

Iron-promoted dealkylative carbene aminocyclization of δ -arylamino- α -diazoesters

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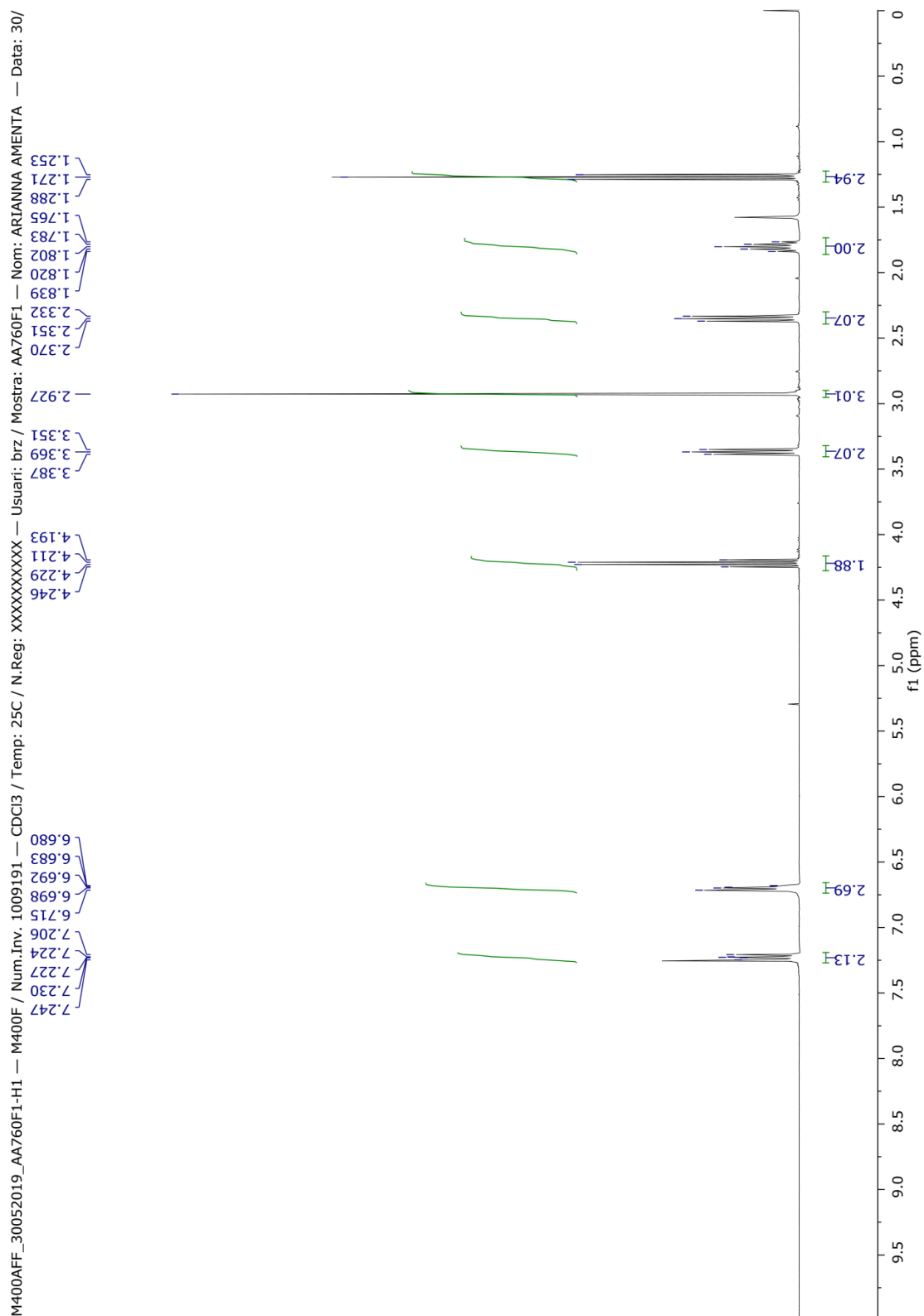
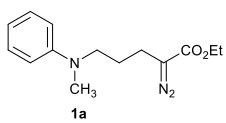
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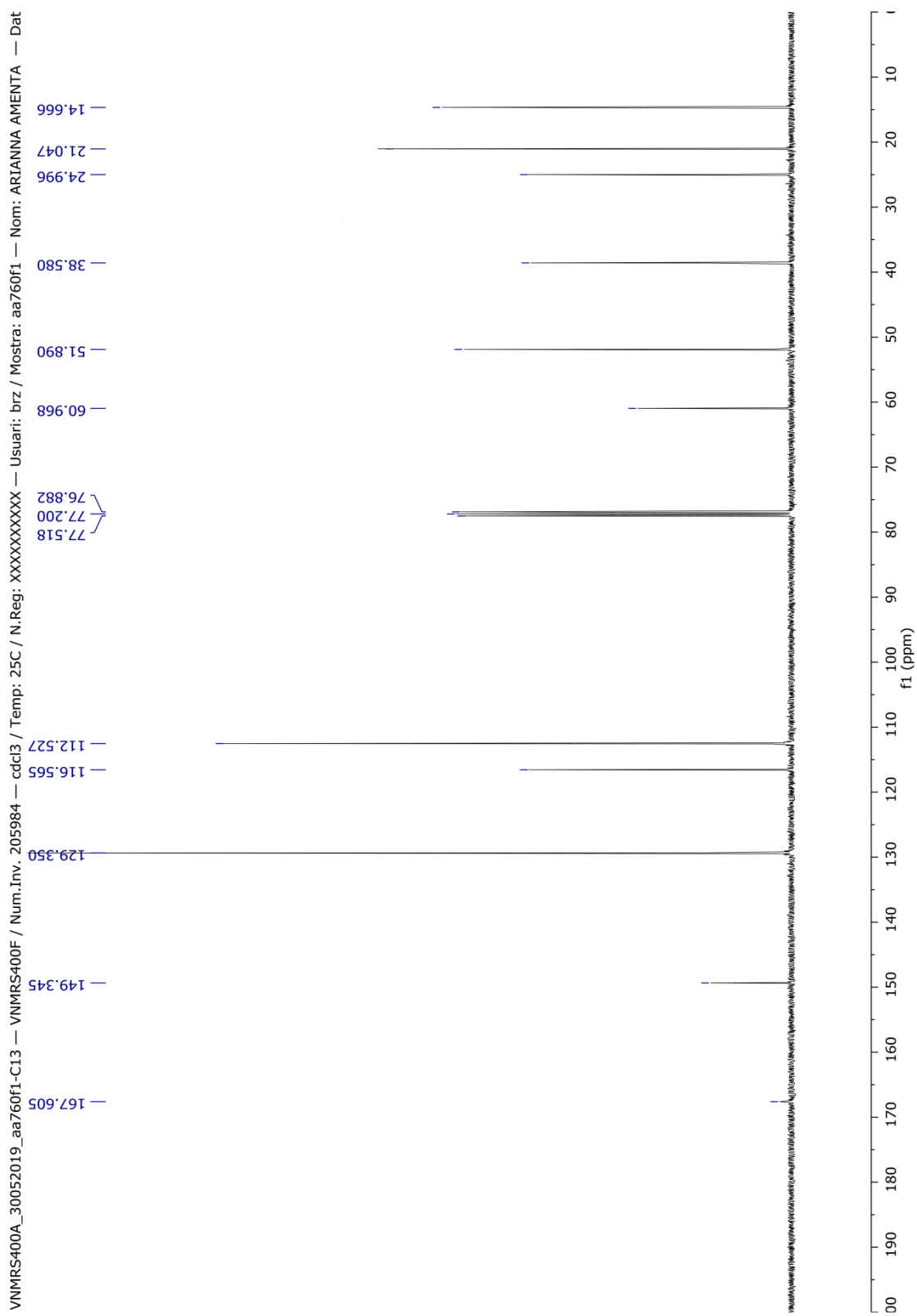
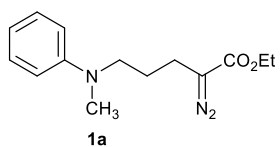
Electronic Supplementary Information

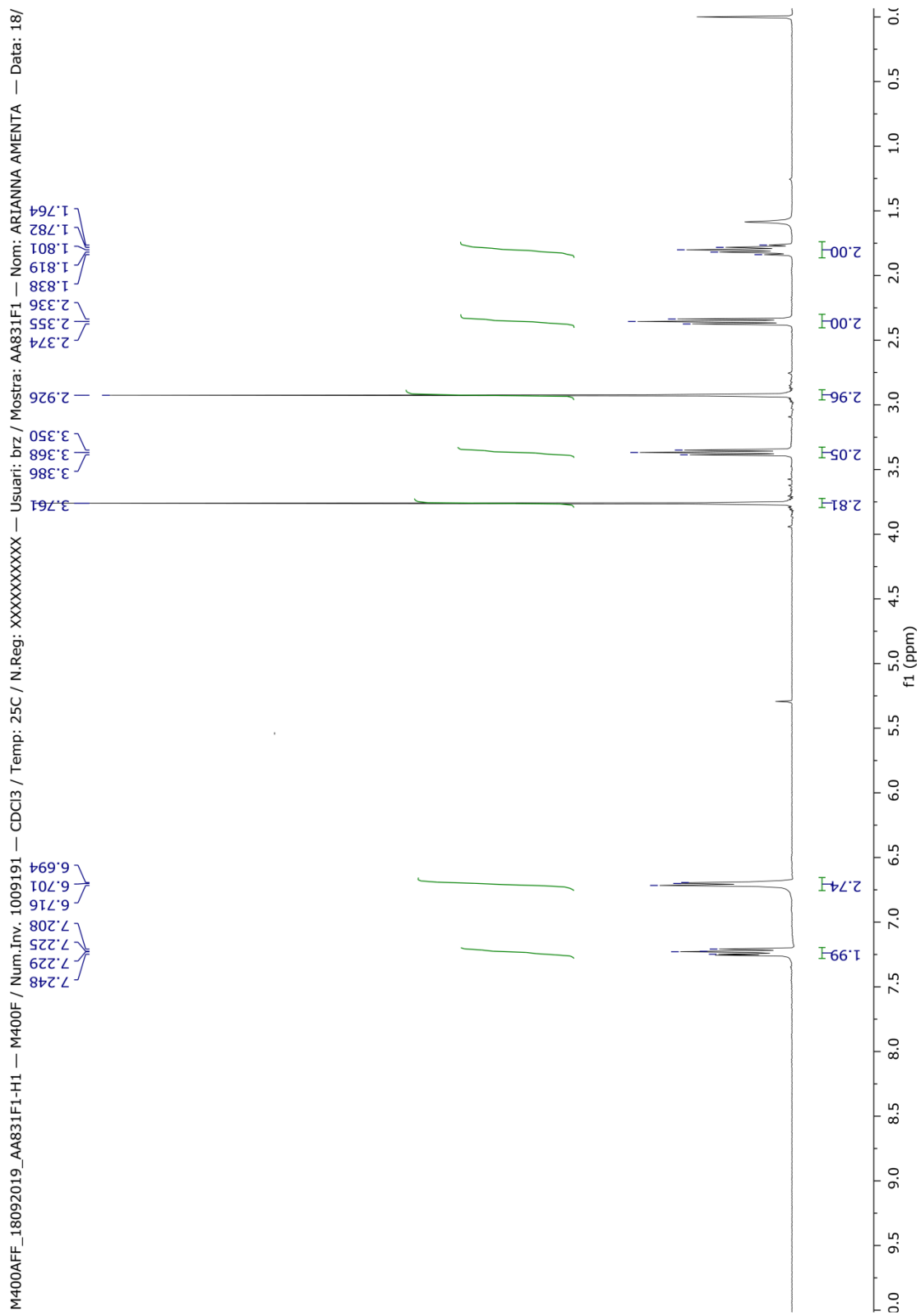
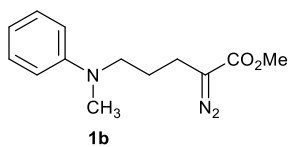
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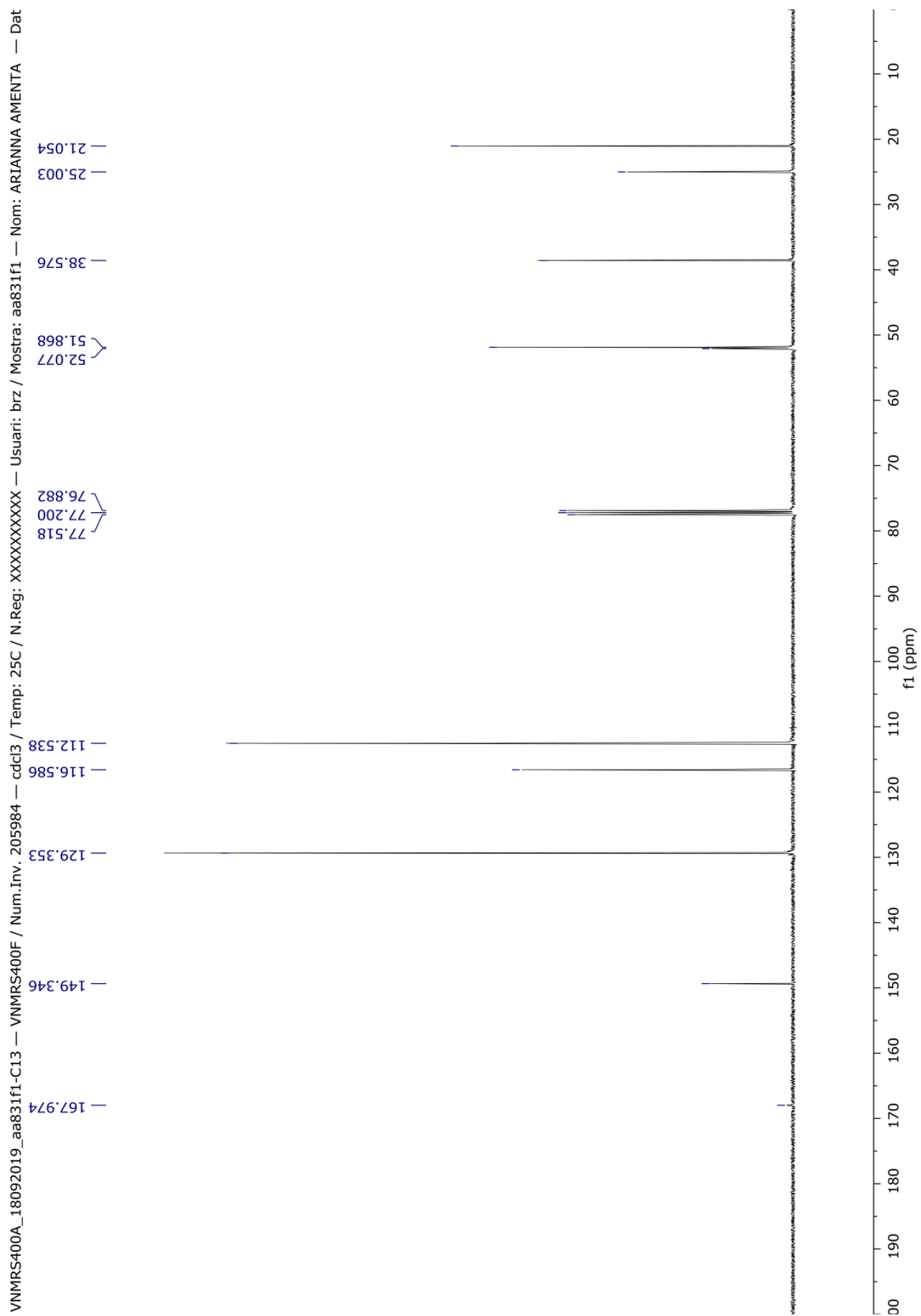
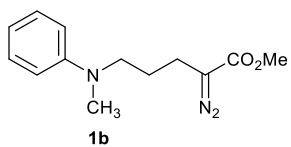
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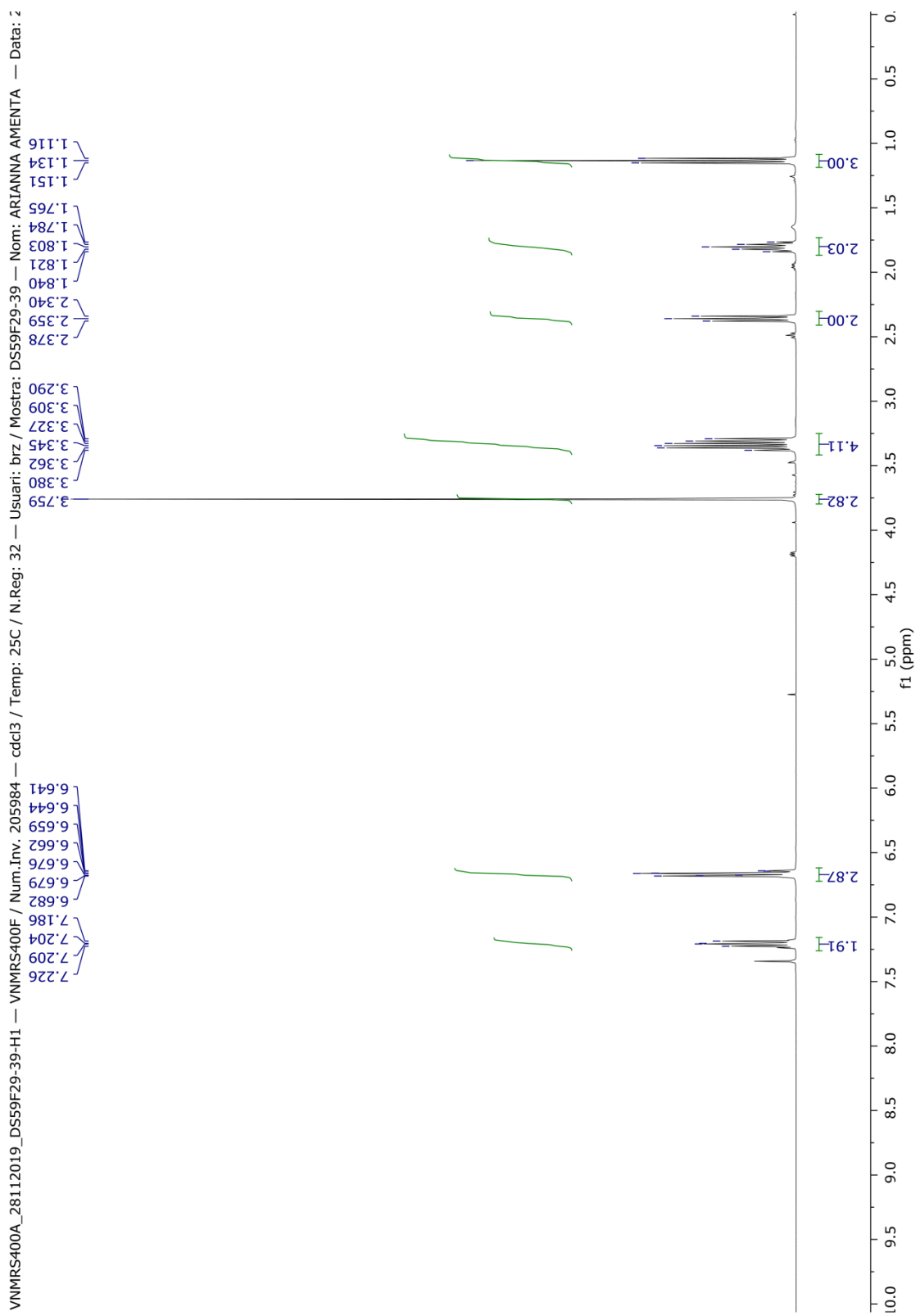
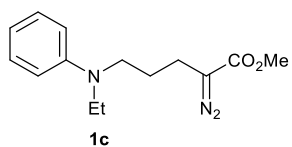
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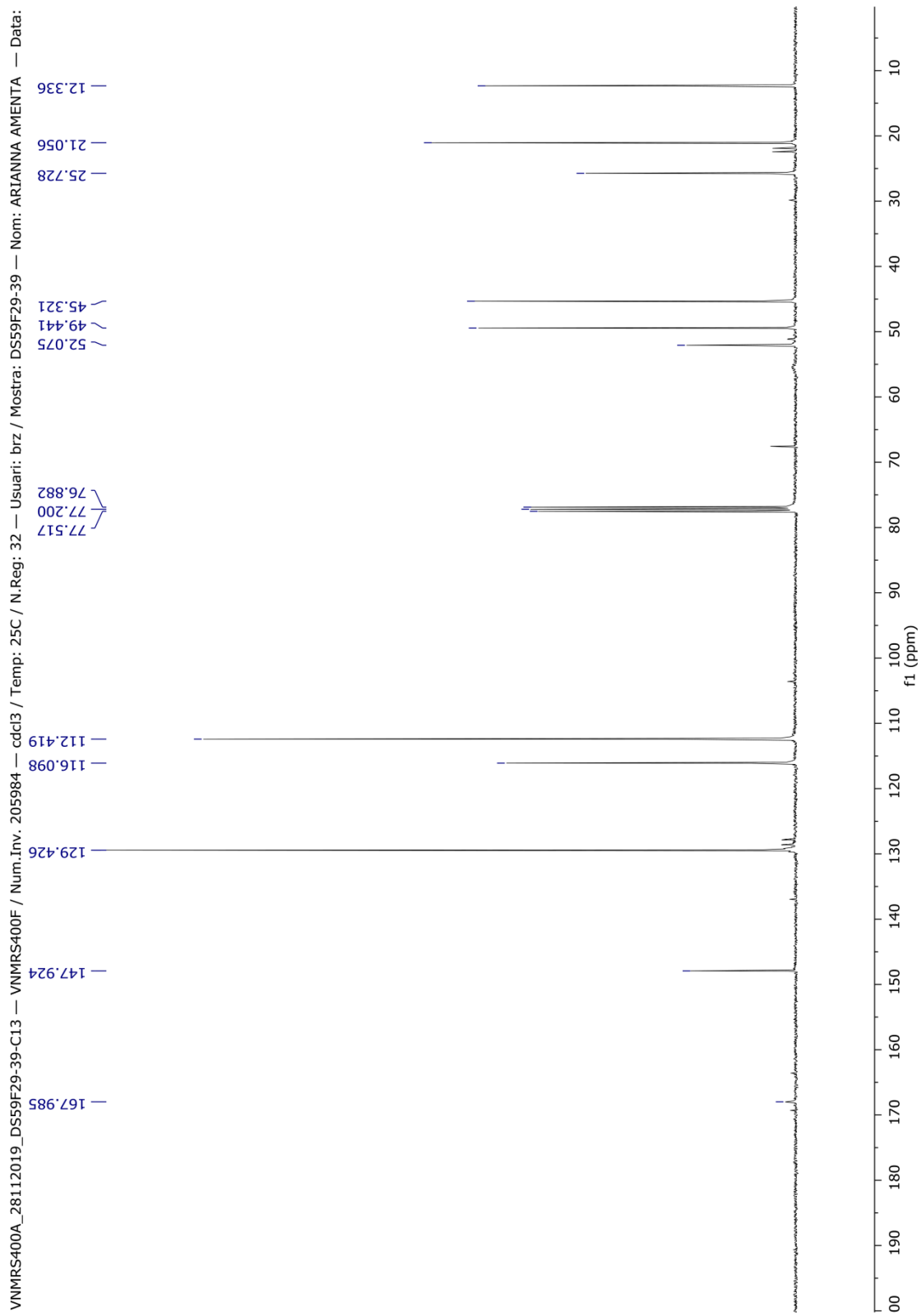
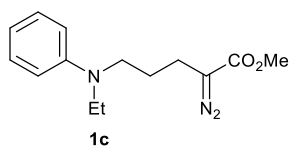


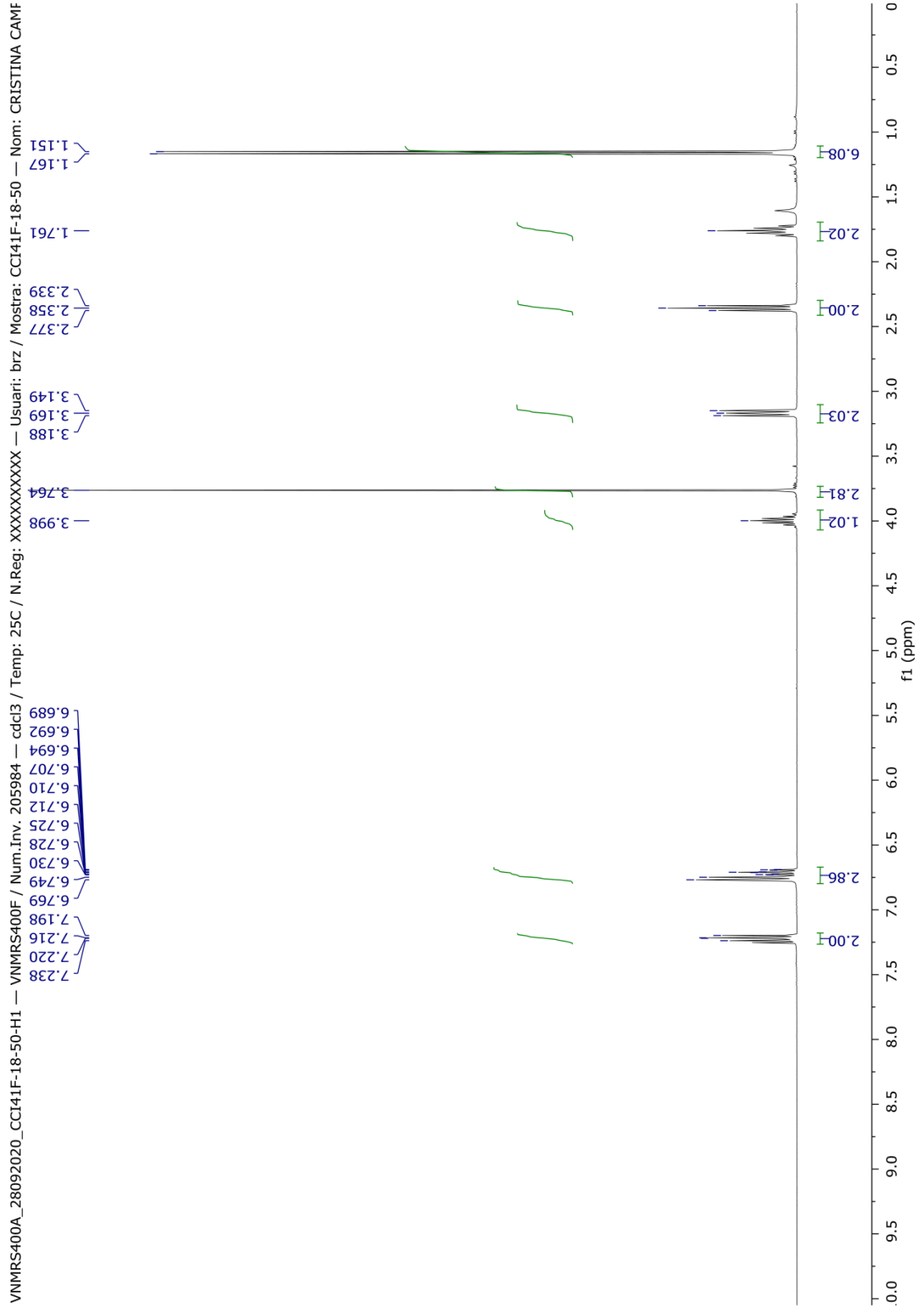
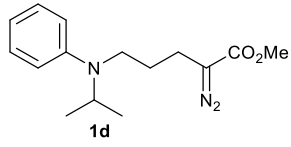


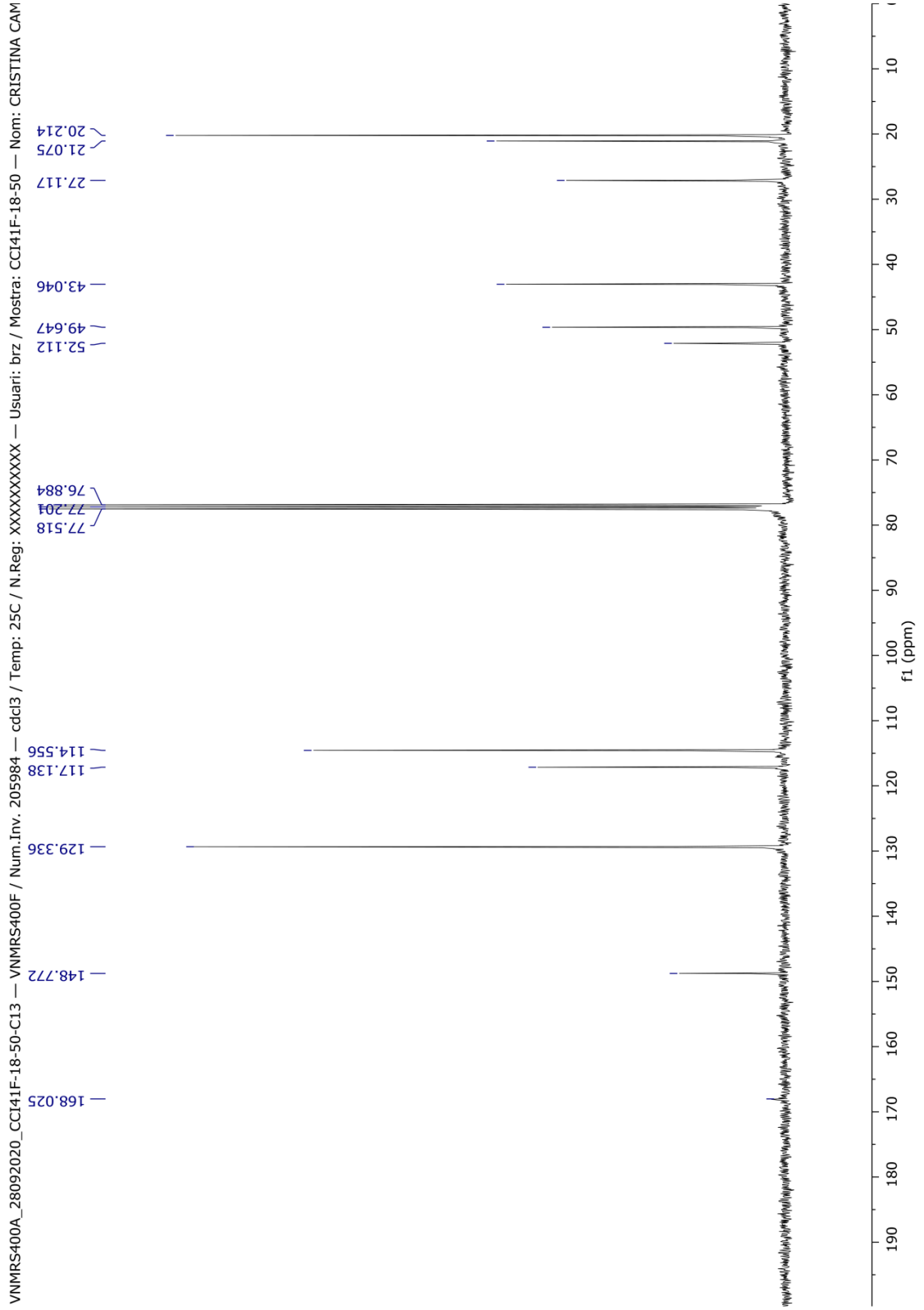
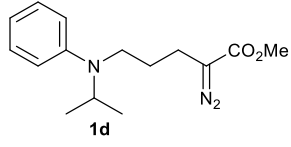


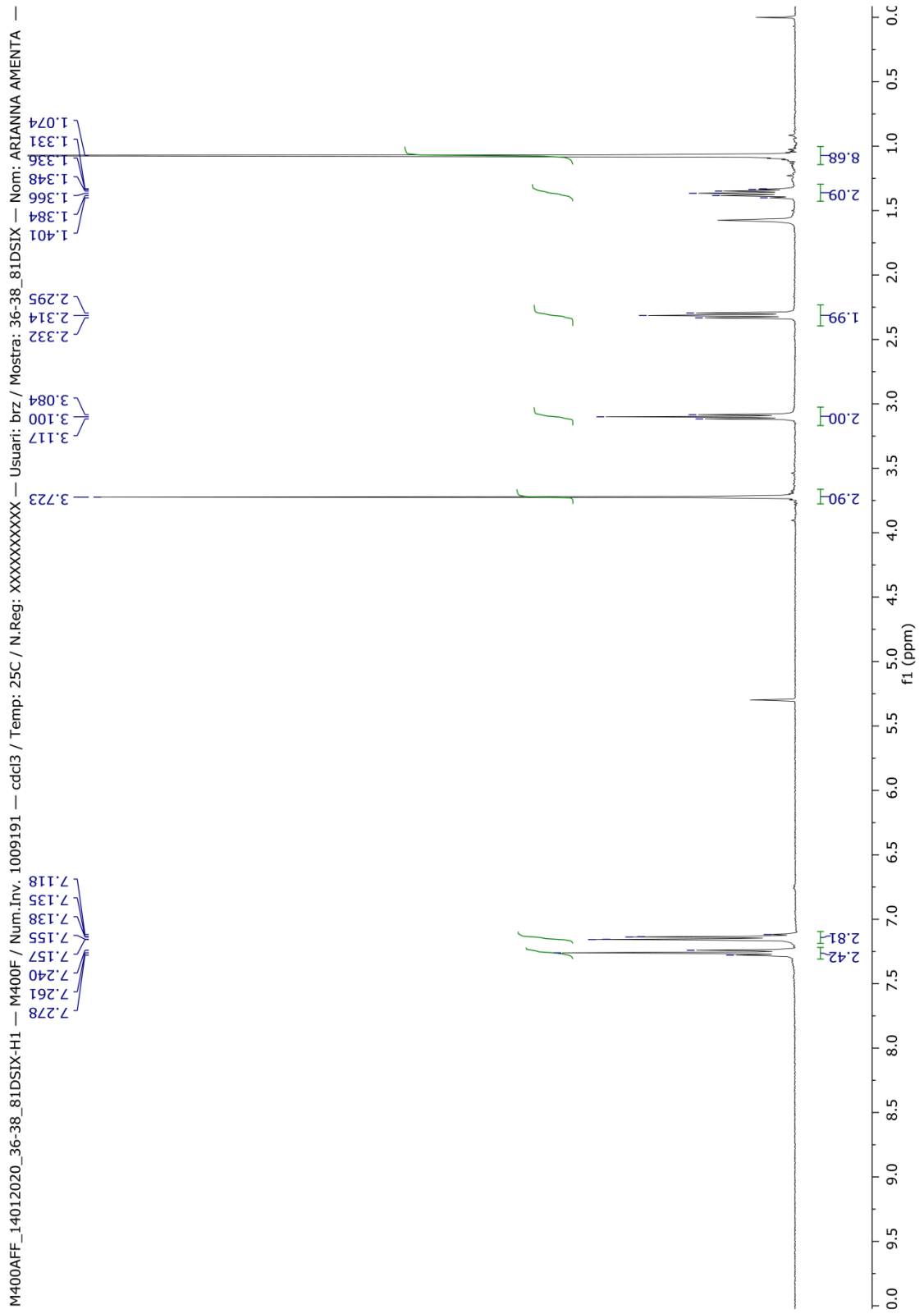
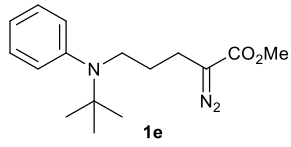


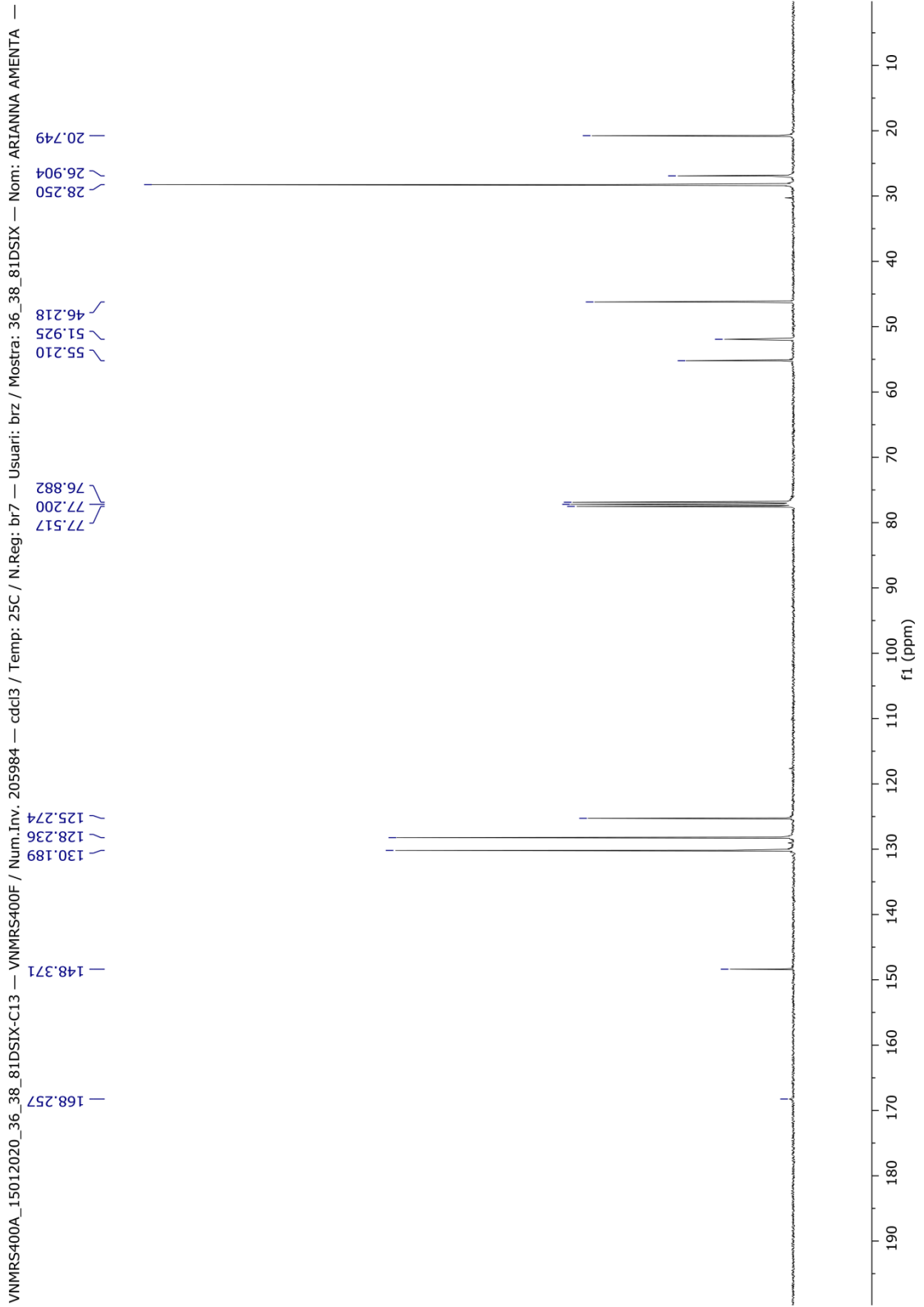
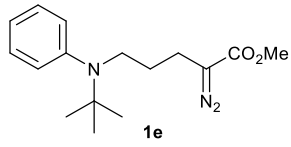


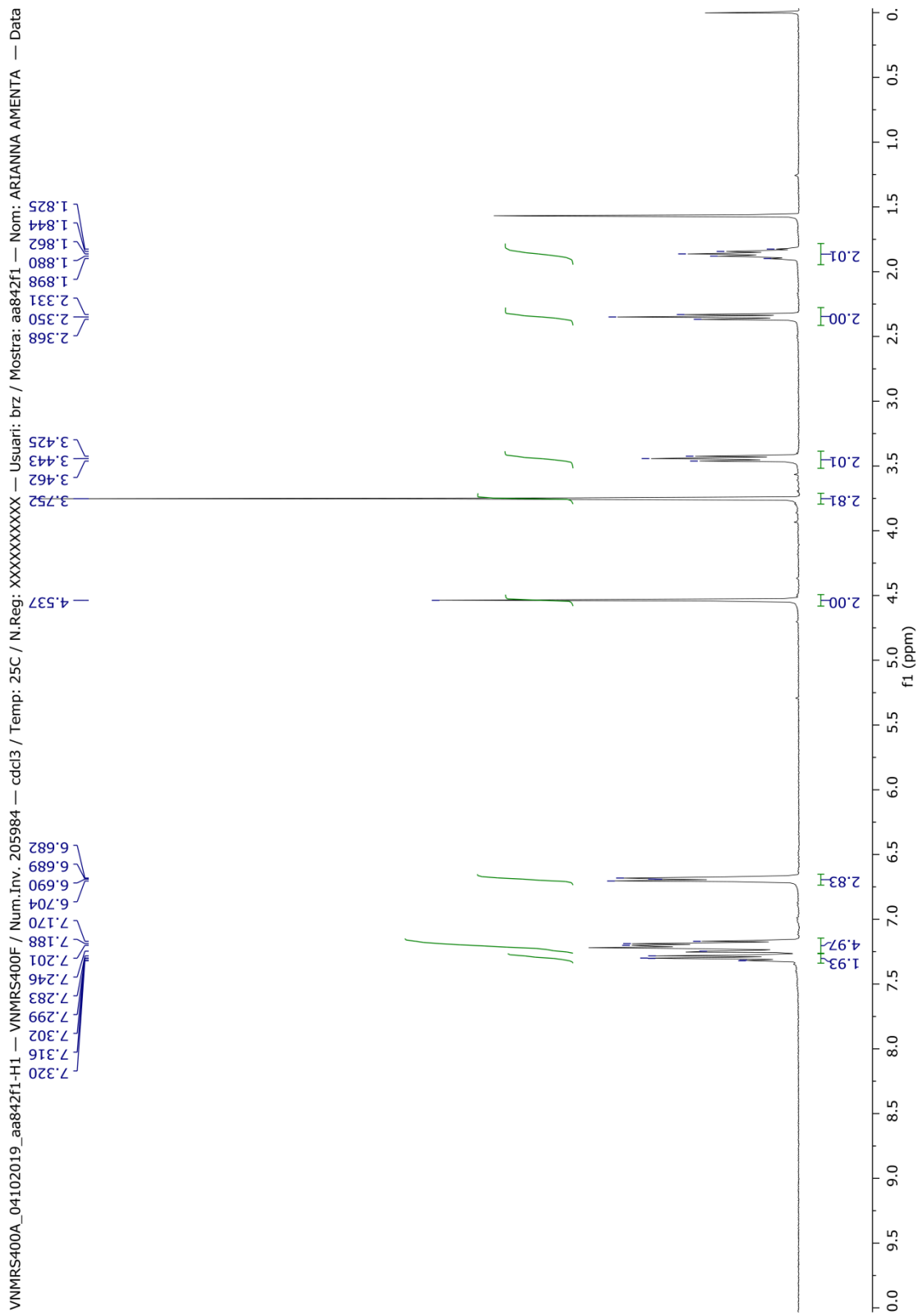
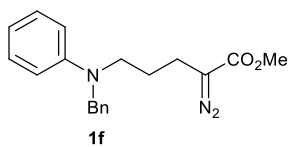


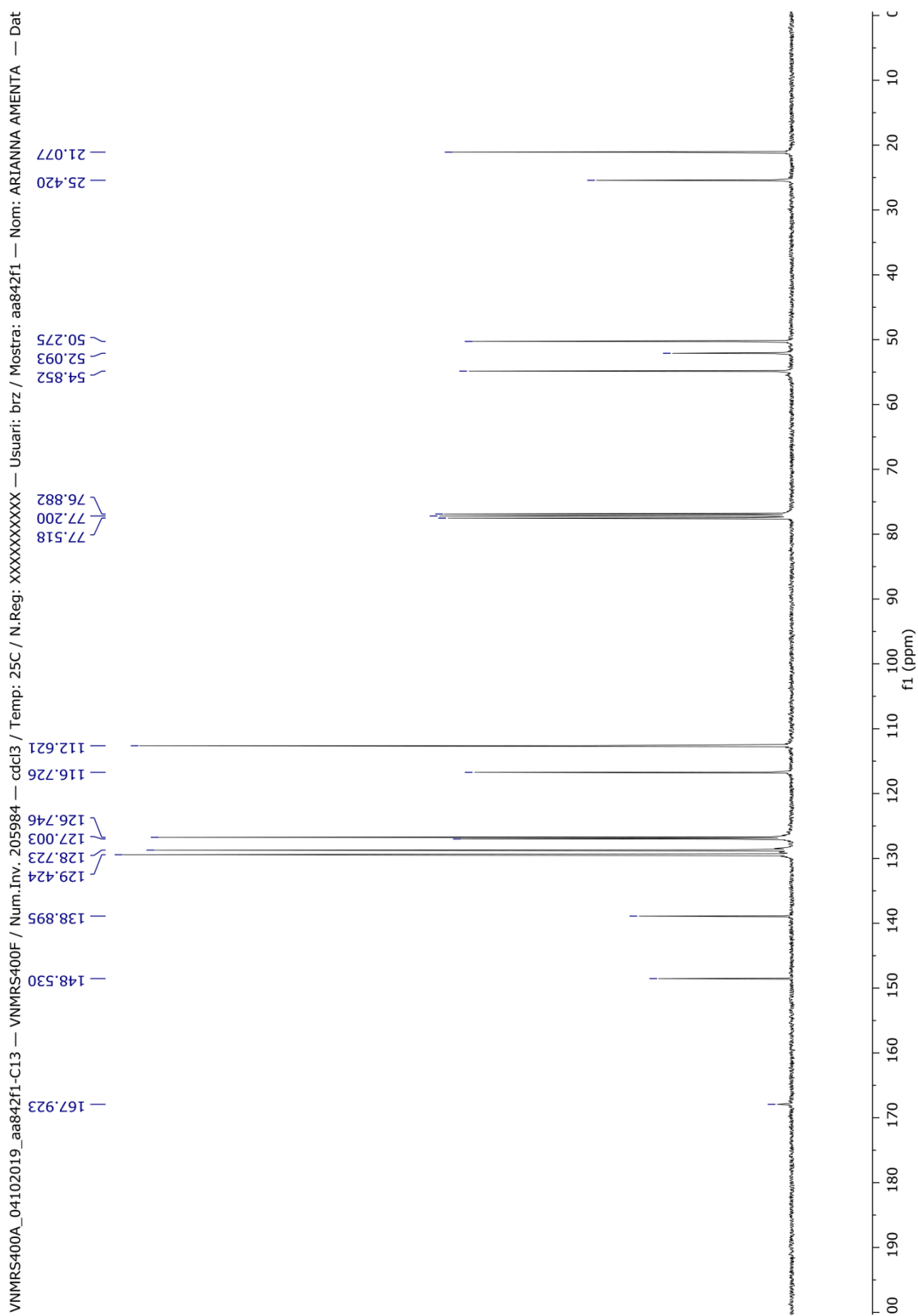
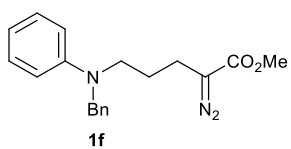


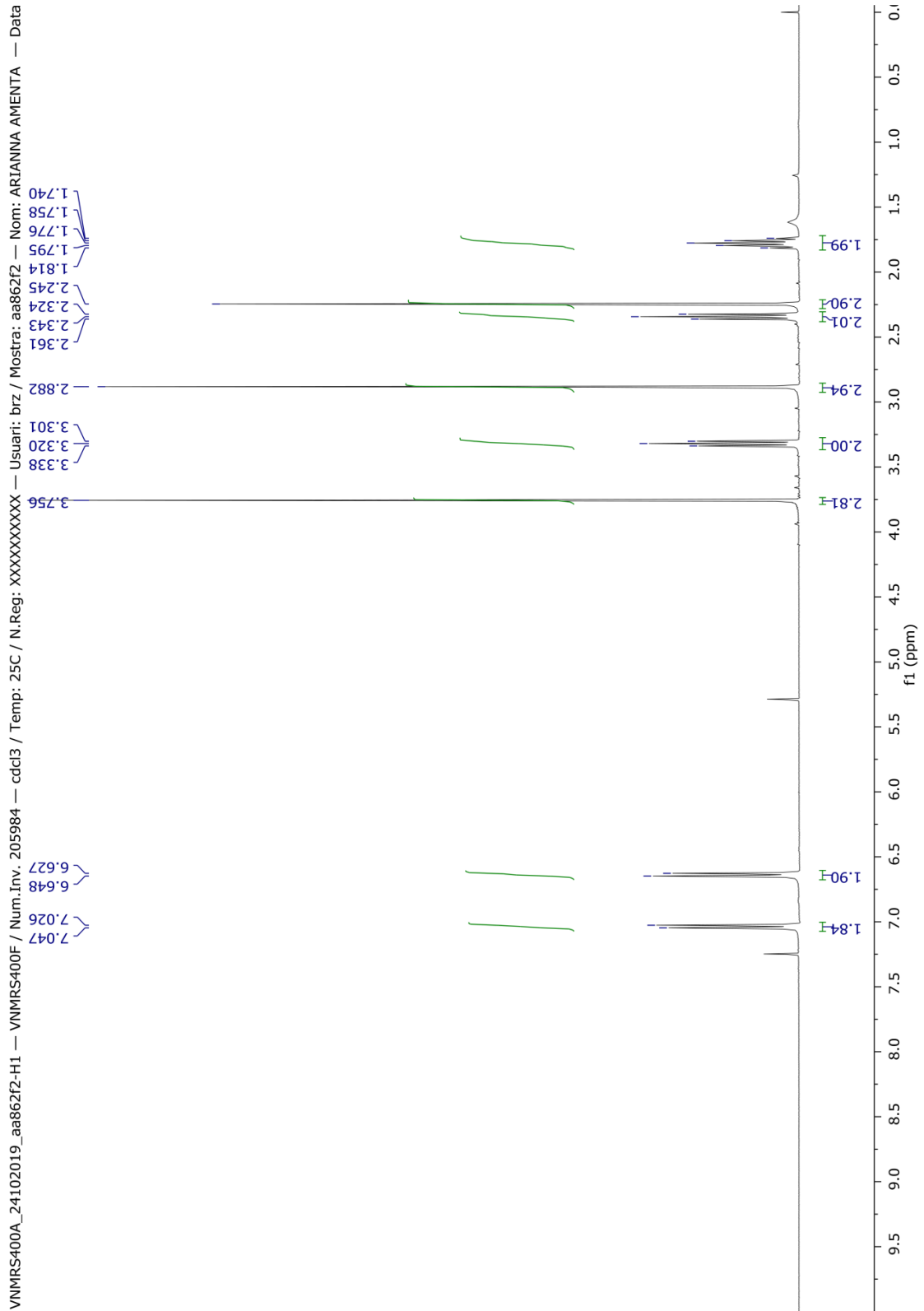
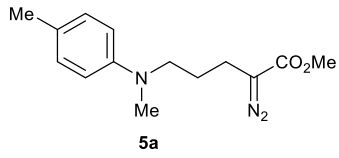


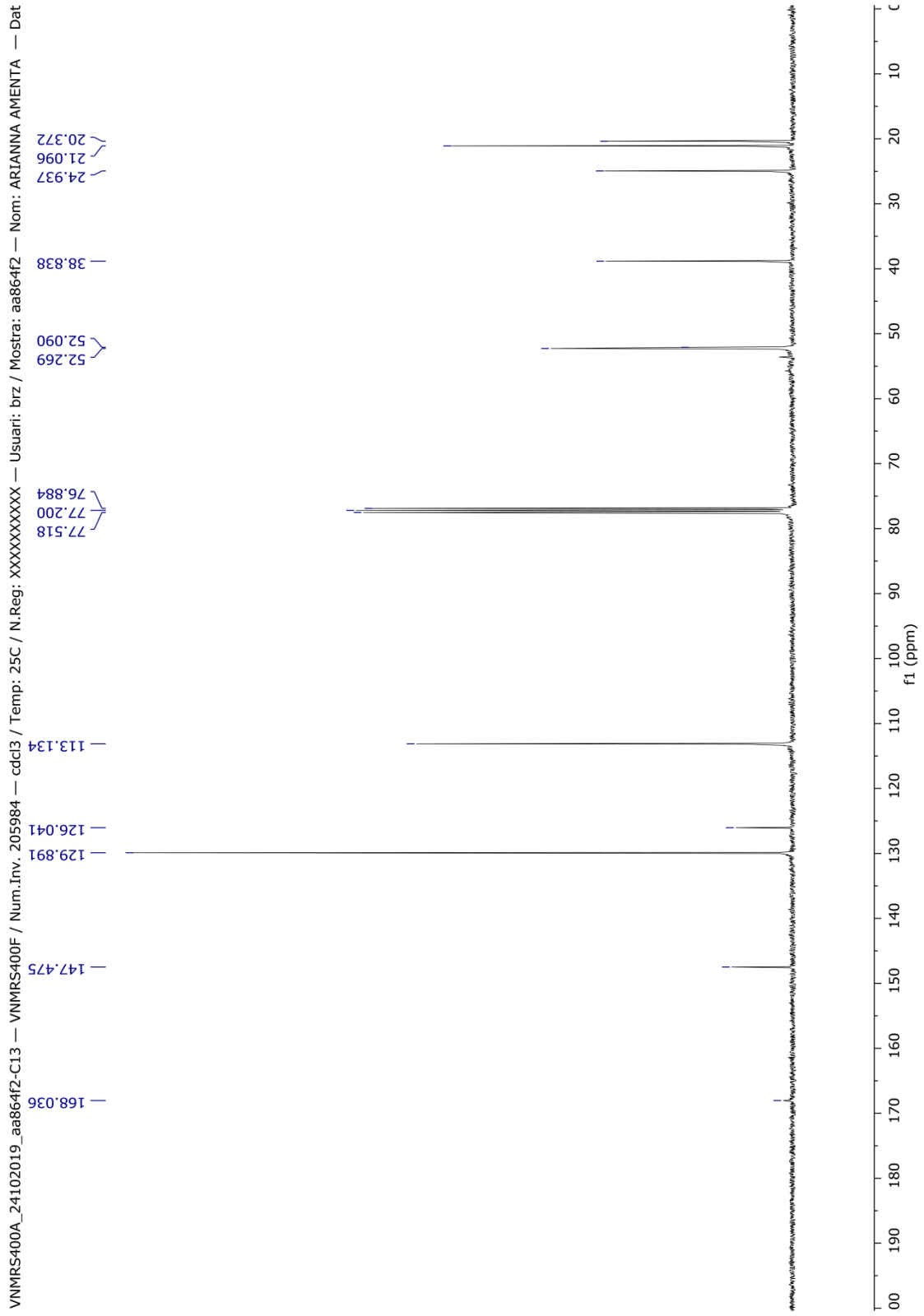
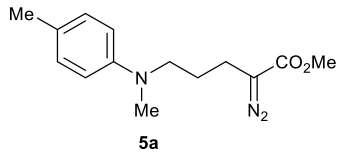


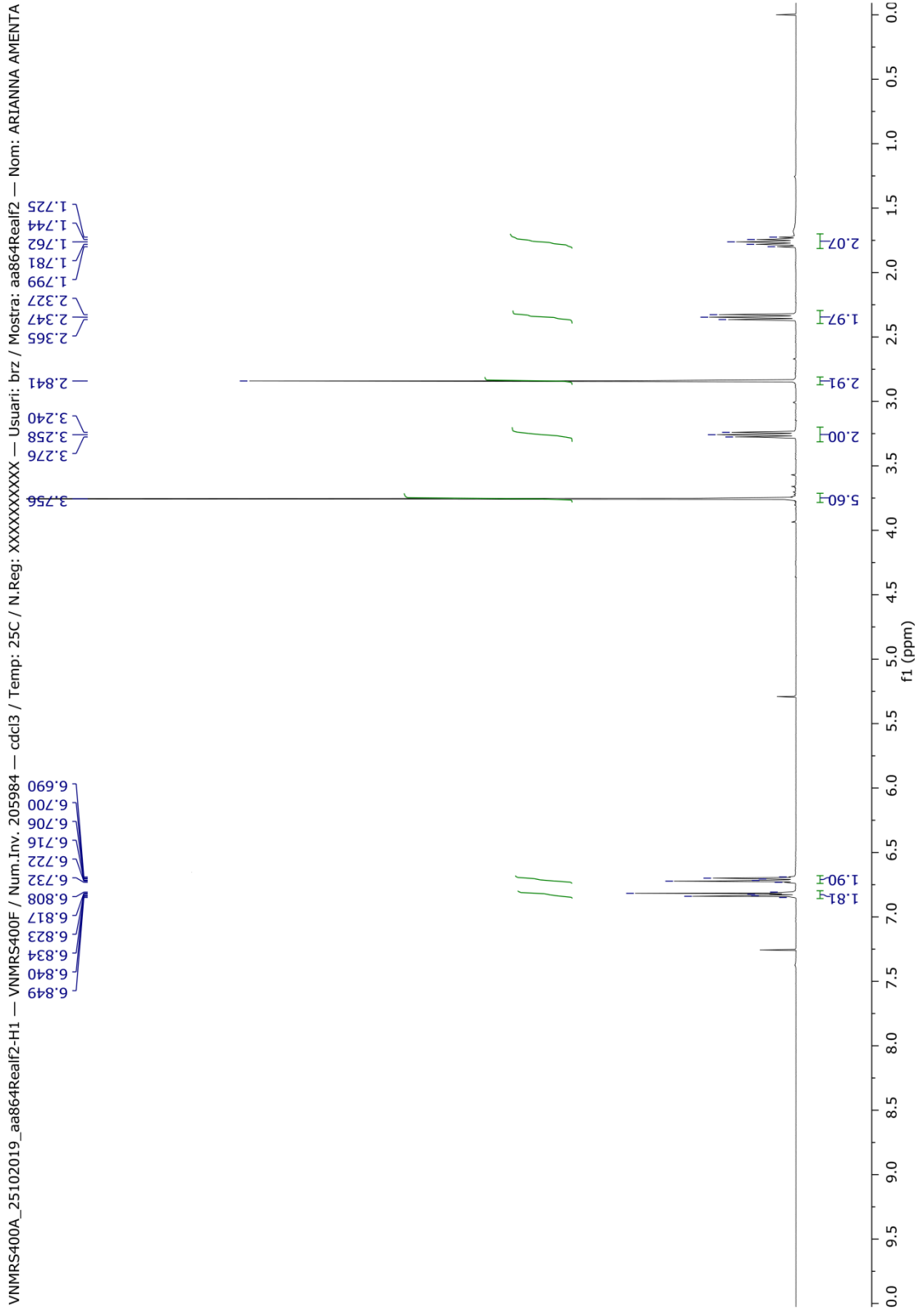
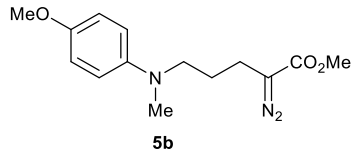


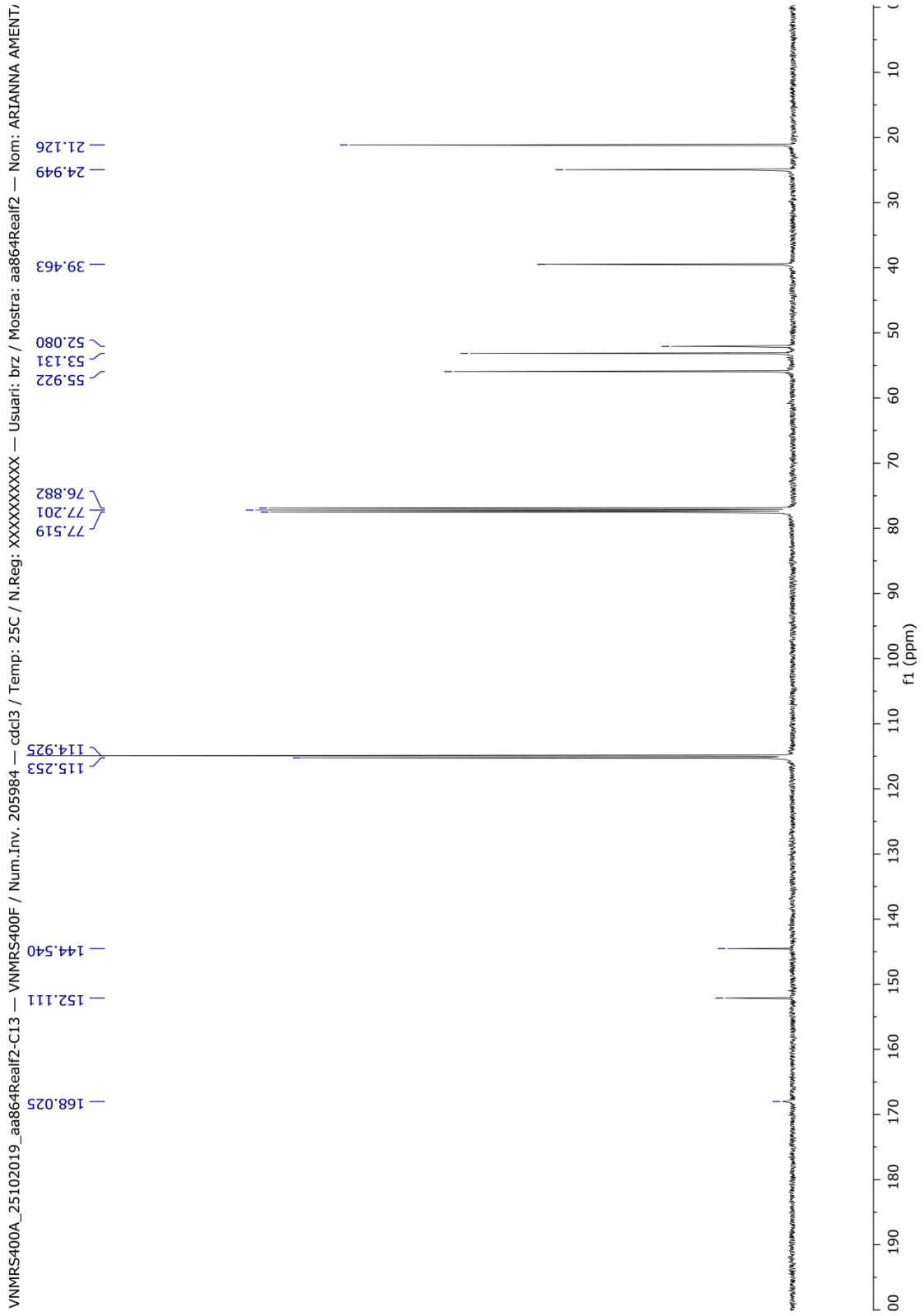
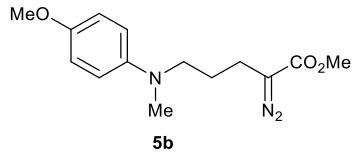


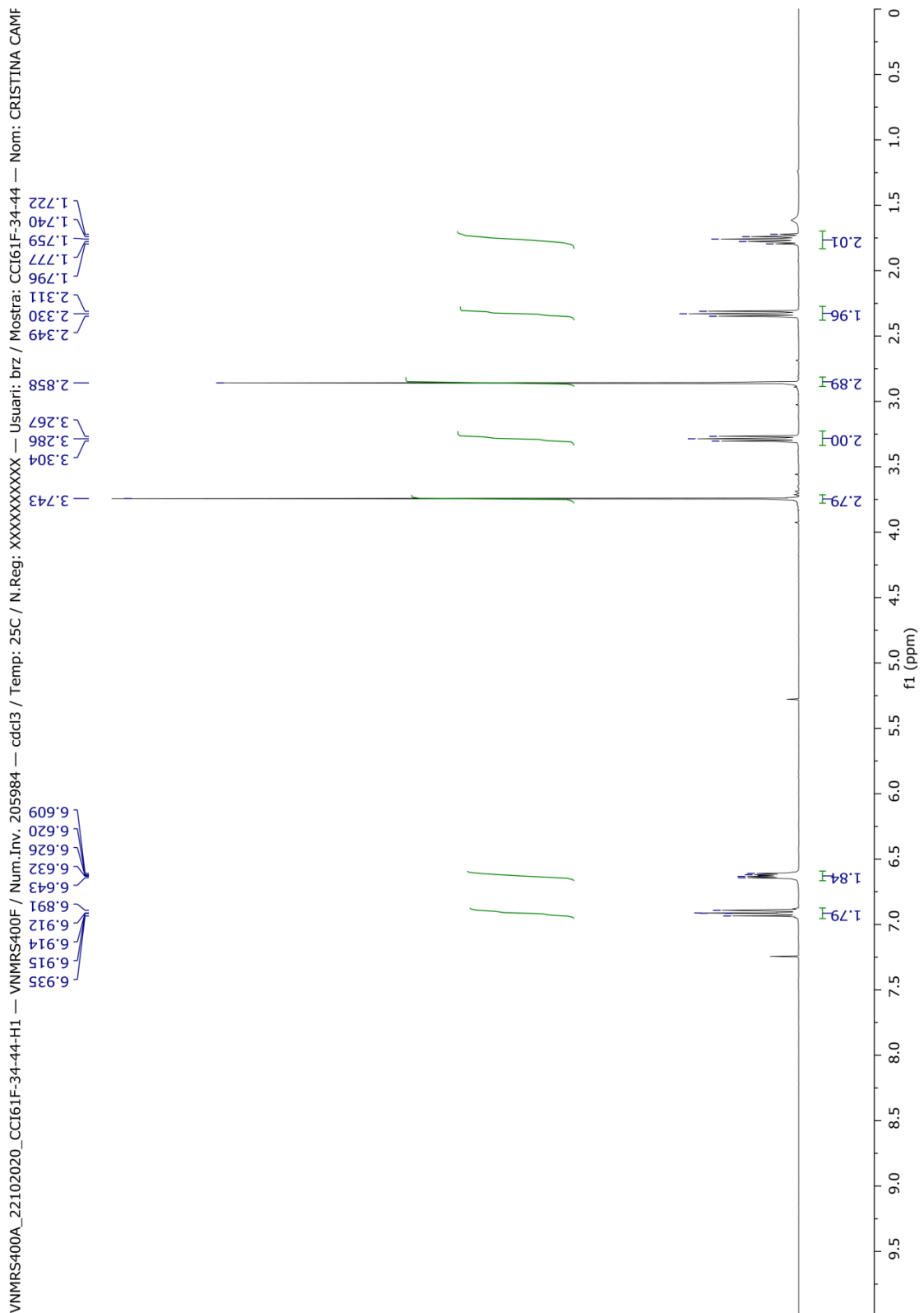
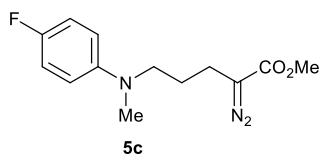


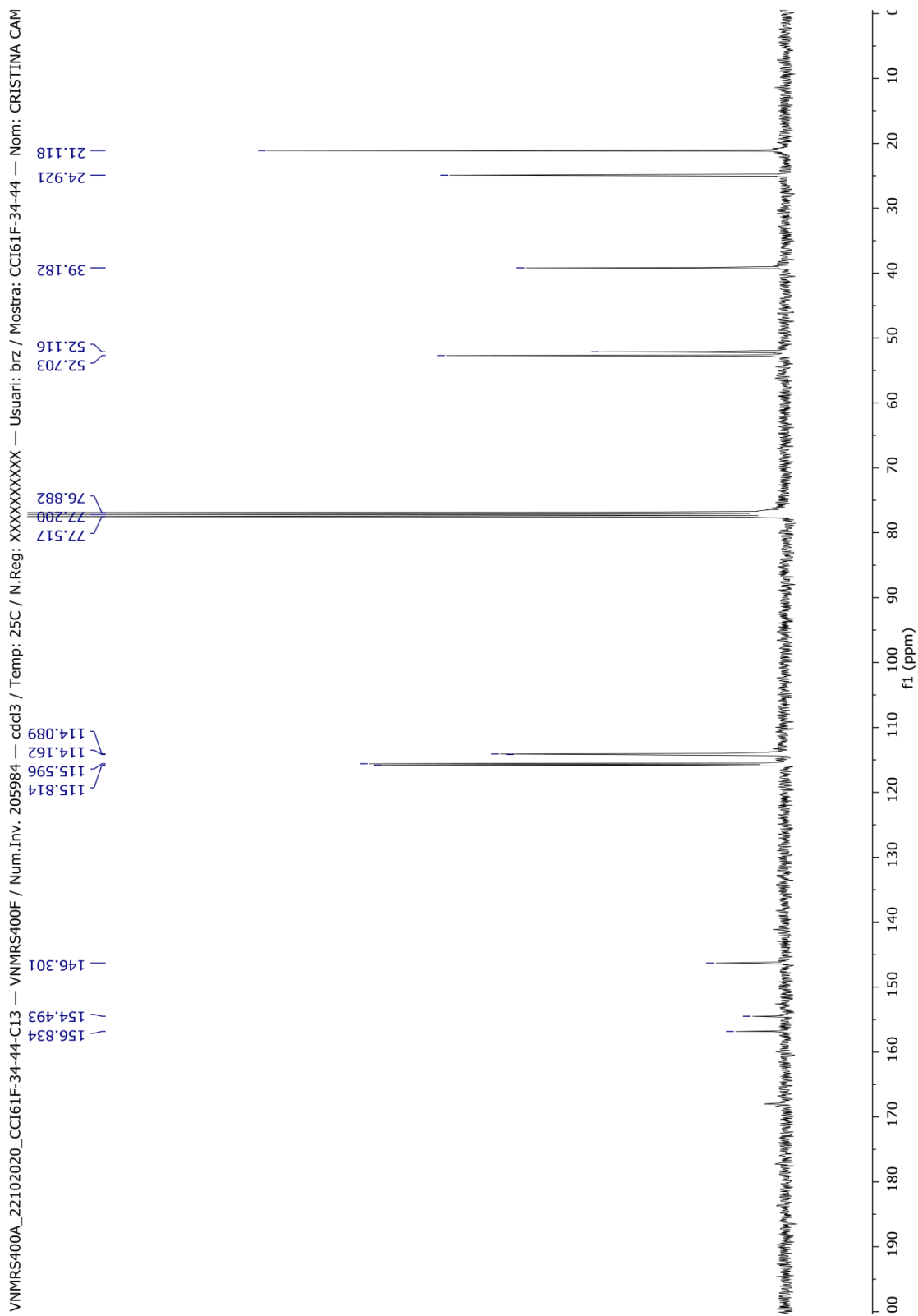
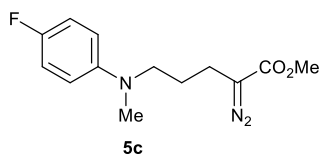


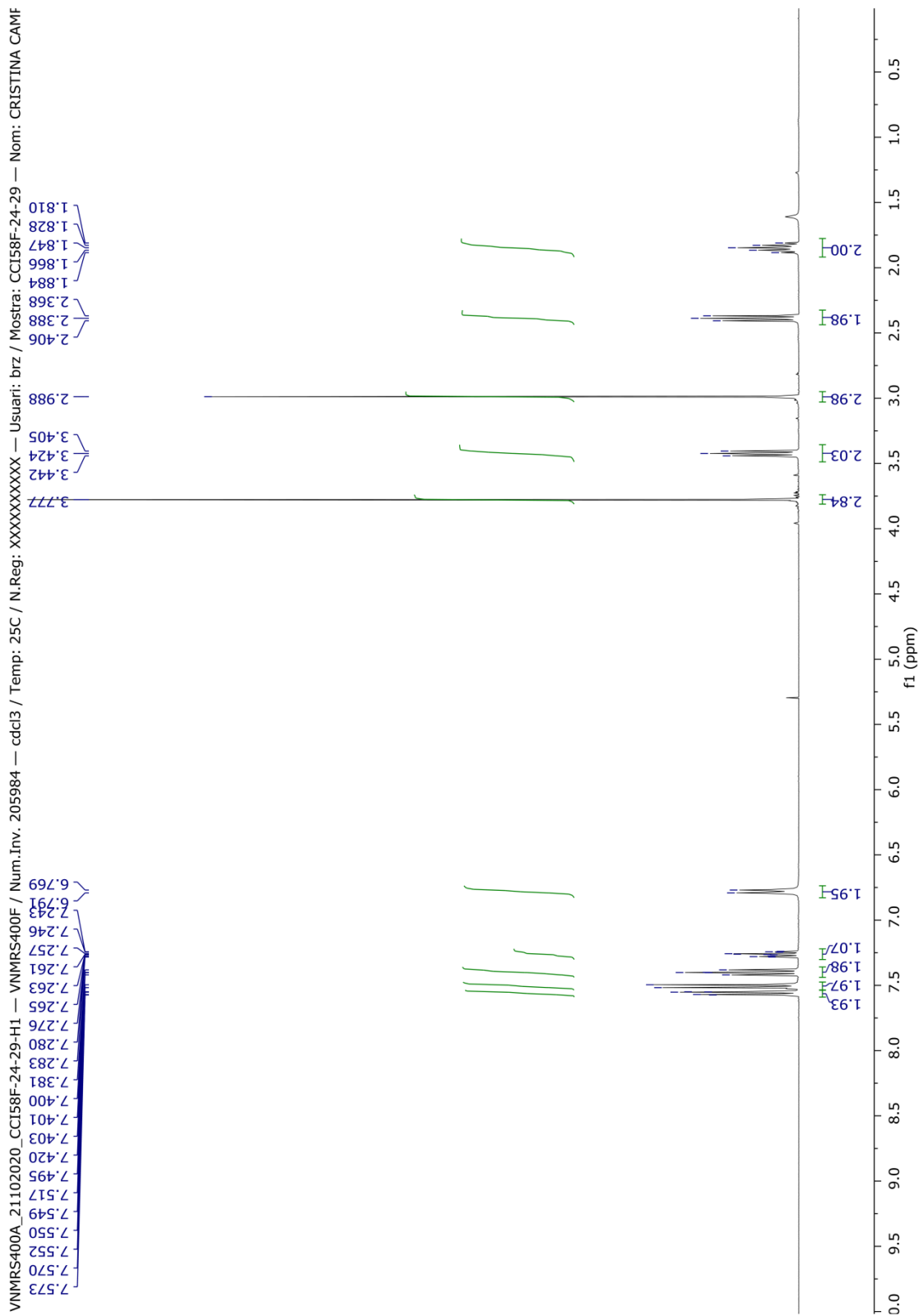
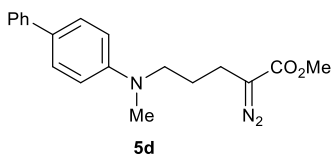


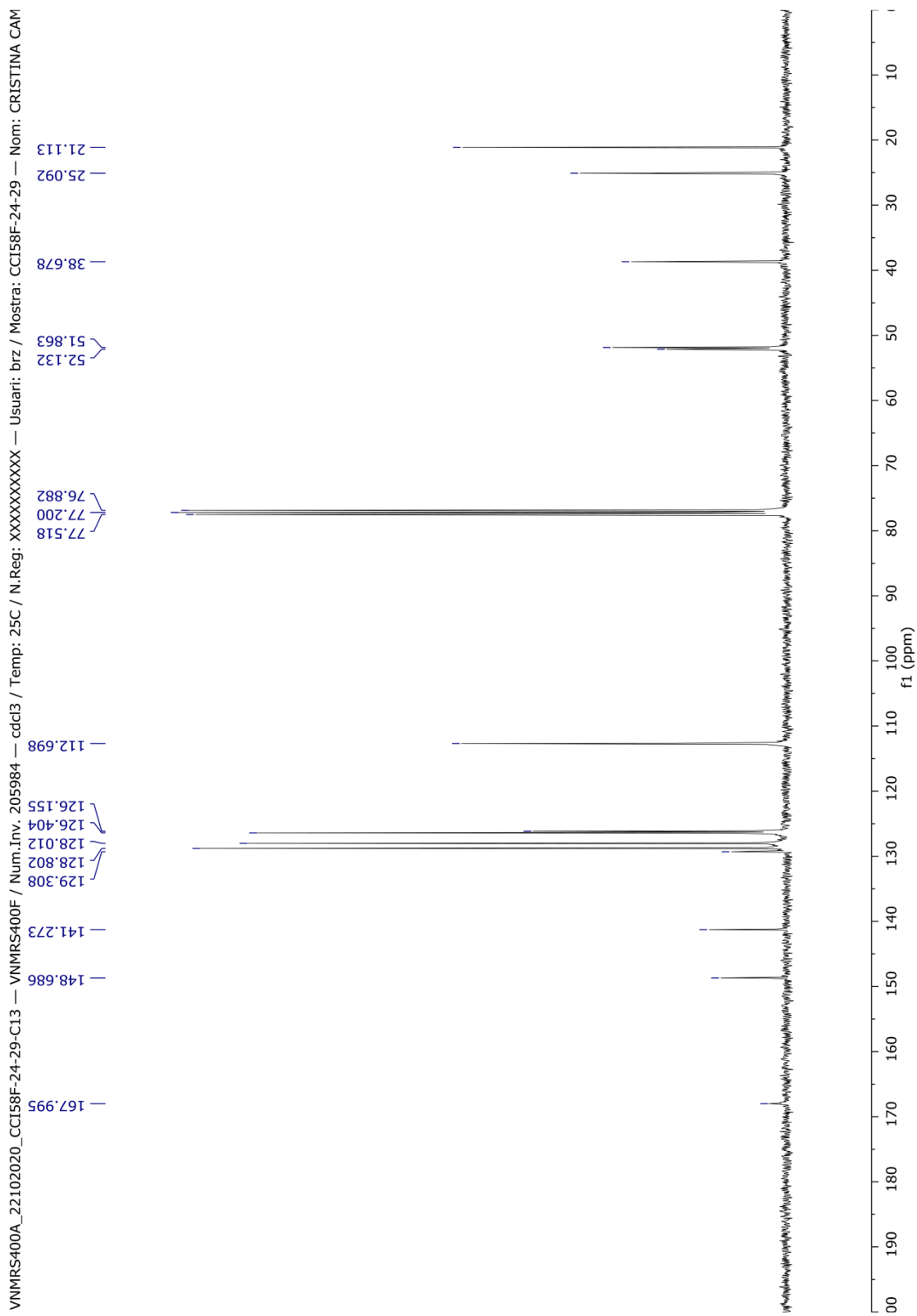
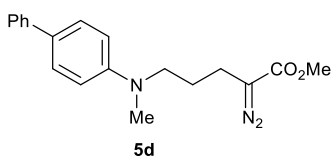


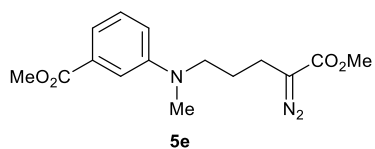




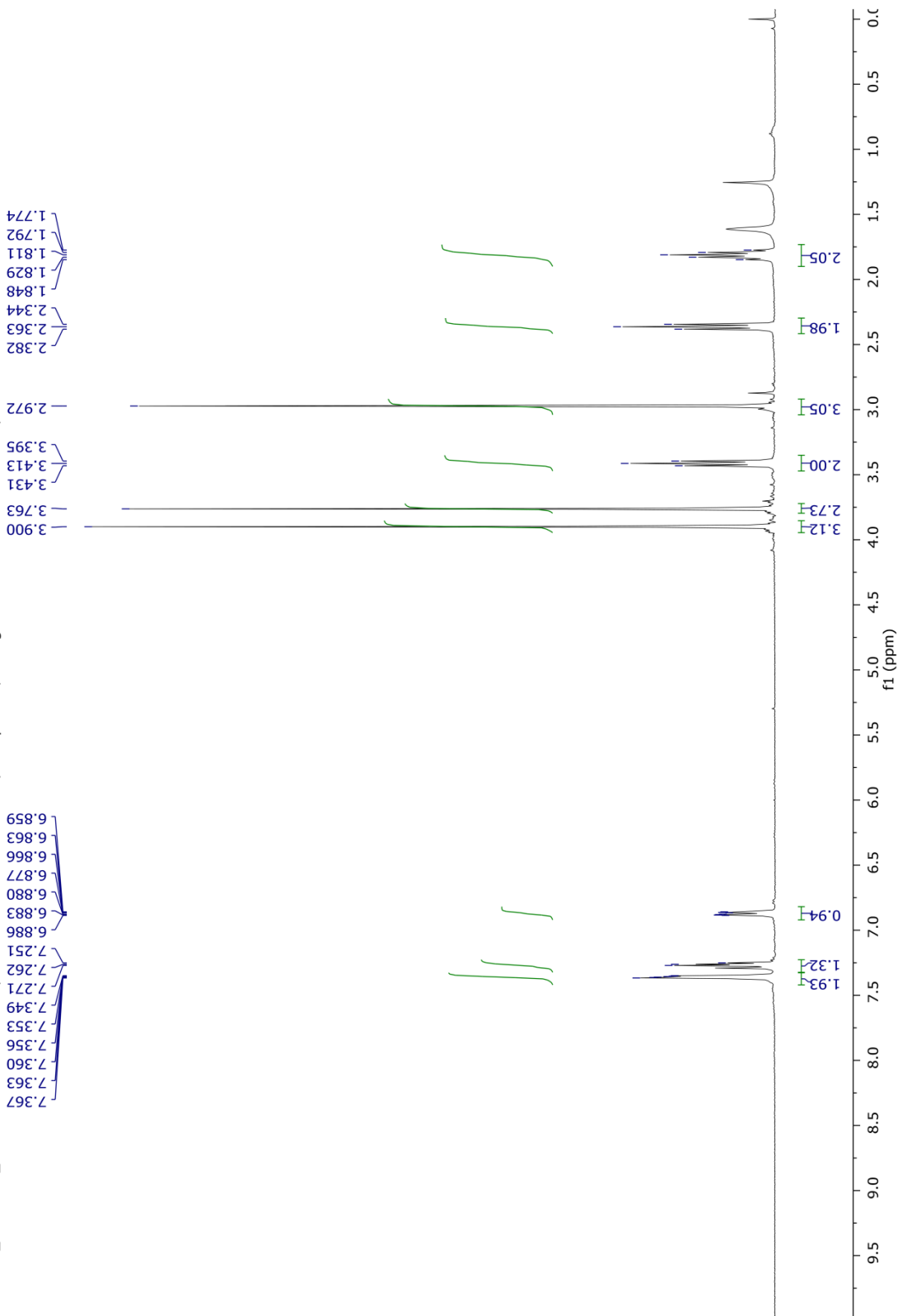


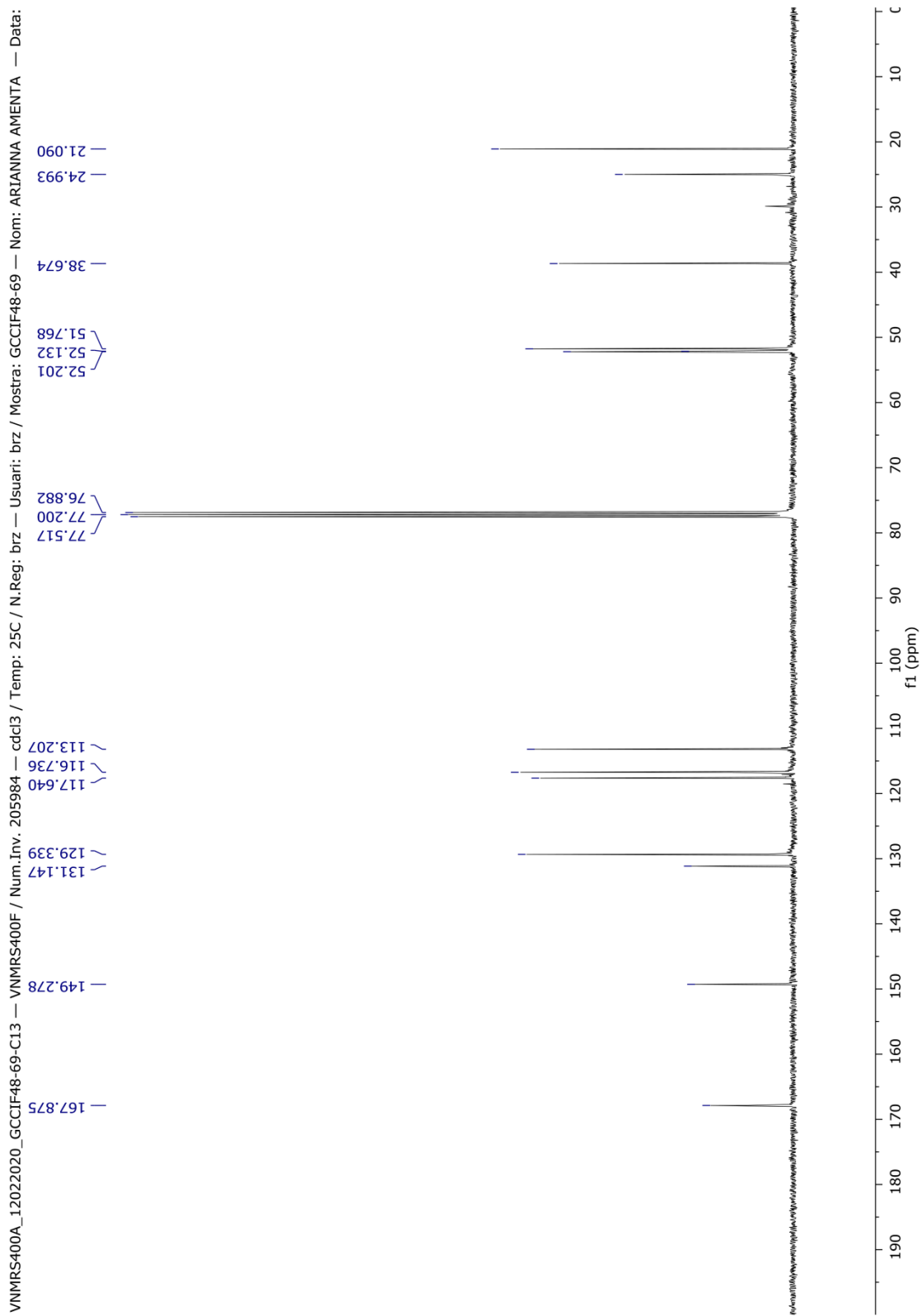
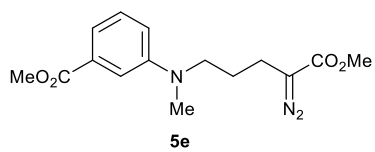


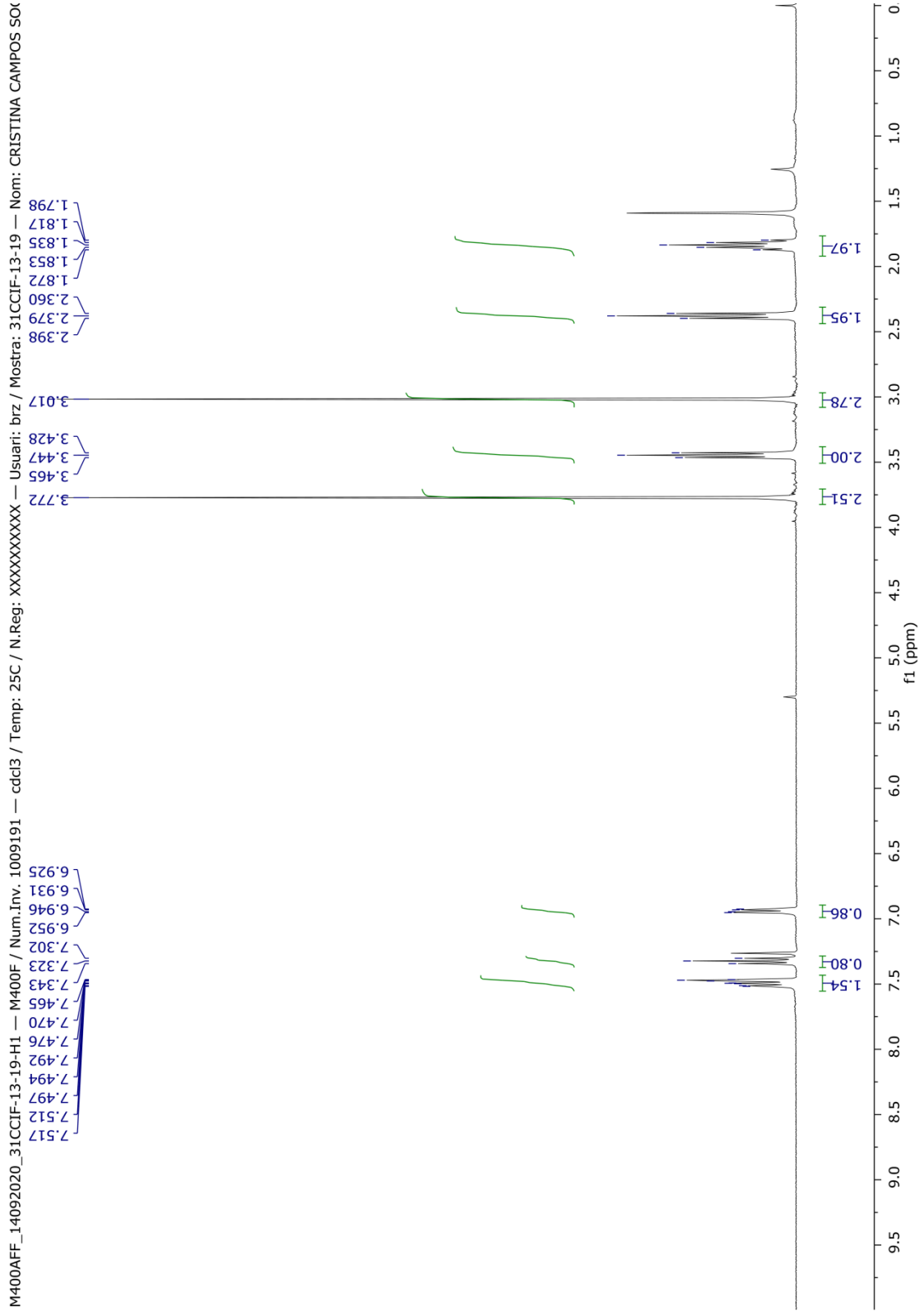
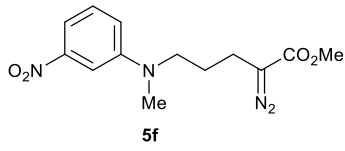


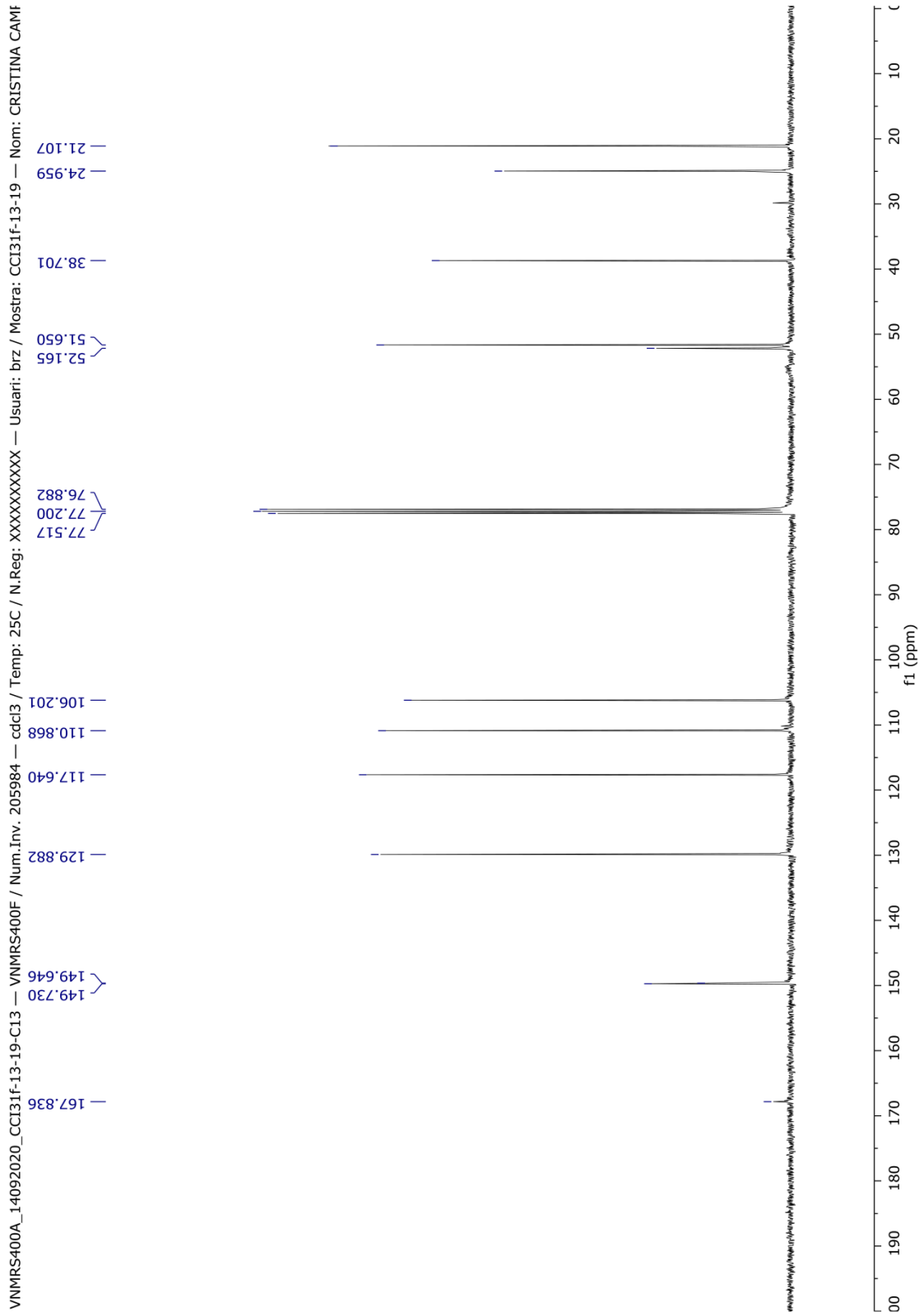
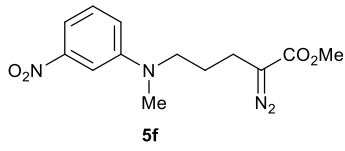


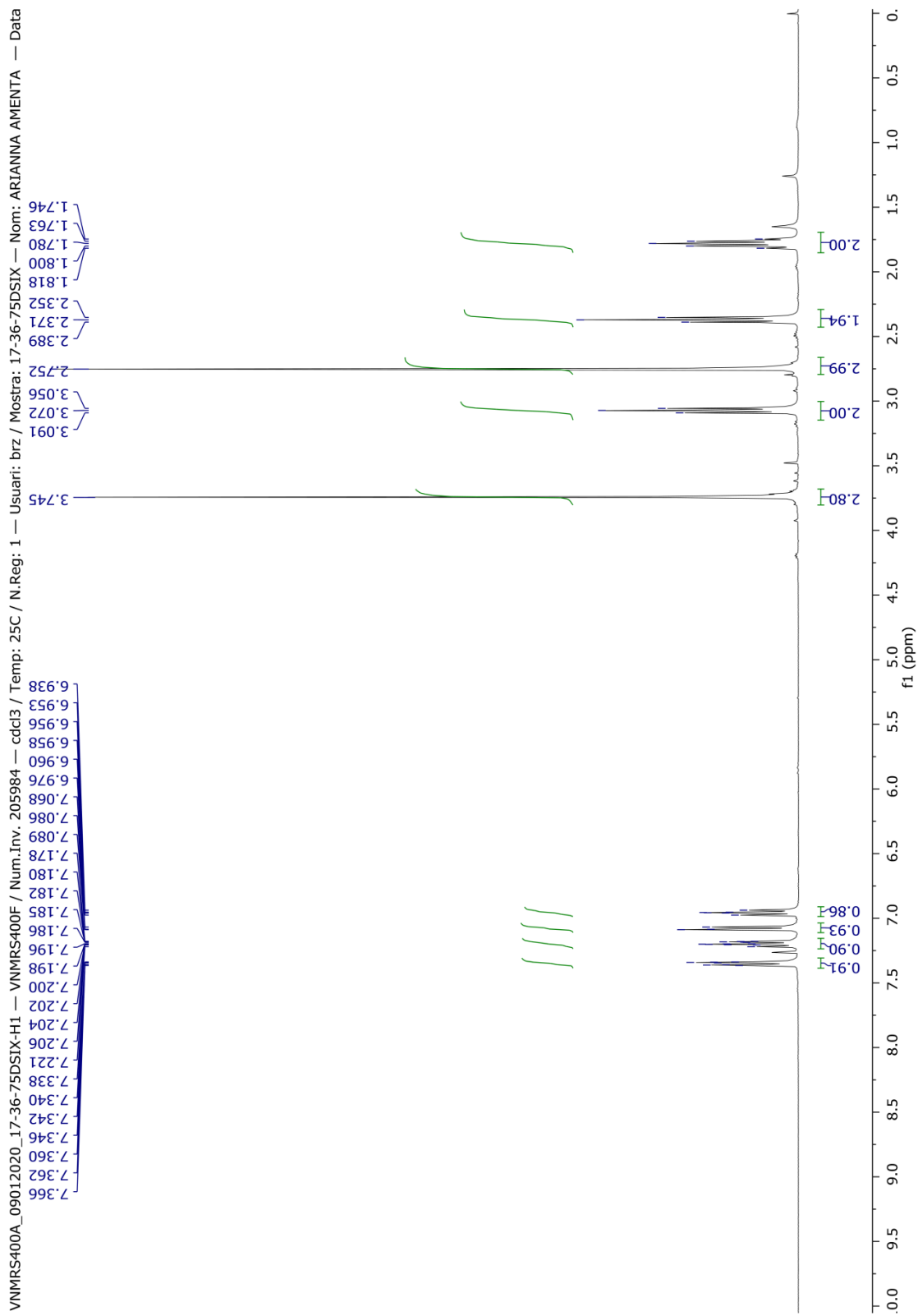
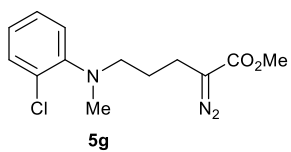
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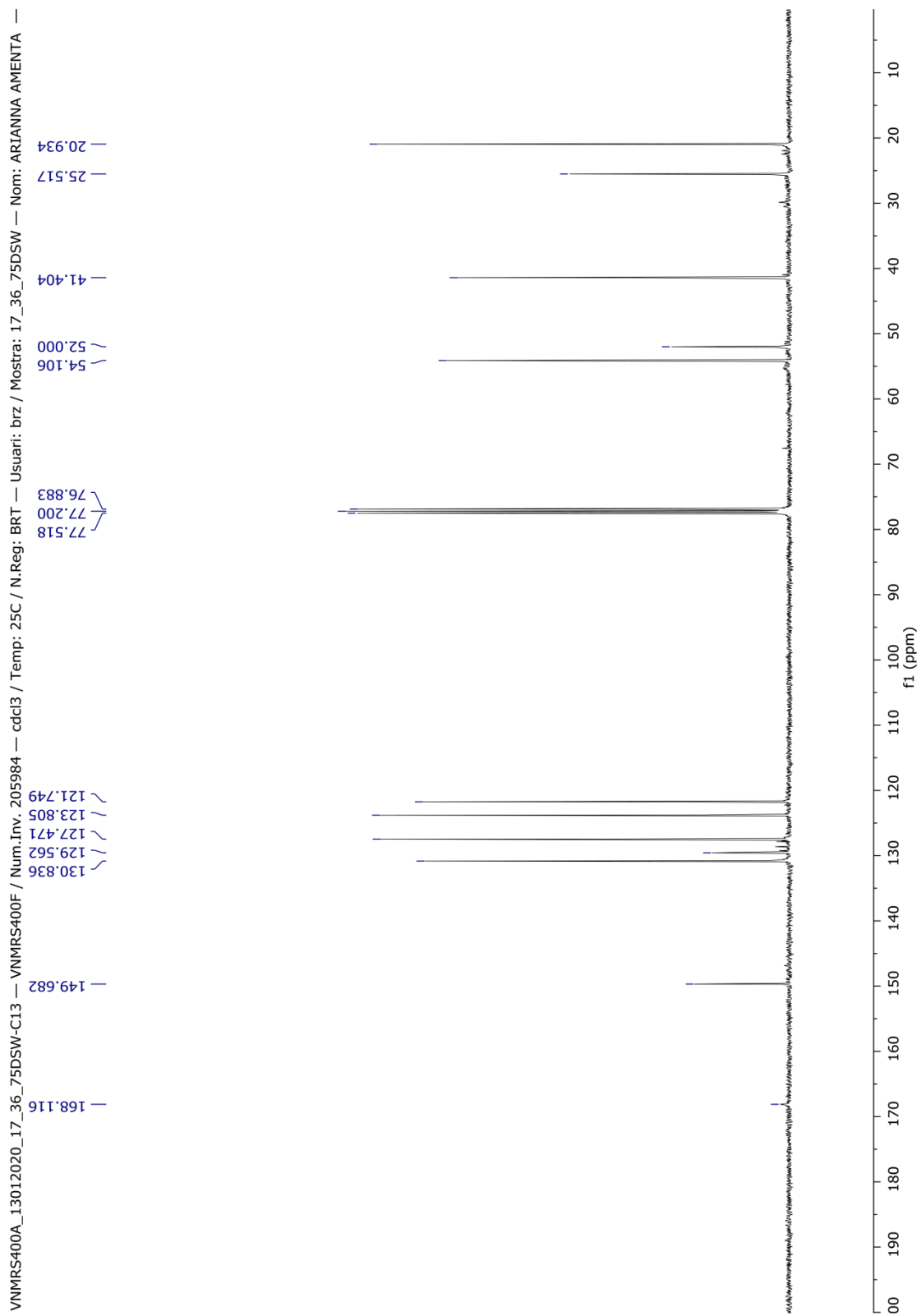
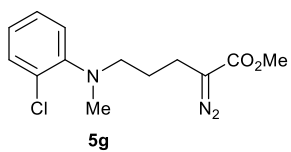


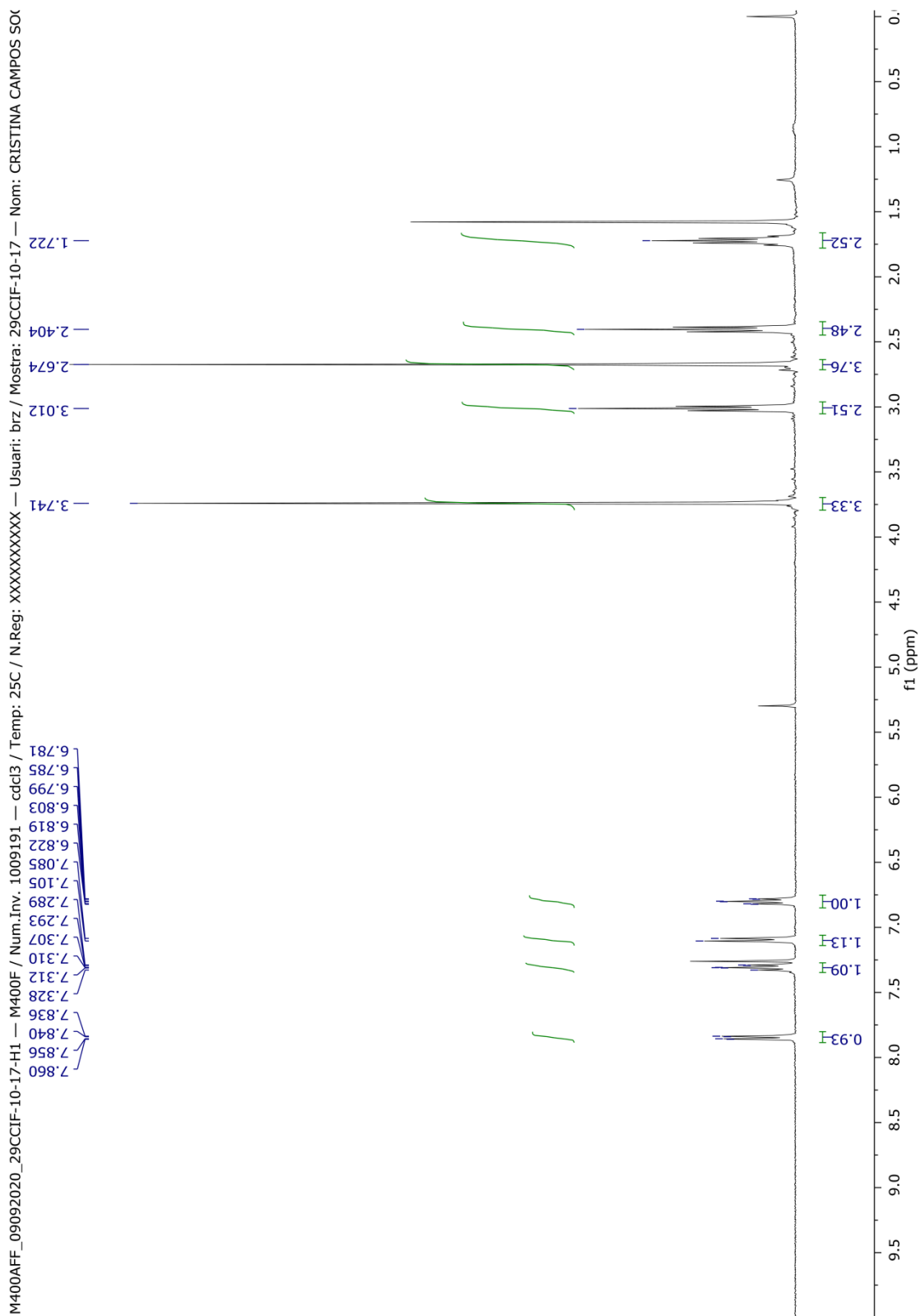
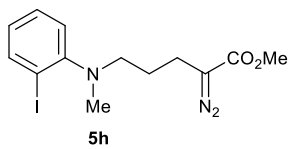


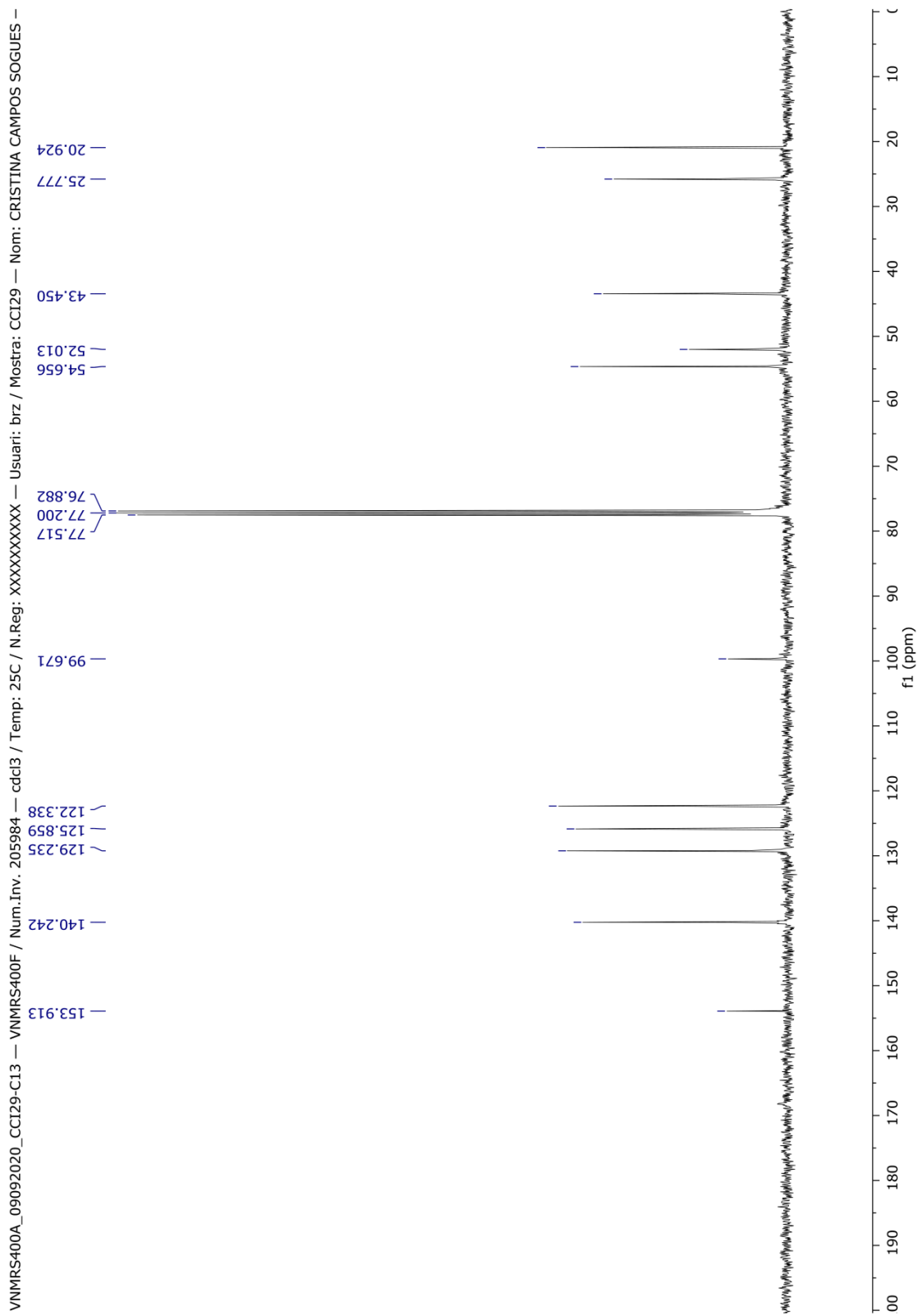
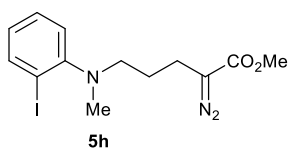


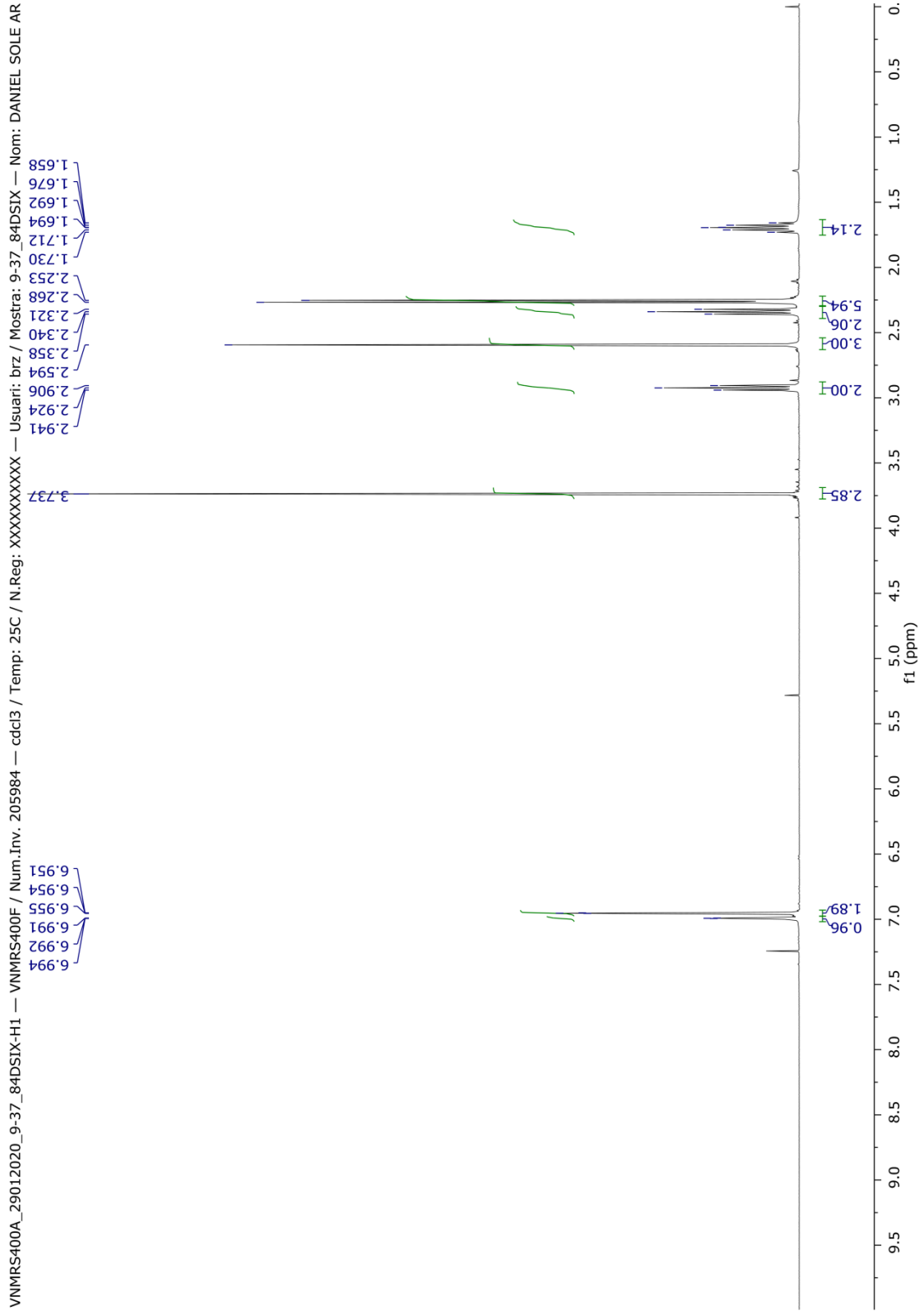
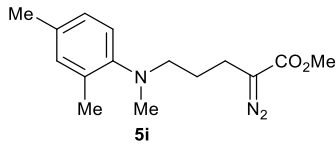


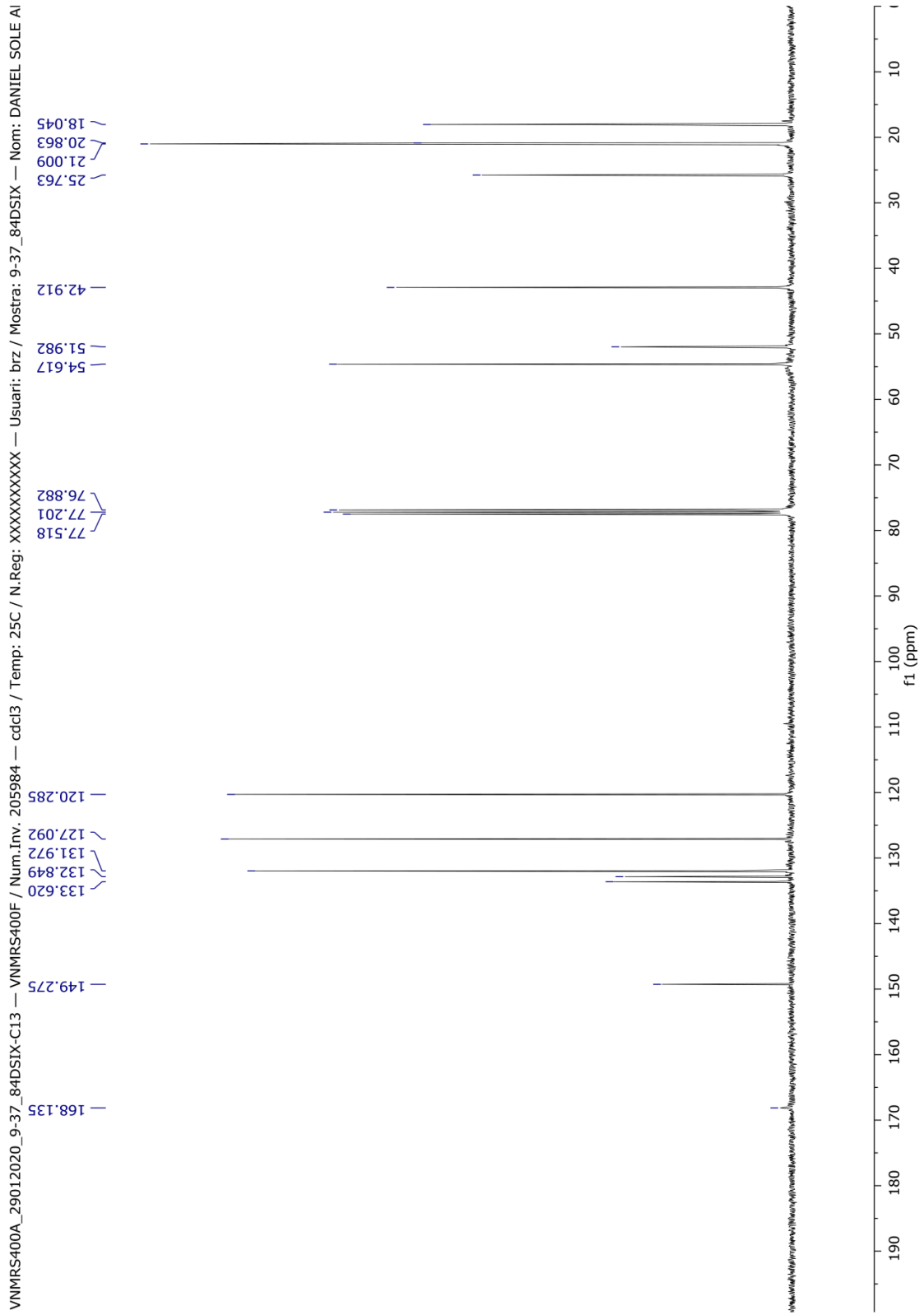
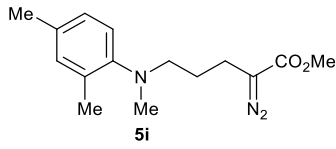


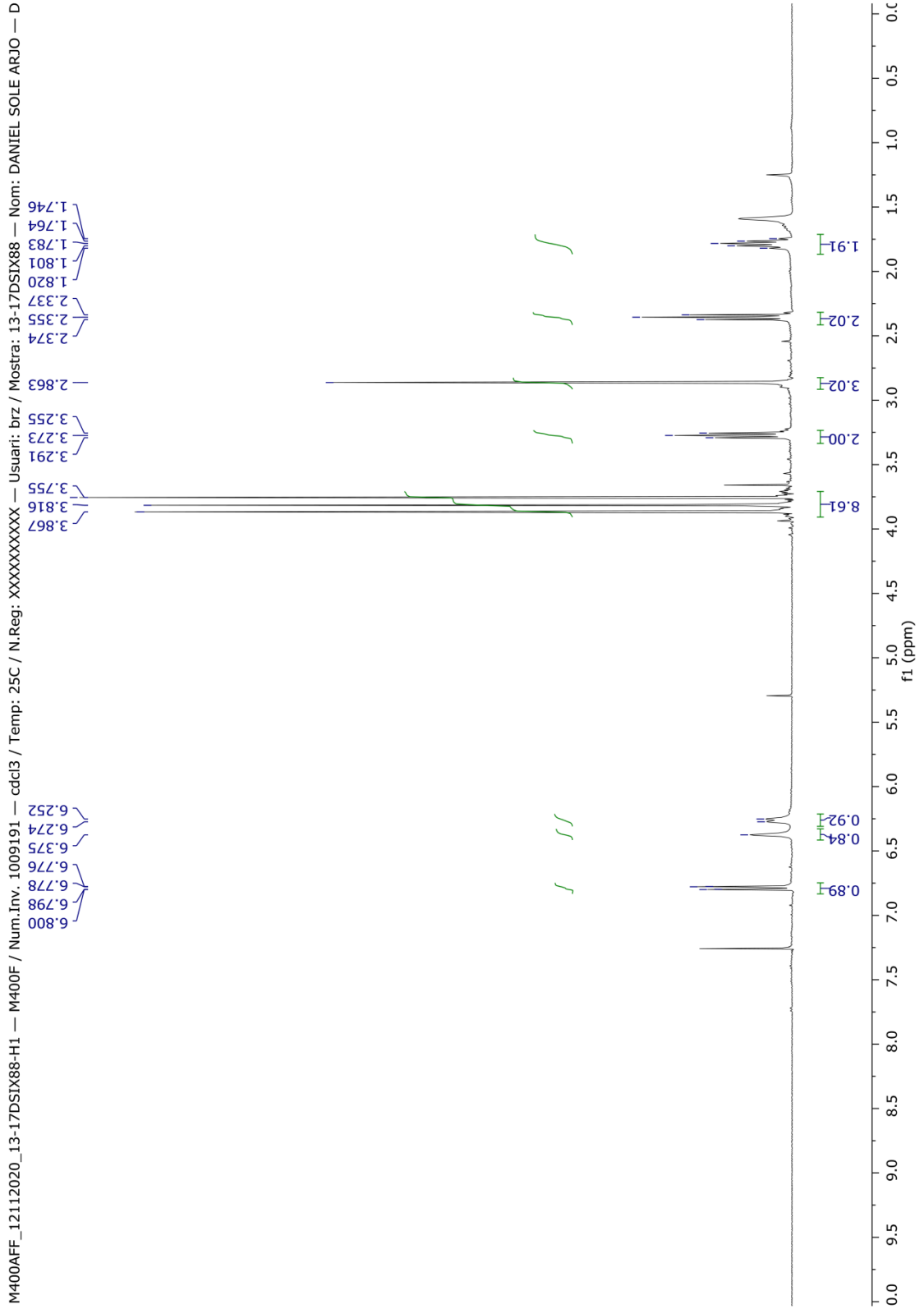
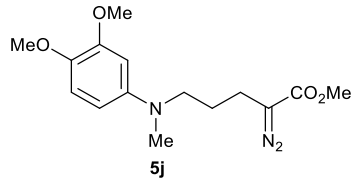


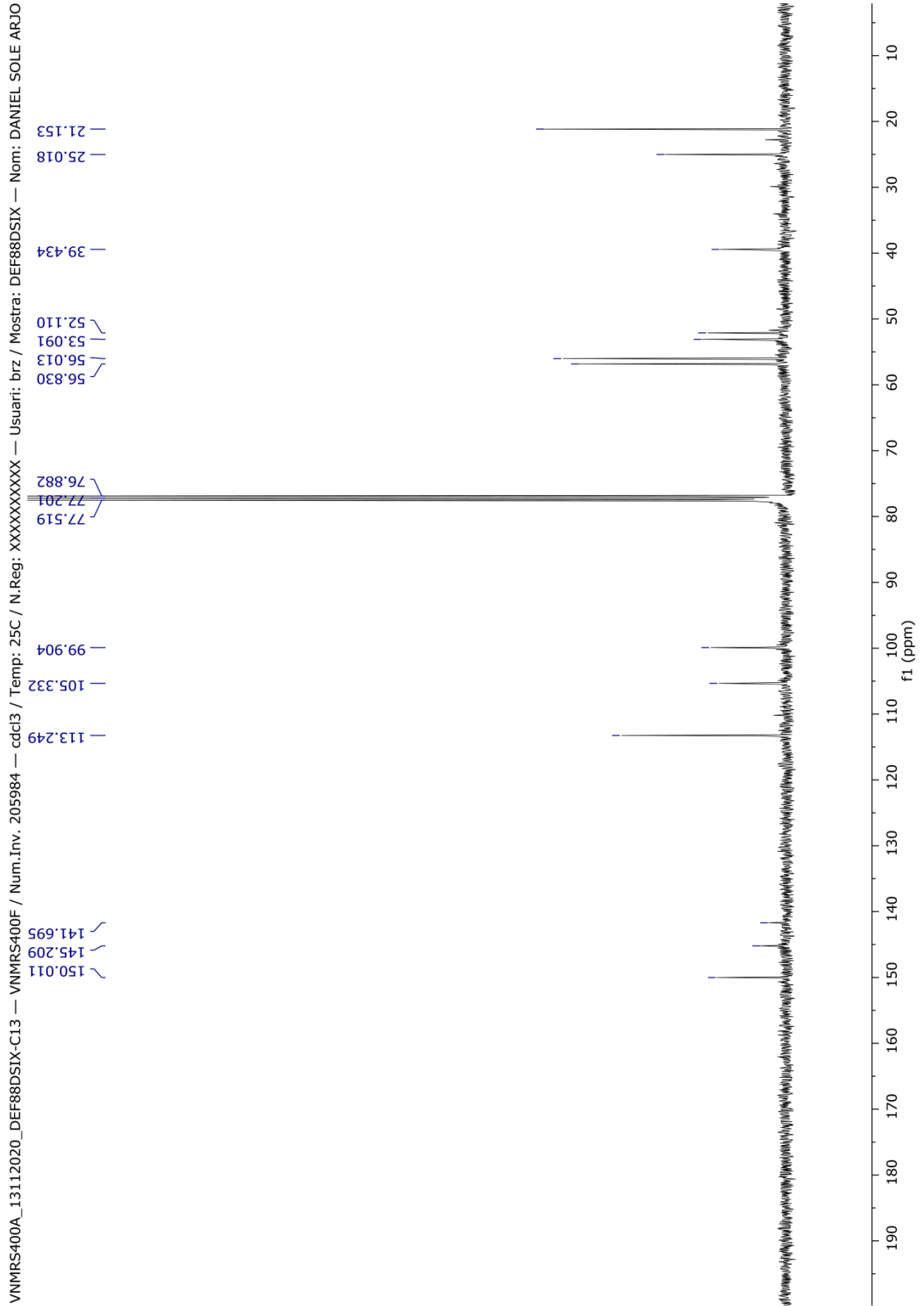
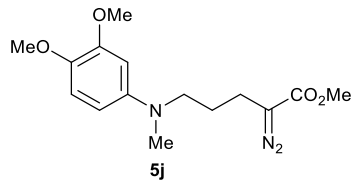


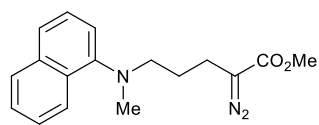




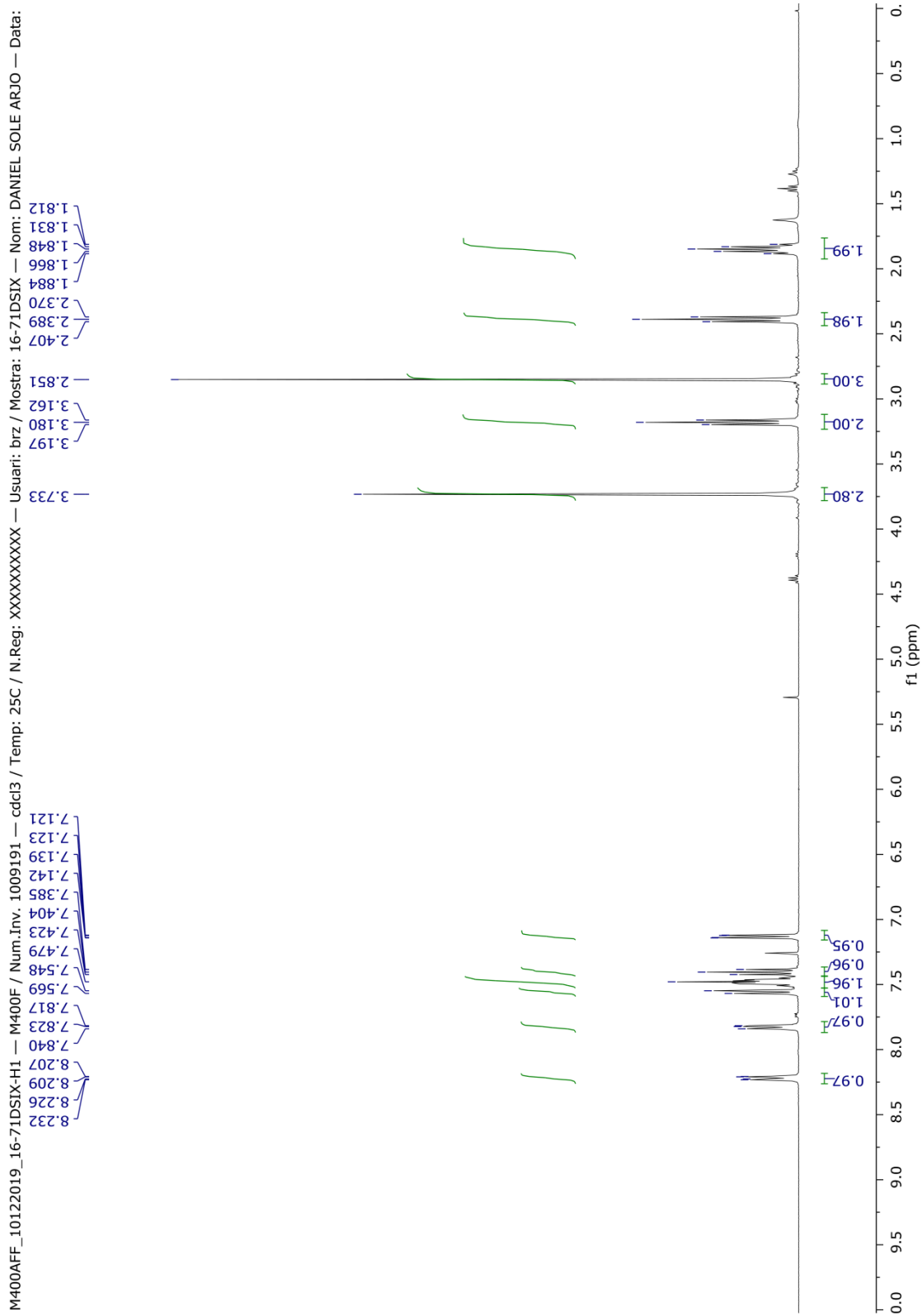


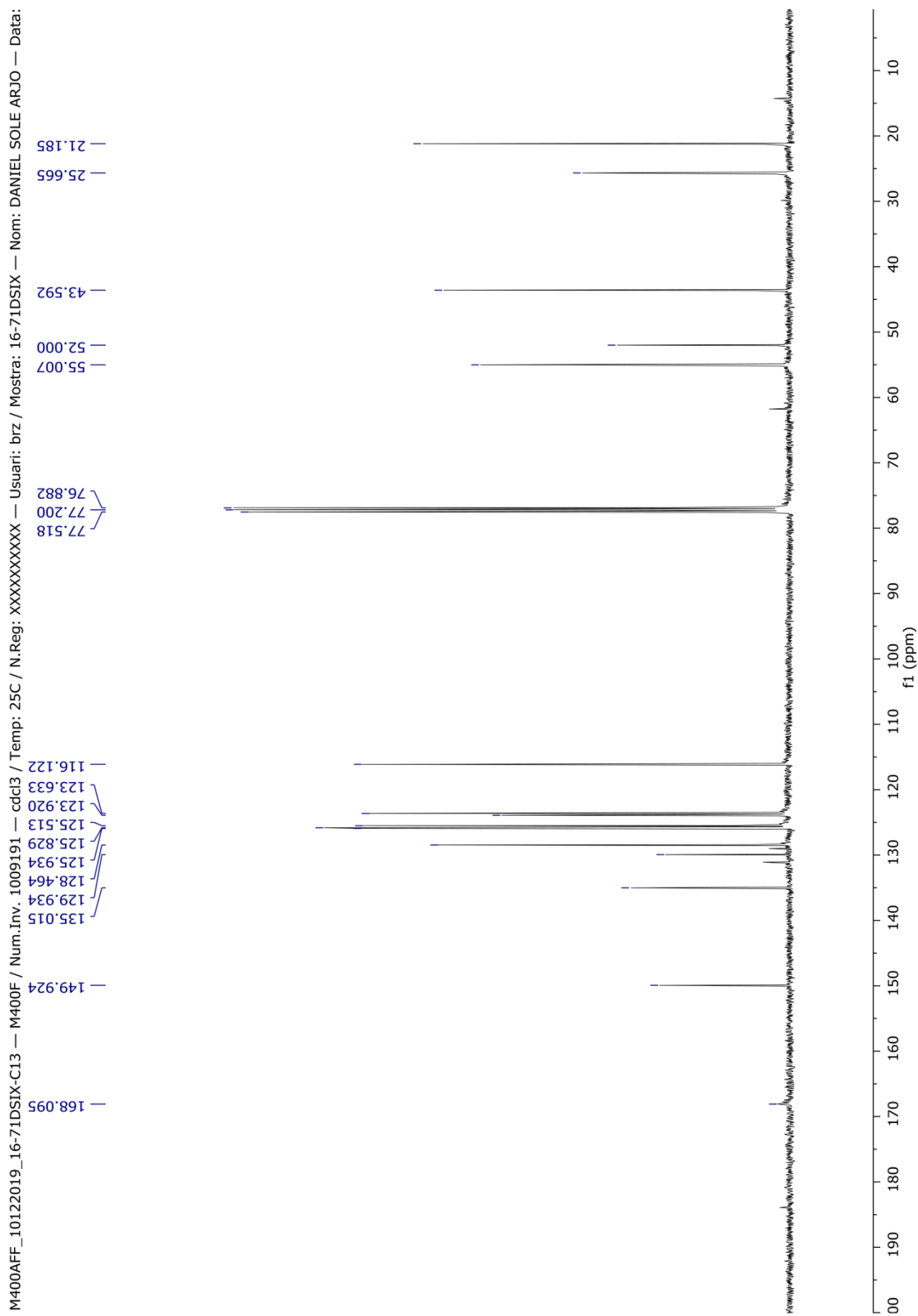
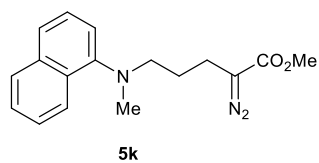


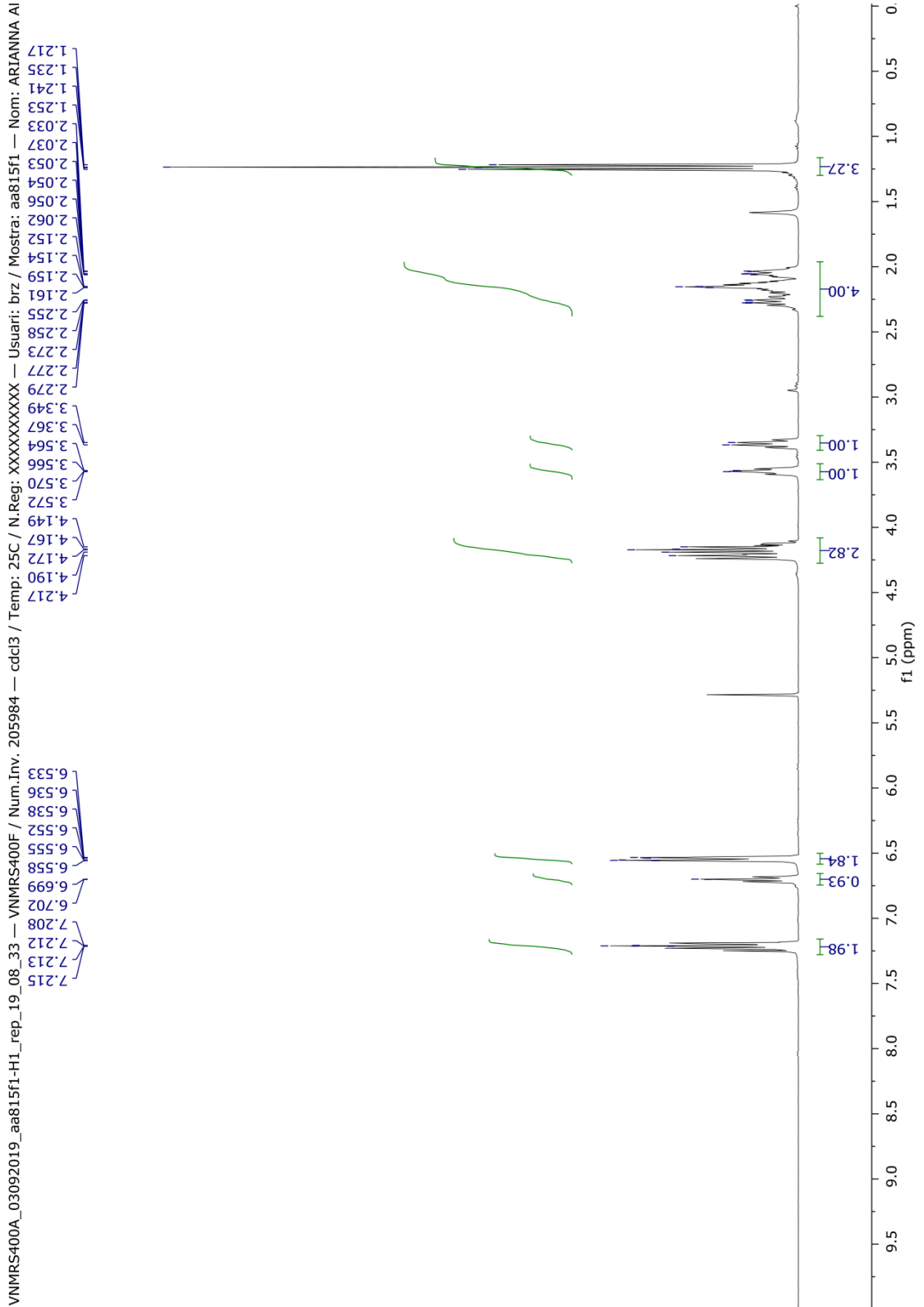
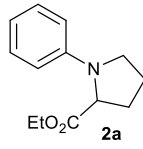


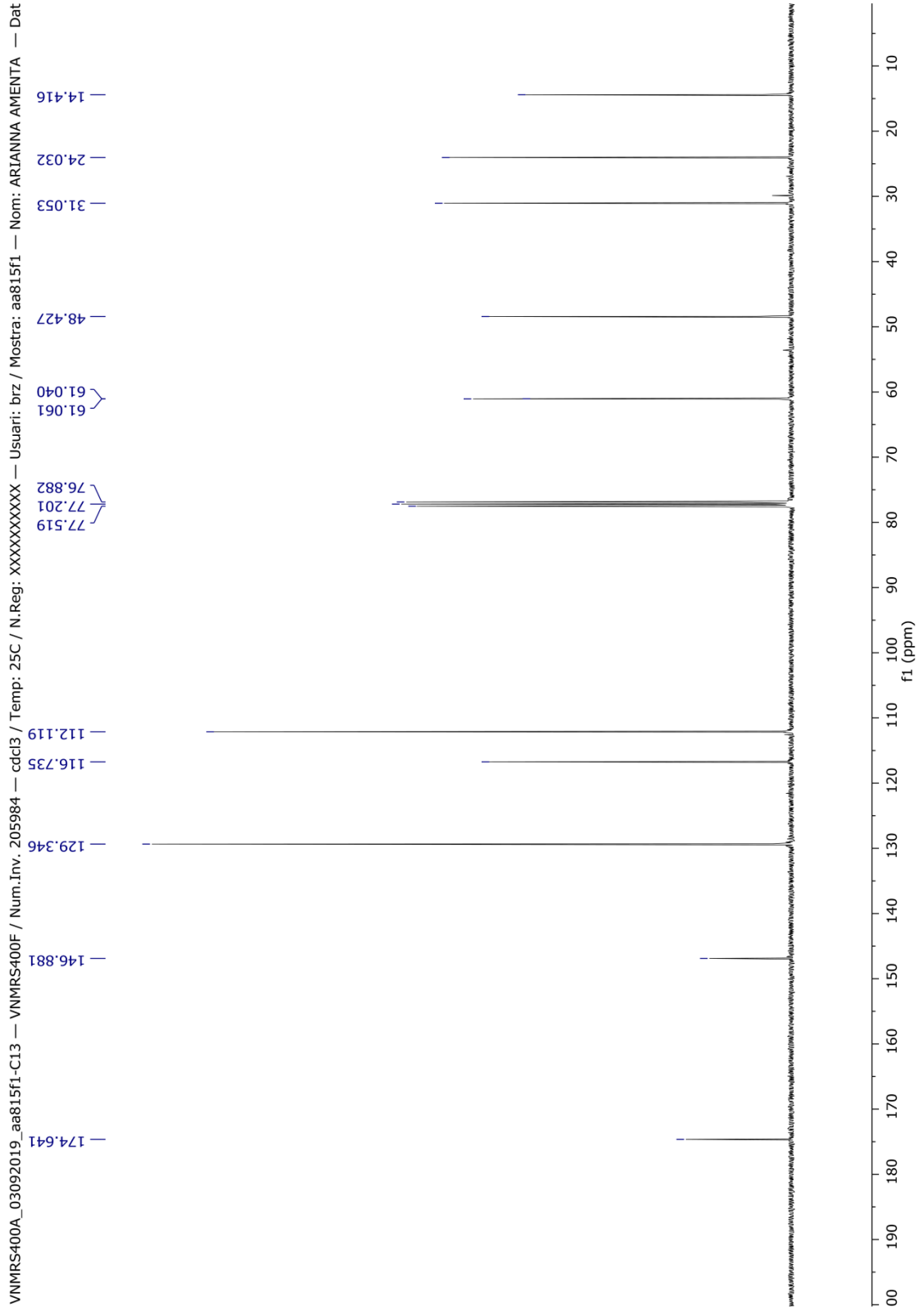
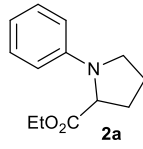


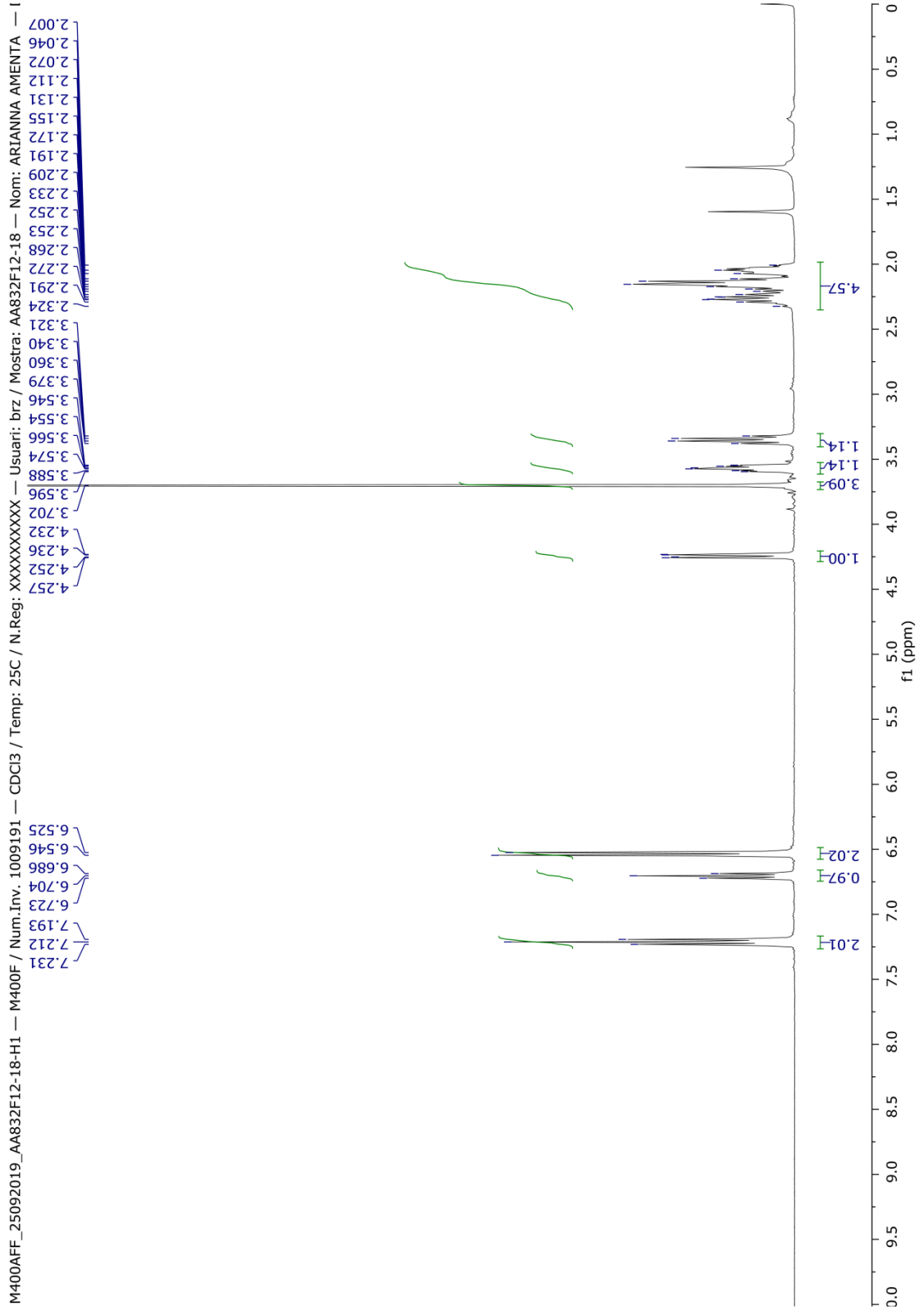
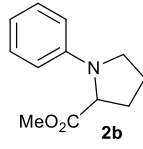
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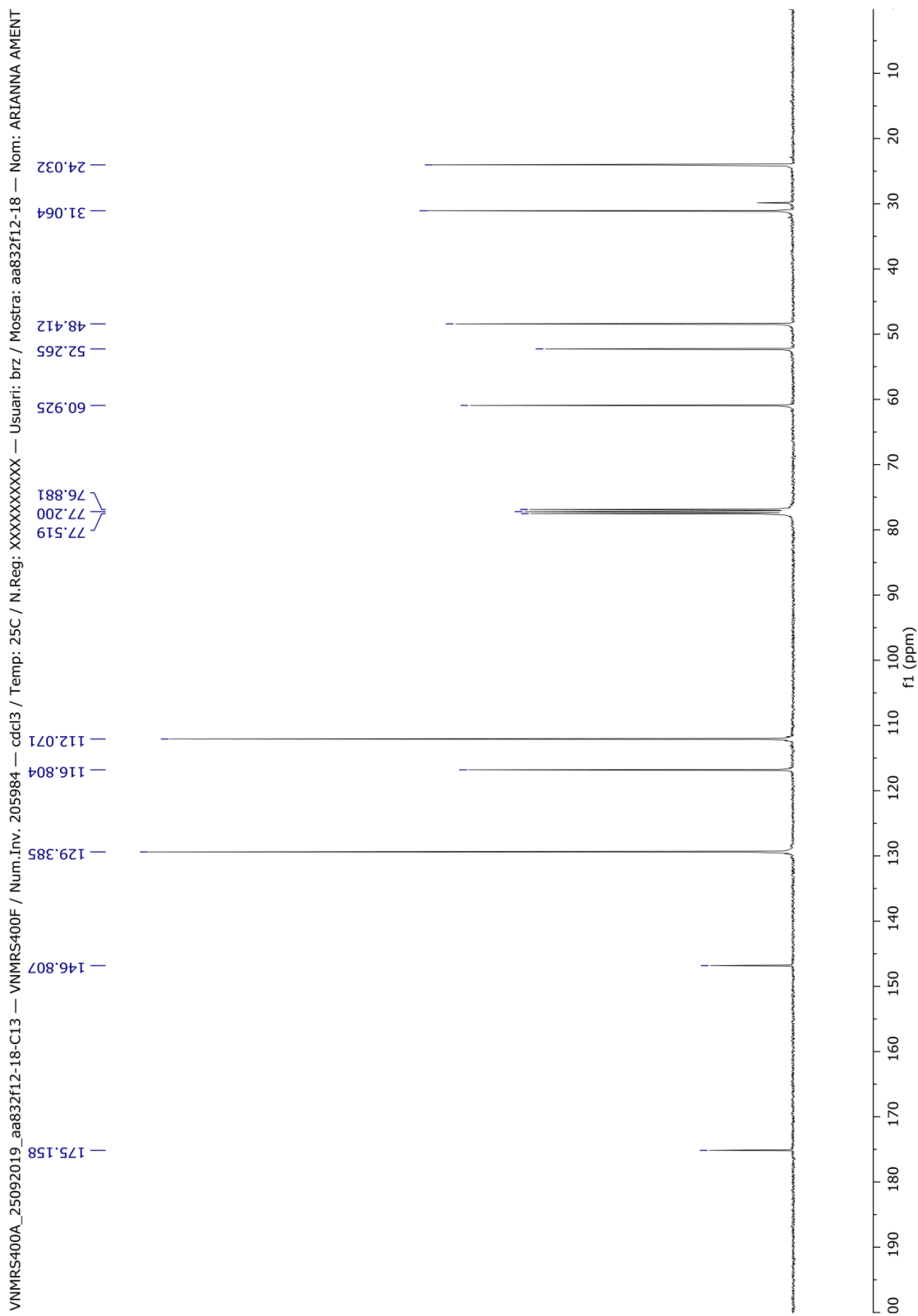
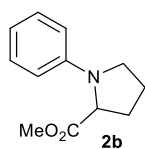


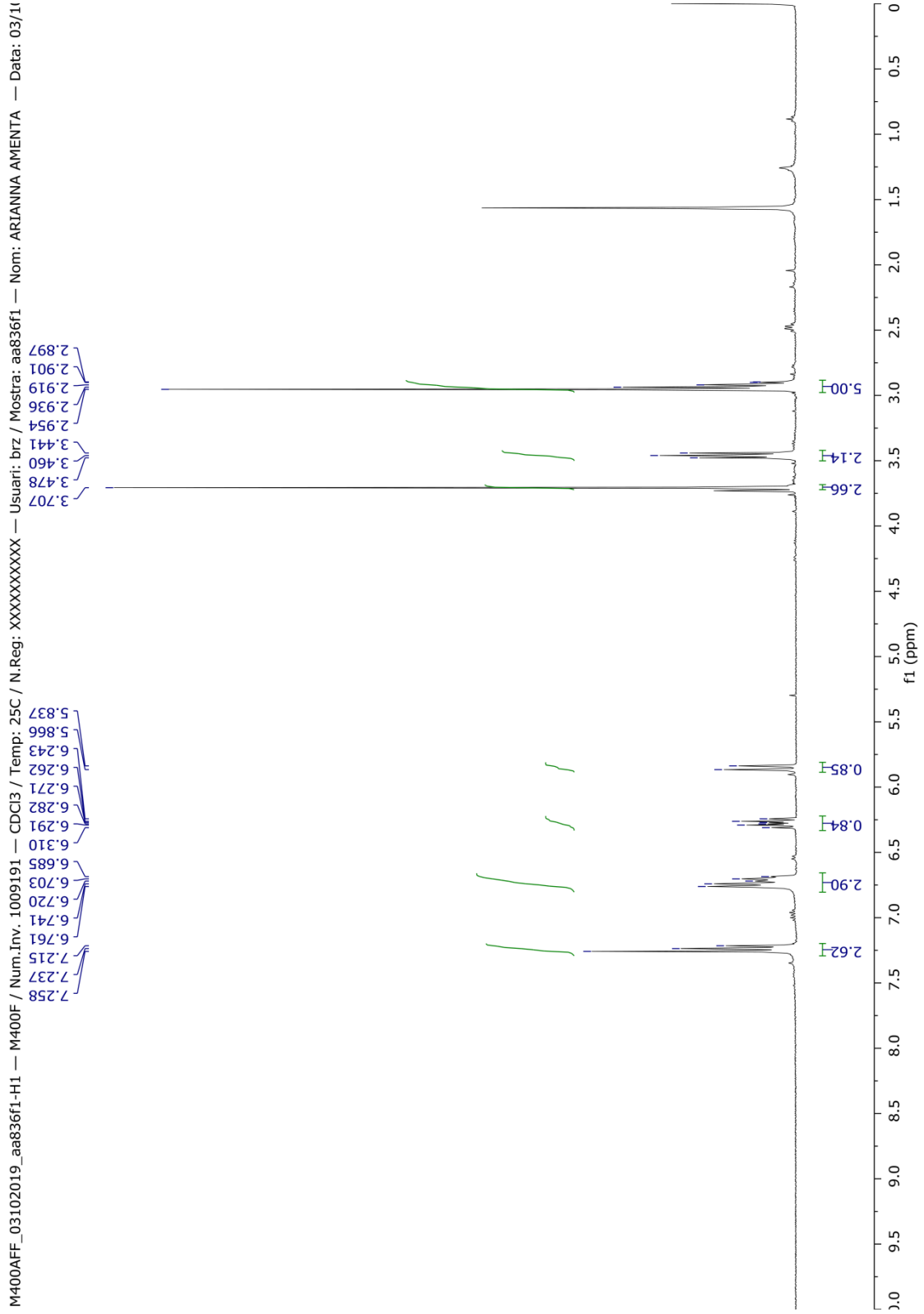
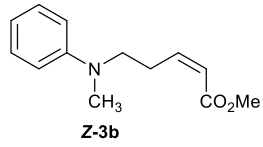


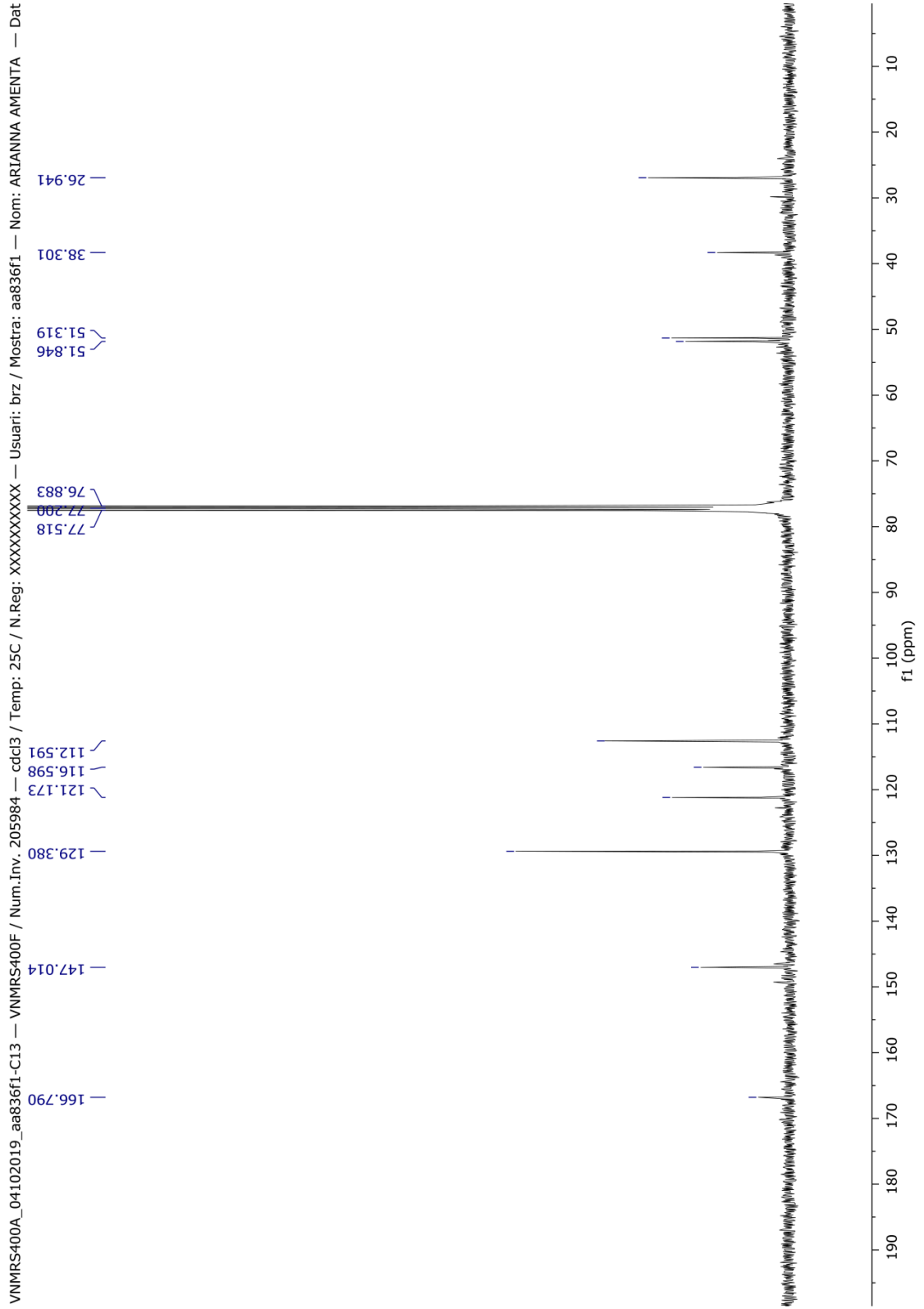
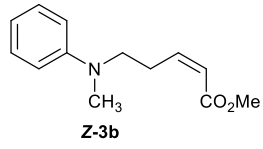


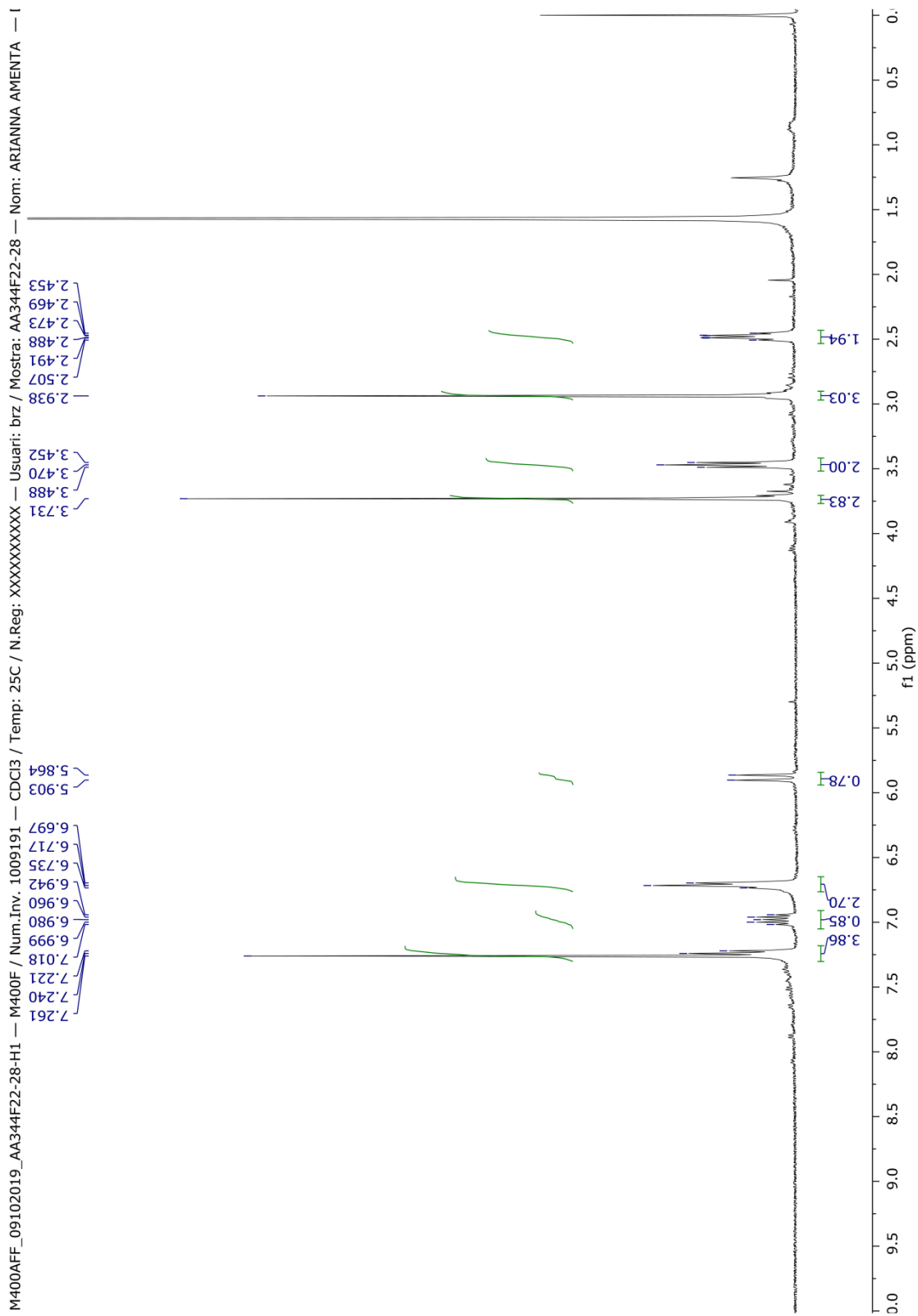
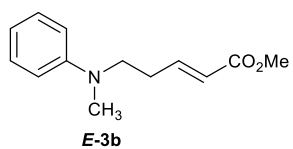


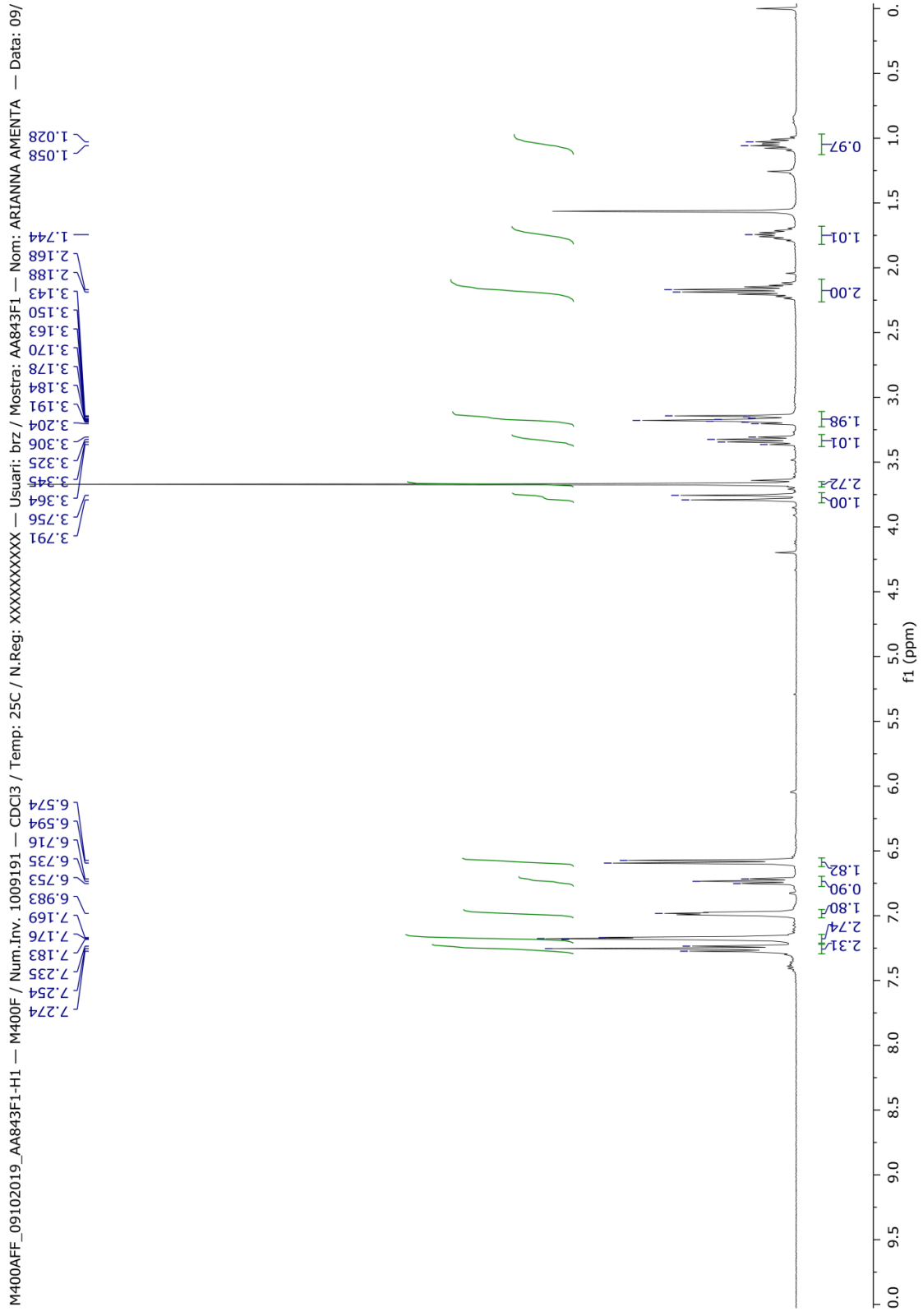
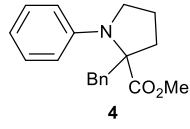


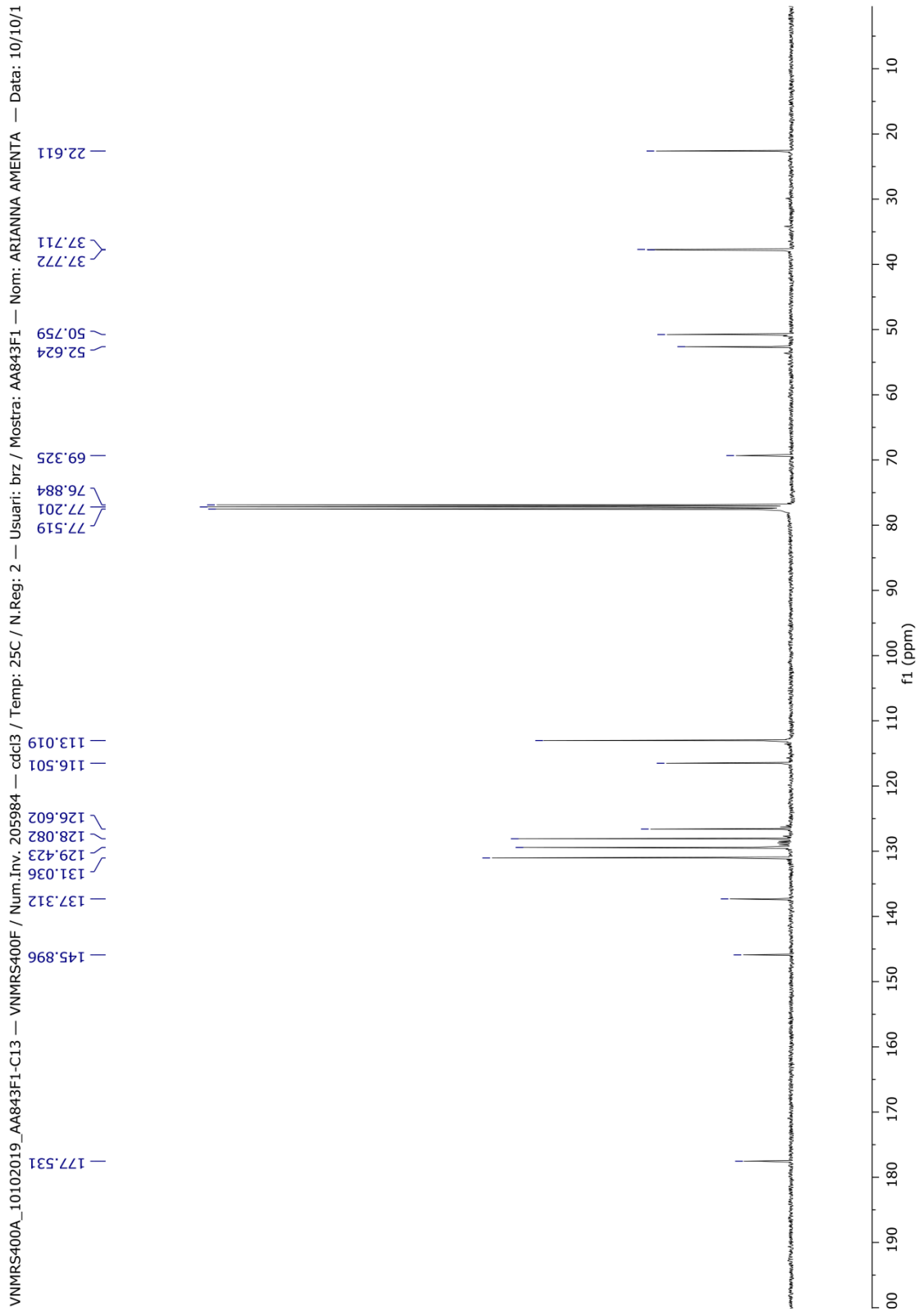
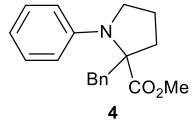


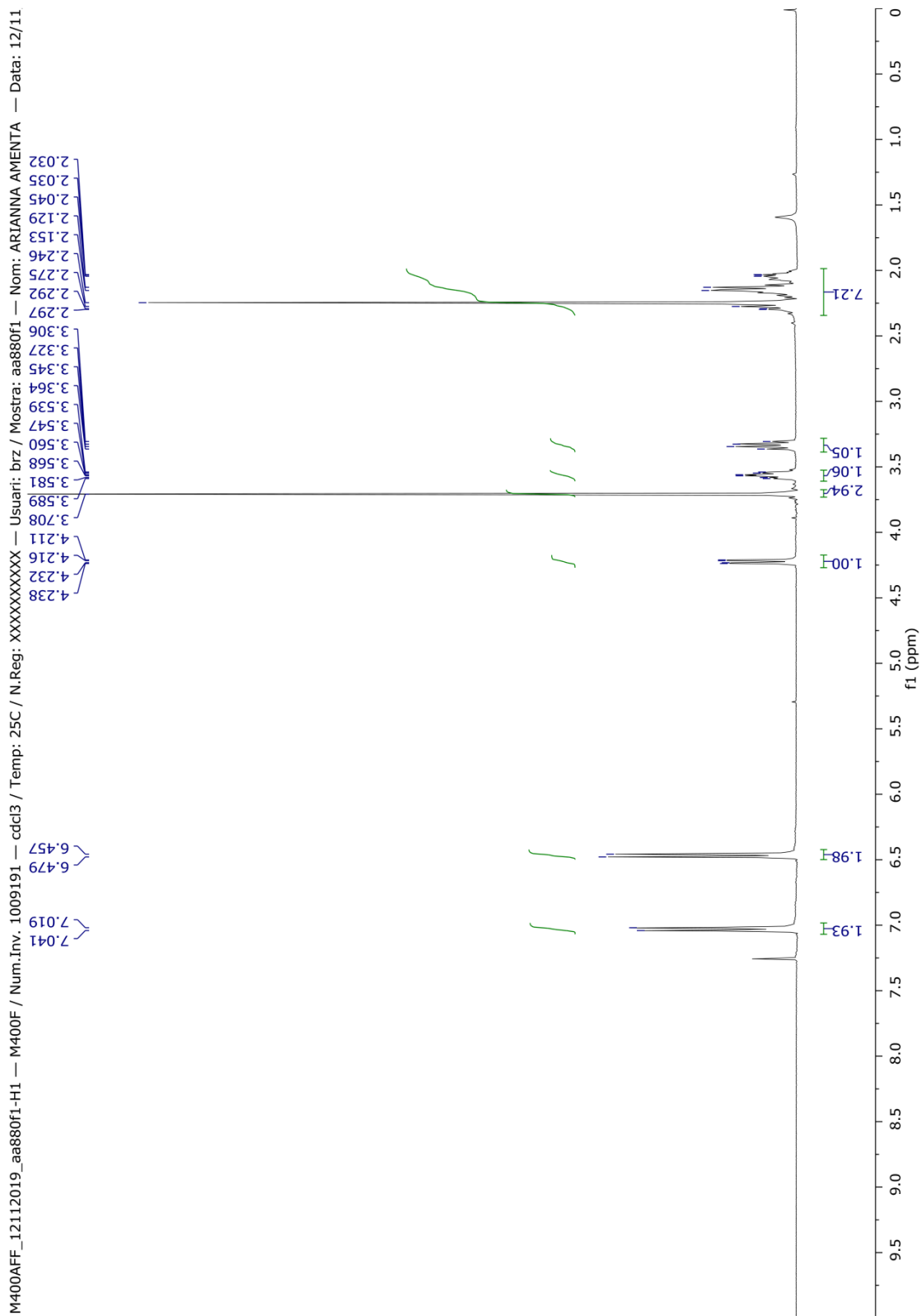
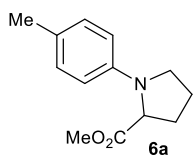


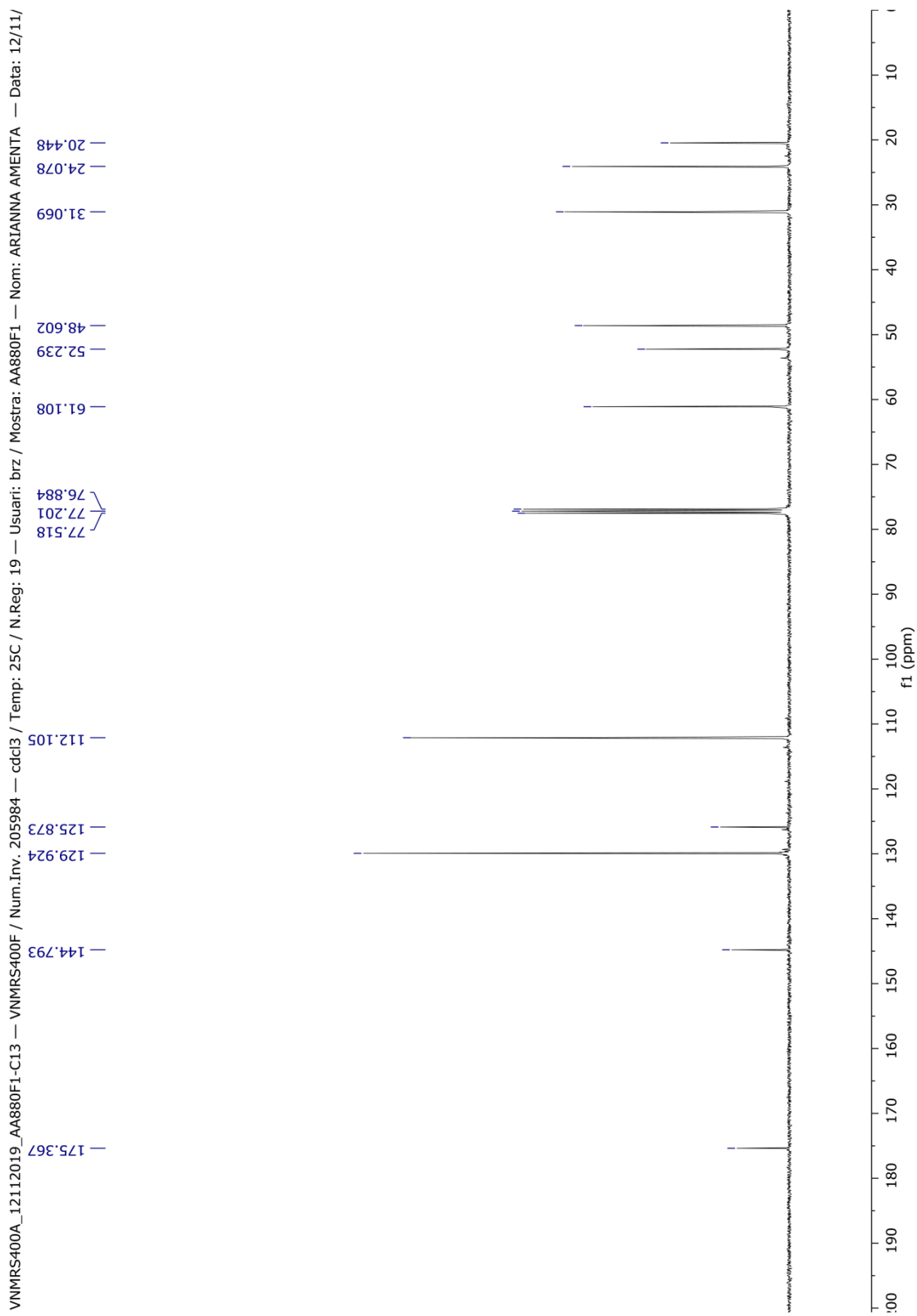
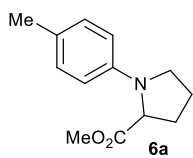


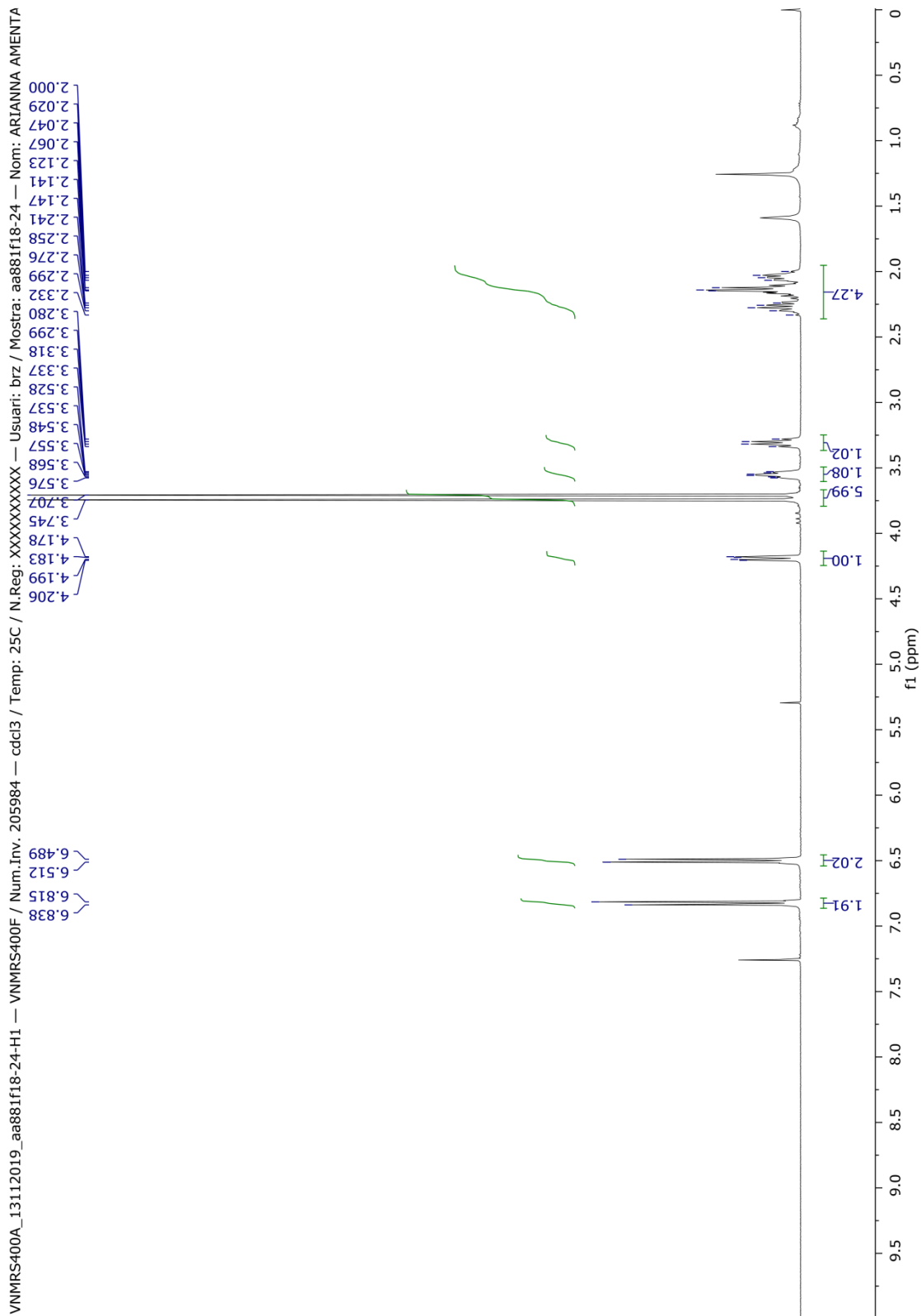
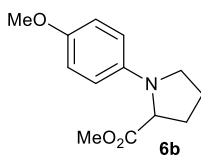


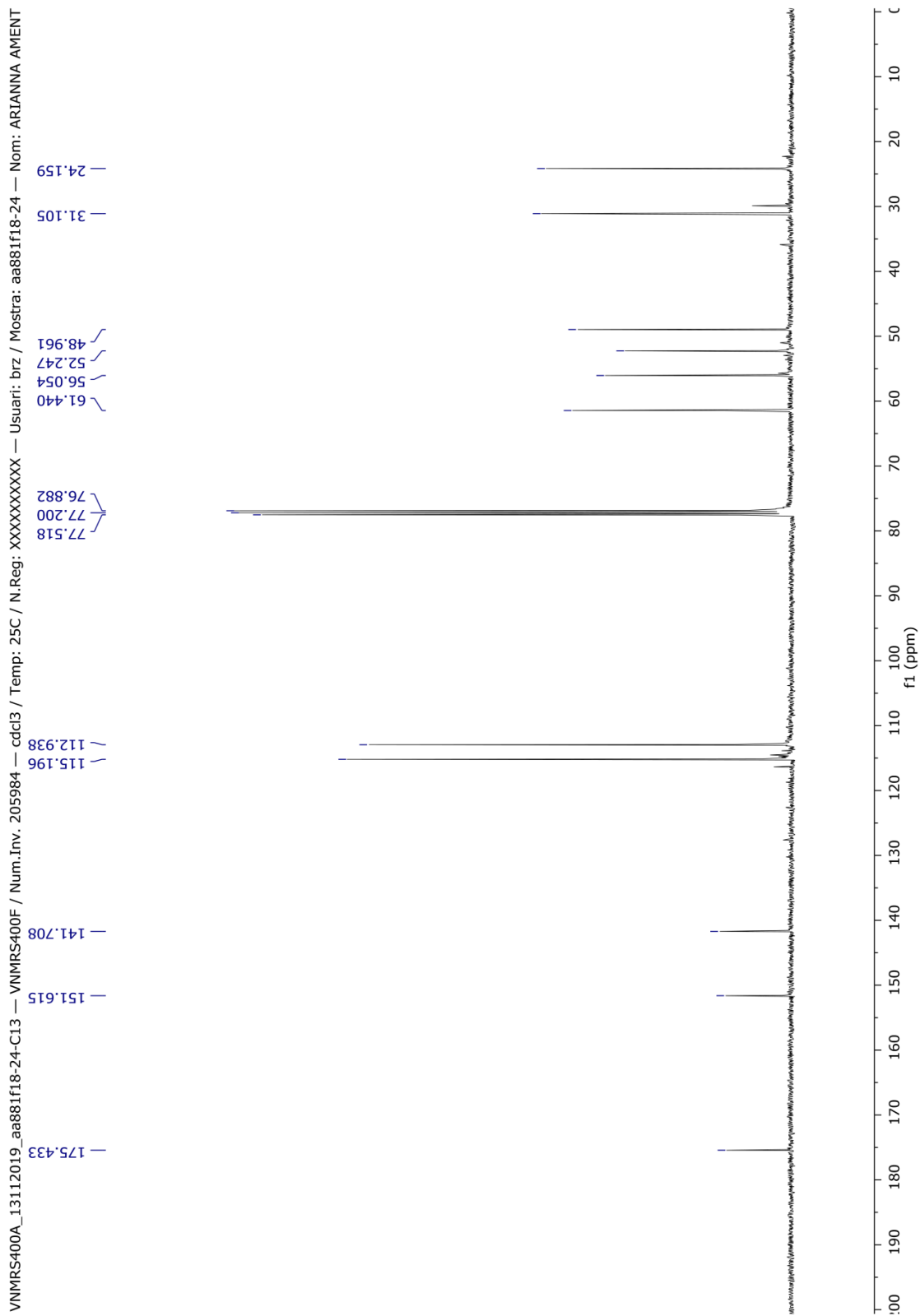
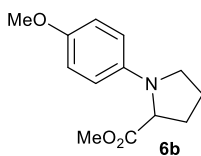


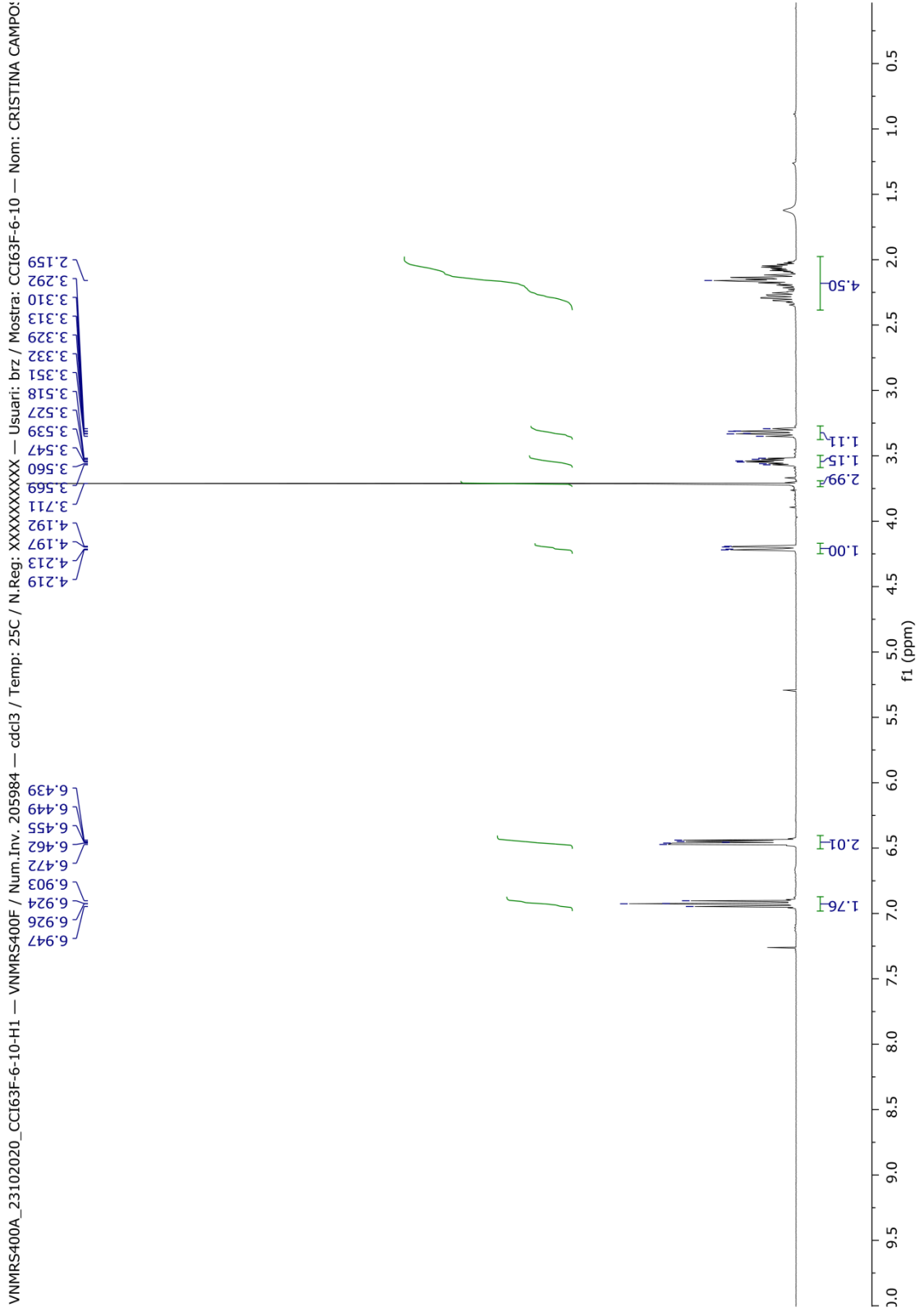
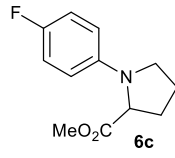


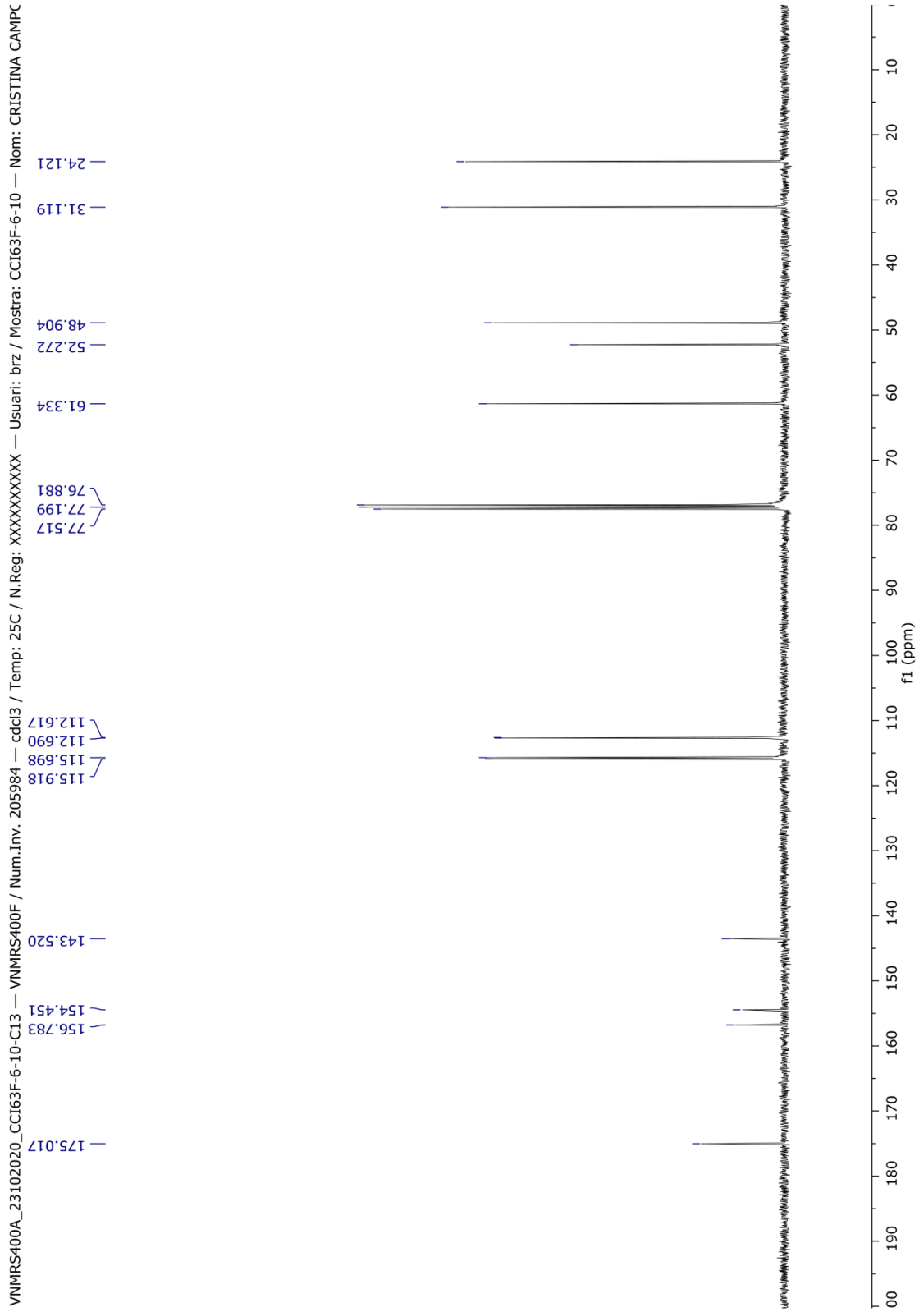
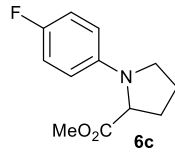


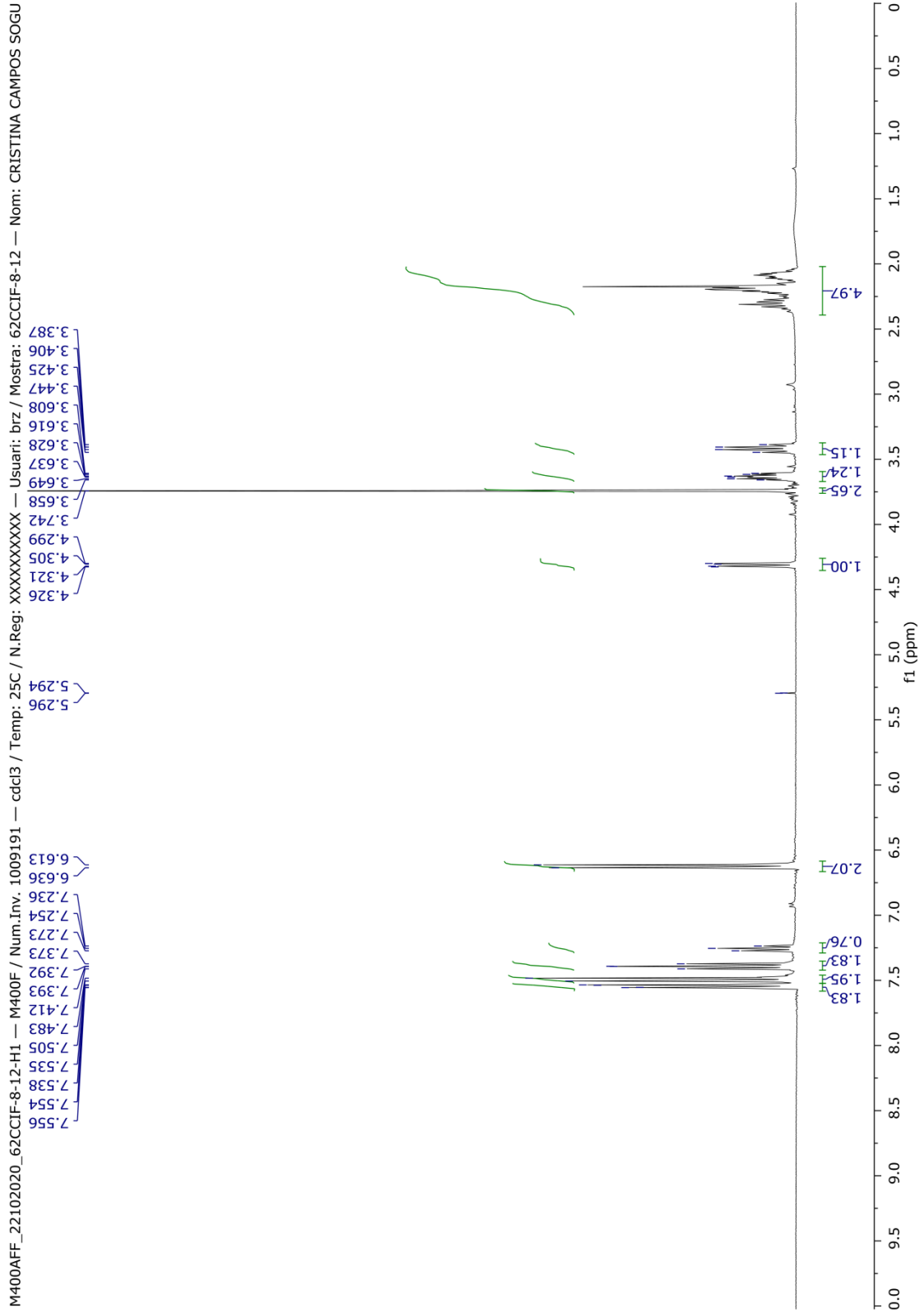
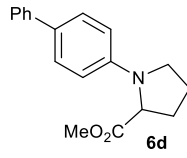


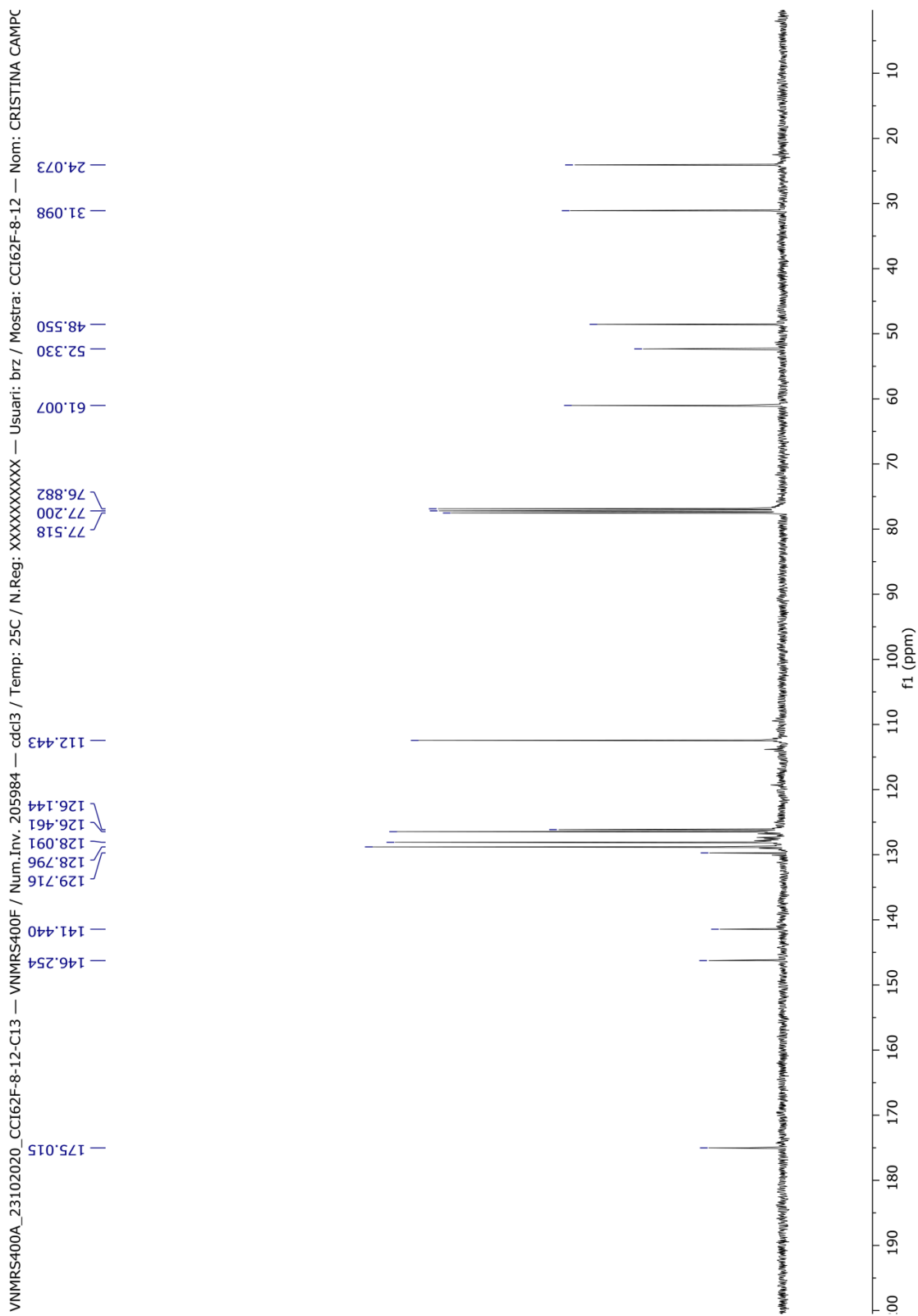
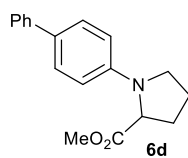


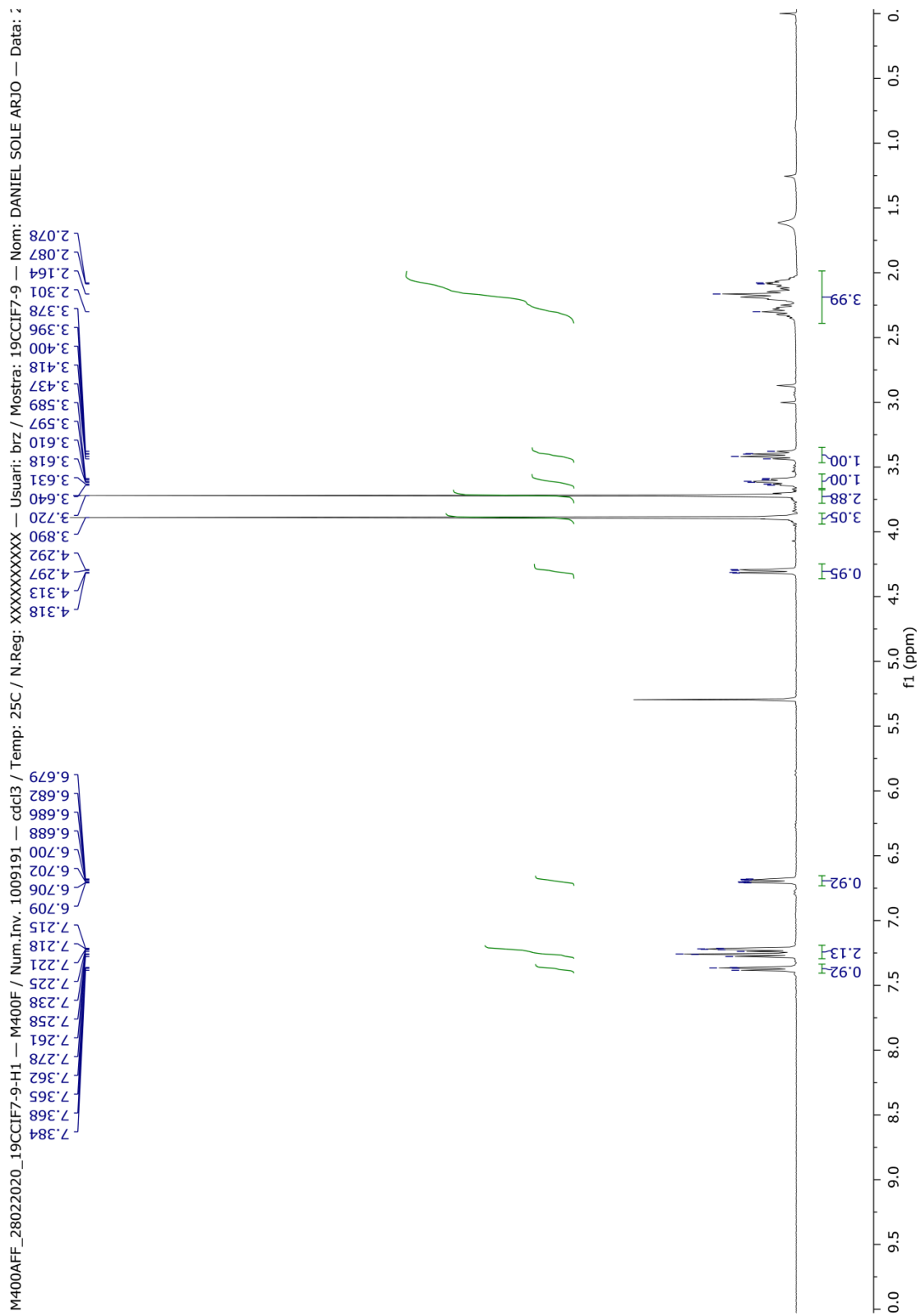
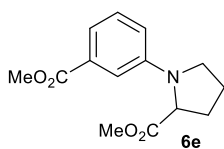


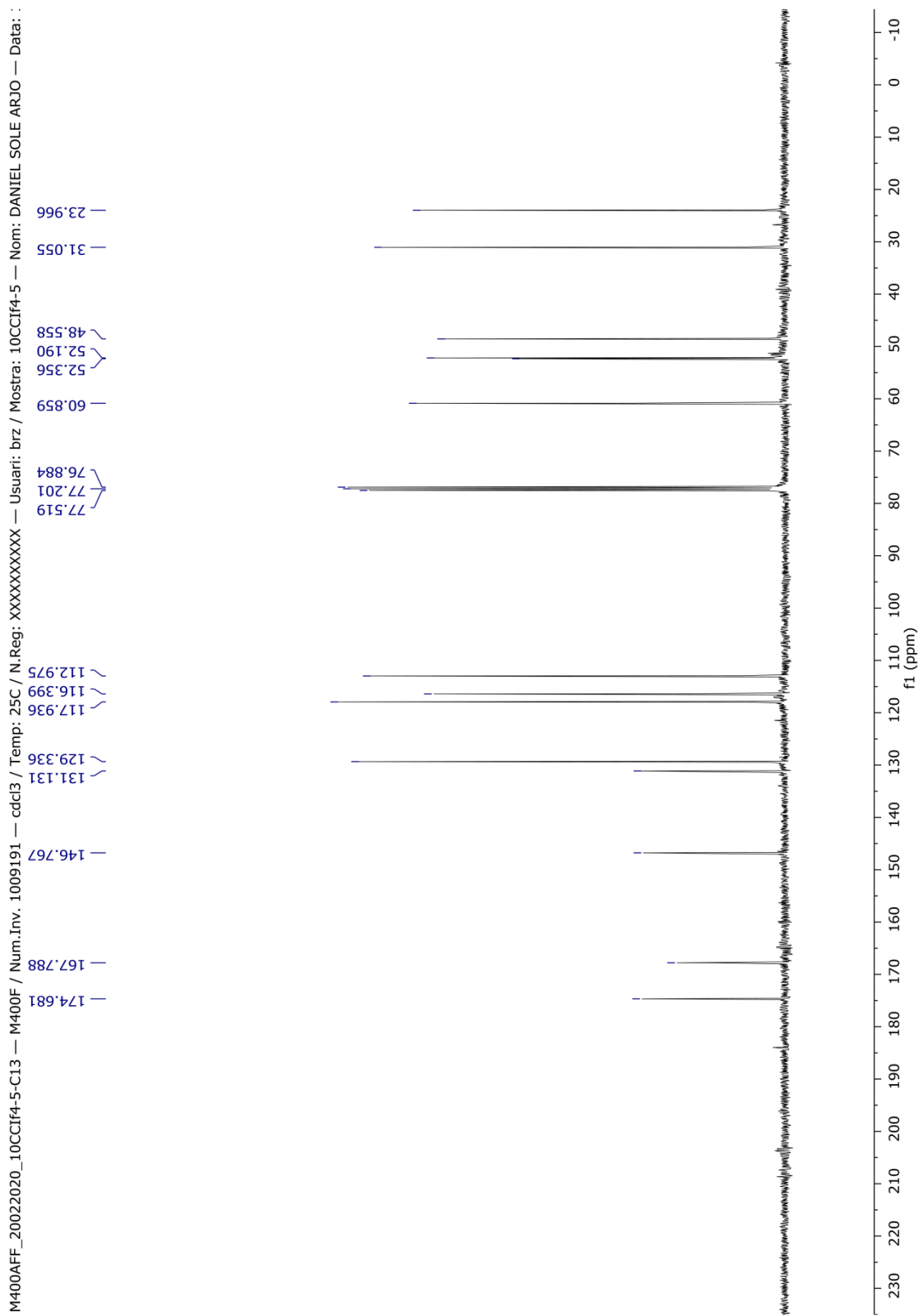
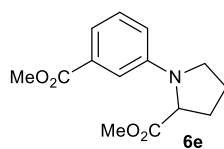


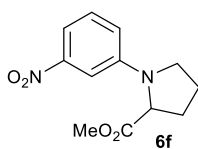




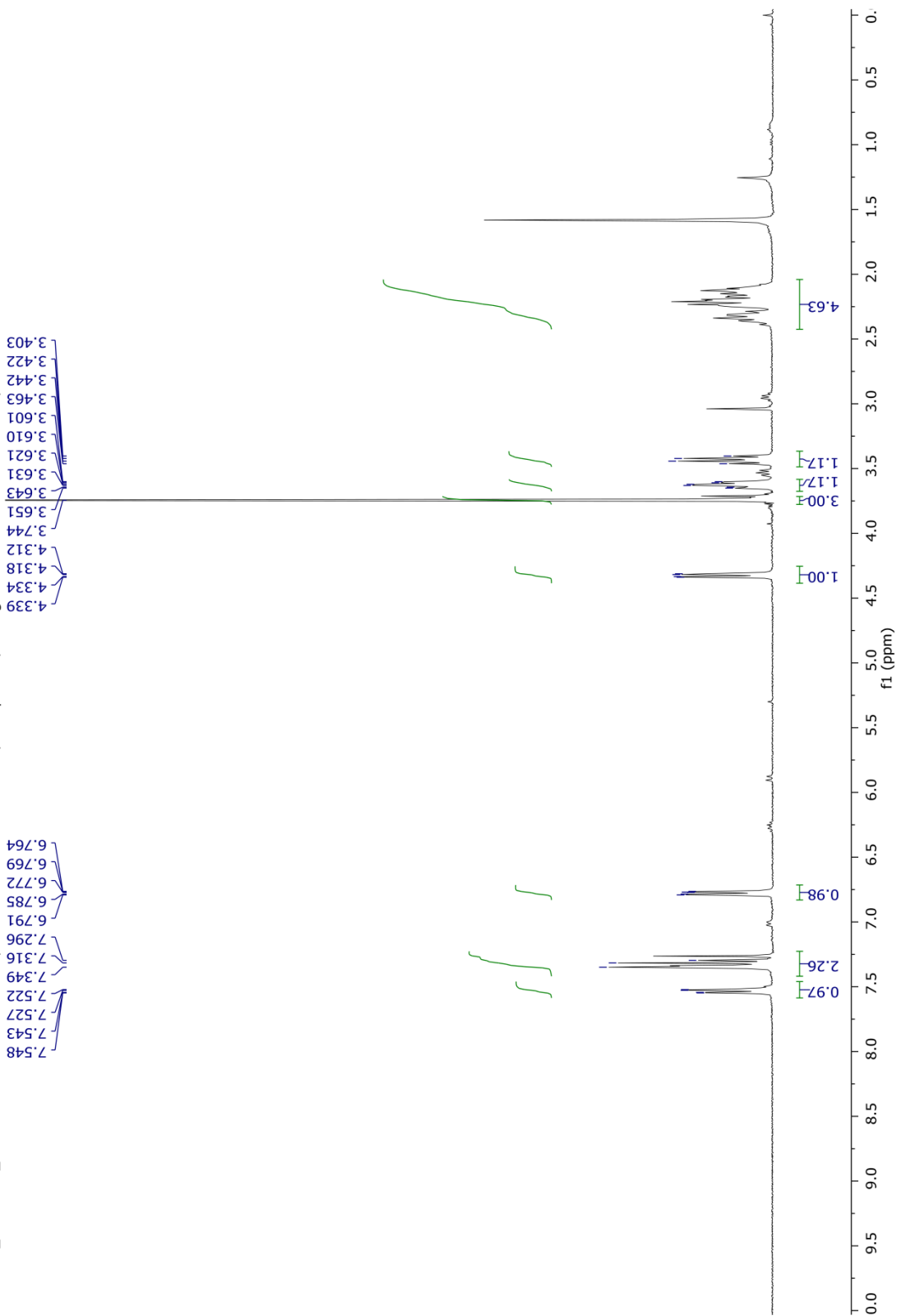


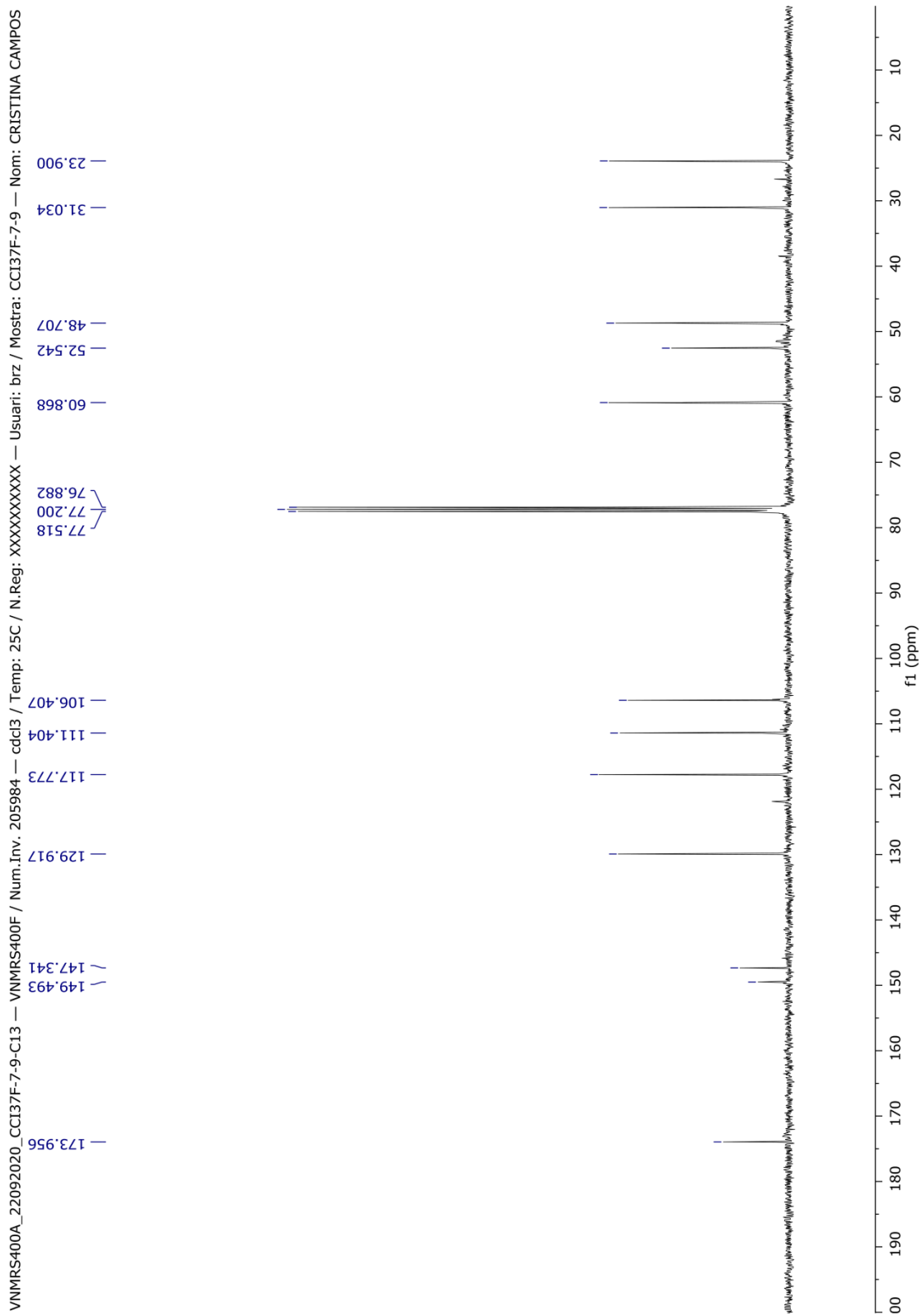
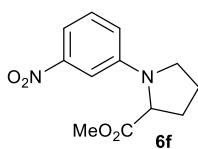


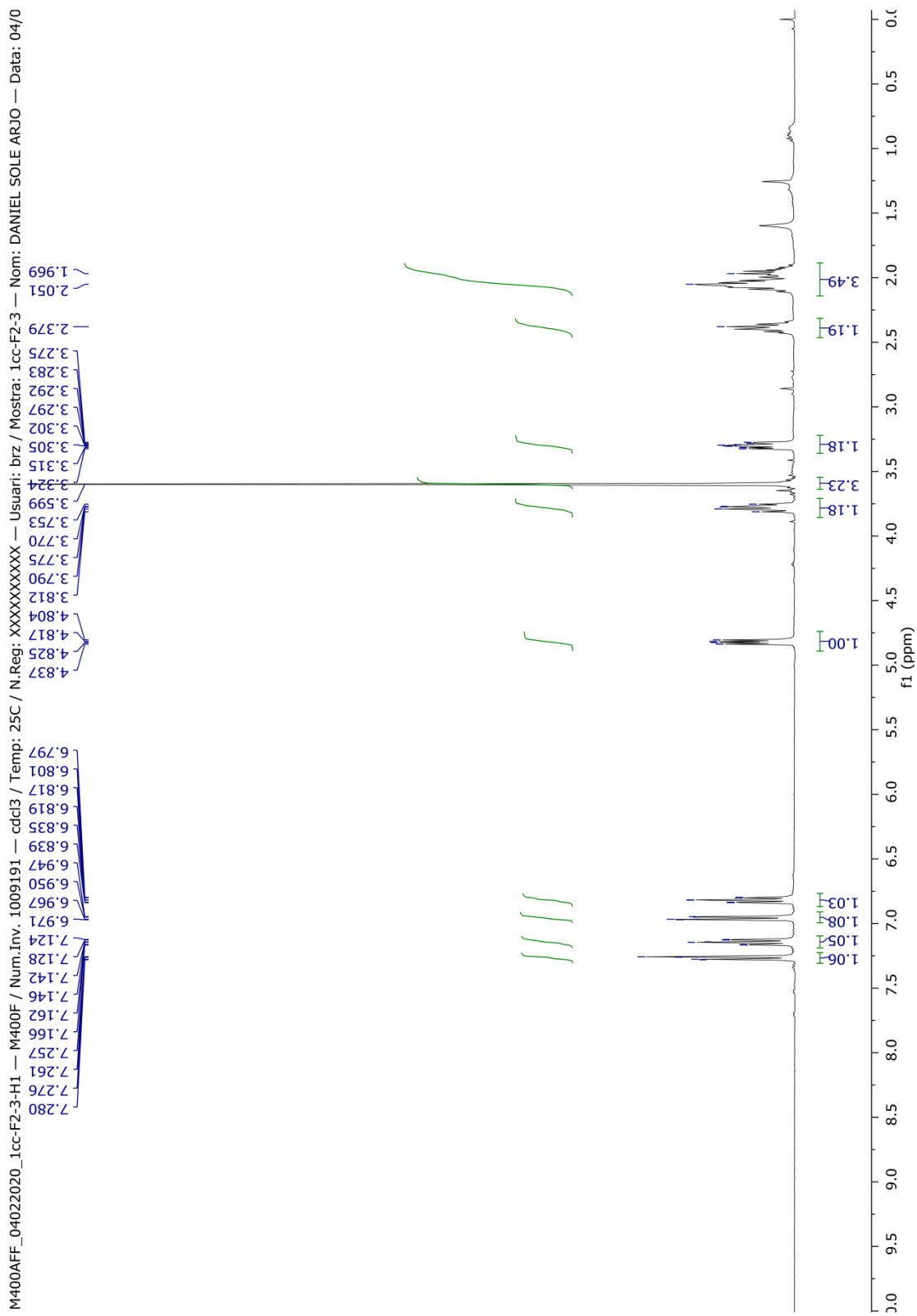
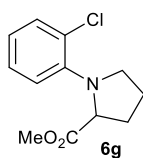


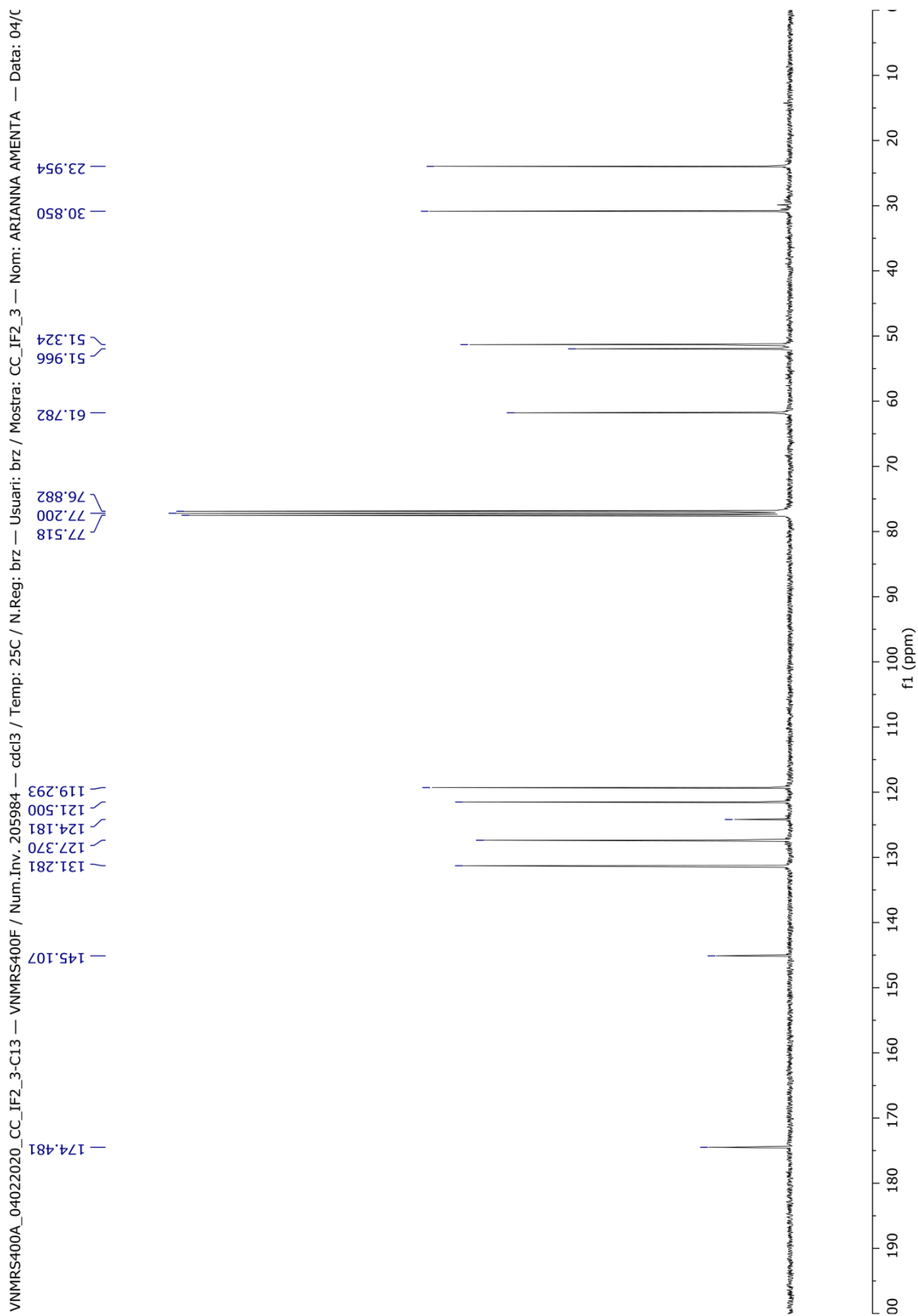
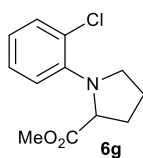


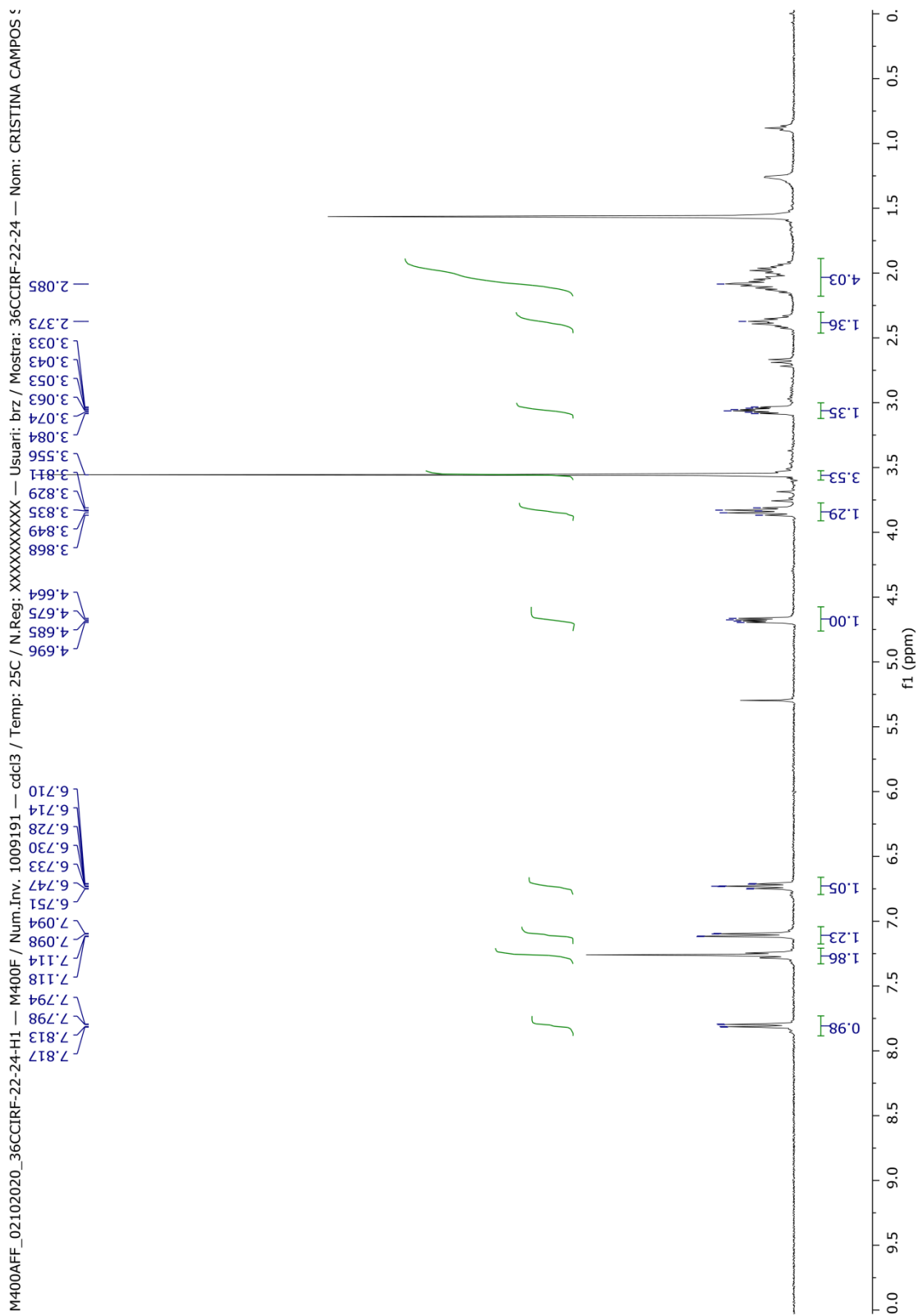
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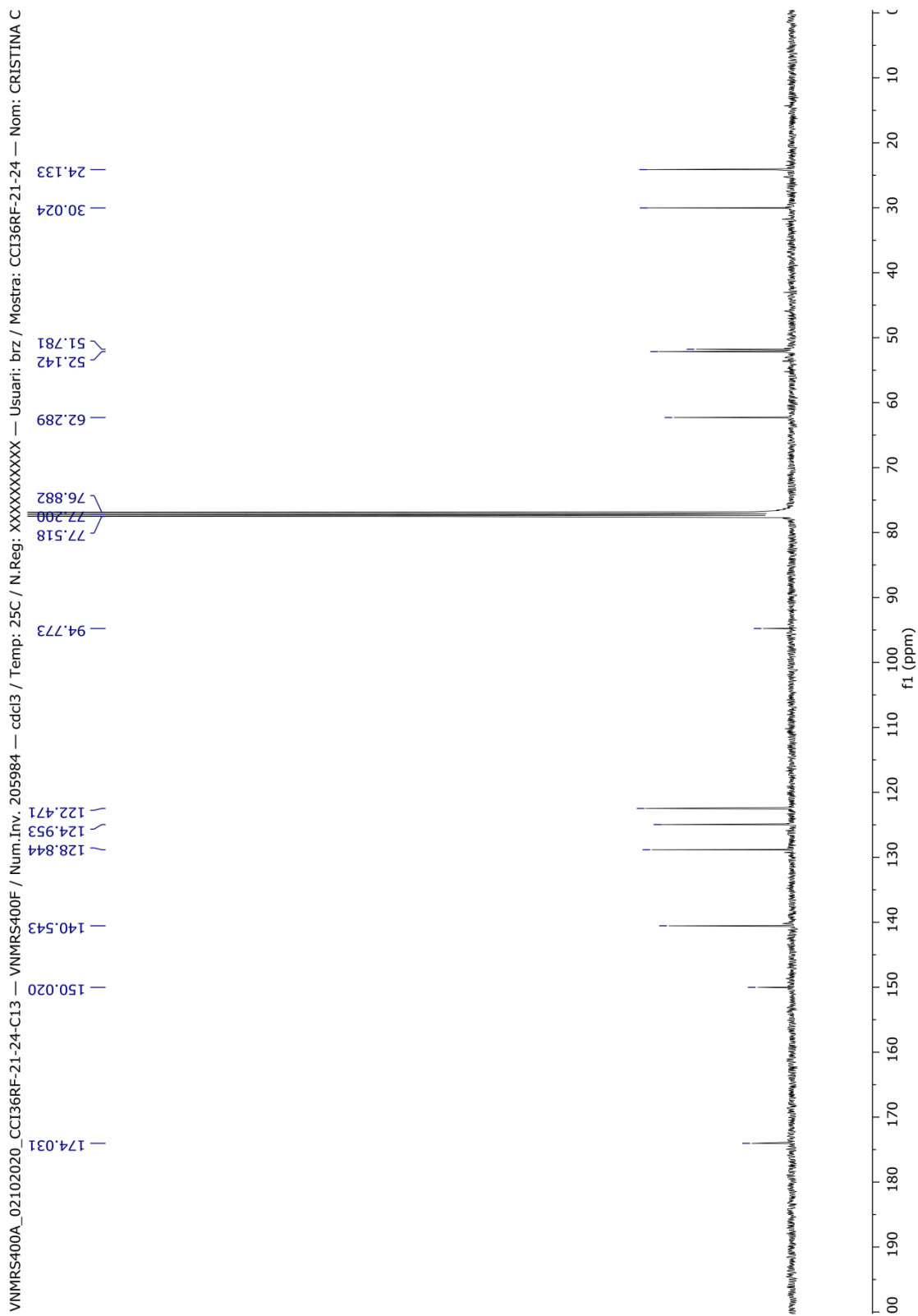
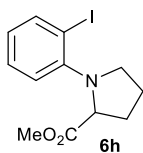


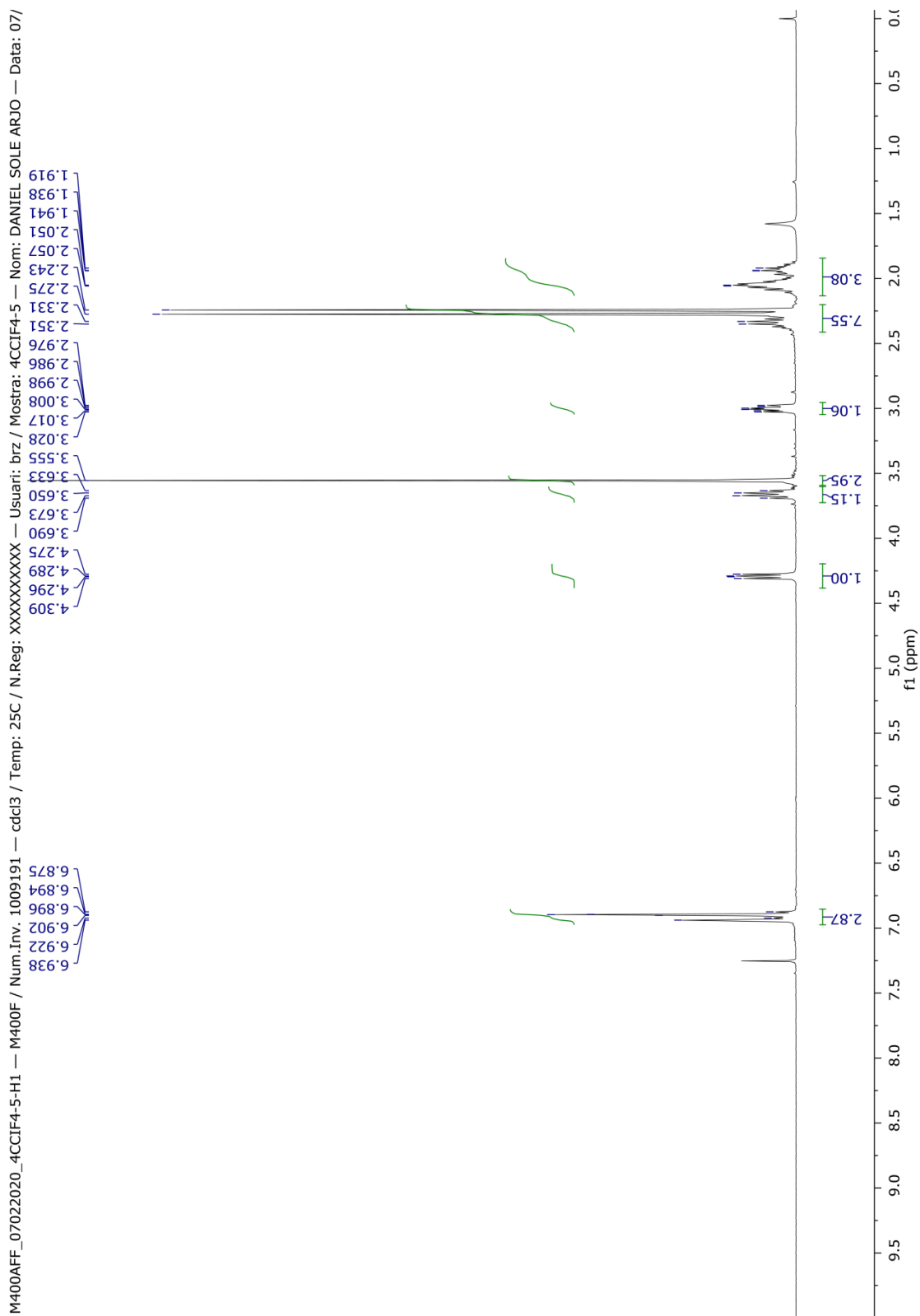
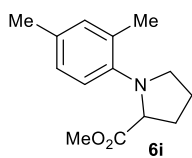


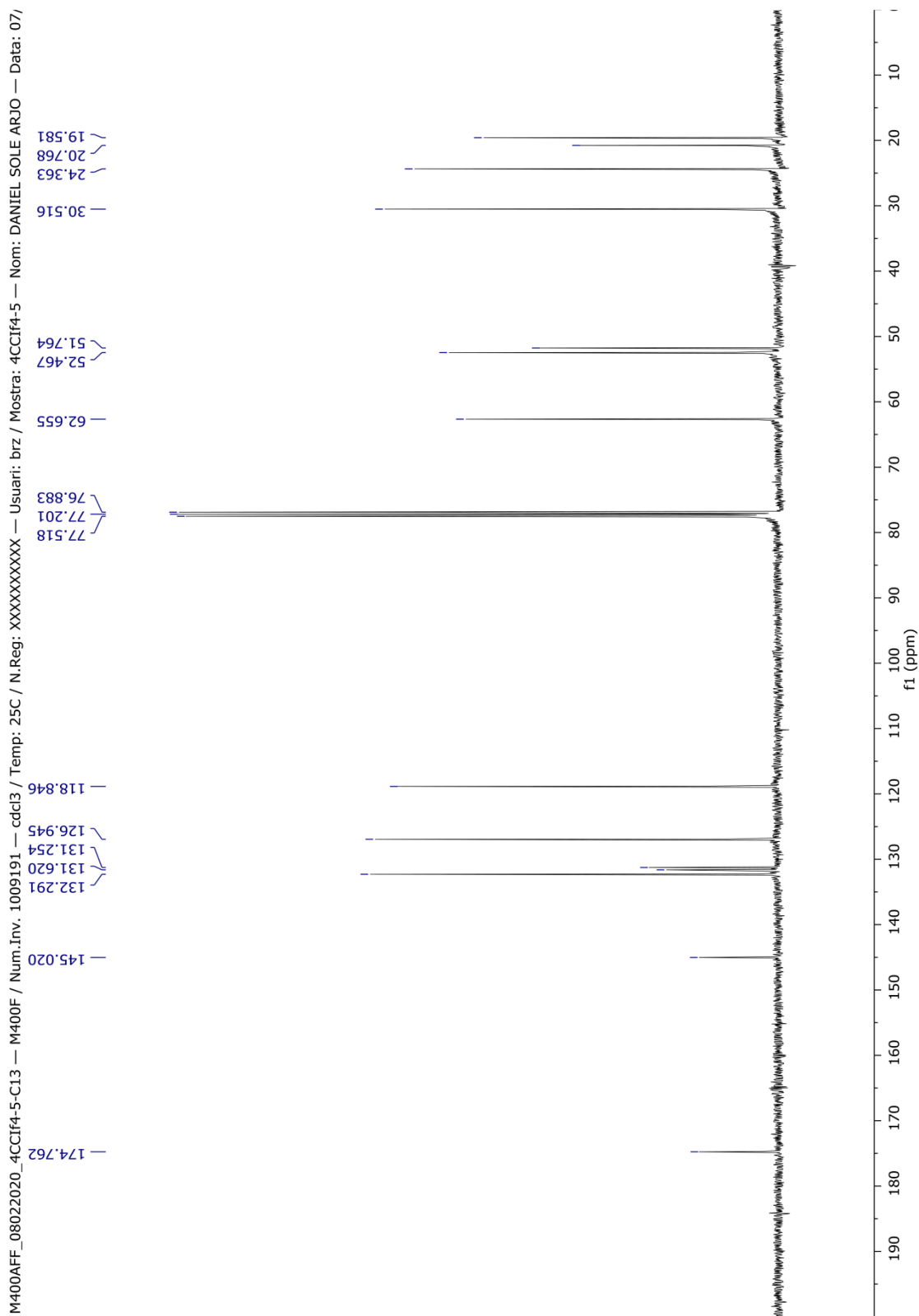
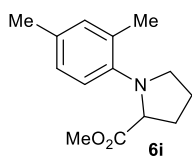


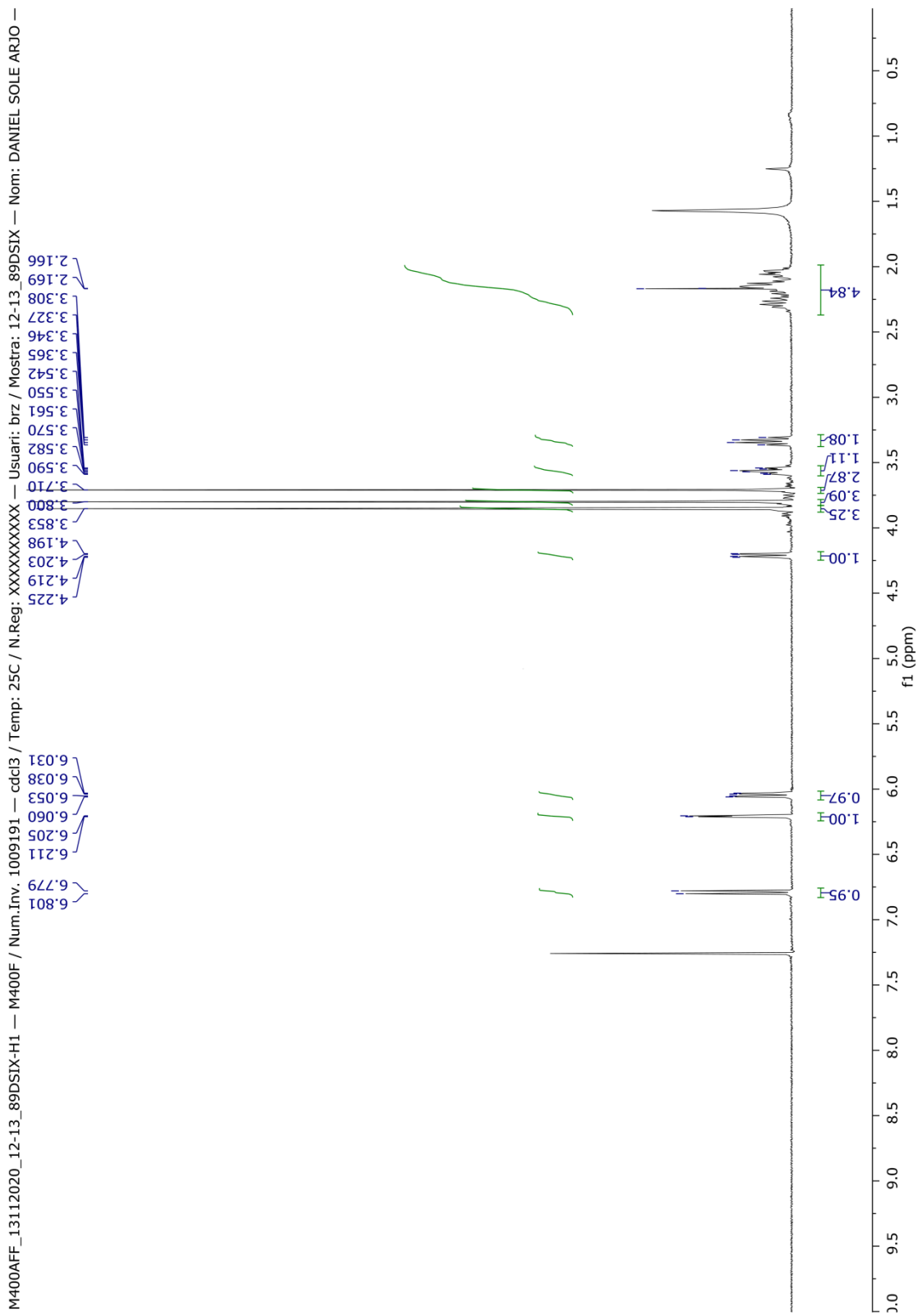
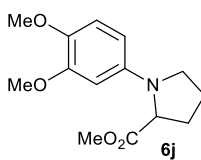


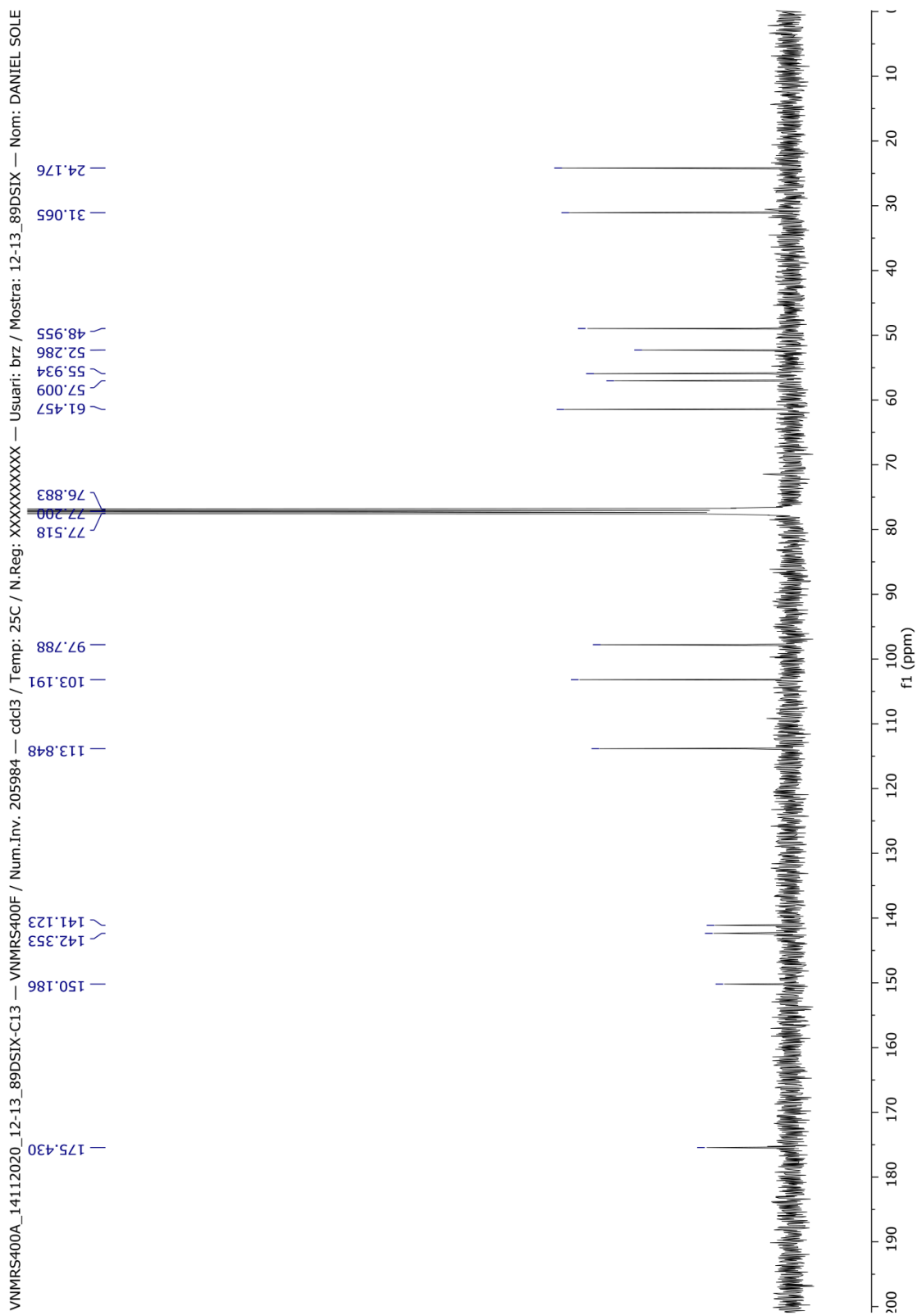
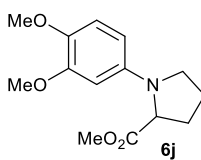


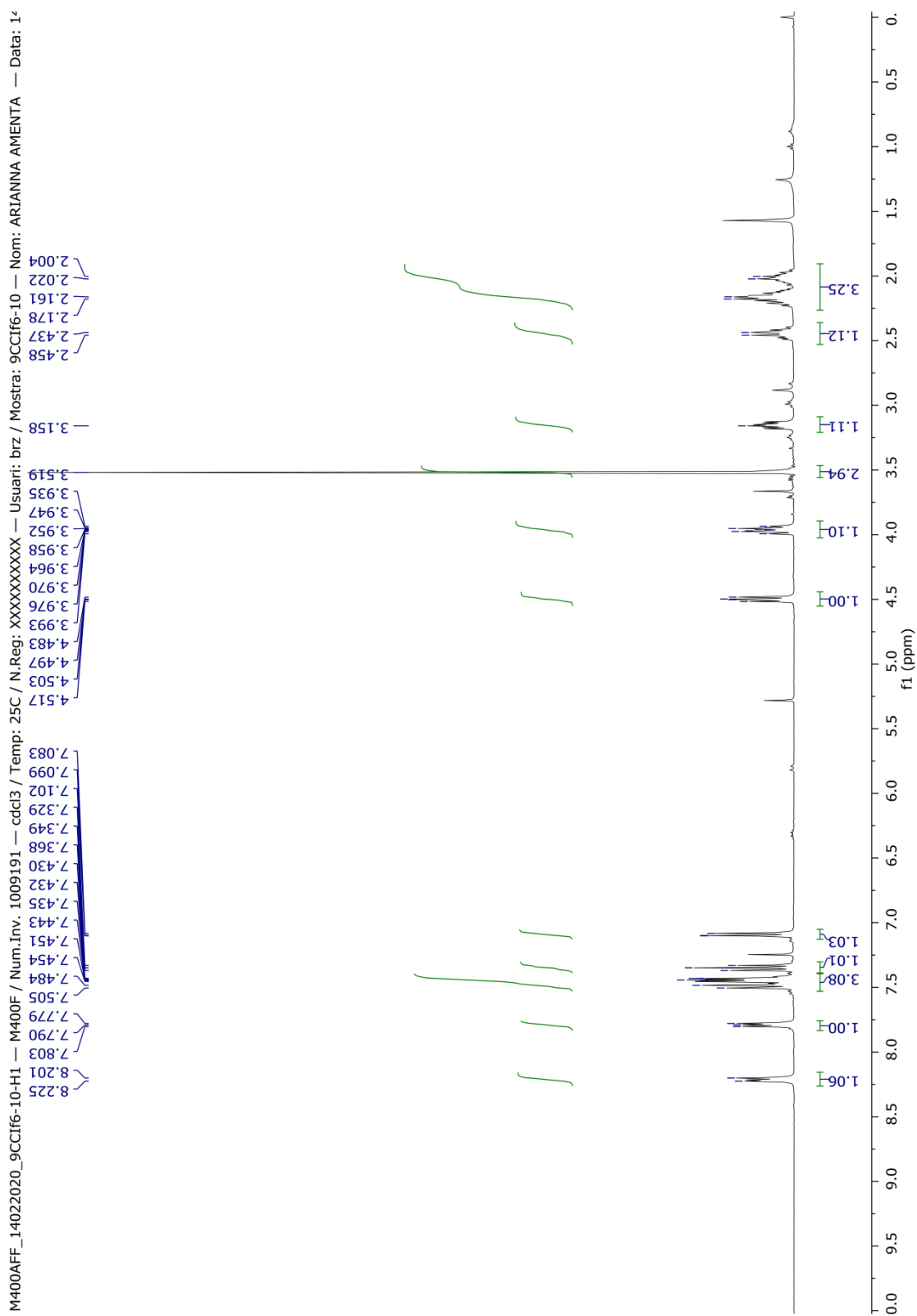
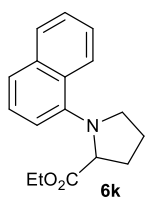


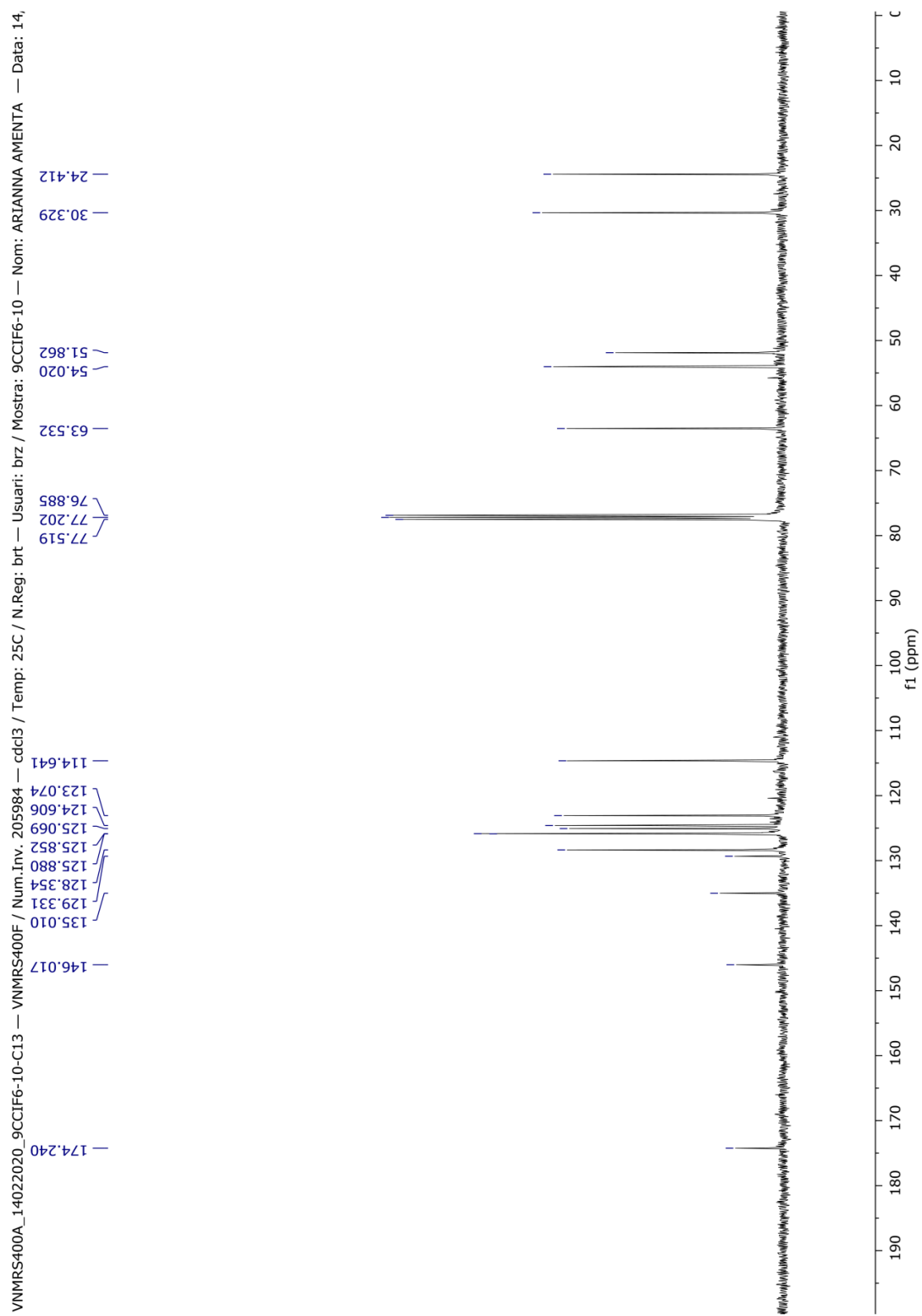
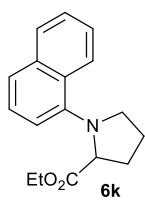












Cartesian coordinates and total energies

Cartesian coordinates (in Å) and total energies (in a.u.) of all the stationary points discussed in the text. All calculations have been performed at the PCM(solvent)-M06L-D3/def2-TZVPP//PCM(solvent)-B3LYP-D3/def2-SVP level.

INT0: E= -7232.361052

C	-0.311976000	1.434155000	-0.766212000
C	-1.445356000	1.243906000	0.253983000
H	-0.078614000	2.507846000	-0.870283000
H	-0.733513000	1.087303000	-1.720355000
C	-2.829574000	1.682002000	-0.181858000
O	-3.631281000	0.768618000	-0.369959000
O	-3.058451000	2.949304000	-0.358499000
C	-4.380235000	3.341970000	-0.815130000
H	-4.561717000	2.921265000	-1.813204000
H	-5.137795000	2.974719000	-0.109776000
H	-4.367239000	4.435795000	-0.845975000
Fe	-2.292865000	-0.653196000	0.435611000
Br	-1.752740000	-1.599239000	-1.706343000
Br	-0.951230000	-1.740395000	2.077809000
C	0.927553000	0.611455000	-0.428507000
H	1.422630000	1.004716000	0.475056000
H	0.609048000	-0.415949000	-0.198927000
C	1.927960000	0.577982000	-1.590483000
H	2.260634000	1.595512000	-1.848517000
H	1.417816000	0.194219000	-2.488549000
N	3.079162000	-0.269132000	-1.331981000
C	2.906535000	-1.695968000	-1.548515000
H	1.929043000	-1.874875000	-2.015011000
H	3.683260000	-2.108903000	-2.216043000
H	2.932722000	-2.268812000	-0.603505000
C	4.163480000	0.188665000	-0.601428000
C	5.242302000	-0.675847000	-0.278069000
C	4.257645000	1.531772000	-0.149327000
C	6.347360000	-0.213579000	0.438734000
C	5.370059000	1.975535000	0.565936000
C	6.430107000	1.114136000	0.870239000
H	5.225972000	-1.718053000	-0.594671000
H	3.453001000	2.239102000	-0.347791000
H	7.158398000	-0.912540000	0.663013000
H	5.400493000	3.017583000	0.897487000
H	7.295750000	1.467988000	1.434686000
N	-1.113026000	1.687351000	1.506390000
N	-0.790959000	1.907909000	2.552256000

TS1: E= -7232.355281

C	-0.305343000	1.205274000	-0.995180000
C	-1.415613000	1.076266000	0.022656000
H	-0.067021000	2.266255000	-1.186513000
H	-0.761927000	0.809174000	-1.919103000
C	-2.740092000	1.715622000	-0.298307000
O	-3.674058000	0.908402000	-0.277987000
O	-2.832815000	2.984683000	-0.568817000
C	-4.148936000	3.521170000	-0.860707000

H	-4.542133000	3.053285000	-1.773404000
H	-4.824908000	3.322061000	-0.018030000
H	-4.004883000	4.596759000	-1.002935000
Fe	-2.290056000	-0.530334000	0.537133000
Br	-2.067084000	-1.783750000	-1.463979000
Br	-0.850028000	-1.486650000	2.163182000
C	0.938119000	0.391276000	-0.652001000
H	1.422634000	0.797510000	0.251009000
H	0.626165000	-0.635355000	-0.408950000
C	1.954541000	0.362023000	-1.799415000
H	2.242264000	1.385760000	-2.086136000
H	1.481544000	-0.073250000	-2.694136000
N	3.143091000	-0.418516000	-1.493971000
C	3.042000000	-1.857732000	-1.666272000
H	2.164814000	-2.085976000	-2.285378000
H	3.928875000	-2.268647000	-2.177586000
H	2.925793000	-2.394831000	-0.705836000
C	4.150642000	0.102636000	-0.694942000
C	5.208254000	-0.717875000	-0.222443000
C	4.182772000	1.471799000	-0.318891000
C	6.238161000	-0.189778000	0.558340000
C	5.219559000	1.981711000	0.462639000
C	6.261793000	1.162938000	0.911522000
H	5.233441000	-1.778934000	-0.466618000
H	3.390012000	2.149872000	-0.632571000
H	7.035035000	-0.857421000	0.898679000
H	5.204120000	3.042434000	0.729595000
H	7.067969000	1.568289000	1.527088000
N	-0.844113000	1.862190000	1.365420000
N	-0.347772000	1.821900000	2.357943000

INT1: E= -7122.853113

C	0.206537000	-0.287075000	2.032431000
C	0.292052000	0.198096000	0.640291000
C	-0.028031000	-1.809033000	2.070598000
N	-1.636541000	-1.478452000	0.182605000
C	-1.391580000	-2.156658000	1.465351000
H	-0.586861000	0.245442000	2.584104000
H	0.787315000	-2.304115000	1.522513000
H	-1.468388000	-3.249108000	1.315873000
H	-2.183211000	-1.885245000	2.171084000
H	0.009176000	-2.173582000	3.108883000
H	1.173139000	-0.060789000	2.514254000
C	-1.000223000	-2.135144000	-0.954181000
H	-0.000406000	-2.477321000	-0.664734000
H	-1.589515000	-2.998431000	-1.313924000
H	-0.878230000	-1.424996000	-1.784154000
C	-2.883393000	-0.854102000	-0.043824000
C	-3.425580000	-0.756241000	-1.344418000
C	-3.601153000	-0.243718000	1.011083000
C	-4.627935000	-0.080306000	-1.572210000
C	-4.803032000	0.419304000	0.773252000
C	-5.330603000	0.510343000	-0.519959000
H	-2.920582000	-1.209359000	-2.194886000
H	-3.204574000	-0.250429000	2.025190000
H	-5.018150000	-0.026589000	-2.591762000
H	-5.326398000	0.883214000	1.613076000
H	-6.271017000	1.034881000	-0.702179000
C	-0.527624000	1.231709000	0.000286000
O	-0.143730000	1.497479000	-1.158356000

O	-1.516577000	1.819245000	0.615329000
C	-2.312752000	2.772411000	-0.124242000
H	-1.662996000	3.523957000	-0.592194000
H	-2.893172000	2.238470000	-0.889733000
H	-2.983685000	3.231414000	0.608667000
Fe	1.480565000	0.201892000	-0.653699000
Br	2.797231000	-1.756420000	-0.480236000
Br	2.855941000	1.888170000	0.272388000

TS2: E= -7122.847594

C	0.094288000	-0.276533000	2.019791000
C	0.053964000	0.034875000	0.567999000
C	0.047924000	-1.800112000	2.175125000
N	-1.387930000	-1.533501000	0.177323000
C	-1.212240000	-2.283380000	1.452460000
H	-0.732991000	0.208398000	2.565594000
H	0.949122000	-2.234089000	1.716752000
H	-1.165511000	-3.359568000	1.225007000
H	-2.094746000	-2.128086000	2.081181000
H	0.023203000	-2.105456000	3.231624000
H	1.041790000	0.126295000	2.413210000
C	-0.793380000	-2.241625000	-0.964794000
H	0.201675000	-2.599272000	-0.679792000
H	-1.423512000	-3.092461000	-1.271899000
H	-0.677077000	-1.559531000	-1.816733000
C	-2.677131000	-0.939180000	-0.054696000
C	-3.225561000	-0.869122000	-1.347832000
C	-3.382917000	-0.335358000	1.005137000
C	-4.445636000	-0.221961000	-1.567161000
C	-4.600649000	0.303354000	0.777319000
C	-5.143258000	0.365681000	-0.510456000
H	-2.717273000	-1.314924000	-2.199836000
H	-2.974934000	-0.332820000	2.014750000
H	-4.850909000	-0.186028000	-2.581159000
H	-5.123302000	0.765363000	1.618139000
H	-6.096720000	0.868559000	-0.686234000
C	-0.657592000	1.154597000	-0.069405000
O	-0.362900000	1.318702000	-1.269753000
O	-1.431004000	1.952923000	0.620151000
C	-2.002485000	3.088441000	-0.063778000
H	-1.203207000	3.695854000	-0.510127000
H	-2.689145000	2.738801000	-0.847636000
H	-2.546364000	3.654377000	0.699678000
Fe	1.353134000	0.154497000	-0.688066000
Br	2.861229000	-1.669493000	-0.431420000
Br	2.528291000	1.998667000	0.270119000

INT2: E= -7122.855269

C	-0.415721000	0.133098000	1.801500000
C	-0.358858000	0.124162000	0.280735000
C	-1.116583000	-1.189502000	2.190527000
N	-1.445047000	-0.874427000	-0.172858000
C	-1.246521000	-1.961830000	0.884830000
H	-0.965175000	1.003528000	2.191366000
H	-0.540364000	-1.776494000	2.918166000
H	-0.306892000	-2.460378000	0.618934000
H	-2.075282000	-2.675498000	0.840898000
H	-2.108288000	-0.997299000	2.624732000
H	0.609161000	0.197320000	2.188048000

C	-1.194650000	-1.412142000	-1.555264000
H	-0.201849000	-1.881350000	-1.575476000
H	-1.943231000	-2.174793000	-1.790792000
H	-1.249715000	-0.584776000	-2.268513000
C	-2.858443000	-0.350374000	-0.094108000
C	-3.908625000	-1.247476000	-0.334263000
C	-3.134376000	0.981325000	0.216625000
C	-5.230633000	-0.806545000	-0.269199000
C	-4.465267000	1.413305000	0.280260000
C	-5.515110000	0.527821000	0.038072000
H	-3.716755000	-2.293884000	-0.572760000
H	-2.346443000	1.699844000	0.418789000
H	-6.039239000	-1.515259000	-0.460230000
H	-4.669781000	2.457653000	0.525591000
H	-6.550348000	0.871924000	0.089762000
C	-0.168903000	1.349041000	-0.488134000
O	0.233307000	1.262215000	-1.685429000
O	-0.261891000	2.510154000	0.149095000
C	0.267595000	3.671172000	-0.514795000
H	1.331637000	3.512576000	-0.736065000
H	-0.286997000	3.864521000	-1.444165000
H	0.139548000	4.501542000	0.188911000
Fe	1.380942000	-0.089707000	-0.664759000
Br	2.281979000	-2.249757000	-0.135583000
Br	2.901910000	1.367840000	0.490054000

TS3: E= -7122.804495

C	0.014844000	0.222079000	-2.002953000
C	0.336118000	0.218921000	-0.517195000
C	0.116564000	-1.259447000	-2.395710000
N	1.366903000	-0.803953000	-0.362534000
C	1.067094000	-1.886916000	-1.350238000
H	0.798330000	0.816314000	-2.508278000
H	-0.871216000	-1.733073000	-2.328250000
H	0.585149000	-2.730665000	-0.836177000
H	2.015896000	-2.232585000	-1.778741000
H	0.495597000	-1.386939000	-3.419060000
H	-0.955382000	0.675956000	-2.227748000
C	0.320694000	-1.197592000	1.480344000
H	-0.611595000	-0.916898000	2.159663000
H	0.358858000	-2.287928000	1.391073000
H	1.185798000	-0.752446000	1.982738000
C	2.740659000	-0.508733000	-0.119979000
C	3.535868000	-1.528396000	0.435063000
C	3.319076000	0.736757000	-0.412649000
C	4.886148000	-1.300665000	0.698264000
C	4.672368000	0.956594000	-0.136716000
C	5.460661000	-0.054449000	0.419350000
H	3.084582000	-2.495190000	0.667137000
H	2.734733000	1.527631000	-0.879424000
H	5.490958000	-2.099870000	1.133279000
H	5.112453000	1.928242000	-0.373617000
H	6.517098000	0.124501000	0.631421000
C	0.433983000	1.515742000	0.214812000
O	0.085379000	1.522247000	1.405573000
O	0.672292000	2.600628000	-0.479055000
C	0.399075000	3.871652000	0.153875000
H	-0.662572000	3.905786000	0.435243000
H	1.030893000	3.995360000	1.043710000
H	0.631999000	4.632504000	-0.598290000

Fe	-1.131435000	-0.128085000	0.822734000
Br	-2.334143000	-2.097898000	0.179348000
Br	-2.722225000	1.420495000	-0.166713000

TS3' : E= -7122.775472

C	-0.339336000	-1.775851000	1.935983000
C	-0.004004000	-1.032847000	0.668214000
C	0.060115000	-0.728634000	2.980942000
N	1.240627000	-0.263821000	0.912140000
C	1.371517000	-0.176829000	2.418031000
H	0.273357000	-2.689862000	2.042364000
H	-0.708175000	0.060084000	3.022830000
H	1.591508000	0.855424000	2.722884000
H	2.219885000	-0.807980000	2.717960000
H	0.196030000	-1.131624000	3.994016000
H	-1.398680000	-2.058073000	1.967829000
C	0.775900000	1.635100000	0.265795000
H	0.265933000	1.878148000	1.190643000
H	1.810618000	1.930452000	0.131927000
H	0.303132000	1.286049000	-0.660220000
C	2.474895000	-0.665494000	0.266073000
C	3.611277000	0.137212000	0.470542000
C	2.589538000	-1.822638000	-0.515463000
C	4.829631000	-0.197564000	-0.121135000
C	3.813710000	-2.148494000	-1.109372000
C	4.936012000	-1.338857000	-0.923047000
H	3.551100000	1.023684000	1.104482000
H	1.746639000	-2.497049000	-0.651871000
H	5.699726000	0.441230000	0.047439000
H	3.883782000	-3.053976000	-1.716731000
H	5.888212000	-1.598036000	-1.391140000
C	-0.334548000	-1.517307000	-0.649624000
O	-0.377921000	-0.685274000	-1.613246000
O	-0.764021000	-2.762053000	-0.768430000
C	-1.503594000	-3.098654000	-1.958637000
H	-2.407315000	-2.474815000	-2.014961000
H	-0.883887000	-2.946209000	-2.852720000
H	-1.771969000	-4.155590000	-1.852095000
Fe	-1.293958000	0.277160000	-0.137525000
Br	-3.450916000	-0.629167000	0.122459000
Br	0.026558000	3.901809000	-0.520413000

INT3 : E= -7122.871024

C	0.164761000	0.486239000	2.508698000
C	-0.283546000	0.568786000	1.074541000
C	0.041031000	-1.007282000	2.847852000
N	-1.065699000	-0.556440000	0.734483000
C	-1.002200000	-1.550968000	1.860031000
H	-0.524306000	1.106211000	3.109299000
H	1.002785000	-1.511154000	2.694133000
H	-0.736448000	-2.536812000	1.457618000
H	-2.008579000	-1.599478000	2.301037000
H	-0.272772000	-1.171567000	3.887393000
H	1.176378000	0.891778000	2.646810000
C	-0.036069000	-0.712568000	-2.055616000
H	0.776764000	-0.546969000	-2.780117000
H	-0.312637000	-1.773006000	-2.007203000
H	-0.899492000	-0.074030000	-2.278293000
C	-2.336434000	-0.500874000	0.062013000

C	-2.758668000	-1.634395000	-0.644503000
C	-3.174190000	0.616587000	0.161329000
C	-4.004621000	-1.636690000	-1.273124000
C	-4.415862000	0.611030000	-0.480290000
C	-4.833323000	-0.511152000	-1.201960000
H	-2.106408000	-2.506390000	-0.703610000
H	-2.879959000	1.481257000	0.757877000
H	-4.326031000	-2.521849000	-1.826767000
H	-5.063724000	1.487041000	-0.400790000
H	-5.805609000	-0.512493000	-1.699787000
C	-0.473186000	1.858339000	0.368326000
O	-0.408096000	1.858664000	-0.856623000
O	-0.562585000	2.930067000	1.124503000
C	-0.521849000	4.210418000	0.455109000
H	0.403133000	4.290289000	-0.132621000
H	-1.391387000	4.314898000	-0.208665000
H	-0.547565000	4.962767000	1.250223000
Fe	0.801600000	-0.143304000	-0.380905000
Br	1.825006000	-2.192638000	0.125941000
Br	2.737981000	1.071090000	-0.855709000

TS4: E= -7122.828284

C	0.173330000	1.350493000	2.548488000
C	-0.189736000	1.165486000	1.108425000
C	-0.048393000	-0.074849000	3.091073000
N	-1.117676000	0.081853000	0.941091000
C	-1.241166000	-0.590038000	2.278882000
H	-0.506490000	2.072821000	3.034922000
H	0.840473000	-0.691781000	2.888877000
H	-1.250631000	-1.679641000	2.149764000
H	-2.197594000	-0.275719000	2.725436000
H	-0.250255000	-0.107641000	4.170279000
H	1.202930000	1.713251000	2.664741000
C	0.002471000	-1.447566000	-2.003909000
H	0.727352000	-0.703402000	-2.347406000
H	0.123904000	-2.408868000	-2.501915000
H	-1.033217000	-1.110879000	-1.922363000
C	-2.354504000	0.196182000	0.210819000
C	-2.983949000	-0.987192000	-0.199946000
C	-2.939202000	1.435644000	-0.068762000
C	-4.194144000	-0.926495000	-0.894268000
C	-4.147332000	1.488112000	-0.770307000
C	-4.778745000	0.311378000	-1.185402000
H	-2.513573000	-1.948680000	0.015003000
H	-2.457885000	2.356034000	0.265297000
H	-4.678197000	-1.852329000	-1.214156000
H	-4.598624000	2.459021000	-0.988752000
H	-5.723013000	0.358281000	-1.732701000
C	0.188683000	1.900962000	-0.048110000
O	-0.006573000	1.350862000	-1.177613000
O	0.840063000	3.043724000	0.114499000
C	1.524181000	3.569353000	-1.038172000
H	2.274430000	2.845696000	-1.386945000
H	0.808367000	3.784723000	-1.844524000
H	2.005748000	4.494633000	-0.701201000
Fe	0.647620000	-0.198735000	-0.074362000
Br	0.623604000	-2.566659000	-0.020728000
Br	3.018539000	0.160462000	-0.482030000

INT4: E= -7122.852235

C	-0.224423000	2.681286000	1.656490000
C	-0.395243000	1.721157000	0.520489000
C	-0.287085000	1.719236000	2.858832000
N	-1.175024000	0.567870000	0.931119000
C	-1.313748000	0.662826000	2.426241000
H	-1.049283000	3.416310000	1.695726000
H	0.700737000	1.255292000	3.008210000
H	-1.152953000	-0.324947000	2.878865000
H	-2.340759000	0.990034000	2.652681000
H	-0.582033000	2.203133000	3.800464000
H	0.722427000	3.232917000	1.586795000
C	2.152400000	-3.322285000	-0.402251000
H	2.873516000	-2.497819000	-0.354778000
H	2.298628000	-4.052974000	0.400418000
H	2.126814000	-3.797886000	-1.388479000
C	-2.381719000	0.164358000	0.248919000
C	-2.858074000	-1.135697000	0.465719000
C	-3.085085000	1.035104000	-0.588941000
C	-4.030680000	-1.563816000	-0.159599000
C	-4.254234000	0.597761000	-1.219218000
C	-4.731575000	-0.699733000	-1.009020000
H	-2.303318000	-1.810796000	1.120916000
H	-2.720951000	2.051324000	-0.746805000
H	-4.393327000	-2.580077000	0.012911000
H	-4.796077000	1.281018000	-1.877964000
H	-5.645092000	-1.036660000	-1.504538000
C	-0.012051000	1.796955000	-0.841500000
O	-0.101995000	0.761327000	-1.576915000
O	0.549605000	2.934898000	-1.260546000
C	1.347376000	2.844831000	-2.450007000
H	2.160533000	2.117412000	-2.303540000
H	0.735199000	2.541088000	-3.311587000
H	1.758234000	3.848431000	-2.614189000
Fe	0.635315000	-0.031729000	0.221332000
Br	0.377773000	-2.494843000	-0.119996000
Br	3.055903000	0.250054000	0.072430000

INT5: E= -4508.854064

C	0.094891000	2.094389000	1.776891000
C	-0.127121000	1.205642000	0.593372000
C	-0.093263000	1.091436000	2.933106000
N	-0.992082000	0.101980000	0.930159000
C	-1.186267000	0.143859000	2.417321000
H	-0.664902000	2.895547000	1.821272000
H	0.844970000	0.537871000	3.100106000
H	-1.127669000	-0.872509000	2.829939000
H	-2.191628000	0.546947000	2.619135000
H	-0.383142000	1.561483000	3.883023000
H	1.086767000	2.564481000	1.757662000
C	-2.176530000	-0.218759000	0.170966000
C	-2.632054000	-1.541983000	0.190352000
C	-2.872971000	0.756891000	-0.548141000
C	-3.790490000	-1.888373000	-0.508375000
C	-4.025560000	0.401849000	-1.255552000
C	-4.489250000	-0.917816000	-1.236115000
H	-2.063109000	-2.293982000	0.741571000
H	-2.509872000	1.786469000	-0.558128000
H	-4.141990000	-2.922898000	-0.493268000
H	-4.564646000	1.163911000	-1.823784000

H	-5.390485000	-1.190754000	-1.790178000
C	0.345083000	1.261406000	-0.741972000
O	0.175631000	0.246558000	-1.501090000
O	1.052267000	2.335254000	-1.108525000
C	1.961712000	2.141227000	-2.202505000
H	2.667088000	1.328989000	-1.964564000
H	1.419553000	1.892246000	-3.125995000
H	2.497475000	3.090500000	-2.322908000
Fe	0.785875000	-0.526780000	0.234416000
Br	3.004604000	-1.283970000	-0.169685000