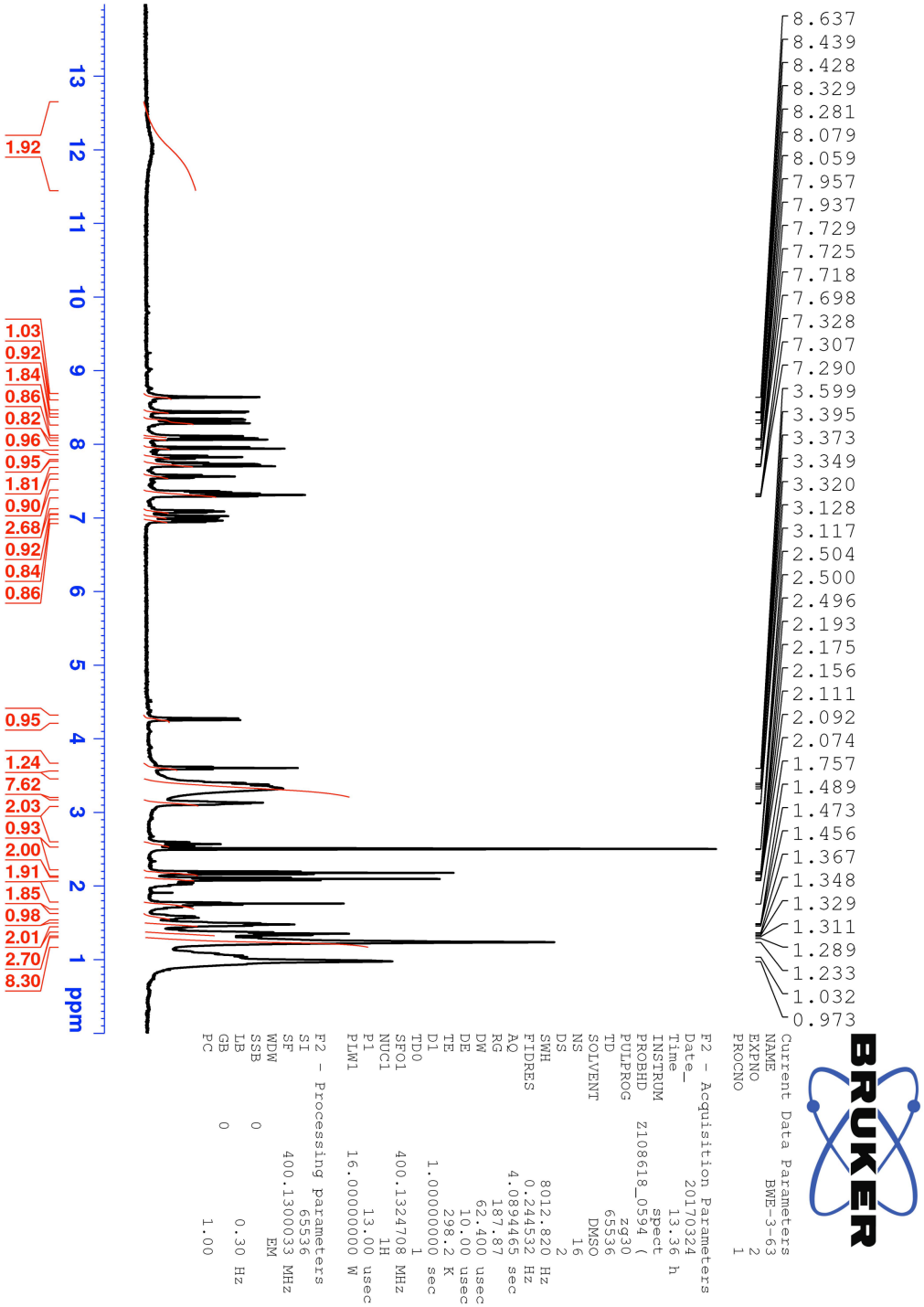
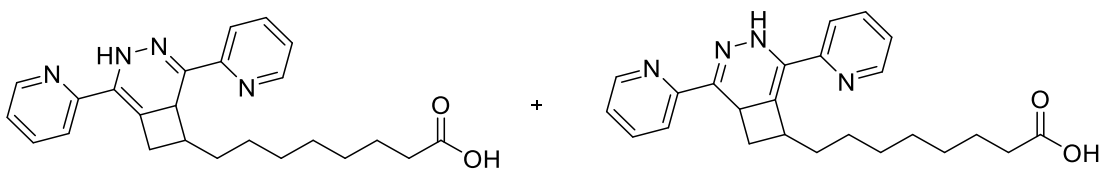
A Genetically Encoded Cyclobutene Probe for Labelling of Live Cells

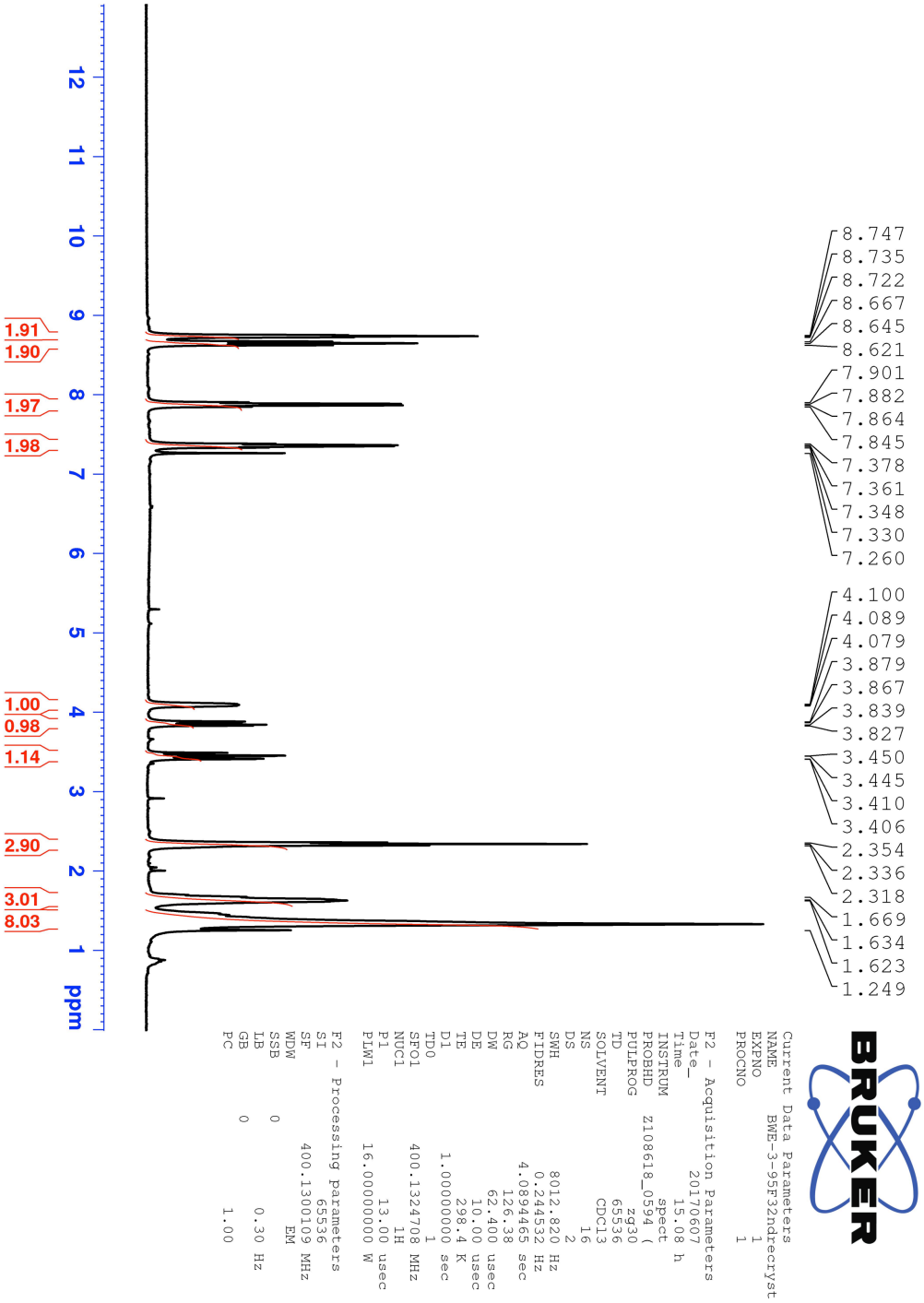
Electronic Supporting Information, Section 2: NMR spectra

Model studies of inverse electron-demand Diels-Alder (IEDDA)

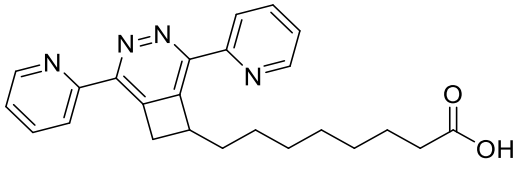


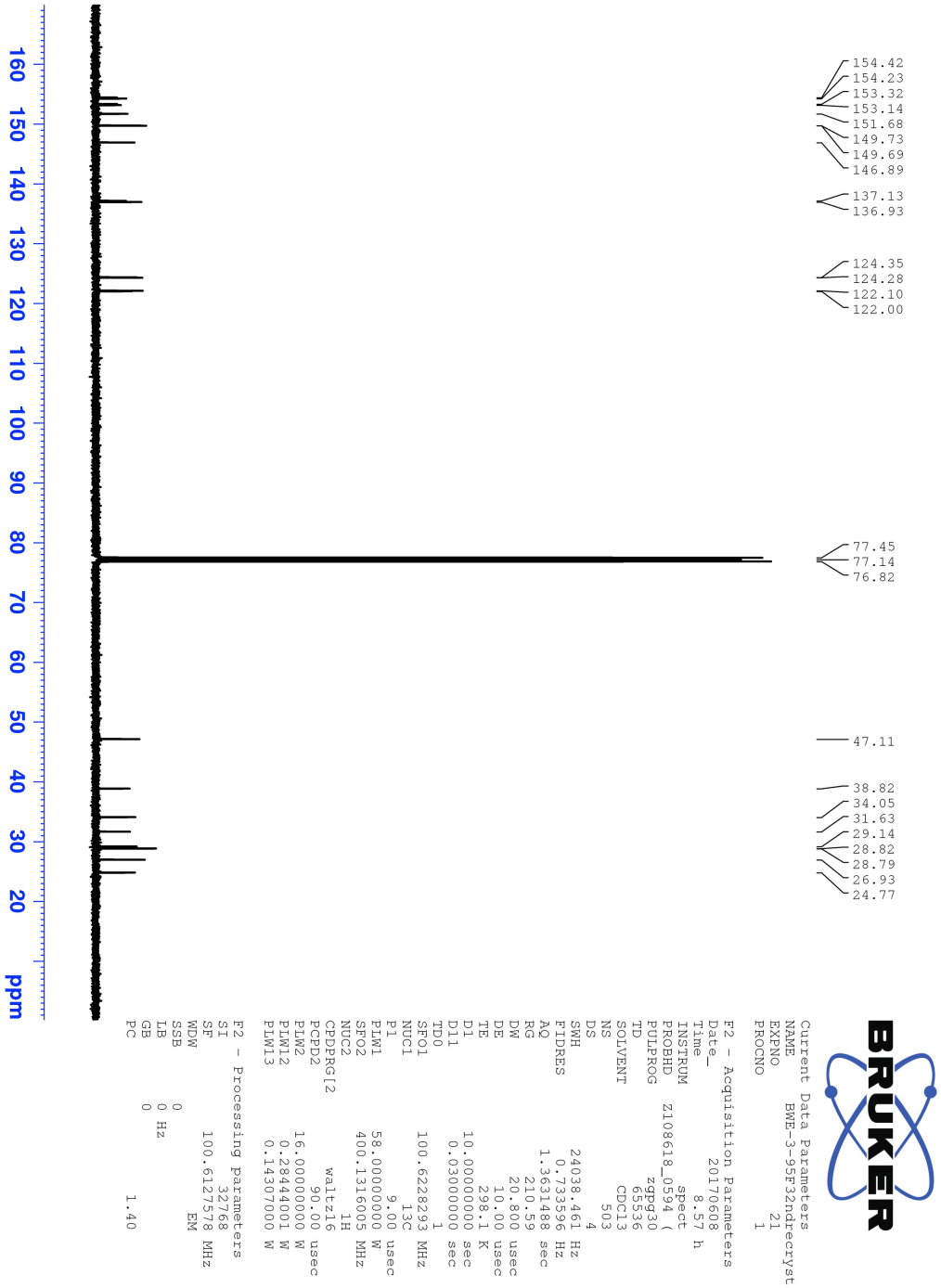
8-(2,5-Di(pyridin-2-yl)-3,4-diazabicyclo[4.2.0]octa-1,4-dien-7-yl)octanoic acid and **-2,5-dien-7-yl *tautomer.* (2a**, **2b)**





8-(2,5-Di(pyridin-2-yl)-3,4-diazabicyclo[4.2.0]octa-1,3,5-trien-7-yl)octanoic acid (one-pot cycloaddition/aromatizatio). ^{1}H spectrum





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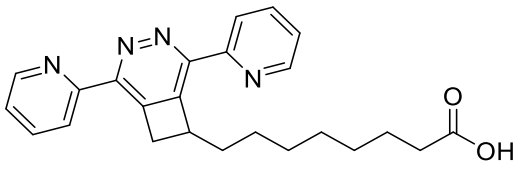
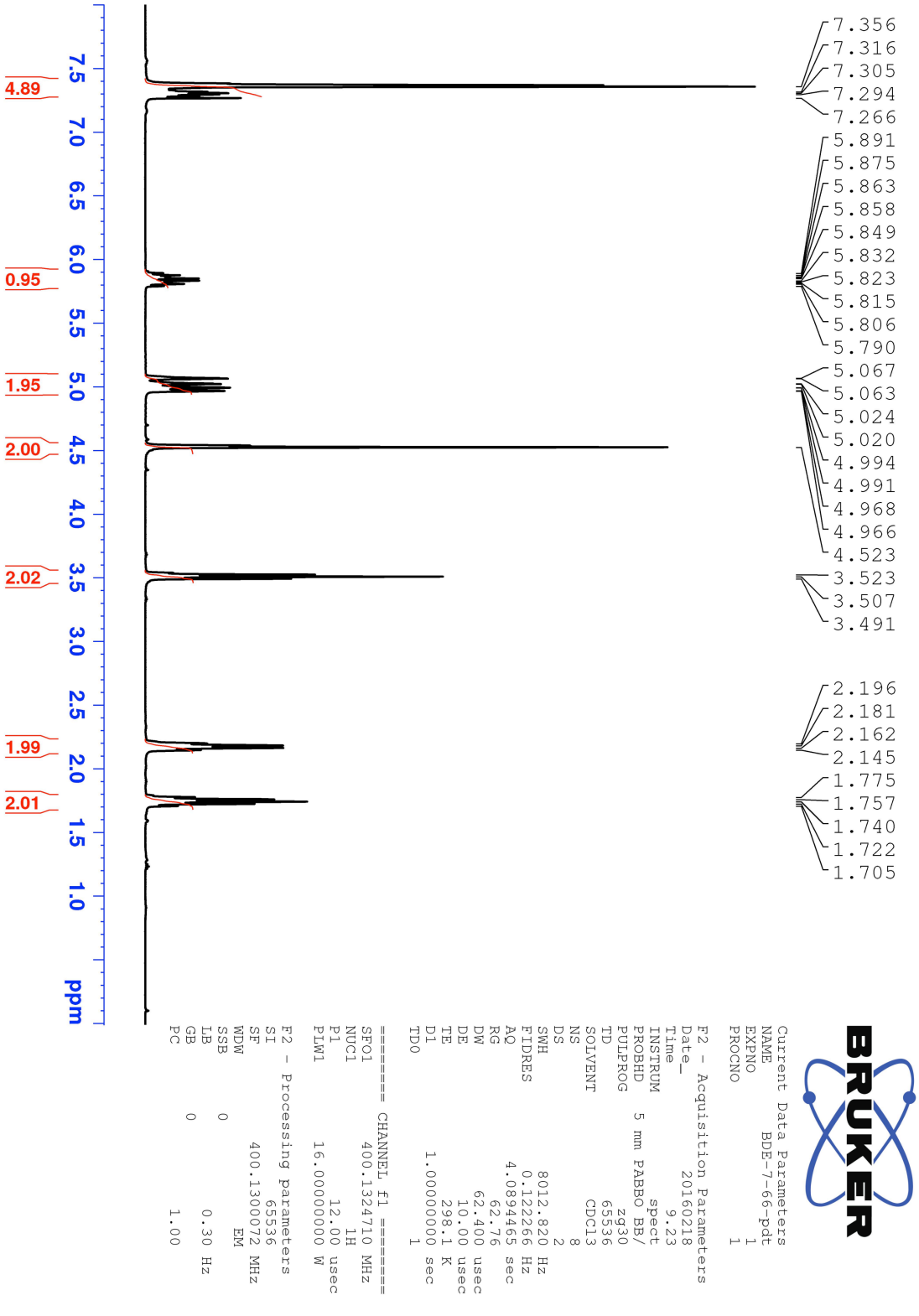
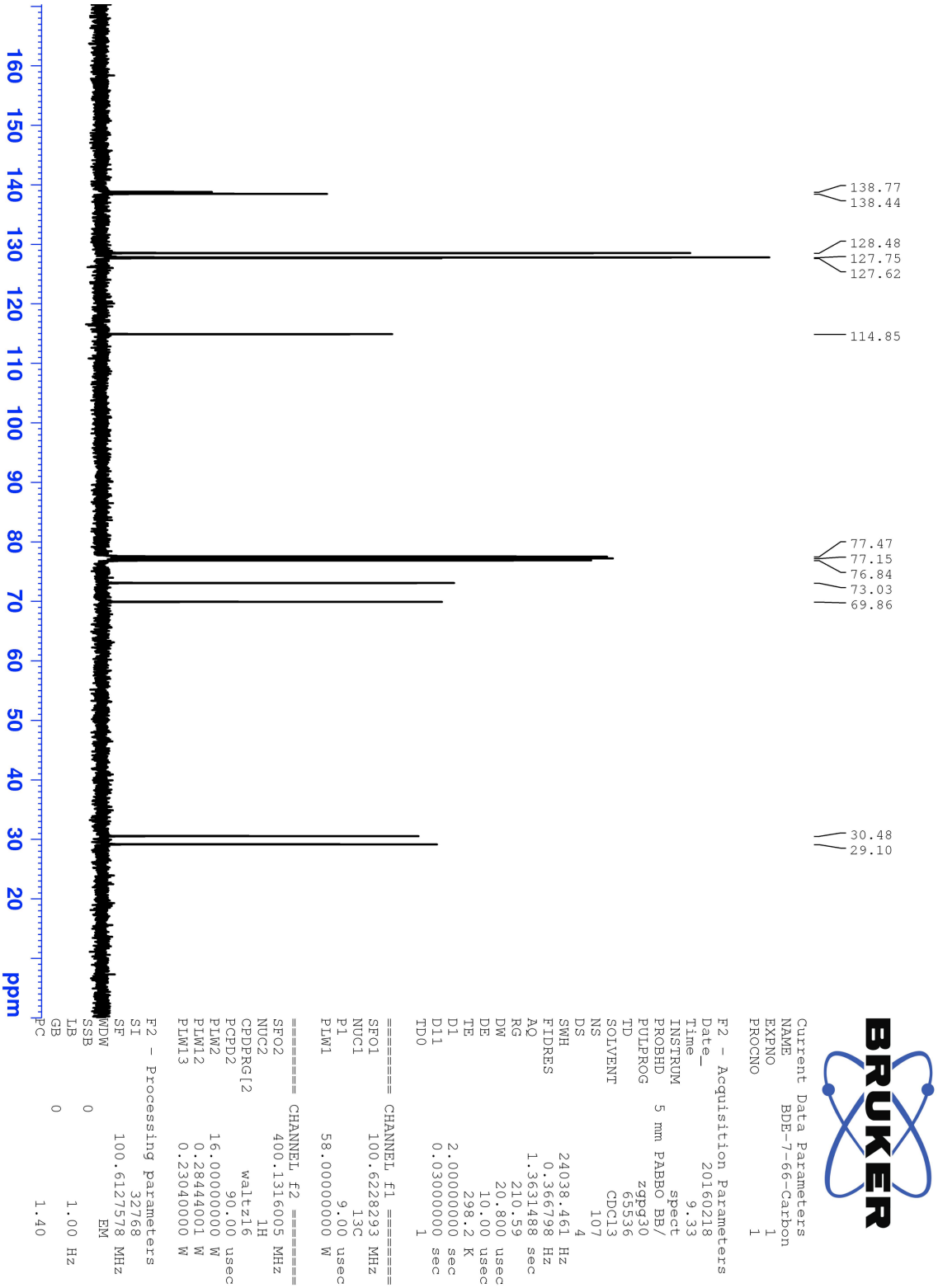
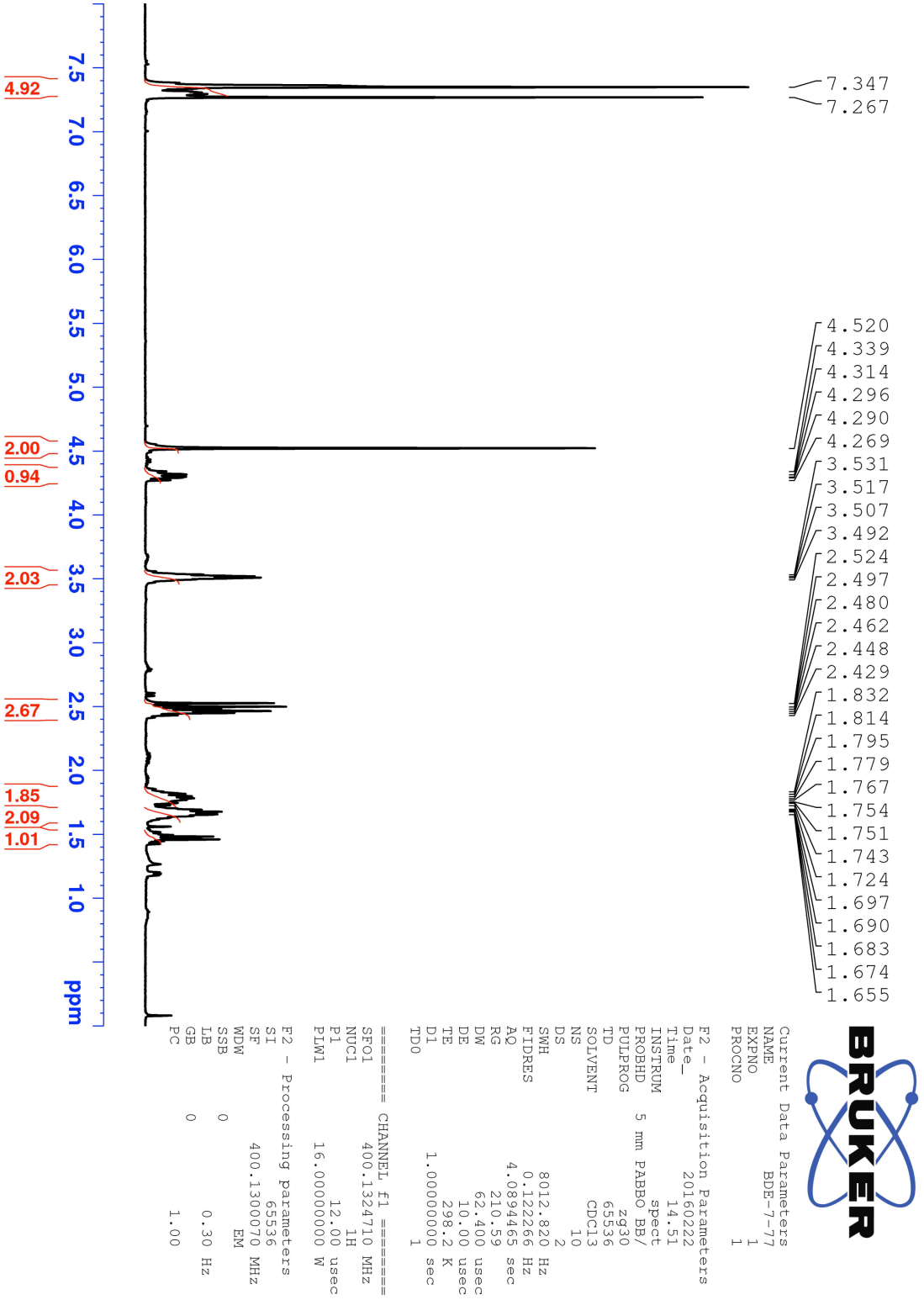




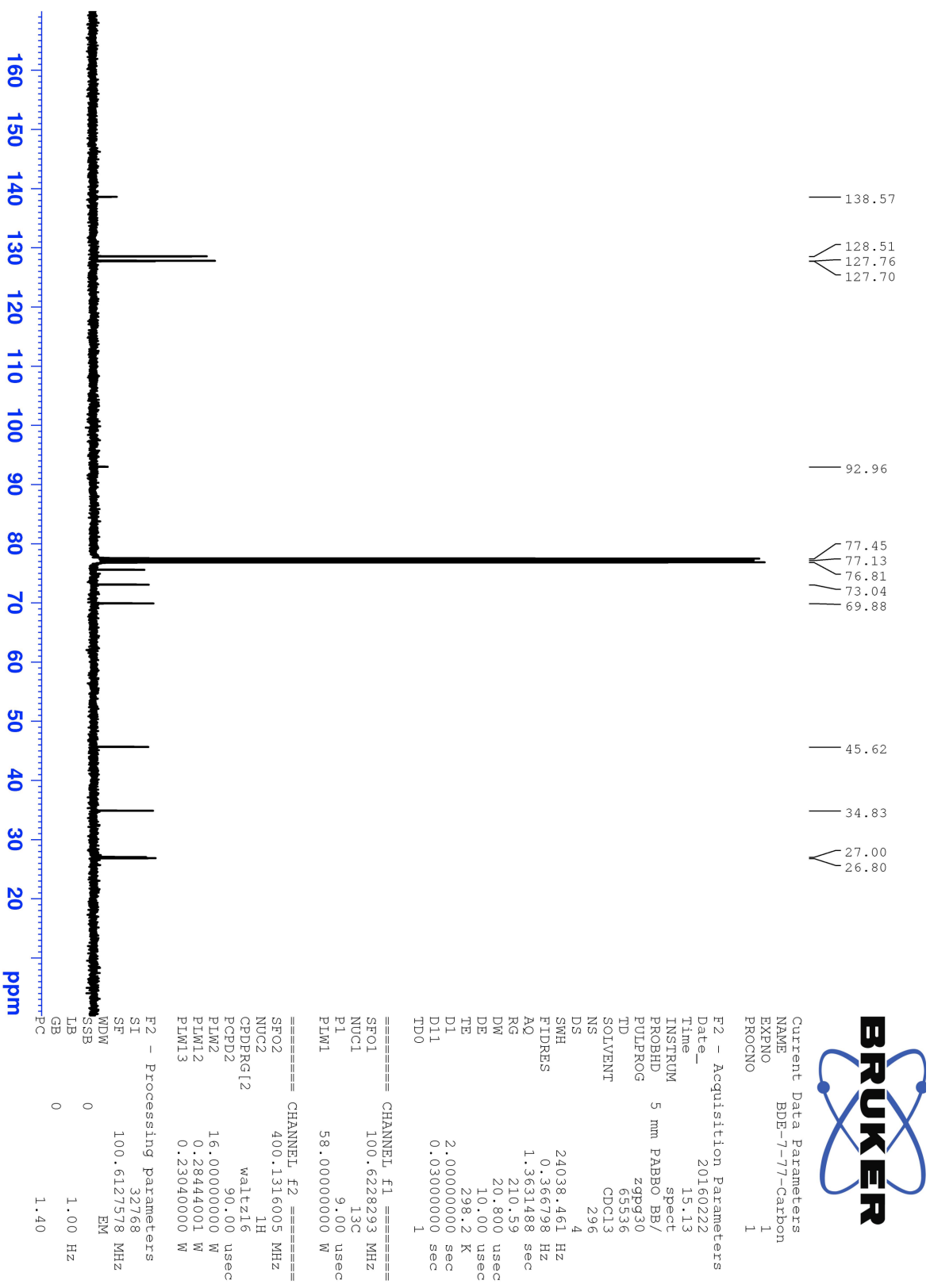
((Pent-4-en-1-yloxy)methyl)benzene (1). ^{1}H spectrum.



((Pent-4-en-1-yloxy)methyl)benzene (1). ^{13}C spectrum.



***cis*-3-(3-(Benzyloxy)propyl)-2,2-dichlorocyclobutan-1-ol (2)**. ^{1}H spectrum.



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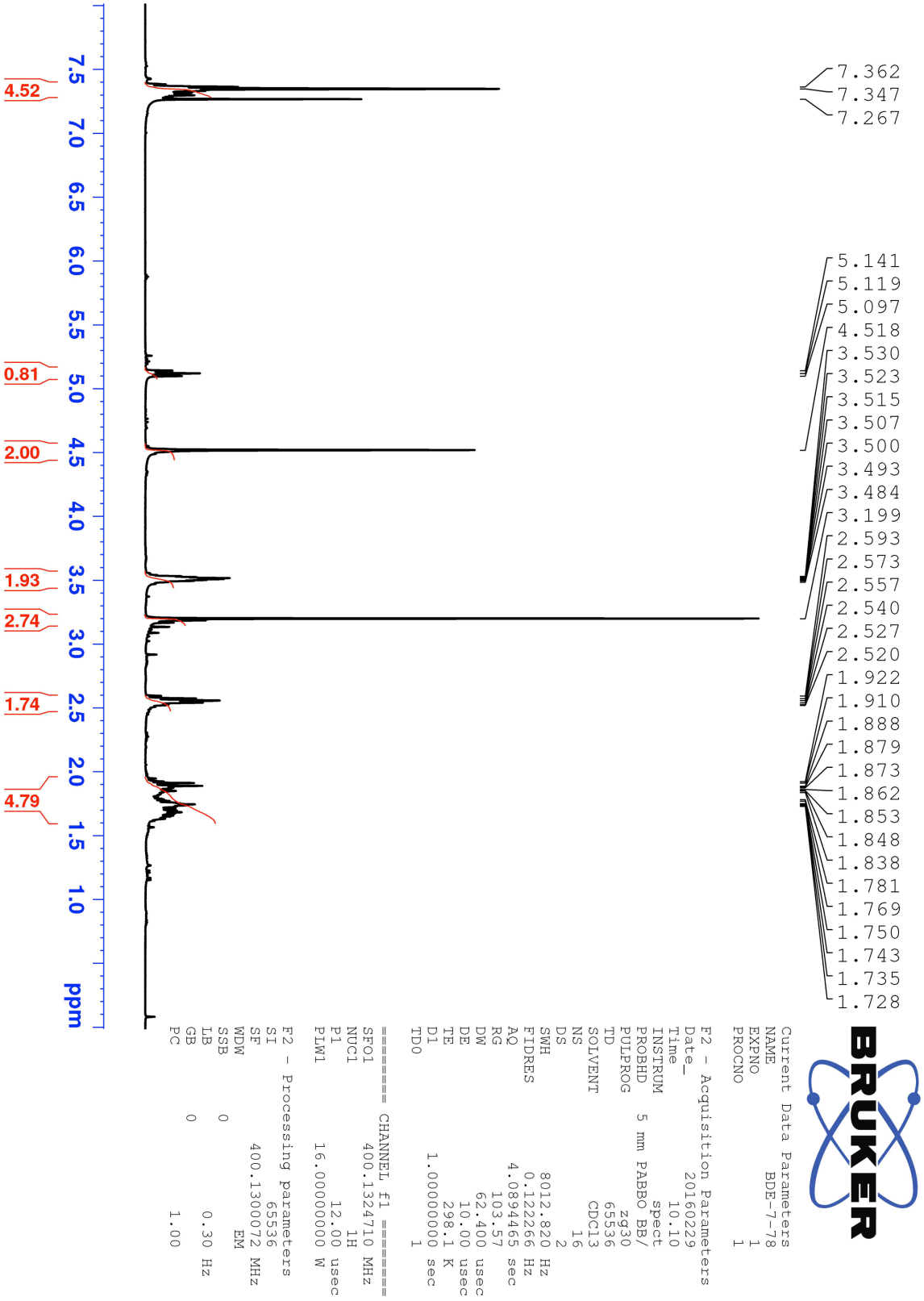
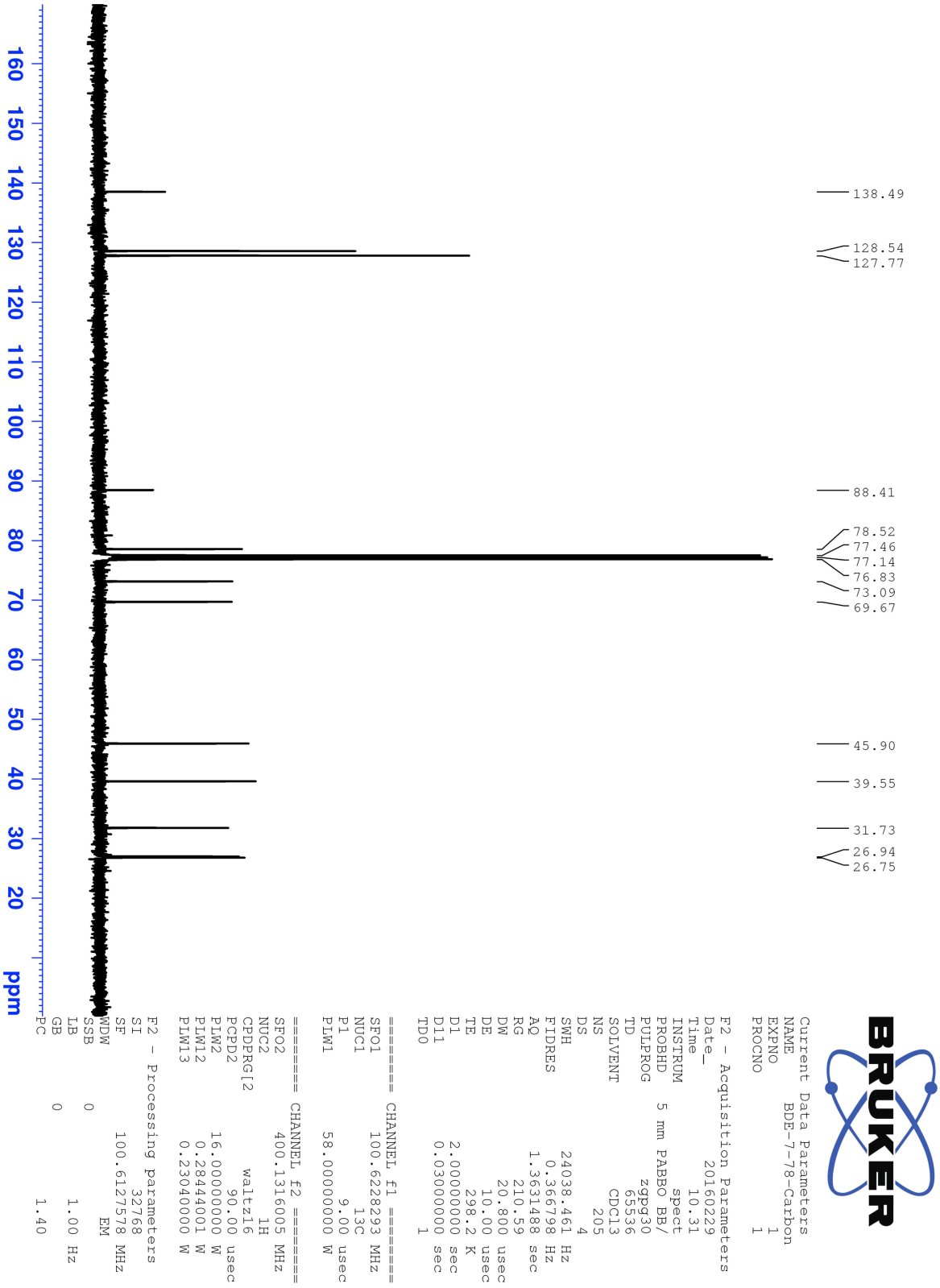


***cis*-3-(3-(Benzyloxy)propyl)-2,2-dichlorocyclobutyl methanesulfonate (3)**. ^{1}H spectrum.



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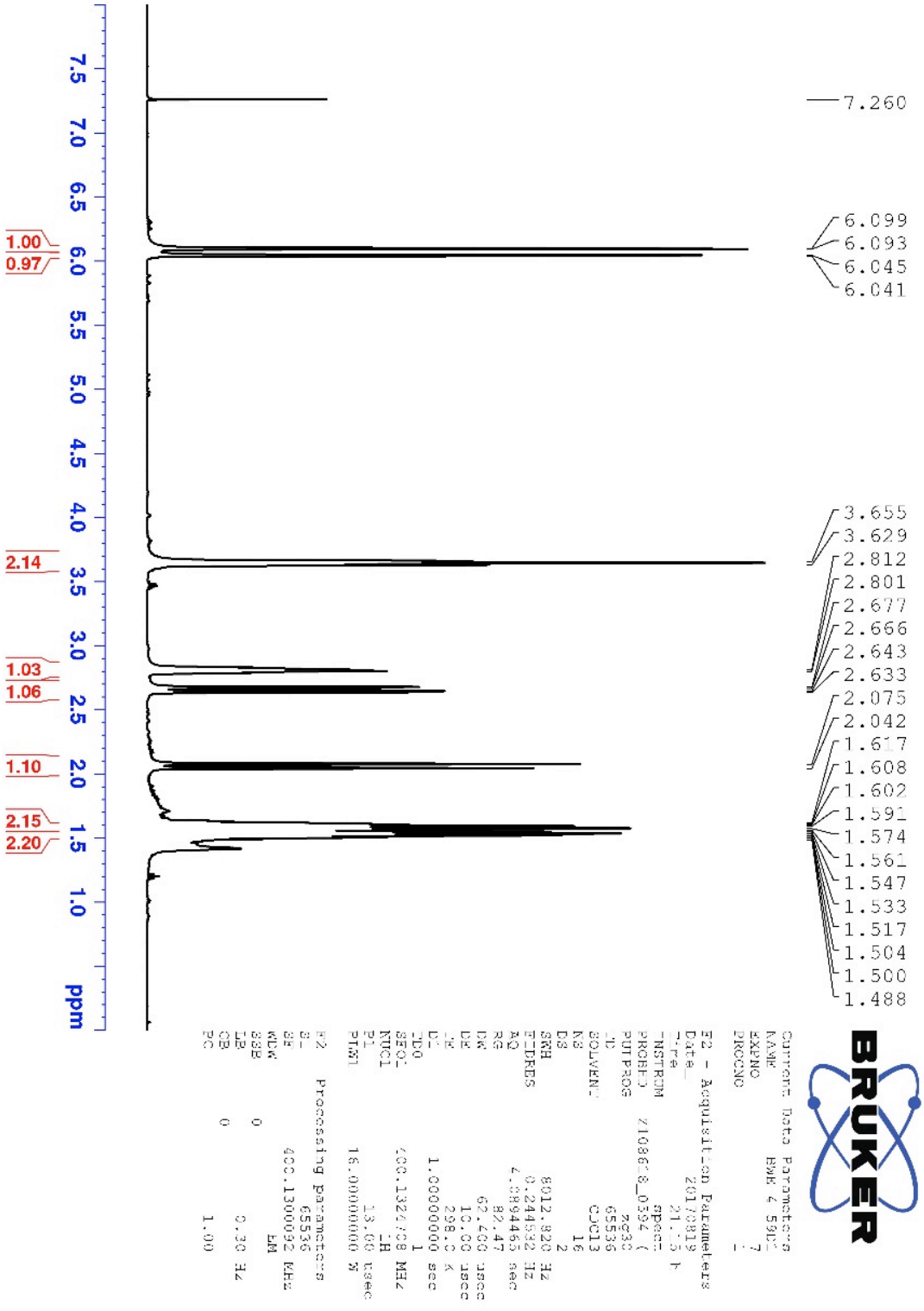
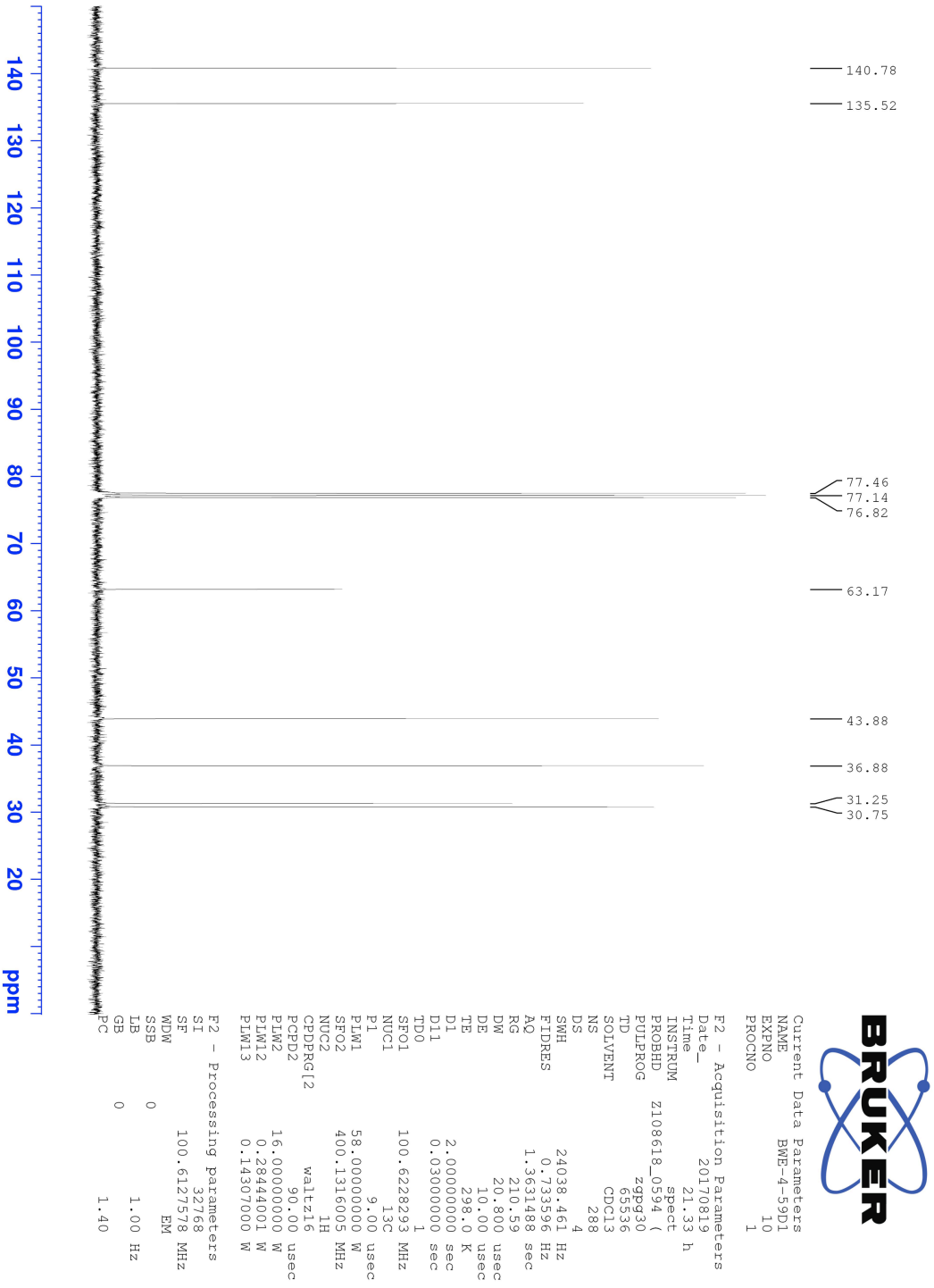
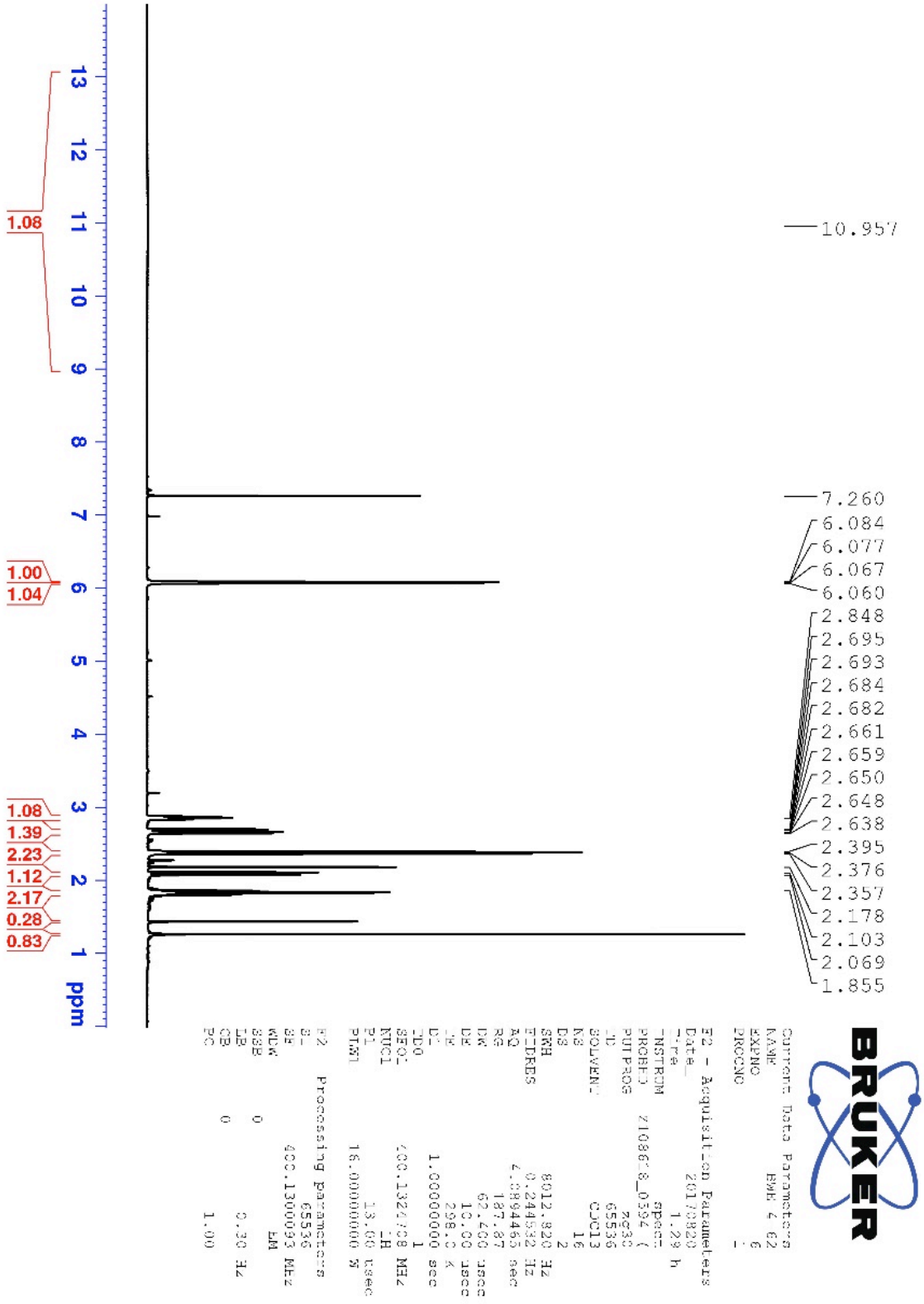


3

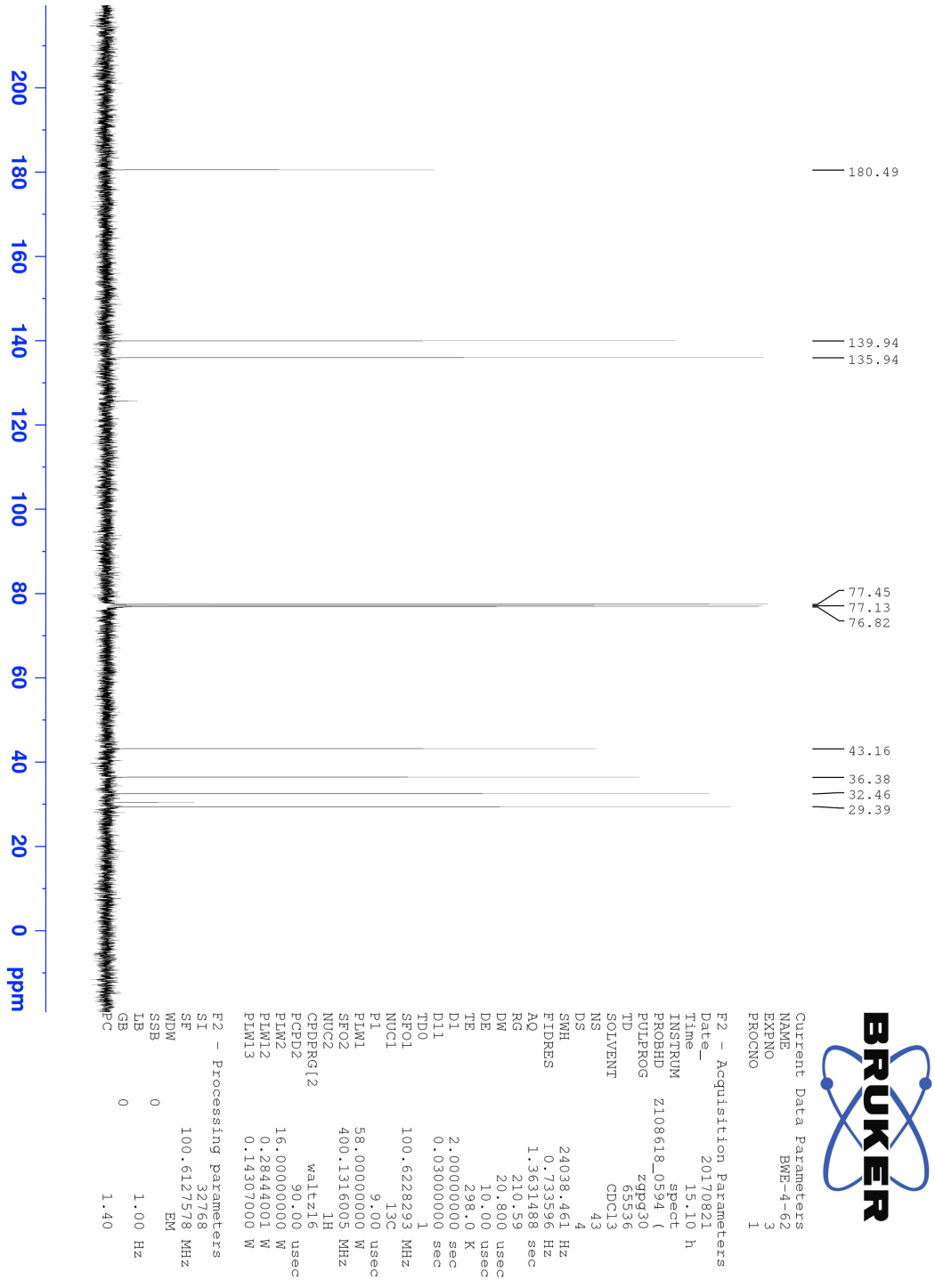
3-(Cyclobut-2-en-1-yl)propanol. ^{1}H spectrum of partially purified reaction aliquot.



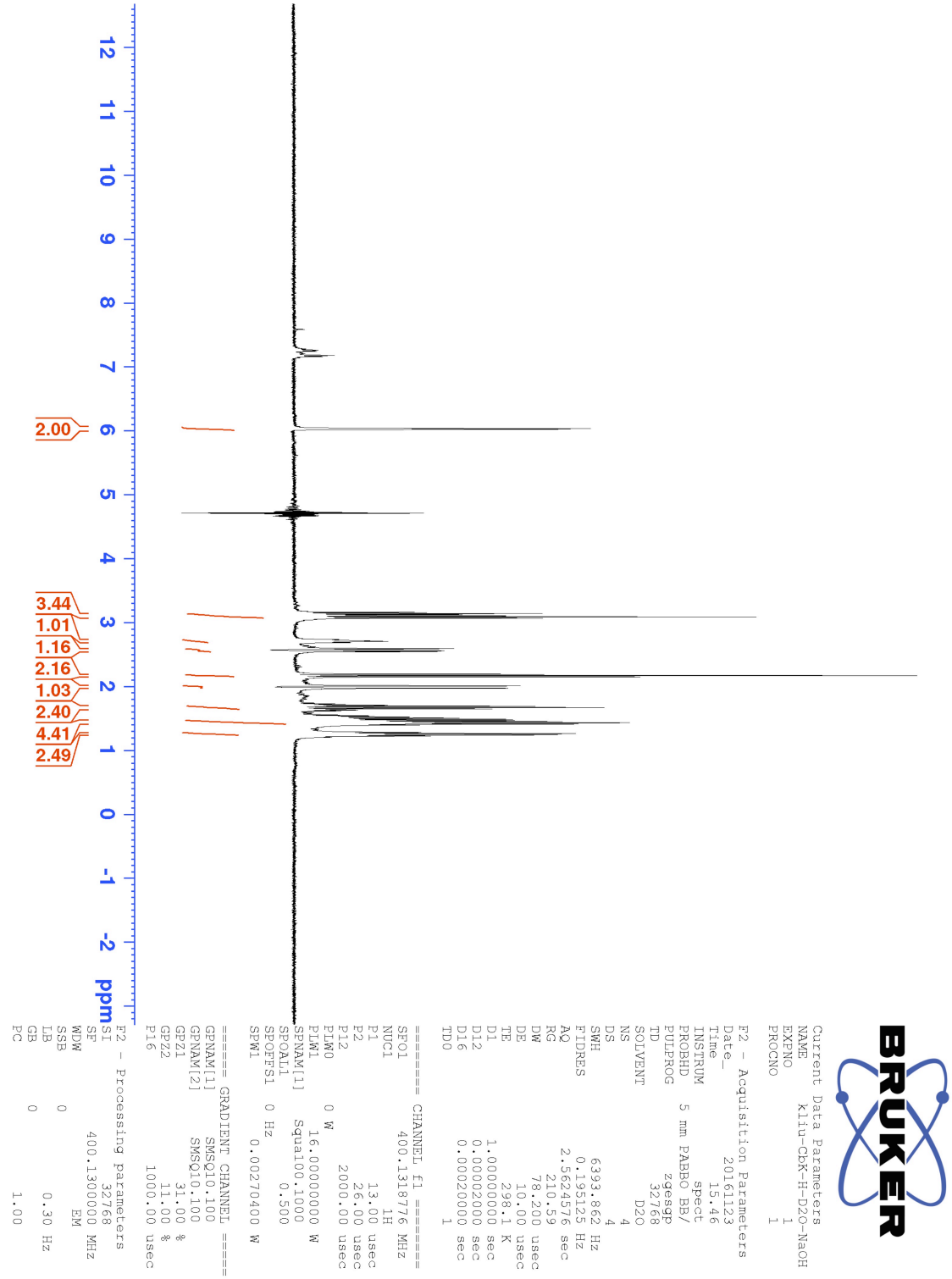
3-(Cyclobut-2-en-1-yl)propanol; ^{13}C spectrum of partially purified reaction aliquot.



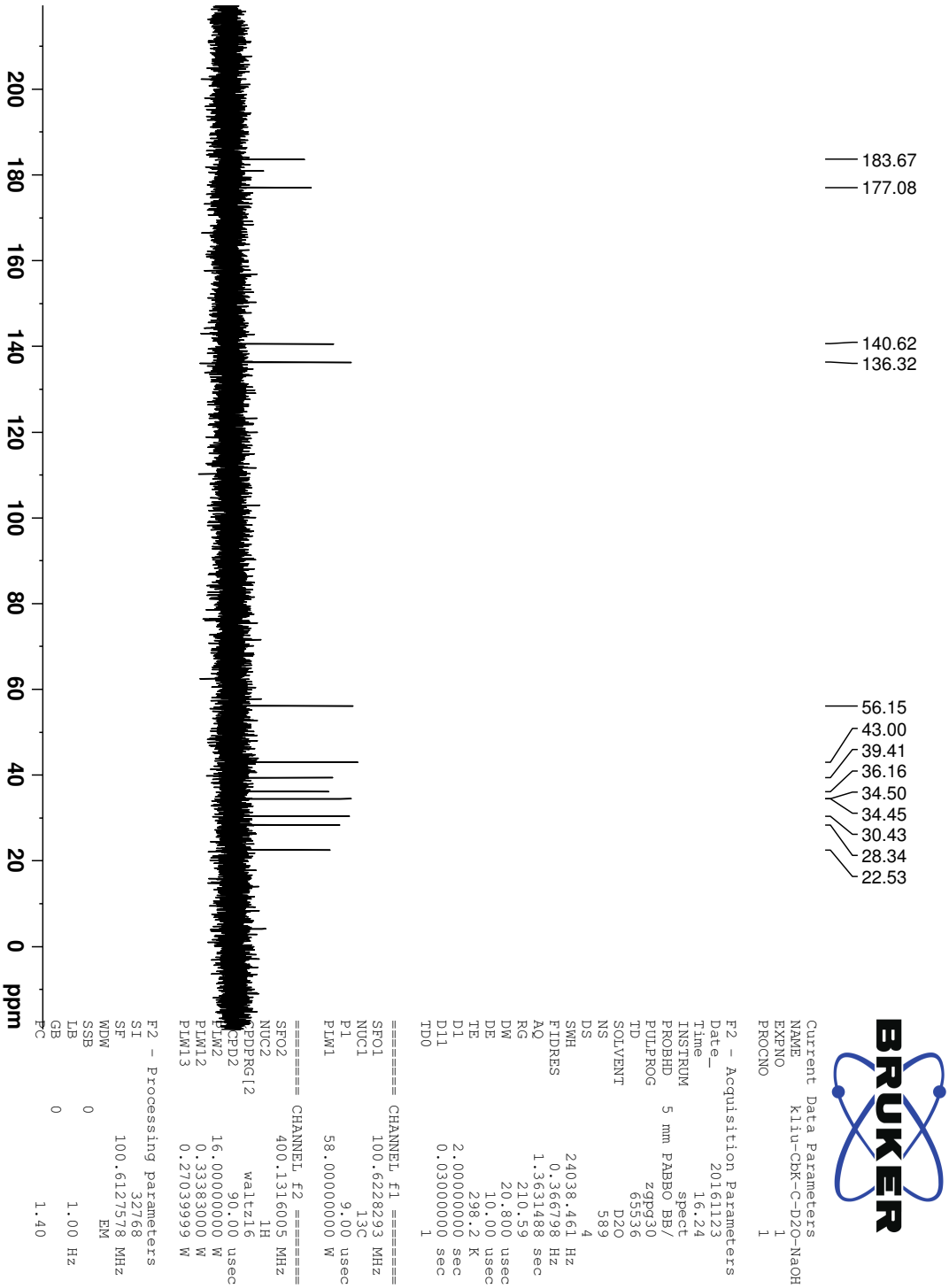
3-(Cyclobut-2-en-1-yl)propanoic acid (4). ^{1}H spectrum



3-(Cyclobut-2-en-1-yl)propanoic acid (4). ^{13}C spectrum.



N_6-(3-(Cyclobut-2-en-1-yl)propionyl)-*L*-lysine (CbK). ^{1}H spectrum



N_6-(3-(Cyclobut-2-en-1-yl)propionyl)-*L*-lysine (CbK). ^{13}C spectrum