

Supplementary Material

Microwave-assisted synthesis of novel 1-[[[(diindolyl)methyl]benzyl]-2-[[[(diindolyl)methyl]phenyl]-1*H*-benzimidazole scaffold via two-consecutive multicomponent reactions

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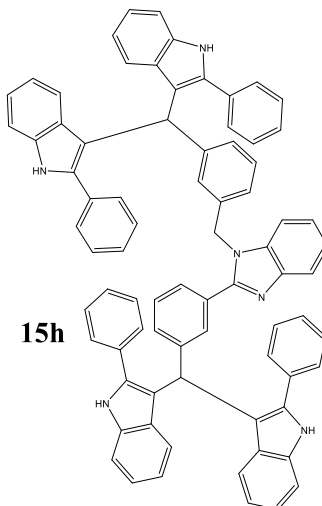
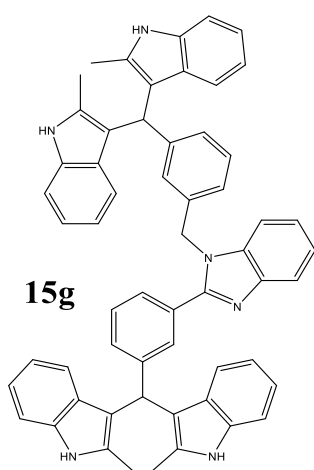
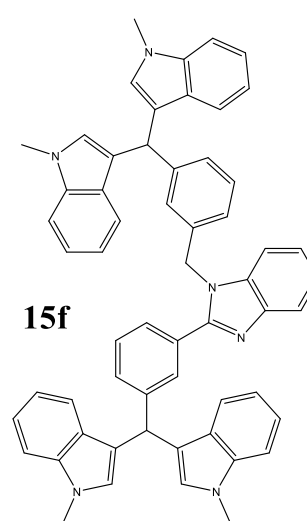
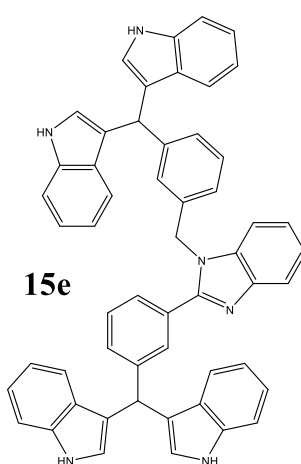
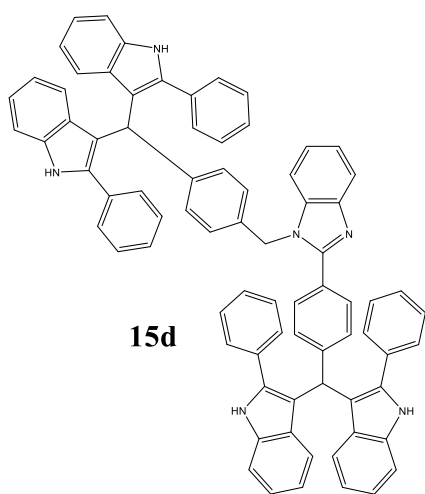
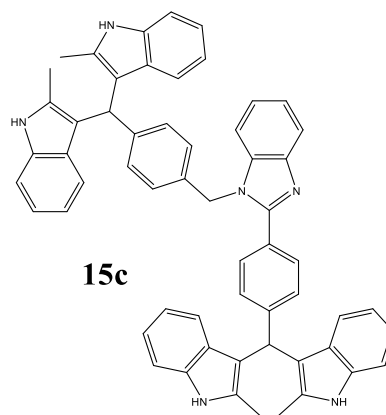
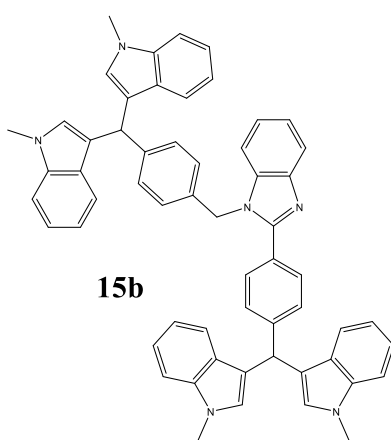
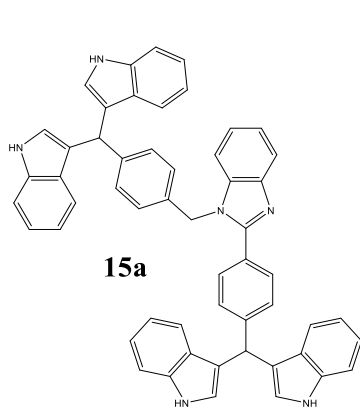
c) Departamento de Alimentos y Biotecnología, Facultad de Química, Edificio E, UNAM, Av. Universidad 3000, C.U., Coyoacán, México, D.F., 04510, México.

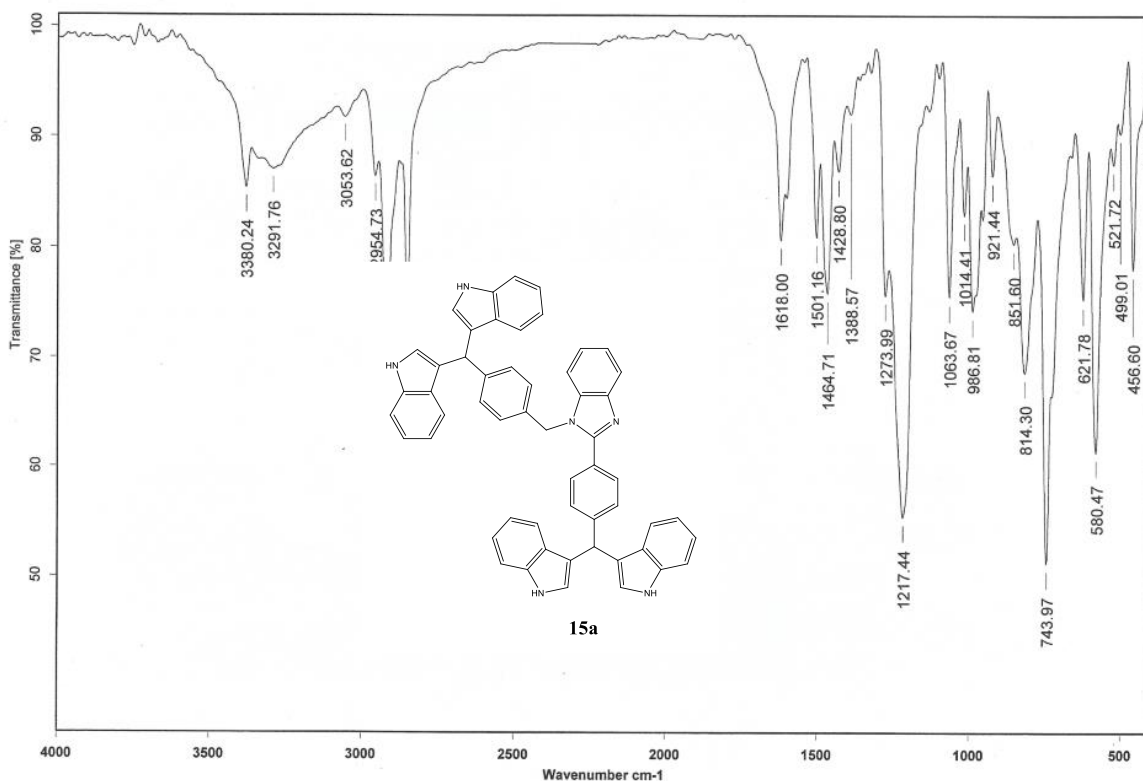
E-mail: penieres@unam.mx

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IR, MS, ^1H NMR, ^{13}C NMR Spectra1-{4-[Bis(1*H*-indol-3-yl)methyl]benzyl}-2-{4-[bis(1*H*-indol-3-yl)methyl]phenyl}-1*H*-benzimidazole (15a)

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Instrument : MStation

Note : -

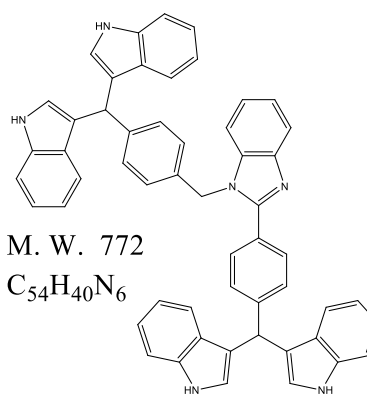
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Mass Tolerance : 1000ppm, 1mmu if m/z > 1

Unsaturation (U.S.) : -0.5 - 40.0

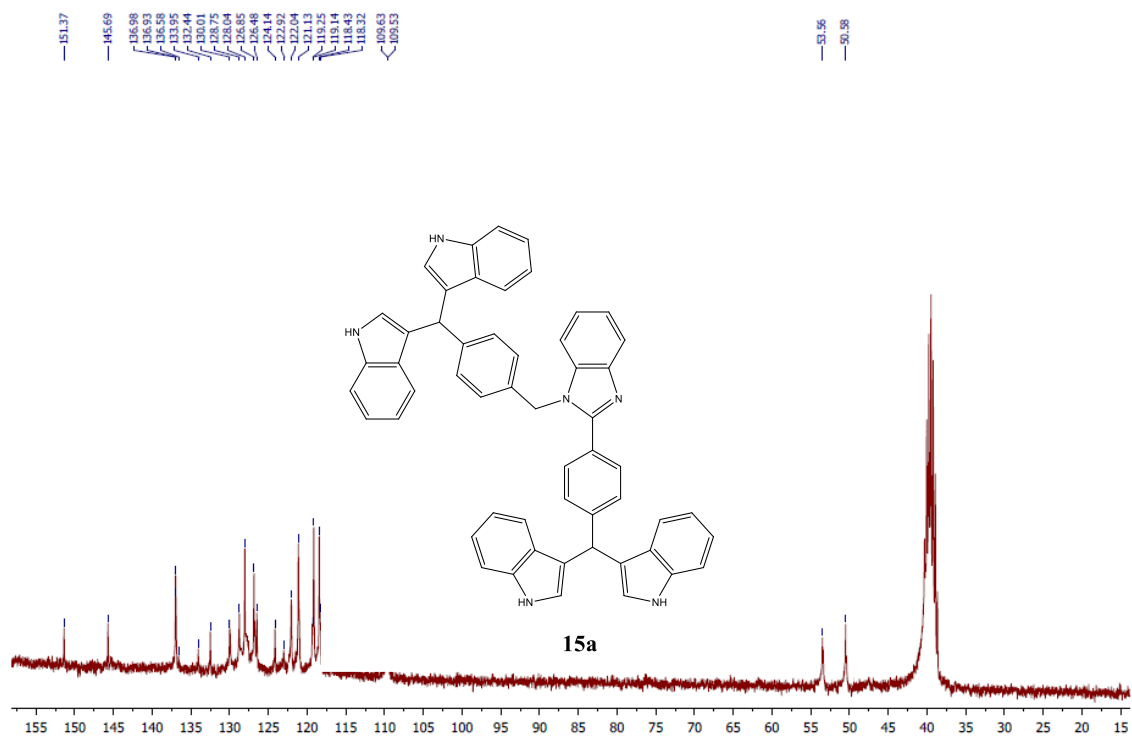
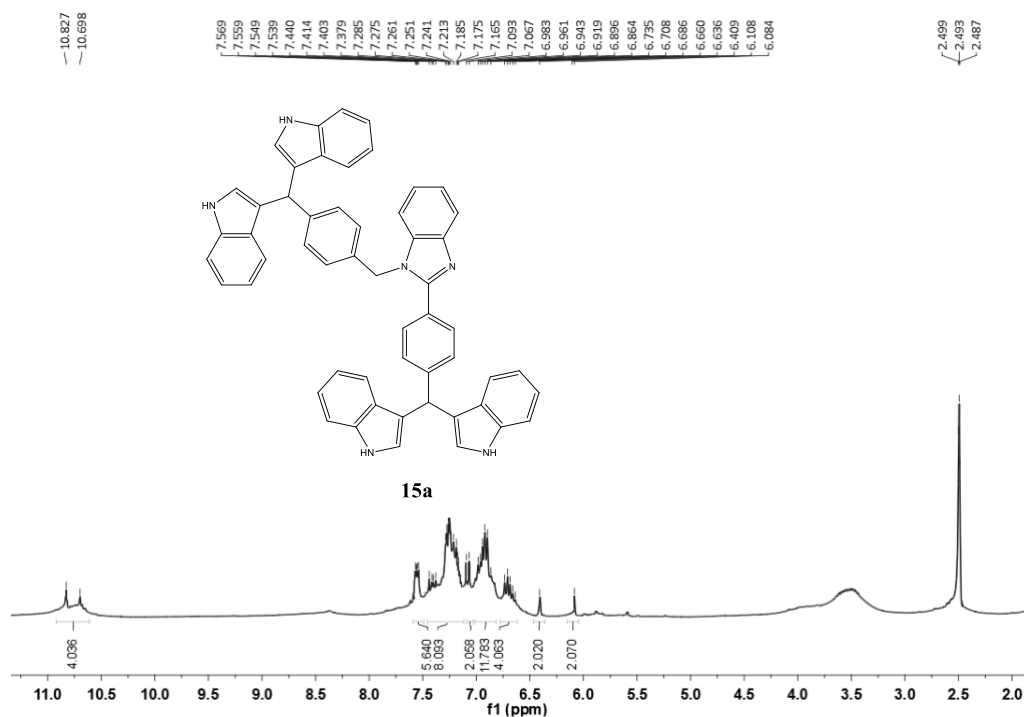


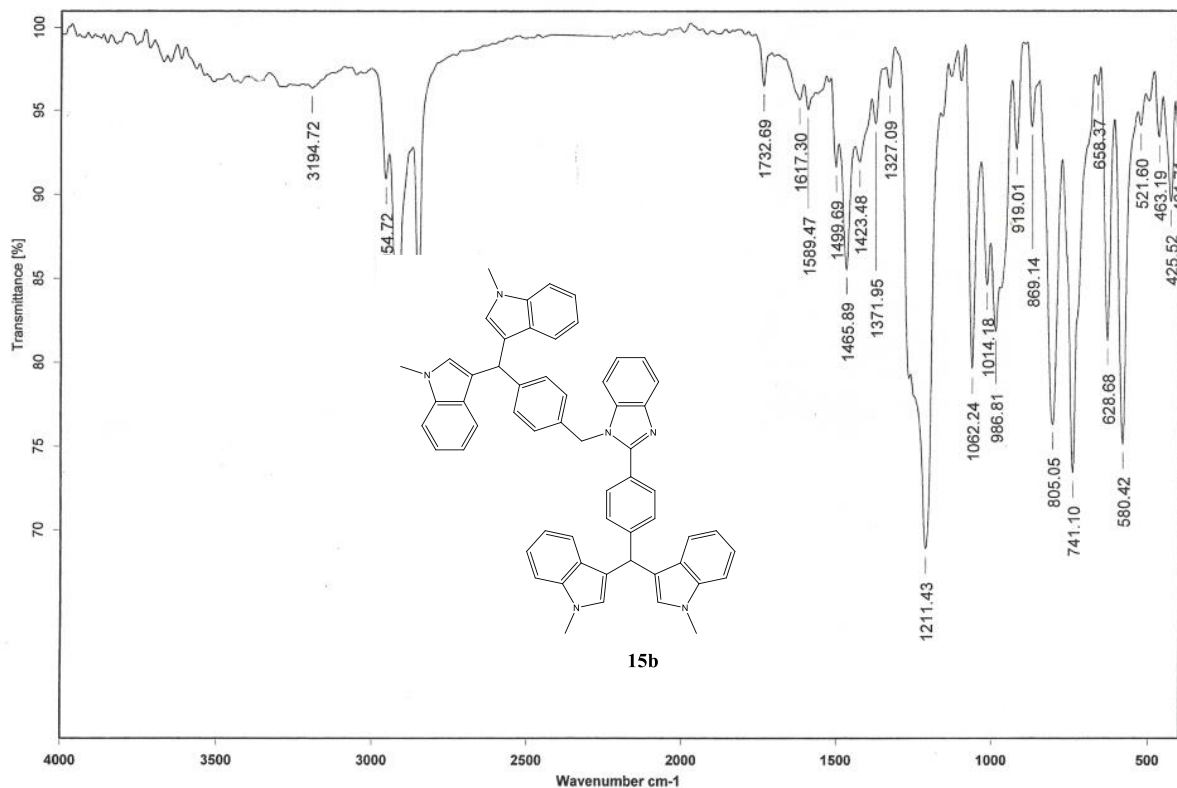
M. W. 772

 $\text{C}_{54}\text{H}_{40}\text{N}_6$

15a

	Observed m/z	Int%			
	772.33105	68.99			
	Estimated m/z	Err [ppm / mmu]	U.S.	C	H
1	772.33145	-1.7 / -0.4	38.0	54	40
					N
					6



1-{4-[Bis(1-methyl-1*H*-indol-3-yl)methyl]benzyl}-2-{4-[bis(1-methyl-1*H*-indol-3-yl)methyl]phenyl}-1*H*-benzimidazole (15b)

Instrument : MStation

Note : -

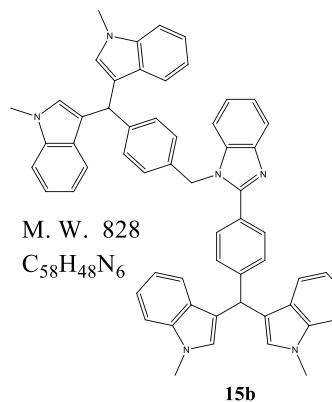
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RT : 0.90 min Scan# : (6,7)

Elements : C 60/0, H 48/0, N 6/0

Mass Tolerance : 1000ppm, 1mmu if m/z > 1

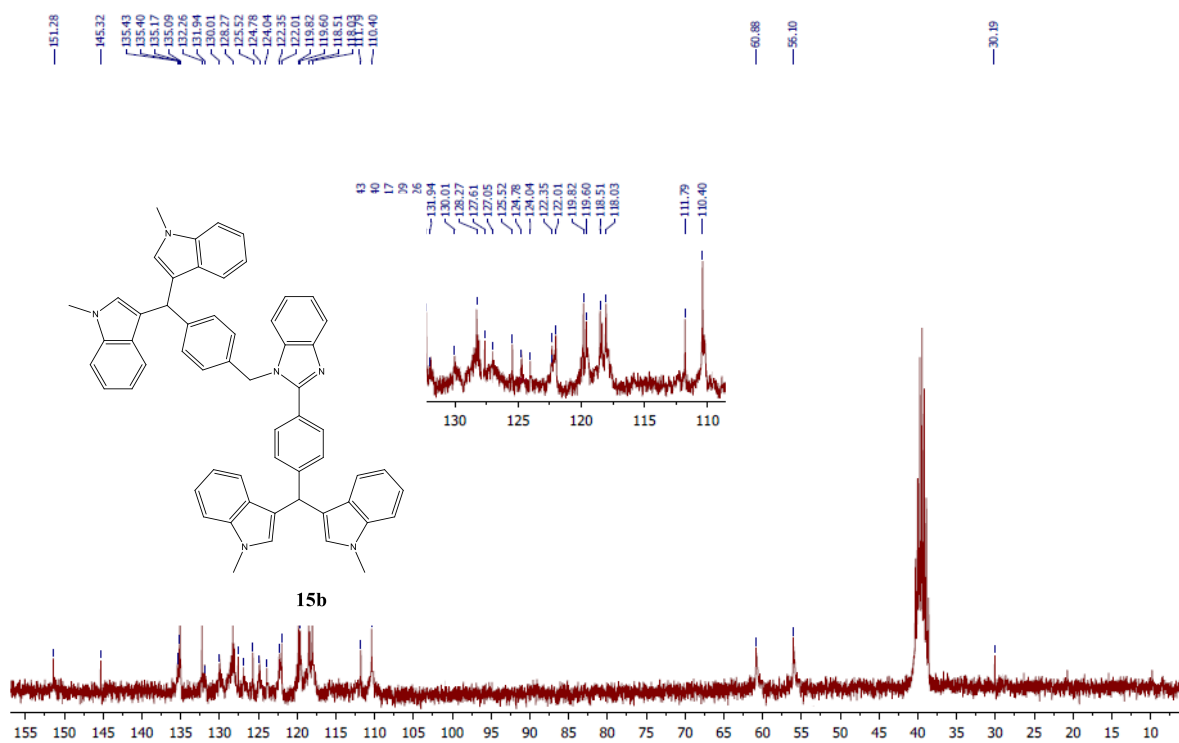
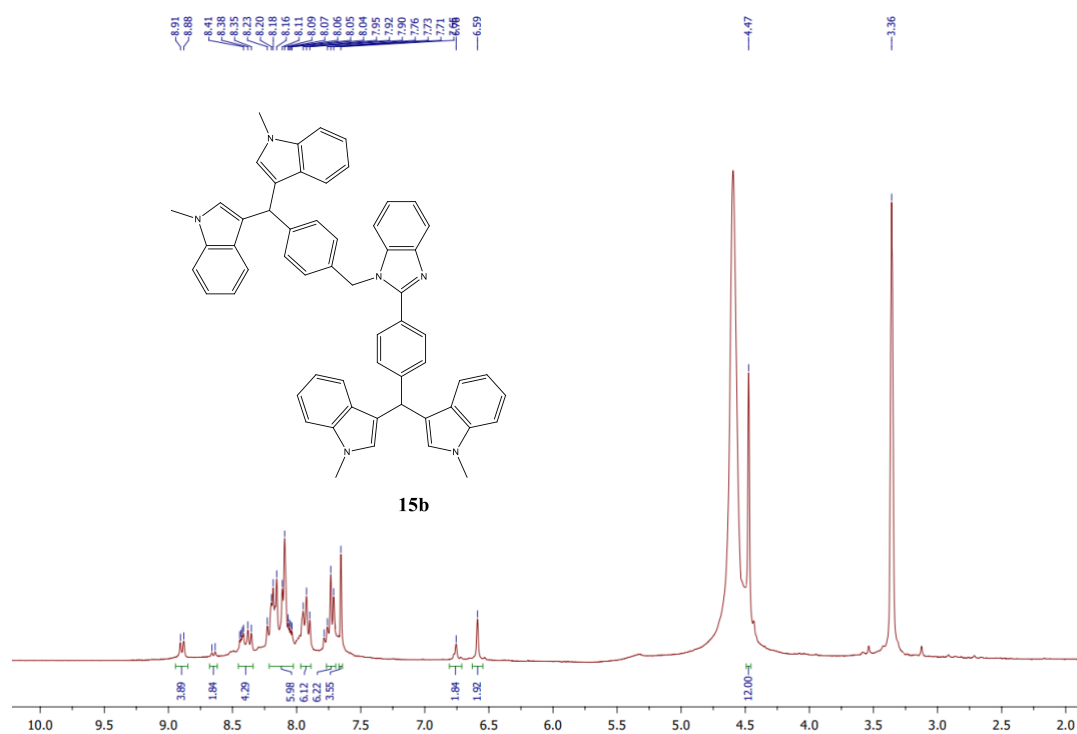
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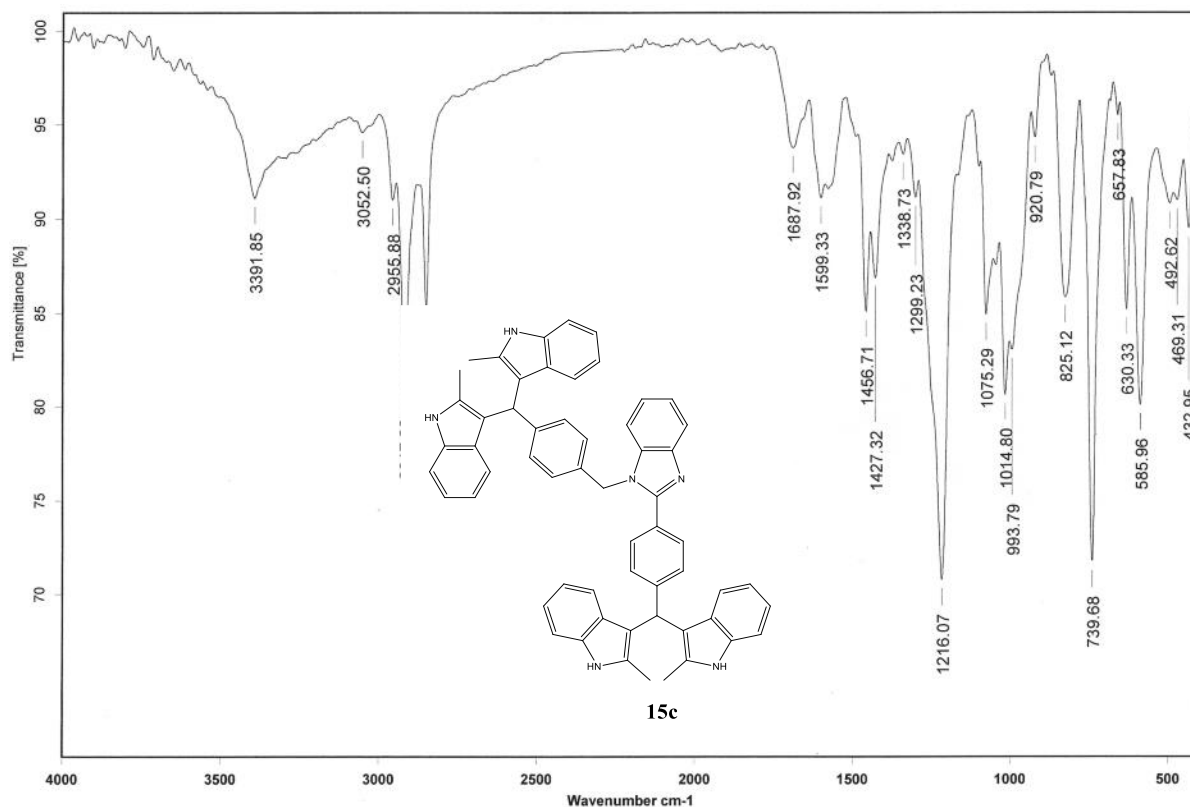


M. W. 828

C₅₈H₄₈N₆

	Observed m/z	Int %			
	828.39365	25.03			
	Estimated m/z	Err [ppm / mmu]	U.S.	C	H
1	828.39405	+0.8 / -0.4	38.5	58	48
					N
					6



1-{4-[Bis(2-methyl-1*H*-indol-3-yl)methyl]benzyl}-2-{4-[bis(2-methyl-1*H*-indol-3-yl)methyl]phenyl}-1*H*-benzimidazole (15c)

Data : para 2 me

Instrument : MStation

Note : -

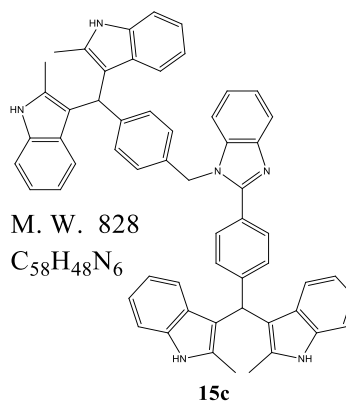
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Elements : C 60/0, H 50/0, N 6/0

Mass Tolerance : 1000ppm, 1mmu if m/z > 1

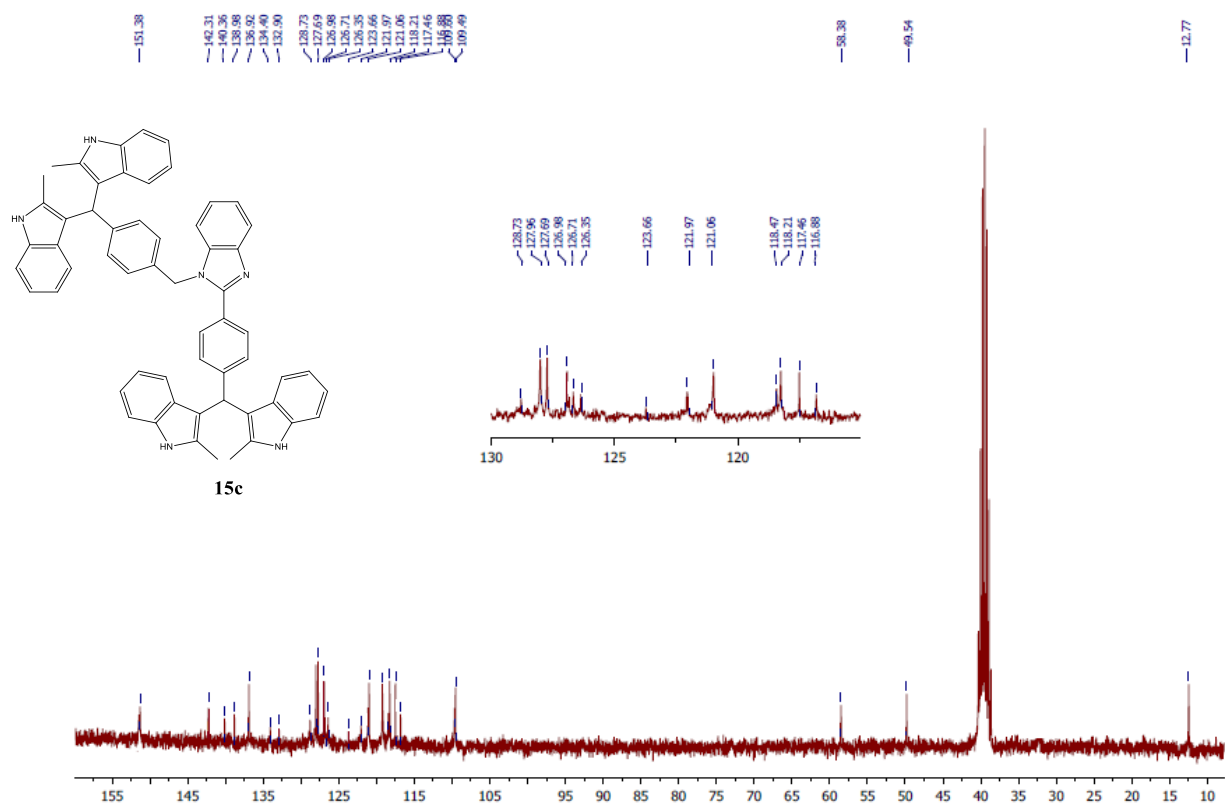
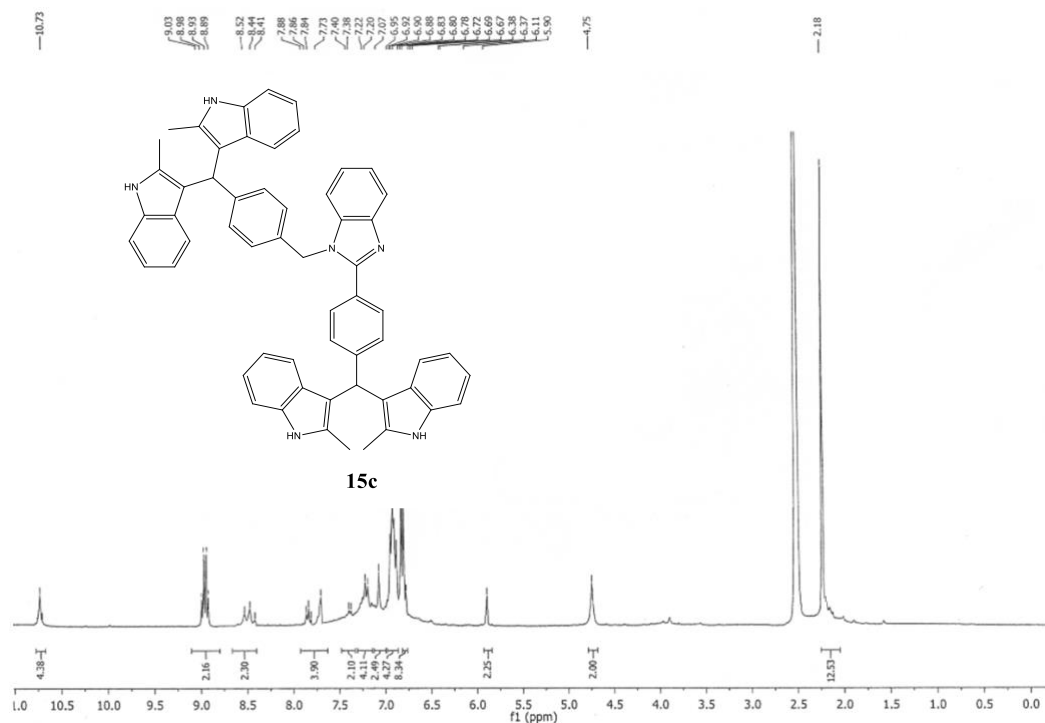
Unsaturation (U.S.) : -0.5 - 40.0

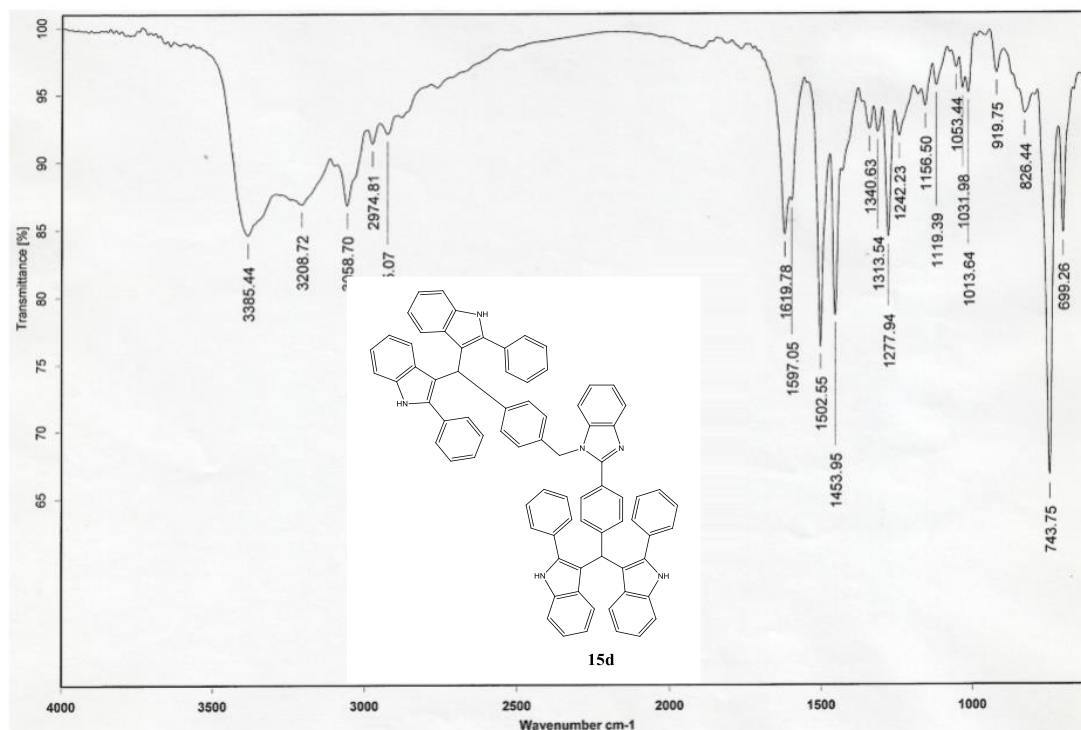


M. W. 828

C₅₈H₄₈N₆

Observed m/z	Int%				
828.39325	68.99				
Estimated m/z	Err [ppm / mmu]	U.S.	C	H	N
1 828.39405	-1.7 / -0.8	38.5	58	48	6



1-{4-[Bis(2-phenyl-1*H*-indol-3-yl)methyl]benzyl}-2-{4-[bis(2-phenyl-1*H*-indol-3-yl)methyl]phenyl}-1*H*-benzimidazole (15d)

Data : para 2ph

Instrument : MStation

Note : -

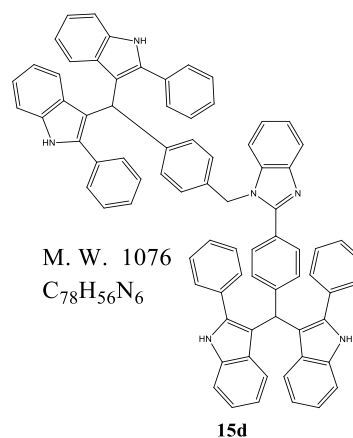
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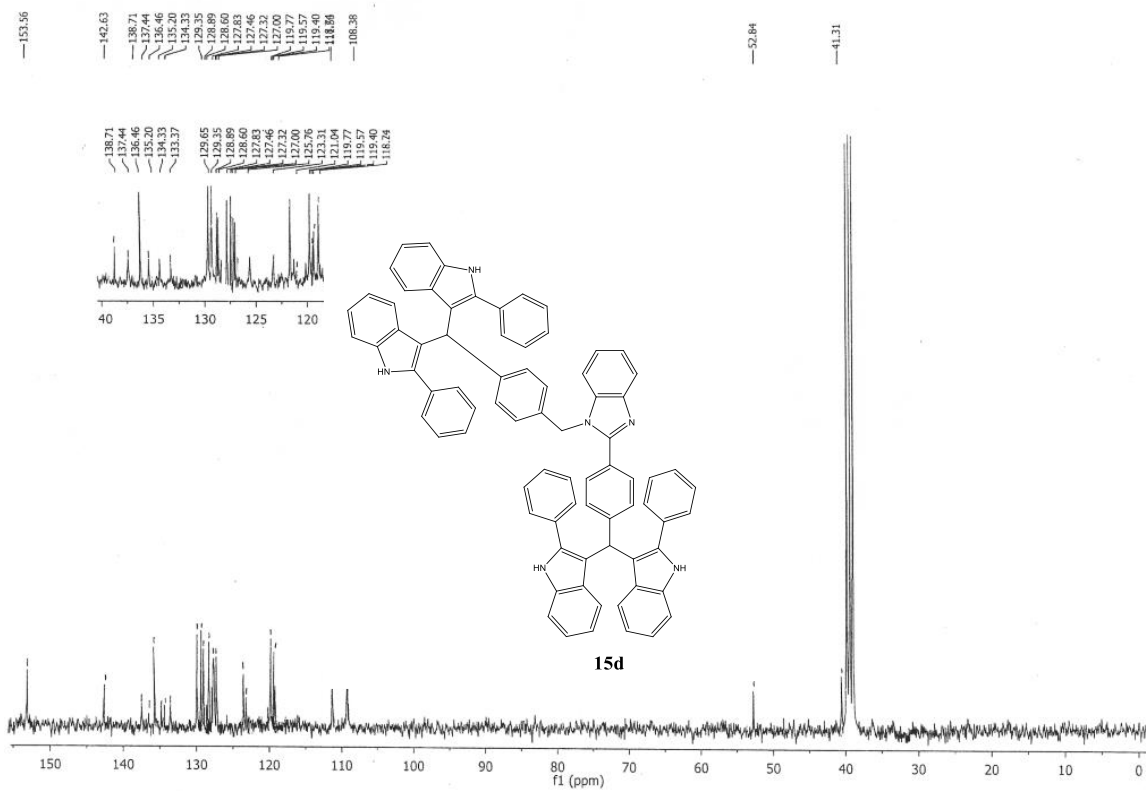
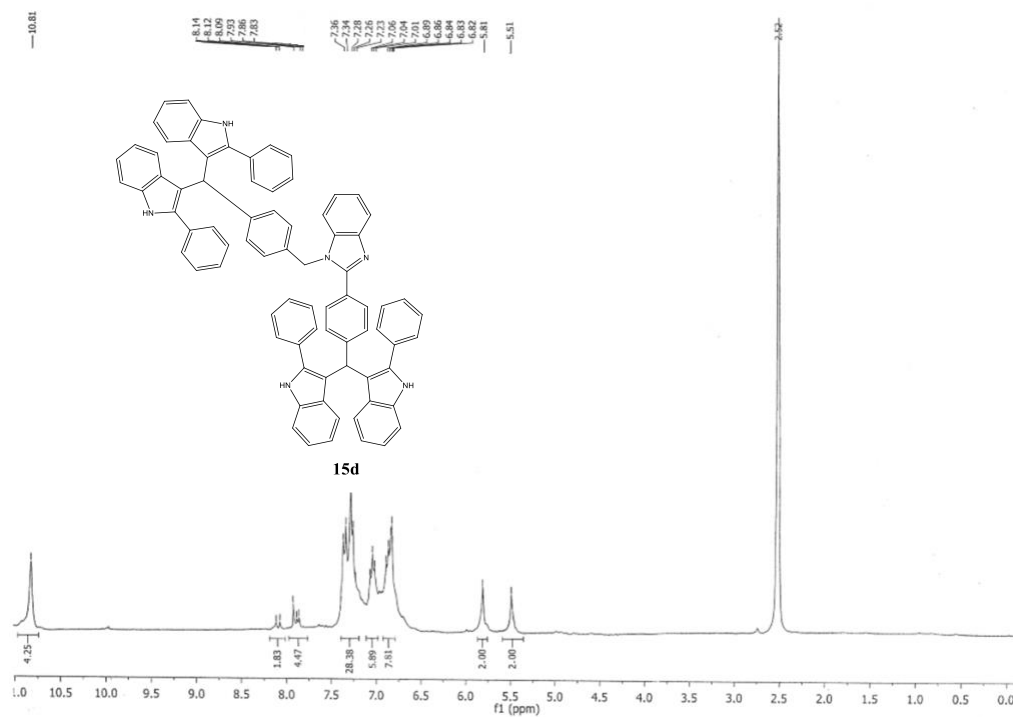
Elements : C 80/0, H 60/0, N 6/0

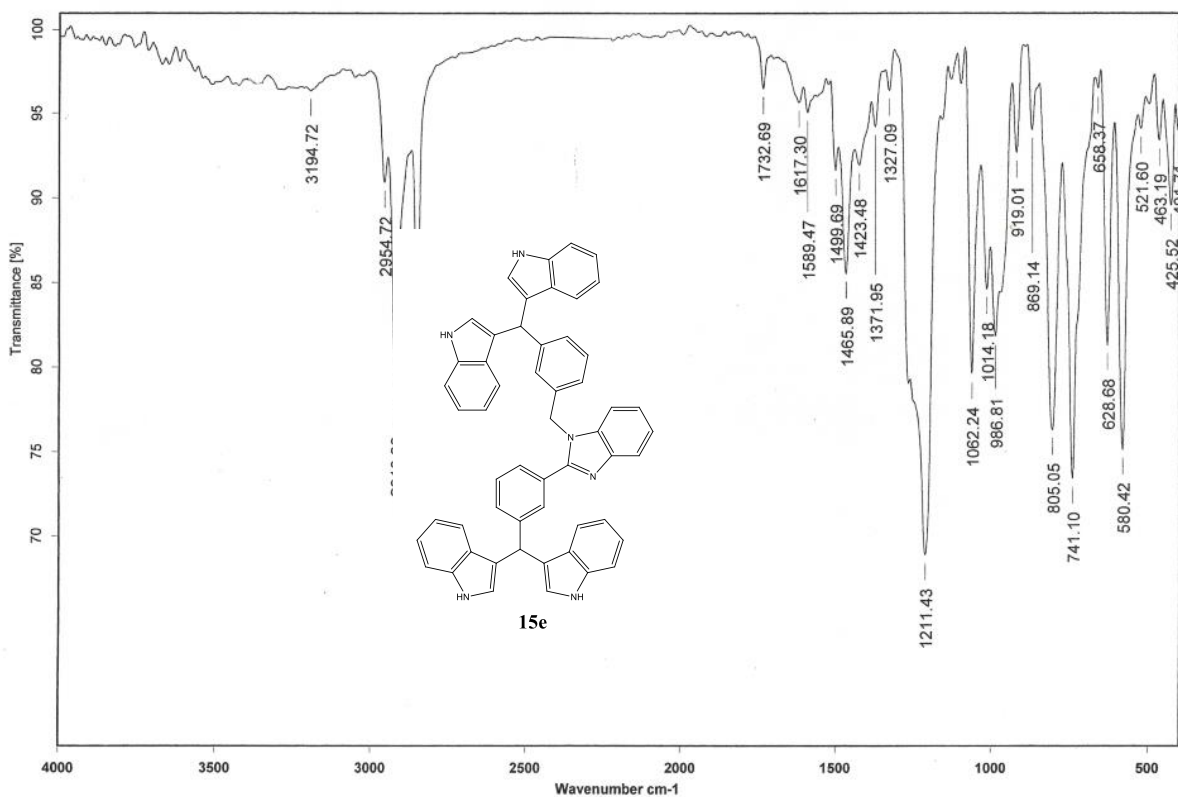
Mass Tolerance : 1000ppm, 1mmu if m/z > 1

Unsaturation (U.S.) : -0.5 - 60.0



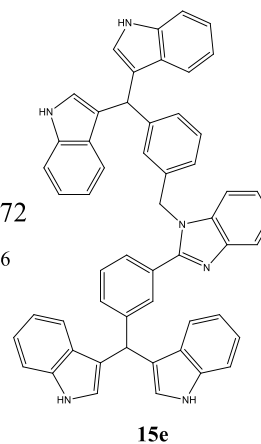
Observed m/z		Int %				
1076.45705		68.99				
Estimated m/z		Err [ppm / mmu]	U.S.	C	H	N
1	1076.45665	-1.5 / 0.4	54.5	78	56	6



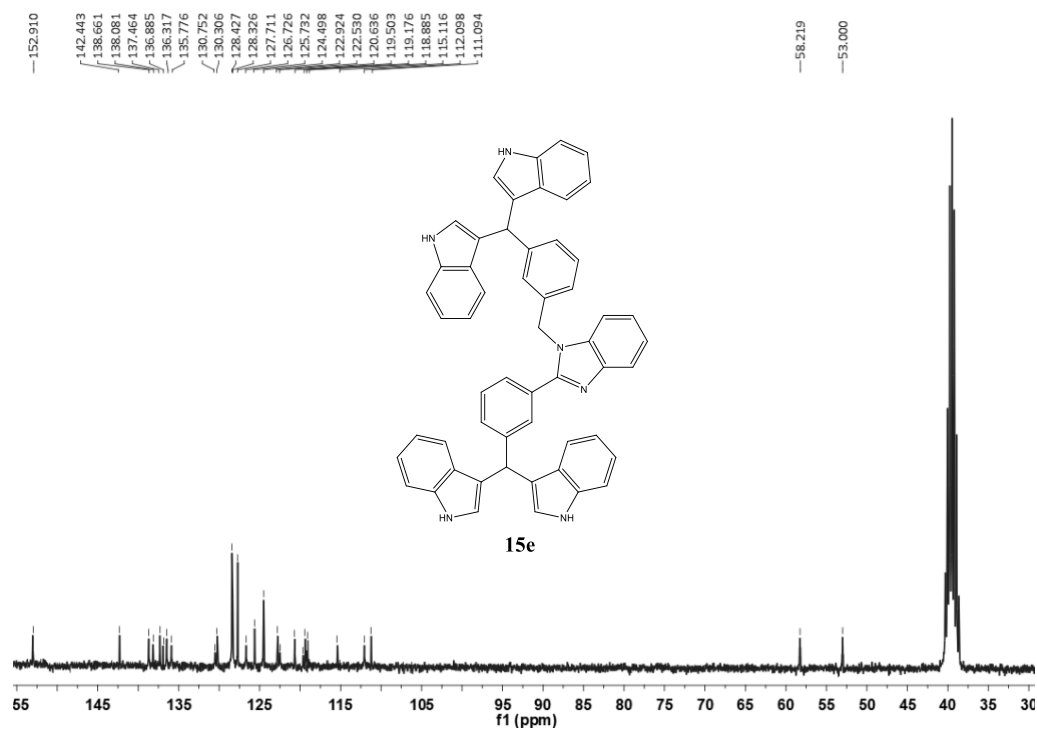
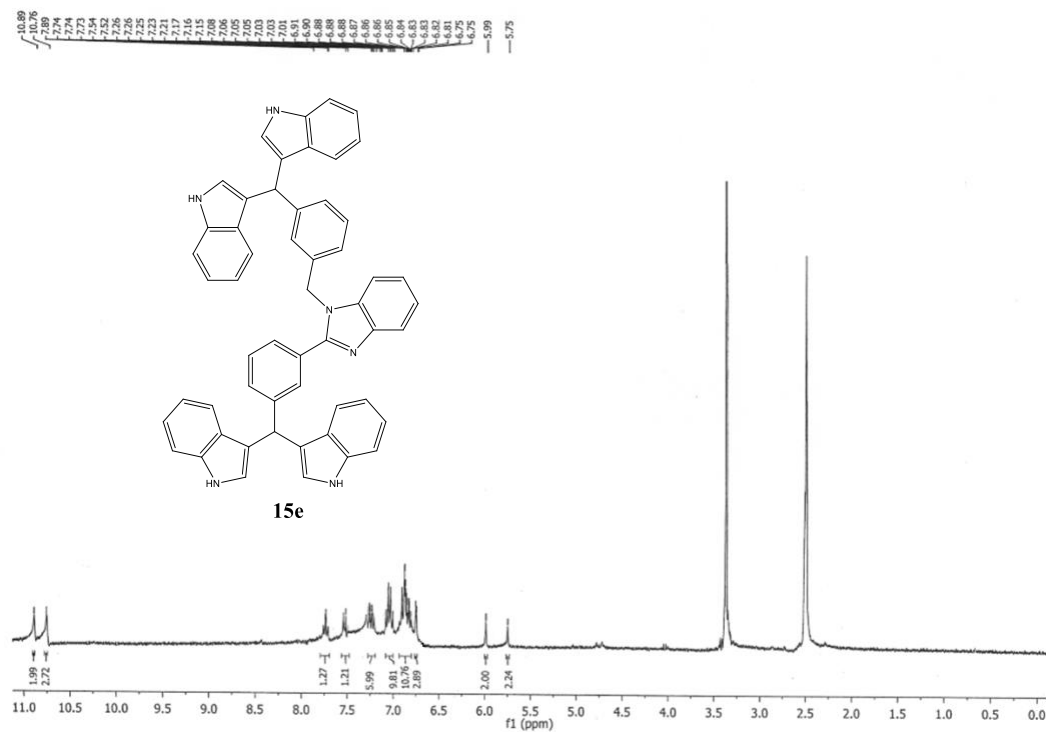
1-{3-[Bis(1*H*-indol-3-yl)methyl]benzyl}-2-{3-[bis(1*H*-indol-3-yl)methyl]phenyl}-1*H*-benzimidazole (15e)

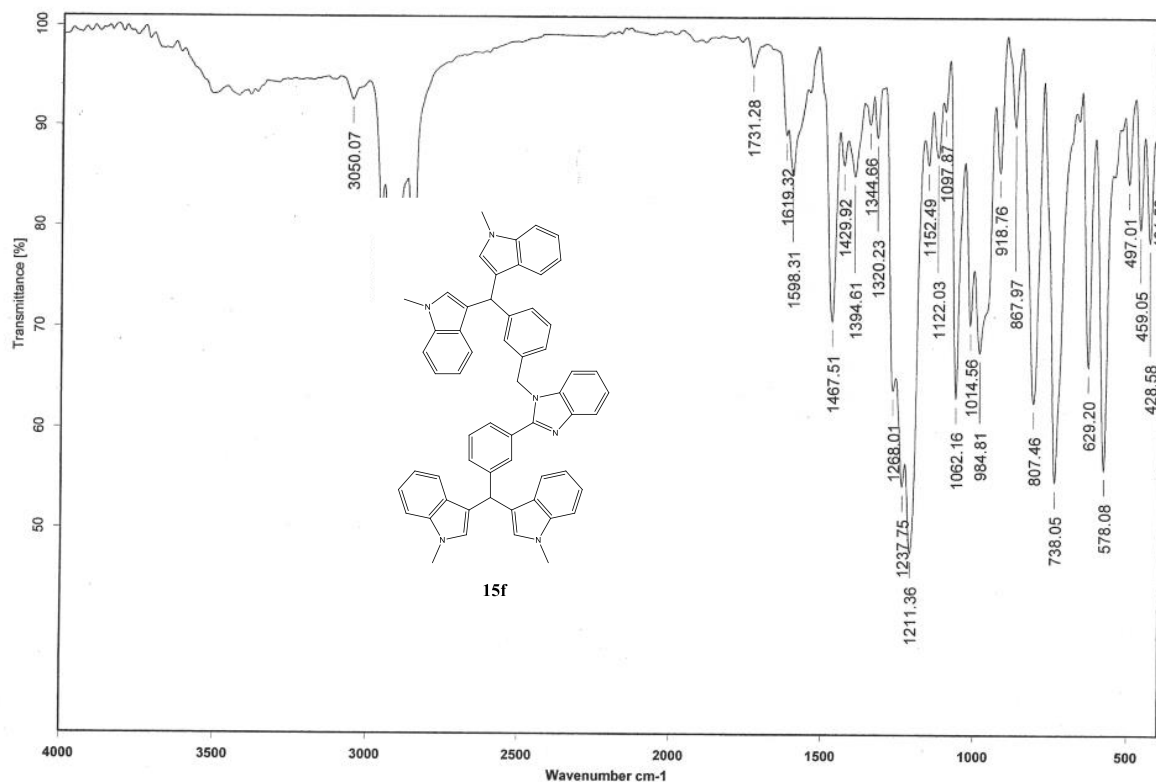
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 Elements : C 60/0, H 49/0, N 6/0
 Mass Tolerance : 1000ppm, 2mmu if m/z > 2
 Unsaturation (U.S.) : -0.5 - 40.0

M. W. 772
 $C_{54}H_{40}N_6$



	Observed m/z	Int%	Estimated m/z	Err [ppm / m/z]					N
	772.33095	2.32							
1	772.33145	-2.2 / -0.5	38.0	54	40	6			



1-{3-[Bis(1-methyl-1*H*-indol-3-yl)methyl]benzyl}-2-{3-[bis(1-methyl-1*H*-indol-3-yl)methyl]phenyl}-1*H*-benzimidazole (15f)

Note : -

Inlet : Direct Ion Mode : FA

RT : 0.85 min Scan# : (6,7)

Elements : C 60/0, H 49/0, N 6/0

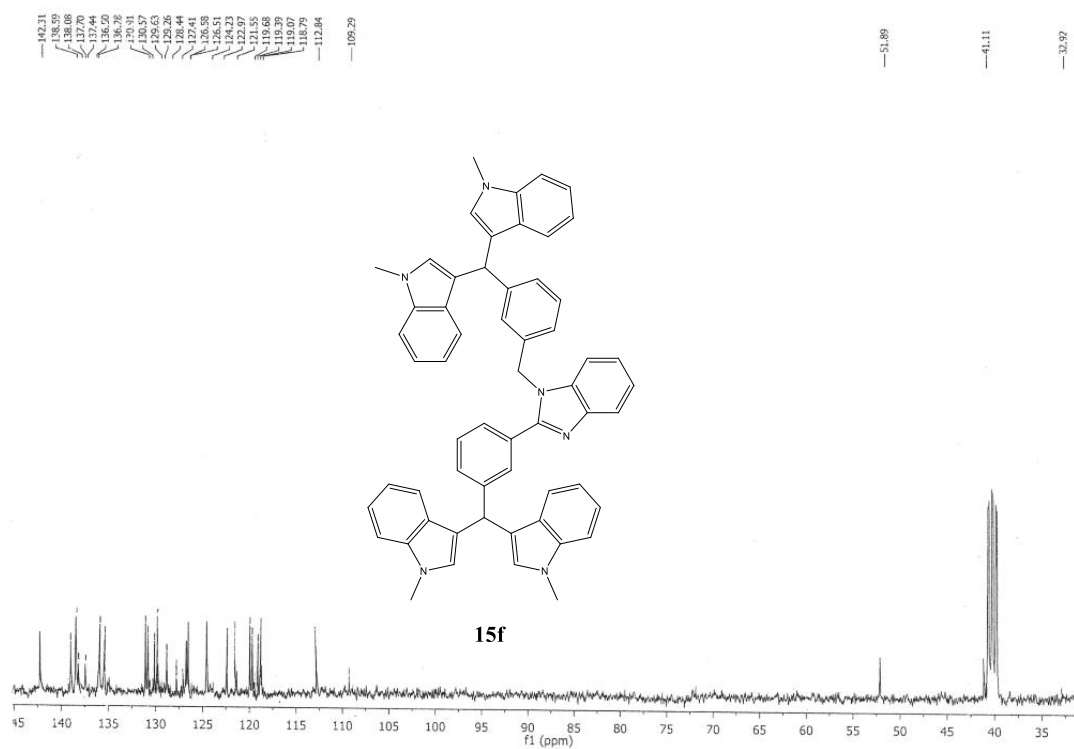
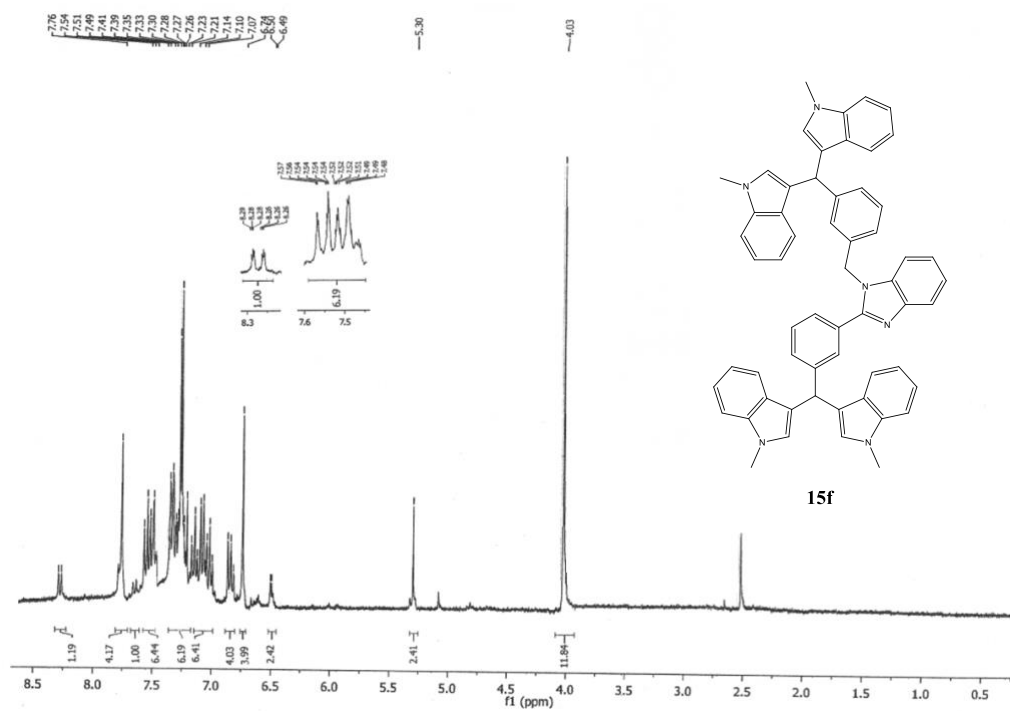
Mass Tolerance : 1000ppm, 1mmu if m/z > 1

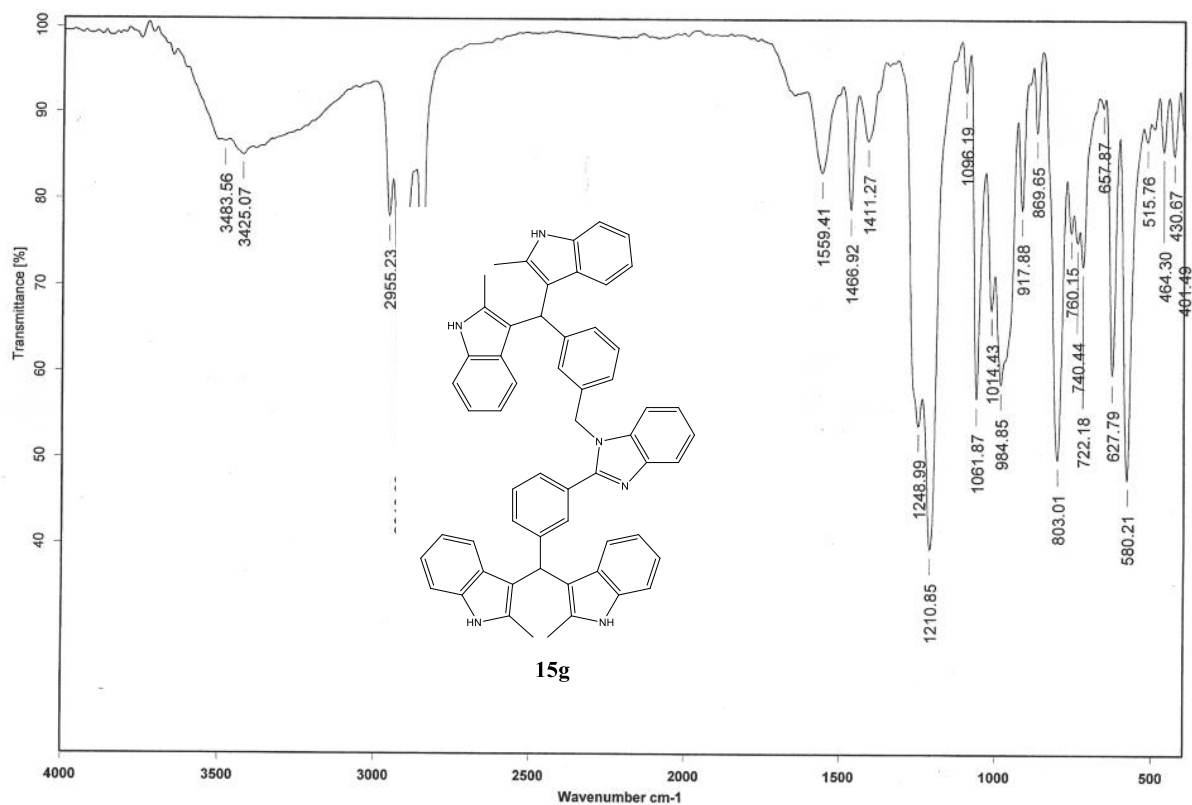
Unsaturation (U.S.) : -0.5 - 45.0

M. W. 828

C₅₈H₄₈N₆

Observed m/z	Int%						
828.39319	25.03						
Estimated m/z	Err [ppm /	15f				H	N
1 828.39405	+0.8 / -0.8	38.5	58		48	6	



1-{3-[Bis(2-methyl-1*H*-indol-3-yl)methyl]benzyl}-2-{3-[bis(2-methyl-1*H*-indol-3-yl)methyl]phenyl}-1*H*-benzimidazole (15g)

Data : meta 2 me

Instrument : MStation

Note : -

Inlet : Direct Ion Mode : FAB+

RT : 3.27 min Scan# : (26,48)

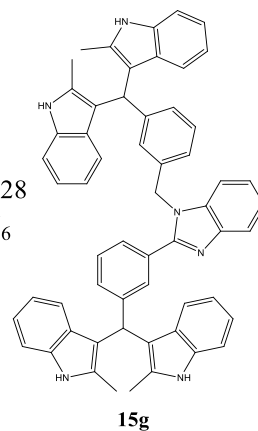
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Mass Tolerance : 1000ppm, 1mmu if m/z > 1

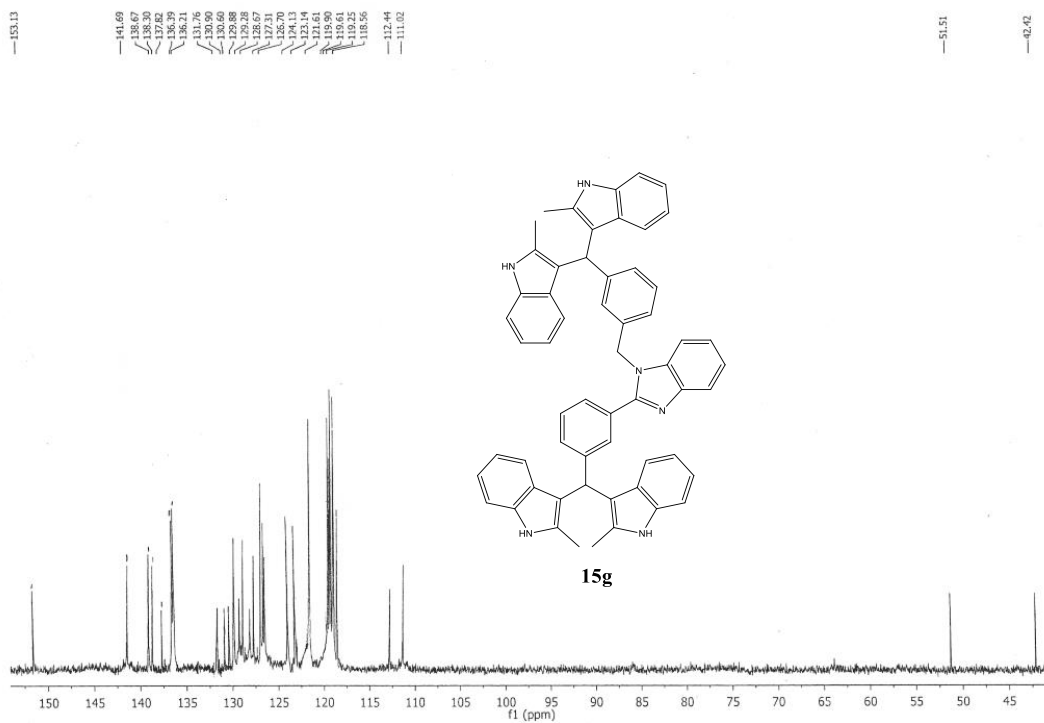
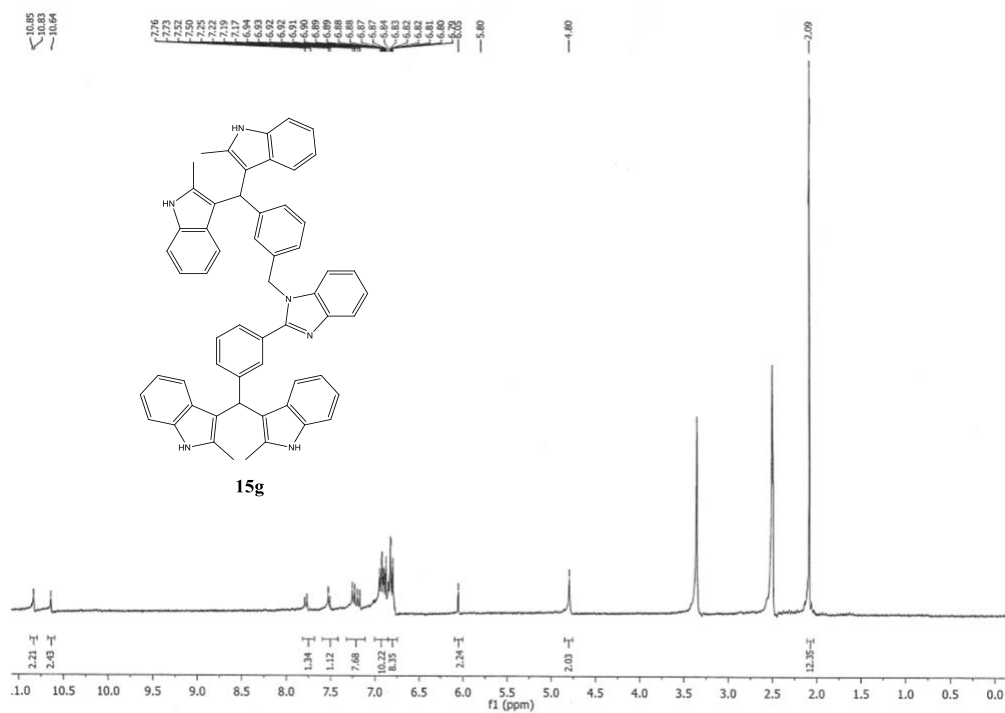
Unsaturation (U.S.) : -0.5 - 40.0

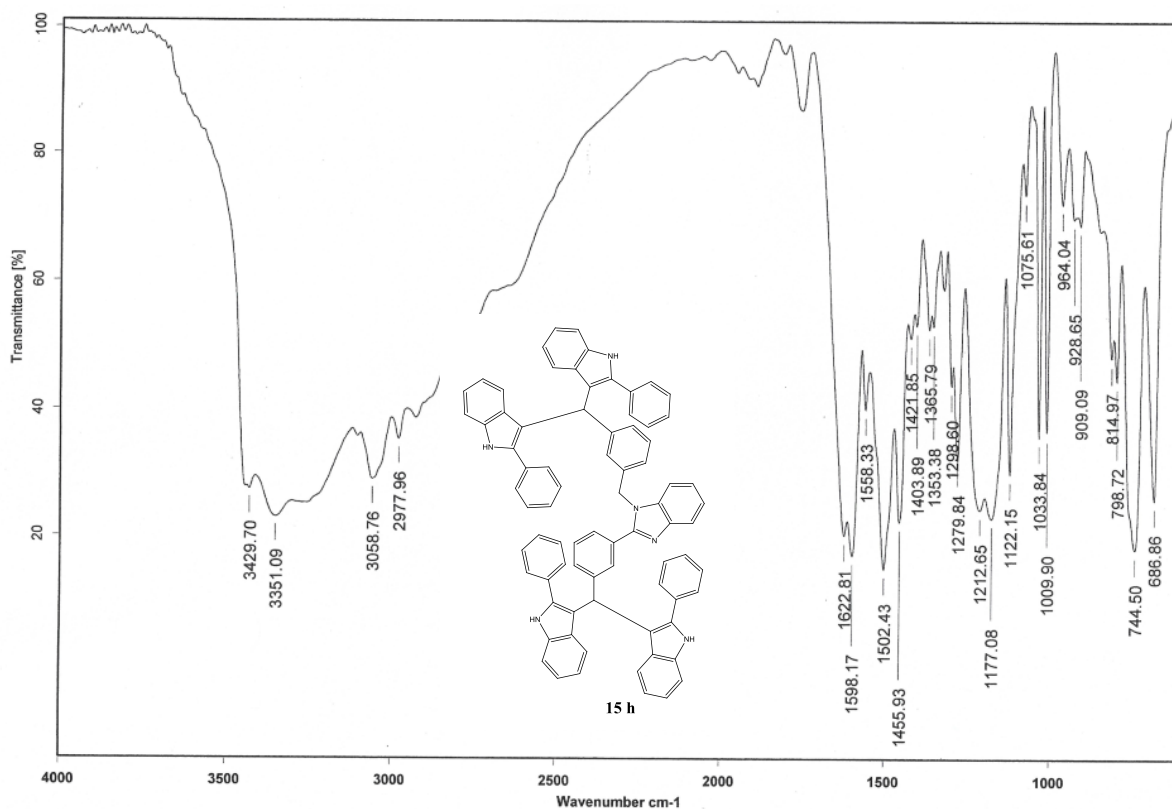
7

M. W. 828

C₅₈H₄₈N₆

	Observed m/z	Int %			
	828.39345	58.99			
	Estimated m/z	Err [ppm / mmu]	U.S.	C	H
1	828.39405	-1.6 / -0.6	38.5	58	48
					N
					6



1-{3-[Bis(2-phenyl-1*H*-indol-3-yl)methyl]benzyl}-2-{3-[bis(2-phenyl-1*H*-indol-3-yl)methyl]phenyl}-1*H*-benzimidazole (15h)

Data : meta 2ph

Instrument : MStation

Note : -

Inlet : Direct Ion Mode : FAB+

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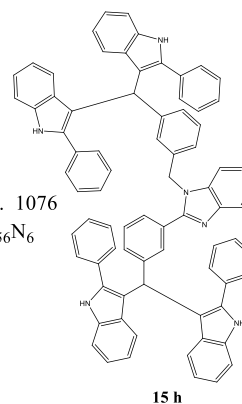
Elements : C 80/0, H 60/0, N 6/0

Mass Tolerance : 1000ppm, 1mmu if m/z > 1

Unsaturation (U.S.) : -0.5 - 60.0

1:

M. W. 1076

C₇₈H₅₆N₆

15 h

	Observed m/z	Int %				
	1076.45715	25.03				
	Estimated m/z	Err [ppm / mmu]	U. S.	C	H	N
1	1076.45665	+0.8 / +0.5	54.5	78	56	6

