Supplementary Information

1,5-Benzosulfonamide anthracenedione analogues of mitoxantrone as antibacterial and anticancer agents

Manu Vatsal, Anjali Sharma & Pamita Awasthi*

Department of Chemistry, National Institute of Technology, Hamirpur 177 005, India

E-mail: pamitawasthi@gmail.com; pamita@nith.ac.in; vatsal.manu9@gmail.com; tanu.anjali.sharma@gmail.com

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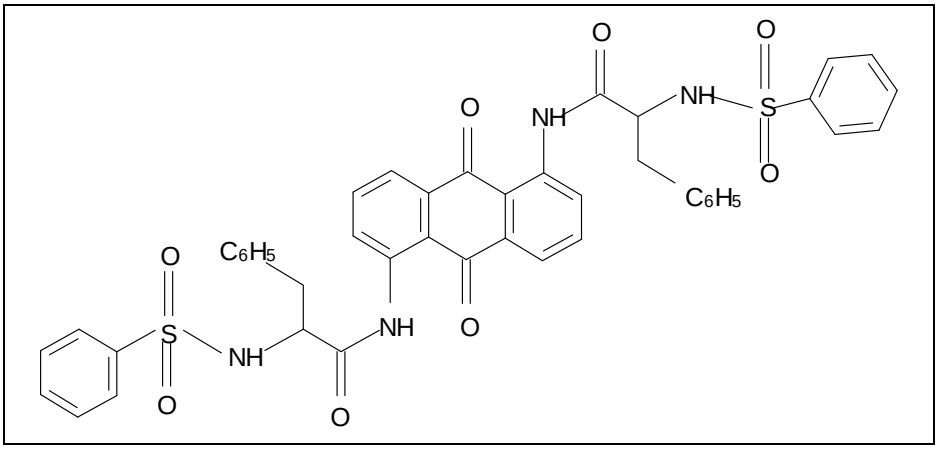
ST.1 General synthetic details

The progress of the reaction was monitored by TLC till single spot and kept overnight. The solution was filtered and distilled to remove excess solvent and monitored by TLC single spot. It was recrystallised with chloroform and pure product was obtained. The HRMS ionization type (ES+) mass spectra were obtained with a XEVO G2-XS Q-TOF micro spectrometer. ^{1}H & $^{13}CNMR$ spectra were recorded in $CDCl_3$ and DMSO on a BRUKER AVANCE II 400 NMR spectrometer. The IR spectra were recorded on NICOLET 6700 supplied by Thermo scientific USA spectrometer using KBr pellets. The spectra range from 500-4000cm^{-1}.

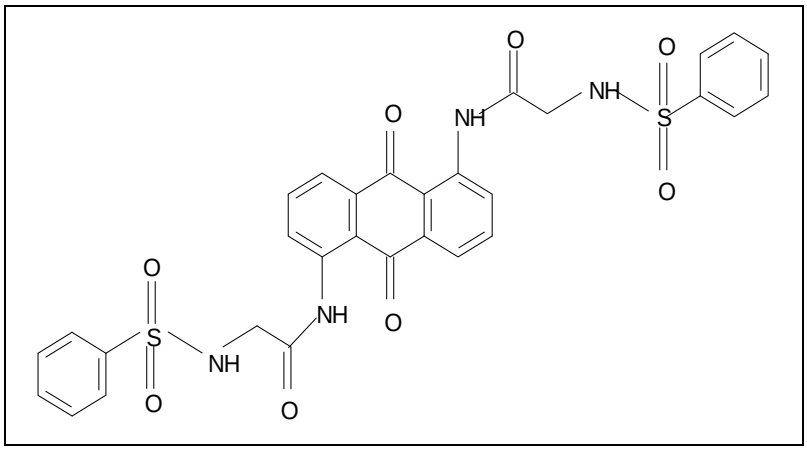
Characterization of bi-substituted series (B1-B5)

1,5 Bis [1-oxo-3-phenyl-2-(benzosulfonamide)-propylamido]-anthracene-9,10-dione (B1)= Yellow crystalline solid



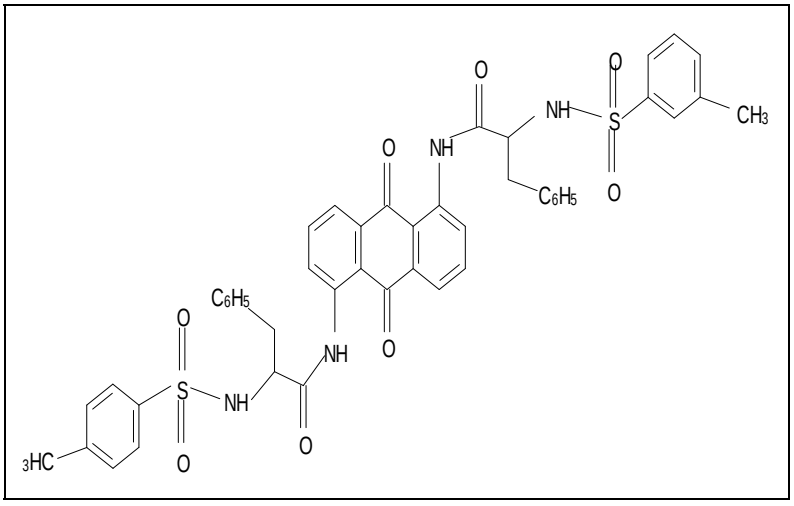
IR(υcm^{-1}): NH str.=3278cm^{-1}, Arm.CN stre.= 1259.2cm^{-1}, -C=O str.=1695cm^{-1}, Alp.CN stre.= 1088.6cm^{-1}, O=S=O str.=1325.2, 1155.7cm^{-1}. (^{1}H-NMR $CDCl_3$) 400MHz= δ 12.63 (1H, s, -NH ar), 8.97-8.95 (1H, d,-N H ar, J=7.92 Hz), 8.08-8.03 (1H, d, H_6 aaq, J=10.08 Hz), 7.94-7.92 (1H, d, H_2 aaq, J=7.32 Hz), 7.77-7.71 (4H, m, Ar-(H_3, H_4, 7_3 and H_8) aaq, J_1=8 Hz, J_2=3.92 Hz), 7.59-7.48 (4H, m, Ar-H ortho to SO_2NH gp, J_1=7.36 Hz, J_2=4.92 Hz), 7.46-7.30 (6H, m, Ar-H, meta and para to SO_2NH gp, J_1=6.4 Hz, J_2=3.32 Hz), 7.26-7.15 (10H, m, Ar-H, J_1=11.36 Hz, J_2=3.96 Hz), 3.50-3.45 (2H, dd, -CH-CH_2-, J=14 Hz), 3.14-3.09 (2H, d, -NH-SO gp, J=5.52 Hz), 1.88-1.25 (4H, dd, -CH_2-, J_1=19.2Hz, J_2=14Hz).^{13}C-NMR 171 (C=O), 15.25 (-CH_2-), 65.86(-CH-NH), 142.80-117.60 (aromatic carbons), HRMS (ESI); m/z Calculated for $C_{44}H_{36}N_4O_8S_2$ $[M + H]^+$: 813.915, found: 813.180 (65.35% , m.p. 215-220°C, Rf = 0.76).

1,5 Bis [1-oxo -2-(benzosulfonamide)-ethylamido]-anthracene-9,10-dione (B2)= Yellow crystalline solid.



IR(υ cm^{-1}): NH str.=3067cm^{-1}, Arm.CN stre.= 1262cm^{-1}, -C=O str.=1689cm^{-1}, Alp.CN stre.= 1091cm^{-1}, O=S=O str.=1336, 1161cm^{-1}. (^{1}H-NMR- $CDCl_3$) 400MHz= δ 12.50 (1H, s, -NH ar), 12.20 (1H, s, -NH ar), 8.96-8.84 (1H, d, H_6 aaq, J=8.52 Hz), 8.09-8.02 (1H, d, H_2 aaq, J=7.40 Hz), 7.95-7.81 (4H, m, Ar-(H_3, H_4, H_7 and H_8) aaq, J_1=3.12 Hz, J_2=4.16 Hz), 7.70-7.68 (2H, m, Ar-H para to SO_2NH gp, J_1=3.36 Hz, J_2=4.88 Hz), 7.59-7.51 (4H, m, Ar-H, ortho to SO_2NH gp, J_1=6.84 Hz, J_2=4.12 Hz), 7.43-7.36 (2H, m, Ar-H meta to SO_2NH gp, J_1=9.68 Hz, J_2=6.96 Hz), 6.99-6.96 (2H, m, Ar-H meta to SO_2NH gp, J_1=12.04 Hz), 4.50 (1H, s, -NH-SO gp), 5.10 (1H, s, -NH-SO gp), 3.84-3.45 (2H, q, -CH_2-, J_1=14.08 Hz, J_2=14 Hz), 1.80-1.25 (2H, dd, -CH_2-, J_1=11.2Hz, J_2=7Hz).^{13}C-NMR: 14.22 (-CH_2-), 133.08-126.43 (aromatic carbons), 171 (C=O). HRMS (ESI); m/z Calculated for $C_{30}H_{24}N_4O_8S_2$ $[M + H]^+$: 633.670, found: 633.090 (57%, m.p. 185-190°C; Rf = 0.50).

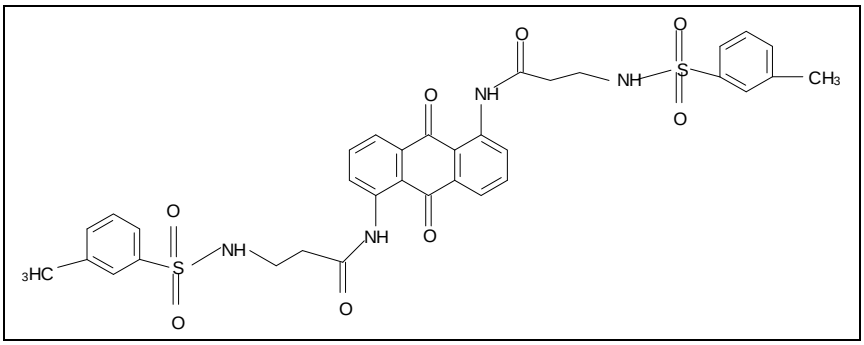
1,5 Bis [1-oxo-3-phenyl-2p-(tosylamide)-propylamido]-anthracene-9,10-dione(B3)= Yellow crystalline solid.



IR(υ cm^{-1}): NH str.=3262cm^{-1}, Arm.CN stre.= 1260cm^{-1}, -C=O str.=1696cm^{-1}, Alp.CN stre.= 1087cm^{-1}, O=S=O str.=1333, 1157cm^{-1}. (^{1}H-NMR- $CDCl_3$) 400MHz= δ 12.65 (1H, s, -NH ar), 12.60 (1H, s, -NH ar), 8.93-8.91 (1H, d, H_6 aaq, J=0.68 Hz), 8.82-8.79 (1H, d, H_2 aaq, J=0.96 Hz), 8.03-7.99 (2H, m, Ar-(H_7 and H_8) aaq, J_1=1 Hz, J_2=8.6 Hz), 7.72-7.69 (2H, m, Ar-(H_3 and H_4) aaq, J_1=8.12 Hz, J_2=4.6 Hz), 7.59-7.41 (5H, m, Ar-H, J_1=6.72 Hz, J_2=0.68 Hz), 7.16-7.10 (9H, m, Ar-H and ortho to SO_2NH gp, J_1=3.8 Hz, J_2=2.04 Hz), 7.08-6.95 (4H, m, Ar-H, meta to SO_2NH gp, J_1=2.08 Hz, J_2=2.6 Hz), 5.44 (1H, s, -NH-SO gp), 5.42 (1H, s, -NH-SO gp), 4.19-

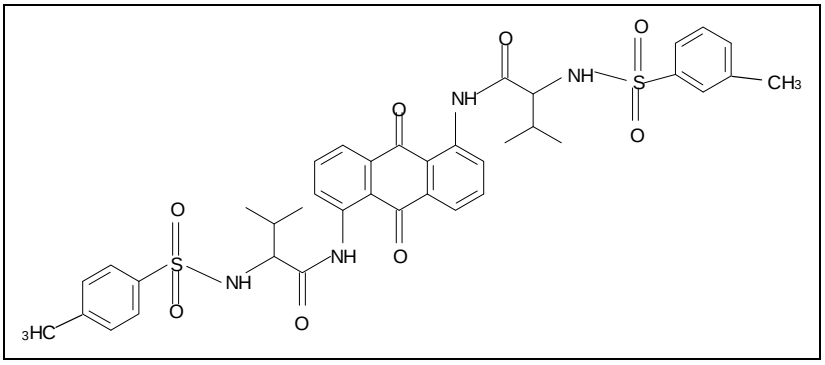
4.17 (1H, d, -CH_2-, J=7 Hz), 3.14-3.13 (2H, d, -CH_2-, J=6 Hz), 3.11 (1H, s, -CH_3), 2.32 (1H, s, -CH_3), 2.27-2.25 (1H, t, -CH-, J=8.48 Hz), 1.22-1.19 (1H, t, -CH-, J=14 Hz).^{13}C-NMR **:** 21.46(-CH_2), 21.53(-CH_2), 38.84 (-CH_3), 39.21(-CH_3), 59.57(-CH-NH), 170.43 (C=O), 170.81 (C=O), 143.71-117.35 (aromatic carbons). HRMS (ESI); m/z Calculated for $C_{46}H_{40}N_4O_8S_2$ $[M + H]^+$: 841.968 found: 841.210 (47.77%, m.p. 255-260°C; Rf = 0.66).

1,5 Bis [1-oxo (-3-p-tosylamide)-propylamido]-anthracene-9,10-dione (B4)=Orange crystalline solid.



IR(υ cm^{-1}): NH str.=3254cm^{-1}, Arm.CN stre.= 1262cm^{-1}, -C=O str.=1694cm^{-1}, Alp.CN stre.= 1091cm^{-1}, O=S=O str.=1328, 1154cm^{-1}. (^{1}H-NMR- $CDCl_3$) 400MHz= δ 12.21 (1H, s, -NH ar), 12.20 (1H, s, -NH ar), 9.01-8.99 (1H, d, -NHSO gp, J=4.52 Hz), 8.07-7.99 (2H, m, Ar H_2 and H_6 aaq, J_1=15.24 Hz, J_2=7.4 Hz), 7.74-7.71 (6H, m, Ar-(H_3, H_4, H_7 and H_8) aaq and 2H meta to SO_2NH gp, J_1=6.32 Hz, J_2=3.48 Hz), 7.47-7.41 (2H, m, Ar-H meta to SO_2NH gp, J_1=8.12 Hz, J_2=10.8 Hz), 7.31-7.26 (4H, m, Ar-H ortho to SO_2NH gp, J_1=8.12 Hz, J_2=10.8 Hz),6.99-6.97 (1H, d, -NHSO gp, J=7.88 Hz), 4.15-4.11 (1H, d, -NH-SO gp, J=14 Hz), 3.48-3.47 (2H, d, -CH_2-, J=7Hz), 3.21-3.14 (2H, t, -CH_2-, J=9.92 Hz), 2.98-2.89 (2H, t, -CH_2-, J=9.96 Hz), 2.79-2.73 (2H, t, -CH_2-, J=11.32 Hz), 2.39-2.33 (6H, m, -CH_3, J_1=12.08 Hz, J_2=4.71 Hz).^{13}C-NMR: 15.26(-CH_2), 21.55(-CH_2), 21.71(-CH_2), 38.93(-CH_3), 186.05 (C=O), 171.01 (C=O), 143.49-122.93 (aromatic carbons. HRMS (ESI); m/z Calculated for $C_{34}H_{32}N_4O_8S_2$ $[M + H]^+$: 689.776, found: 689.151 (55.80% , m.pt 130°C ; Rf = 0.84).

1,5 Bis [1-oxo -3-methyl-2-(-p-tosylamide)-butylamido]-anthracene-9,10-dione (B5)= Yellow crystalline solid.



IR(υ cm^{-1}): NH str.=3256cm^{-1}, Arm.CN stre.= 1262cm^{-1}, -C=O str.=1685cm^{-1}, Alp.CN stre.= 1089cm^{-1}, O=S=O str.=1337, 1167cm^{-1}. (^{1}H-NMR- $CDCl_3$) 400MHz= δ 12.34 (1H, s, -NH ar), 11.90 (1H, s, -NH ar), 8.78-8.76 (1H, d, H_6, J=8.32 Hz), 8.07-7.99 (1H, d, Ar H_2 aaq, J_1=7.6 Hz), 7.68-7.62 (10H, m, Ar-H ortho and para to –NHSO gp and Ar-(H_3, H_4, H_7 and H_8) aaq, J_1=7.96 Hz, J_2=3.12 Hz), 7.12-7.00 (4H, m, Ar-H meta to SO_2NH gp, J_1=10.8 Hz, J_2=7.76 Hz), 5.48-5.46 (1H, d, -NHSO gp, J=7.56 Hz), 3.68-3.66 (1H, d, -NHSO gp, J=8.08 Hz), 2.35-2.27 (4H, q, -CH-, J_1=28.6 Hz, J_2=17.28 Hz), 2.22-2.02 (6H, m, -CH_3, J_1=7.2Hz, J_2=20.56 Hz), 1.28-1.01 (6H, m, -CH_3, J_1=7.2 Hz, J_2=11.6 Hz), 0.93-0.80 (6H, m, -CH_3, J_1=6.44 Hz, J_2=11.92 Hz).^{13}C-NMR **:** 15.27 (-CH_3), 17.64(-CH_3), 19.27 (-CH_3), 31.81(-CH), 65.87(-CH-NH), 143.71-123.28 (aromatic carbons), 171.22 (C=O), 174.27 (C=O). HRMS (ESI); m/z Calculated for $C_{38}H_{40}N_4O_8S_2$ $[M + H]^+$: 745.883, found: 745.210 (52.52%, m.pt 305-310°C; Rf = 0.33).

Fig. S1 [1]HNMR of 1,5 Bis [1-oxo-3-phenyl-2-(benzosulfonamide)-propylamido]-anthracene-9,10-dione (B1)

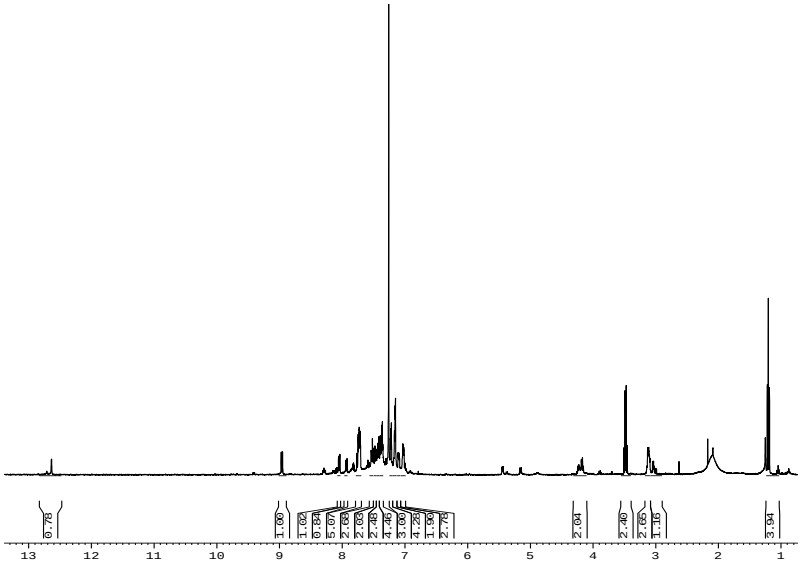


Fig. S2 [13]CNMR of 1,5 Bis [1-oxo-3-phenyl-2-(benzosulfonamide)-propylamido]-anthracene-9,10-dione (B1)

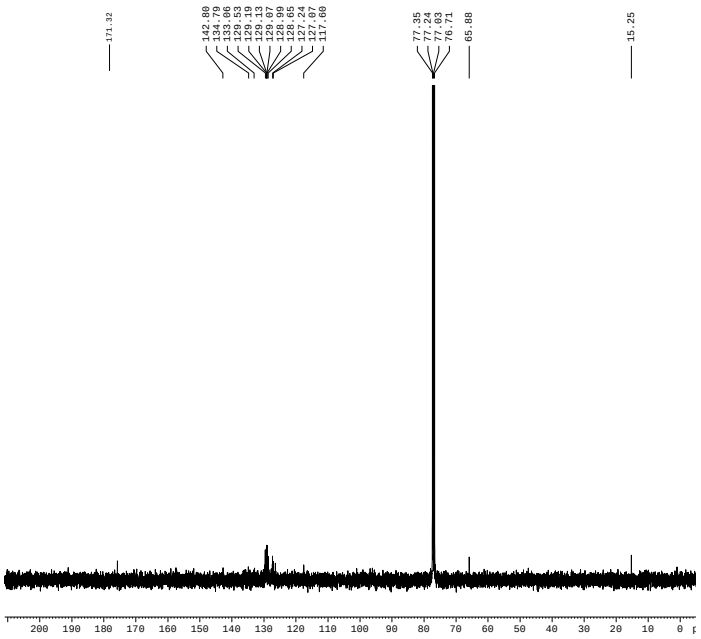


Fig. S3 [1]HNMR of 1,5 Bis [1-oxo -2-(benzosulfonamide)-ethylamido]-anthracene-9,10-dione (B2)

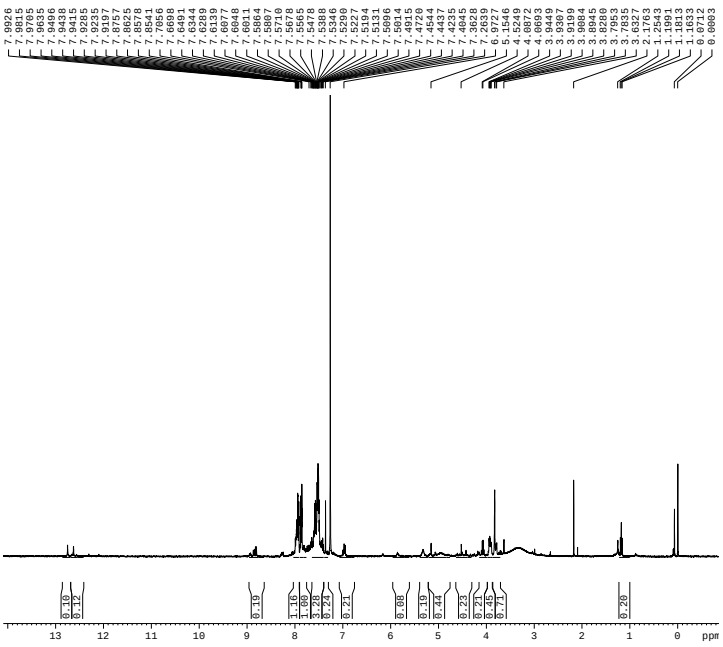


Fig. S4 [13]CNMR of 1,5 Bis [1-oxo -2-(benzosulfonamide)-ethylamido]-anthracene-9,10-dione (B2)

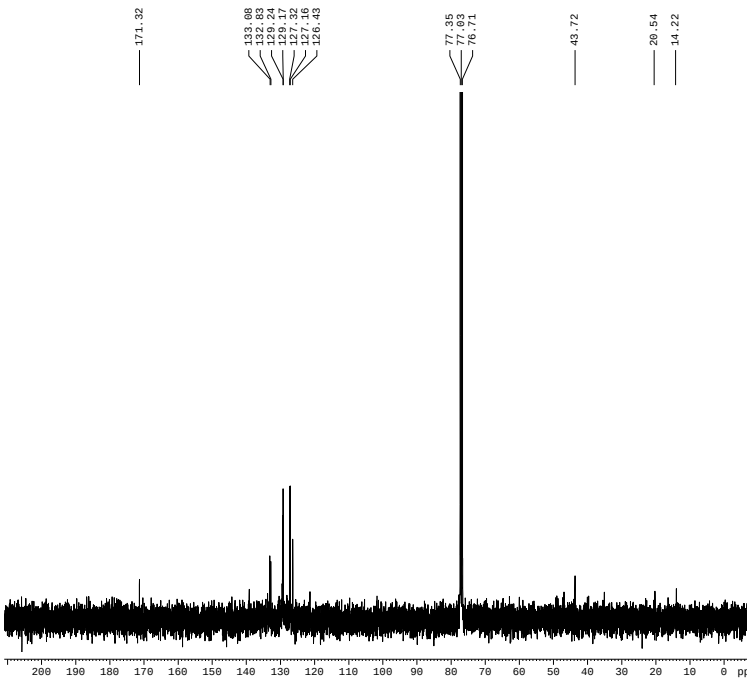


Fig. S5 [1]HNMR of 1,5 Bis [1-oxo-3-phenyl-2p-(tosylamide)-propylamido]-anthracene-9,10-dione(B3)

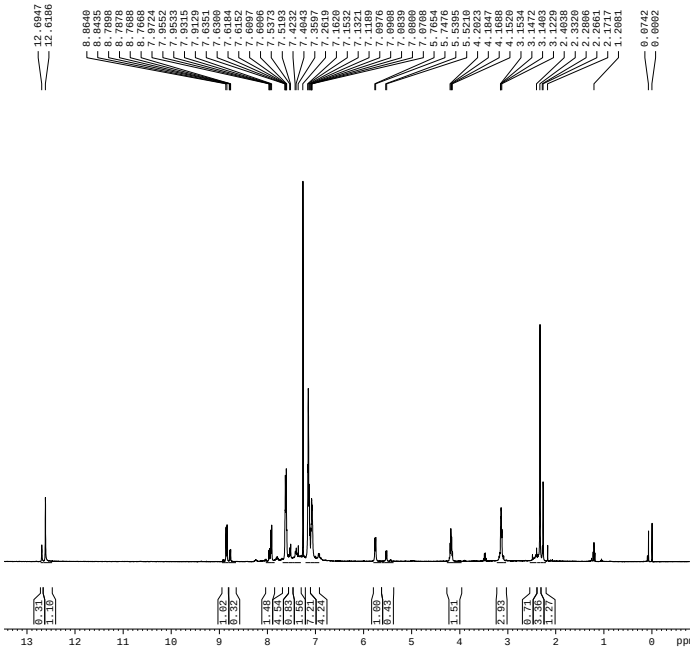


Fig. S6 [13]CNMR of 1,5 Bis [1-oxo-3-phenyl-2p-(tosylamide)-propylamido]-anthracene-9,10-dione(B3)

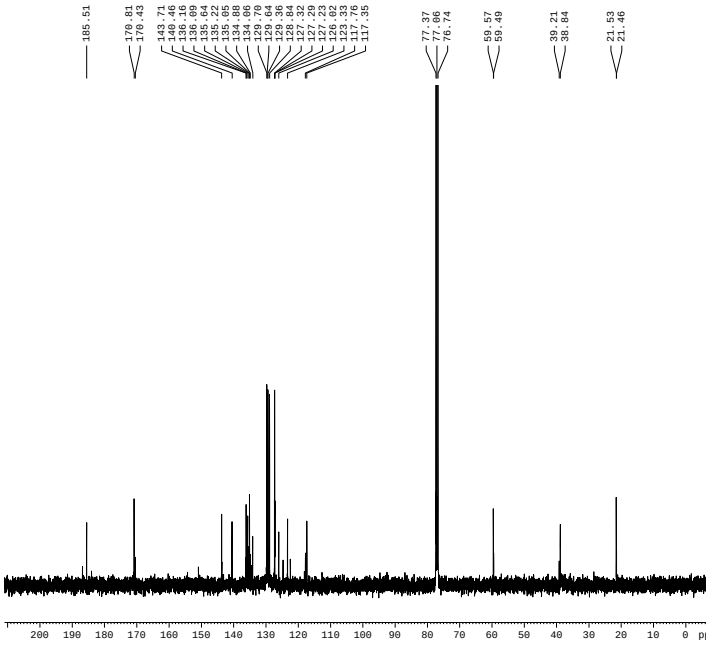


Fig. S7 [1]HNMR 1,5 Bis [1-oxo (-3-p-tosylamide)-propylamido]-anthracene-9,10-dione (B4)

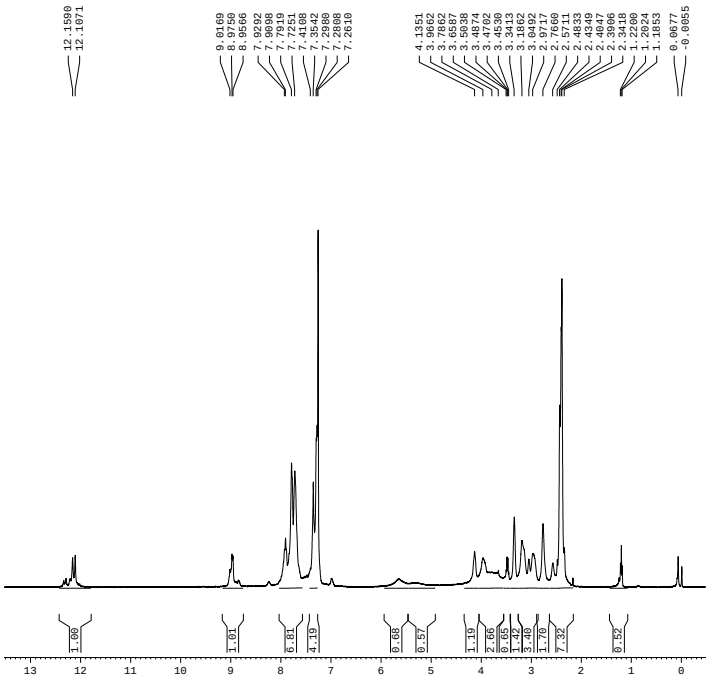


Fig. S8 [13]CNMR 1,5 Bis [1-oxo (-3-p-tosylamide)-propylamido]-anthracene-9,10-dione (B4)

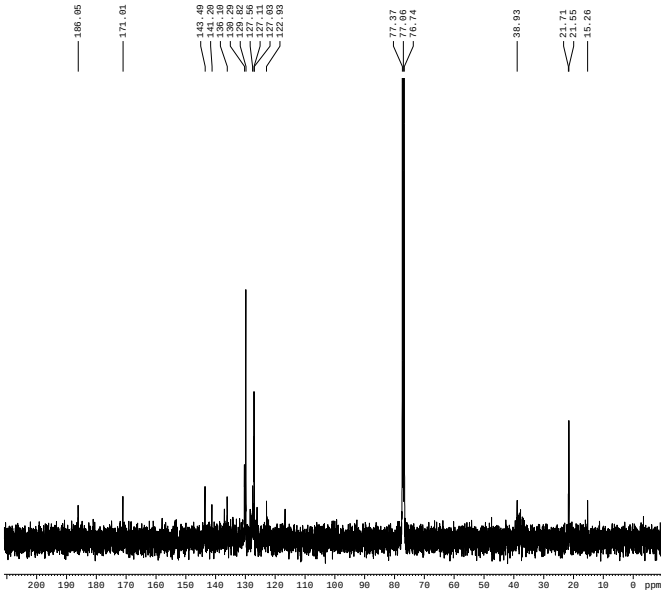


Fig. S9 [1] HNMR 1,5 Bis [1-oxo -3-methyl-2-(-p-tosylamide)-butylamido]-anthracene-9,10-dione (B5)

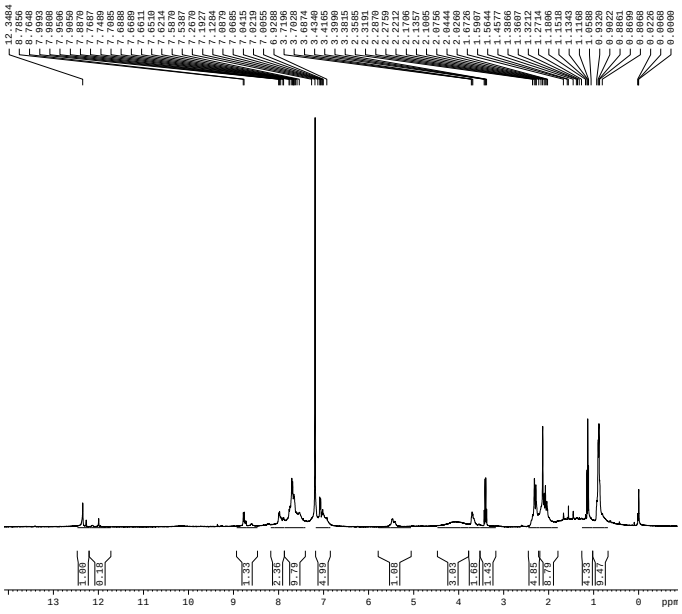


Fig. S10 [13]CNMR 1,5 Bis [1-oxo -3-methyl-2-(-p-tosylamide)-butylamido]-anthracene-9,10-dione (B5)