

Supporting Information

Threefold and chemoselective couplings of triarylbismuths with benzylic chlorides and iodides using palladium catalysis

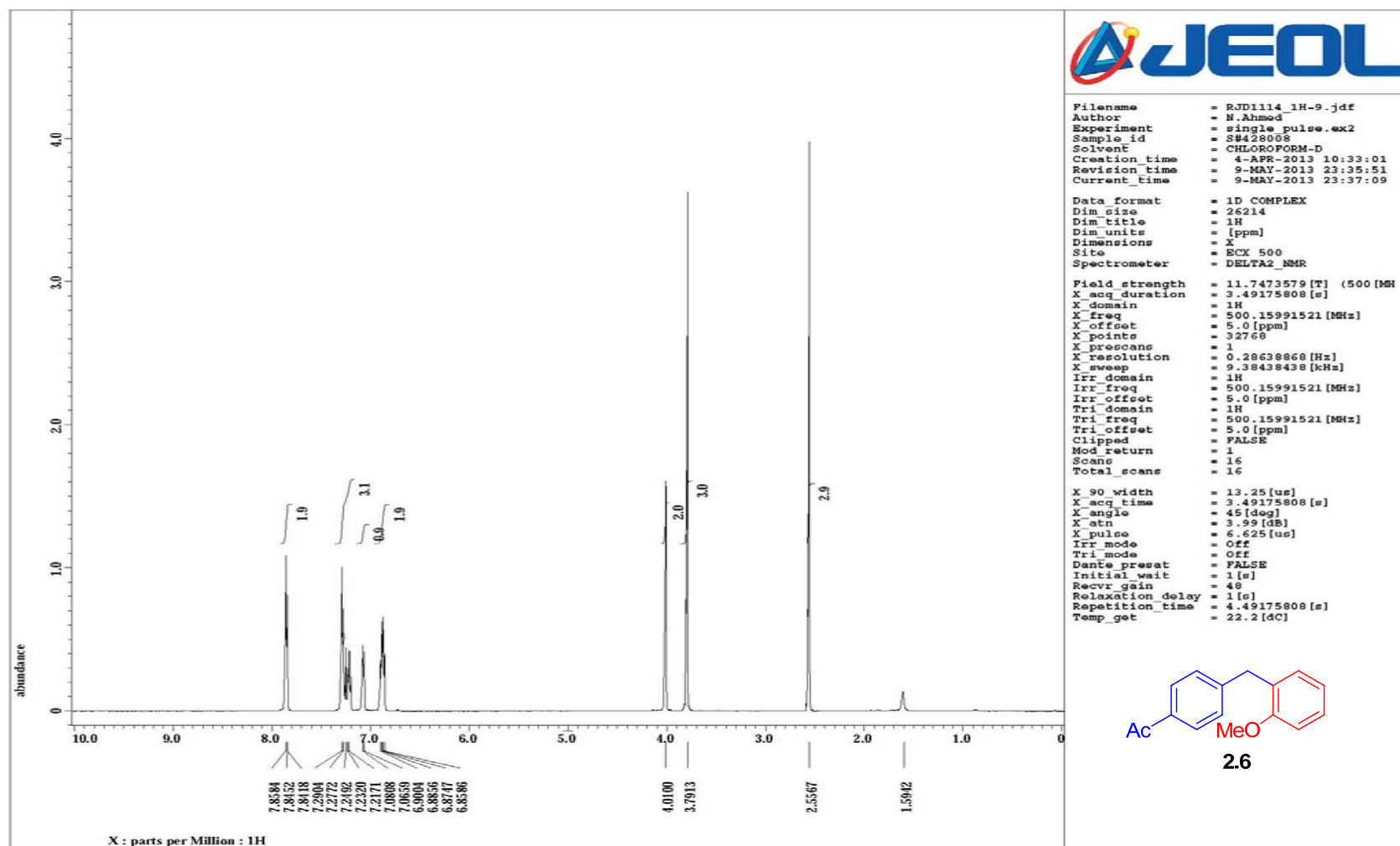
Maddali L.N. Rao^{*}, Ritesh J. Dhanorkar

Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur-208016, India

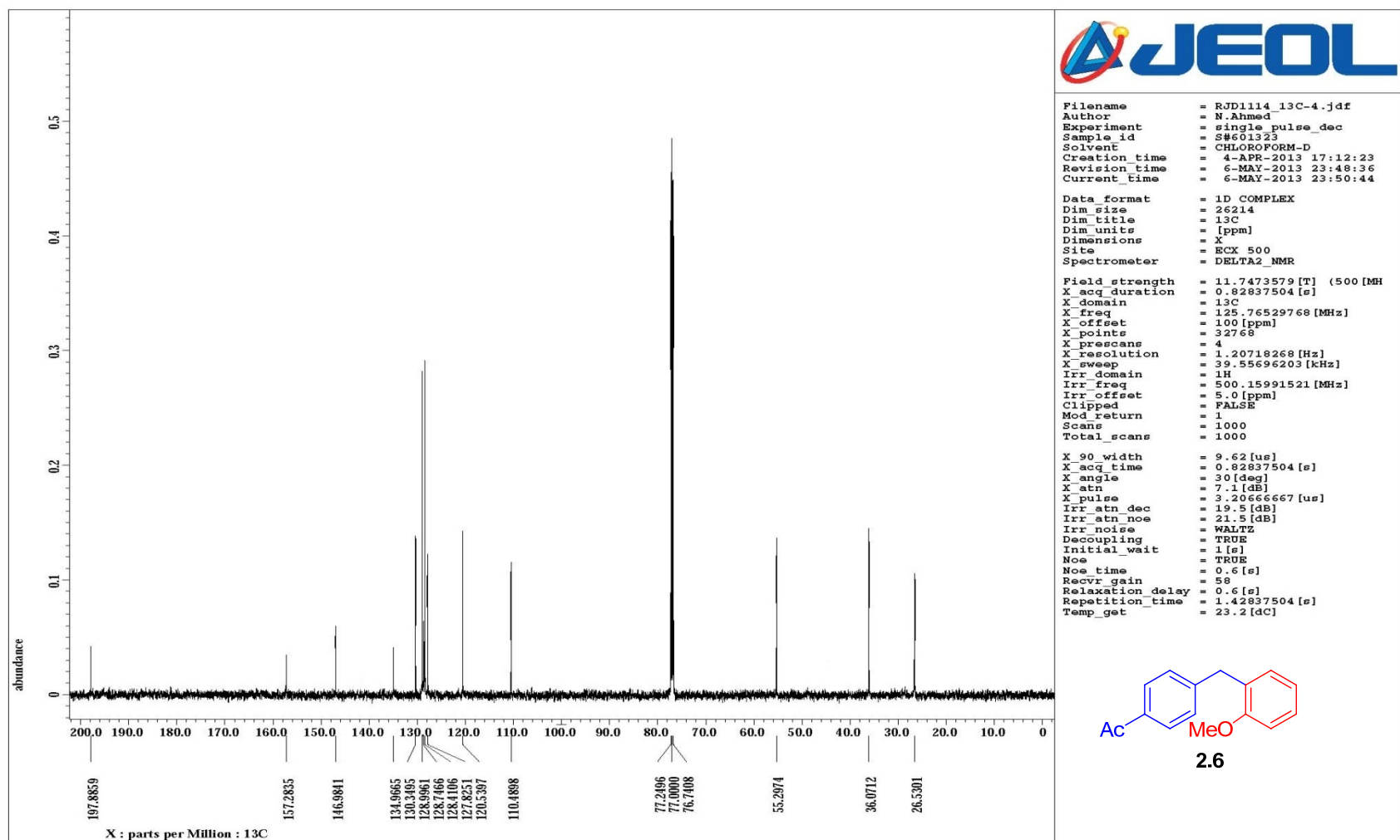
maddali@iitk.ac.in

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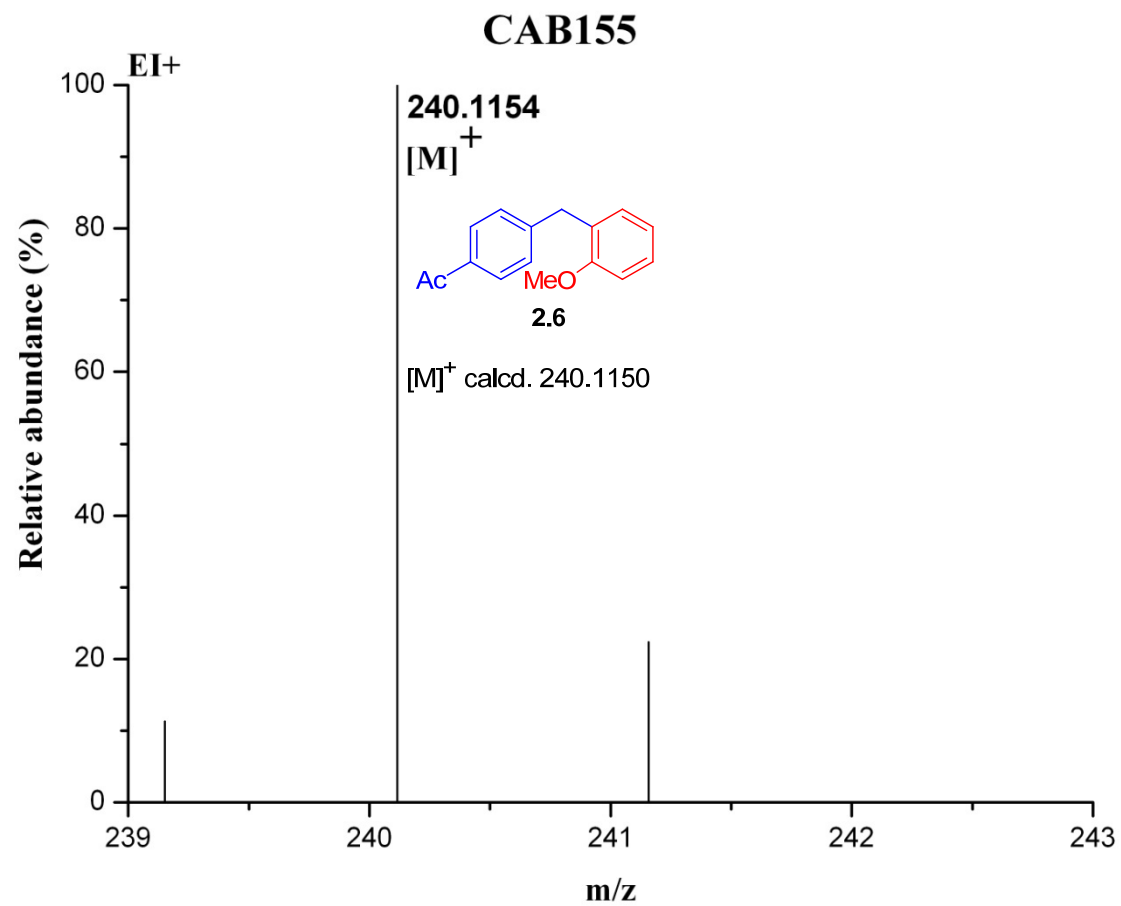
Copies of ¹H NMR, ¹³C NMR and HRMS spectra.....S2-S112



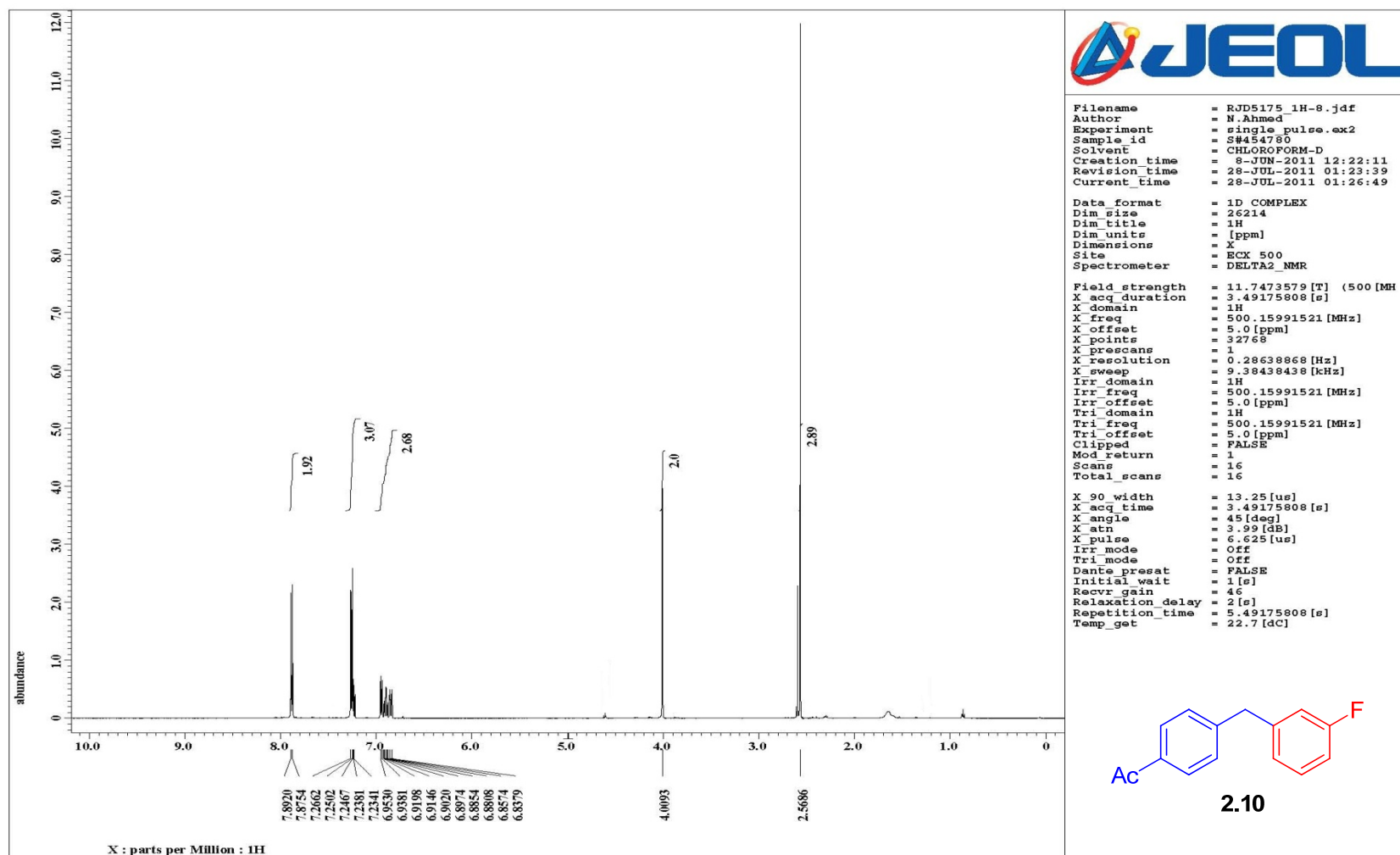
¹H NMR spectrum of 1-(4-(2-methoxybenzyl)phenyl)ethanone (2.6)



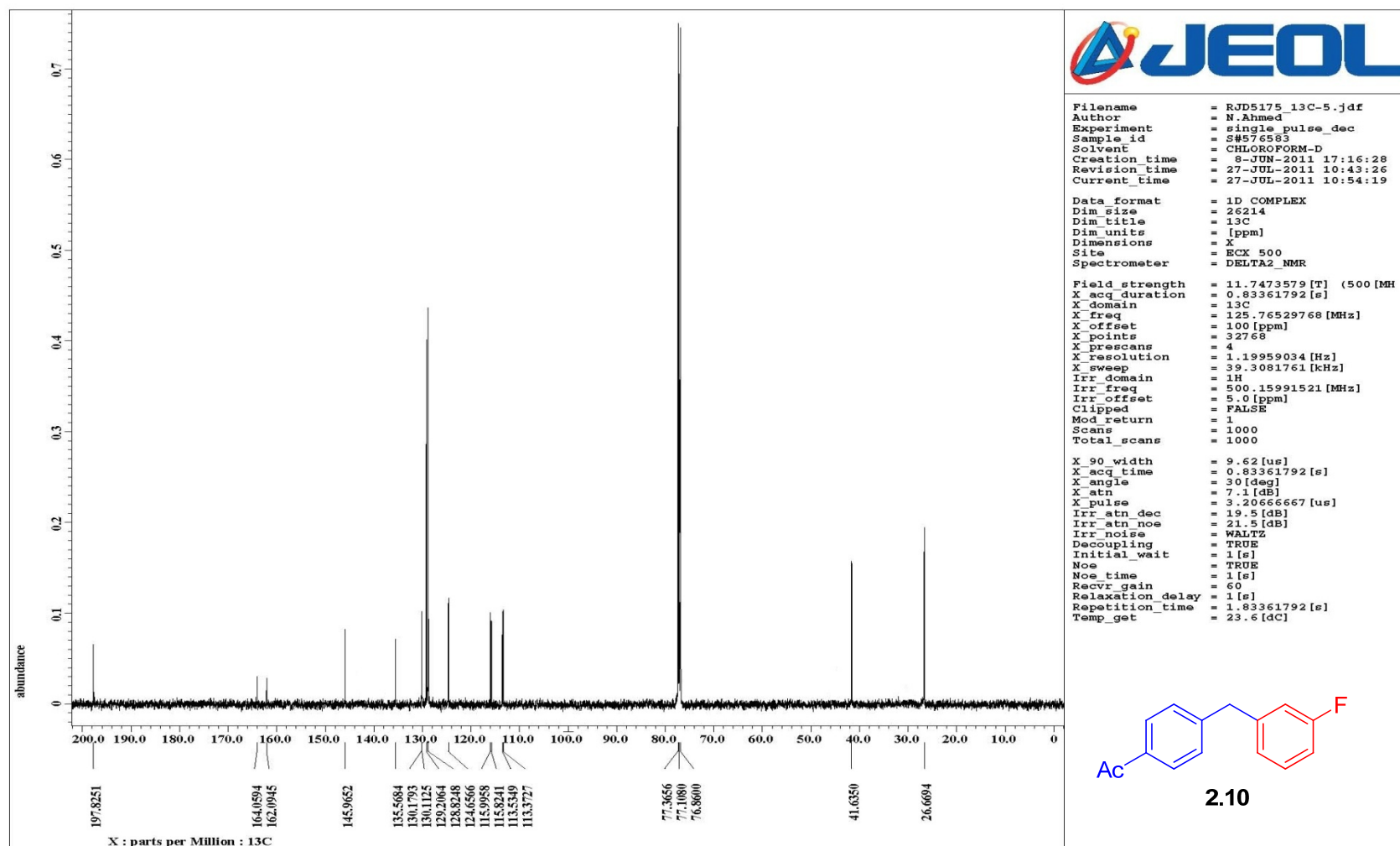
^{13}C NMR spectrum of 1-(4-(2-methoxybenzyl)phenyl)ethanone (2.6)



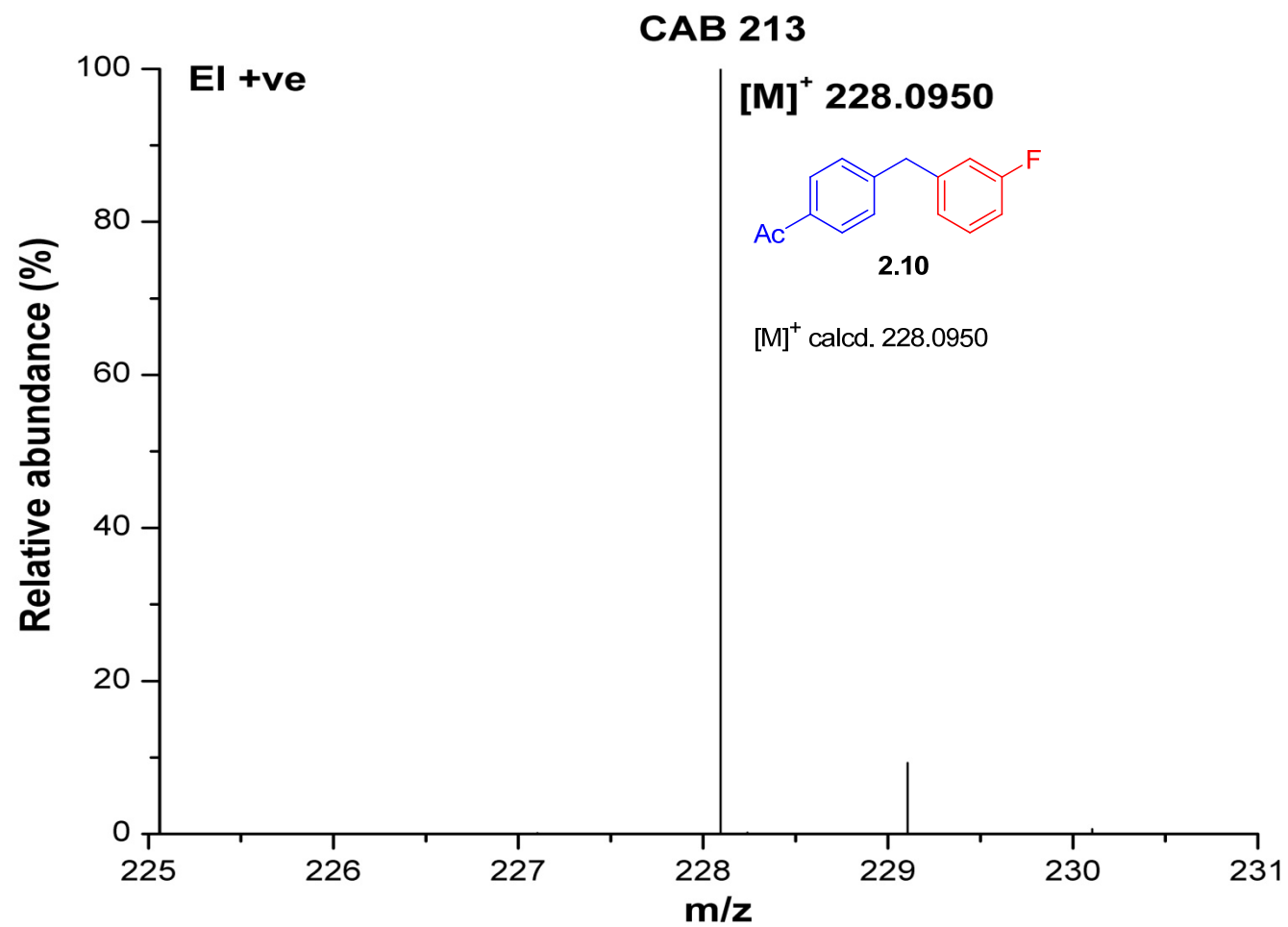
HRMS spectrum of 1-(4-(2-methoxybenzyl)phenyl)ethanone (**2.6**)



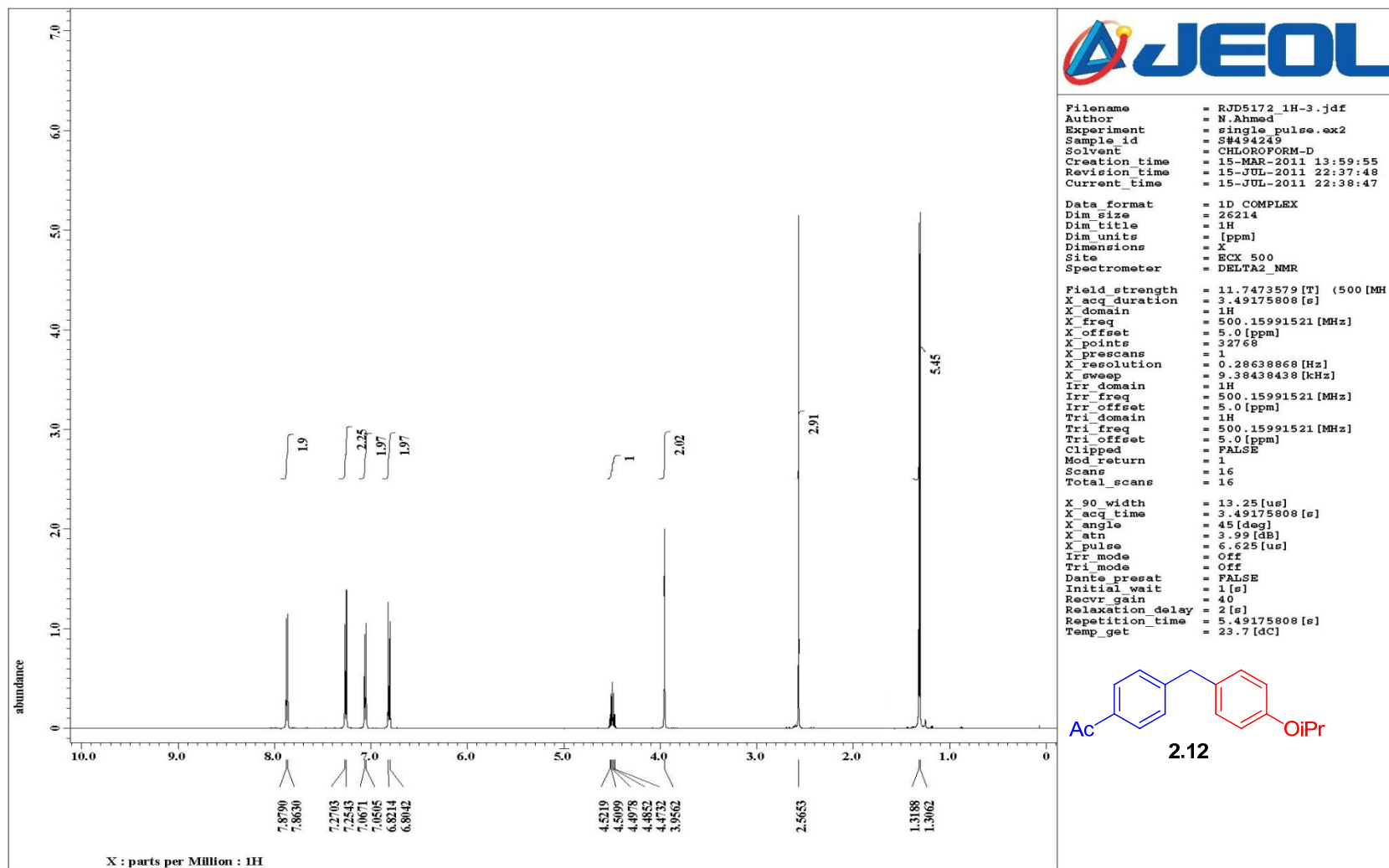
¹H NMR spectrum of 1-(4-(3-florobenzyl)phenyl)ethanone (2.10)



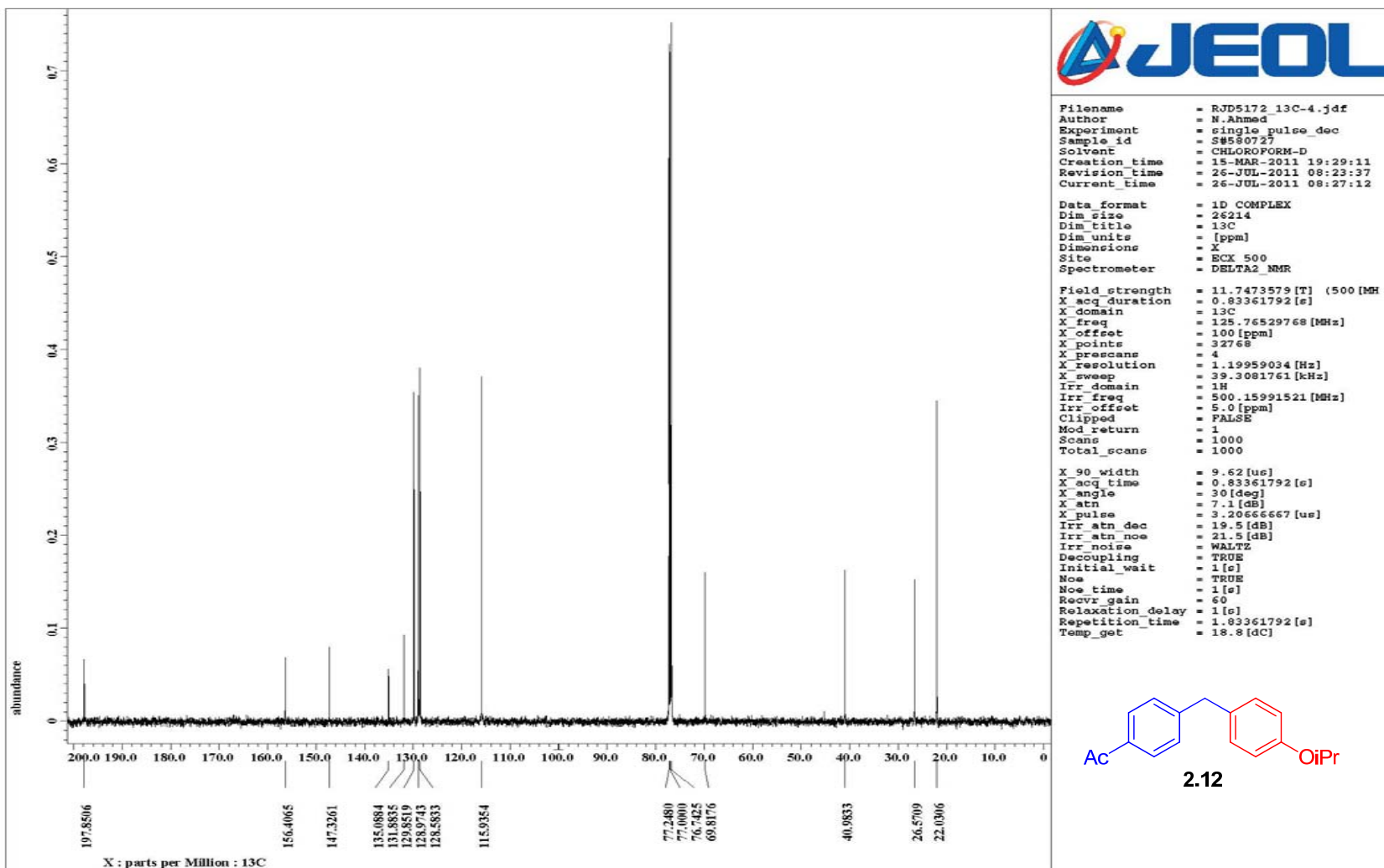
¹³C NMR spectrum of 1-(4-(3-fluorobenzyl)phenyl)ethanone (2.10)



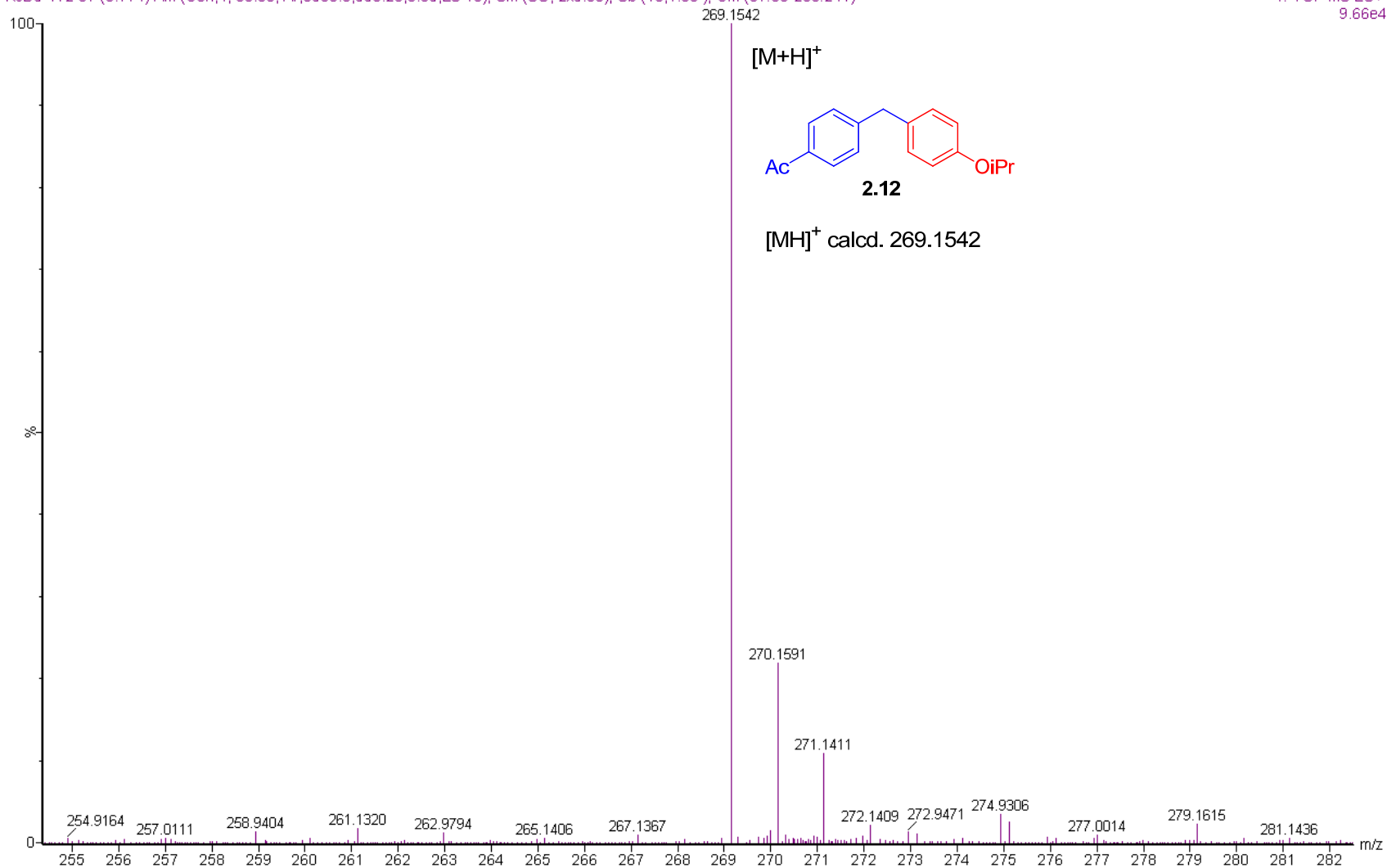
HRMS spectrum of 1-(4-(3-florobenzyl)phenyl)ethanone (**2.10**)



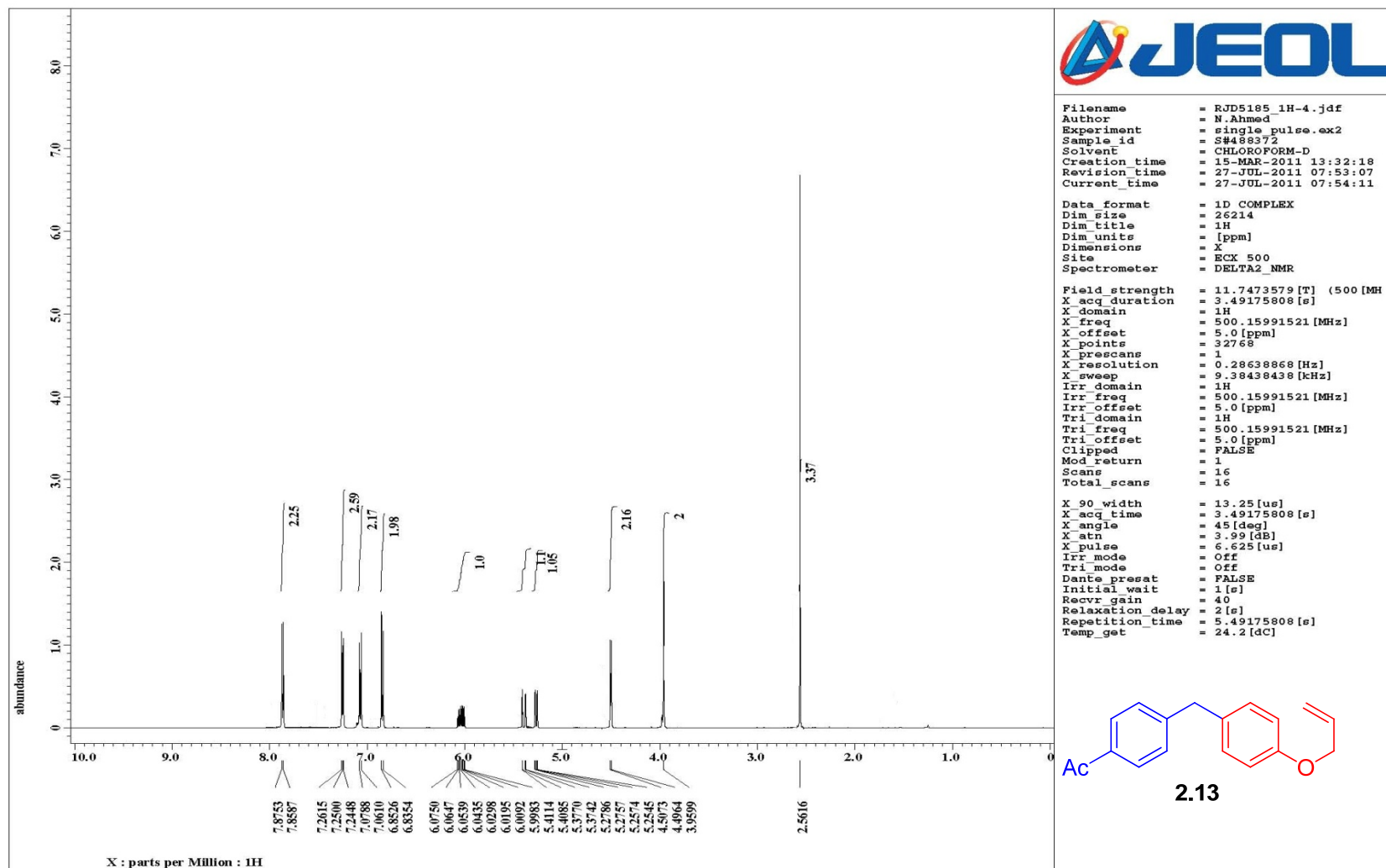
¹H NMR spectrum of 1-(4-(4-isopropoxybenzyl)phenyl)ethanone (2.12)



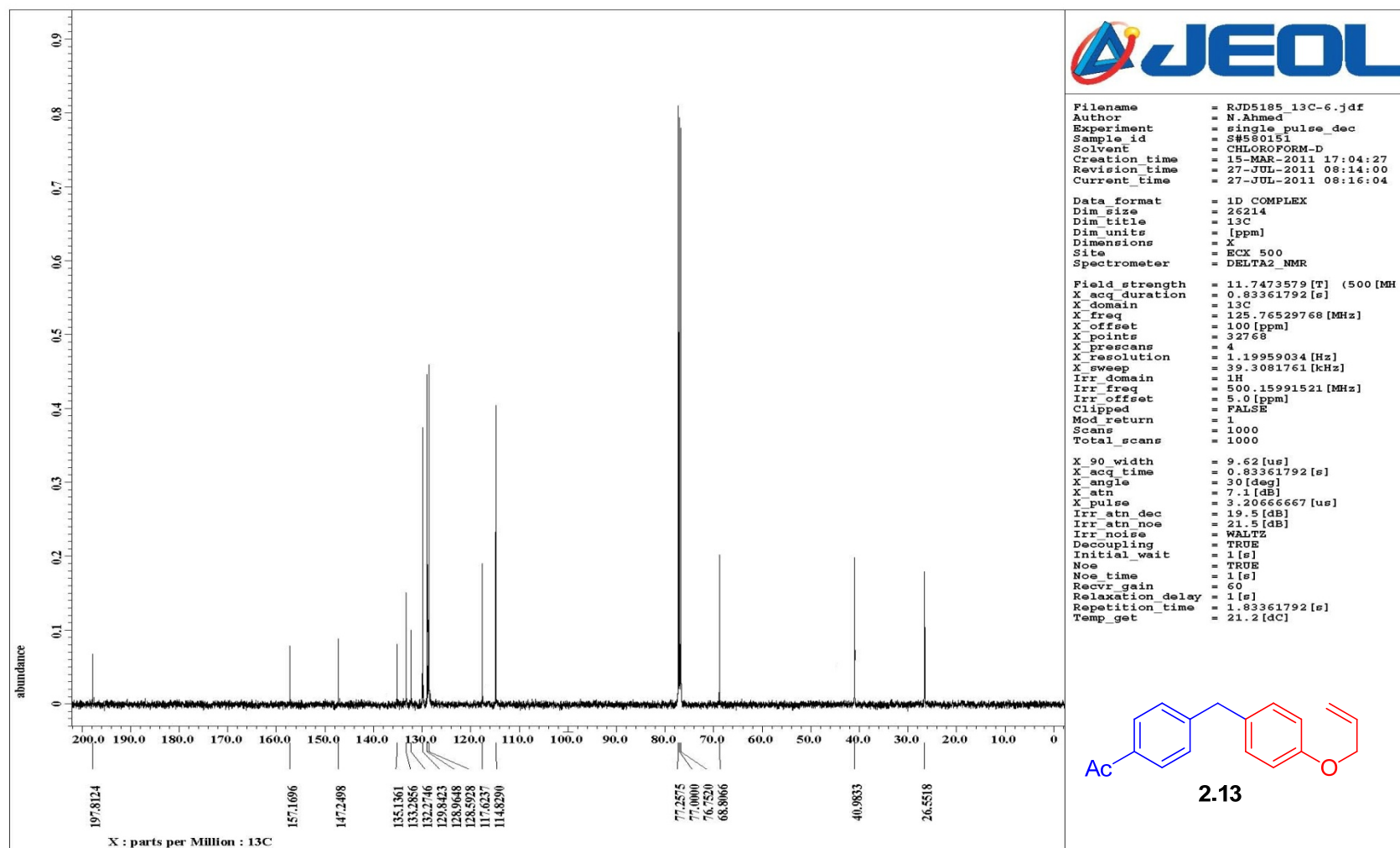
¹³C NMR spectrum of 1-(4-(4-isopropoxybenzyl)phenyl)ethanone (2.12)



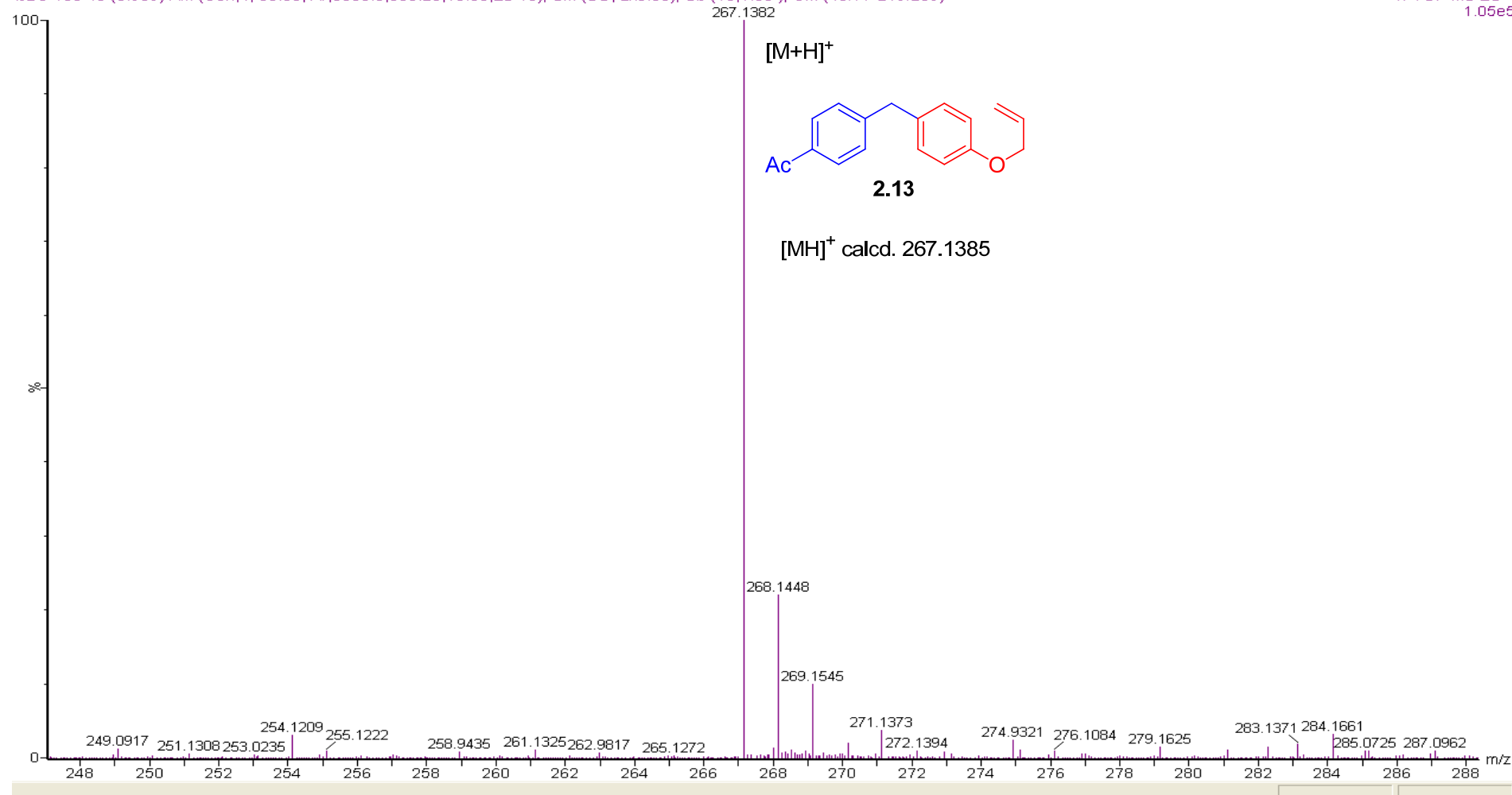
HRMS spectrum of 1-(4-(4-isopropoxybenzyl)phenyl)ethanone



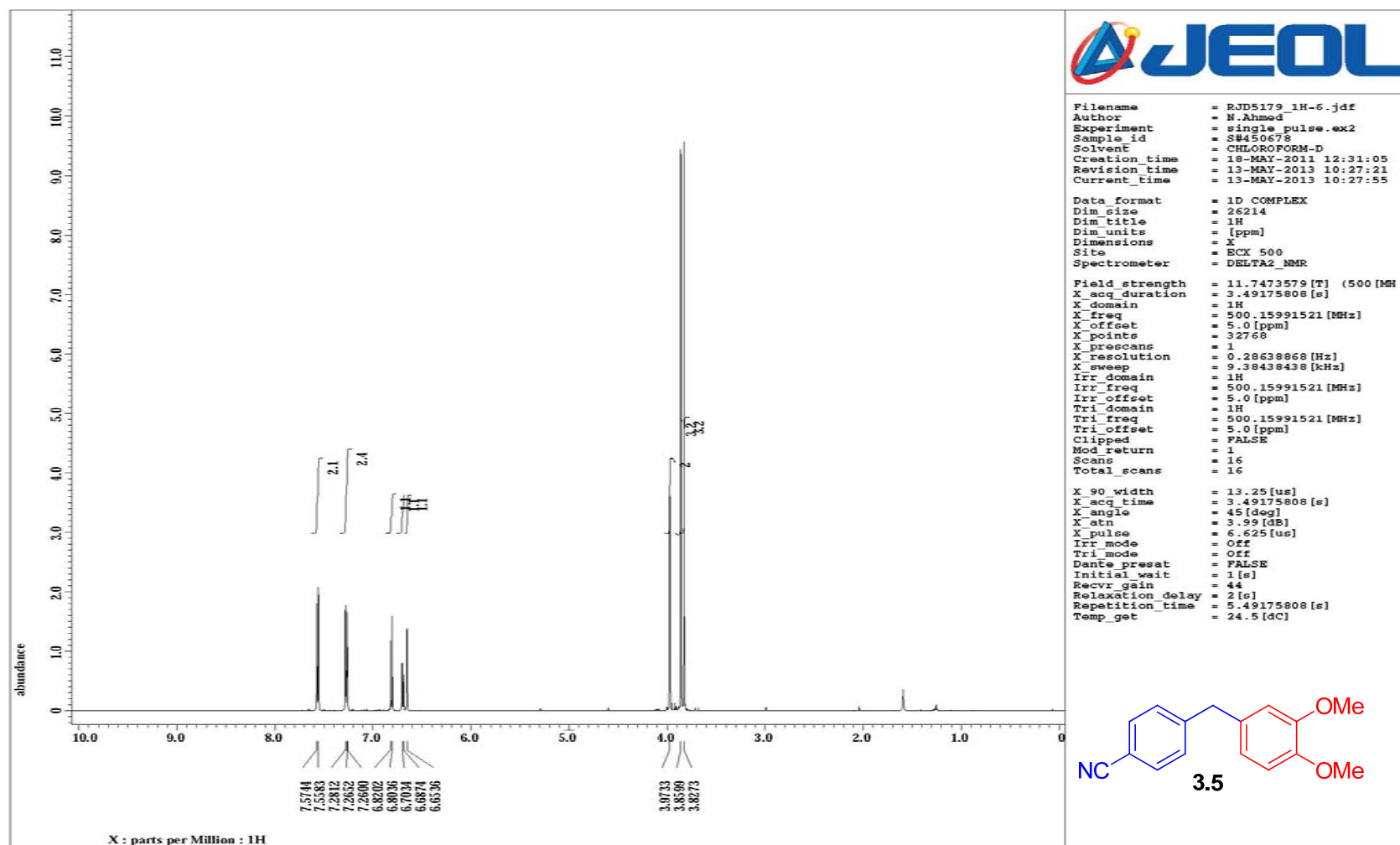
¹H NMR spectrum of 1-(4-(4-(allyloxy)benzyl)phenyl)ethanone (2.13)



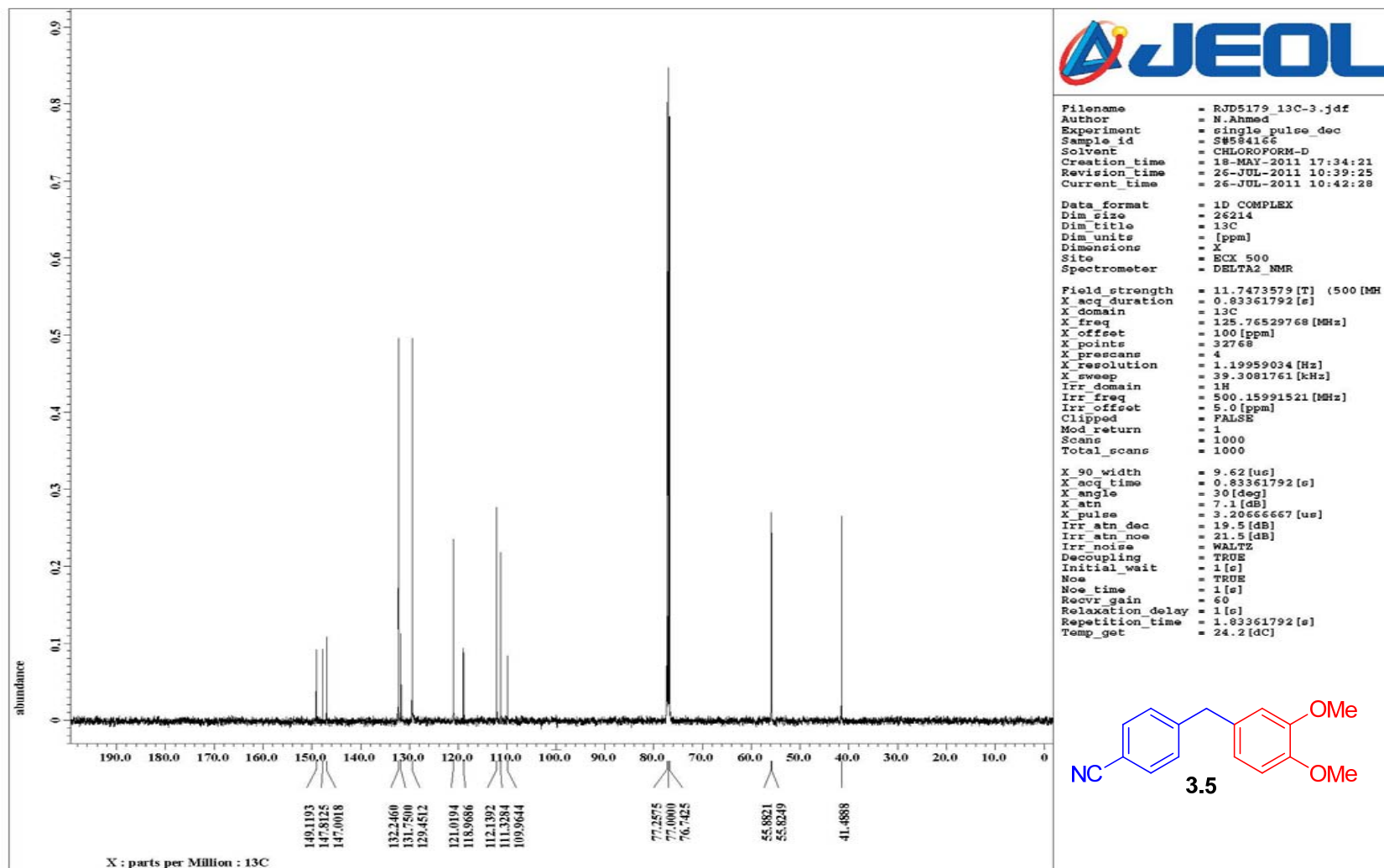
¹³C NMR spectrum of 1-(4-(4-(allyloxy)benzyl)phenyl)ethanone (2.13)



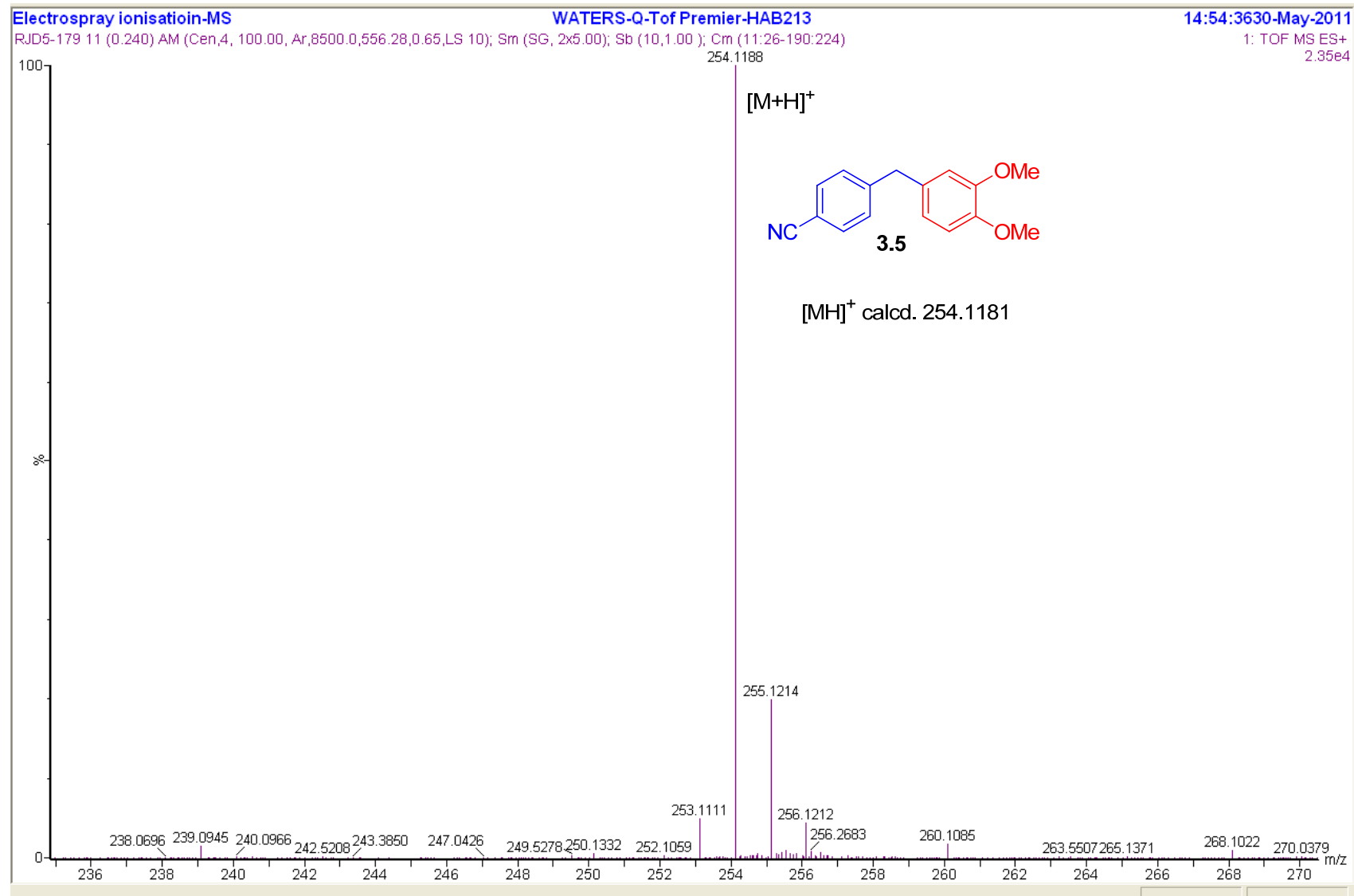
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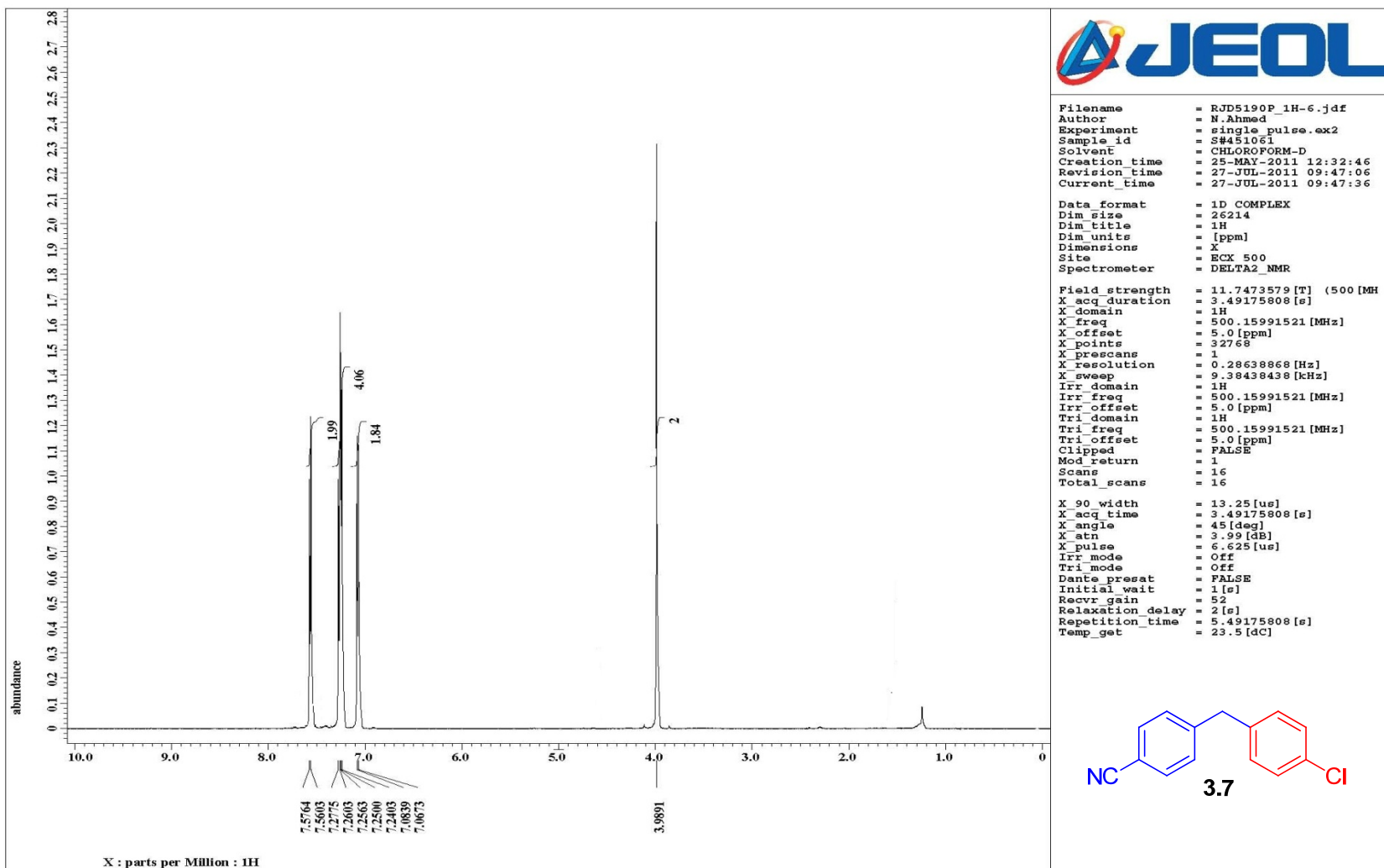
¹H NMR spectrum of 4-(3,4-dimethoxybenzyl)benzonitrile (3.5)



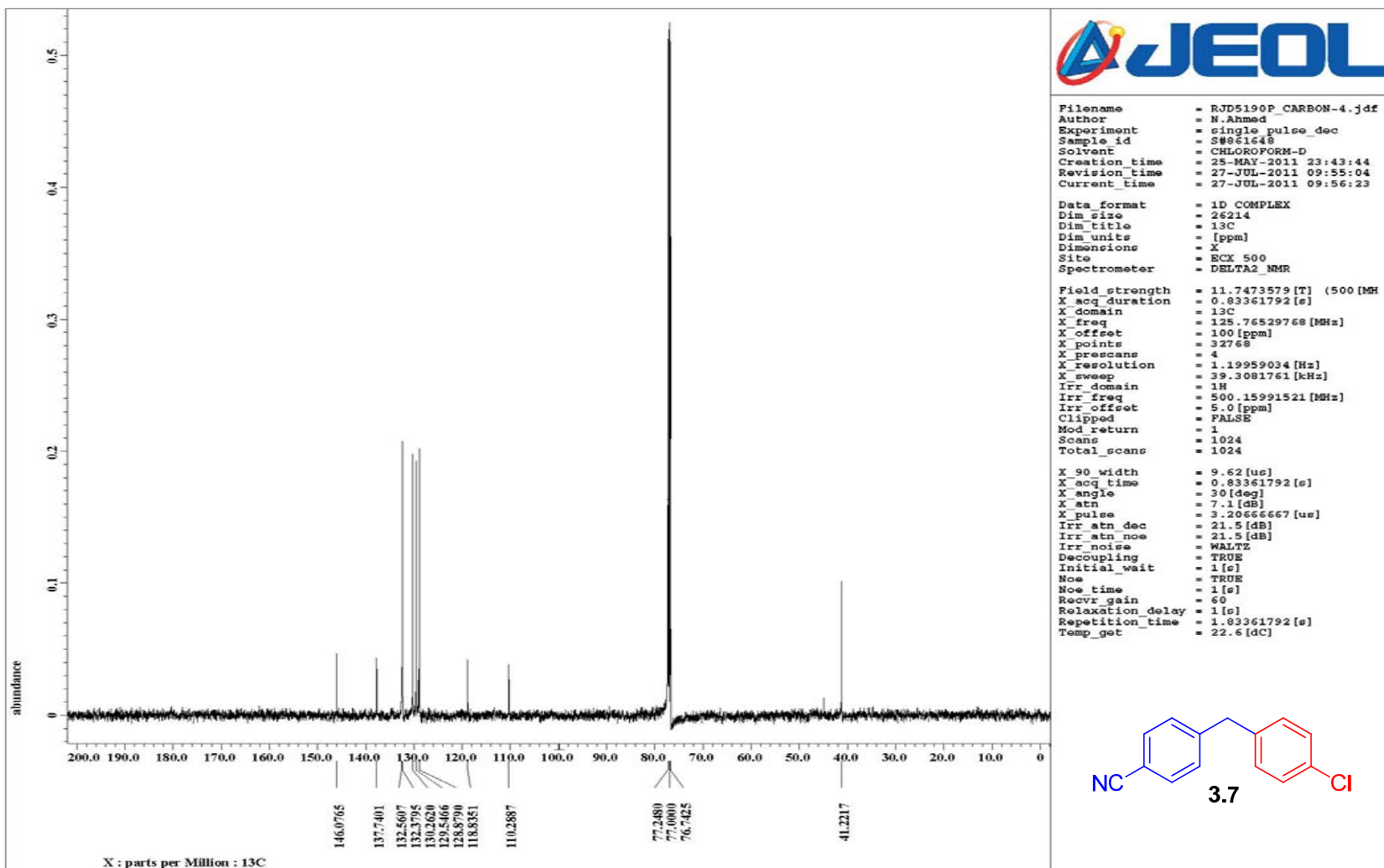
¹³C NMR spectrum of 4-(3,4-dimethoxybenzyl)benzonitrile (3.5)



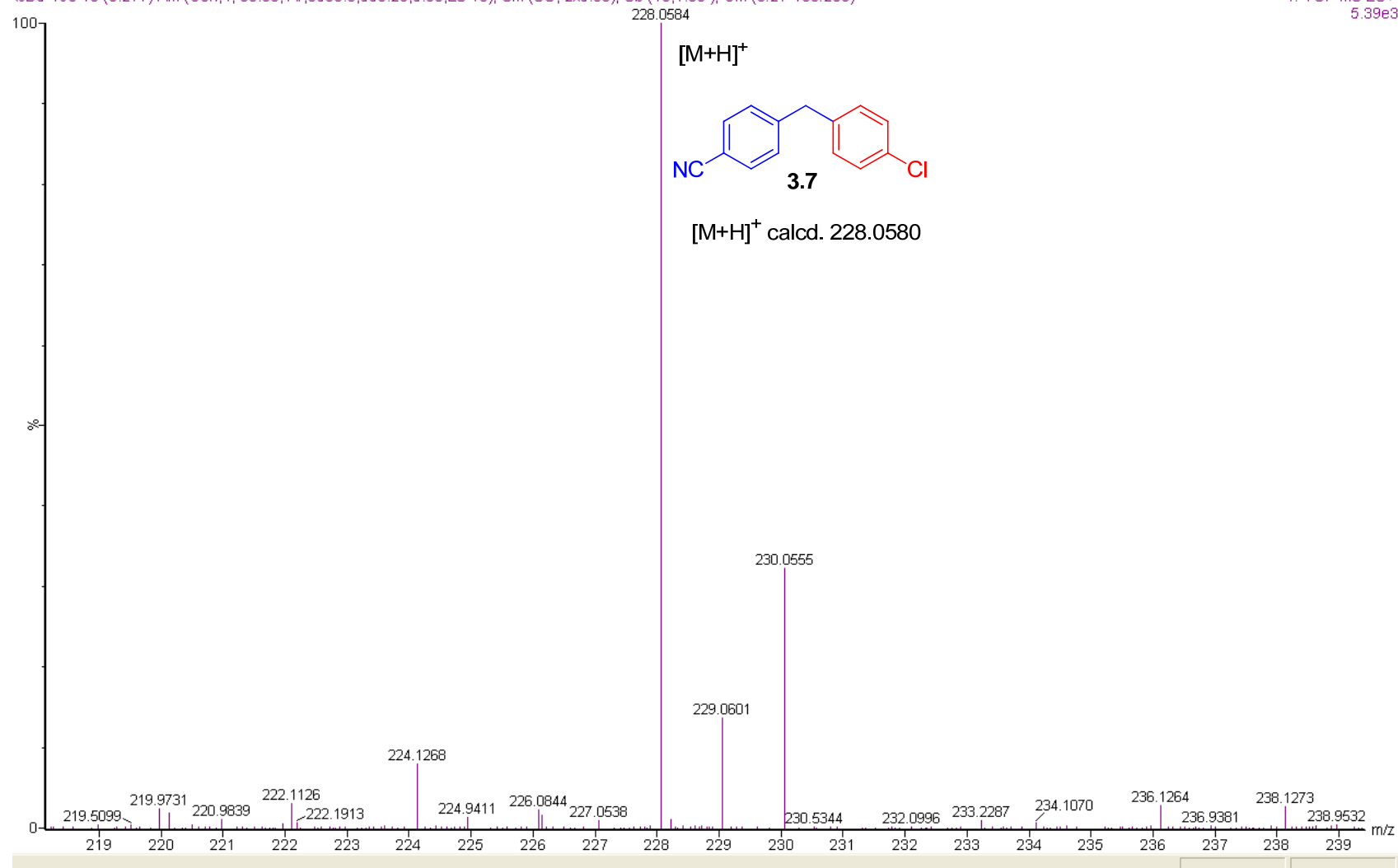
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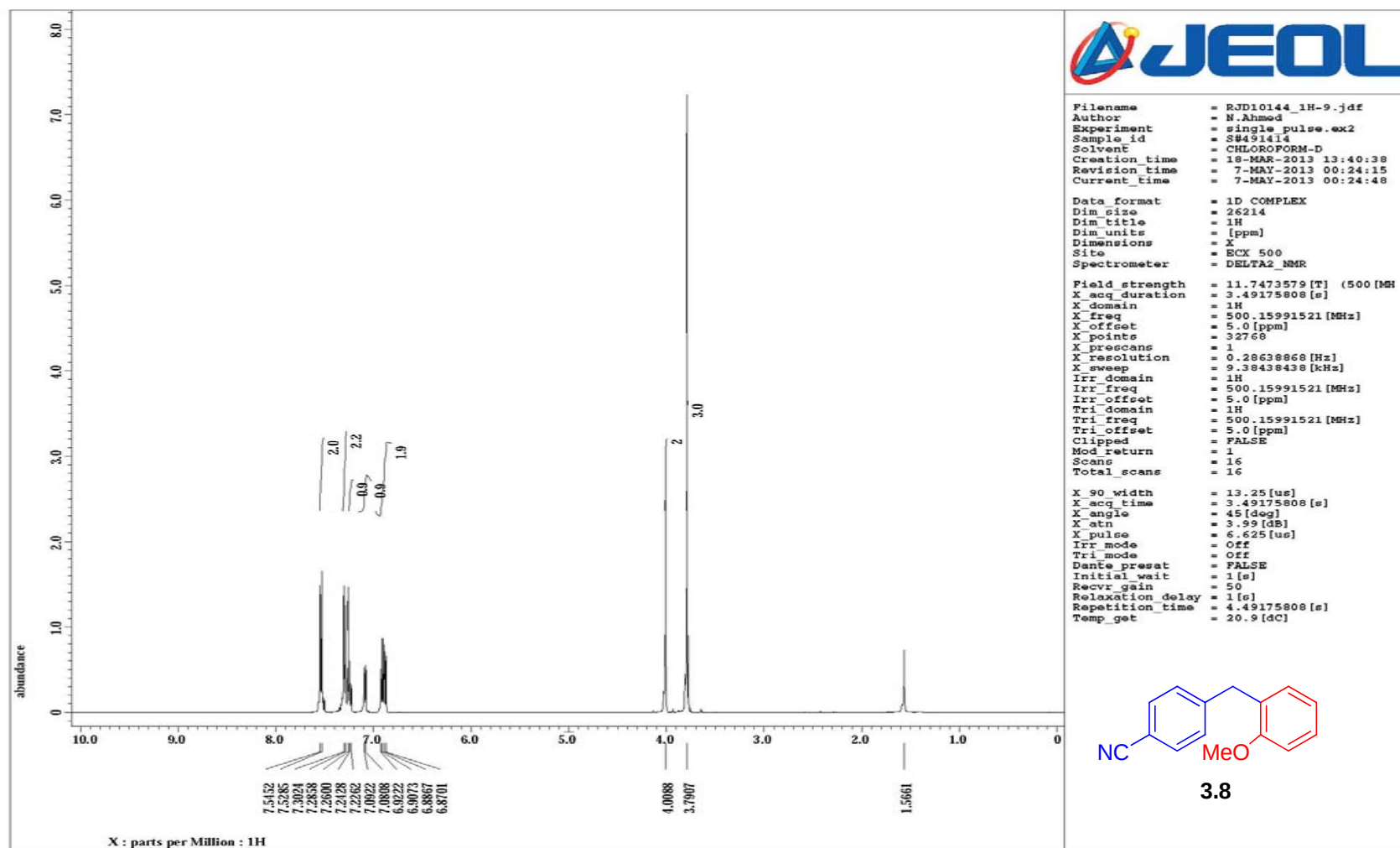


¹H NMR spectrum of 4-(4-chlorobenzyl)benzonitrile (3.7)

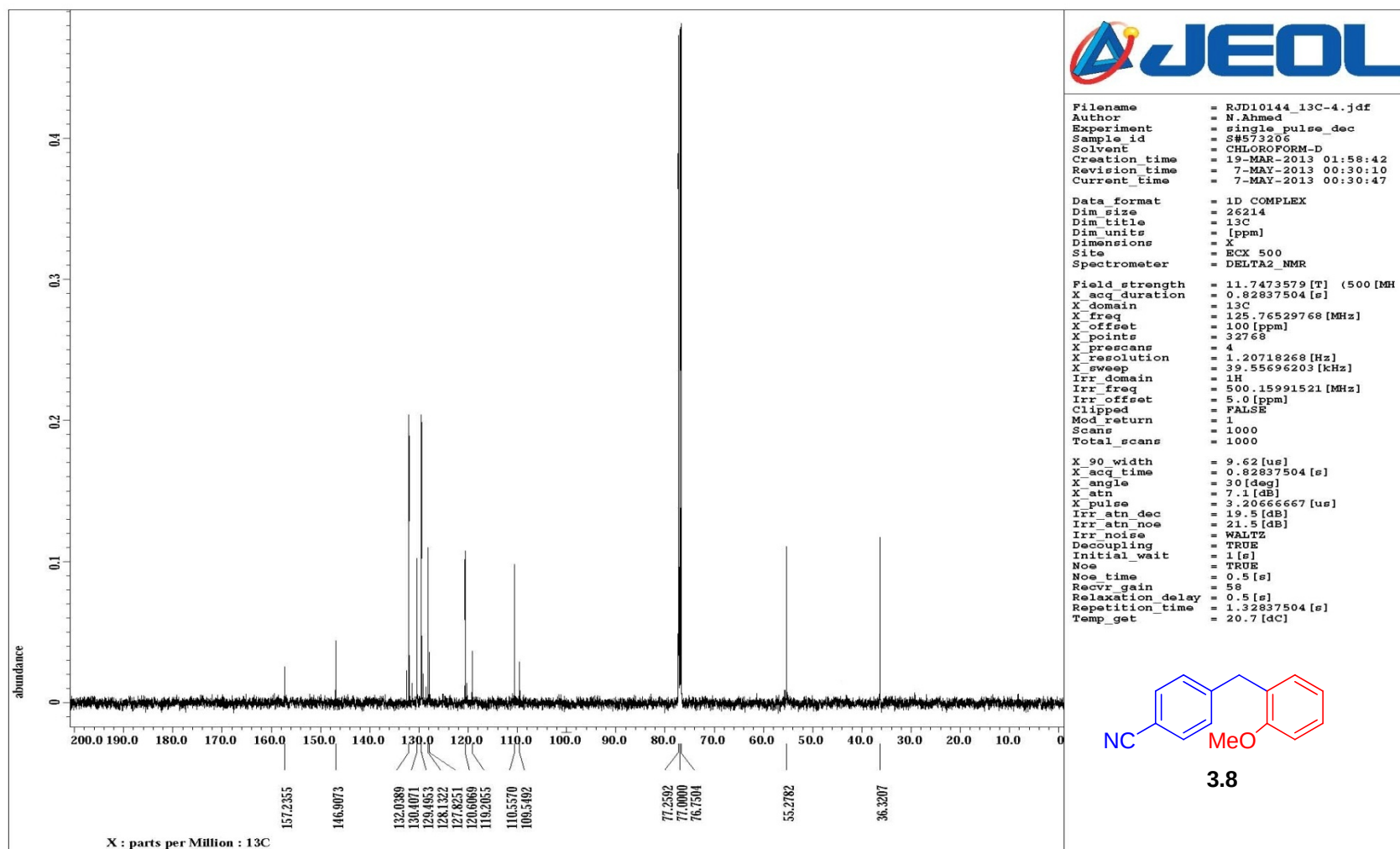


^{13}C NMR spectrum of 4-(4-chlorobenzyl)benzonitrile (3.7)

HRMS spectrum of 4-(4-chlorobenzyl)benzonitrile (**3.7**)

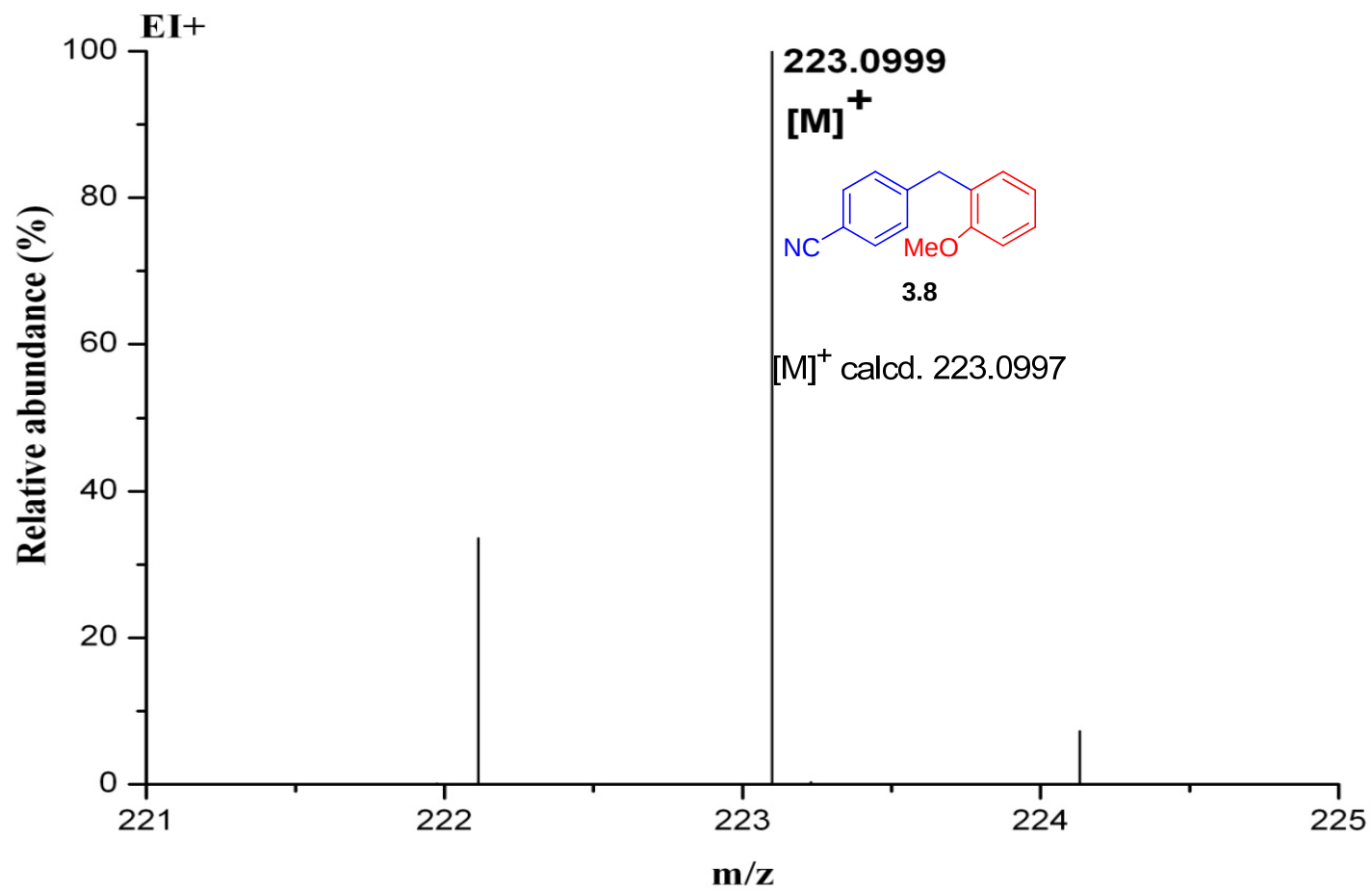


¹H NMR spectrum of . 4-(2-methoxybenzyl)benzonitrile (3.8)

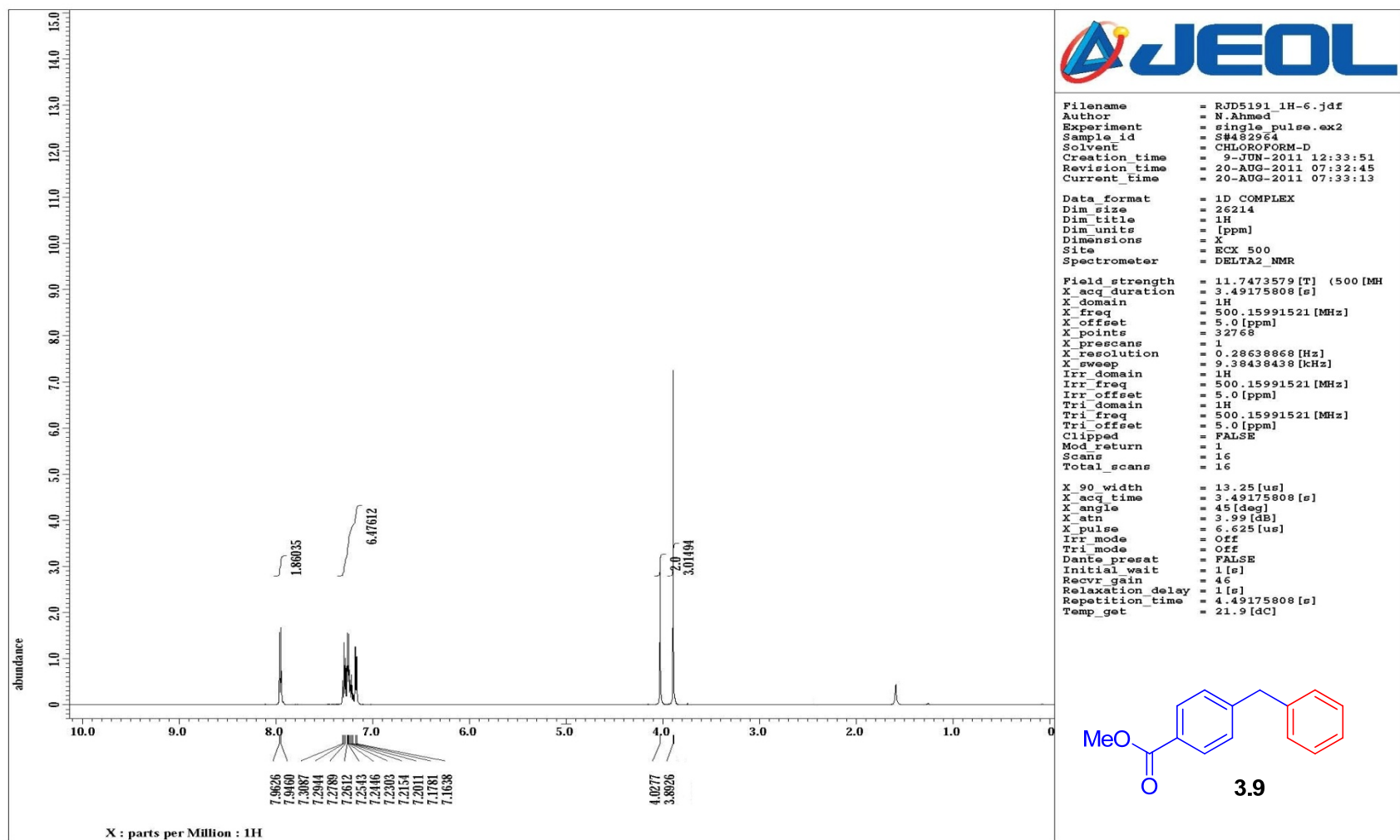


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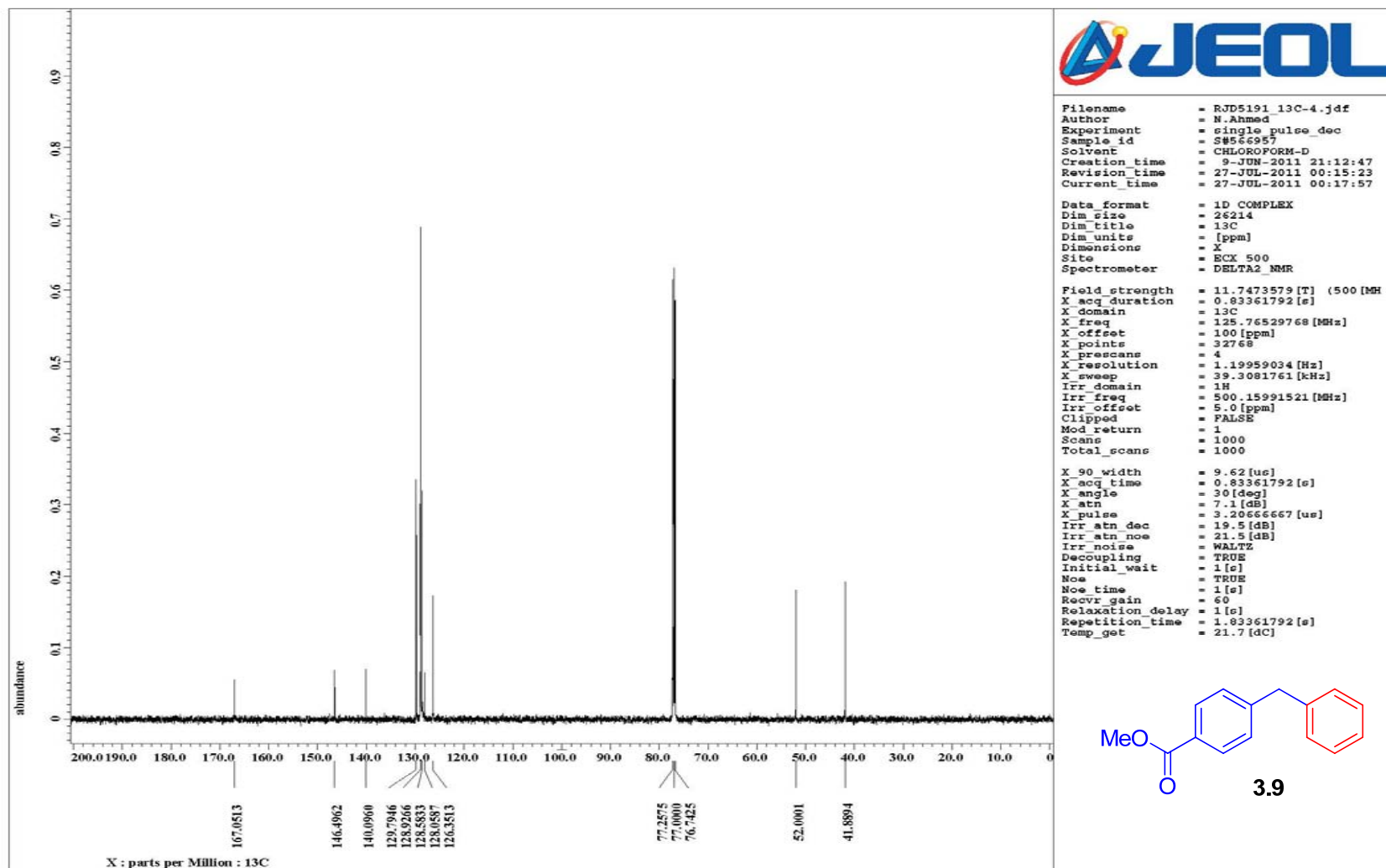
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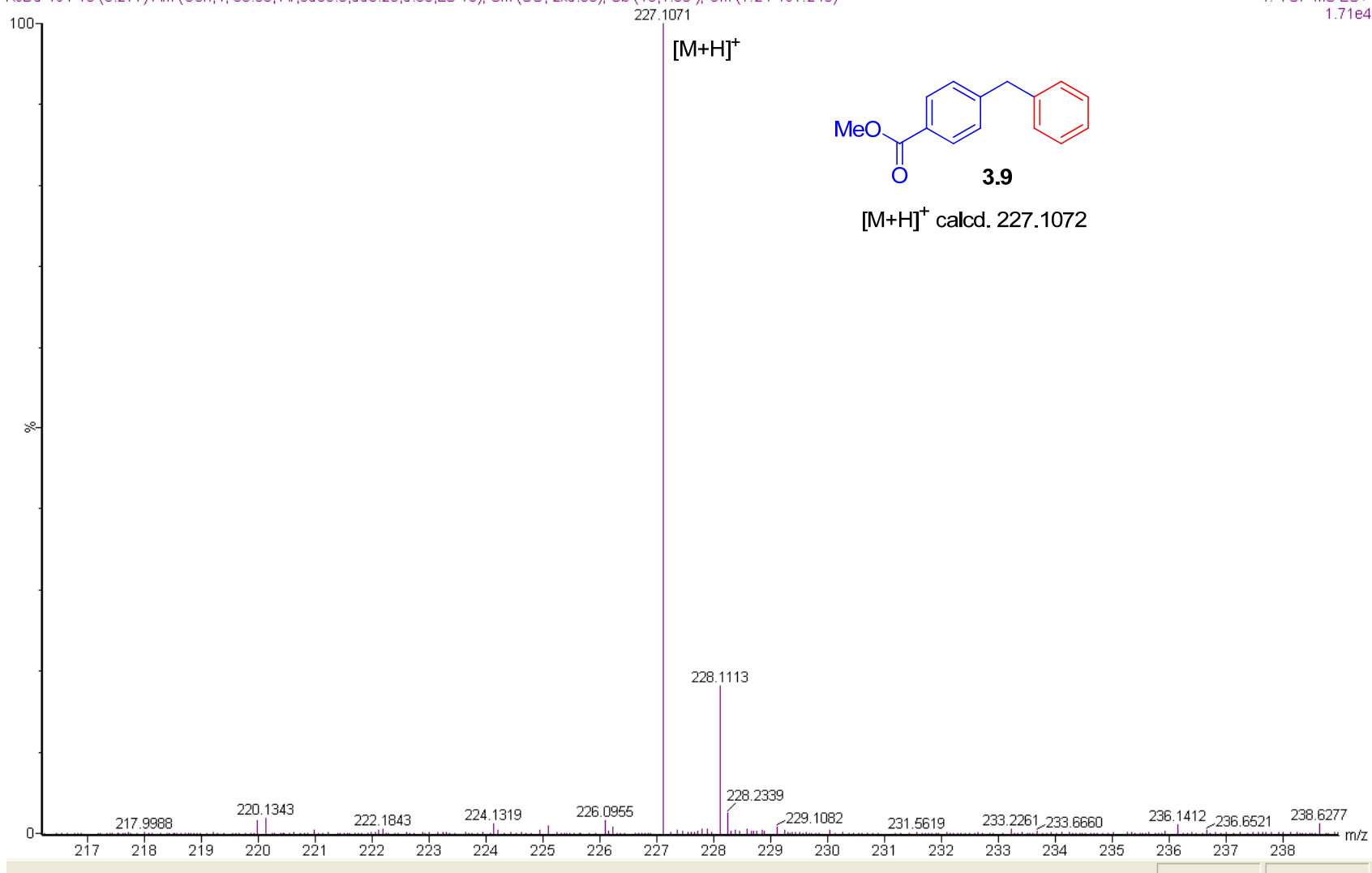
HRMS spectrum of . 4-(2-methoxybenzyl)benzonitrile (**3.8**)



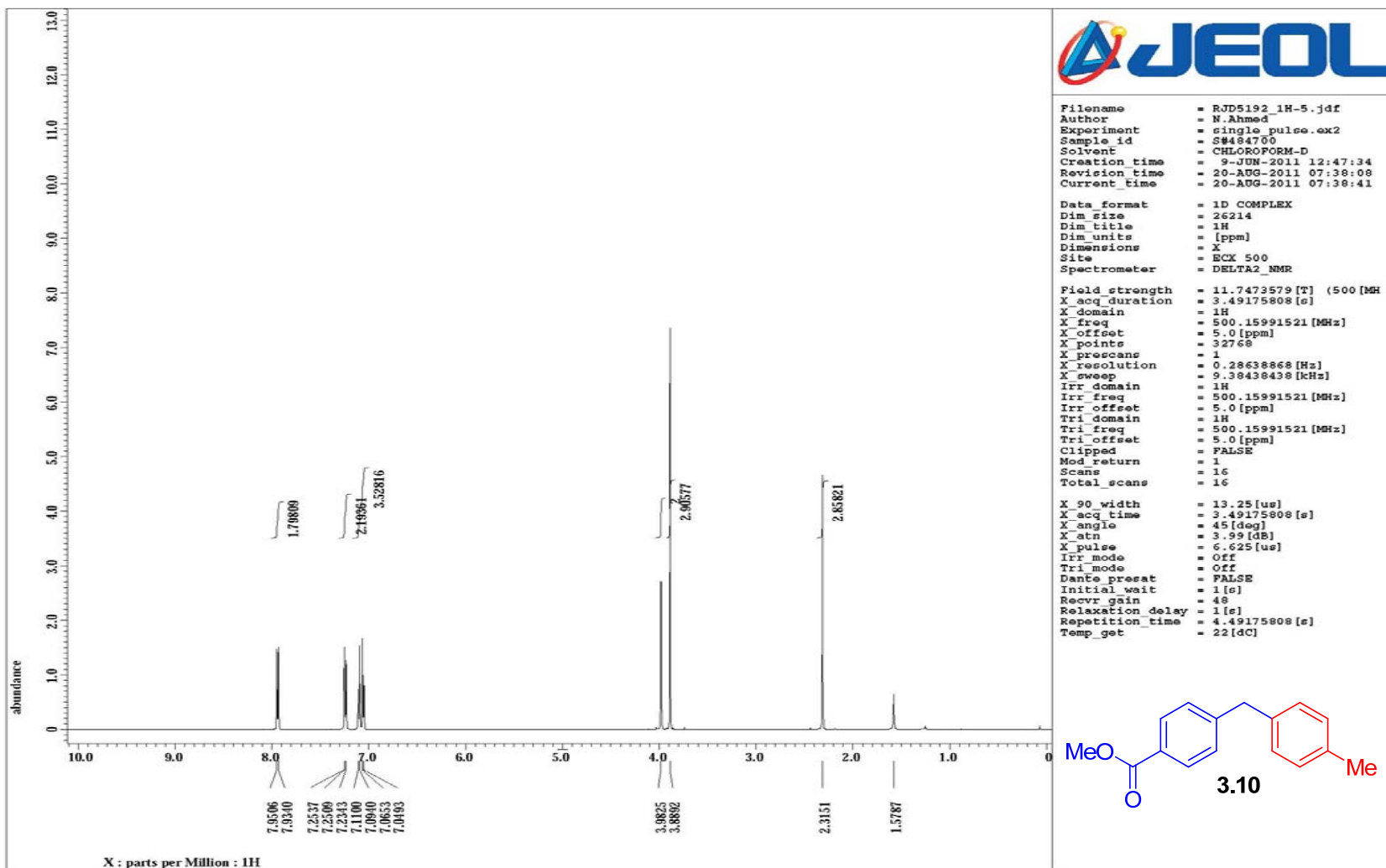
^1H NMR spectrum of Methyl 4-benzylbenzoate (3.9)



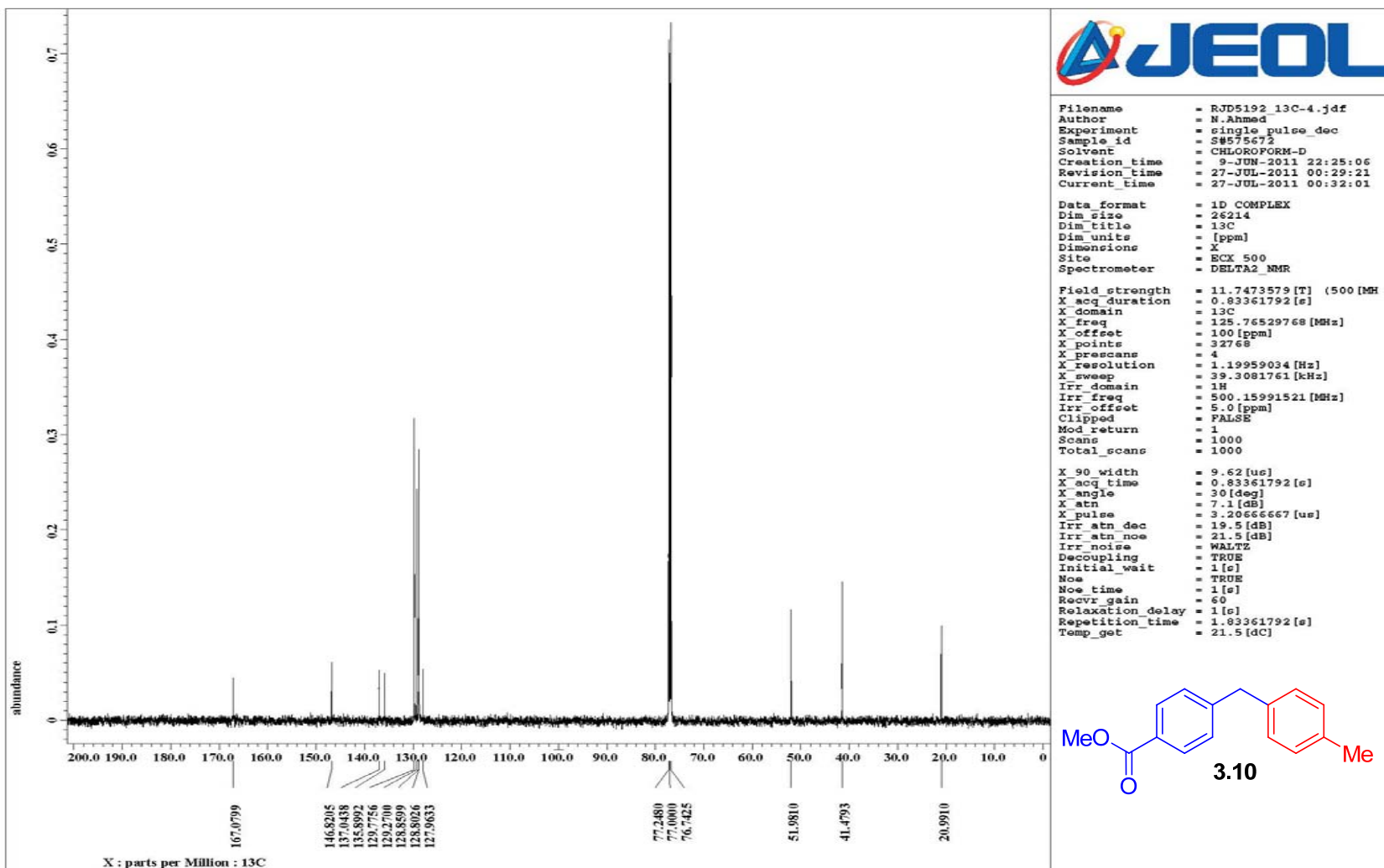
^{13}C NMR spectrum of Methyl 4-benzylbenzoate (3.9)



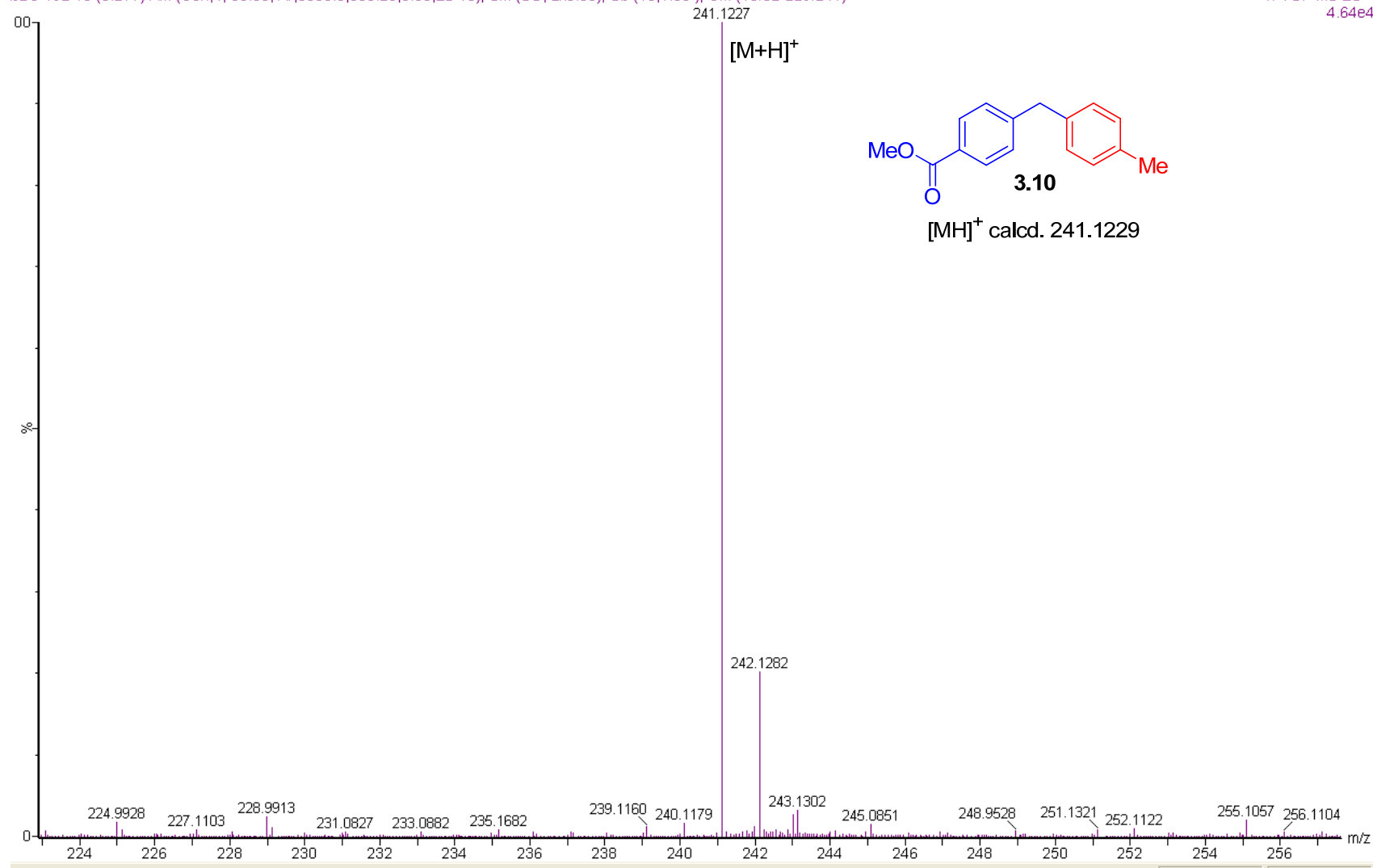
HRMS spectrum of Methyl 4-benzylbenzoate (3.9)



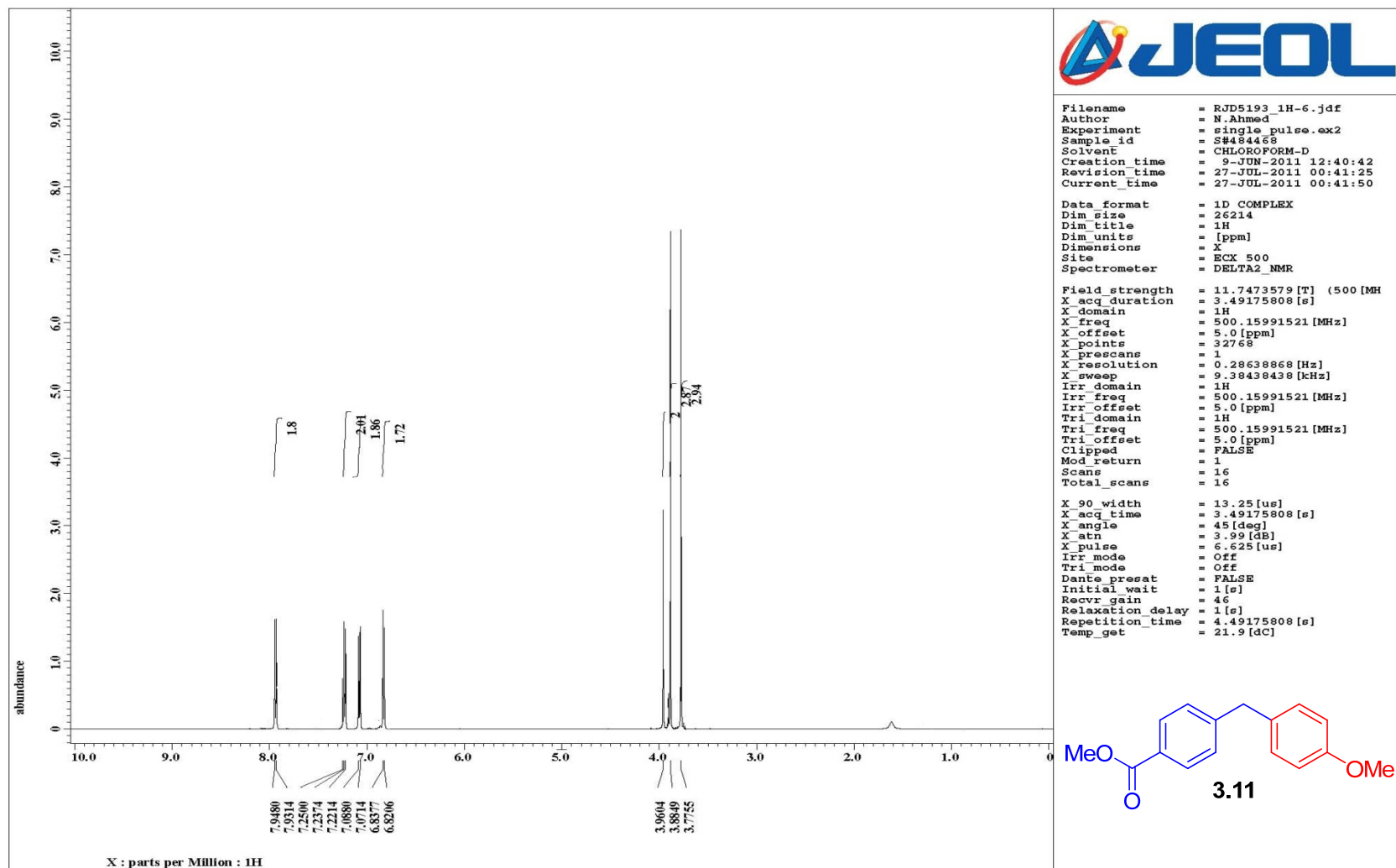
¹H NMR spectrum of Methyl 4-(4-methylbenzyl)benzoate (**3.10**)



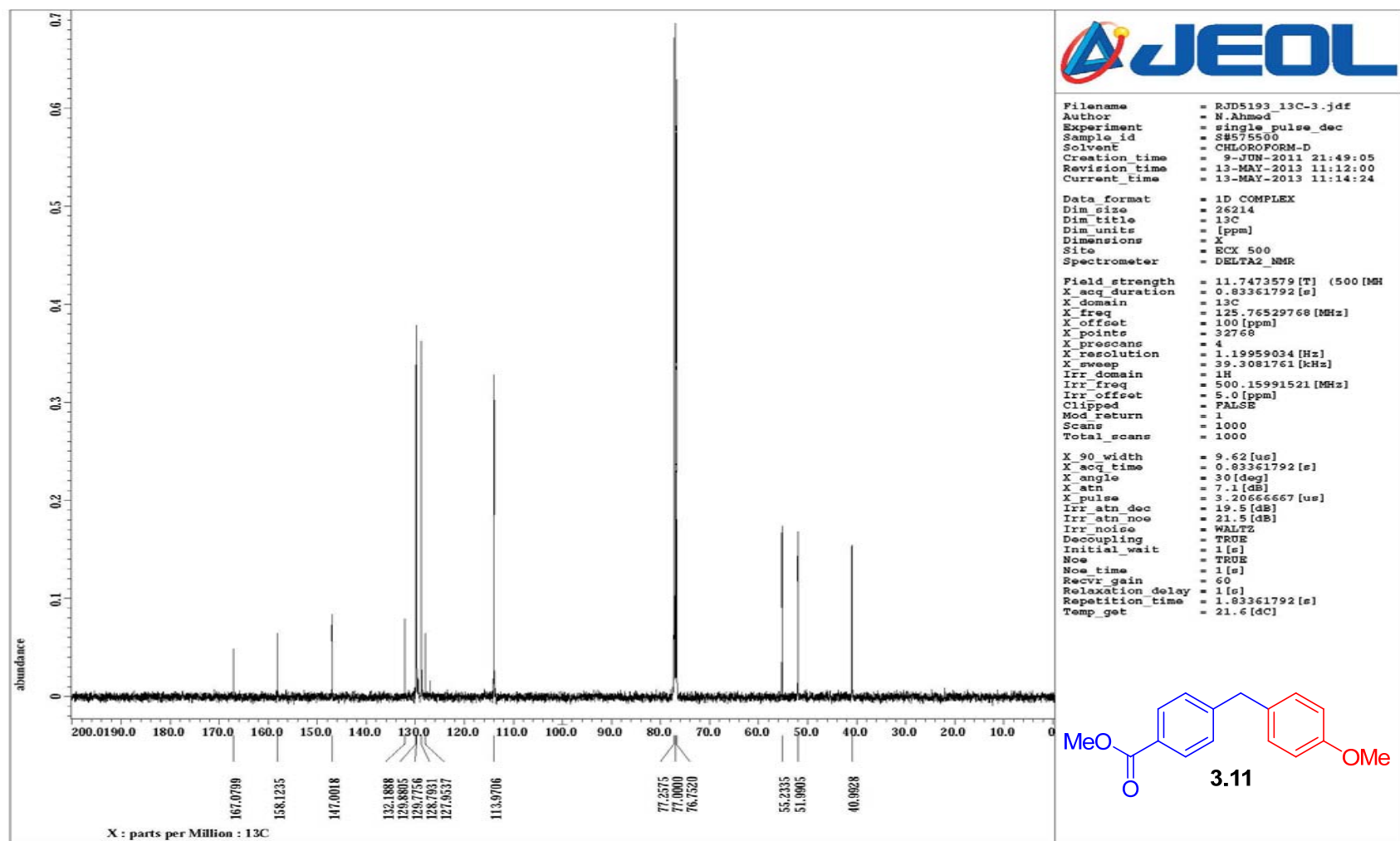
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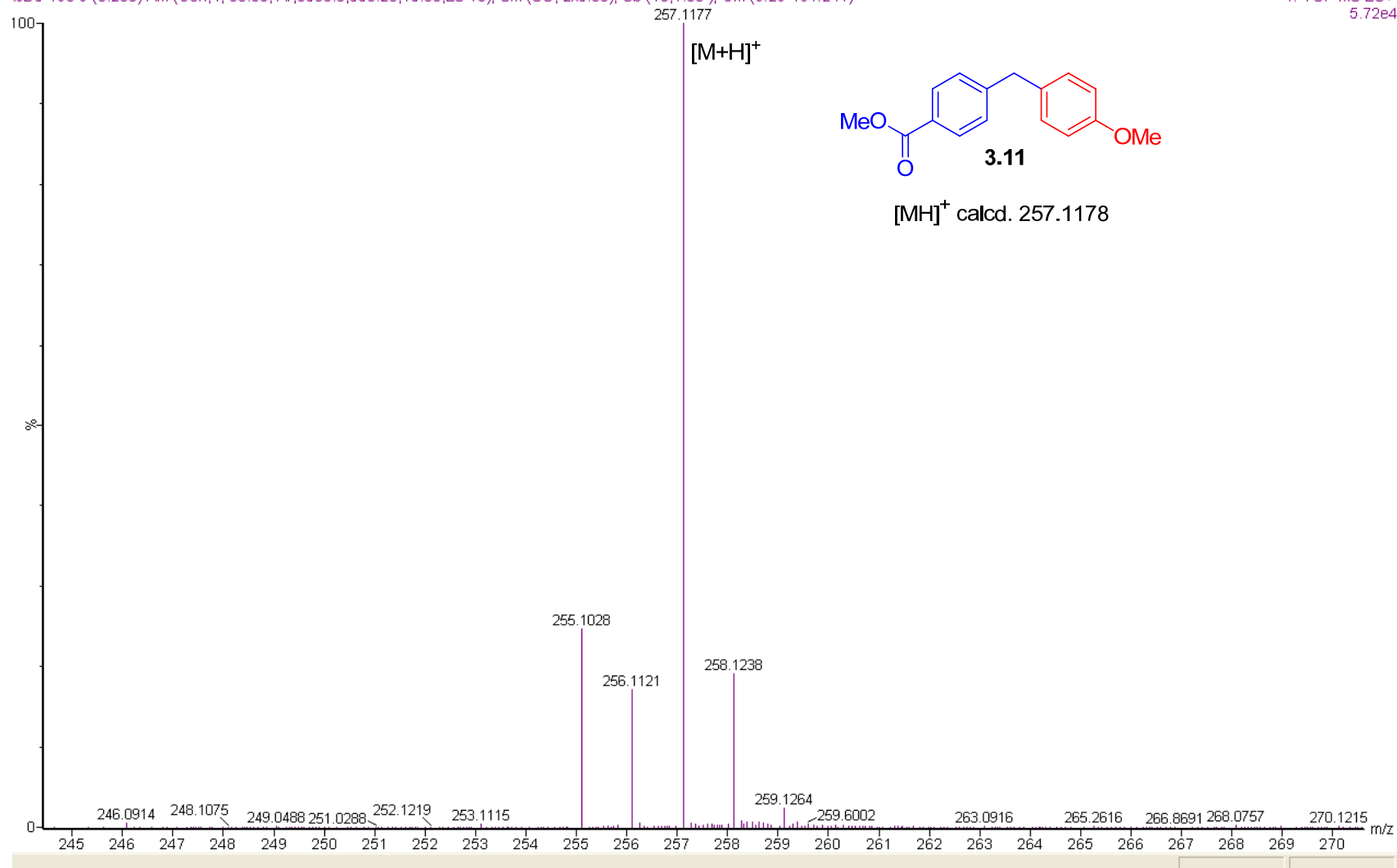
HRMS spectrum of Methyl 4-(4-methylbenzyl)benzoate (3.10)

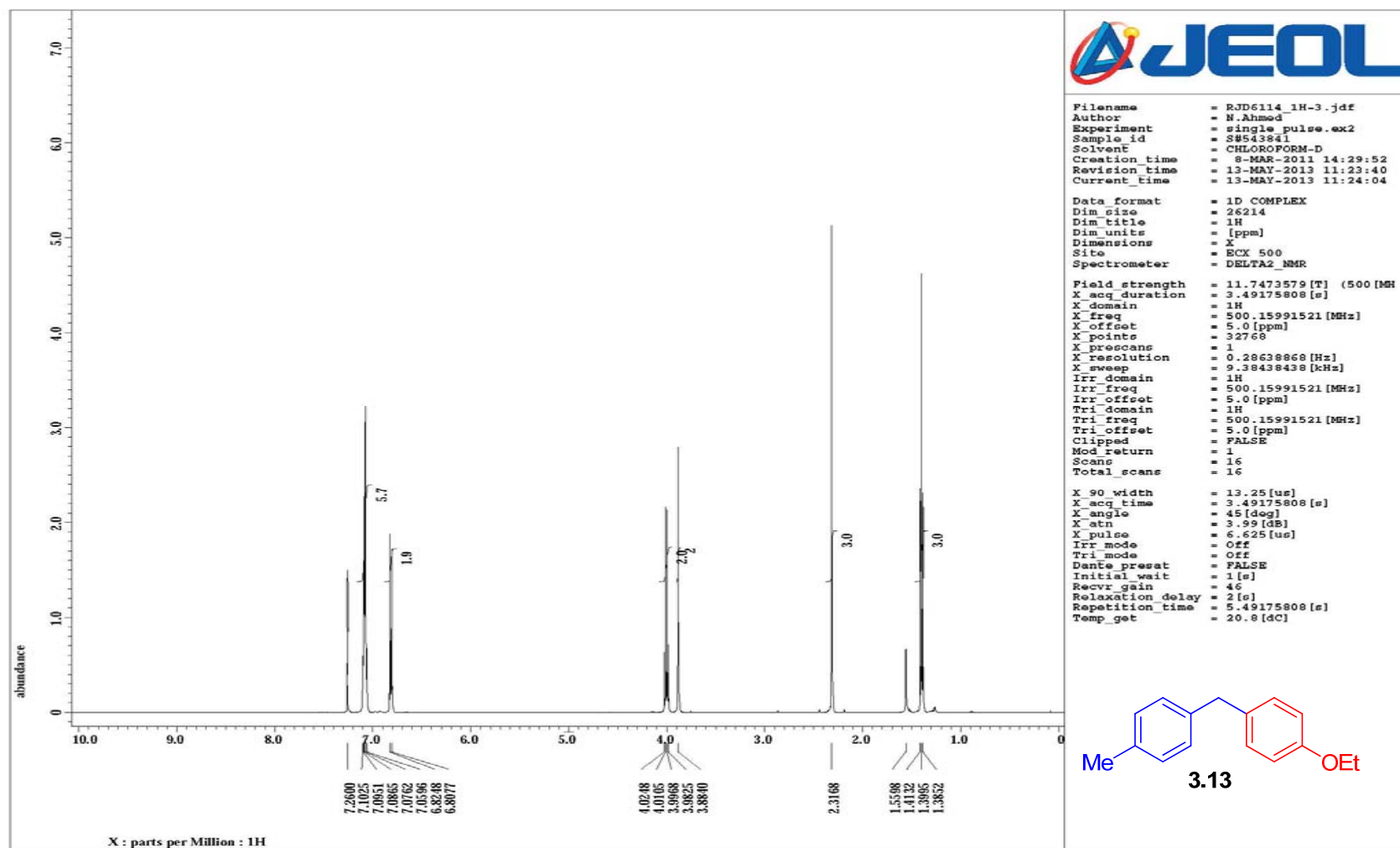


¹H NMR spectrum of Methyl 4-(4-methoxybenzyl)benzoate (3.11)

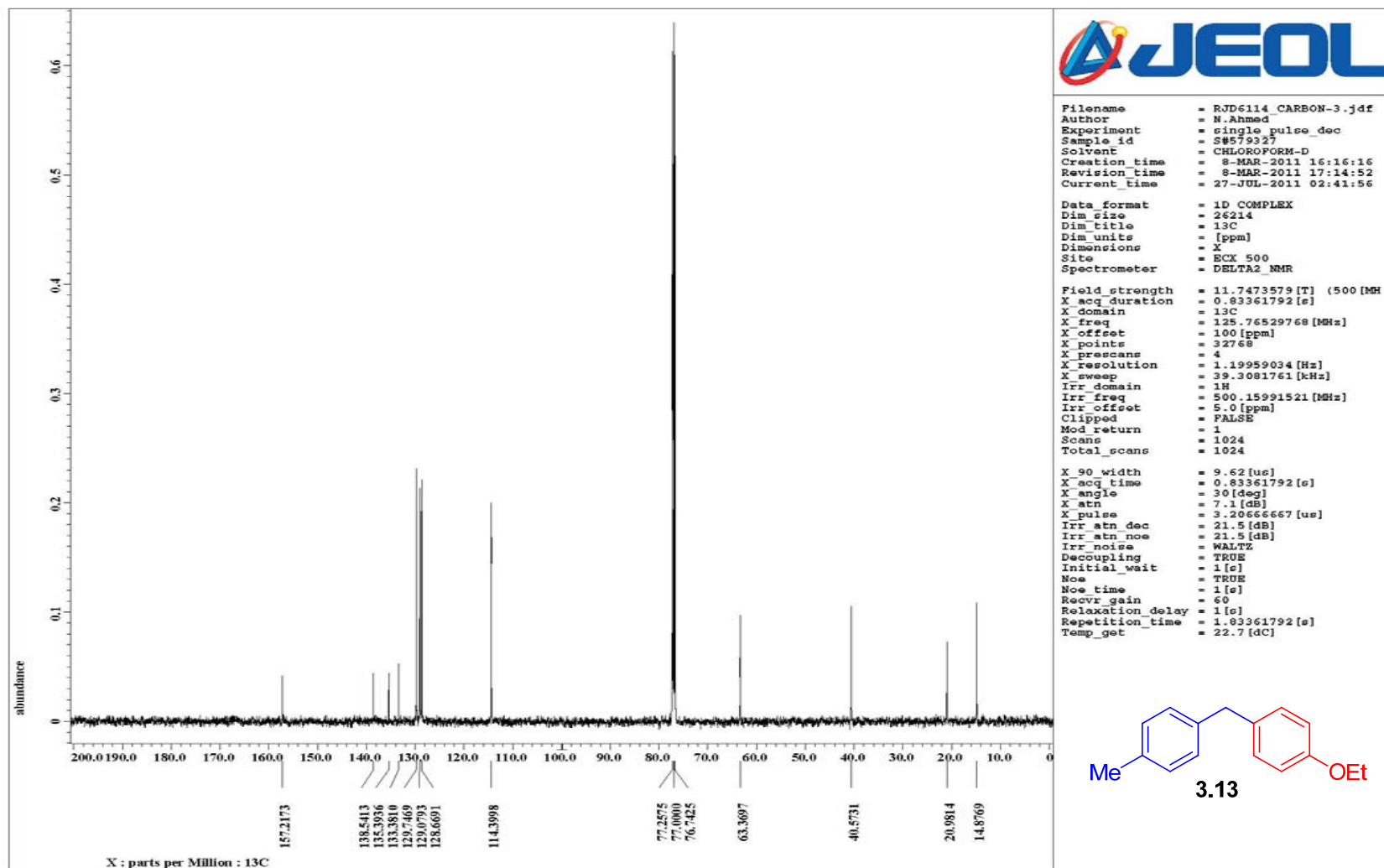


^{13}C NMR spectrum of Methyl 4-(4-methoxybenzyl)benzoate (**3.11**)

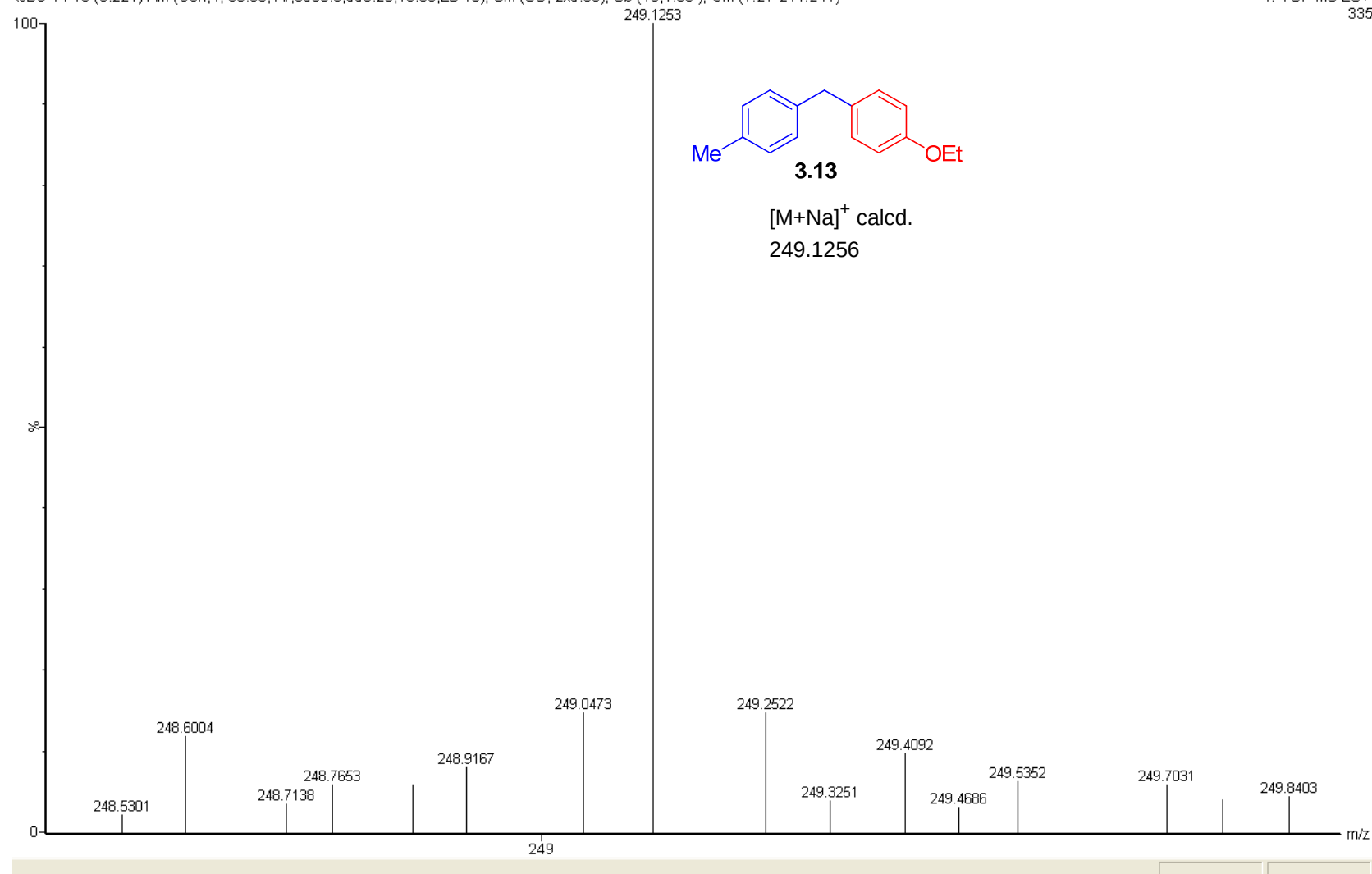
HRMS spectrum of Methyl 4-(4-methoxybenzyl)benzoate (**3.11**)



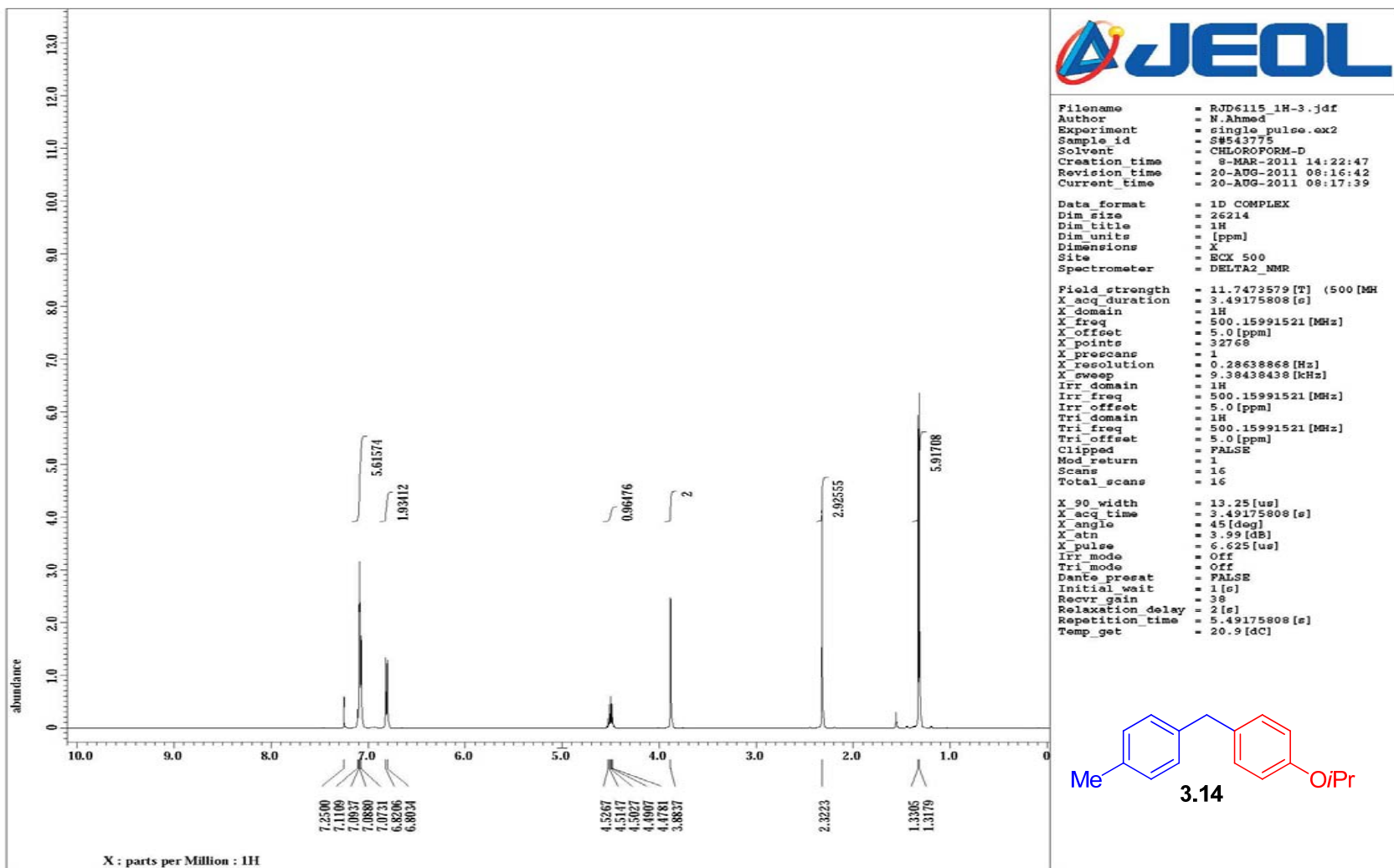
¹H NMR spectrum of 1-ethoxy-4-(4-methylbenzyl)benzene (3.13)



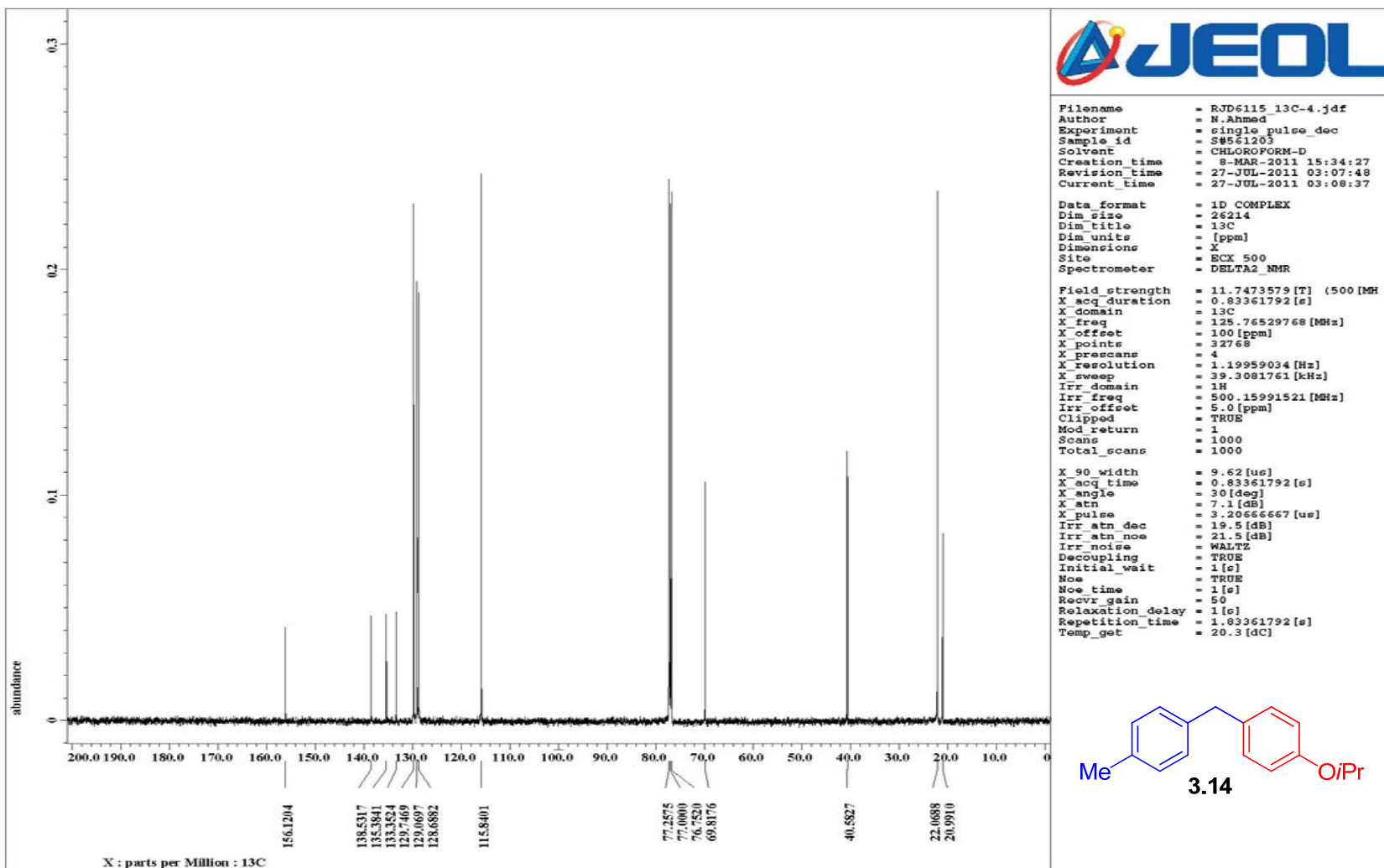
¹³C NMR spectrum of 1-ethoxy-4-(4-methylbenzyl)benzene (3.13)



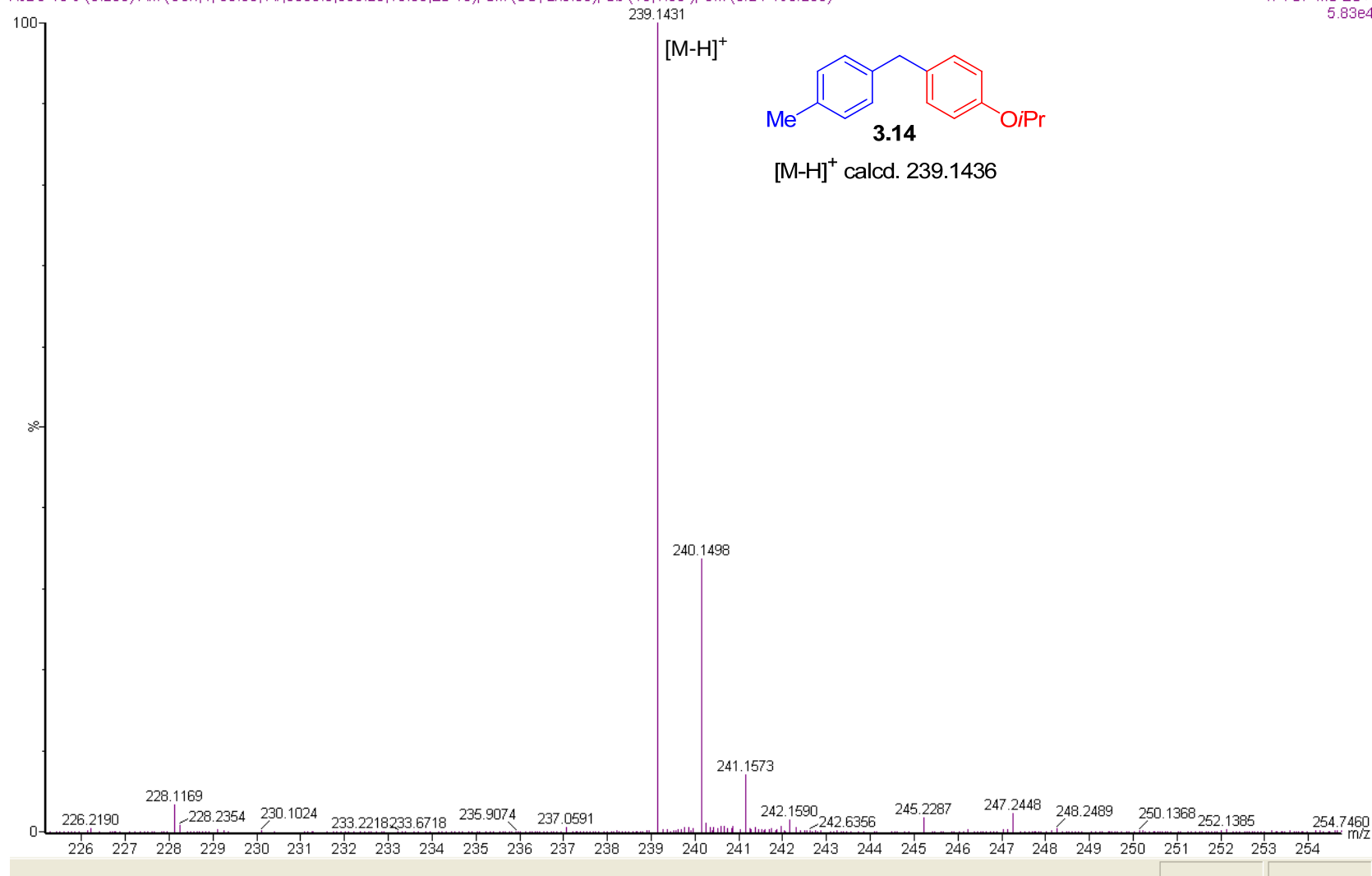
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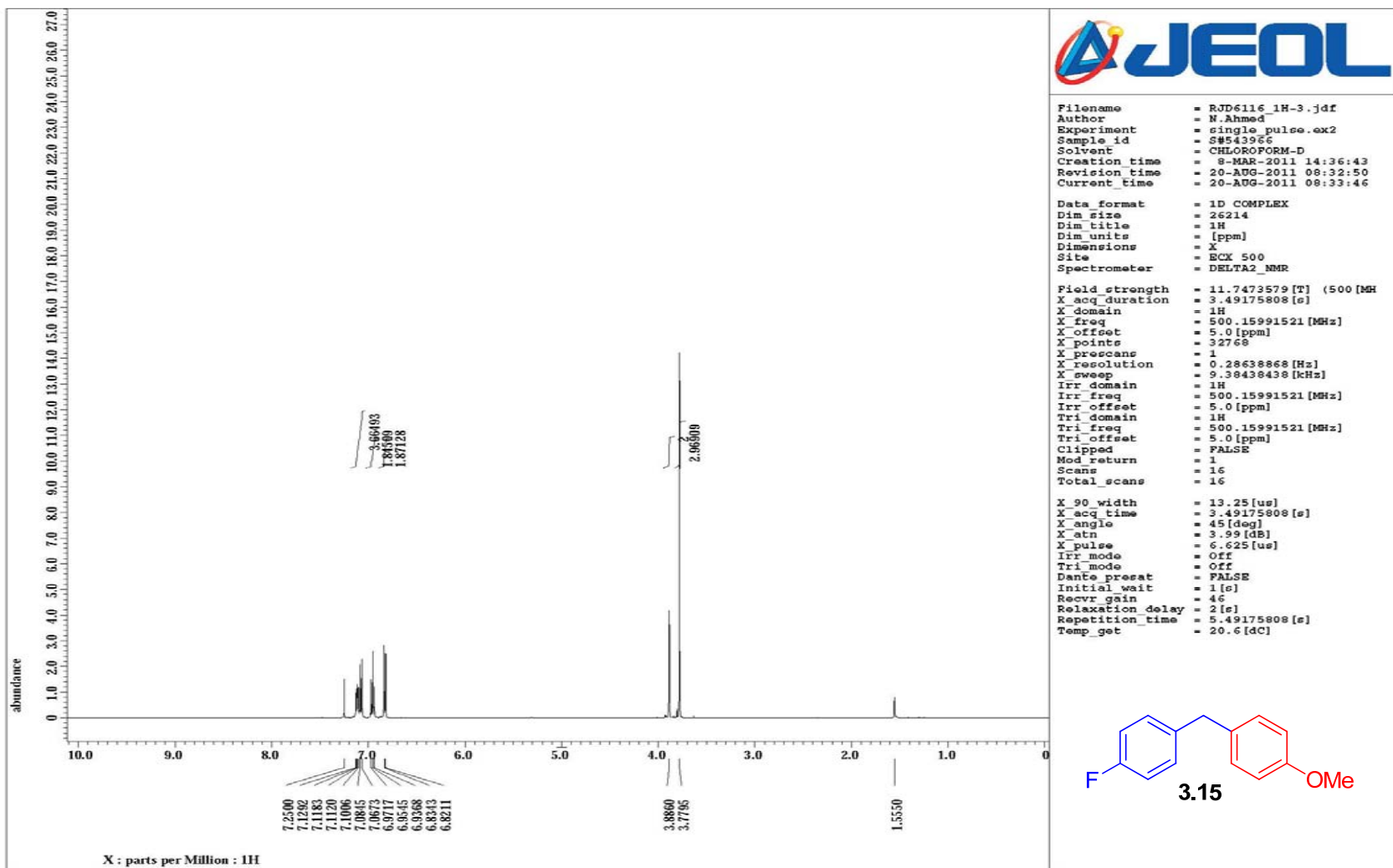


¹H NMR spectrum of 1-isopropoxy-4-(4-methylbenzyl)benzene (3.14)

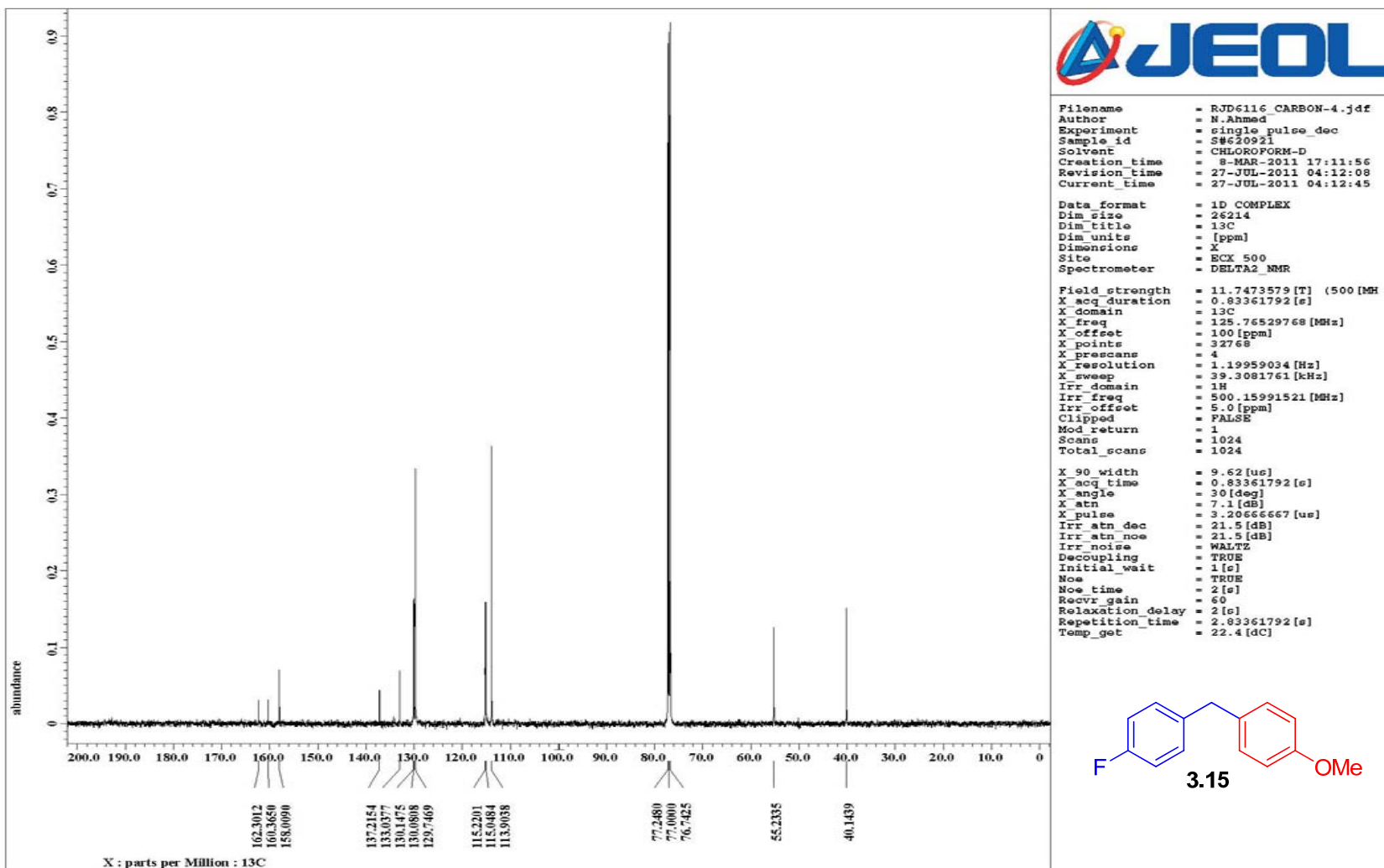


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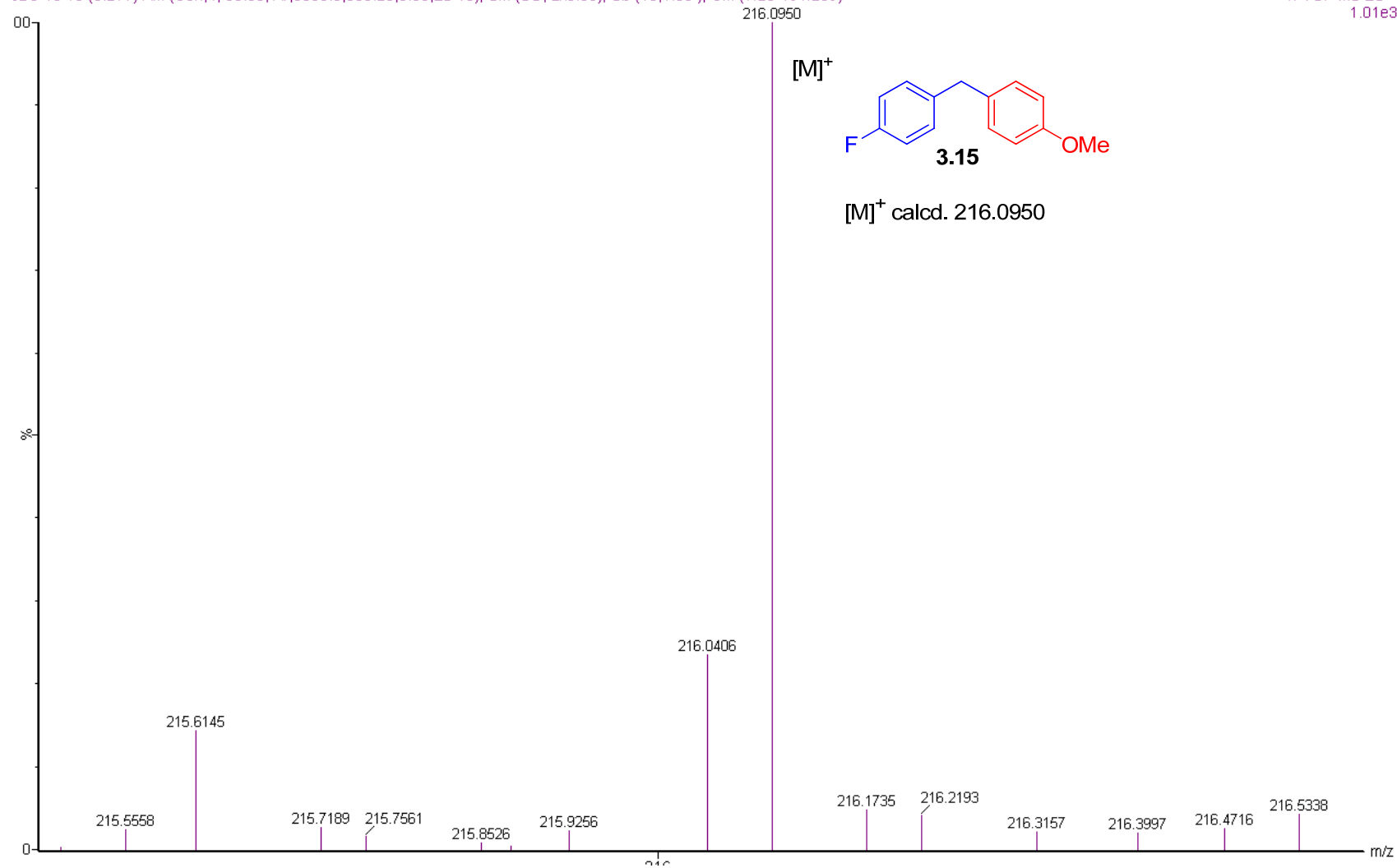
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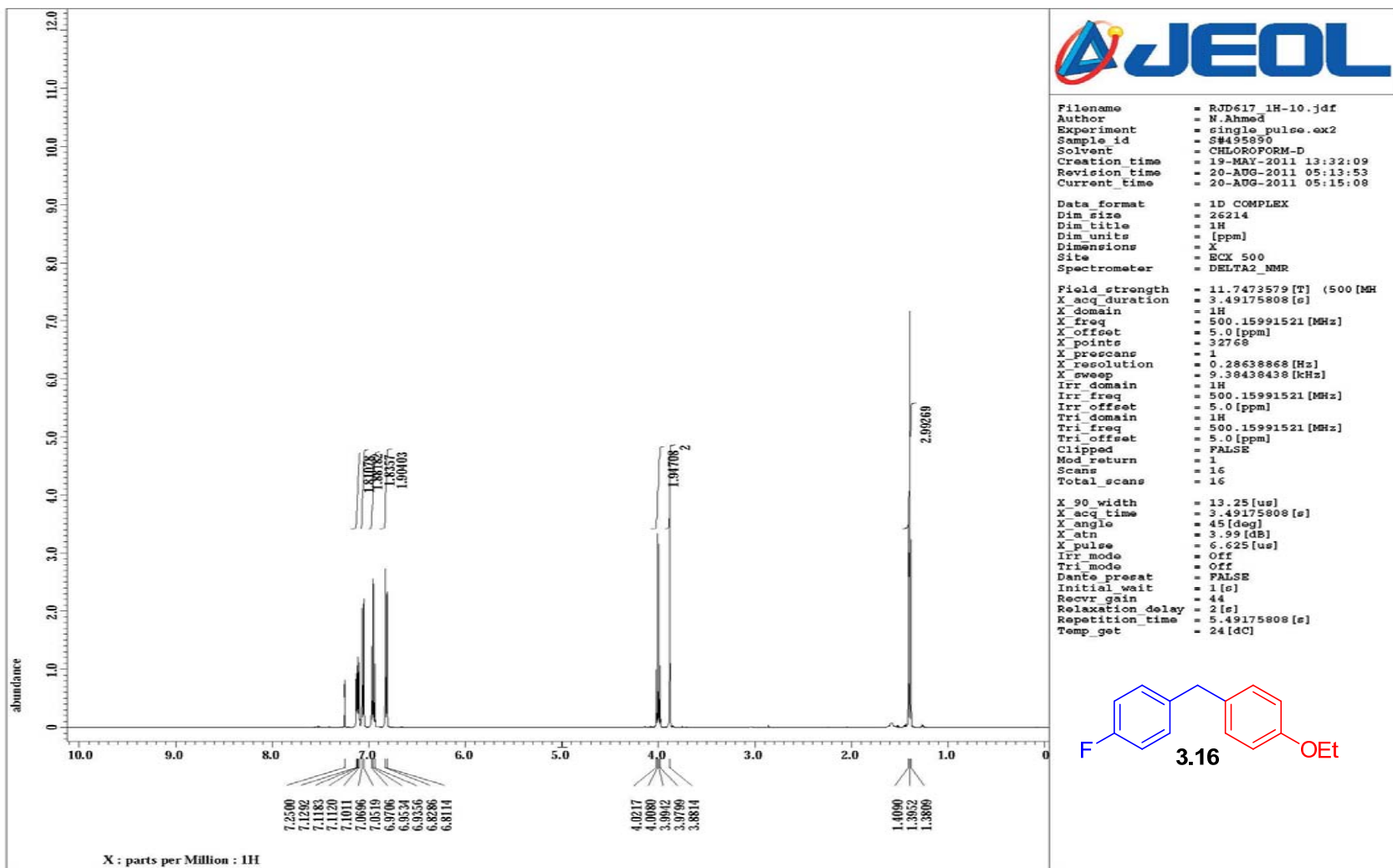


¹H NMR spectrum of 1-methoxy-4-(4-fluorobenzyl)benzene (3.15)

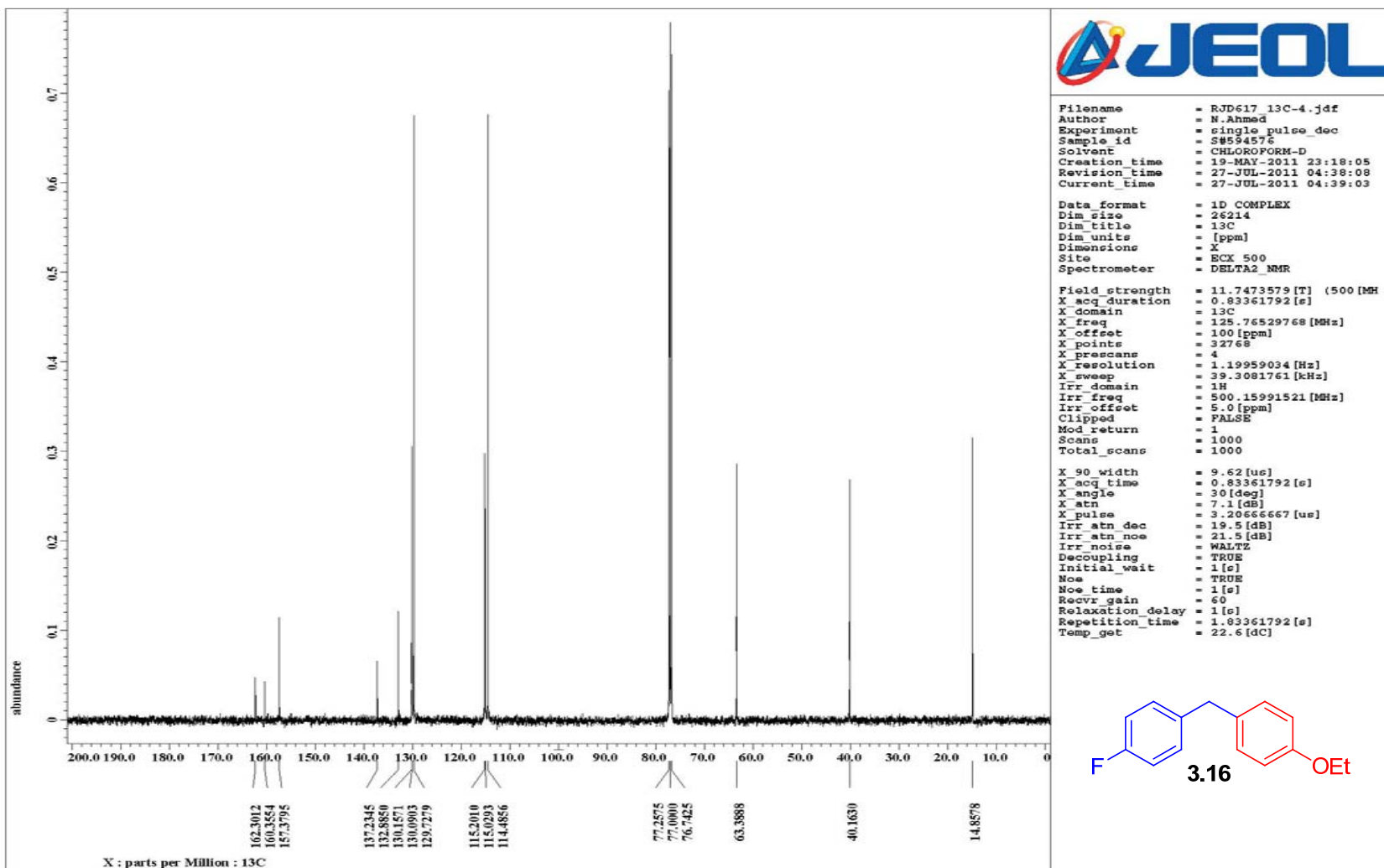


^{13}C NMR spectrum of 1-methoxy-4-(4-fluorobenzyl)benzene (3.15)

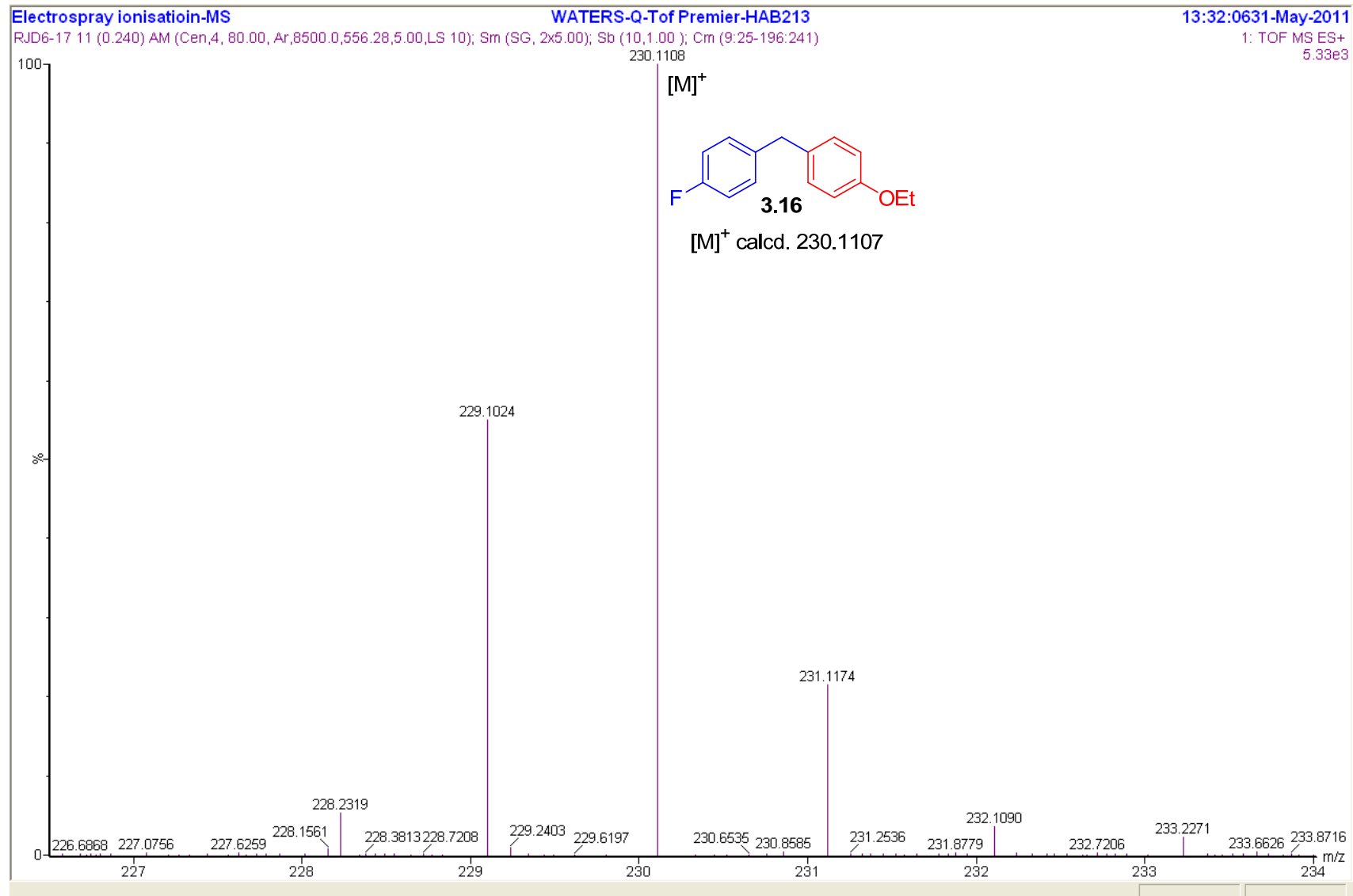
HRMS spectrum of 1-methoxy-4-(4-fluorobenzyl)benzene (**3.15**)



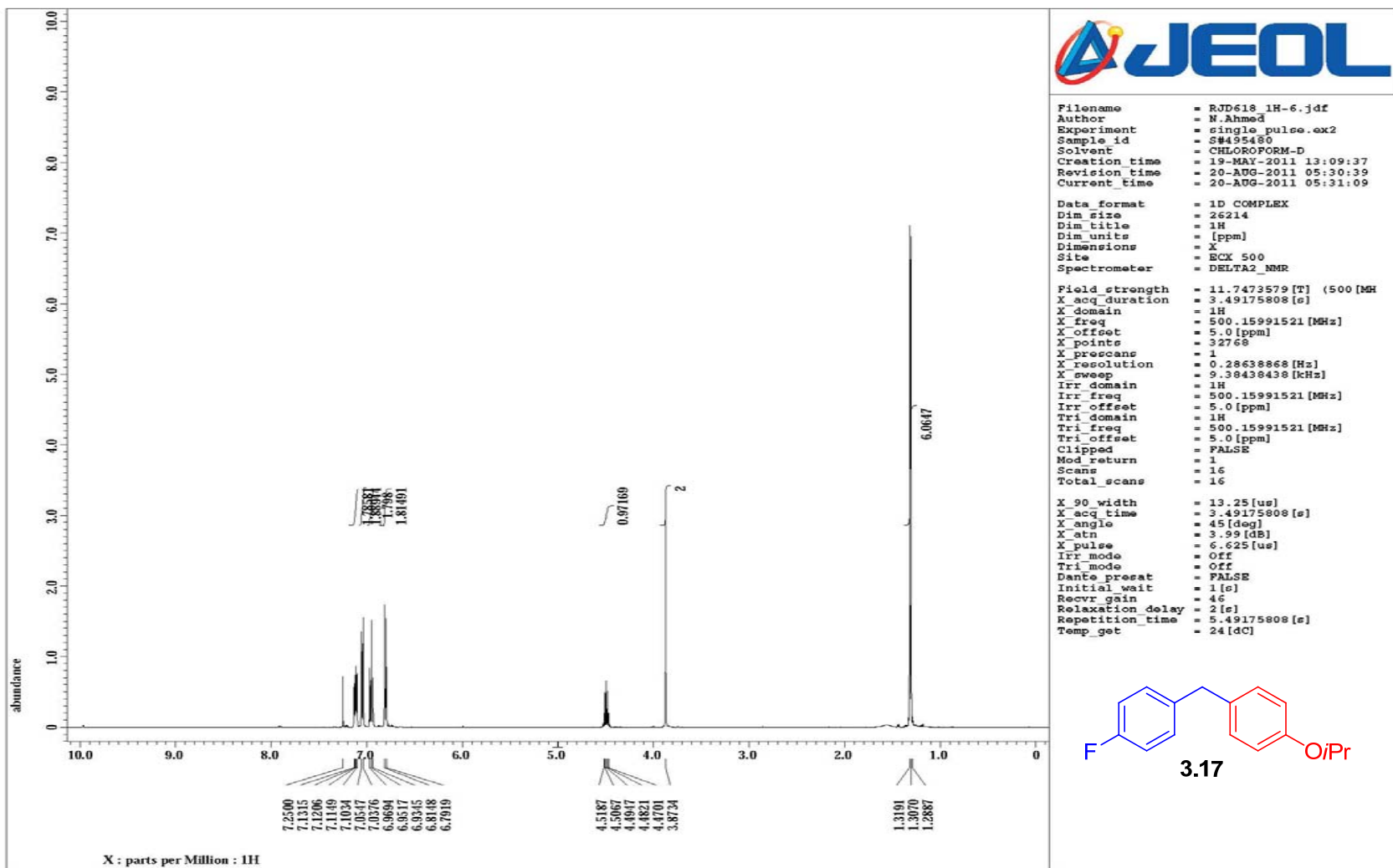
^1H NMR spectrum of 1-ethoxy-4-(4-fluorobenzyl)benzene (**3.16**)



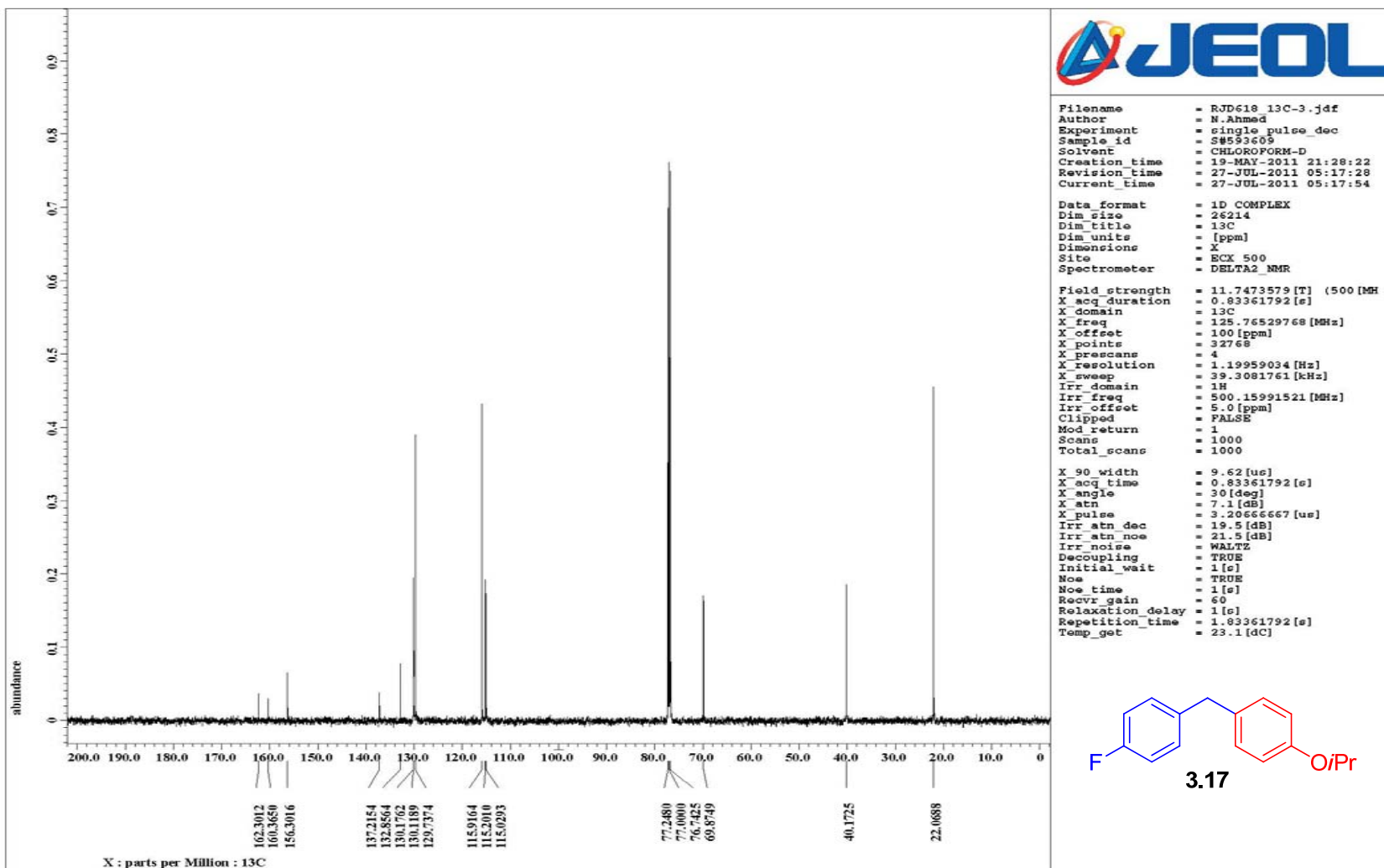
^{13}C NMR spectrum of 1-ethoxy-4-(4-fluorobenzyl)benzene (**3.16**)



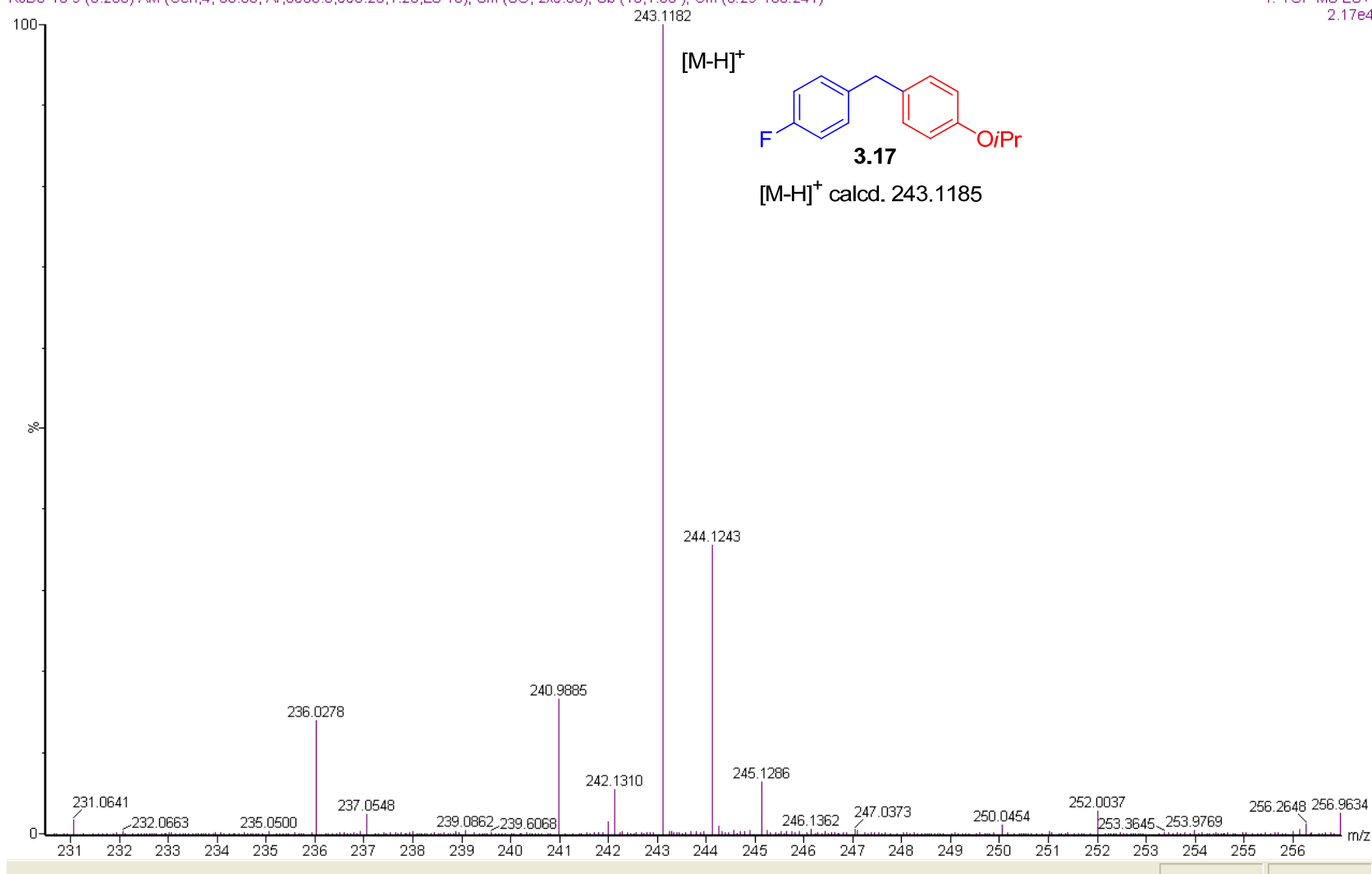
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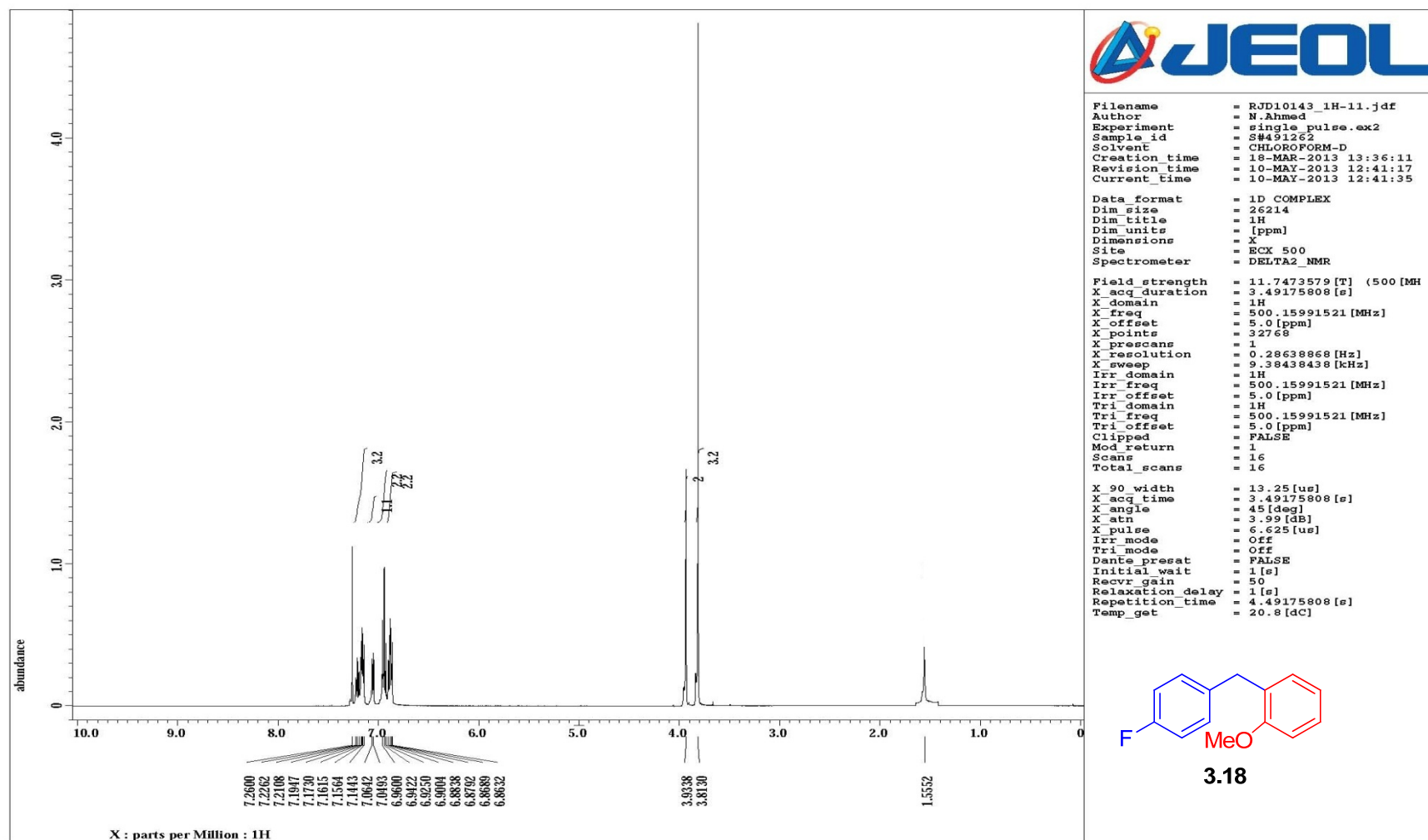


¹H spectrum of 1-isopropoxy-4-(4-fluorobenzyl)benzene (3.17)

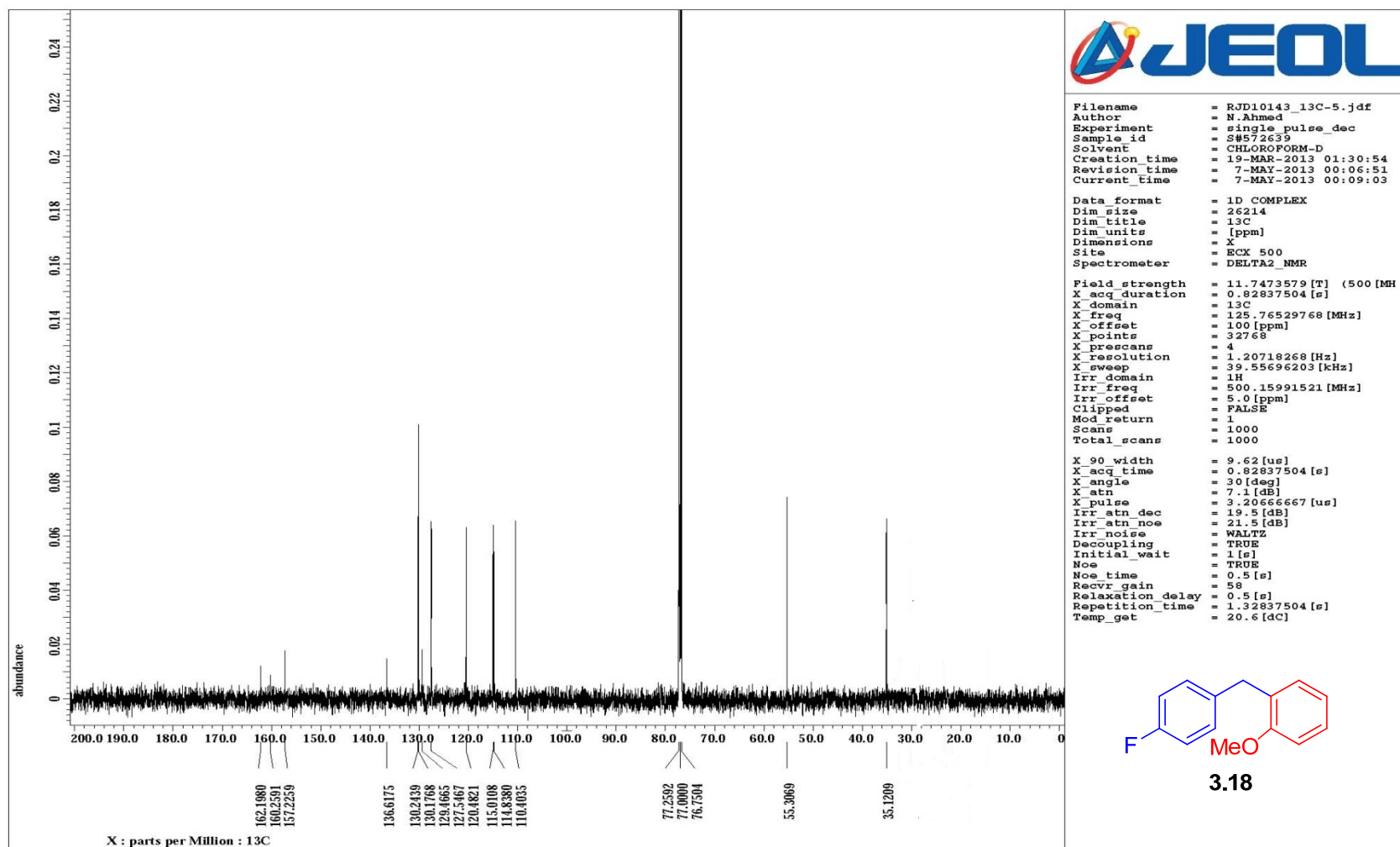


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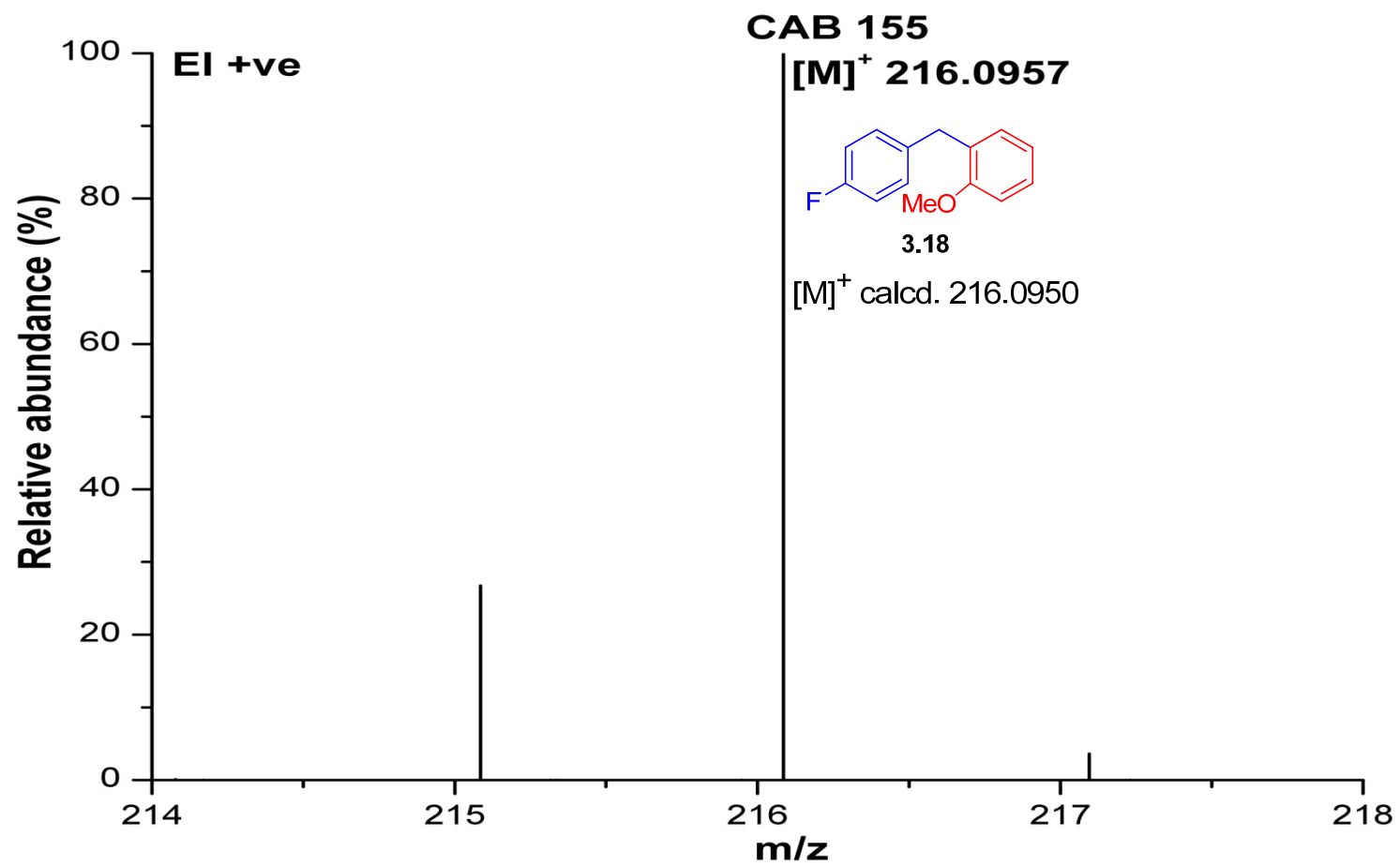
HRMS spectrum of 1-isopropoxy-4-(4-fluorobenzyl)benzene (**3.17**)



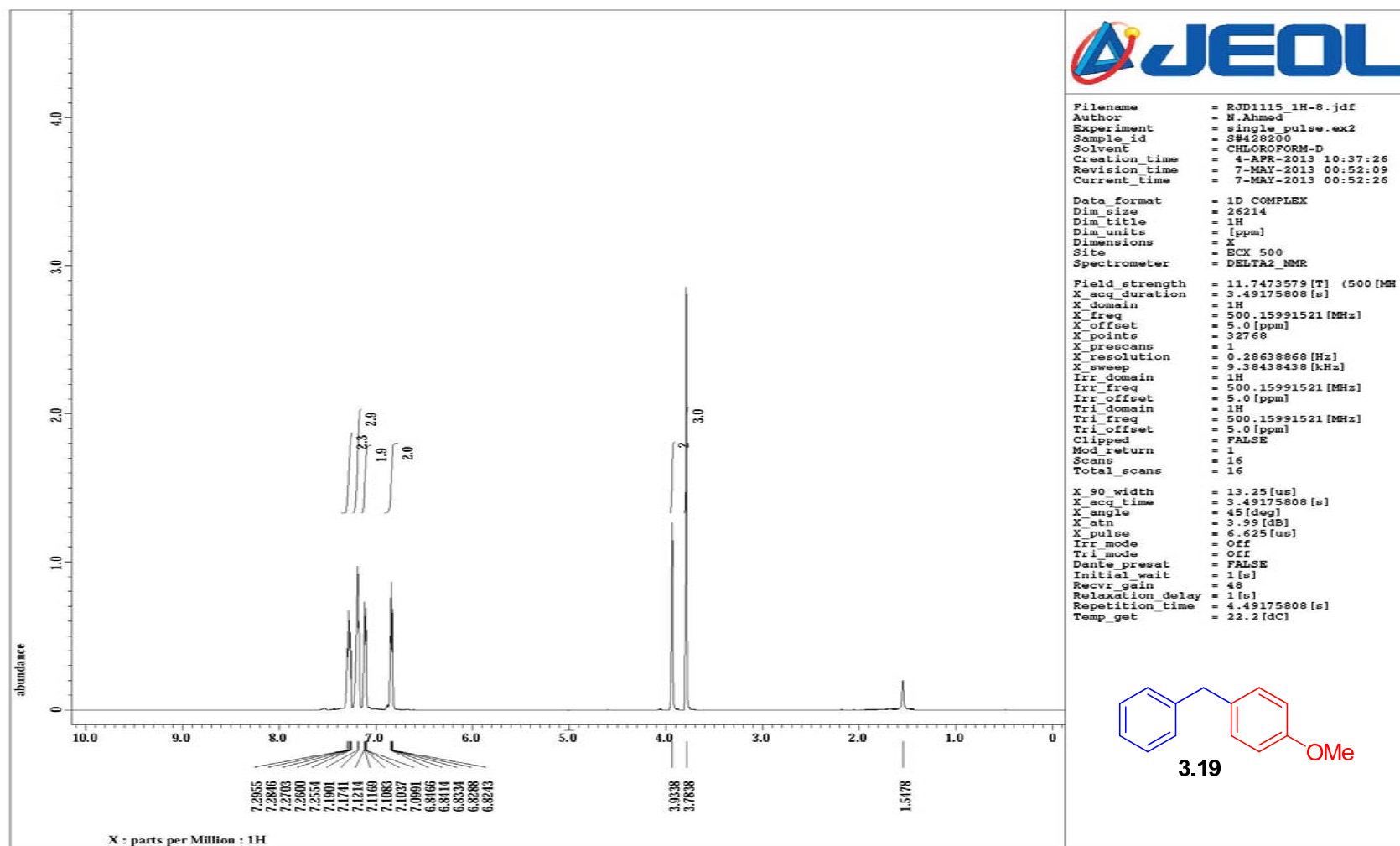
¹H spectrum of 1-(4-fluorobenzyl)-2-methoxybenzene (3.18)



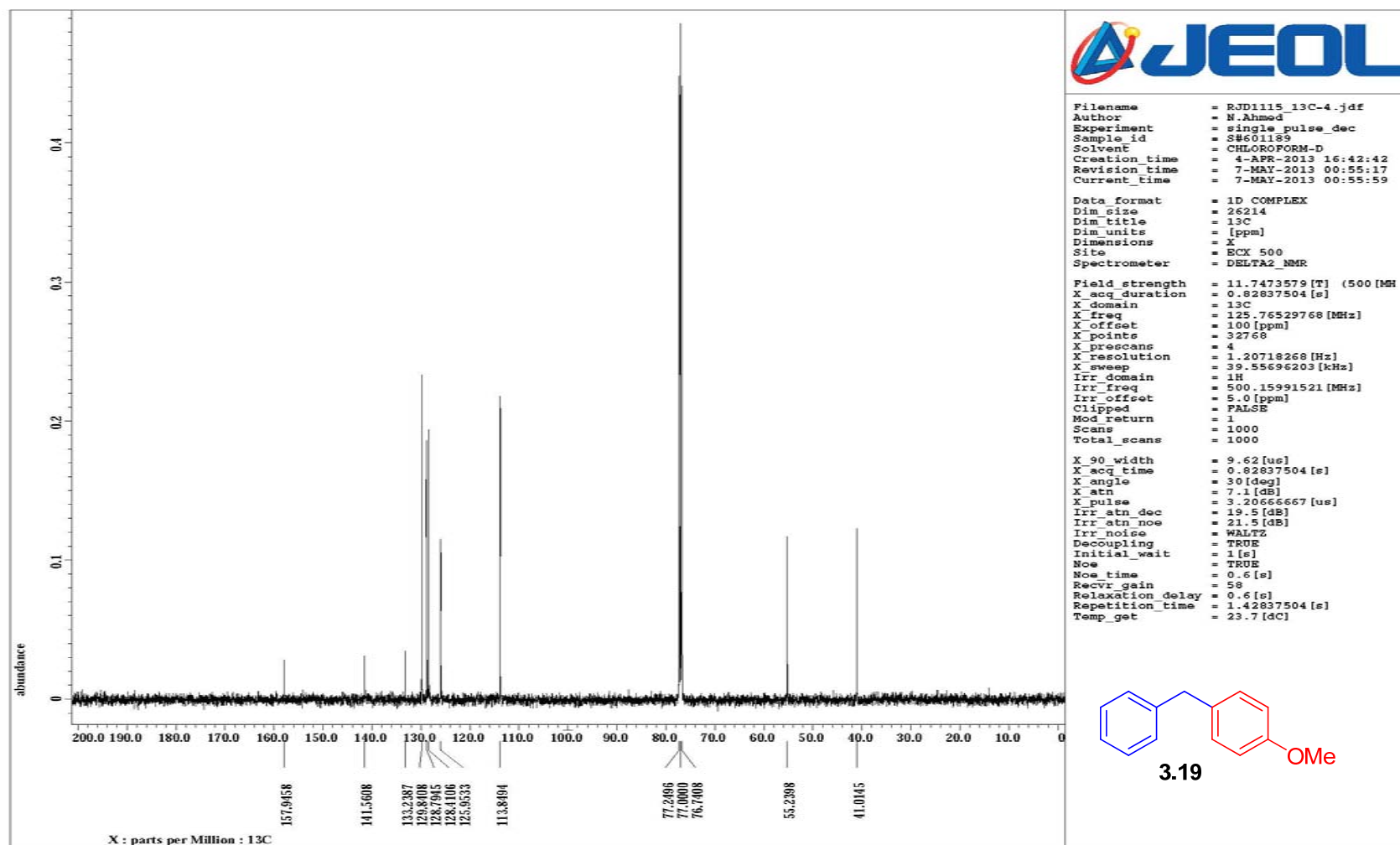
^{13}C spectrum of 1-(4-fluorobenzyl)-2-methoxybenzene (3.18)



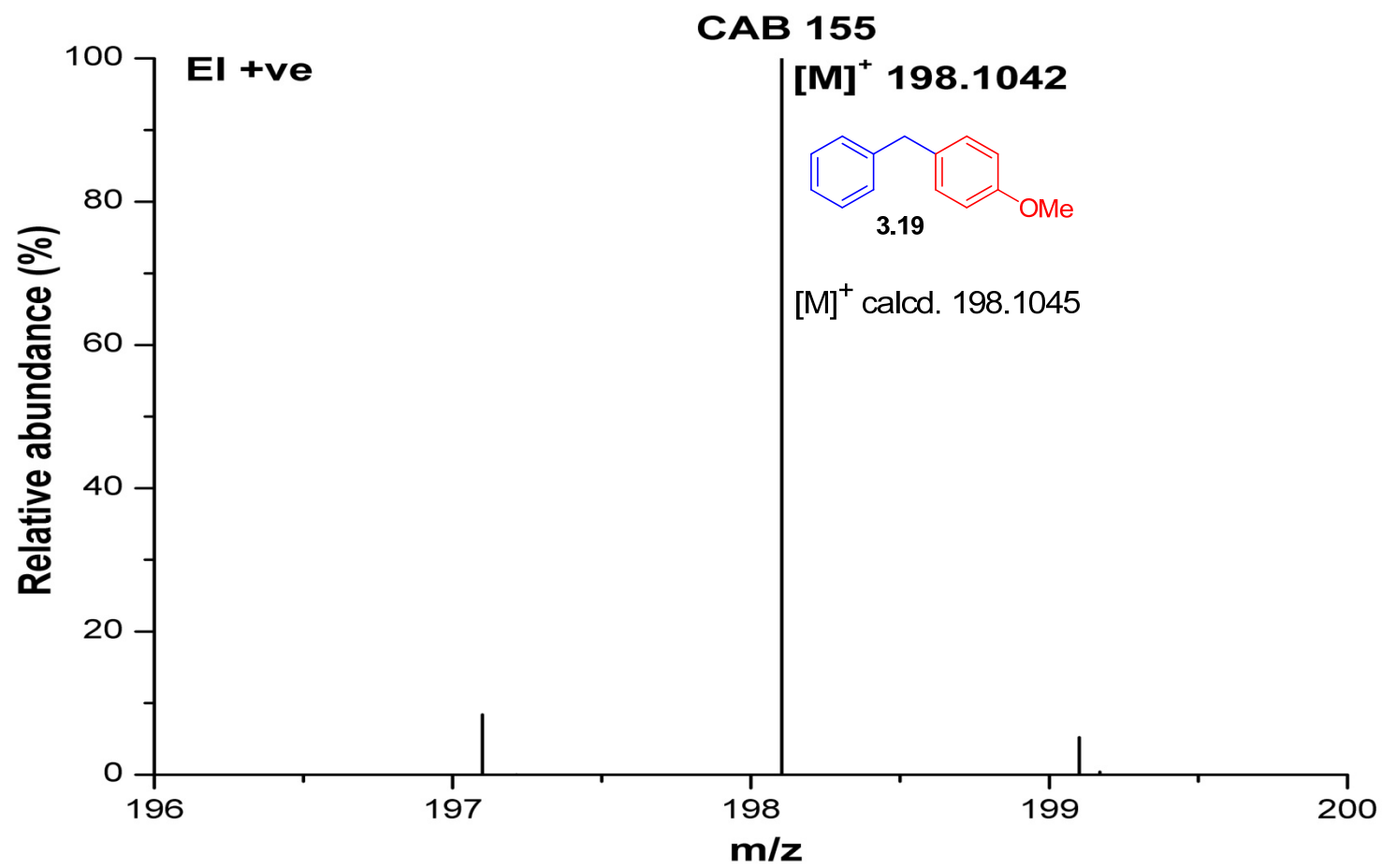
HRMS spectrum of 1-(4-fluorobenzyl)-2-methoxybenzene (**3.18**)



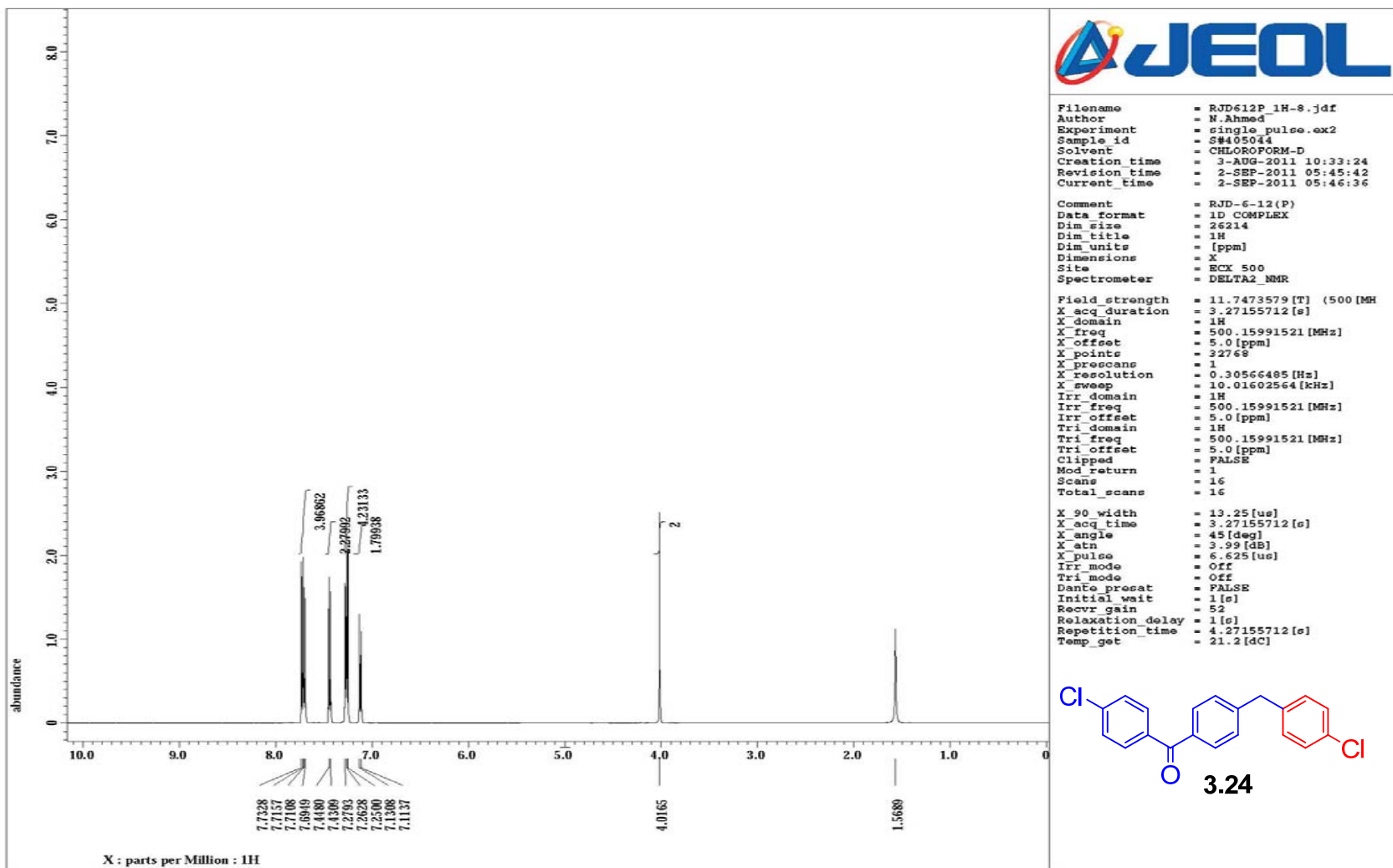
¹H spectrum of 1-benzyl-4-methoxybenzene (3.19)



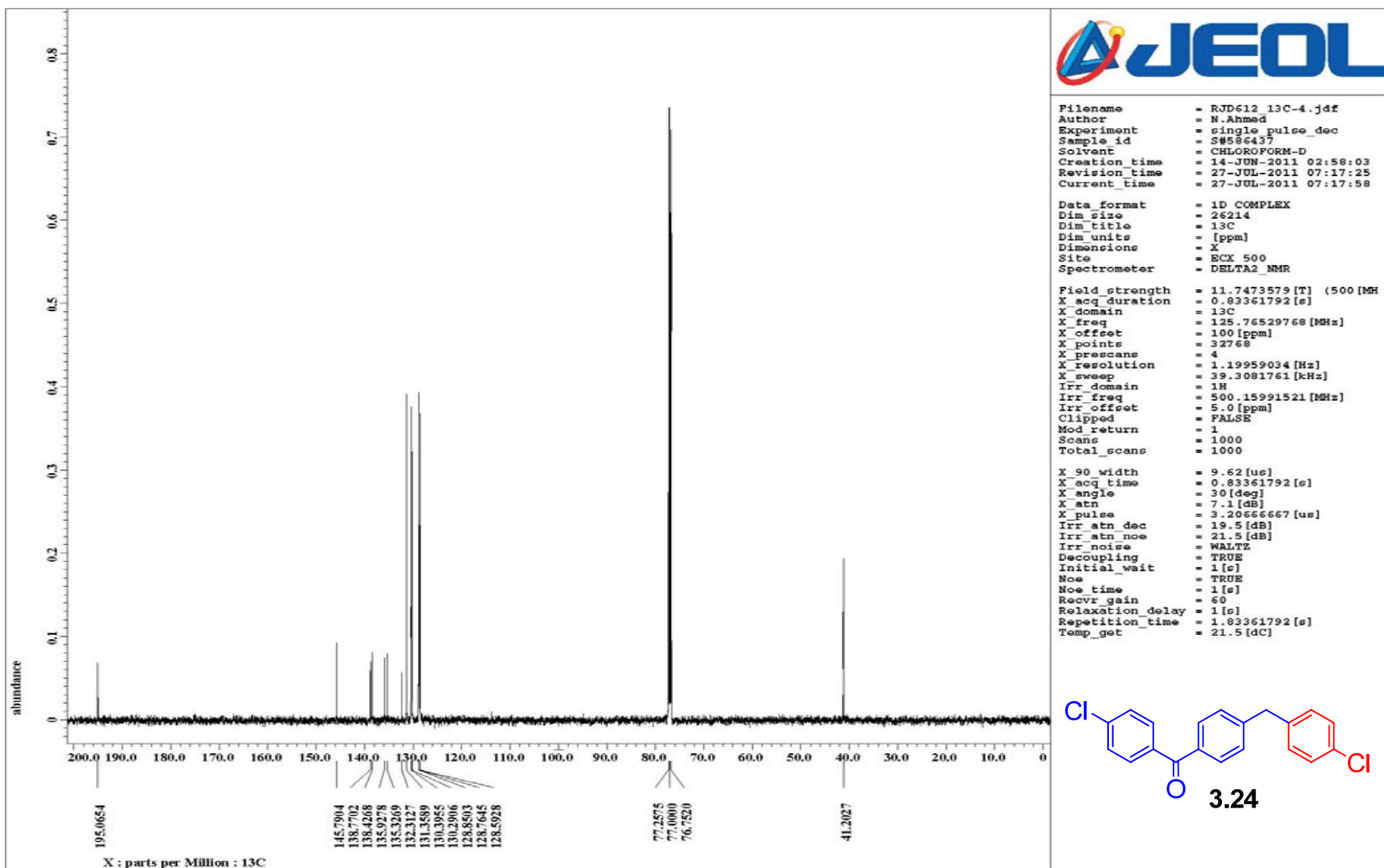
^{13}C spectrum of 1-benzyl-4-methoxybenzene (3.19)



HRMS spectrum of 1-benzyl-4-methoxybenzene (**3.19**)

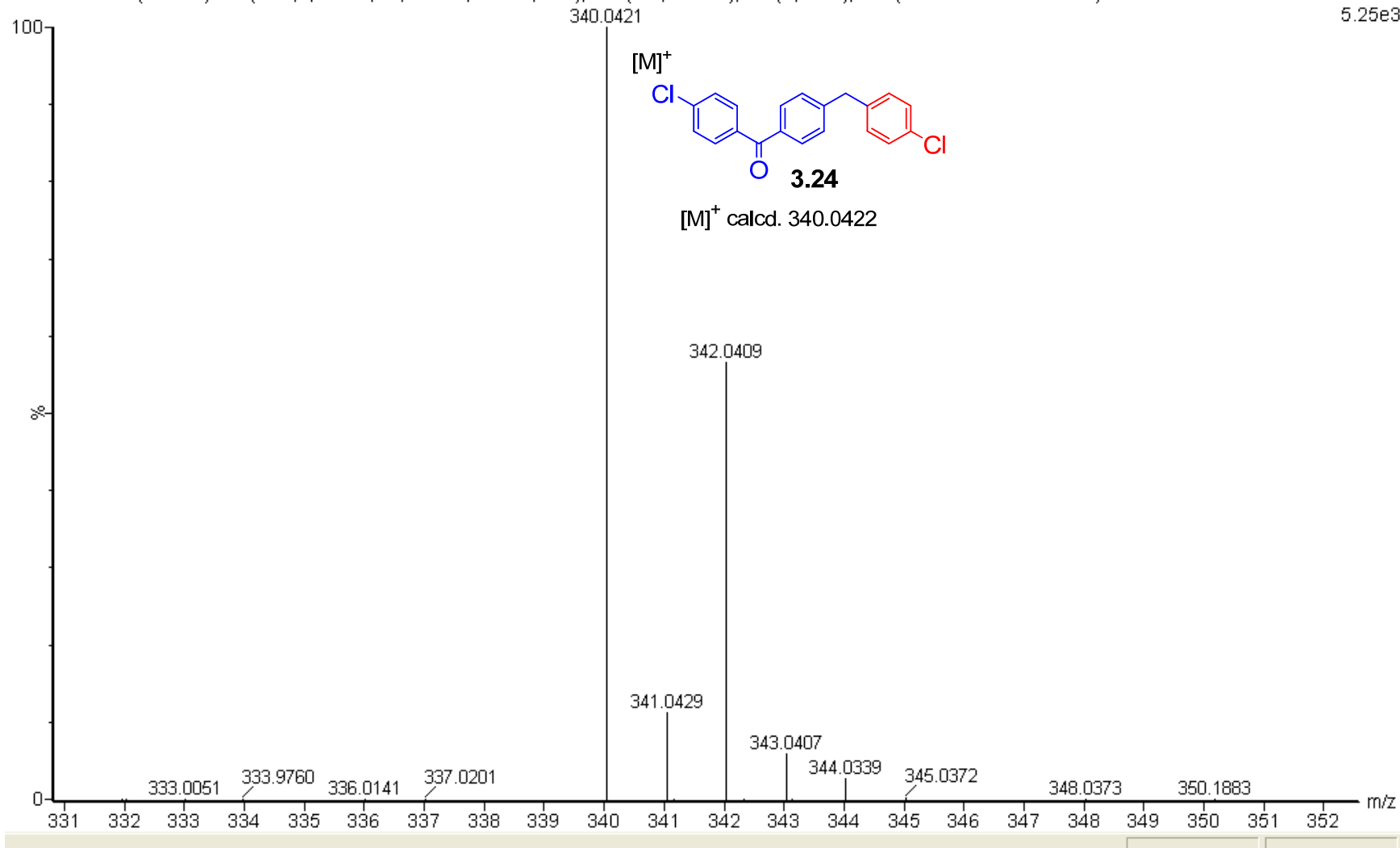


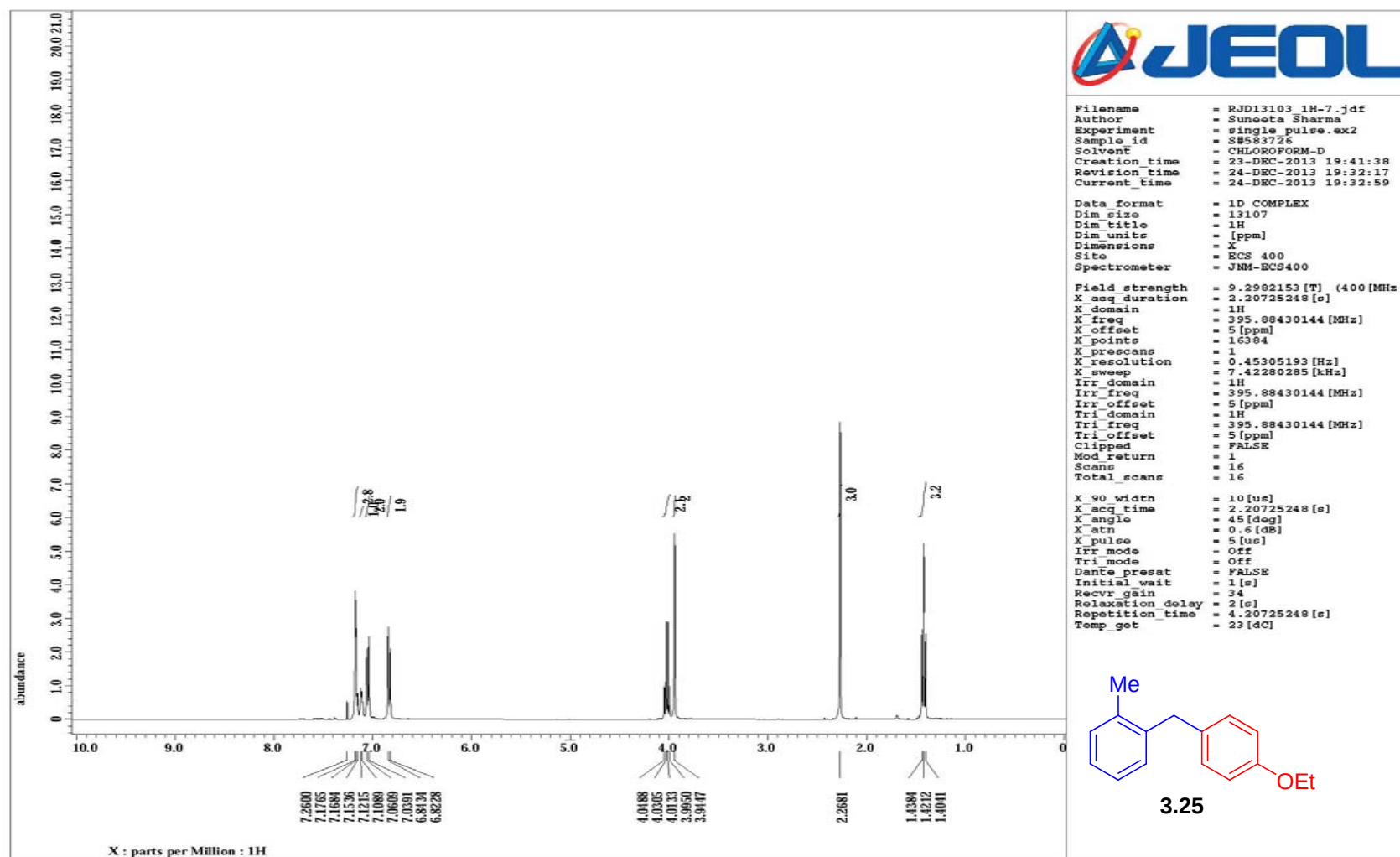
¹H spectrum of (4-chlorophenyl)(4-(4-chlorobenzyl)phenyl)methanone (3.24)



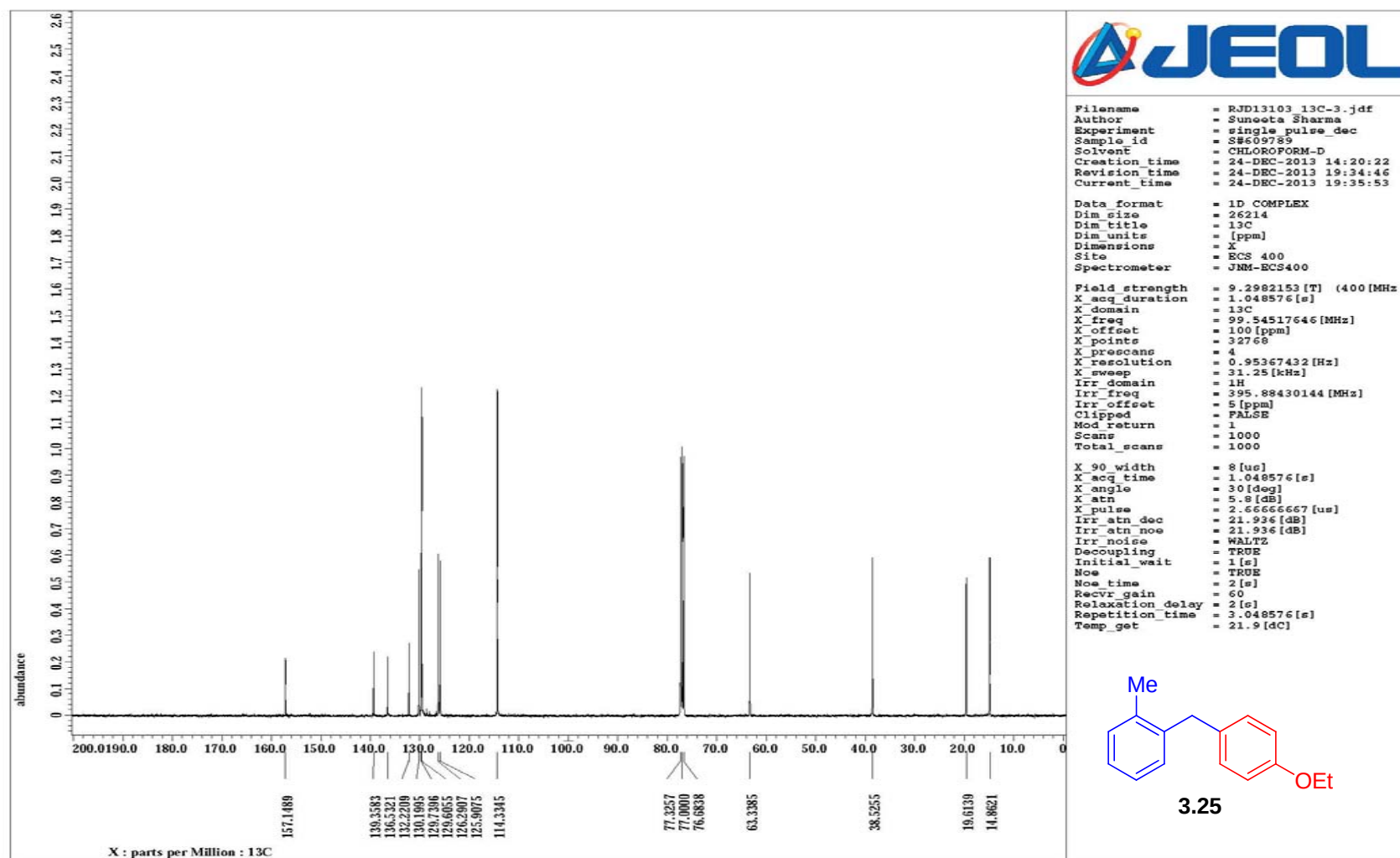
^{13}C spectrum of (4-chlorophenyl)(4-(4-chlorobenzyl)phenyl)methanone (3.24)

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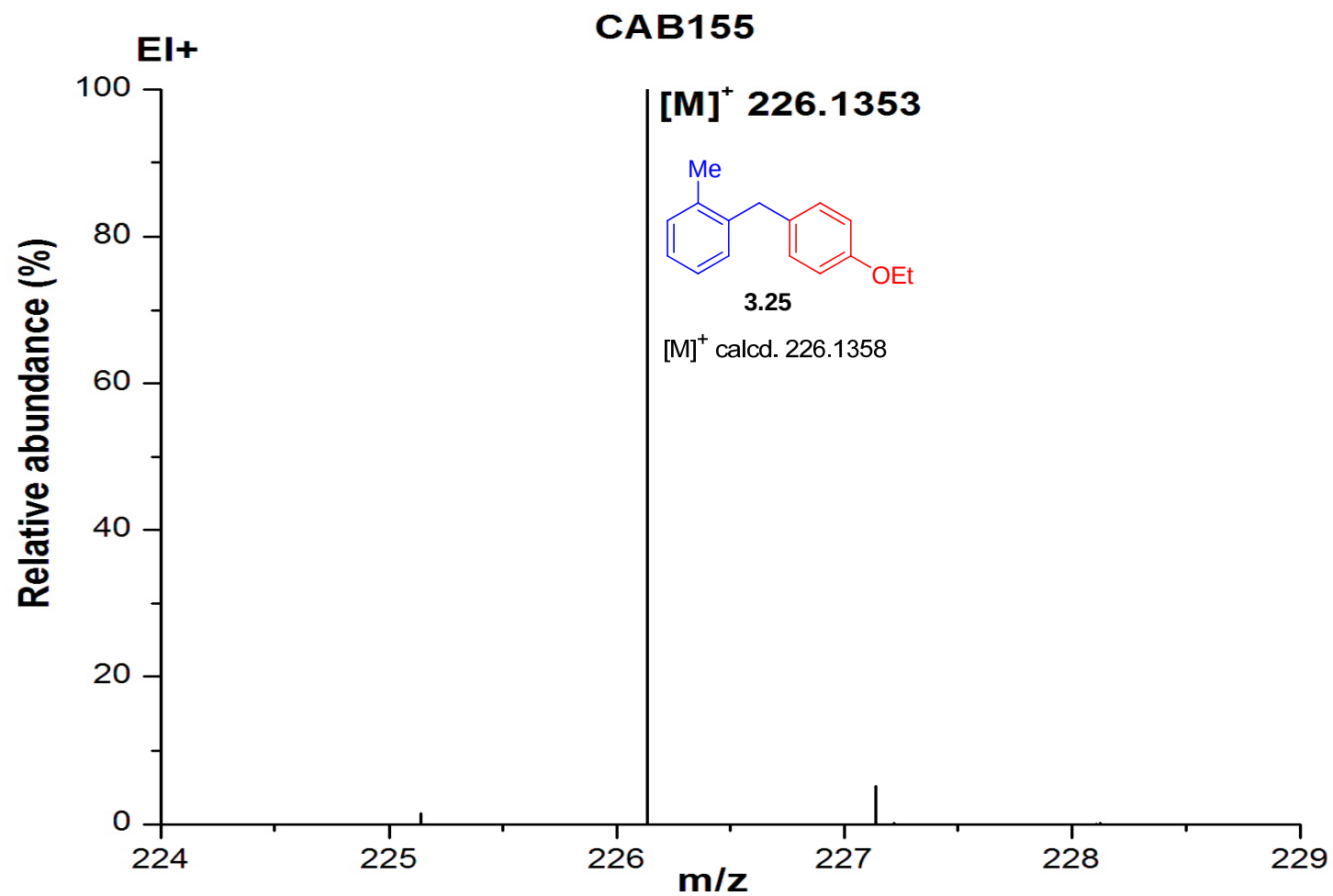
TOF MS EI+
5.25e3HRMS spectrum of (4-chlorophenyl)(4-(4-chlorobenzyl)phenyl)methanone (**3.24**)



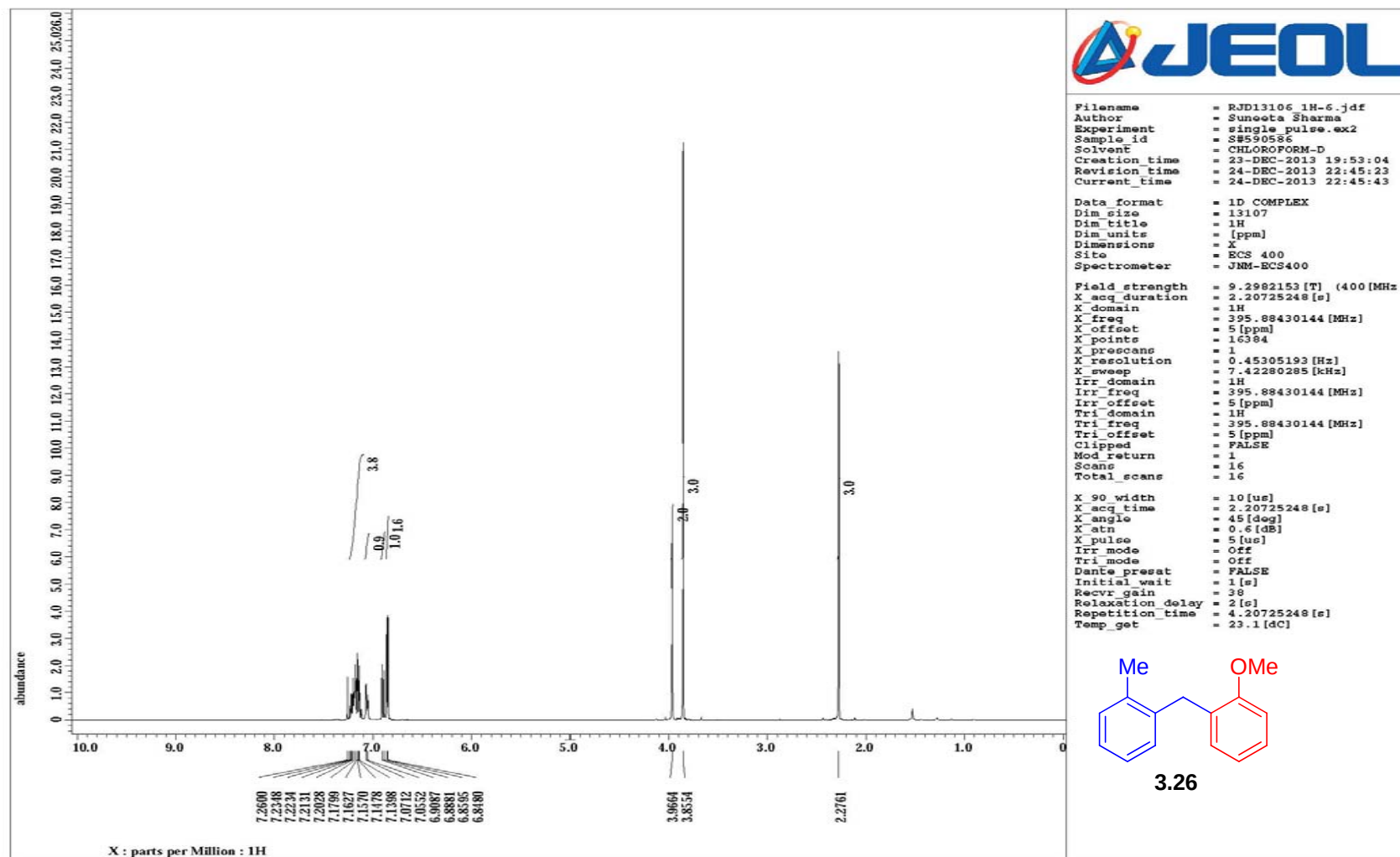
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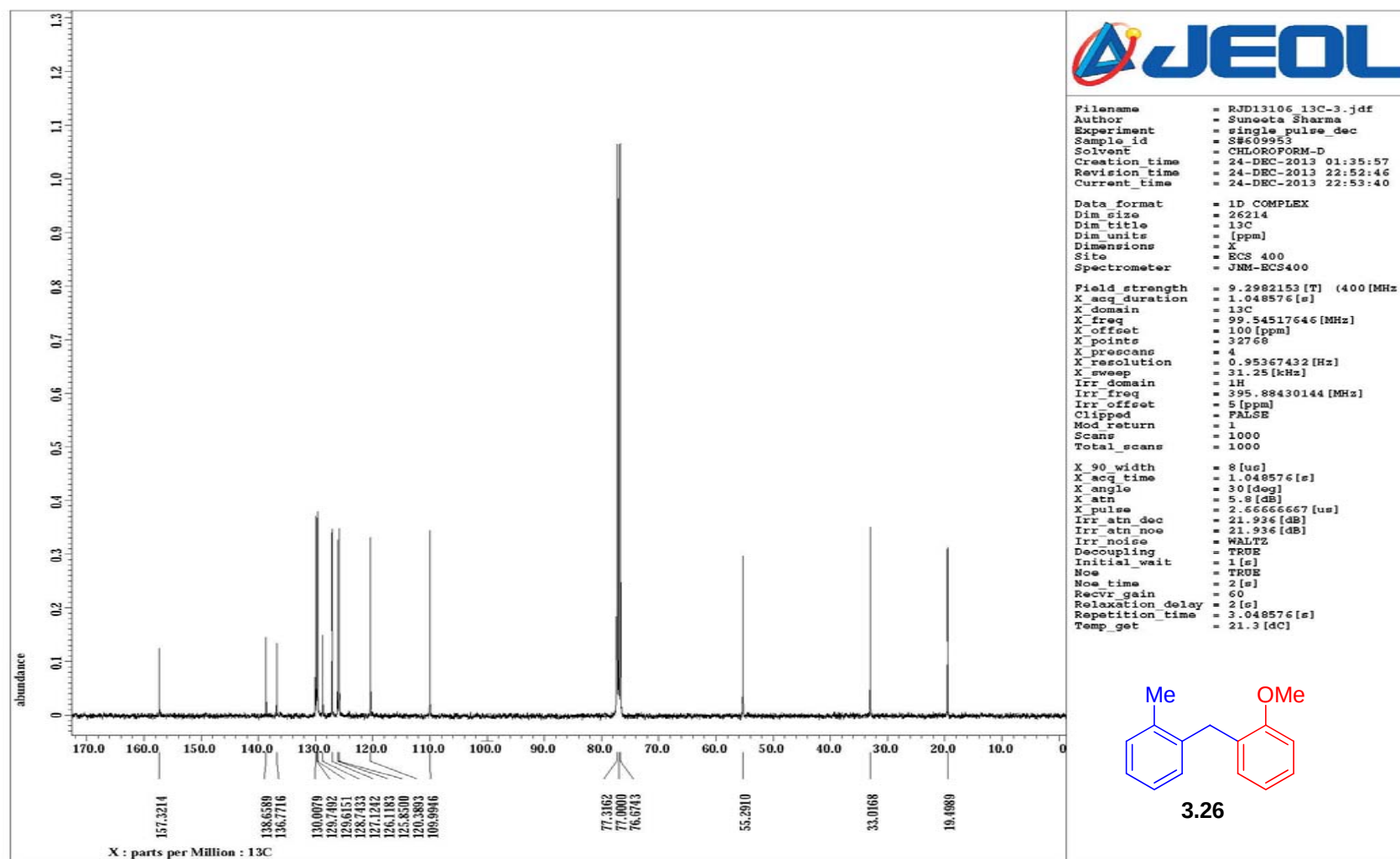
¹³C NMR spectrum of 1-(4-ethoxybenzyl)-2-methylbenzene (3.25)



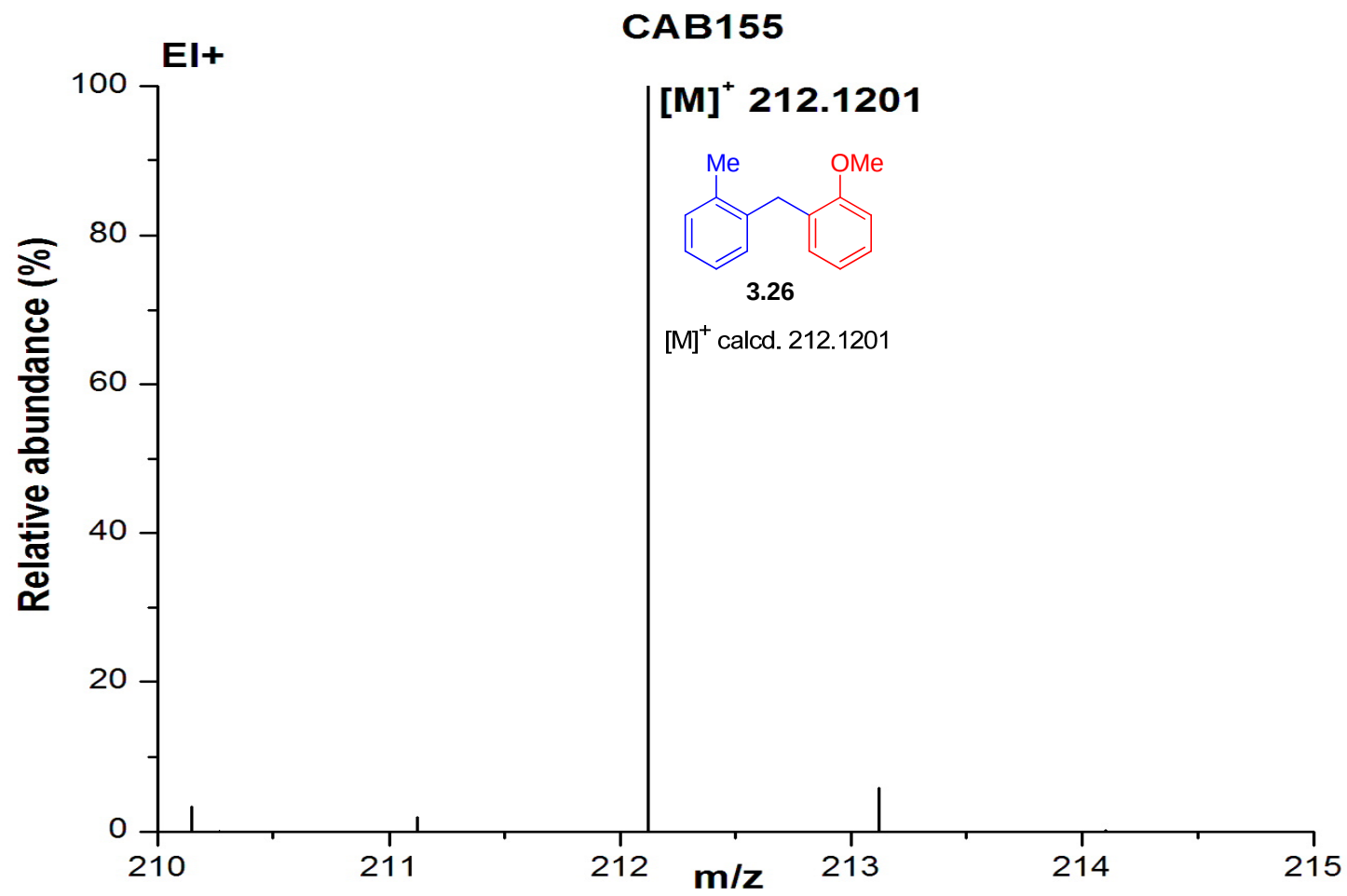
HRMS spectrum of 1-(4-ethoxybenzyl)-2-methylbenzene (3.25)



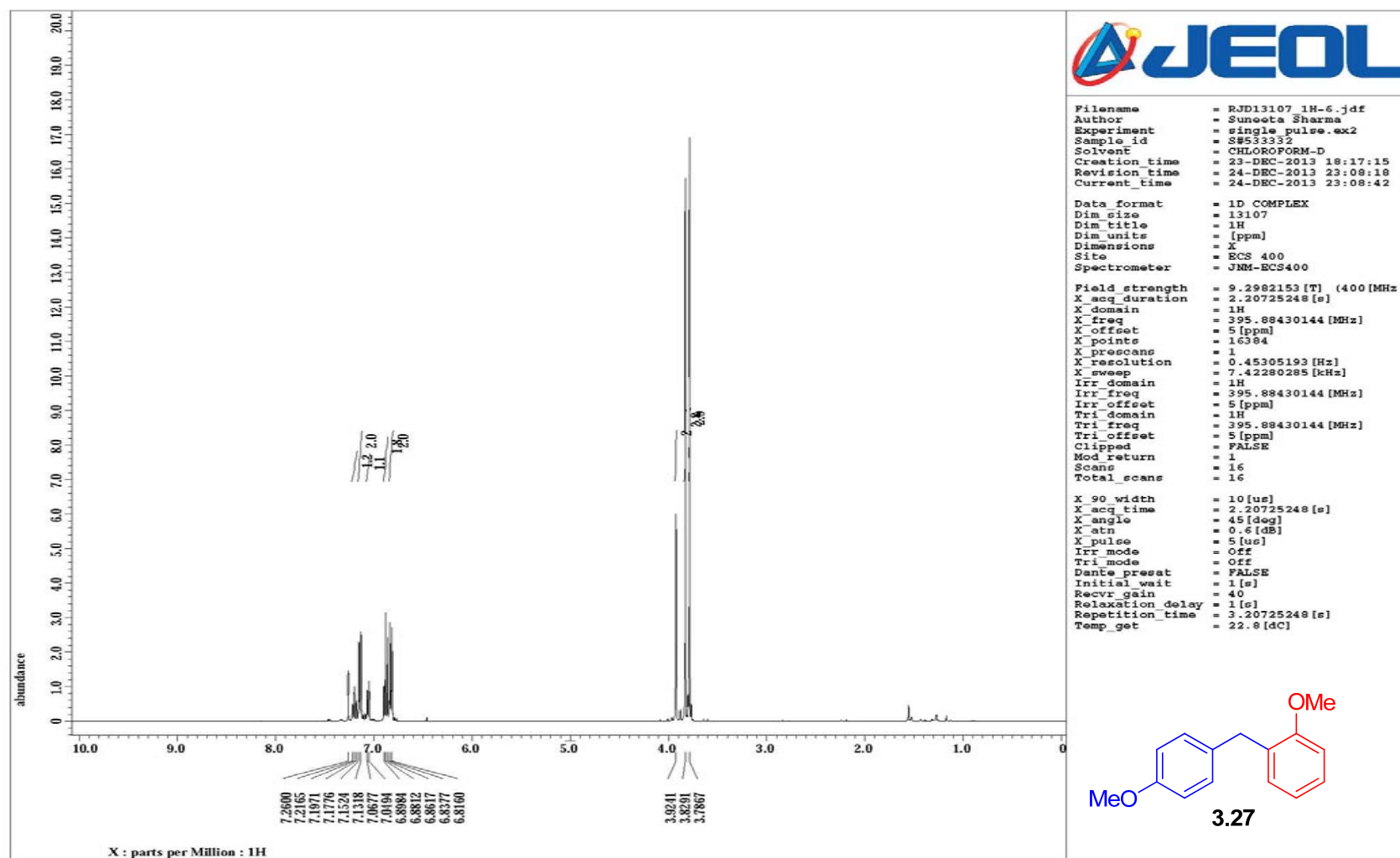
^1H NMR spectrum of 1-methoxy-2-(2-methylbenzyl)benzene (3.26)



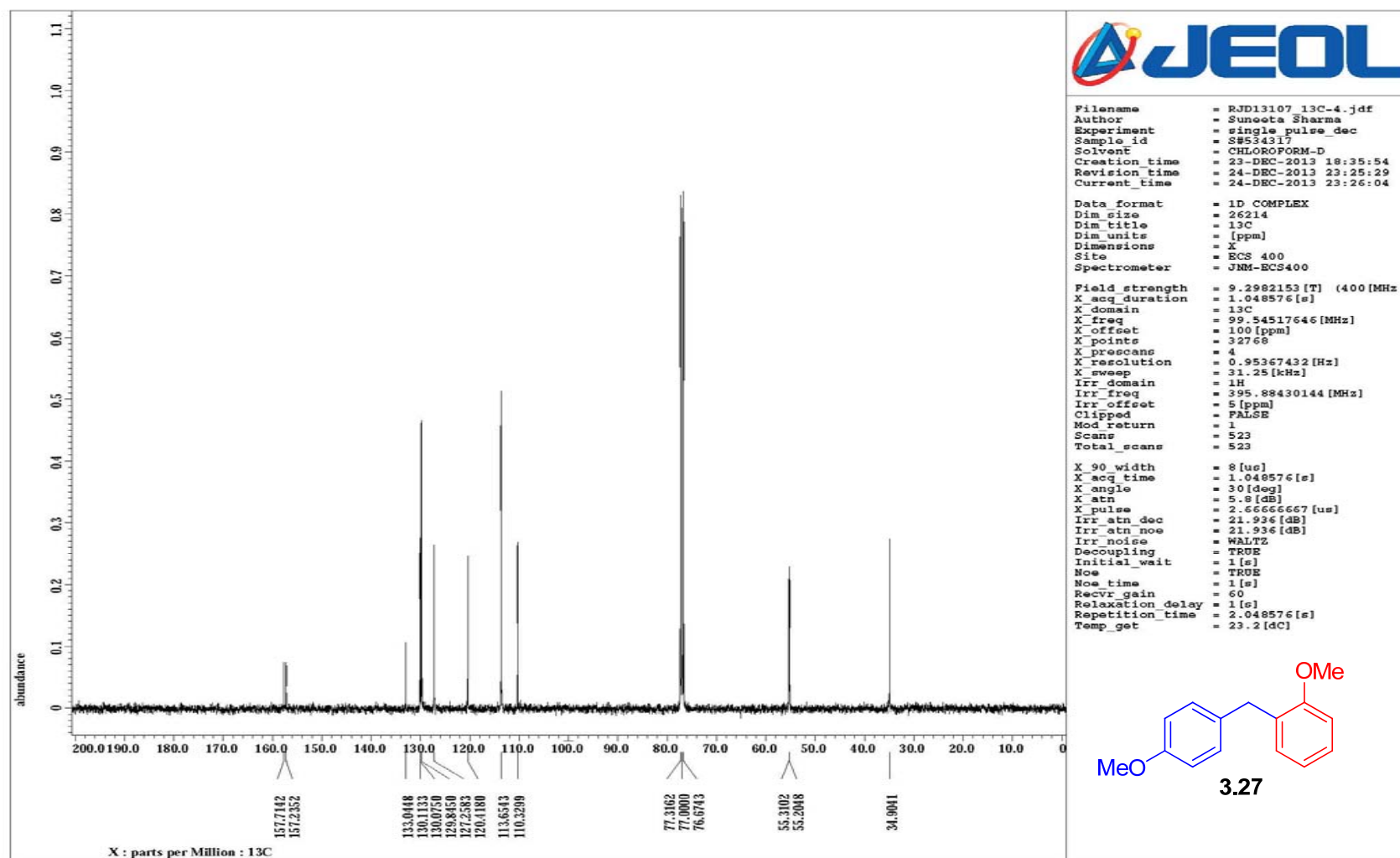
¹³C NMR spectrum of 1-methoxy-2-(2-methylbenzyl)benzene (3.26)



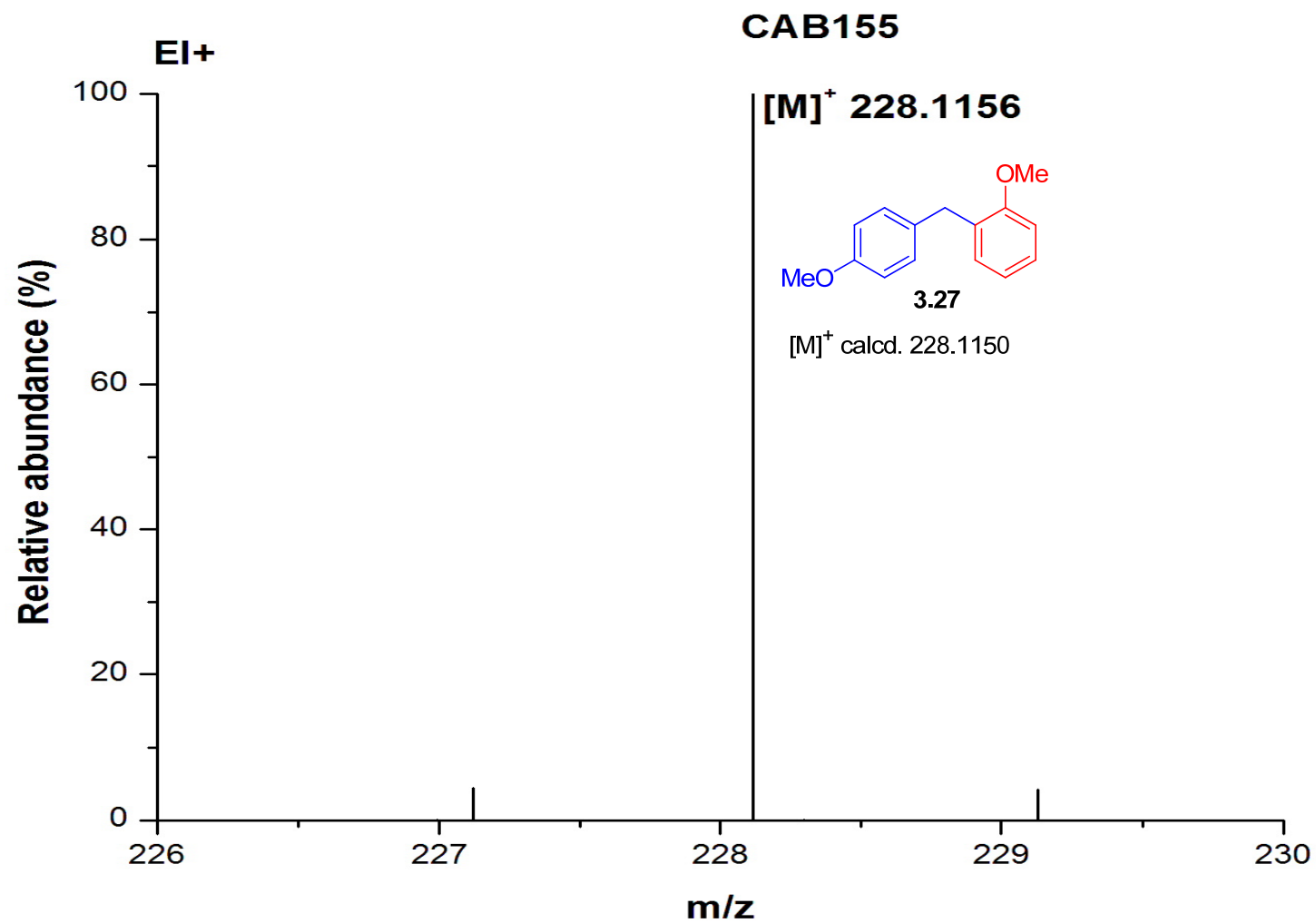
HRMS spectrum of 1-methoxy-2-(2-methylbenzyl)benzene (**3.26**)



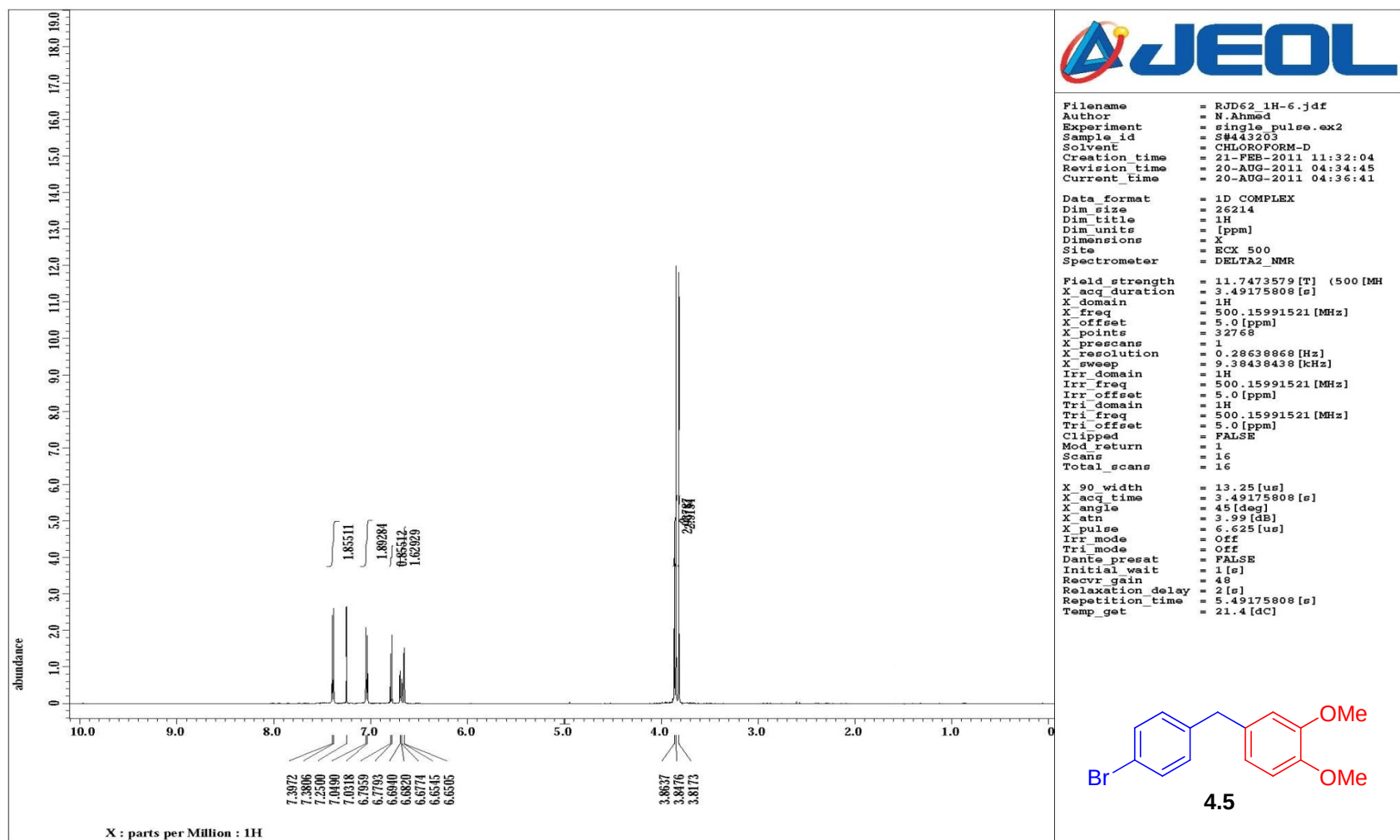
¹H NMR spectrum of 1-methoxy-2-(4-methoxybenzyl)benzene (3.27)



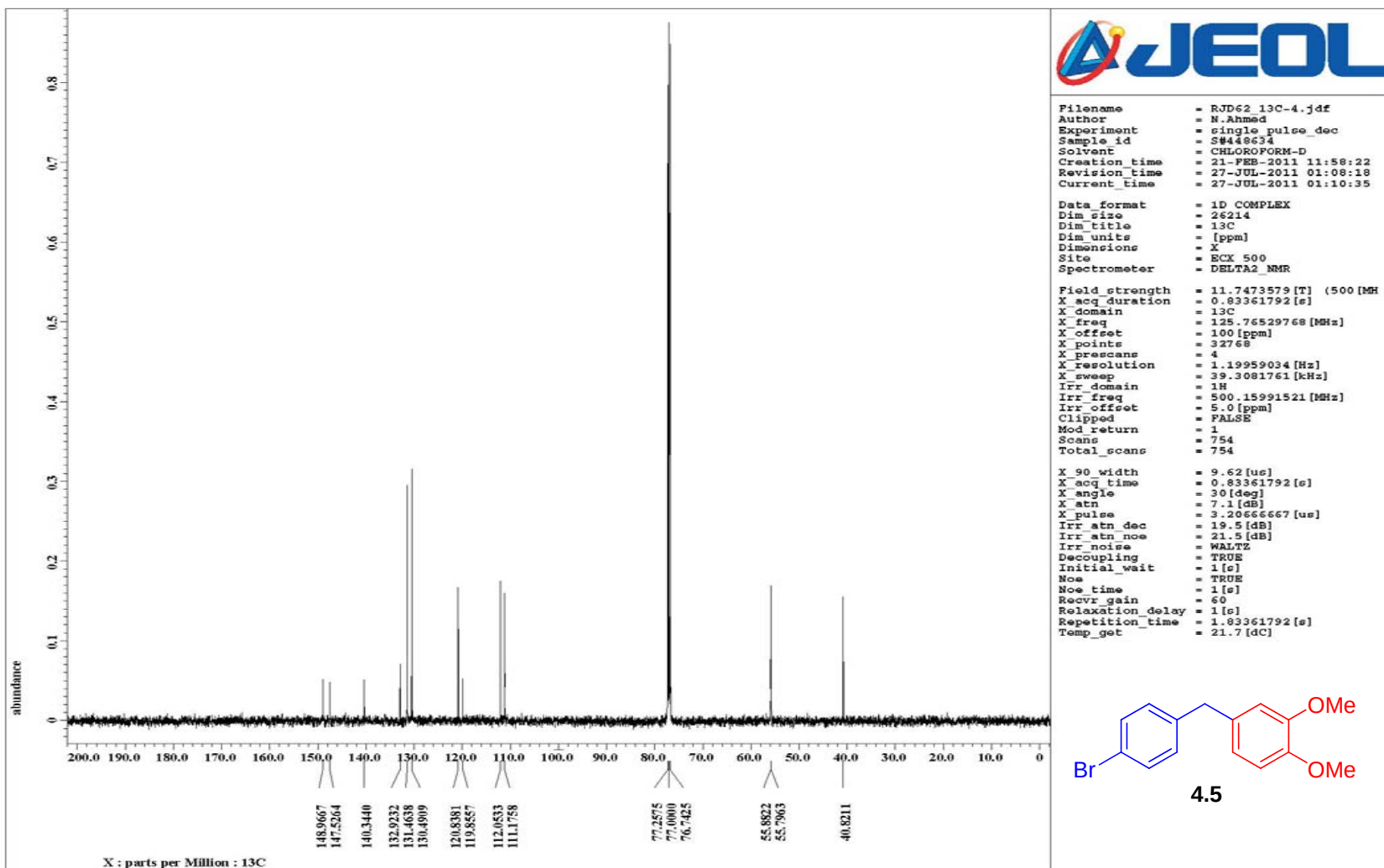
^{13}C NMR spectrum of 1-methoxy-2-(4-methoxybenzyl)benzene (3.27)



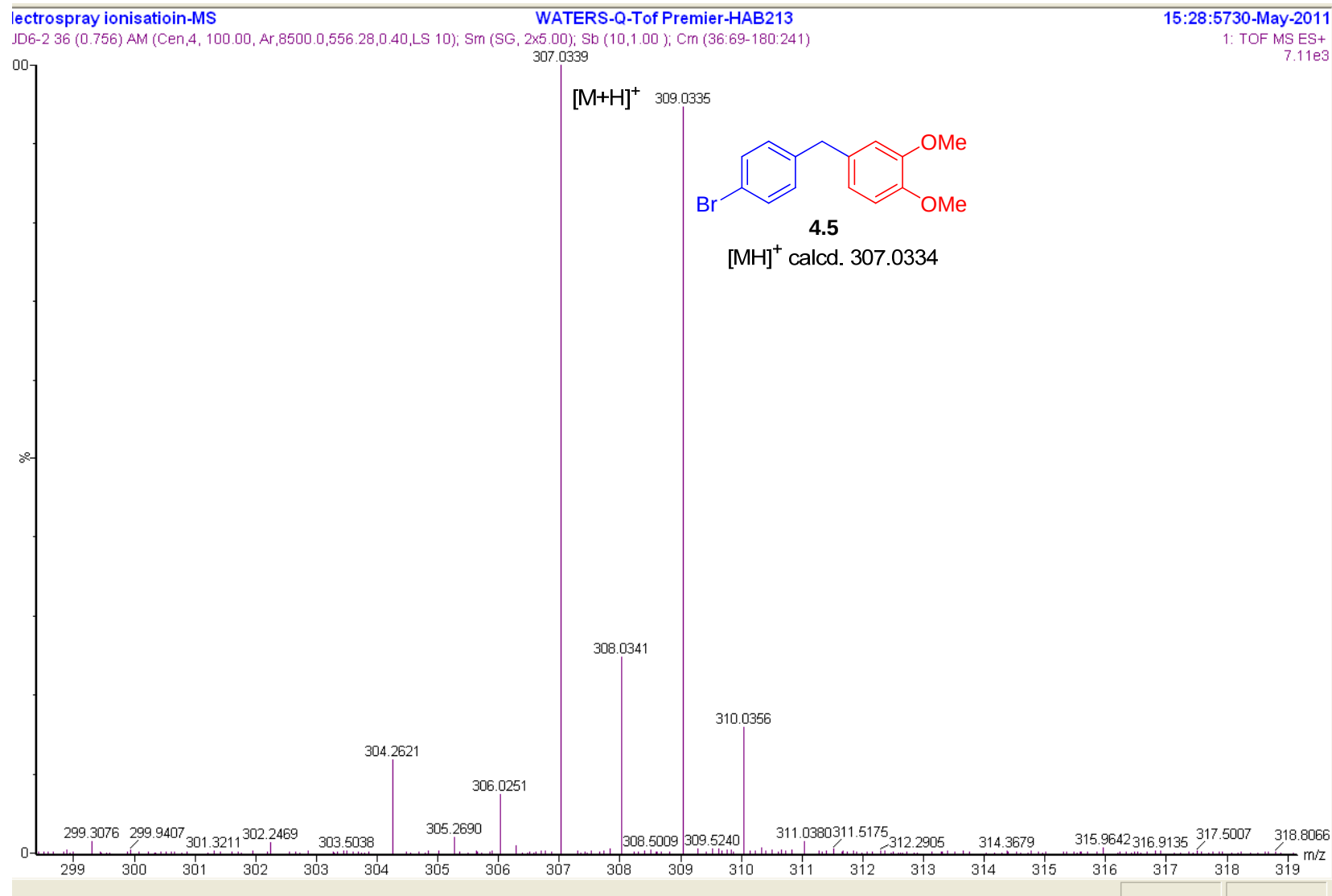
HRMS spectrum of 1-methoxy-2-(4-methoxybenzyl)benzene (**3.27**)



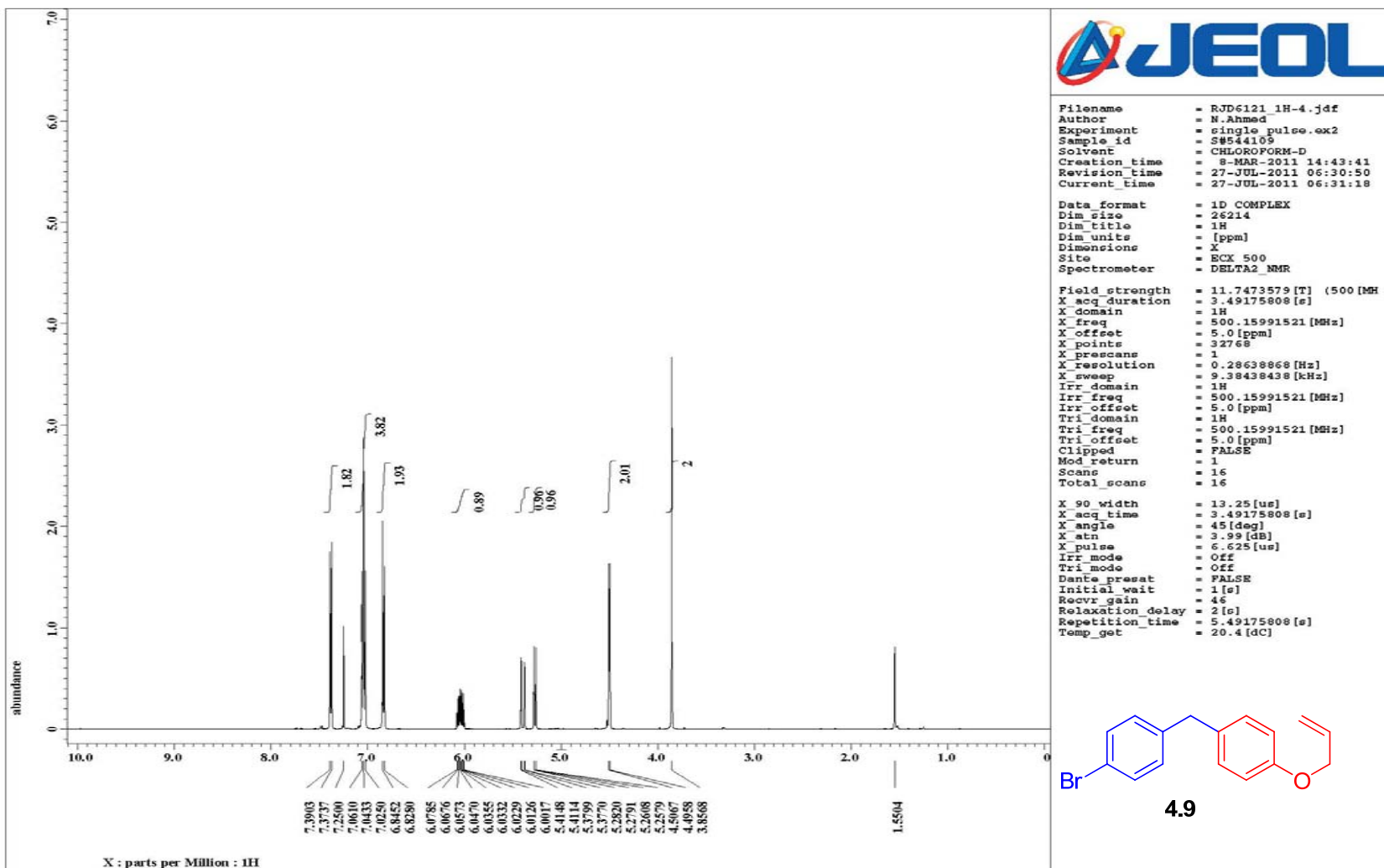
¹H NMR spectrum of 4-(4-bromobenzyl)-1,2-dimethoxybenzene (4.5)



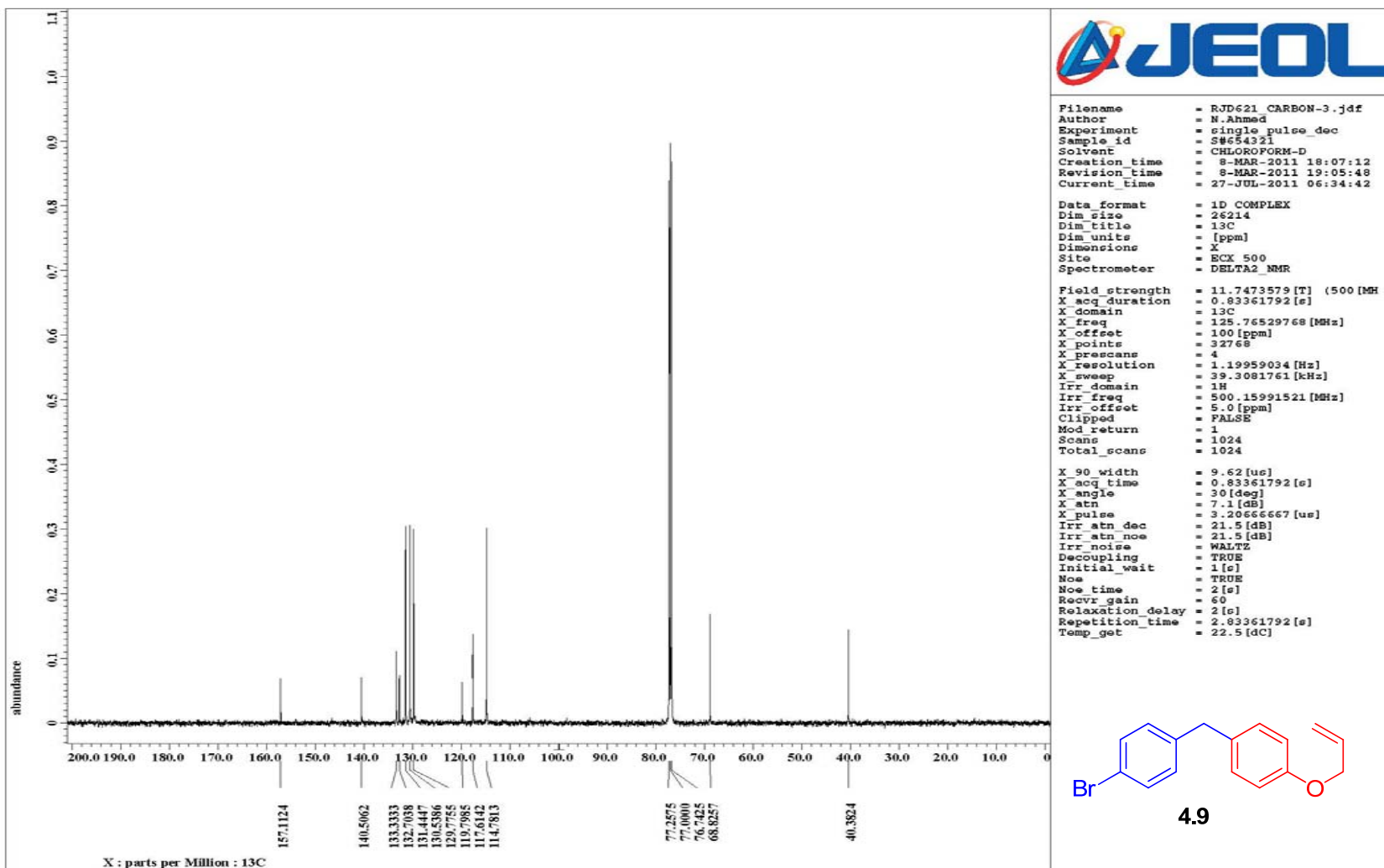
^{13}C NMR spectrum of 4-(4-bromobenzyl)-1,2-dimethoxybenzene (4.5)



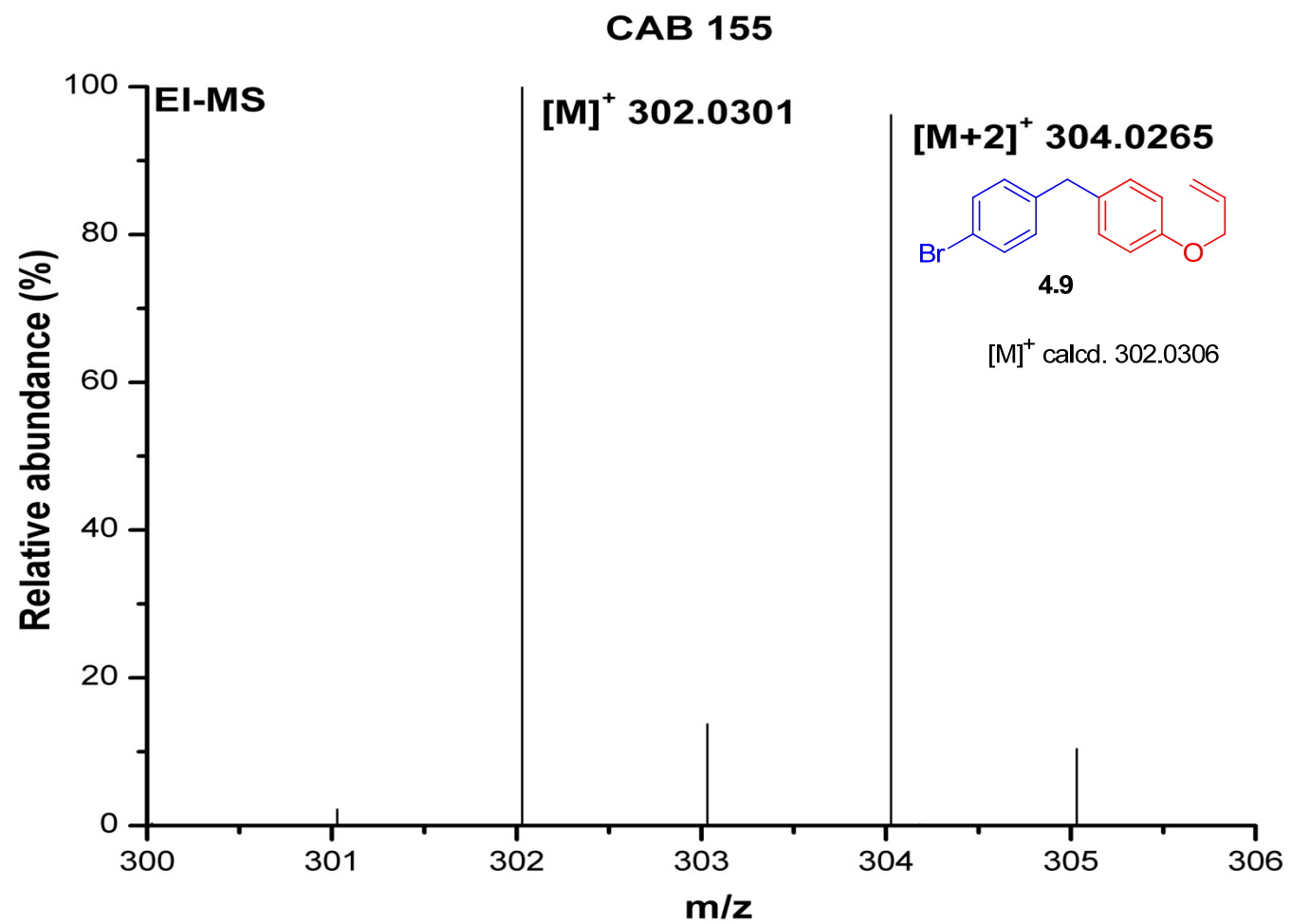
HRMS spectrum of 4-(4-bromobenzyl)-1,2-dimethoxybenzene (4.5)



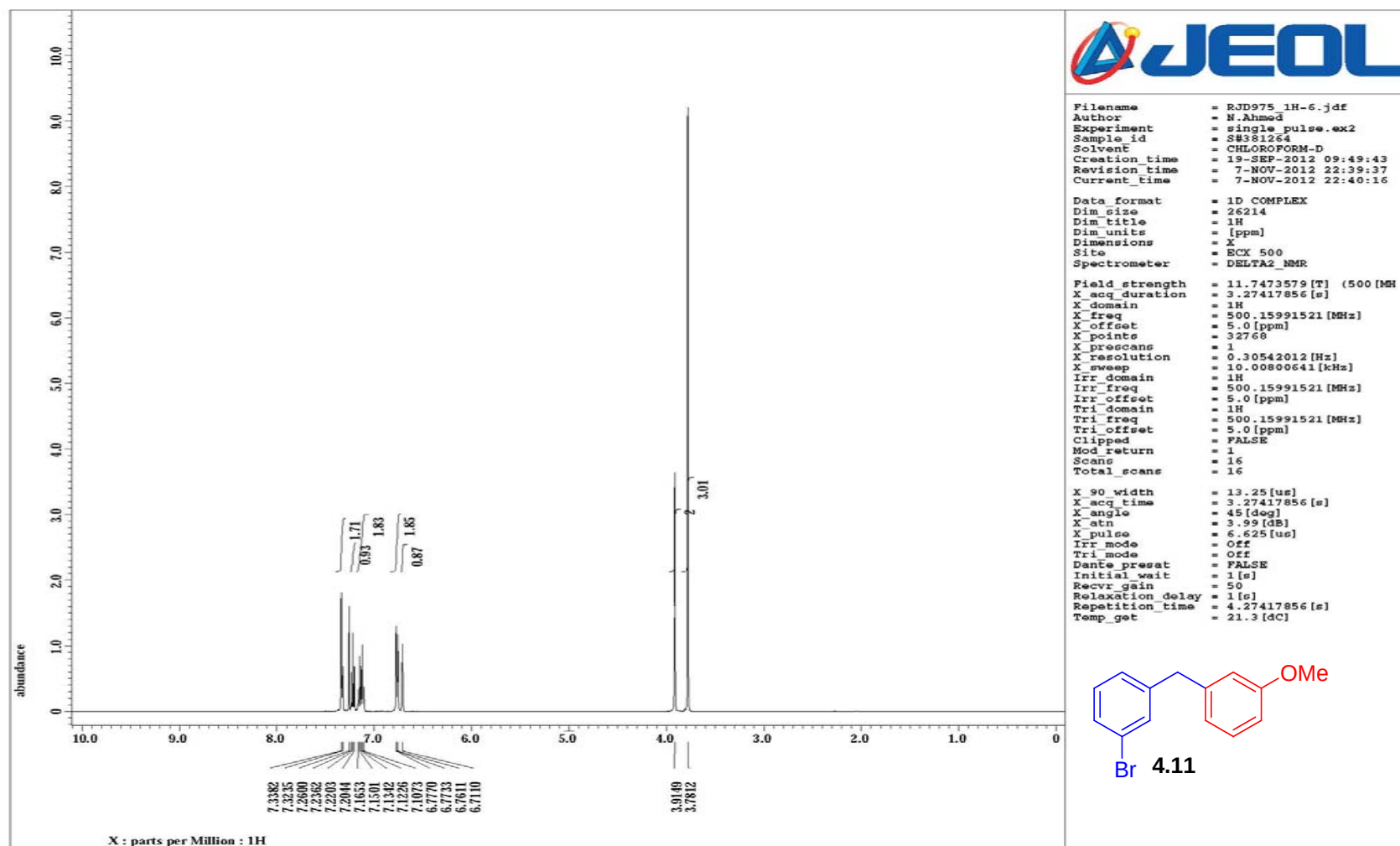
¹H NMR spectrum of 1-(allyloxy)-4-(4-bromobenzyl)benzene (4.9)



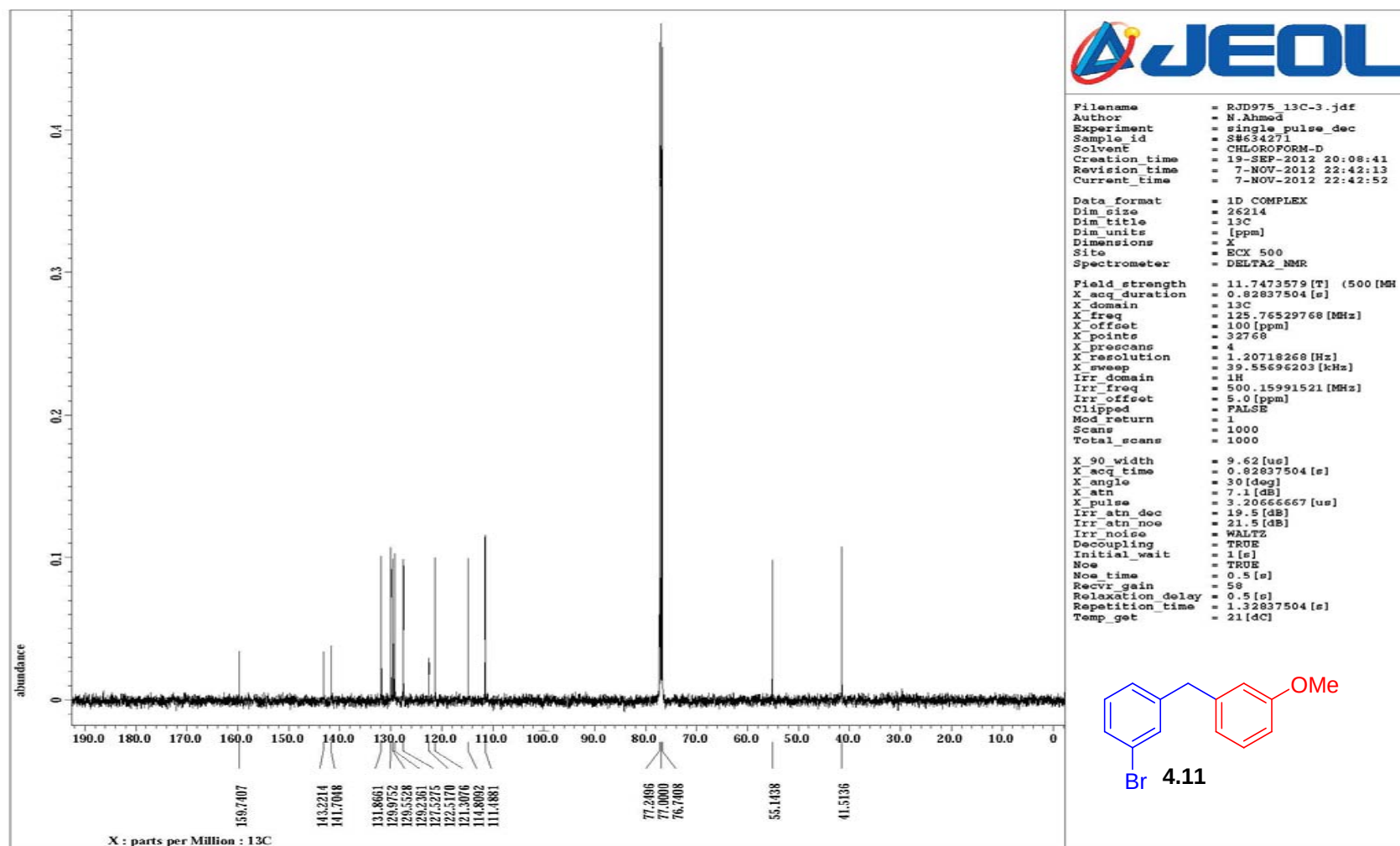
¹³C NMR spectrum of 1-(allyloxy)-4-(4-bromobenzyl)benzene (**4.9**)



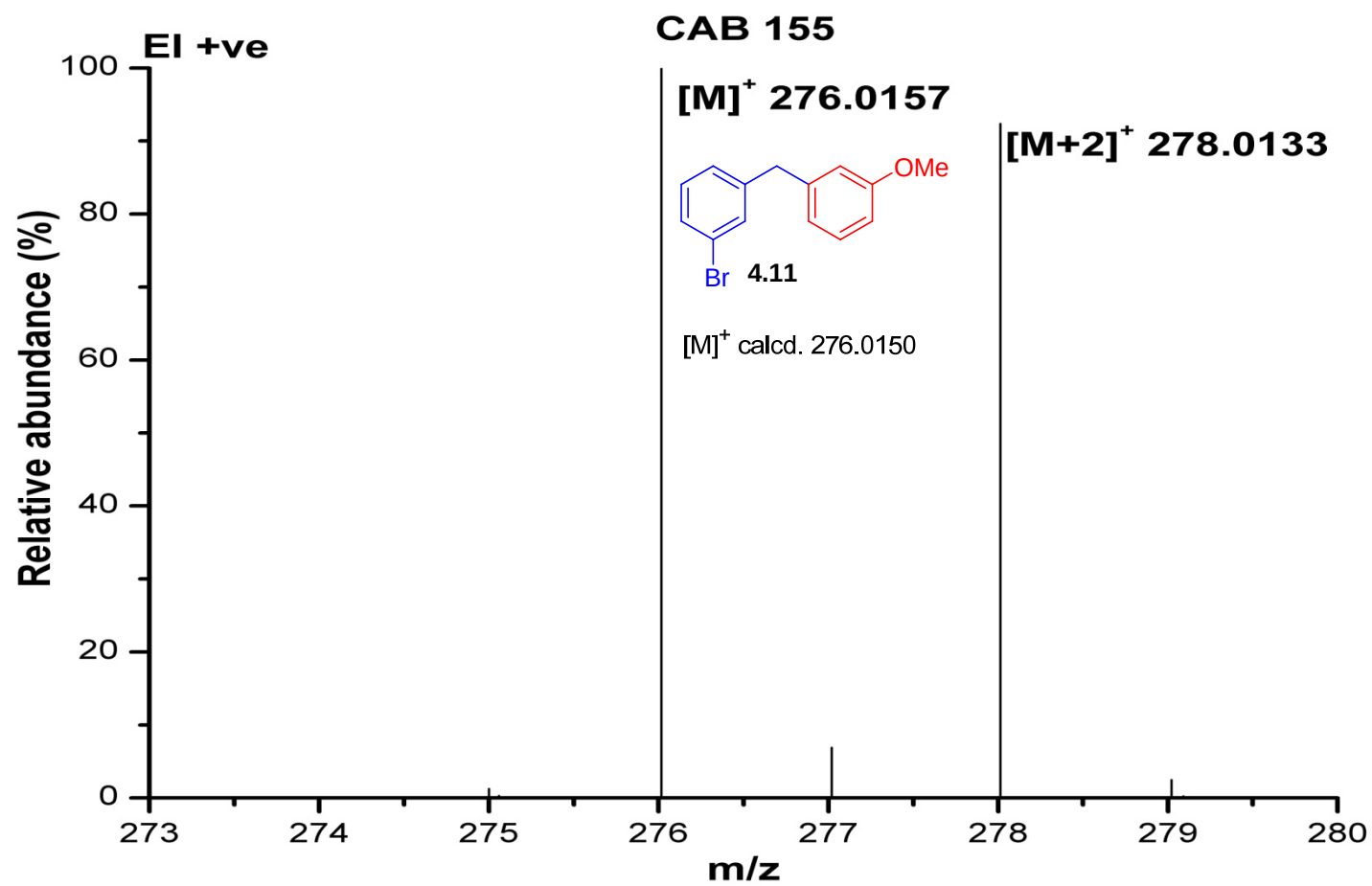
HRMS spectrum of 1-(allyloxy)-4-(4-bromobenzyl)benzene (**4.9**)



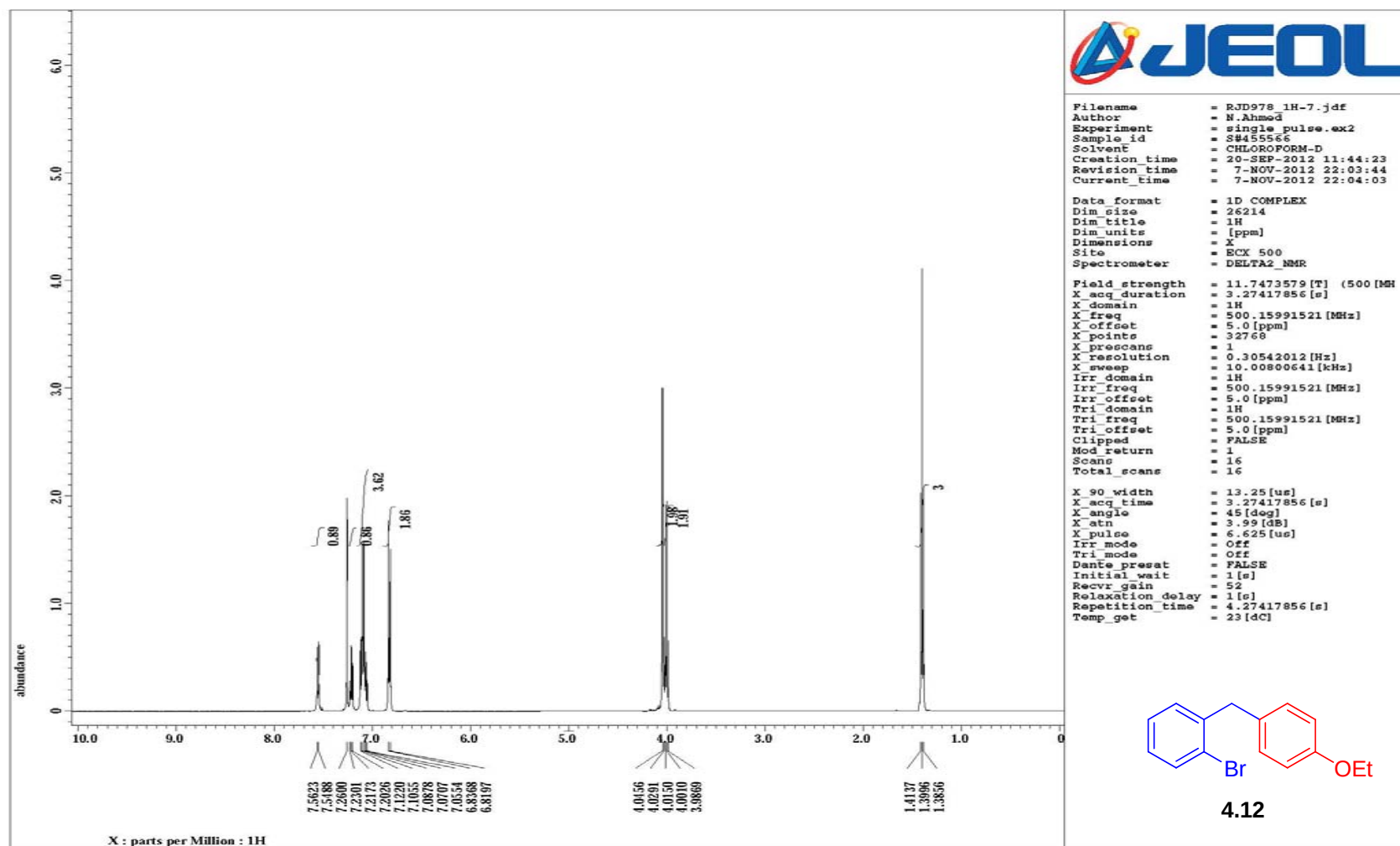
¹H NMR spectrum of 1-Bromo-3-(3-methoxybenzyl)benzene (**4.11**)



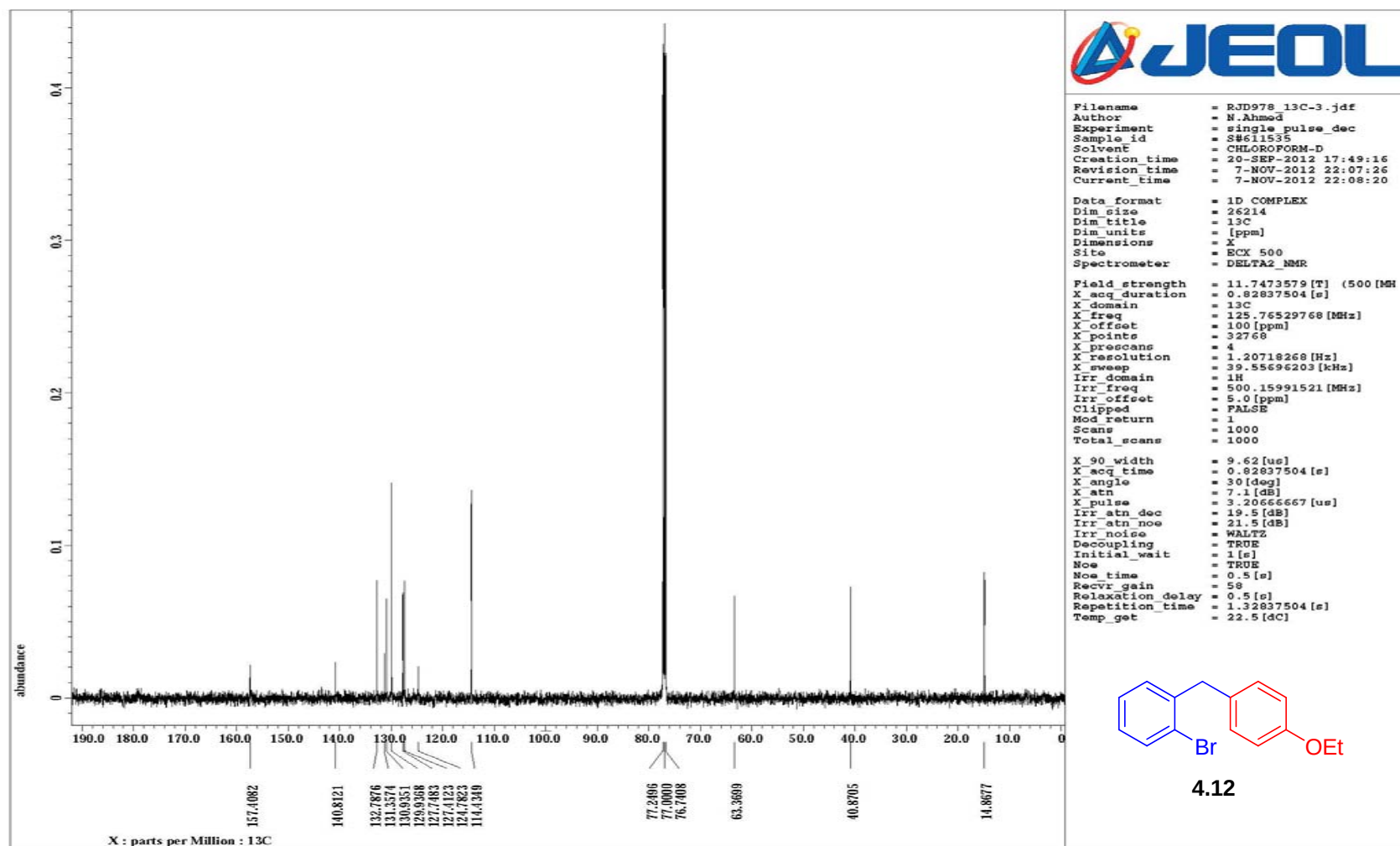
^{13}C NMR spectrum of 1-Bromo-3-(3-methoxybenzyl)benzene (**4.11**)



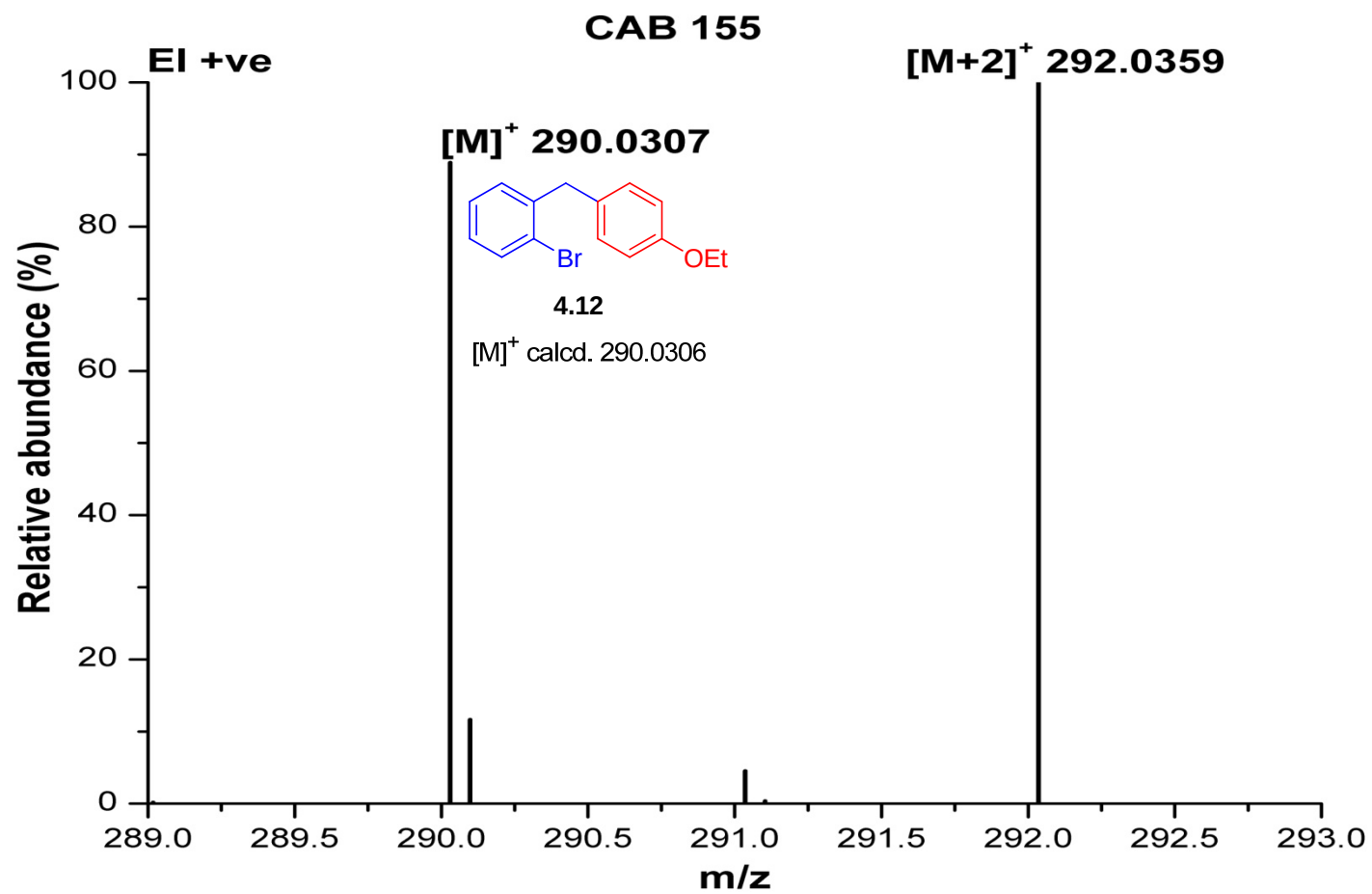
HRMS spectrum of 1-Bromo-3-(3-methoxybenzyl)benzene (**4.11**)



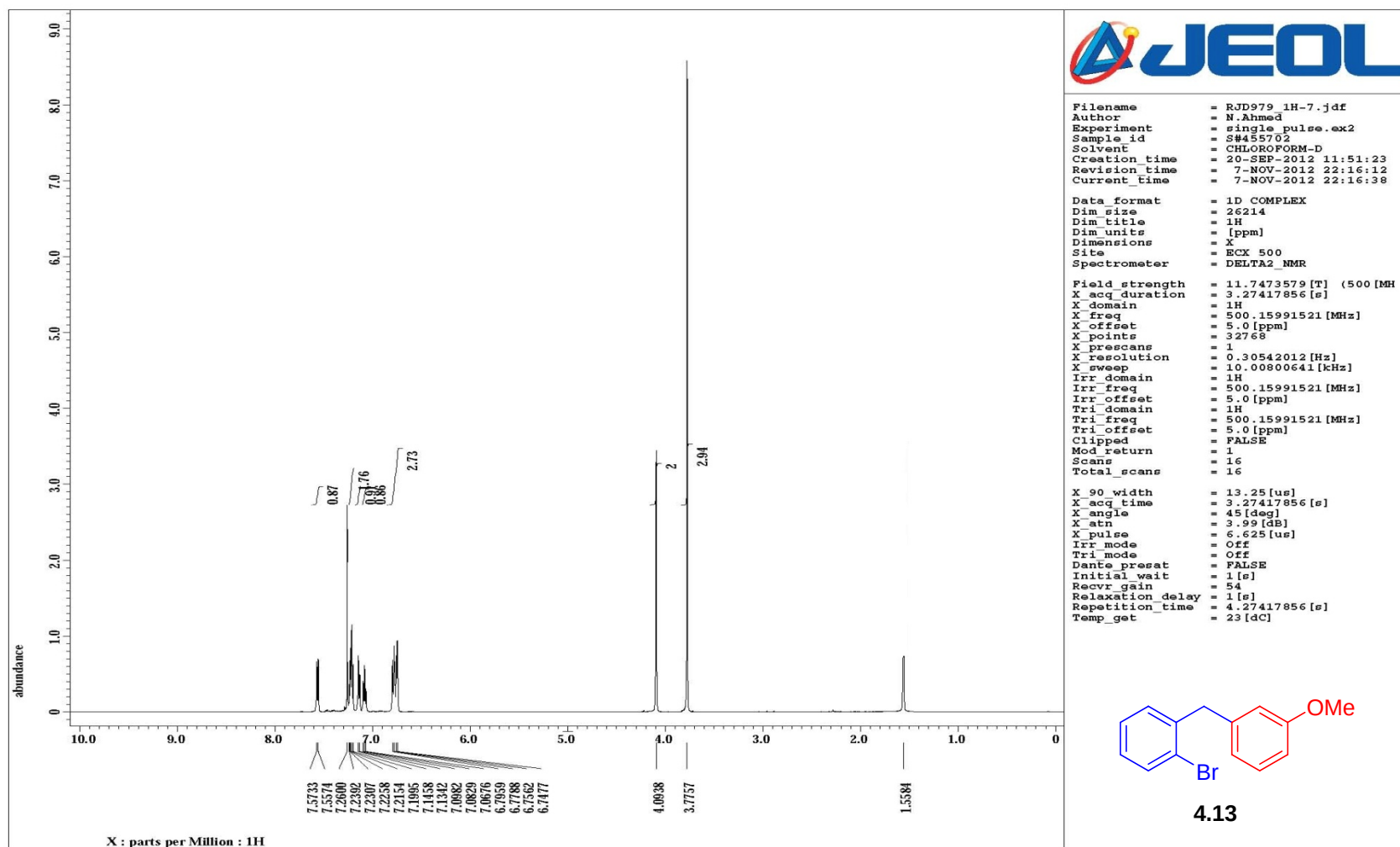
¹H NMR spectrum of 1-Bromo-2-(4-ethoxybenzyl)benzene (4.12)



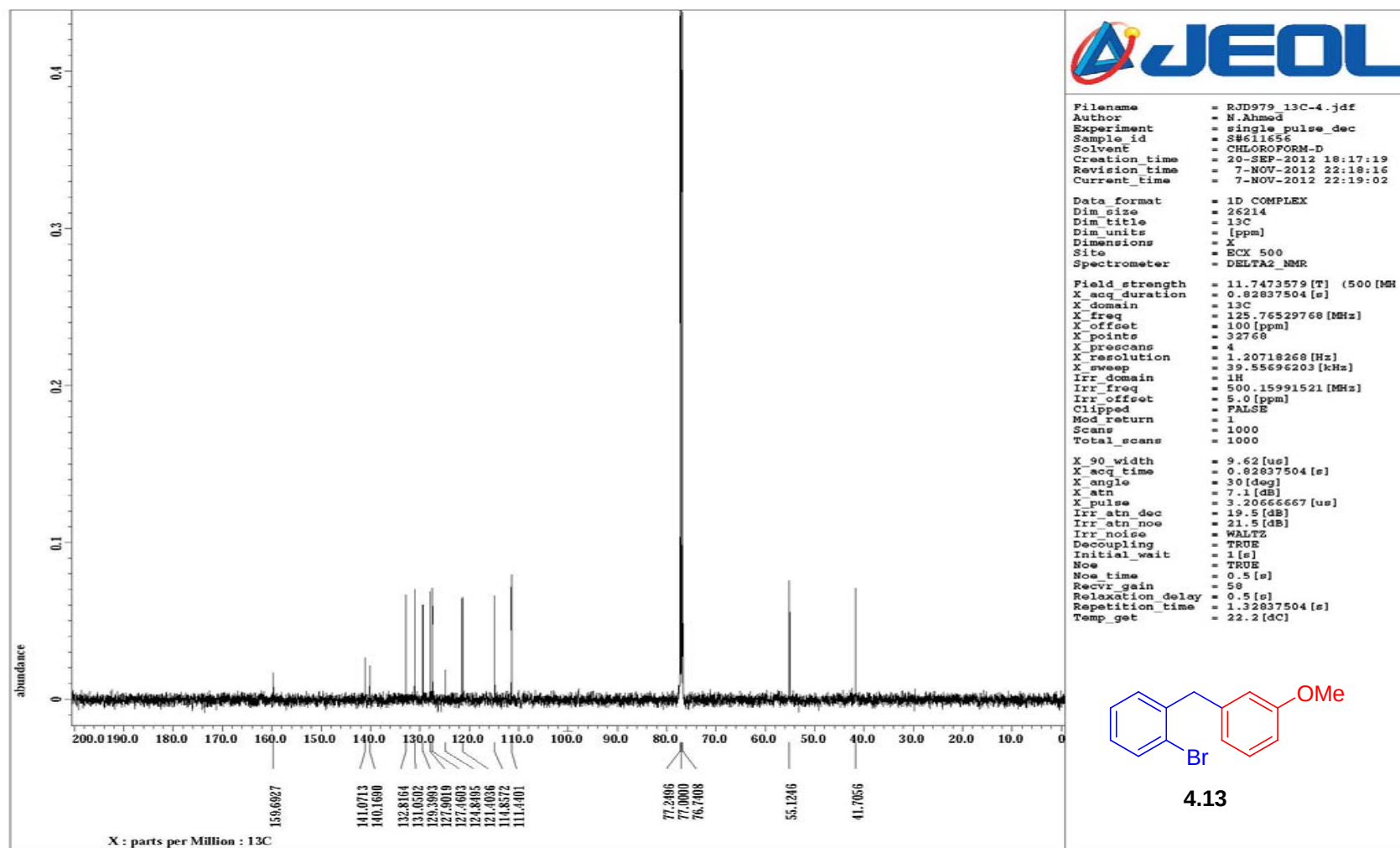
^{13}C NMR spectrum of 1-Bromo-2-(4-ethoxybenzyl)benzene (4.12)



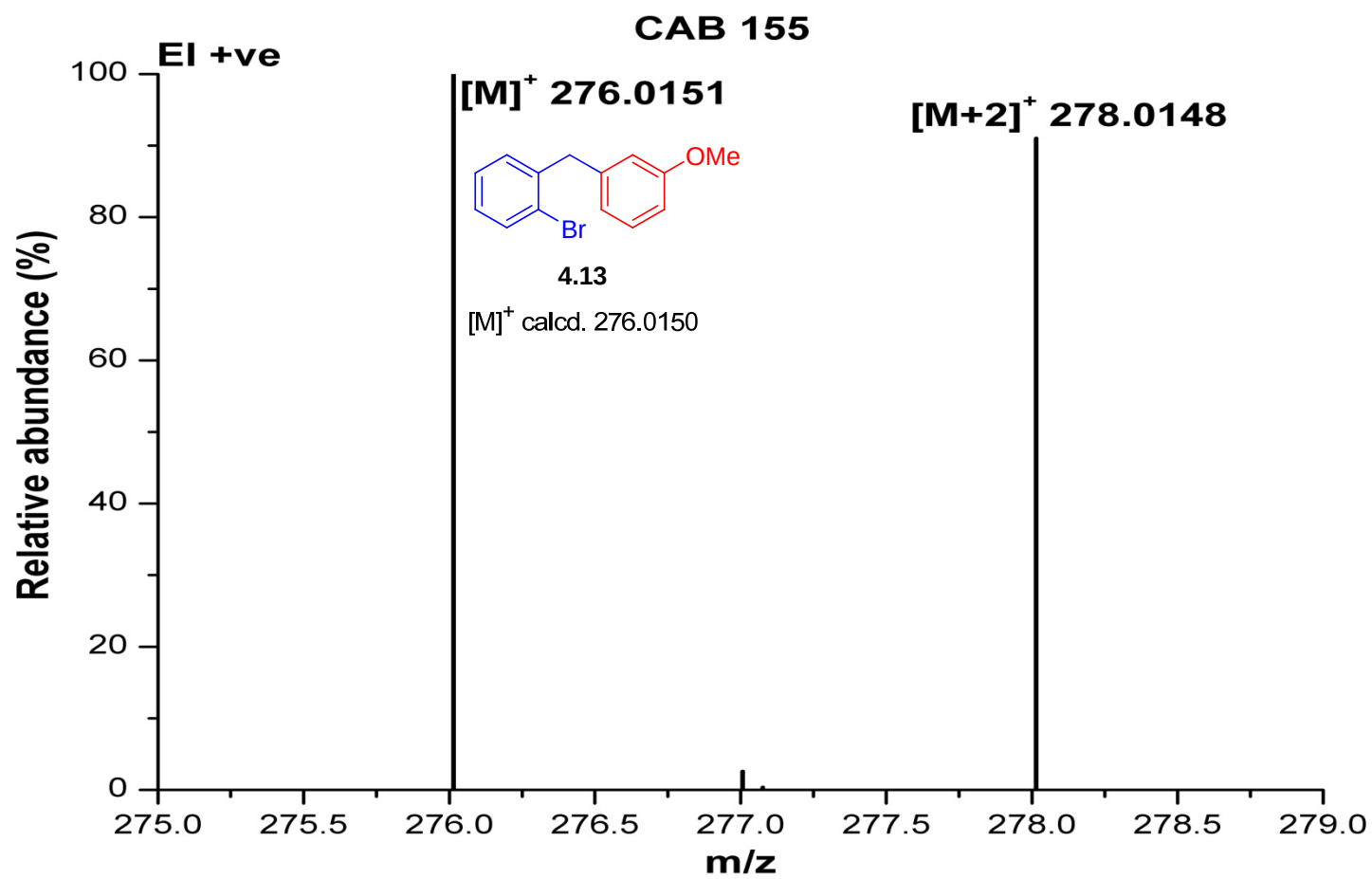
HRMS spectrum of 1-Bromo-2-(4-ethoxybenzyl)benzene (**4.12**)



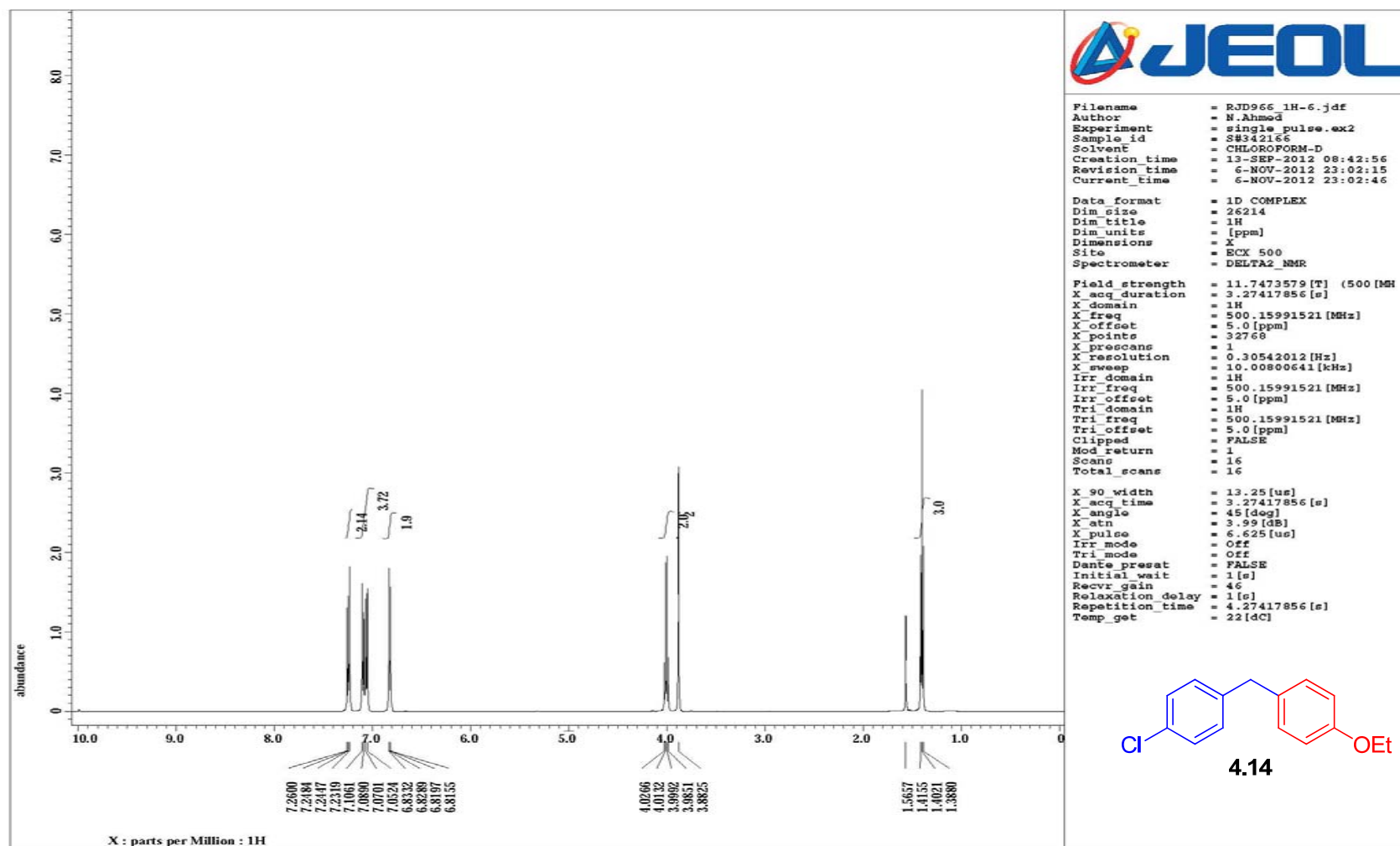
¹H NMR spectrum of 1-Bromo-2-(3-methoxybenzyl)benzene (4.13)



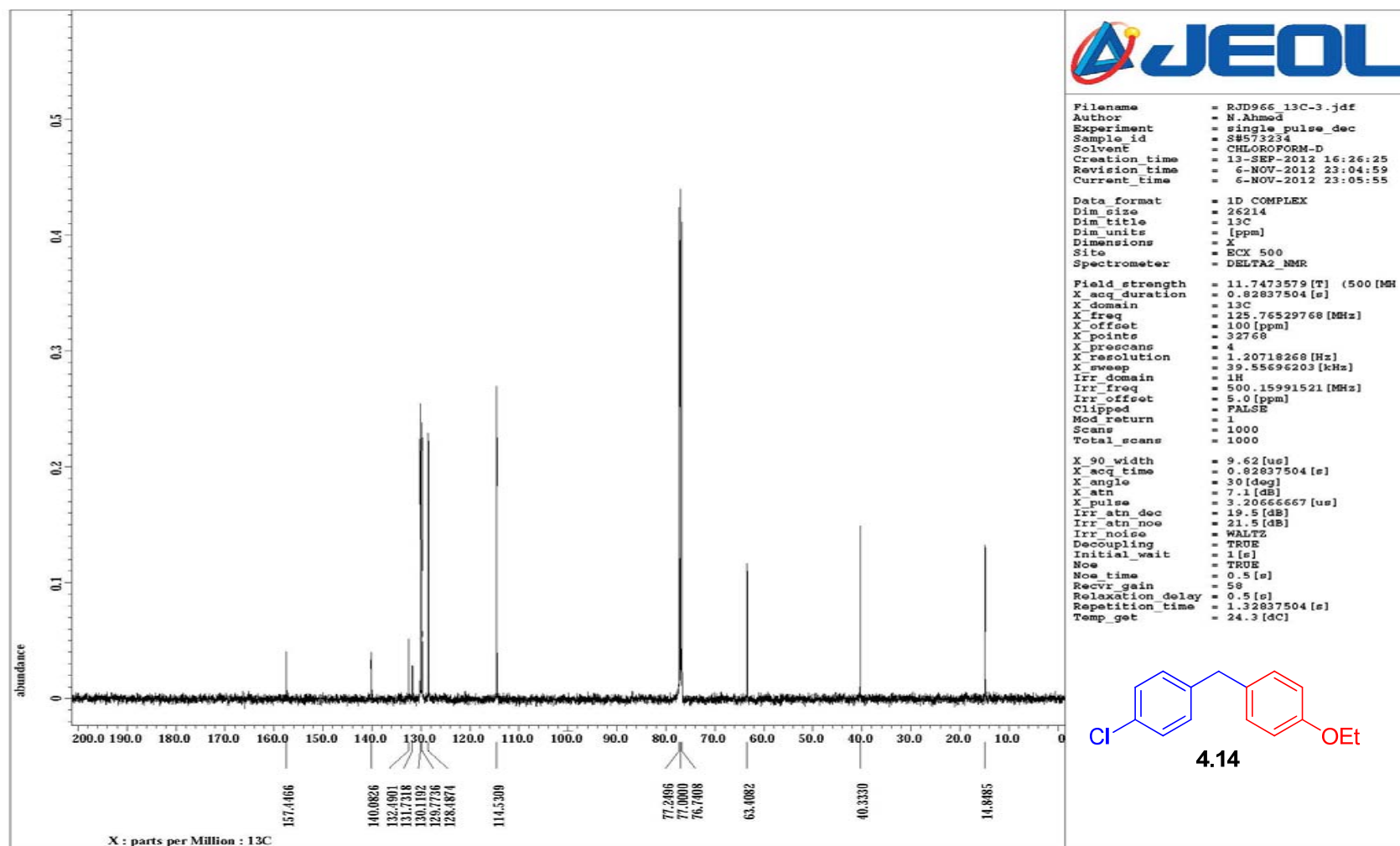
^{13}C NMR spectrum of 1-Bromo-2-(3-methoxybenzyl)benzene (**4.13**)



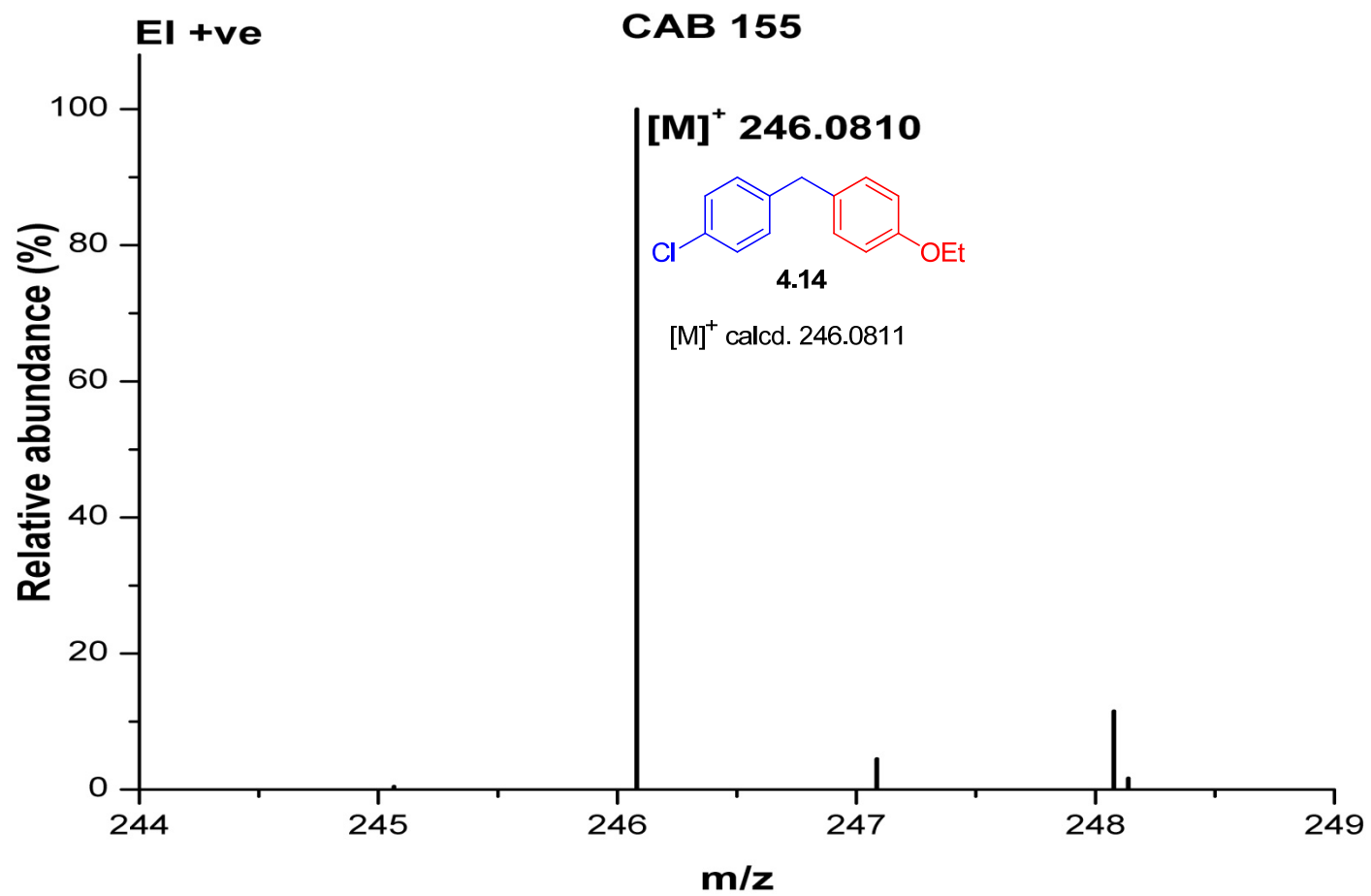
HRMS spectrum of 1-Bromo-2-(3-methoxybenzyl)benzene (**4.13**)



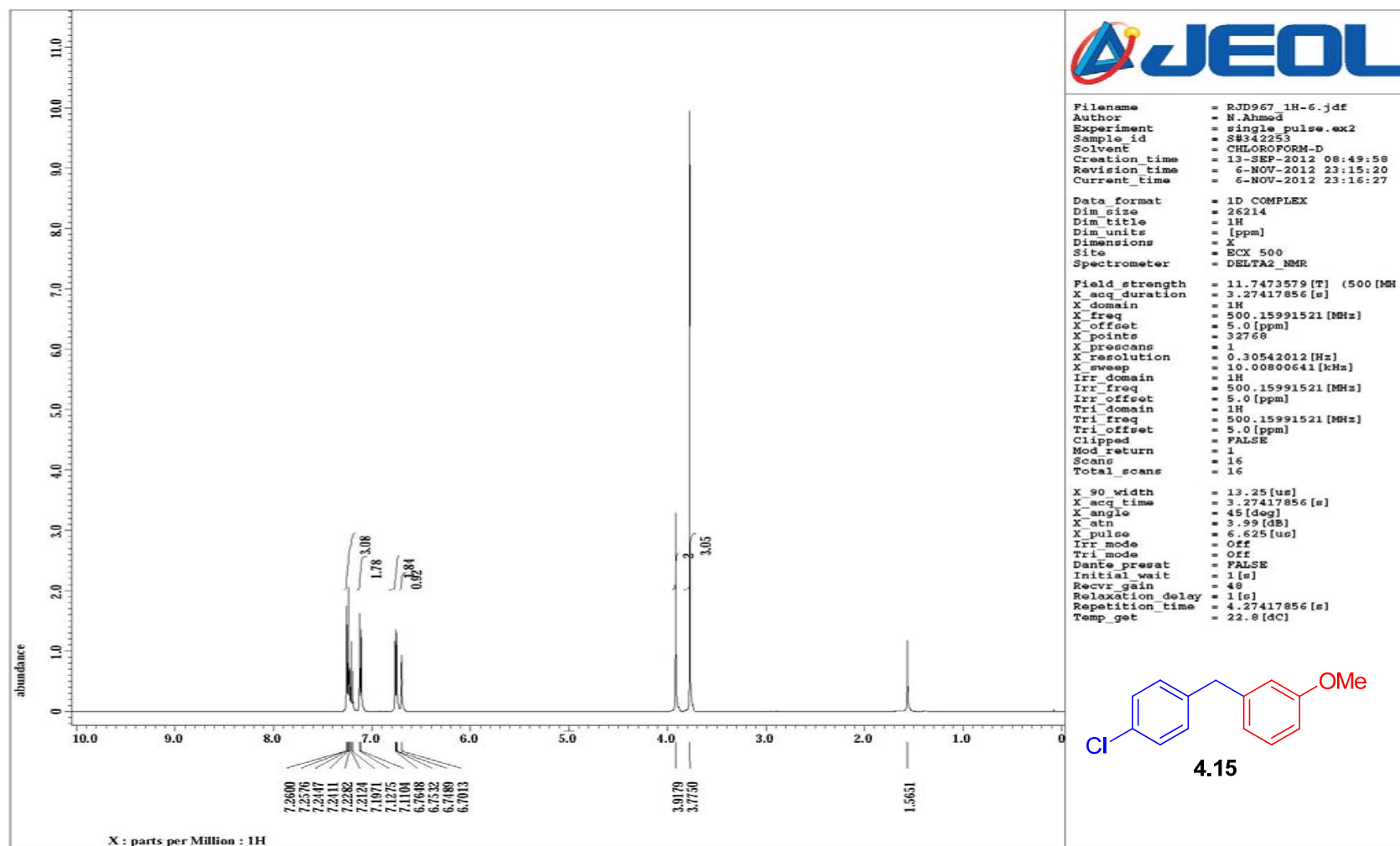
¹H NMR spectrum of 1-Chloro-4-(4-ethoxybenzyl)benzene (4.14)



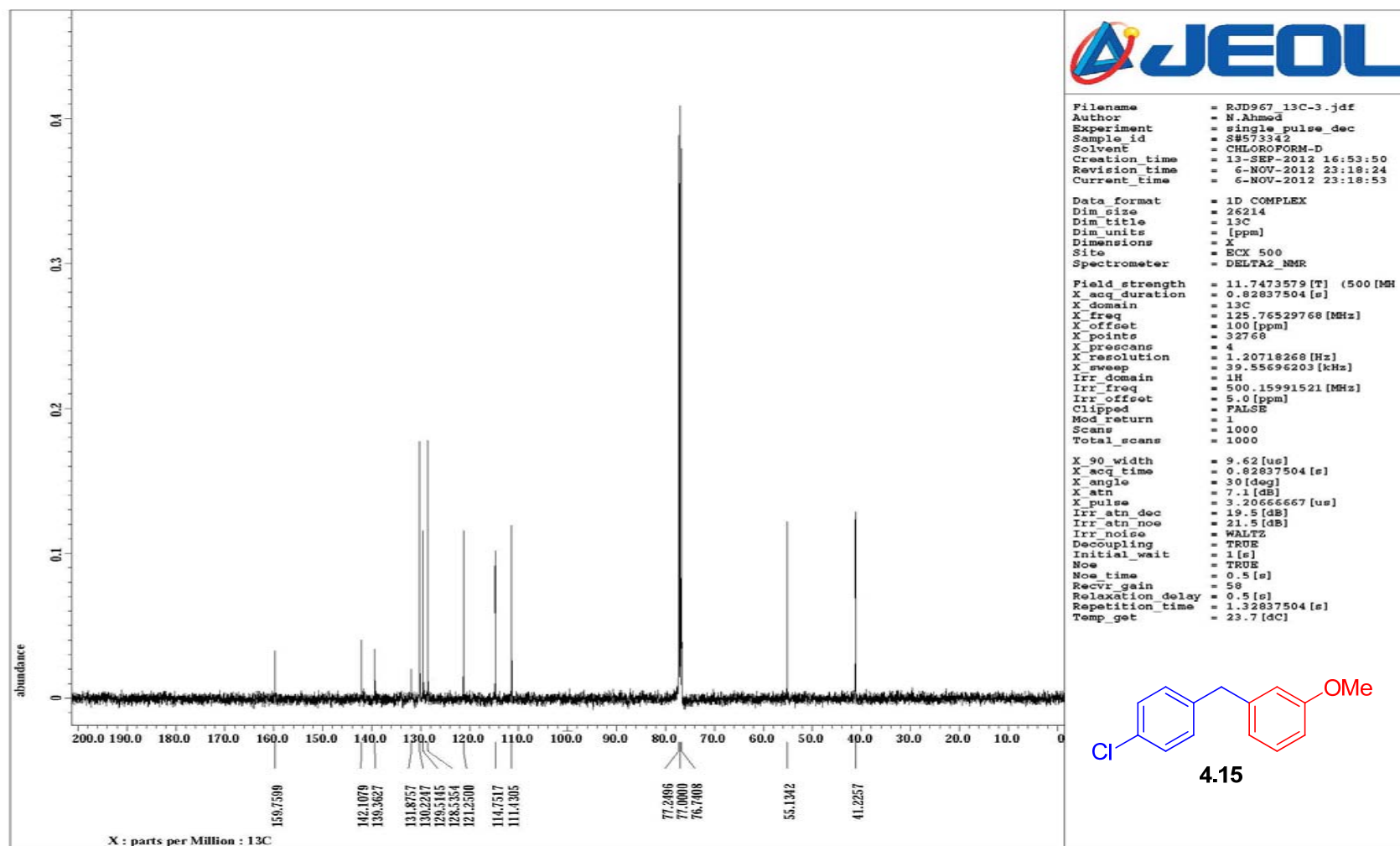
^{13}C NMR spectrum of 1-Chloro-4-(4-ethoxybenzyl)benzene (4.14)



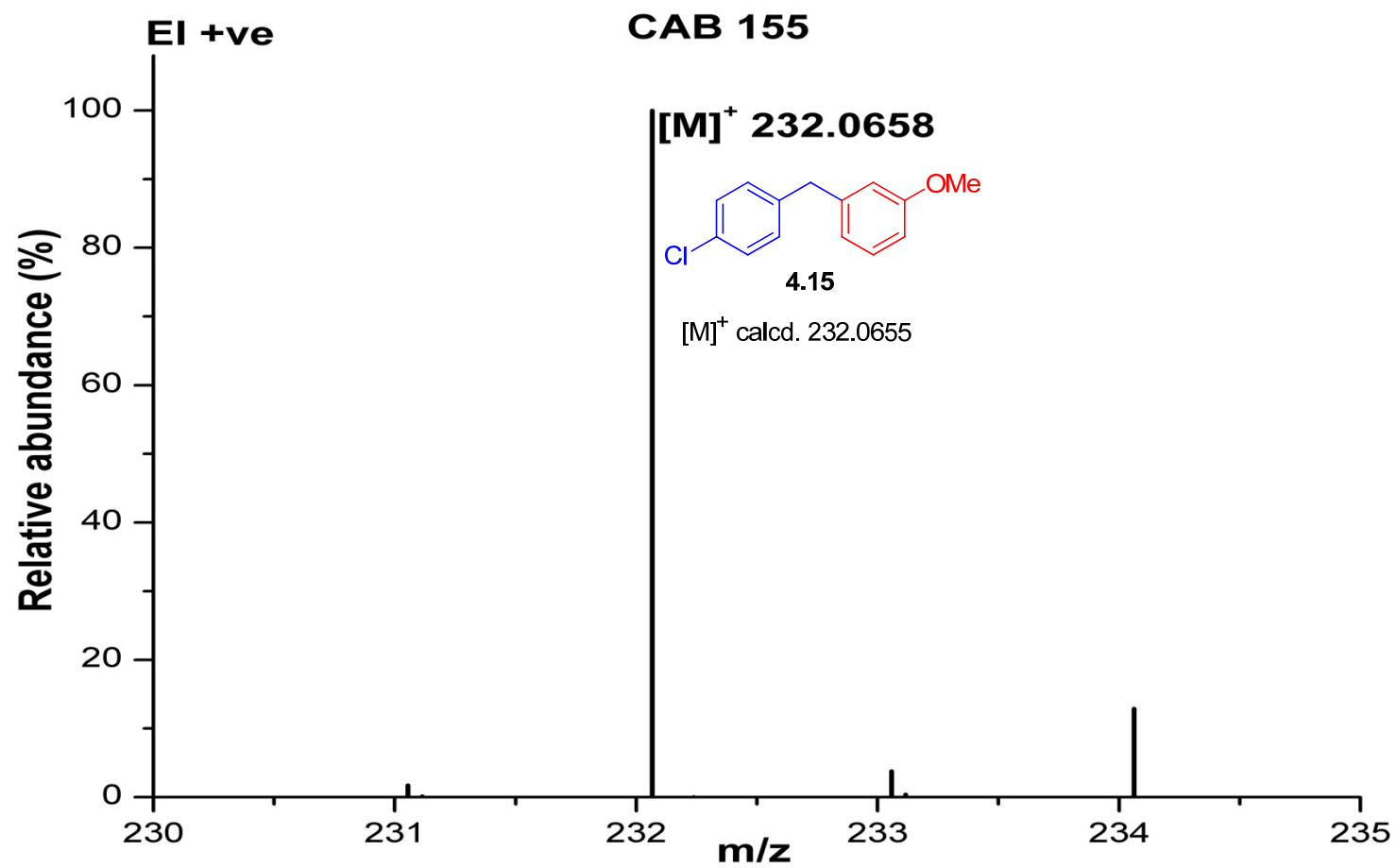
HRMS spectrum of 1-Chloro-4-(4-ethoxybenzyl)benzene (**4.14**)



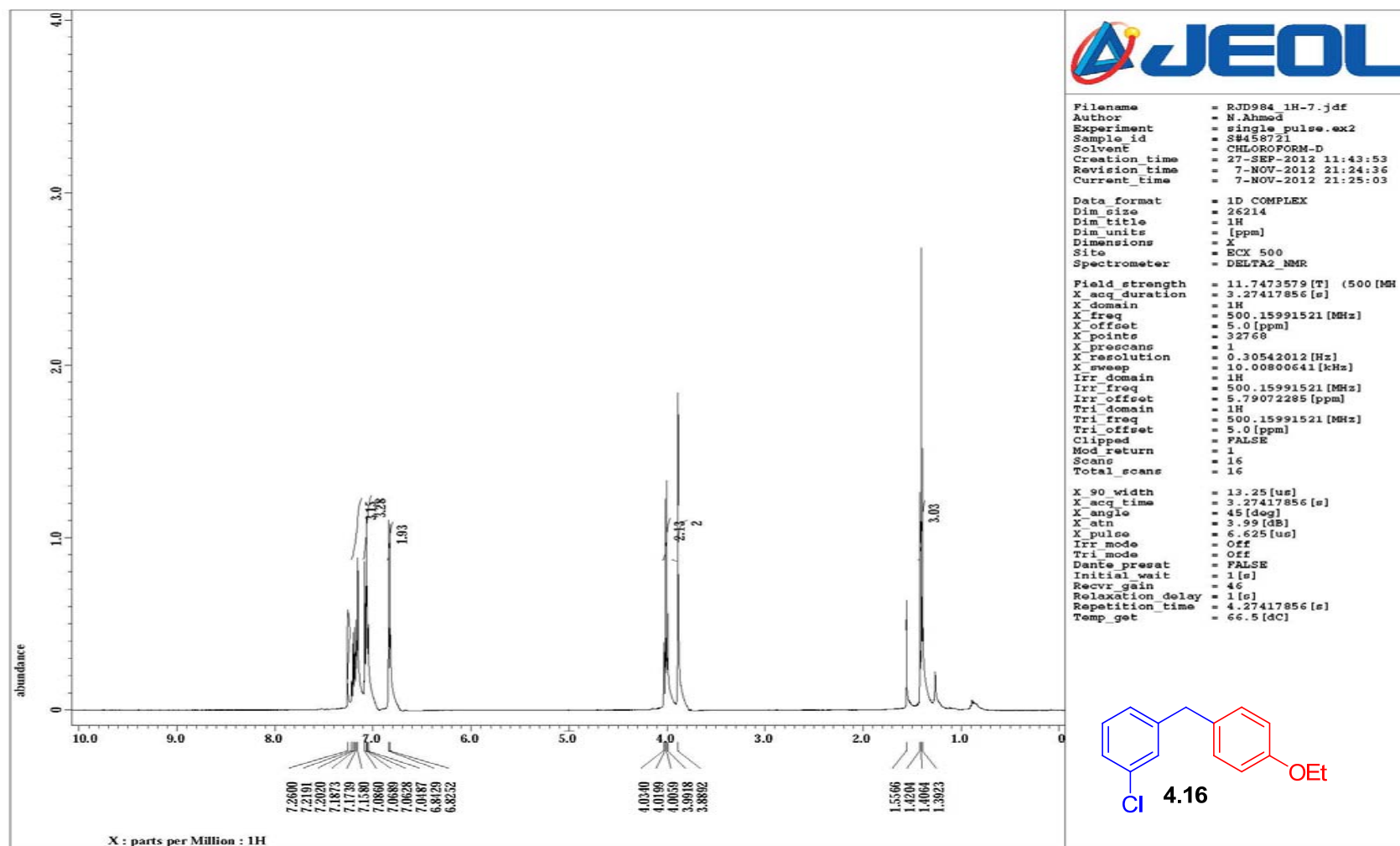
¹H NMR spectrum of 1-(4-chlorobenzyl)-3-methoxybenzene (4.15)



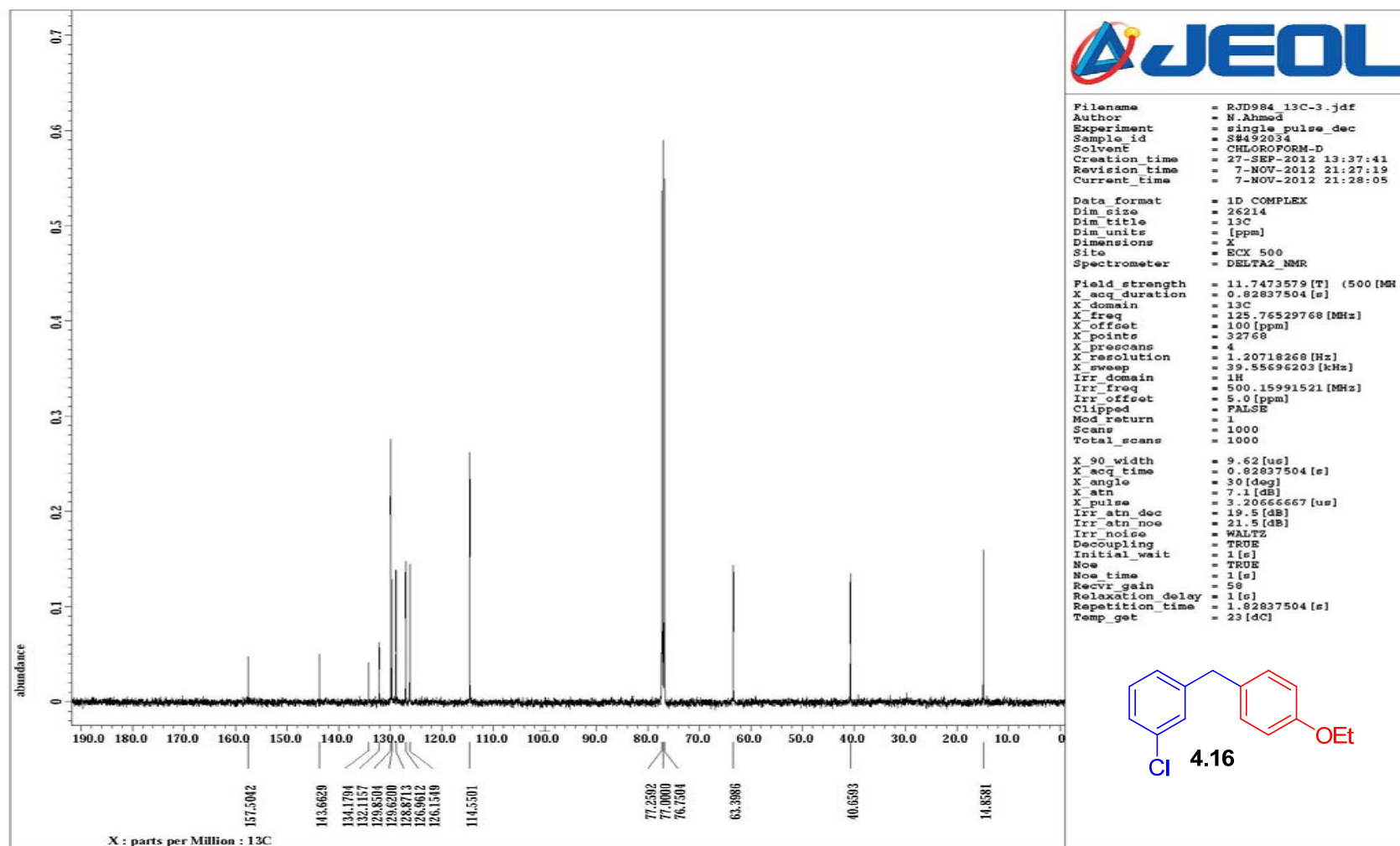
^{13}C NMR spectrum of 1-(4-Chlorobenzyl)-3-methoxybenzene (**4.15**)



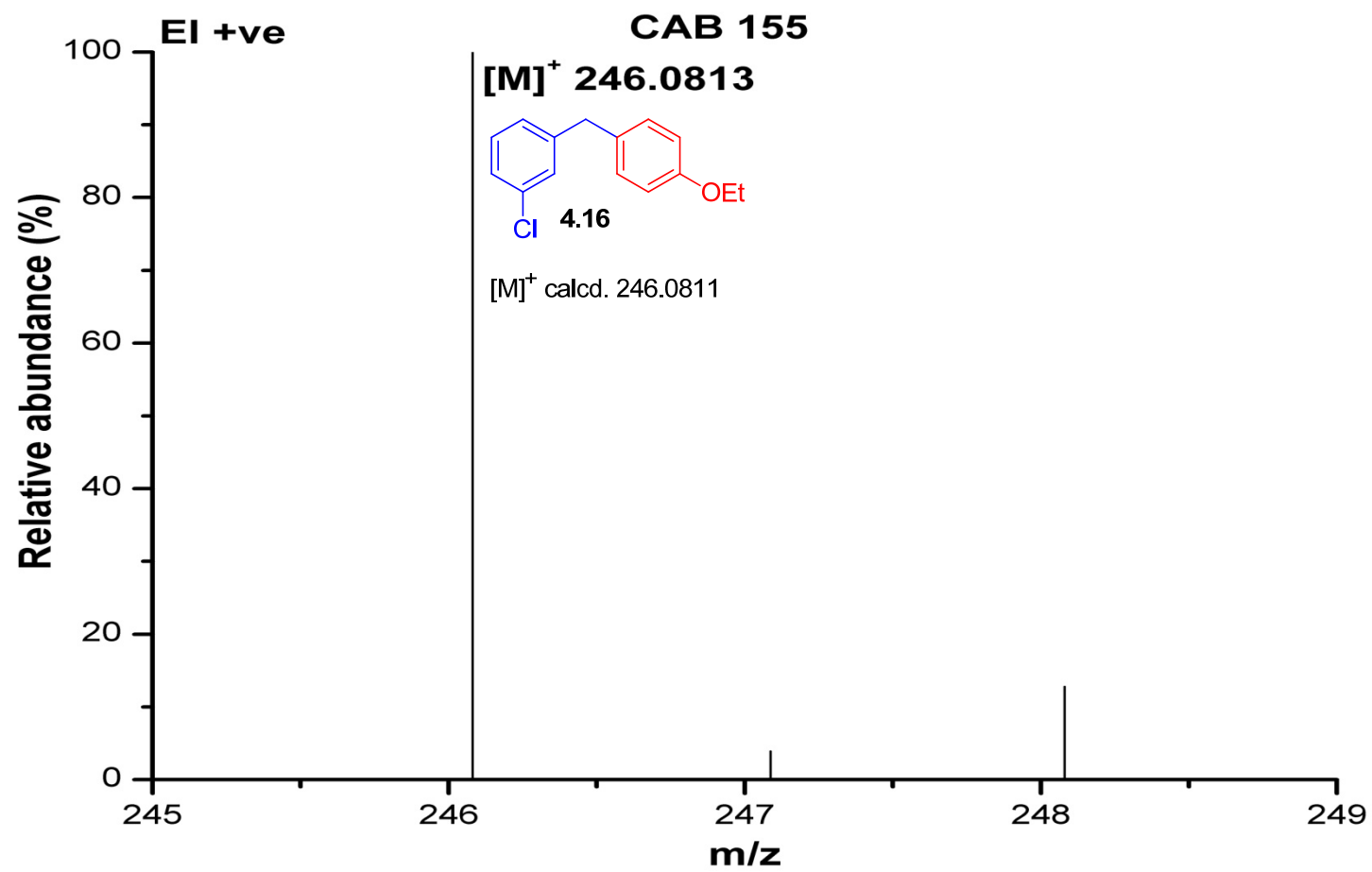
HRMS spectrum of 1-(4-Chlorobenzyl)-3-methoxybenzene (4.15)



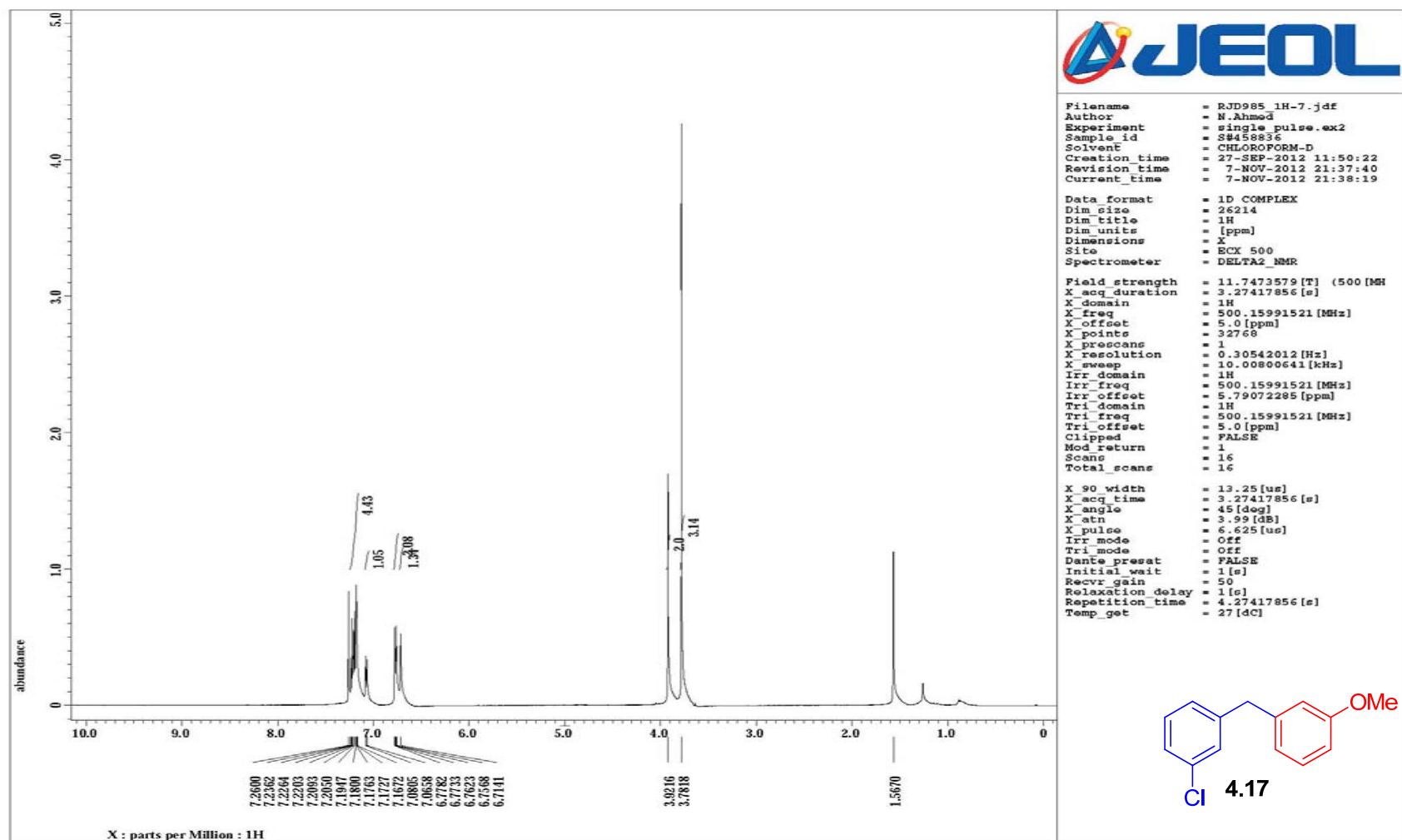
¹H NMR spectrum of 1-Chloro-3-(4-ethoxybenzyl)benzene (4.16)



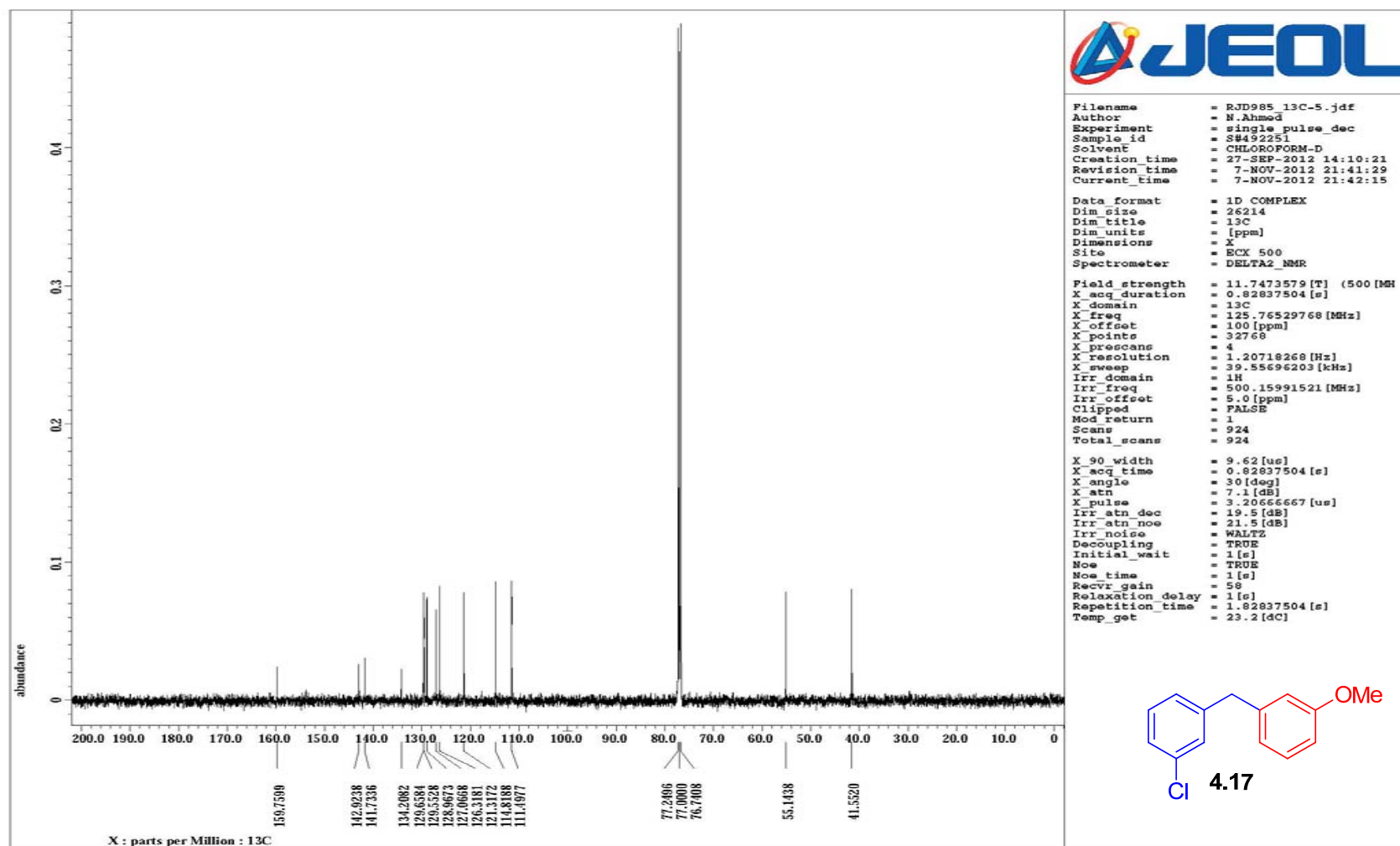
¹³C NMR spectrum of 1-Chloro-3-(4-ethoxybenzyl)benzene (4.16)



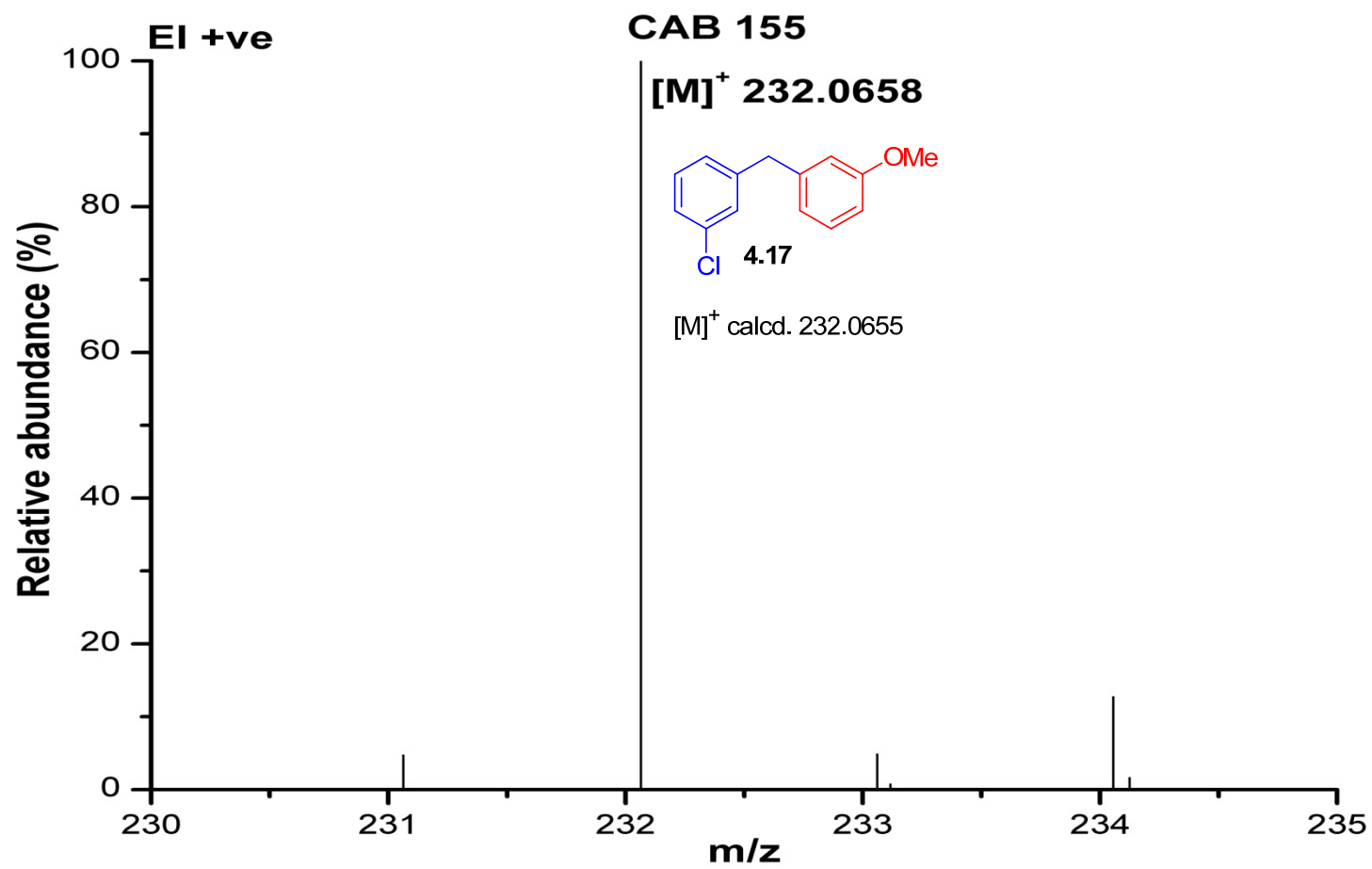
HRMS spectrum of 1-Chloro-3-(4-ethoxybenzyl)benzene (**4.16**)



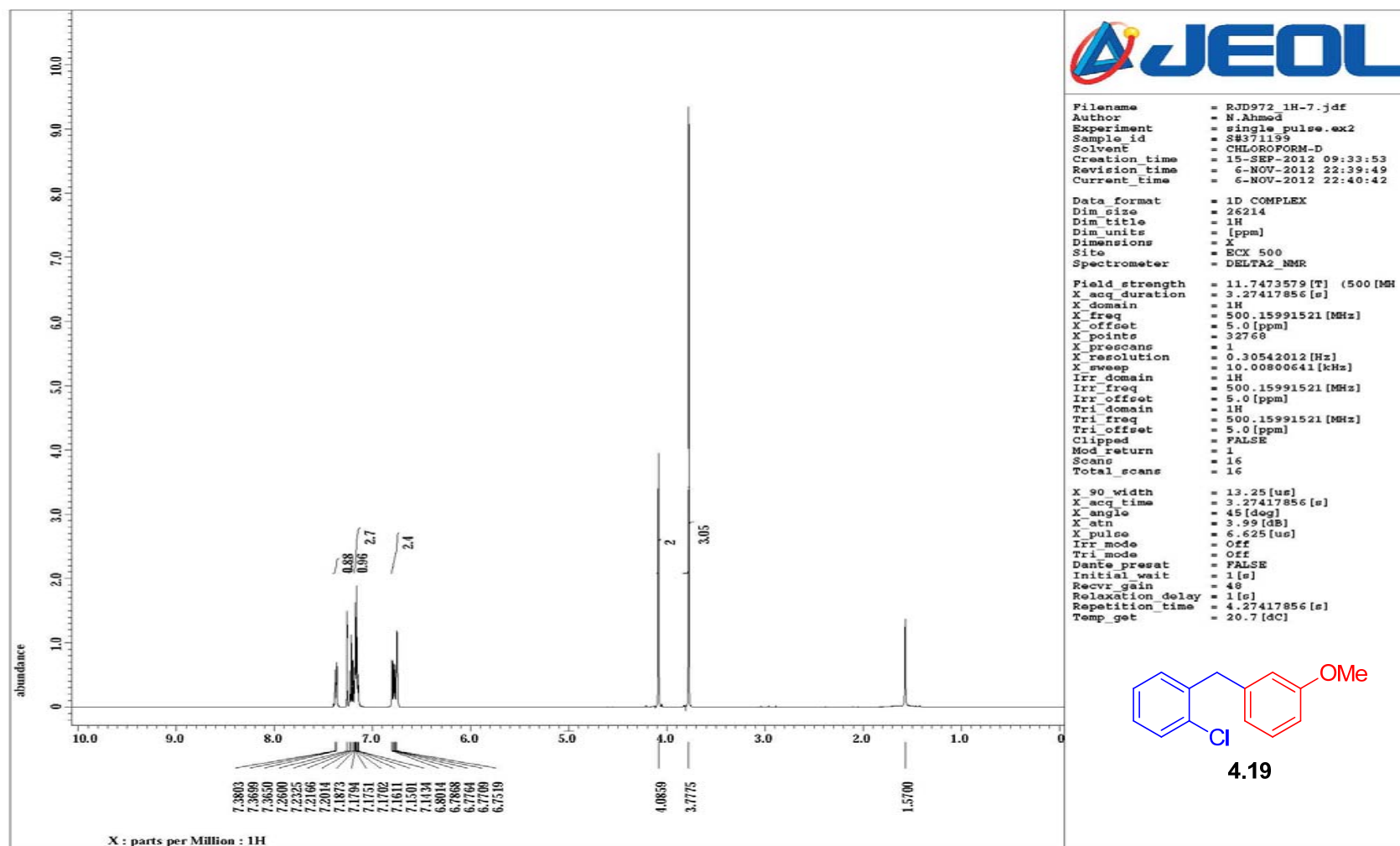
¹H NMR spectrum of 1-Chloro-3-(3-methoxybenzyl)benzene (4.17)



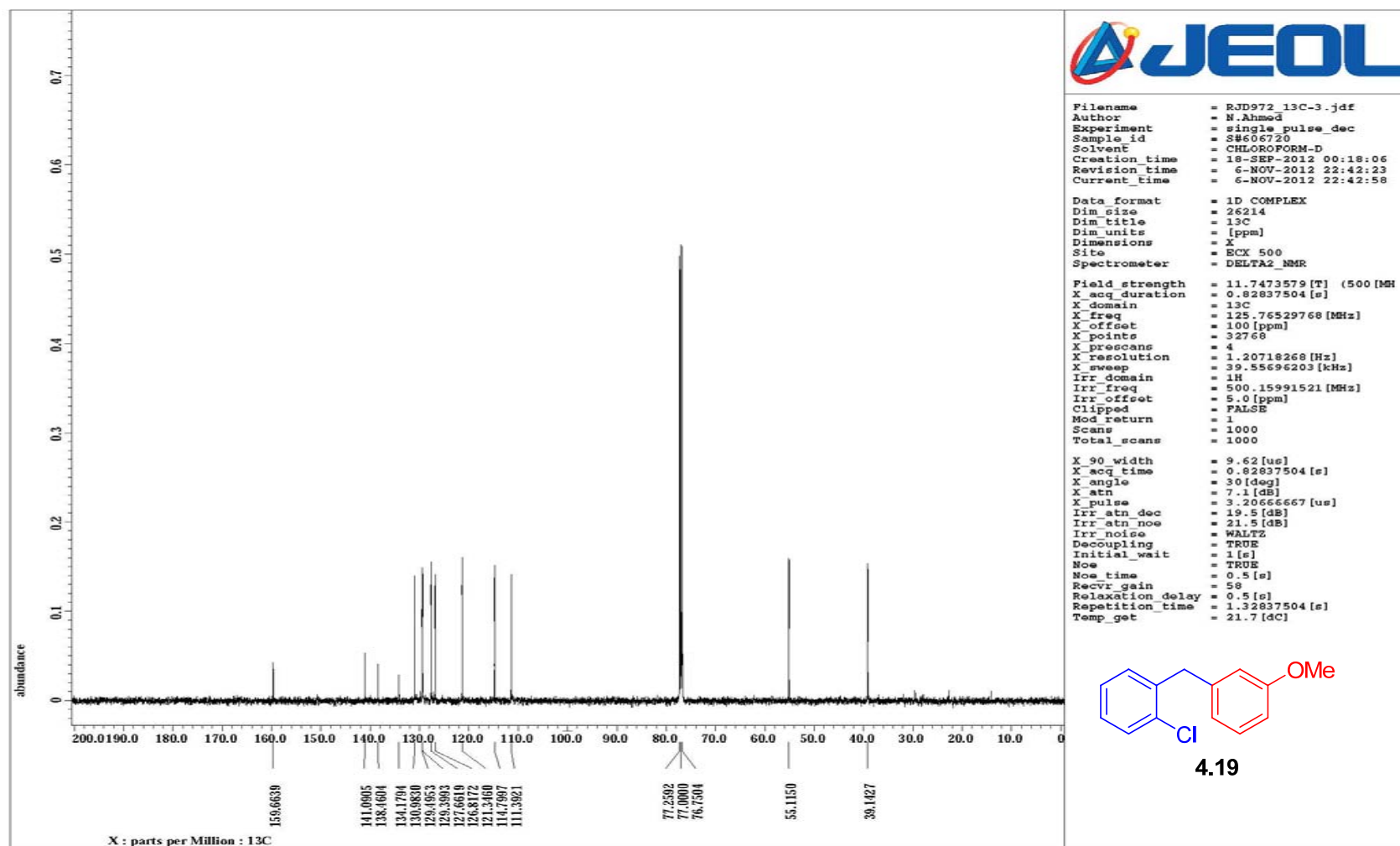
^{13}C NMR spectrum of 1-Chloro-3-(3-methoxybenzyl)benzene (**4.17**)



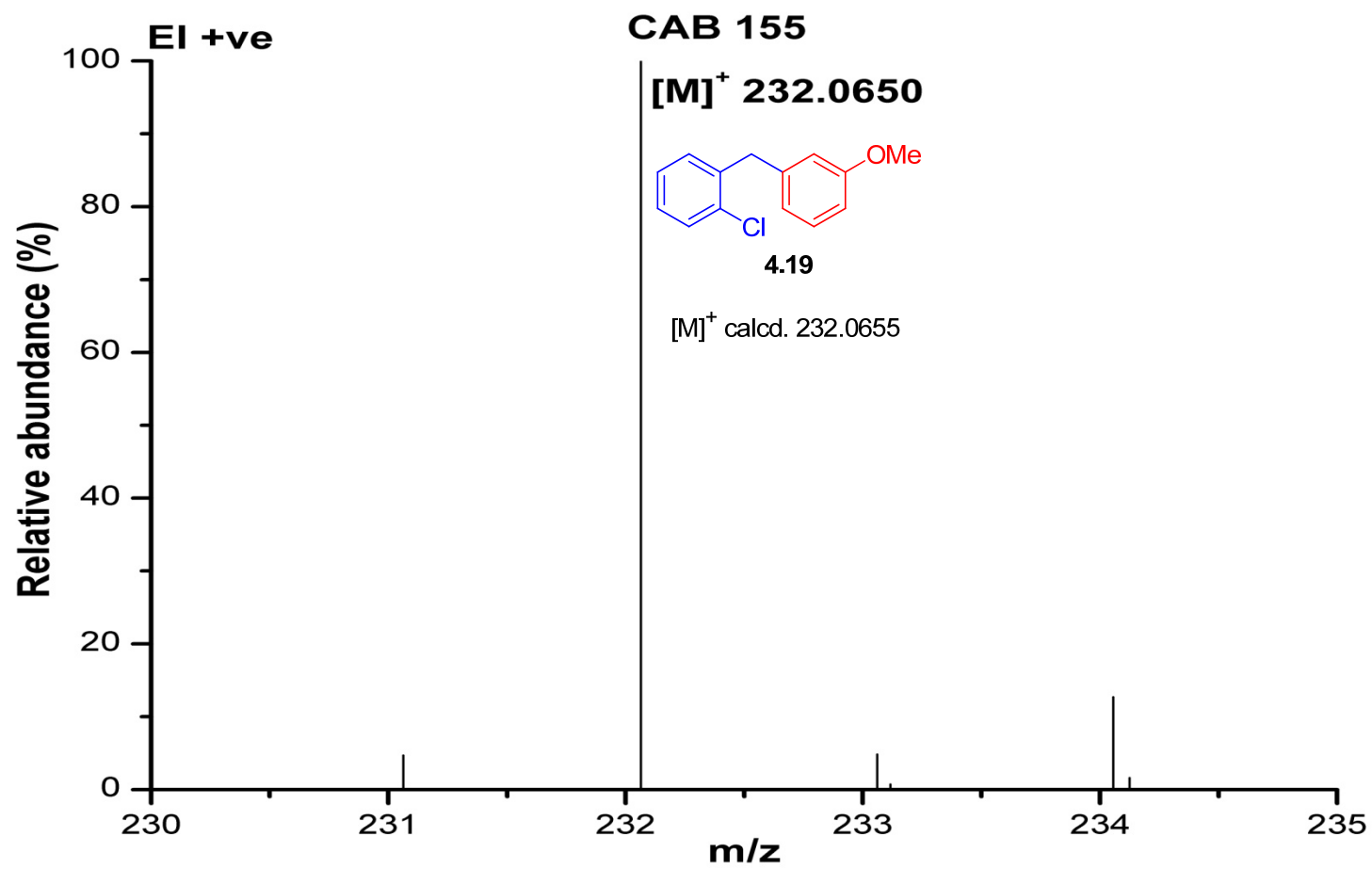
HRMS spectrum of 1-Chloro-3-(3-methoxybenzyl)benzene (**4.17**)



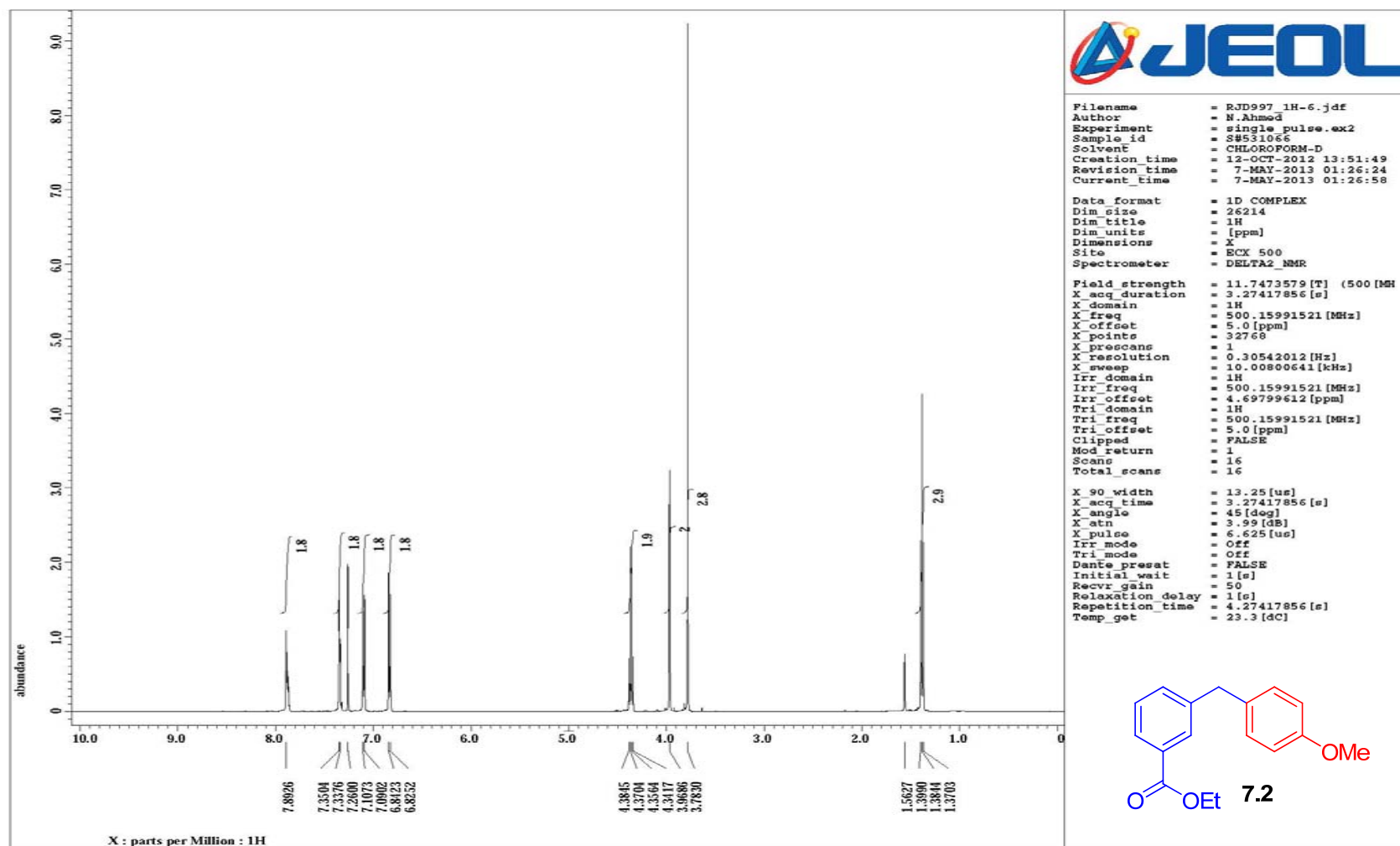
¹H NMR spectrum of 1-Chloro-2-(3-methoxybenzyl)benzene (4.19)



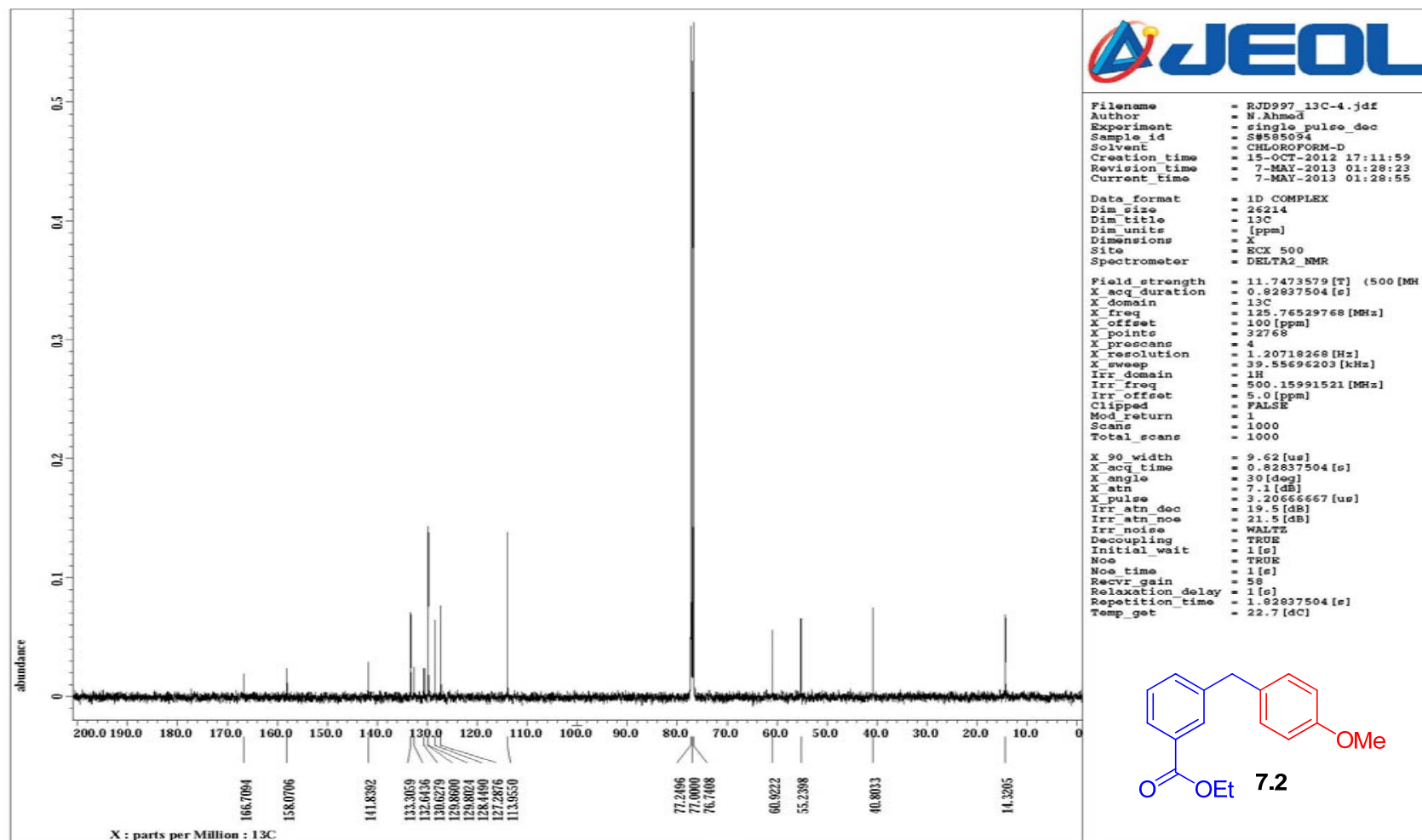
^{13}C NMR spectrum of 1-Chloro-2-(3-methoxybenzyl)benzene (**4.19**)



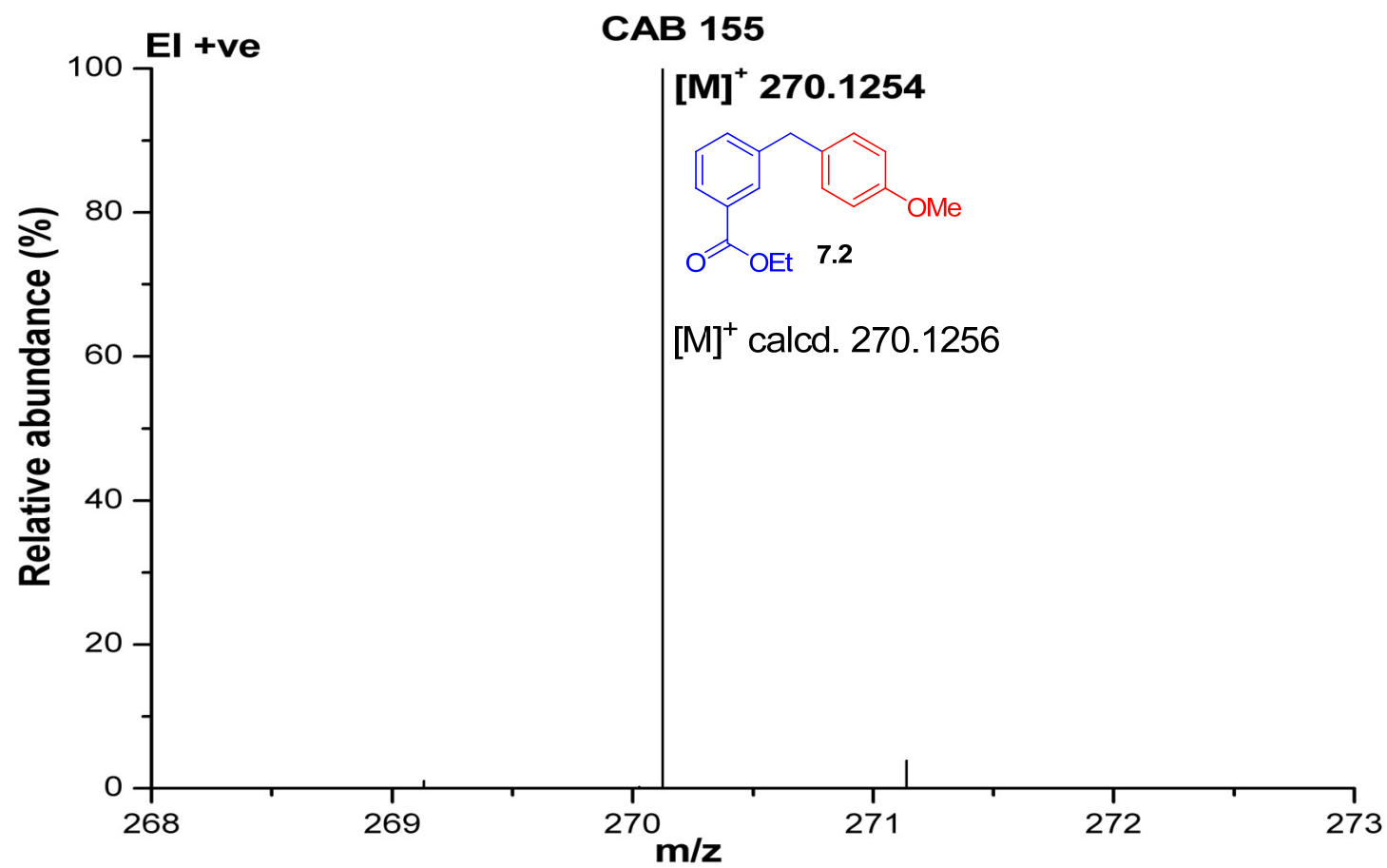
HRMS spectrum of 1-Chloro-2-(3-methoxybenzyl)benzene (**4.19**)



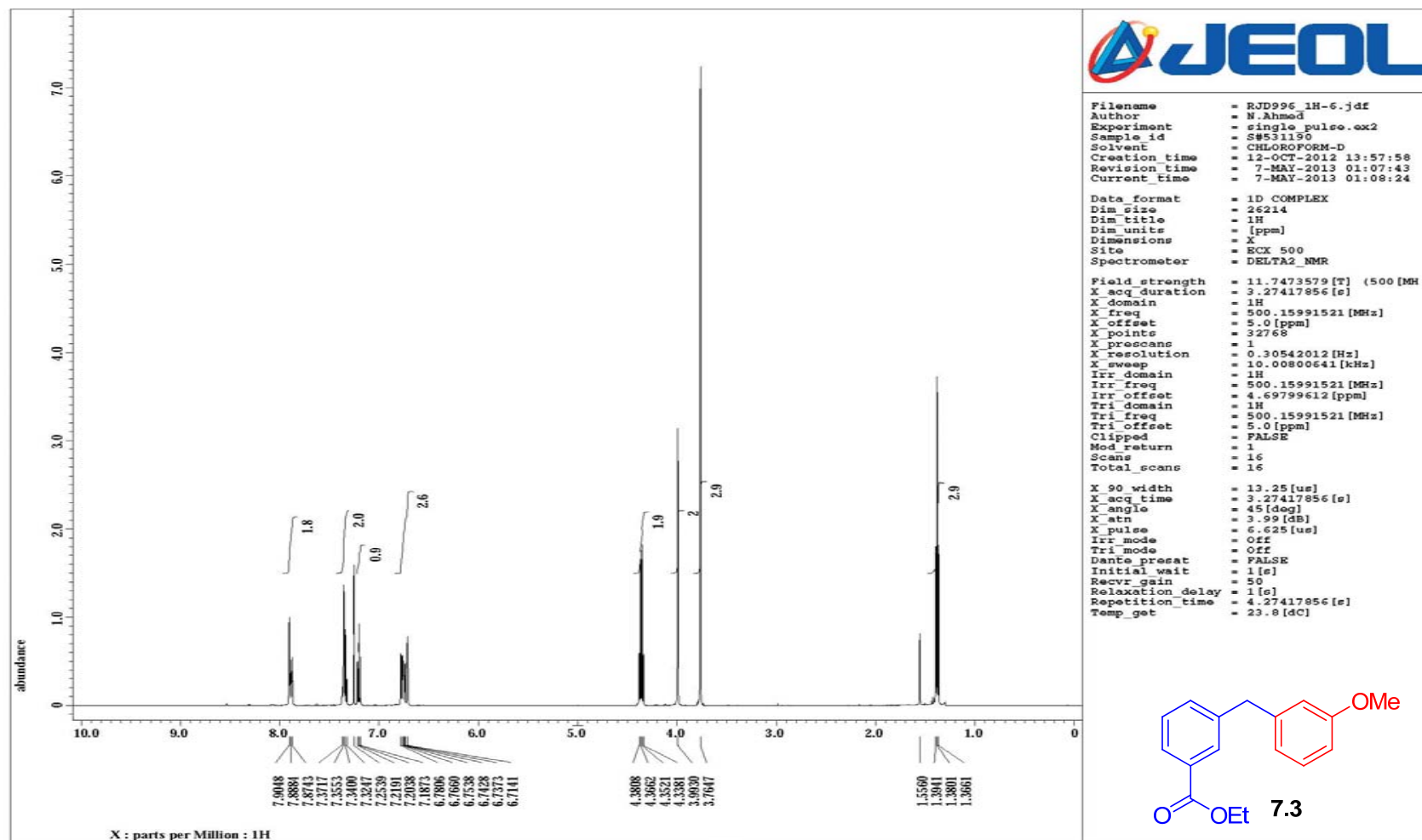
¹H NMR spectrum of Ethyl 3-(4-methoxybenzyl)benzoate (7.2)



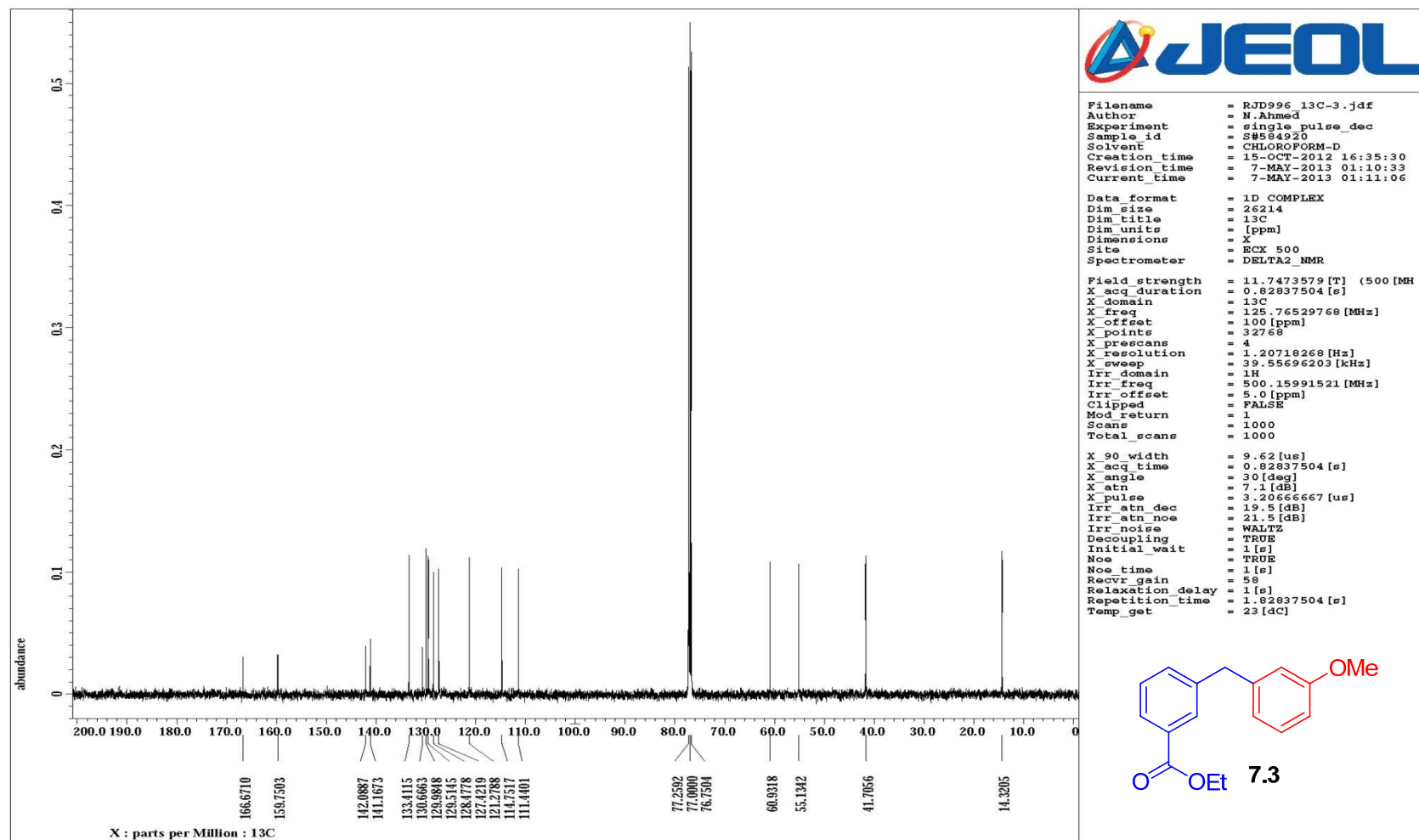
¹³C NMR spectrum of Ethyl 3-(4-methoxybenzyl)benzoate (7.2)



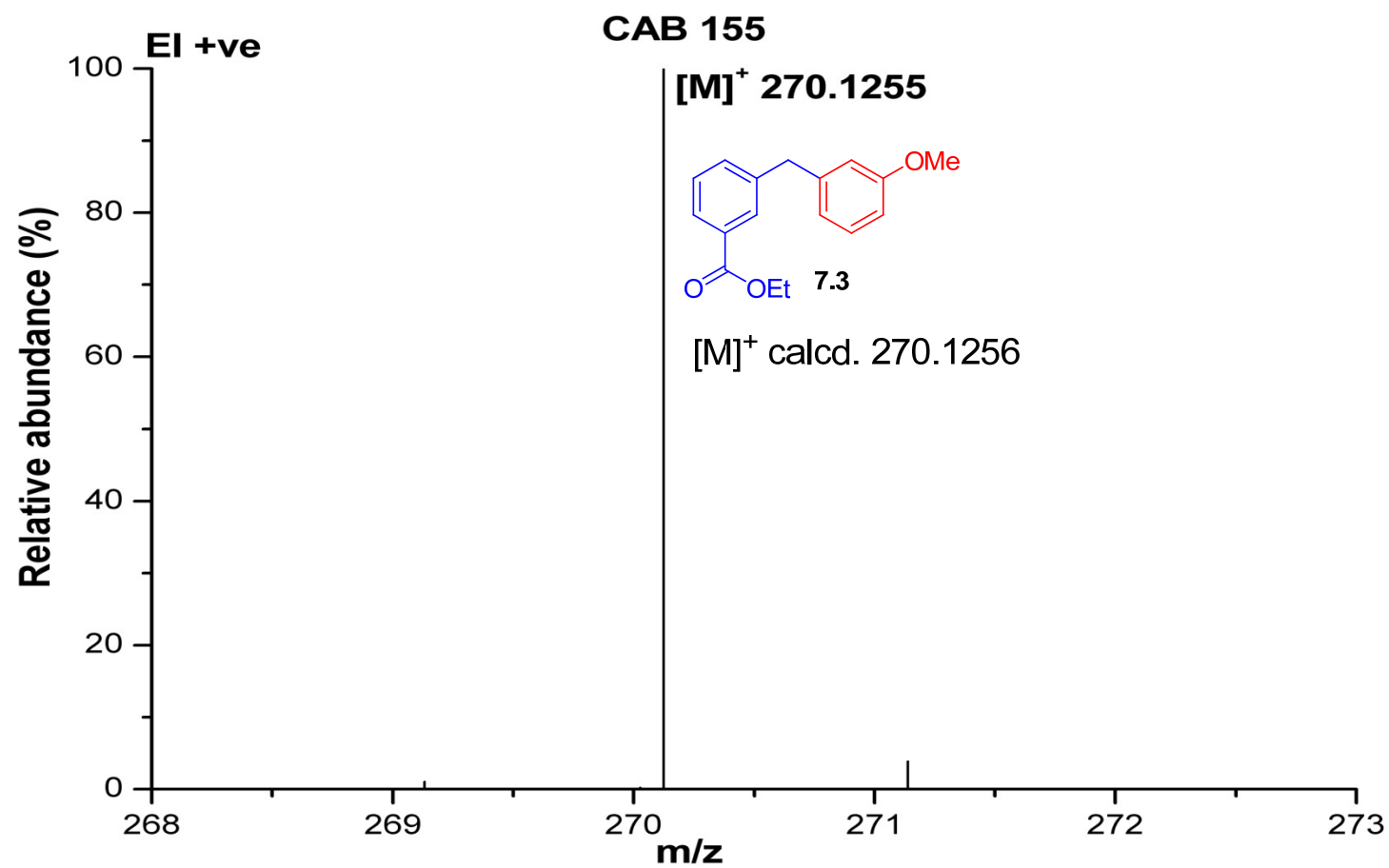
HRMS spectrum of Ethyl 3-(4-methoxybenzyl)benzoate (7.2)



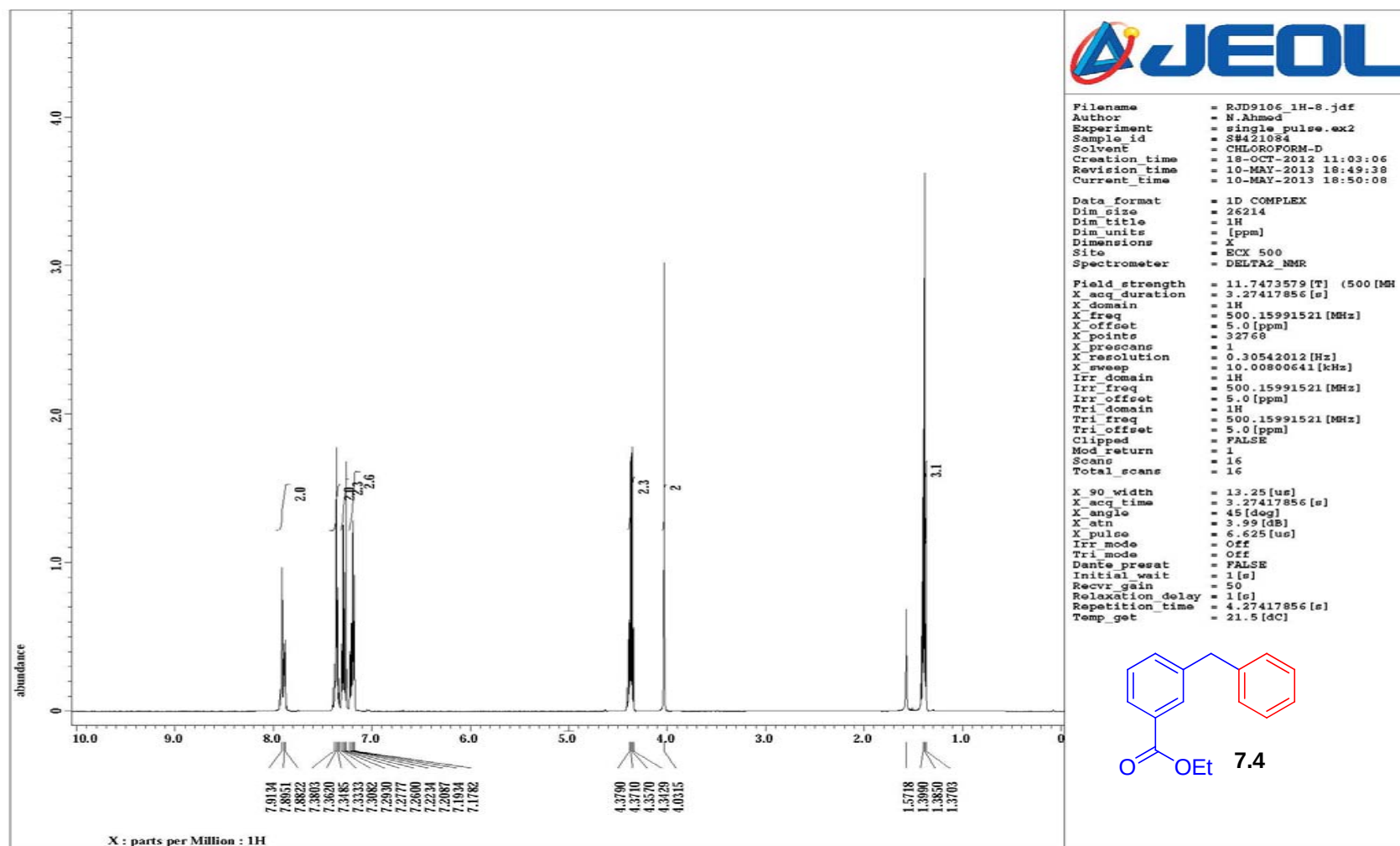
¹H NMR spectrum of Ethyl 3-(3-methoxybenzyl)benzoate (7.3)



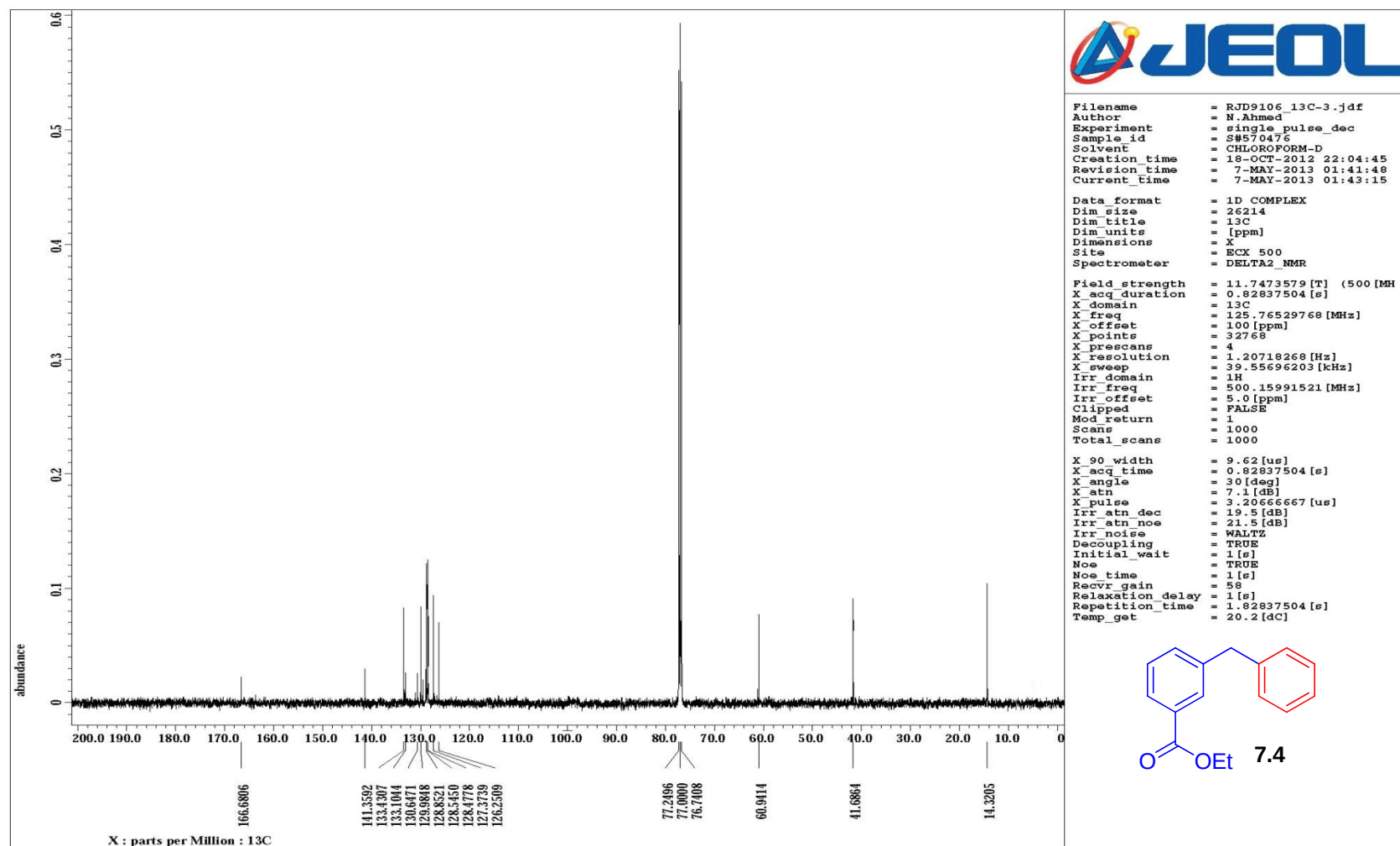
^{13}C NMR spectrum of Ethyl 3-(3-methoxybenzyl)benzoate (**7.3**)



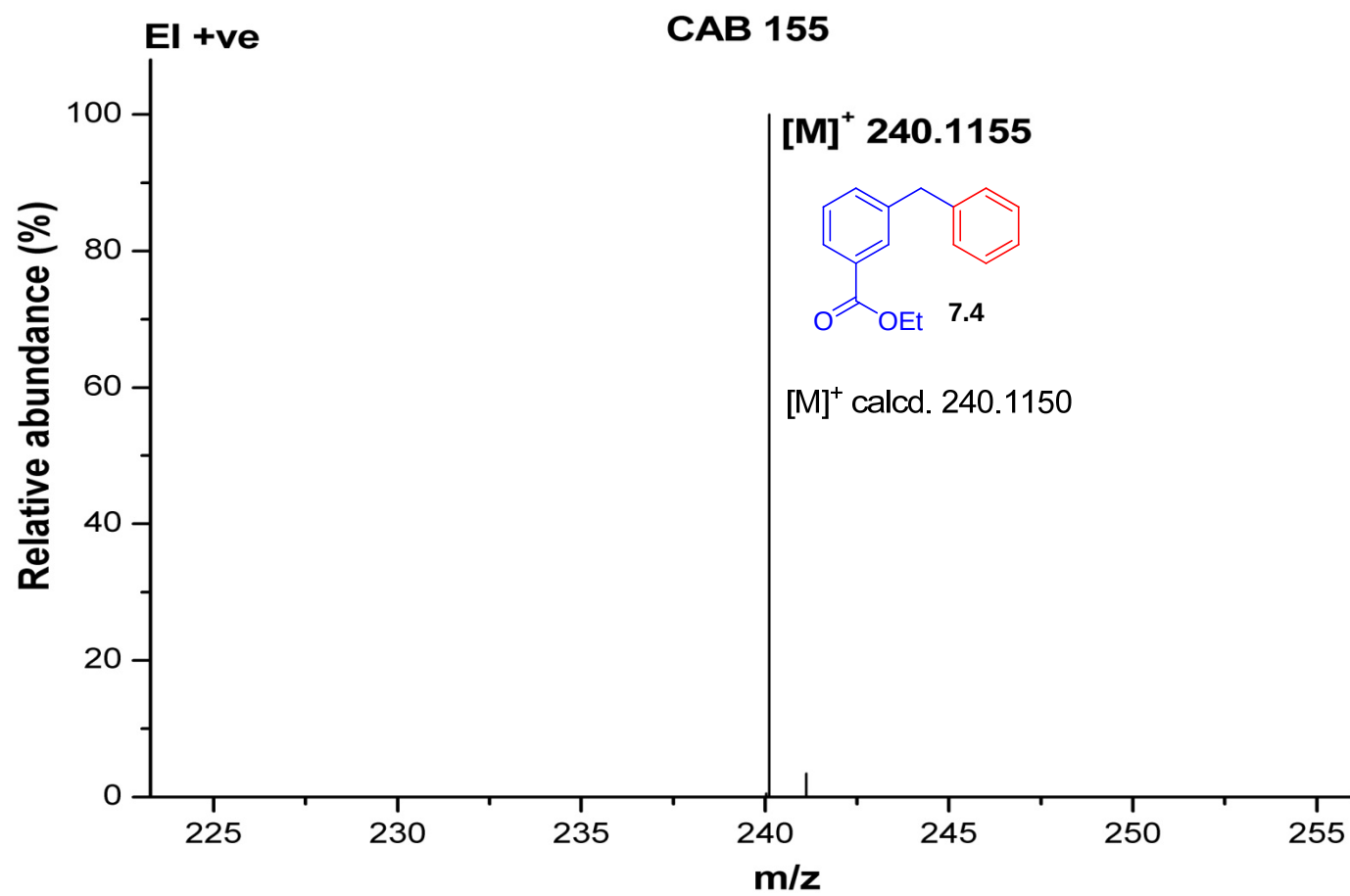
HRMS spectrum of Ethyl 3-(3-methoxybenzyl)benzoate (**7.3**)



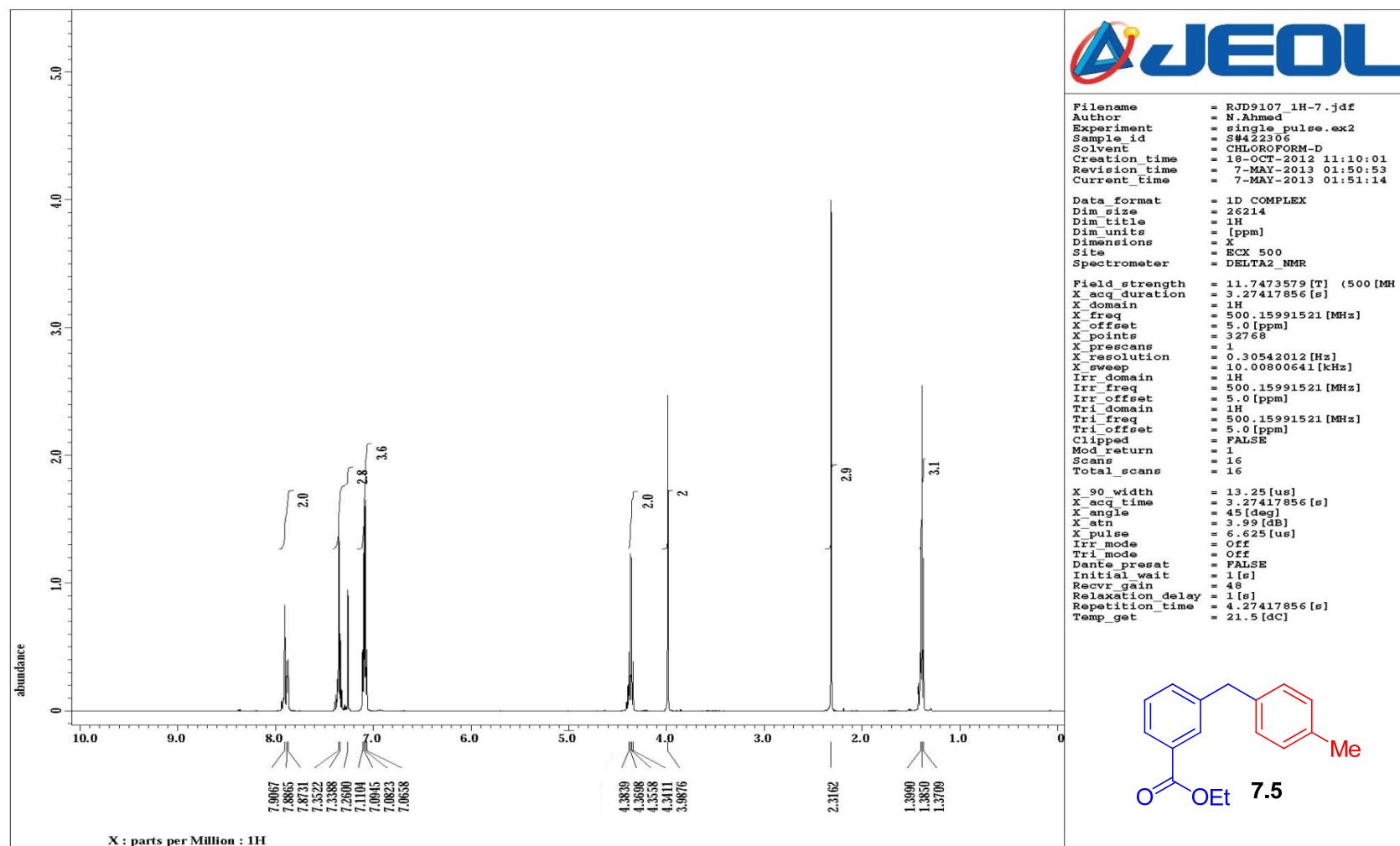
^1H NMR spectrum of Ethyl 3-benzylbenzoate (7.4)



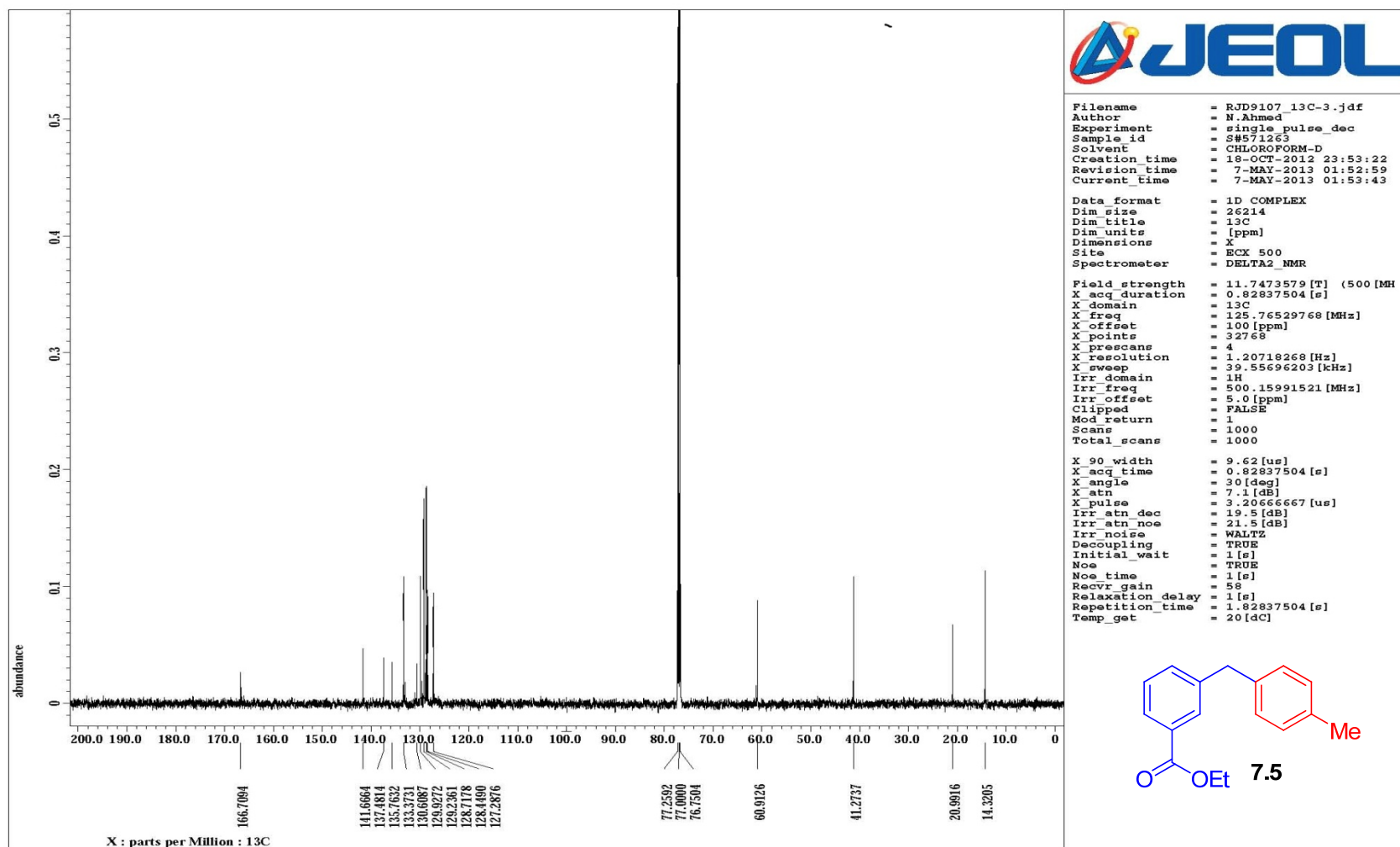
¹³C NMR spectrum of Ethyl 3-benzylbenzoate (7.4)



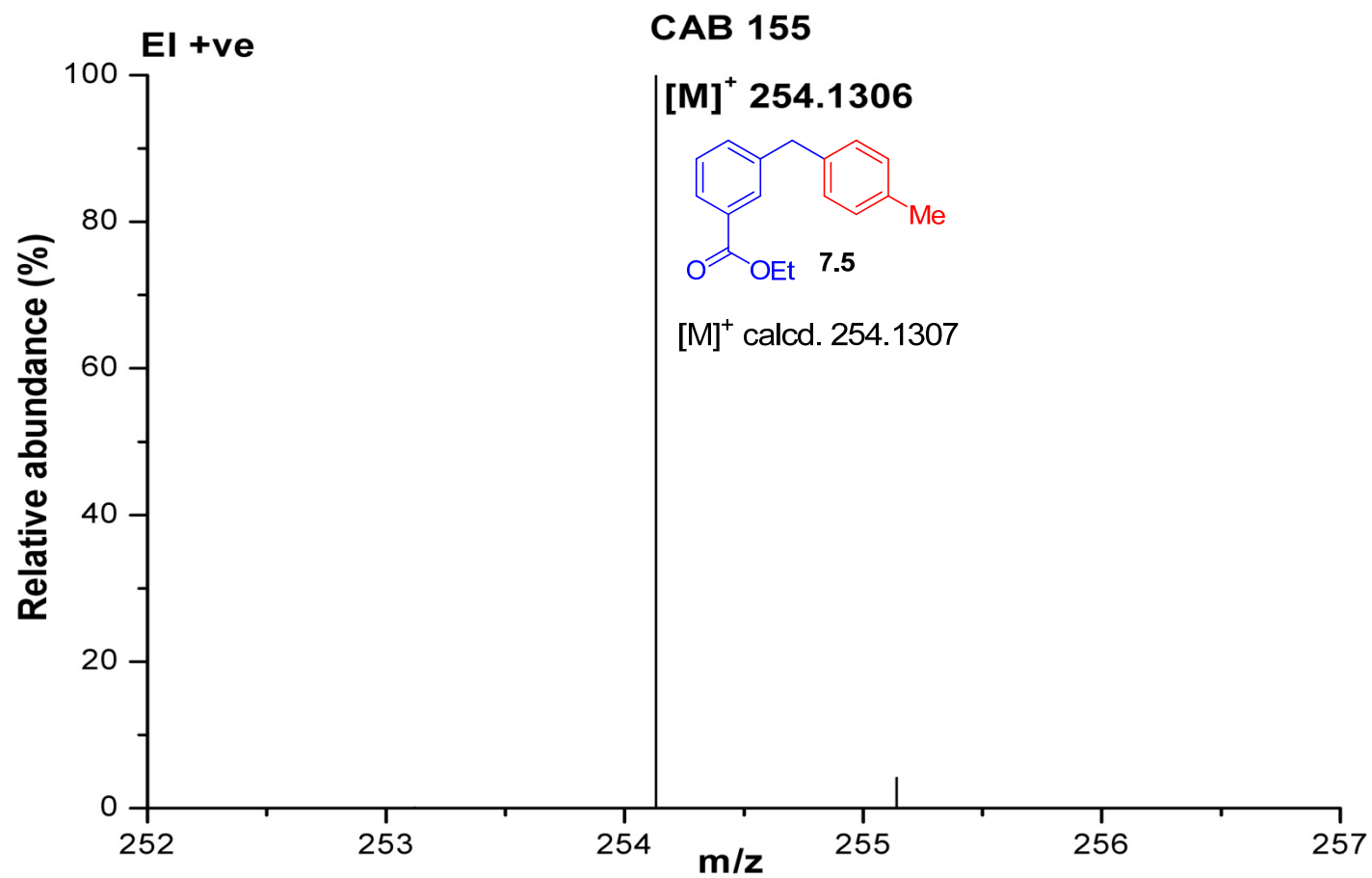
HRMS spectrum of Ethyl 3-benzylbenzoate (7.4)



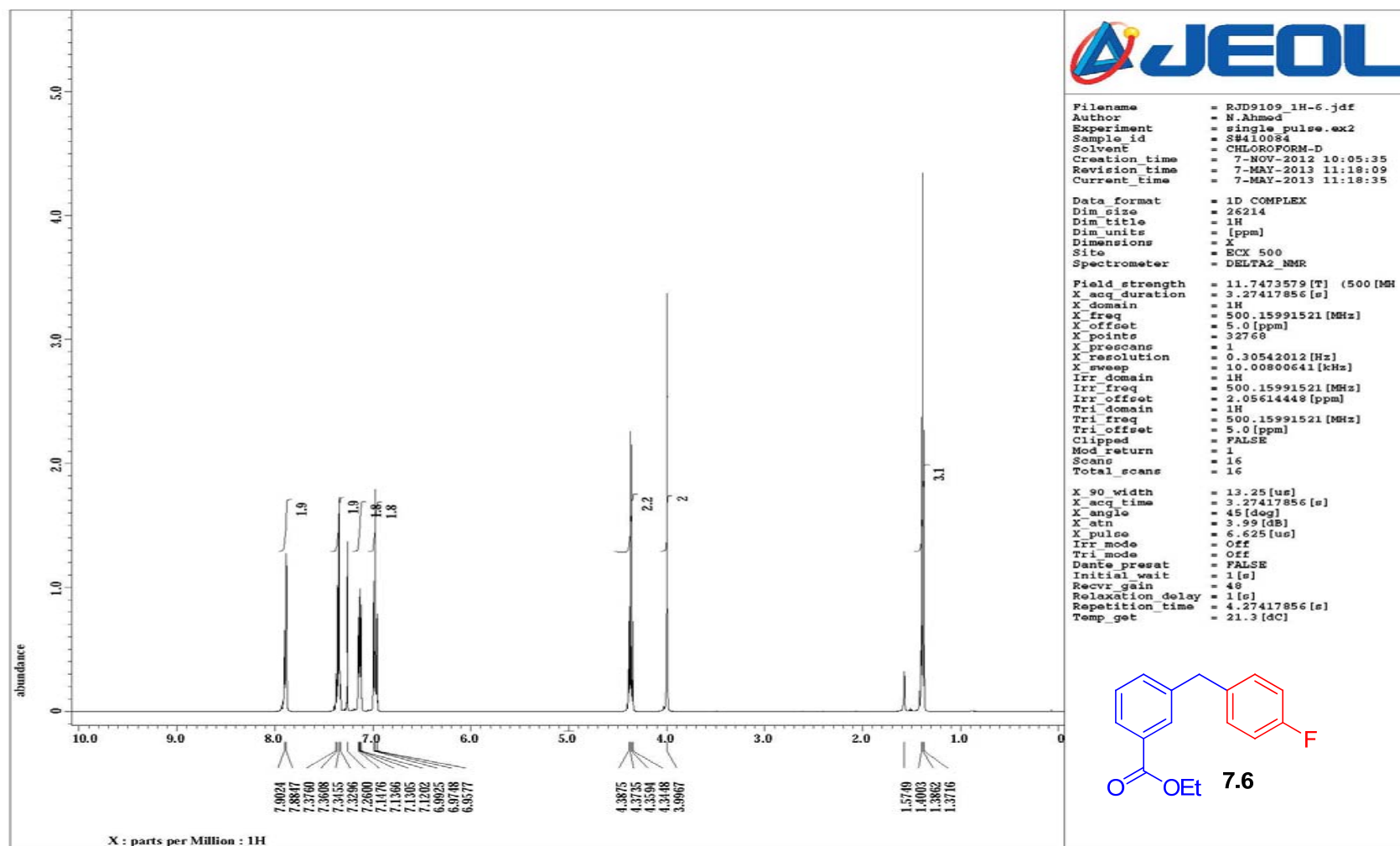
¹H NMR spectrum of Ethyl 3-(4-methylbenzyl)benzoate (7.5)



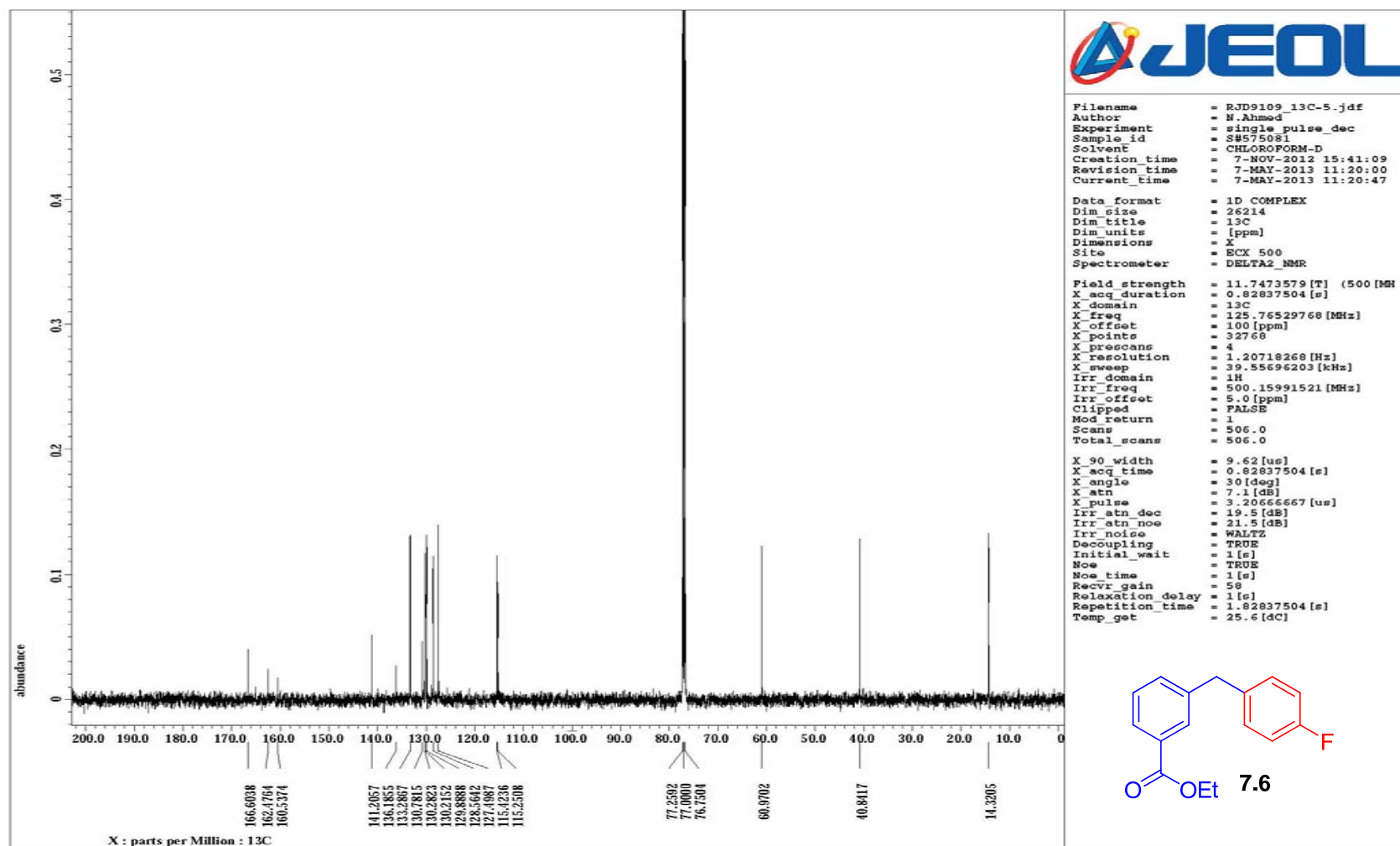
¹³C NMR spectrum of Ethyl 3-(4-methylbenzyl)benzoate (7.5)



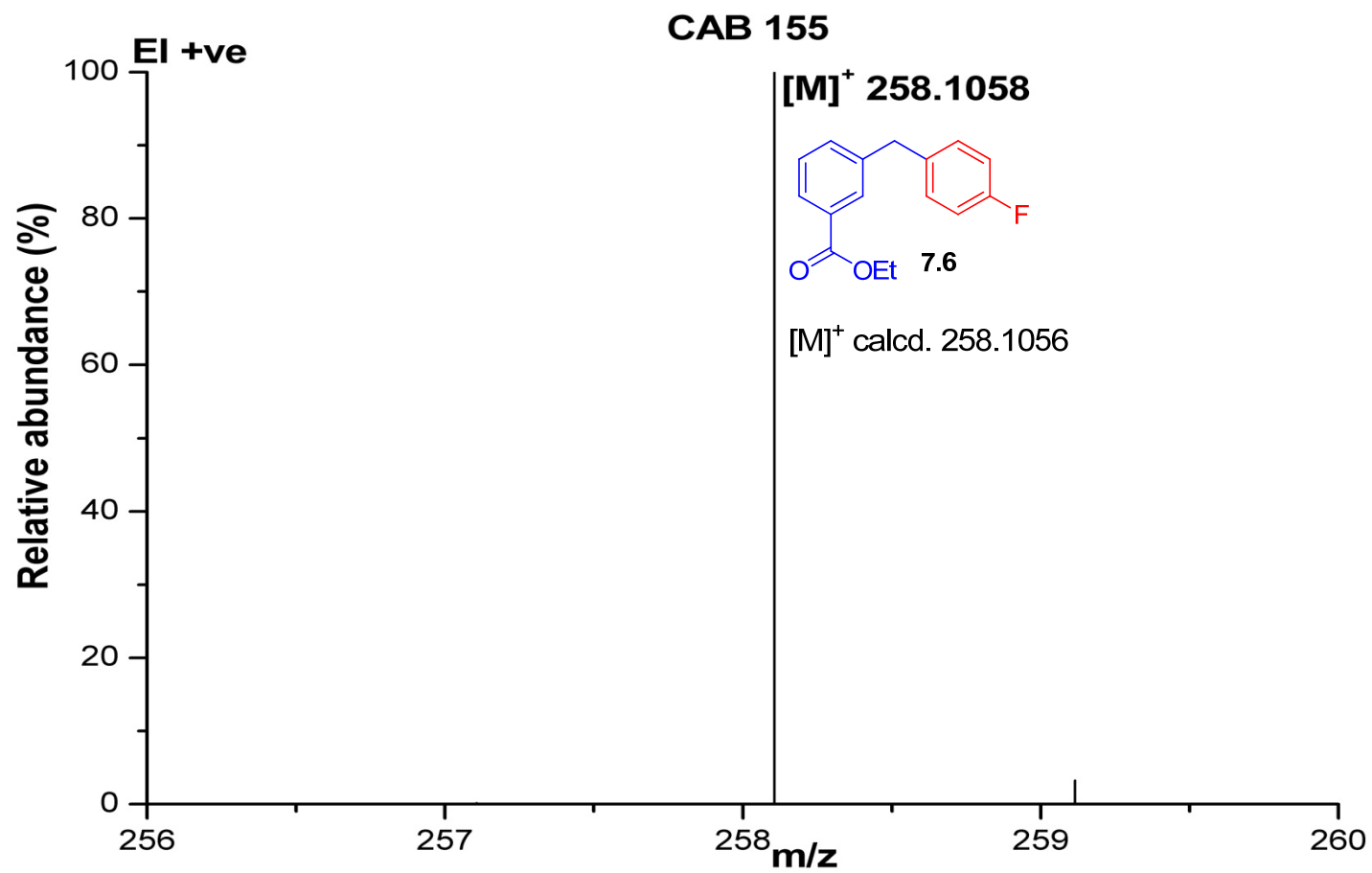
HRMS spectrum of Ethyl 3-(4-methylbenzyl)benzoate (**7.5**)



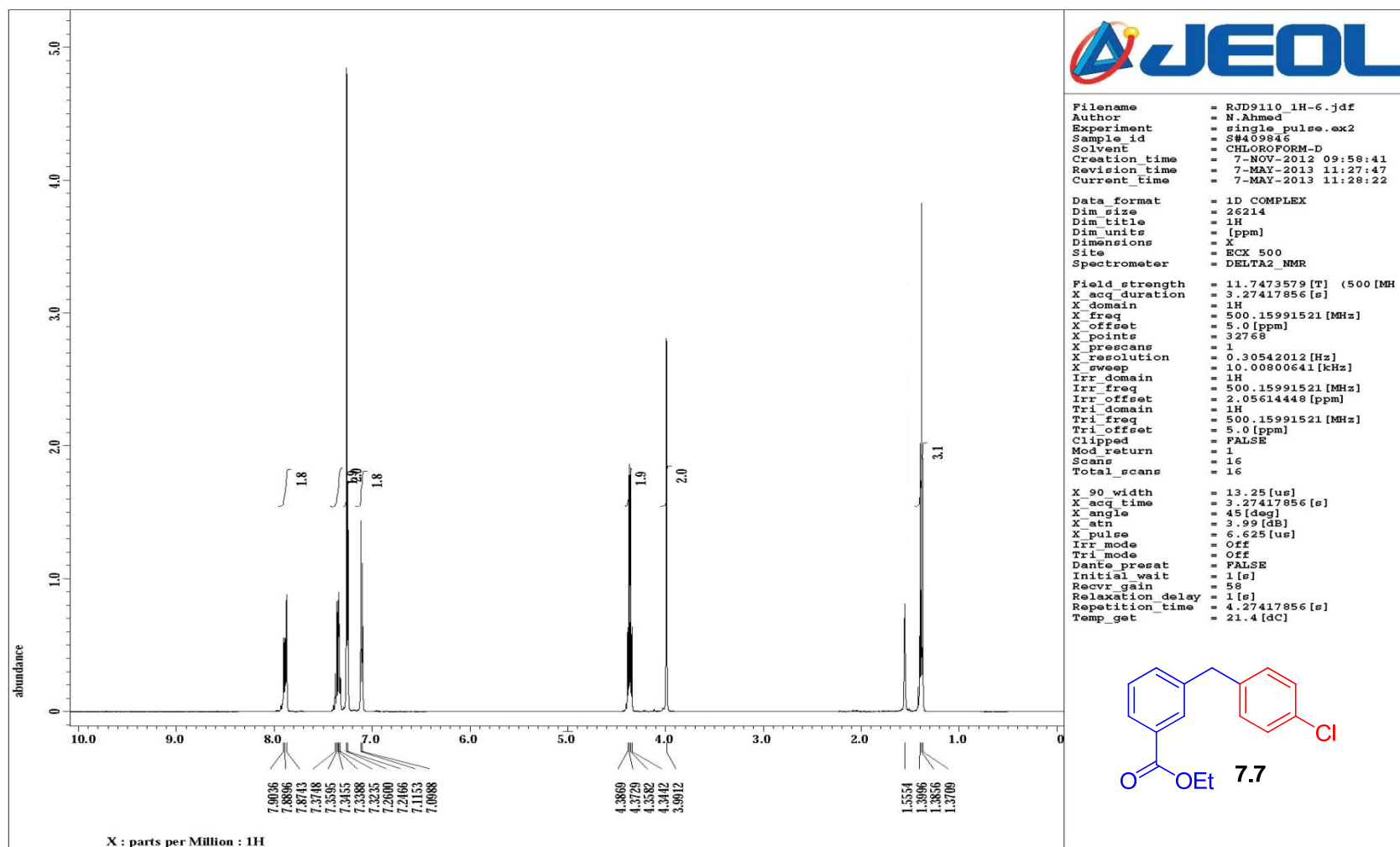
¹H NMR spectrum of Ethyl 3-(4-fluorobenzyl)benzoate (7.6)



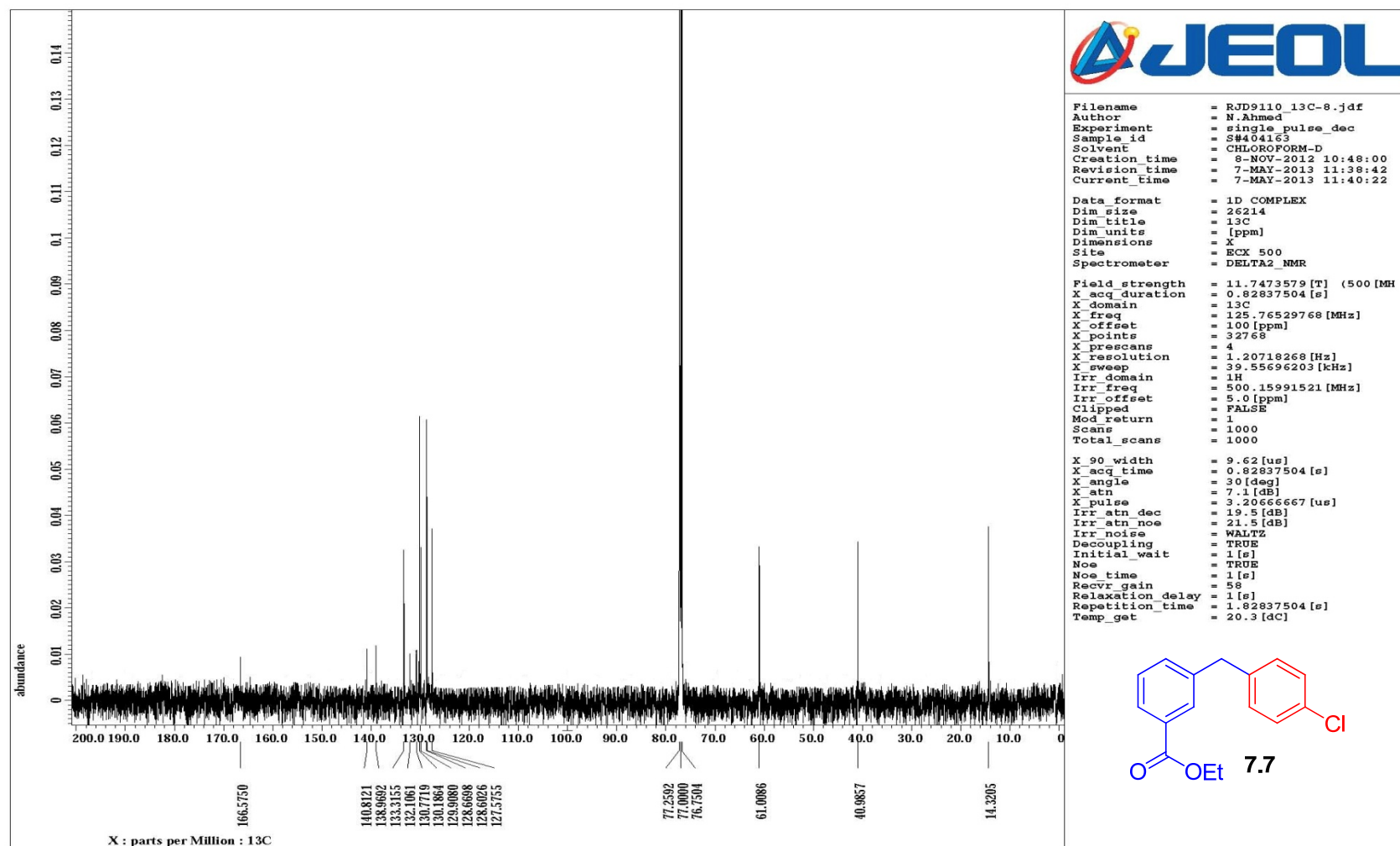
^{13}C NMR spectrum of Ethyl 3-(4-fluorobenzyl)benzoate (7.6)



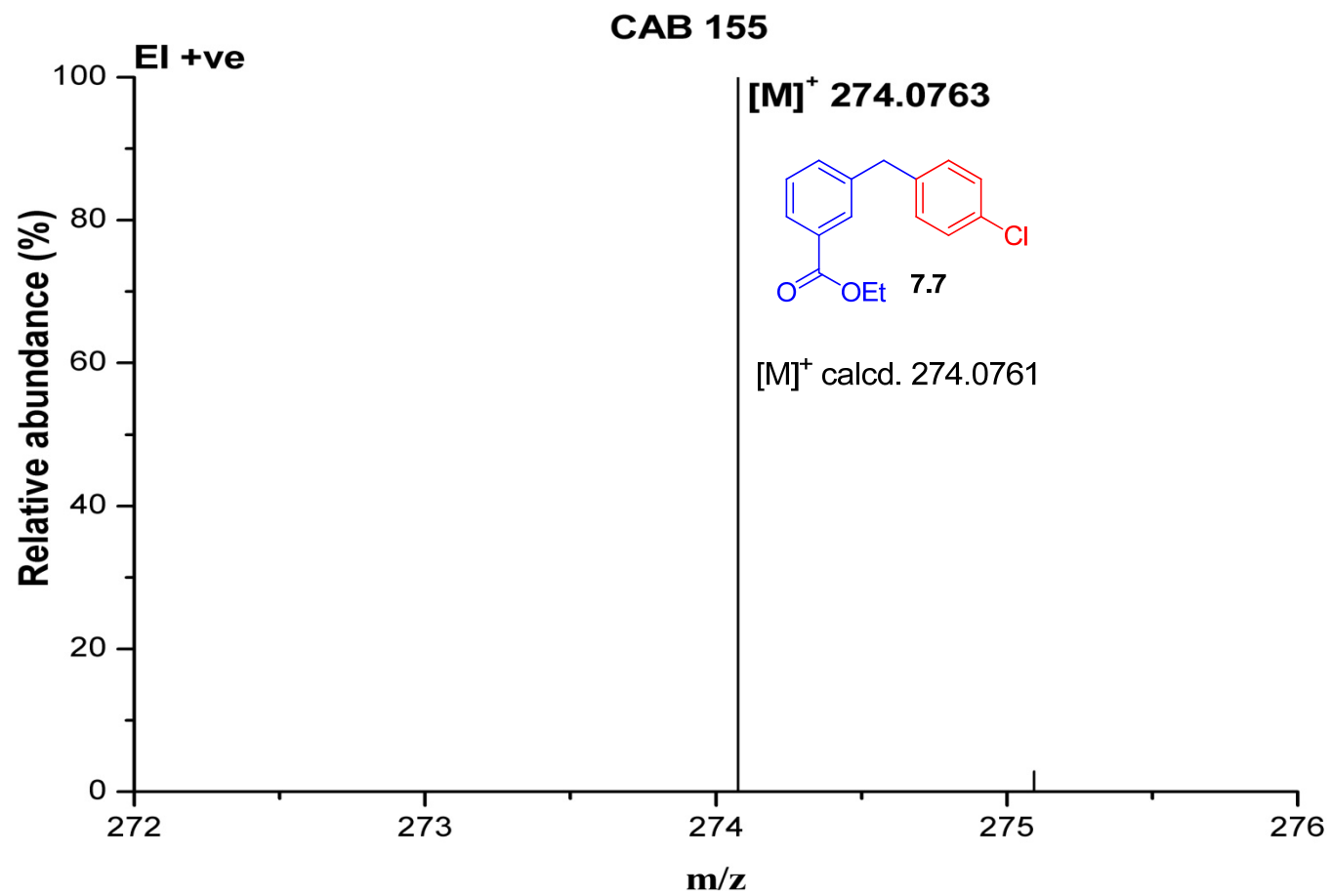
HRMS spectrum of Ethyl 3-(4-fluorobenzyl)benzoate (**7.6**)



¹H NMR spectrum of Ethyl 3-(4-chlorobenzyl)benzoate (7.7)



¹³C NMR spectrum of Ethyl 3-(4-chlorobenzyl)benzoate (7.7)



HRMS spectrum of Ethyl 3-(4-chlorobenzyl)benzoate (7.7)