

Supplementary Material

Synthesis of 4-Alkyl-4*H*-1,2,4-triazole Derivatives by Suzuki Cross-coupling Reactions and Their Luminescence Properties

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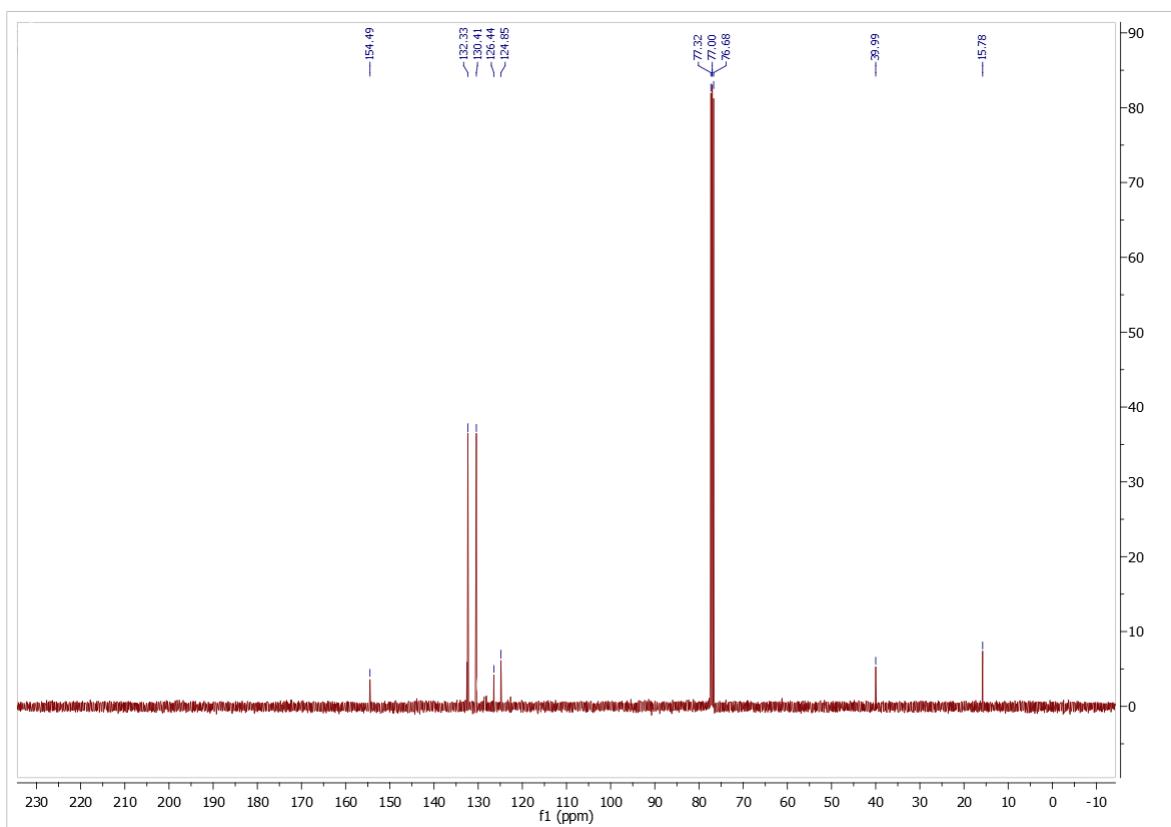
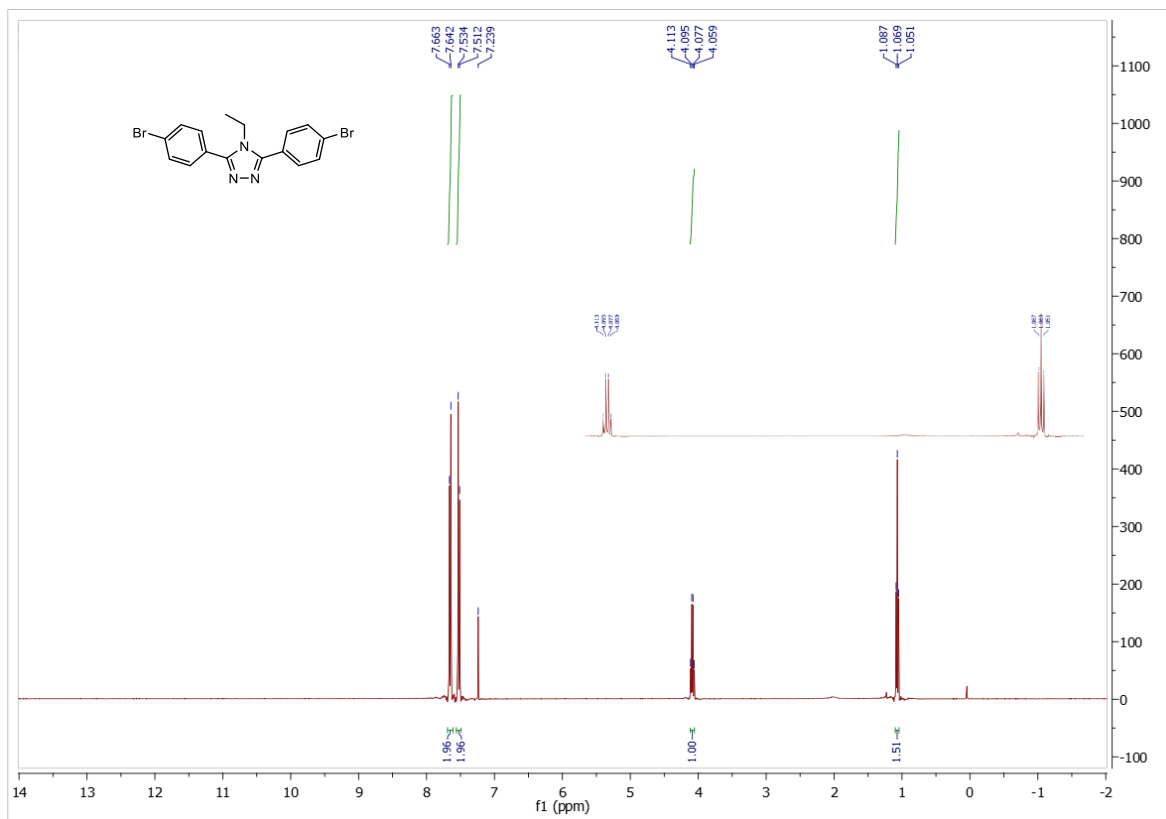
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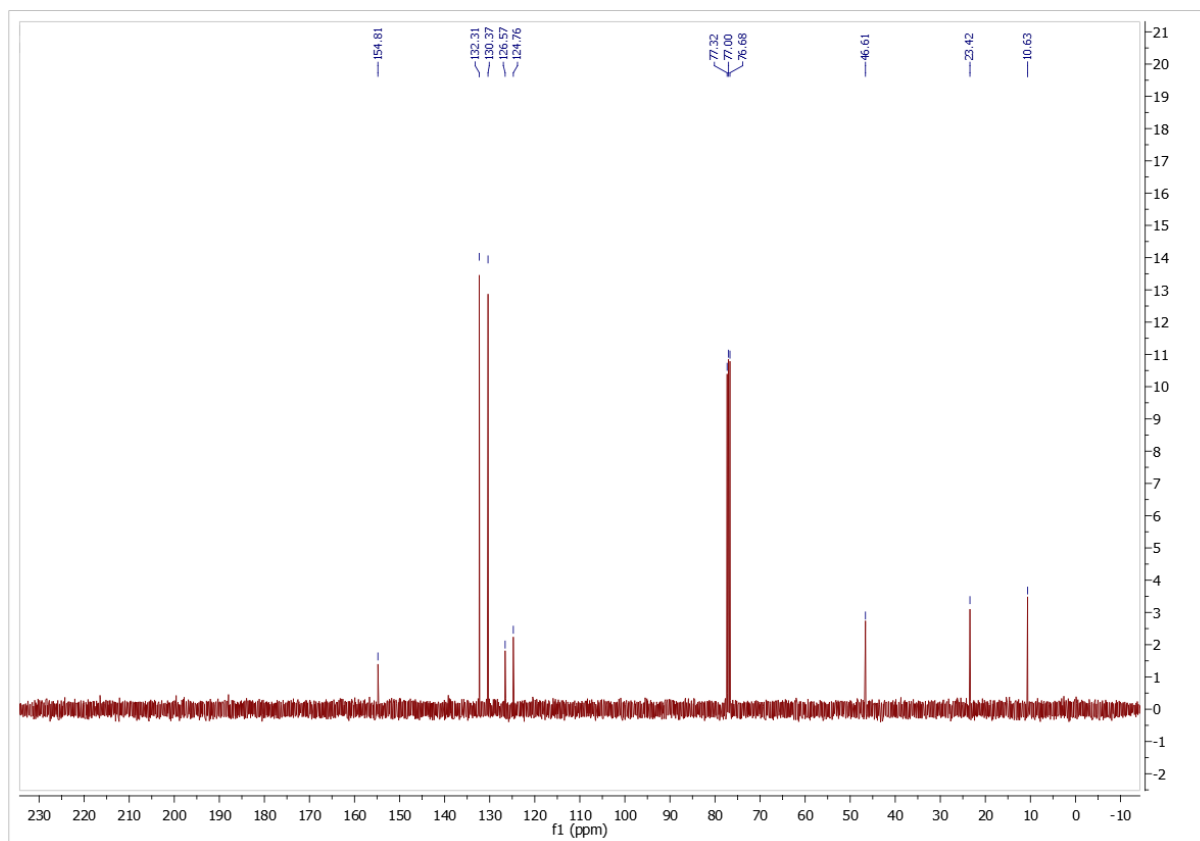
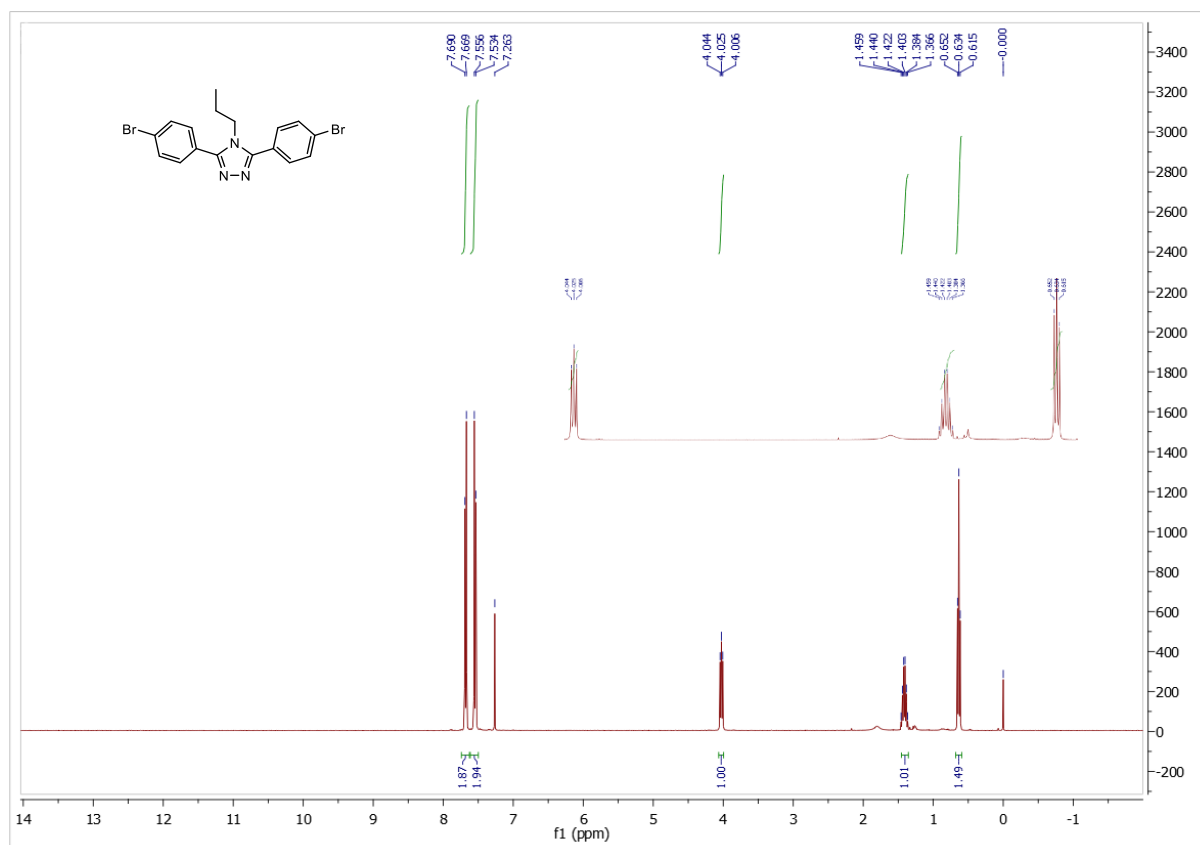
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1. ^1H NMR and ^{13}C NMR spectra of compounds

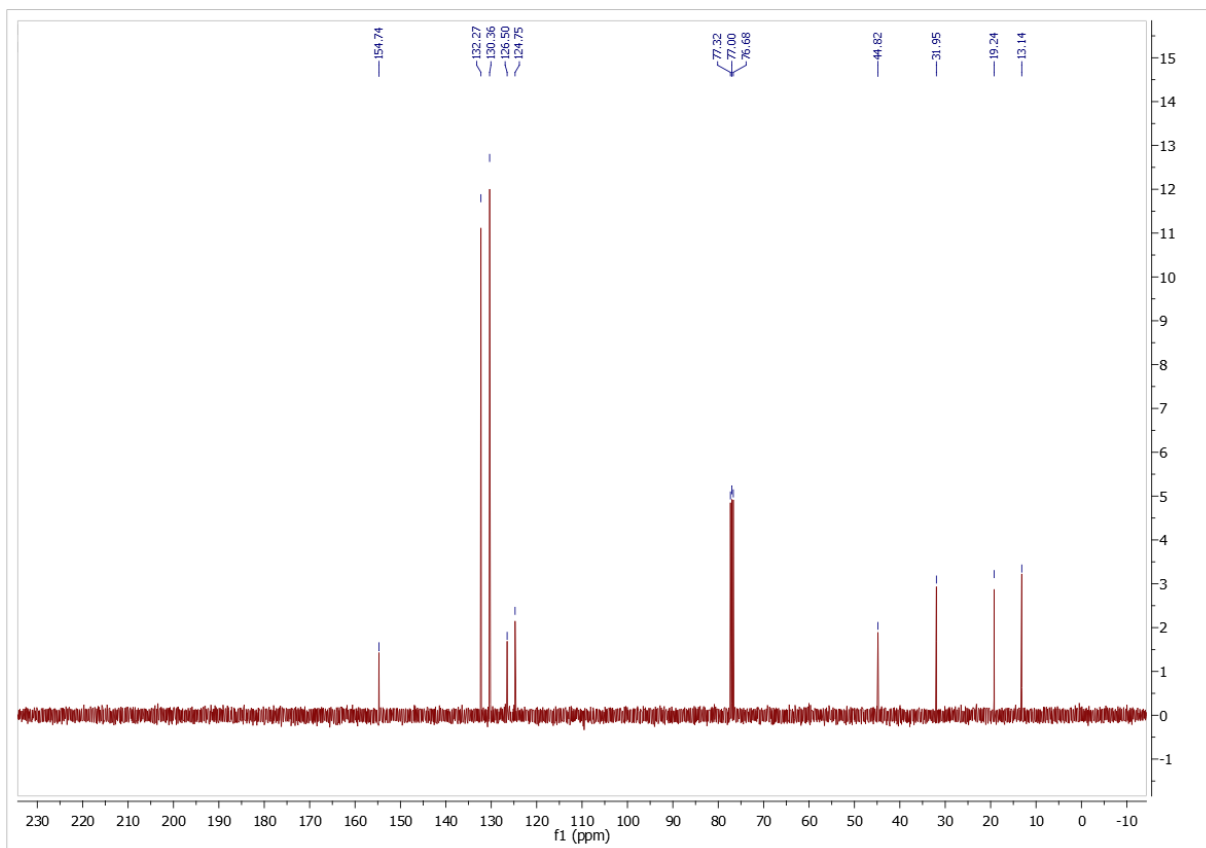
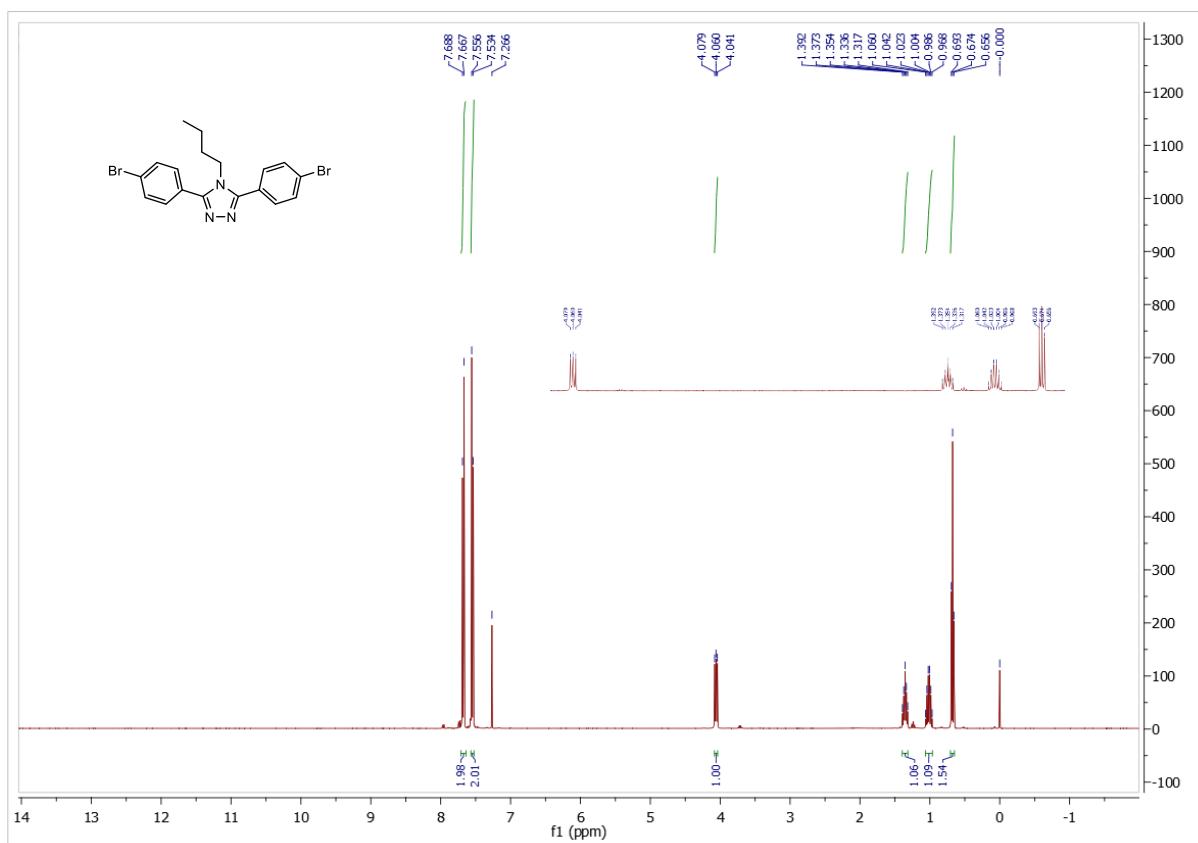
^1H and ^{13}C NMR of 3,5-bis(4-bromophenyl)-4-ethyl-4*H*-1,2,4-triazole (**3a**)



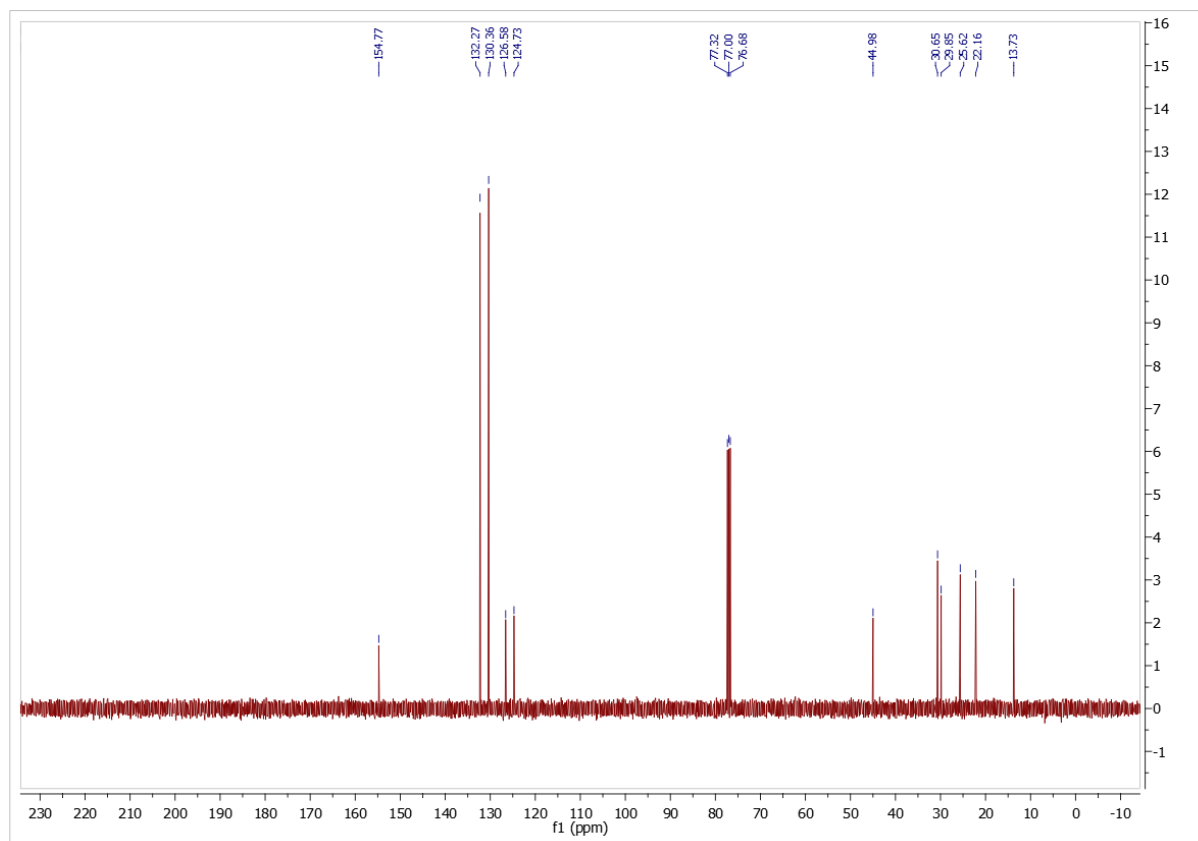
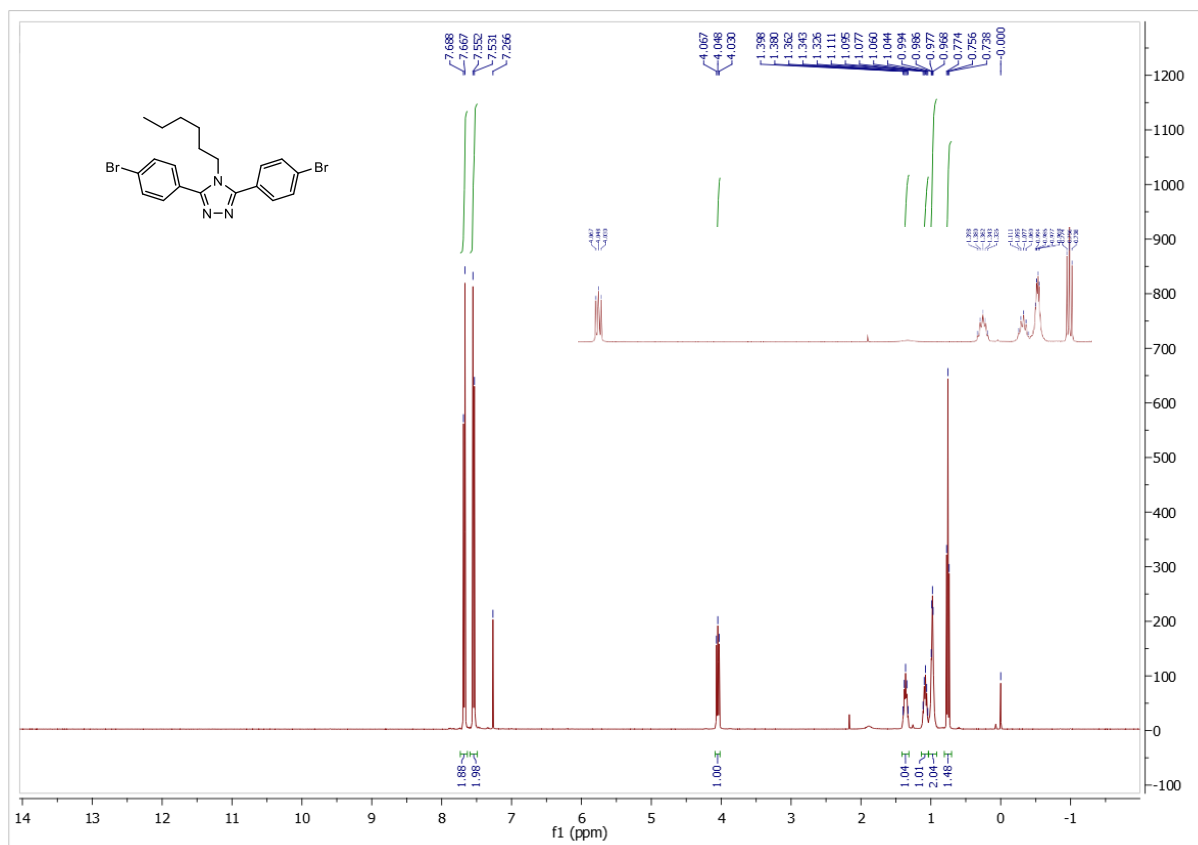
^1H and ^{13}C NMR of 3,5-bis(4-bromophenyl)-4-propyl-4*H*-1,2,4-triazole (**3b**)



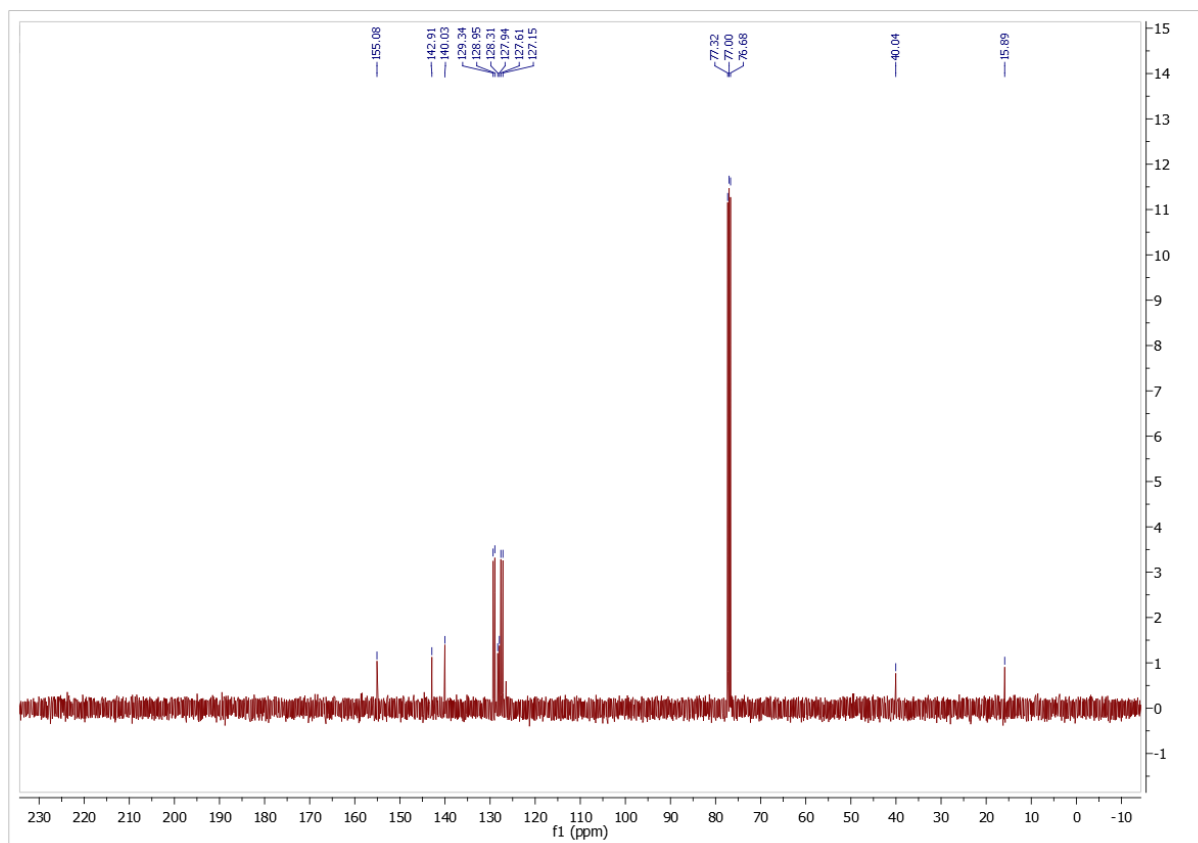
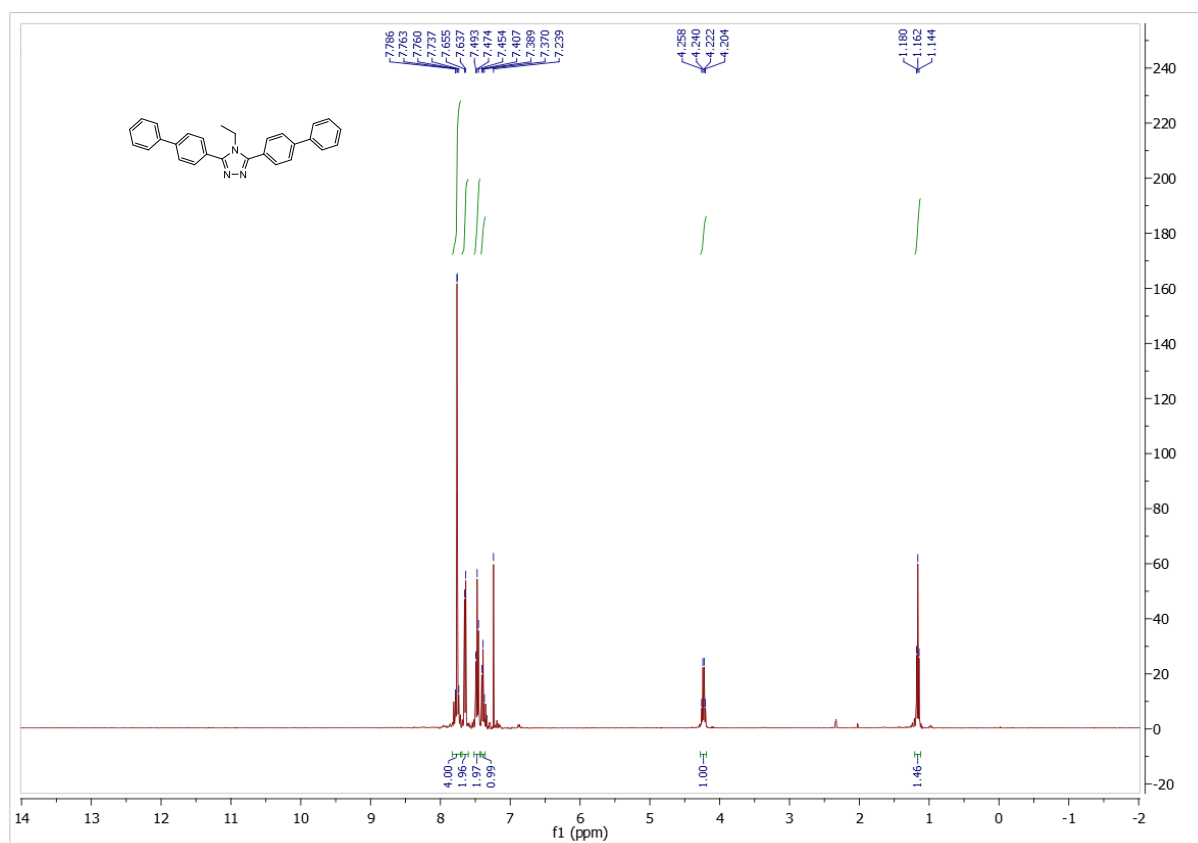
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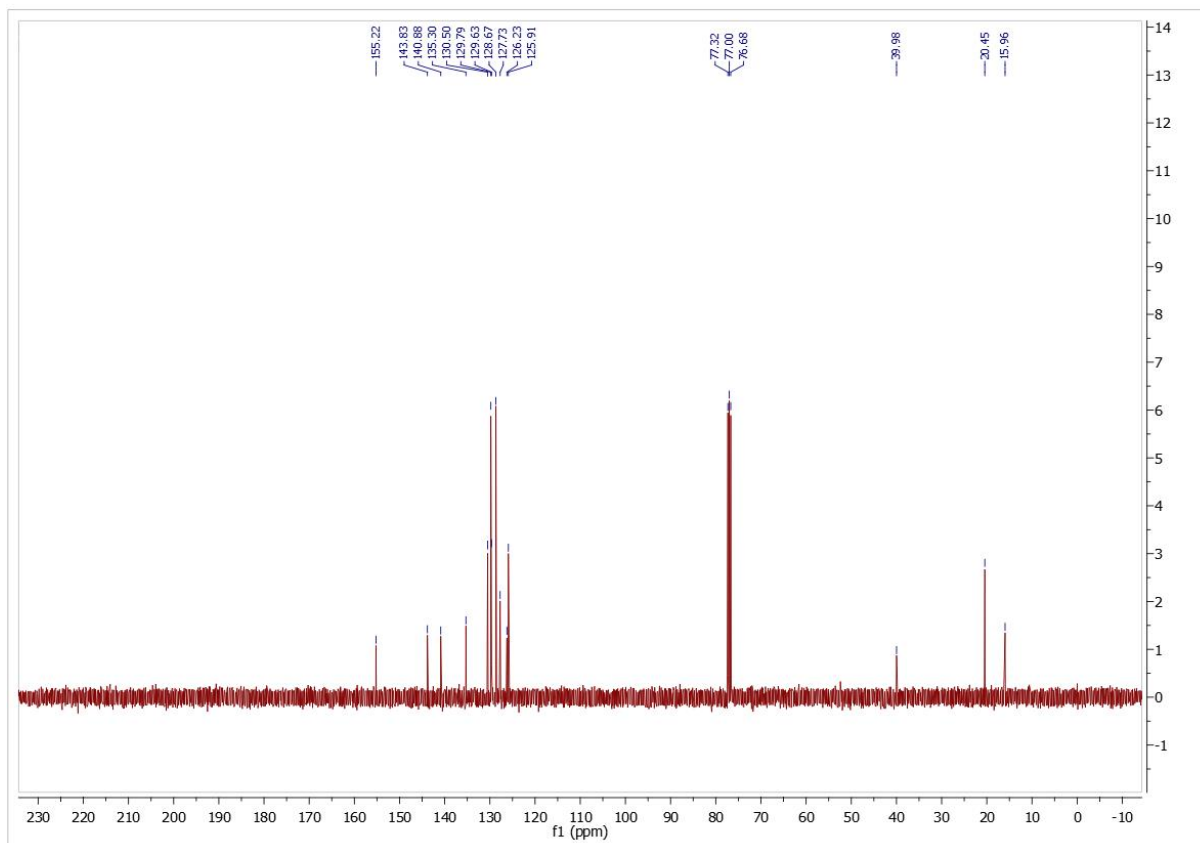
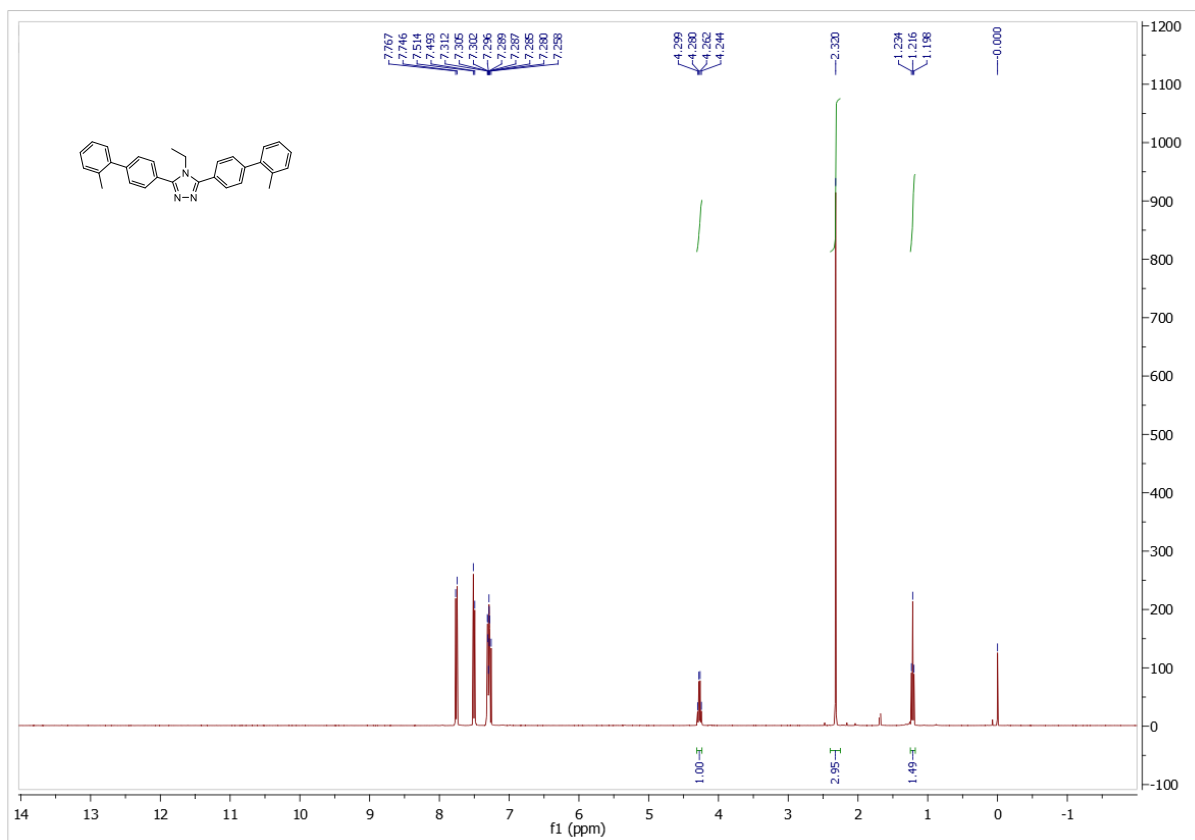
^1H and ^{13}C NMR of 3,5-bis(4-bromophenyl)-4-hexyl-4*H*-1,2,4-triazole (**3d**)



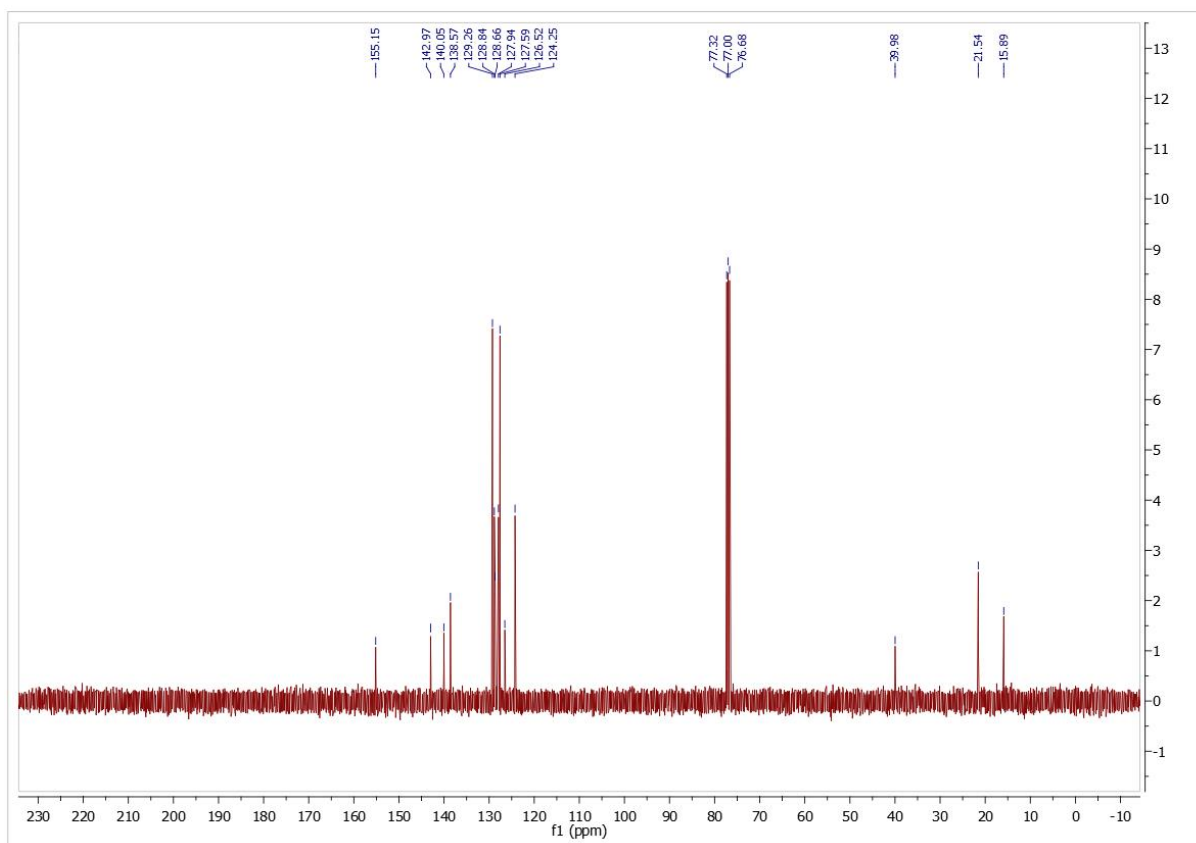
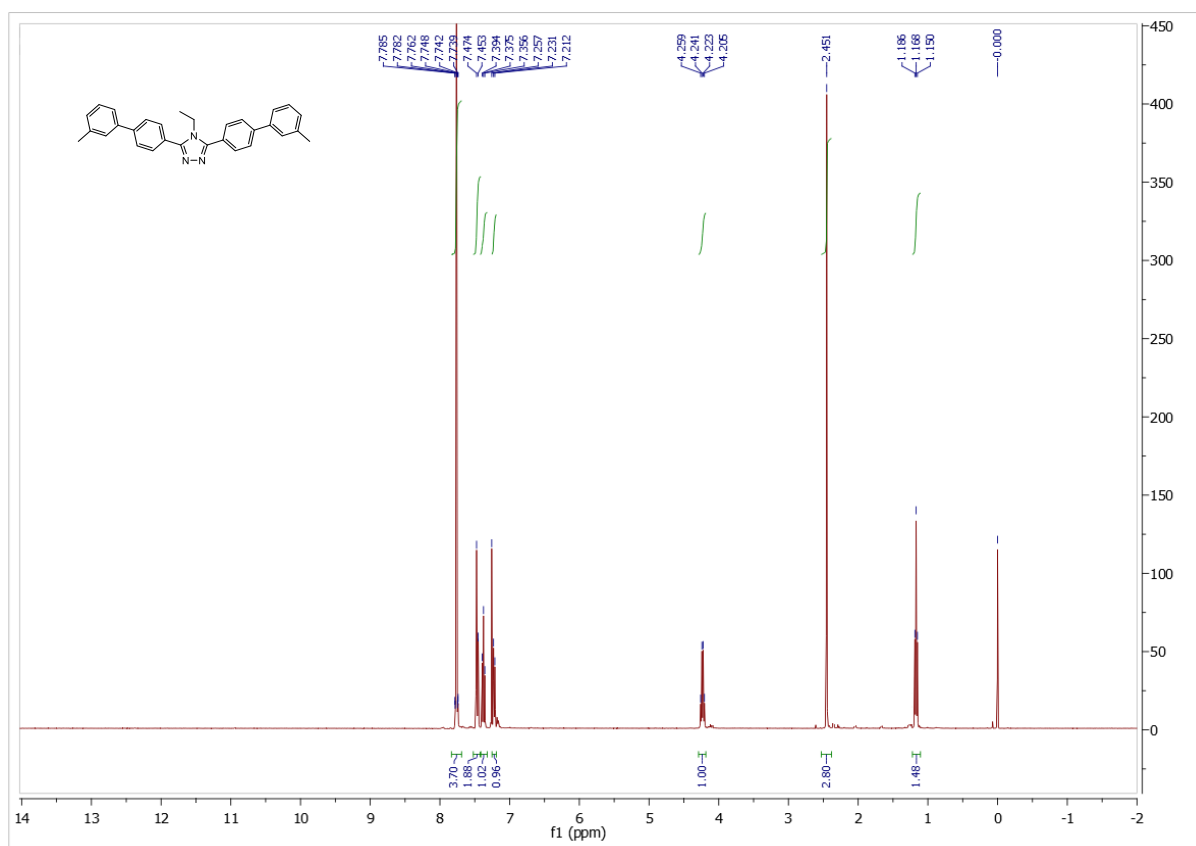
^1H and ^{13}C NMR of 3,5-bis(biphenyl-4-yl)-4-ethyl-4*H*-1,2,4-triazole (**5a**)



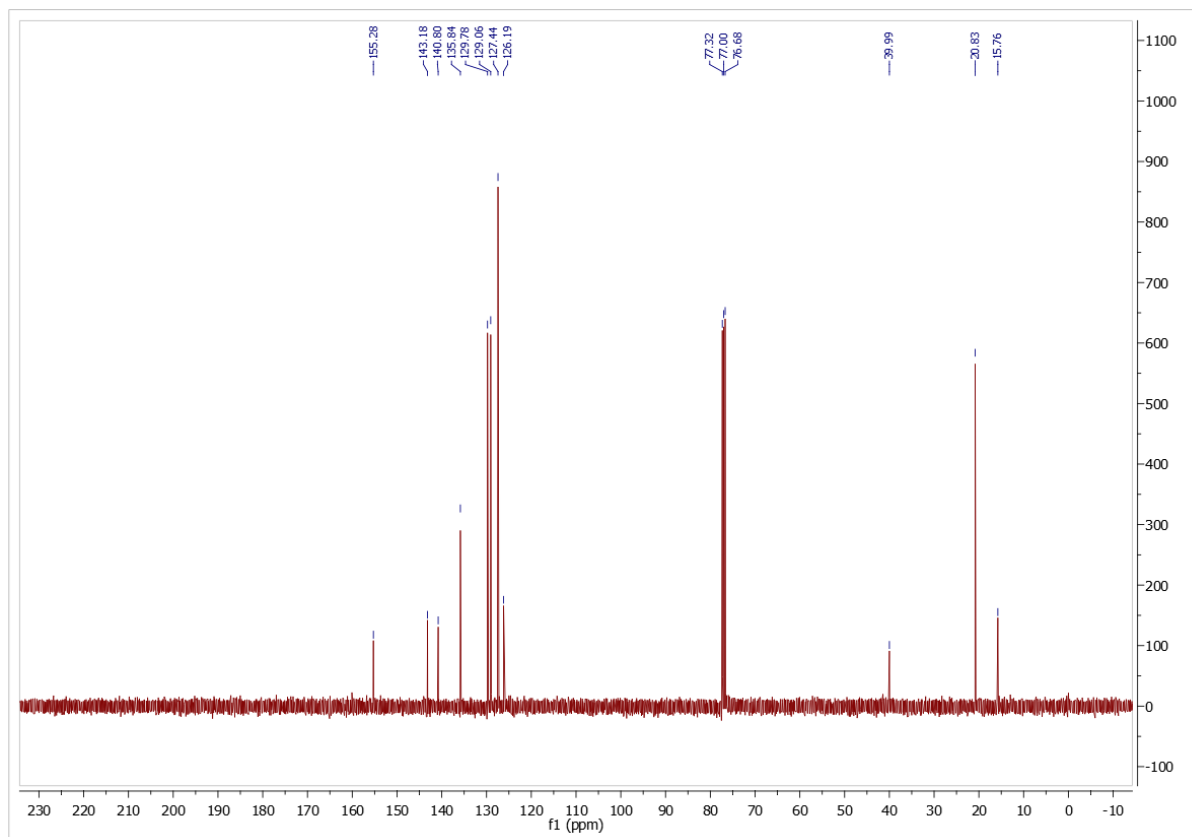
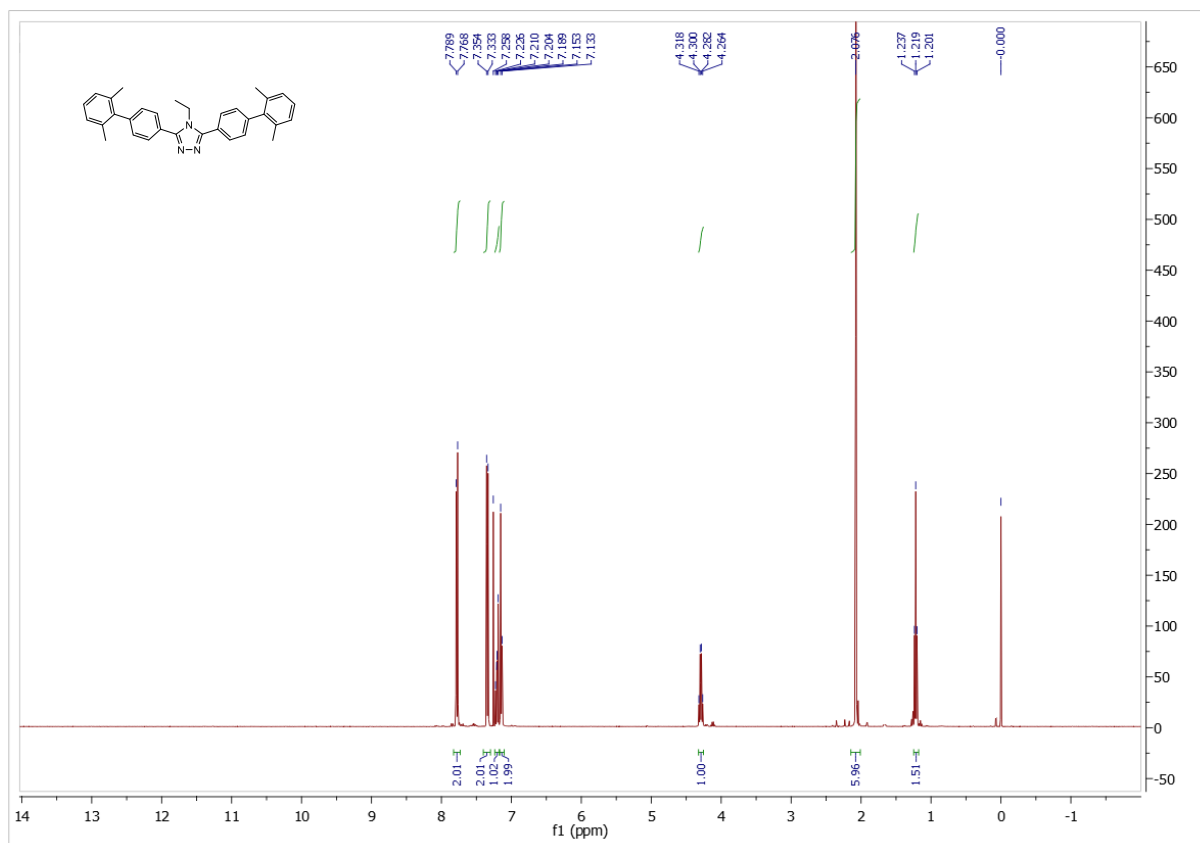
^1H and ^{13}C NMR of 4-ethyl-3,5-bis(2'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**5b**)



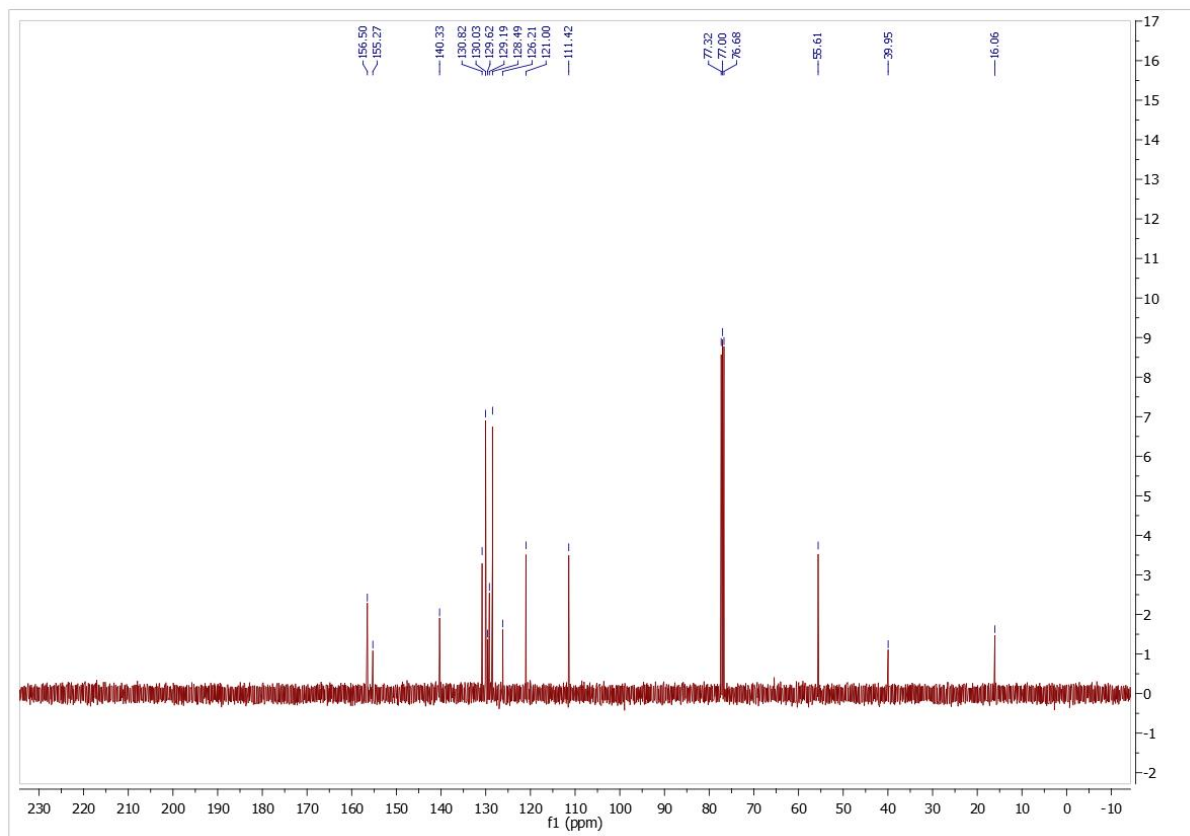
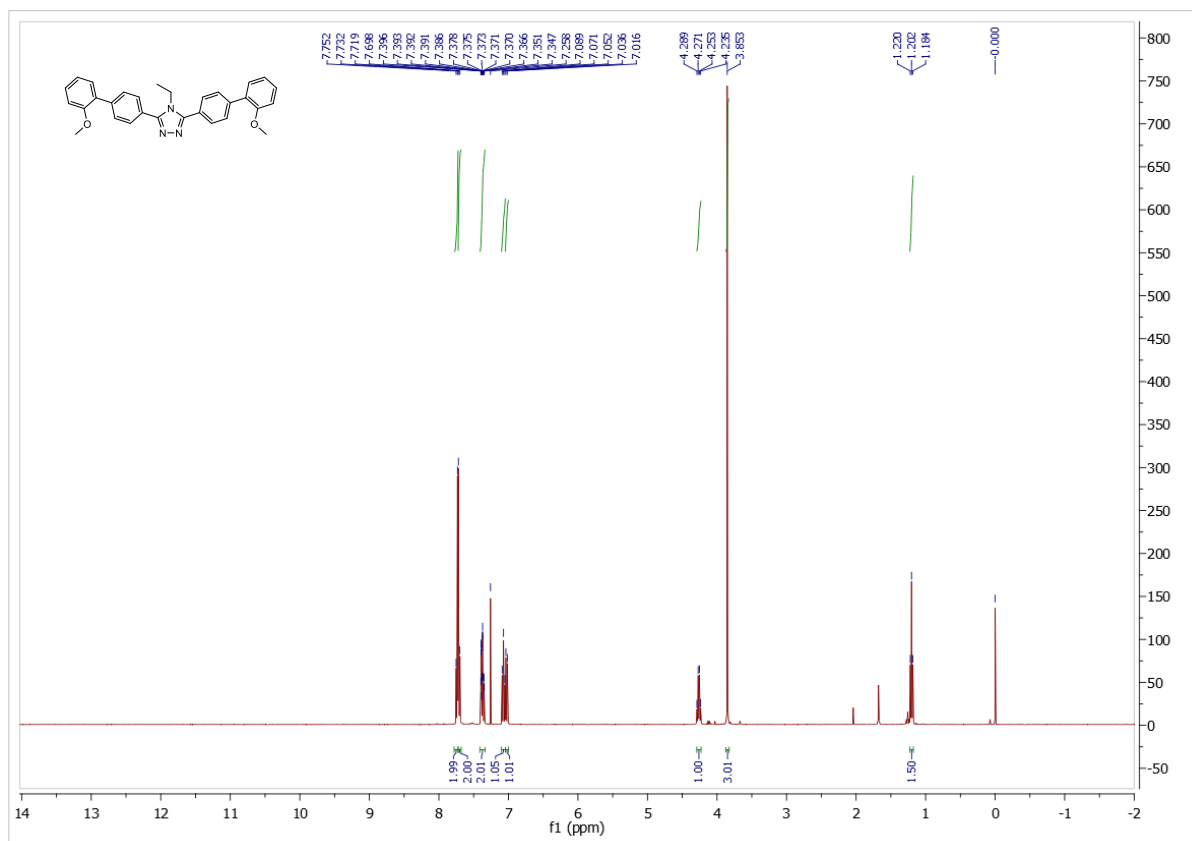
^1H and ^{13}C NMR of 4-ethyl-3,5-bis(3'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**5c**)



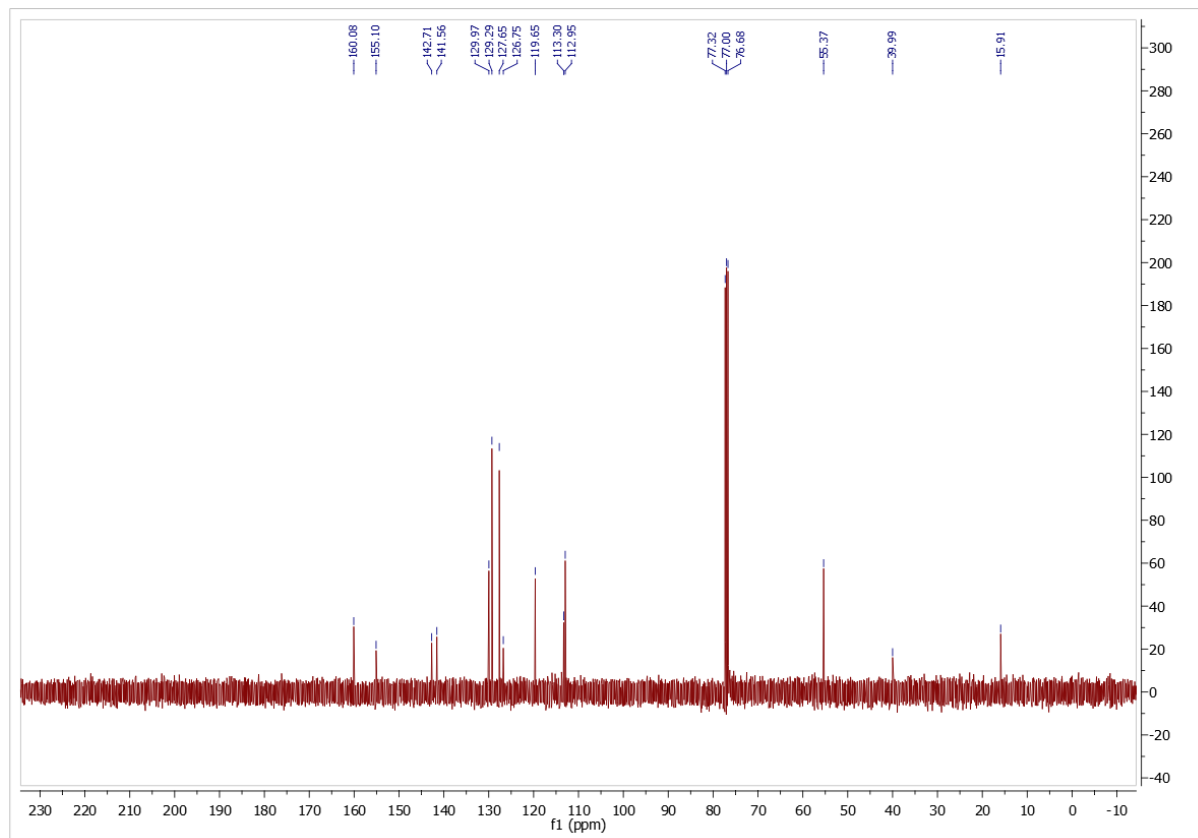
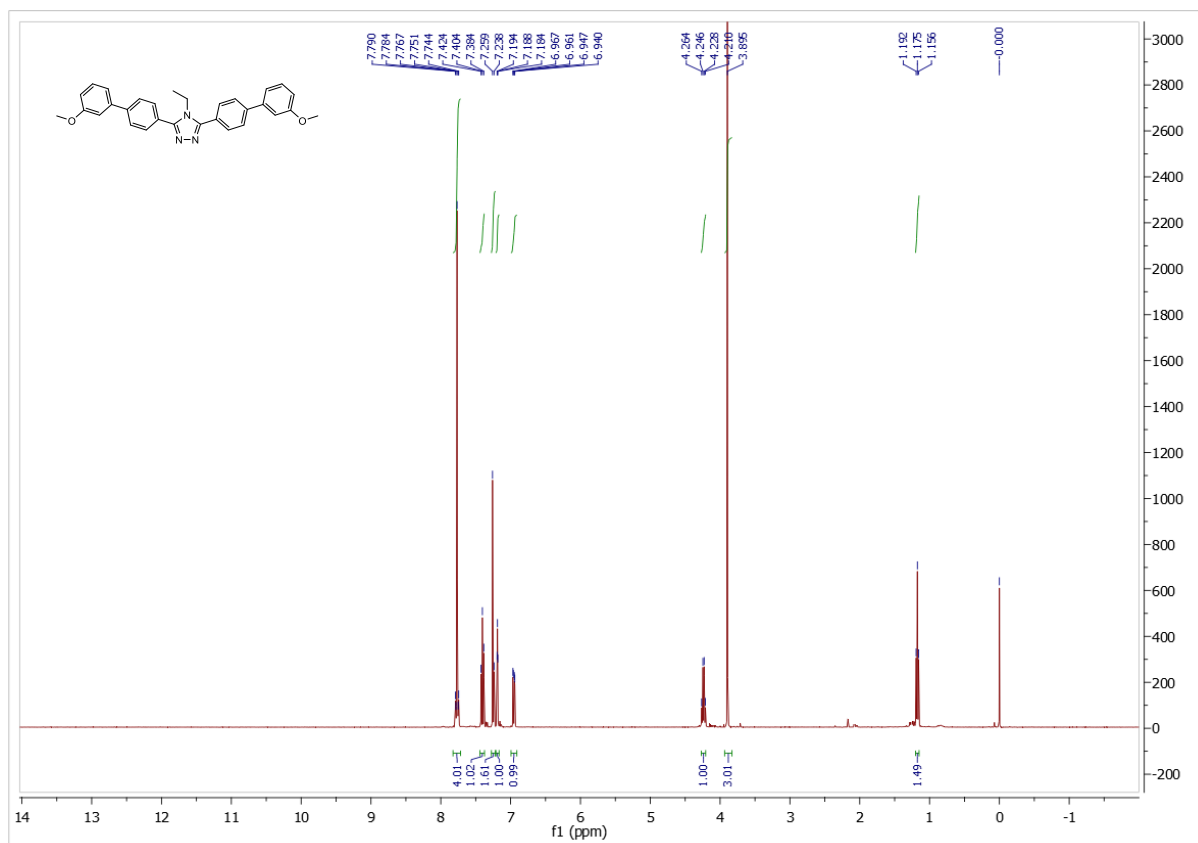
^1H and ^{13}C NMR of 4-ethyl-3,5-bis(2',6'-dimethylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**5d**)



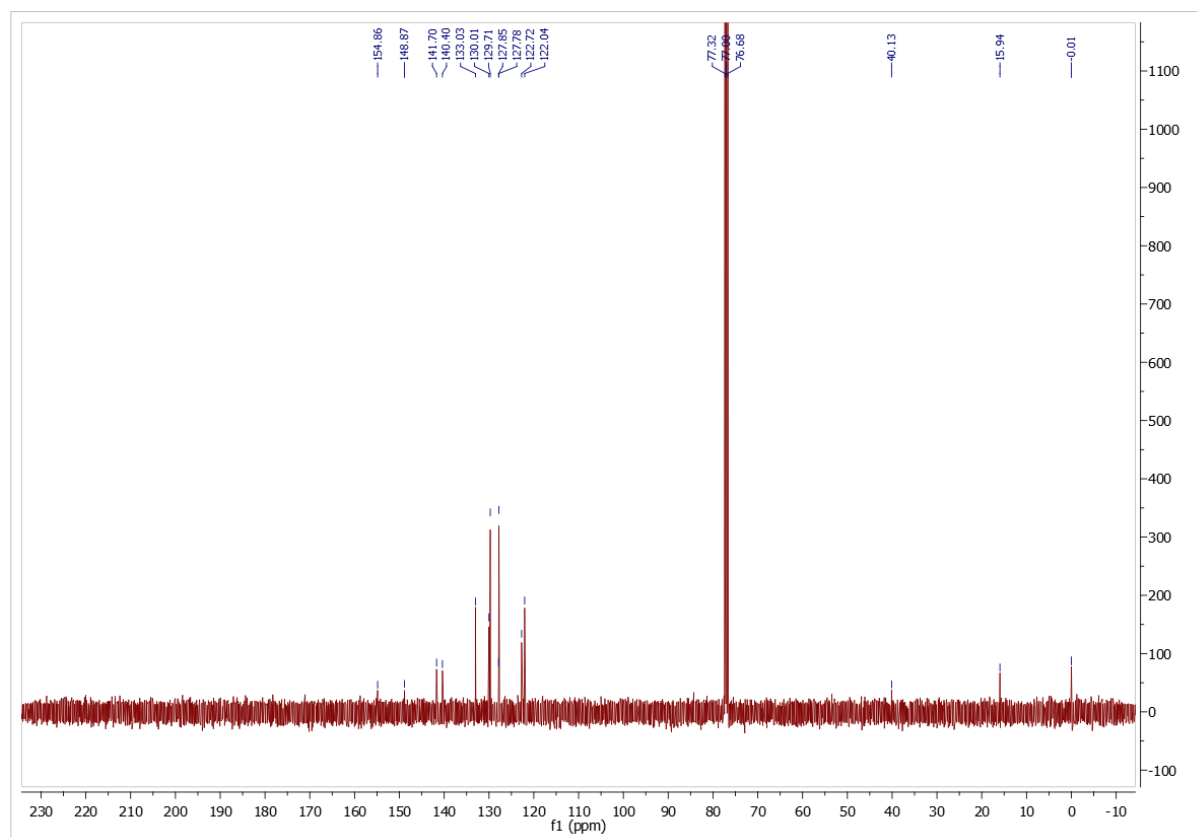
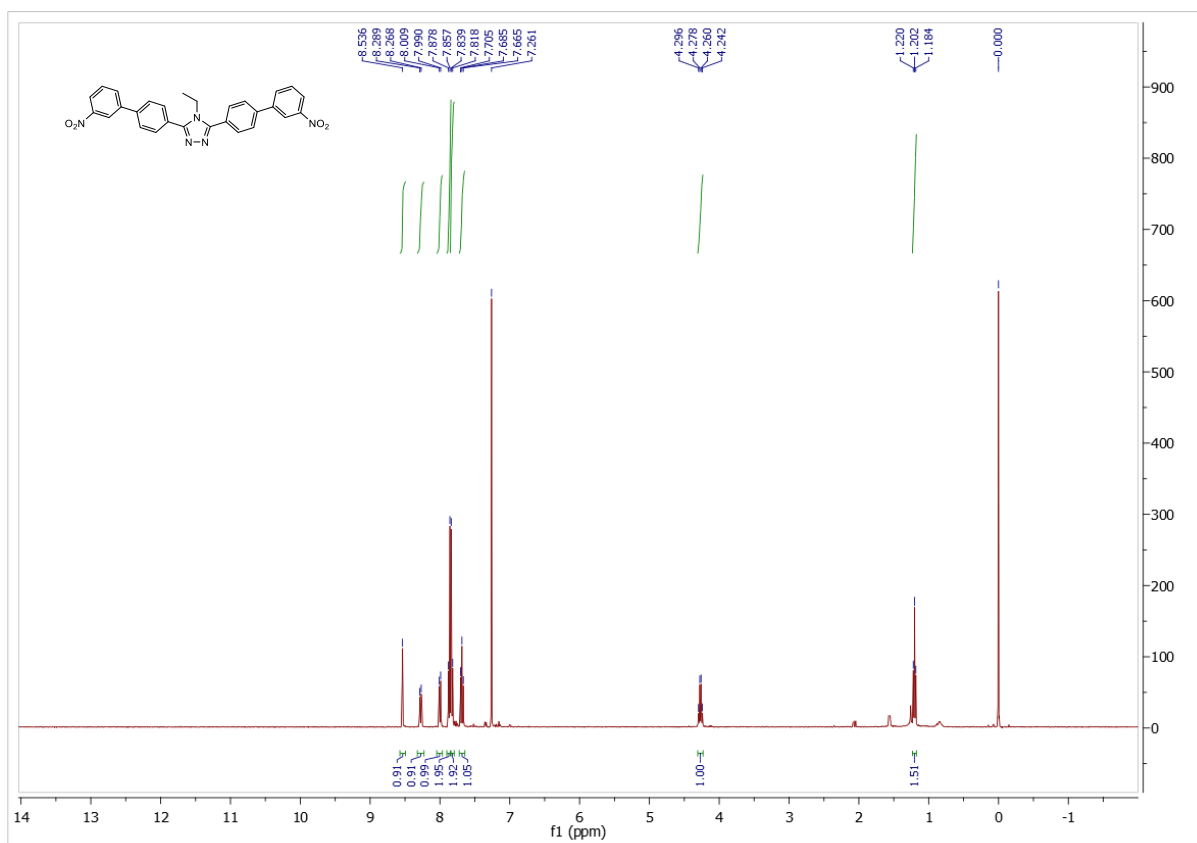
^1H and ^{13}C NMR of 4-ethyl-3,5-bis(2'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**5e**)



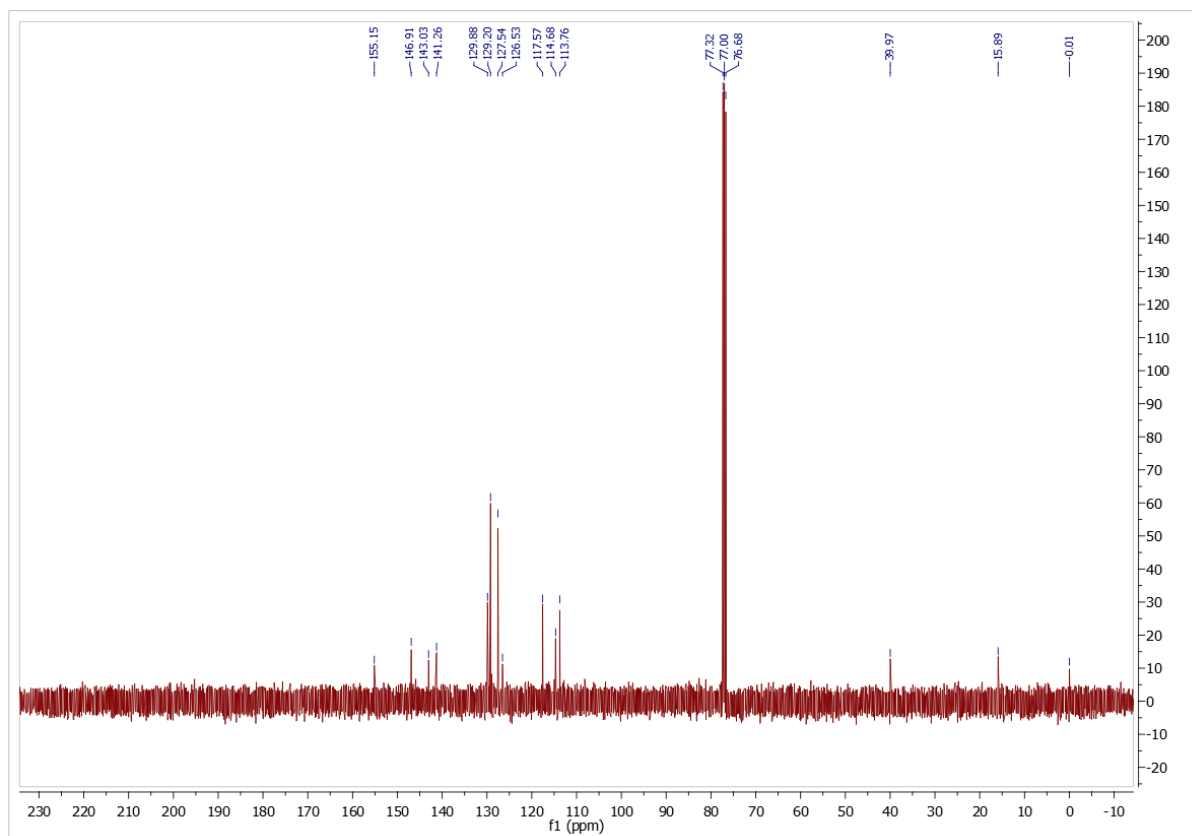
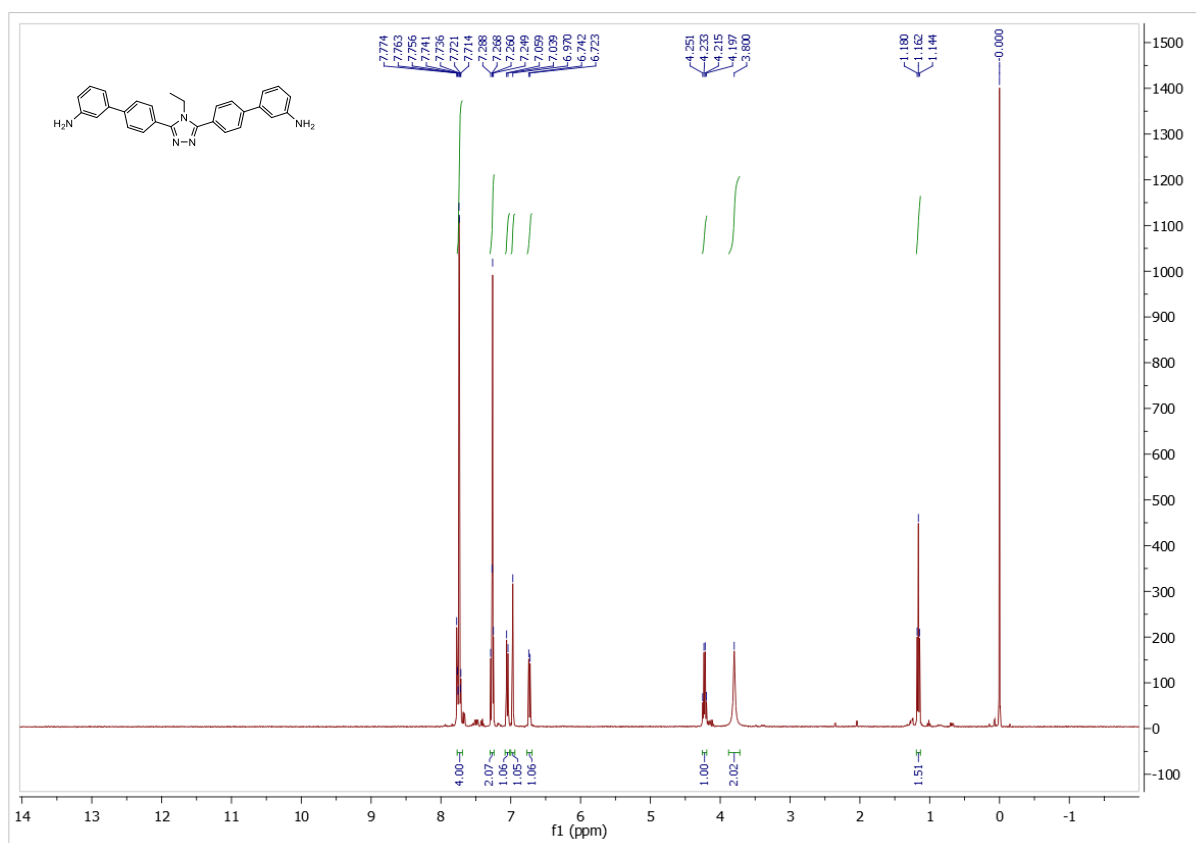
^1H and ^{13}C NMR of 4-ethyl-3,5-bis(3'-methoxyphenyl-4-yl)-4*H*-1,2,4-triazole (**5f**)



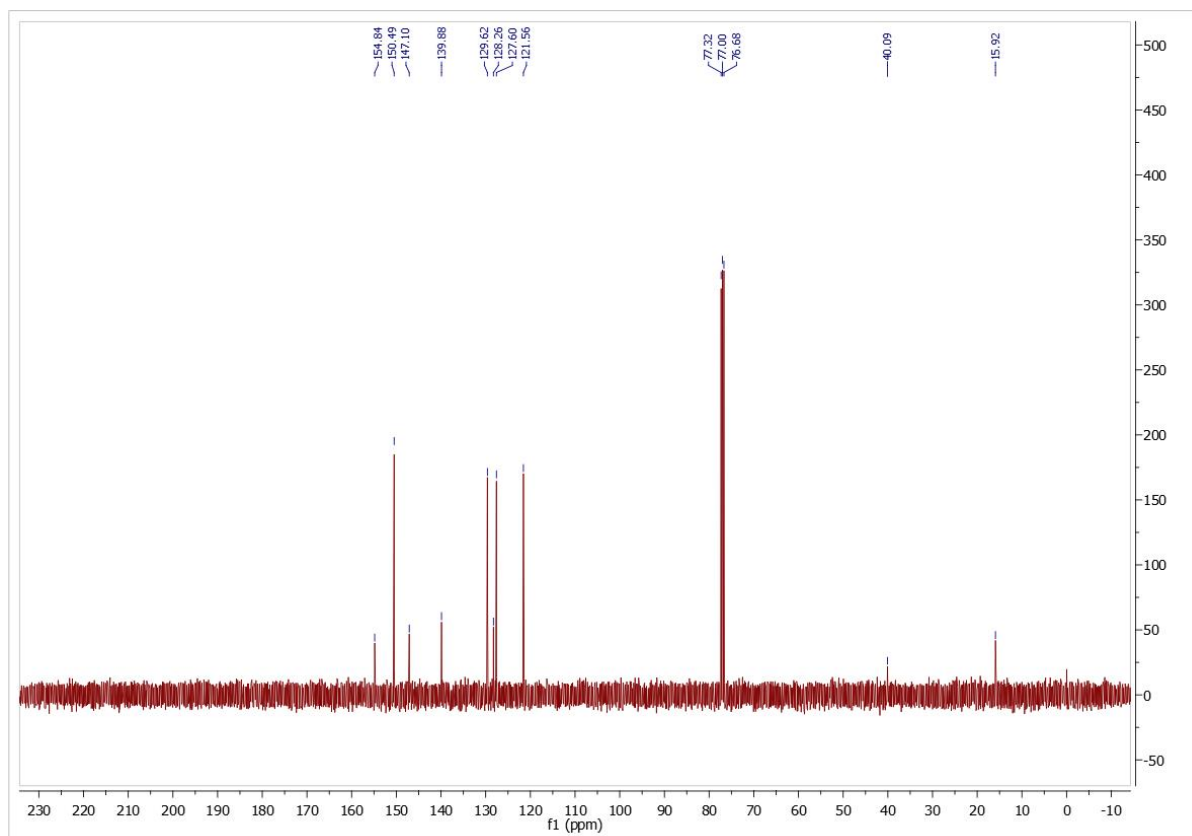
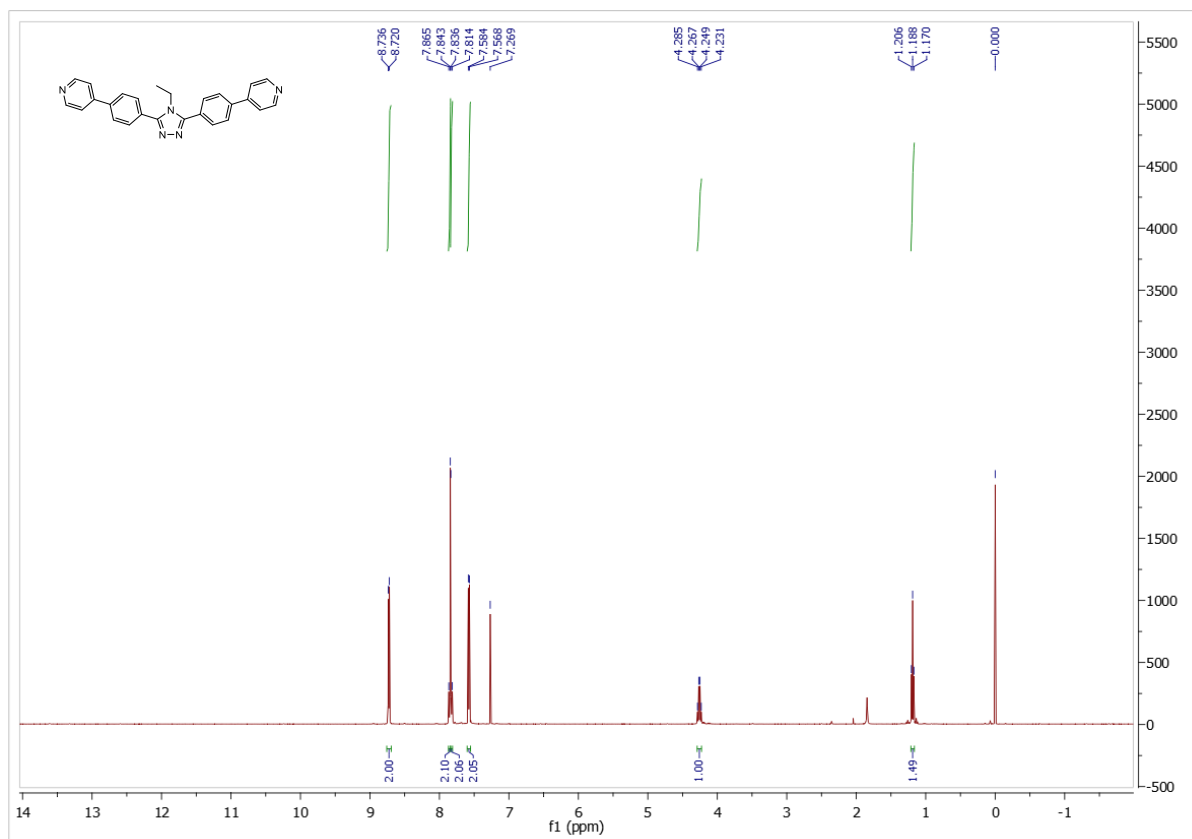
^1H and ^{13}C NMR of 4-ethyl-3,5-bis(3'-nitrophenyl-4-yl)-4*H*-1,2,4-triazole (**5g**)



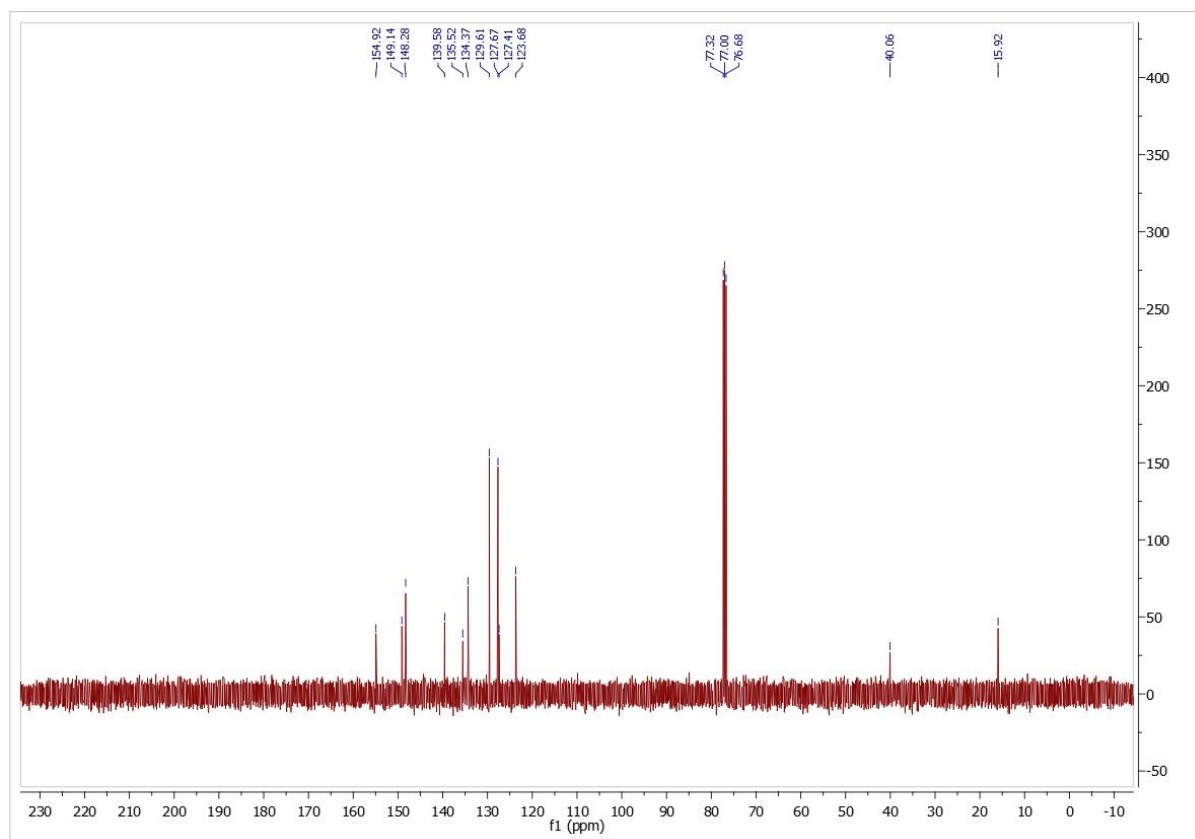
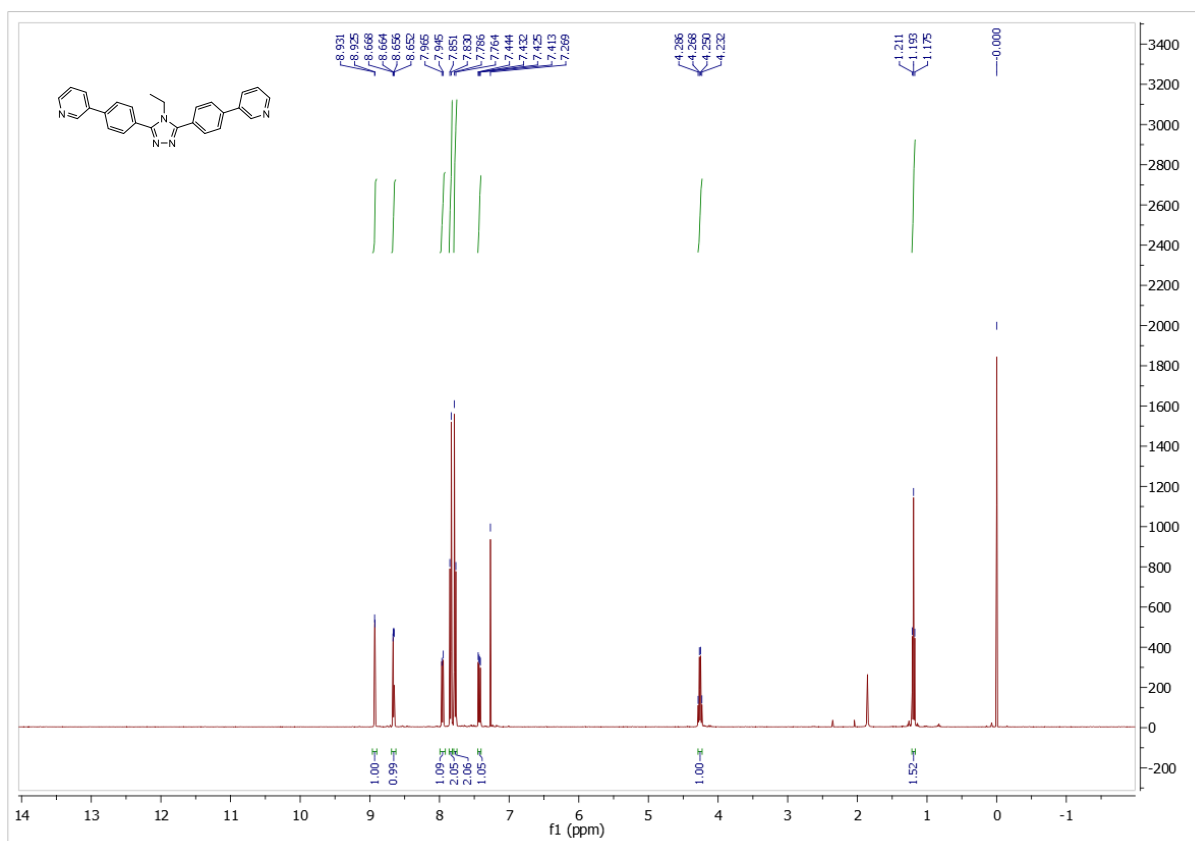
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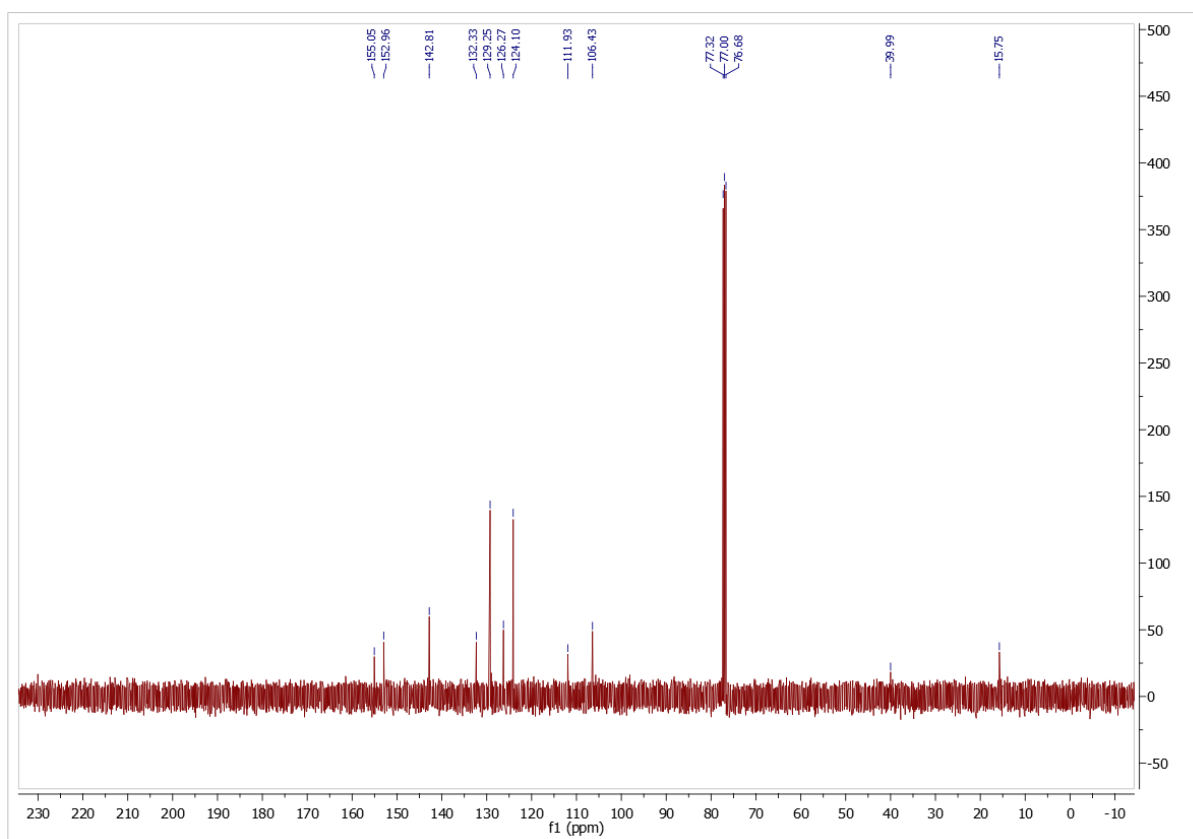
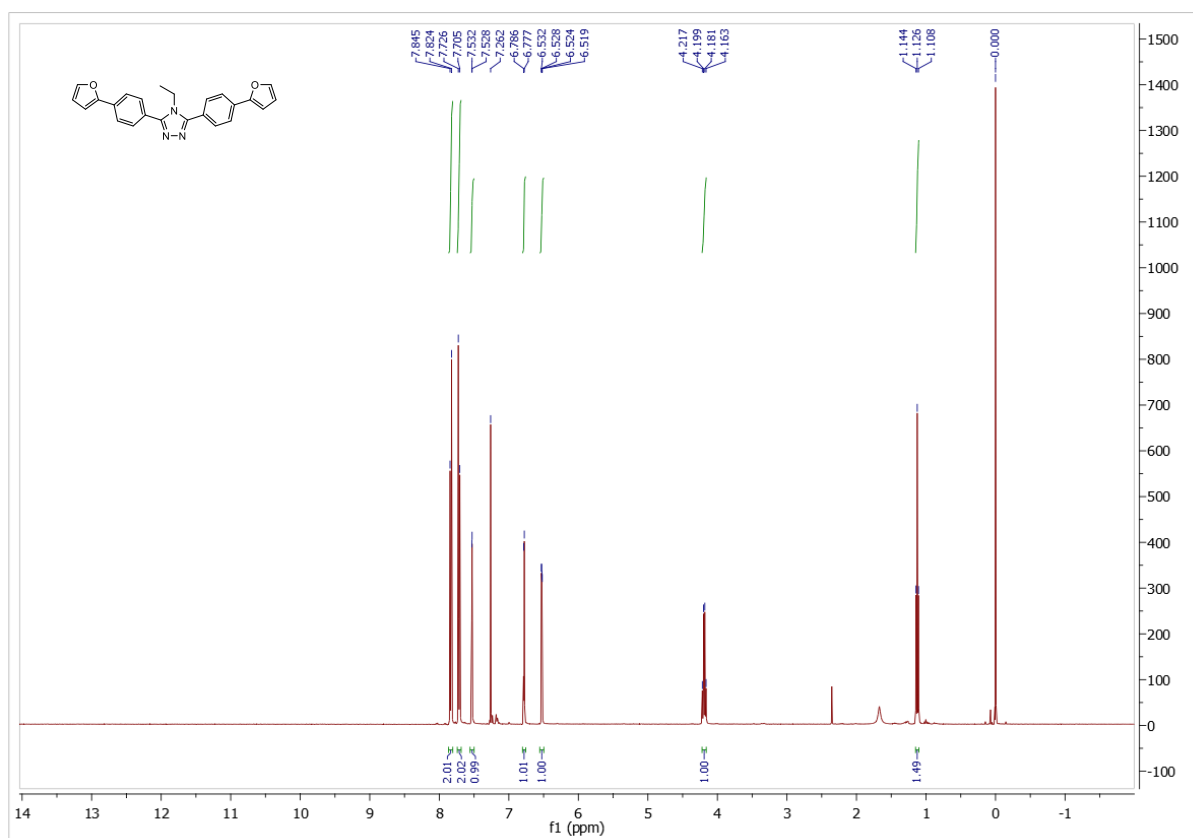
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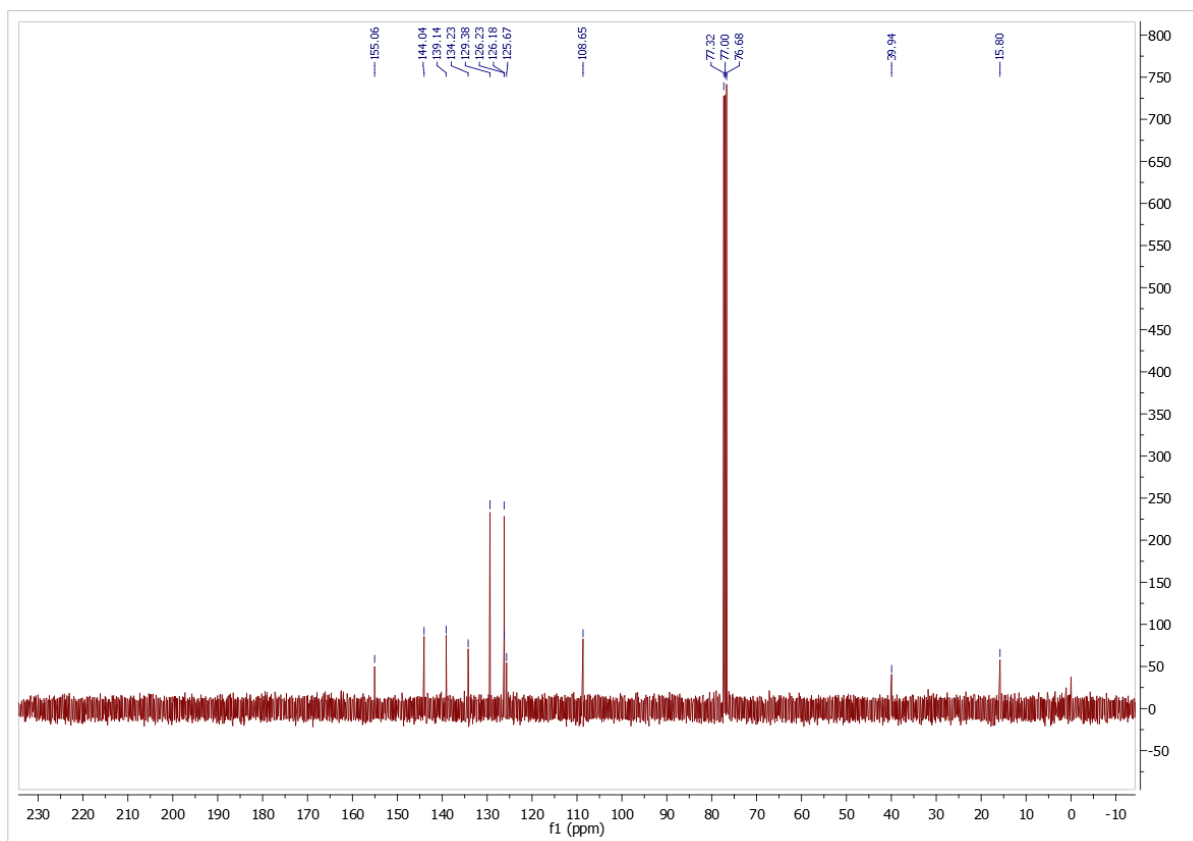
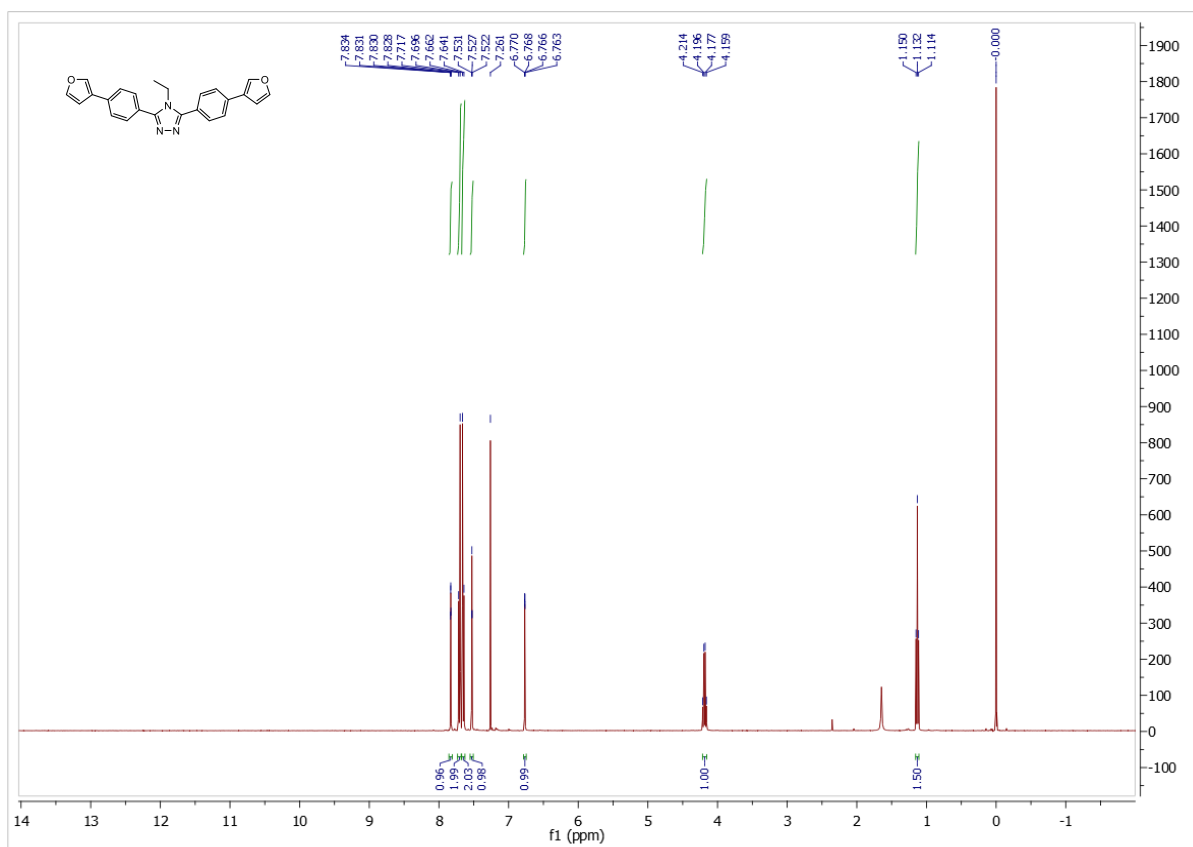
^1H and ^{13}C NMR of 4-ethyl-3,5-bis[4-(pyridin-3-yl)phenyl]-4*H*-1,2,4-triazole (**5j**)



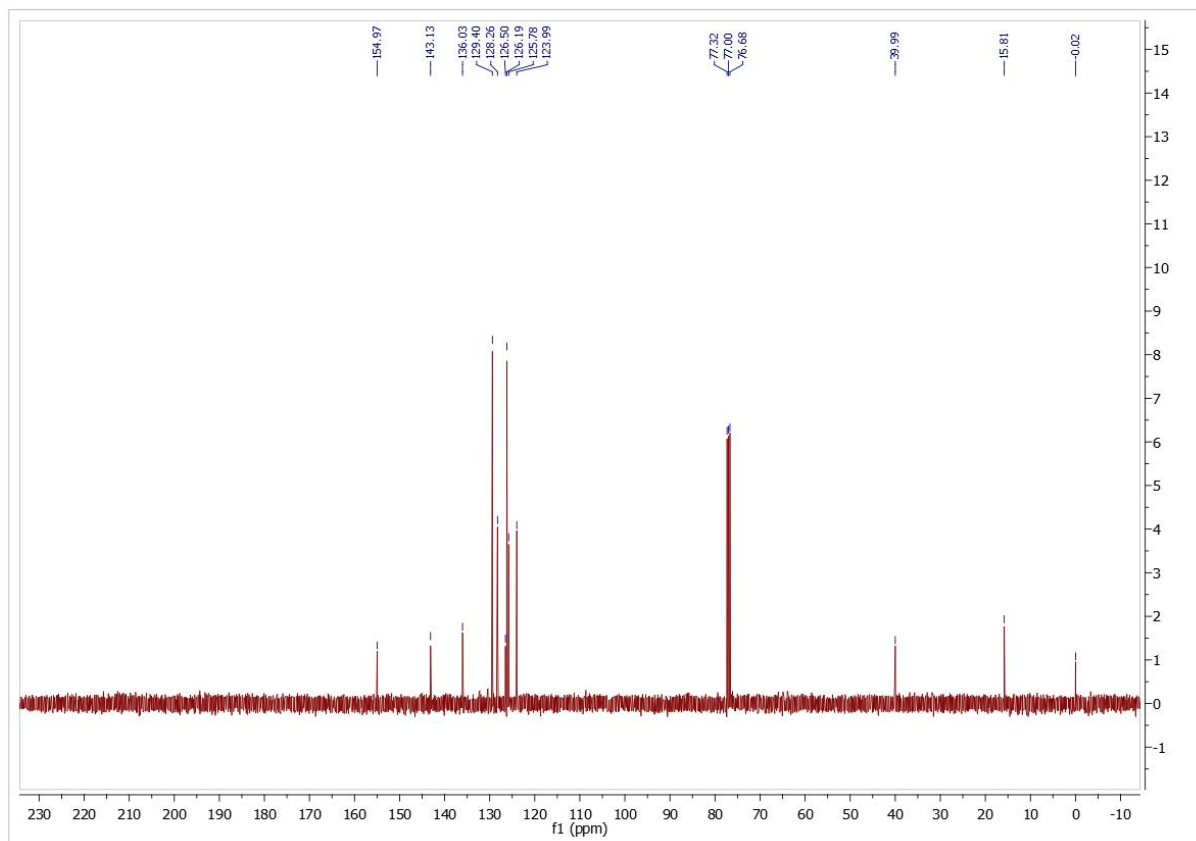
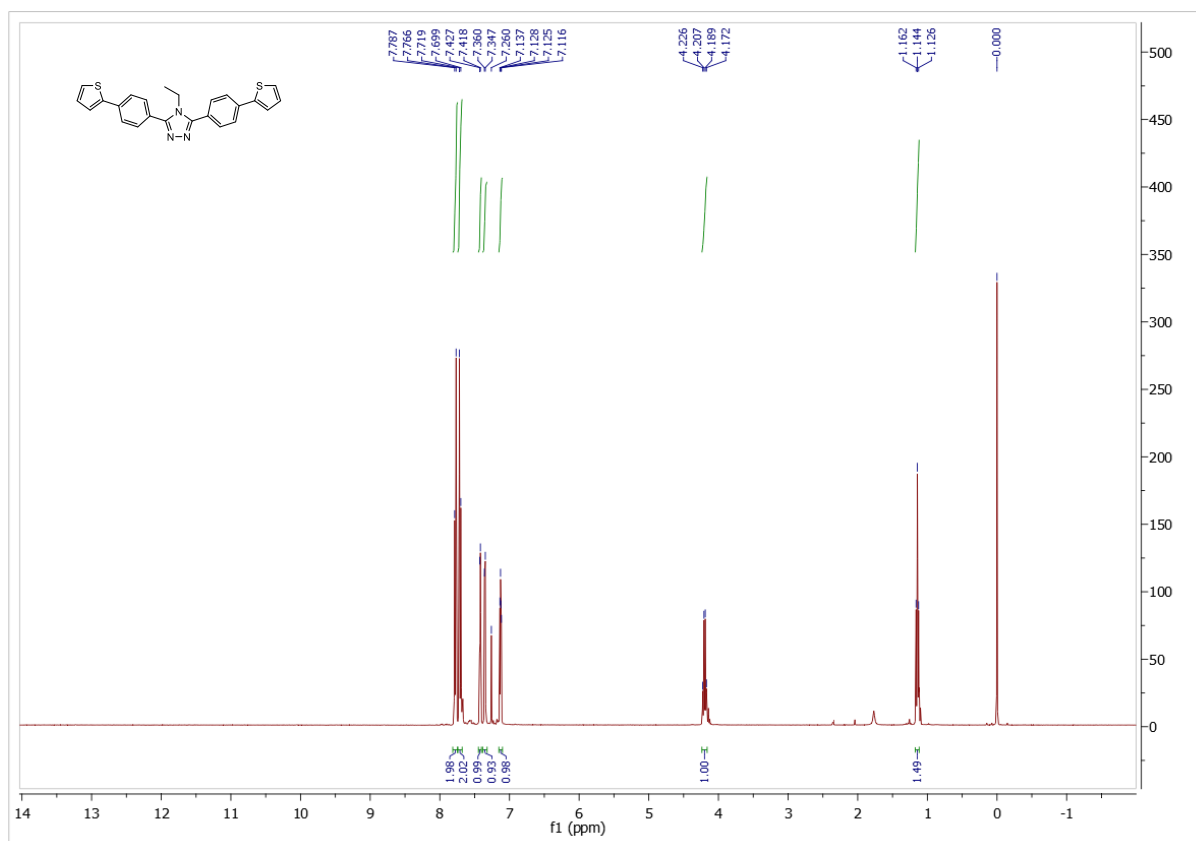
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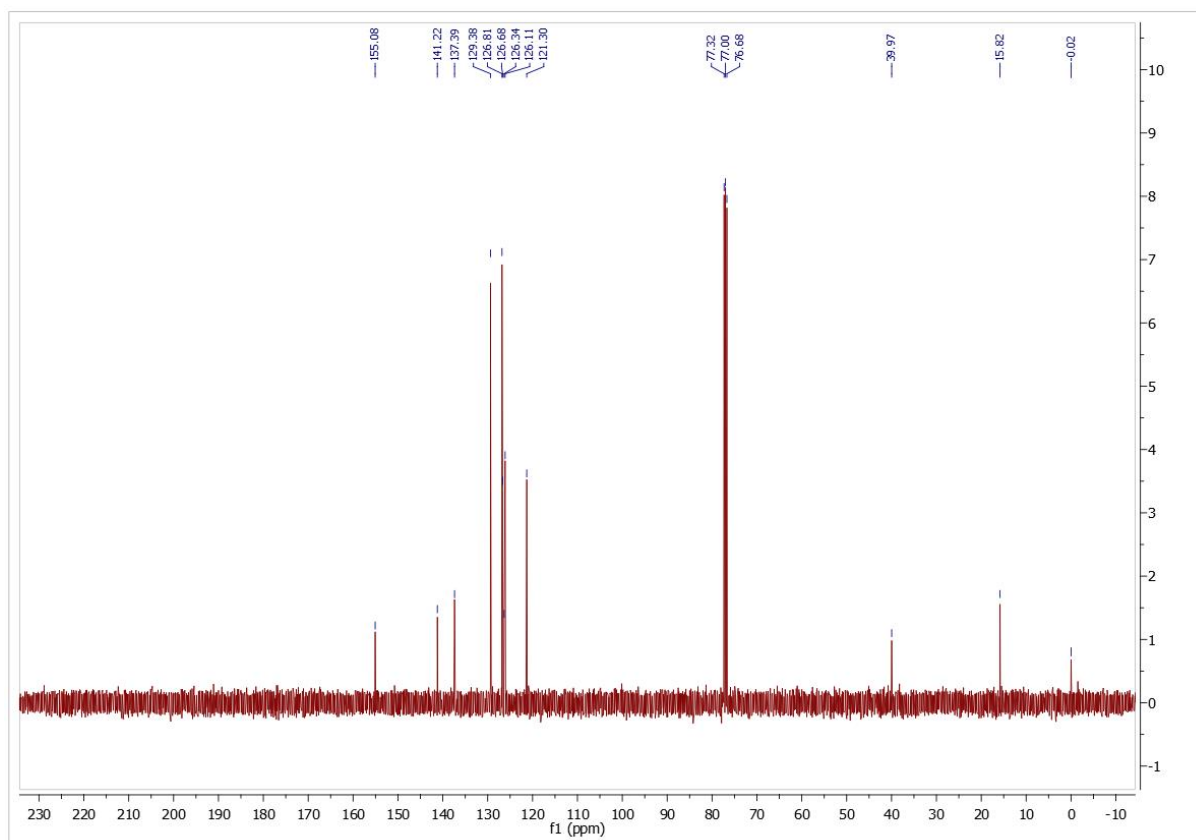
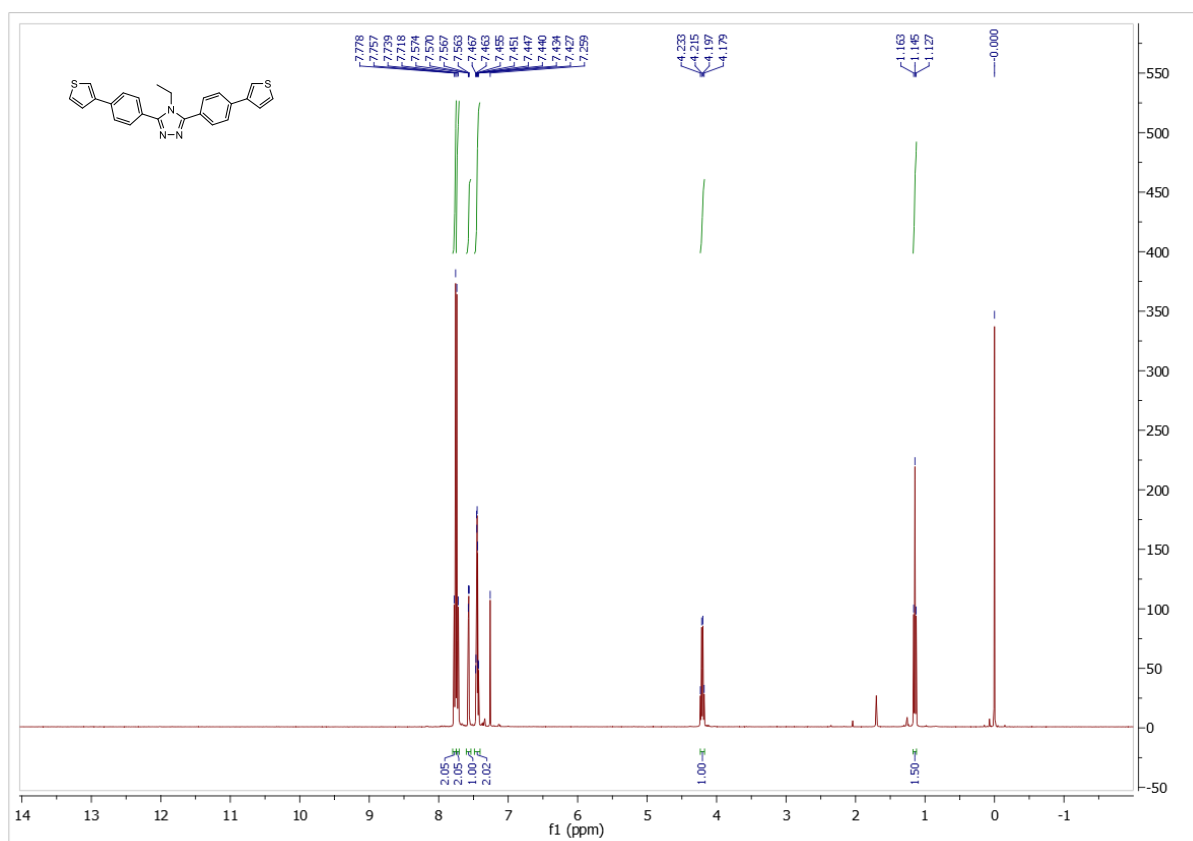
^1H and ^{13}C NMR of 4-ethyl-3,5-bis[4-(furan-3-yl)phenyl]-4*H*-1,2,4-triazole (**5**)



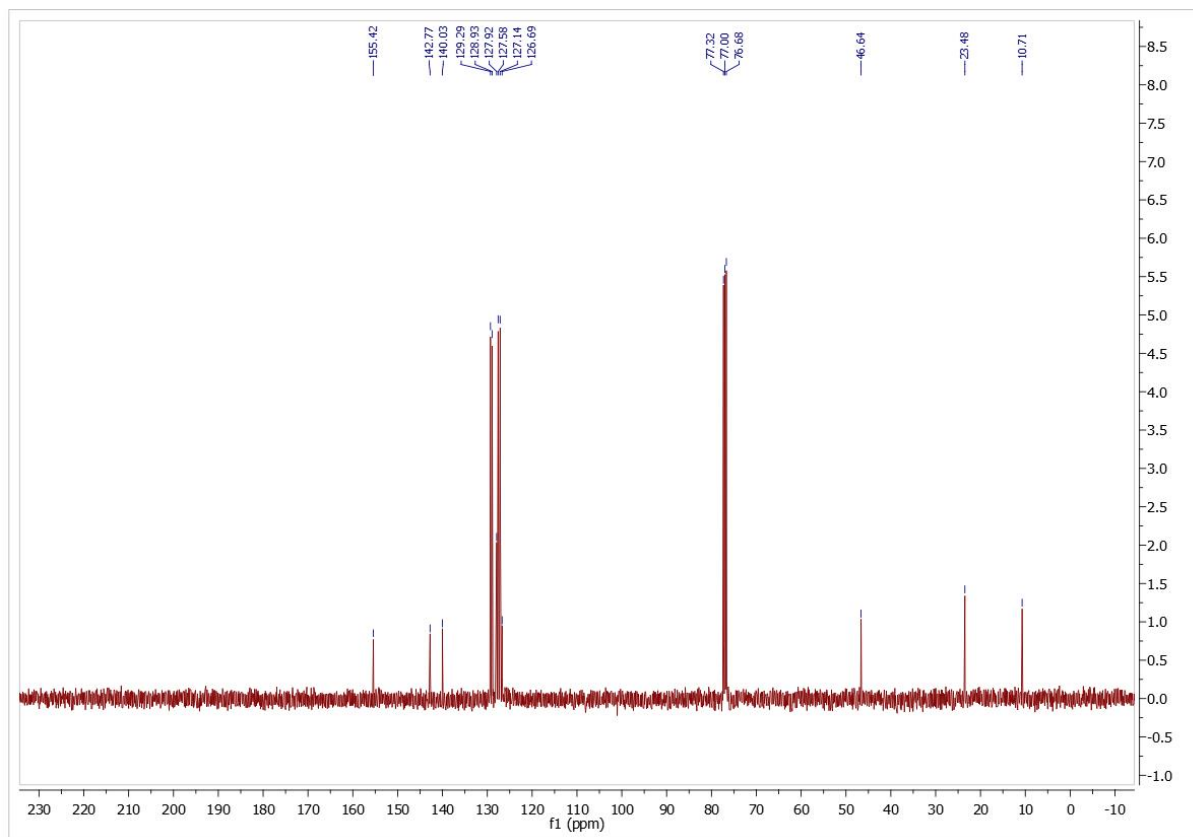
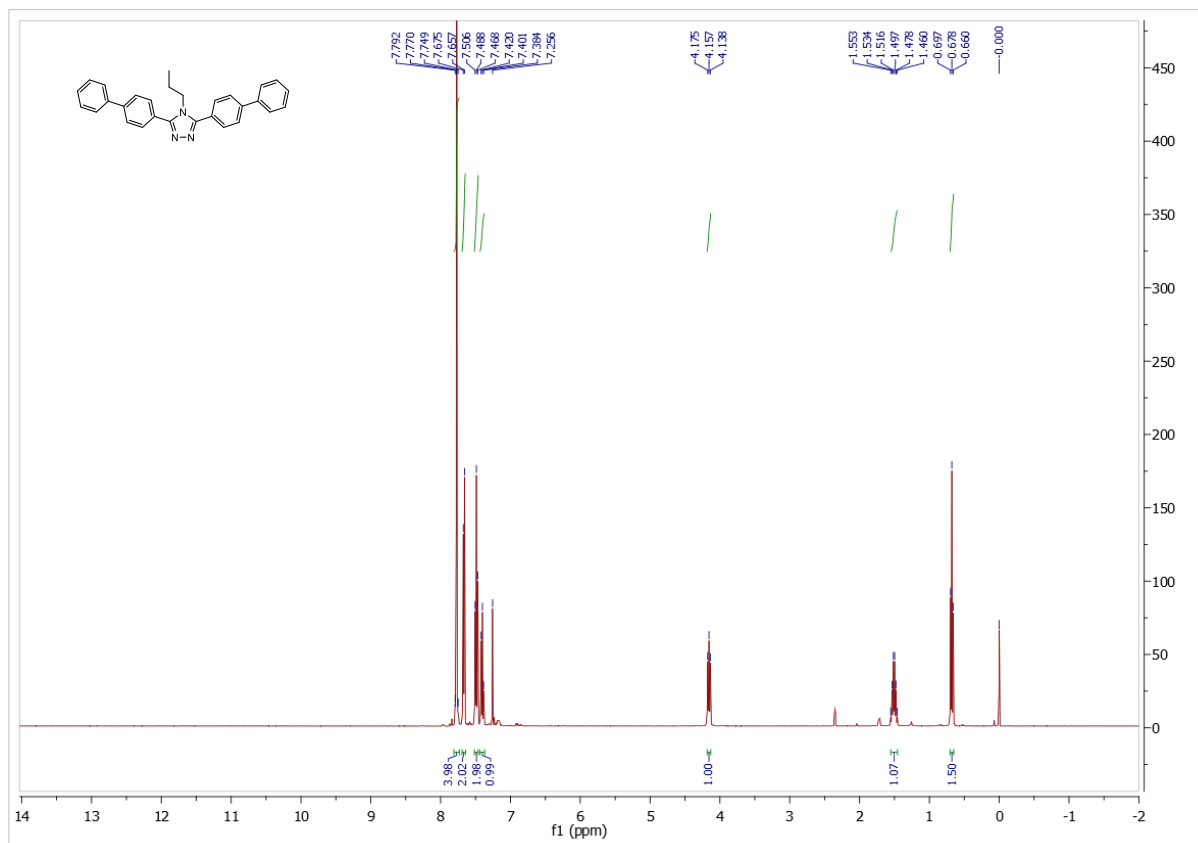
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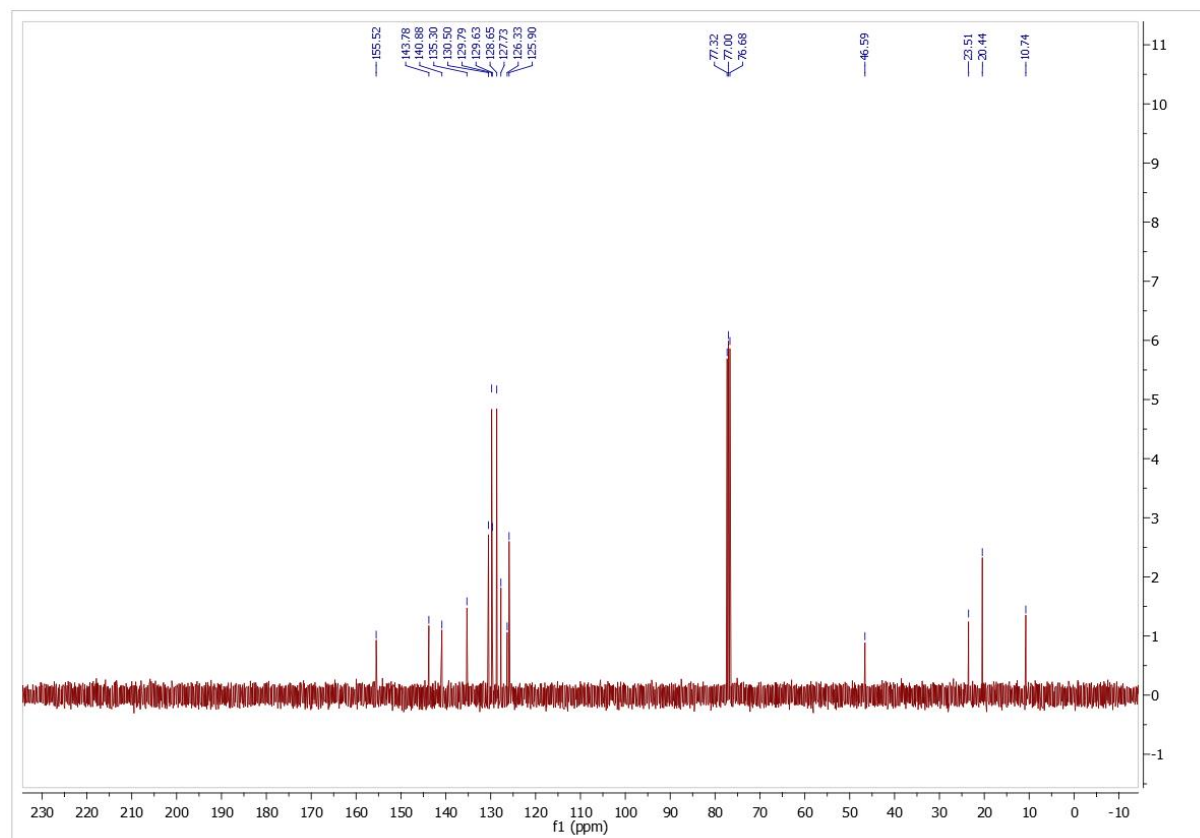
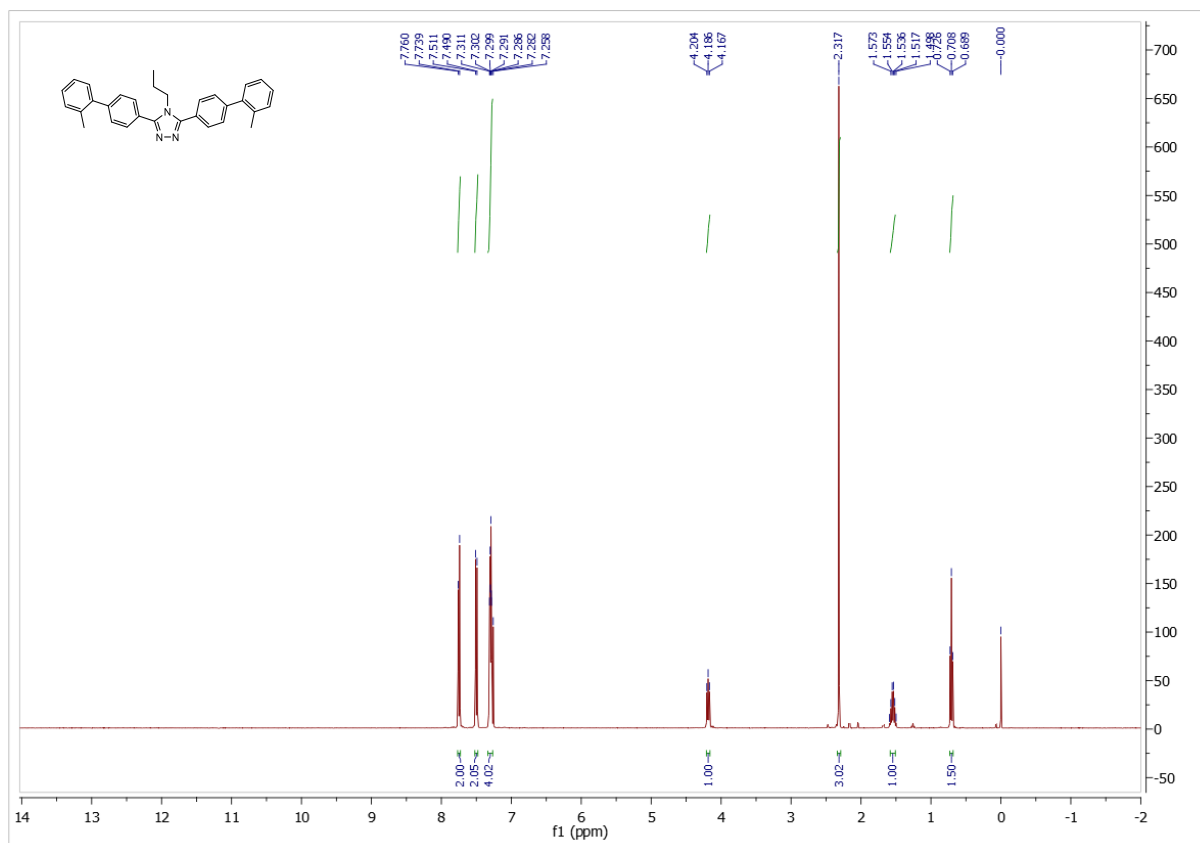
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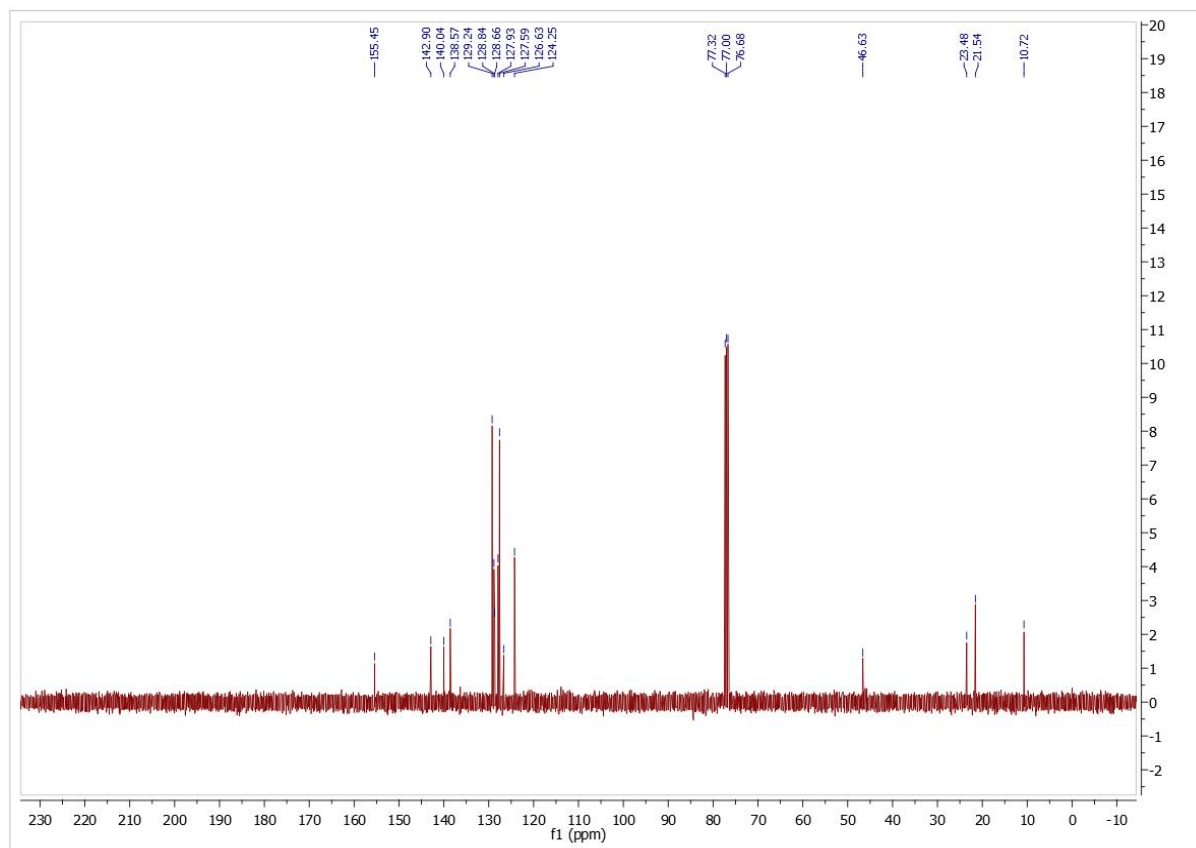
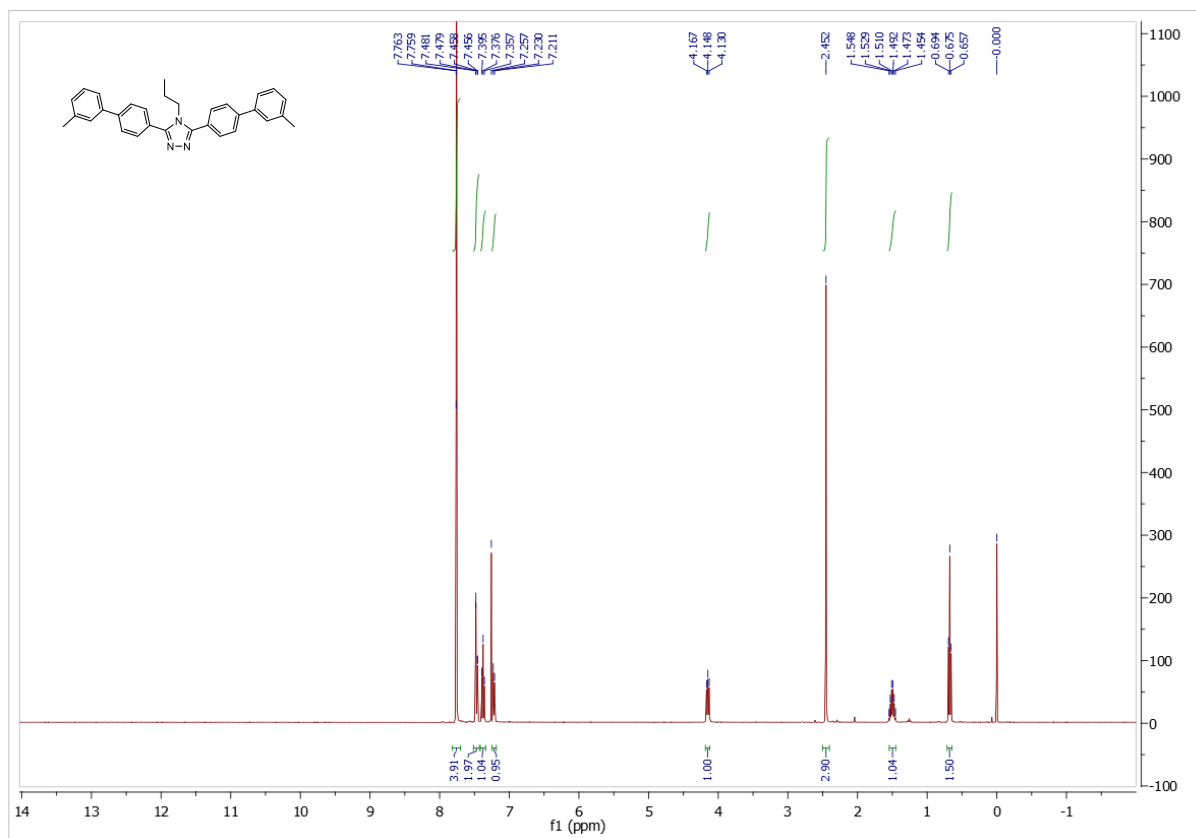
^1H and ^{13}C NMR of 3,5-bis(biphenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6a**)



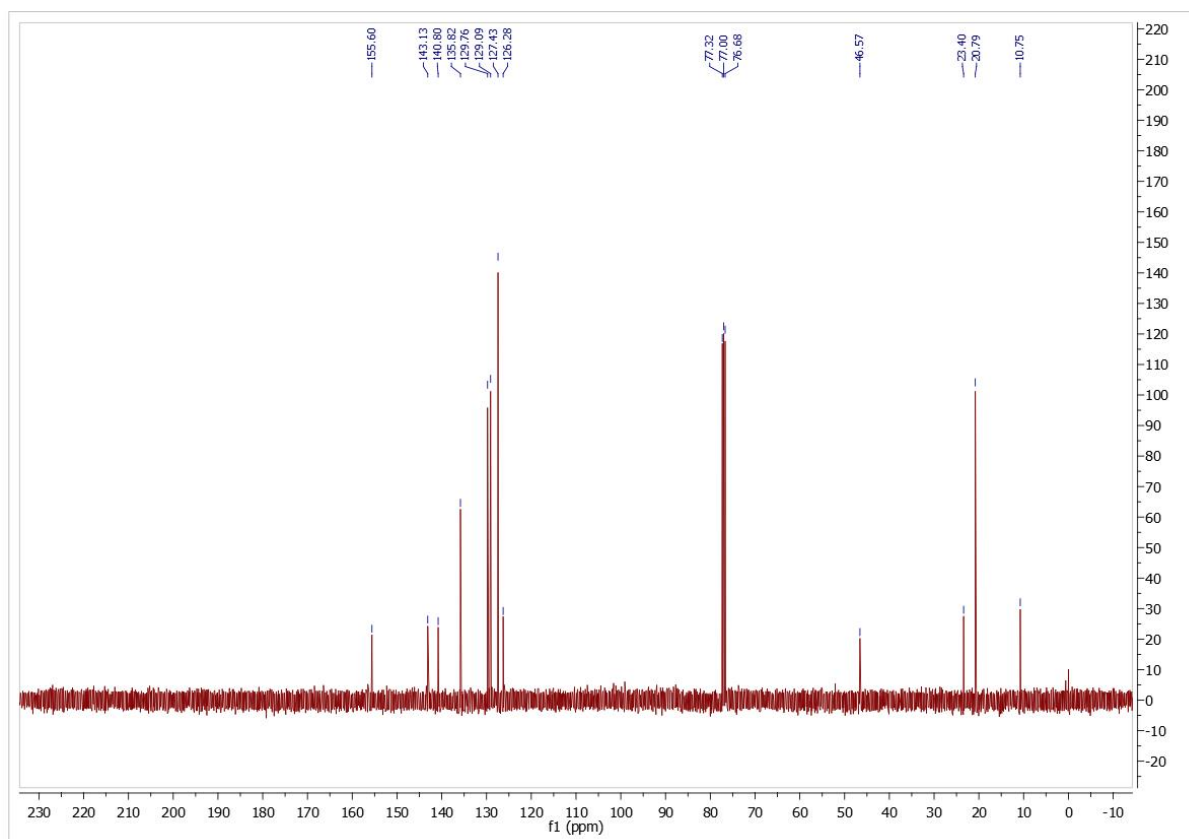
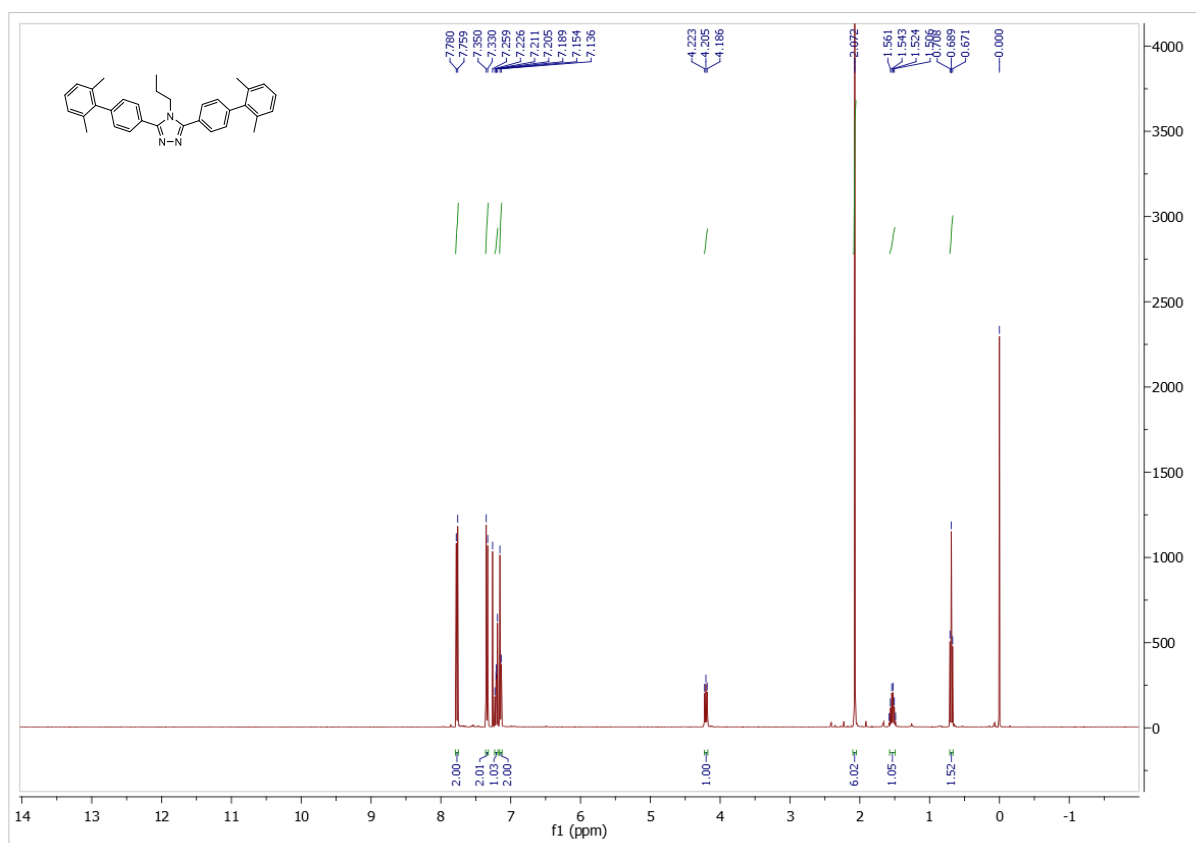
^1H and ^{13}C NMR of 3,5-bis(2'-methylbiphenyl-4-yl)-4-propyl-4H-1,2,4-triazole (**6b**)



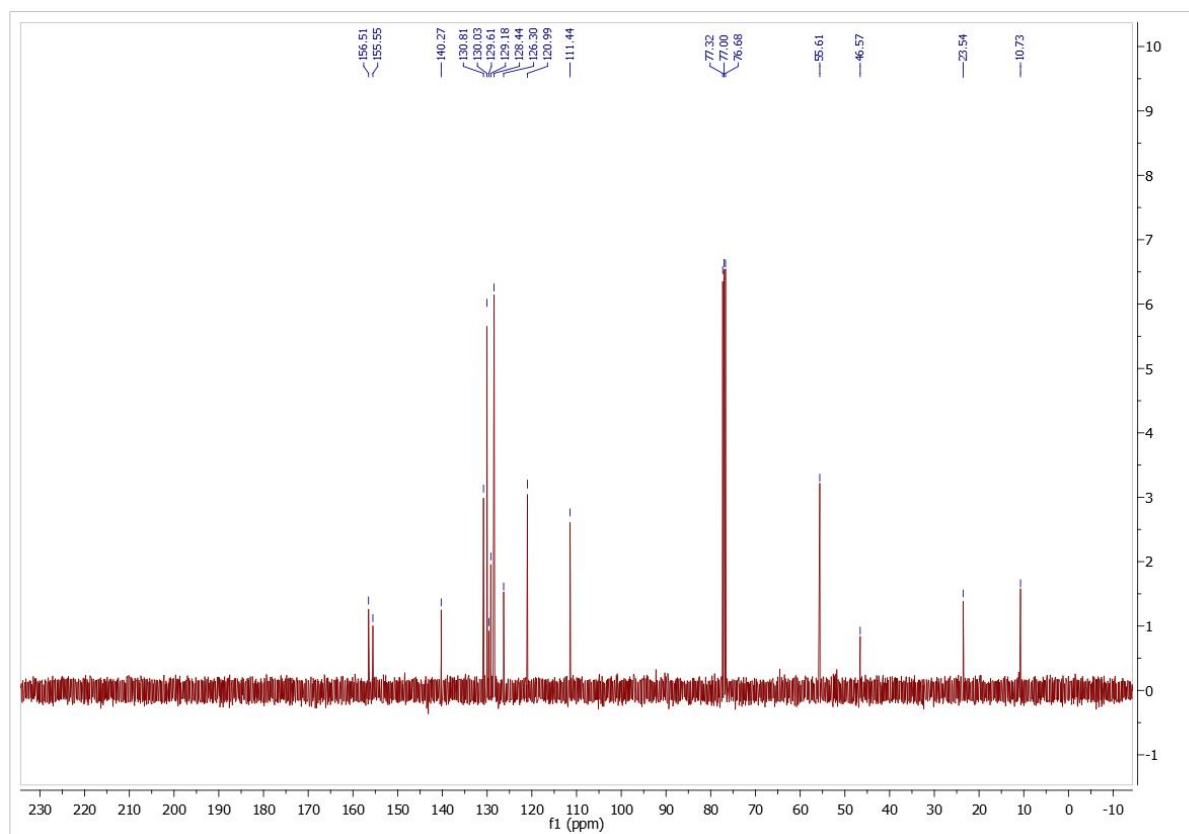
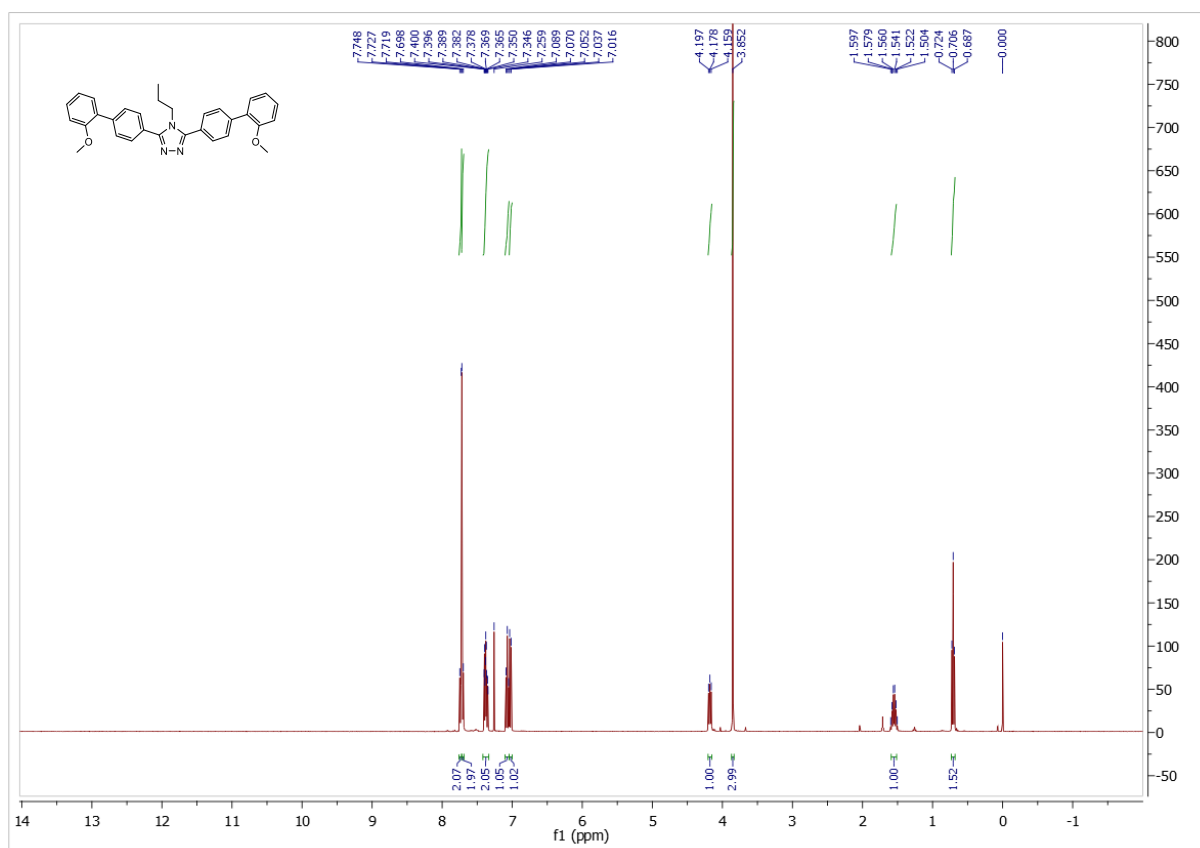
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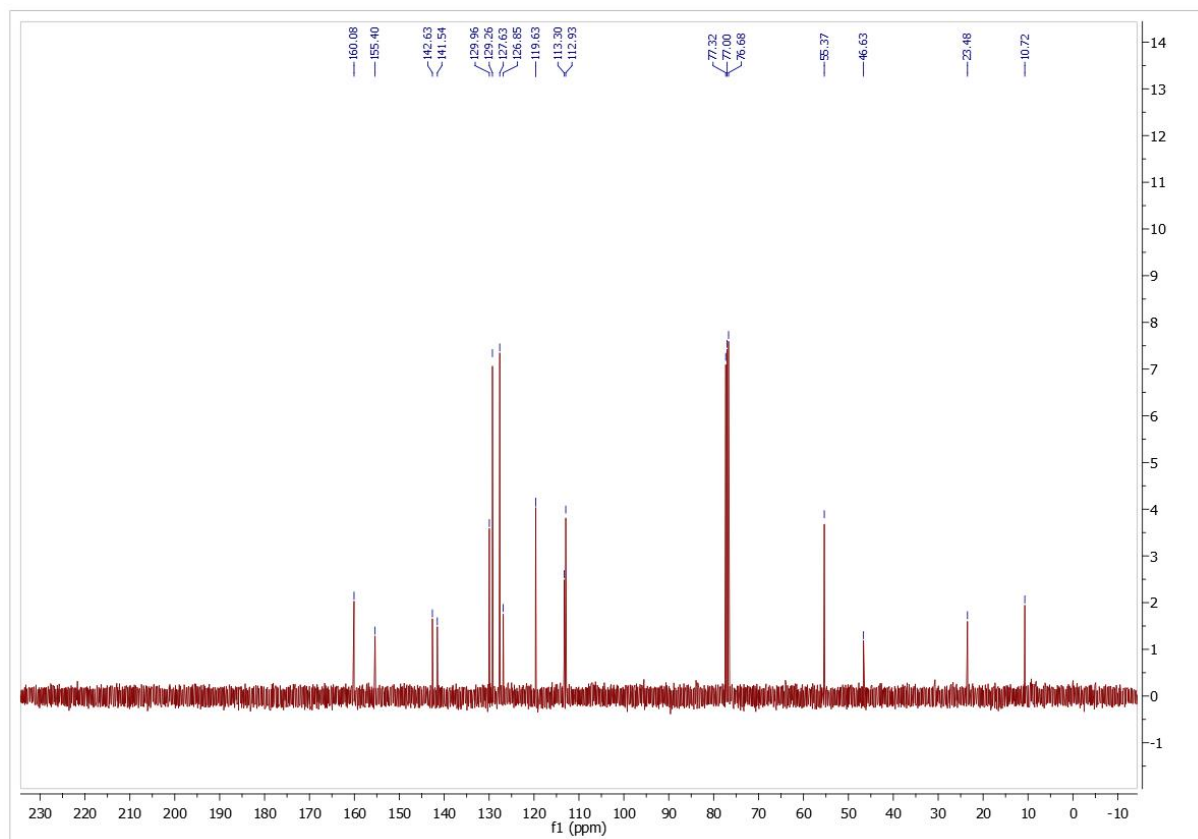
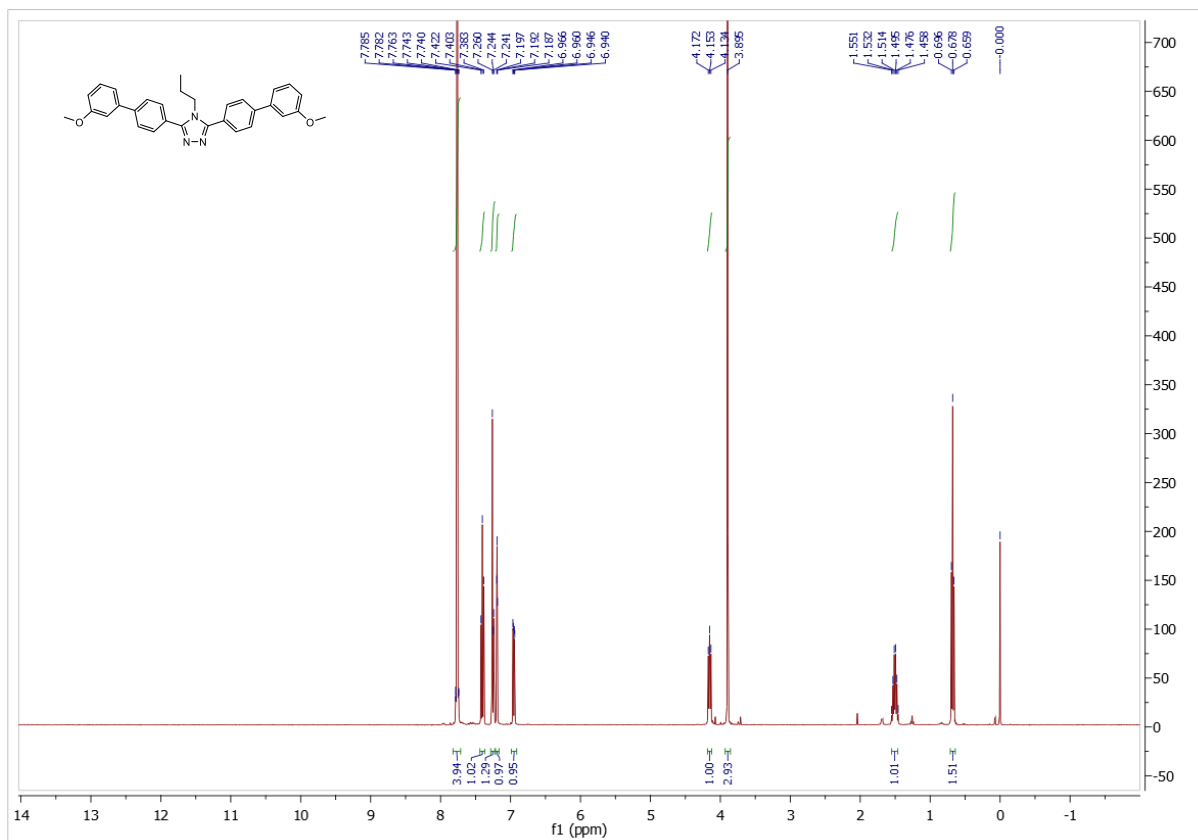
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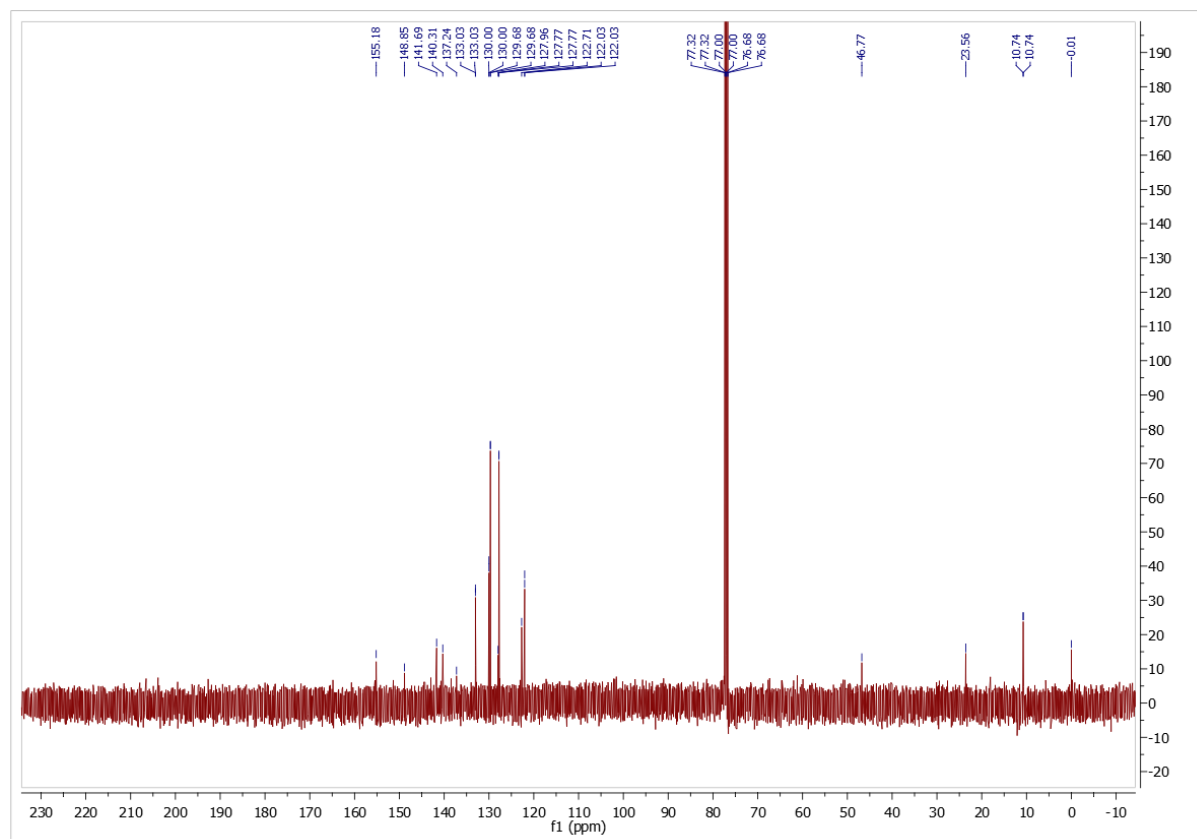
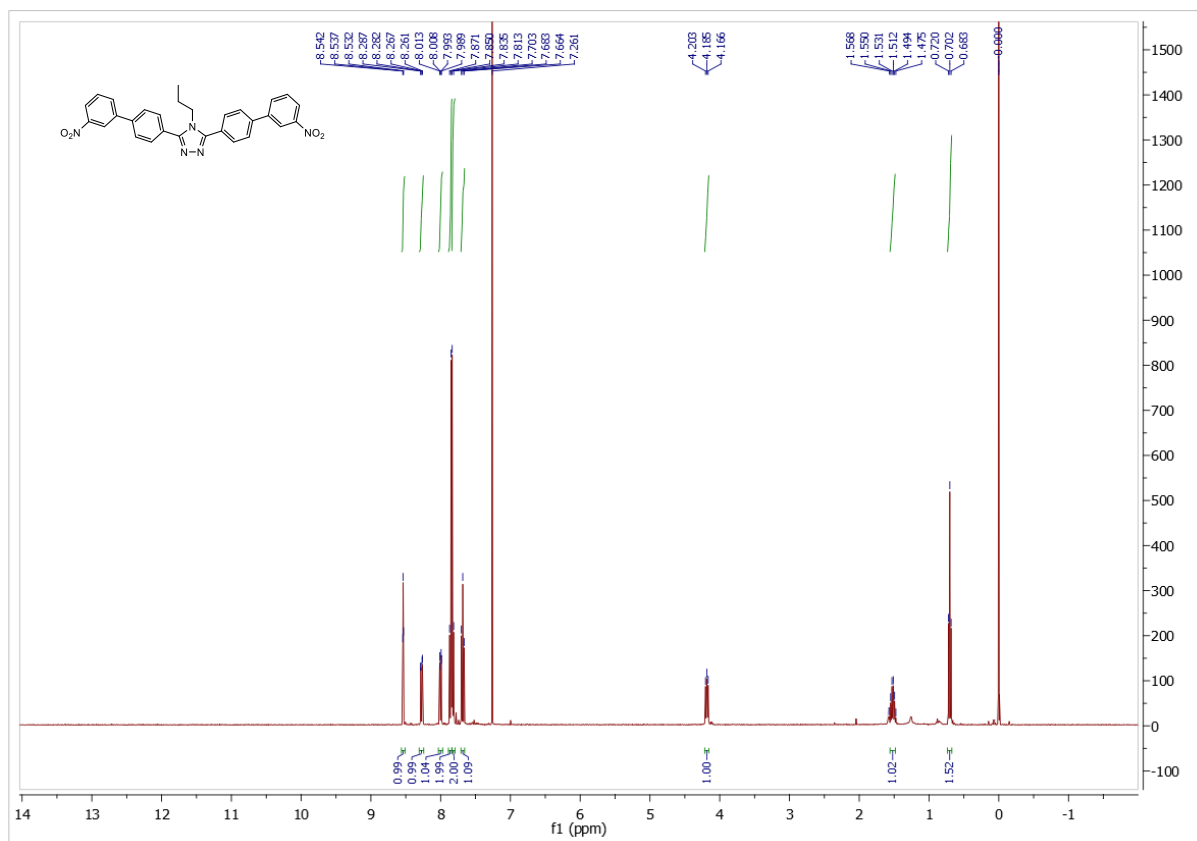
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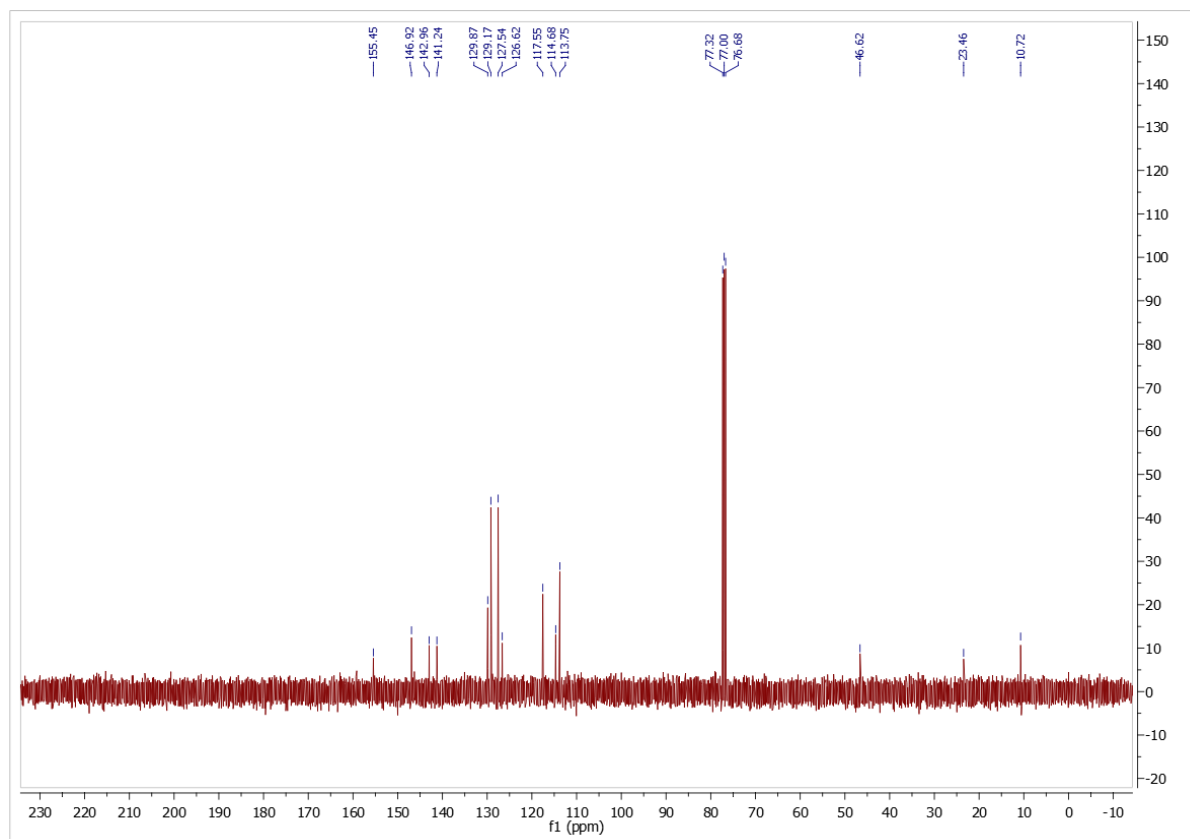
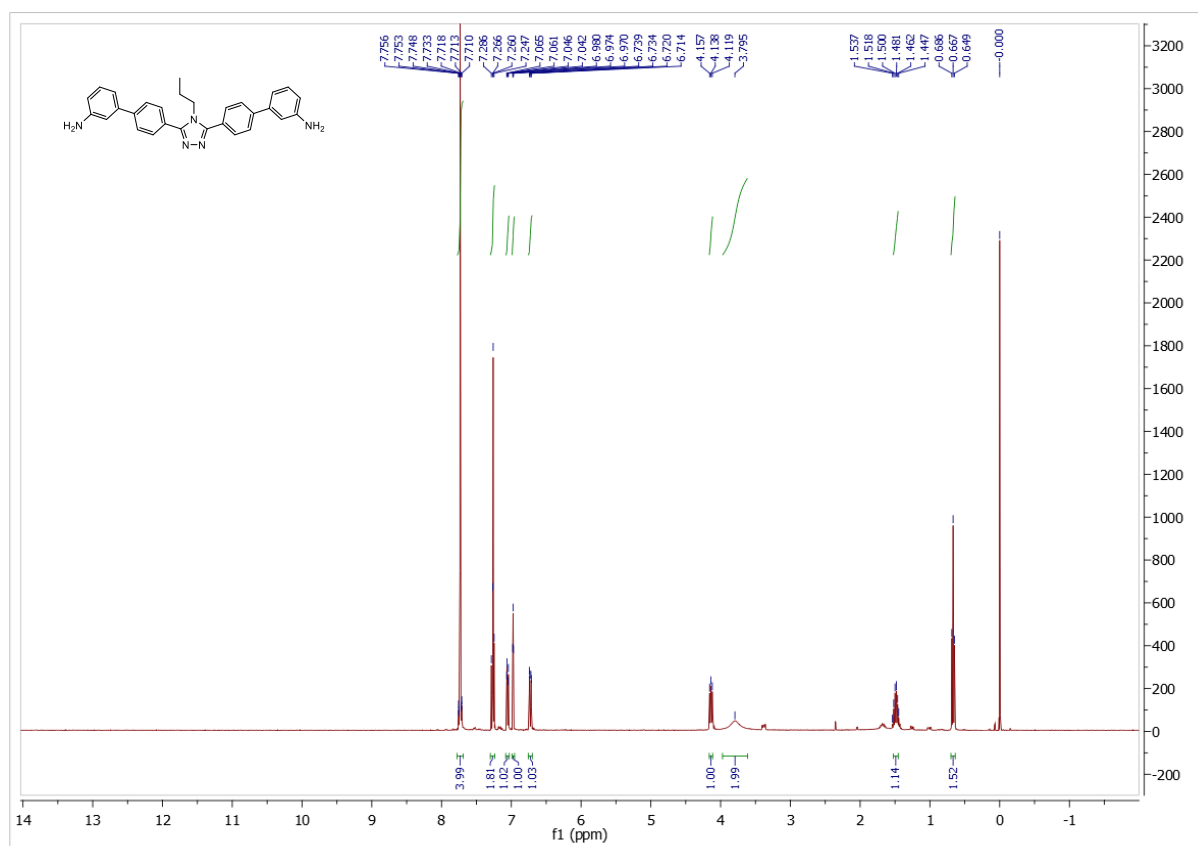
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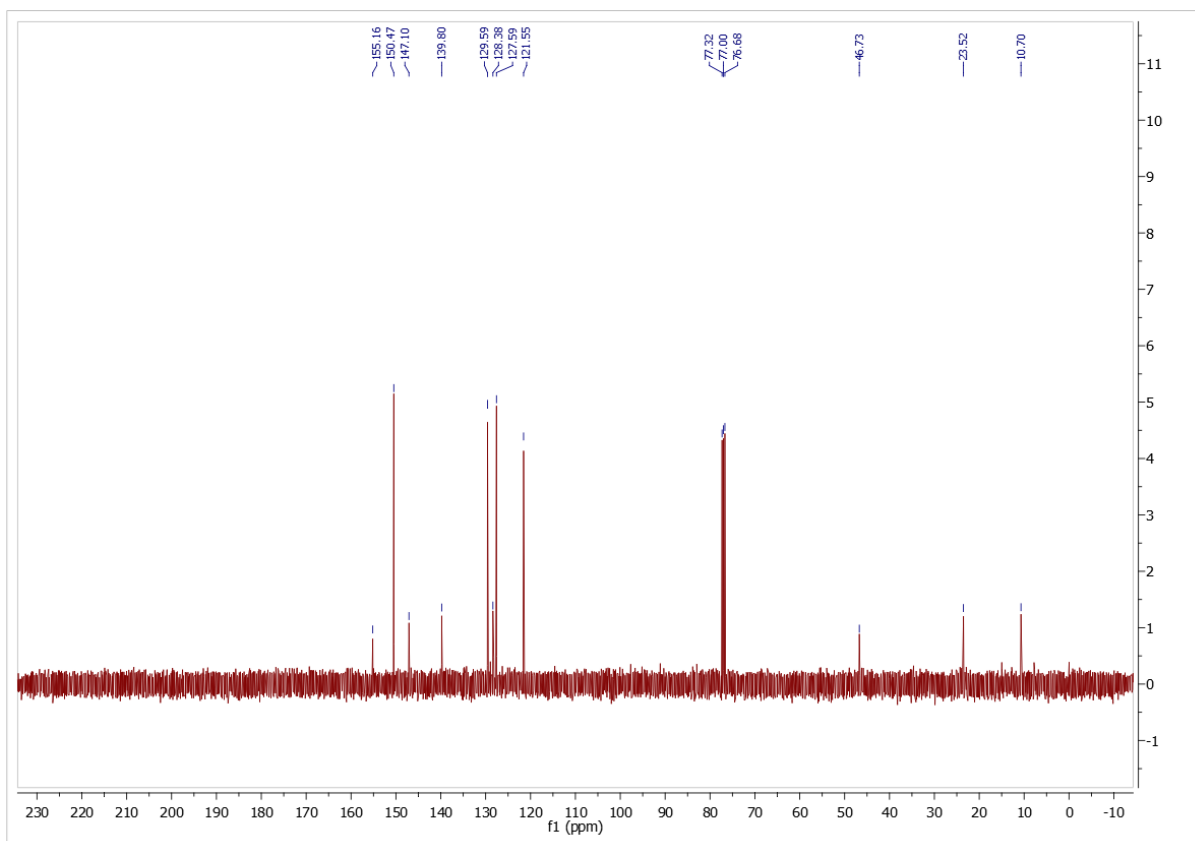
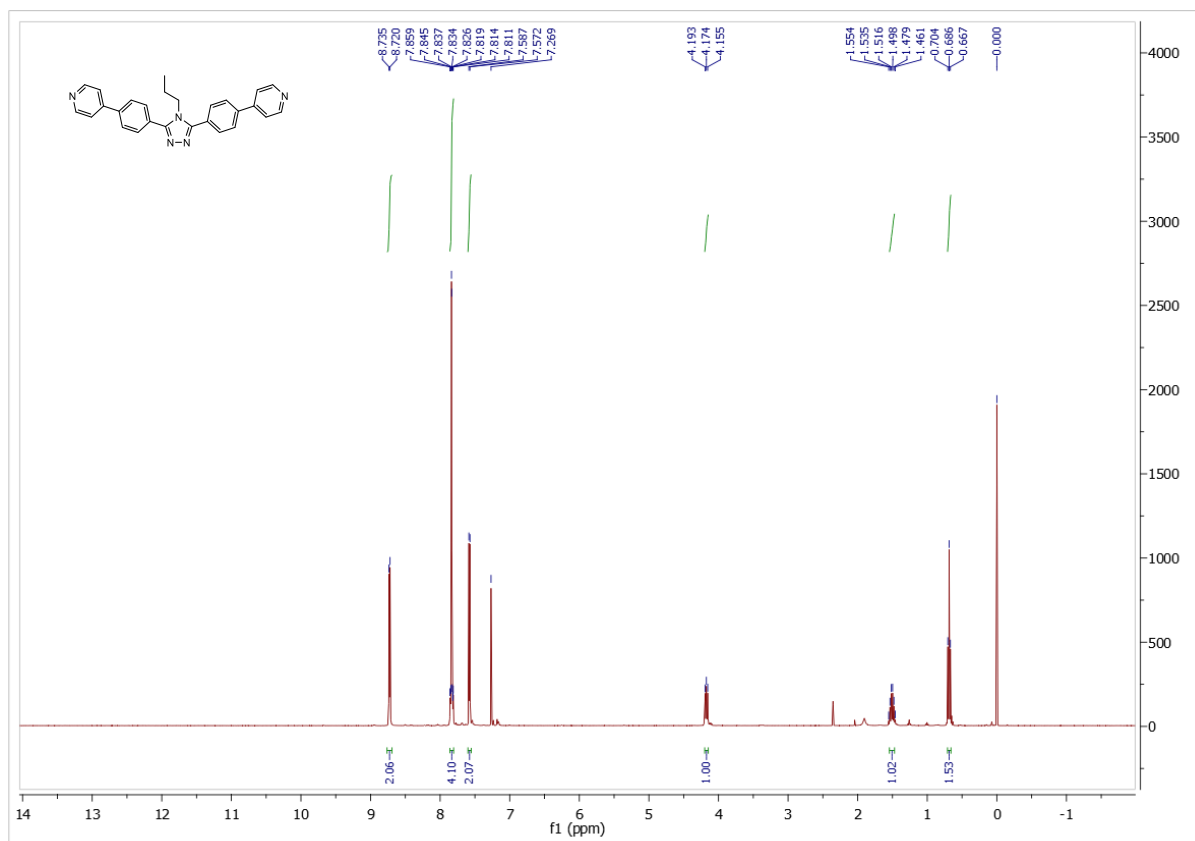
^1H and ^{13}C NMR of 3,5-bis(3'-nitrophenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6g**)



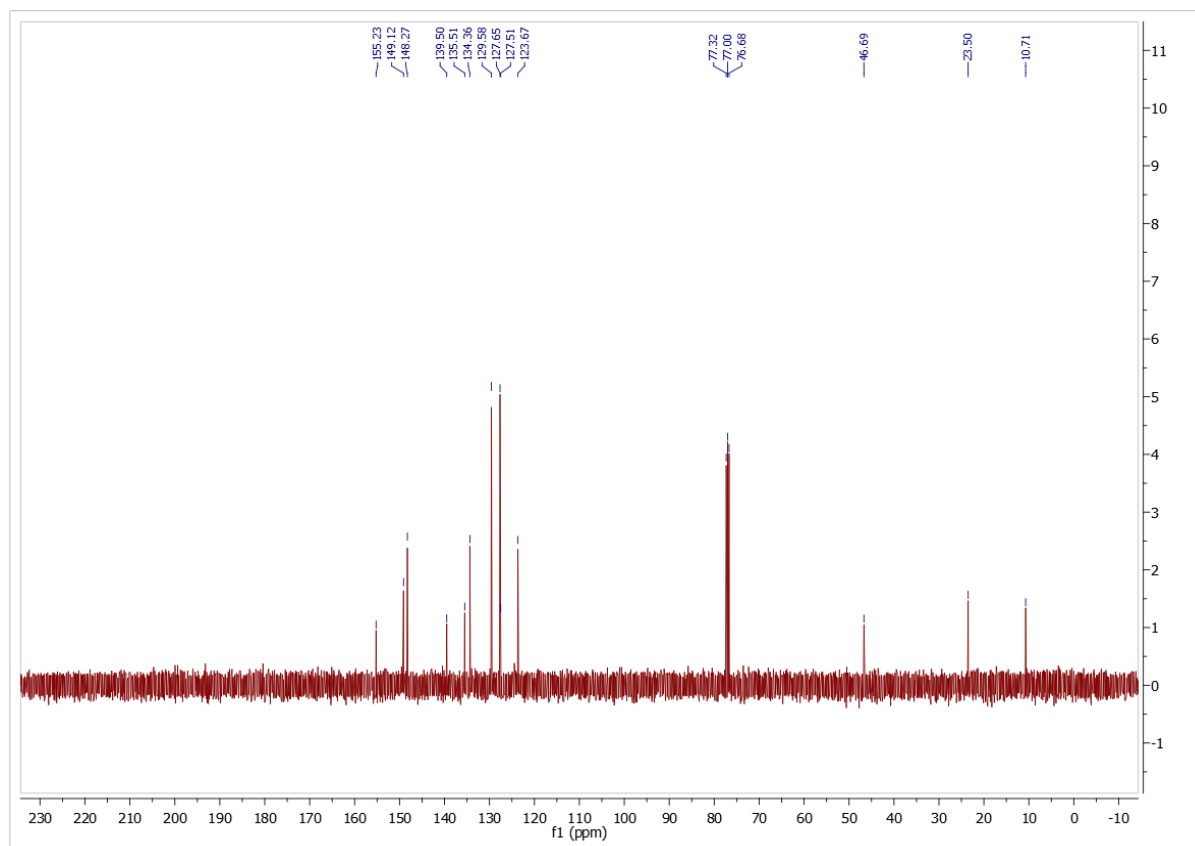
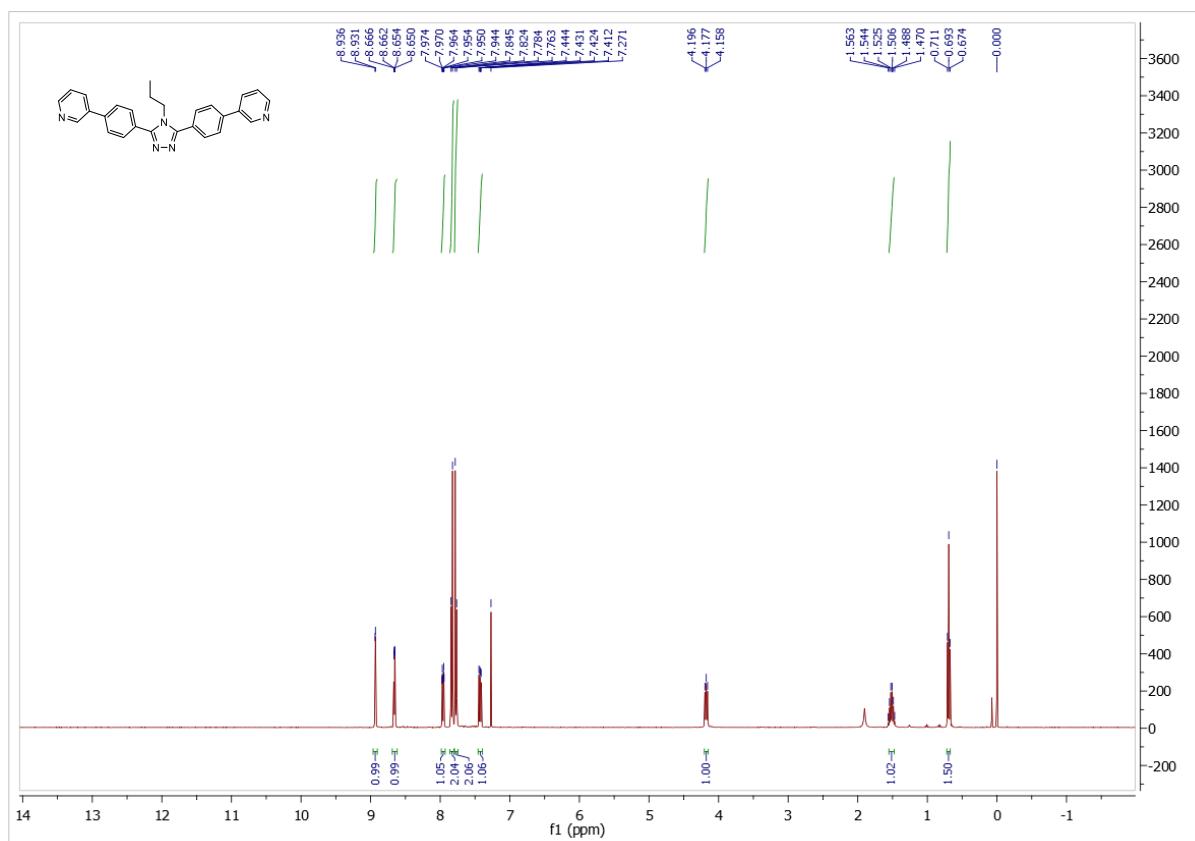
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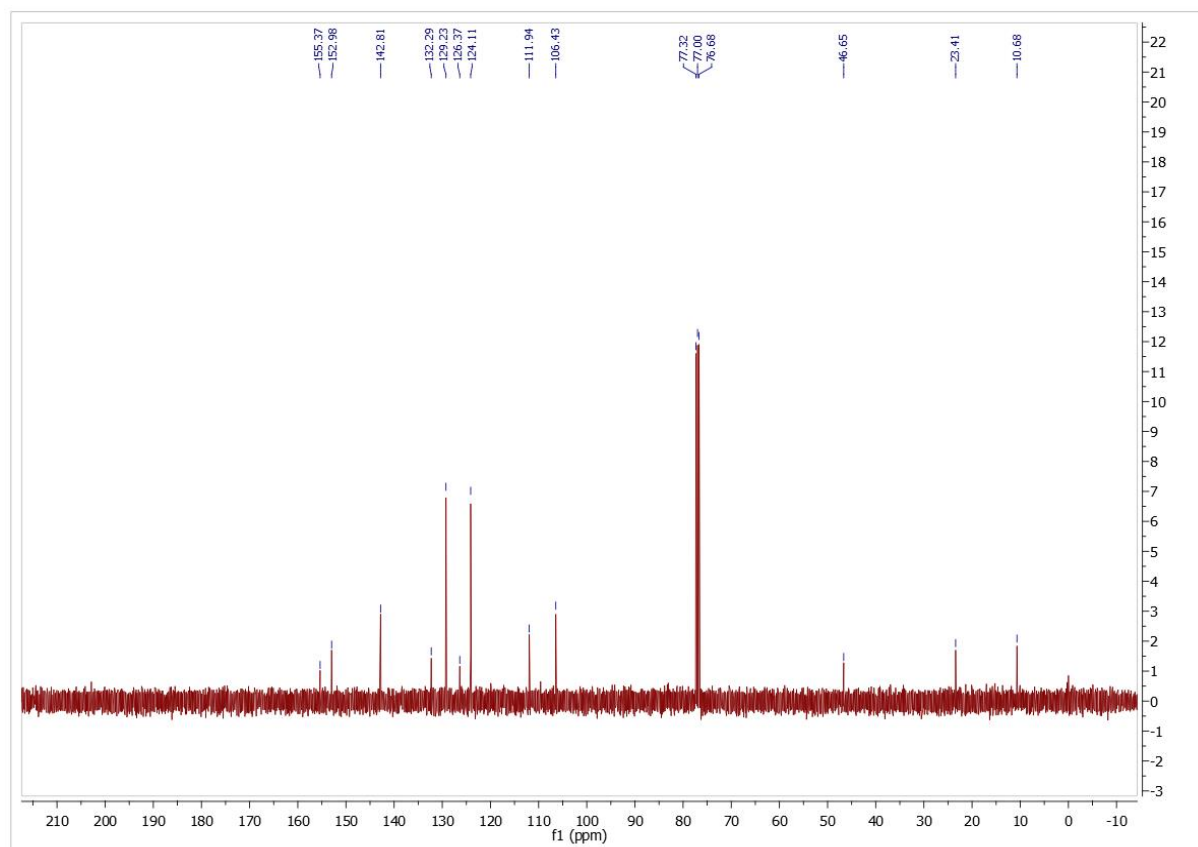
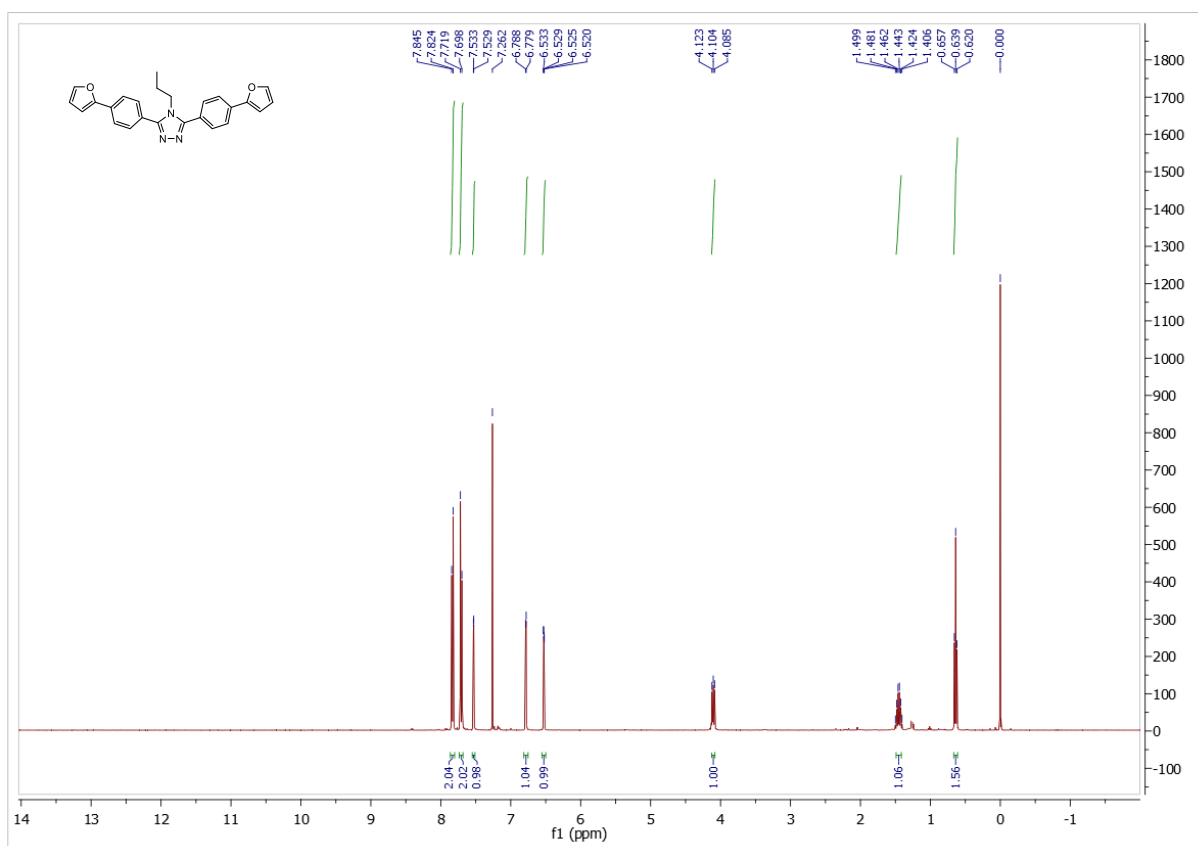
^1H and ^{13}C NMR of 4-propyl-3,5-bis[4-(pyridin-4-yl)phenyl]-4*H*-1,2,4-triazole (**6i**)



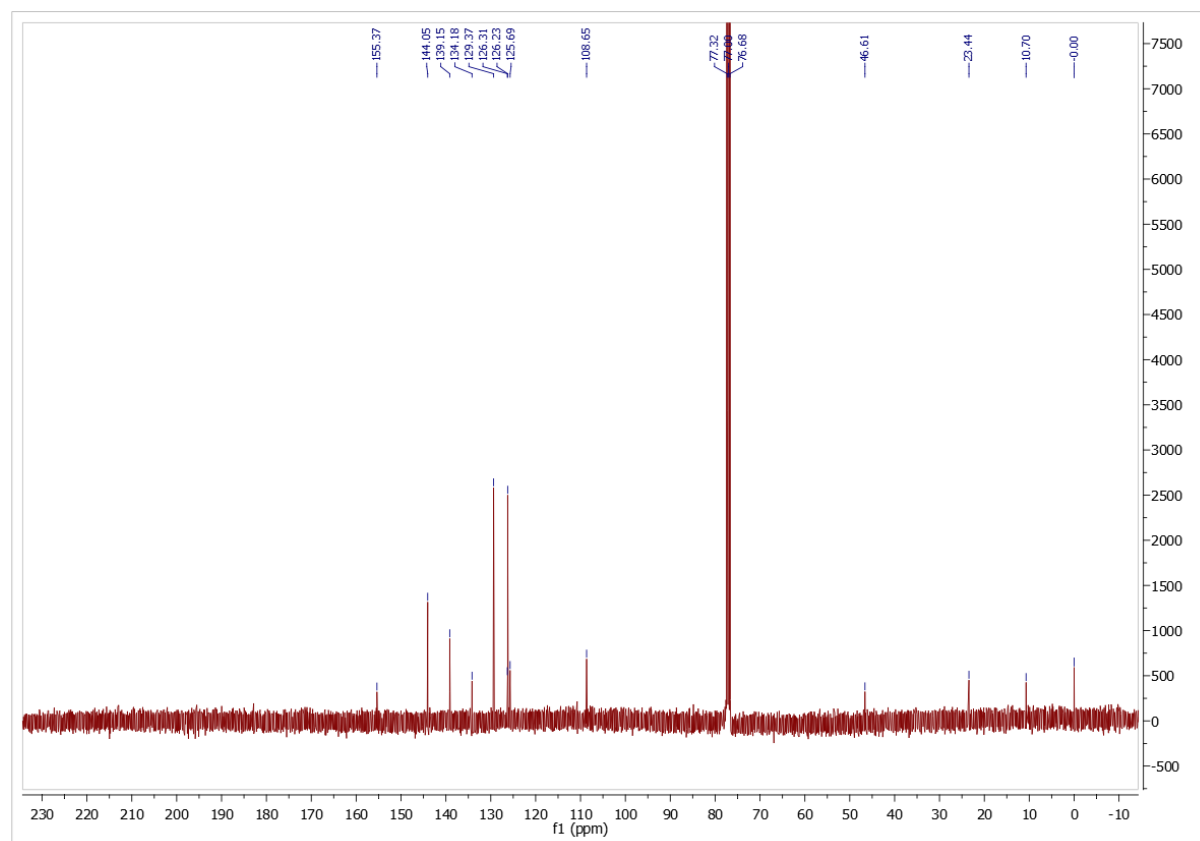
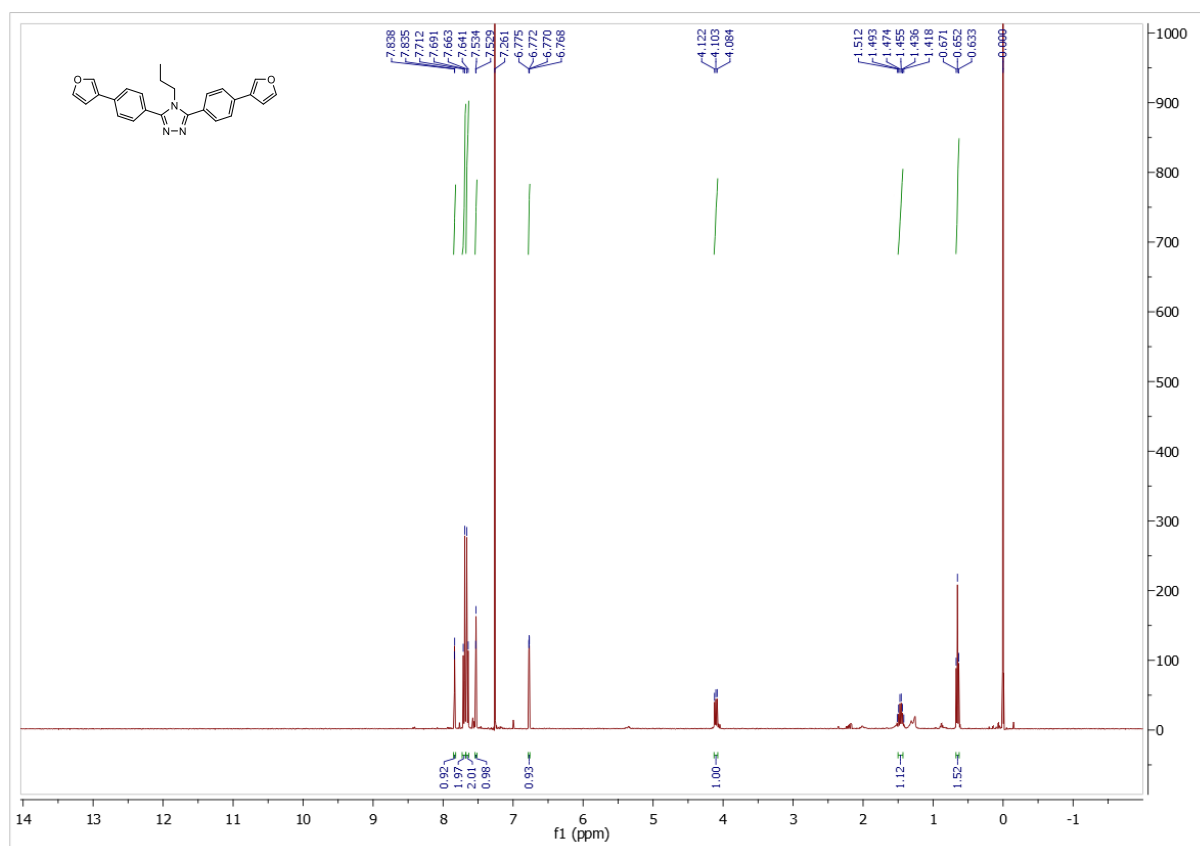
^1H and ^{13}C NMR of 4-propyl-3,5-bis[4-(pyridin-3-yl)phenyl]-4*H*-1,2,4-triazole (**6j**)



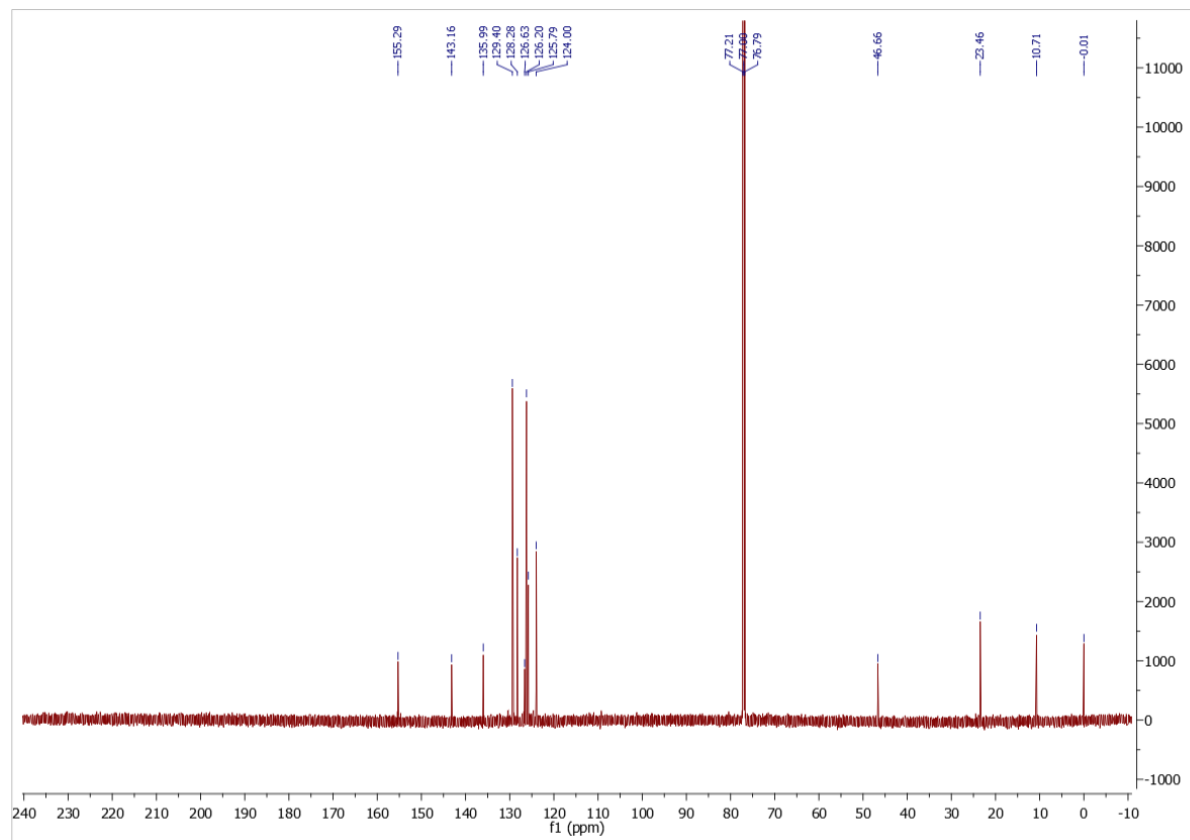
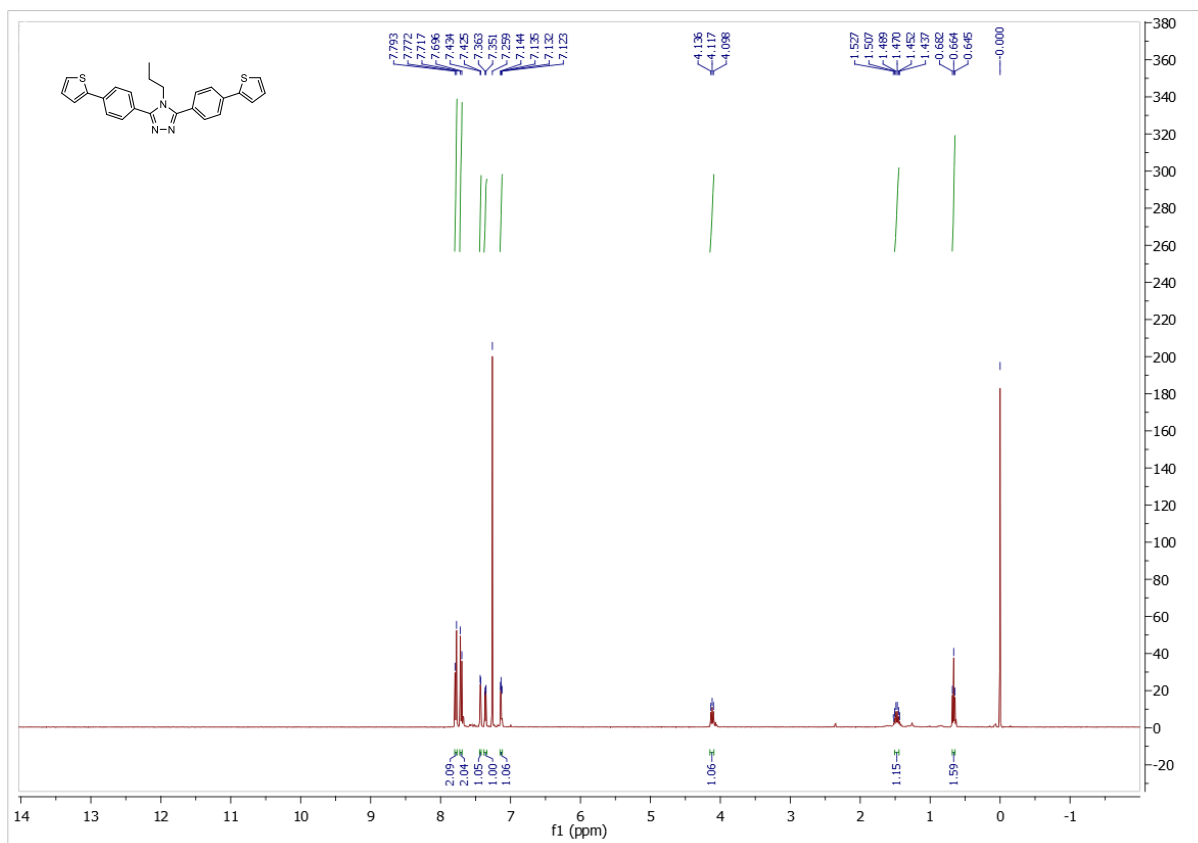
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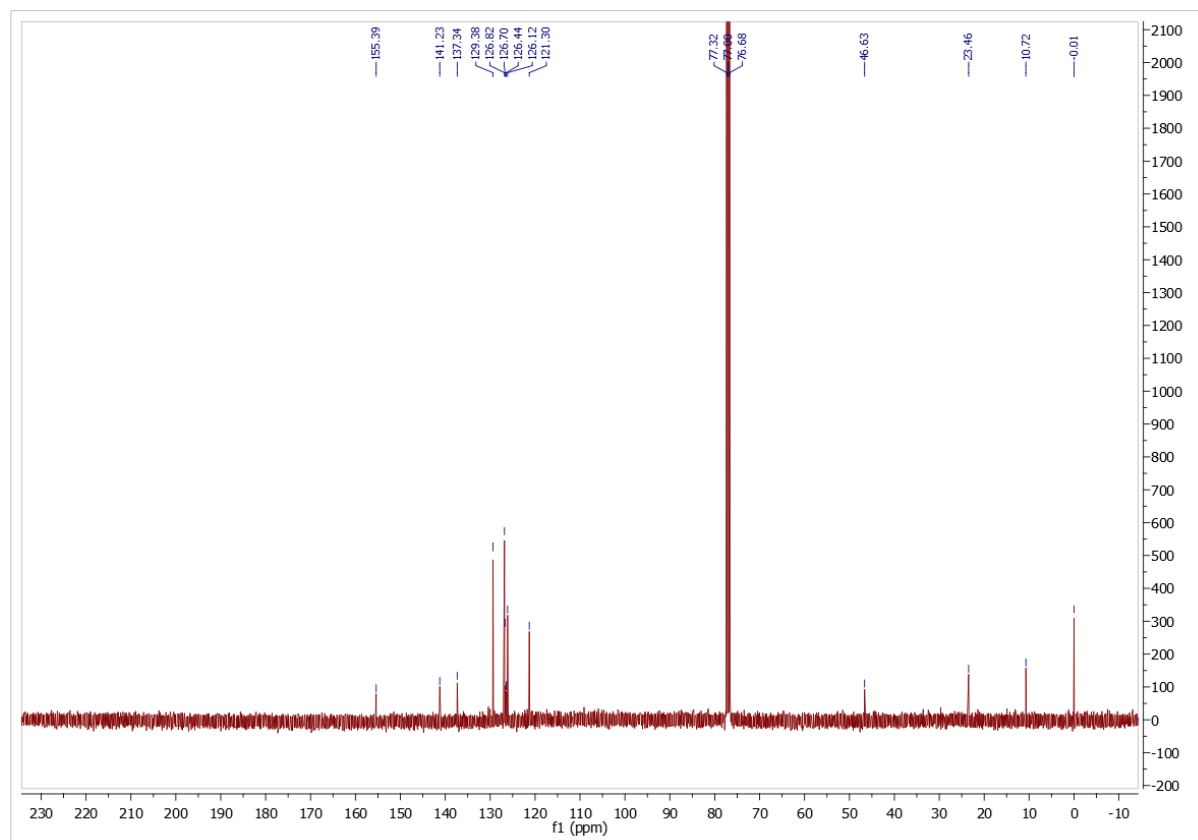
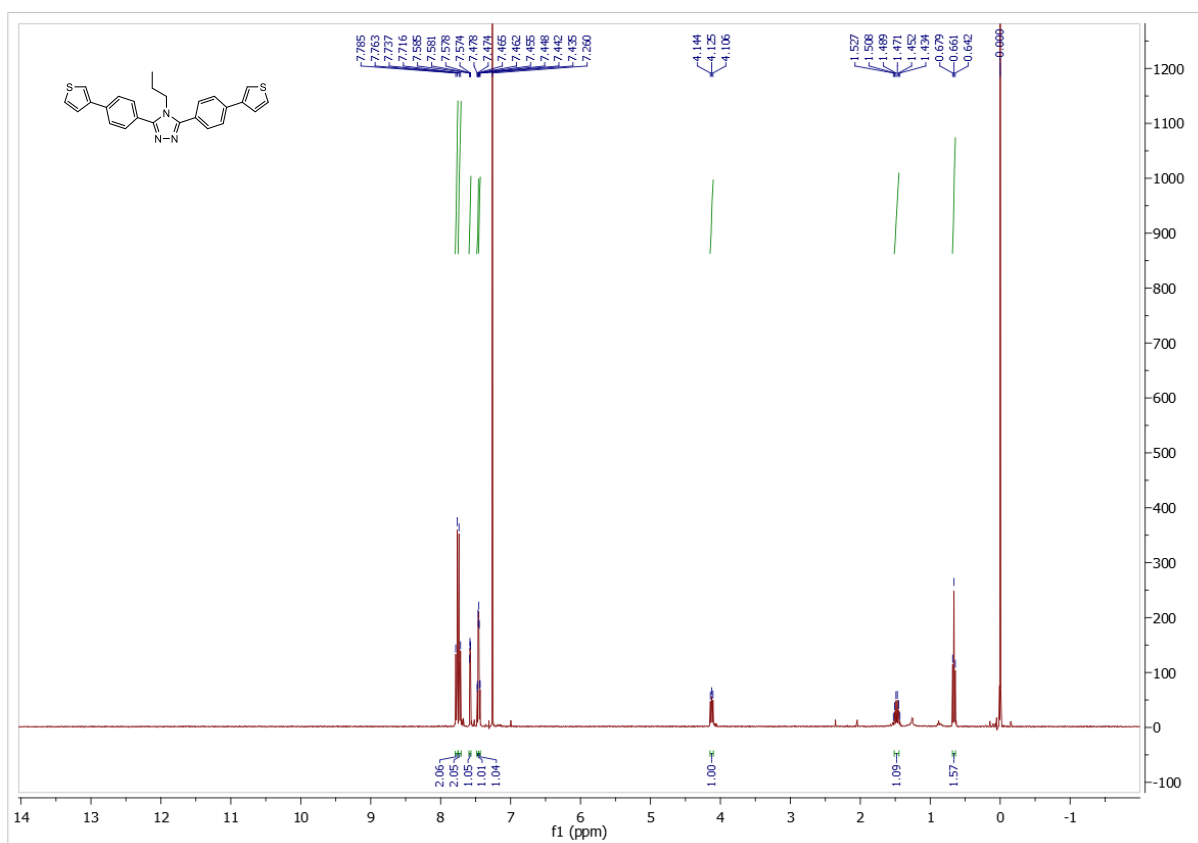
^1H and ^{13}C NMR of 3,5-bis[4-(furan-3-yl)phenyl]-4-propyl-4*H*-1,2,4-triazole (**6l**)



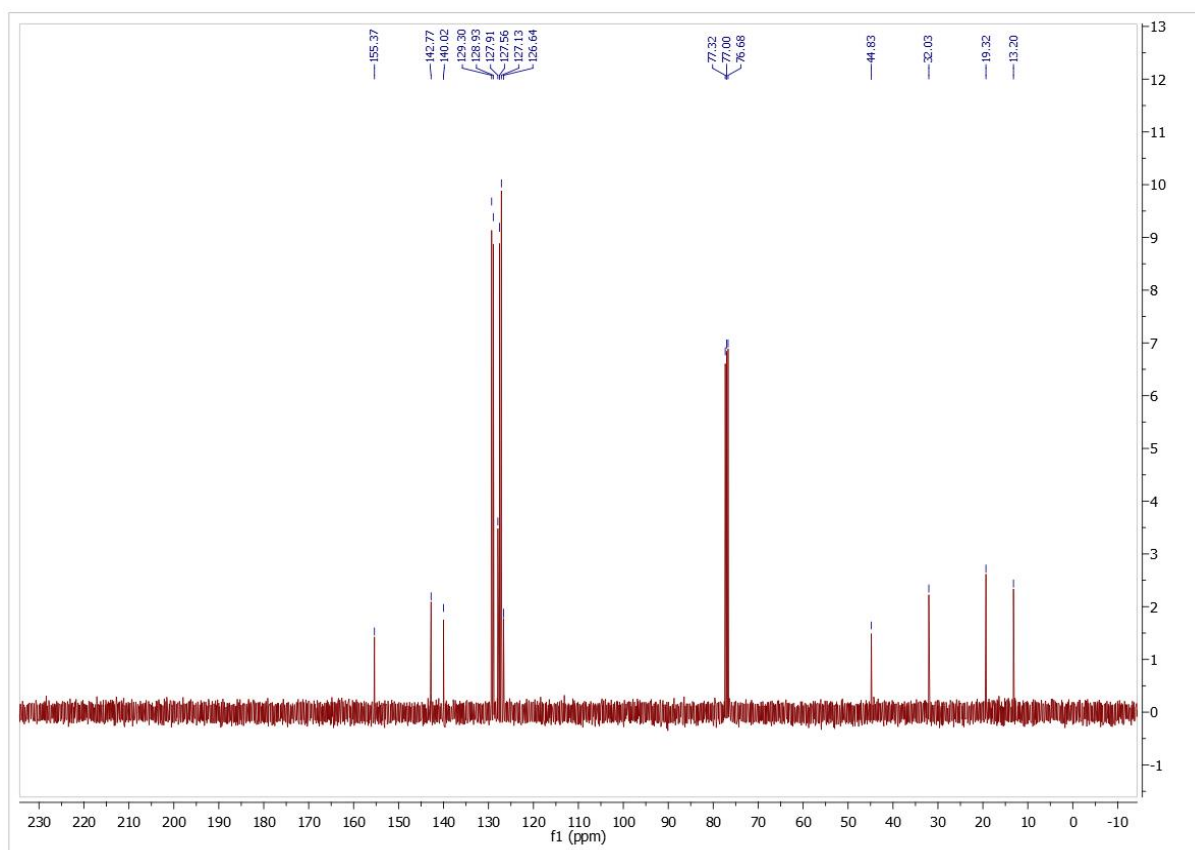
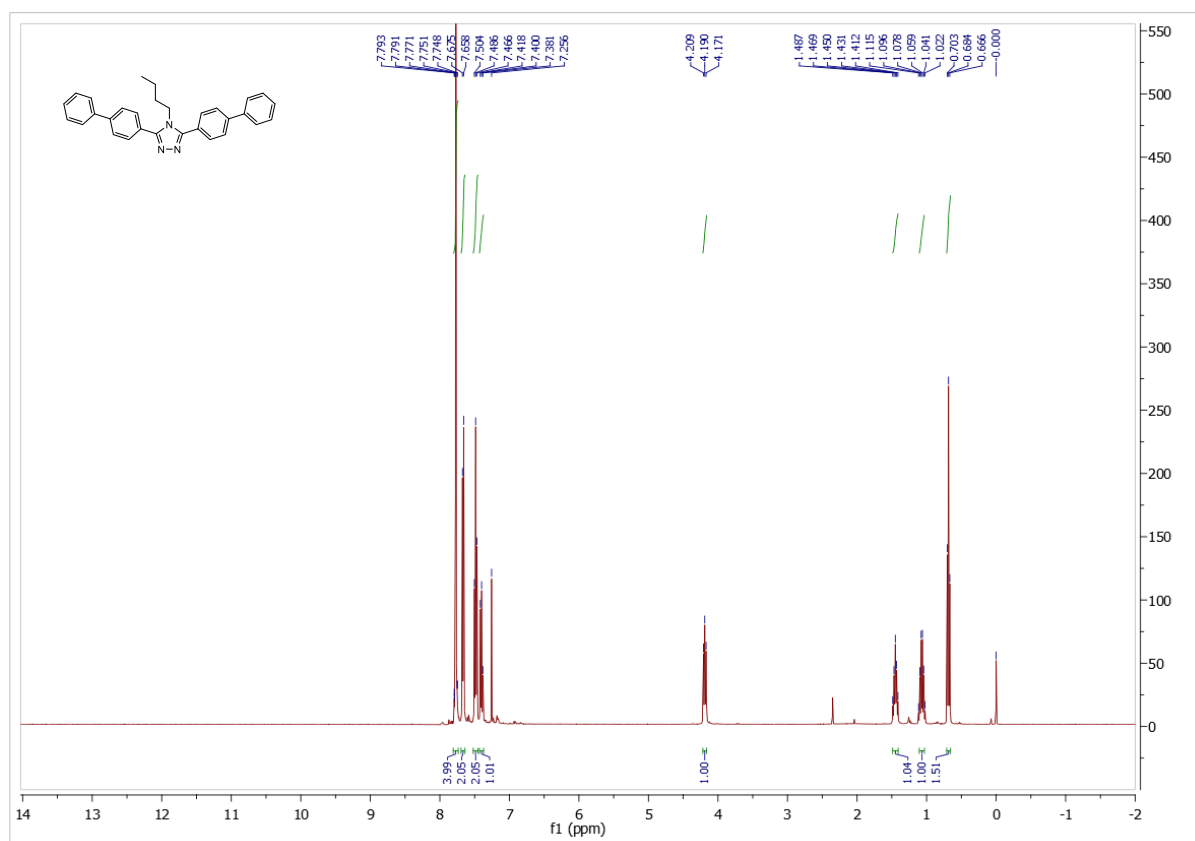
^1H and ^{13}C NMR of 4-propyl-3,5-bis[4-(thiophen-2-yl)phenyl]-4*H*-1,2,4-triazole (**6m**)



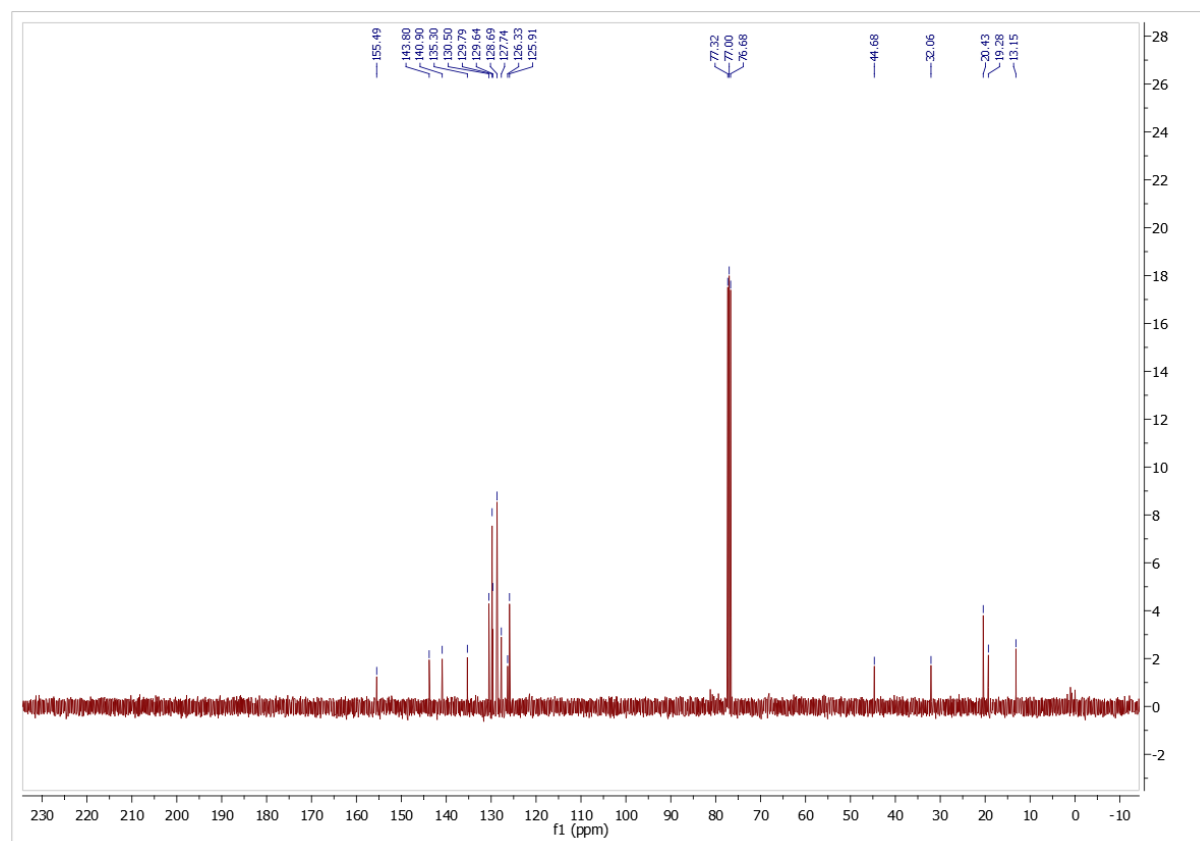
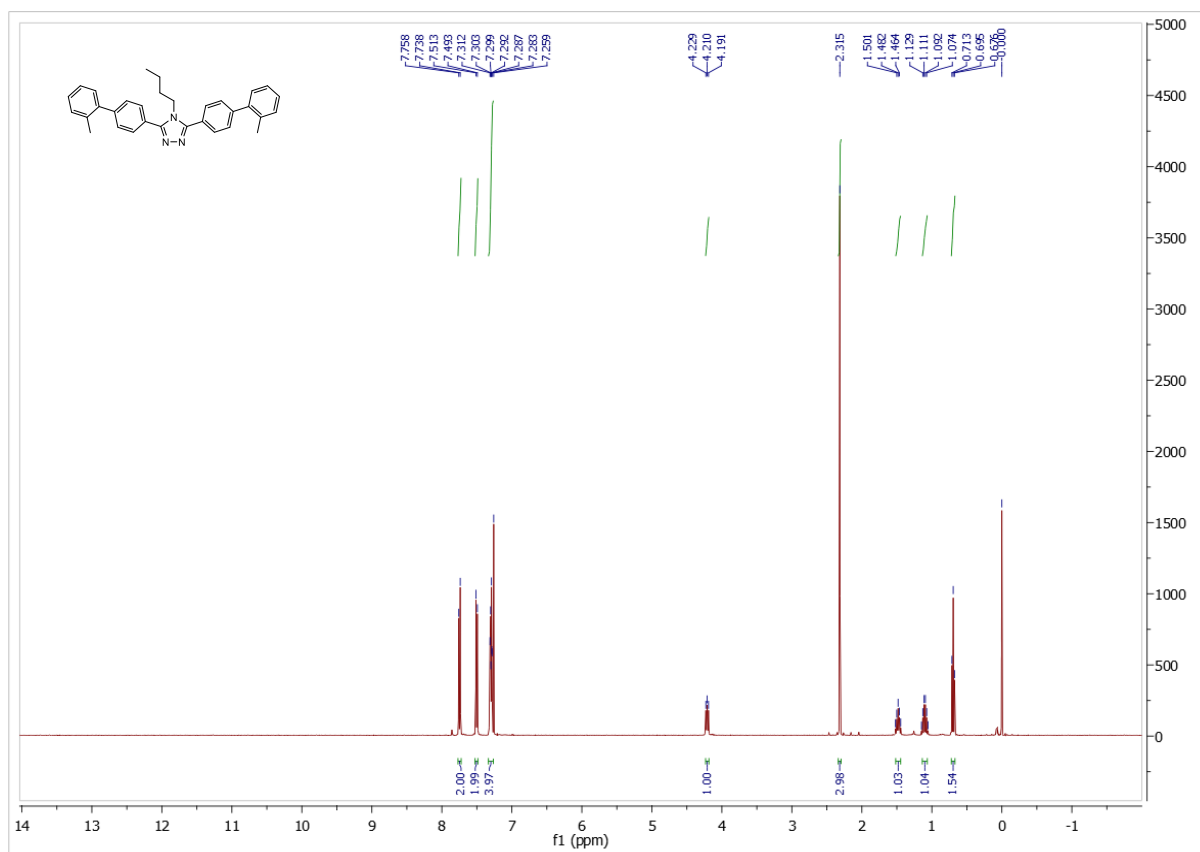
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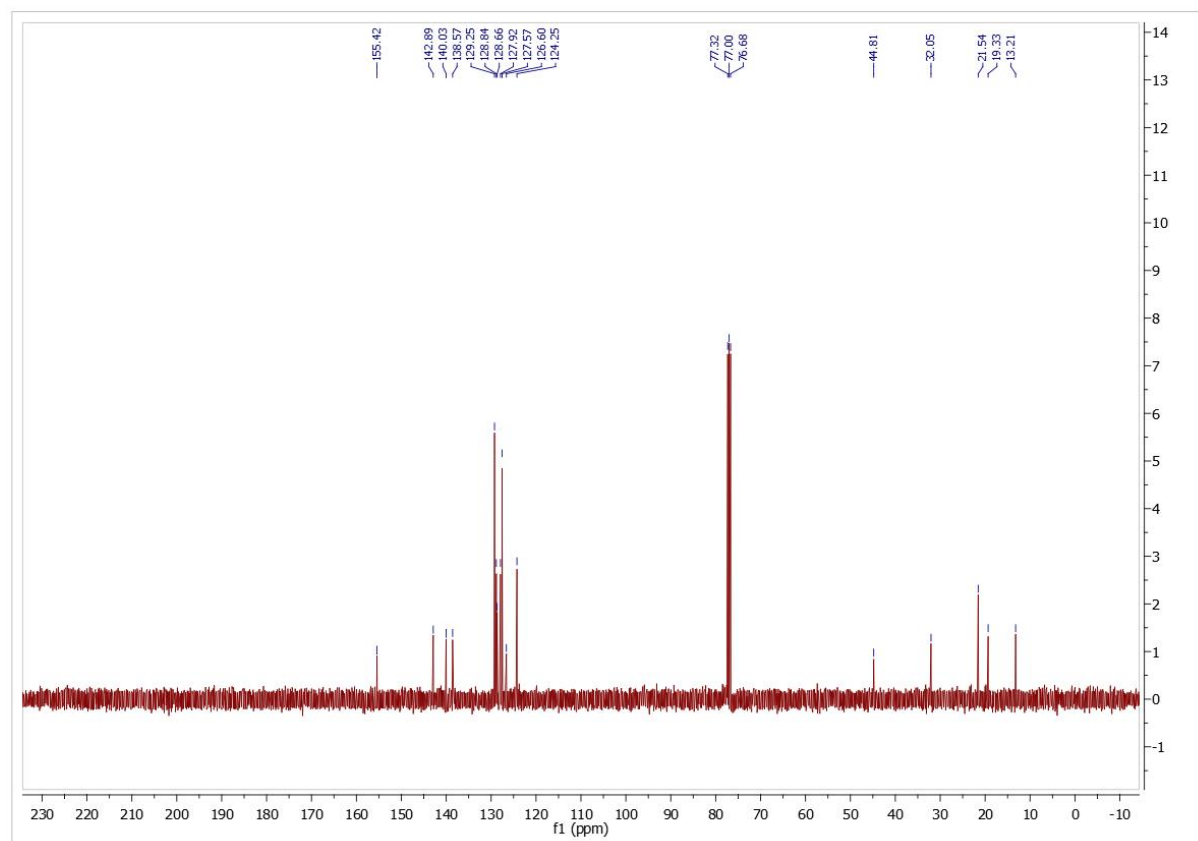
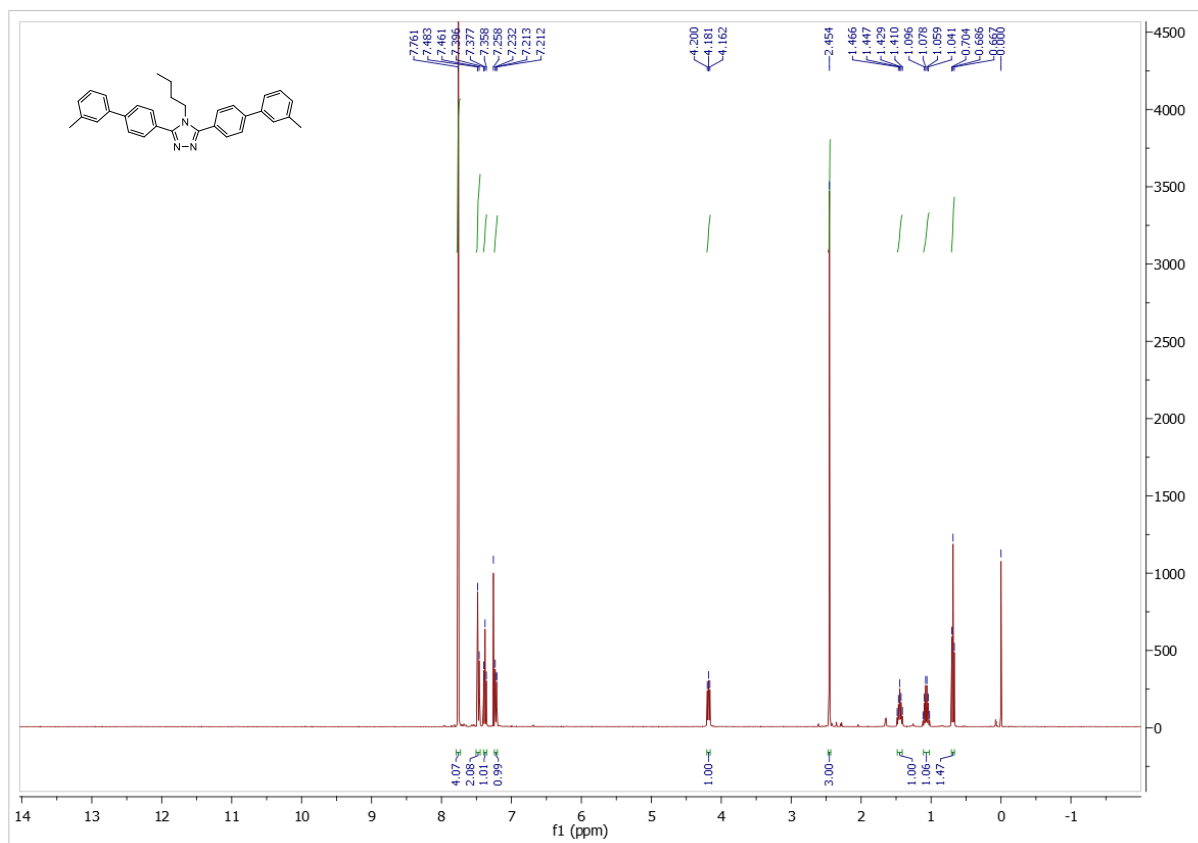
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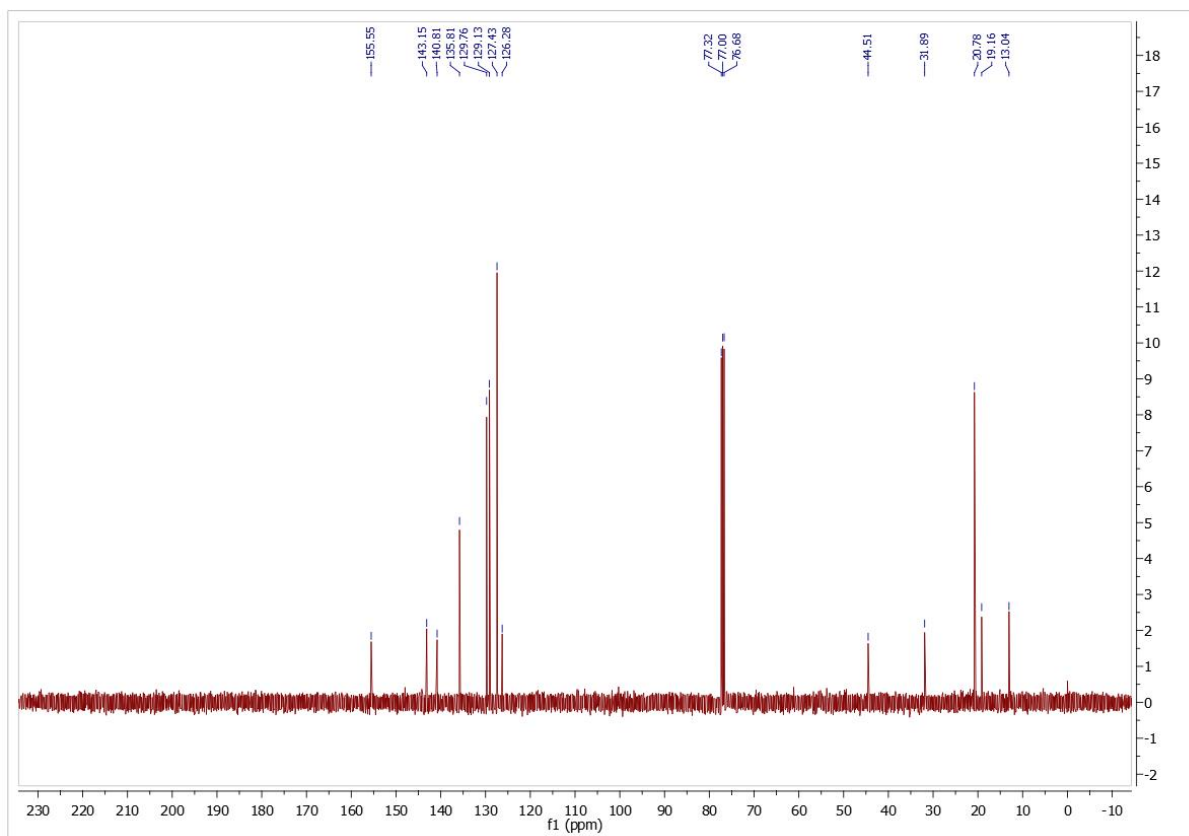
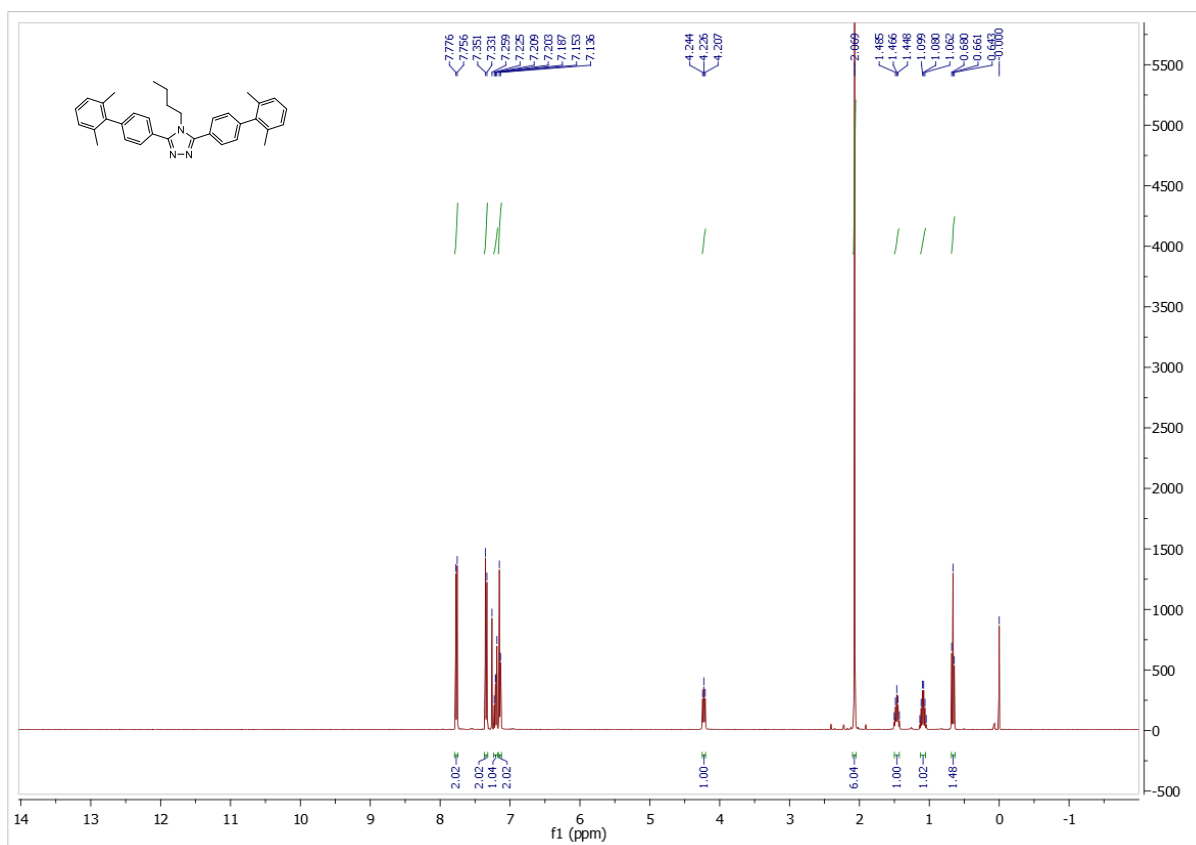
^1H and ^{13}C NMR of 4-butyl-3,5-bis(2'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**7b**)



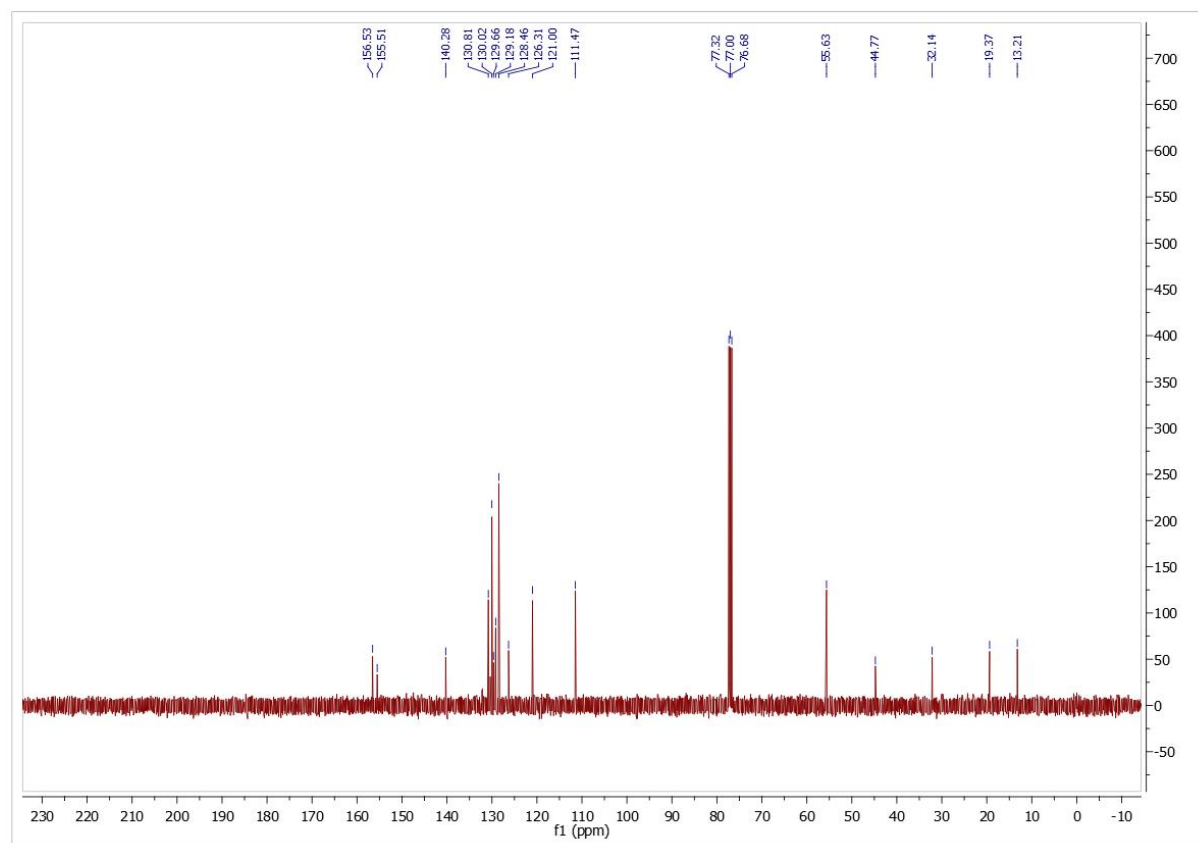
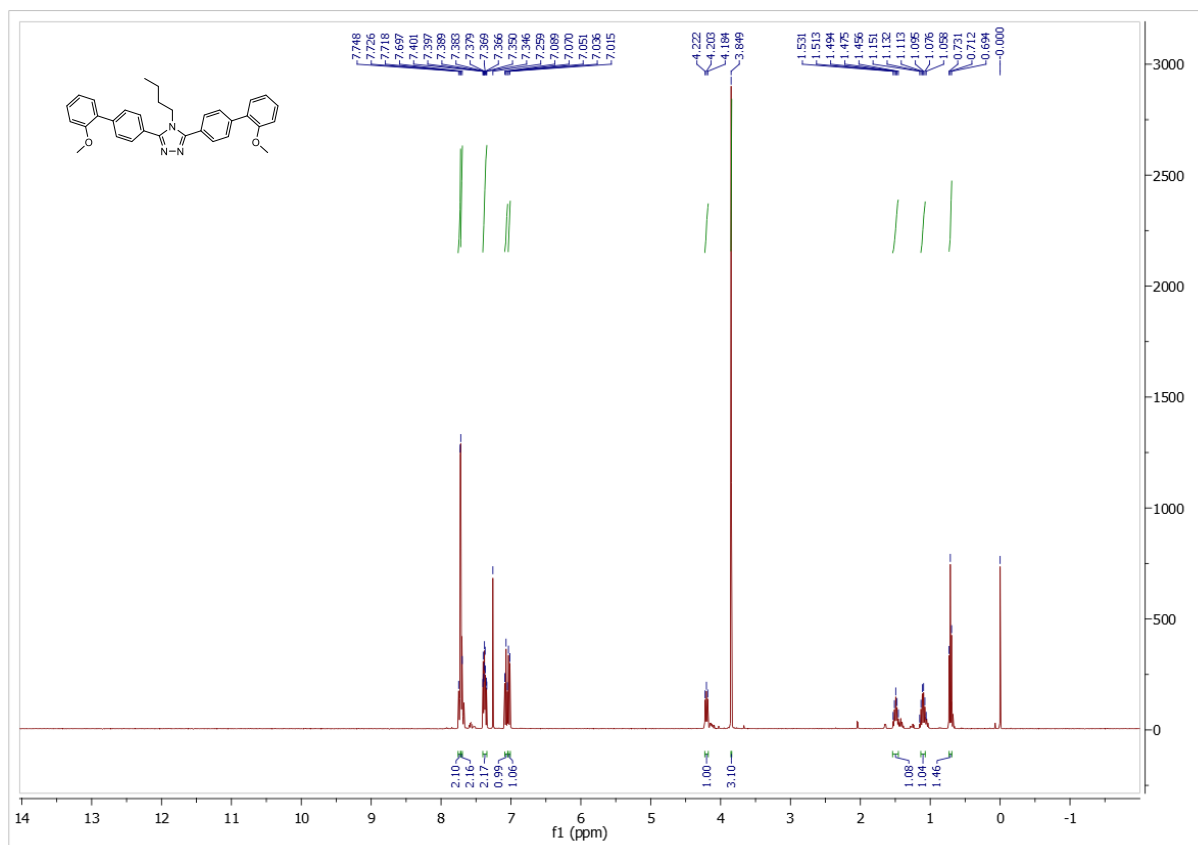
^1H and ^{13}C NMR of 4-butyl-3,5-bis(3'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**7c**)



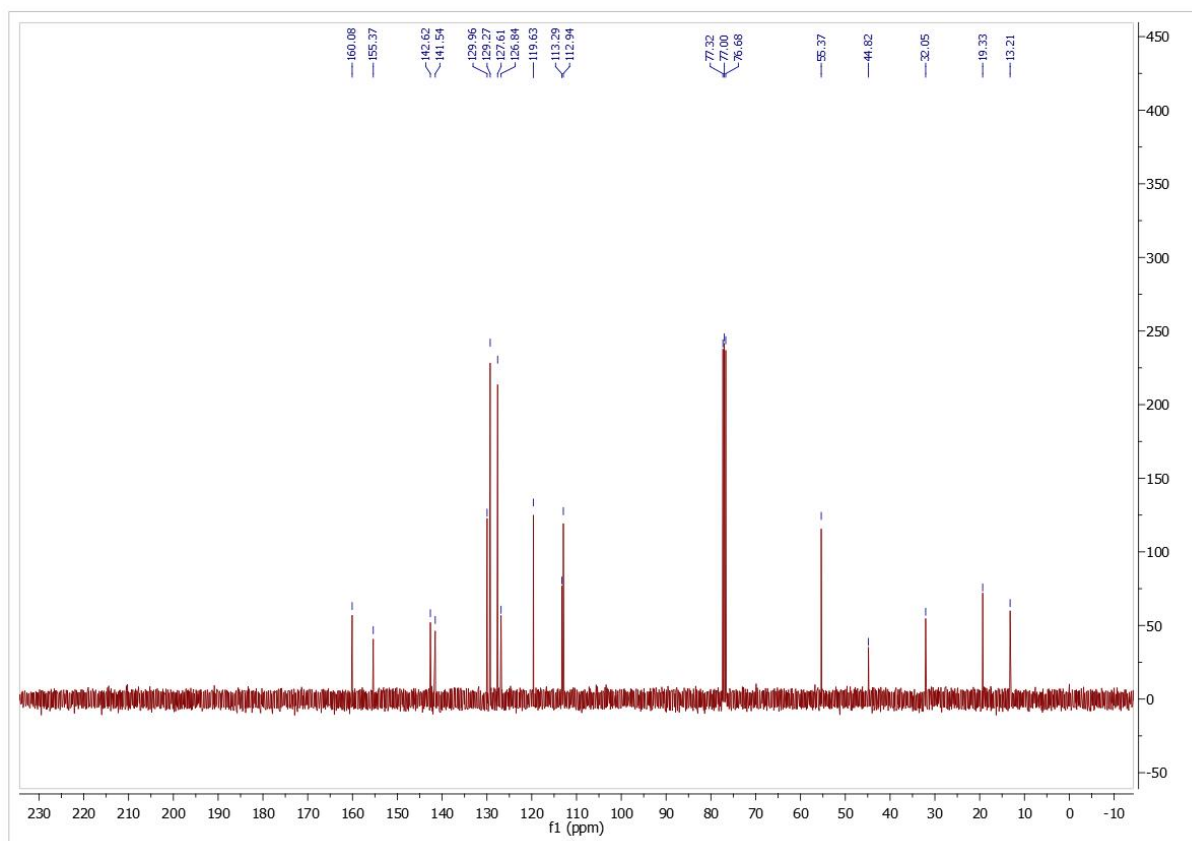
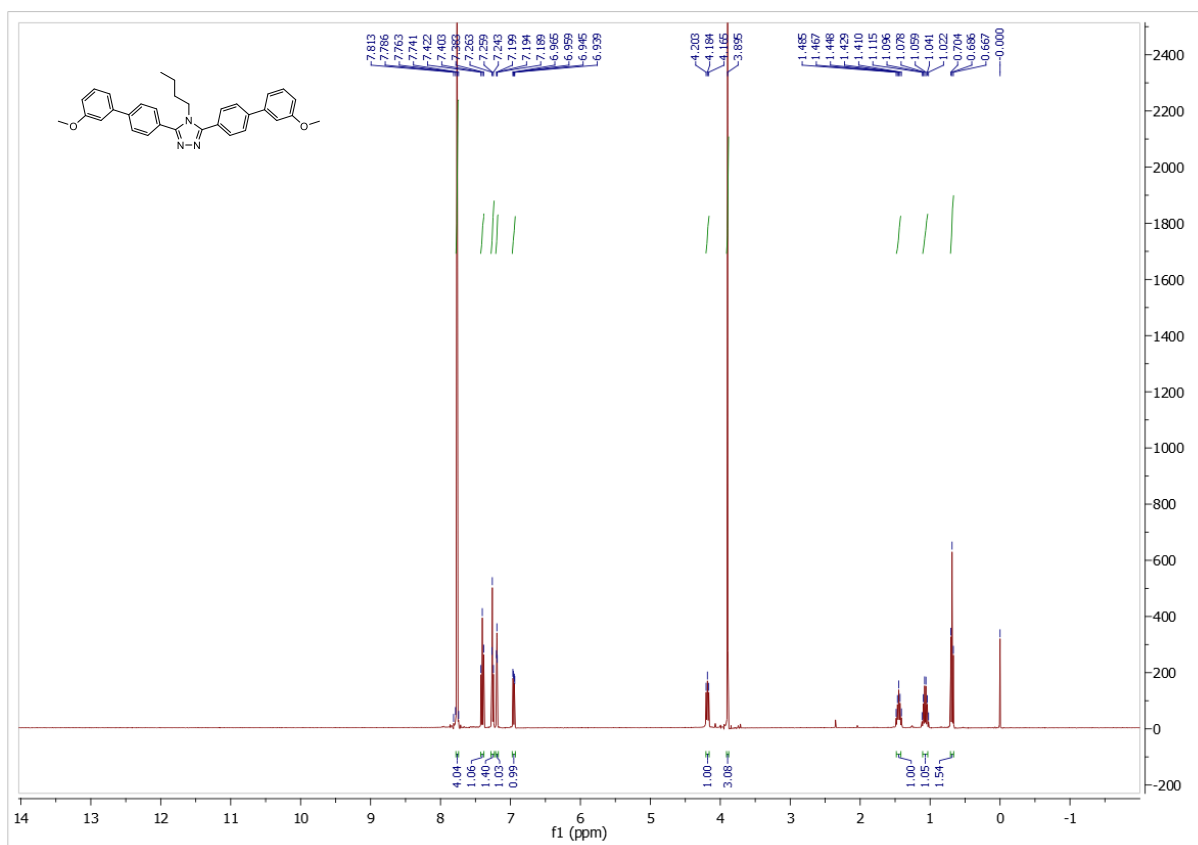
^1H and ^{13}C NMR of 4-butyl-3,5-bis(2',6'-dimethylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**7d**)



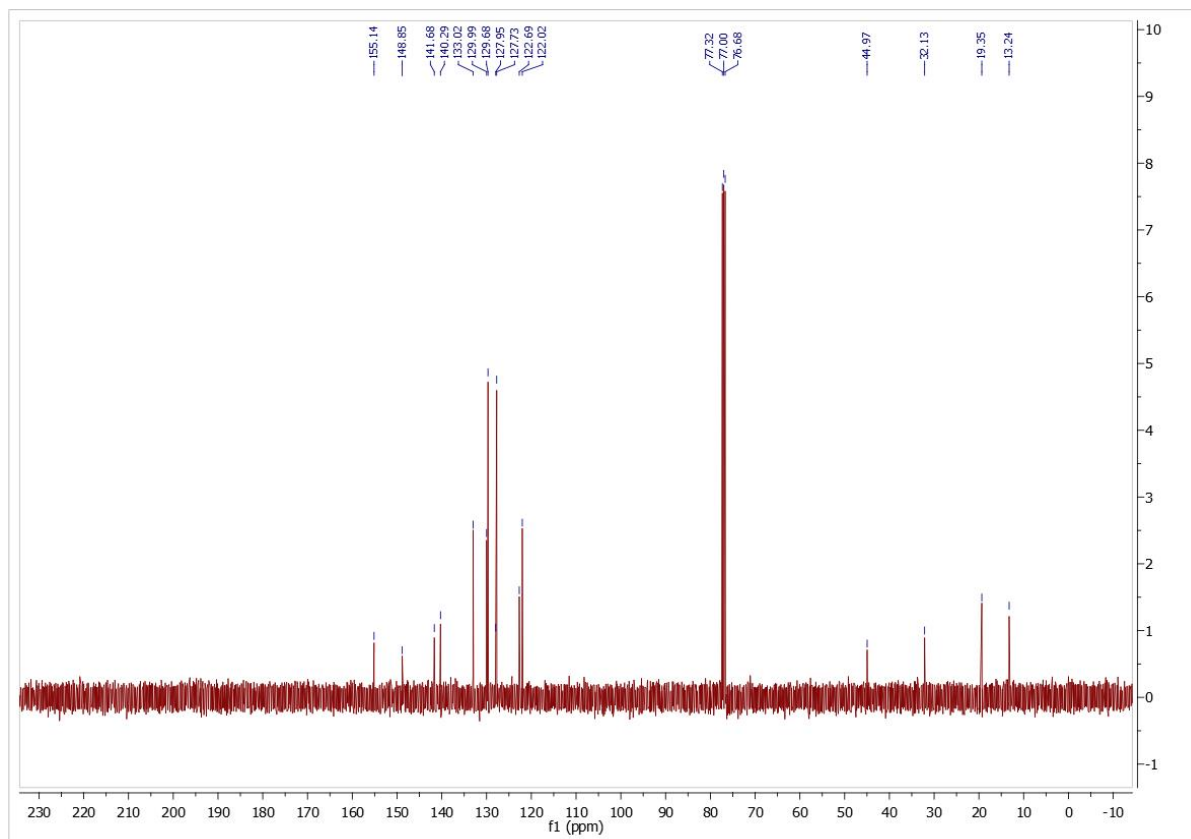
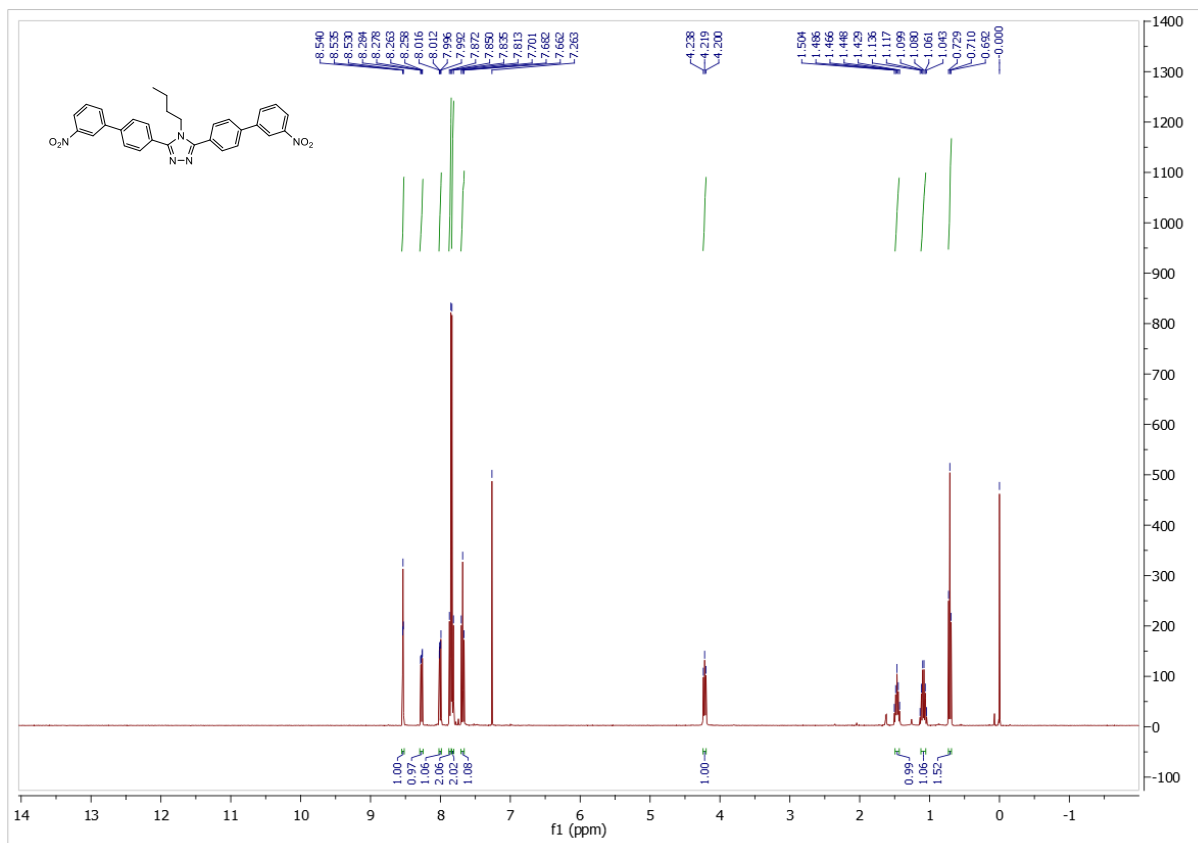
^1H and ^{13}C NMR of 4-butyl-3,5-bis(2'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**7e**)



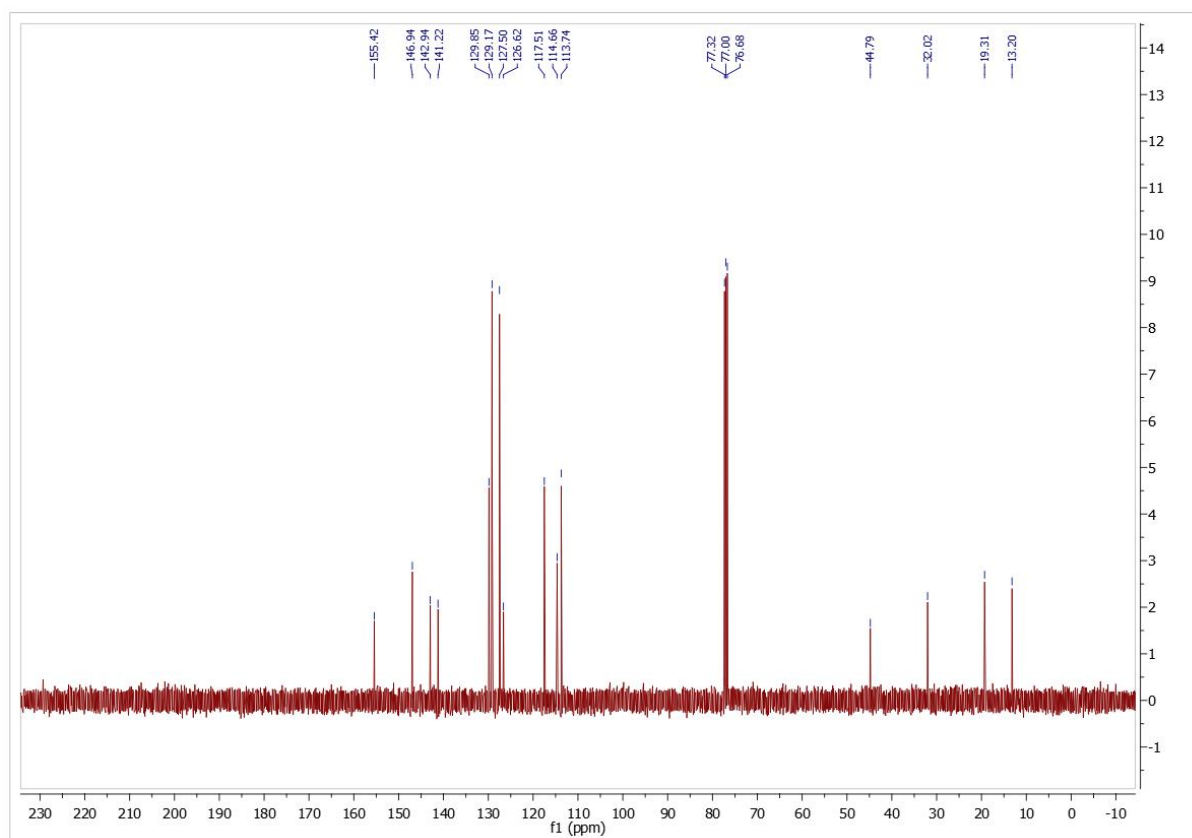
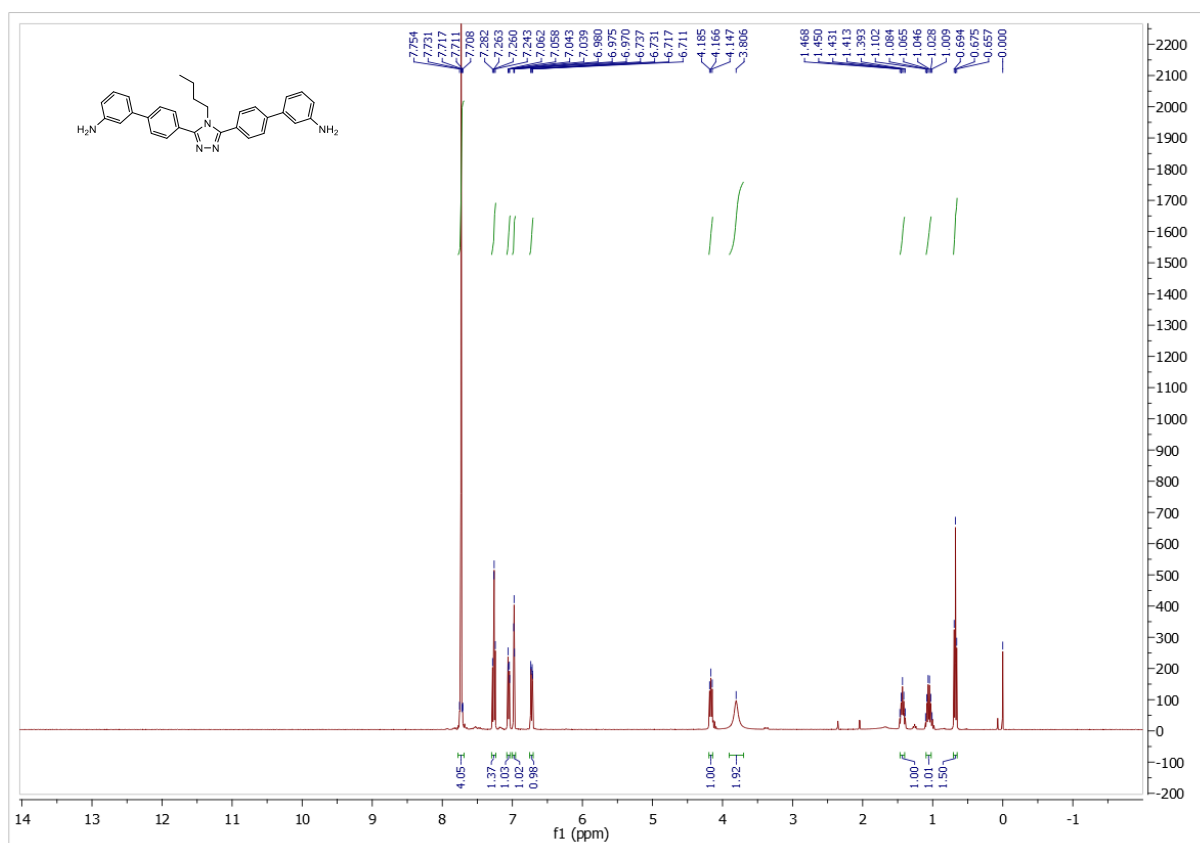
^1H and ^{13}C NMR of 4-butyl-3,5-bis(3'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**7f**)



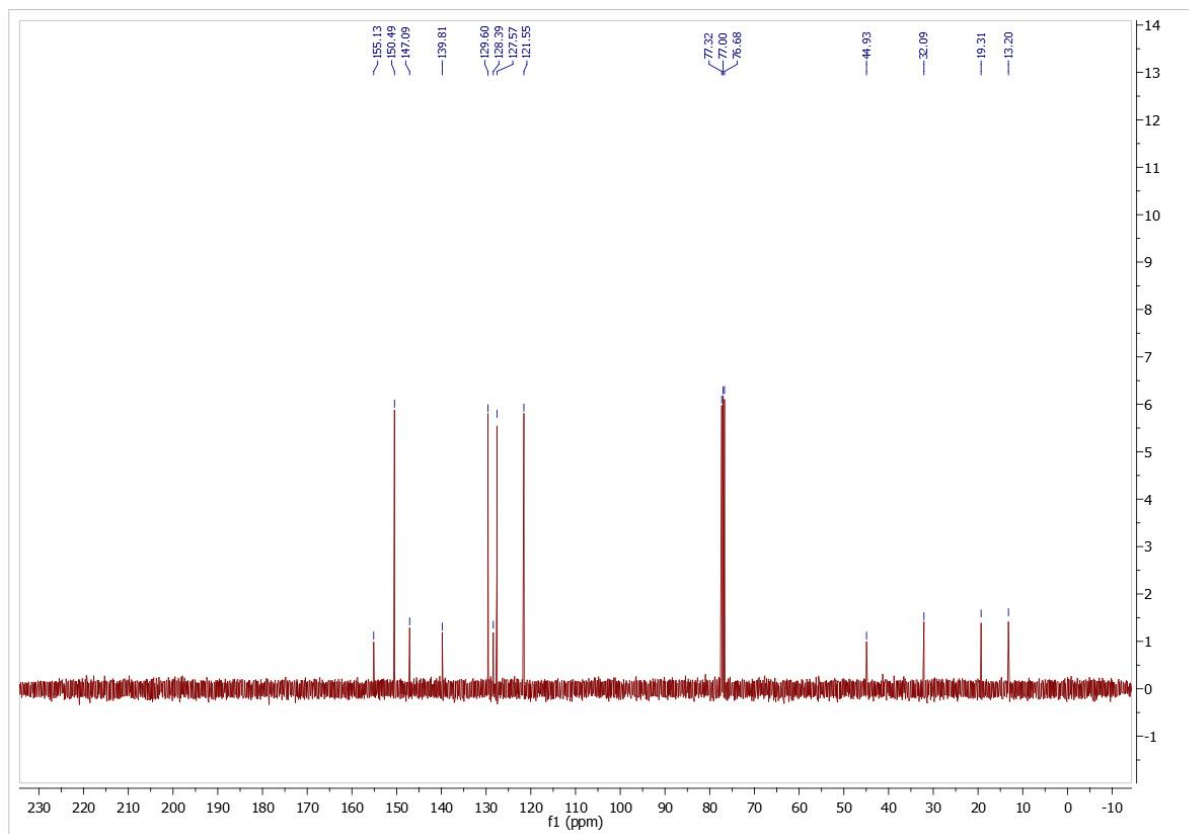
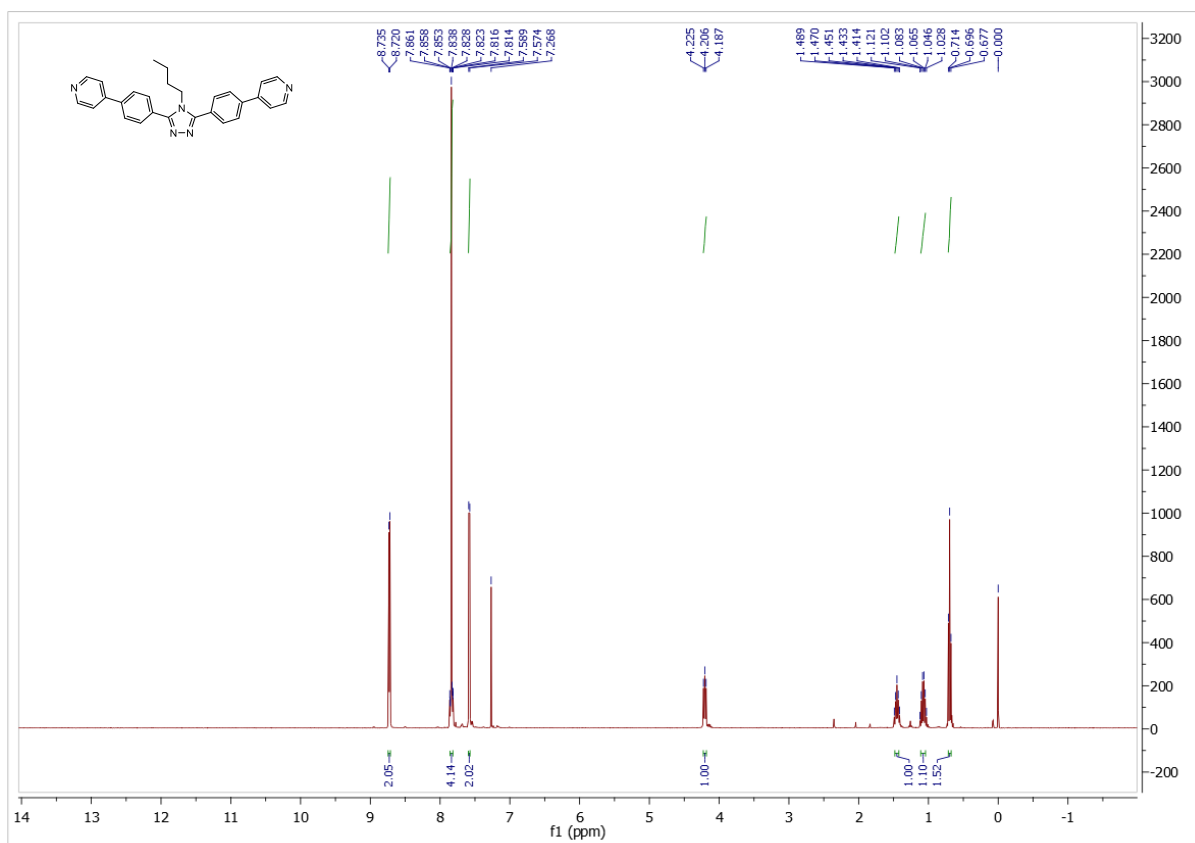
^1H and ^{13}C NMR of 4-butyl-3,5-bis(3'-nitrophenyl-4-yl)-4*H*-1,2,4-triazole (**7g**)



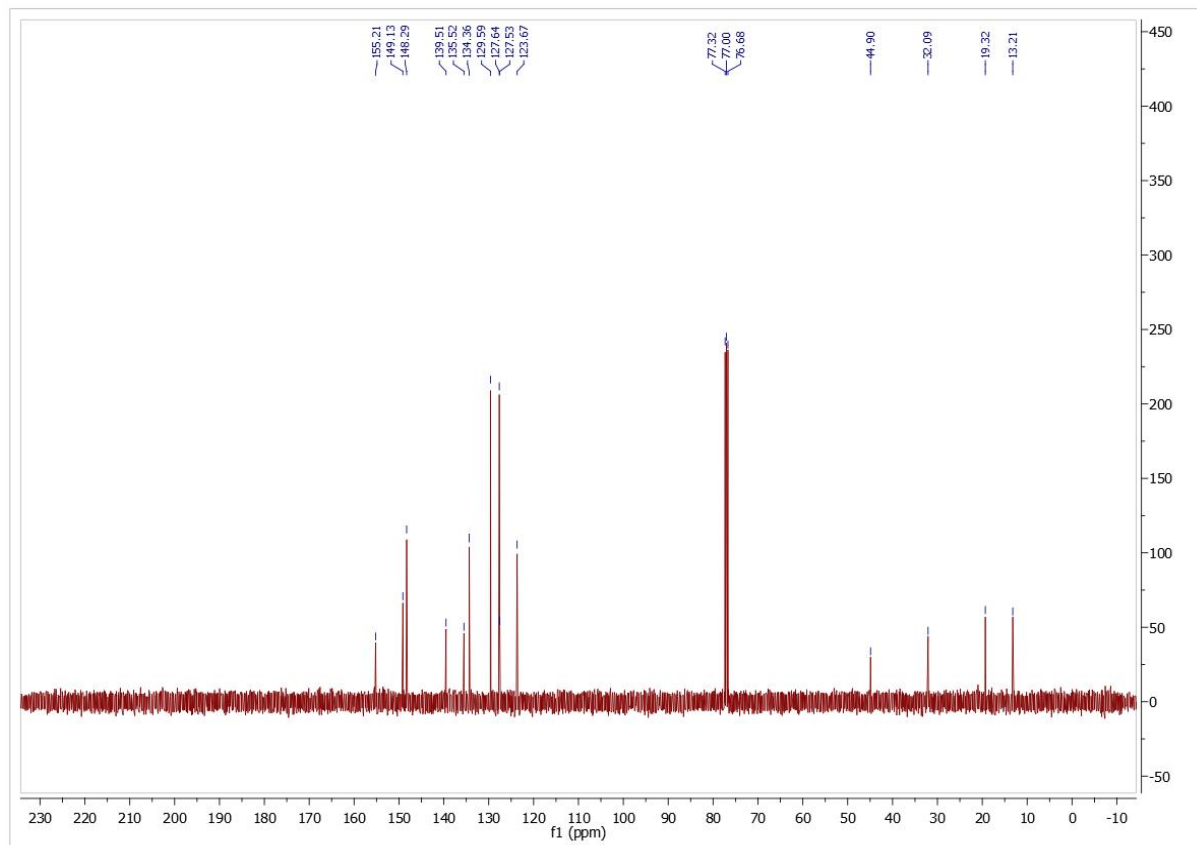
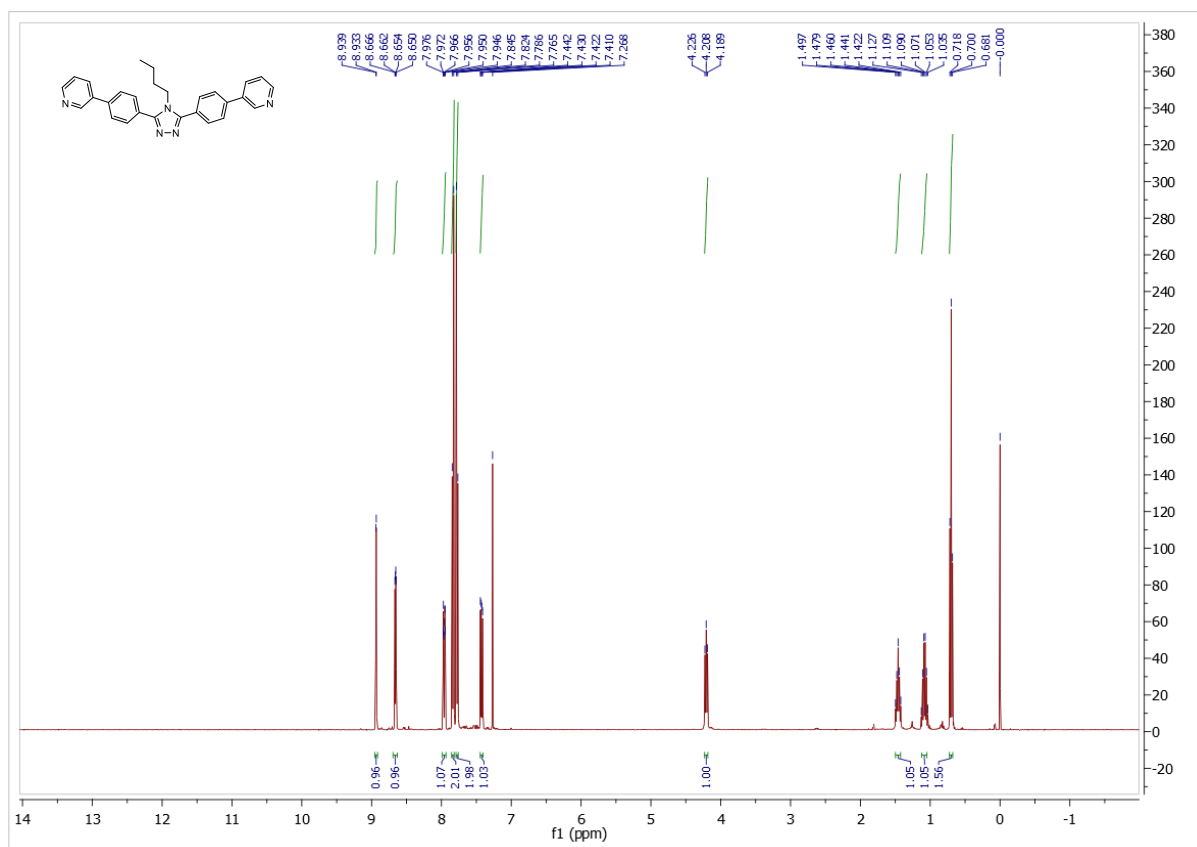
^1H and ^{13}C NMR of 3,5-bis(3'-aminobiphenyl-4-yl)-4-butyl-4*H*-1,2,4-triazole (**7h**)



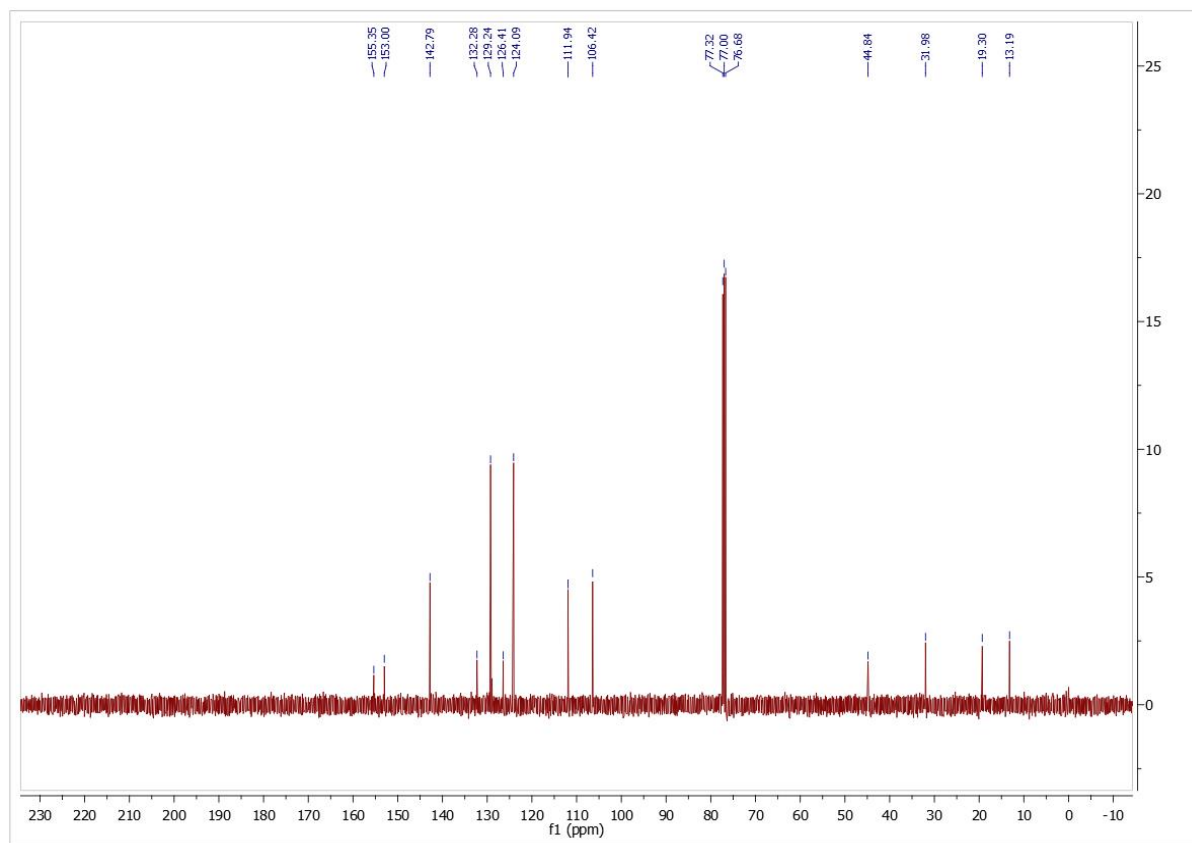
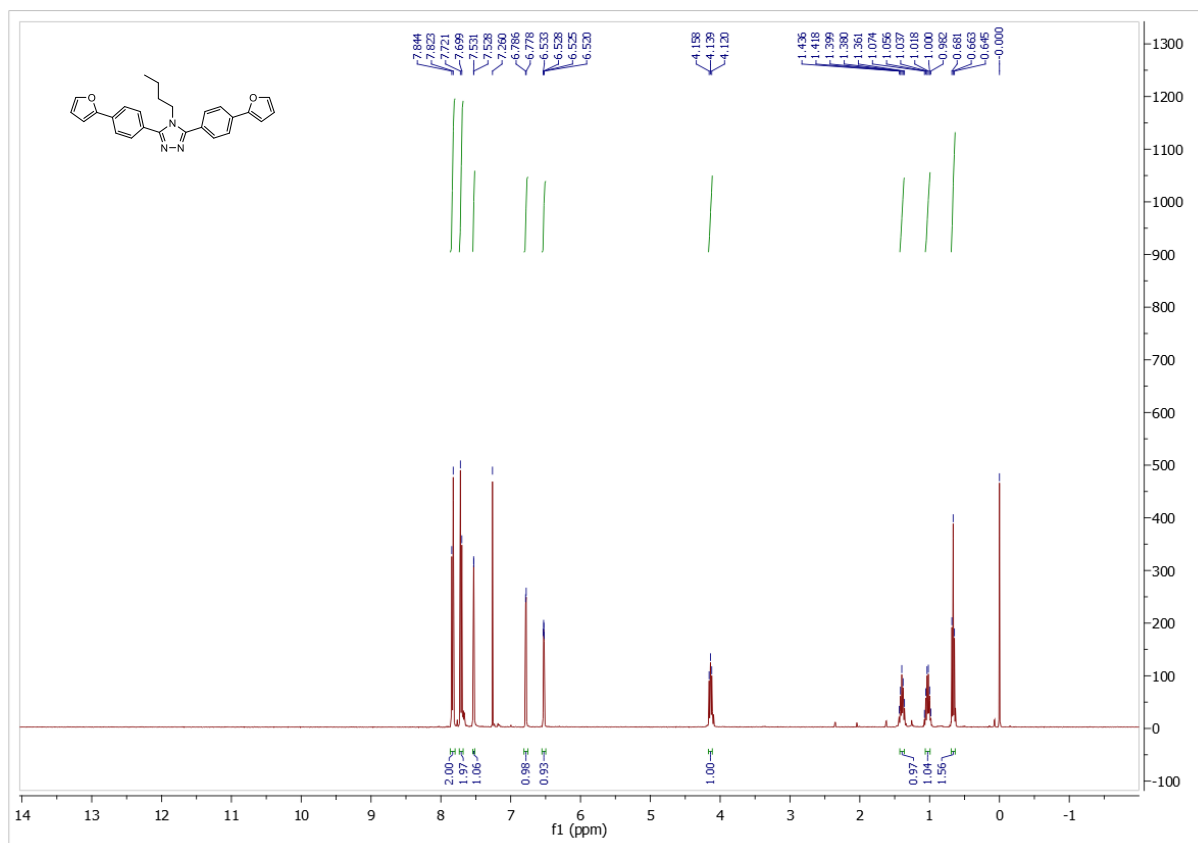
^1H and ^{13}C NMR of 4-butyl-3,5-bis[4-(pyridin-4-yl)phenyl]-4*H*-1,2,4-triazole (**7i**)



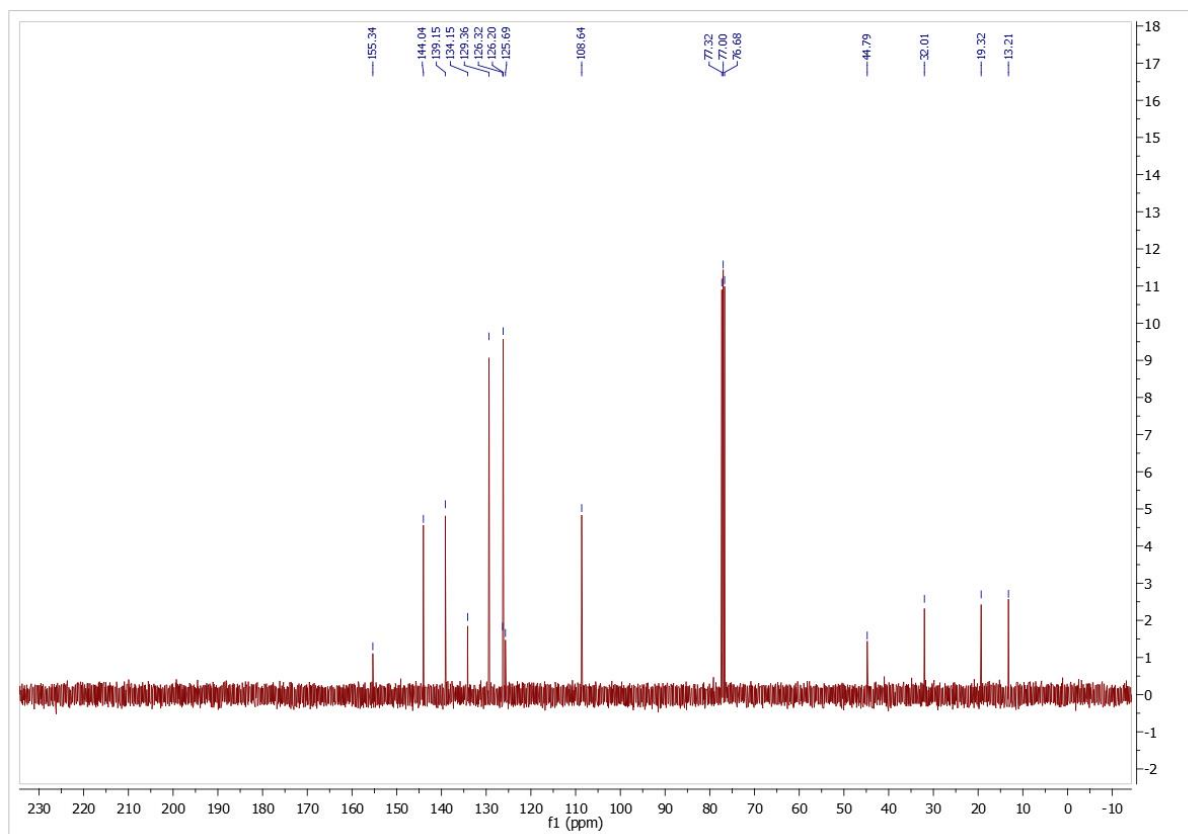
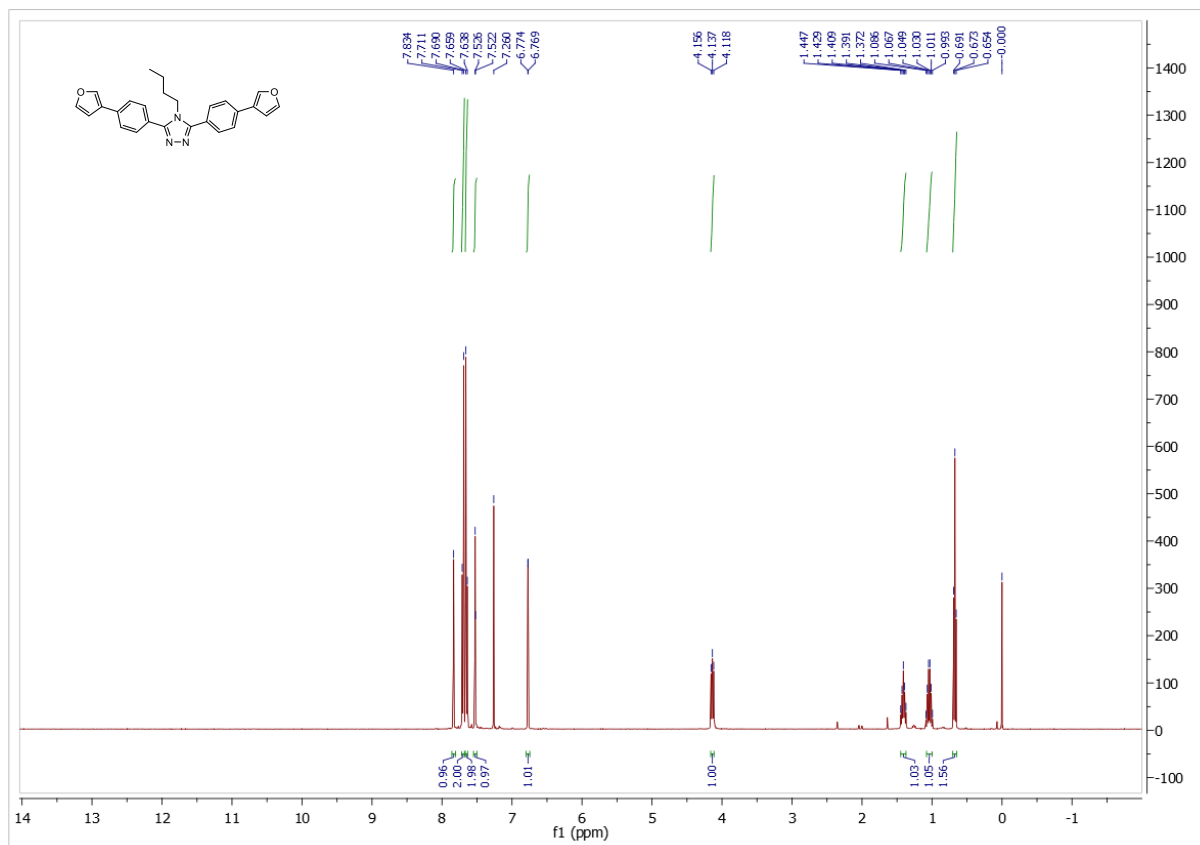
^1H and ^{13}C NMR of 4-butyl-3,5-bis[4-(pyridin-3-yl)phenyl]-4*H*-1,2,4-triazole (**7j**)



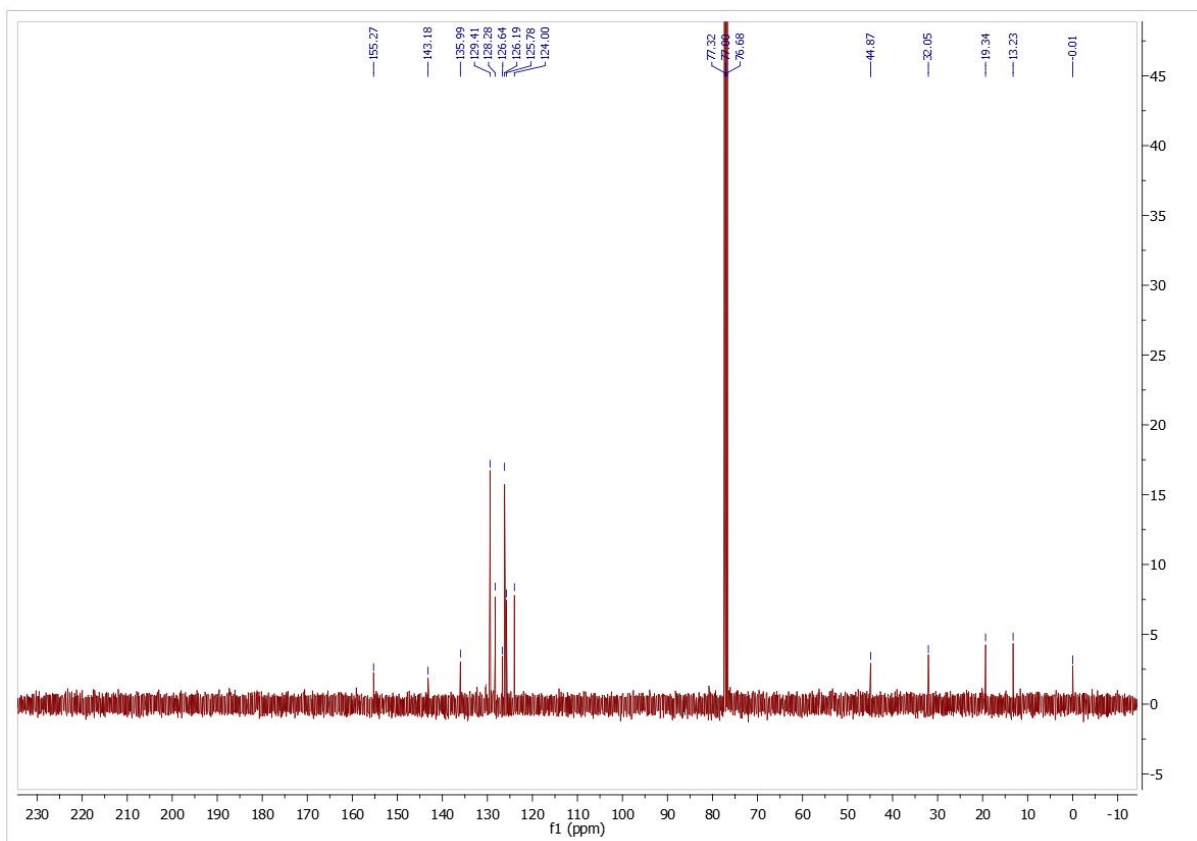
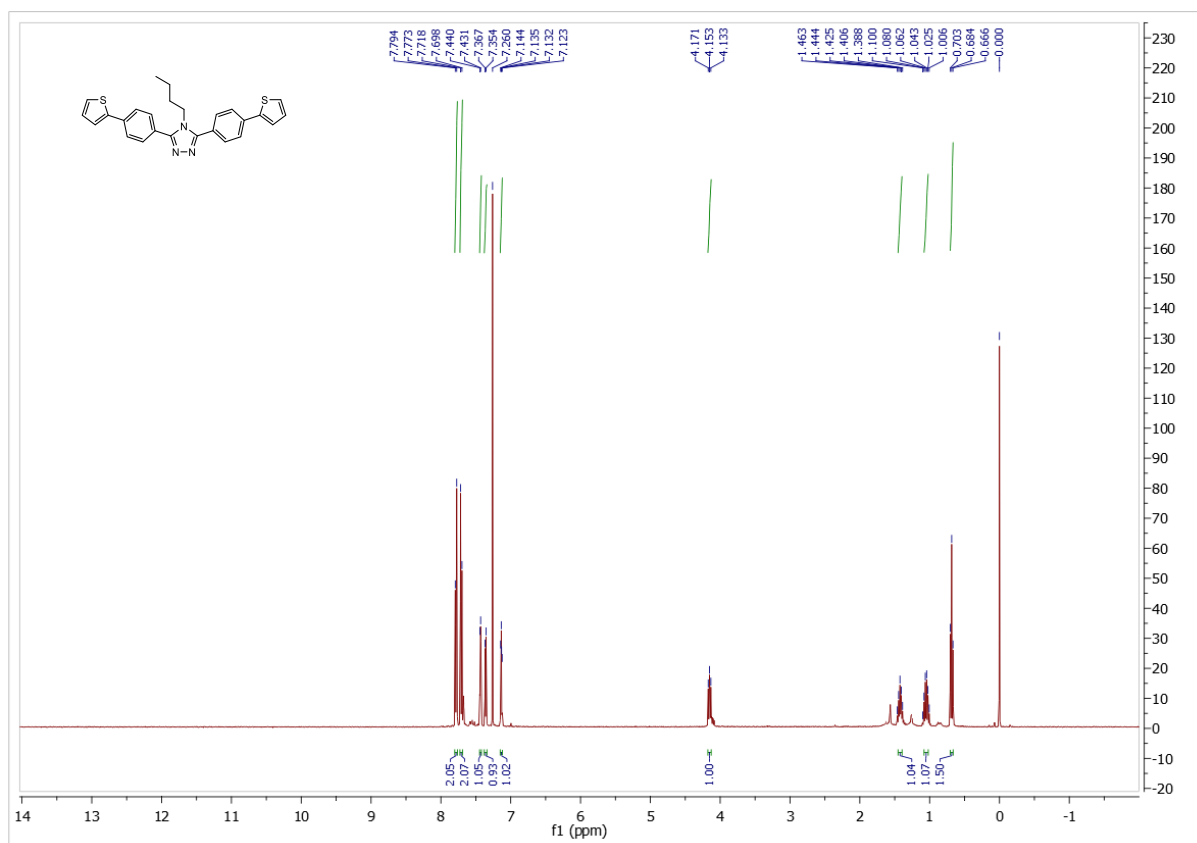
^1H and ^{13}C NMR of 4-butyl-3,5-bis[4-(furan-2-yl)phenyl]-4*H*-1,2,4-triazole (**7k**)



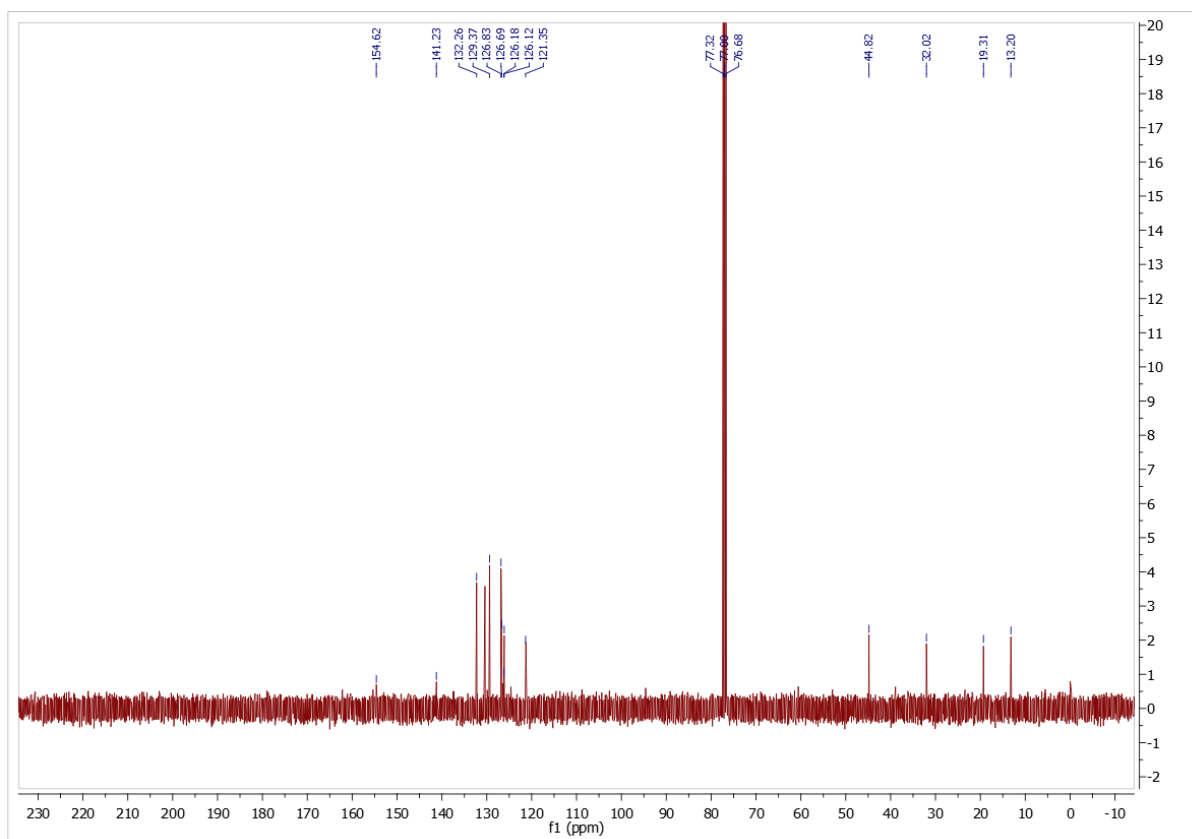
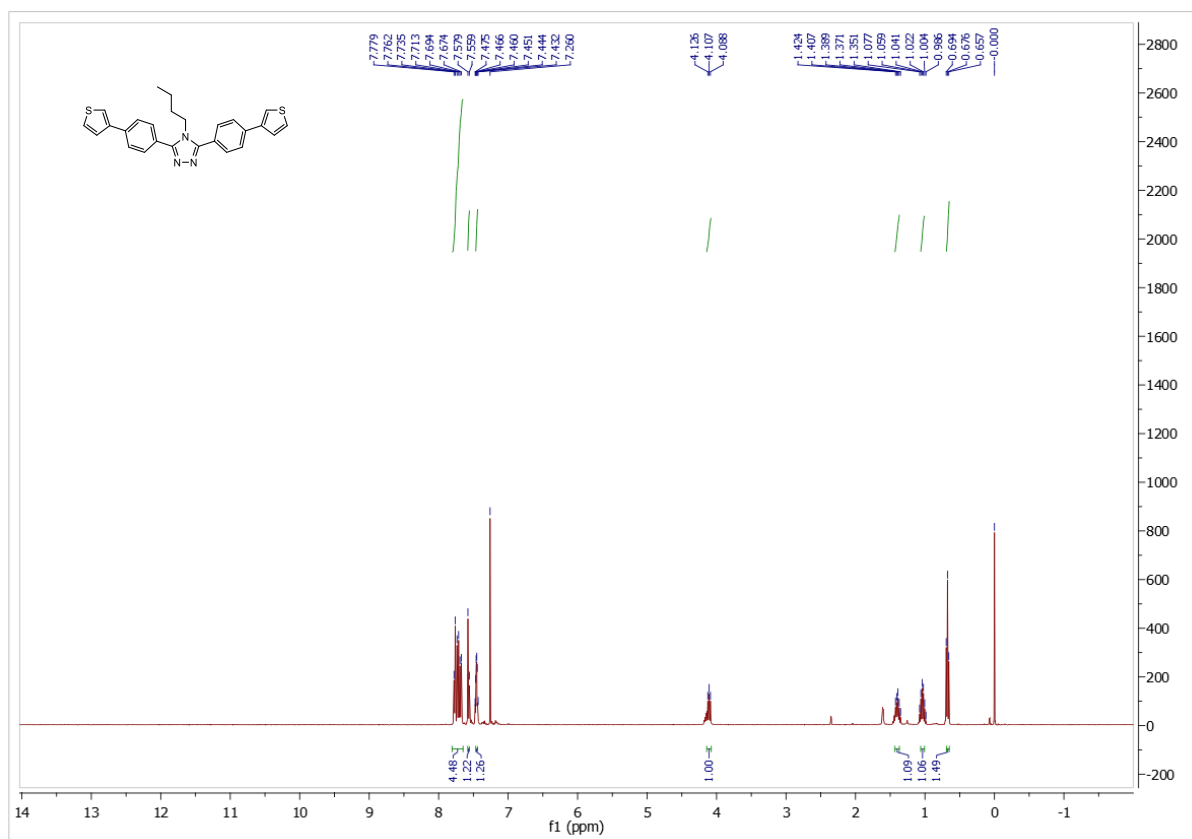
^1H and ^{13}C NMR of 4-butyl-3,5-bis[4-(furan-3-yl)phenyl]-4*H*-1,2,4-triazole (**7I**)



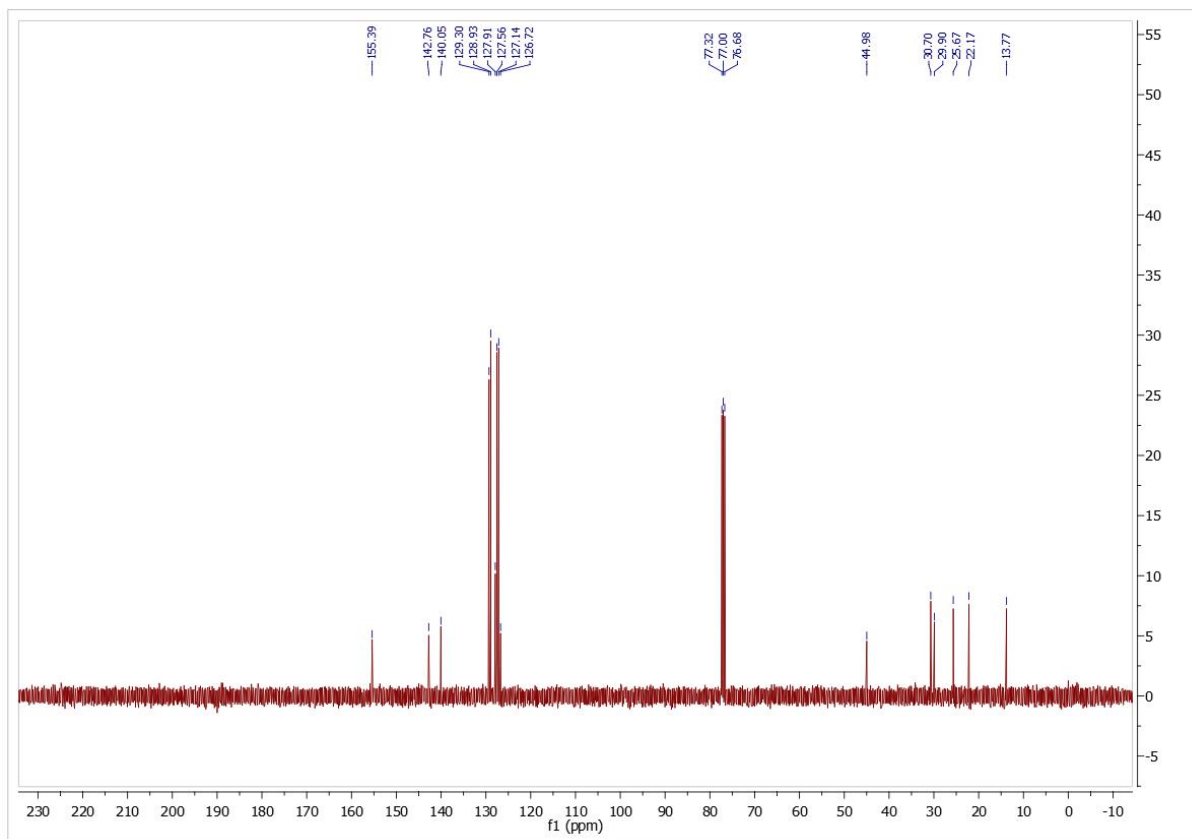
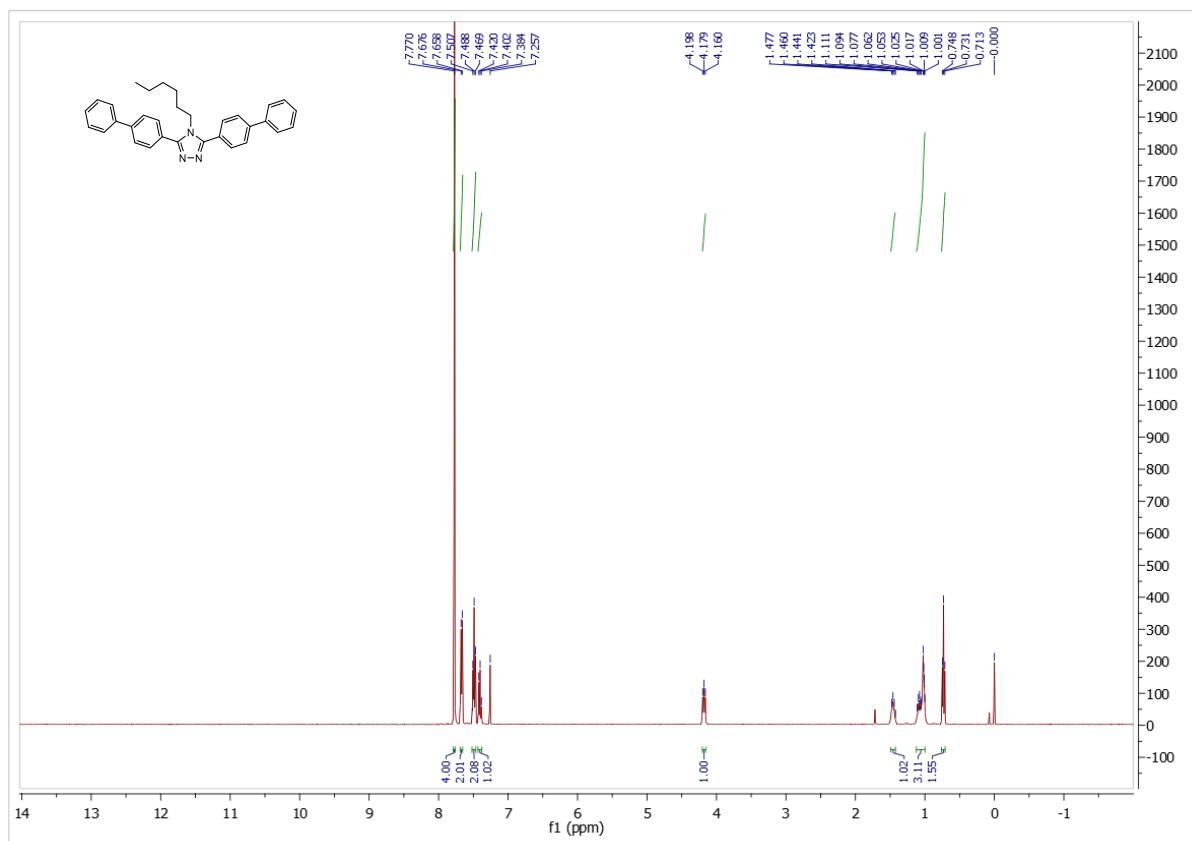
^1H and ^{13}C NMR of 4-butyl-3,5-bis[4-(thiophen-2-yl)phenyl]-4H-1,2,4-triazole (**7m**)



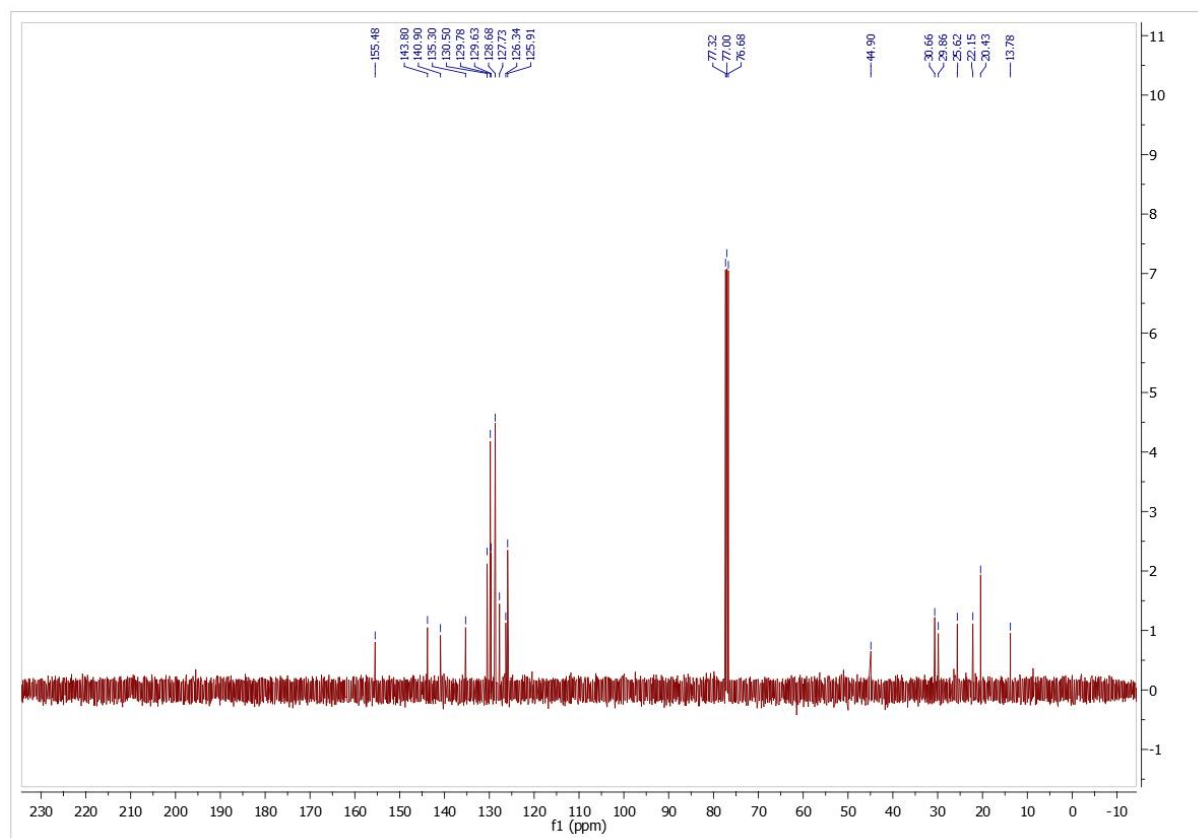
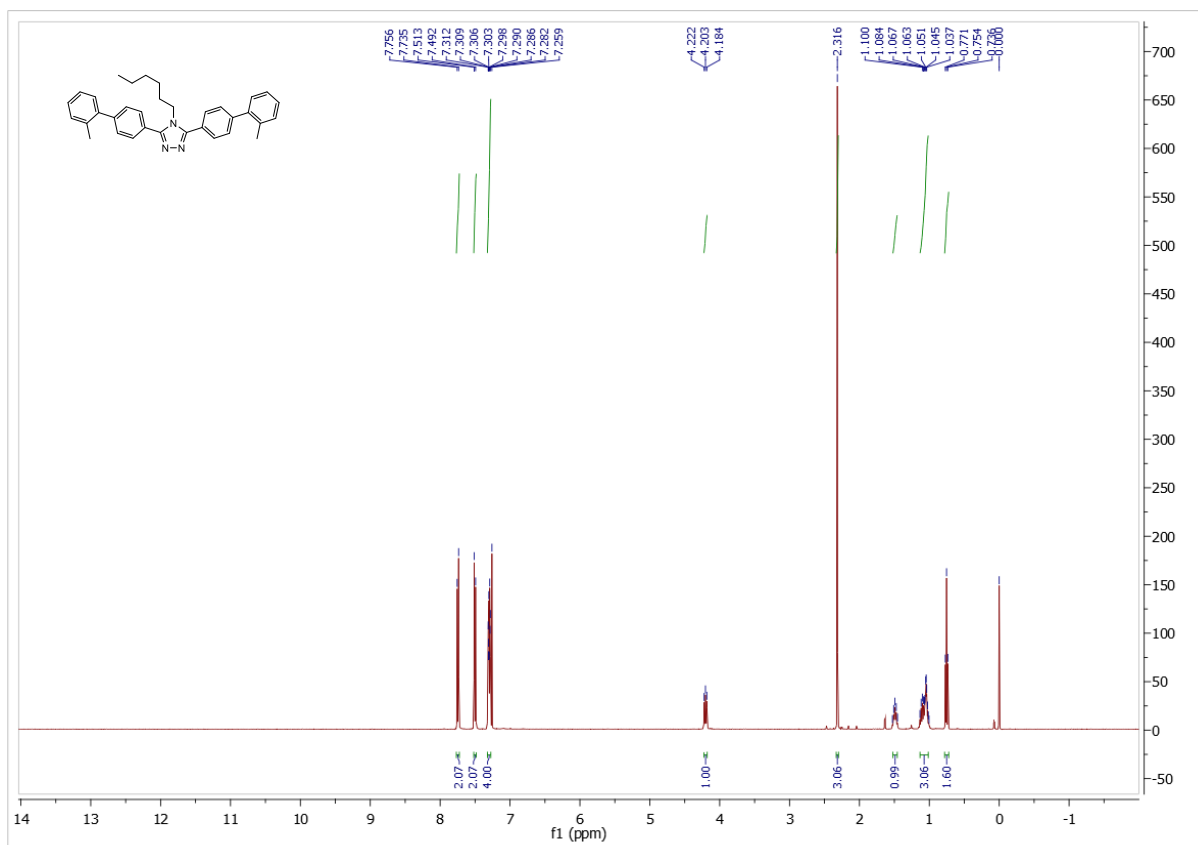
^1H and ^{13}C NMR of 4-butyl-3,5-bis[4-(thiophen-3-yl)phenyl]-4*H*-1,2,4-triazole (**7n**)



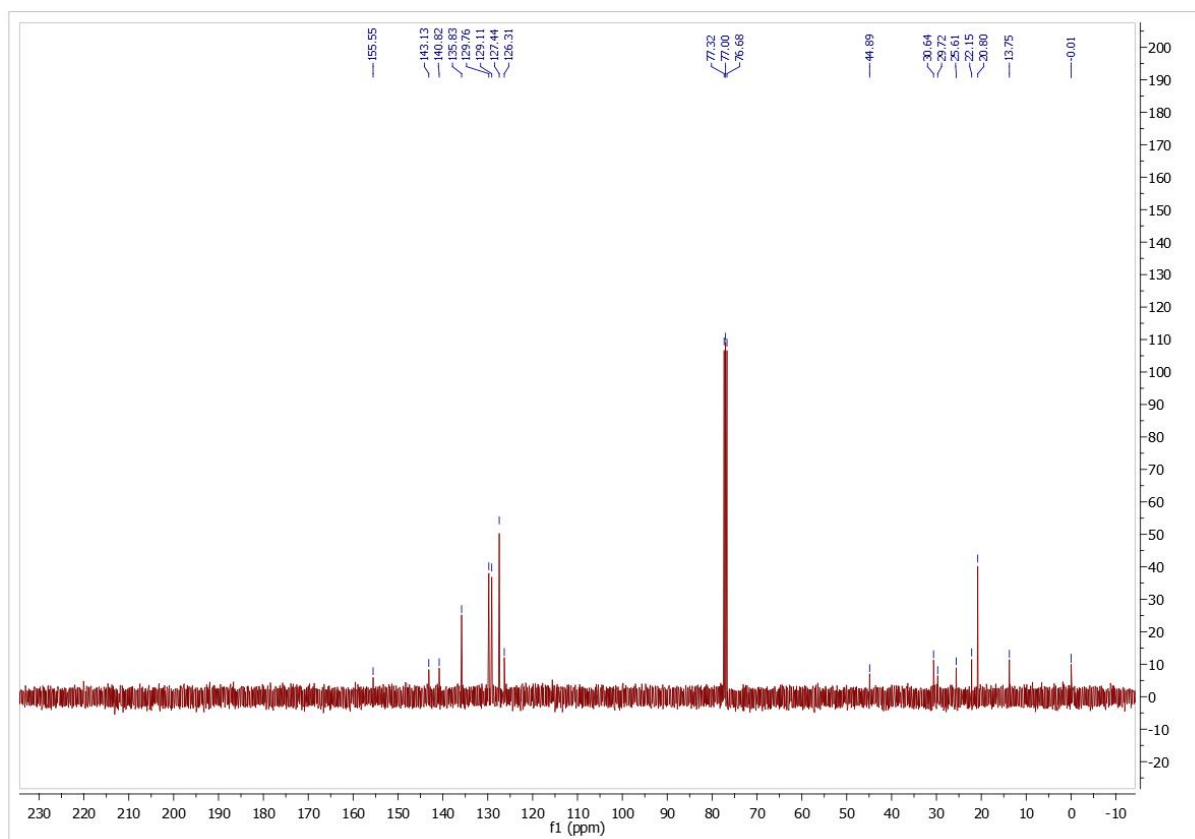
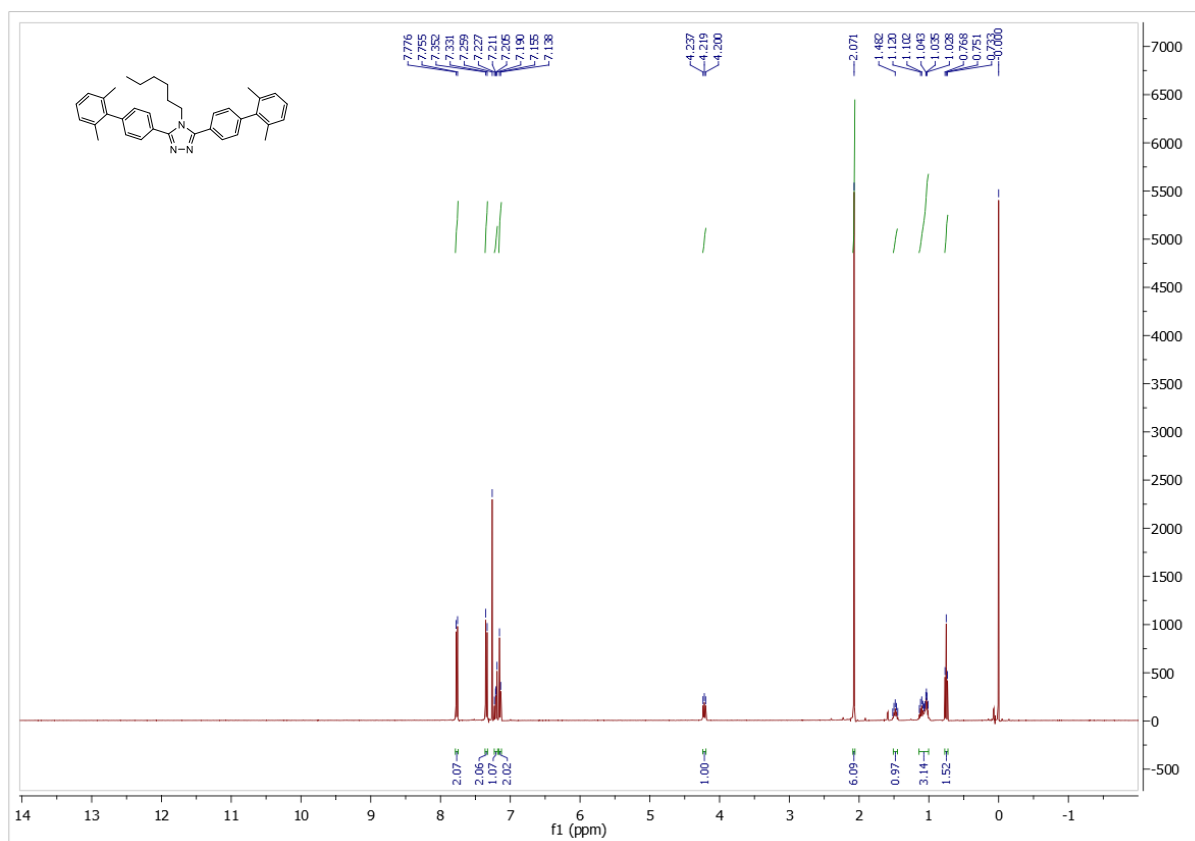
^1H and ^{13}C NMR of 3,5-bis(biphenyl-4-yl)-4-hexyl-4*H*-1,2,4-triazole (**8a**)



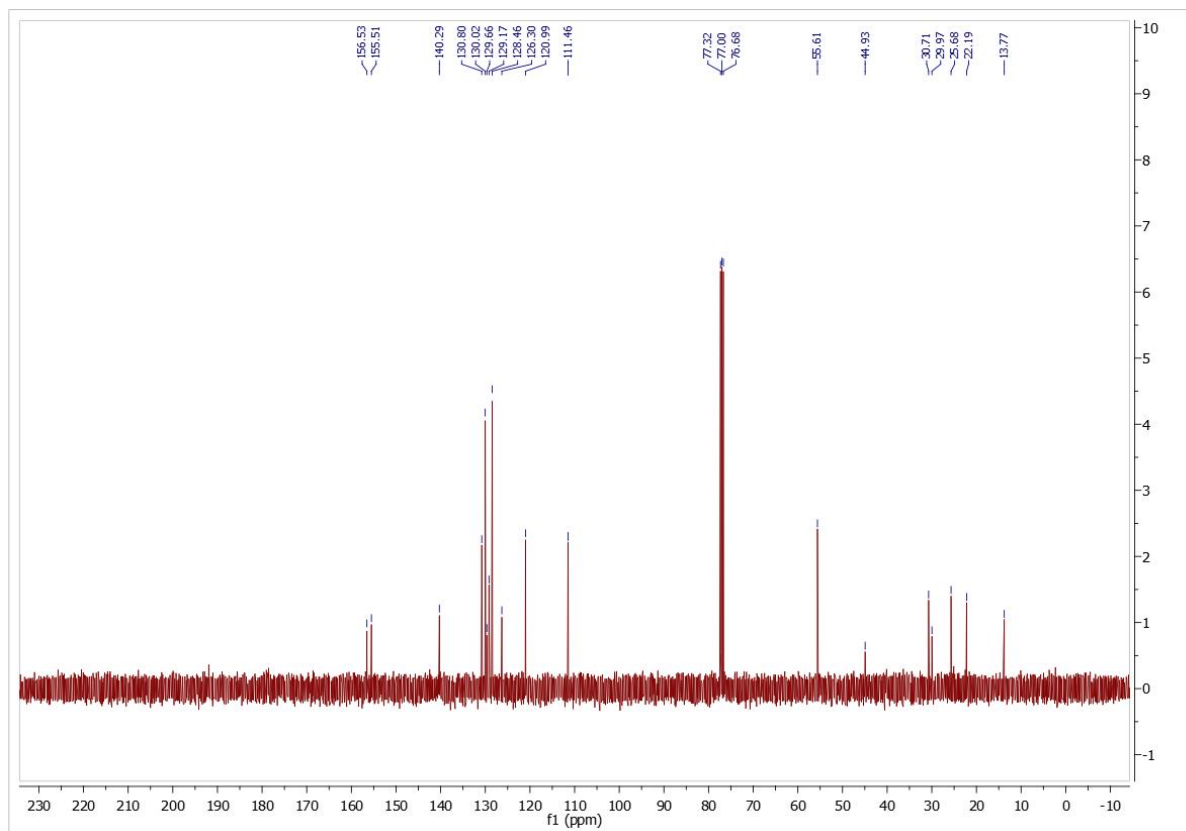
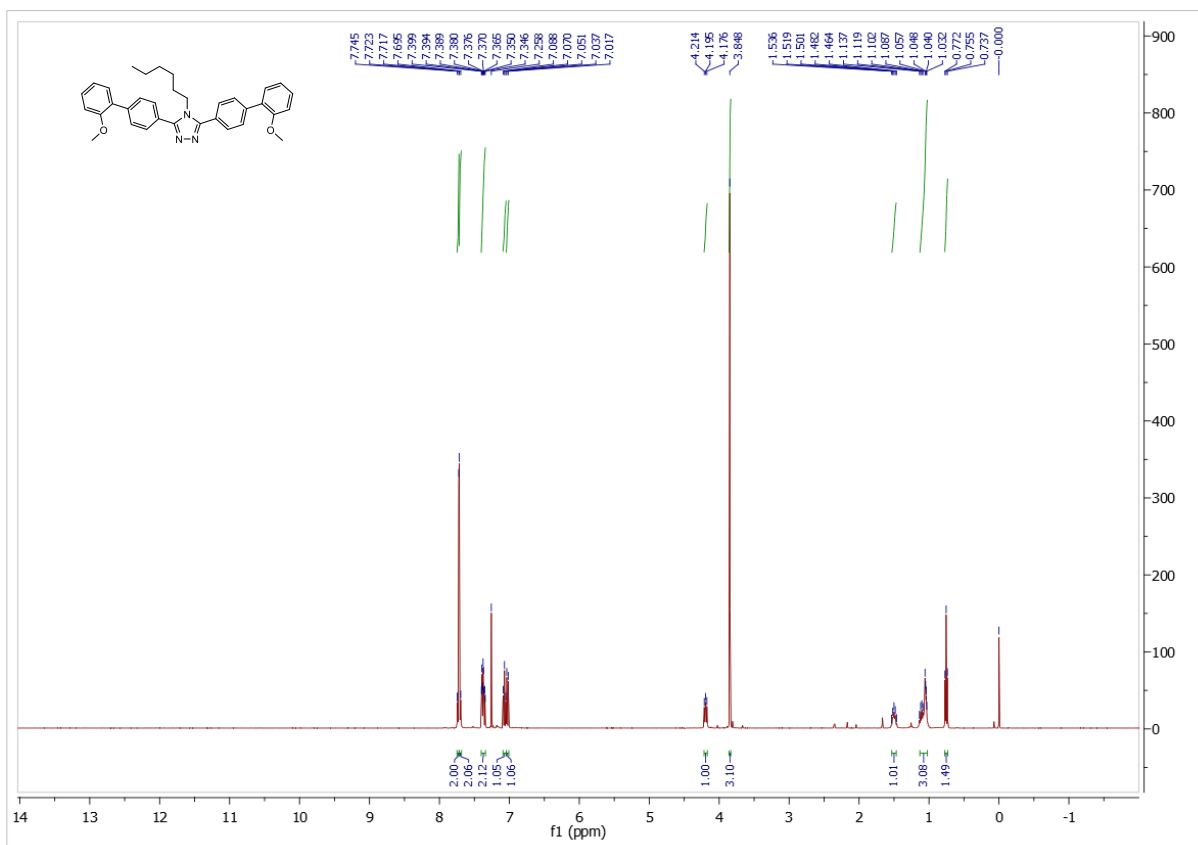
^1H and ^{13}C NMR of 4-hexyl-3,5-bis(2'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**8b**)



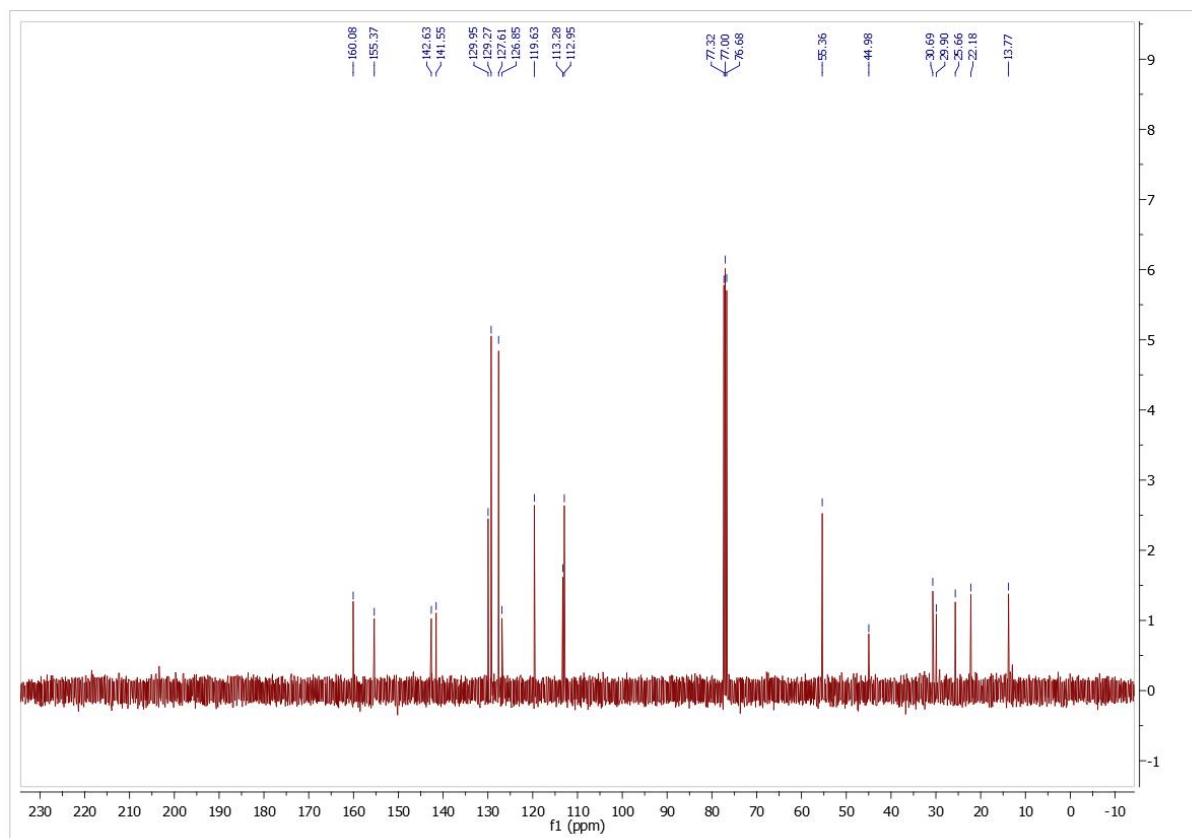
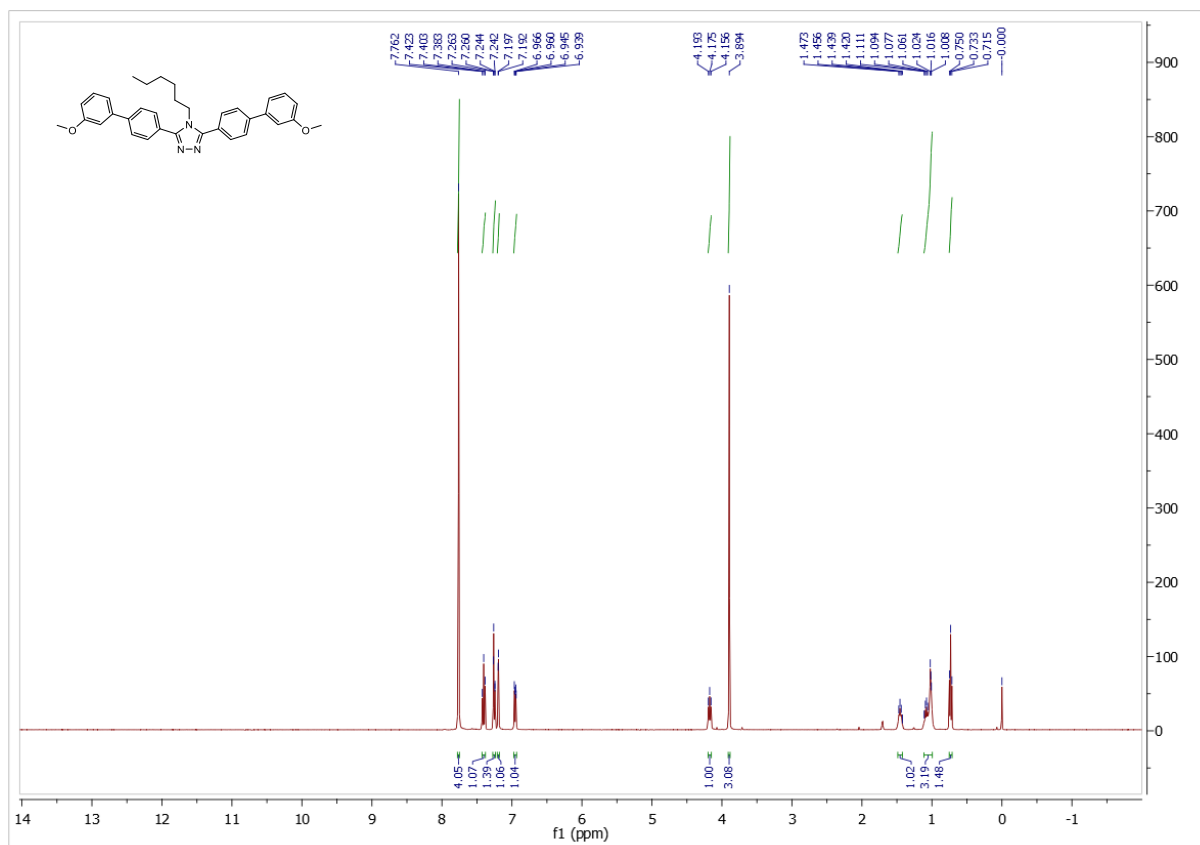
^1H and ^{13}C NMR of 4-hexyl-3,5-bis(2',6'-dimethylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**8d**)



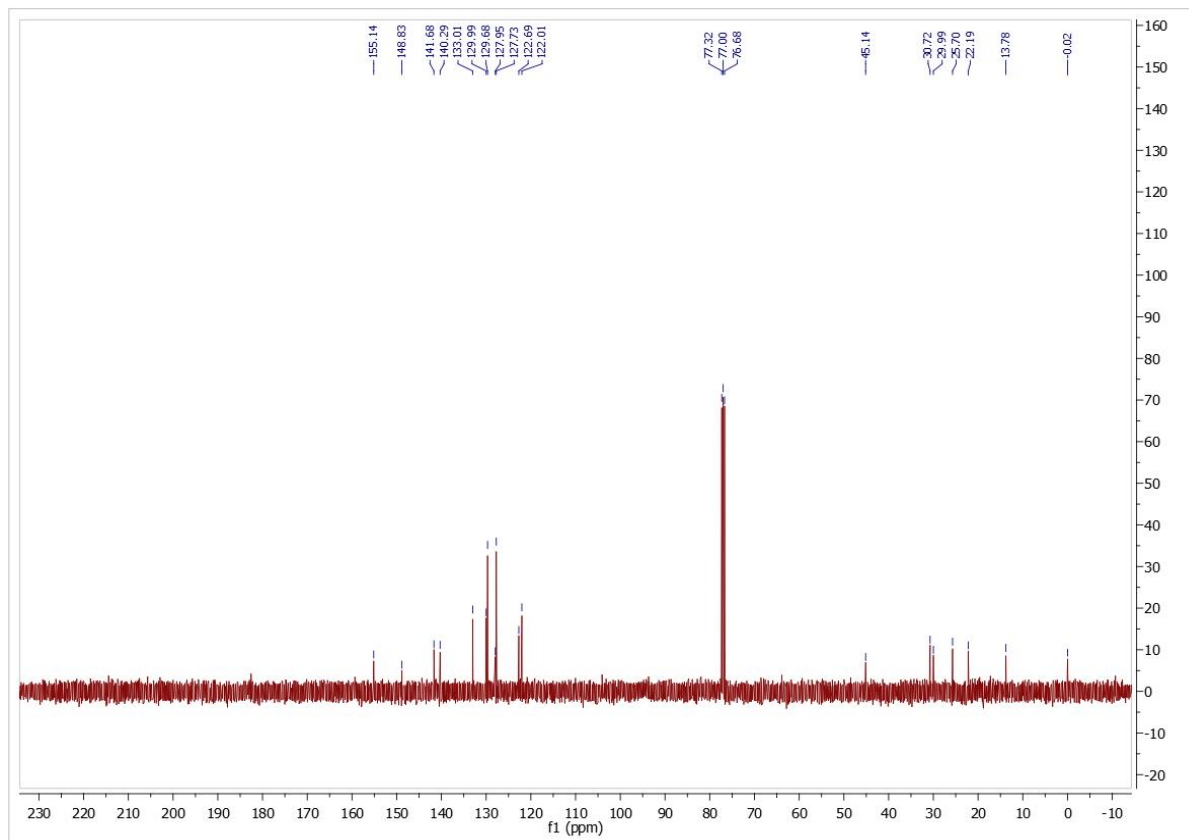
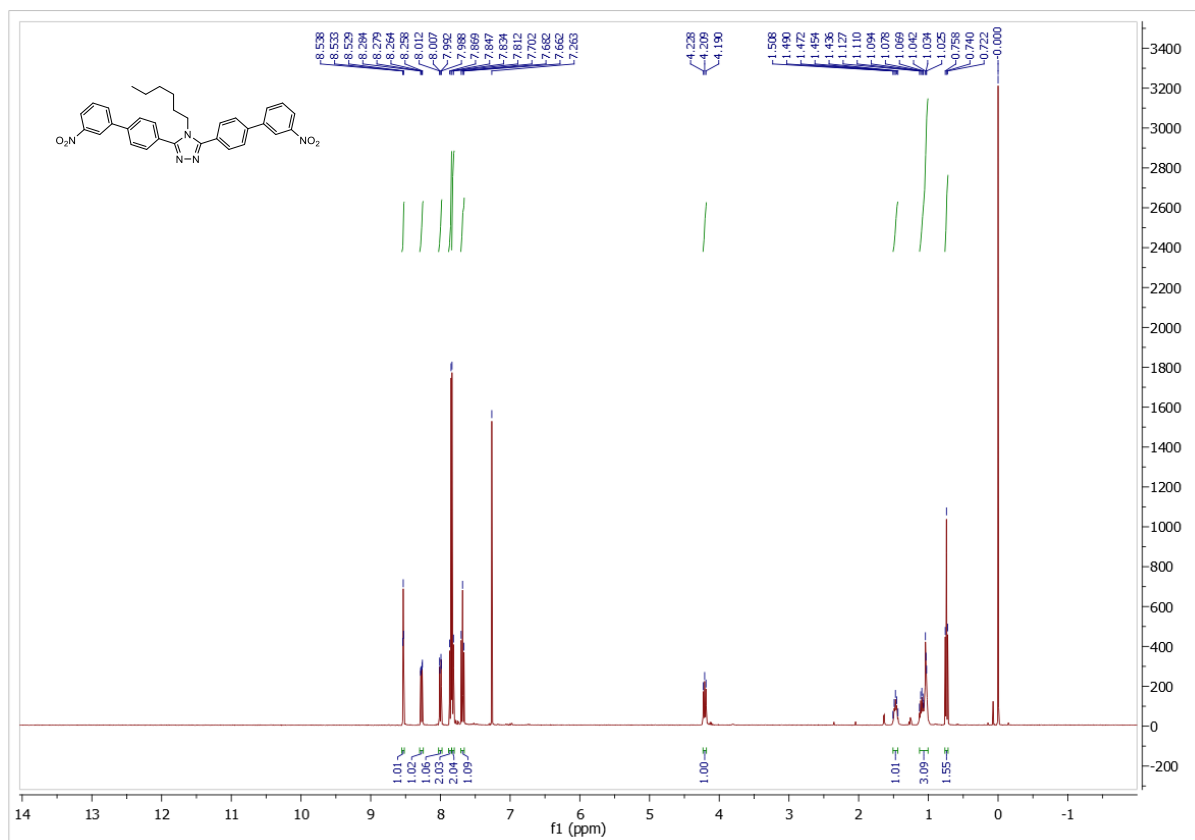
^1H and ^{13}C NMR of 4-hexyl-3,5-bis(2'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**8e**)



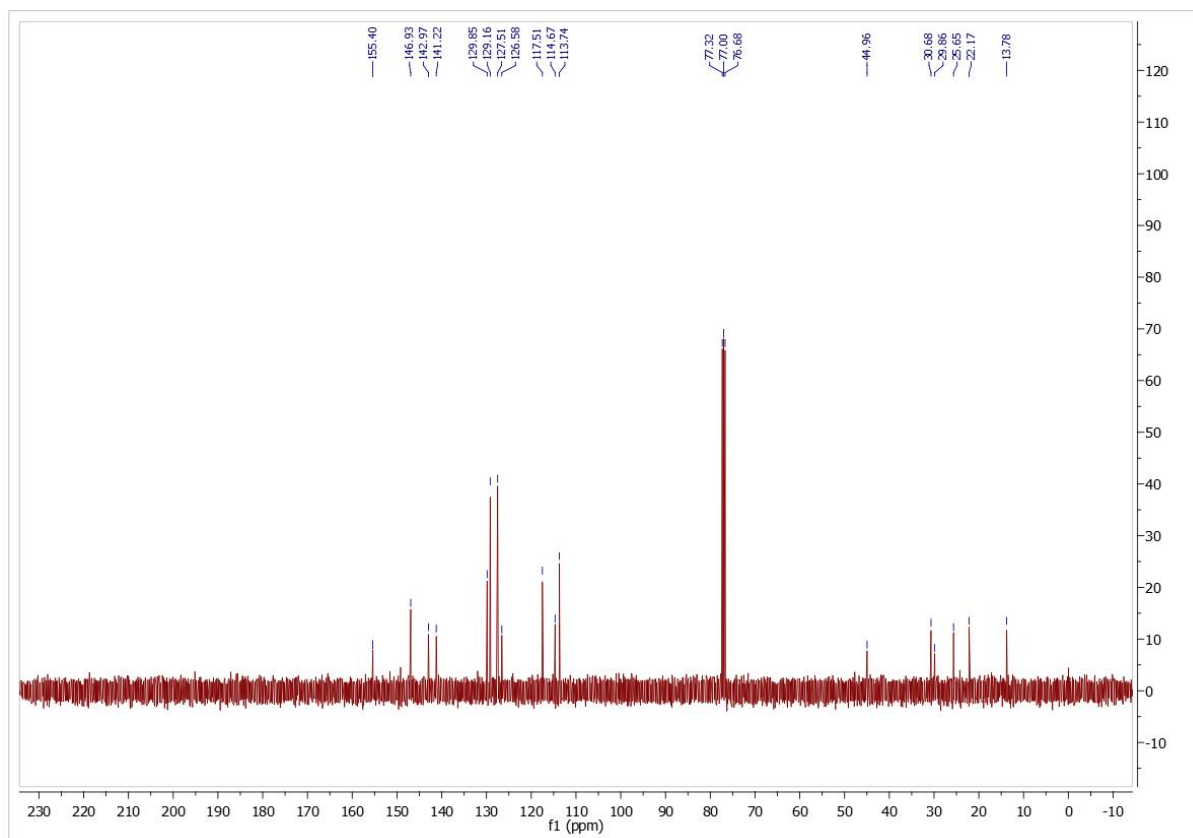
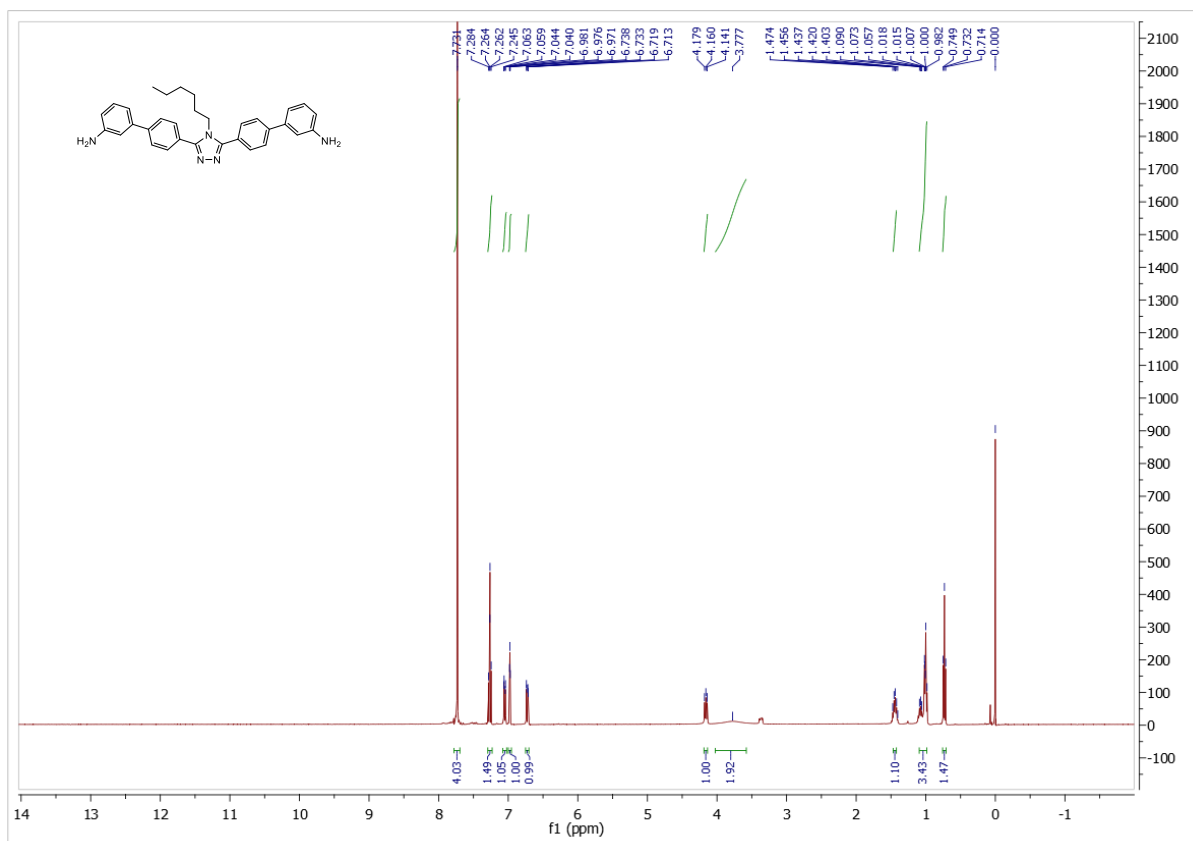
^1H and ^{13}C NMR of 4-hexyl-3,5-bis(3'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**8f**)



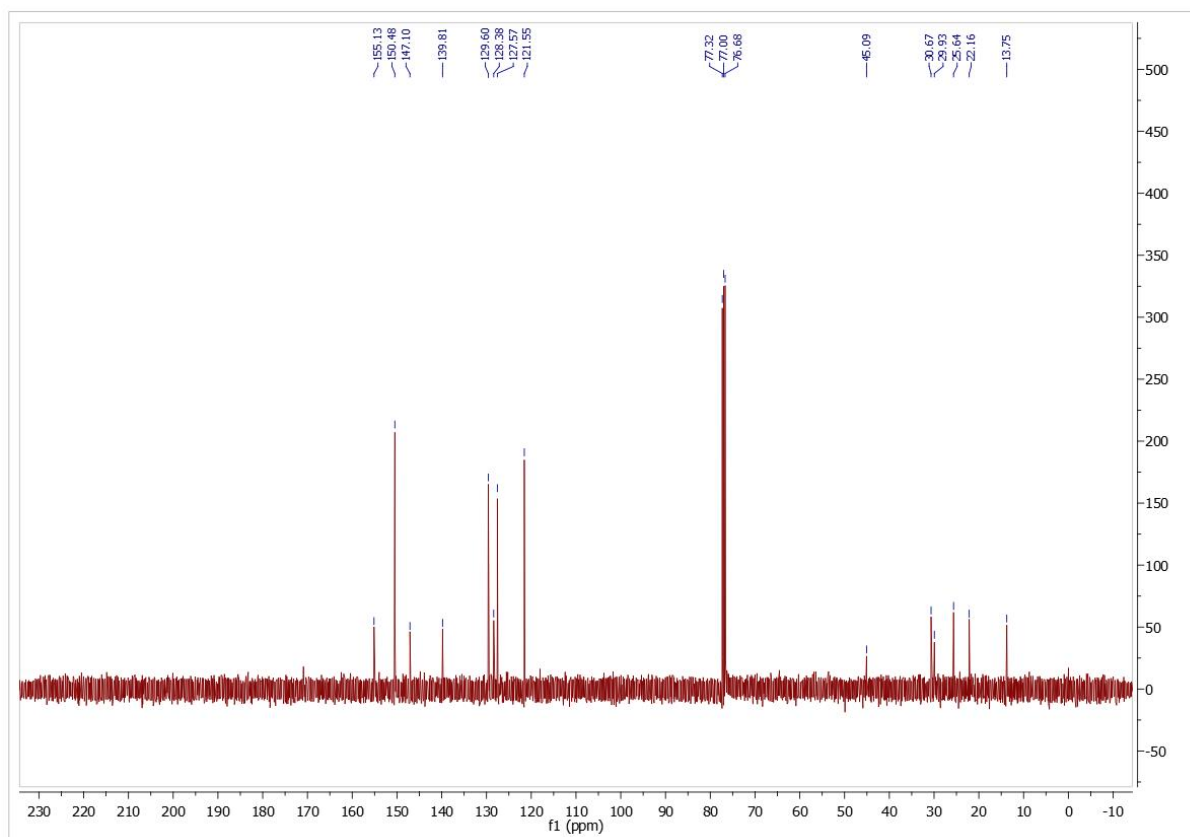
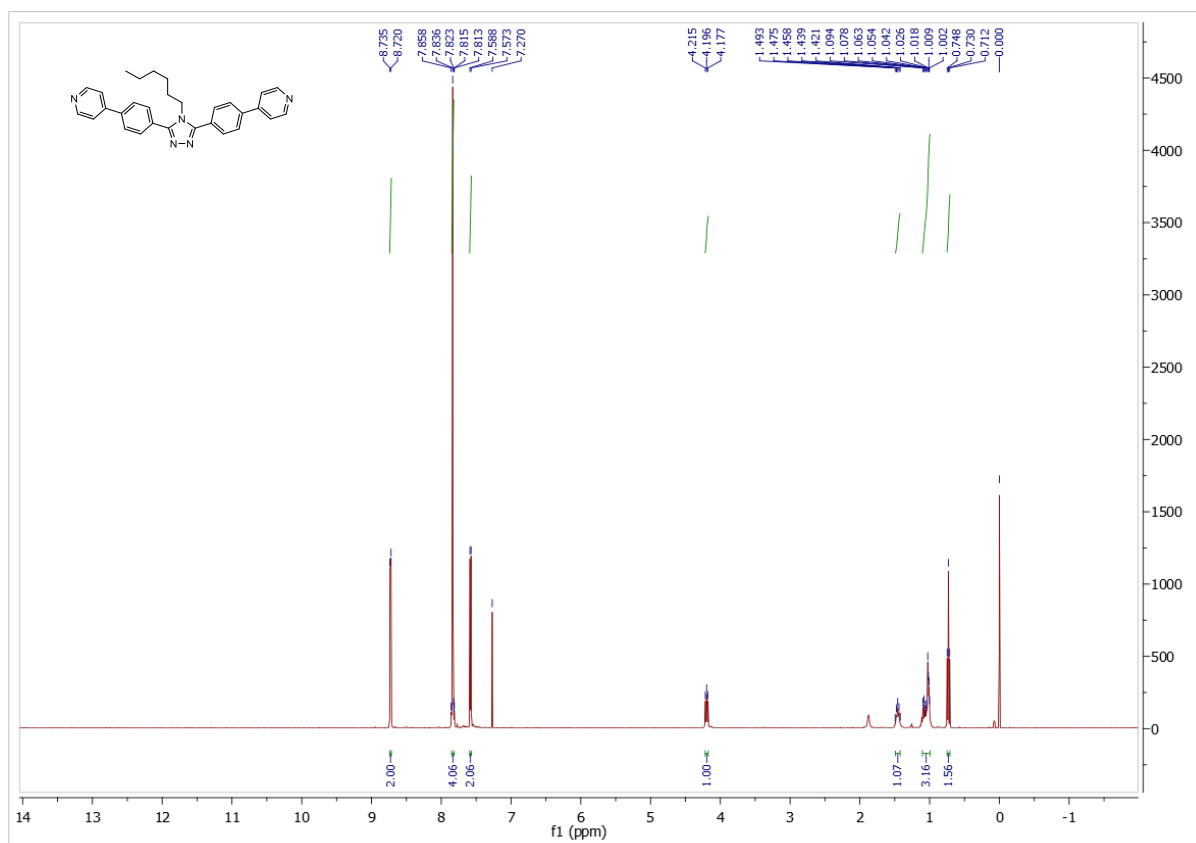
^1H and ^{13}C NMR of 4-hexyl-3,5-bis(3'-nitrophenyl-4-yl)-4*H*-1,2,4-triazole (**8g**)



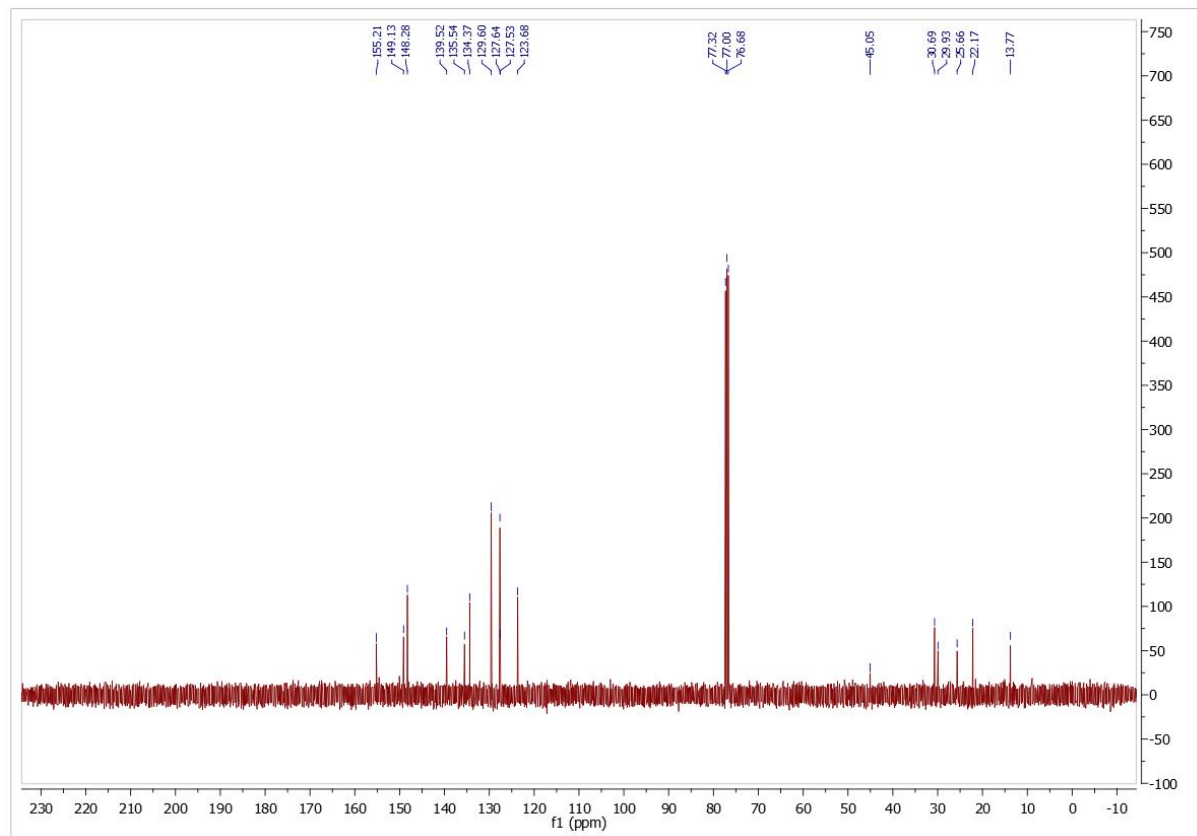
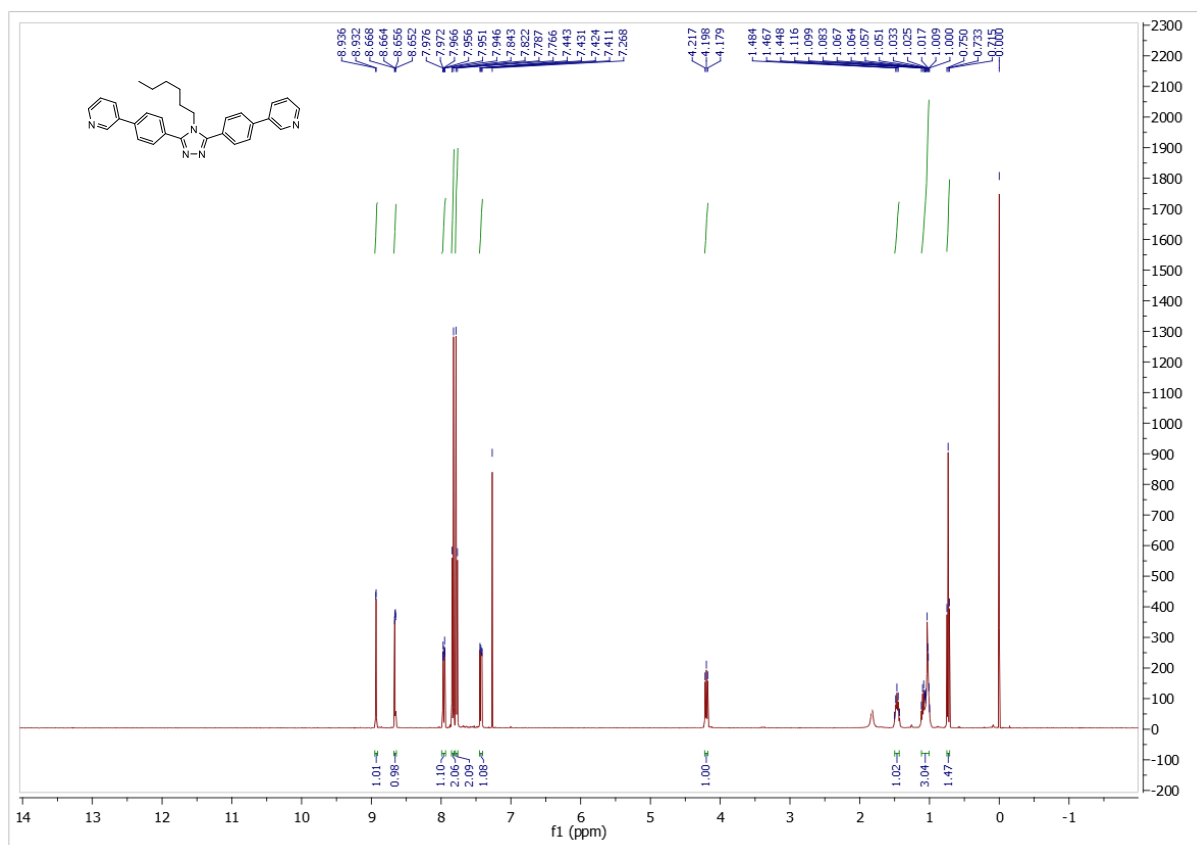
^1H and ^{13}C NMR of 3,5-bis(3'-aminobiphenyl-4-yl)-4*H*-1,2,4-triazole (**8h**)



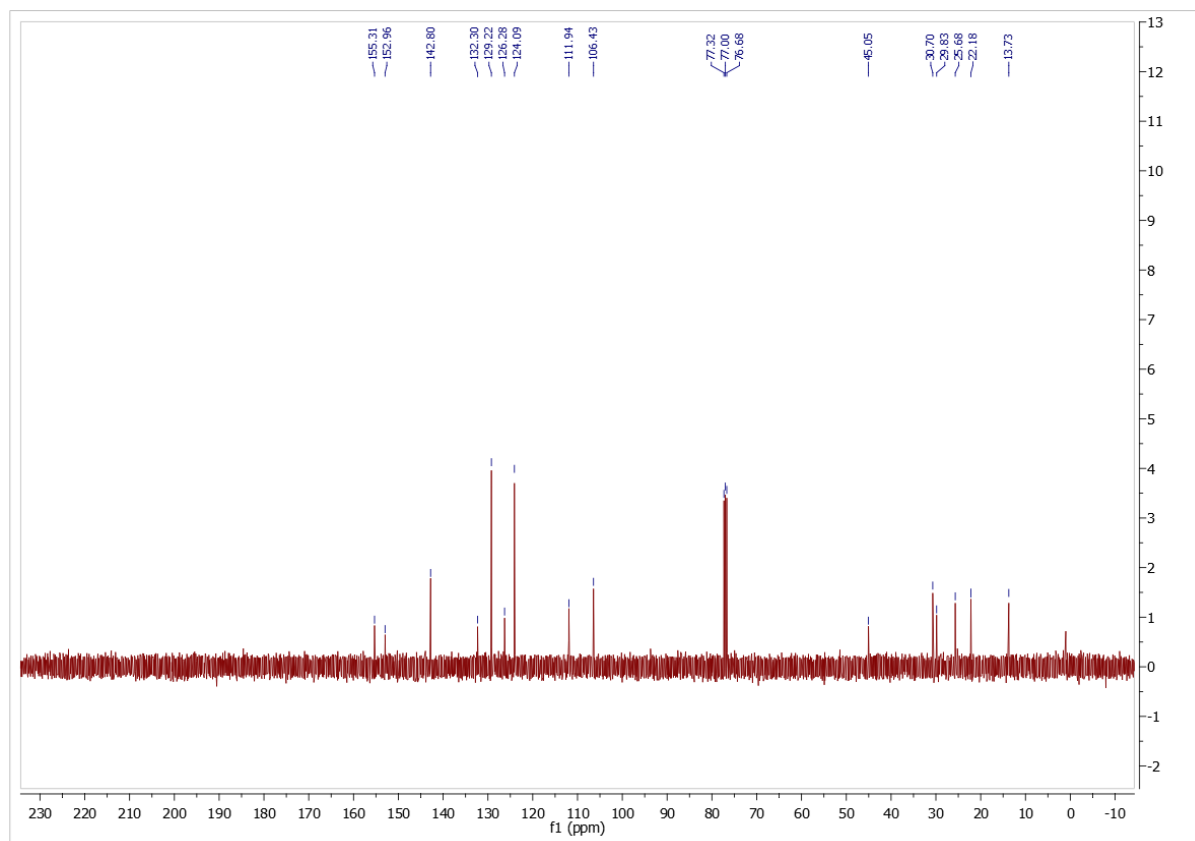
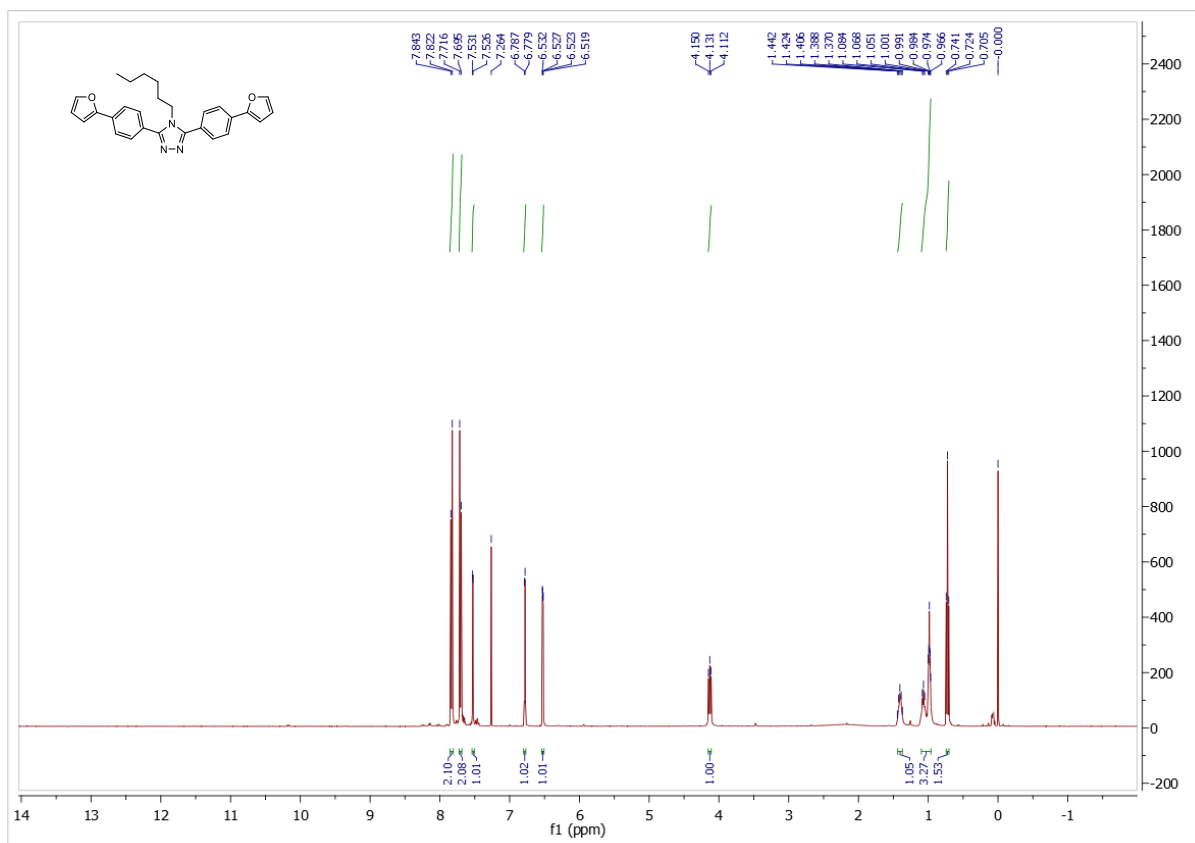
^1H and ^{13}C NMR of 4-hexyl-3,5-bis[4-(pyridin-4-yl)phenyl]-4*H*-1,2,4-triazole (**8i**)



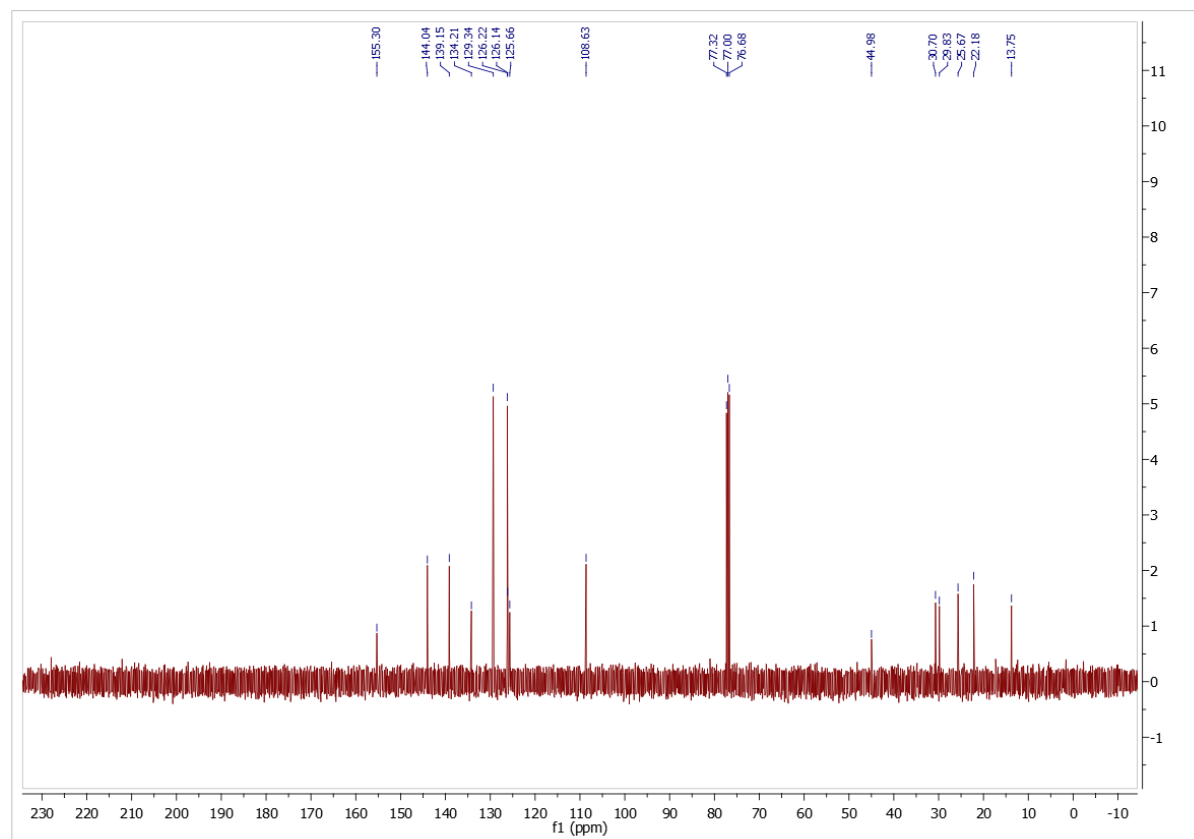
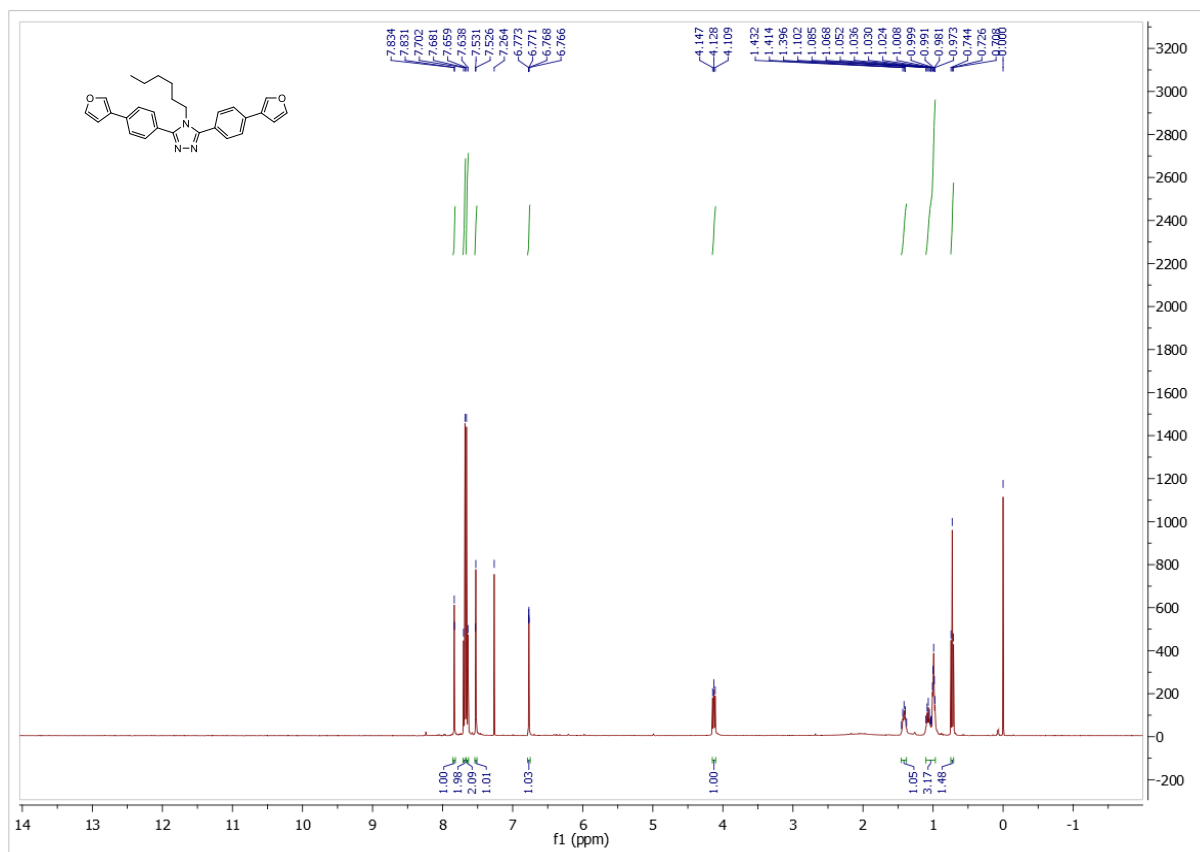
^1H and ^{13}C NMR of 4-hexyl-3,5-bis[4-(pyridin-3-yl)phenyl]-4*H*-1,2,4-triazole (**8j**)



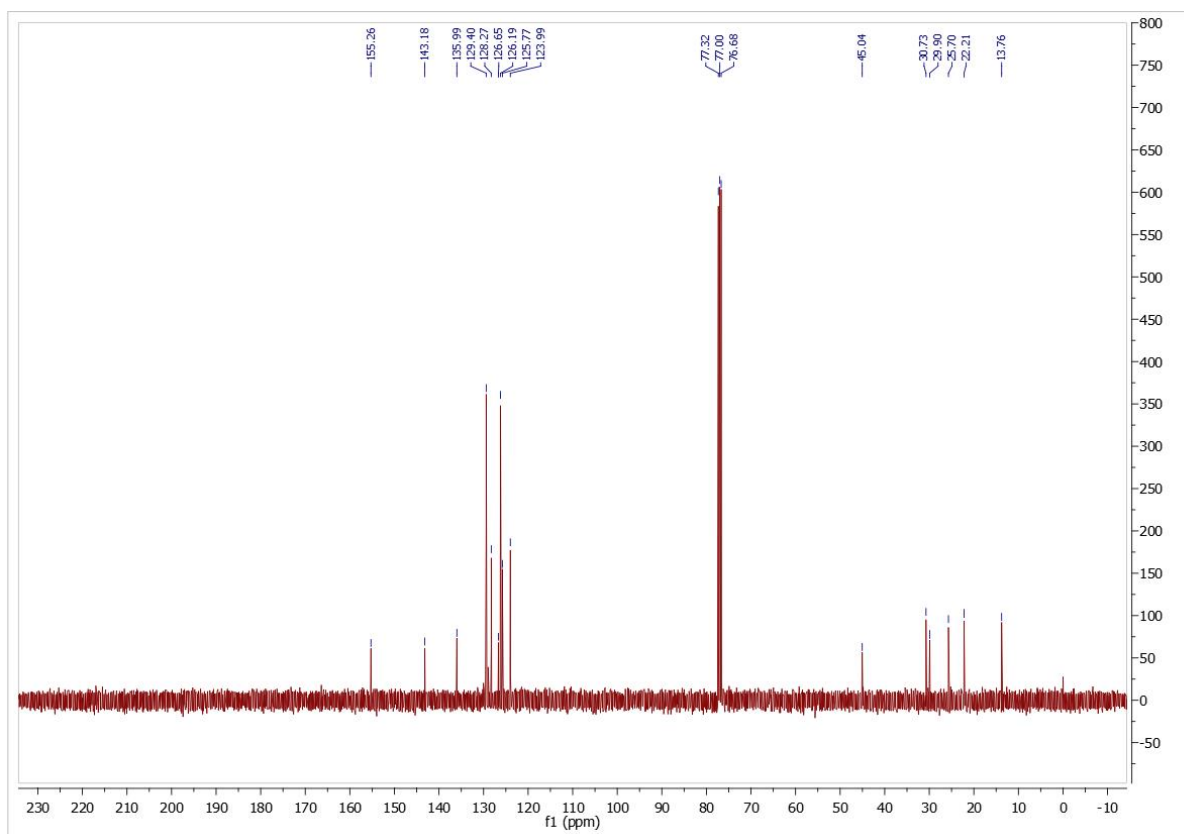
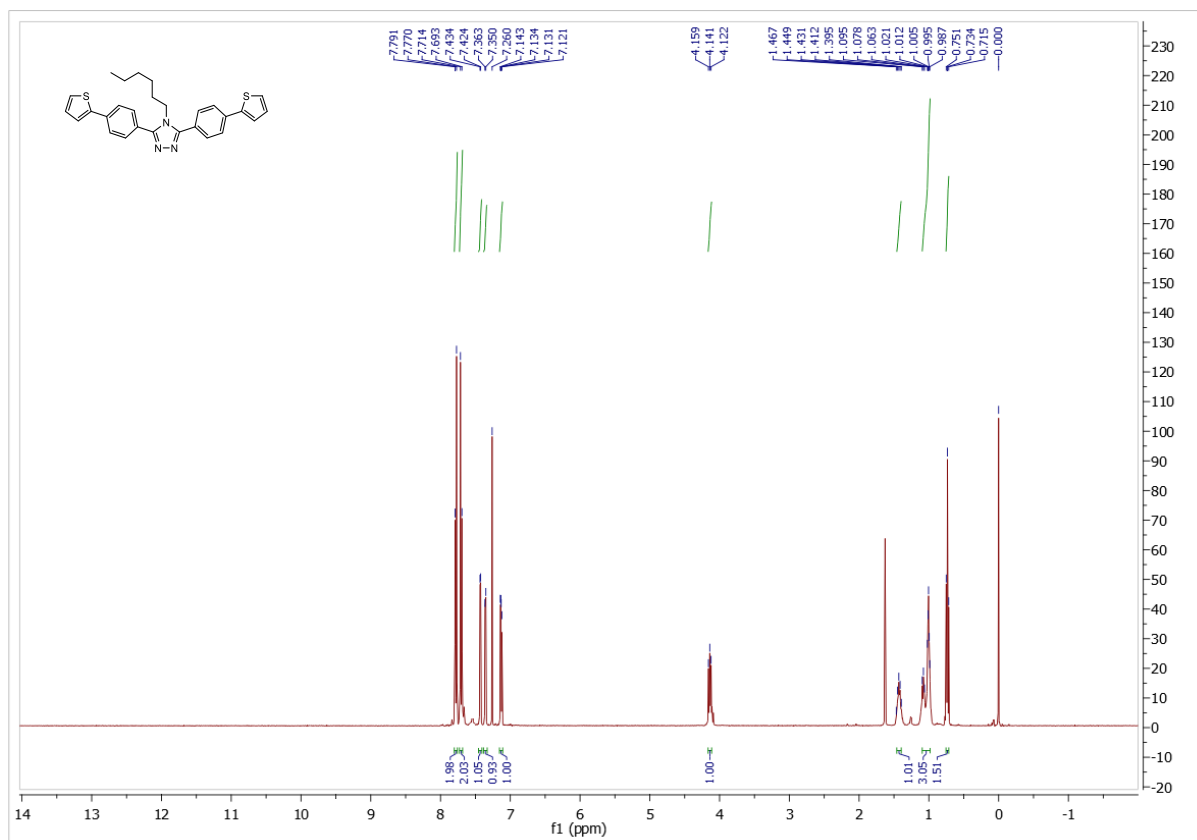
^1H and ^{13}C NMR of 3,5-bis[4-(furan-2-yl)phenyl]-4-hexyl-4H-1,2,4-triazole (**8k**)



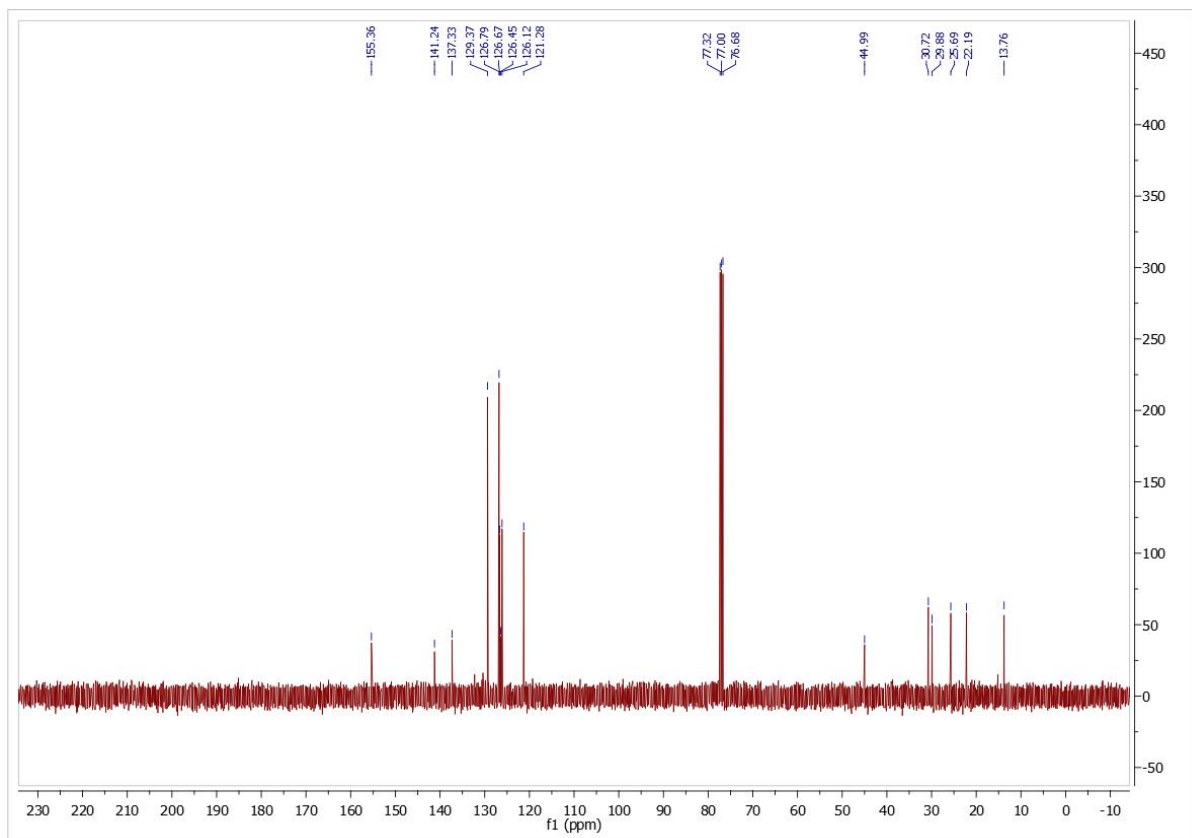
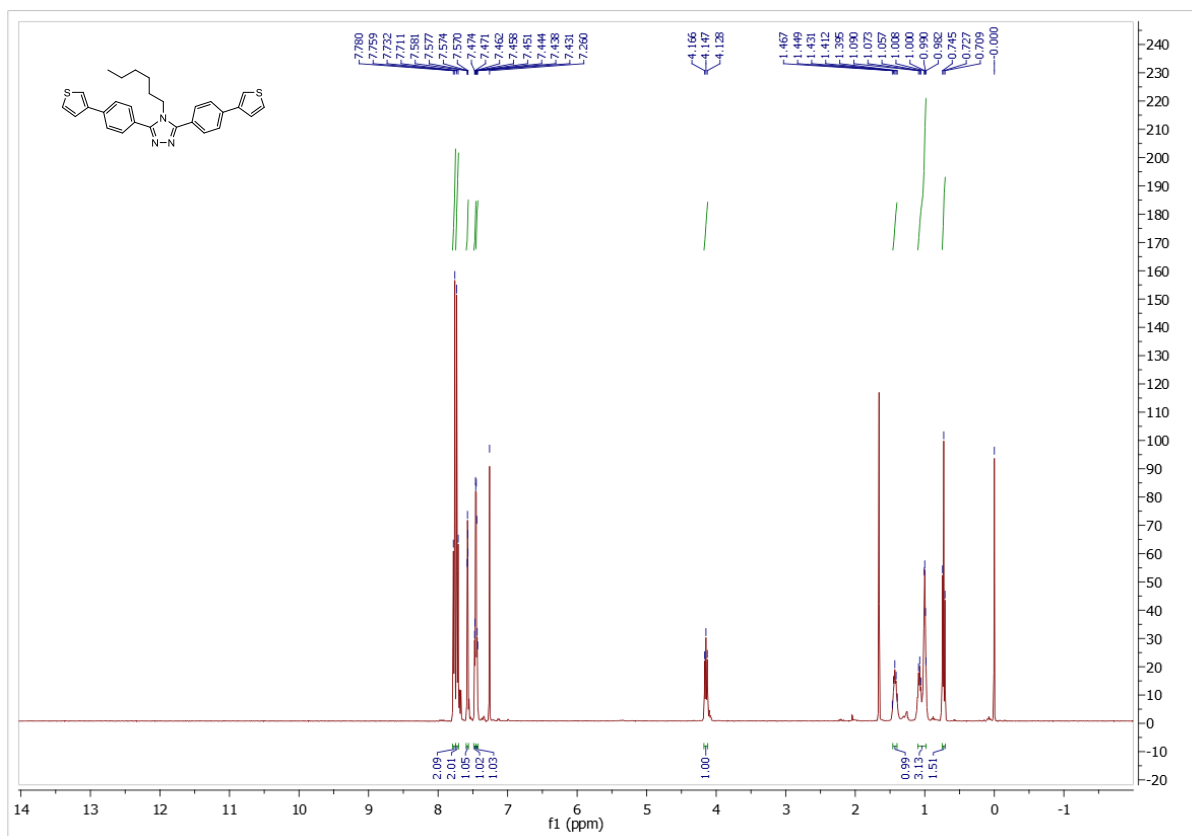
^1H and ^{13}C NMR of 3,5-bis[4-(furan-3-yl)phenyl]-4-hexyl-4*H*-1,2,4-triazole (**81**)



^1H and ^{13}C NMR of 4-hexyl-3,5-bis[4-(thiophen-2-yl)phenyl]-4*H*-1,2,4-triazole (**8m**)

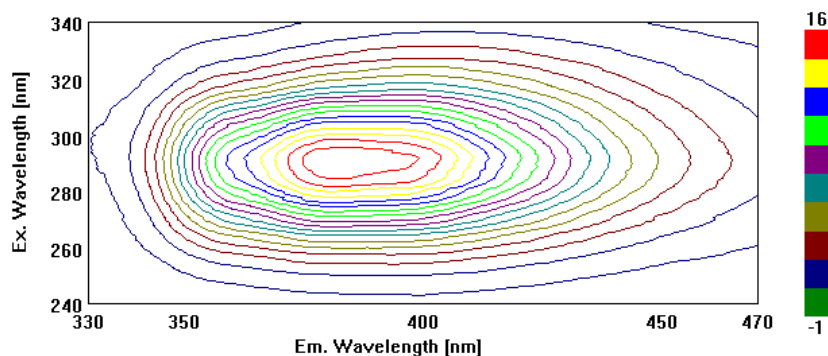
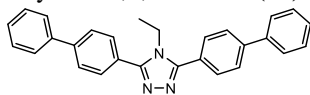


^1H and ^{13}C NMR of 4-hexyl-3,5-bis[4-(thiophen-3-yl)phenyl]-4*H*-1,2,4-triazole (**8n**)

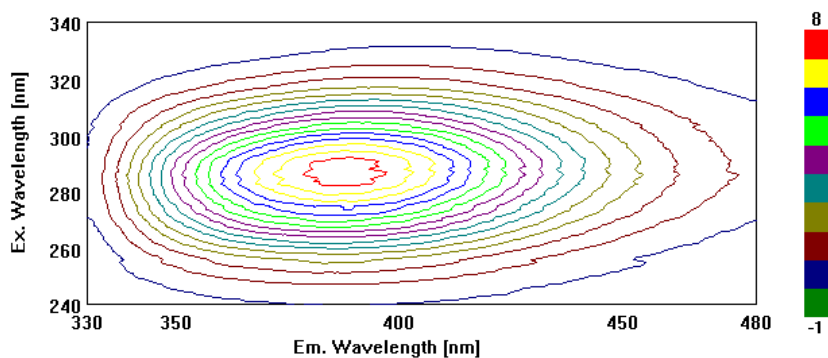
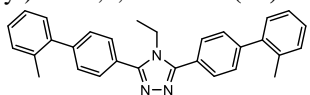


2. 3D emission spectra of compounds

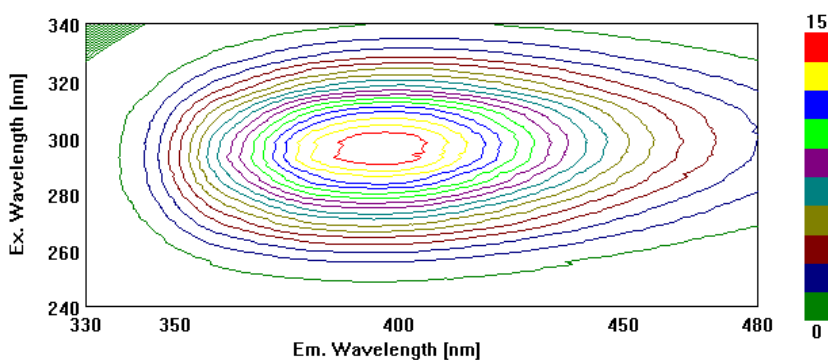
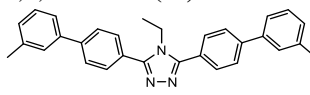
Emission spectrum of 3,5-bis(biphenyl-4-yl)-4-ethyl-4*H*-1,2,4-triazole (**5a**)



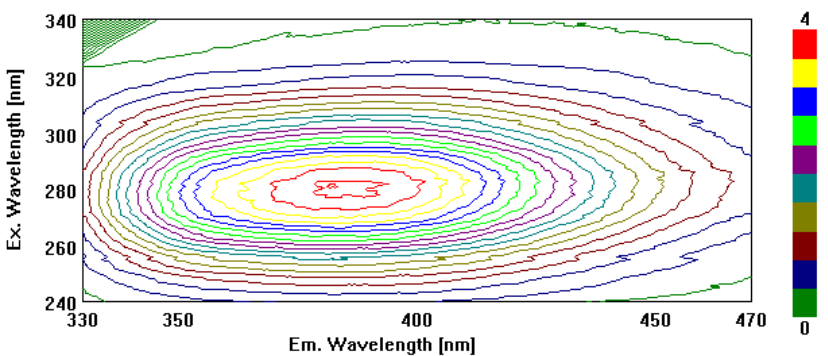
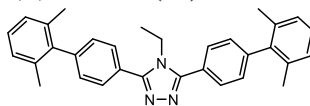
Emission spectrum of 4-ethyl-3,5-bis(2'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**5b**)



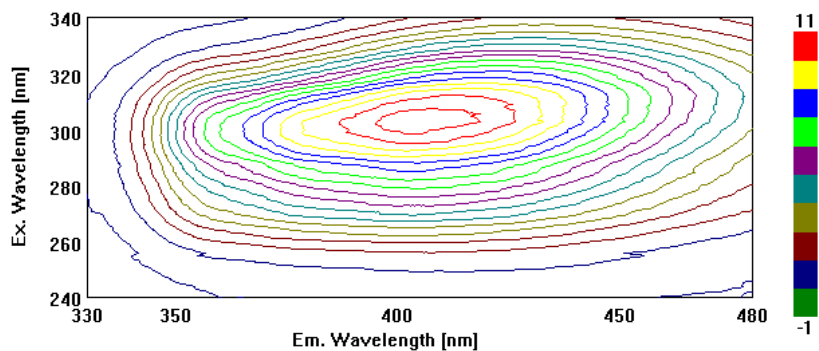
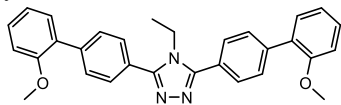
Emission spectrum of 4-ethyl-3,5-bis(3'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**5c**)



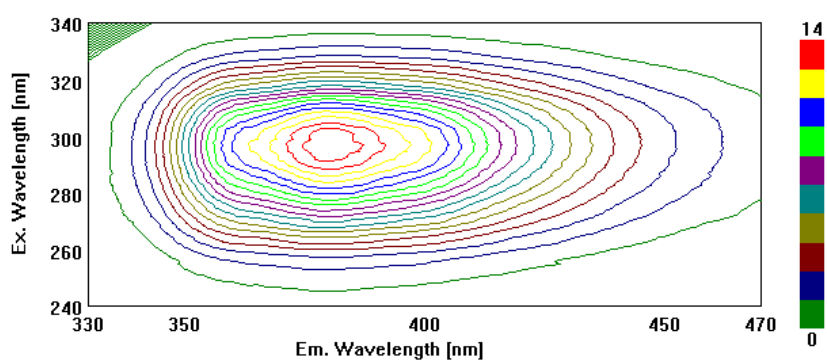
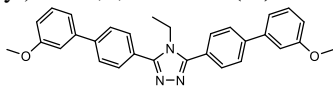
Emission spectrum of 4-ethyl-3,5-bis(2',6'-dimethylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**5d**)



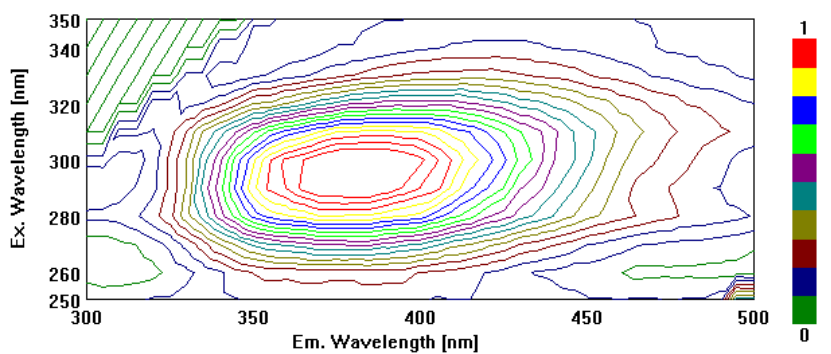
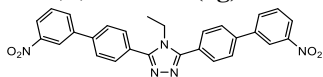
Emission spectrum of 4-ethyl-3,5-bis(2'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**5e**)



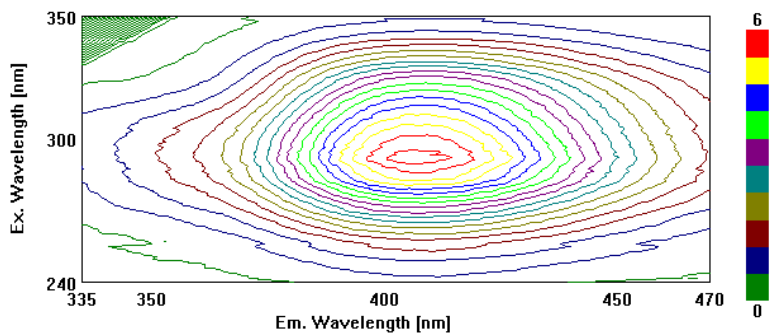
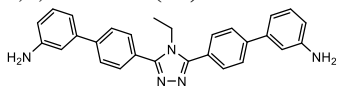
Emission spectrum of 4-ethyl-3,5-bis(3'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**5f**)



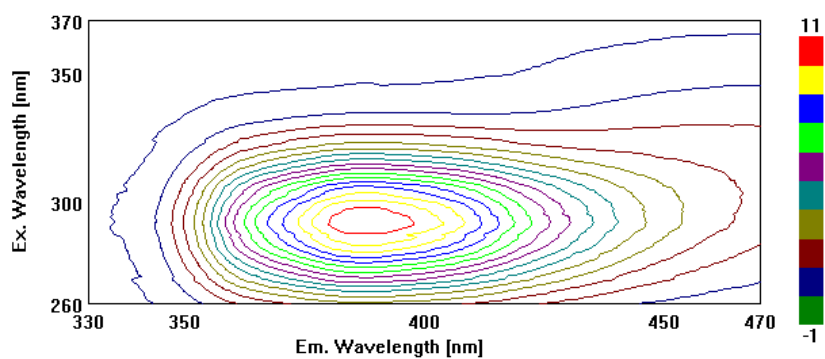
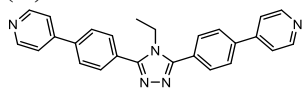
Emission spectrum of 4-ethyl-3,5-bis(3'-nitrobiphenyl-4-yl)-4*H*-1,2,4-triazole (**5g**)



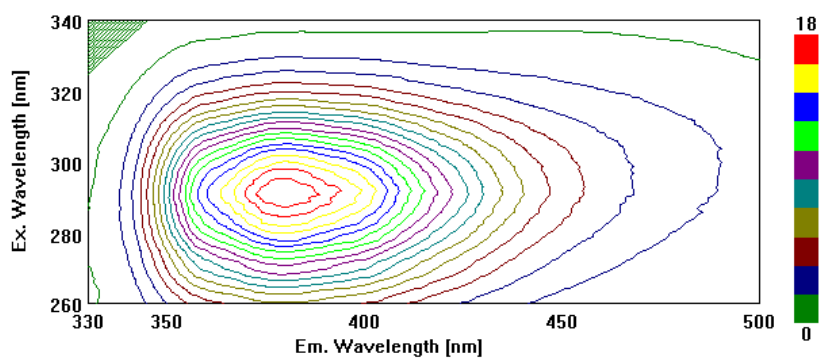
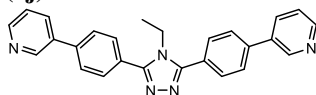
Emission spectrum of 3,5-bis(3'-aminobiphenyl-4-yl)-4-ethyl-4*H*-1,2,4-triazole (**5h**)



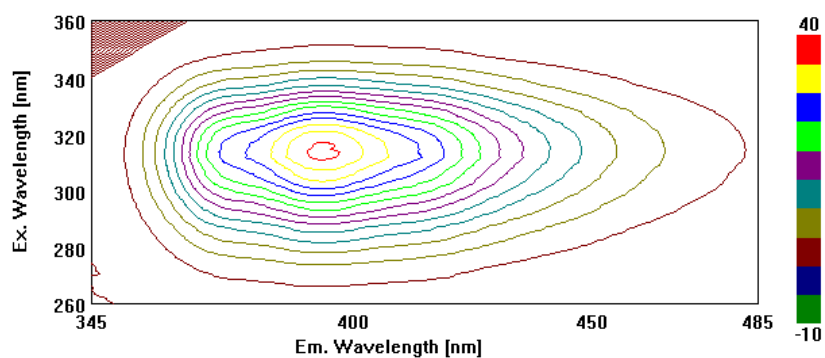
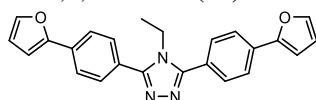
Emission spectrum of 4-ethyl-3,5-bis[4-(pyridin-4-yl)phenyl]-4*H*-1,2,4-triazole (**5i**)



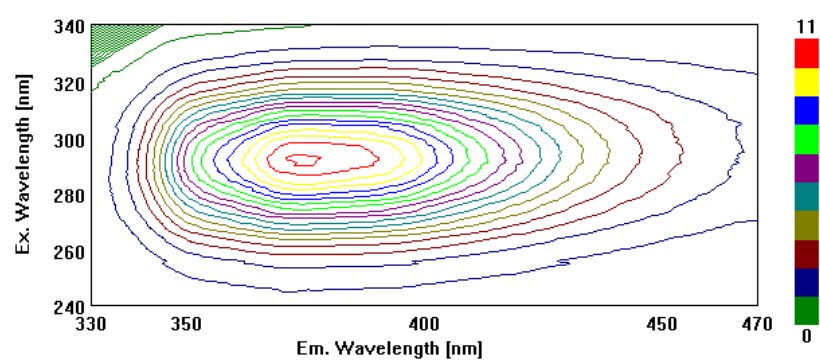
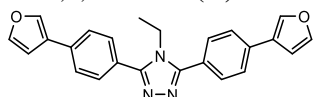
Emission spectrum of 4-ethyl-3,5-bis[4-(pyridin-3-yl)phenyl]-4*H*-1,2,4-triazole (**5j**)



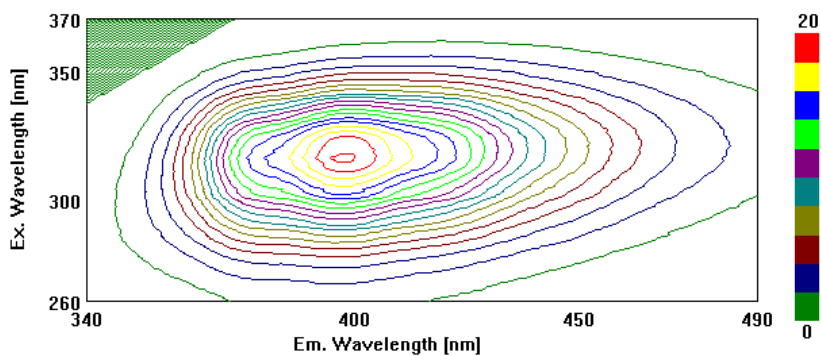
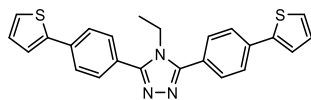
Emission spectrum of 4-ethyl-3,5-bis[4-(furan-2-yl)phenyl]-4*H*-1,2,4-triazole (**5k**)



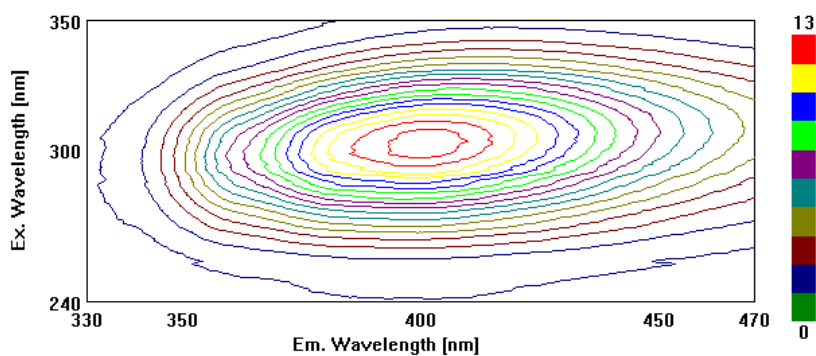
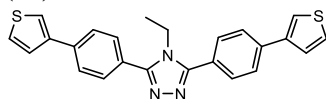
Emission spectrum of 4-ethyl-3,5-bis[4-(furan-3-yl)phenyl]-4*H*-1,2,4-triazole (**5l**)



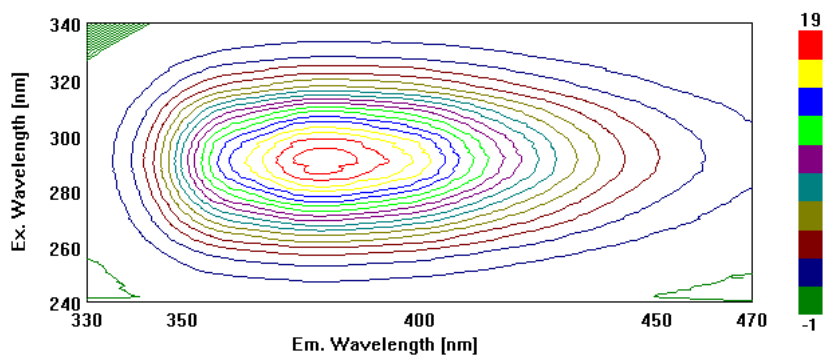
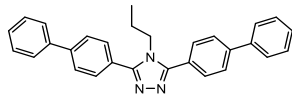
Emission spectrum of 4-ethyl-3,5-bis[4-(thiophen-2-yl)phenyl]-4*H*-1,2,4-triazole (**5m**)



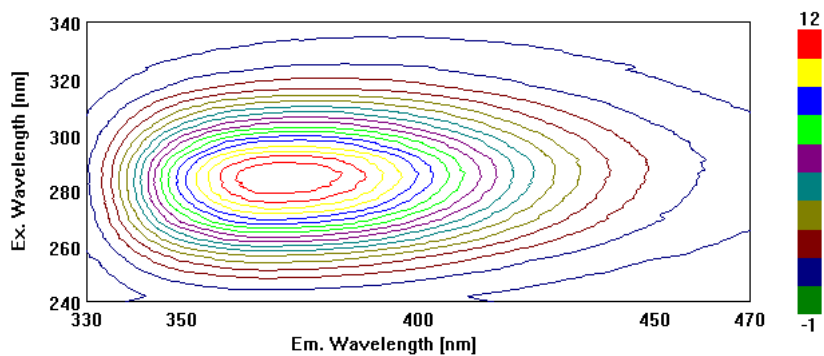
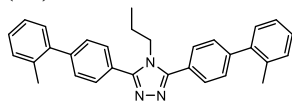
Emission spectrum of 4-ethyl-3,5-bis[4-(thiophen-3-yl)phenyl]-4*H*-1,2,4-triazole (**5n**)



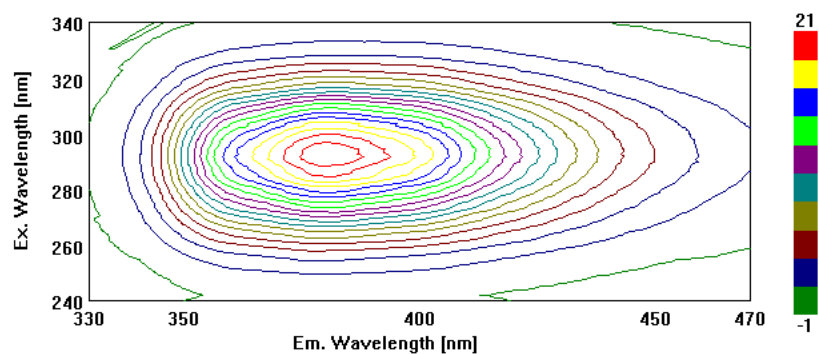
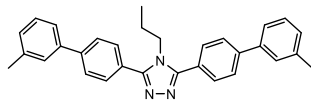
Emission spectrum of 3,5-bis(biphenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6a**)



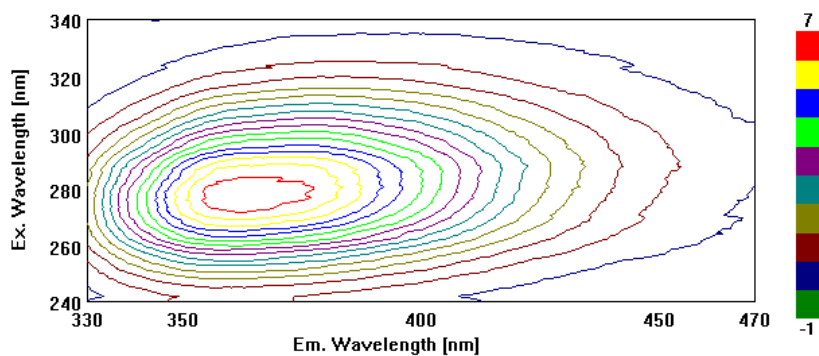
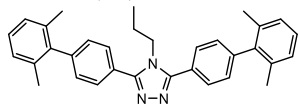
Emission spectrum of 3,5-bis(2'-methylbiphenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6b**)



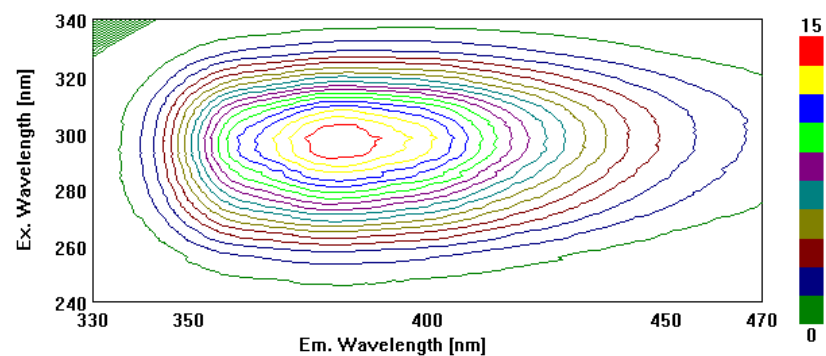
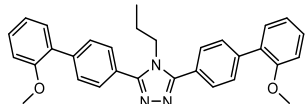
Emission spectrum of 3,5-bis(3'-methylbiphenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6c**)



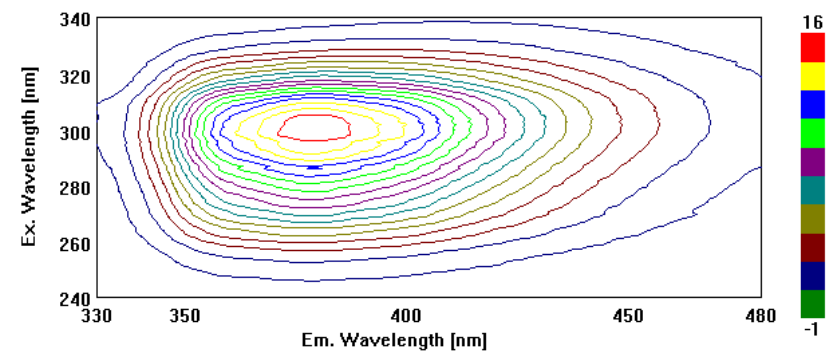
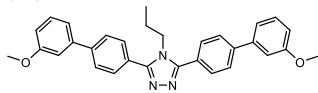
Emission spectrum of 3,5-bis(2',6'-dimethylbiphenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6d**)



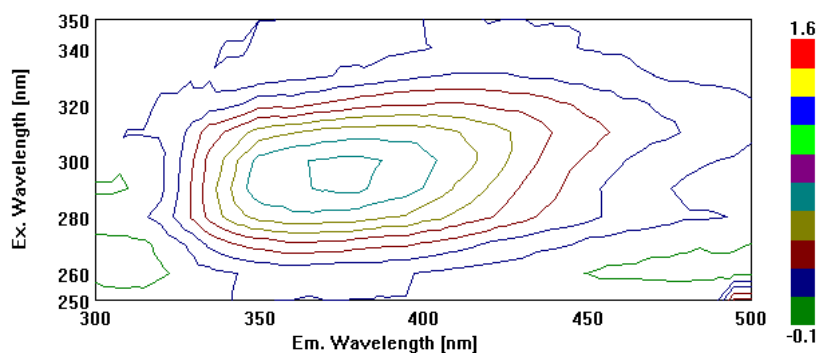
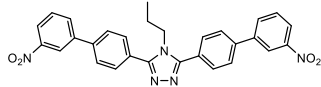
Emission spectrum of 3,5-bis(2'-methoxybiphenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6e**)



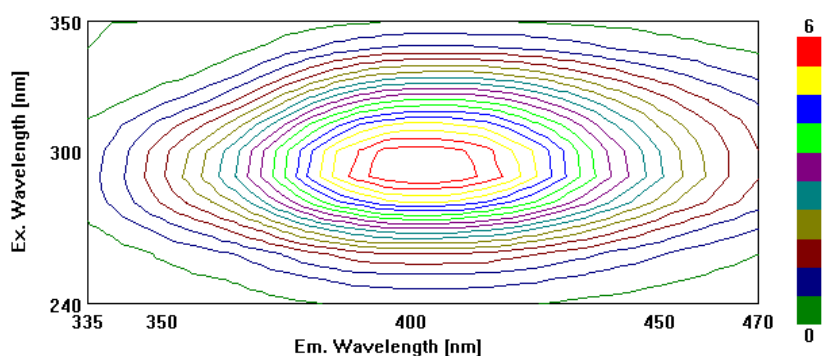
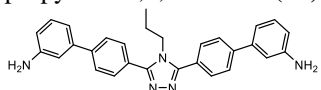
Emission spectrum of 3,5-bis(3'-methoxybiphenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6f**)



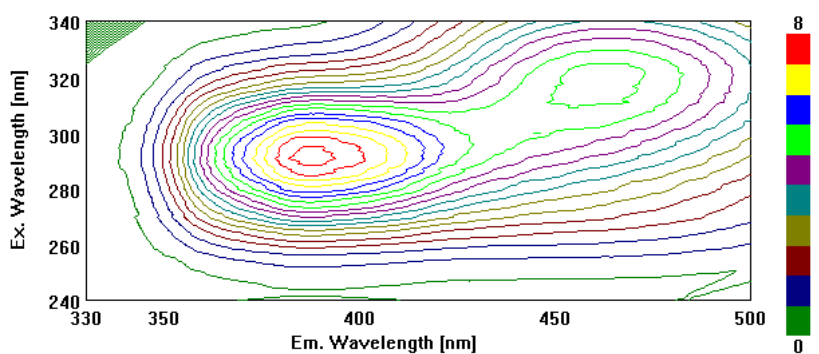
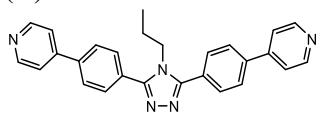
Emission spectrum of 3,5-bis(3'-nitrophenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6g**)



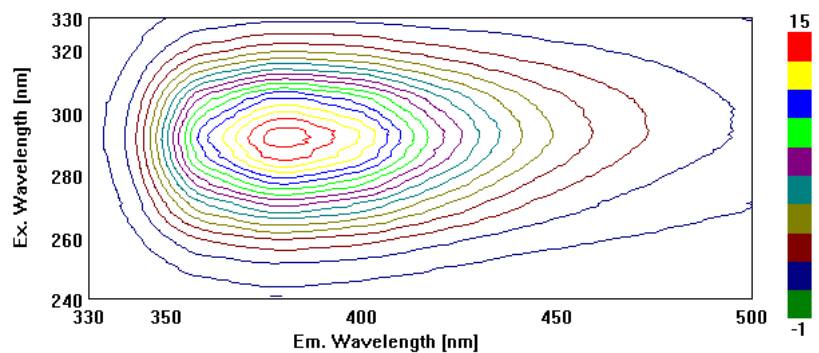
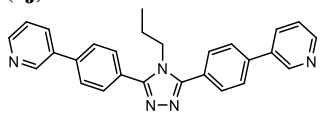
Emission spectrum of 3,5-bis(3'-aminophenyl-4-yl)-4-propyl-4*H*-1,2,4-triazole (**6h**)



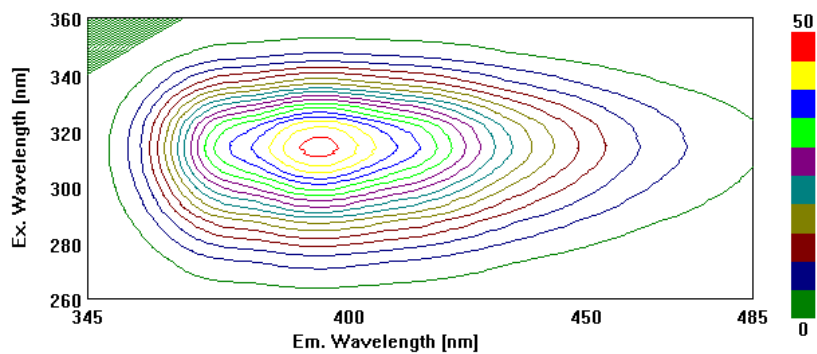
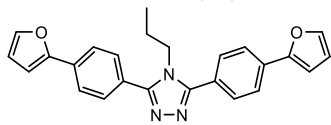
Emission spectrum of 4-propyl-3,5-bis[4-(pyridin-4-yl)phenyl]-4*H*-1,2,4-triazole (**6i**)



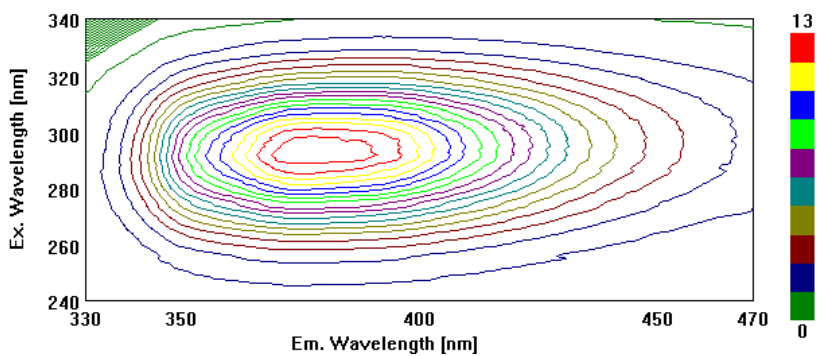
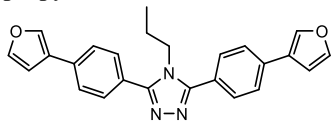
Emission spectrum of 4-propyl-3,5-bis[4-(pyridin-3-yl)phenyl]-4*H*-1,2,4-triazole (**6j**)



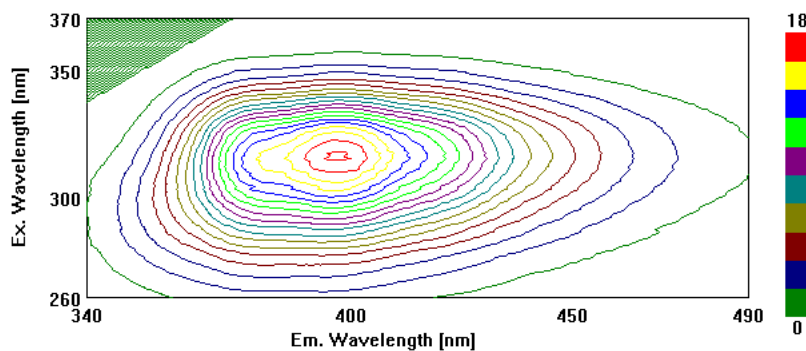
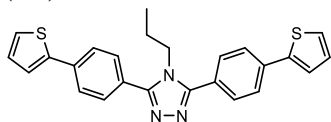
Emission spectrum of 3,5-bis[4-(furan-2-yl)phenyl]-4-propyl-4*H*-1,2,4-triazole (**6k**)



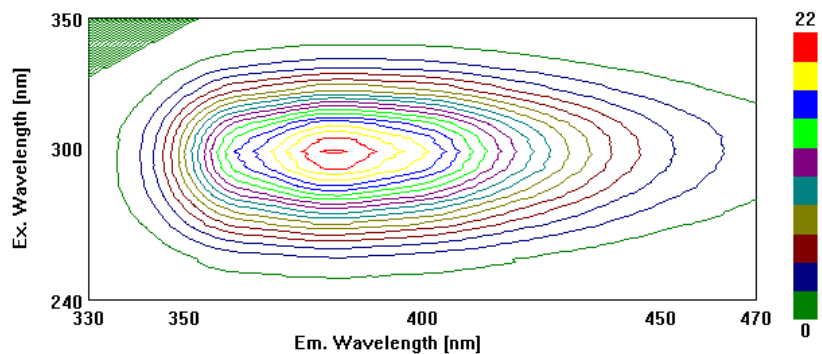
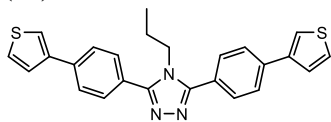
Emission spectrum of 3,5-bis[4-(furan-3-yl)phenyl]-4-propyl-4*H*-1,2,4-triazole (**6l**)



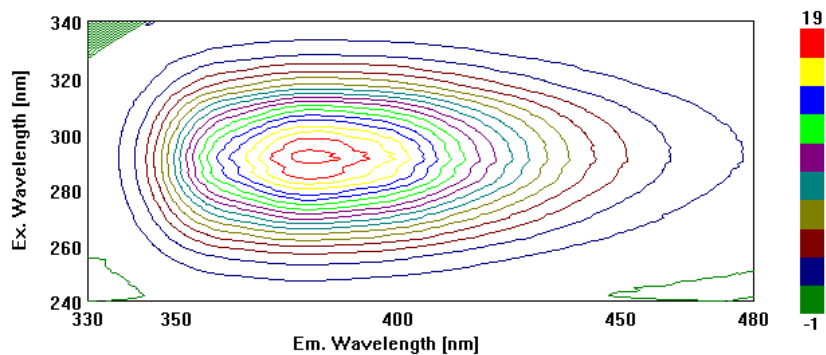
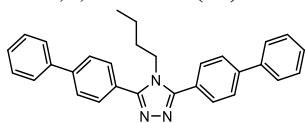
Emission spectrum of 4-propyl-3,5-bis[4-(thiophen-2-yl)phenyl]-4*H*-1,2,4-triazole (**6m**)



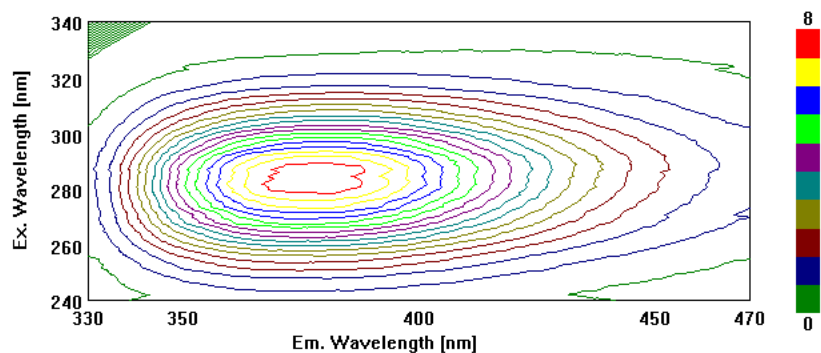
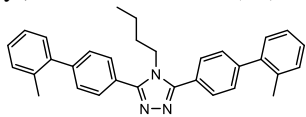
Emission spectrum of 4-propyl-3,5-bis[4-(thiophen-3-yl)phenyl]-4*H*-1,2,4-triazole (**6n**)



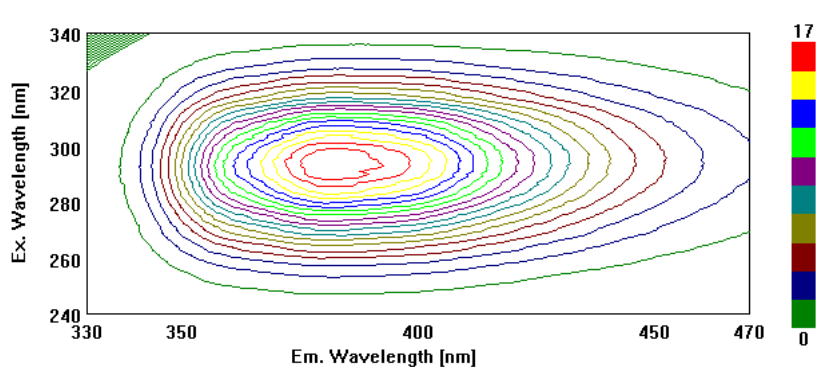
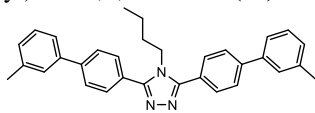
Emission spectrum of 3,5-bis(biphenyl-4-yl)-4-butyl-4*H*-1,2,4-triazole (**7a**)



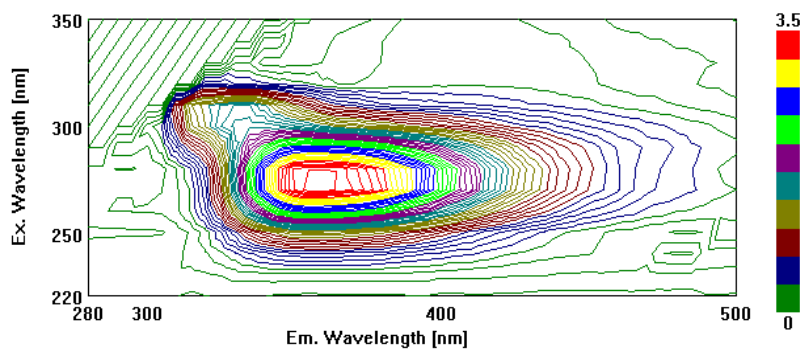
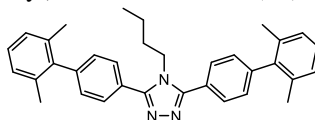
Emission spectrum of 4-butyl-3,5-bis(2'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**7b**)



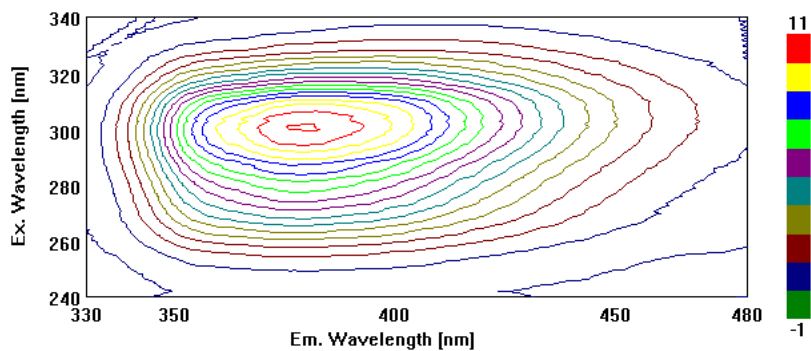
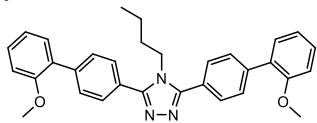
Emission spectrum of 4-butyl-3,5-bis(3'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**7c**)



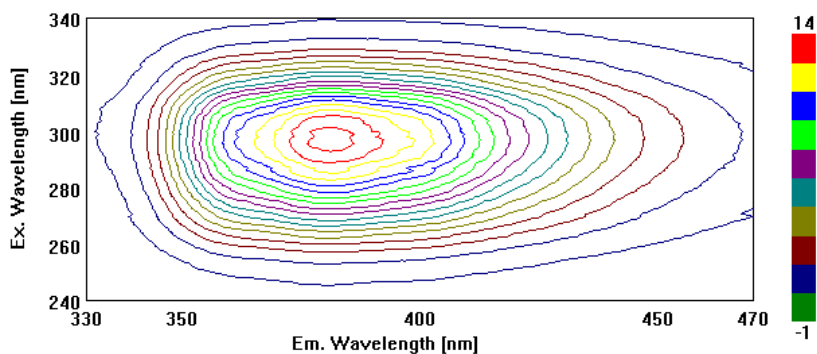
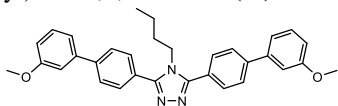
Emission spectrum of 4-butyl-3,5-bis(2',6'-dimethylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**7d**)



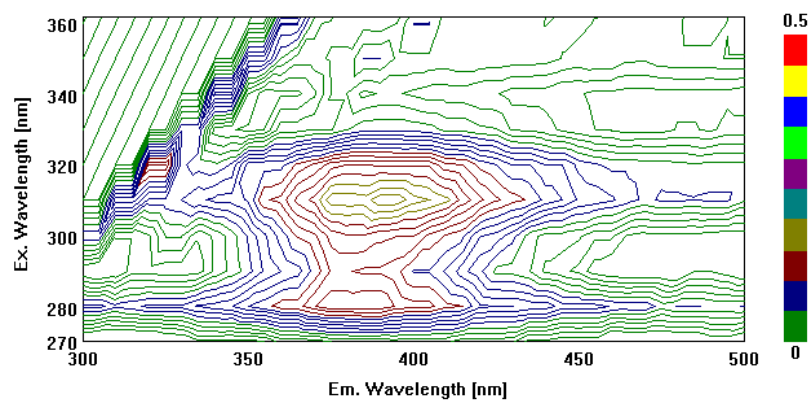
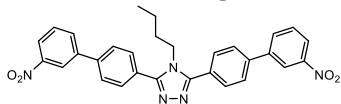
Emission spectrum of 4-butyl-3,5-bis(2'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**7e**)



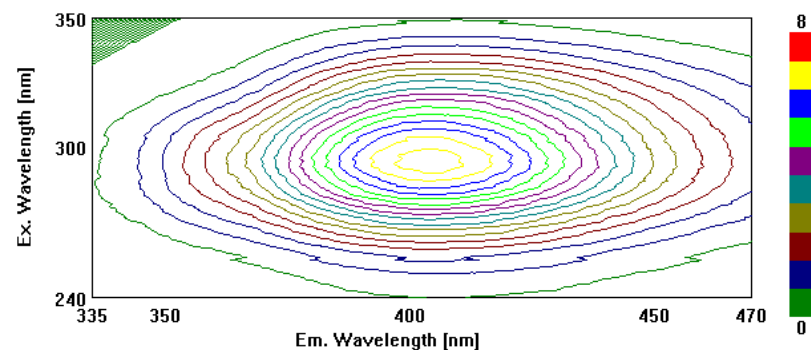
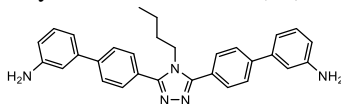
Emission spectrum of 4-butyl-3,5-bis(3'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**7f**)



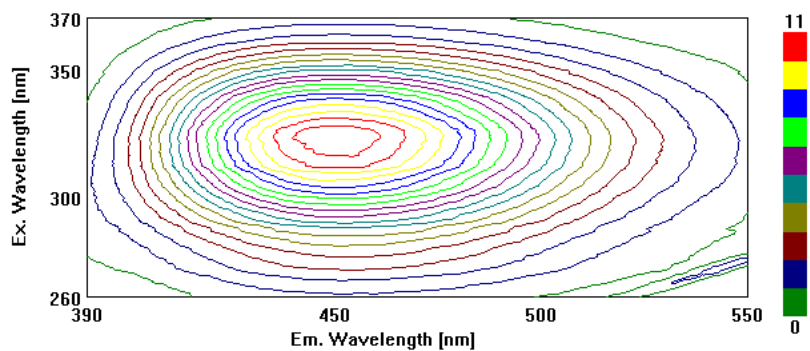
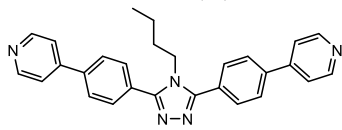
Emission spectrum of 4-butyl-3,5-bis[(3'-nitrobiphenyl-4-yl)-4*H*-1,2,4-triazole (**7g**)



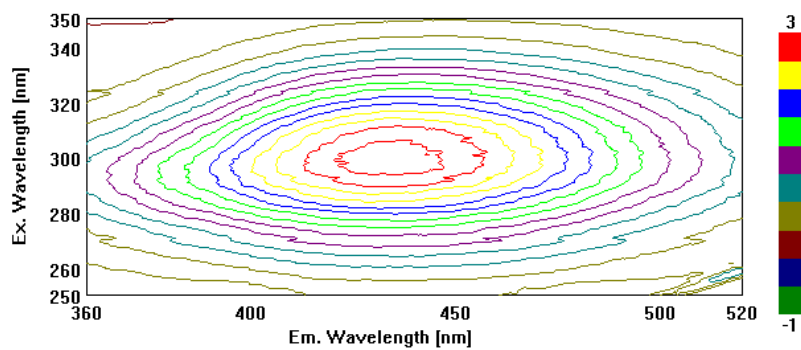
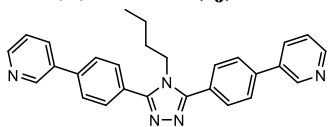
Emission spectrum of 3,5-bis(3'-aminobiphenyl-4-yl)-4-butyl-4*H*-1,2,4-triazole (**7h**)



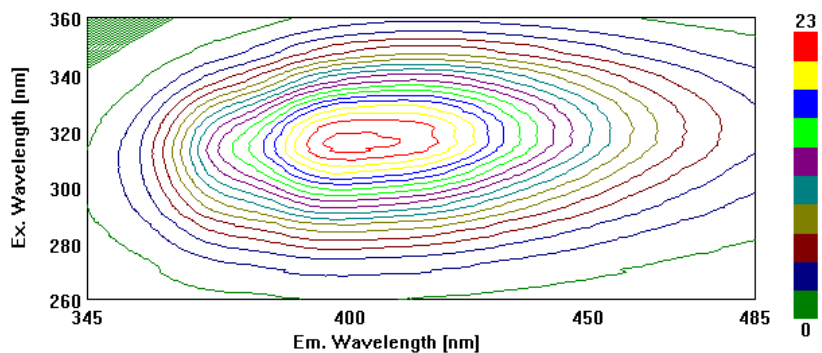
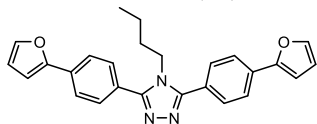
Emission spectrum of 4-butyl-3,5-bis[4-(pyridin-4-yl)phenyl]-4*H*-1,2,4-triazole (**7i**)



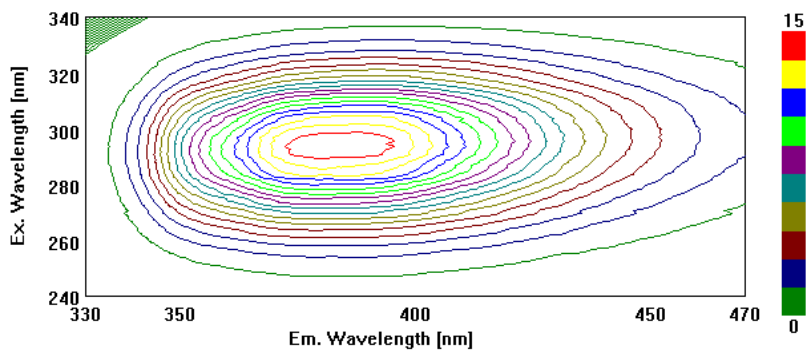
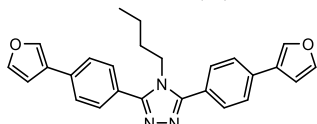
Emission spectrum of 4-butyl-3,5-bis[4-(pyridin-3-yl)phenyl]-4*H*-1,2,4-triazole (**7j**)



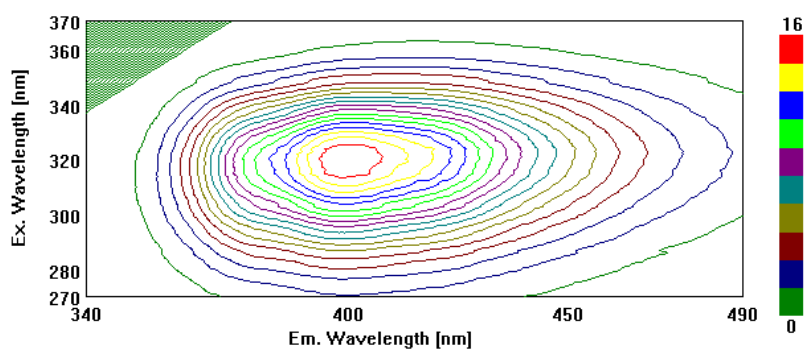
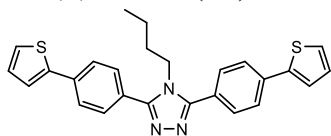
Emission spectrum of 4-butyl-3,5-bis[4-(furan-2-yl)phenyl]-4*H*-1,2,4-triazole (**7k**)



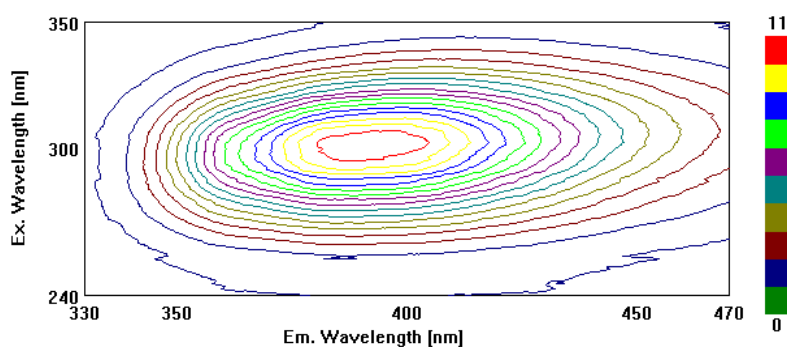
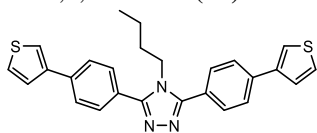
Emission spectrum of 4-butyl-3,5-bis[4-(furan-3-yl)phenyl]-4*H*-1,2,4-triazole (**7l**)



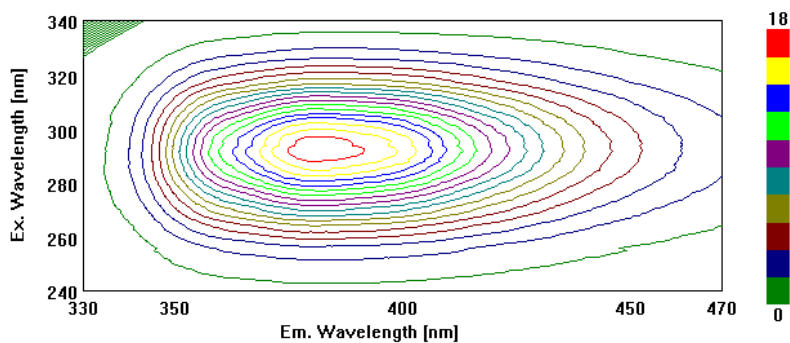
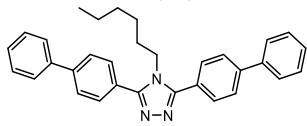
Emission spectrum of 4-butyl-3,5-bis[4-(thiophen-2-yl)phenyl]-4*H*-1,2,4-triazole (**7m**)



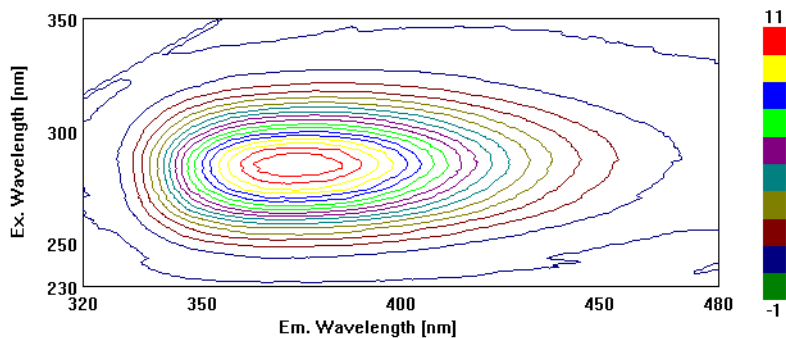
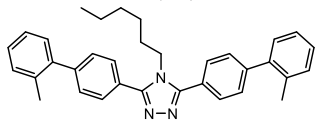
Emission spectrum of 4-butyl-3,5-bis[4-(thiophen-3-yl)phenyl]-4*H*-1,2,4-triazole (**7n**)



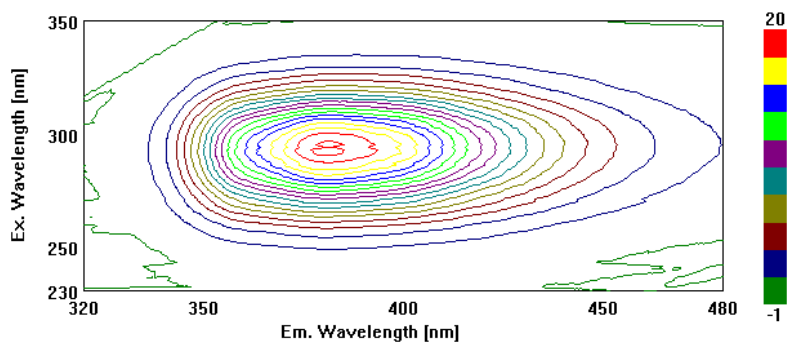
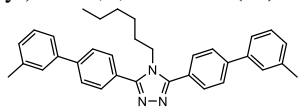
Emission spectrum of 3,5-bis(biphenyl-4-yl)-4-hexyl-4*H*-1,2,4-triazole (**8a**)



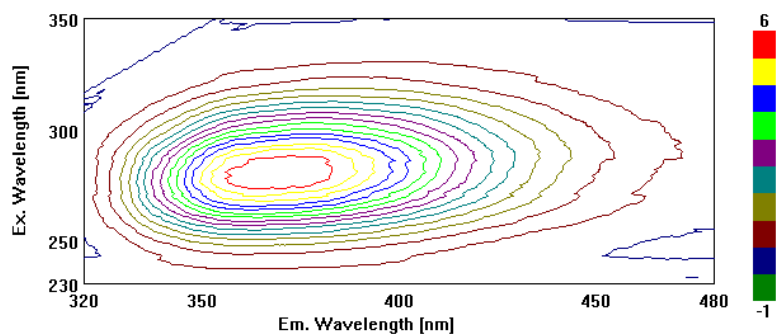
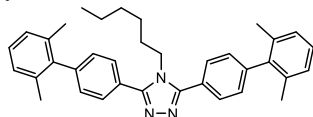
Emission spectrum of 4-hexyl-3,5-bis(2'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**8b**)



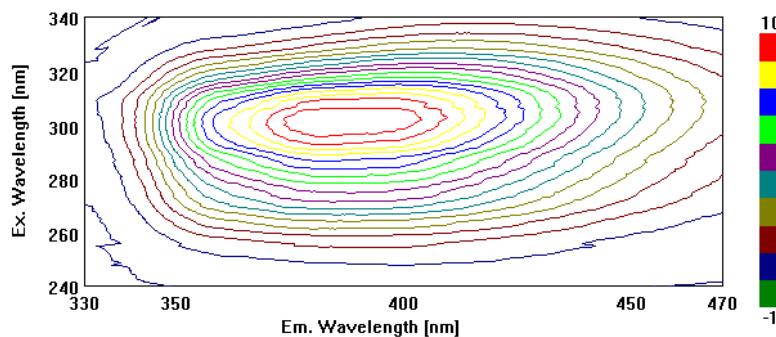
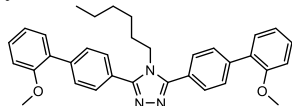
Emission spectrum of 4-hexyl-3,5-bis(3'-methylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**8c**)



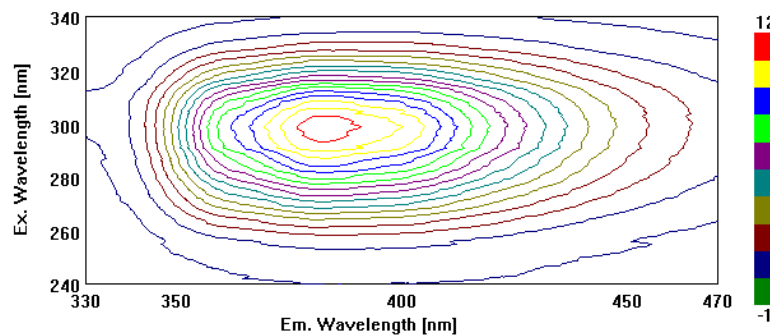
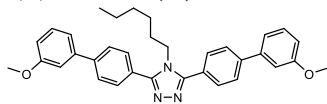
Emission spectrum of 4-hexyl-3,5-bis(2',6'-dimethylbiphenyl-4-yl)-4*H*-1,2,4-triazole (**8d**)



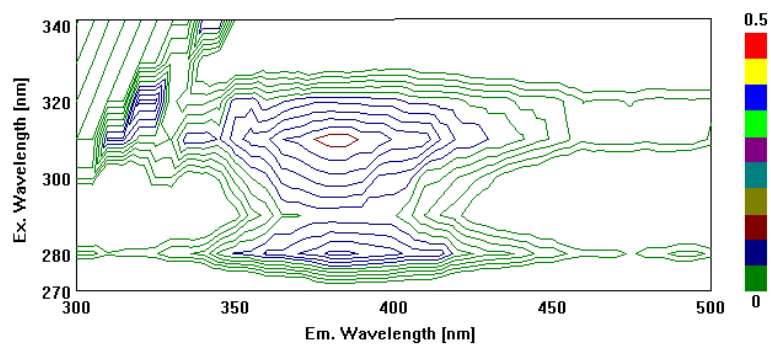
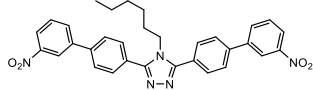
Emission spectrum of 4-hexyl-3,5-bis(2'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**8e**)



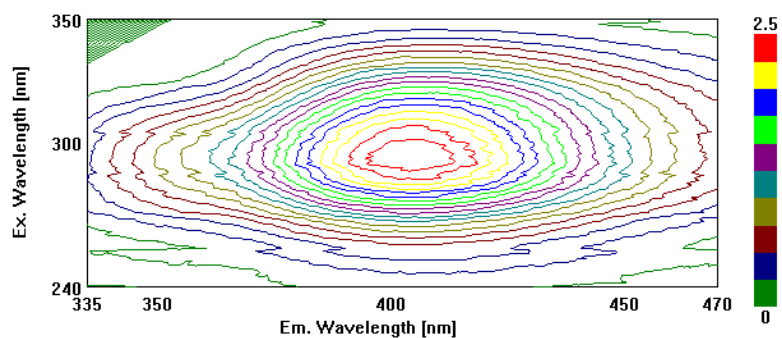
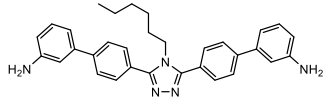
Emission spectrum of 4-hexyl-3,5-bis(3'-methoxybiphenyl-4-yl)-4*H*-1,2,4-triazole (**8f**)



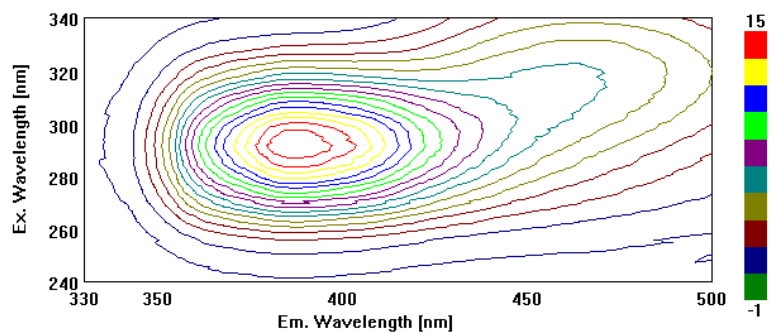
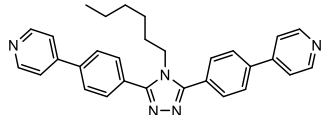
Emission spectrum of 4-hexyl-3,5-bis(3'-nitrophenyl-4-yl)-4*H*-1,2,4-triazole (**8g**)



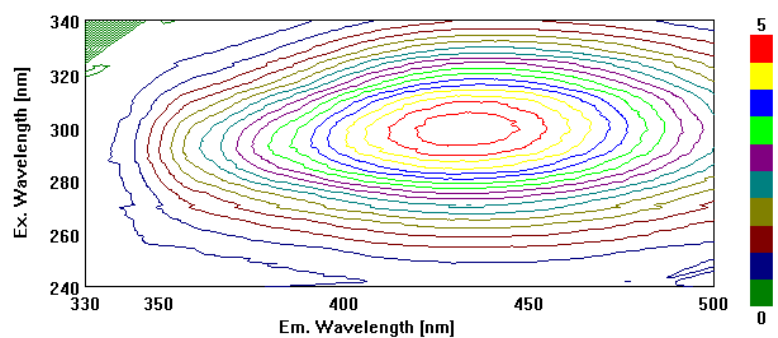
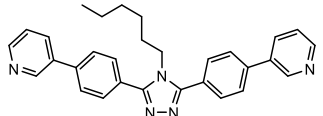
Emission spectrum of 3,5-bis(3'-aminobiphenyl-4-yl)-4-hexyl-4*H*-1,2,4-triazole (**8h**)



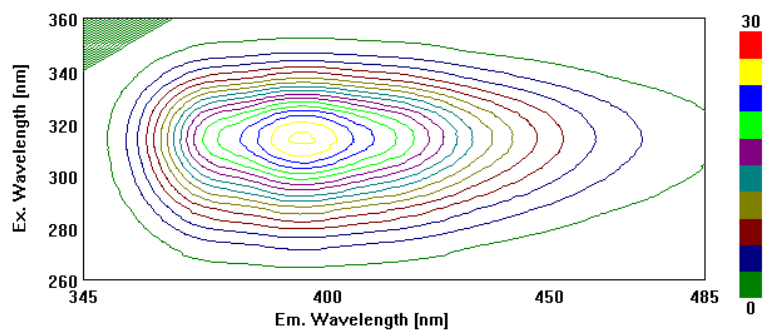
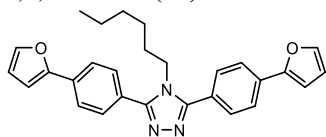
Emission spectrum of 4-hexyl-3,5-bis[4-(pyridin-4-yl)phenyl]-4*H*-1,2,4-triazole (**8i**)



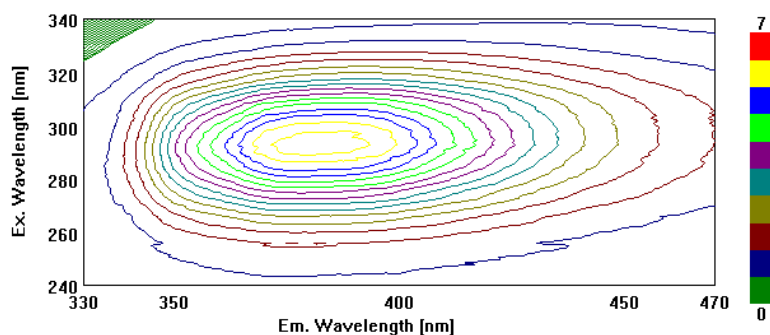
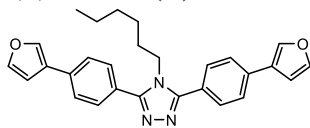
Emission spectrum of 4-hexyl-3,5-bis[4-(pyridin-3-yl)phenyl]-4*H*-1,2,4-triazole (**8j**)



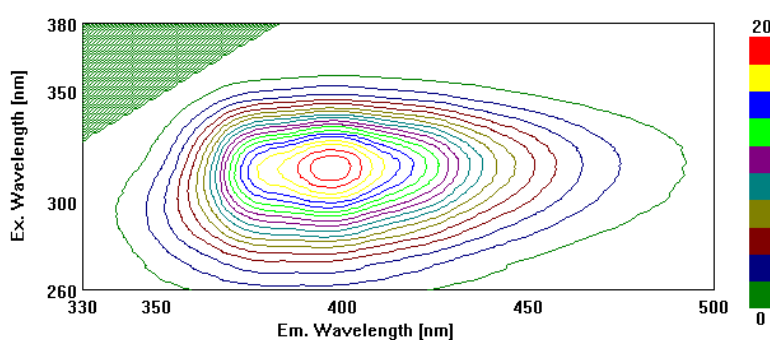
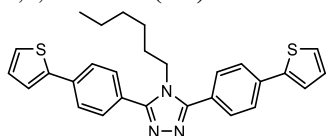
Emission spectrum of 3,5-bis[4-(furan-2-yl)phenyl]-4-hexyl-4*H*-1,2,4-triazole (**8k**)



Emission spectrum of 3,5-bis[4-(furan-3-yl)phenyl]-4-hexyl-4*H*-1,2,4-triazole (**8l**)



Emission spectrum of 4-hexyl-3,5-bis[4-(thiophen-2-yl)phenyl]-4*H*-1,2,4-triazole (**8m**)



Emission spectrum of 4-hexyl-3,5-bis[4-(thiophen-3-yl)phenyl]-4*H*-1,2,4-triazole (**8n**)

