Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Unravelling the role of anchoring groups on the ground and excited states of Pyrene by computational and spectroscopic methods

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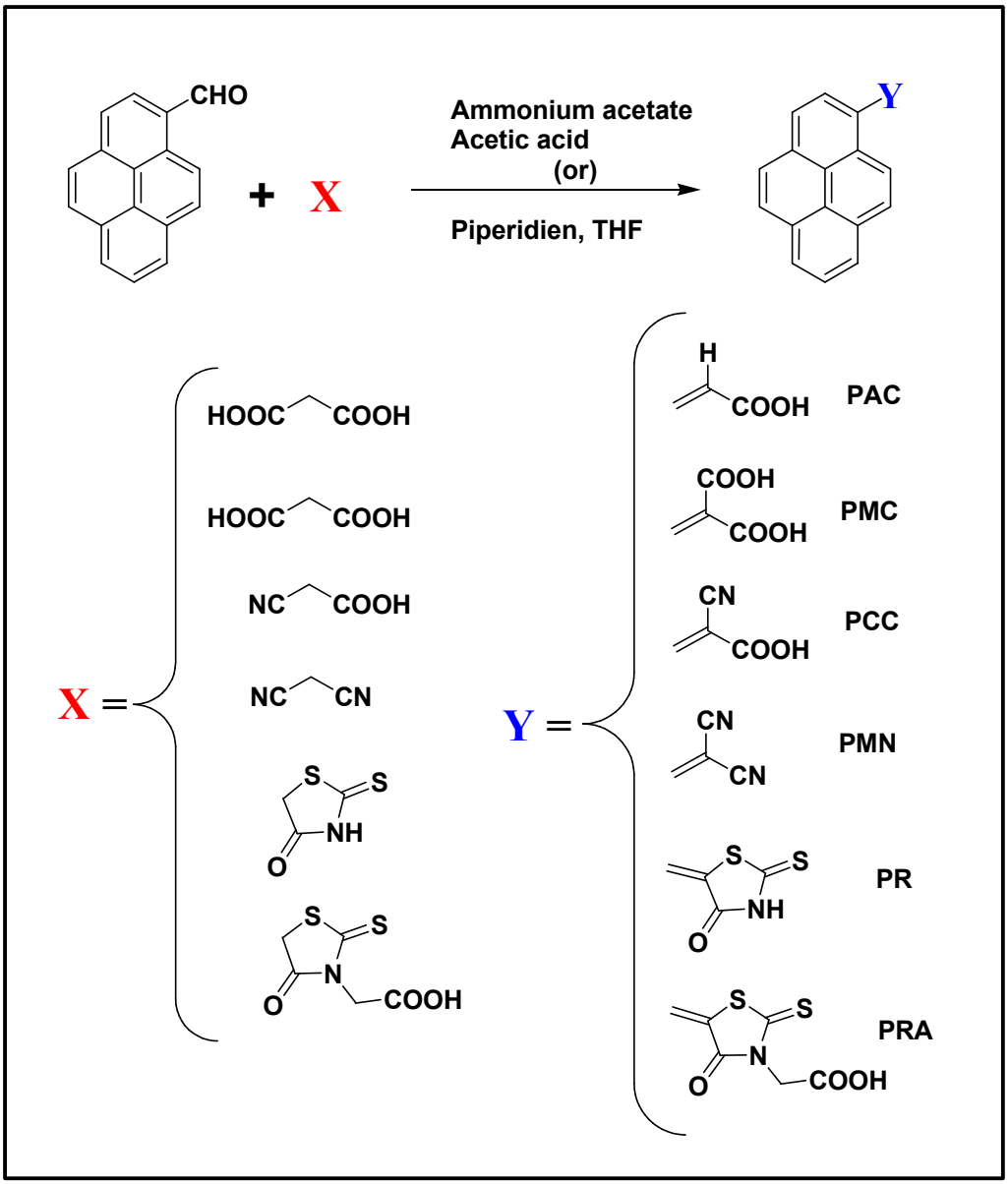

Scheme S1: Synthetic route of pyrene derivatives

Preparation of 3-(pyren-1-yl) acrylic acid (PAC)

A mixture of pyrene-1-carboxaldehyde (0.10 g, 0.43 mmol), malonic acid (0.1 g; 0.86 mmol), acetic acid (5 mL) and ammonium acetate (2 mg) was mixed together and reflux at 120 °C for 15 h. The resulting yellow solution was poured into ice-cold water, to produce a yellow precipitate. This was filtered, washed thoroughly with water, dried at vacuum to give the crude product which was then purified by silica gel column chromatography using chloroform-methanol (v/v: 10:0.1) yielded yellow solid. Yield 0.07 g (58%). Melting point > 200 °C. IR (cm^{-1}): ~3070 (aromatic C–H Stretch); 2921 (acid O–H); 1672 (acid C=O); 1609 (alkene –C=C–); 1409 (aromatic –C–C– stretch); 698, 743, 757 (aromatic C–H bend); 972 (R_2alkene C–H bend). ^{1}H NMR (DMSO-d_6, 400 MHz) δ ppm: 12.64 (s, 1H), 8.70-8.74 (d, J = 16 Hz, 1H), 8.50-8.54 (m, 2H), 8.29-8.37 (m, 4H), 8.19-8.26 (q , 1H), 8.10-8.14 (t, J = 7.6 Hz, 1H), 6.84-6.88 (d, J = 16 Hz, 1H). ^{13}C NMR (DMSO-d_6, 100 MHz) δ ppm: 168.12, 140.35, 132.53, 131.28, 130.62, 129.35, 129.11, 128.90, 128.28, 127.78, 127.05, 126.55, 126.29, 125.75, 125.03, 124.46, 124.21, 122.70, 122.07. MS-EI *m/z* calcd for ($C_{19}H_{12}O_2$): 272.2974. Found: 272.4220.

Preparation of 2-(pyren-1-ylmethylene) malonic acid (PMC)

A mixture of pyrene-1-carboxaldehyde (0.50 g, 2.17 mmol), malonic acid (2.26 g, 21.7 mmol) and piperidine (0.5 mL) in 10 mL of THF were heated to reflux under a nitrogen atmosphere for 8 hr. After cooling to room temperature, 20 mL of water was added. The solution was acidified with10% aqueous hydrochloric acid and extracted with dichloromethame (3 × 15 mL). The organic phase was dried over anhydrous sodium sulphate. The solvent was removed under vacuum and the residue was purified on a silica gel column chromatography using chloroform/methanol (v/v: 10:0.2) yielded yellow solid. Yield 0.40 g (59%).Melting point > 200 °C. IR (cm^{-1}): ~3390 (acid O–H), 1670 (acid -C=O), 1606 (alkene -C=C-).^{1}H NMR (DMSO-d_6, 400 MHz) δ ppm: 12.78 (br s, 2H), 8.70-8.74 (d, J = 16 Hz, 1H), 8.51-8.55 (m, 2H), 8.31-8.38 (m, 4H), 8.21-8.28 (q, 2H), 8.10-8.14 (t, J = 8 Hz, 1H), 6.82-6.86 (d, J = 16 Hz, 1H). ^{13}C NMR (DMSO-d_6, 100 MHz) δ ppm: 168.09, 167.86, 140.37, 132.56, 131.30, 130.64, 129.37, 129.16, 128.93, 128.31, 127.81, 127.09, 126.58, 126.32, 125.78, 125.07, 124.48, 124.23, 122.74, 122.11. MS-EI: *m/z* calcd for ($C_{20}H_{12}O_4$): 316.3069. Found: 316.2090.

Preparation of 2-cyano-3-(pyren-1-yl)acrylic acid (PCC)

PCC was prepared by using a procedure similar to that adopted for preparing PAC, and cyanoacetic acid (0.054 g, 0.65 mmol) was used to obtain the product as anorange precipitate, which was used for complex preparation without further purification.This was filtered, washed thoroughly with water and then dried. The crude product was purified by silica gel column chromatography using chloroform-methanol (v/v: 10:0.2) to obtain a orange solid. Yield 0.08 g (66%). Melting point > 200 °C. IR (cm^{-1}): 2363 (acid O–H); 2216 (C≡N); 1678 (acid C=O); 1609 (alkene –C=C–); 1561, 1409 (aromatic –C–C– stretch); 762, 711 (aromatic C–H bend); 845 (R_3alkene C–H bend). ^{1}H NMR (DMSO-d_6, 400 MHz) δ ppm: 9.23 (s, 1H), 8.64-8.66 (d, J = 8 Hz, 1H), 8.32-8.42 (m, 6H), 8.22-8.24 (d, J = 8 Hz, 1H), 8.14-8.18 (t, J = 8 Hz, 1H). ^{13}C NMR (DMSO-d_6, 100 MHz) δ ppm: 163.80, 150.77, 133.78, 131.08, 130.50, 130.35, 130.06, 129.85, 127.70, 127.35, 127.27, 127.09, 126.43, 126.12, 125.36, 124.11, 123.80, 122.88, 117.55. MS-EI *m/z* calcd for ($C_{20}H_{11}NO_2$): 297.3068. Found ($C_{19}H_{10}N$): [M–COOH] 252.6362.

Preparation of 2-(pyren-1-ylmethylene) malononitrile (PMN)

PMN was prepared by using a procedure similar to that used for preparing PAC, and malononitrile (0.10 mL, 1.7 mmol) was used to obtain PMN as an orange precipitate. This was filtered, washed thoroughly with water and then dried. The crude product was purified by silica gel column chromatography using petroleum ether/chloroform (v/v: 3:7) to obtain an orange solid. Yield 0.18 g (75%). Melting point > 200 °C. IR (cm^{-1}): 2214 (nitrile -C≡N), 1556 (alkene -C=C-) cm^{-1}. ^{1}H NMR (DMSO-d_6, 400 MHz) δ ppm: 9.63 (s, 1H), 8.68-8.74 (m, 2H), 8.43-8.52 (m, 5H), 8.30-8.32 (d, J = 8 Hz, 1H), 8.20-8.24 (t, J = 8 Hz, 1H). MS-EI: *m/*z calcd for ($C_{20}H_{10}N_2$): 278.3068. Found: 278.0725.

Preparation of 5-(pyren-1-ylmethylene)-2-thioxothiazolidin-4-one (PR)

A general procedure adopted for the preparation of PAC was used for preparing PR, and rhodanine (0.33 g; 2.5 mmol) was used to obtain PR as a red precipitate. This was filtered, washed thoroughly with water and then dried. The crude product was purified by silica gel column chromatography using chloroform-methanol (v/v: 10:0.2) to obtain a red solid. Yield 0.47 g (78%). Melting point > 200 °C. IR (cm^{-1}): 1680 (carbonyl –C=O), 1565 (alkene -C=C-), 1176 (Thiocorbonyl –C=S) cm^{-1}. ^{1}H NMR (DMSO-d_6, 400 MHz) δ ppm: 8.60 (s, 1H), 8.50-8.52

(d, *J* = 8 Hz, 1H), 8.44-8.46 (d, *J* = 8 Hz, 1H), 8.40-8.42 (d, *J* = 8 Hz, 3H), 8.31-8.38 (m, 3H), 8.22-8.28 (m, 2H), 8.10-8.20 (m, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz) δ ppm: 132.86, 131.30, 130.70, 130.49, 129.89, 129.75, 128.88, 127.78, 127.44, 127.12, 126.95, 126.14, 125.91, 124.27, 123.03. MS-EI: *m/z* calcd for ($C_{20}H_{11}NOS_2$): 345.4374. Found: 345.0709.

Preparation of 2-(4-oxo-5-(pyren-1-ylmethylene)-2-thioxothiazolidin-3-yl)acetic acid (PRA)

PRA was synthesized by using a procedure similar to that followed for preparation of L3, and rhodanine-3-acetic acid (0.48 g, 2.5 mmol) was used to obtain the final compound as a red precipitate. This was filtered, washed thoroughly with water and then dried. The crude product was purified by silica gel column chromatography using chloroform-methanol (v/v: 10:0.2) to obtain a red solid. Yield 0.58 g (83%).Melting point > 200 °C. IR (cm^{-1}): 1736(Carbonyl -C=O), 1706 (acid -C=O), 1575 (alkene -C=C-), 1182 (Thiocorbonyl –C=S) cm^{-1}.^{1}H NMR (DMSO-d_6, 400 MHz) δ ppm: 8.71 (s, 1H), 8.43-8.45 (d, *J* = 8 Hz, 1H), 8.31-8.37 (m, 4H), 8.26-8.28 (d, *J* = 8 Hz, 1H), 8.16-8.18 (d, *J* = 8 Hz, 1H), 8.07-8.11 (t, J= 8 Hz, 2H), 4.73 (s, 2H).^{13}C NMR (DMSO-d_6, 100 MHz) δ ppm: 194.09, 167.81, 166.49, 133.19, 131.25, 131.14, 130.71, 130.64, 130.16, 129.92, 127.77, 127.49, 127.28, 127.11, 126.84, 126.31, 125.97, 124.75, 124.45, 123.85, 122.99, 45.61. MS-EI: *m/z* calcd for ($C_{22}H_{13}NO_3S_2$): 403.4735. Found: 403.8627.

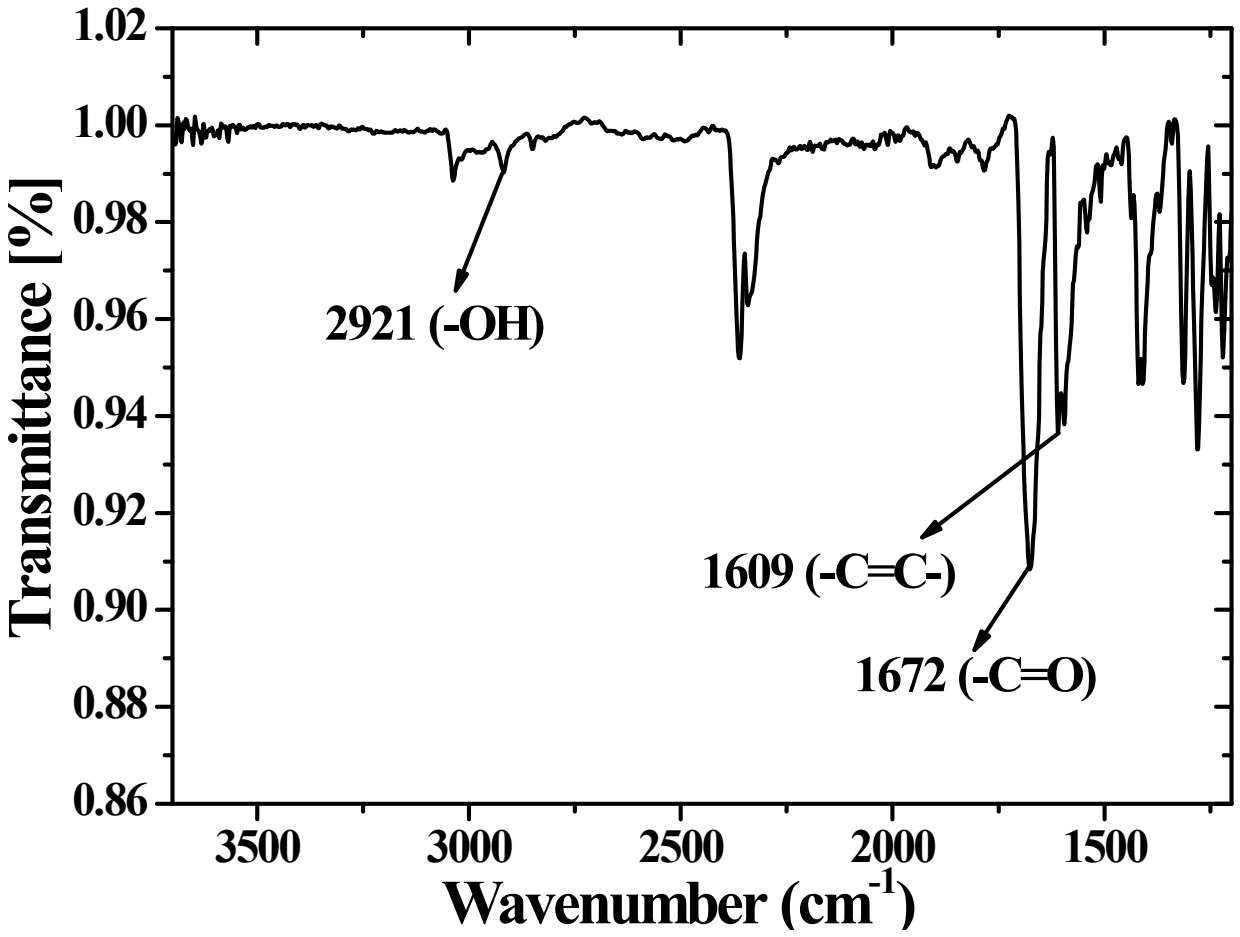

Figure S1. IR spectrum of **PAC**

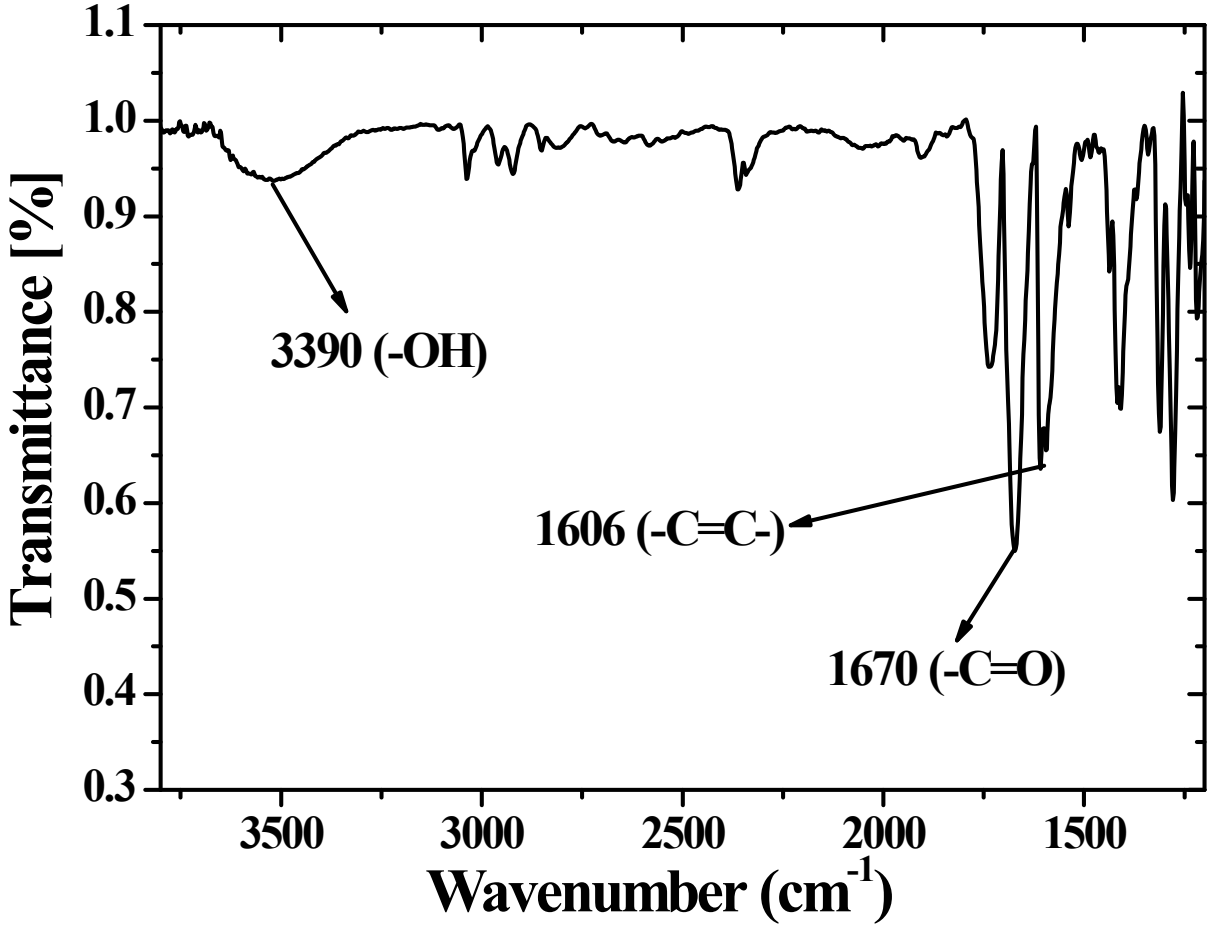

Figure S2. IR spectrum of **PMC**

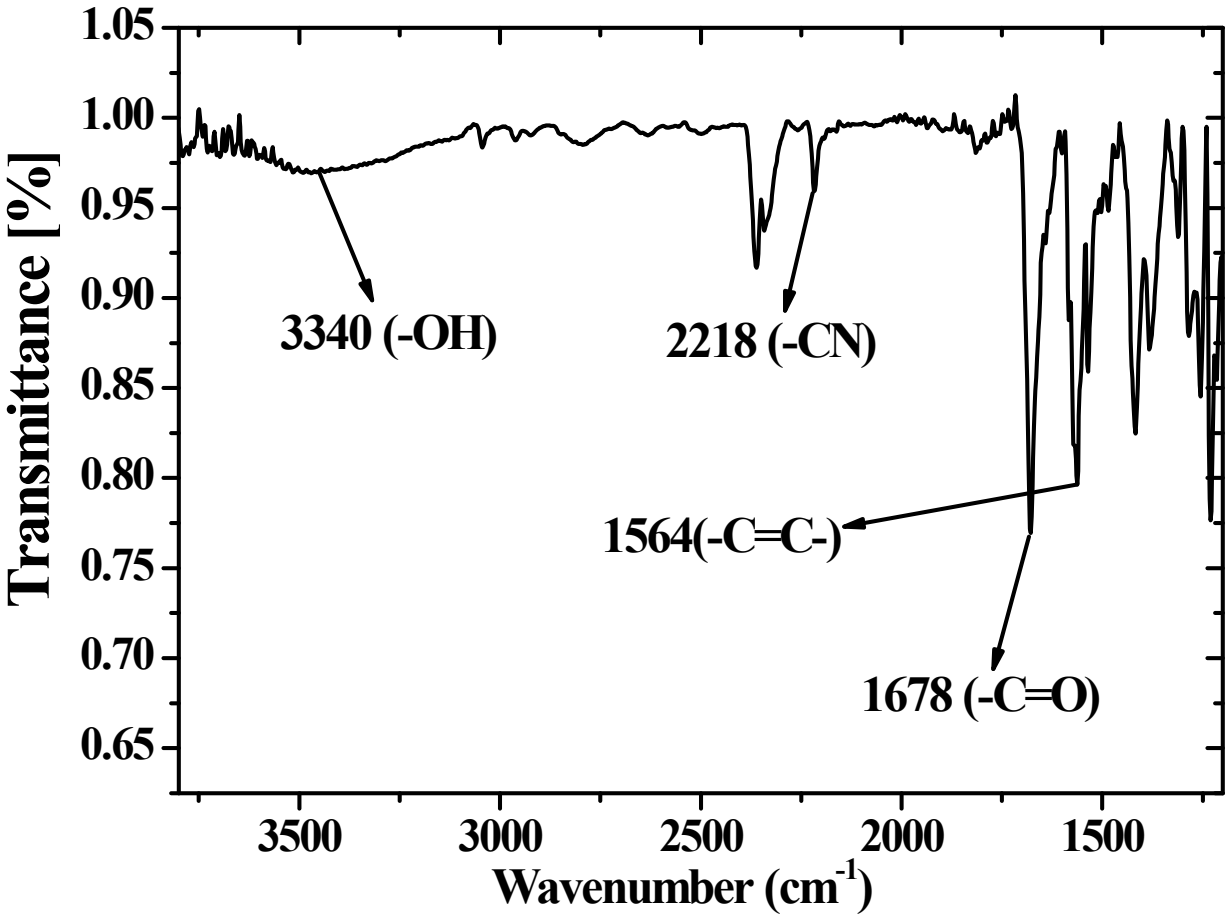

Figure S3. IR spectrum of **PCC**

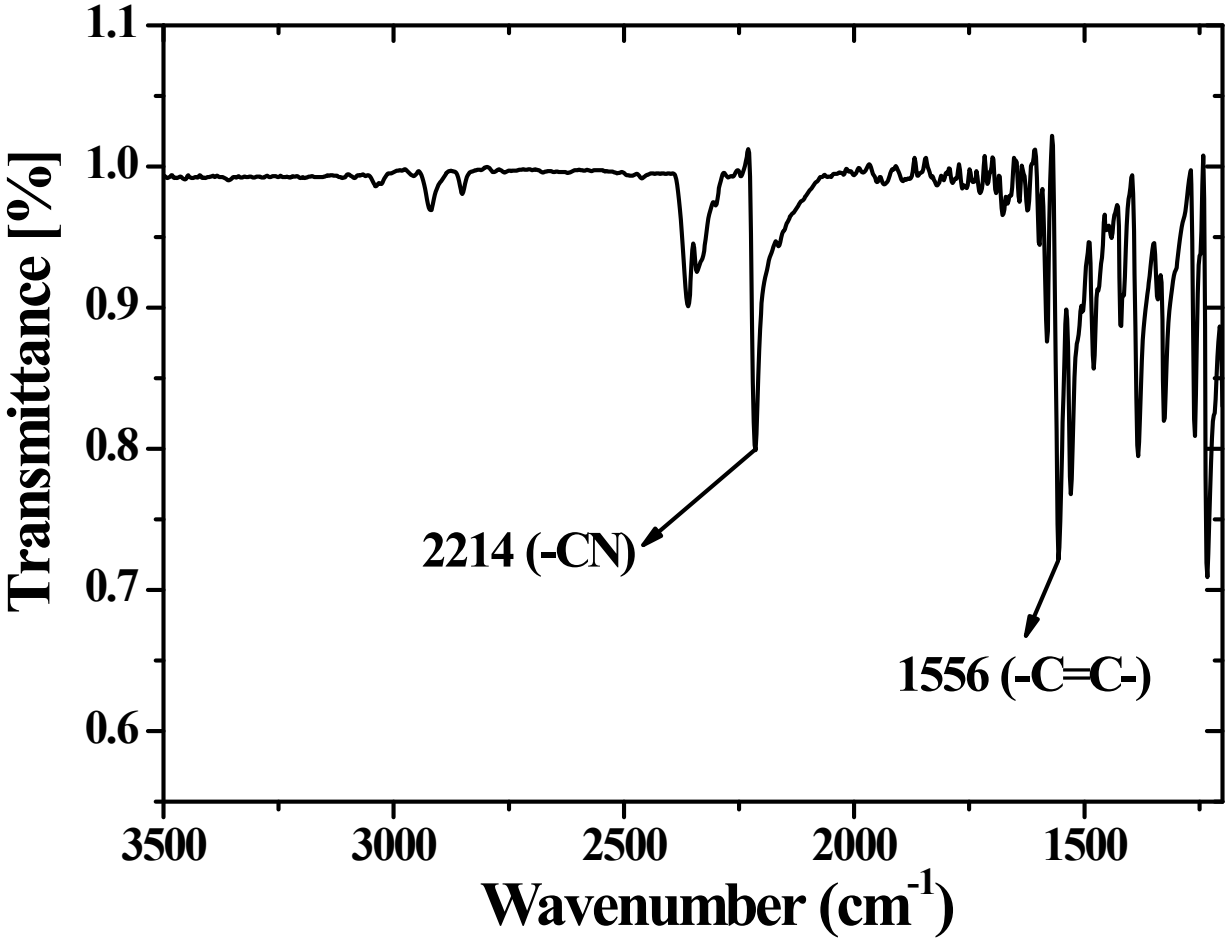

Figure S4. IR spectrum of **PMN**

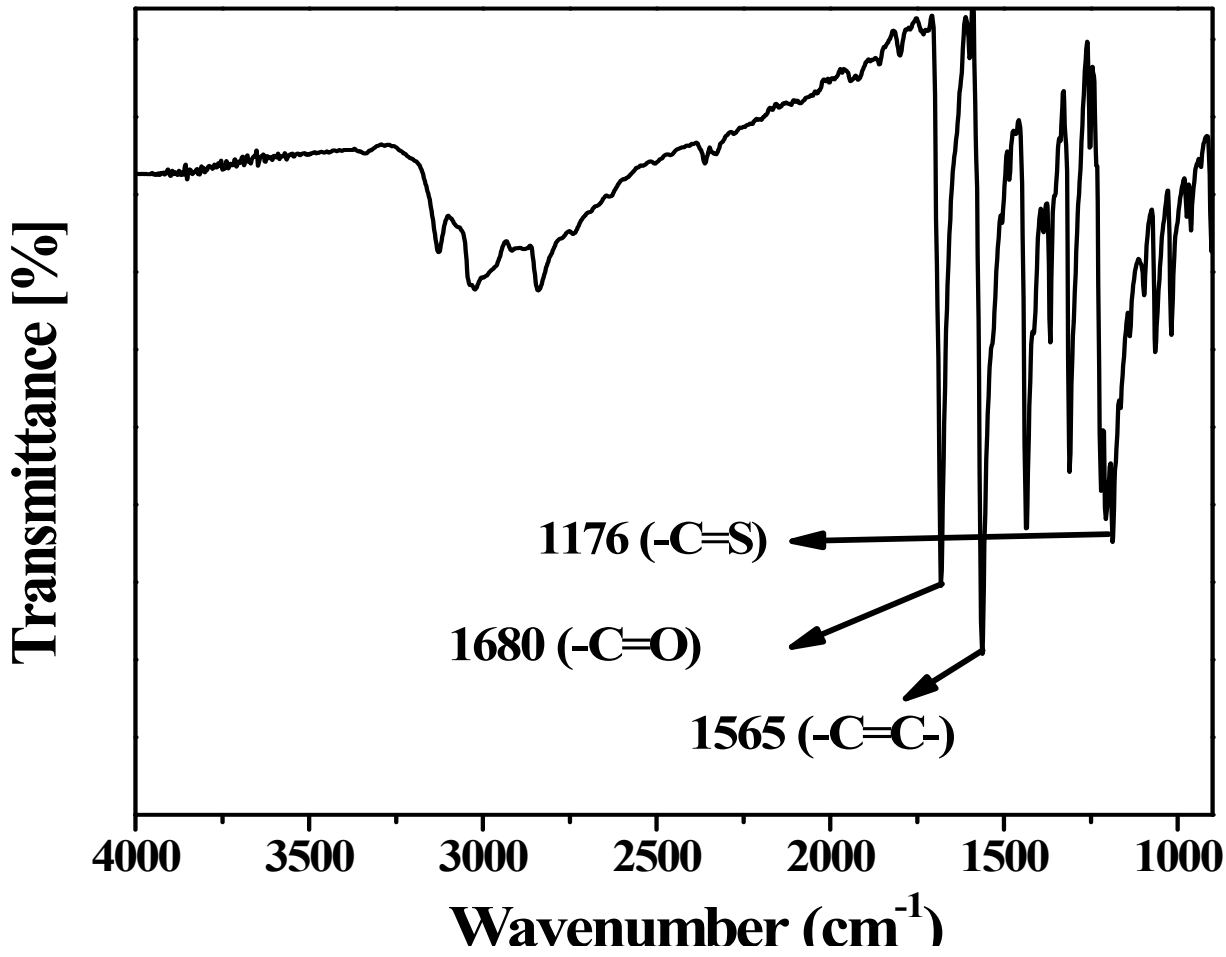

Figure S5. IR spectrum of **PR**

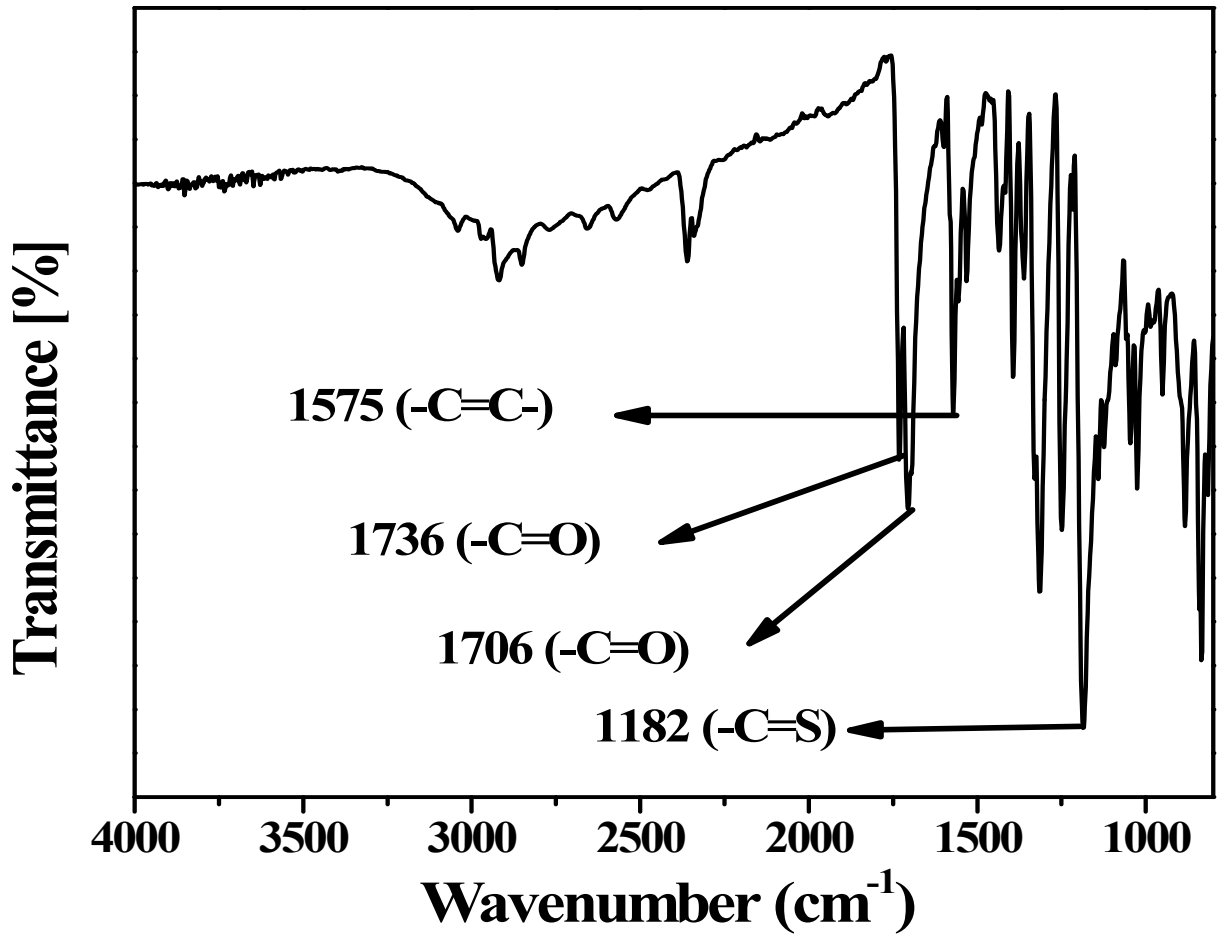

Figure S6: IR spectrum of **PRA**

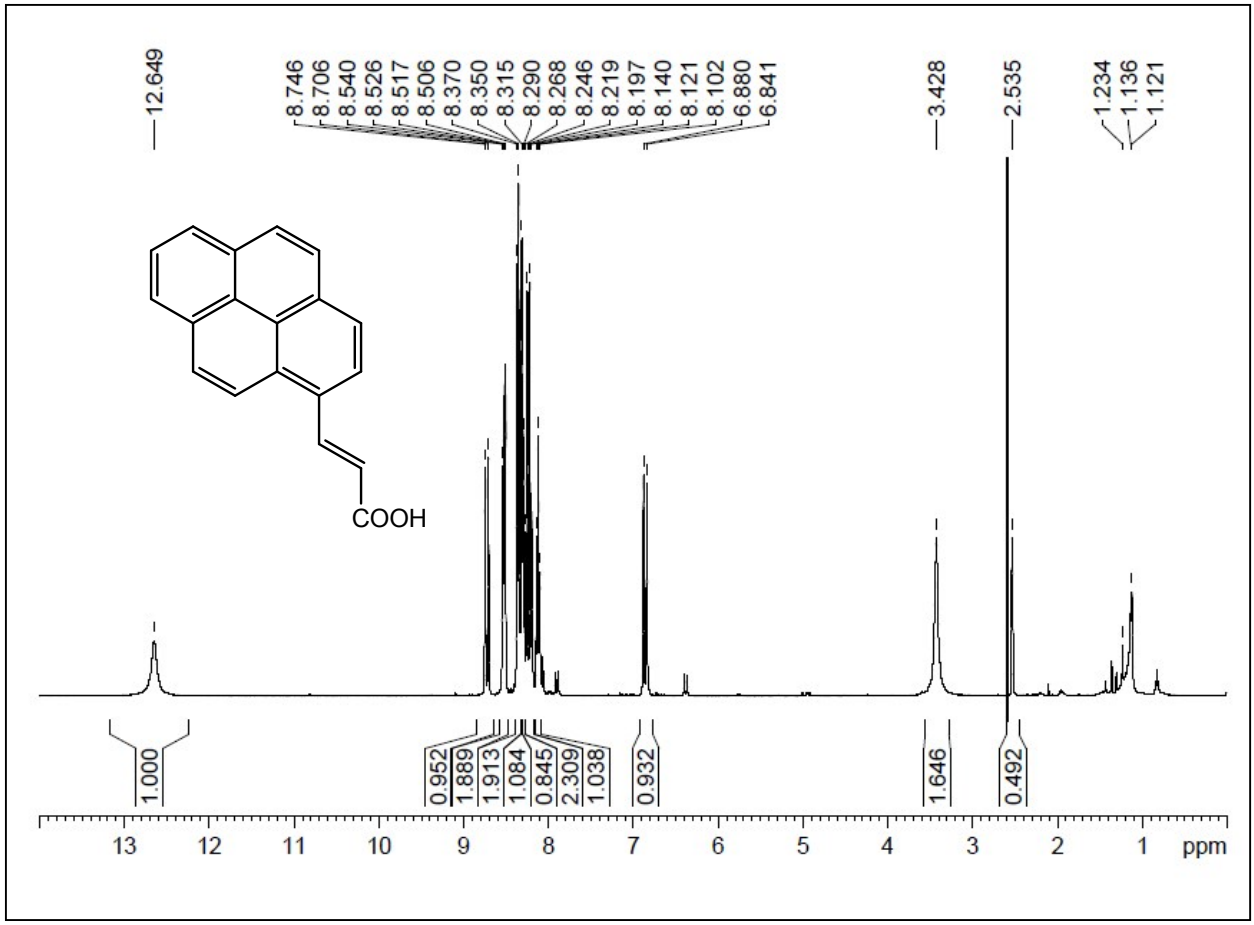

Figure S7: ^{1}H NMR spectrum of **PAC** in DMSO-d_6.

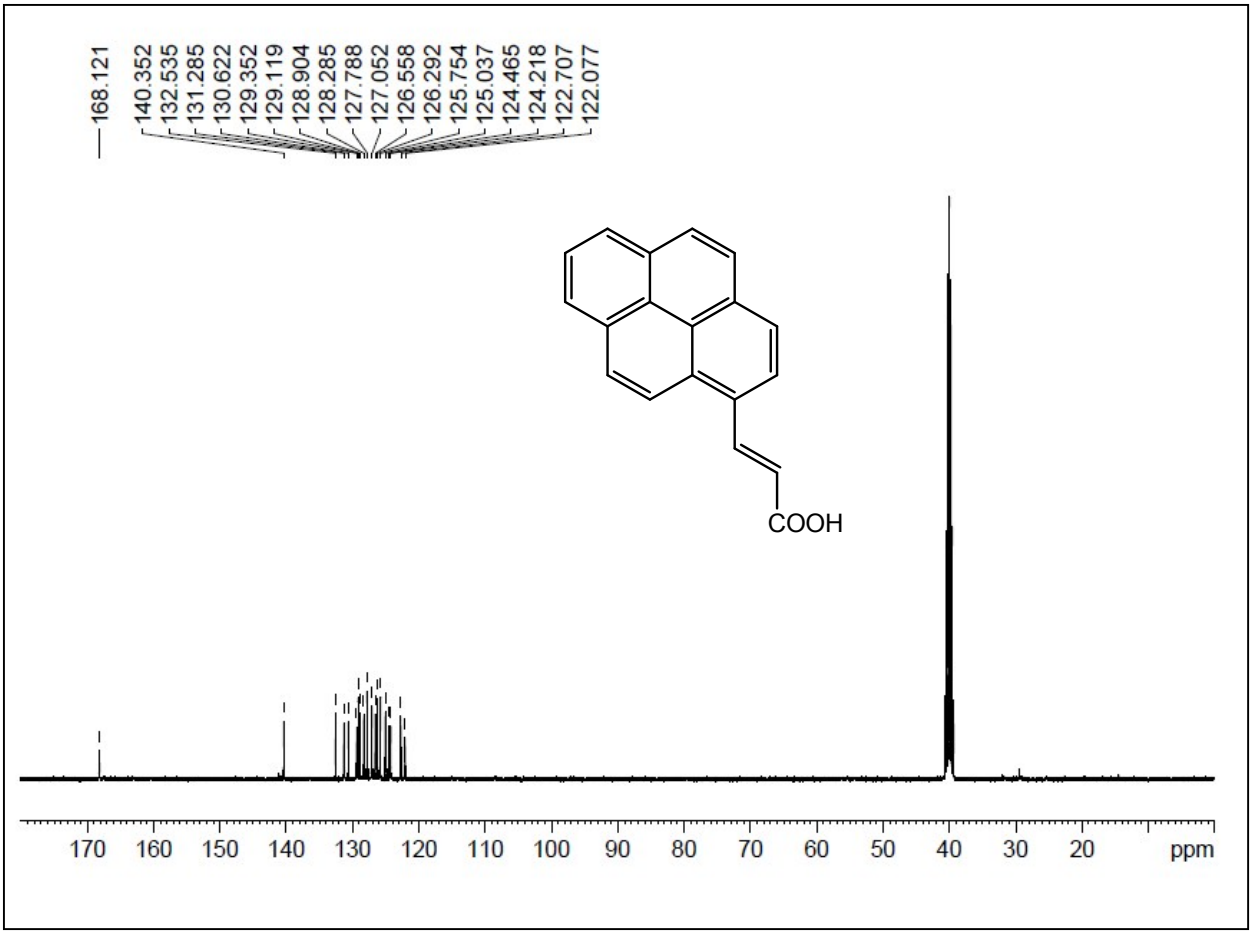

Figure S8: ^{13}C NMR spectrum of **PAC** in DMSO-d_6.

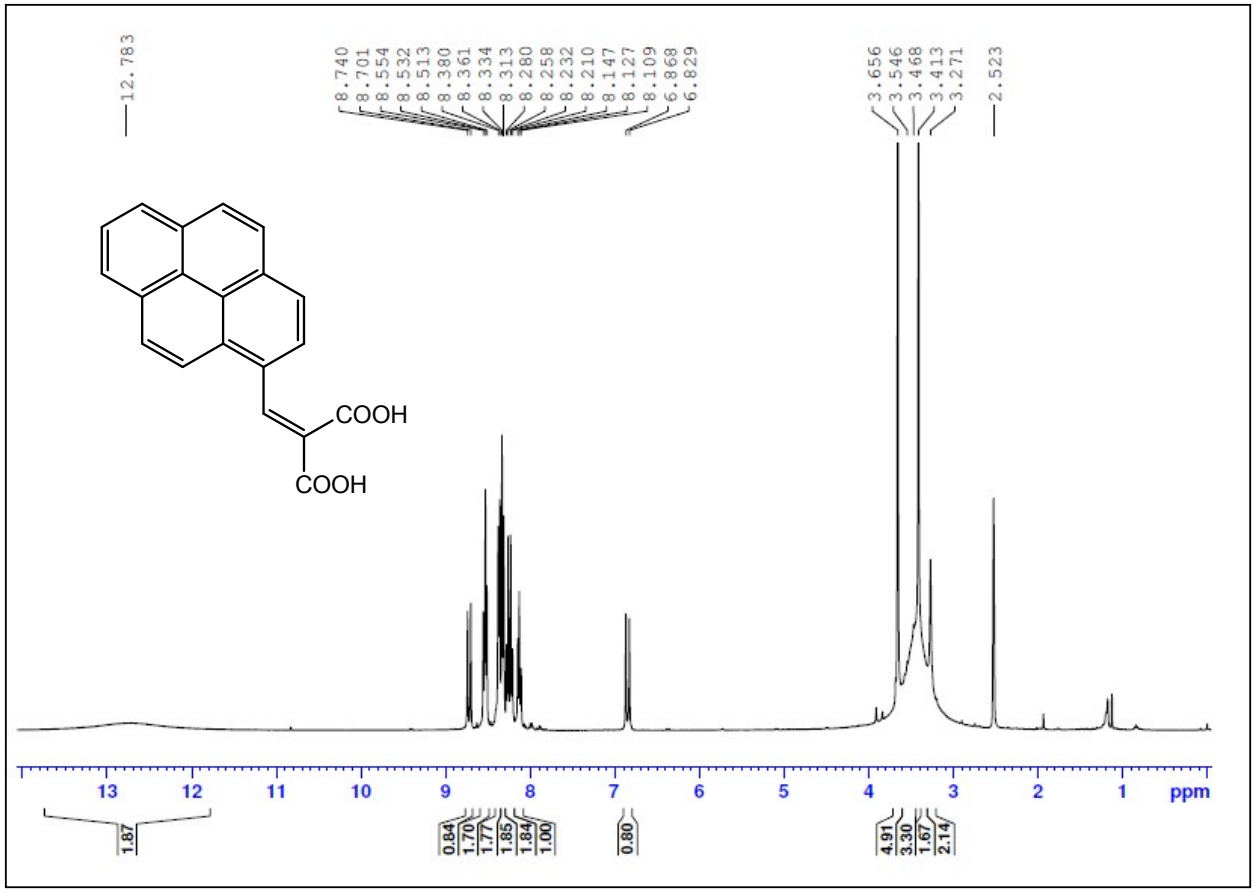

Figure S9: ^{1}H NMR spectrum of **PMC** in DMSO-d_6.

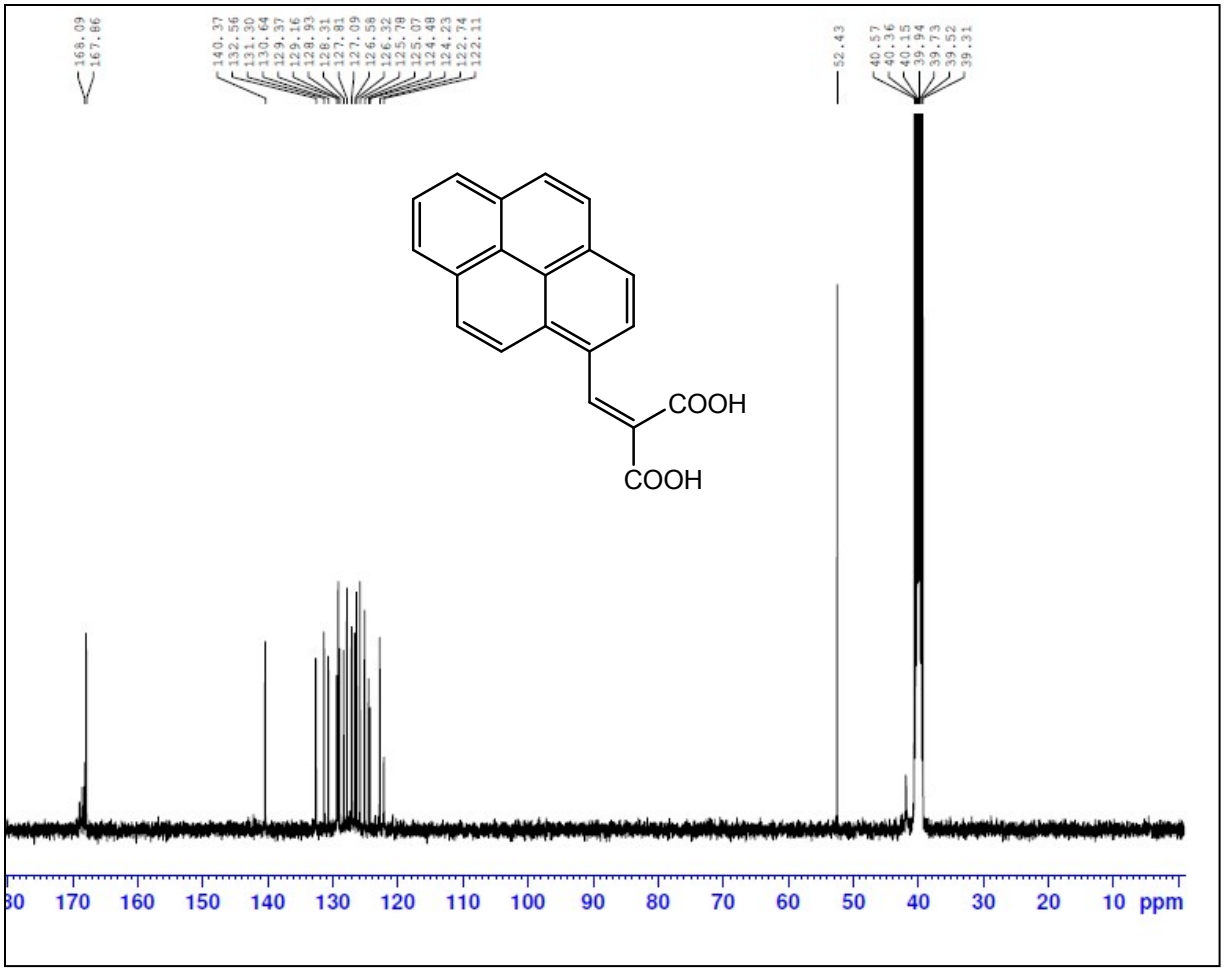

Figure S10: ^{13}C NMR spectrum of **PMC** in DMSO-d_6.

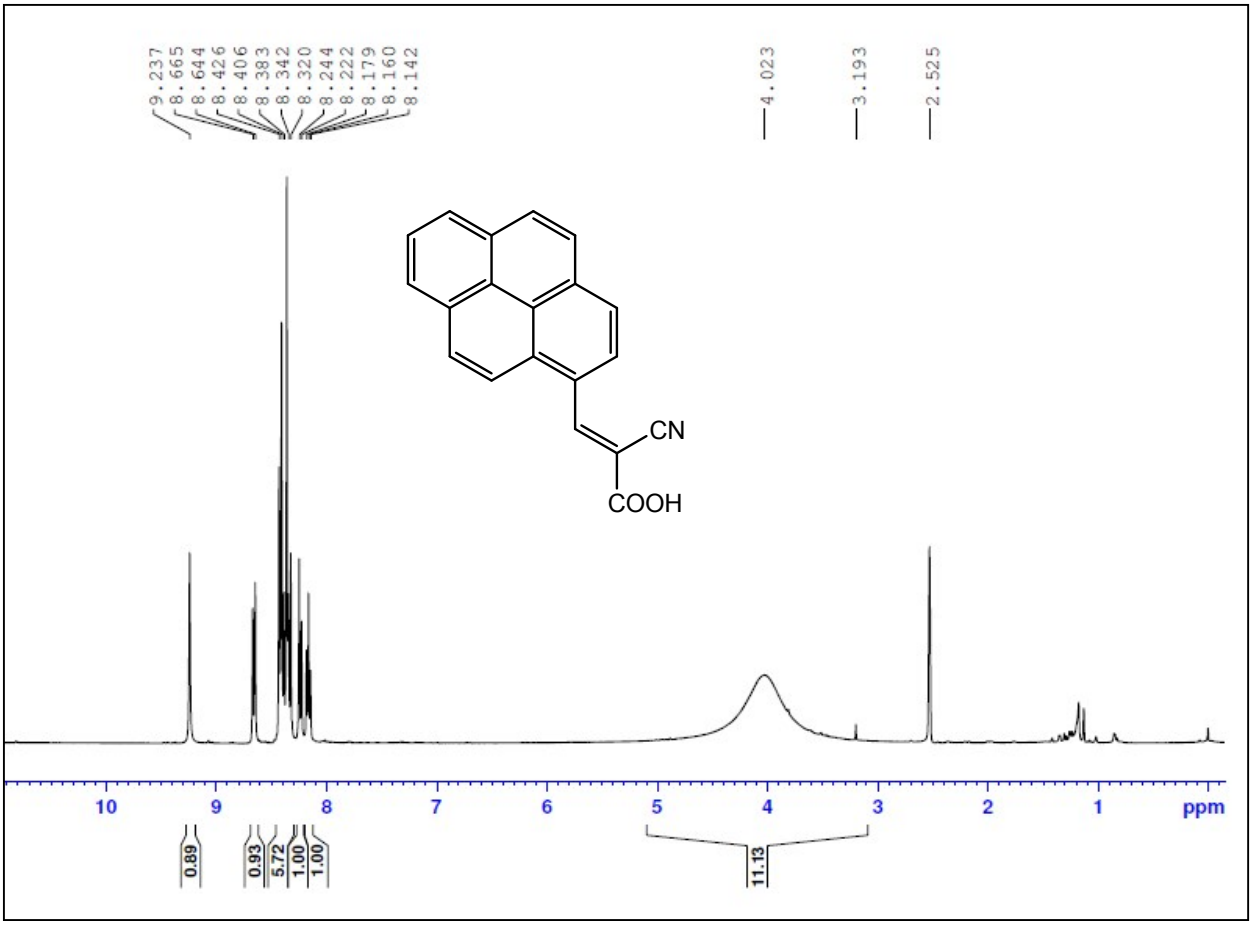

Figure S11: ^{1}H NMR spectrum of **PCC** in DMSO-d_6.

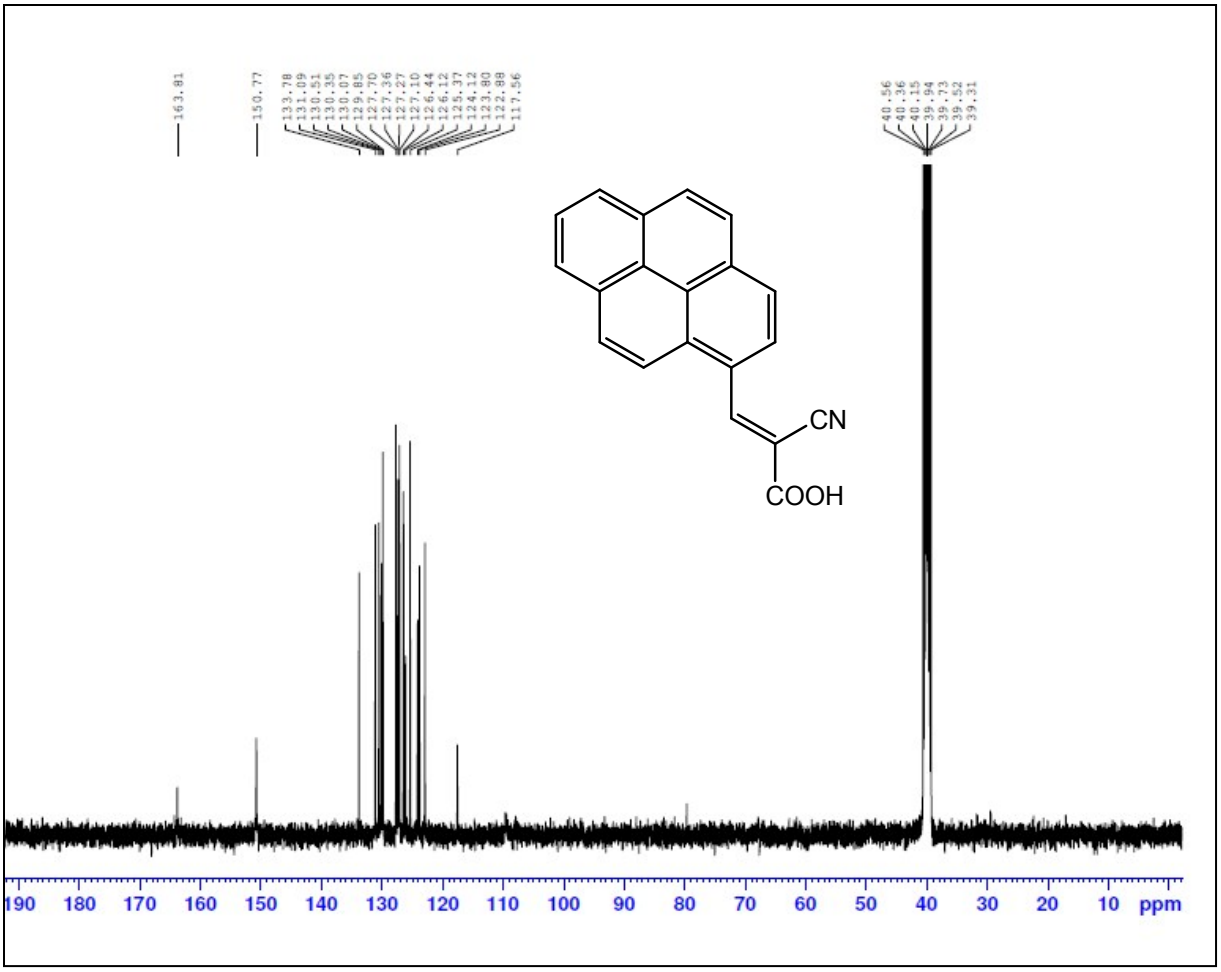

Figure S12: ^{13}C NMR spectrum of **PCC** in DMSO-d_6.

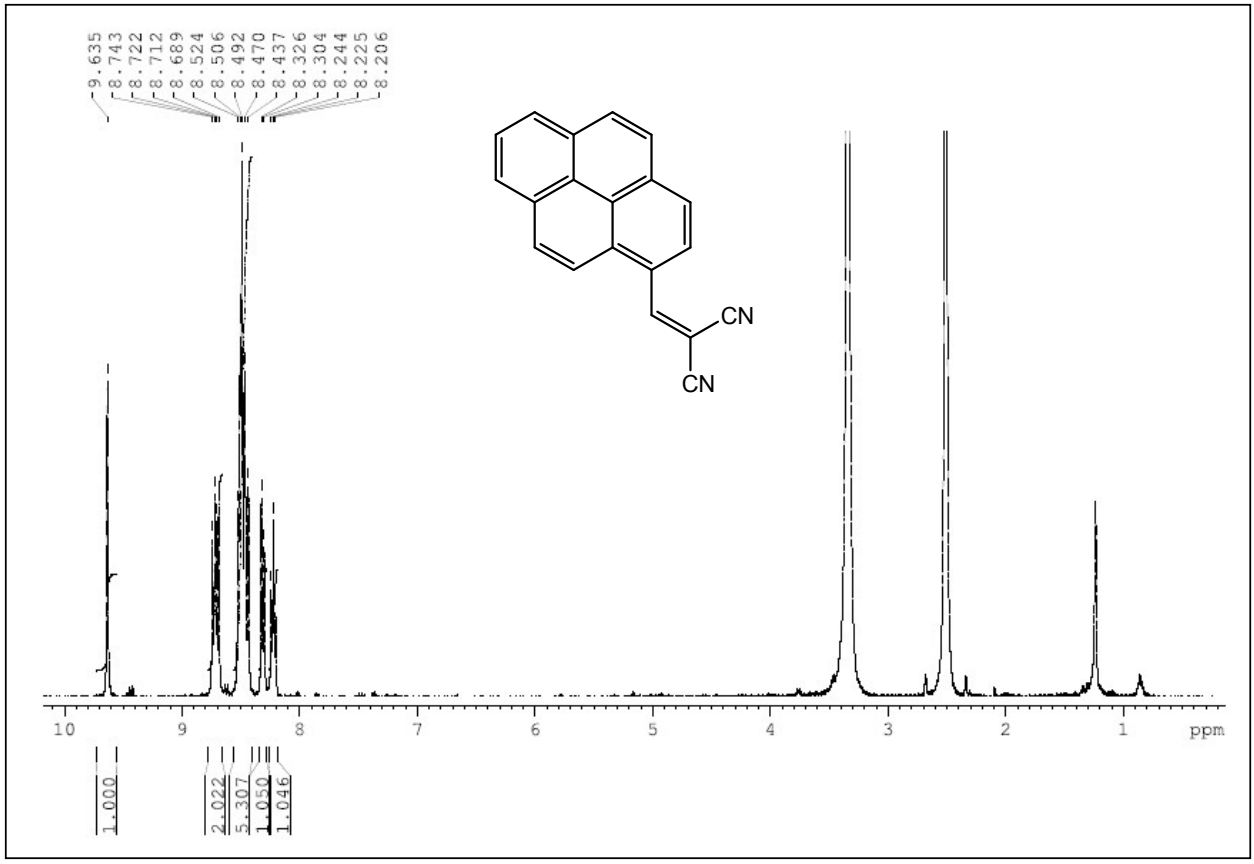

Figure S13: ^{1}H NMR spectrum of **PMN** in DMSO-d_6.

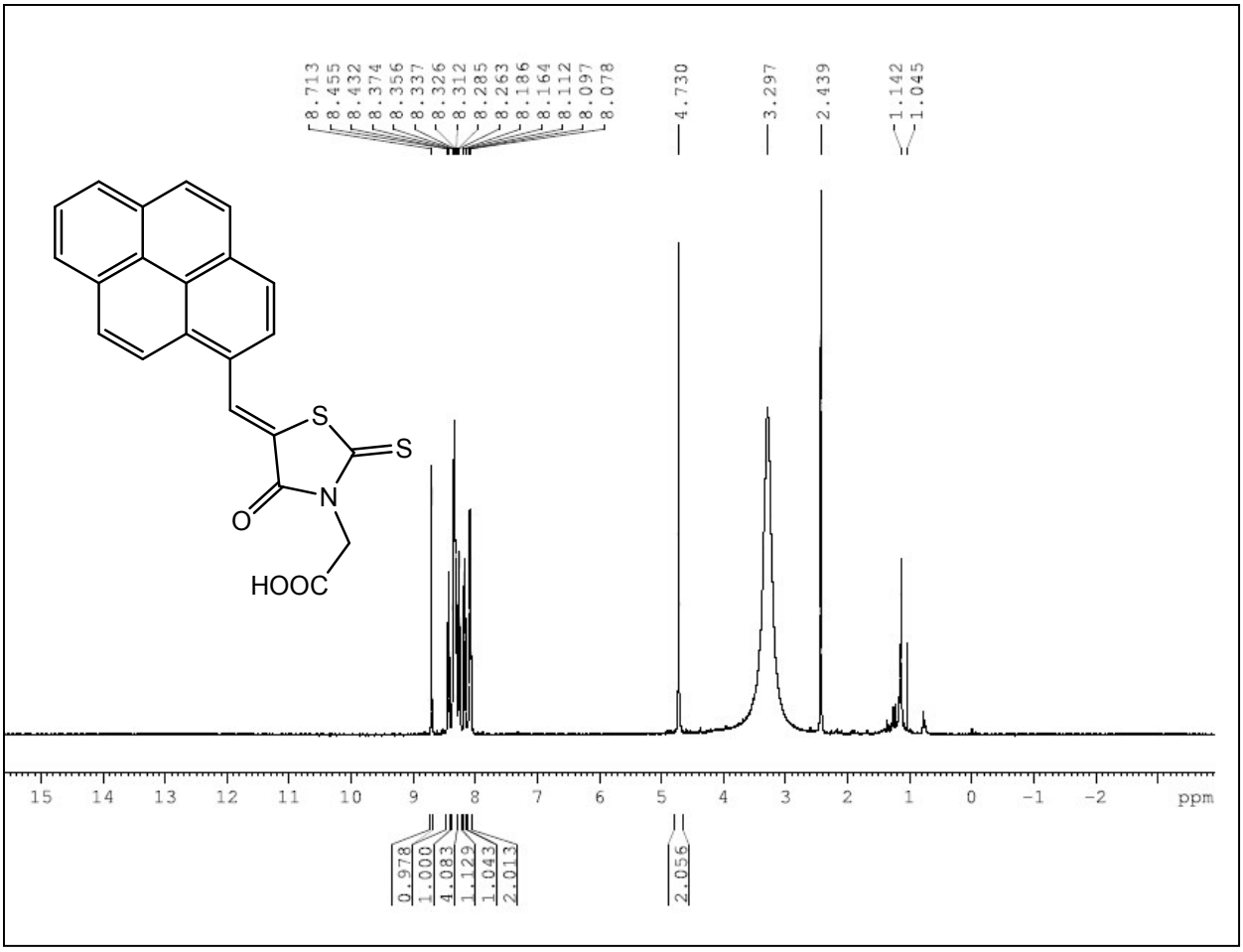

Figure S14: ^{1}H NMR spectrum of **PRA** in DMSO-d_6.

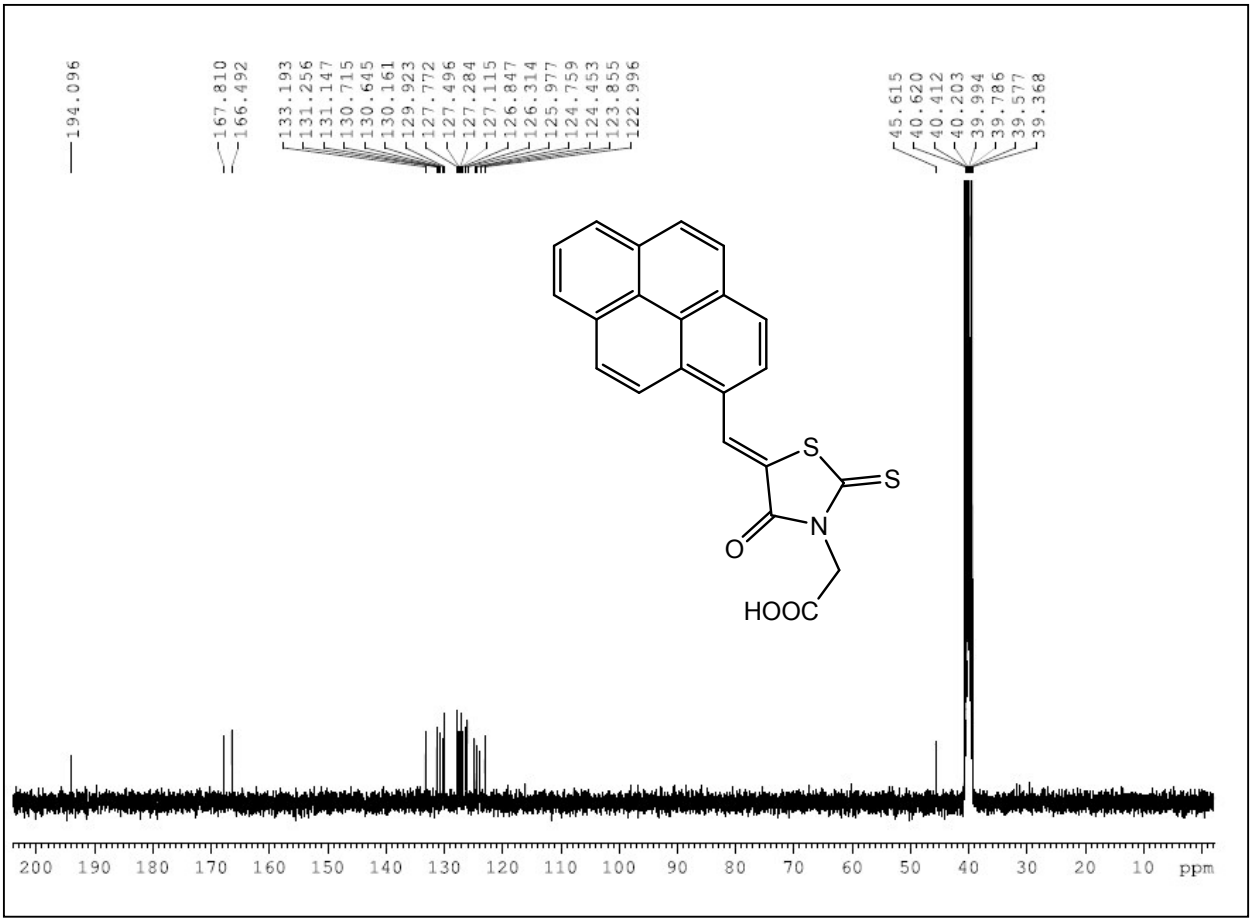

Figure S15: ^{13}C NMR spectrum of **PRA** in DMSO-d_6.

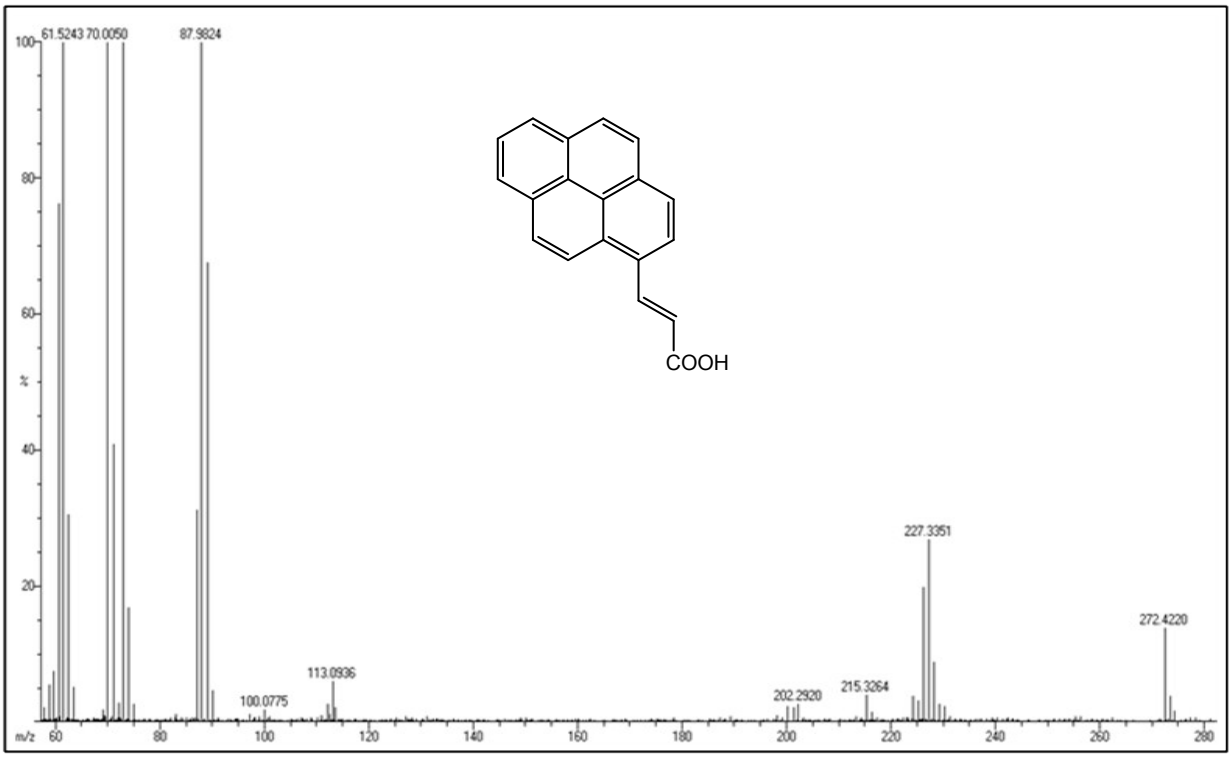

Figure S16: Mass spectrum of **PAC**

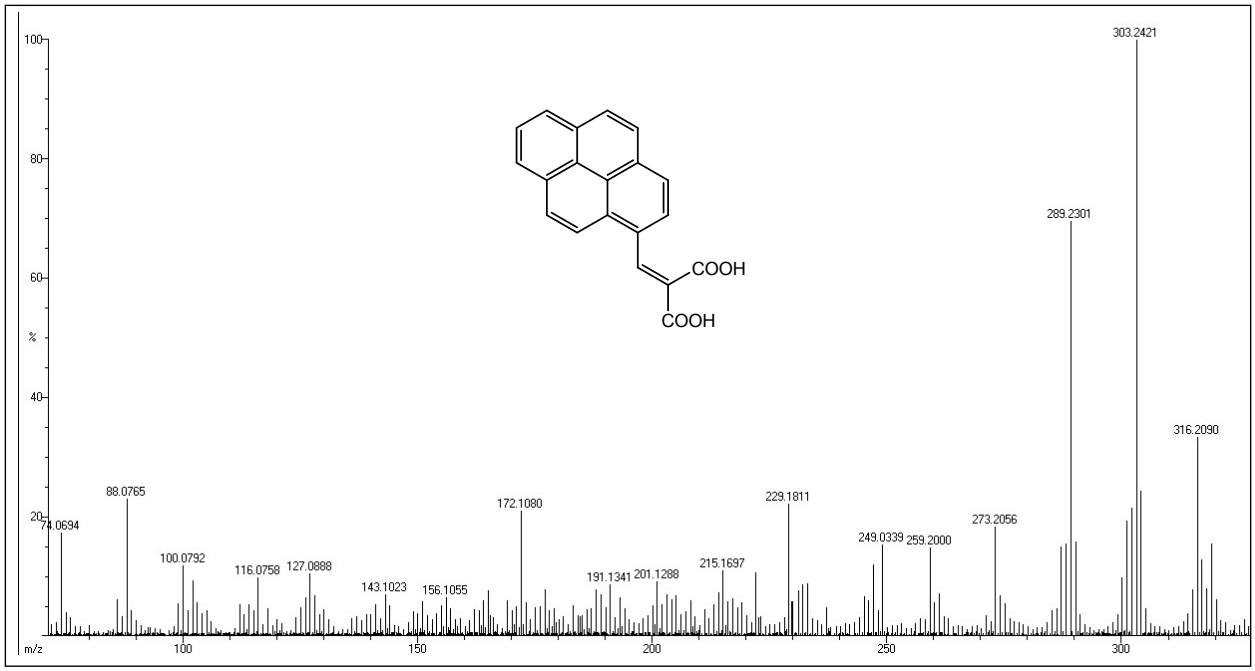

Figure S17: Mass spectrum of **PMC**

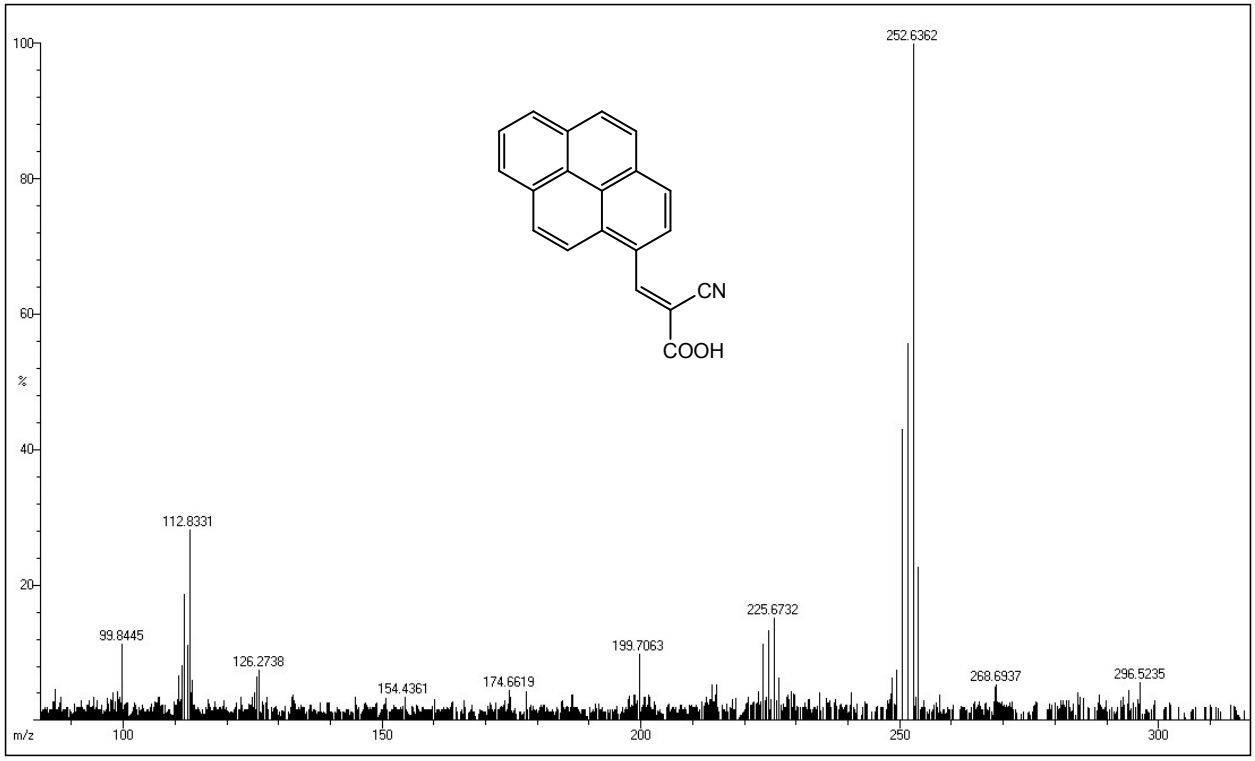

Figure S18: Mass spectrum of **PCC**

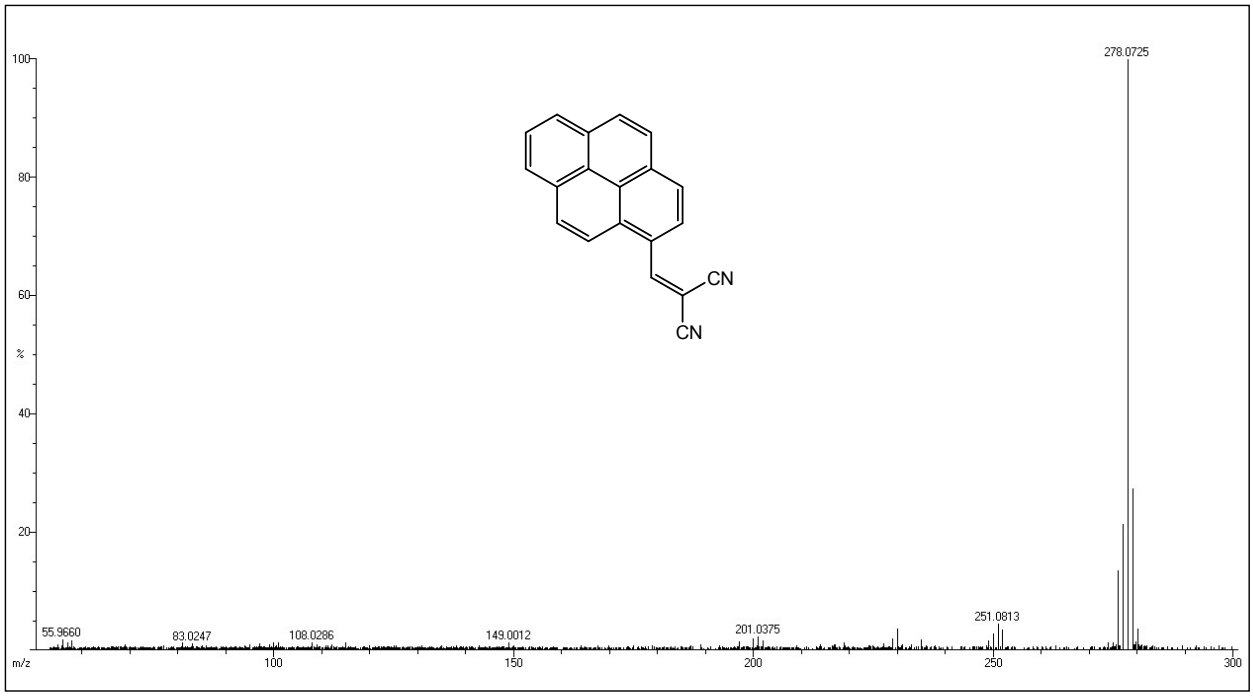

Figure S19: Mass spectrum of **PMN**

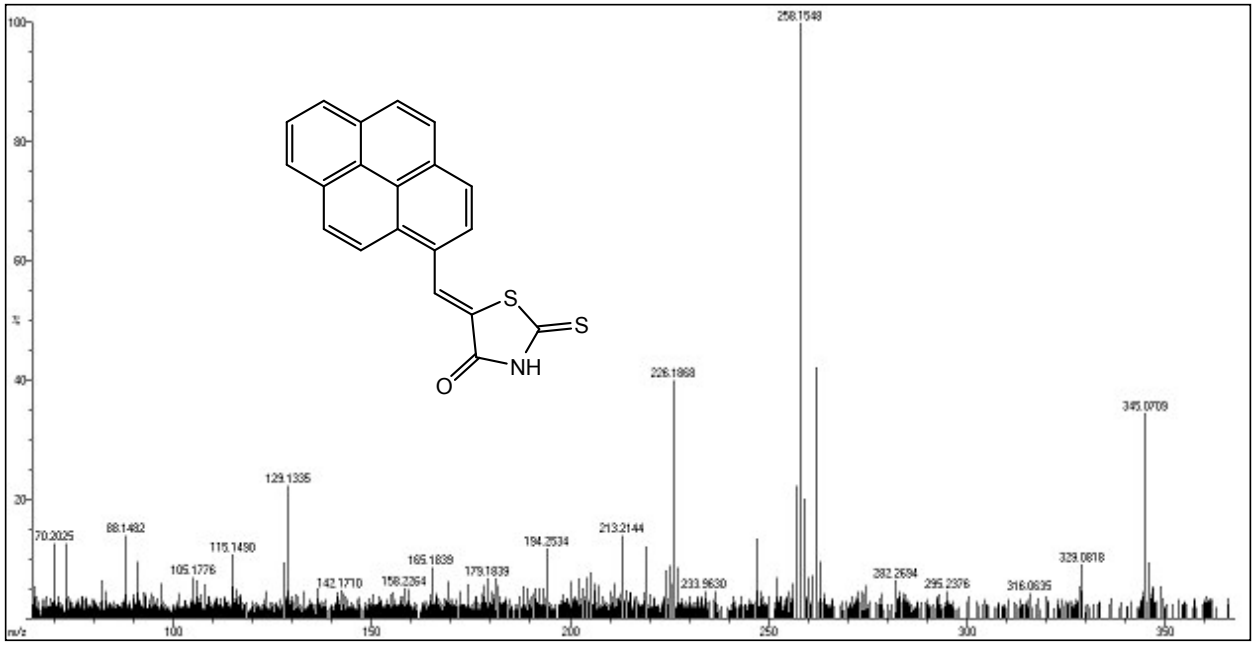

Figure S20: Mass spectrum of **PR**

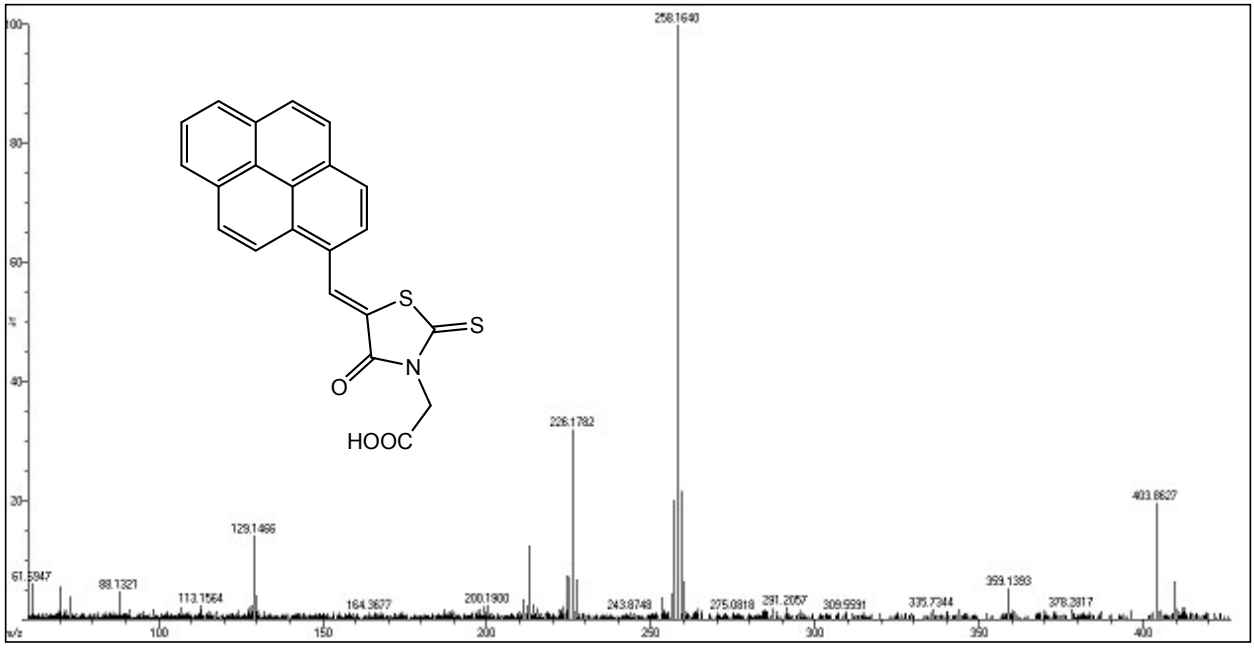

Figure S21: Mass spectrum of **PRA**

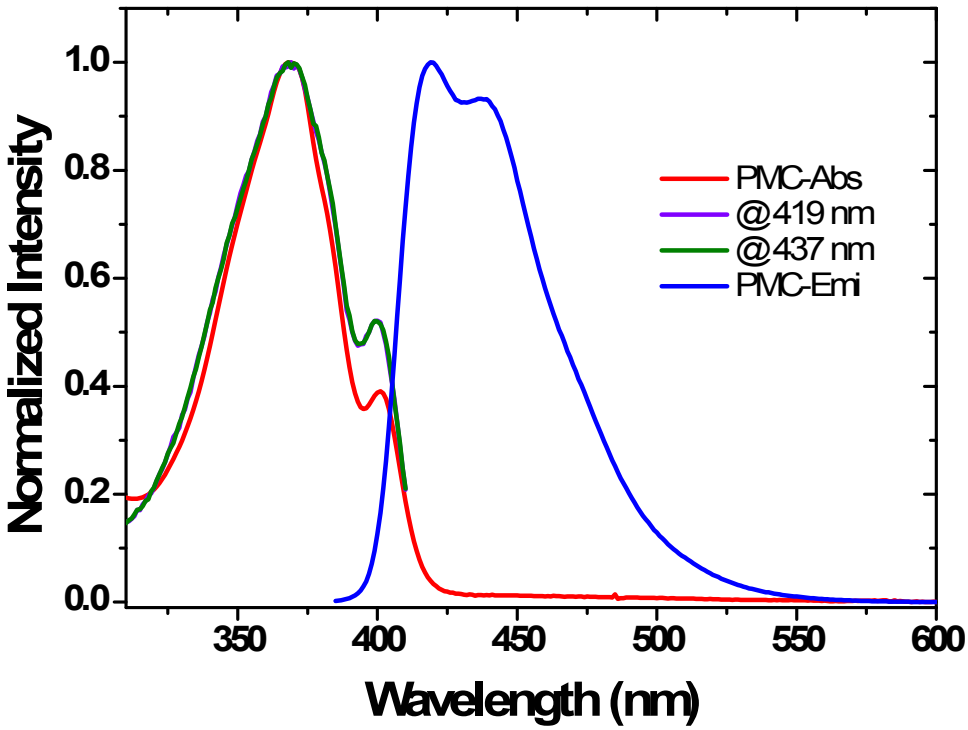

Figure S22: Excitation and emission spectrum of PMC.

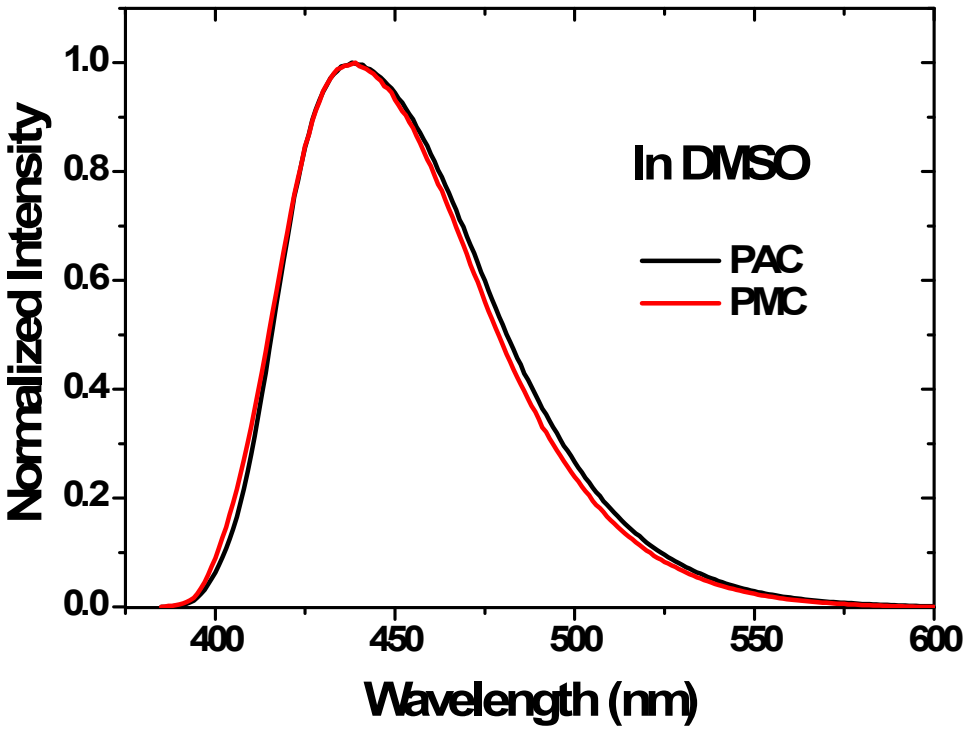

Figure S23: Emission spectra of PAC and PMC in DMSO solvent.

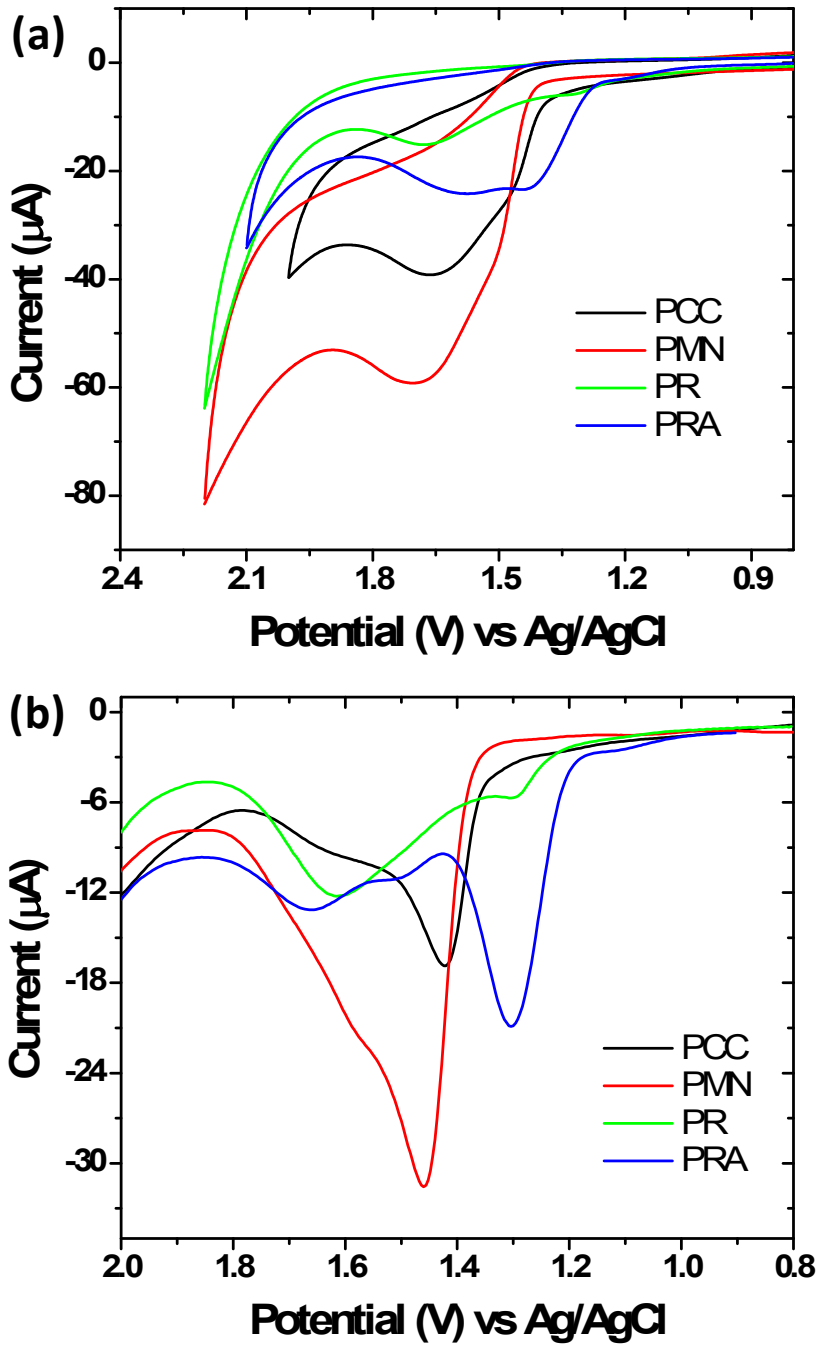

Figure S24: (a) CV and (b) DPV plots of pyrene derivatives.

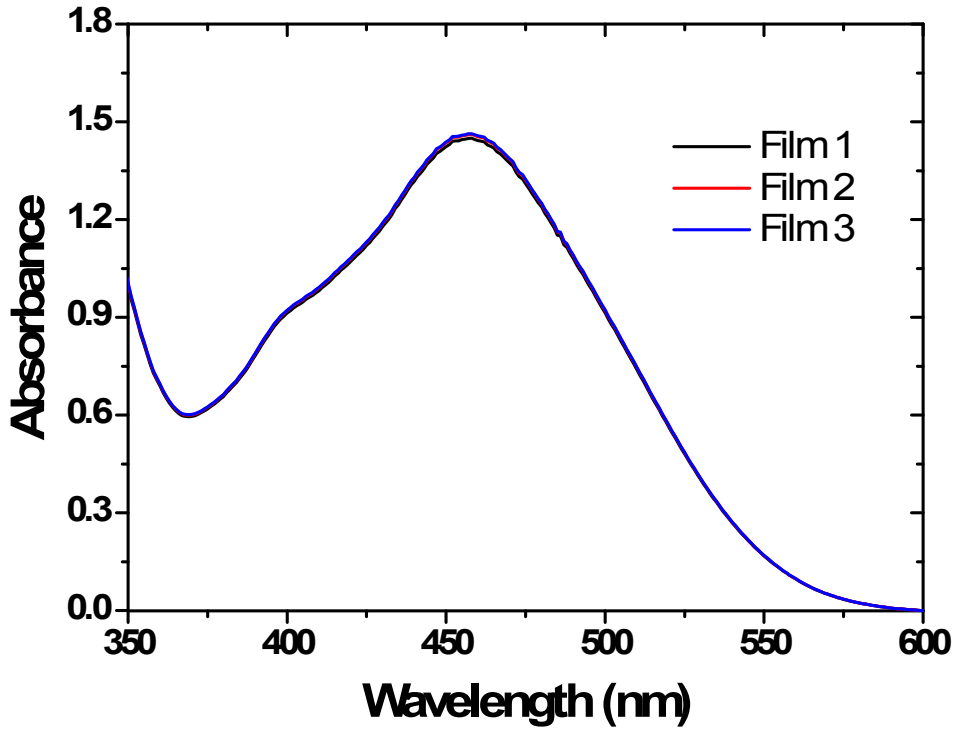

Figure S25: Absorption spectrum of PRA/TiO_2 films.

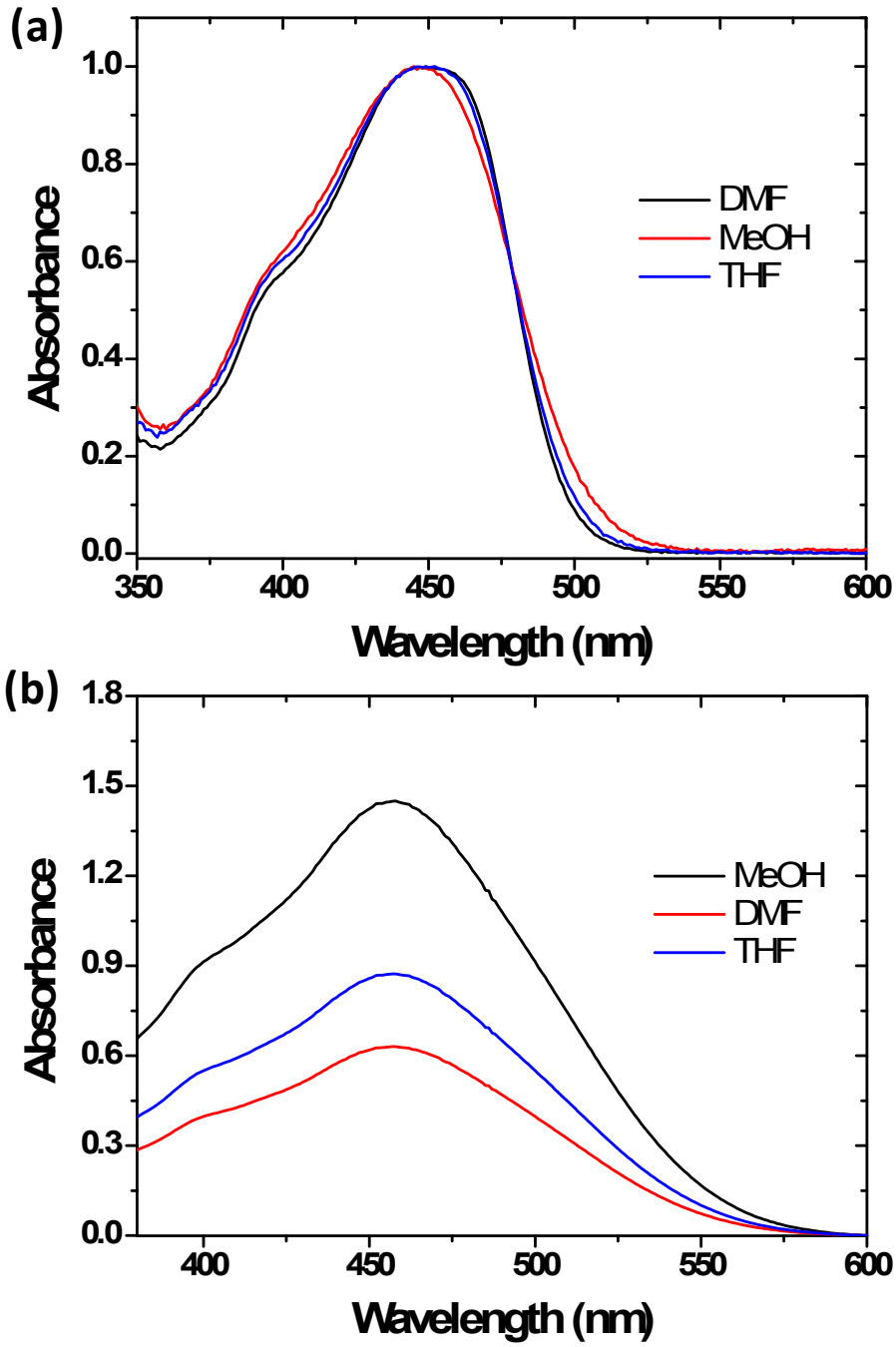

Figure S26: Absorption spectra of PRA and PRA/TiO_2 in various solvents.

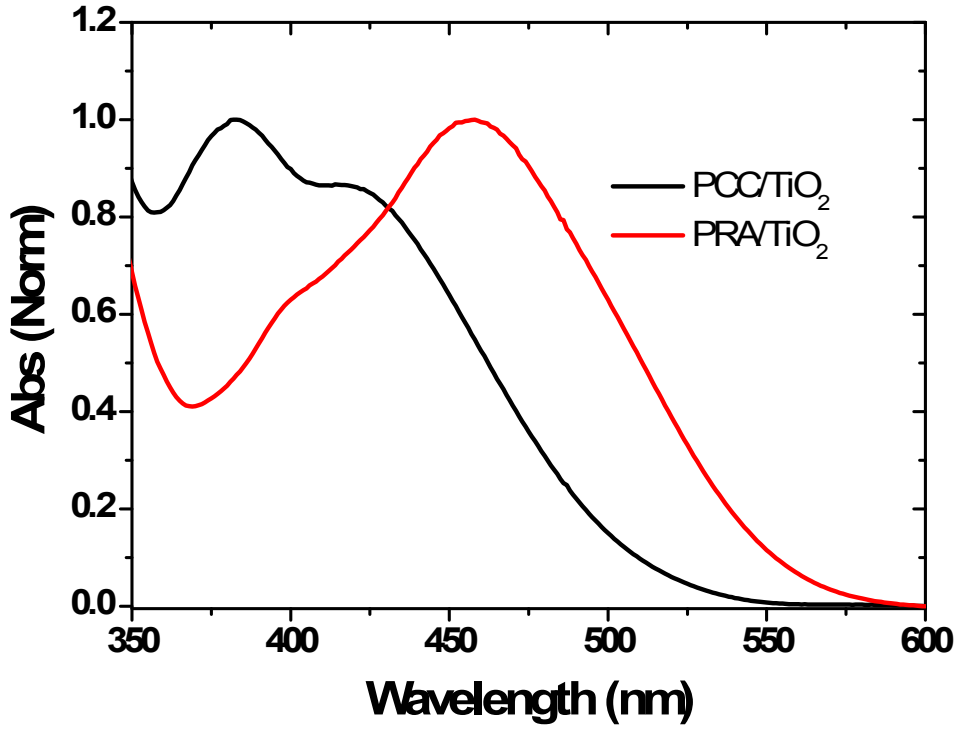

Figure S27: Absorption spectra of PCC/TiO_2 and PRA/TiO_2 films.

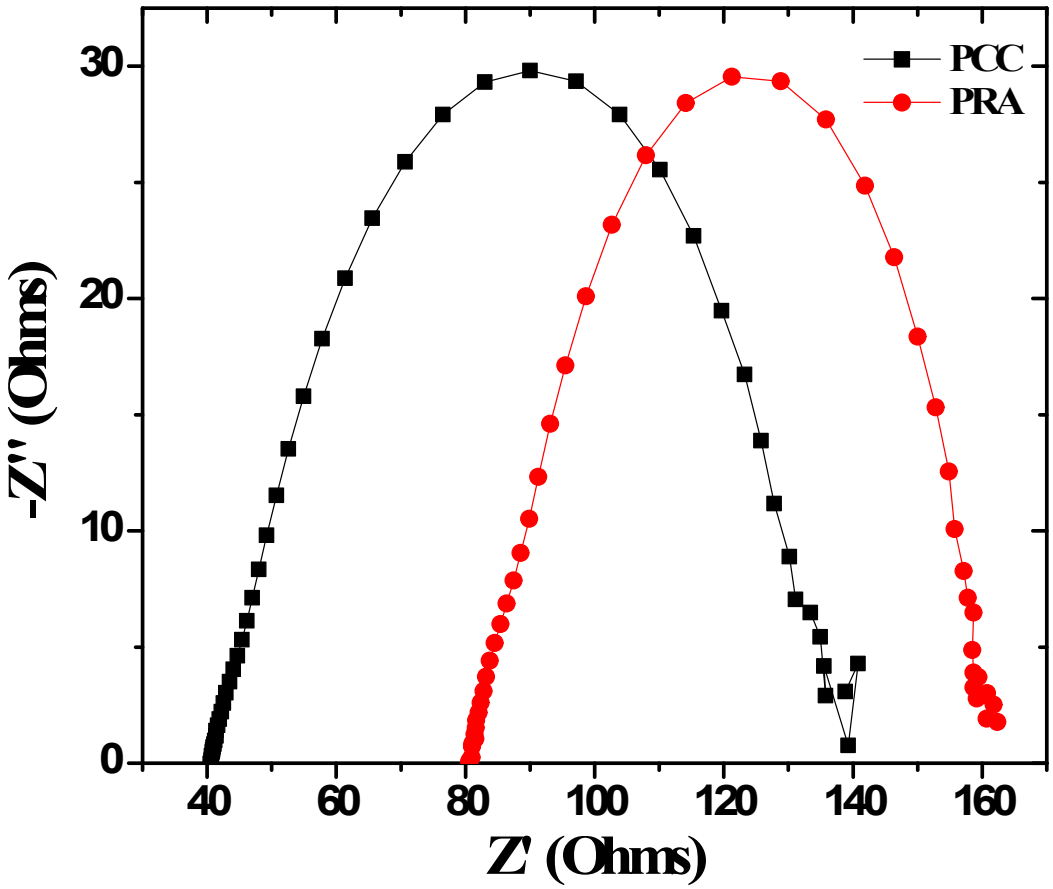

Figure S28: Nyquist plots of PCC and PRA devices.

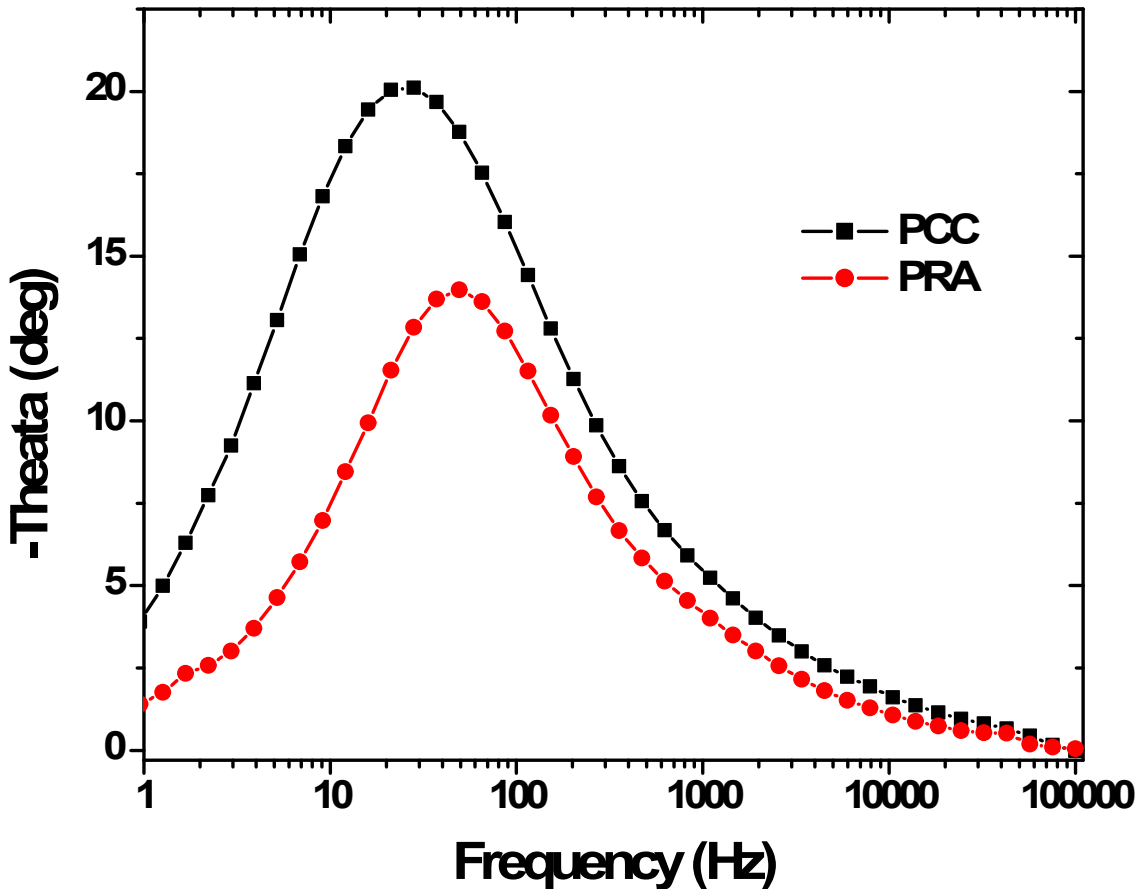

Figure S29: Bode phase plots of PCC and PRA devices.

Table S1: Molecular orbital composition (%) of the designed pyrene based dyes.

	HOMO		LUMO	
	Donor	Acceptor	Donor	Acceptor
P	100	-	100	-
PC	89	11	98	2
PAC	95	5	88	12
PMC	83	17	78	21
PCC	92	8	87	13
PMN	88	12	87	13
PR	86	14	75	24
PRA	81	19	55	45

Table S2: Calculated absorption maxima in various level of theory at TD-DFT/6-311+G(d,p) along with experimentally observed absorption maxima.

Molecule	**B3LYP**	**PBE**	**M06**	**ωb97xd-D3**	**Expt.**
P	345	370	349	318	336
PC	381	413	381	346	353
PAC	422	471	416	369	367
PMC	436	505	424	366	367
PCC	471	534	459	400	383
PMN	478	539	468	409	438
PR	499	576	482	418	442
PRA	504	578	487	422	452

Table S3: Calculated ground state dipole moment (in Debye) of pyrene derivatives at B3LYP/6-311+G(d,p) level.

Molecule	**Dipole moment**	
	Gas	**THF**
P	0.0	0.0
PC	2.9	3.9
PAC	3.6	4.5
PMC	4.4	5.7
PCC	5.9	7.8
PMN	7.5	9.4
PR	5.5	7.1
PRA	4.4	6.0

Table S4: Cartesian coordinates (X, Y and Z in angstrom, Å) of optimized structure of pyrene derivatives at the B3LYP/6-311+G(d,p) level of theory in vacuum.

For P:

	X	Y	Z
C	-3.51913600	0.00002000	0.00014000
C	-2.82944800	1.20934600	-0.00009800
C	-1.42739100	1.23481400	-0.00010400
C	-0.71321400	0.00015000	-0.00003600
C	-1.42725900	-1.23464000	-0.00001500
C	-2.83025900	-1.20900800	0.00007900
C	-0.67921000	2.46124300	0.00000100
C	0.71237000	0.00010300	-0.00001400
C	1.42763000	1.23441900	-0.00001100
C	0.68017400	2.46109800	0.00003800
C	2.83017000	1.20867100	0.00002000
H	3.37594700	2.14625500	0.00004600
C	3.51970900	-0.00036900	0.00005500
C	2.82945500	-1.20919300	0.00002000
C	1.42710600	-1.23443100	-0.00001300
C	0.67949000	-2.46131900	-0.00005400
C	-0.67979600	-2.46115500	-0.00003700
H	-1.22785800	-3.39758800	-0.00010500
H	1.22694500	-3.39804700	-0.00012000
H	-1.22610700	3.39847100	-0.00015300
H	-4.60357900	0.00142600	0.00027900
H	-3.37720900	-2.14591300	0.00013300
H	1.22679000	3.39844000	0.00010500
H	4.60391500	-0.00106800	0.00009300
H	3.37538700	-2.14673400	0.00004400
H	-3.37657200	2.14626500	-0.00014300

For PC:

	X	Y	Z
C	2.27261400	0.21697100	-0.00816300
C	0.99066900	-0.40065600	-0.00925400
C	-0.16910800	0.44636900	0.00214000
C	-0.03165200	1.86665300	0.01990600
C	1.25317200	2.42717600	0.00851900
C	2.37100800	1.61705100	-0.01227000
C	-1.48170700	-0.11941400	-0.00419900
C	-1.20603300	2.68972200	0.04238500
H	1.36427000	3.50586100	0.01634700
H	3.36171400	2.05201300	-0.02706400
C	-2.45014200	2.14487900	0.04253700
C	-2.63376100	0.72324400	0.01710100
H	-1.07659900	3.76656300	0.05819400
H	-3.32926500	2.78049600	0.05949900
C	0.76857200	-1.82269900	-0.05019400
C	-3.91034700	0.14181400	0.01199100
C	-4.06554200	-1.24070000	-0.01637300
C	-2.94998800	-2.07084300	-0.04042200
C	-1.65461700	-1.53192100	-0.03465600
C	-0.48360000	-2.35247900	-0.06248500
H	-4.78258000	0.78659400	0.02989600
H	-5.06013400	-1.67184400	-0.02042600
H	-3.07273500	-3.14842600	-0.06409300
H	1.62057200	-2.48164200	-0.06810200
C	3.59587500	-0.47128100	-0.01080300
O	4.64525100	0.08655300	-0.24657400
O	3.57844500	-1.79372300	0.30479200
H	4.50192600	-2.08567000	0.27009000
H	-0.60921100	-3.42990500	-0.09464700

For PAC:

	X	Y	Z
C	-1.43214500	0.96770300	-0.21448500
C	-0.33198100	0.06497800	-0.20835800
C	0.99266600	0.58717300	-0.06041200
C	1.20904300	1.99386600	0.04529600
C	0.10634600	2.85619700	-0.03649700
C	-1.17288200	2.34992900	-0.17569500
C	2.11543300	-0.29482100	-0.01943900
C	2.54439700	2.48752900	0.21585300
H	0.26348300	3.92799200	0.01664600
H	-2.01259400	3.03506900	-0.22236700
C	3.60723600	1.64291100	0.27563400
C	3.43347900	0.22382800	0.15735700
H	2.68917400	3.55952700	0.29780500
H	4.61125900	2.03171600	0.40893600
C	-0.47105400	-1.35182900	-0.40183100
C	4.51764300	-0.66471500	0.20698100
C	4.32283900	-2.03674600	0.07684100
C	3.04402900	-2.55139100	-0.10788200
C	1.92942400	-1.70027900	-0.15902700
C	0.60126600	-2.18836600	-0.37629200
H	5.51781100	-0.26877400	0.34731900
H	5.17344000	-2.70765200	0.11665100
H	2.89724100	-3.62072400	-0.21597800
H	-1.45023100	-1.75976700	-0.60538200
C	-2.84636400	0.58952400	-0.23379100
C	-3.44024700	-0.48905900	0.31066000
C	-4.89032400	-0.72387000	0.27532600
O	-5.43731800	-1.67285100	0.79400400
O	-5.59489600	0.22692800	-0.40033900
H	-6.52572600	-0.03283400	-0.34650800
H	-3.50289600	1.32591900	-0.68950300
H	0.46065000	-3.25209200	-0.53735100
H	-2.89671400	-1.24635500	0.85896500

For PMC:

	X	Y	Z
C	0.97000900	1.21542000	-0.39844200
C	-0.08008400	0.26218000	-0.43115200
C	-1.41465700	0.69481800	-0.14966300
C	-1.68466300	2.06593900	0.13555600
C	-0.62835500	2.98792900	0.09081200
C	0.66030500	2.56971000	-0.18983600
C	-2.49020200	-0.24370700	-0.15621200
C	-3.02818400	2.46554000	0.43885600
H	-0.82853900	4.03670400	0.28096100
H	1.46373400	3.29820300	-0.21074100
C	-4.04614400	1.56504500	0.45319600
C	-3.81713200	0.18094700	0.15303100
H	-3.21658200	3.51093600	0.65909200
H	-5.05657800	1.88276200	0.68800800
C	0.11835600	-1.11338100	-0.79455400
C	-4.85490300	-0.76291400	0.15095500
C	-4.60487200	-2.09701200	-0.15663200
C	-3.31667300	-2.51843700	-0.47057300
C	-2.24681800	-1.61083500	-0.47567400
C	-0.91050600	-2.00210700	-0.81230800
H	-5.86214300	-0.44005600	0.39186100
H	-5.41997200	-2.81173600	-0.15468600
H	-3.12824300	-3.55794300	-0.71662200
H	1.10672000	-1.44852900	-1.07693600
C	2.39338700	0.90502200	-0.58538800
C	3.15754400	-0.04091500	-0.00094900
C	4.61377000	-0.13190300	-0.28447500
O	5.40604600	-0.74201500	0.39118500
O	4.99167500	0.57867800	-1.38057900
H	5.95468900	0.49762100	-1.44103100
H	2.92033100	1.58001300	-1.25426700
C	2.67340900	-1.03157600	1.01830400
O	2.78312300	-2.22533700	0.91387900
O	2.09653600	-0.42898300	2.08077600
H	1.79343700	-1.13165600	2.67686900
H	-0.72742300	-3.03362700	-1.09372000

For PCC:

	X	Y	Z
C	-1.17184600	1.11667500	-0.28865800
C	-0.09527100	0.18697600	-0.32825800
C	1.23339400	0.66282400	-0.09243000
C	1.47452700	2.04733900	0.15277100
C	0.39530500	2.94472900	0.10298200
C	-0.88600500	2.48846800	-0.13569800
C	2.33388600	-0.24554100	-0.10689300
C	2.81190500	2.48889400	0.41729900
H	0.57514200	4.00302000	0.25607700
H	-1.70701500	3.19691800	-0.16161300
C	3.85341600	1.61484500	0.43052500
C	3.65483300	0.22005500	0.16411200
H	2.97725400	3.54350900	0.60959500
H	4.85951000	1.96390200	0.63769700
C	-0.26102400	-1.19465300	-0.67479600
C	4.71763400	-0.69557500	0.15855800
C	4.49770300	-2.04153400	-0.11879600
C	3.21529400	-2.50202700	-0.39888900
C	2.12149900	-1.62310900	-0.39853100
C	0.79190700	-2.05443100	-0.70617400
H	5.72021300	-0.34152500	0.37341600
H	5.33106800	-2.73469000	-0.11835600
H	3.04951600	-3.55066600	-0.62093400
H	-1.24434600	-1.55985900	-0.93374800
C	-2.58688500	0.78727600	-0.39666800
C	-3.30909200	-0.22058500	0.16418400
C	-4.77455900	-0.34758300	-0.06922100
O	-5.47435800	-1.19584500	0.42493700
O	-5.26071500	0.60026500	-0.91284700
H	-6.21208200	0.43804800	-0.99041200
H	-3.17897400	1.50933000	-0.95036300
H	0.63232800	-3.09389300	-0.97146400
C	-2.77122700	-1.16705000	1.08771200
N	-2.34205800	-1.91505900	1.85637100

For PMN:

	X	Y	Z
C	-1.53526900	1.08755700	-0.35409800
C	-0.44959100	0.16630100	-0.36023700
C	0.87100500	0.66036800	-0.11733800
C	1.09623200	2.05301200	0.09609100
C	0.00995300	2.93958000	0.00799200
C	-1.26402500	2.46632800	-0.23315400
C	1.97967000	-0.23757800	-0.09486300
C	2.42523200	2.51345100	0.36853500
H	0.17866900	4.00297900	0.13542300
H	-2.09079800	3.16656600	-0.28462400
C	3.47414300	1.64936000	0.41879800
C	3.29206400	0.24687800	0.18394800
H	2.57855400	3.57394000	0.53640700
H	4.47384300	2.01290900	0.63165100
C	-0.59697200	-1.22323400	-0.68094700
C	4.36309900	-0.65858200	0.21561300
C	4.15974900	-2.01284100	-0.03285100
C	2.88620000	-2.49181000	-0.32168800
C	1.78445400	-1.62340700	-0.35756900
C	0.46435900	-2.07378400	-0.67703200
H	5.35913100	-0.29013900	0.43638900
H	4.99949200	-2.69757800	-0.00470200
H	2.73373100	-3.54656900	-0.52315900
H	-1.57113600	-1.60312500	-0.95357100
C	-2.94357300	0.74267400	-0.45975000
C	-3.65408300	-0.27273300	0.11135400
H	-3.54735000	1.45448100	-1.01694000
H	0.31889800	-3.11936100	-0.92572100
C	-3.12571000	-1.21642100	1.04423700
N	-2.73482000	-1.97534400	1.82301500
C	-5.05977500	-0.37440300	-0.14241700
N	-6.19318100	-0.45299900	-0.35428500

For PR:

	X	Y	Z
C	0.21556100	-0.10318700	0.35122600
C	-1.08868200	0.44594000	0.15752300
C	-2.21756900	-0.43034200	0.12024500
C	-2.04306300	-1.83791200	0.27364000
C	-0.74699900	-2.34290900	0.46119700
C	0.34526100	-1.49792100	0.49694400
C	-3.53260800	0.09209200	-0.07057400
C	-3.19054400	-2.69508700	0.23889000
H	-0.60714000	-3.41032300	0.59210800
H	1.32028300	-1.92720100	0.68794300
C	-4.44149400	-2.19258600	0.06171300
C	-4.65845600	-0.78429300	-0.09987400
H	-3.03899000	-3.76248400	0.35829200
H	-5.30069500	-2.85450300	0.03867100
C	-1.32790700	1.84943300	-0.03140700
C	-5.94022400	-0.24517500	-0.28520700
C	-6.12231000	1.12577700	-0.44180900
C	-5.03101500	1.98773900	-0.41846200
C	-3.73077000	1.49261900	-0.23480600
C	-2.58192600	2.34569700	-0.21129500
H	-6.79513200	-0.91253800	-0.30576500
H	-7.12055600	1.52359400	-0.58417800
H	-5.17733900	3.05529400	-0.54302000
H	-0.49407700	2.53800600	-0.04562300
C	1.36918500	0.77107200	0.43908800
H	-2.72606600	3.41212100	-0.34887100
H	1.18620300	1.81058800	0.69093500
C	2.68562400	0.51815500	0.25671800
S	3.50539800	-0.97344900	-0.24694800
C	3.68030800	1.61184600	0.41243800
O	3.46909300	2.75847300	0.74221000
N	4.95236000	1.11905200	0.10306000
C	5.09865400	-0.18972700	-0.26690600
S	6.50262100	-0.94088500	-0.66561900
H	5.75977100	1.72824000	0.14578600

For PRA:

	X	Y	Z
C	0.79342200	0.28862500	0.19050700
C	2.04593900	-0.37747000	0.02077600
C	3.25824700	0.36727600	0.16183600
C	3.21748400	1.76054900	0.46595900
C	1.96958400	2.38252500	0.62545200
C	0.79723300	1.66502400	0.48997200
C	4.52389500	-0.27367700	0.00091000
C	4.44558300	2.48439700	0.60780900
H	1.93043400	3.43779300	0.87225900
H	-0.13992900	2.17645500	0.66659000
C	5.64865600	1.86895700	0.45798600
C	5.73234200	0.47086100	0.14998400
H	4.39491000	3.54257700	0.84076400
H	6.57027700	2.43020400	0.56973200
C	2.15493900	-1.77028700	-0.31227900
C	6.96283400	-0.18390300	-0.00811100
C	7.01571900	-1.54172200	-0.30940500
C	5.84361700	-2.27502000	-0.46098800
C	4.59038100	-1.66172500	-0.30998900
C	3.36196700	-2.37984000	-0.46352400
H	7.88040400	0.38299100	0.10755700
H	7.97625800	-2.02993000	-0.42805700
H	5.88912700	-3.33232600	-0.69897100
H	1.25865600	-2.35681800	-0.46142000
C	-0.44772700	-0.45534300	0.09968100
H	-0.39197900	-1.53112800	0.22736800
H	3.40666900	-3.43447600	-0.71407300
C	-1.71507800	-0.03327400	-0.12030100
S	-2.33752200	1.58558300	-0.46879400
C	-2.82557700	-1.01186900	-0.14977800
O	-2.75317200	-2.20756100	0.03775000
N	-4.03682200	-0.36149400	-0.46124000
C	-3.99813000	0.99889400	-0.65564200
S	-5.25974100	1.98725700	-1.02309300
C	-5.26879800	-1.12222900	-0.49748600
C	-5.95764900	-1.15086100	0.86012700
O	-5.53527500	-0.67294100	1.87630400
O	-7.12978800	-1.81489300	0.76477700
H	-7.53498400	-1.82225100	1.64521900
H	-5.94433800	-0.68727500	-1.23406000
H	-5.02895700	-2.14697500	-0.78565600