How Do Amides Affect the Electronic Properties of Pyrene? (Supporting Information)

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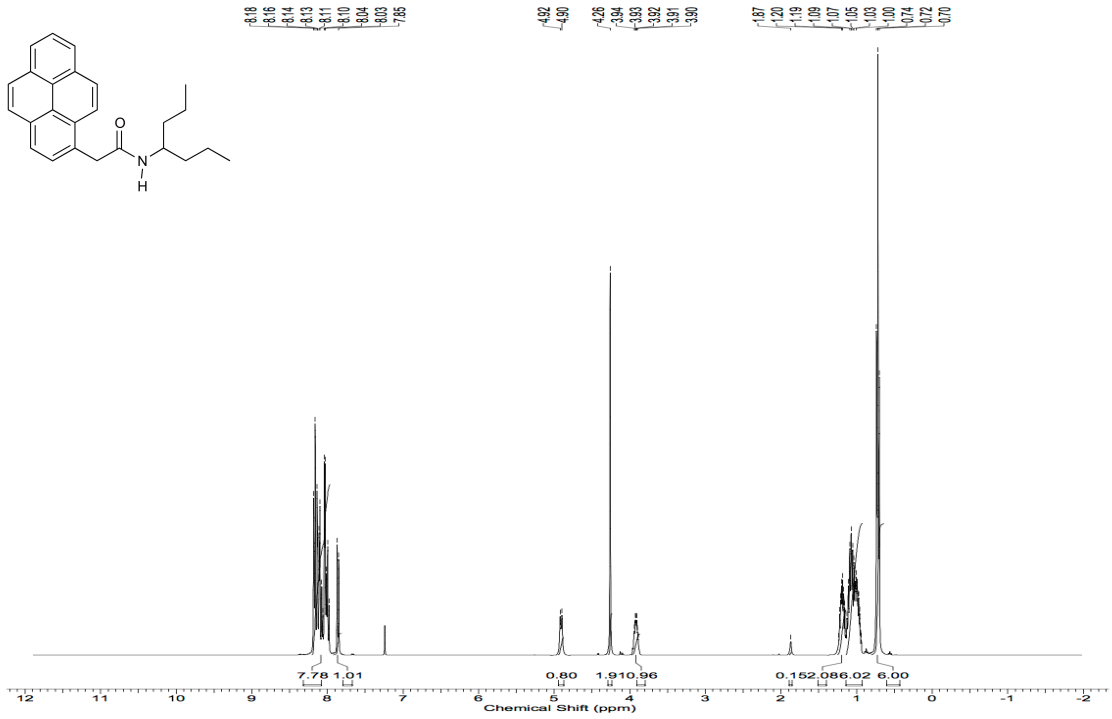
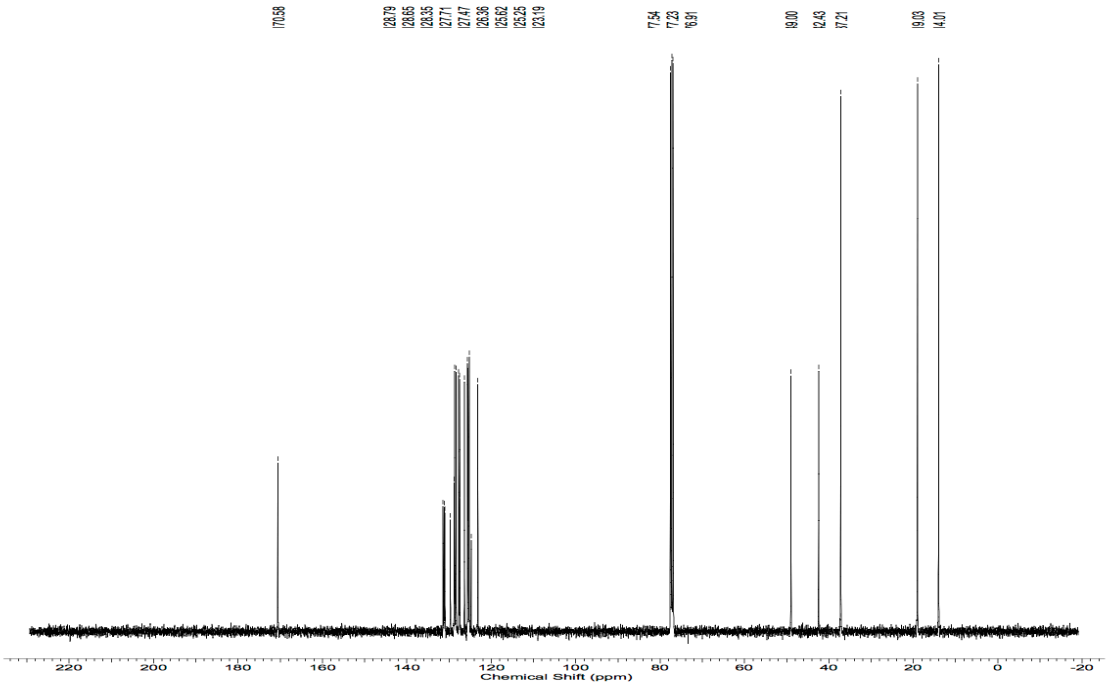
NMR spectra of pyrene derivatives

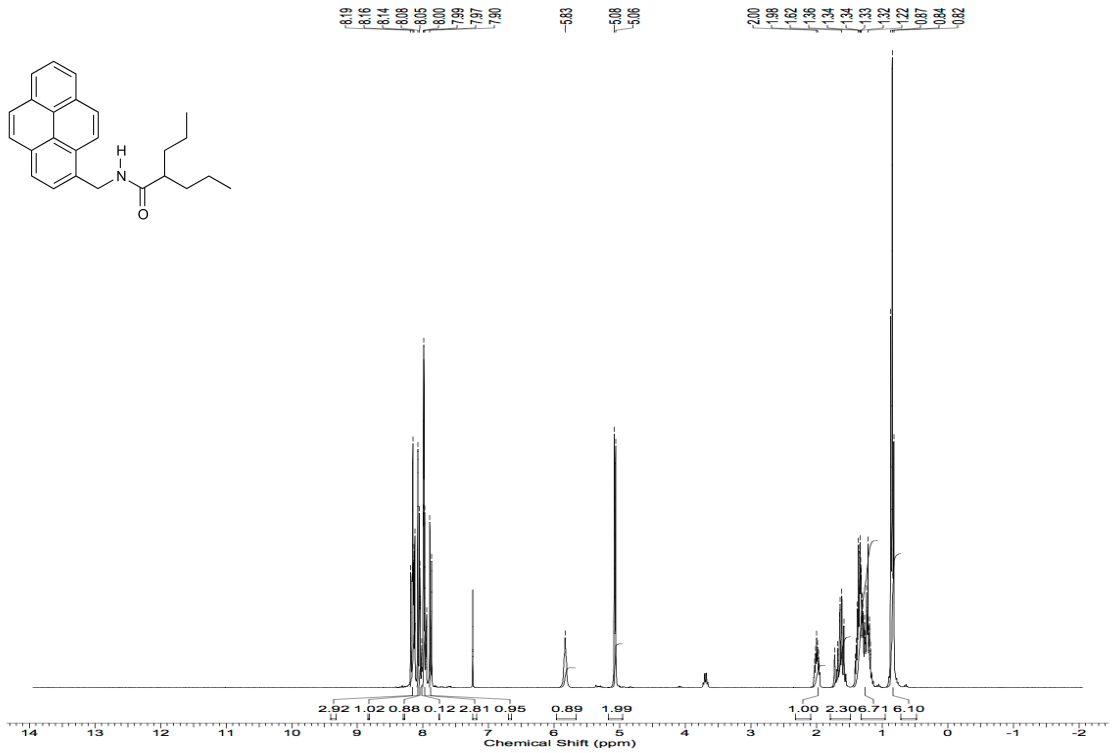


a



b

Figure S1. (a) ^{1}HNMR of $\mathbf{Py_{mC\text{-}N}}$ (300 MHz, $CDCl_3$); (b) ^{13}C NMR of $\mathbf{Py_{mC\text{-}N}}$ (300 MHz, $CDCl_3$)



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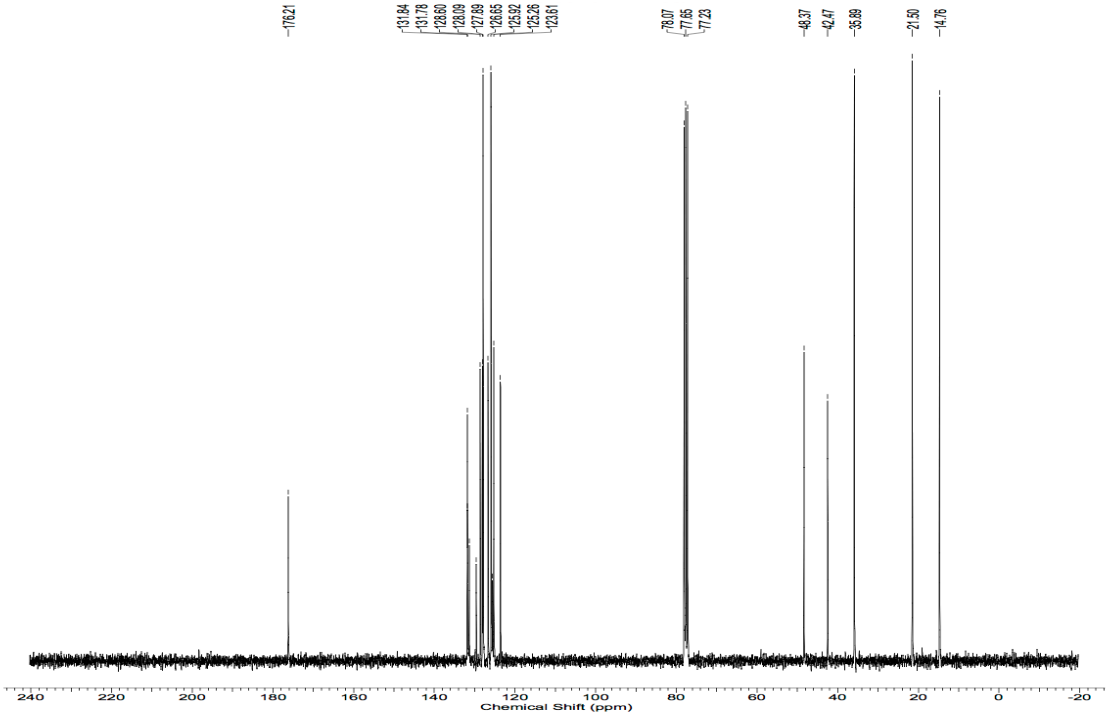
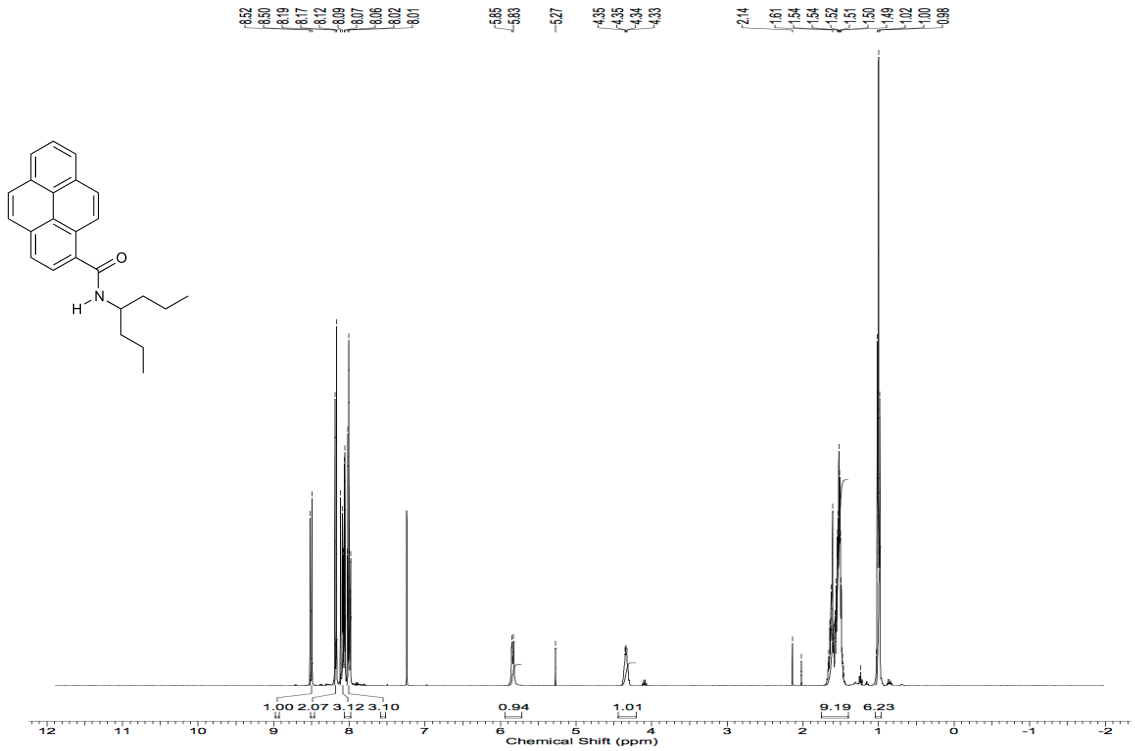


b

Figure S2. (a) ^{1}HNMR of $\mathbf{Py_{mN\text{-}C}}$ (300 MHz, $CDCl_3$); (b) ^{13}C NMR of $\mathbf{Py_{mN\text{-}C}}$ (300 MHz, $CDCl_3$)



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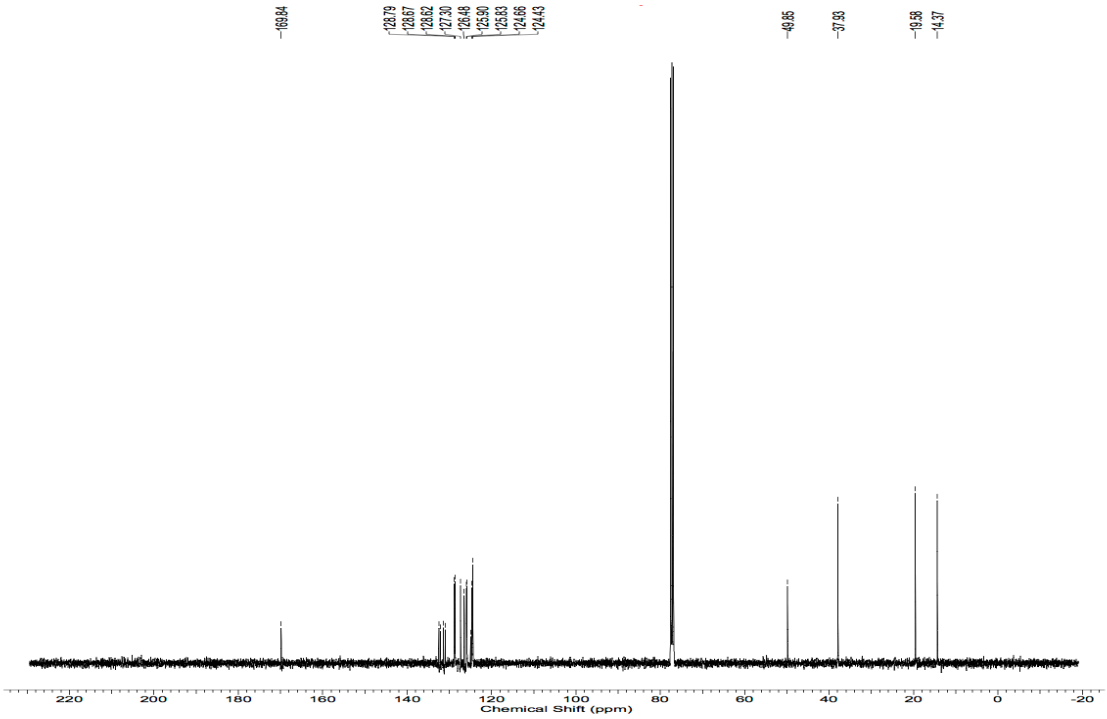
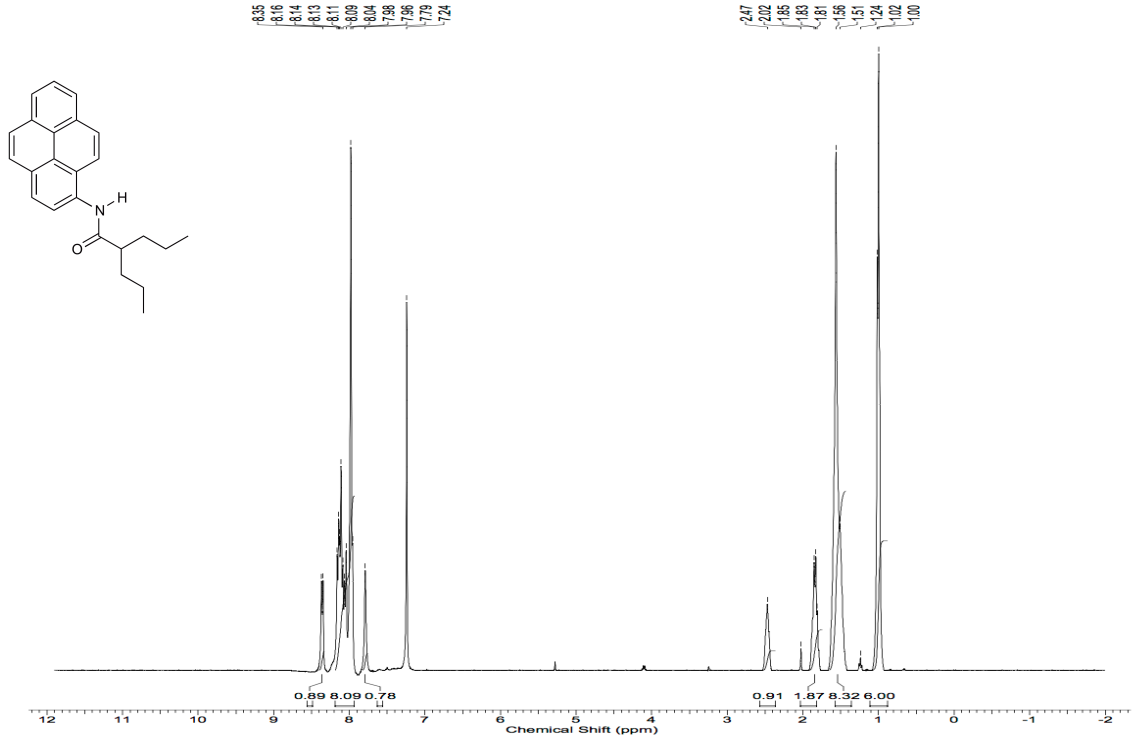


b

Figure S3. (a) ^{1}HNMR of **Py$_{C\text{-}N}$** (400 MHz, $CDCl_3$); (b) ^{13}C NMR of **Py$_{C\text{-}N}$** (400 MHz, $CDCl_3$).



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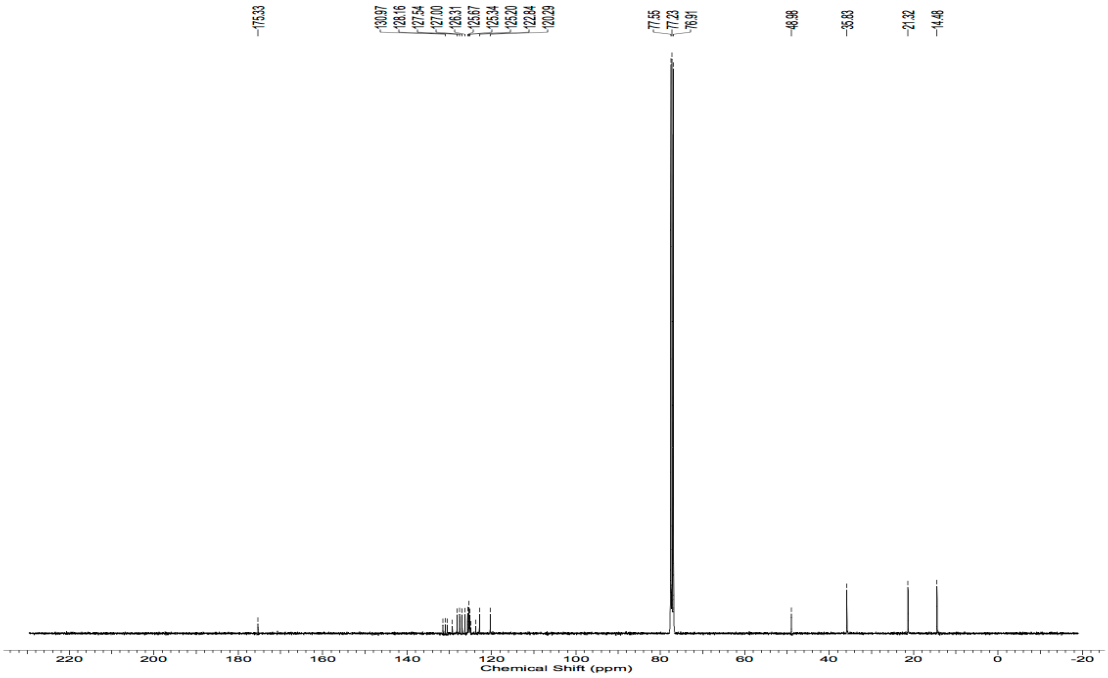

b

Figure S4. (a)[1] HNMR of $\mathbf{Py_{N\text{-}C}}$ (400 MHz, $CDCl_3$); (b) ^{13}C NMR of $\mathbf{Py_{N\text{-}C}}$ (400 MHz, $CDCl_3$).

Table S1. Ionization energies and electron affinities of the pyrene-amide derivatives obtained from the difference between the energies of the ground state and the radical ions calculated using the 6-311+G(d,p) basis set with different DFT functionals.

	Solvent	B3LYP		CAM-B3LYP		PEB0	
		IE / eV	EA / eV	IE / eV	EA / eV	IE / eV	EA / eV
$\mathbf{Py_{mN\text{-}C}}$	MeCN	5.58	2.35	5.70	2.28	5.62	2.32
	DCM	5.74	2.17	5.80	2.09	5.74	2.20
	$CHCl_3$	5.82	2.00	5.95	1.92	5.87	2.00
$\mathbf{Py_{mC\text{-}N}}$	MeCN	5.55	2.32	5.73	2.26	5.66	2.36
	DCM	5.65	2.18	5.81	2.11	5.73	2.17
	$CHCl_3$	5.81	2.00	5.95	1.94	5.87	2.03
$\mathbf{Py_{N\text{-}C}}$	MeCN	5.36	2.33	5.49	2.26	5.41	2.34
	DCM	5.48	2.17	5.60	2.09	5.52	2.17
	$CHCl_3$	5.62	1.98	5.73	1.90	5.66	1.98
$\mathbf{Py_{C\text{-}N}}$	MeCN	5.63	2.49	5.80	2.42	5.73	2.52
	DCM	5.75	2.34	5.88	2.27	5.95	2.19
	$CHCl_3$	5.89	2.17	6.03	2.09	5.95	2.18