

Supporting Information

Recombinant Squalene Synthase. Synthesis of Non-Head to Tail Triterpenes

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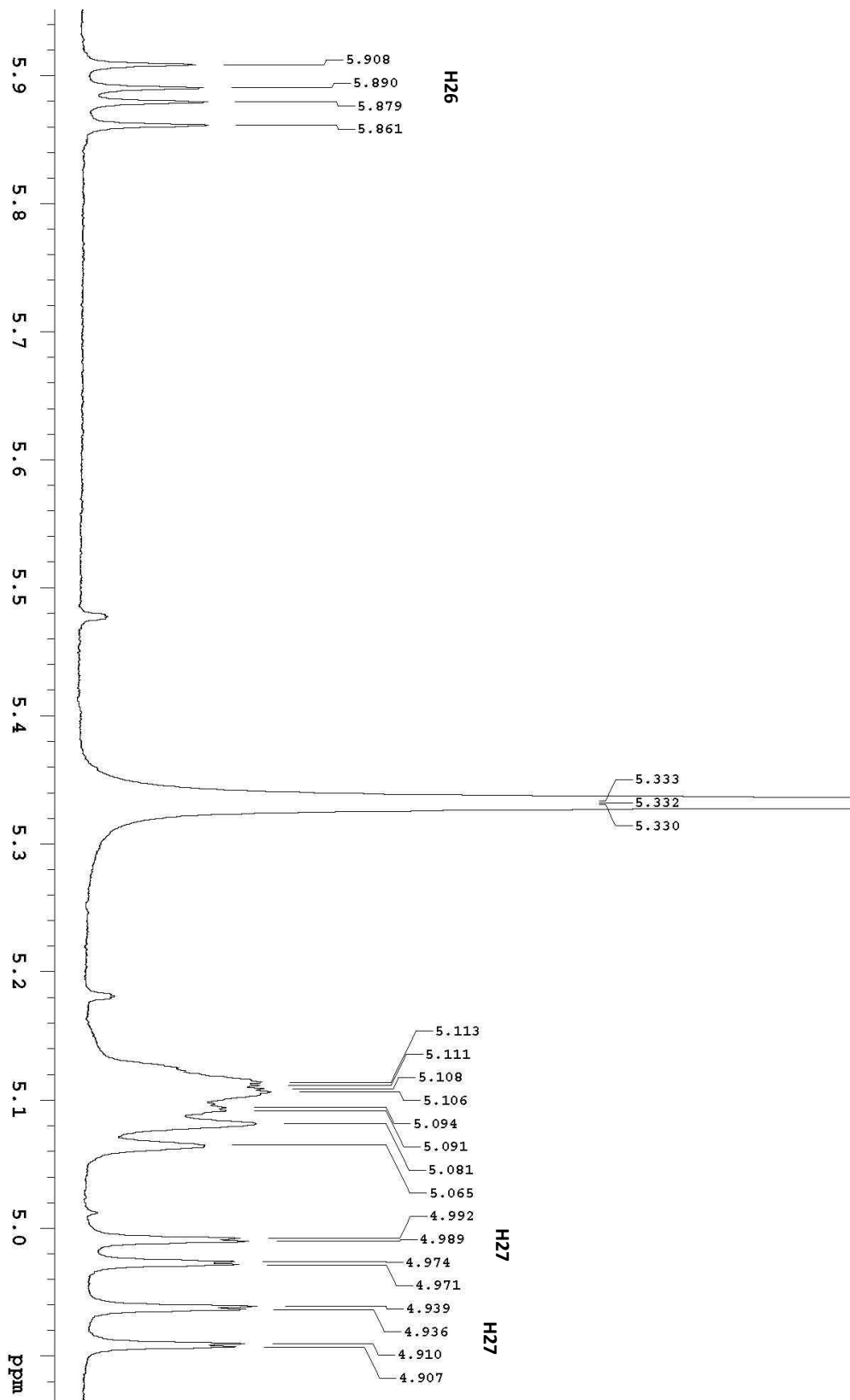
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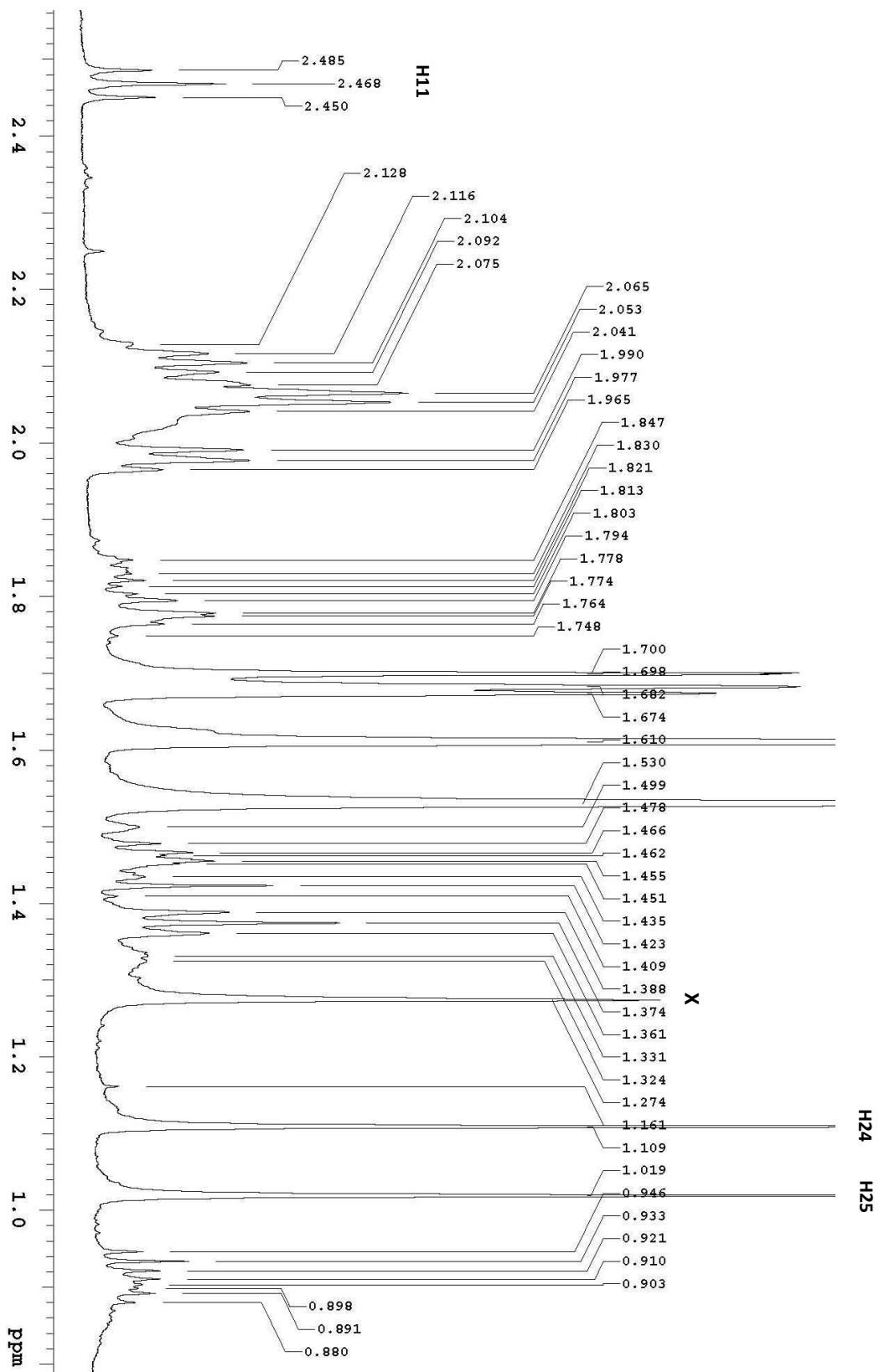
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Materials. Designed PCR primers were ordered from Integrated DNA Technologies. All restriction enzymes and T4 DNA ligase were purchased from New England Biolabs. pGEM-T Easy vector was purchased from Promega. Easy-A PCR cloning enzyme and XL1-Blue competent cells were purchased from Stratagene. pET28b+ vector and BL21(DE3) were purchased from Novagen. EDTA-free protease inhibitor cocktail tablets were purchased from Roche Diagnostics. Ni-nitrilotriacetic acid (Ni-NTA) agarose resin was purchased from Qiagen. *N*-[2-Hydroxyethyl]-piperazine-*N'*-[2-ethanesulfonic acid] (HEPES) was from USB Corporation. β -Mercaptoethanol (BME) and 3-(*N*-Morpholino)-propanesulfonic acid (MOPS) were from Sigma. HPLC grade hexanes and methyl *tert*-butyl ether (MTBE) were from EMD Chemicals and Mallinckrodt Chemicals, respectively.

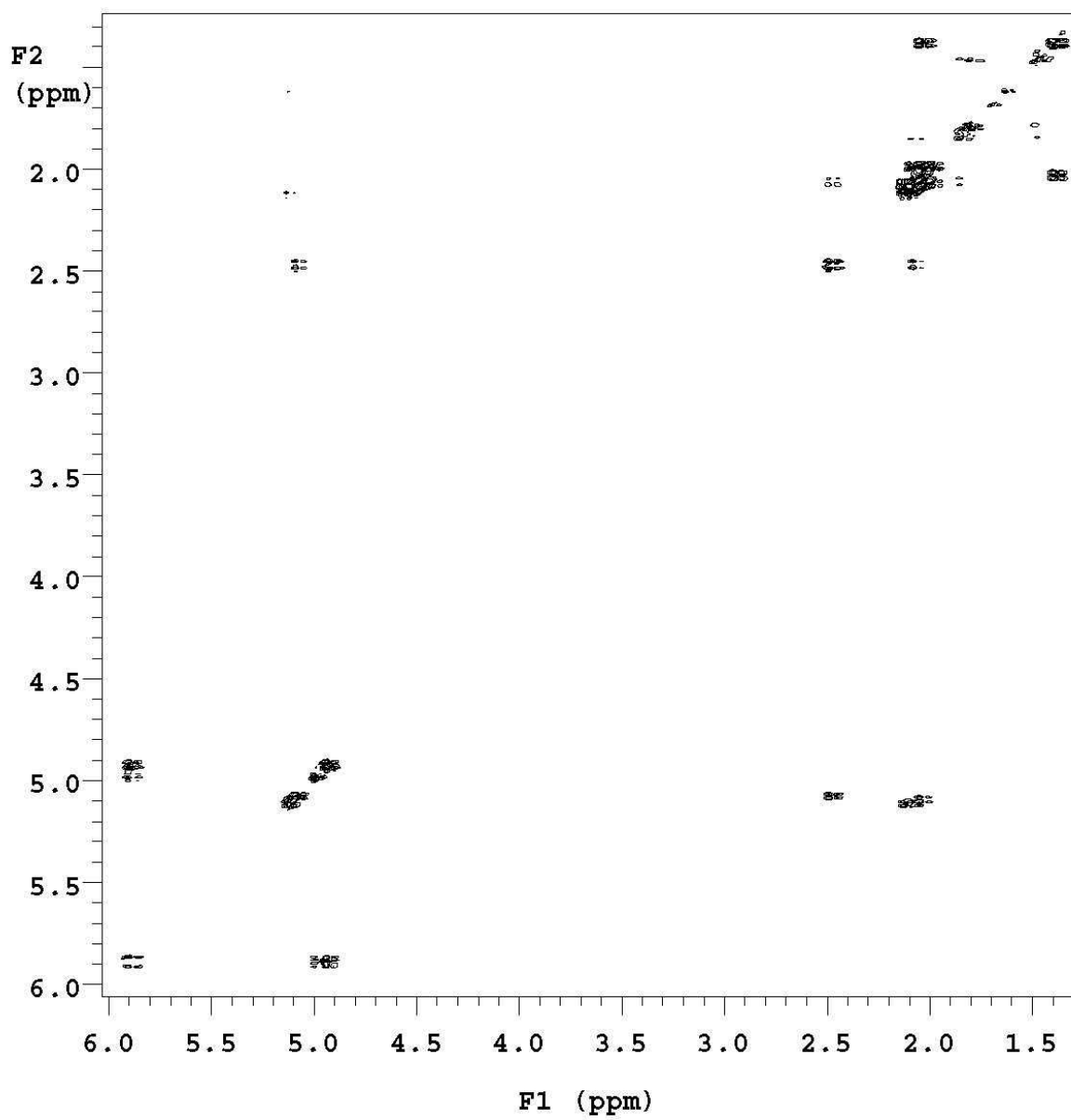
¹H-NMR



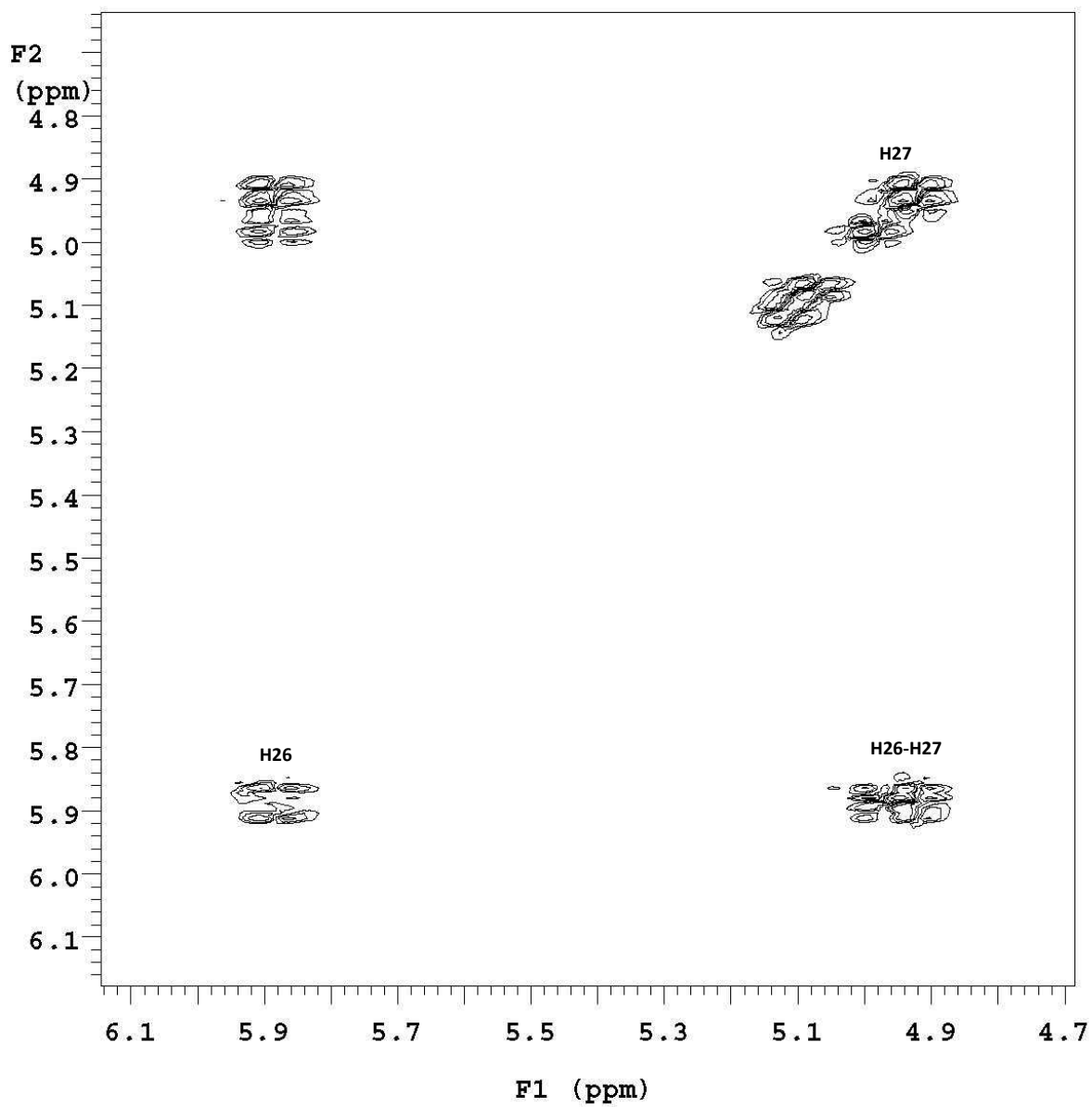
¹H-NMR



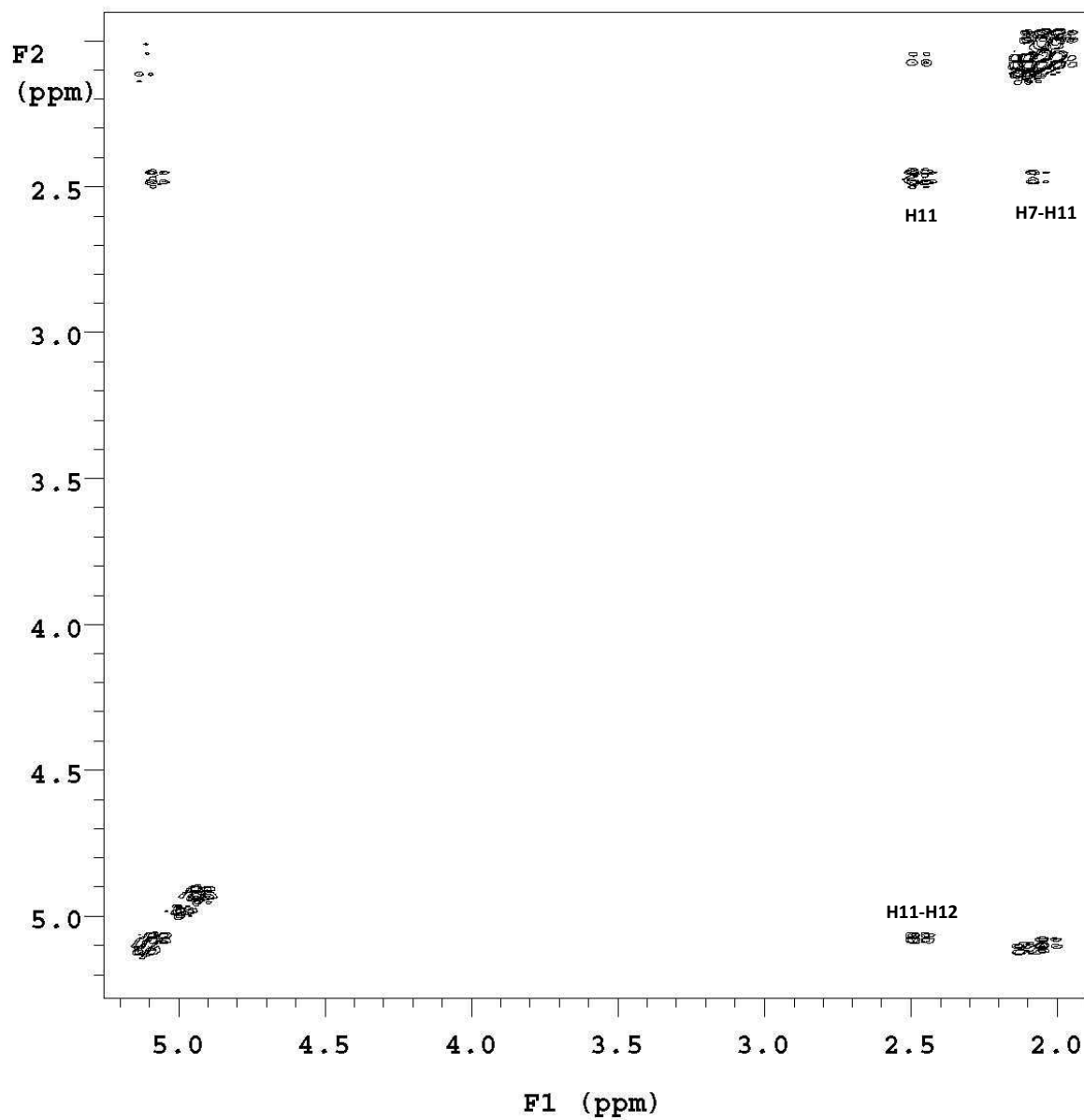
^1H - ^1H DQCOSY



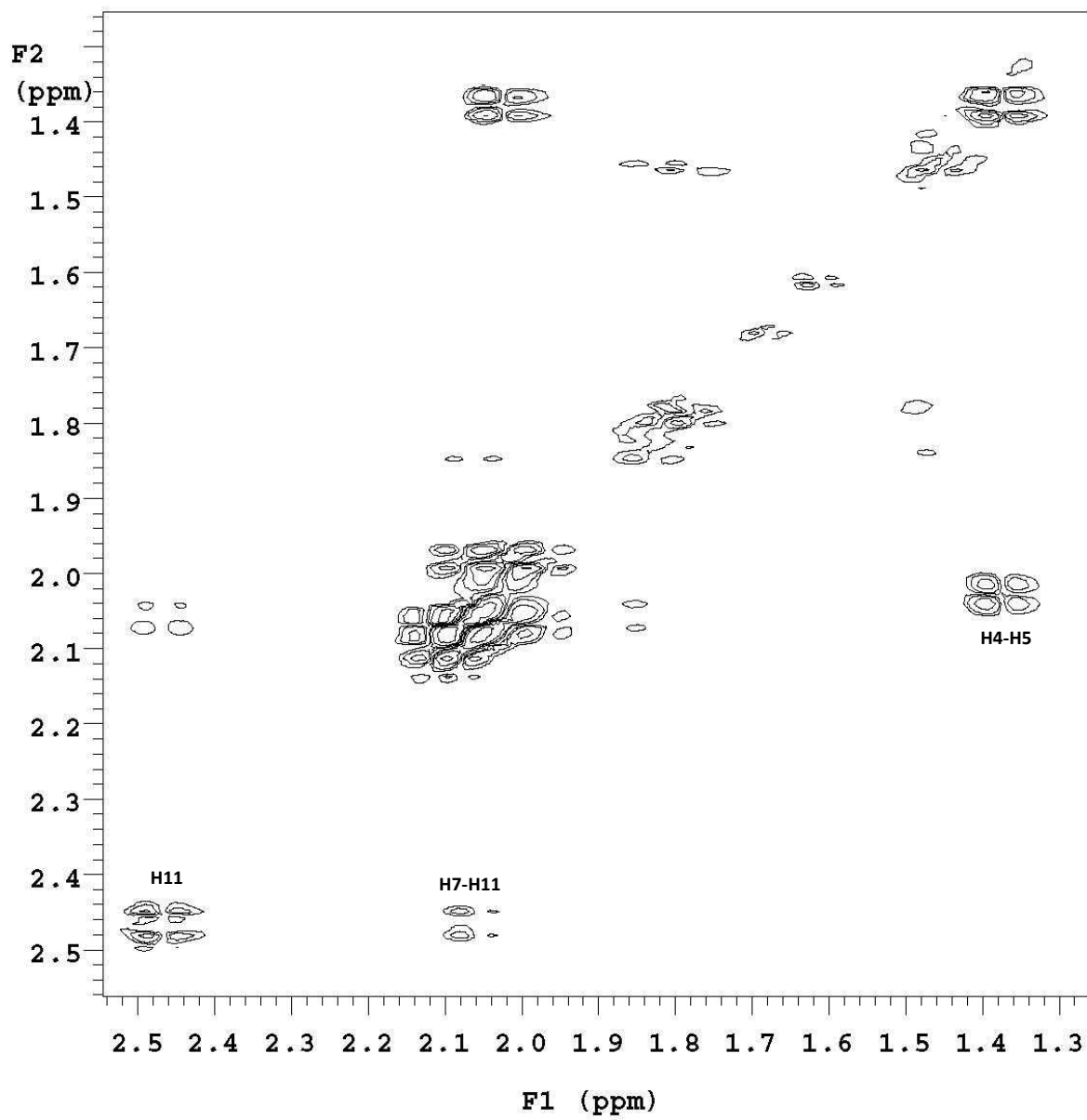
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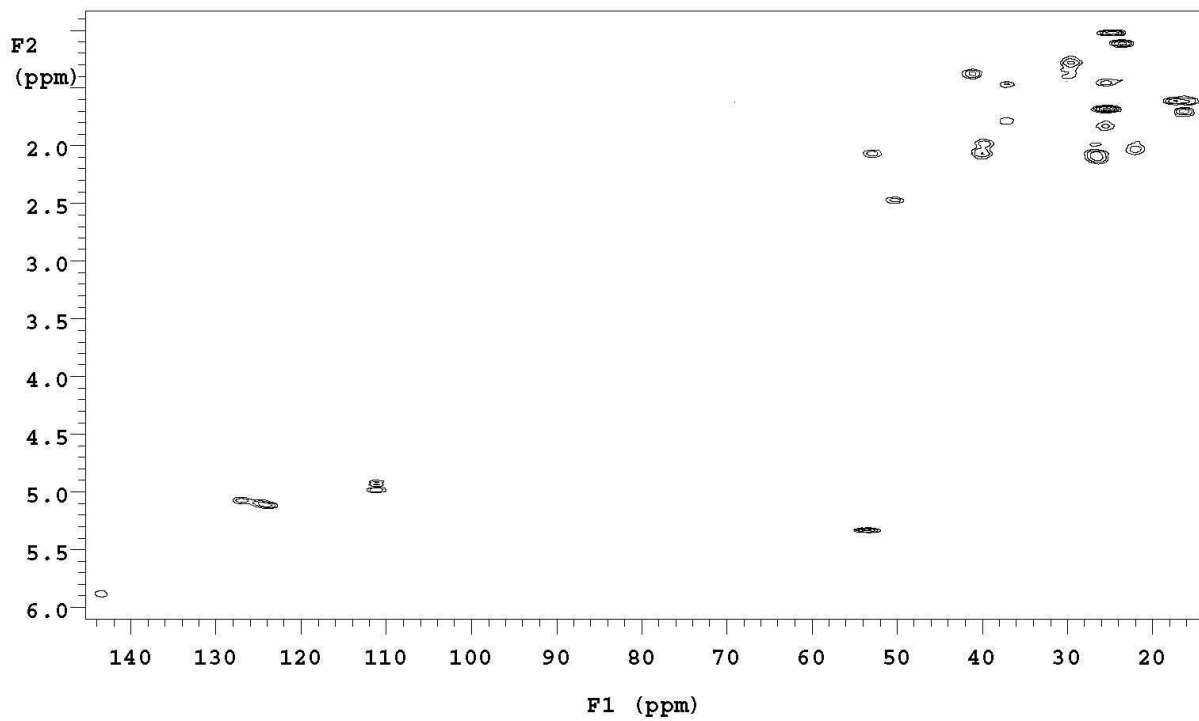
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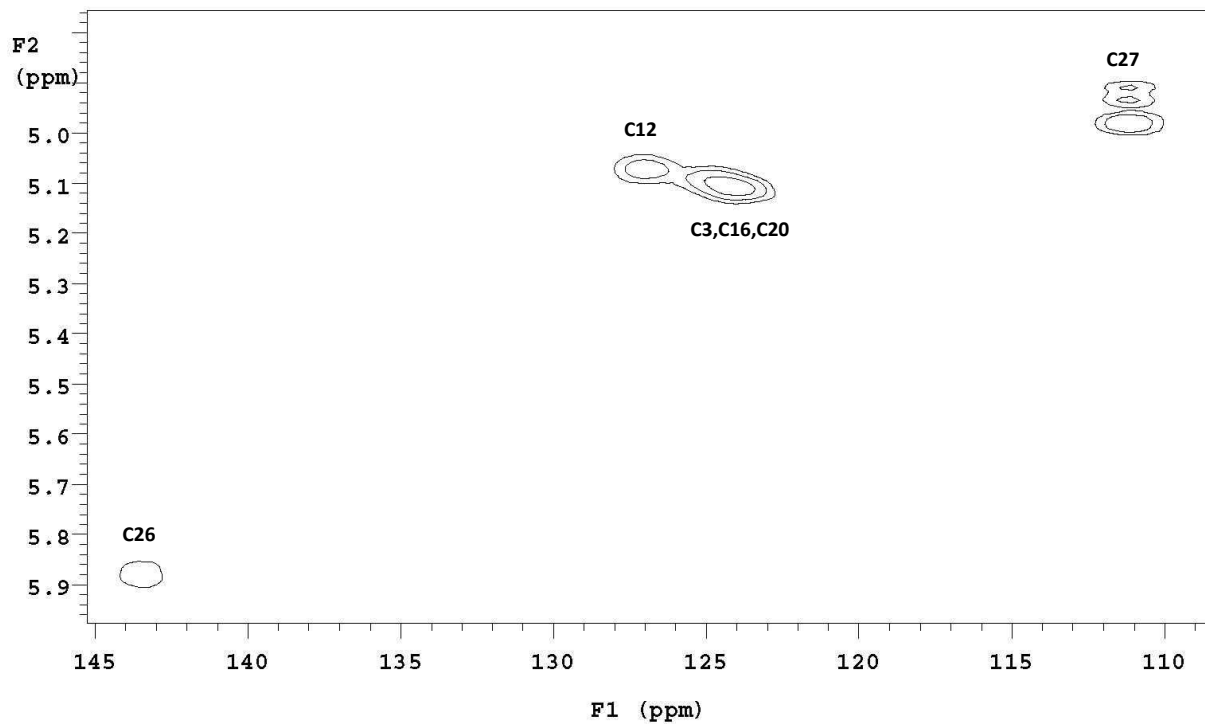
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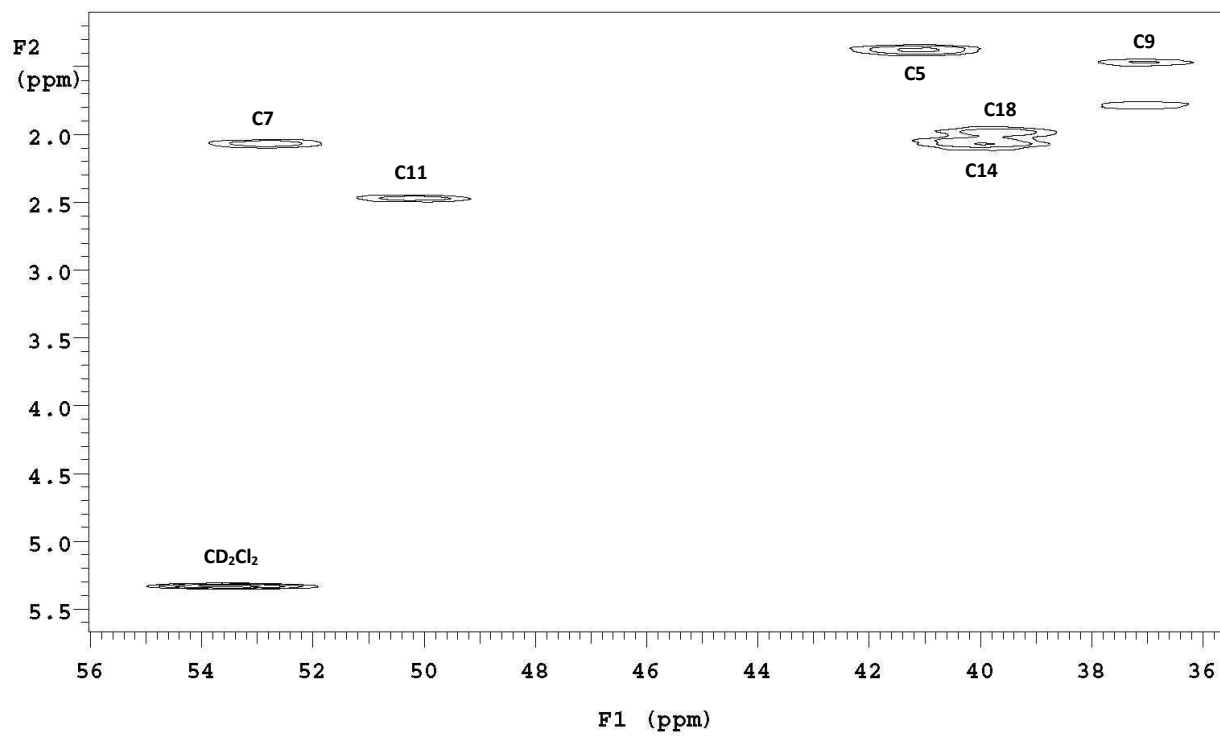
^1H - ^{13}C HSQC



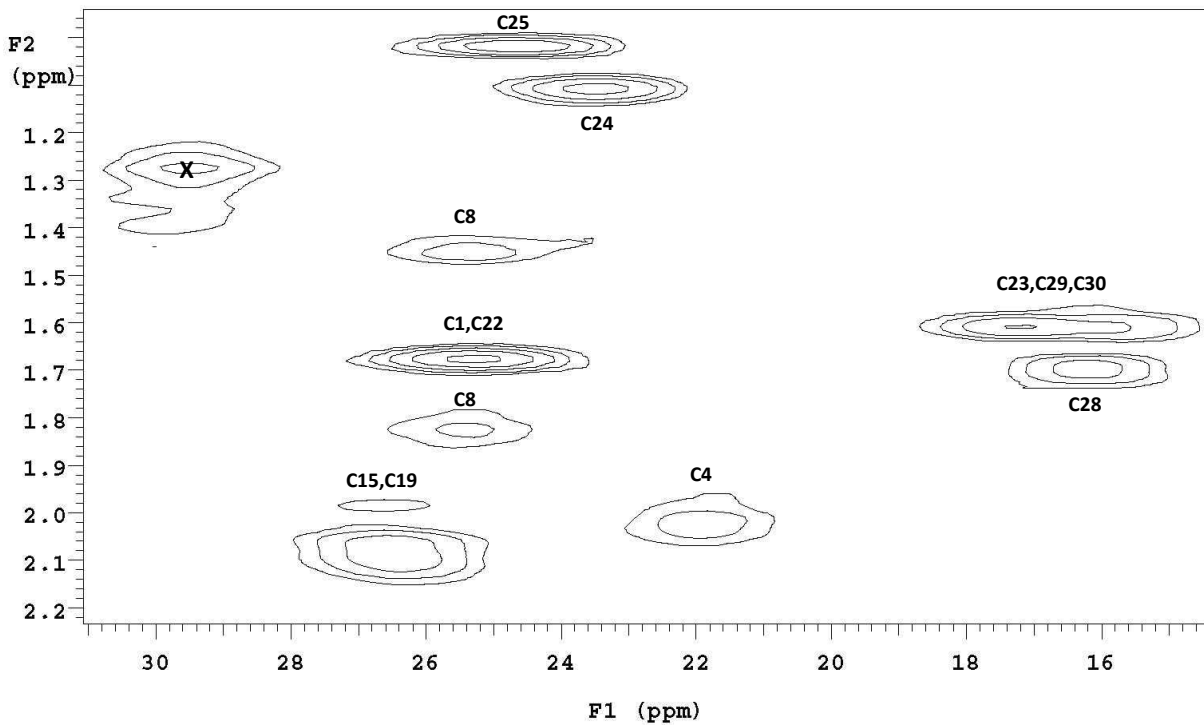
$^1\text{H}-^{13}\text{C}$ HSQC



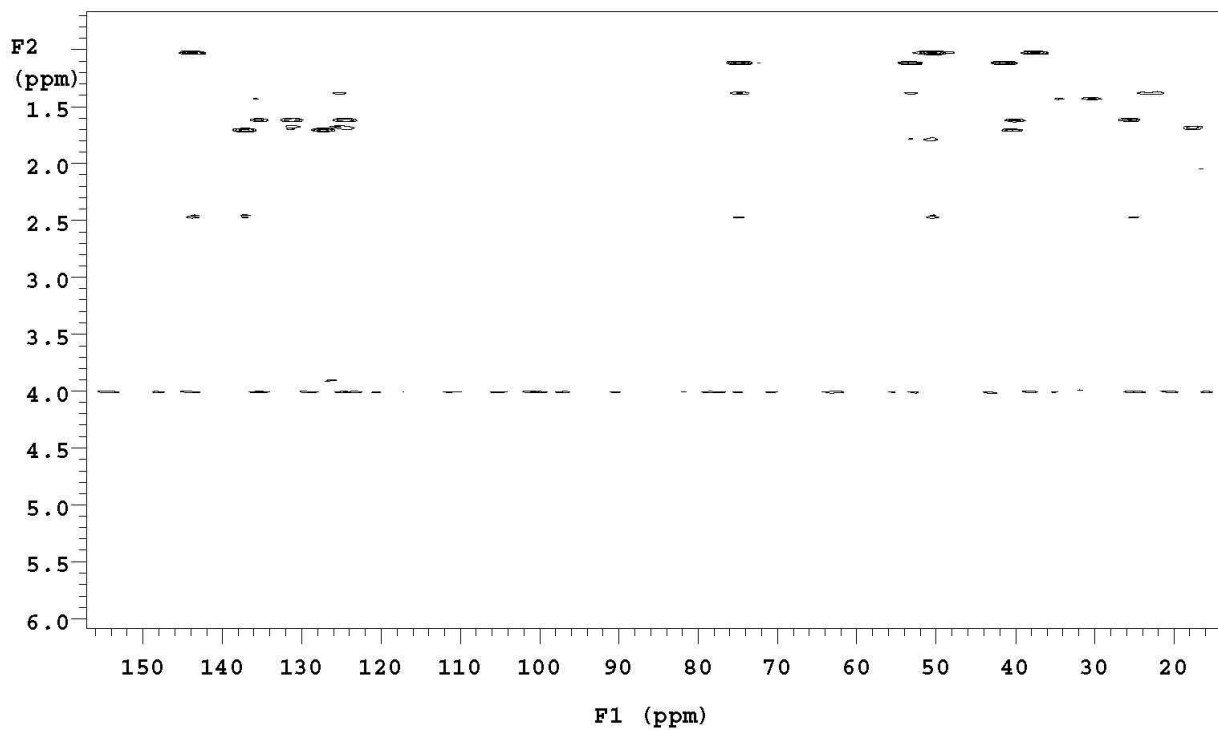
$^1\text{H}-^{13}\text{C}$ HSQC



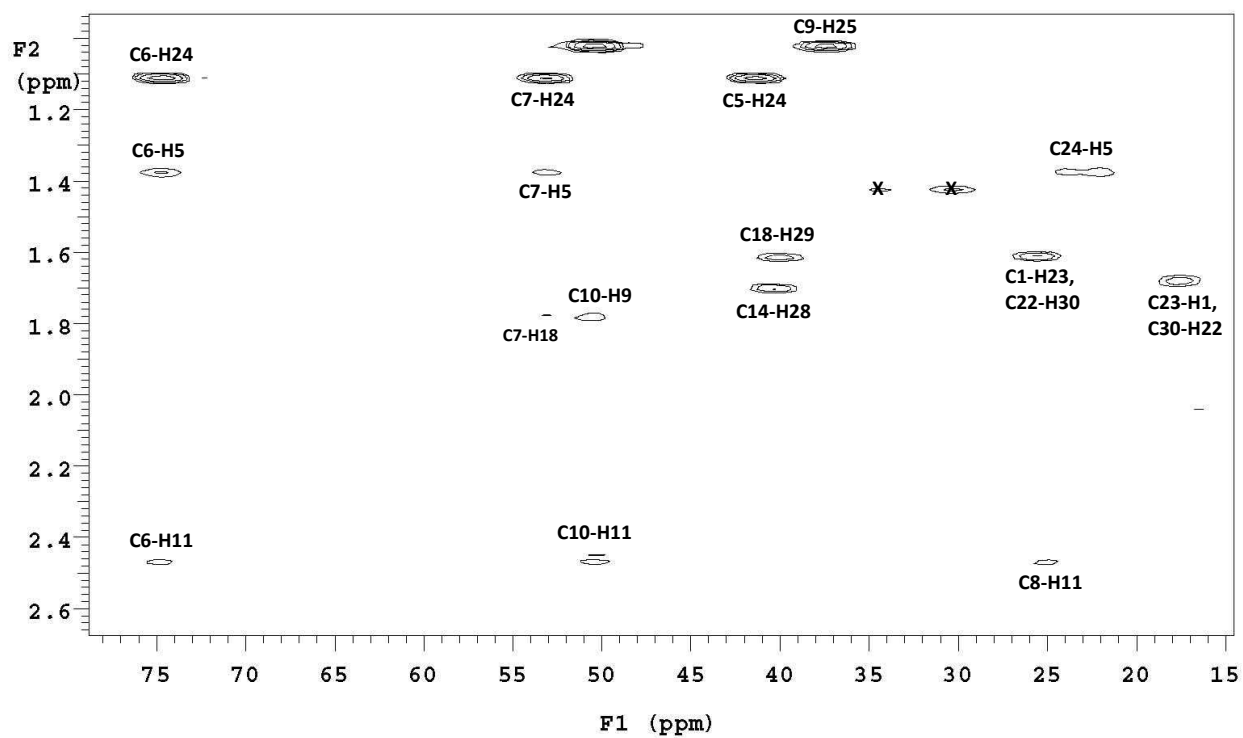
$^1\text{H}-^{13}\text{C}$ HSQC



$^1\text{H}-^{13}\text{C}$ HMBC

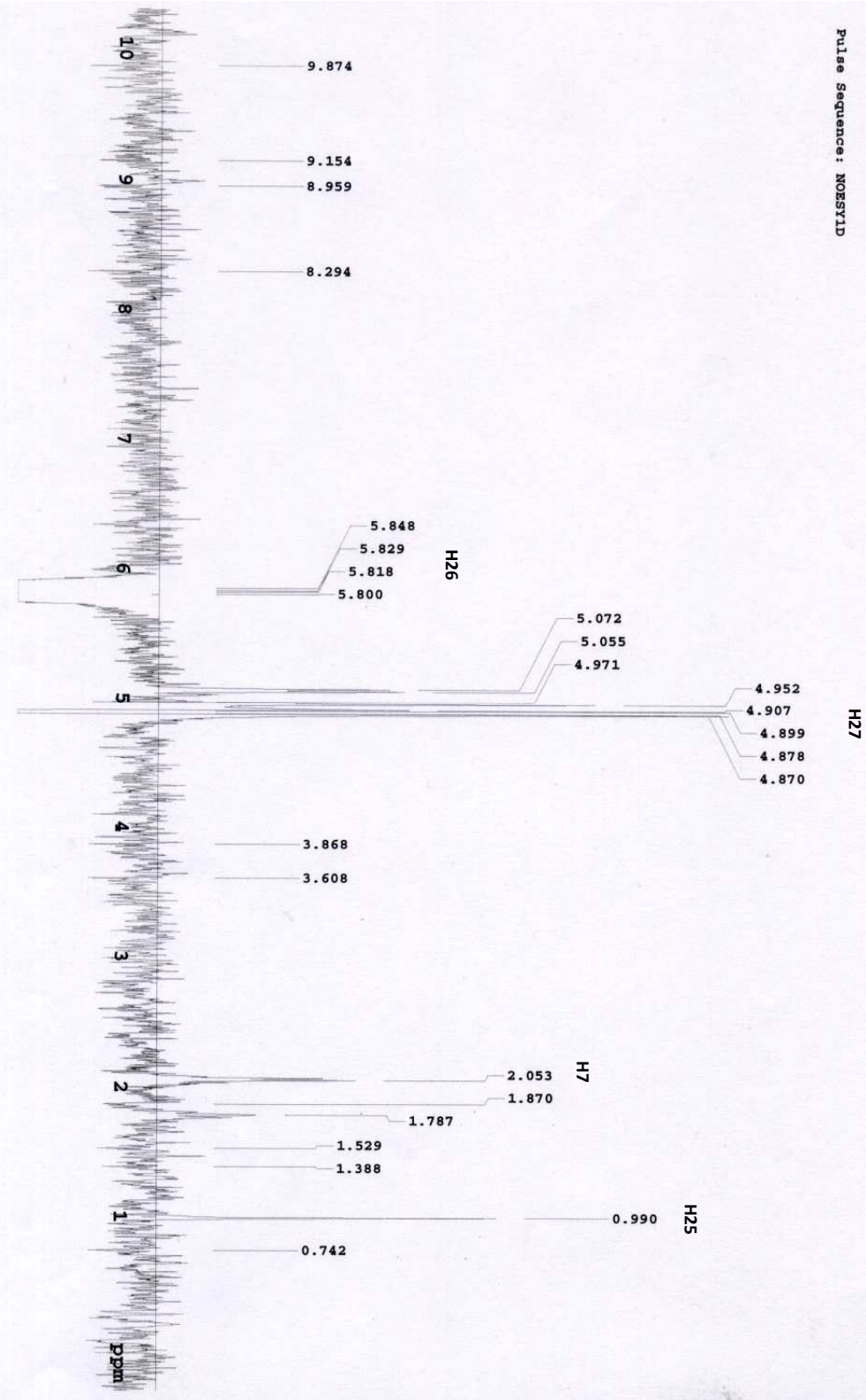


$^1\text{H}-^{13}\text{C}$ HMBC



600 MHz, 25C
5mm tube
Cryoprobe
Sample 2
01 Dec 2008
CDC13

Pulse Sequence: NOESY1D



600 MHz, 25C
5mm tube
Cryoprobe
Sample 2
01 Dec 2008
CDC13

Pulse Sequence: NOESY1D

500ms Mixing time

