Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Pd-catalyzed Threefold Arylations of Mono, Di and Tetra-bromoquinones using Triarylbismuth Reagents

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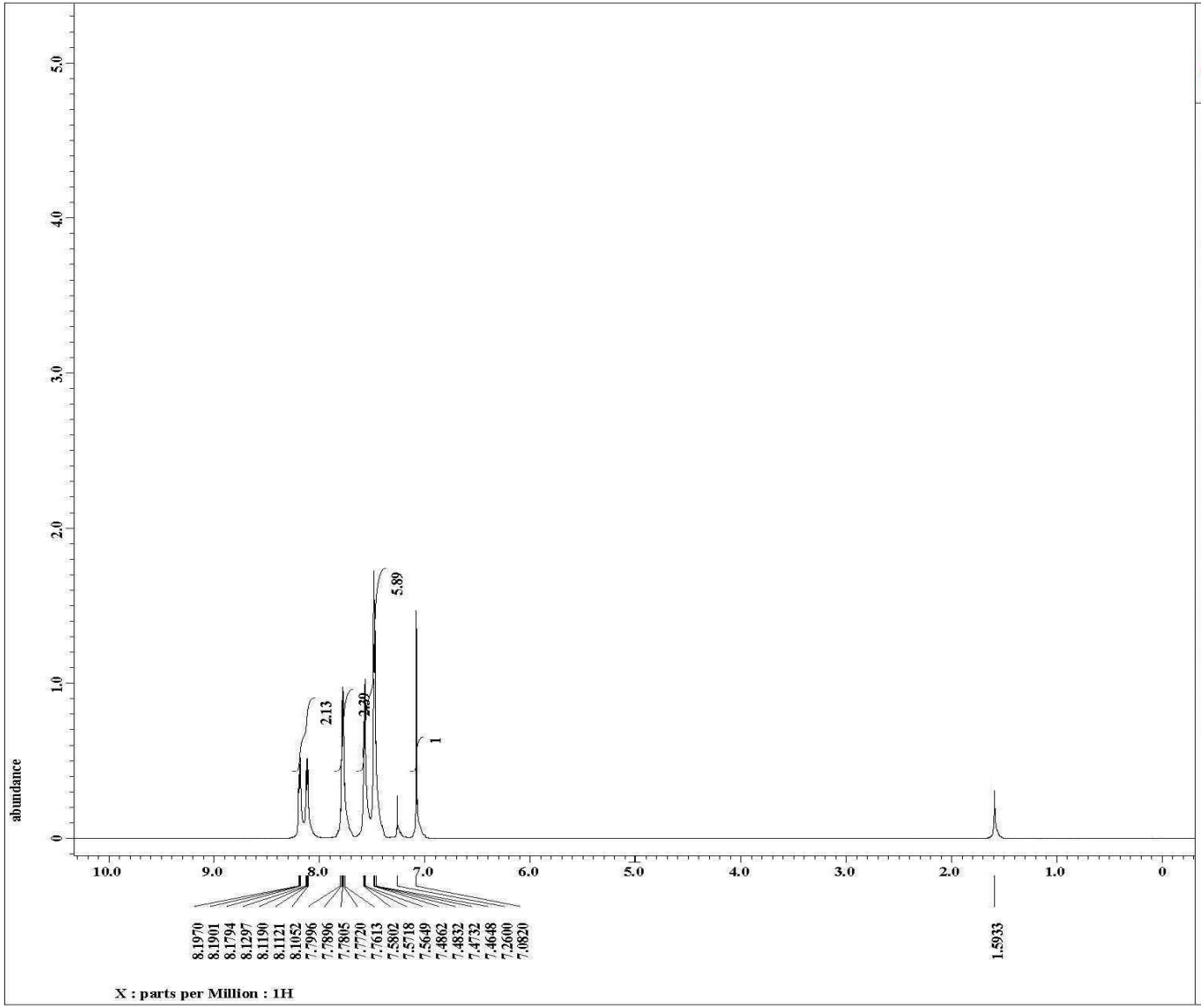
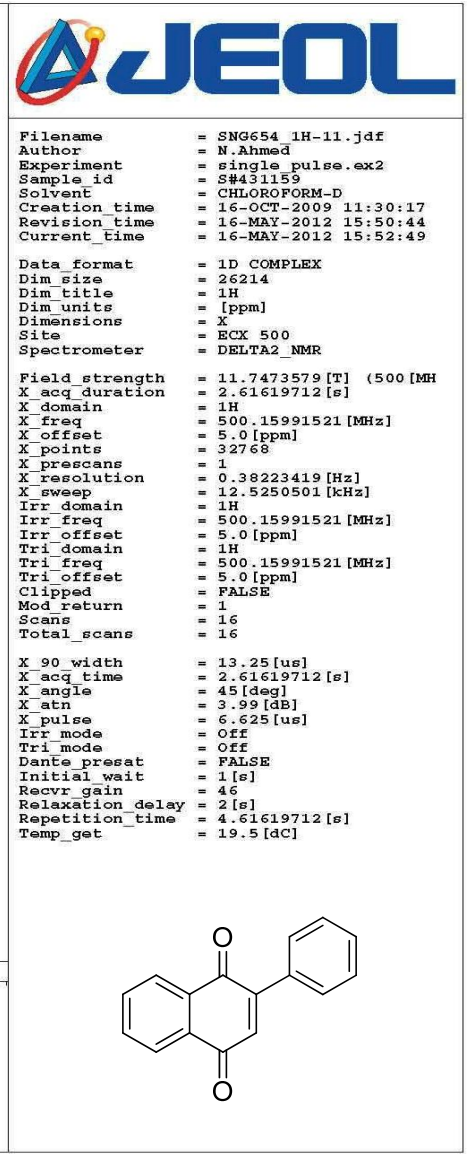
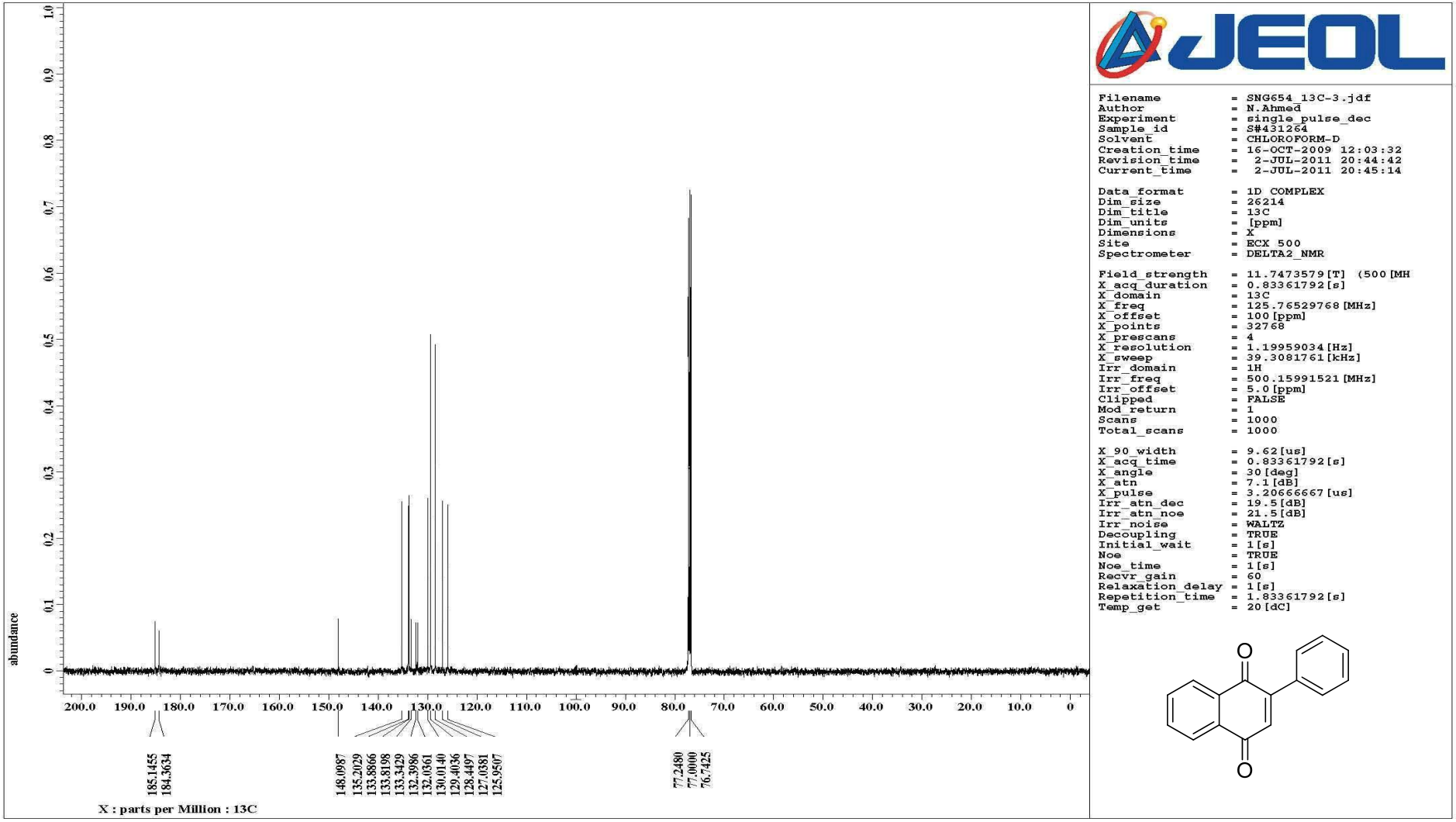




^{1}H NMR spectrum of 2-phenyl-1,4-naphthoquinone **(2.1)**



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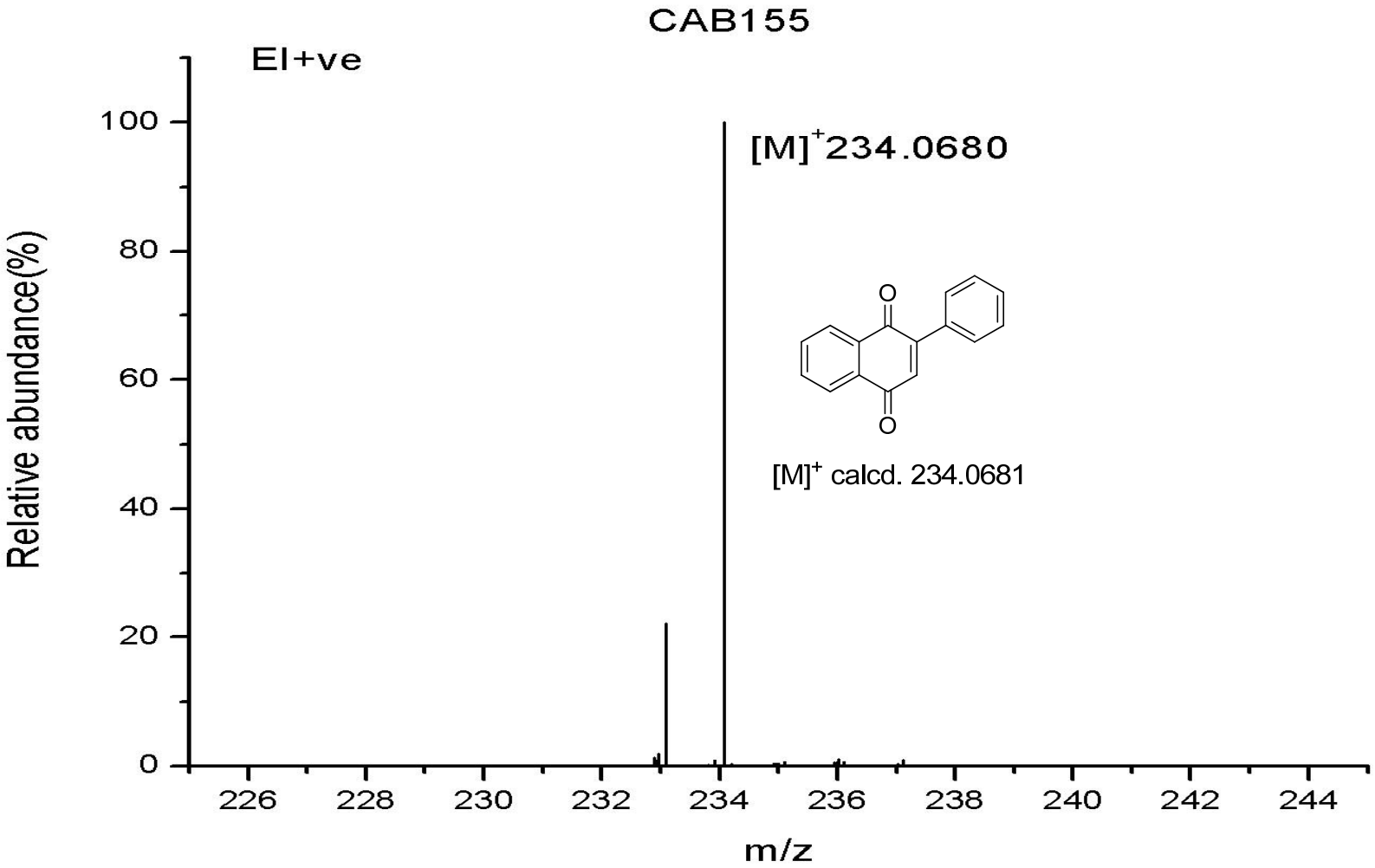
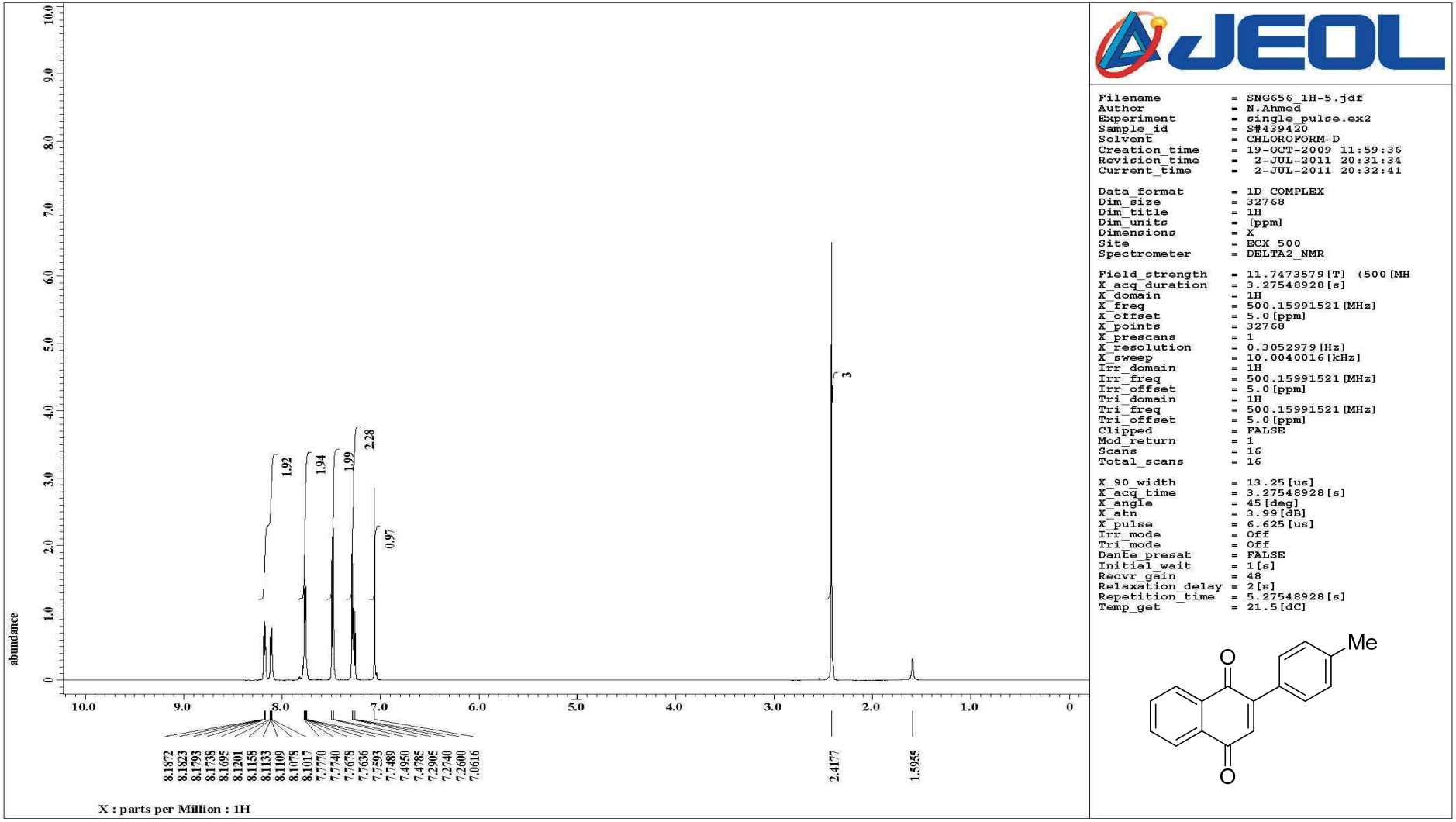


HRMS spectrum of 2-phenyl-1,4-naphthoquinone **(2.1)**



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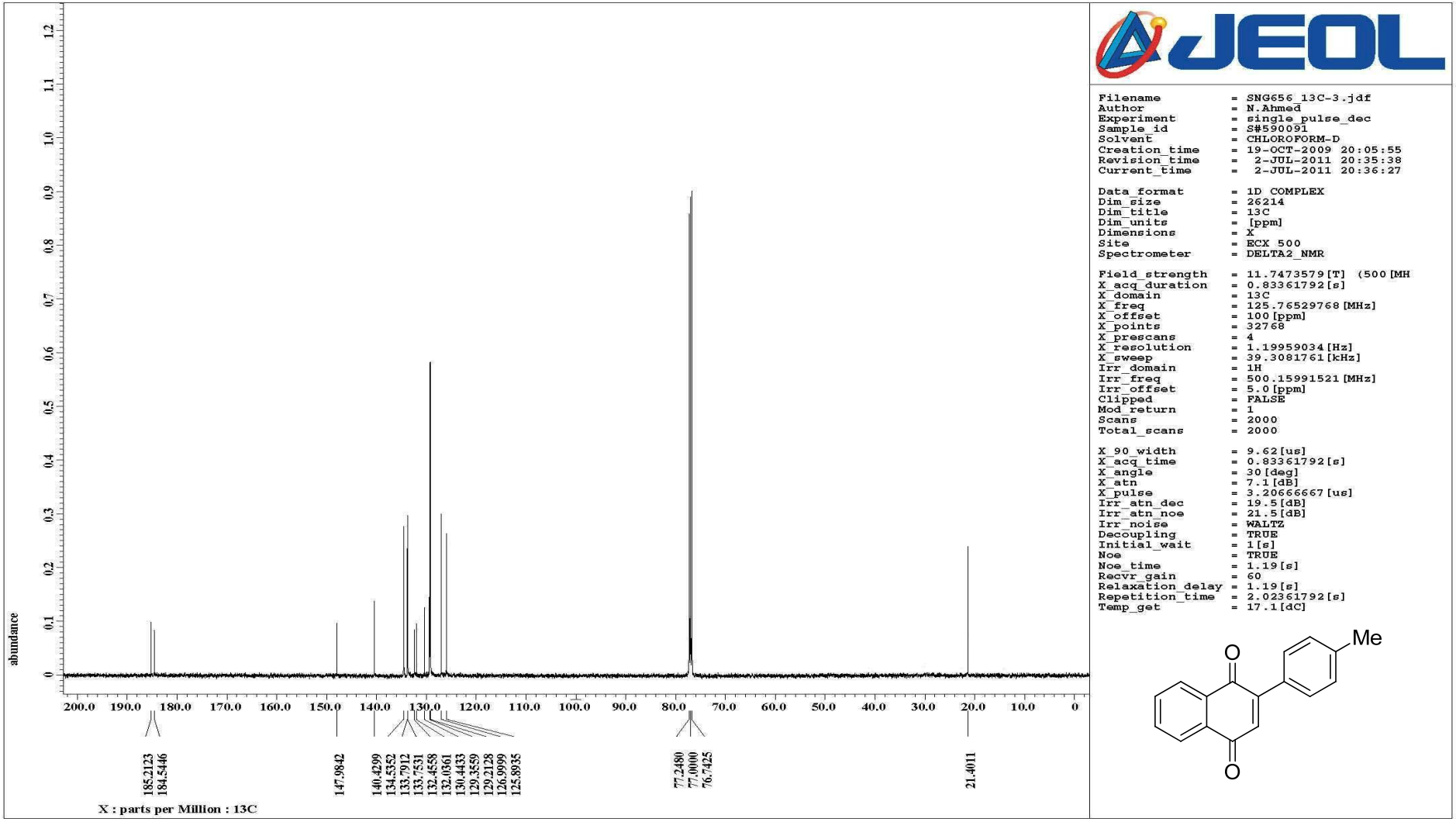
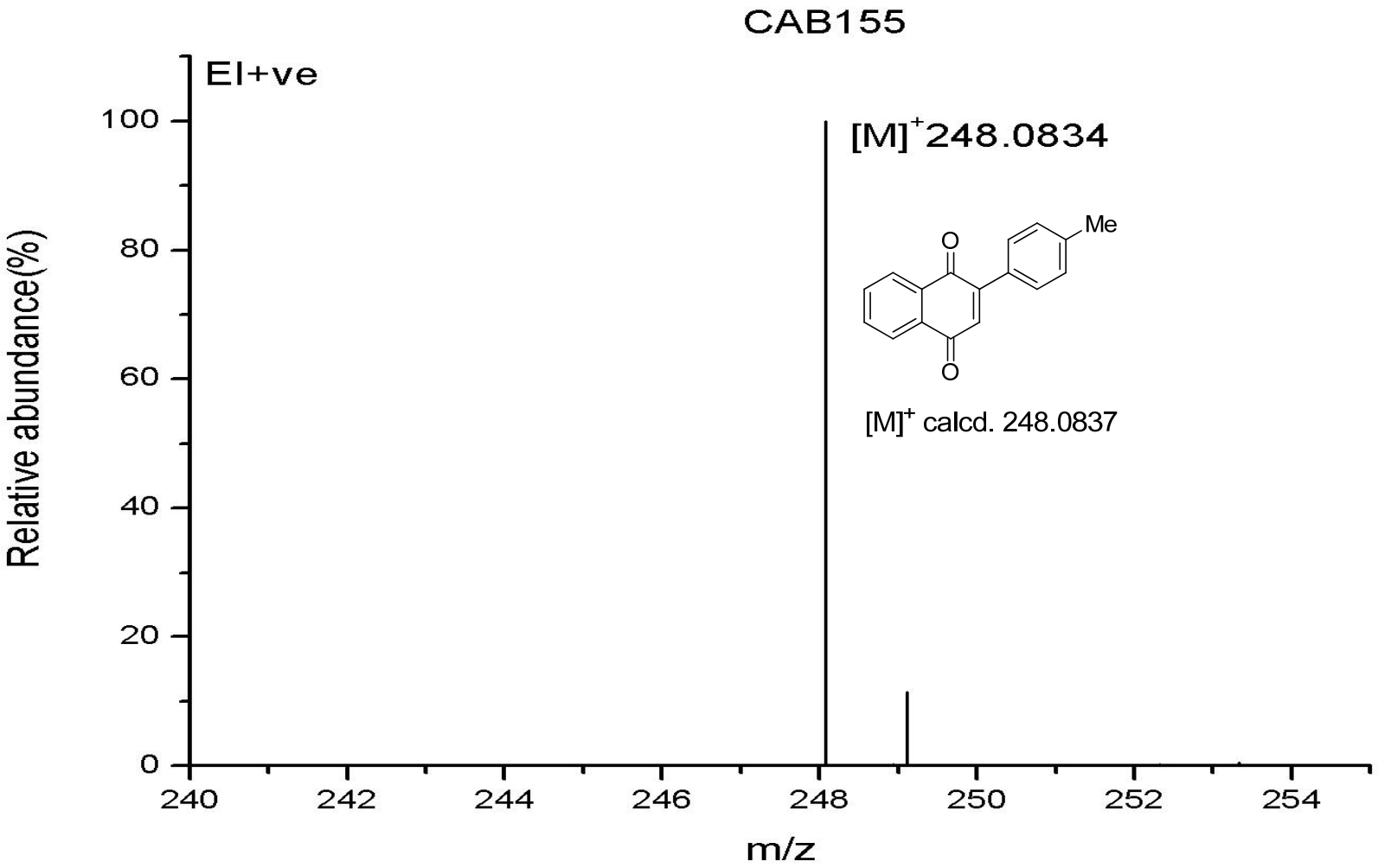
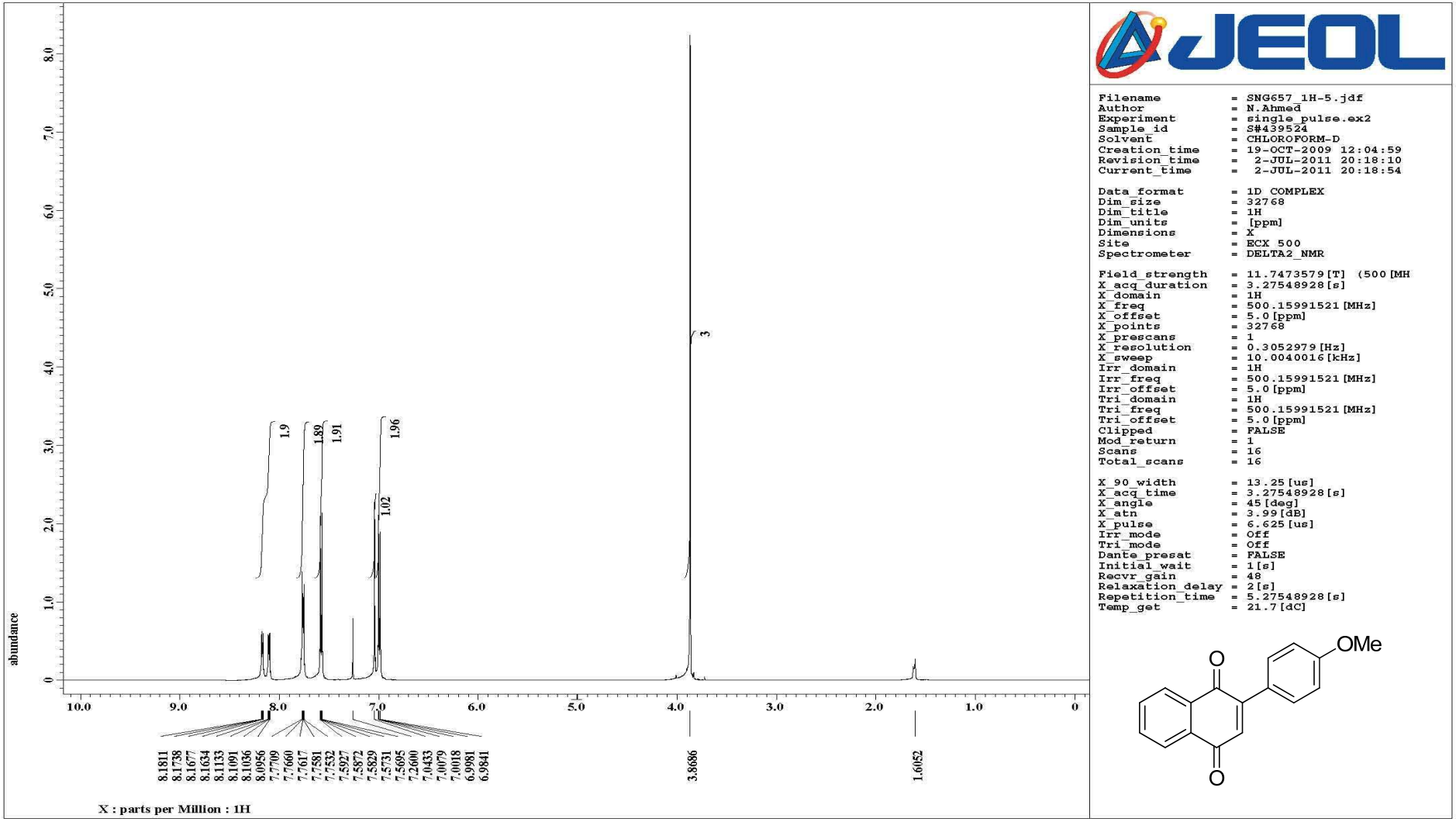


^{13}C NMR spectrum of 2-*p*-tolyl-1,4-naphthoquinone **(2.2)**



HRMS spectrum of 2-*p*-tolyl-1,4-naphthoquinone **(2.2)**



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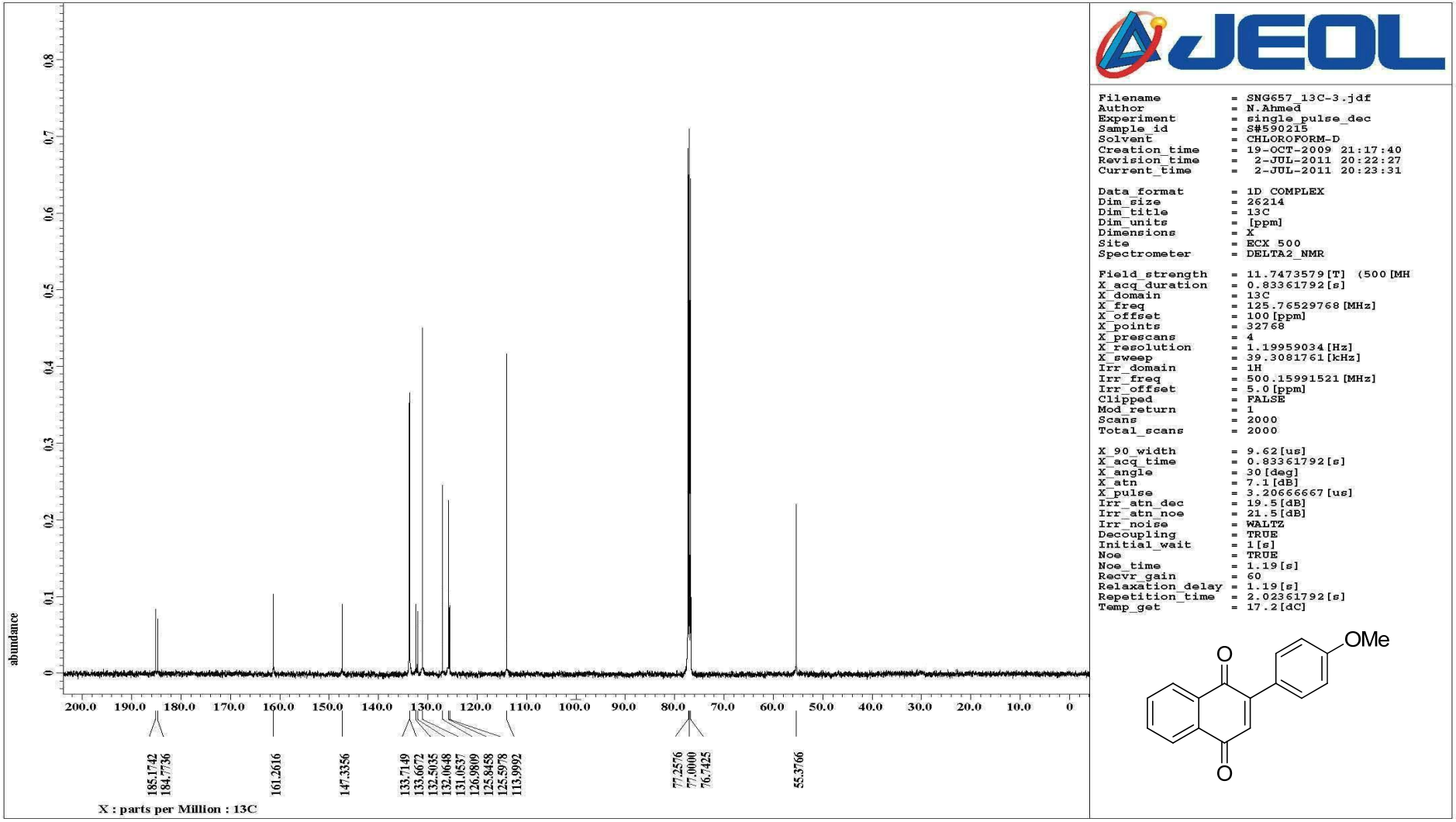

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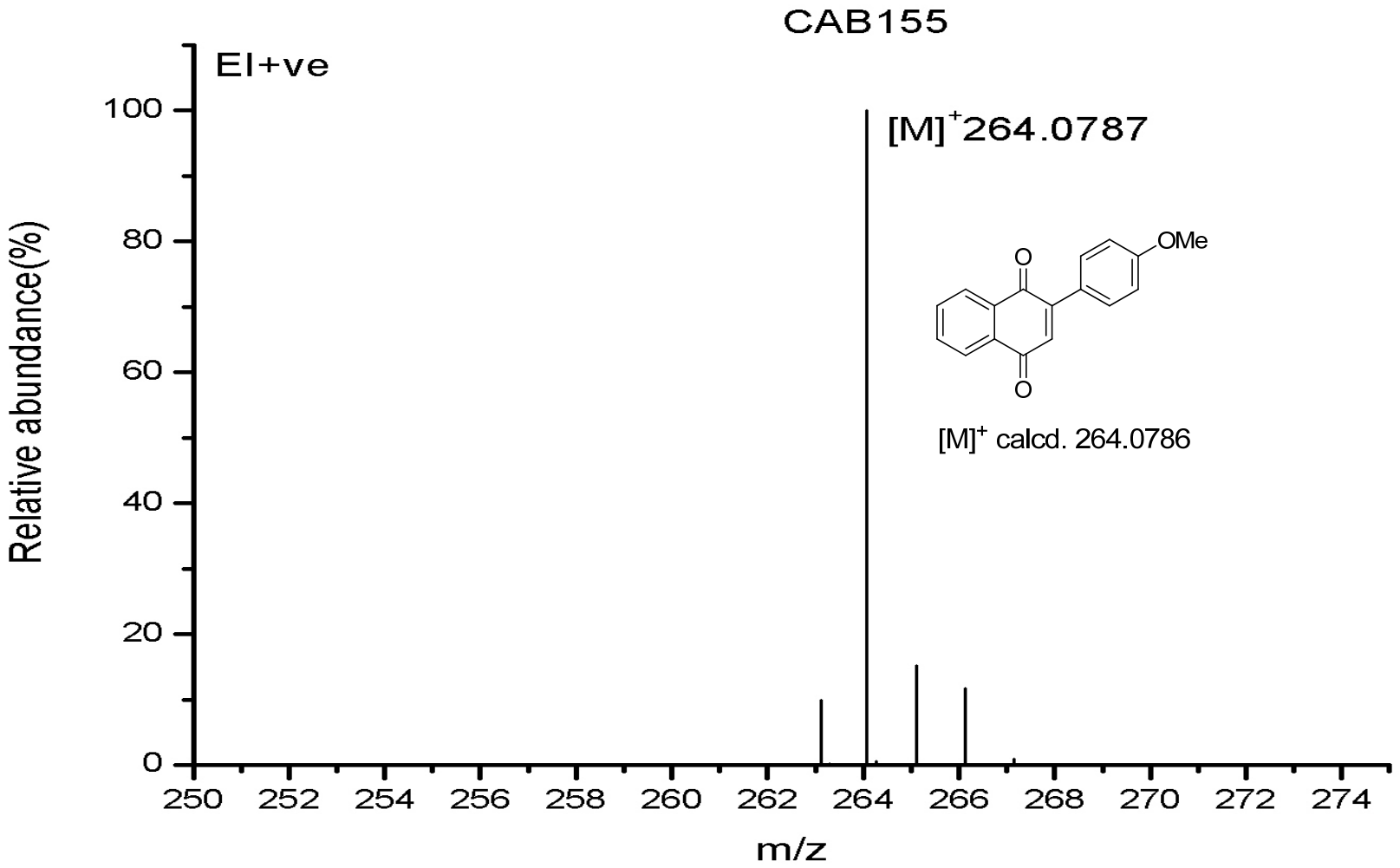
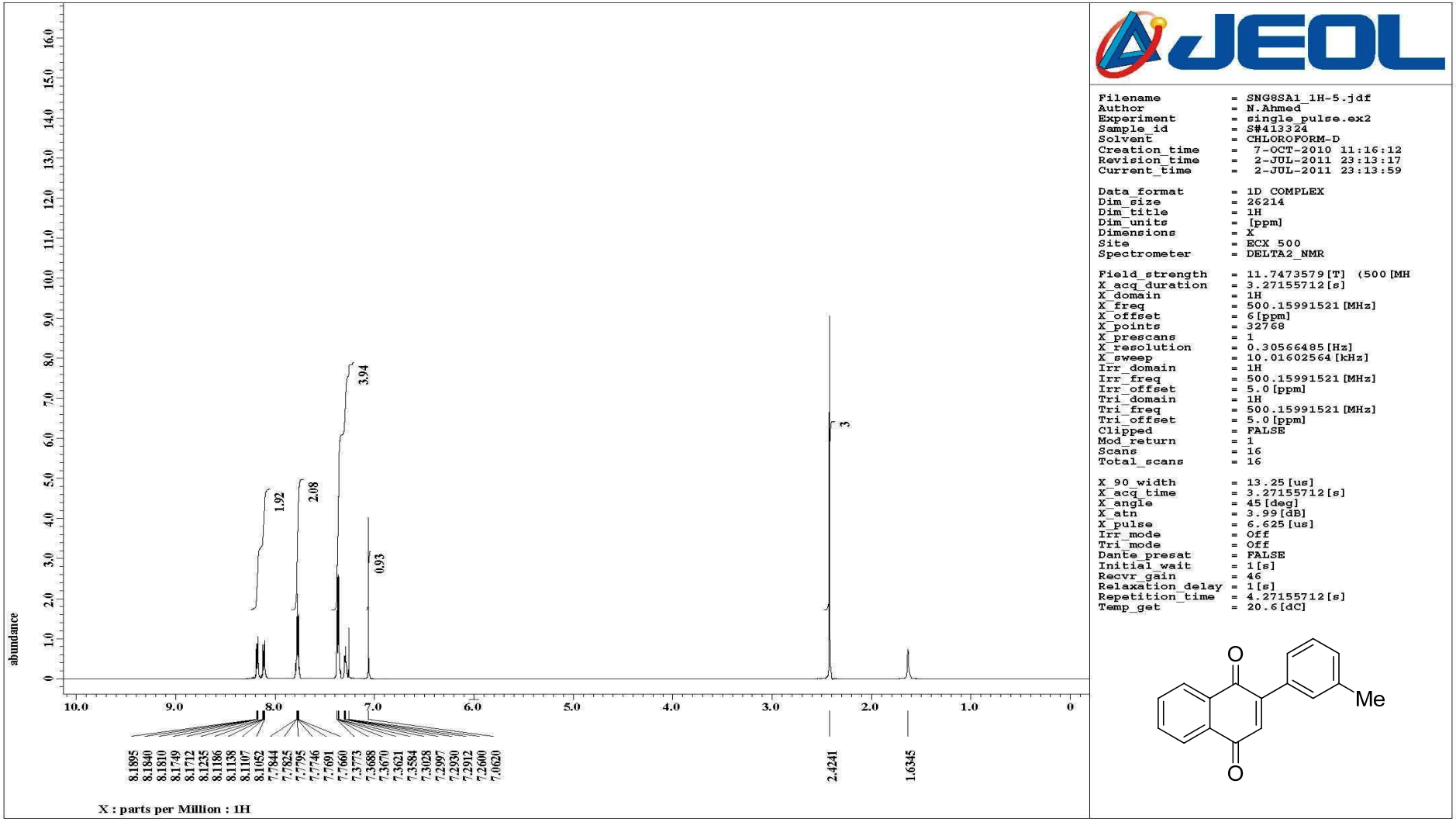


HRMS spectrum of 2-(4-methoxyphenyl)-1,4-naphthoquinone **(2.3)**



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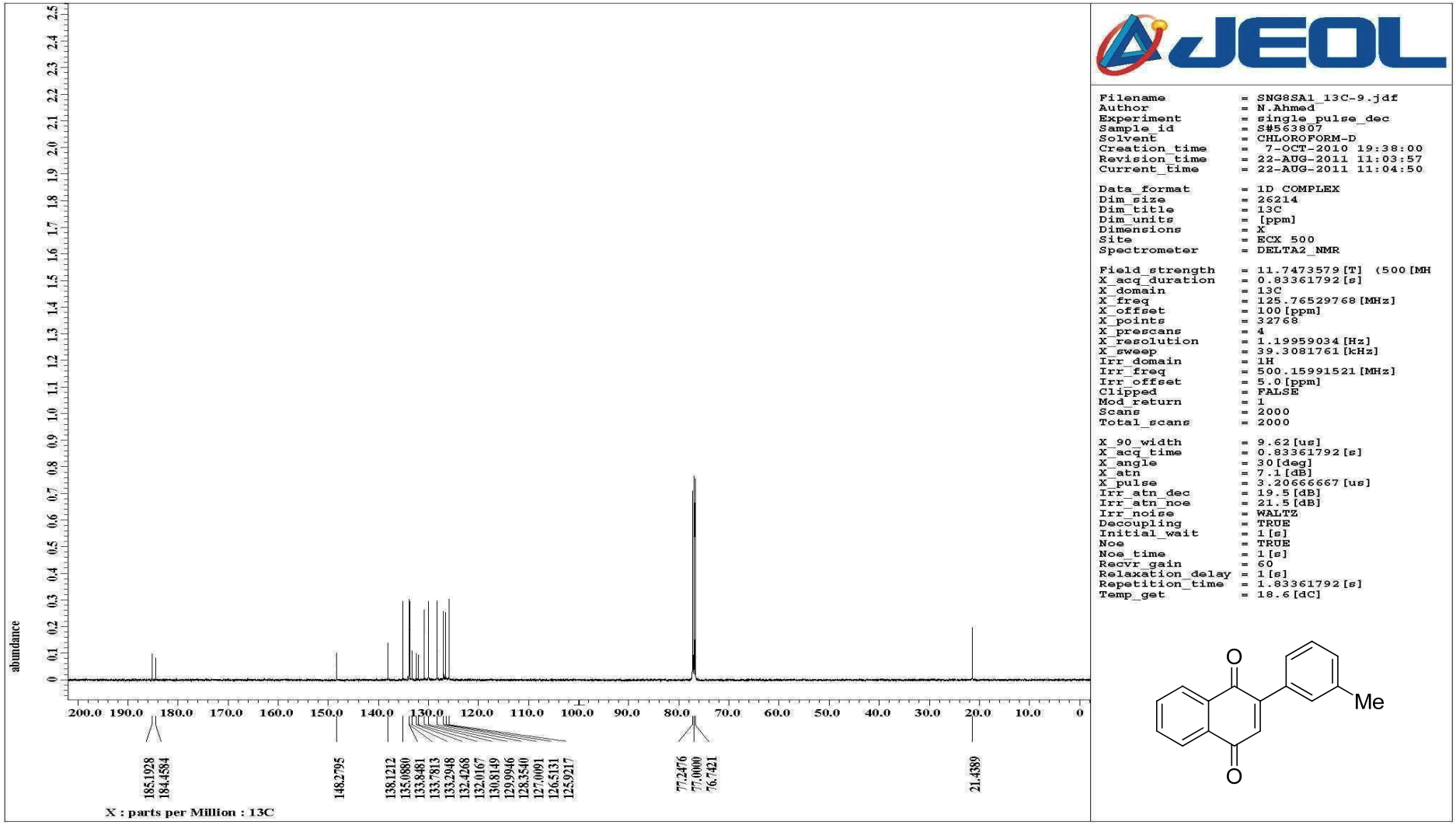

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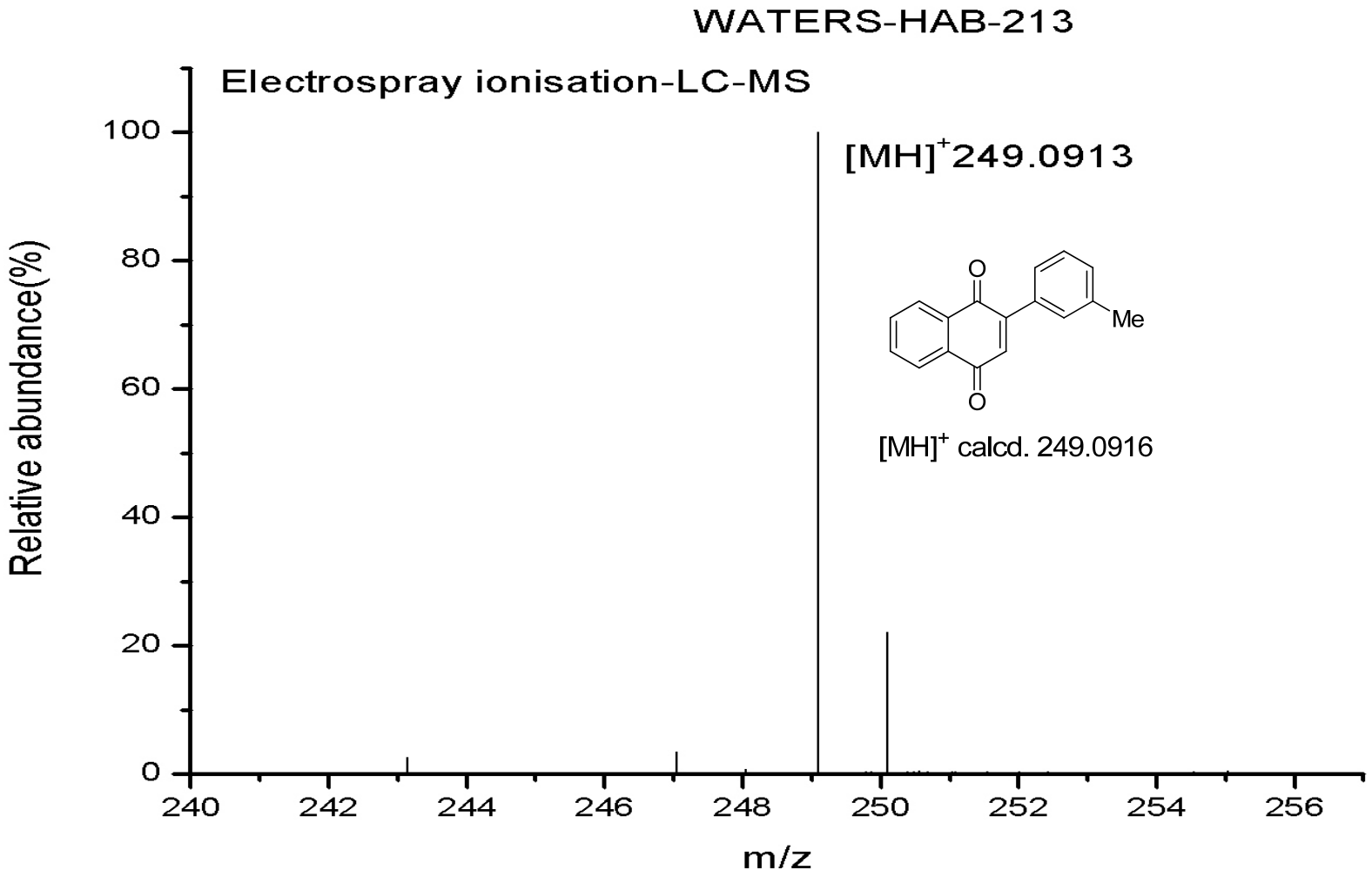

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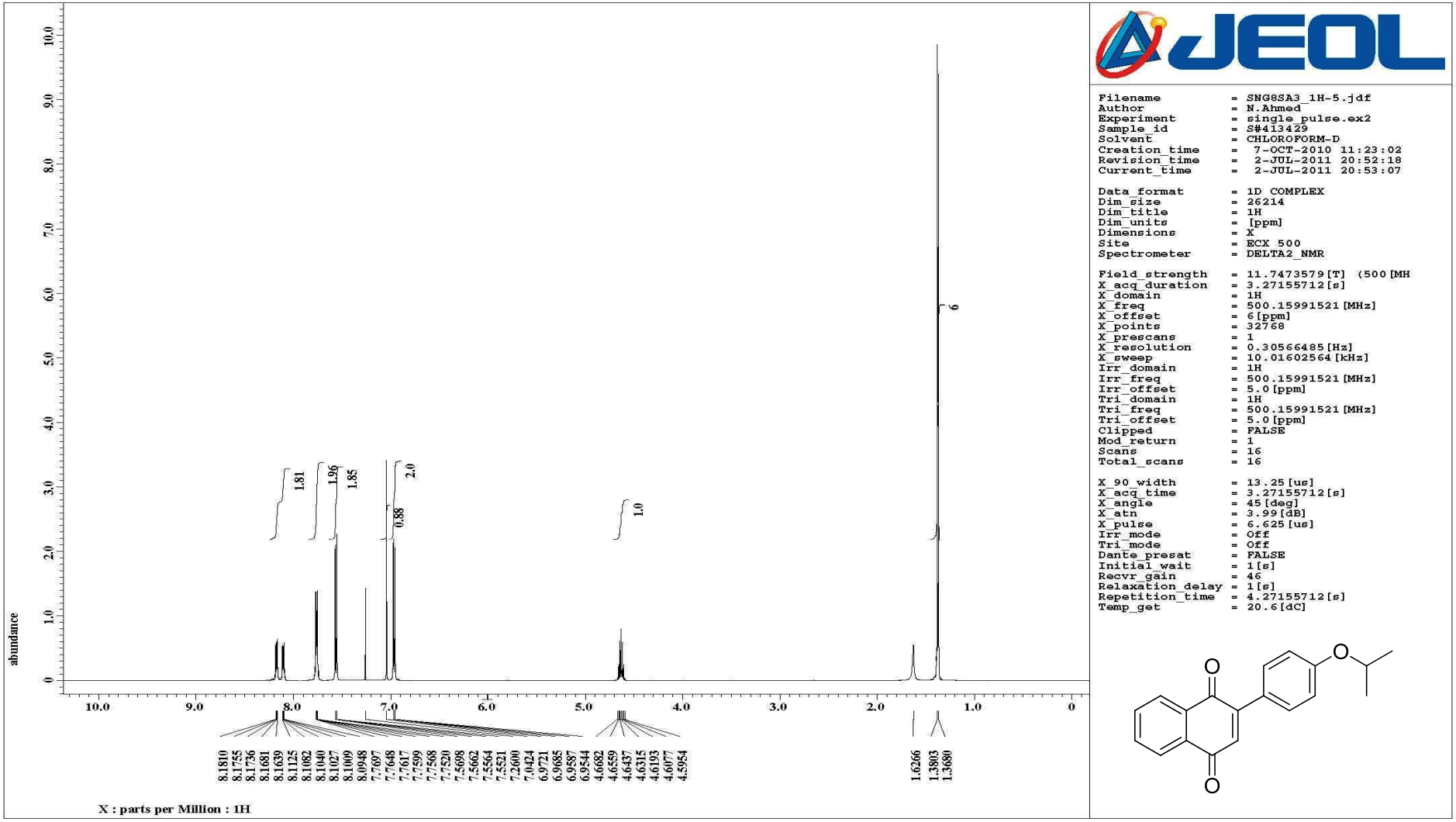

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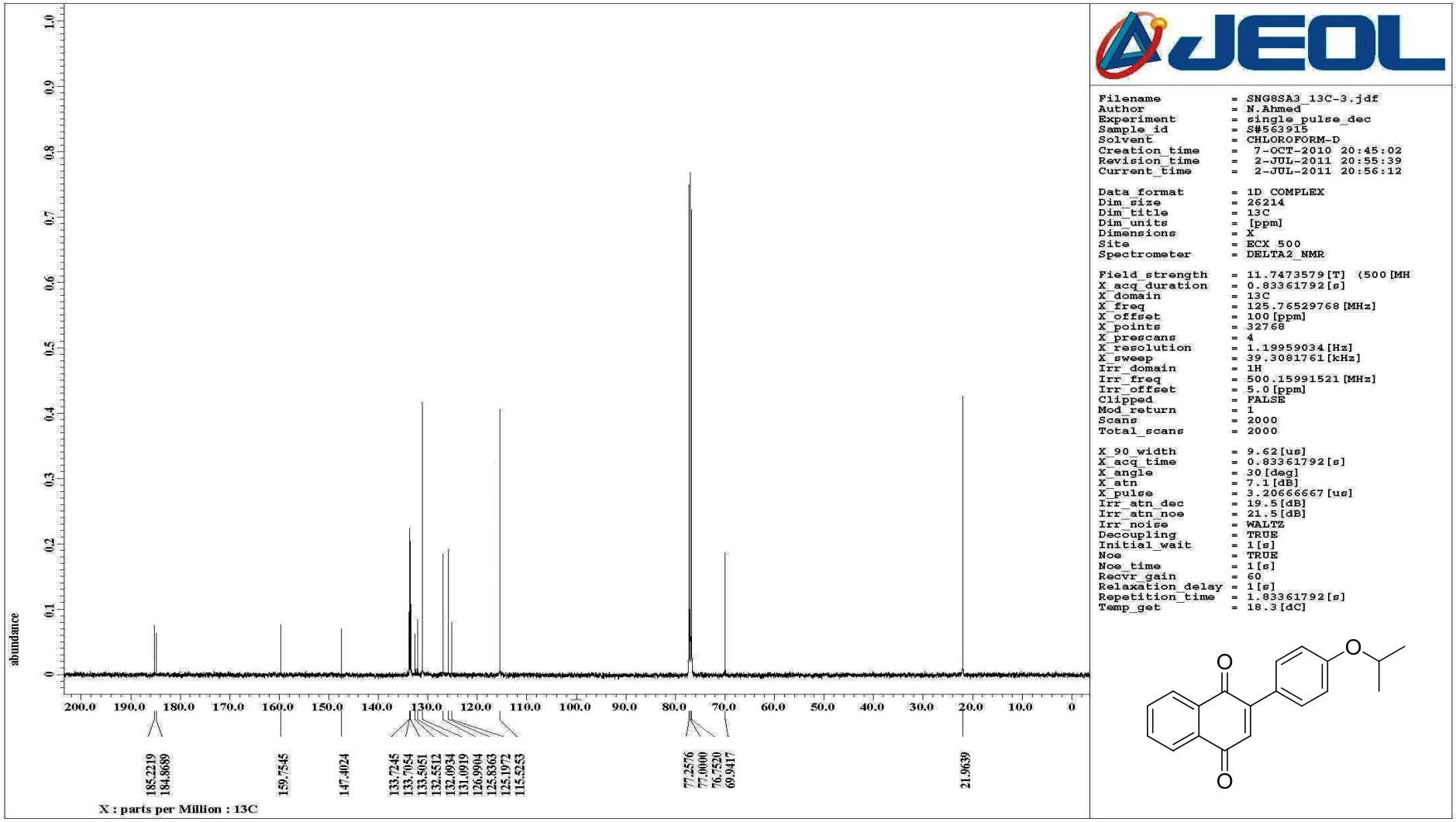
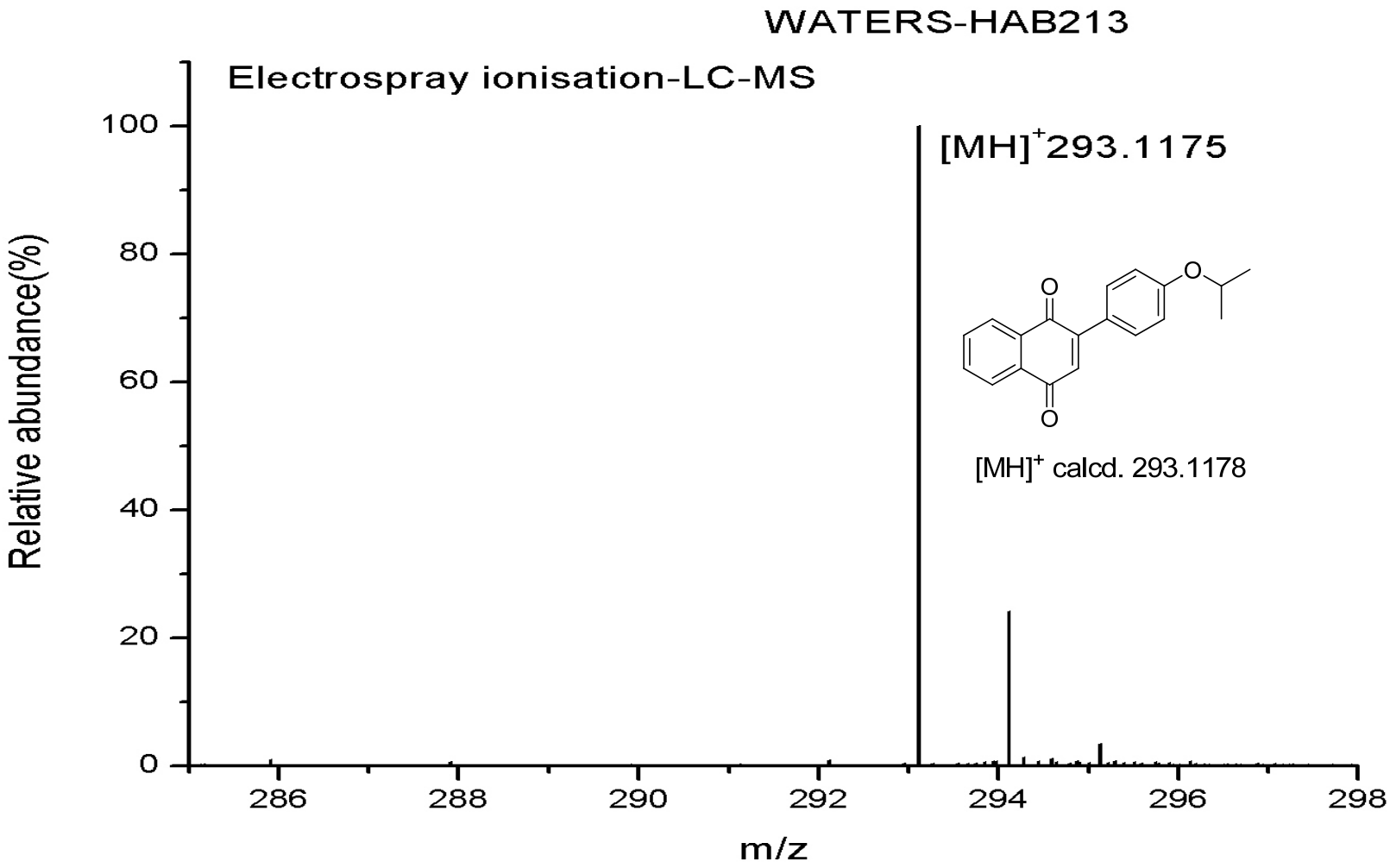


^{13}C NMR spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone **(2.5)**



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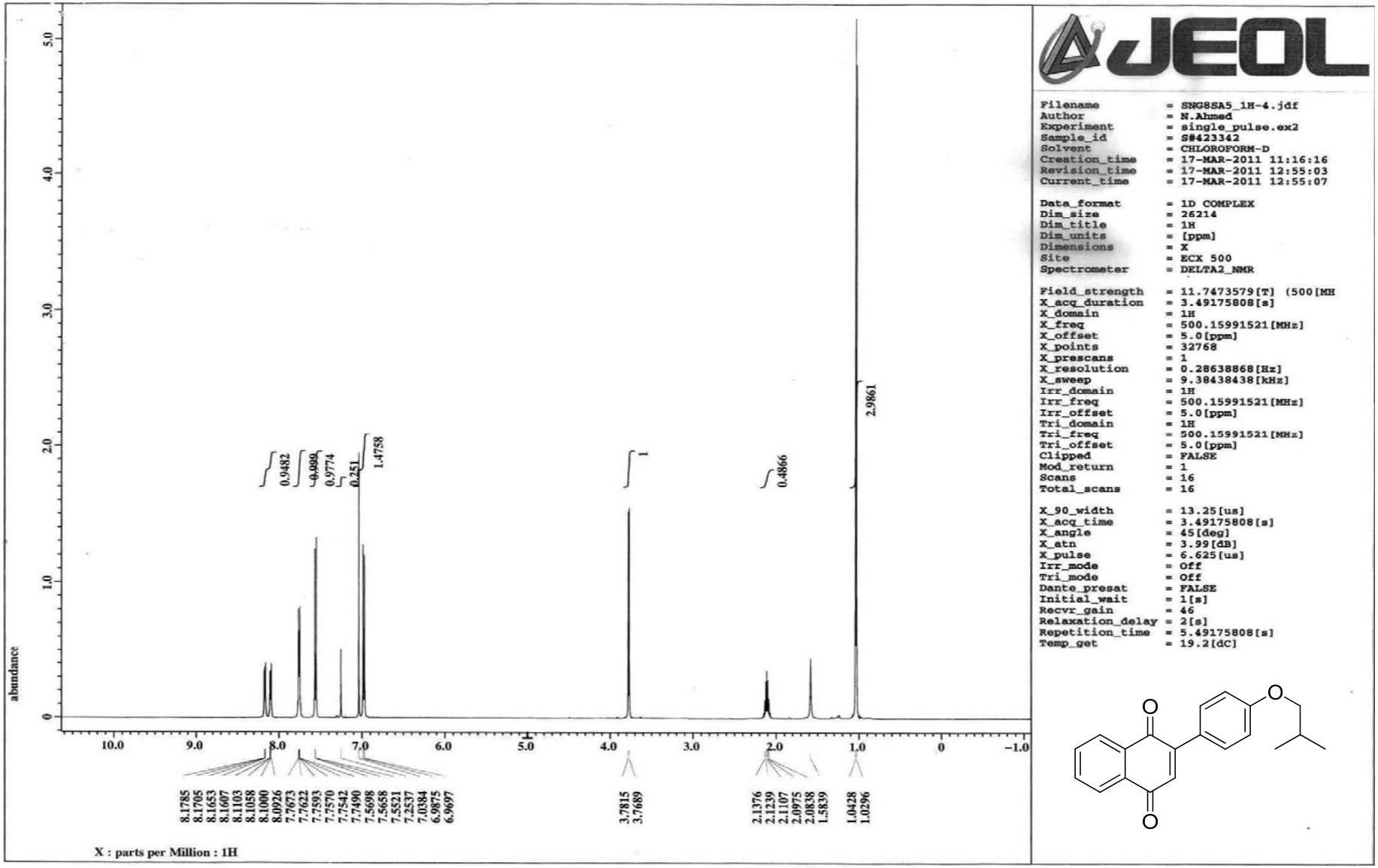
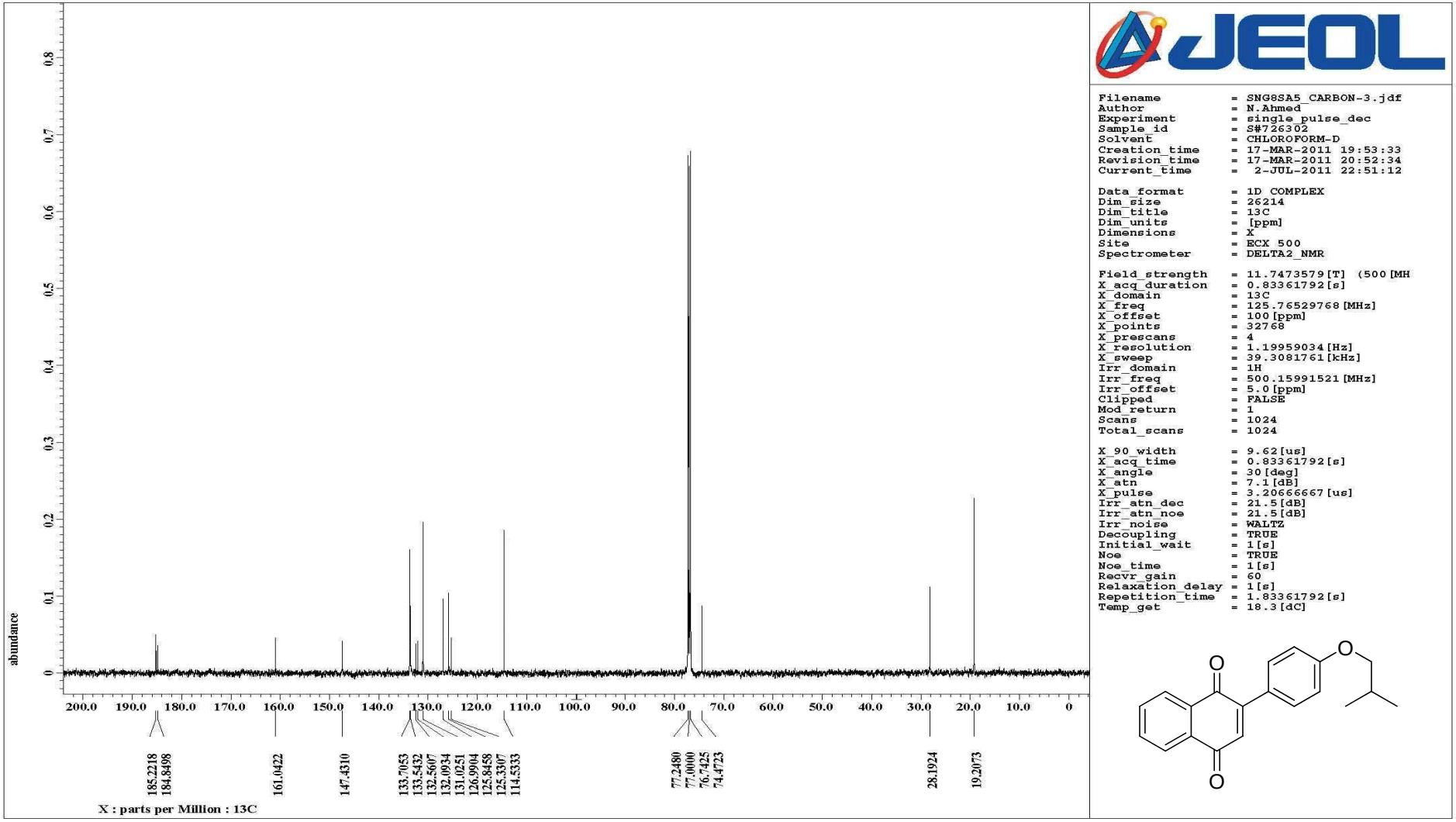
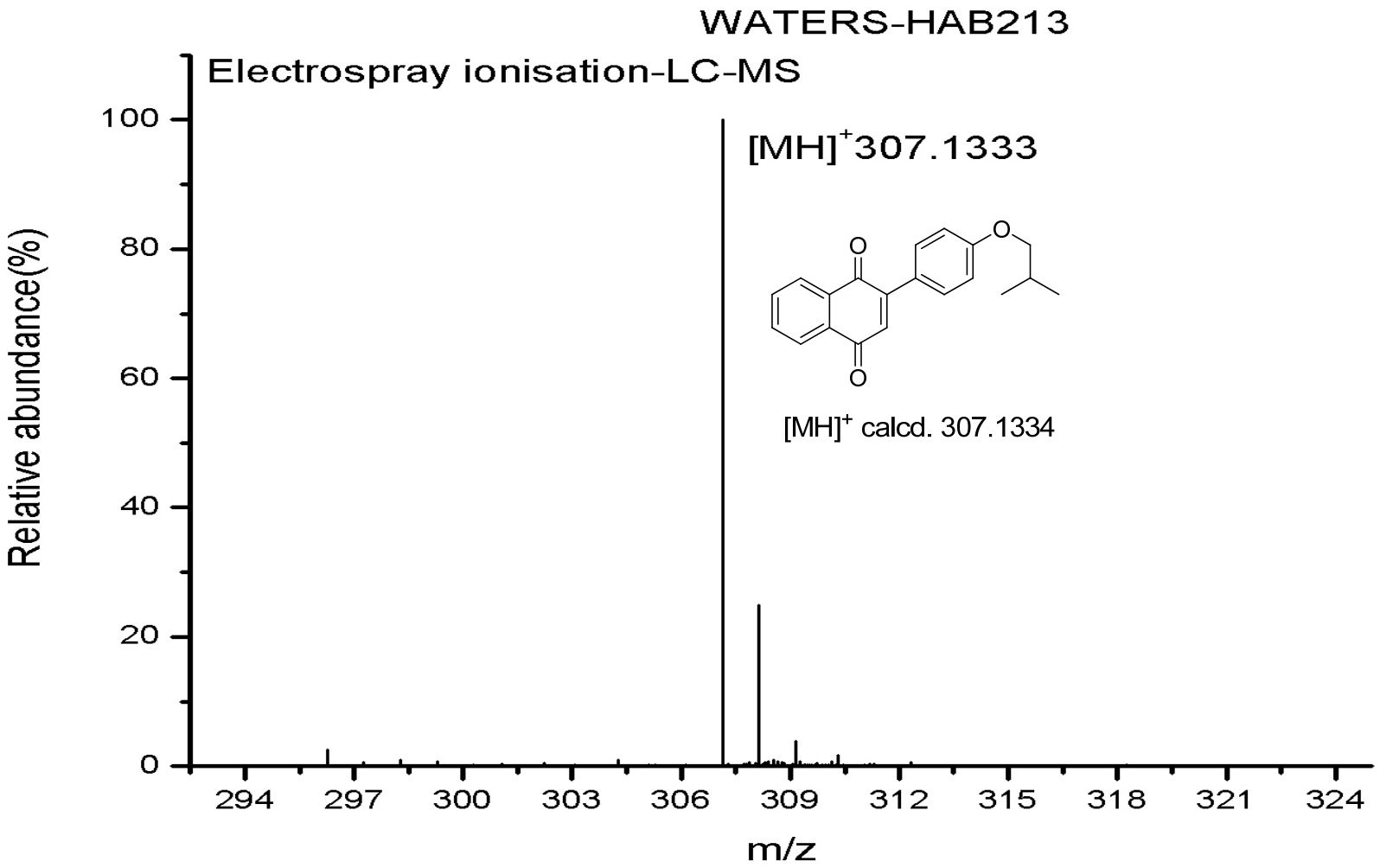


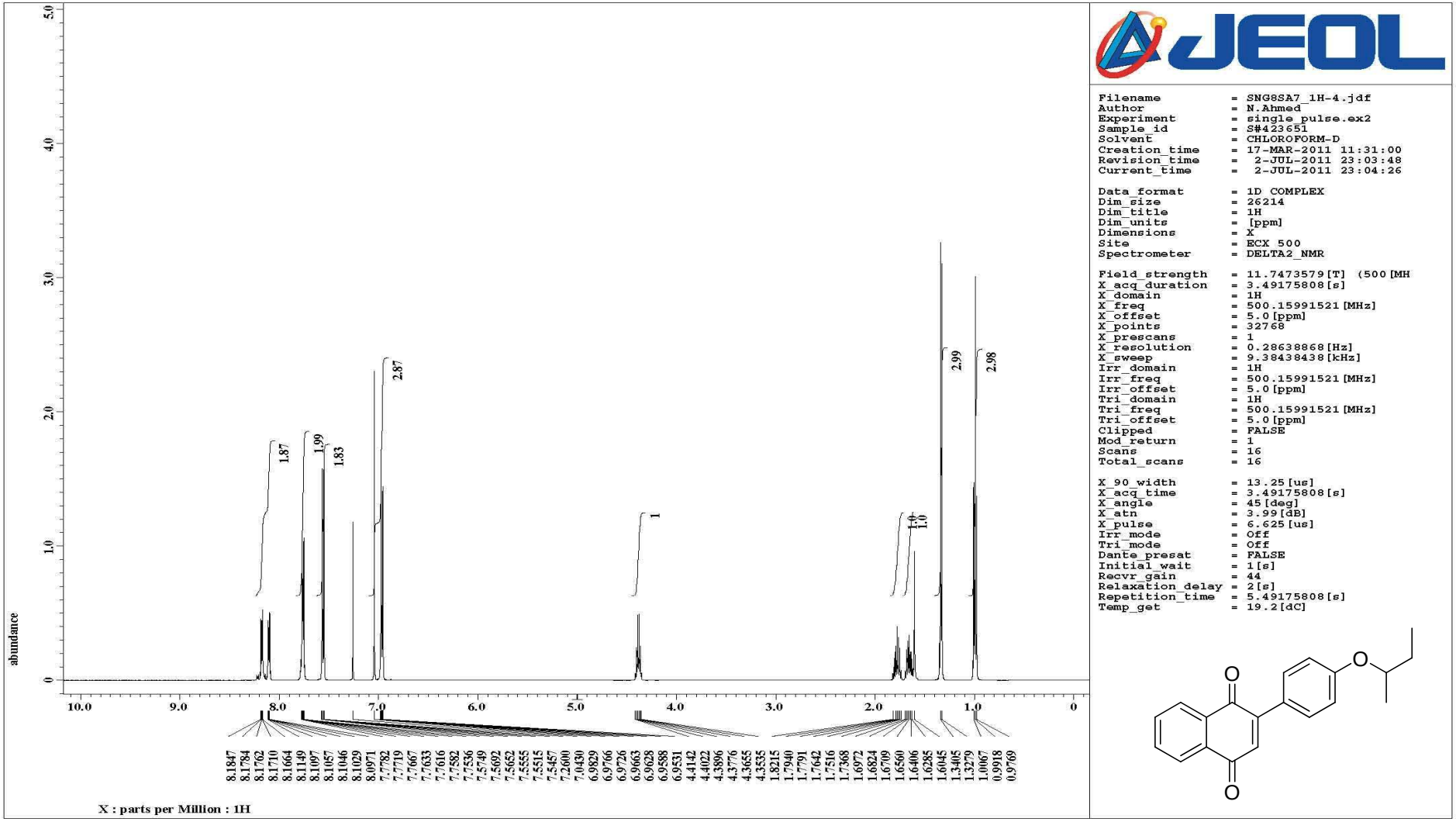
^{1}H NMR spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone **(2.6)**



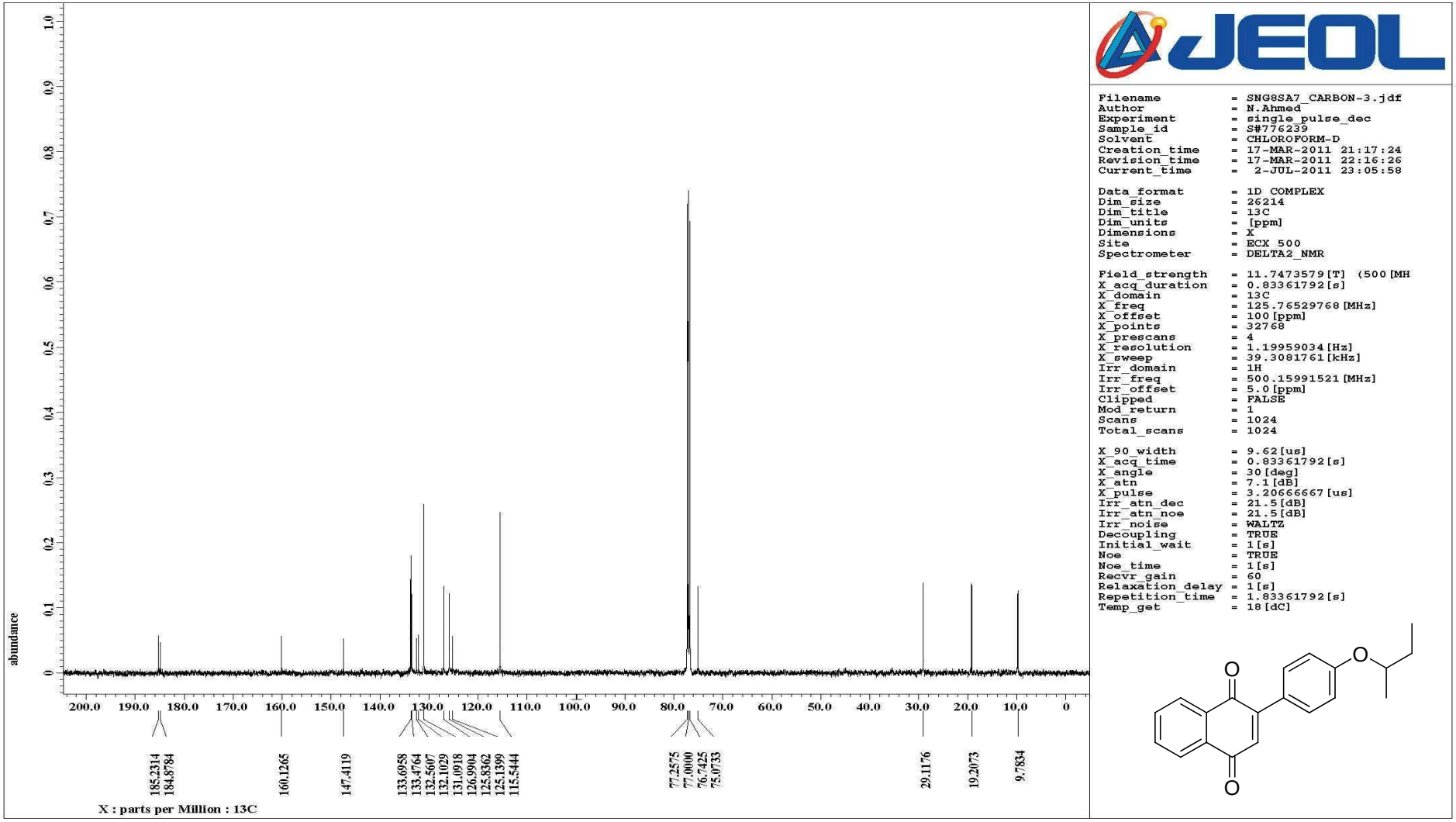
^{13}C NMR spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone **(2.6)**



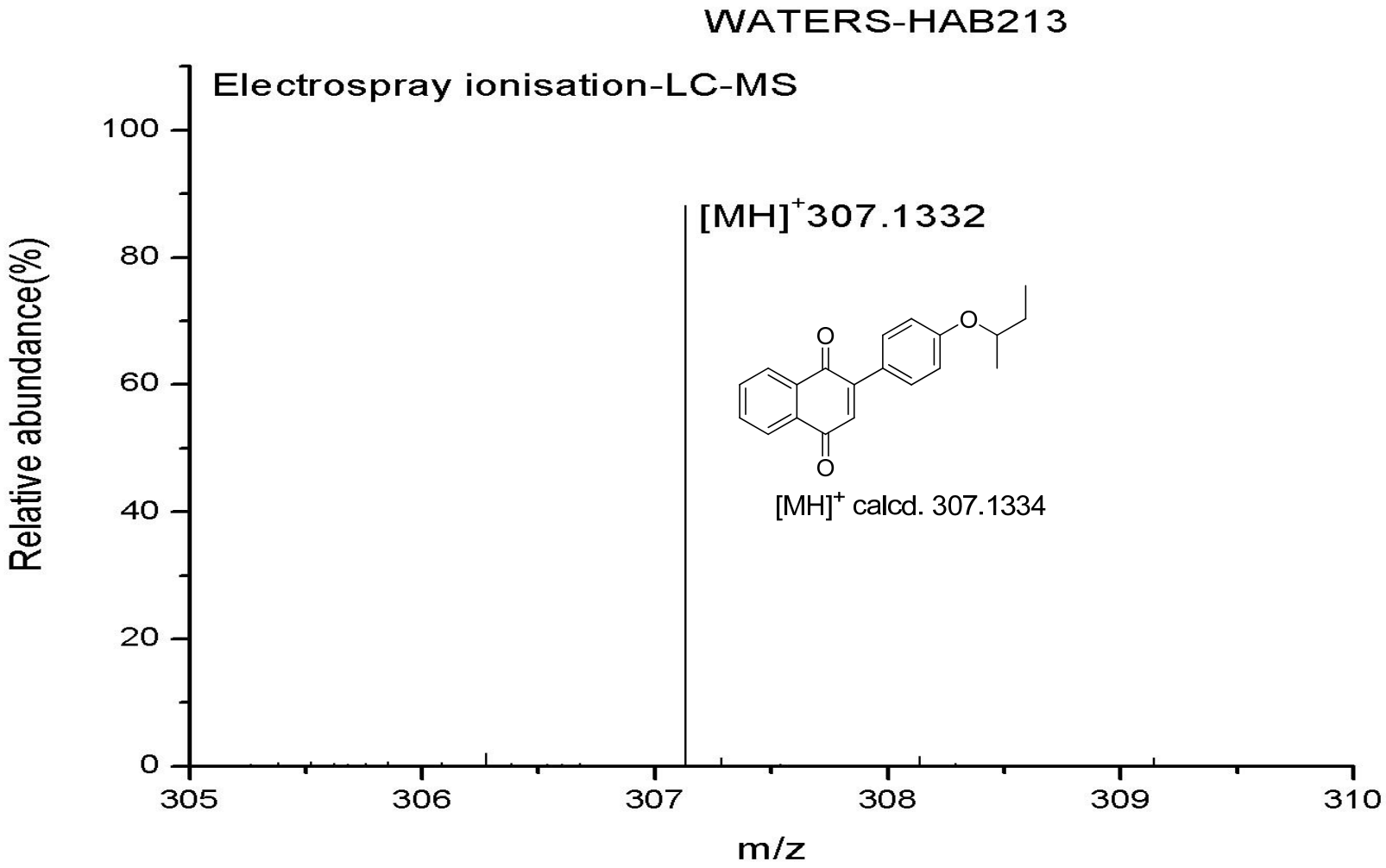
HRMS spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone **(2.6)**



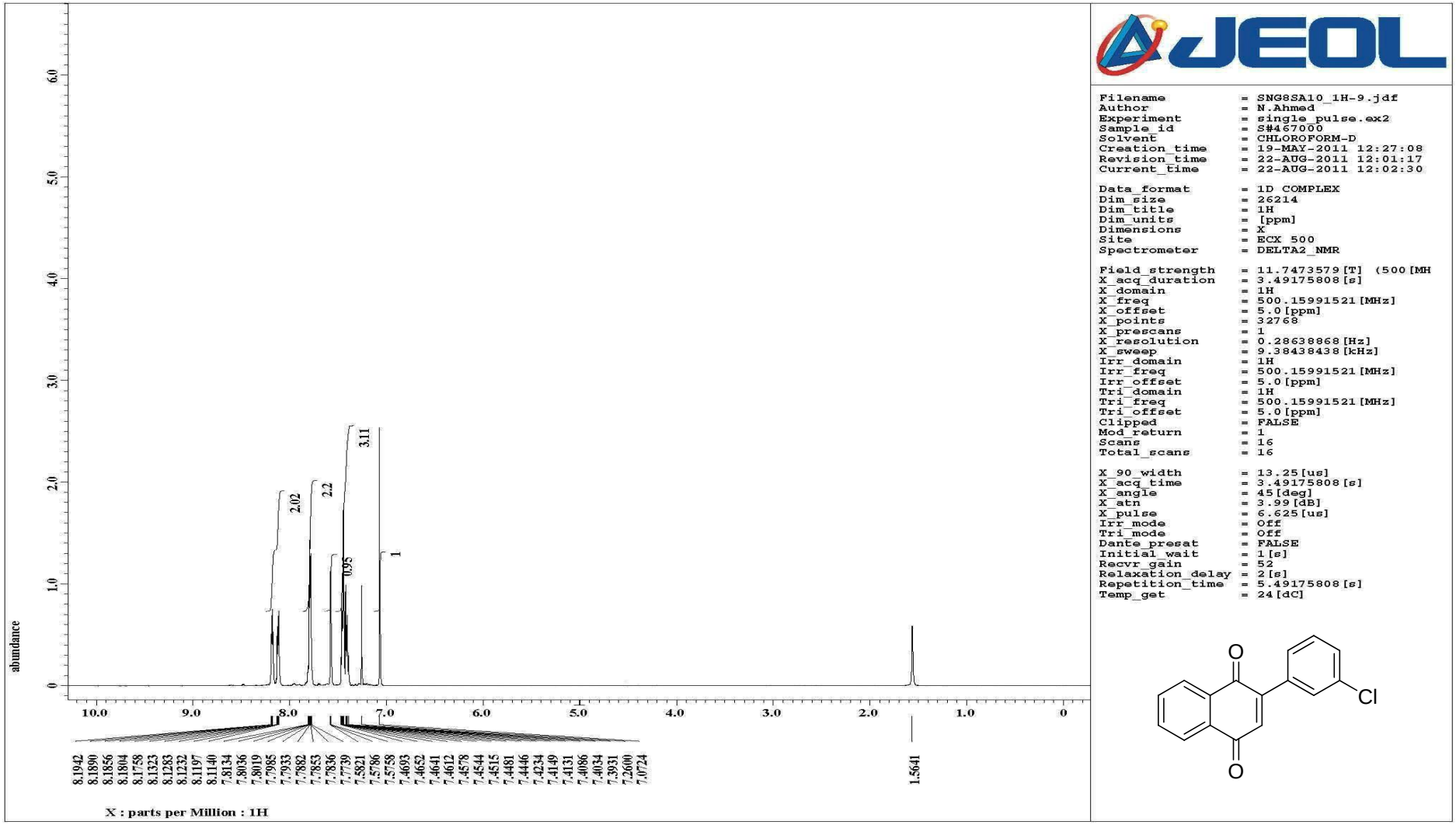
^{1}H NMR spectrum of 2-(4-sec-butoxyphenyl)-1,4-naphthoquinone **(2.7)**



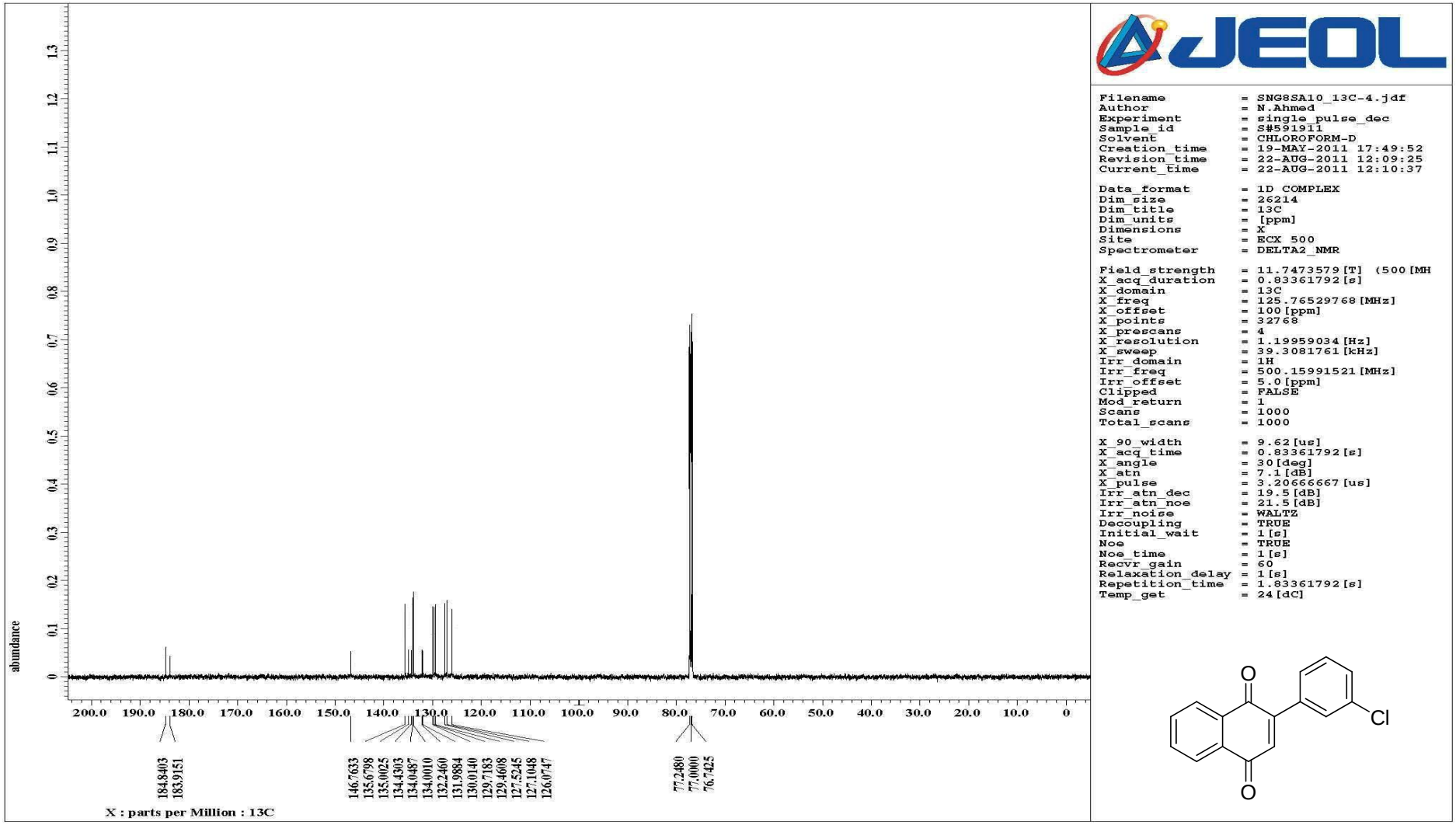
^{13}C spectrum of 2-(4-sec-butoxyphenyl)-1,4-naphthoquinone **(2.7)**



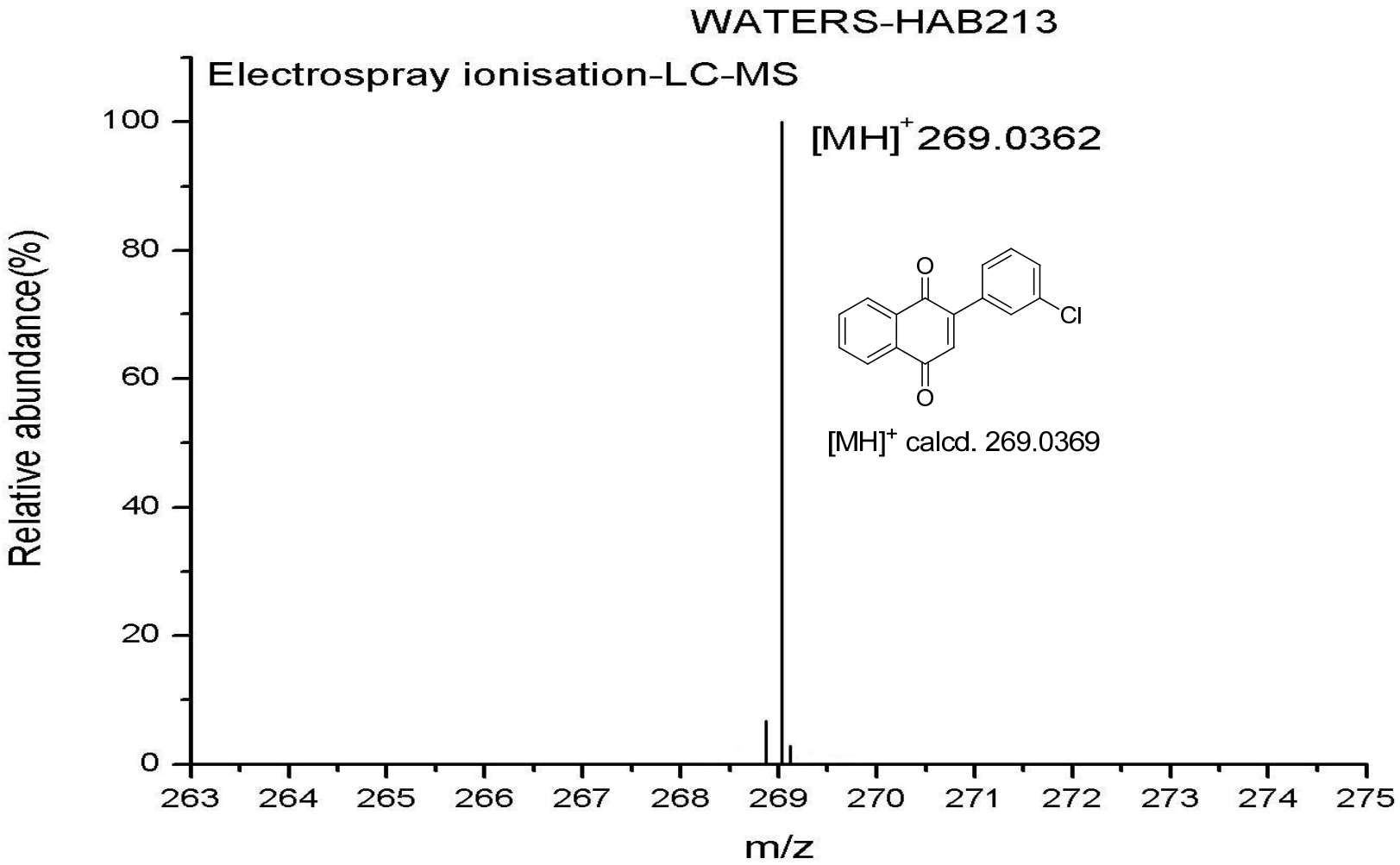
HRMS spectrum of 2-(4-sec-butoxyphenyl)-1,4-naphthoquinone **(2.7)**



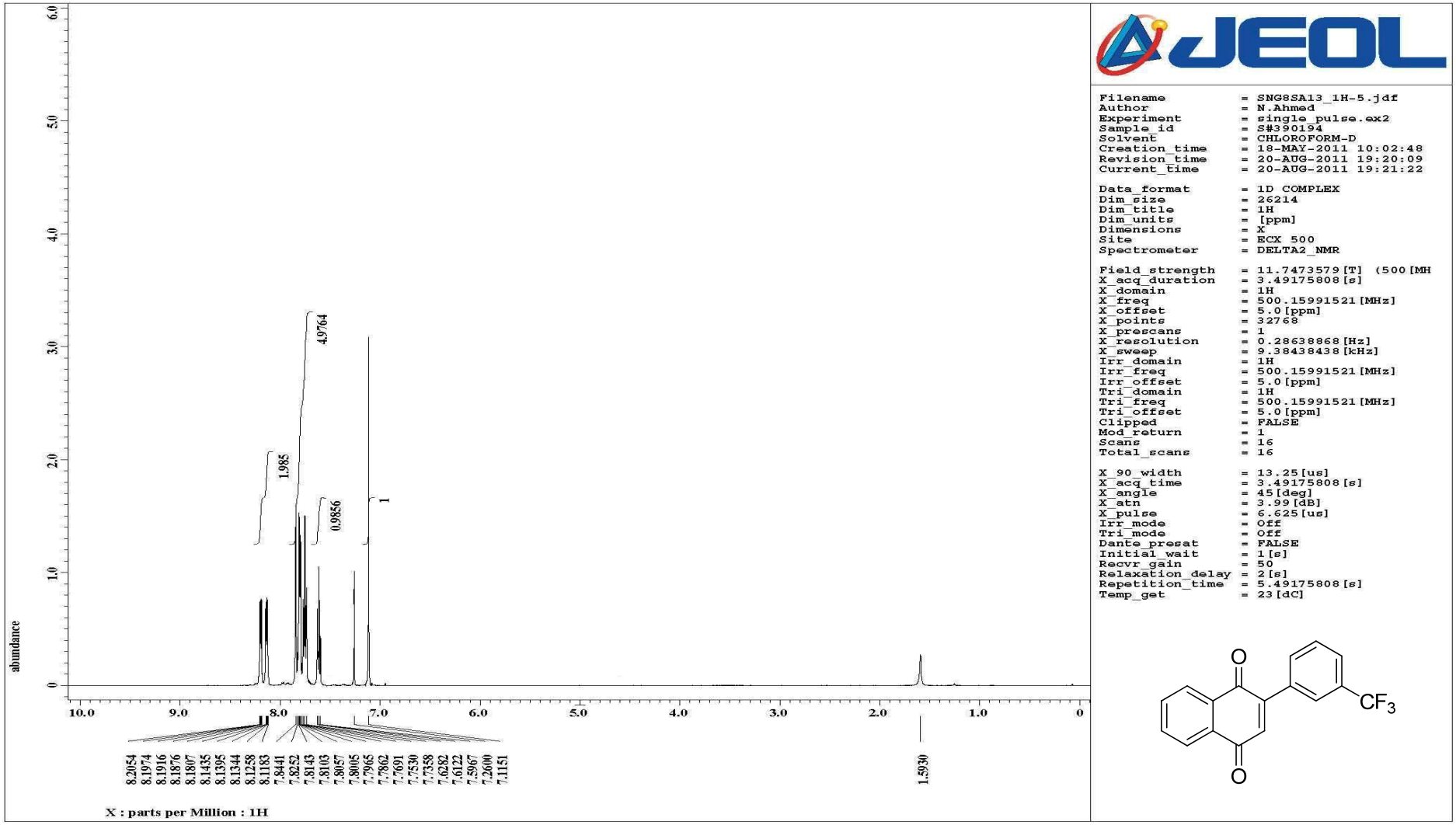
^{1}H NMR spectrum of 2-(3-chlorophenyl)-1,4-naphthoquinone **(2.8)**



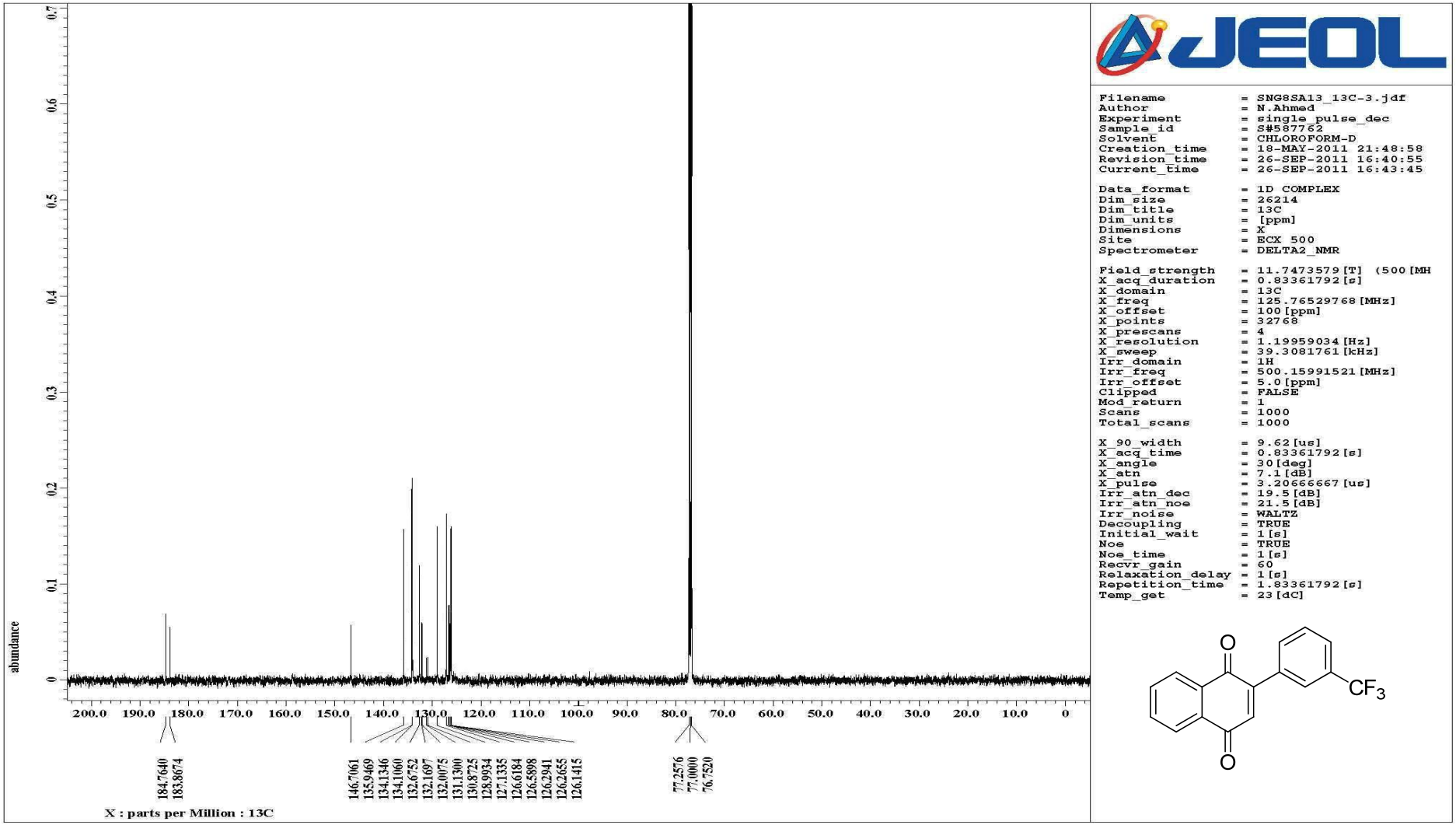
^{13}C NMR spectrum of 2-(3-chlorophenyl)-1,4-naphthoquinone **(2.8)**



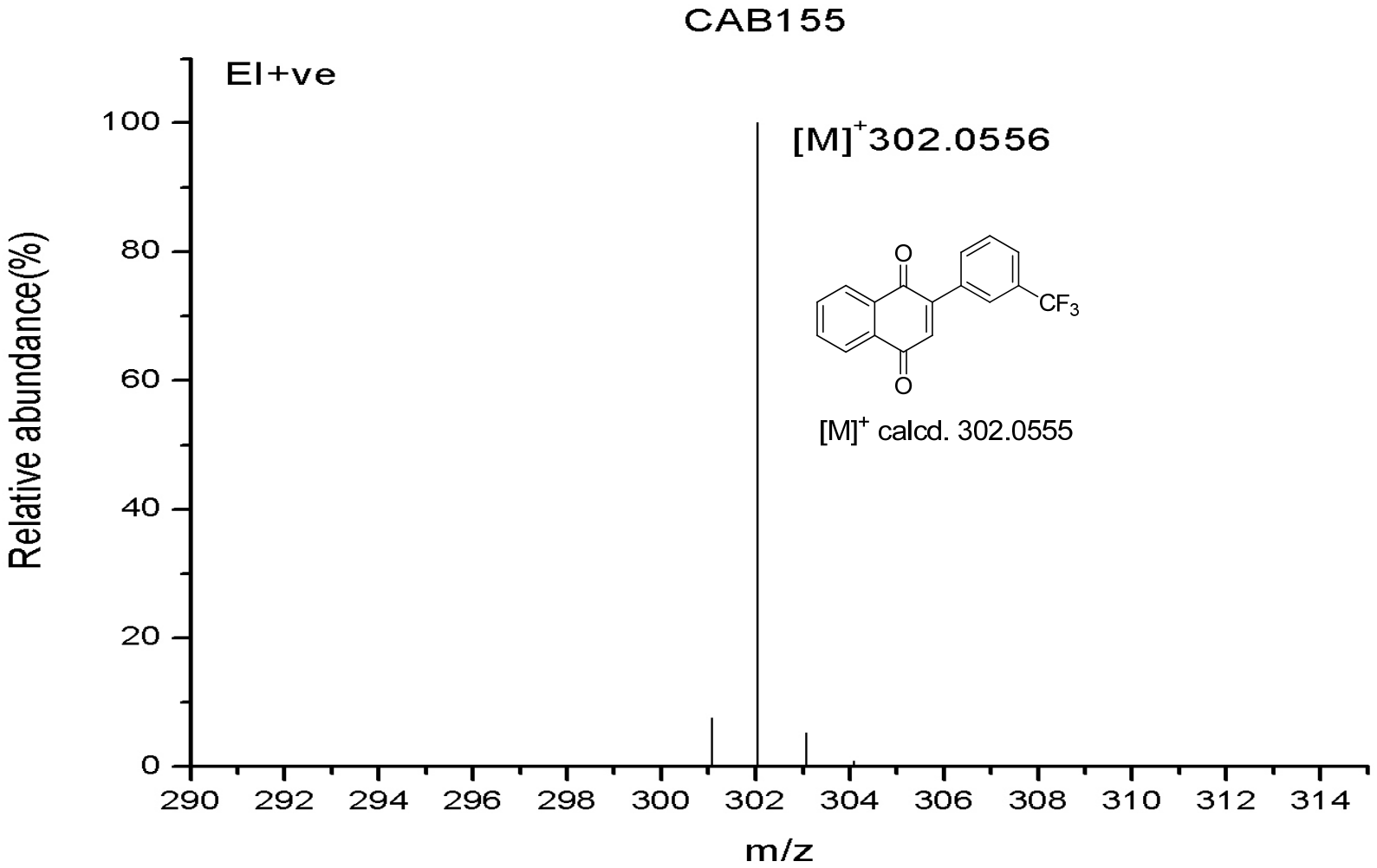
HRMS spectrum of 2-(3-chlorophenyl)-1,4-naphthoquinone **(2.8)**



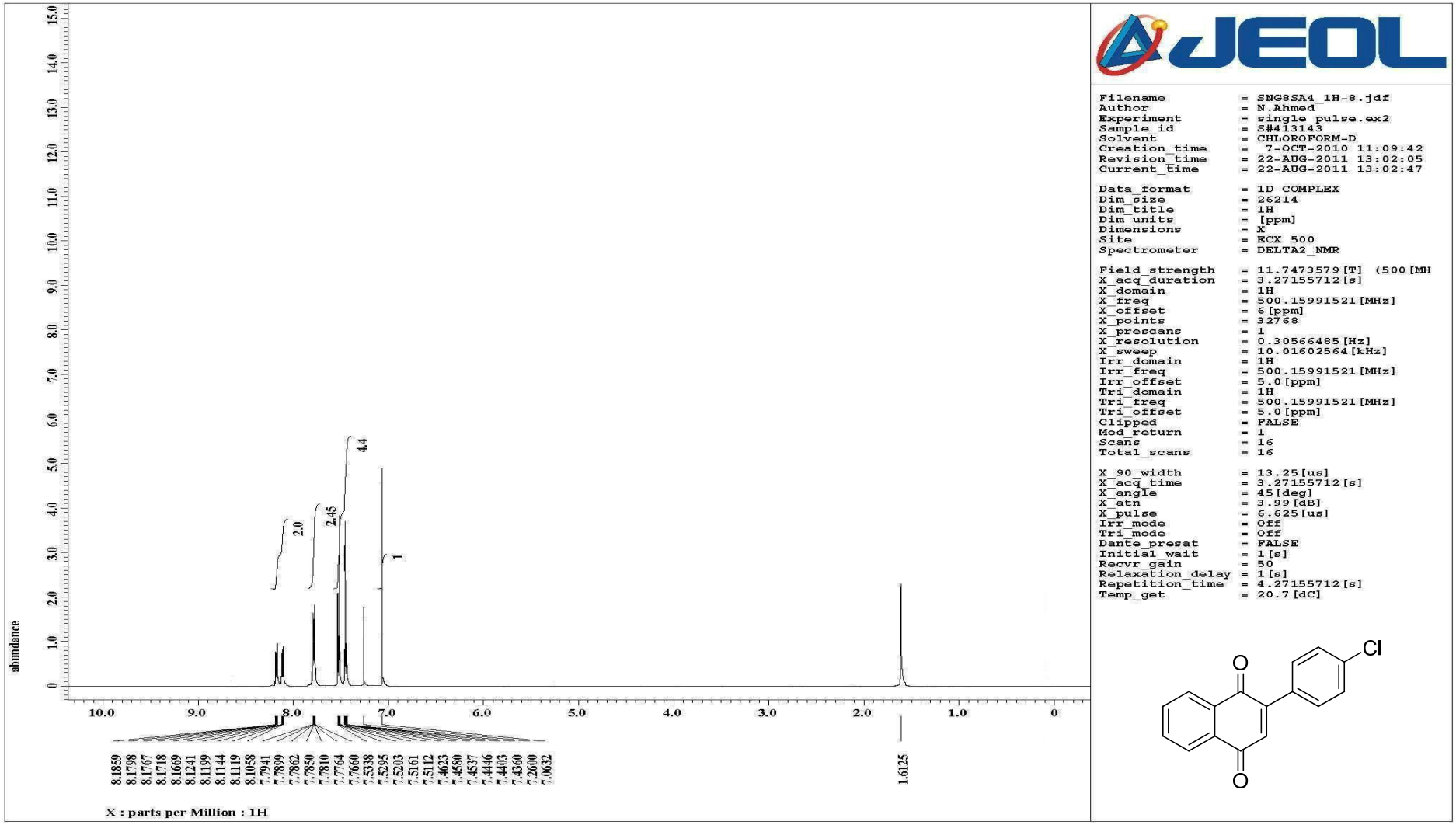
^{1}H NMR spectrum of 2-(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone **(2.9)**



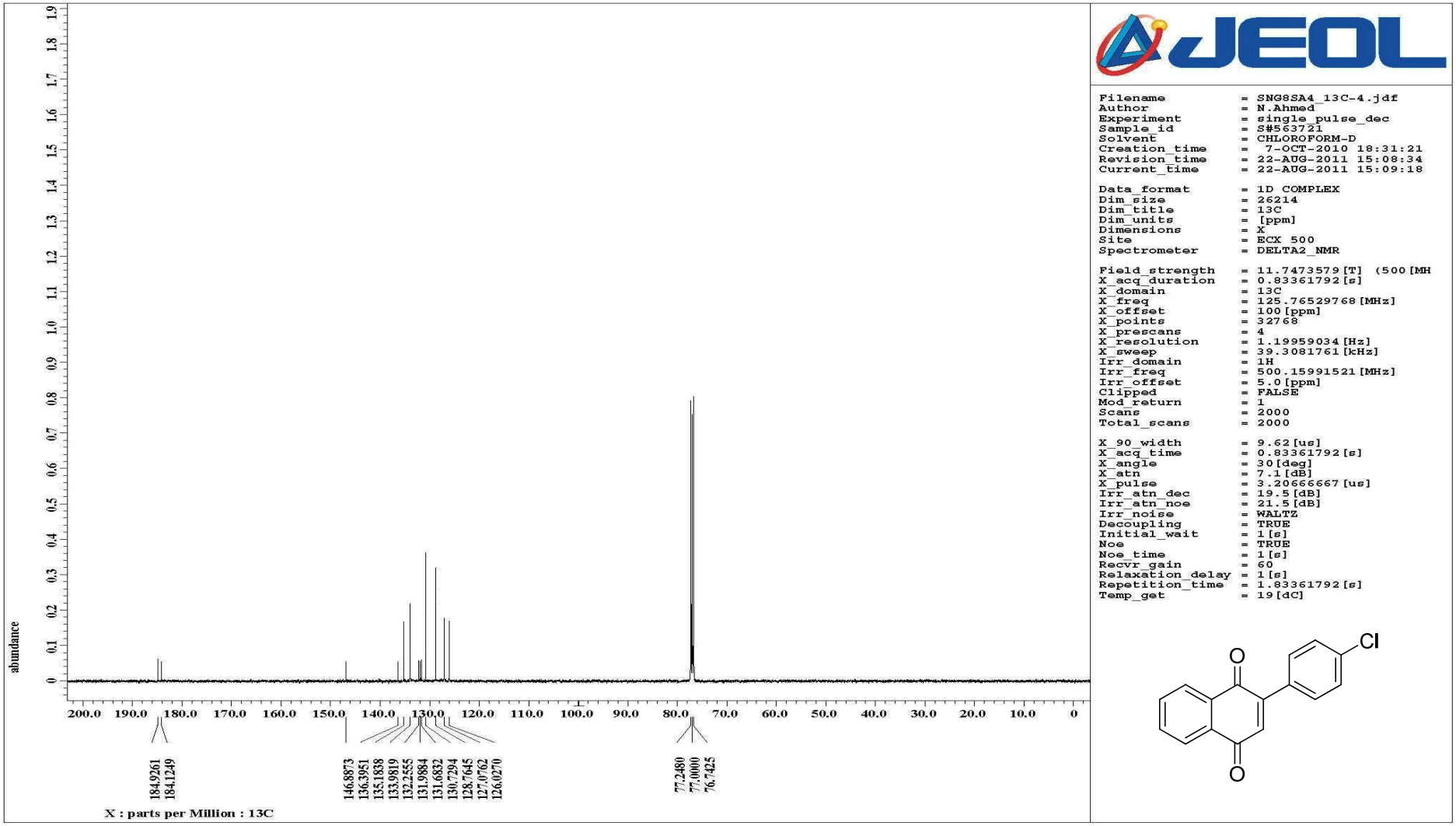
^{13}C spectrum of 2-(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone **(2.9)**



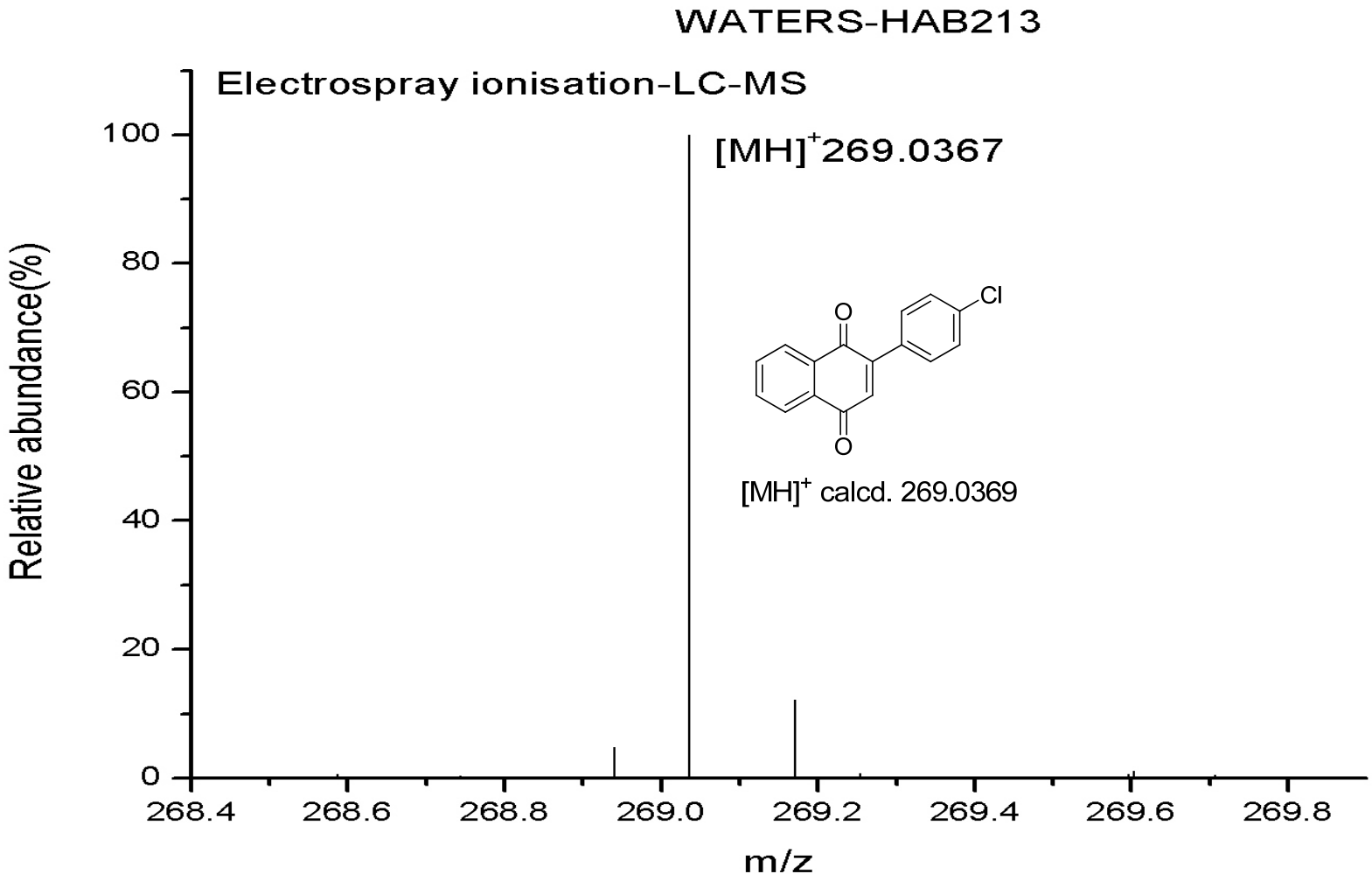
HRMS spectrum of 2-(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone **(2.9)**



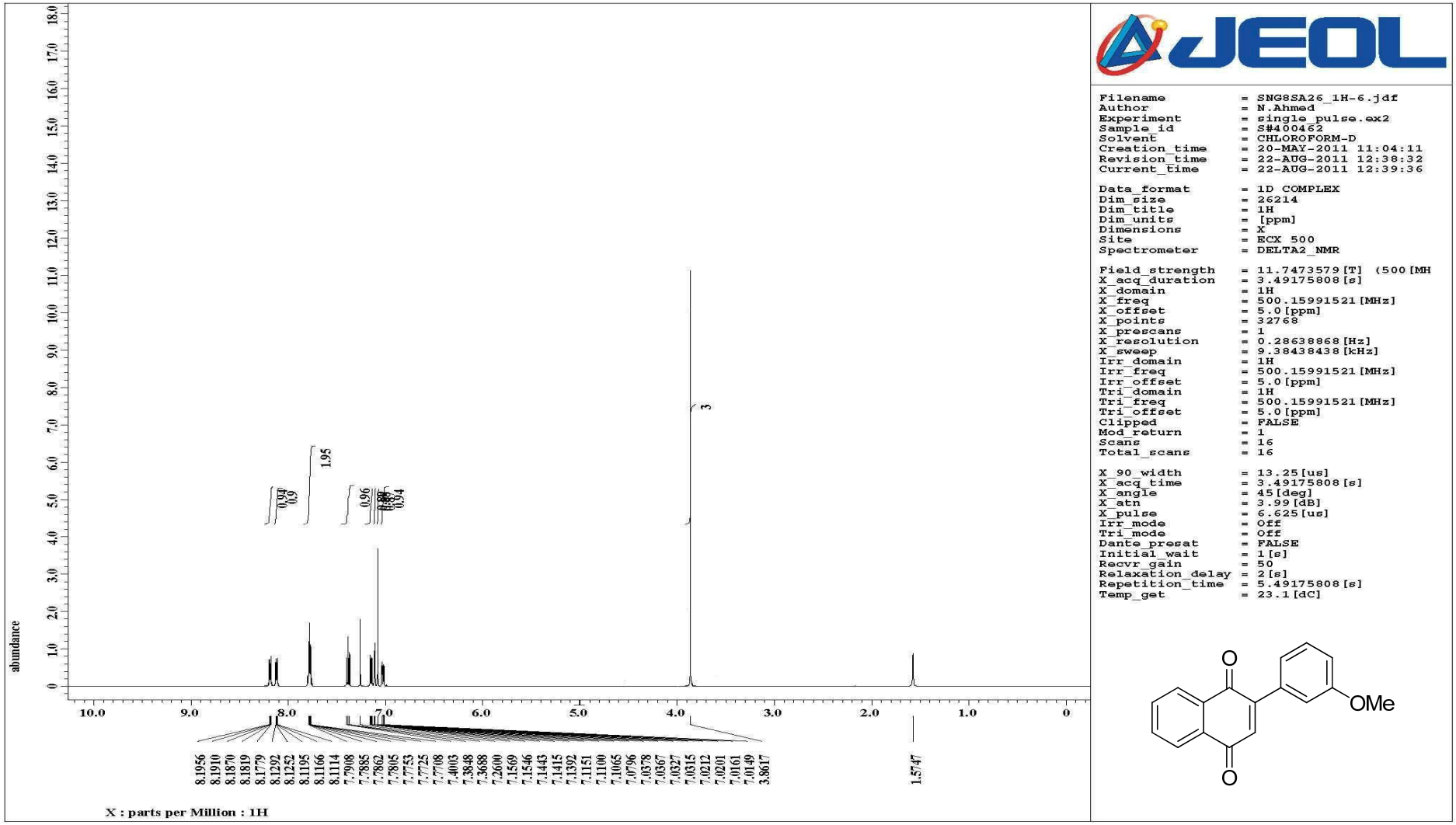
^{1}H NMR spectrum of 2-(4-chlorophenyl)-1,4-naphthoquinone **(2.10)**



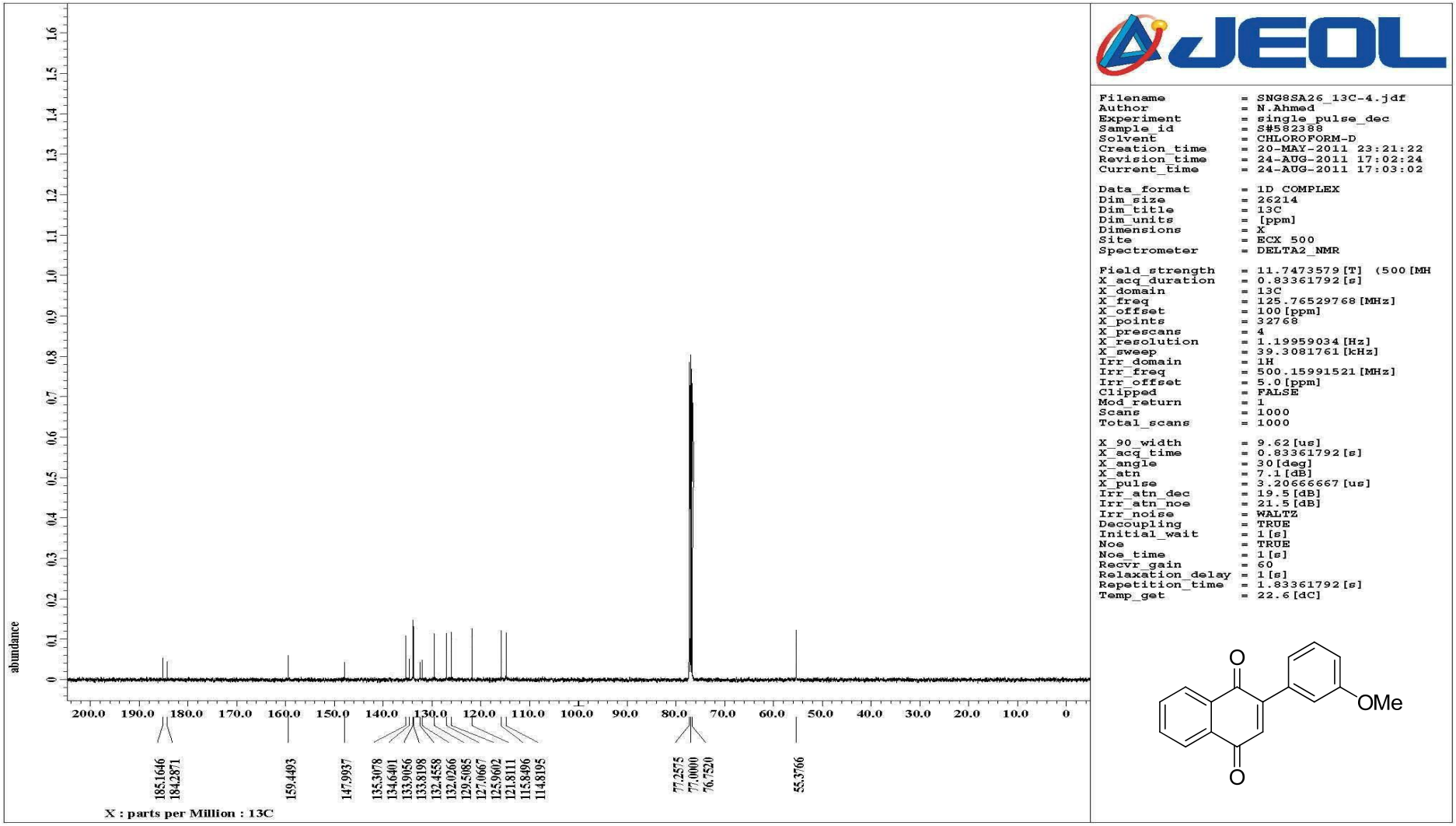
^{13}C spectrum of 2-(4-chlorophenyl)-1,4-naphthoquinone **(2.10)**



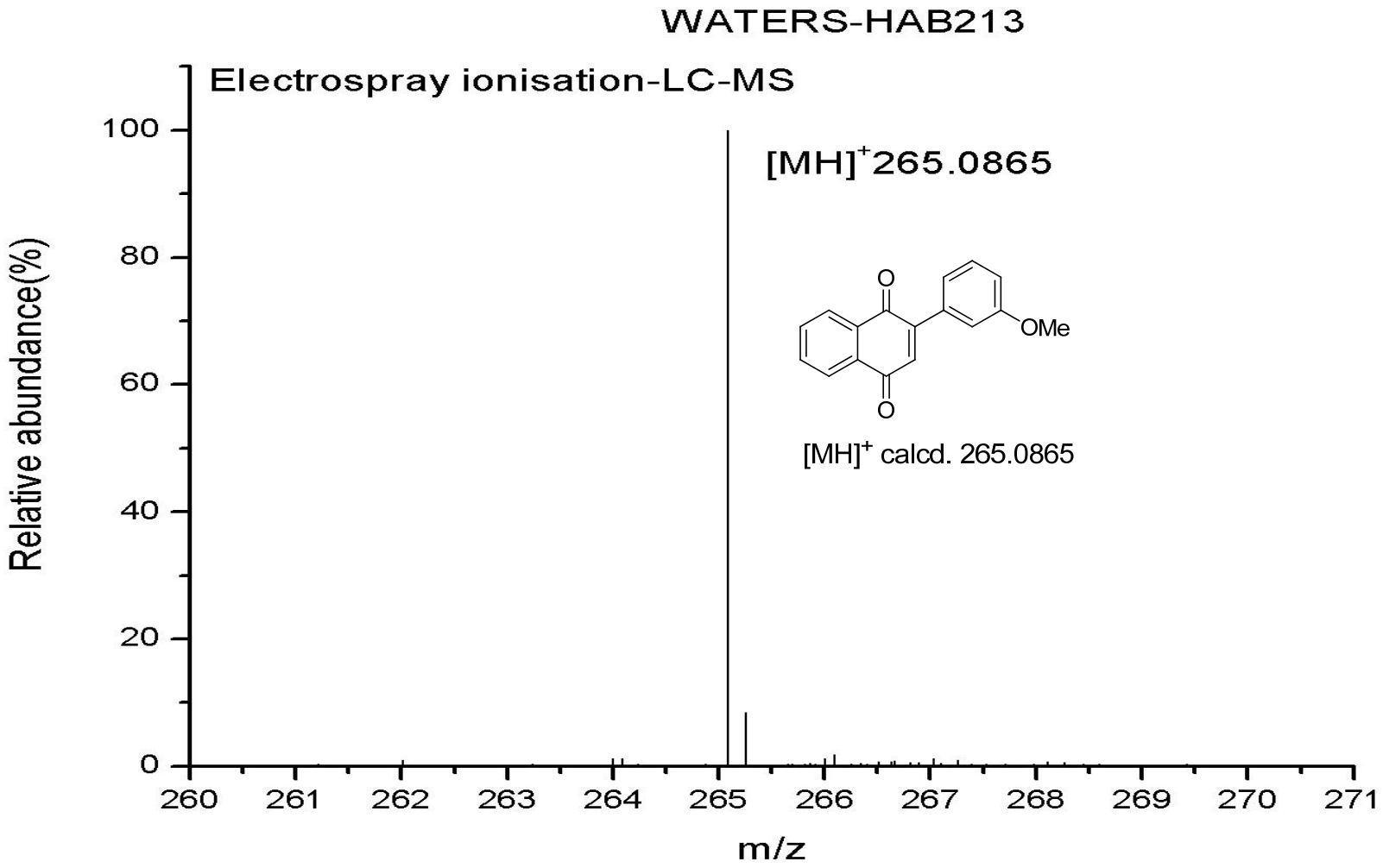
HRMS spectrum of 2-(4-chlorophenyl)-1,4-naphthoquinone **(2.10)**



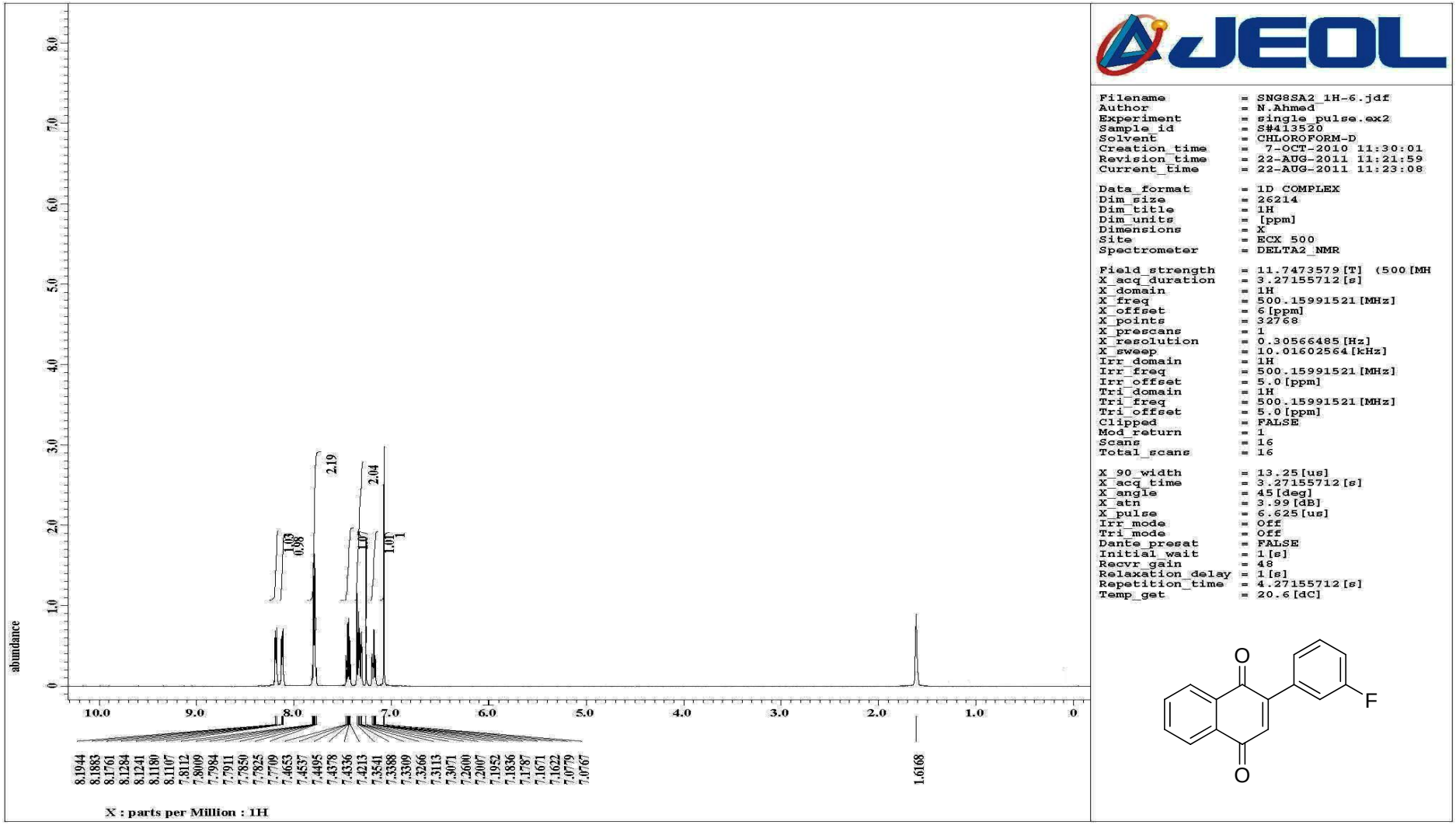
^{1}H NMR spectrum of 2-(3-methoxyphenyl)-1,4-naphthoquinone **(2.11)**



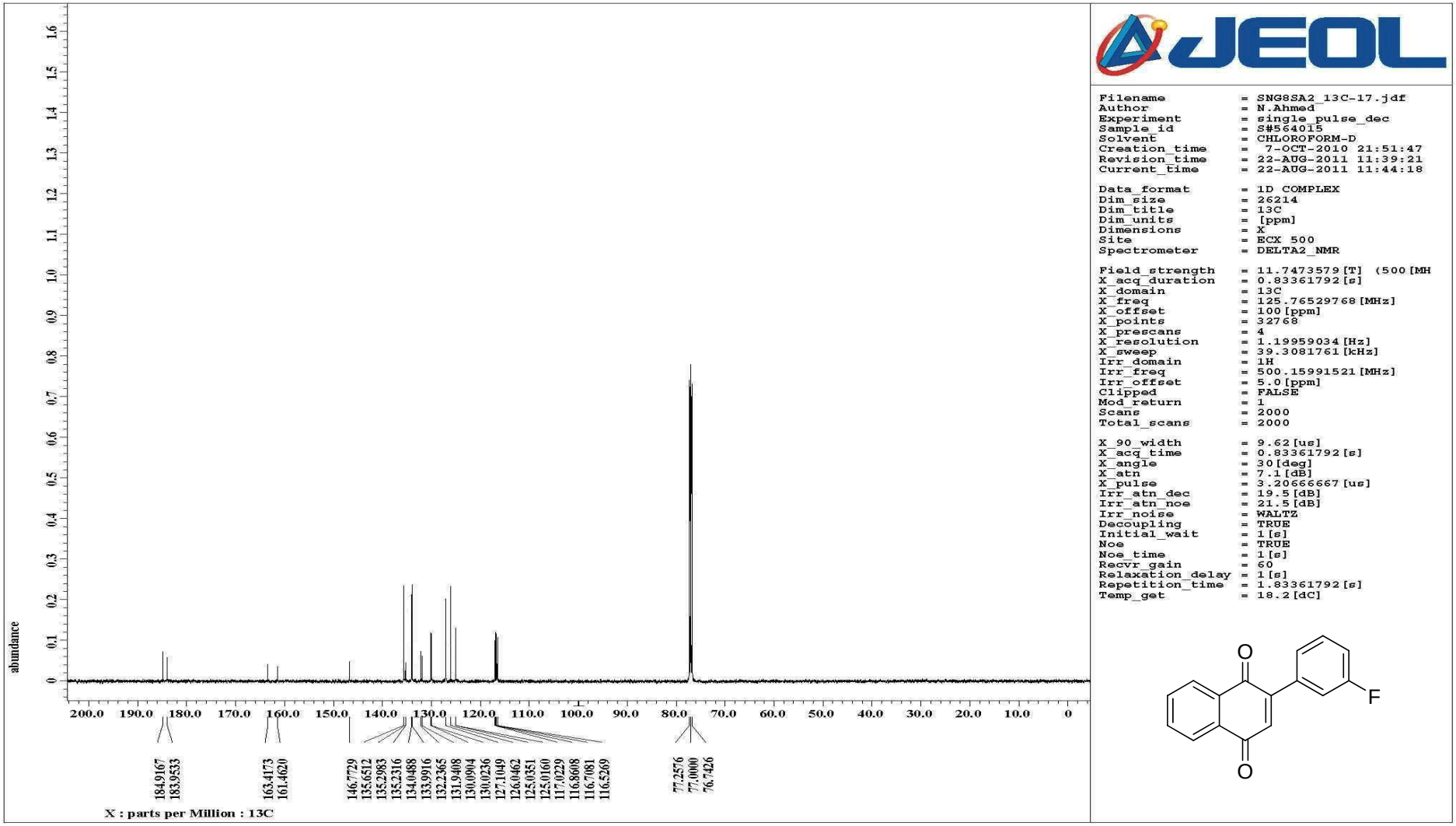
^{13}C spectrum of 2-(3-methoxyphenyl)-1,4-naphthoquinone **(2.11)**



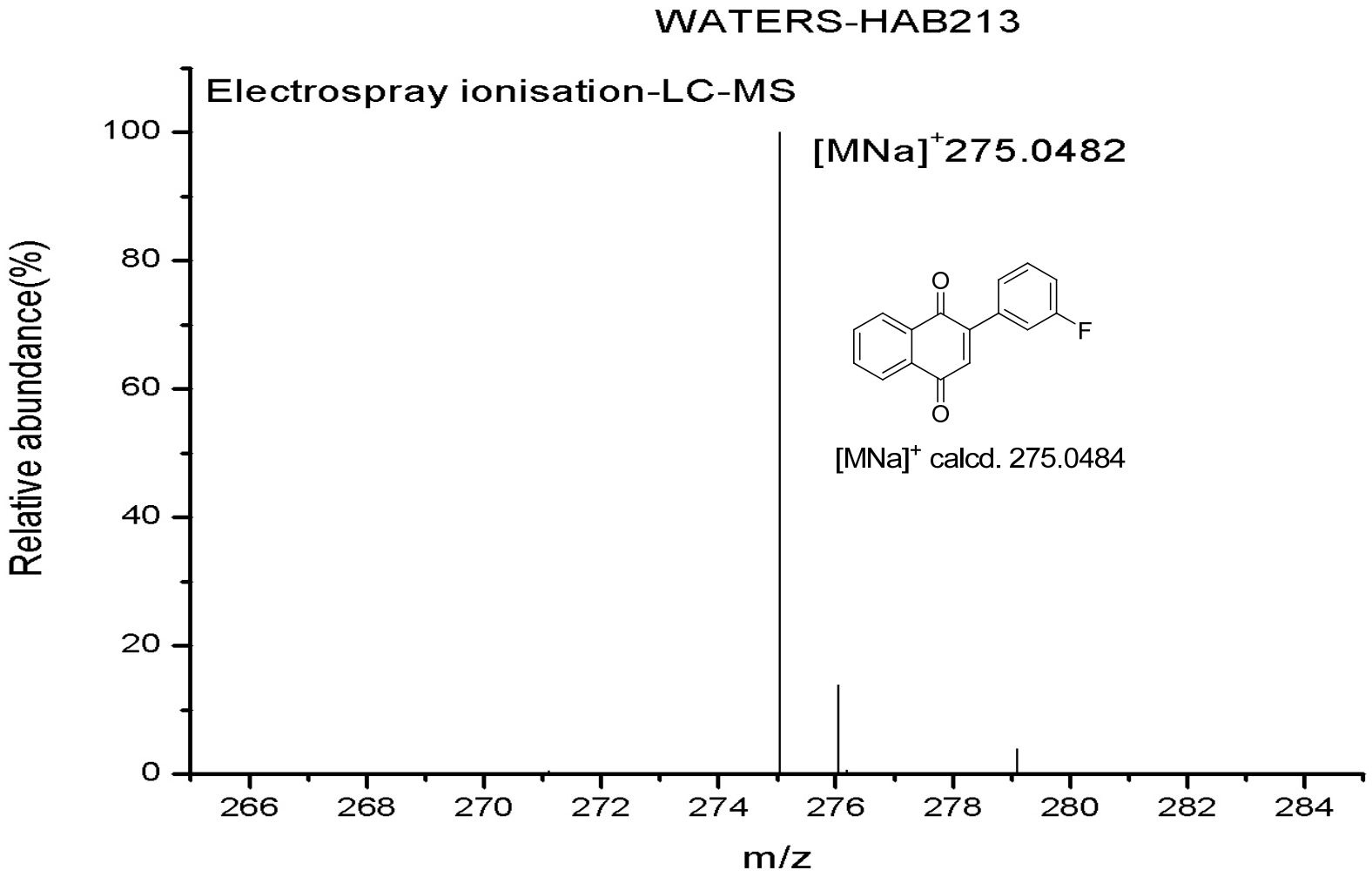
HRMS spectrum of 2-(3-methoxyphenyl)-1,4-naphthoquinone **(2.11)**



^{1}H NMR spectrum of 2-(3-fluorophenyl)-1,4-naphthoquinone **(2.12)**



^{13}C NMR spectrum of 2-(3-fluorophenyl)-1,4-naphthoquinone **(2.12)**



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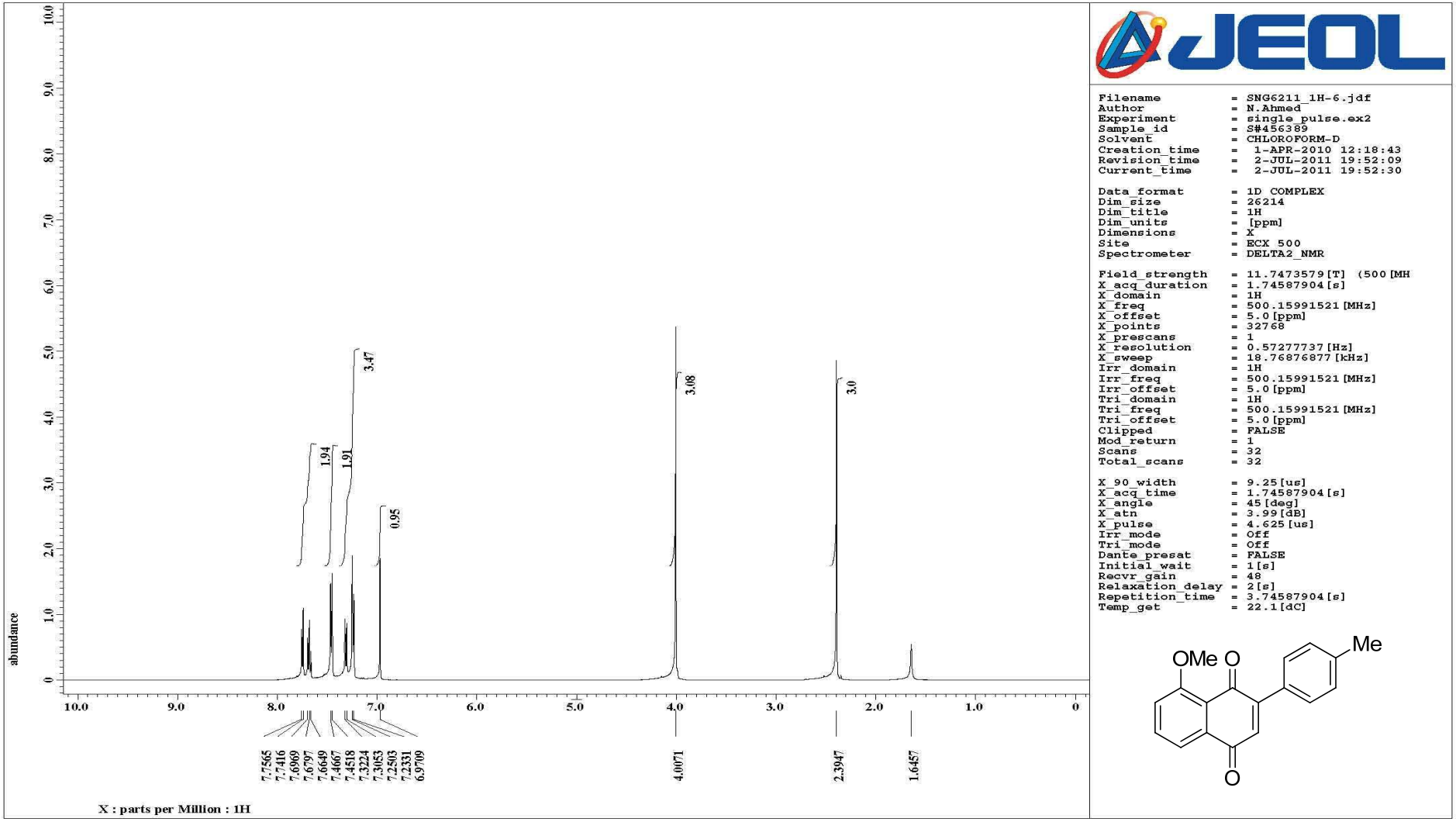
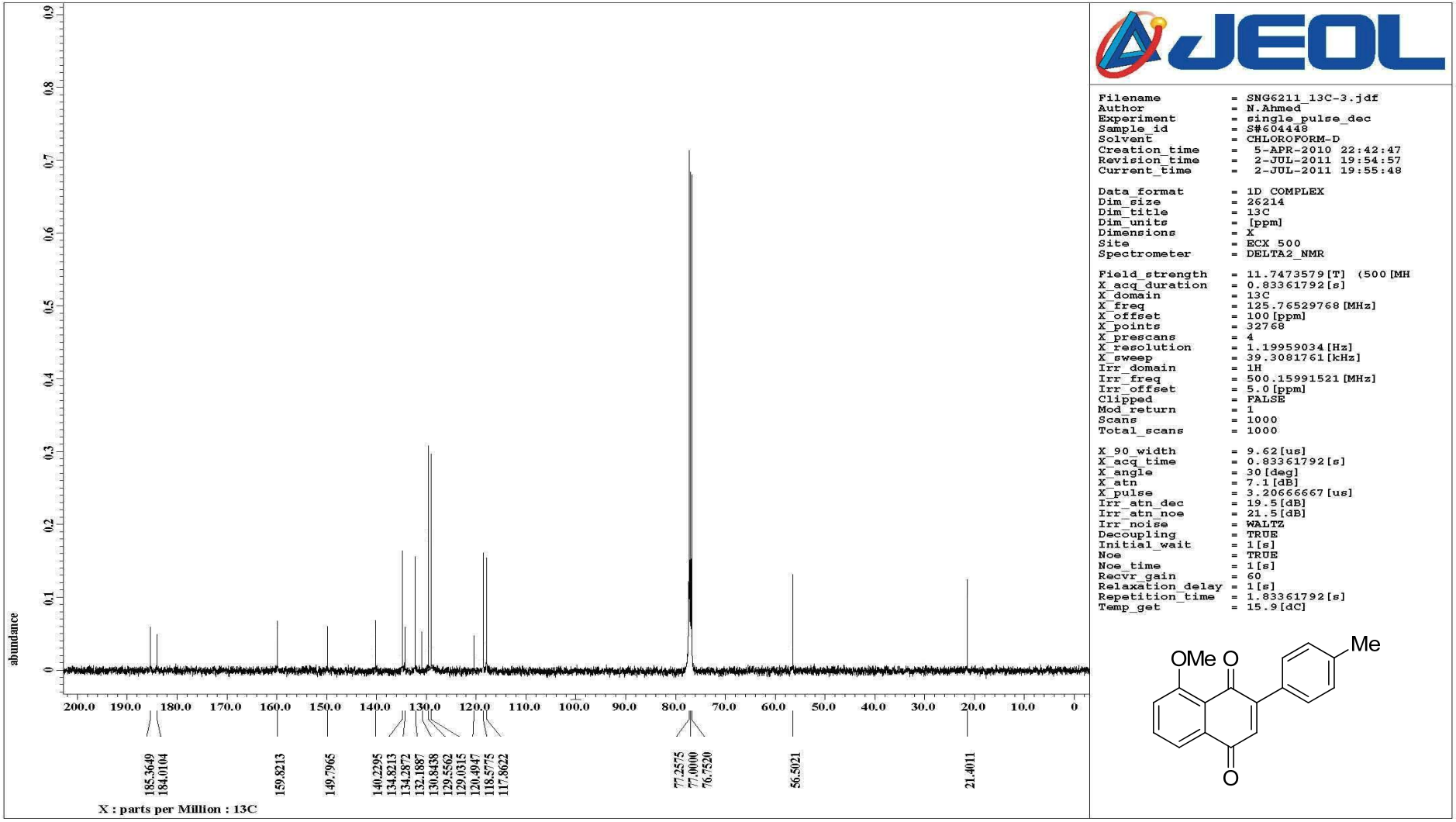
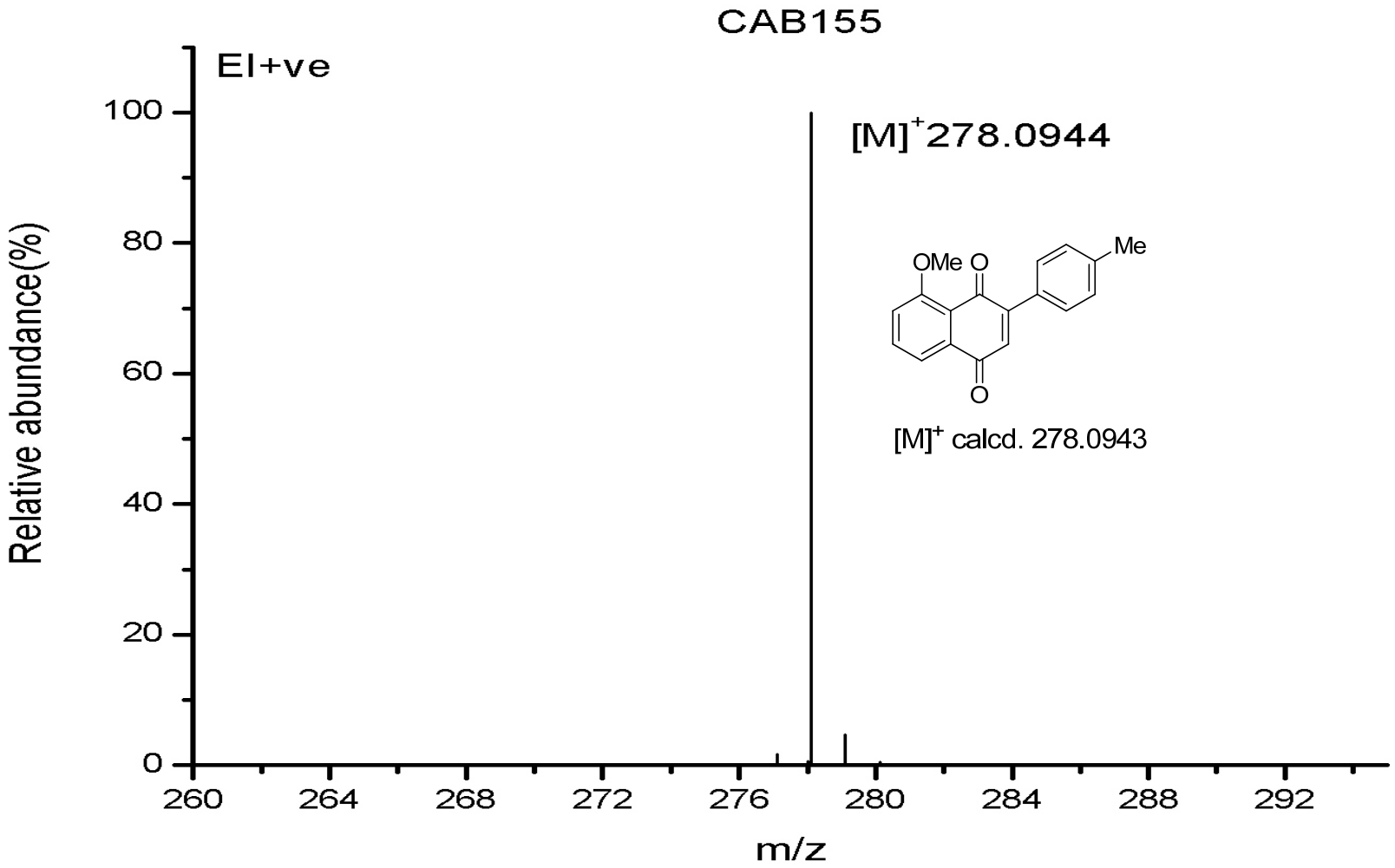


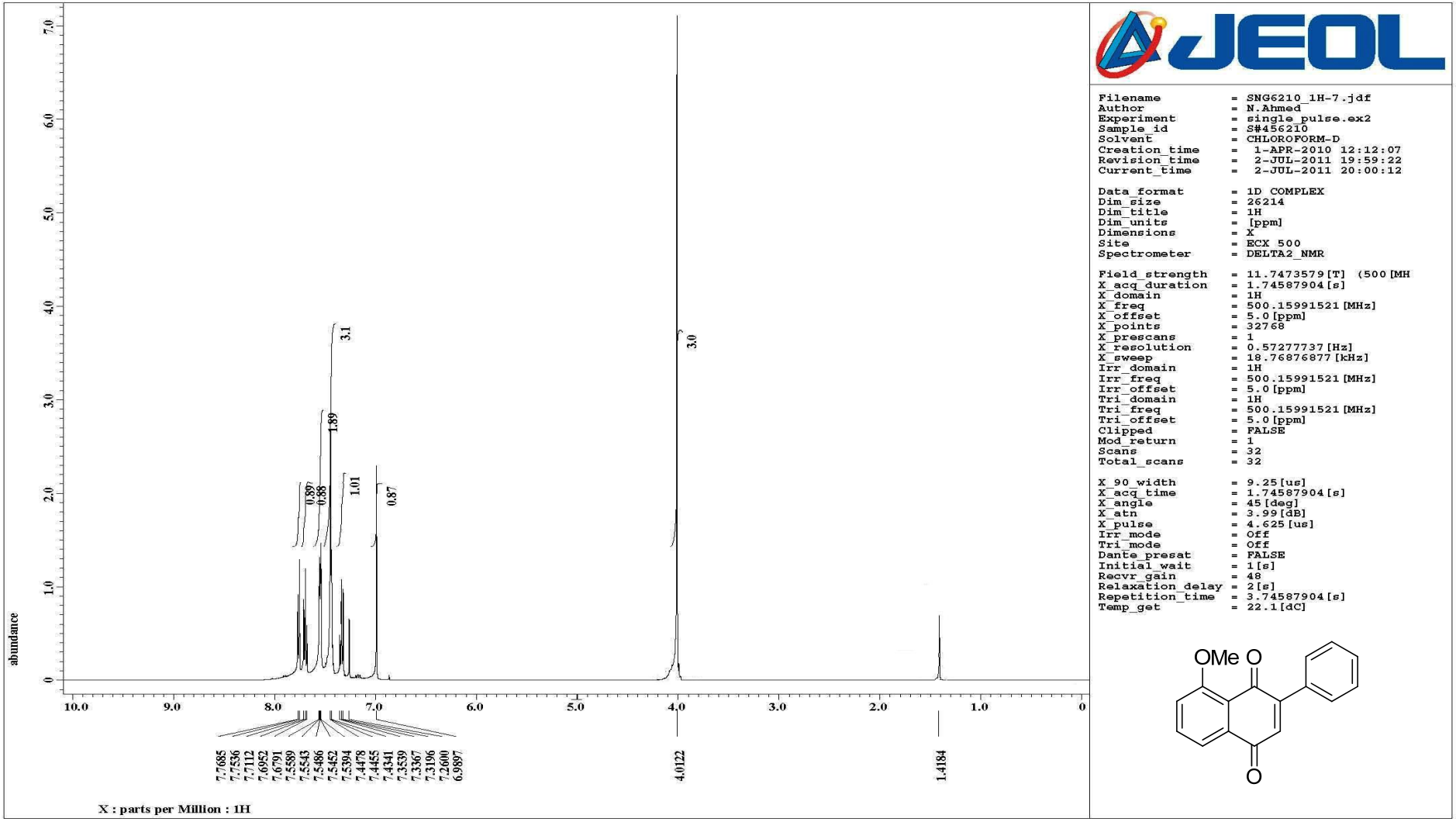
^{1}H NMR spectrum of 8-methoxy-2-*p*-tolyl-1,4-naphthoquinone **(3.1)**



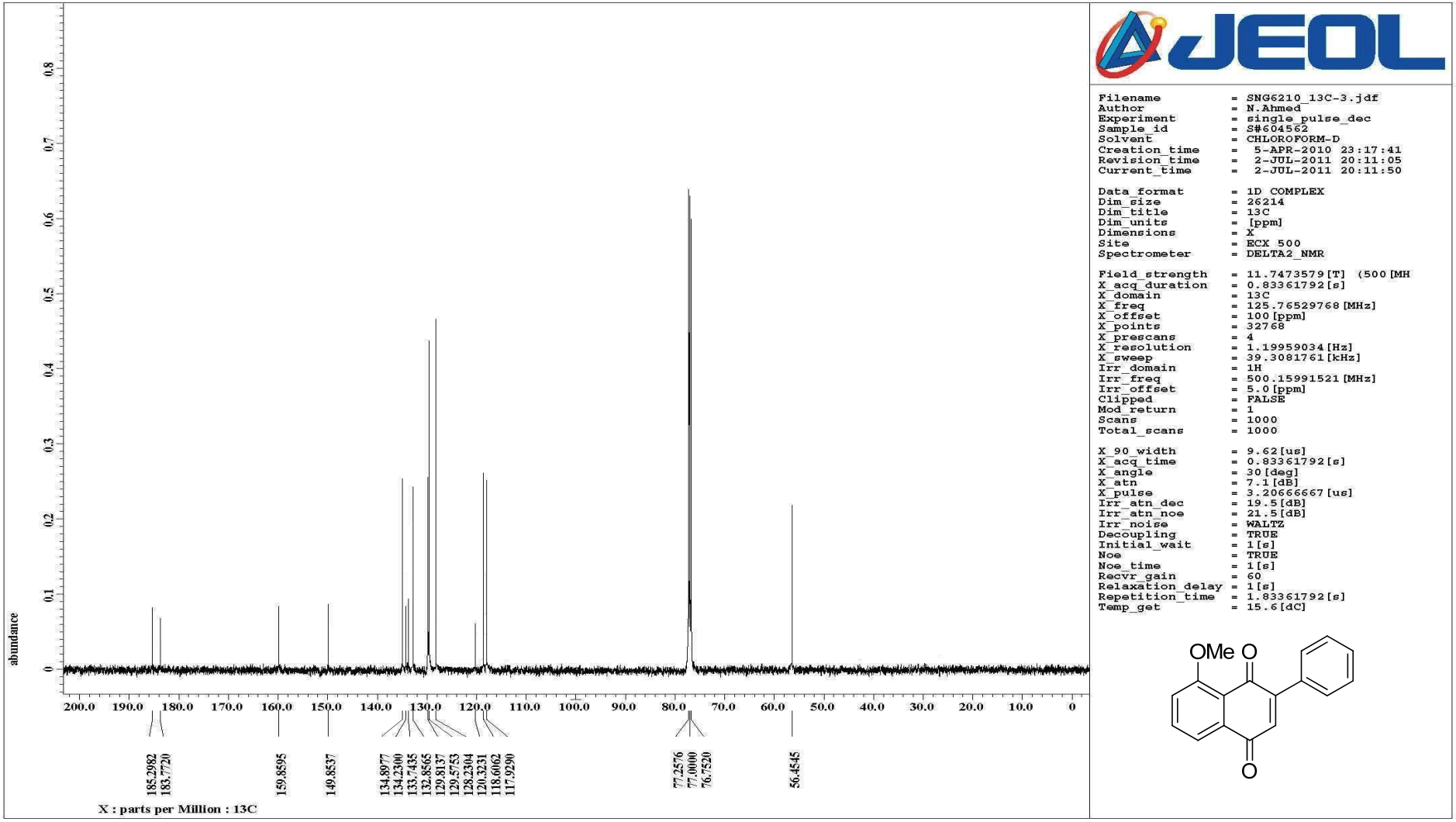
^{13}C NMR spectrum of 8-methoxy-2-*p*-tolyl-1,4-naphthoquinone **(3.1)**



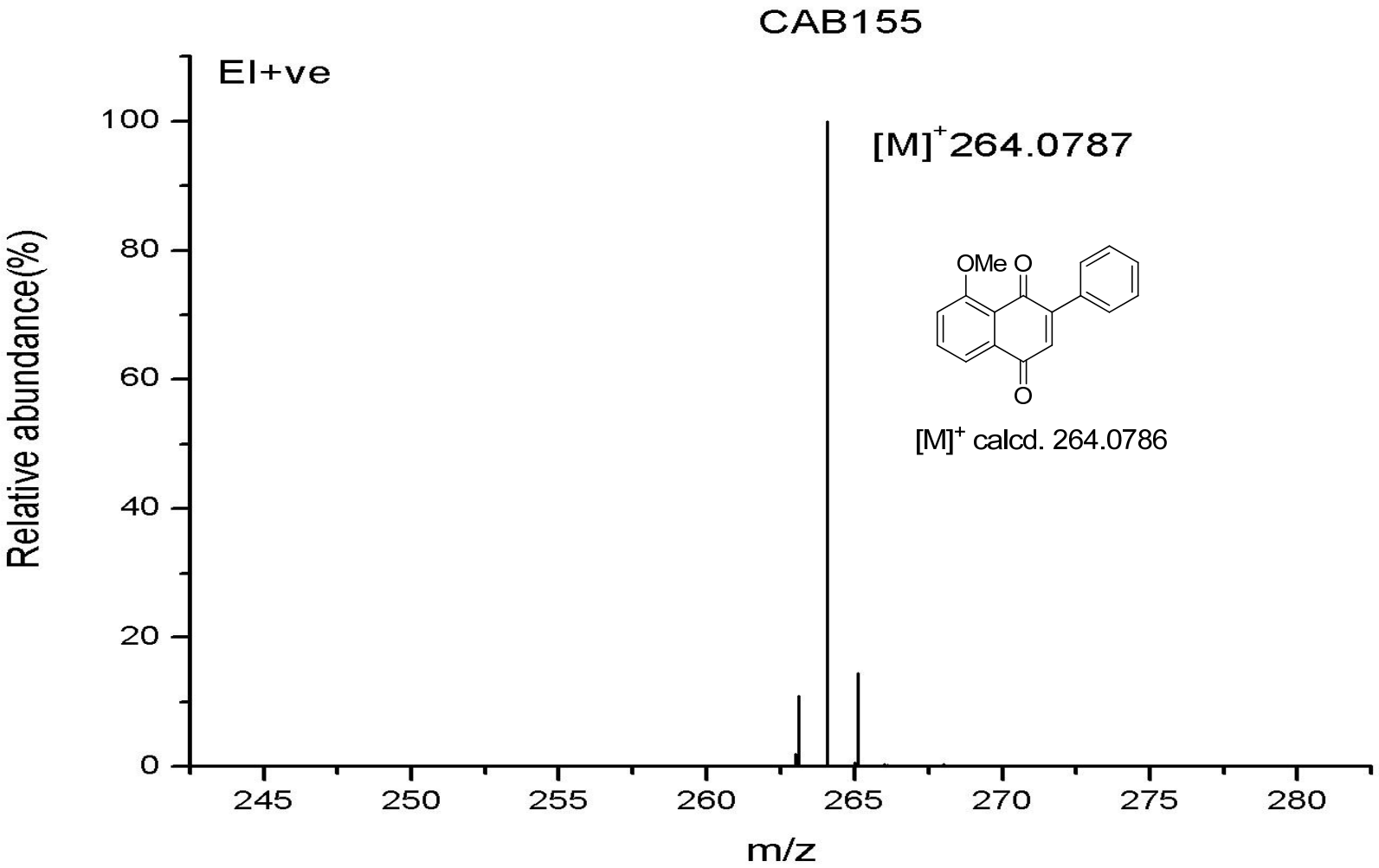
HRMS spectrum of 8-methoxy-2-*p*-tolyl-1,4-naphthoquinone **(3.1)**



^{1}H NMR spectrum of 8-methoxy-2-phenyl-1,4-naphthoquinone **(3.2)**



^{13}C NMR spectrum of 8-methoxy-2-phenyl-1,4-naphthoquinone **(3.2)**



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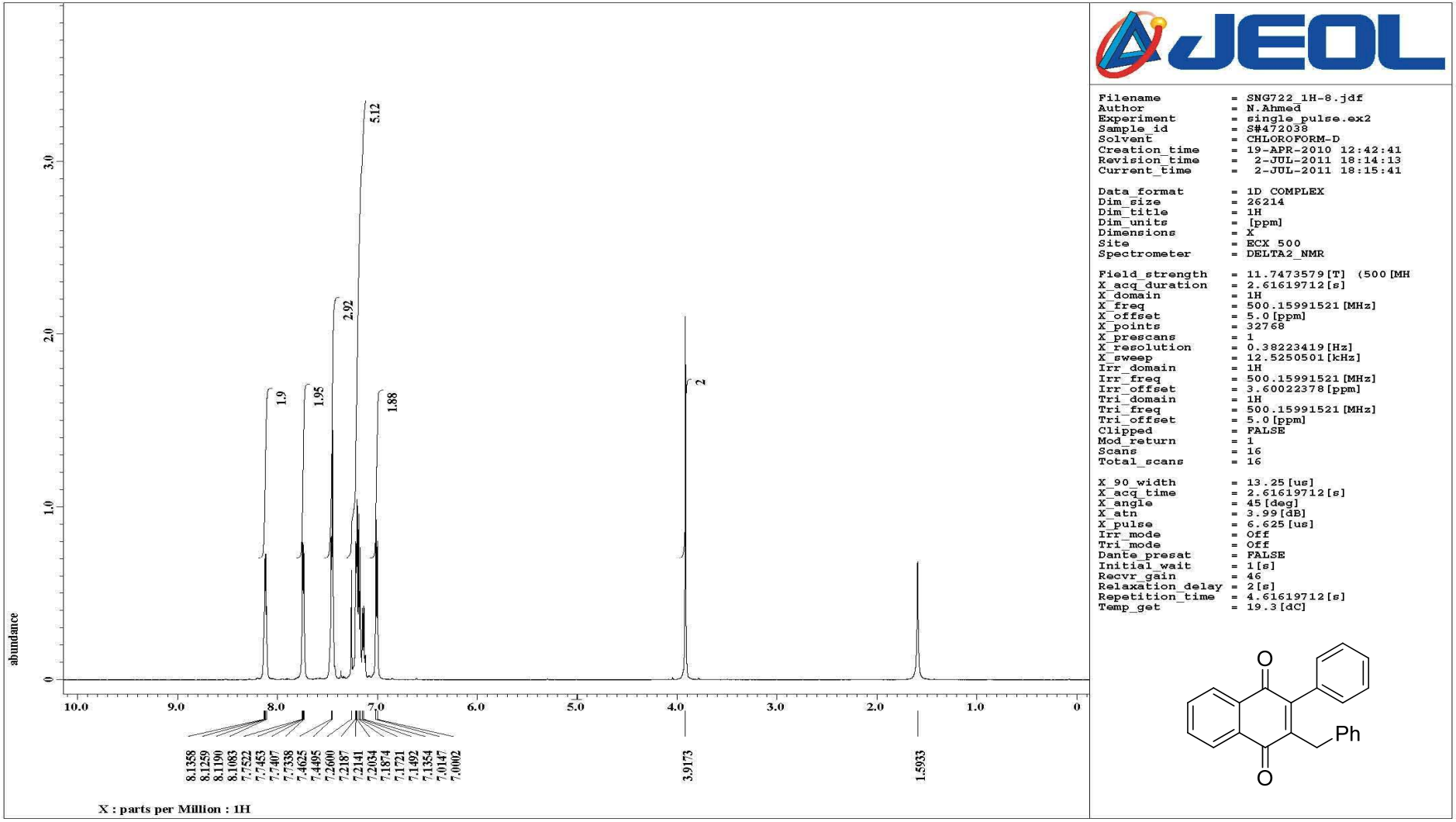
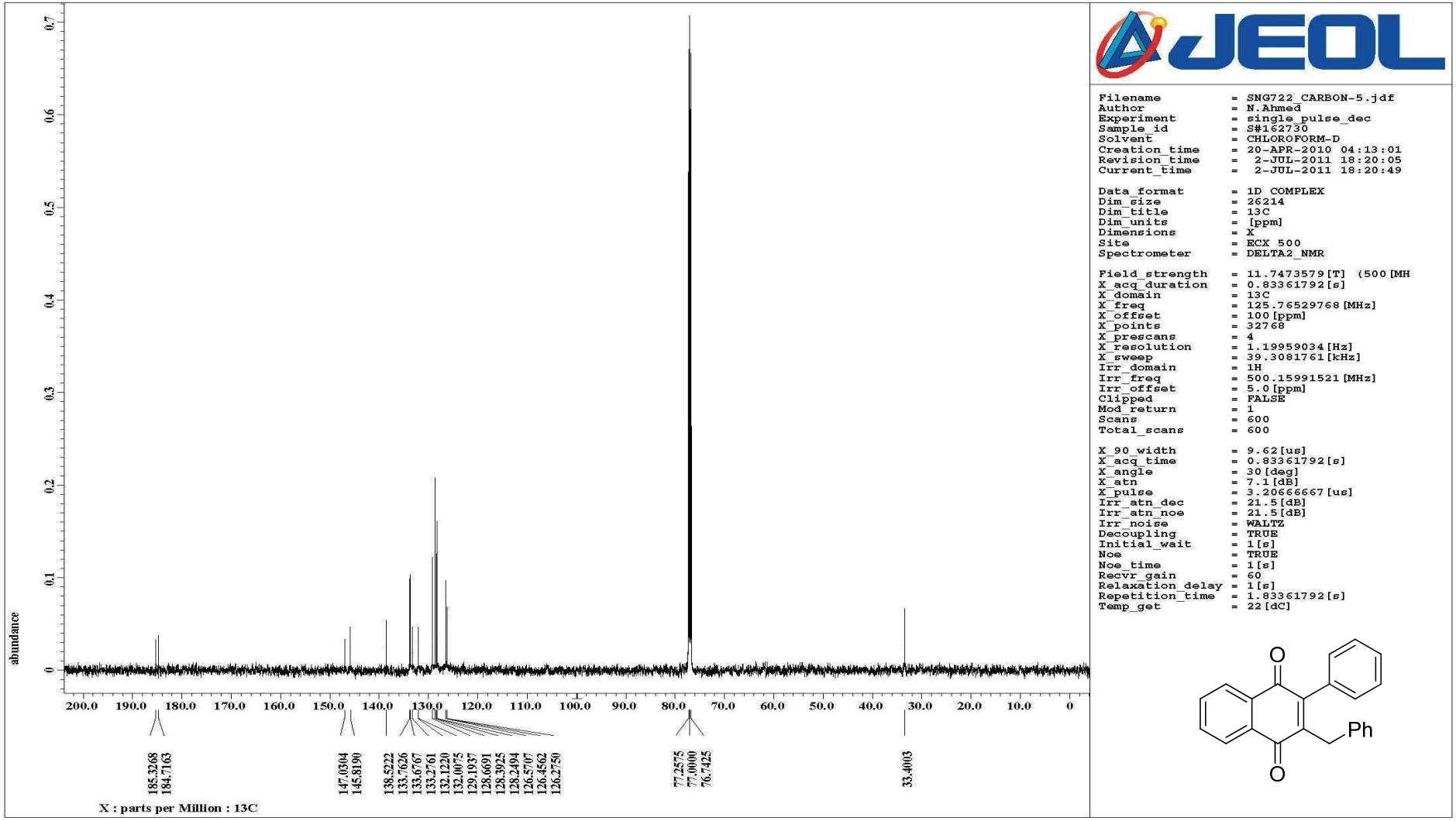
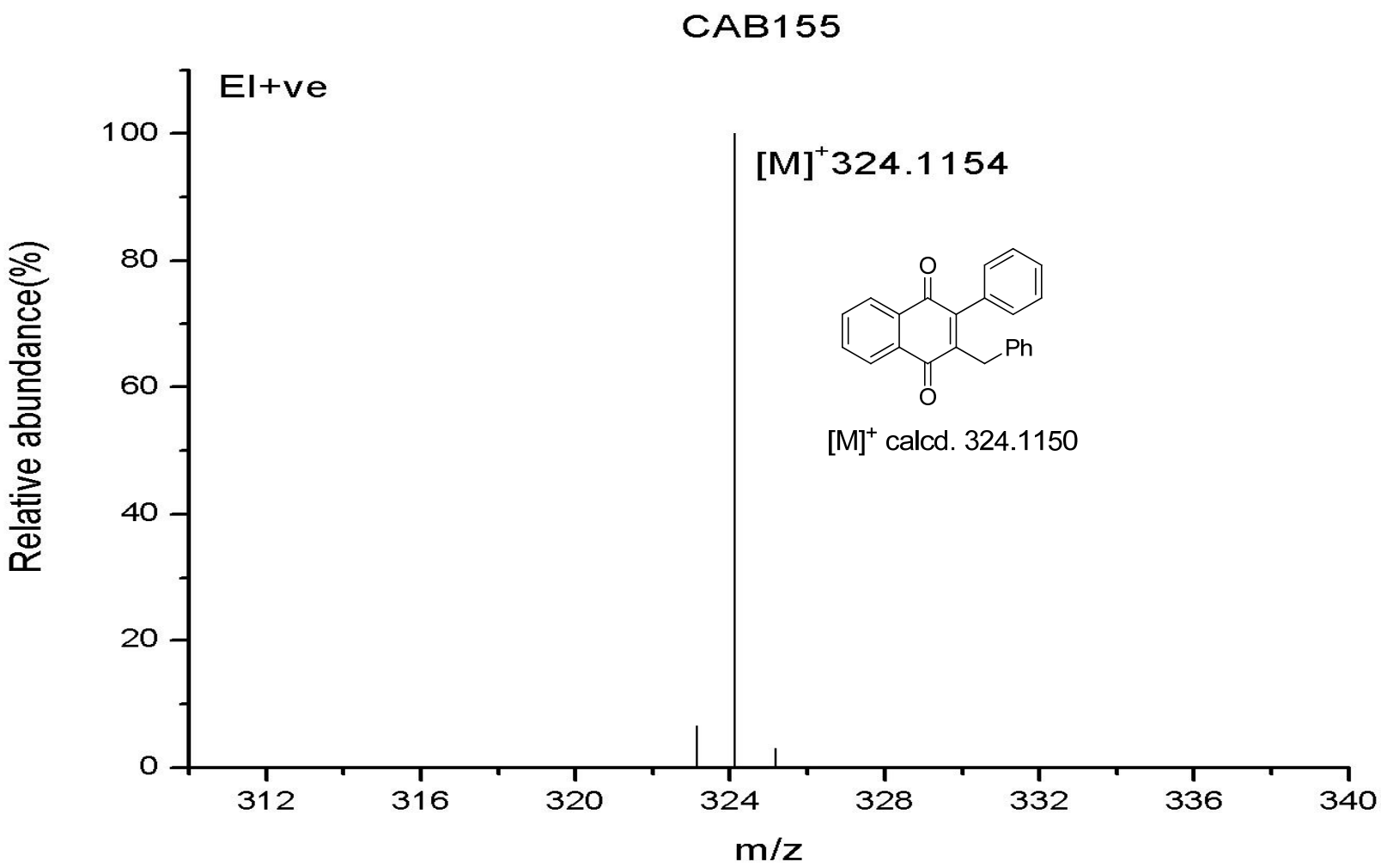


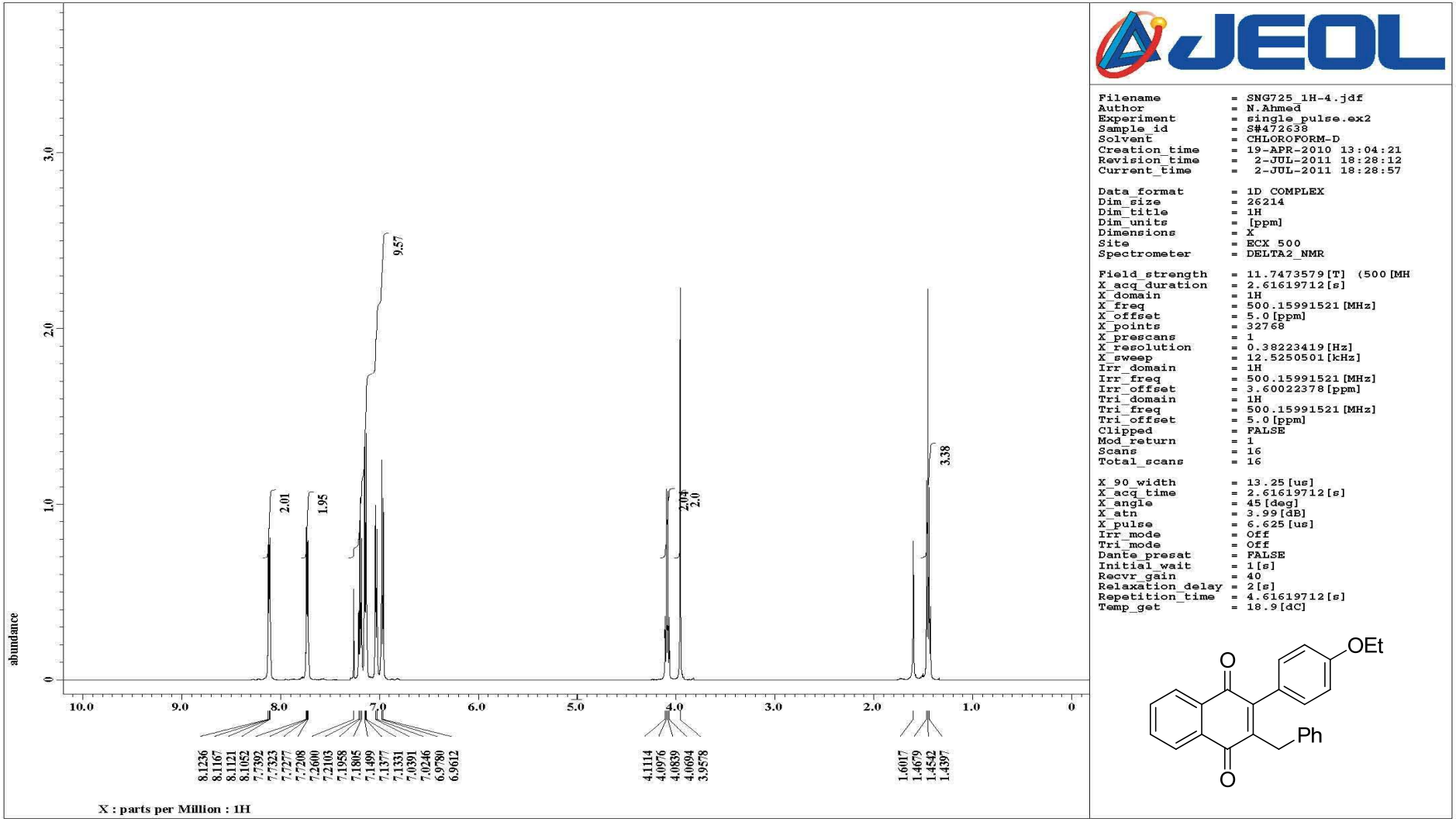
^{1}H NMR spectrum of 2-benzyl-3-phenyl-1,4-naphthoquinone **(3.3)**



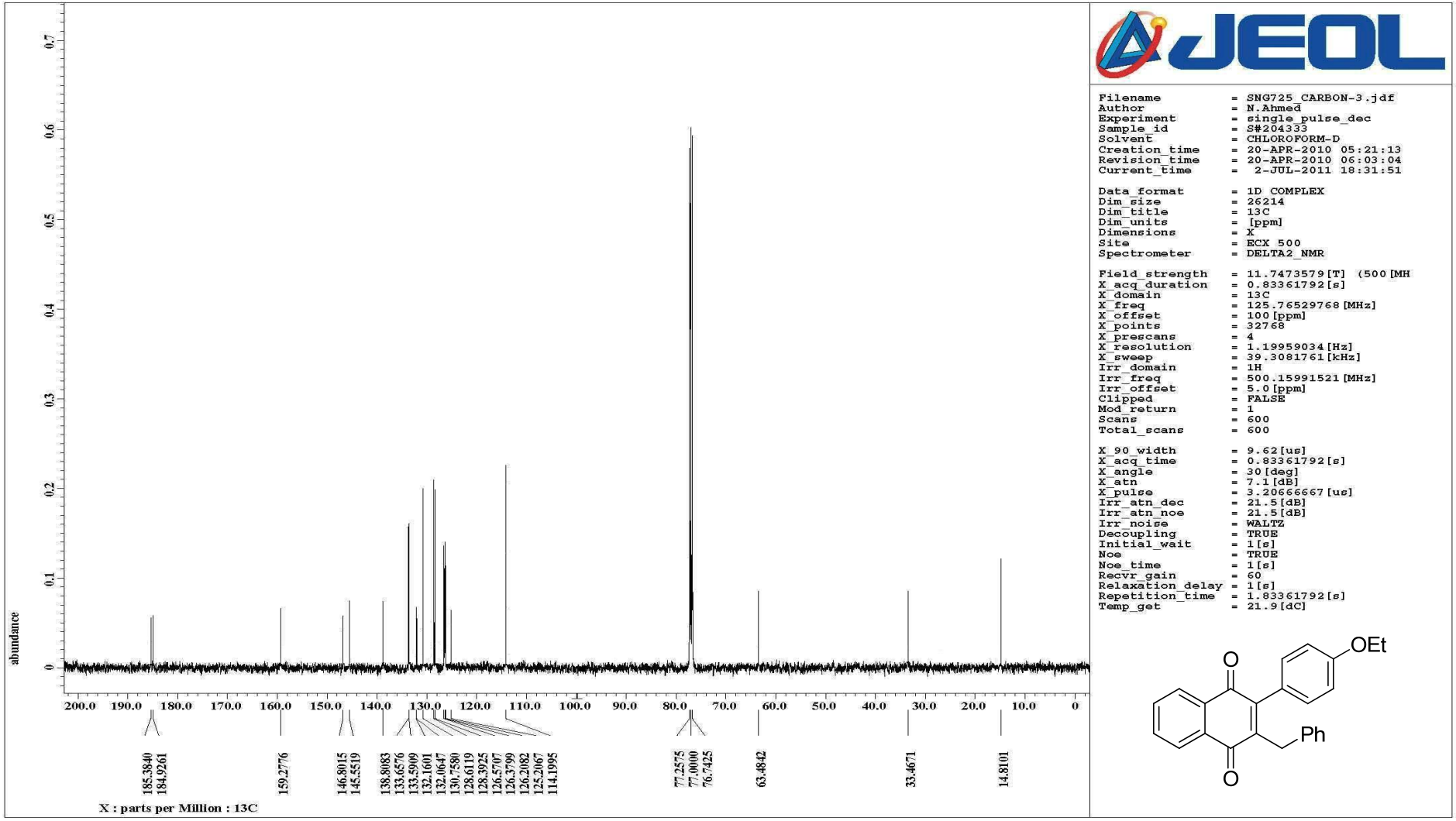
^{13}C NMR spectrum of 2-benzyl-3-phenyl-1,4-naphthoquinone **(3.3)**



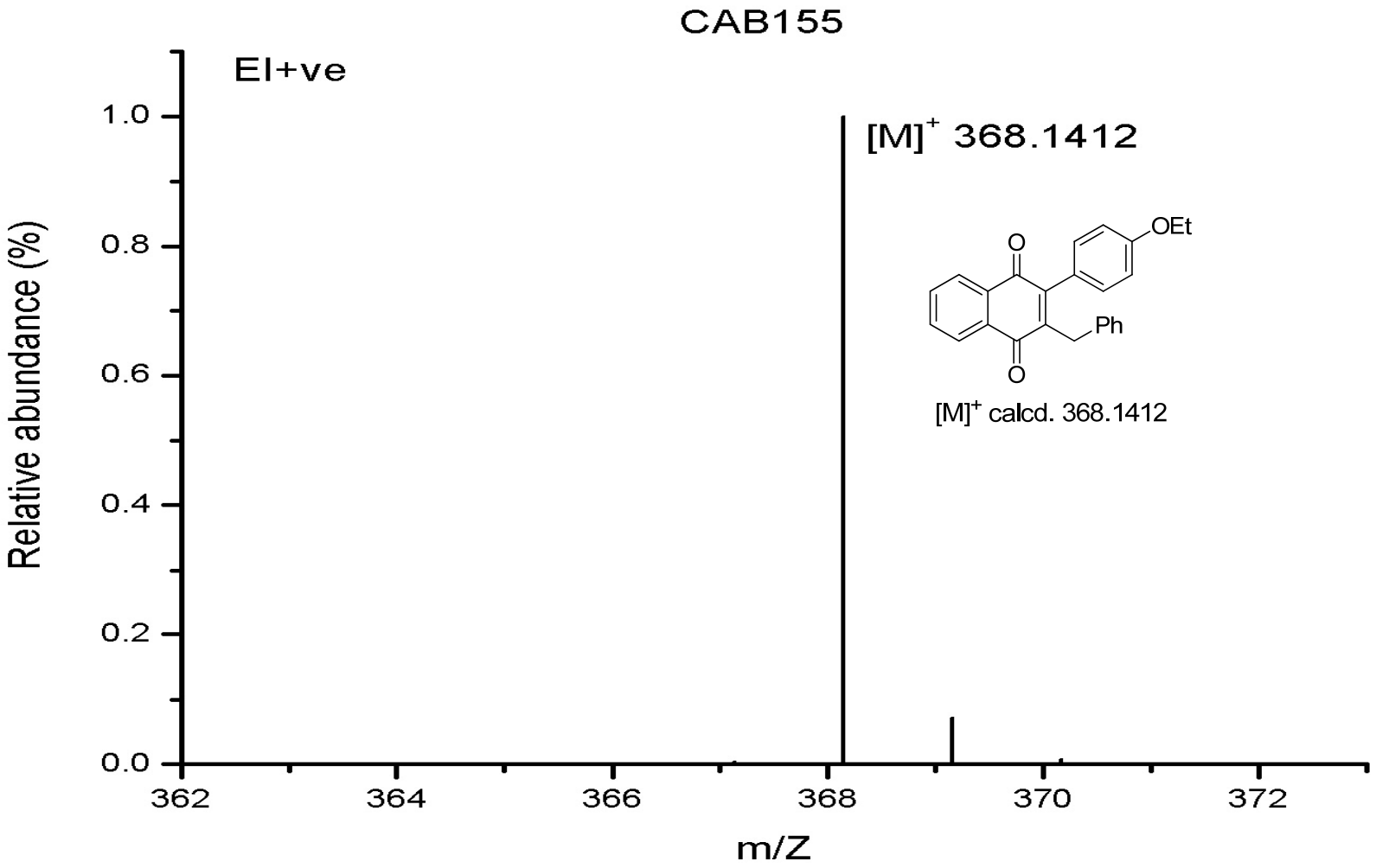
HRMS spectrum of 2-benzyl-3-phenyl-1,4-naphthoquinone **(3.3)**



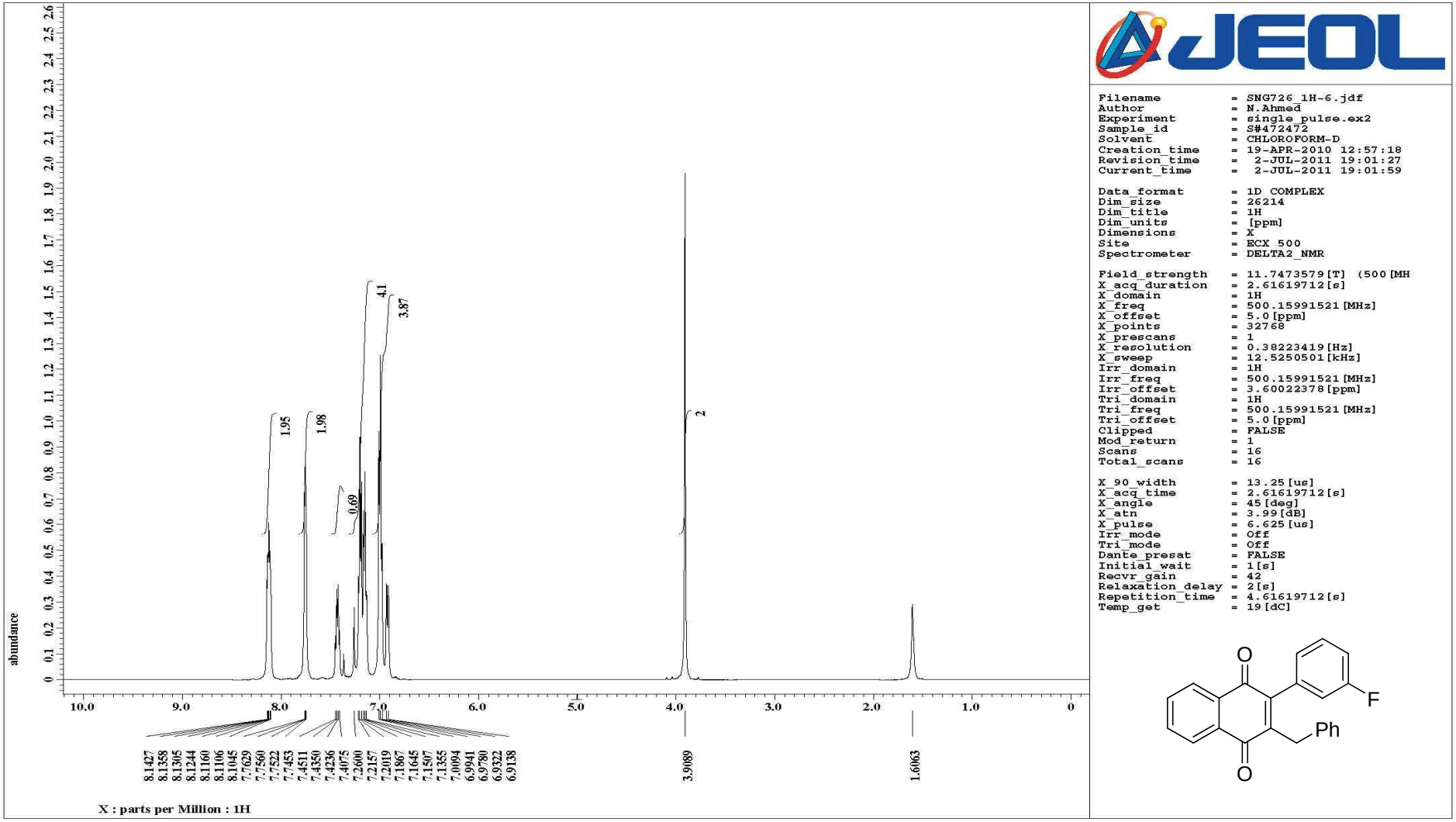
^{1}H NMR spectrum of 2-benzyl-3-(4-ethoxyphenyl)-1,4-naphthoquinone **(3.4)**



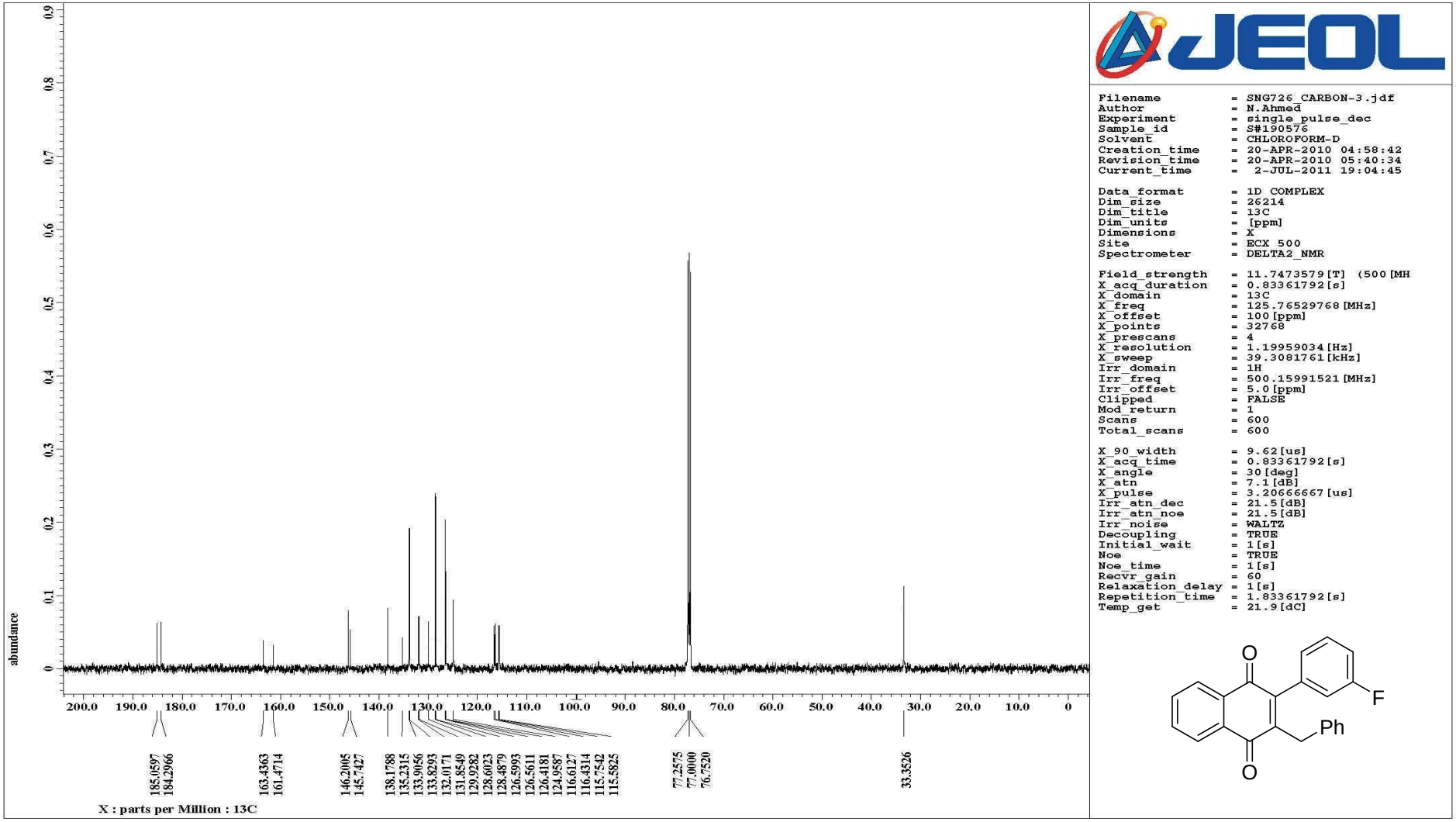
^{1}H NMR spectrum of 2-benzyl-3-(4-ethoxyphenyl)-1,4-naphthoquinone **(3.4)**



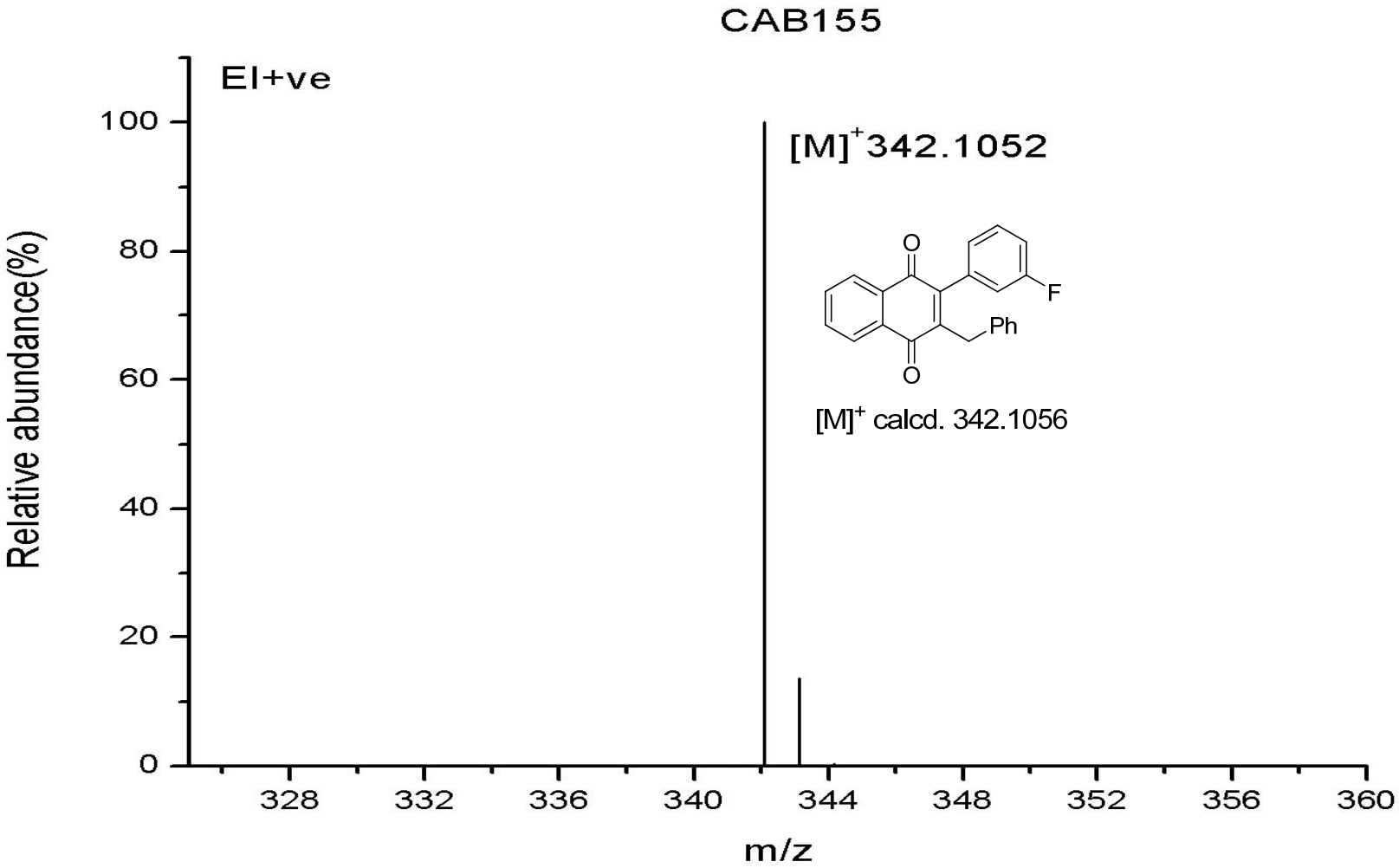
HRMS spectrum of 2-benzyl-3-(4-ethoxyphenyl)-1,4-naphthoquinone **(3.4)**



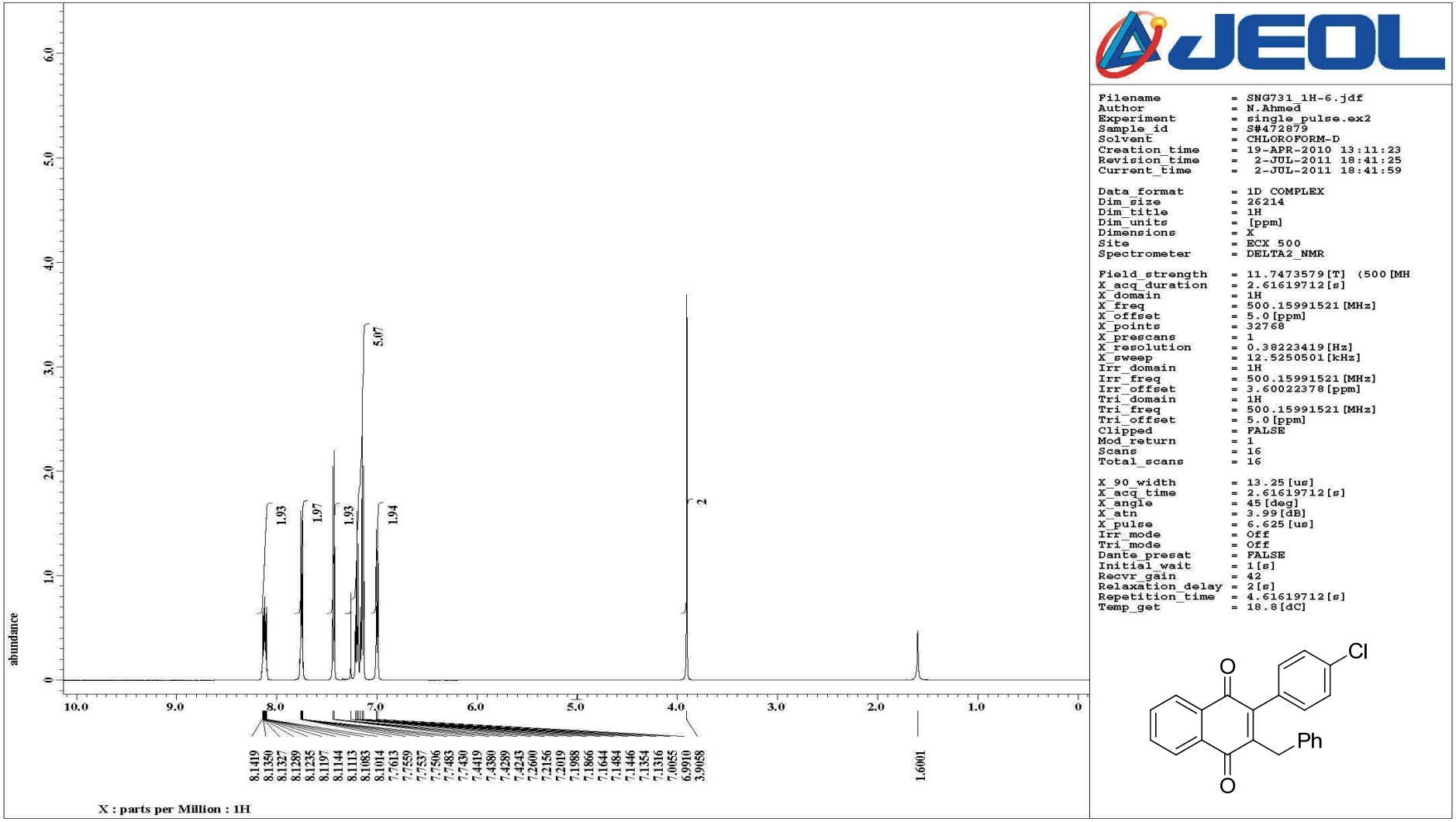
^{1}H NMR spectrum of 2-benzyl-3-(3-fluorophenyl)-1,4-naphthoquinone **(3.5)**



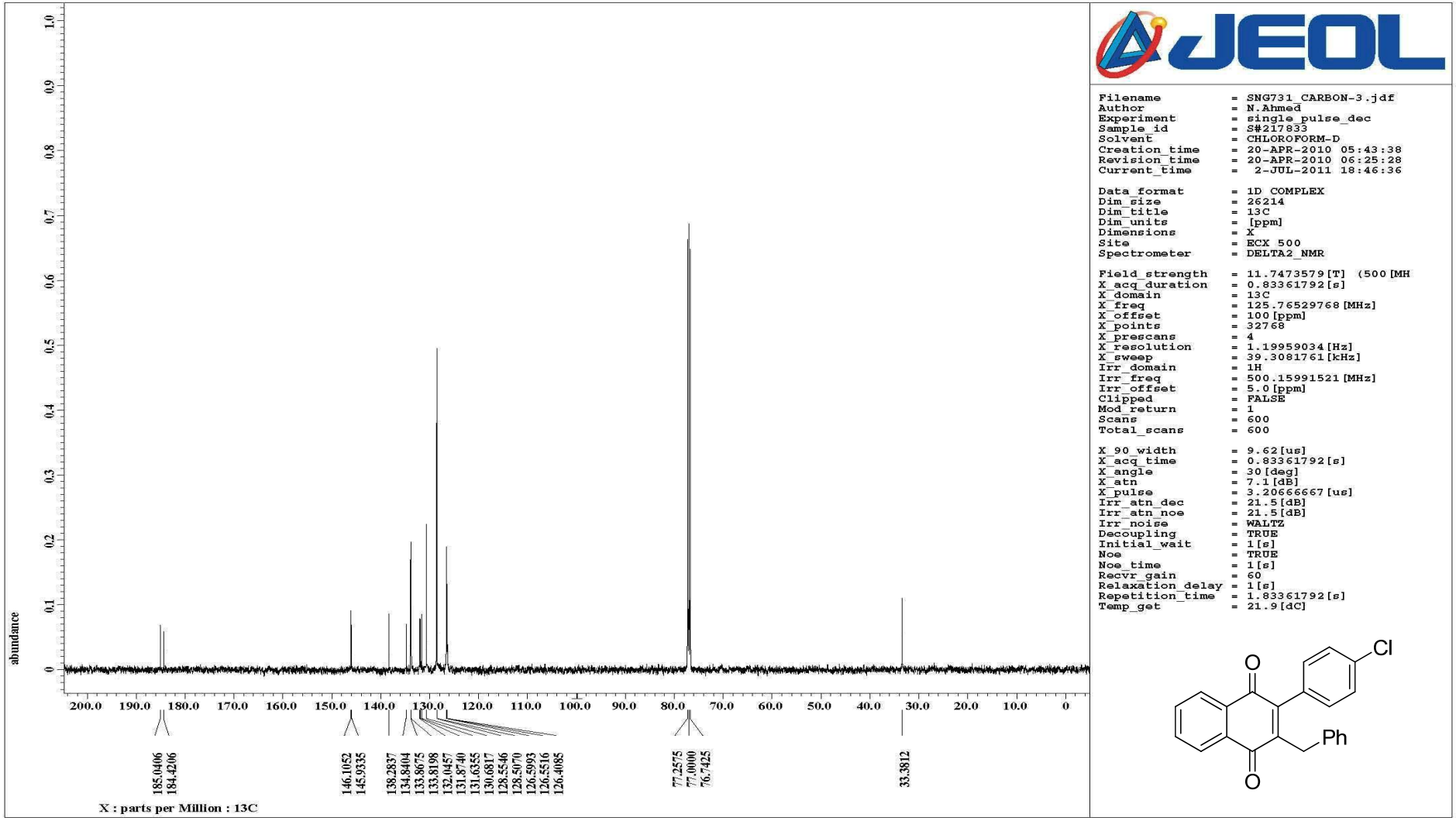
^{13}C NMR spectrum of 2-benzyl-3-(3-fluorophenyl)-1,4-naphthoquinone **(3.5)**



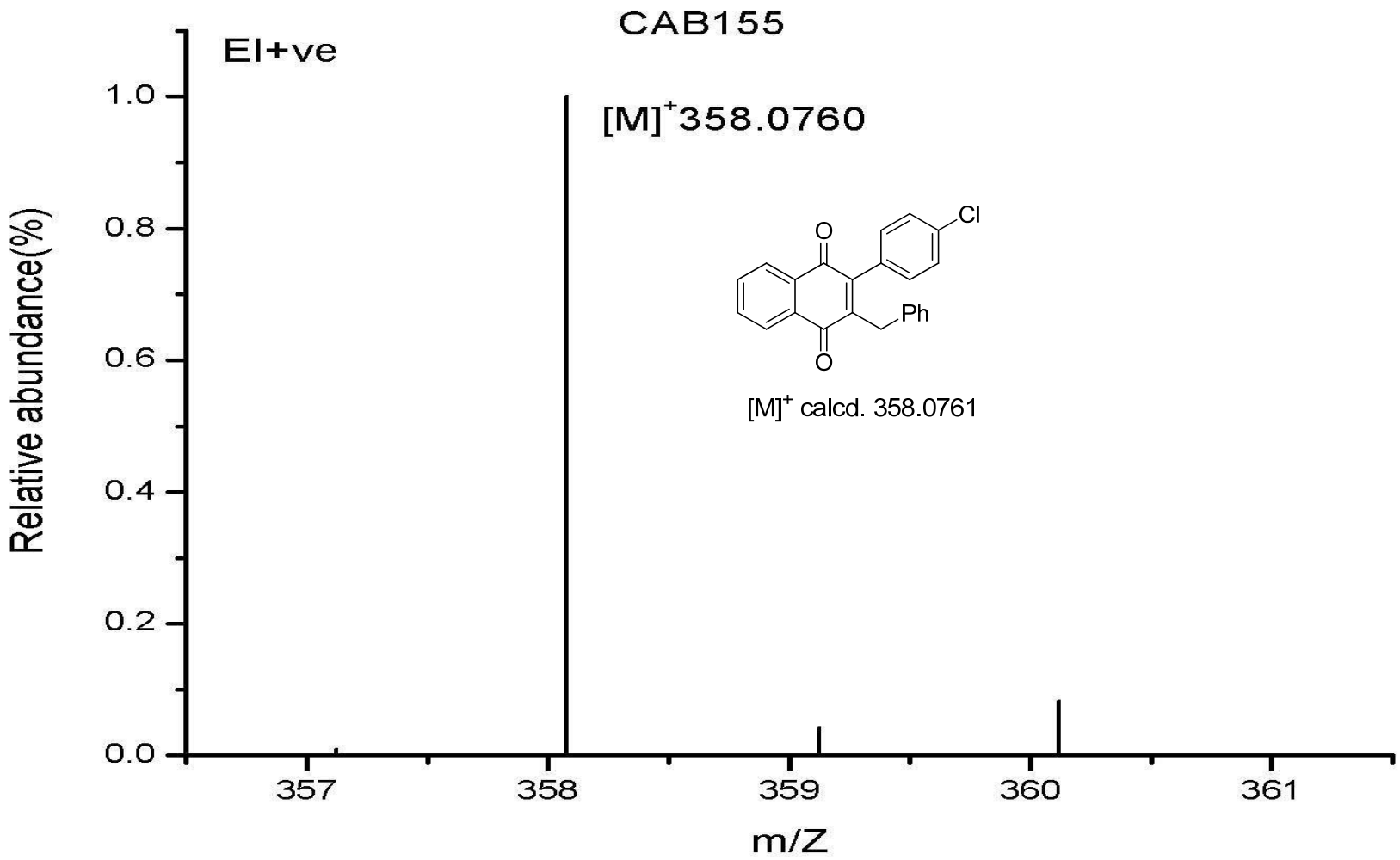
HRMS spectrum of 2-benzyl-3-(3-fluorophenyl)-1,4-naphthoquinone **(3.5)**



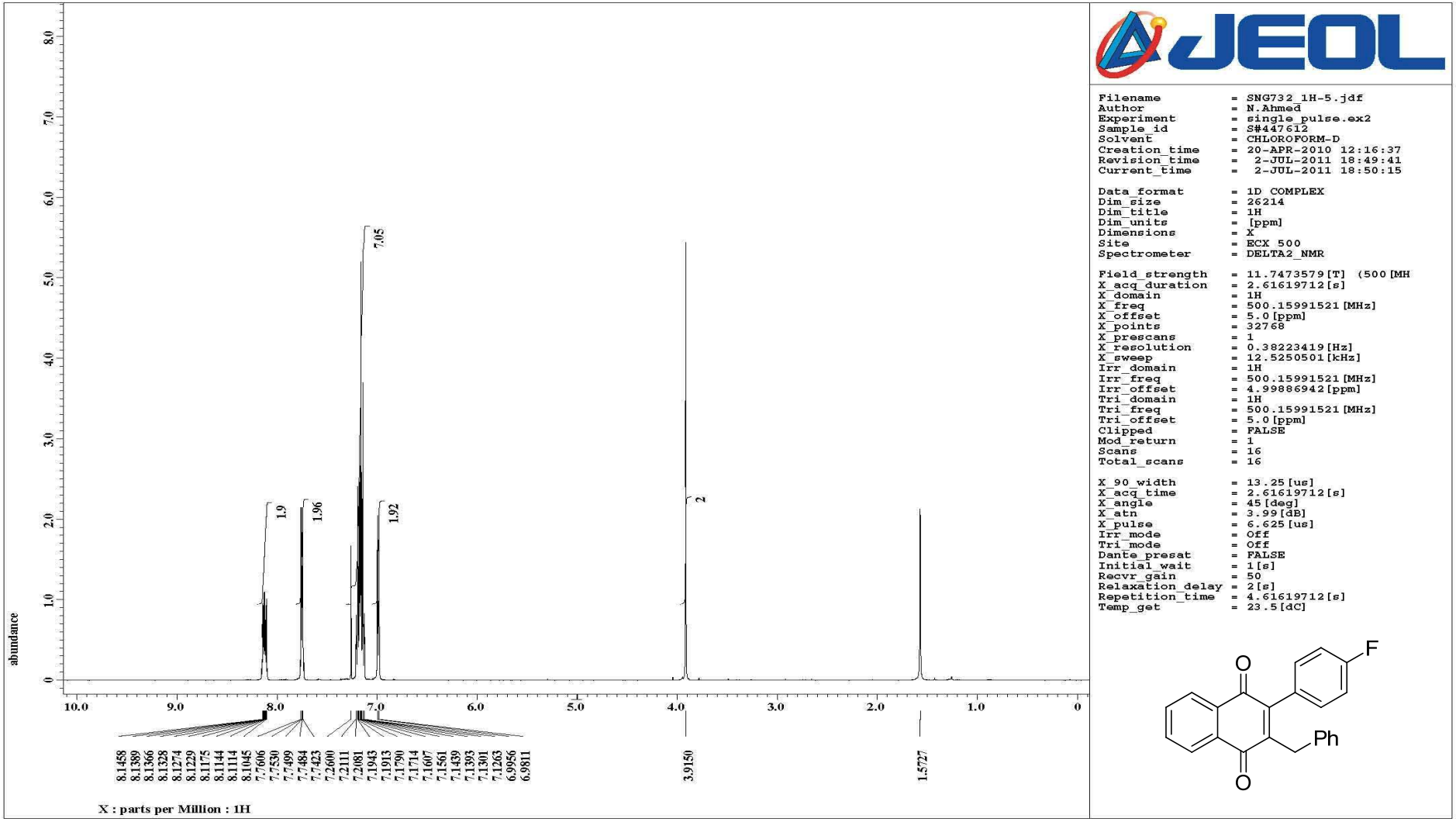
^{1}H NMR spectrum of 2-benzyl-3-(4-chlorophenyl)-1,4-naphthoquinone **(3.6)**



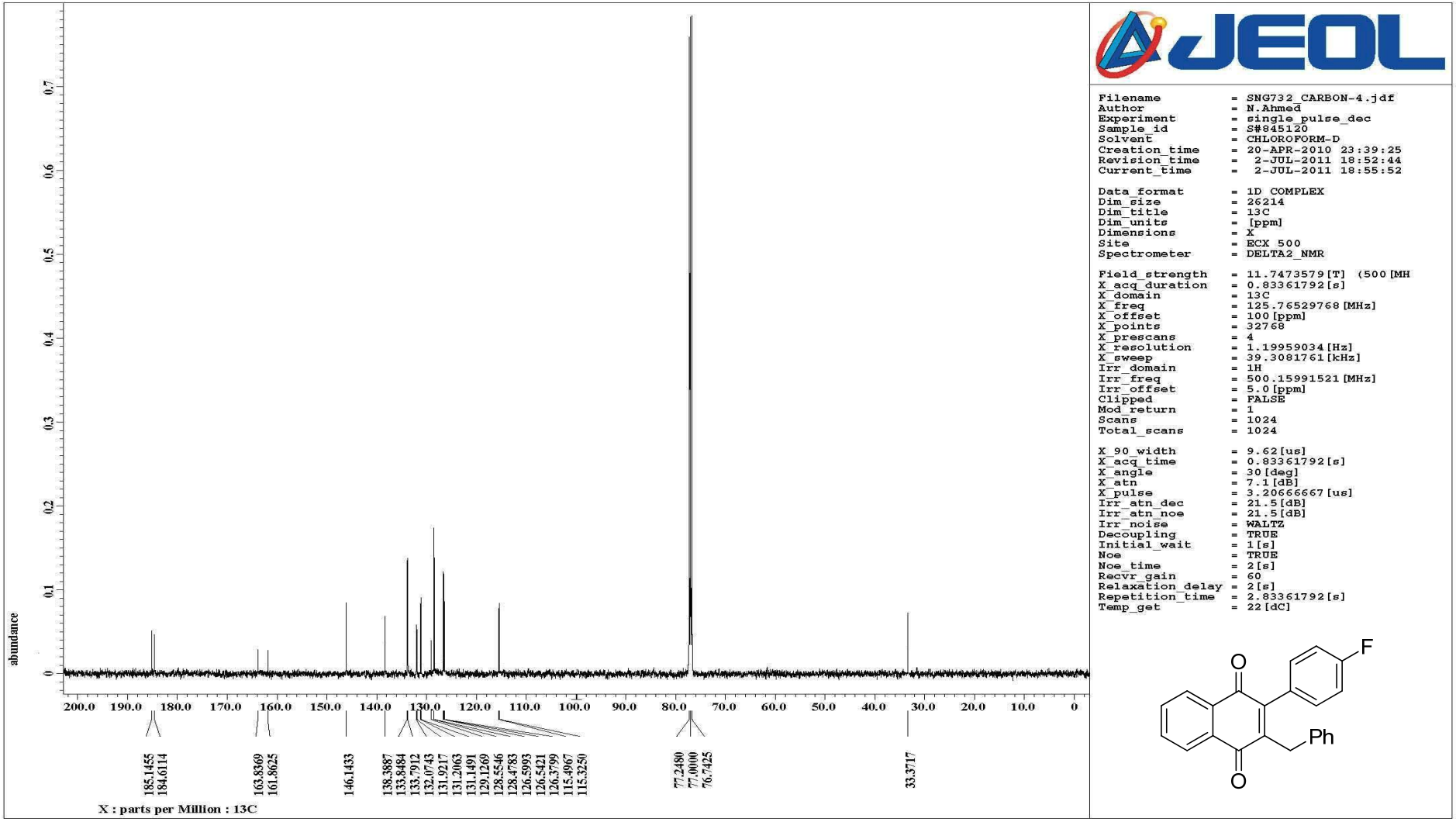
^{13}C NMR spectrum of 2-benzyl-3-(4-chlorophenyl)-1,4-naphthoquinone **(3.6)**



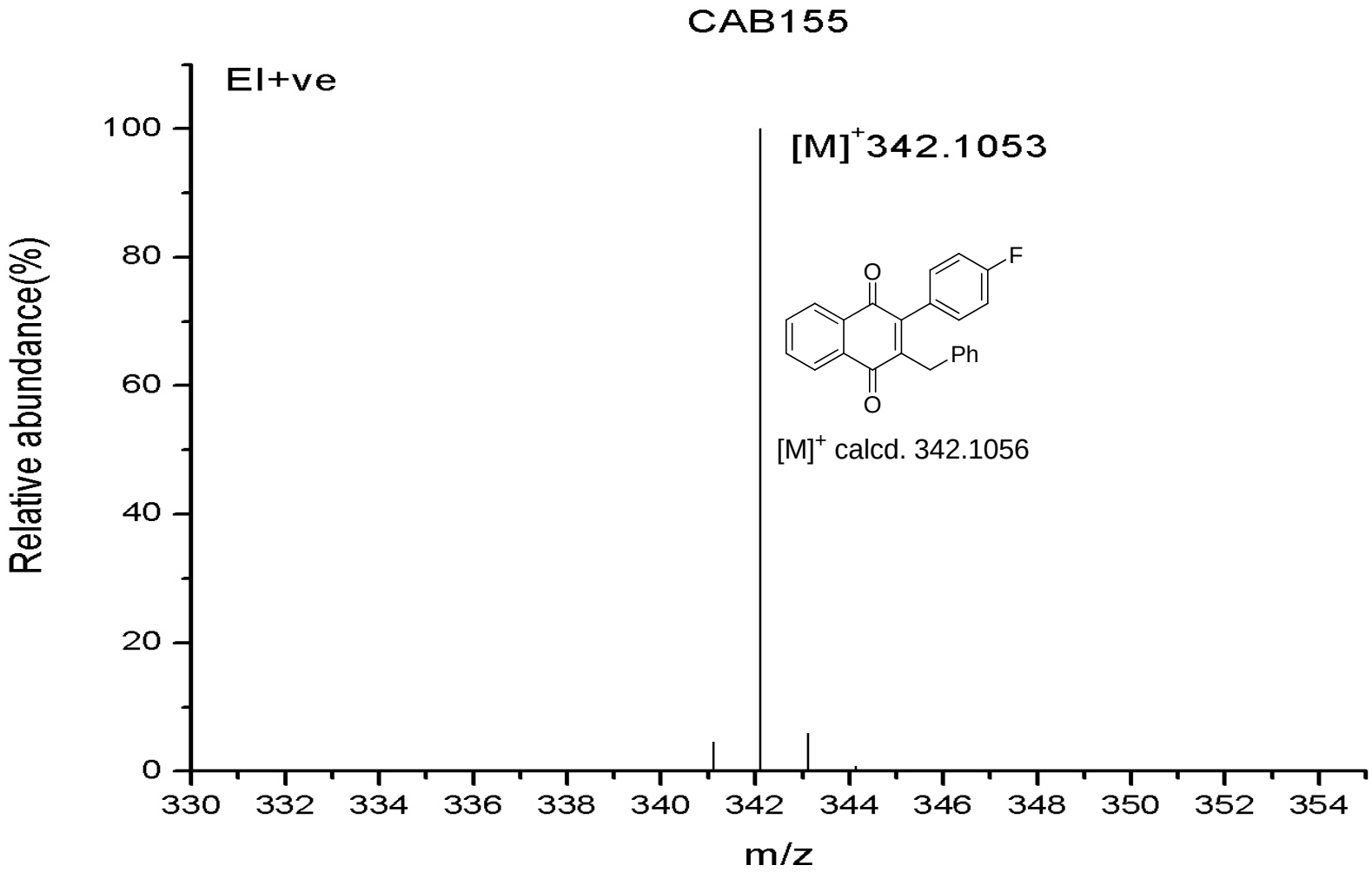
HRMS spectrum of 2-benzyl-3-(4-chlorophenyl)-1,4-naphthoquinone **(3.6)**



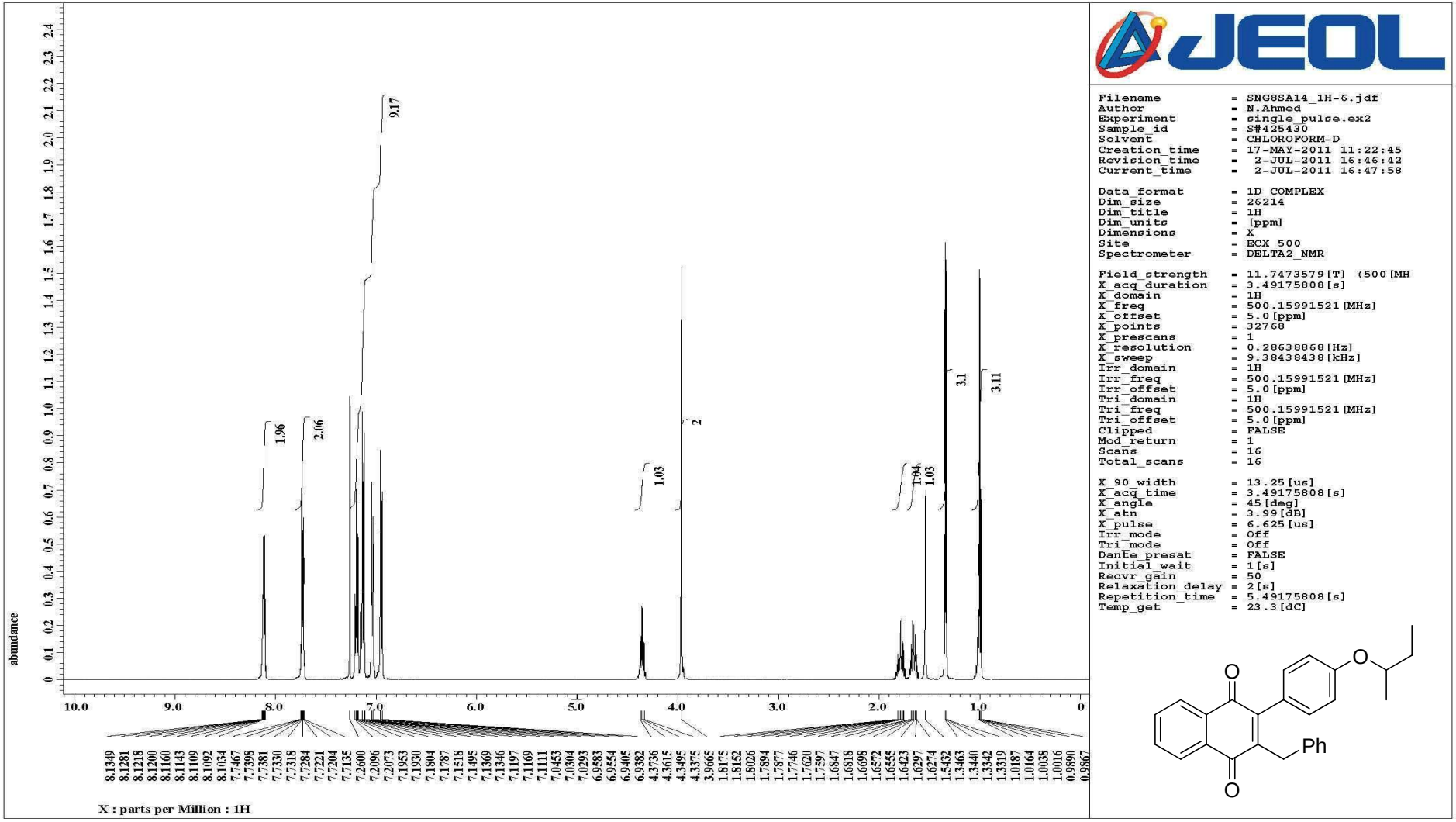
^{1}H NMR spectrum of 2-benzyl-3-(4-fluorophenyl)-1,4-naphthoquinone **(3.7)**



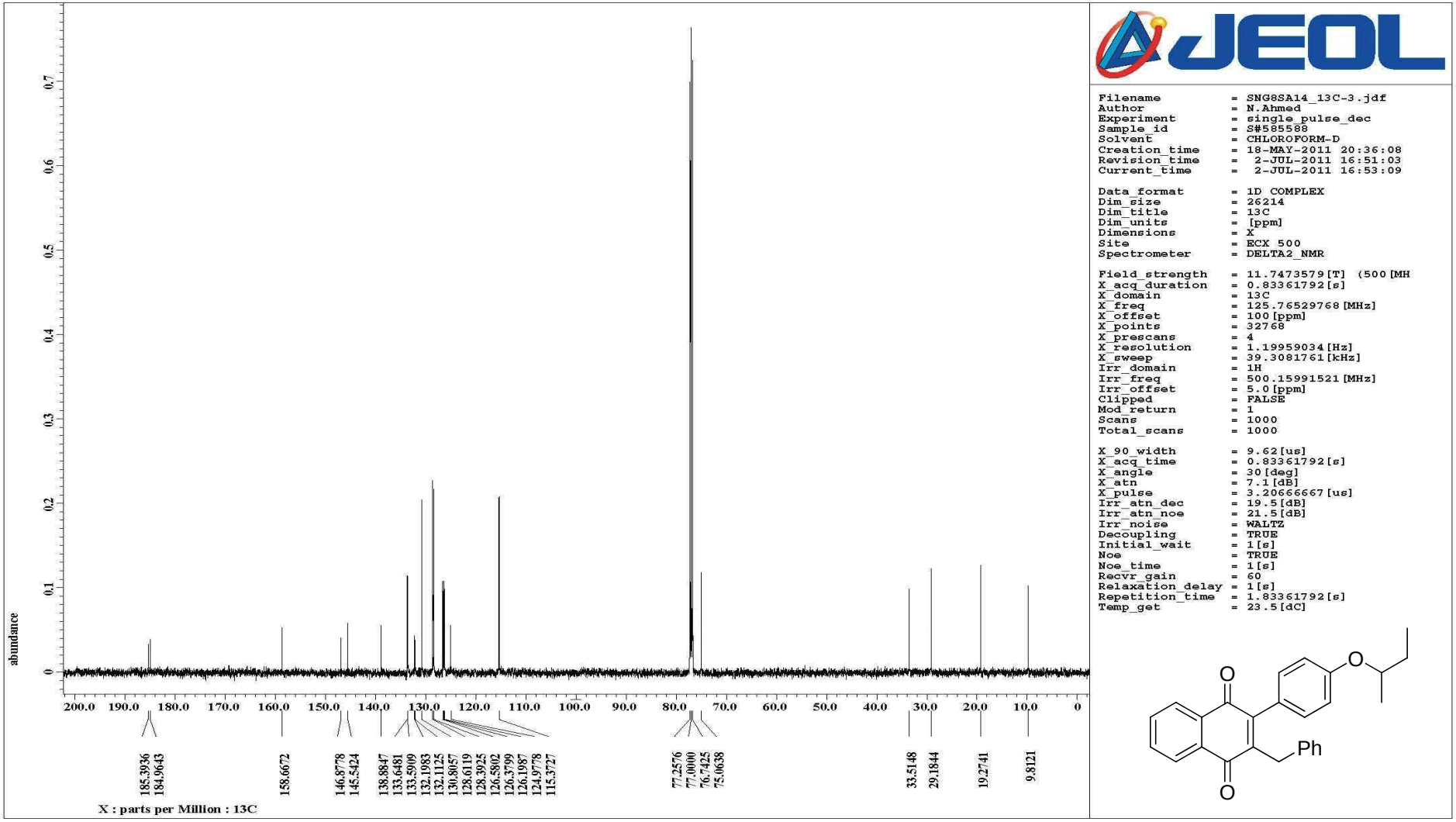
^{13}C NMR spectrum of 2-benzyl-3-(4-fluorophenyl)-1,4-naphthoquinone **(3.7)**



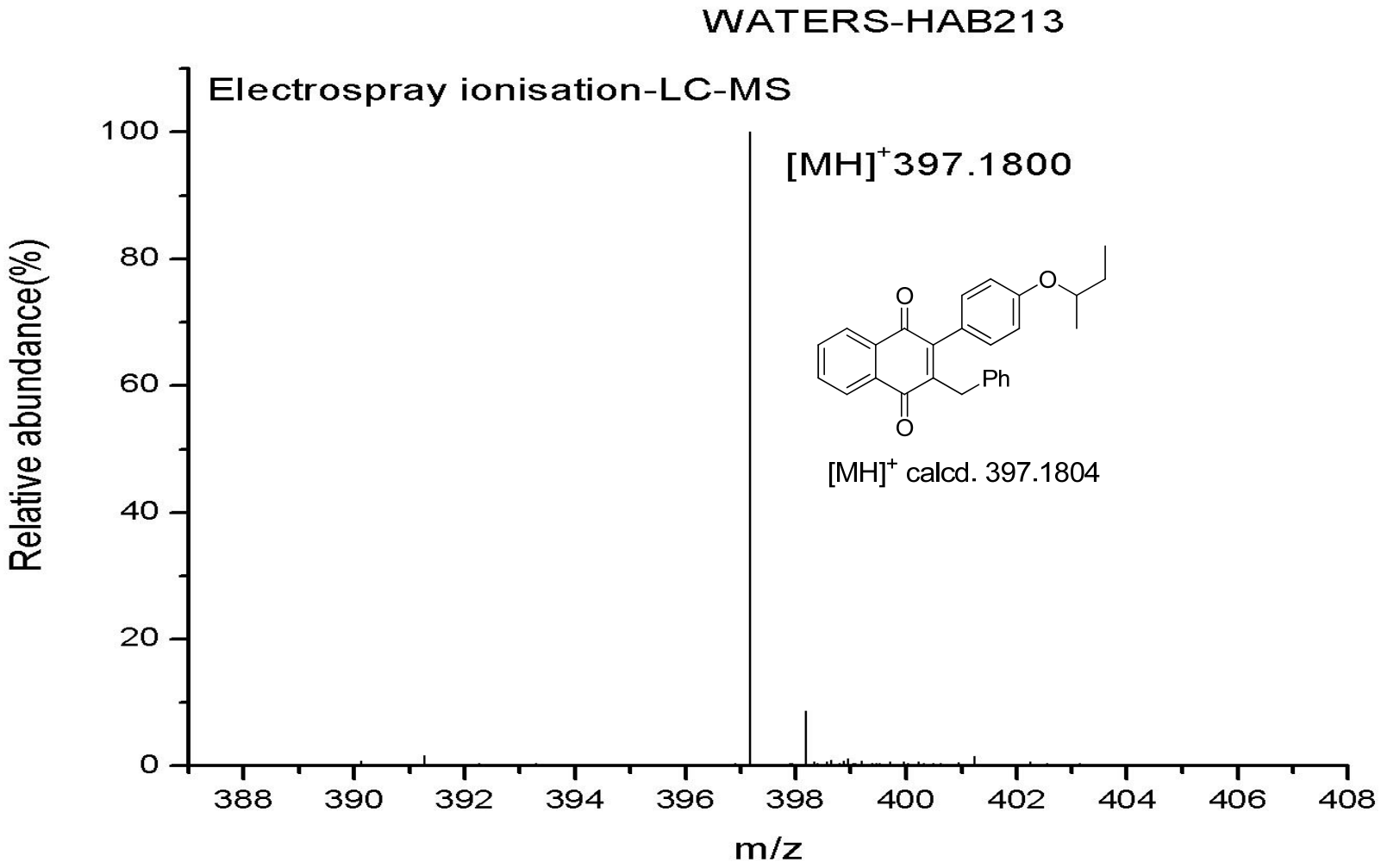
HRMS spectrum of 2-benzyl-3-(4-fluorophenyl)-1,4-naphthoquinone **(3.7)**



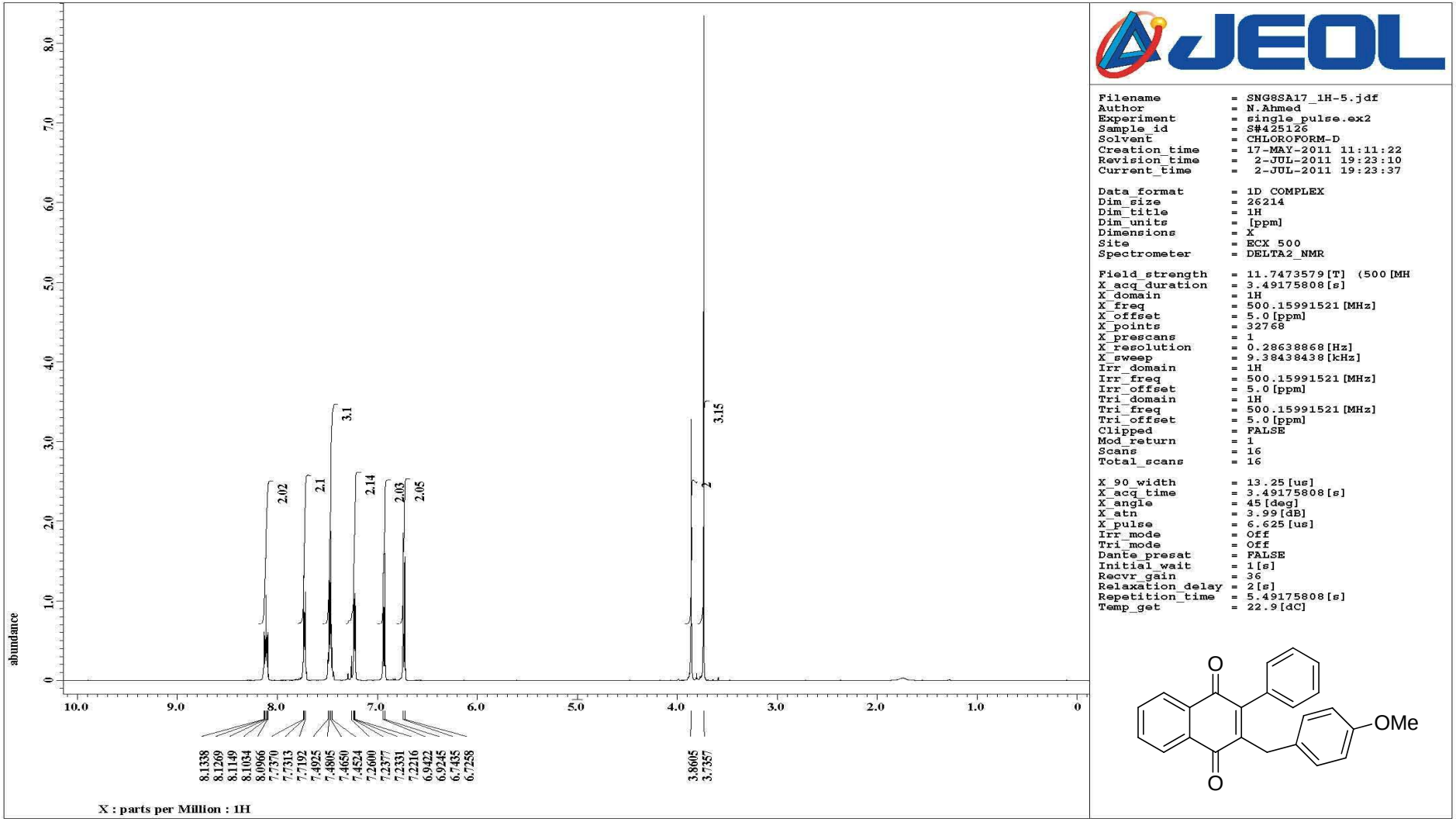
^{1}H NMR spectrum of 2-benzyl-3-(4-sec-butoxyphenyl)-1,4-naphthoquinone **(3.8)**



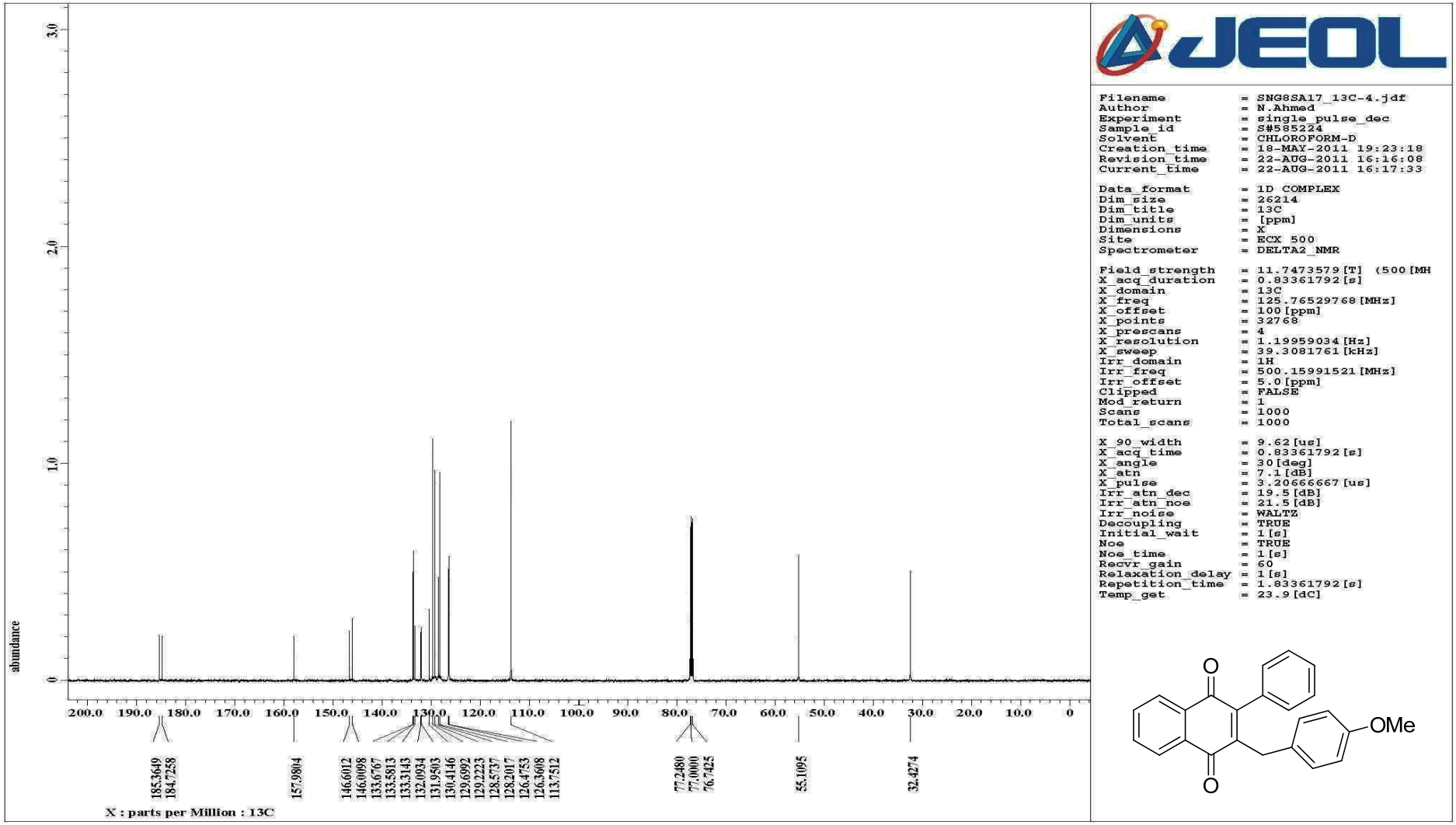
^{13}C NMR spectrum of 2-benzyl-3-(4-sec-butoxyphenyl)-1,4-naphthoquinone **(3.8)**



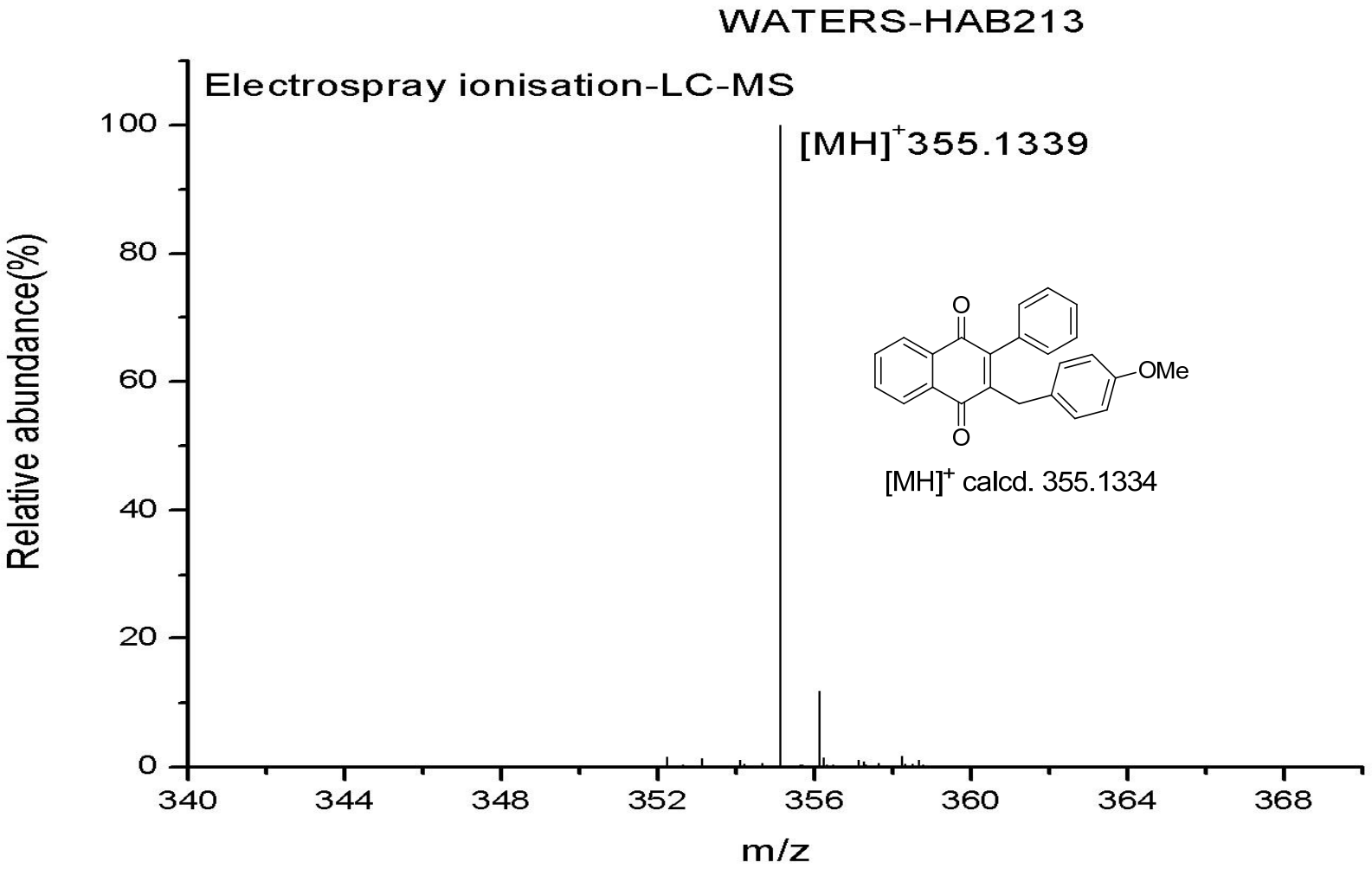
HRMS spectrum of 2-benzyl-3-(4-sec-butoxyphenyl)-1,4-naphthoquinone **(3.8)**



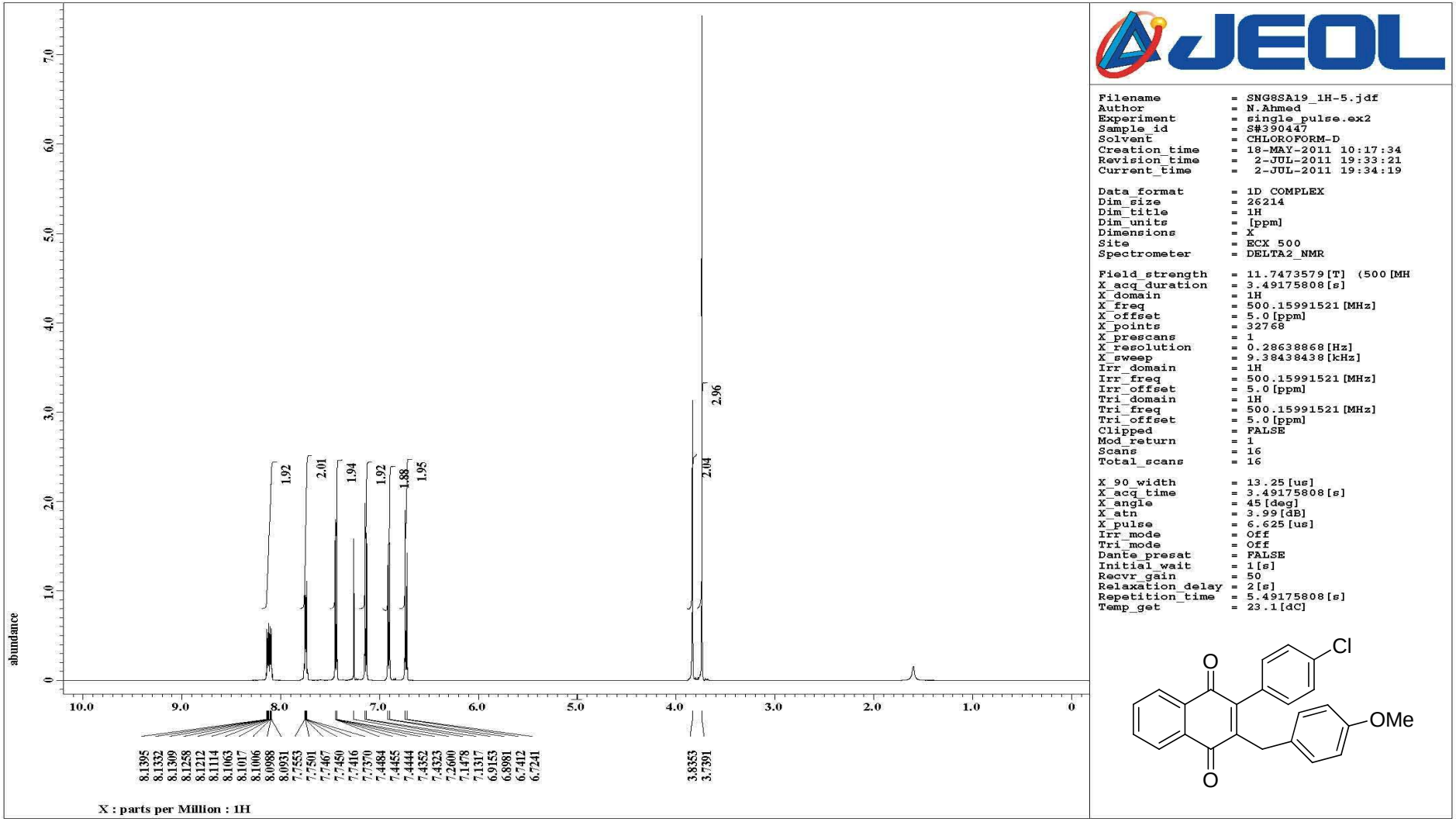
^{1}H NMR spectrum of 2-(4-methoxybenzyl)-3-phenyl-1,4-naphthoquinone **(3.9)**



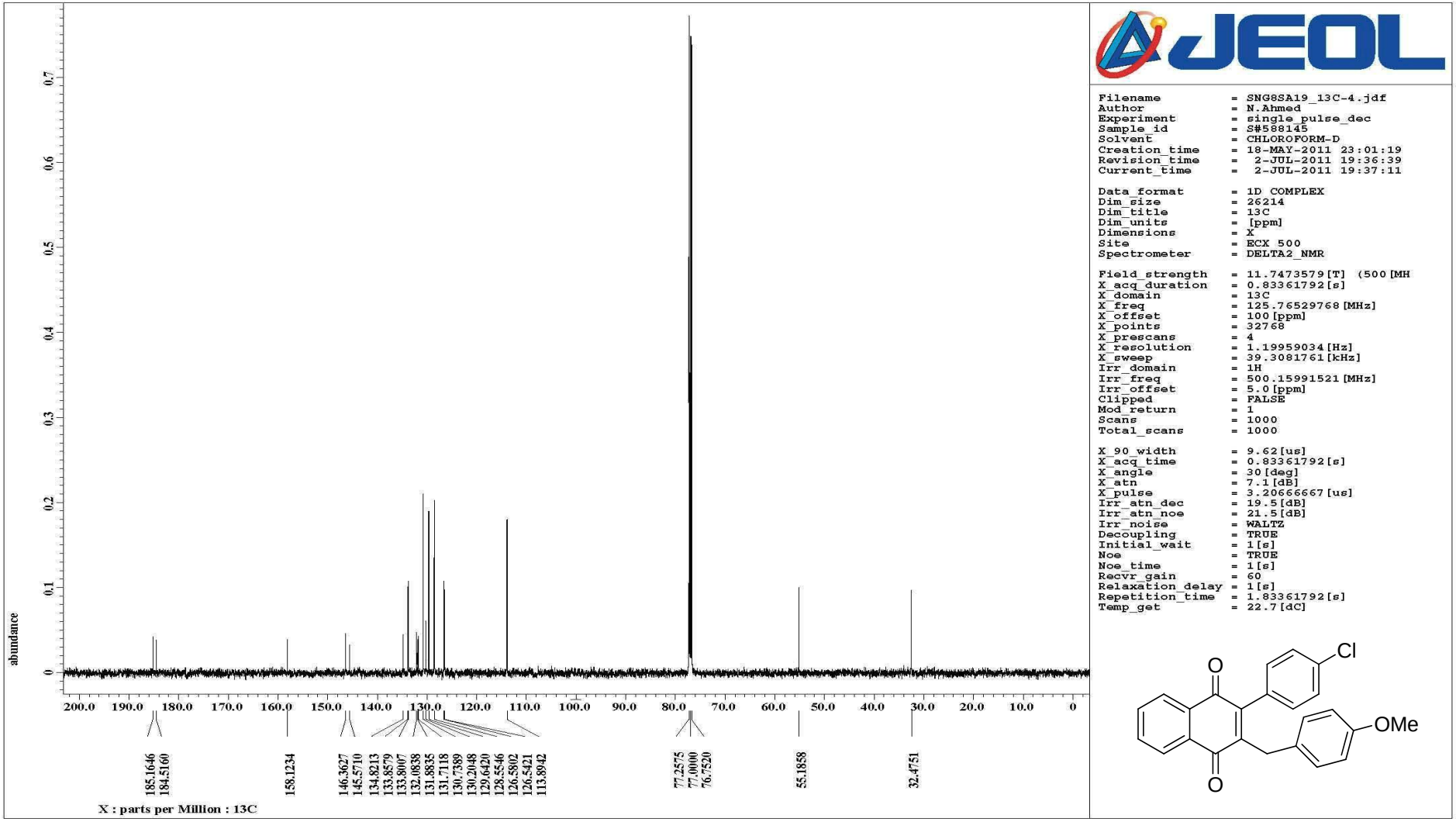
^{13}C NMR spectrum of 2-(4-methoxybenzyl)-3-phenyl-1,4-naphthoquinone **(3.9)**



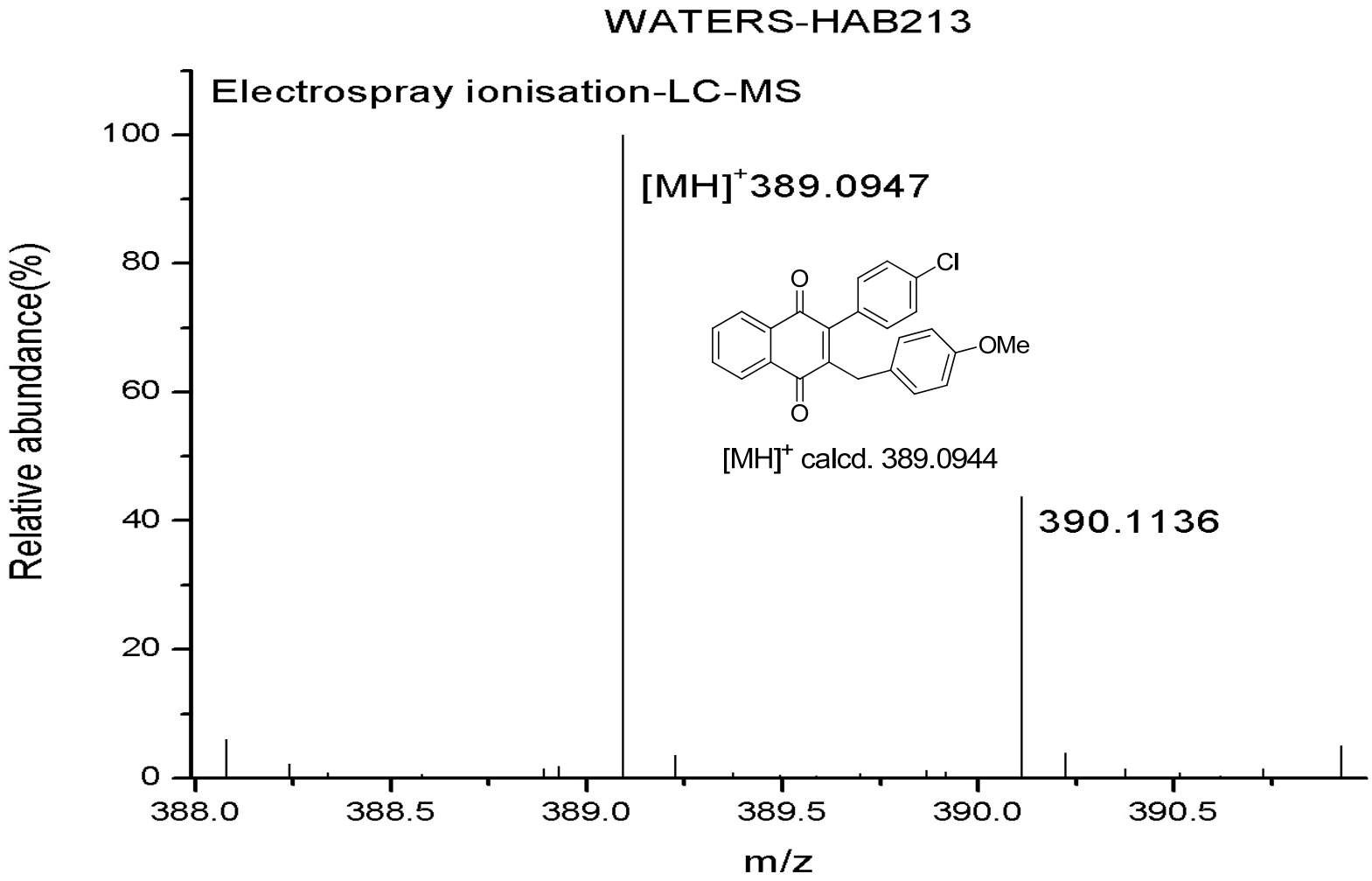
HRMS spectrum of 2-(4-methoxybenzyl)-3-phenyl-1,4-naphthoquinone **(3.9)**



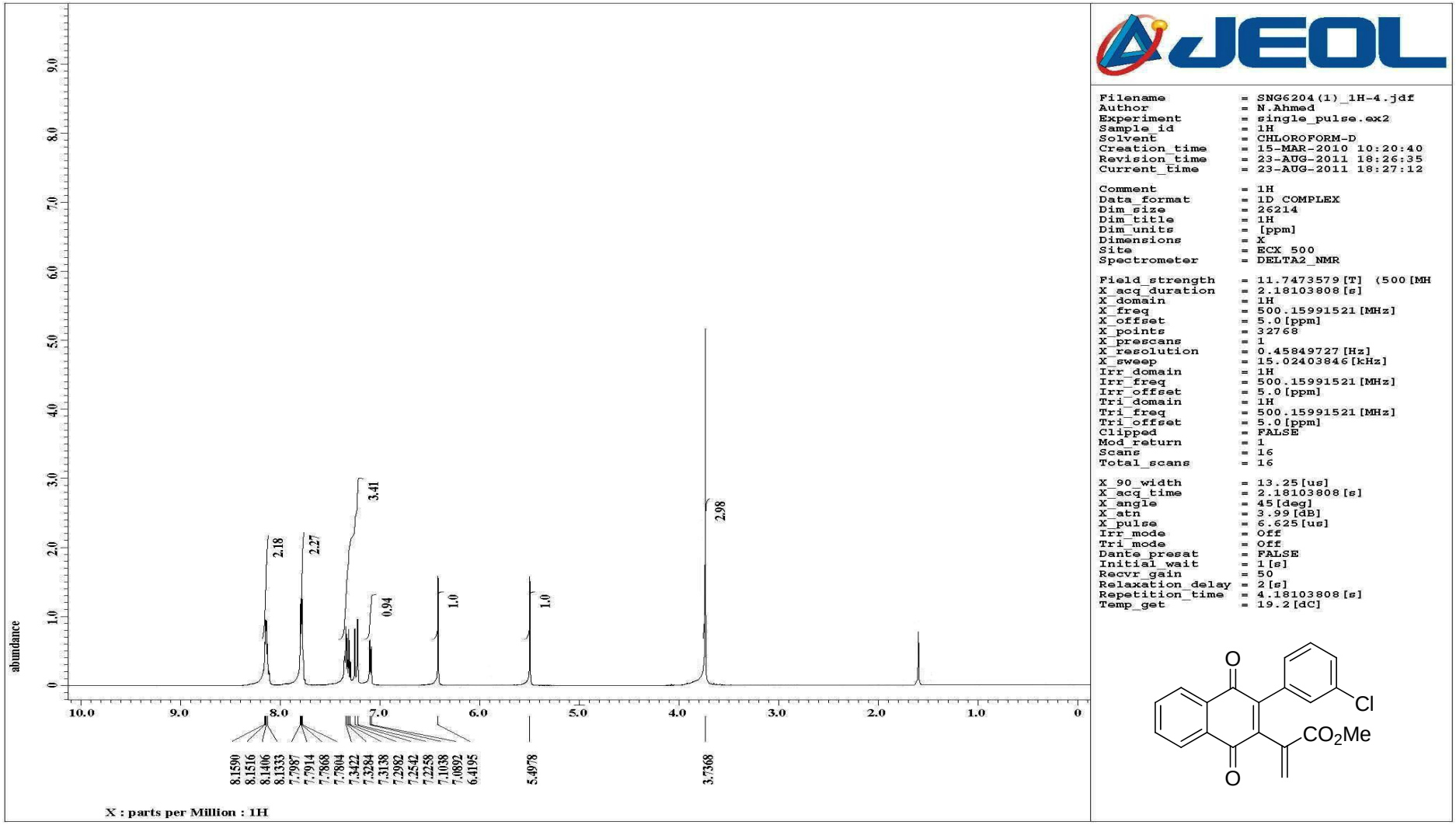
^{1}H NMR spectrum of 2-(4-chlorophenyl)-3-(4-methoxybenzyl)-1,4-naphthoquinone **(3.10)**



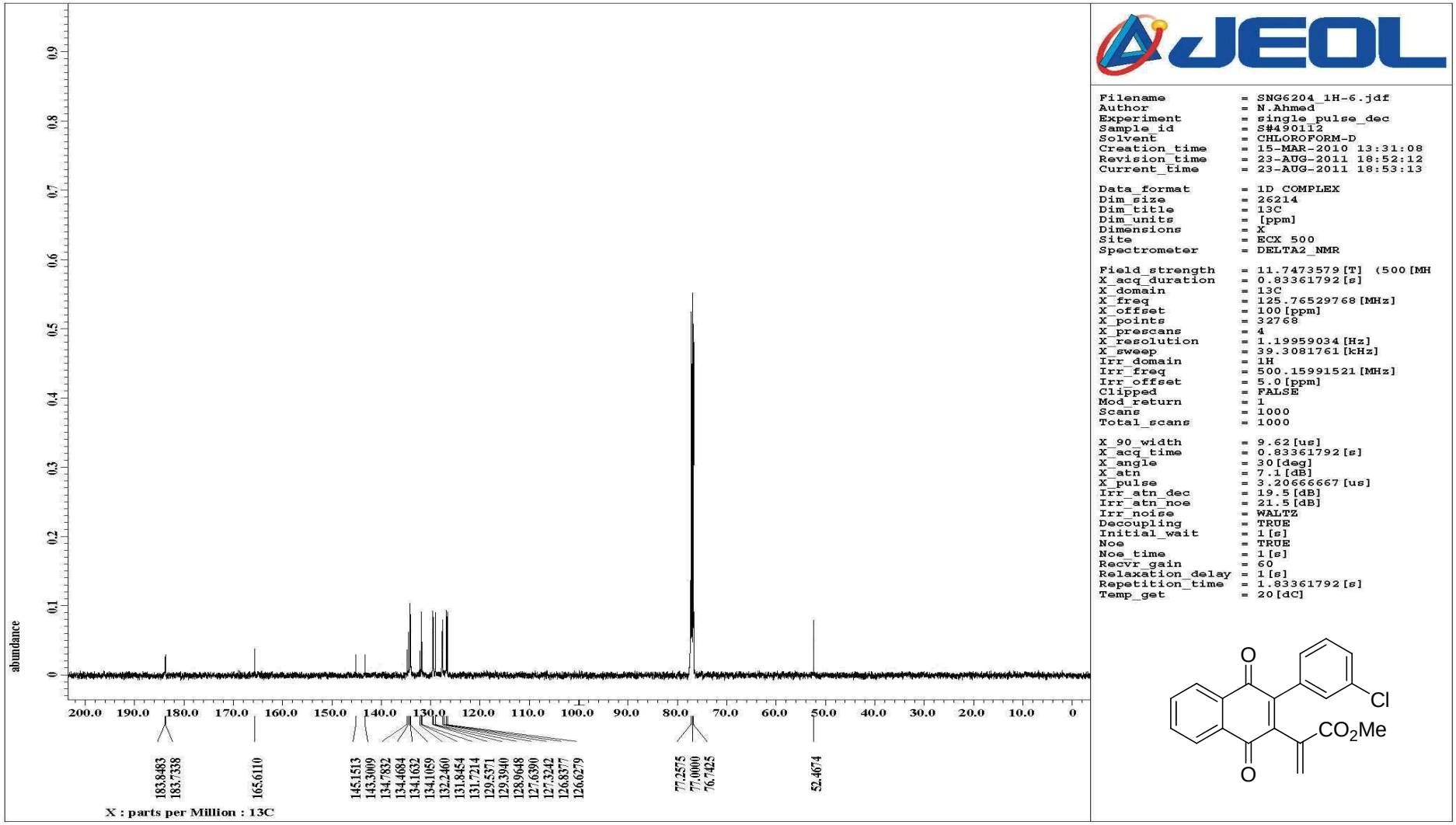
^{13}C NMR spectrum of 2-(4-chlorophenyl)-3-(4-methoxybenzyl)-1,4-naphthoquinone **(3.10)**



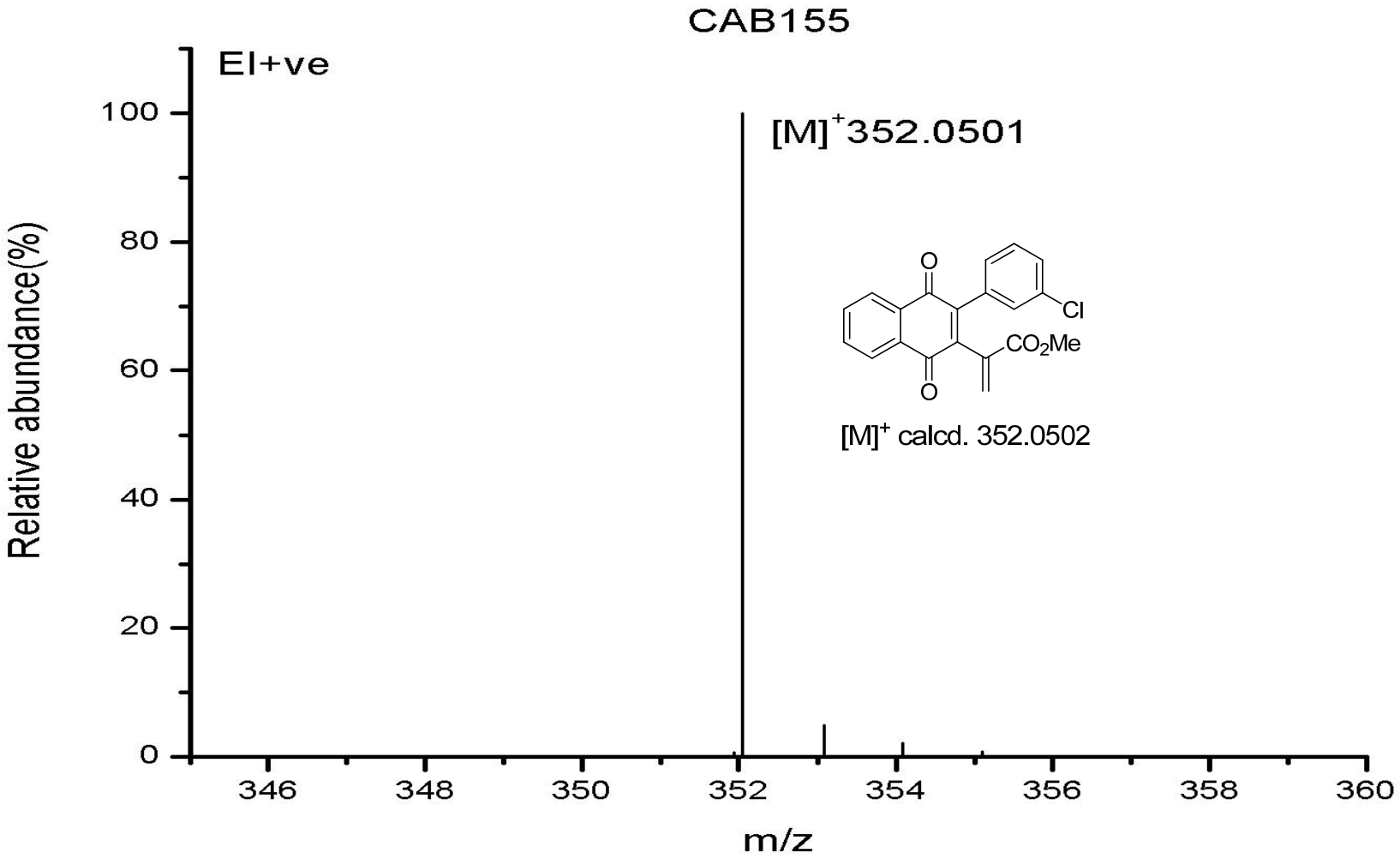
HRMS spectrum of 2-(4-chlorophenyl)-3-(4-methoxybenzyl)-1,4-naphthoquinone **(3.10)**



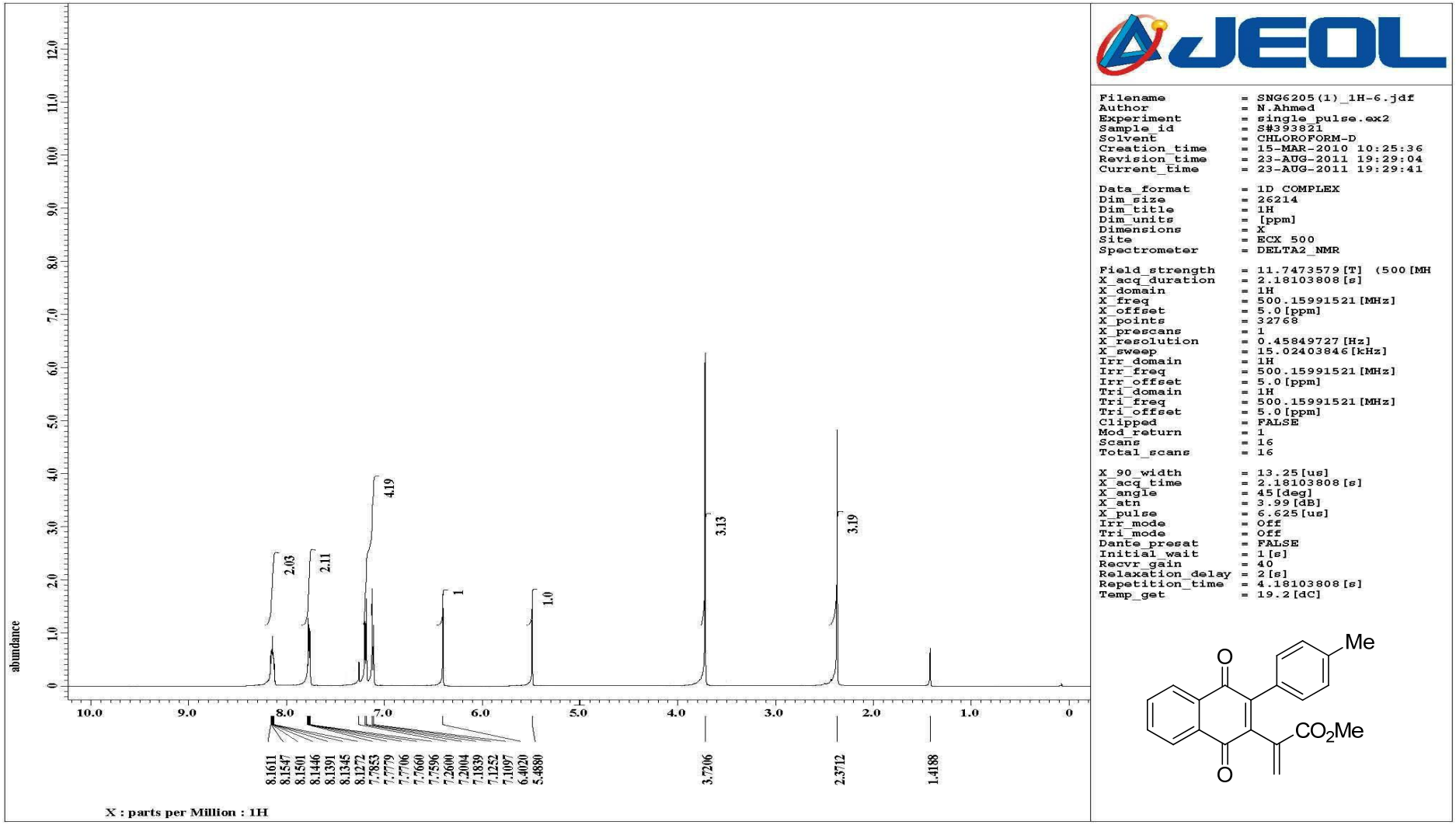
^{1}H NMR spectrum of methyl 2-(3-(3-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.11)**



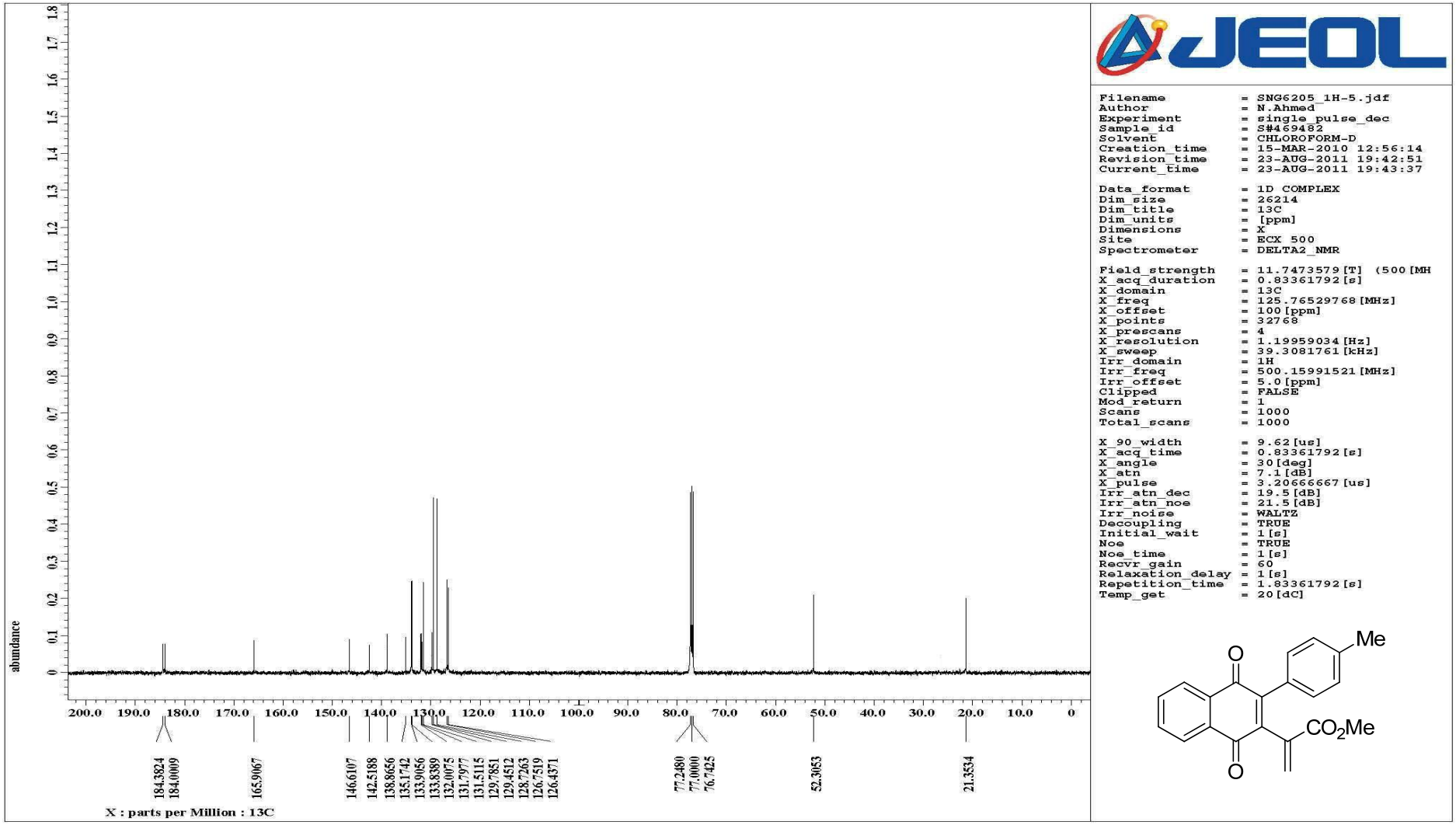
^{13}C NMR spectrum of methyl 2-(3-(3-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.11)**



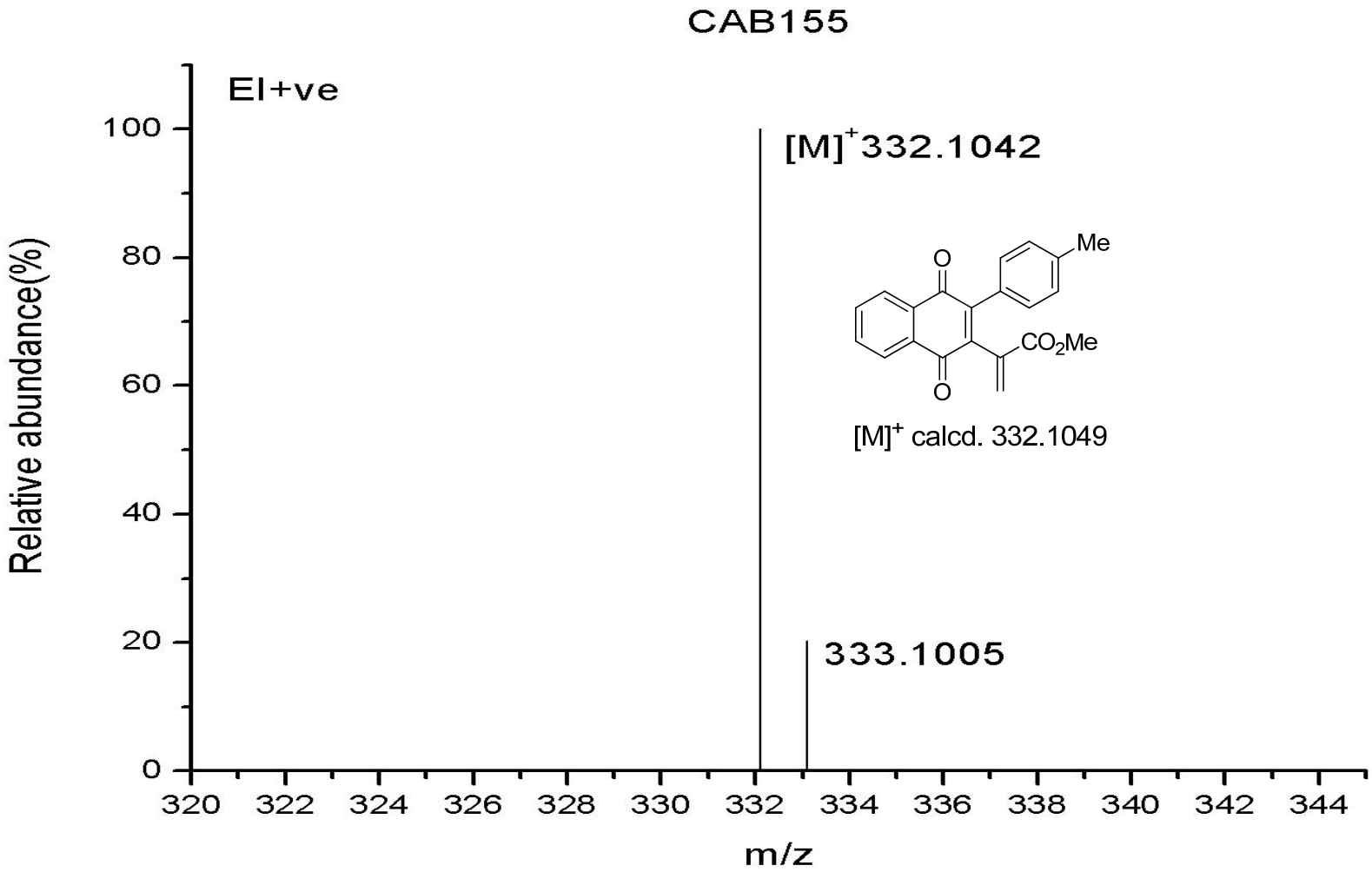
HRMS spectrum of methyl 2-(3-(3-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.11)**



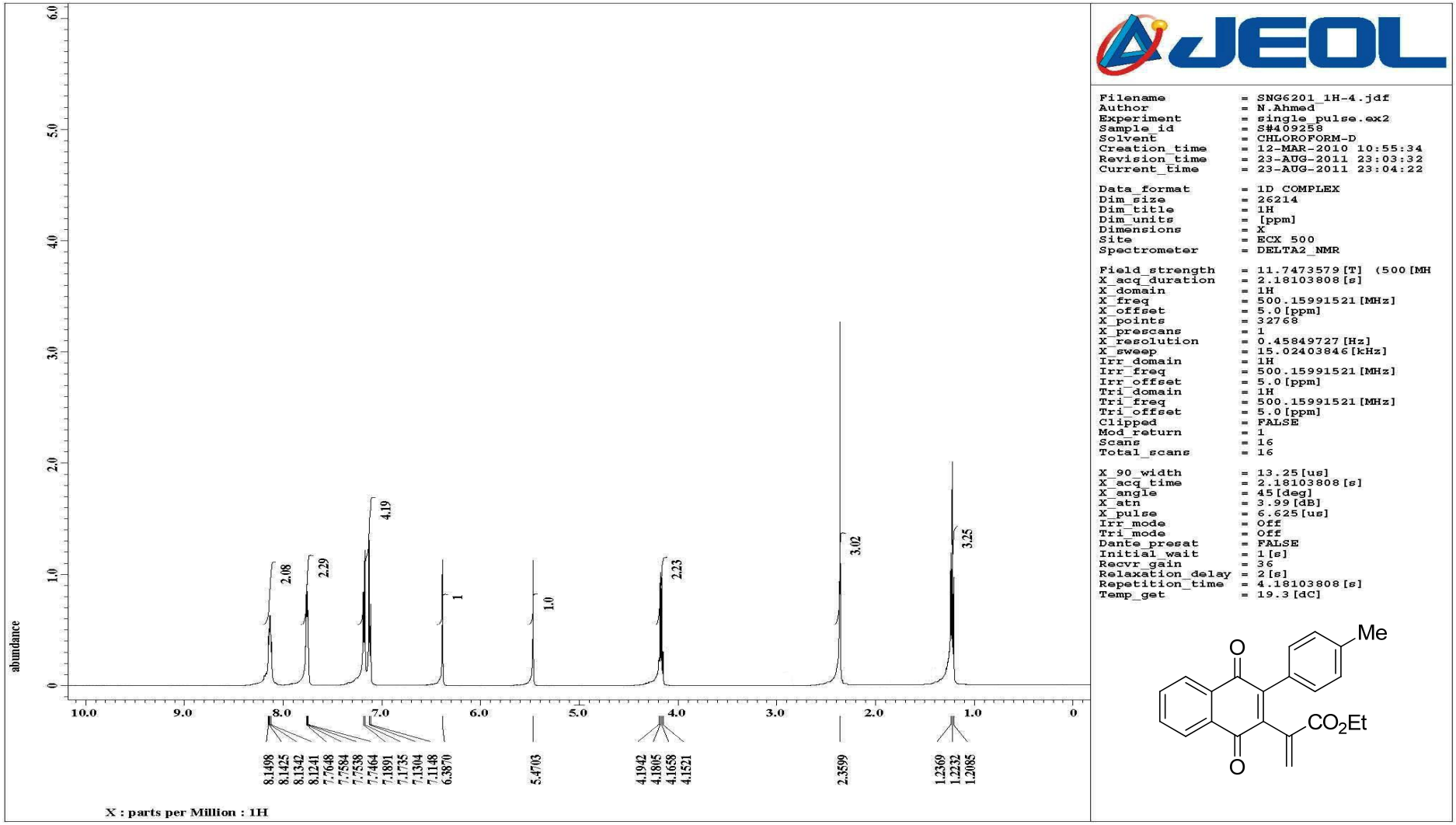
^{1}H NMR spectrum of methyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate **(3.12)**



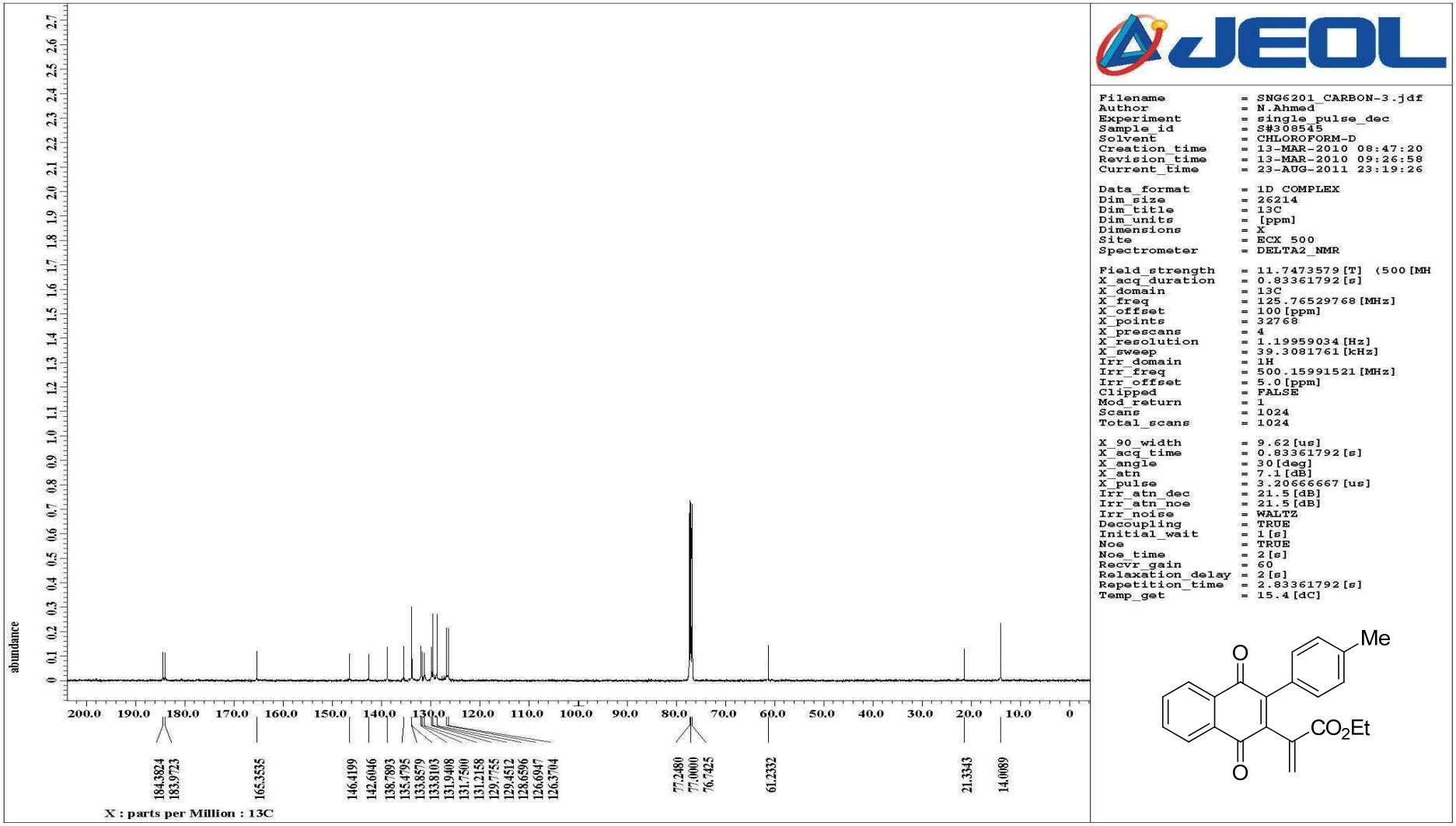
^{13}C NMR spectrum of methyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate **(3.12)**



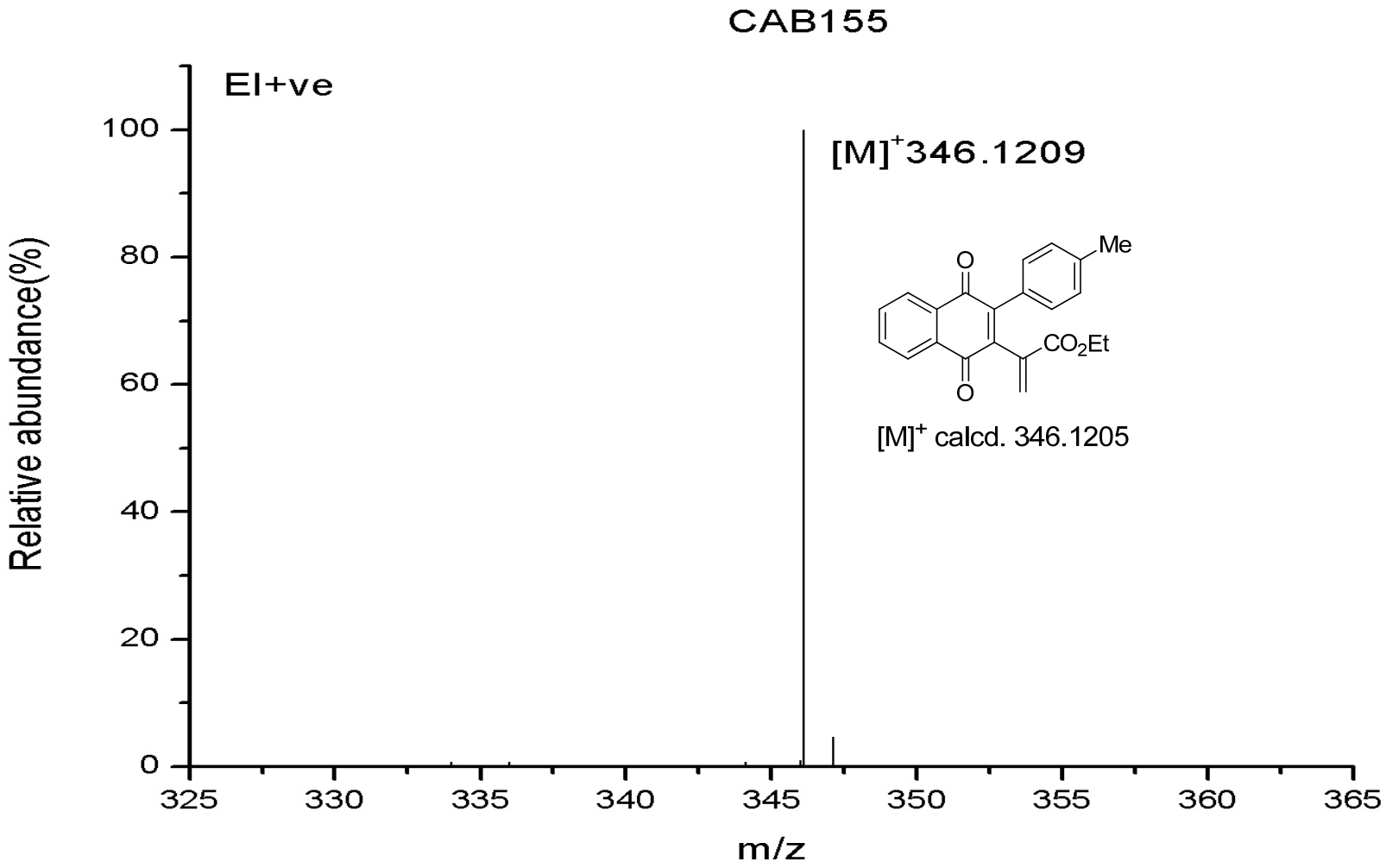
HRMS spectrum of methyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate **(3.12)**



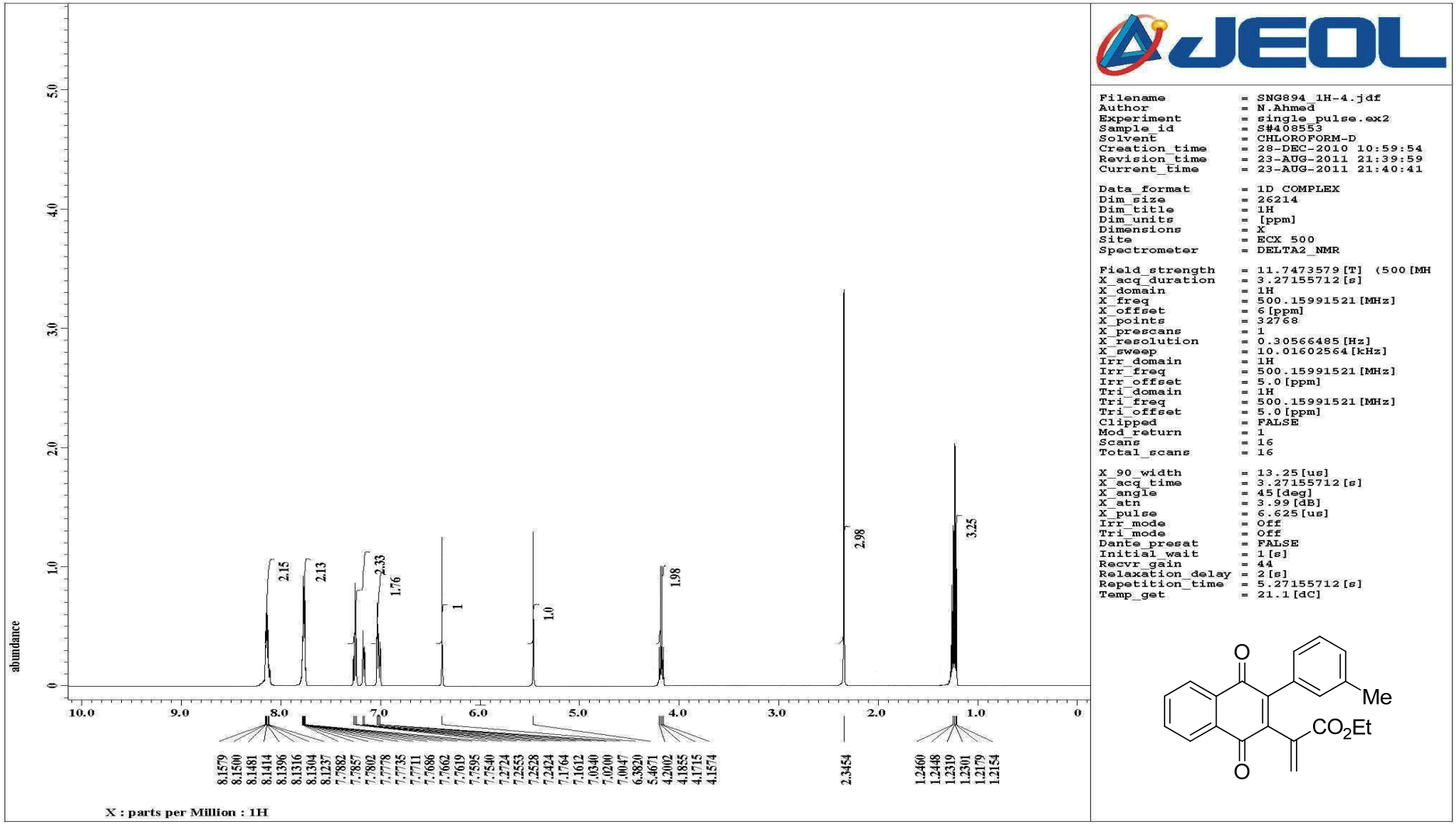
^{1}H NMR spectrum of ethyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate **(3.13)**



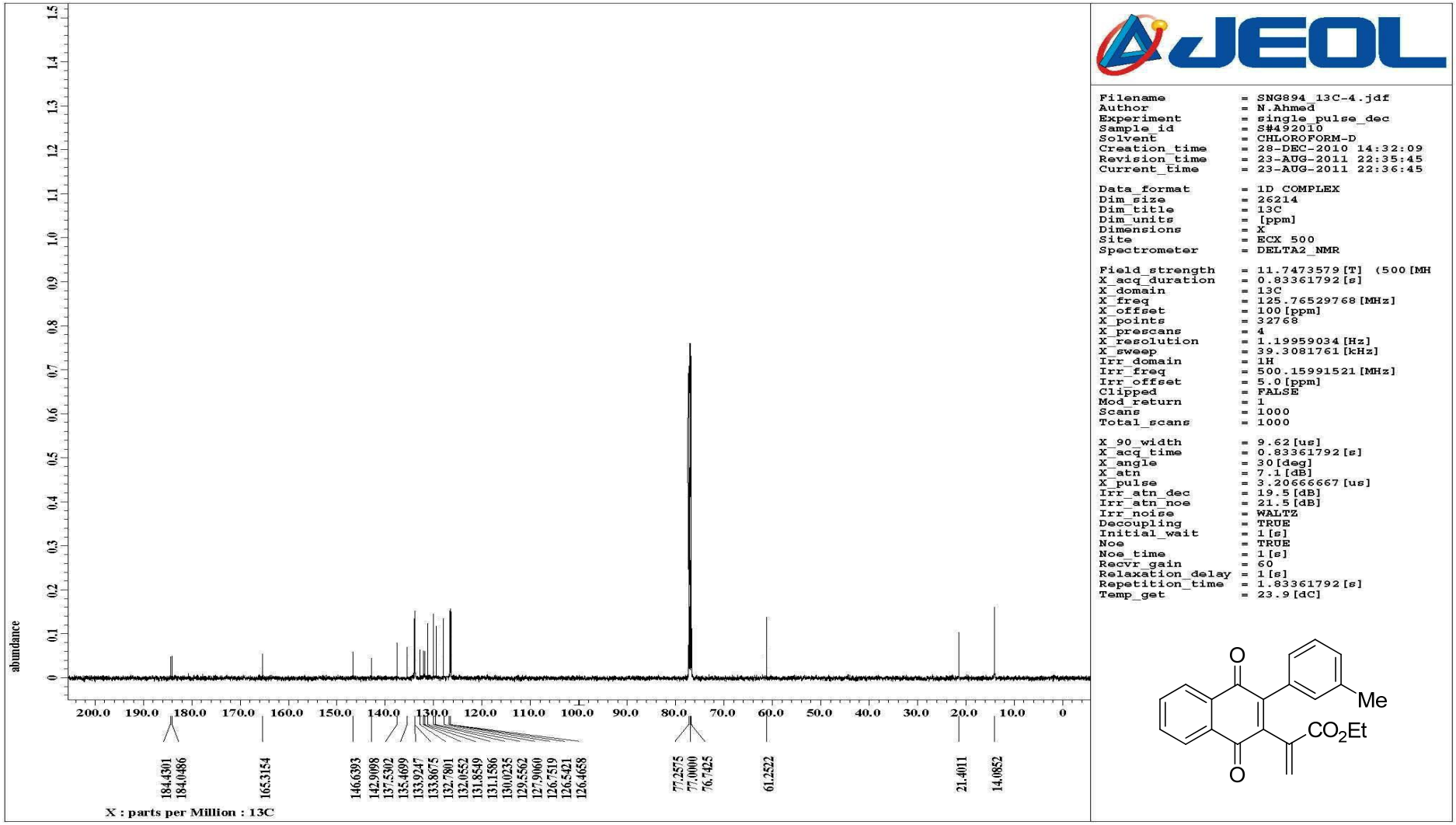
^{13}C NMR spectrum of ethyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate **(3.13)**



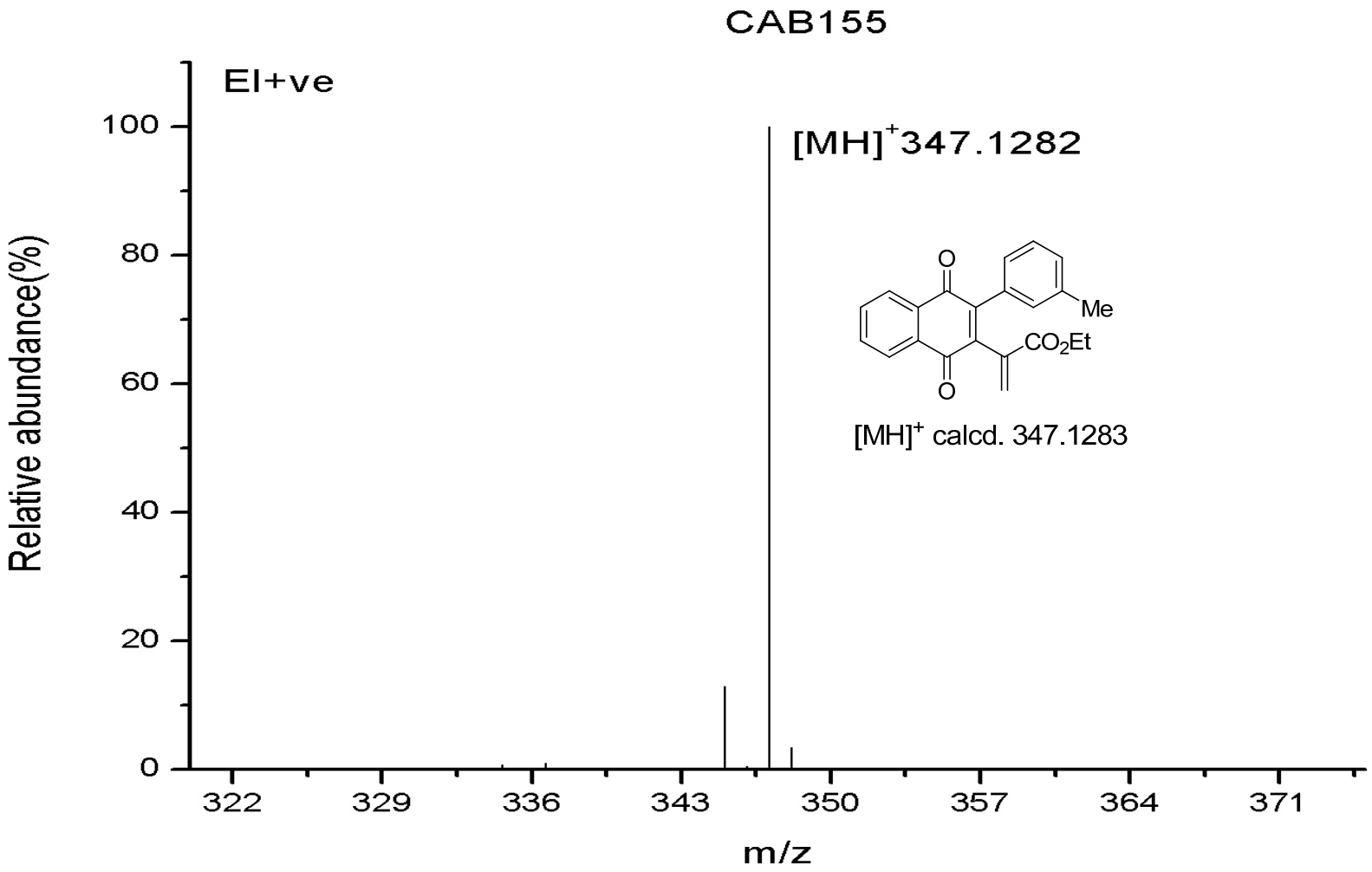
HRMS spectrum of ethyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate **(3.13)**



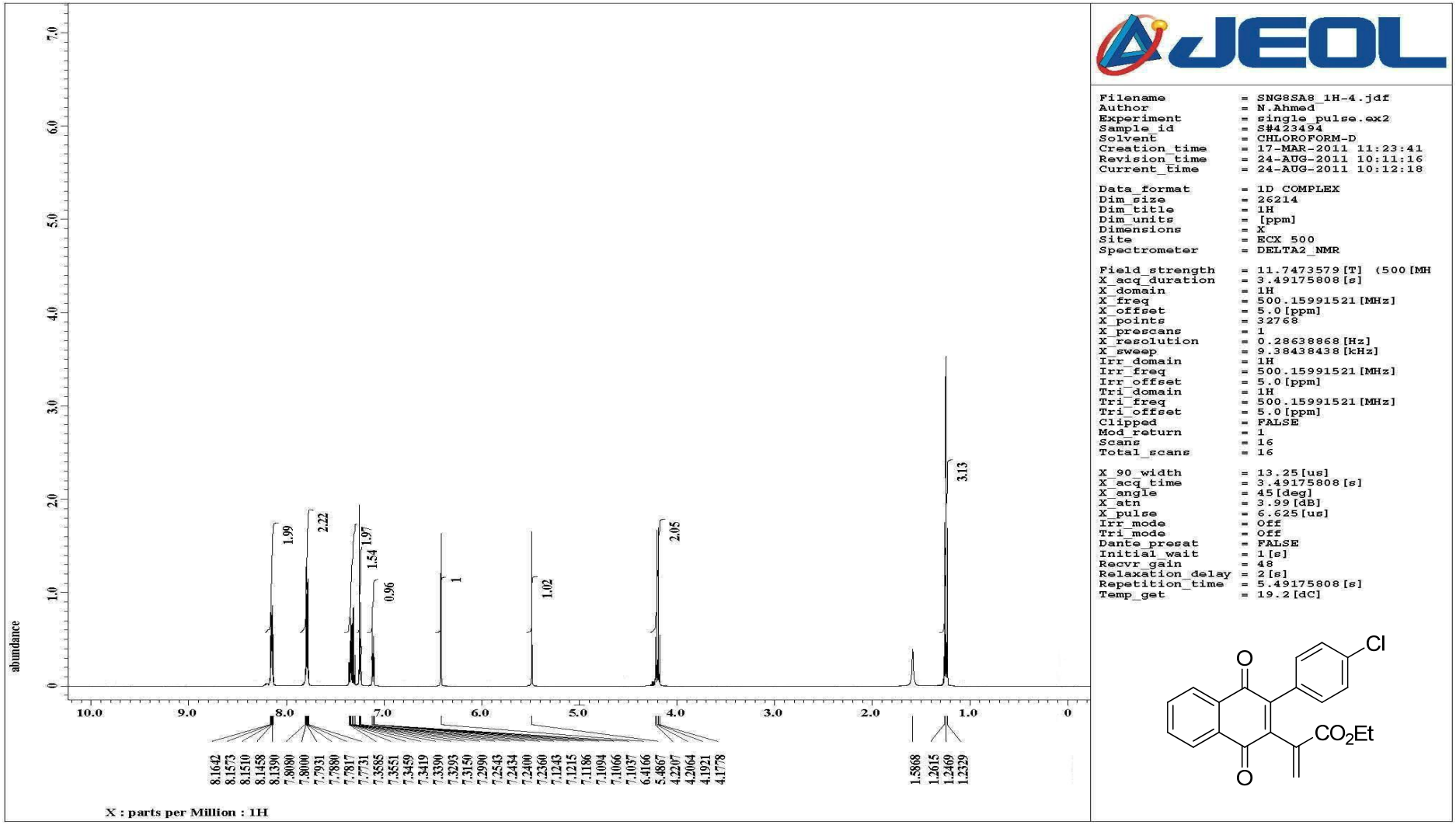
^{1}H NMR spectrum of ethyl 2-(1,4-dioxo-3-*m*-tolyl-1,4-dihydronaphthalen-2-yl)acrylate **(3.14)**



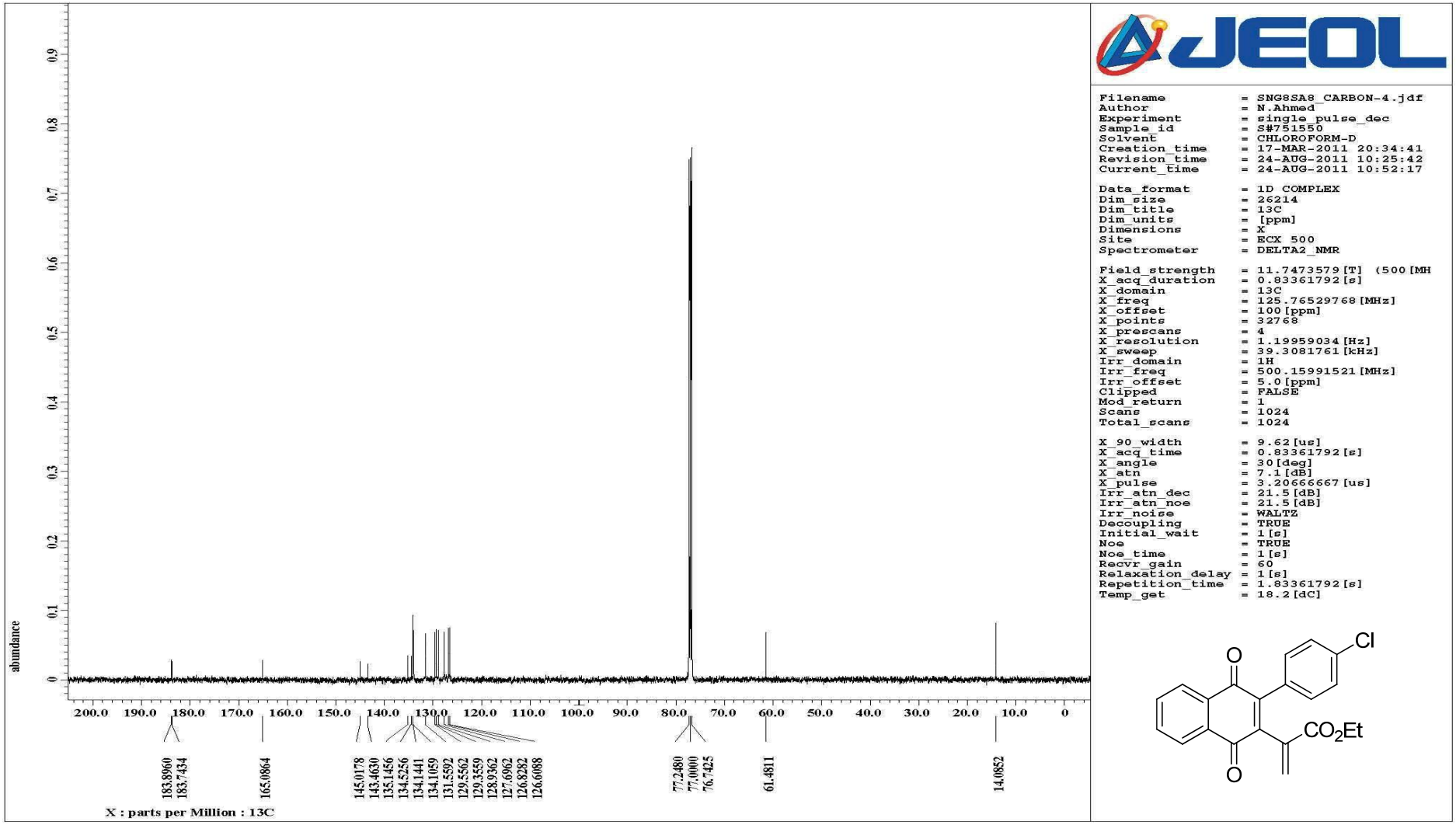
^{13}C NMR spectrum of ethyl 2-(1,4-dioxo-3-*m*-tolyl-1,4-dihydronaphthalen-2-yl)acrylate **(3.14)**



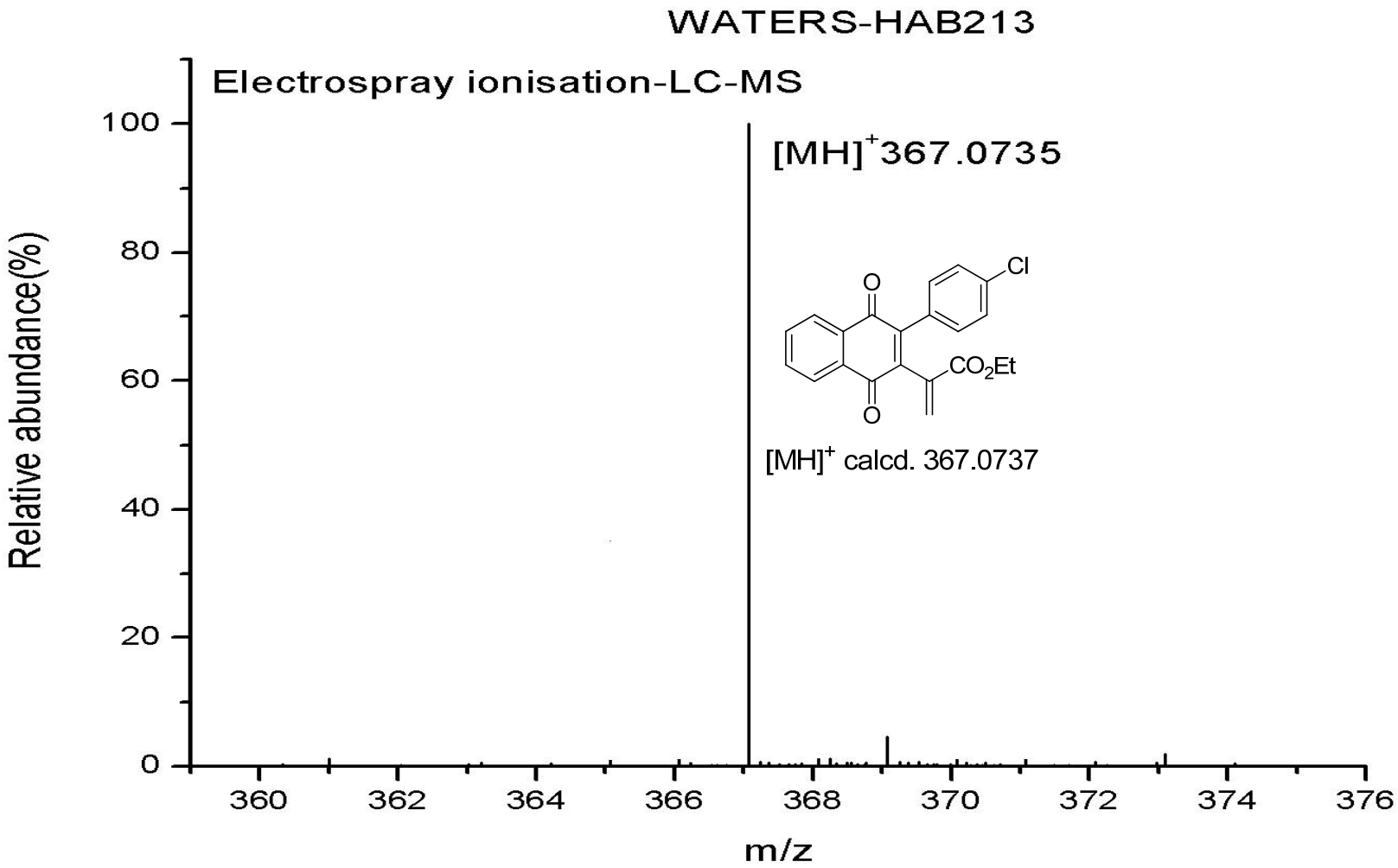
HRMS spectra of ethyl 2-(1,4-dioxo-3-*m*-tolyl-1,4-dihydronaphthalen-2-yl)acrylate **(3.14)**



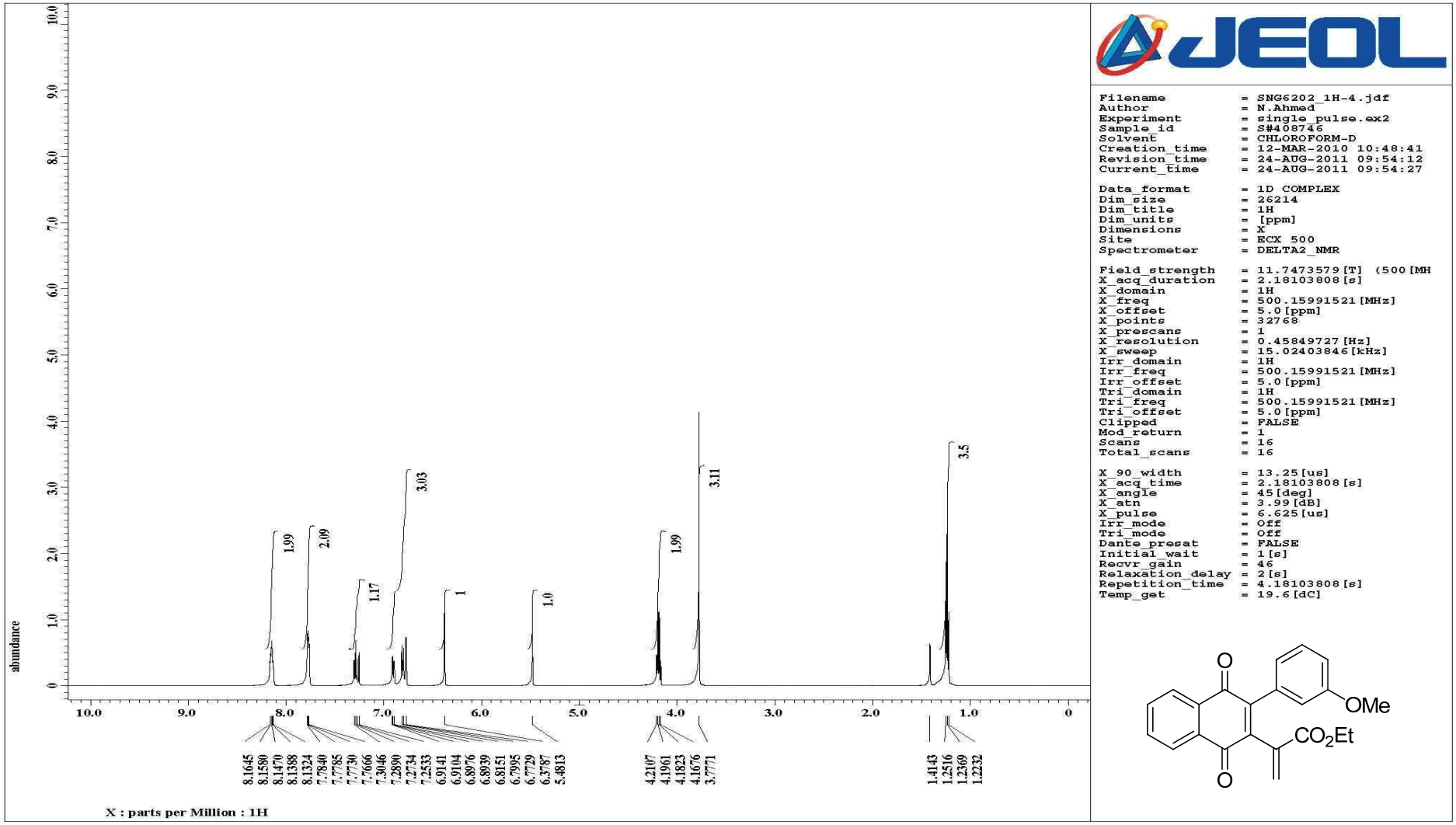
^{1}H NMR spectrum of ethyl 2-(3-(4-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.15)**



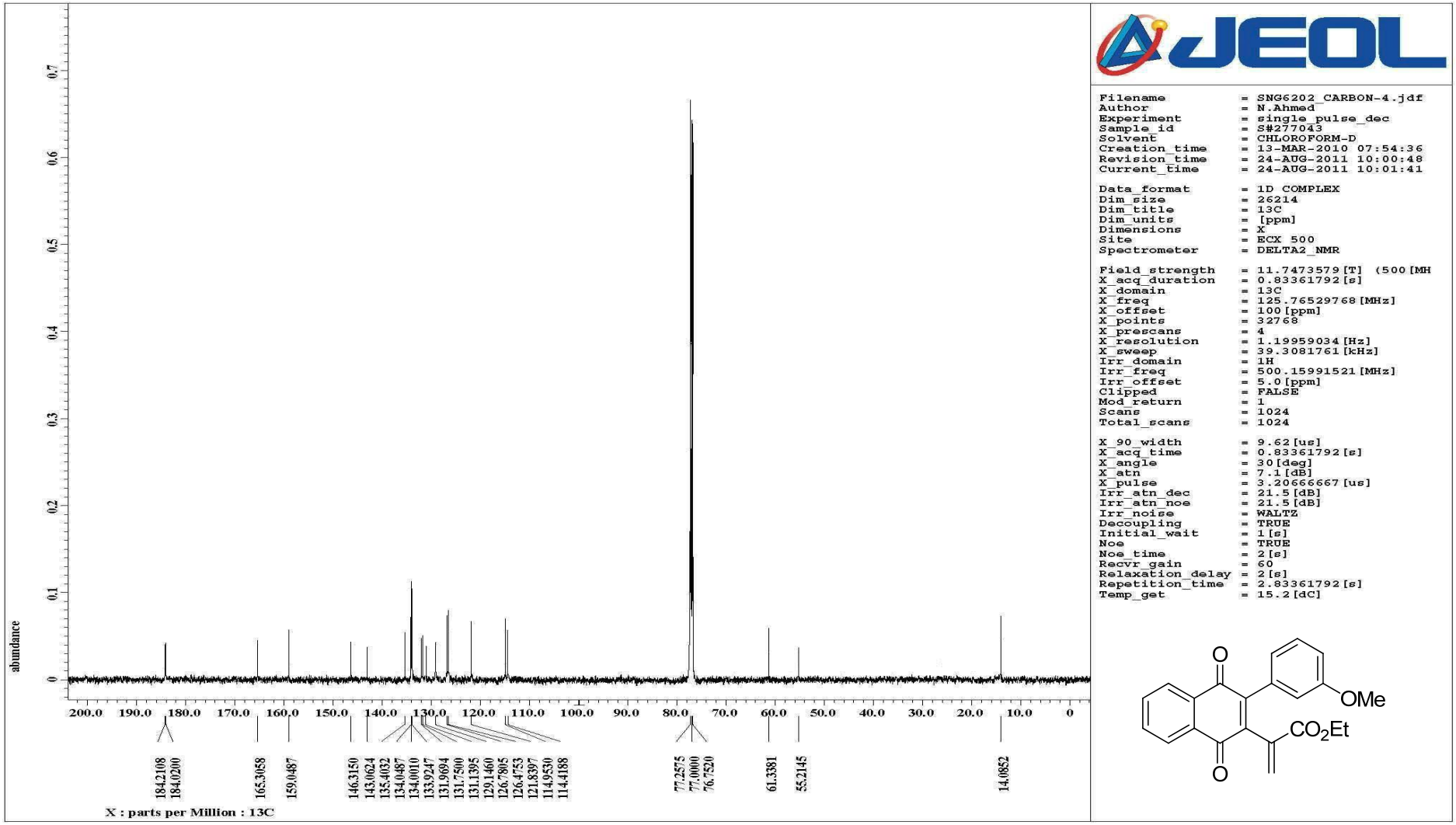
^{13}C NMR spectrum of ethyl 2-(3-(4-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.15)**



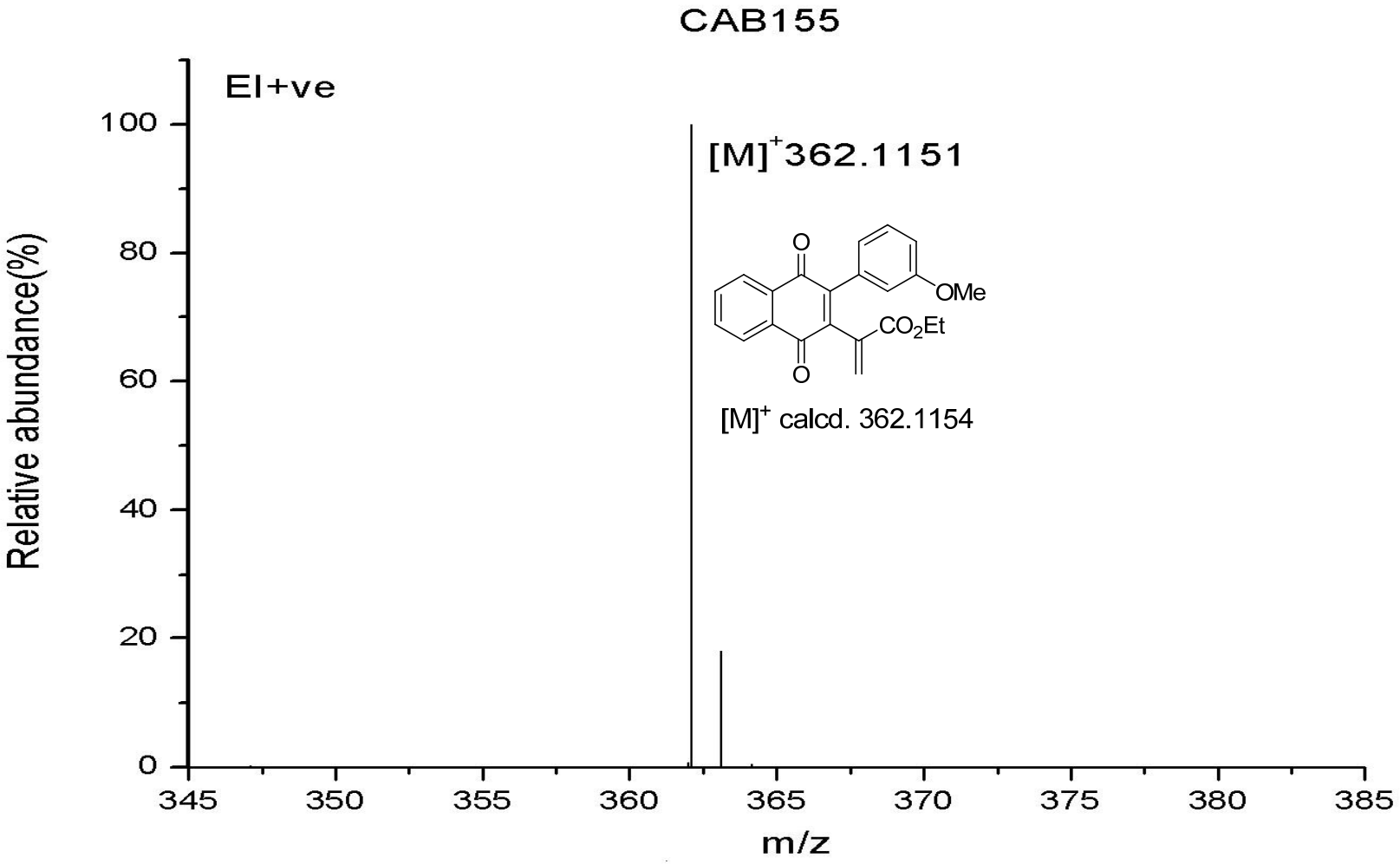
HRMS spectrum of ethyl 2-(3-(4-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.15)**



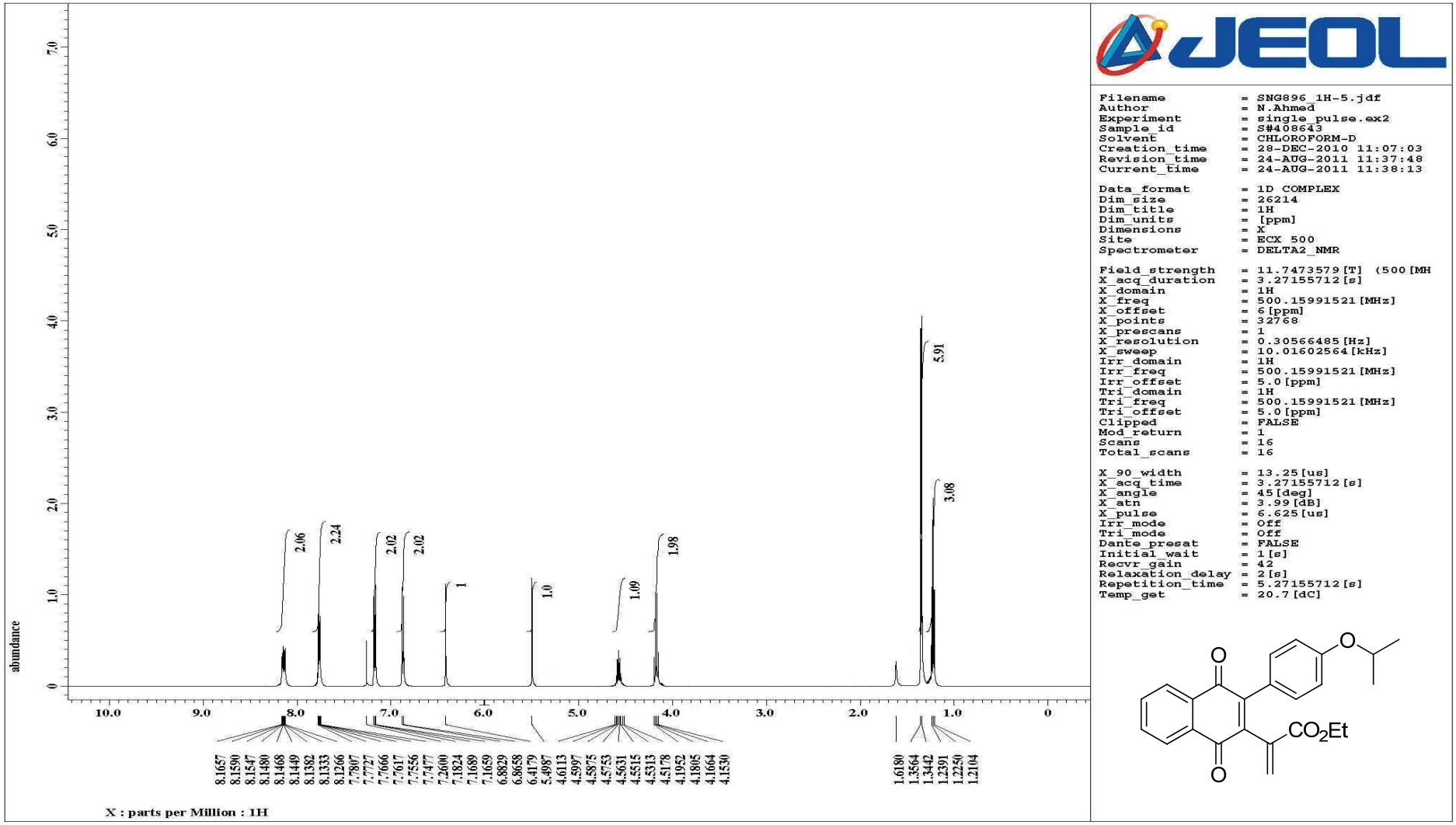
^{1}H NMR spectrum of ethyl 2-(3-(3-methoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.16)**



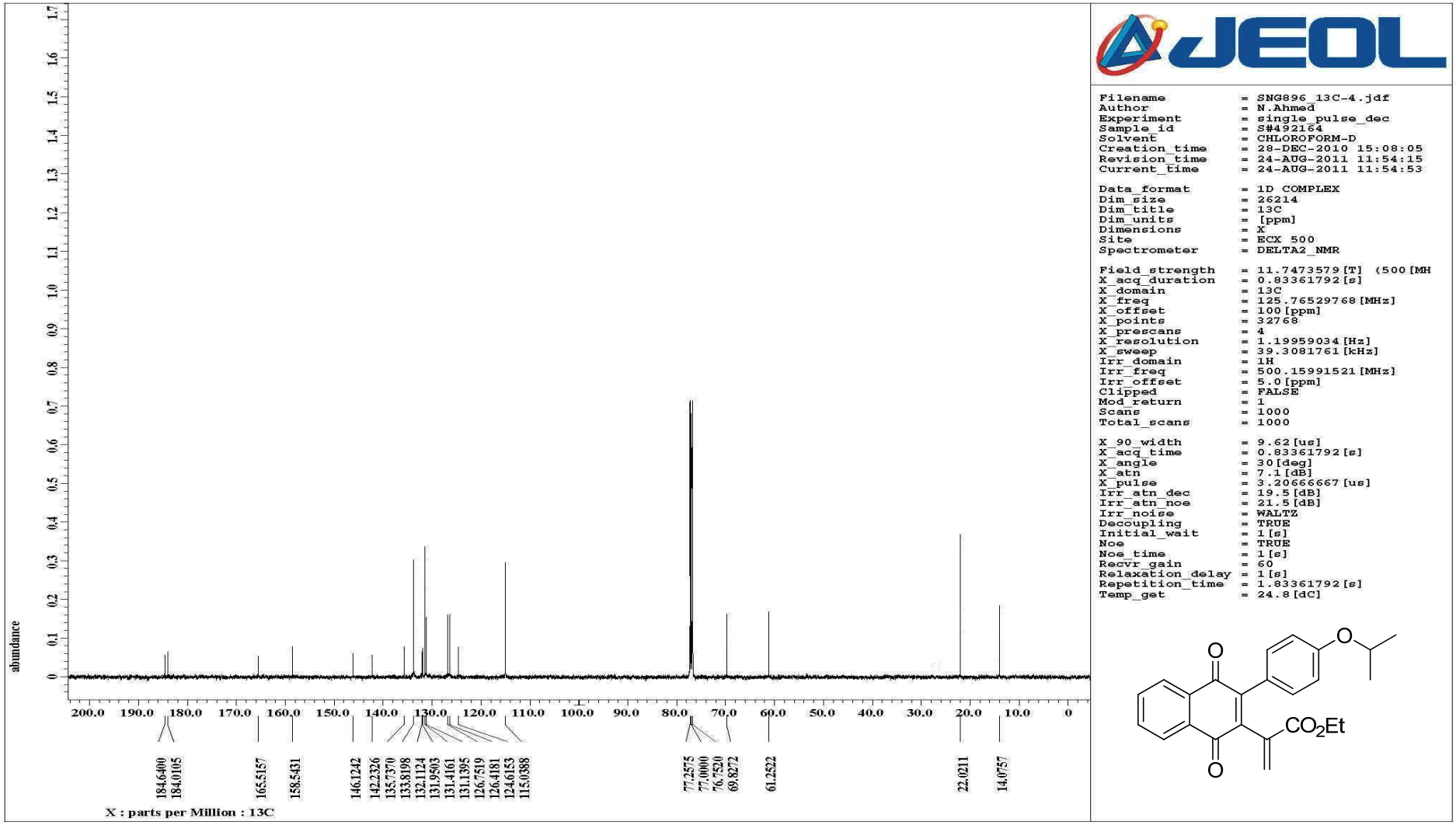
^{13}C NMR spectrum of ethyl 2-(3-(3-methoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.16)**



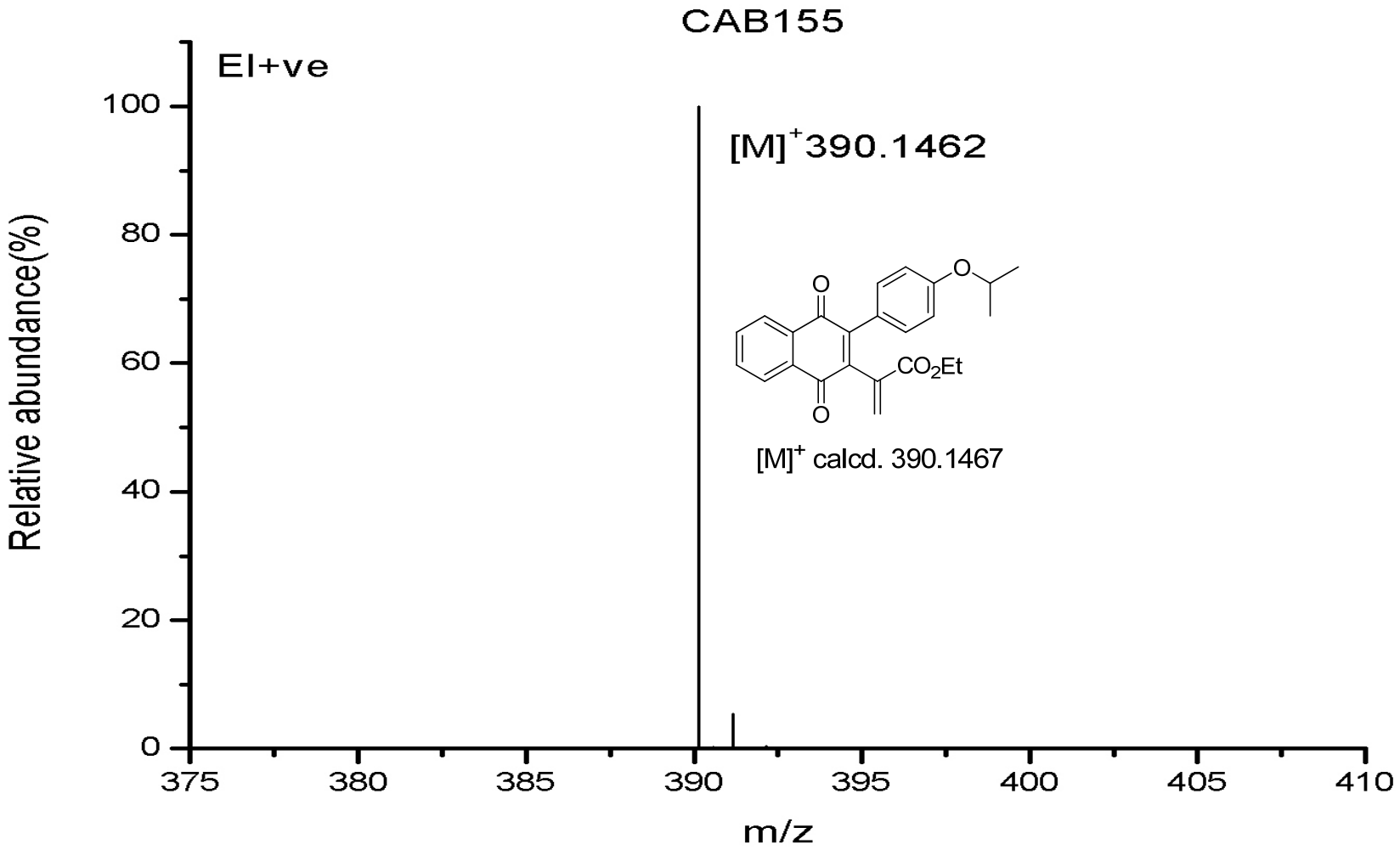
HRMS spectrum of ethyl 2-(3-(3-methoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.16)**



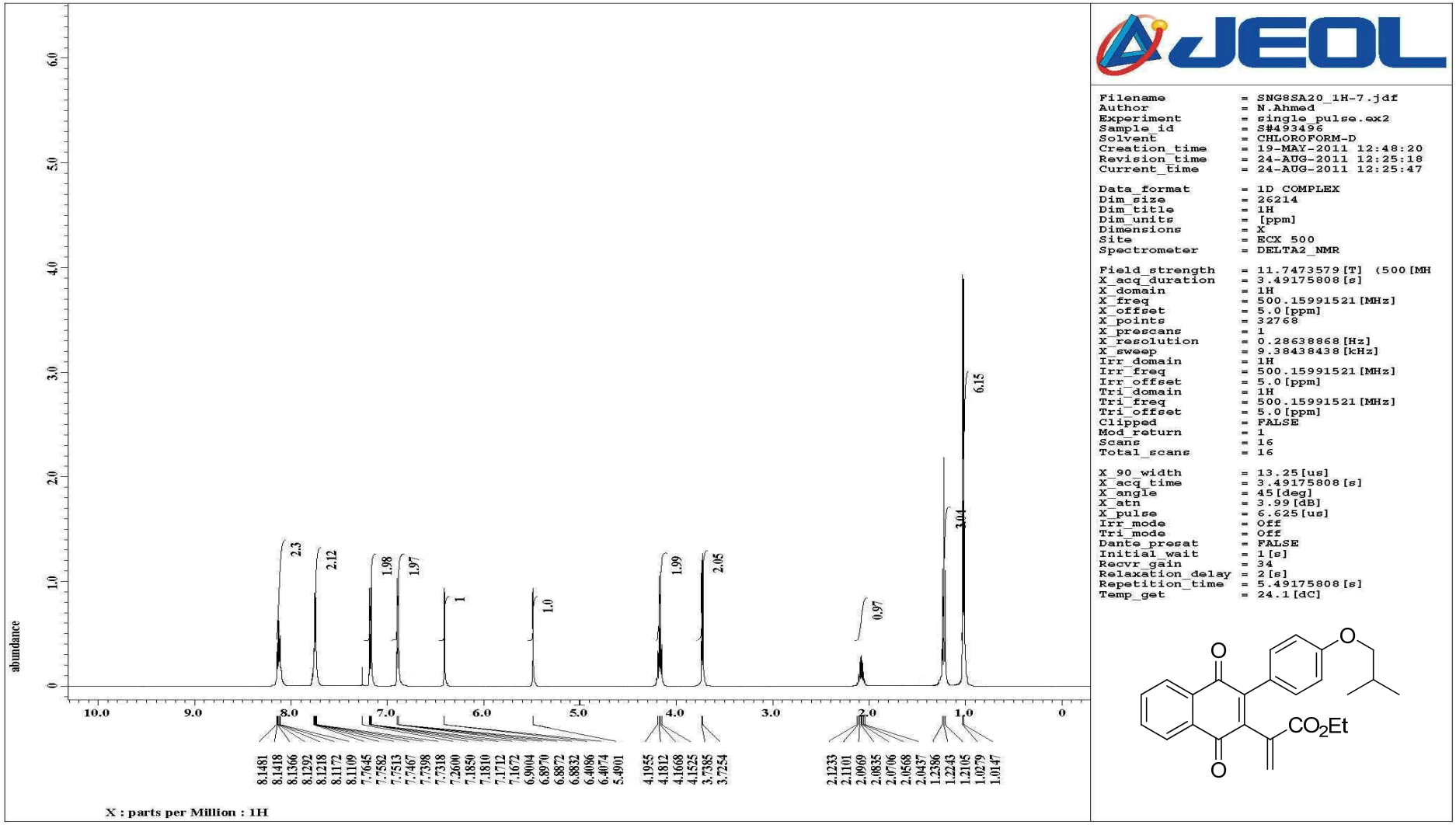
^{1}H NMR spectrum of ethyl 2-(3-(4-isopropoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.17)**



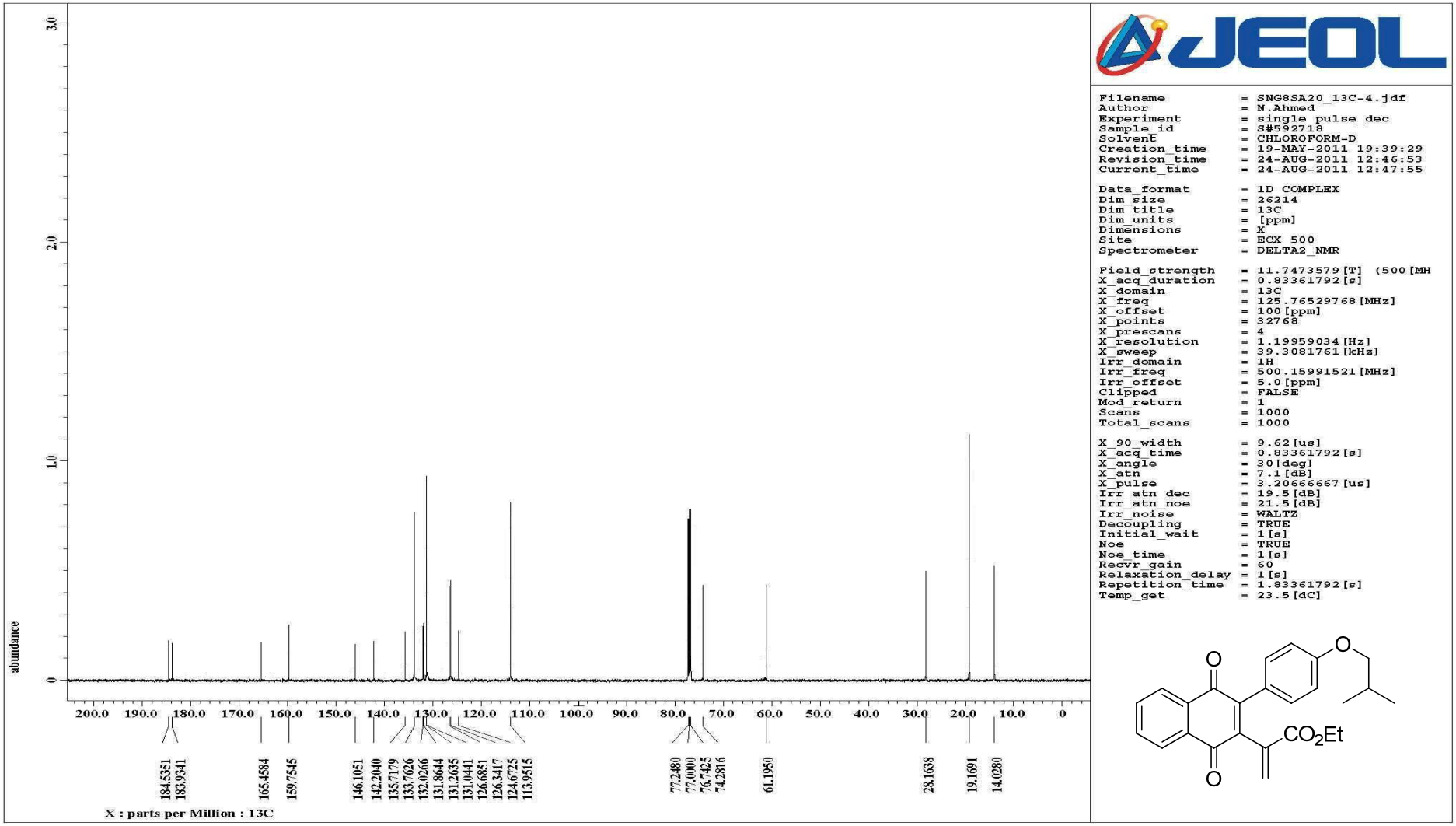
^{13}C NMR spectrum of ethyl 2-(3-(4-isopropoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.17)**



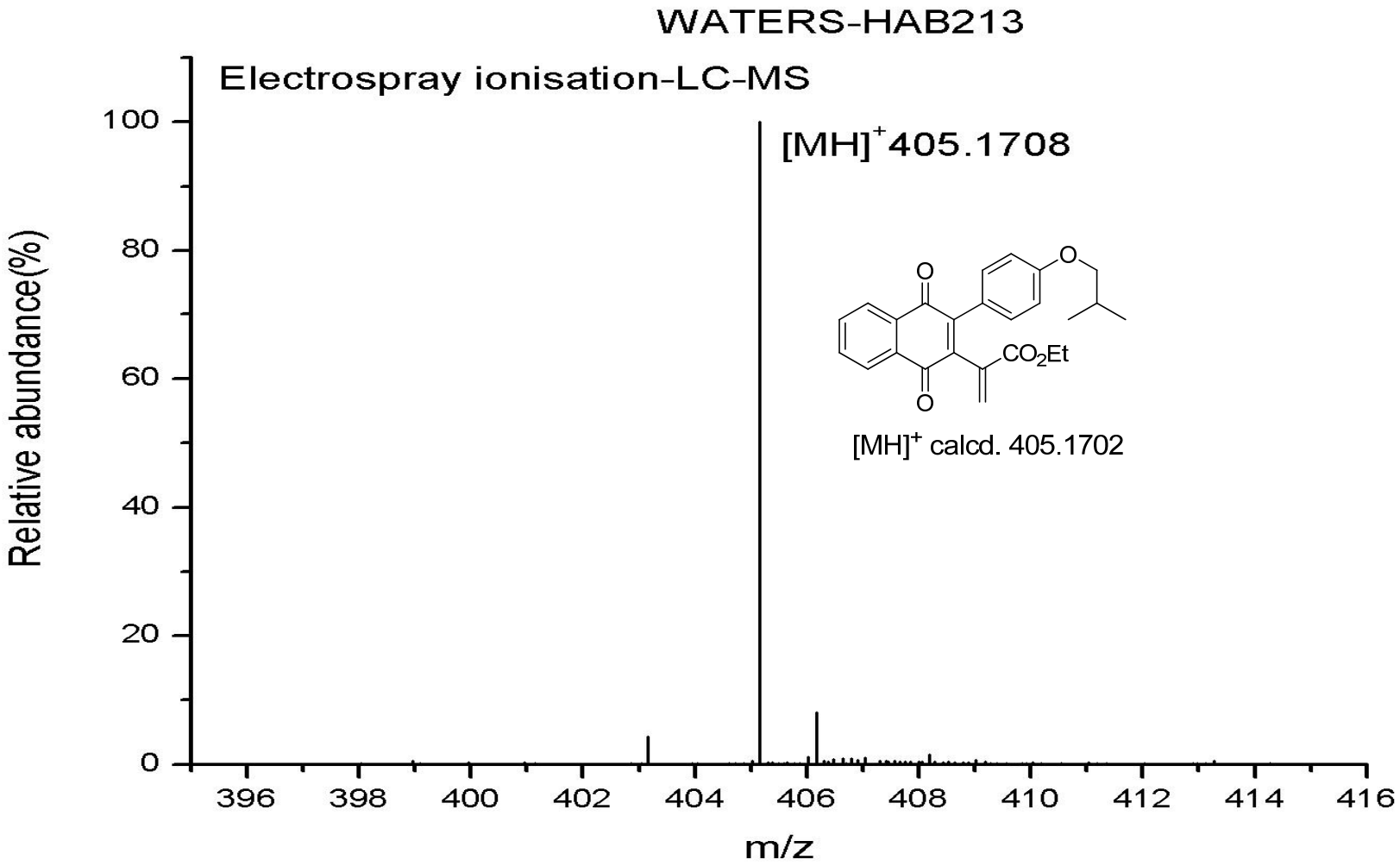
HRMS spectrum of ethyl 2-(3-(4-isopropoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.17)**



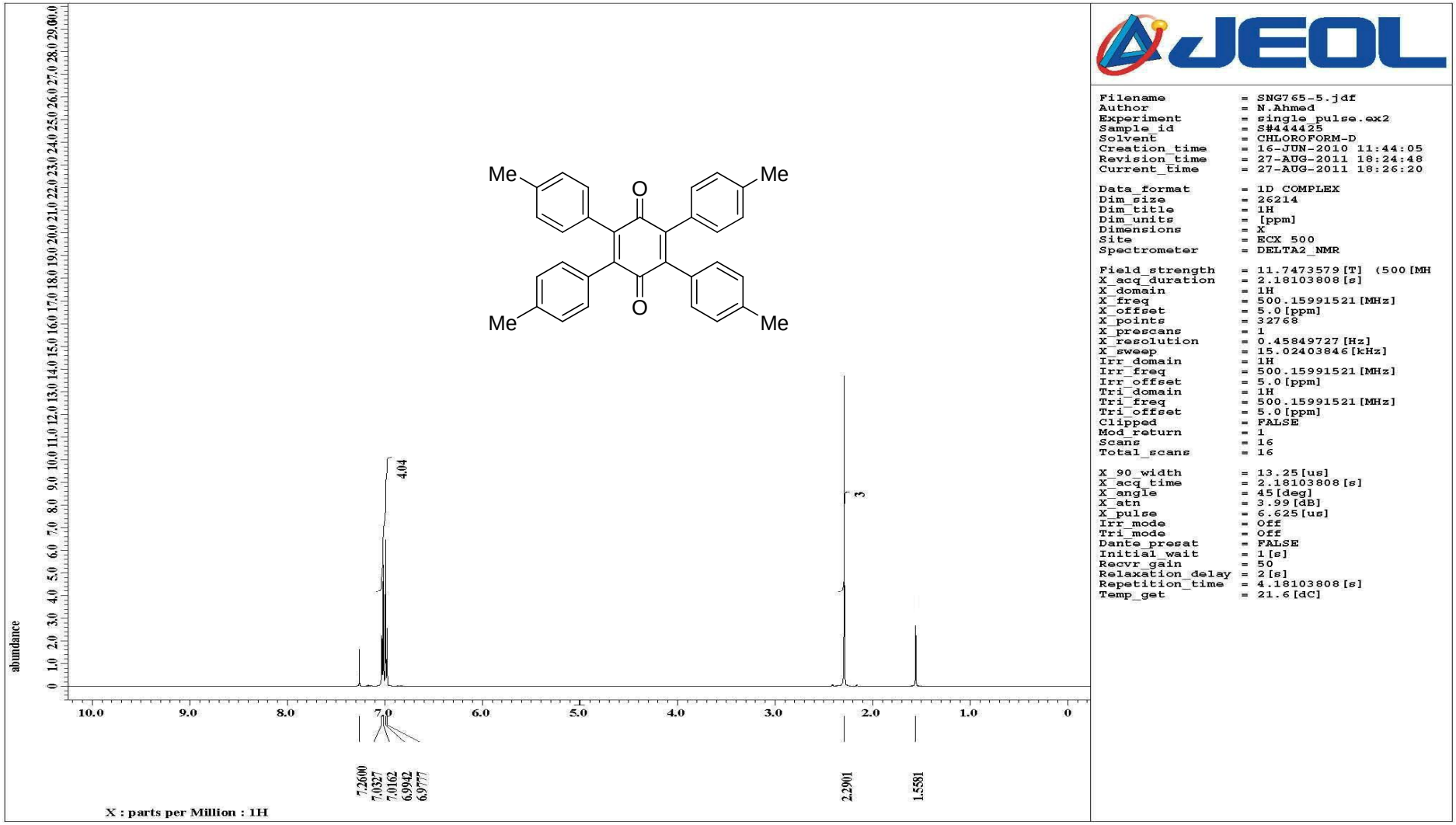
^{1}H NMR spectrum of ethyl 2-(3-(4-isobutoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.18)**



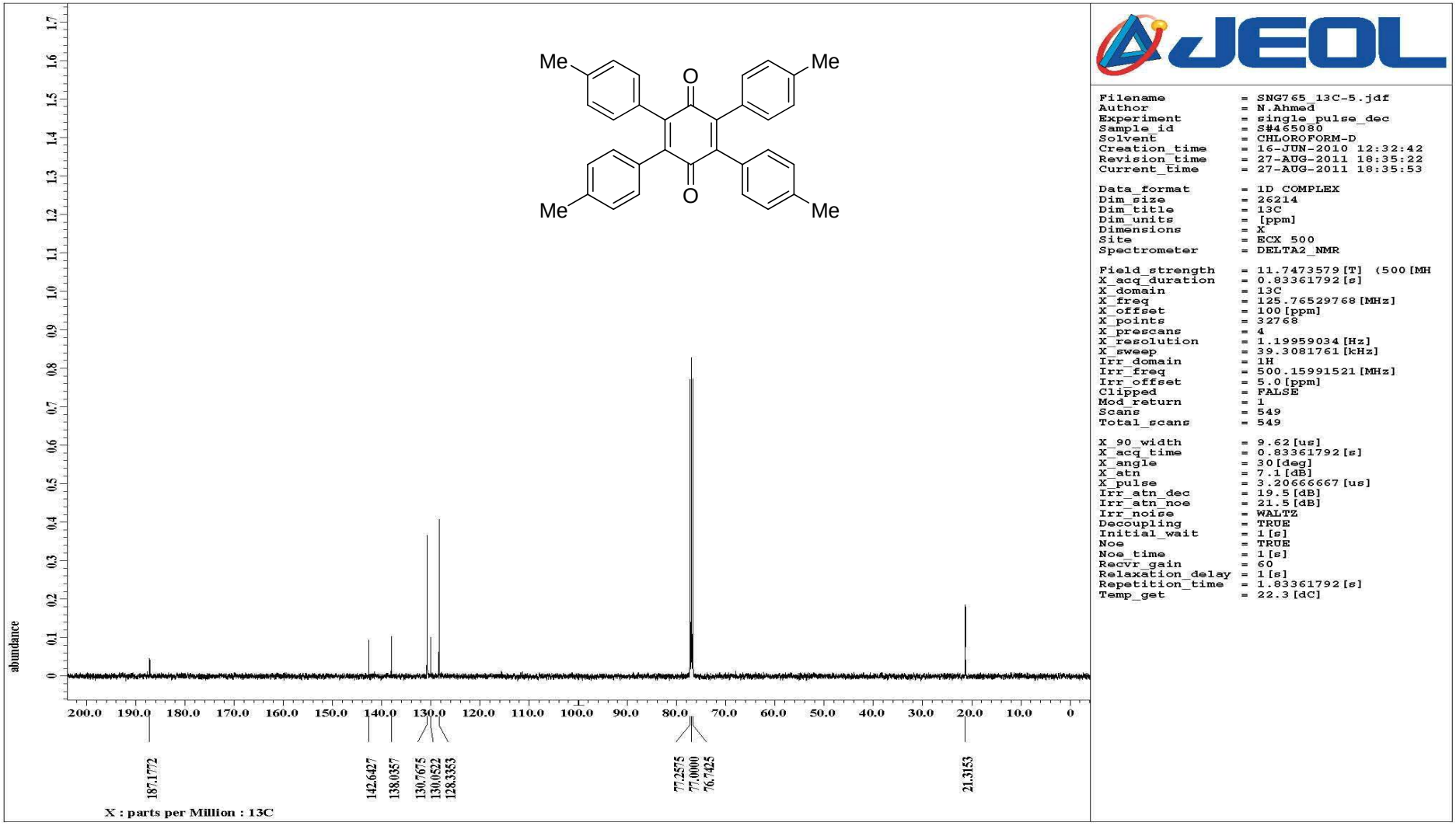
^{13}C NMR spectrum of ethyl 2-(3-(4-isobutoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate **(3.18)**



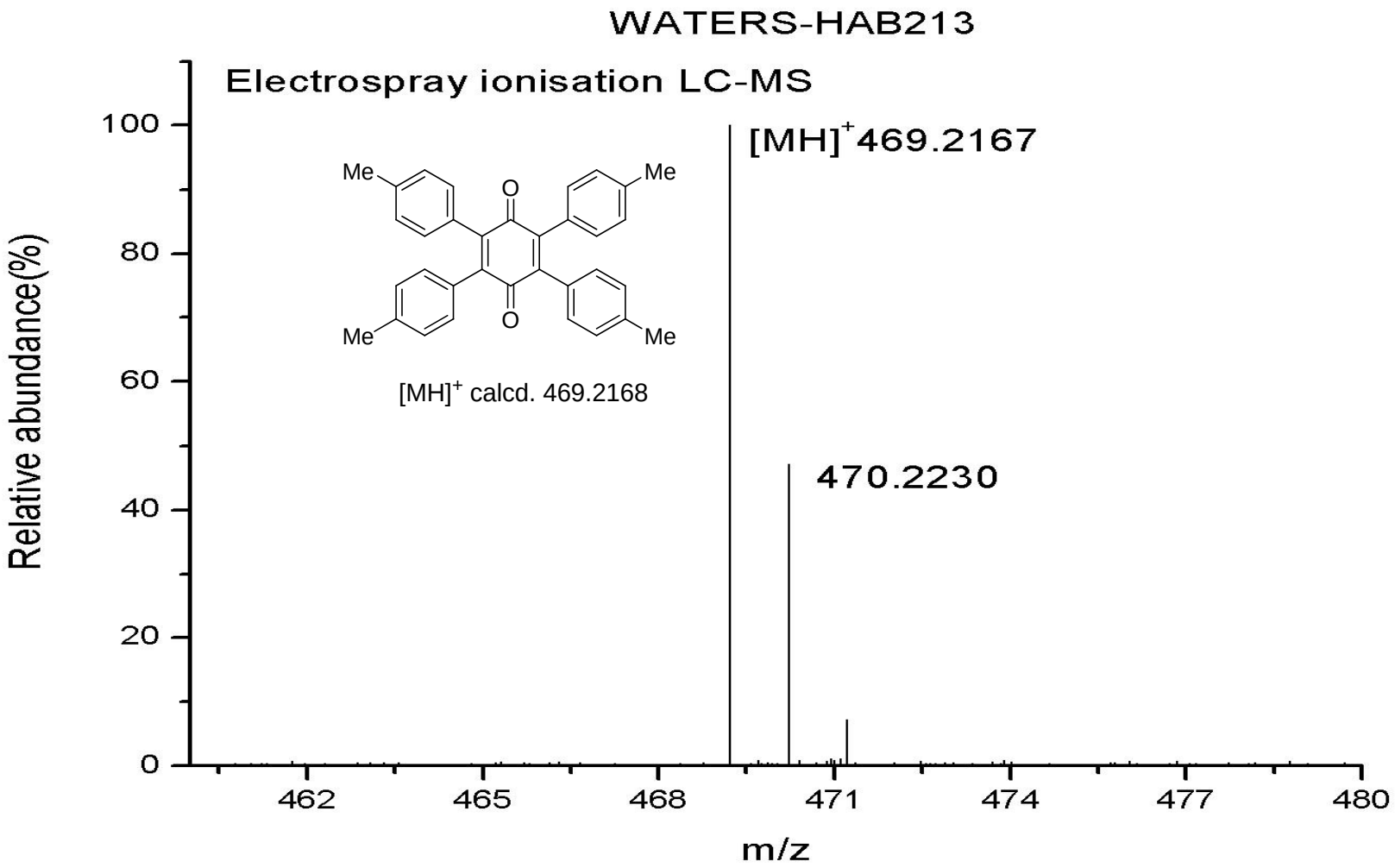
HRMS spectrum of ethyl 2-(3-(4-isobutoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.18**)



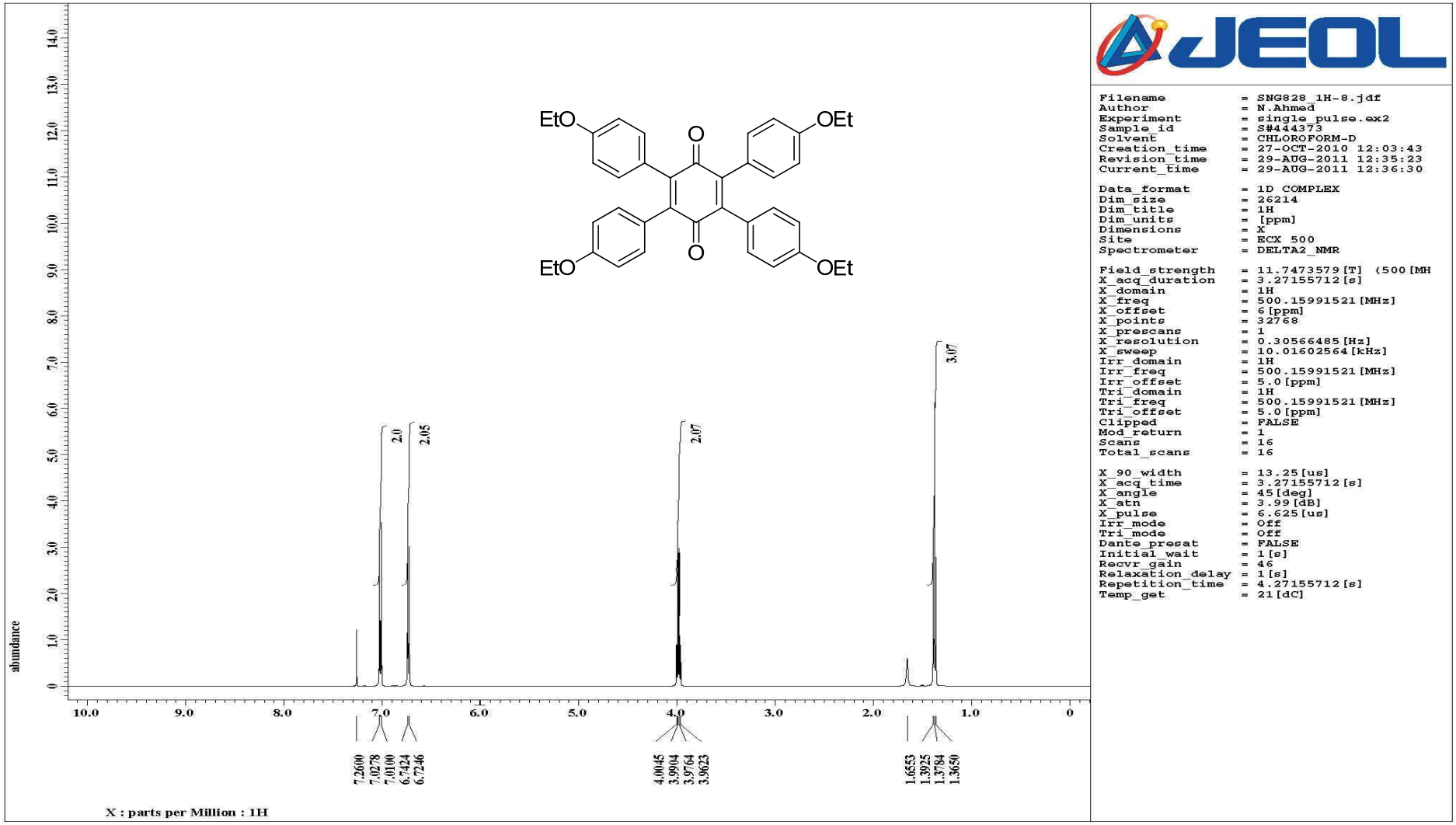
^{1}H NMR spectrum of 2,3,5,6-tetra4-tolylcyclohexa-2,5-diene-1,4-dione (**5.1**)



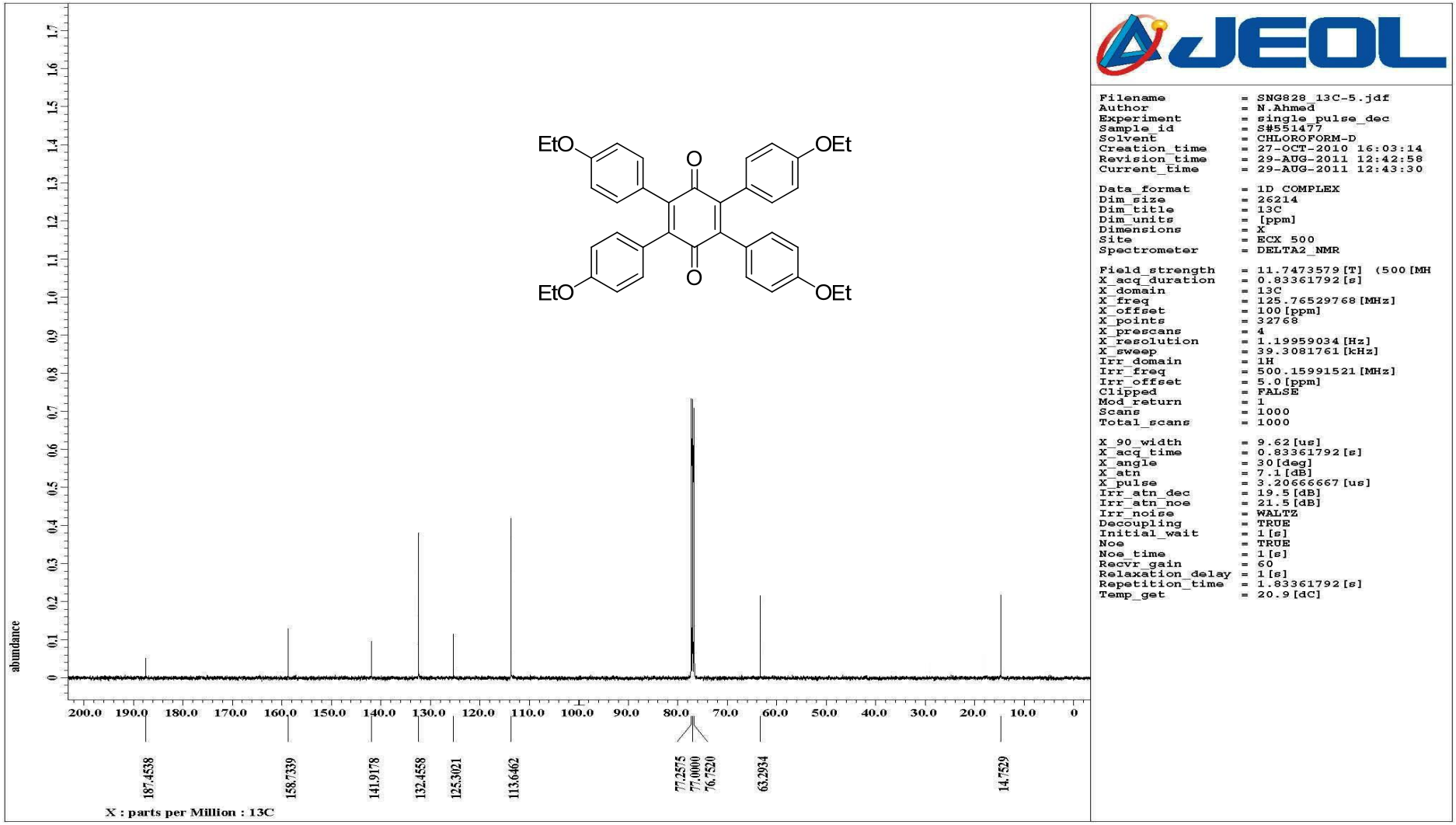
^{13}C NMR spectrum of 2,3,5,6-tetra4-tolylcyclohexa-2,5-diene-1,4-dione (**5.1**)



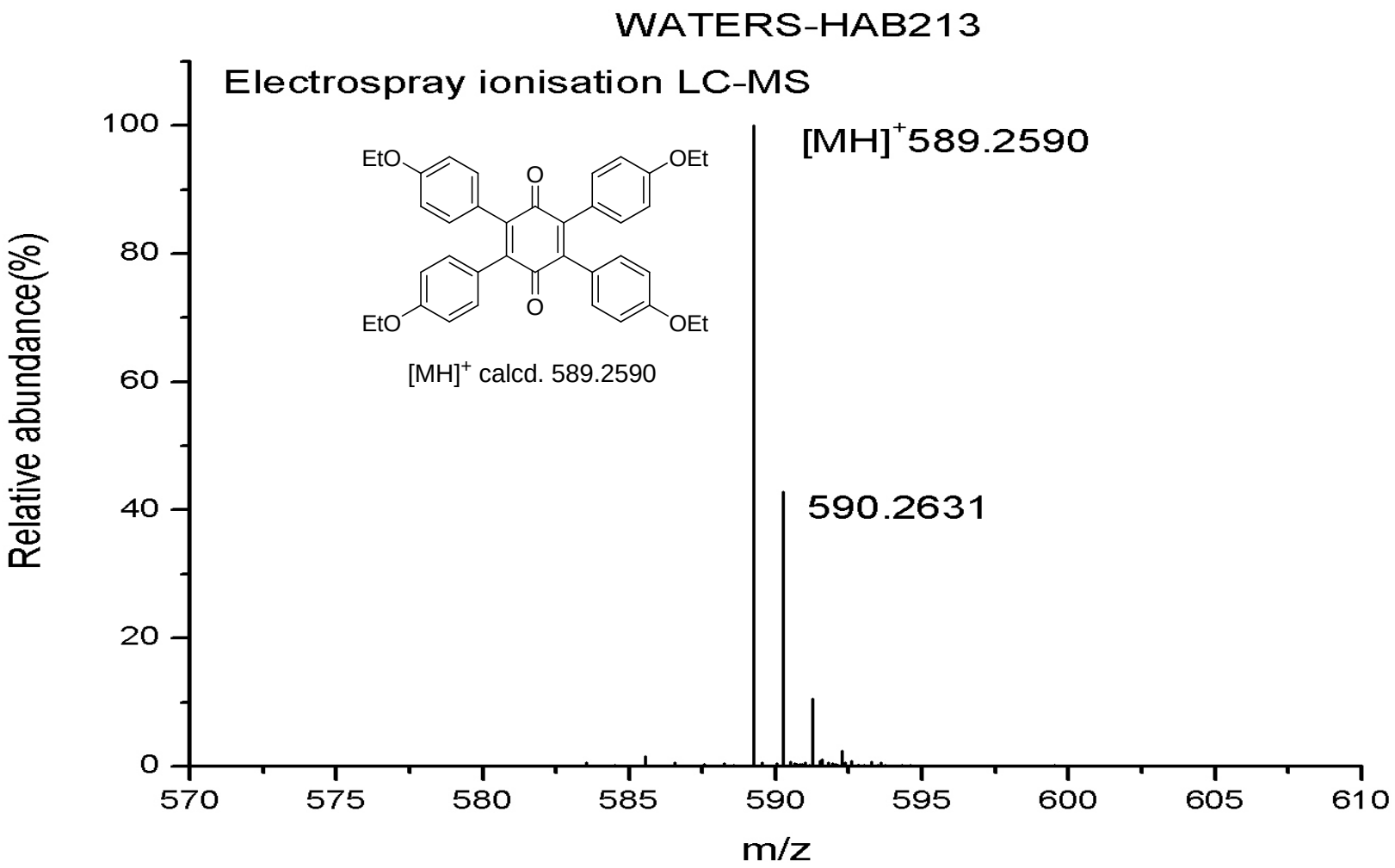
HRMS spectrum of 2,3,5,6-tetra4-tolylcyclohexa-2,5-diene-1,4-dione (**5.1**)



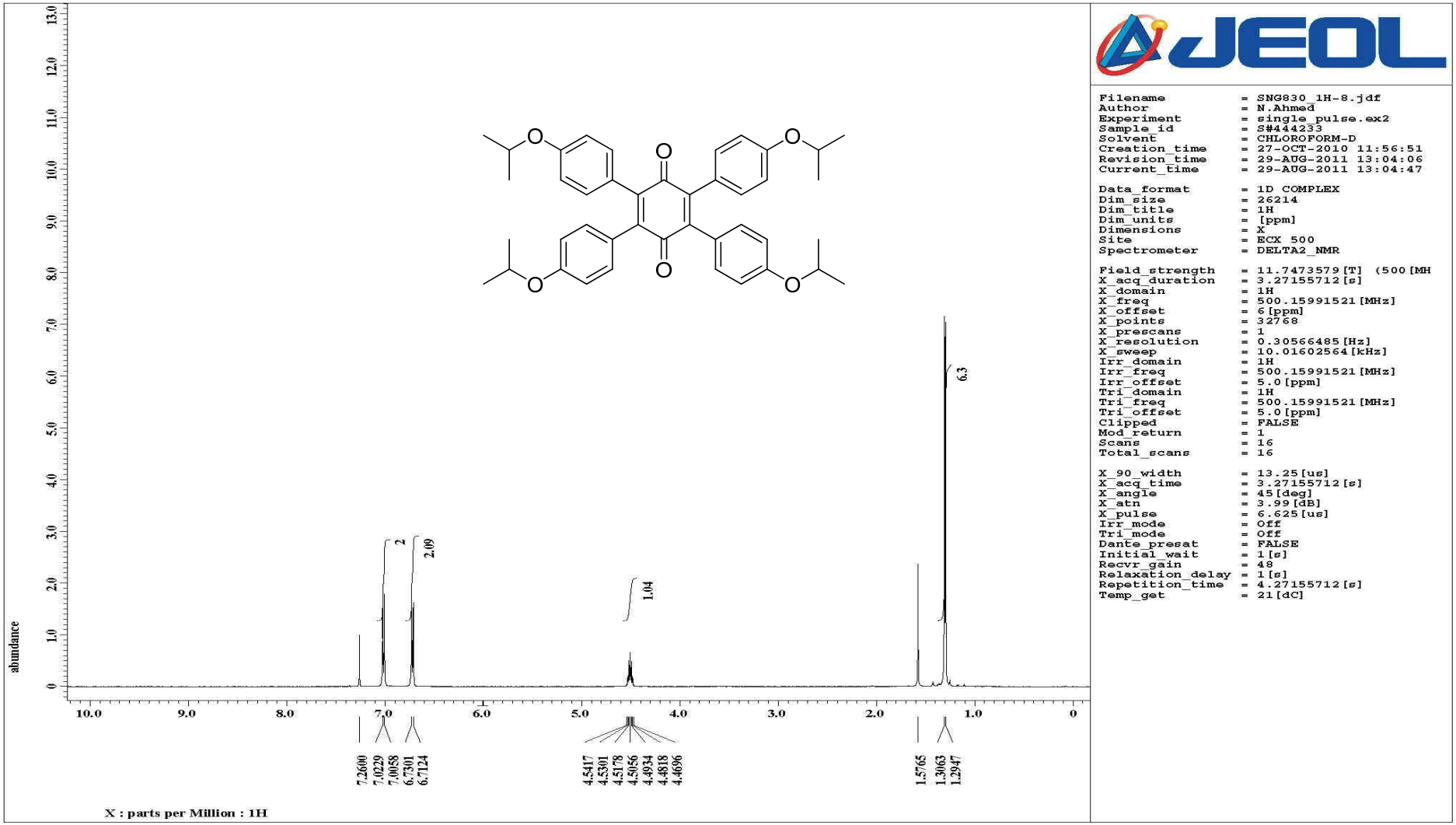
^{1}H NMR spectrum of 2,3,5,6-tetrakis(4-ethoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.2**)



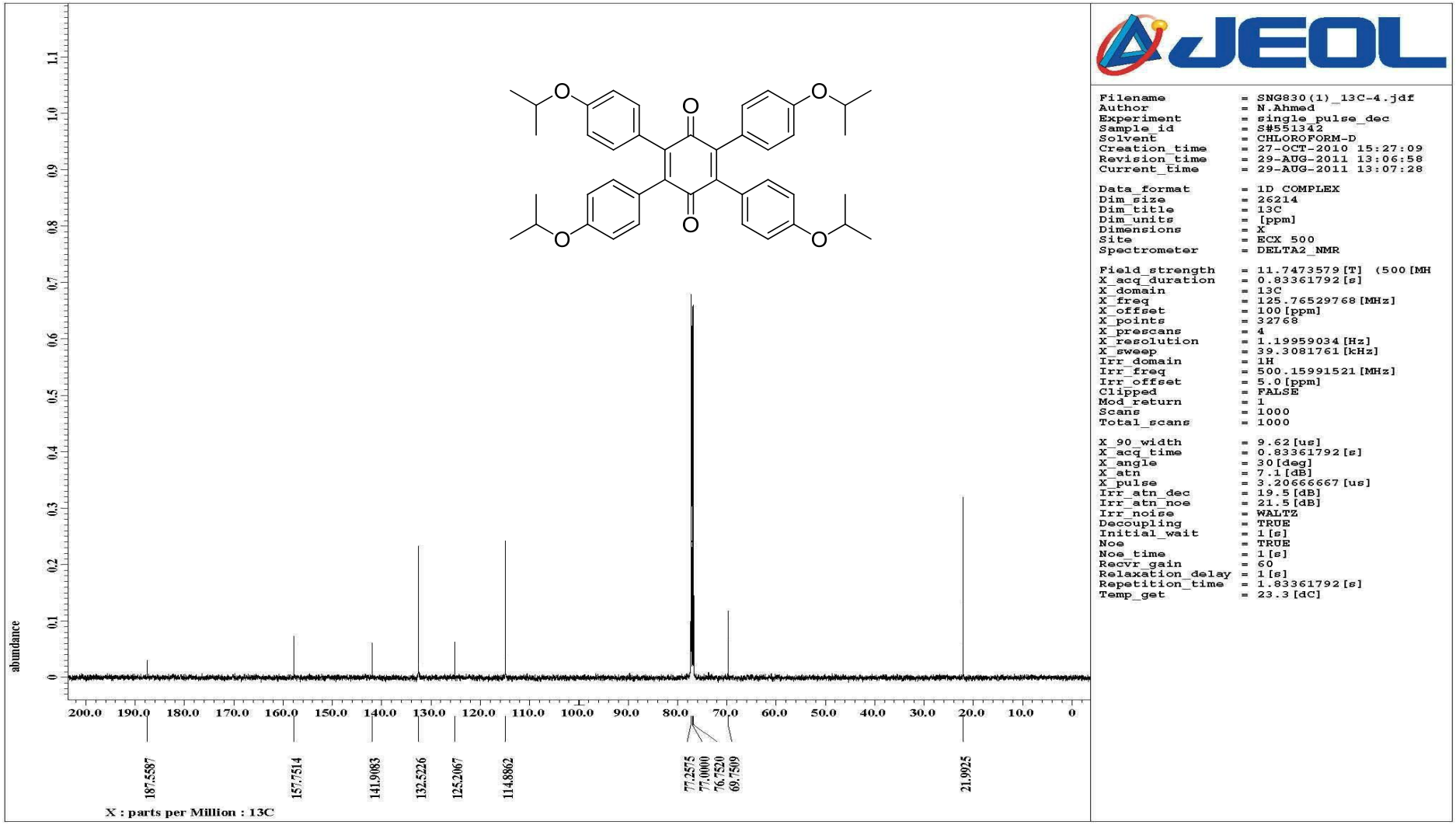
^{13}C NMR spectrum of 2,3,5,6-tetrakis(4-ethoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.2**)



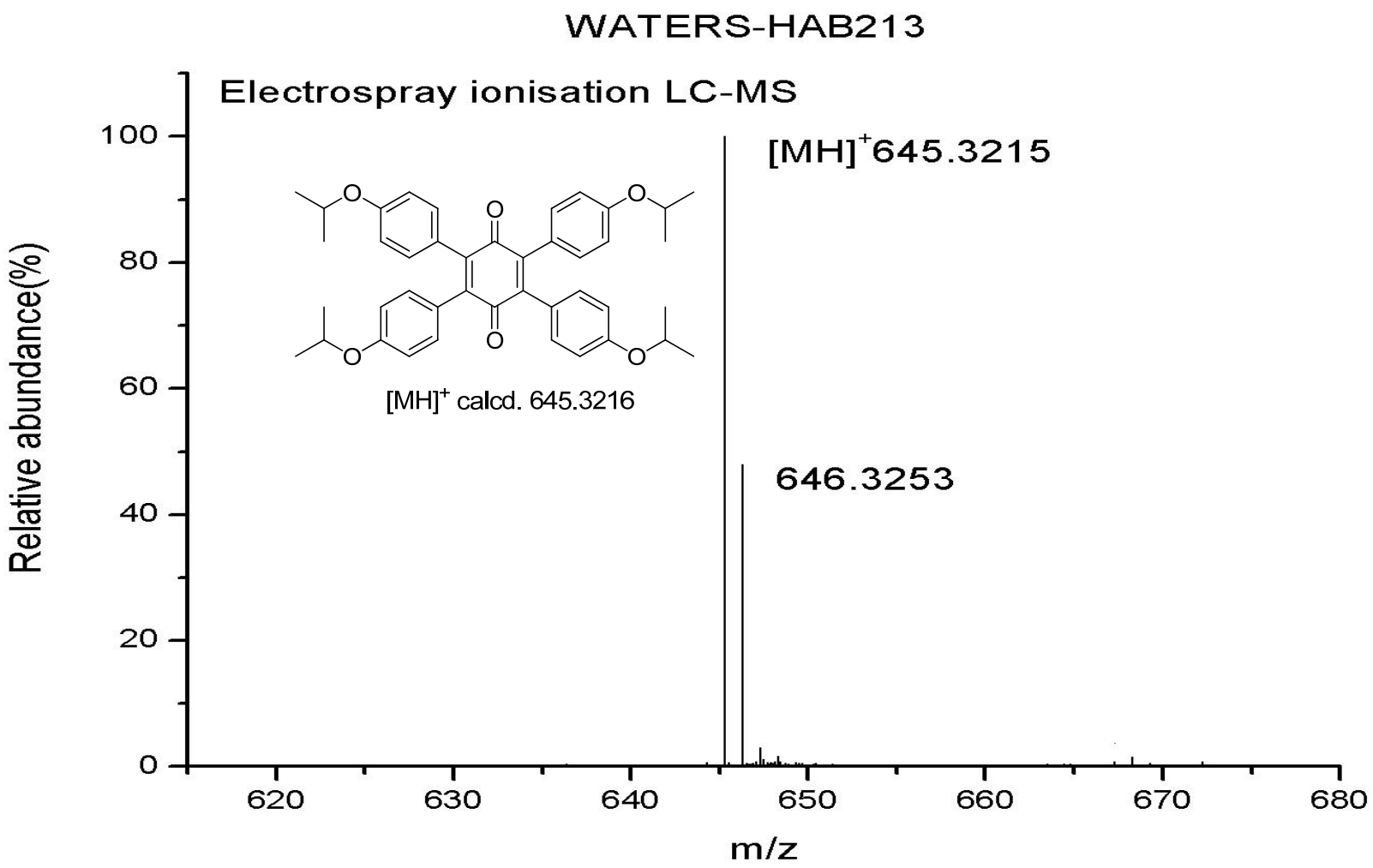
HRMS spectrum of 2,3,5,6-tetrakis(4-ethoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.2**)



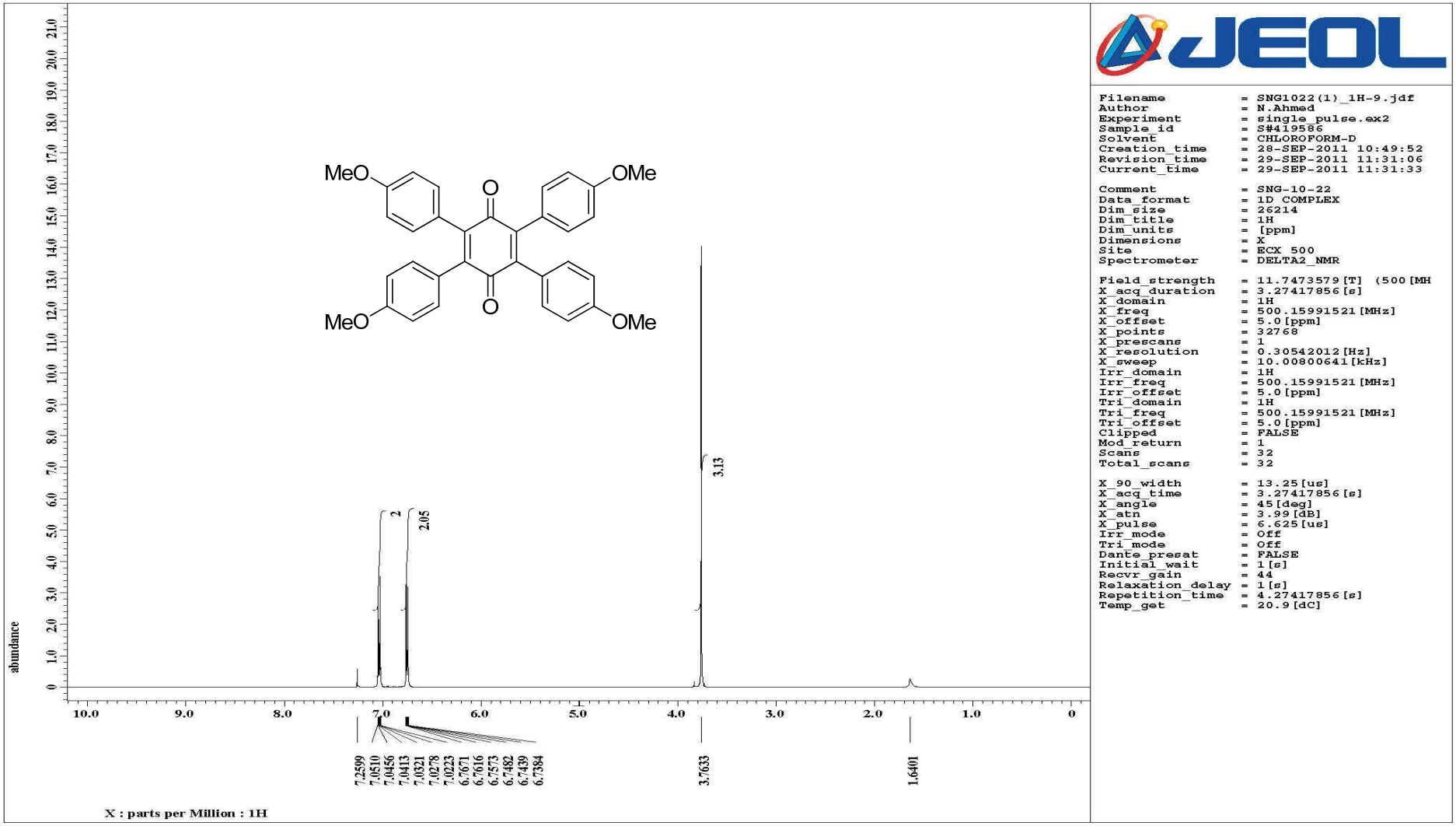
^{1}H NMR spectrum of 2,3,5,6-tetrakis(4-isopropoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.3**)



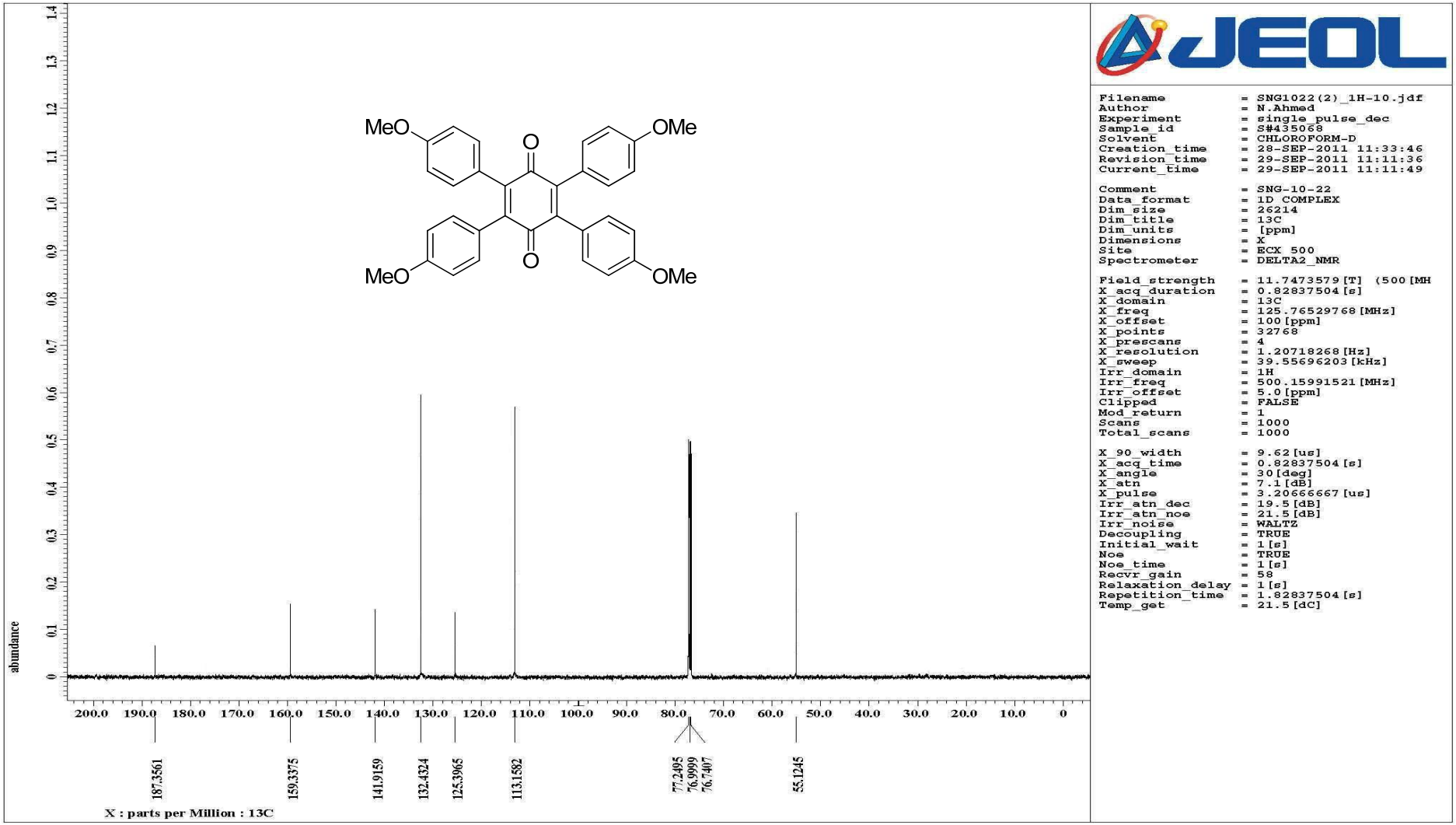
^{13}C NMR spectrum of 2,3,5,6-tetrakis(4-isopropoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.3**)



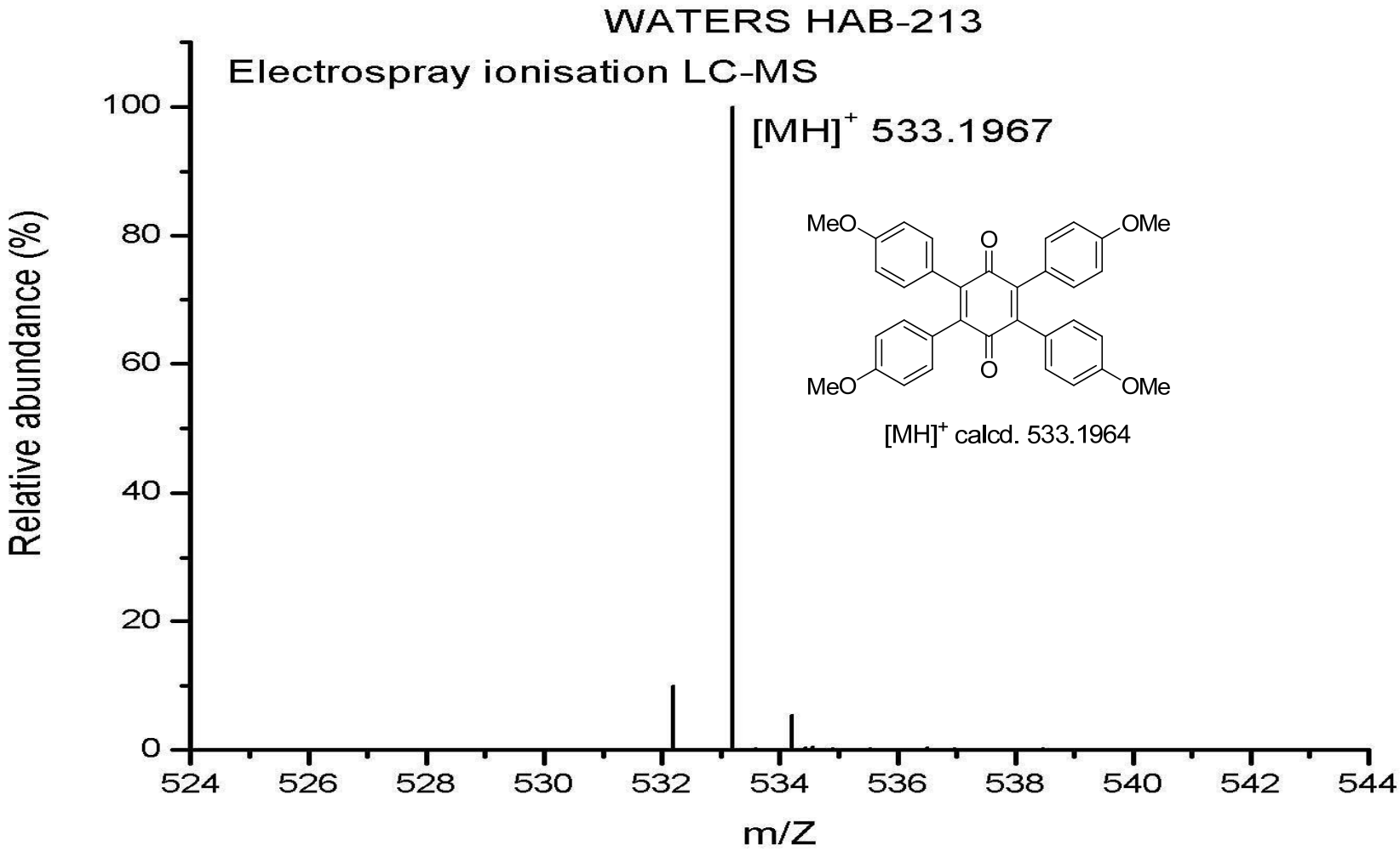
HRMS spectrum of 2,3,5,6-tetrakis(4-isopropoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.3**)



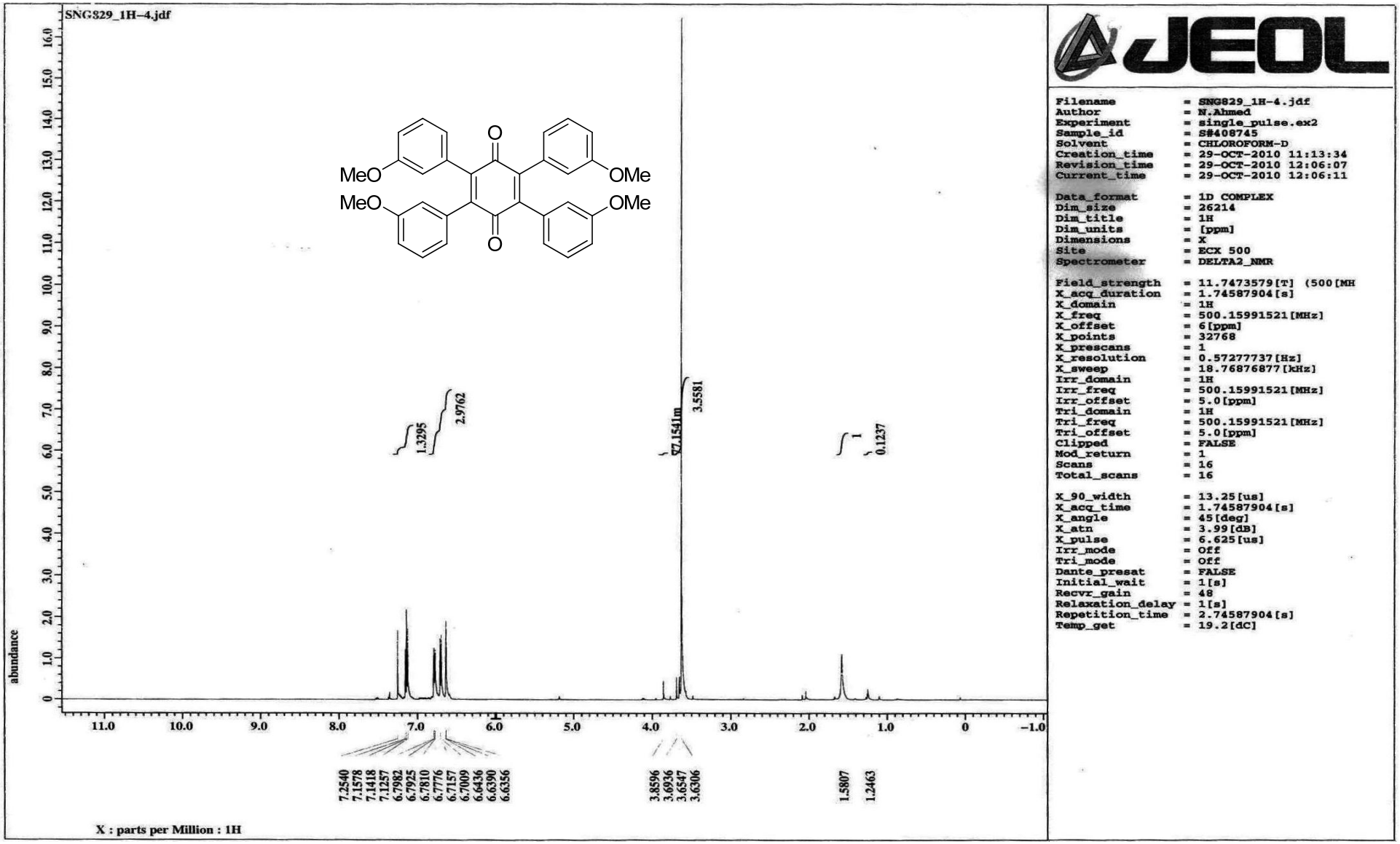
^{1}H NMR spectrum of 2,3,5,6-tetrakis(4-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.4**)



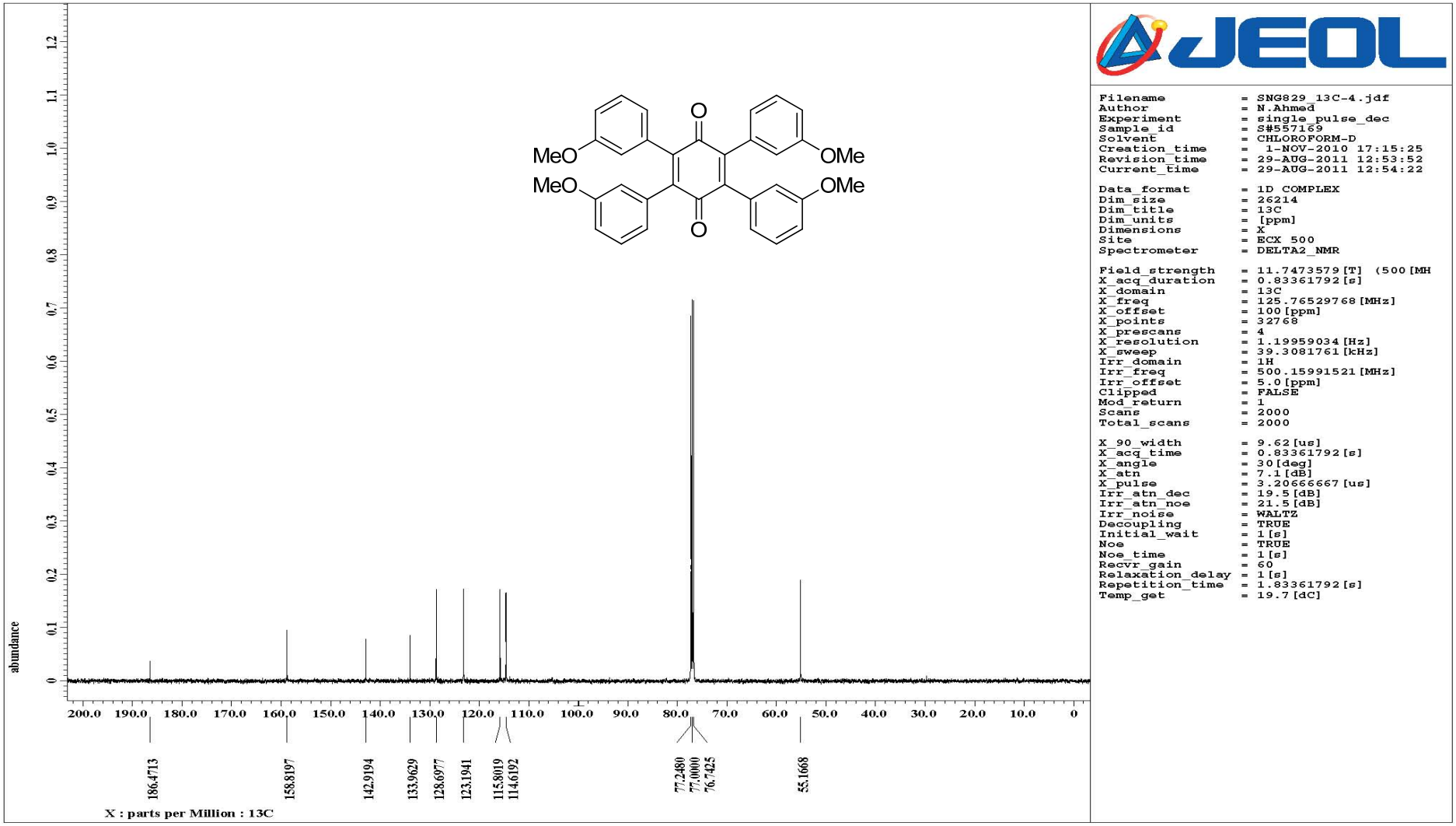
^{13}C NMR spectrum of 2,3,5,6-tetrakis(4-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.4**)



HRMS spectrum of 2,3,5,6-tetrakis(4-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.4**)



^{1}H NMR spectrum of 2,3,5,6-tetrakis(3-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.5**)

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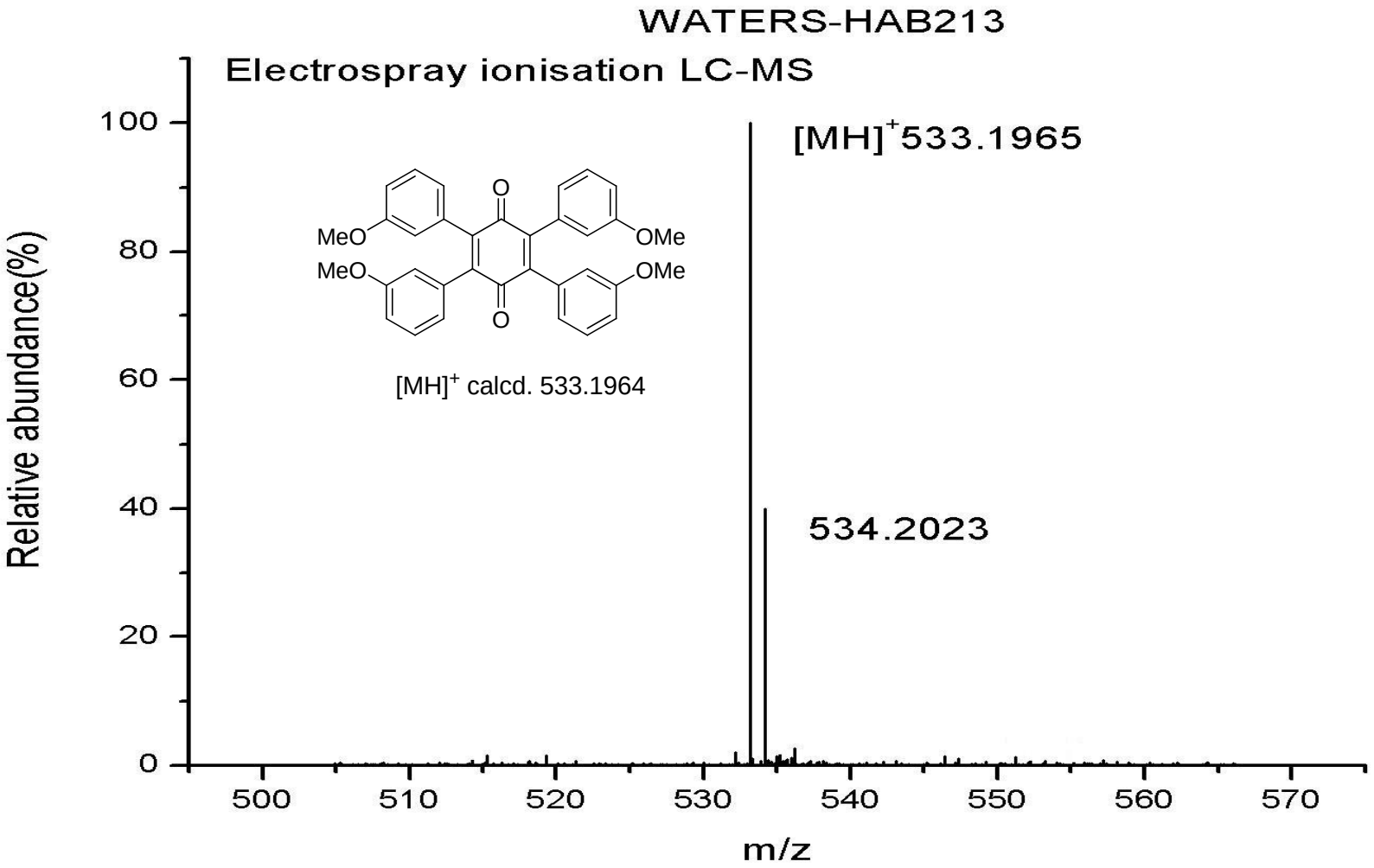
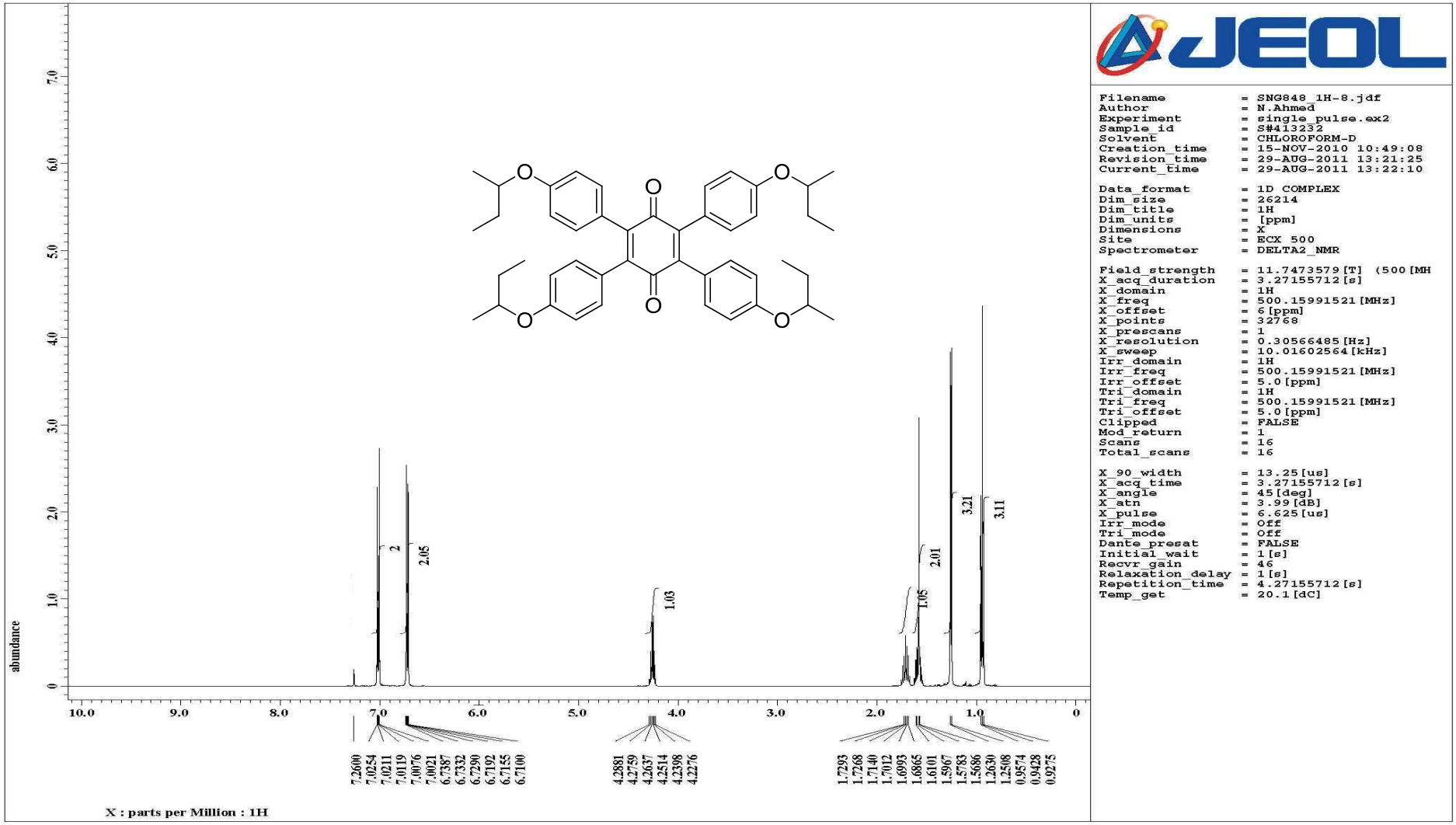
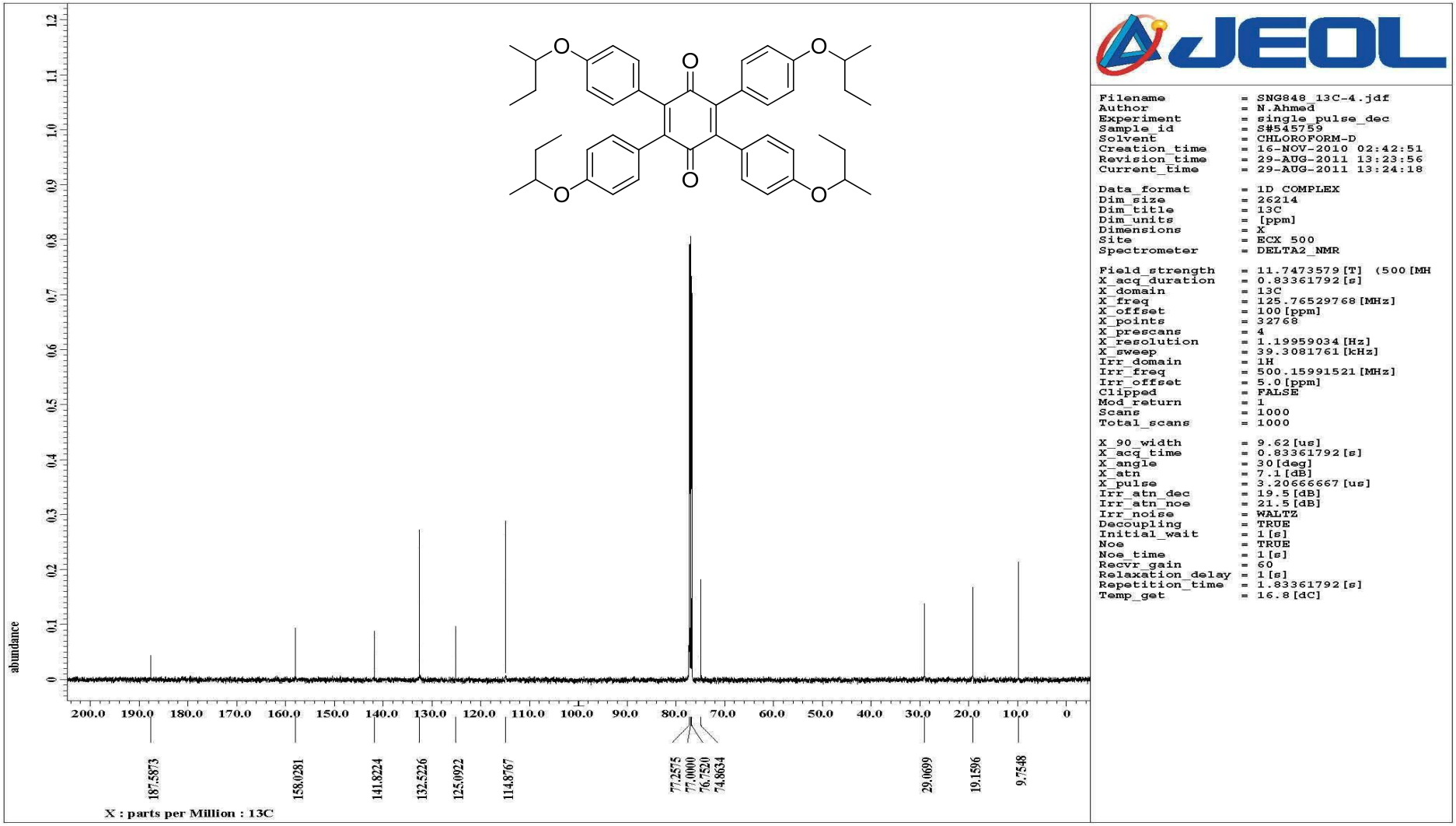
^{13}C NMR spectrum of 2,3,5,6-tetrakis(3-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.5**)



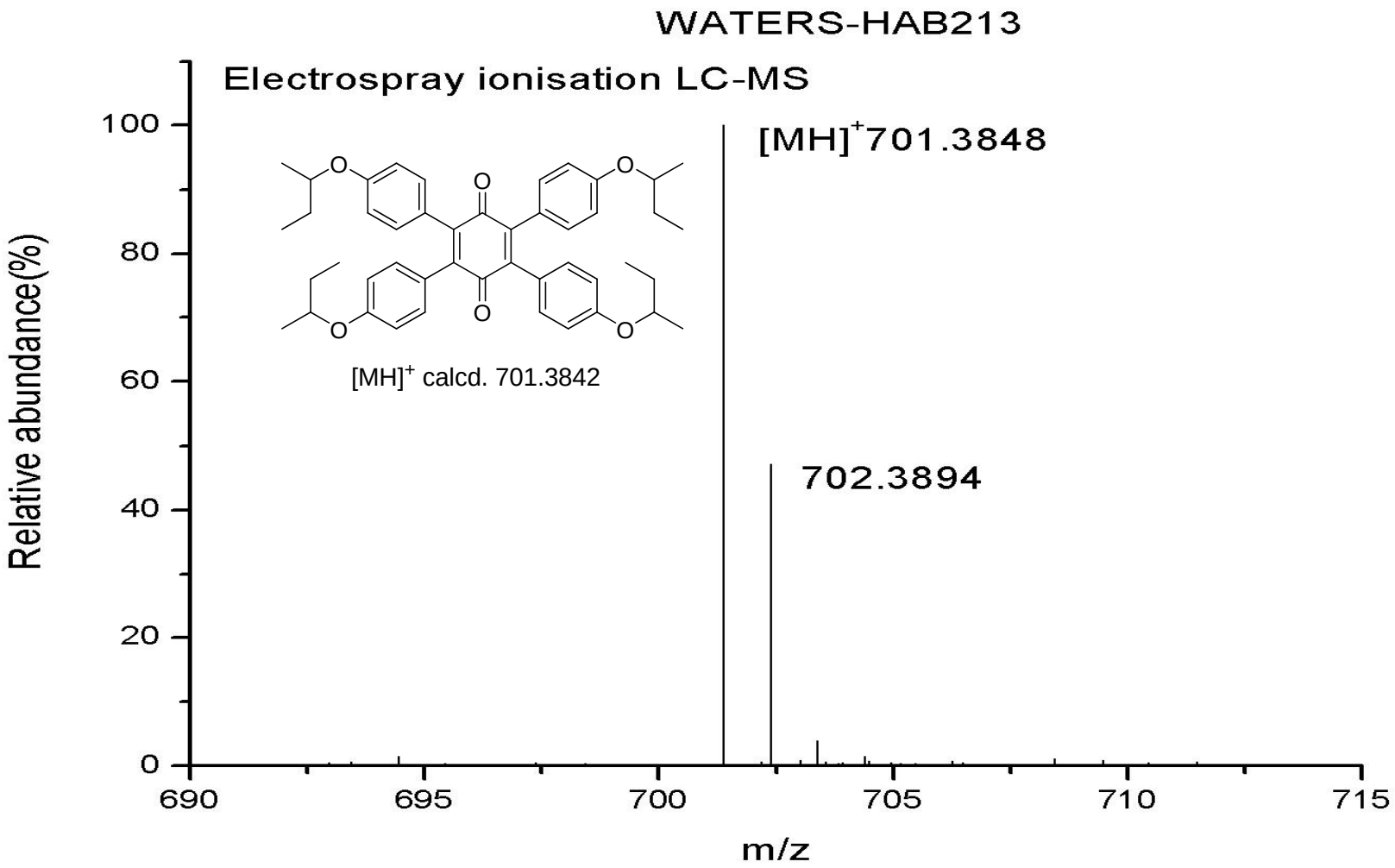
HRMS spectrum of 2,3,5,6-tetrakis(3-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.5**)



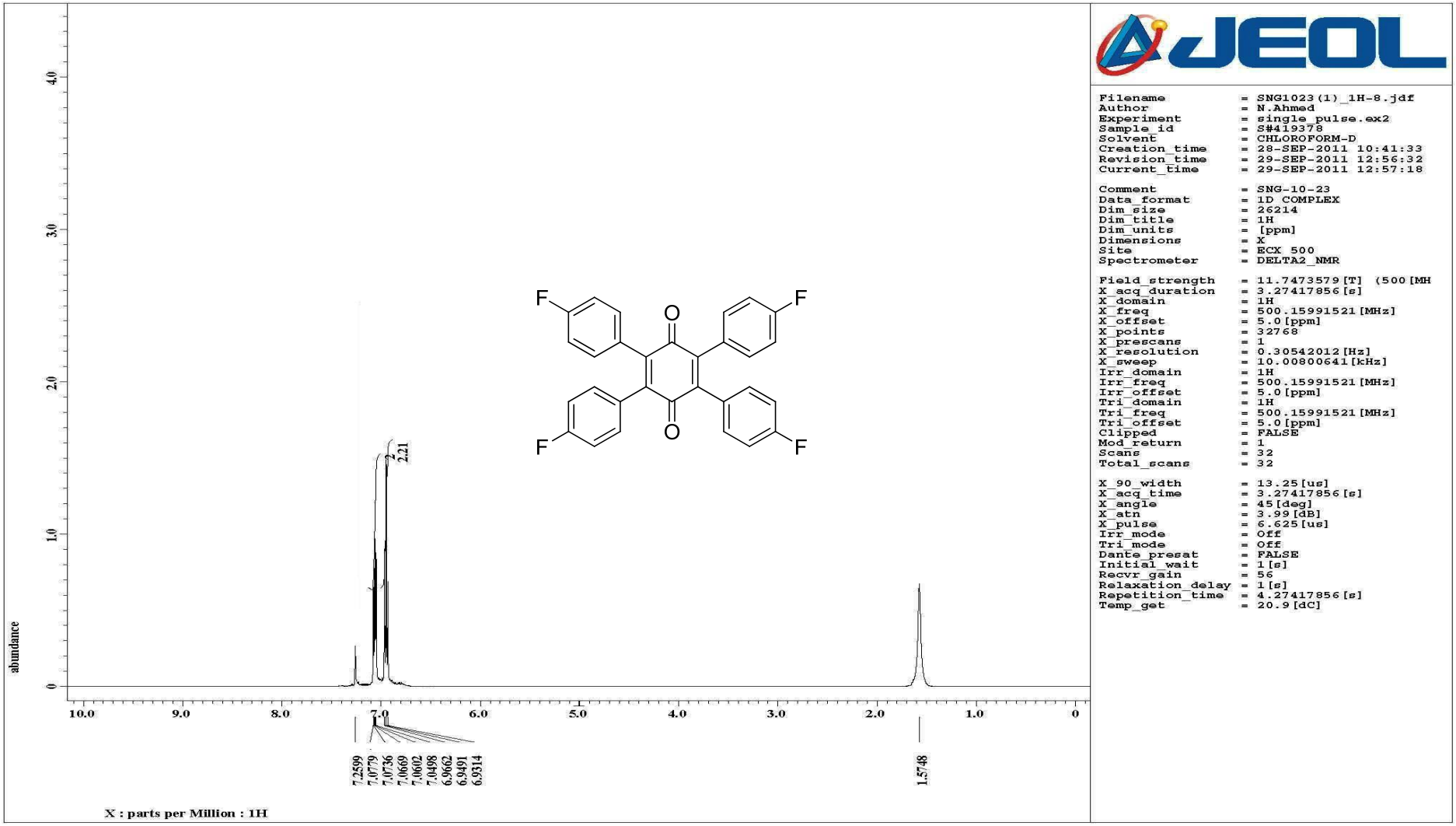
^{1}H NMR spectrum of 2,3,5,6-tetrakis(4-*sec*-butoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.6**)



^{13}C NMR spectrum of 2,3,5,6-tetrakis(4-*sec*-butoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.6**)



HRMS spectrum of 2,3,5,6-tetrakis(4-*sec*-butoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.6**)

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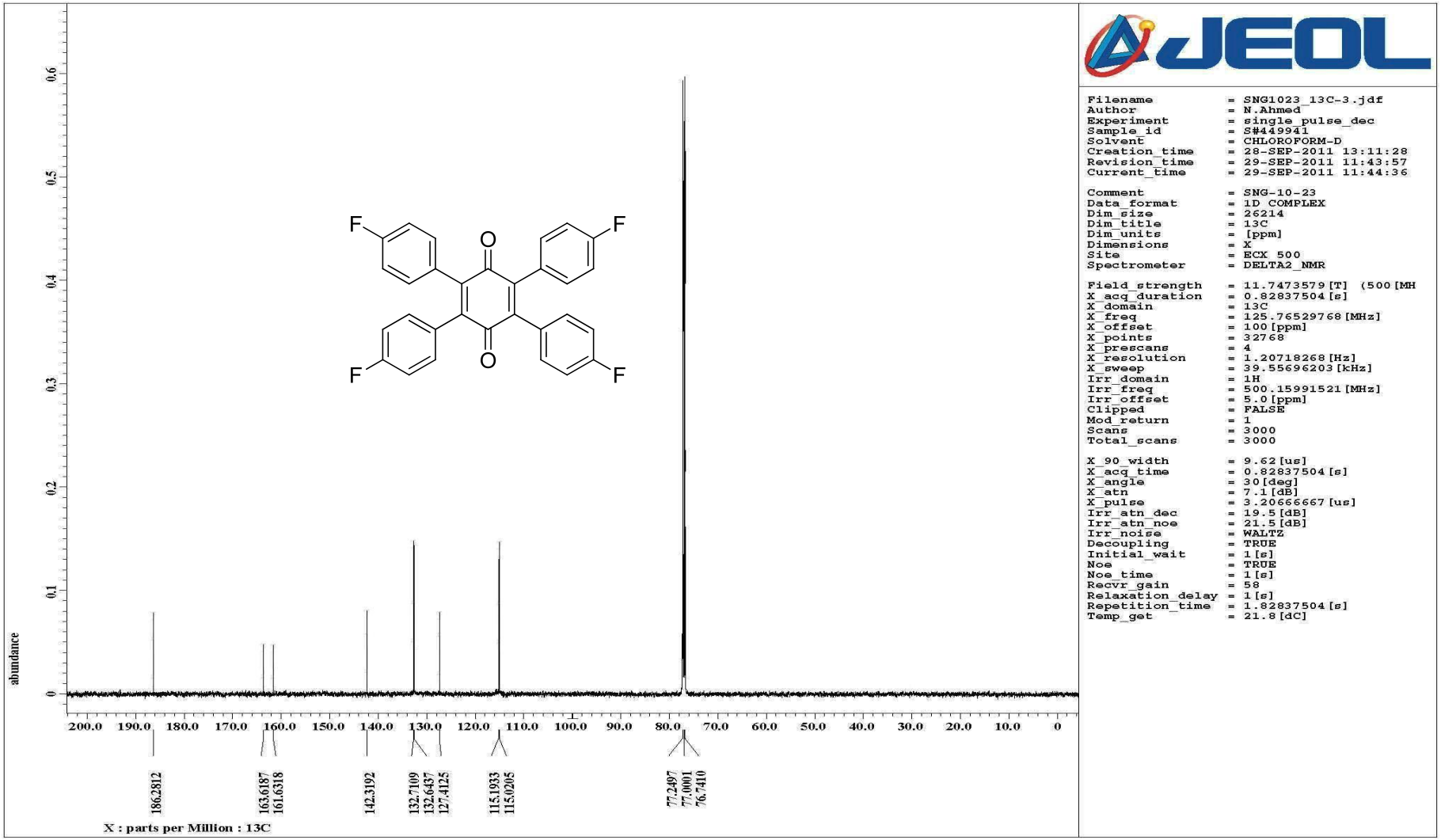
^{1}H NMR spectrum of 2,3,5,6-tetrakis(4-fluorophenyl)cyclohexa-2,5-diene-1,4-dione (**5.7**)

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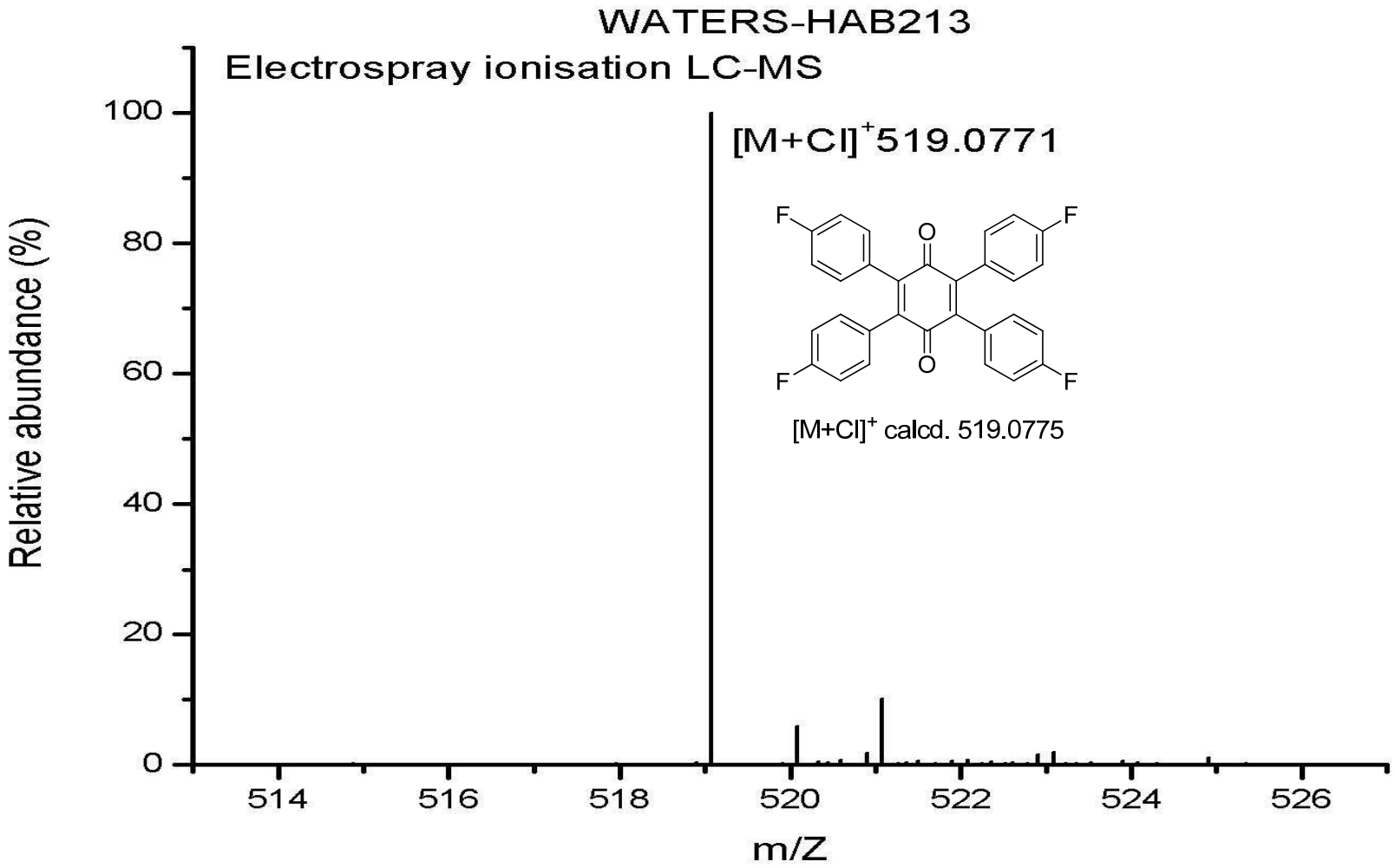
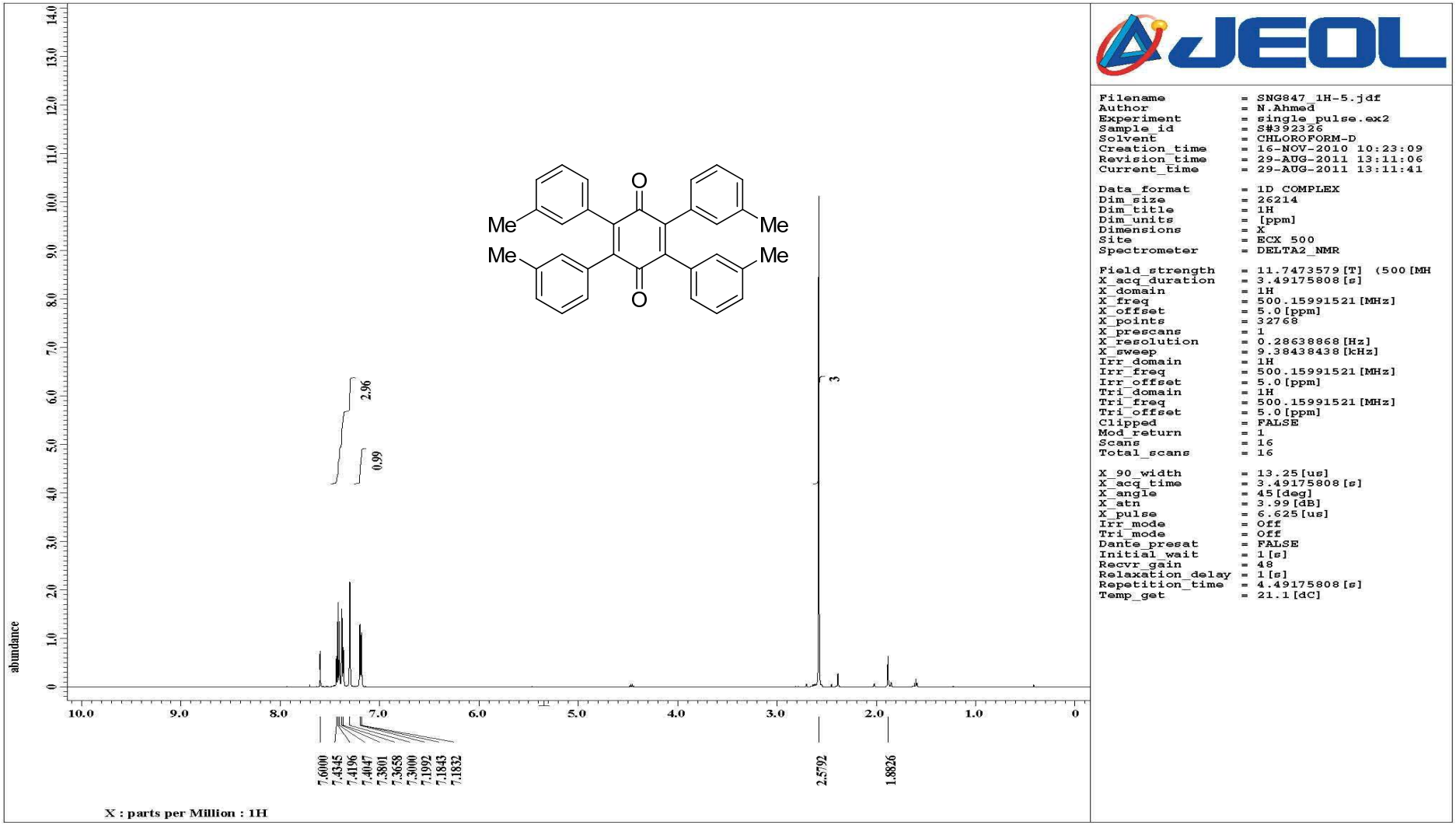
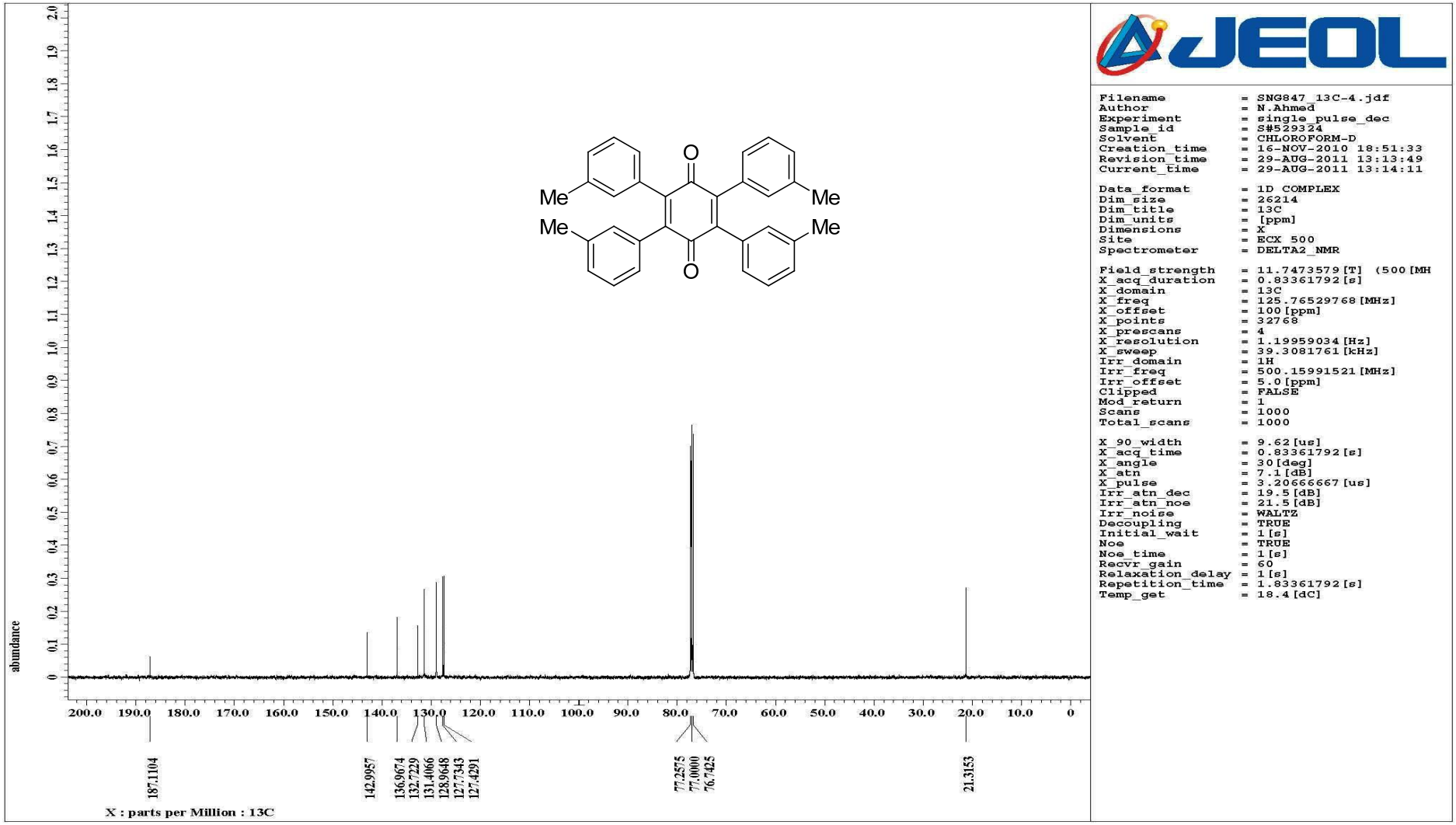
^{13}C NMR spectrum of 2,3,5,6-tetrakis(4-fluorophenyl)cyclohexa-2,5-diene-1,4-dione (**5.7**)



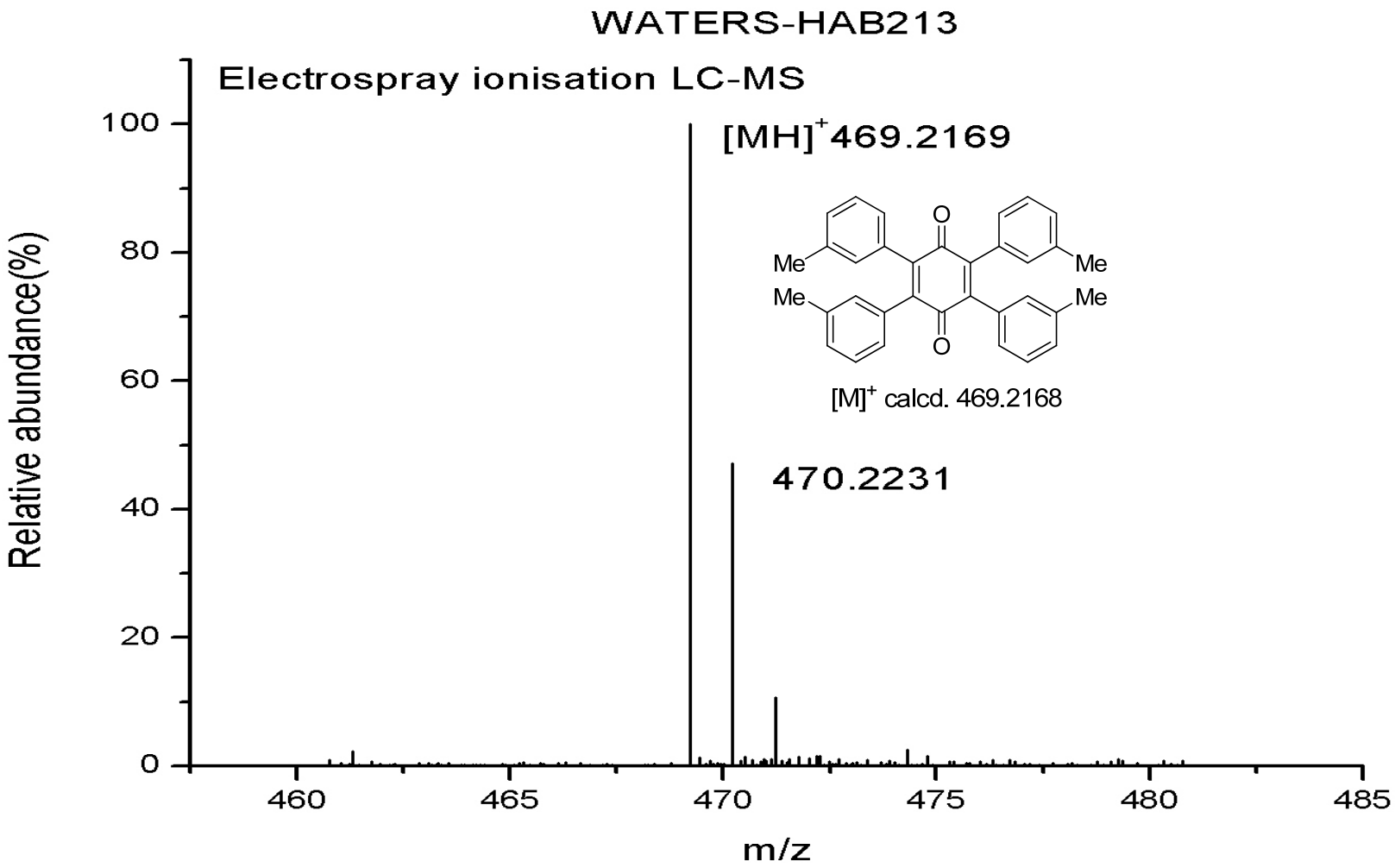
HRMS spectrum of 2,3,5,6-tetrakis(4-fluorophenyl)cyclohexa-2,5-diene-1,4-dione (**5.7**)



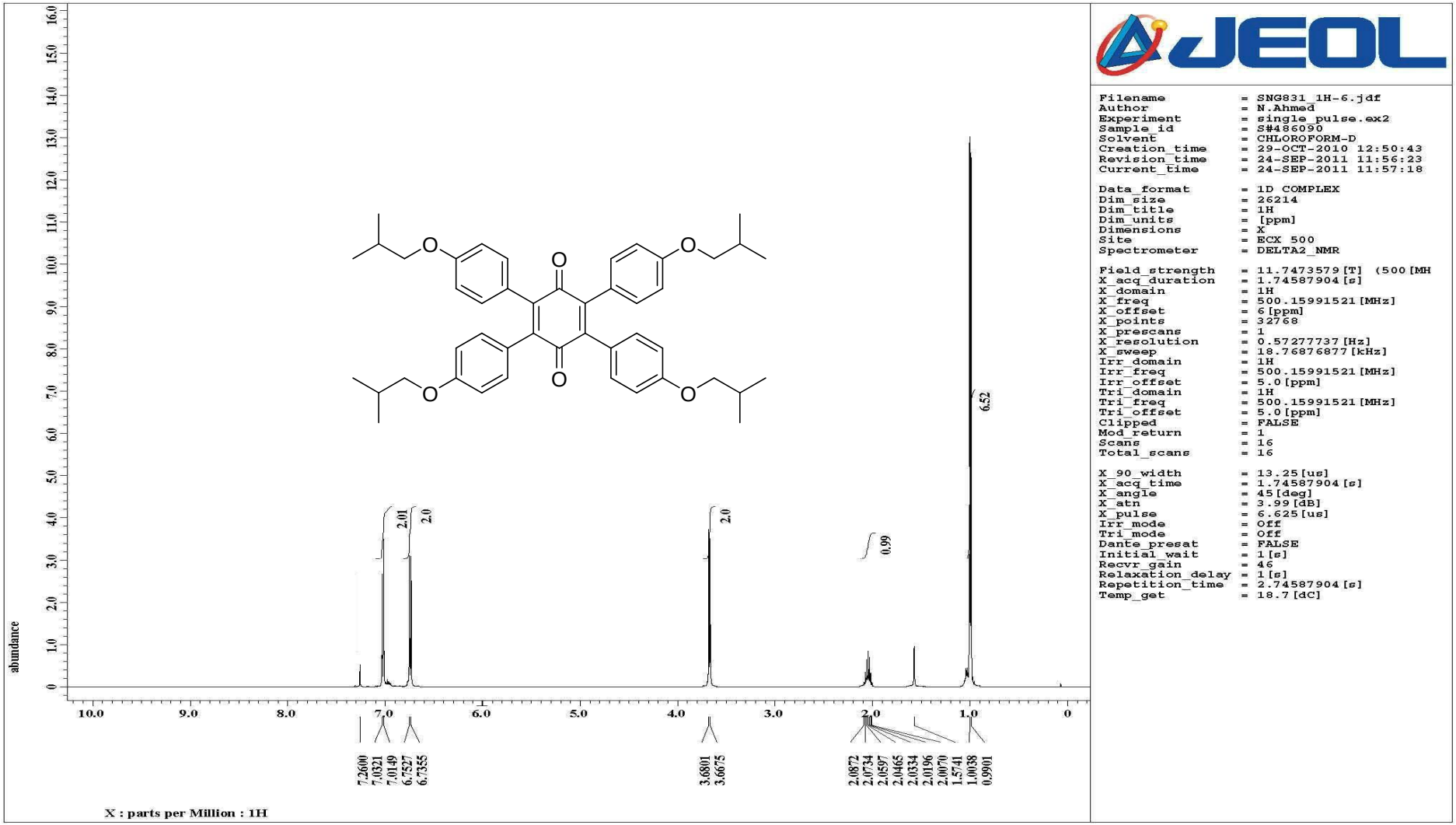
^{1}H NMR spectrum of 2,3,5,6-tetra 3-tolylcyclohexa-2,5-diene-1,4-dione (**5.8**)



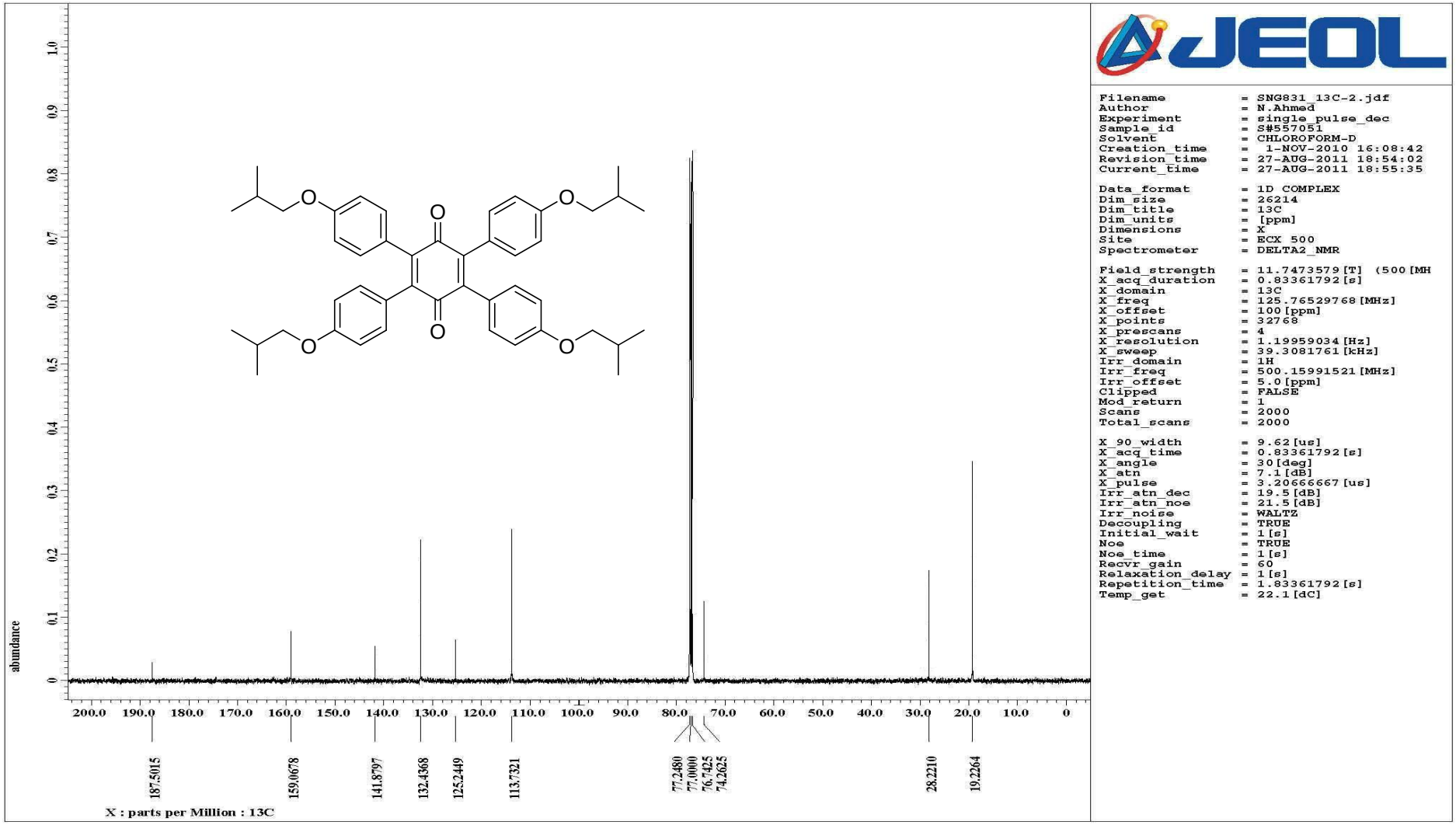
^{13}C NMR spectrum of 2,3,5,6-tetra 3-tolylcyclohexa-2,5-diene-1,4-dione (**5.8**)



HRMS spectrum of 2,3,5,6-tetra 3-tolylcyclohexa-2,5-diene-1,4-dione (**5.8**)



^{1}H NMR spectrum of 2,3,5,6-tetrakis(4-isobutoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.9**)



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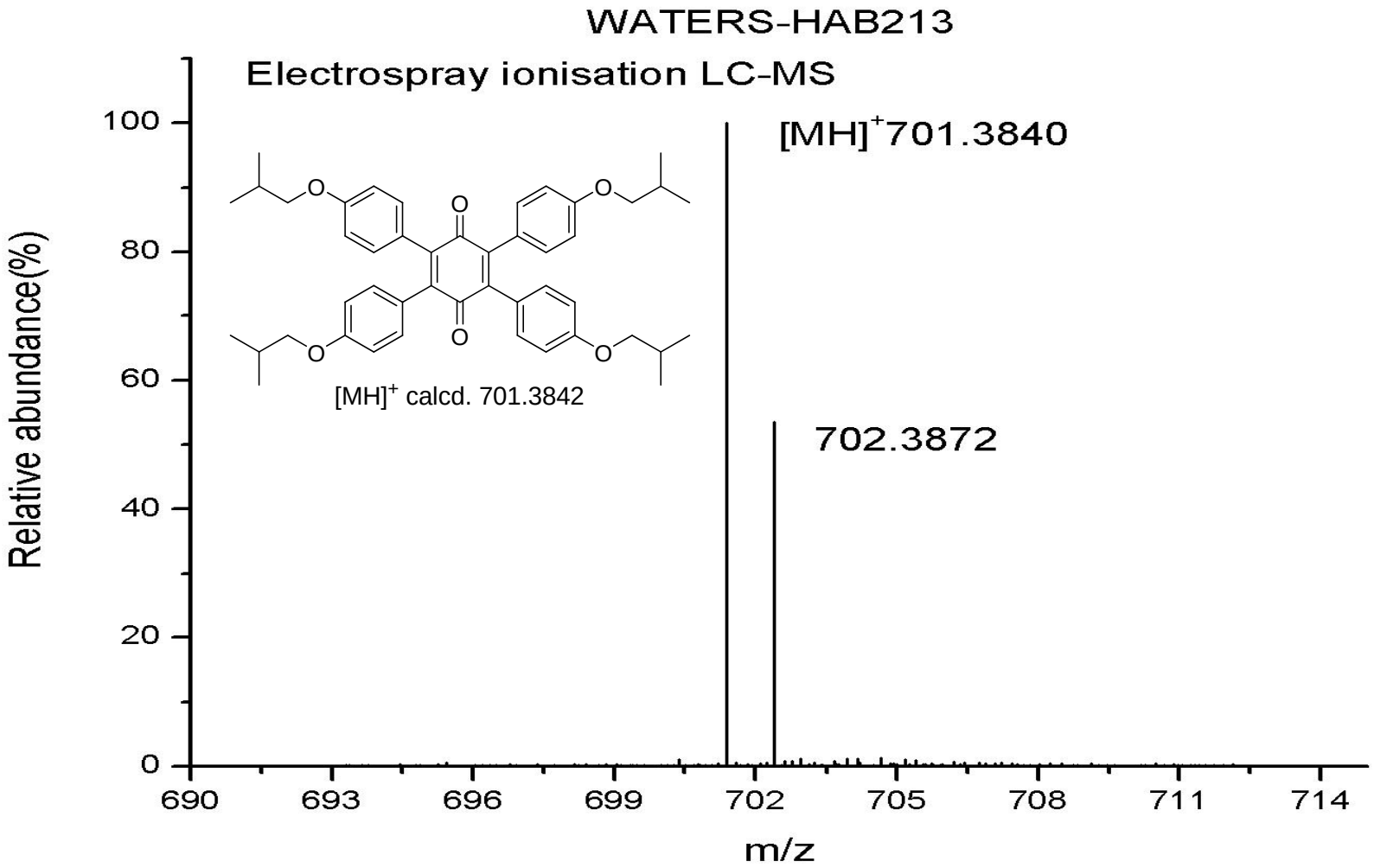

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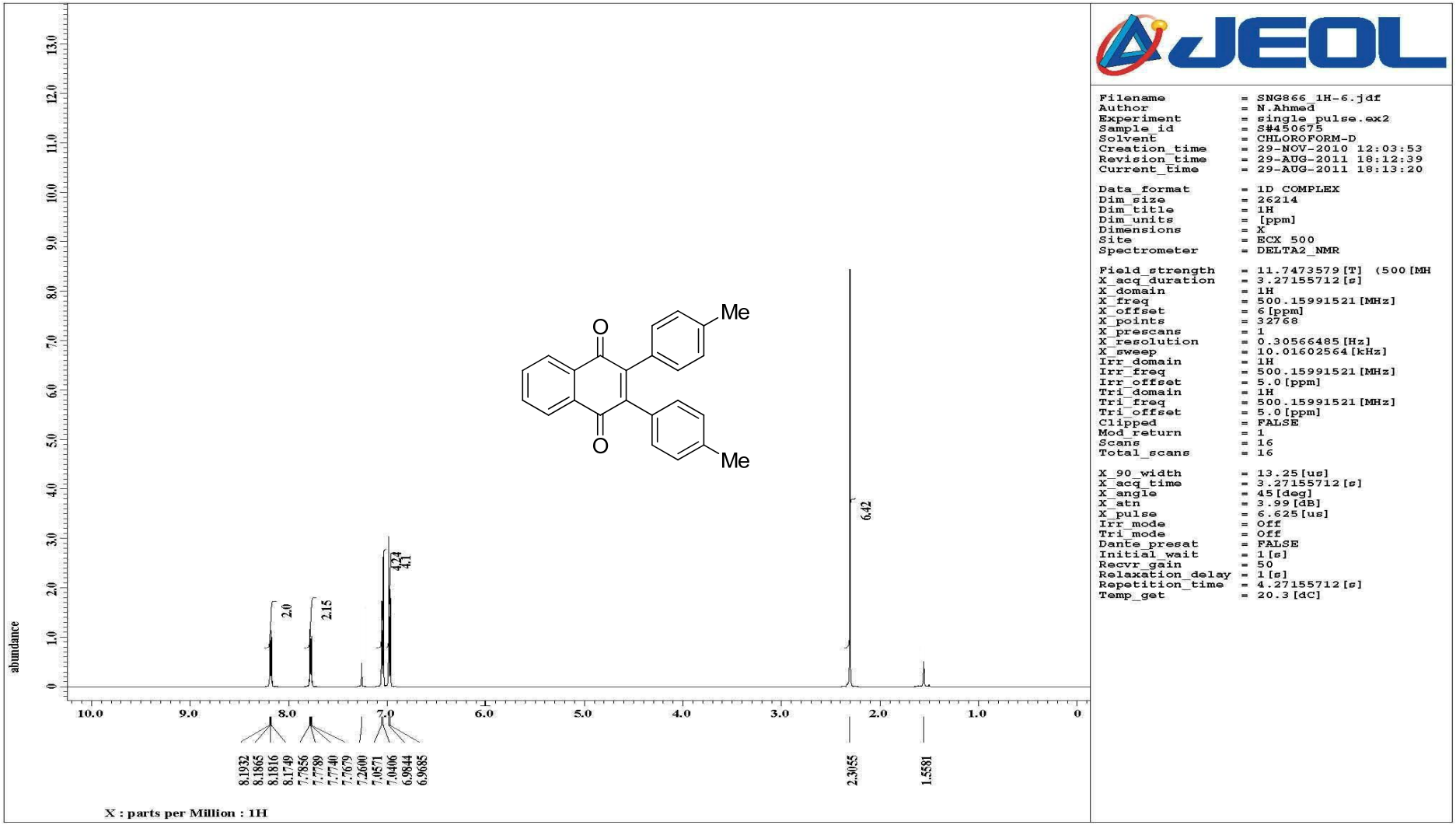
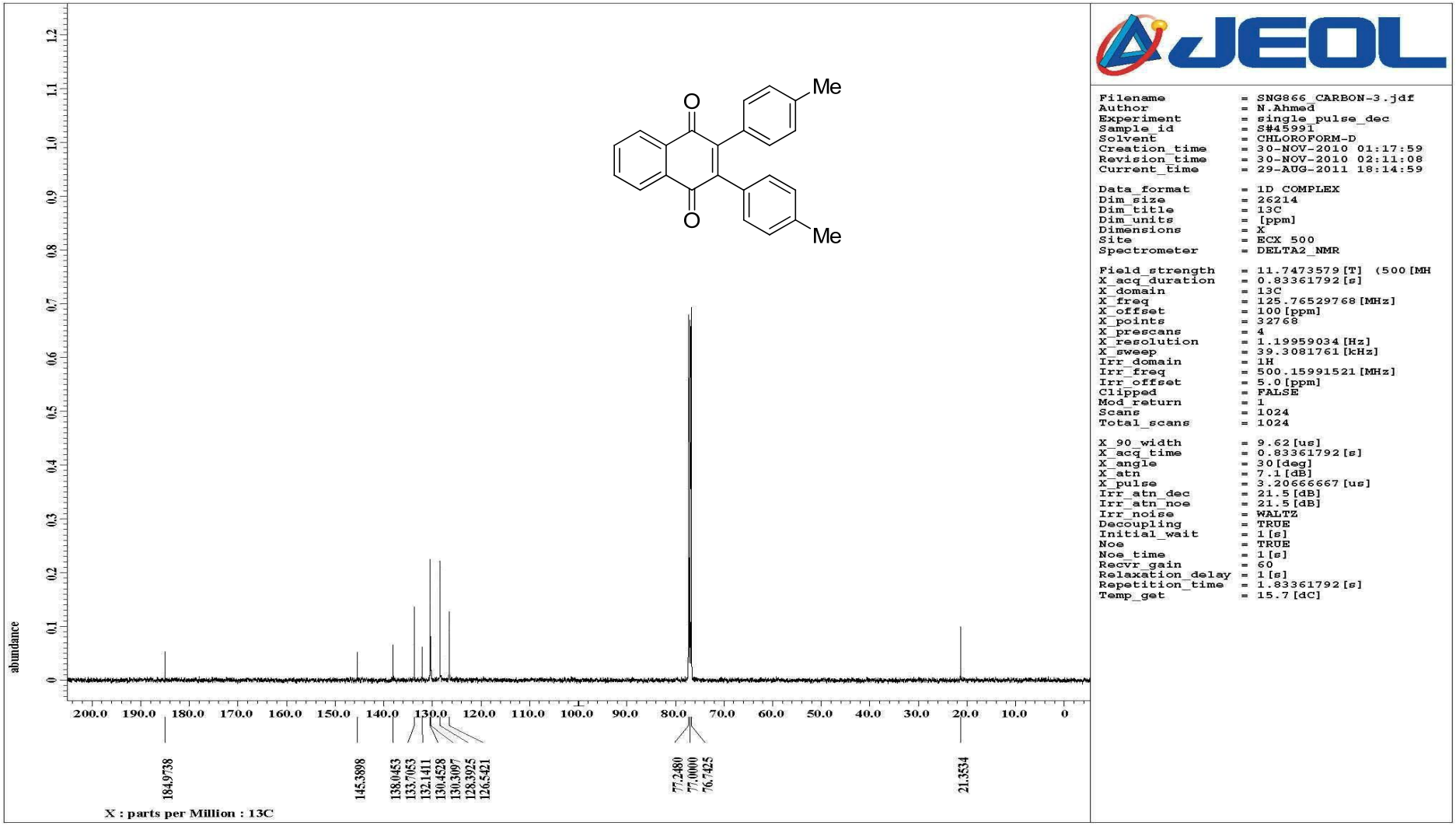
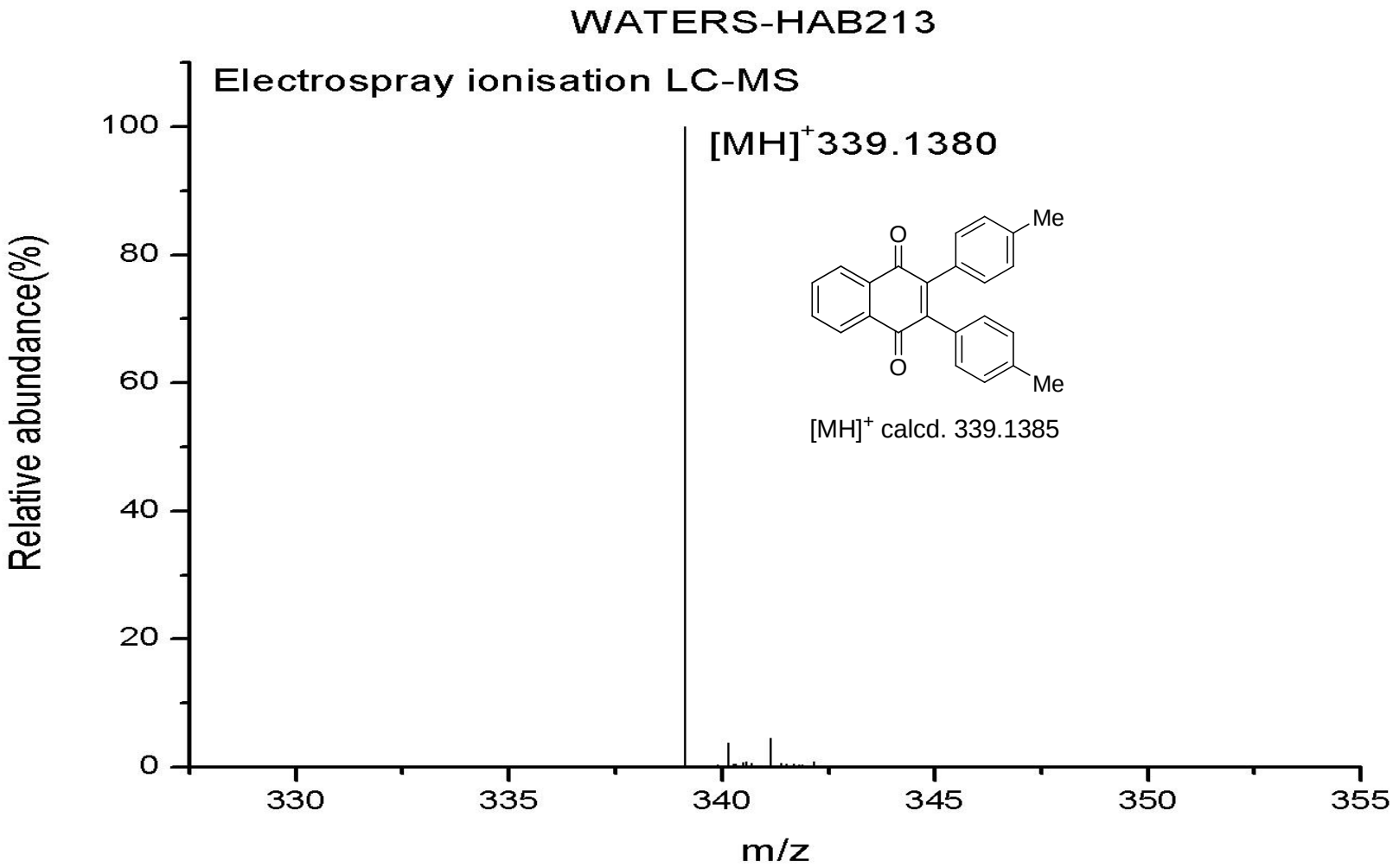


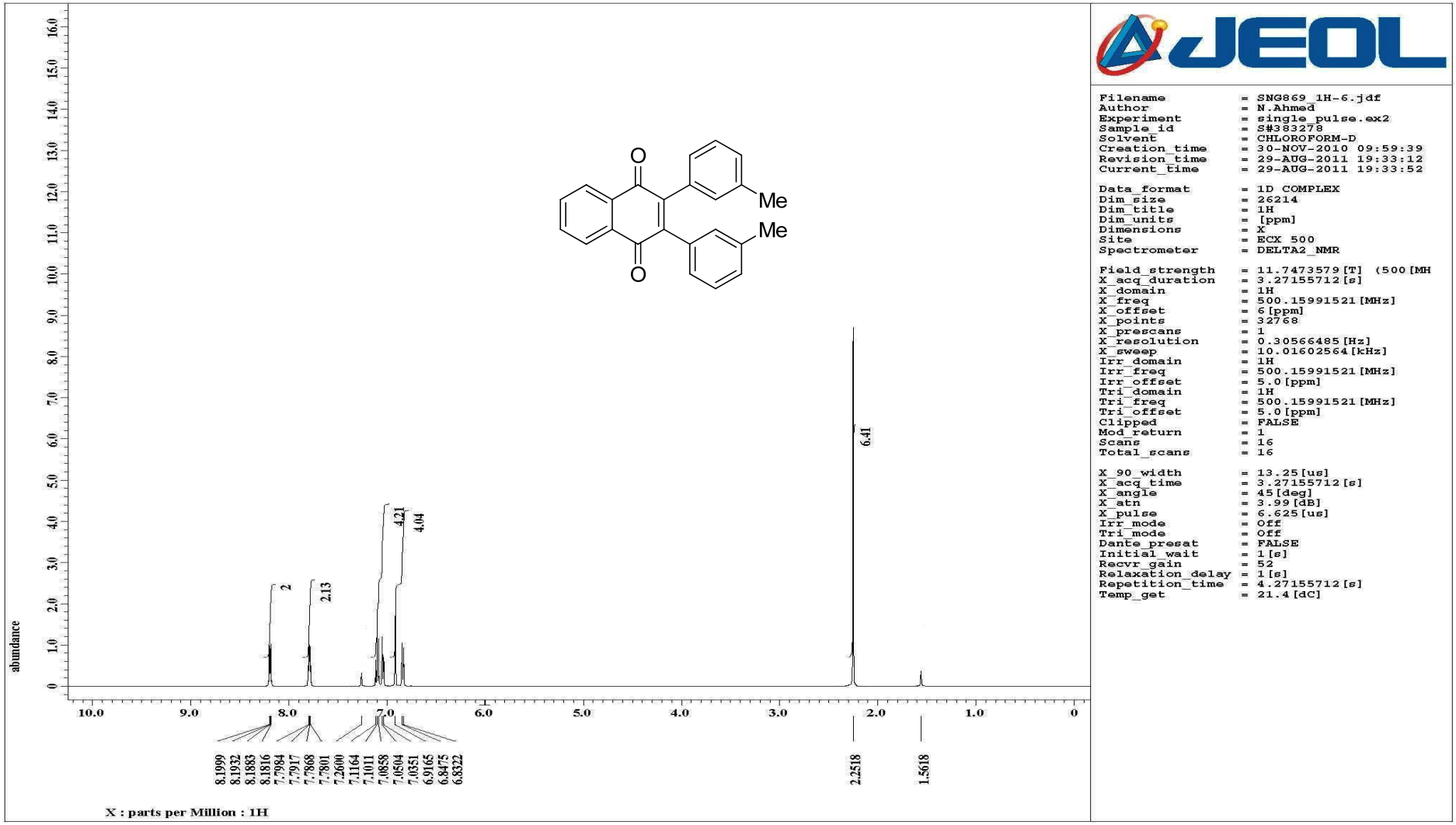
^{1}H NMR spectrum of 2,3-di-4-tolyl-1,4-naphthoquinone (**6.1**)



^{13}C NMR spectrum of 2,3-di-4-tolyl-1,4-naphthoquinone (**6.1**)



HRMS spectrum of 2,3-di-4-tolyl-1,4-naphthoquinone (**6.1**)



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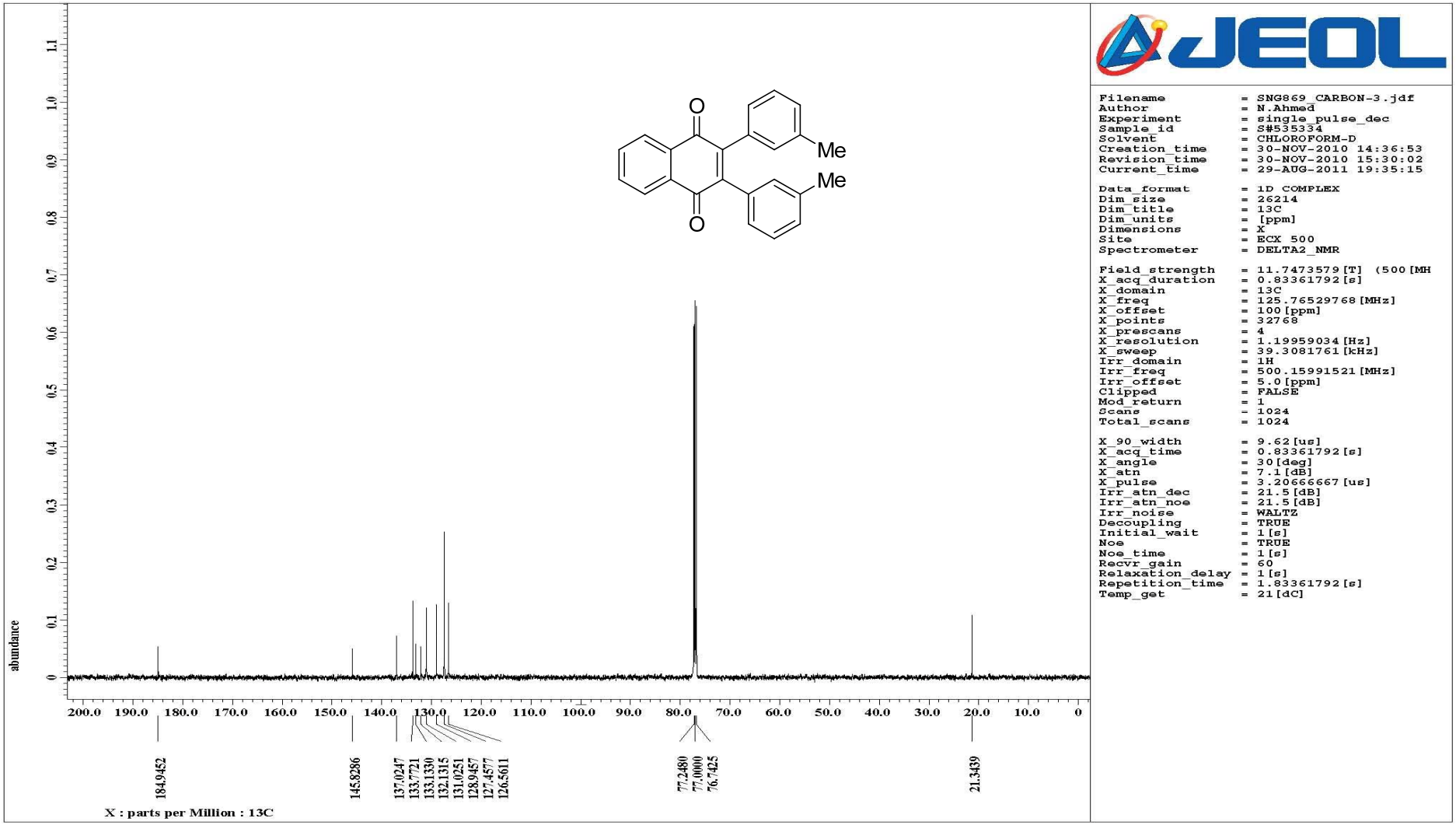
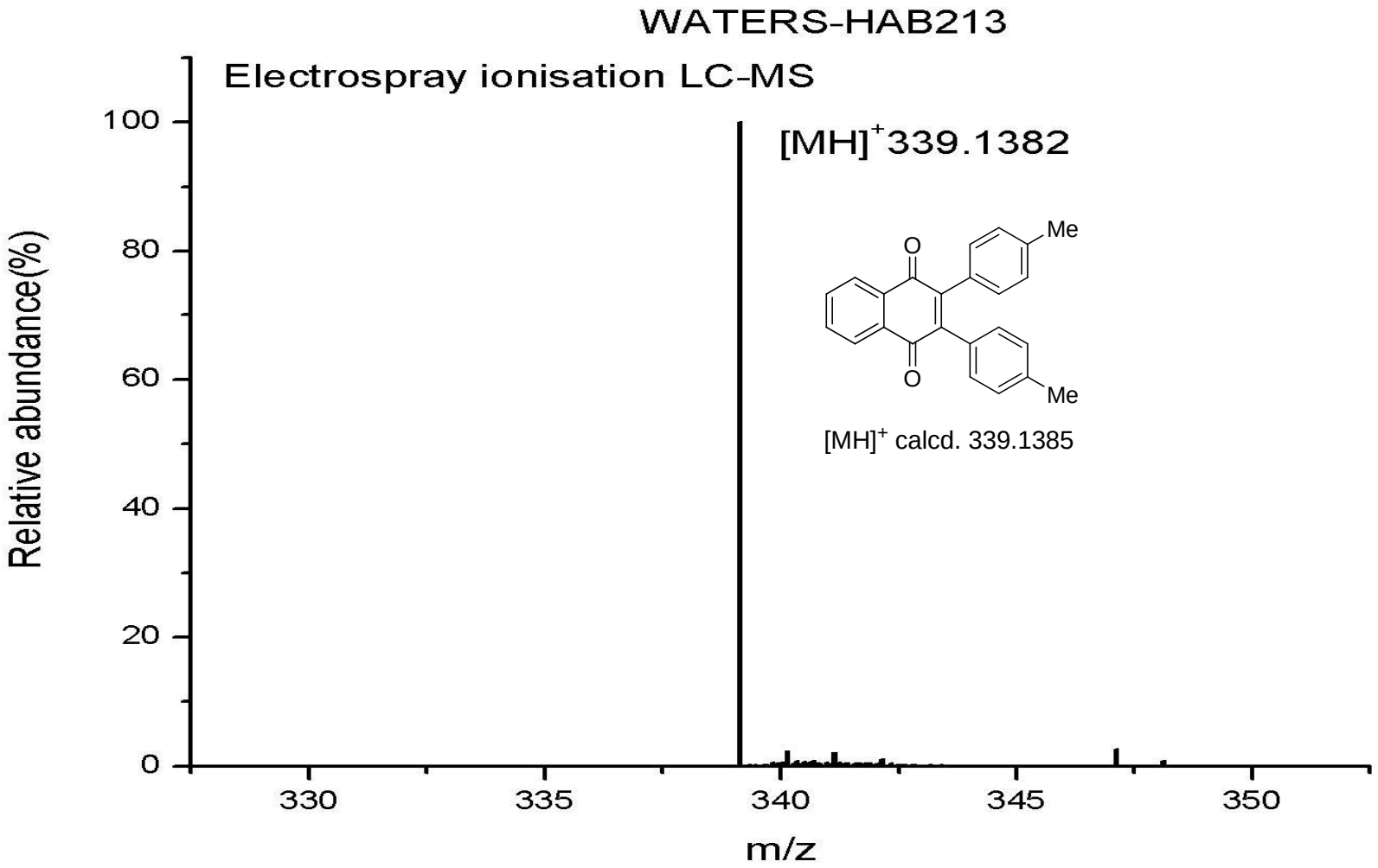
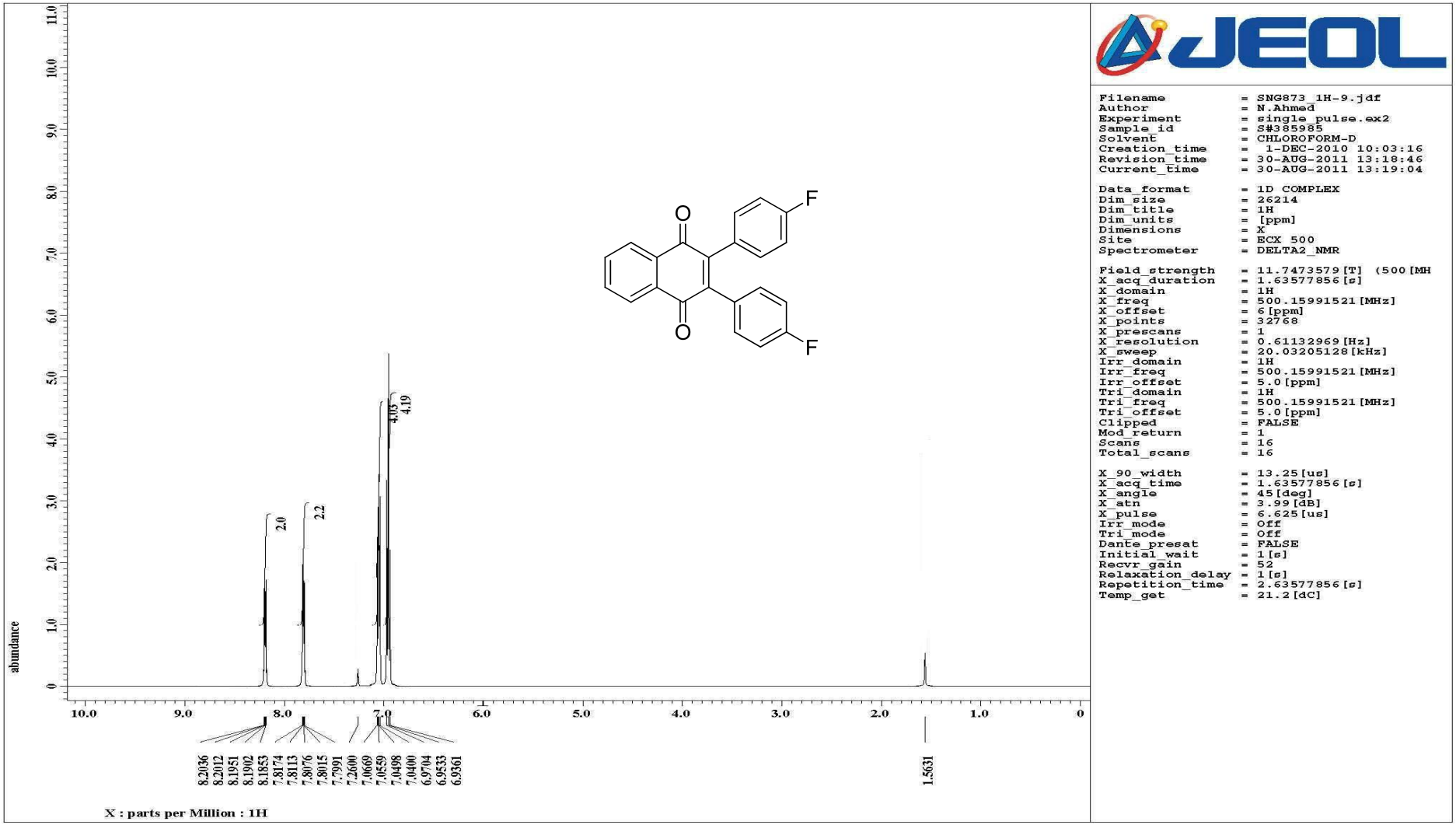


^{13}C NMR spectrum of 2,3-di-3-tolyl-1,4-naphthoquinone (**6.2**)



HRMS spectrum of 2,3-di-3-tolyl-1,4-naphthoquinone (**6.2**)



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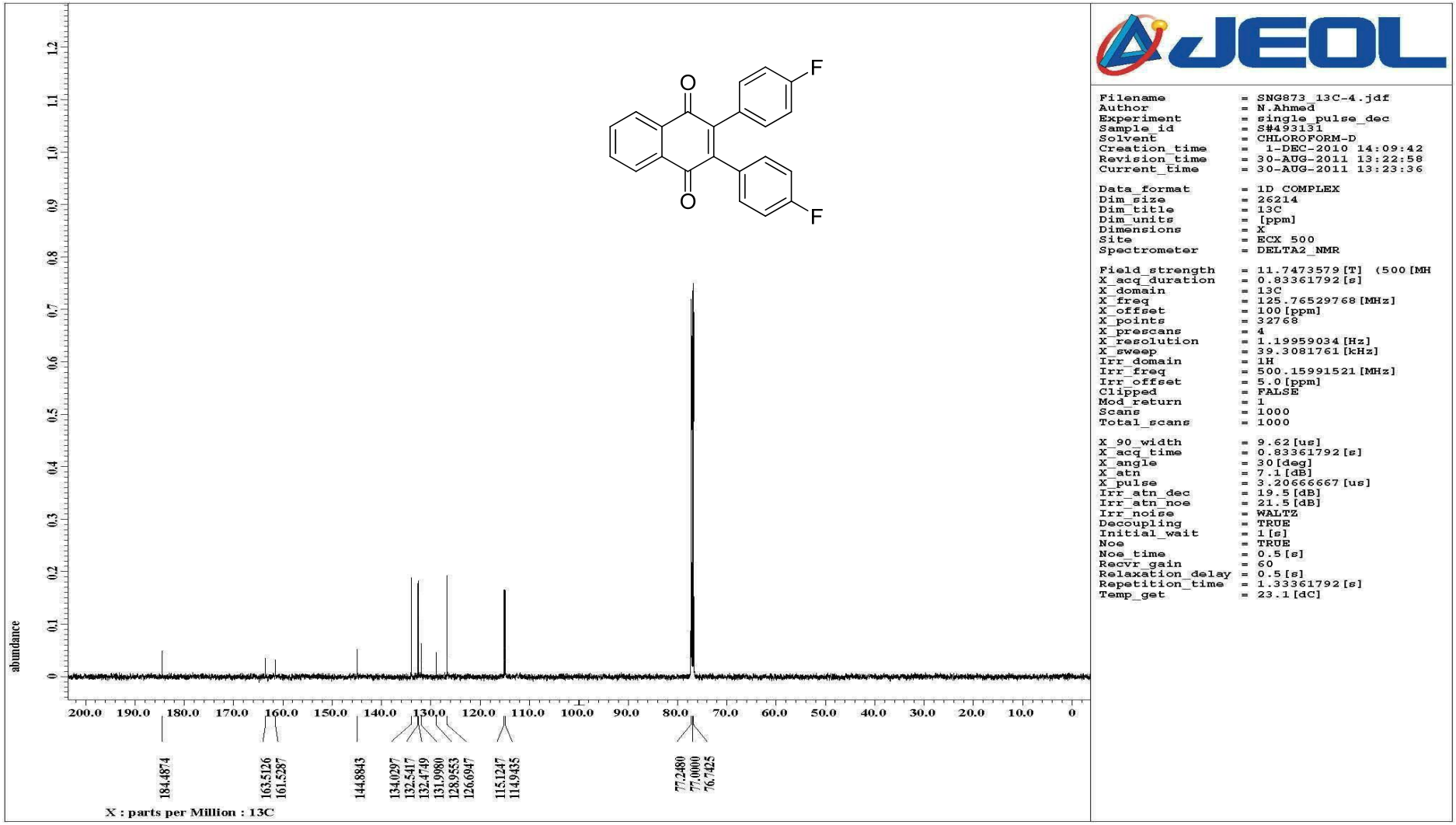

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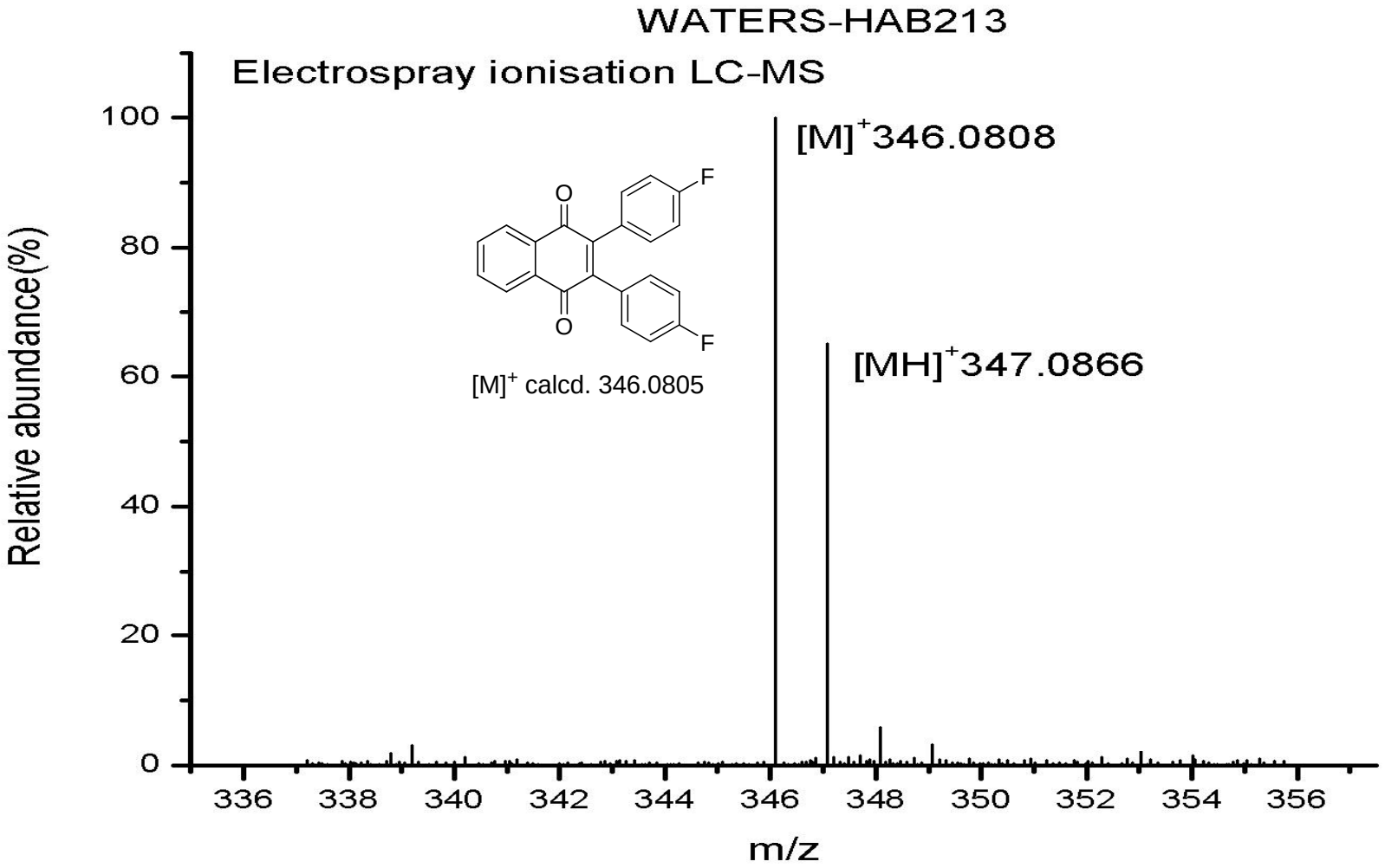
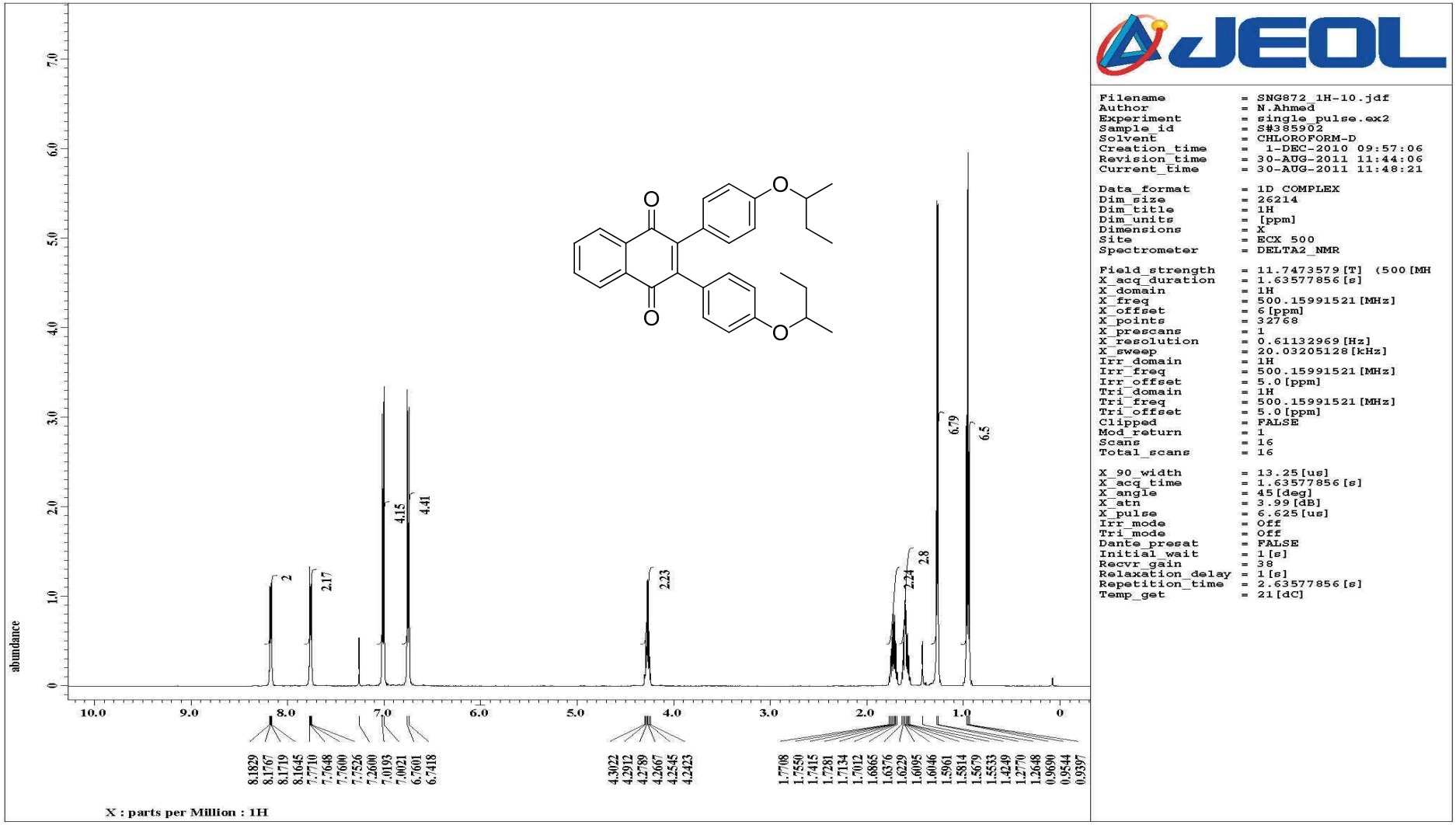


HRMS spectrum of 2,3-bis(4-fluorophenyl)-1,4-naphthoquinone (**6.3**)



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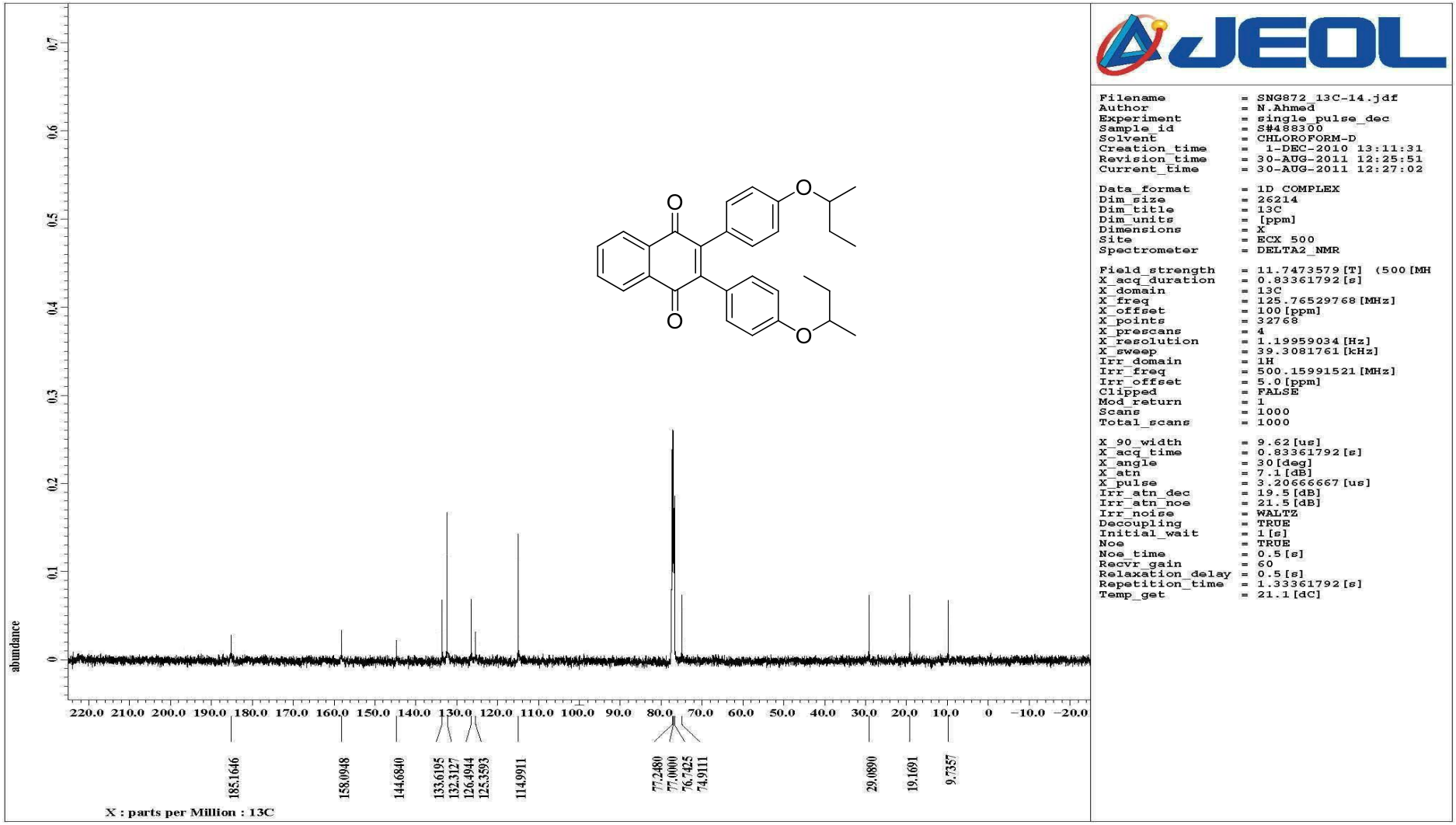


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Scans             = 1000
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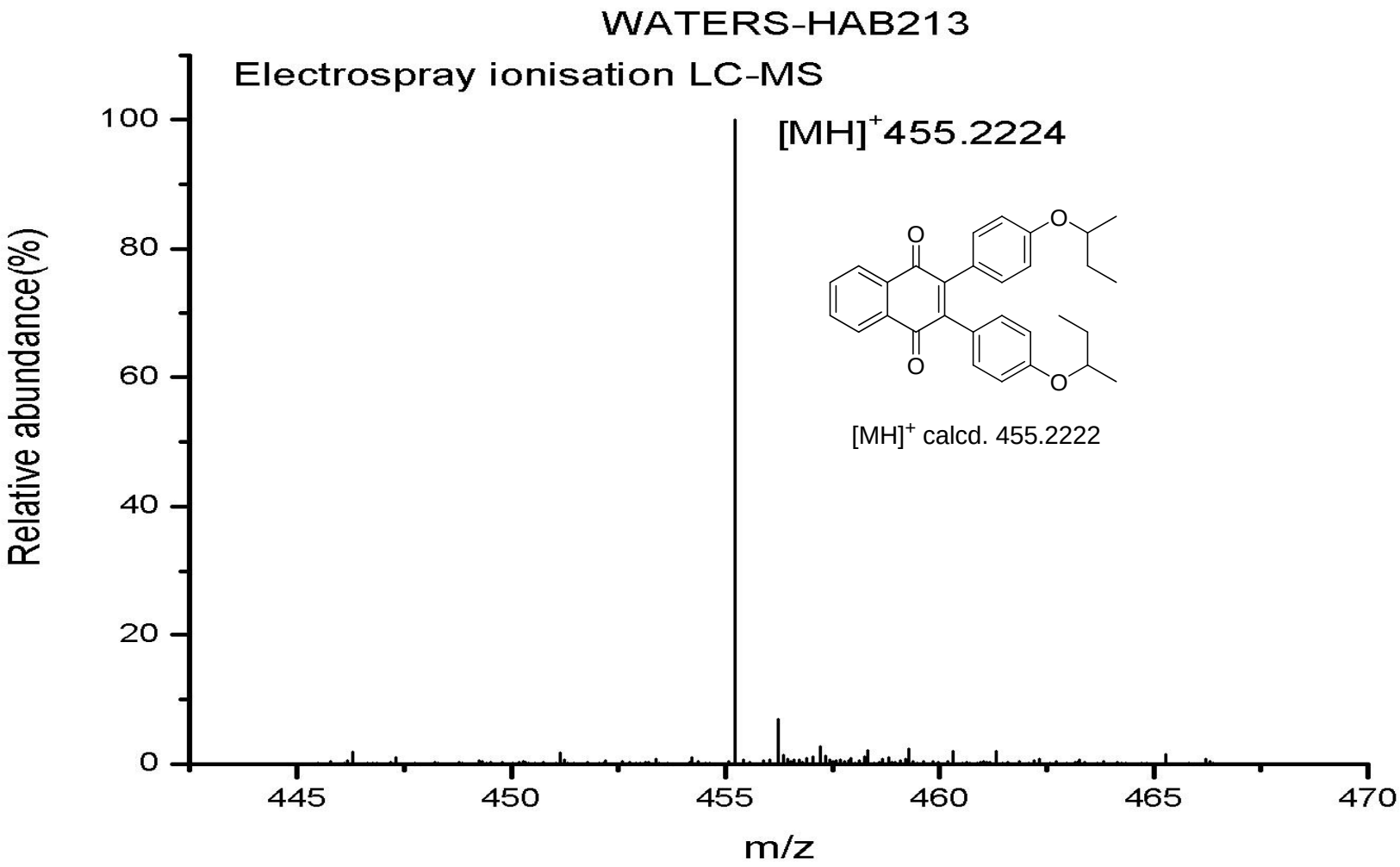
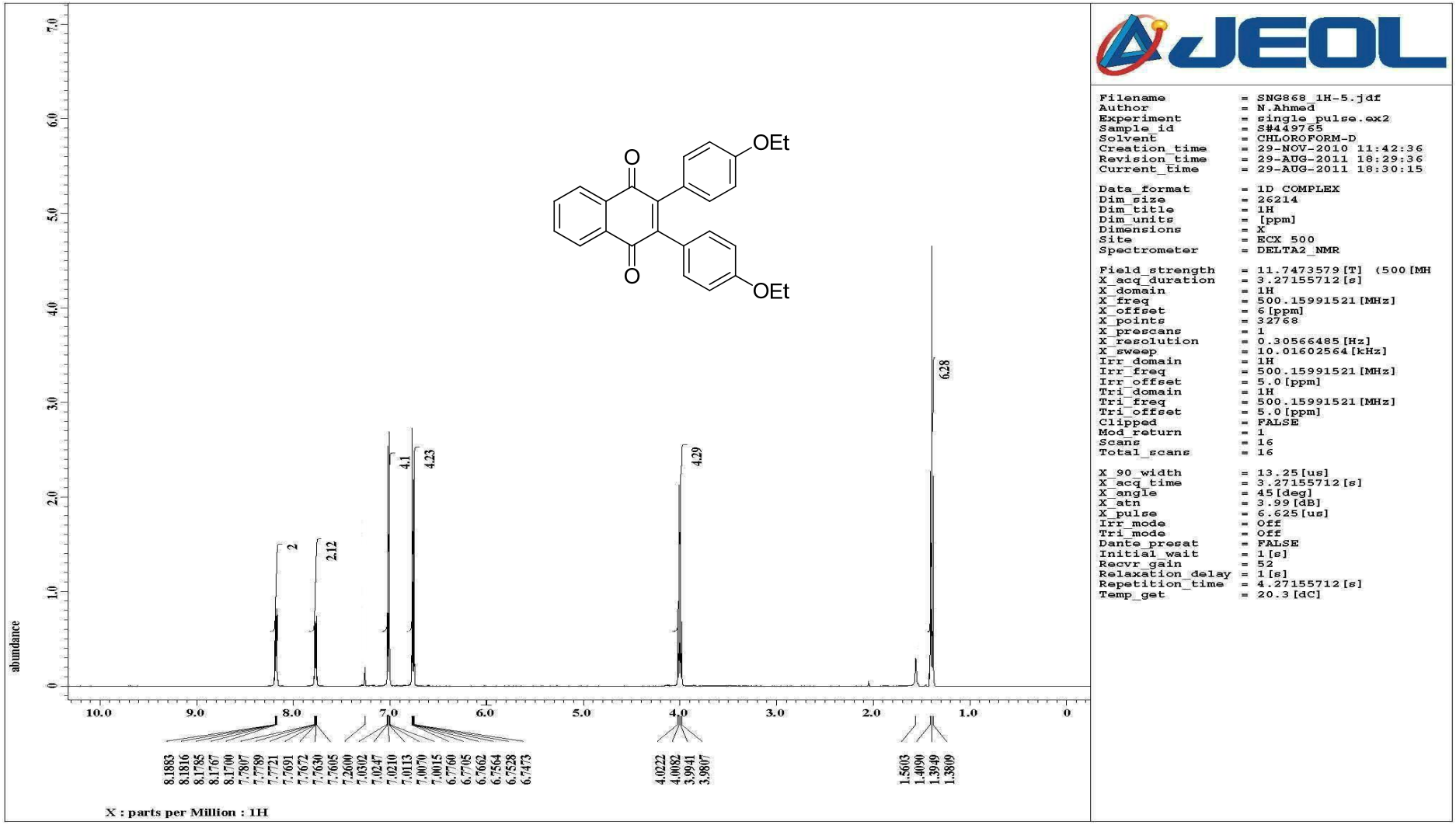
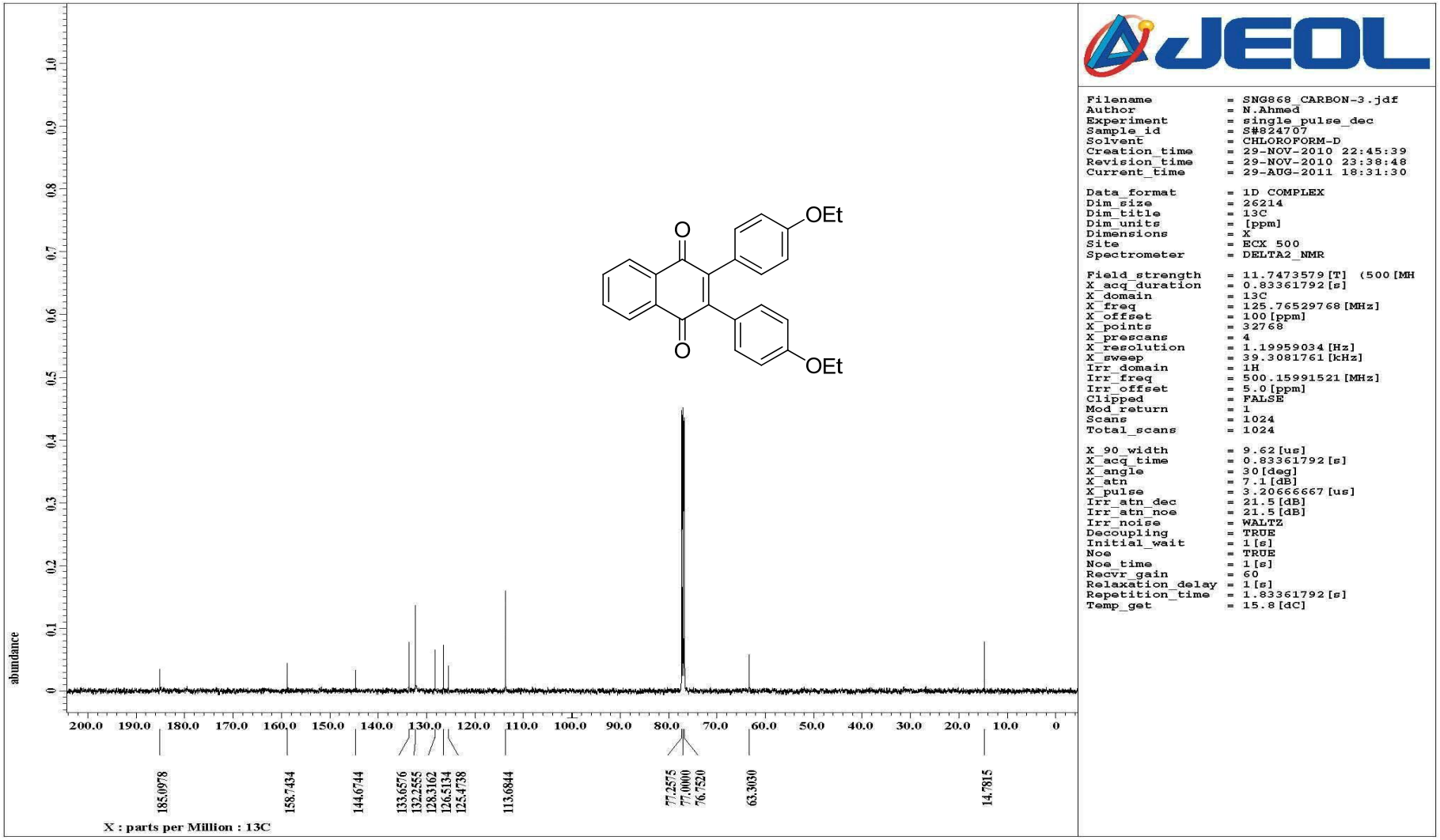
^{13}C NMR spectrum of 2,3-bis(4-sec-butoxyphenyl)-1,4-naphthoquinone (**6.4**)



HRMS spectrum of 2,3-bis(4-sec-butoxyphenyl)-1,4-naphthoquinone (**6.4**)



^{1}H NMR spectrum of 2,3-bis(4-ethoxyphenyl)-1,4-naphthoquinone (**6.5**)

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Noe_time          = 1[s]
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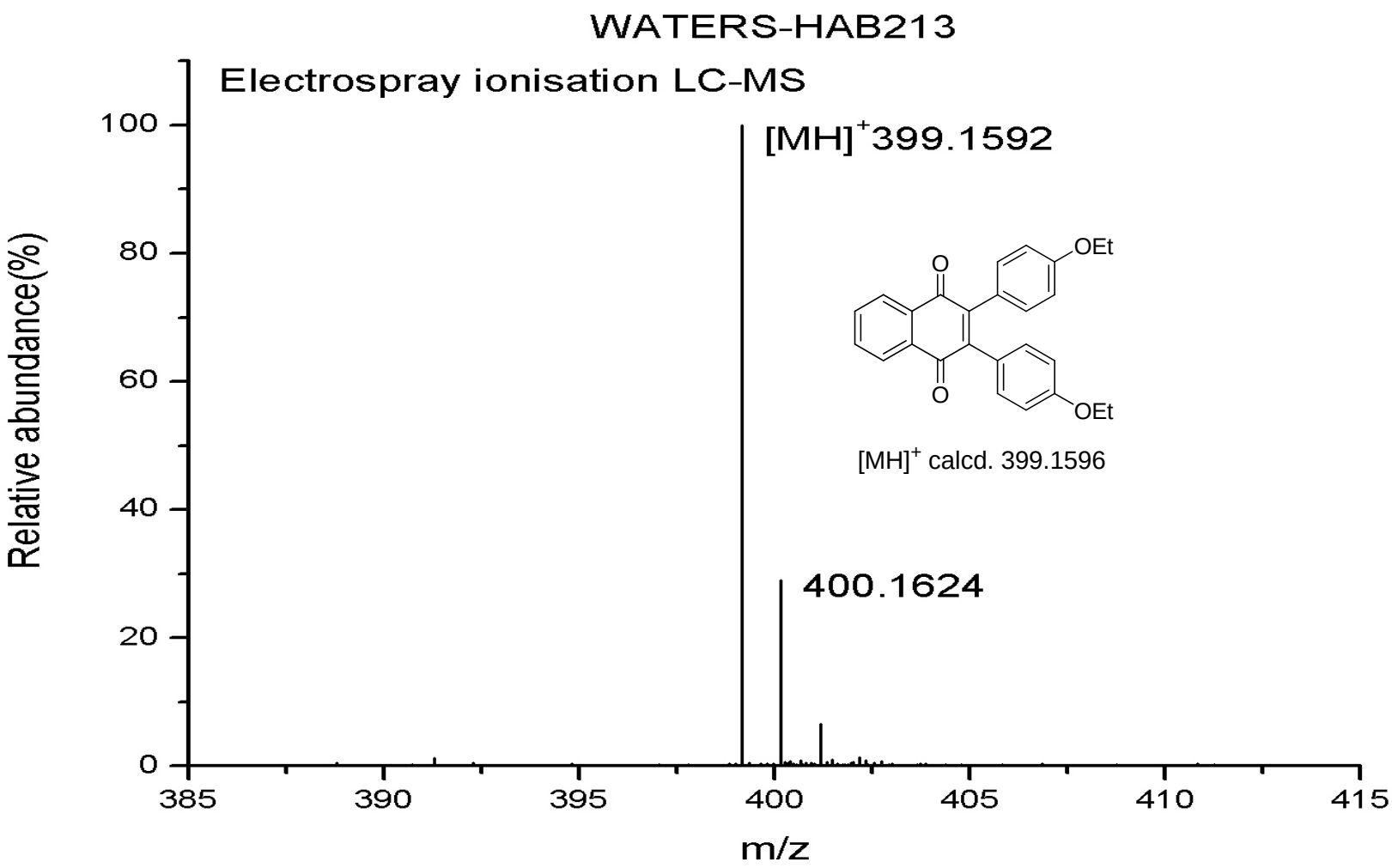
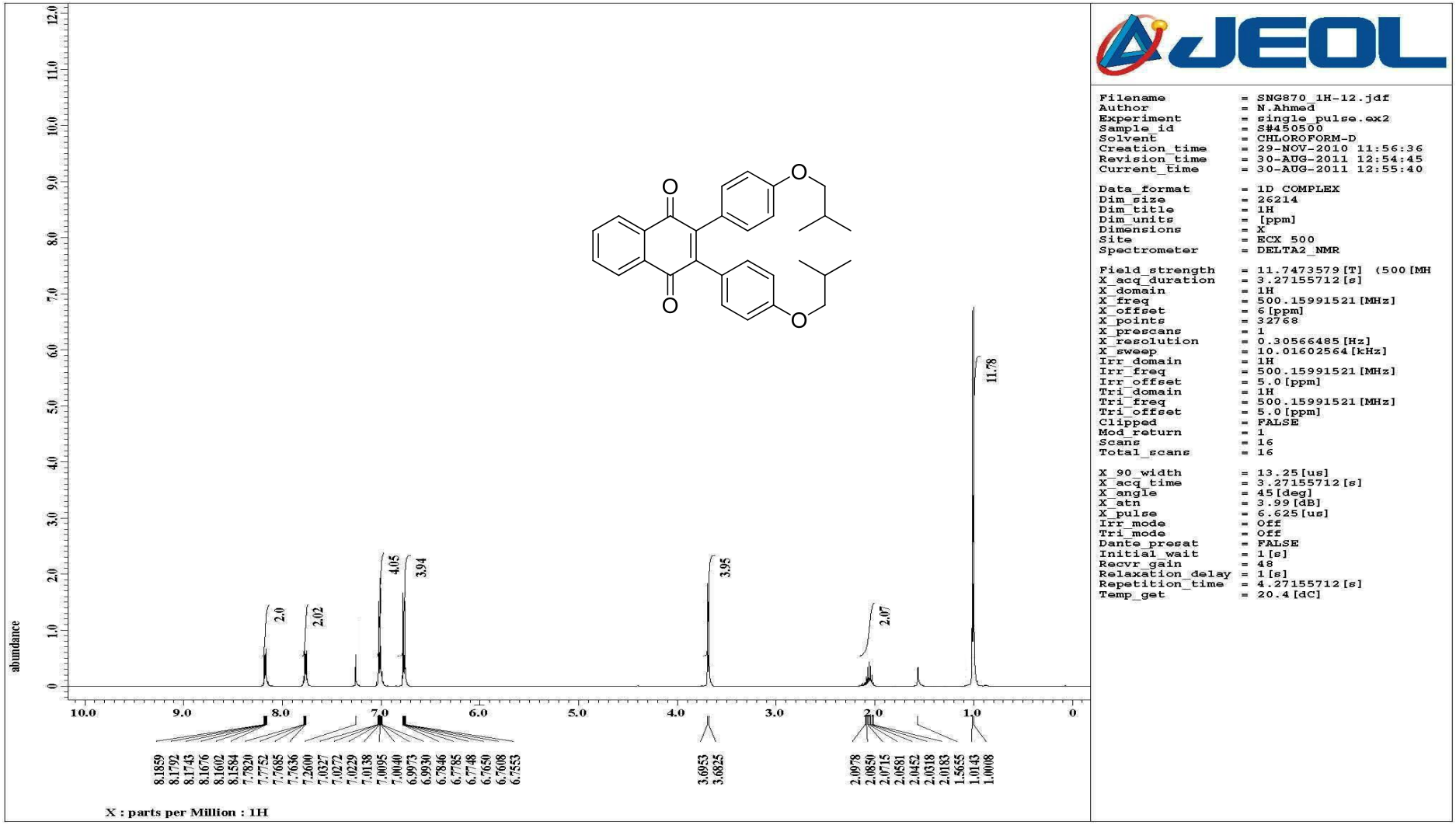
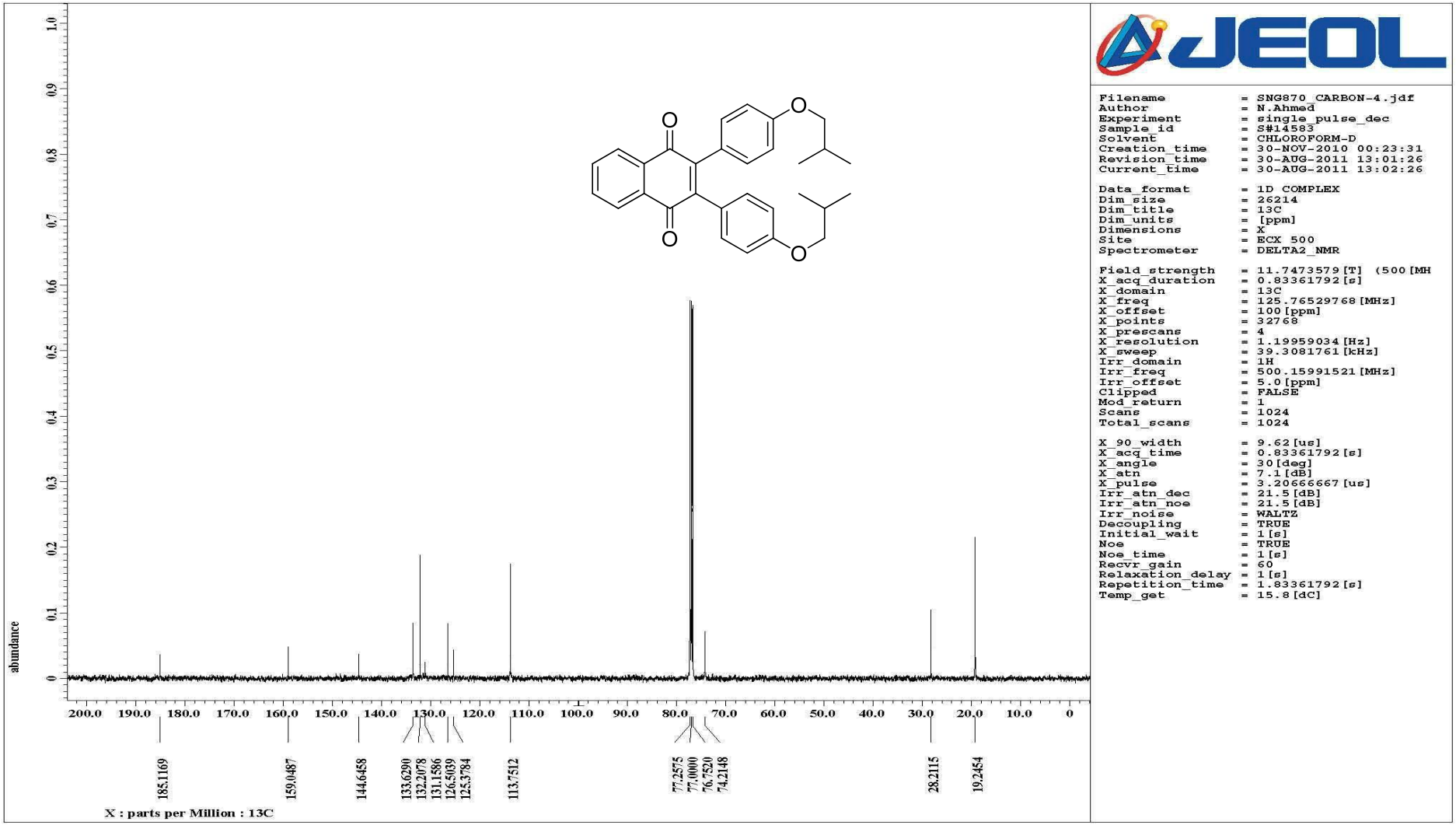
^{13}C NMR spectrum of 2,3-bis(4-ethoxyphenyl)-1,4-naphthoquinone (**6.5**)



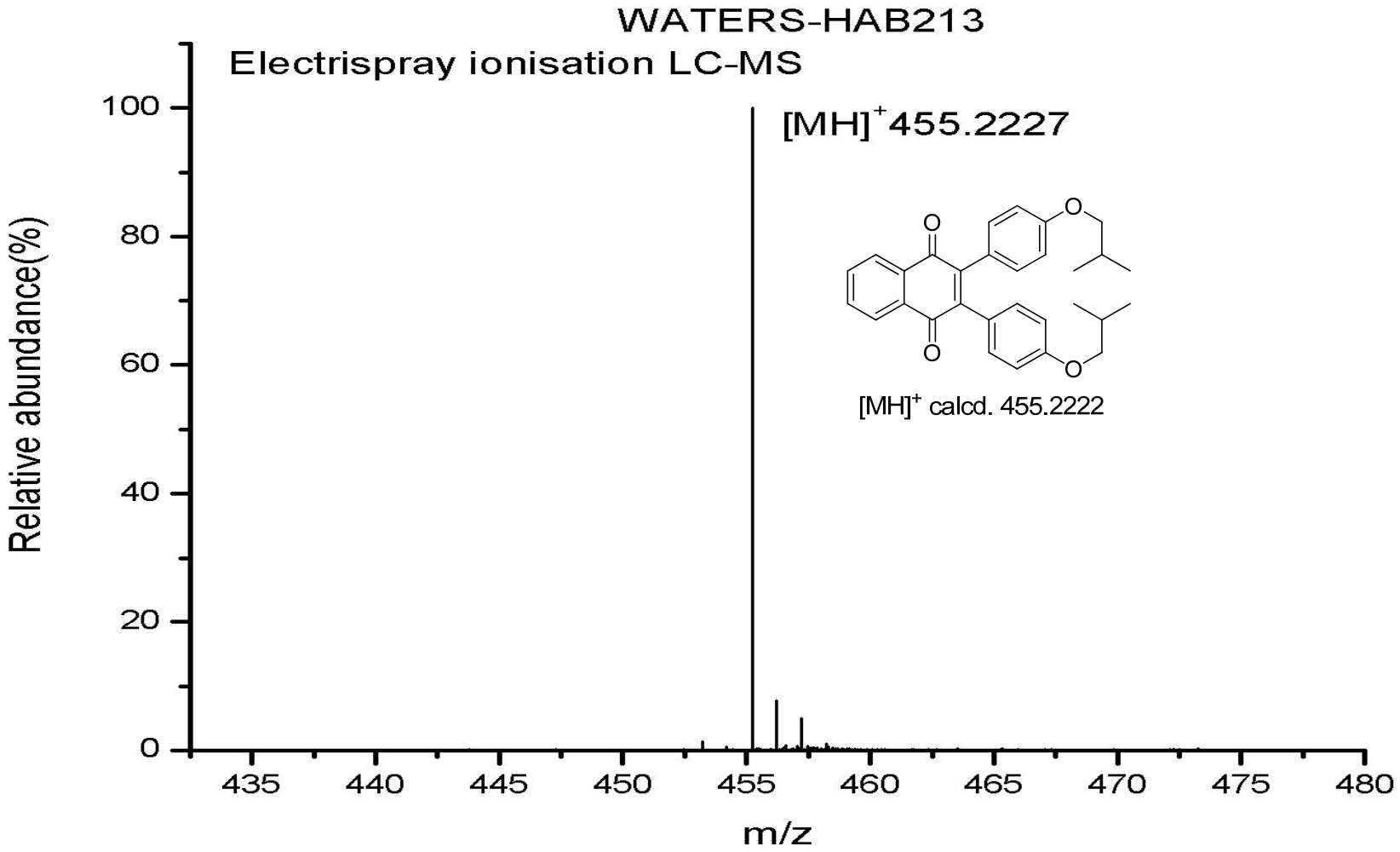
HRMS spectrum of 2,3-bis(4-ethoxyphenyl)-1,4-naphthoquinone (**6.5**)



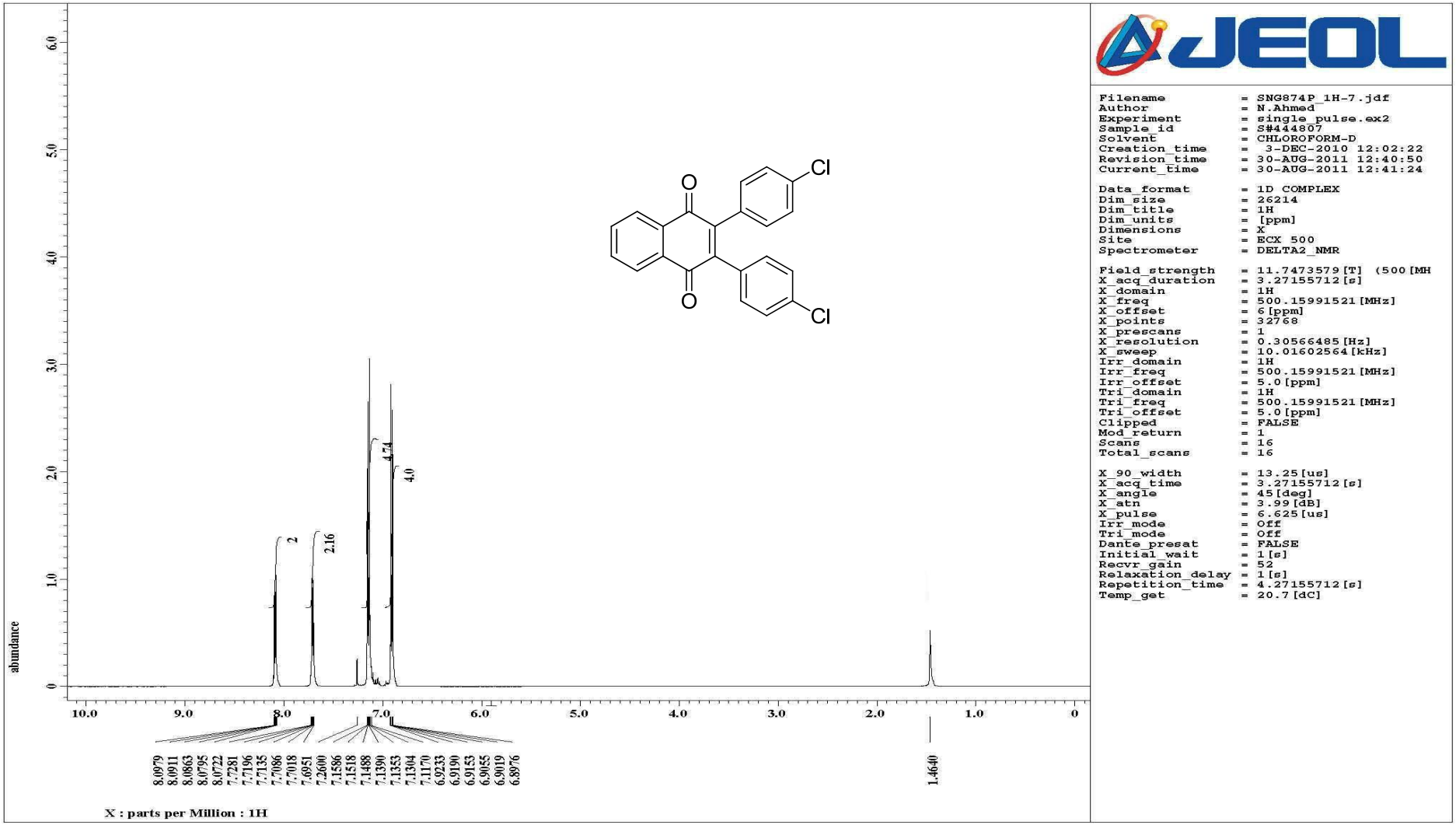
^{1}H NMR spectrum of 2,3-bis(4-isobutoxyphenyl)-1,4-naphthoquinone (**6.6**)



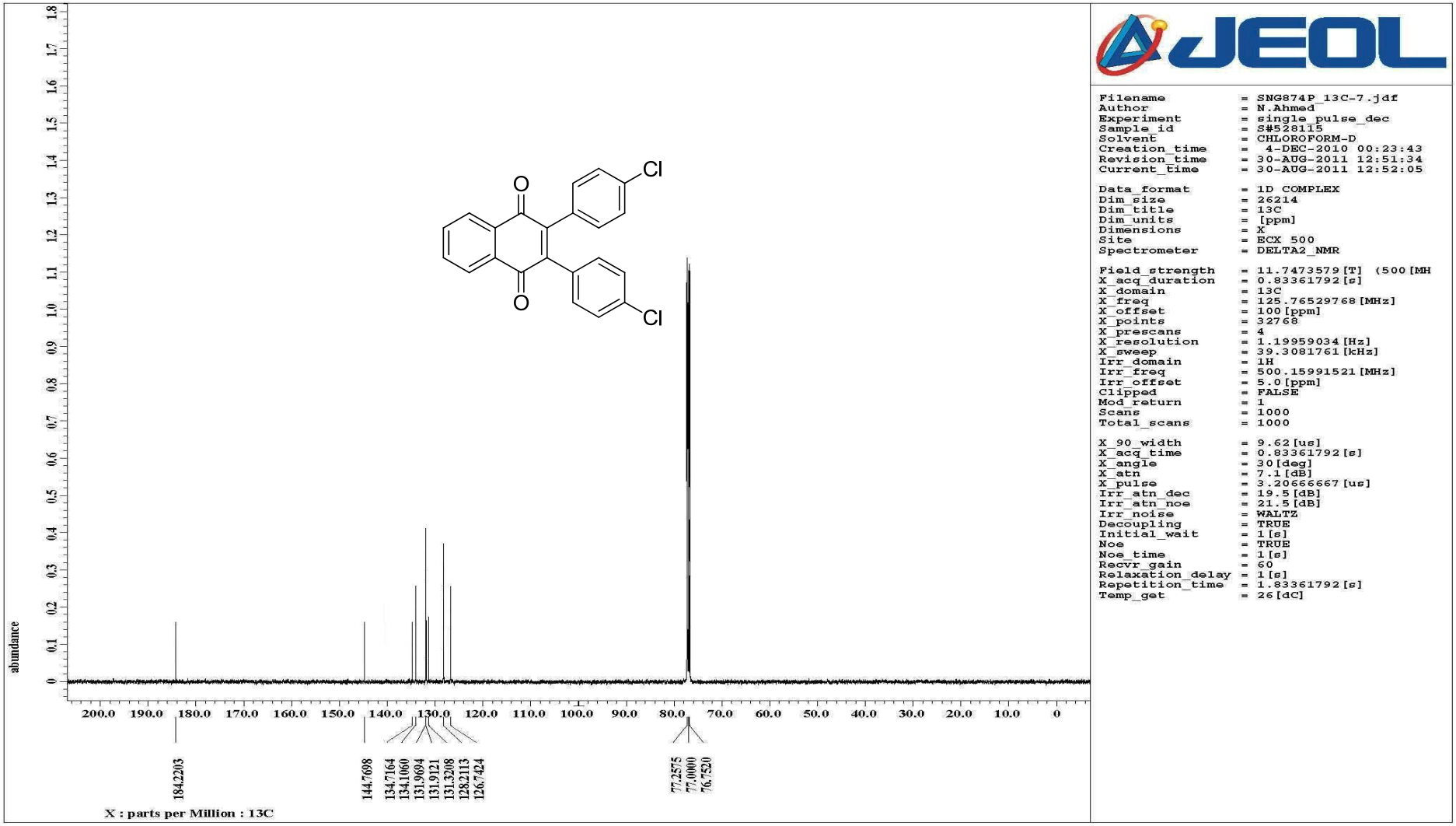
^{13}C NMR spectrum of 2,3-bis(4-isobutoxyphenyl)-1,4-naphthoquinone (**6.6**)



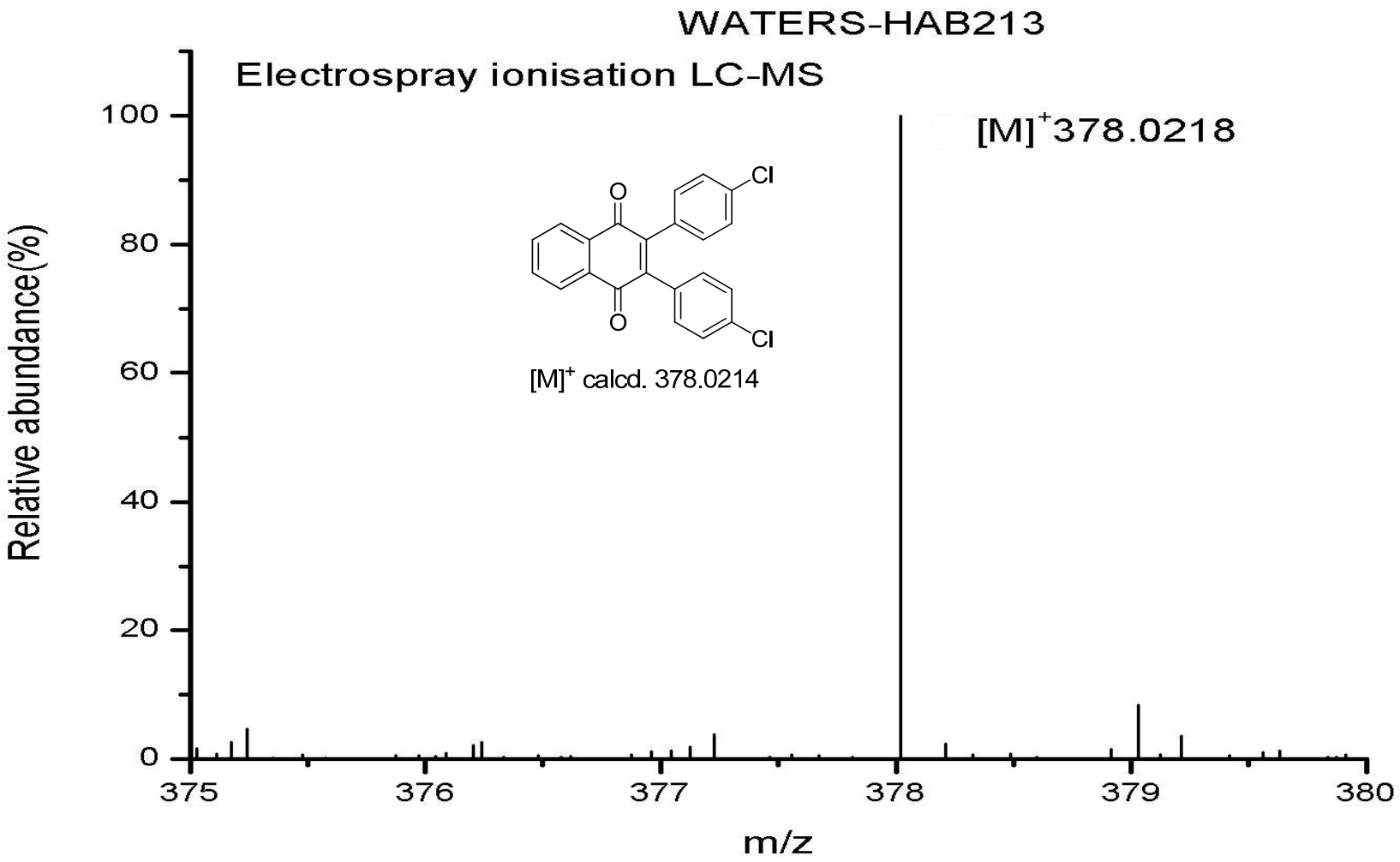
HRMS spectrum of 2,3-bis(4-isobutoxyphenyl)-1,4-naphthoquinone (**6.6**)



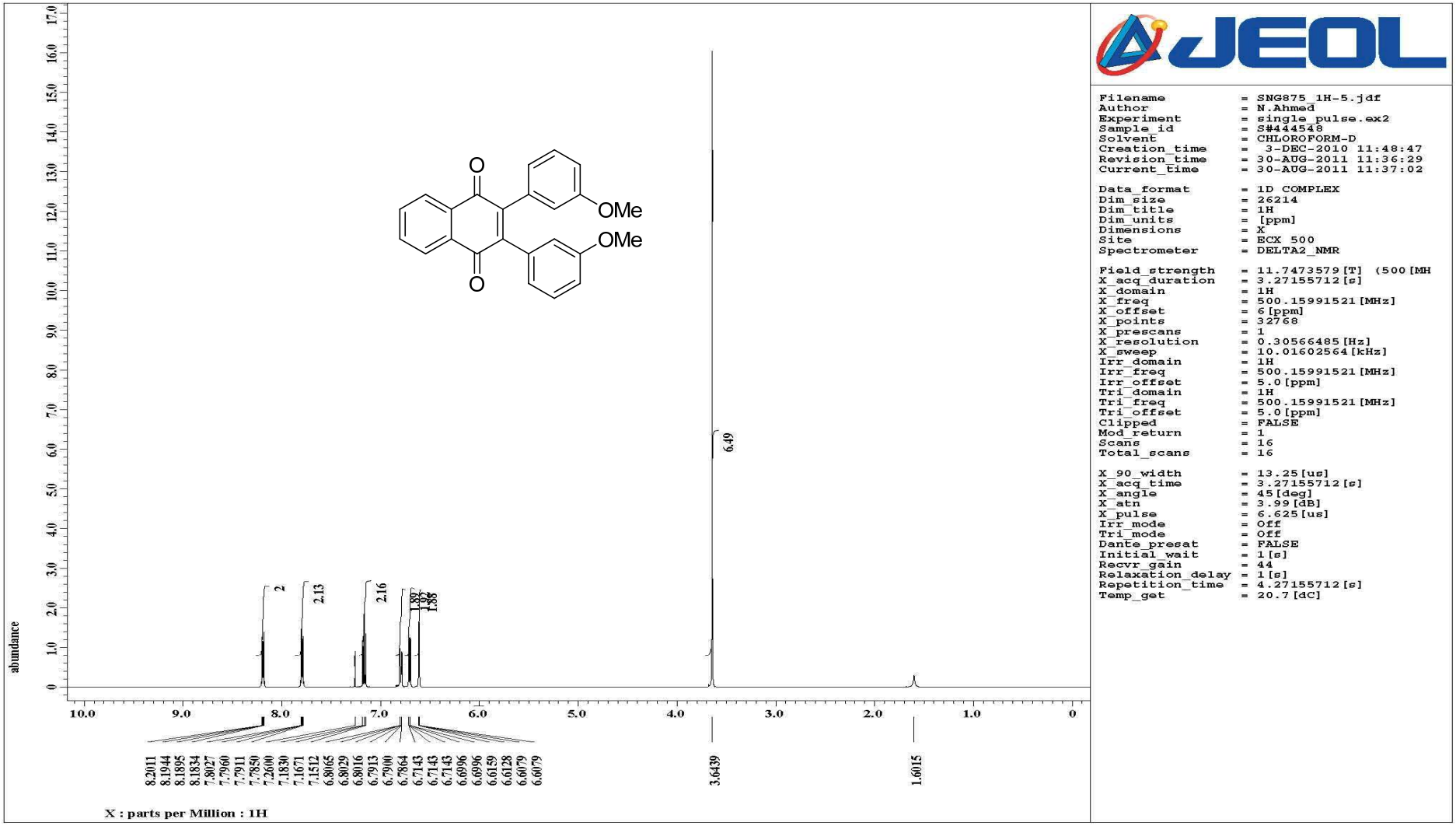
^{1}H NMR spectrum of 2,3-bis(4-chlorophenyl)-1,4-naphthoquinone (**6.7**)



^{13}C NMR spectrum of 2,3-bis(4-chlorophenyl)-1,4-naphthoquinone (**6.7**)



HRMS spectrum of 2,3-bis(4-chlorophenyl)-1,4-naphthoquinone (**6.7**)

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Revision_time     = 30-AUG-2011 11:36:29
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X_offset          = 6[ppm]
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Tri_freq          = 500.15991521[MHz]
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Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
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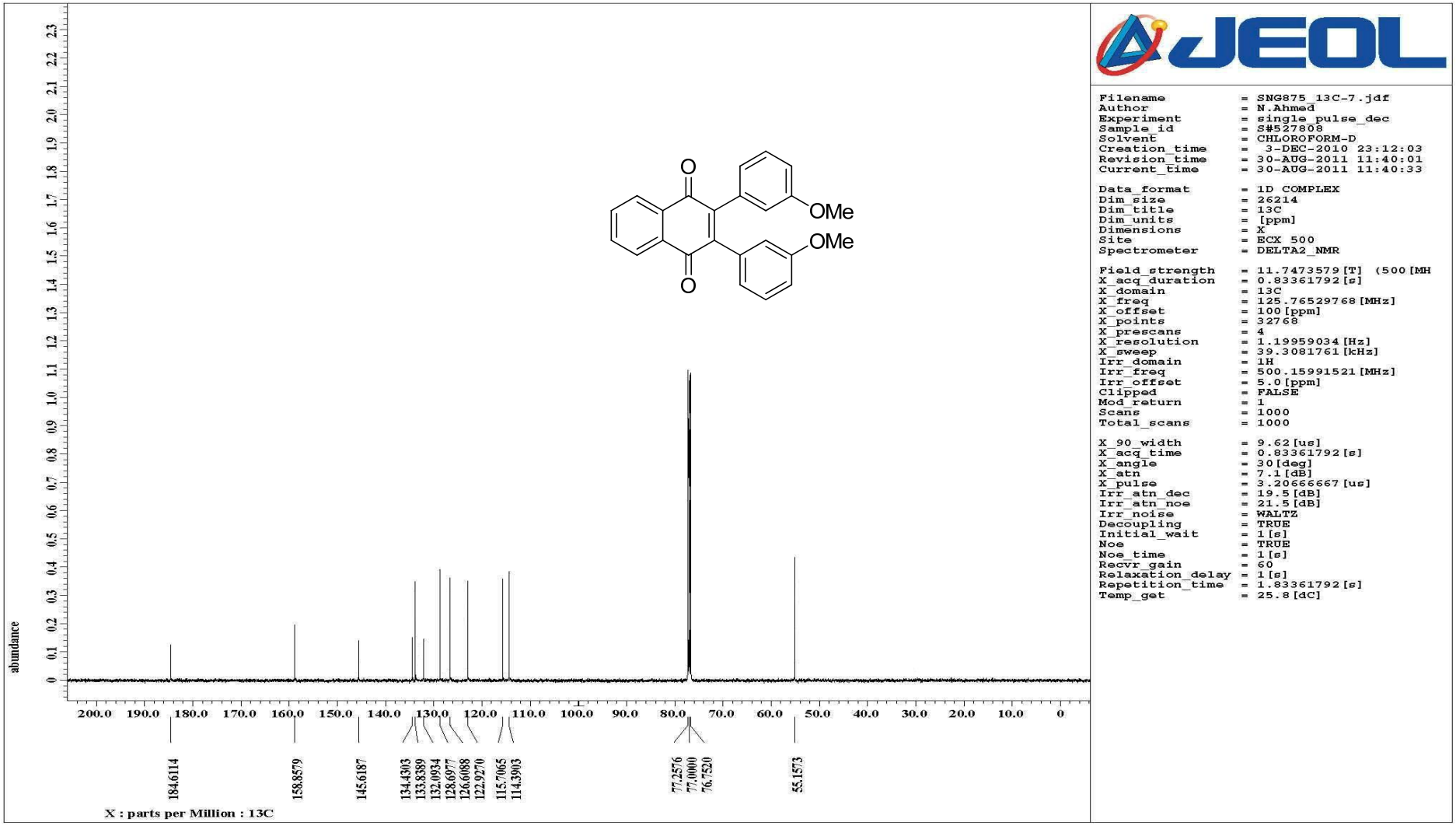
^{1}H NMR spectrum of 2,3-bis(3-methoxyphenyl)-1,4-naphthoquinone (**6.8**)



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Noe_time = 1[s]
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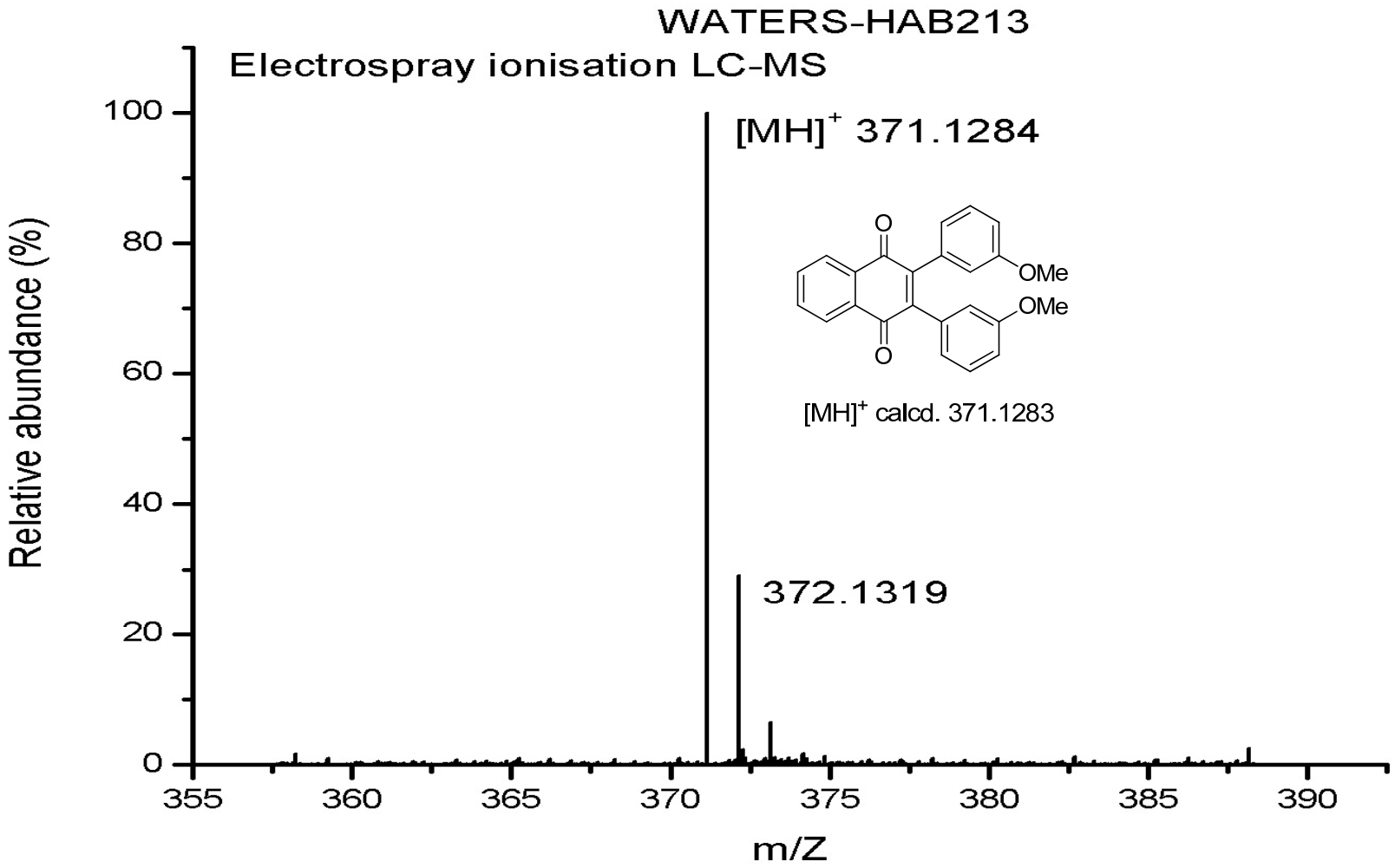
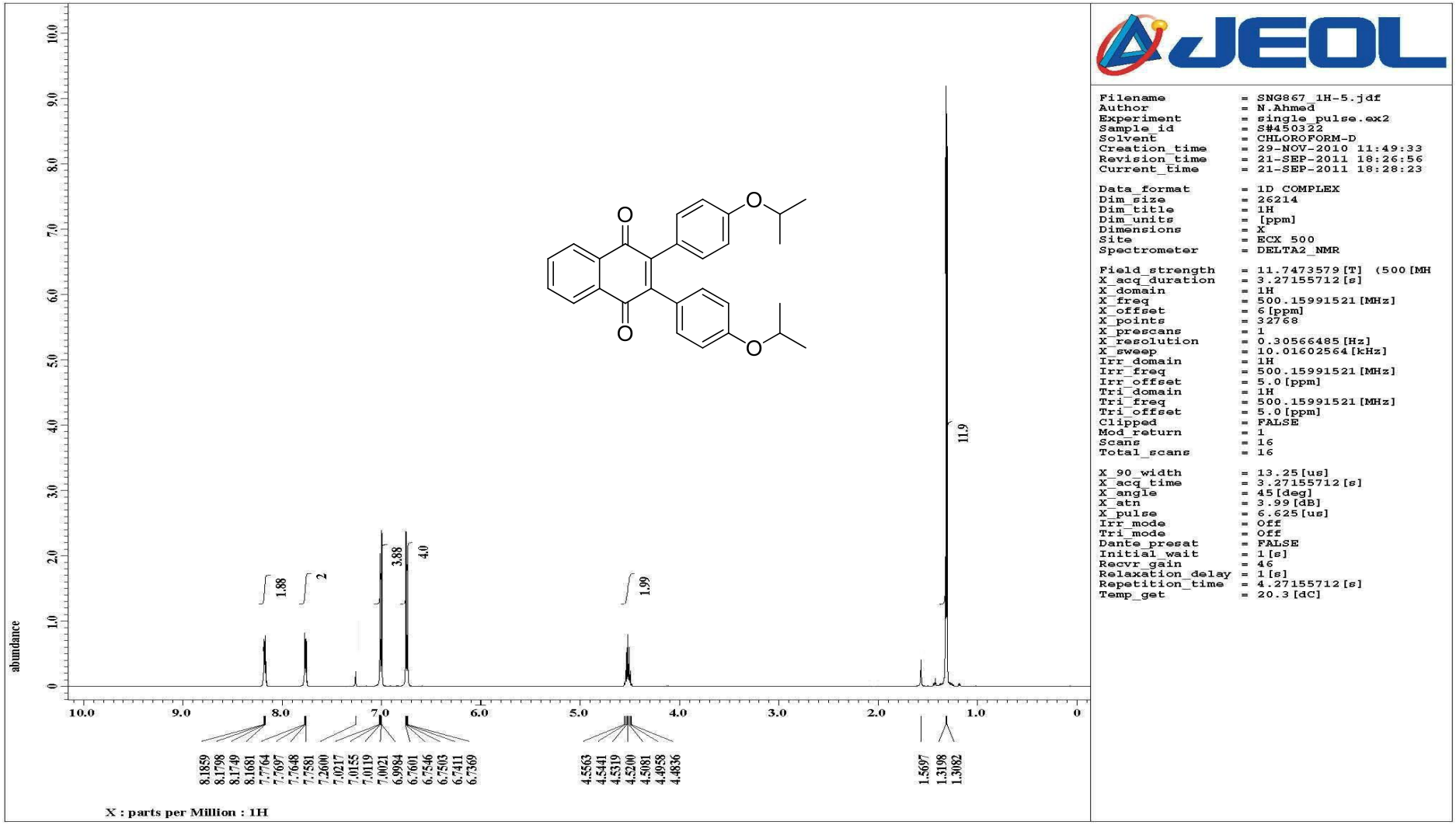
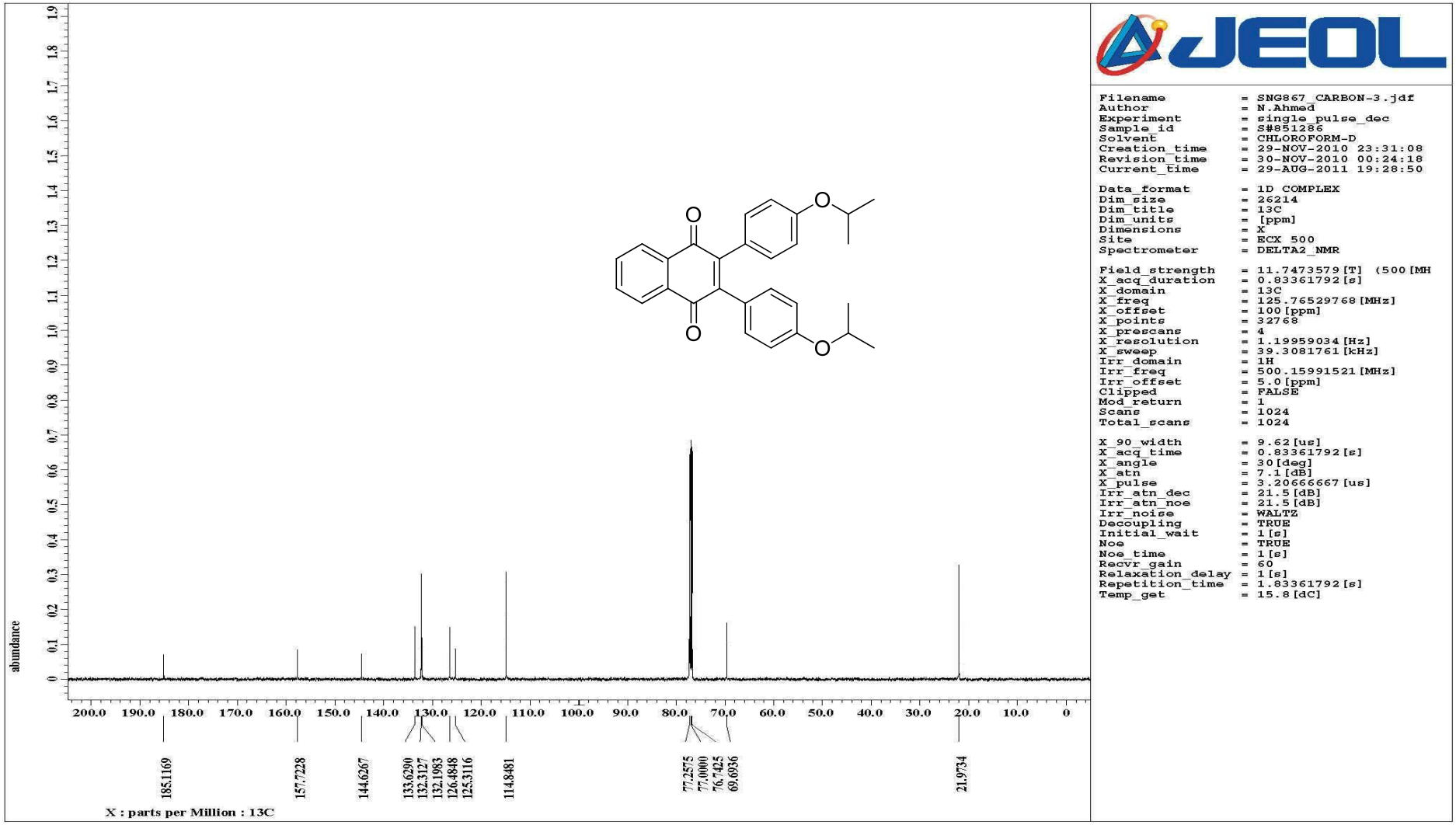
^{13}C NMR spectrum of 2,3-bis(3-methoxyphenyl)-1,4-naphthoquinone (**6.8**)



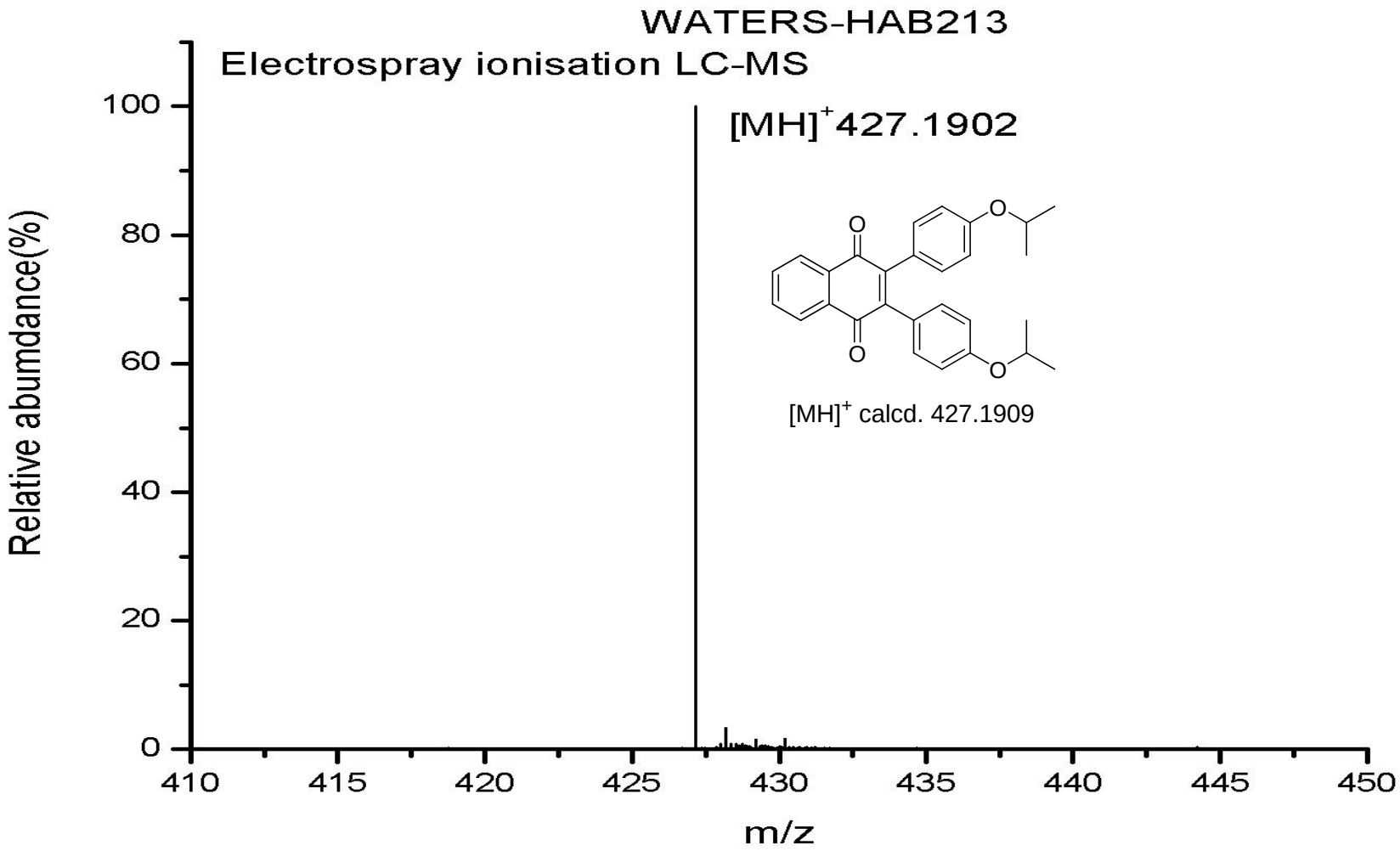
HRMS spectrum of 2,3-bis(3-methoxyphenyl)-1,4-naphthoquinone (**6.8**)



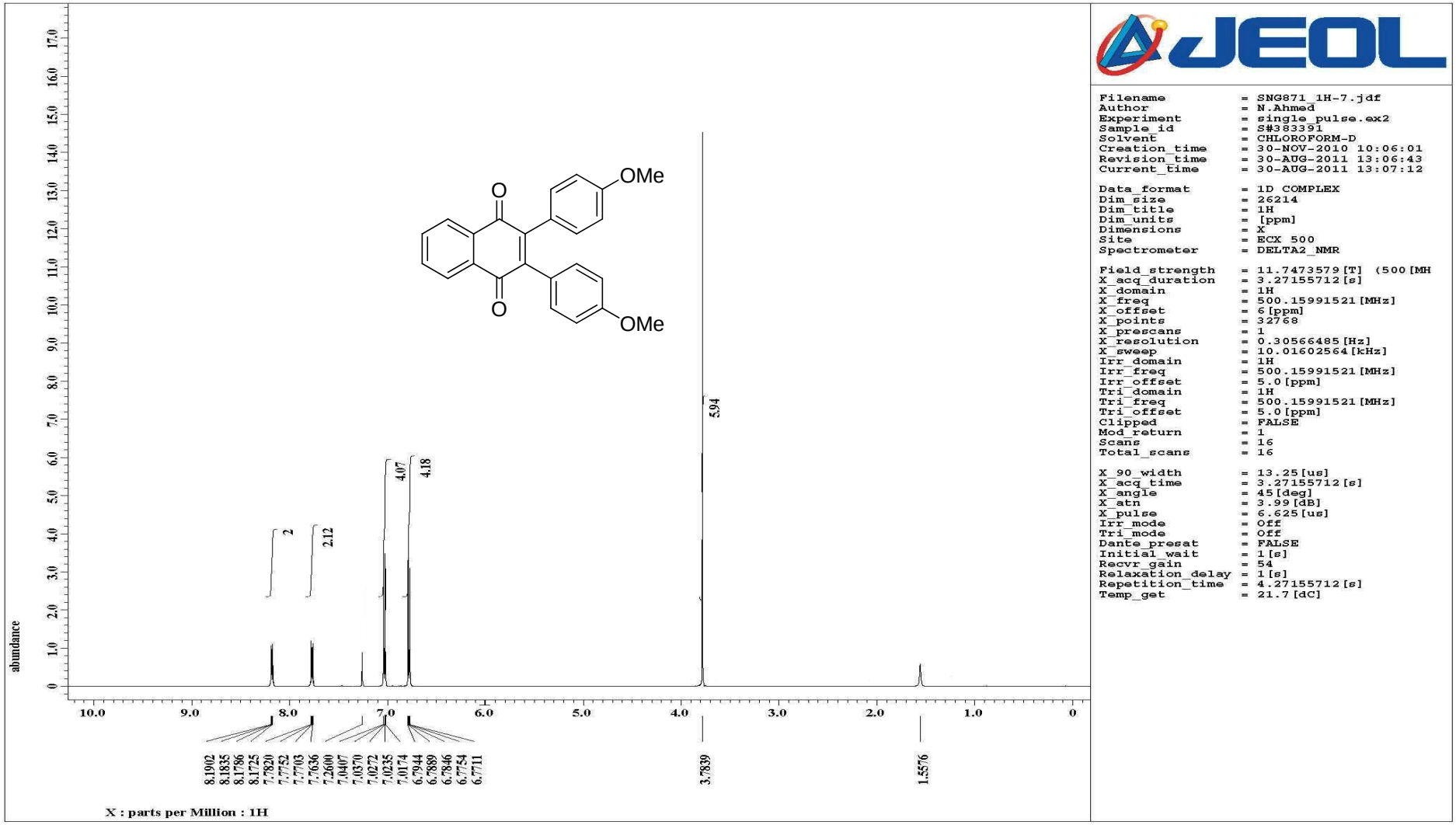
^{1}H NMR spectrum of 2,3-bis(4-isopropoxyphenyl)-1,4-naphthoquinone (**6.9**)



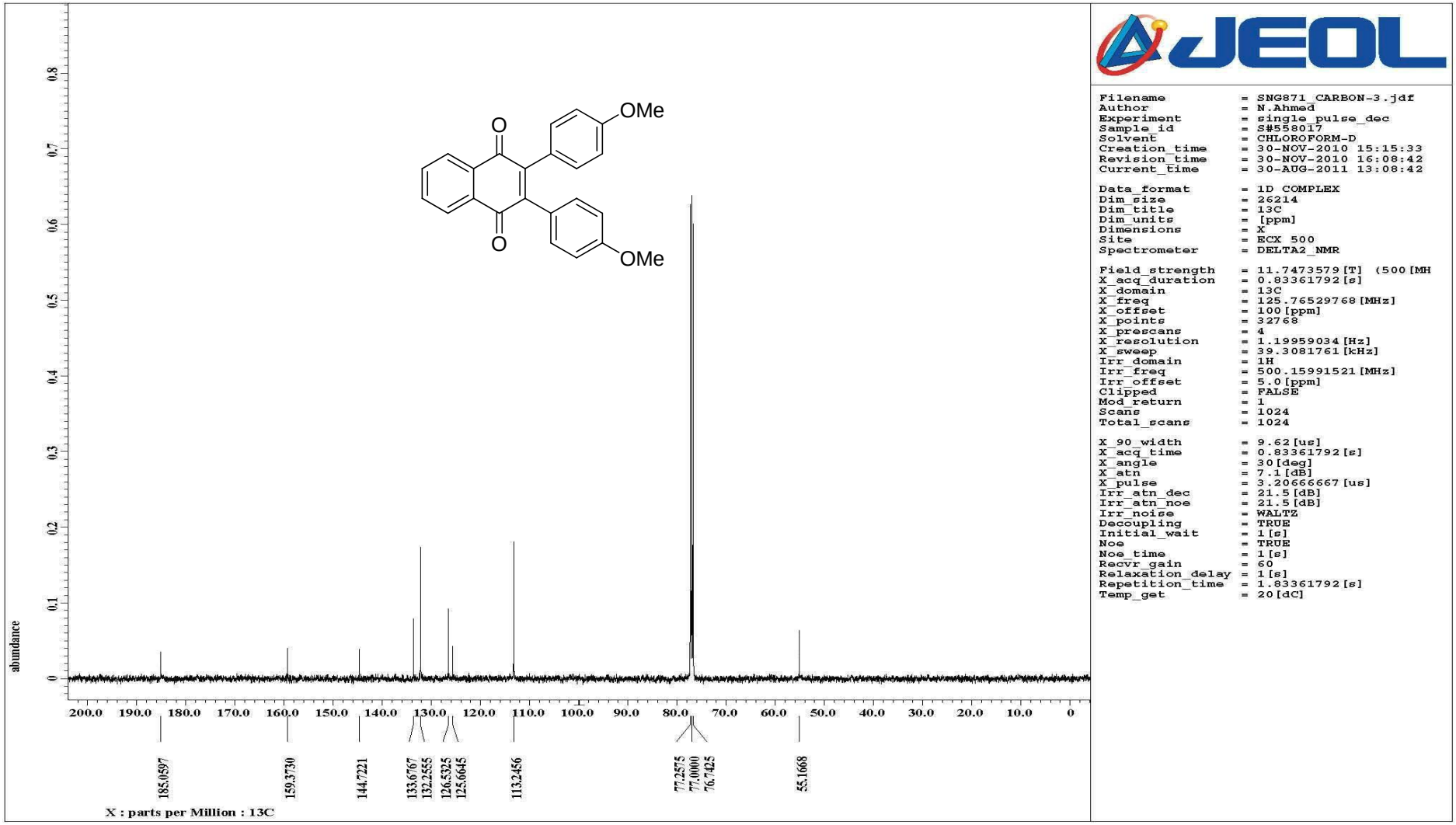
^{13}C NMR spectrum of 2,3-bis(4-isopropoxyphenyl)-1,4-naphthoquinone (**6.9**)



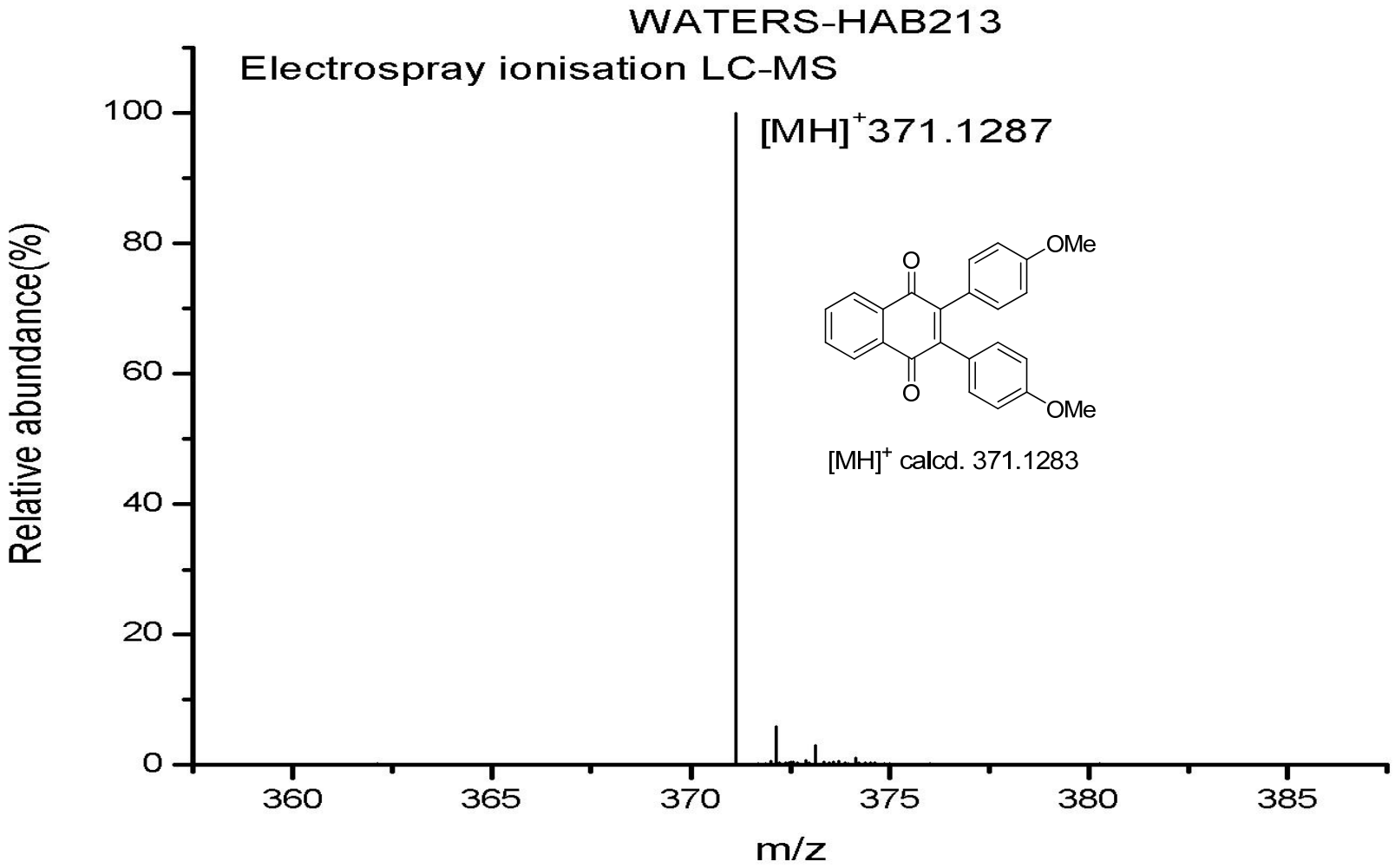
HRMS spectrum of 2,3-bis(4-isopropoxyphenyl)-1,4-naphthoquinone (**6.9**)



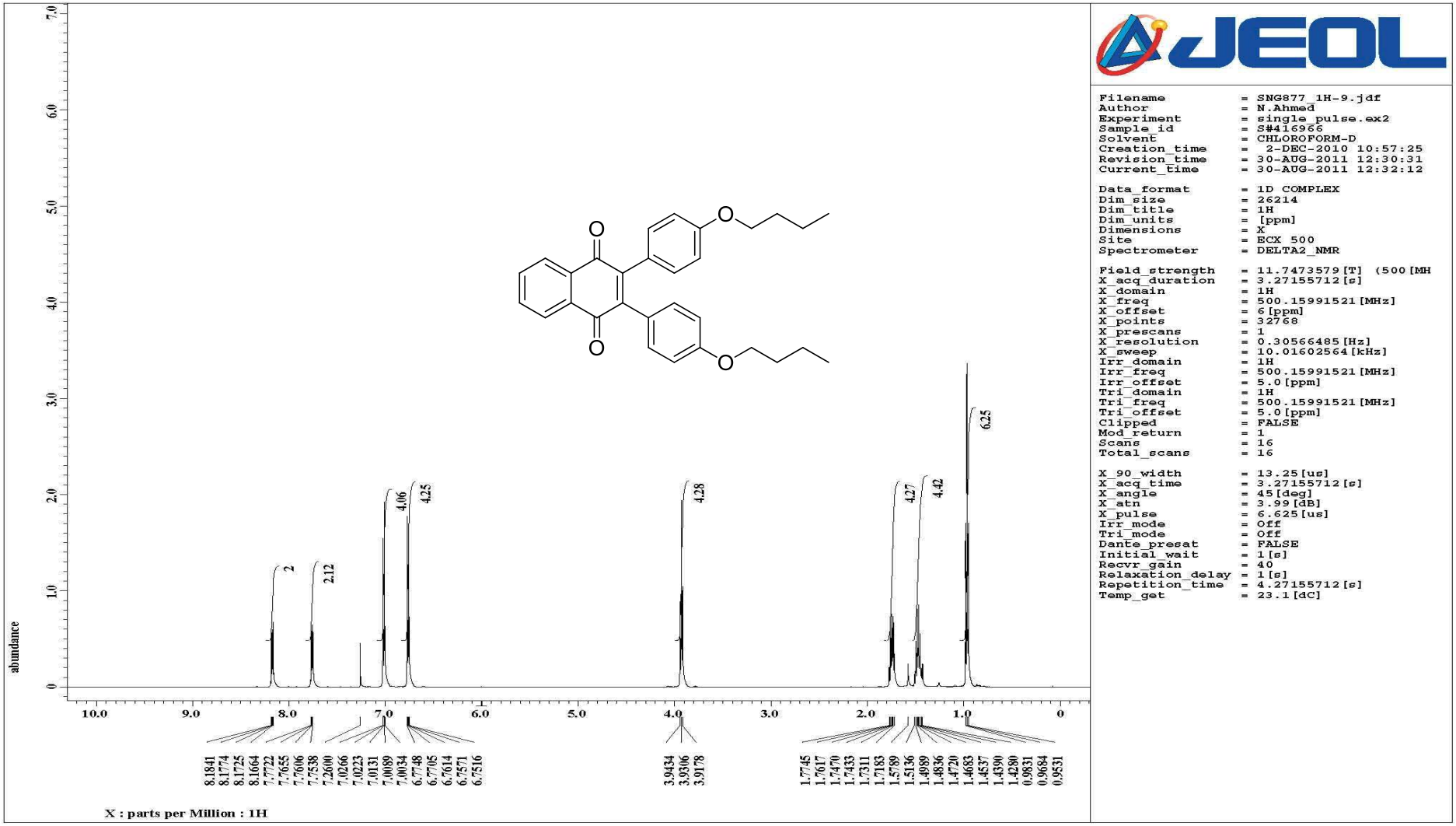
^{1}H NMR spectrum of 2,3-bis(4-methoxyphenyl)-1,4-naphthoquinone (**6.10**)



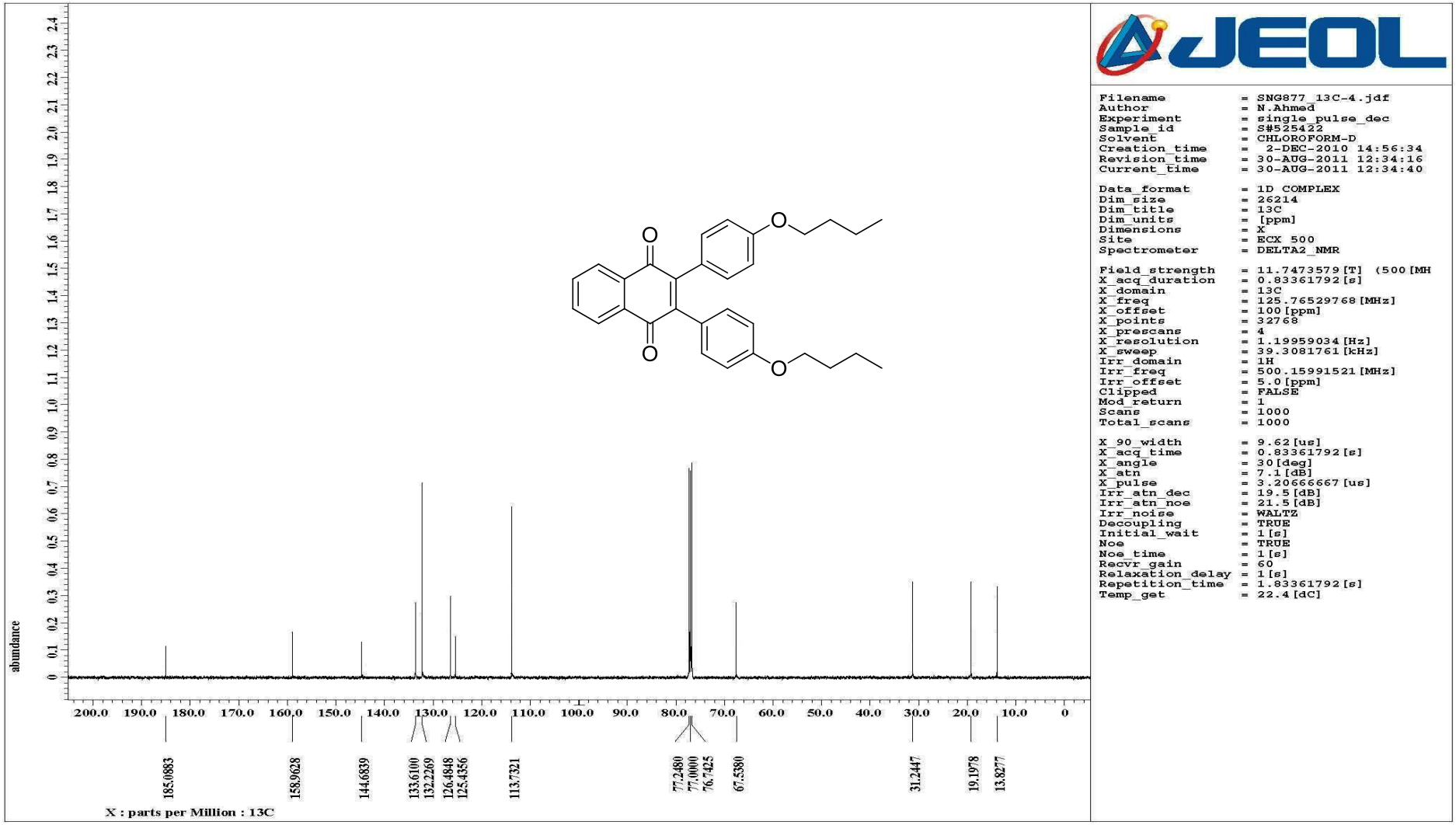
^{13}C NMR spectrum of 2,3-bis(4-methoxyphenyl)-1,4-naphthoquinone (**6.10**)



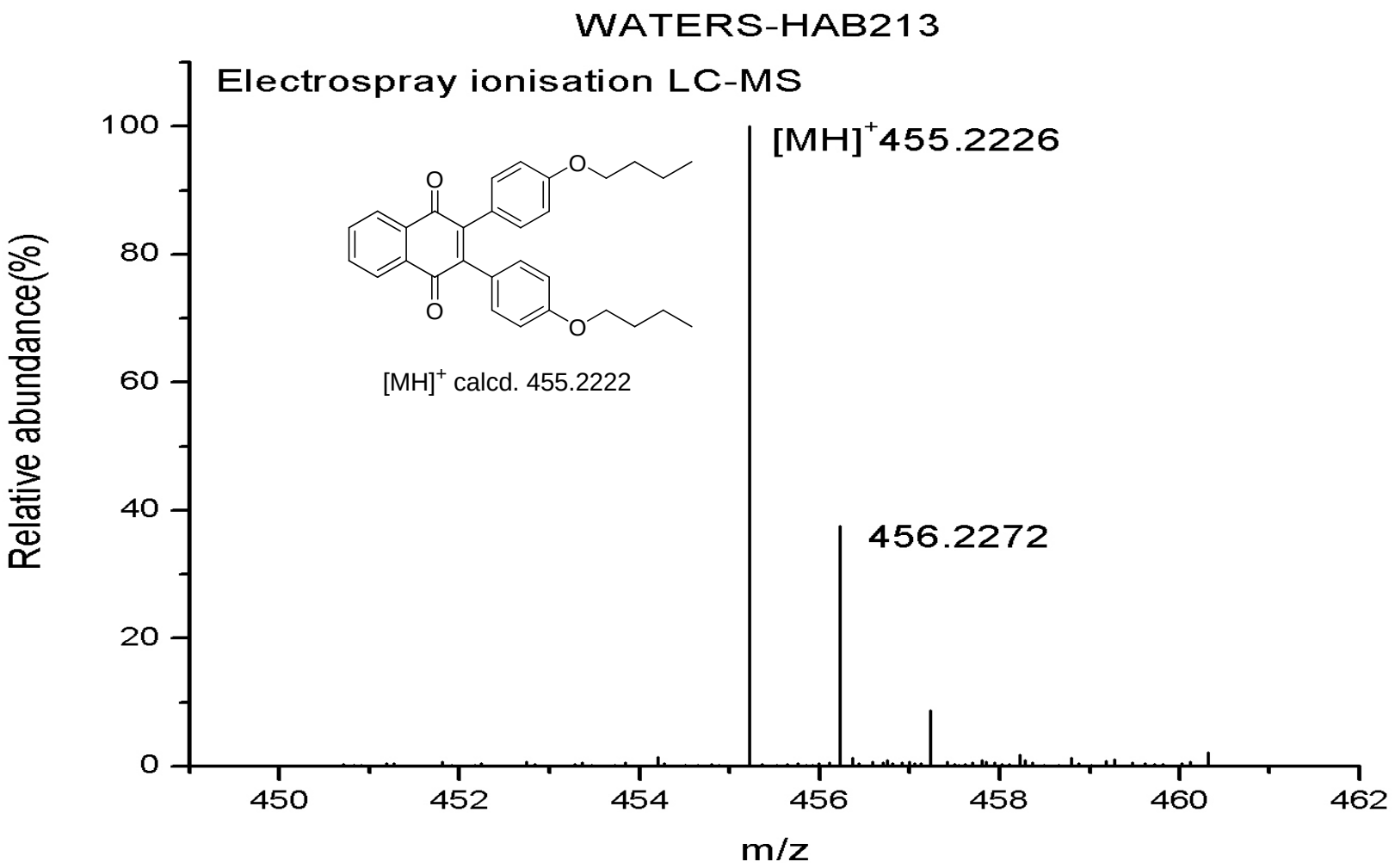
HRMs spectrum of 2,3-bis(4-methoxyphenyl)-1,4-naphthoquinone (**6.10**)



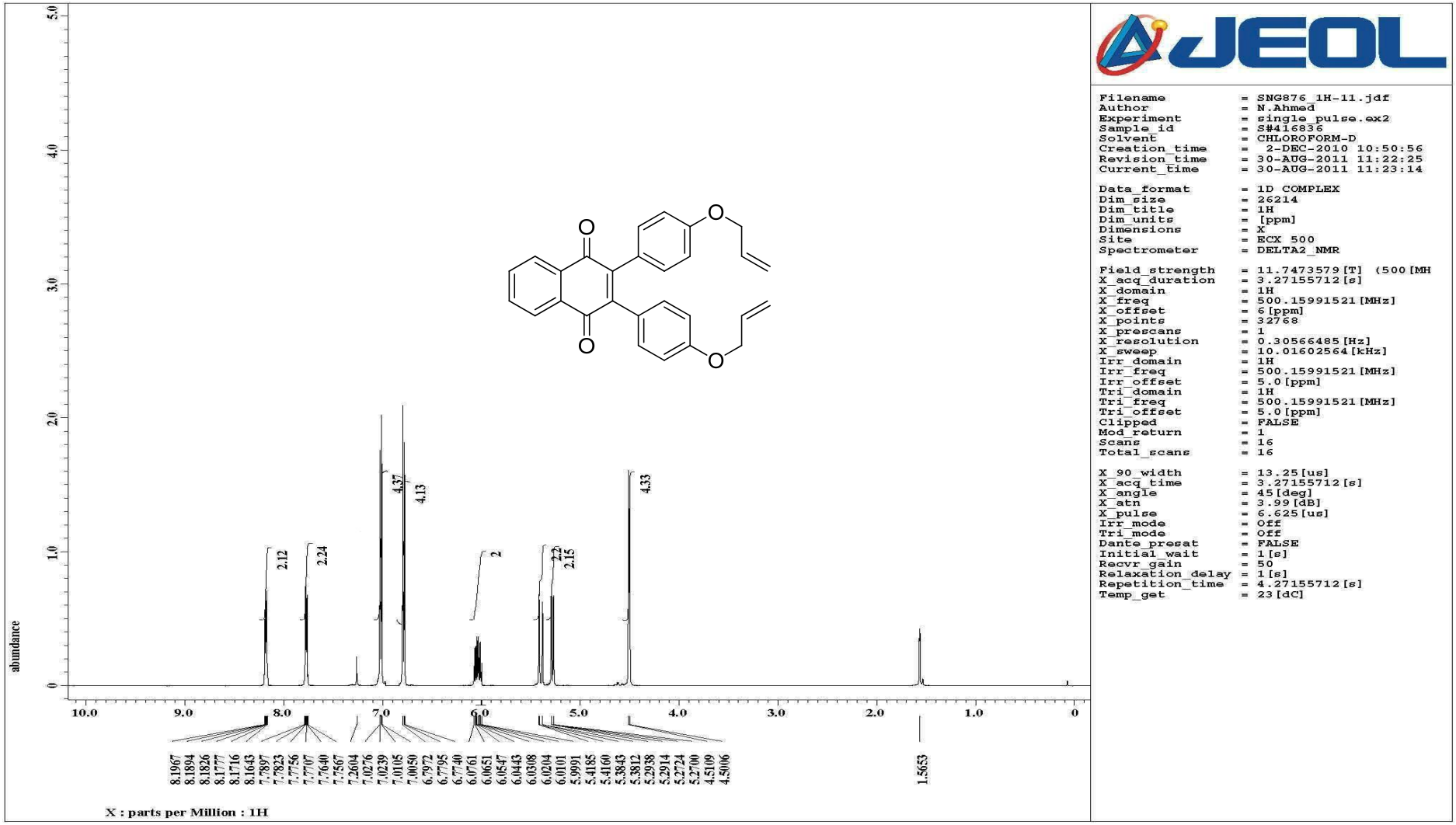
^{1}H NMR spectrum of 2,3-bis(4-butoxyphenyl)-1,4-naphthoquinone (**6.11**)



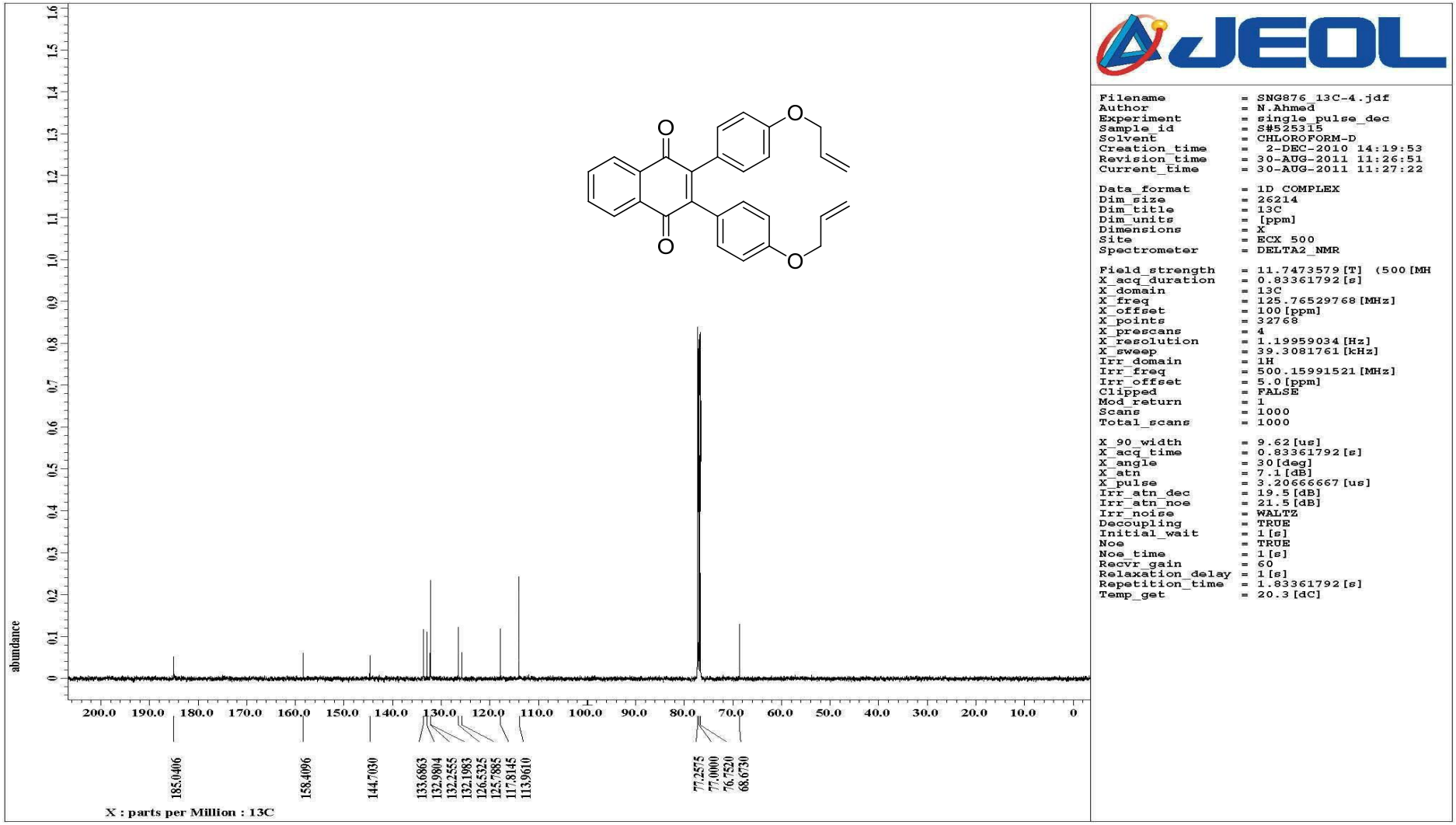
^{13}C NMR spectrum of 2,3-bis(4-butoxyphenyl)-1,4-naphthoquinone (**6.11**)



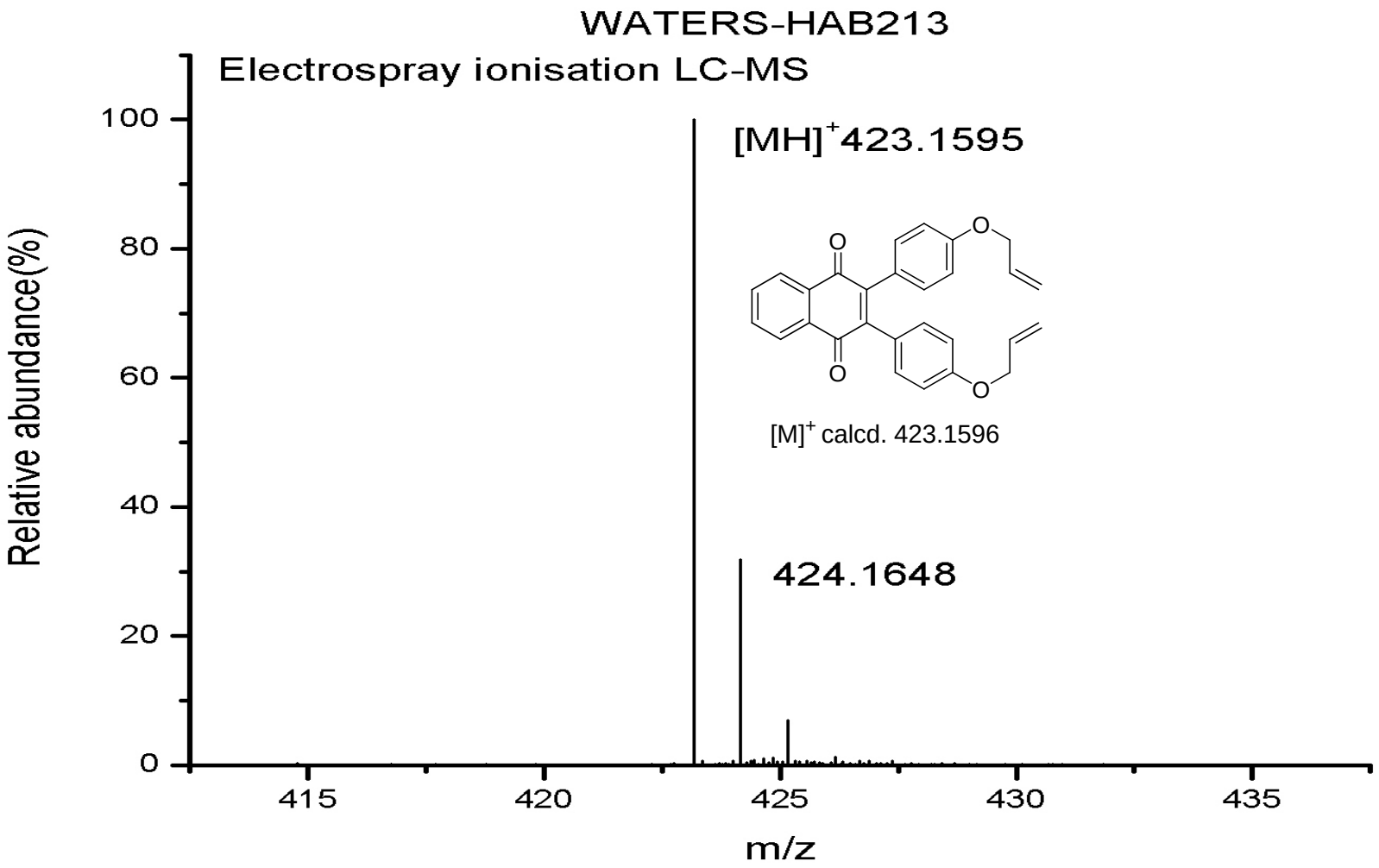
HRMS spectrum of 2,3-bis(4-butoxyphenyl)-1,4-naphthoquinone (**6.11**)



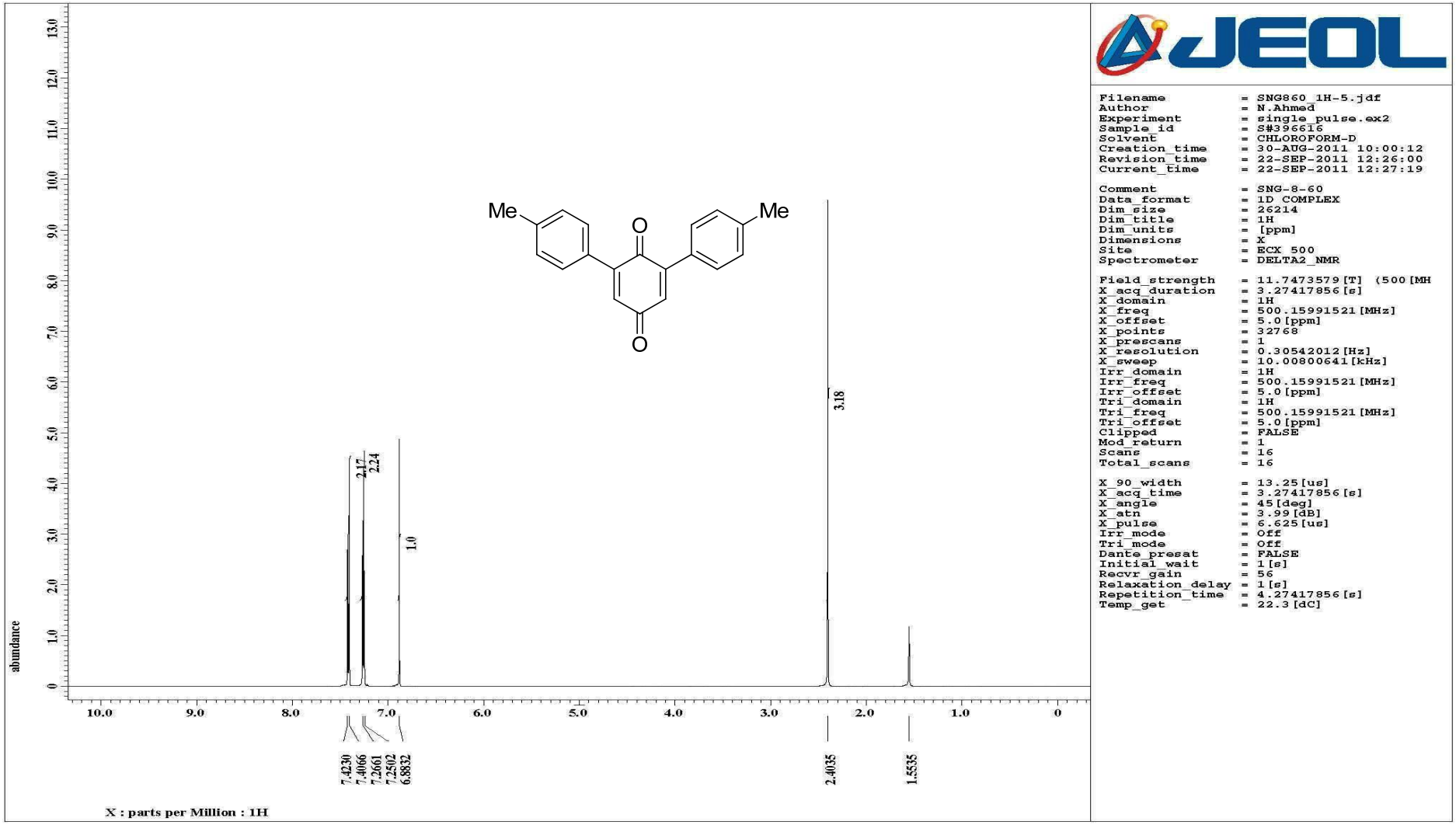
^{1}H NMR spectrum of 2,3-bis(4-(allyloxy)phenyl-1,4-naphthoquinone (**6.12**)



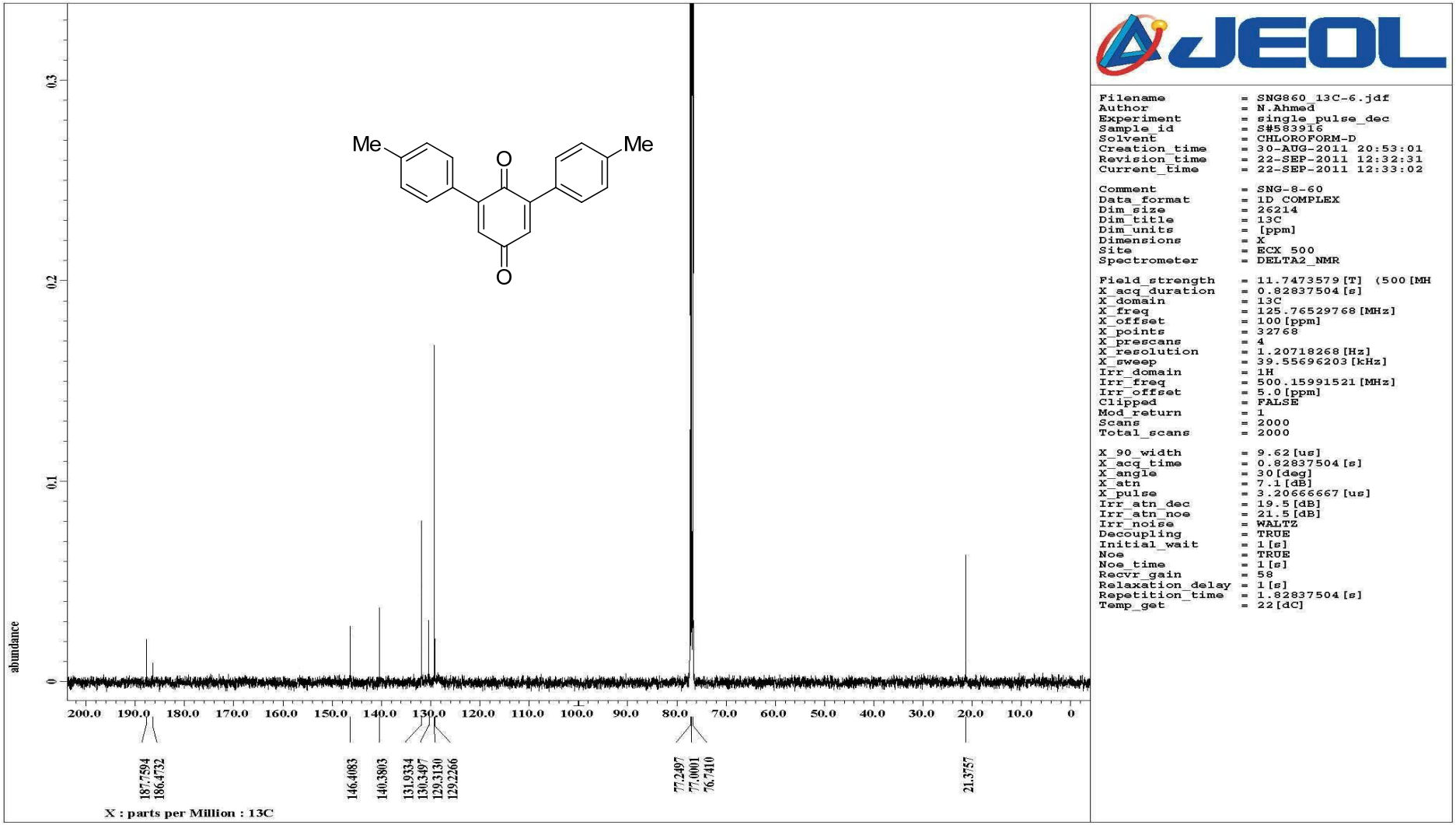
^{13}C NMR spectrum of 2,3-bis(4-(allyloxy)phenyl-1,4-naphthoquinone (**6.12**)



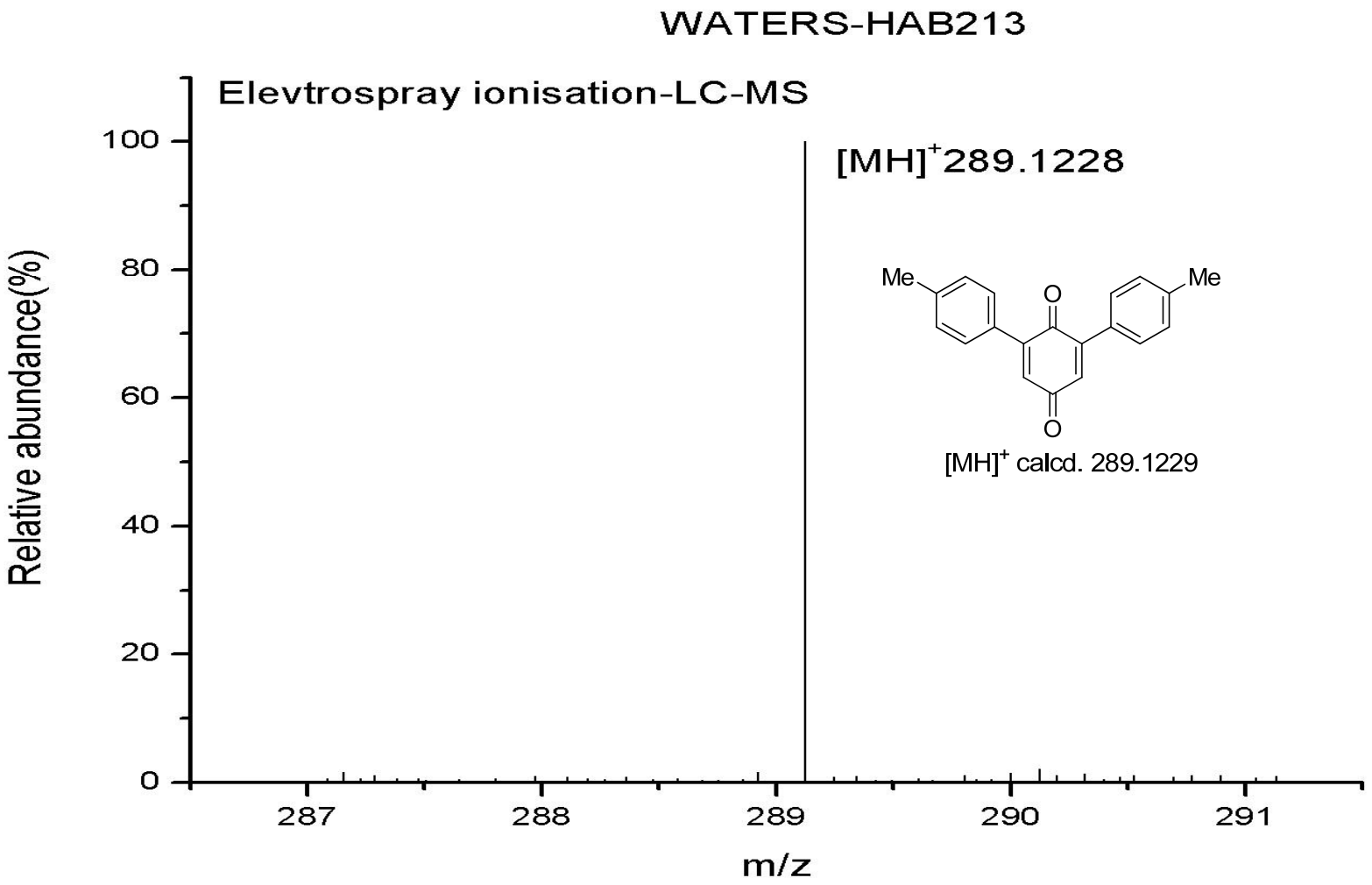
HRMS spectrum of 2,3-bis(4-(allyloxy)phenyl-1,4-naphthoquinone (**6.12**)



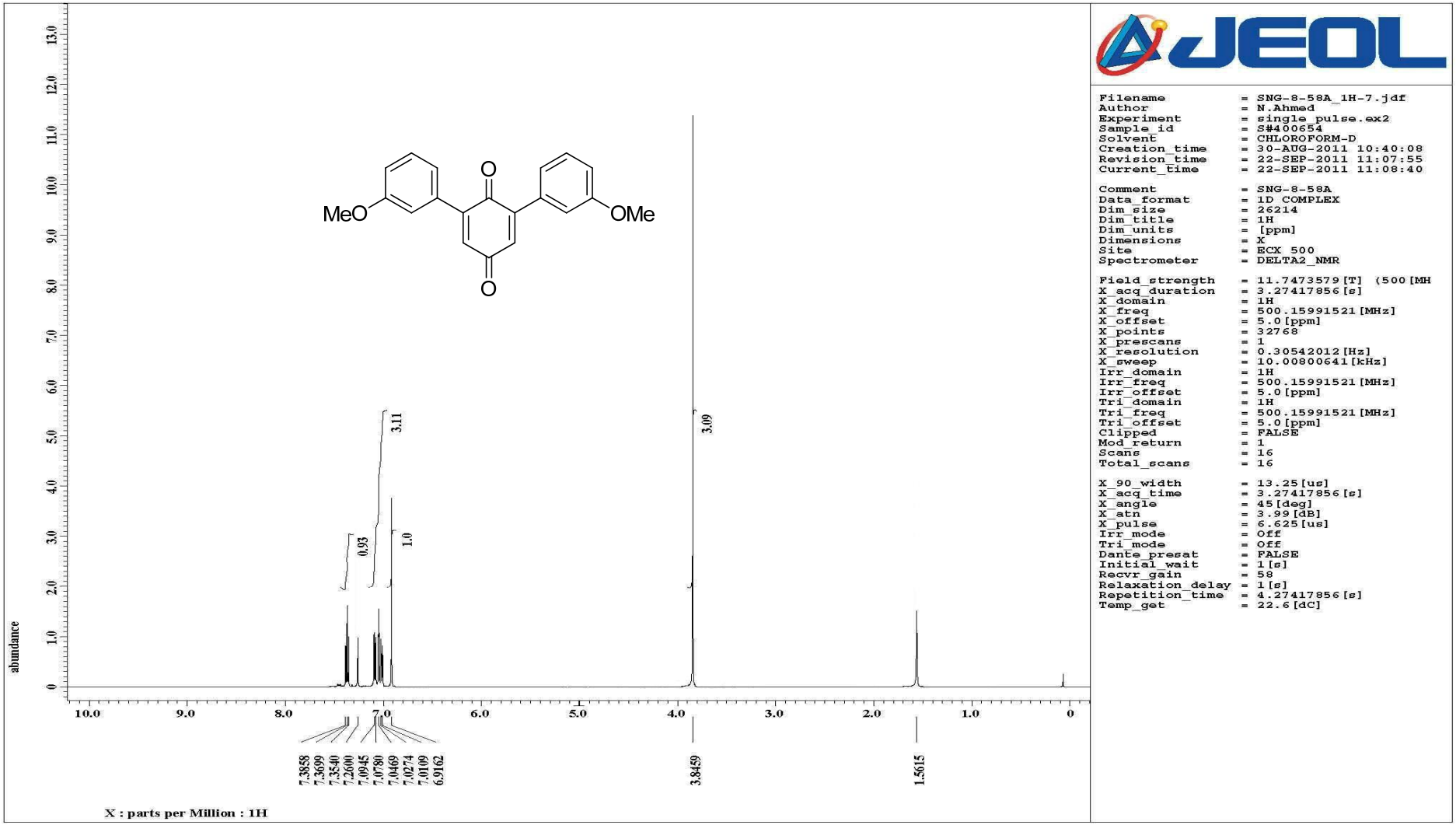
^{1}H NMR spectrum of 2,6-di-(4-methylphenyl)-1,4-benzoquinone (**7.1**)



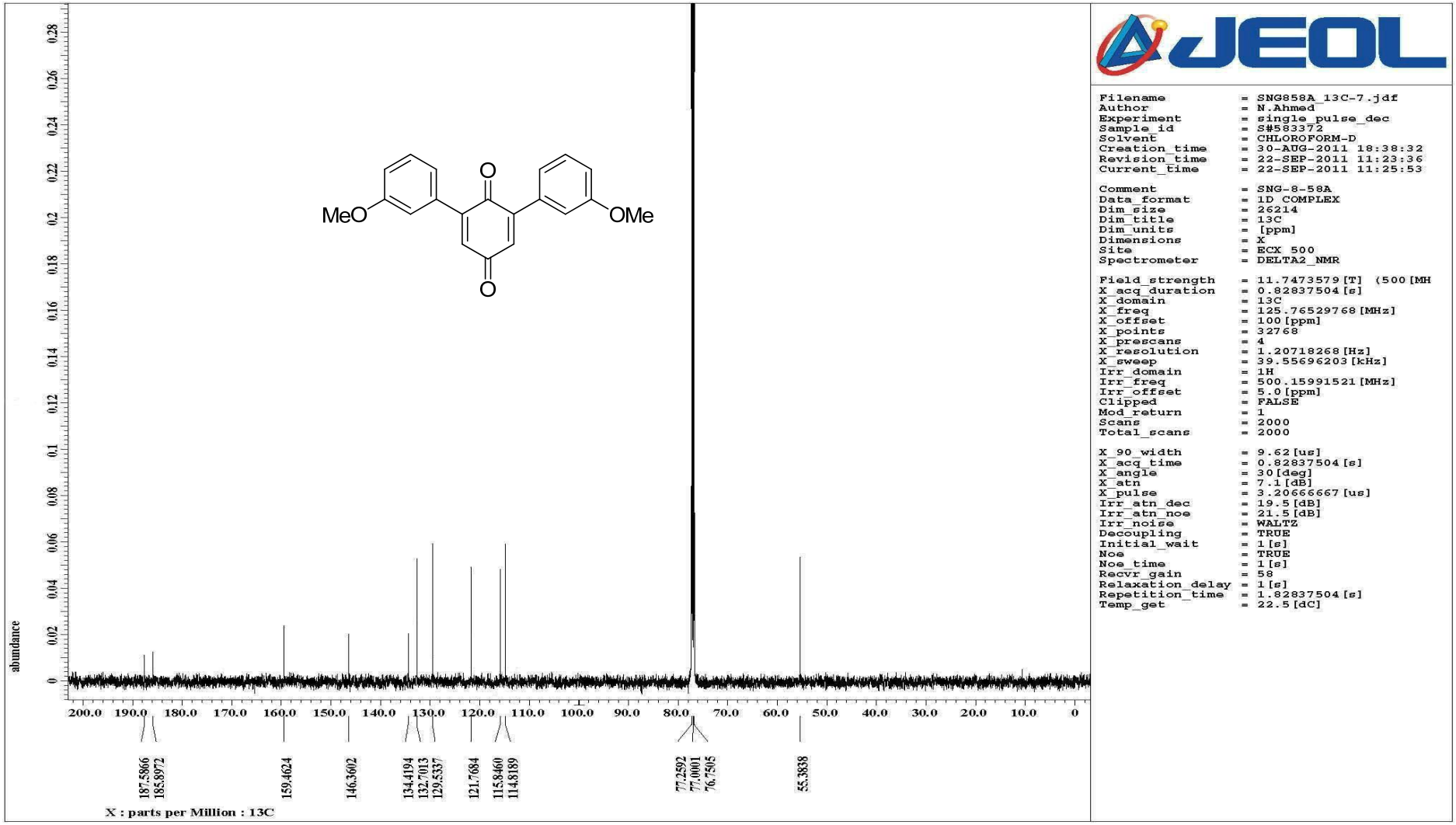
^{13}C NMR spectrum of 2,6-di-(4-methylphenyl)-1,4-benzoquinone (**7.1**)



HRMS spectrum of 2,6-di-(4-methylphenyl)-1,4-benzoquinone (**7.1**)



^{1}H NMR spectrum of 2,6-bis(3-methoxyphenyl)-1,4-benzoquinone (**7.2**)

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Solvent           = CHLOROFORM-D
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Revision_time     = 22-SEP-2011 11:23:36
Current_time      = 22-SEP-2011 11:25:53

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X_sweep           = 39.55696203[kHz]
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Irr_offset        = 5.0[ppm]
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Total_scans       = 2000

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X_pulse           = 3.20666667[us]
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Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
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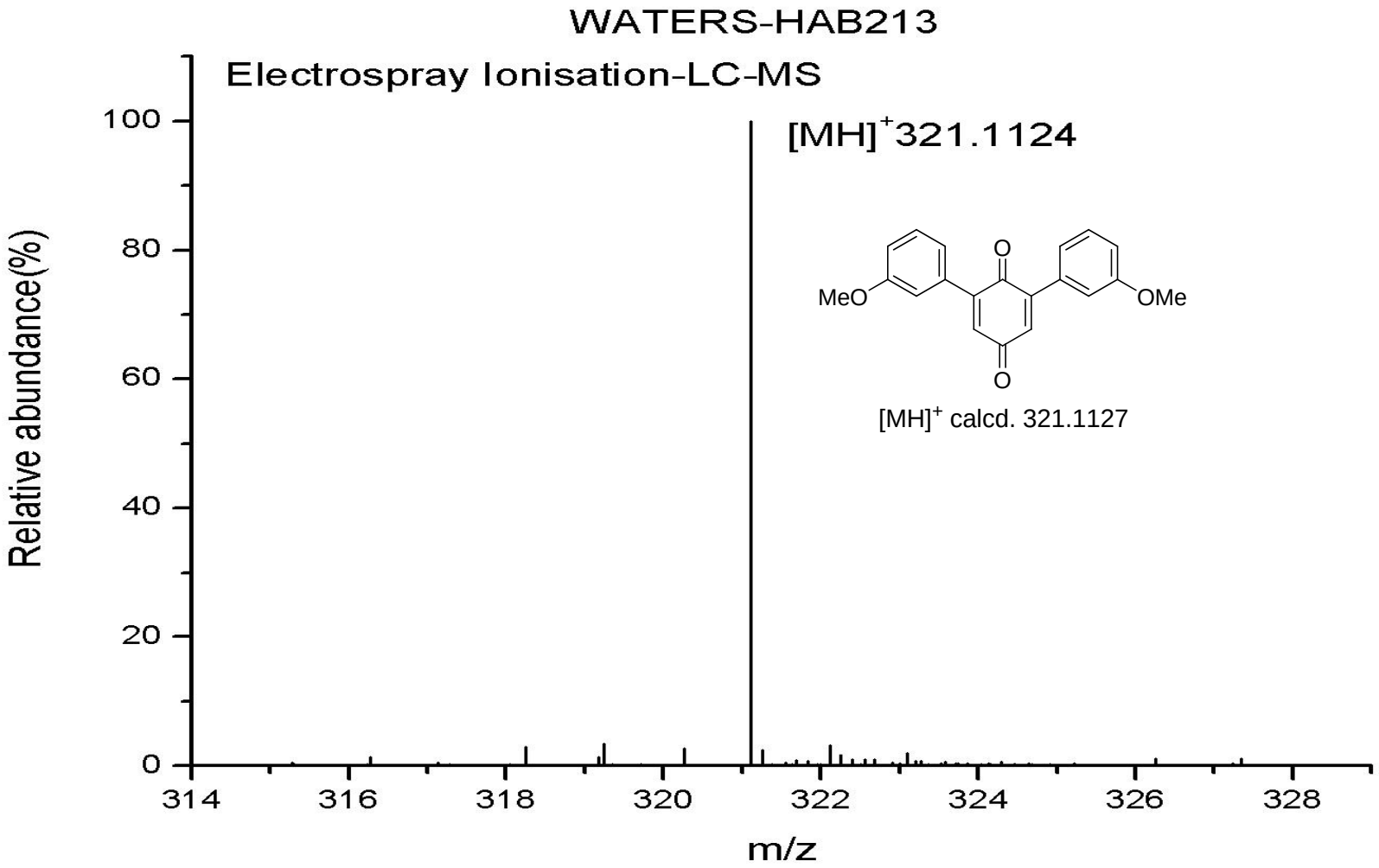
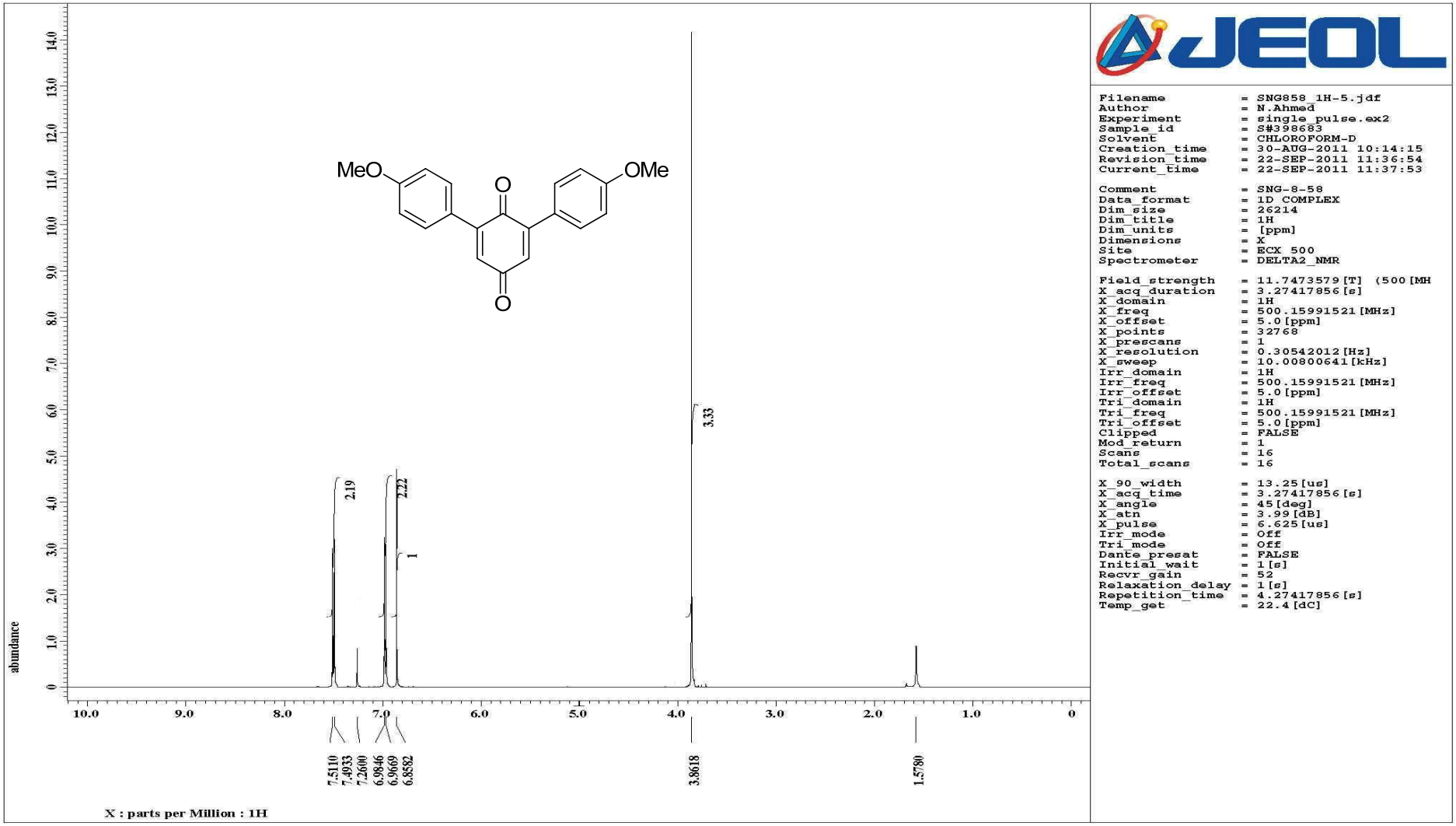
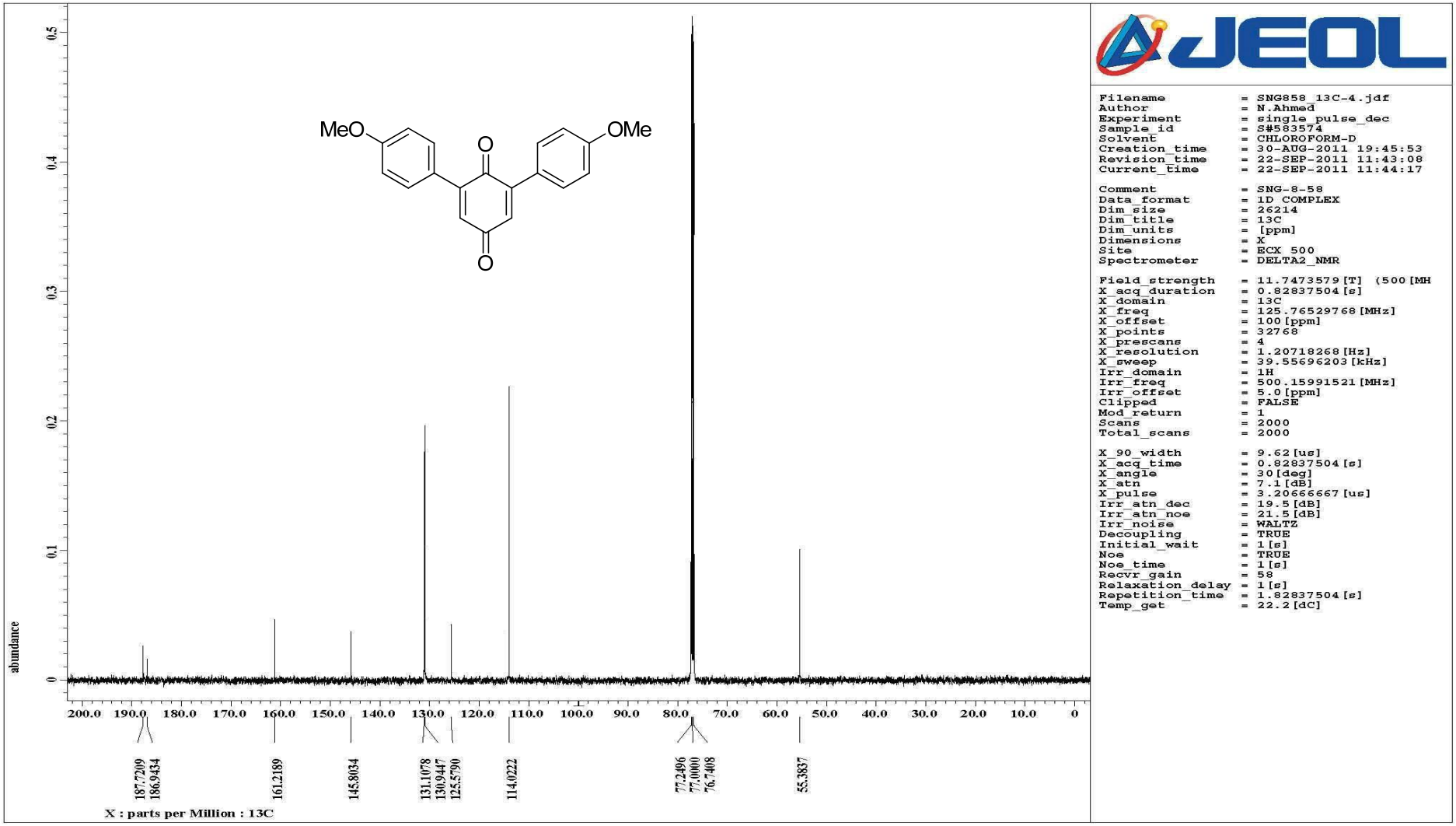
^{13}C NMR spectrum of 2,6-bis(3-methoxyphenyl)-1,4-benzoquinone (**7.2**)



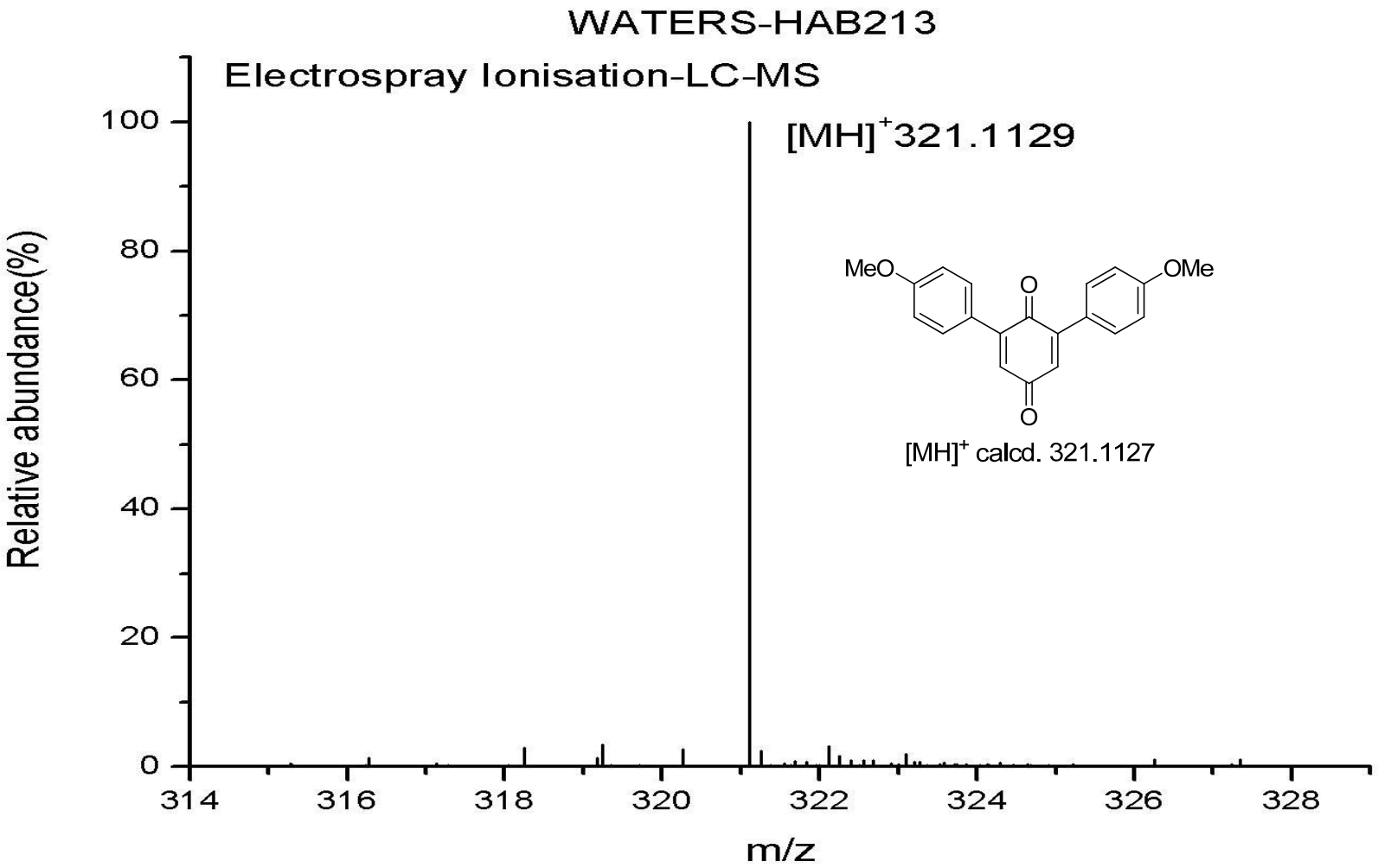
HRMS spectrum of 2,6-bis(3-methoxyphenyl)-1,4-benzoquinone (**7.2**)



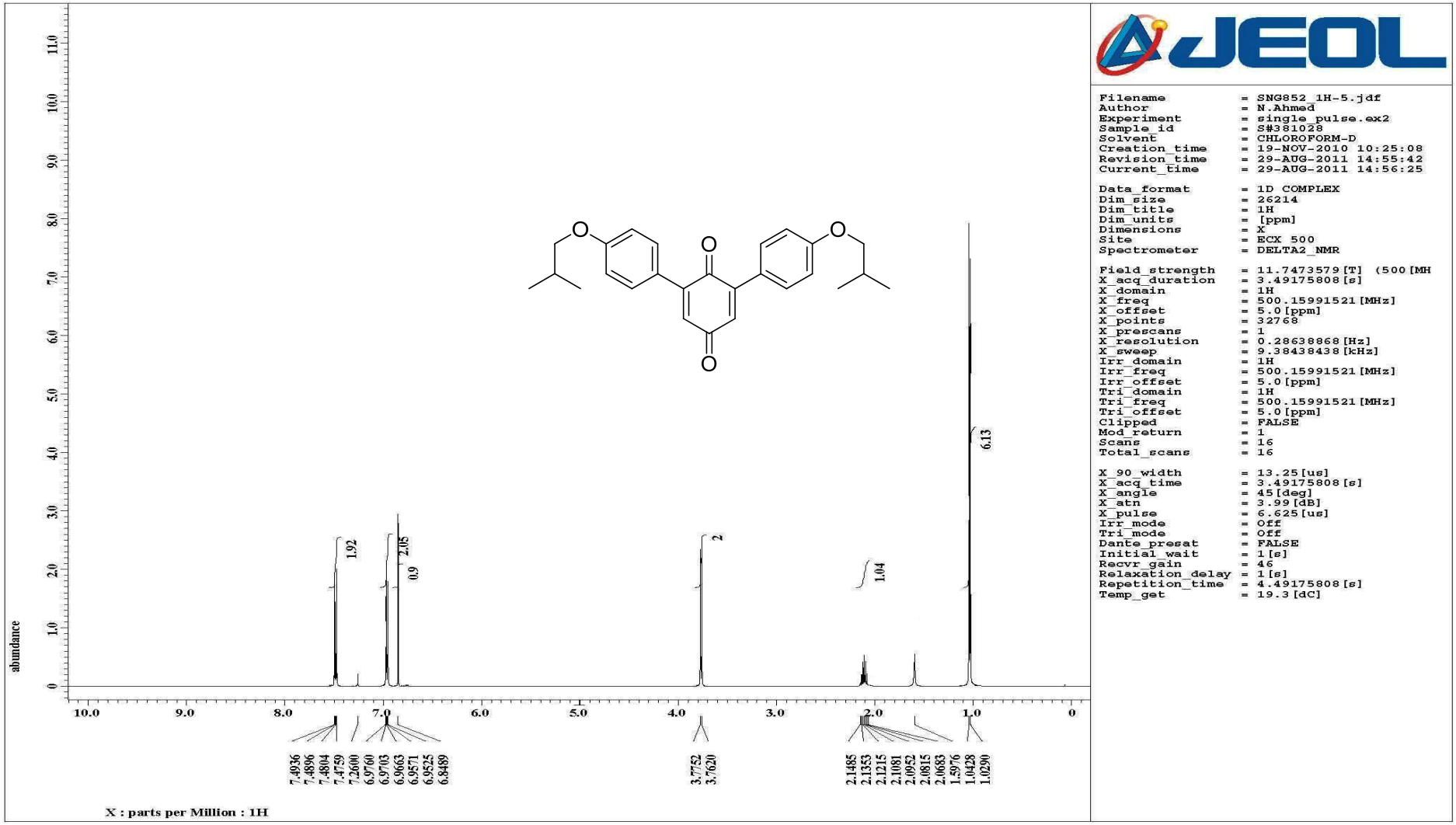
^{1}H NMR spectrum of 2,6-bis(4-methoxyphenyl)-1,4-benzoquinone (**7.3**)



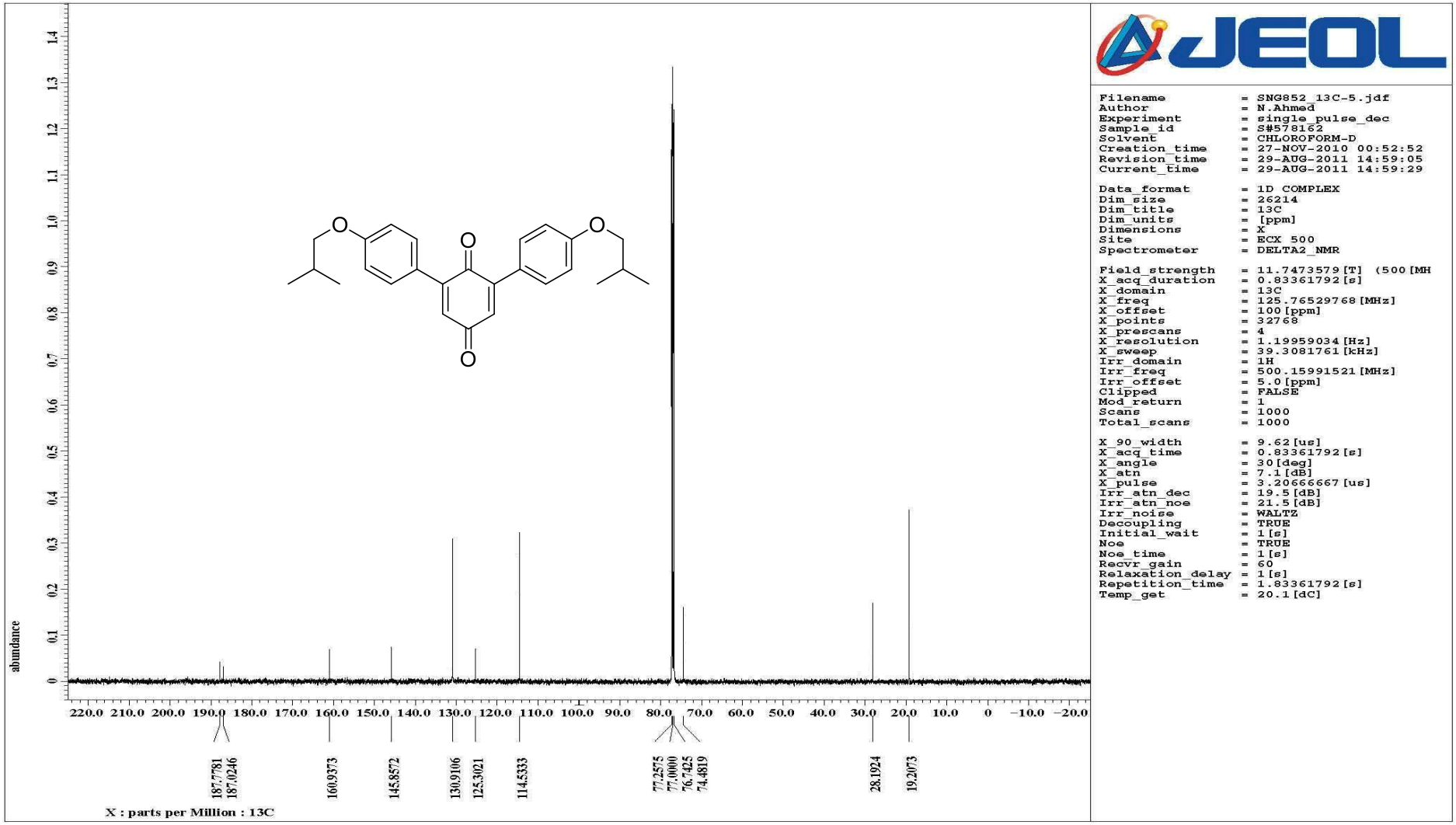
^{13}C NMR spectrum of 2,6-bis(4-methoxyphenyl)-1,4-benzoquinone (**7.3**)



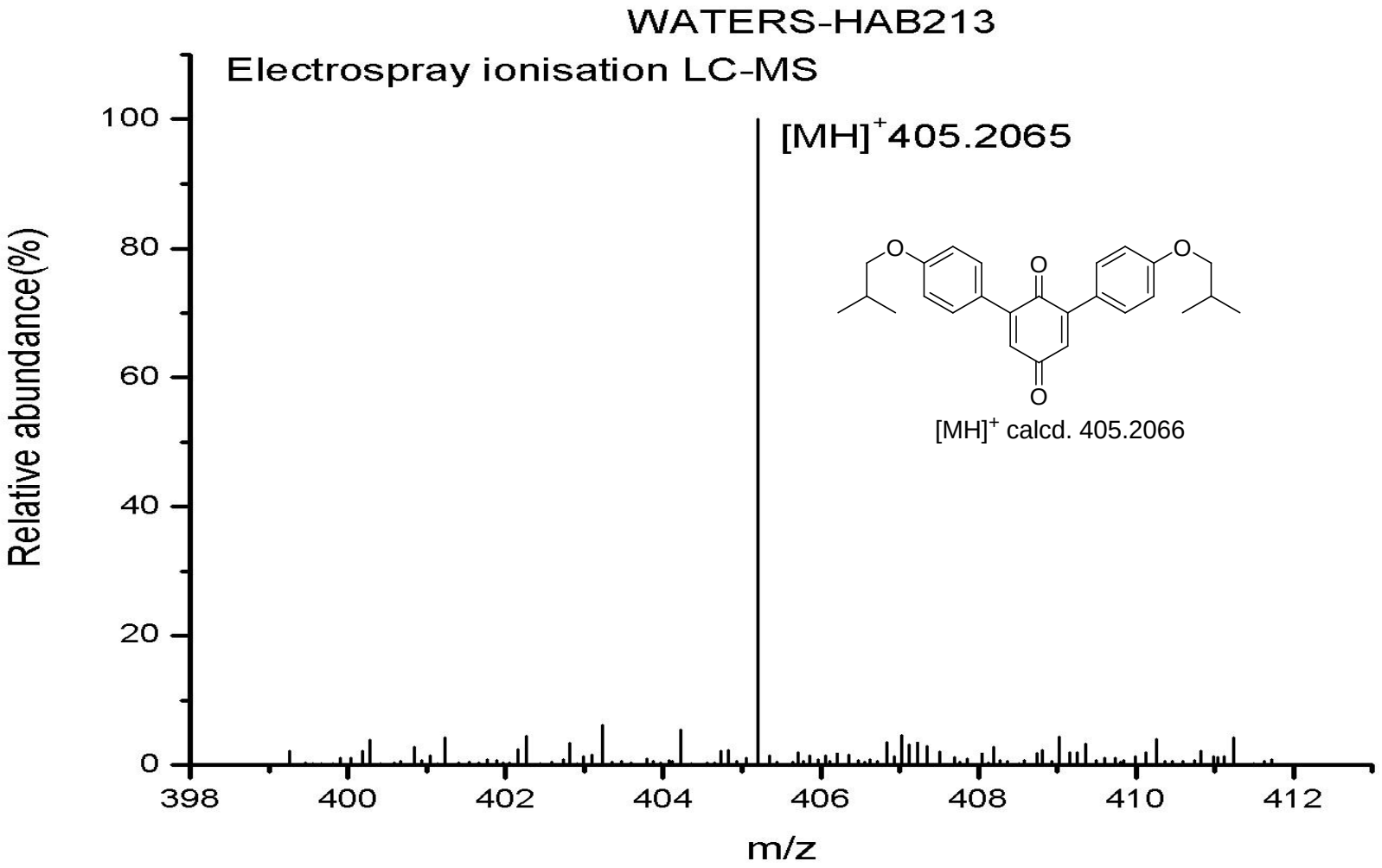
HRMS spectrum of 2,6-bis(4-methoxyphenyl)-1,4-benzoquinone (**7.3**)



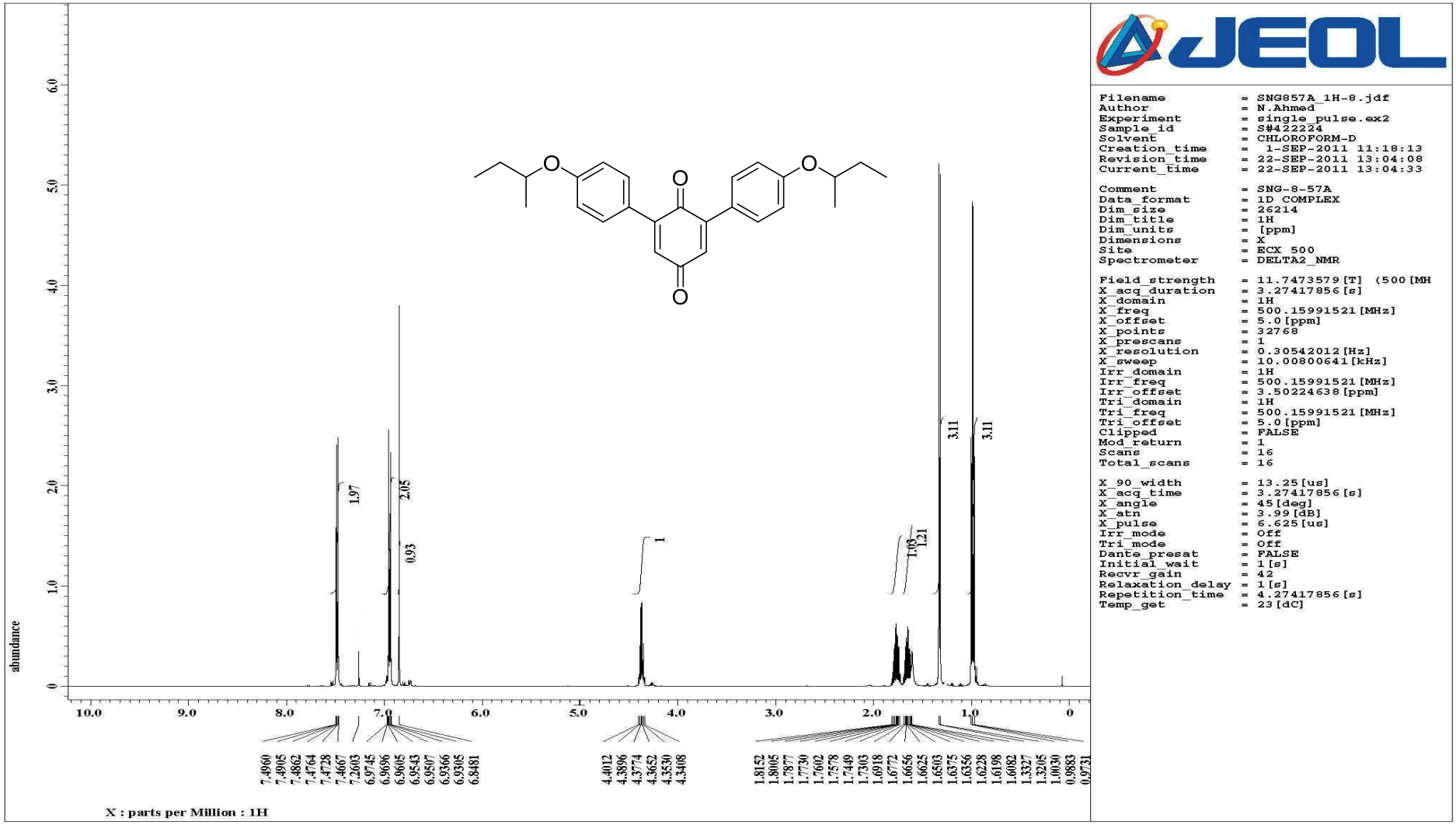
^{1}H NMR spectrum of 2,6-bis(4-isobutoxyphenyl)-1,4-benzoquinone (**7.4**)



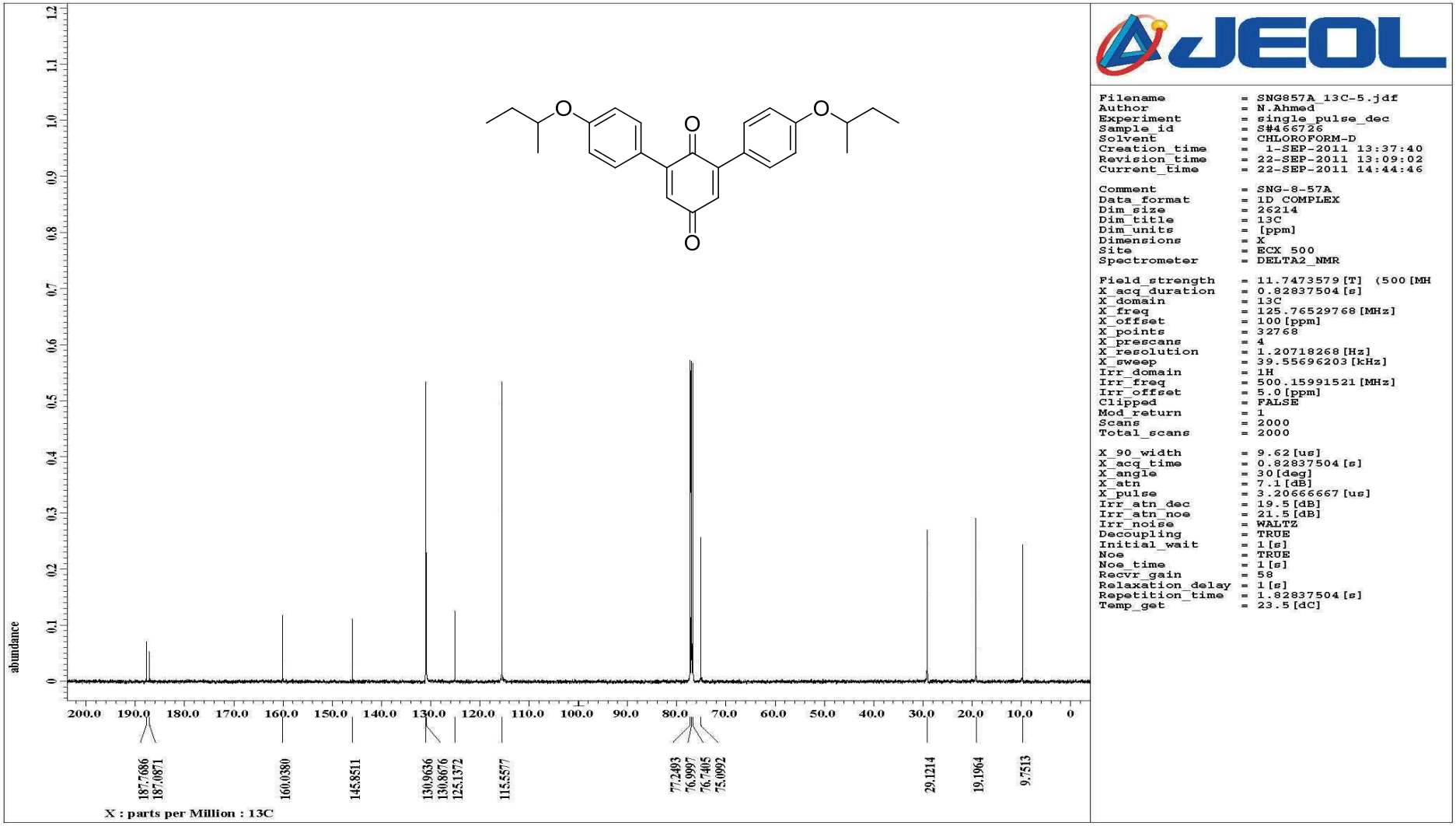
^{13}C NMR spectrum of 2,6-bis(4-isobutoxyphenyl)-1,4-benzoquinone (**7.4**)



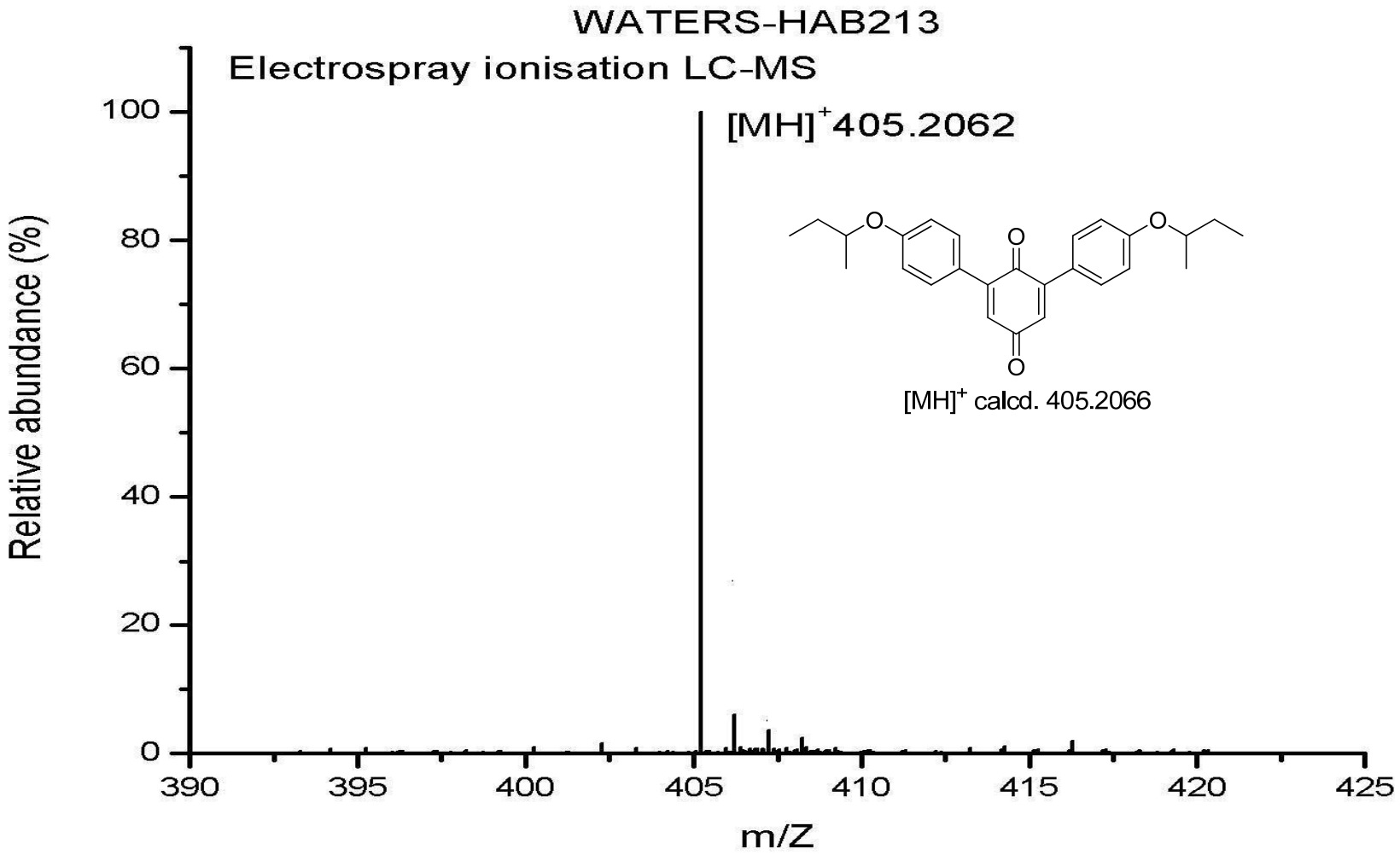
HRMS spectrum of 2,6-bis(4-isobutoxyphenyl)-1,4-benzoquinone (**7.4**)



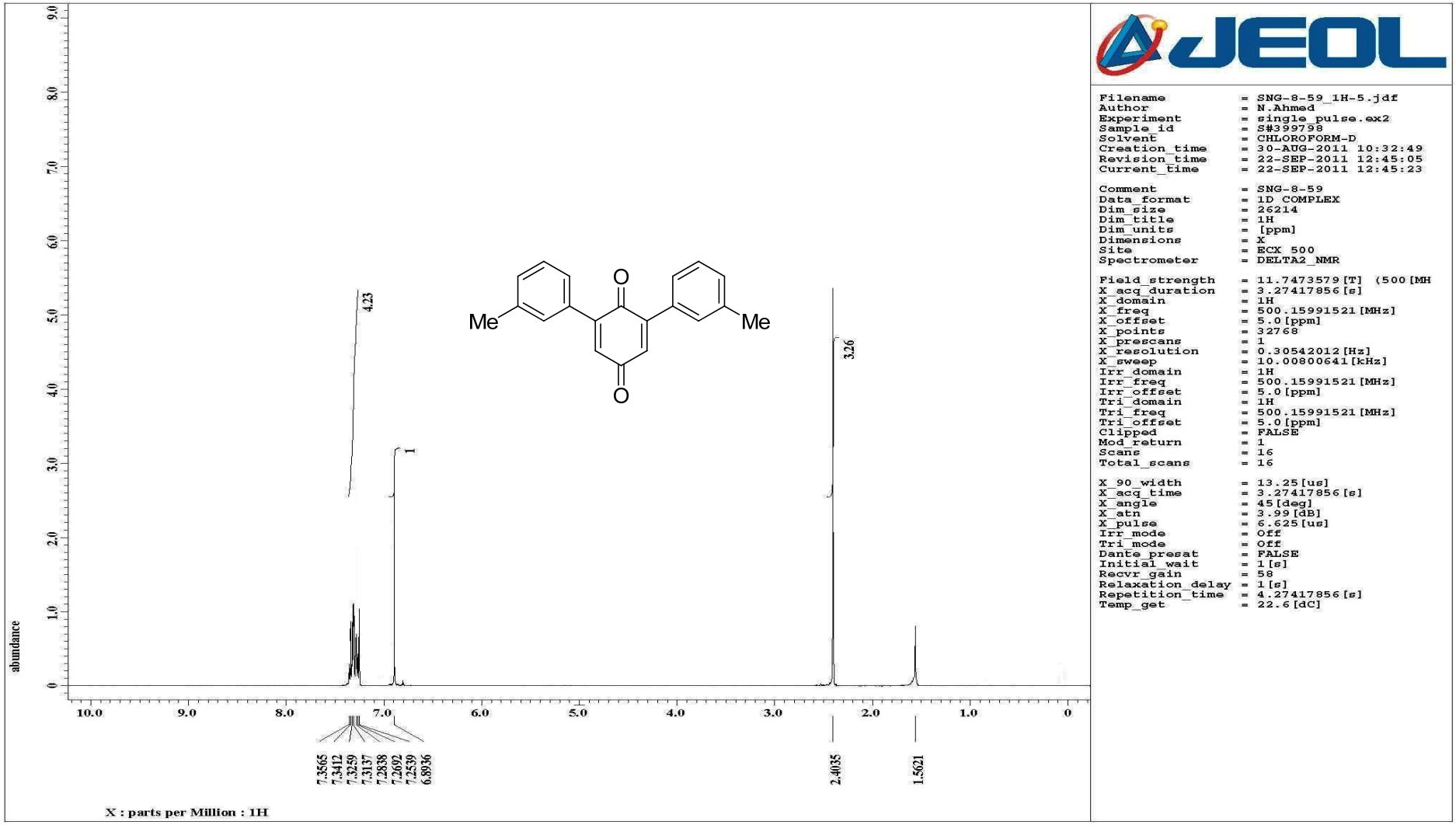
^{1}H NMR spectrum of 2,6-bis(4-sec-butoxyphenyl)-1,4-benzoquinone (**7.5**)



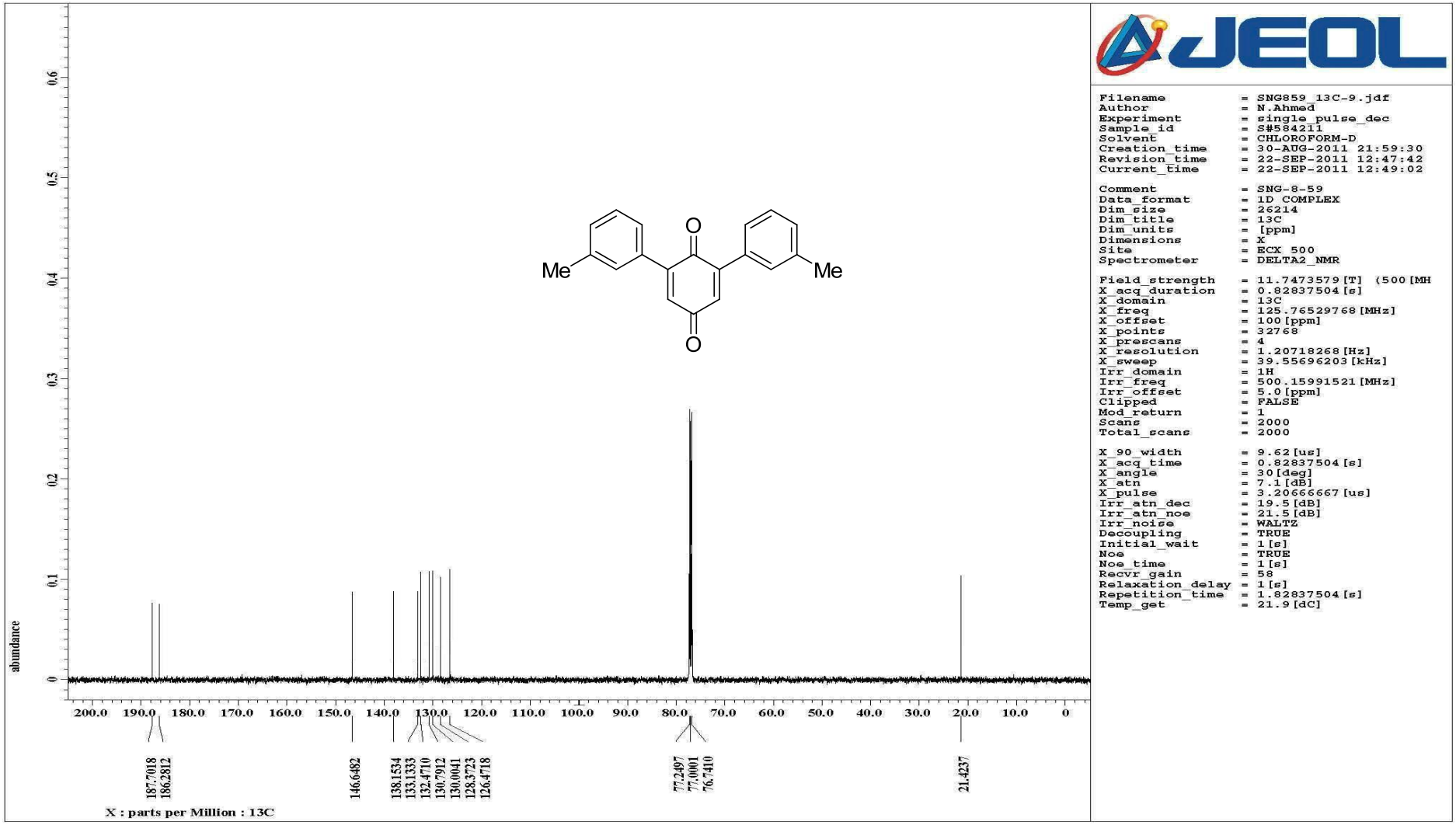
^{13}C NMR spectrum of 2,6-bis(4-sec-butoxyphenyl)-1,4-benzoquinone (**7.5**)



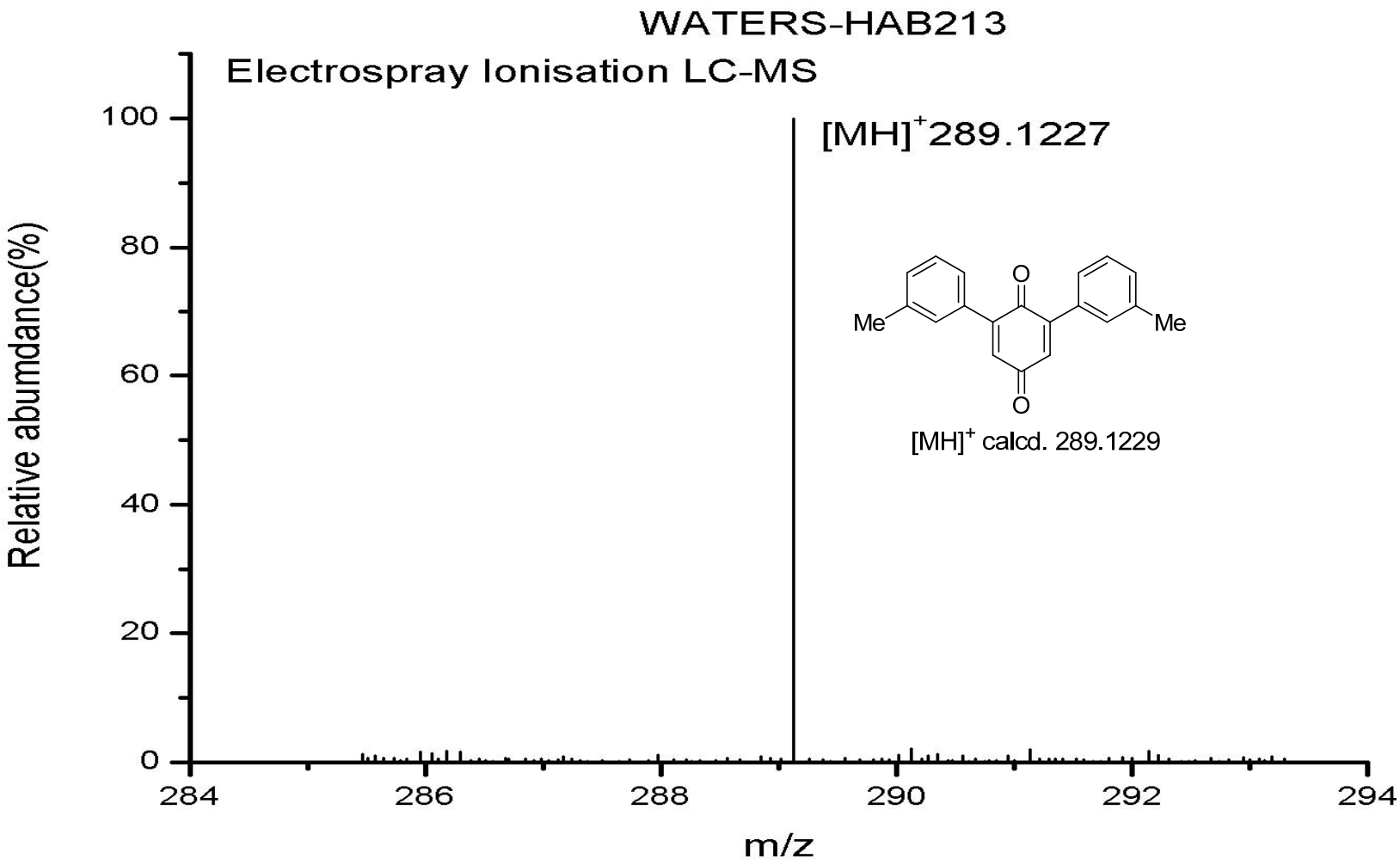
HRMS spectrum of 2,6-bis(4-sec-butoxyphenyl)-1,4-benzoquinone (**7.5**)



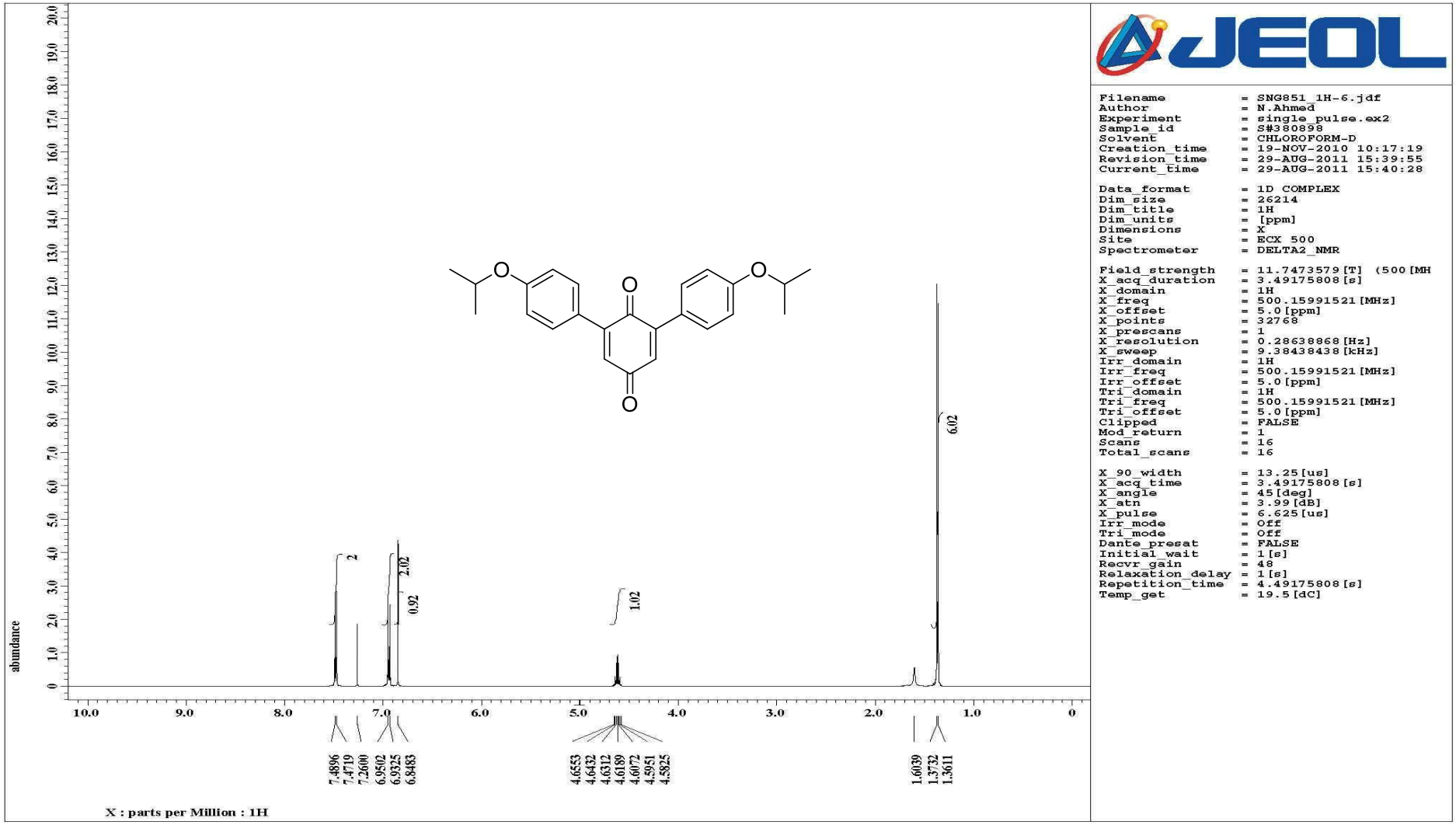
^{1}H NMR spectrum of 2,6-di-(3-methylphenyl)-1,4-benzoquinone (**7.6**)



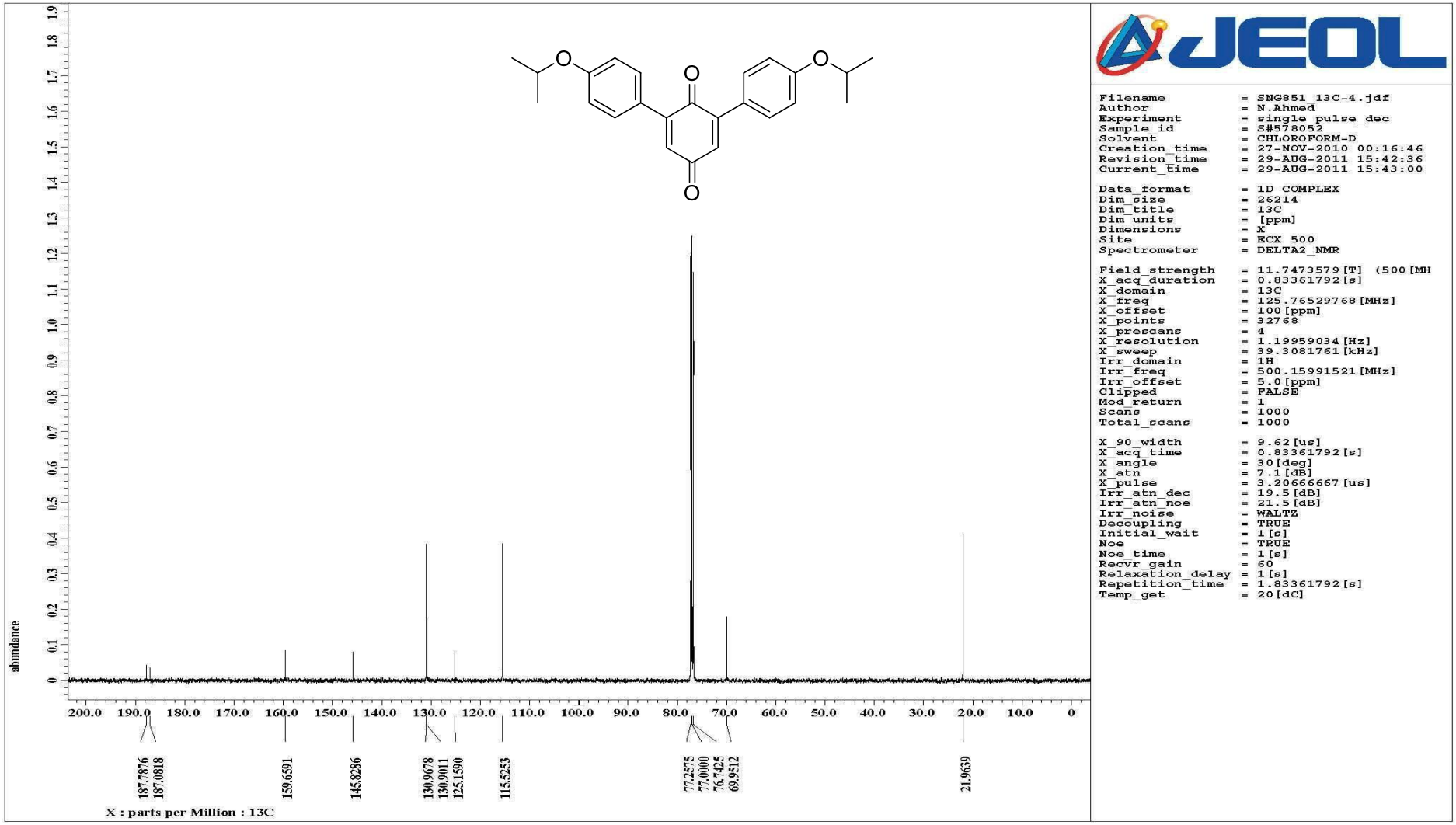
^{13}C NMR spectrum of 2,6-di-(3-methylphenyl)-1,4-benzoquinone (**7.6**)



HRMS spectrum of 2,6-di-(3-methylphenyl)-1,4-benzoquinone (**7.6**)



^{1}H spectrum of 2,6-bis(4-isopropoxyphenyl)-1,4-benzoquinone (**7.7**)



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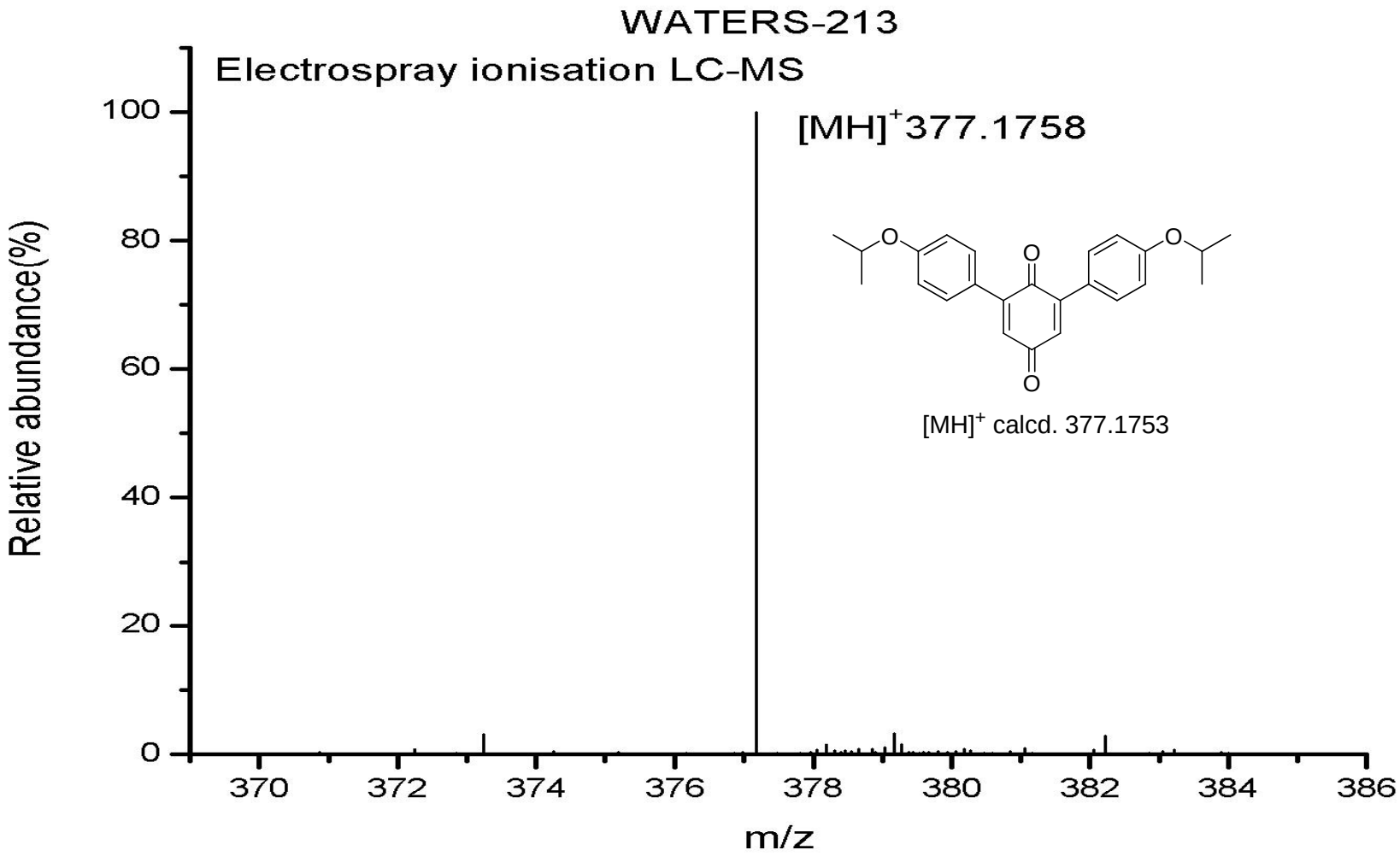
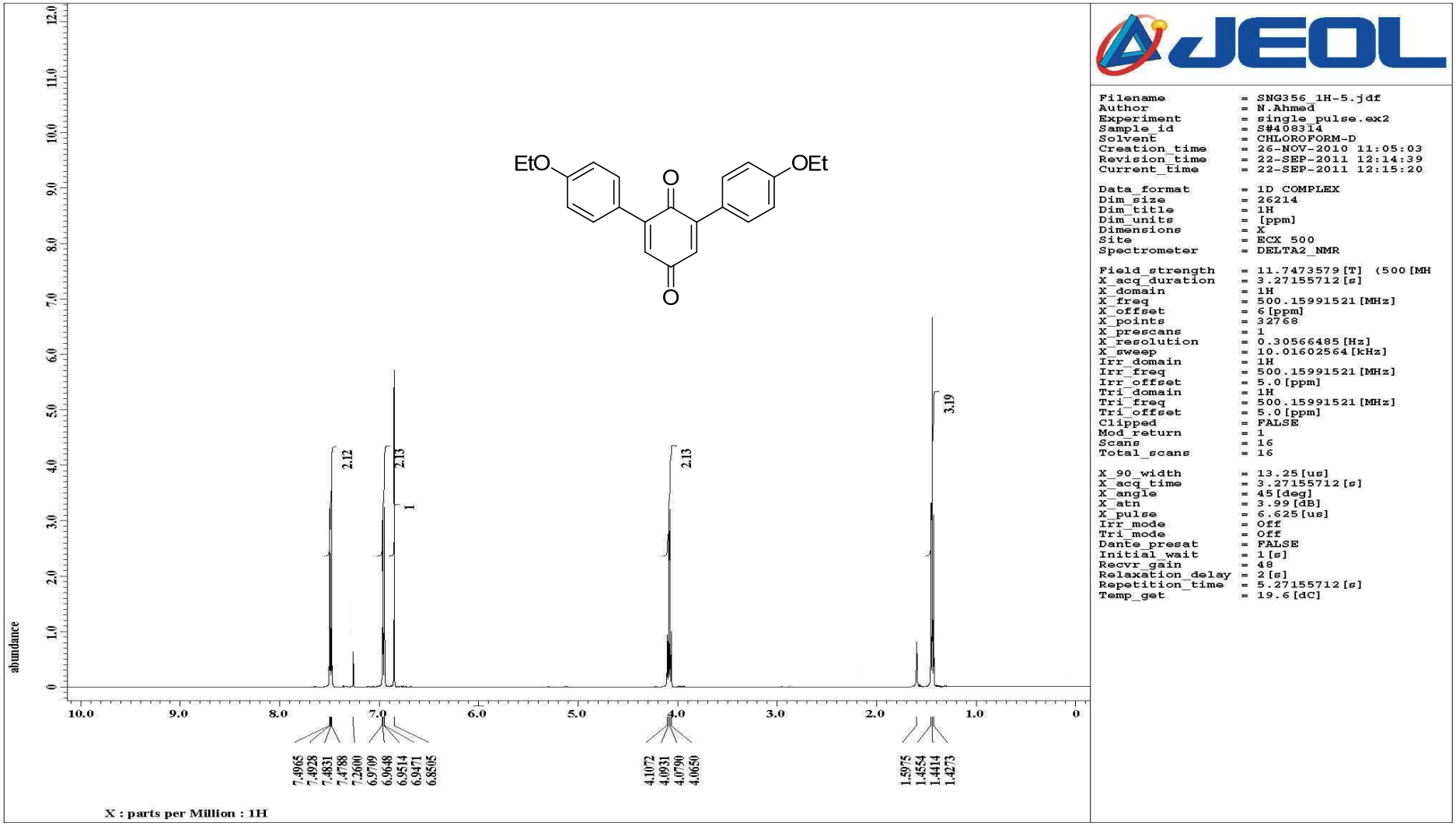
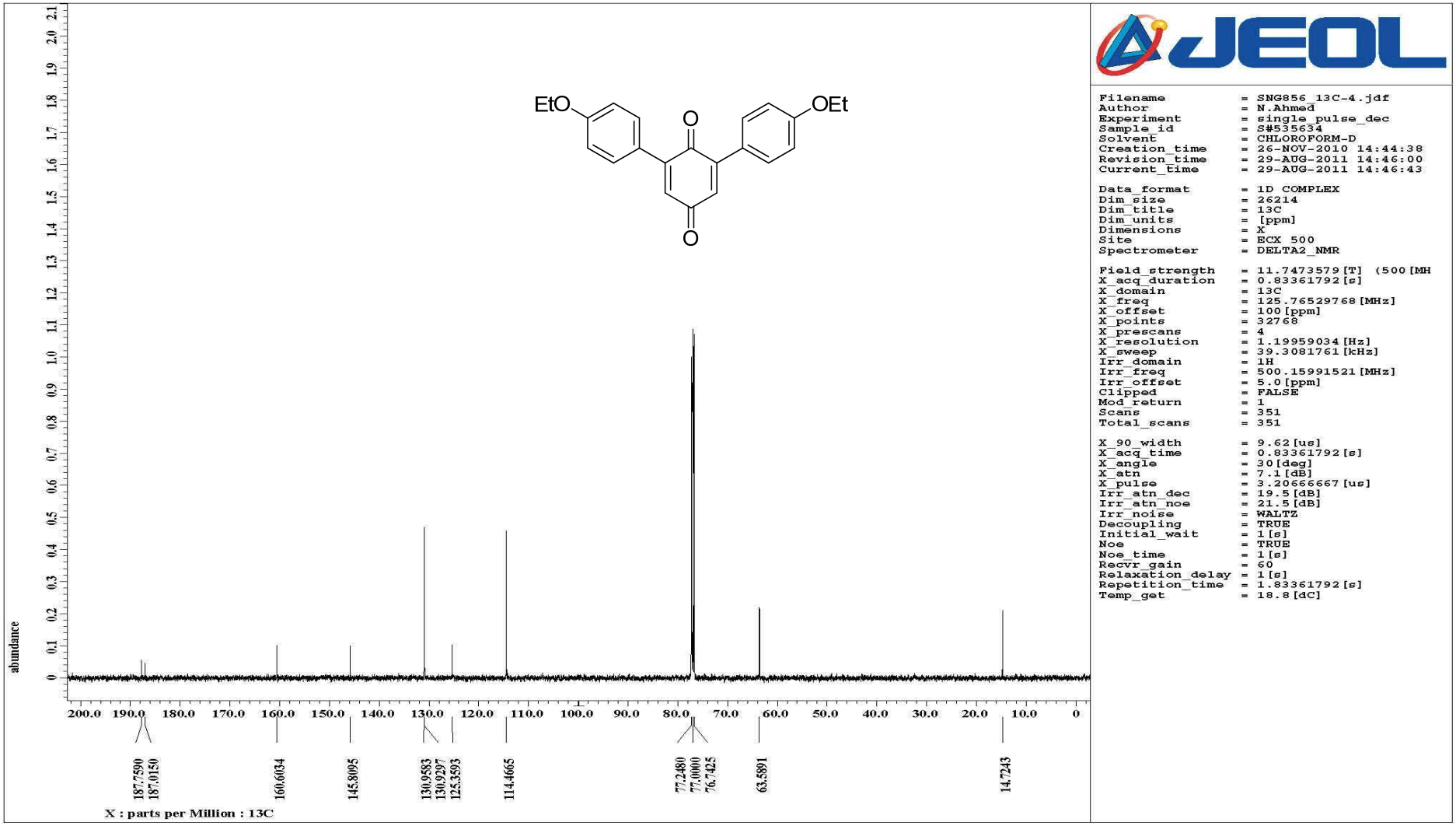
^{13}C NMR spectrum of 2,6-bis(4-isopropoxyphenyl)-1,4-benzoquinone (**7.7**)



HRMS spectrum of 2,6-bis(4-isopropoxyphenyl)-1,4-benzoquinone (**7.7**)



^{1}H NMR spectrum of 2,6-bis(4-ethoxyphenyl)-1,4-benzoquinone (**7.8**)

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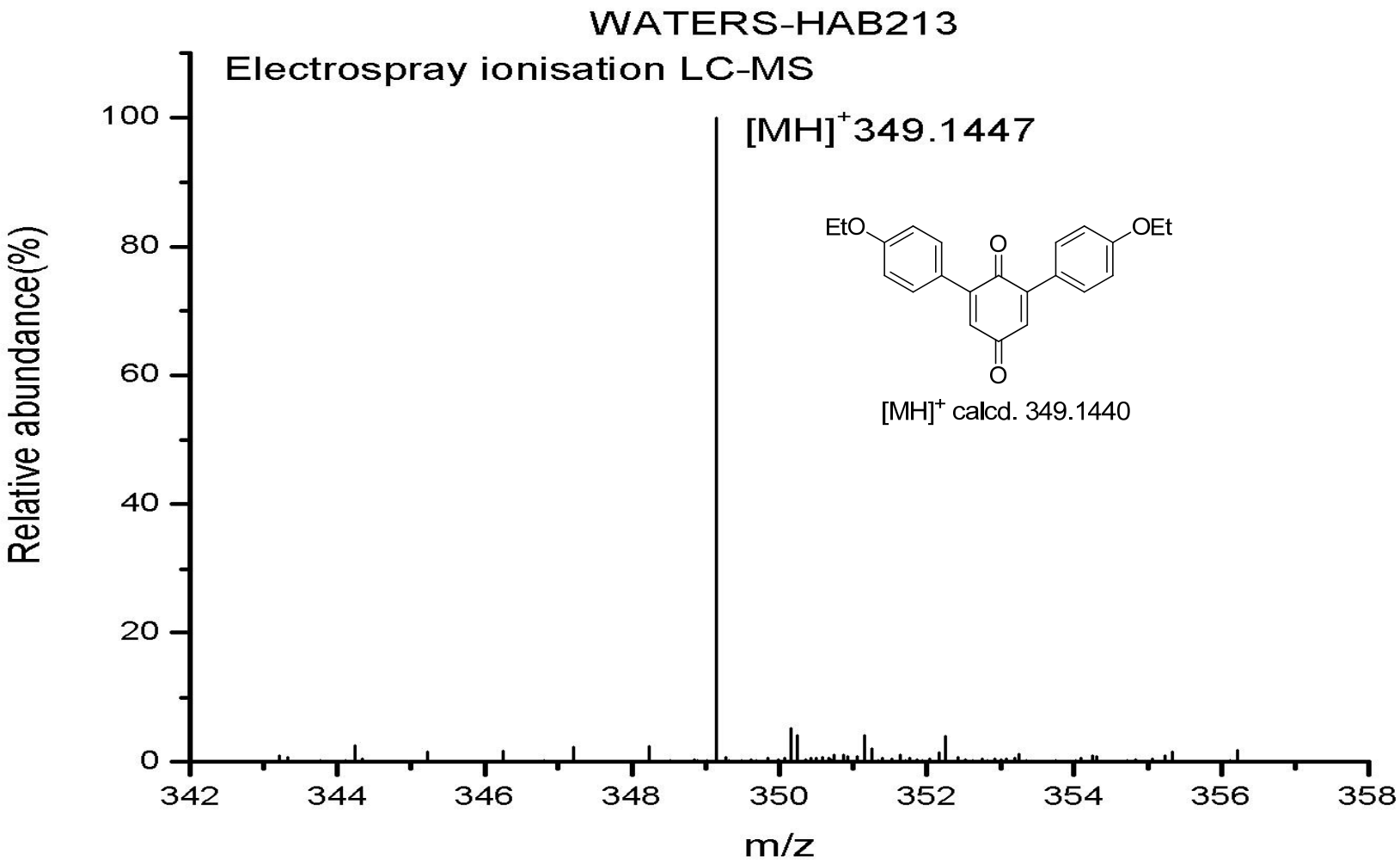
^{13}C NMR spectrum of 2,6-bis(4-ethoxyphenyl)-1,4-benzoquinone (**7.8**)



HRMS spectrum of 2,6-bis(4-ethoxyphenyl)-1,4-benzoquinone (**7.8**)