

Supporting information

Highly Efficient Photoinitiation Systems Based on Dibenzo[a,c]phenazine Sensitivity to Visible Light for Dentistry

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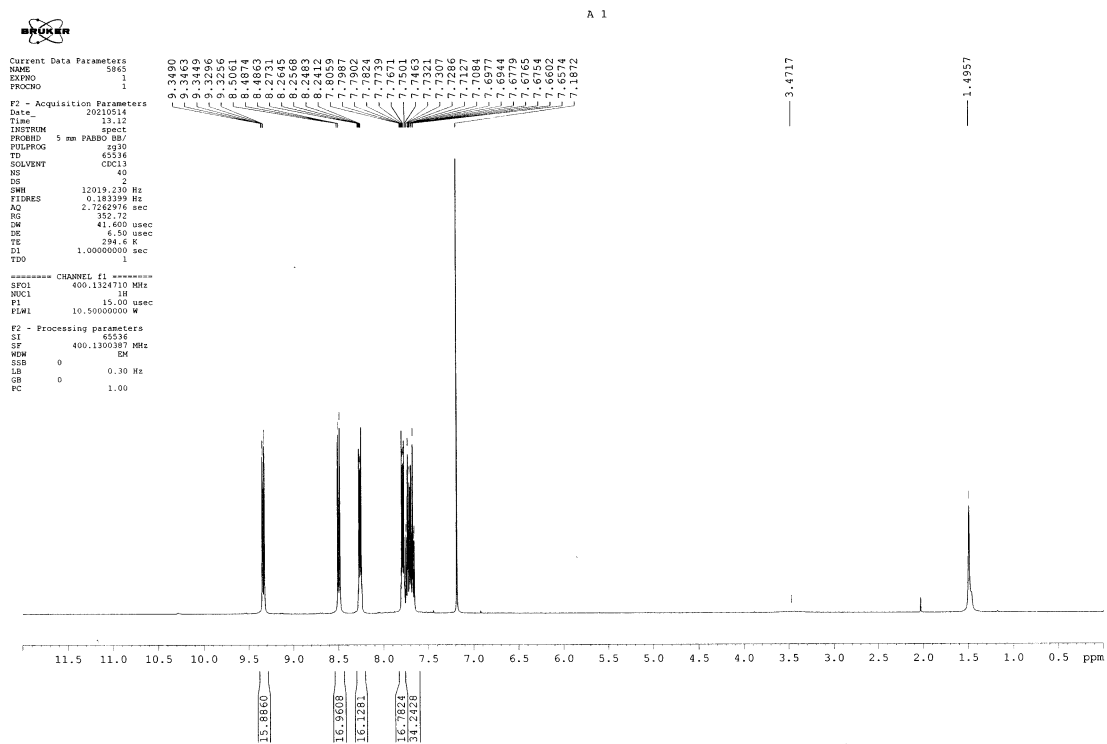
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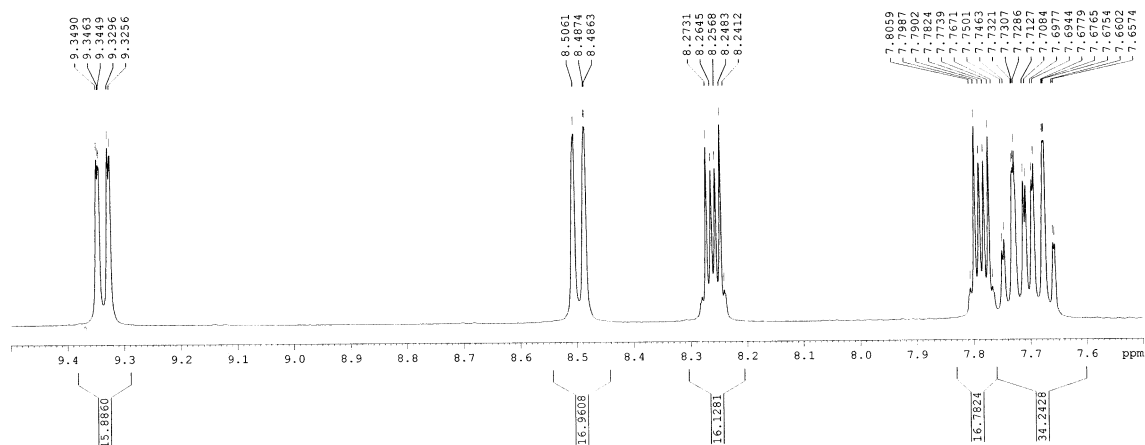
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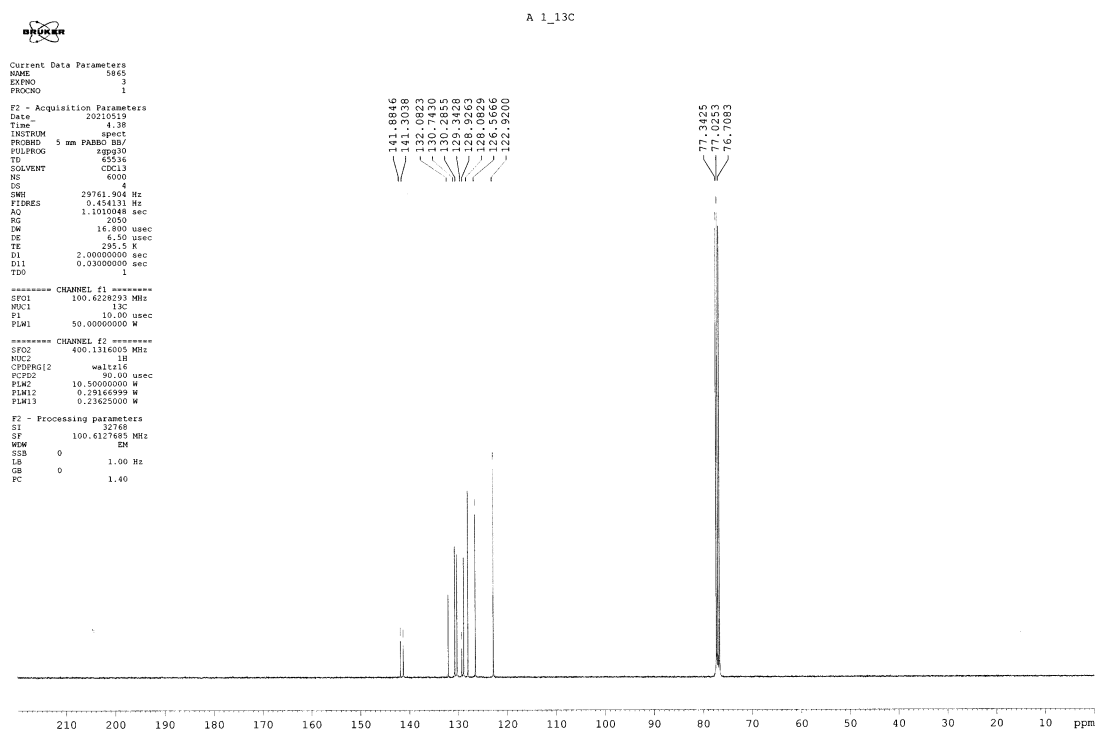
¹H spectrum of DBPh1



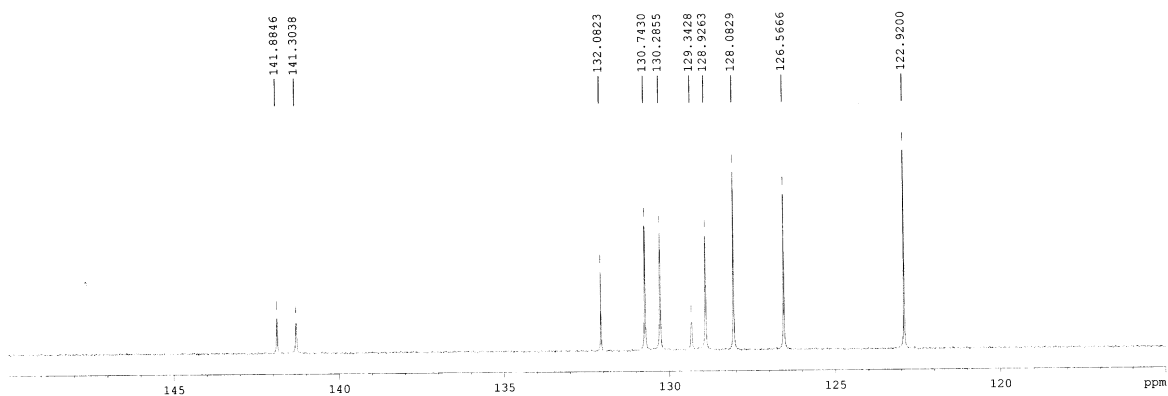
Enlarged spectrum in the range of 6-9 ppm.



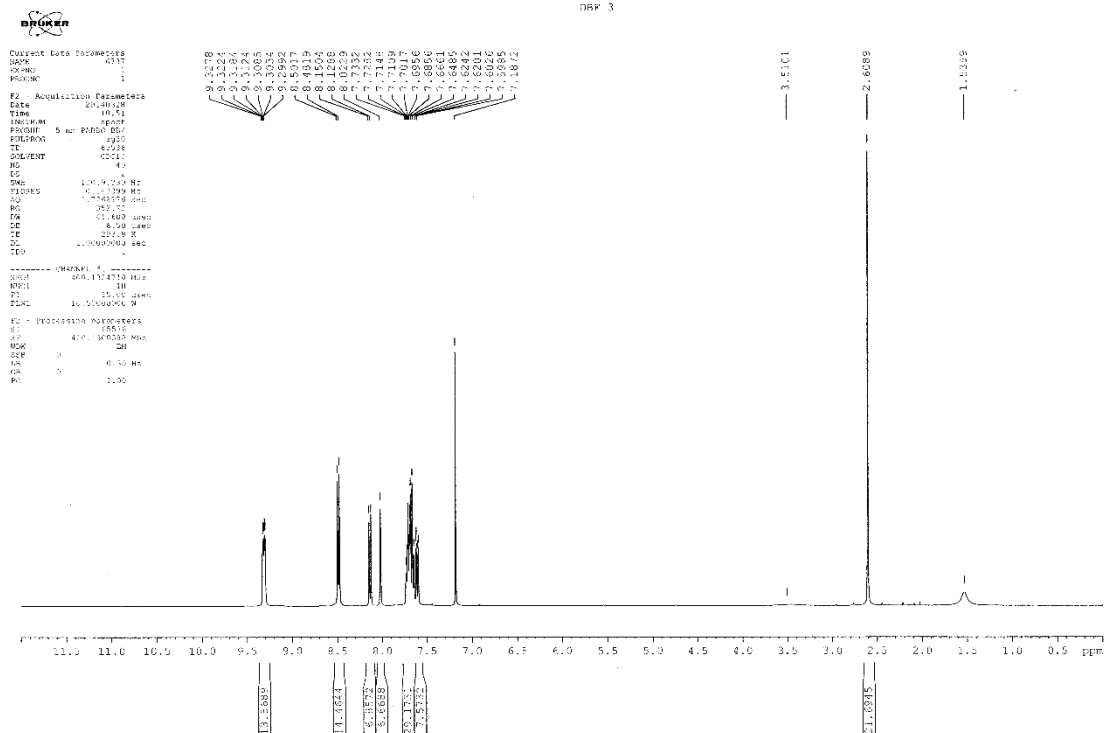
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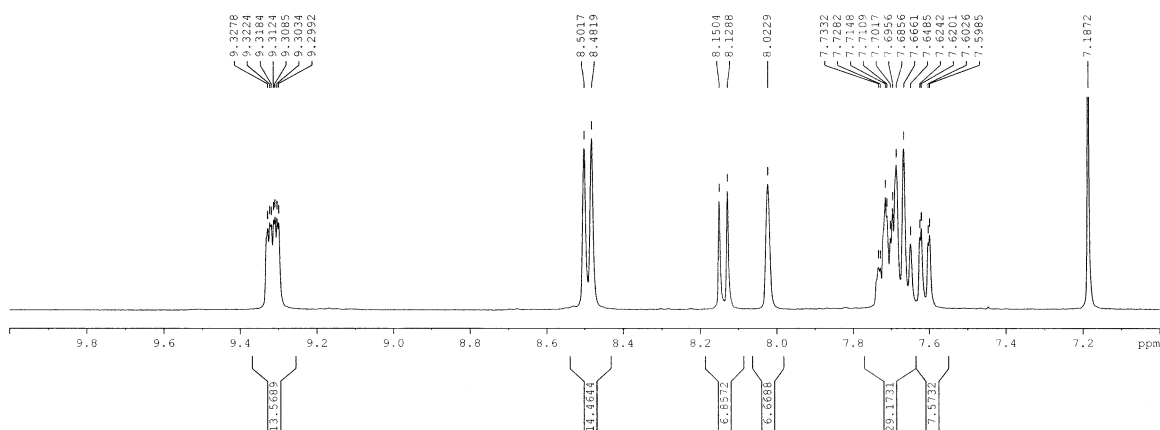
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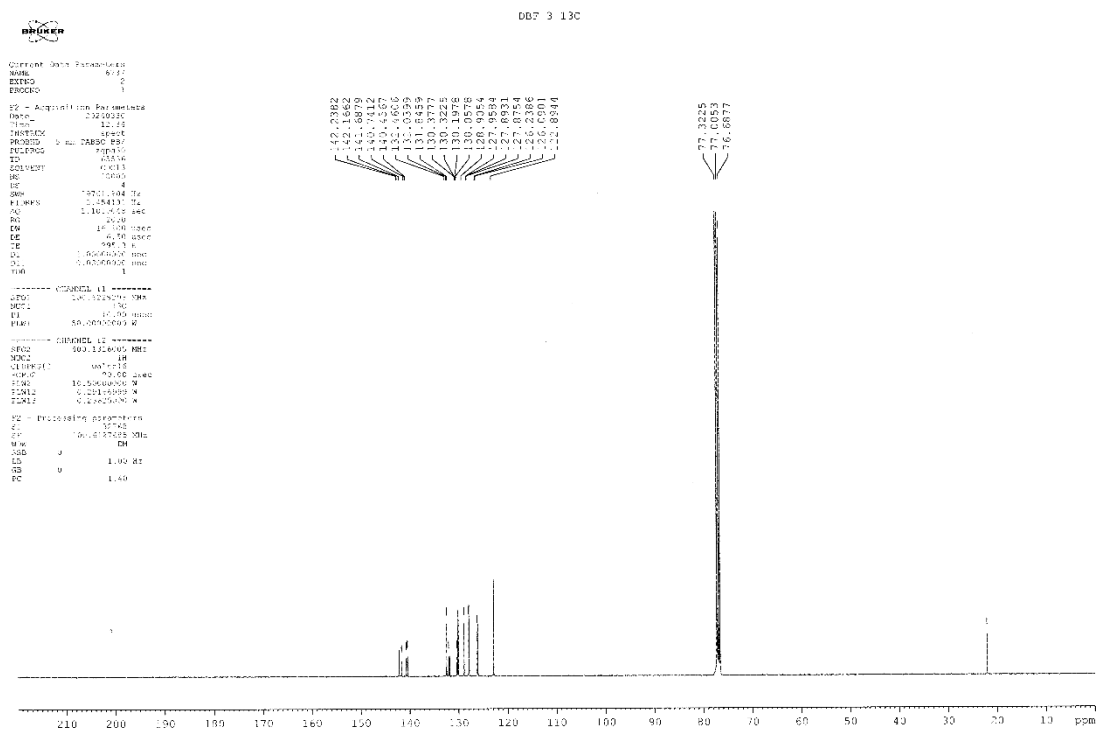
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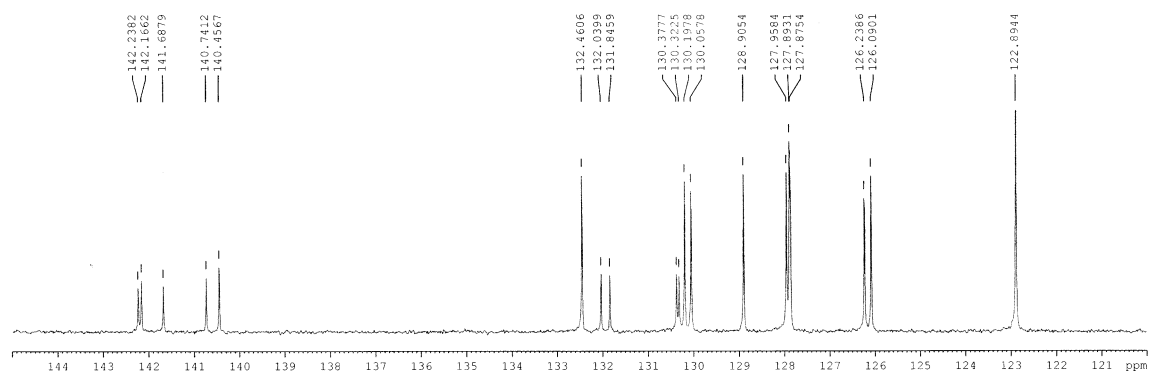
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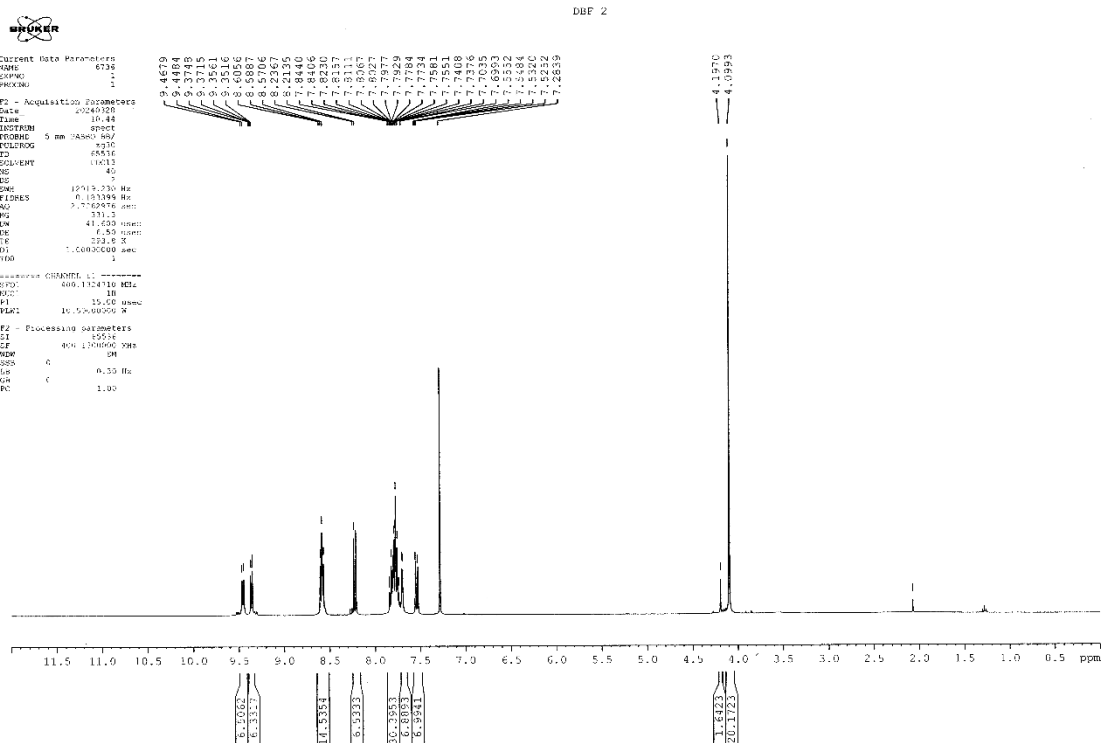
^{13}C spectrum of DBPh2



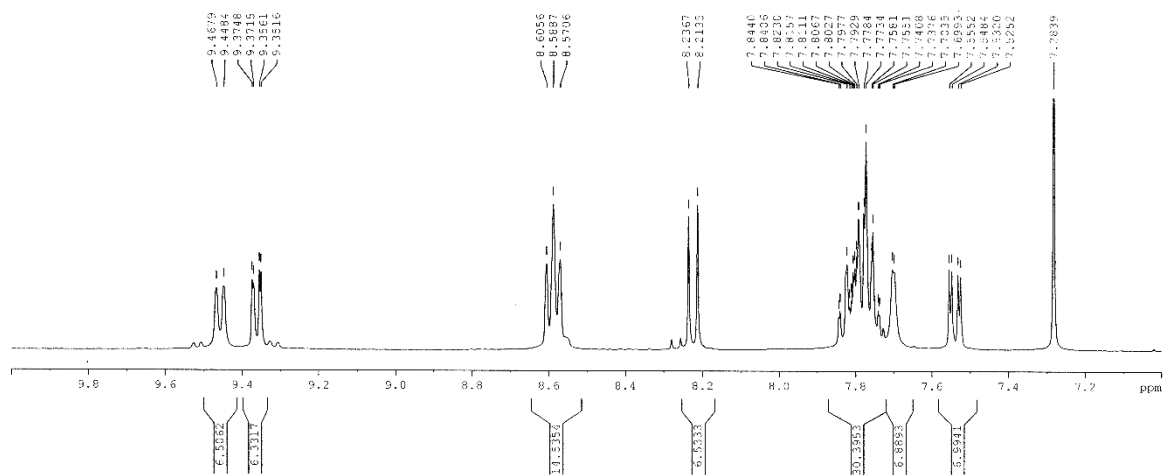
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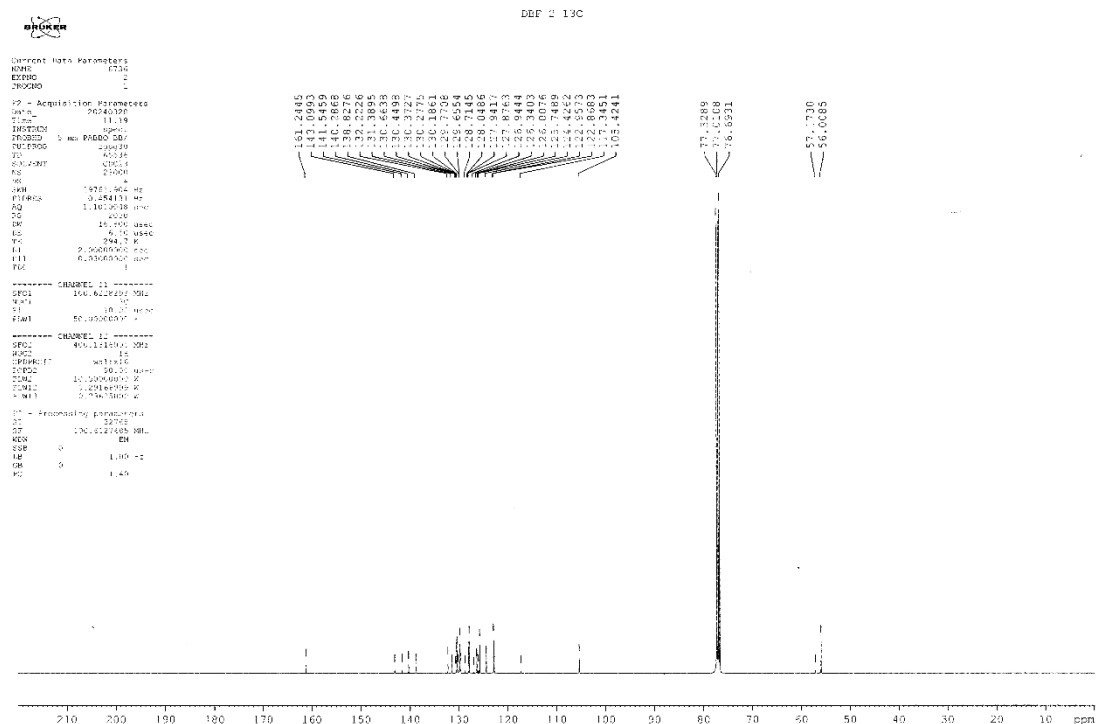
¹H spectrum of DBPh3



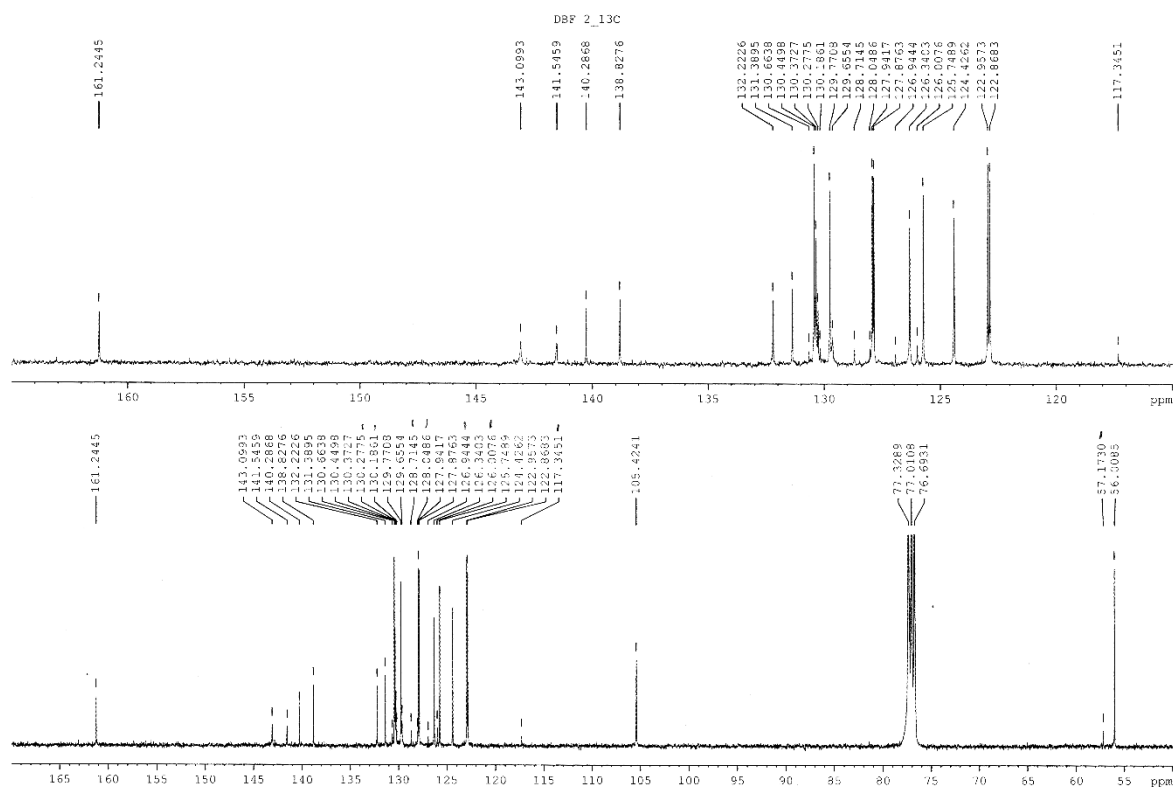
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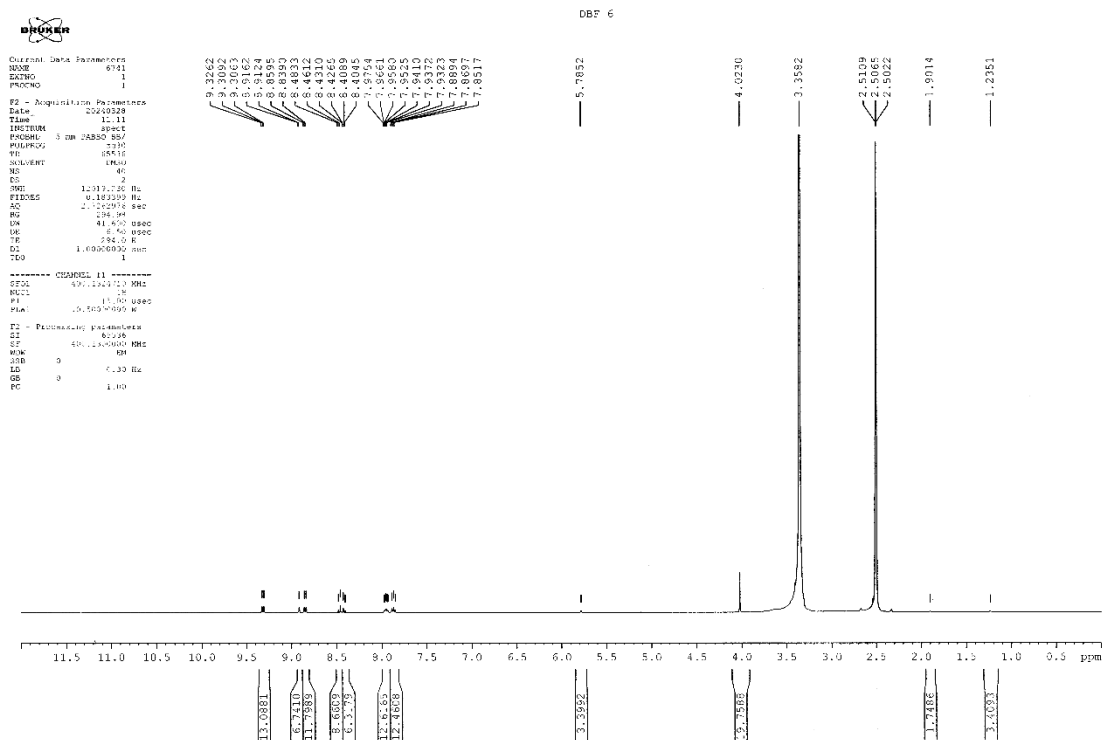
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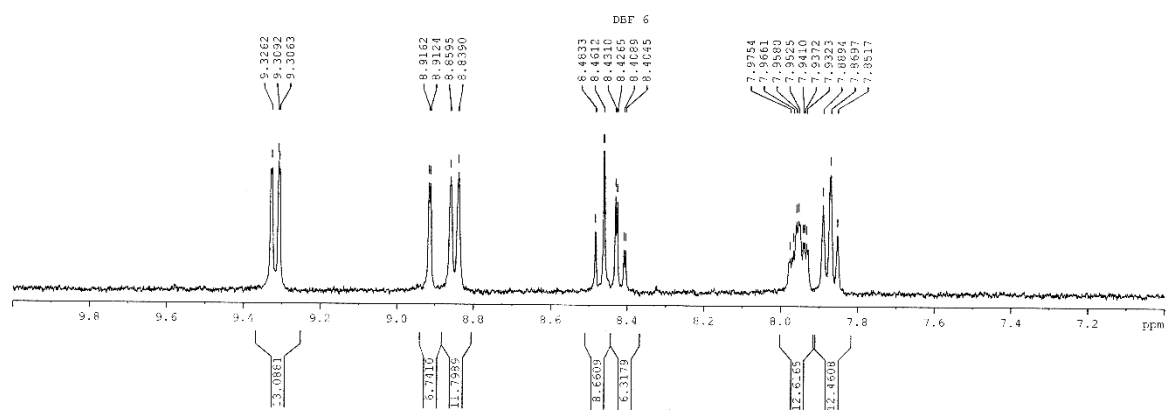
Enlarged spectrum in the range of 50-165 ppm.



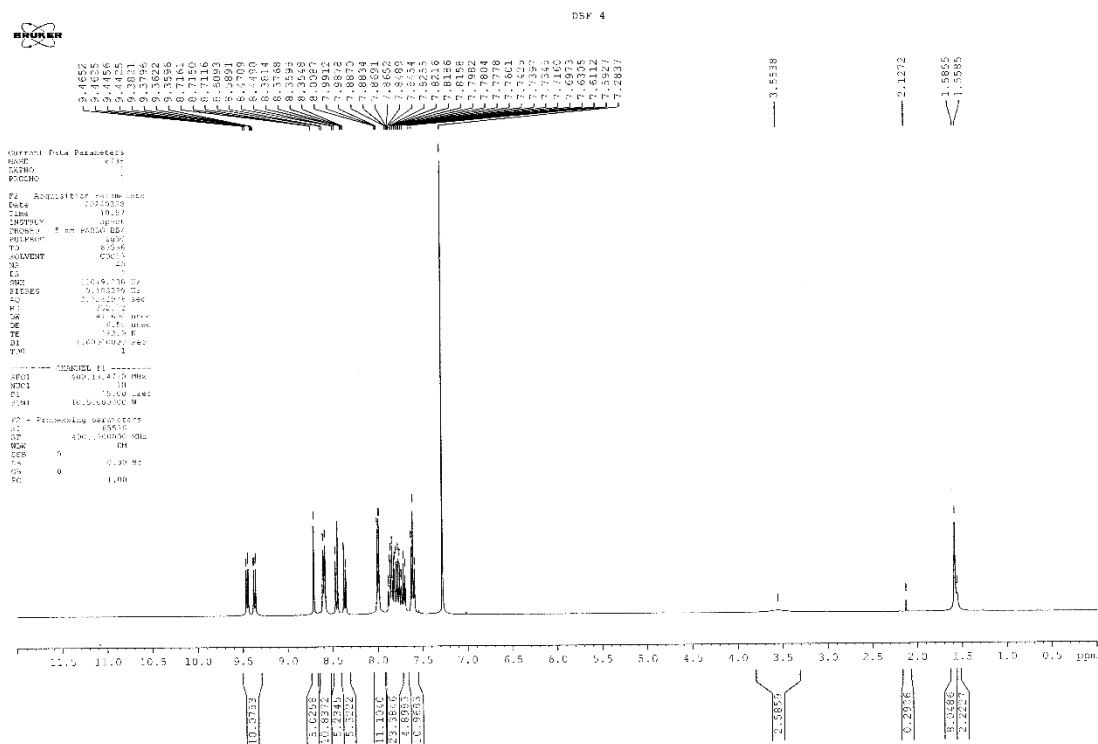
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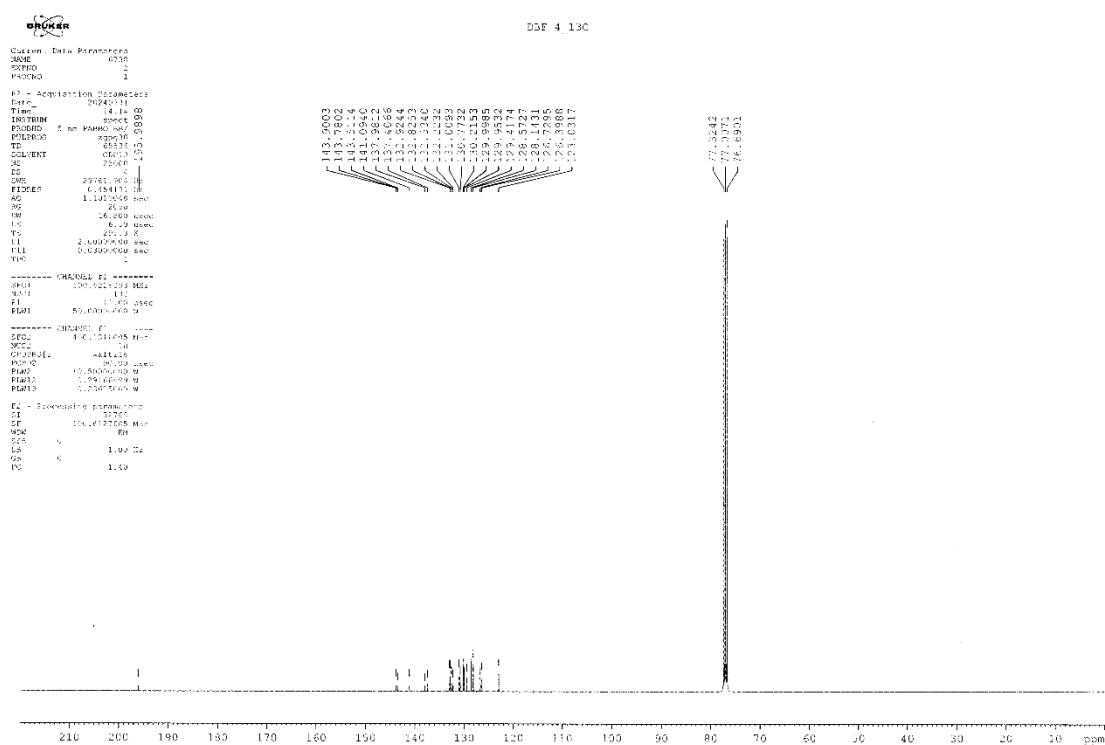
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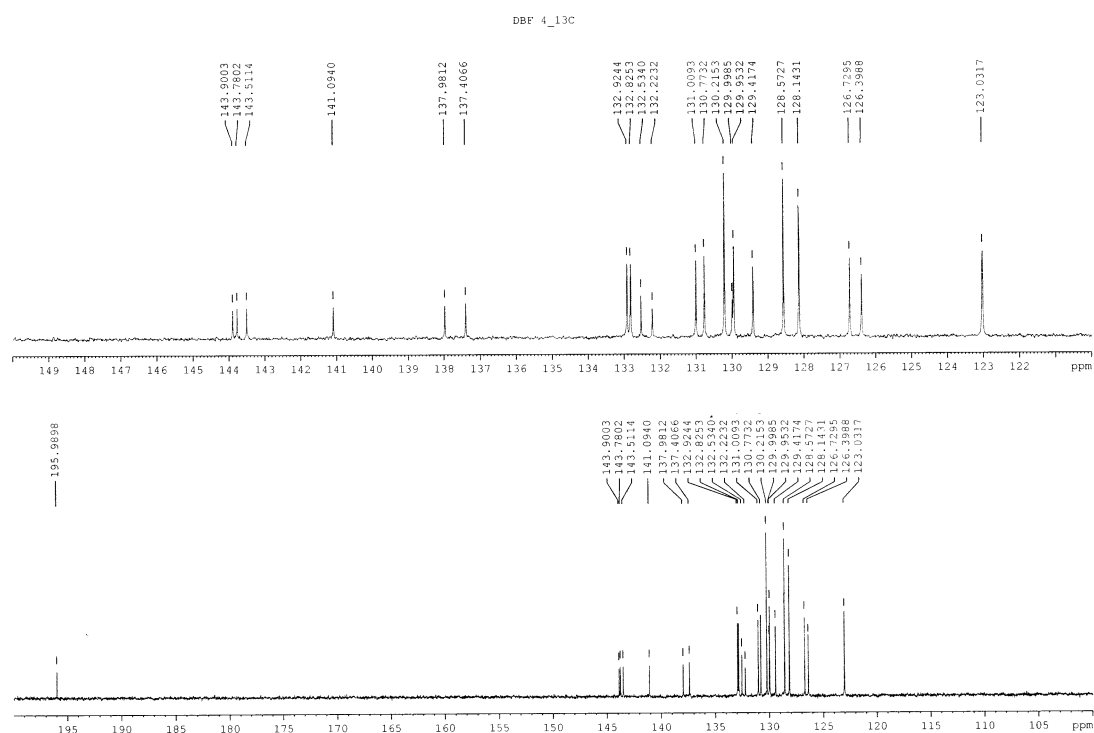
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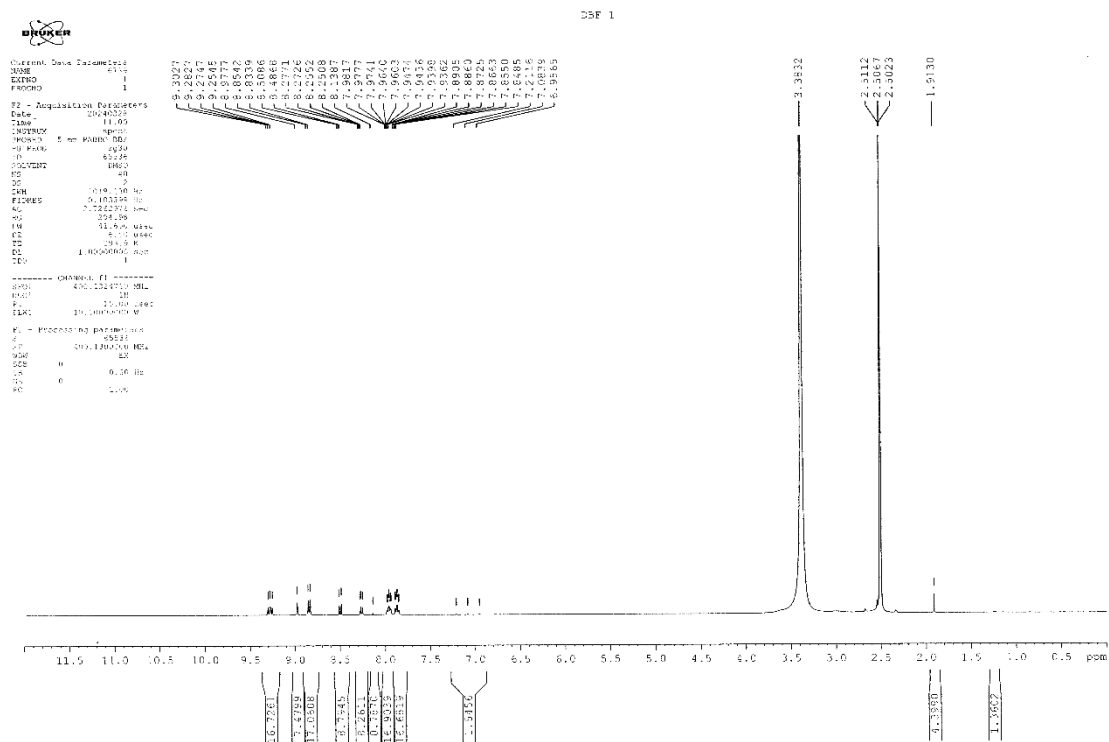
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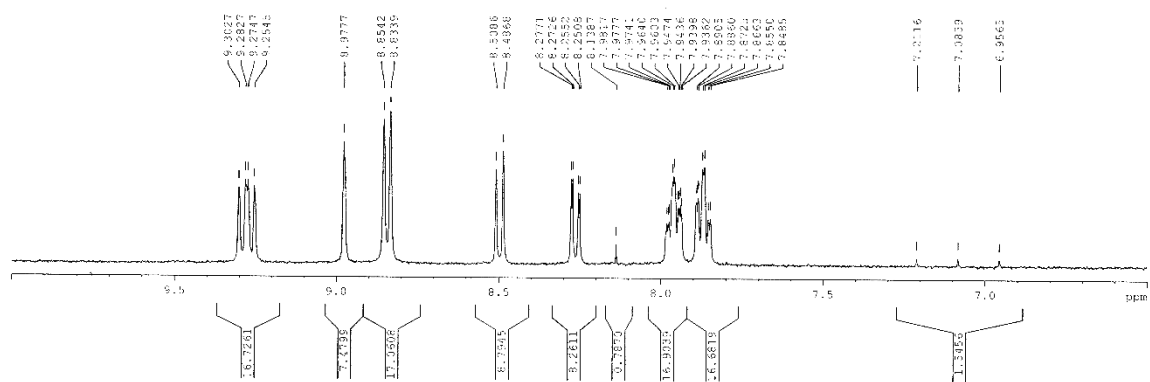
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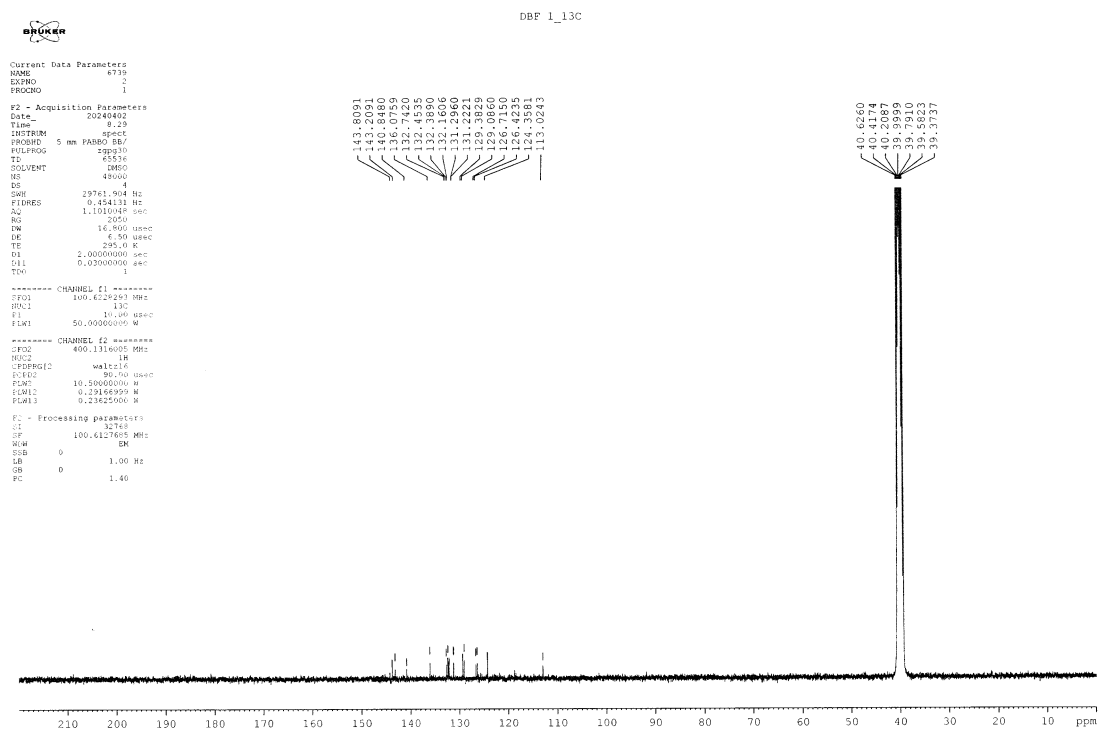
¹H spectrum of DBPh7



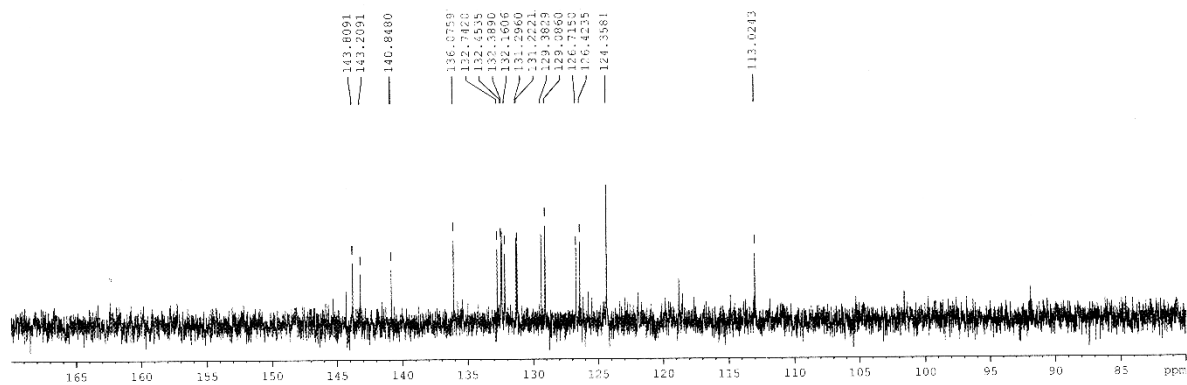
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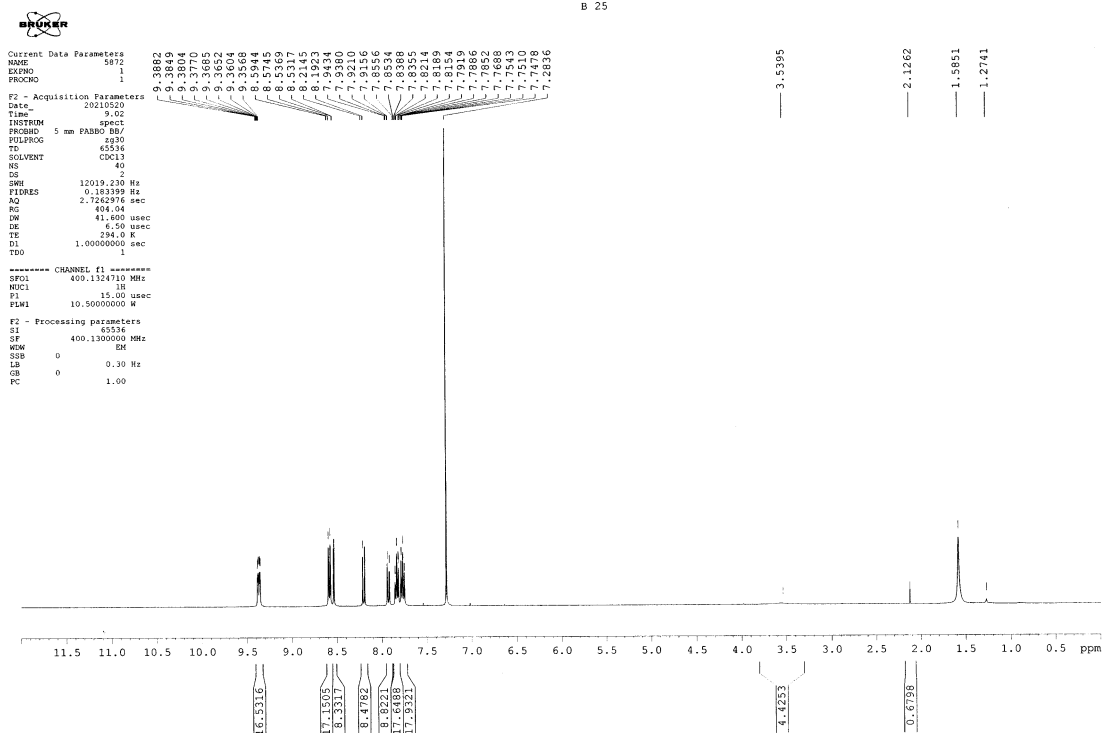
¹³C spectrum of DBPh7



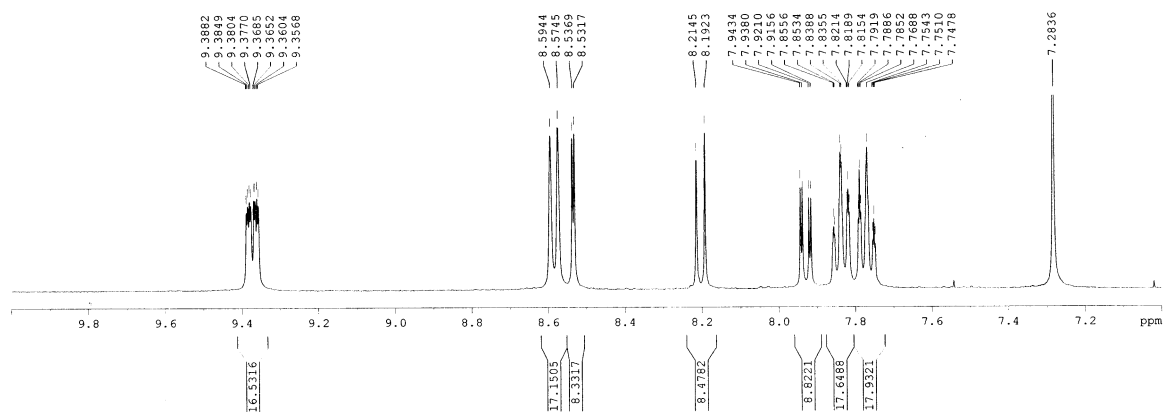
Enlarged spectrum in the range of 100-170 ppm.



¹H spectrum of DBPh8



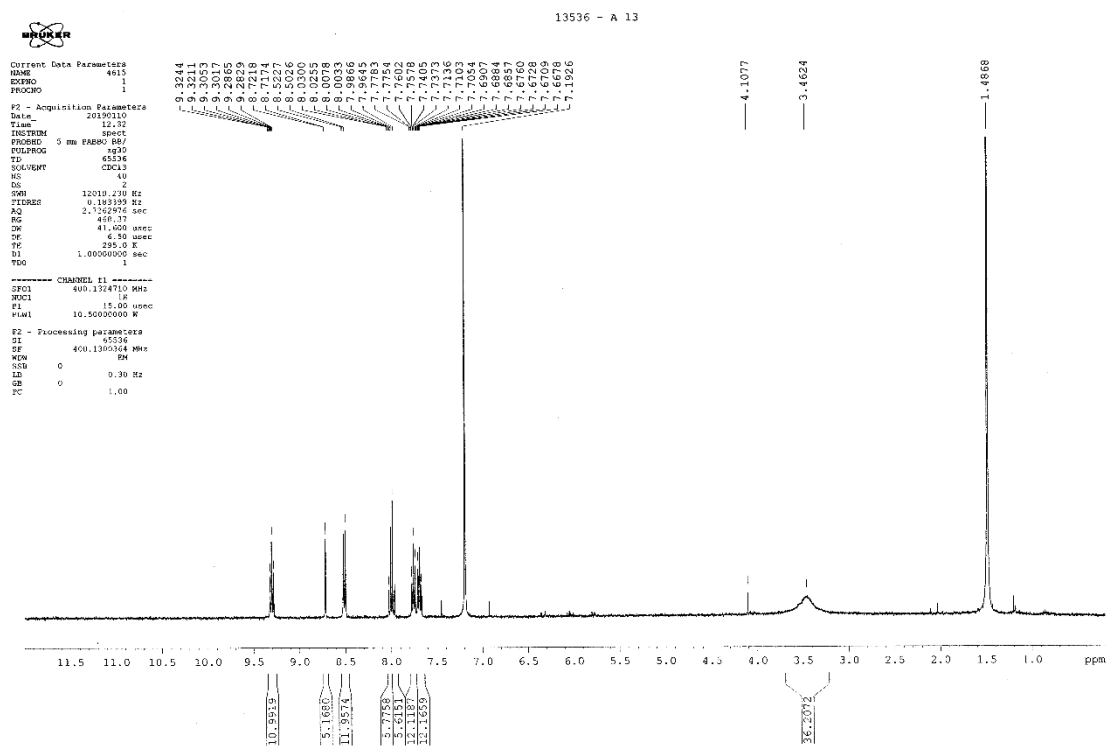
Enlarged spectrum in the range of 6-9 ppm.



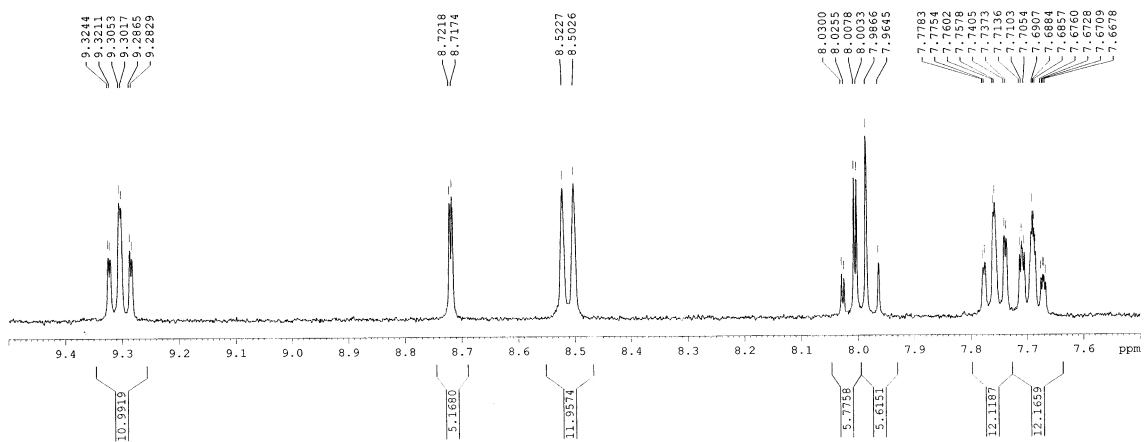
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133.7525
132.3802
132.2629
131.2777
131.0713
130.9856
130.2668
128.2201
128.1262
126.6799
126.6213
123.0591
123.0289

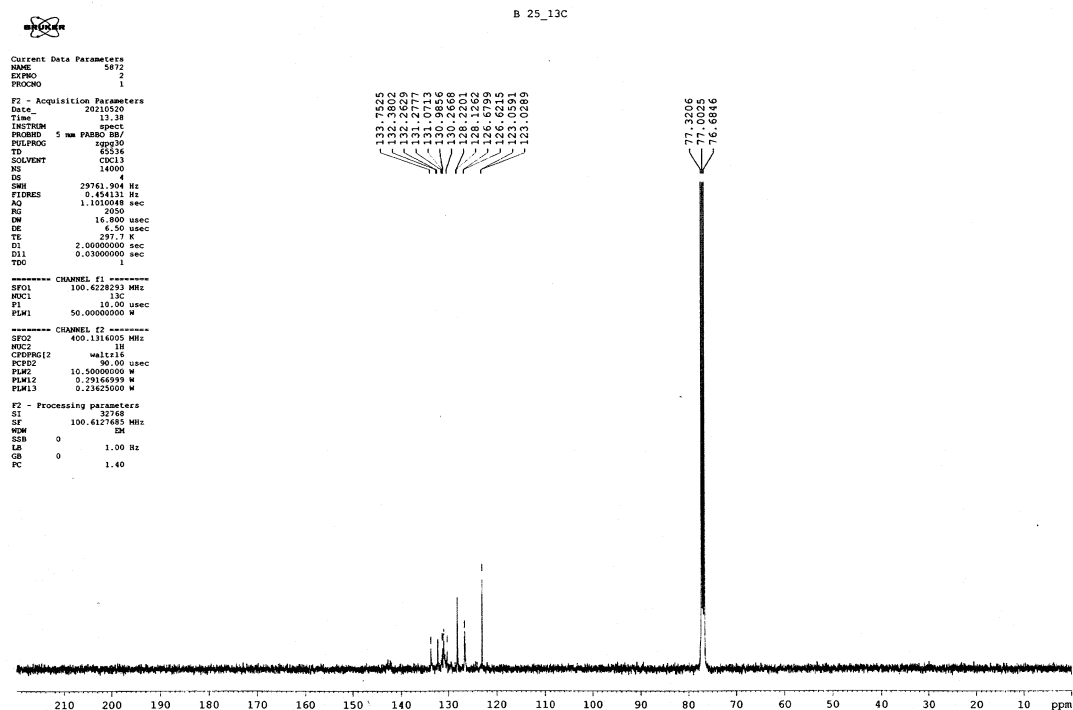
145 140 135 130 125 120 115 ppm

¹H spectrum of DBPh9

Enlarged spectrum in the range of 7-10ppm.

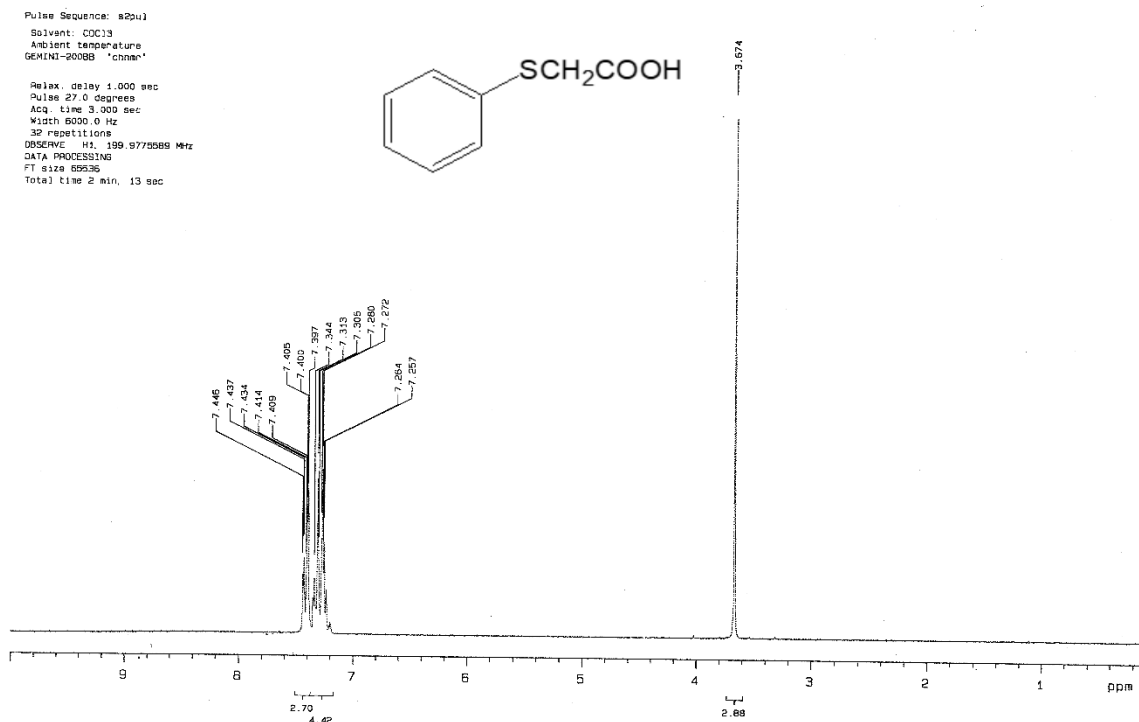


¹³C spectrum of DBPh9

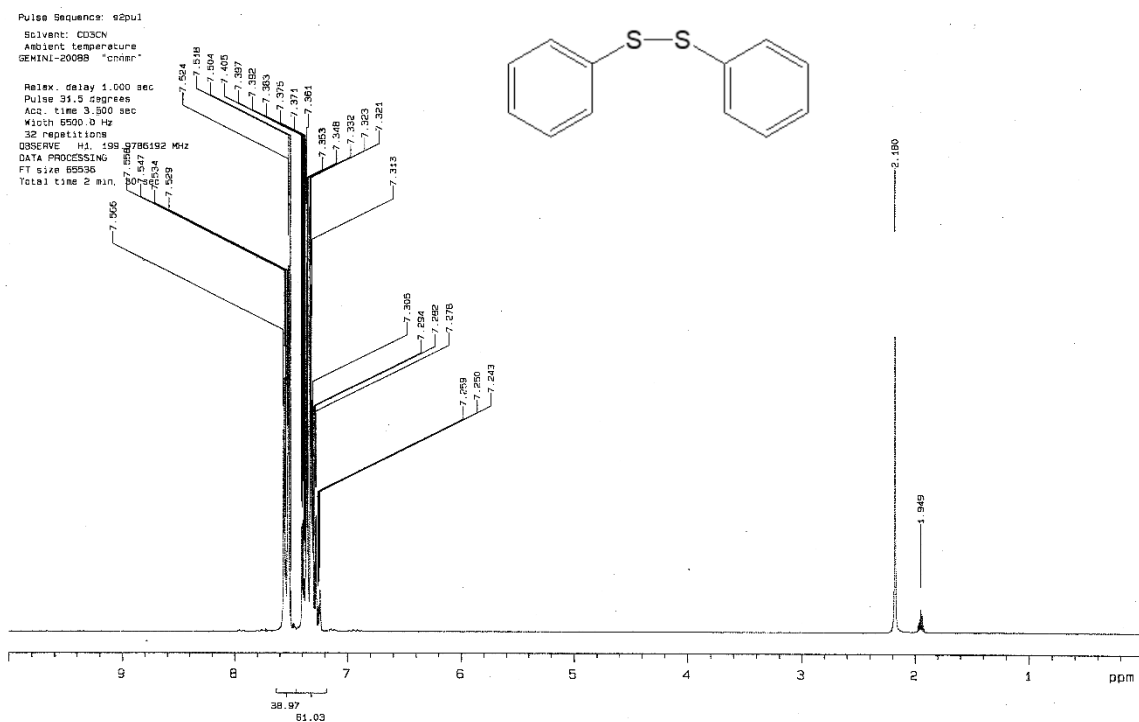


¹H NMR spectra of samples containing standards of products formed from (phenylthio)acetic acid (PhTAA) under photoreduction conditions

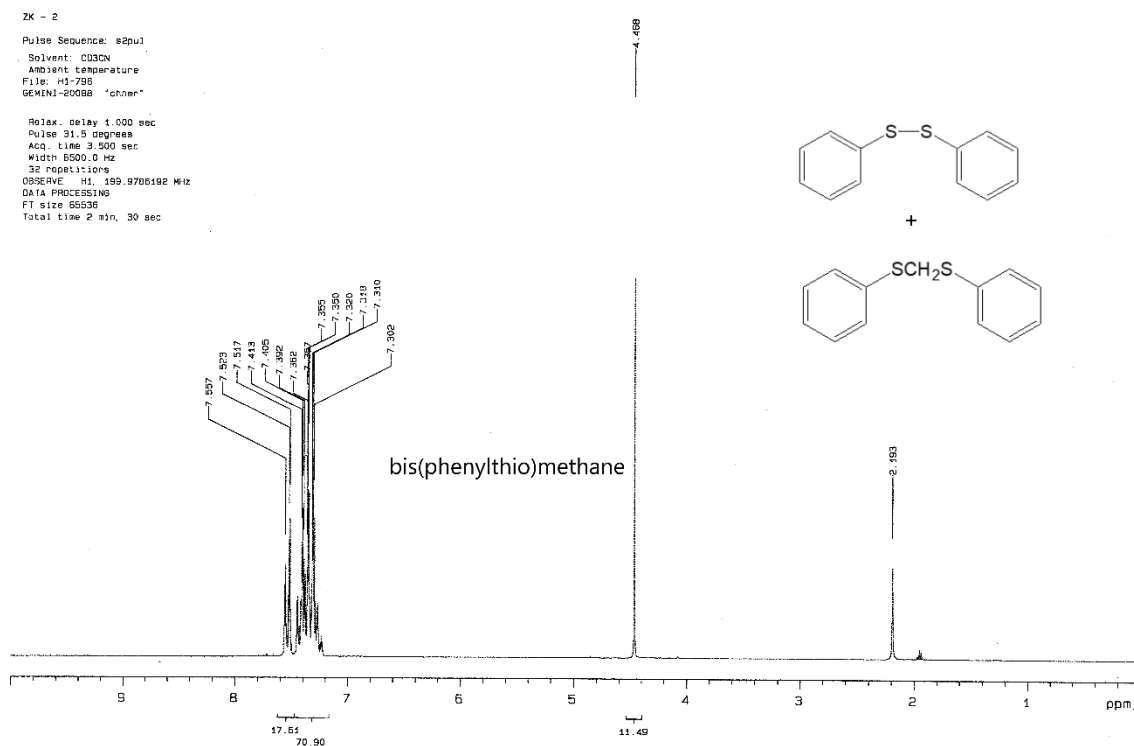
¹H NMR spectrum of (phenylthio)acetic acid (PhTAA)



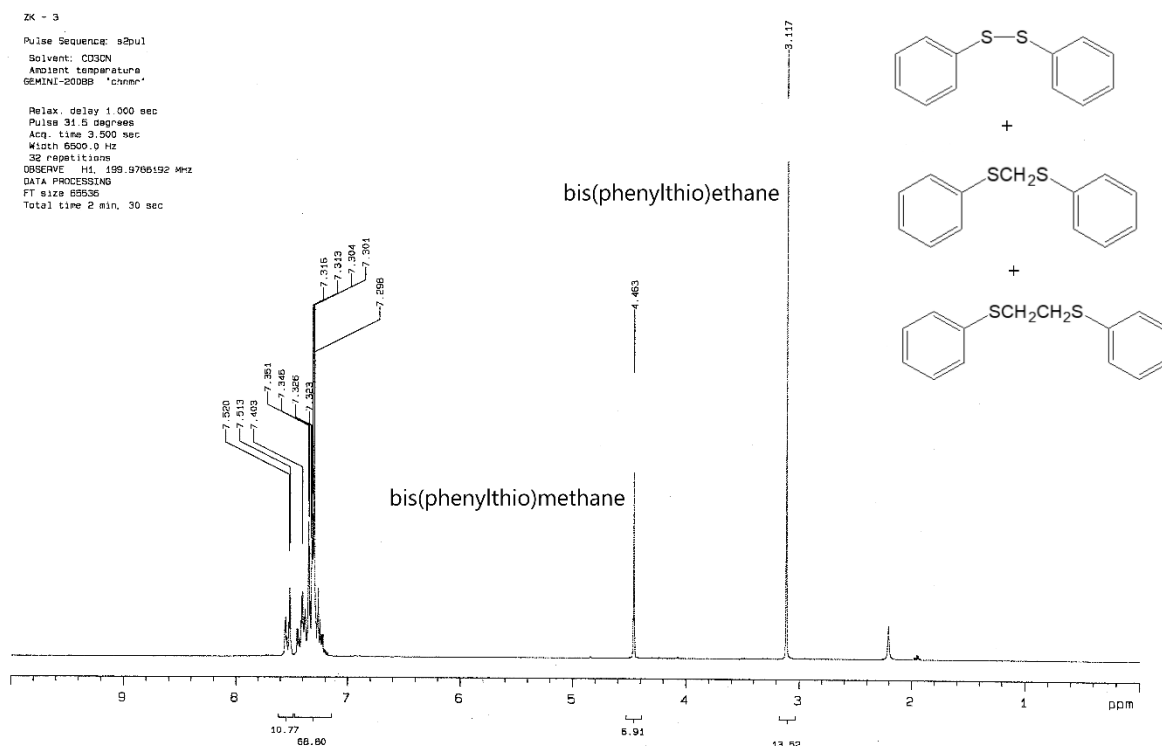
¹H NMR spectrum of diphenyl-disulfide



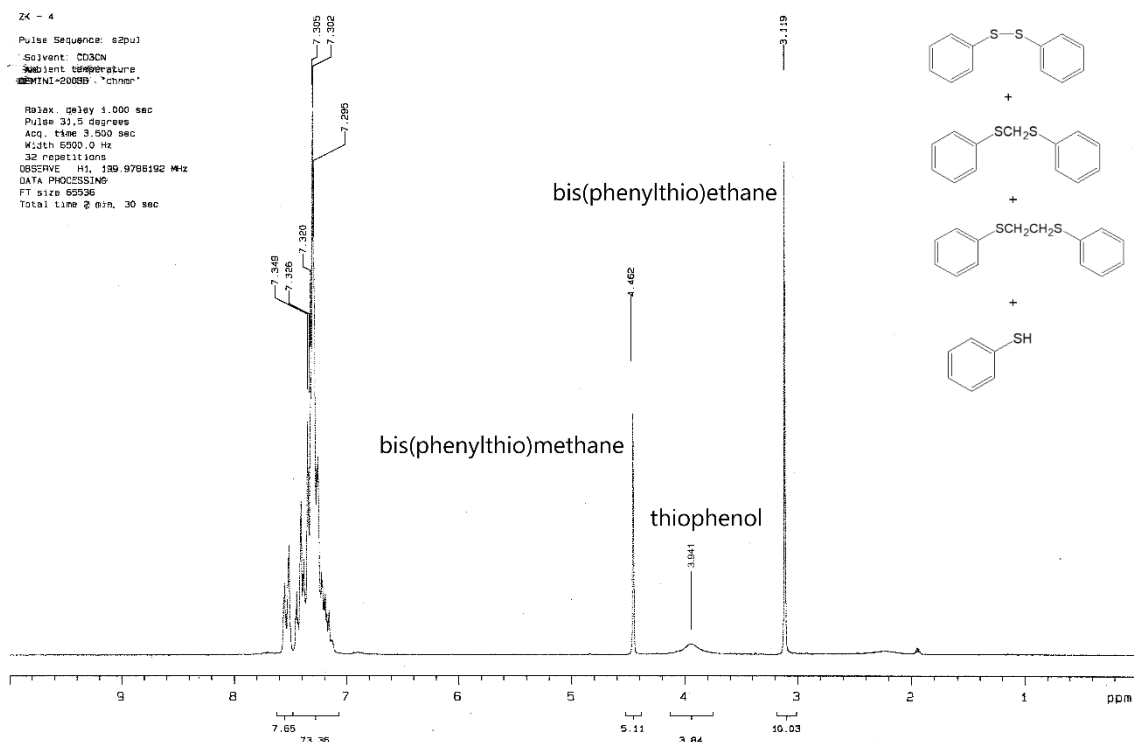
¹H NMR spectrum of a sample containing: diphenyl-disulfide, bis(phenylthio)methane



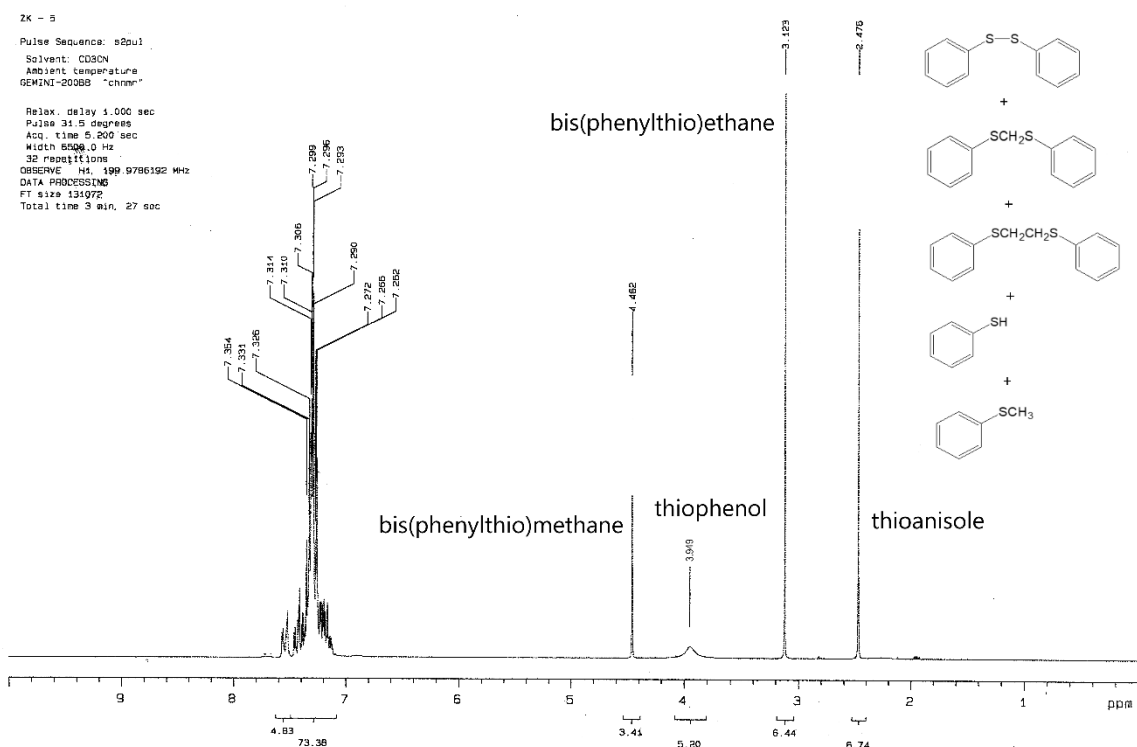
¹H NMR spectrum of a sample containing: diphenyl-disulfide, bis(phenylthio)methane, bis(phenylthio)ethane



¹H NMR spectrum of a sample containing: diphenyl-disulfide, bis(phenylthio)methane, bis(phenylthio)ethane, thiophenol



¹H NMR spectrum of a sample containing: diphenyl-disulfide, bis(phenylthio)methane, bis(phenylthio)ethane, thiophenol, thioanisole



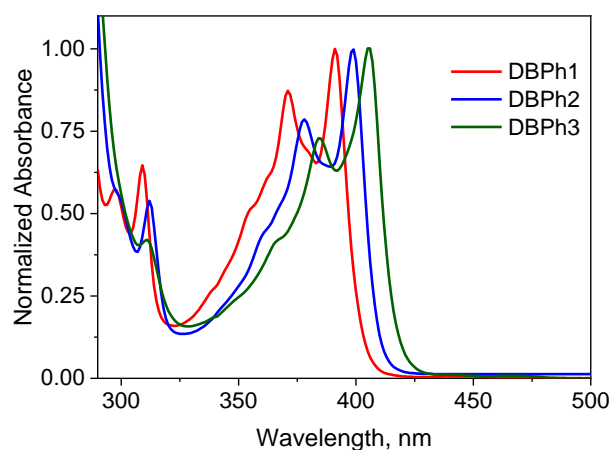


Figure S1. Normalized electronic absorption spectra of the dyes differing in the electron-releasing substituent (DBPh1 vs. DBPh2 and DBPh3) in ethyl acetate.

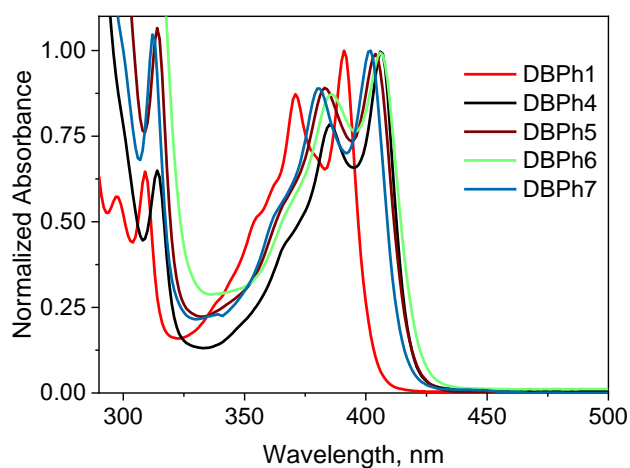


Figure S2. Normalized electronic absorption spectra of dyes differing in the electron-withdrawing substituent (DBPh1 vs. DBPh4–DBPh7) in ethyl acetate.

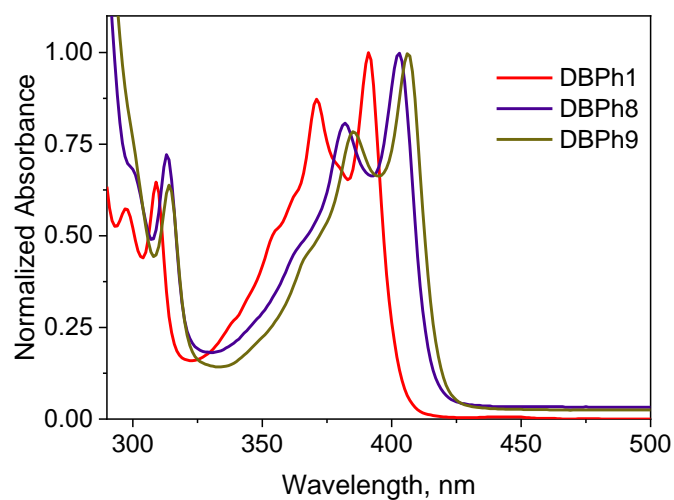


Figure S3. Normalized electronic absorption spectra of dyes differing in heavy atoms (DBPh1 vs. DBPh8 and DBPh9) in ethyl acetate.

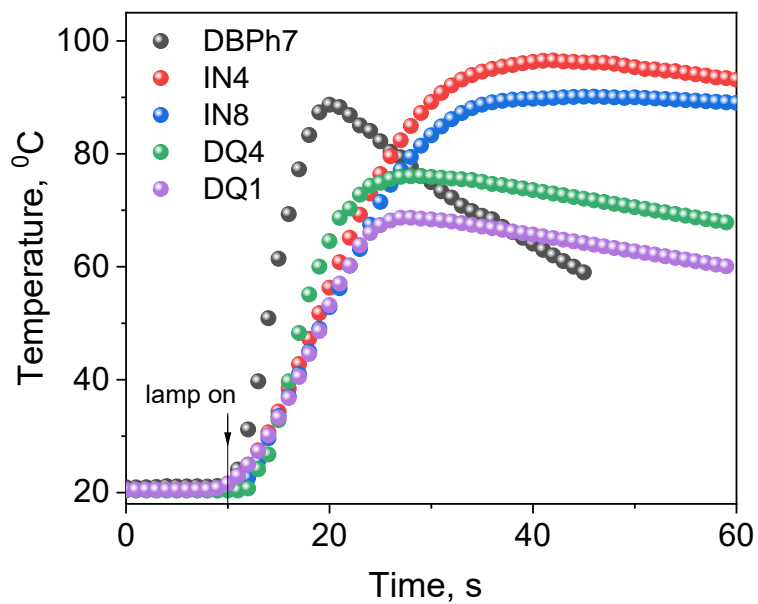
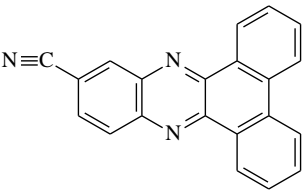
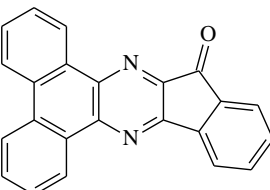
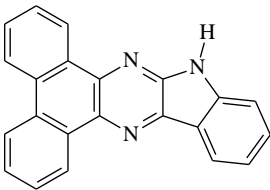
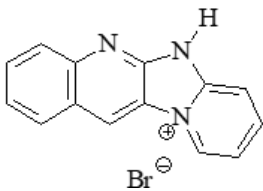
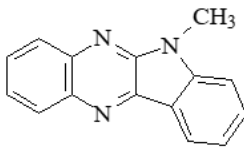


Figure S4. Comparison of kinetic curves of TMPTA polymerization photoinitiated by the tested dibenzo[a,c]phenazine (DBPh7) and other dyes coupled with co-initiator – thiophenoxyacetic acid (0.1 M). The light intensity emitted by the dental lamp was 20 mW cm⁻².

Table S1. Initial rate of photoinitiated free radical polymerization of TMPTA (R_p) initiated by different photoredox pairs in the same experimental conditions.

No	Photoinitiators tested	R_p (μmol/s)
DBPh7	 11-Carbonitriledibenzo[a,c]phenazine	194.55
IN4	 13H-Dibenzo[f,h]indeno[1,2-b]quinoxalin-13-one	104.30
IN8	 10H-Dibenzo[f,h]indolo[2,3-b]quinoxaline	88.50

DQ1	 <p>Quinoline[2,3-b]-1H-imidazo[1,2-a]pyridinium bromide</p>	109.06
DQ4	 <p>6-Methyl-6H-indolo[2,3-b]quinoxaline</p>	115.30

References:

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