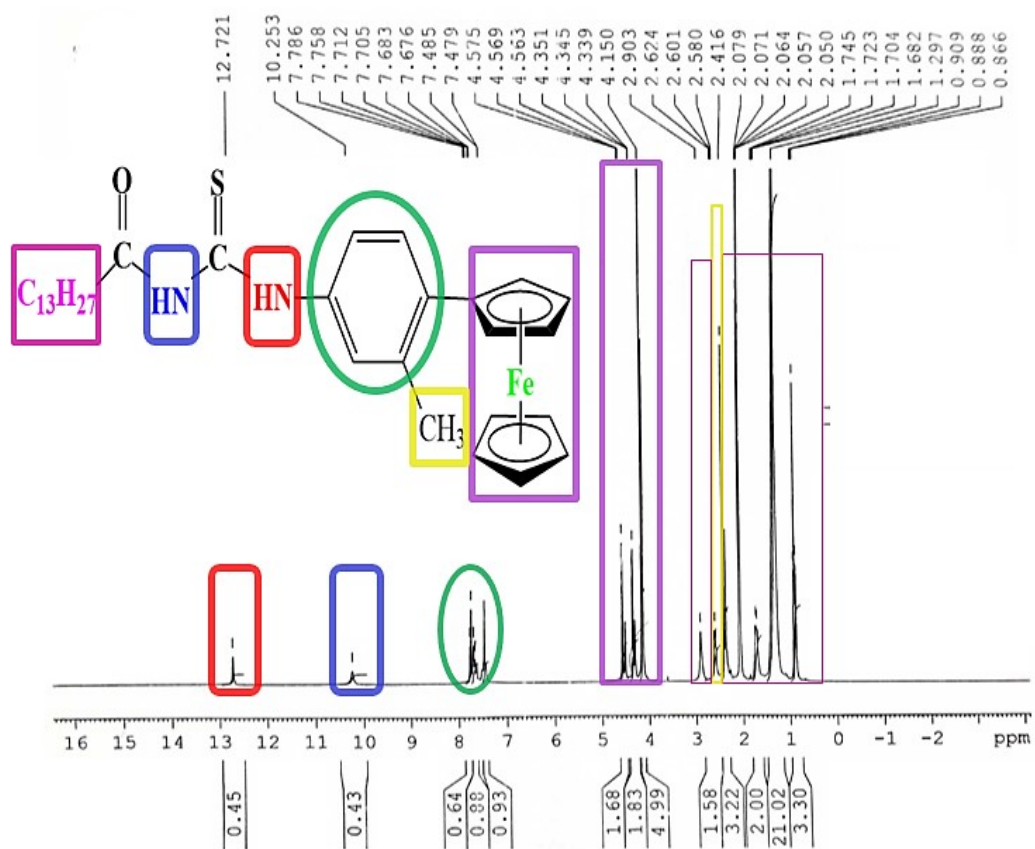
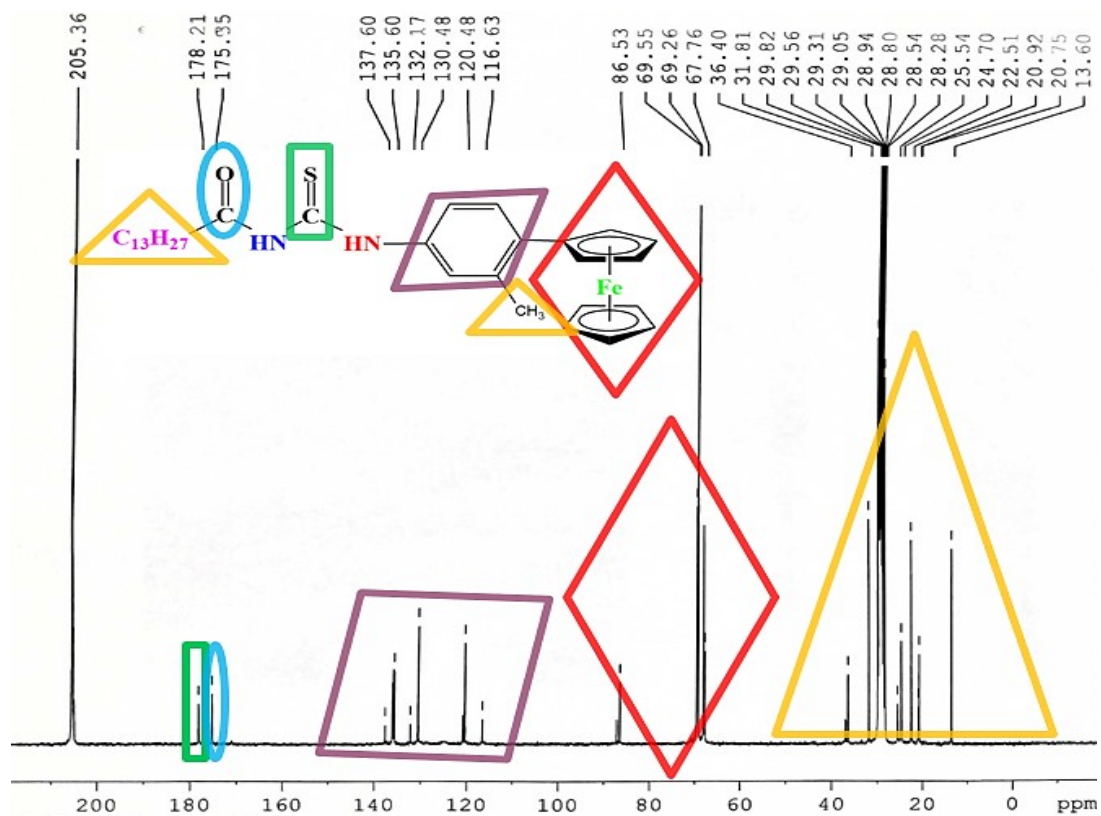


**Figure S1:** FT-IR spectrum of G-7.

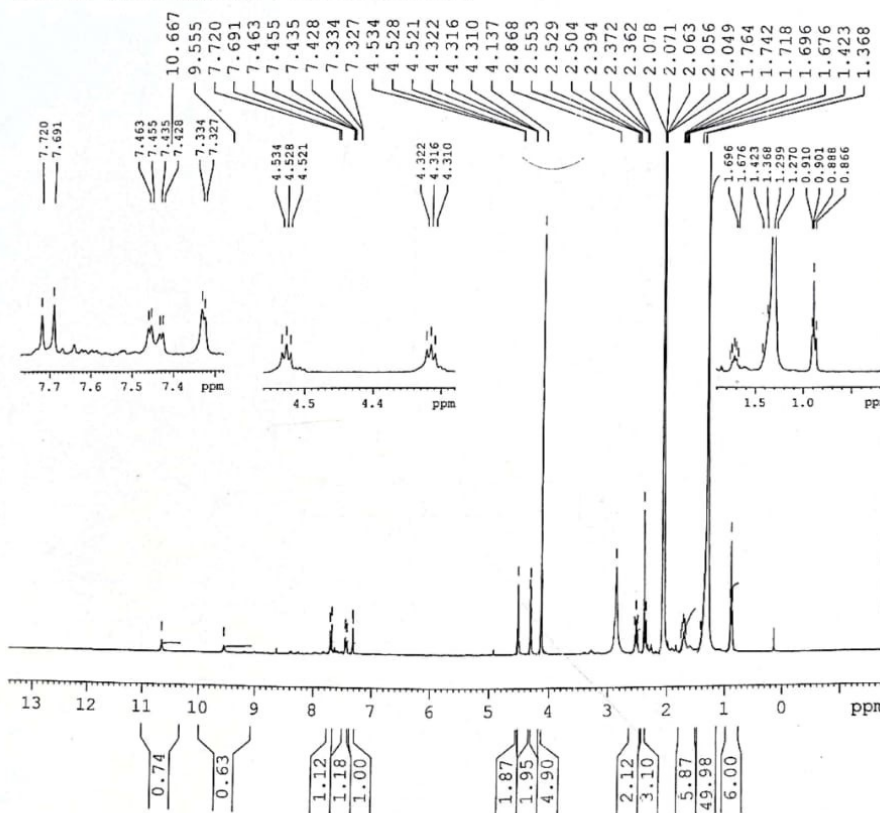


**Figure S2 (a):** <sup>1</sup>H-NMR spectrum for ferrocenyl thiourea (**13C4N**)



**Figure S2 (b):**  $^{13}\text{C}$ -NMR spectrum for ferrocenyl (13C4N) thiourea

DR.AMIN BADSHAH/SAMEEN/G-18\_1HNMR\_ACETONE



Current Data Parameters  
NAME G-18\_1HNMR\_ACETONE  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180716  
Time\_ 13.32  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT Acetone  
NS 8  
DS 0  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 456.1  
DW 81.000 usec  
DE 6.00 usec  
TE 295.3 K  
D1 1.0000000 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 9.00 usec  
PL1 2.00 dB  
SF01 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S3 (a): <sup>1</sup>H-NMR spectrum of G-18.

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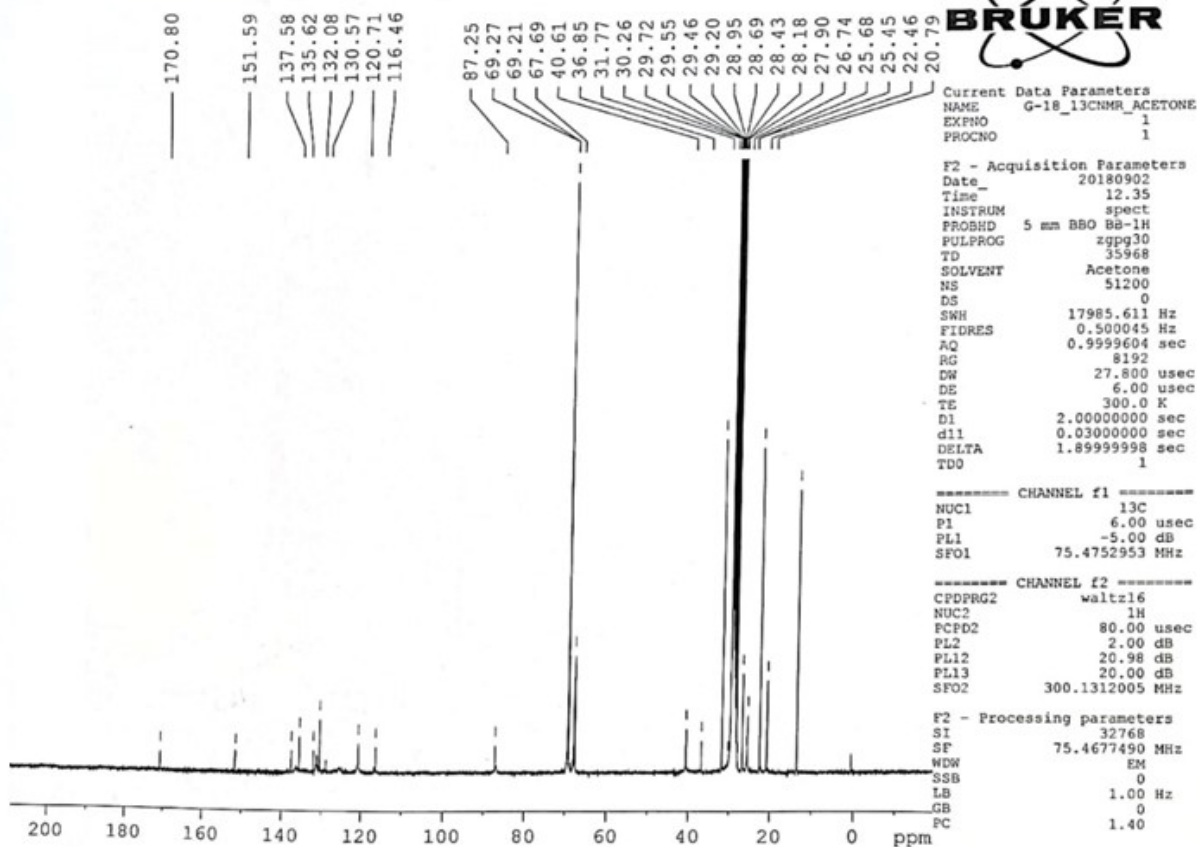
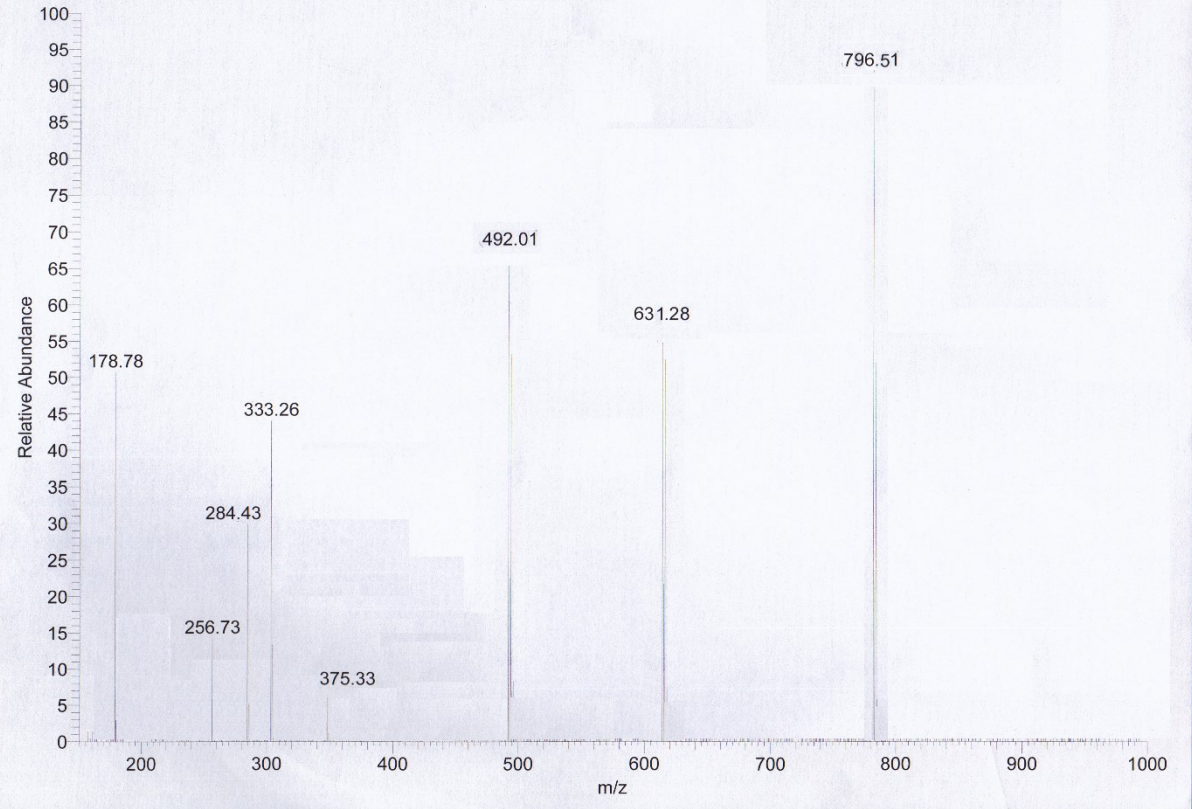


Figure S3 (b): <sup>13</sup>C-NMR spectrum of G-18.

C:\LCQusers\...lasghar\140729-DC1  
ESI, Methanol  
140729-DC1 #1 RT: 0.01 AV: 1 NL: 3.47E6  
T: + c ESI Full ms [ 150.00-1000.00]

7/29/2019 12:30:25 PM

DC1

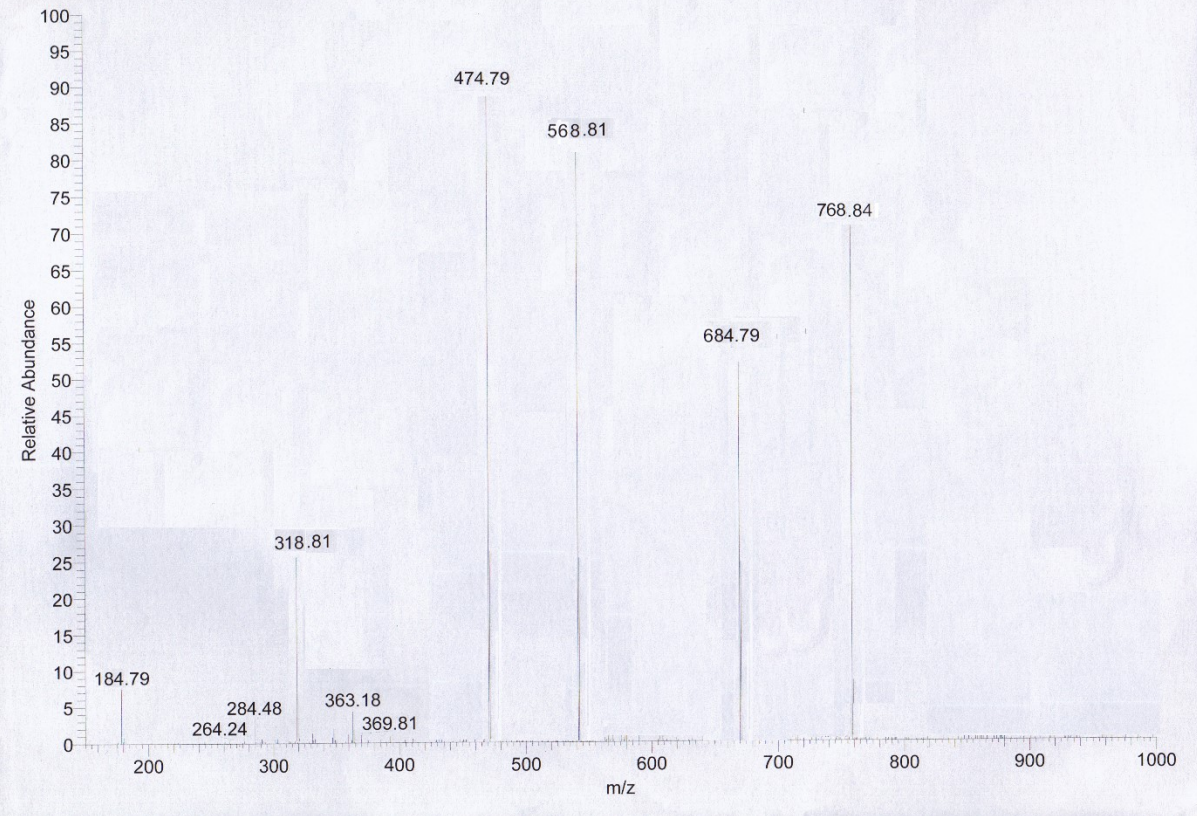


**Figure S4:** ESI-MS spectrum of **G-18**.

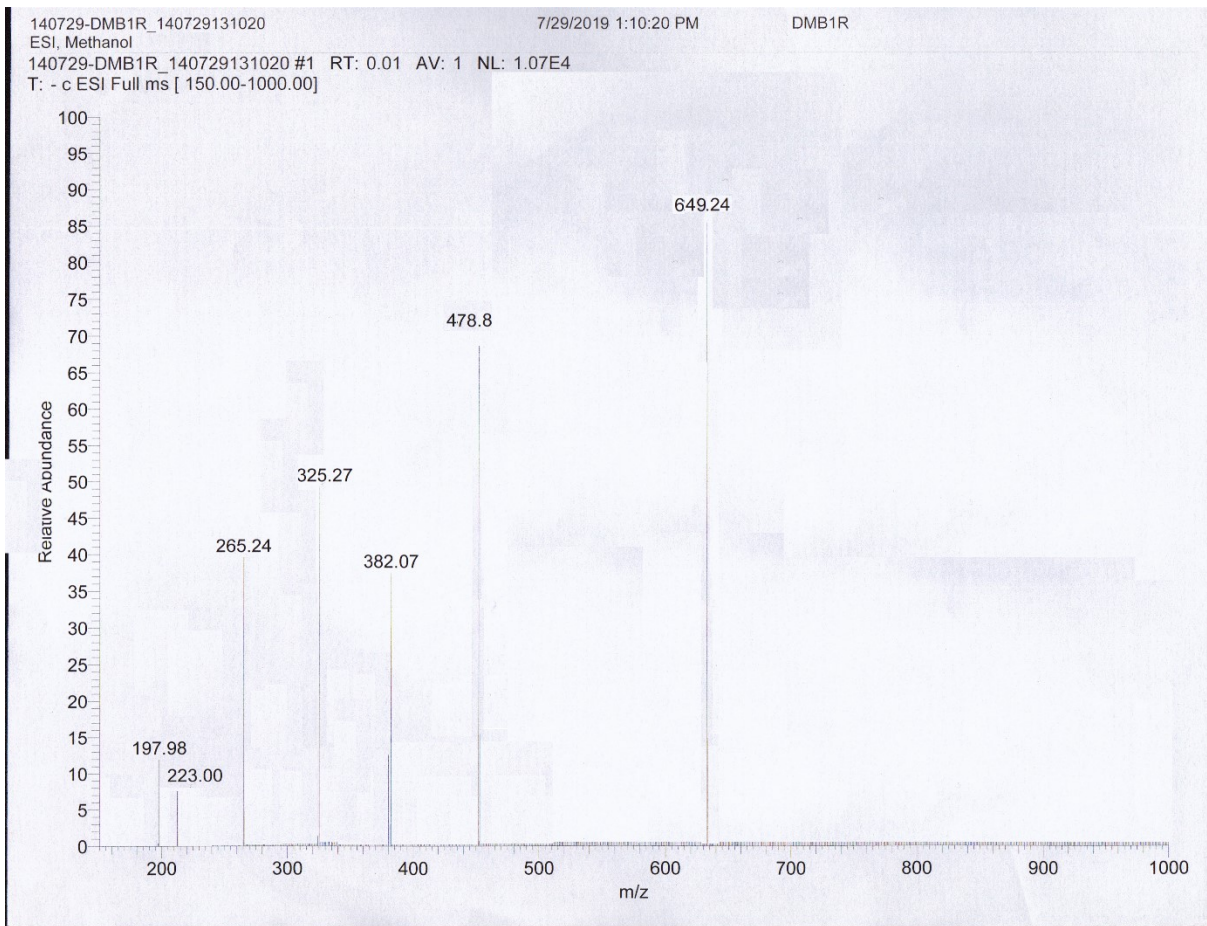
C:\LCQusers\...lasghar\140729-DMB1  
ESI, Methanol  
140729-DMB1 #1 RT: 0.01 AV: 1 NL: 4.43E7  
T: + c ESI Full ms [ 150.00-1000.00]

7/29/2019 12:23:07 PM

DMB1



**Figure S5:** ESI-MS spectrum of **G-16**.



**Figure S6:** ESI-MS spectrum of G-7.



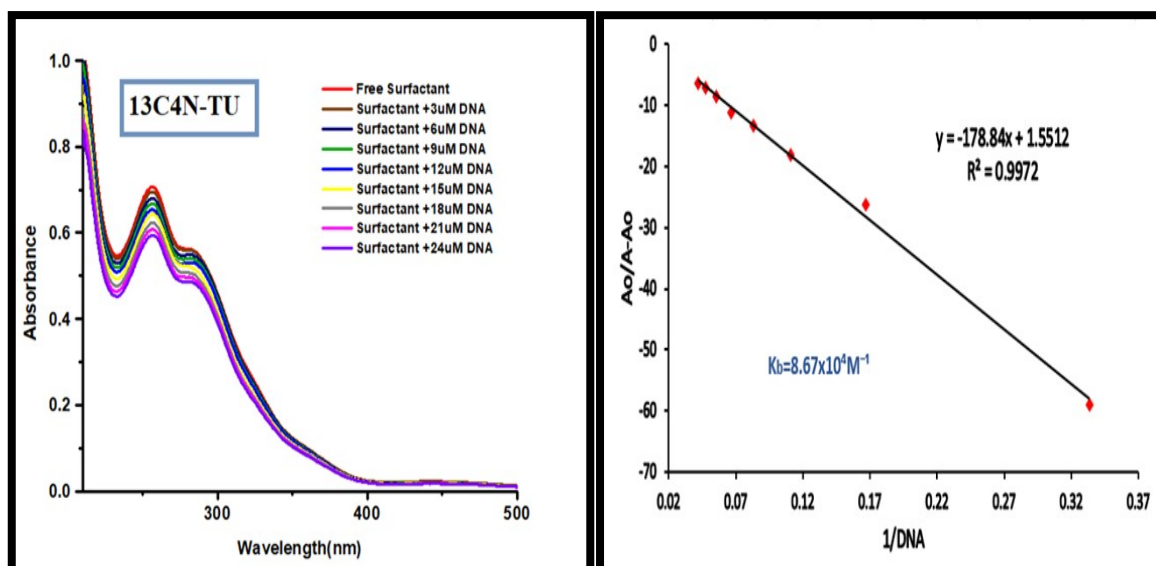
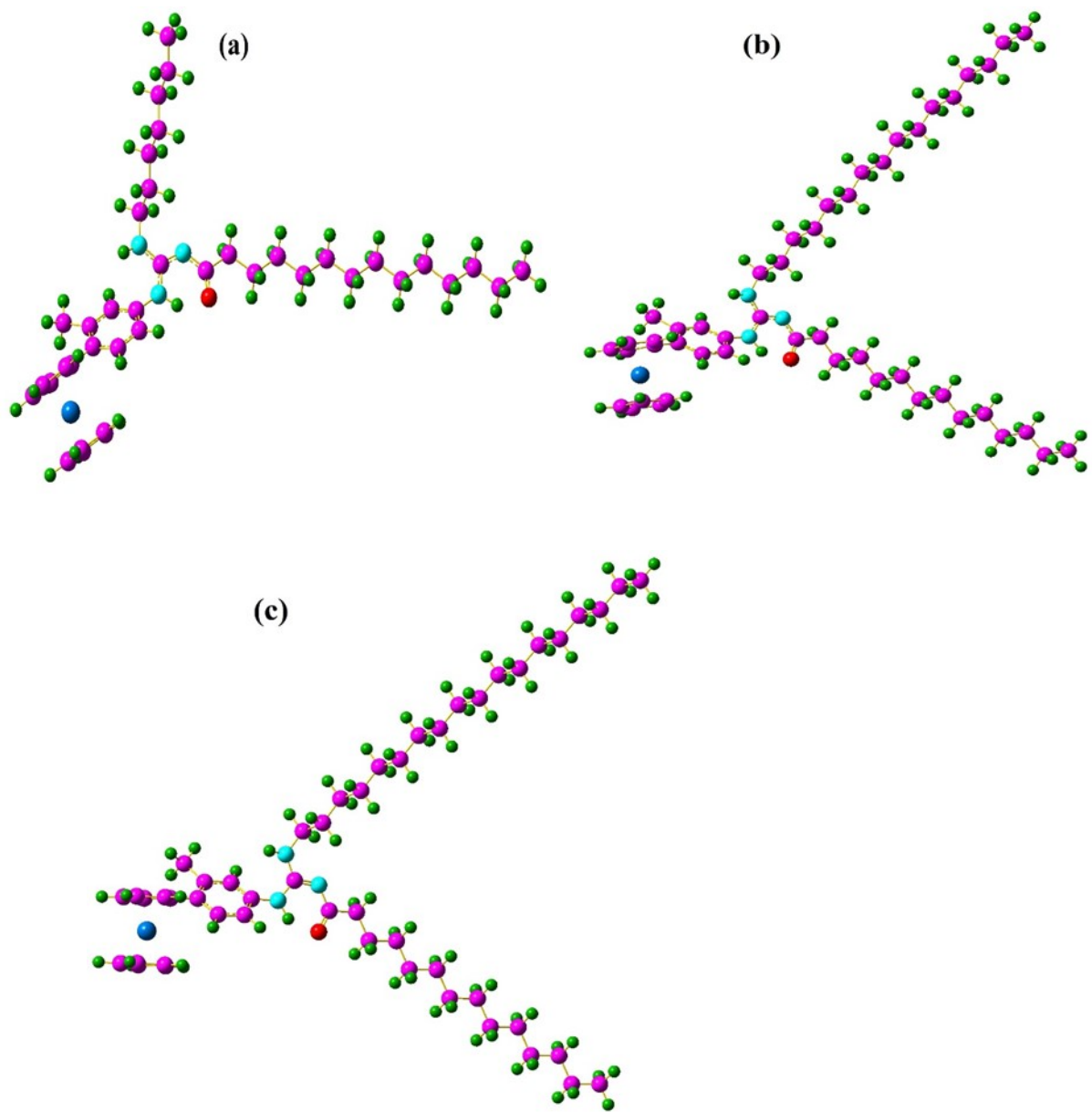
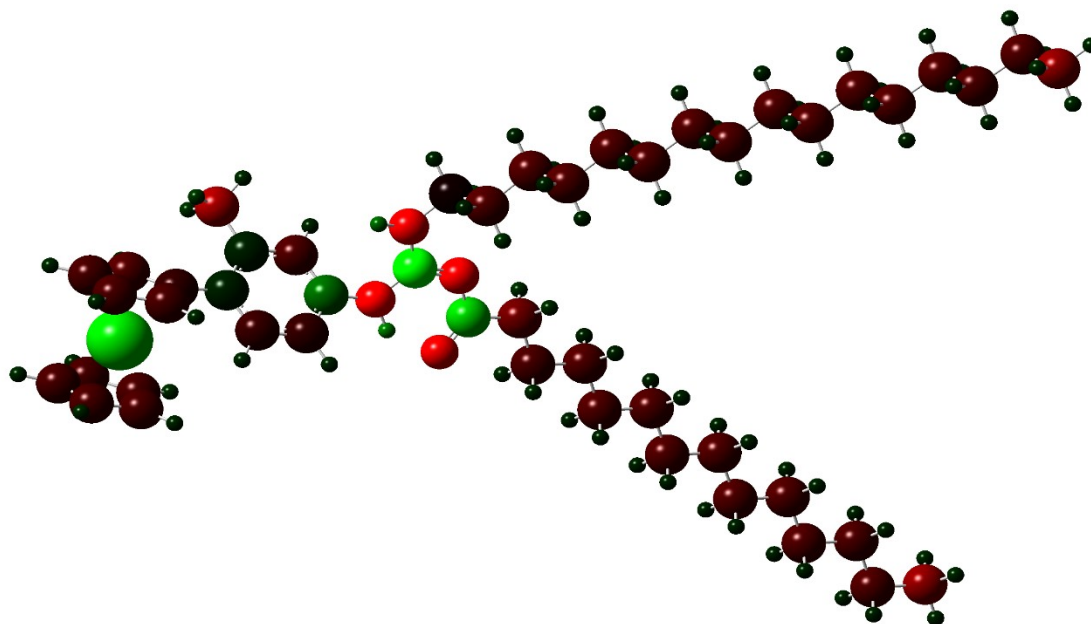


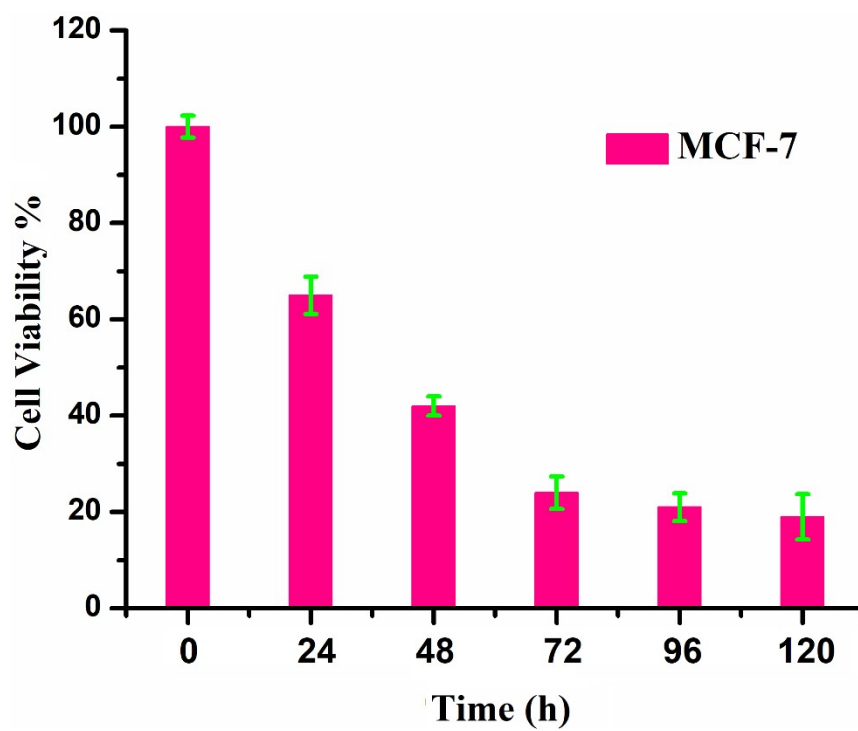
Figure S7: UV-visible spectrum and binding constant plot for 13C4N.



**Figure S8:** (a) Optimized structures of G-7, (b) G-16, (c) G-18.



**Figure S9:** Mulliken charge distribution for **G-16** by colors. The lighter to darker color scheme representing positive to negative charge distribution.



**Figure S10:** Cell viability (%) of cancerous cells (MCF-7) after regular time intervals (24-120 h) of a representative compound **G-18** (25  $\mu$ M).