Supplementary Information

Synthesis and Three-Dimensional Structure, Conformation and Correct Chemical Shift Assignment Determination of Pharmaceutical Molecules by NMR

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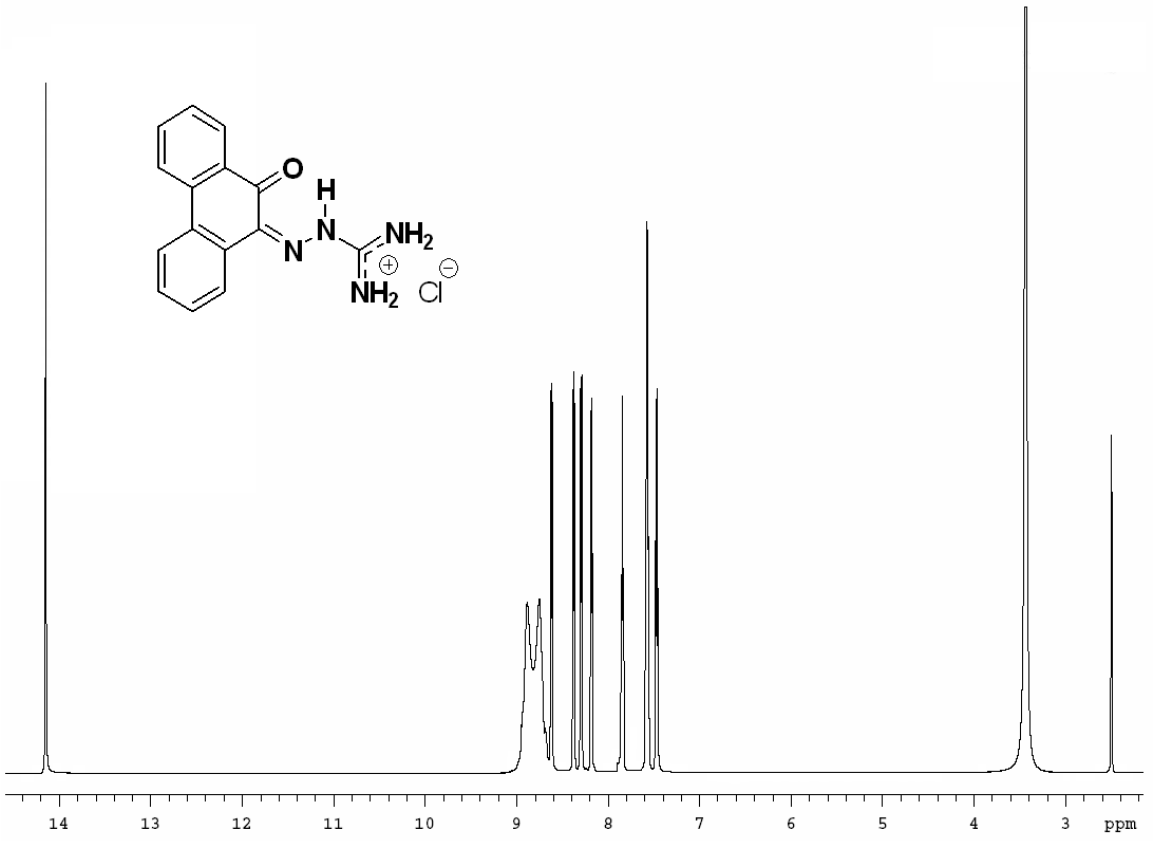

Figure S1. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of phenanthrenequinone guanylhydrazone (**3**).

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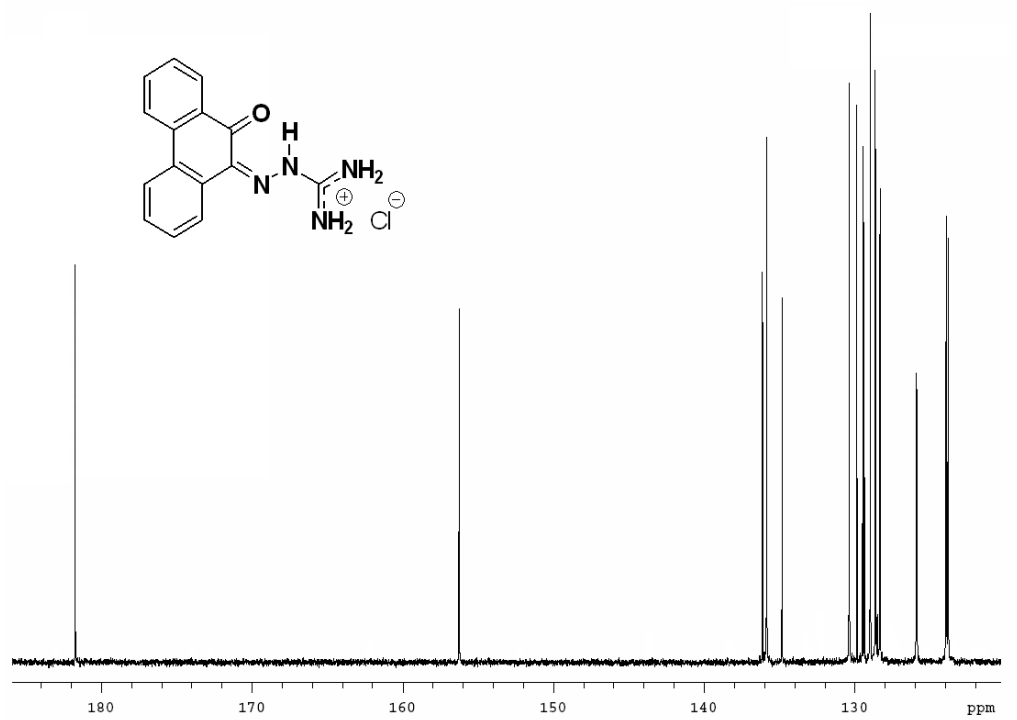

Figure S2. ^{13}C NMR spectrum (150 MHz, DMSO-d_6) of phenanthrenequinone guanylhydrazone (**3**).

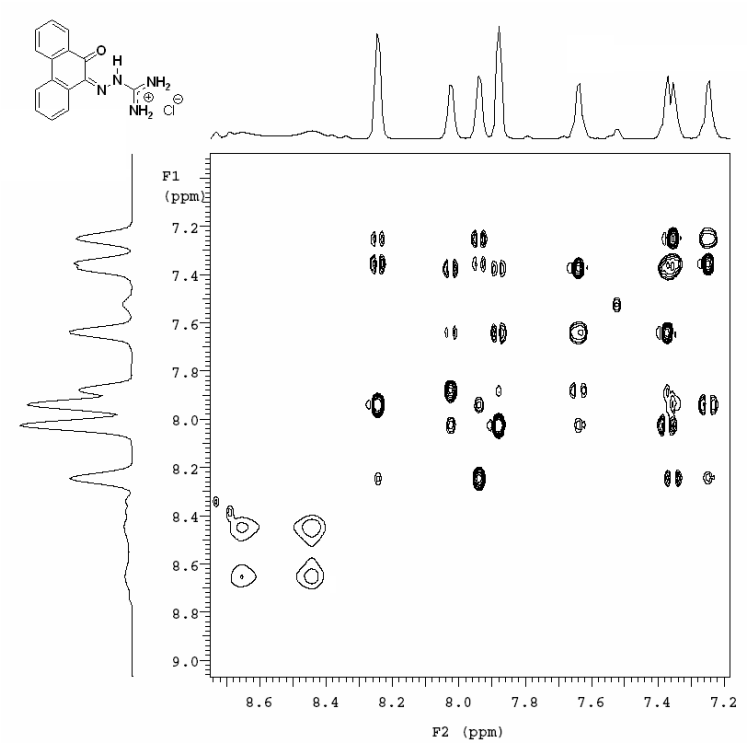

Figure S3. COSY spectrum (600 MHz, DMSO-d_6) of phenanthrenequinone guanylhydrazone (**3**).

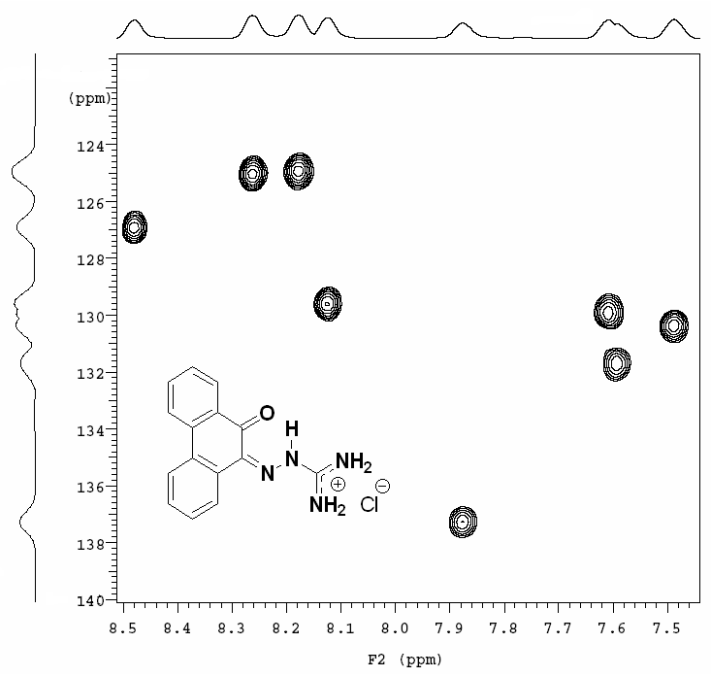

Figure S4. gHSQC spectrum (600 MHz, DMSO-d_6) of phenanthrenequinone guanylhydrazone (**3**).

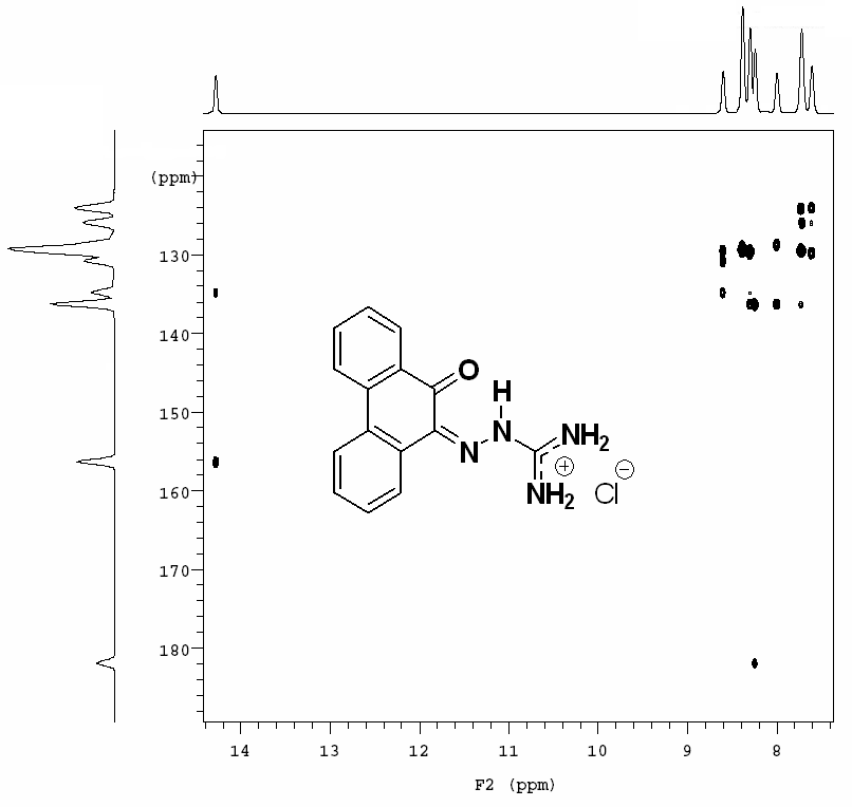

Figure S5. gHMBC spectrum (600 MHz, DMSO-d_6) of phenanthrenequinone guanylhydrazone (**3**).

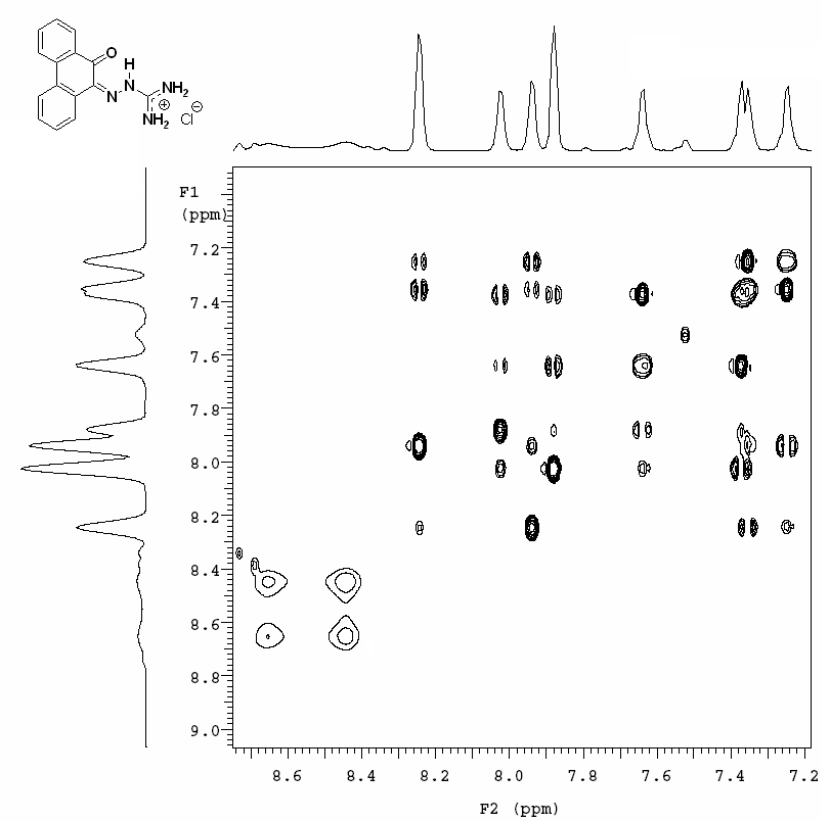

Figure S6. TOCSY spectrum (600 MHz, DMSO-d_6) of phenanthrenequinone guanylhydrazone (**3**).

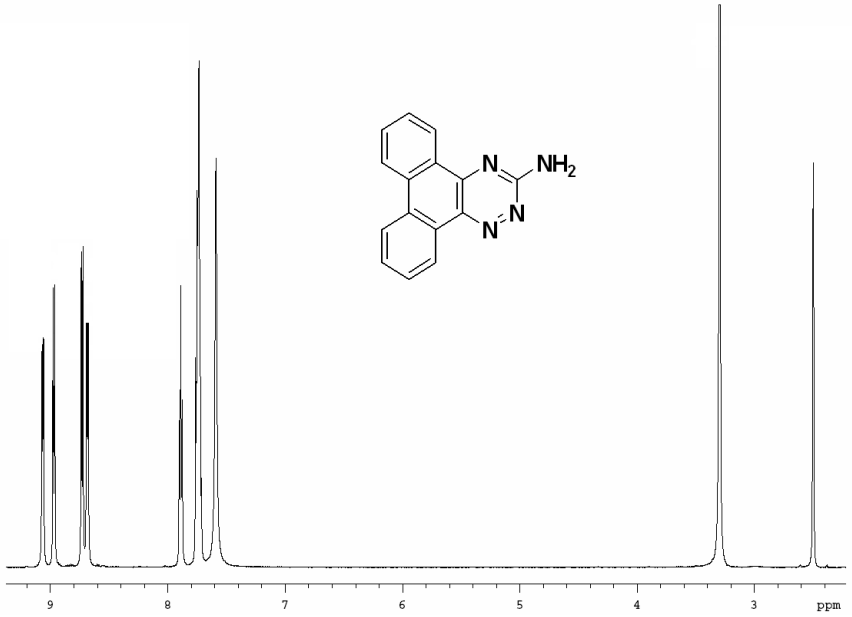

Figure S7. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of phenanthro[9,6-*e*][1,2,4]trizin-3-amine (**4**).

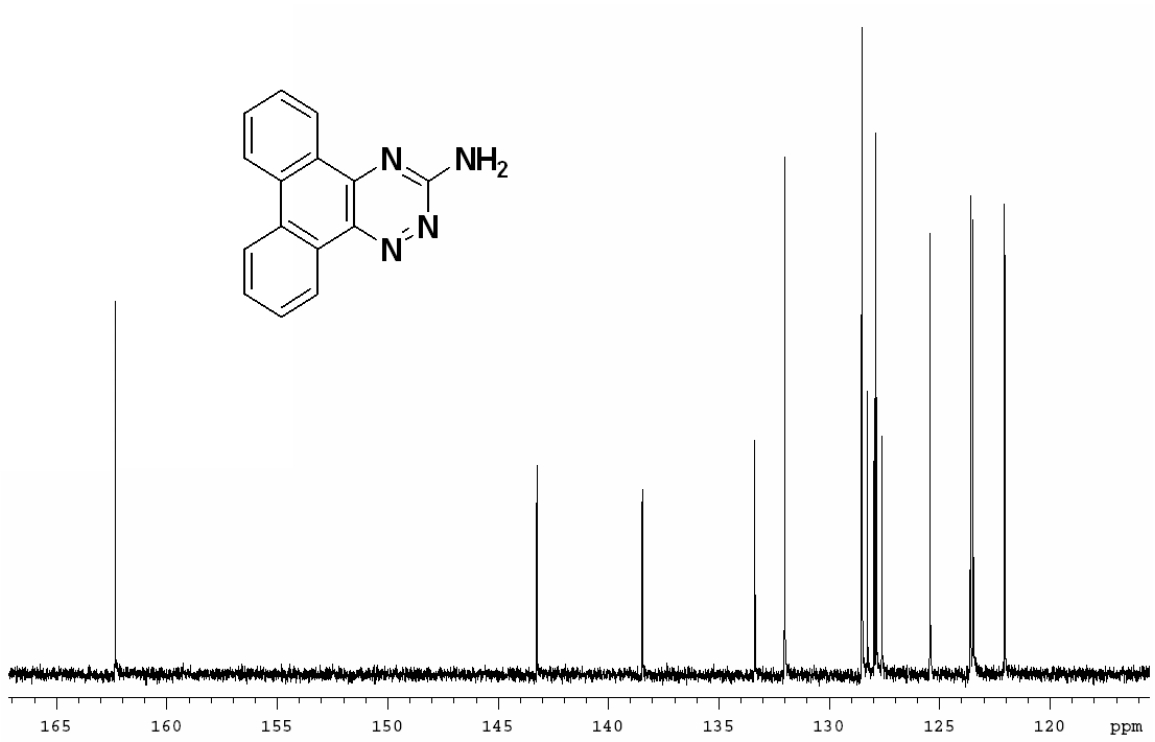

Figure S8. ^{13}C NMR spectrum (150 MHz, DMSO-d_6) of phenanthro[9,10-*e*][1,2,4]triazin-3-amine (**4**).

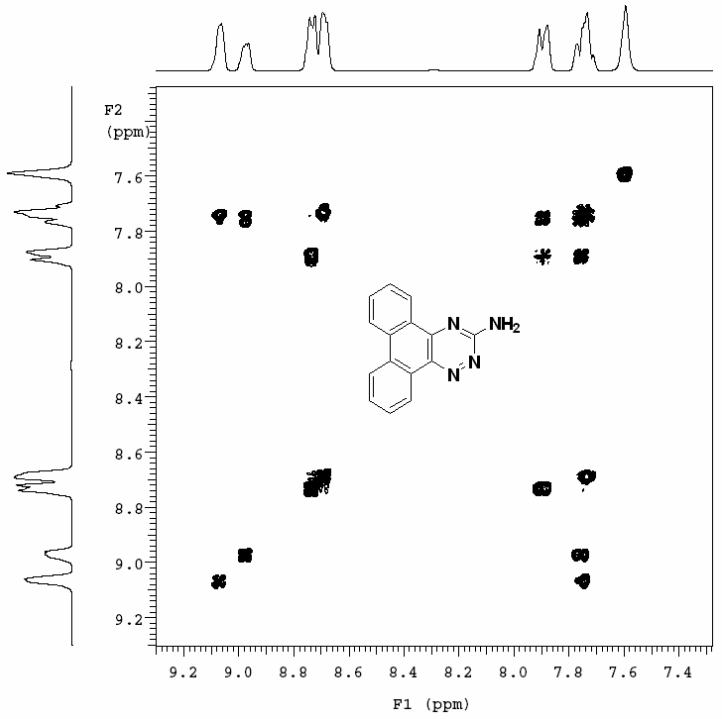

Figure S9. COSY spectrum (600 MHz, DMSO-d_6) of phenanthro[9,10-*e*][1,2,4]triazin-3-amine (**4**).

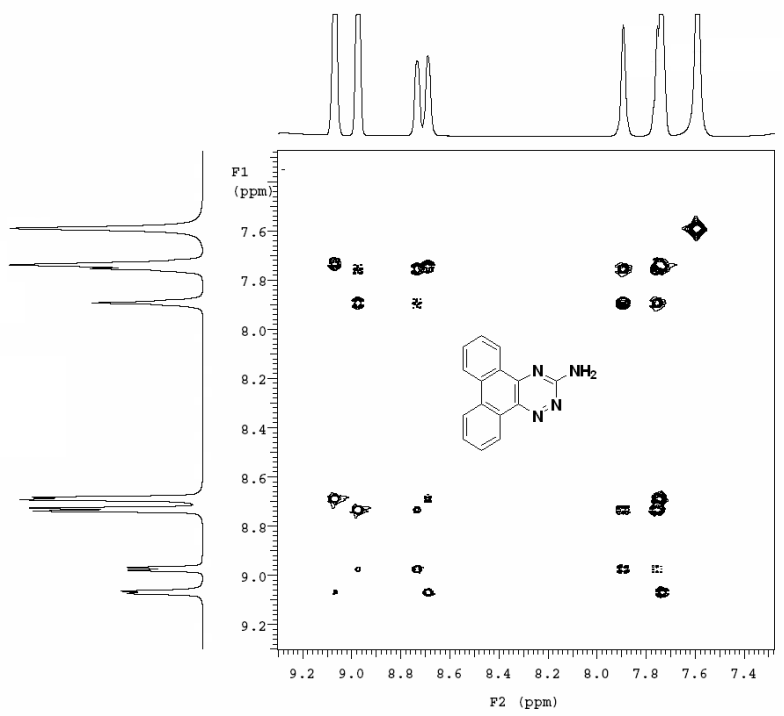

Figure S10. TOCSY spectrum (600 MHz, DMSO-d_6) of phenanthro[9,10-*e*][1,2,4]triazin-3-amine (**4**).

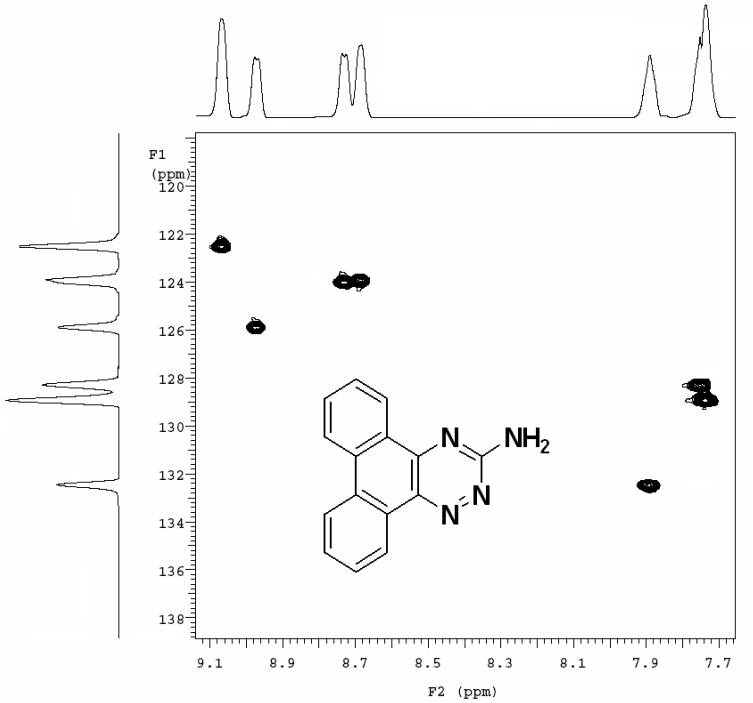

Figure S11. gHSQC spectrum (600 MHz, DMSO-d_6) of phenanthro[9,10-*e*][1,2,4]triazin-3-amine (**4**).

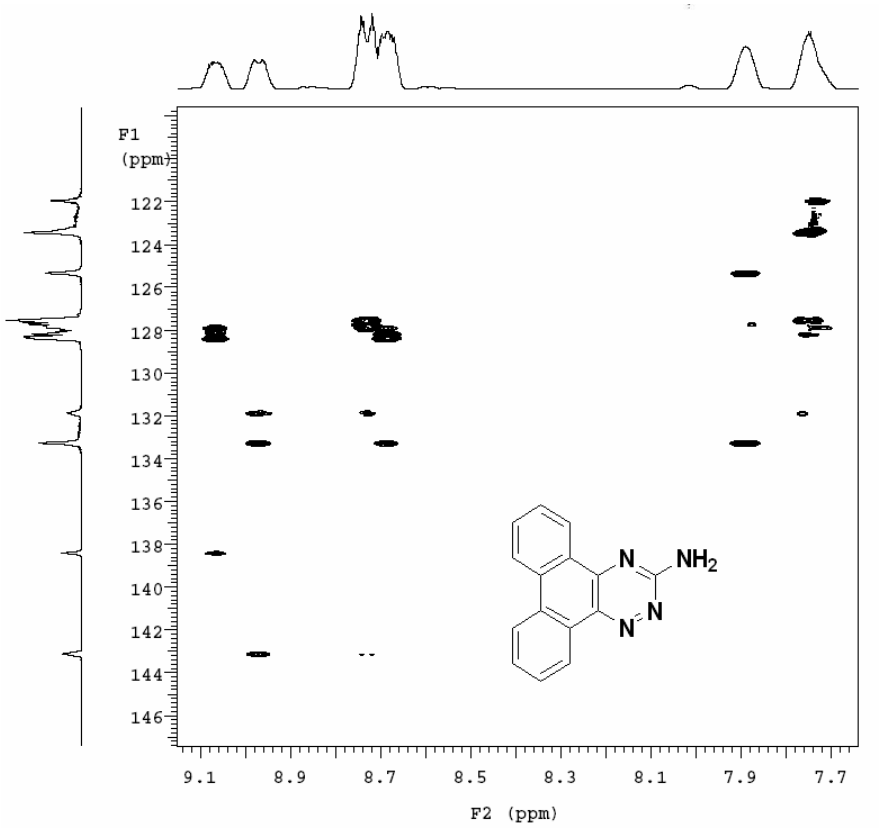

Figure S12. gHMBC spectrum (600 MHz, DMSO-d_6) of phenanthro[9,10-*e*][1,2,4]triazin-3-amine (**4**).

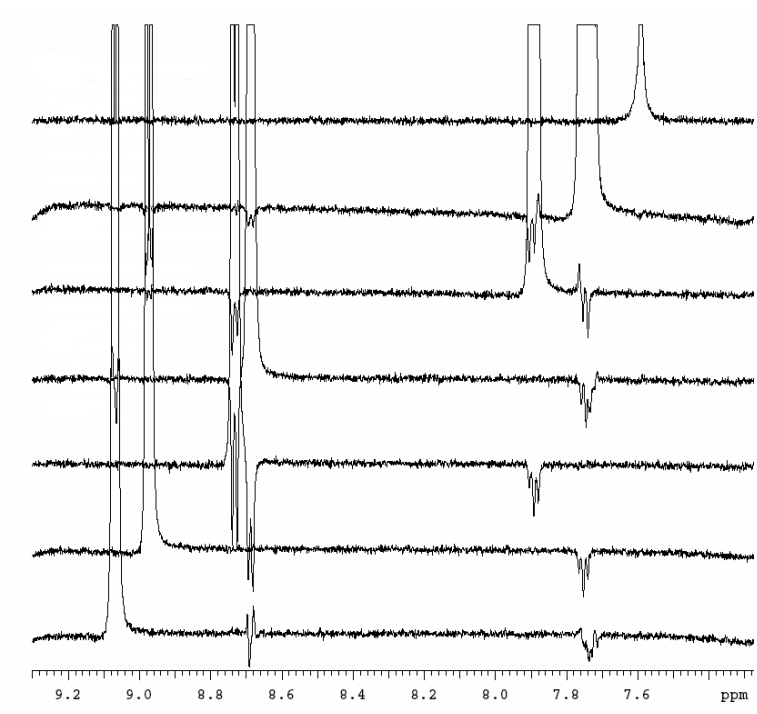

Figure S13. NOESY-1D spectrum (600 MHz, DMSO-d_6) of phenanthro[9,10-*e*][1,2,4]triazin-3-amine (**4**).

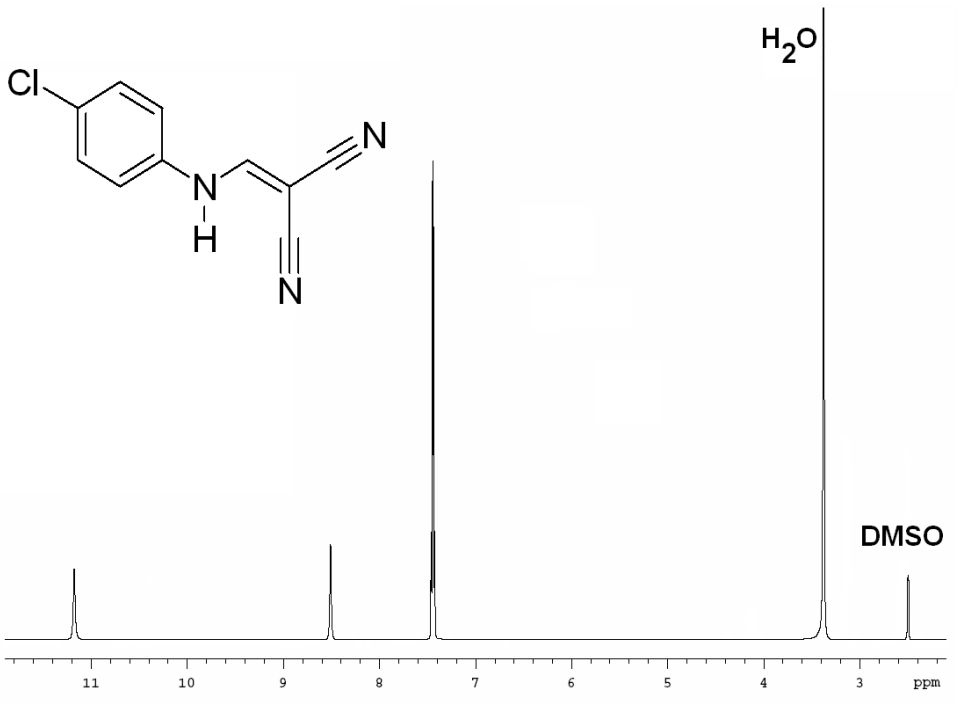

Figure S14. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of 2-[(4-chlorophenylamino)methylene]malononitrile (**5**).

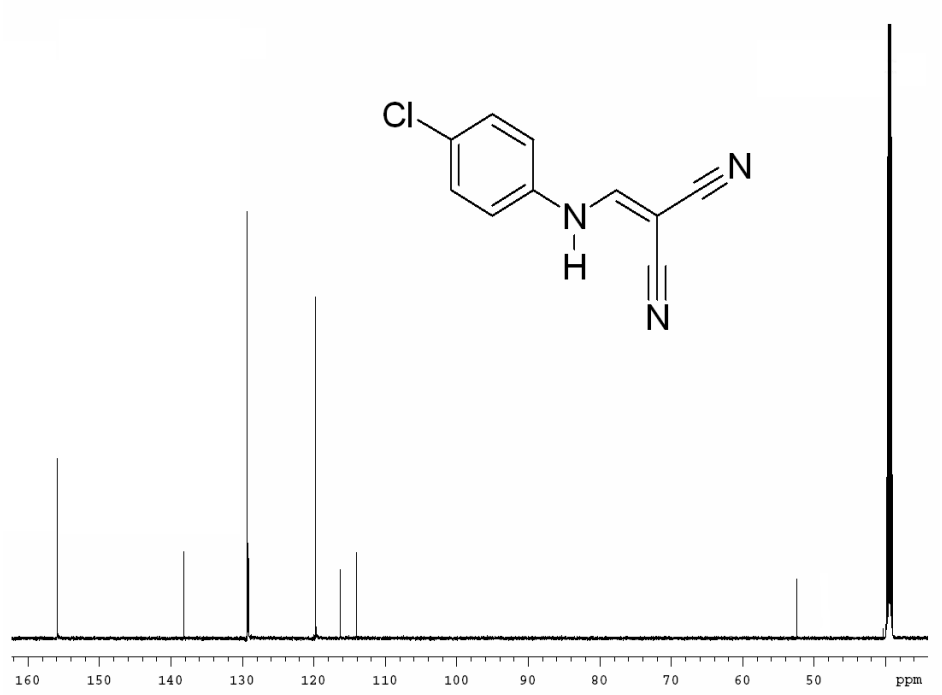

Figure S15. ^{13}C NMR spectrum (150 MHz, DMSO-d_6) of 2-[(4-chlorophenylamino)methylene]malononitrile (**5**).

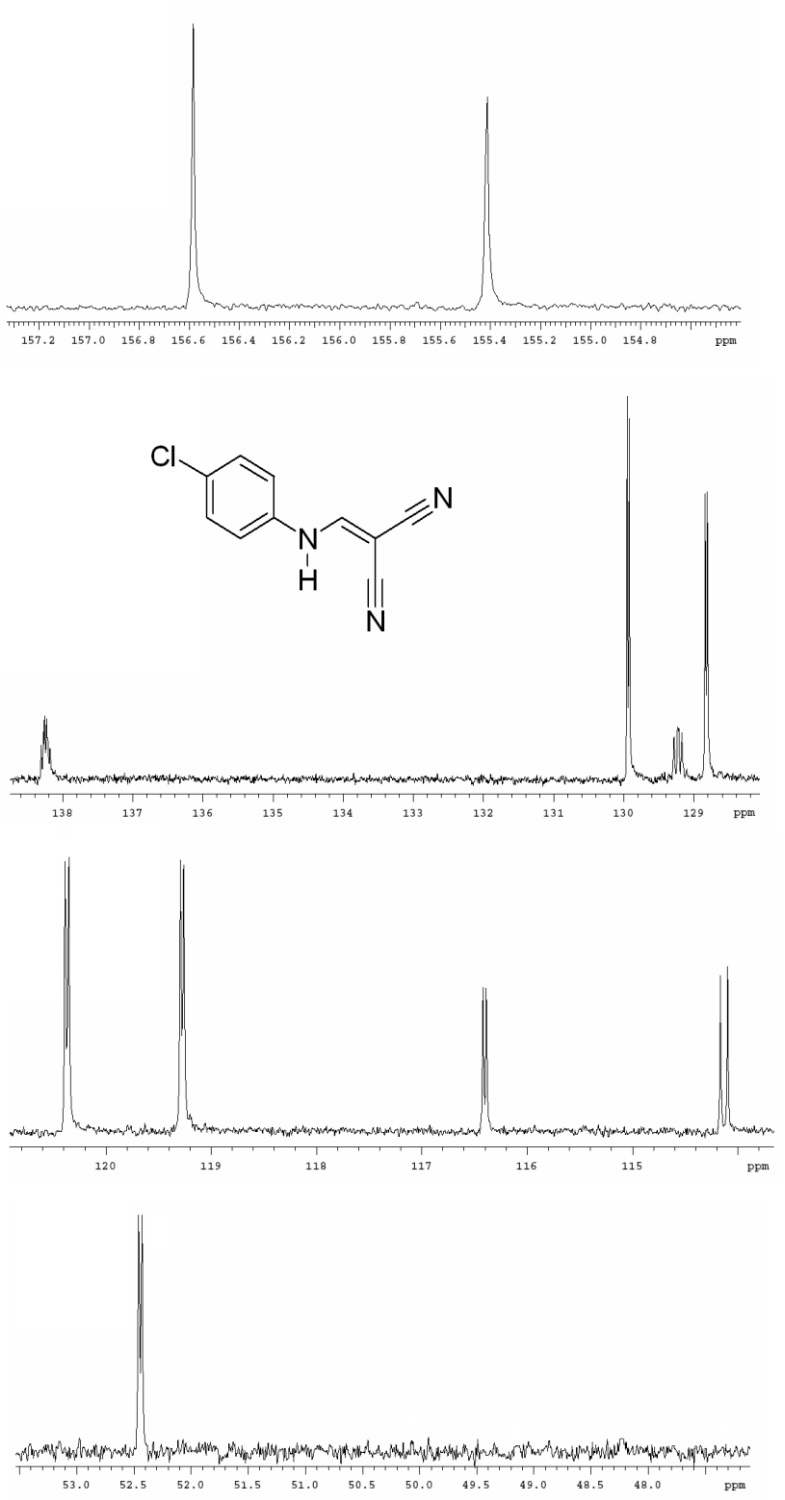

Figure S16. Gated decoupling ^{13}C NMR spectrum (150 MHz, DMSO-d_6) of 2-[(4-chlorophenylamino)methylene]malononitrile (**5**).

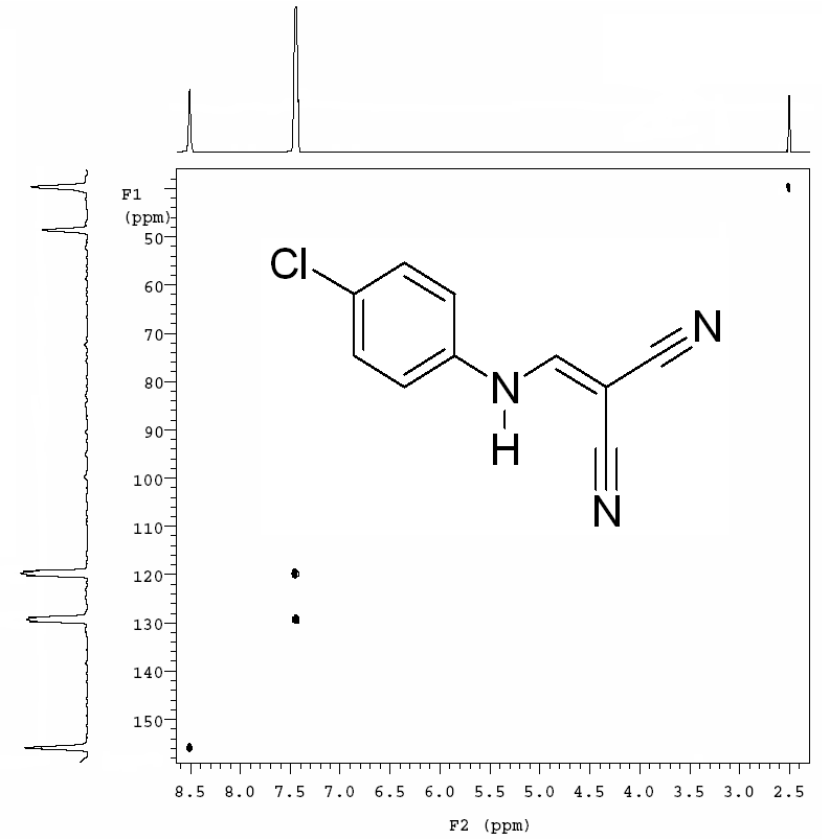

Figure S17. gHSQC spectrum (600 MHz, DMSO-d_6) of 2-[(4-chlorophenylamino) methylene]malononitrile (**5**).

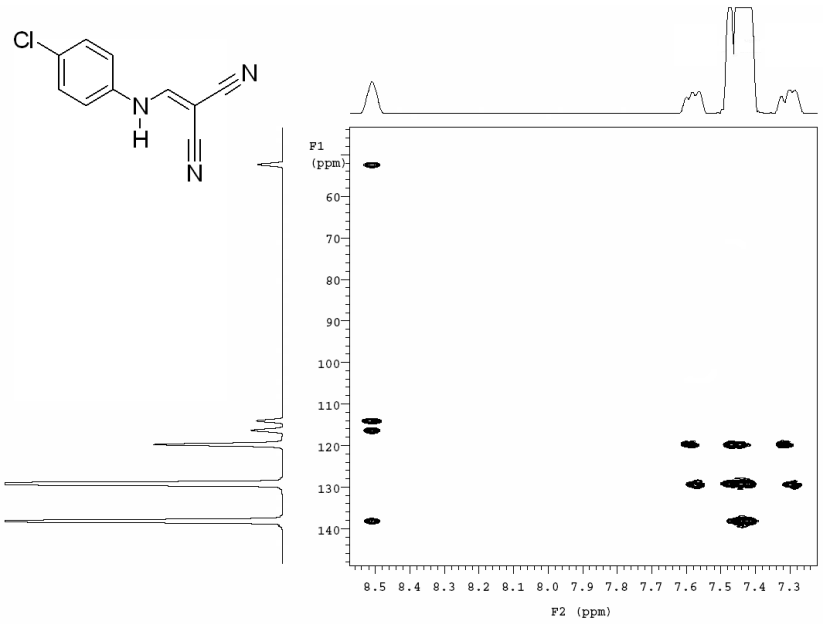

Figure S18. gHMBC spectrum (600 MHz, DMSO-d_6) of 2-[(4-chlorophenylamino)methylene]malononitrile (**5**).

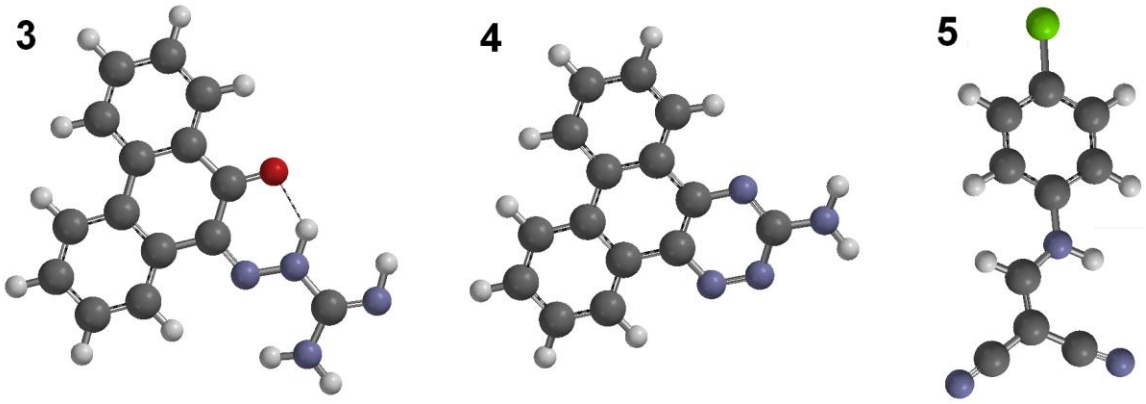

Figure S19. Molecular modeling structure of compounds **3**, **4** and **5** by Spartan'10 using density functional theory (DFT) with the B3LYP method and 6-311G* basis set.

Table S1. The confirmation of the NMR chemical shift of compound 3 by NMR and molecular modeling (density functional, M06 by 6-311G*)

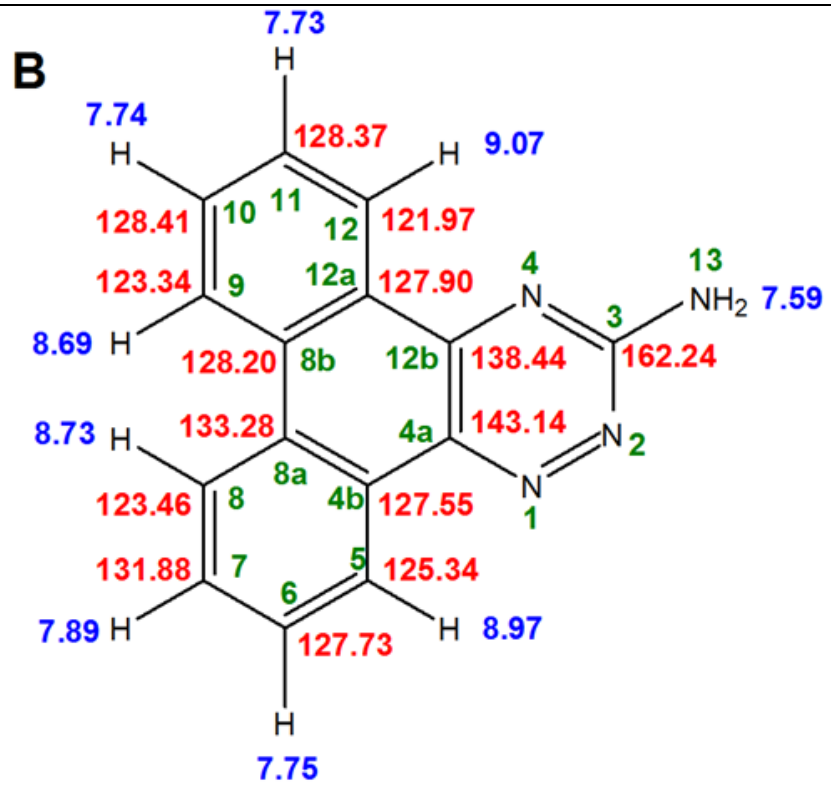

Table S1. The confirmation of the NMR chemical shift of compound 3 by NMR and molecular modeling (Density Functional, M06 by 6-311G*) (cont.)

Carbon			Hydrogen		
^{13}C	Molecular modeling	NMR	^{1}H	Molecular modeling	NMR
C3	159.95	162.24	–	–	–
C4a	147.63	143.14	–	–	–
C4b	128.22	127.55	–	–	–
C5	125.09	125.34	H5	9.80	8.97
C6	127,13	127.73	H6	8.01	7.75
C7	129,90	131.88	H7	7.96	7.89
C8	122.09	123.46	H8	8.75	8.74
C8a	130.65	133.28	–	–	–
C8b	128.32	128.20	–	–	–
C9	123.38	123.34	H9	8.71	8.69
C10	129.01	128.41	H10	8.18	7.74
C11	127.54	128.37	H11	7.88	7.73
C12	122.00	121.97	H12	9.72	9.07
C12a	127.84	127.90	–	–	–
C12b	139.88	138.44	–	–	–
–	–	–	H13	3.82	7.59
–	–	–	H13	4.35	7.59