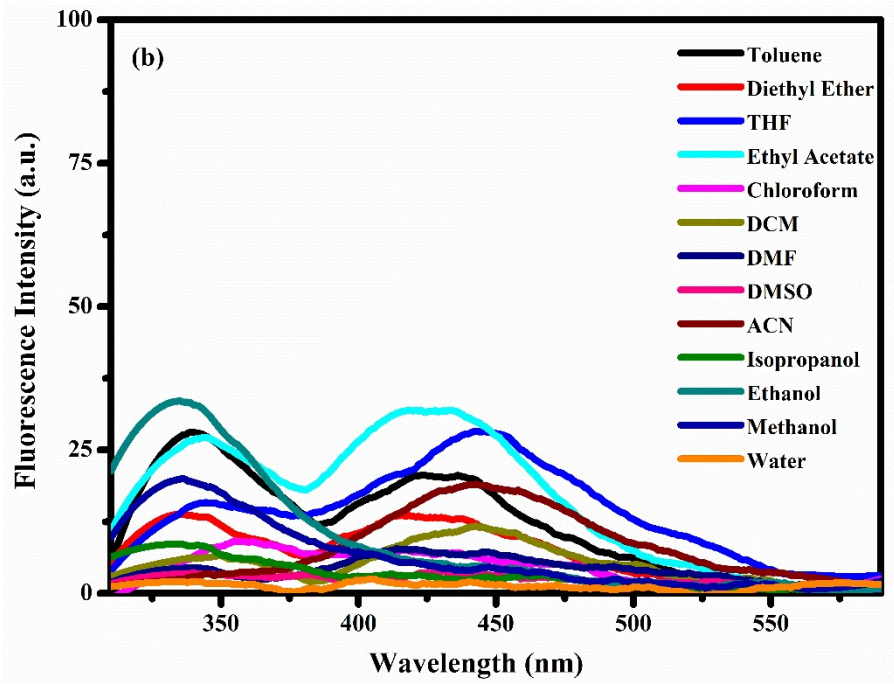


Figure 6. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_6}$ (10 μM) in different solvents





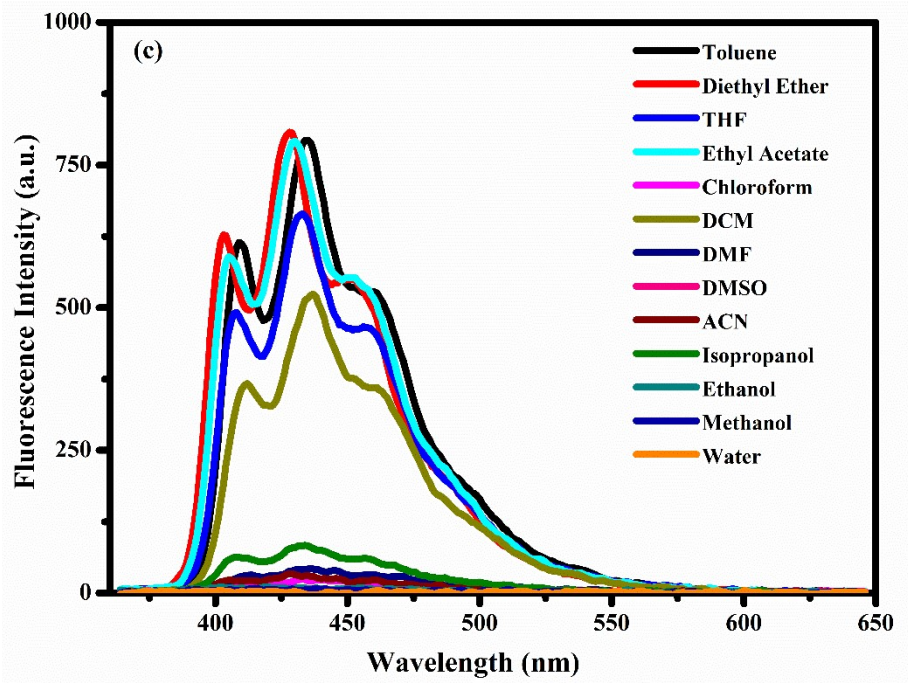
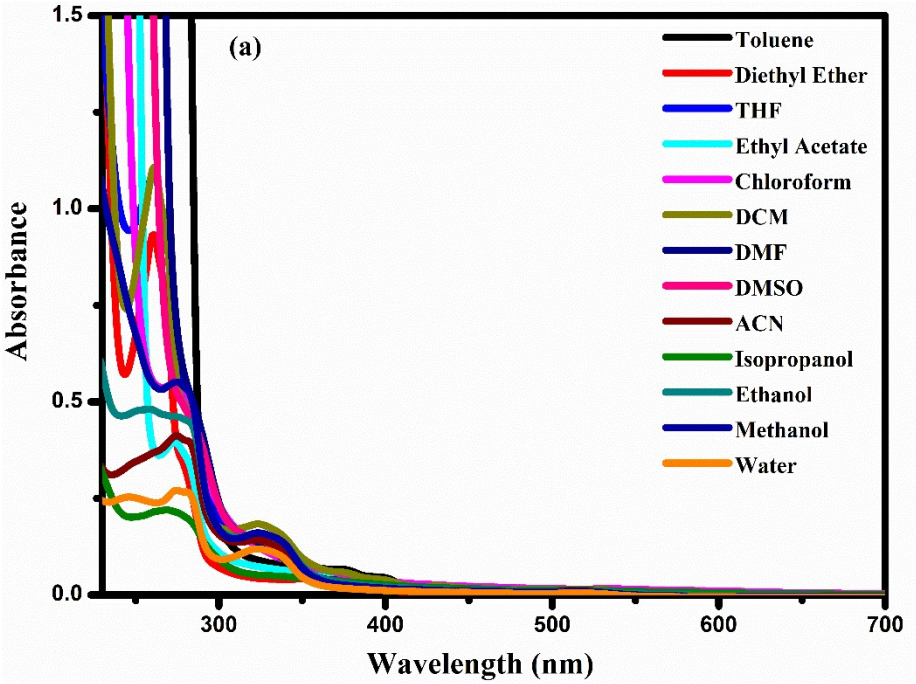
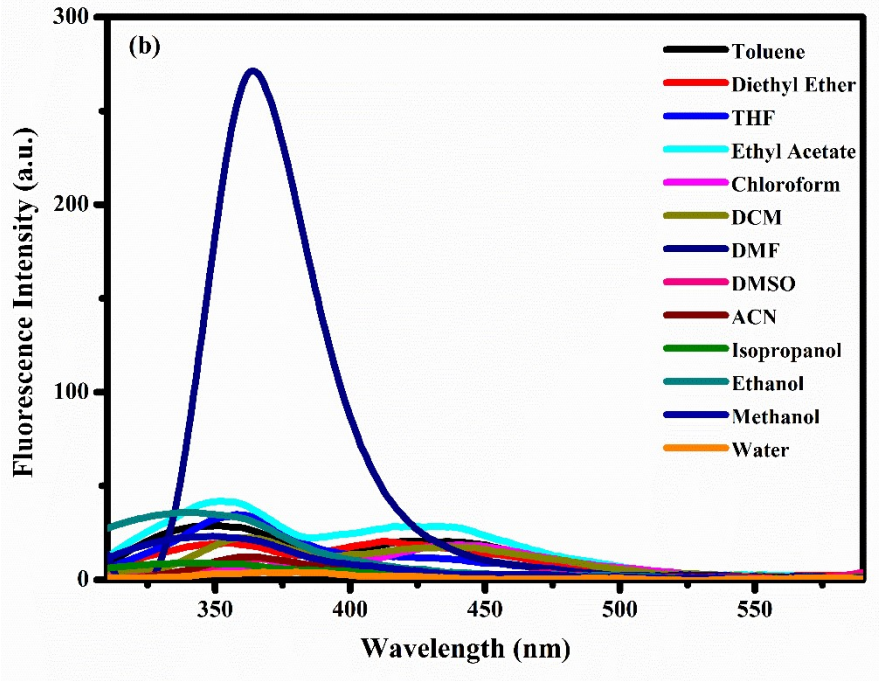


Figure 7. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound **C**$_7$ (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
1.5
1.0
0.5
0.0
300
400
500
600
700
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
300
200
100
0
350
400
450
500
550
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

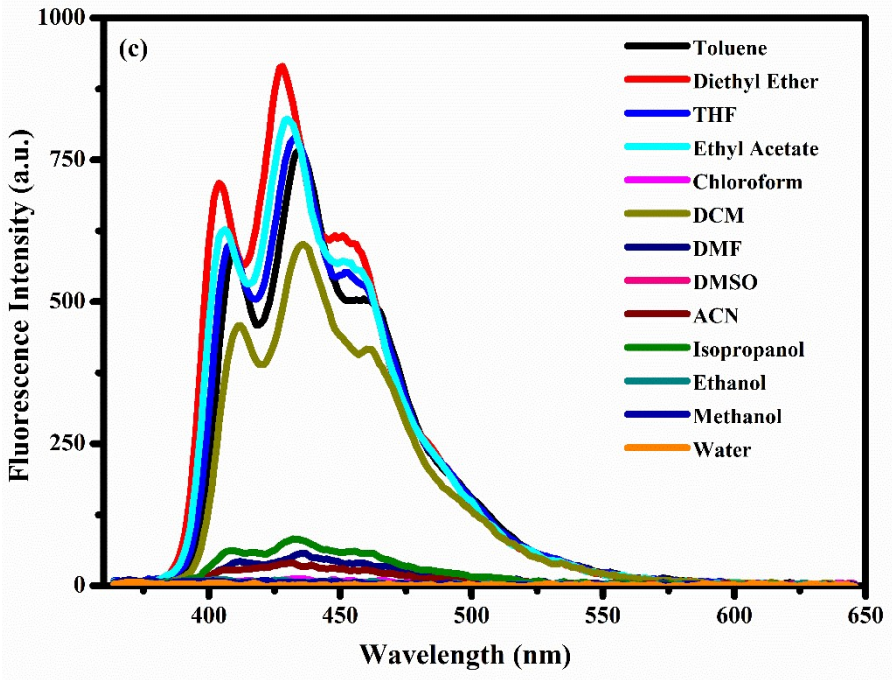
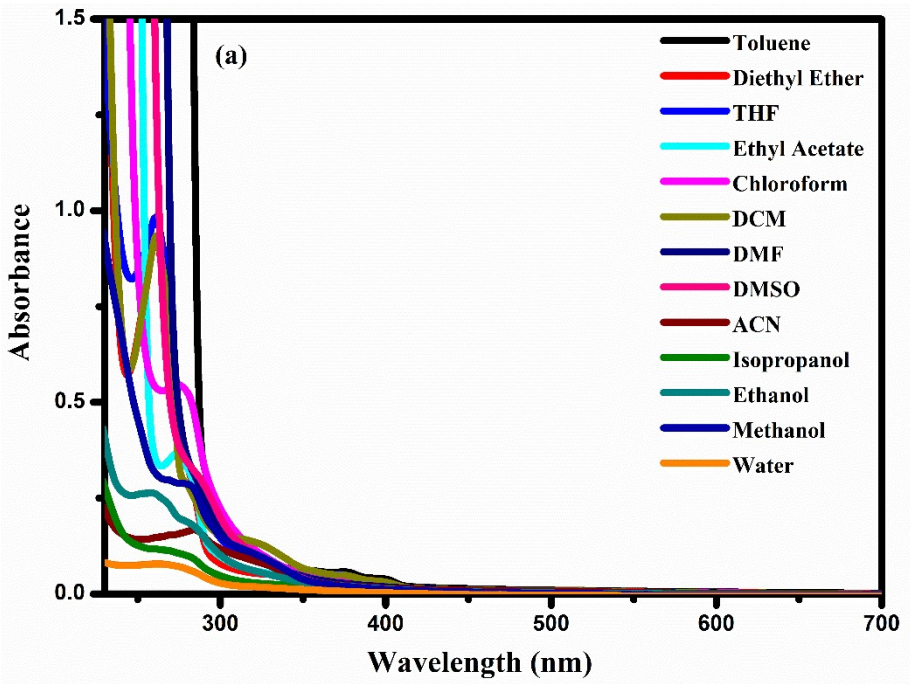
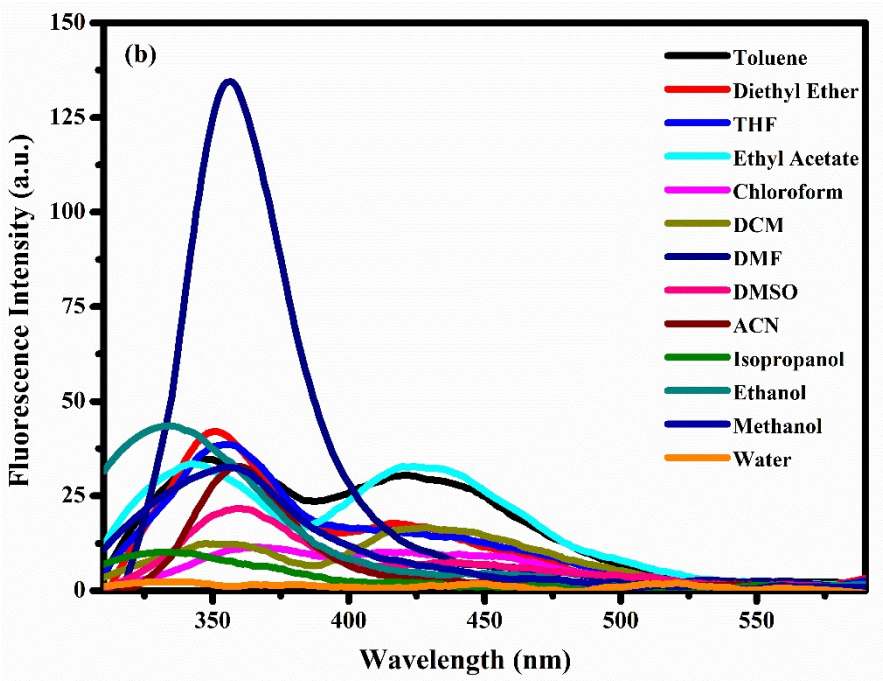


Figure 8. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_8}$ (10 μM) in different solvents





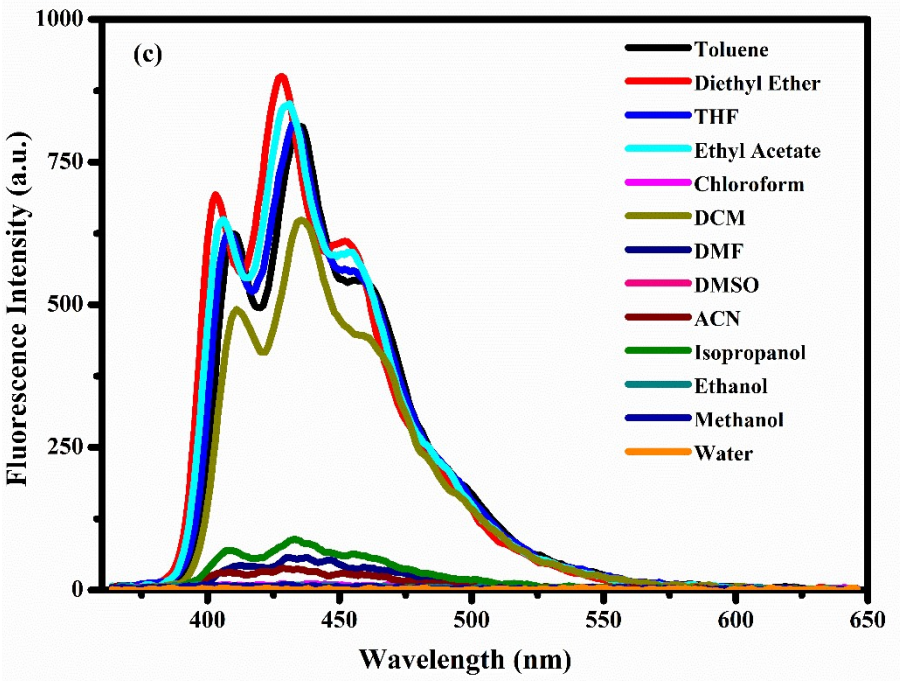
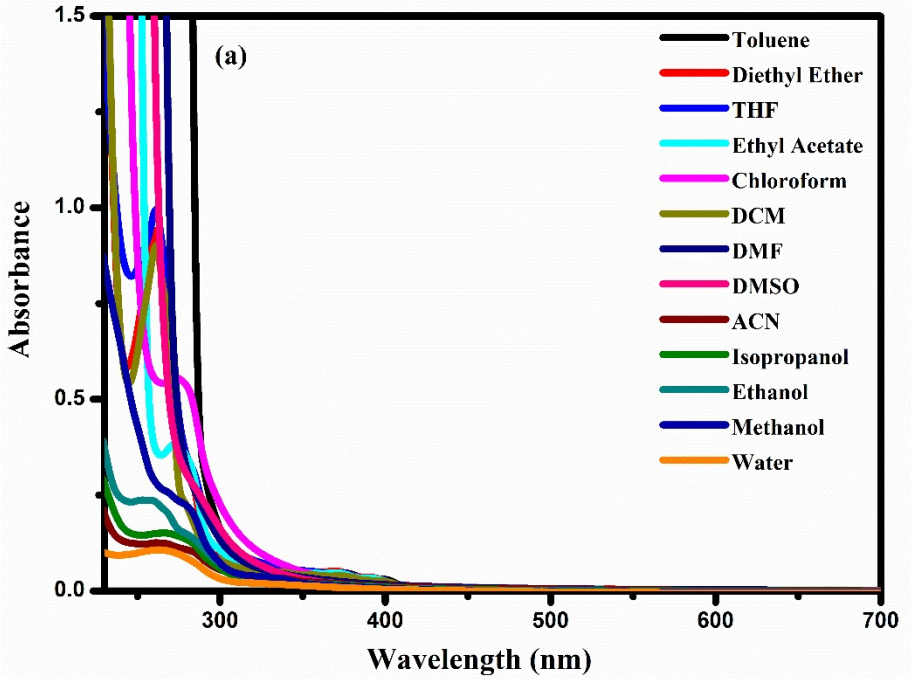
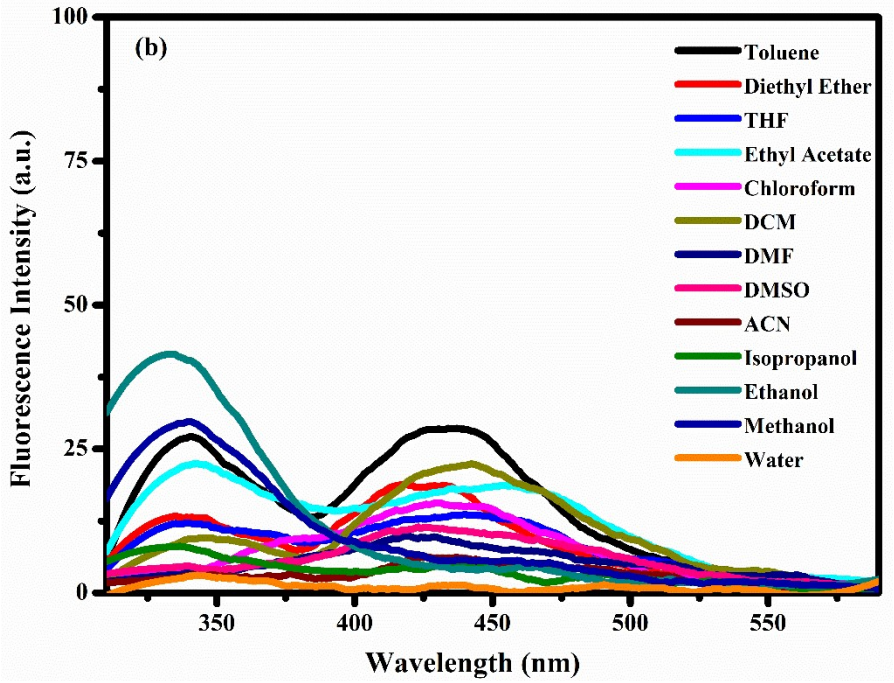


Figure 9. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound **C$_9$** (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
1.5
1.0
0.5
0.0
300
400
500
600
700
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
100
75
50
25
0
350
400
450
500
550
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

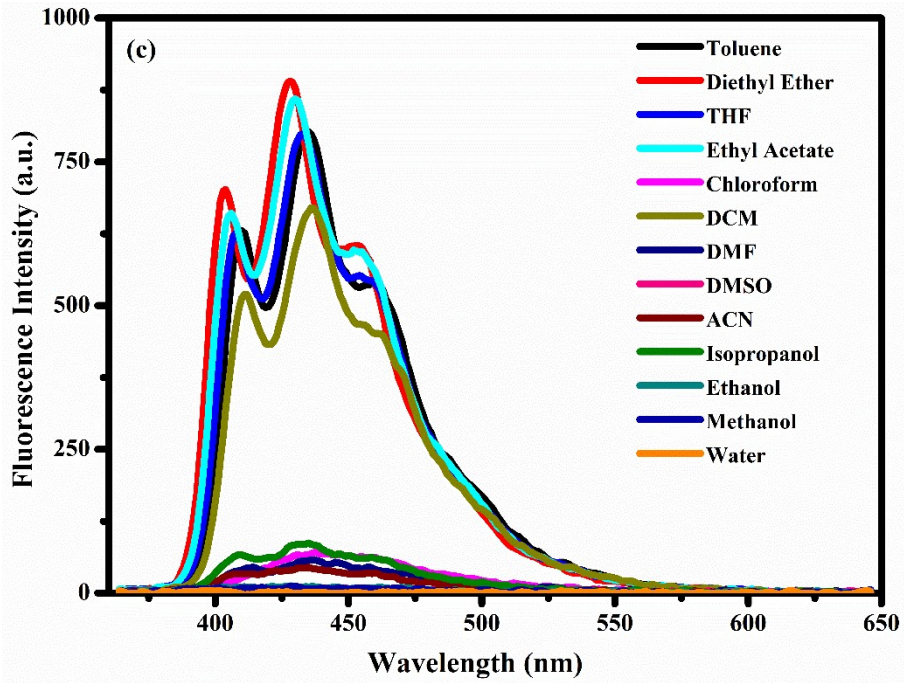
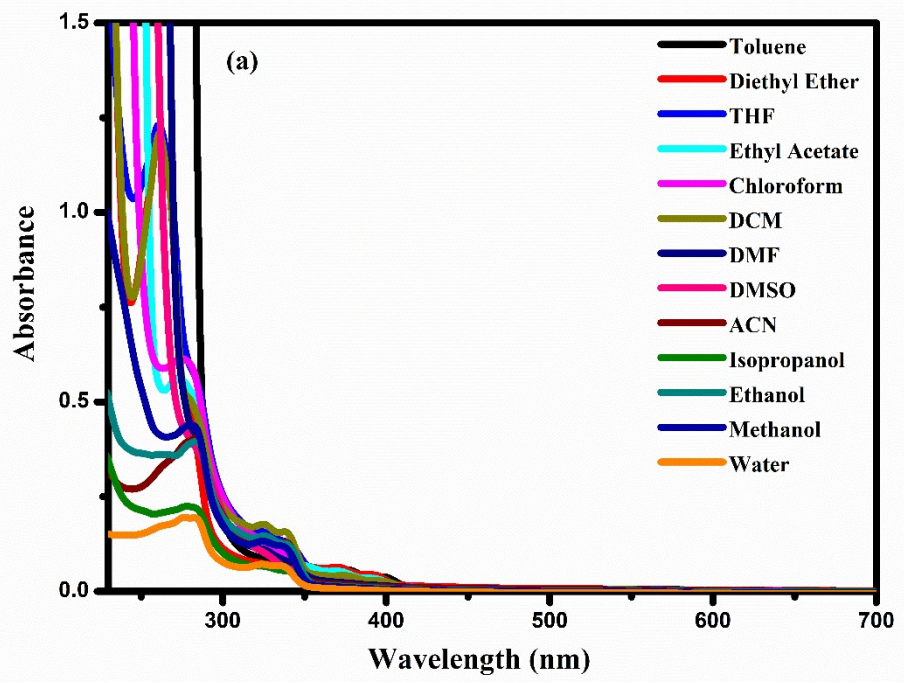
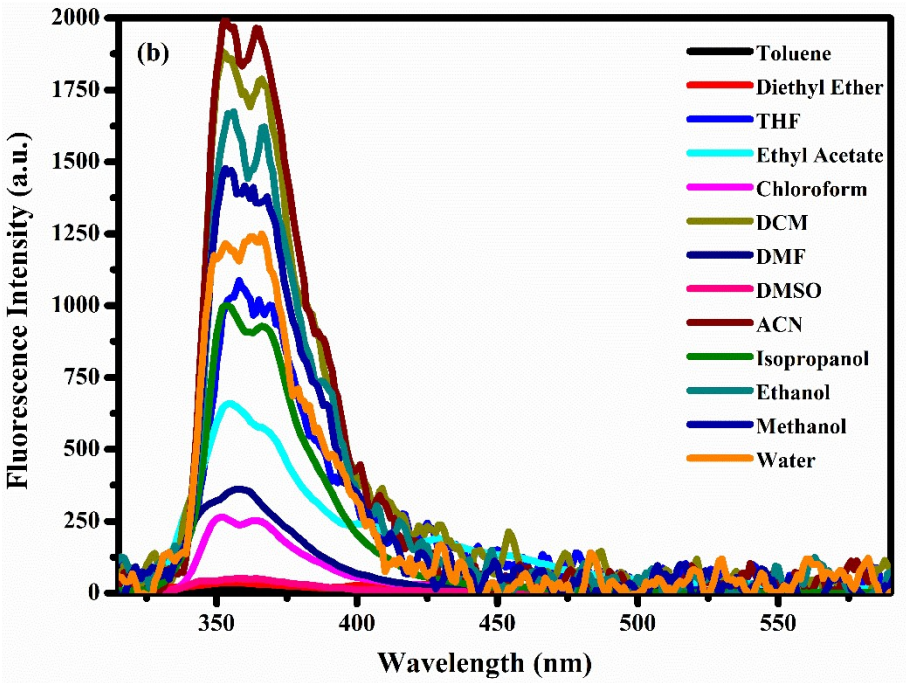


Figure 10. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{10}}$ (10 μM) in different solvents





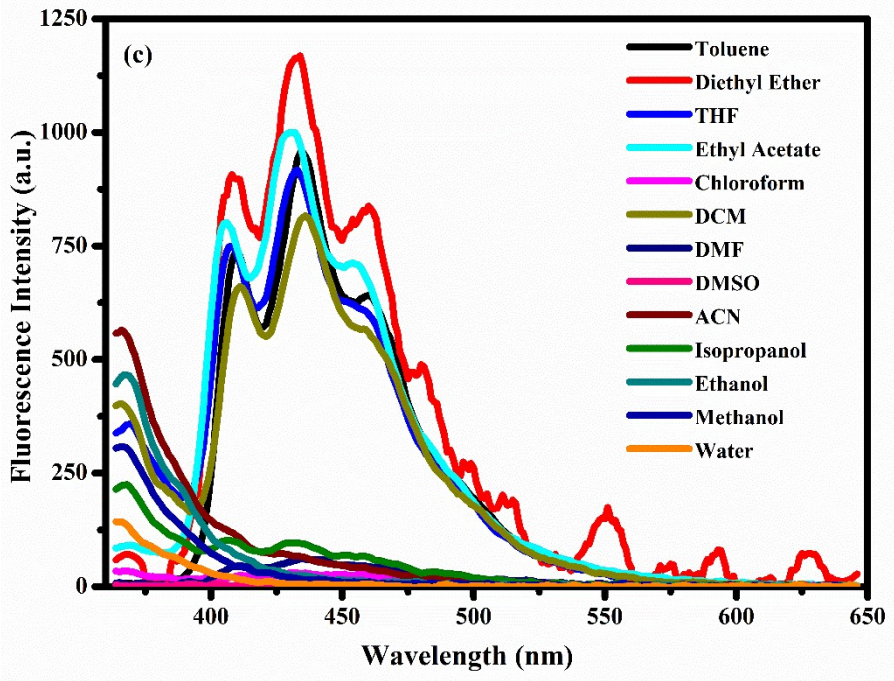
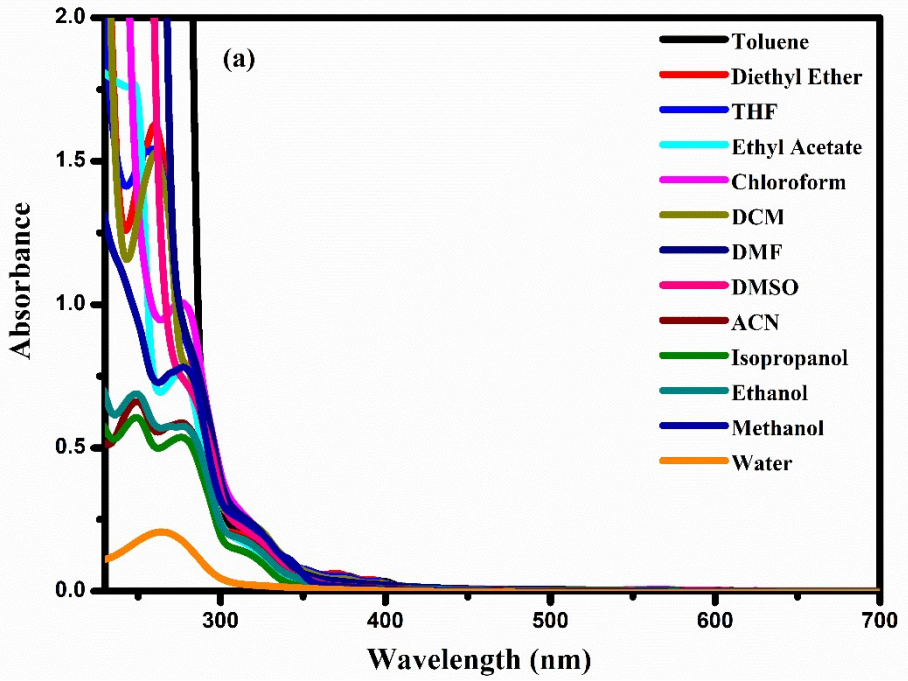
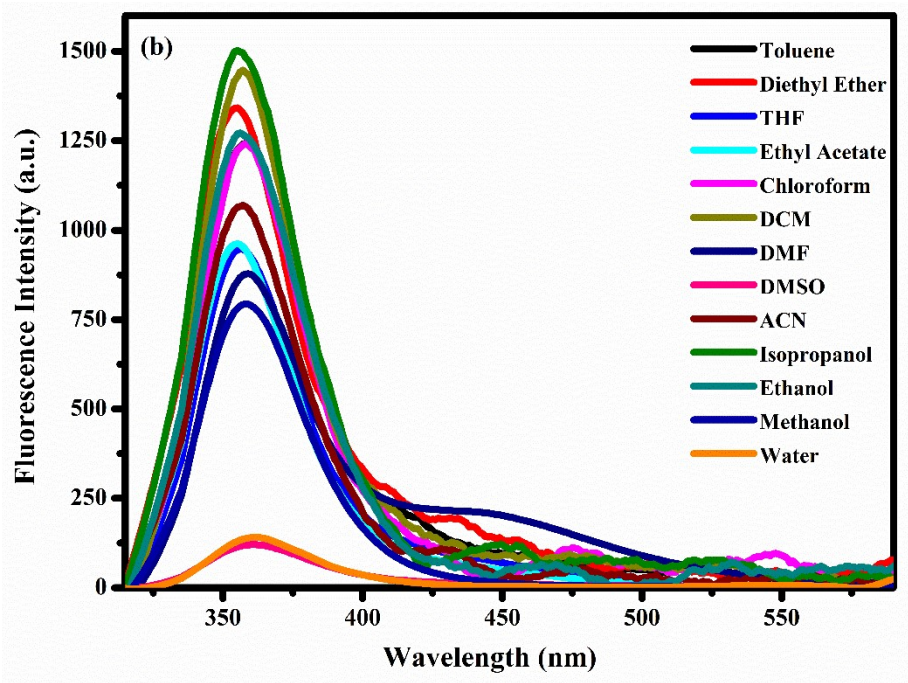


Figure 11. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{11}}$ (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
2.0
1.5
1.0
0.5
0.0
300
400
500
600
700
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
1500
1250
1000
750
500
250
0
350
400
450
500
550
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

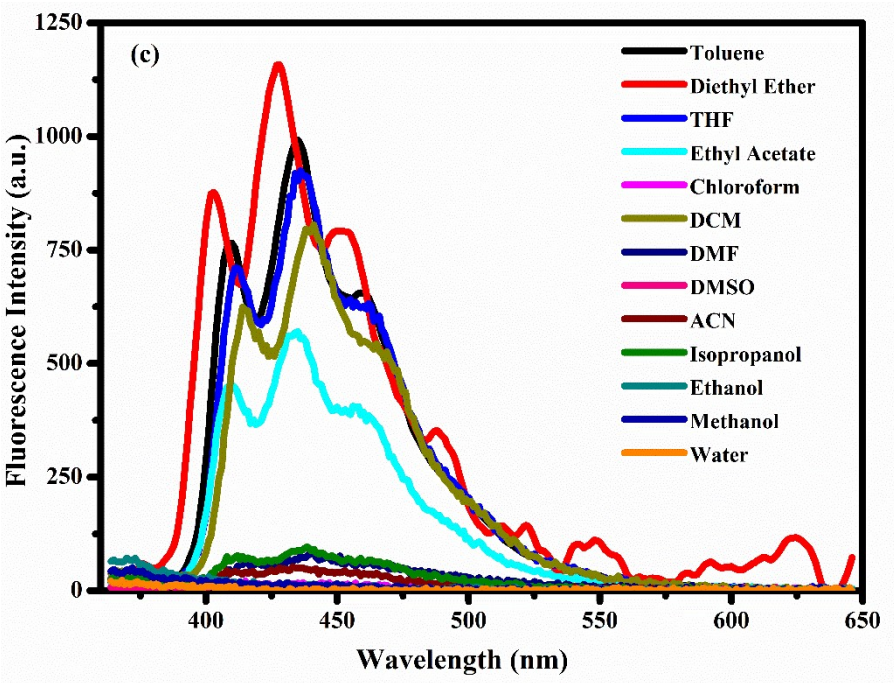
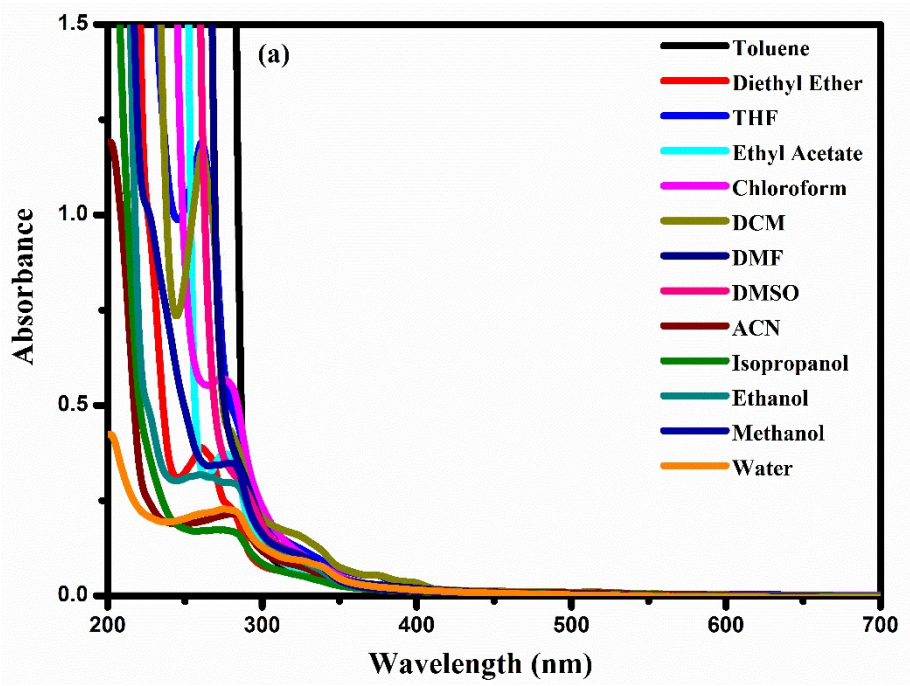


Figure 12. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{12}}$ (10 μM) in different solvents



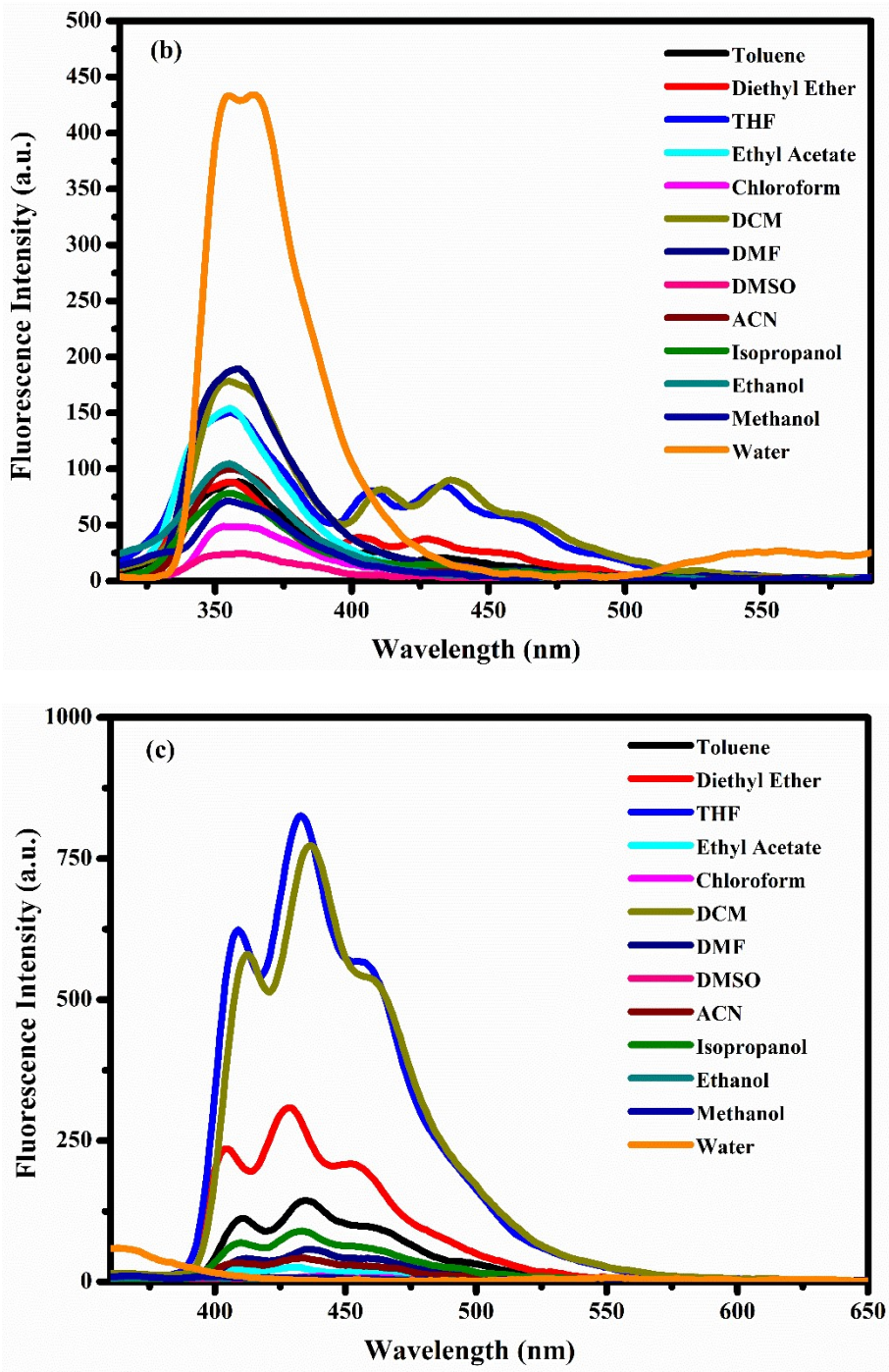
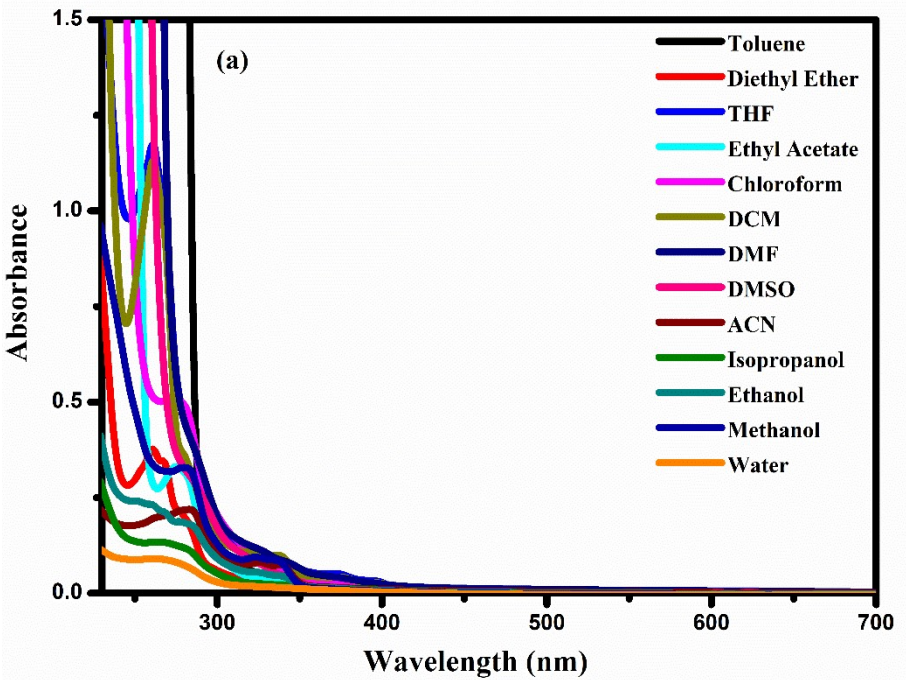
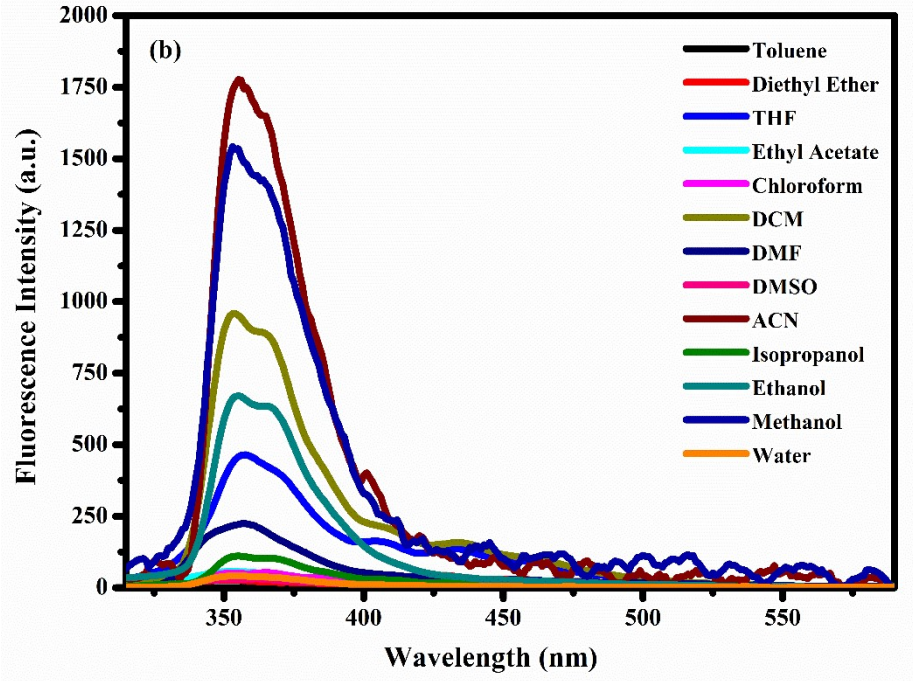


Figure 13. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{13}}$ (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
1.5
1.0
0.5
0.0
300
400
500
600
700
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
2000
1750
1500
1250
1000
750
500
250
0
350
400
450
500
550
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

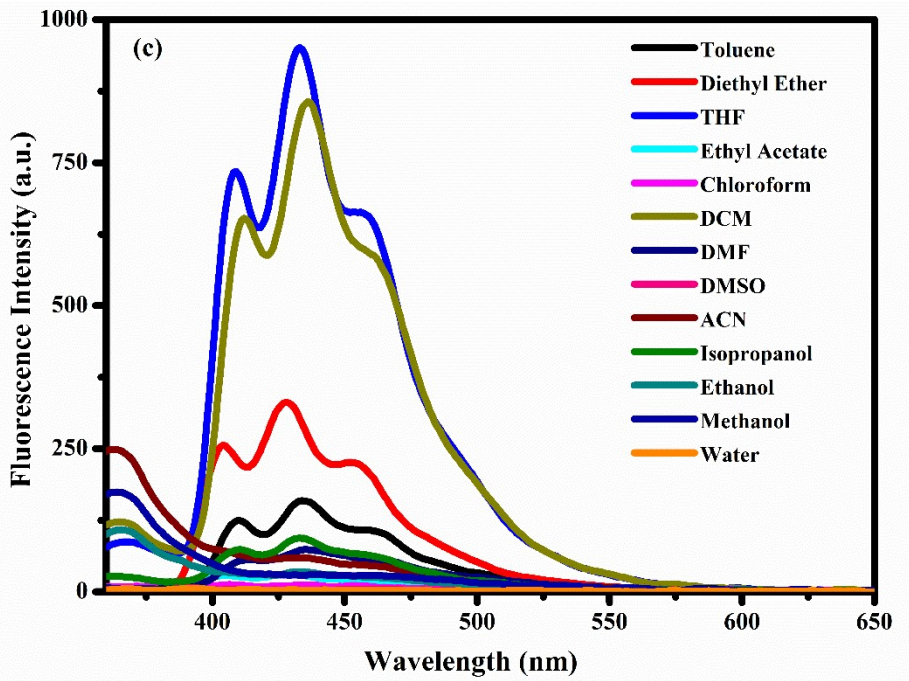
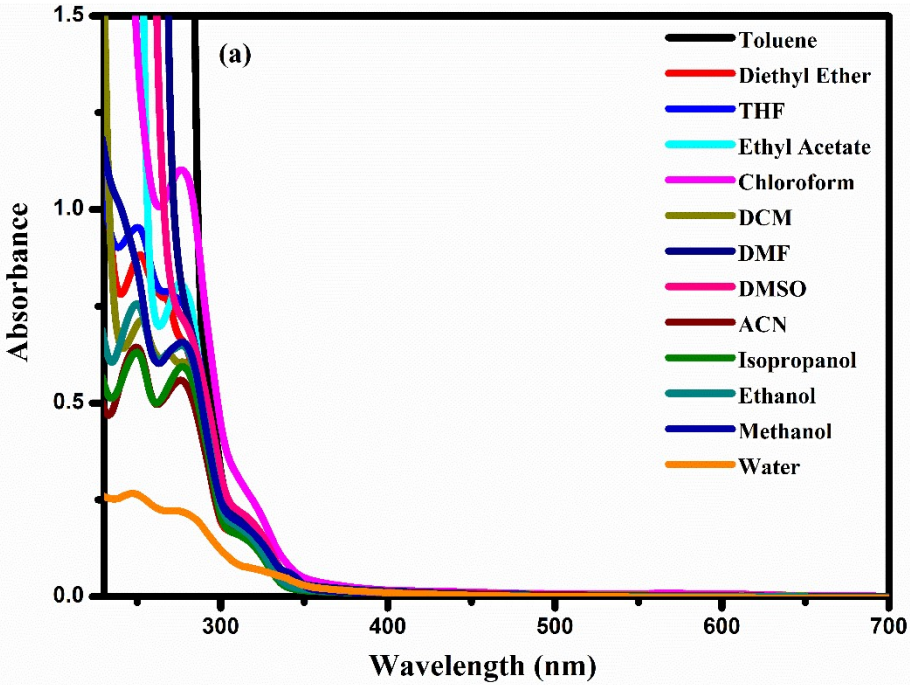
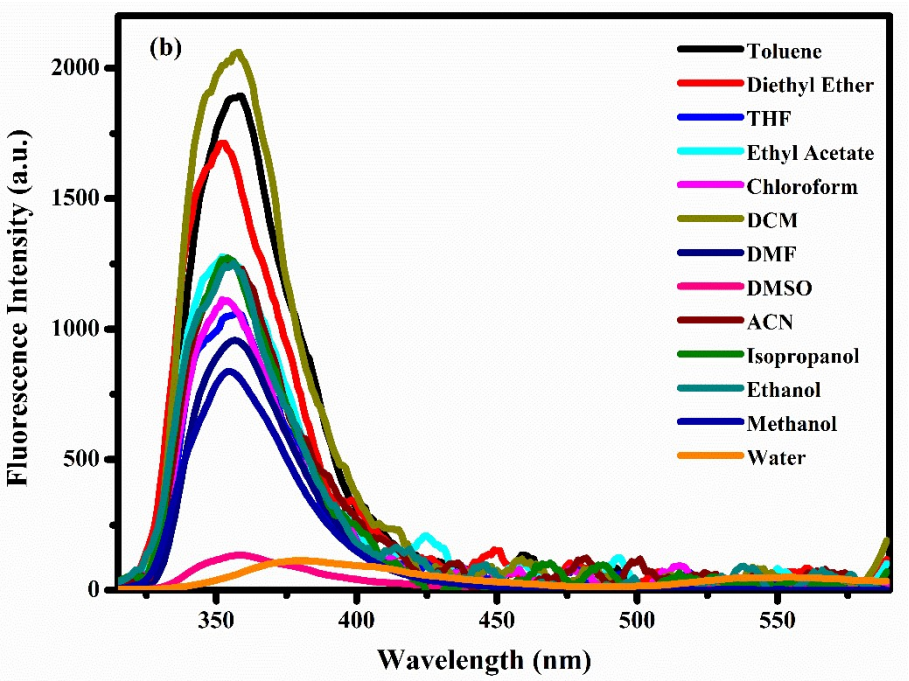


Figure 14. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{14}}$ (10 μM) in different solvents





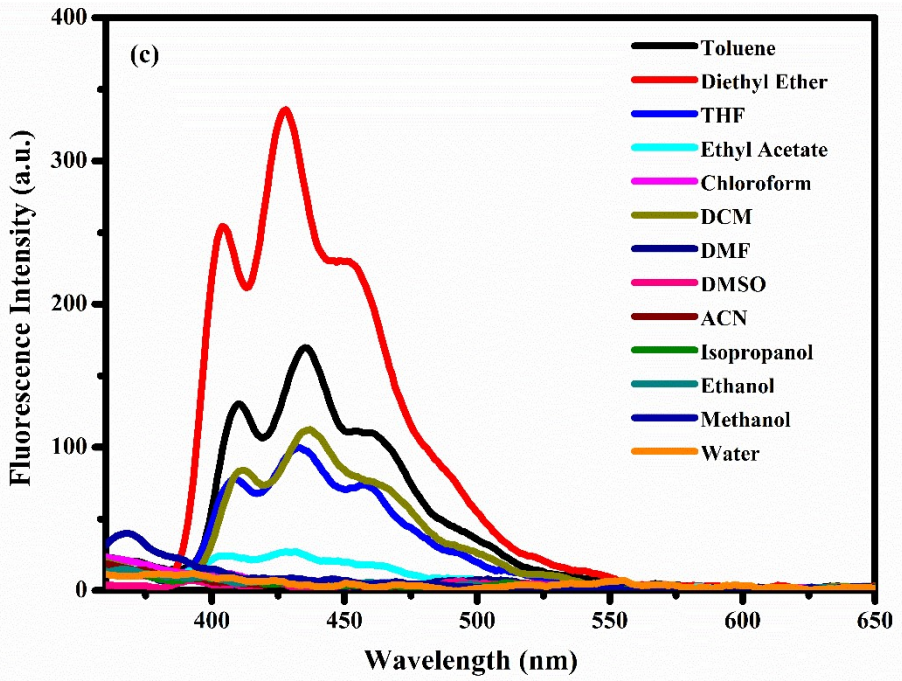
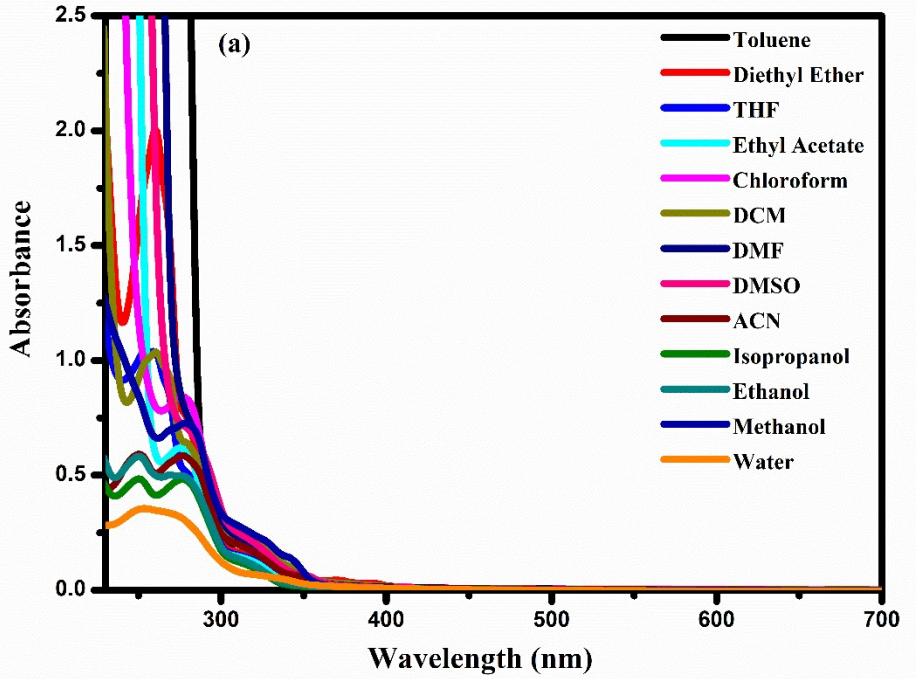
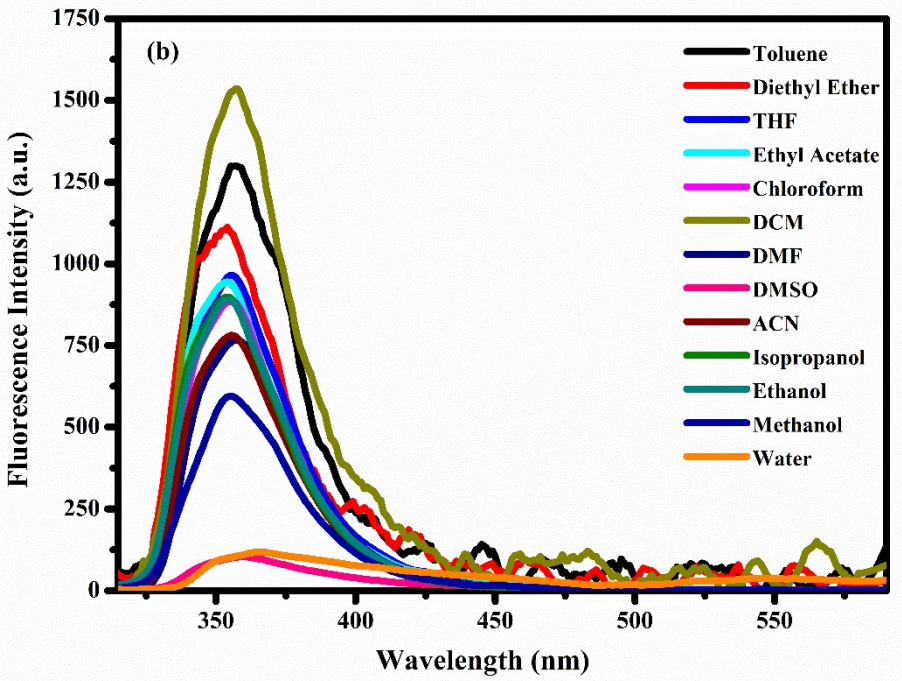


Figure 15. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{15}}$ (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

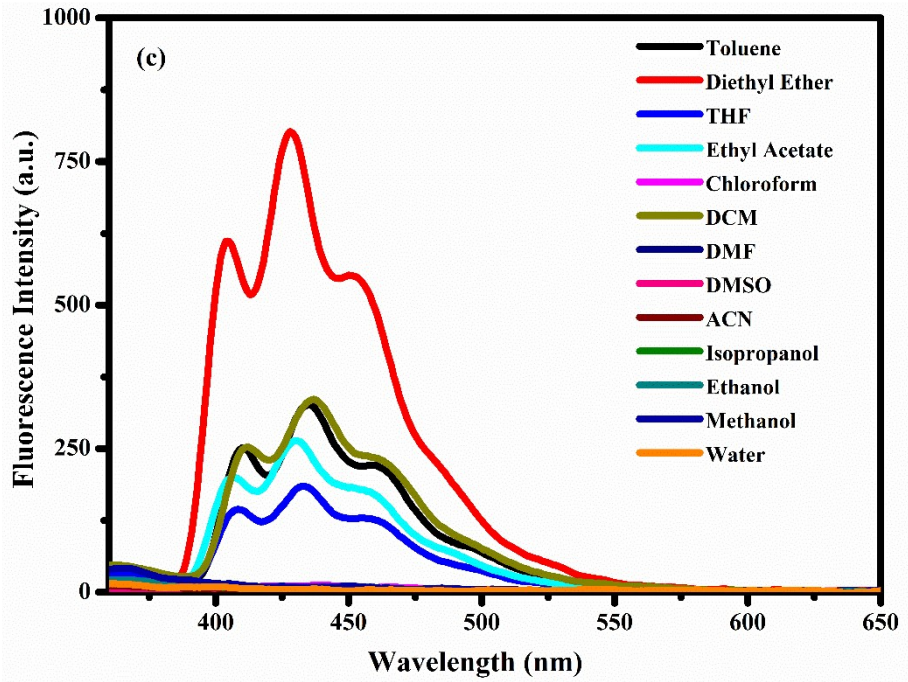
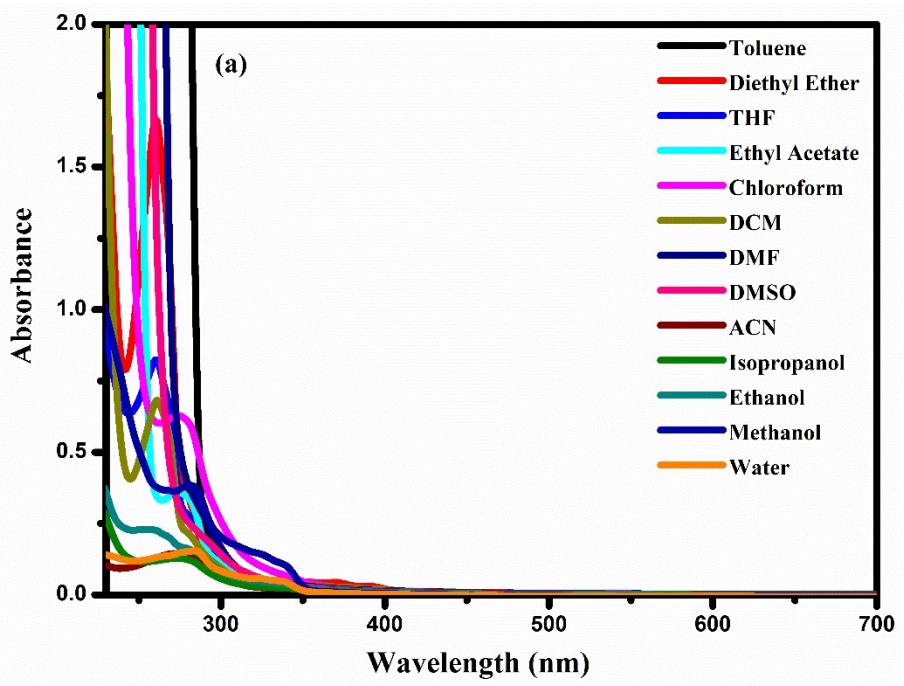


Figure 16. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{16}}$ (10 μM) in different solvents



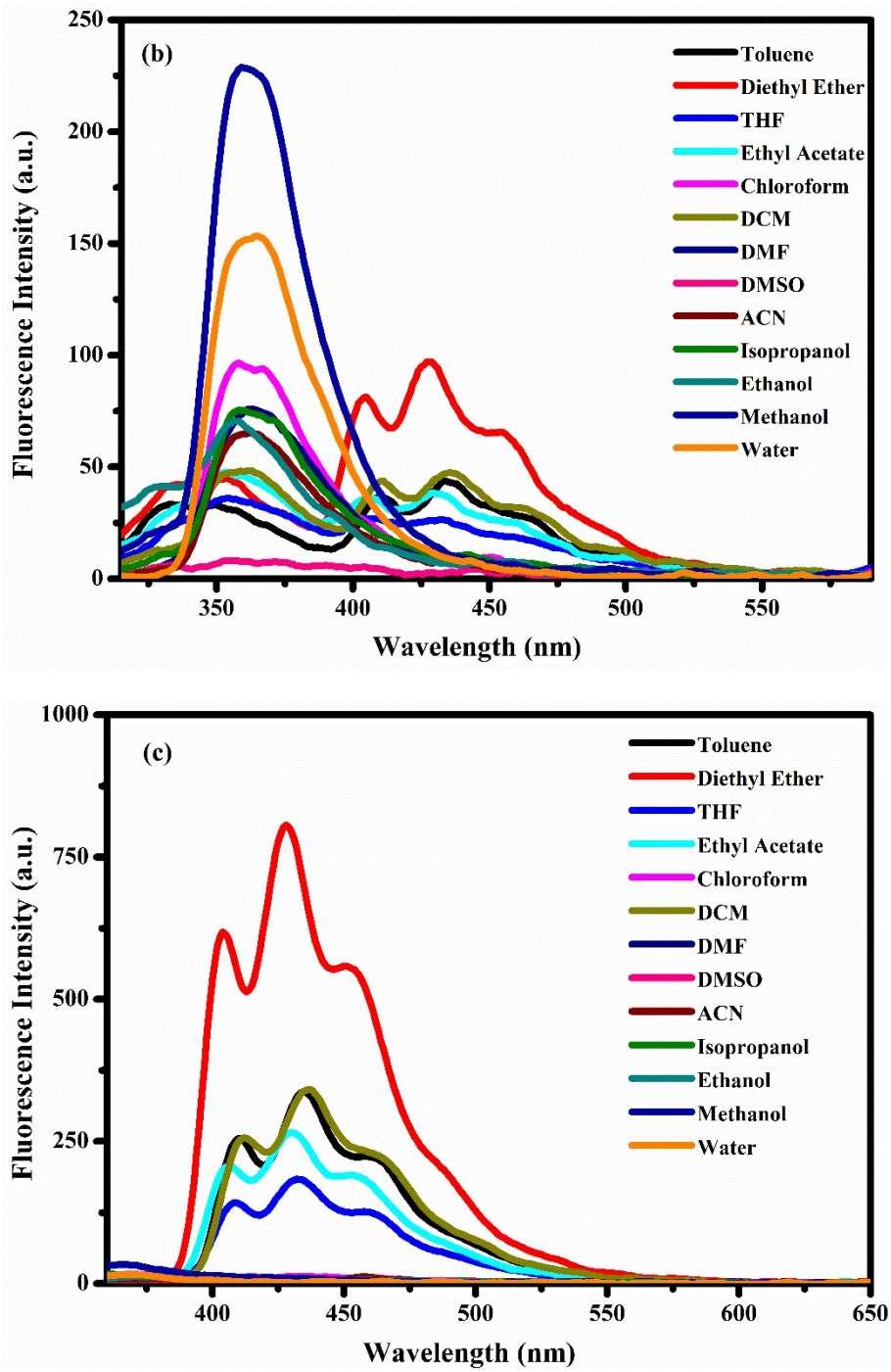
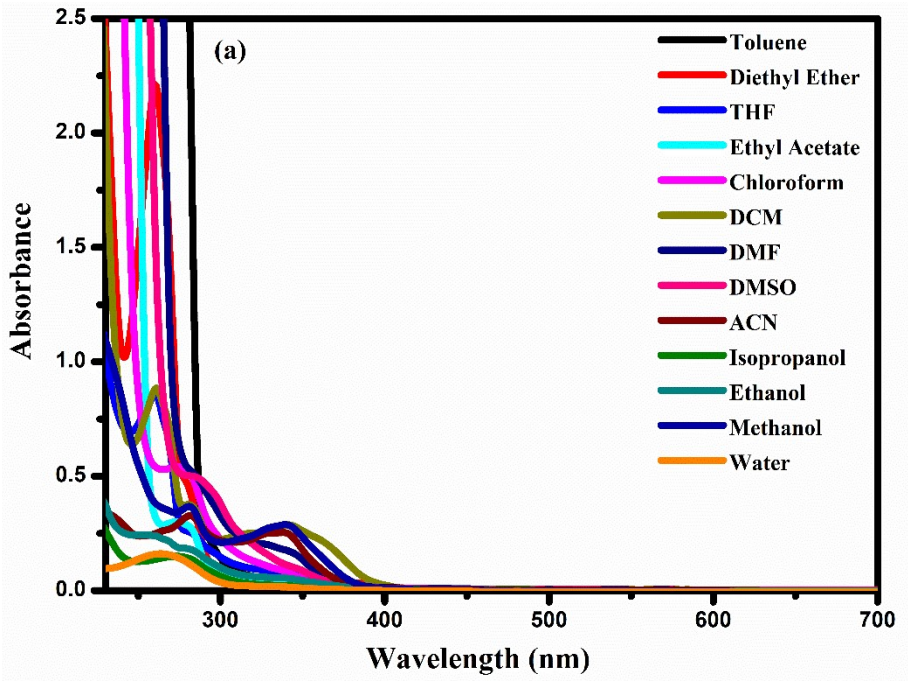
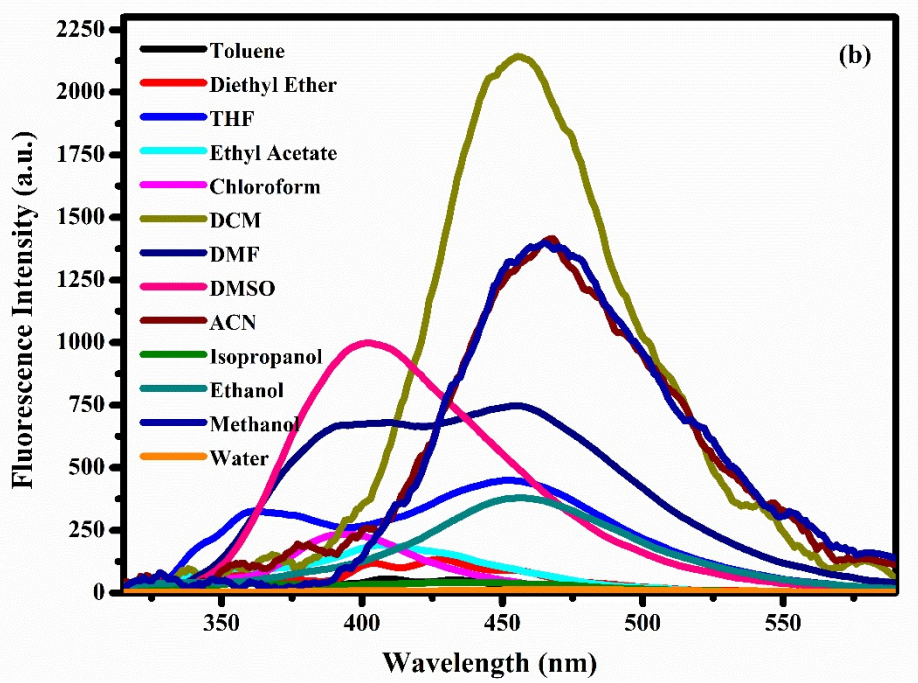


Figure 17. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{17}}$ (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

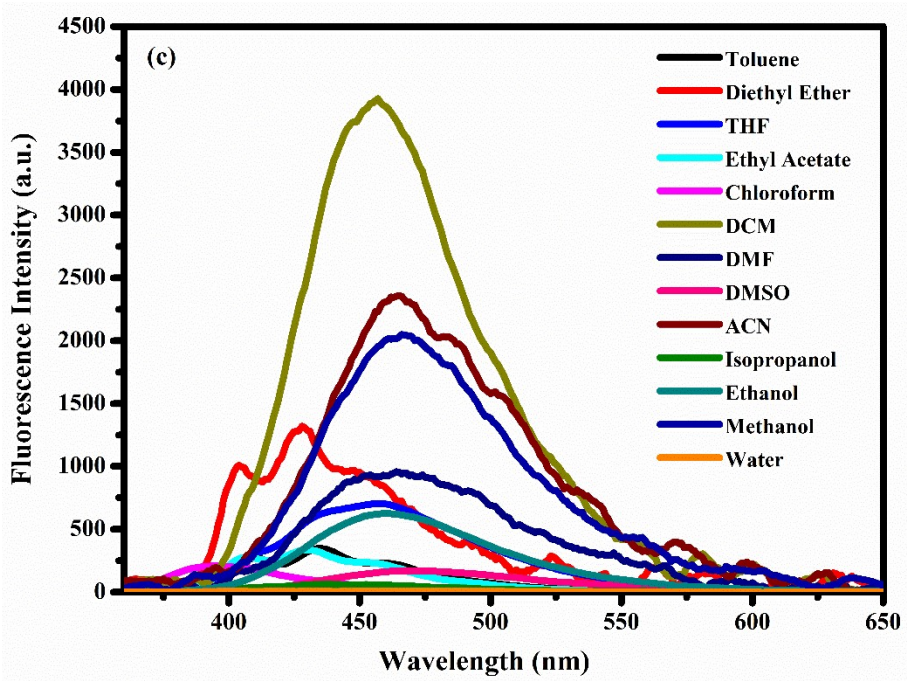
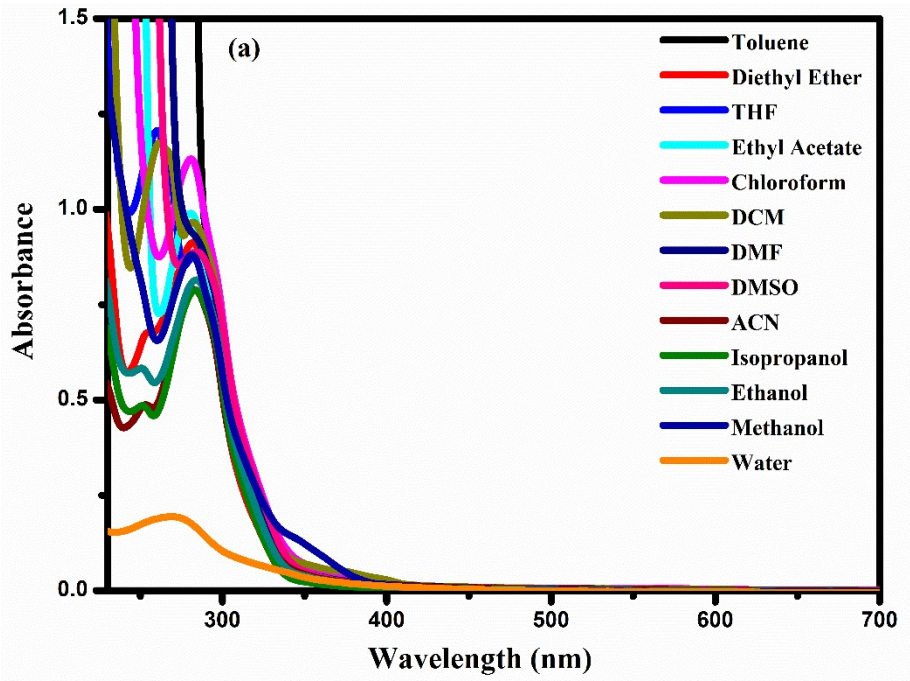


Figure 18. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{18}}$ (10 μM) in different solvents



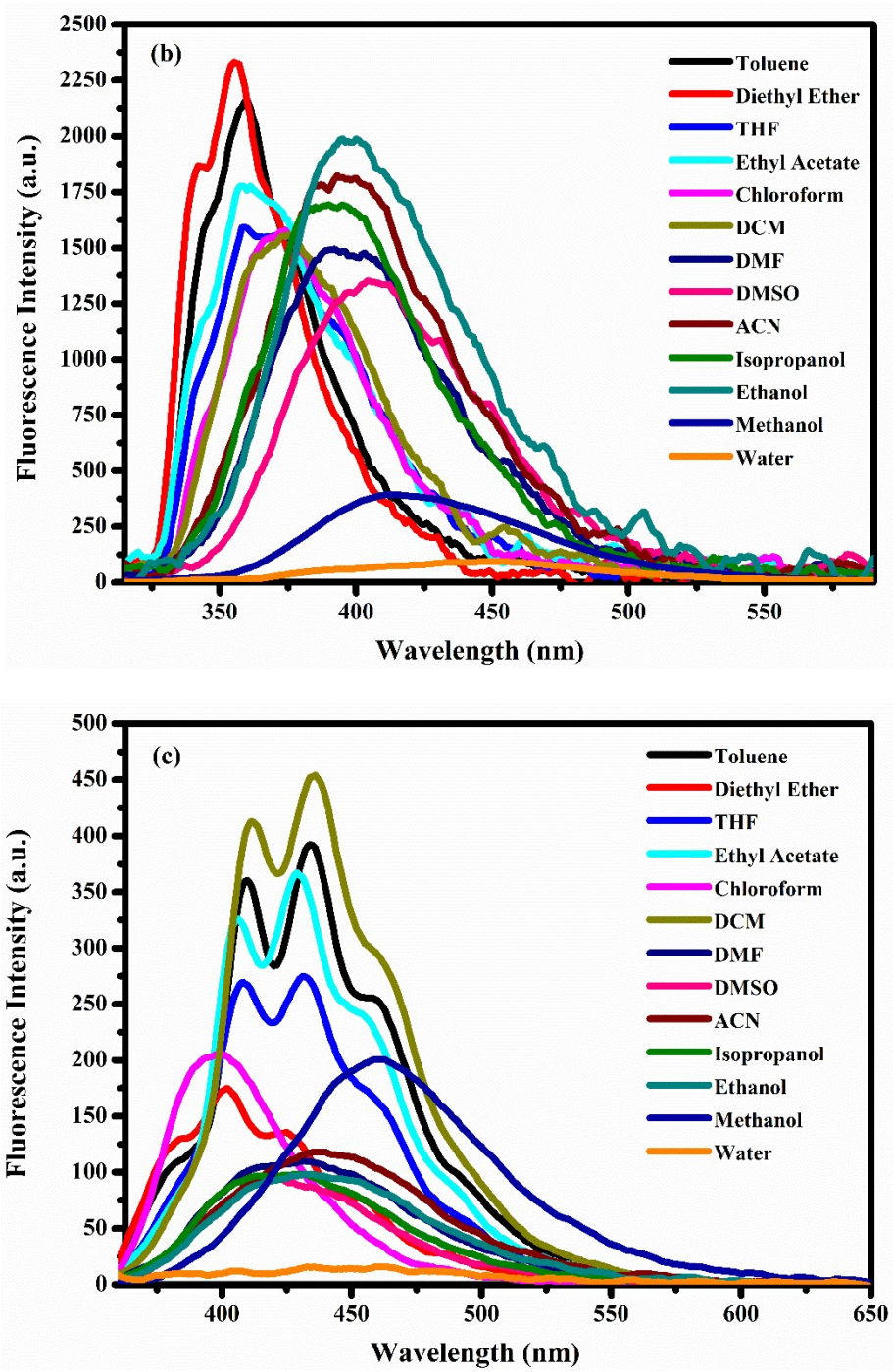
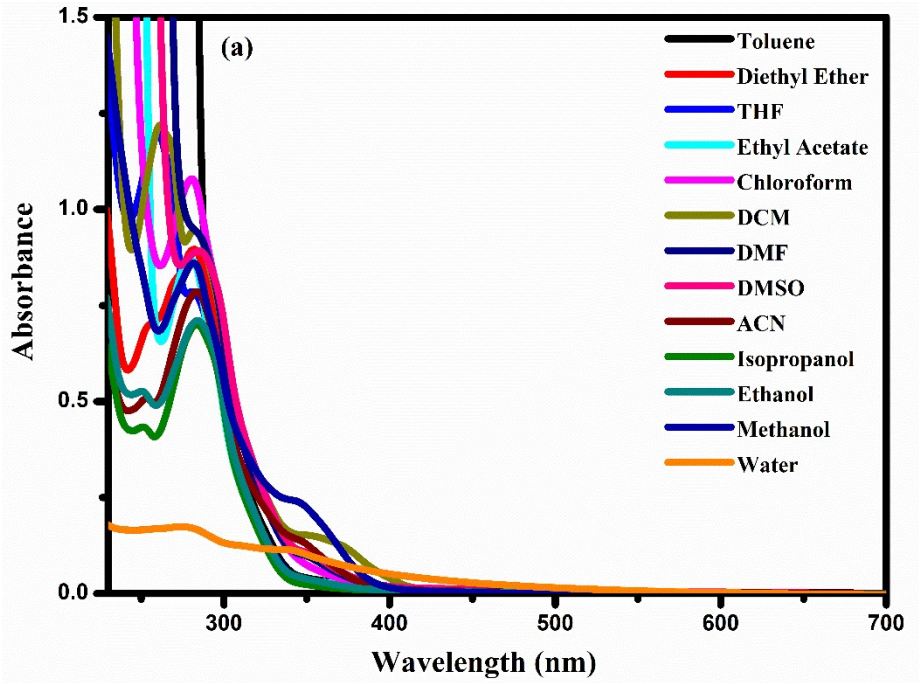
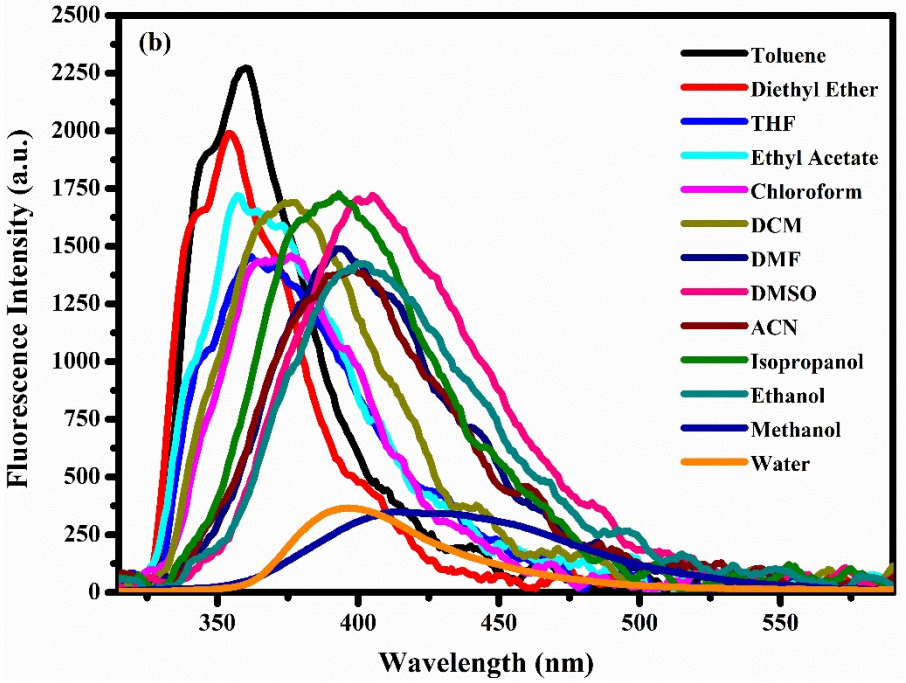


Figure 19. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{19}}$ (10 μM) in different solvents


(a)
Absorbance
Wavelength (nm)
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water


(b)
Fluorescence Intensity (a.u.)
Wavelength (nm)
Toluene
Diethyl Ether
THF
Ethyl Acetate
Chloroform
DCM
DMF
DMSO
ACN
Isopropanol
Ethanol
Methanol
Water

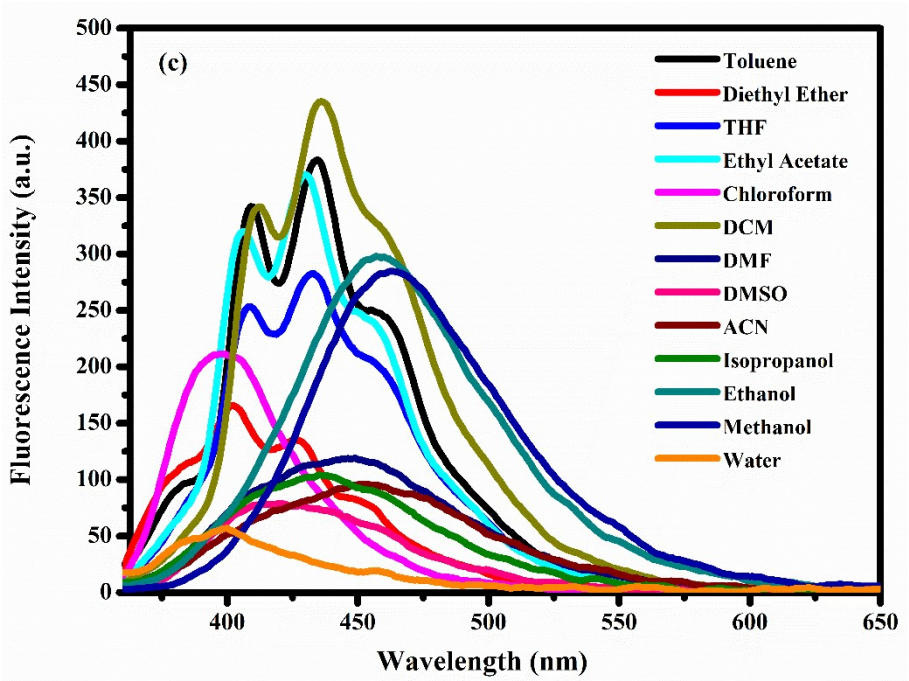
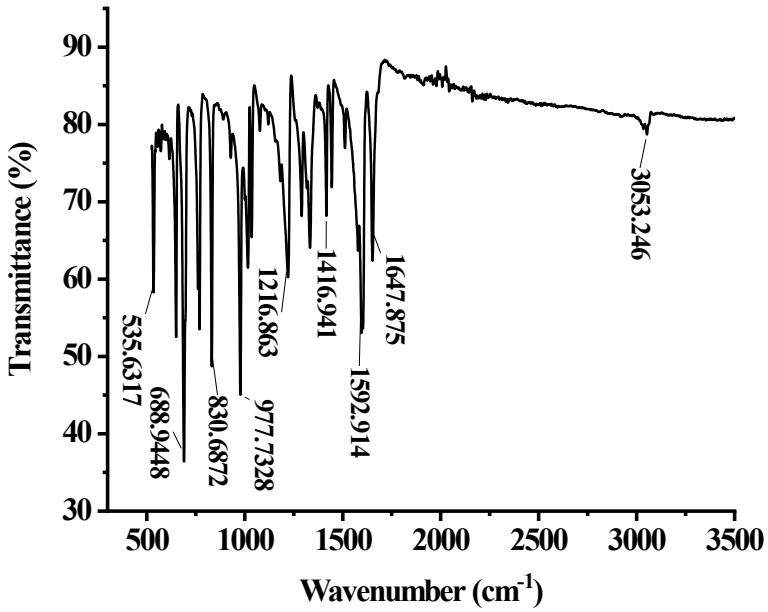
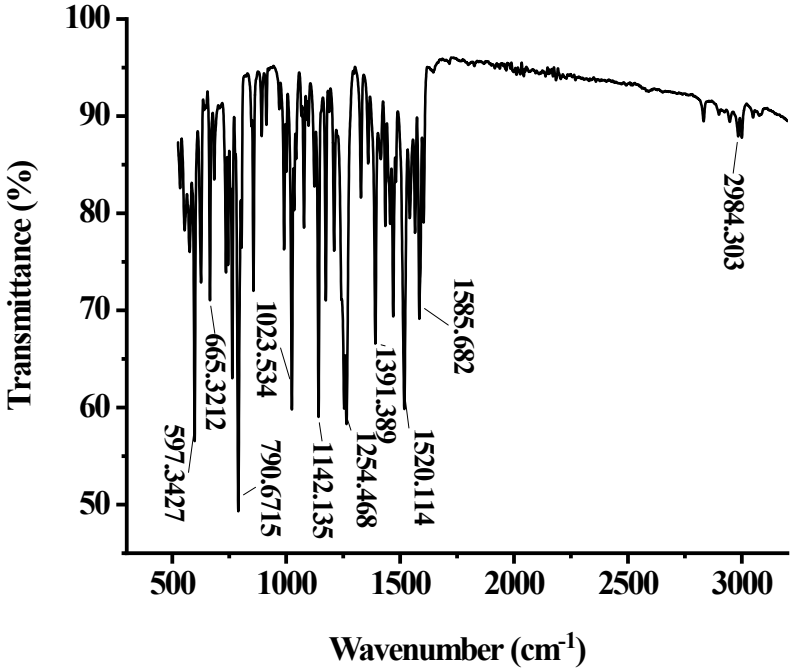


Figure 20. (a) The UV-vis. absorption and (b) λ_{exc}=300 nm fluorescence spectra and (c) λ_{exc}=350 nm fluorescence spectra of compound $\mathbf{C_{20}}$ (10 μM) in different solvents

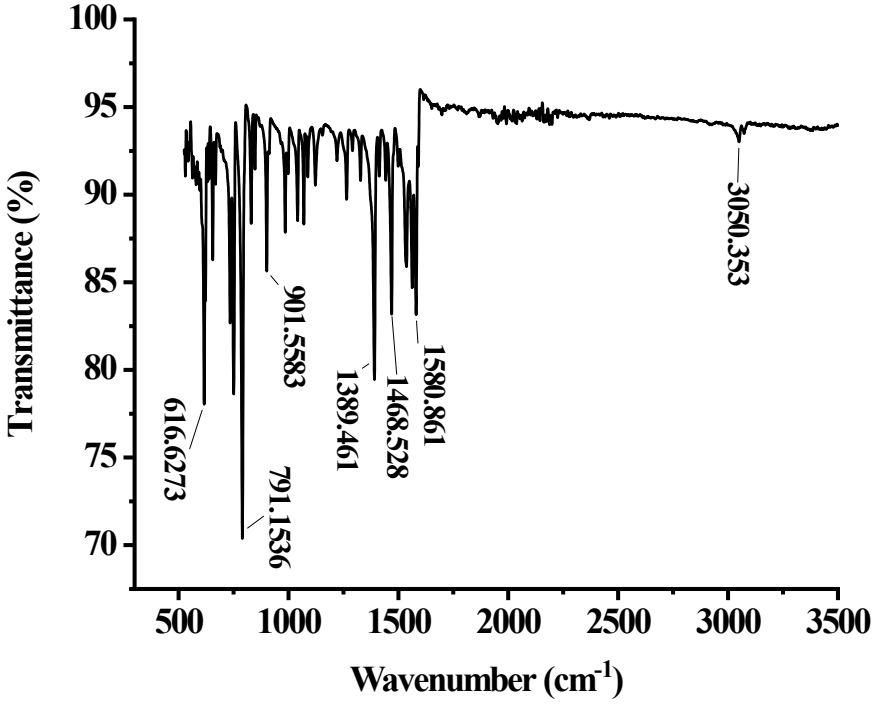
Table S2. FTIR Spectra of All of the Newly Synthesized Ligands & Complexes

Compound No.	FTIR Graphs
L_4	

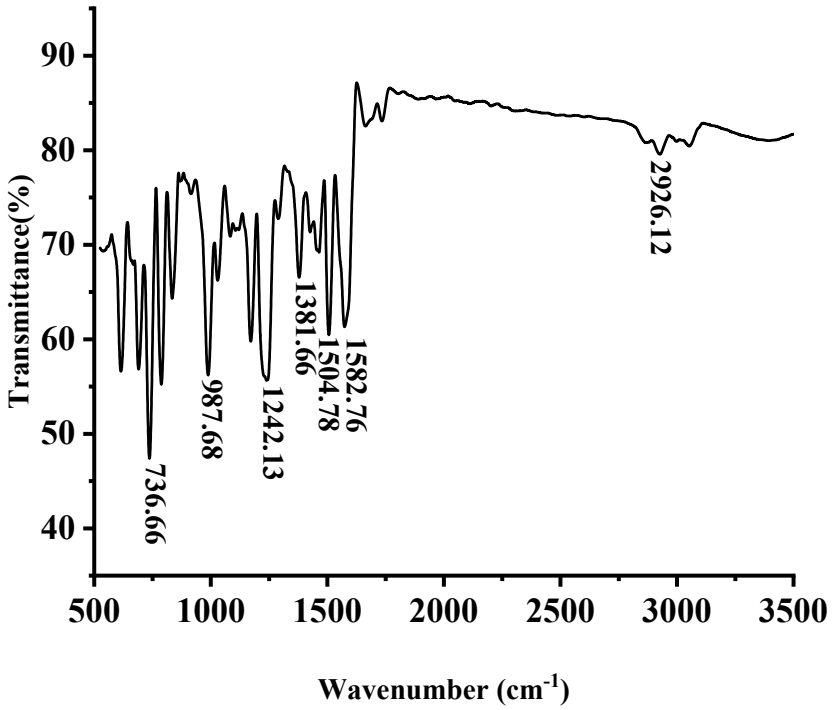
L_5


Transmittance (%)
Wavenumber (cm-1)
597.3427
665.3212
790.6715
1023.534
1142.135
1254.468
1391.389
1520.114
1585.682
2984.303

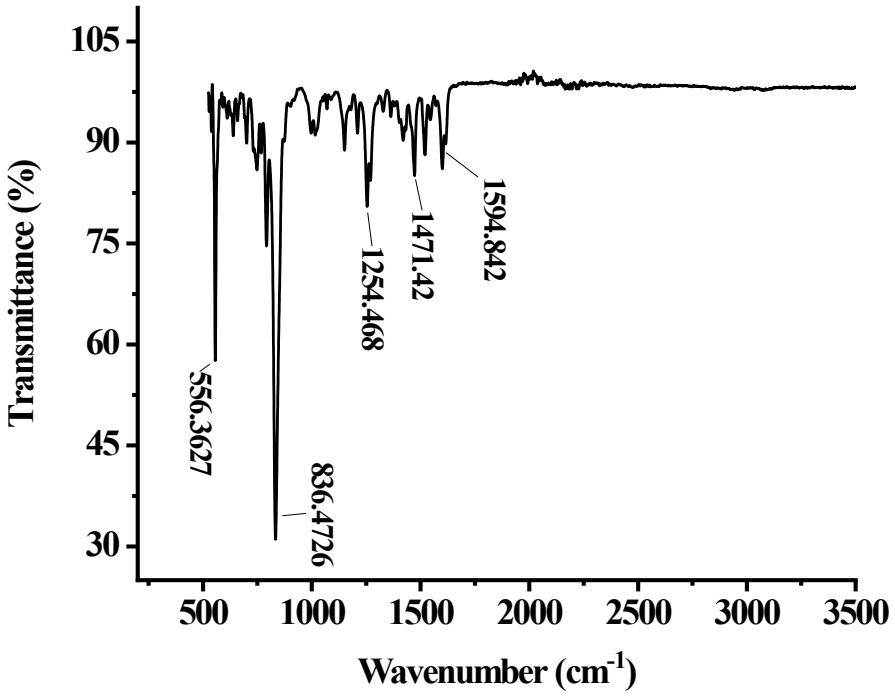
L_9


Transmittance (%)
Wavenumber (cm-1)
616.6273
791.1536
901.5583
1389.461
1468.528
1580.861
3050.353

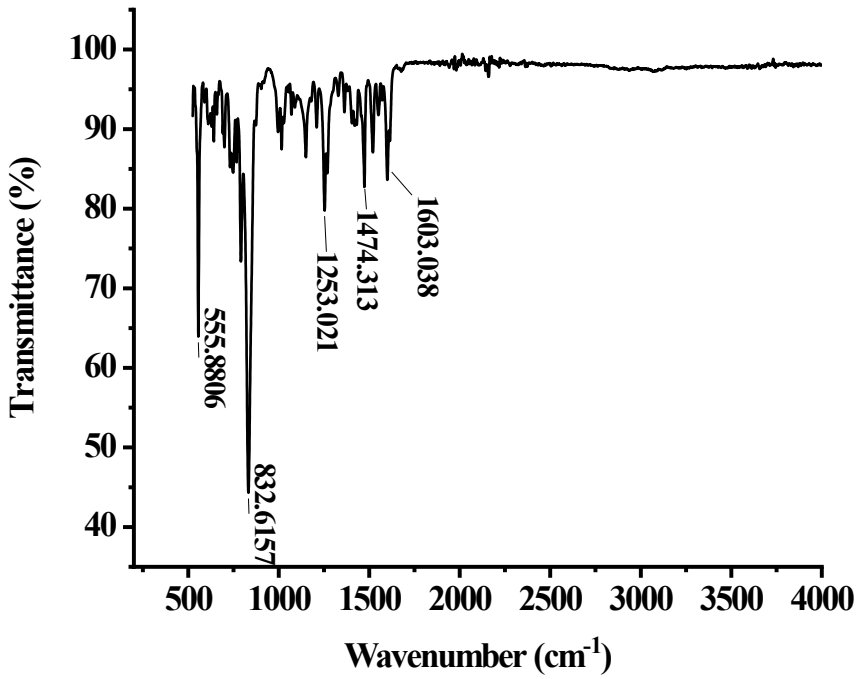
L_{10}


Transmittance(%)
90
80
70
60
50
40
736.66
987.68
1242.13
1381.66
1504.78
1582.76
2926.12
500
1000
1500
2000
2500
3000
3500
Wavenumber (cm-1)

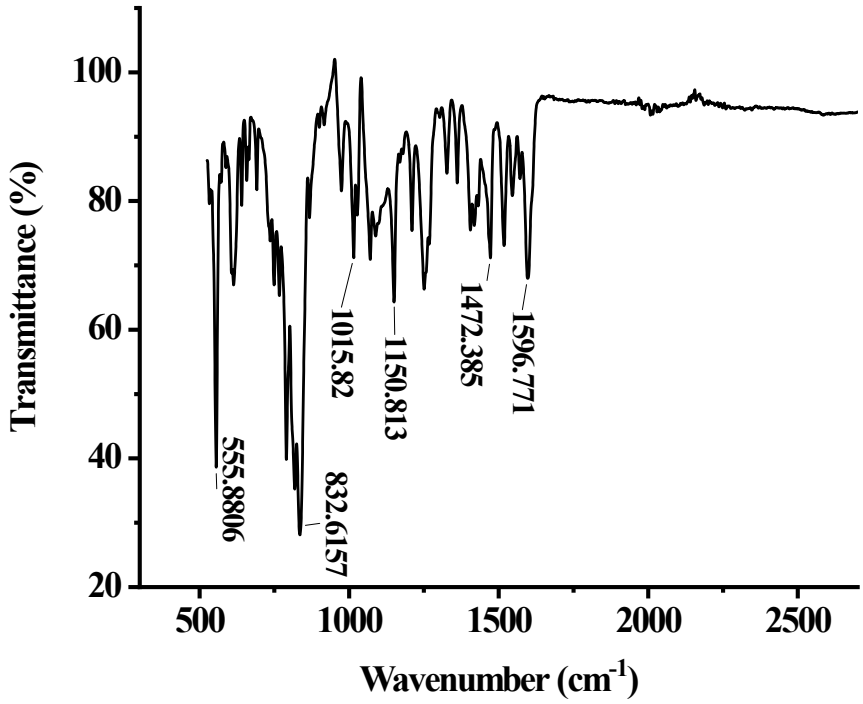
C_1


Transmittance (%)
105
90
75
60
45
30
556.3627
836.4726
1254.468
1471.42
1594.842
500
1000
1500
2000
2500
3000
3500
Wavenumber (cm-1)

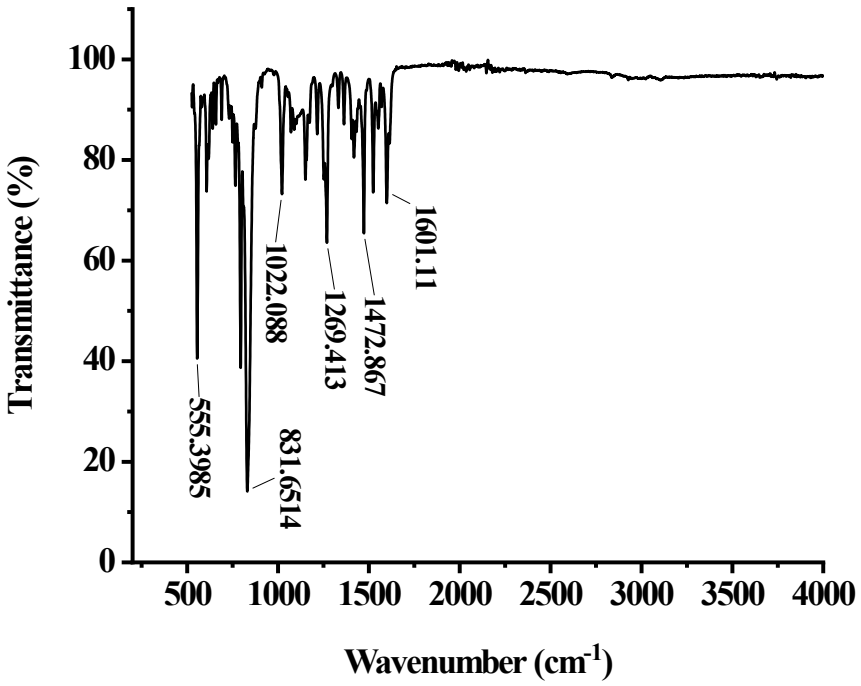
C_2


Transmittance (%)
Wavenumber (cm-1)
555.8806
832.6157
1253.021
1474.313
1603.038

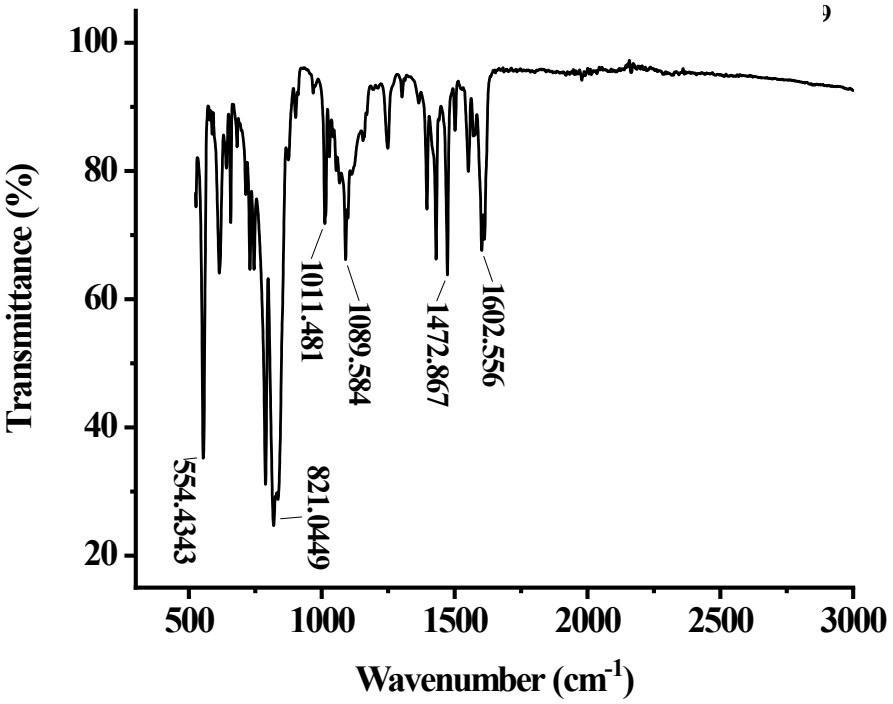
C_4


Transmittance (%)
Wavenumber (cm-1)
555.8806
832.6157
1015.82
1150.813
1472.385
1596.771

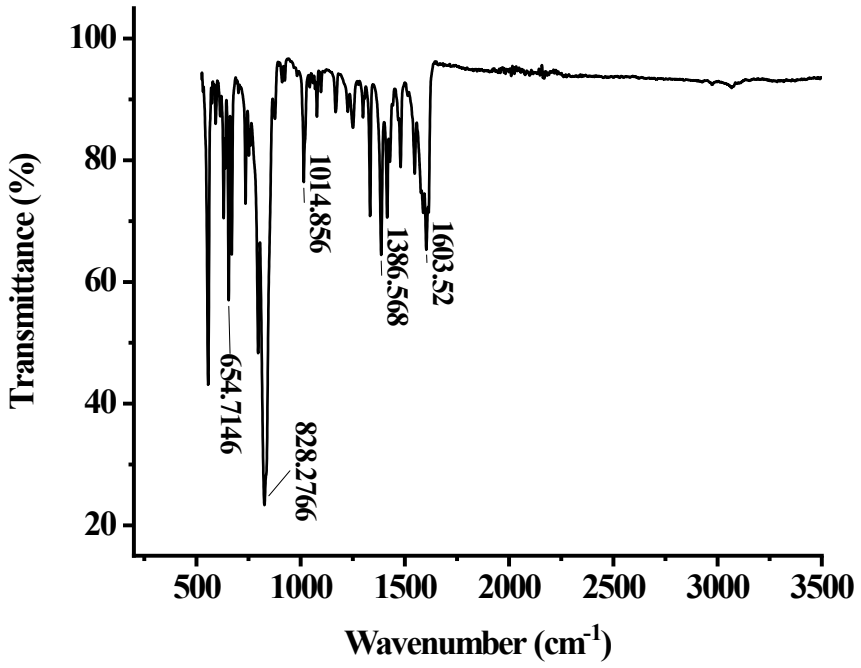
C_5


Transmittance (%)
Wavenumber (cm-1)
555.3985
831.6514
1022.088
1269.413
1472.867
1601.11

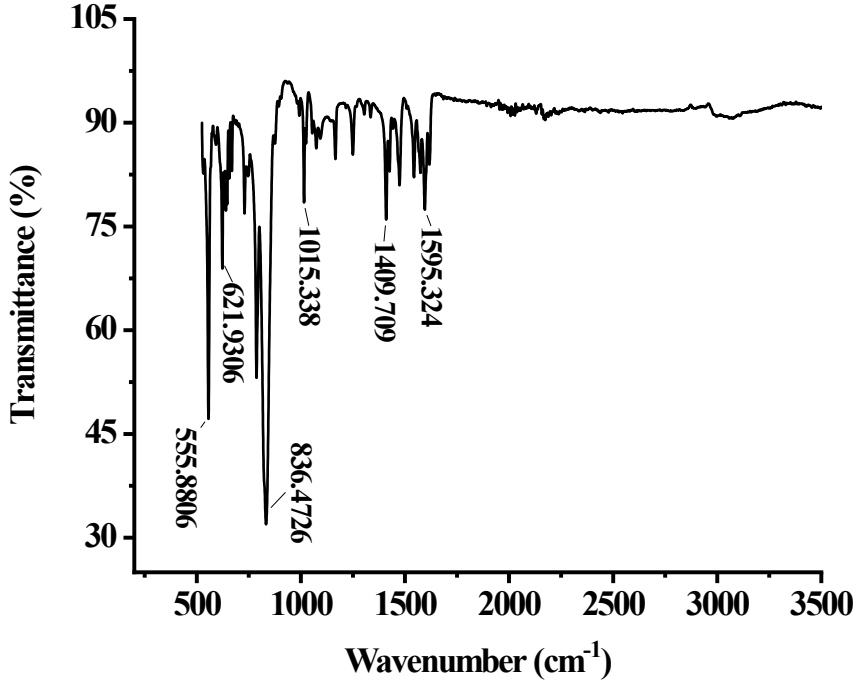
C_6


Transmittance (%)
Wavenumber (cm-1)
554.4343
821.0449
1011.481
1089.584
1472.867
1602.556

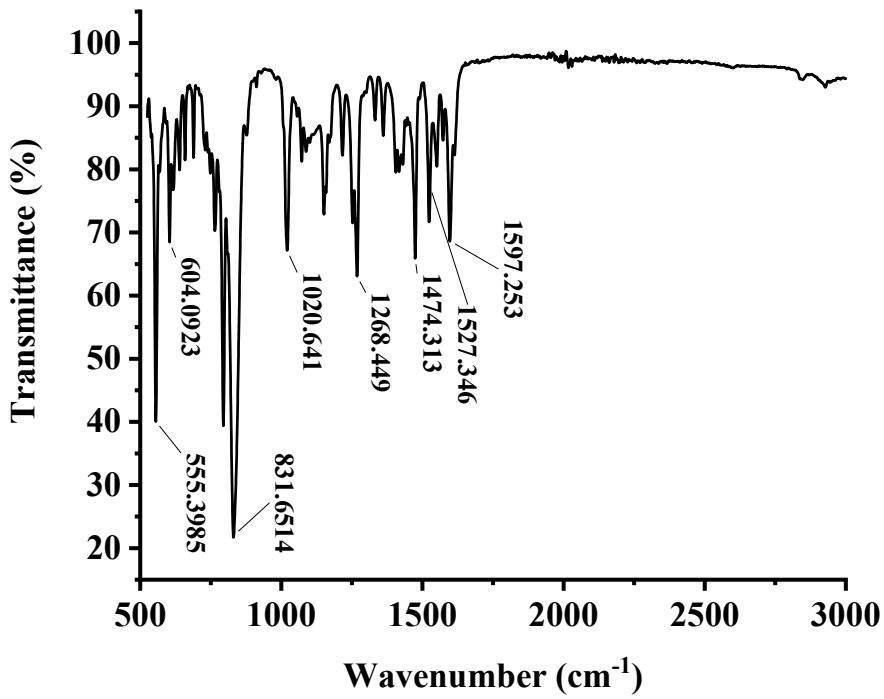
C_7


Transmittance (%)
Wavenumber (cm-1)
654.7146
828.2766
1014.856
1386.568
1603.52

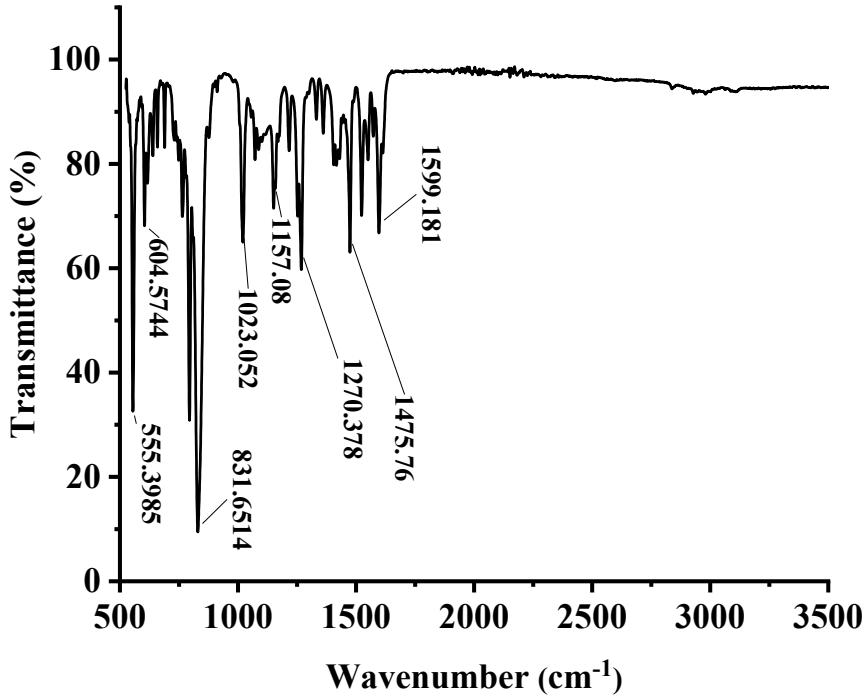
C_8


Transmittance (%)
Wavenumber (cm-1)
555.8806
621.9306
836.4726
1015.338
1409.709
1595.324

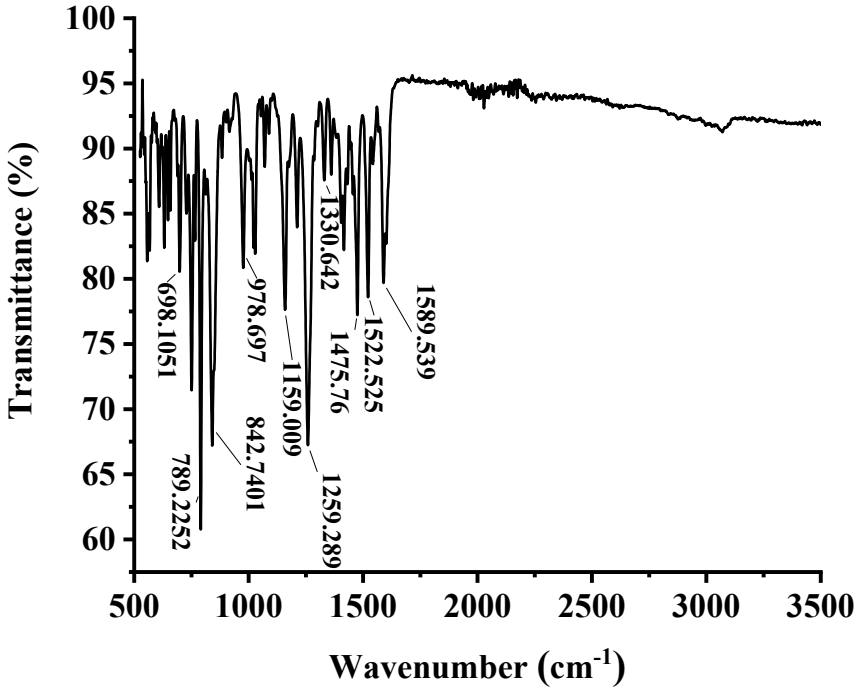
C_{11}


Transmittance (%)
Wavenumber (cm-1)
604.0923
555.3985
831.6514
1020.641
1268.449
1474.313
1527.346
1597.253

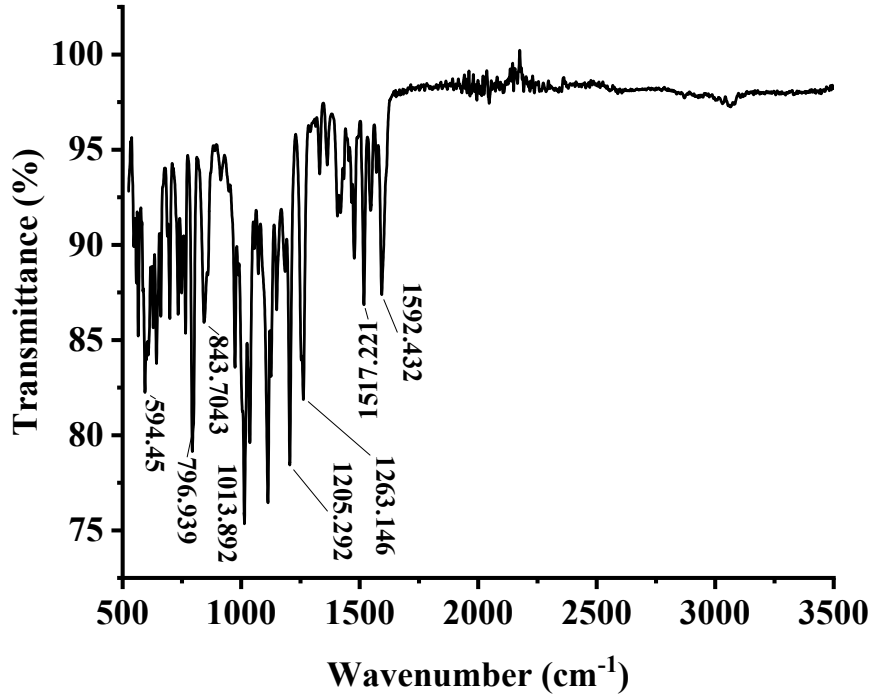
C_{12}


Transmittance (%)
Wavenumber (cm-1)
604.5744
555.3985
831.6514
1023.052
1157.08
1270.378
1475.76
1599.181

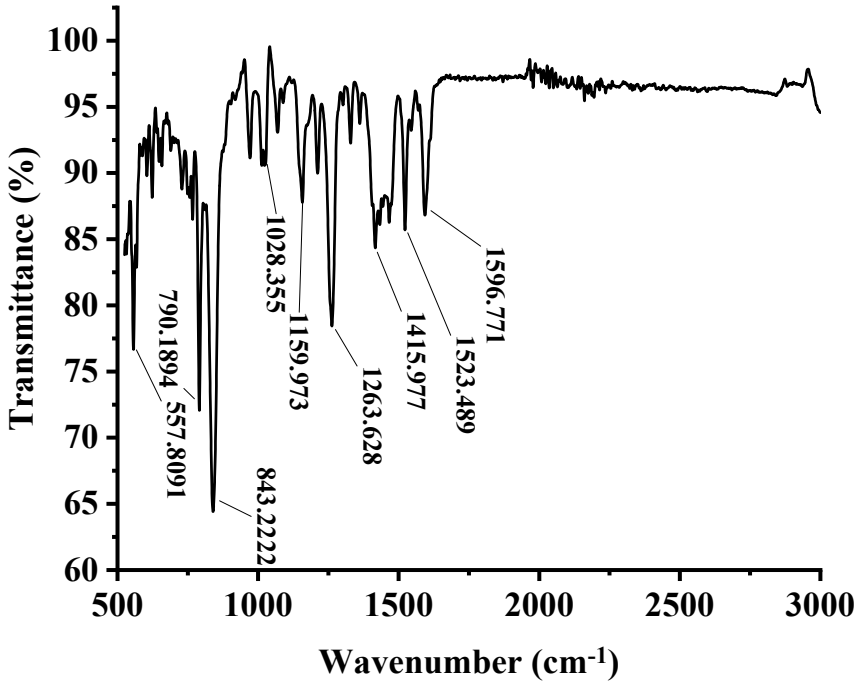
C_{13}


Transmittance (%)
Wavenumber (cm-1)
698.1051
789.2252
842.7401
978.697
1159.009
1259.289
1330.642
1475.76
1522.525
1589.539

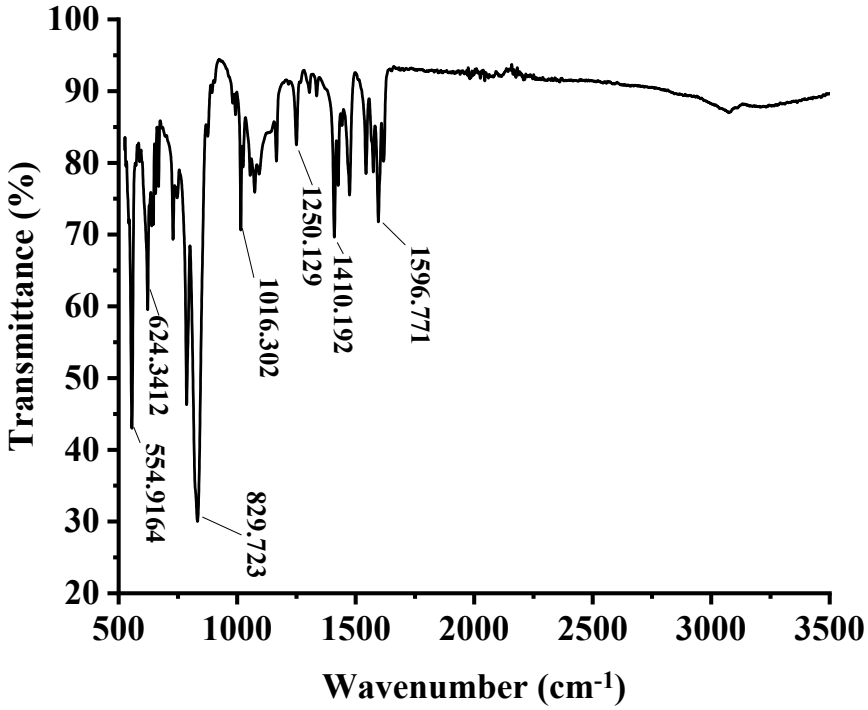
C_{14}


Transmittance (%)
Wavenumber (cm-1)
594.45
796.939
843.7043
1013.892
1205.292
1263.146
1517.221
1592.432

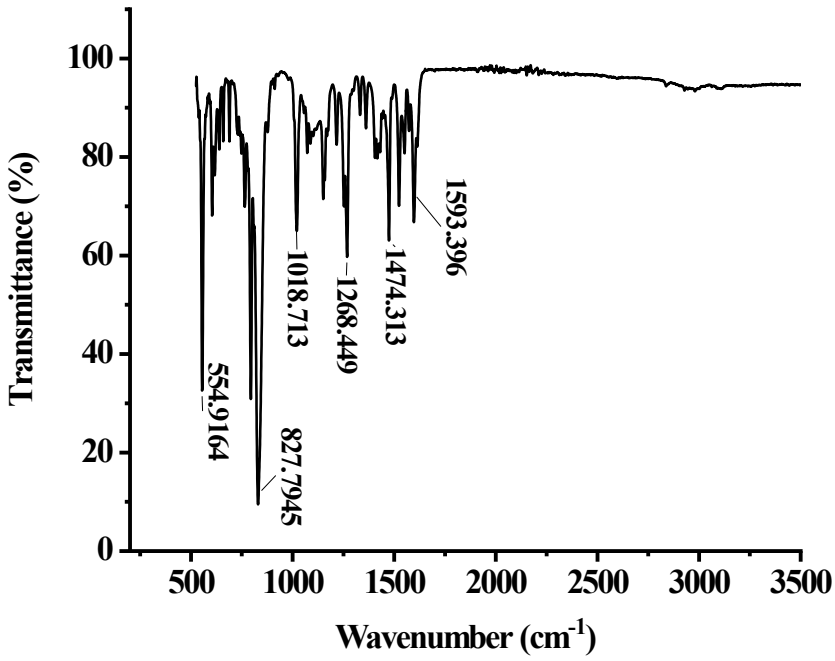
C_{15}


Transmittance (%)
Wavenumber (cm-1)
1028.355
1159.973
1263.628
1415.977
1523.489
1596.771
790.1894
557.8091
843.2222

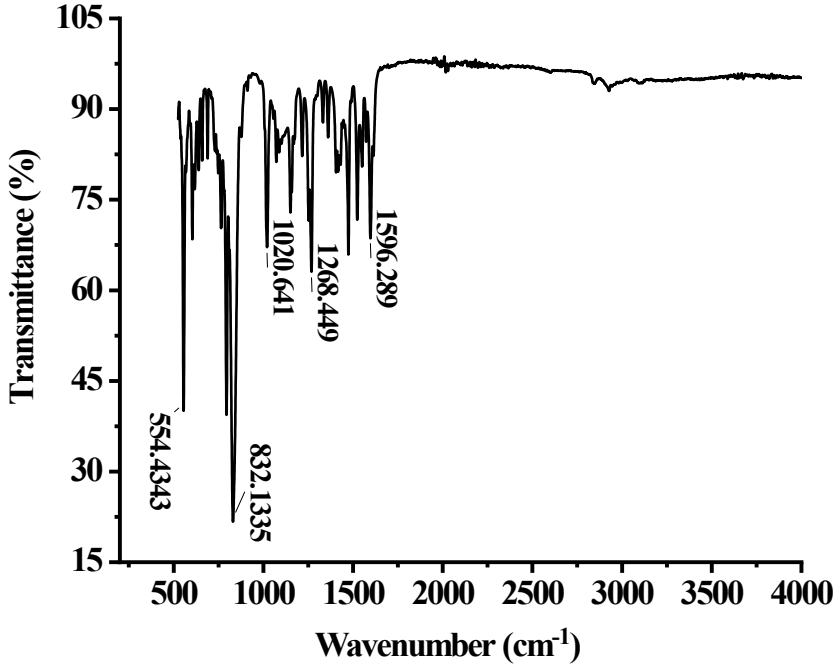
C_{16}


Transmittance (%)
Wavenumber (cm-1)
1250.129
1410.192
1596.771
1016.302
624.3412
554.9164
829.723

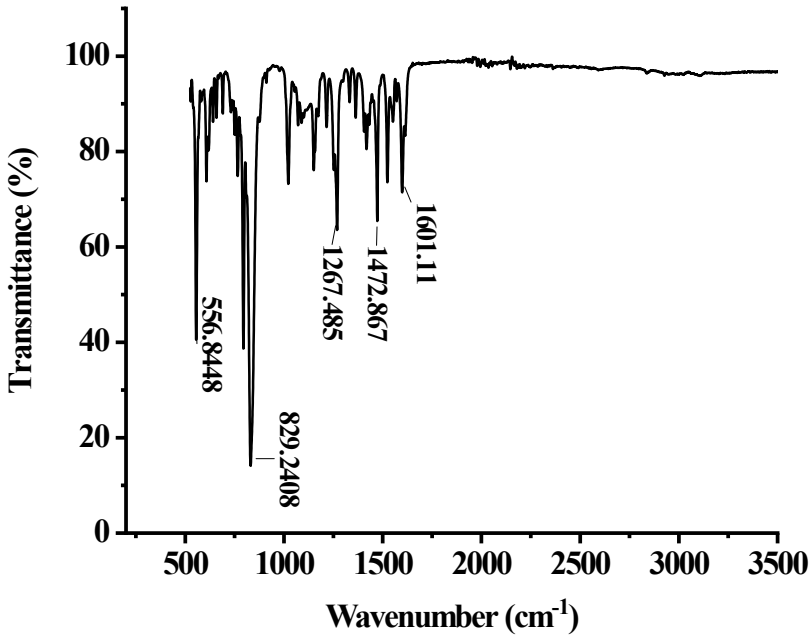
C_{17}


Transmittance (%)
Wavenumber (cm-1)
554.9164
827.7945
1018.713
1268.449
1474.313
1593.396

C_{18}


Transmittance (%)
Wavenumber (cm-1)
554.4343
832.1335
1020.641
1268.449
1596.289

C_{19}


Transmittance (%)
Wavenumber (cm-1)
556.8448
829.2408
1267.485
1472.867
1601.11

C_{20}

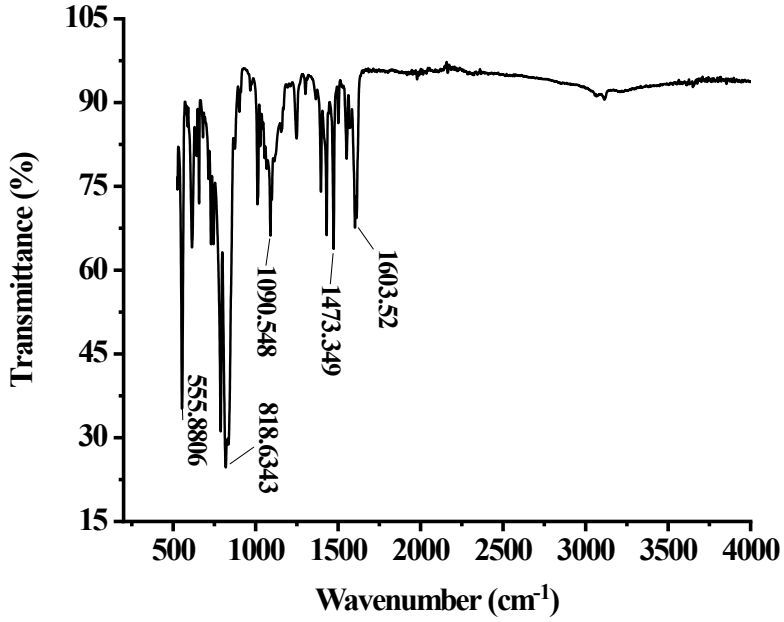
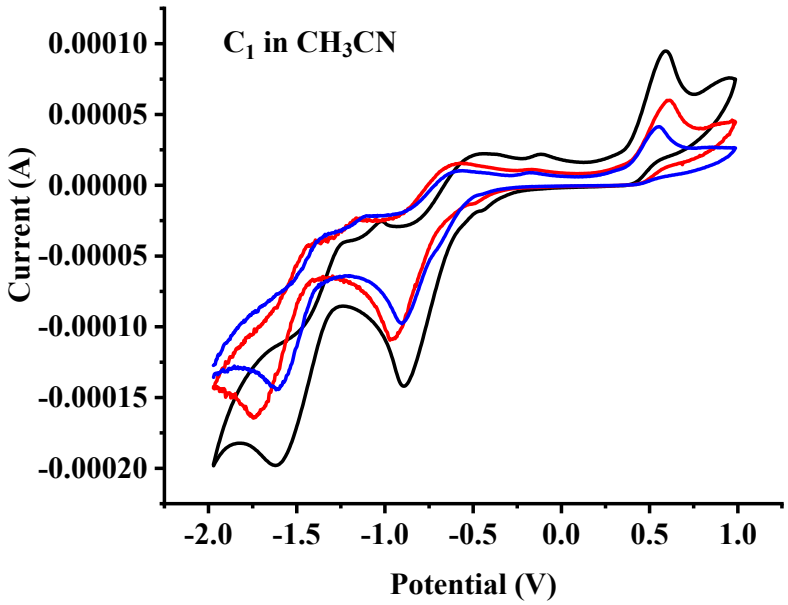
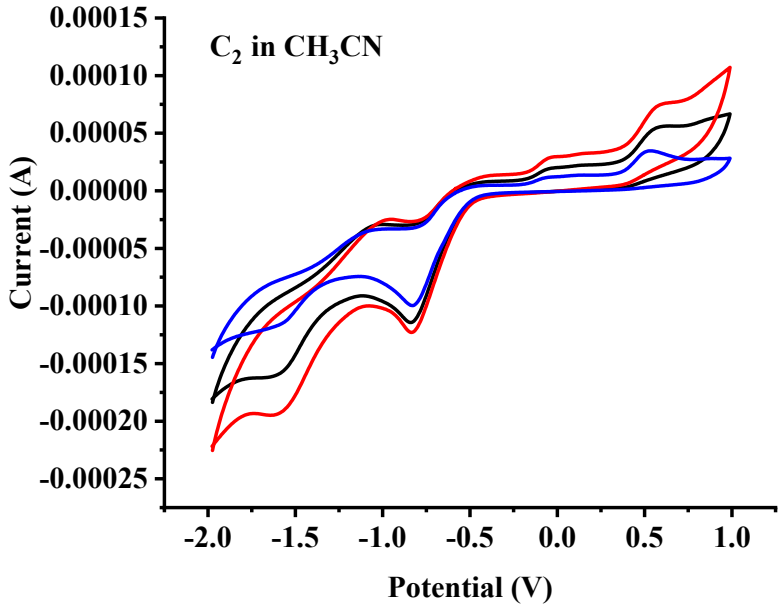

Transmittance (%)
Wavenumber (cm-1)
555.8806
818.6343
1090.548
1473.349
1603.52

Table S3. CV Graphs of All the Synthesized Complexes (C_1-C_{20}) at (200, 100 & 40 mVs^{-1})

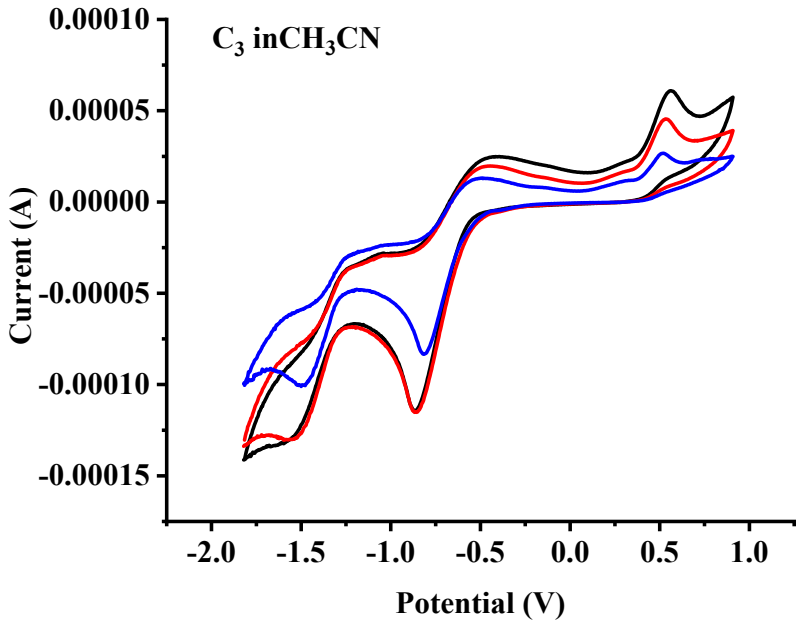
In these graphs, the black voltammogram corresponds to a scan rate of 200 mVs^{-1}, the red voltammogram represents 100 mVs^{-1}, and the blue voltammogram indicates 40 mVs^{-1}.

Compound No.	CV Graphs
C_1	

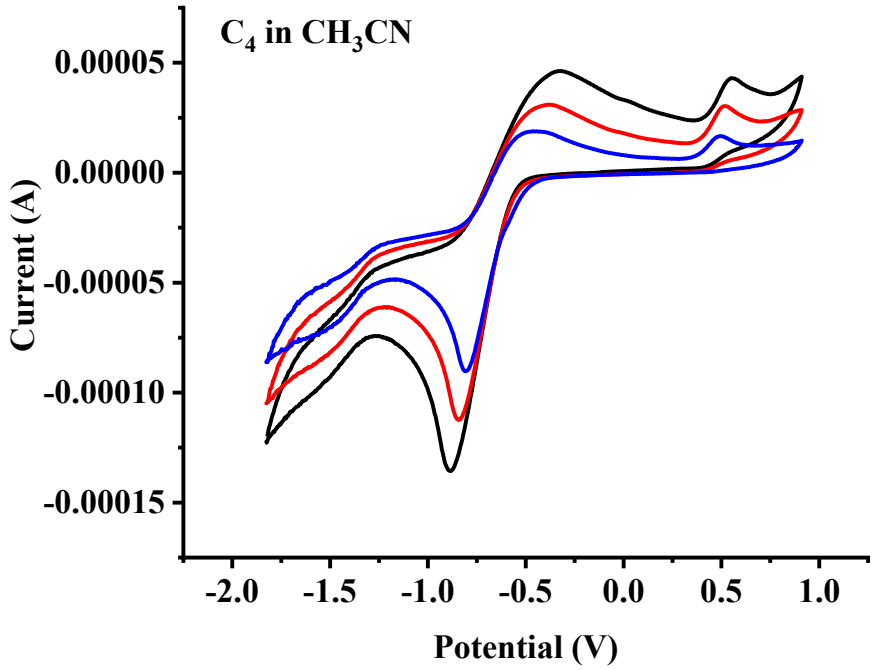
C_2


C2 in CH3CN
Current (A)
Potential (V)
0.00015
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
-0.00020
-0.00025
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0

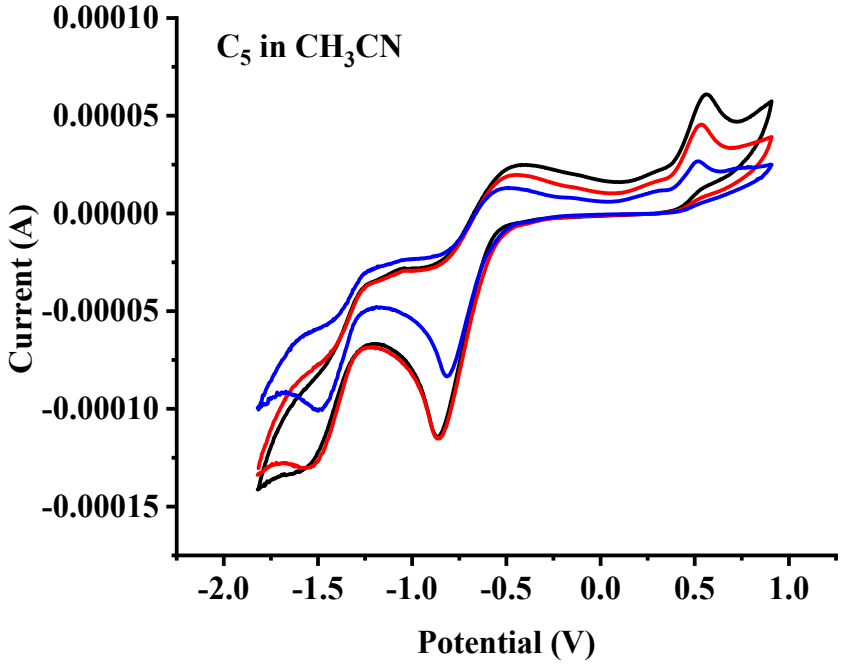
C_3


C3 inCH3CN
Current (A)
Potential (V)
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0

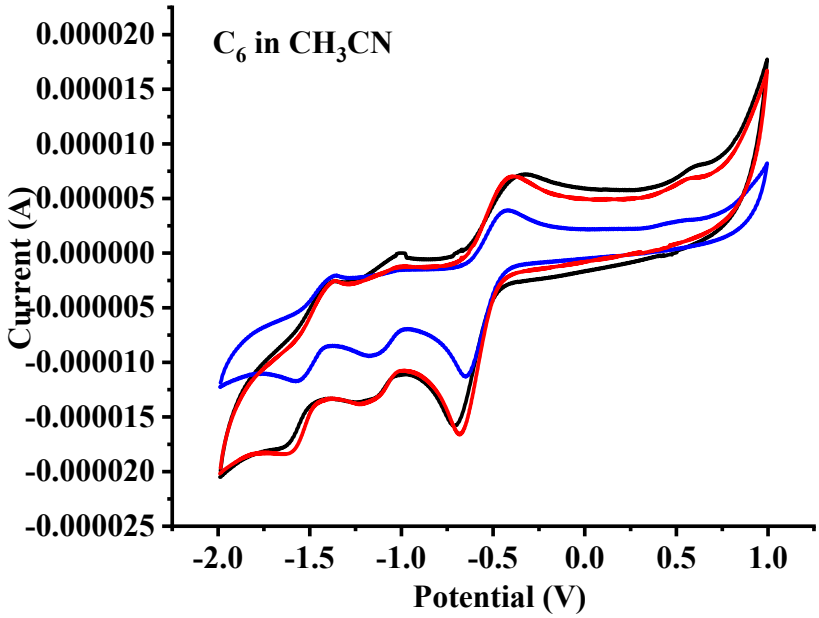
C_4


C4 in CH3CN
0.00005
0.00000
-0.00005
-0.00010
-0.00015
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

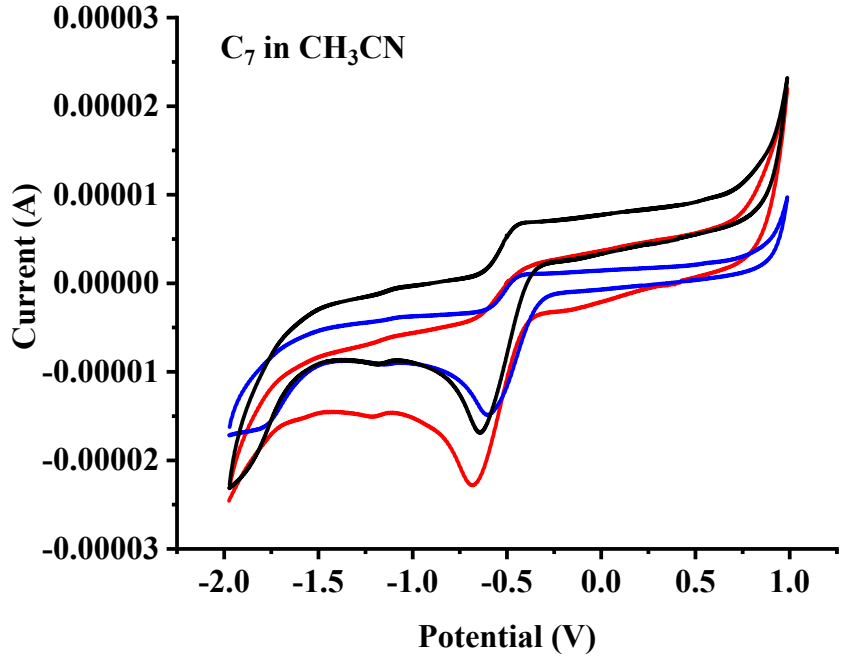
C_5


C5 in CH3CN
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

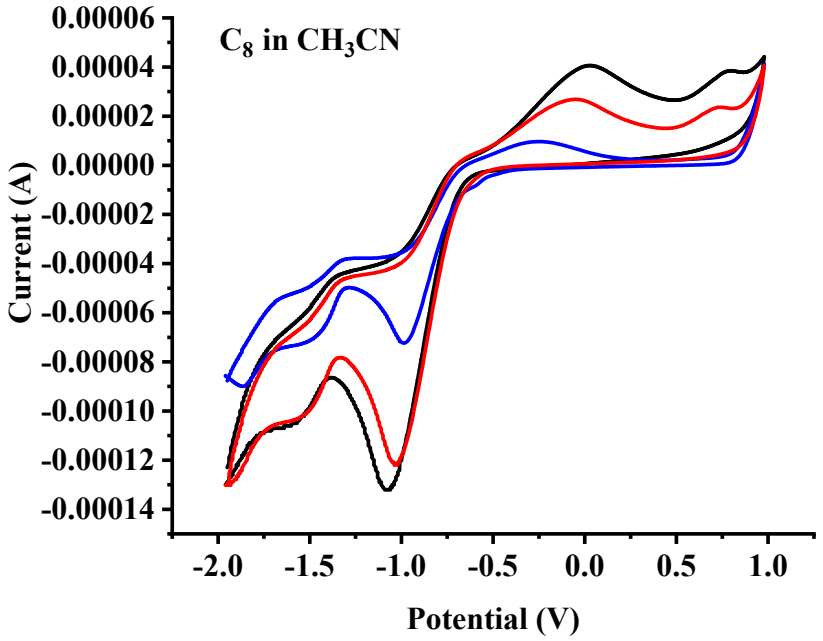
C_6


C6 in CH3CN
0.000020
0.000015
0.000010
0.000005
0.000000
-0.000005
-0.000010
-0.000015
-0.000020
-0.000025
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

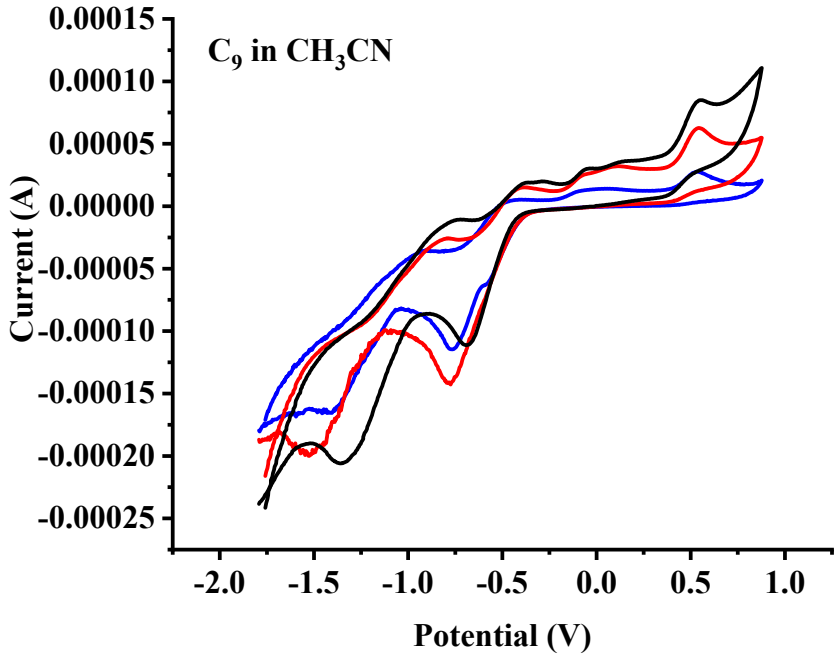
C_7


C7 in CH3CN
0.00003
0.00002
0.00001
0.00000
-0.00001
-0.00002
-0.00003
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

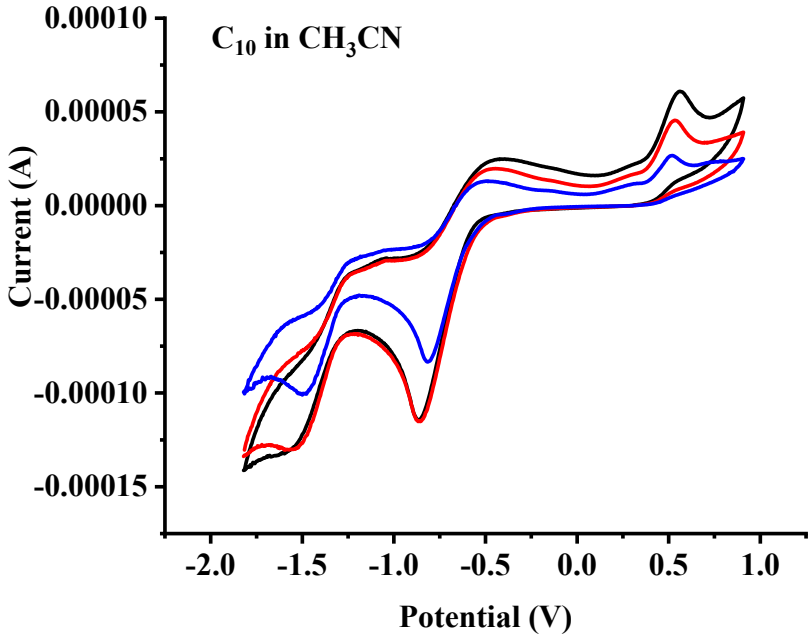
C_8


C8 in CH3CN
Current (A)
Potential (V)
0.00006
0.00004
0.00002
0.00000
-0.00002
-0.00004
-0.00006
-0.00008
-0.00010
-0.00012
-0.00014
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0

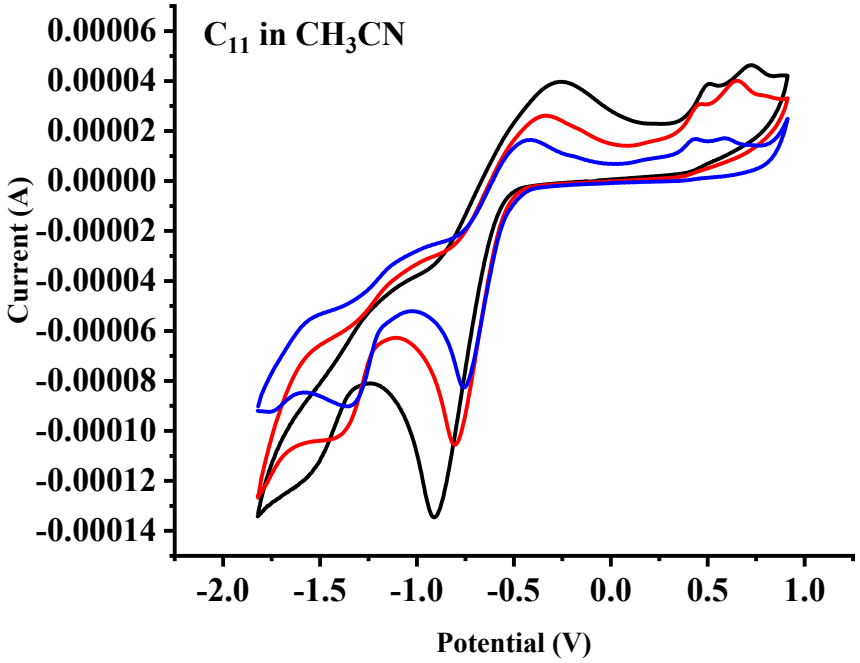
C_9


C9 in CH3CN
Current (A)
Potential (V)
0.00015
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
-0.00020
-0.00025
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0

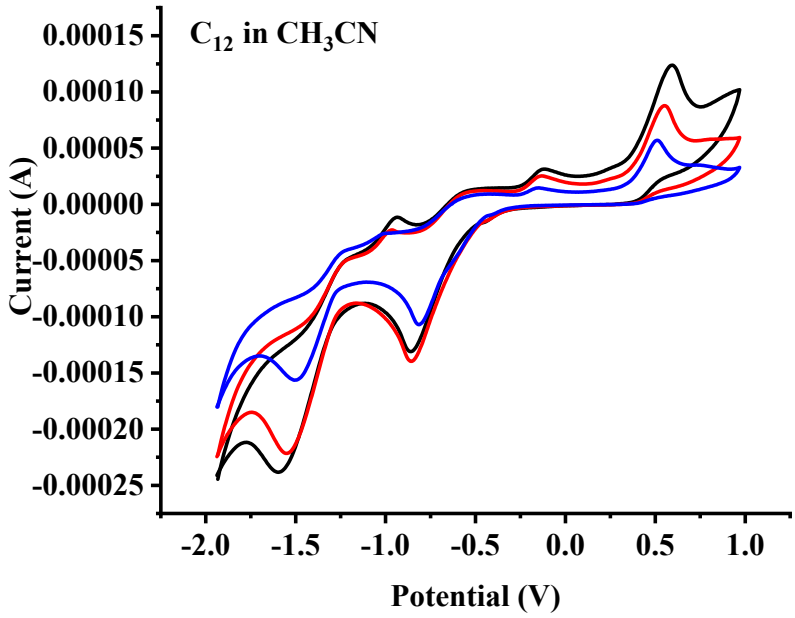
C_{10}


C10 in CH3CN
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

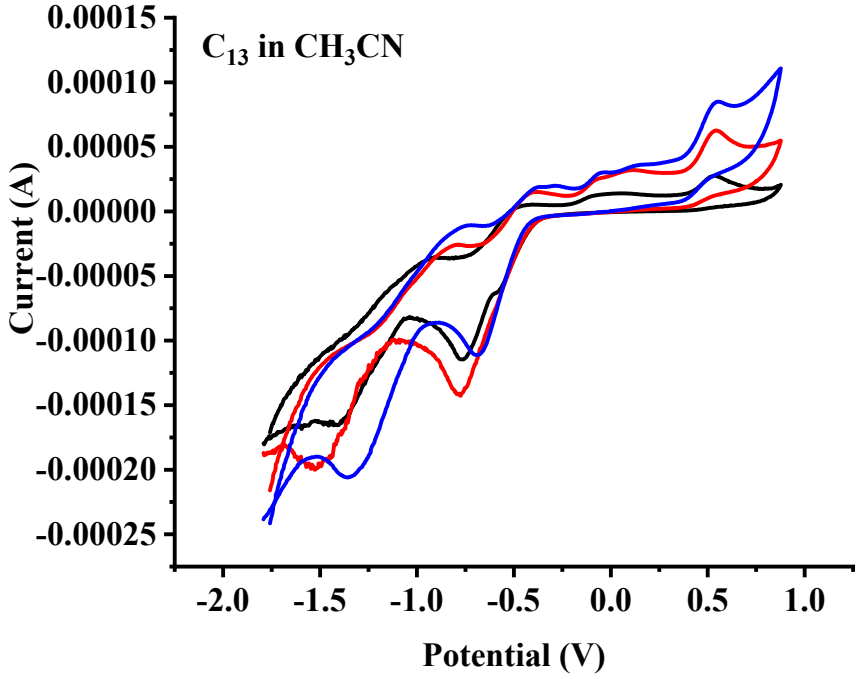
C_{11}


C11 in CH3CN
0.00006
0.00004
0.00002
0.00000
-0.00002
-0.00004
-0.00006
-0.00008
-0.00010
-0.00012
-0.00014
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

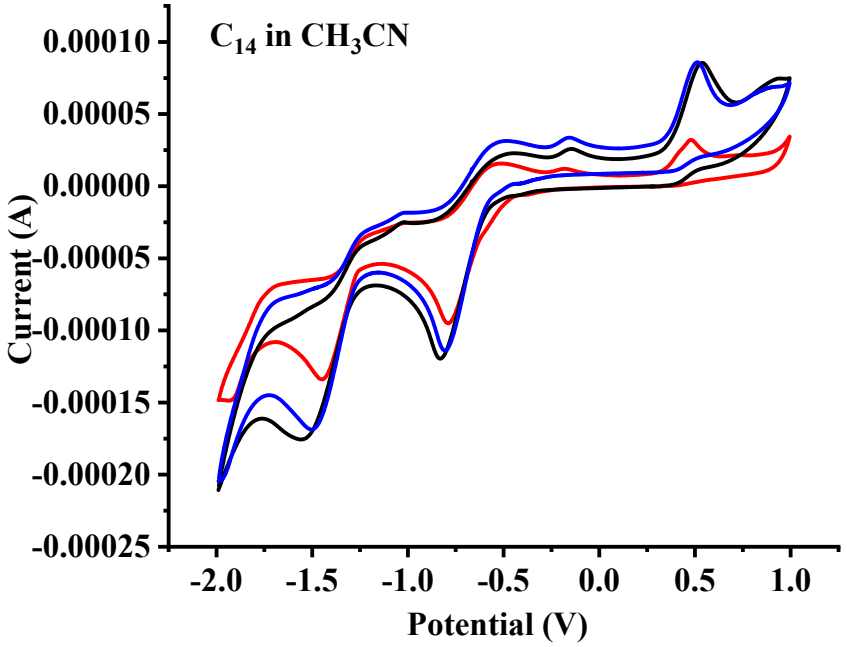
C_{12}


C12 in CH3CN
0.00015
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
-0.00020
-0.00025
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

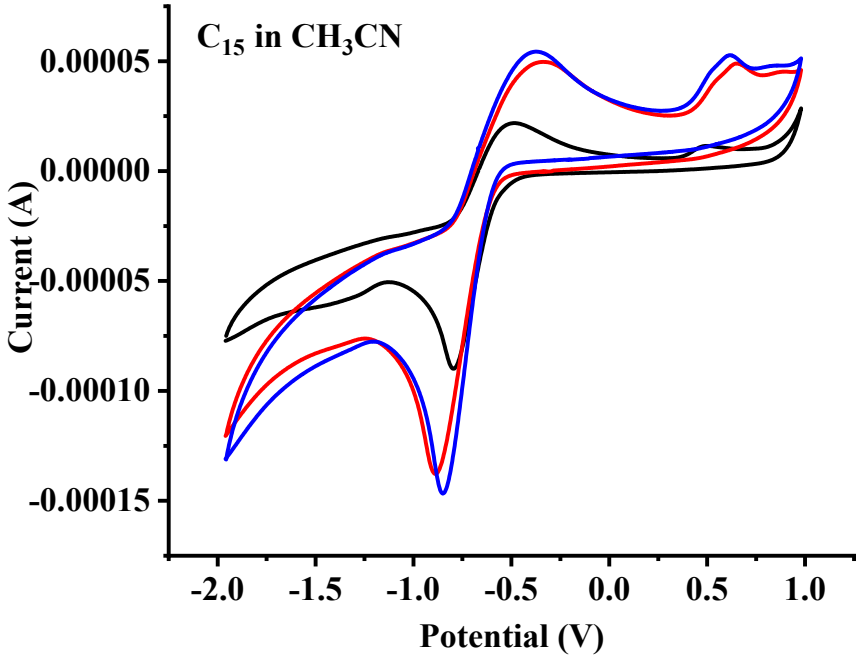
C_{13}


C13 in CH3CN
0.00015
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
-0.00020
-0.00025
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

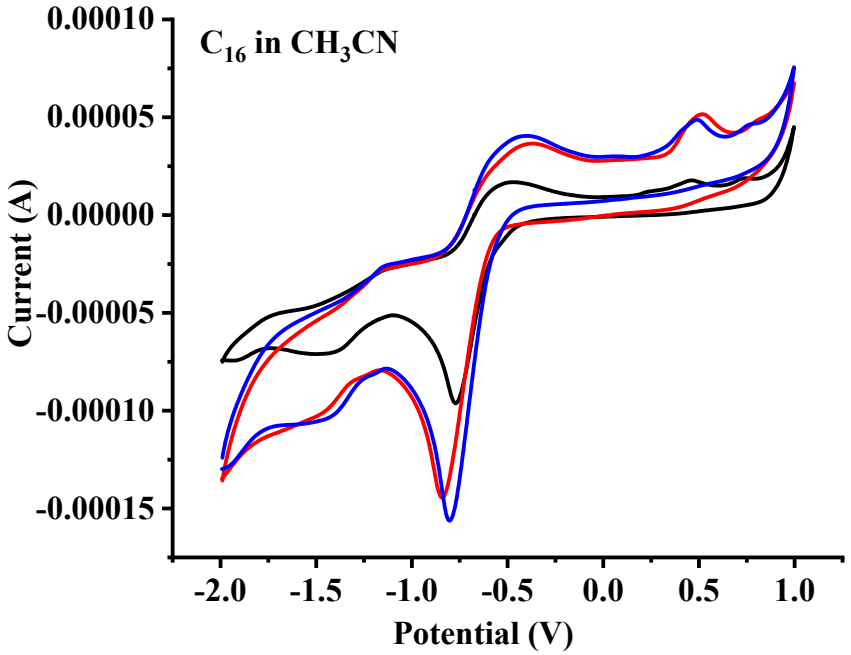
C_{14}


C14 in CH3CN
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
-0.00020
-0.00025
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

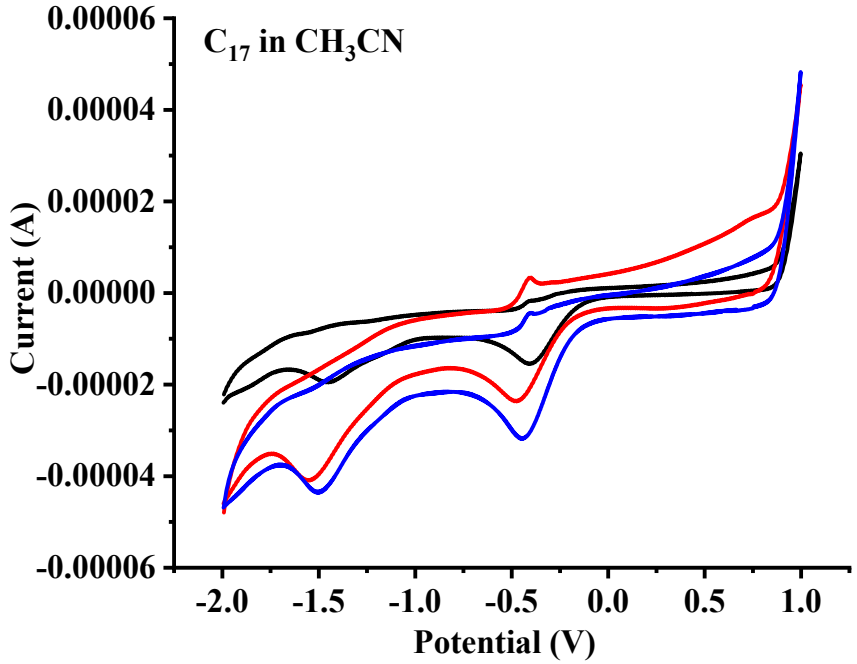
C_{15}


C15 in CH3CN
0.00005
0.00000
-0.00005
-0.00010
-0.00015
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

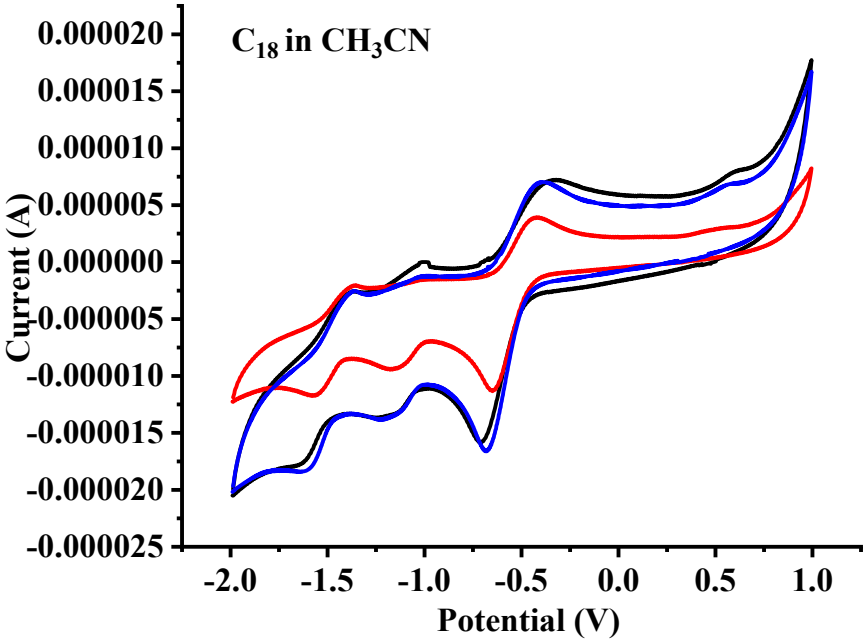
C_{16}


C16 in CH3CN
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

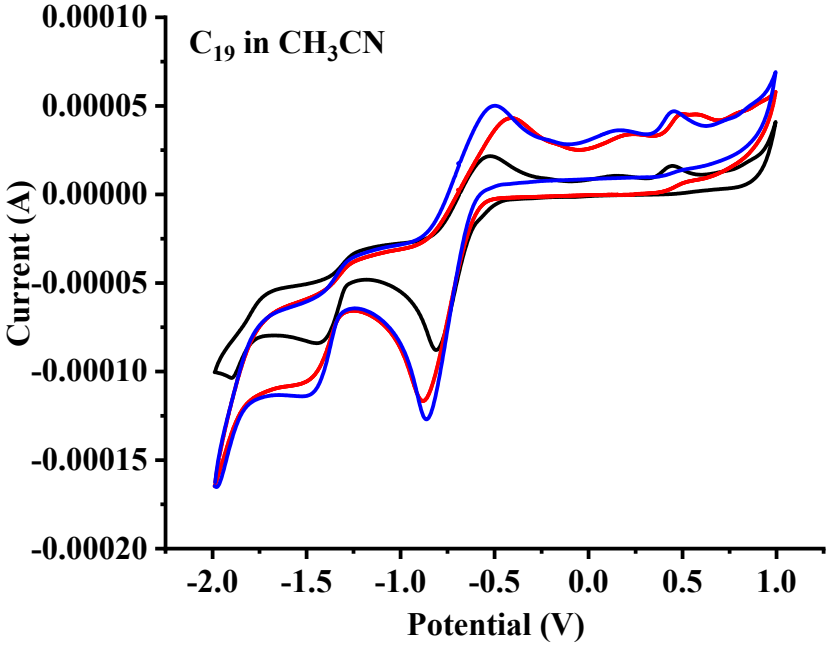
C_{17}


C17 in CH3CN
0.00006
0.00004
0.00002
0.00000
-0.00002
-0.00004
-0.00006
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

C_{18}


C18 in CH3CN
0.000020
0.000015
0.000010
0.000005
0.000000
-0.000005
-0.000010
-0.000015
-0.000020
-0.000025
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

C_{19}


C19 in CH3CN
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
-0.00020
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

C_{20}

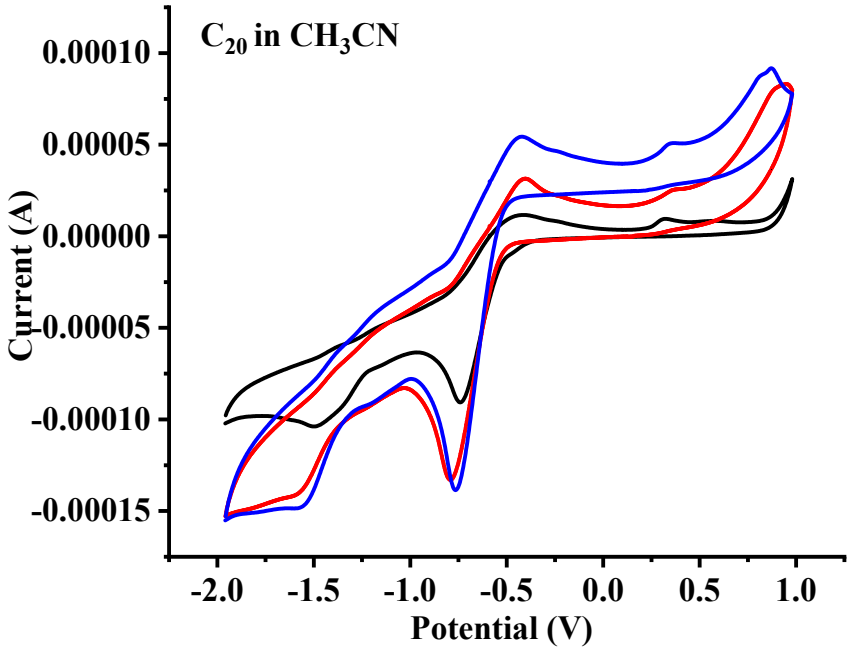
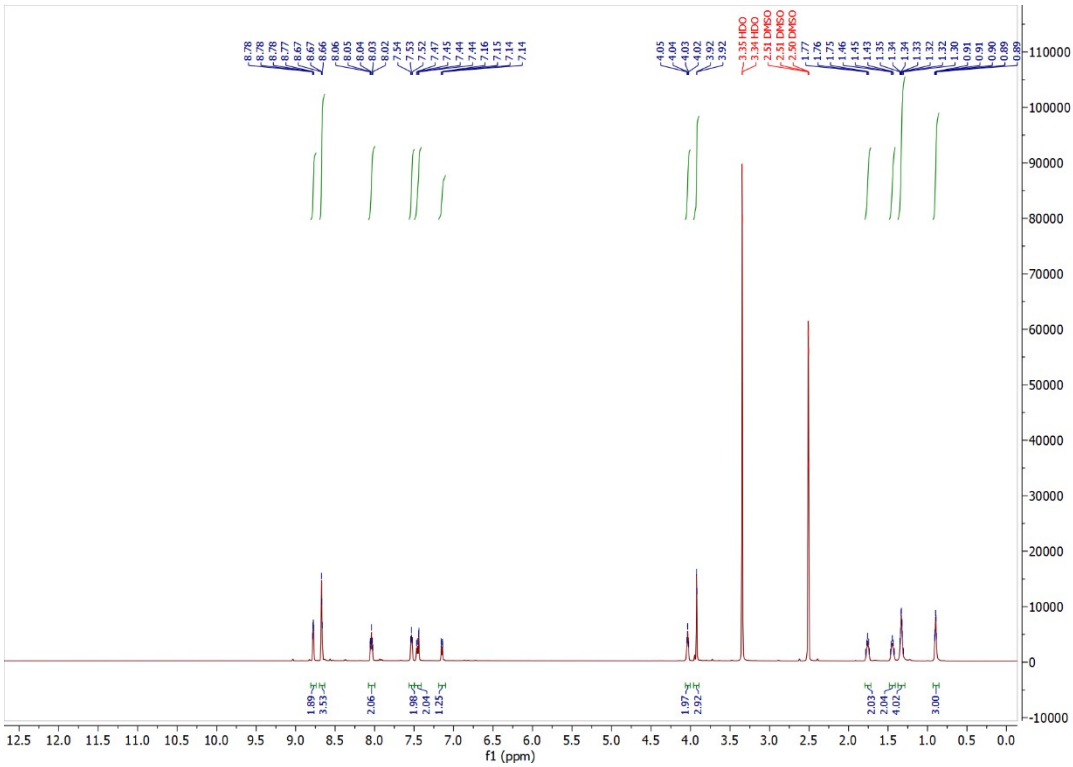

C20 in CH3CN
0.00010
0.00005
0.00000
-0.00005
-0.00010
-0.00015
Current (A)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Potential (V)

Table S4. Quantum chemical descriptors for the TPY-based complexes

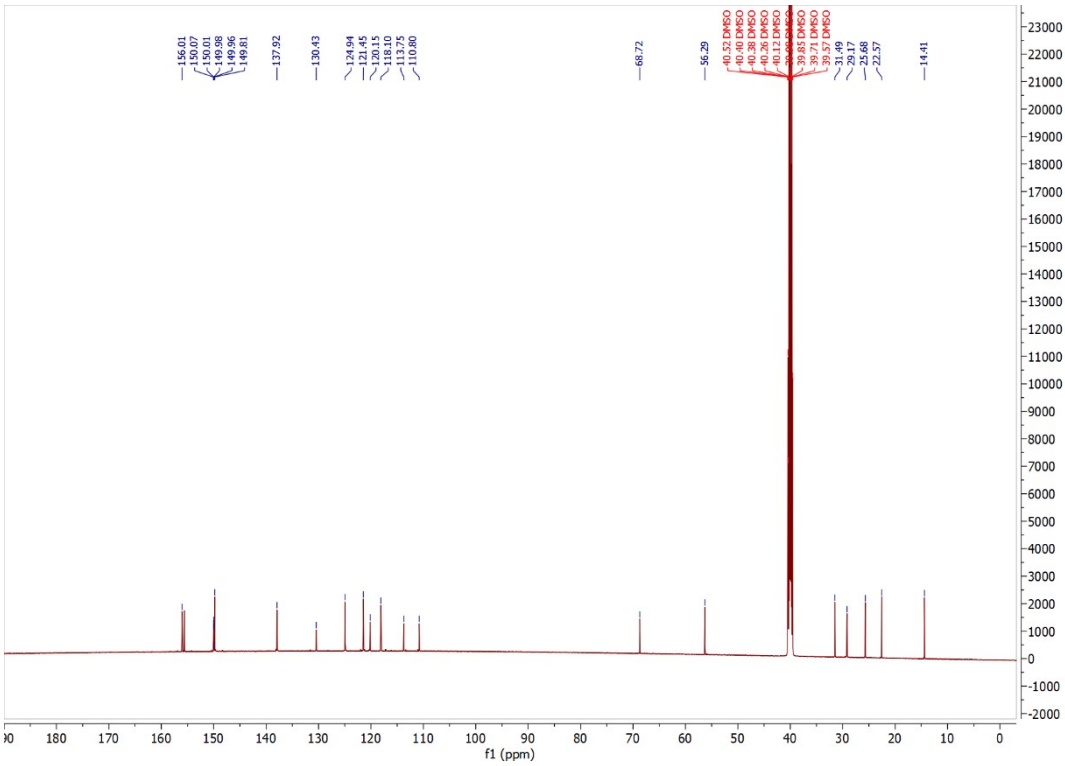
Molecules	Global Hardness (η)	Global Softness (σ)	Chemical Potential (μ)	Electro-negativity (x)	Electro-philicity (ω)	Total charge transfer ΔN_{max}
C_1	0.61	1.646	-2.26	2.26	1.56	3.70
C_4	0.315	3.17	-2.22	2.22	0.77	7.03
C_5	0.305	3.28	-2.27	2.27	0.78	7.43
C_6	0.64	1.56	-2.36	2.36	1.78	3.69
C_8	0.32	3.13	-2.77	2.77	1.23	8.66
C_9	0.57	1.75	-2.54	2.54	1.84	4.46
C_{11}	0.5	2.00	-3.04	3.04	2.31	6.08
C_{16}	0.53	1.89	-2.65	2.65	1.86	5.00
C_{18}	0.425	2.35	-3.015	3.015	1.93	7.09
C_{19}	0.325	3.08	-2.38	2.38	0.92	7.31

Figure S2: NMR Spectra of the Newly Synthesized Ligands and Complexes

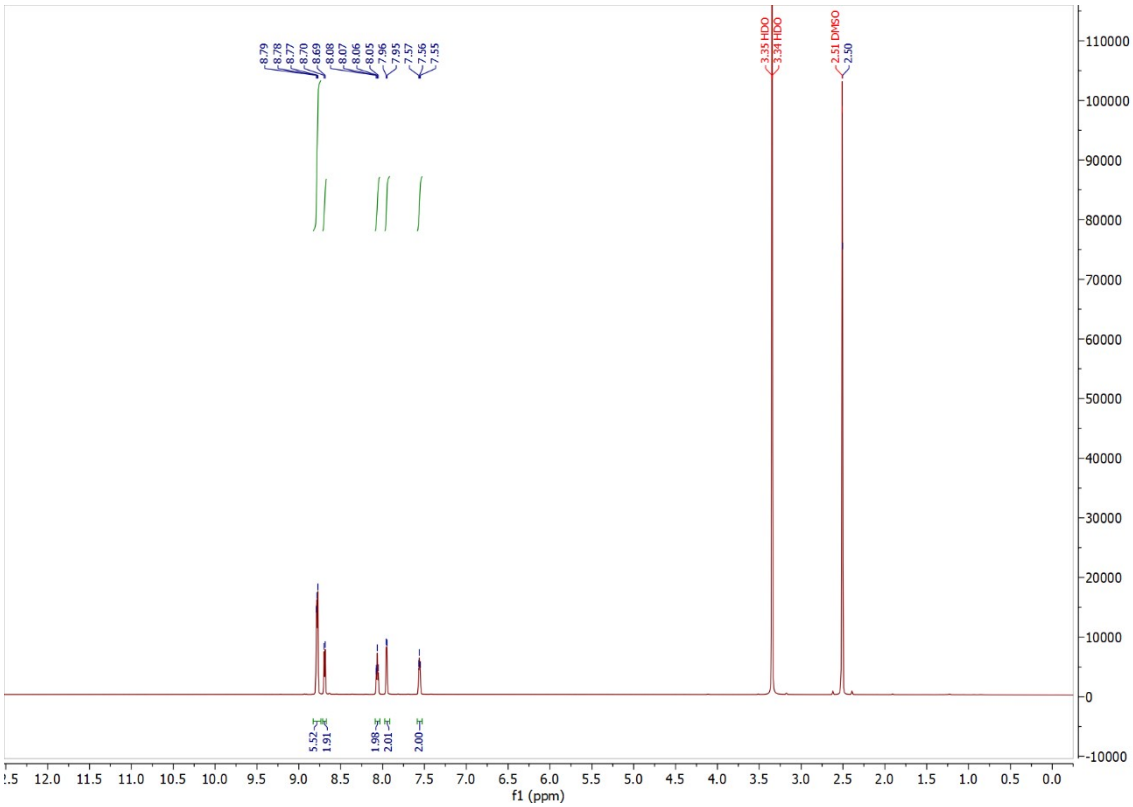
^{1}H-NMR Spectrum (600 MHz, DMSO-d_6) of Compound L_4



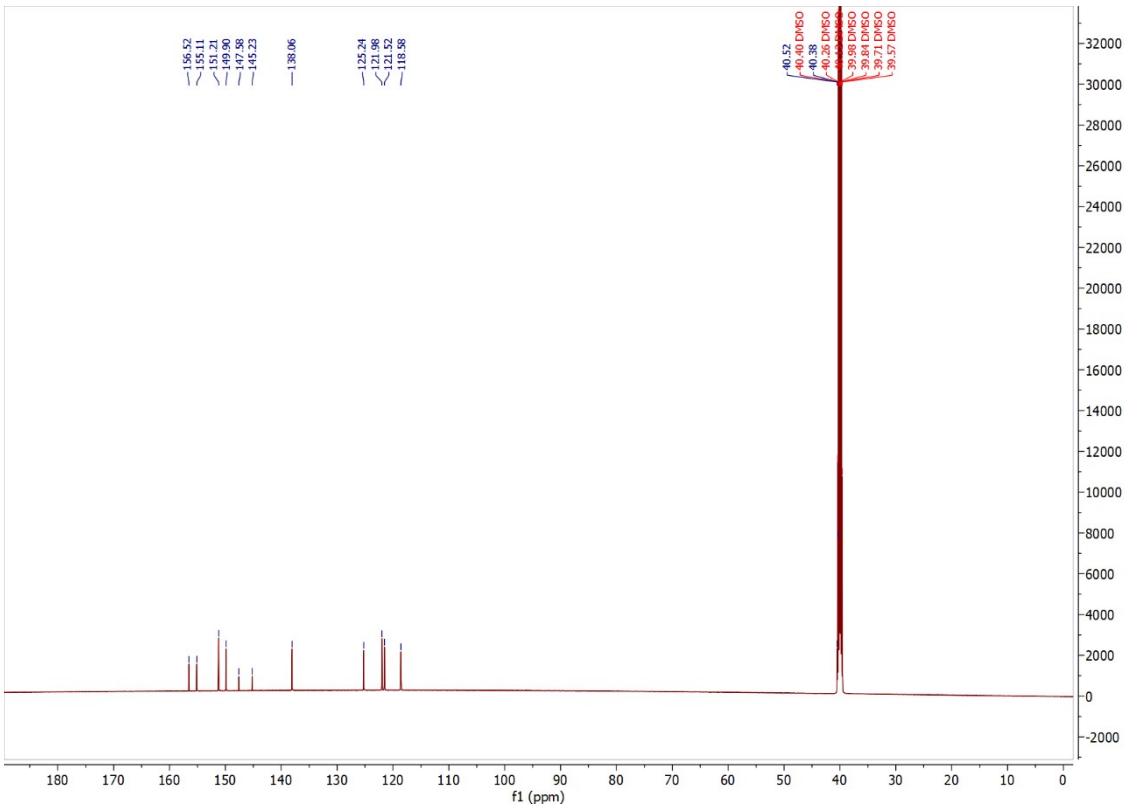
^{13}C-NMR Spectrum (151 MHz, DMSO-d_6) of Compound L_4



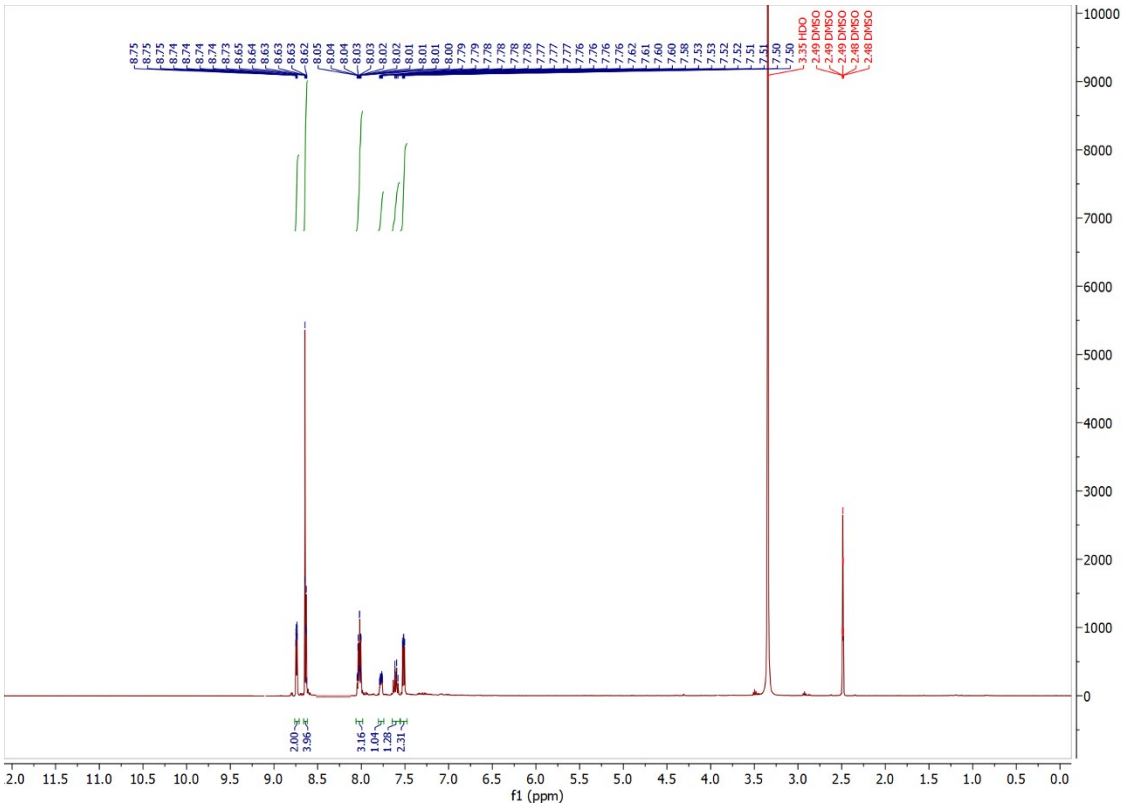
^{1}H-NMR Spectrum (600 MHz, DMSO-d_6) of Compound L_5



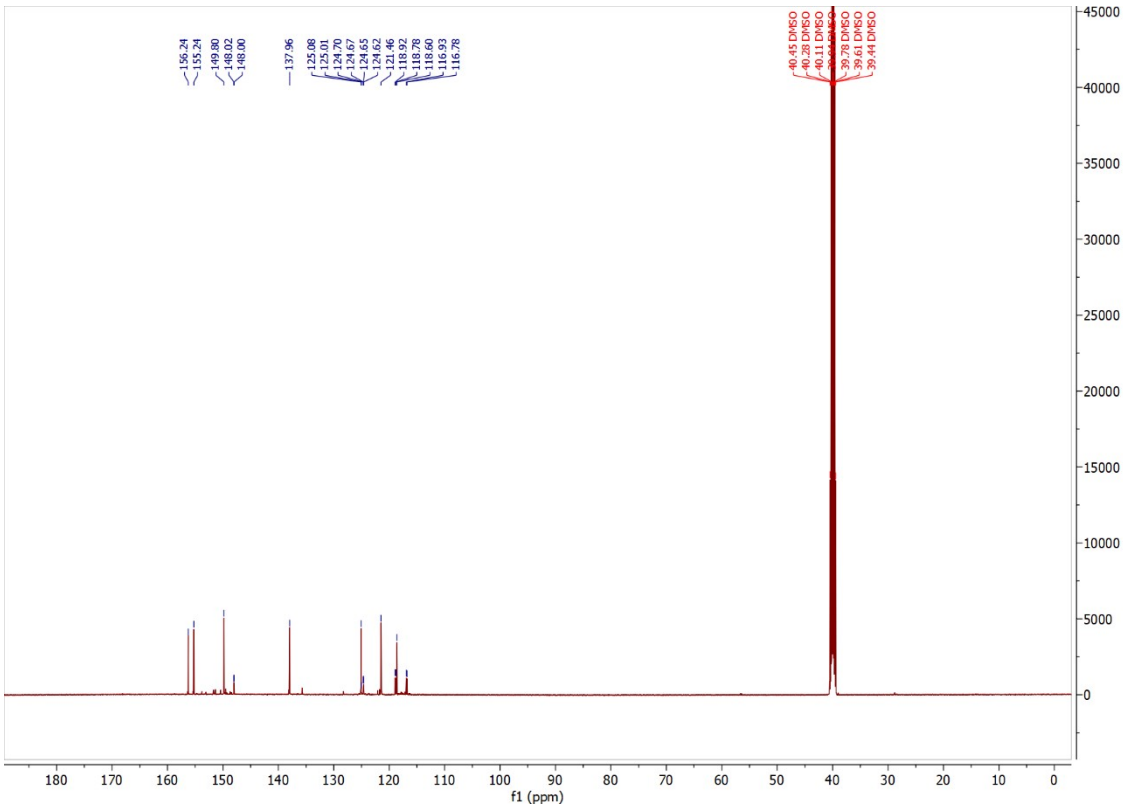
^{13}C-NMR Spectrum (151 MHz, DMSO-d_6) of Compound L_5



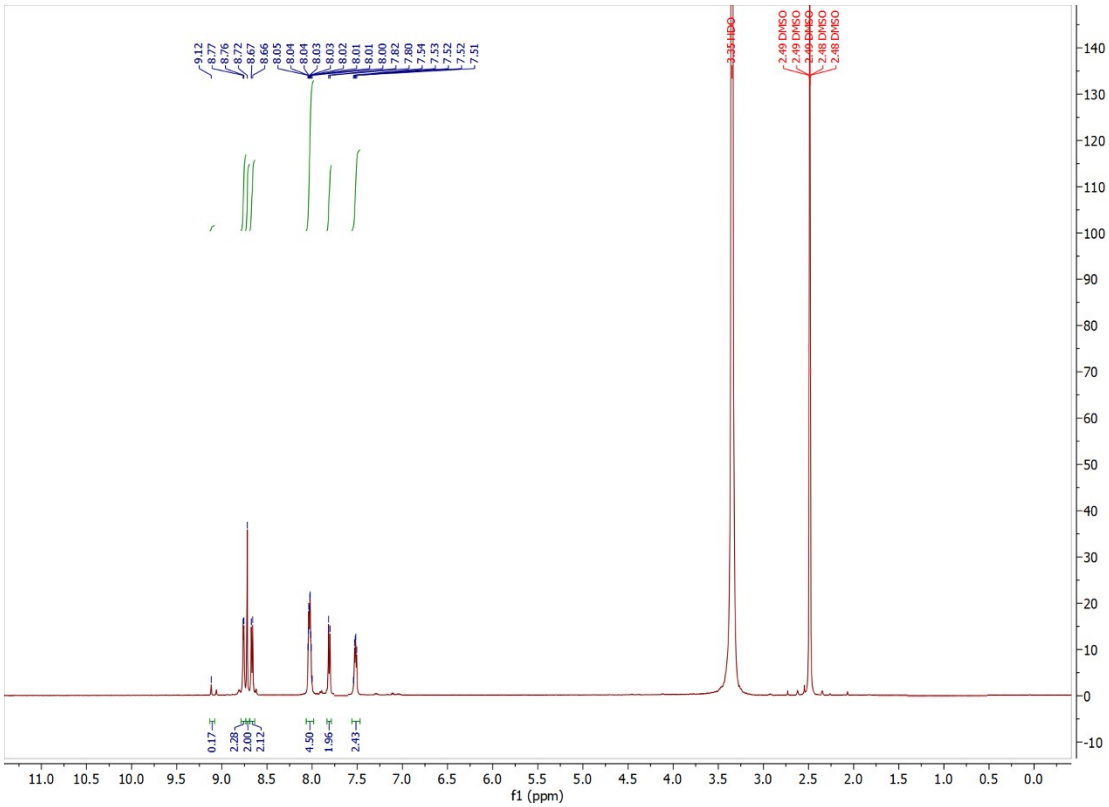
^{1}H-NMR Spectrum (500 MHz, DMSO-d_6) of Compound L_9



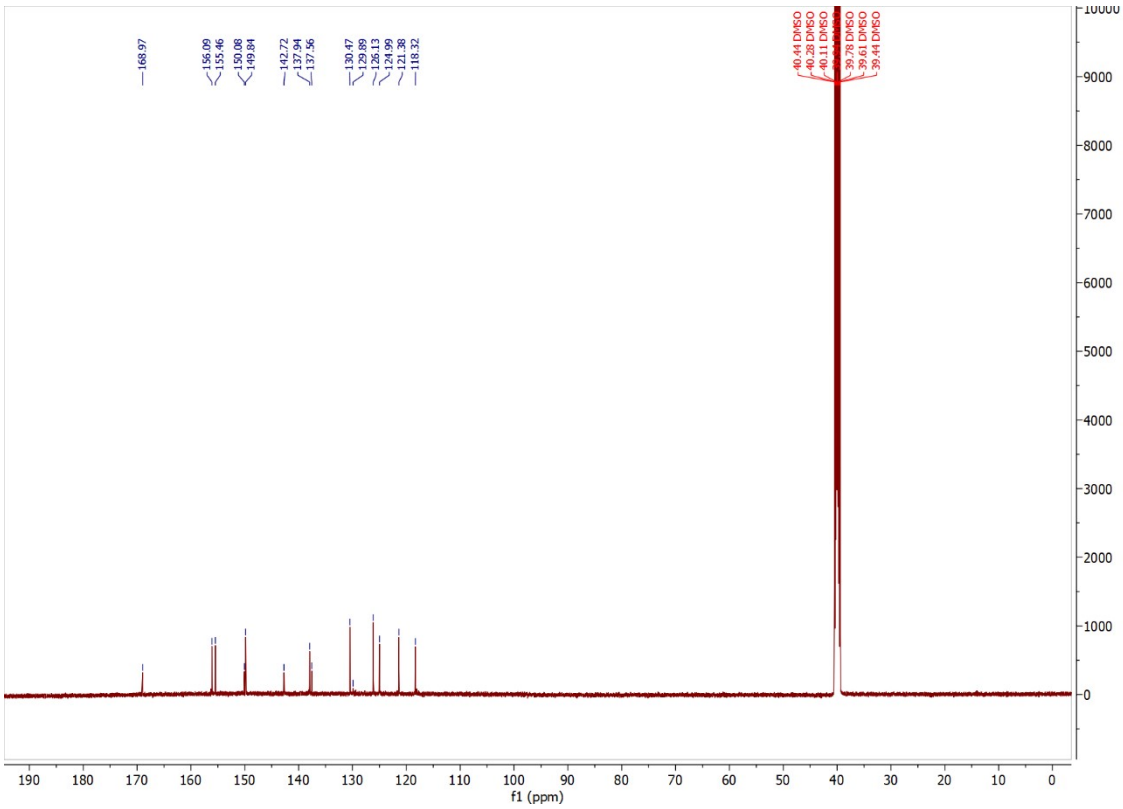
^{13}C-NMR Spectrum (126 MHz, DMSO-d_6) of Compound L_9



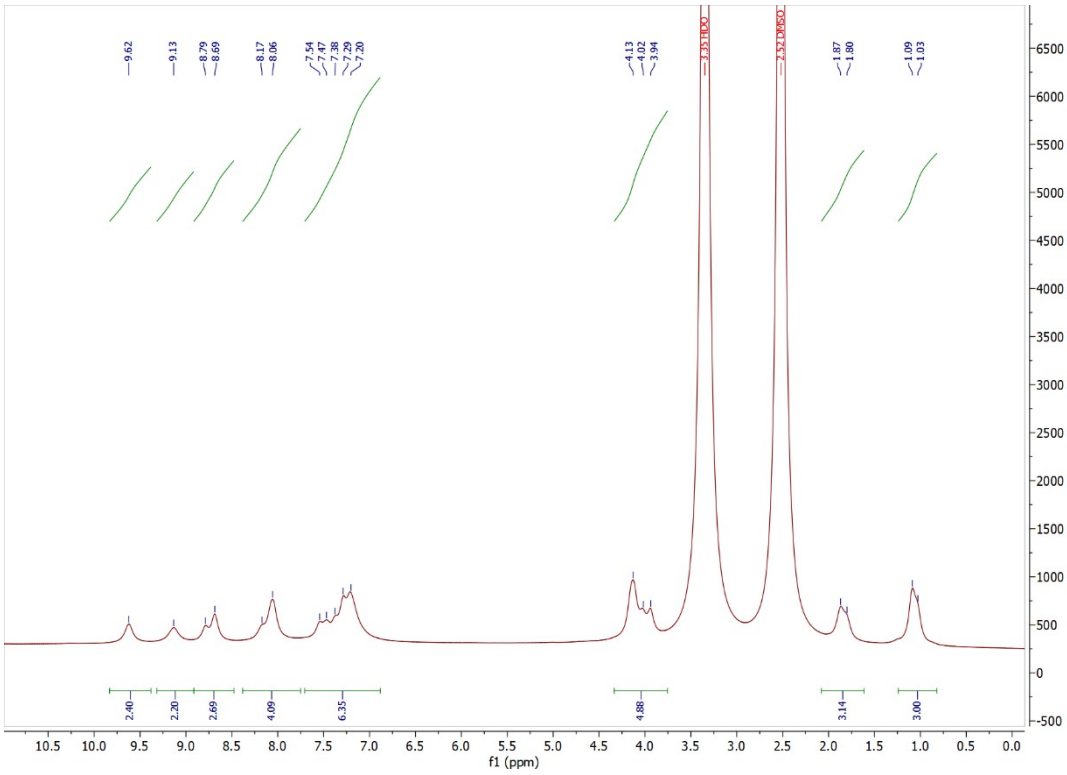
^{1}H-NMR Spectrum (500 MHz, DMSO-d_6) of Compound L_{10}



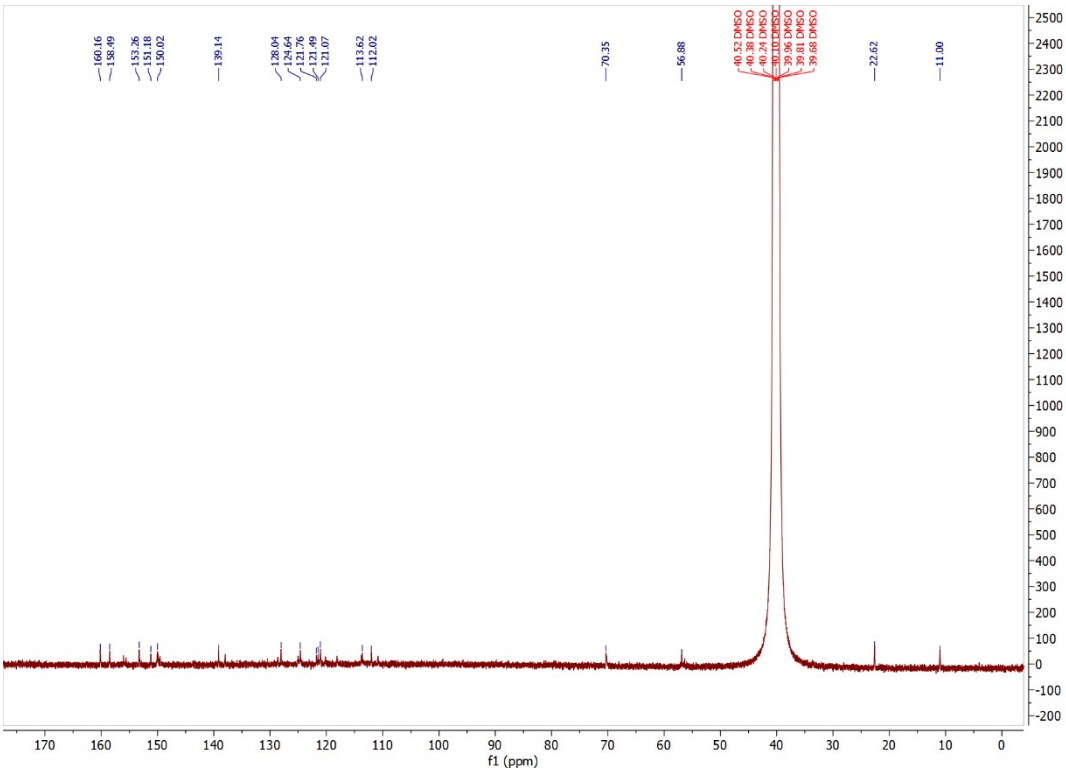
^{13}C-NMR Spectrum (126 MHz, DMSO-d_6) of Compound L_{10}



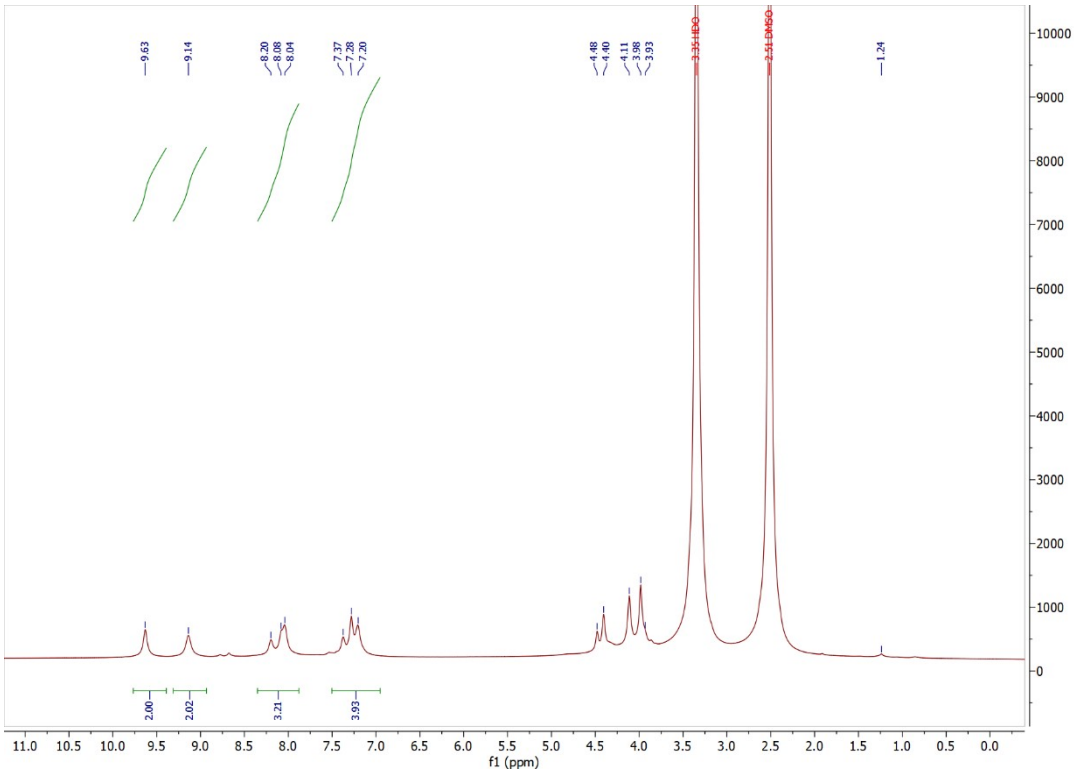
^{1}H-NMR Spectrum (600 MHz, DMSO-d_6) of Compound C_4



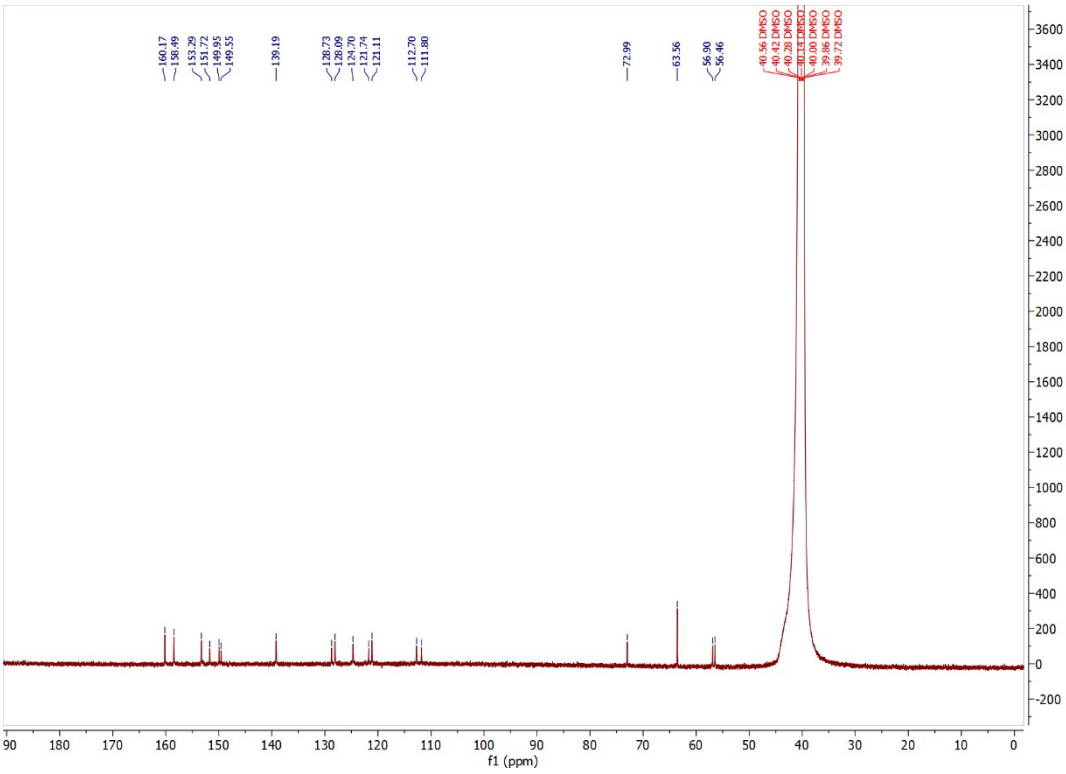
^{13}C-NMR Spectrum (151 MHz, DMSO-d_6) of Compound C_4



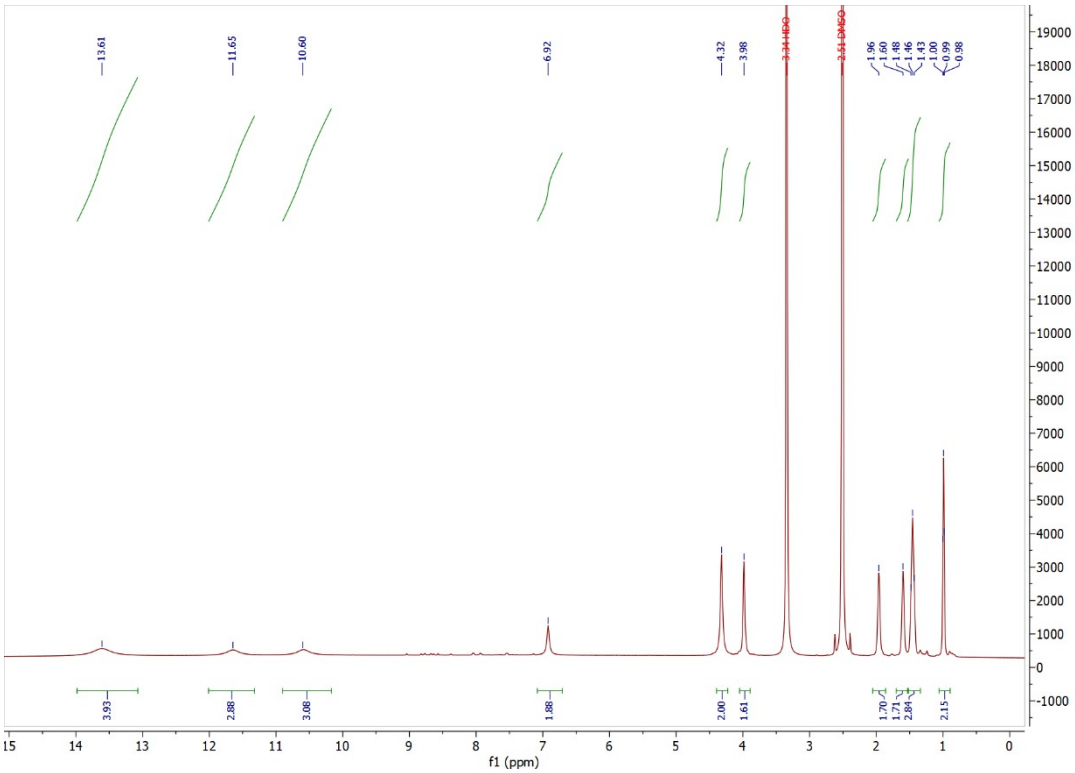
^{1}H-NMR Spectrum (600 MHz, DMSO-d_6) of Compound C_5



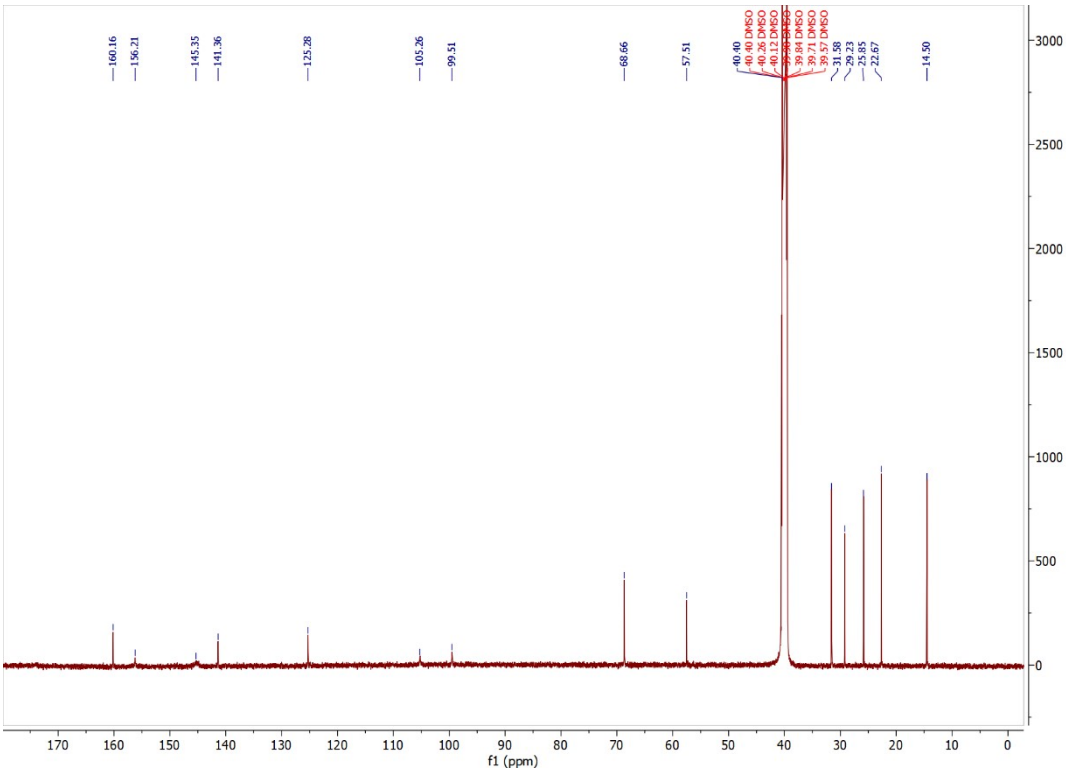
^{13}C-NMR Spectrum (151 MHz, DMSO-d_6) of Compound C_5



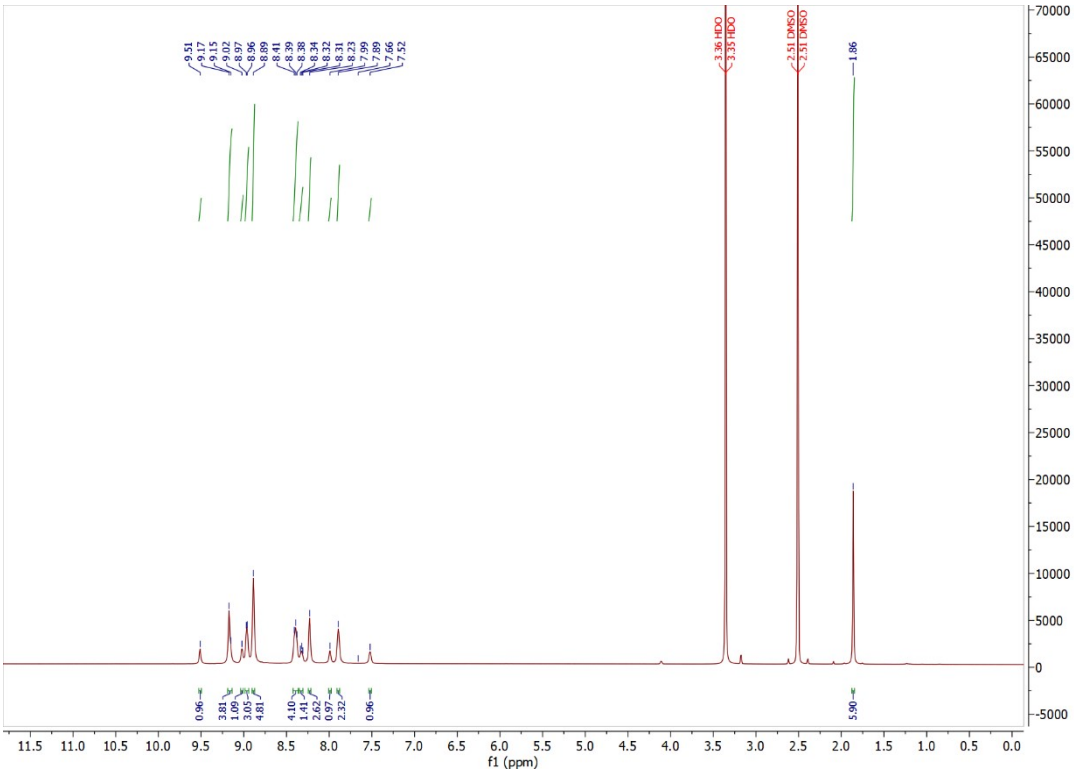
^{1}H-NMR Spectrum (600 MHz, DMSO-d_6) of Compound C_7



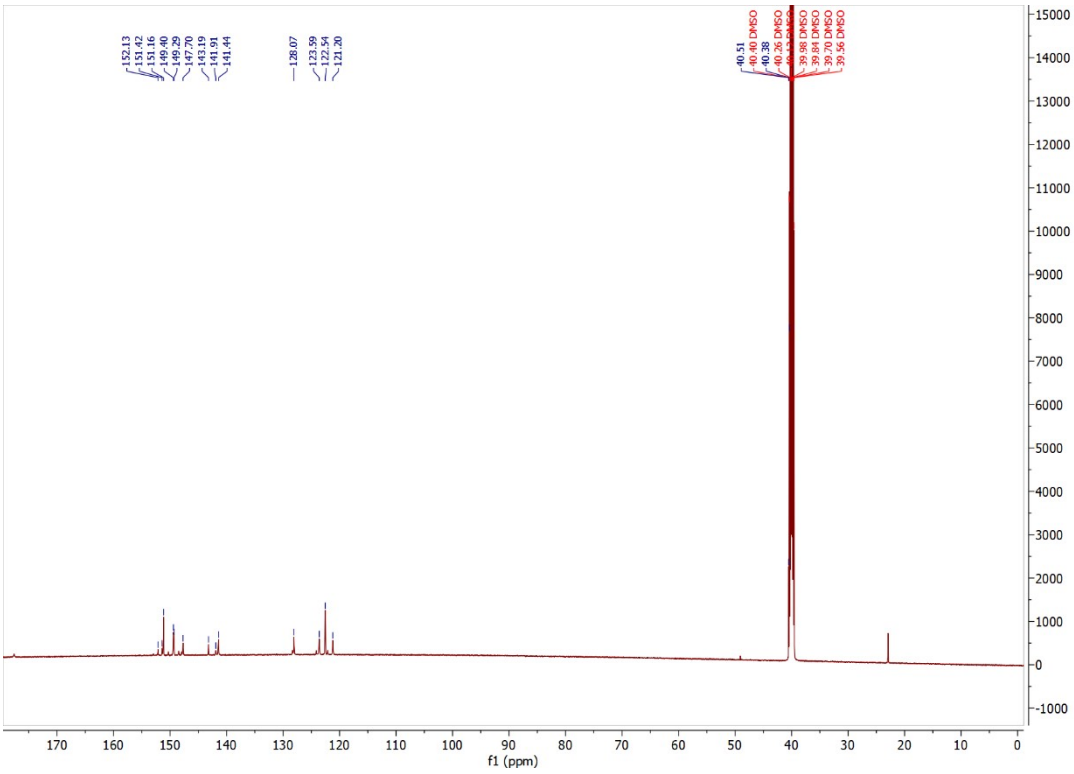
^{13}C-NMR Spectrum (151 MHz, DMSO-d_6) of Compound C_7



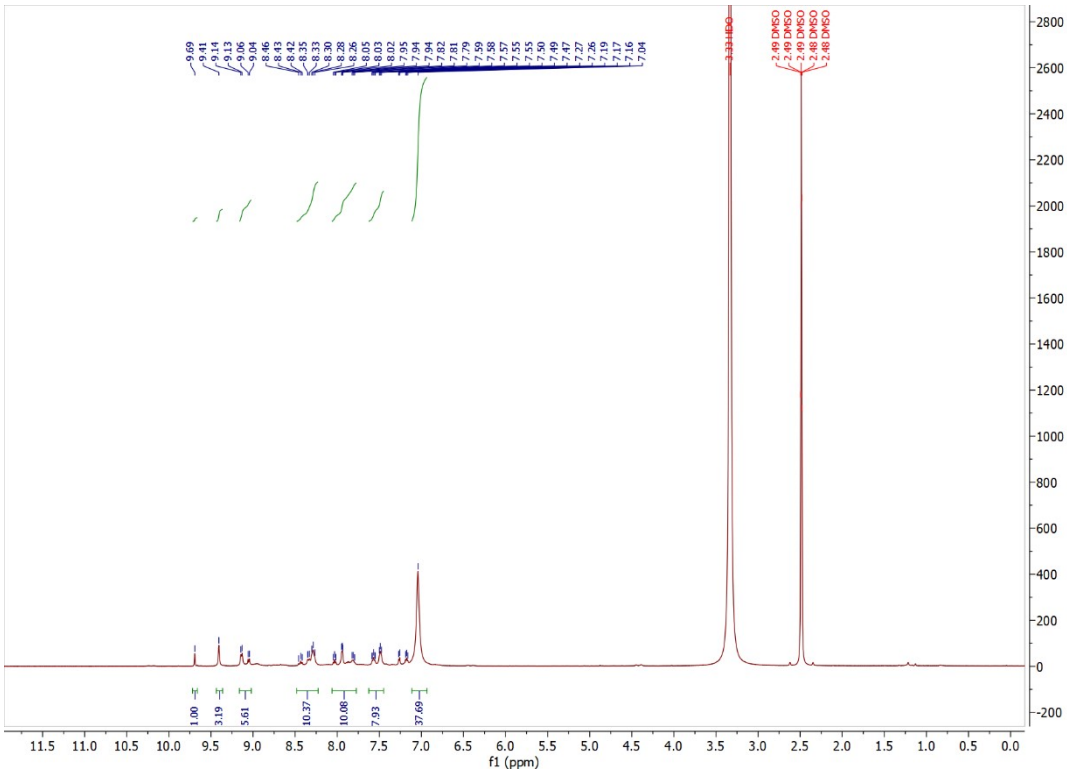
^{1}H-NMR Spectrum (600 MHz, DMSO-d_6) of Compound C_8



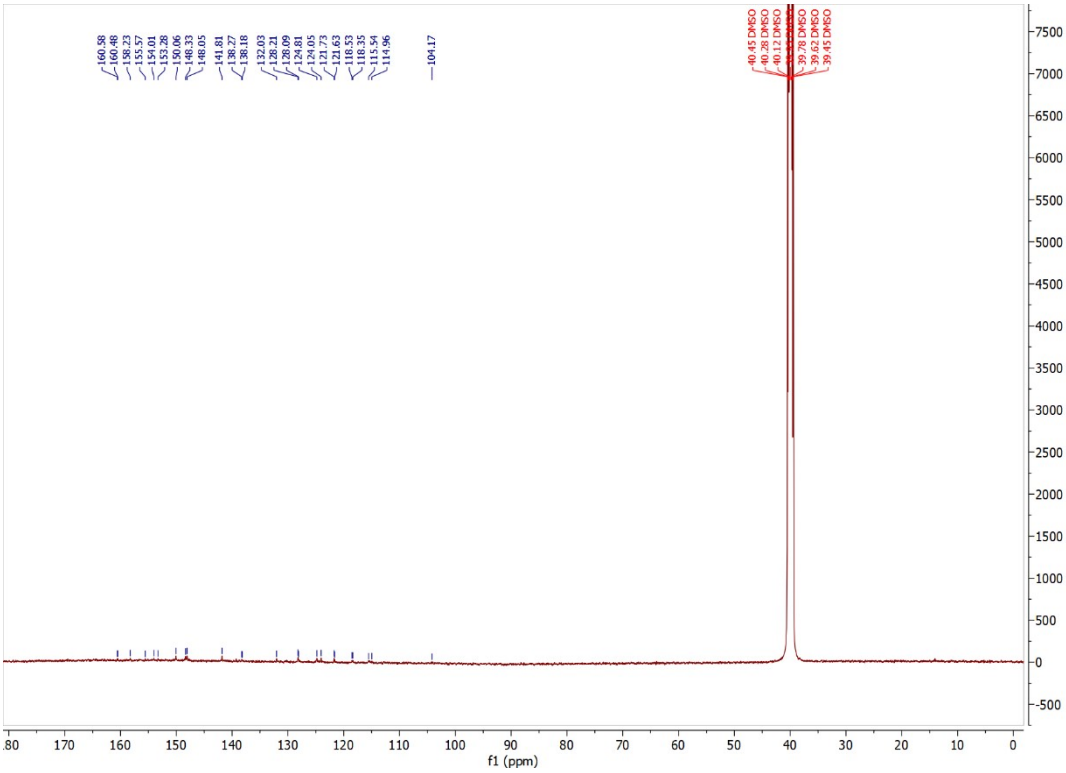
^{13}C-NMR Spectrum (151 MHz, DMSO-d_6) of Compound C_8



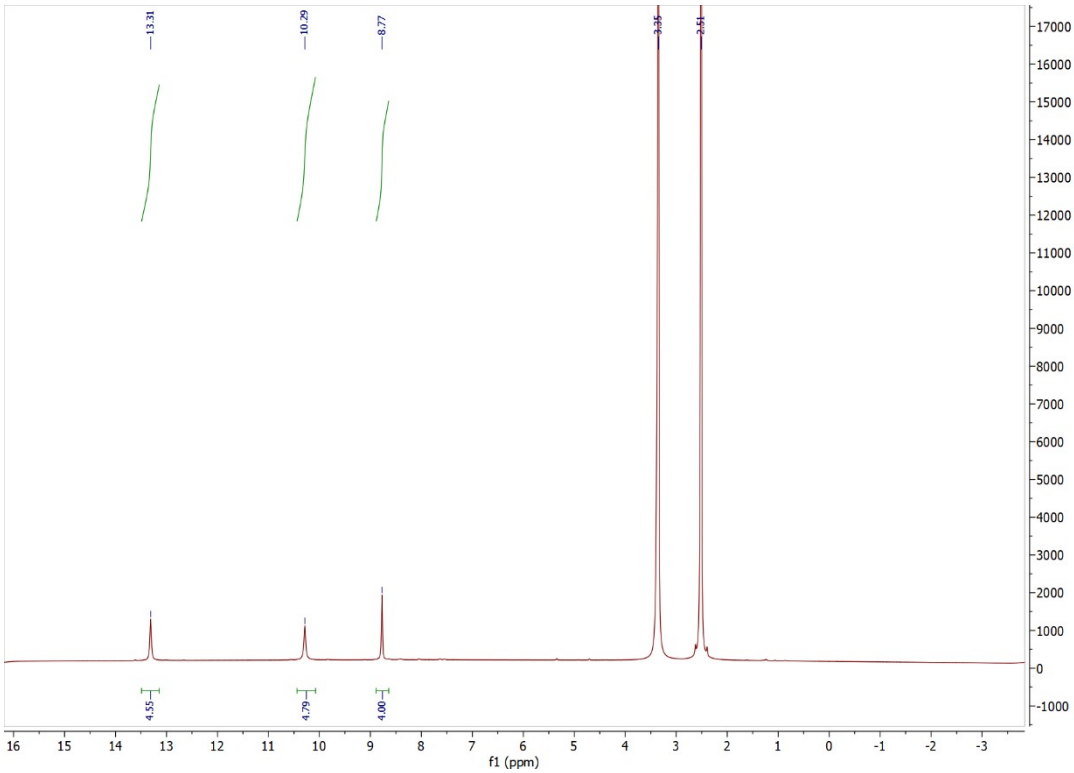
^{1}H-NMR Spectrum (500 MHz, DMSO-d_6) of Compound C_{11}



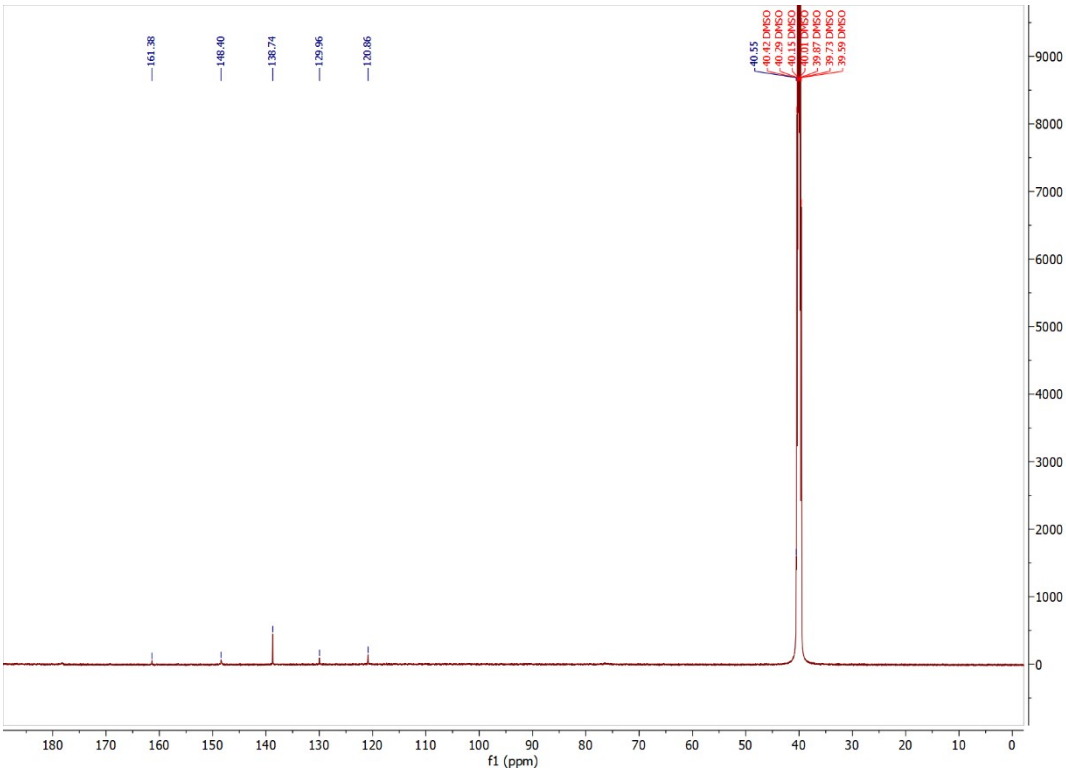
^{13}C-NMR Spectrum (126 MHz, DMSO-d_6) of Compound C_{11}



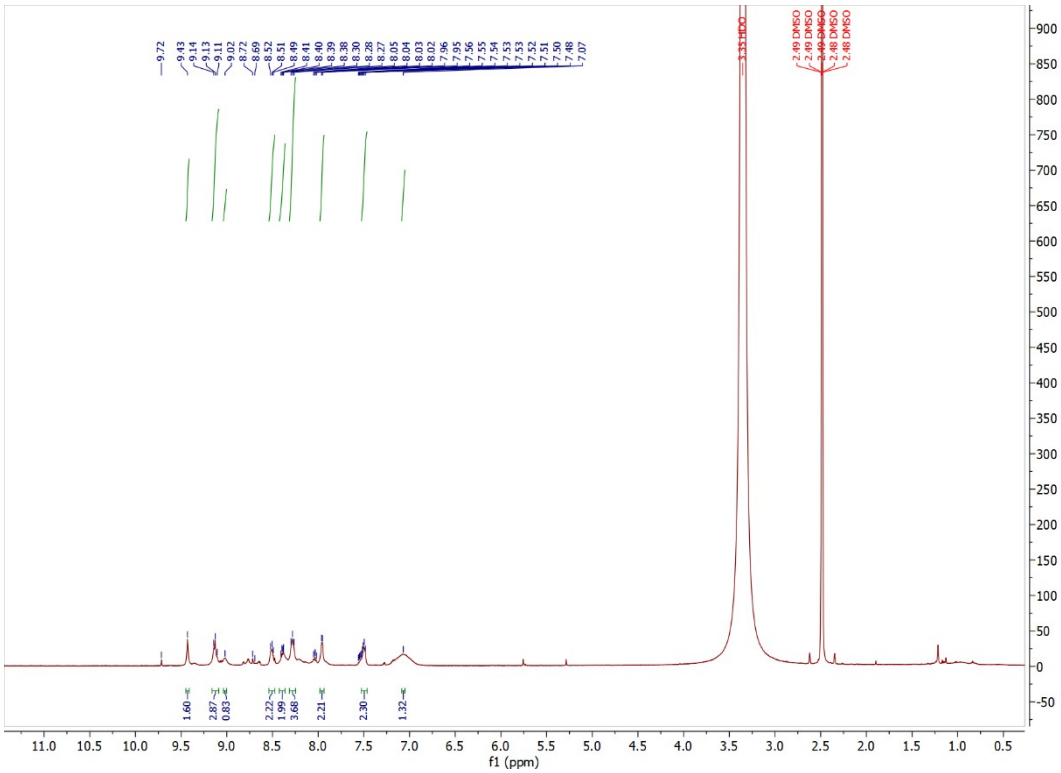
^{1}H-NMR Spectrum (600 MHz, DMSO-d_6) of Compound C_{12}



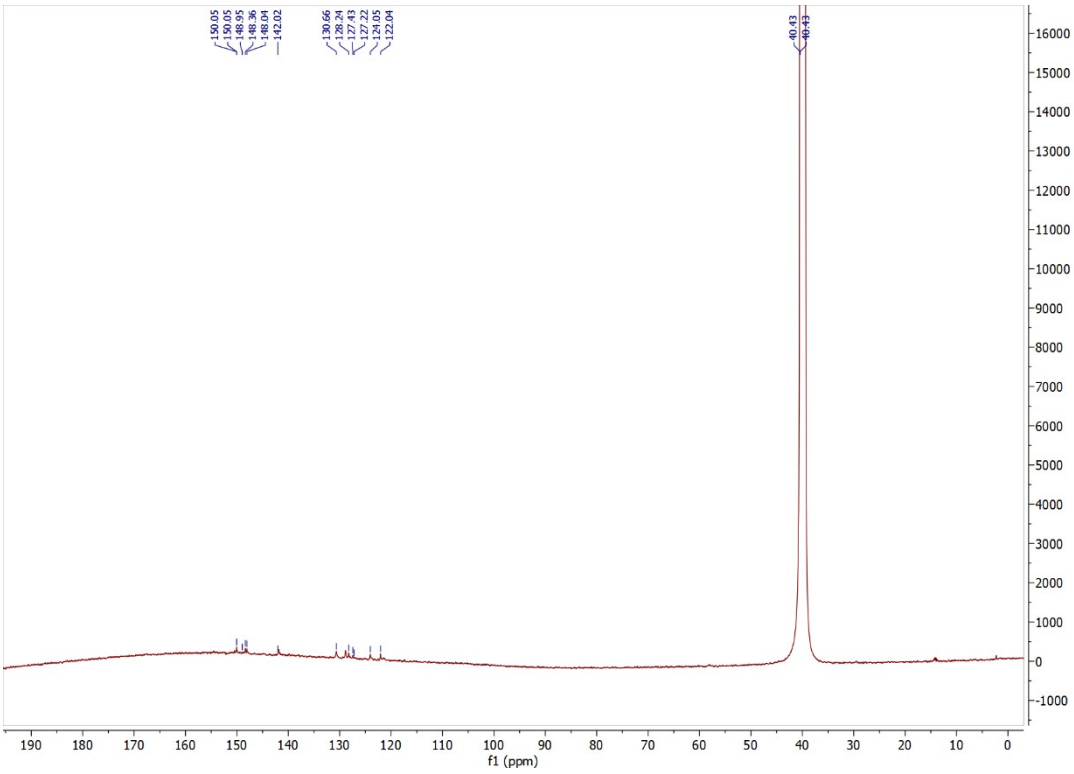
^{13}C-NMR Spectrum (151 MHz, DMSO-d_6) of Compound C_{12}



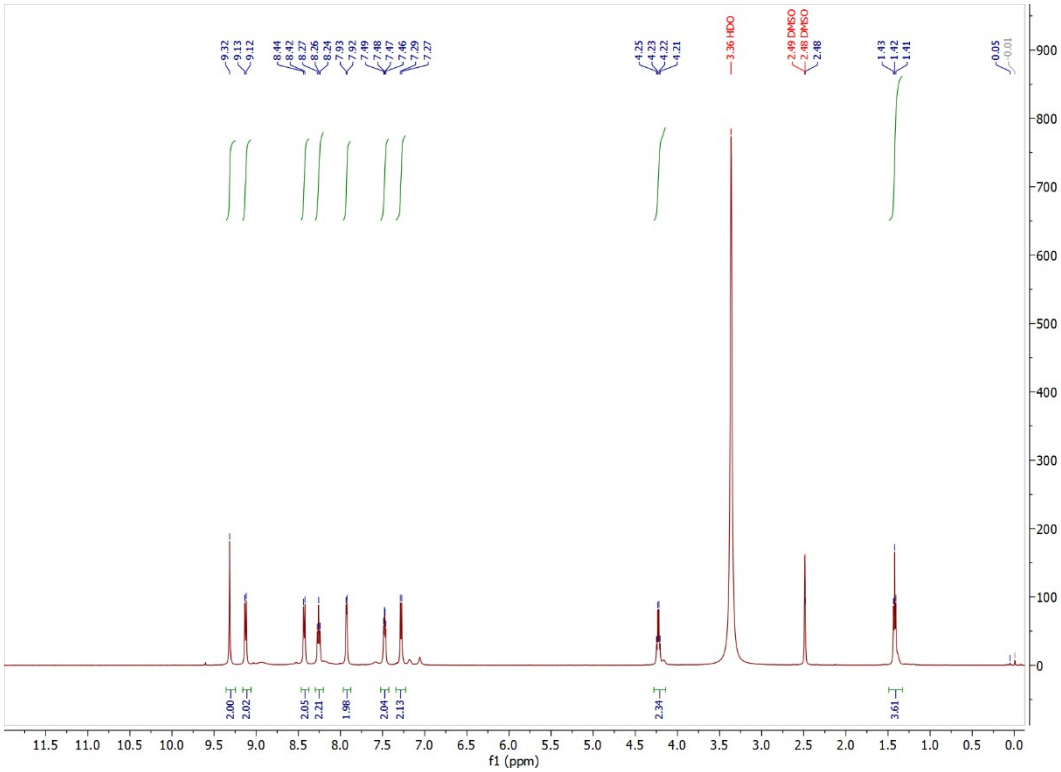
^{1}H-NMR Spectrum (500 MHz, DMSO-d_6) of Compound C_{17}



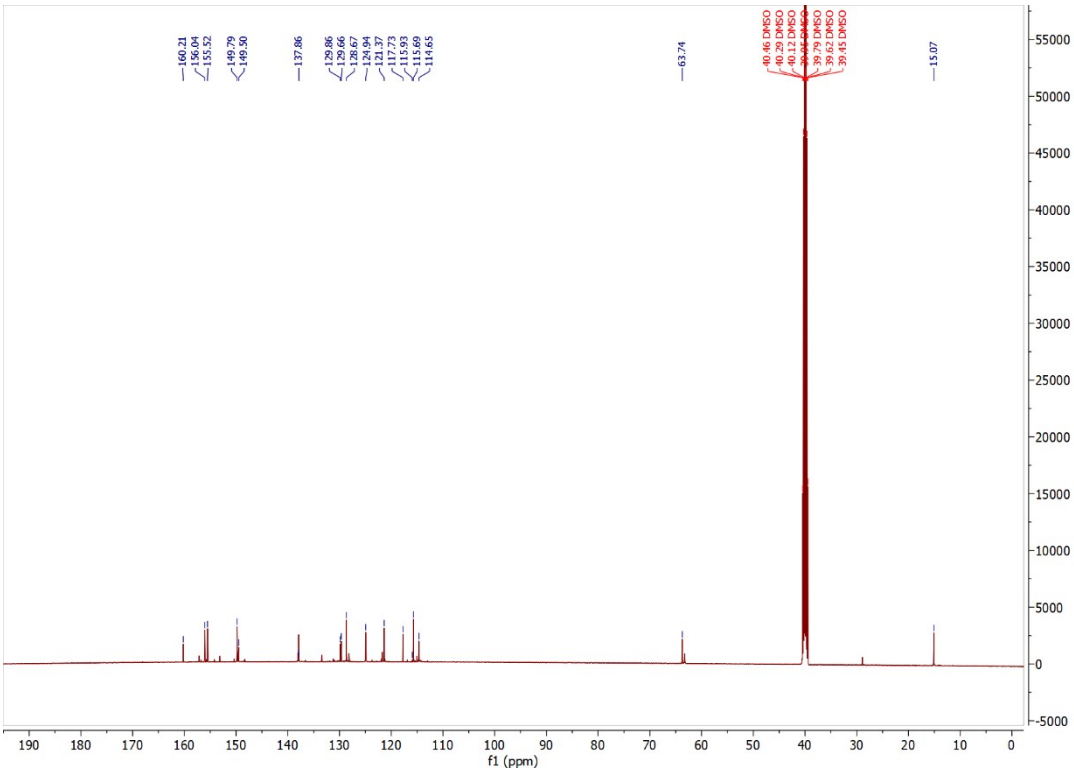
^{13}C-NMR Spectrum (126 MHz, DMSO-d_6) of Compound C_{17}



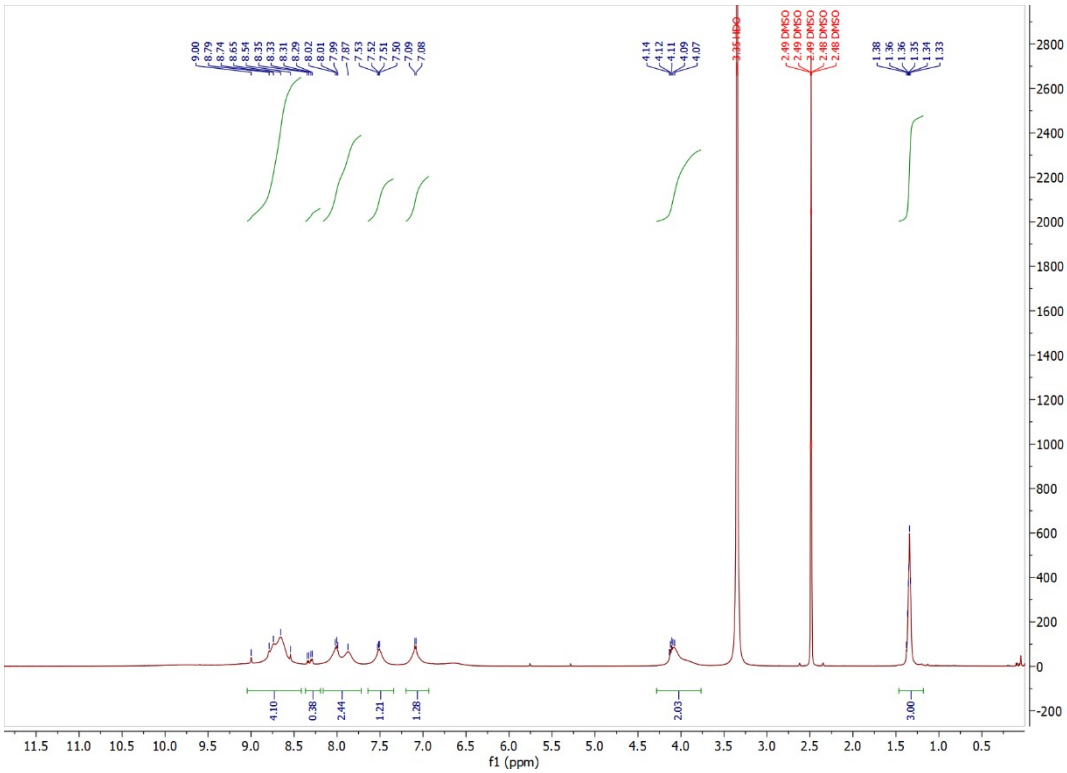
^{1}H-NMR Spectrum (500 MHz, DMSO-d_6) of Compound C_{18}



^{13}C-NMR Spectrum (126 MHz, DMSO-d_6) of Compound C_{18}



^{1}H-NMR Spectrum (500 MHz, DMSO-d_6) of Compound C_{19}



^{13}C-NMR Spectrum (126 MHz, DMSO-d_6) of Compound C_{19}

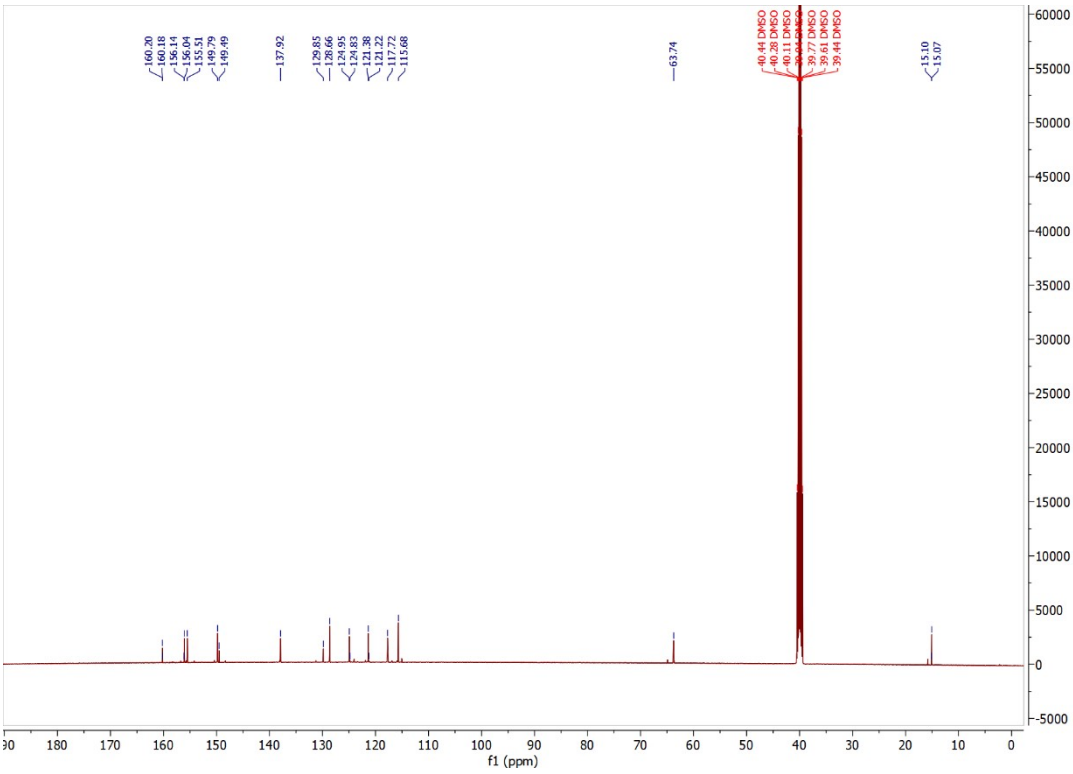


Figure S3: Representative ESI Mass Spectrum of the Synthesized Compound

ESI Mass Spectrum of Compound C_{19}