

De novo synthesis of functionalized 1,3-enynes and extended conjugated molecular systems

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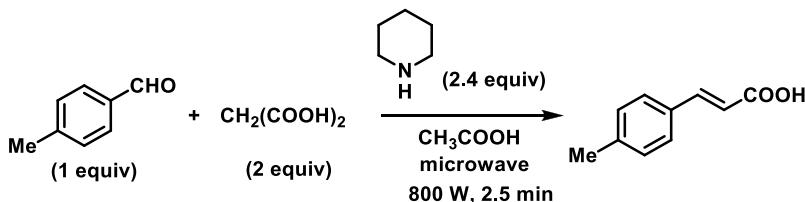
Supporting Information

Contents

| | | |
|----|--|----------|
| 1. | Representative Experimental Procedures..... | S2-S5 |
| 2. | Control Reaction | S6 |
| 3. | References..... | S7 |
| 4. | ^1H , ^{13}C and HRMS Spectras of 1,3-Dienyldibromides (1a-1m)..... | S8-S47 |
| 5. | ^1H , ^{13}C and HRMS Spectras of groups of 1,3-Enynes (2-18)..... | S48-S261 |

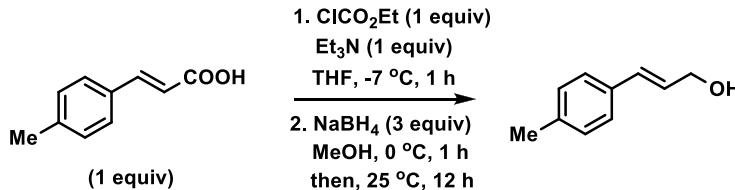
1. Experimental Procedure for Substrate Preparation:

1.1 Preparation of (*E*)-3-(*p*-tolyl)acrylic acid¹:



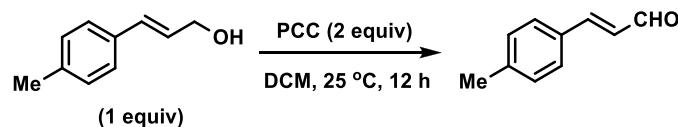
To an oven-dried beaker, added 4-methylbenzaldehyde (4 g, 33.29 mmol, 1 equiv), malonic acid (6.9 g, 66.58 mmol, 2 equiv) and glacial acetic acid (50 mL). Then piperidine (6.8 g, 79.89 mmol, 2.4 equiv) was added dropwise and was irradiated at 800 W for 2.5 minutes with 1 minute interval. The mixture was quenched with water to obtain a colourless solid and it was air-dried to afford (*E*)-3-(*p*-tolyl) acrylic acid (5.1g, 95%). This was directly used in the next reaction in **1.2**.

1.2 Preparation of (*E*)-3-(*p*-tolyl)prop-2-en-1-ol:



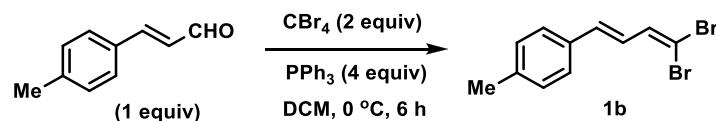
To a stirred solution of (*E*)-3-(*p*-tolyl)acrylic acid (6.9 g, 42.54 mmol, 1 equiv) in THF was added NEt_3 (4.3 g, 42.54 mmol, 1 equiv) under N_2 atmosphere. The mixture was cooled to -7°C and ClCO_2Et (4.6 g, 42.54 mmol, 1 equiv) was slowly added. The reaction mixture was stirred for 1 h at -7°C and was brought to r.t. The mixture was filtered and the filtrate was reduced with NaBH_4 . It was done in a three-neck round bottom flask using NaBH_4 (4.8 g, 127.62 mmol, 3 equiv) and with the slow addition of MeOH at 0°C . The mixture was further stirred at r.t for 12 h. After removing the solvent under reduced pressure, the product was extracted with ethyl acetate, washed with water, brine and dried over anhydrous MgSO_4 and concentrated. The crude product was purified by silica-gel column chromatography using 20% ethyl acetate/hexane as eluent to obtain (*E*)-3-*p*-tolylprop-2-en-1-ol (4.2 g, 67%).

1.3 Preparation of (*E*)-3-*p*-tolylacrylaldehyde:



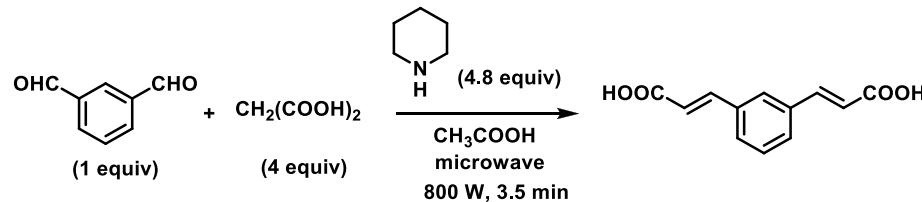
To an oven-dried round bottom flask containing (*E*)-3-*p*-tolylprop-2-en-1-ol (4.2 g, 28.34 mmol, 1 equiv) in DCM, pyridinium chlorochromate (PCC) was added in portions (12.2 g, 56.68 mmol, 2 equiv). The reaction mixture was stirred at r.t under nitrogen for 12 h. It was passed through celite and washed with DCM. The filtrate was concentrated under reduced pressure. The crude was purified by silica-gel column chromatography using 10% ethyl acetate/hexane to obtain (*E*)-3-*p*-tolylacrylaldehyde (1.9 g, 45%).

1.4 Preparation of (*E*)-1-(4,4-dibromobuta-1,3-dienyl)-4-methylbenzene²:



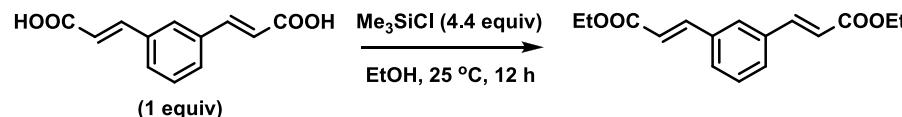
To an oven-dried round bottom flask, added (*E*)-3-*p*-tolylacrylaldehyde (1 g, 6.84 mmol, 1 equiv) in DCM followed by the addition of CBr₄ (4.53 g, 13.68 mmol, 2 equiv) and PPh₃ (7.17 g, 27.36 mmol, 4 equiv) in portions at 0 °C under N₂ atmosphere. The mixture was stirred at 0 °C for 6 h. To the product mixture, hexane solvent was added and filtered through a small silica-gel pad and concentrated. The crude product was purified by silica gel column chromatography using hexane as eluent to obtain (*E*)-1-(4,4-dibromobuta-1,3-dienyl)-4-methylbenzene as colourless solid (1.56 g, 76%).

1.5 Preparation of (2*E*,2'*E*)-3,3'-(1,3-phenylene)diacrylic acid¹:



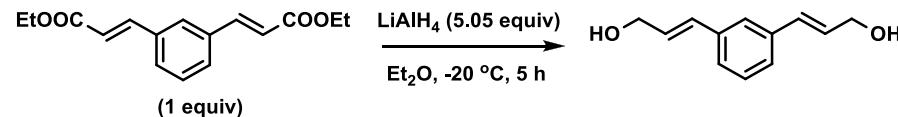
To an oven-dried beaker, added isophthalaldehyde (4 g, 29.82 mmol, 1 equiv), malonic acid (12.4 g, 119.28 mmol, 4 equiv) and glacial acetic acid (60 mL). Then piperidine (12.2 g, 143.13 mmol, 4.8 equiv) was added dropwise and was irradiated at 800 W for 3.5 minutes with 1 minute interval. The mixture was thoroughly washed with water to obtain a colourless solid and it was air-dried to afford (*2E,2'E*)-3,3'-(1,3-phenylene)diacrylic acid (4.5 g, 69%). This was directly used in the next reaction in **1.6**.

1.6 Preparation of Ethyl (*2E,2'E*)-3,3'-(1,3-phenylene)diacrylate³:



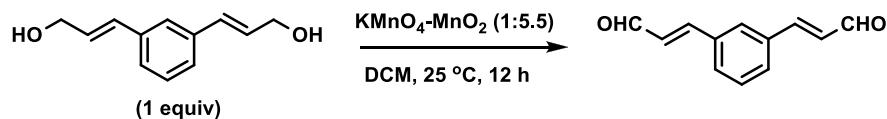
To a round bottom flask, added (*2E,2'E*)-3,3'-(1,3-phenylene)diacrylic acid (1 g, 4.58 mmol, 1 equiv) in ethanol (20 mL) followed by addition of Me_3SiCl (2.2 g, 20.24 mmol, 4.4 equiv) in portions at r.t under nitrogen condition. The resulting white turbidity slowly disappeared to form yellow transparent colored solution. This was stirred for 12 h after which, ethanol was removed under reduced pressure. The resultant residue was extracted with ethyl acetate, washed with saturated NaHCO_3 solution, water and brine, dried over anhydrous MgSO_4 and concentrated. The crude was purified by silica-gel column chromatography using 10% ethyl acetate in hexane as eluent to obtain the diester product (1.1 g, 87%).

1.7 Preparation of (*2E,2'E*)-3,3'-(1,3-phenylene)diprop-2-en-1-ol:



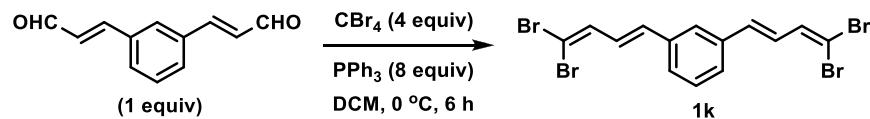
To an oven-dried round bottom flask equipped with a dropping funnel, added the diester (6.3 g, 23 mmol, 1 equiv) in diethyl ether (400 mL). After it was cooled to -20 °C, a suspension of LiAlH_4 (4.4 g, 116.15 mmol, 5.05 equiv) in ether was slowly added under N_2 atmosphere. The reaction mixture was stirred for 5 h. After the reaction is over, it was quenched at 0 °C, using saturated solution of NH_4Cl . The resulting mixture was filtered through a celite bed and the filtrate was washed with ethyl acetate and brine. The organic extract was dried over anhydrous MgSO_4 and concentrated. The crude was purified by silica-gel column chromatography using 30% ethyl acetate in hexane as eluent to obtain the diol, (*2E,2'E*)-3,3'-(1,3-phenylene)diprop-2-en-1-ol as product (2.4 g, 54%).

1.8 Preparation of (2E,2'E)-3,3'-(1,3-phenylene)diprop-2-en-1-al:



To an oven-dried round bottom flask, added the diol (1.4 g, 7.36 mmol, 1 equiv) and a crushed 1:5.5 mixture of KMnO_4 (4.6 g, 29.4 mmol, 4 equiv) and MnO_2 (25 g, 287.04 mmol, 39 equiv) in DCM (75 mL) under N_2 atmosphere. The reaction mixture was stirred at rt for 12 h. After that, the mixture was filtered through celite and washed with DCM. The resulting filtrate was concentrated and crude was purified by silica gel column chromatography using 10% ethyl acetate/hexane to obtain the dialdehyde product (0.97 g, 71%).

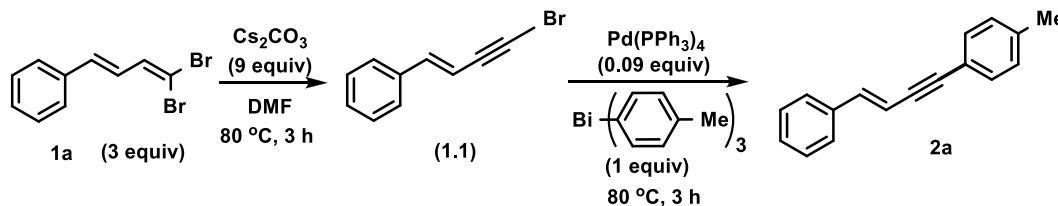
1.9 Preparation of 1,3-bis((E)-4,4-dibromobuta-1,3-dienyl)benzene (**1k**)²:



To an oven-dried round bottom flask, added the dialdehyde (1 g, 5.37 mmol, 1 equiv) in DCM and cooled to 0 °C under nitrogen. Then CBr_4 (7.1 g, 21.48 mmol, 4 equiv) and PPh_3 (11.3 g, 42.96 mmol, 8 equiv) were added in small portions. The reaction was stirred at 0 °C under nitrogen for 6 h. The mixture was quenched with hexane, passed through a silica gel pad. The filtrate obtained was concentrated and purified by silica gel column chromatography using hexane as eluent to obtain the product **1k** as colourless solid (1.8 g, 67%).

2. Control Reaction:

2.1 Sequential Addition Reaction in Two Step-One-pot Protocol:

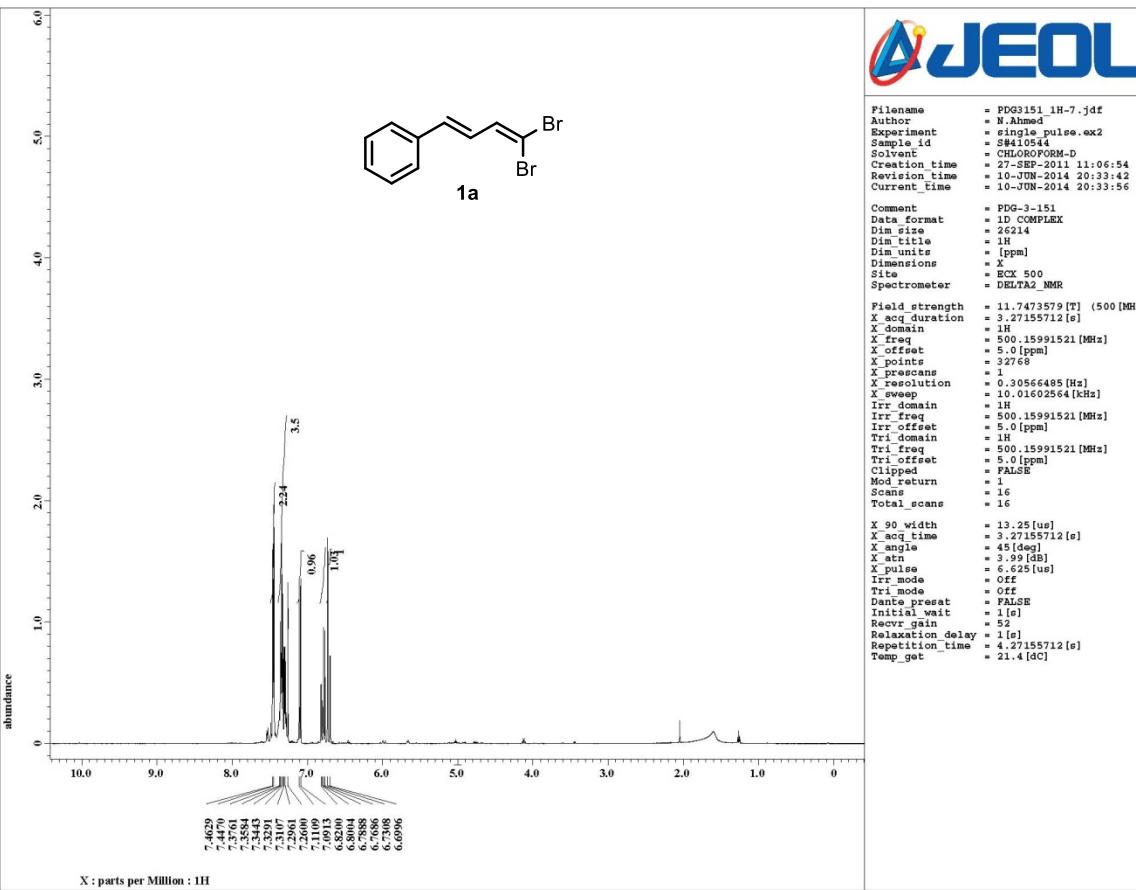


To an oven-dried Schlenk tube under N_2 atmosphere, added (*E*)-(4,4-dibromobuta-1,3-dienyl)benzene (0.108 g, 0.375 mmol, 3 equiv), Cs_2CO_3 (0.367 g, 1.125 mmol, 9 equiv) and DMF (6 mL). The reaction mixture was stirred at 80°C in an oil bath for 3 h. It was then brought to rt and tri(*p*-tolyl)bismuth (0.060 g, 0.125 mmol, 1 equiv) and $\text{Pd}(\text{PPh}_3)_4$ (0.013 g, 0.0112 mmol, 0.09 equiv) were added under N_2 atmosphere. The mixture was further stirred at 80°C for 3 h. After the stipulated time, work up was carried out with ethyl acetate (50 mL), washing with water (15 mL), brine (15 mL), drying with anhydrous MgSO_4 and concentrated. The crude was purified by silica gel column chromatography using hexane as eluent to obtain **2a** (0.070 g, 86%).

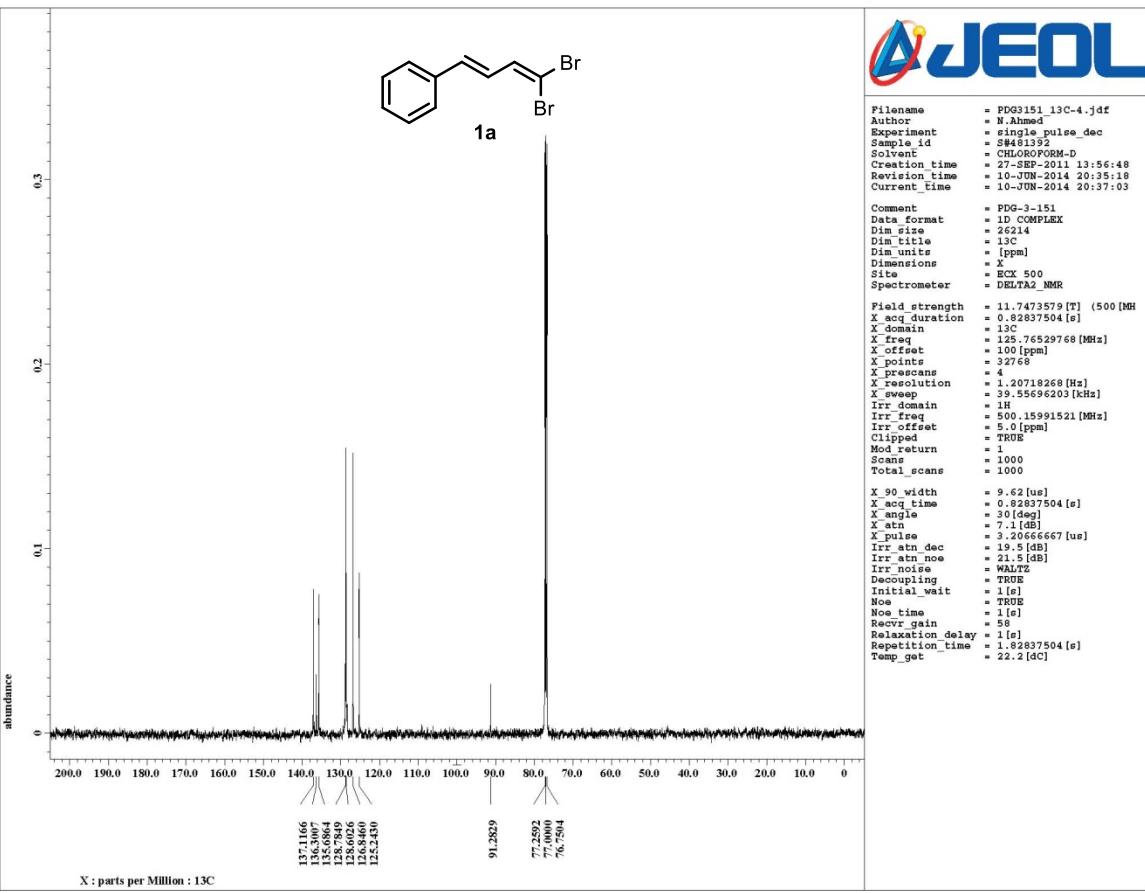
3. References:

1. A. Sharma, B. P. Joshi and A. K.Sinha, *Chem. Lett.*, 2003, **32**, 1186.
2. F. Ramirez, N. B. Desai and N. Mckelvie, *J. Am. Chem. Soc.*, 1962, **84**, 1745.
3. G. Rai, C. J. Thomas, W. Leister and D. J. Maloney, *Tetrahedron Lett.*,2009, **50**, 1710.

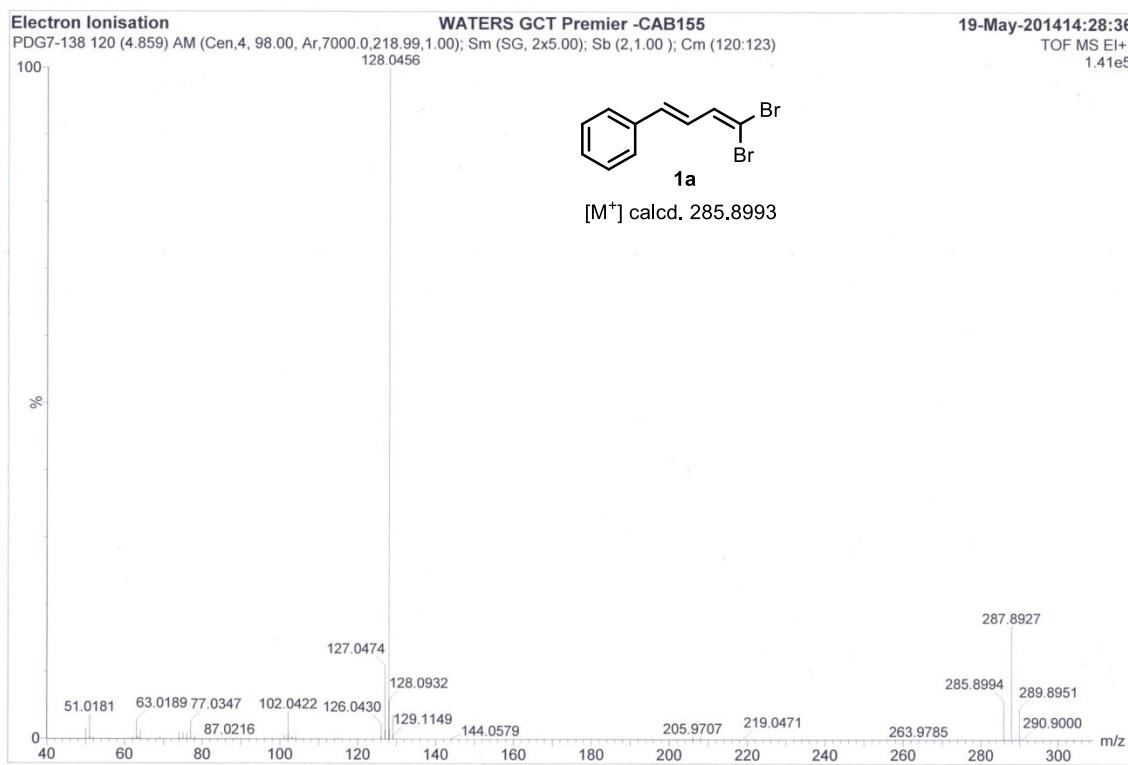
4. ^1H , ^{13}C and HRMS Spectras of 1,3-Dienyldibromides (1a-1m):



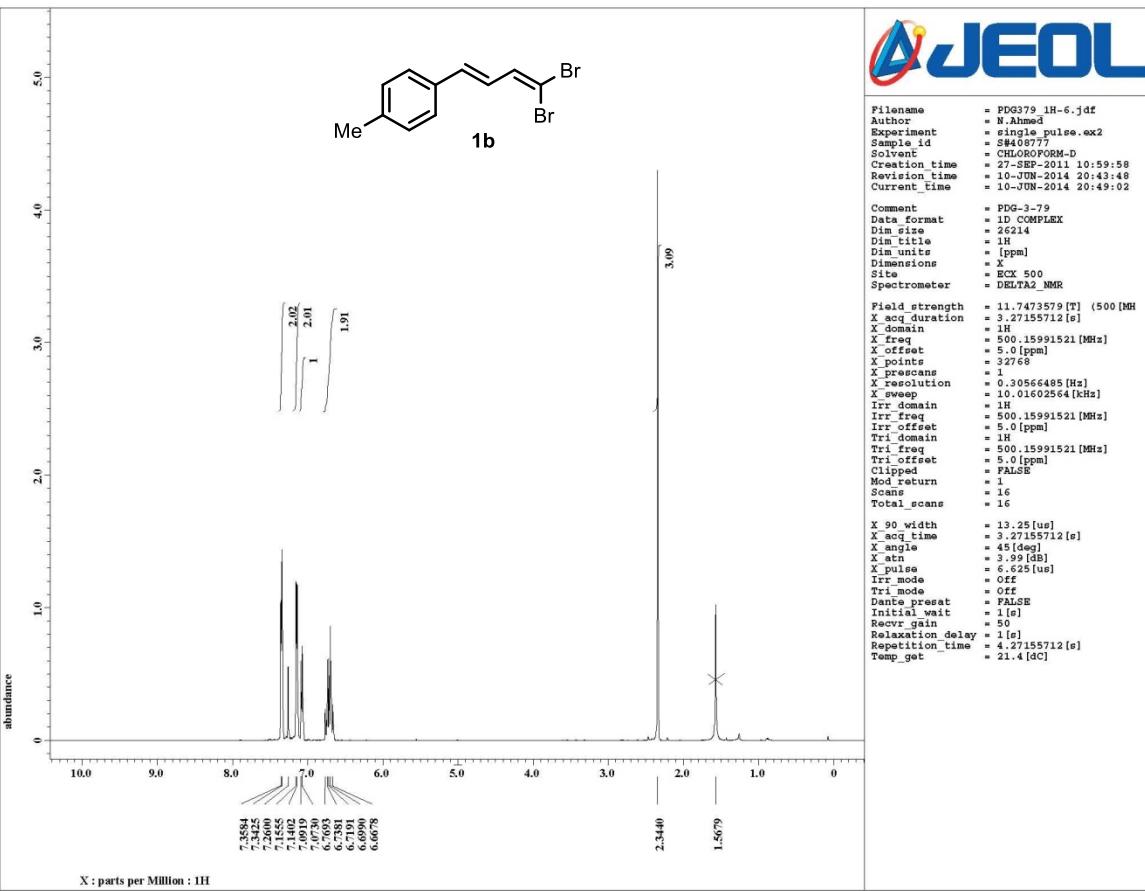
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-(4,4-dibromobuta-1,3-dienyl)benzene (**1a**)



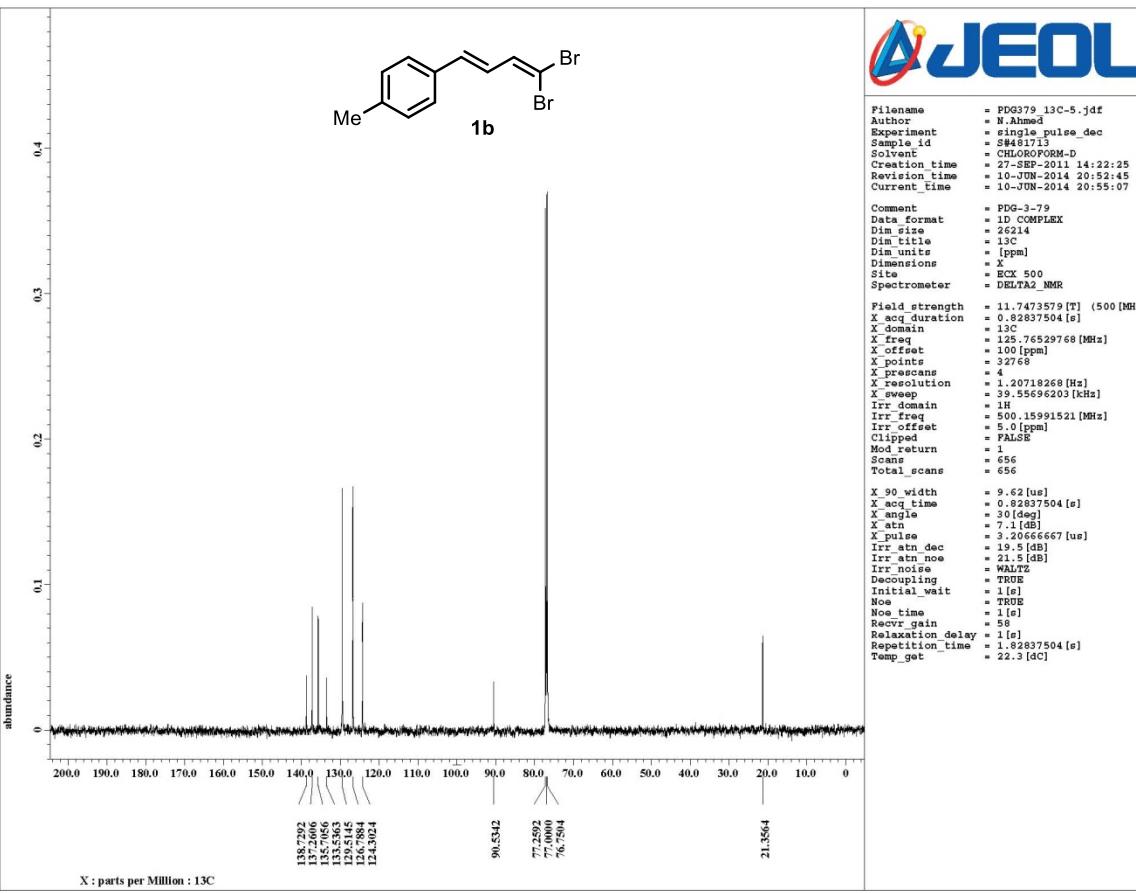
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-(4,4-dibromobuta-1,3-dienyl)benzene (**1a**)



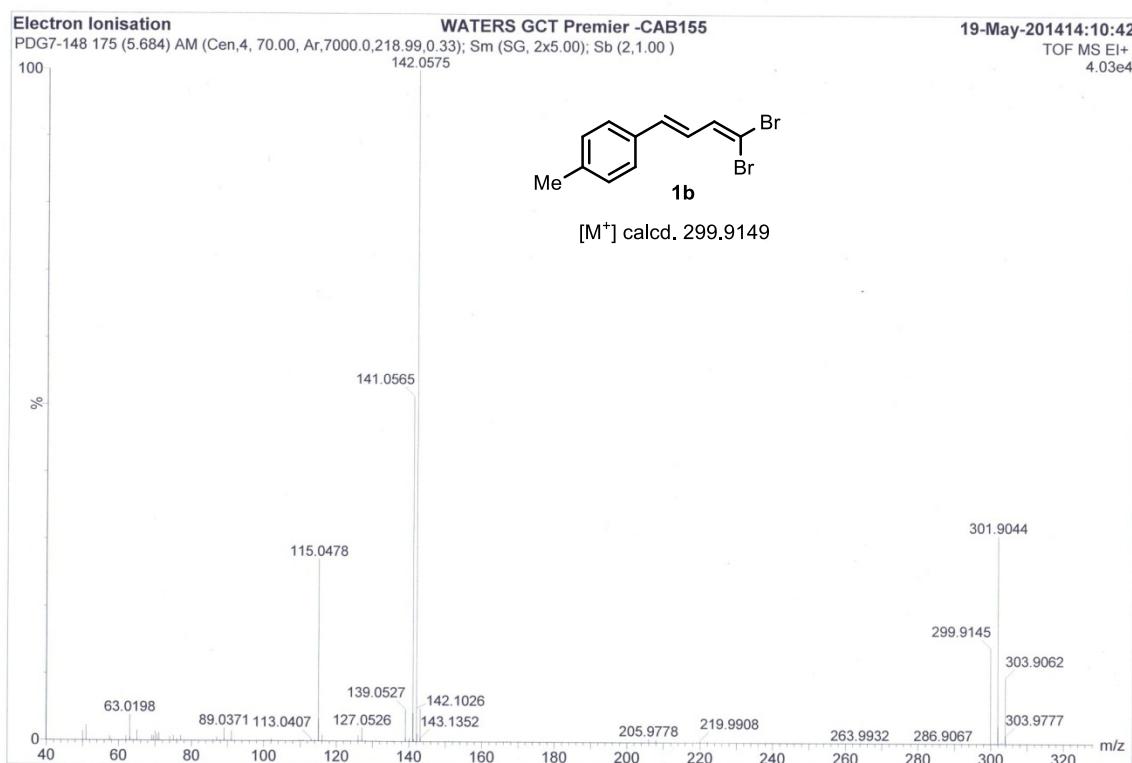
EI (HRMS) spectrum of (*E*)-(4,4-dibromobuta-1,3-dienyl)benzene (**1a**)



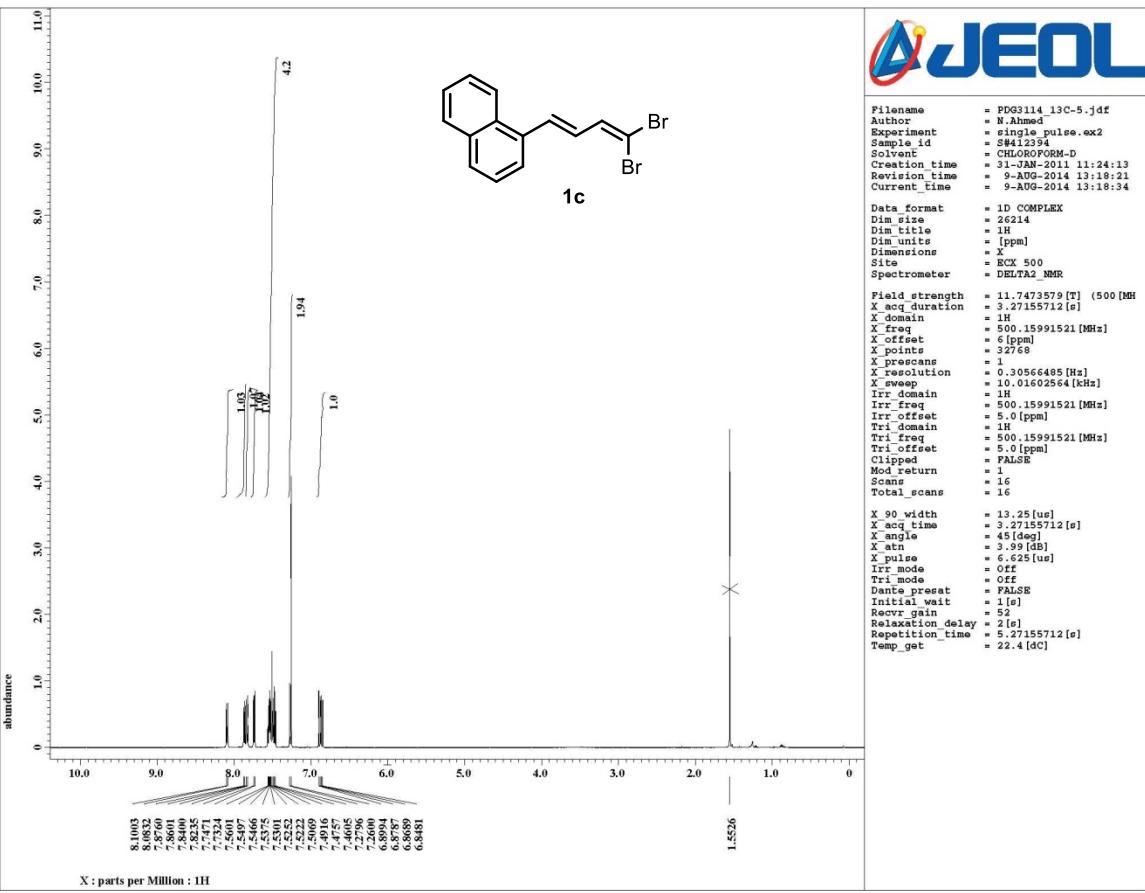
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4,4-dibromobuta-1,3-dienyl)-4-methylbenzene (**1b**)



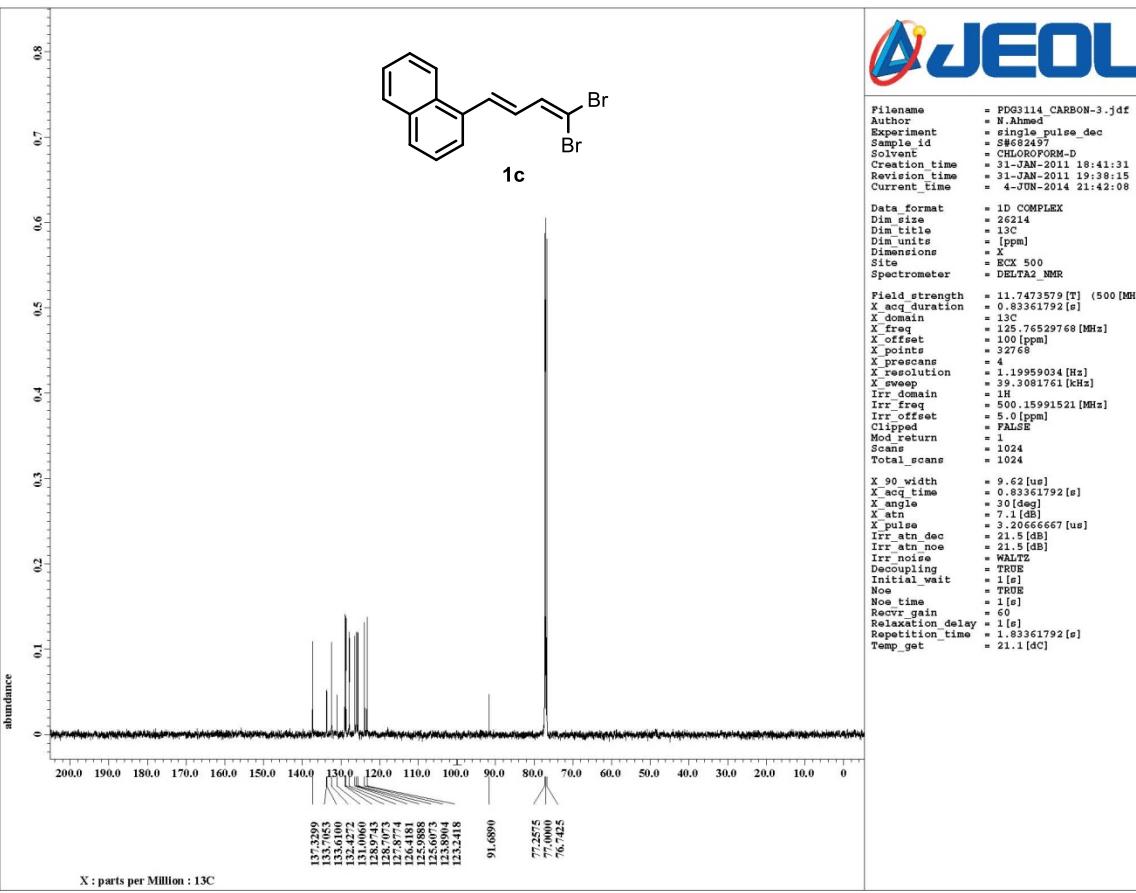
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4,4-dibromobuta-1,3-dienyl)-4-methylbenzene (**1b**)



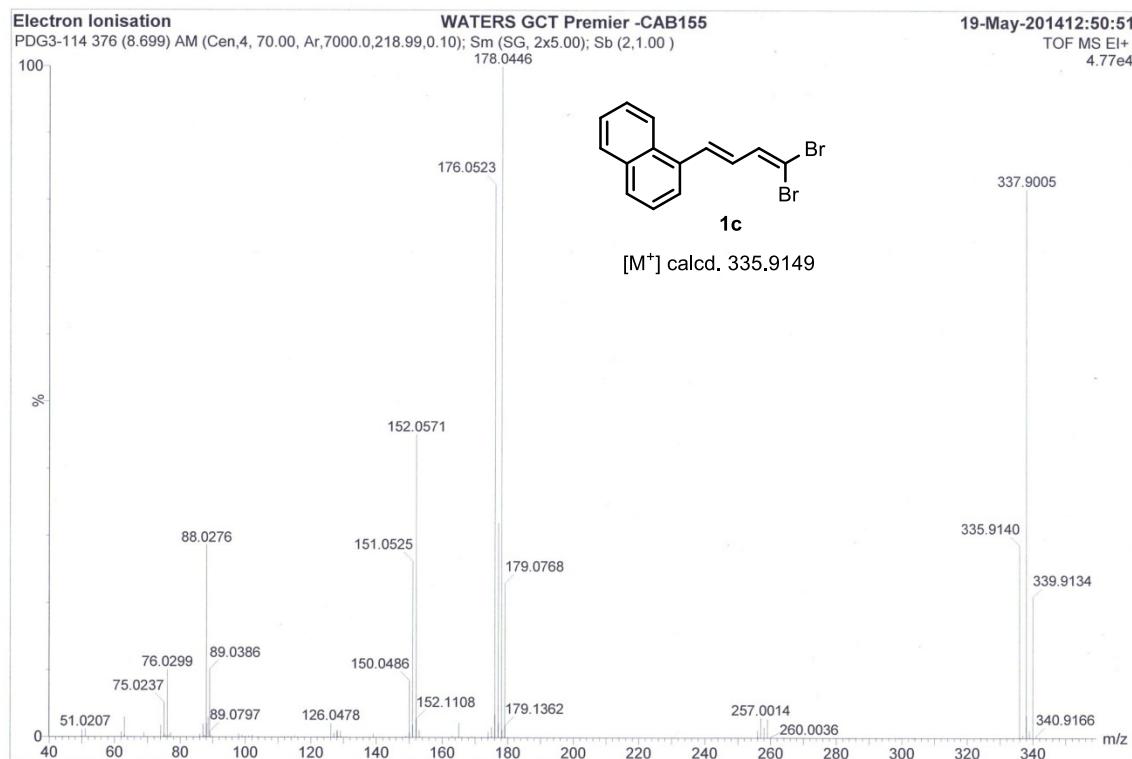
EI (HRMS) spectrum of (*E*)-1-(4,4-dibromobuta-1,3-dienyl)-4-methylbenzene (**1b**)



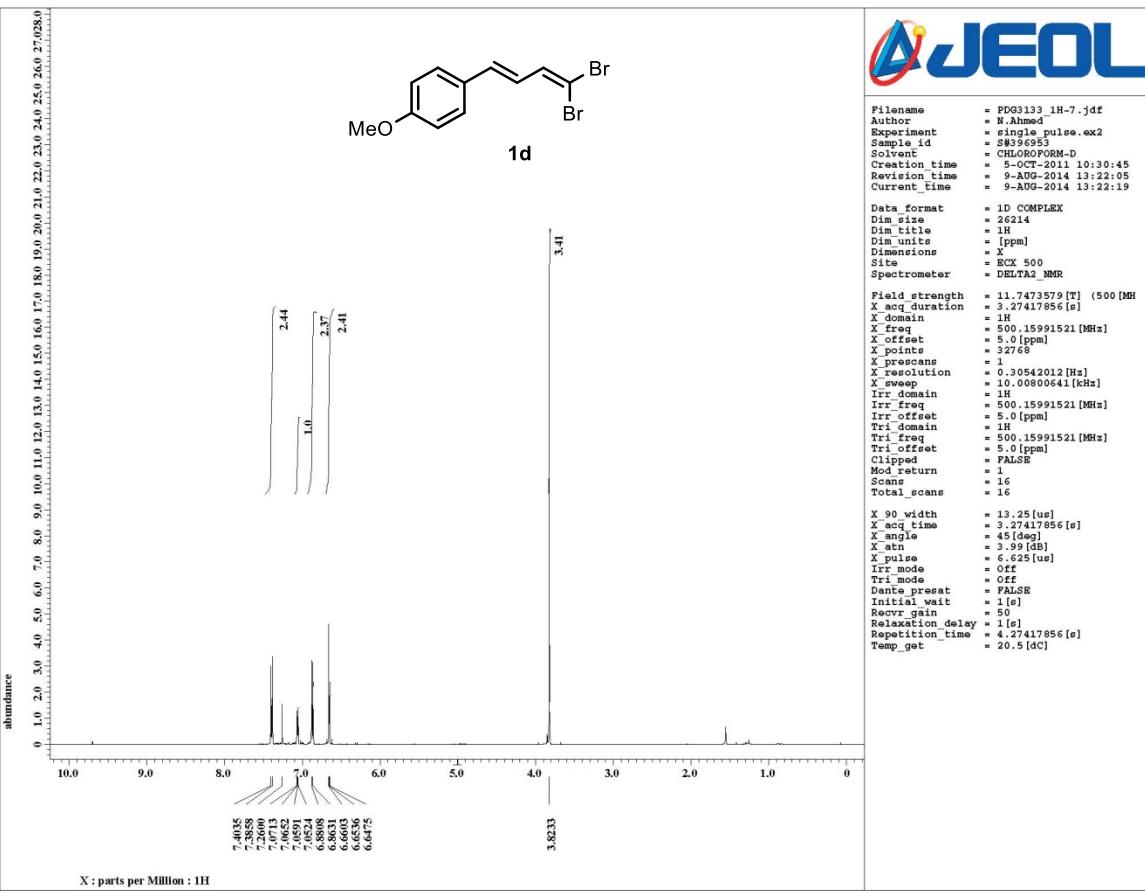
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4,4-dibromobuta-1,3-dienyl)naphthalene (**1c**)



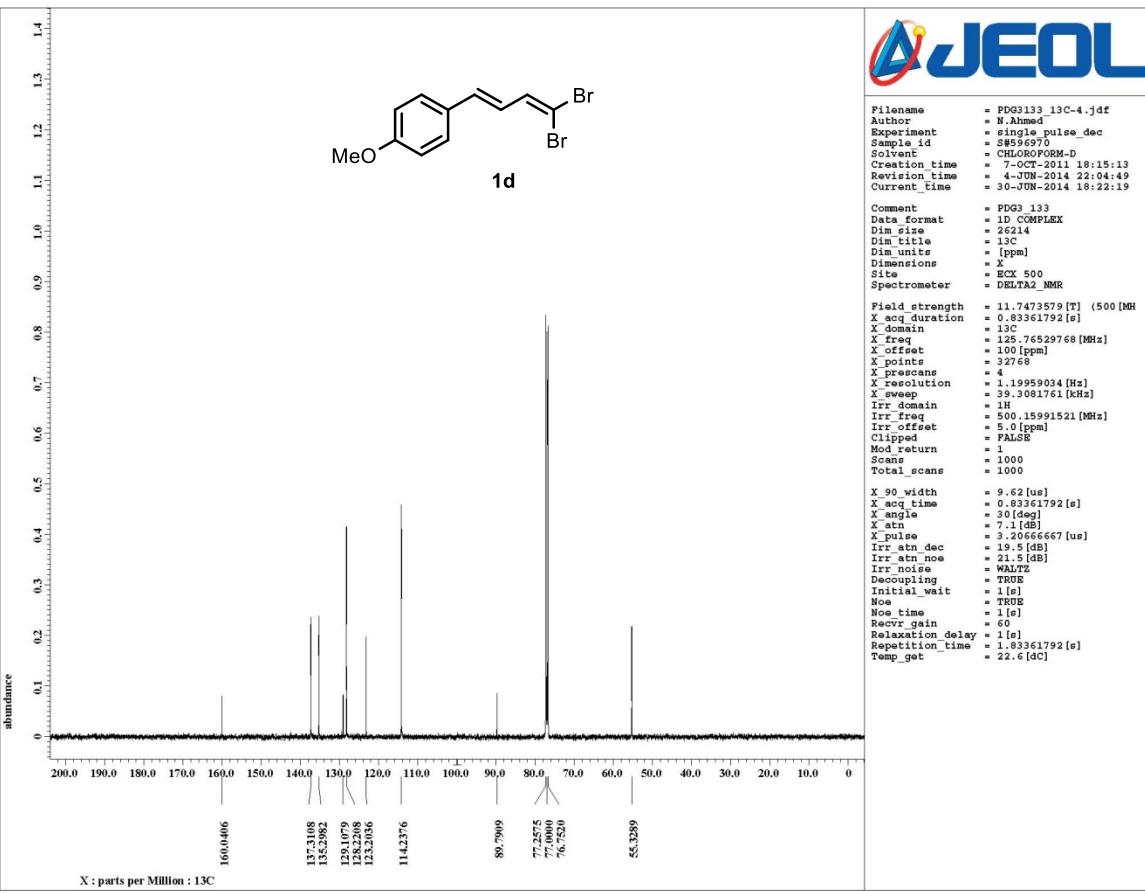
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4,4-dibromobuta-1,3-dienyl)naphthalene (**1c**)



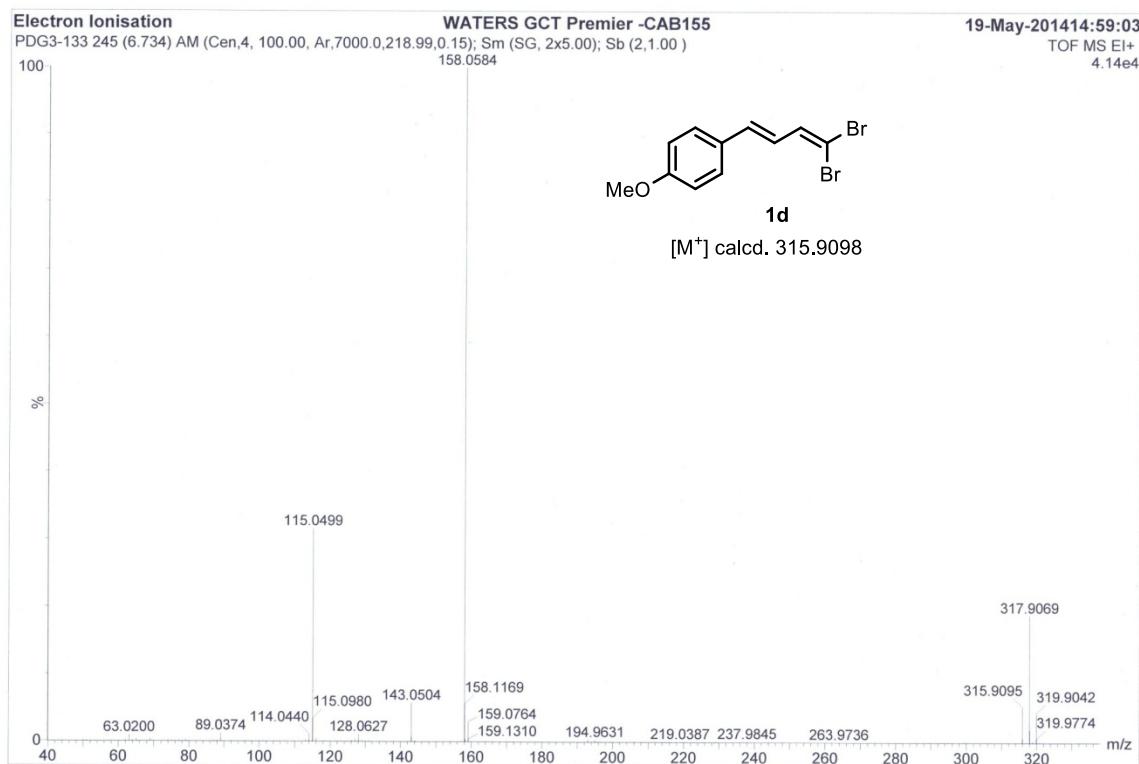
EI (HRMS) spectrum of (*E*)-1-(4,4-dibromobuta-1,3-dienyl)naphthalene (**1c**)



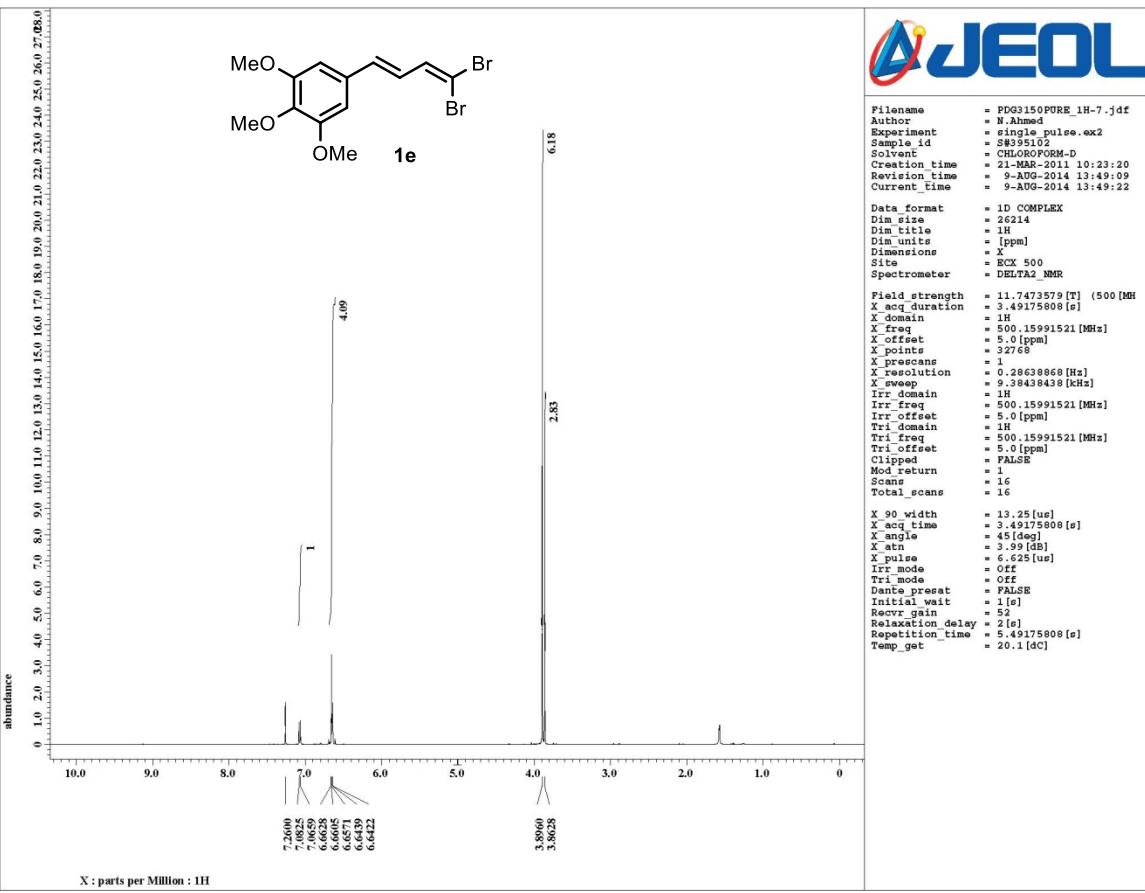
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-(4,4-dibromobuta-1,3-dienyl)-4-methoxybenzene(**1d**)



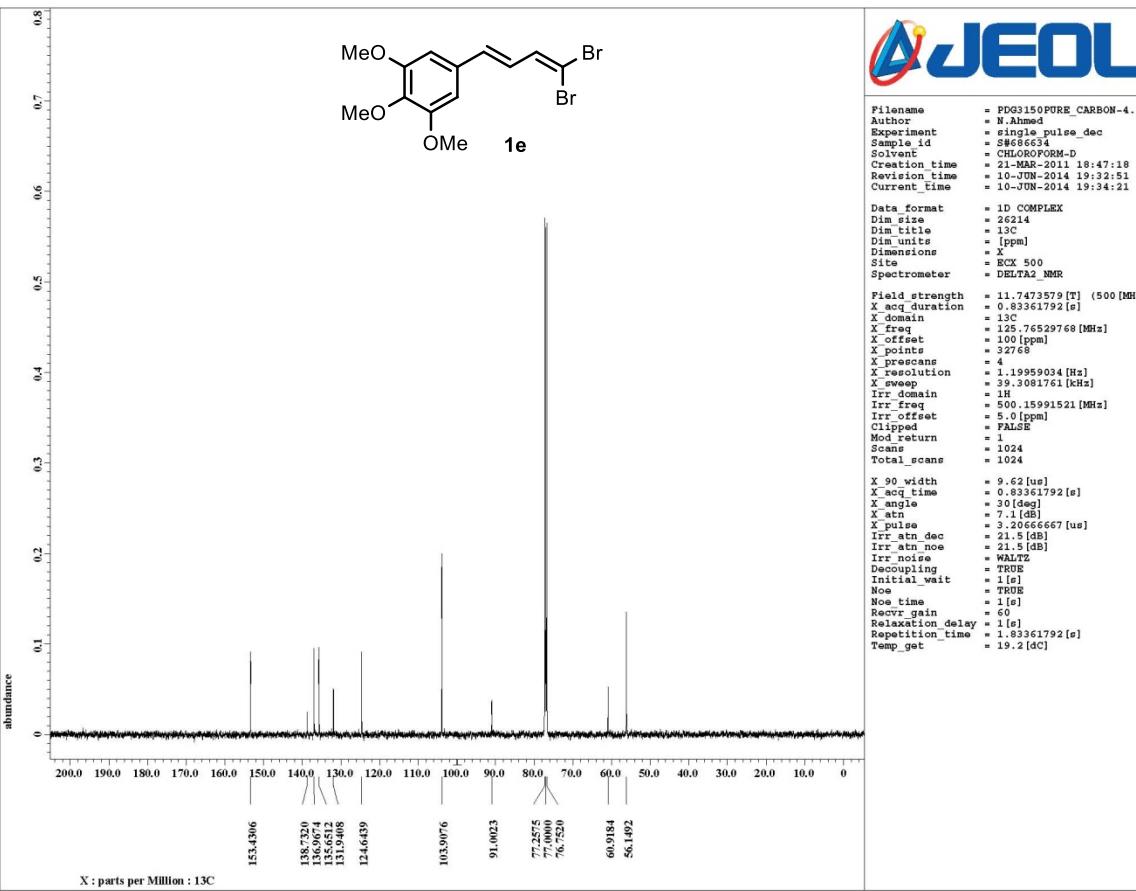
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4,4-dibromobuta-1,3-dienyl)-4-methoxybenzene (**1d**)



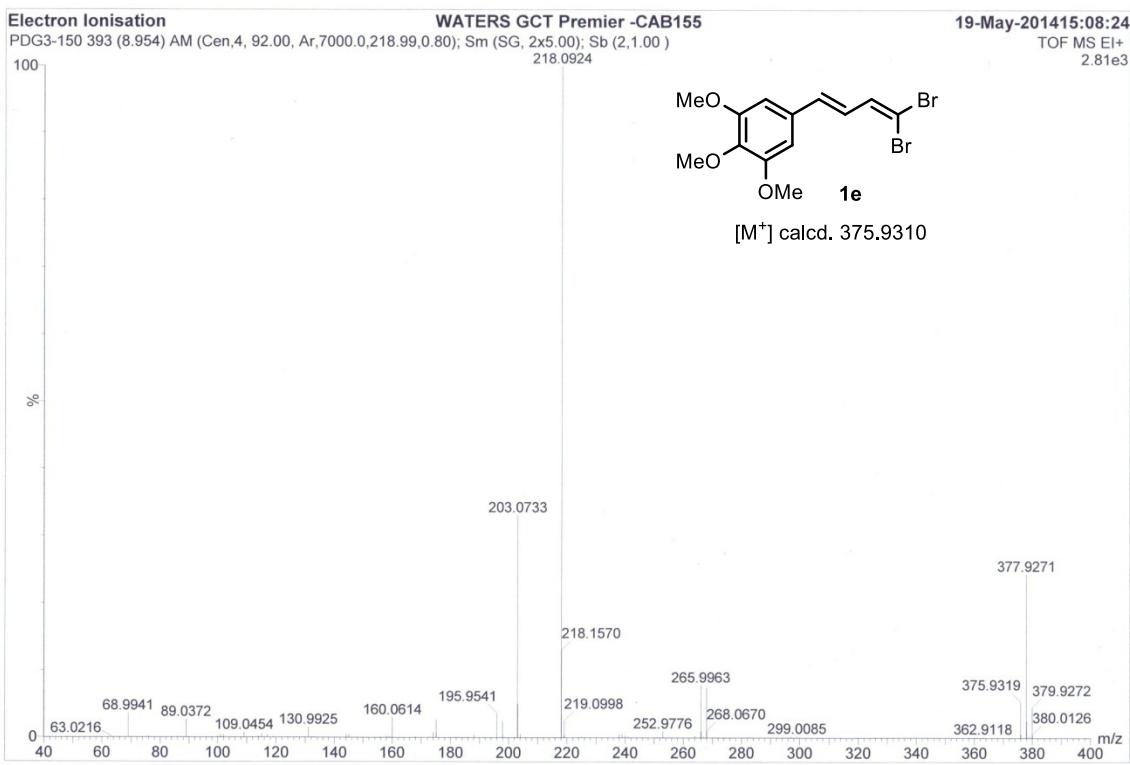
EI (HRMS) spectrum of (*E*)-1-(4,4-dibromobuta-1,3-dienyl)-4-methoxybenzene (**1d**)



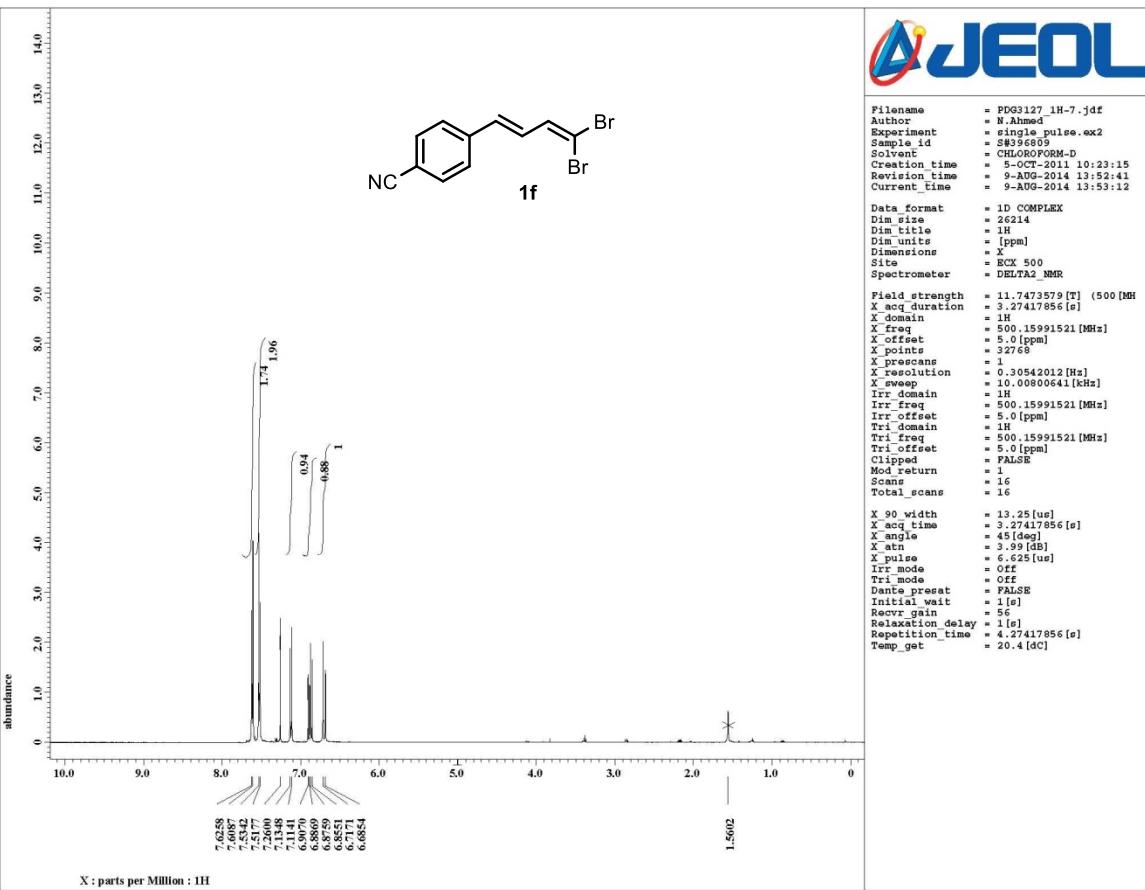
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-5-(4,4-dibromobuta-1,3-dienyl)-1,2,3-trimethoxybenzene(**1e**)



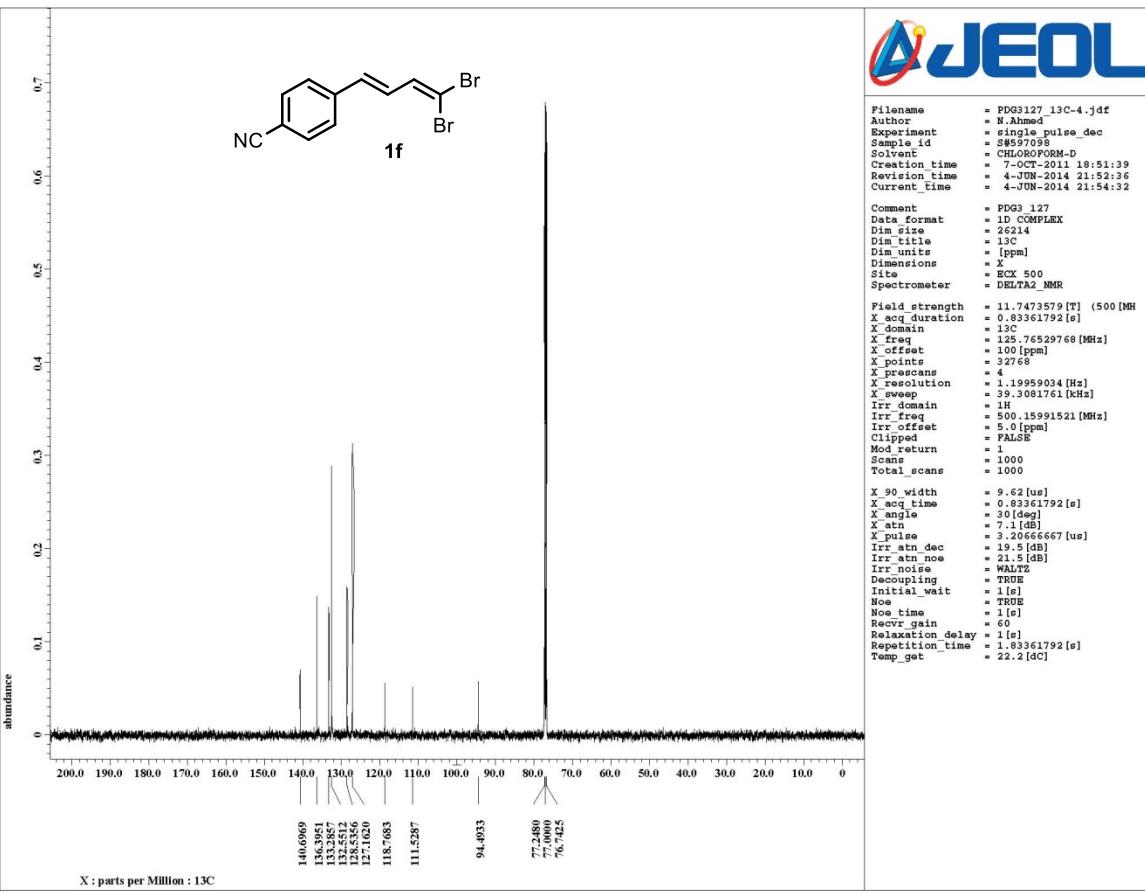
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-5-(4,4-dibromobuta-1,3-dienyl)-1,2,3-trimethoxybenzene (**1e**)



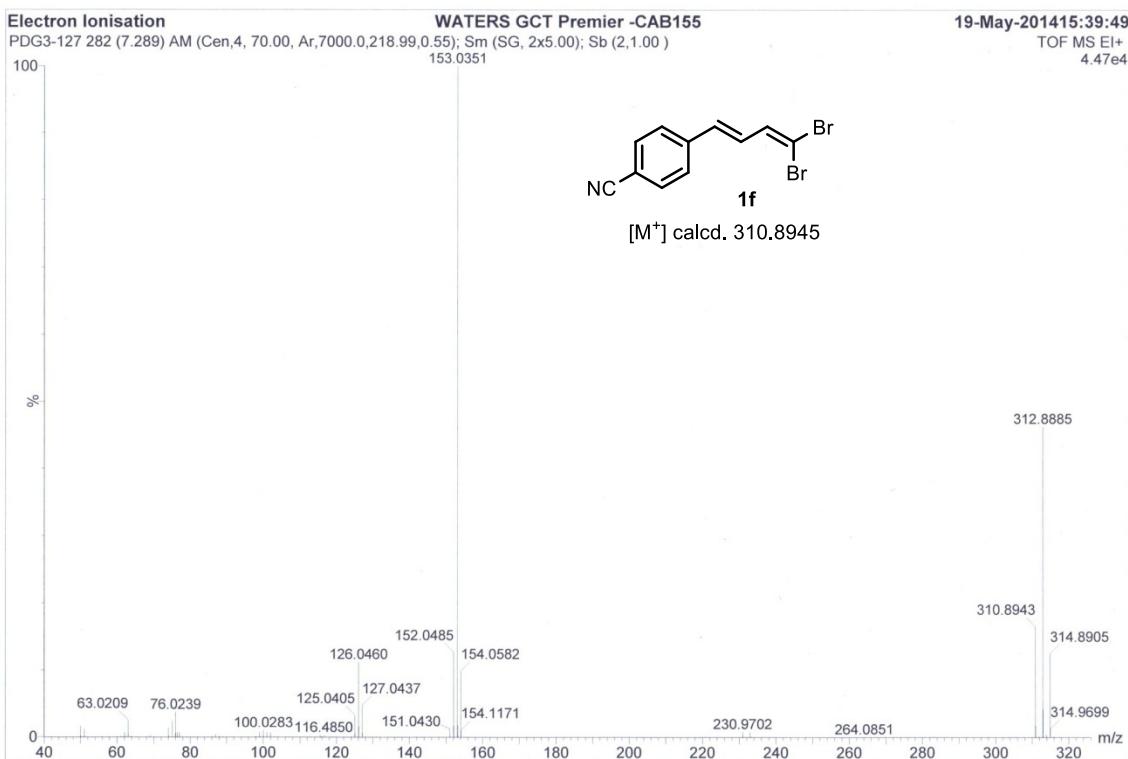
EI (HRMS) spectrum of (*E*)-5-(4,4-dibromobuta-1,3-dienyl)-1,2,3-trimethoxybenzene (**1e**)



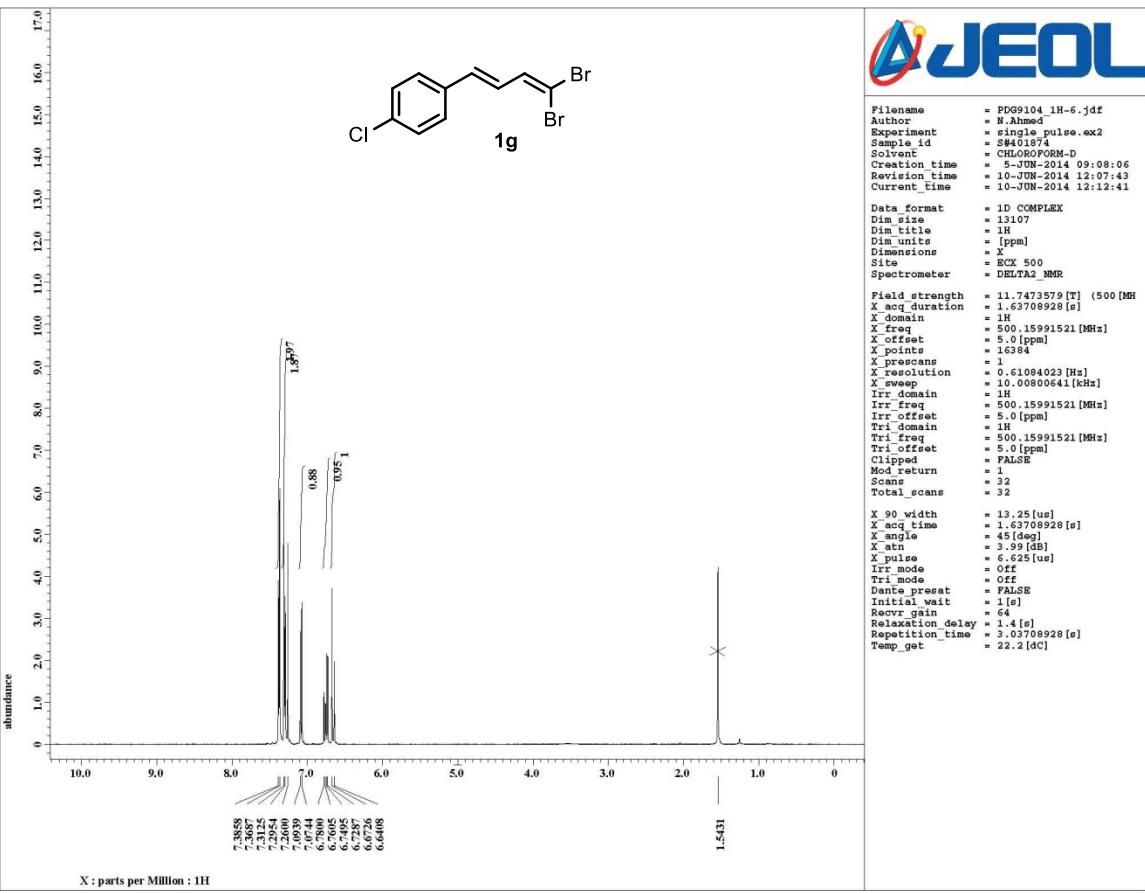
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-4-(4,4-dibromobuta-1,3-dienyl)benzonitrile (**1f**)



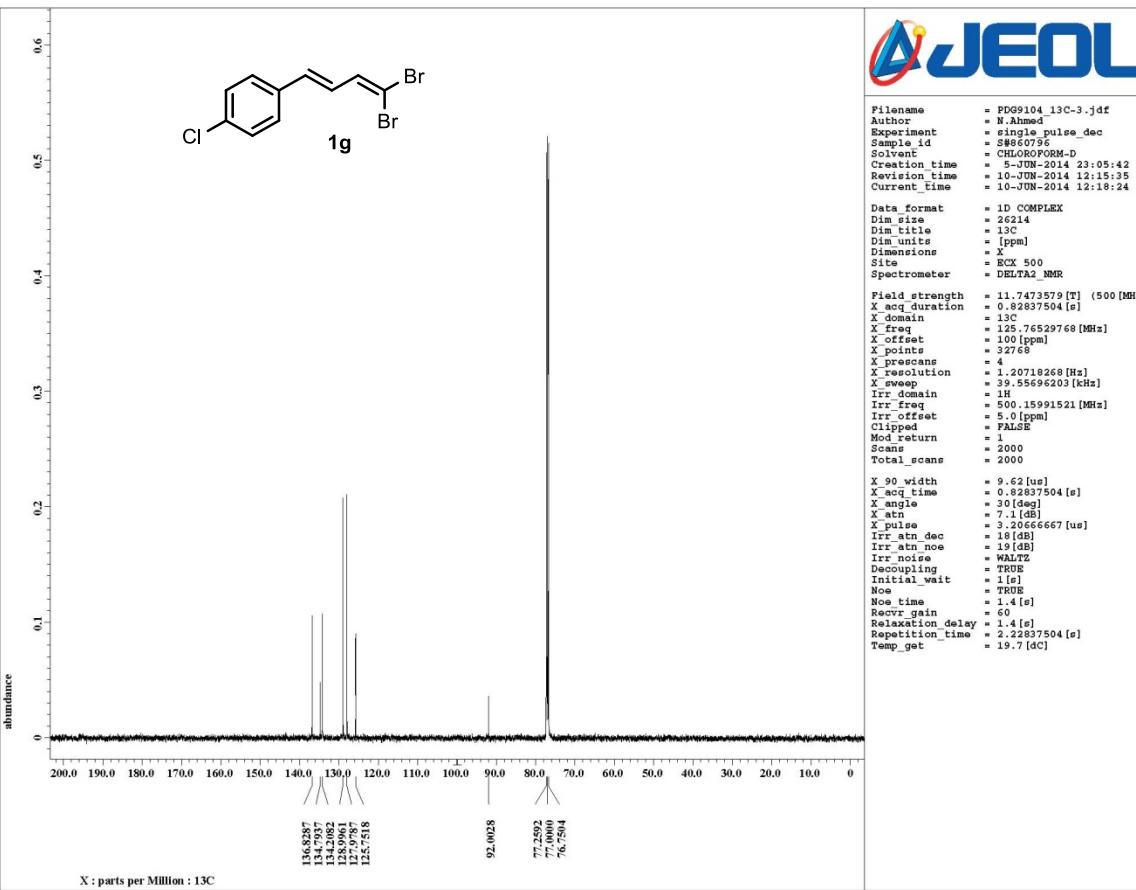
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-4-(4,4-dibromobuta-1,3-dienyl)benzonitrile (**1f**)



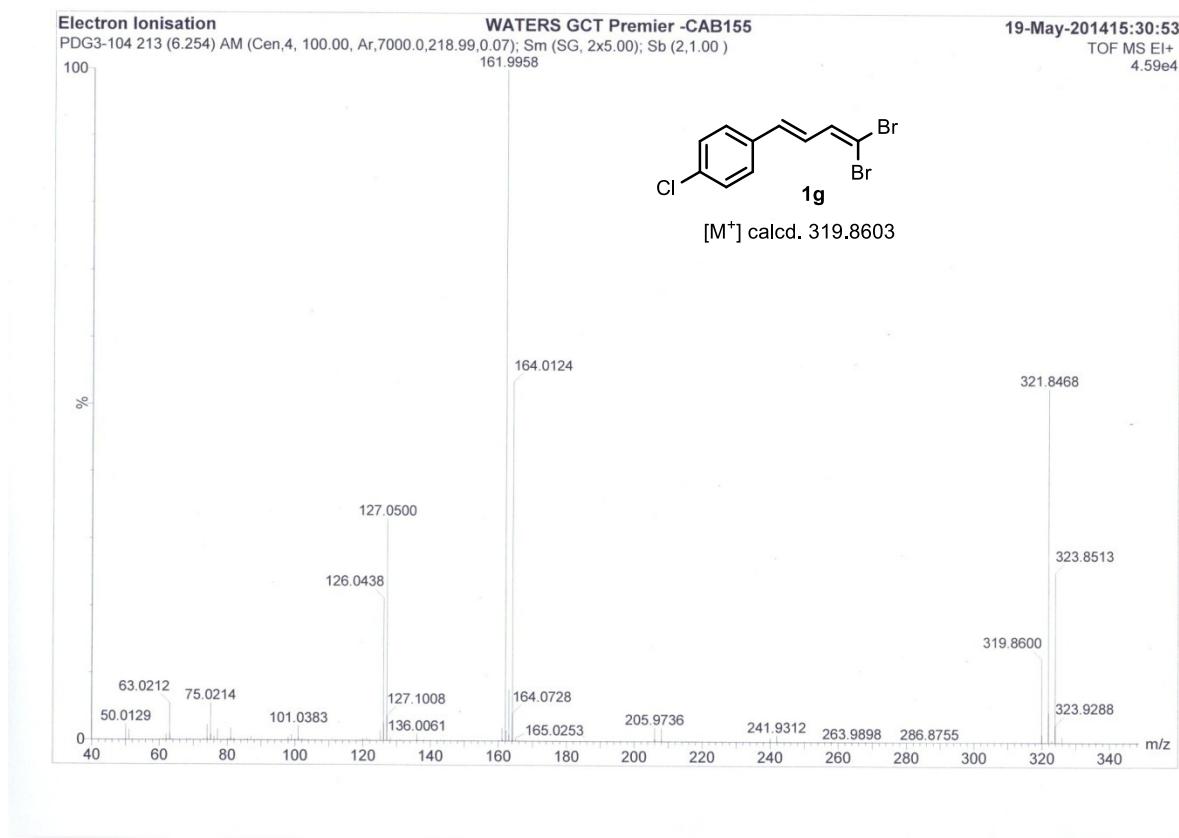
EI (HRMS) spectrum of (*E*)-4-(4,4-dibromobuta-1,3-dienyl)benzonitrile (**1f**)



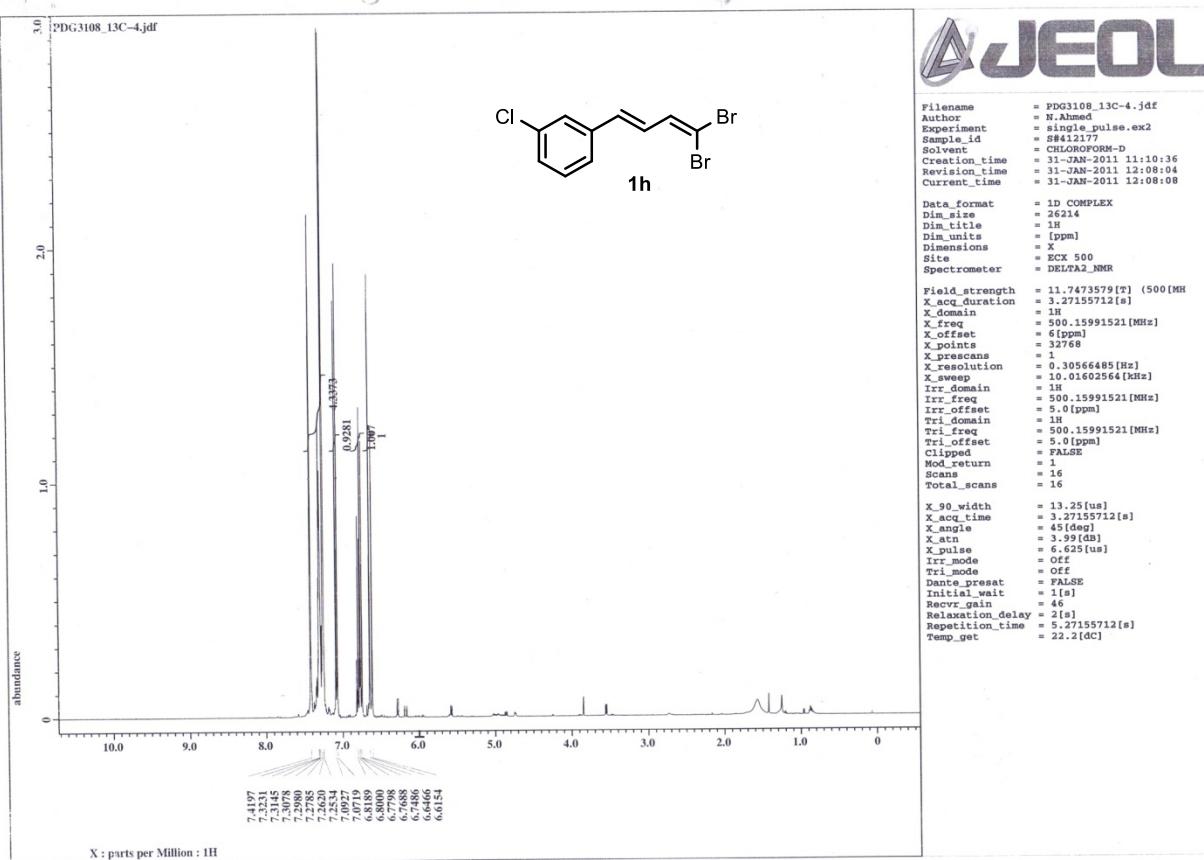
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4,4-dibromobuta-1,3-dienyl)benzene (**1g**)

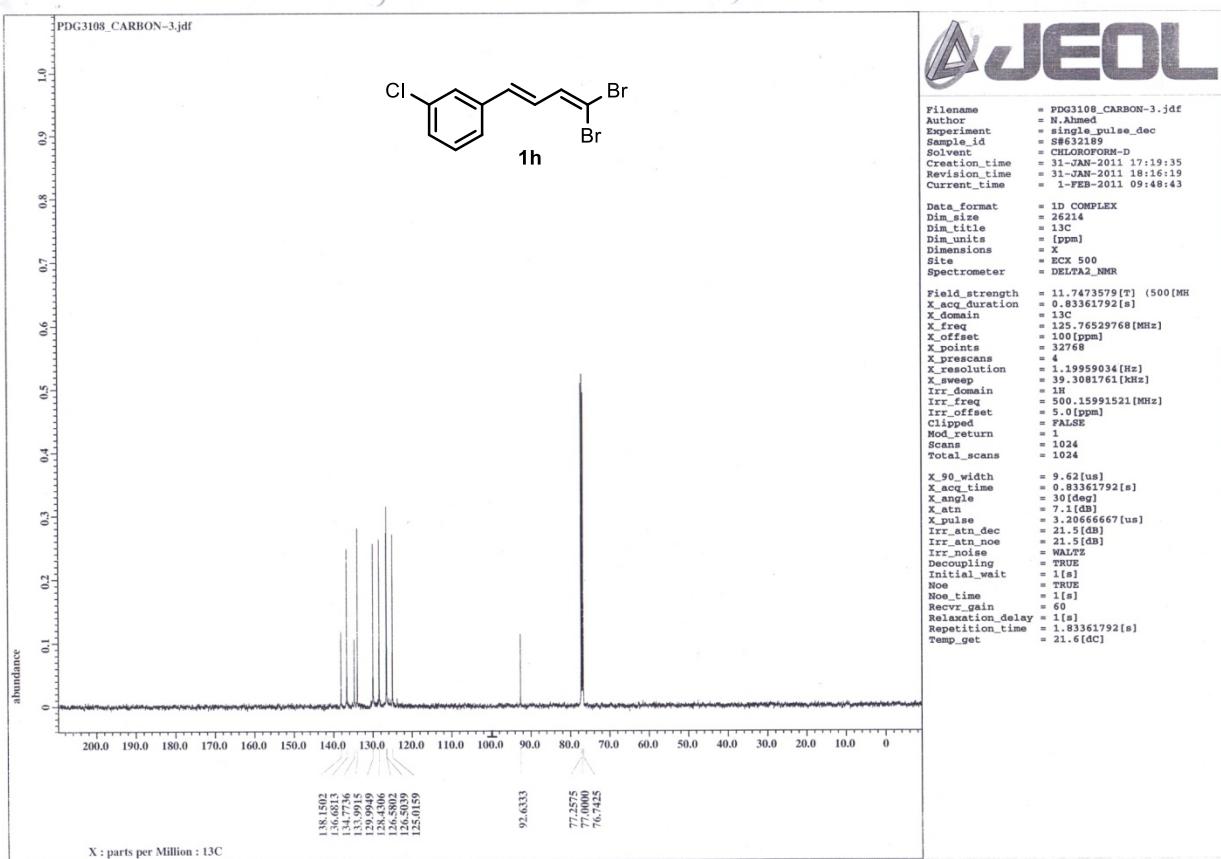


¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-chloro-4-(4,4-dibromobuta-1,3-dienyl)benzene (**1g**)

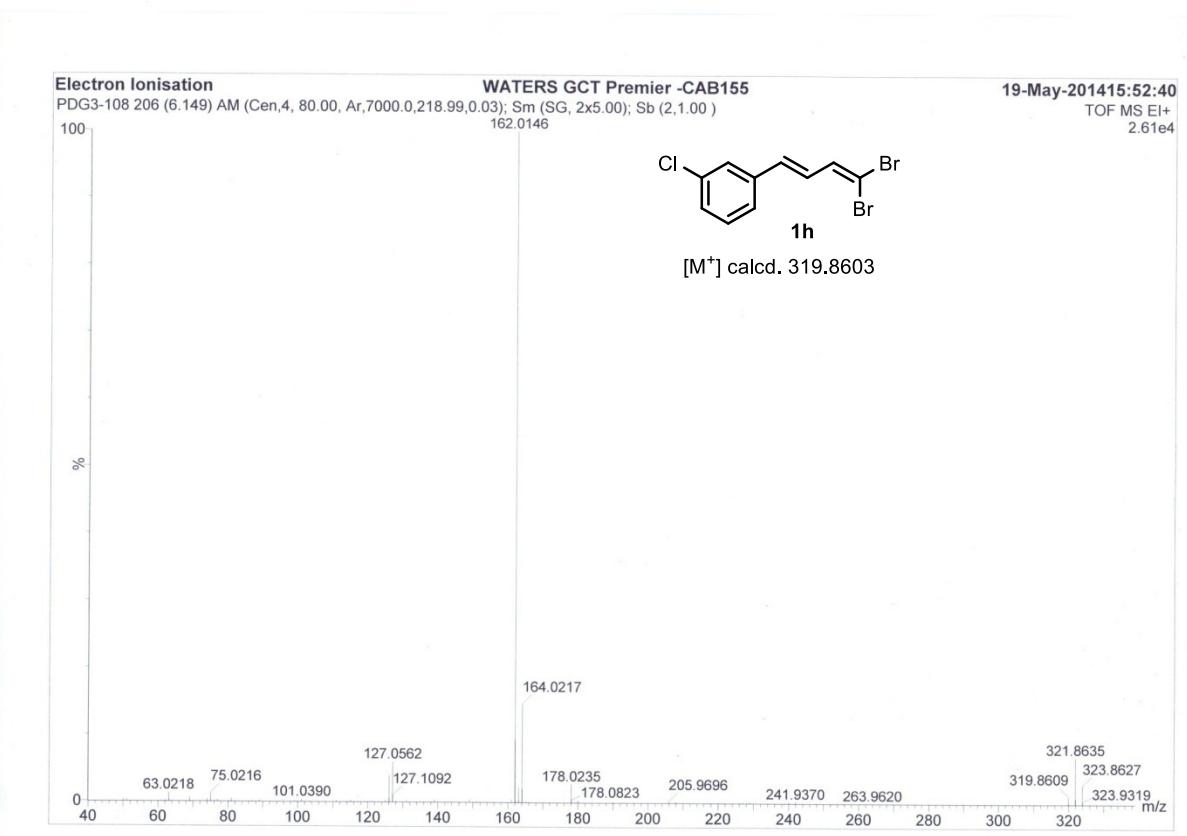


EI (HRMS) spectrum of (*E*)-1-chloro-4-(4,4-dibromobuta-1,3-dienyl)benzene (**1g**)

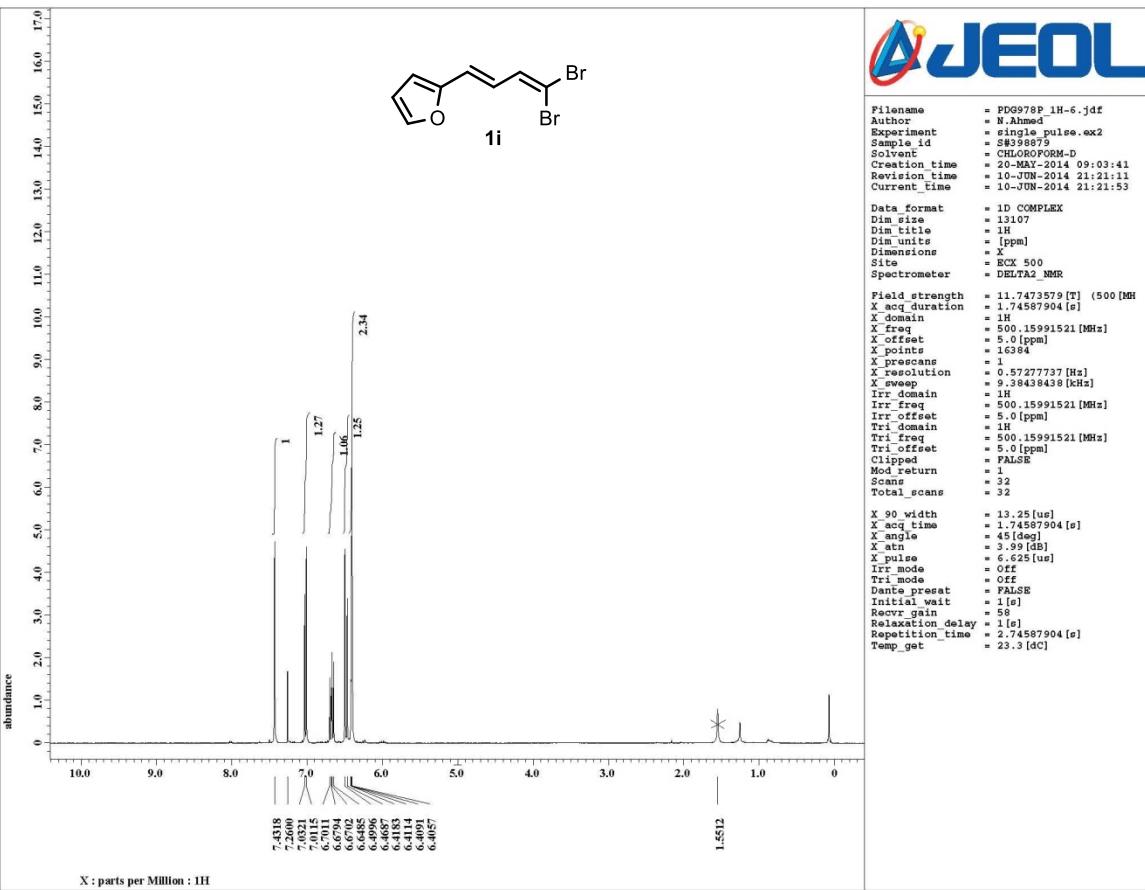




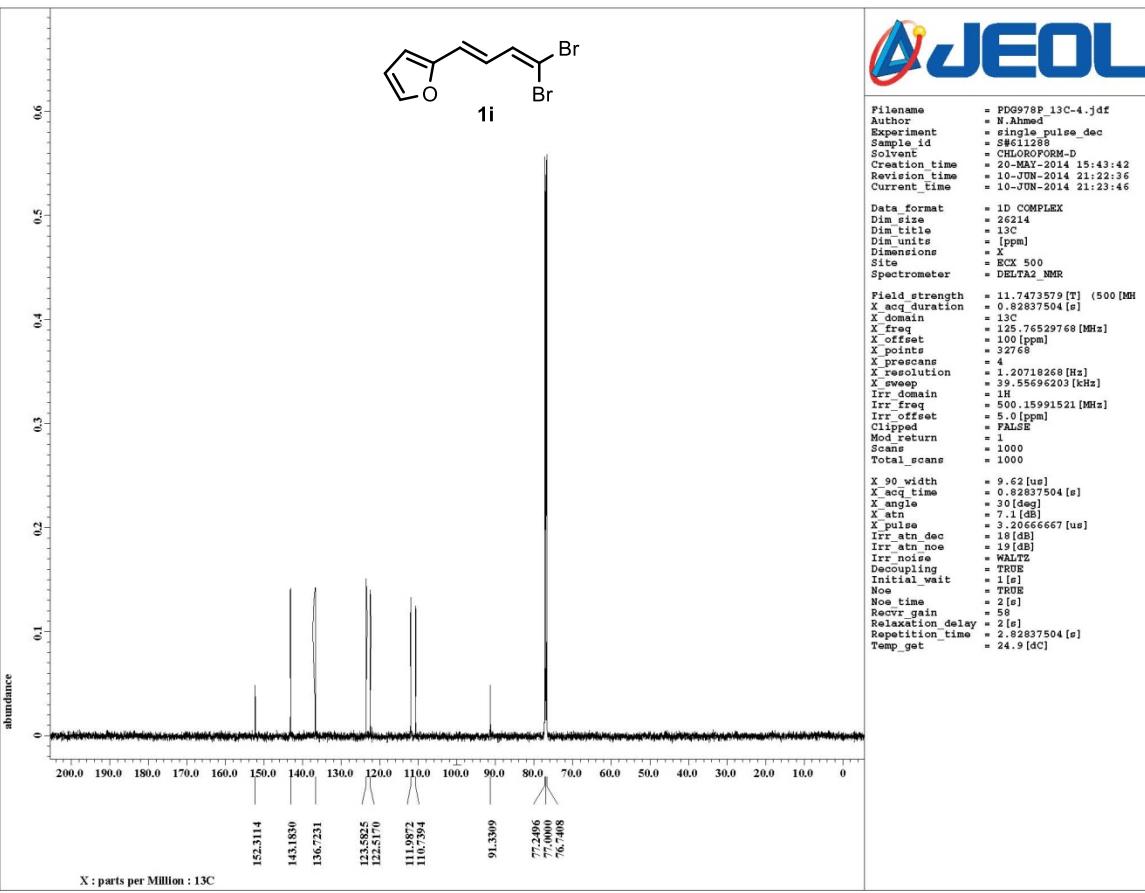
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-chloro-3-(4,4-dibromobuta-1,3-dienyl)benzene (**1h**)

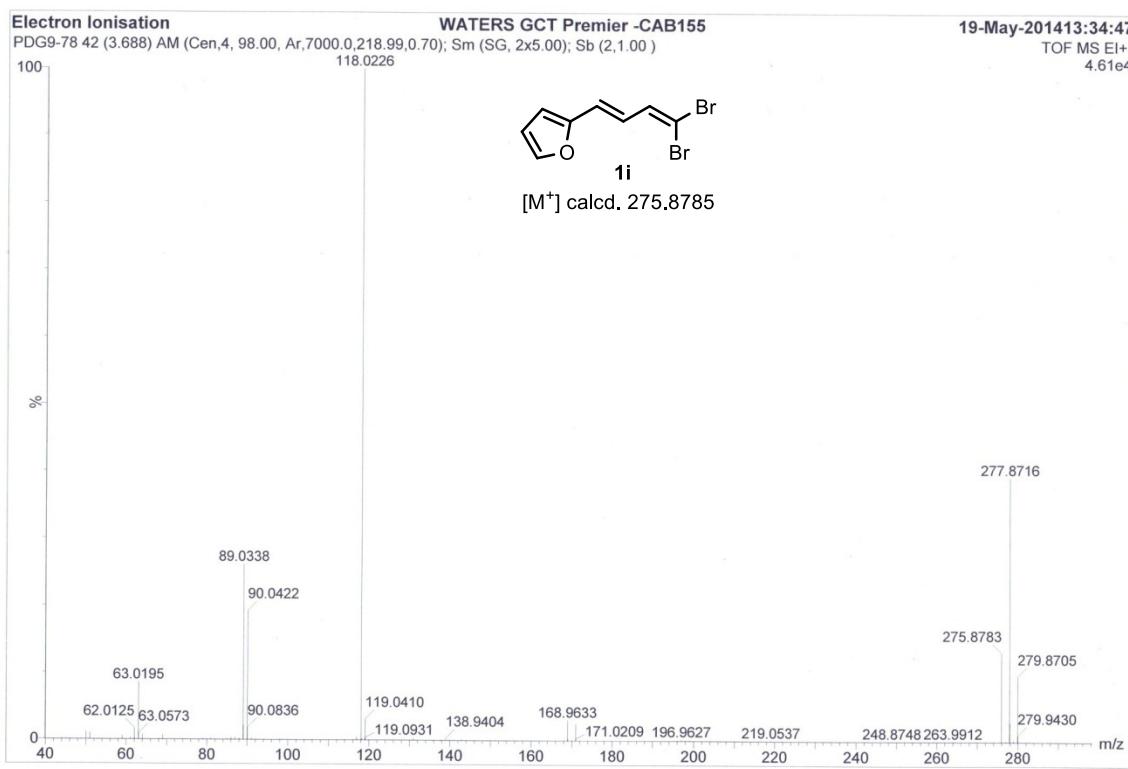


EI (HRMS) spectrum of (*E*)-1-chloro-3-(4,4-dibromobuta-1,3-dienyl)benzene (**1h**)

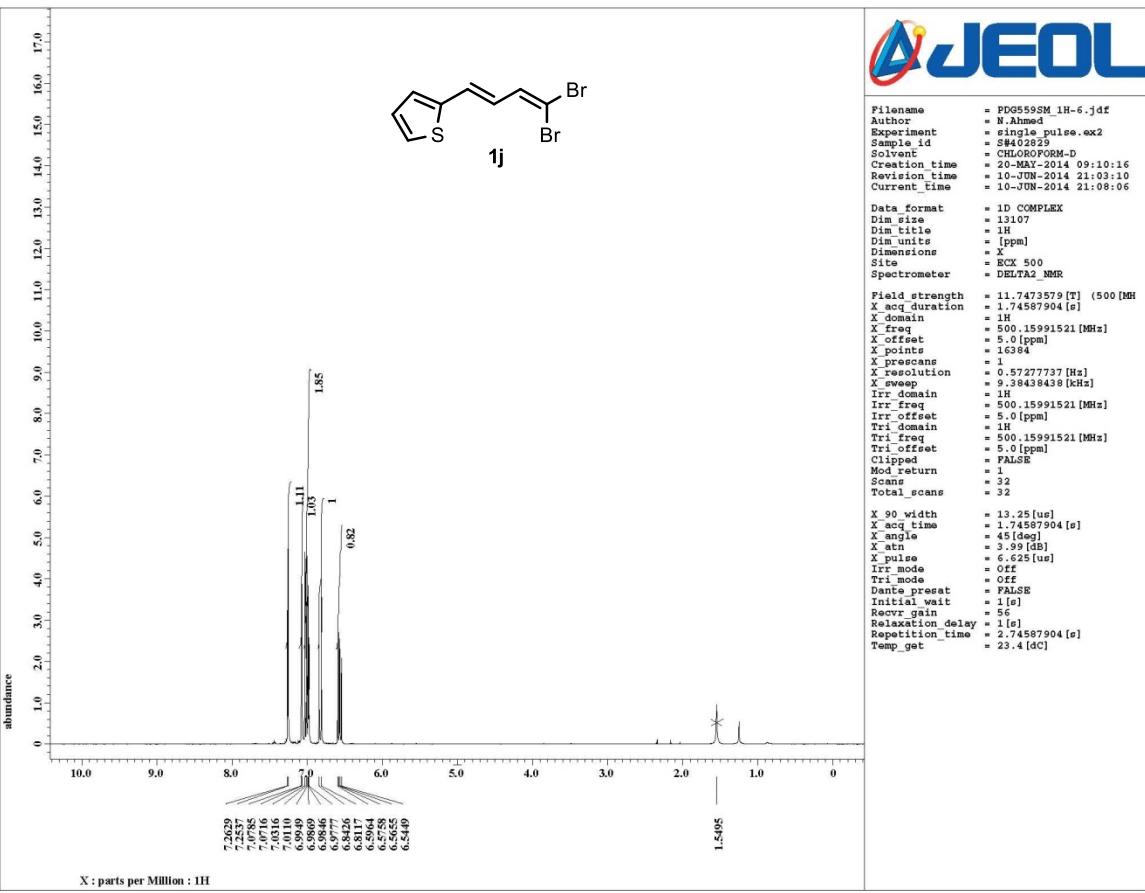


¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-2-(4,4-dibromobuta-1,3-dienyl)furan (**1i**)

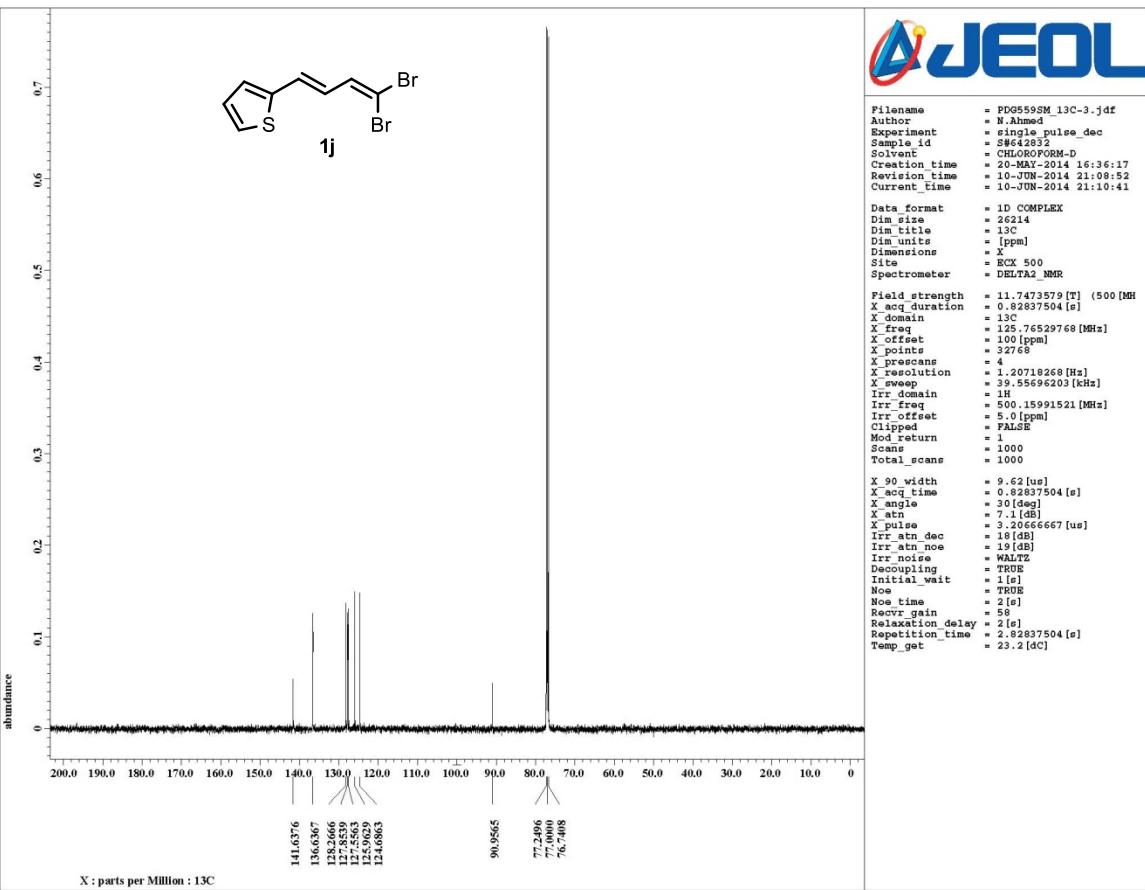




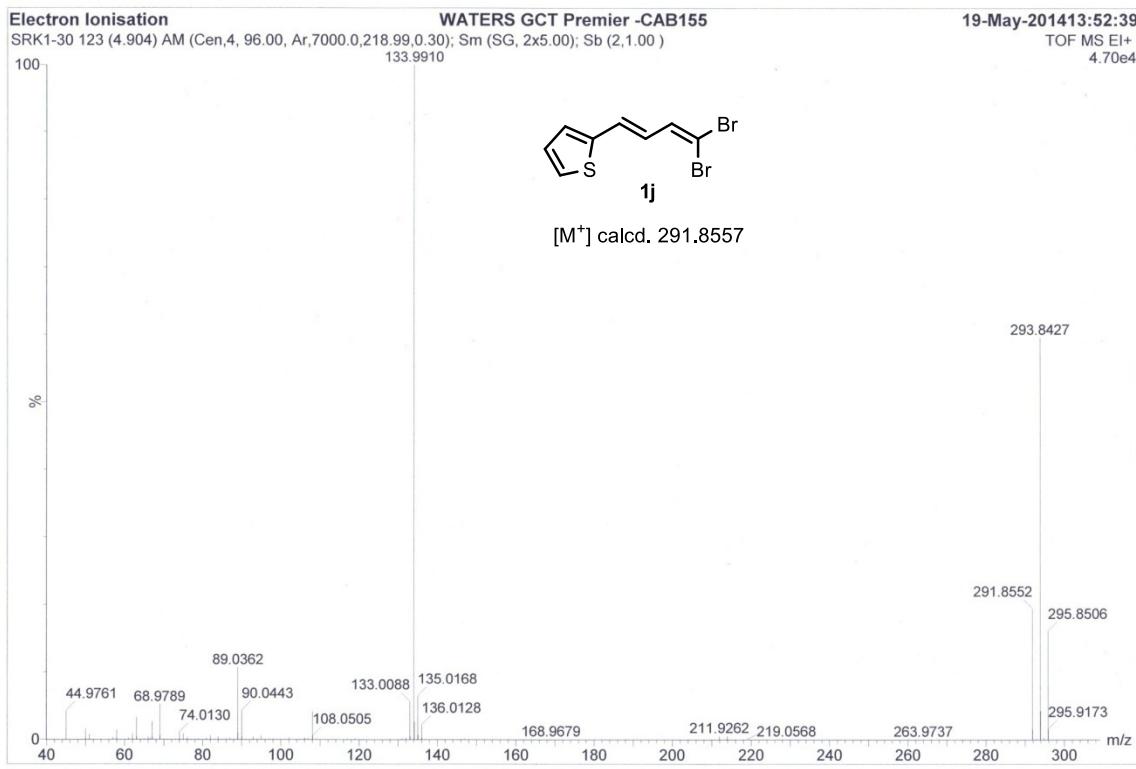
EI (HRMS) spectrum of (*E*)-2-(4,4-dibromobuta-1,3-dienyl)furan (**1i**)



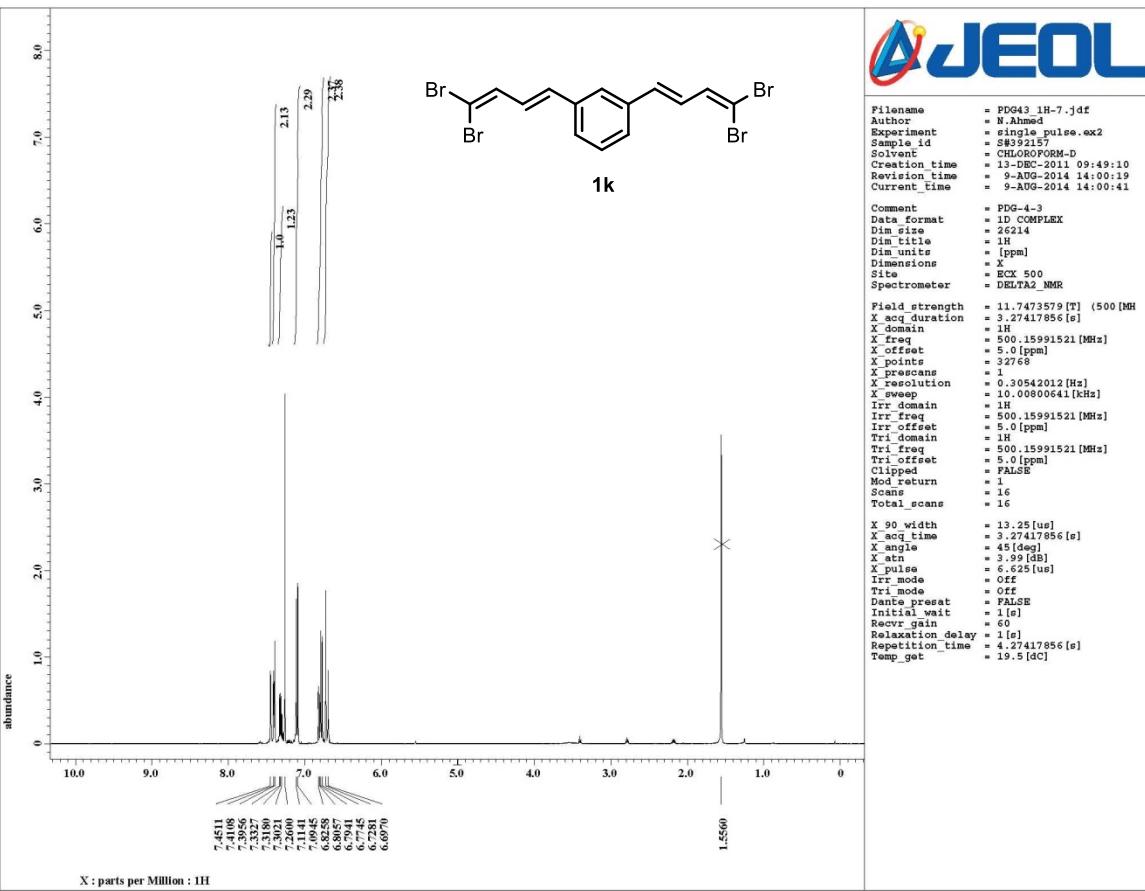
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-2-(4,4-dibromobuta-1,3-dienyl)thiophene (**1j**)



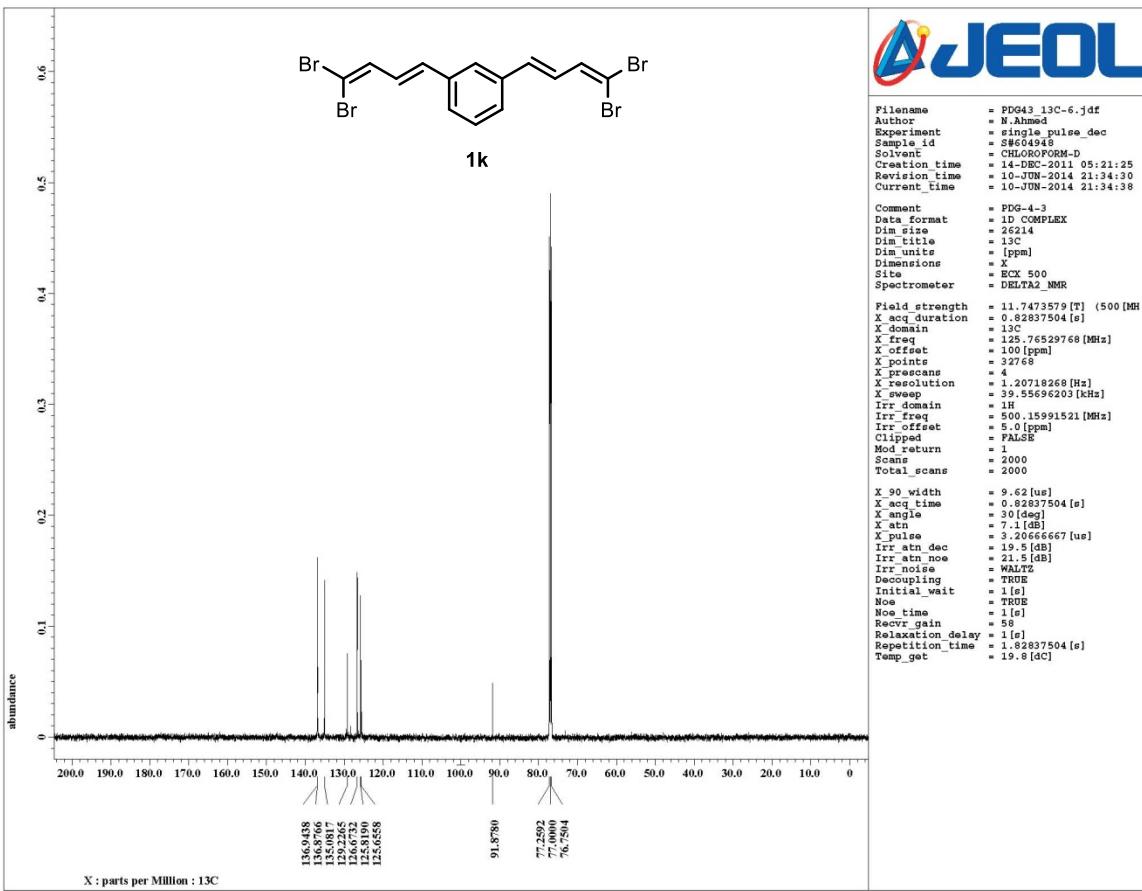
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-2-(4,4-dibromobuta-1,3-dienyl)thiophene (**1j**)



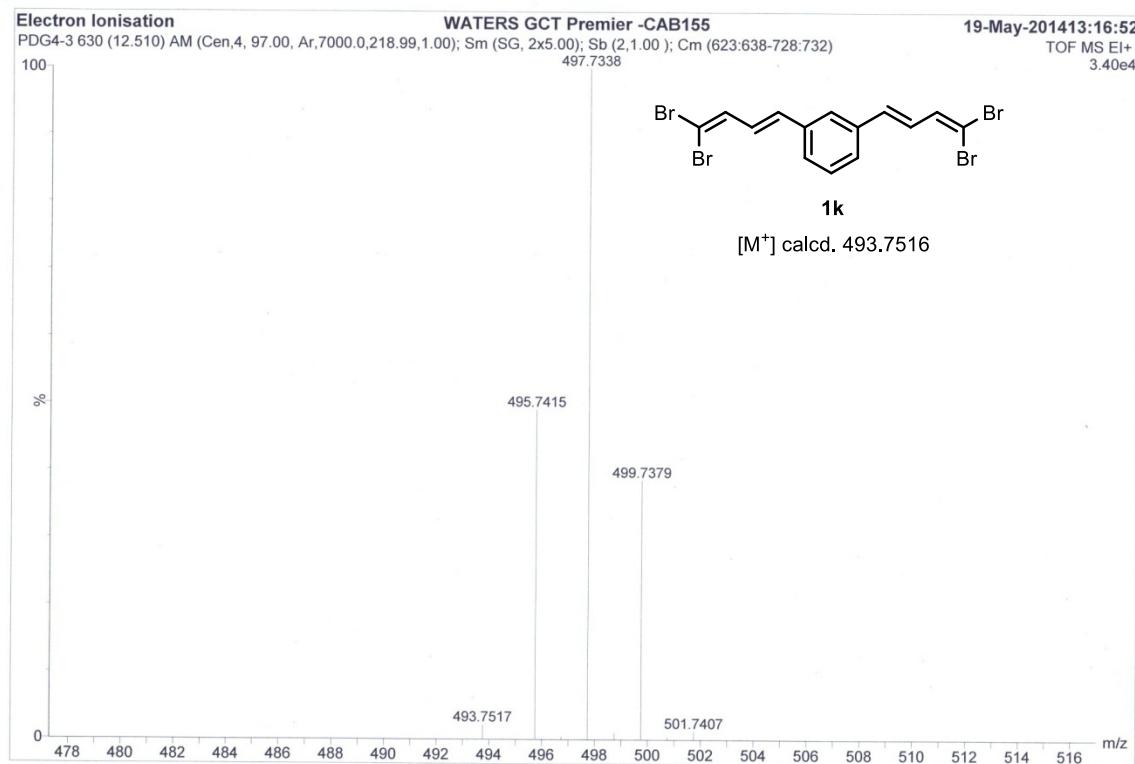
EI (HRMS) spectrum of (*E*)-2-(4,4-dibromobuta-1,3-dienyl)thiophene (**1j**)



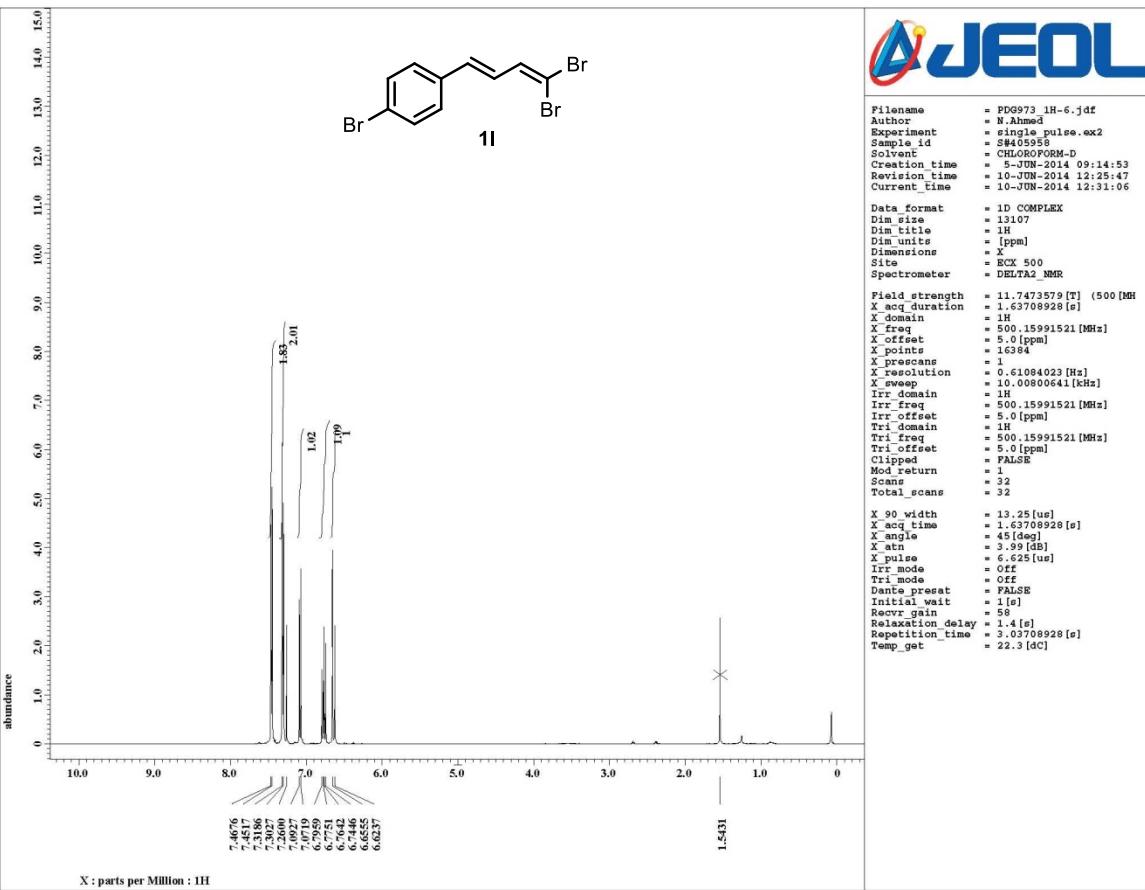
¹H NMR (500 MHz, CDCl₃) spectrum of 1,3-bis((E)-4,4-dibromobuta-1,3-dienyl)benzene (**1k**)



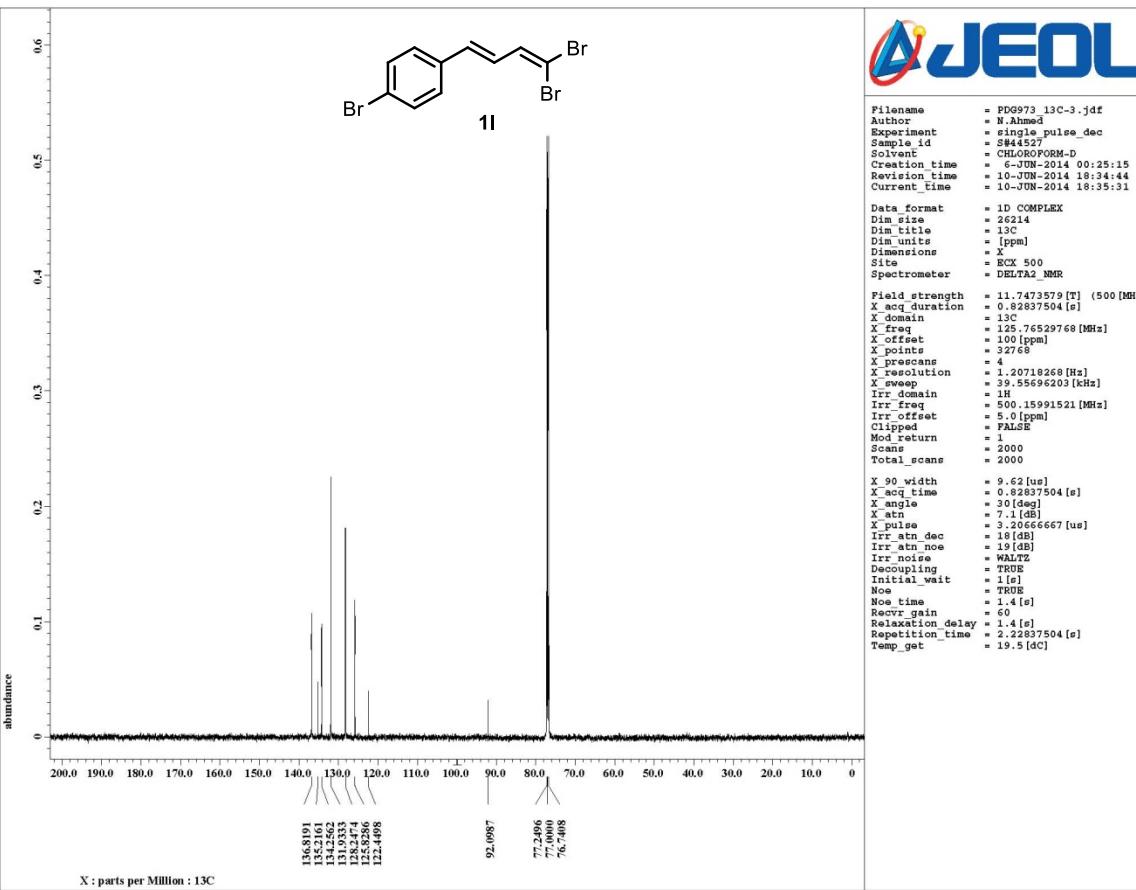
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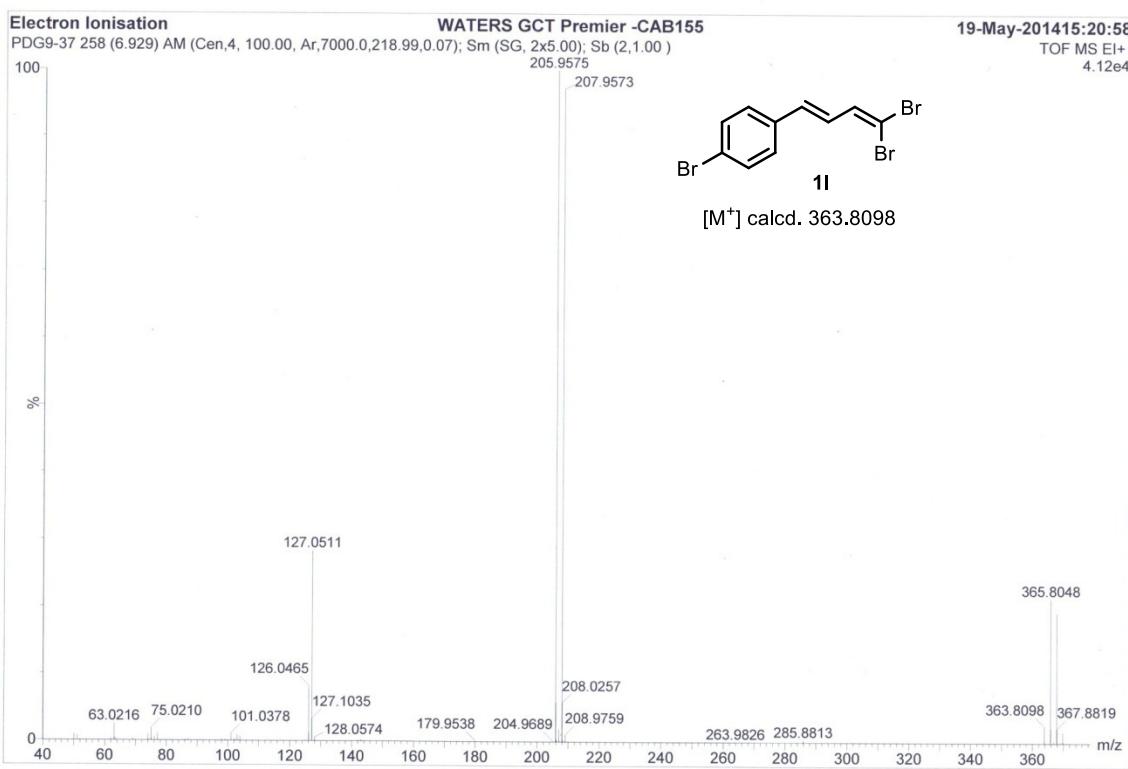
EI (HRMS) spectrum of 1,3-bis((E)-4,4-dibromobuta-1,3-dienyl)benzene (**1k**)



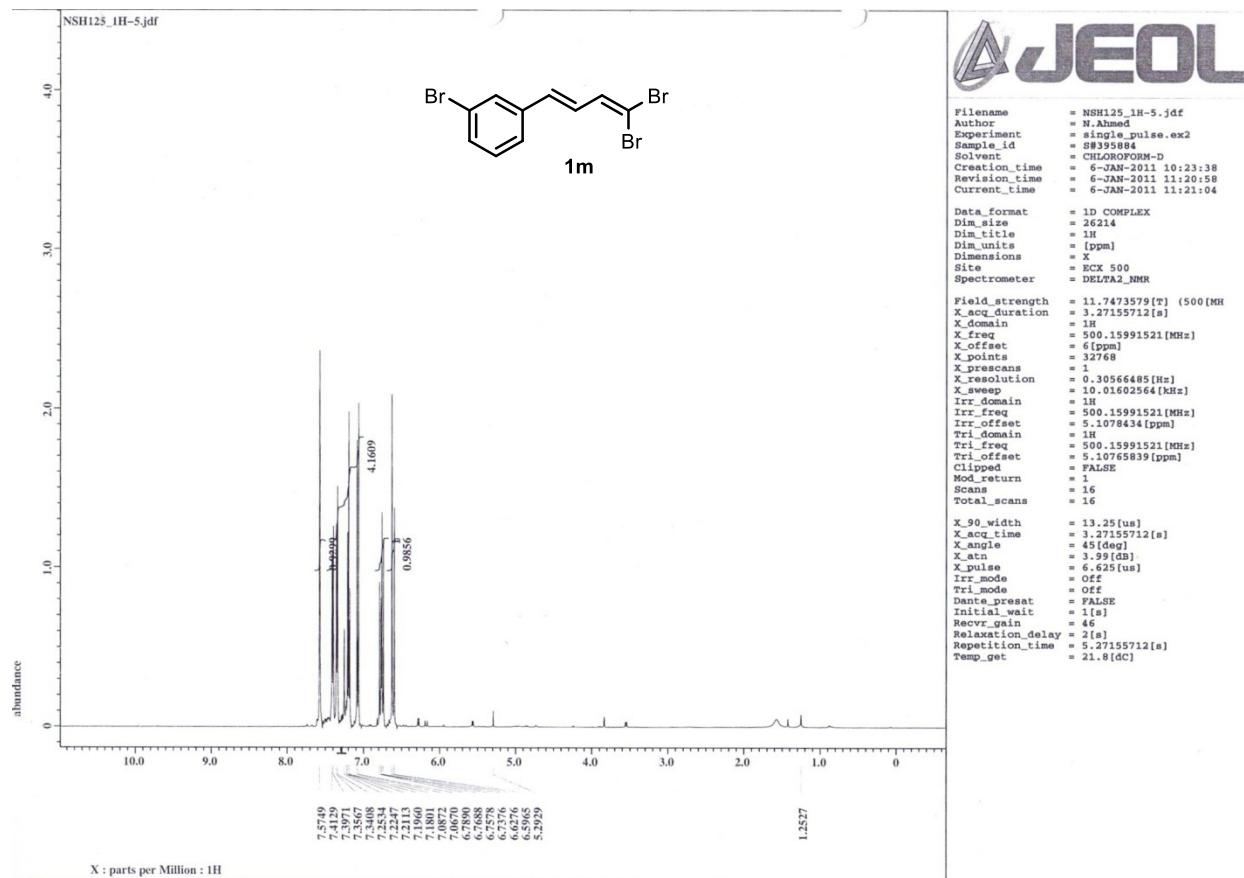
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4,4-dibromobuta-1,3-dienyl)benzene (**1l**)



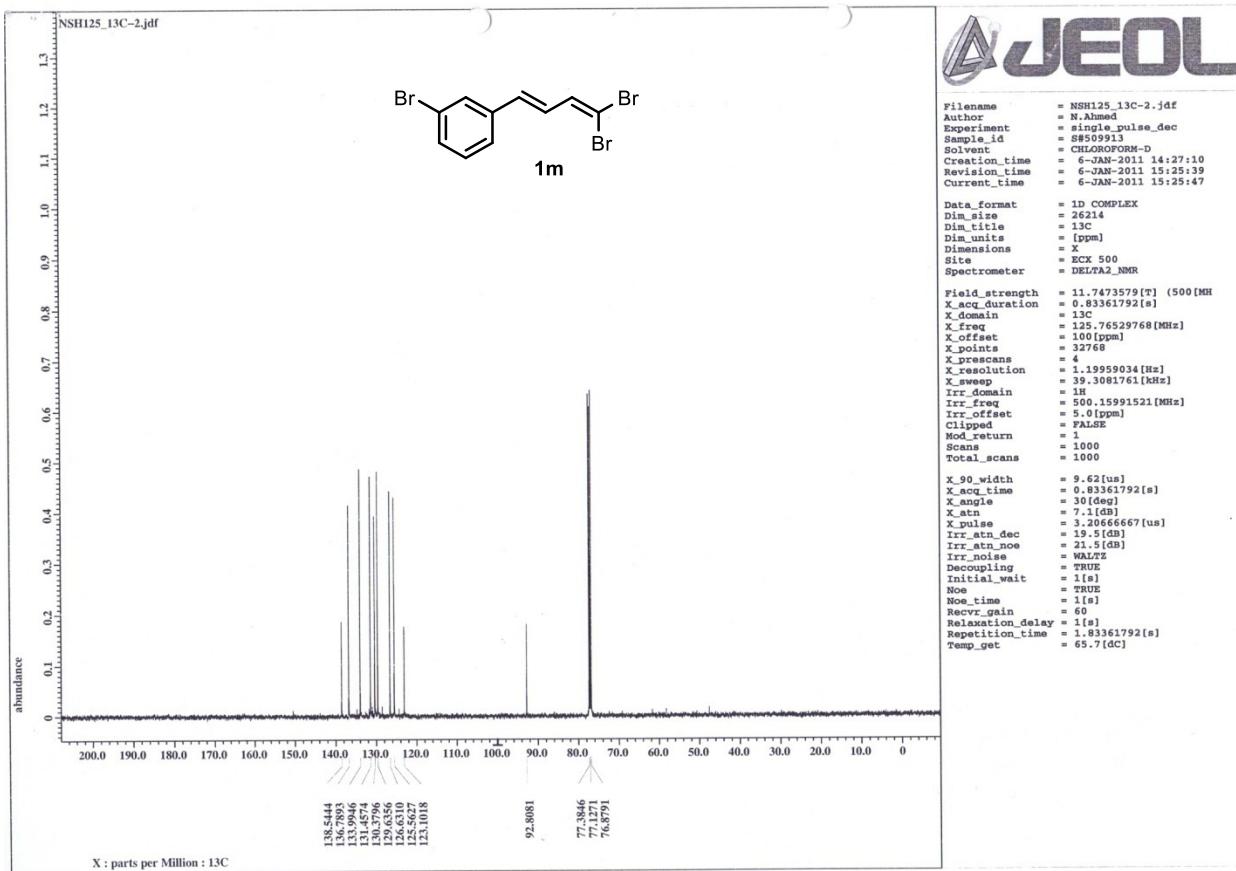
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-bromo-4-(4,4-dibromobuta-1,3-dienyl)benzene (**1I**)



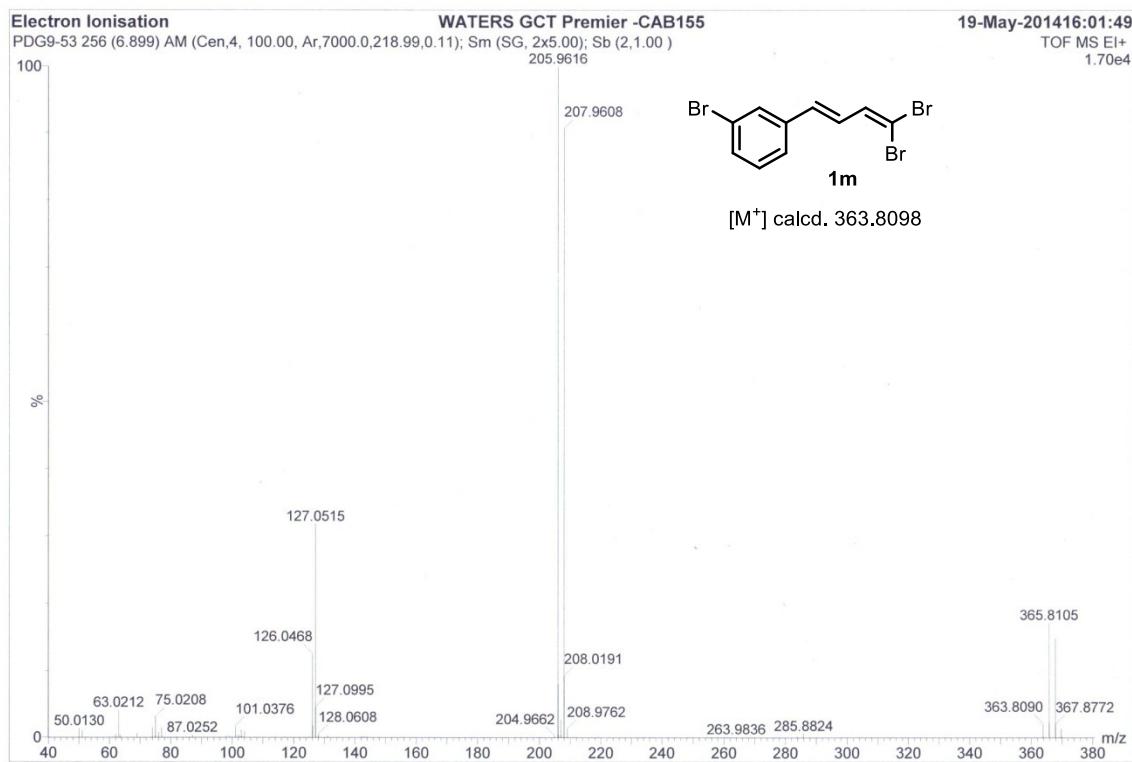
EI (HRMS) spectrum of (*E*)-1-bromo-4-(4,4-dibromobuta-1,3-dienyl)benzene (**1l**)



¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-bromo-3-(4,4-dibromobuta-1,3-dienyl)benzene (**1m**)

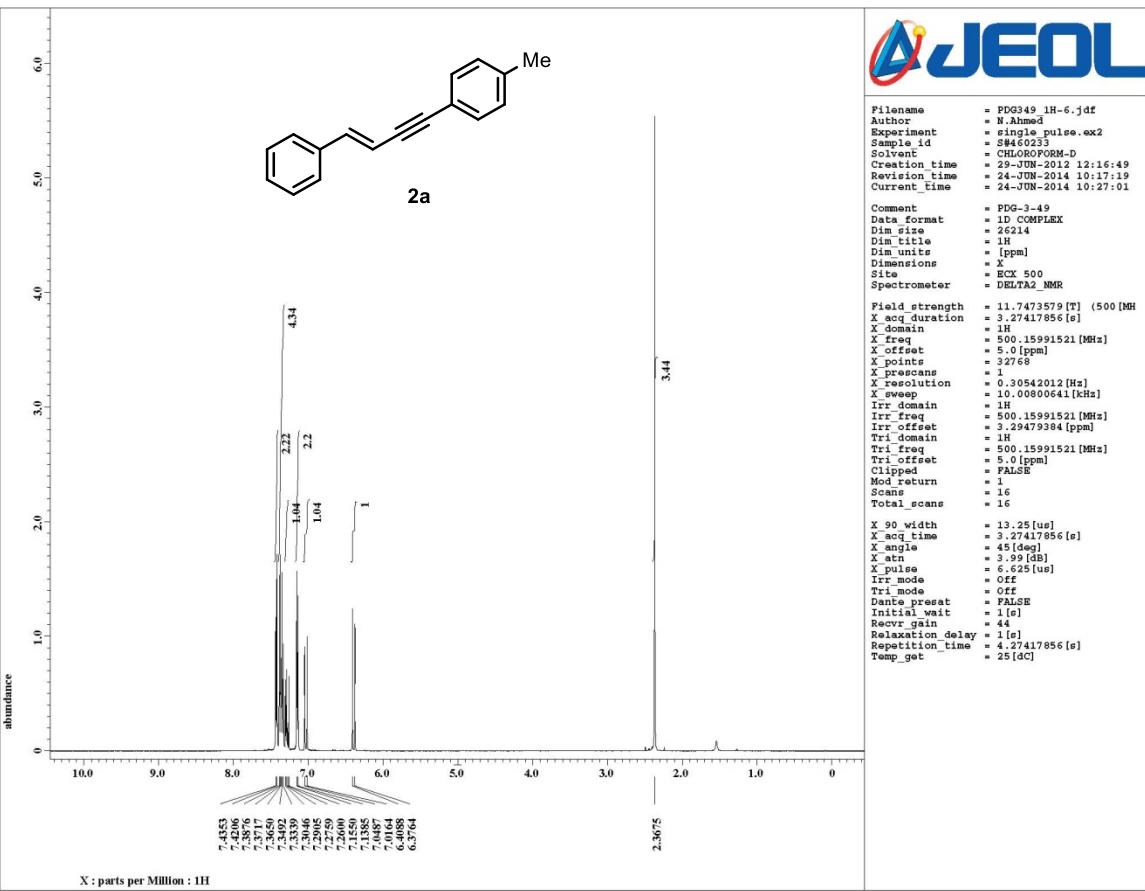


¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-bromo-3-(4,4-dibromobuta-1,3-dienyl)benzene (**1m**)

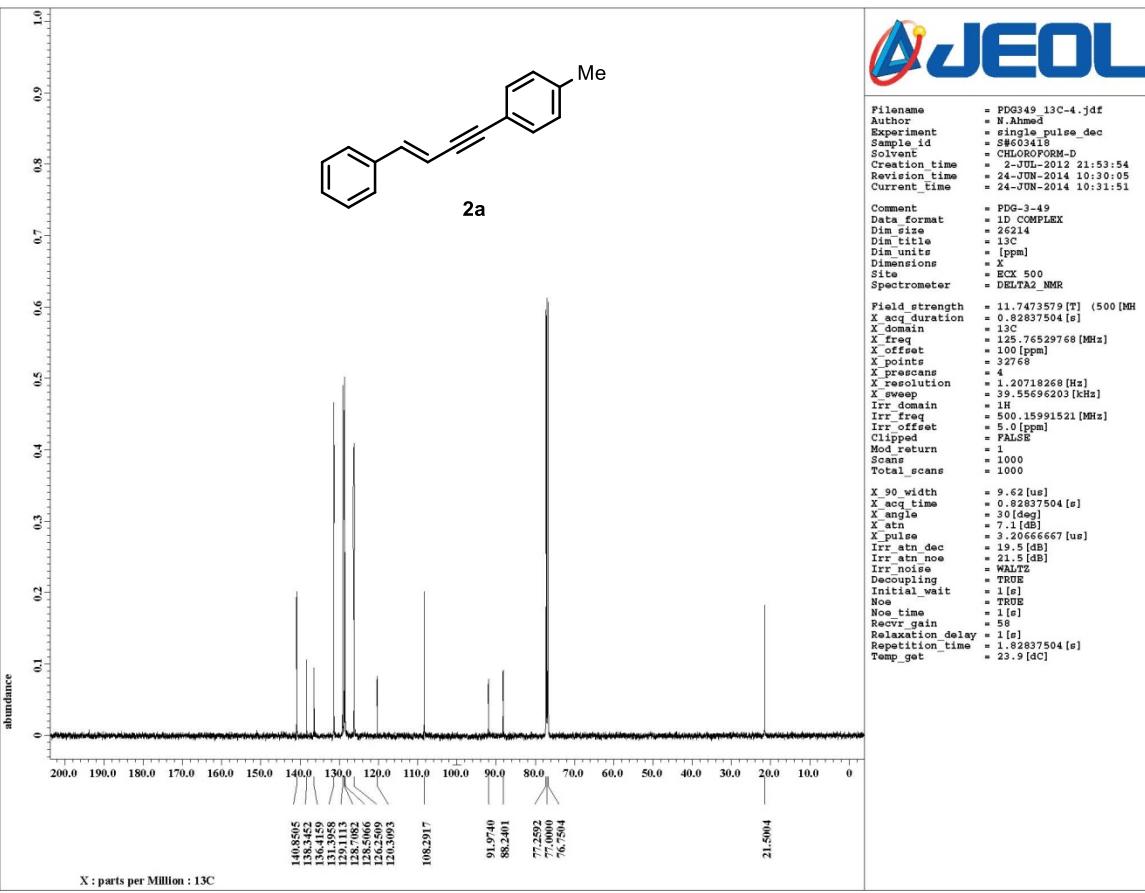


EI (HRMS) spectrum of (*E*)-1-bromo-3-(4,4-dibromobuta-1,3-dienyl)benzene (**1m**)

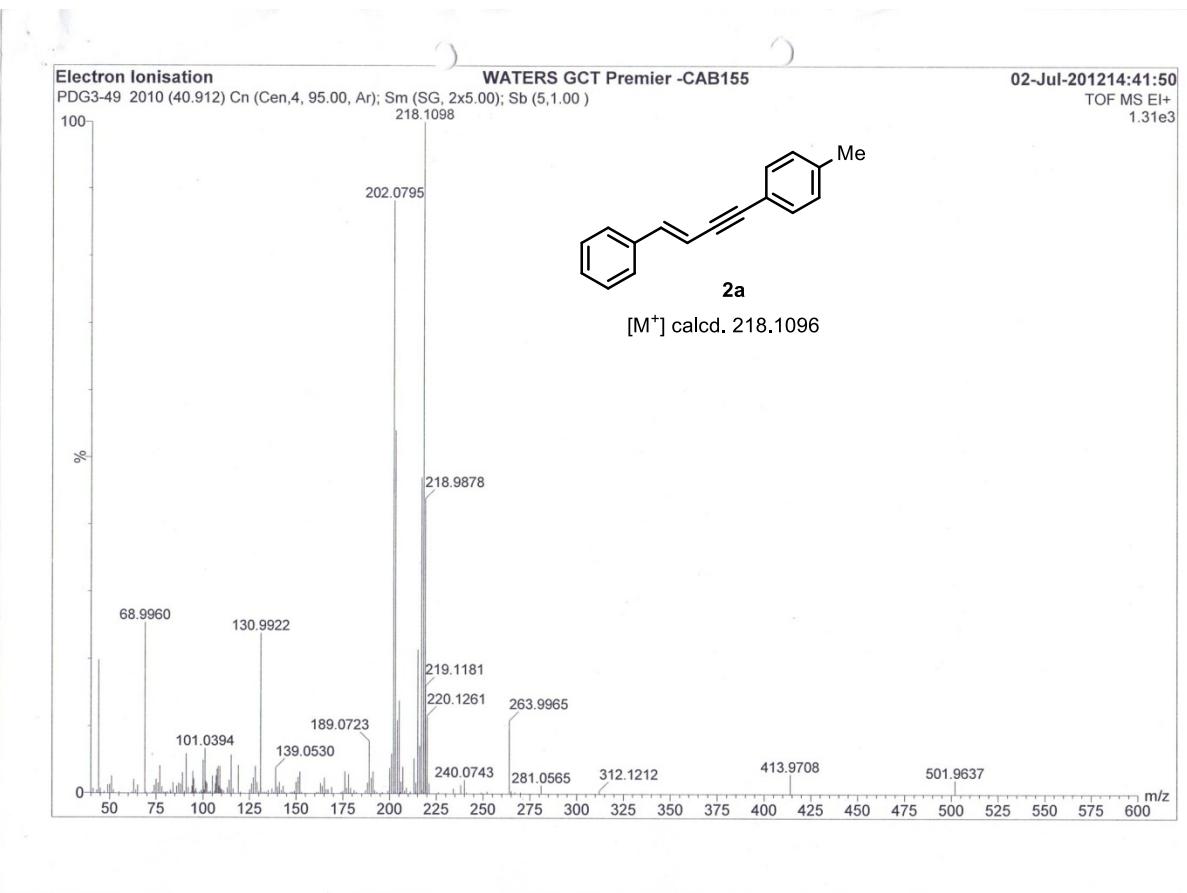
5. ^1H , ^{13}C and HRMS Spectras of groups of 1,3-Enynes (2-18):



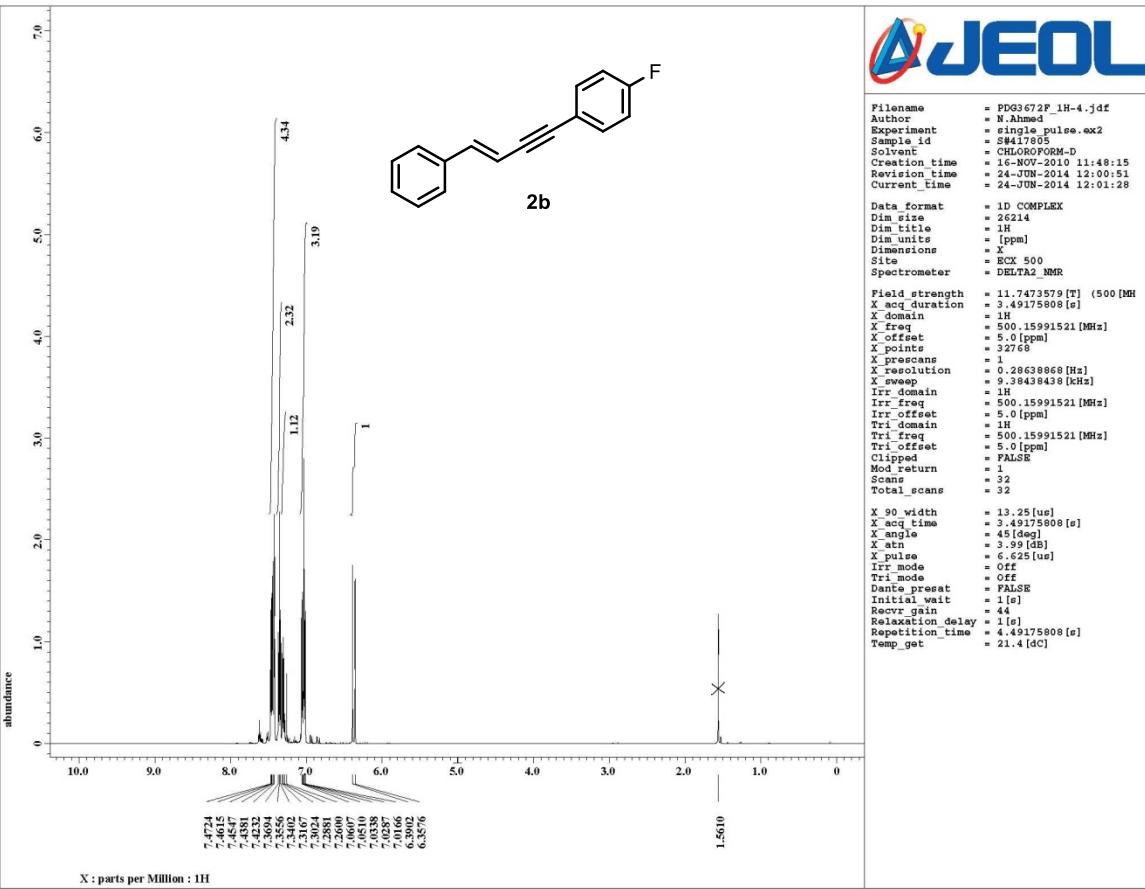
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-methyl-4-(4-phenylbut-3-en-1-ynyl)benzene (**2a**)

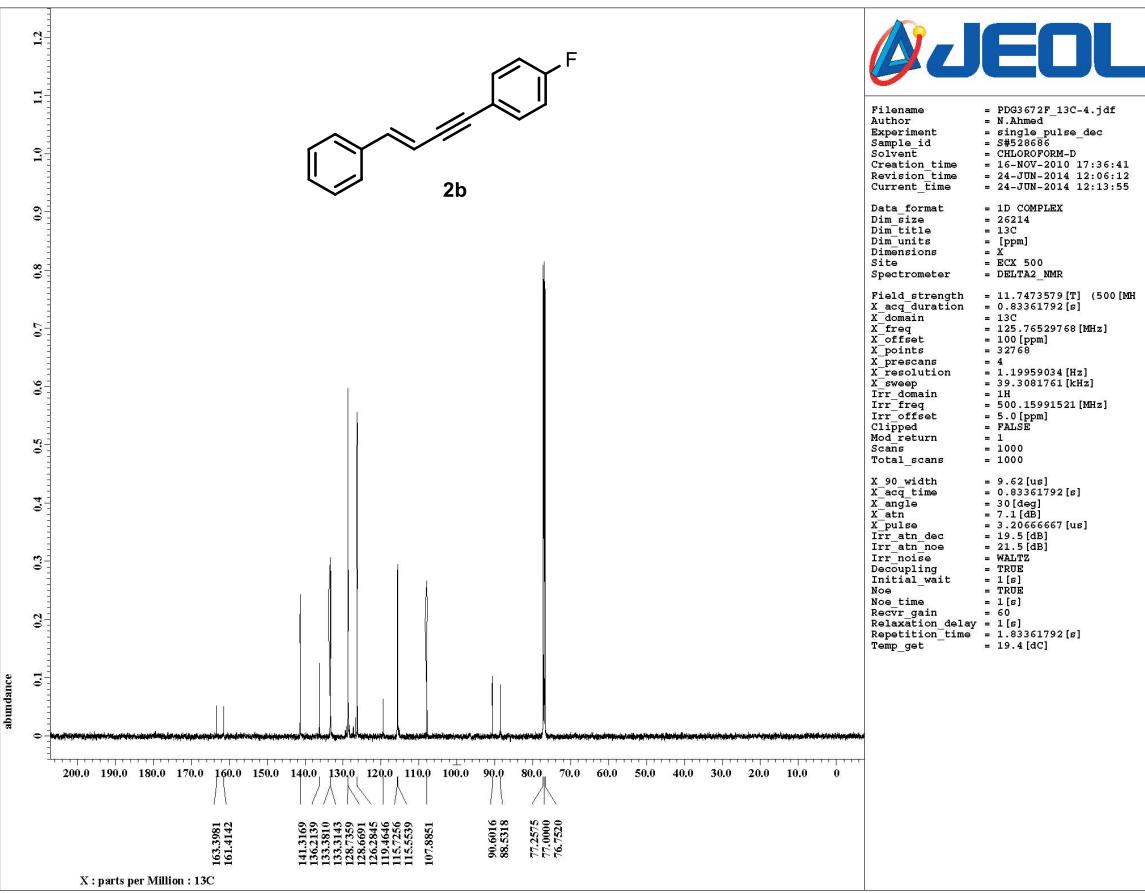


^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-1-methyl-4-(4-phenylbut-3-en-1-ynyl)benzene (**2a**)

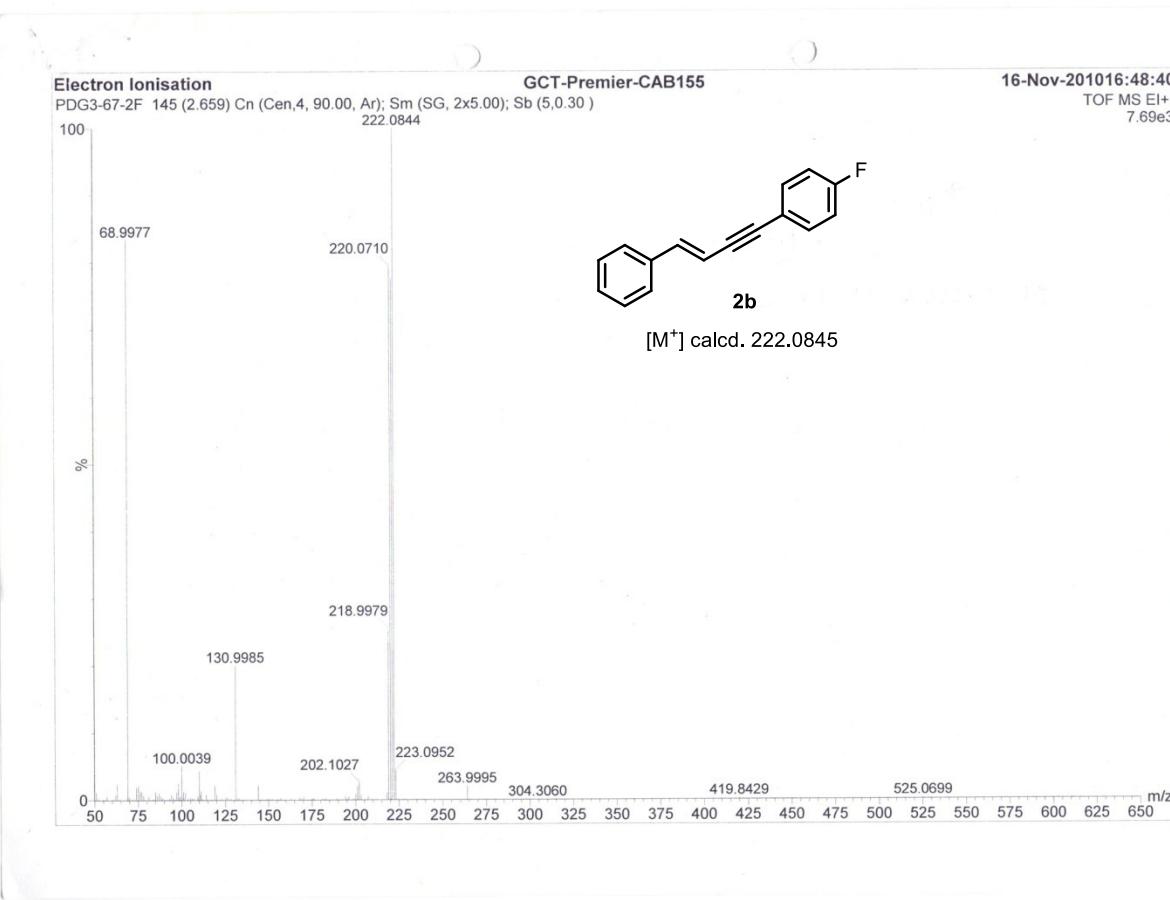


EI (HRMS) spectrum of (E)-1-methyl-4-(4-phenylbut-3-en-1-ynyl)benzene (**2a**)

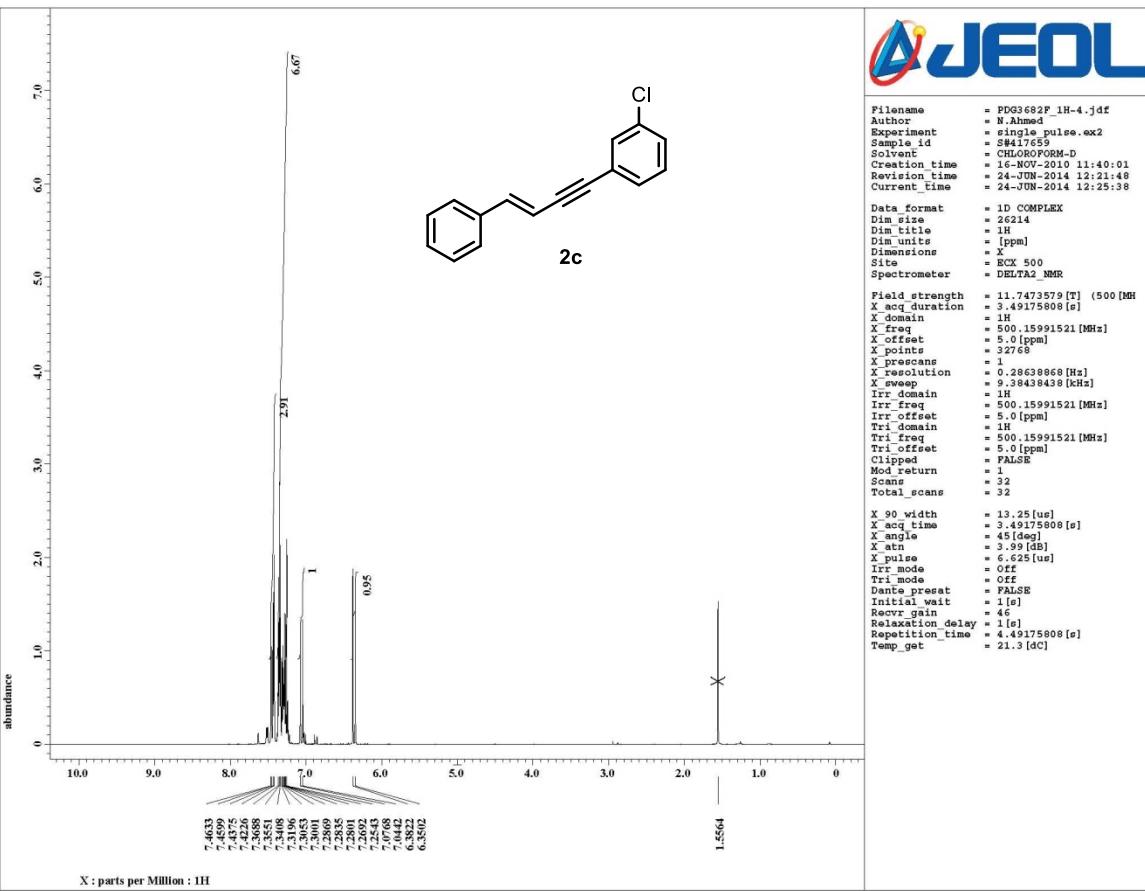




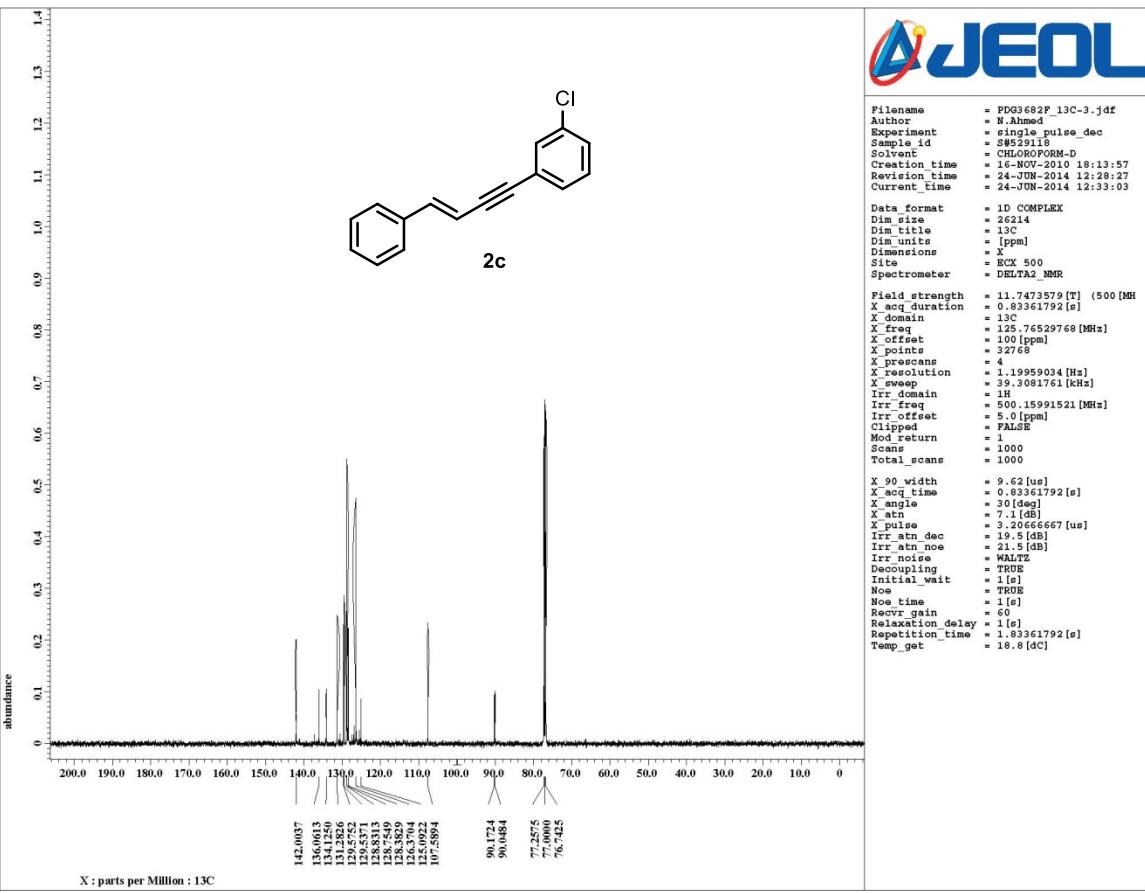
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-fluoro-4-(4-phenylbut-3-en-1-ynyl)benzene (**2b**)



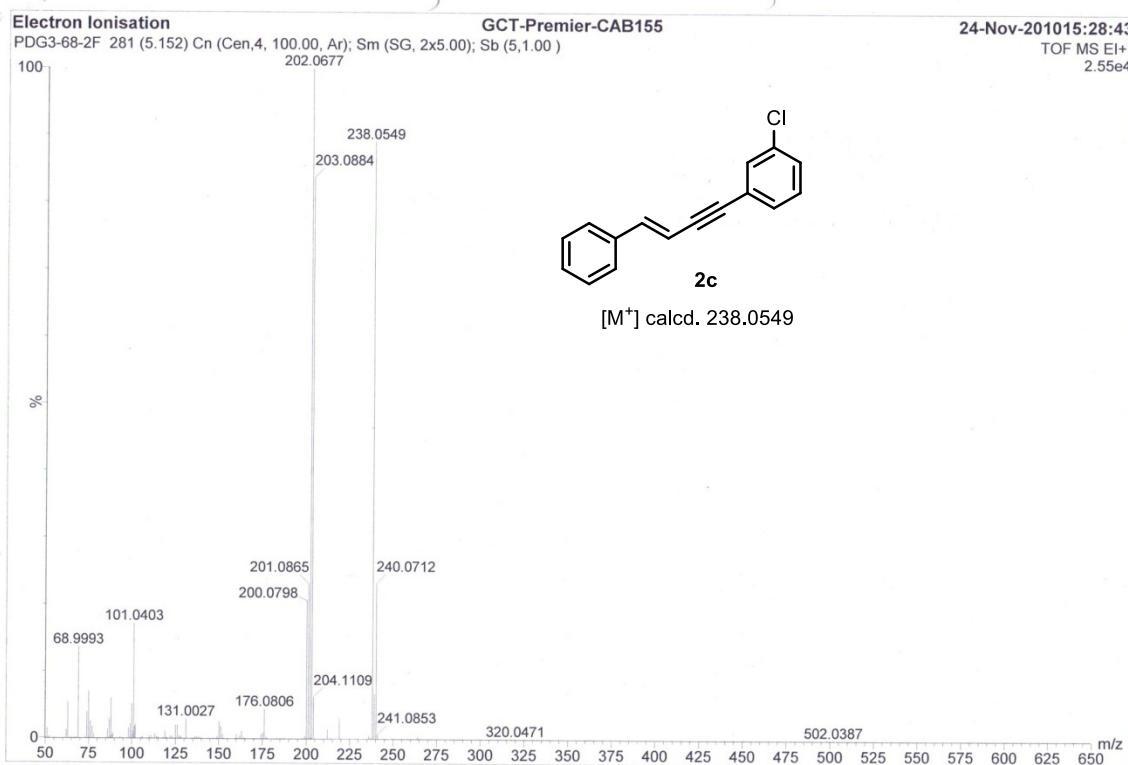
EI (HRMS) spectrum of (*E*)-1-fluoro-4-(4-phenylbut-3-en-1-ynyl)benzene (**2b**)



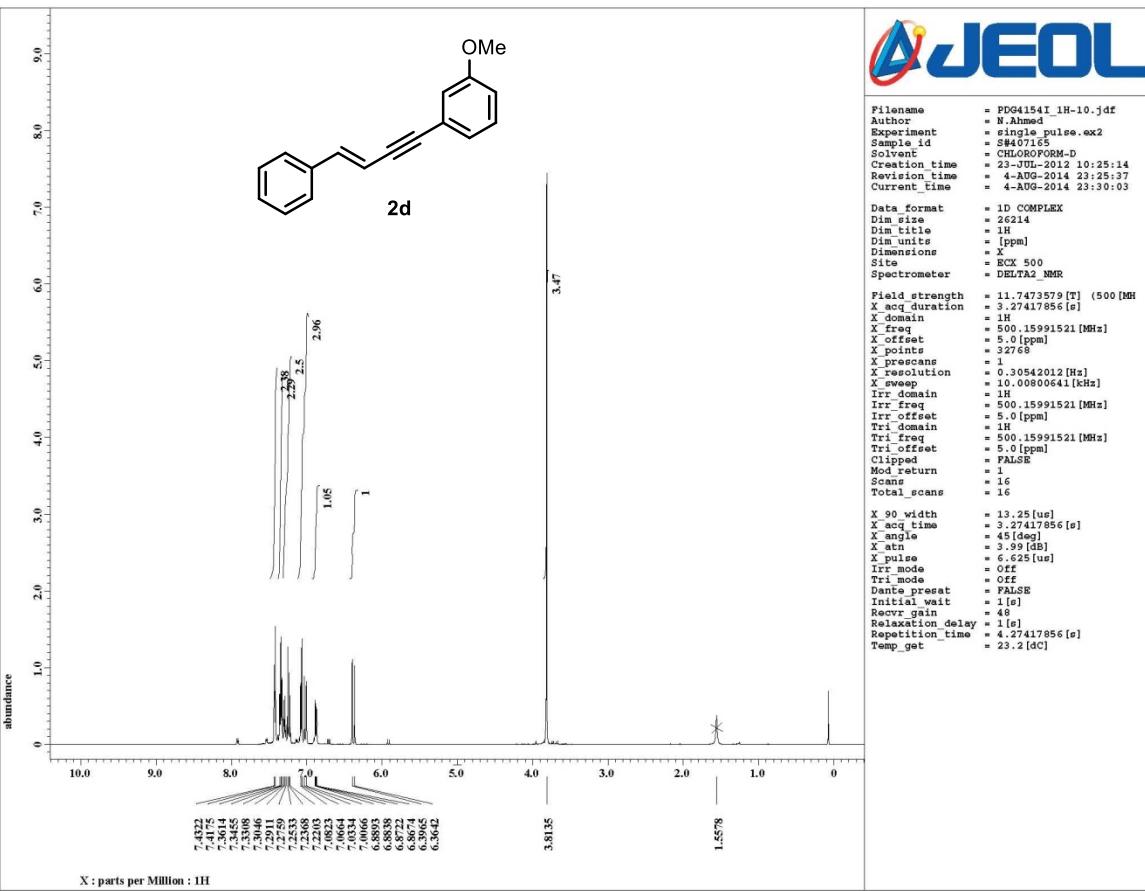
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-chloro-3-(4-phenylbut-3-en-1-ynyl)benzene (**2c**)



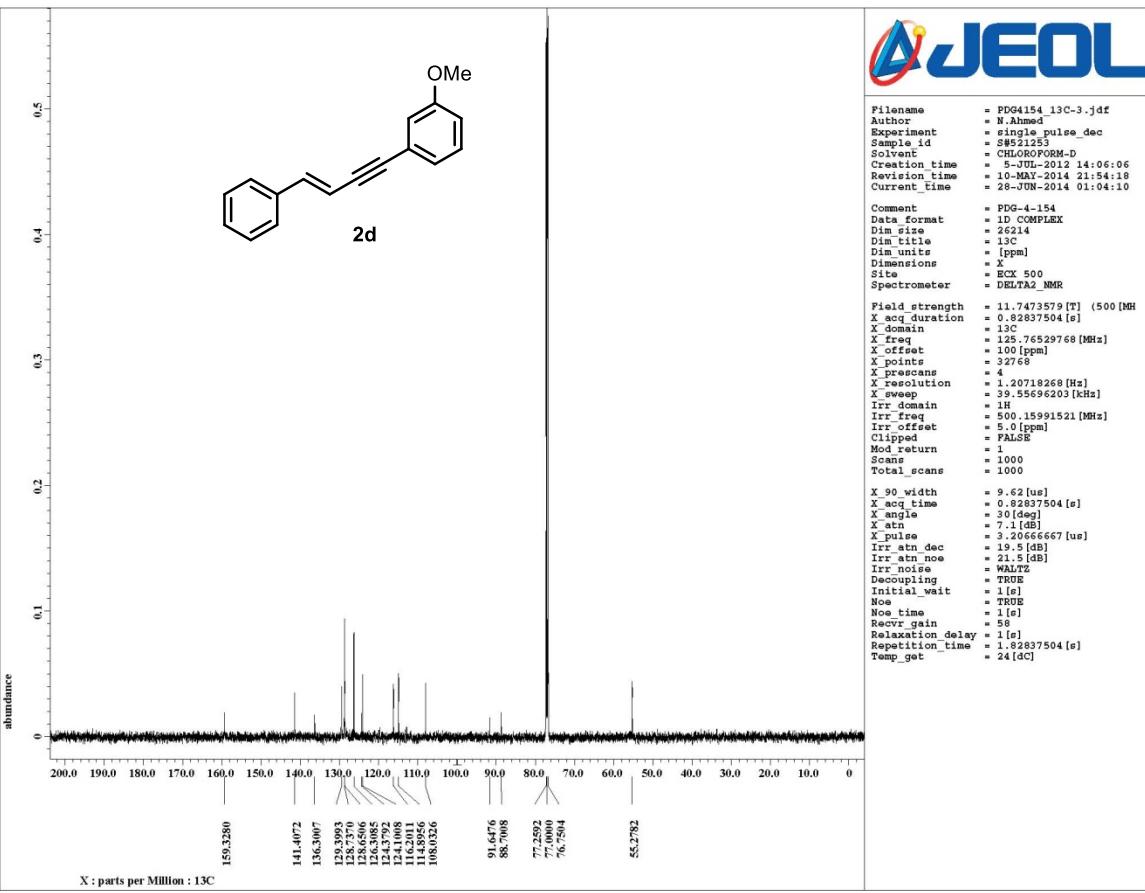
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-chloro-3-(4-phenylbut-3-en-1-ynyl)benzene (**2c**)



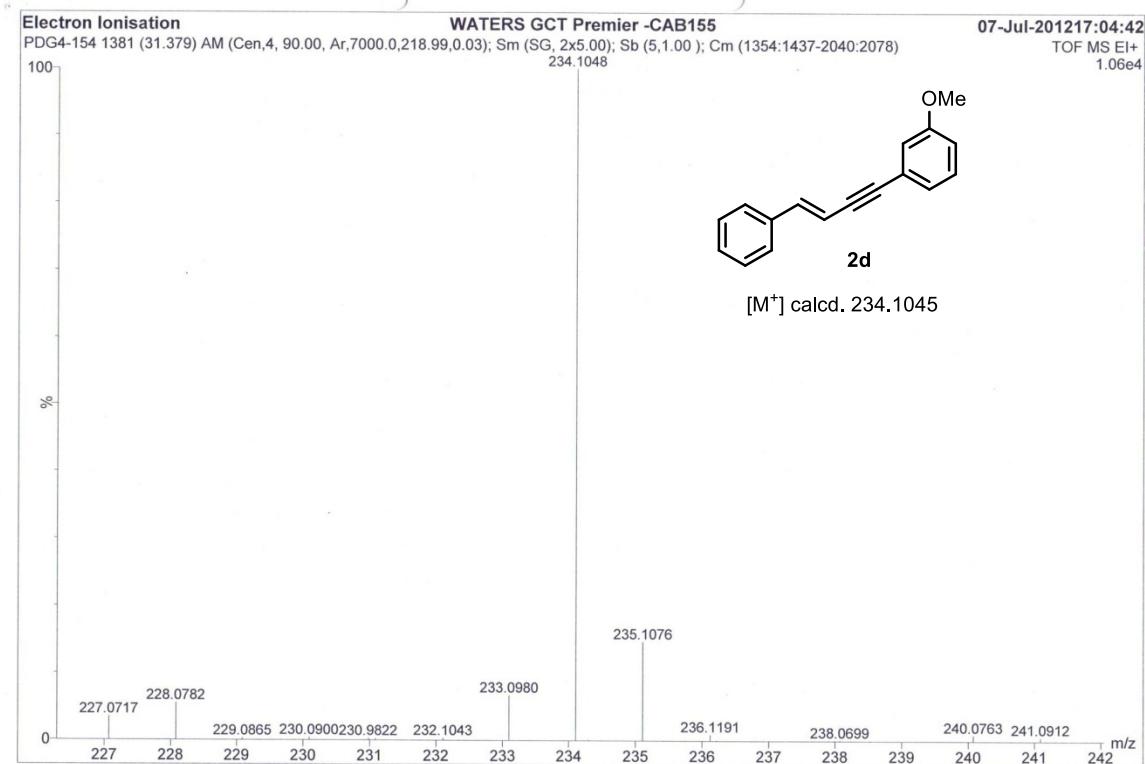
EI (HRMS) spectrum of (*E*)-1-chloro-3-(4-phenylbut-3-en-1-ynyl)benzene (**2c**)



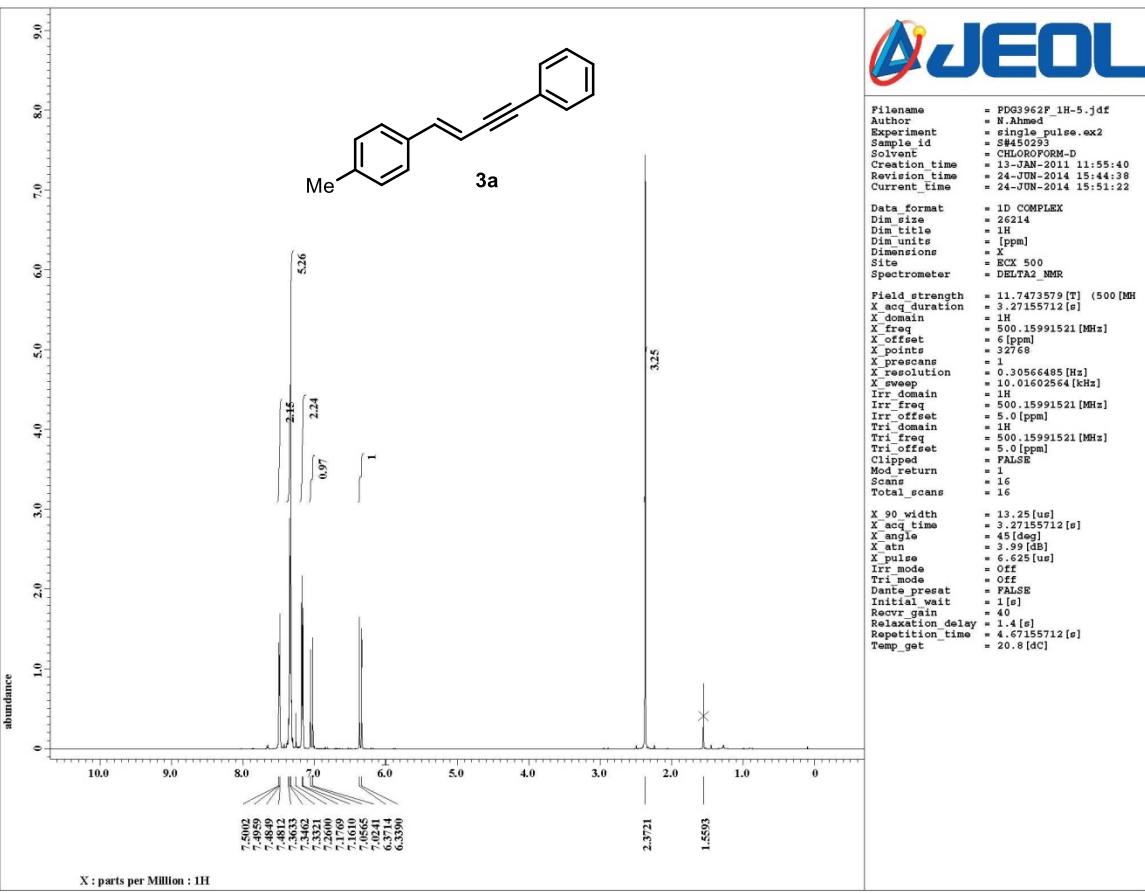
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-methoxy-3-(4-phenylbut-3-en-1-ynyl)benzene (**2d**)



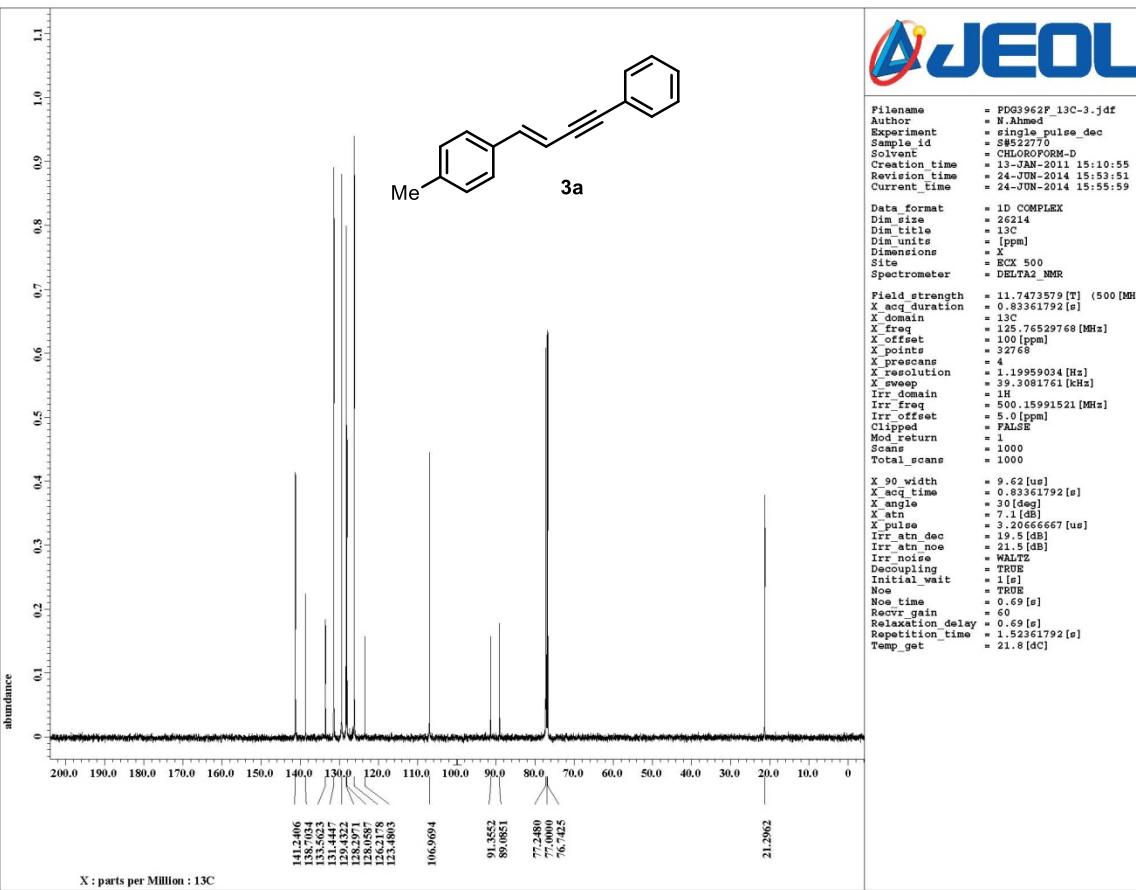
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-methoxy-3-(4-phenylbut-3-en-1-ynyl)benzene (**2d**)



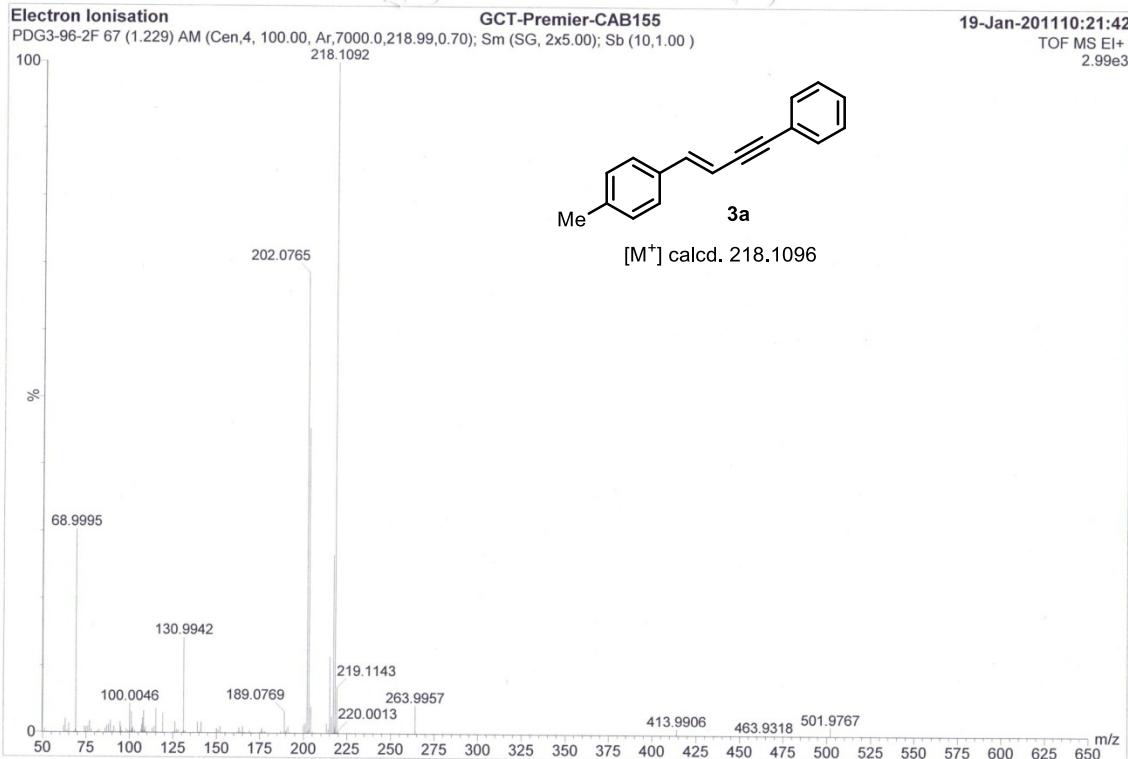
EI (HRMS) spectrum of (*E*)-1-methoxy-3-(4-phenylbut-3-en-1-ynyl)benzene (**2d**)



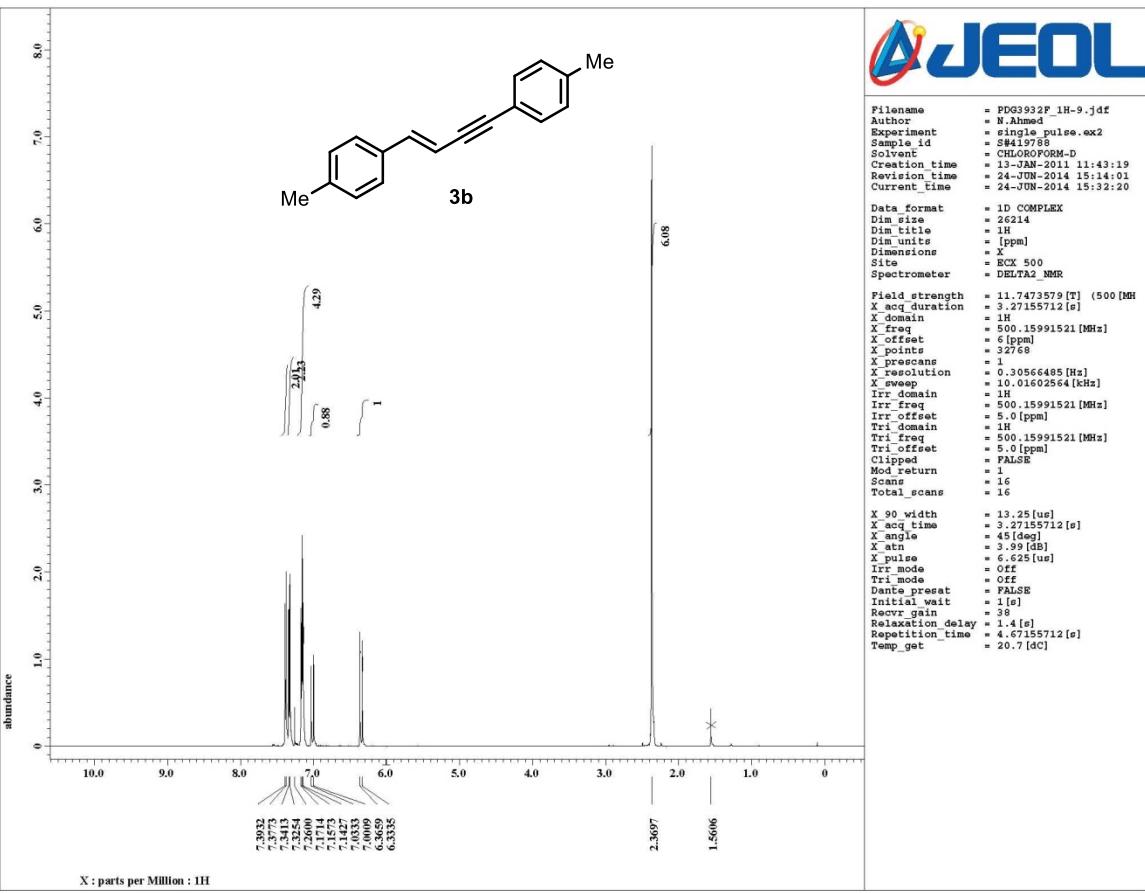
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-methyl-4-(4-phenylbut-1-en-3-ynyl)benzene (**3a**)



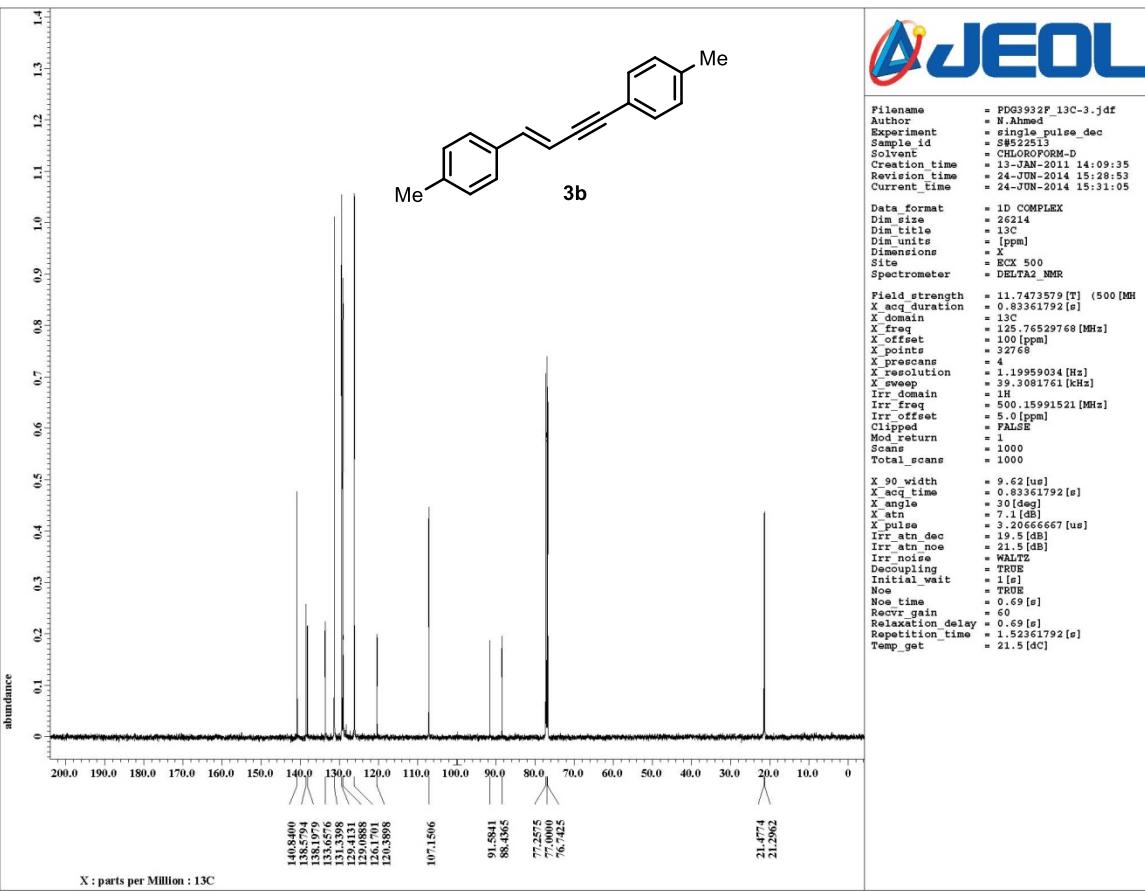
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-methyl-4-(4-phenylbut-1-en-3-ynyl)benzene (**3a**)



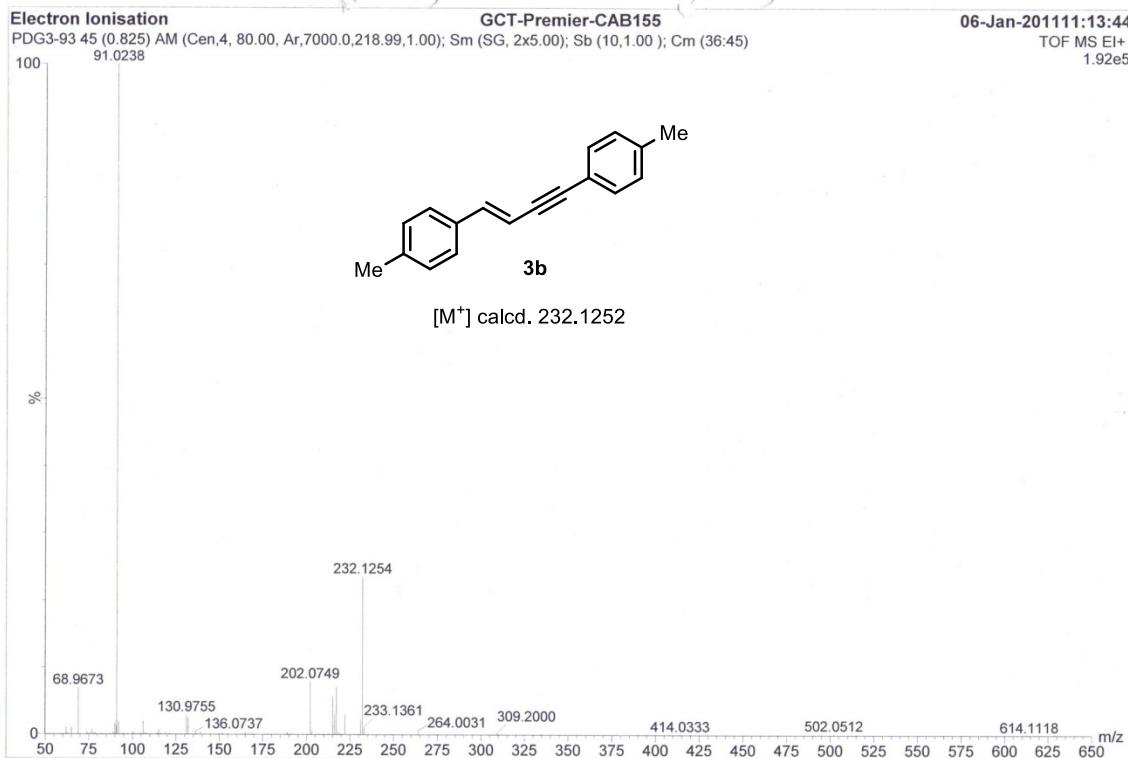
EI (HRMS) spectrum of (*E*)-1-methyl-4-(4-phenylbut-1-en-3-ynyl)benzene (**3a**)



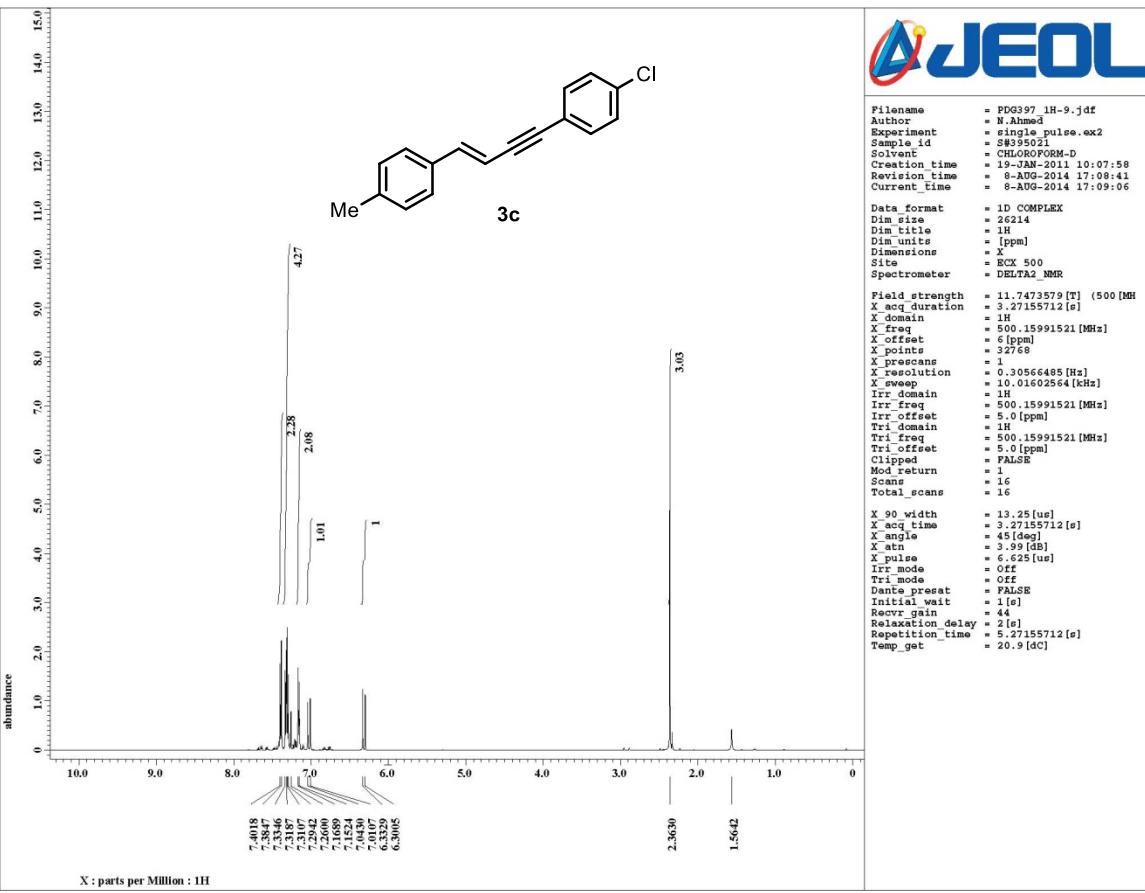
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(methylbenzene) (**3b**)



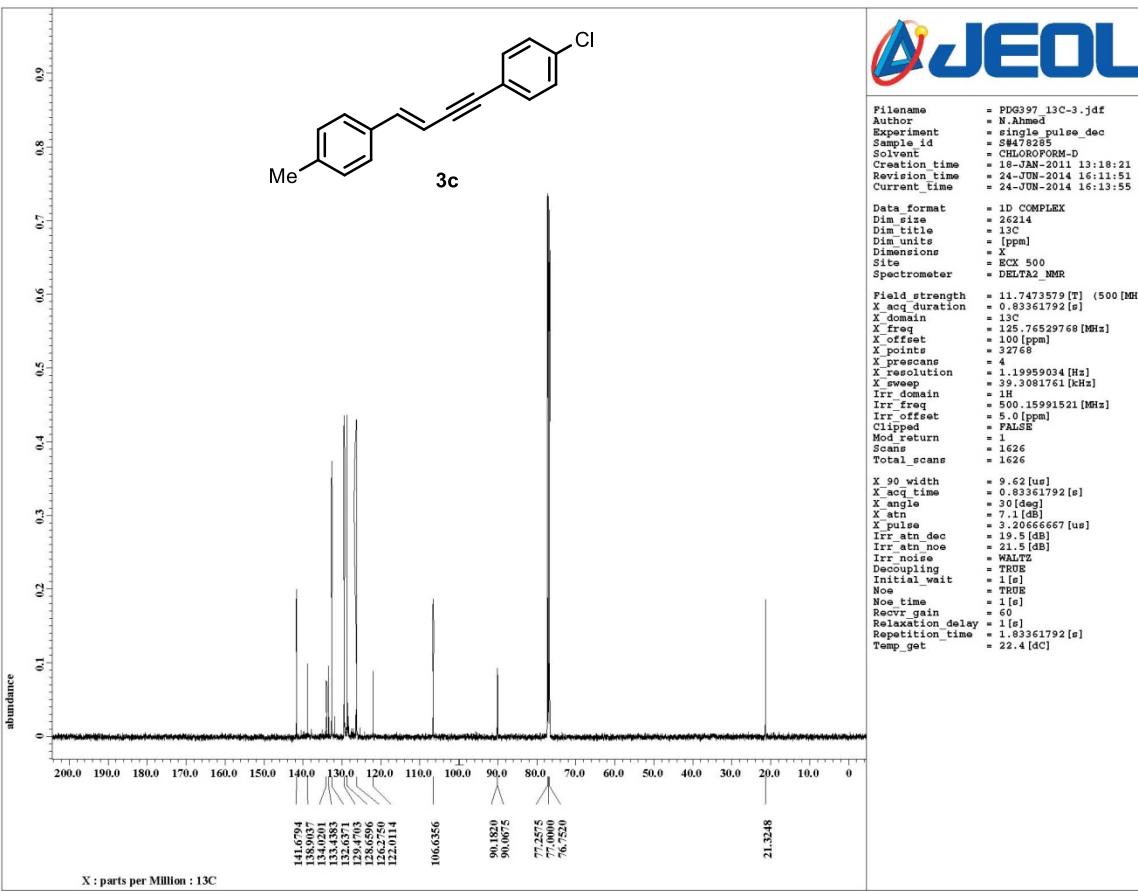
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(methylbenzene) (**3b**)



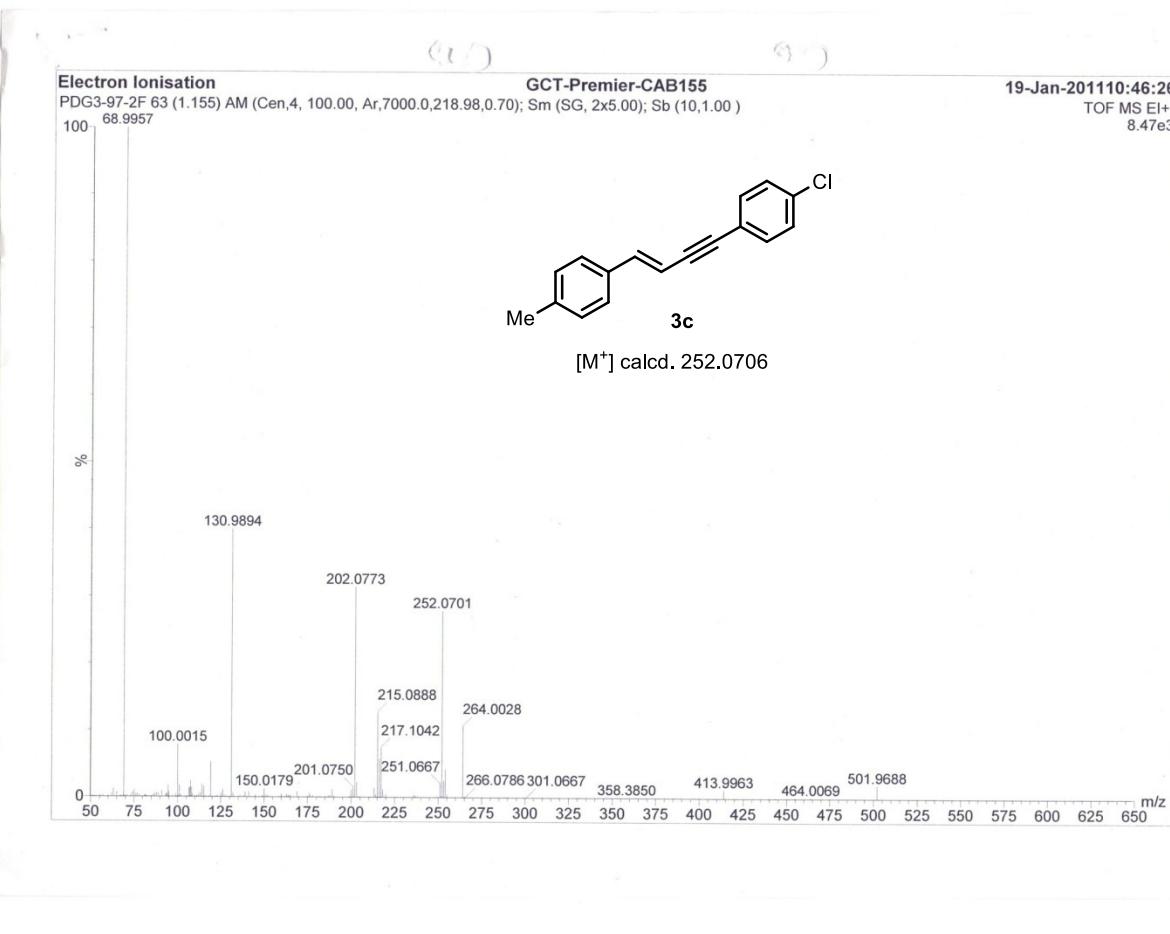
EI (HRMS) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(methylbenzene) (**3b**)



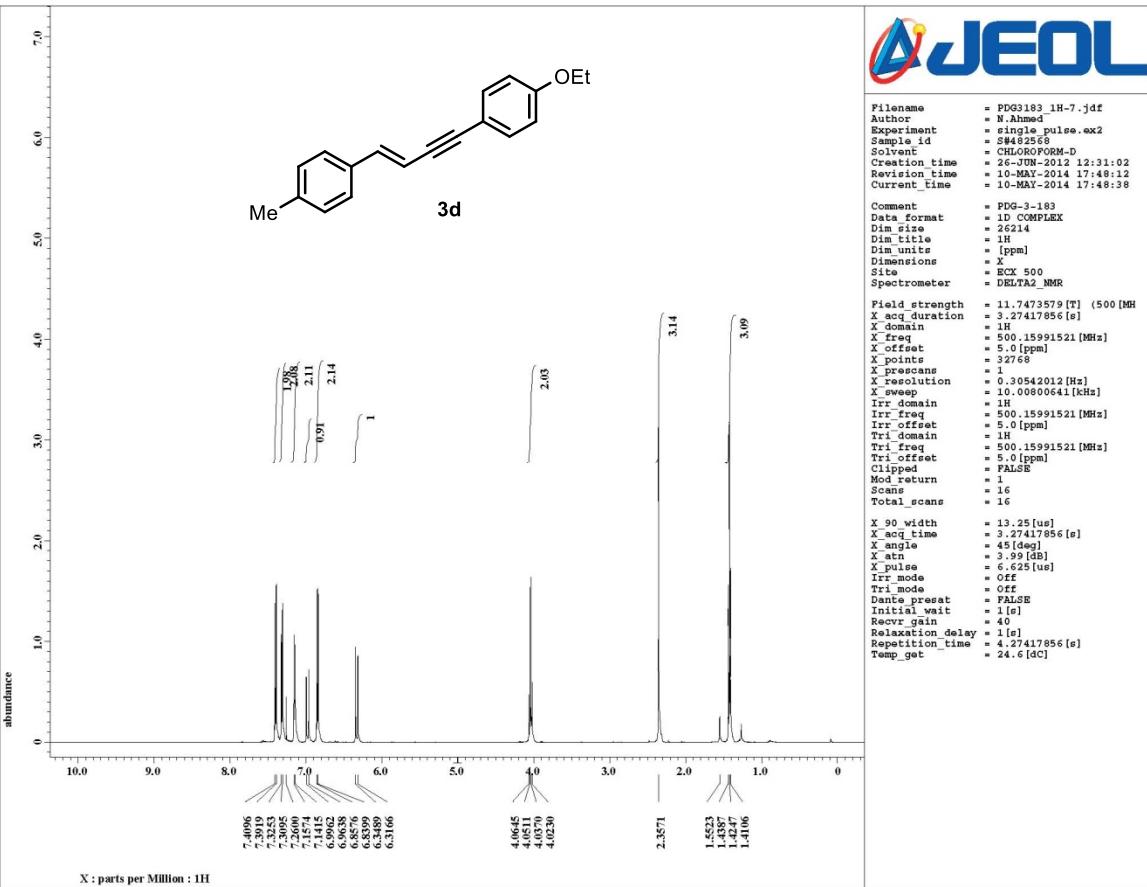
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-*p*-tolylbut-3-en-1-ynyl)benzene (**3c**)



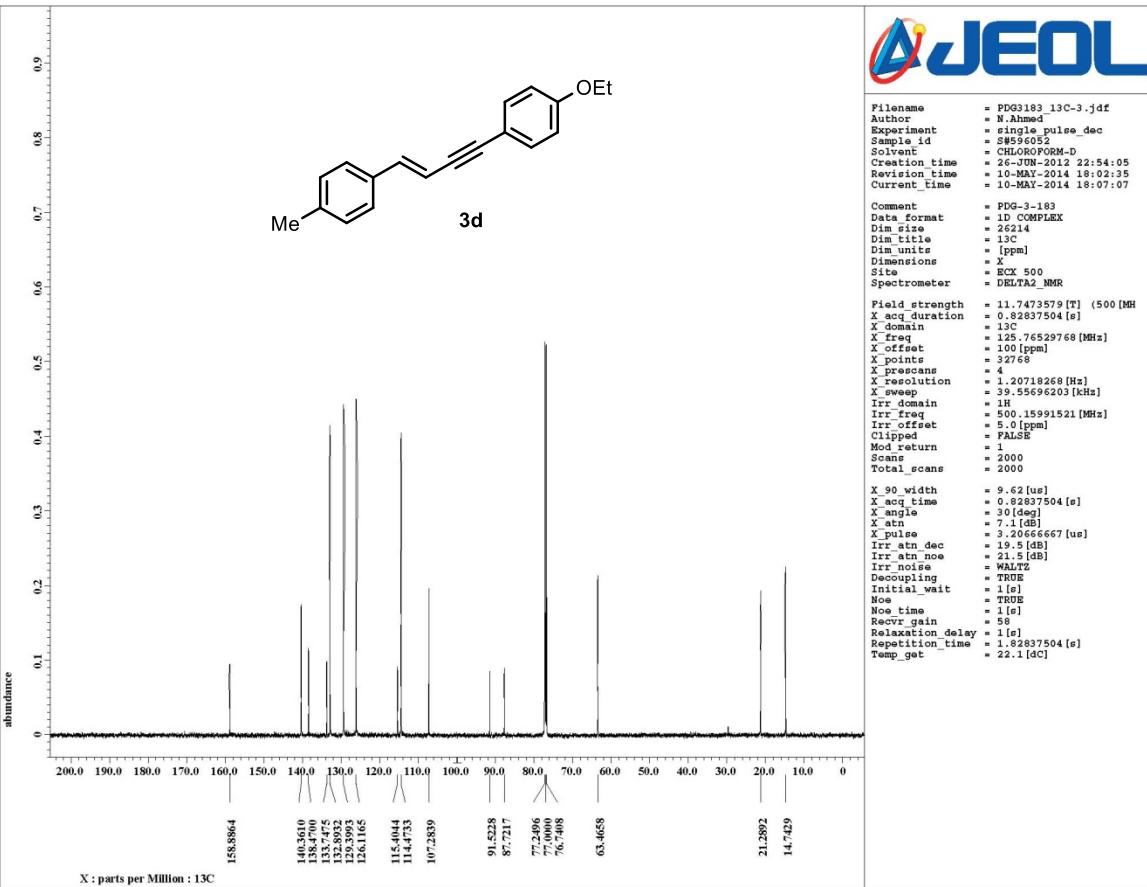
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-*p*-tolylbut-3-en-1-ynyl)benzene (**3c**)



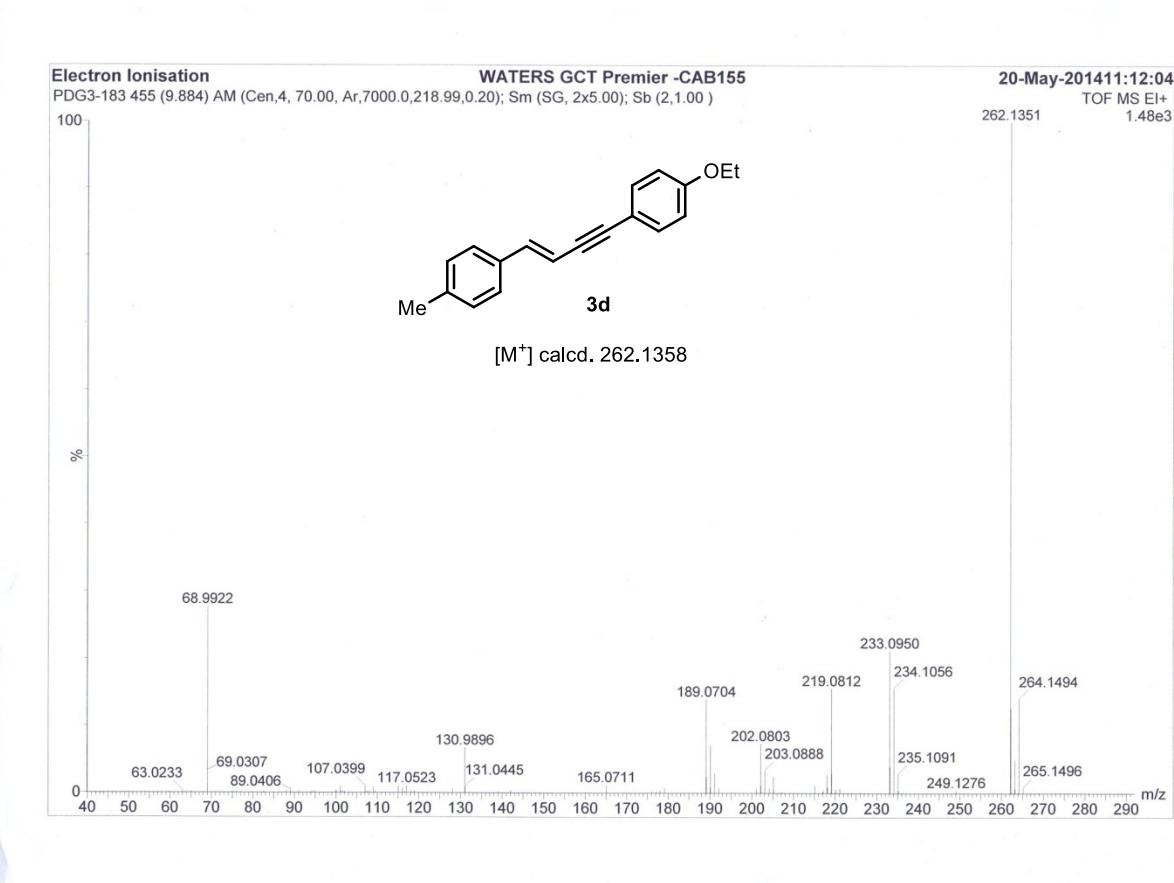
EI (HRMS) spectrum of (*E*)-1-chloro-4-(4-*p*-tolylbut-3-en-1-ynyl)benzene (**3c**)



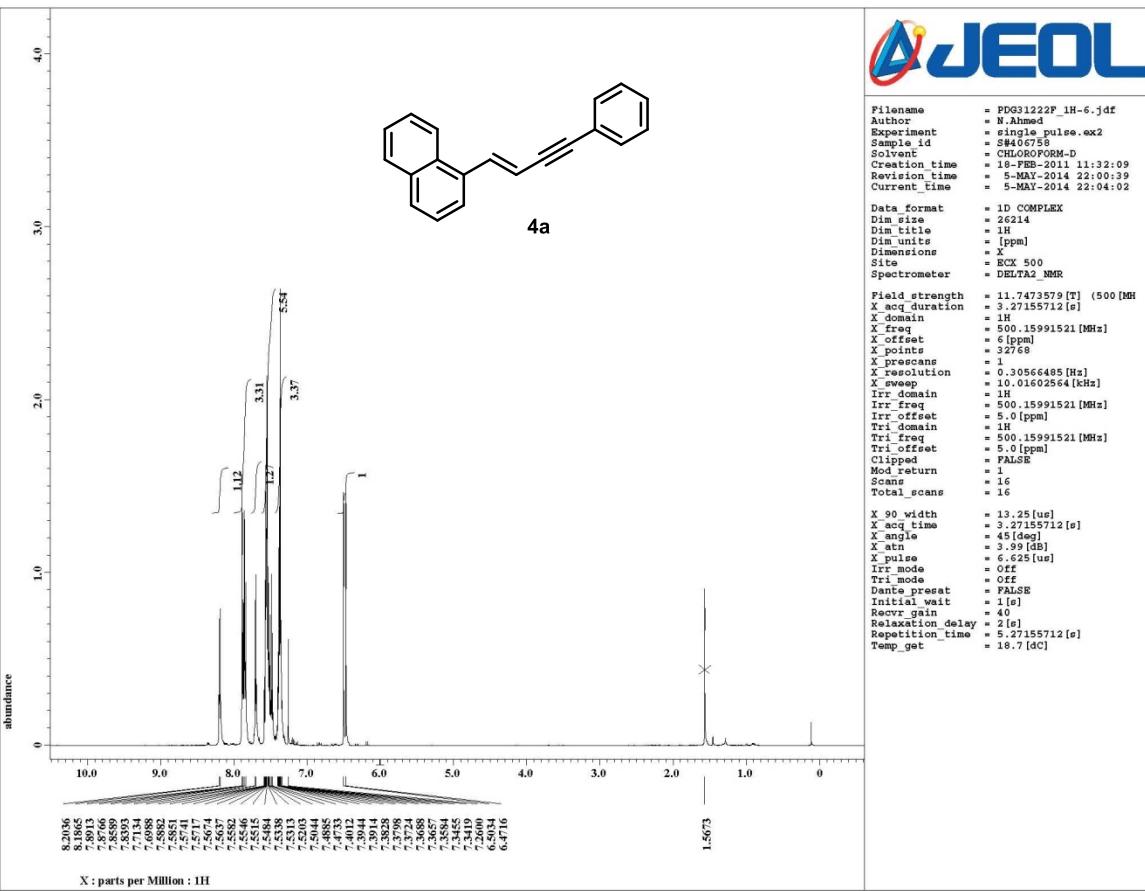
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-ethoxy-4-(4-p-tolylbut-3-en-1-ynyl)benzene (**3d**)



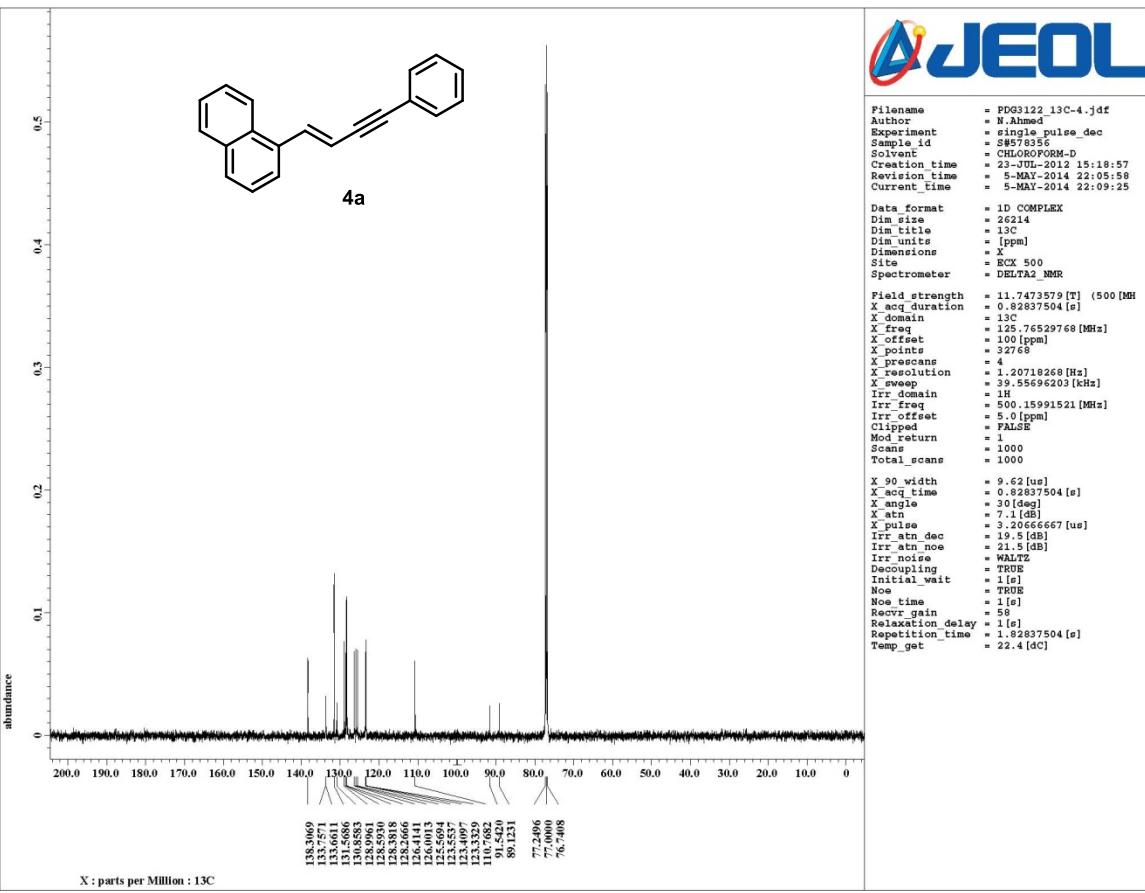
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-ethoxy-4-(4-*p*-tolylbut-3-en-1-ynyl)benzene (**3d**)



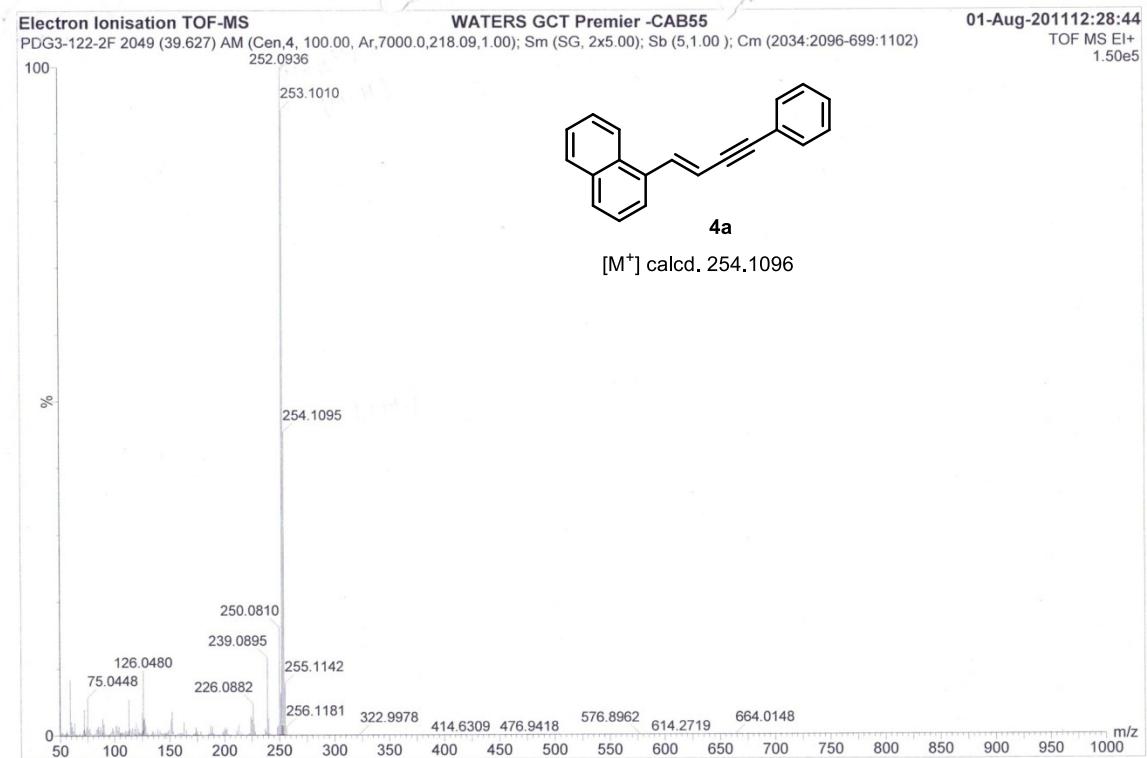
EI (HRMS) spectrum of (*E*)-1-ethoxy-4-(4-*p*-tolylbut-3-en-1-ynyl)benzene (**3d**)



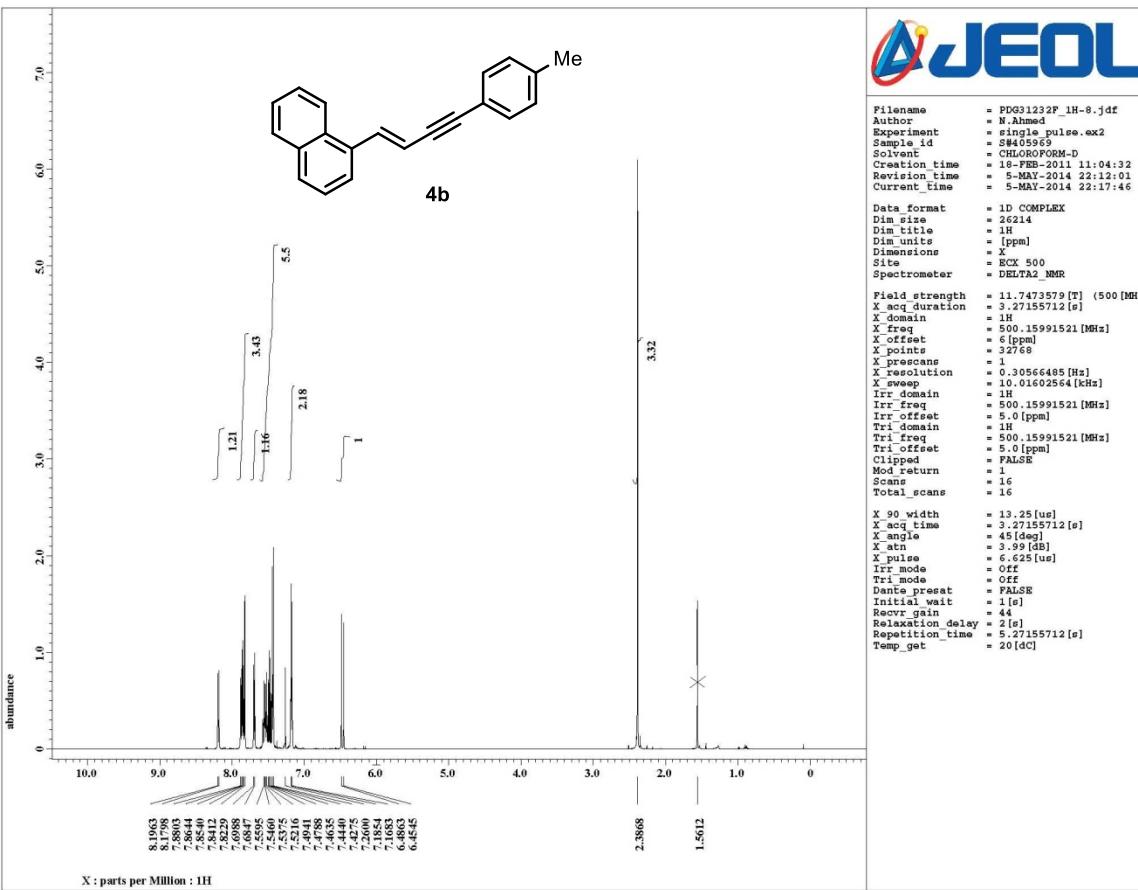
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-phenylbut-1-en-3-ynyl)naphthalene (**4a**)



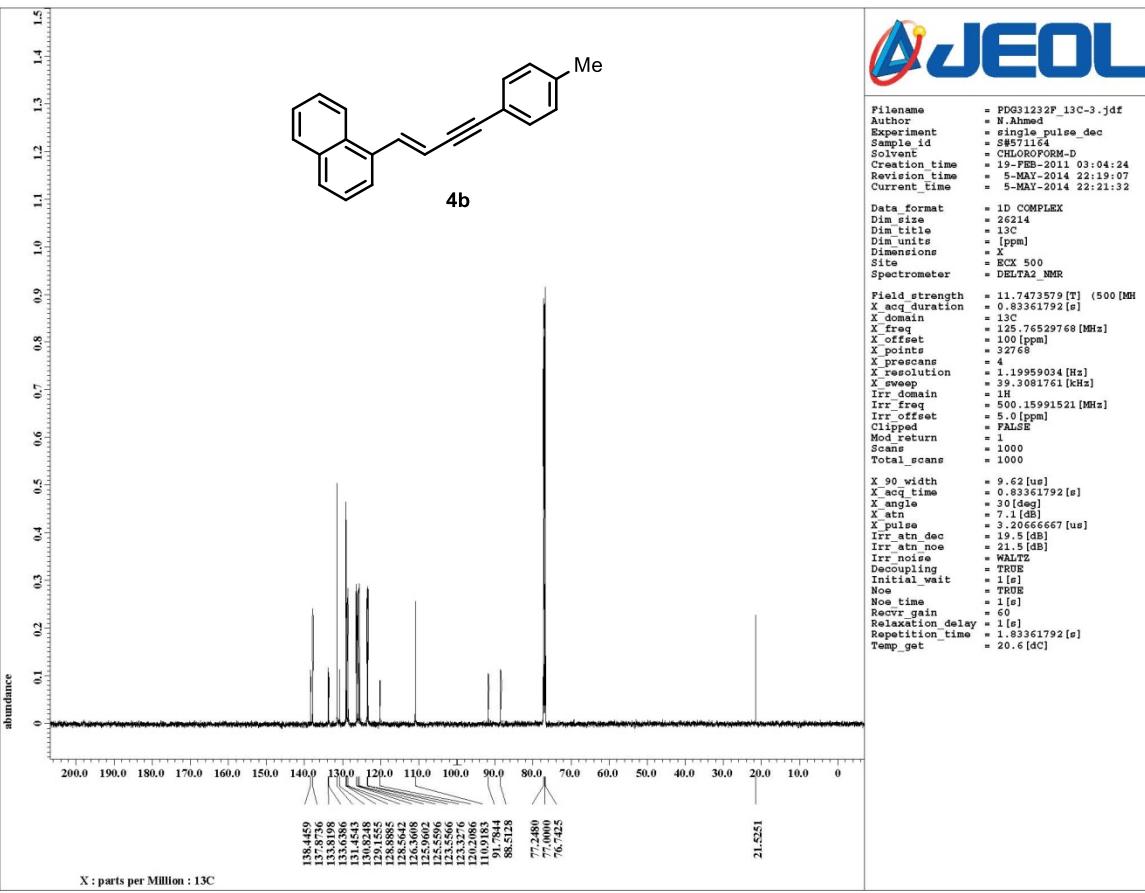
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4-phenylbut-1-en-3-ynyl)naphthalene (**4a**)



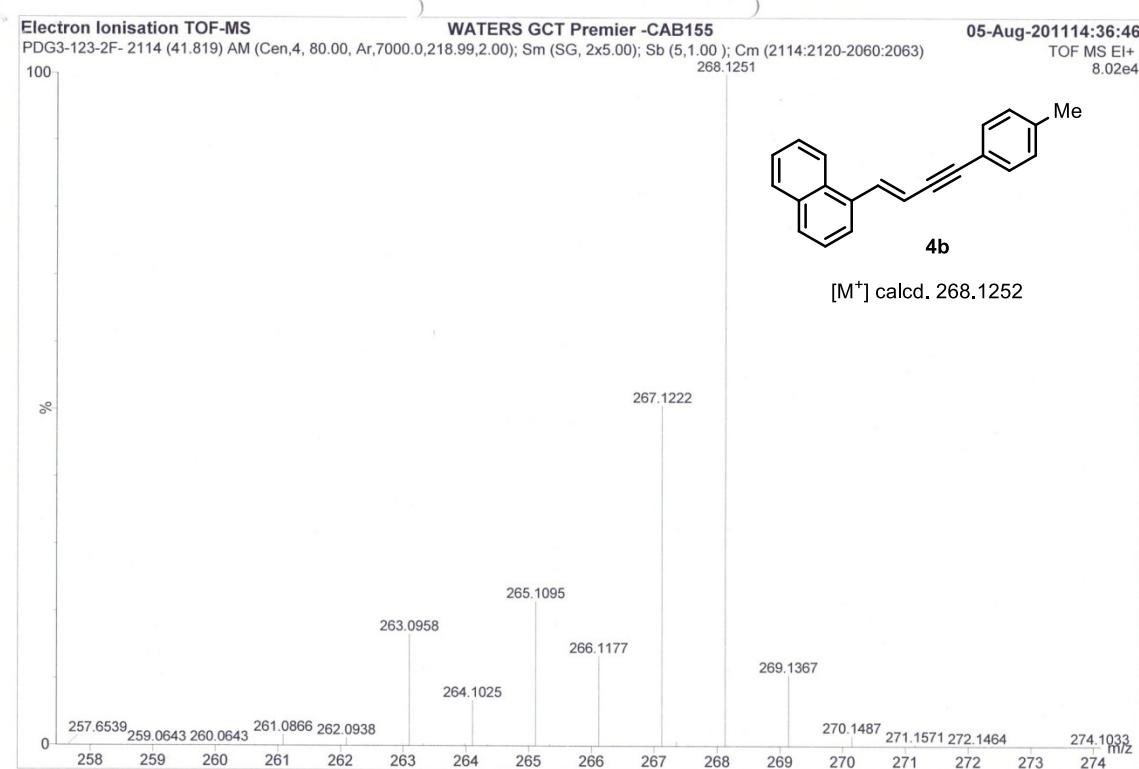
EI (HRMS) spectrum of (*E*)-1-(4-phenylbut-1-en-3-ynyl)naphthalene (**4a**)



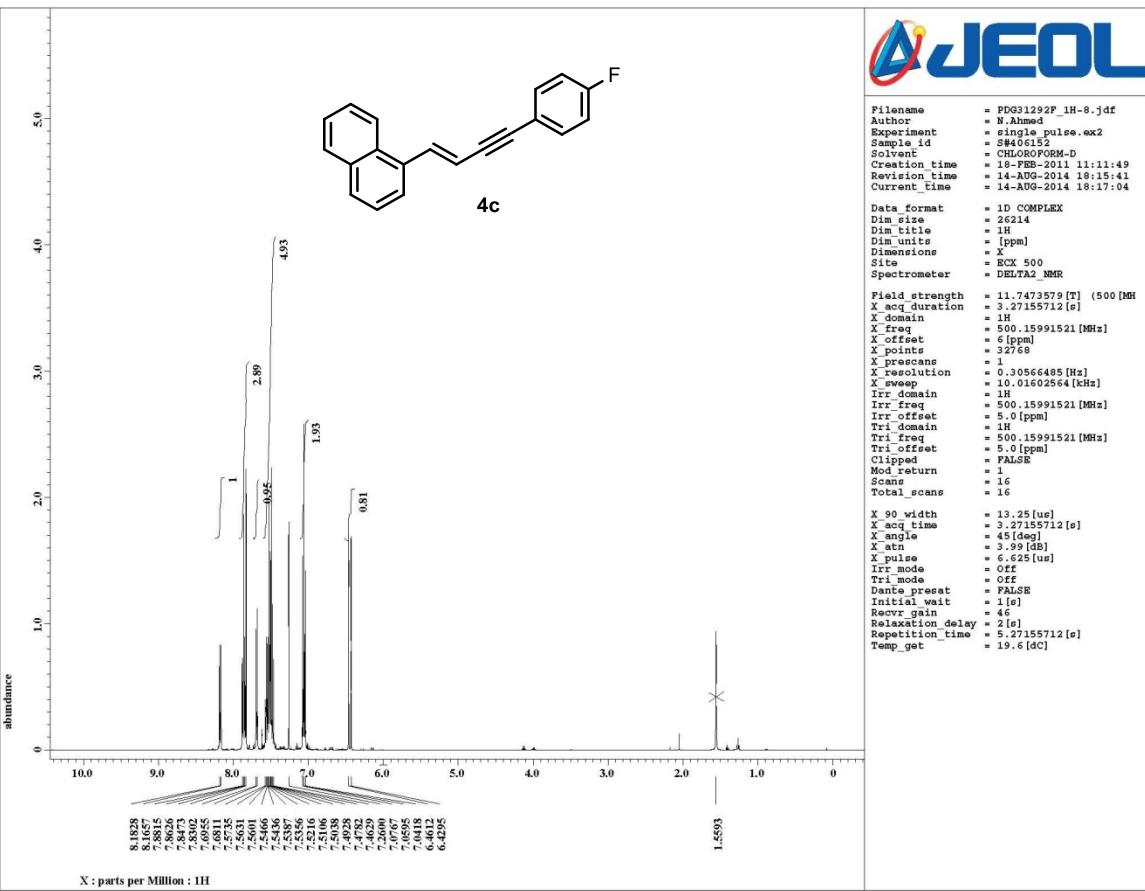
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-*p*-tolylbut-1-en-3-ynyl)naphthalene (**4b**)



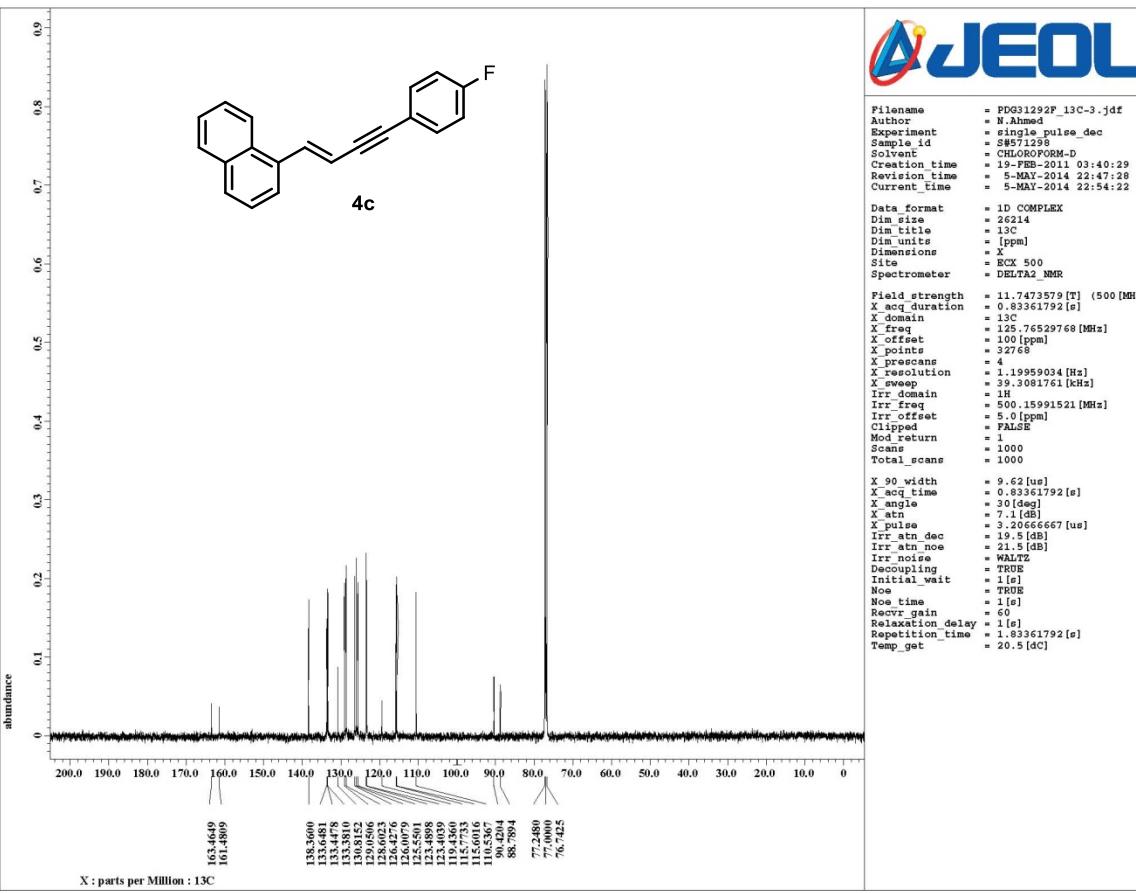
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-(4-p-tolylbut-1-en-3-ynyl)naphthalene (**4b**)



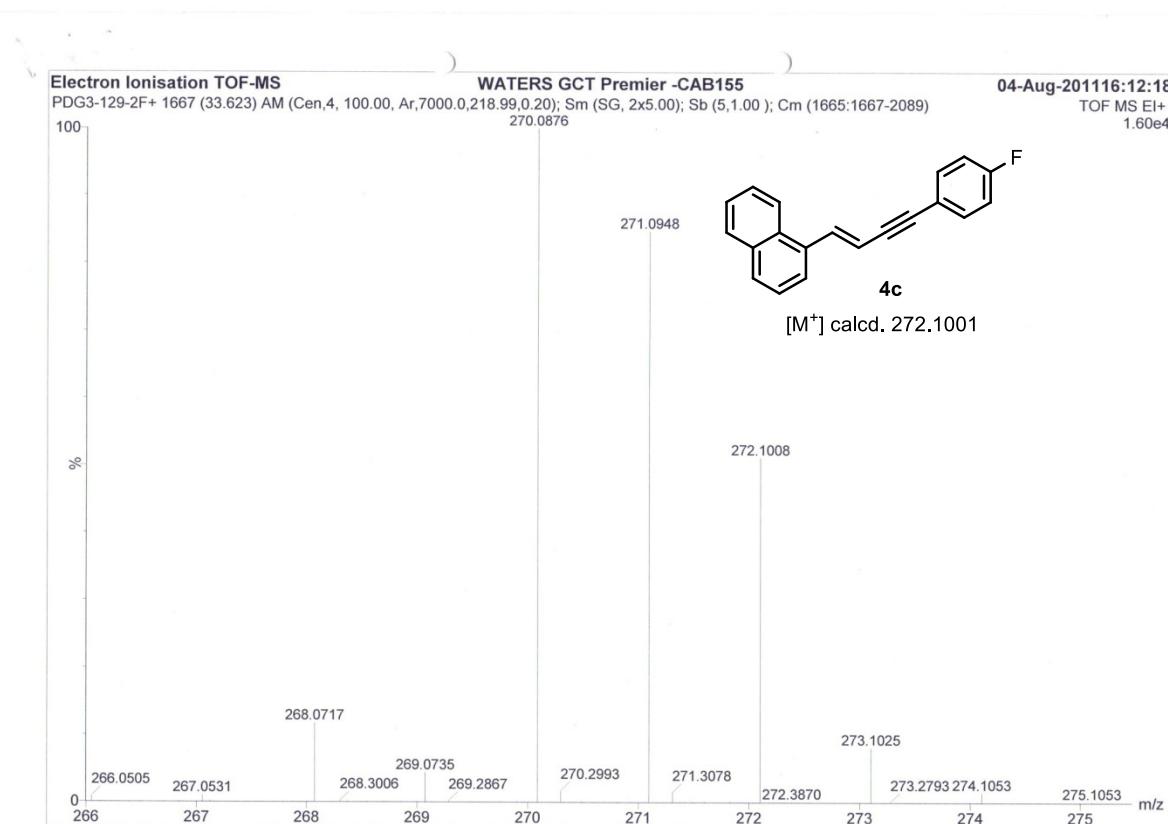
EI (HRMS) spectrum of (*E*)-1-(4-*p*-tolylbut-1-en-3-ynyl)naphthalene (**4b**)



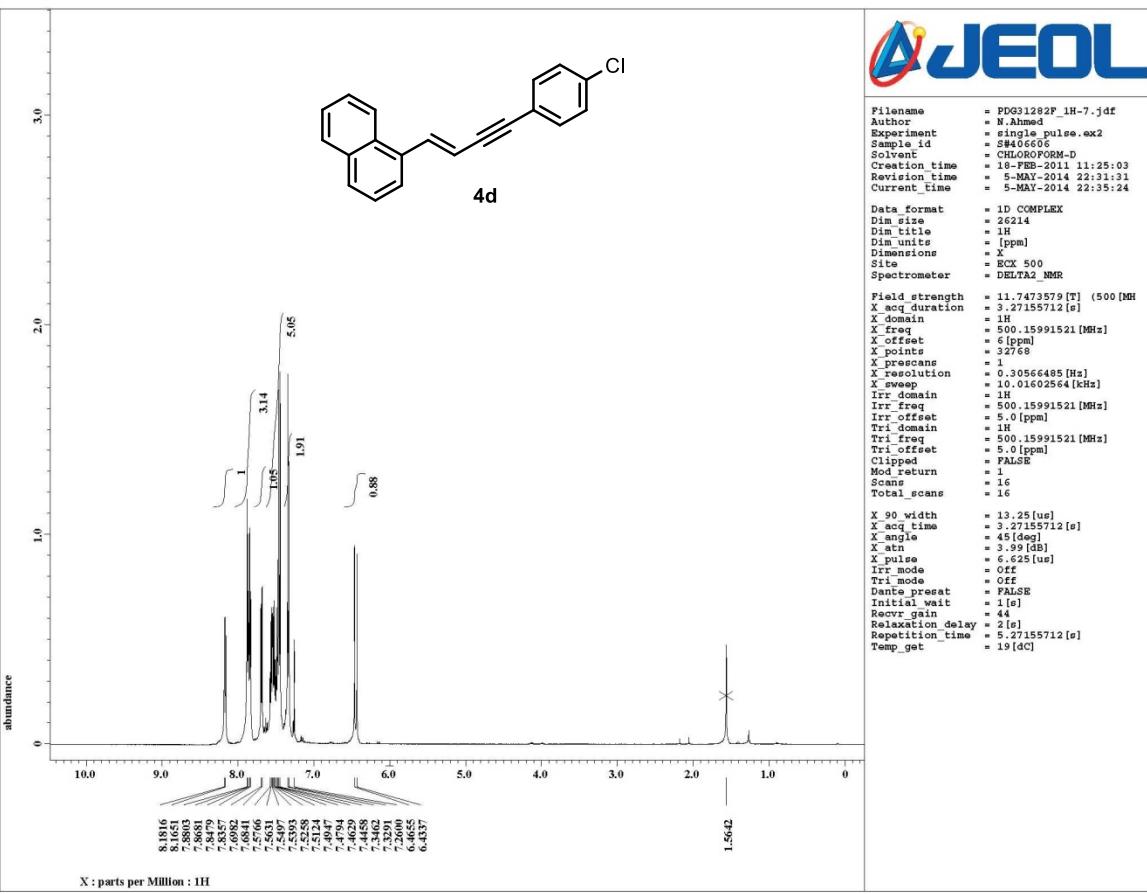
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-fluorophenyl)but-1-en-3-ynyl)naphthalene (**4c**)



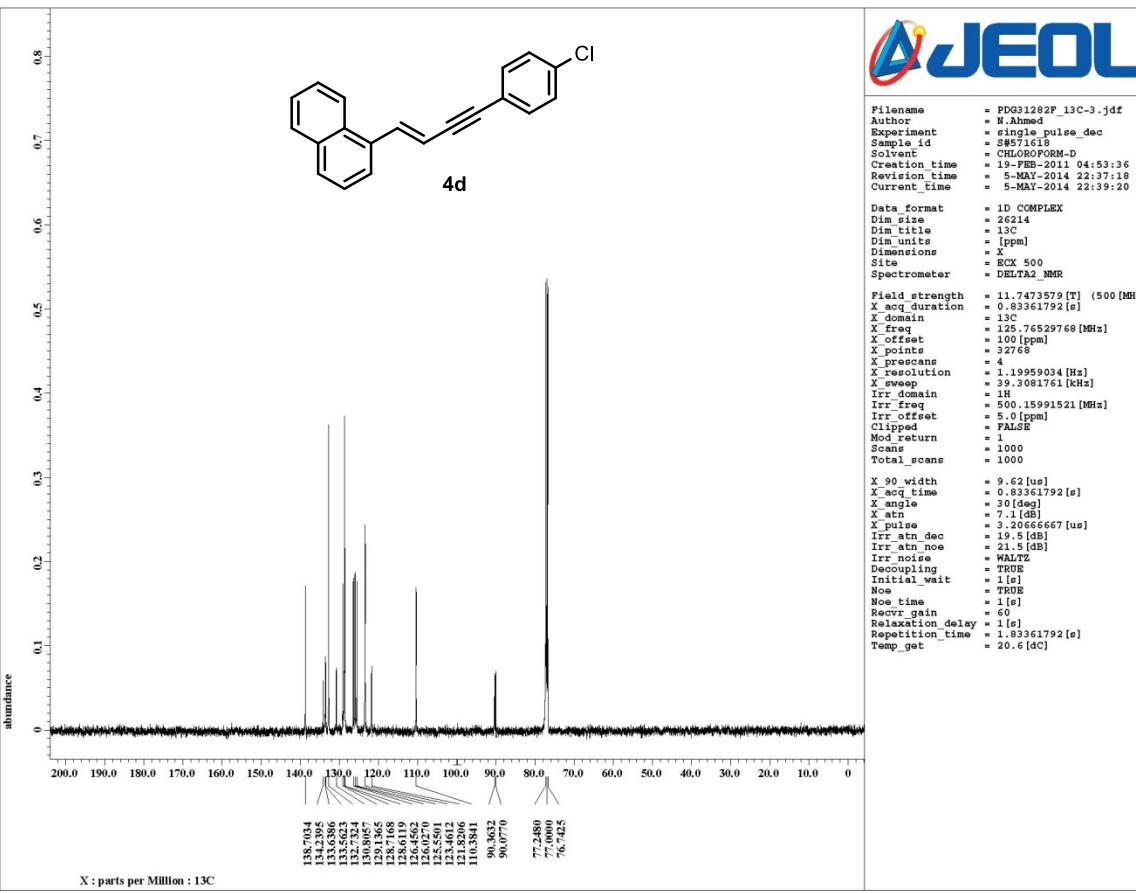
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-(4-(4-fluorophenyl)but-1-en-3ynyl)naphthalene (**4c**)



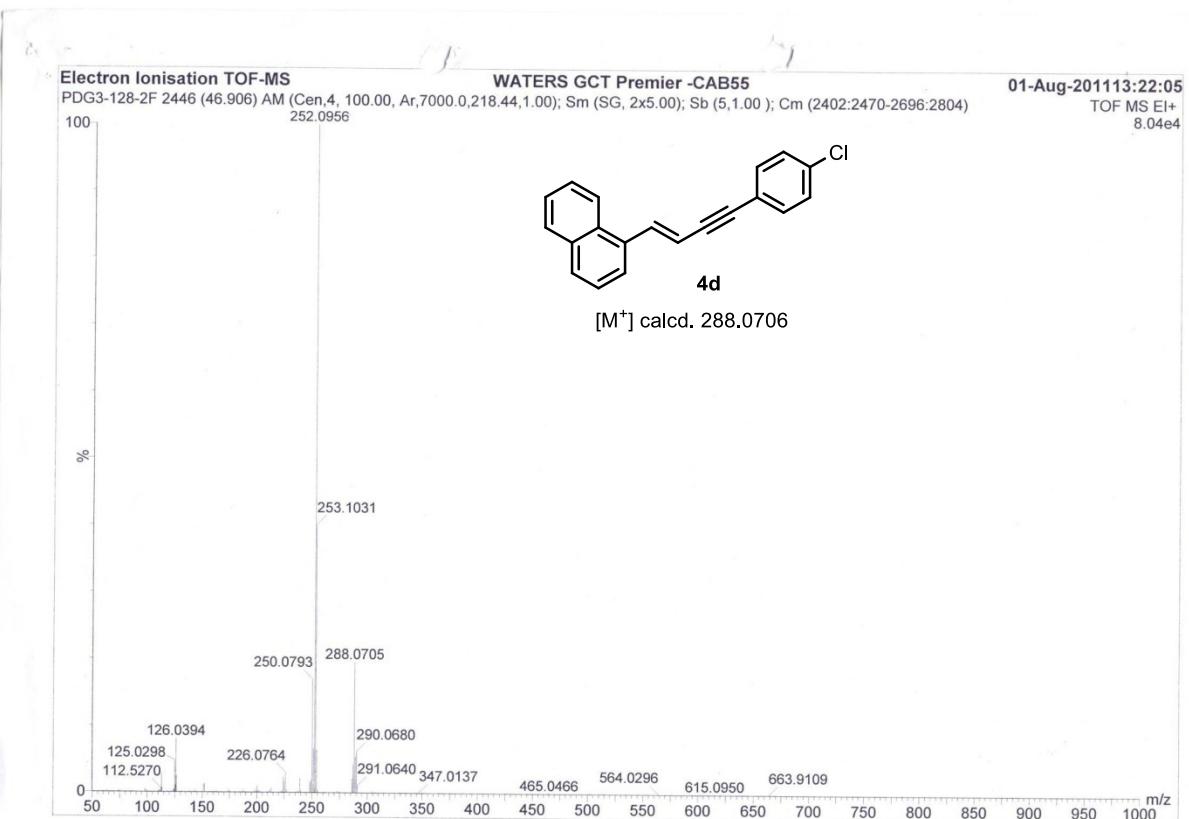
EI (HRMS) spectrum of (*E*)-1-(4-(4-fluorophenyl)but-1-en-3-ynyl)naphthalene (**4c**)



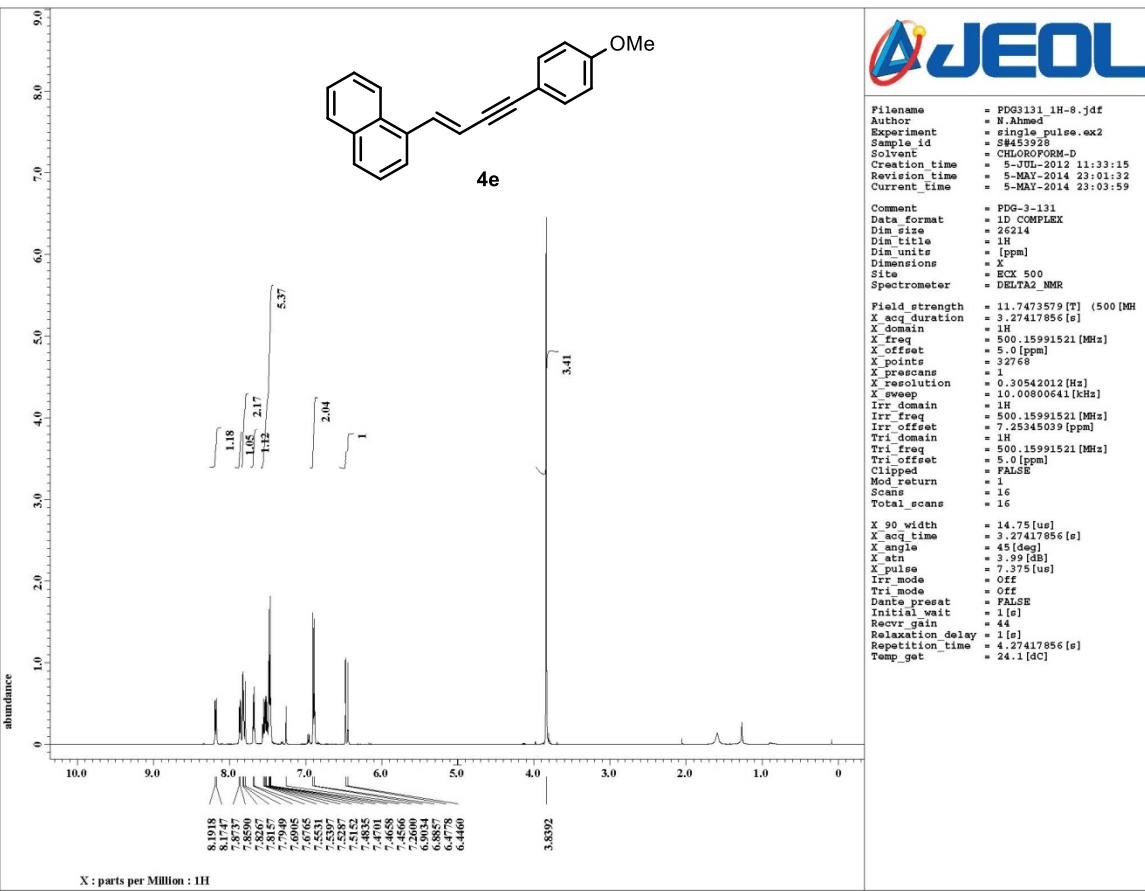
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-chlorophenyl)but-1-en-3-ynyl)naphthalene (**4d**)



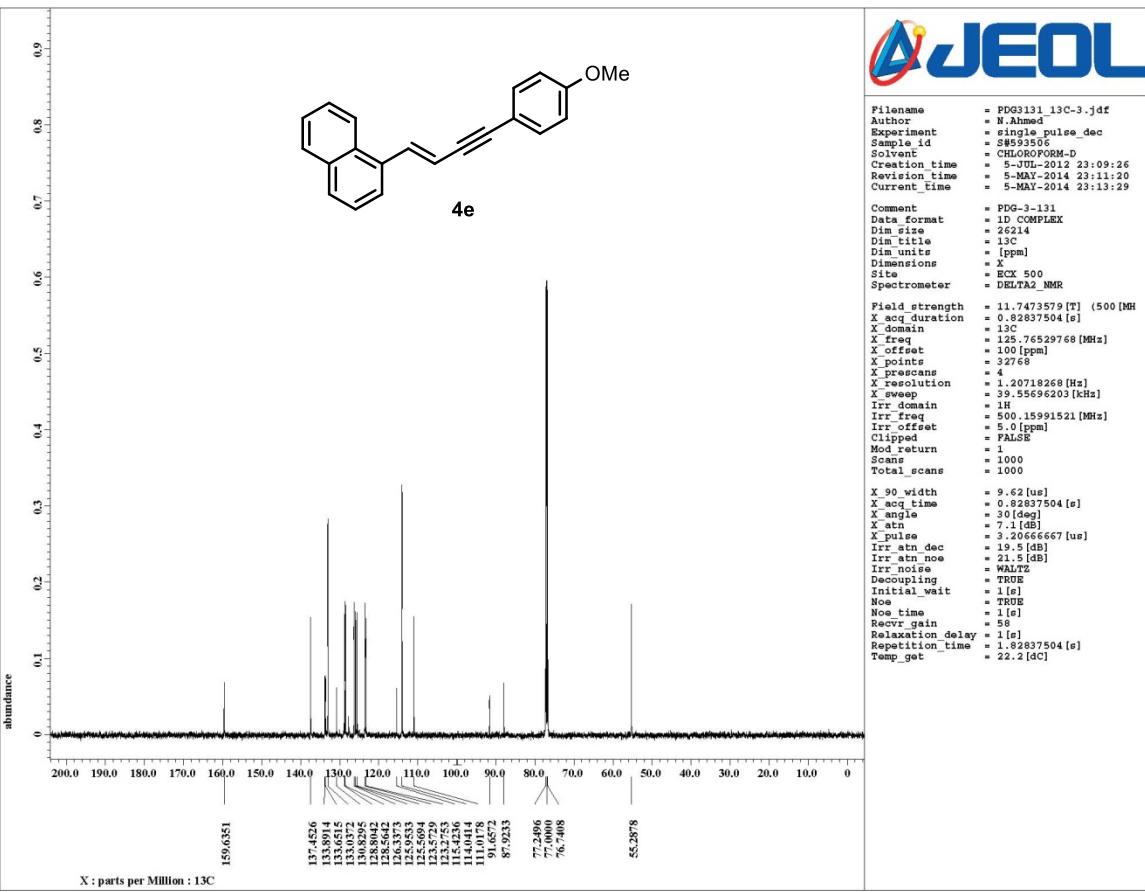
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-chlorophenyl)but-1-en-3-ynyl)naphthalene (**4d**)



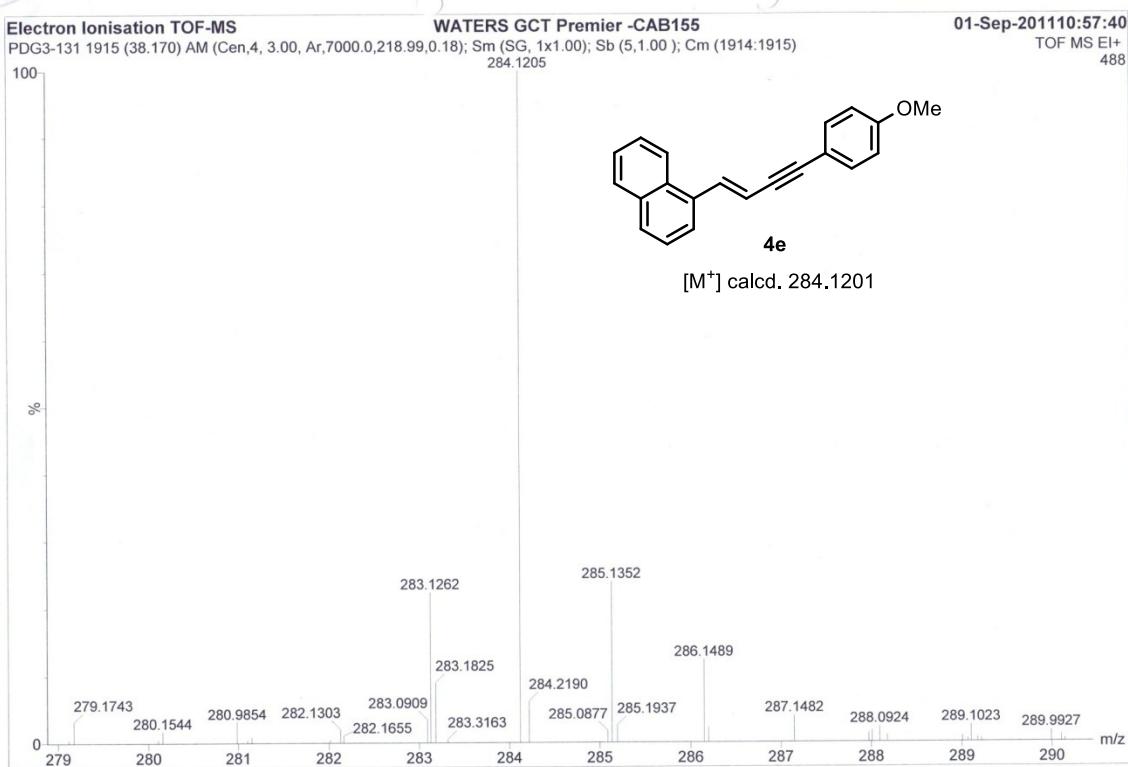
EI (HRMS) spectrum of (*E*)-1-(4-(4-chlorophenyl)but-1-en-3-ynyl)naphthalene (**4d**)



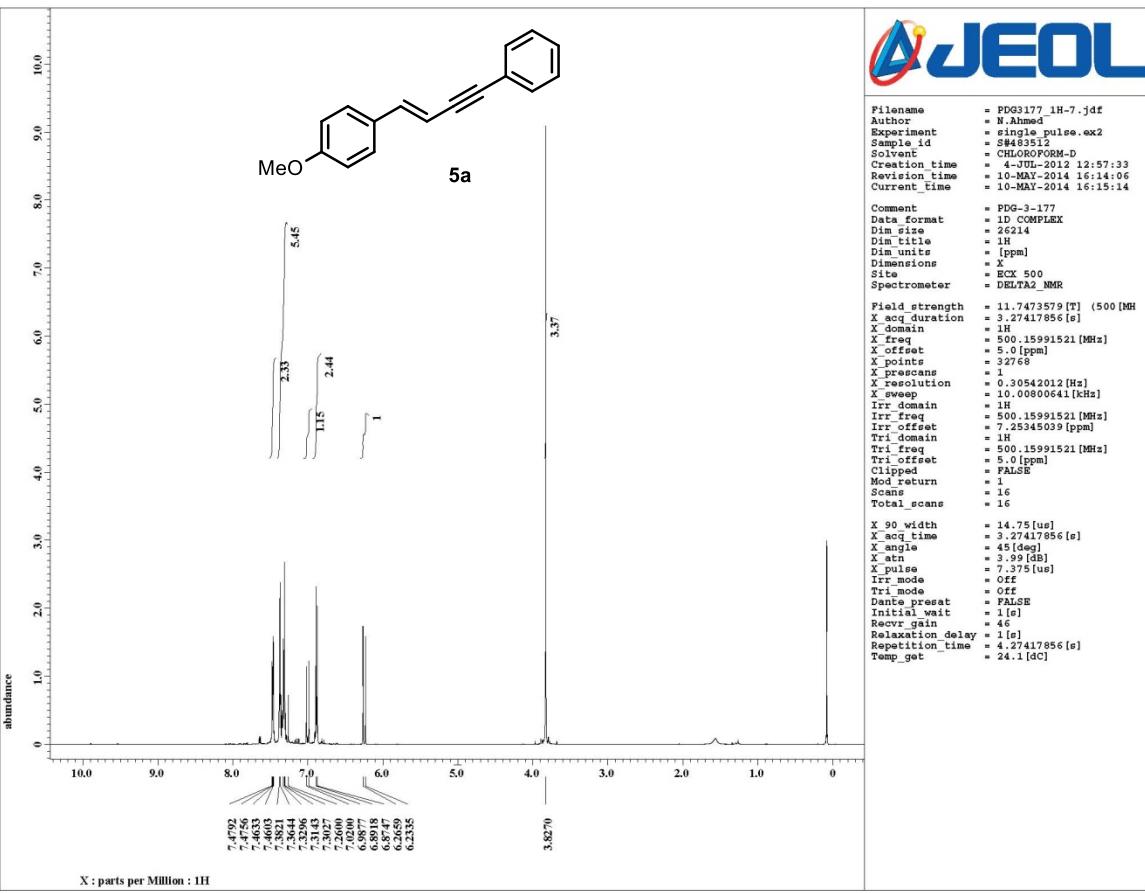
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-methoxyphenyl)but-1-en-3-ynyl)naphthalene (**4e**)



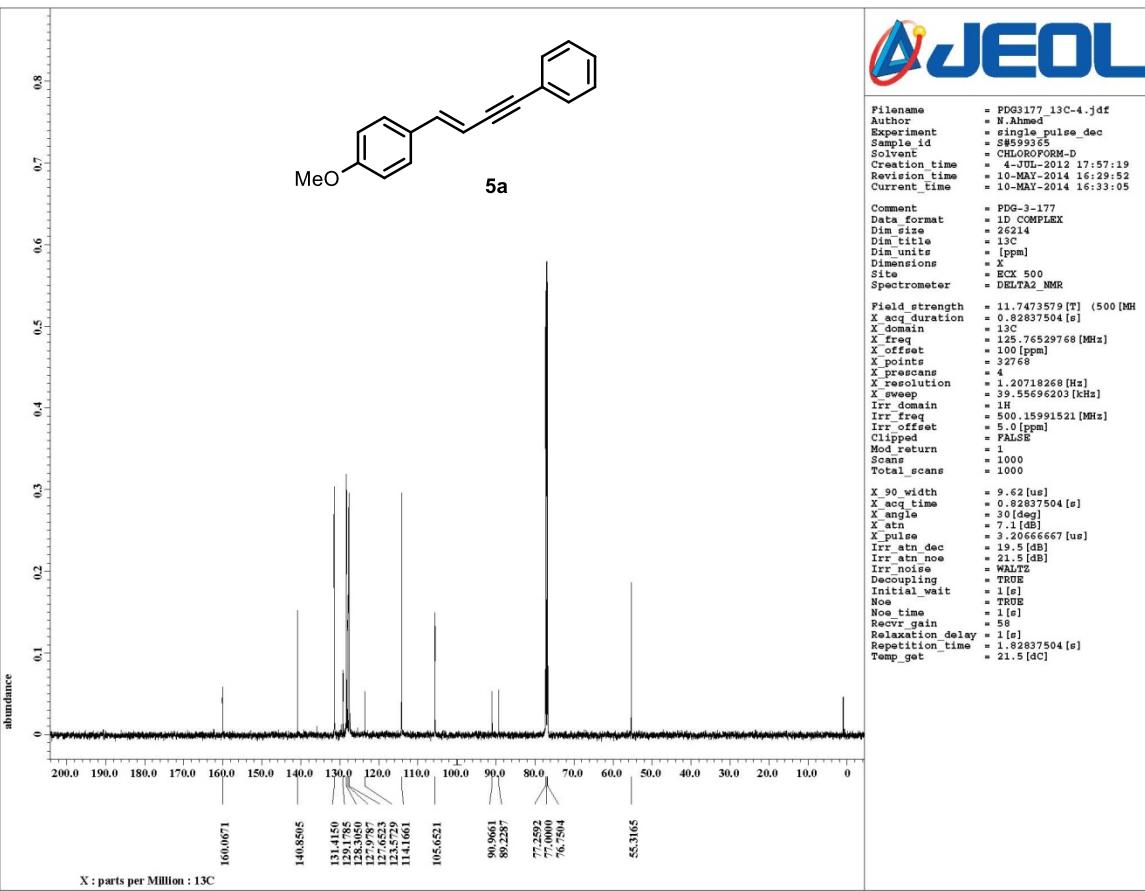
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-methoxyphenyl)but-1-en-3-ynyl)naphthalene (**4e**)



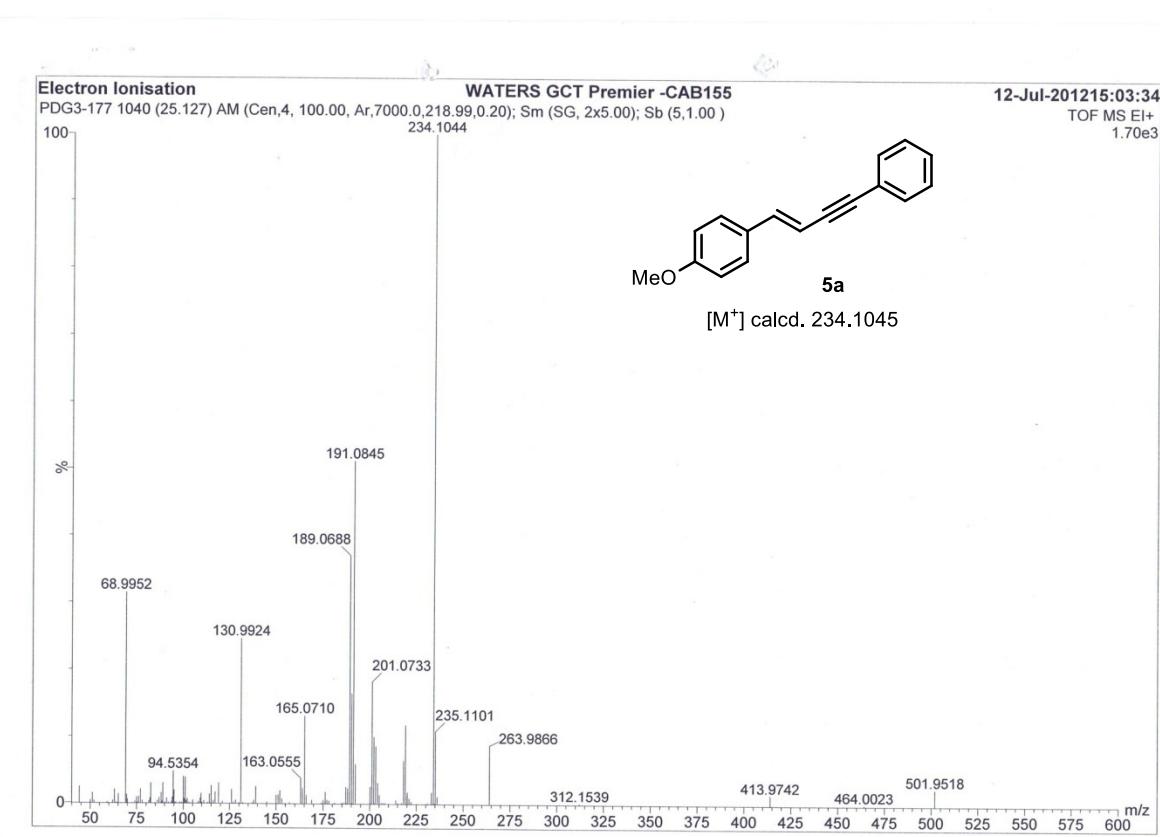
EI (HRMS) spectrum of (*E*)-1-(4-(4-methoxyphenyl)but-1-en-3-ynyl)naphthalene (**4e**)



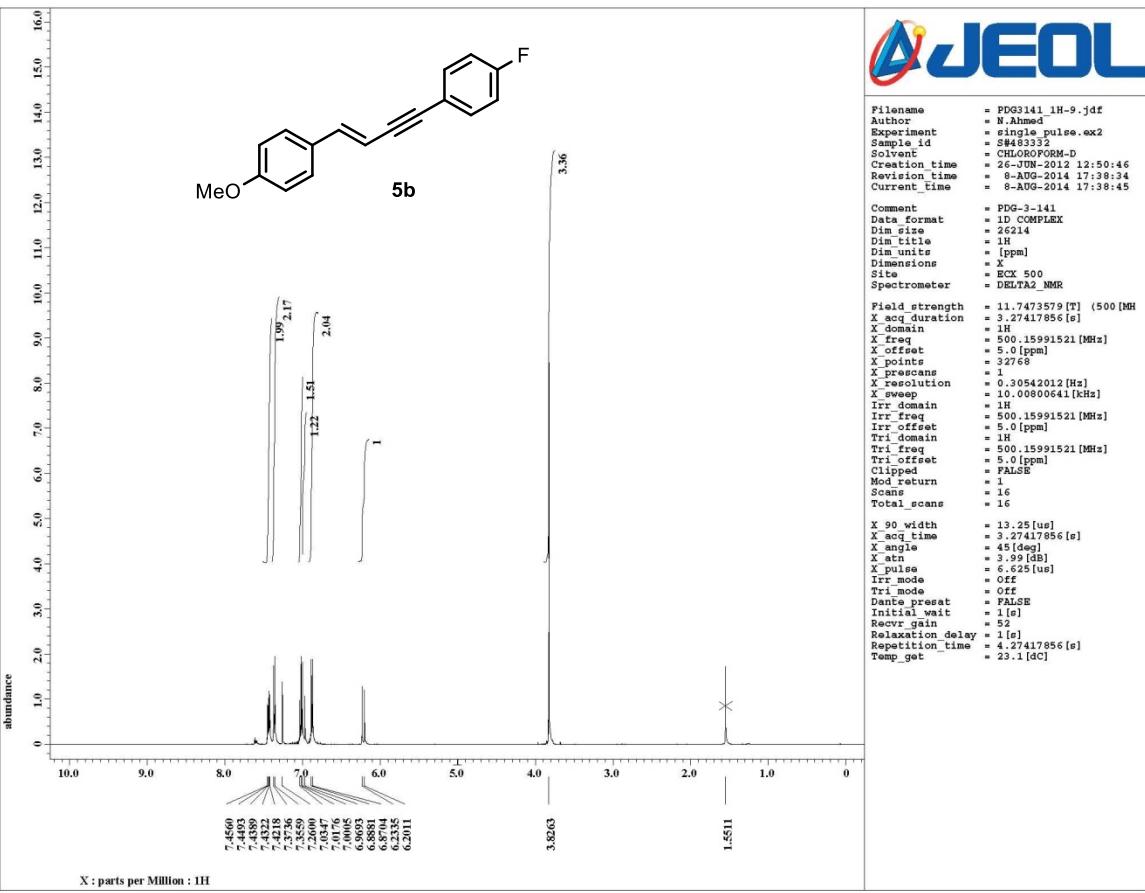
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-methoxy-4-(4-phenylbut-1-en-3-ynyl)benzene (**5a**)

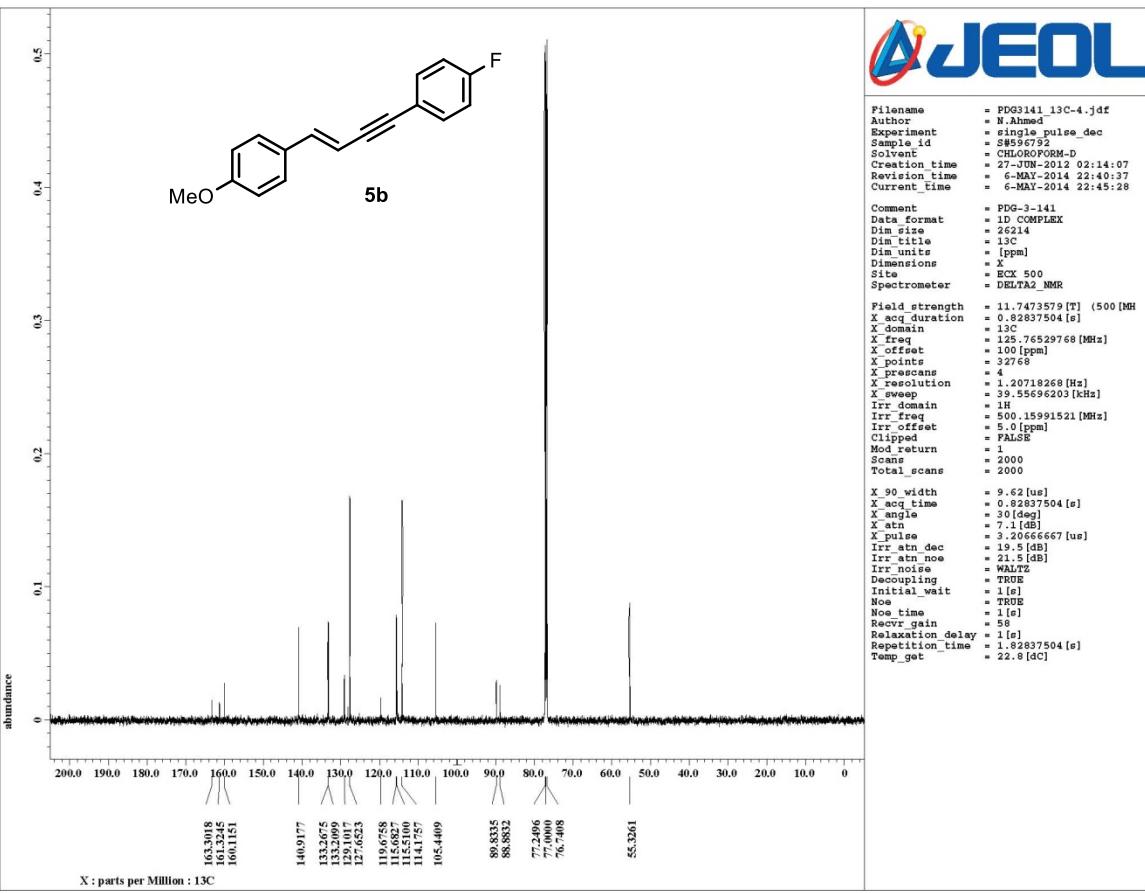


¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-methoxy-4-(4-phenylbut-1-en-3-ynyl)benzene (**5a**)

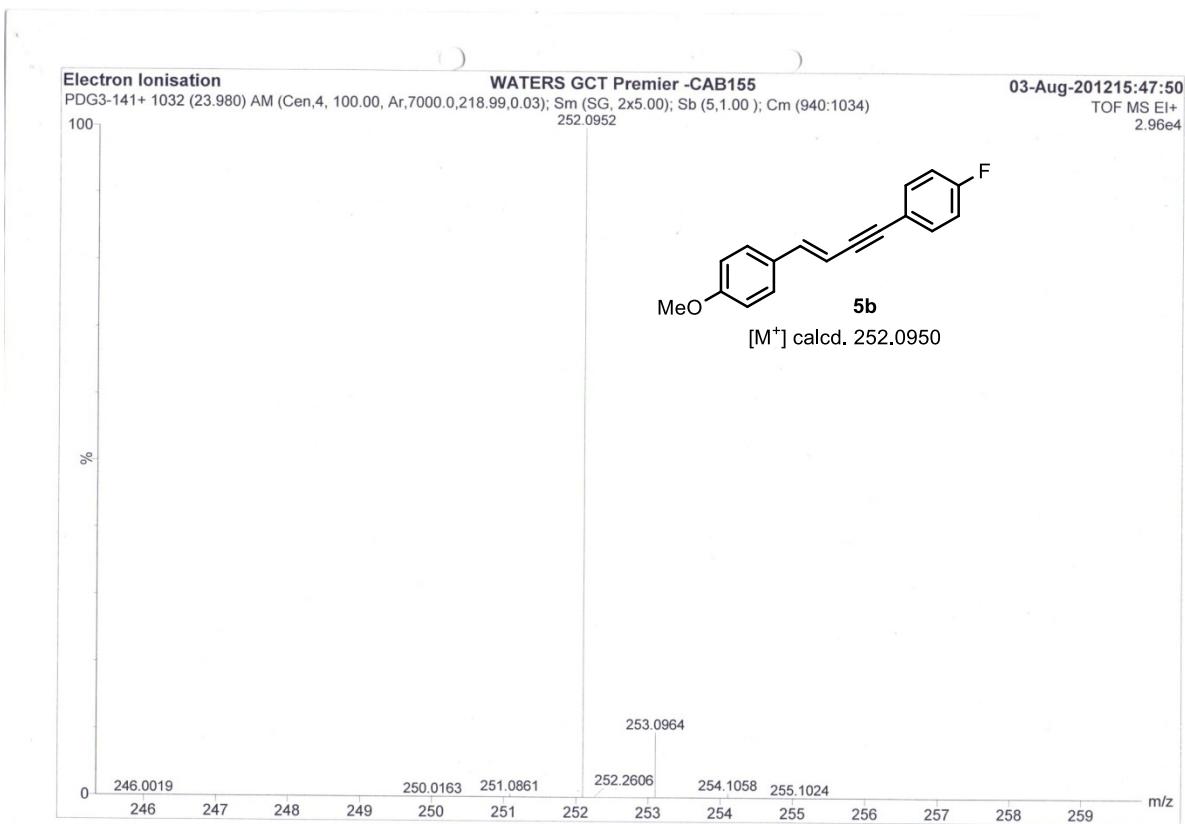


EI (HRMS) spectrum of (*E*)-1-methoxy-4-(4-phenylbut-1-en-3-ynyl)benzene (**5a**)

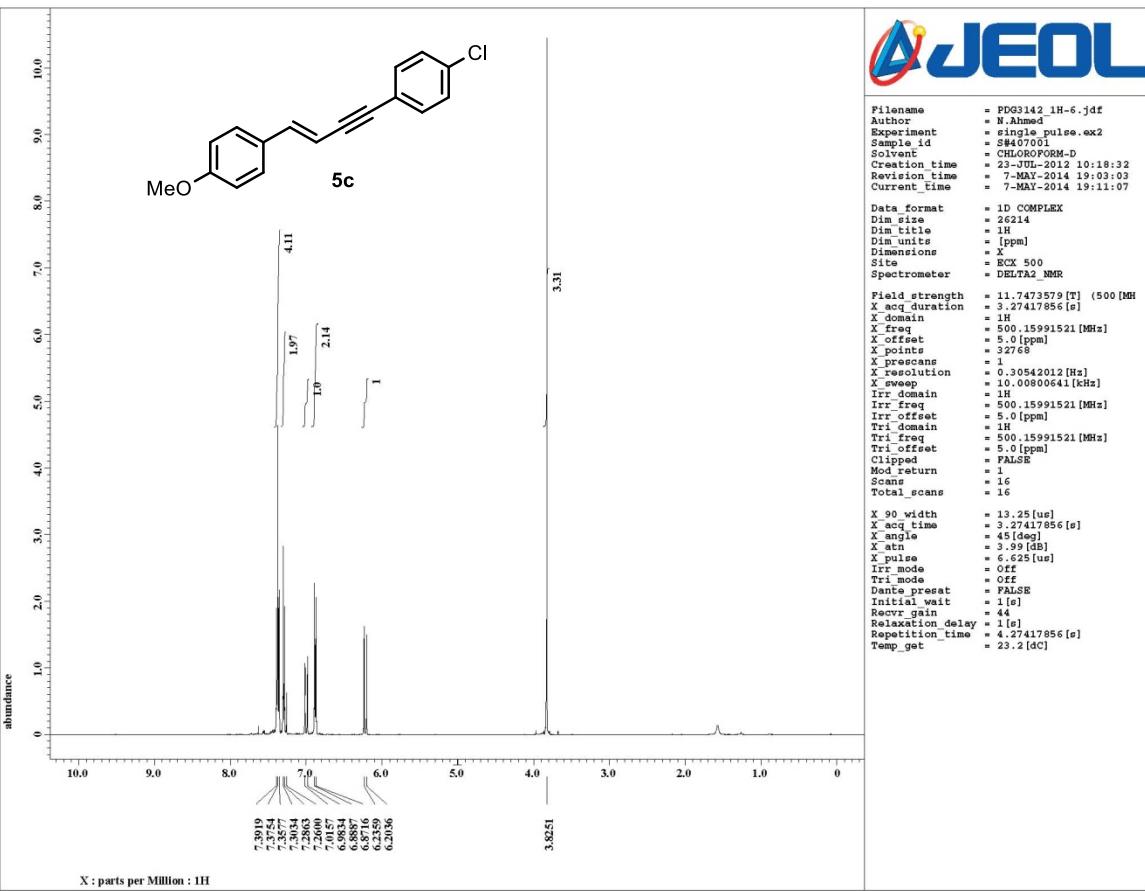




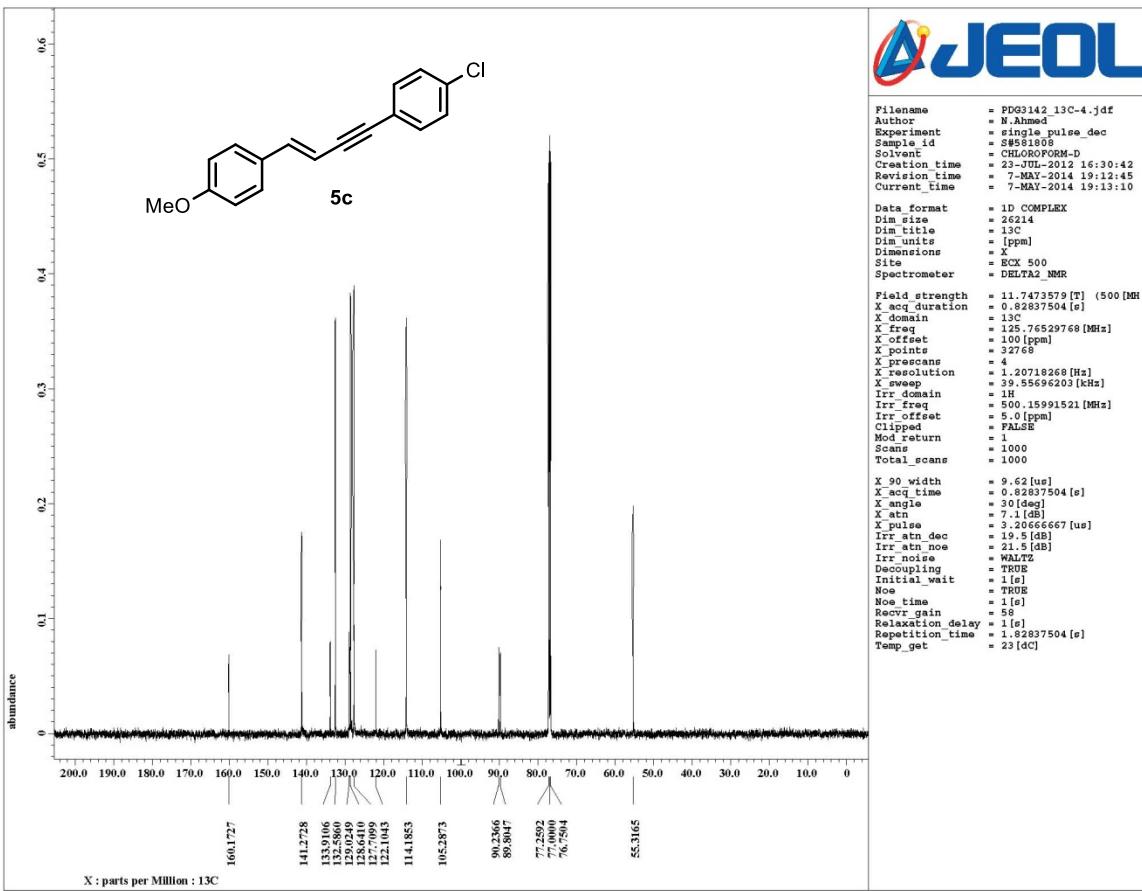
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-1-fluoro-4-(4-(4-methoxyphenyl)but-3-en-1-ynyl)benzene (**5b**)



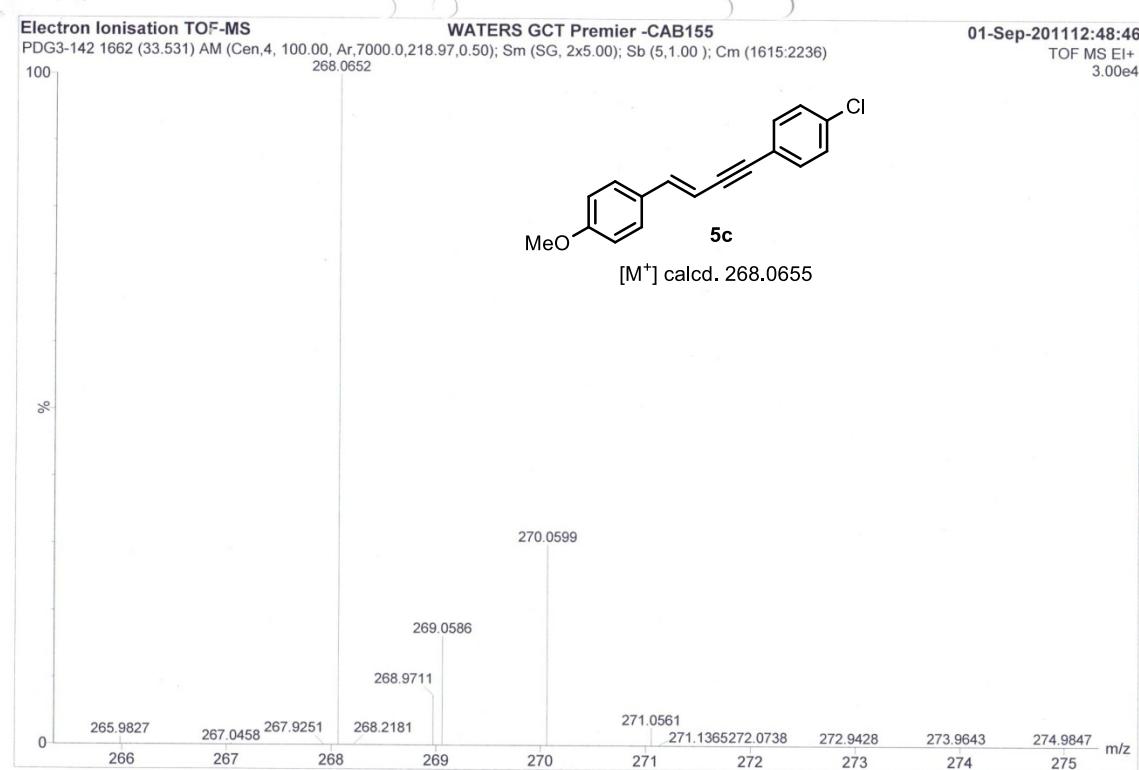
EI (HRMS) spectrum of (*E*)-1-fluoro-4-(4-(4-methoxyphenyl)but-3-en-1-ynyl)benzene (**5b**)



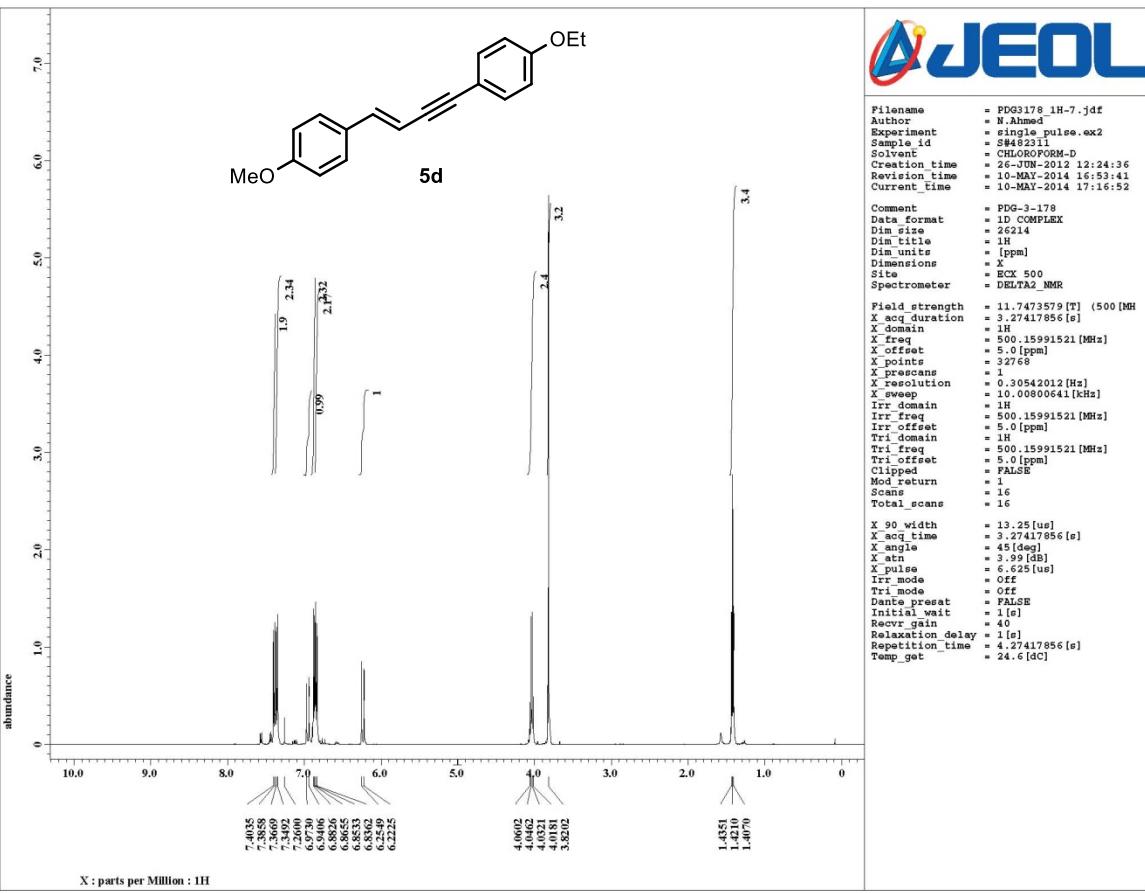
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-chloro-4-(4-(4-methoxyphenyl)but-3-en-1-ynyl)benzene (**5c**)



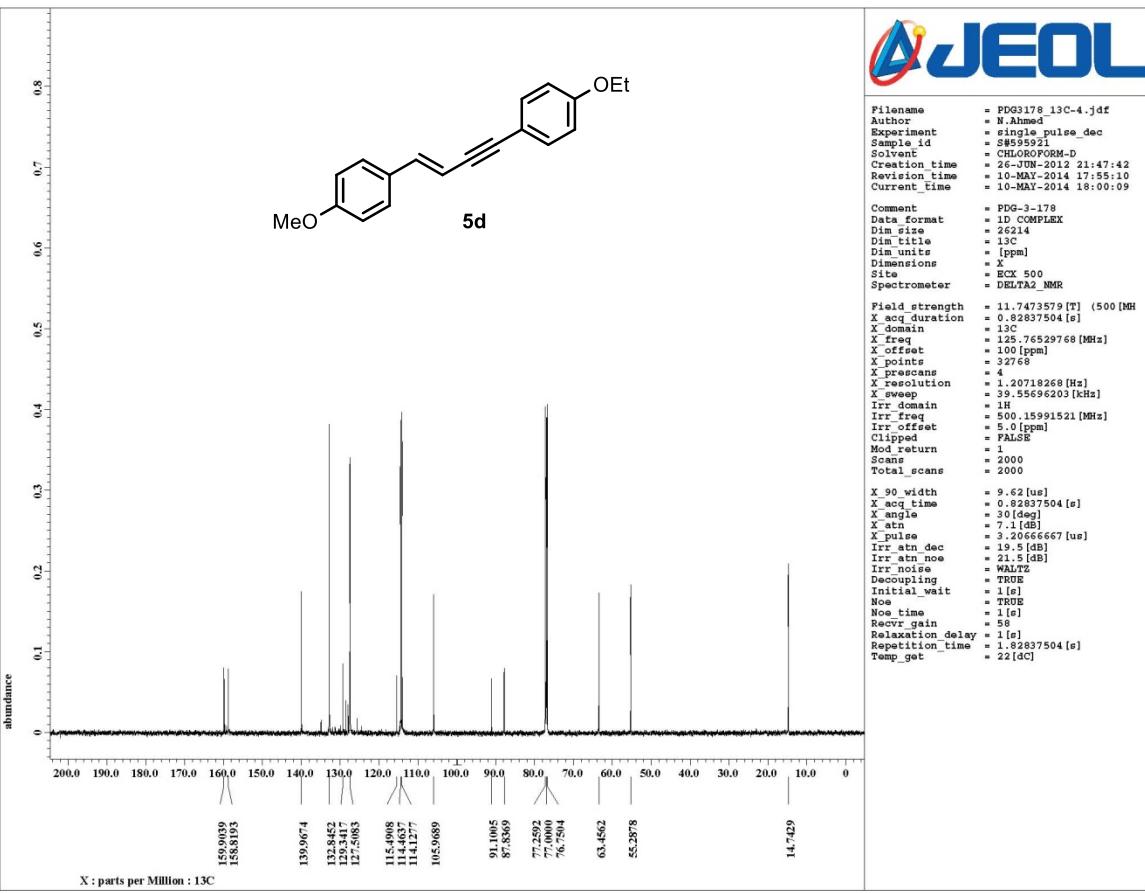
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-(4-methoxyphenyl)but-3-en-1-ynyl)benzene (**5c**)



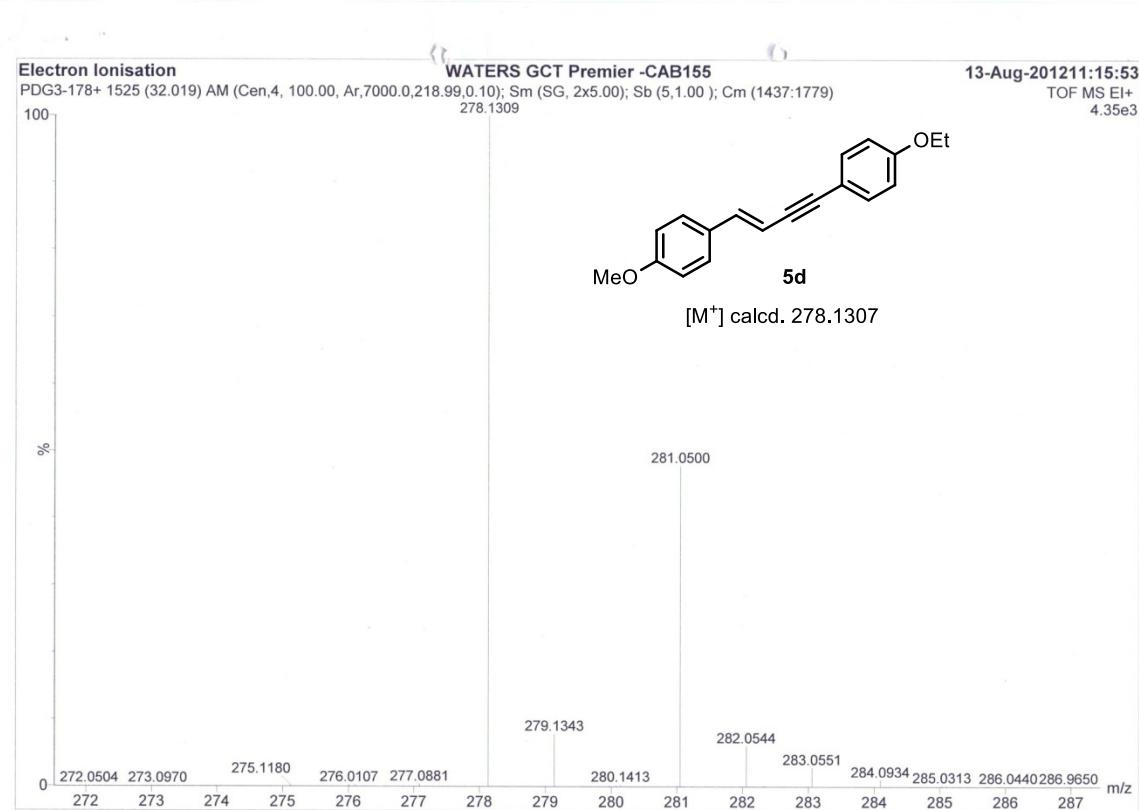
EI (HRMS) spectrum of (*E*)-1-chloro-4-(4-methoxyphenyl)but-3-en-1-ynylbenzene (**5c**)



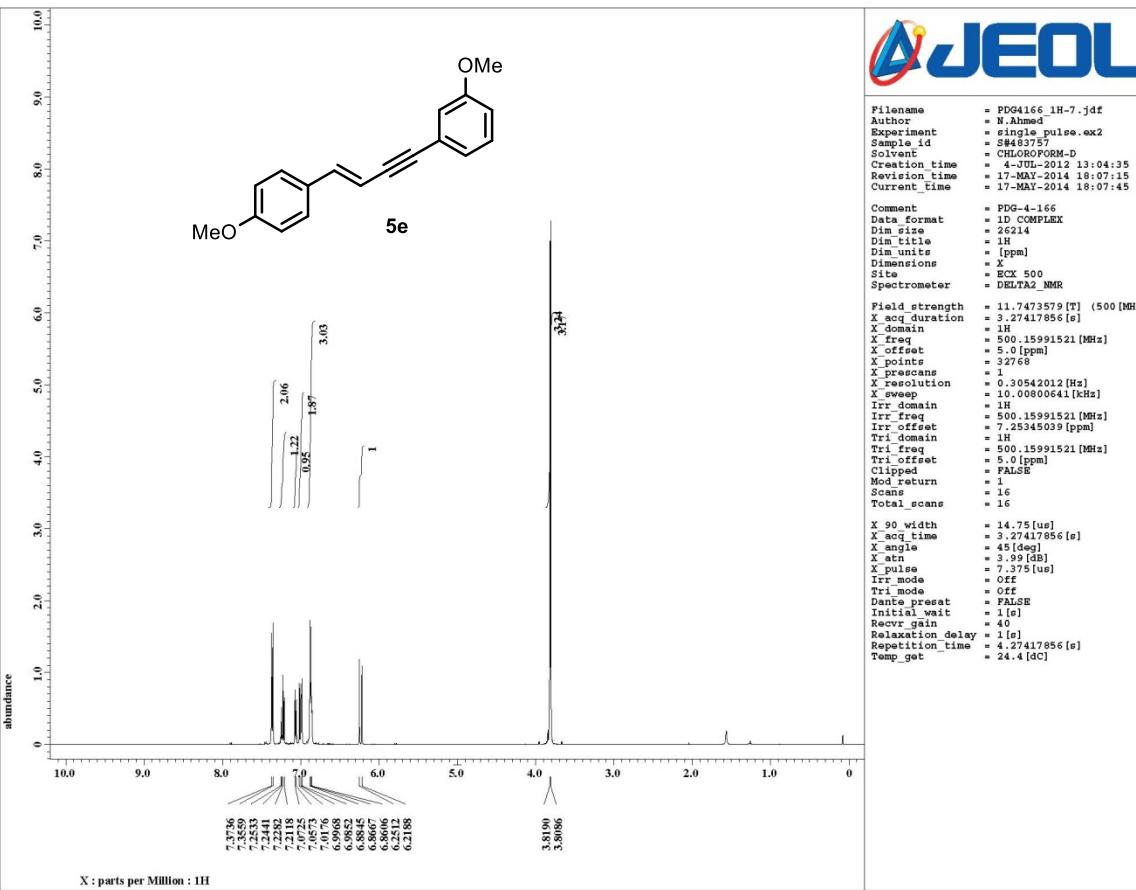
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-ethoxy-4-(4-(4-methoxyphenyl)but-3-en-1-ynyl)benzene (**5d**)



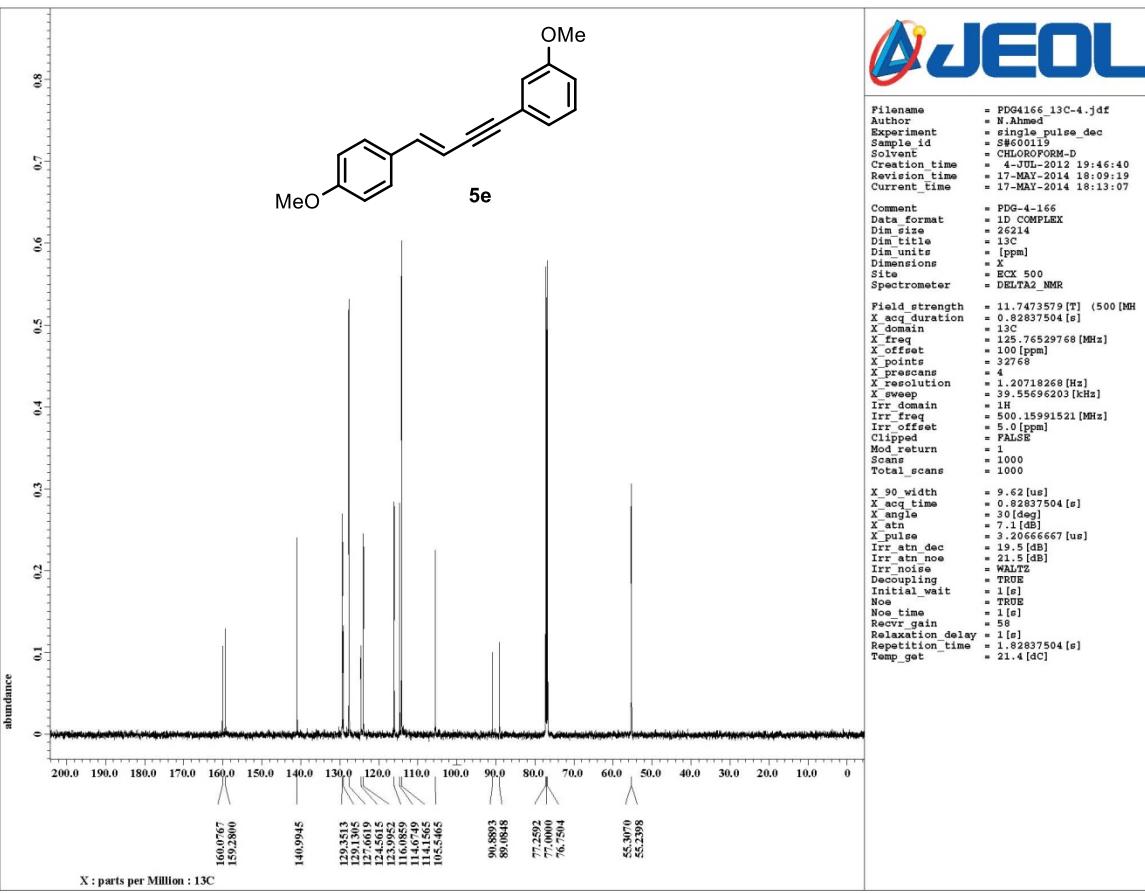
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-ethoxy-4-(4-methoxyphenyl)but-3-en-1-ynylbenzene (**5d**)



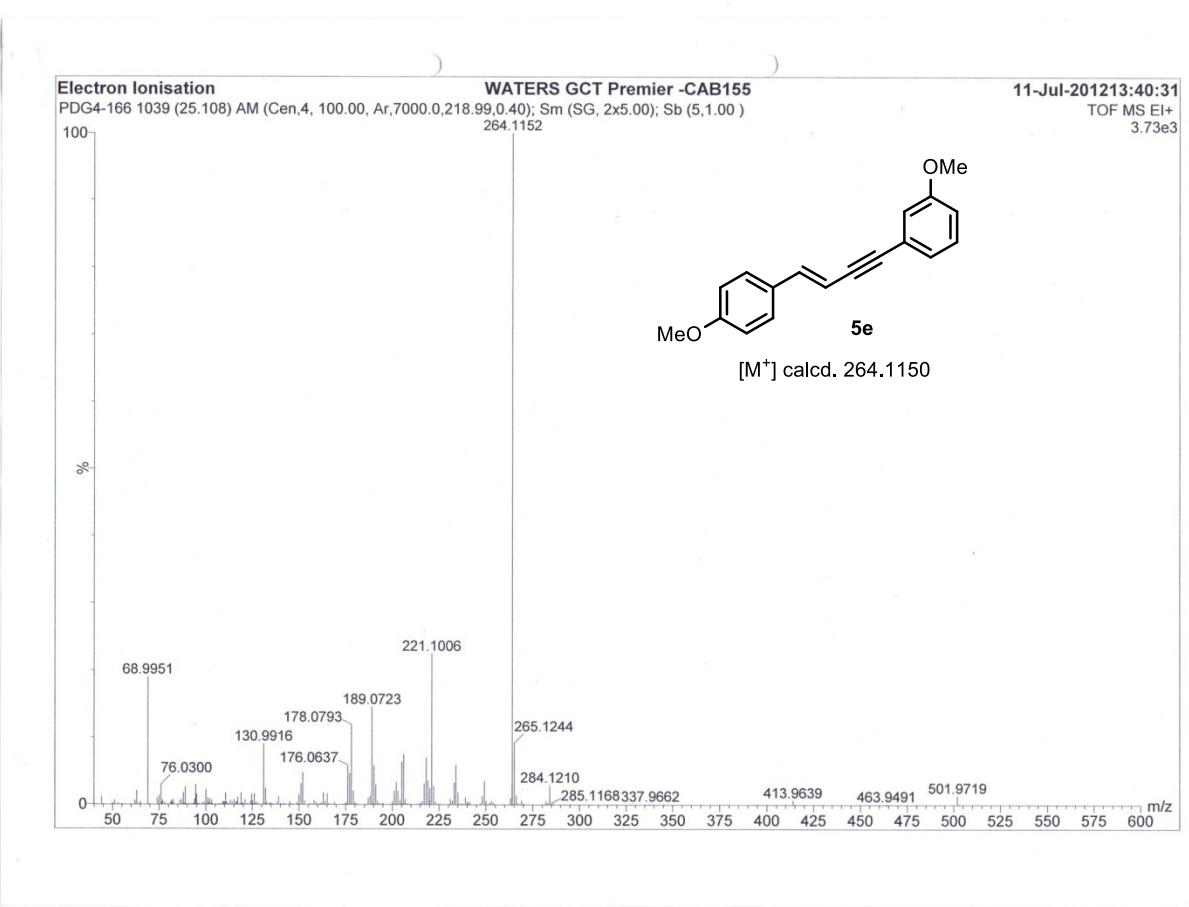
EI (HRMS) spectrum of (*E*)-1-ethoxy-4-(4-(4-methoxyphenyl)but-3-en-1-ynyl)benzene (**5d**)



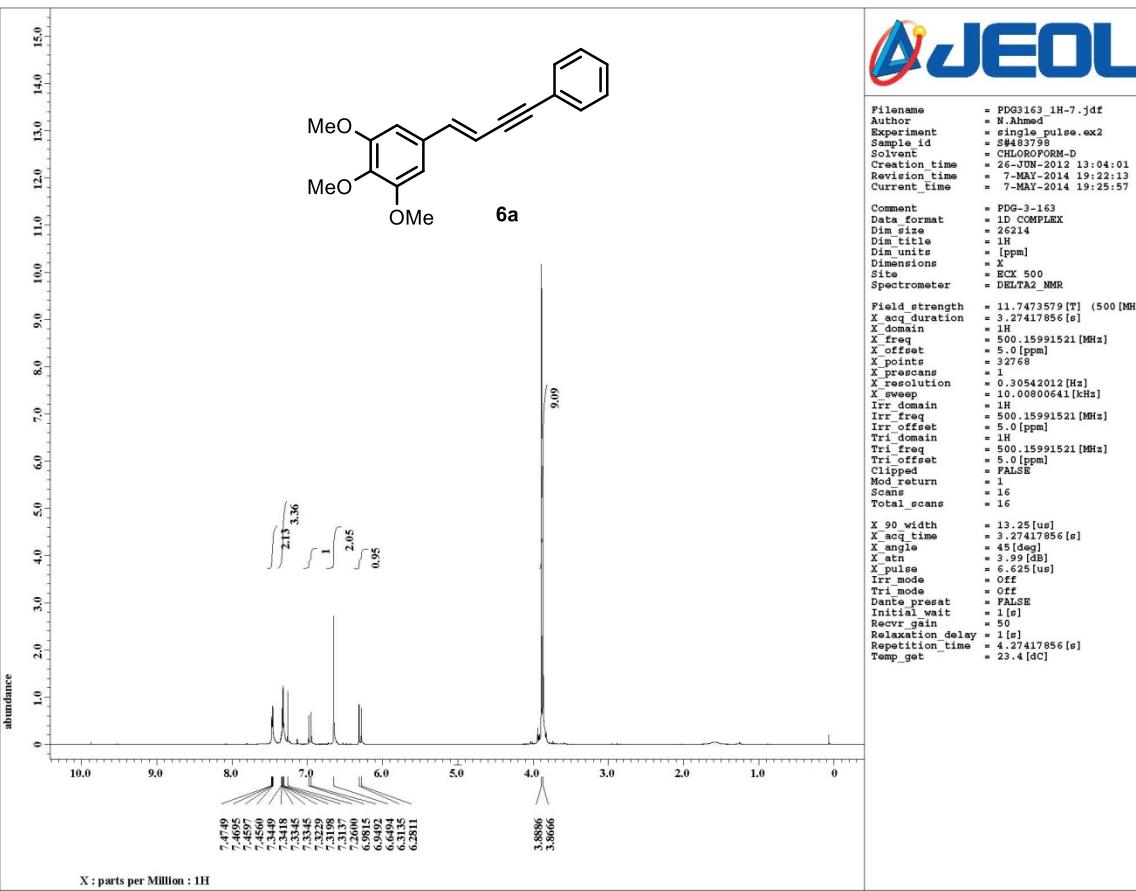
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-methoxy-3-(4-(4-methoxyphenyl)but-3-en-1-ynyl)benzene (**5e**)



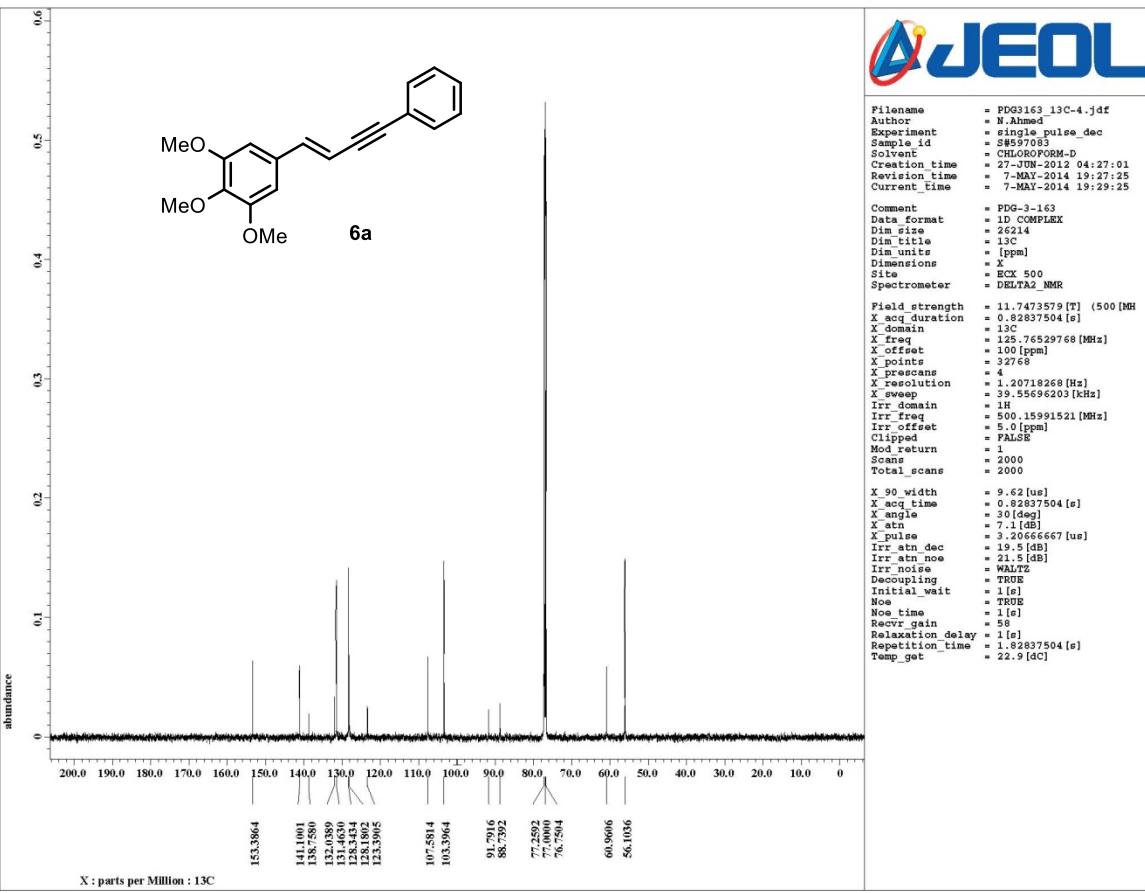
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-methoxy-3-(4-(4-methoxyphenyl)but-3-en-1-ynyl)benzene (**5e**)



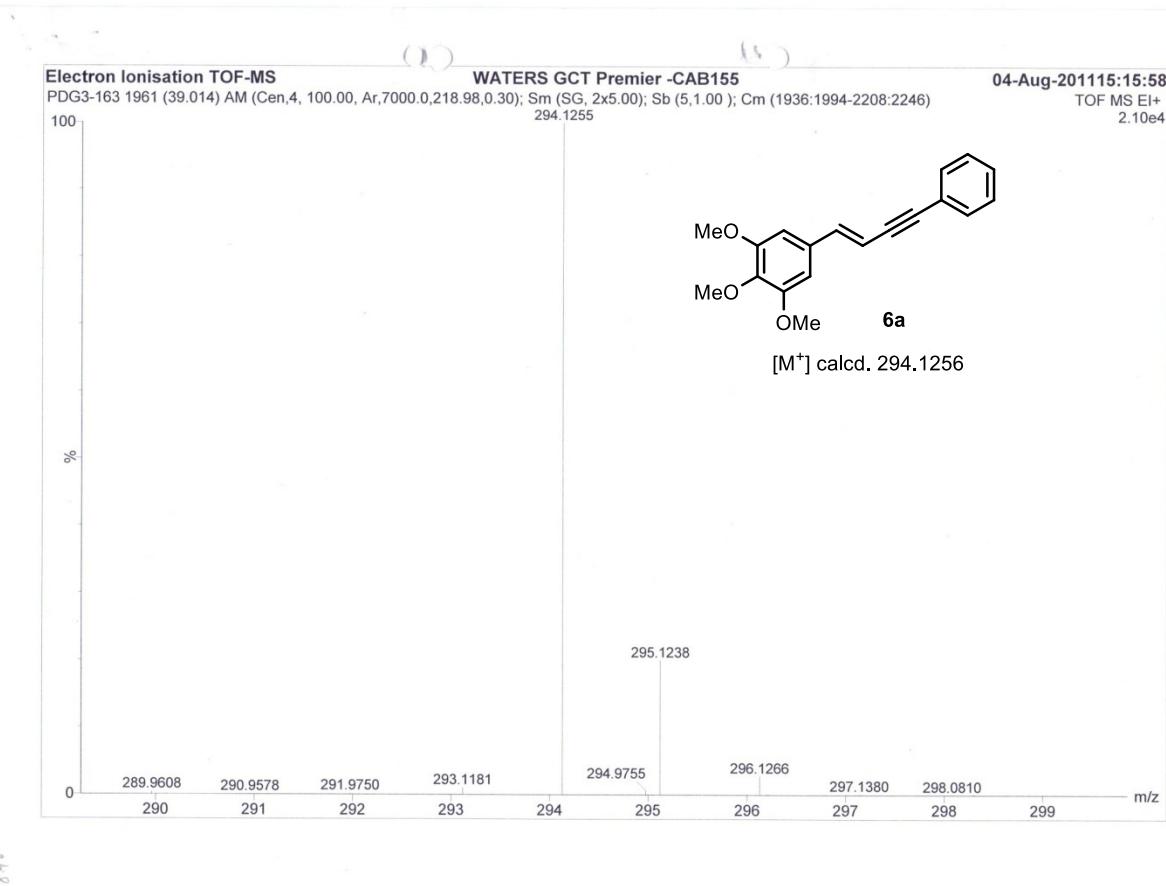
EI (HRMS) spectrum of (*E*)-1-methoxy-3-(4-(4-methoxyphenyl)but-3-en-1-ynyl)benzene (**5e**)



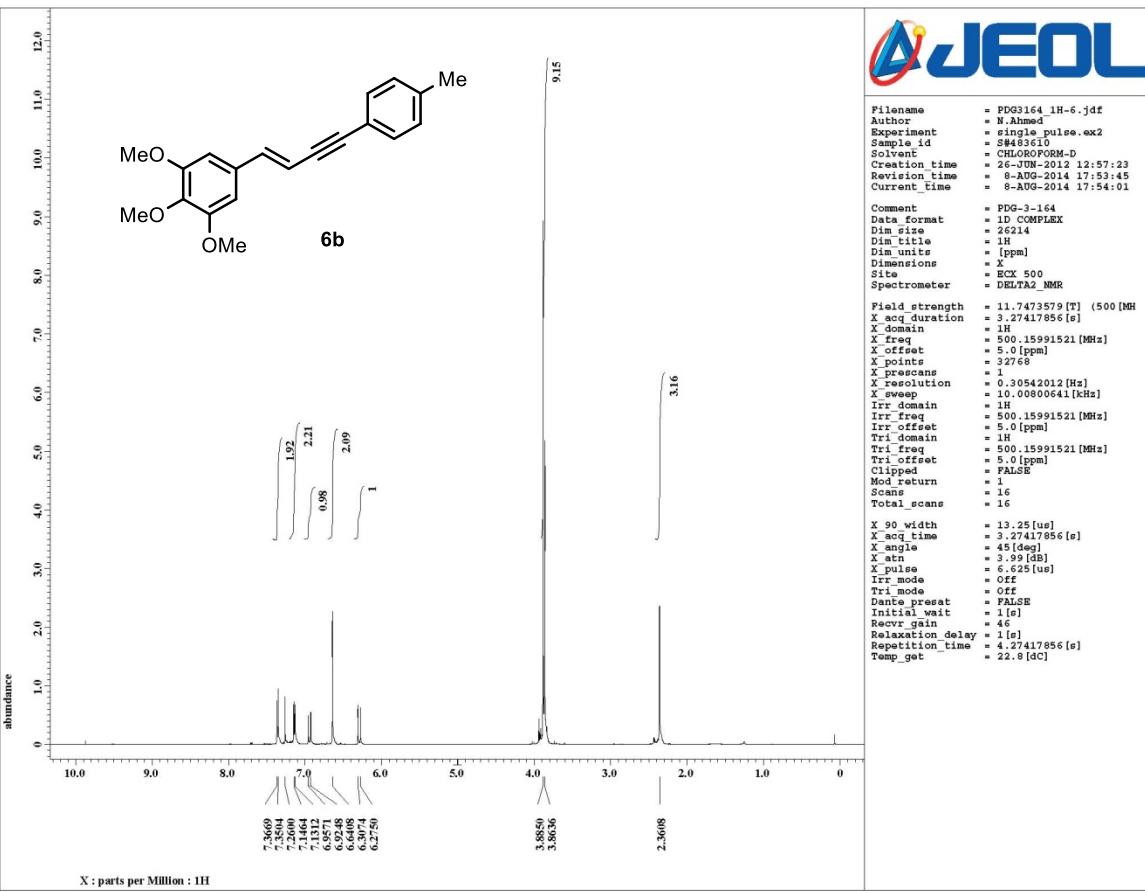
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1,2,3-trimethoxy-5-(4-phenylbut-1-en-3-ynyl)benzene (**6a**)



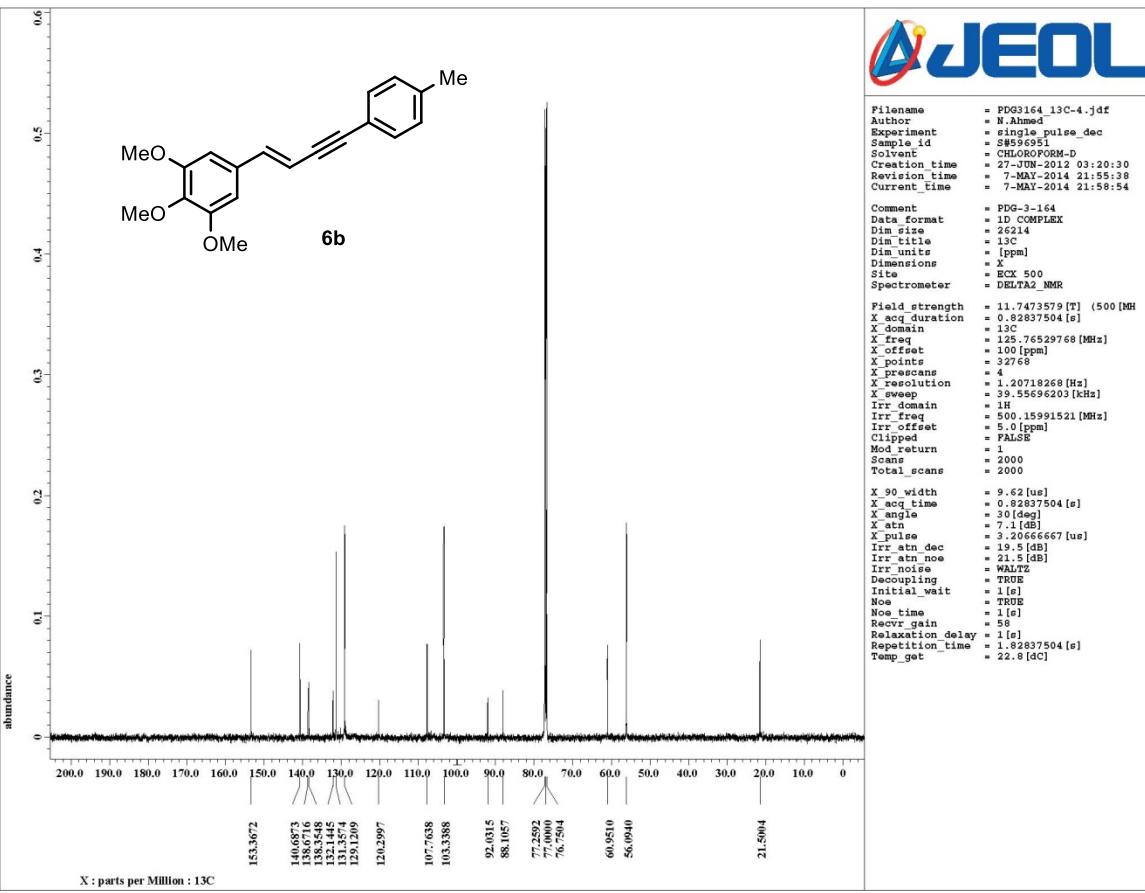
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-1,2,3-trimethoxy-5-(4-phenylbut-1-en-3-ynyl)benzene (**6a**)



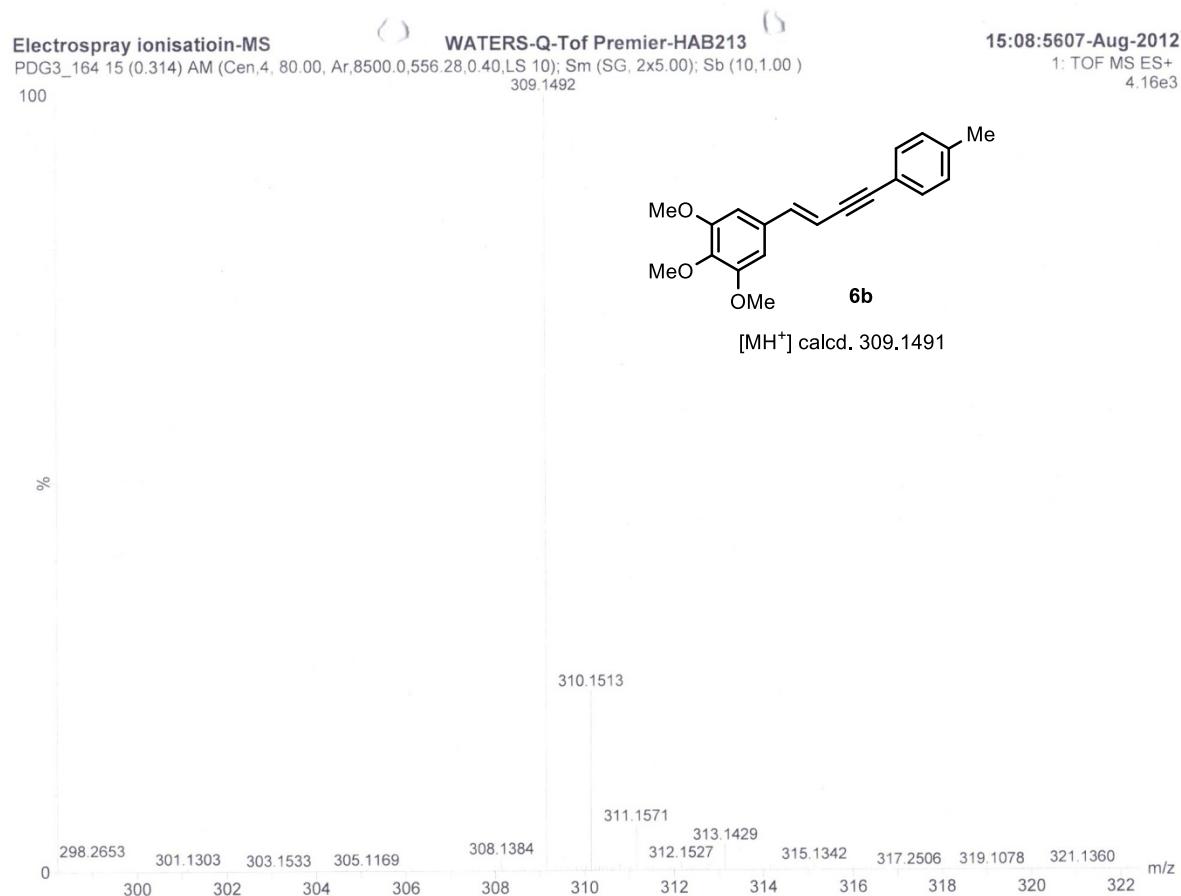
EI (HRMS) spectrum of (*E*)-1,2,3-trimethoxy-5-(4-phenylbut-1-en-3-ynyl)benzene (**6a**)



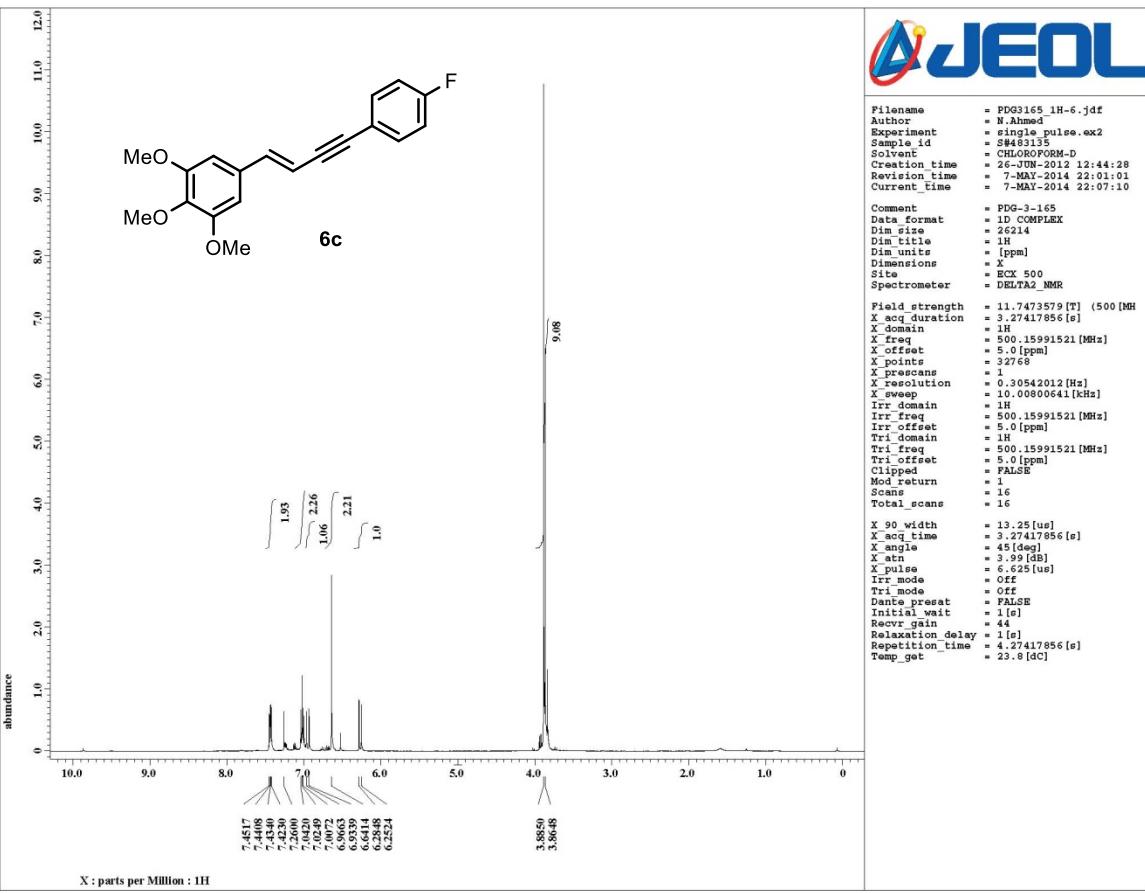
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1,2,3-trimethoxy-5-(4-p-tolylbut-1-en-3-ynyl)benzene (**6b**)



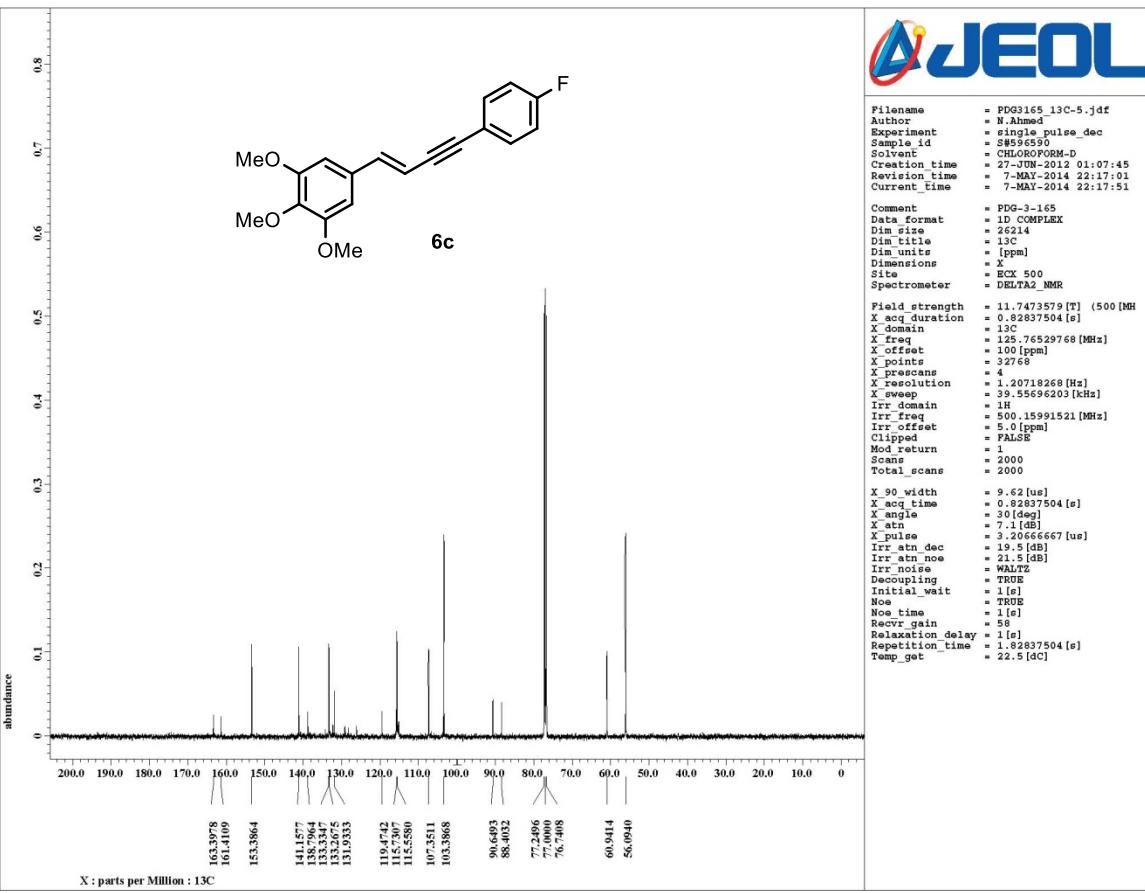
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1,2,3-trimethoxy-5-(4-*p*-tolylbut-1-en-3-ynyl)benzene (**6b**)



ESI (HRMS) spectrum of (*E*)-1,2,3-trimethoxy-5-(4-*p*-tolylbut-1-en-3-ynyl)benzene (**6b**)



¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-5-(4-fluorophenyl)but-1-en-3-yne-1,2,3-trimethoxybenzene (**6c**)



¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-5-(4-(4-fluorophenyl)but-1-en-3-yynyl)-1,2,3-trimethoxybenzene (**6c**)

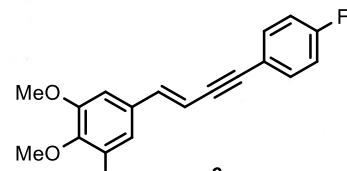
Electrospray ionisation-MS

PDG3-165 18 (0.388) AM (Cen,4, 90.00, Ar,8500.0,556.28,0.96,LS 10); Sm (SG, 2x5.00); Sb (10,1.00)
100 313.1245 647.2197

WATERS-Q-ToF Premier-HAB213

15:31:3729-Jun-2012

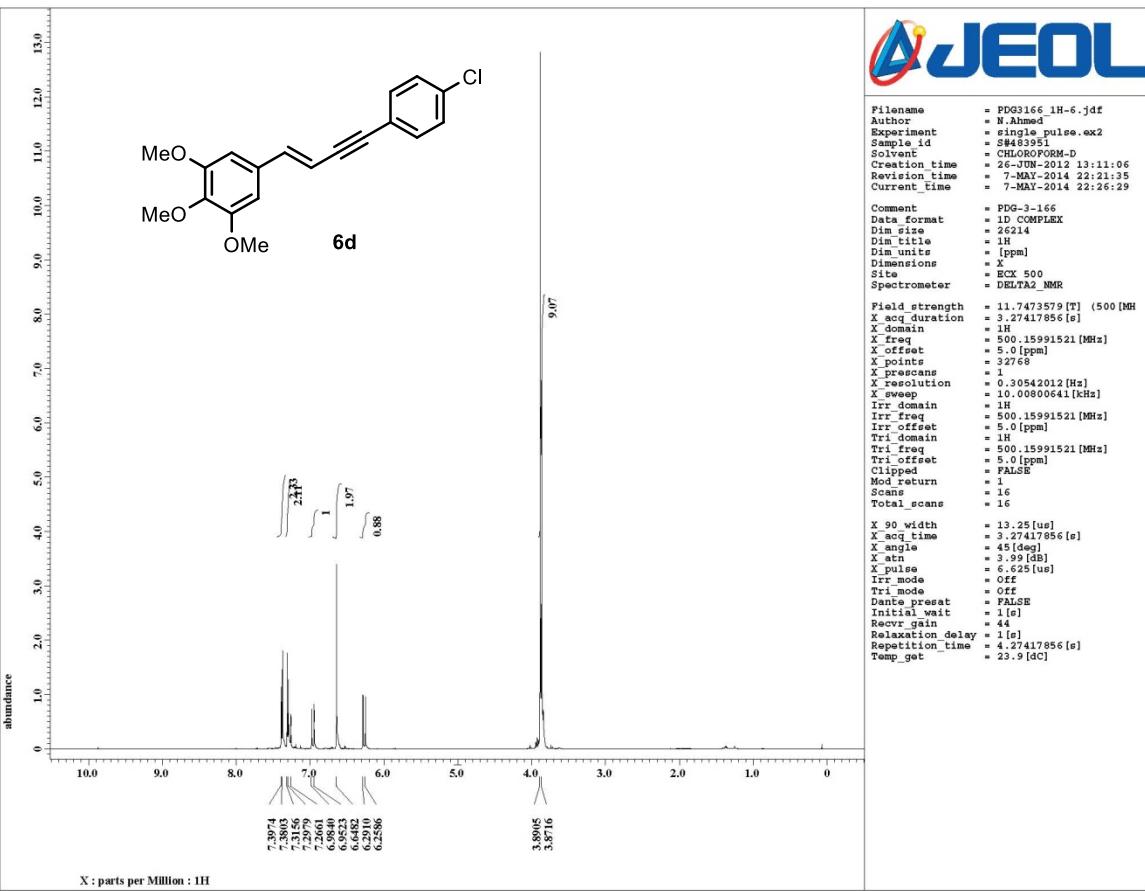
1: TOF MS ES+
3.25e3



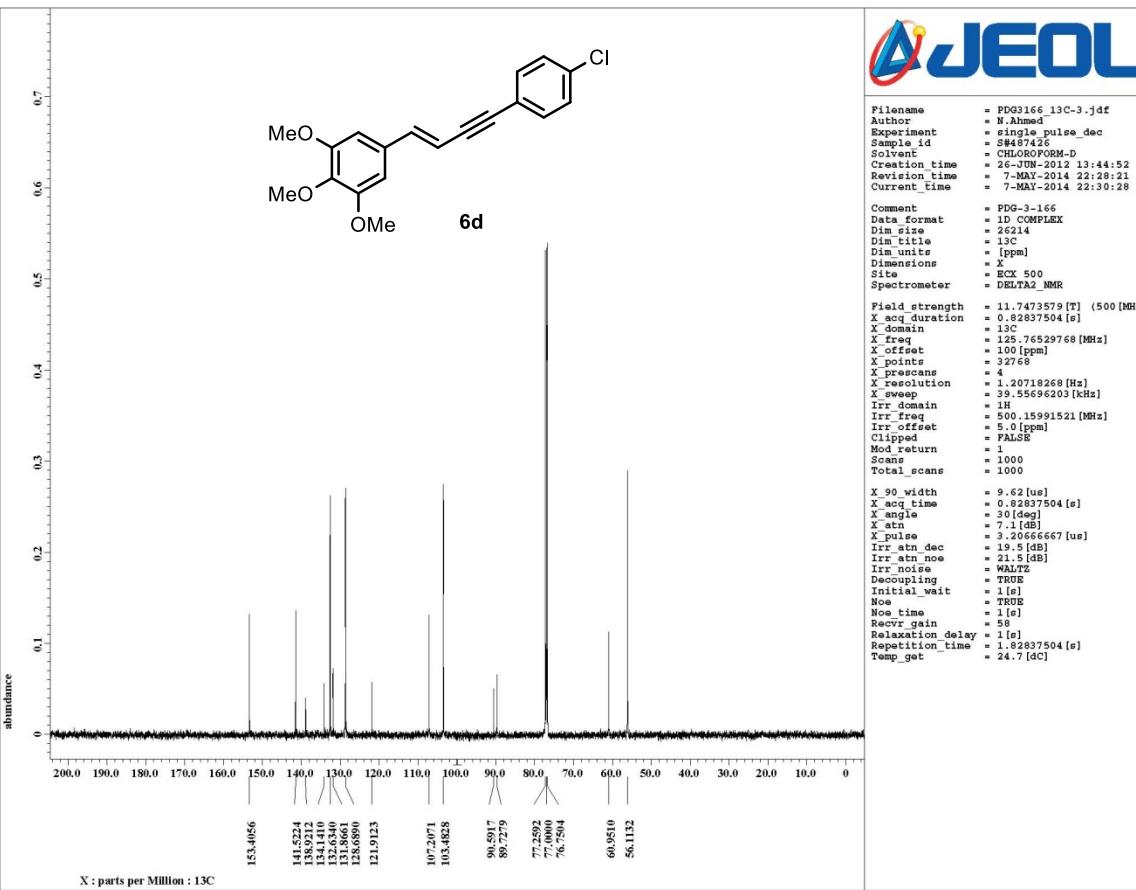
[MH⁺] calcd. 313.1240



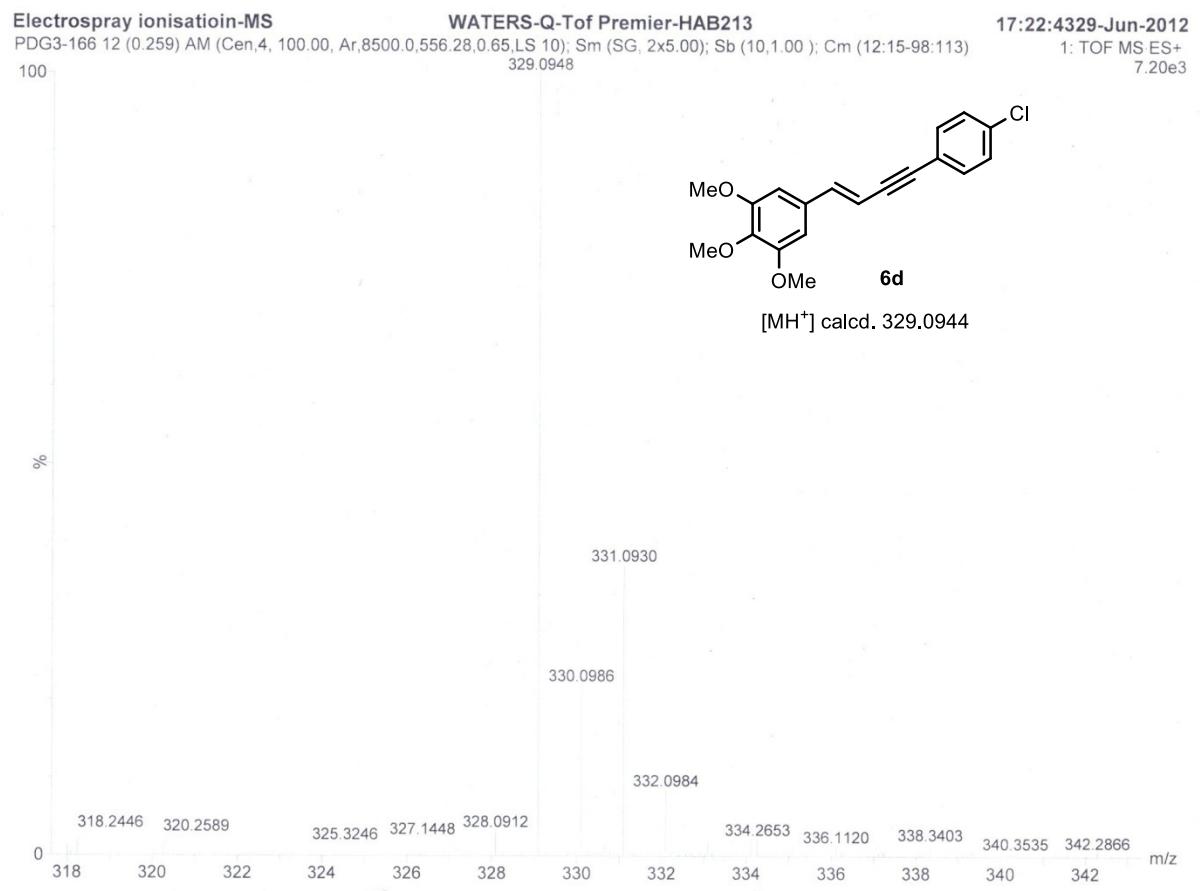
ESI (HRMS) spectrum of (*E*)-5-(4-(4-fluorophenyl)but-1-en-3ynyl)-1,2,3-trimethoxybenzene (**6c**)



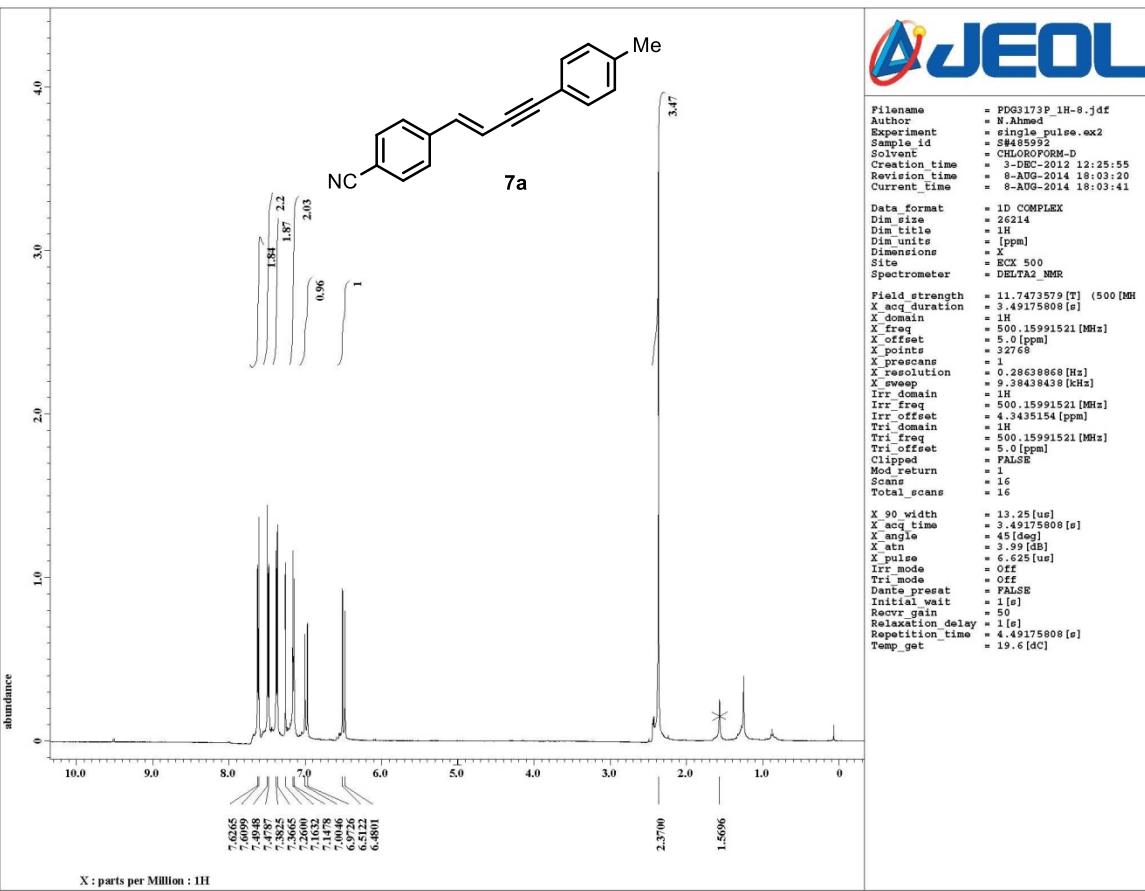
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-5-(4-(4-chlorophenyl)but-1-en-3-ynyl)-1,2,3-trimethoxybenzene (**6d**)



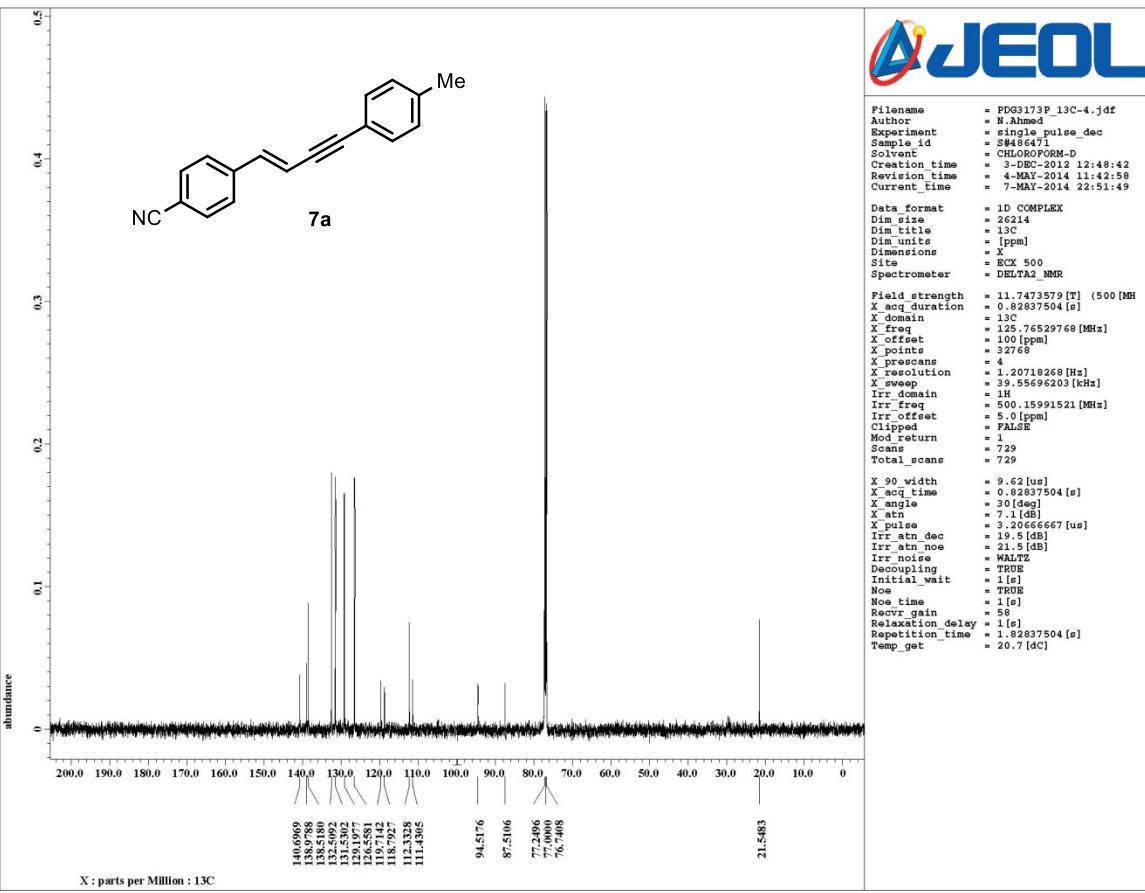
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-5-(4-(4-chlorophenyl)but-1-en-3-ynyl)-1,2,3-trimethoxybenzene (**6d**)



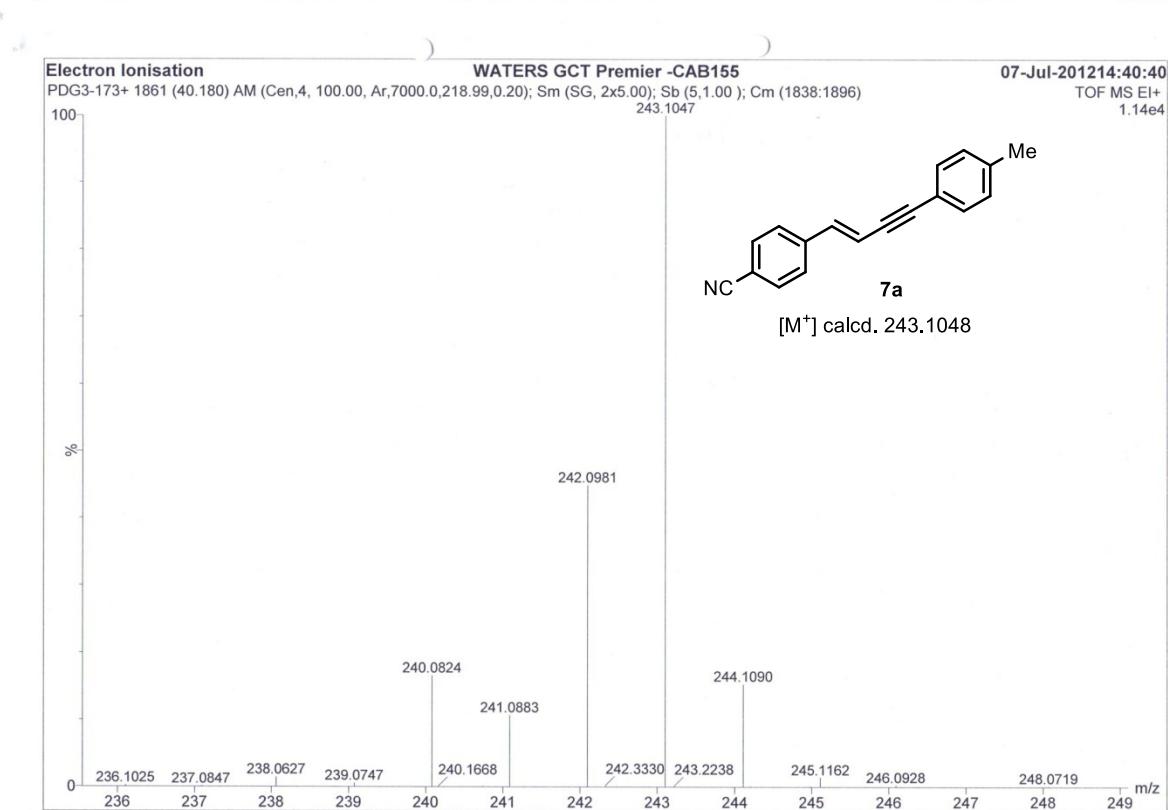
ESI (HRMS) spectrum of (*E*)-5-(4-(4-chlorophenyl)but-1-en-3ynyl)-1,2,3-trimethoxybenzene (**6d**)



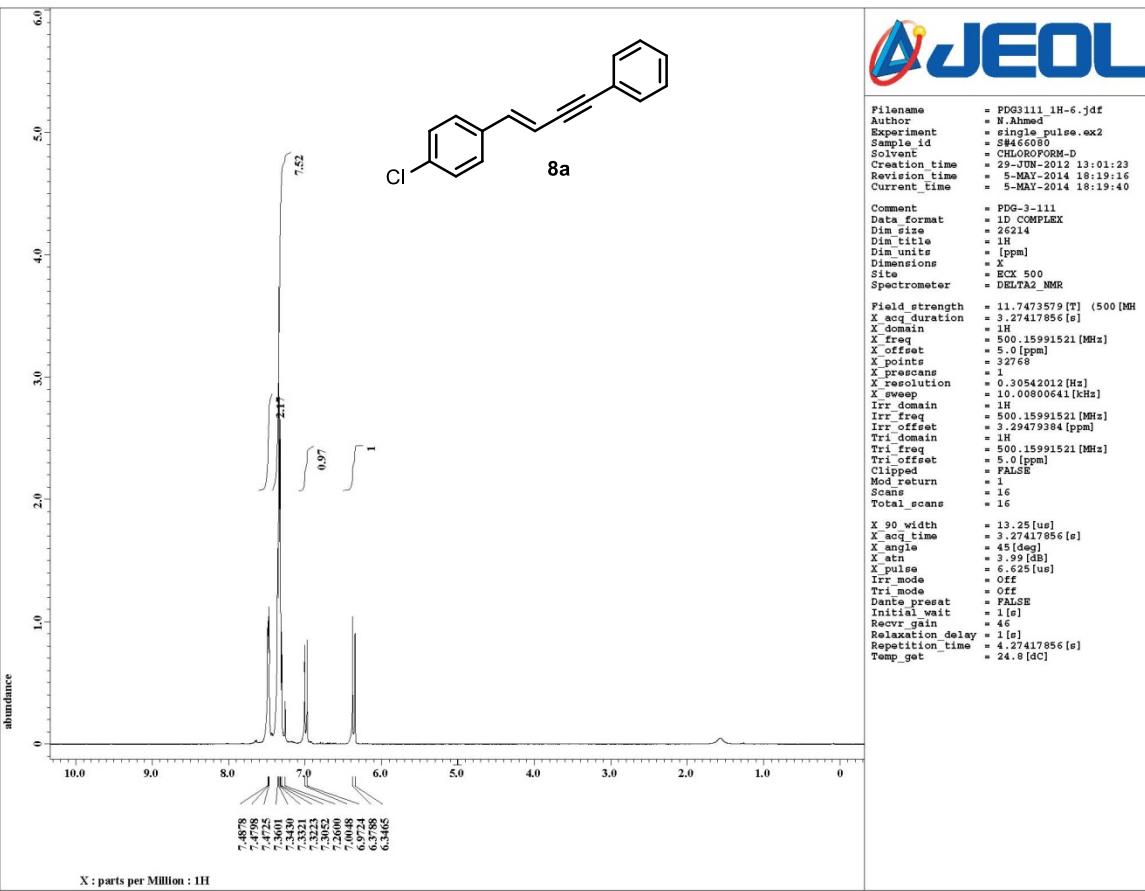
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-4-(4-(p-tolyl)but-1-en-3-ynyl)benzonitrile (**7a**)



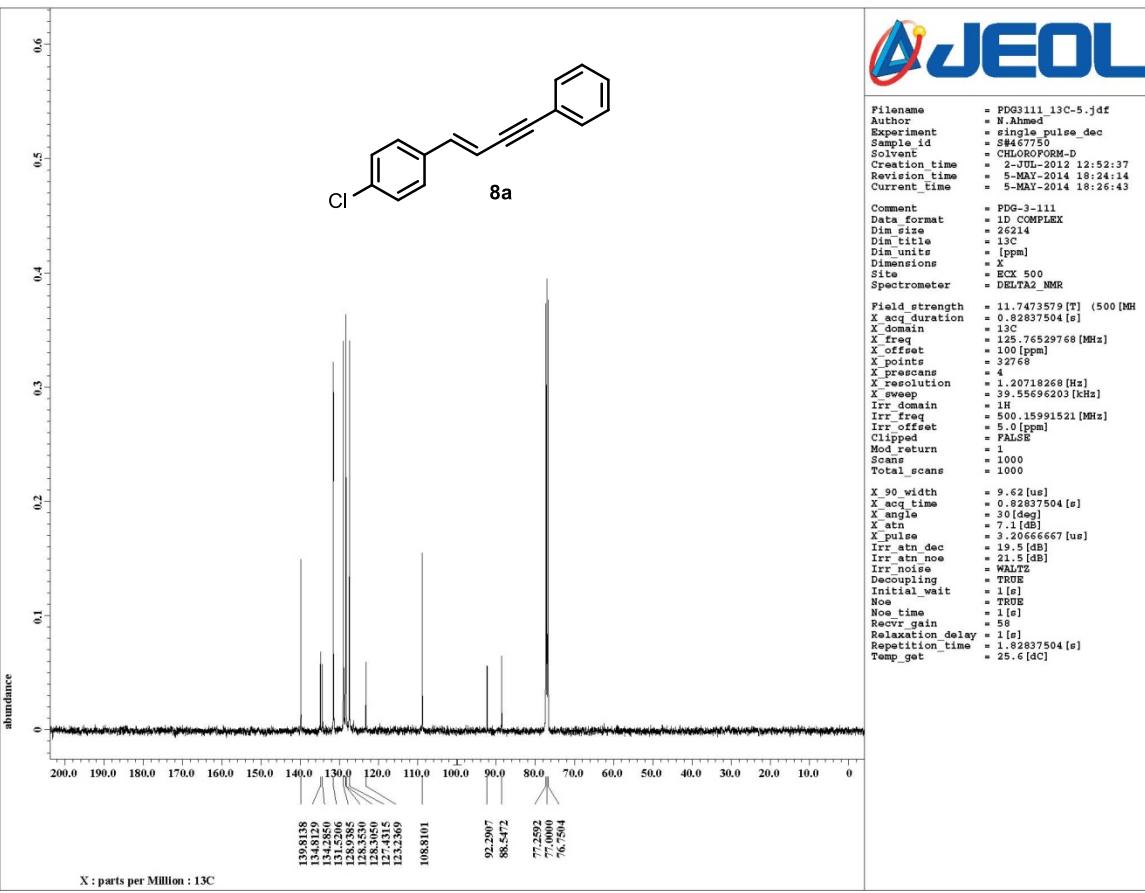
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-4-(4-(*p*-tolyl)but-1-en-3-ynyl)benzonitrile (**7a**)



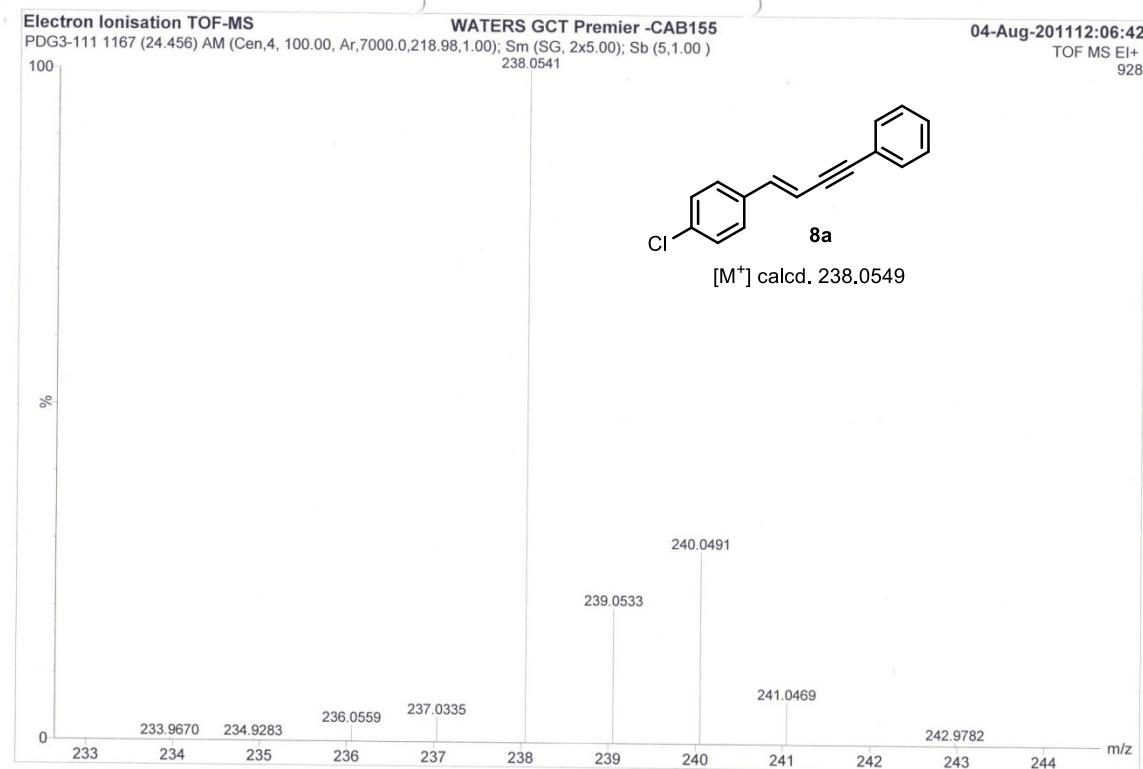
EI (HRMS) spectrum of (*E*)-4-(4-(*p*-tolyl)but-1-en-3-ynyl)benzonitrile (**7a**)



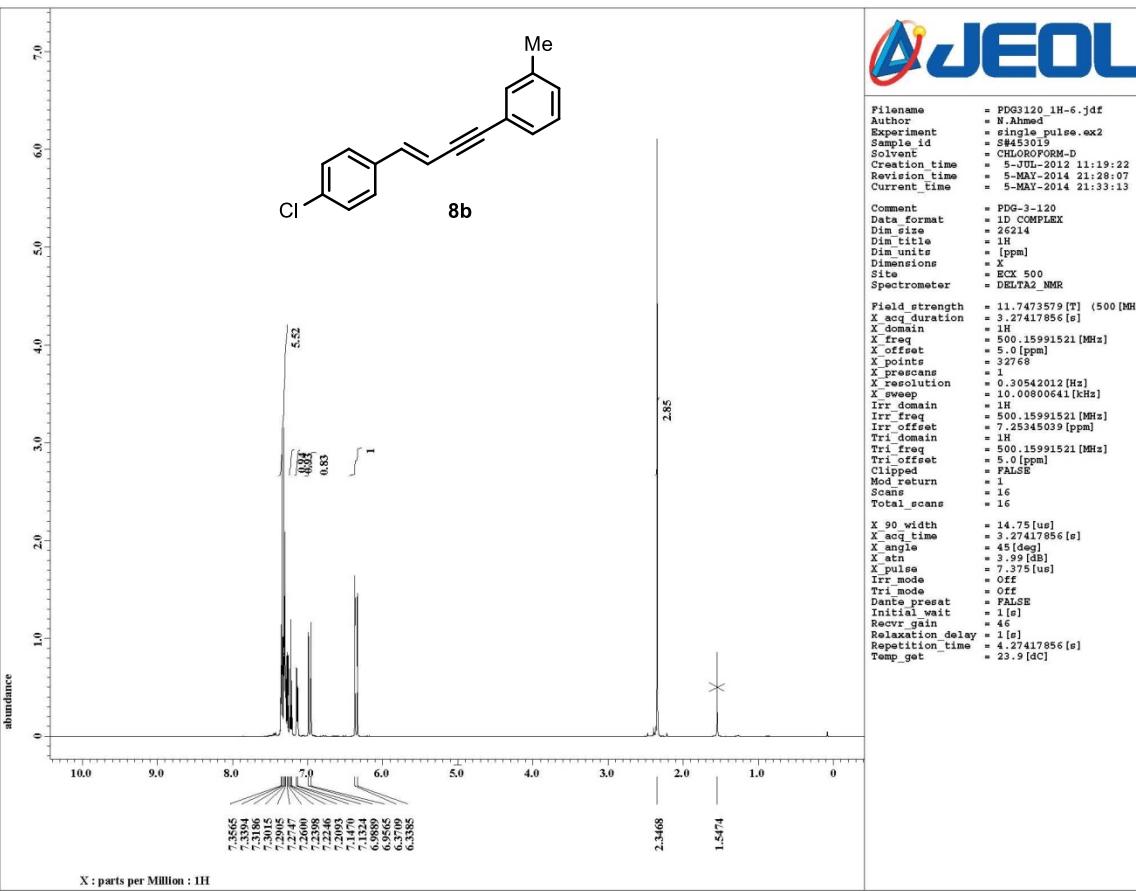
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-chloro-4-(4-phenylbut-1-en-3-ynyl)benzene (**8a**)



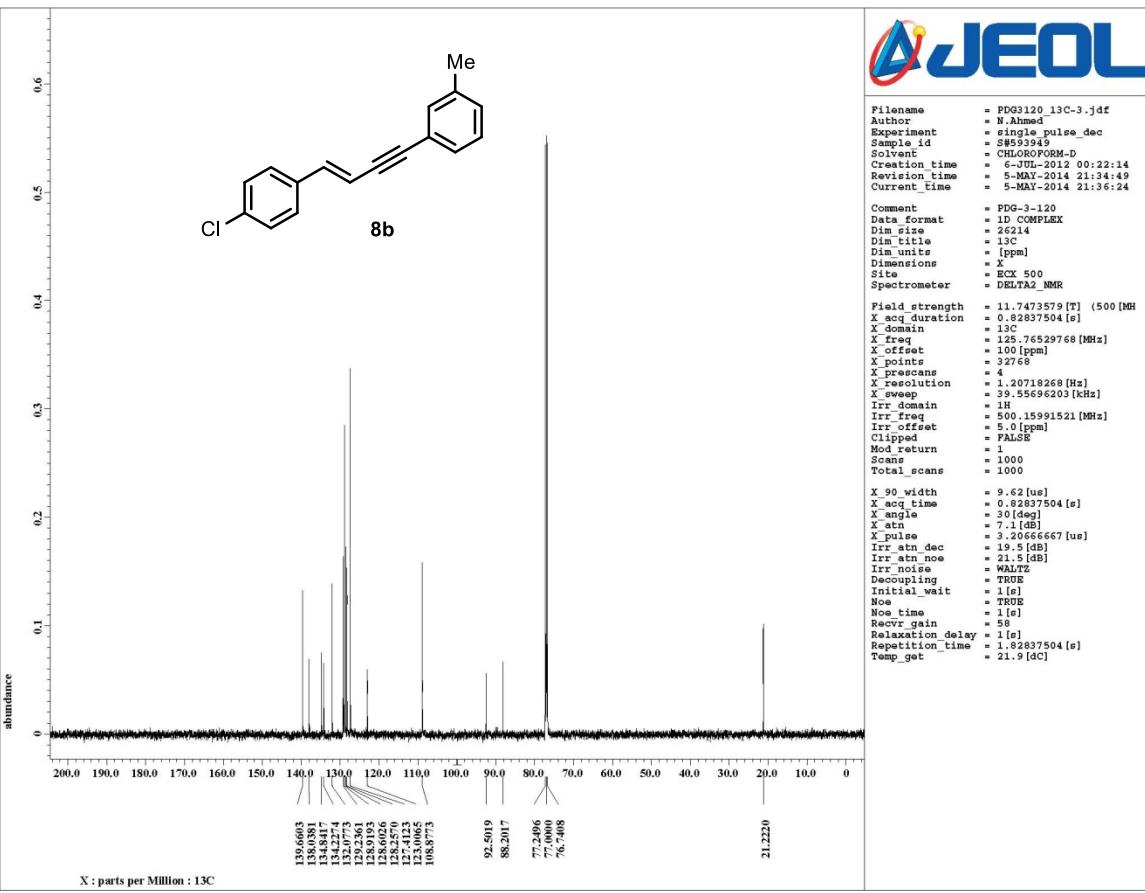
^{13}C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-phenylbut-1-en-3-ynyl)benzene (**8a**)



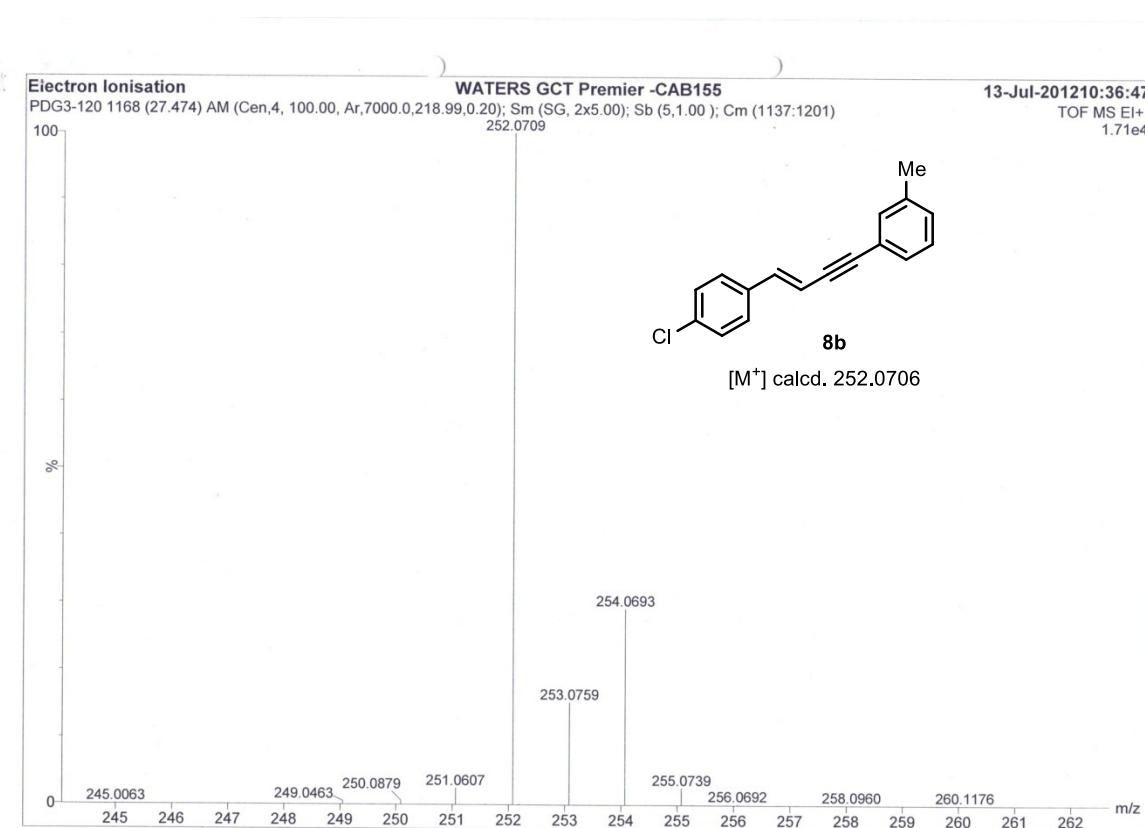
EI (HRMS) spectrum of (E)-1-chloro-4-(4-phenylbut-1-en-3-ynyl)benzene (**8a**)



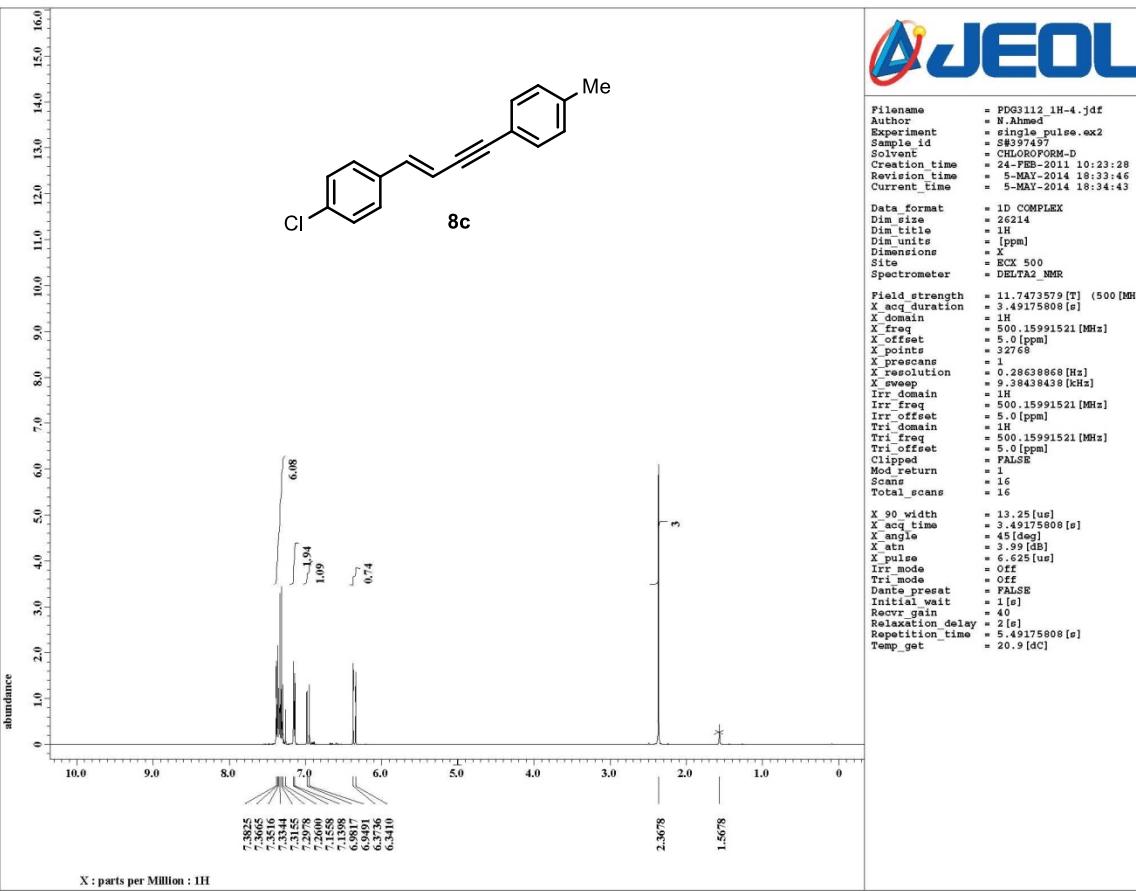
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-chlorophenyl)but-3-en-1-ynyl)-3-methylbenzene (**8b**)



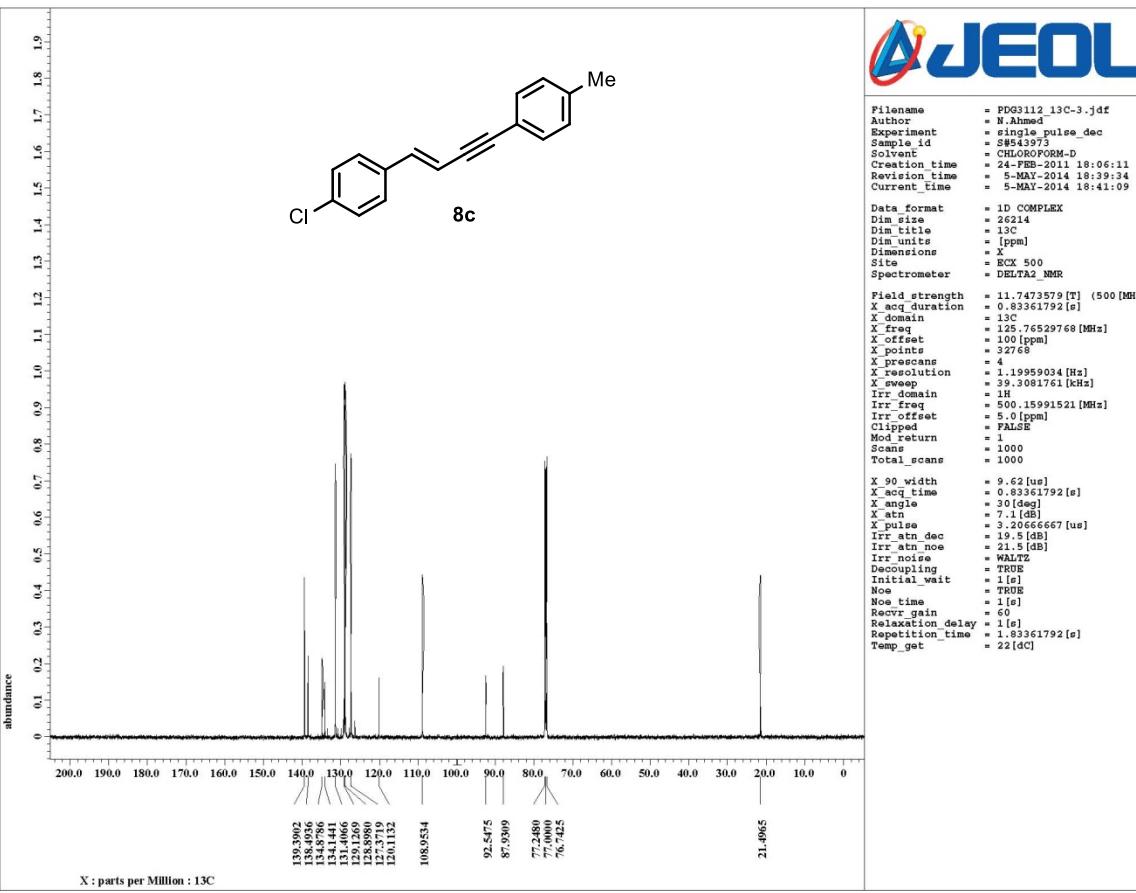
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-chlorophenyl)but-3-en-1-ynyl)-3-methylbenzene (**8b**)



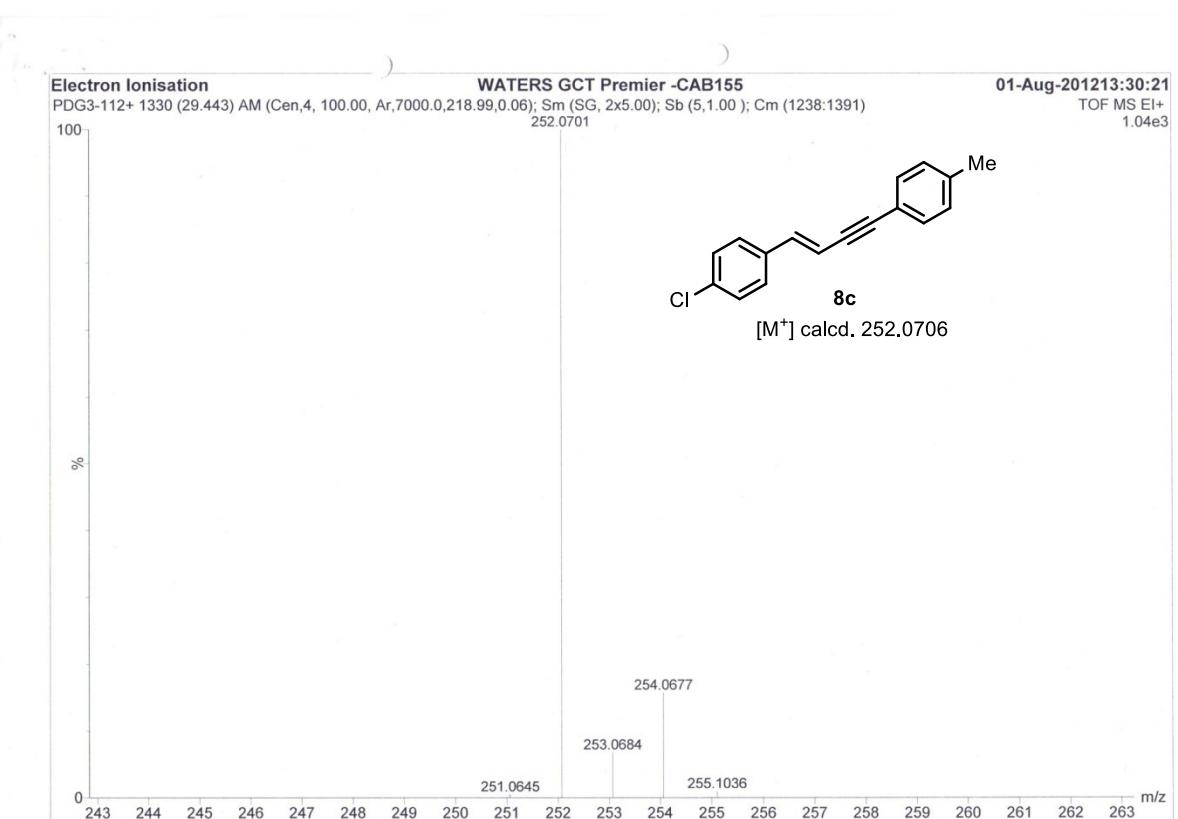
EI (HRMS) spectrum of (*E*)-1-(4-(4-chlorophenyl)but-3-en-1-ynyl)-3-methylbenzene (**8b**)

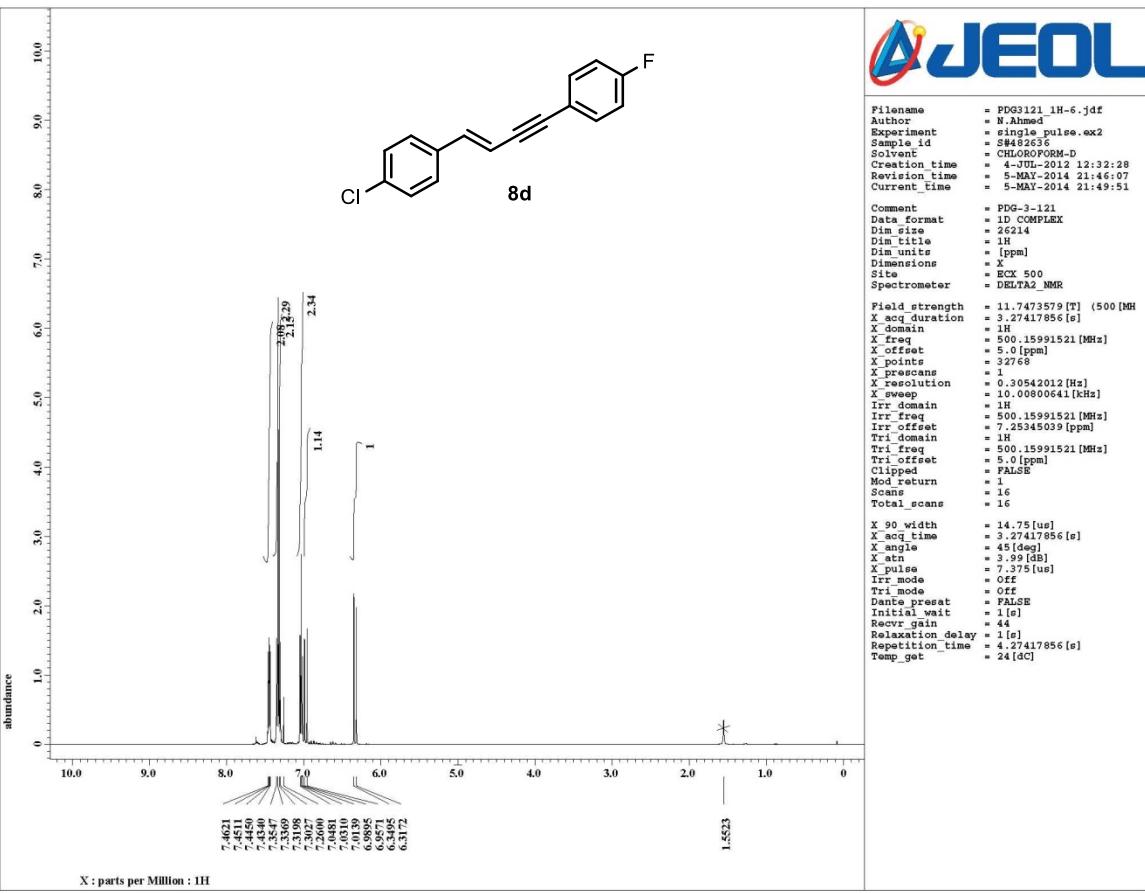


¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-*p*-tolylbut-1-en-3-ynyl)benzene (**8c**)

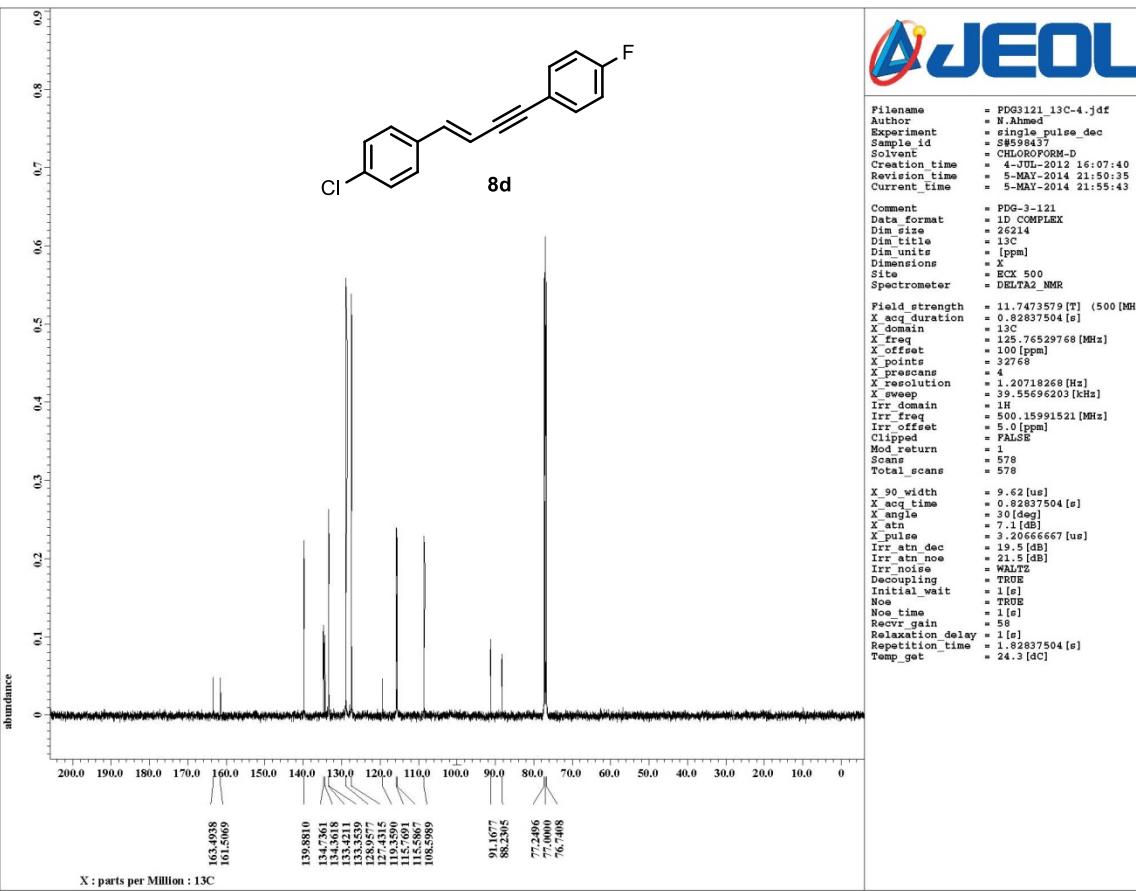


^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-1-chloro-4-(4-*p*-tolylbut-1-en-3ynyl)benzene (**8c**)

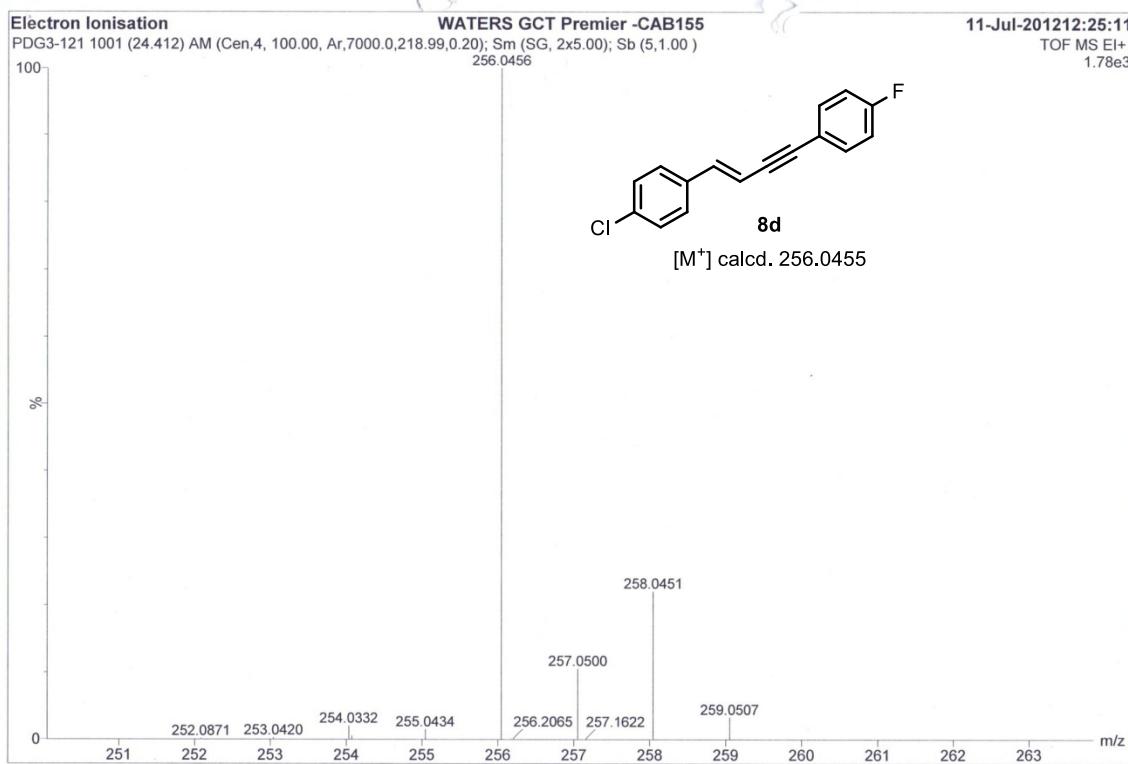




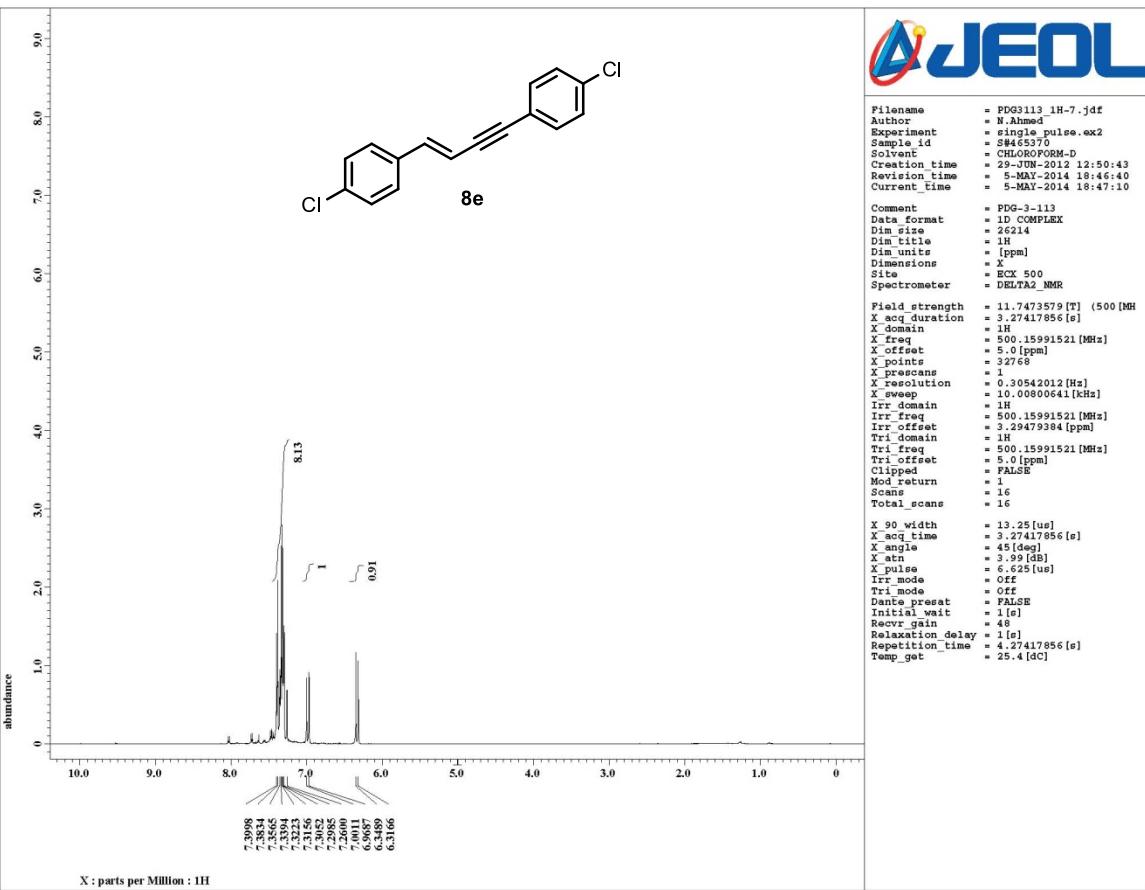
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-chloro-4-(4-fluorophenyl)but-1-en-3-yne (8d)

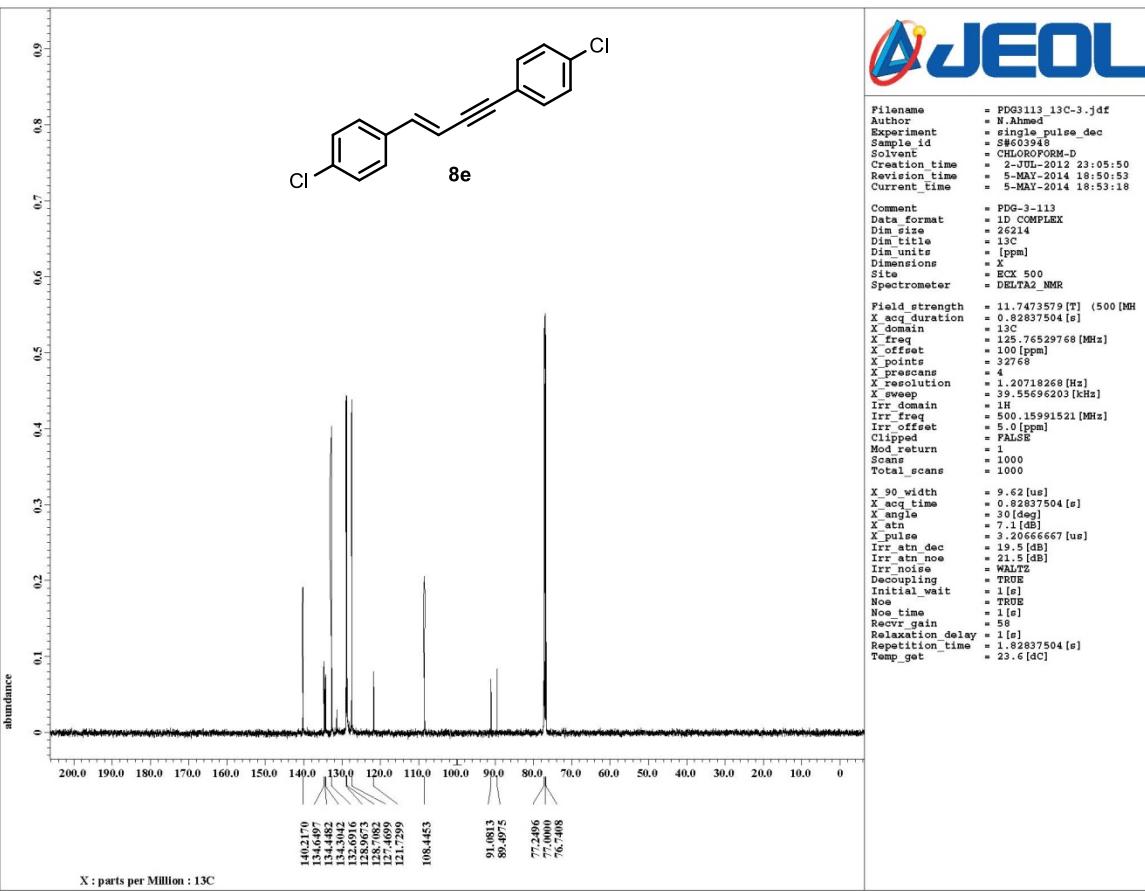


^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-1-chloro-4-(4-(4-fluorophenyl)but-1-en-3-ynyl)benzene (**8d**)

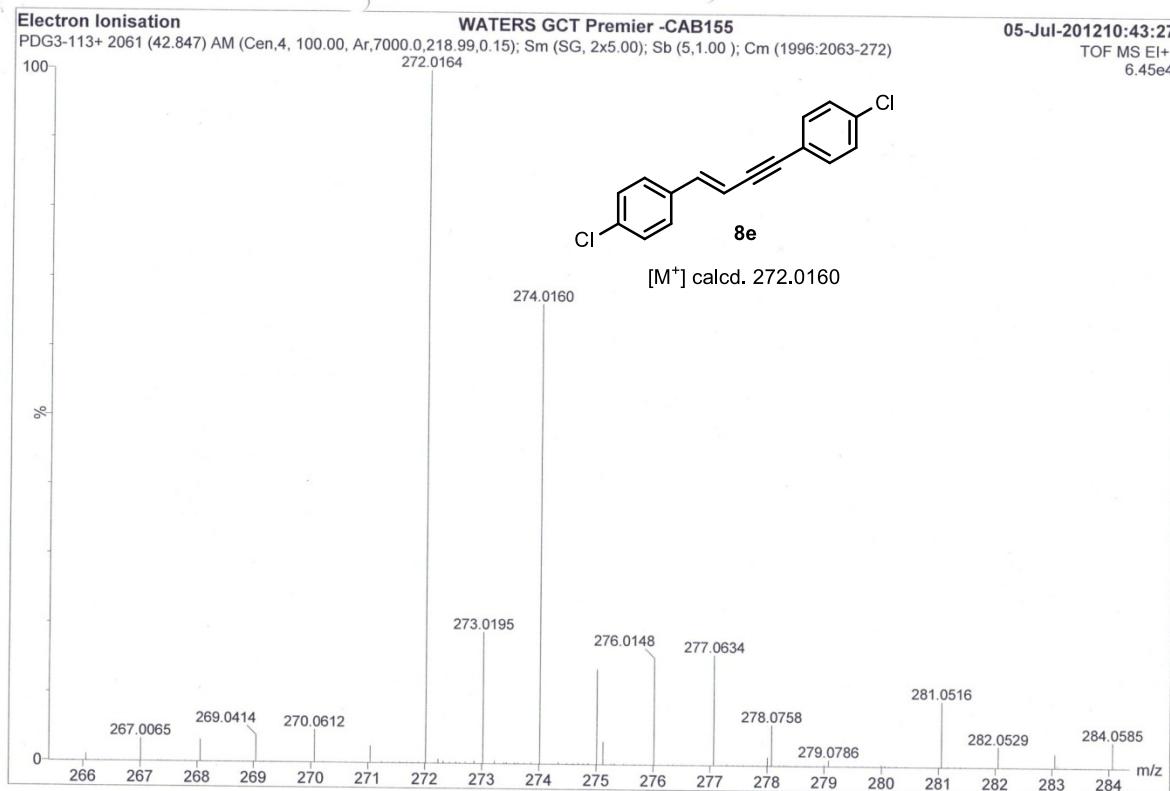


EI (HRMS) spectrum of (*E*)-1-chloro-4-(4-(4-fluorophenyl)but-1-en-3-ynyl)benzene (**8d**)

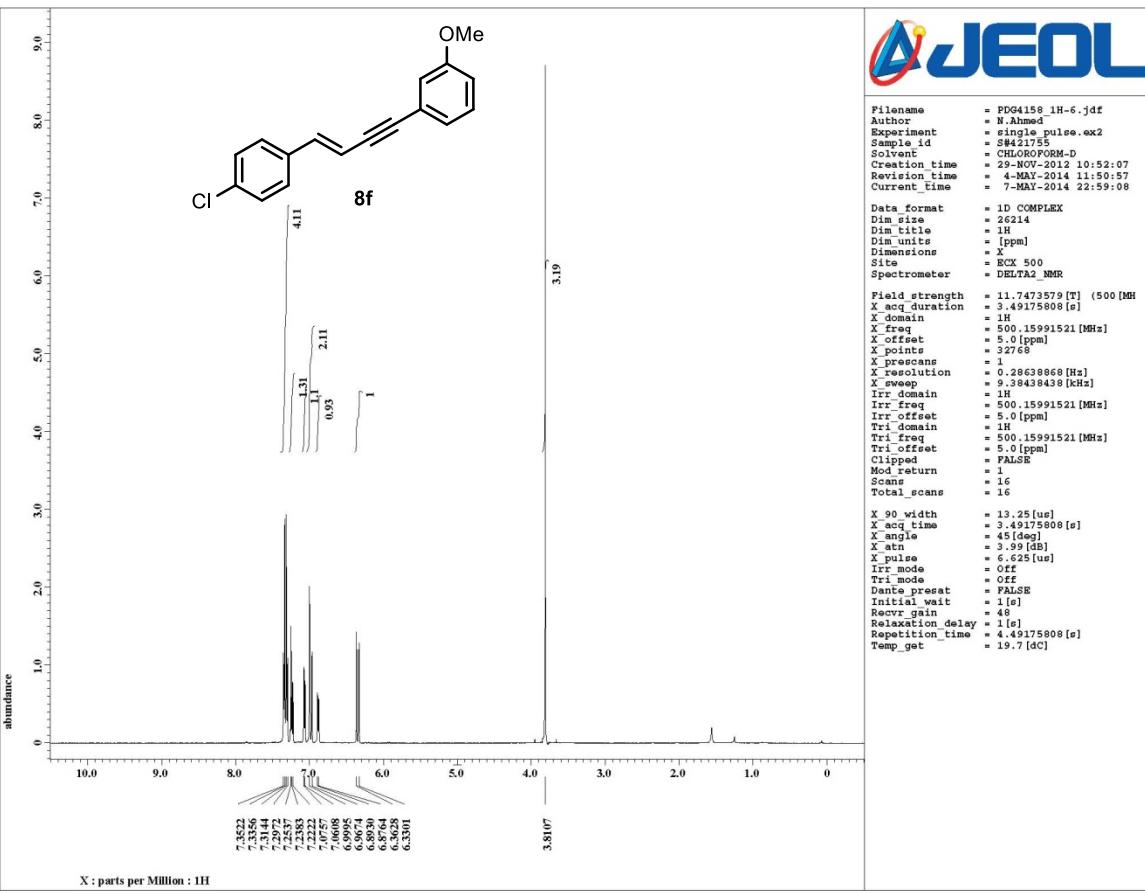




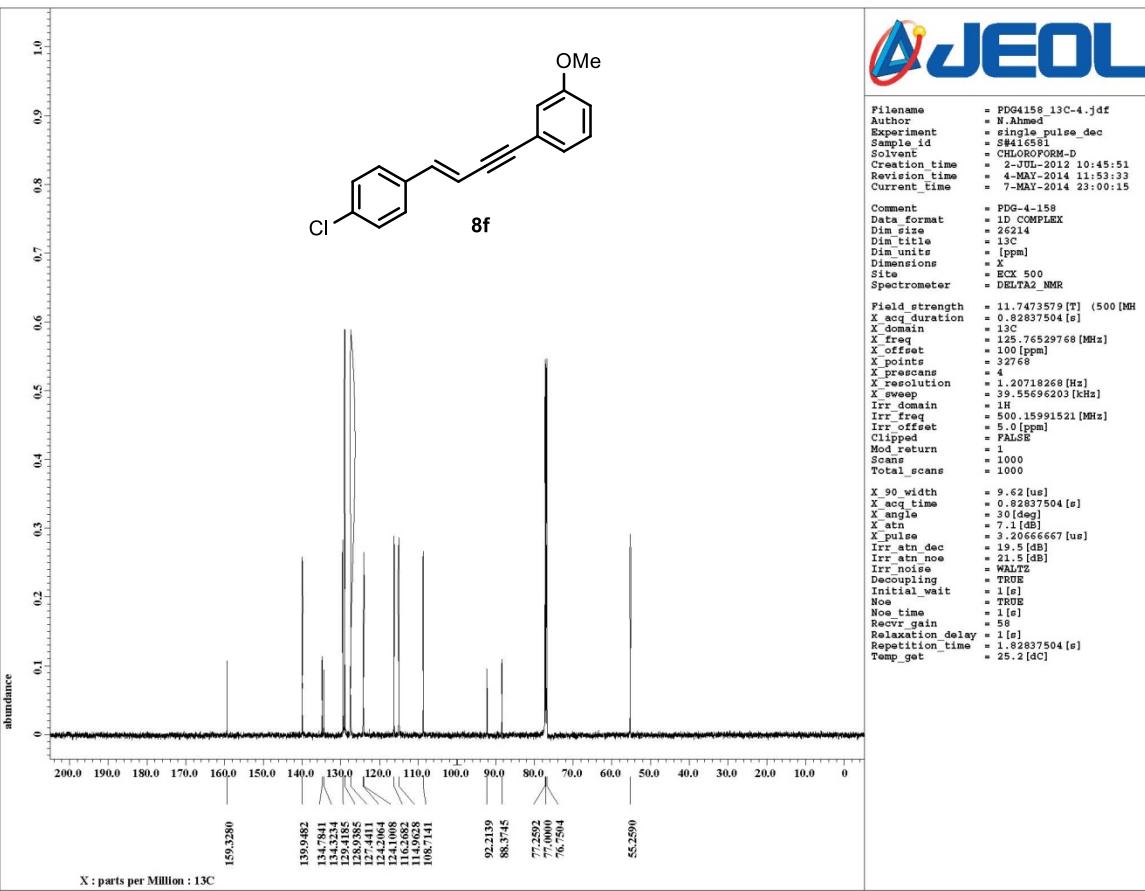
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(chlorobenzene) (**8e**)



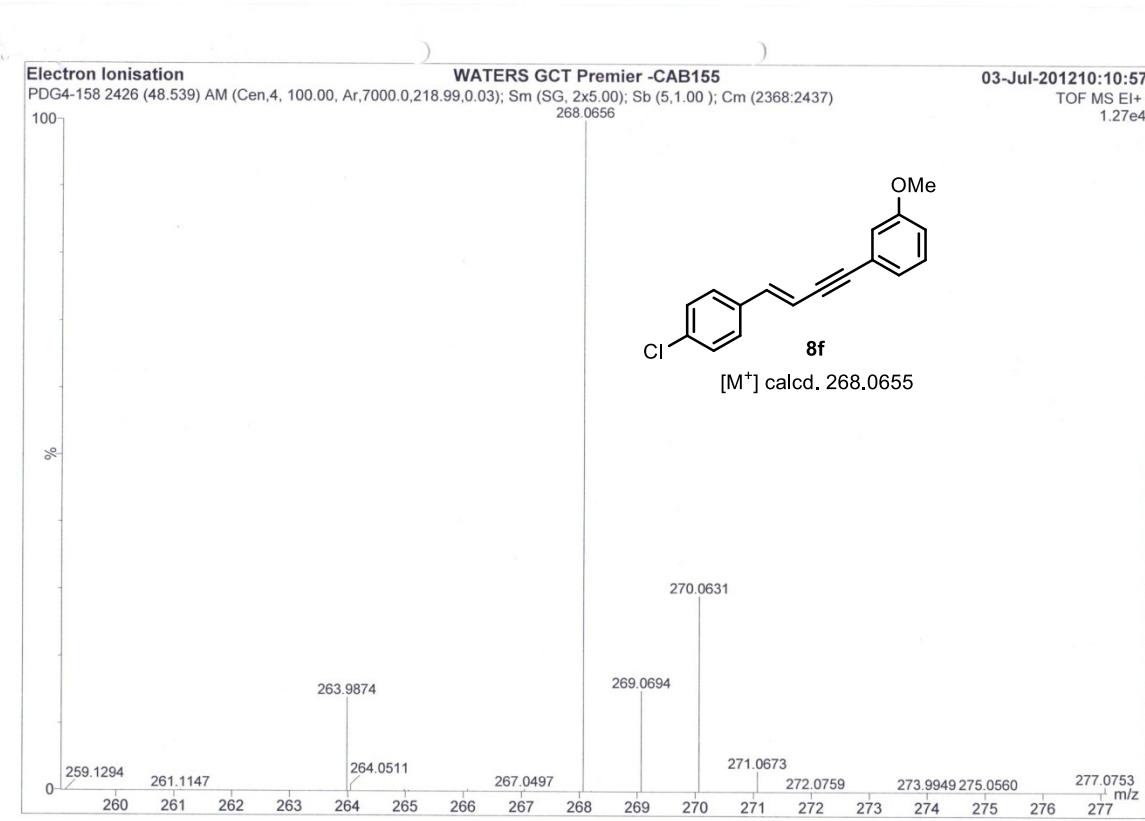
EI (HRMS) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(chlorobenzene) (**8e**)



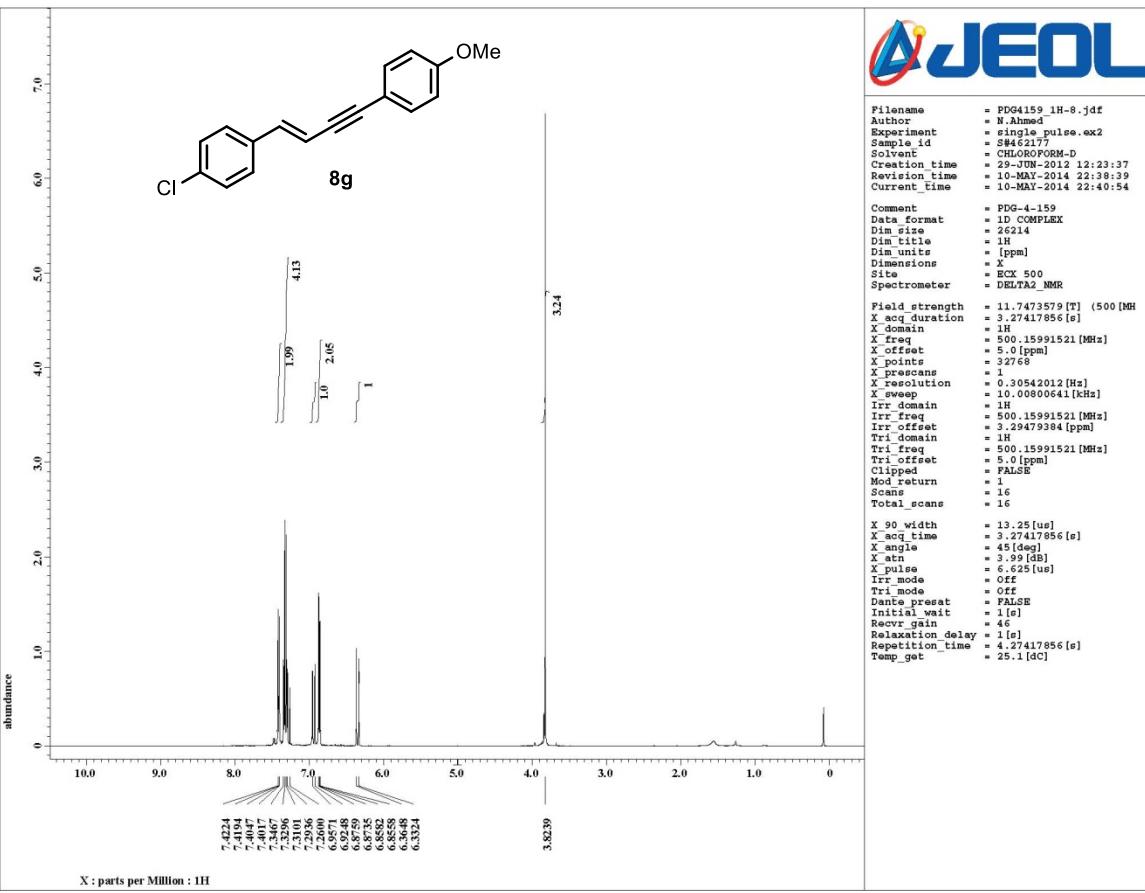
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-chlorophenyl)but-3-en-1-ynyl)-3-methoxybenzene (**8f**)



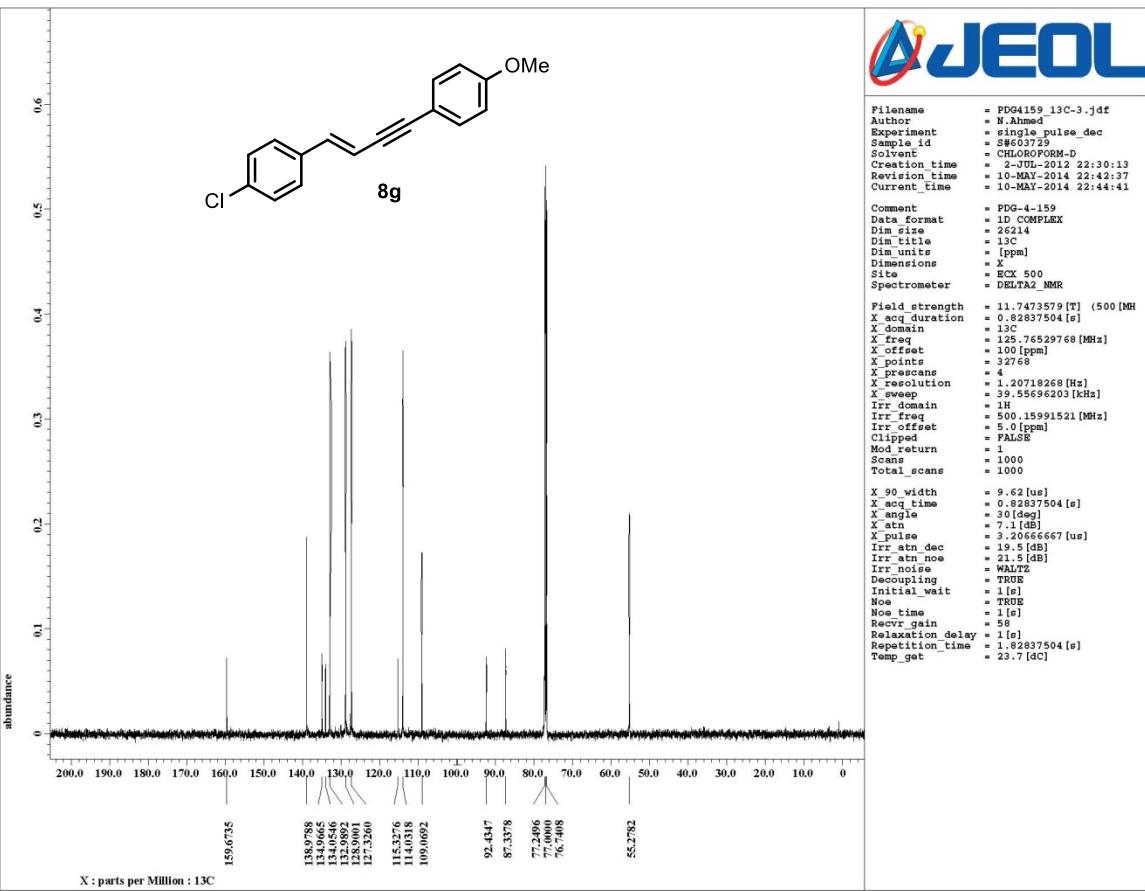
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-chlorophenyl)but-3-en-1-ynyl)-3-methoxybenzene (**8f**)



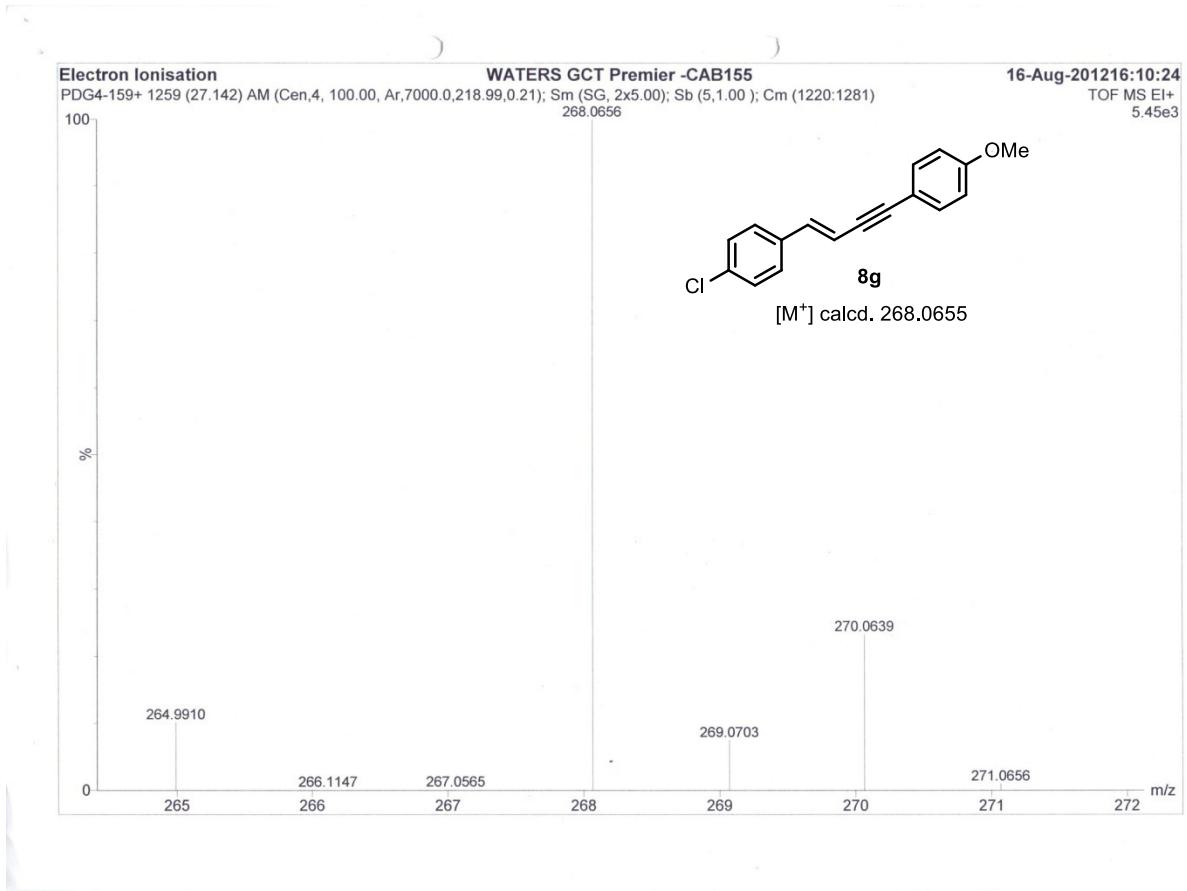
EI (HRMS) spectrum of (*E*)-1-(4-(4-chlorophenyl)but-3-en-1-ynyl)-3-methoxybenzene (**8f**)



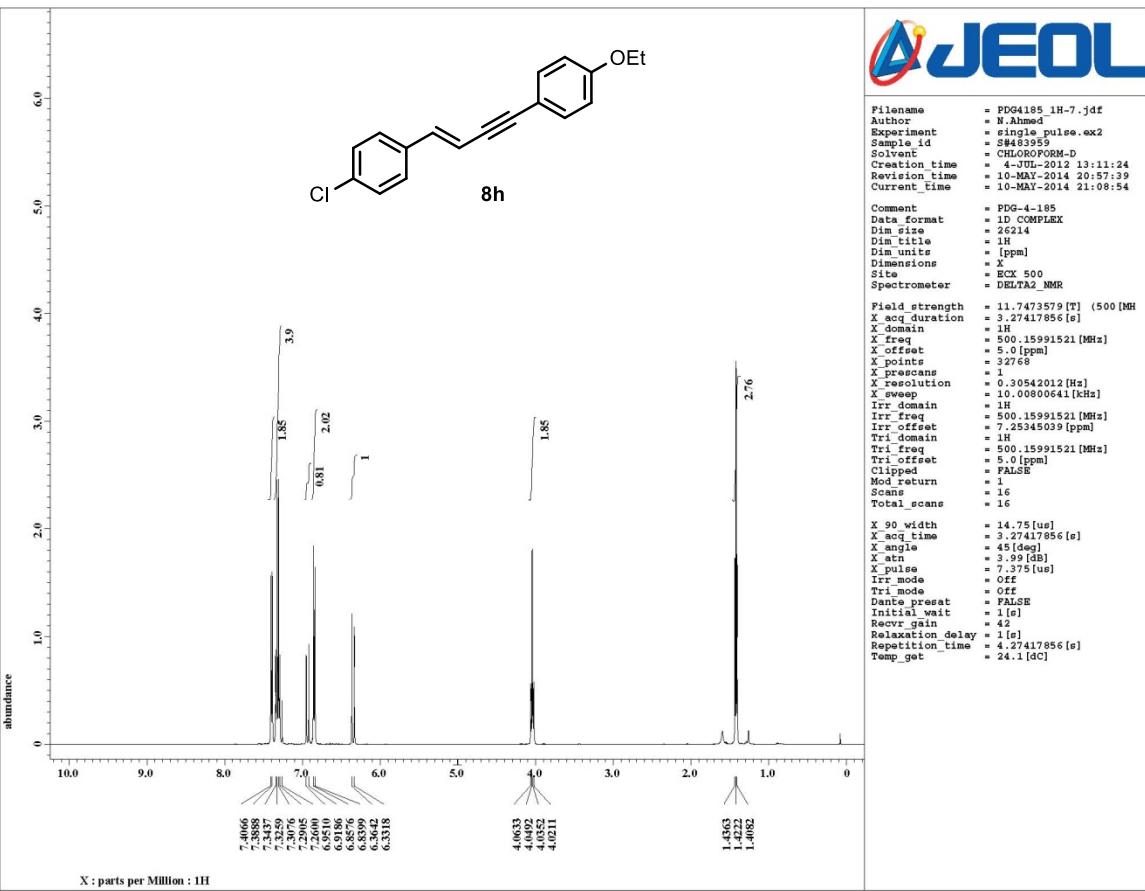
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-(4-methoxyphenyl)but-1-en-3-ynyl)benzene (**8g**)

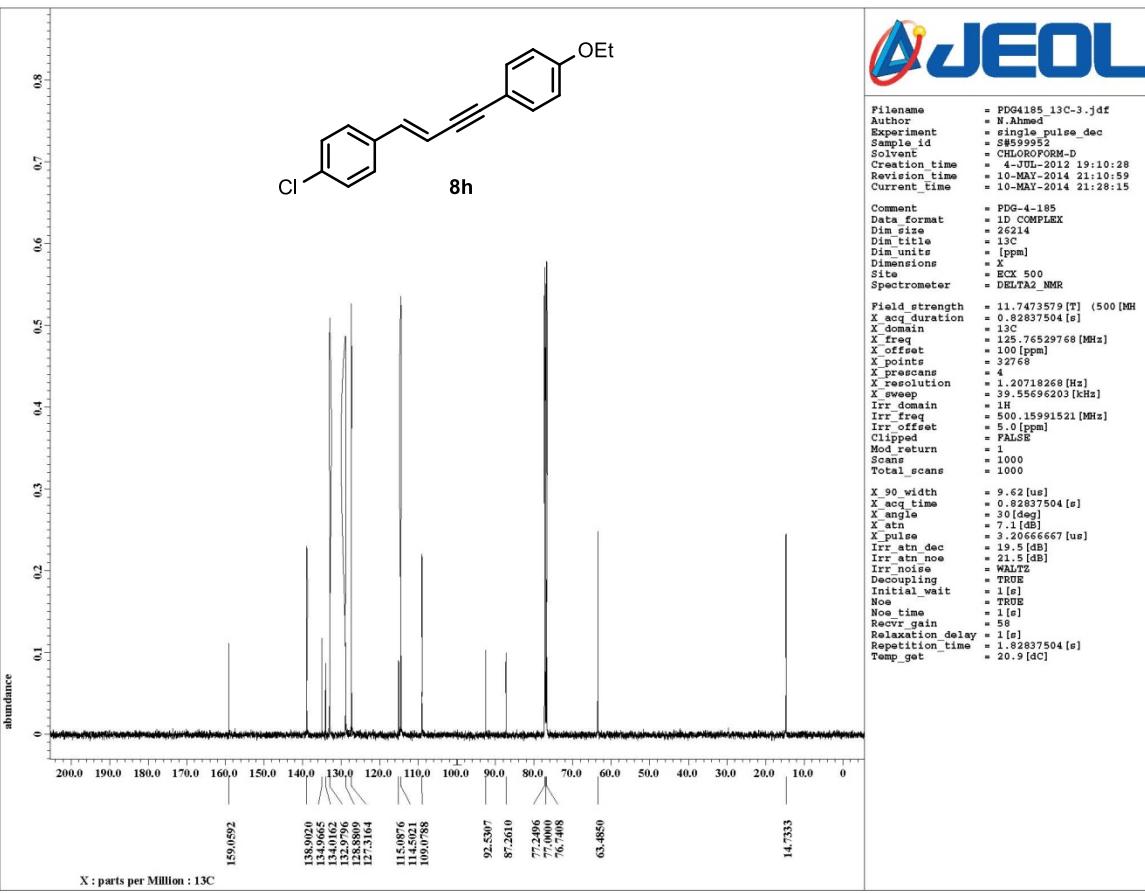


¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-(4-methoxyphenyl)but-1-en-3-ynyl)benzene (**8g**)

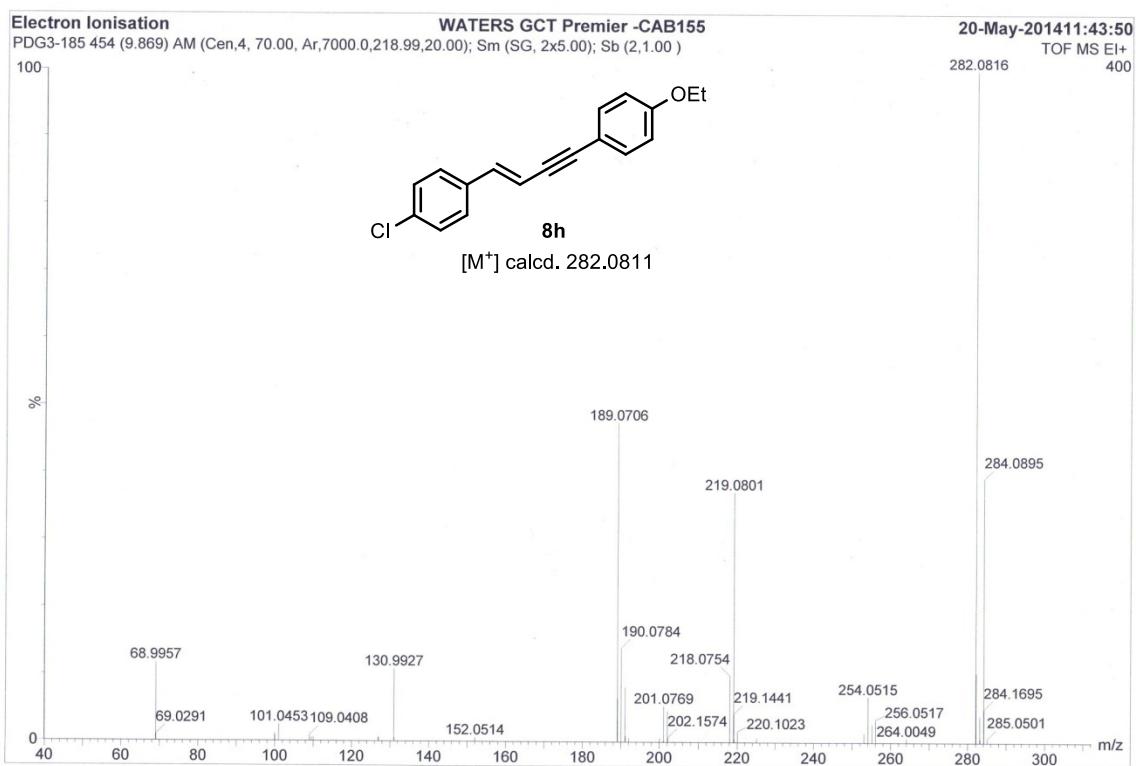


EI (HRMS) spectrum of (*E*)-1-chloro-4-(4-(4-methoxyphenyl)but-1-en-3-ynyl)benzene (**8g**)

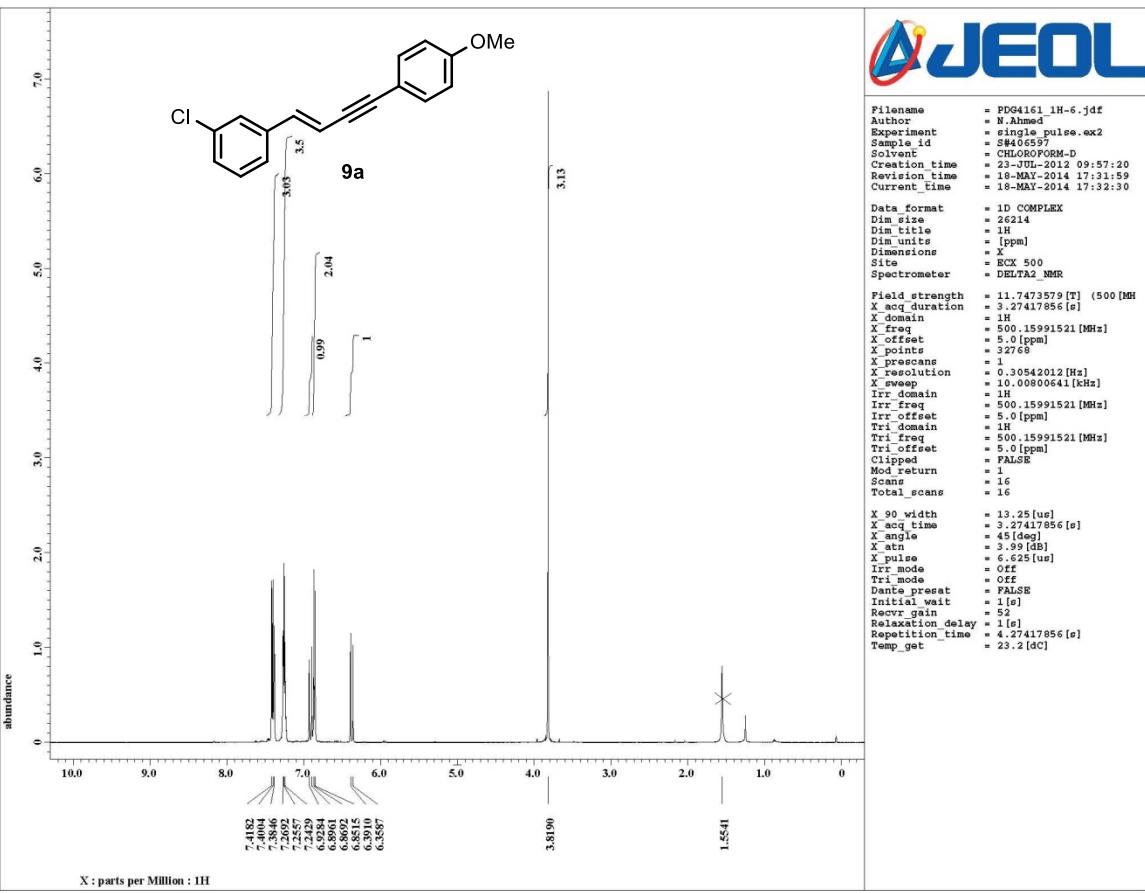




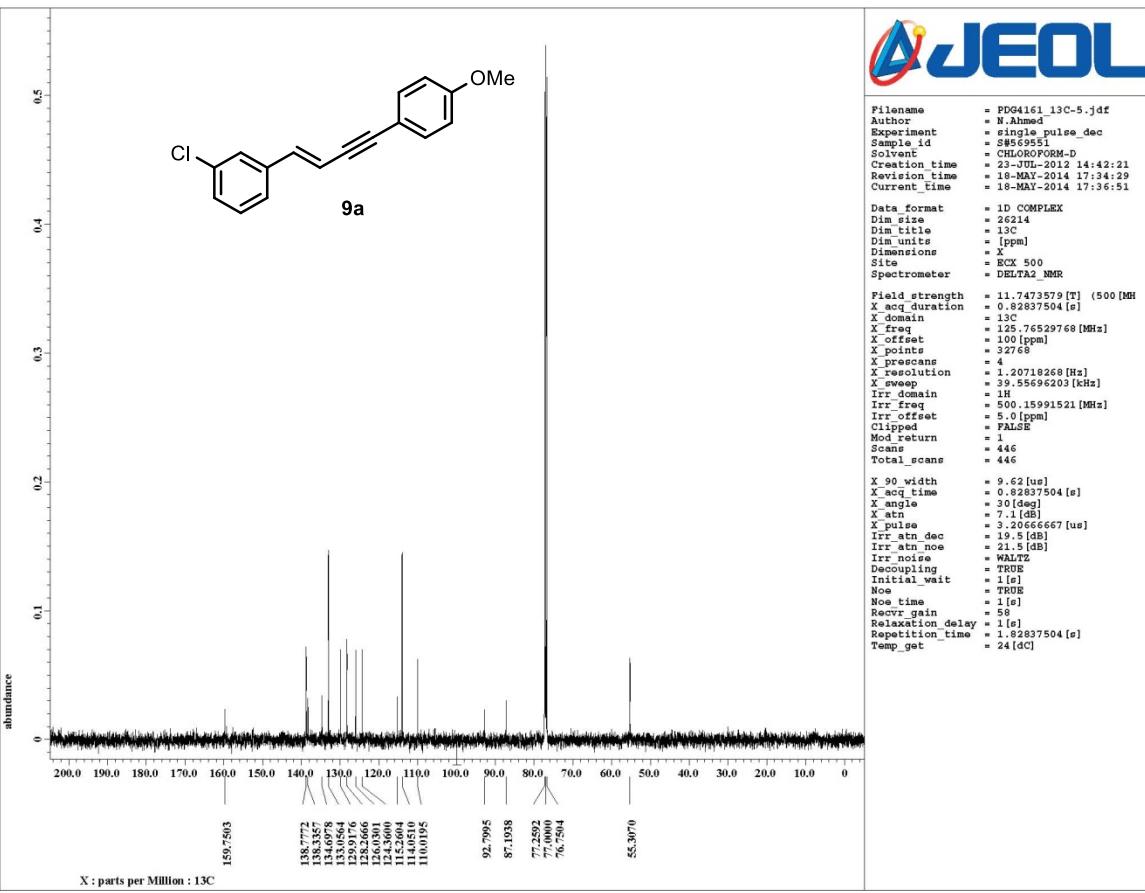
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-(4-ethoxyphenyl)but-1-en-3-ynyl)benzene (**8h**)



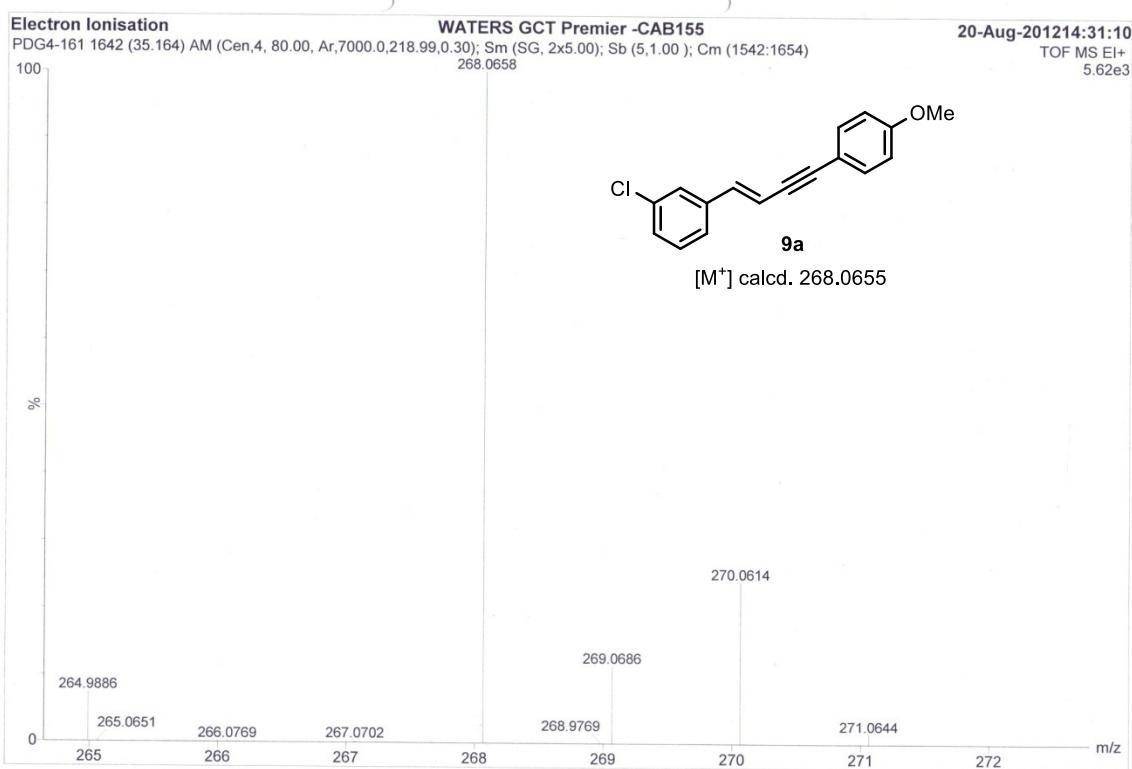
EI (HRMS) spectrum of (*E*)-1-chloro-4-(4-ethoxyphenyl)but-1-en-3-ynylbenzene (**8h**)



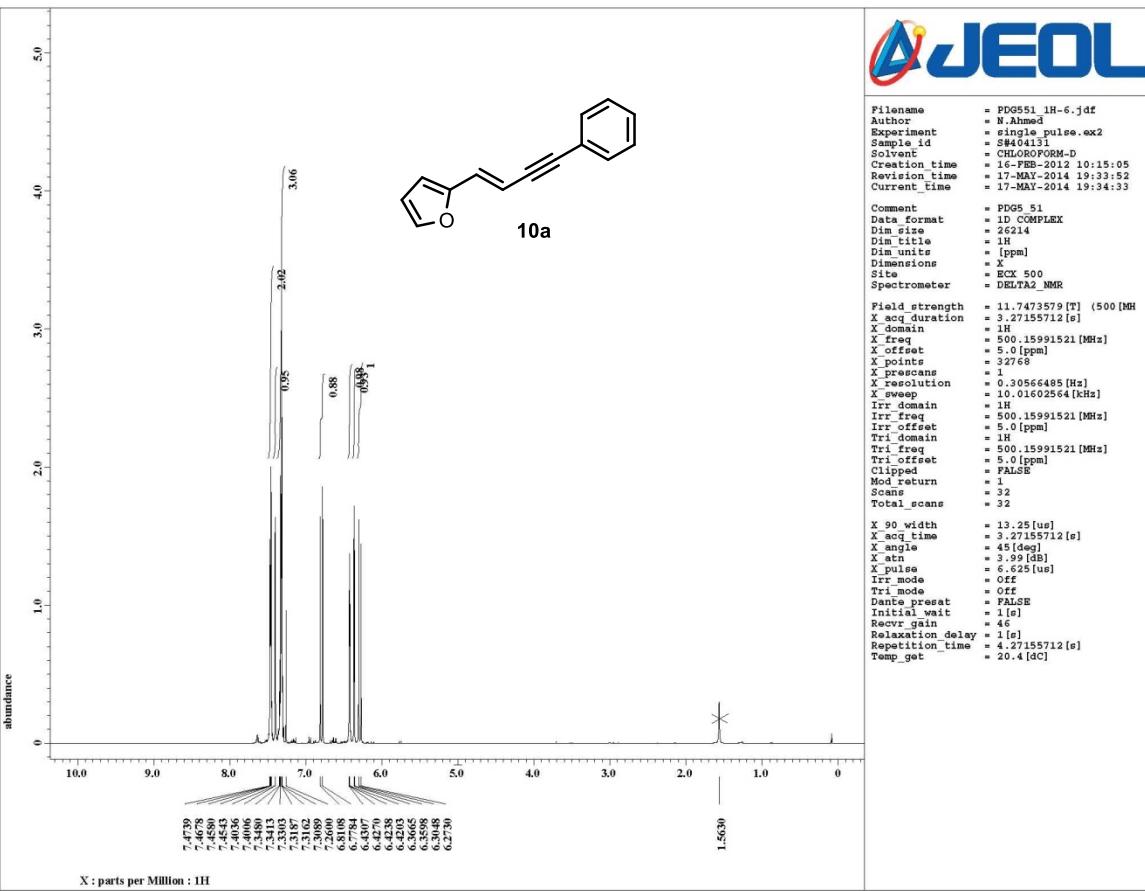
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-chloro-3-(4-(4-methoxyphenyl)but-1-en-3-ynyl)benzene (**9a**)



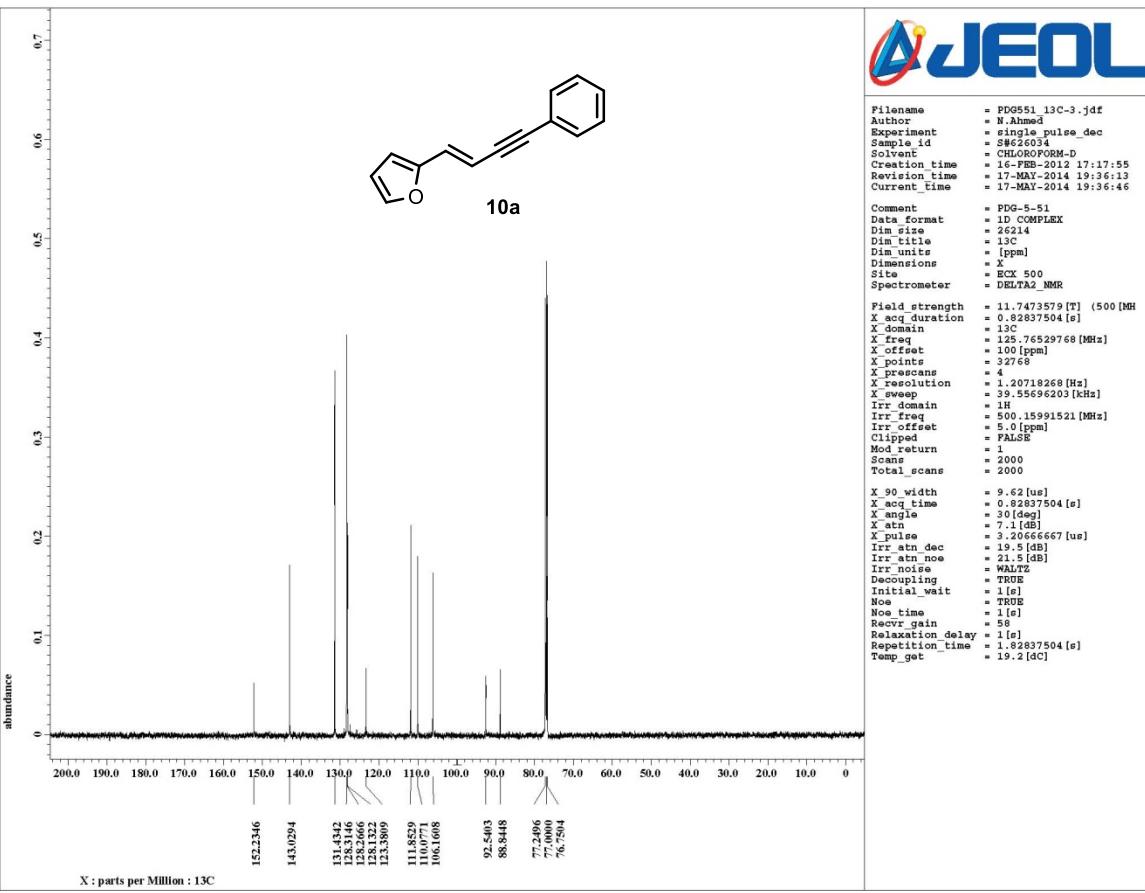
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-chloro-3-(4-(4-methoxyphenyl)but-1-en-3-ynyl)benzene (**9a**)



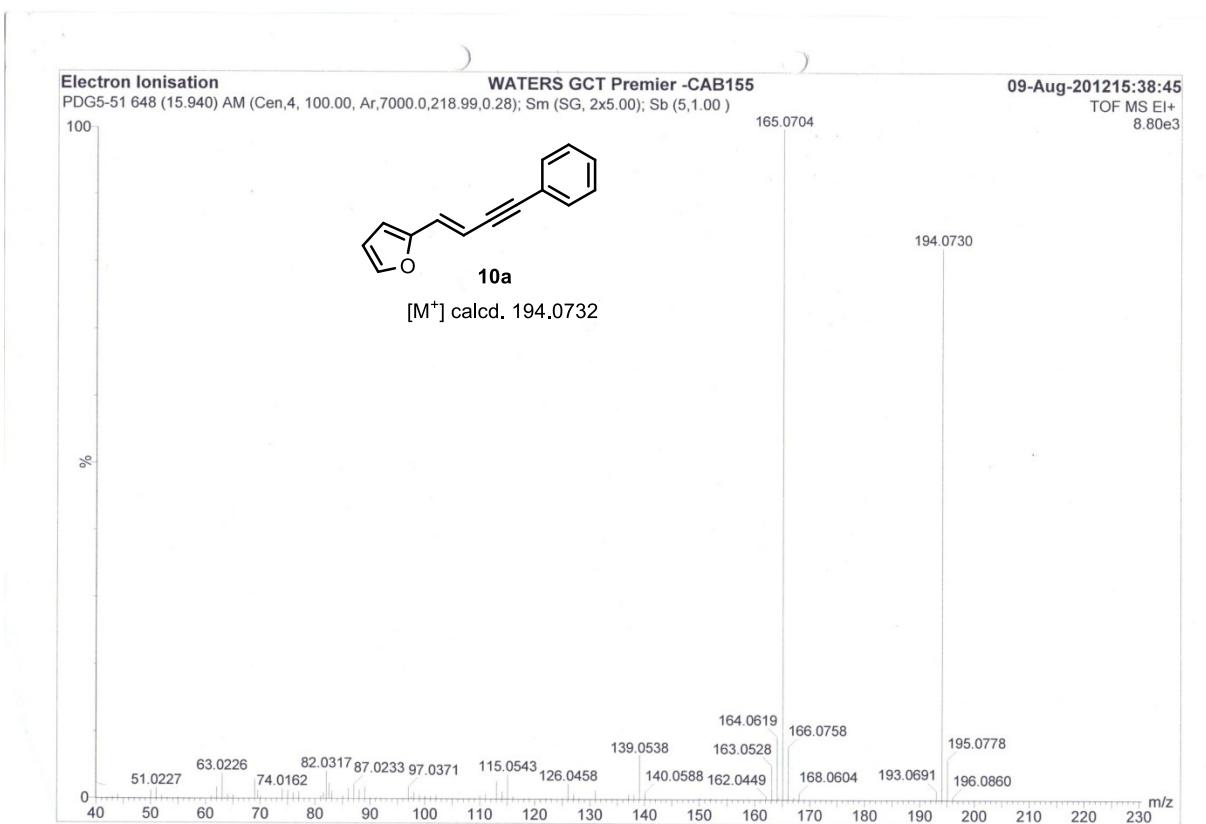
EI (HRMS) spectrum of (*E*)-1-chloro-3-(4-(4-methoxyphenyl)but-1-en-3-ynyl)benzene (**9a**)



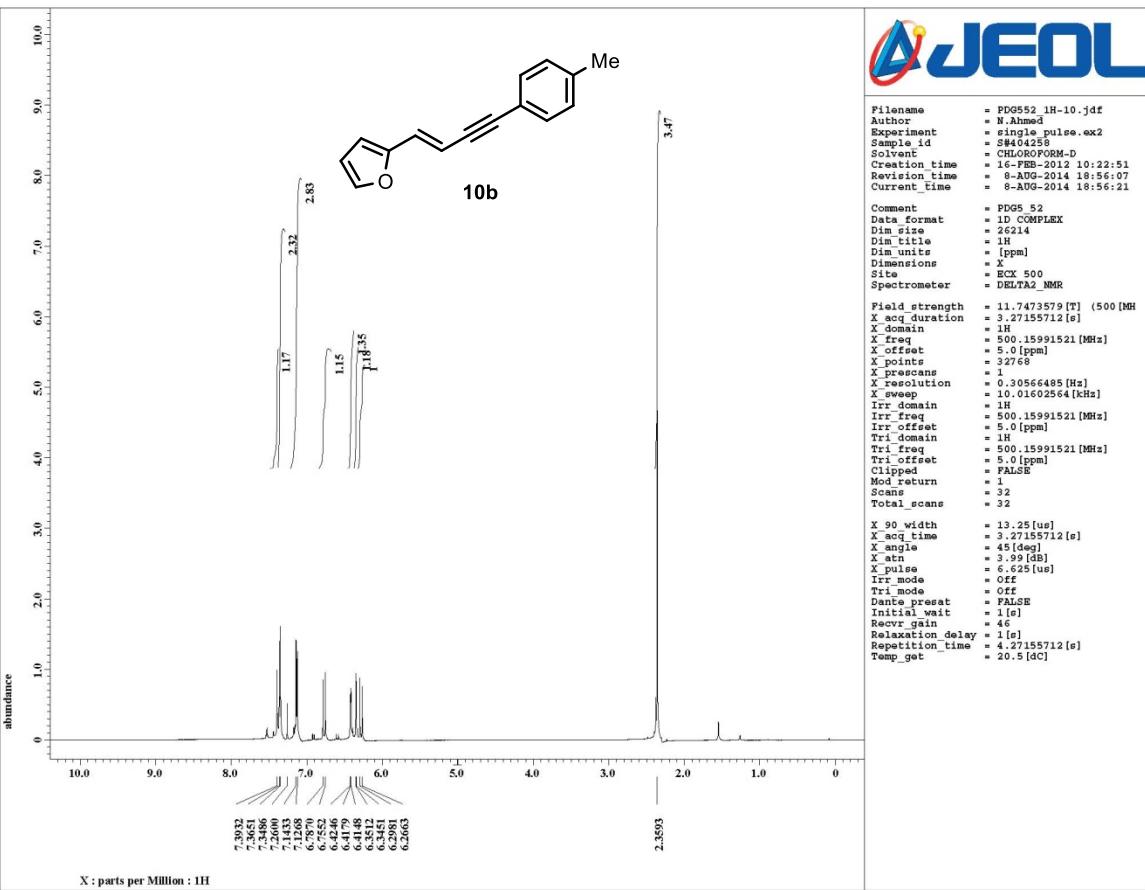
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-2-(4-phenylbut-1-en-3ynyl)furan (**10a**)



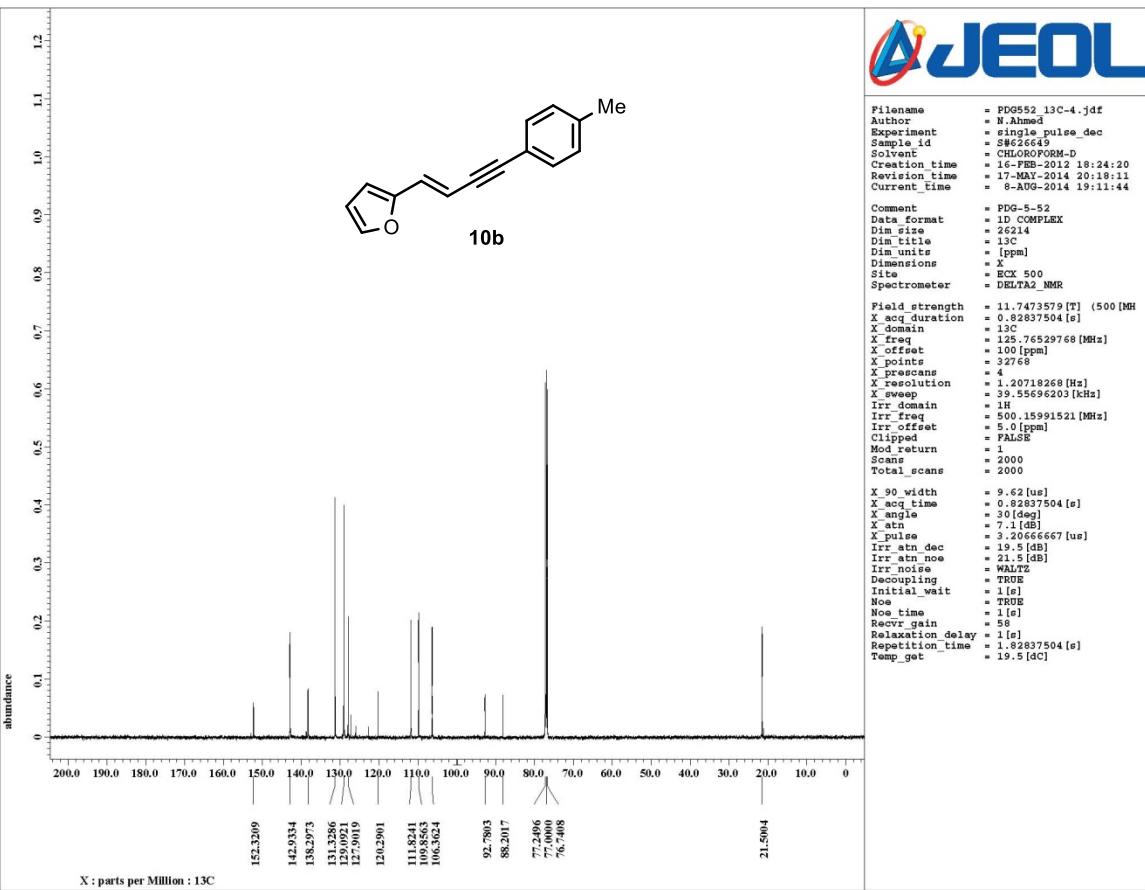
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-2-(4-phenylbut-1-en-3-ynyl)furan (**10a**)



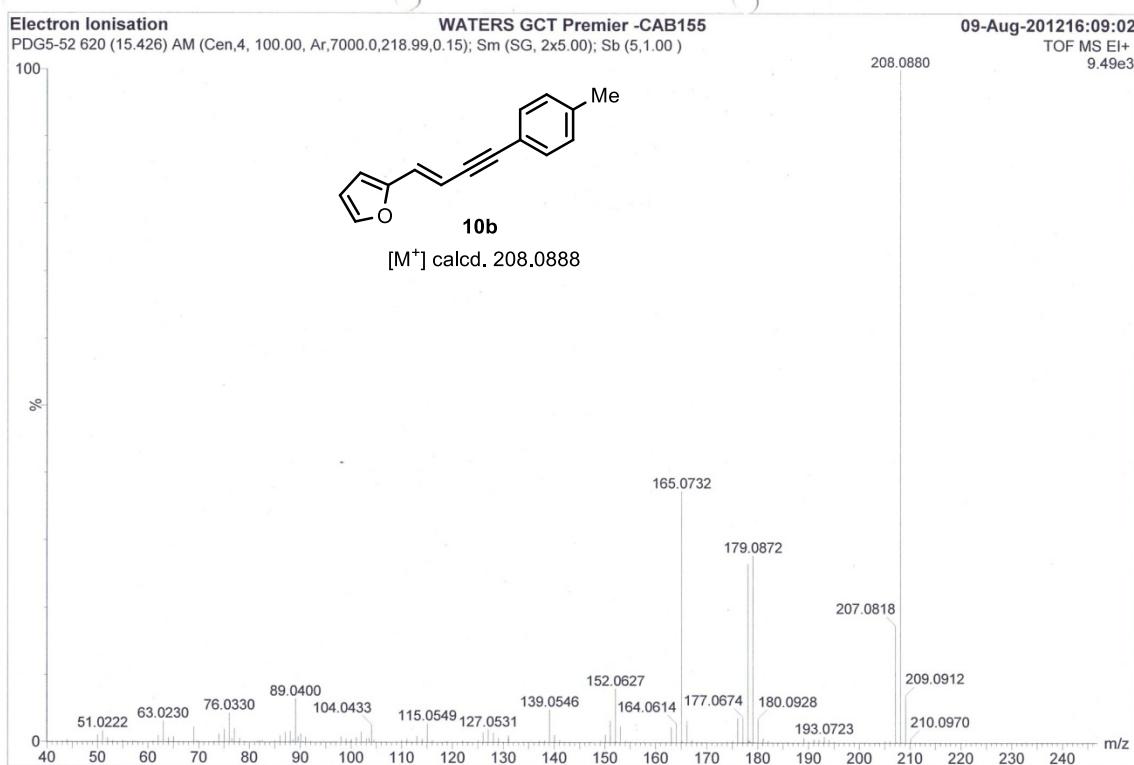
EI (HRMS) spectrum of (*E*)-2-(4-phenylbut-1-en-3-ynyl)furan (**10a**)



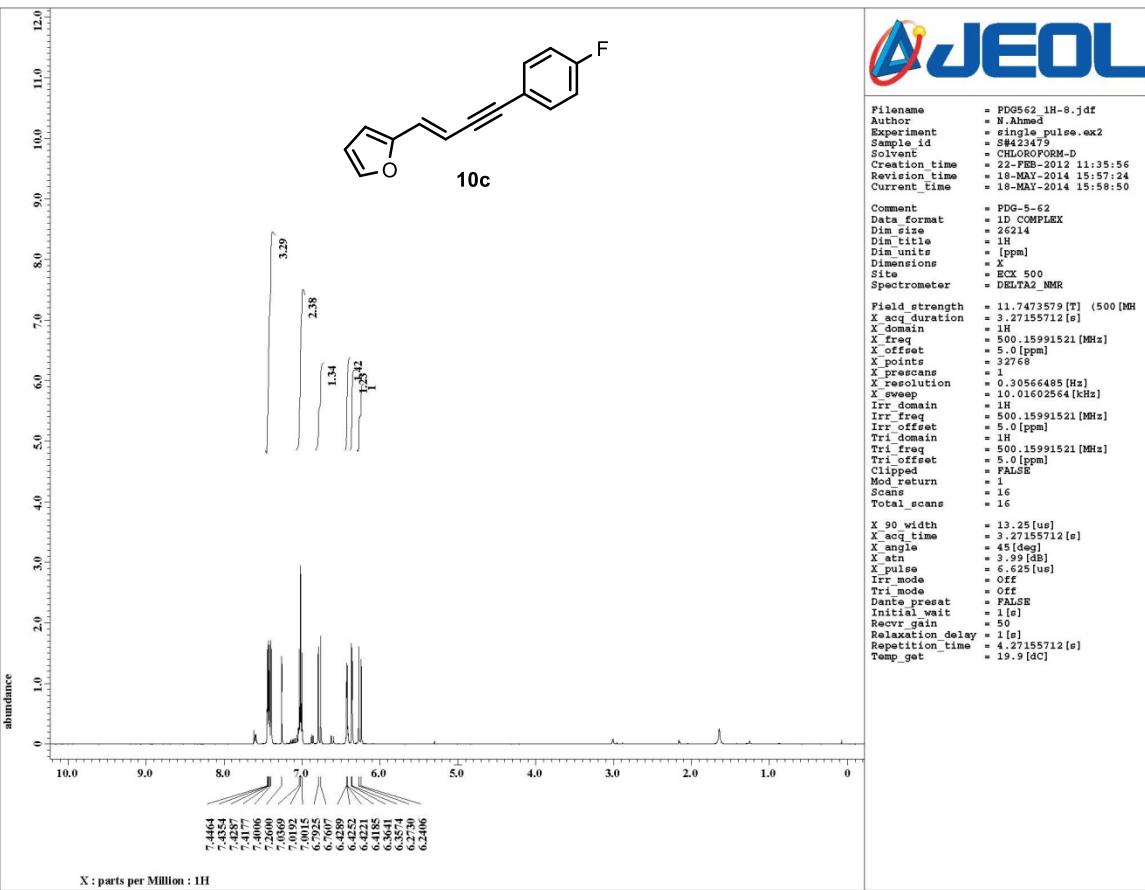
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-2-(4-p-tolylbut-1-en-3-ynyl)furan (**10b**)



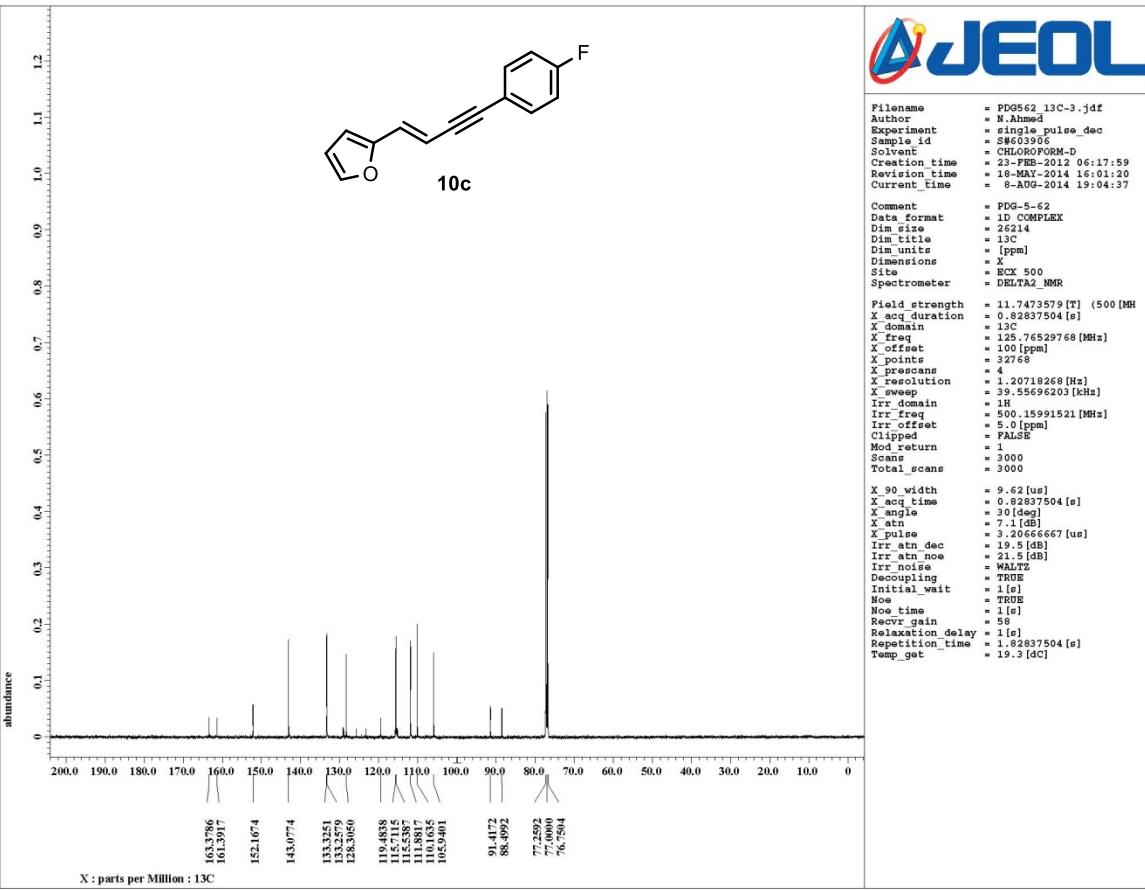
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-2-(4-*p*-tolylbut-1-en-3-ynyl)furan (**10b**)



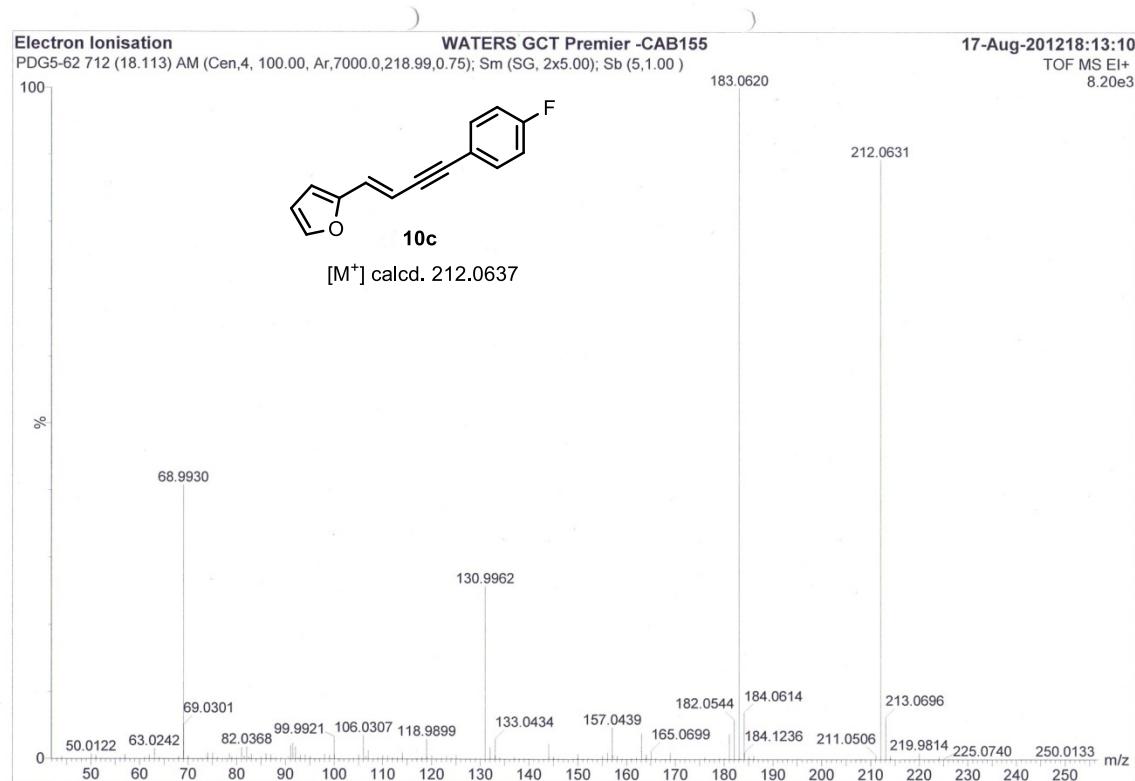
EI (HRMS) spectrum of (*E*)-2-(4-*p*-tolylbut-1-en-3-ynyl)furan (**10b**)



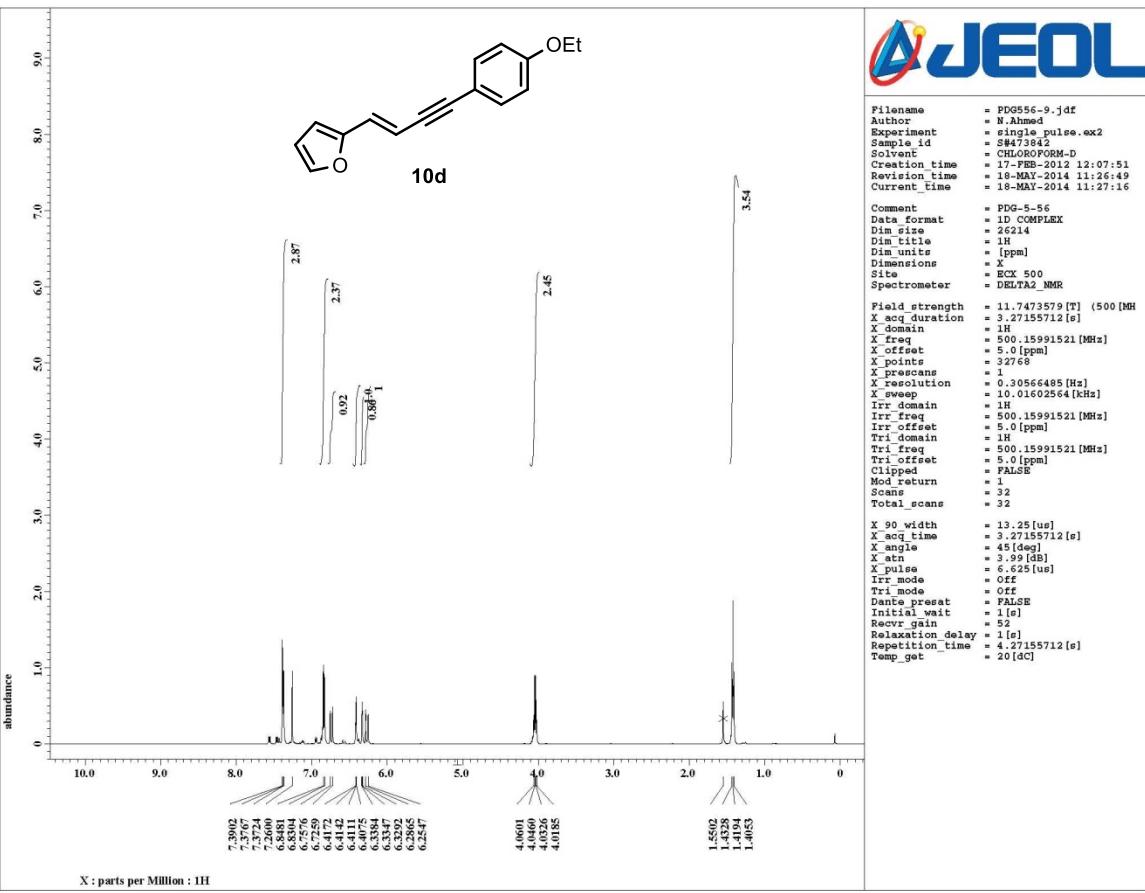
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-2-(4-(4-fluorophenyl)but-1-en-3-ynyl)furan (**10c**)



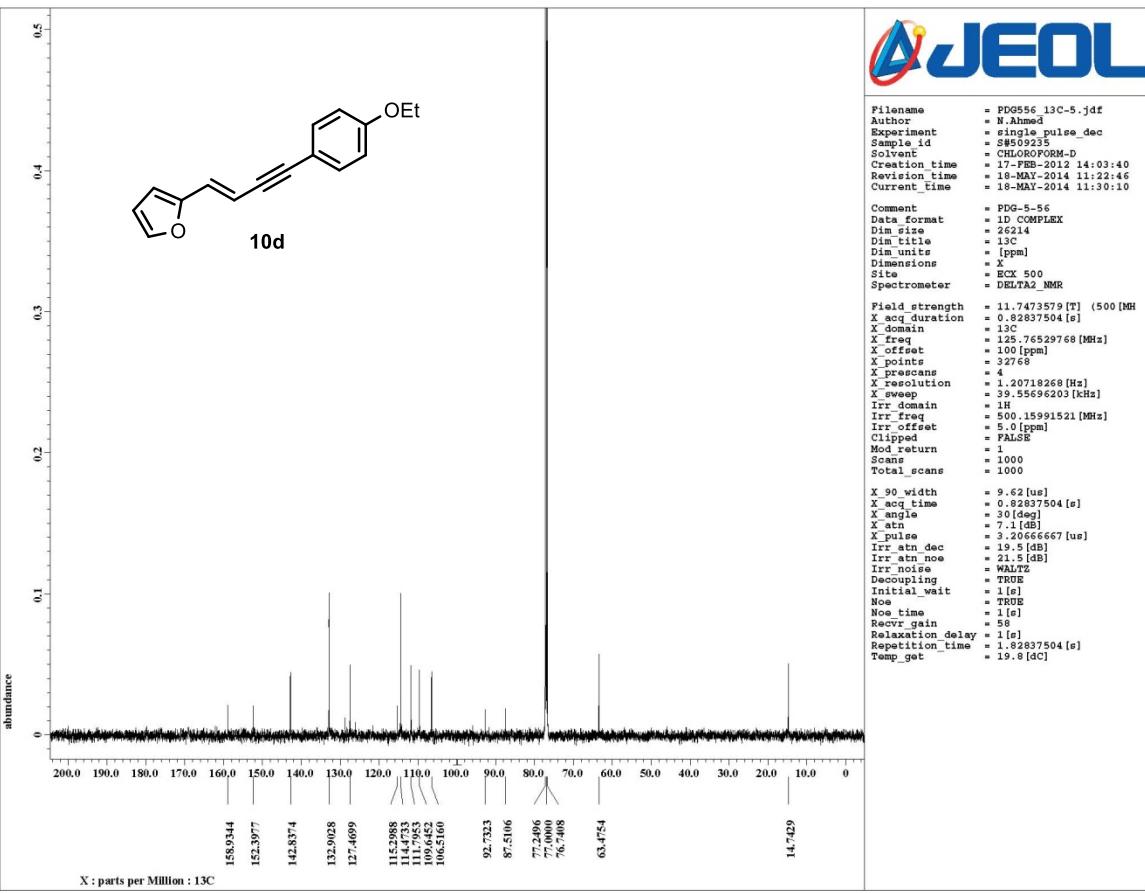
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-2-(4-(4-fluorophenyl)but-1-en-3-ynyl)furan (**10c**)



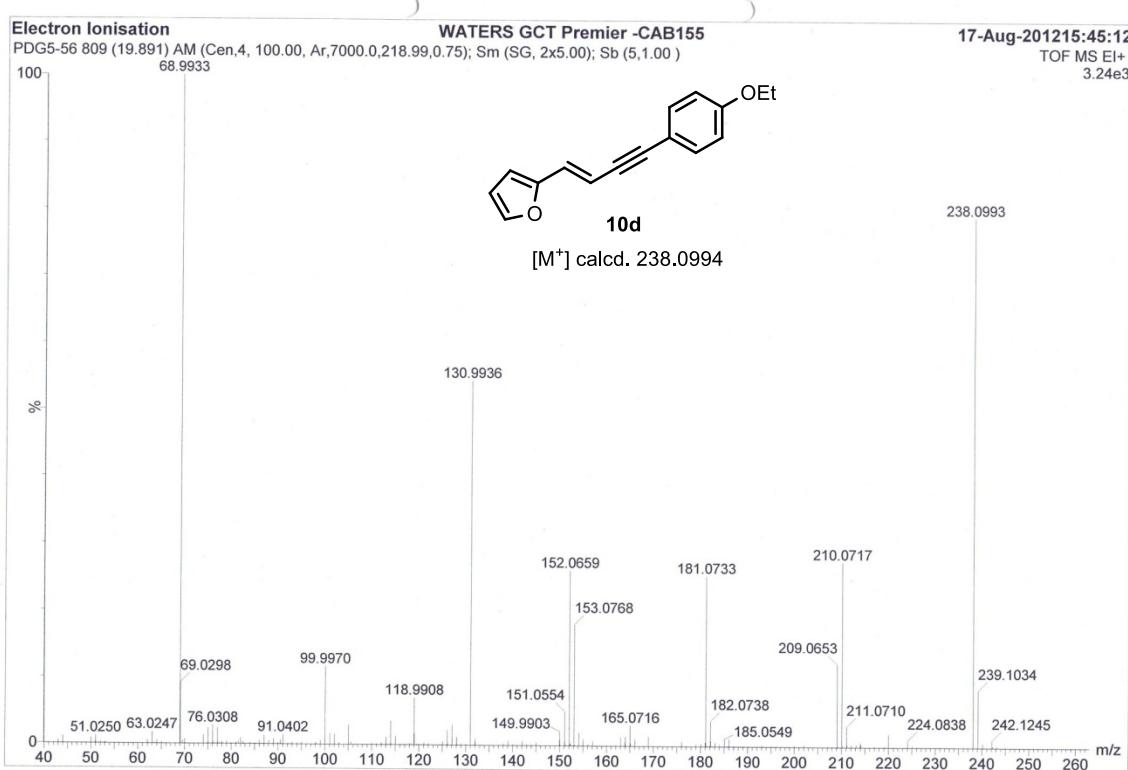
EI (HRMS) spectrum of (*E*)-2-(4-(4-fluorophenyl)but-1-en-3-ynyl)furan (**10c**)



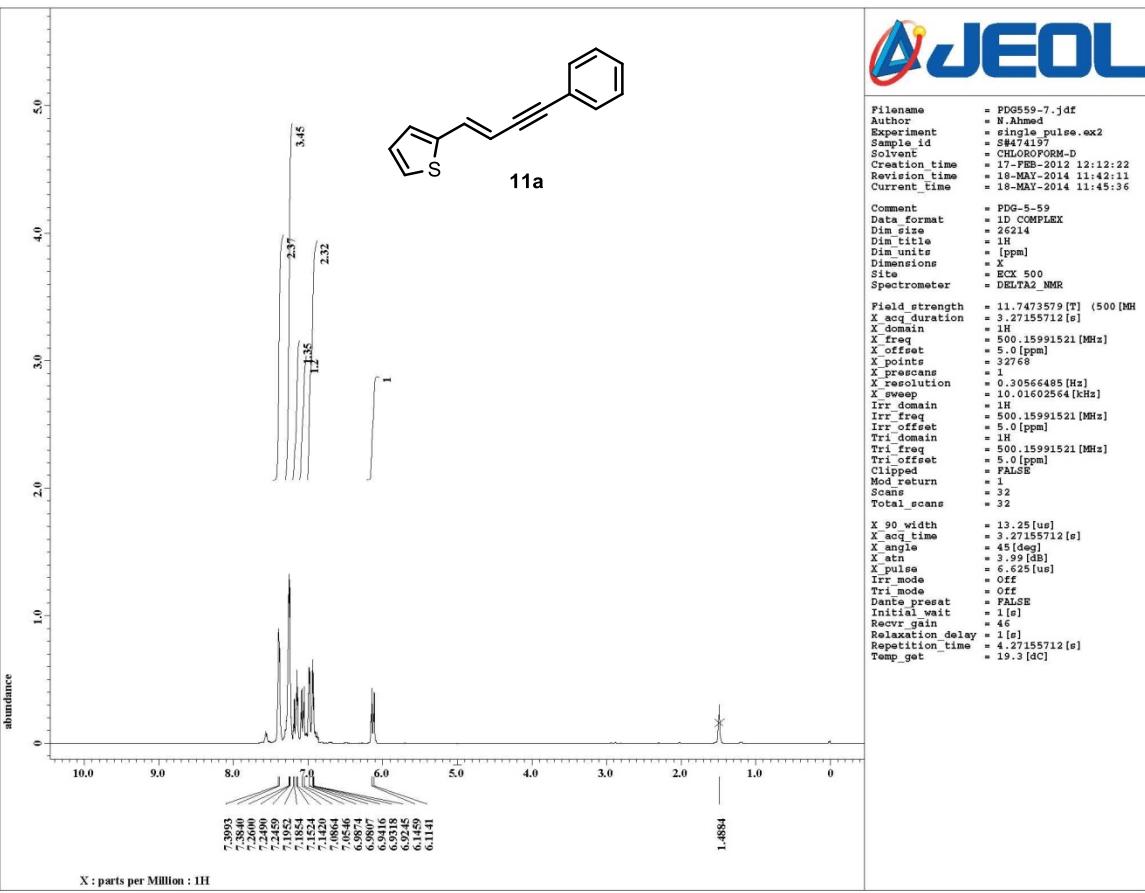
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-2-(4-(4-ethoxyphenyl)but-1-en-3-ynyl)furan (**10d**)



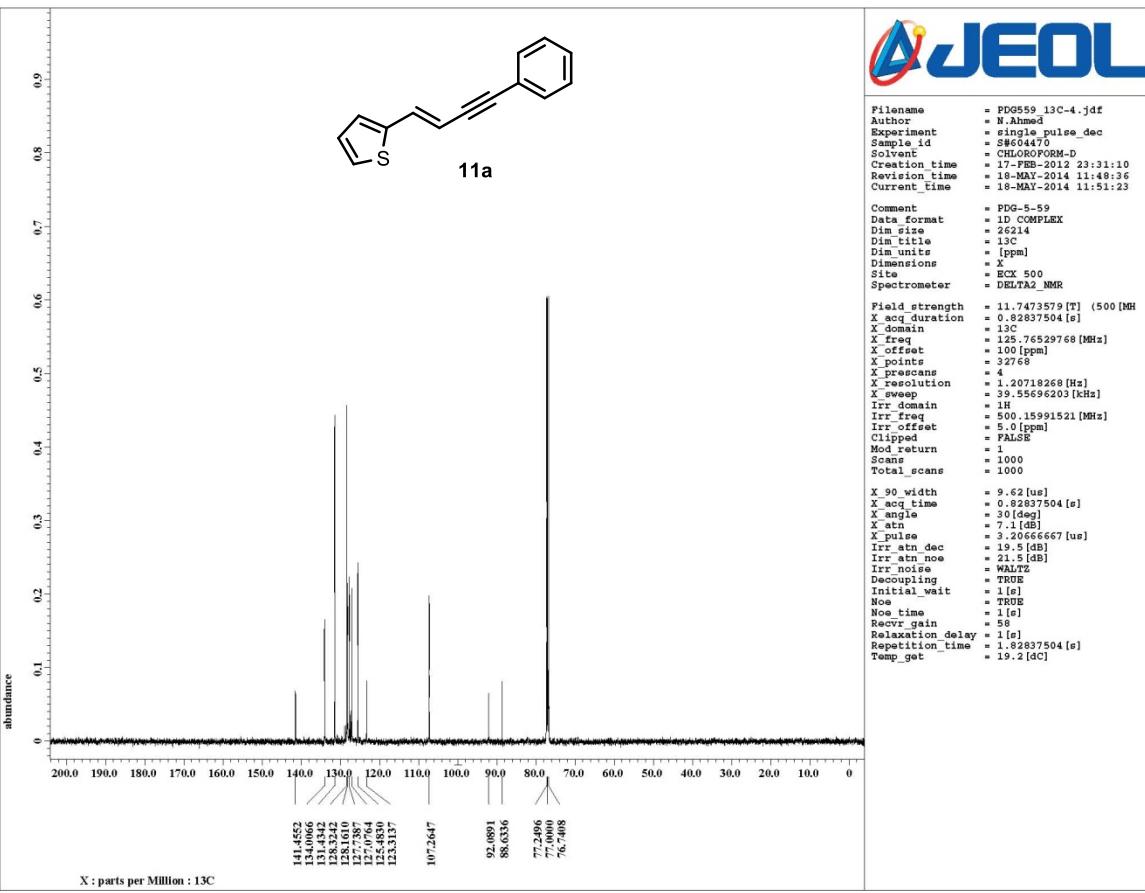
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-2-(4-(4-ethoxyphenyl)but-1-en-3-ynyl)furan (**10d**)



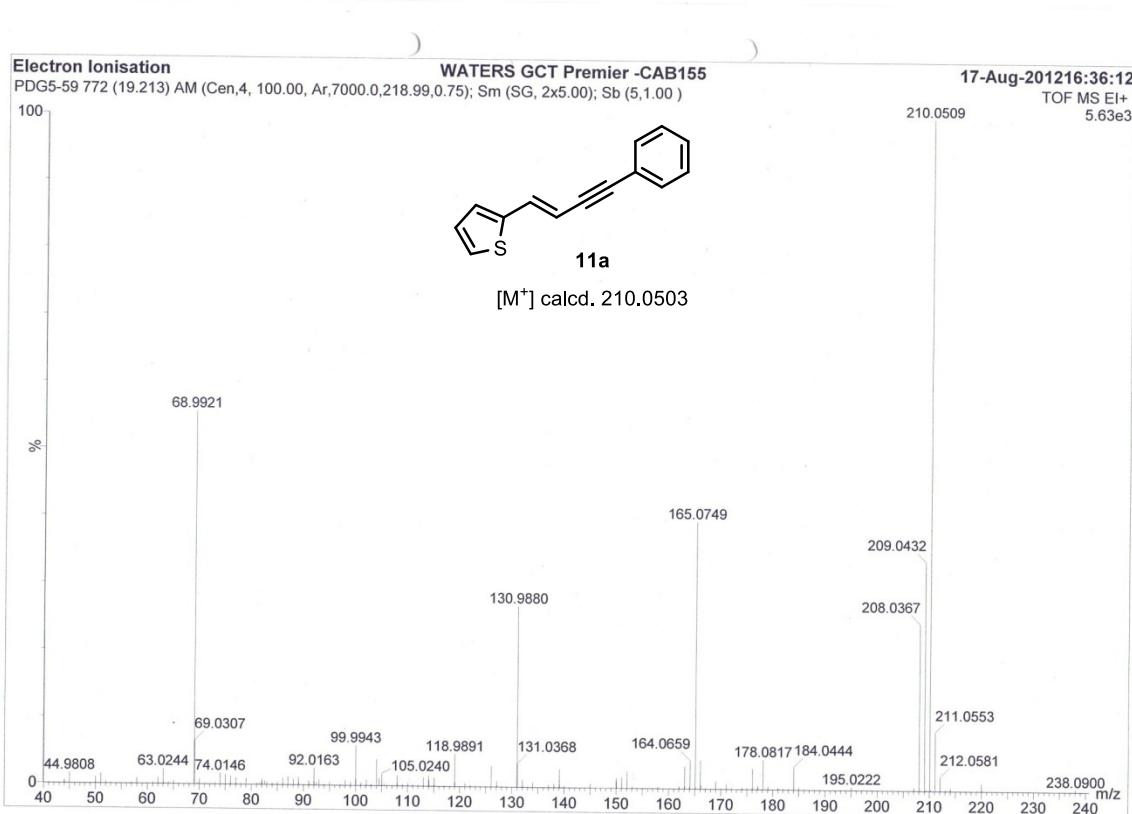
EI (HRMS) spectrum of (*E*)-2-(4-(4-ethoxyphenyl)but-1-en-3-ynyl)furan (**10d**)



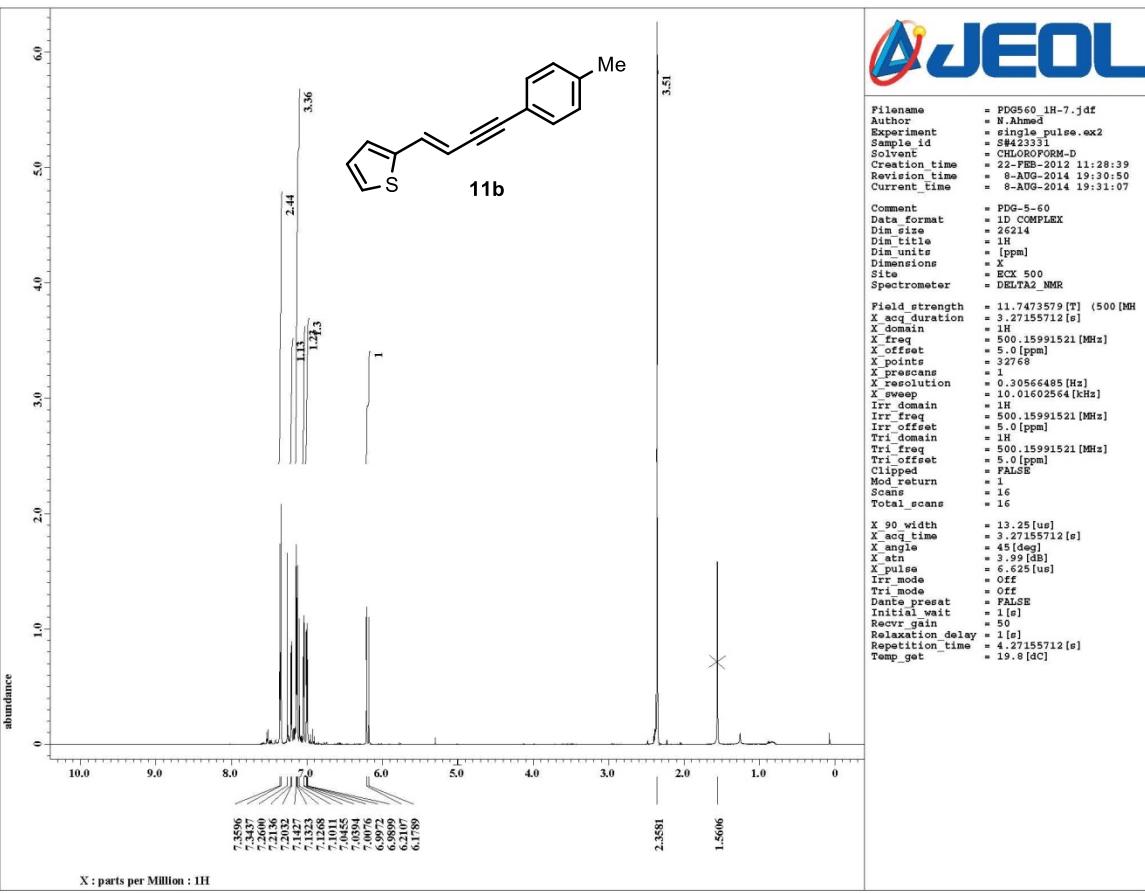
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-2-(4-phenylbut-1-en-3-ynyl)thiophene (**11a**)



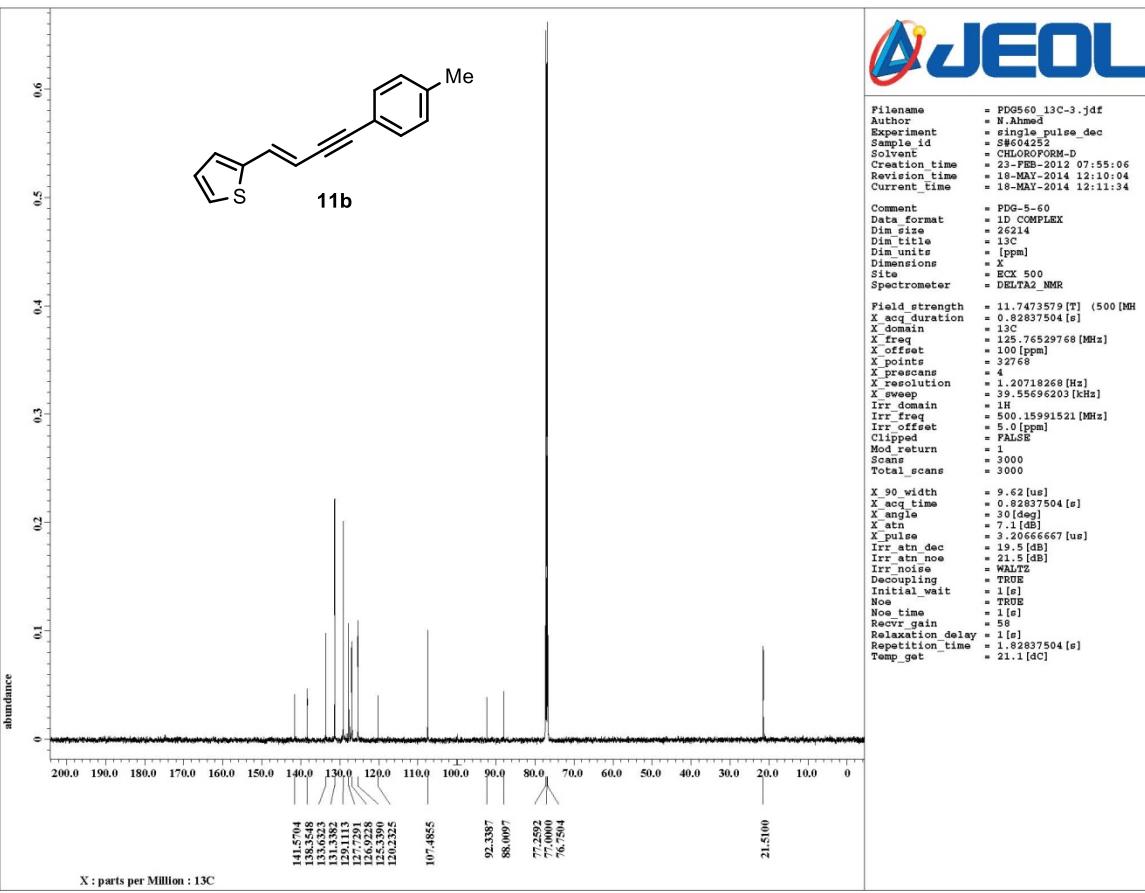
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-2-(4-phenylbut-1-en-3-ynyl)thiophene (**11a**)



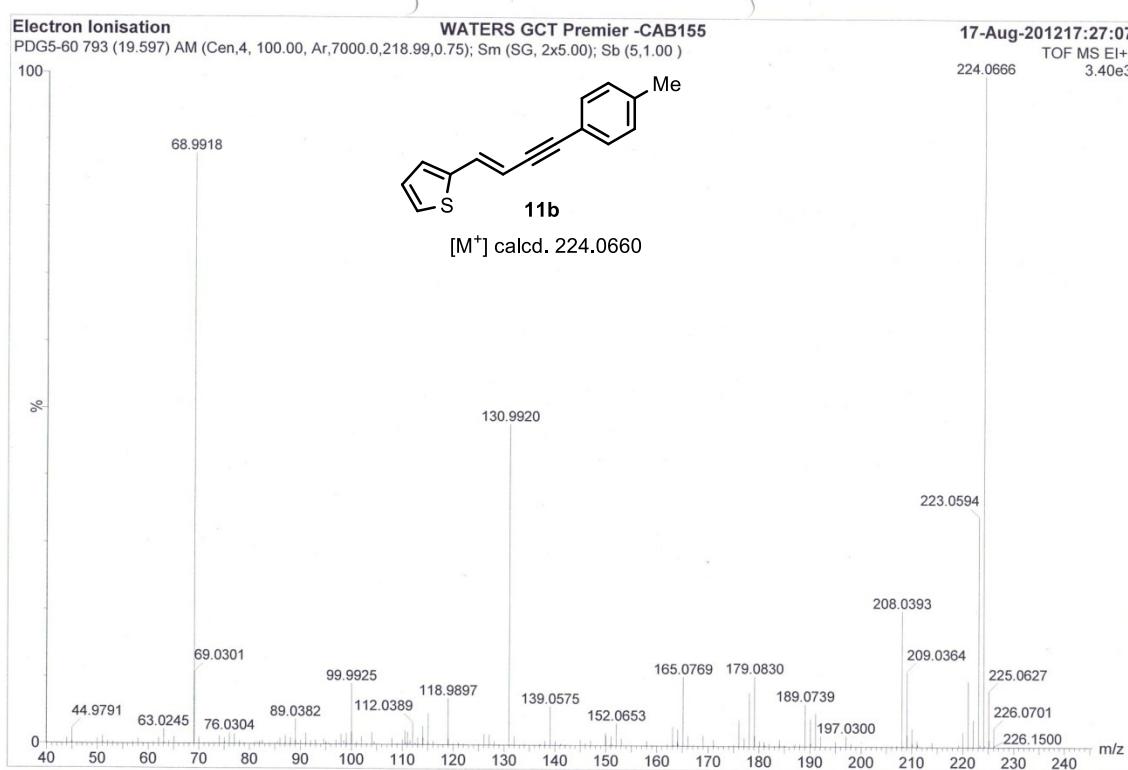
EI (HRMS) spectrum of (*E*)-2-(4-phenylbut-1-en-3-ynyl)thiophene (**11a**)



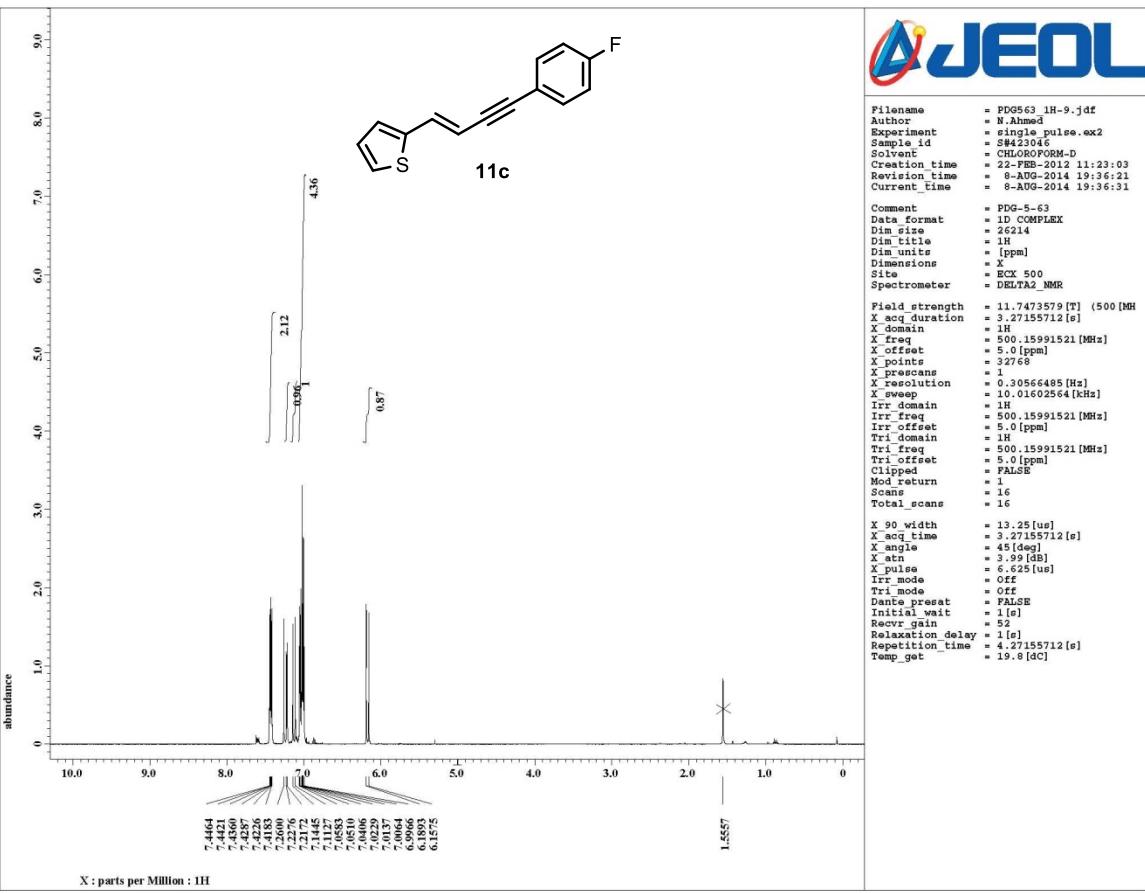
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-2-(4-*p*-tolylbut-1-en-3-ynyl)thiophene (**11b**)



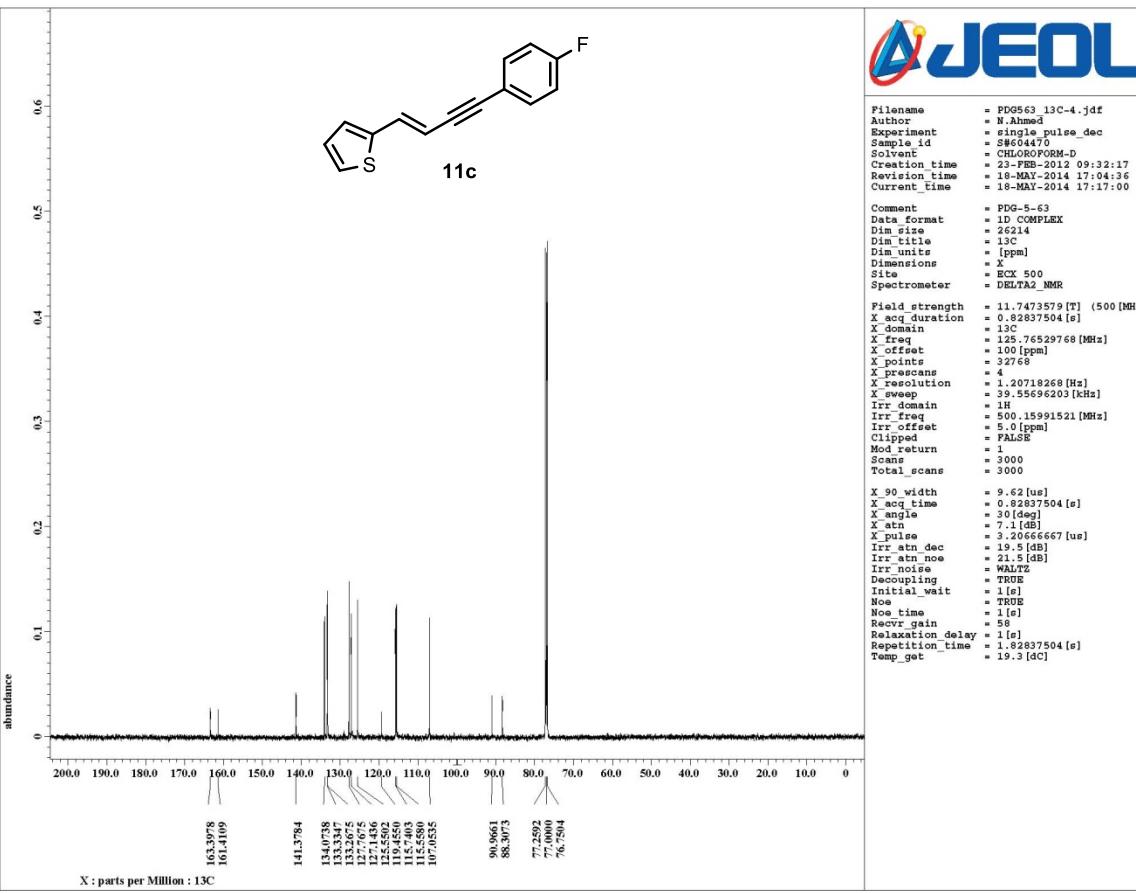
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-2-(4-*p*-tolylbut-1-en-3-ynyl)thiophene (**11b**)



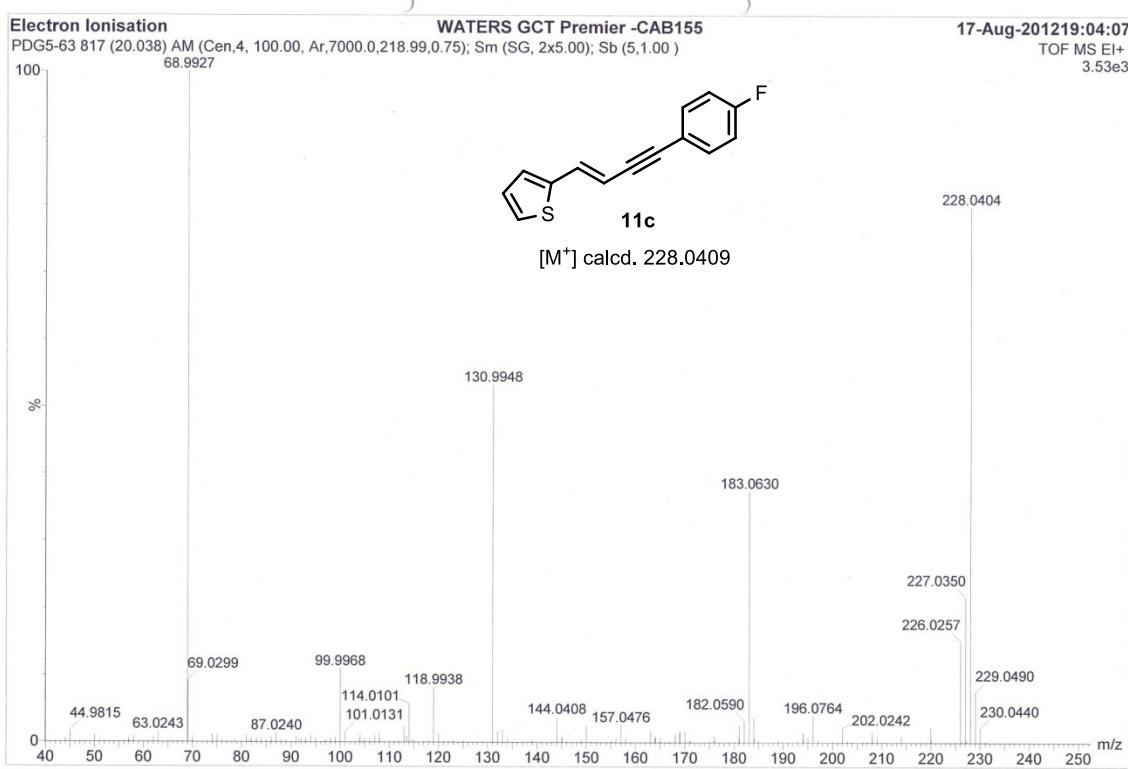
EI (HRMS) spectrum of (*E*)-2-(4-*p*-tolylbut-1-en-3-ynyl)thiophene (**11b**)



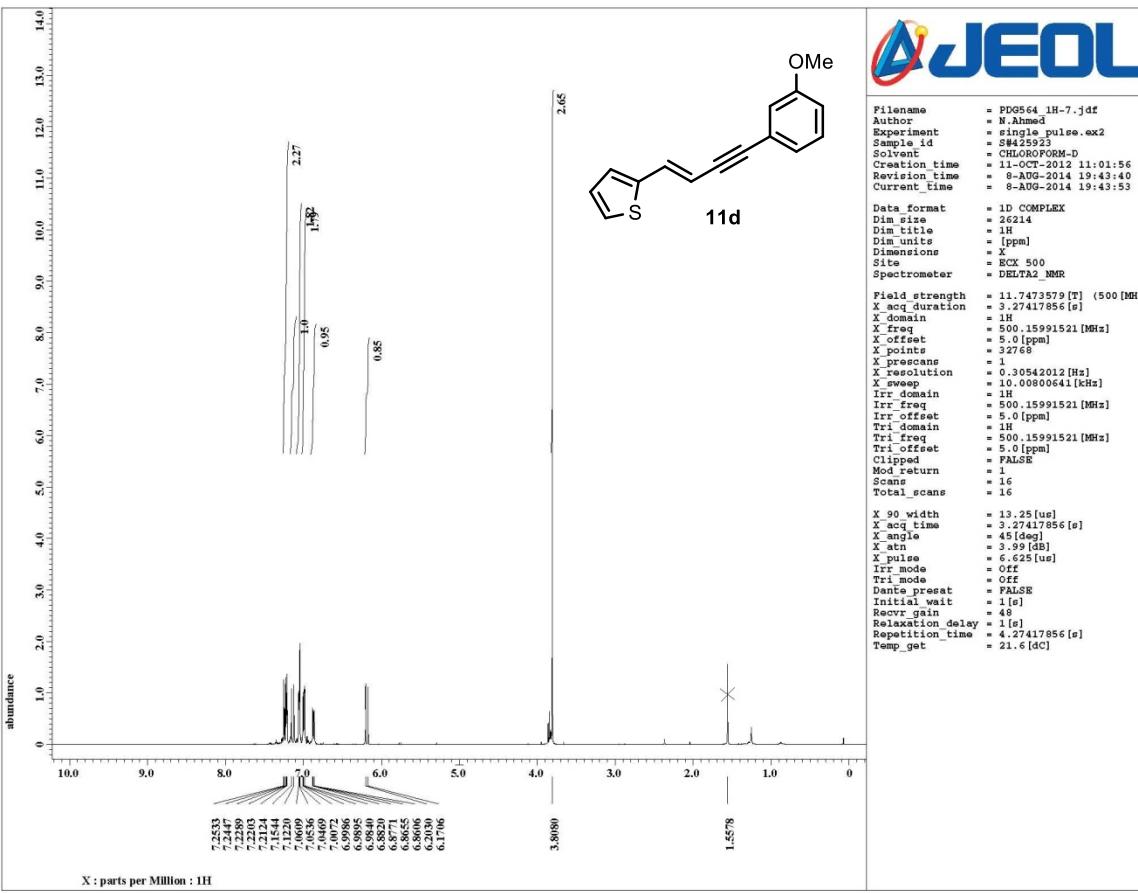
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-2-(4-(4-fluorophenyl)but-1-en-3-ynyl)thiophene (**11c**)



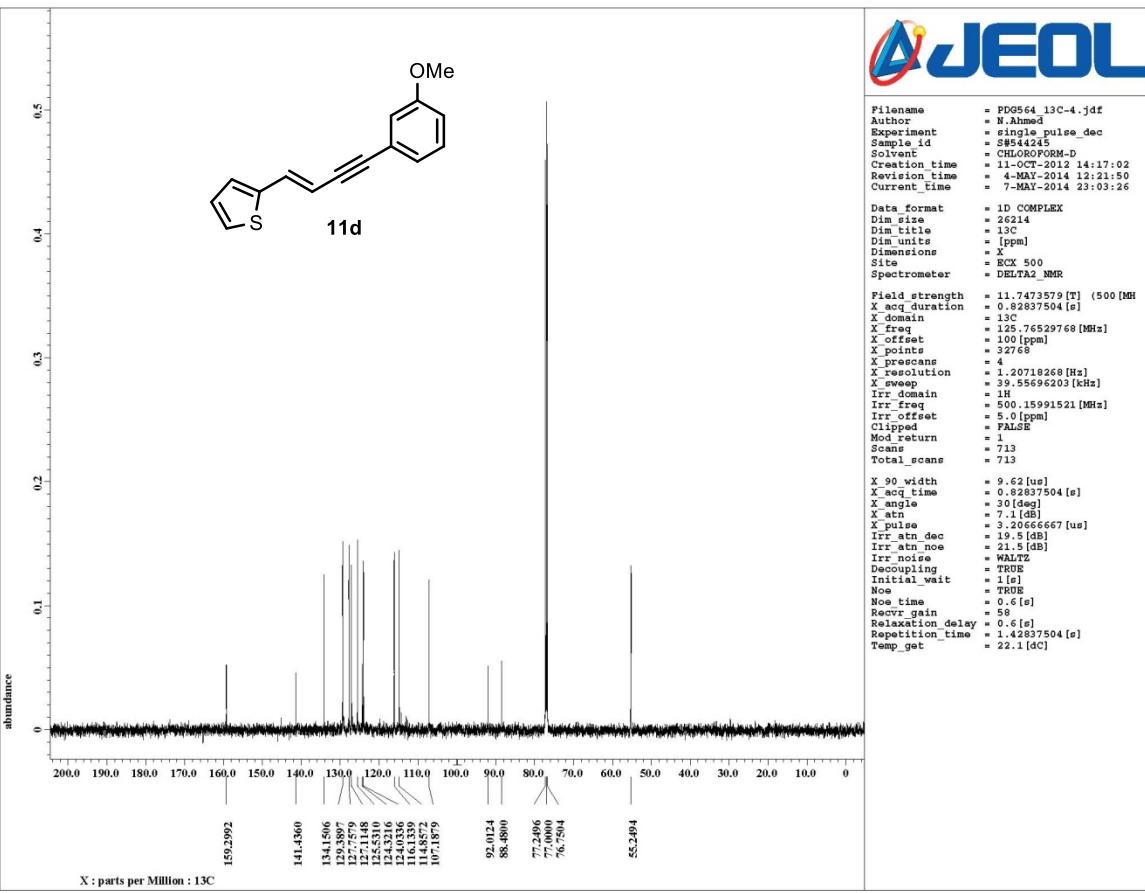
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-2-(4-(4-fluorophenyl)but-1-en-3-ynyl)thiophene (**11c**)



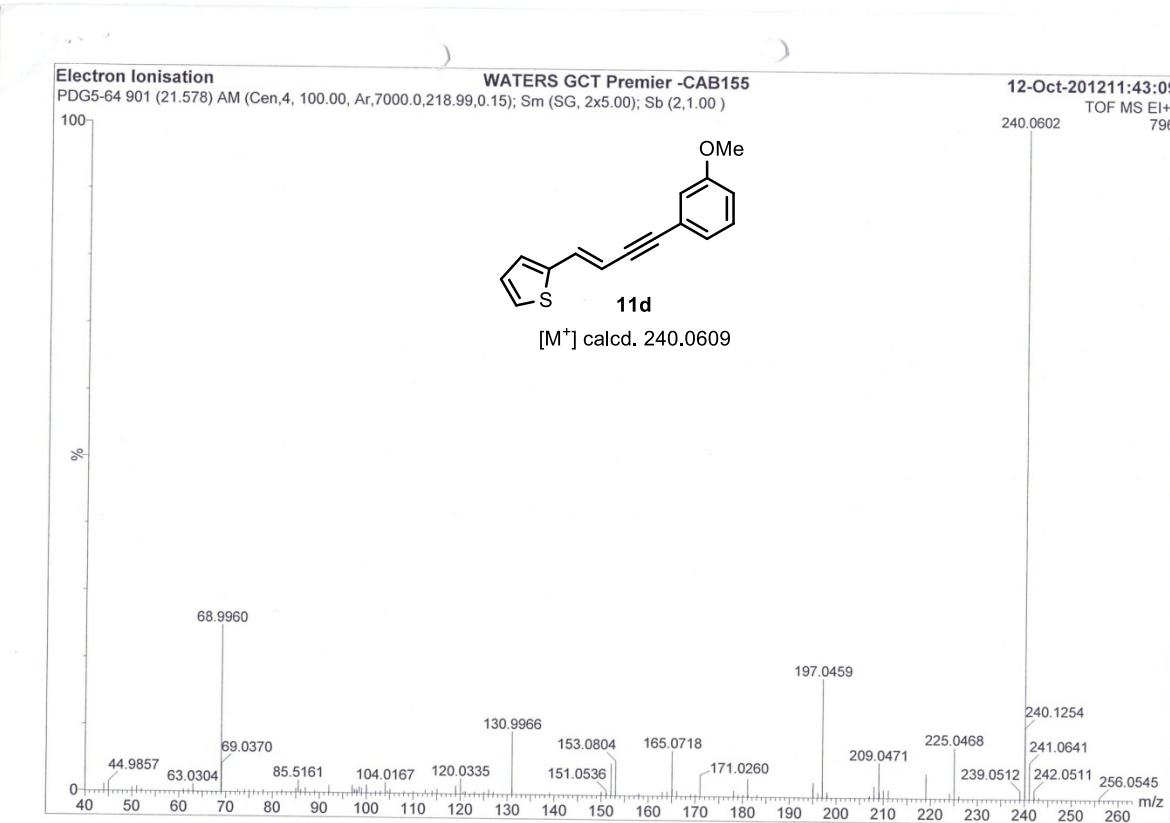
EI (HRMS) spectrum of (*E*)-2-(4-(4-fluorophenyl)but-1-en-3-ynyl)thiophene (**11c**)



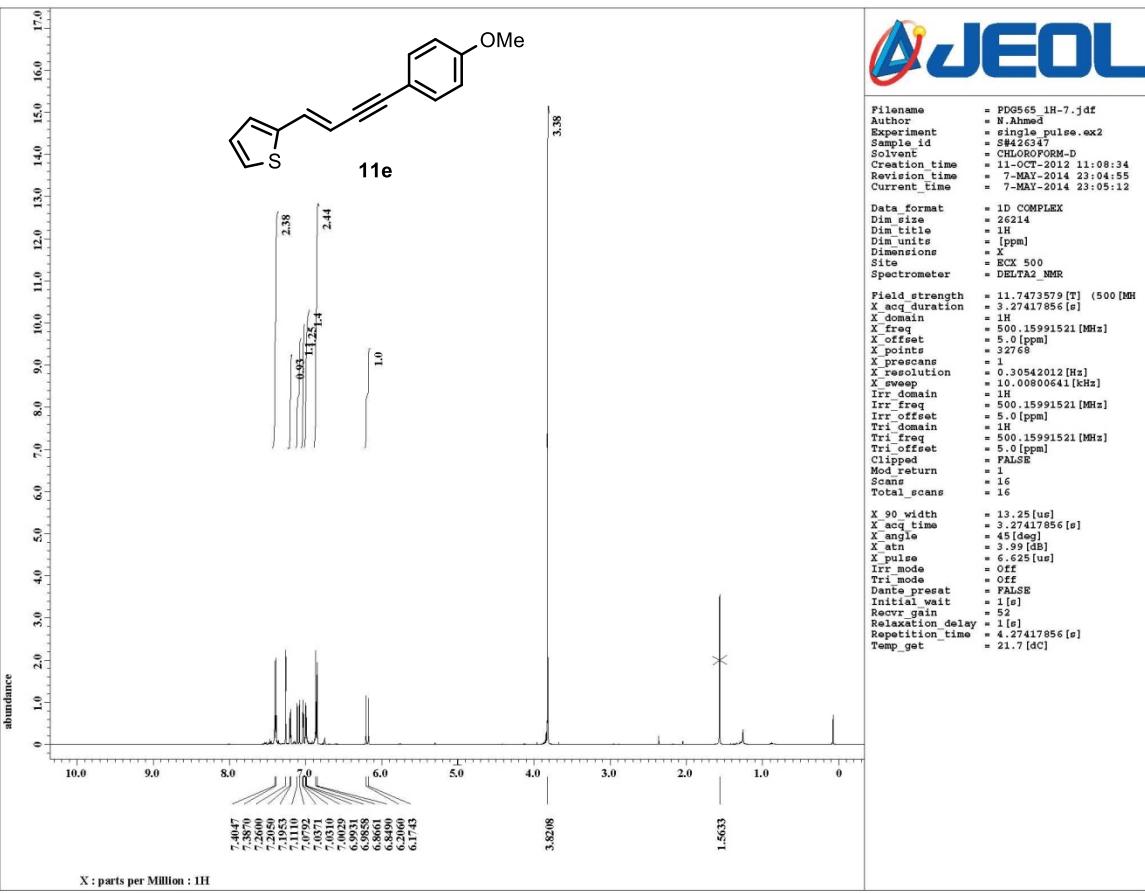
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-2-(4-(3-methoxyphenyl)but-1-en-3-ynyl)thiophene (**11d**)



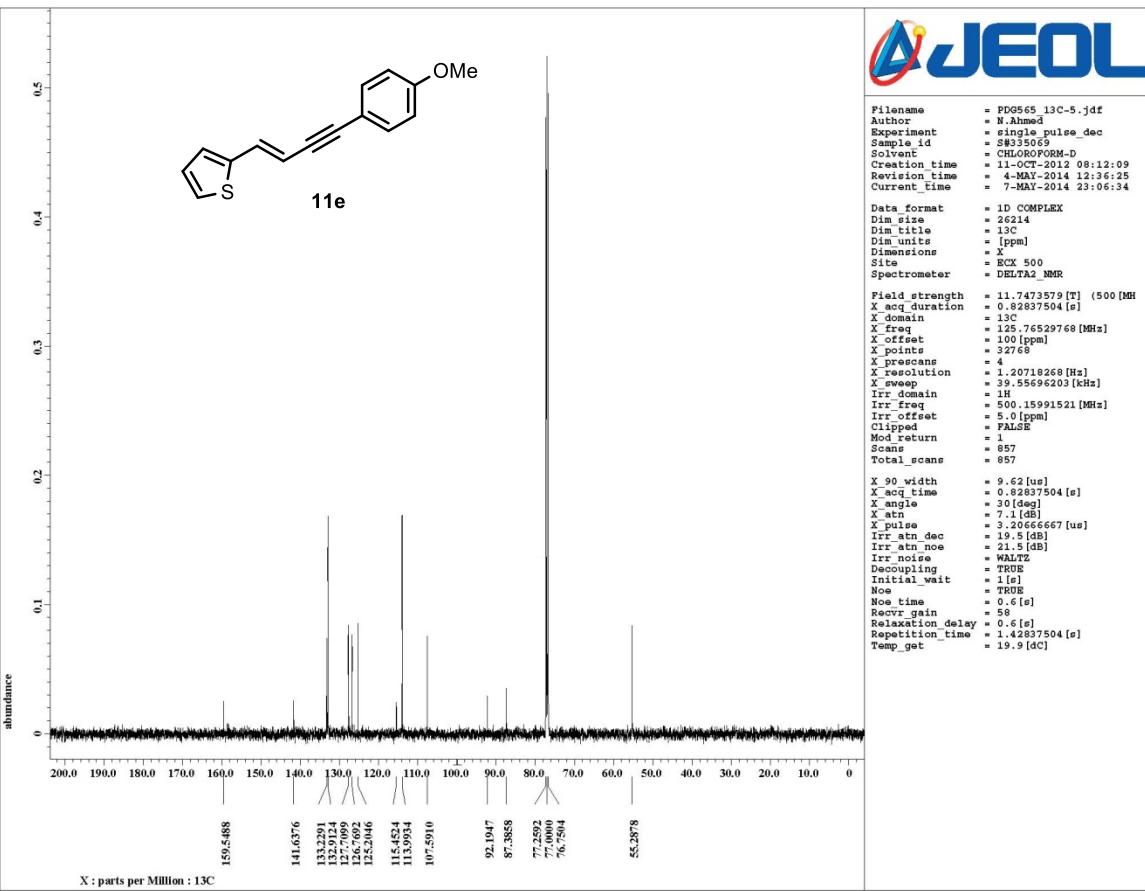
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-2-(4-(3-methoxyphenyl)but-1-en-3-ynyl)thiophene (**11d**)



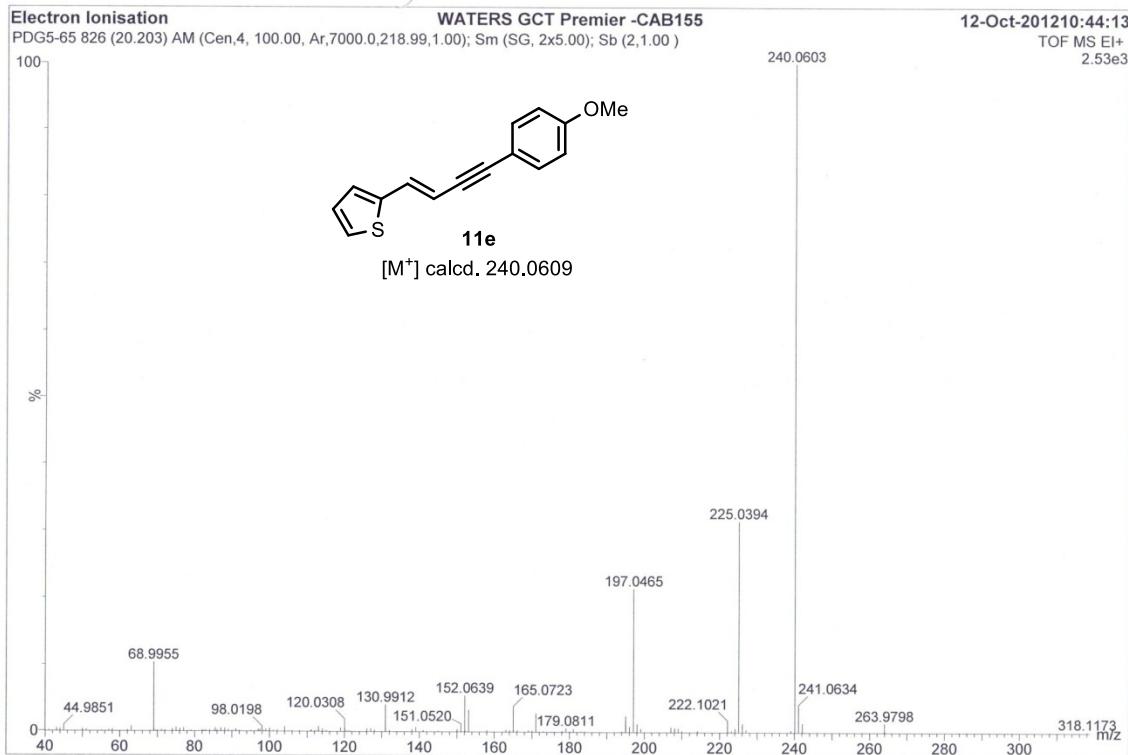
EI (HRMS) spectrum of (*E*)-2-(4-(3-methoxyphenyl)but-1-en-3-ynyl)thiophene (**11d**)



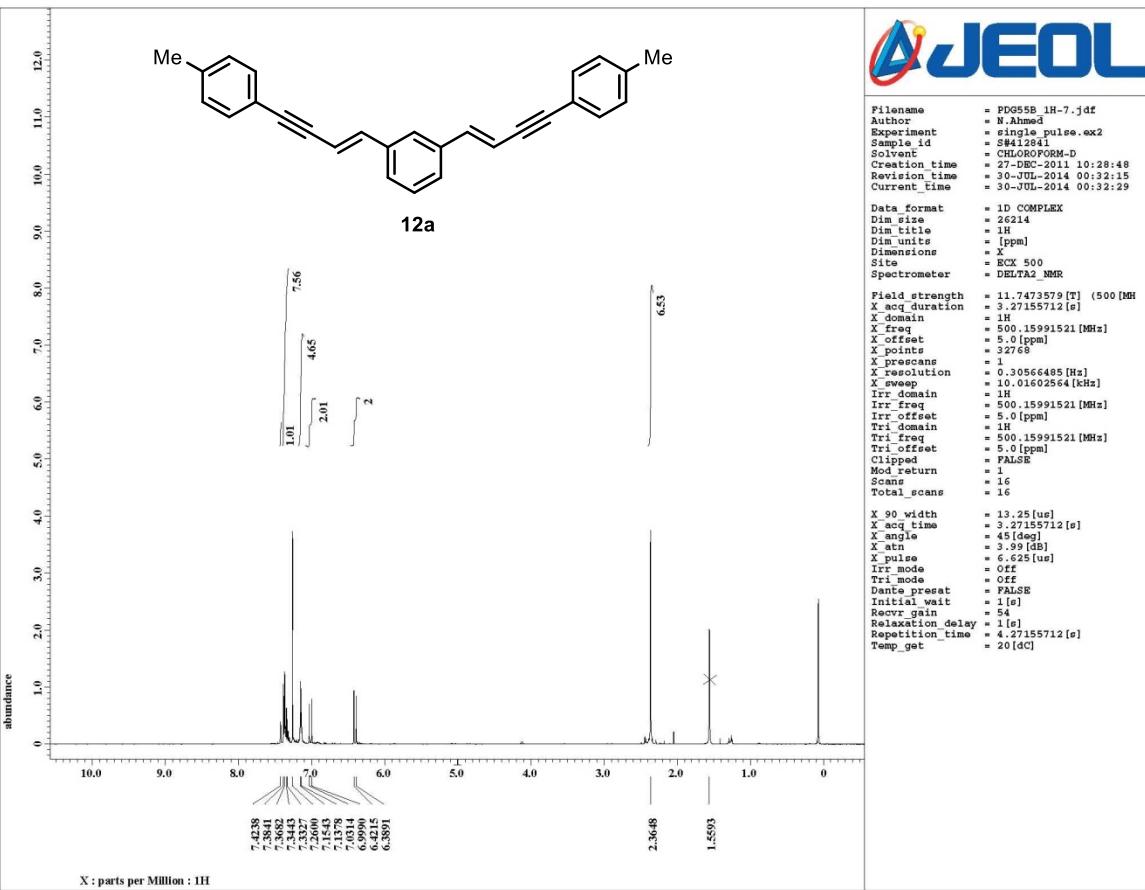
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-2-(4-(4-methoxyphenyl)but-1-en-3-ynyl)thiophene (**11e**)



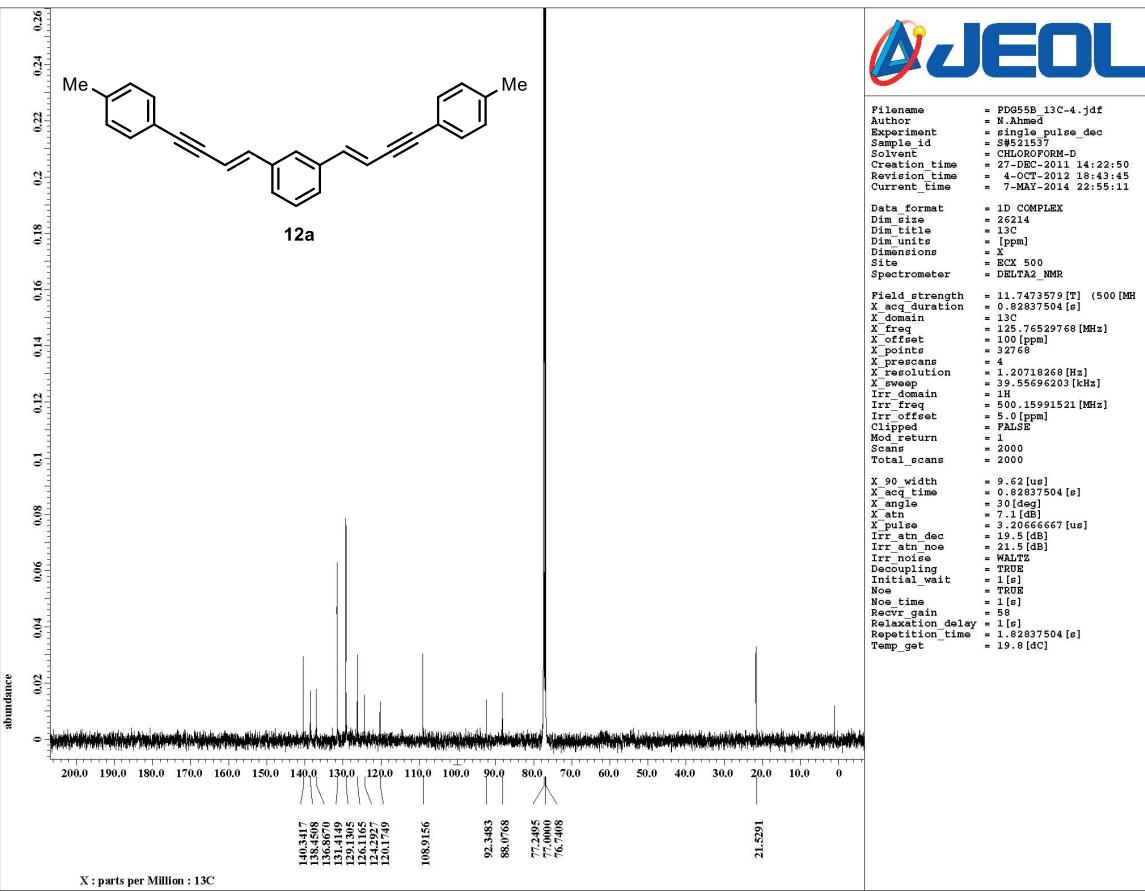
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-2-(4-(4-methoxyphenyl)but-1-en-3-ynyl)thiophene (**11e**)



EI (HRMS) spectrum of (*E*)-2-(4-(4-methoxyphenyl)but-1-en-3-ynyl)thiophene (**11e**)



¹H NMR (500 MHz, CDCl₃) spectrum of 1,3-bis((E)-4-(p-tolyl)but-1-en-3-ynyl)benzene (**12a**)



¹³C NMR (125 MHz, CDCl₃) spectrum of 1,3-bis((E)-4-(*p*-tolyl)but-1-en-3-ynyl)benzene (**12a**)

Electrospray ionisation-MS

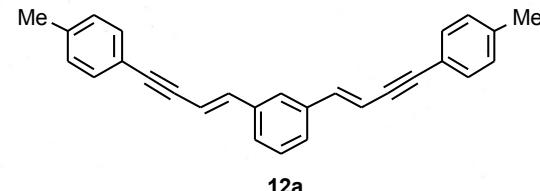
PDG5-5+ 10 (0.221) AM (Cen.4, 100.00, Ar,8500.0,556.28,0.25,LS 10); Sm (SG, 2x5.00); Sb (10,1.00); Cm (10:21-161:193)
376.2067

WATERS-Q-ToF Premier-HAB2

17:03:1021-Aug-2012

1: TOF MS ES+
219

100

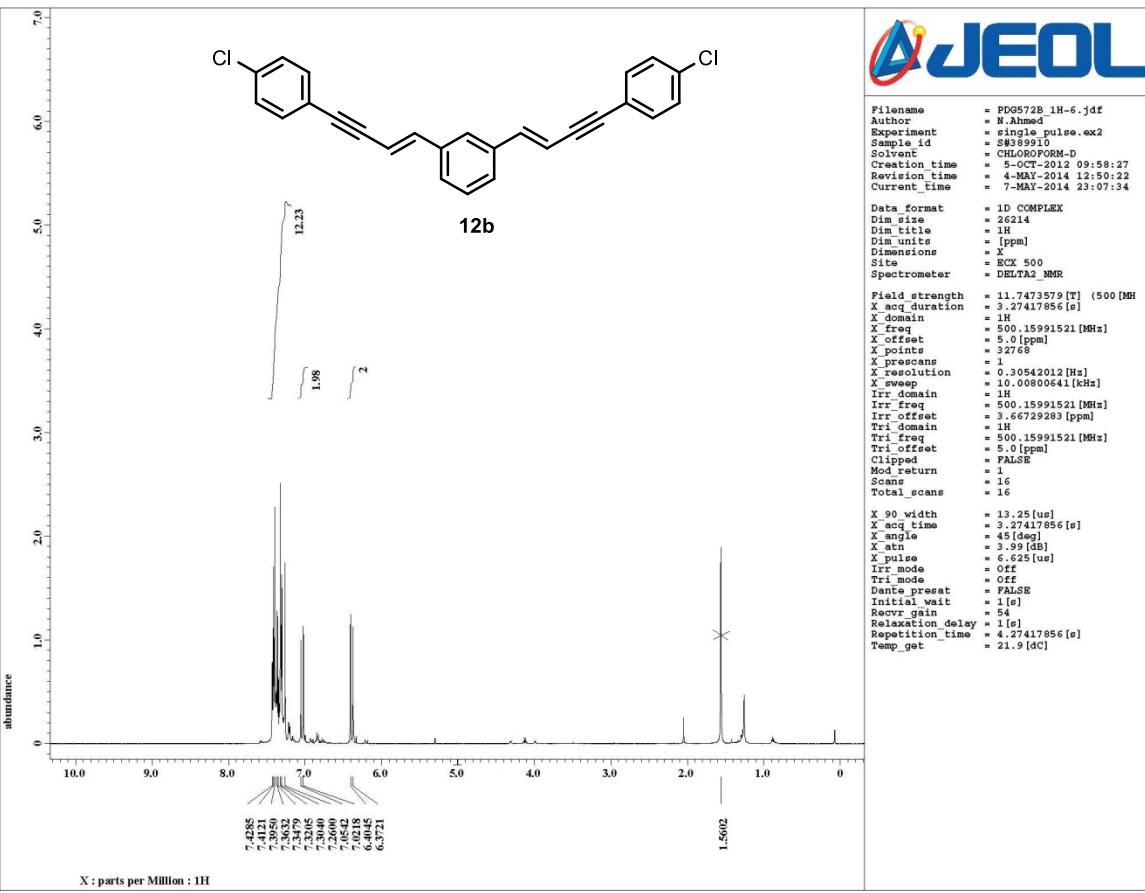


12a

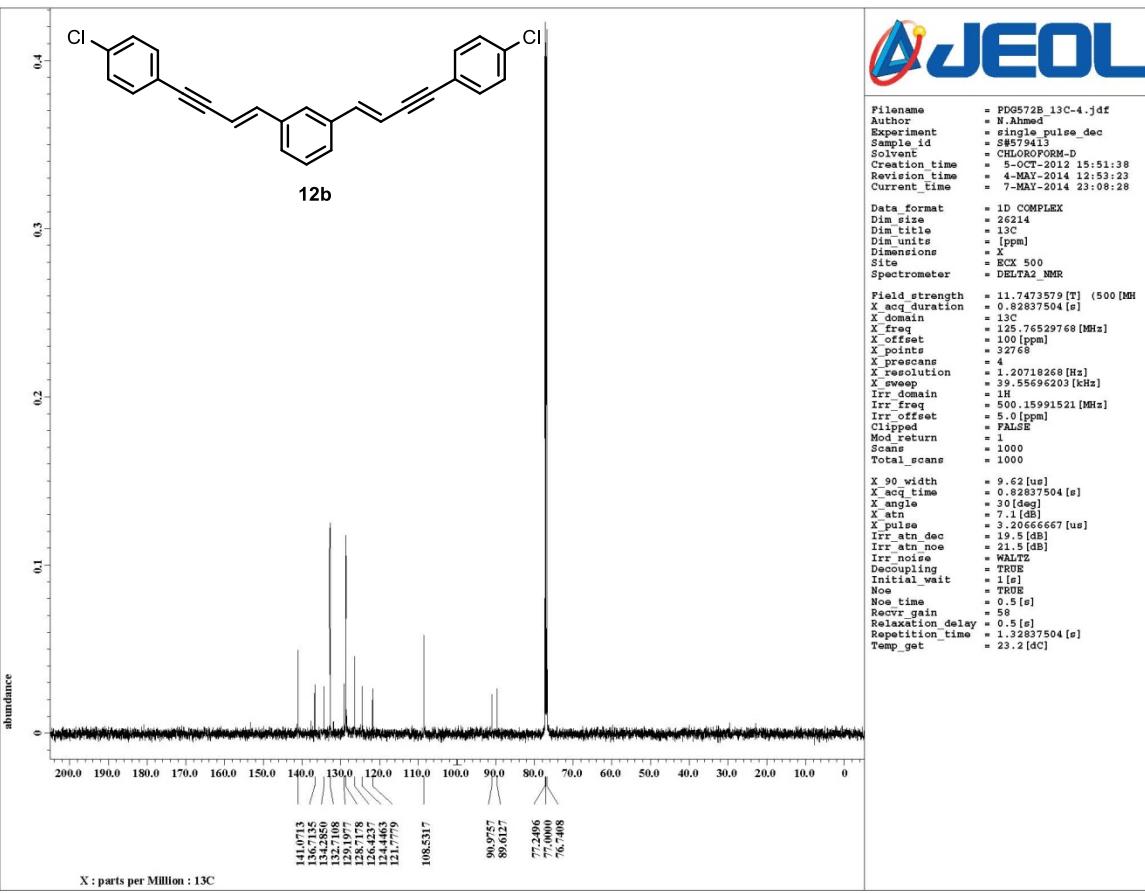
[MNH₄⁺] calcd. 376.2065



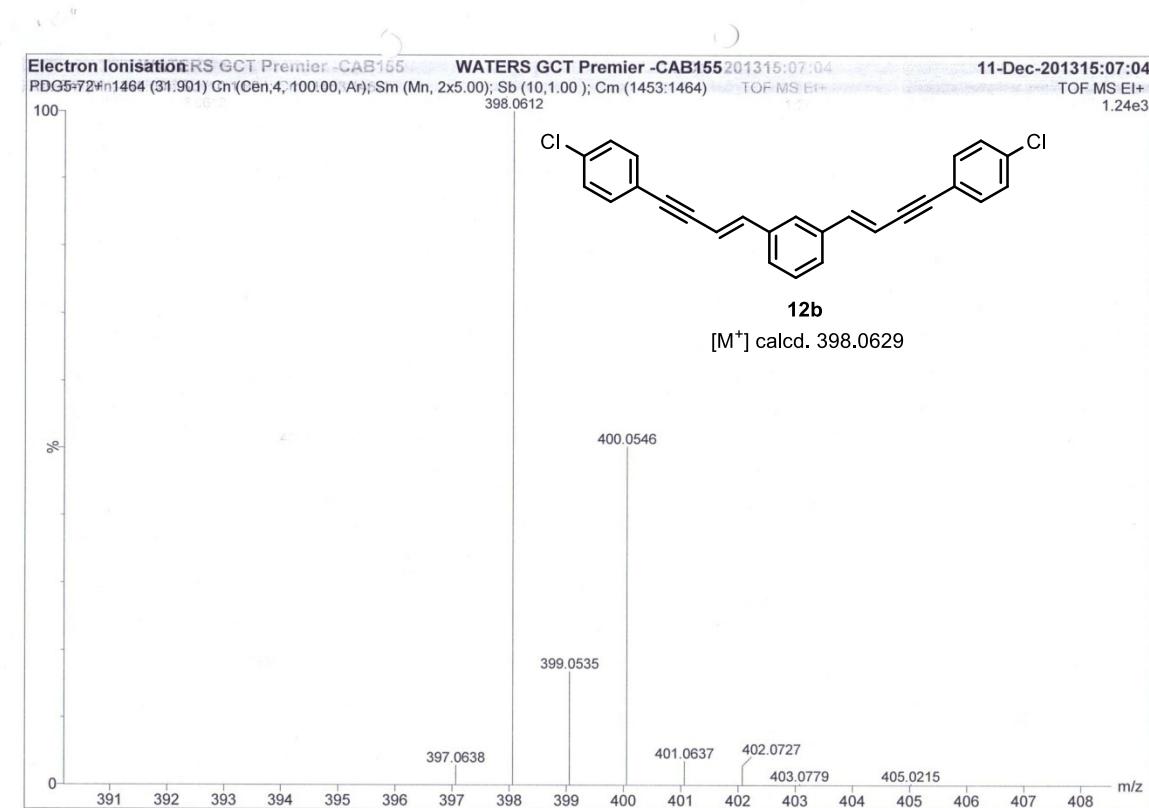
ESI (HRMS) spectrum of 1,3-bis((E)-4-(*p*-tolyl)but-1-en-3-ynyl)benzene (**12a**)



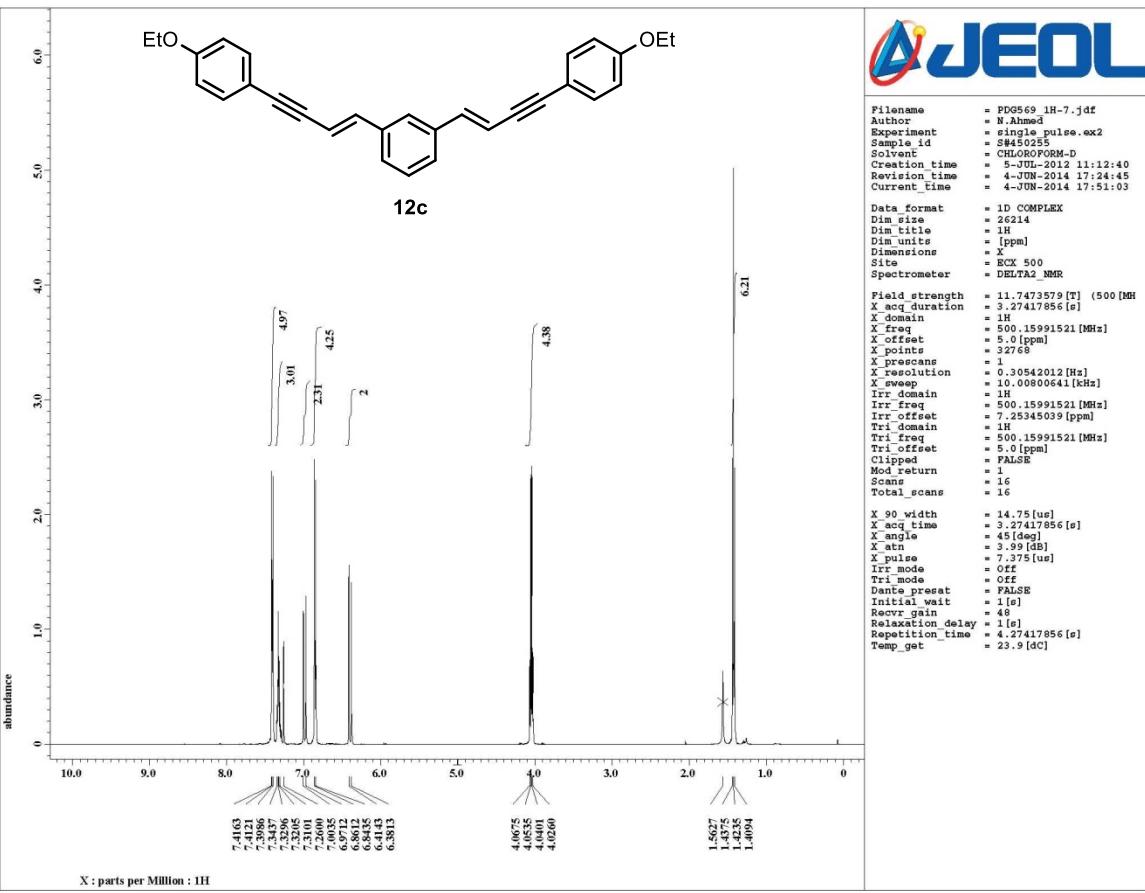
¹H NMR (500 MHz, CDCl₃) spectrum of 1,3-bis((E)-4-(4-chlorophenyl)but-1-en-3-ynyl)benzene (**12b**)



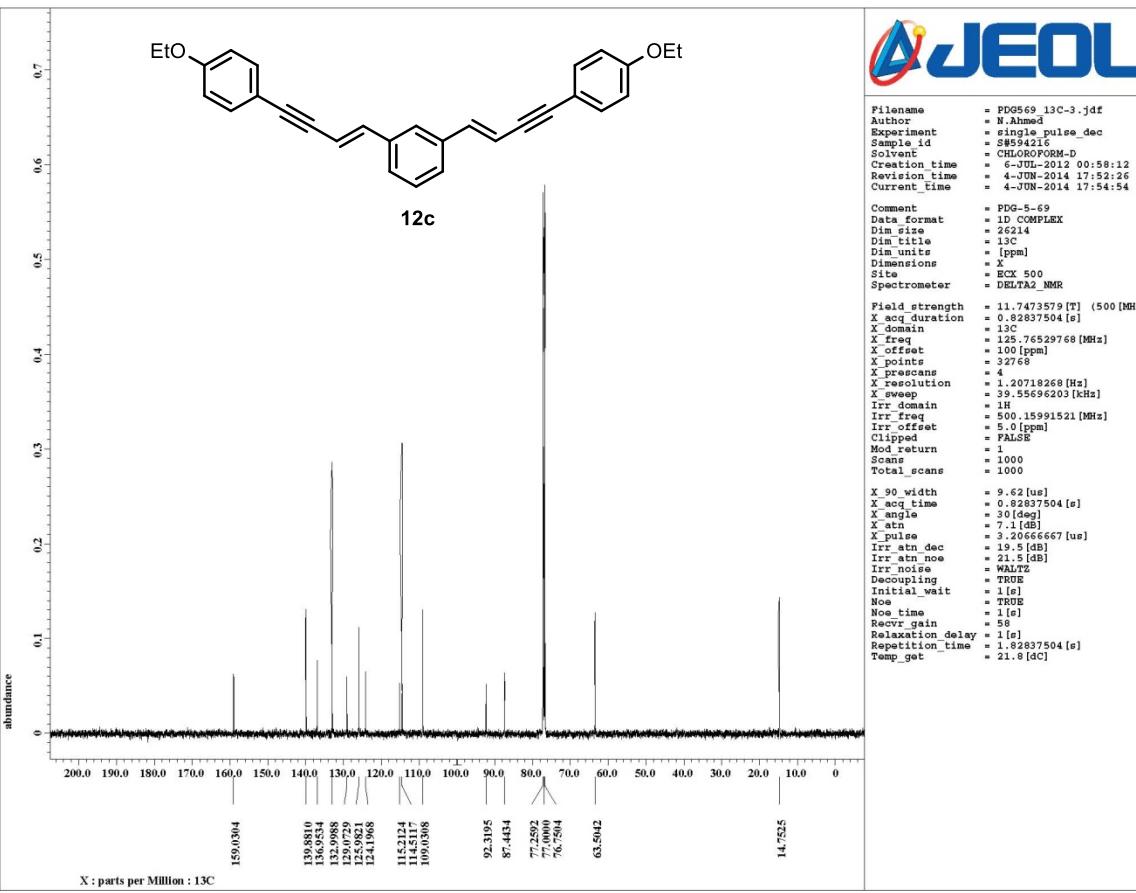
^{13}C NMR (125 MHz, CDCl_3) spectrum of 1,3-bis(*(E*)-4-(4-chlorophenyl)but-1-en-3-ynyl)benzene (**12b**)



EI (HRMS) spectrum of 1,3-bis((E)-4-(4-chlorophenyl)but-1-en-3-ynyl)benzene (**12b**)



¹H NMR (500 MHz, CDCl₃) spectrum of 1,3-bis((E)-4-(4-ethoxyphenyl)but-1-en-3-ynyl)benzene (**12c**)



¹³C NMR (125 MHz, CDCl₃) spectrum of 1,3-bis((E)-4-(4-ethoxyphenyl)but-1-en-3-ynyl)benzene (**12c**)

Electrospray ionisation-MS

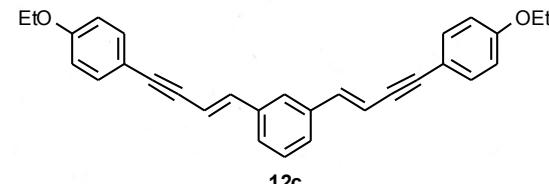
PDG5-69 11 (0.240) AM (Cen,4, 45.00, Ar,8500.0,556.28,0.25,LS 10); Sm (SG, 2x5.00); Sb (10,1.00); Cm (4:27-56:70)
419.2017

WATERS-Q-ToF Premier-HAB213

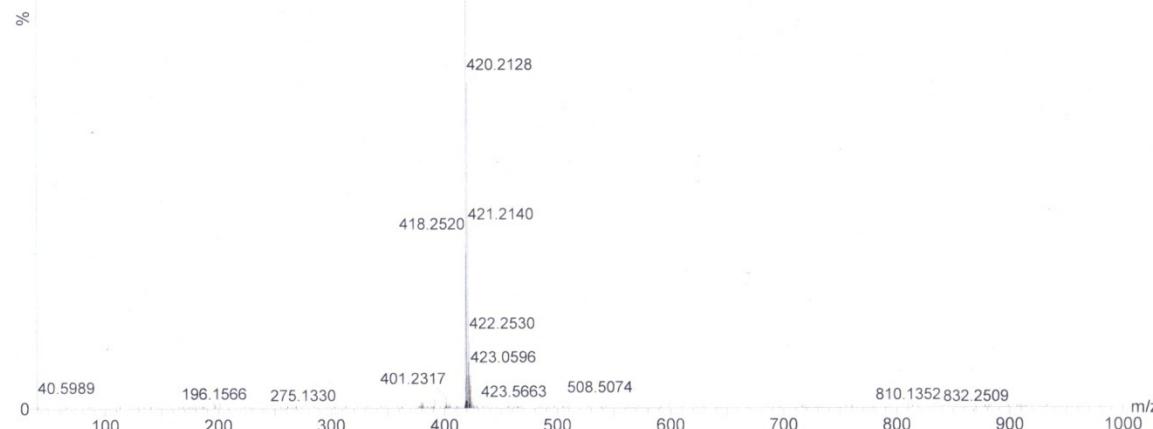
16:38:57 21-Aug-2012

1: TOF MSMS 419.20ES+
446

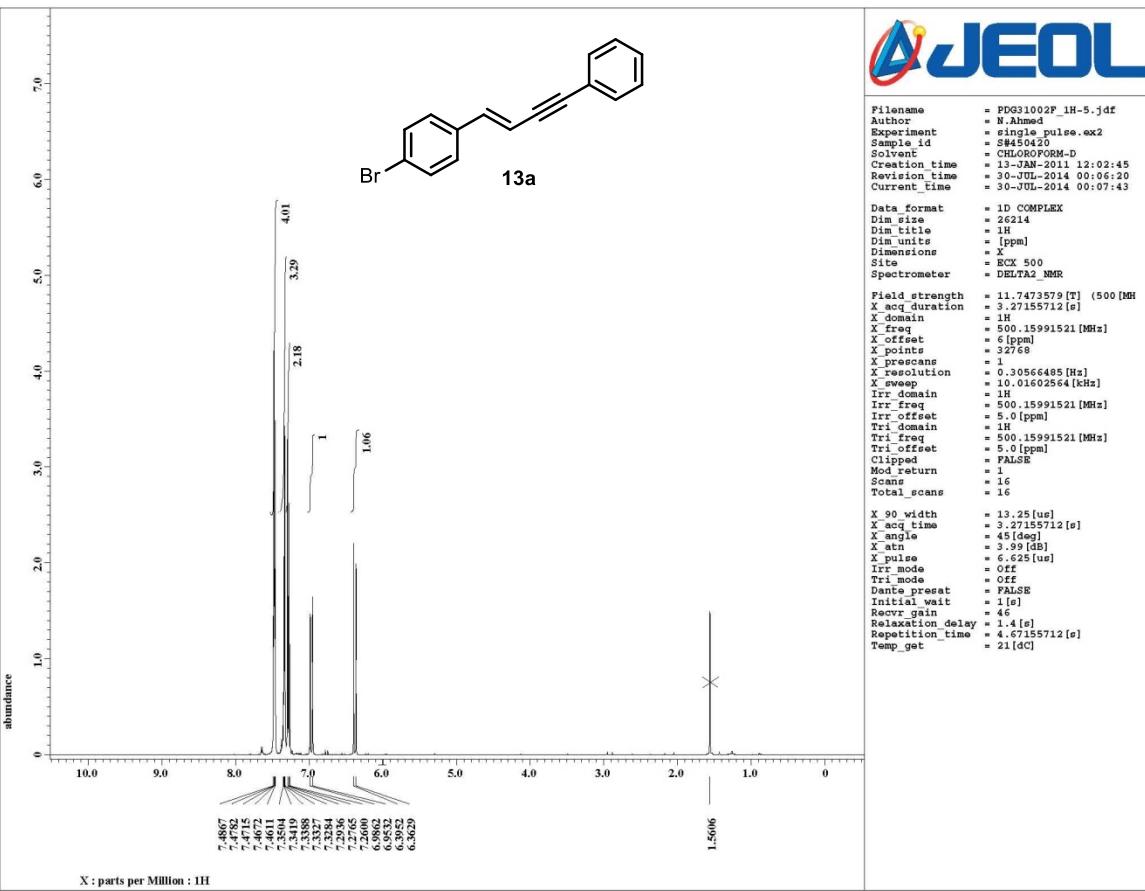
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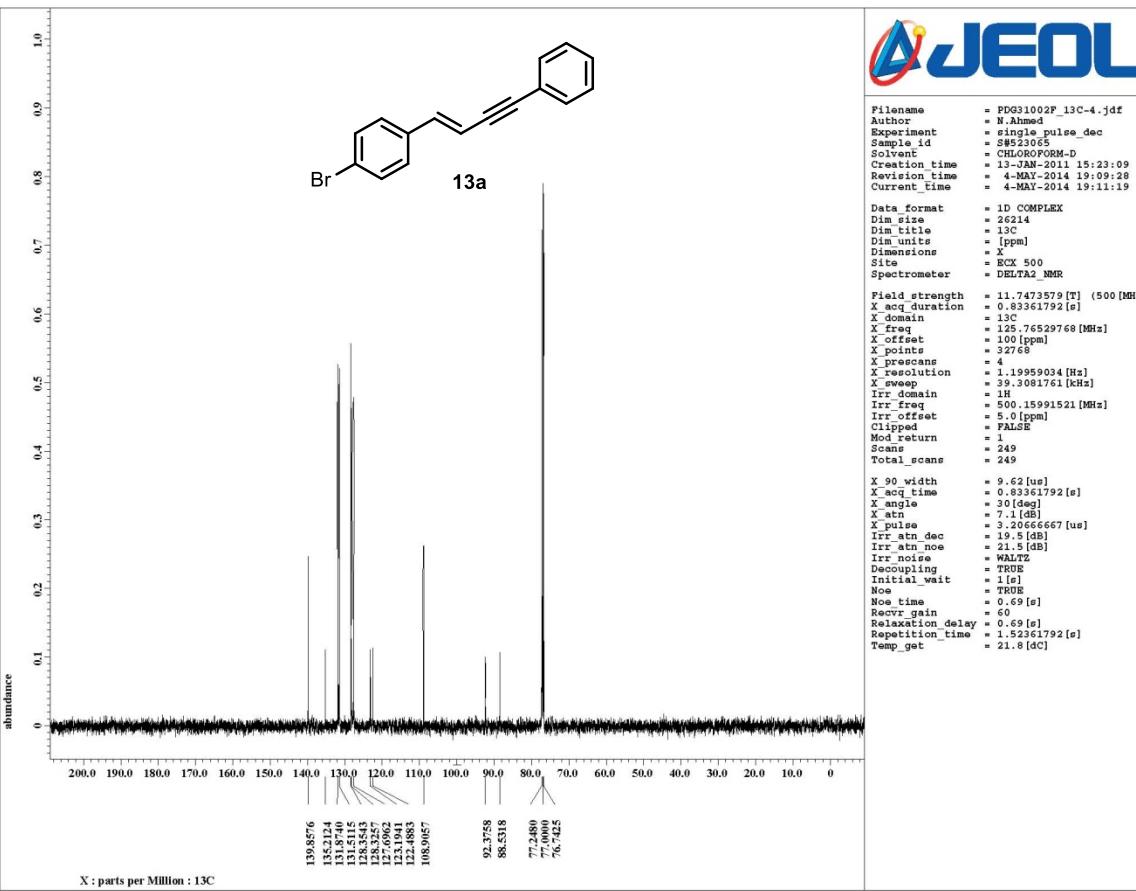
[MH⁺] calcd. 419.2011



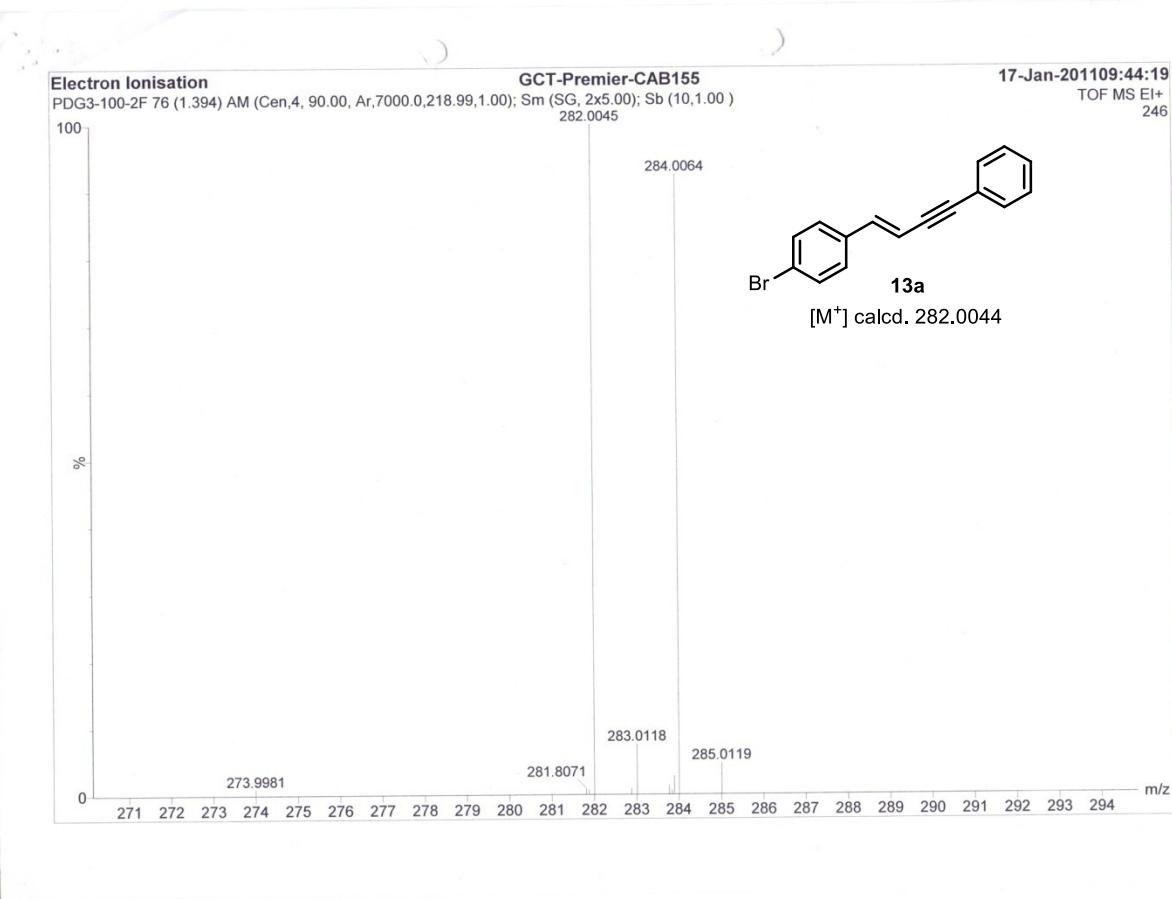
ESI (HRMS) spectrum of 1,3-bis((E)-4-(4-ethoxyphenyl)but-1-en-3-ynyl)benzene (**12c**)



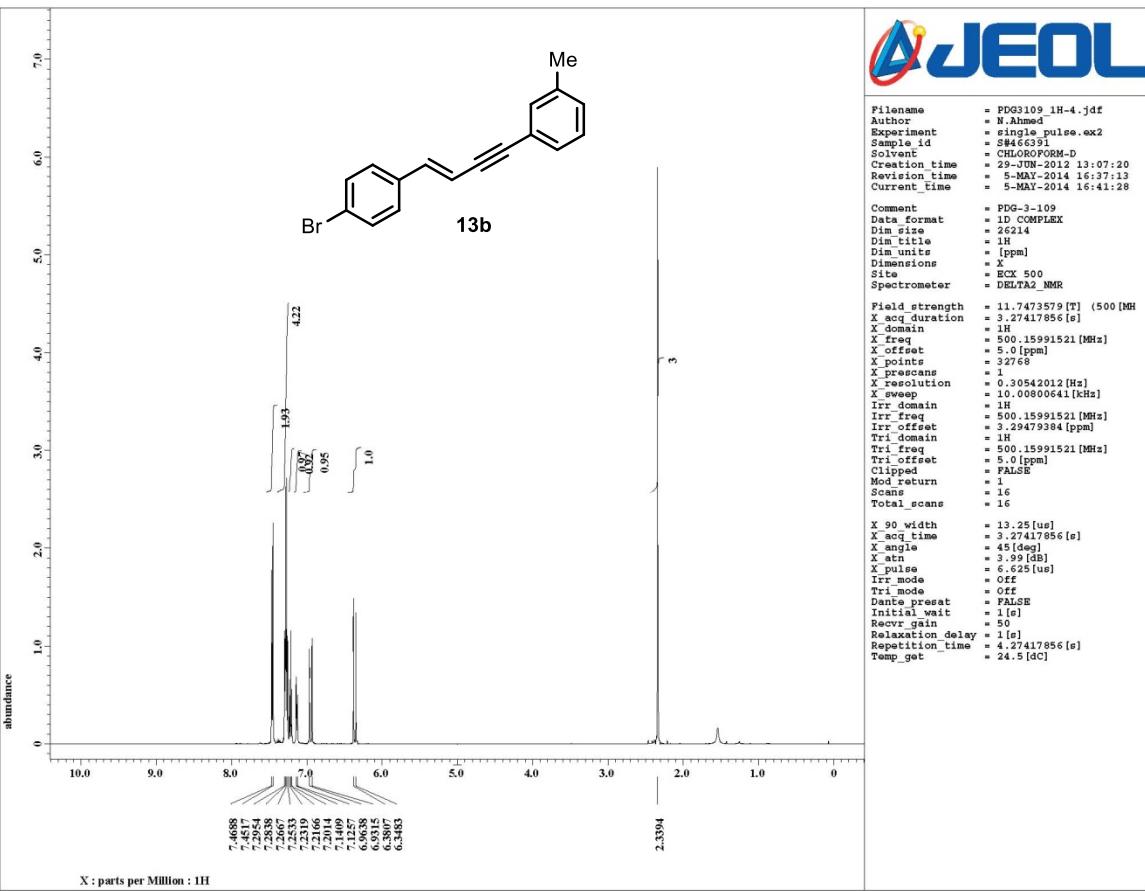
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4-phenylbut-1-en-3-ynyl)benzene (**13a**)



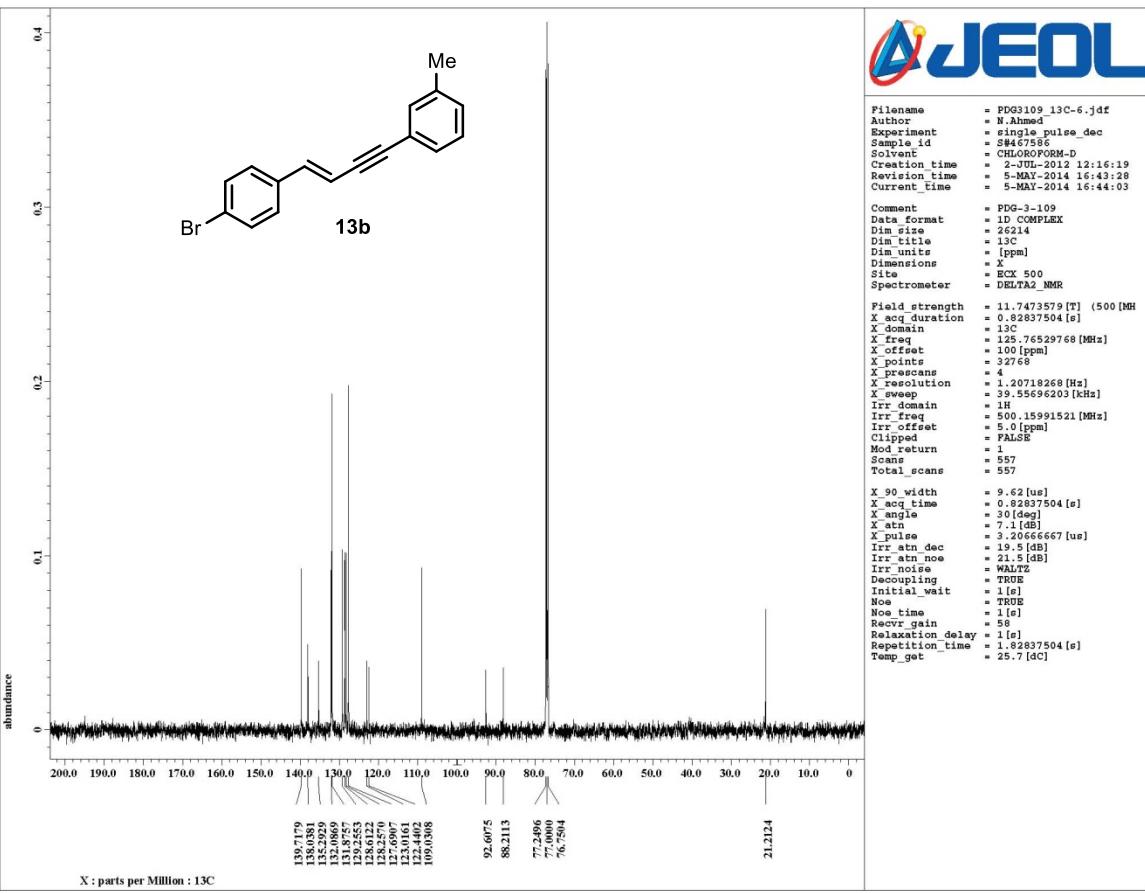
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-1-bromo-4-(4-phenylbut-1-en-3-ynyl)benzene (**13a**)



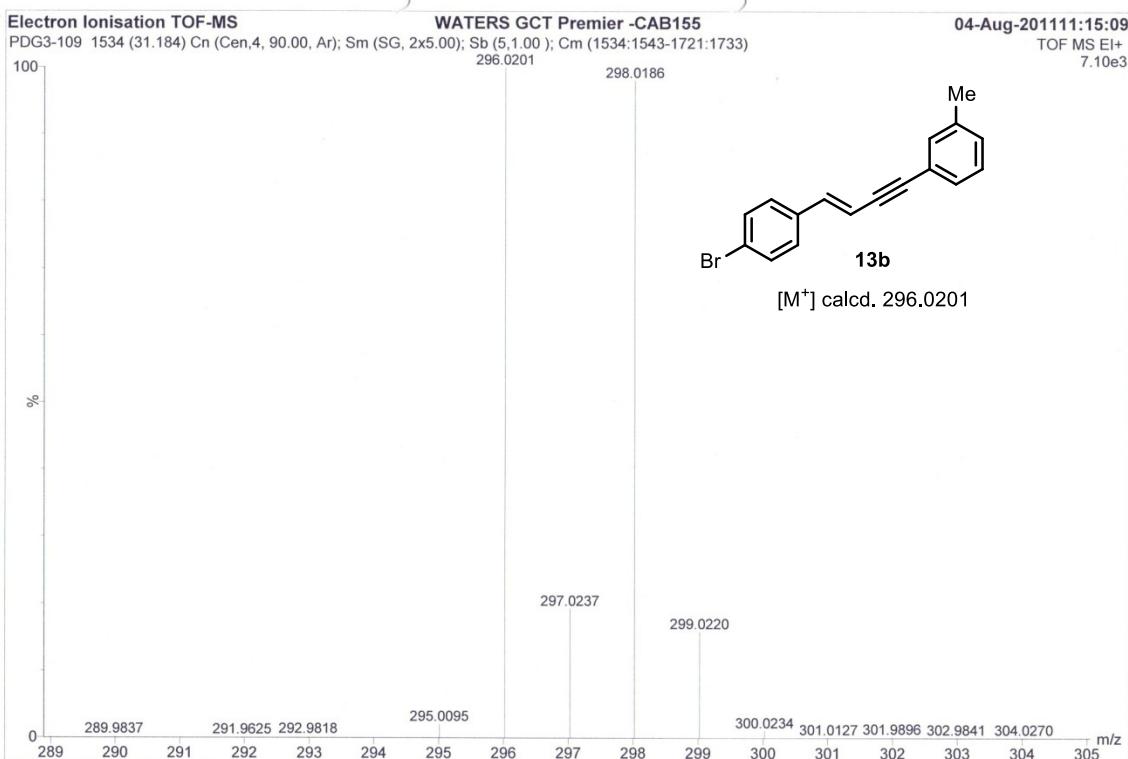
EI (HRMS) spectrum of (*E*)-1-bromo-4-(4-phenylbut-1-en-3-ynyl)benzene (**13a**)



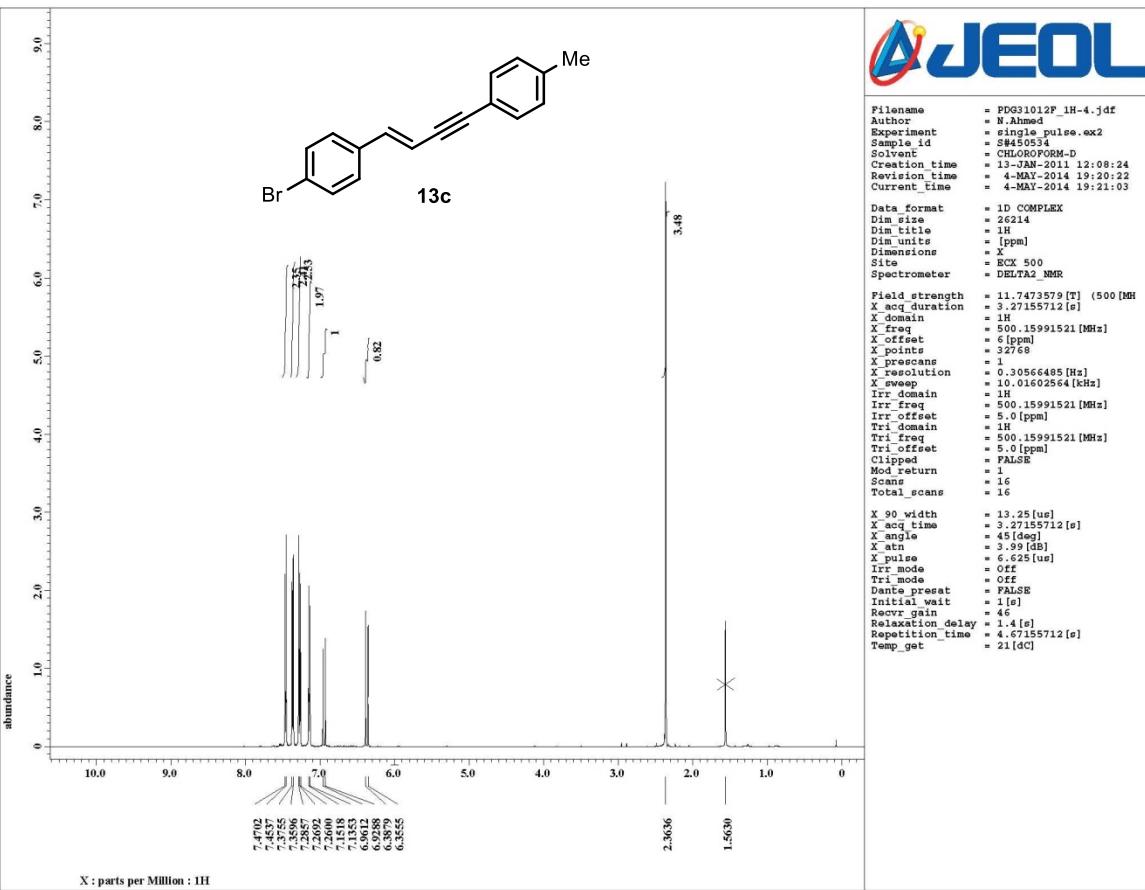
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-methylbenzene (**13b**)



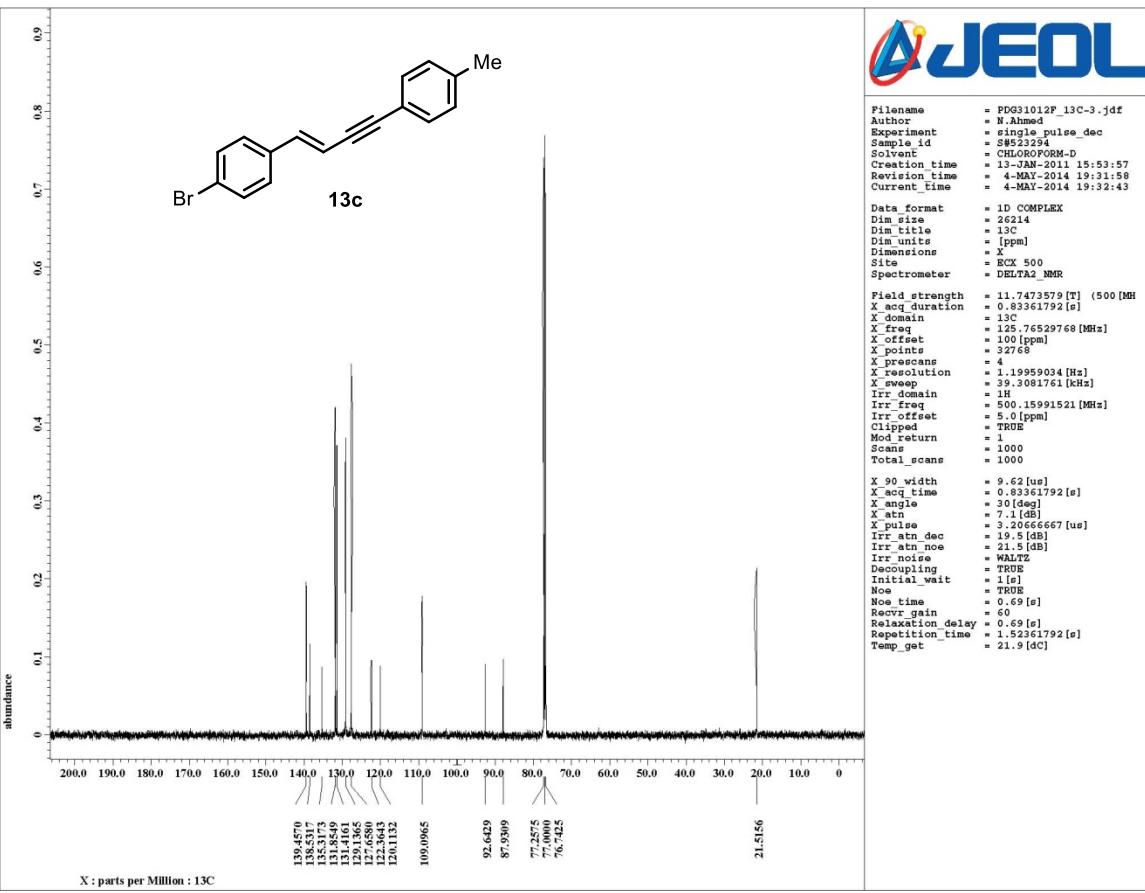
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-methylbenzene (**13b**)



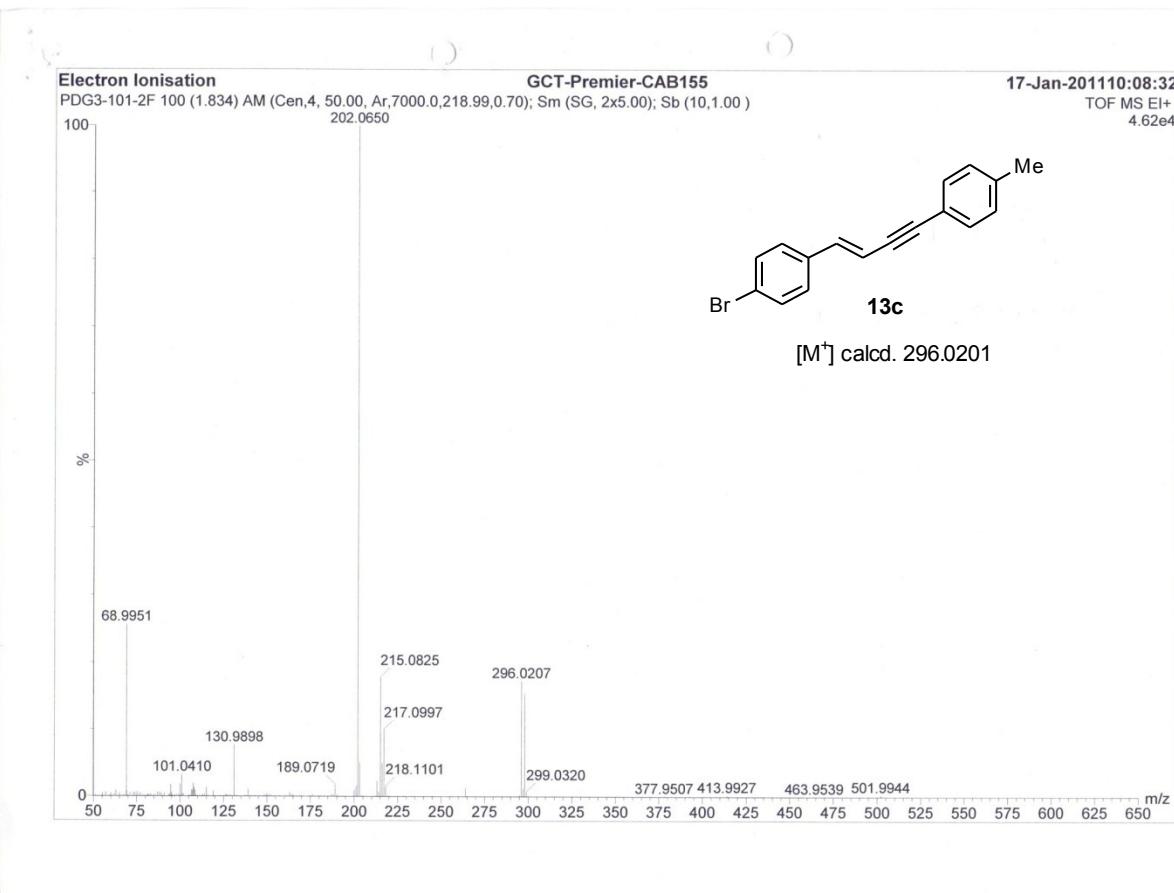
EI (HRMS) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-methylbenzene (**13b**)



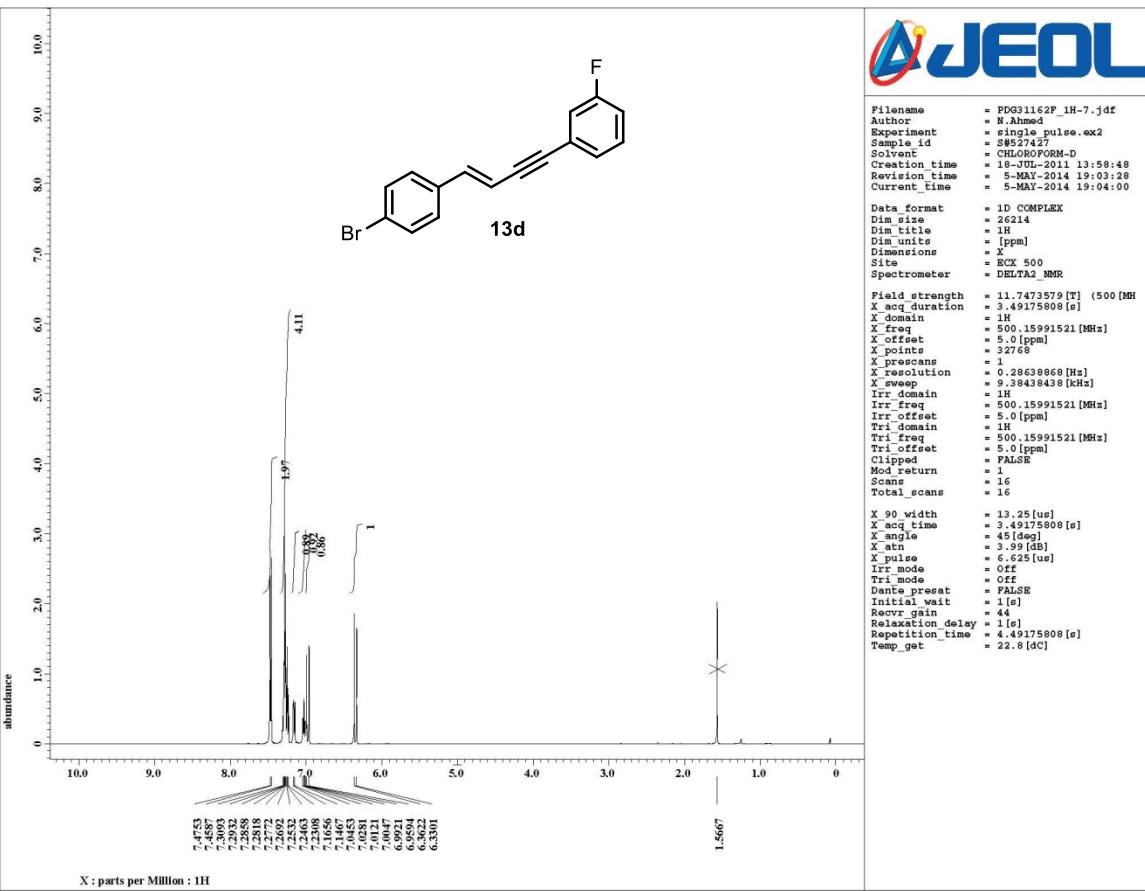
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4-*p*-tolylbut-1-en-3ynyl)benzene (**13c**)



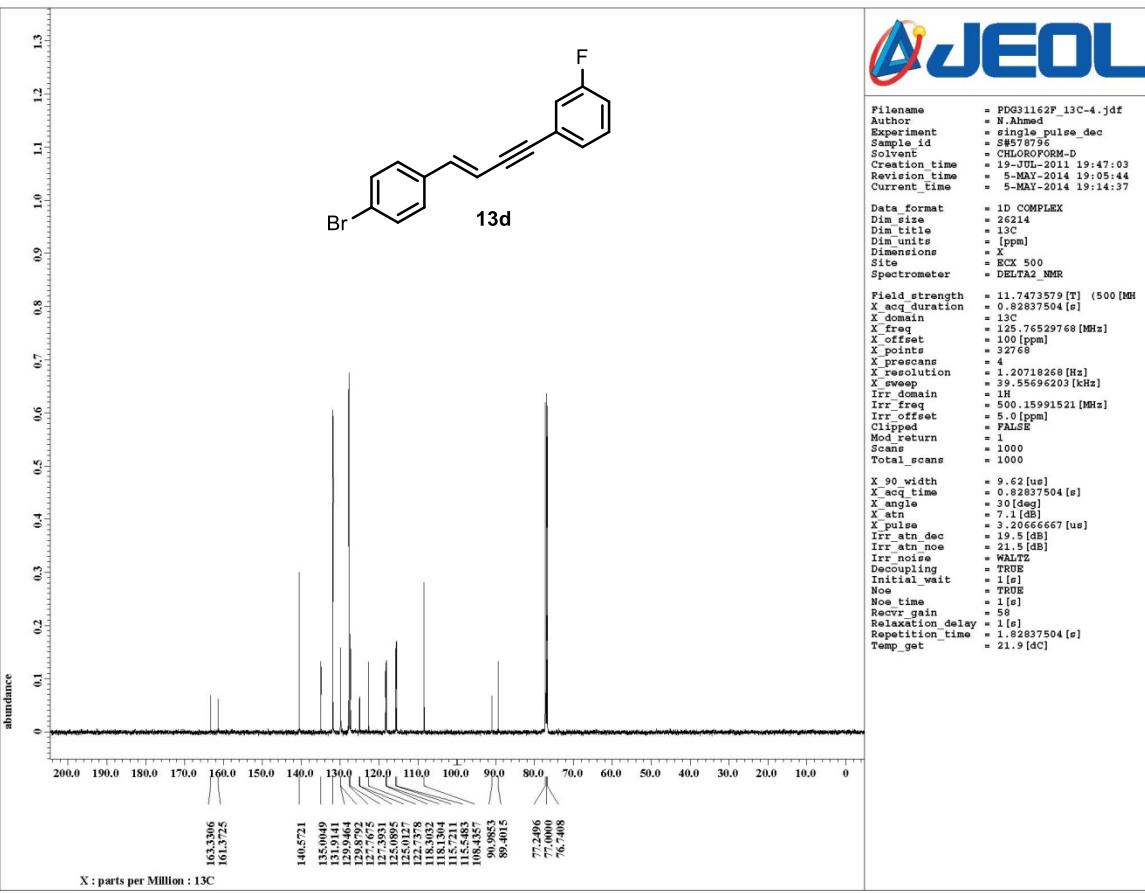
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-bromo-4-(4-p-tolylbut-1-en-3-ynyl)benzene (**13c**)



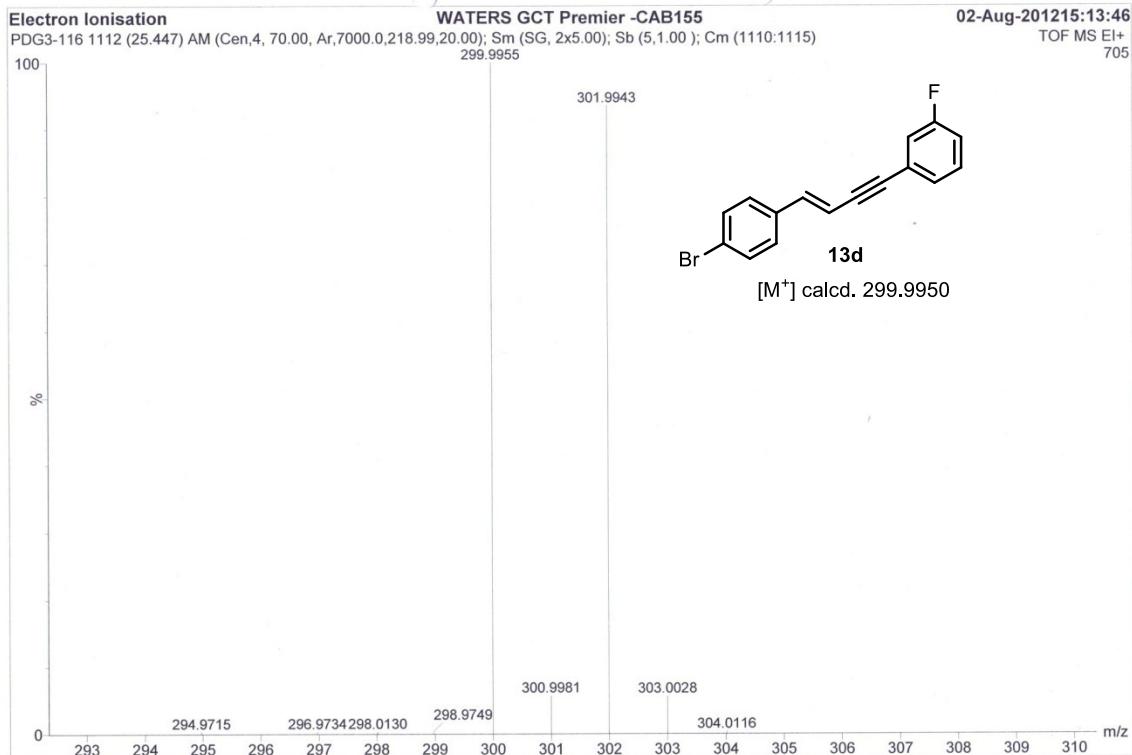
EI (HRMS) spectrum of (*E*)-1-bromo-4-(4-*p*-tolylbut-1-en-3ynyl)benzene (**13c**)



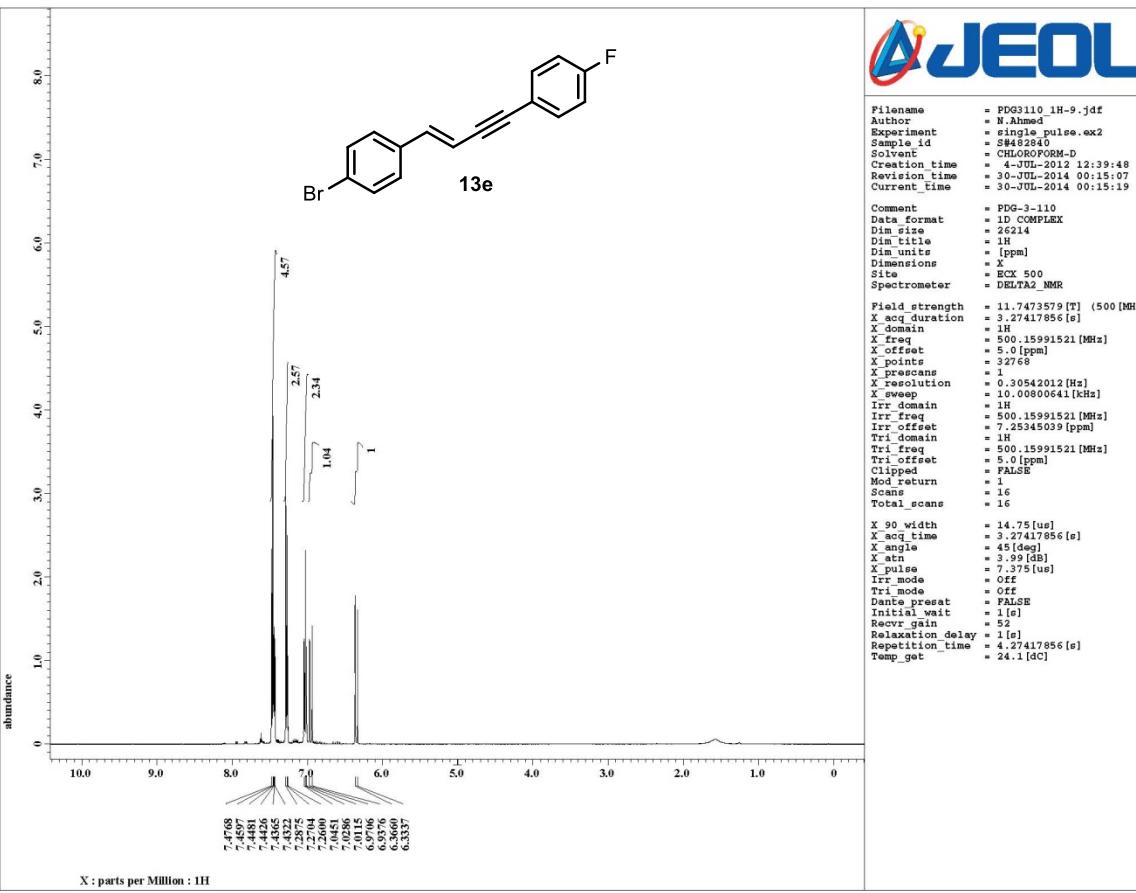
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-fluorobenzene (**13d**)



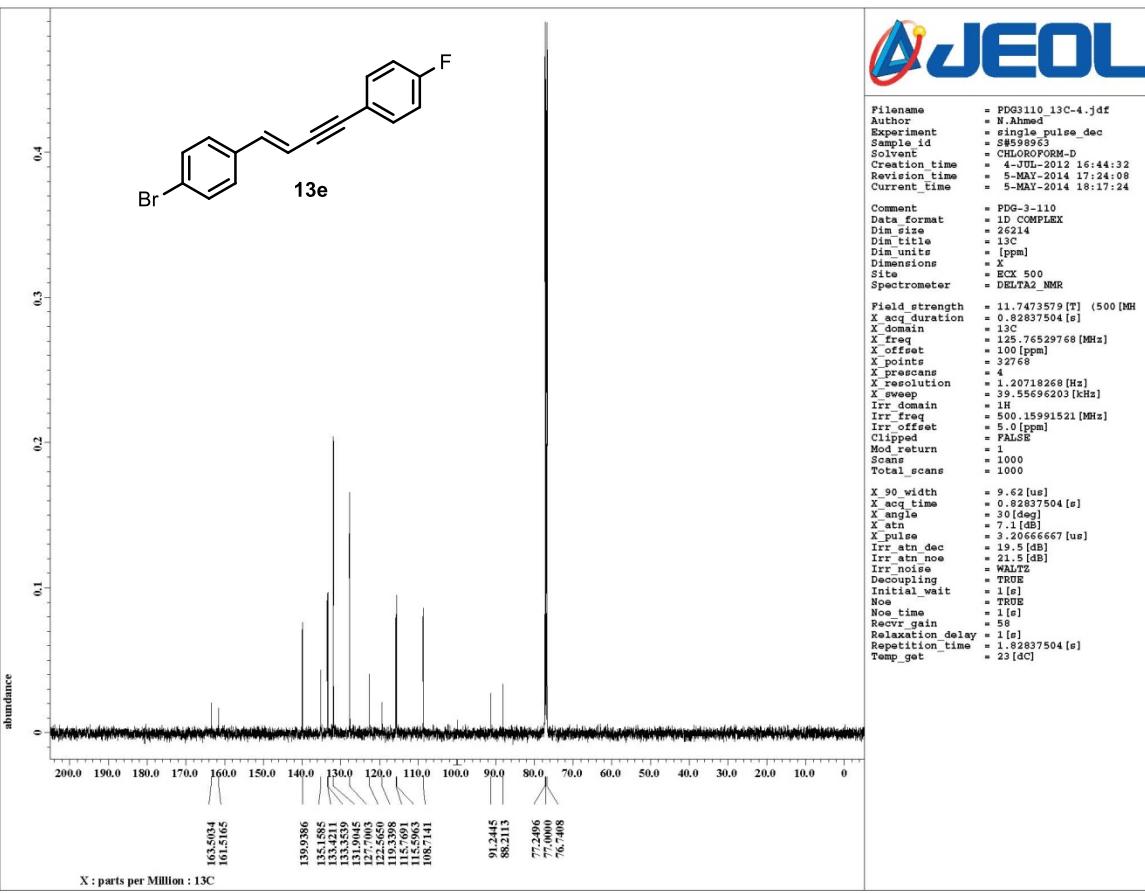
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-fluorobenzene (**13d**)



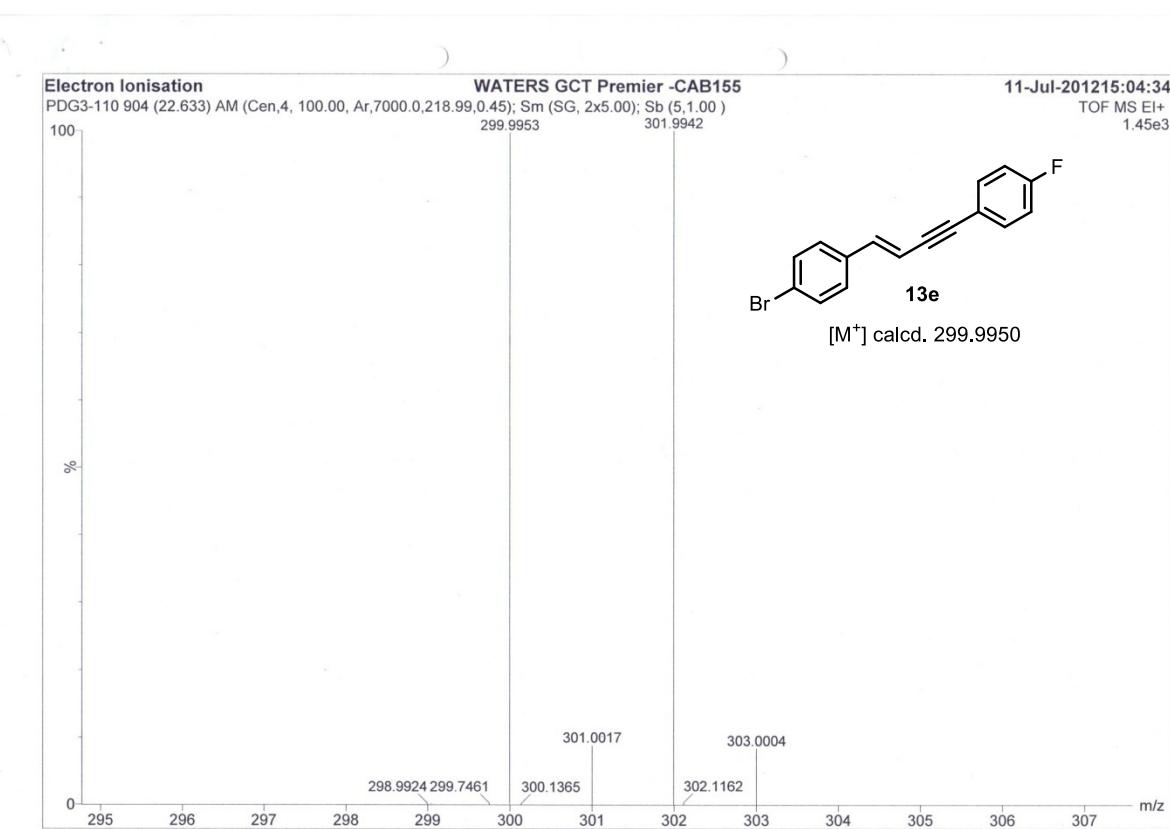
EI (HRMS) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-fluorobenzene (**13d**)



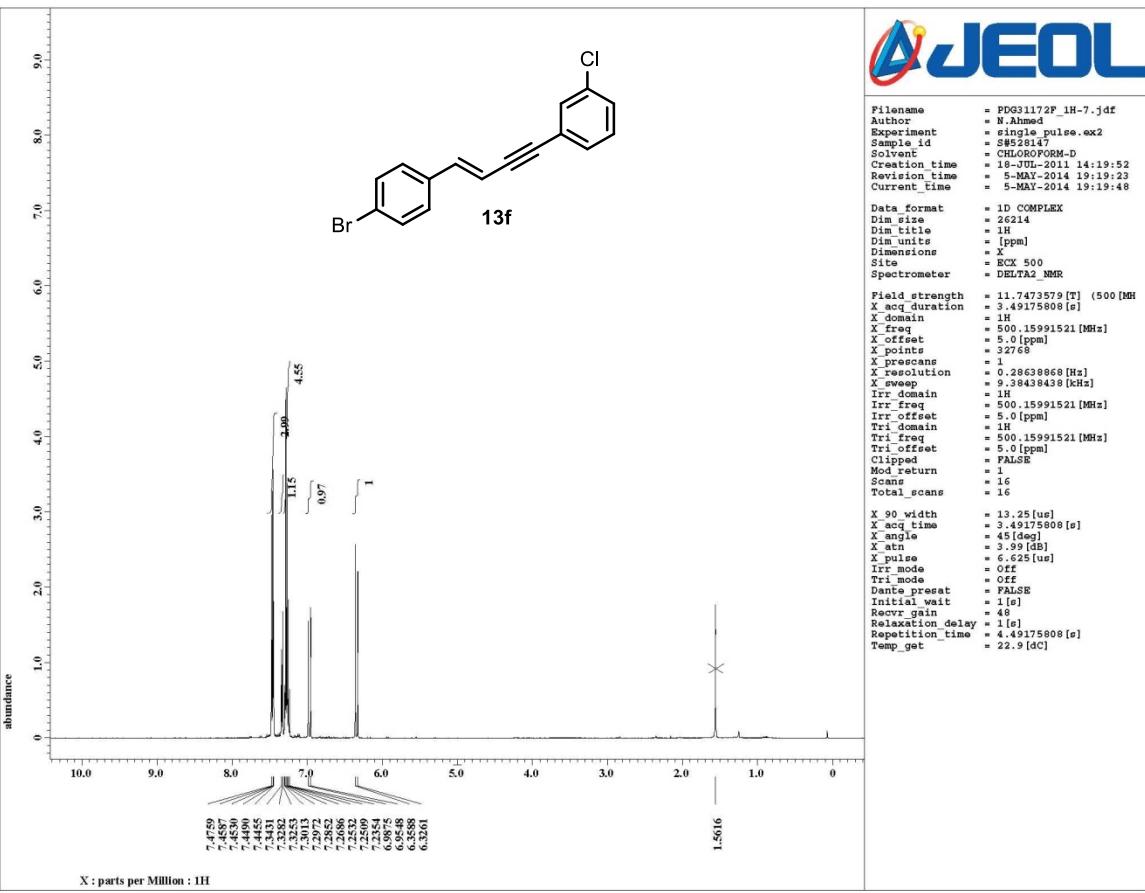
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4-(4-fluorophenyl)but-1-en-3-ynyl)benzene (**13e**)



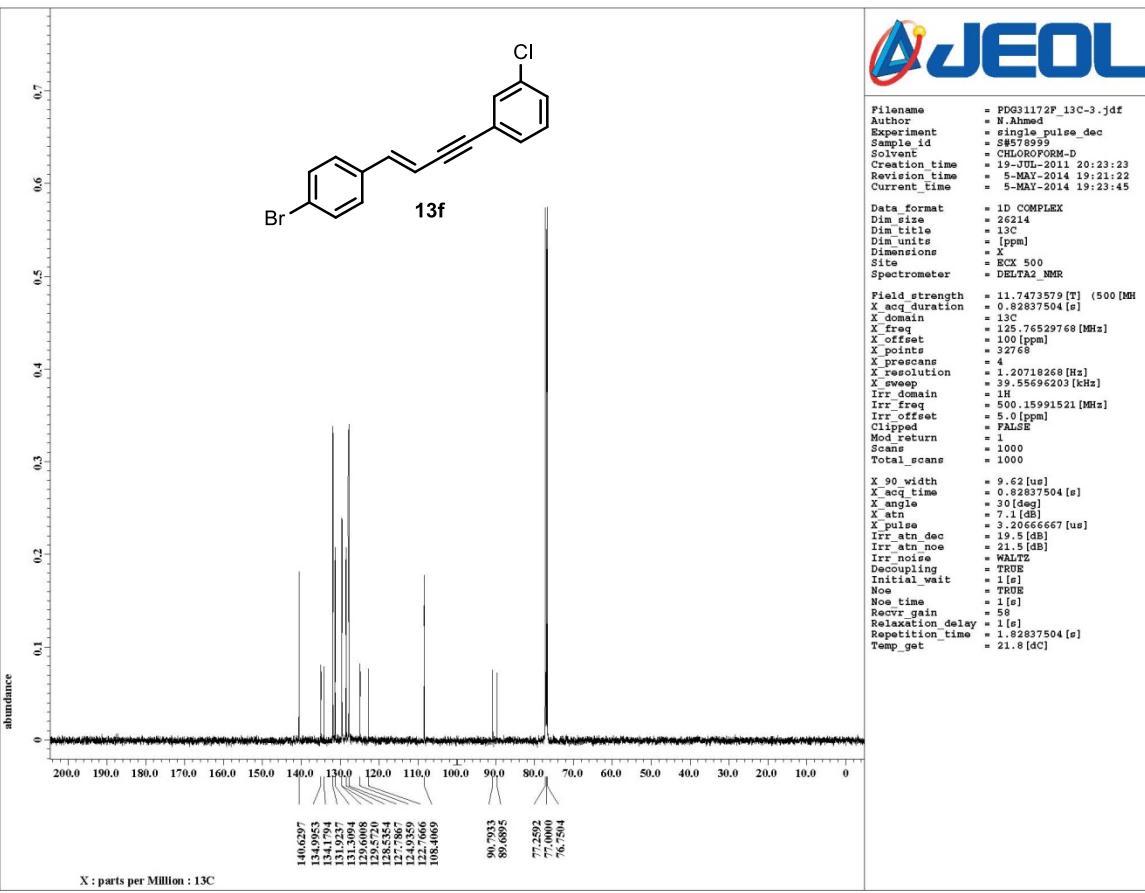
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4-fluorophenyl)but-1-en-3-ynebenzene (**13e**)



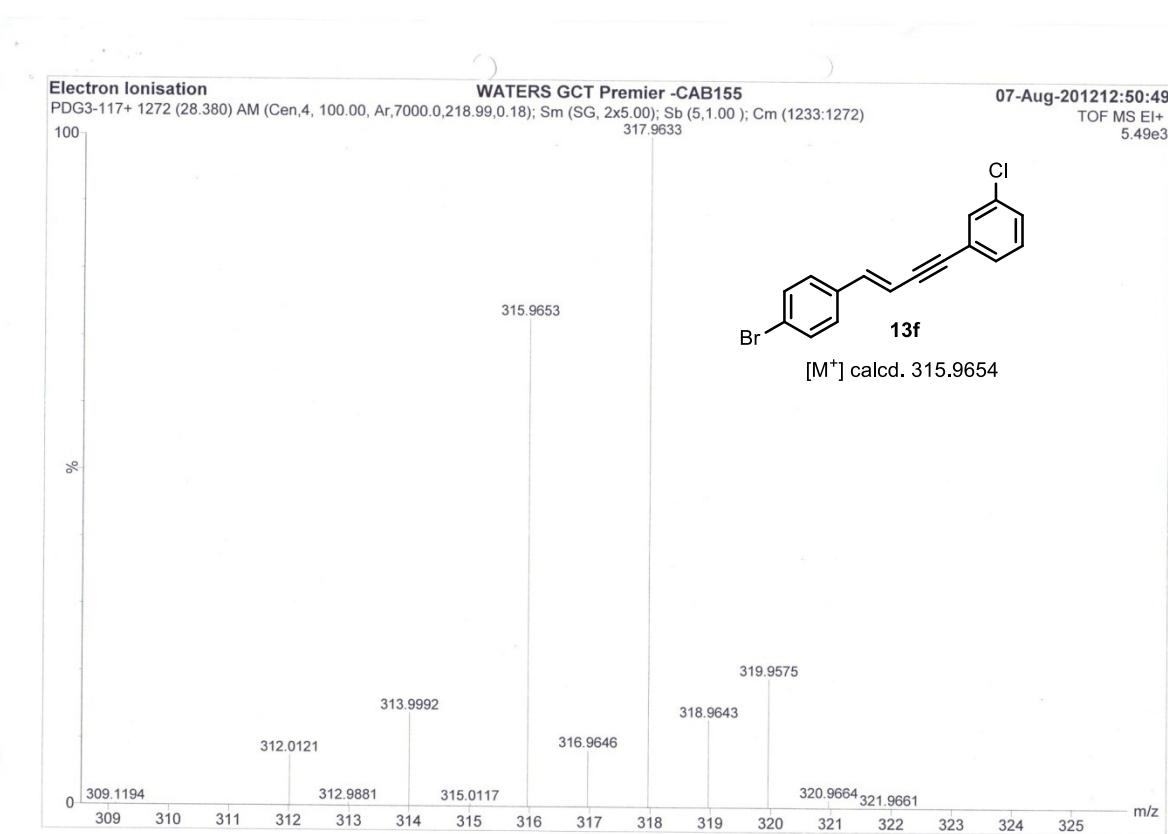
EI (HRMS) spectrum of (*E*)-1-bromo-4-(4-(4-fluorophenyl)but-1-en-3-ynyl)benzene (**13e**)



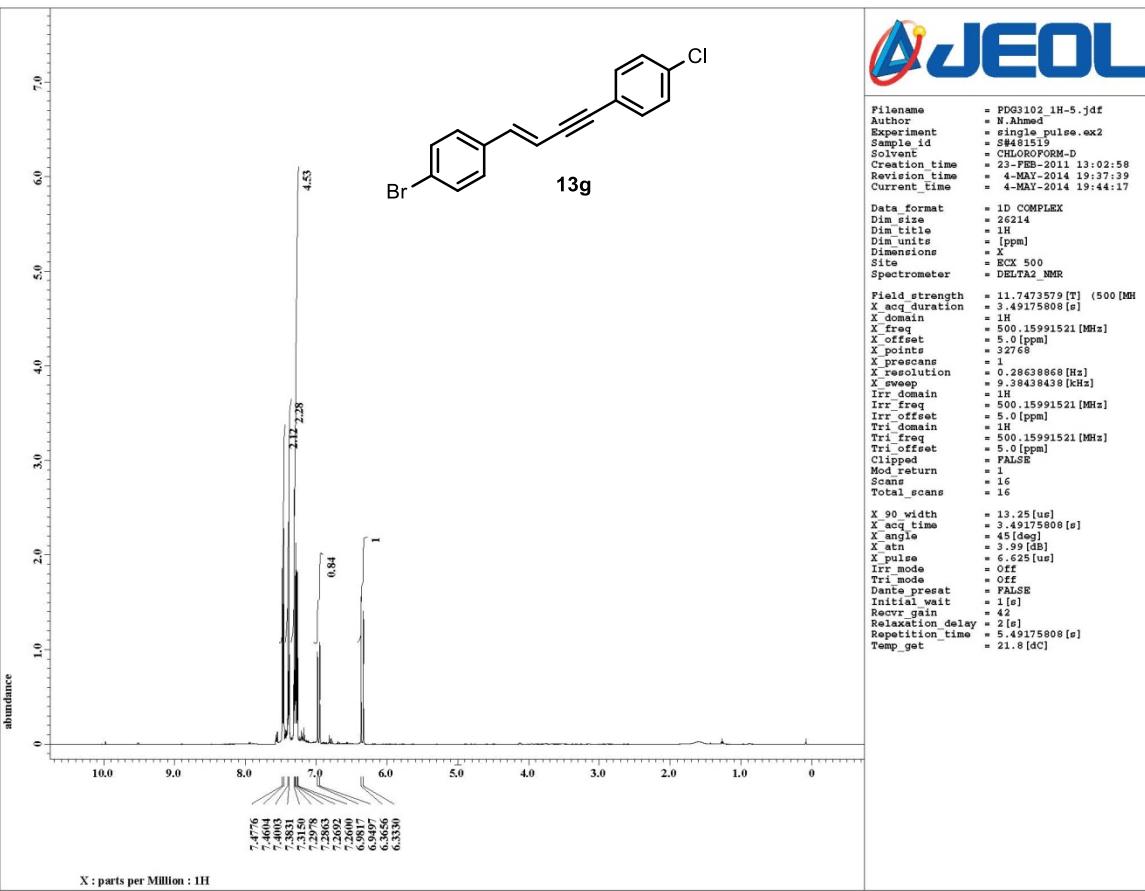
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-chlorobenzene (**13f**)



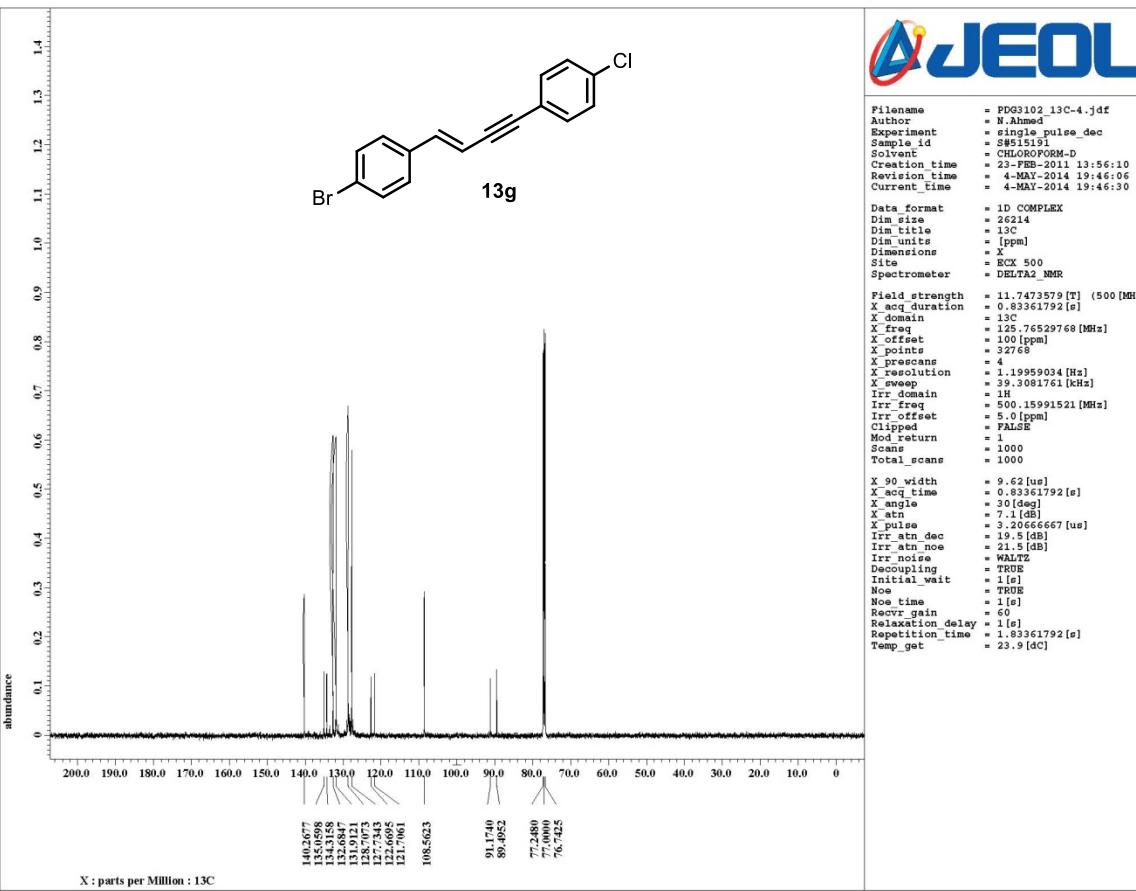
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-chlorobenzene (**13f**)



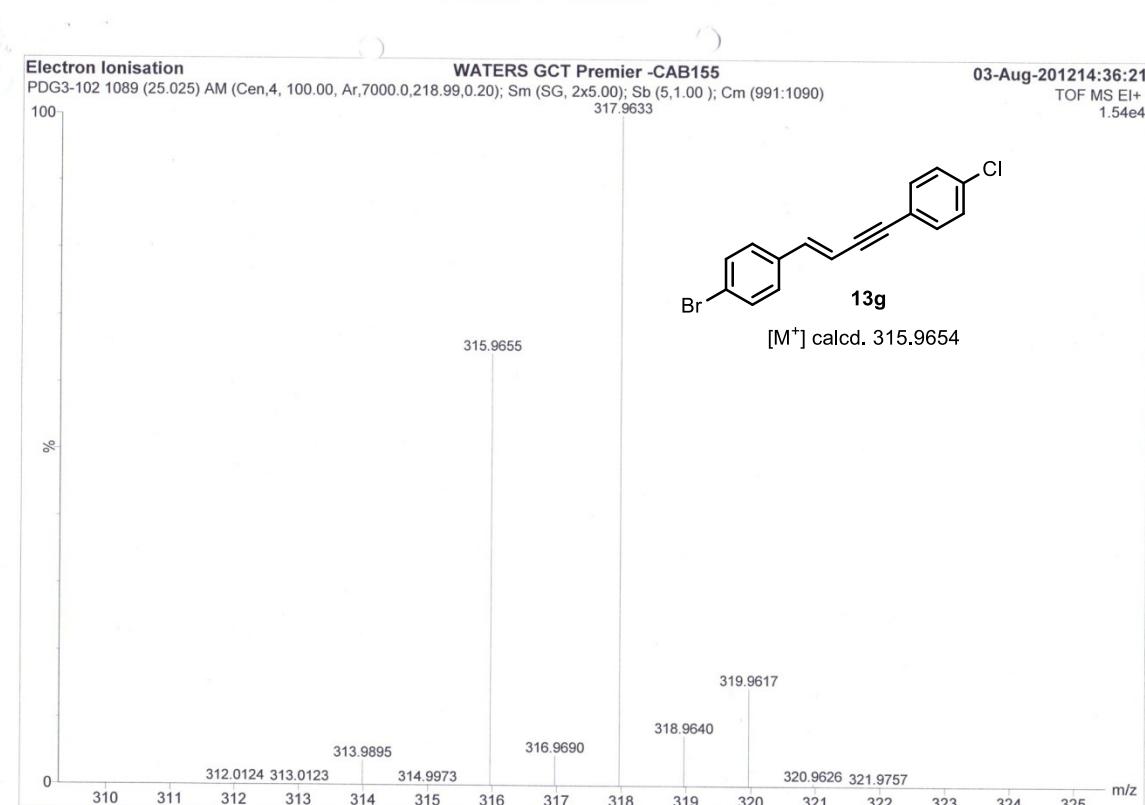
EI (HRMS) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-chlorobenzene (**13f**)



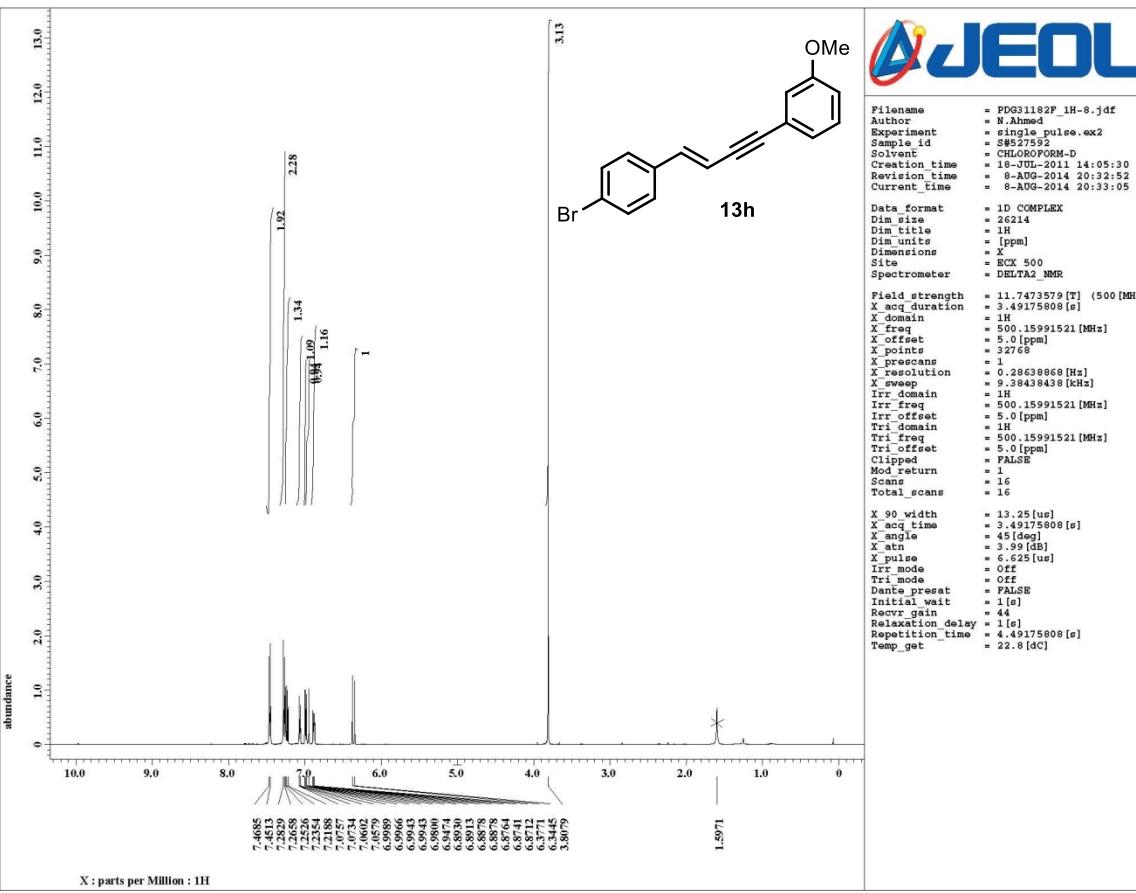
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4-(4-chlorophenyl)but-1-en-3-ynyl)benzene (**13g**)



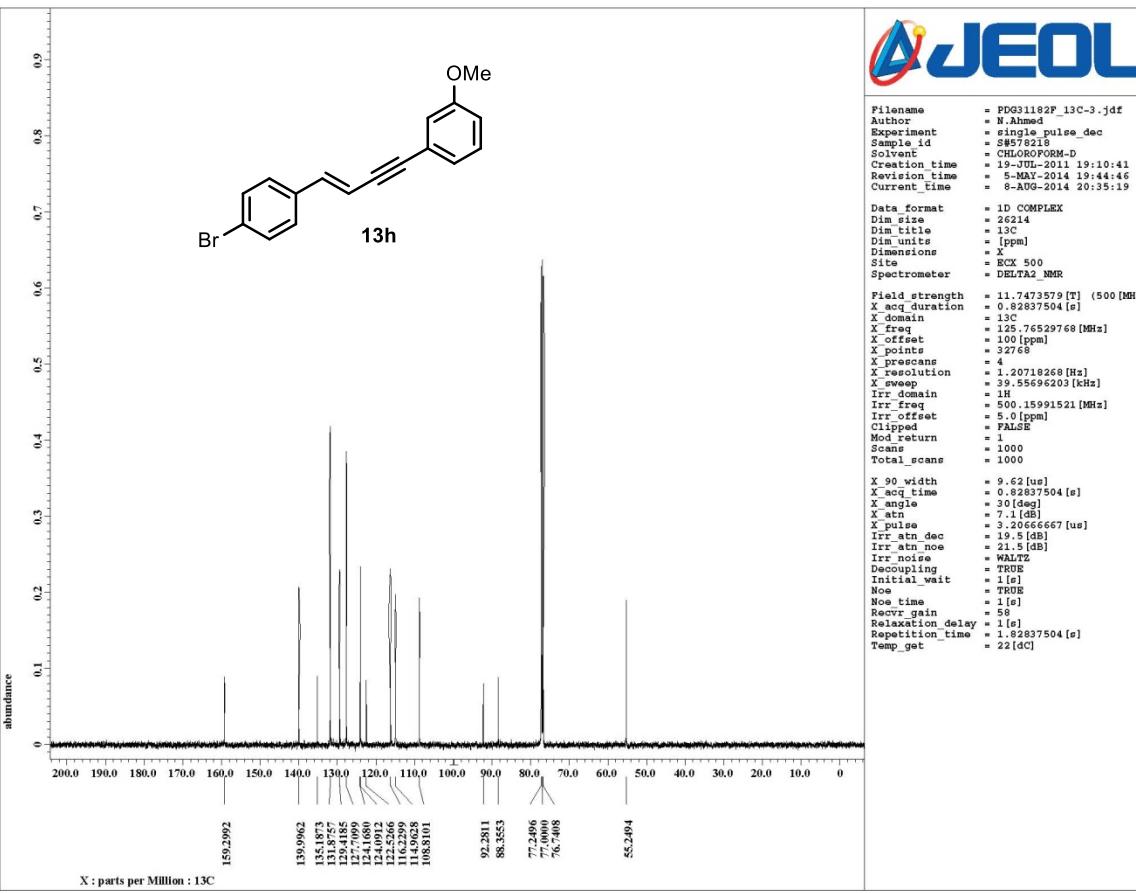
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-1-bromo-4-(4-chlorophenyl)but-1-en-3ynylbenzene (**13g**)



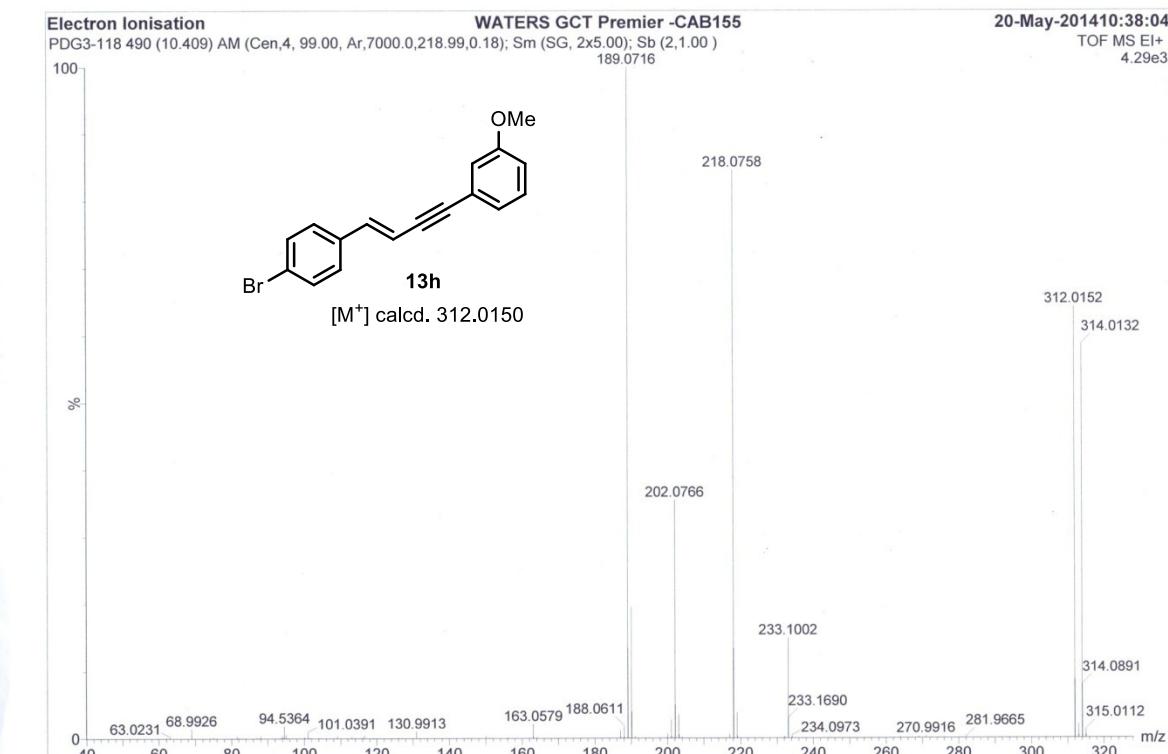
EI (HRMS) spectrum of (*E*)-1-bromo-4-(4-(4-chlorophenyl)but-1-en-3-ynyl)benzene (**13g**)



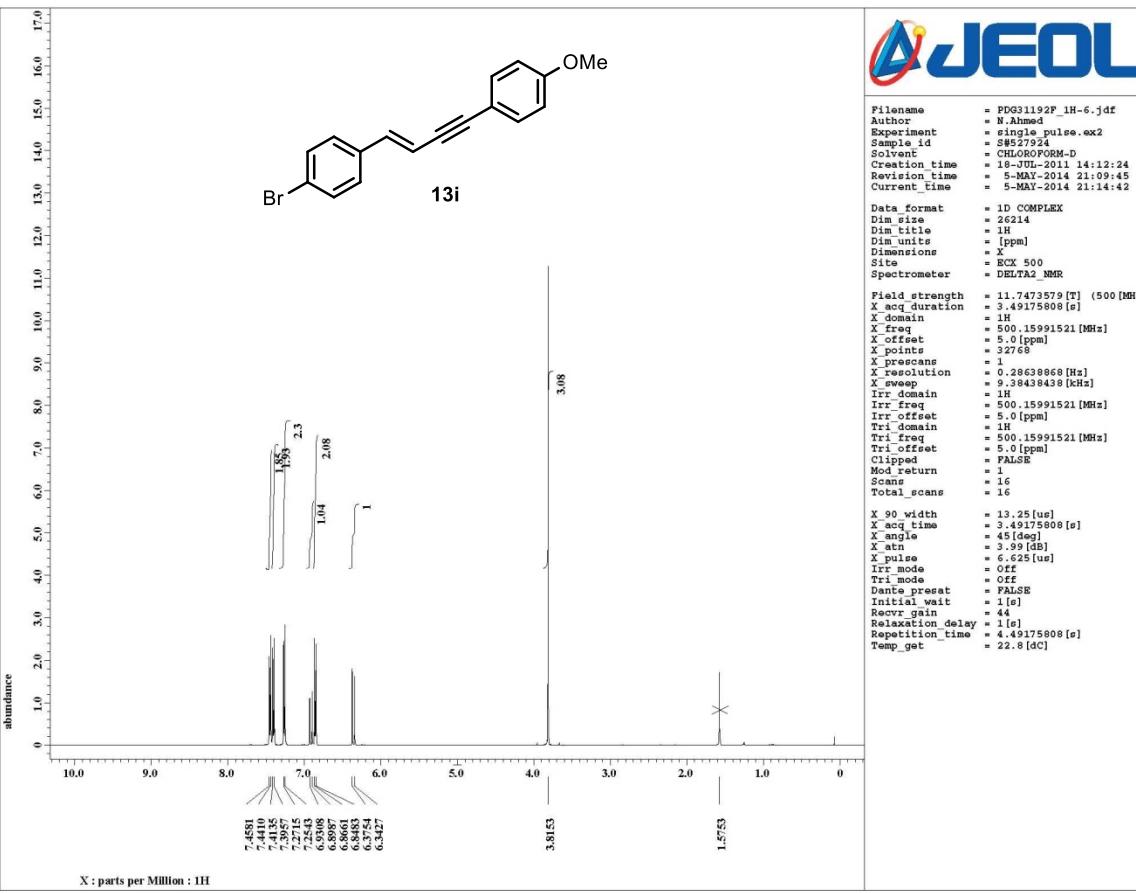
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-methoxybenzene (**13h**)



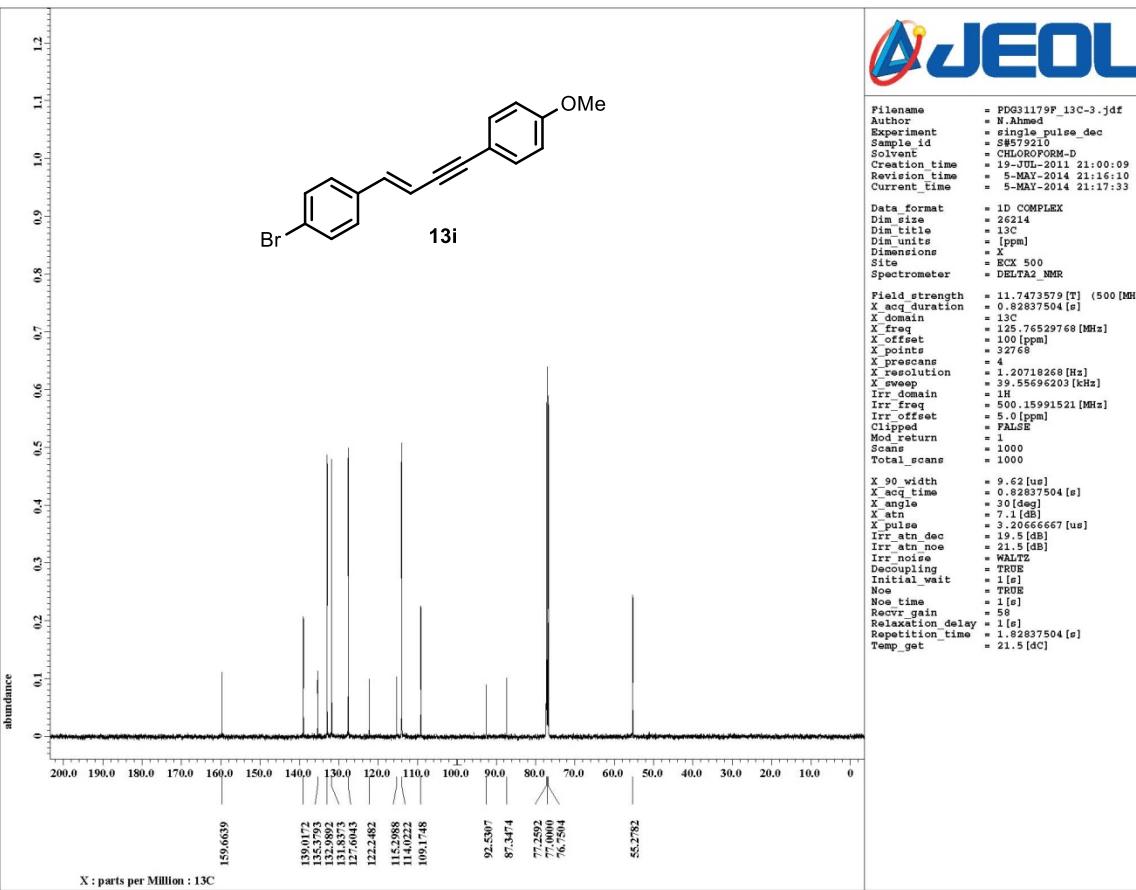
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-methoxybenzene (**13h**)



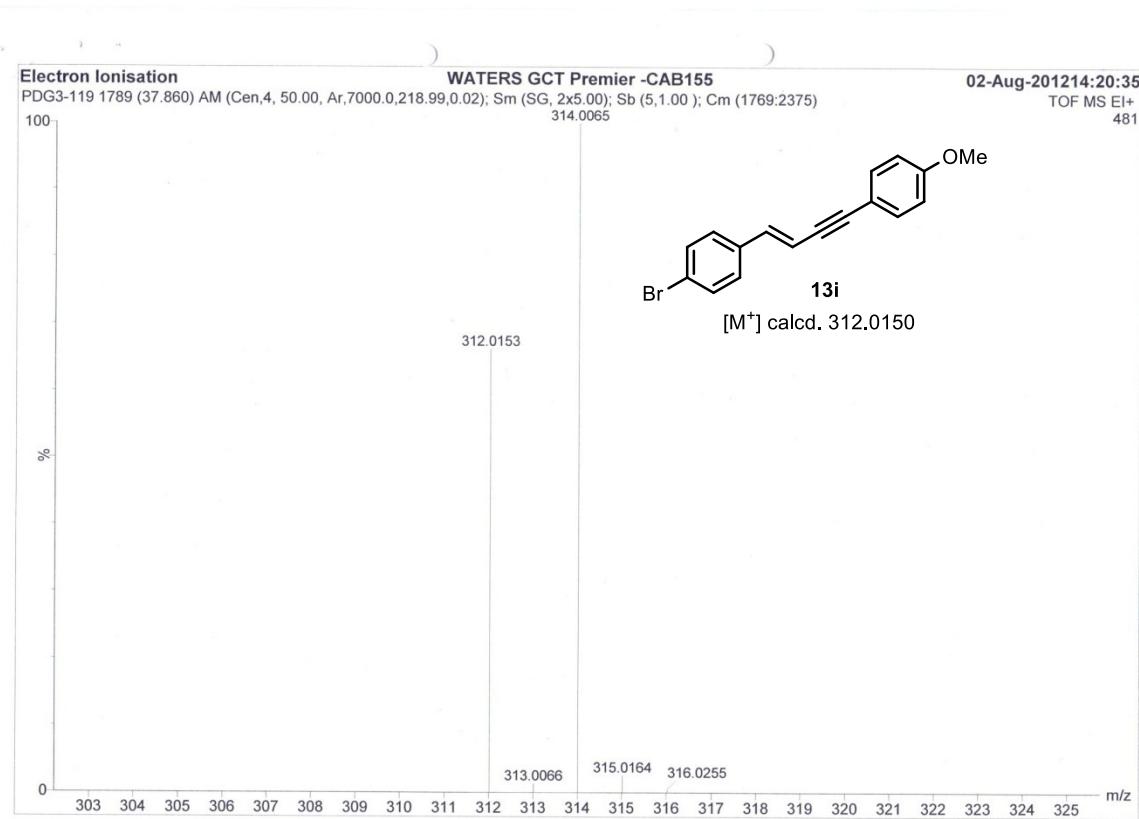
EI (HRMS) spectrum of (*E*)-1-(4-(4-bromophenyl)but-3-en-1-ynyl)-3-methoxybenzene (**13h**)



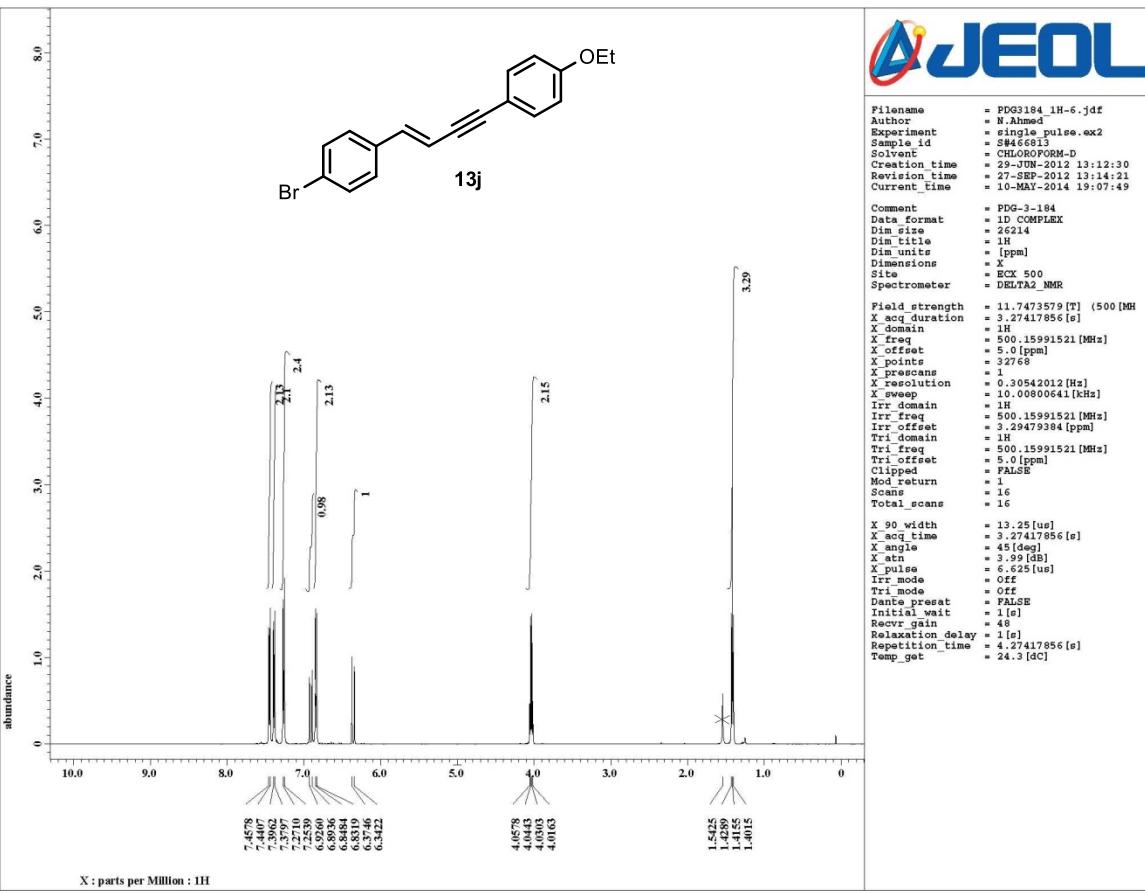
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4-(4-methoxyphenyl)but-1-en-3-ynyl)benzene (**13i**)



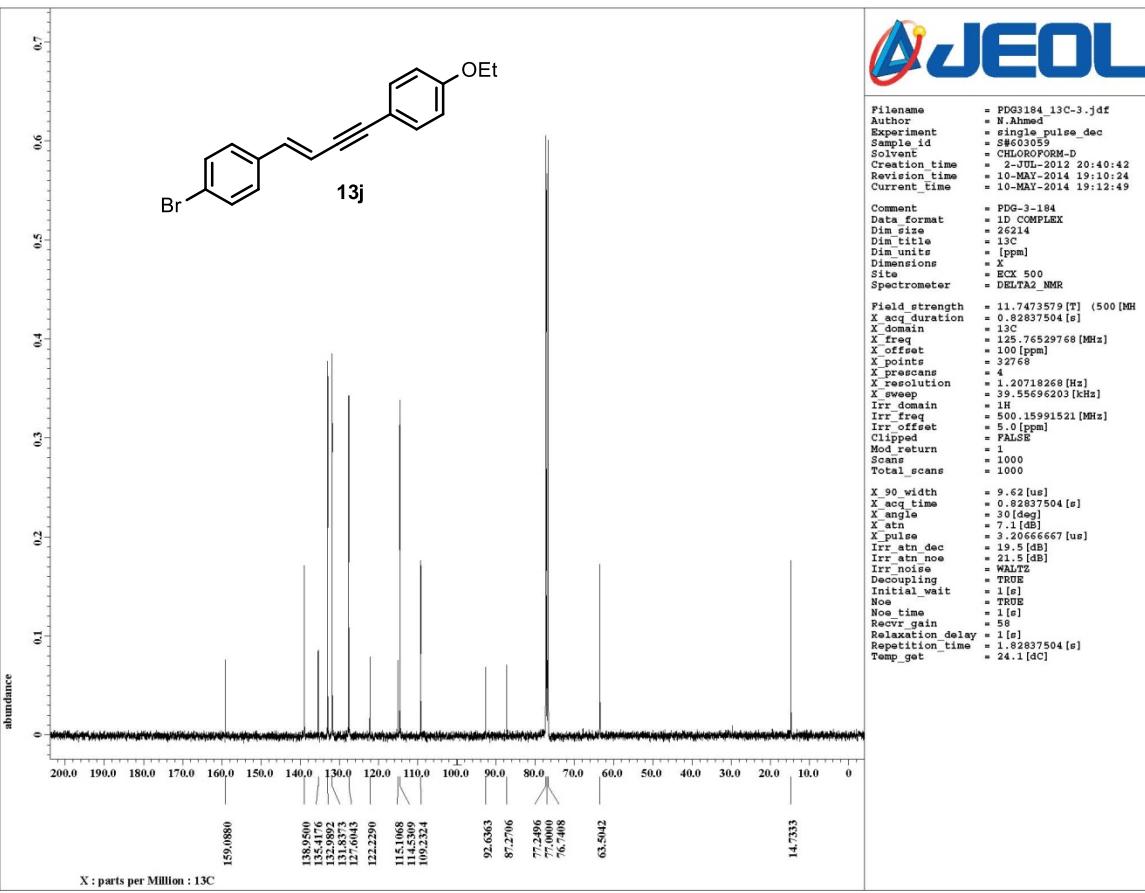
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4-(4-methoxyphenyl)but-1-en-3-ynyl)benzene (**13i**)



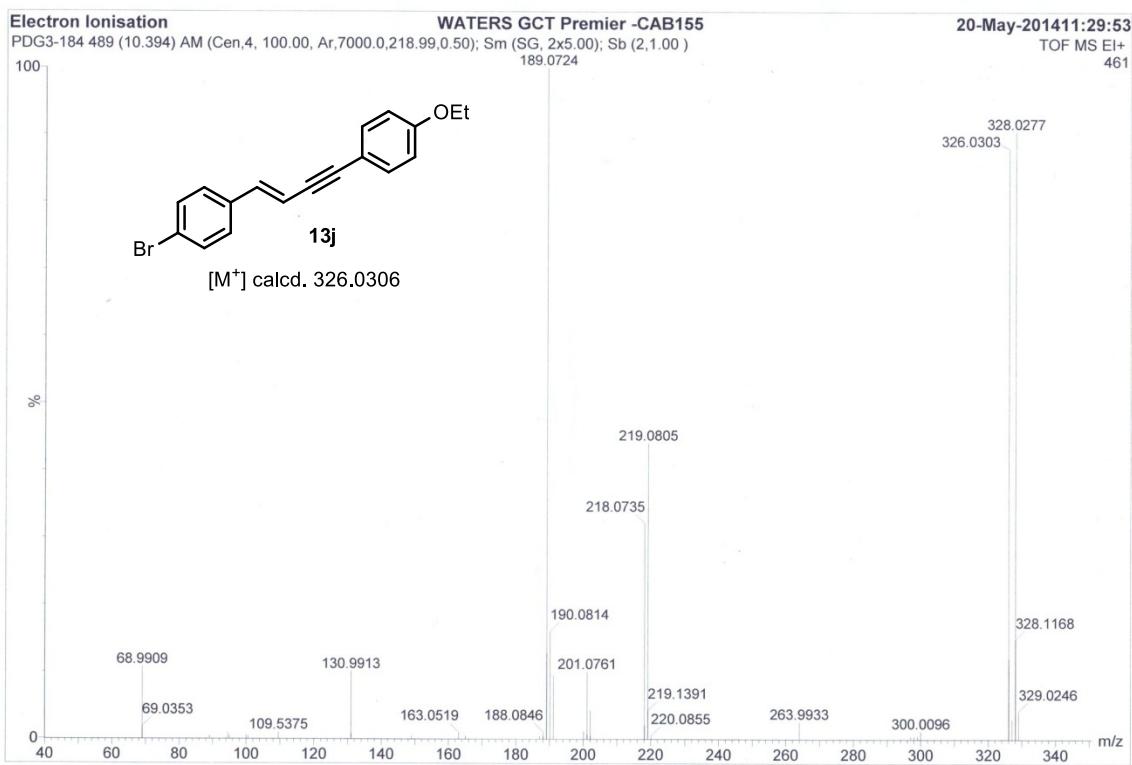
EI (HRMS) spectrum of (*E*)-1-bromo-4-(4-(4-methoxyphenyl)but-1-en-3-ynyl)benzene (**13i**)



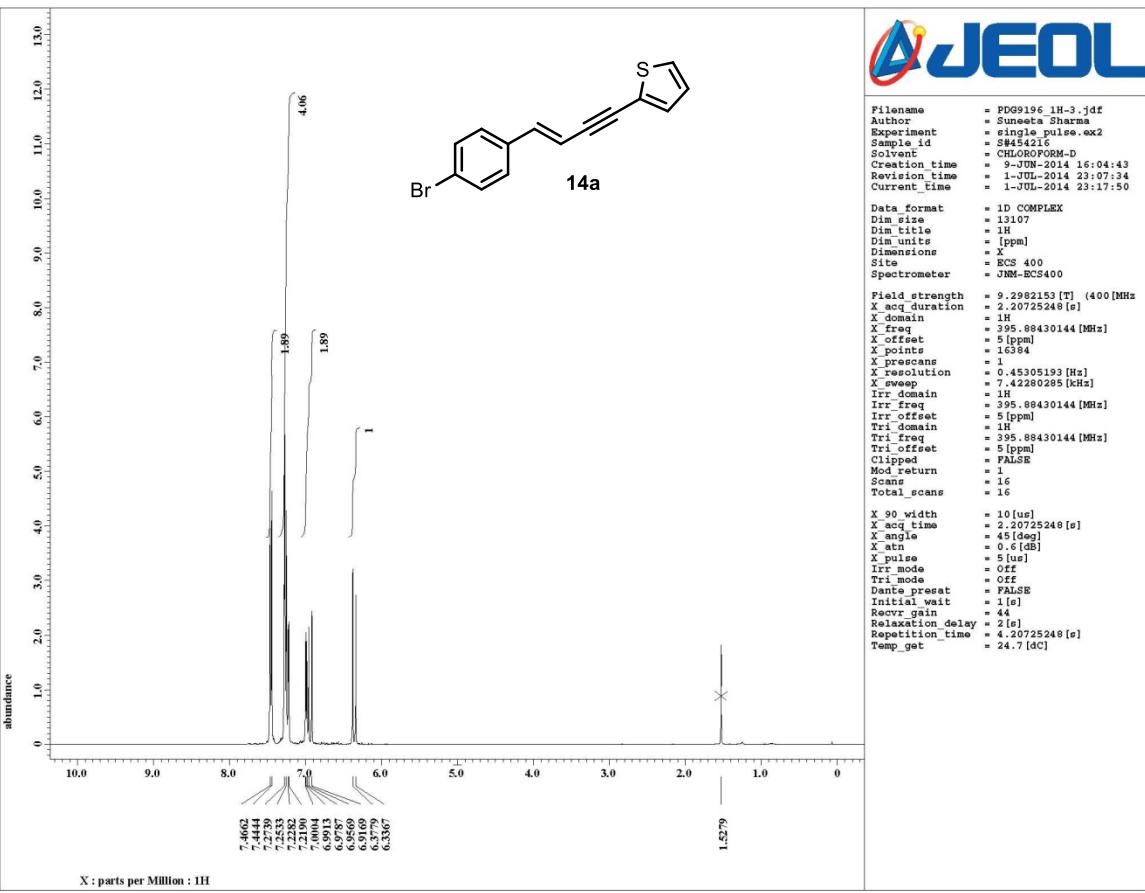
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4-(4-ethoxyphenyl)but-1-en-3-ynyl)benzene (**13j**)



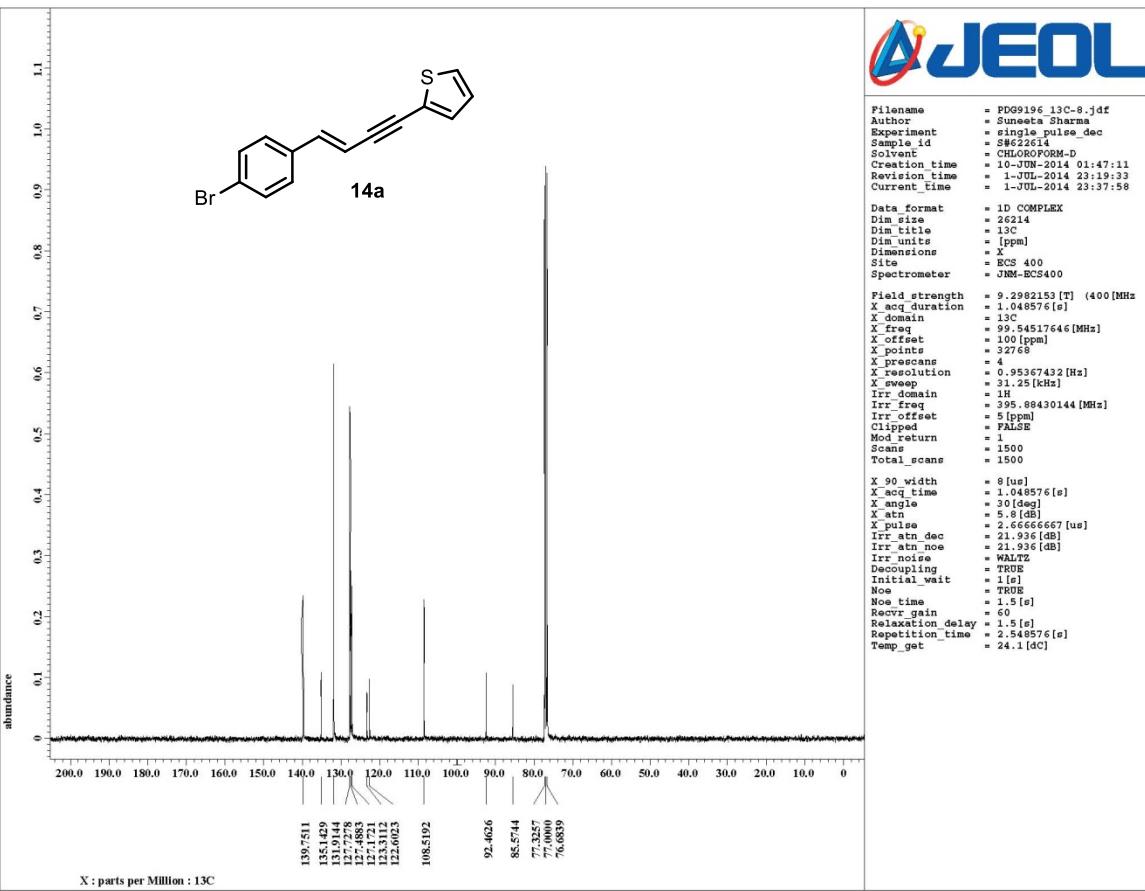
¹³C NMR (125 MHz, CDCl₃) spectrum of (*E*)-1-bromo-4-(4-(4-ethoxyphenyl)but-1-en-3-ynyl)benzene (**13j**)



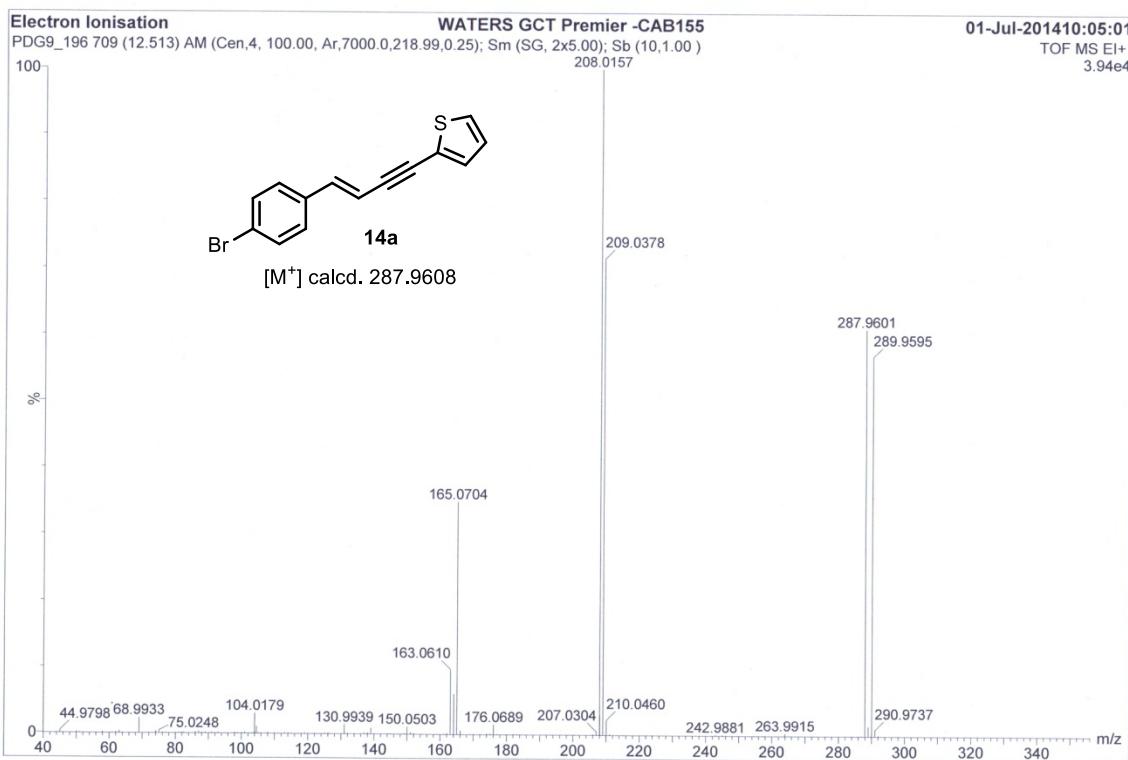
EI (HRMS) spectrum of (*E*)-1-bromo-4-(4-ethoxyphenyl)but-1-en-3-yne (**13j**)



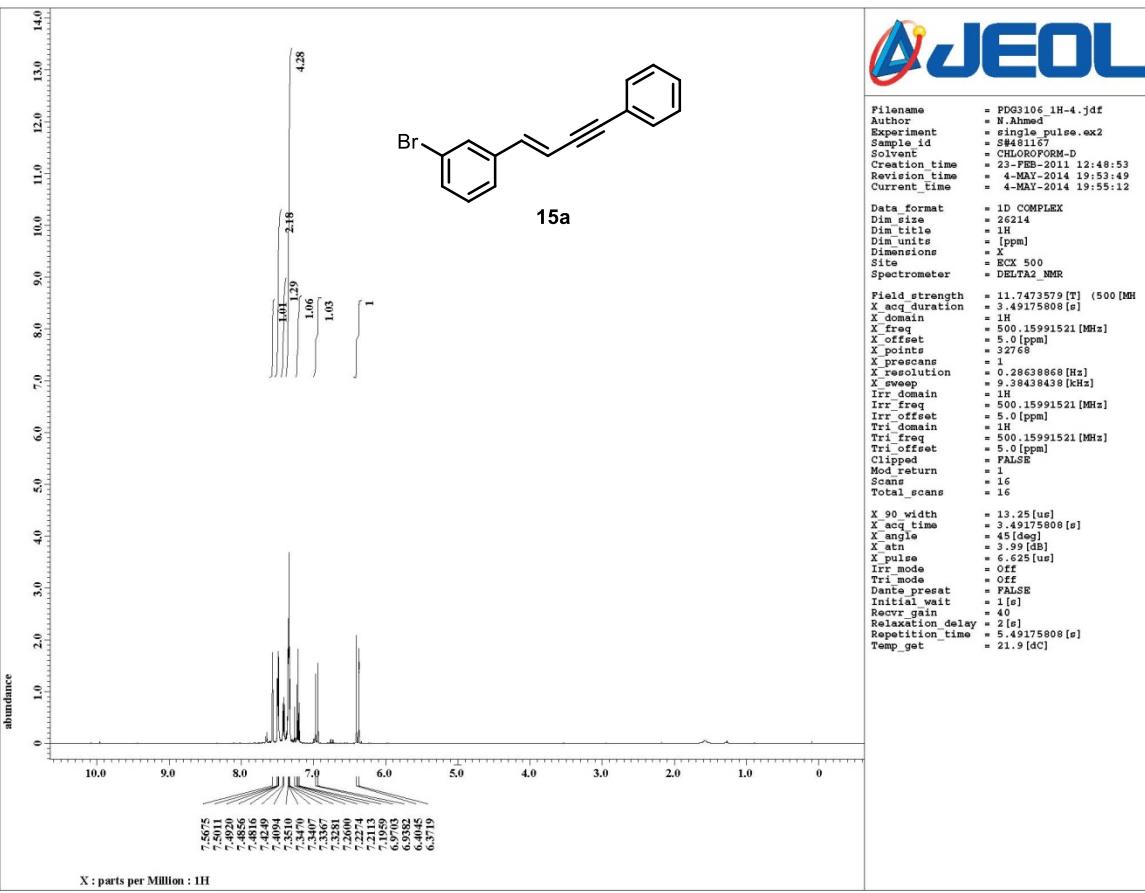
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-2-(4-(4-bromophenyl)but-3-en-1-ynyl)thiophene (**14a**)



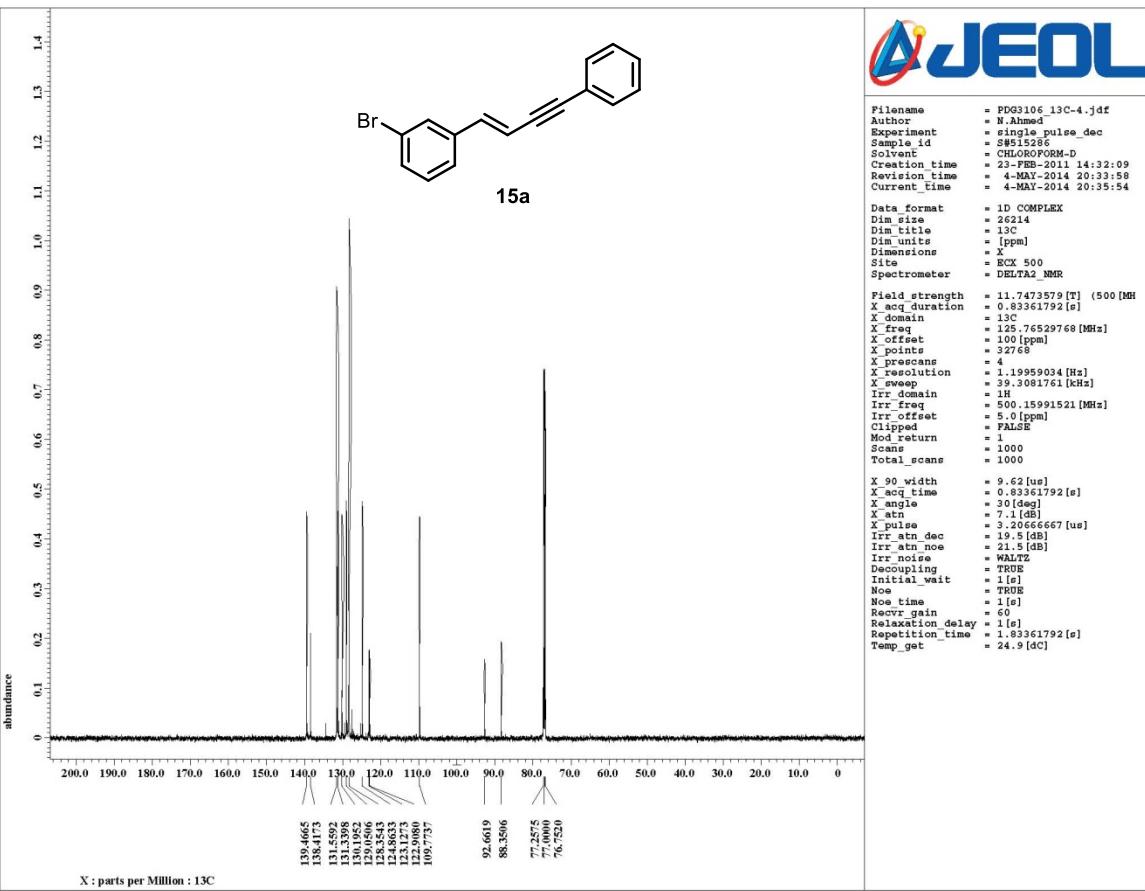
¹³C NMR (100 MHz, CDCl₃) spectrum of (*E*)-2-(4-(4-bromophenyl)but-3-en-1-ynyl)thiophene (**14a**)



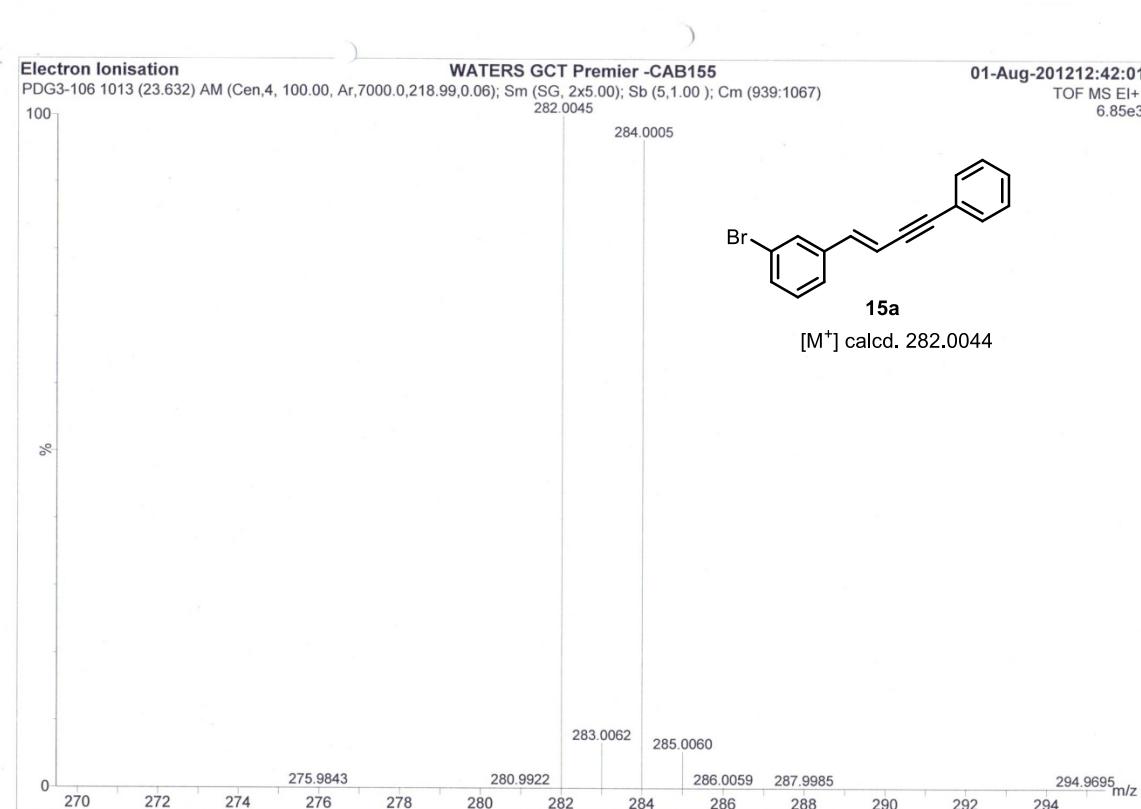
EI (HRMS) spectrum of (*E*)-2-(4-(4-bromophenyl)but-3-en-1-ynyl)thiophene (**14a**)



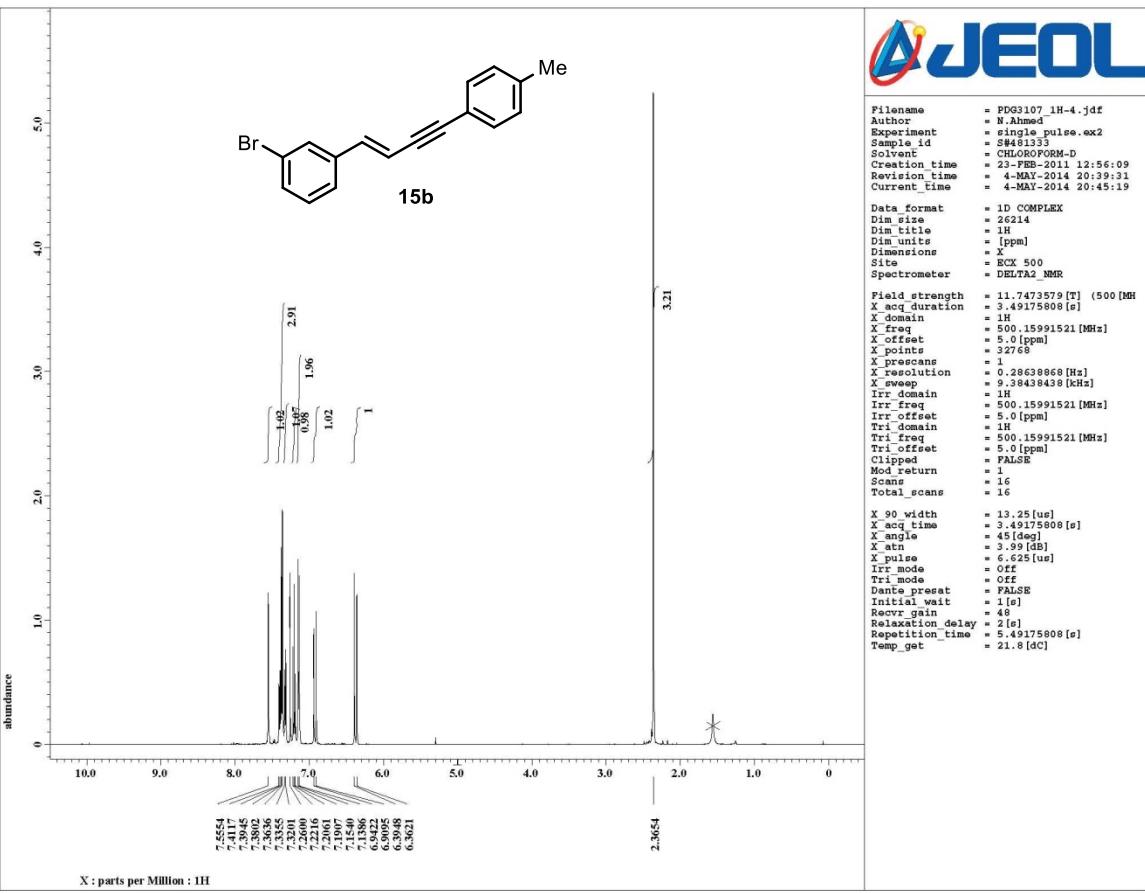
¹H NMR (500 MHz, CDCl₃) spectrum of (E)-1-bromo-3-(4-phenylbut-1-en-3-ynyl)benzene (**15a**)



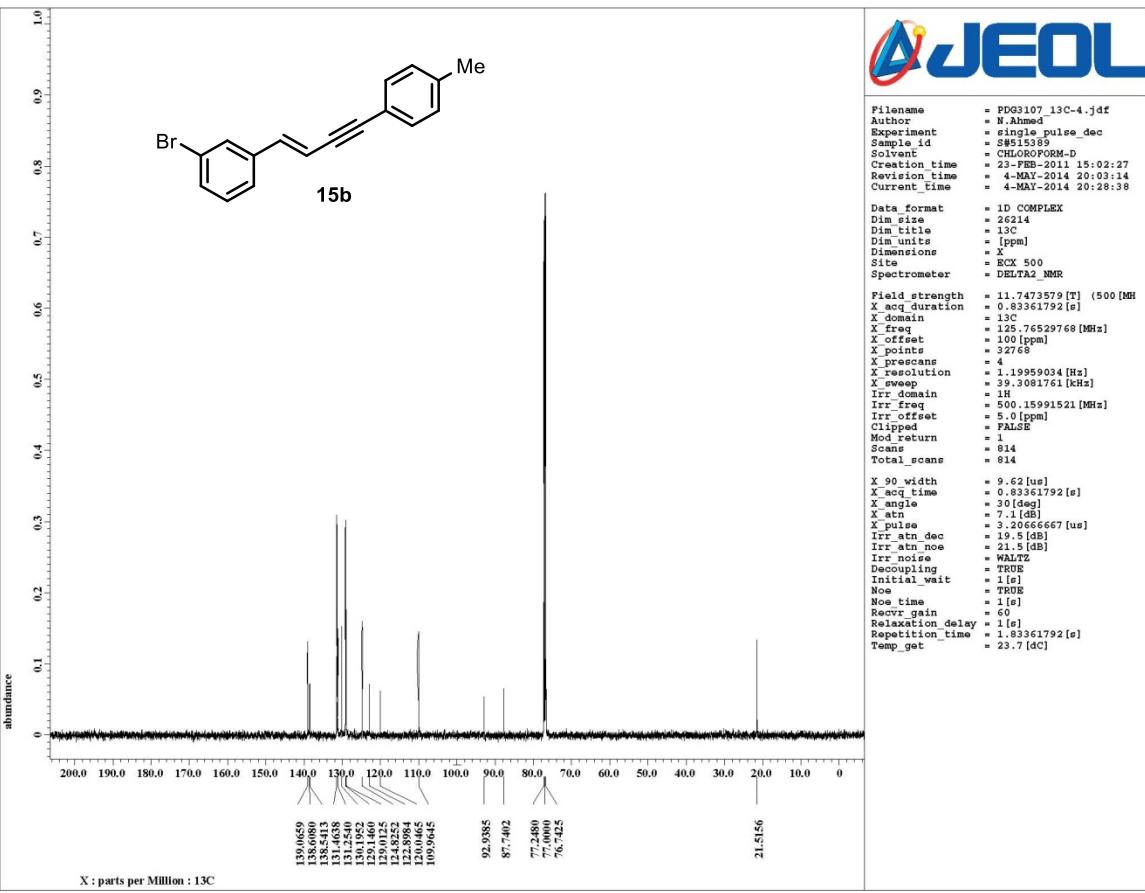
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-bromo-3-(4-phenylbut-1-en-3-ynyl)benzene (**15a**)



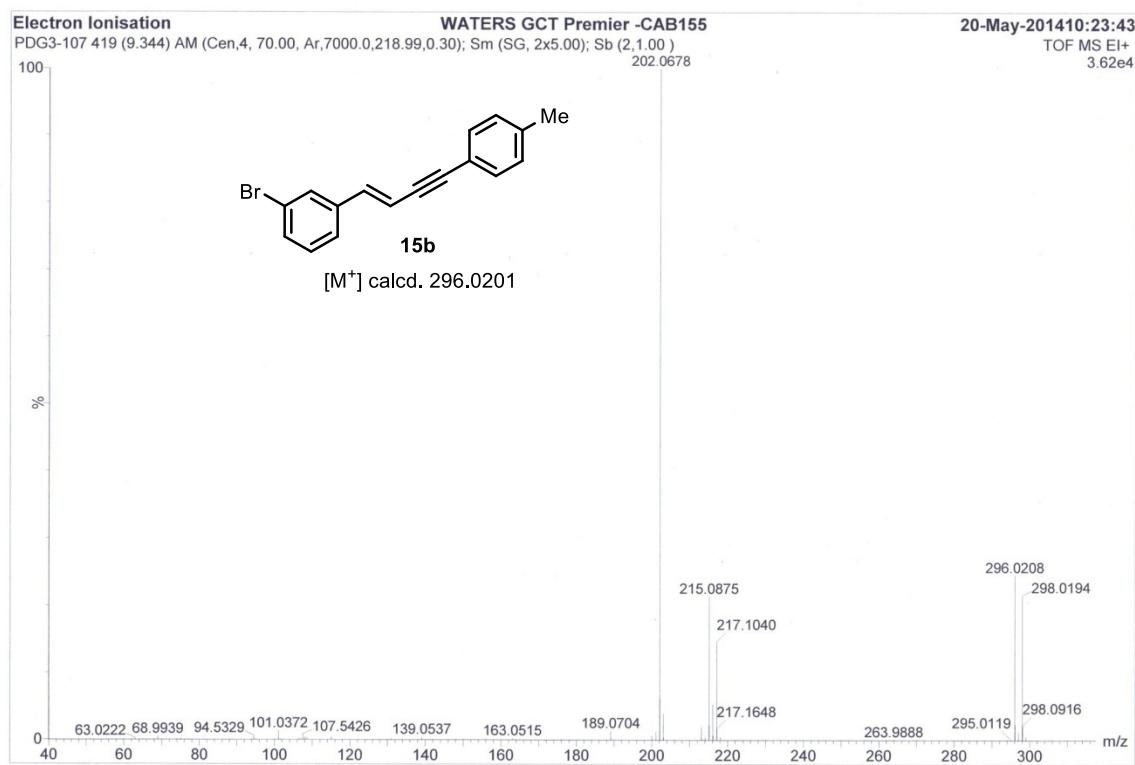
EI (HRMS) spectrum of (*E*)-1-bromo-3-(4-phenylbut-1-en-3-ynyl)benzene (**15a**)



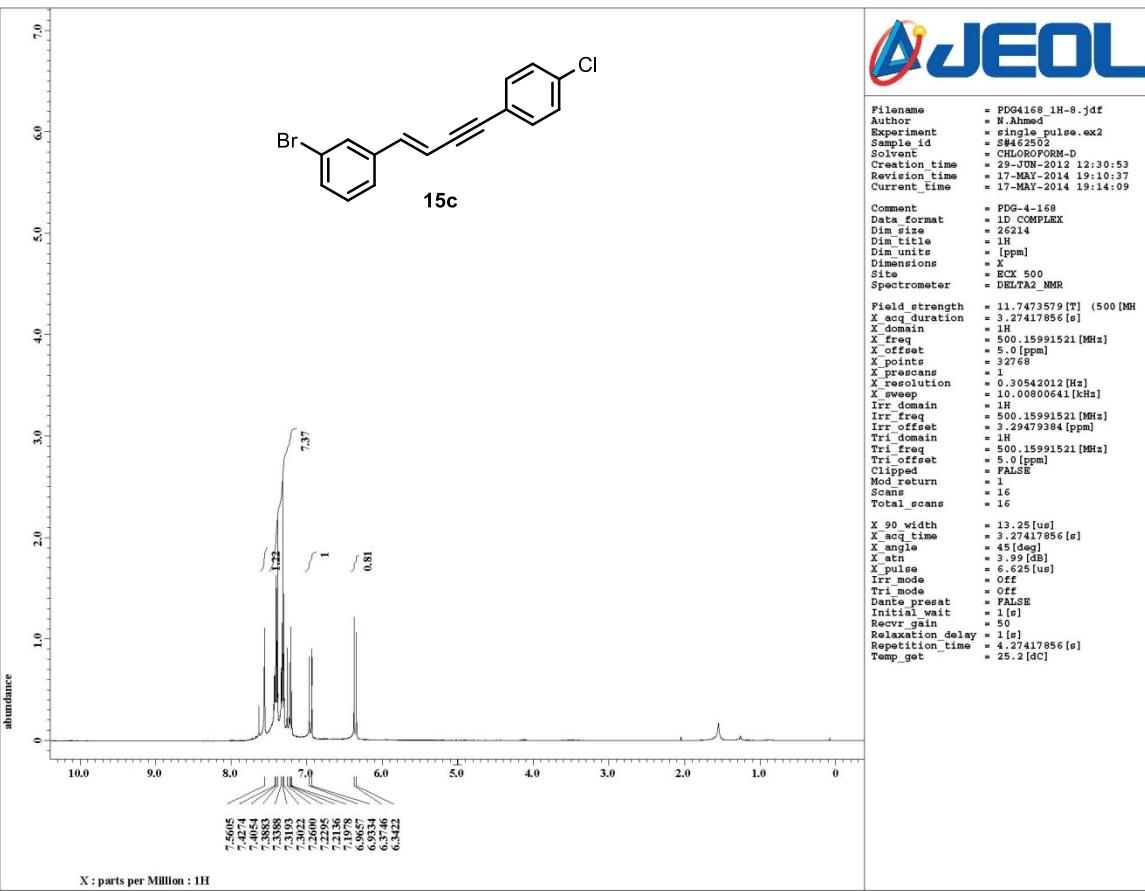
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-bromo-3-(4-*p*-tolylbut-1-en-3-ynyl)benzene (**15b**)



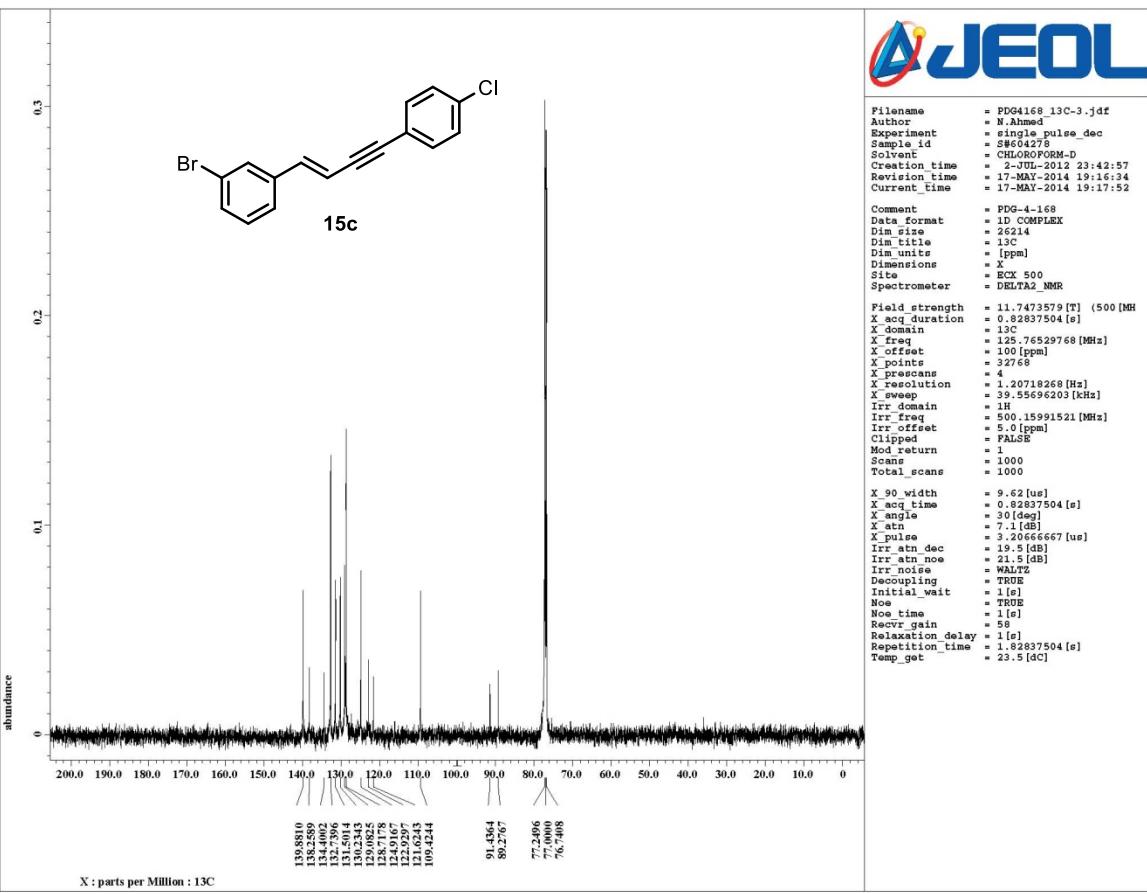
^{13}C NMR (125 MHz, CDCl_3) spectrum of (*E*)-1-bromo-3-(4-*p*-tolylbut-1-en-3-ynyl)benzene (**15b**)



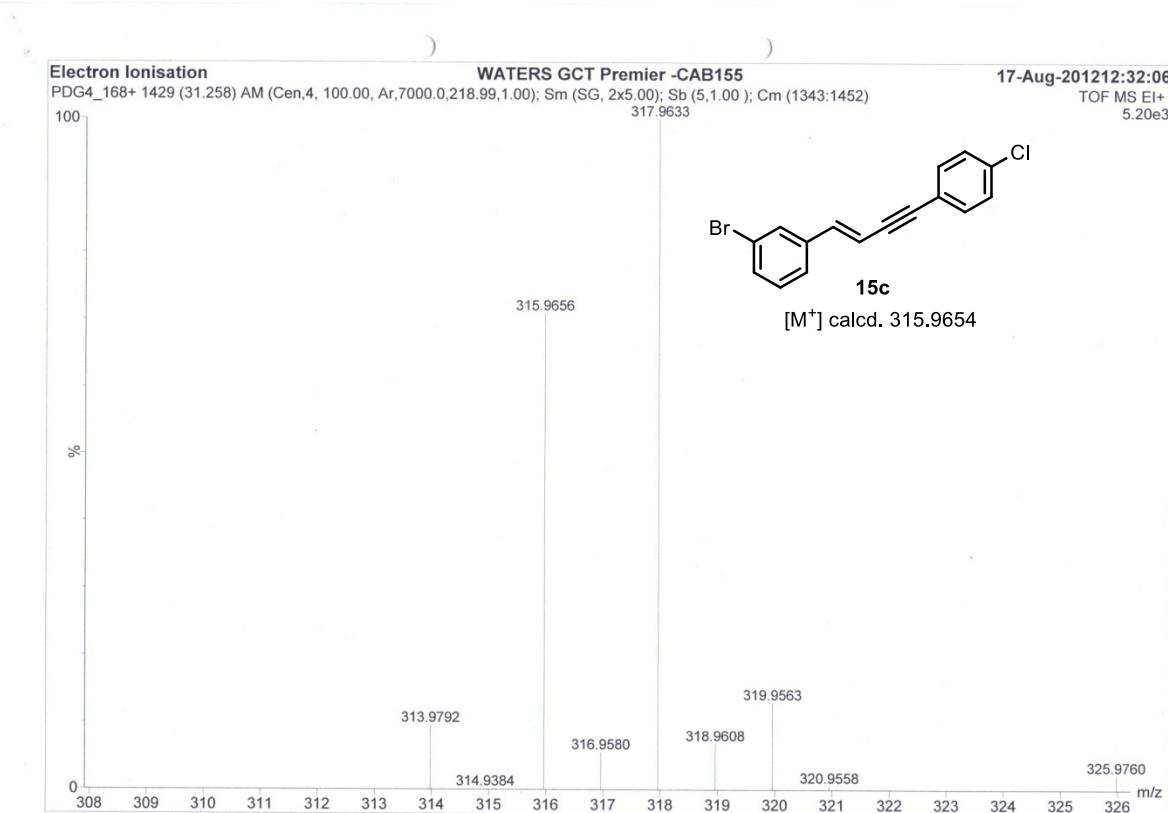
EI (HRMS) spectrum of (*E*)-1-bromo-3-(4-*p*-tolylbut-1-en-3-ynyl)benzene (**15b**)



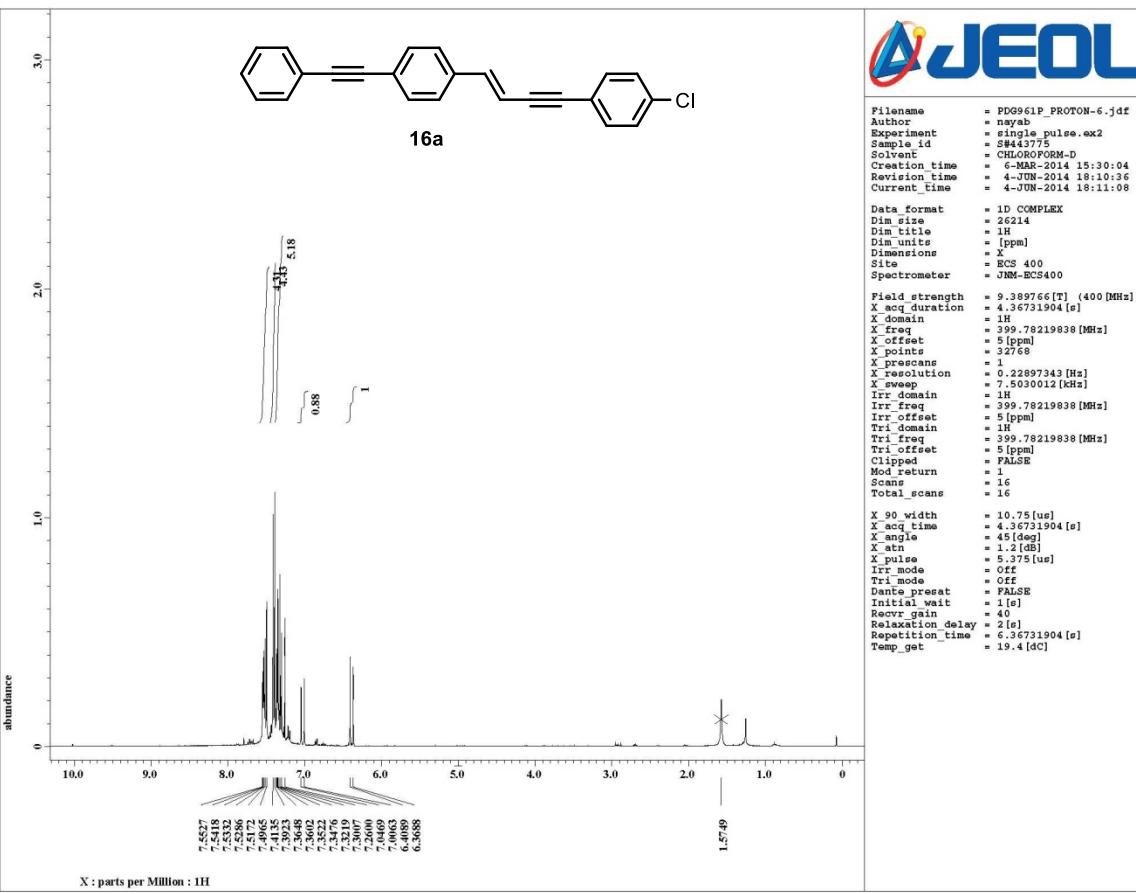
¹H NMR (500 MHz, CDCl₃) spectrum of (*E*)-1-bromo-3-(4-(4-chlorophenyl)but-1-en-3-ynyl)benzene (**15c**)



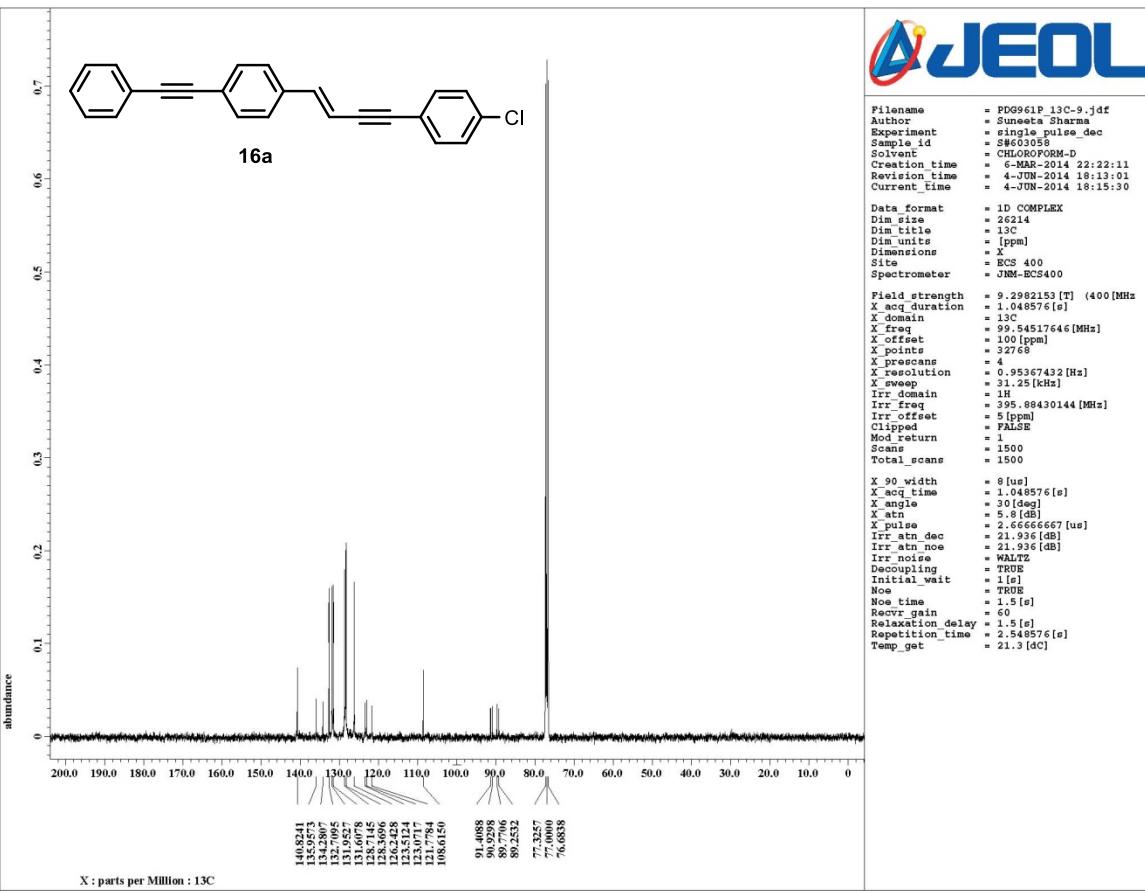
¹³C NMR (125 MHz, CDCl₃) spectrum of (E)-1-bromo-3-(4-(4-chlorophenyl)but-1-en-3-ynyl)benzene (**15c**)



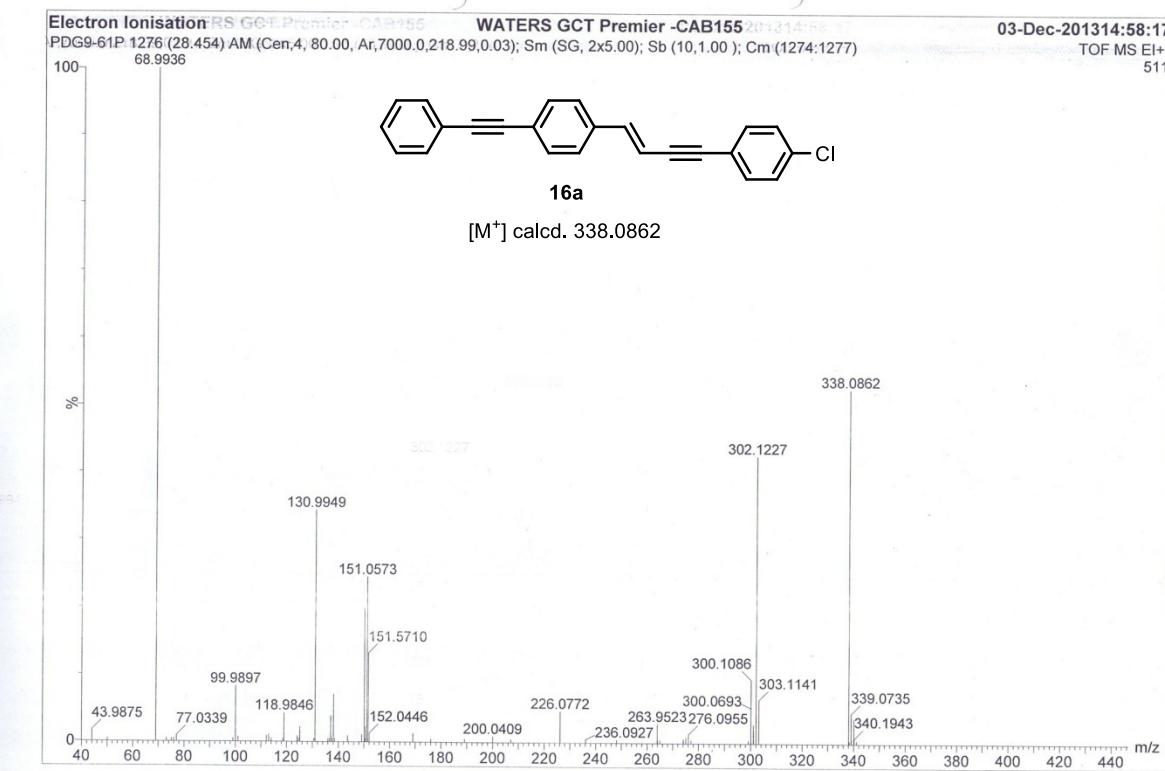
EI (HRMS) spectrum of (*E*)-1-bromo-3-(4-(4-chlorophenyl)but-1-en-3-ynyl)benzene (**15c**)



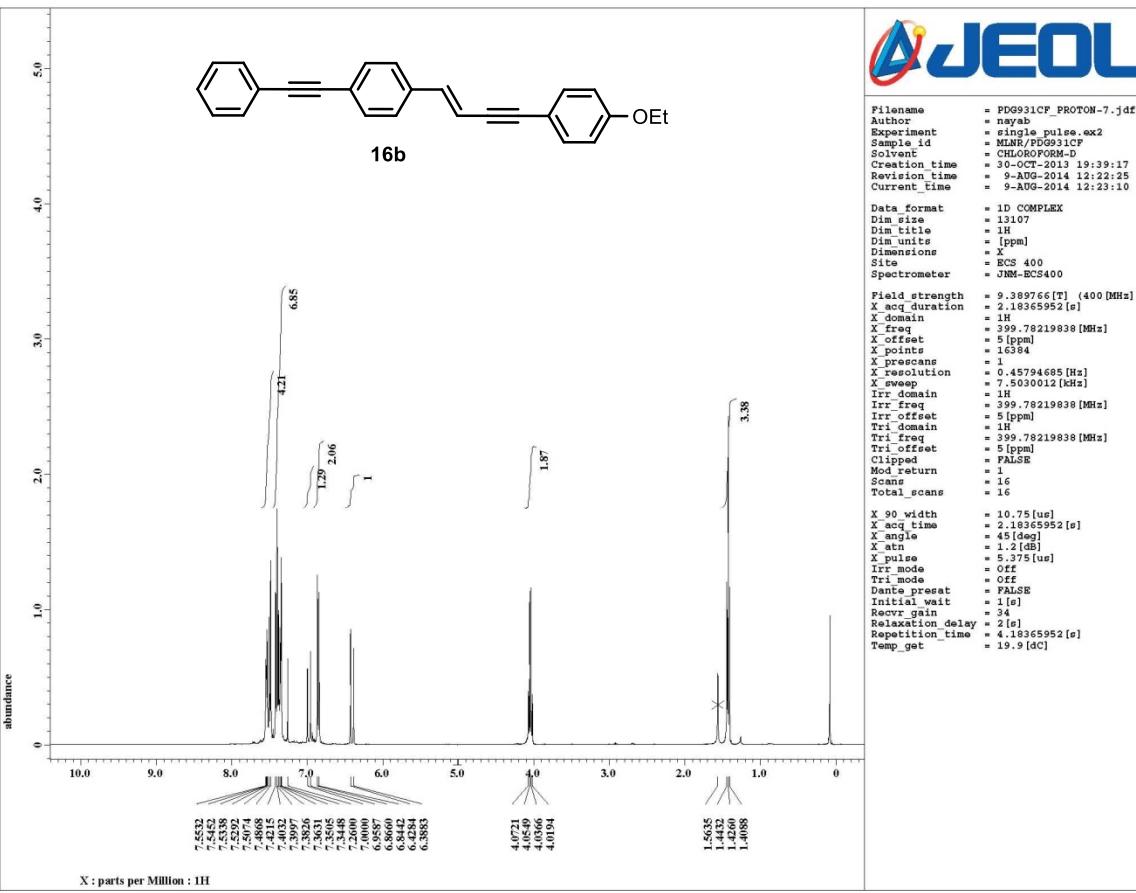
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-(4-(phenylethynyl)phenyl)but-3-en-1-ynyl)benzene (**16a**)



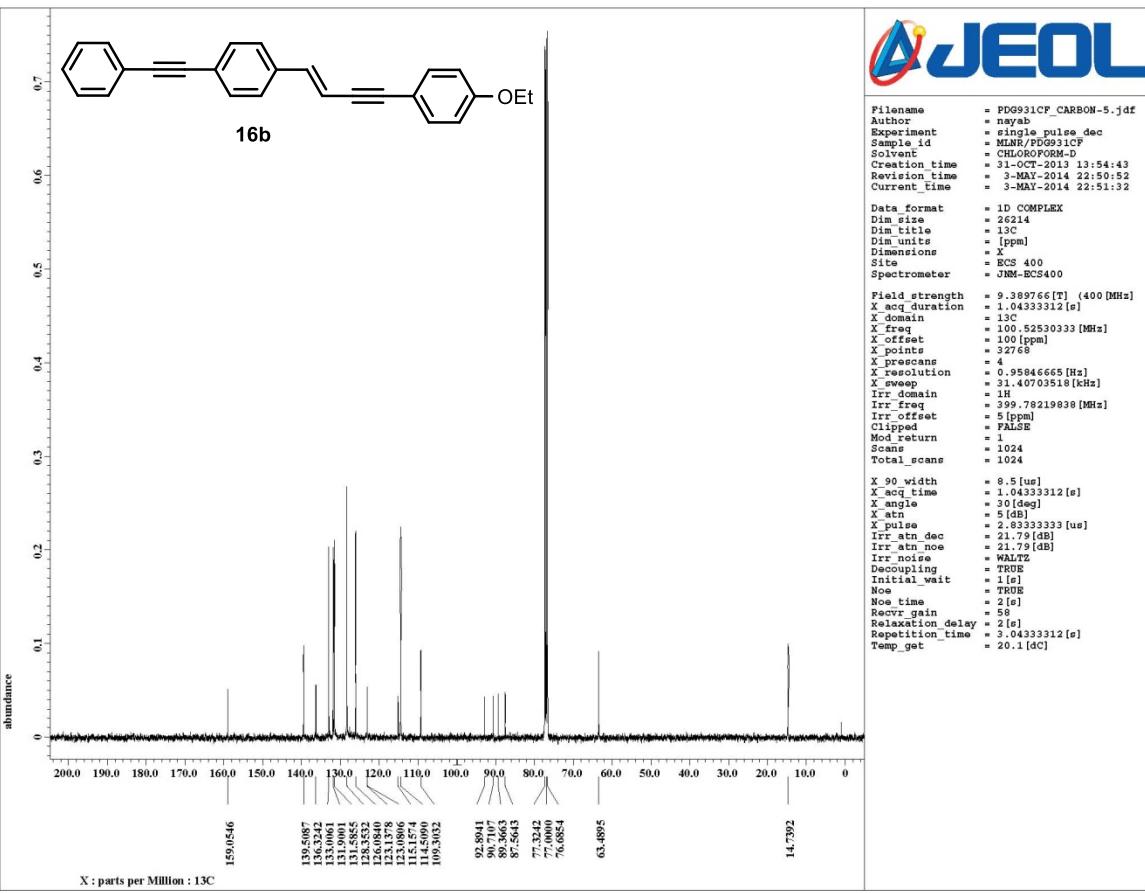
¹³C NMR (100 MHz, CDCl₃) spectrum of (*E*)-1-chloro-4-(4-(4-(phenylethynyl)phenyl)but-3-en-1-ynyl)benzene (**16a**)



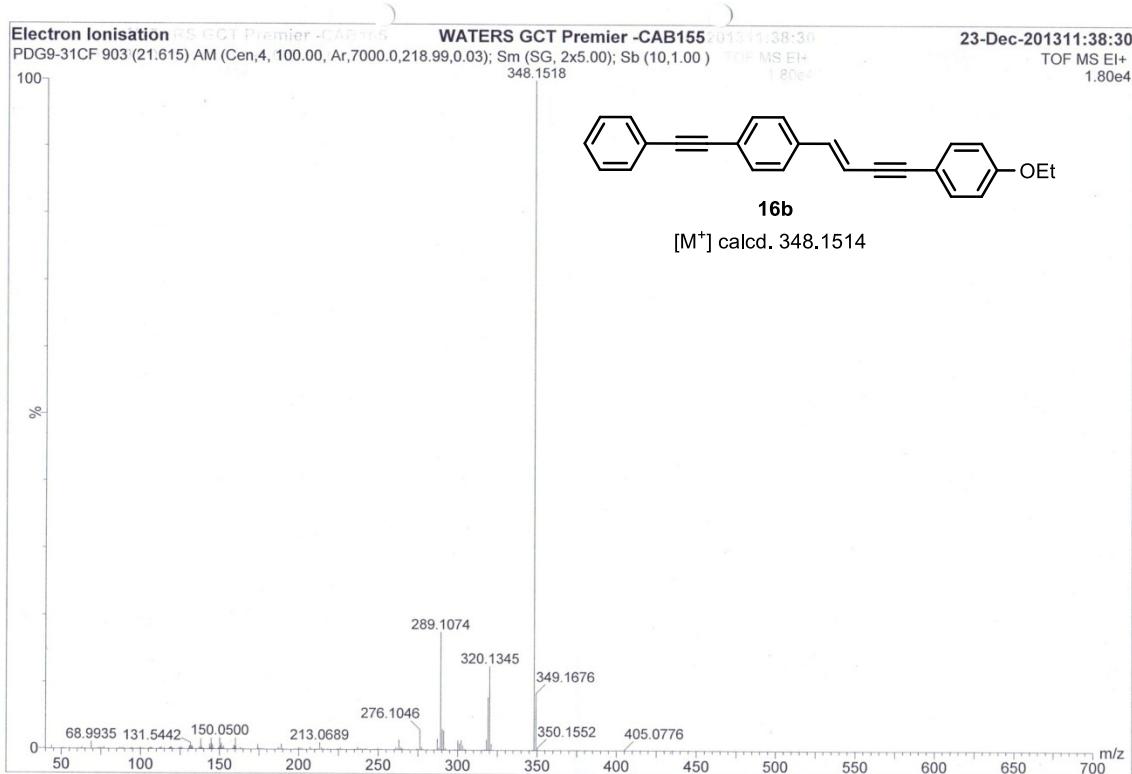
EI (HRMS) spectrum of (*E*)-1-chloro-4-(4-(phenylethynyl)phenyl)but-3-en-1-ynylbenzene (**16a**)



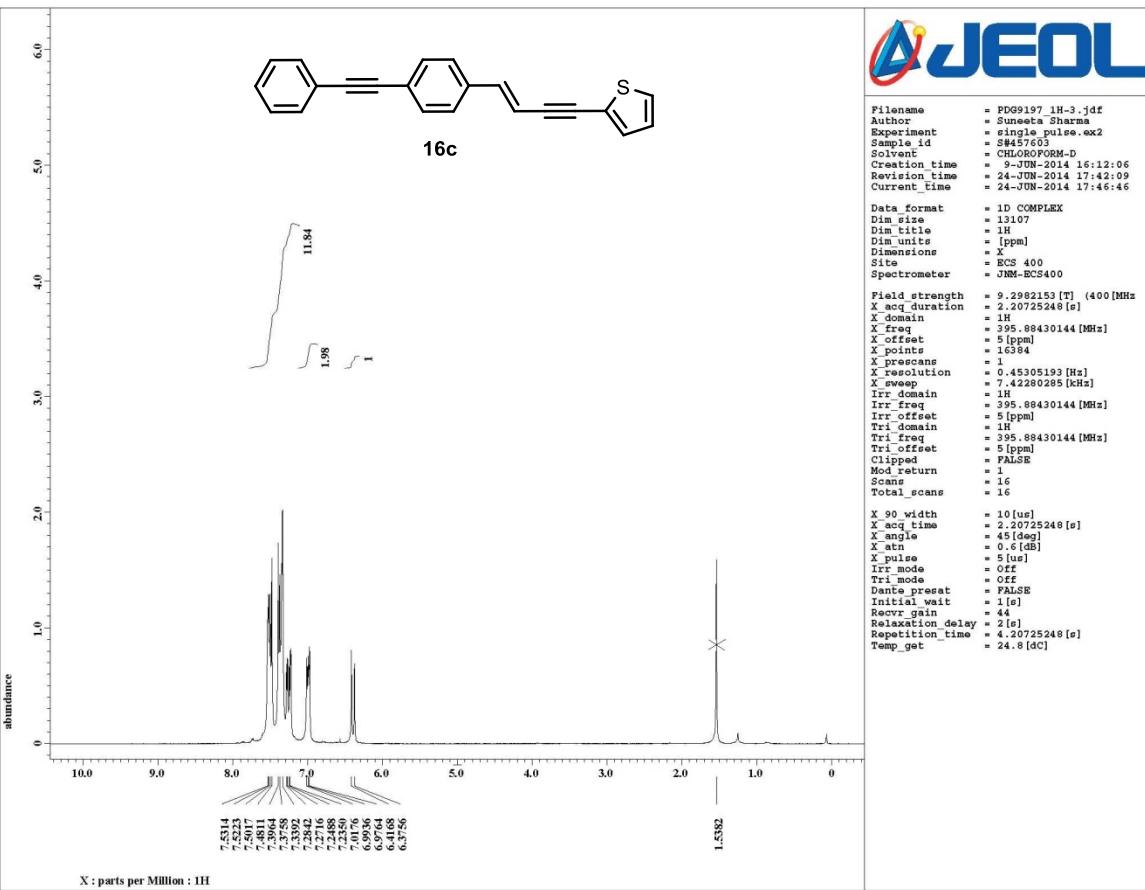
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-1-ethoxy-4-(4-(phenylethynyl)phenyl)but-3-en-1-ynylbenzene (**16b**)



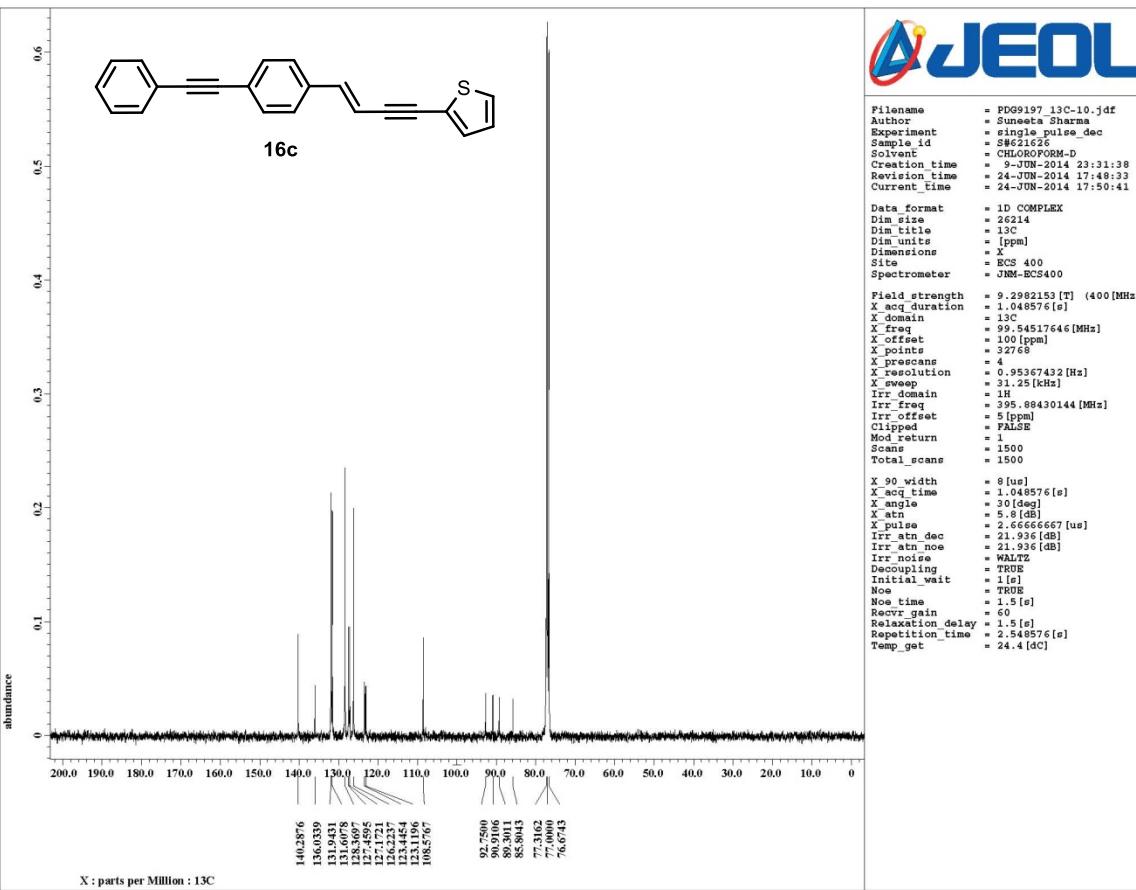
¹³C NMR (100 MHz, CDCl₃) spectrum of (*E*)-1-ethoxy-4-(4-(phenylethyynyl)phenyl)but-3-en-1-ynylbenzene (**16b**)



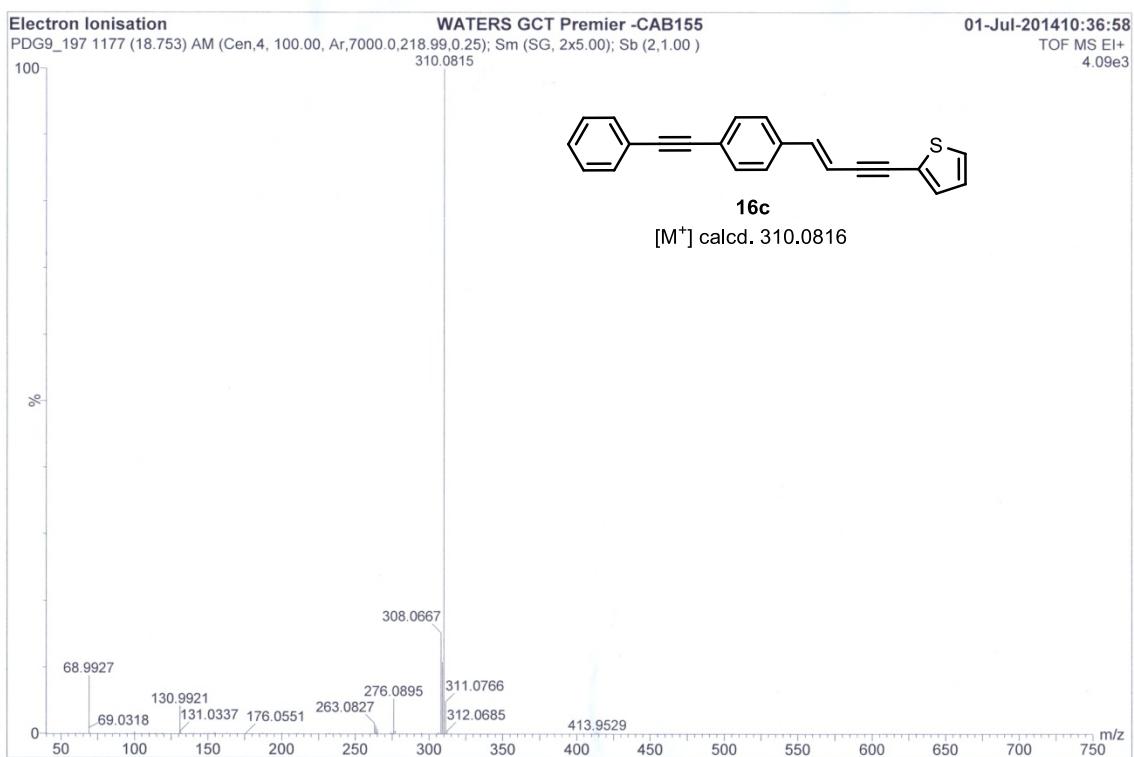
EI (HRMS) spectrum of (*E*)-1-ethoxy-4-(4-(phenylethyynyl)phenyl)but-3-en-1-ynyl)benzene (**16b**)



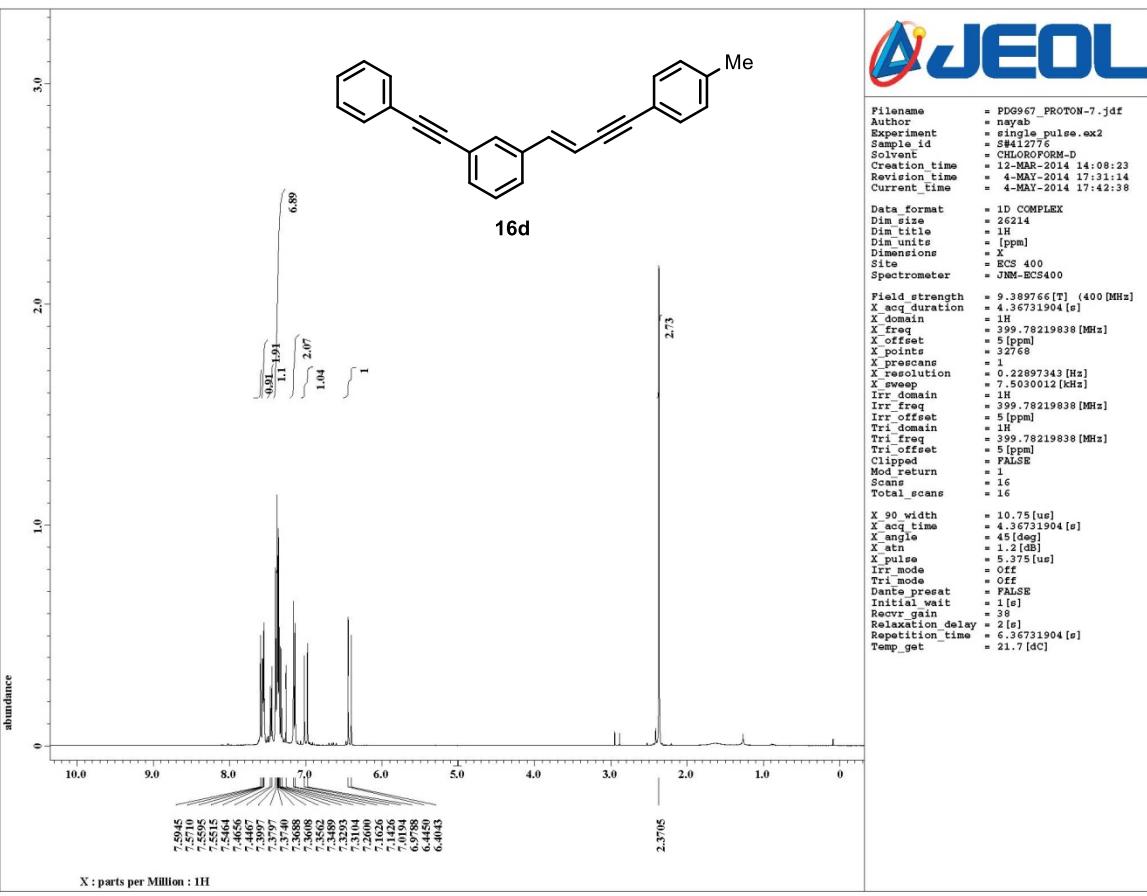
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-2-(4-(phenylethynyl)phenyl)but-3-en-1-ynyl thiophene (**16c**)



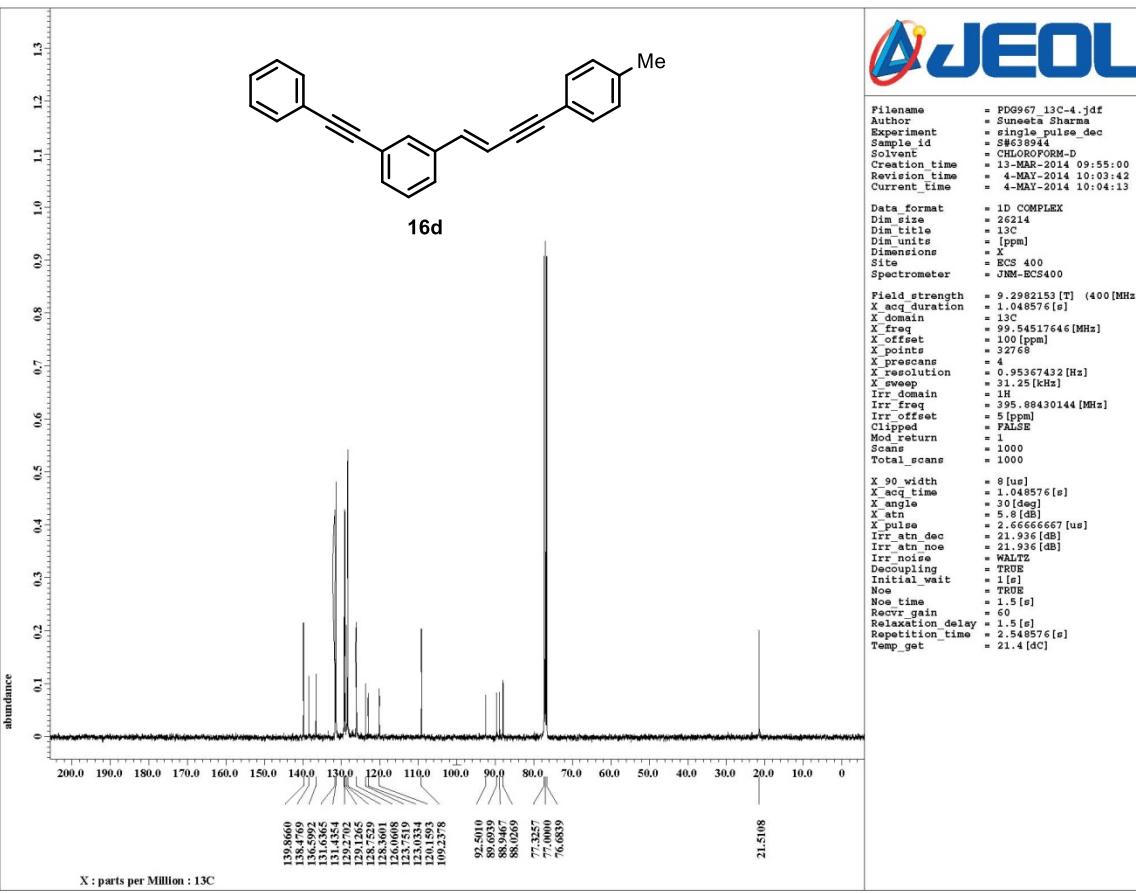
¹³C NMR (100 MHz, CDCl₃) spectrum of (*E*)-2-(4-(4-(phenylethynyl)phenyl)but-3-en-1-ynyl)thiophene (**16c**)



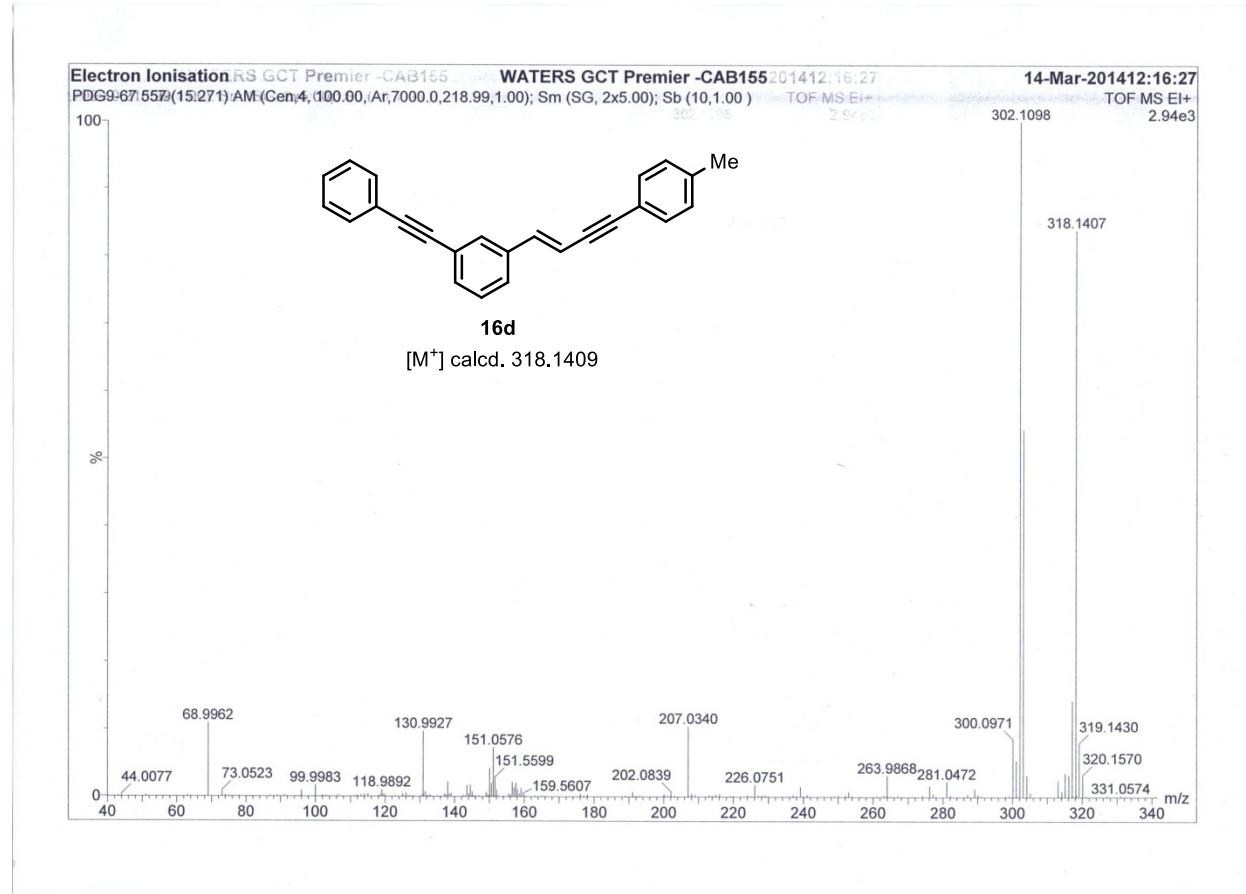
EI (HRMS) spectrum of (*E*)-2-(4-(4-(phenylethynyl)phenyl)but-3-en-1-ynyl)thiophene (**16c**)



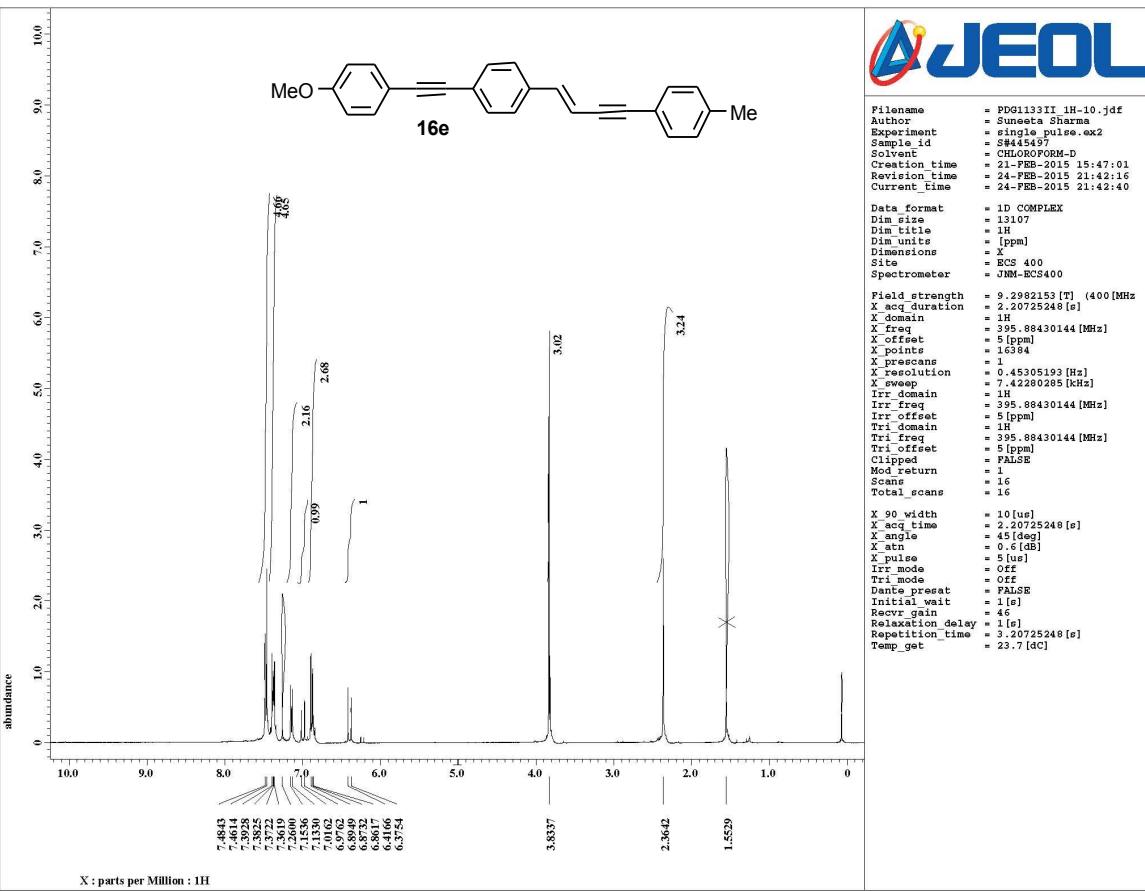
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-1-(phenylethynyl)-3-(4-*p*-tolylbut-1-en-3-ynyl)benzene (**16d**)



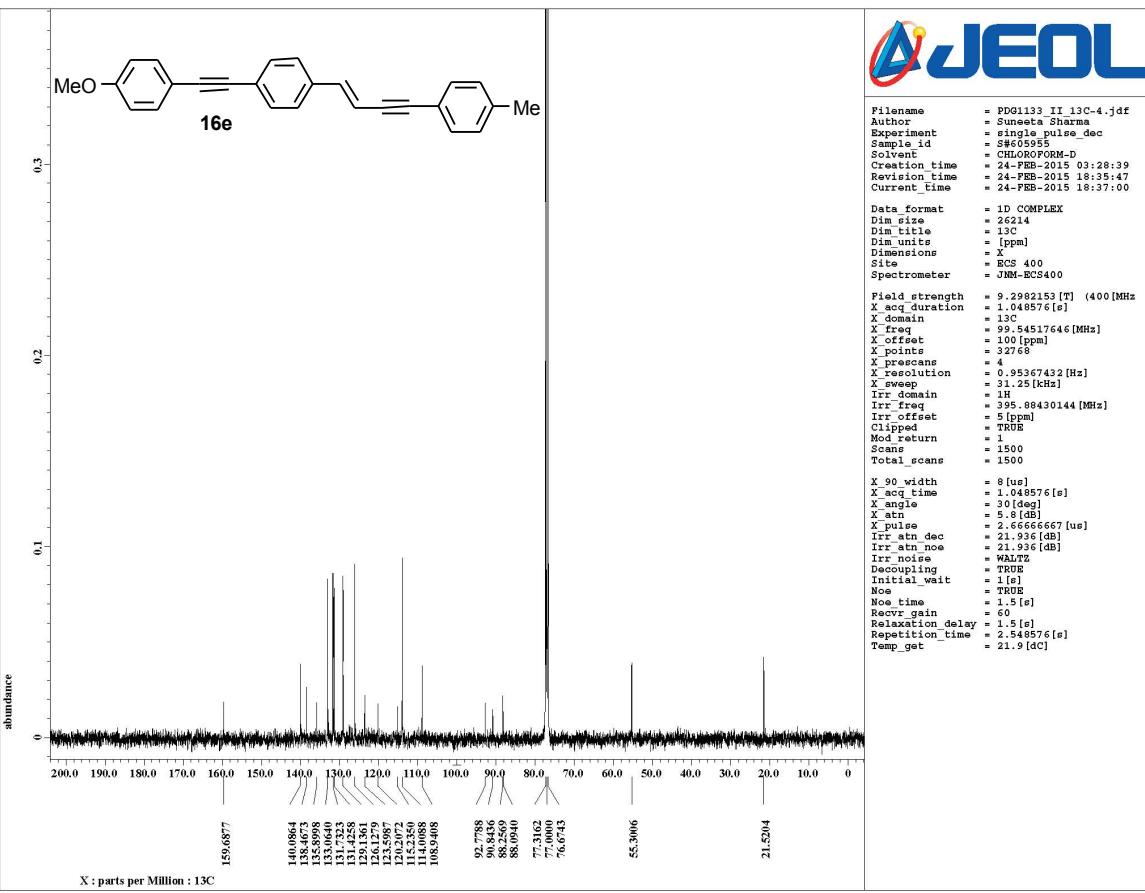
^{13}C NMR (100 MHz, CDCl_3) spectrum of (*E*)-1-(phenylethynyl)-3-(4-*p*-tolylbut-1-en-3-ynyl)benzene (**16d**)



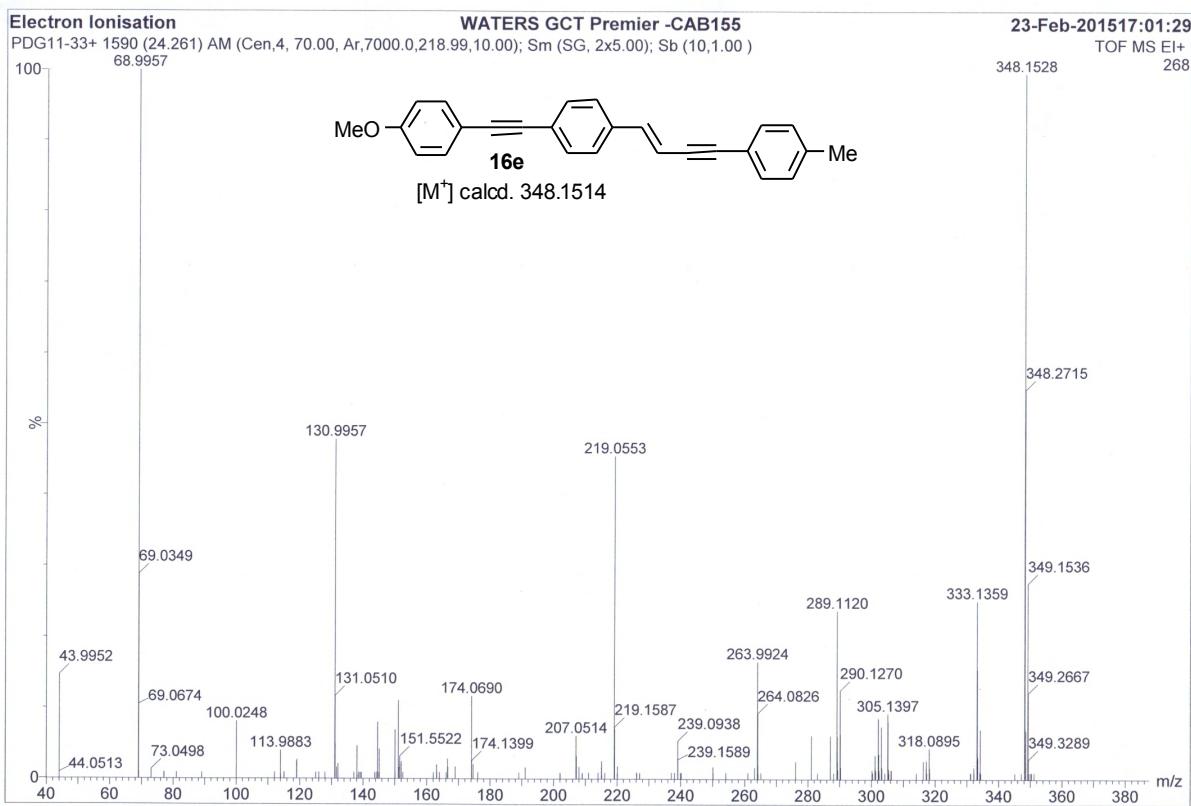
EI (HRMS) spectrum of (*E*)-1-(phenylethynyl)-3-(4-*p*-tolylbut-1-en-3-ynyl)benzene (**16d**)



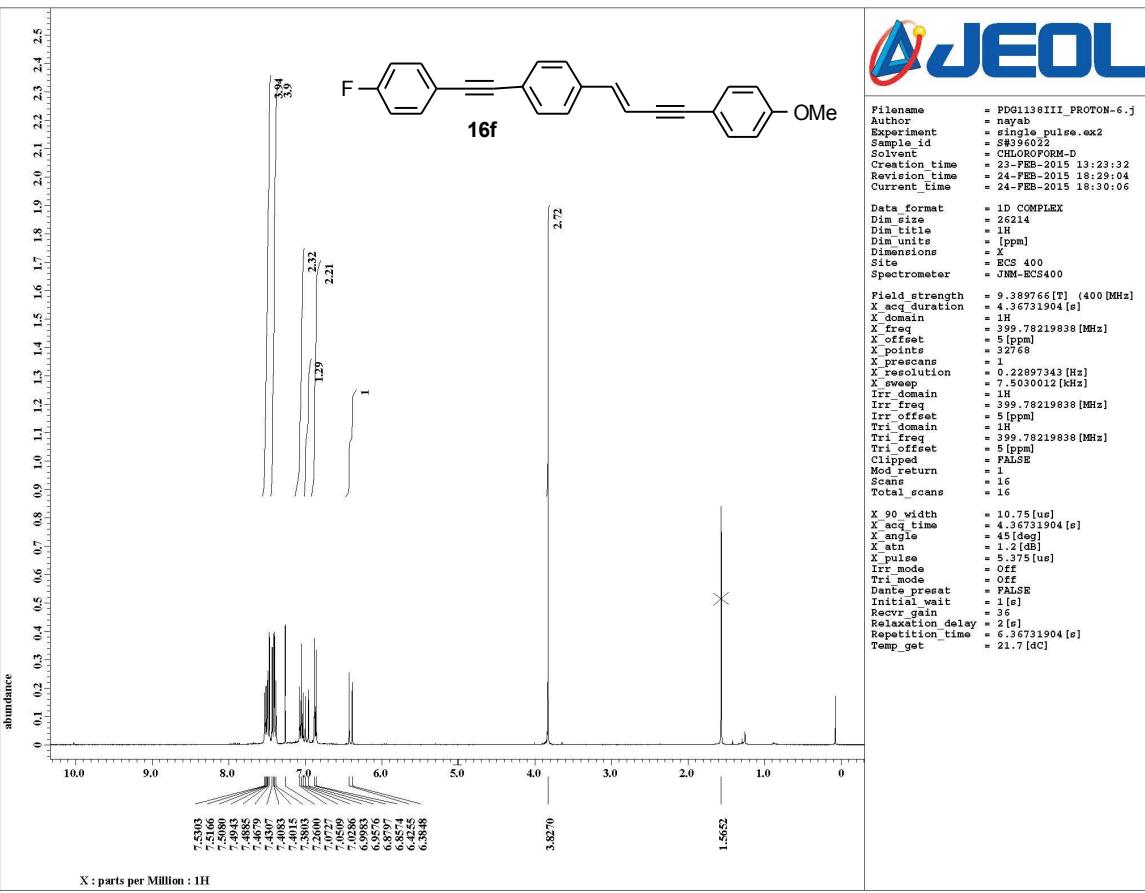
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-1-methoxy-4-((4-(4-*p*-tolylbut-1-en-3-ynyl)phenyl)ethynyl)benzene (**16e**)



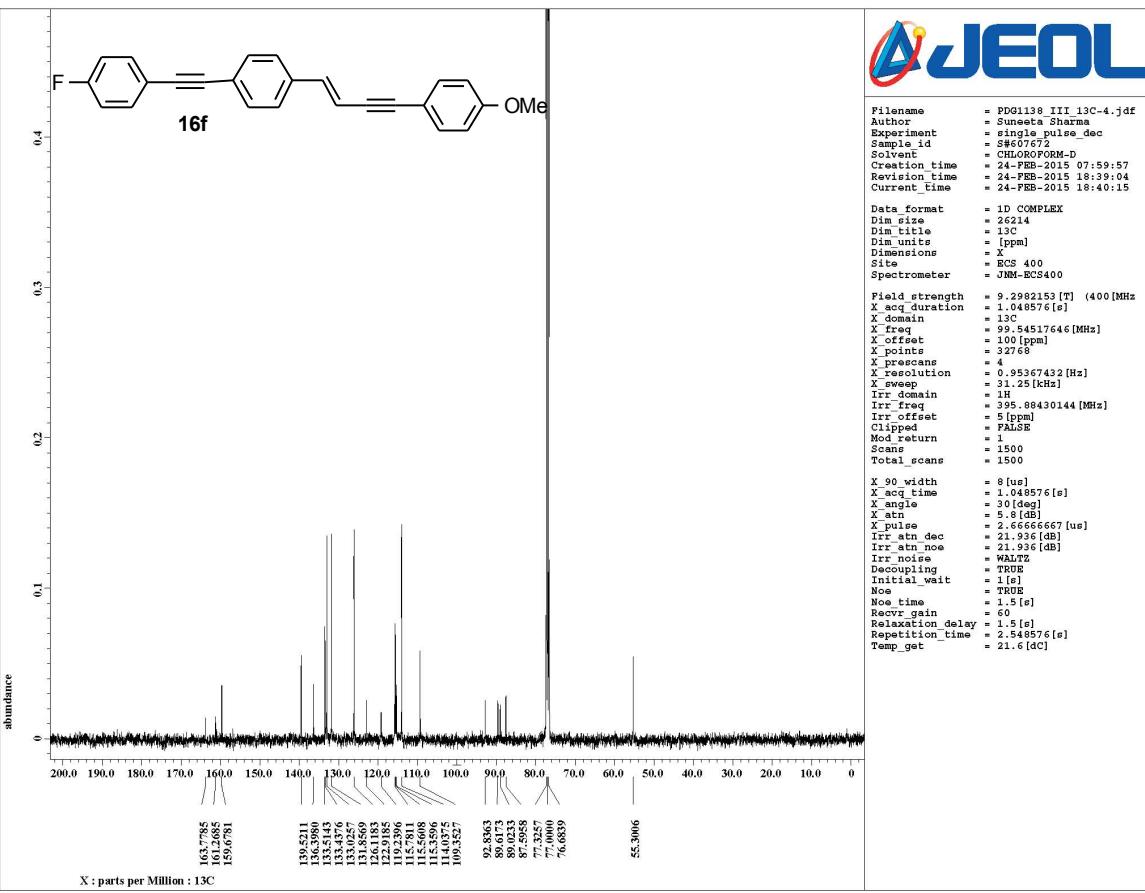
¹³C NMR (100 MHz, CDCl₃) spectrum of (*E*)-1-methoxy-4-((4-(4-*p*-tolylbut-1-en-3-ynyl)phenyl)ethynyl)benzene (**16e**)



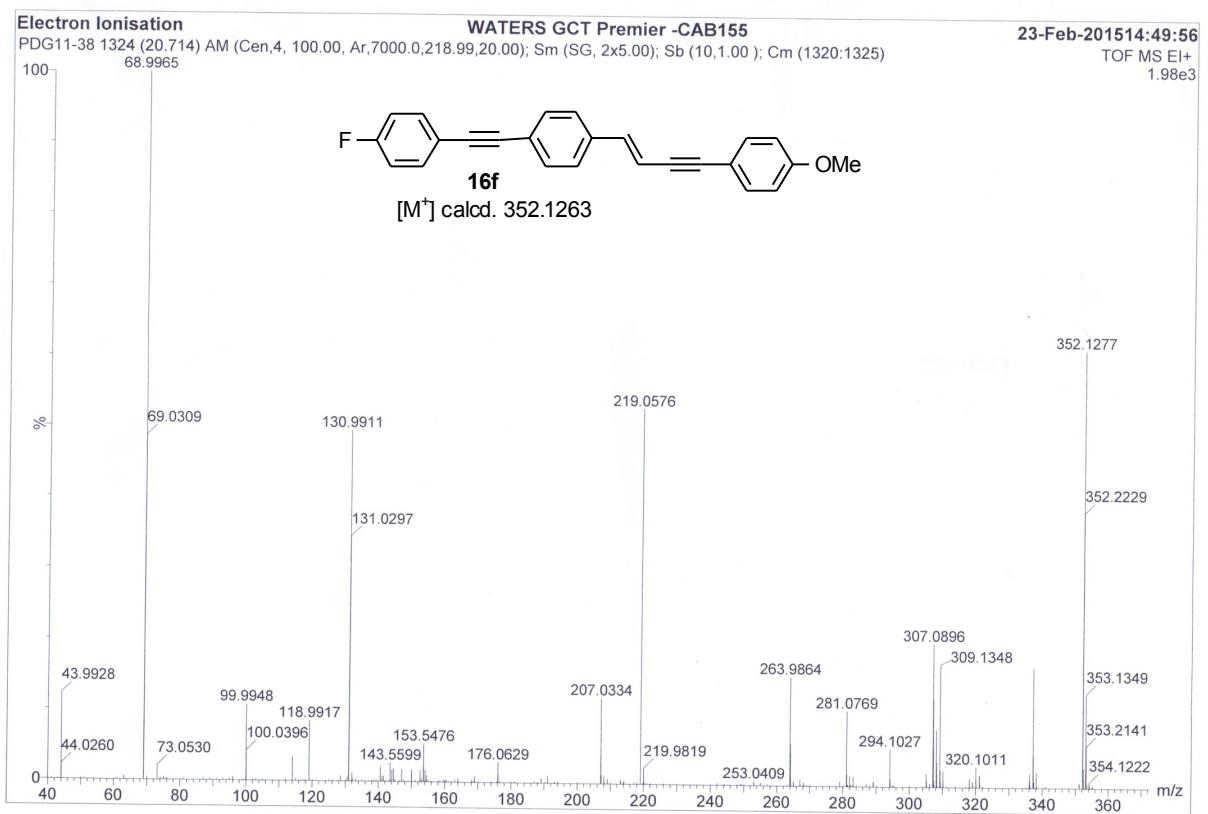
EI (HRMS) spectrum of (*E*)-1-methoxy-4-((4-(4-*p*-tolylbut-1-en-3-ynyl)phenyl)ethynyl)benzene (**16e**)



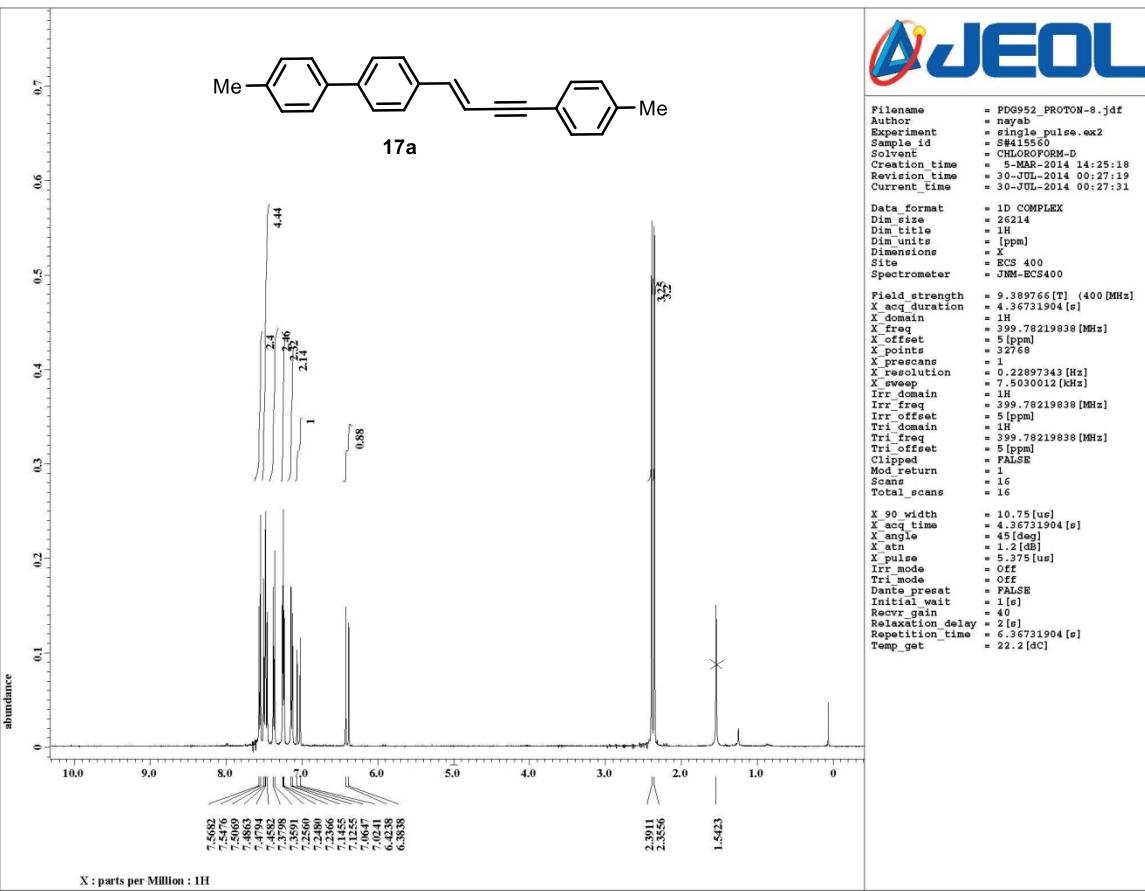
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-1-fluoro-4-((4-(4-methoxyphenyl)but-1-en-3-ynyl)phenyl)ethynylbenzene (**16f**)



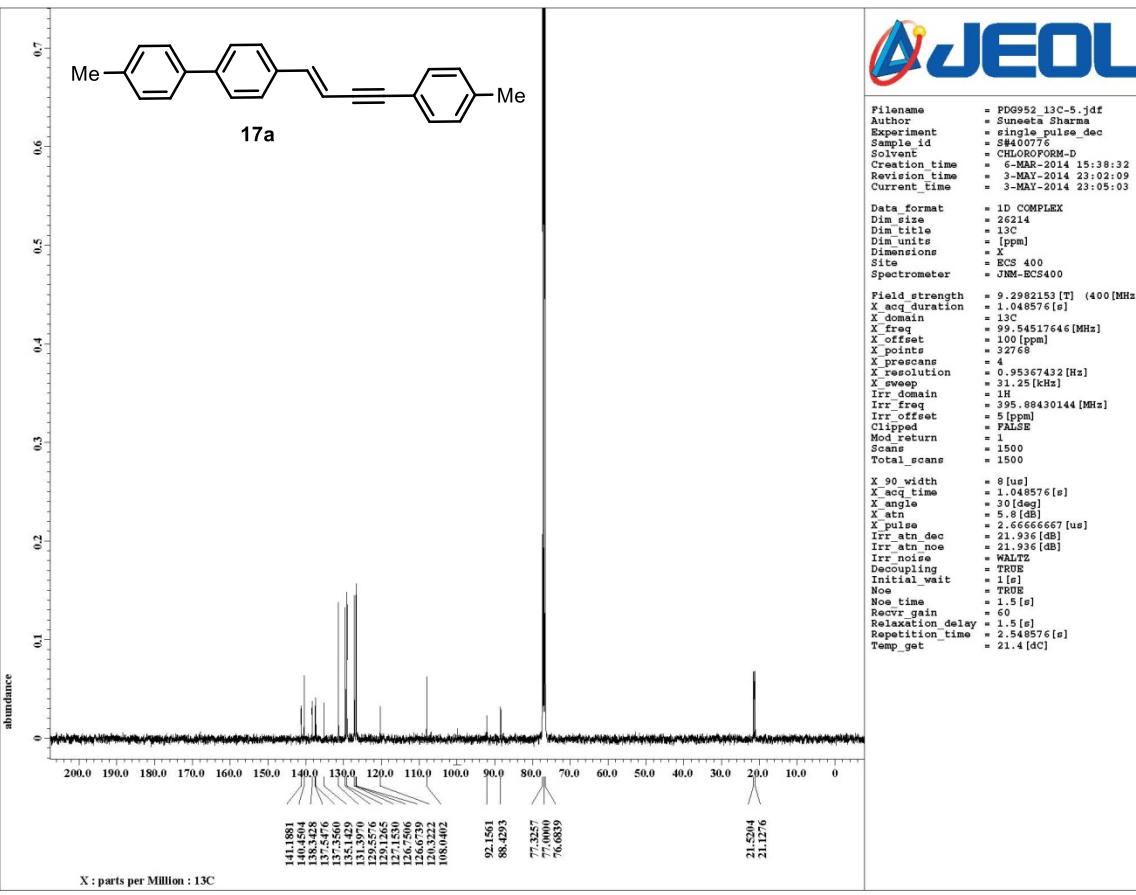
^{13}C NMR (100 MHz, CDCl_3) spectrum of (*E*)-1-fluoro-4-((4-(4-methoxyphenyl)but-1-en-3-ynyl)phenyl)ethynylbenzene (**16f**)



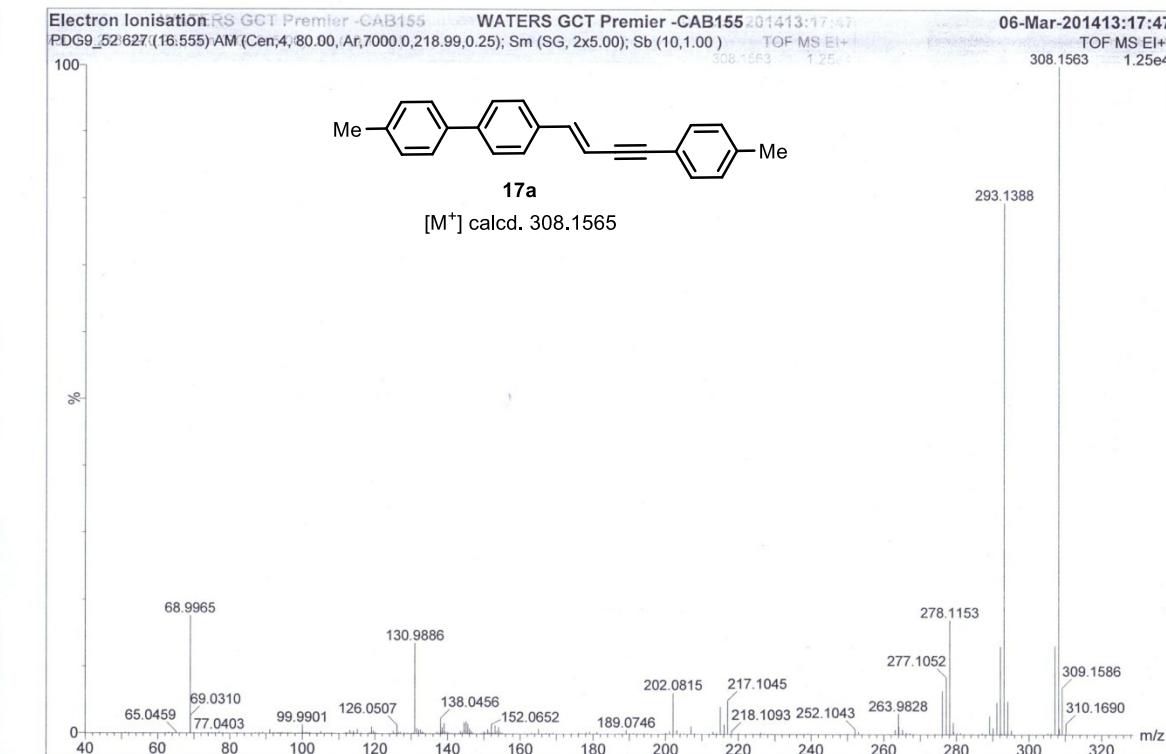
EI (HRMS) spectrum of (*E*)-1-fluoro-4-((4-(4-methoxyphenyl)but-1-en-3-ynyl)phenyl)ethynyl)benzene (**16f**)



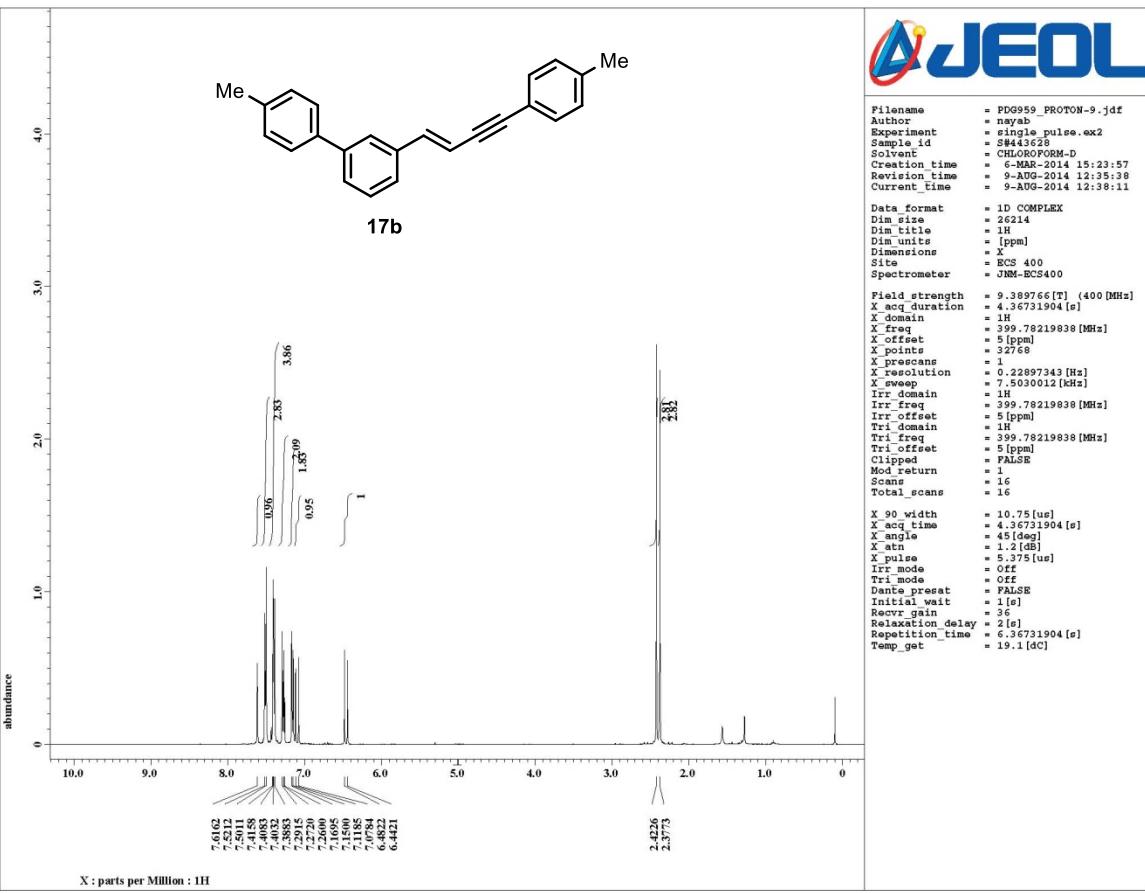
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-4-methyl-4'-(4-*p*-tolylbut-1-en-3-ynyl)biphenyl (**17a**)



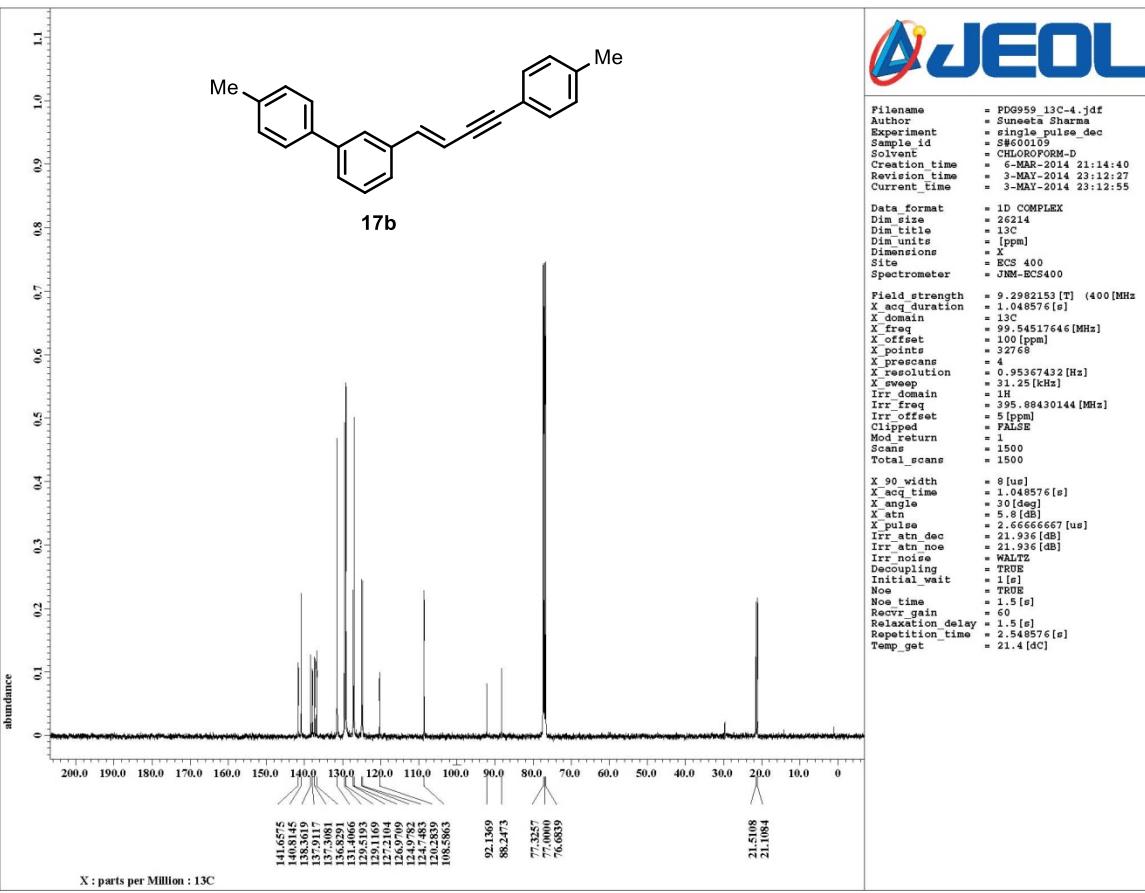
¹³C NMR (100 MHz, CDCl₃) spectrum of (*E*)-4-methyl-4'-(4-*p*-tolylbut-1-en-3-ynyl)biphenyl (**17a**)



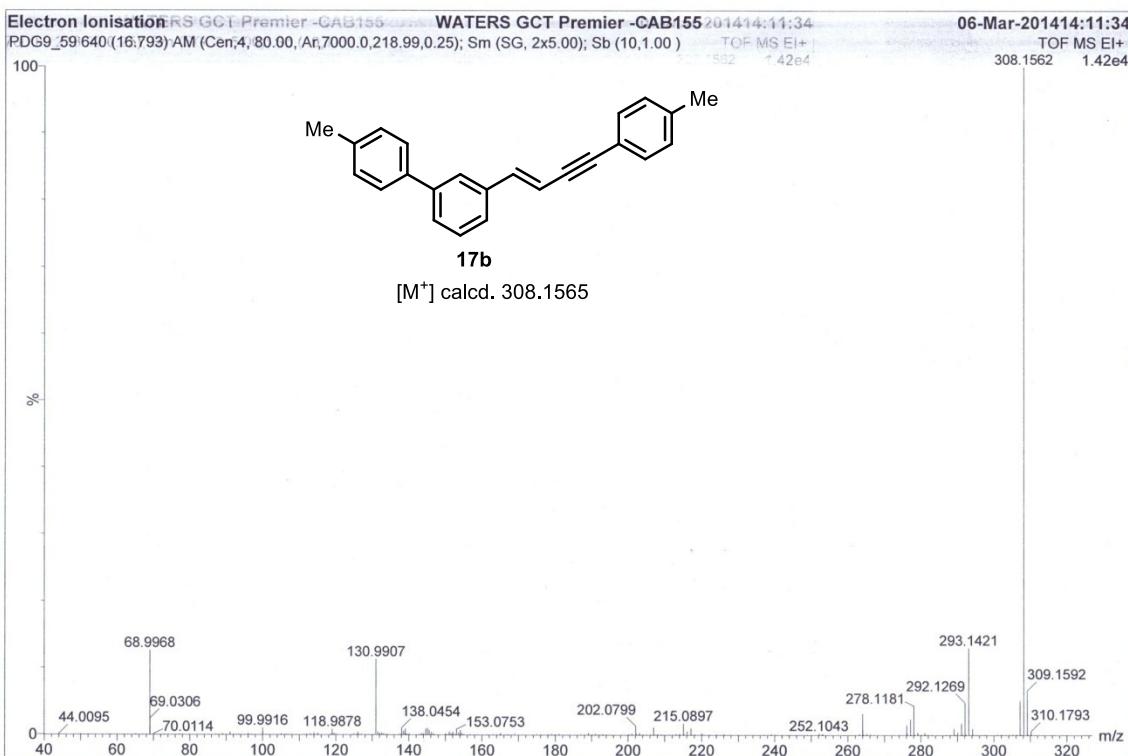
EI (HRMS) spectrum of (*E*)-4-methyl-4'-(4-*p*-tolylbut-1-en-3ynyl)biphenyl (**17a**)



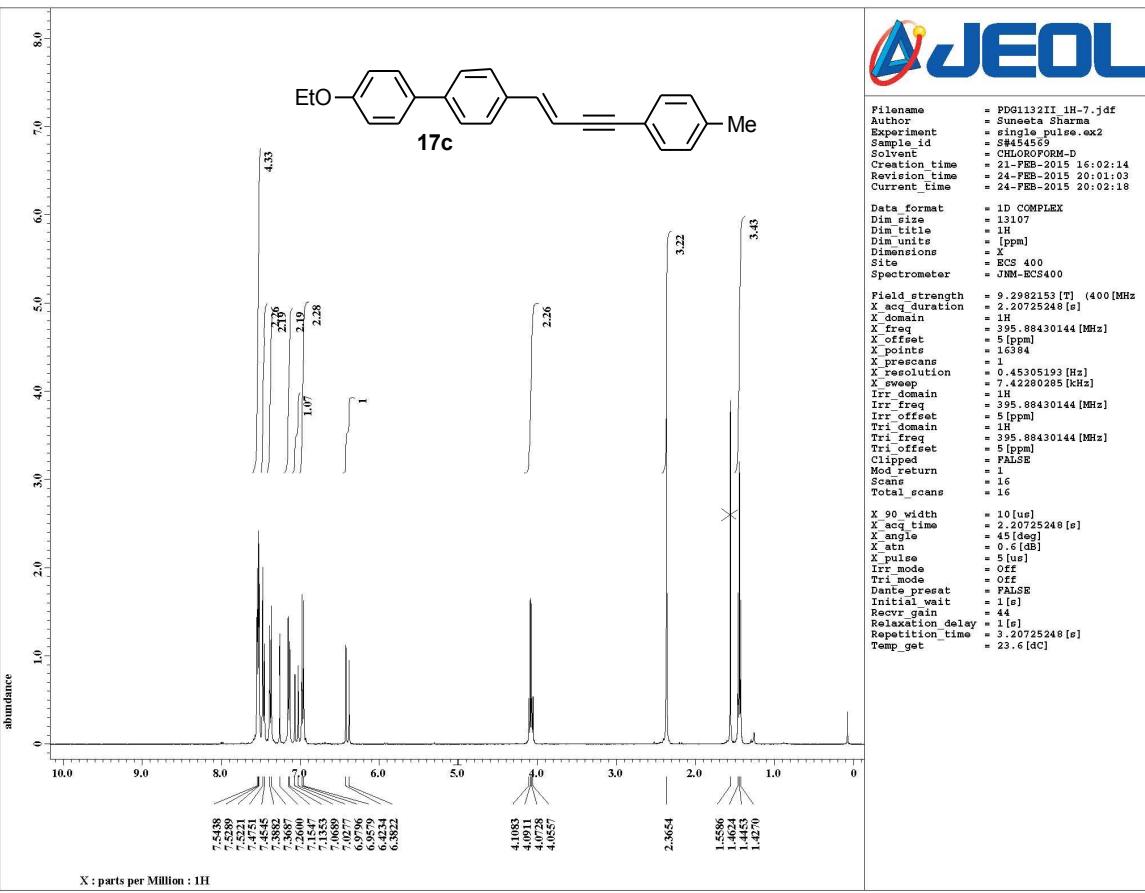
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-4'-methyl-3-(4-p-tolylbut-1-en-3-ynyl)biphenyl (**17b**)



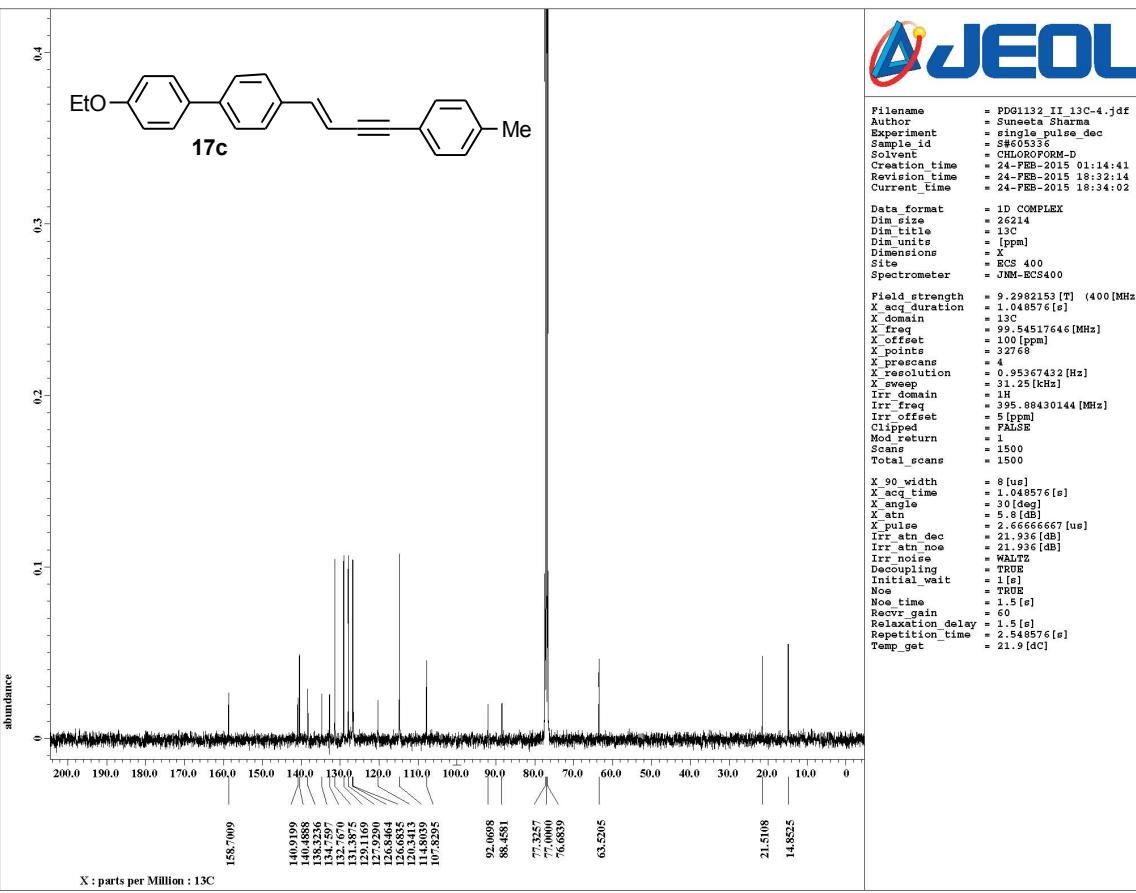
^{13}C NMR (100 MHz, CDCl_3) spectrum of (*E*)-4'-methyl-3-(4-*p*-tolylbut-1-en-3-ynyl)biphenyl (**17b**)



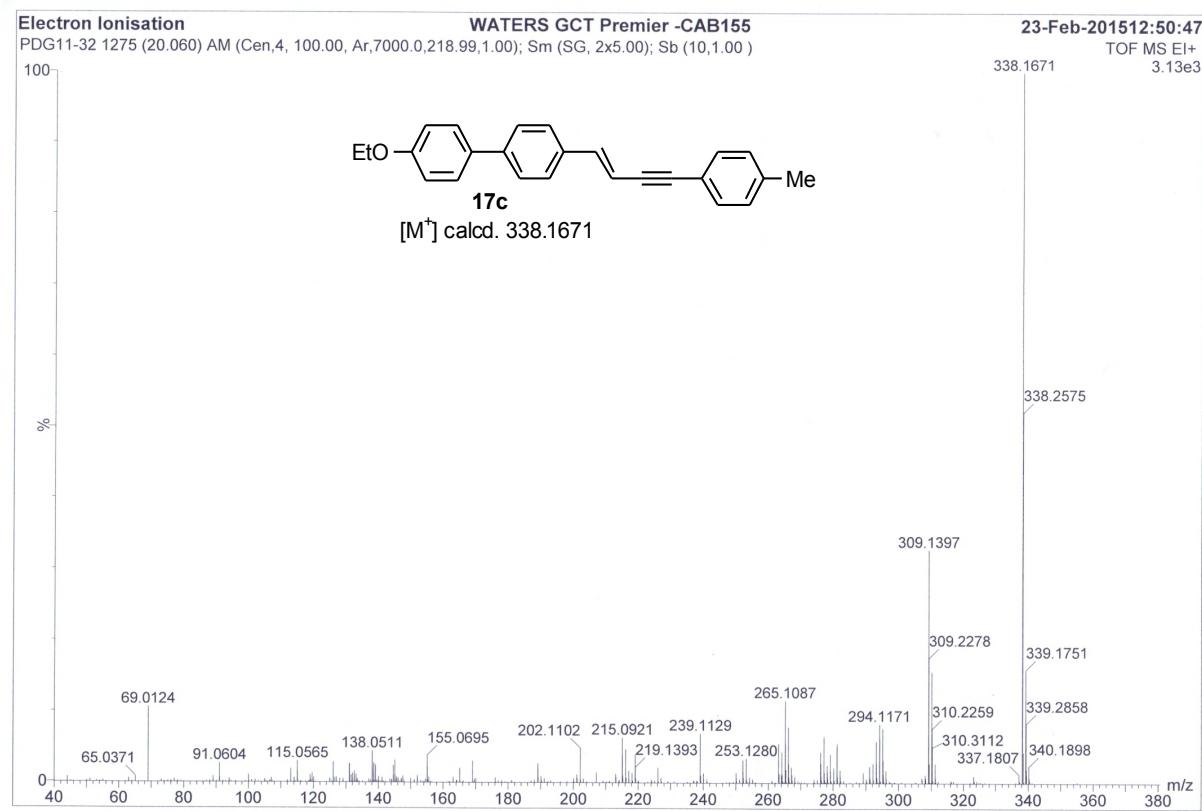
EI (HRMS) spectrum of (*E*)-4'-methyl-3-(4-*p*-tolylbut-1-en-3-ynyl)biphenyl (**17b**)



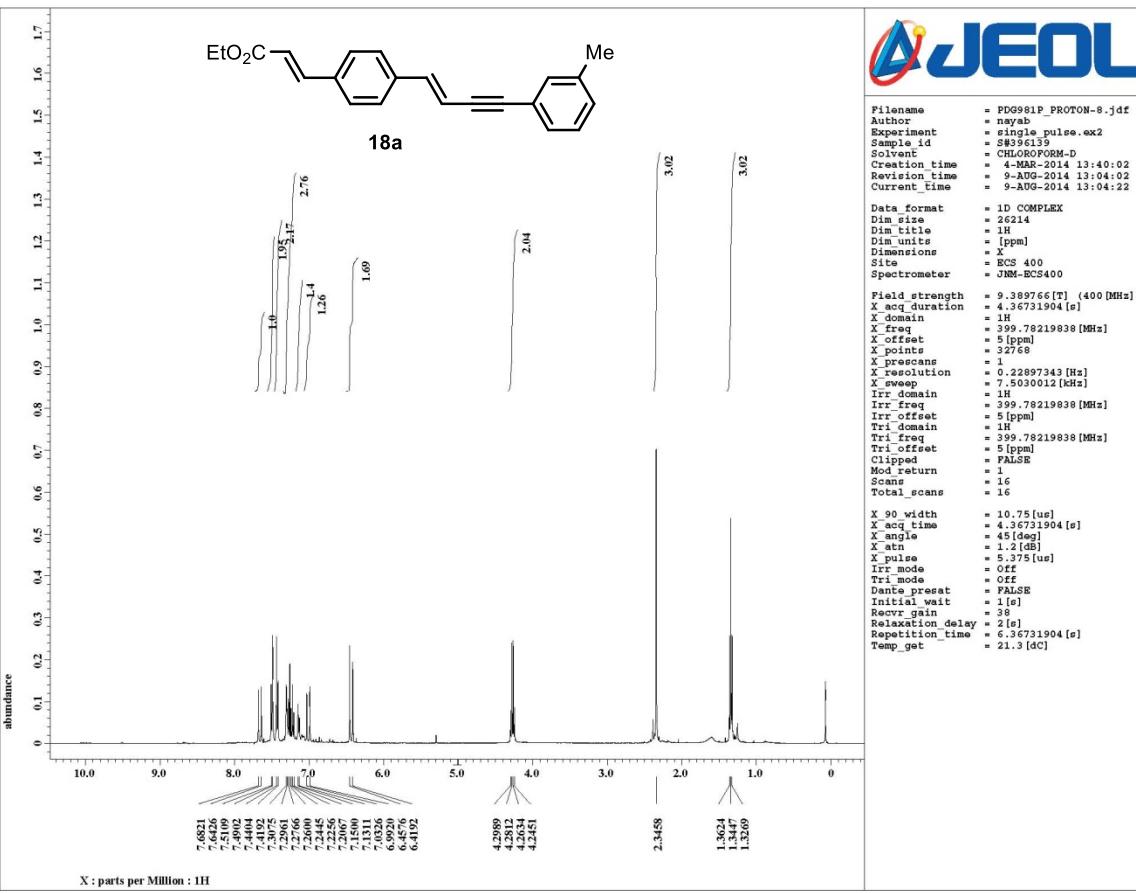
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-4-ethoxy-4'-(4-*p*-tolylbut-1-en-3-ynyl)biphenyl (**17c**)



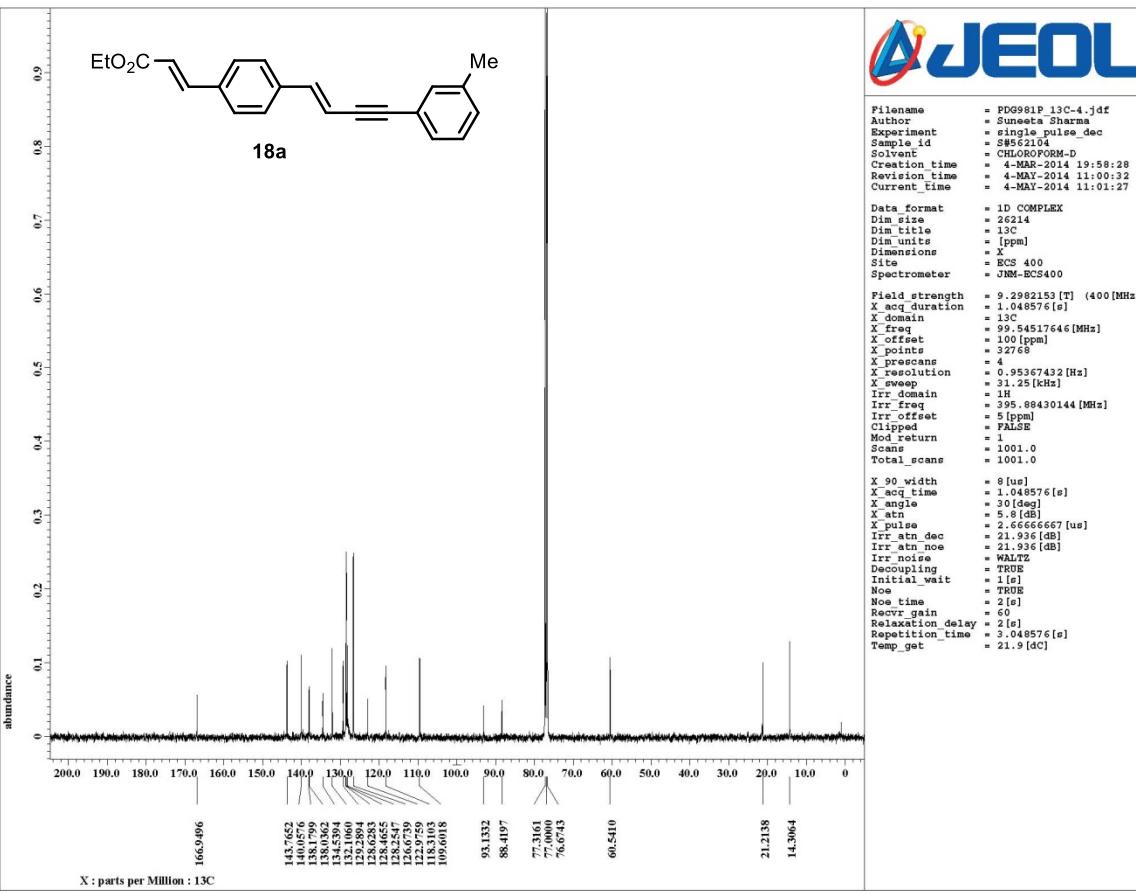
¹³C NMR (100 MHz, CDCl₃) spectrum of (*E*)-4-ethoxy-4'-(4-*p*-tolylbut-1-en-3-ynyl)biphenyl (**17c**)

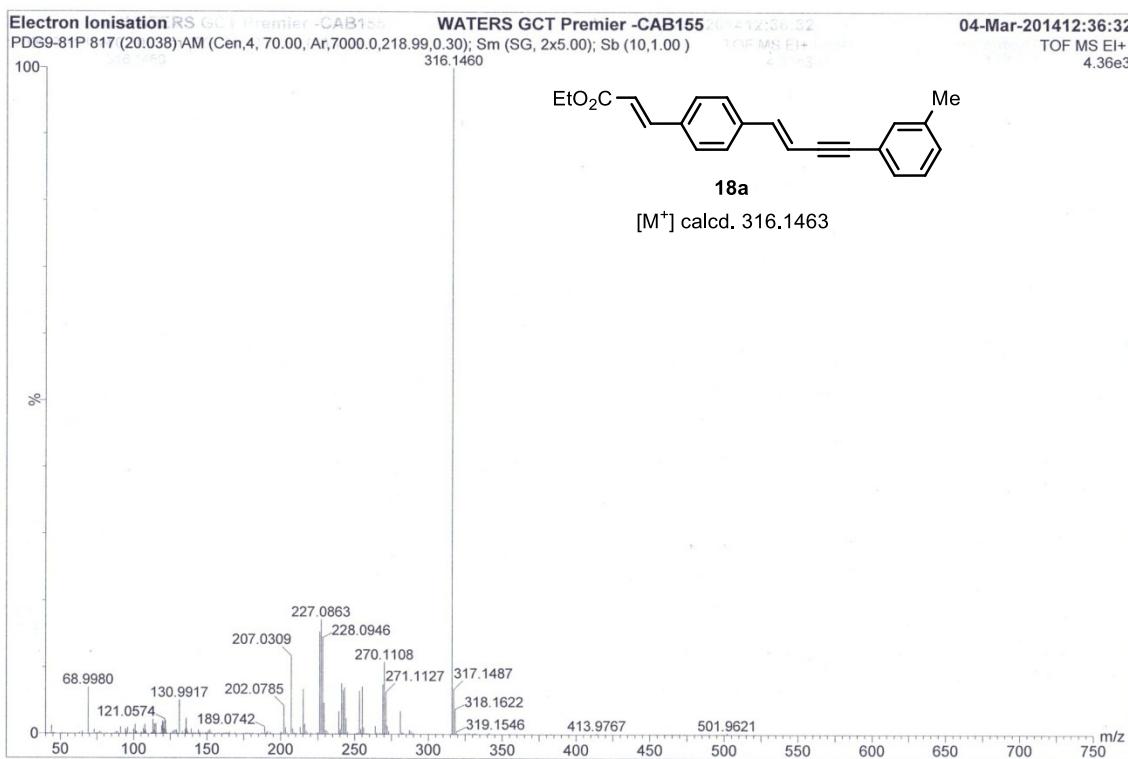


EI (HRMS) spectrum of (*E*)-4-ethoxy-4'-(4-*p*-tolylbut-1-en-3-ynyl)biphenyl (**17c**)

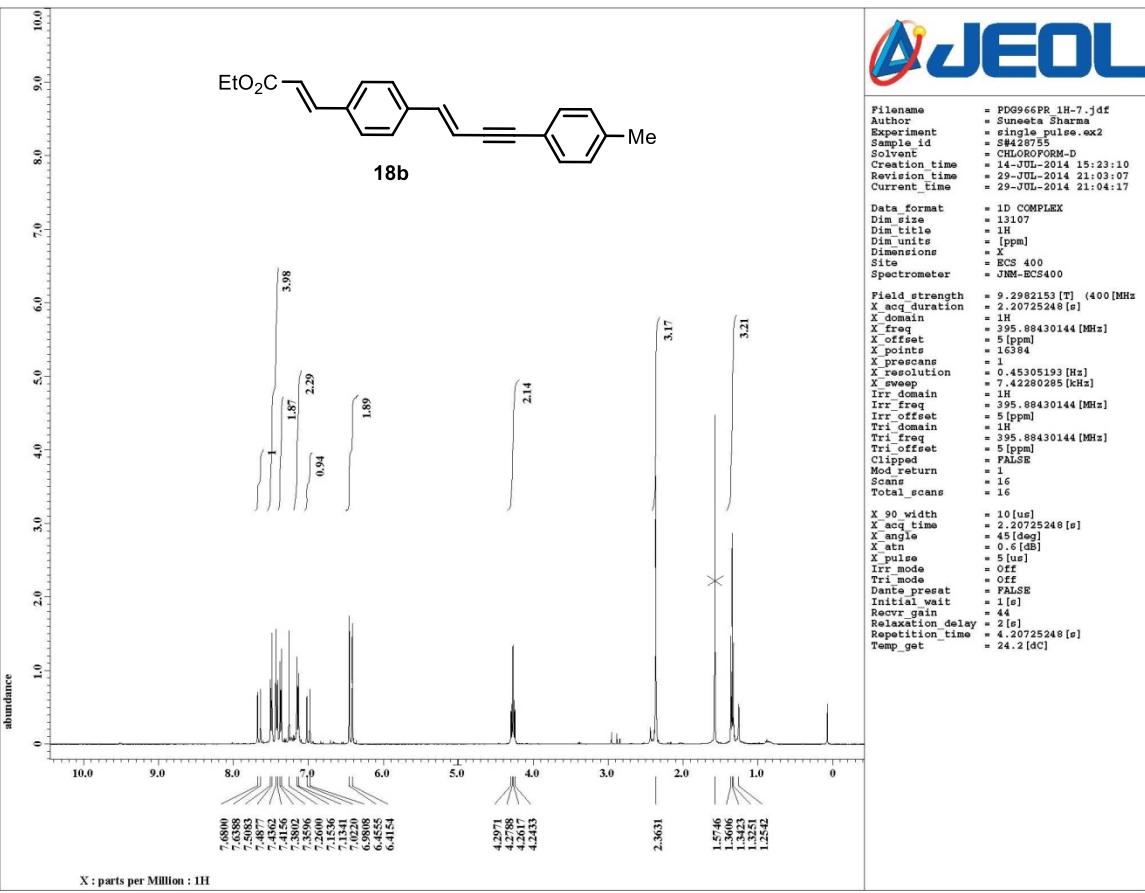


¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-ethyl 3-((*E*)-4-(4-*m*-tolylbut-1-en-3-ynyl)phenyl)acrylate (**18a**)

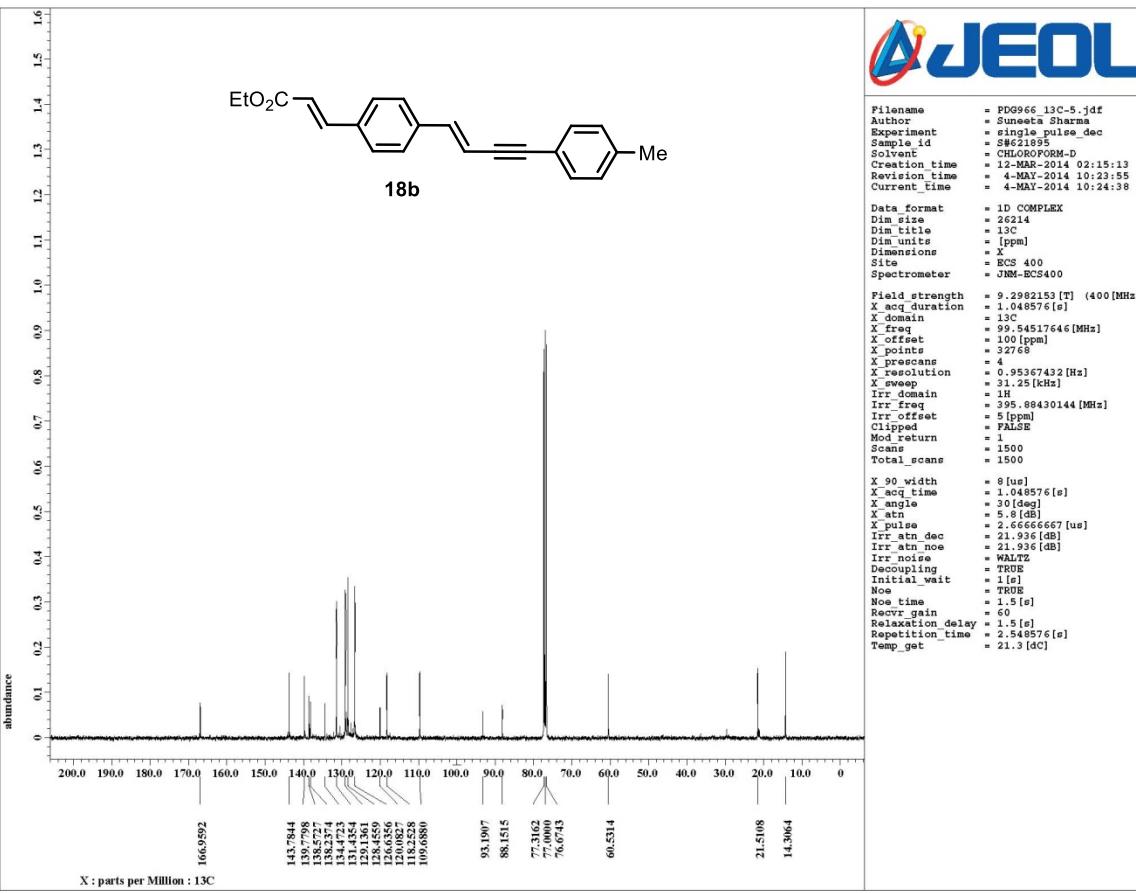




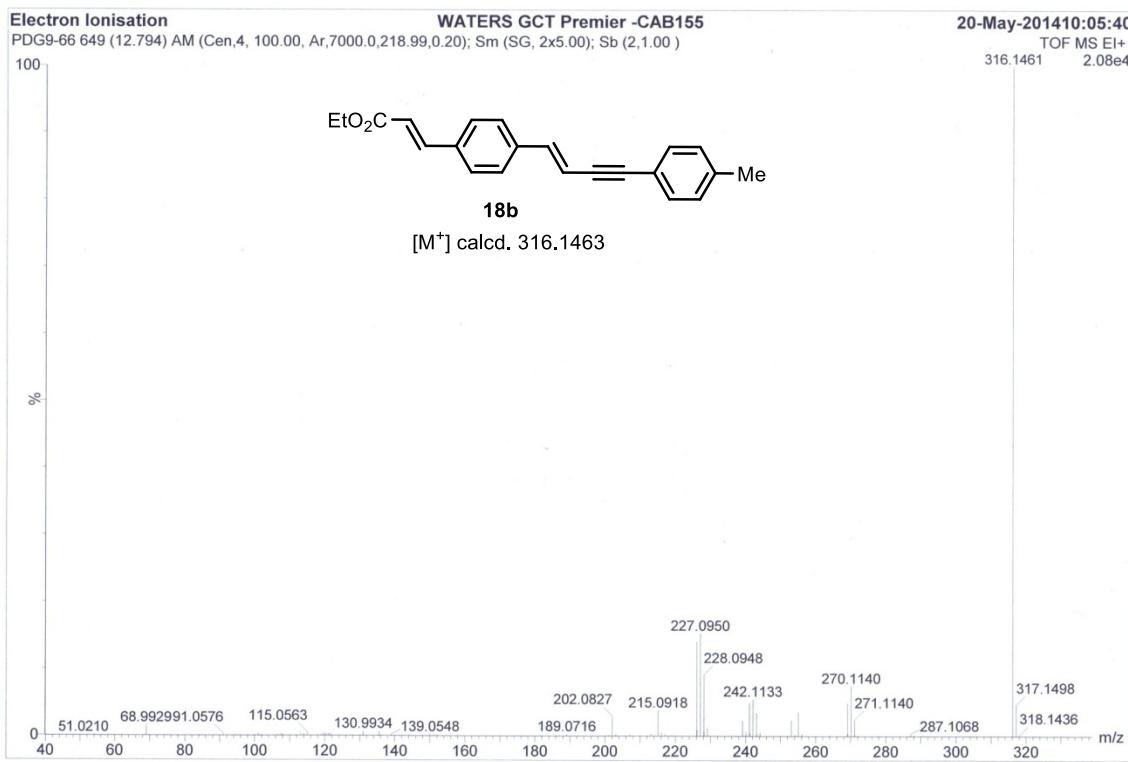
EI (HRMS) spectrum of (*E*)-ethyl 3-((*E*)-4-((*E*)-4-*m*-tolylbut-1-en-3-ynyl)phenyl)acrylate (**18a**)



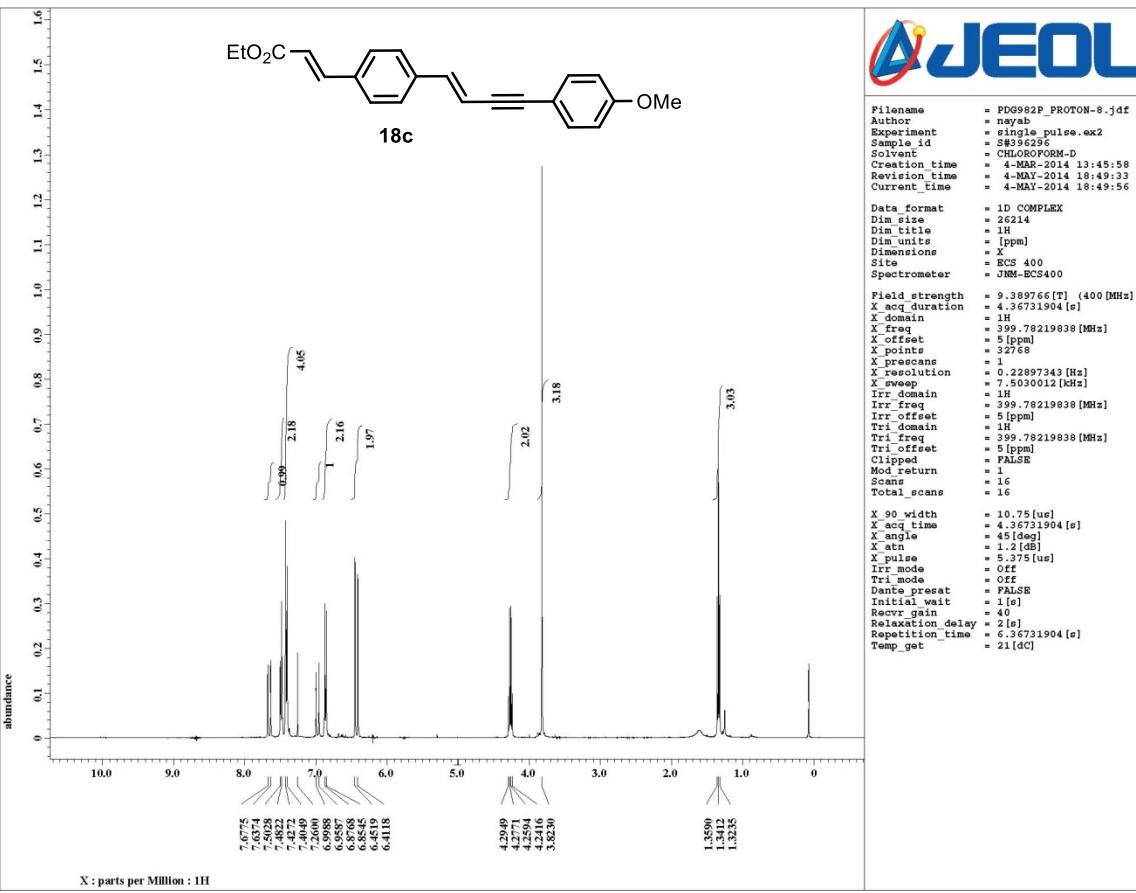
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-ethyl 3-(4-((*E*)-4-*p*-tolylbut-1-en-3-ynyl)phenyl)acrylate (**18b**)



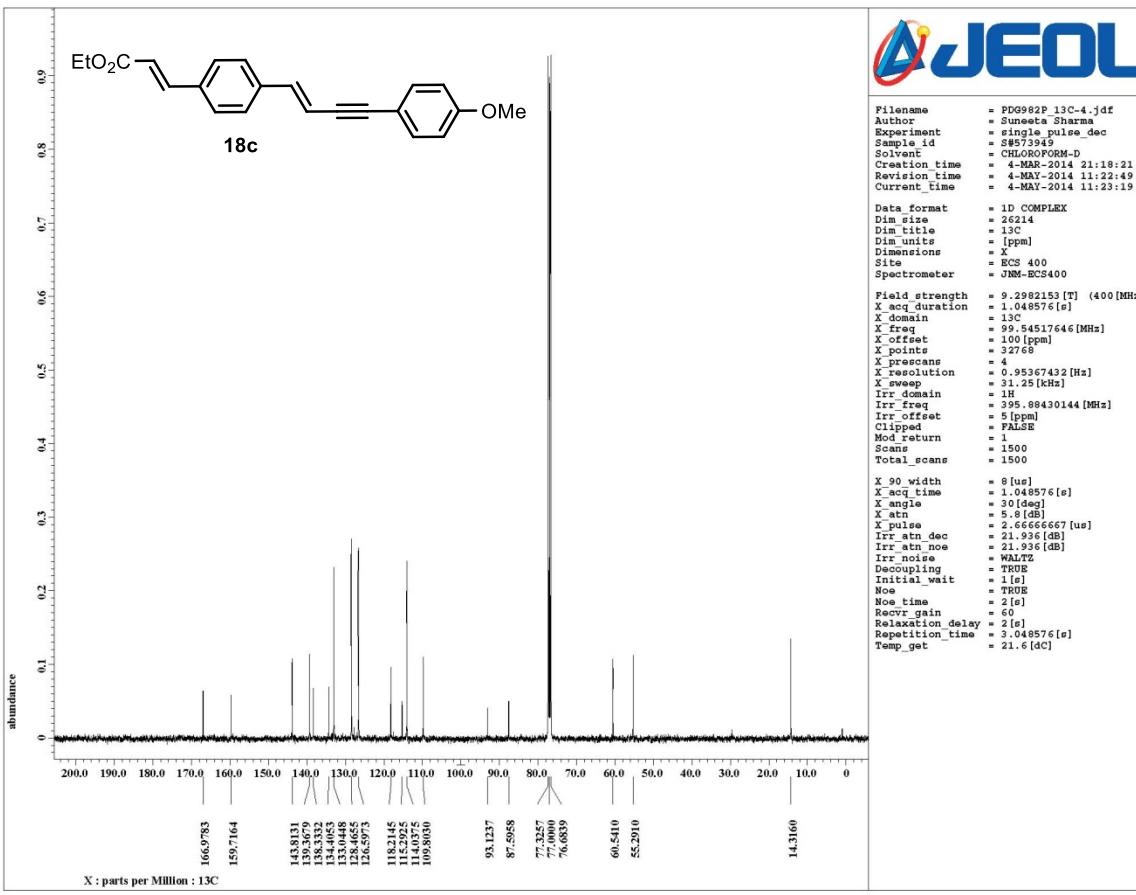
¹³C NMR (100 MHz, CDCl₃) spectrum of (*E*)-ethyl 3-(4-((*E*)-4-*p*-tolylbut-1-en-3-ynyl)phenyl)acrylate (**18b**)



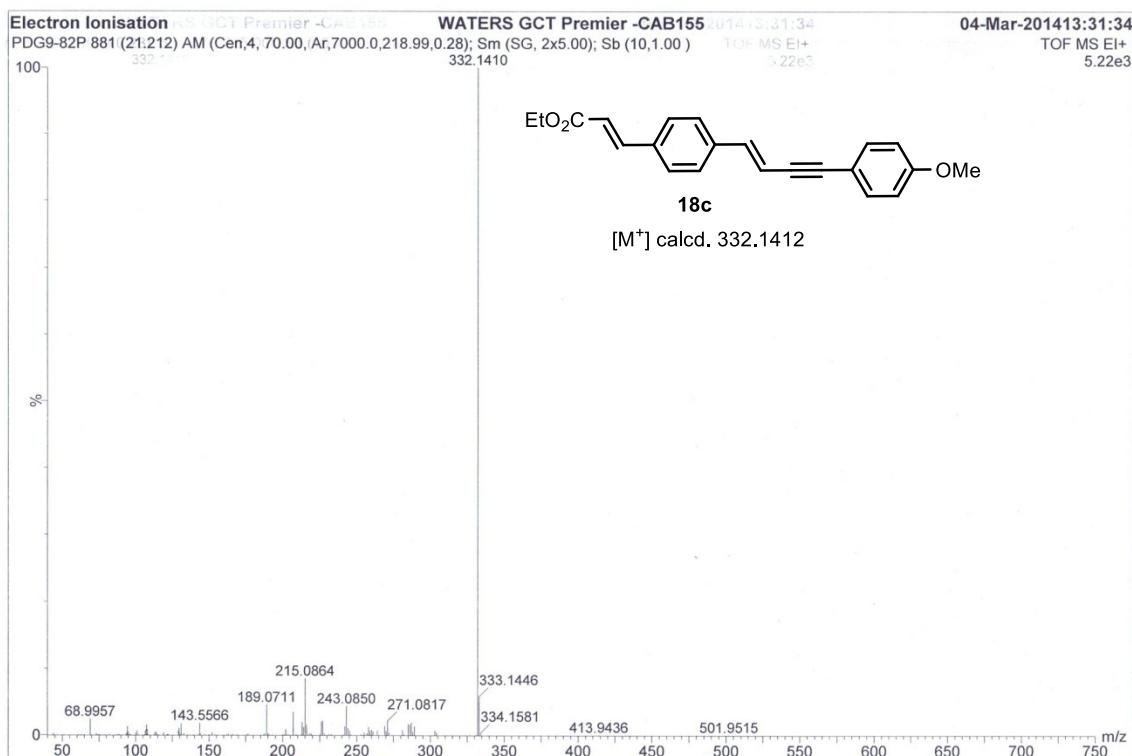
EI (HRMS) spectrum of (*E*)-ethyl 3-((*E*)-4-((*E*)-4-*p*-tolylbut-1-en-3-ynyl)phenyl)acrylate (**18b**)



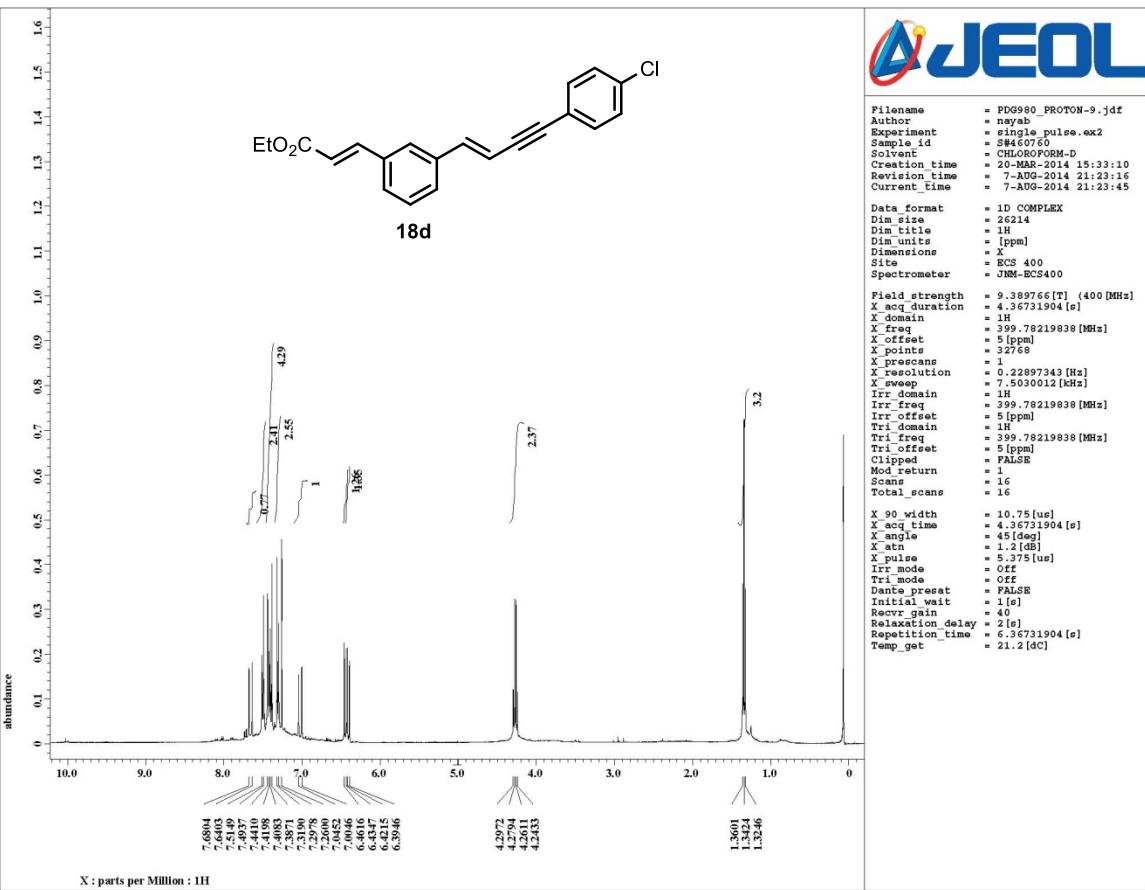
¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-ethyl 3-((*E*)-4-(4-methoxyphenyl)but-1-en-3-ynyl)phenylacrylate (**18c**)



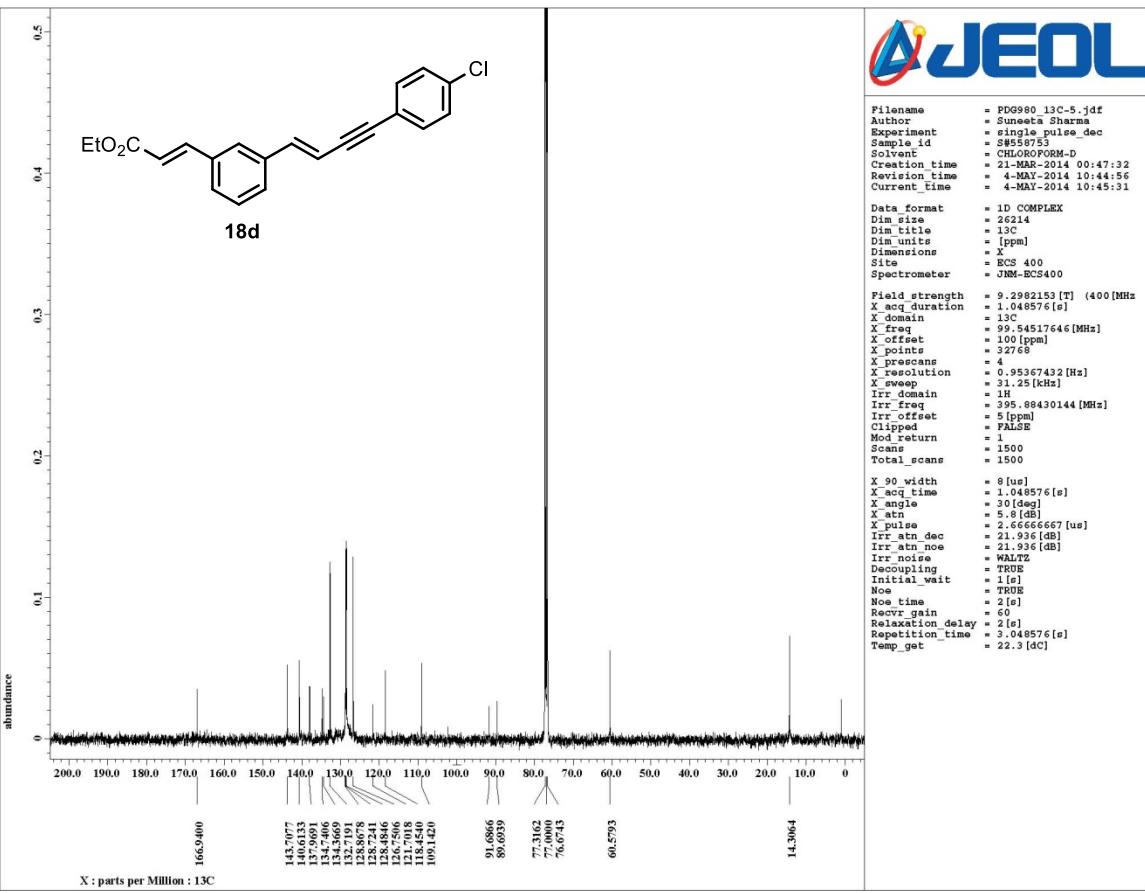
¹³C NMR (100 MHz, CDCl₃) spectrum of (E)-ethyl 3-((E)-4-(4-methoxyphenyl)but-1-en-3-ynyl)phenyl)acrylate (**18c**)



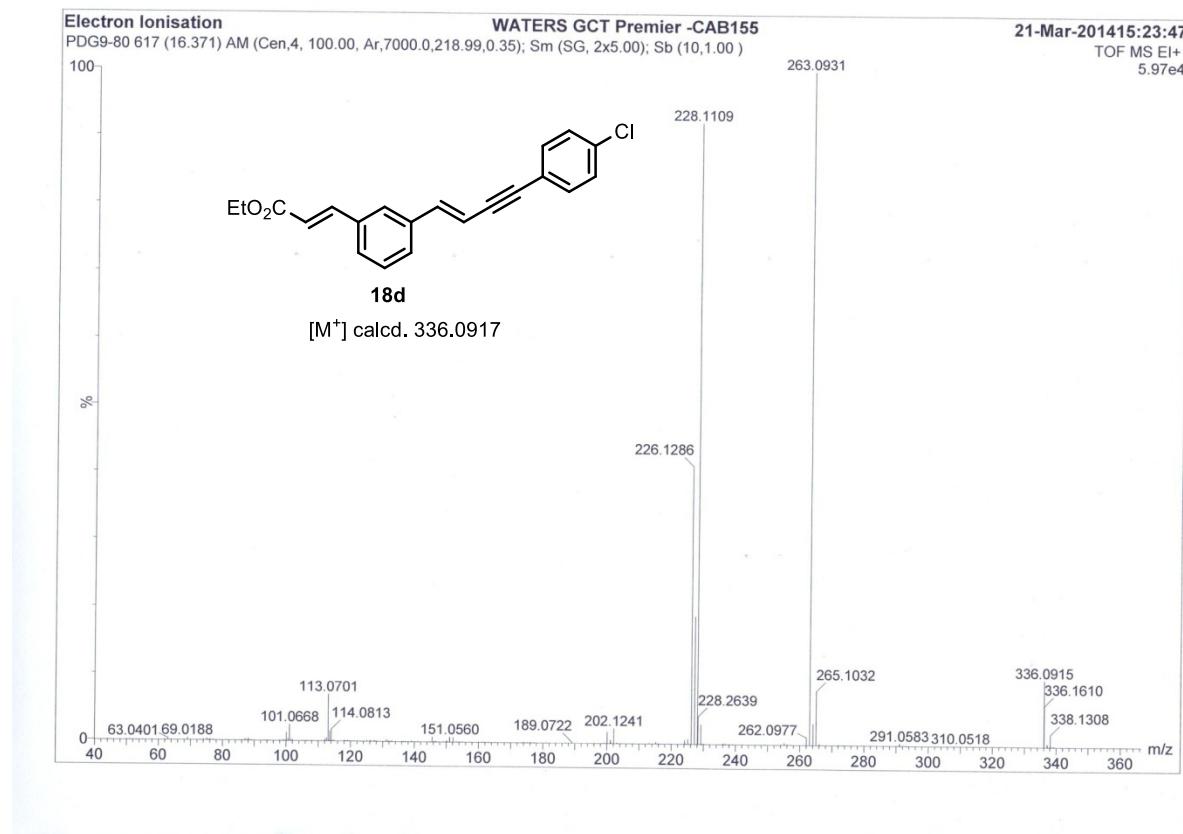
EI (HRMS) spectrum of (*E*)-ethyl 3-((*E*)-4-(4-methoxyphenyl)but-1-en-3-ynyl)phenyl)acrylate (**18c**)



¹H NMR (400 MHz, CDCl₃) spectrum of (*E*)-ethyl 3-((*E*)-4-(4-chlorophenyl)but-1-en-3-ynyl)phenyl)acrylate (**18d**)



¹³C NMR (100 MHz, CDCl₃) spectrum of (*E*)-ethyl 3-((*E*)-4-(4-chlorophenyl)but-1-en-3-ynyl)phenyl)acrylate (**18d**)



EI (HRMS) spectrum of (*E*)-ethyl 3-((*E*)-4-(4-chlorophenyl)but-1-en-3-ynyl)phenyl)acrylate (**18d**)