

Supporting information

Towards new descriptors of basic nitrogen compounds in middle distillates by 2D NMR

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This document contains the full list of the nitrogen compounds used for the simulation and the cartographies obtained by simulation for each family with the software Advanced Chemistry Development/Laboratory.

Tableau S-1. Full list of the nitrogen compounds simulated

Pyridine Family	Quinoline Family	Isoquinoline Family	Acridine Family
Pyridine	Quinoline	Isoquinoline	Acridine
Methylpyridine	Methylquinoline	Methylisoquinoline	Methylacridine
2-methylpyridine	2-methylquinoline	1-methylisoquinoline	1-methylacridine
3-methylpyridine	3-methylquinoline	3-methylisoquinoline	2-methylacridine
4-methylpyridine	4-methylquinoline	4-methylisoquinoline	3-methylacridine
Dimethylpyridine	5-methylquinoline	5-methylisoquinoline	4-methylacridine
2,3-dimethylpyridine	6-methylquinoline	6-methylisoquinoline	9-methylacridine
2,4-dimethylpyridine	7-methylquinoline	7-methylisoquinoline	Dimethylacridine
2,5-dimethylpyridine	8-methylquinoline	8-methylisoquinoline	1,2-dimethylacridine
2,6-dimethylpyridine	Dimethylquinoline	Dimethylisoquinoline	1,3-dimethylacridine
3,4-dimethylpyridine	2,3-dimethylquinoline	1,3-dimethylisoquinoline	1,4-dimethylacridine
3,5-dimethylpyridine	2,4-dimethylquinoline	1,4-dimethylisoquinoline	1,9-dimethylacridine
Tetrahydroquinoline	2,5-dimethylquinoline	1,5-dimethylisoquinoline	1,5-dimethylacridine
5,6,7,8-tetrahydroquinoline	2,6-dimethylquinoline	1,6-dimethylisoquinoline	1,6-dimethylacridine
2-methyl-5,6,7,8-tetrahydroquinoline	2,7-dimethylquinoline	1,7-dimethylisoquinoline	1,7-dimethylacridine
3-methyl-5,6,7,8-tetrahydroquinoline	2,8-dimethylquinoline	1,8-dimethylisoquinoline	1,8-dimethylacridine
4-methyl-5,6,7,8-tetrahydroquinoline	3,4-dimethylquinoline	3,4-dimethylisoquinoline	2,3-dimethylacridine
Octahydroacridine	3,5-dimethylquinoline	3,5-dimethylisoquinoline	2,4-dimethylacridine
1,2,3,4,5,6,7,8-octahydroacridine	3,6-dimethylquinoline	3,6-dimethylisoquinoline	2,9-dimethylacridine
	3,7-dimethylquinoline	3,7-dimethylisoquinoline	2,5-dimethylacridine
	3,8-dimethylquinoline	3,8-dimethylisoquinoline	2,6-dimethylacridine
	4,5-dimethylquinoline	4,5-dimethylisoquinoline	2,7-dimethylacridine
	4,6-dimethylquinoline	4,6-dimethylisoquinoline	3,4-dimethylacridine
	4,7-dimethylquinoline	4,7-dimethylisoquinoline	3,9-dimethylacridine
	4,8-dimethylquinoline	4,8-dimethylisoquinoline	3,5-dimethylacridine
	5,6-dimethylquinoline	5,6-dimethylisoquinoline	3,6-dimethylacridine

	5,7-dimethylquinoline	5,7-dimethylisoquinoline	4,9-dimethylacridine
	5,8-dimethylquinoline	5,8-dimethylisoquinoline	4,5-dimethylacridine
	6,7-dimethylquinoline	6,7-dimethylisoquinoline	Trimethylacridine
	6,8-dimethylquinoline	6,8-dimethylisoquinoline	1,2,3-trimethylacridine
	7,8-dimethylquinoline	7,8-dimethylisoquinoline	1,2,4-trimethylacridine
	Benzo(h)quinoline	Benzo(h)isoquinoline	1,3,4-trimethylacridine
	benzo(h)quinoline	benzo(h)isoquinoline	1,2,8-trimethylacridine
	2-methylbenzo(h)quinoline *	1-methylbenzo(h)isoquinoline *	1,3,8-trimethylacridine
	3-methylbenzo(h)quinoline *	3-methylbenzo(h)isoquinoline *	1,4,8-trimethylacridine
	4-methylbenzo(h)quinoline *	4-methylbenzo(h) isoquinoline *	Autre Methylacridine
	2,5-dimethylbenzo(h)quinoline *	1,5-dimethylbenzo(h)isoquinoline *	2,3,6,7-tetramethylacridine
	3,5-dimethylbenzo(h)quinoline *	3,5-dimethylbenzo(h)isoquinoline *	1,2,3,6,7,8-hexamethylacridine
	4,5-dimethylbenzo(h)quinoline *	4,5-dimethylbenzo(h)isoquinoline *	1,2,3,4,5,6,7,8-octamethylacridine
	Benzo(f)quinoline	Benzo(f)isoquinoline	Benz[a]acridine
	benzo(f)quinoline	benzo(f)isoquinoline	benz[a]acridine
	2-methylbenzo(f)quinoline *	1-methylbenzo(f)isoquinoline *	1-methyl benz[a]acridine *
	3-methylbenzo(f)quinoline *	3-methylbenzo(f)isoquinoline *	1,1-methyl benz[a]acridine *
	4-methylbenzo(f)quinoline *	4-methylbenzo(f)isoquinoline *	1,1,1-dimethyl benz[a]acridine *
	2,8-dimethylbenzo(f)quinoline *	1,8-dimethylbenzo(f)isoquinoline *	Benz[c]acridine
	3,8-dimethylbenzo(f)quinoline *	3,8-dimethylbenzo(f)isoquinoline *	benz[c]acridine
	4,8-dimethylbenzo(f)quinoline *	4,8-dimethylbenzo(f)quinoline *	1-methyl benz[c]acridine *
	Autres	Autres	8-methyl benz[c]acridine *
	8-hydroxyquinoline	8-hydroxyisoquinoline	1,8-dimethyl benz[c]acridine *
	Phenanthridine	Phenanthridine	
	2',2-bisquinoline		
	4',4-dimethyl-2',2-bisquinoline		

* does not really correspond to IUPAC names but keeps a similarity with families

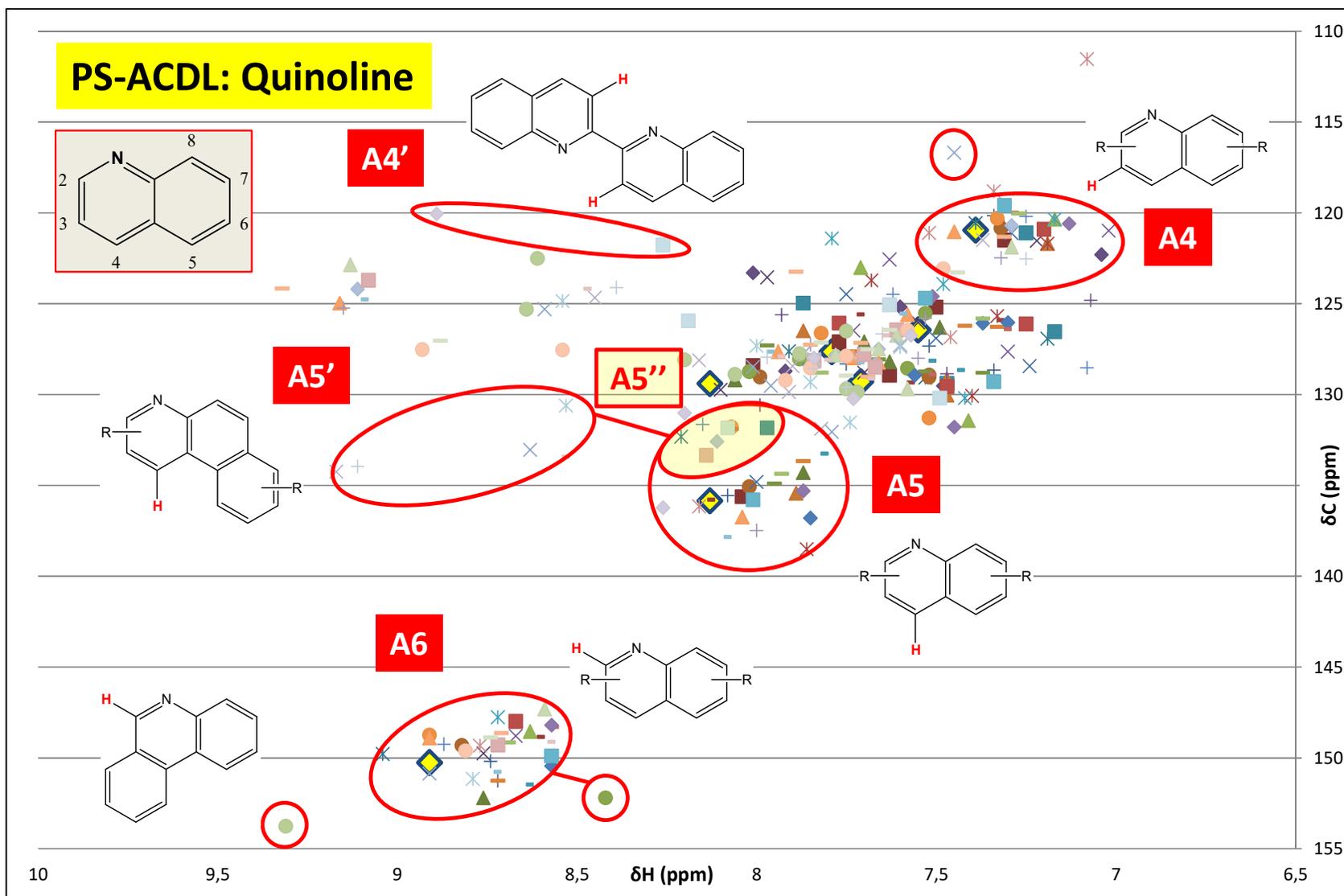


Figure S1. $\{^1\text{H}, ^{13}\text{C}\}$ HSQC spectrum of quinoline derivatives simulated by PS-ACDL

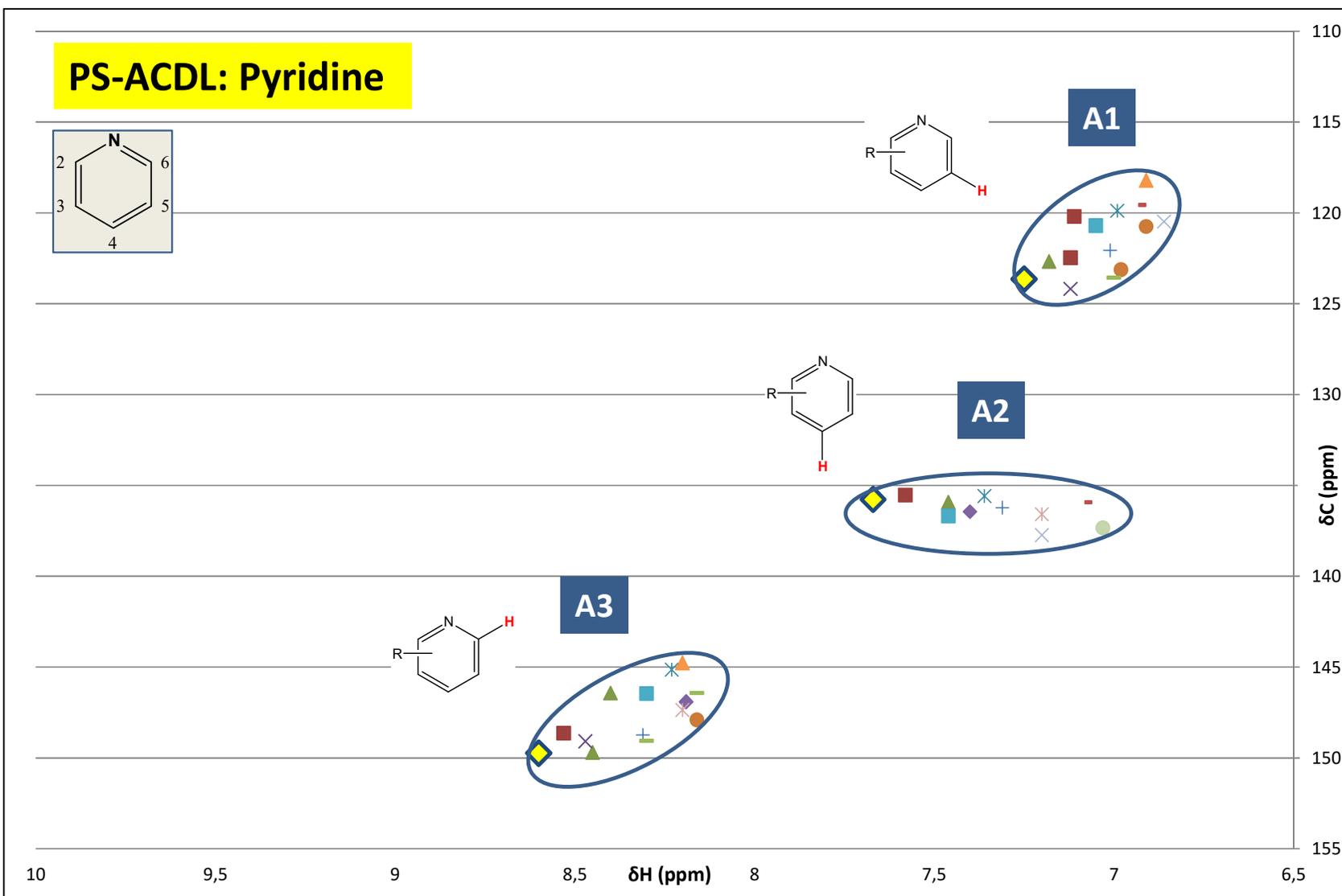


Figure S2. $\{^1H, ^{13}C\}$ HSQC spectrum of pyridine derivatives simulated by PS-ACDL

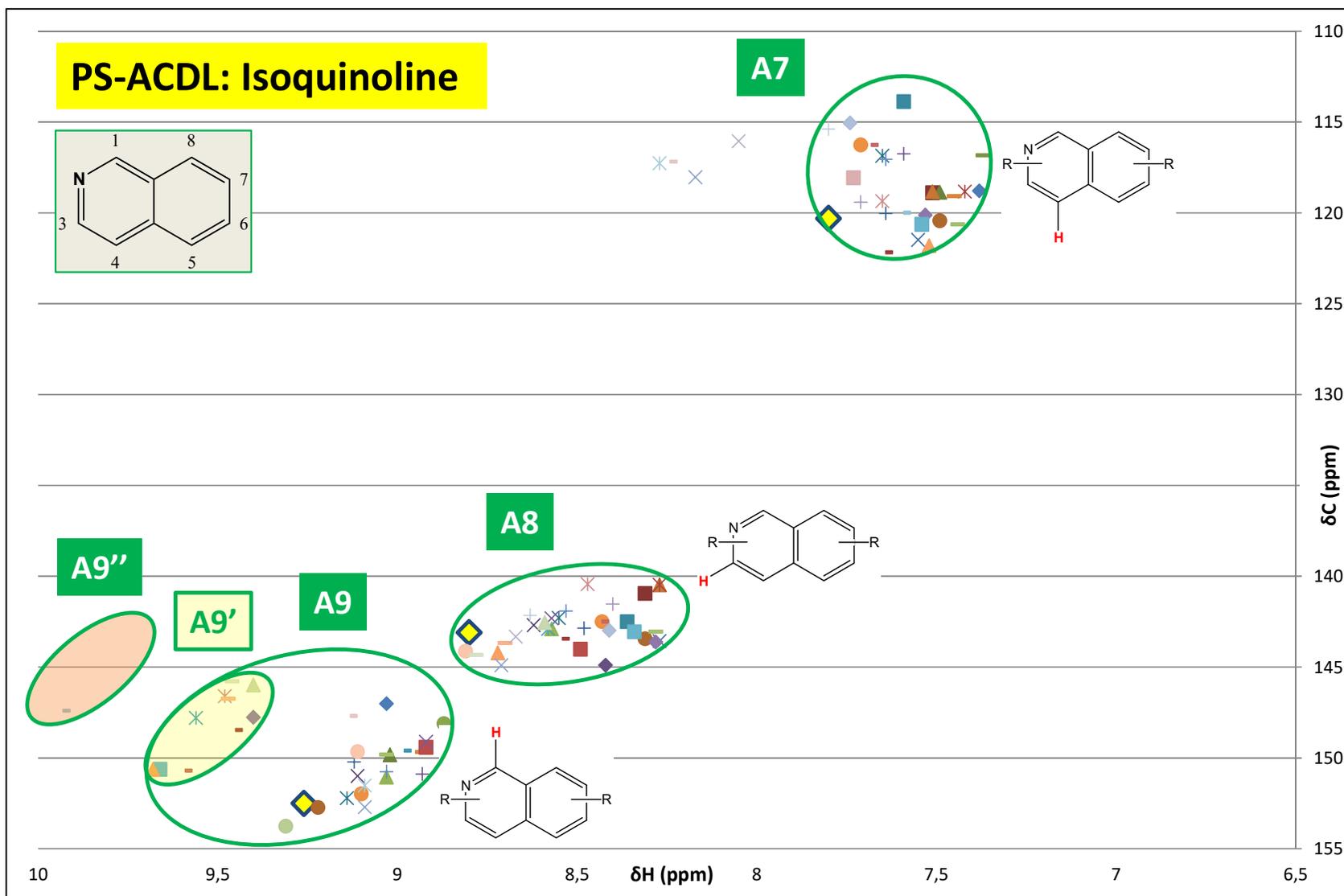


Figure S3. $\{^1\text{H}, ^{13}\text{C}\}$ HSQC spectrum of Isoquinoline derivatives simulated by PS-ACDL without benzenic correlations

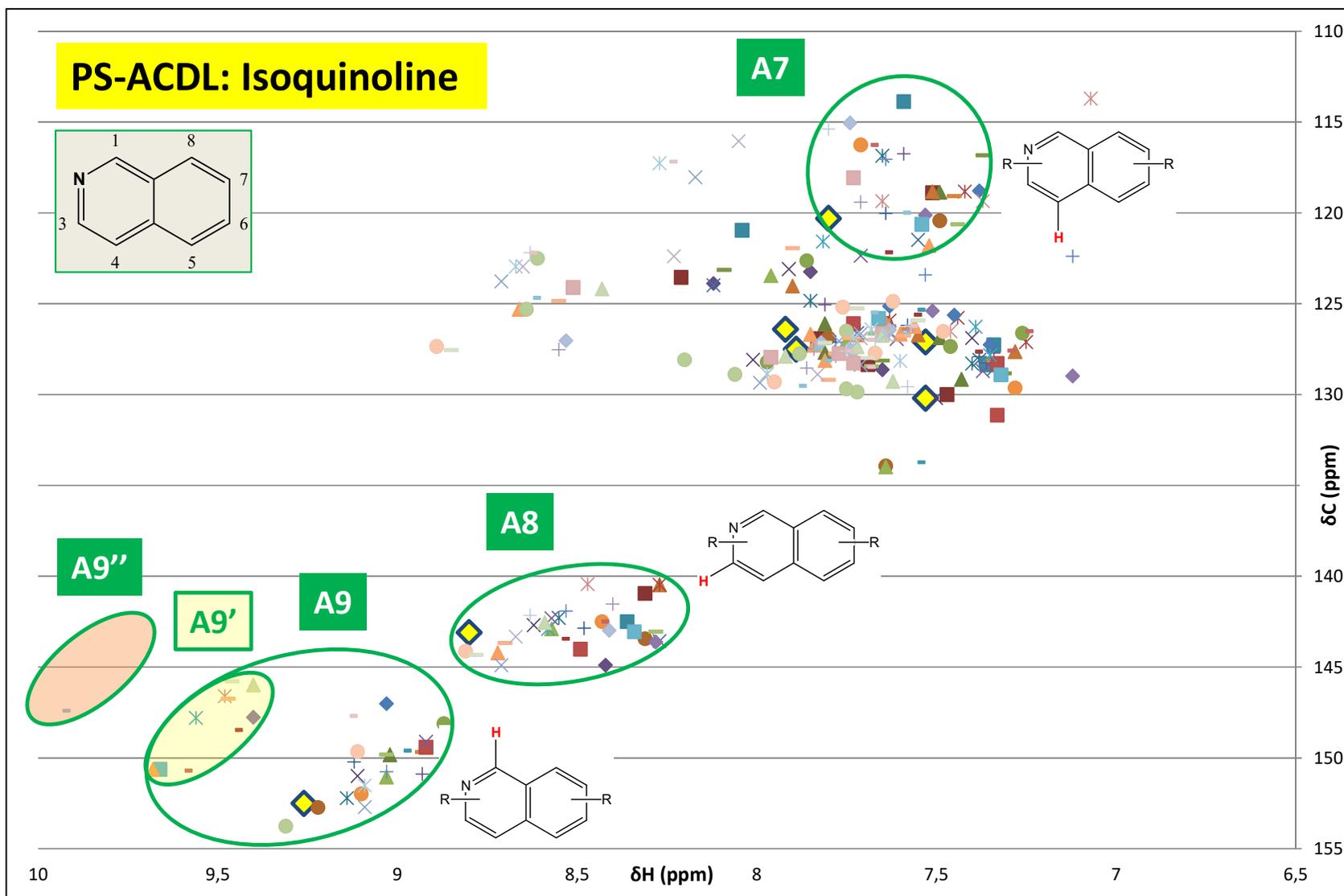


Figure S4. $\{^1H, ^{13}C\}$ HSQC spectrum of Isoquinoline derivatives simulated by PS-ACDL

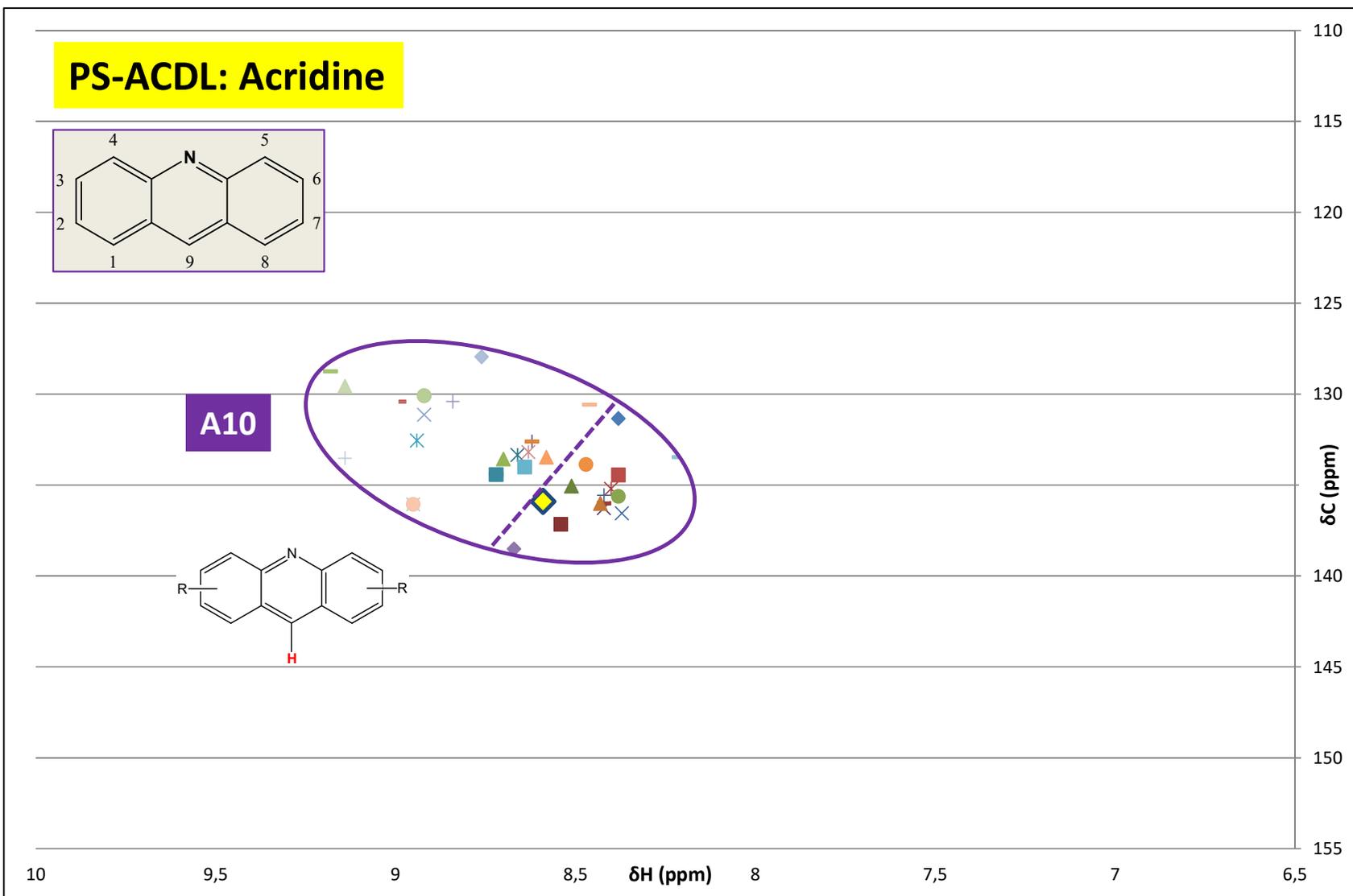


Figure S5. $\{^1H, ^{13}C\}$ HSQC spectrum of Acridine derivatives simulated by PS-ACDL without benzenic correlations

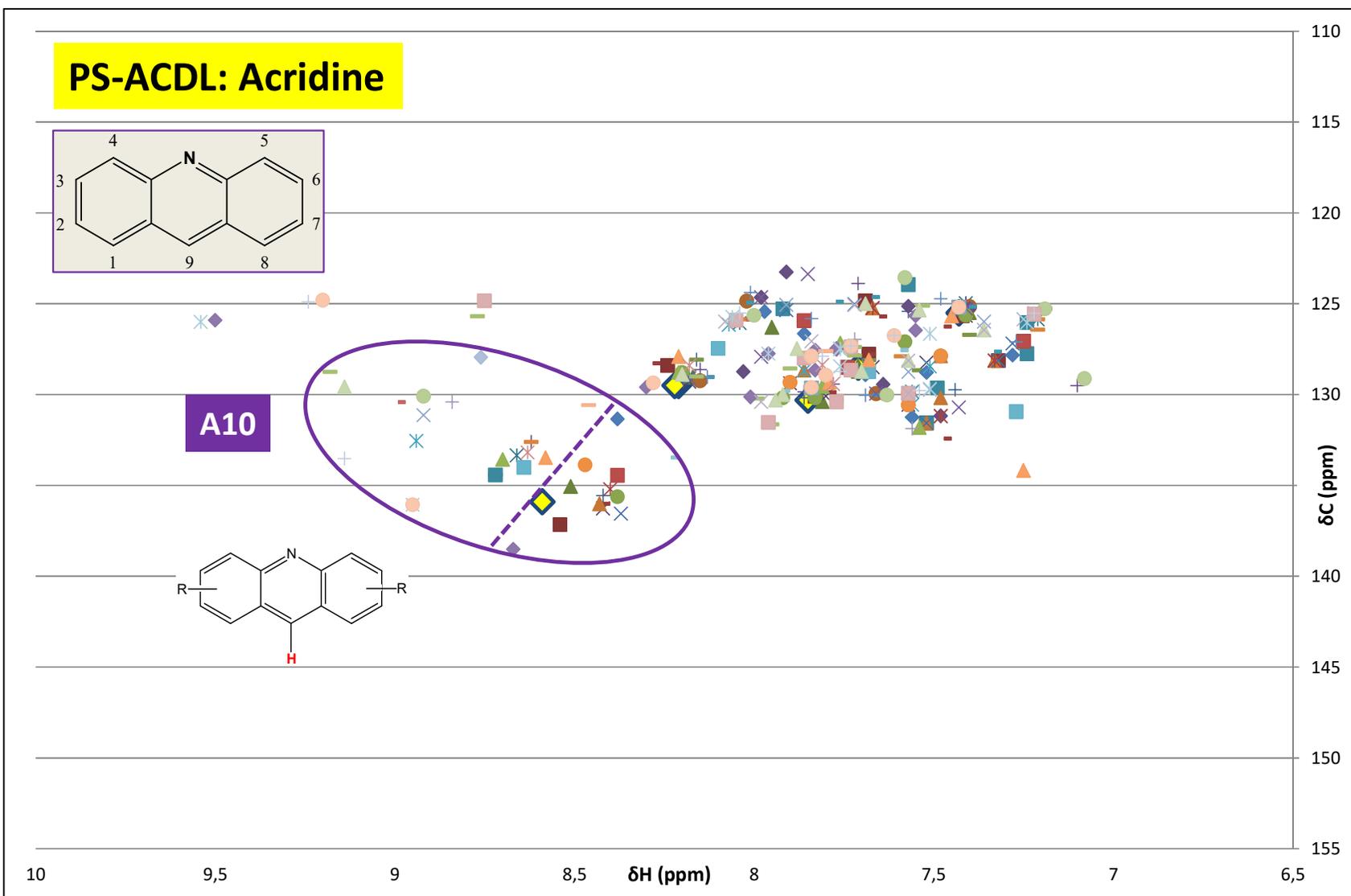


Figure S6. $\{^1H, ^{13}C\}$ HSQC spectrum of Acridine derivatives simulated by PS-ACDL