

Supporting information

Structure-Based Kinetic Control in a Domino Process: A Powerful Tool Toward Molecular Diversity in Chromone Series

Thomas Lepitre,^{*,§} Clement Denhez,^{†,‡} Jan Moncol,^δ Mohamed Othman,[§] Ata Martin Lawson^{*,§}
and Adam Daïch[§]

thomas.lepitre@univ-lehavre.fr

lawsona@univ-lehavre.fr

[§] Normandie Univ., France; UNILEHAVRE, URCOM, F-76600 Le Havre, France; EA 3221, FR 3038 CNRS, F-76600 Le Havre, France

[†] Université de Reims Champagne Ardenne, Institut de Chimie Moléculaire de Reims, CNRS UMR 7312, UFR de Pharmacie, 51 rue Cognacq-Jay, F-51096 Reims Cedex, France.

[‡] Université de Reims Champagne Ardenne, Multiscale Molecular Modelling, UFR Sciences Exactes et Naturelle, F-51687 Cedex 2 Reims, France.

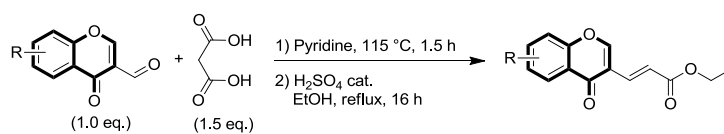
^δ Slovak University of Technology, Department of Inorganic Chemistry, Institute of Inorganic Chemistry, Technology and Materials, Radlinskeho 9, SK-81237 Bratislava, Slovakia.

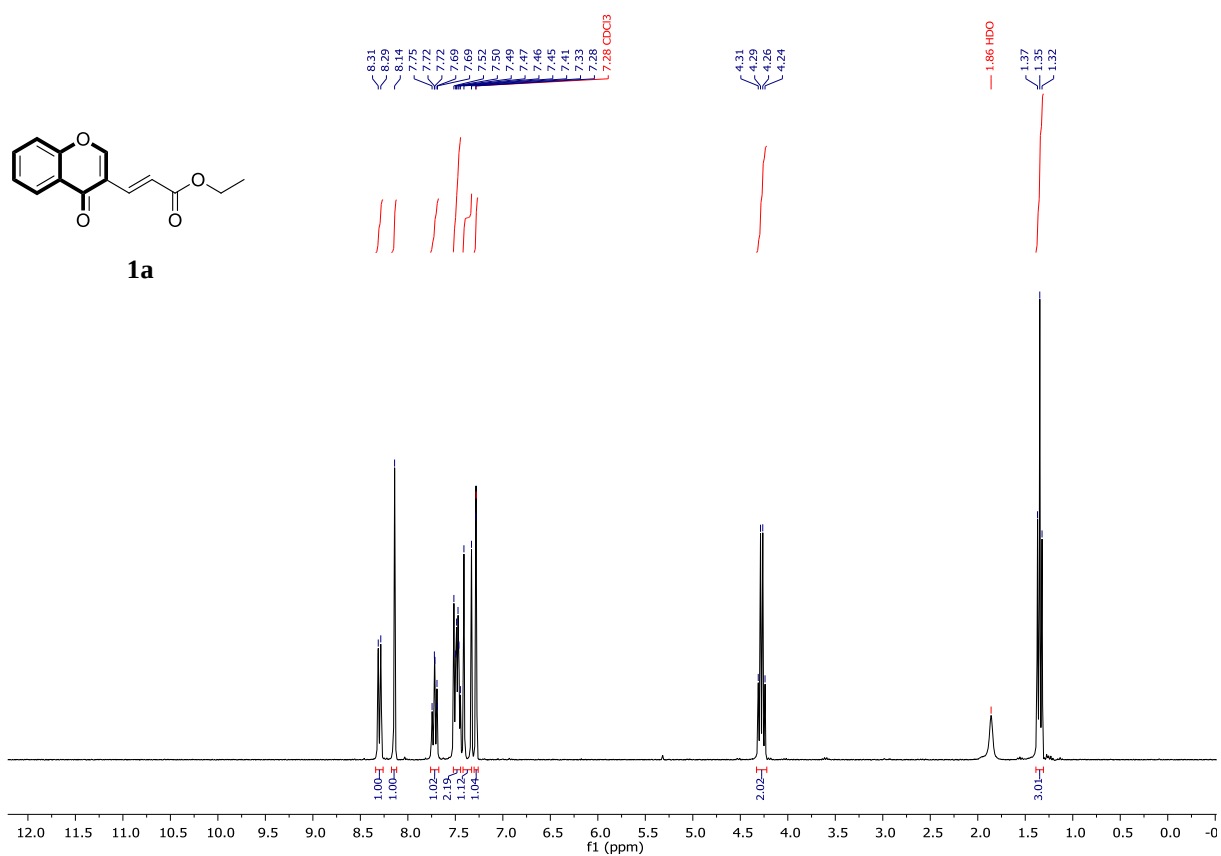
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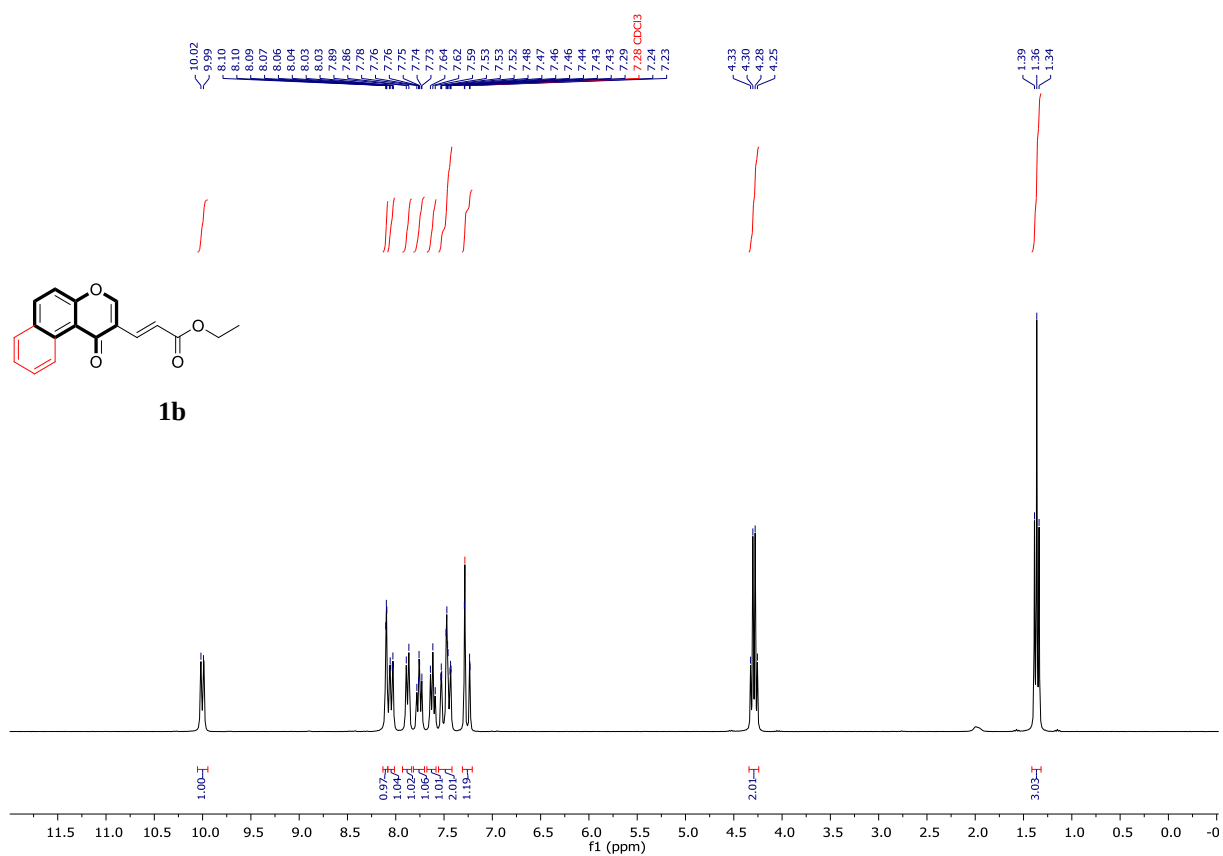
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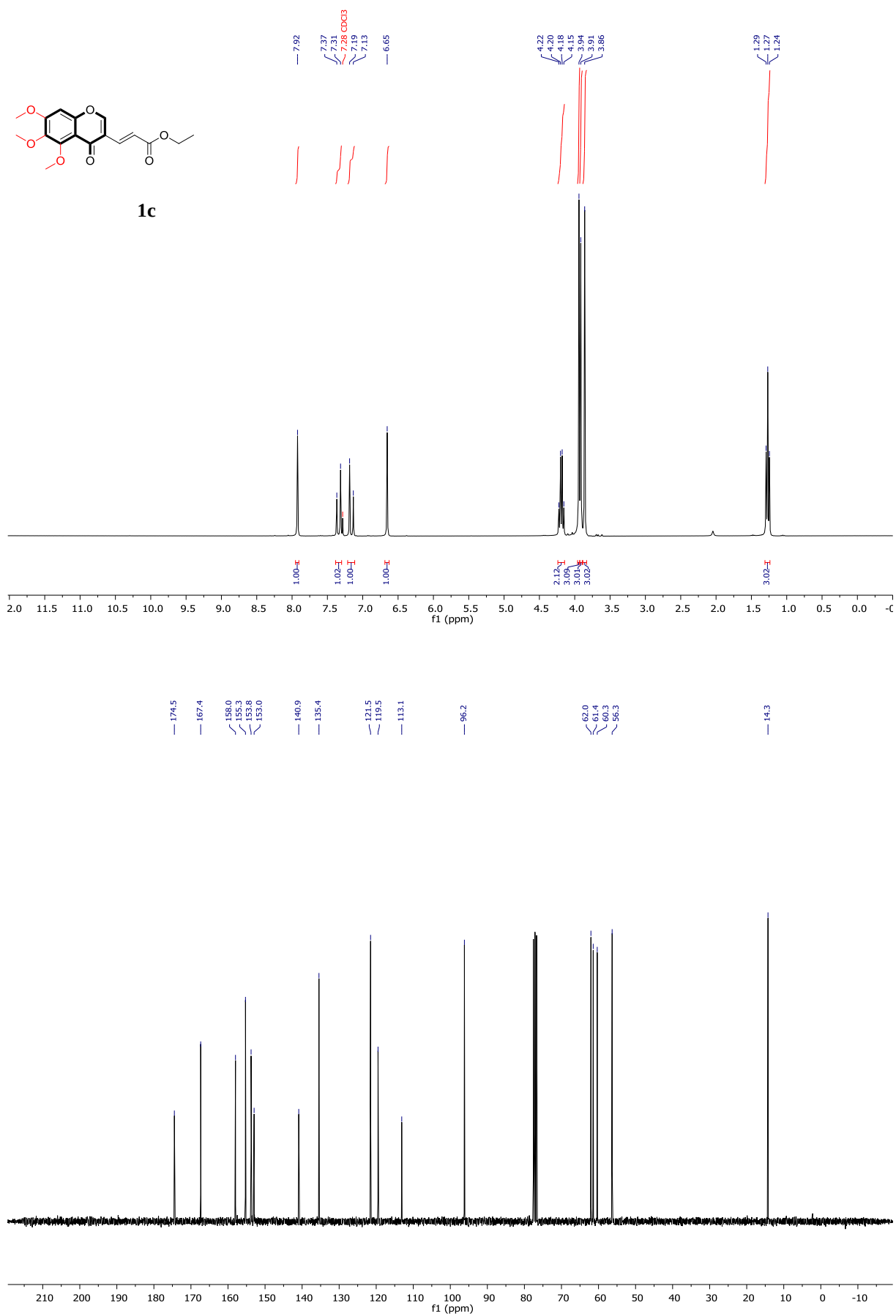
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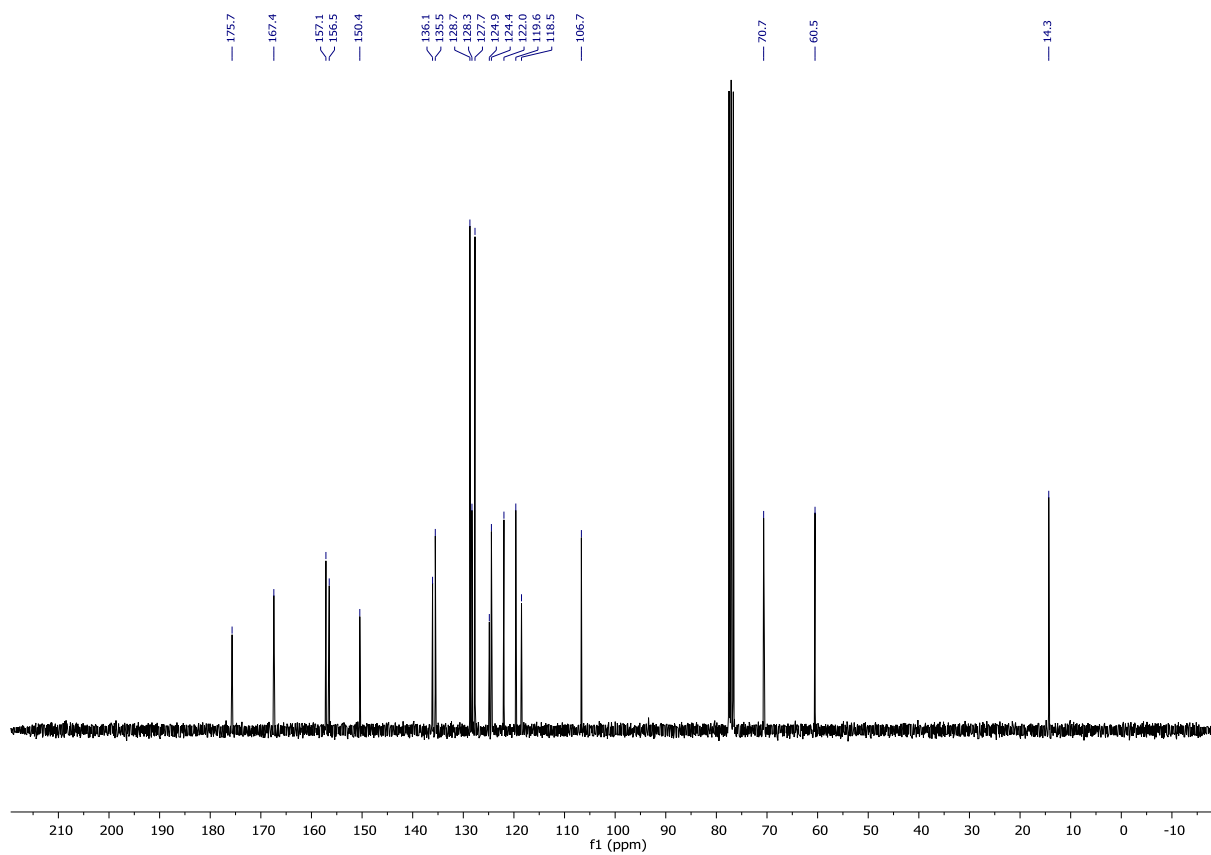
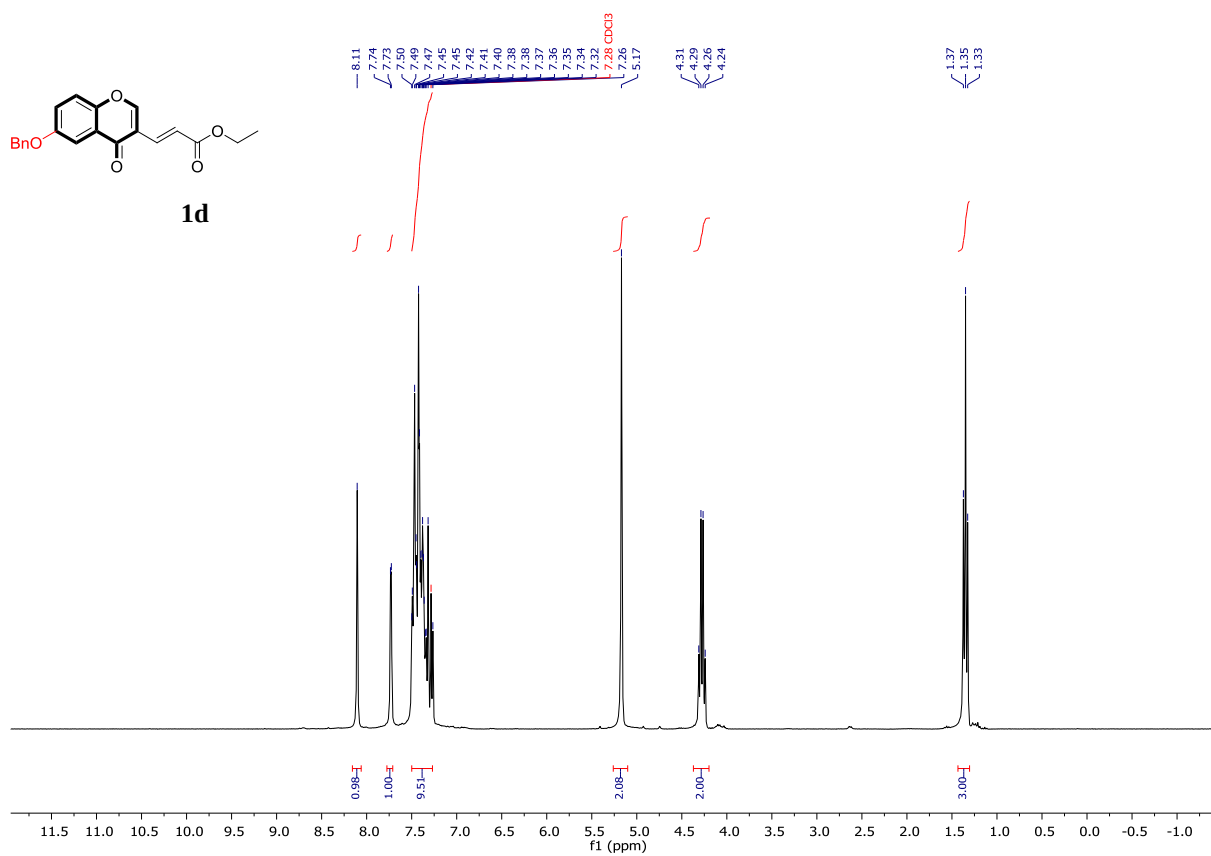
I. a. General procedure for chromone-based Michael acceptors synthesis.

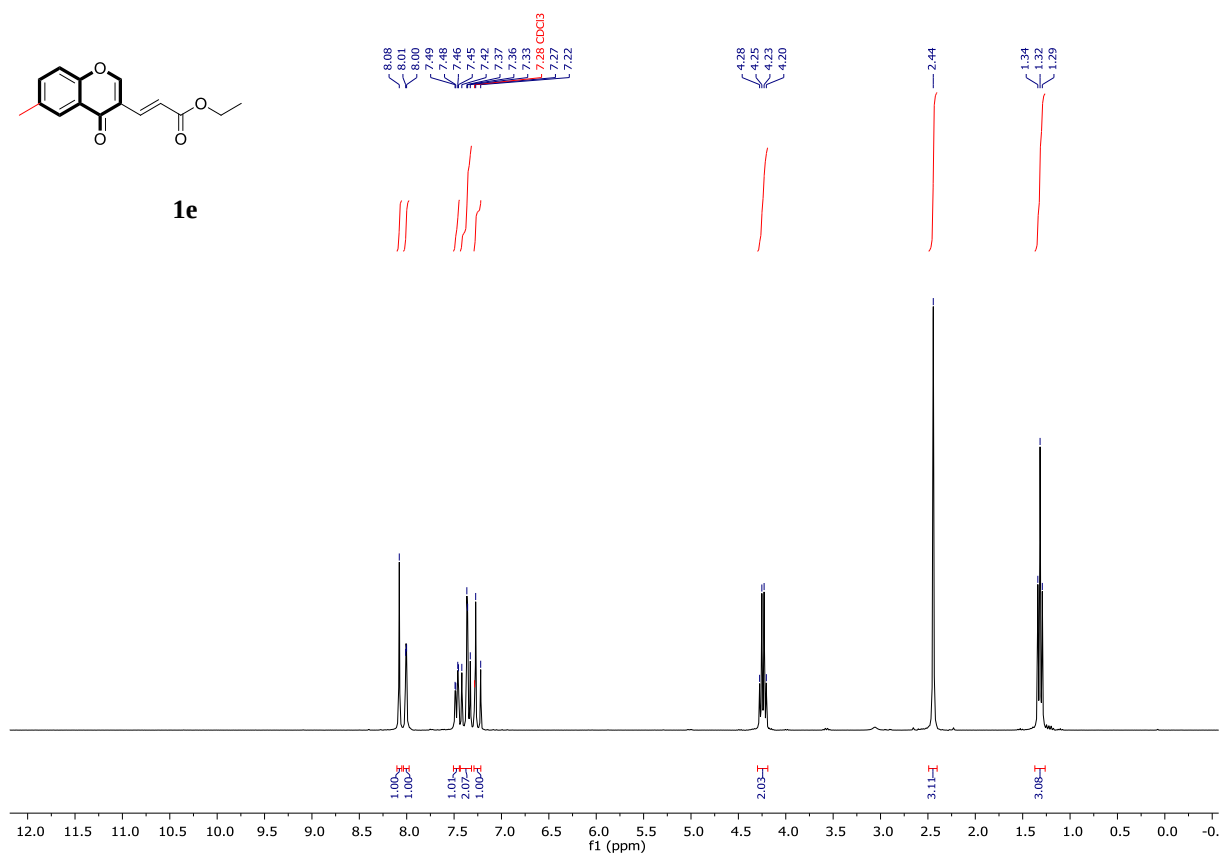


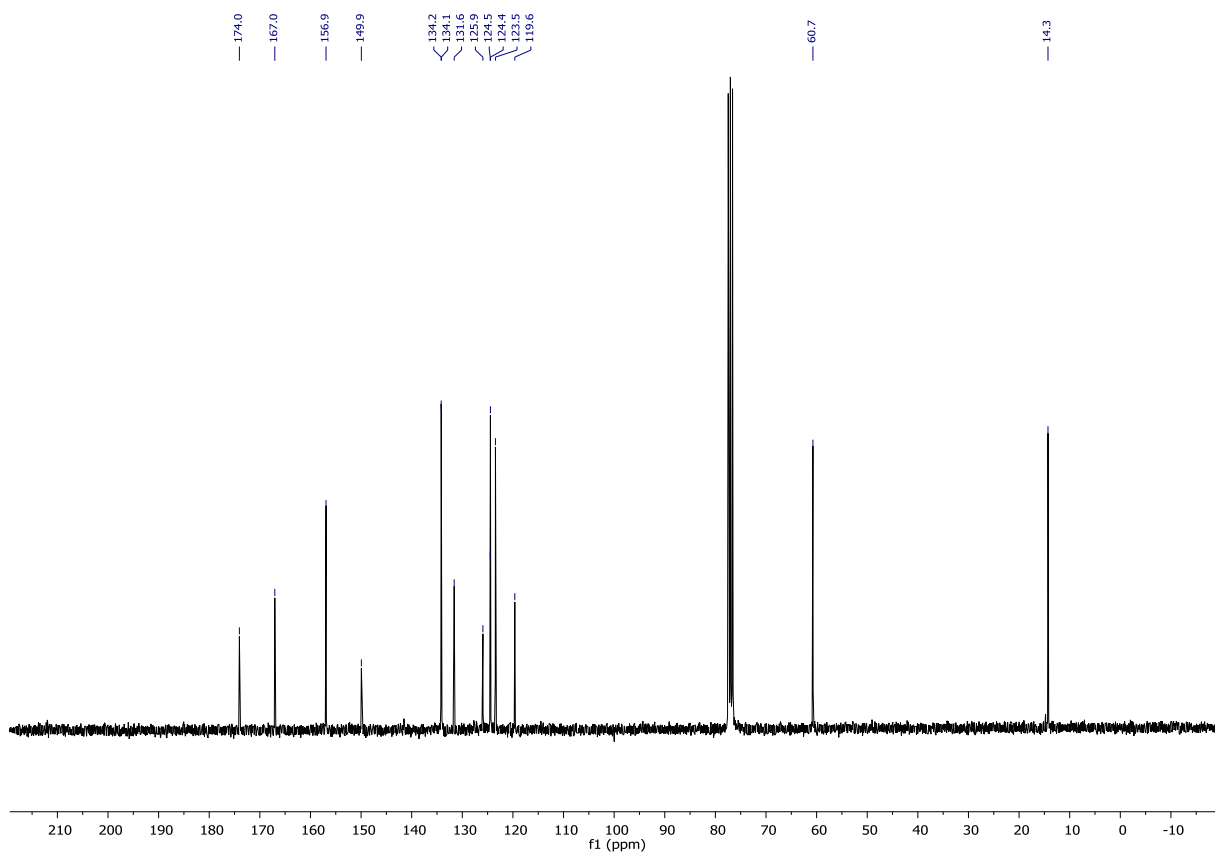
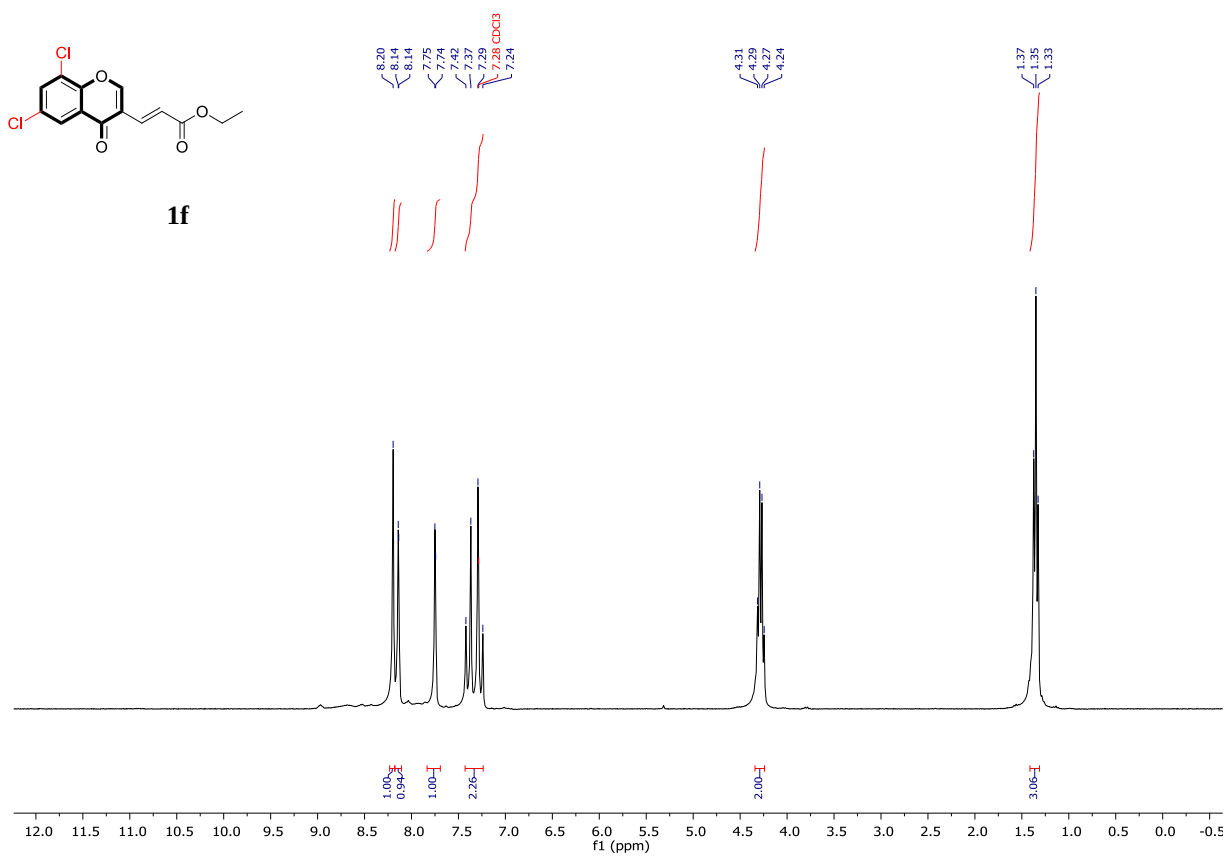


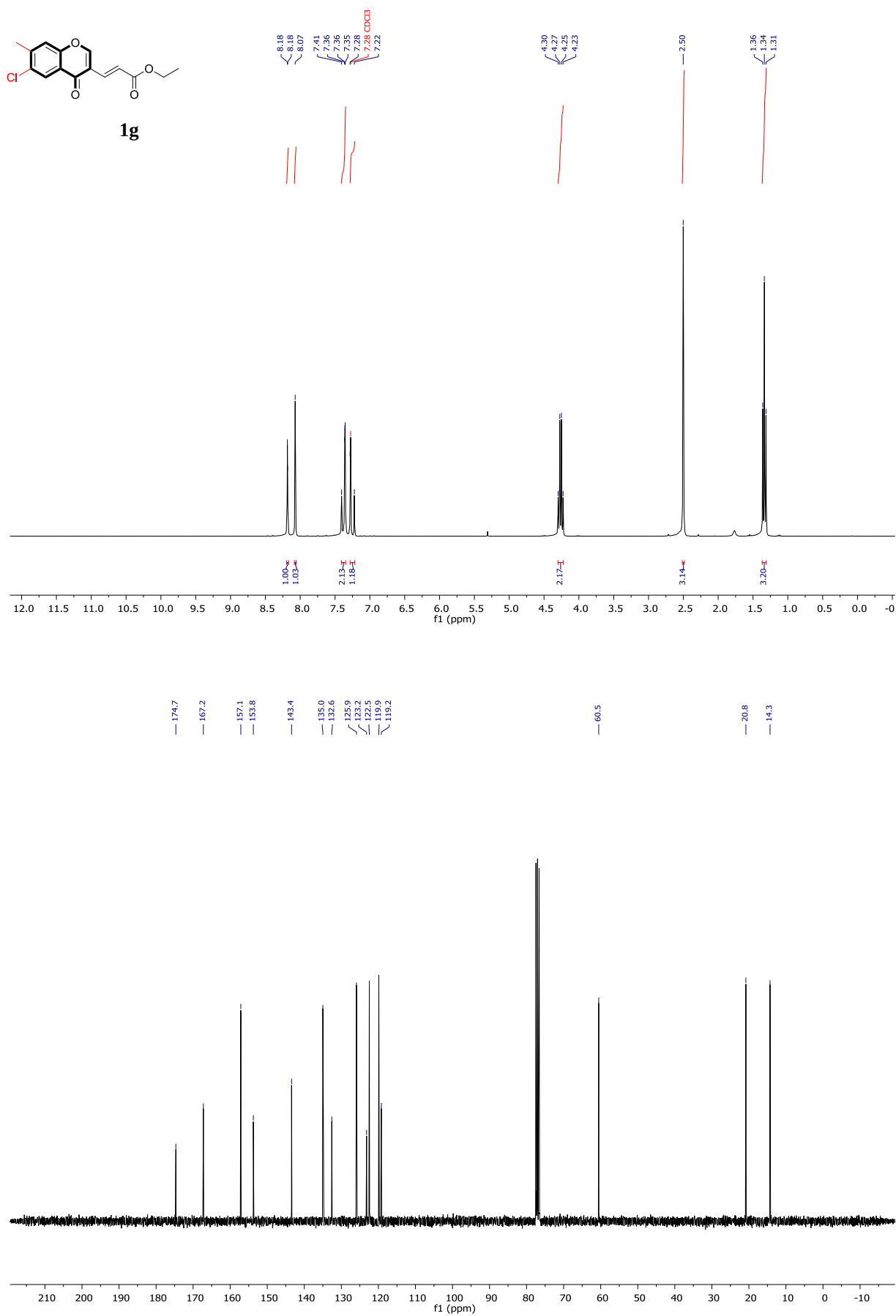




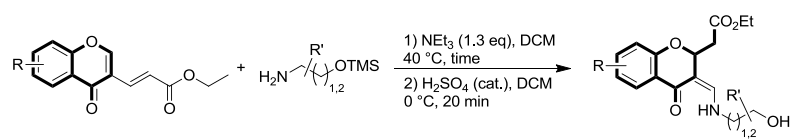


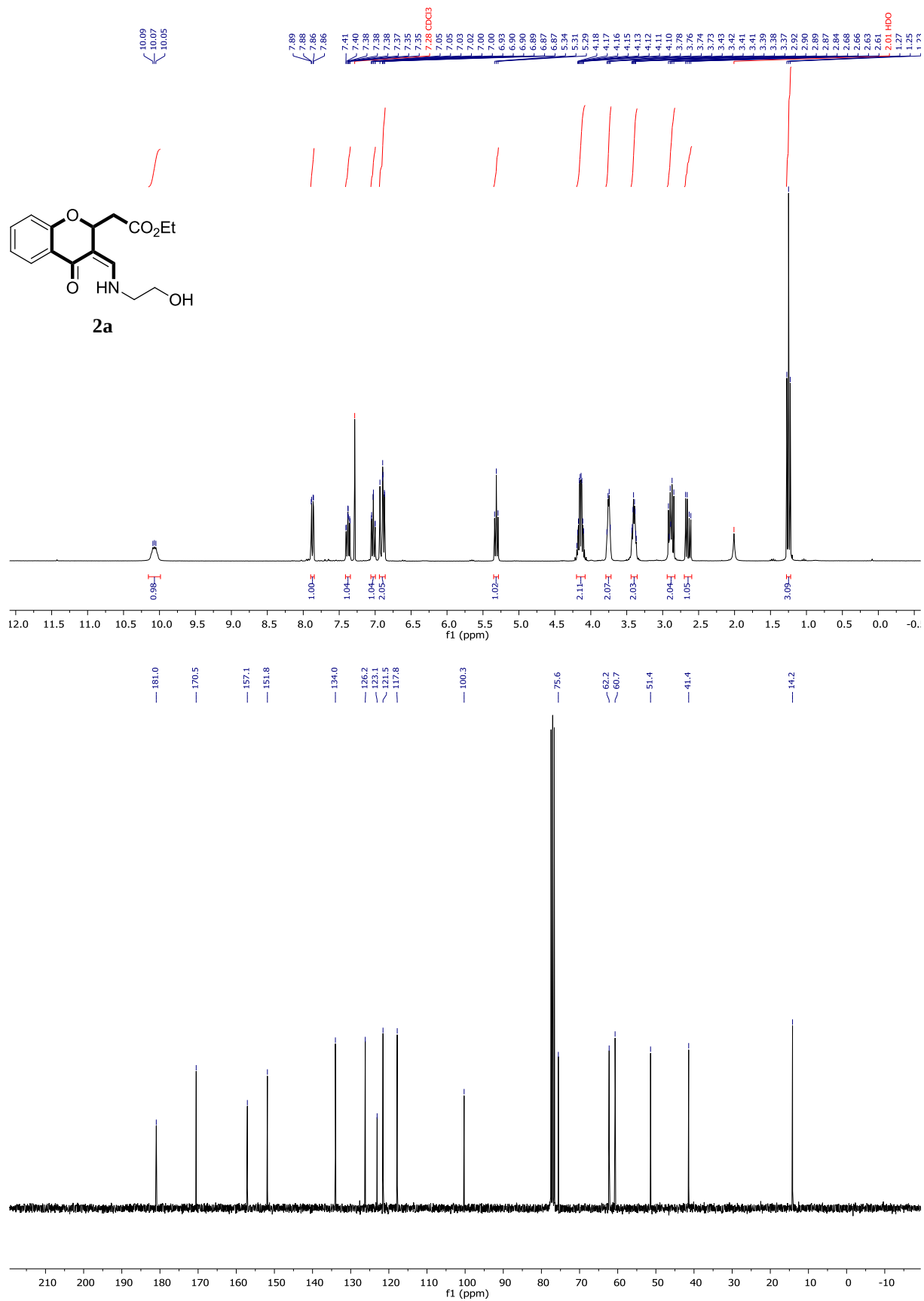


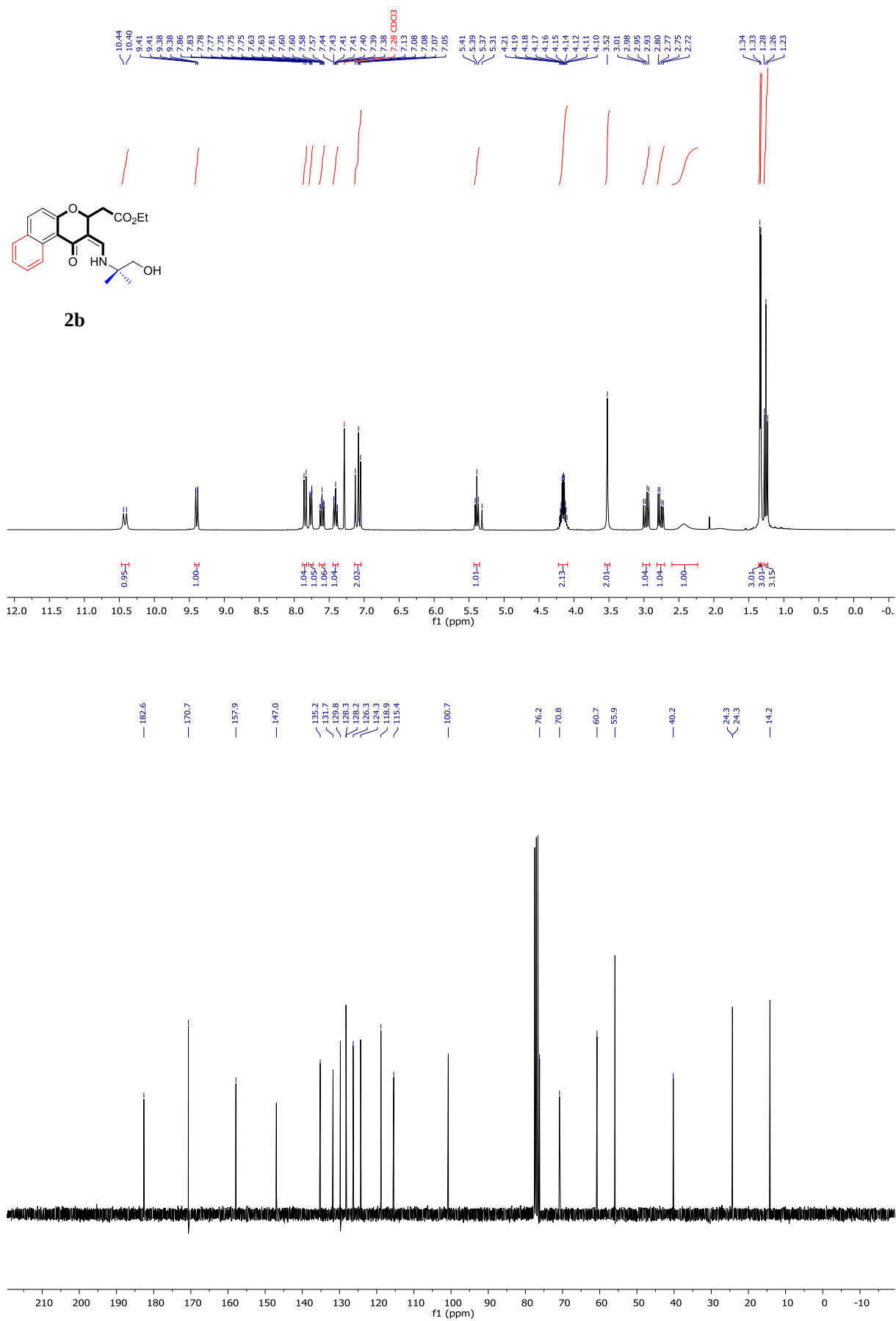


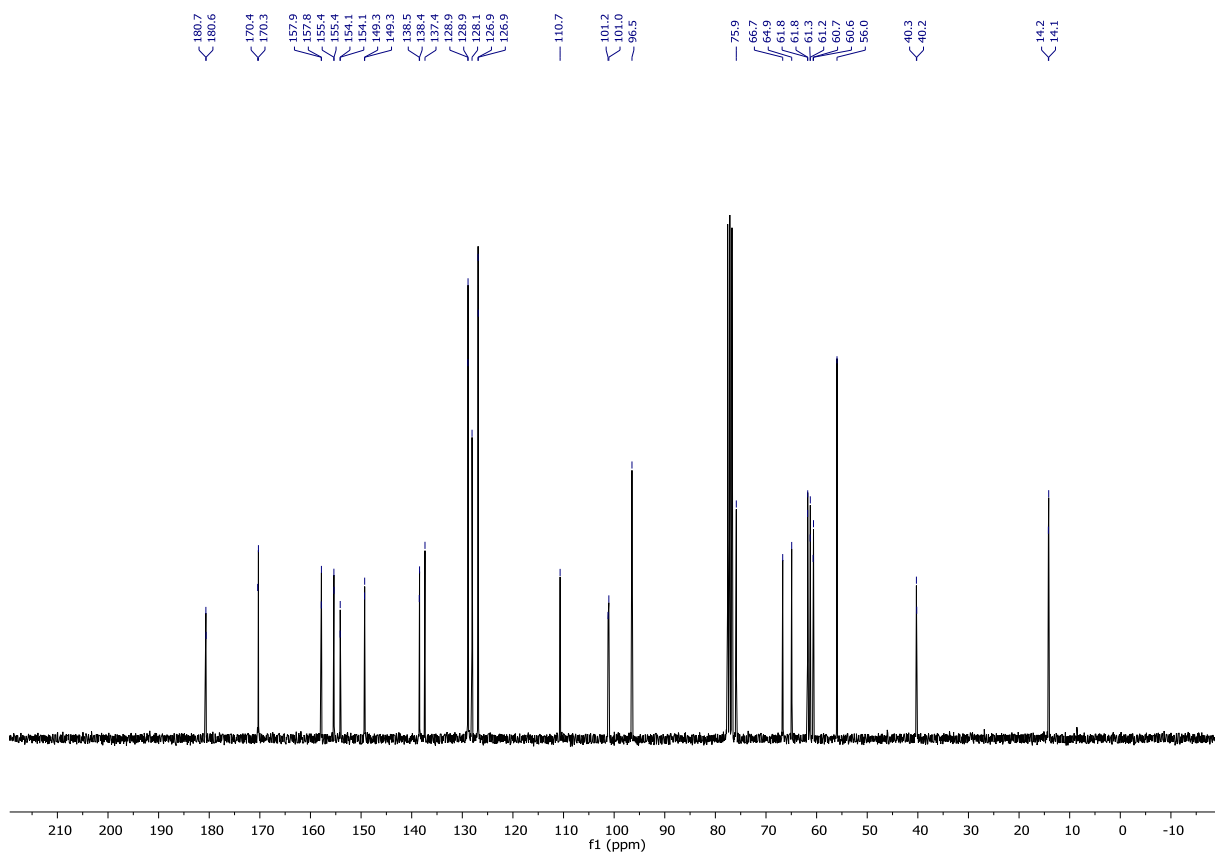
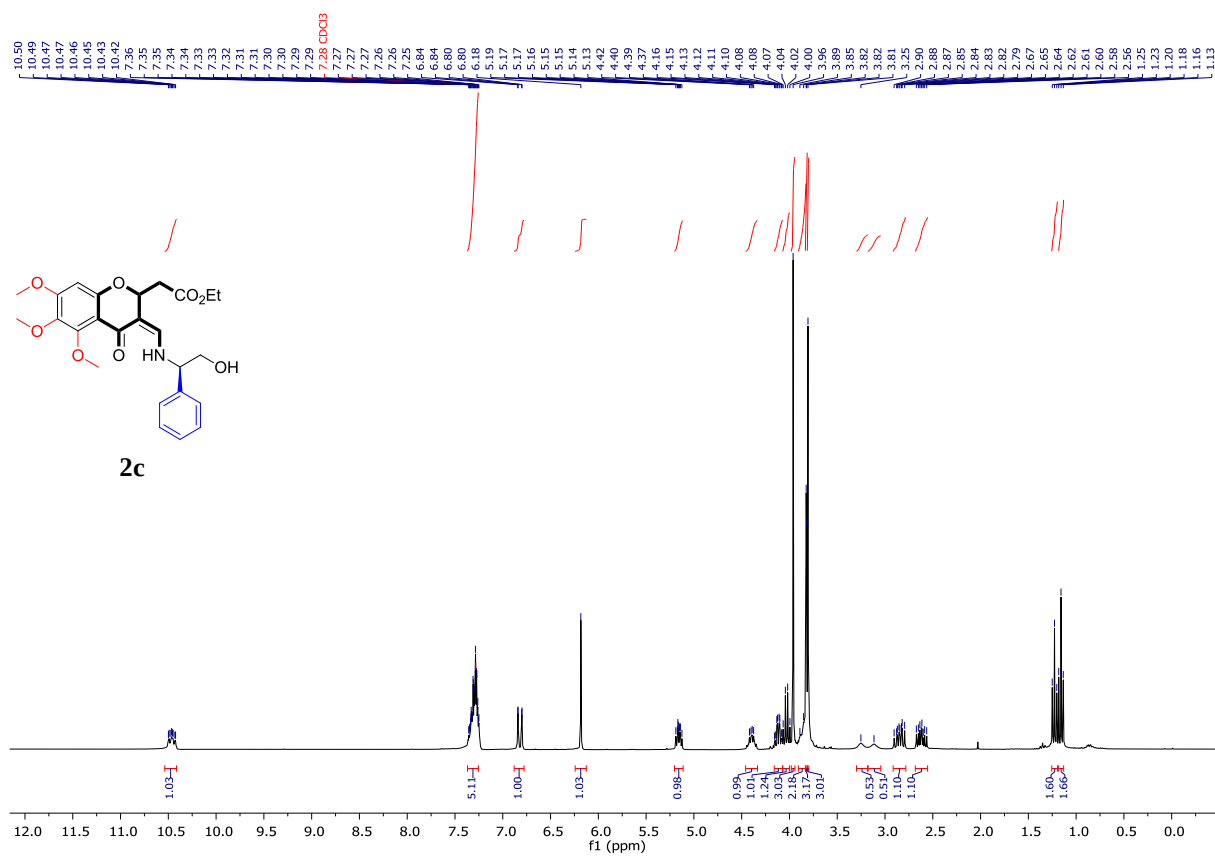


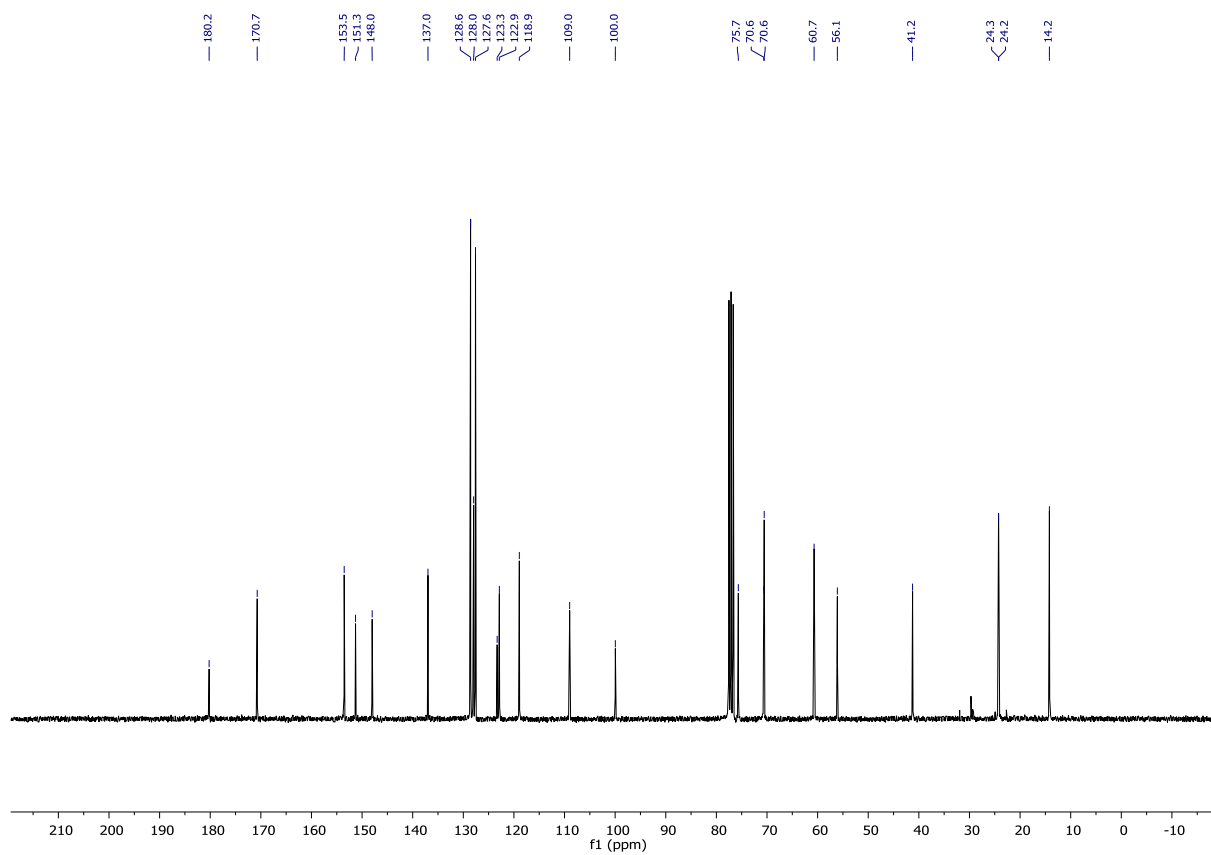
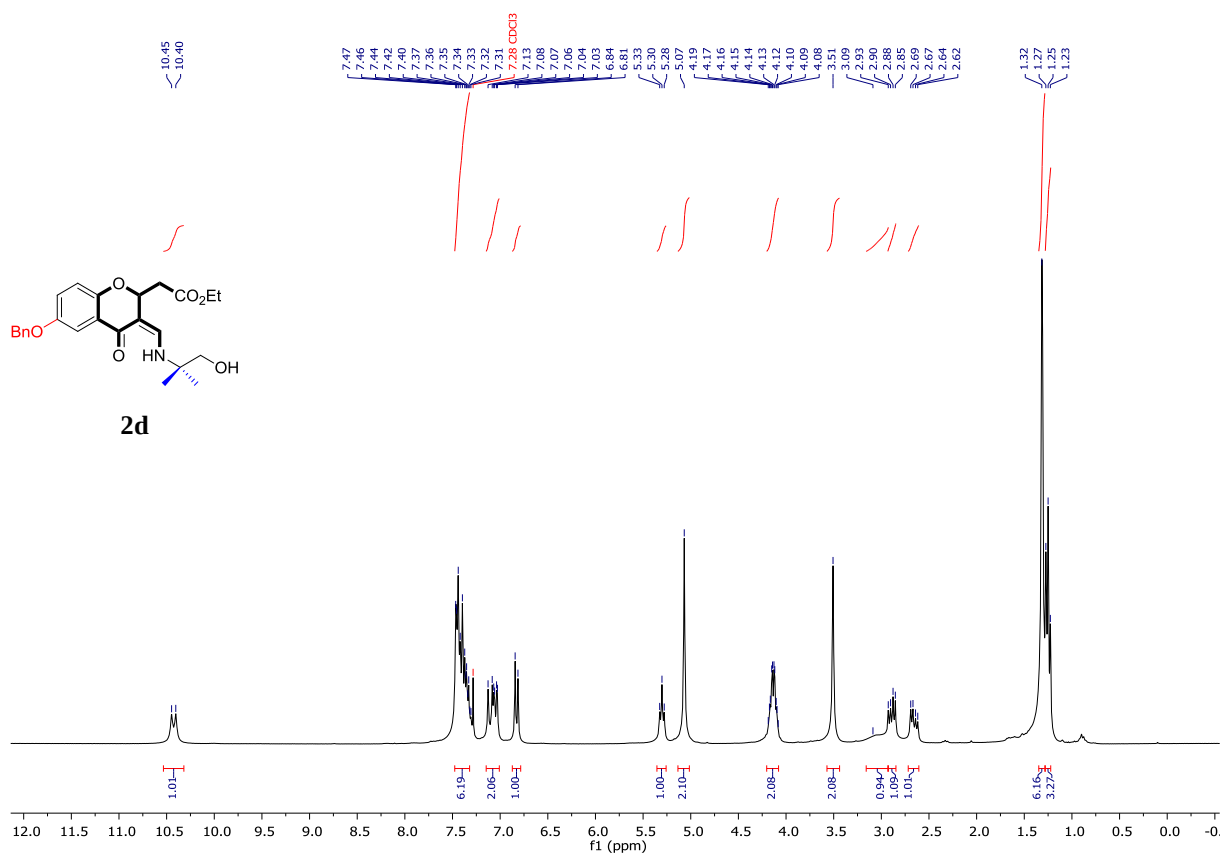
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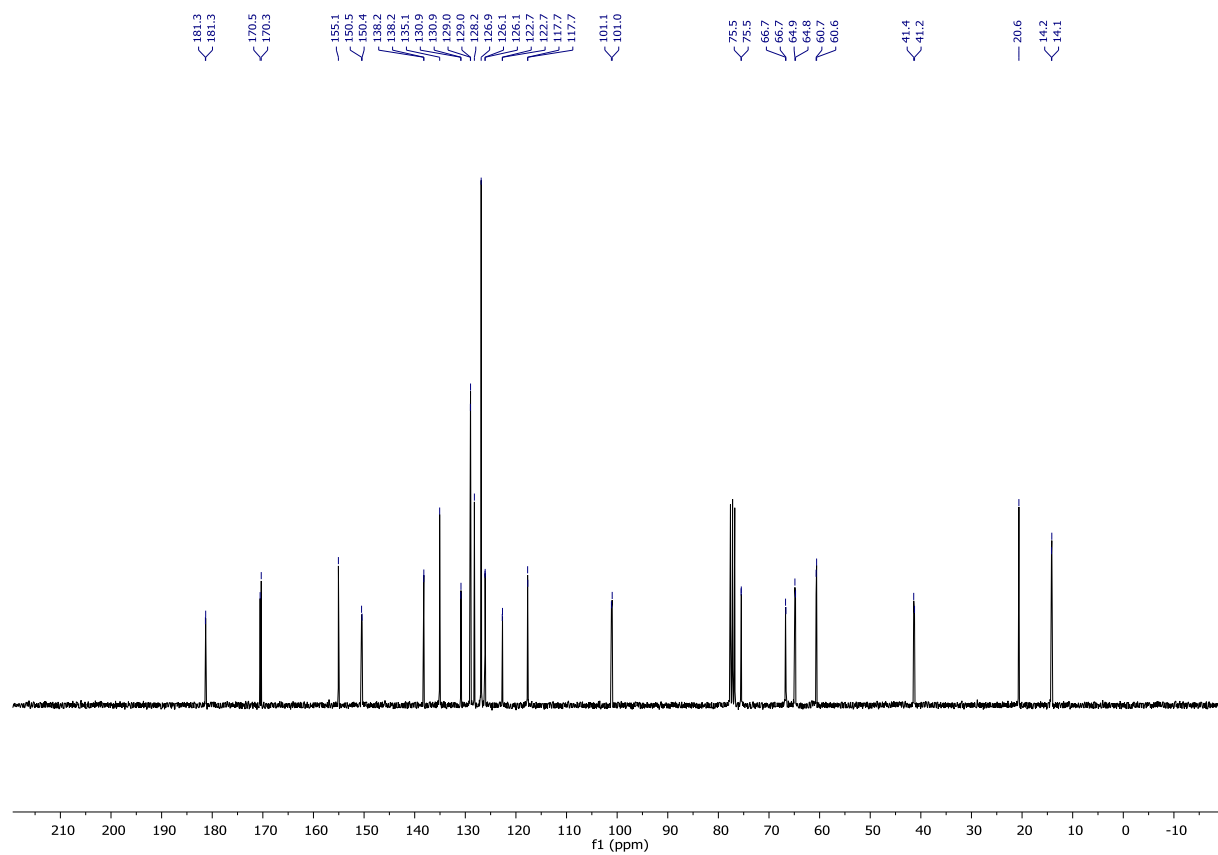
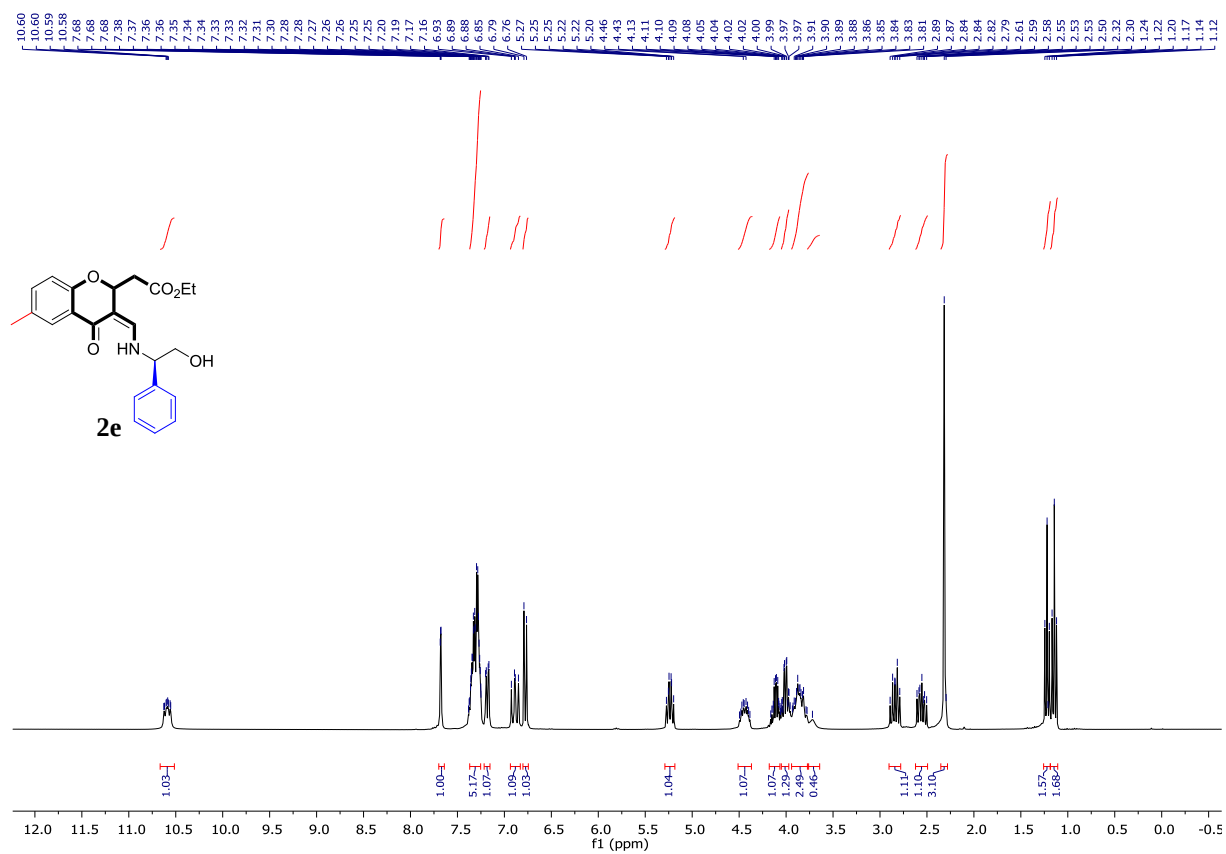


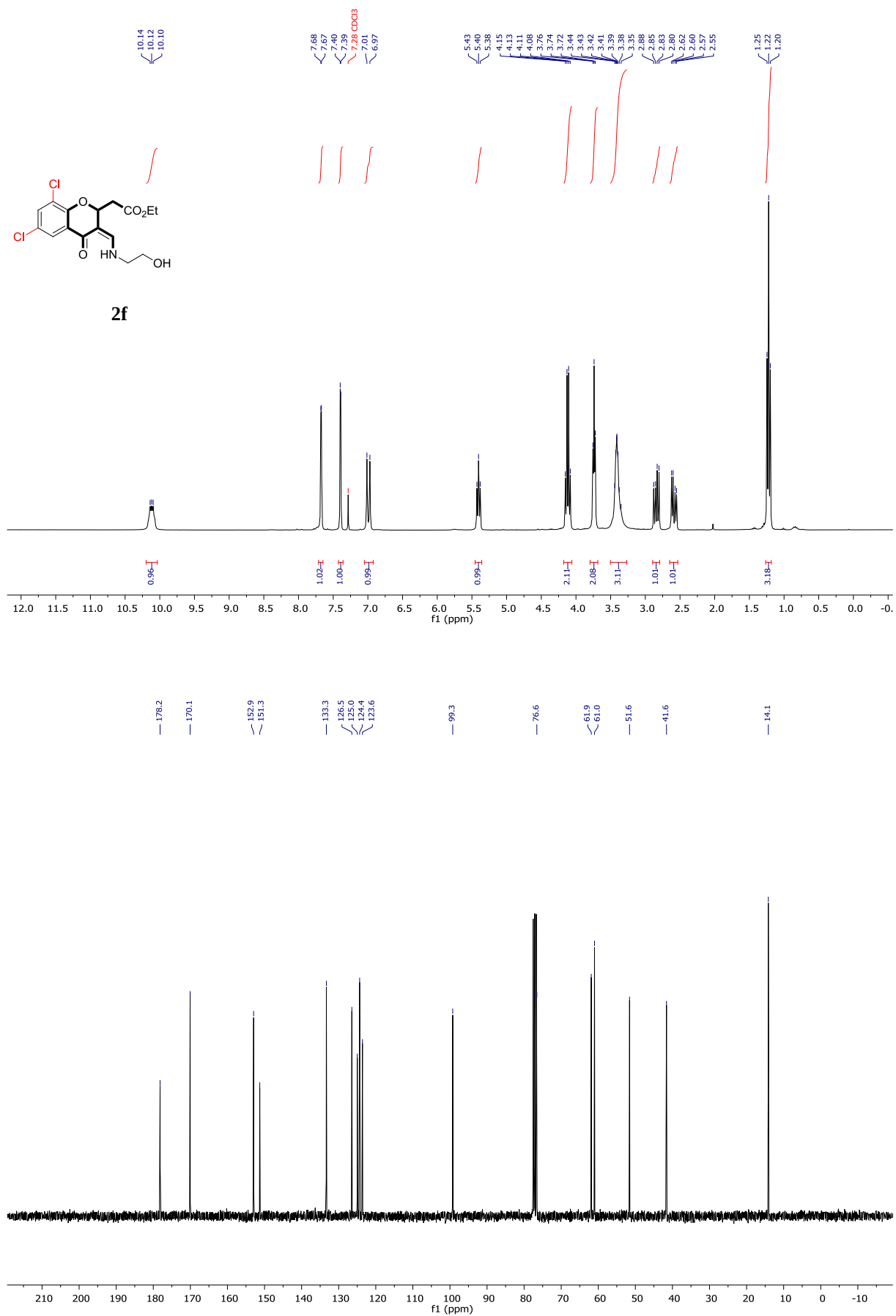


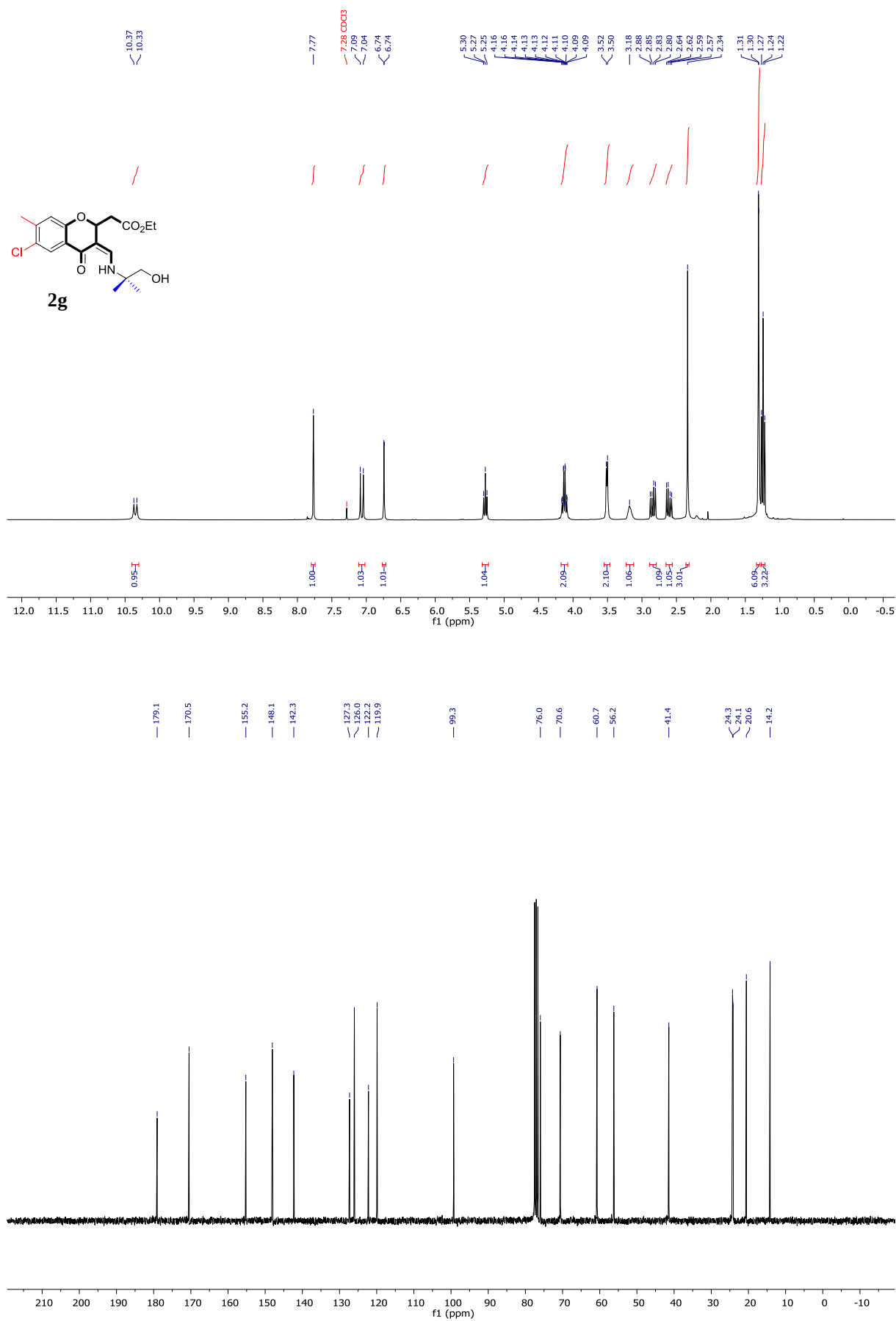


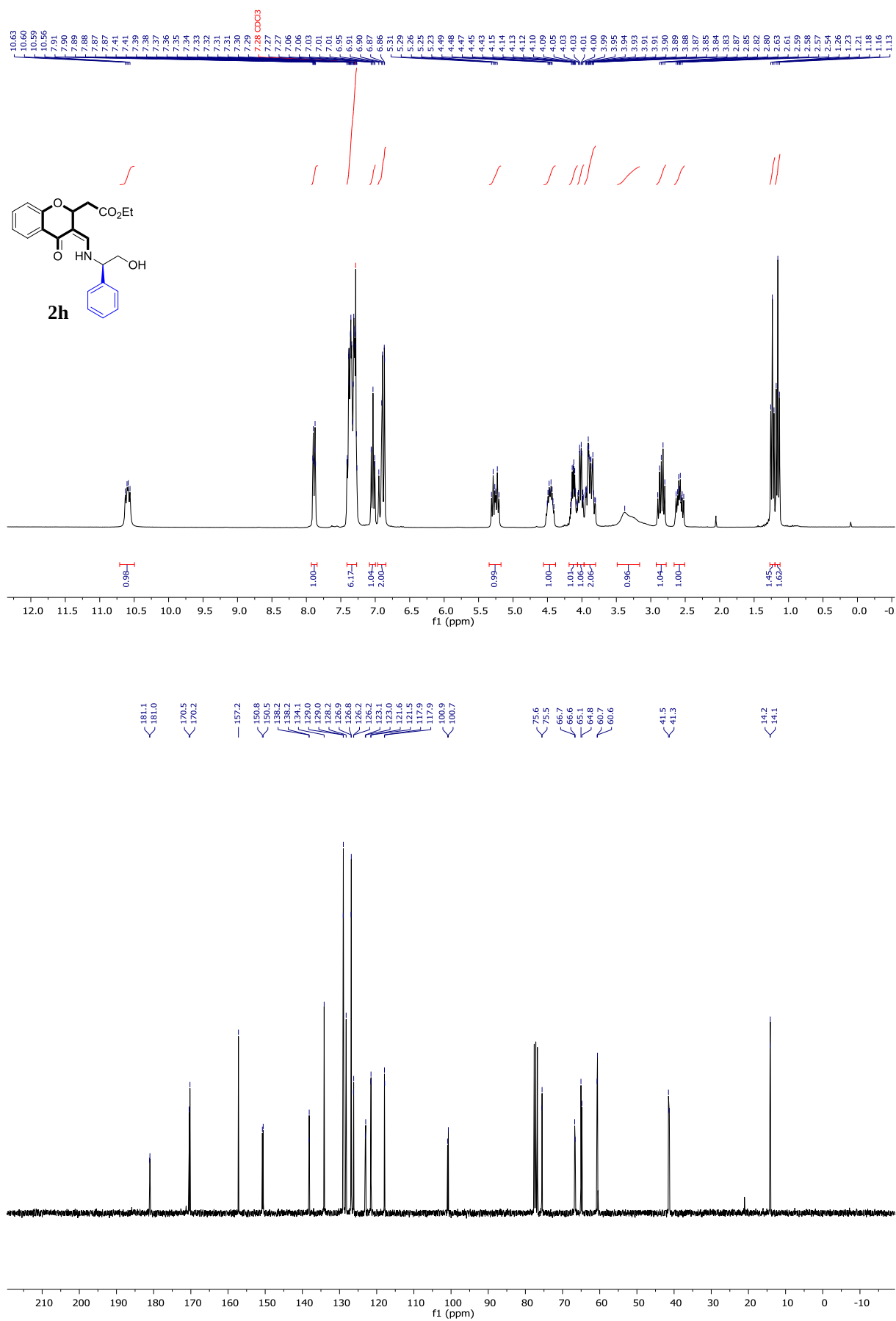


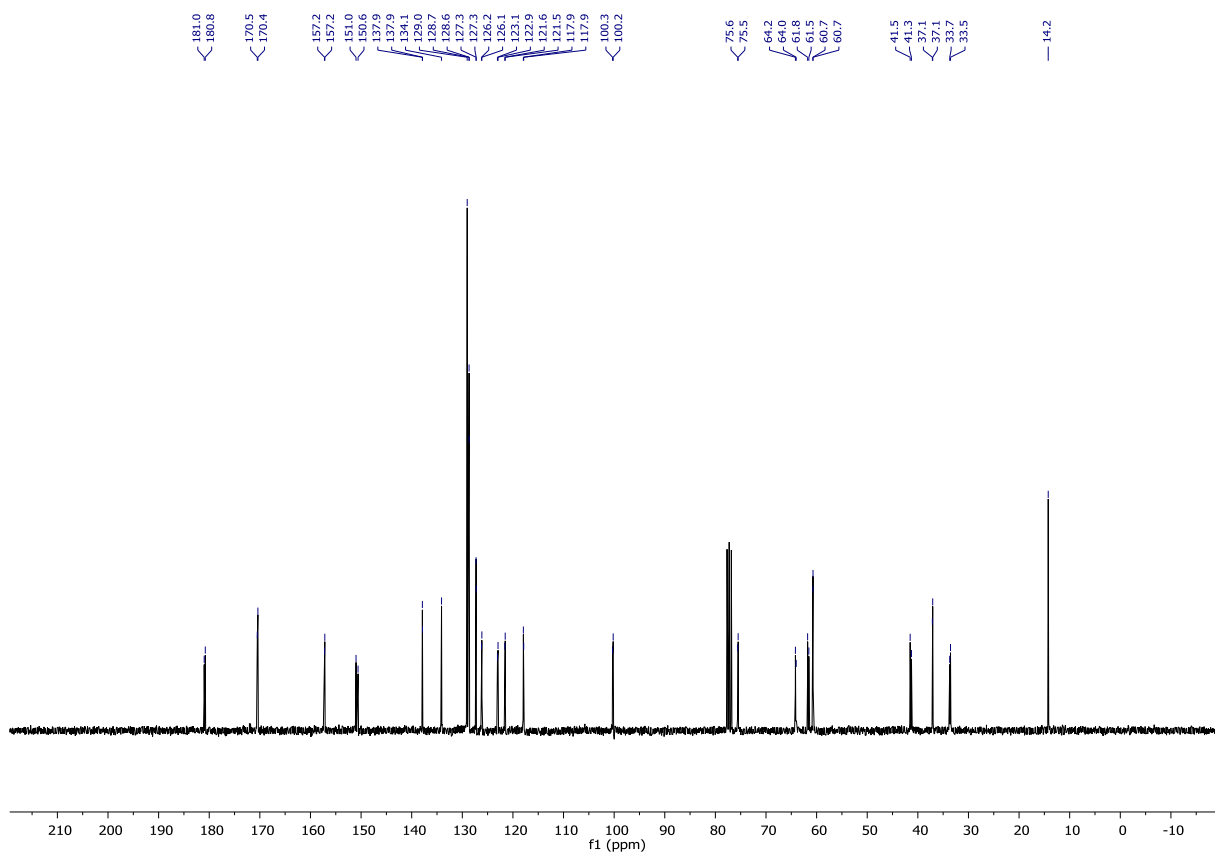
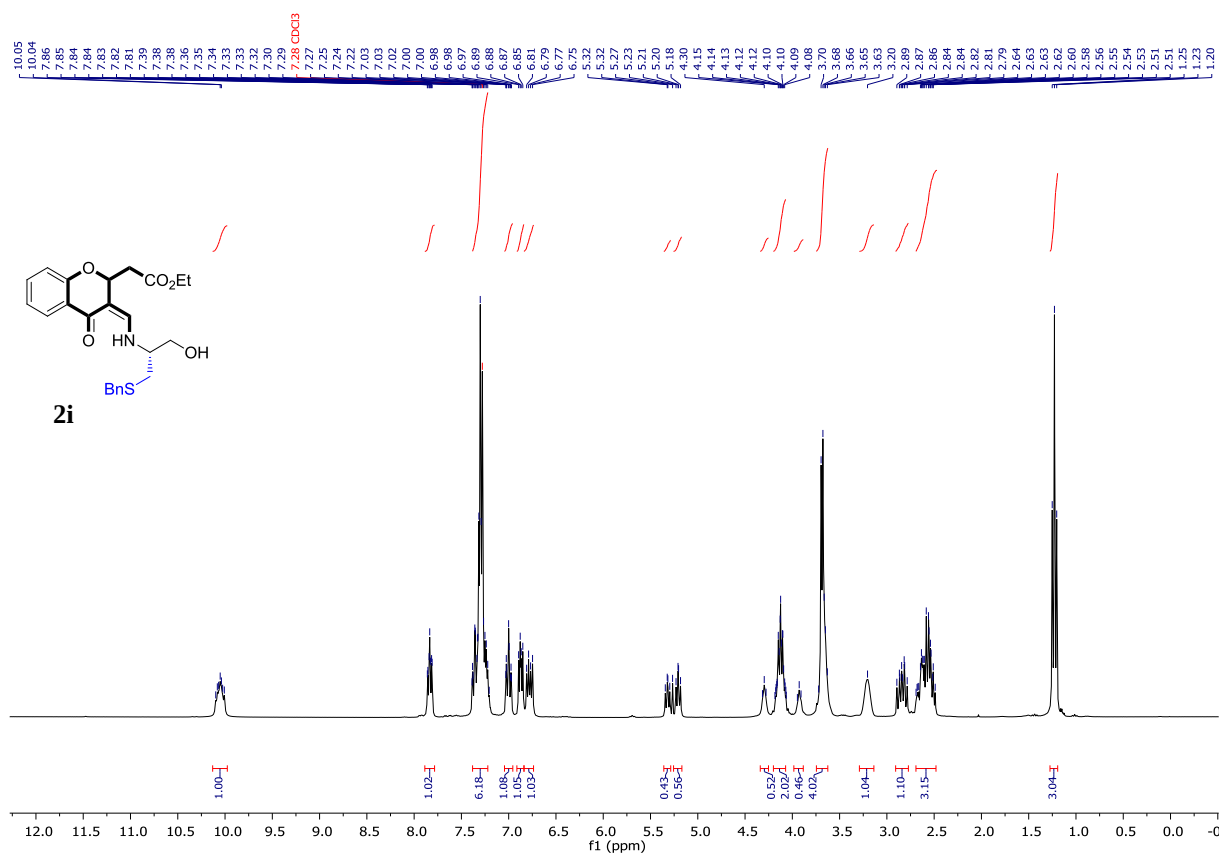


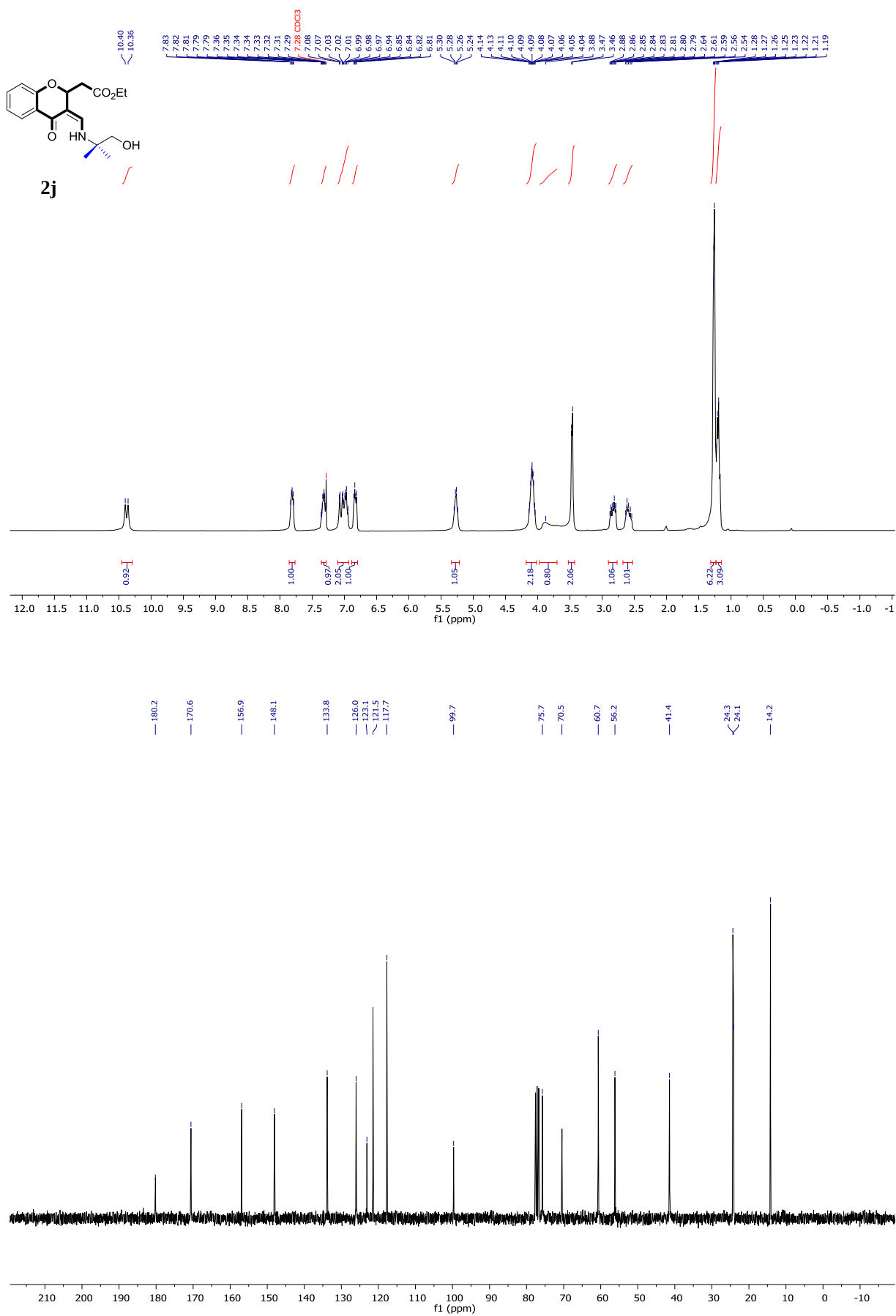


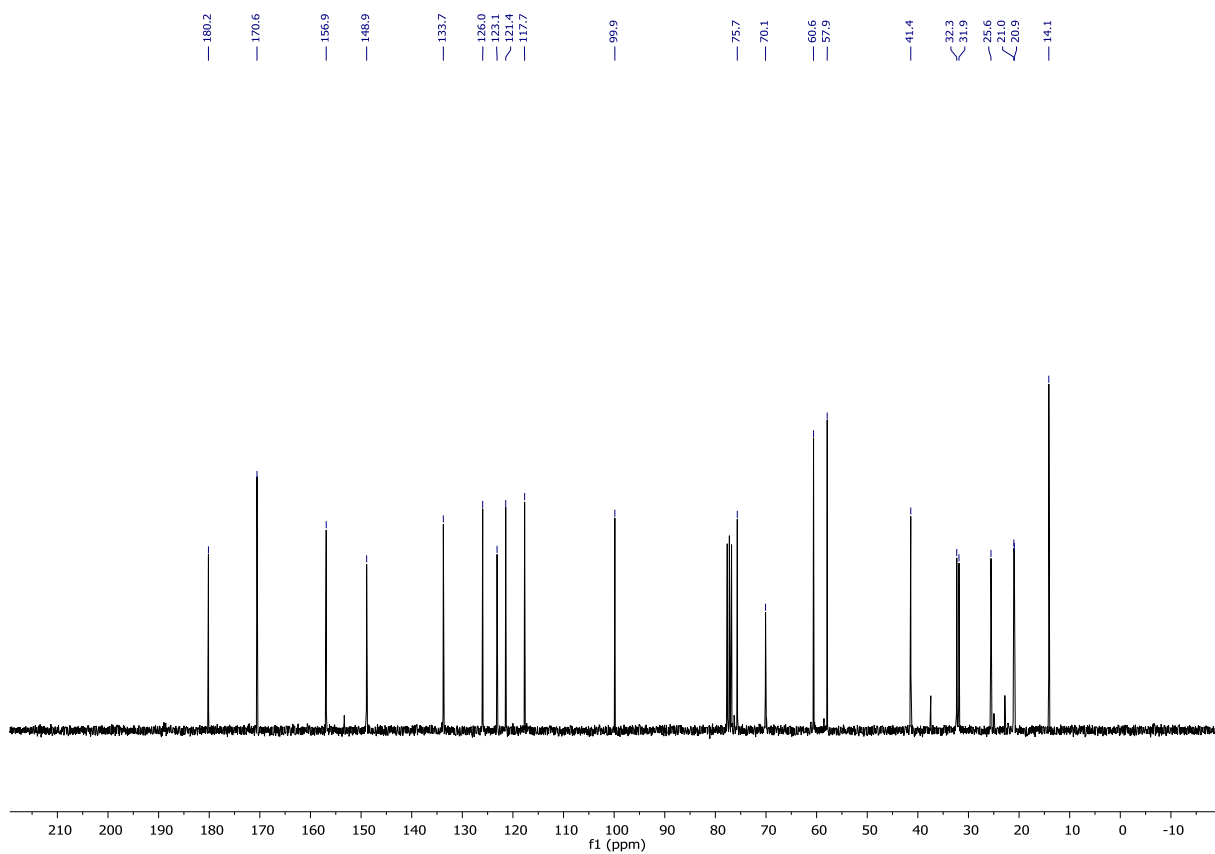
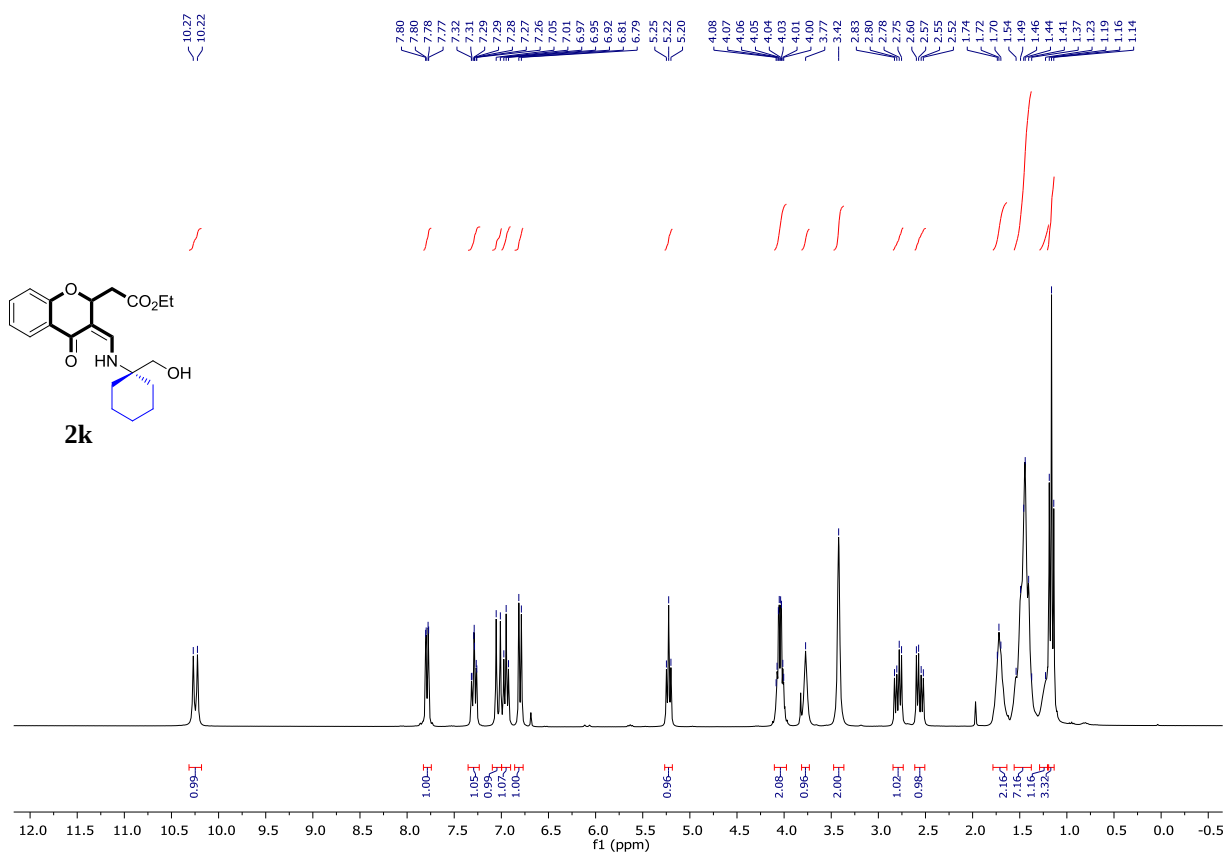


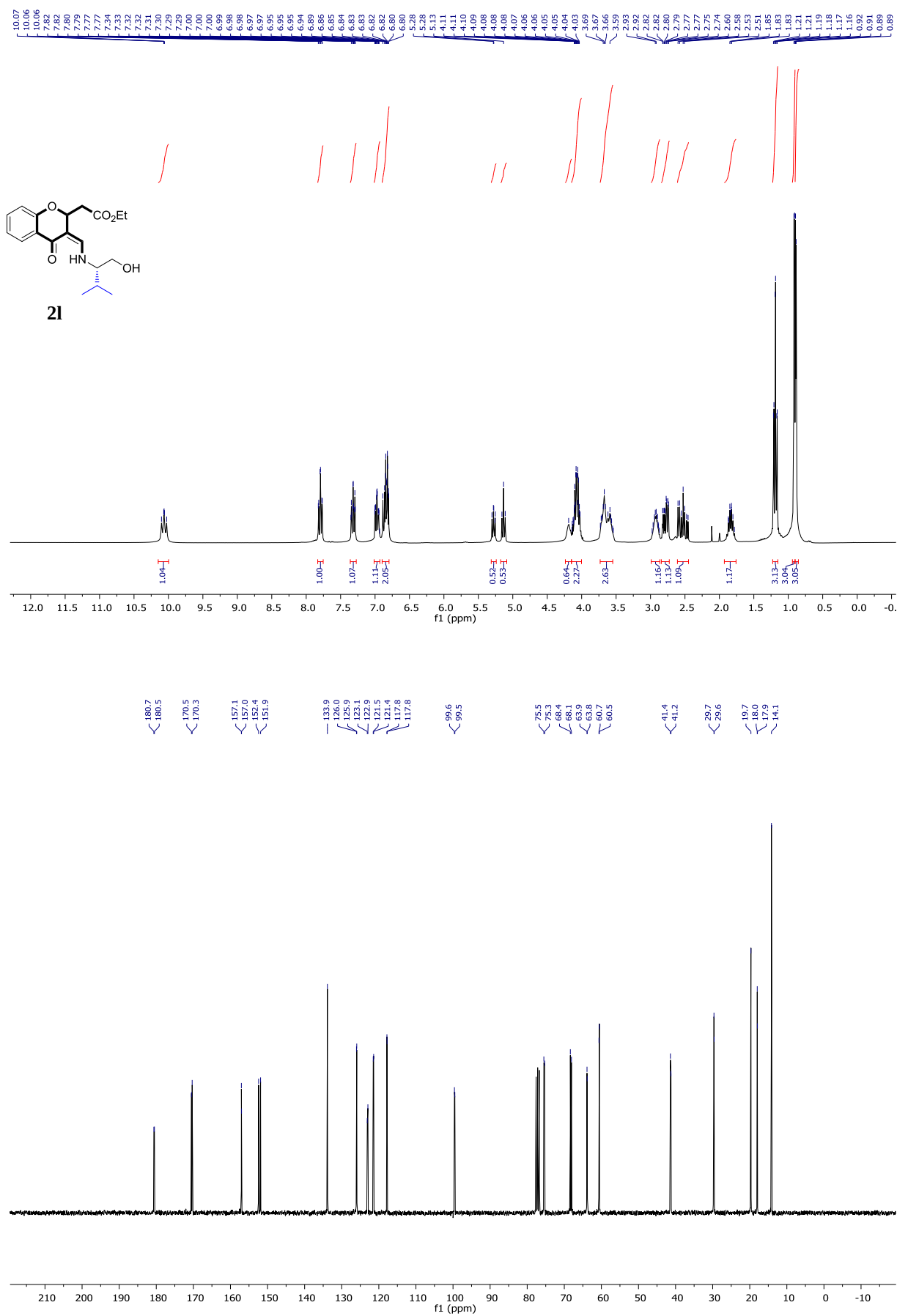


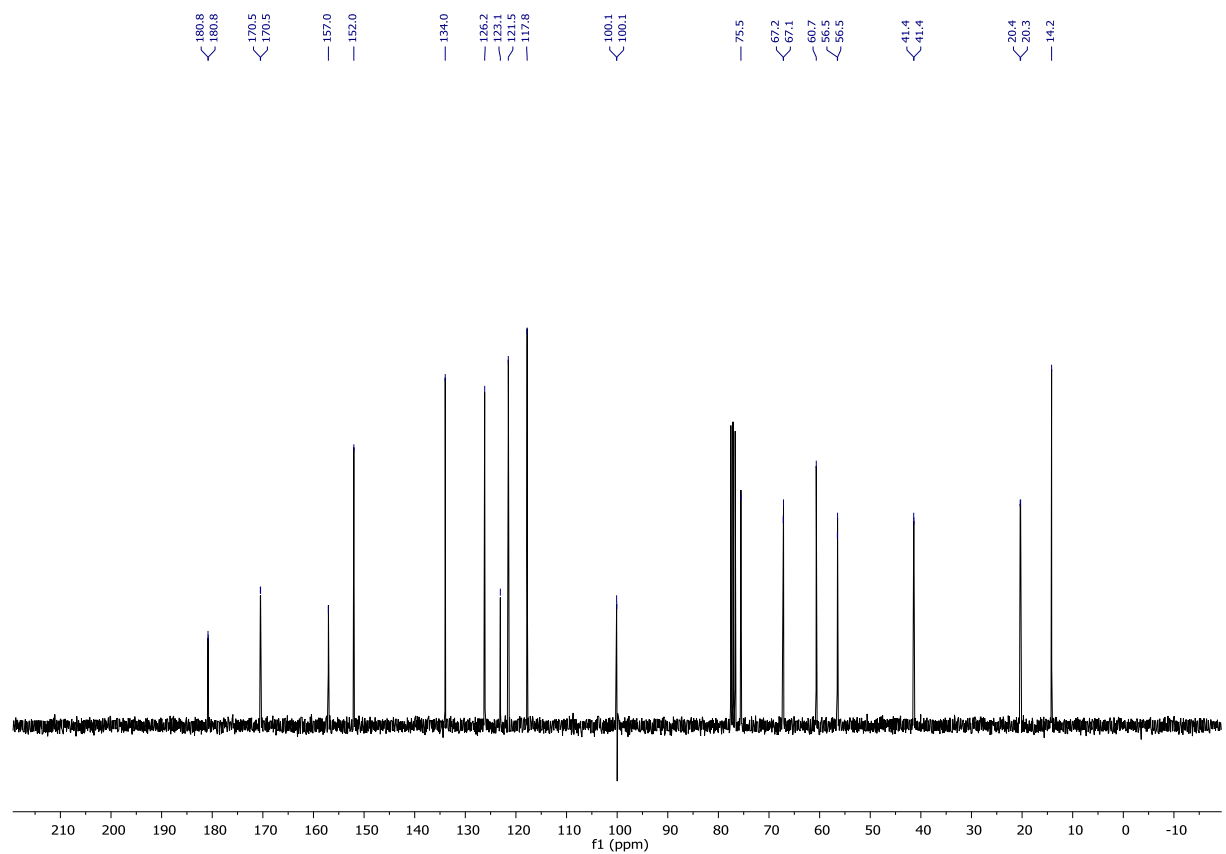
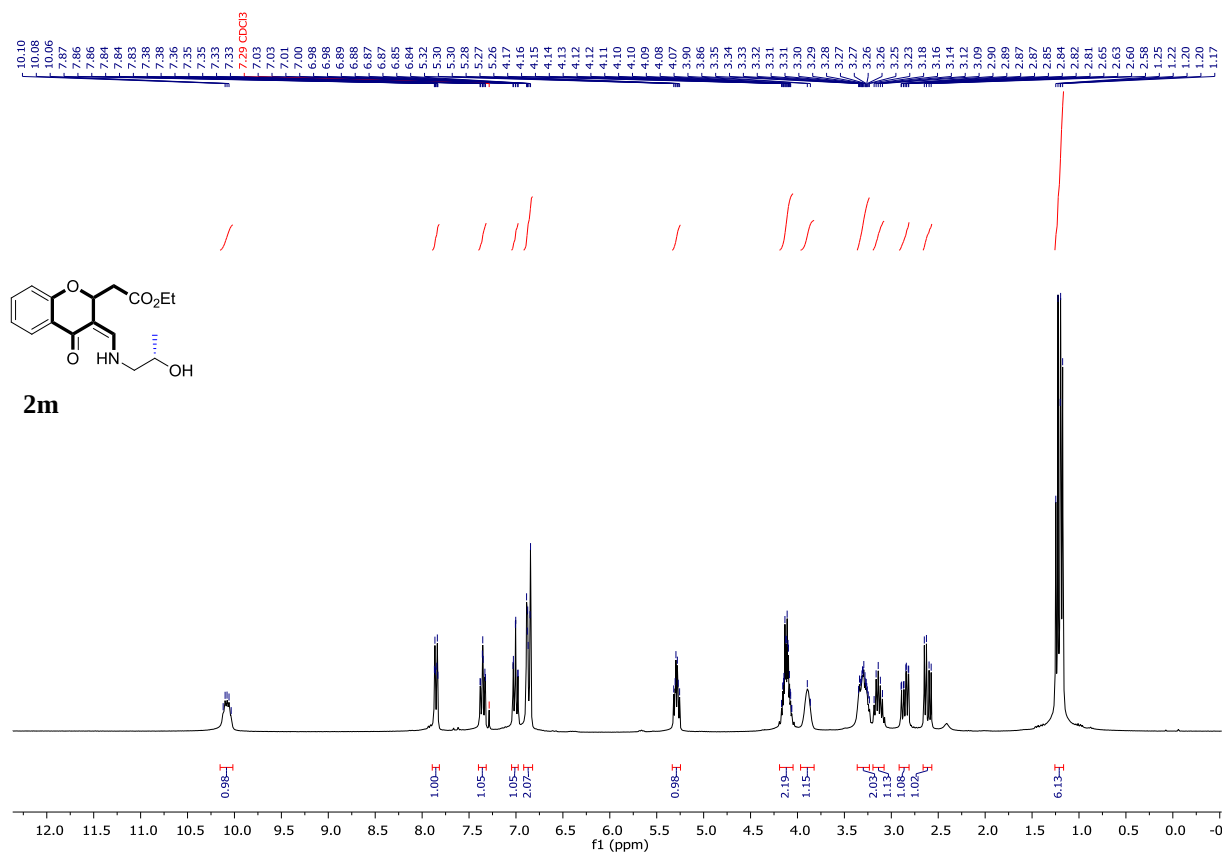


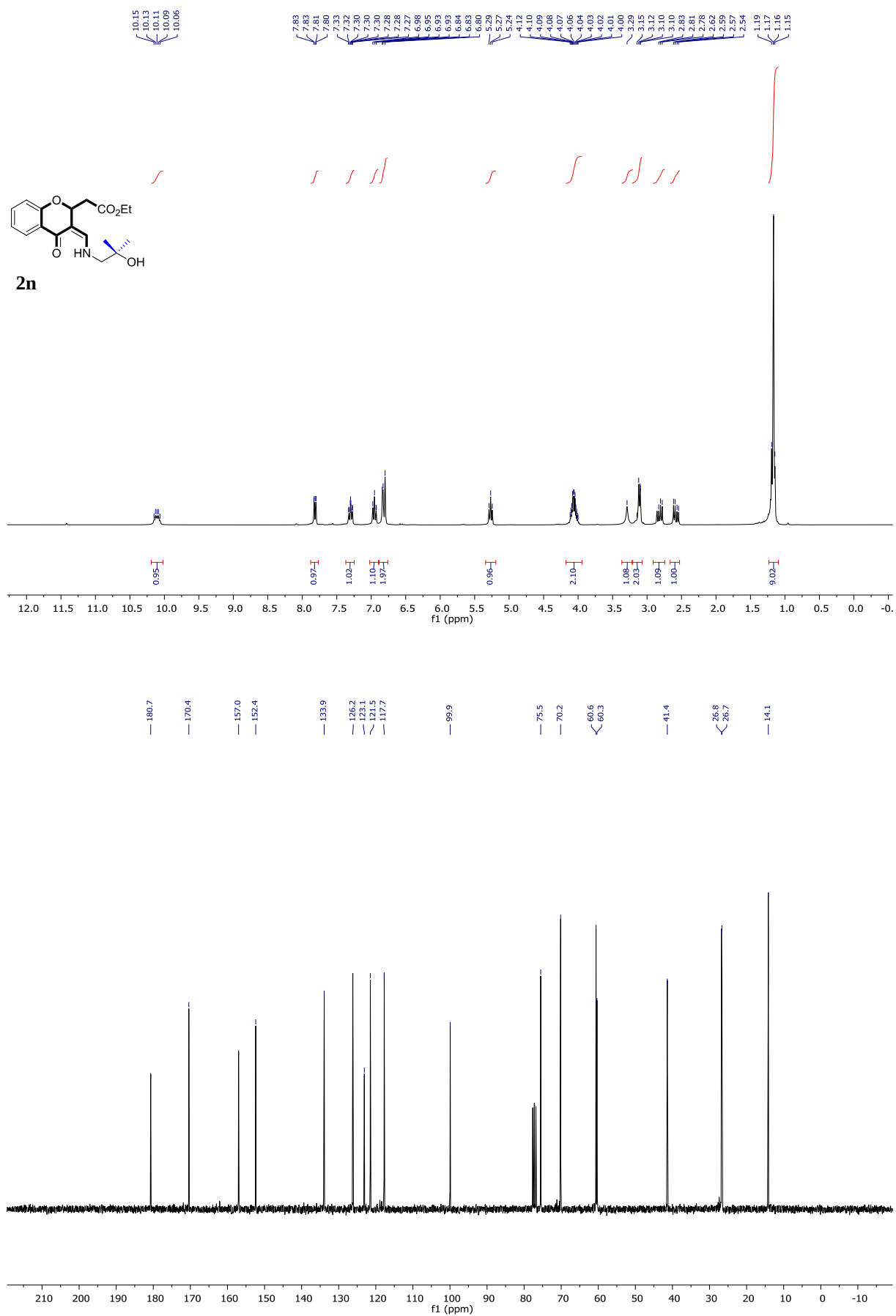


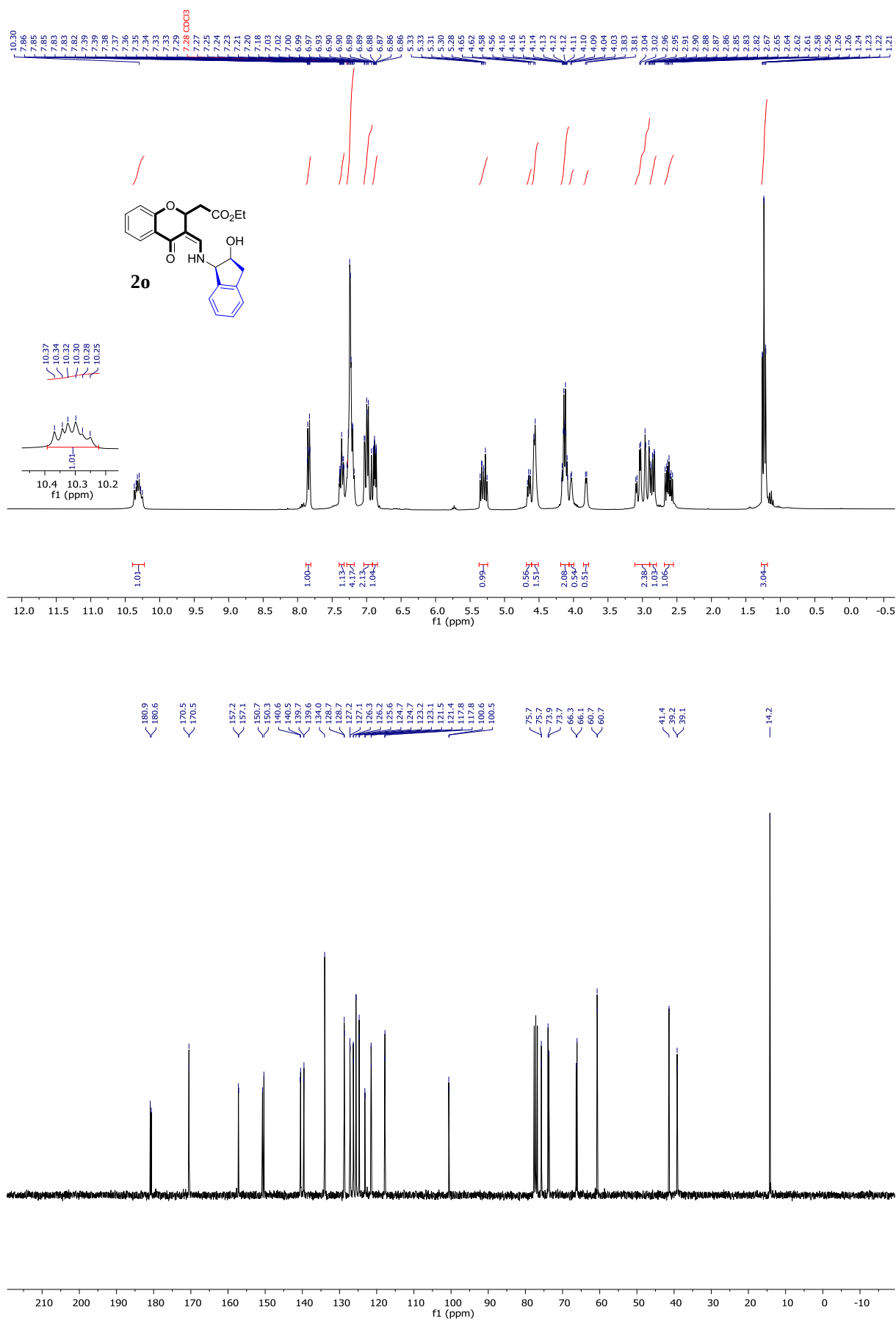


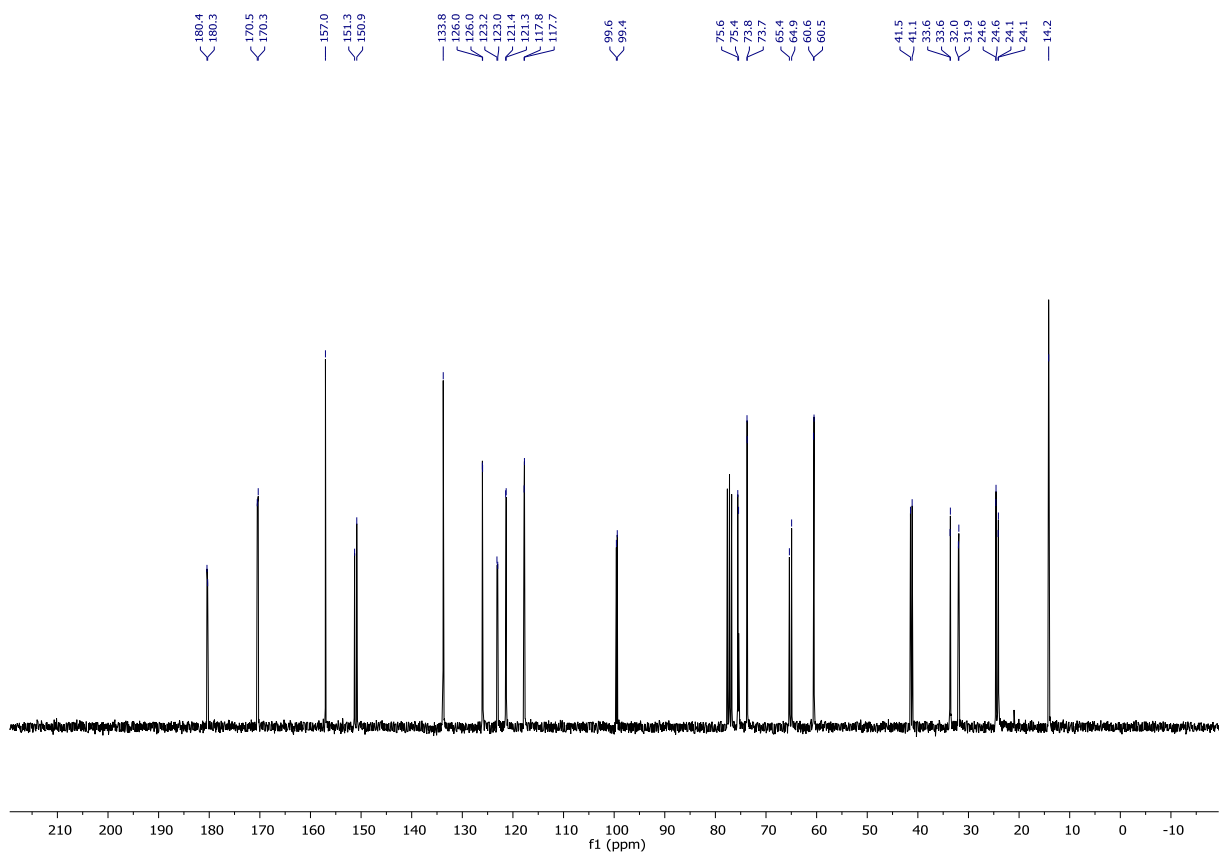
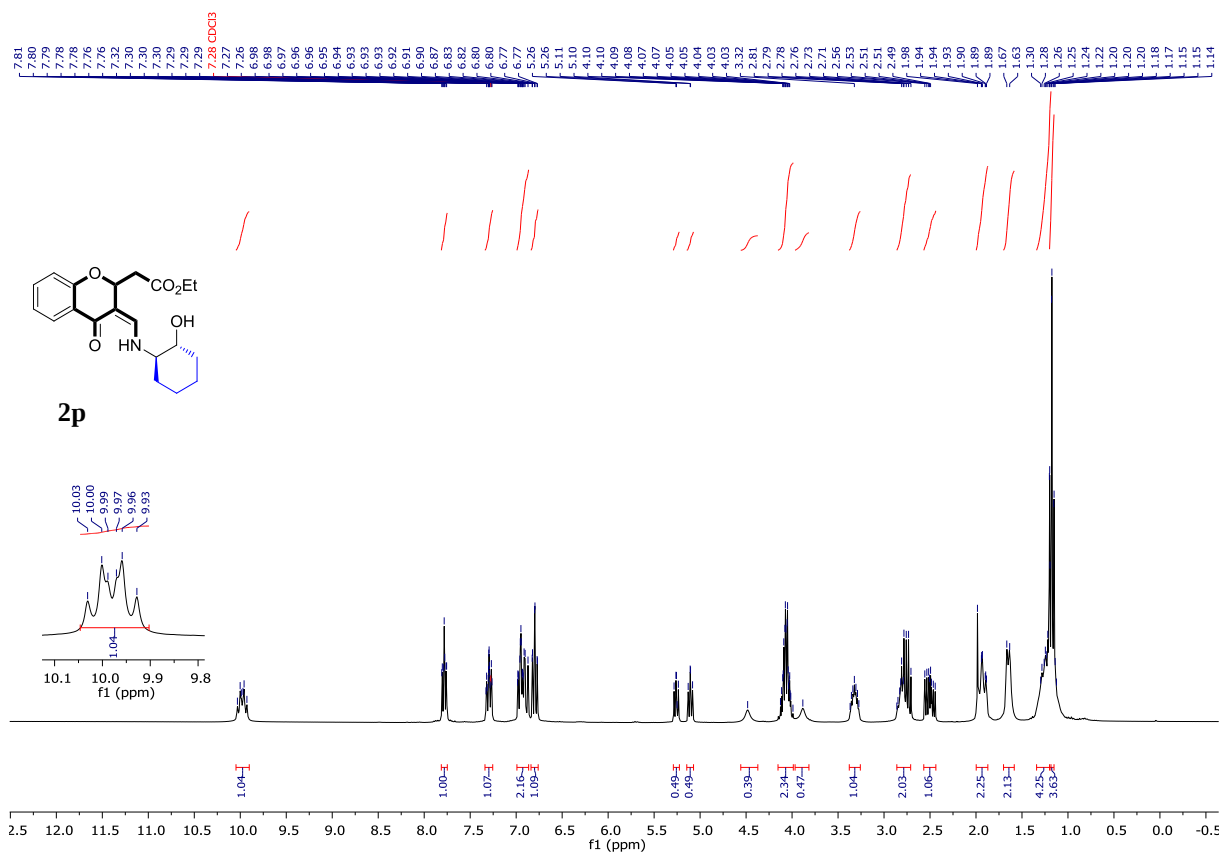


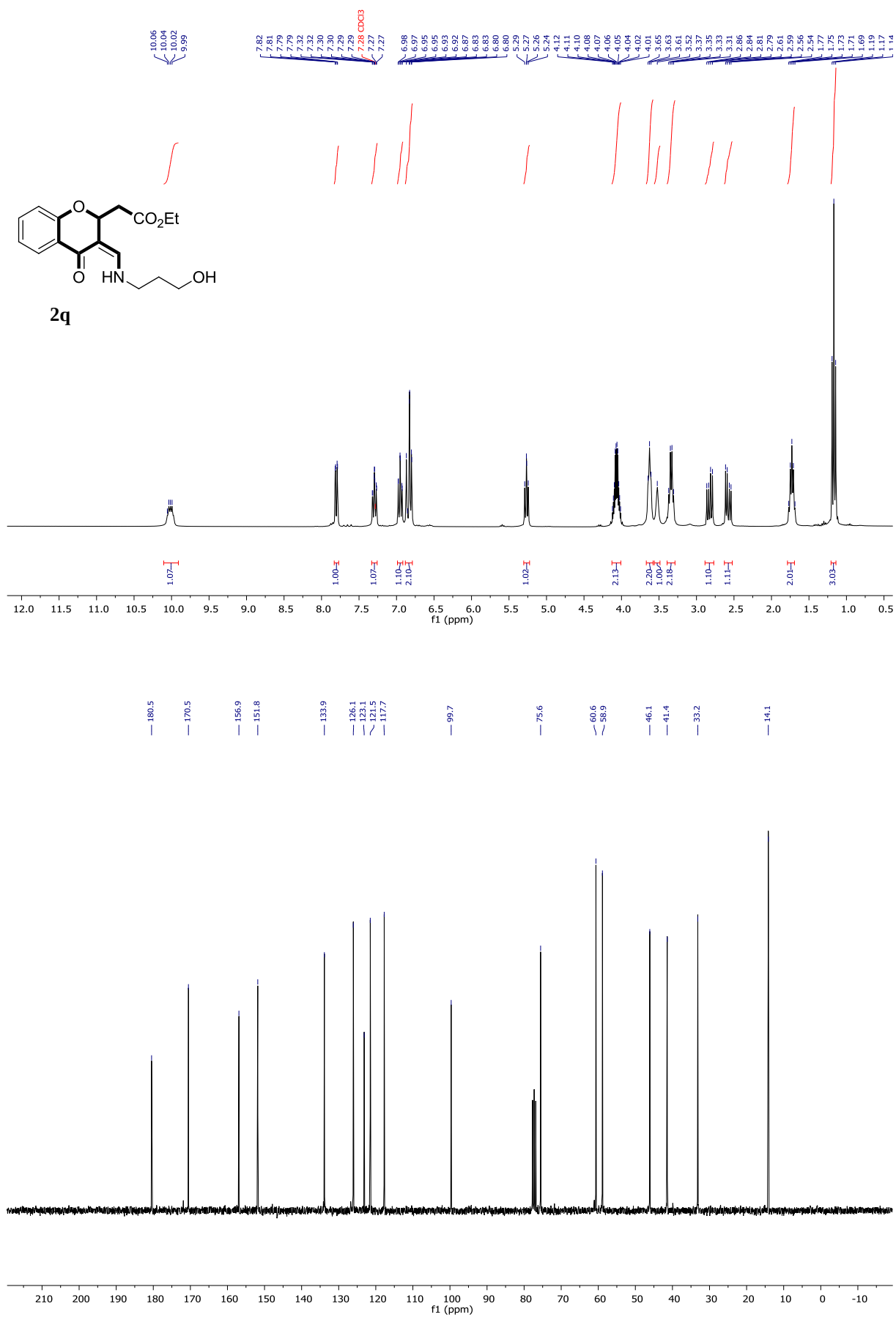




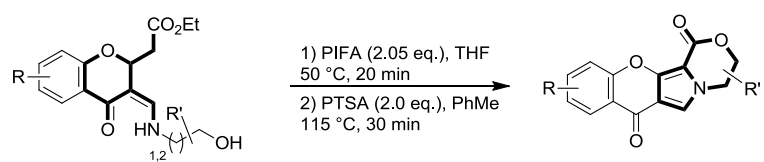


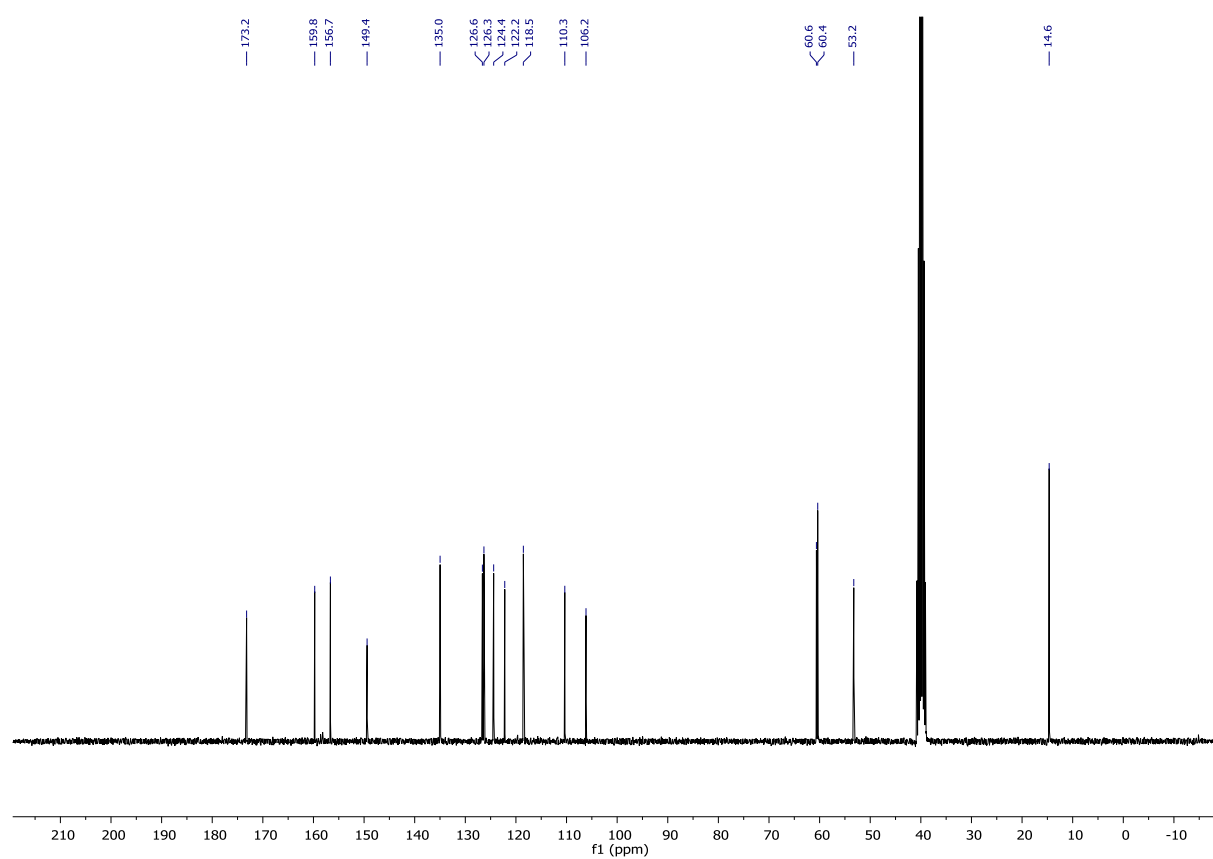
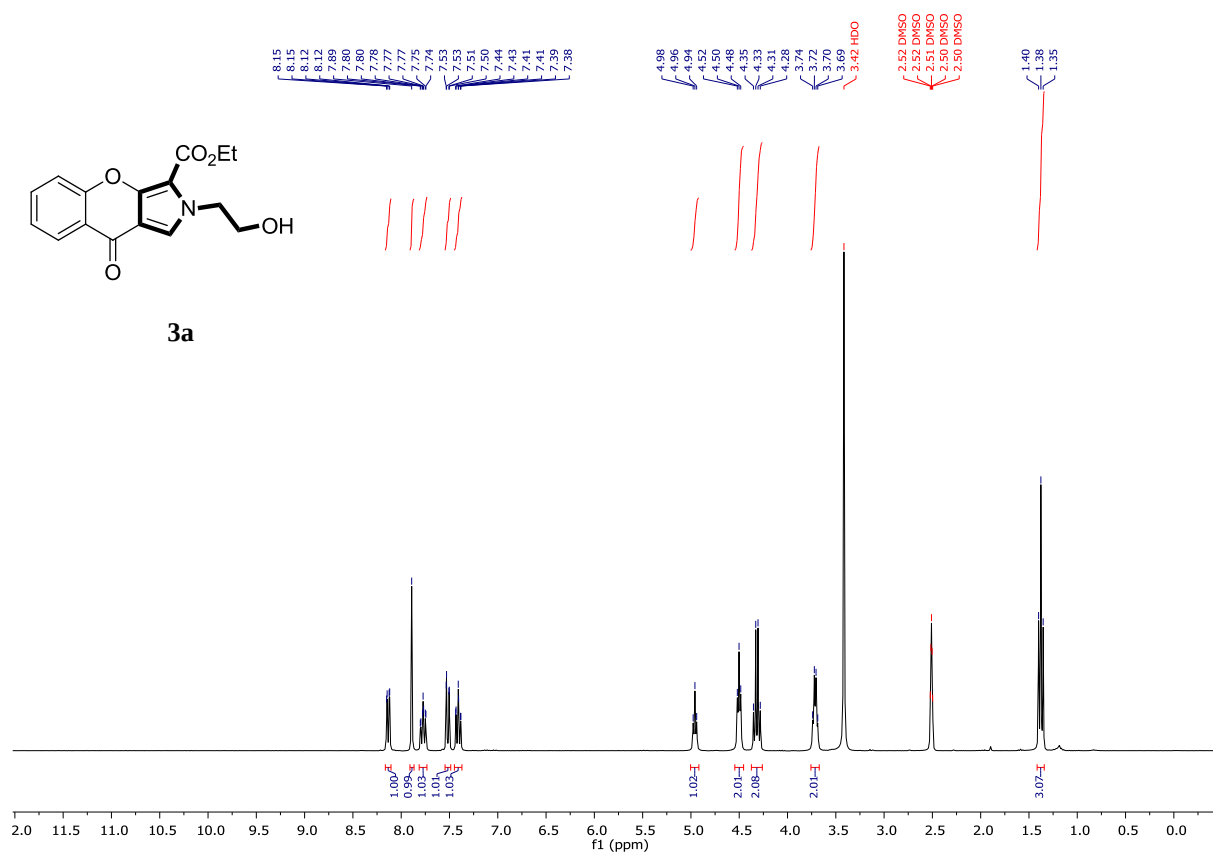


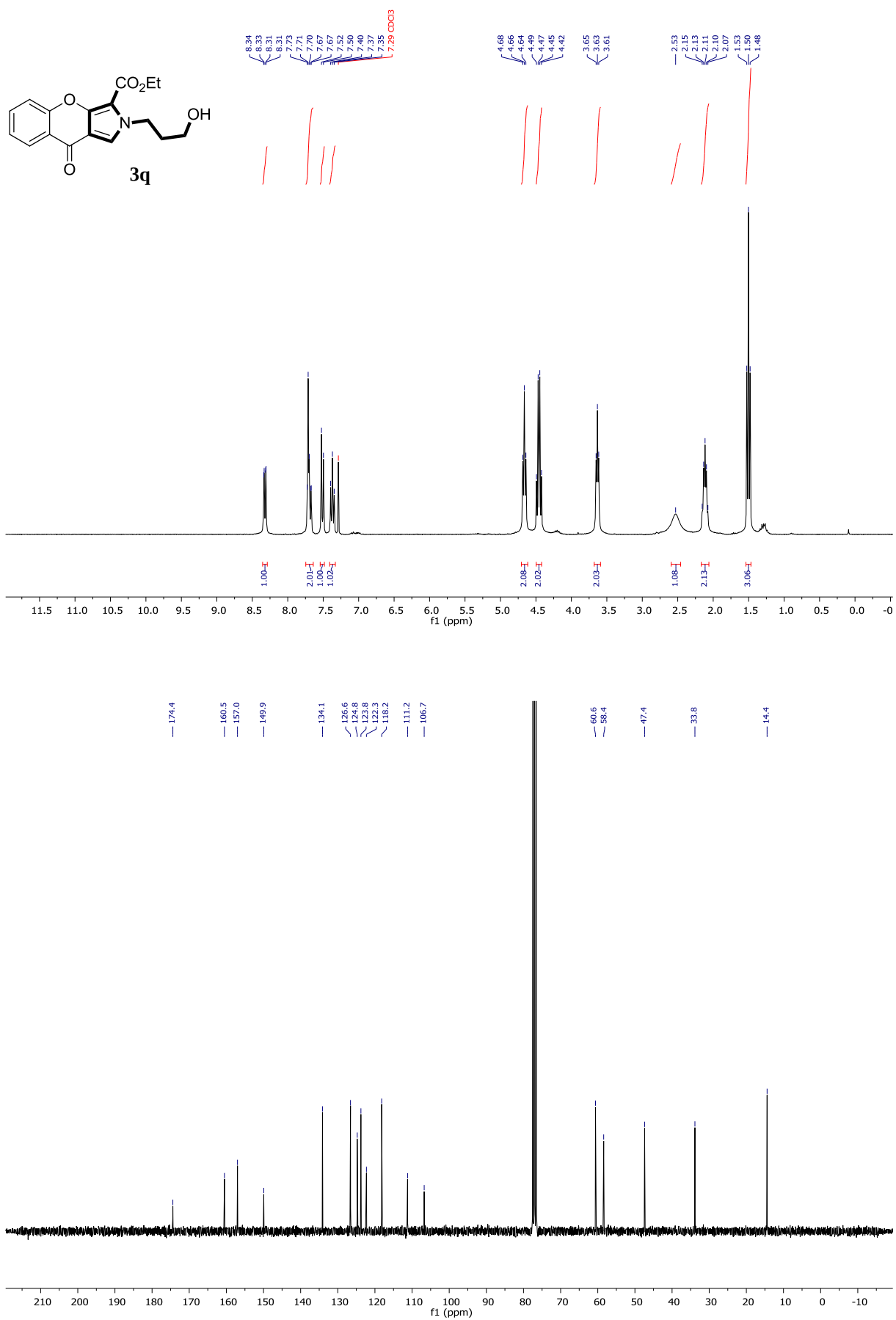


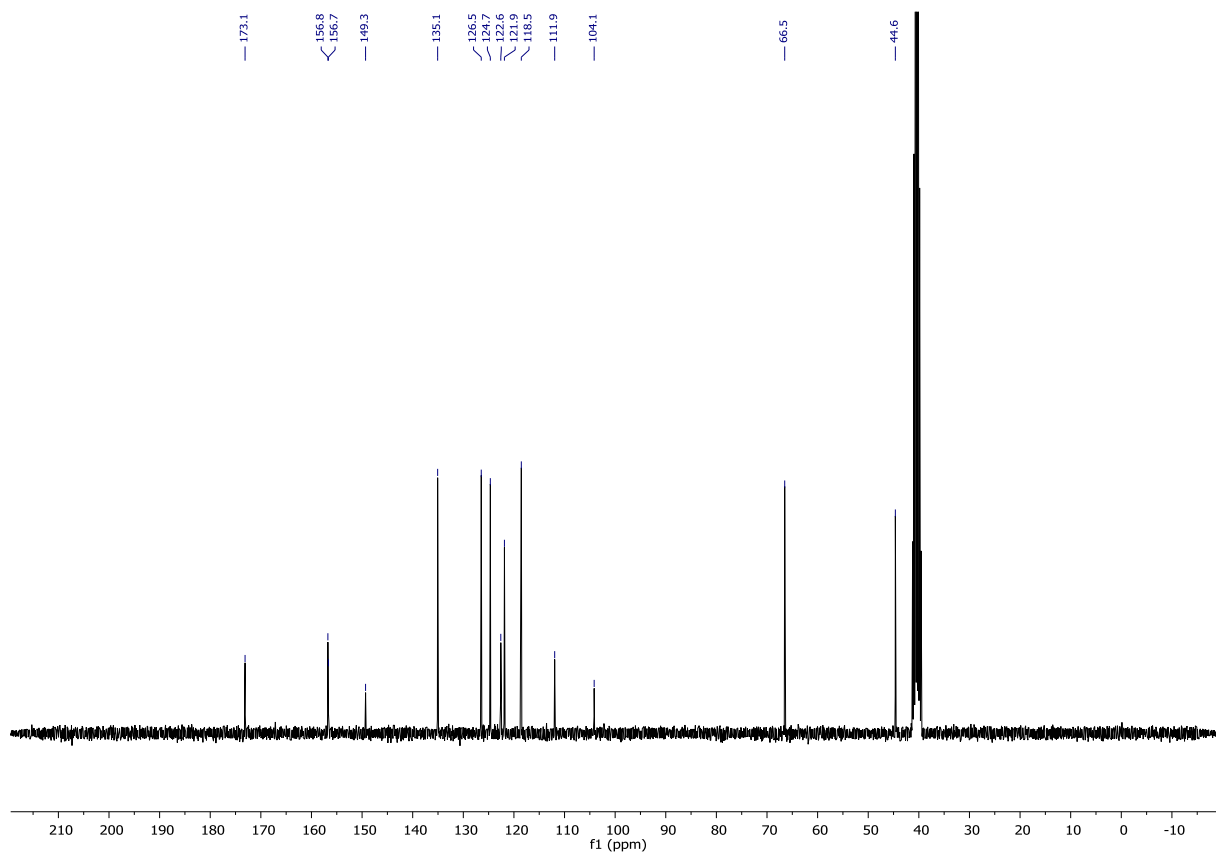
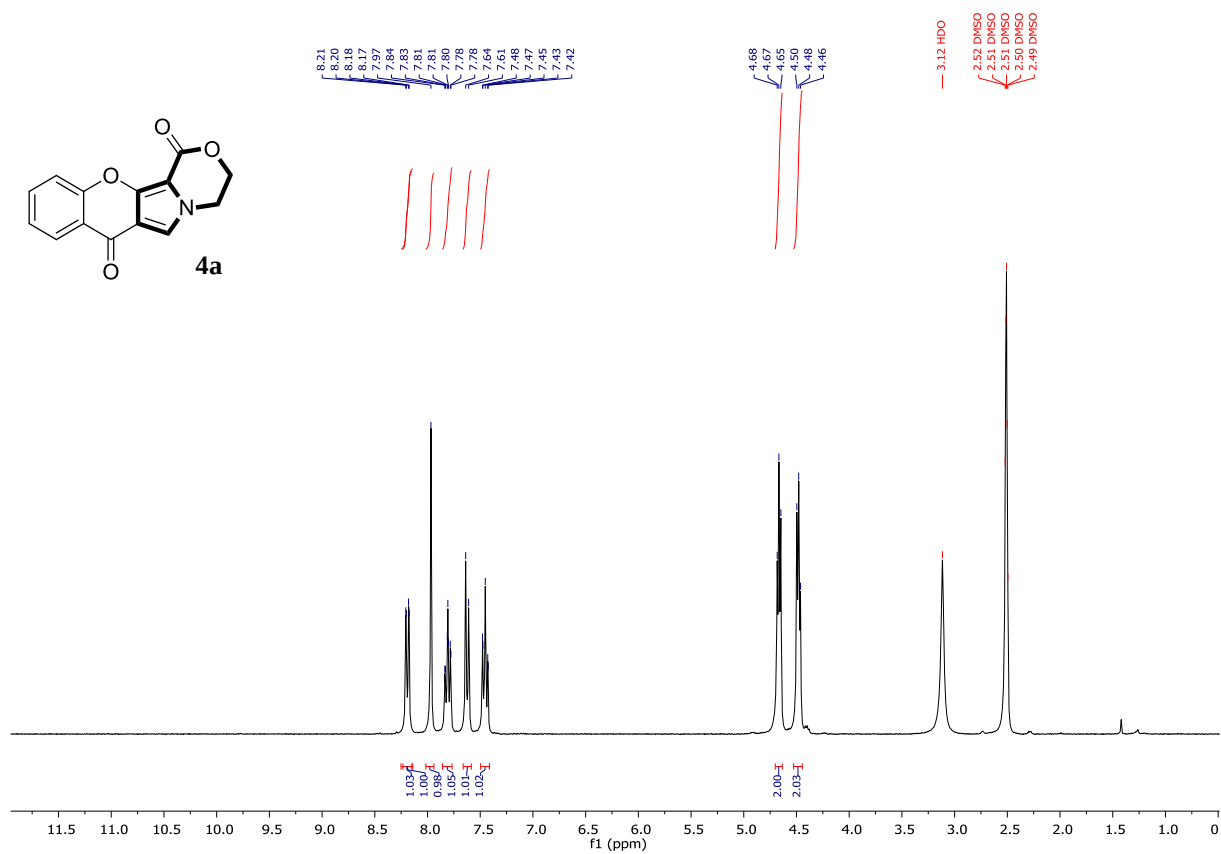


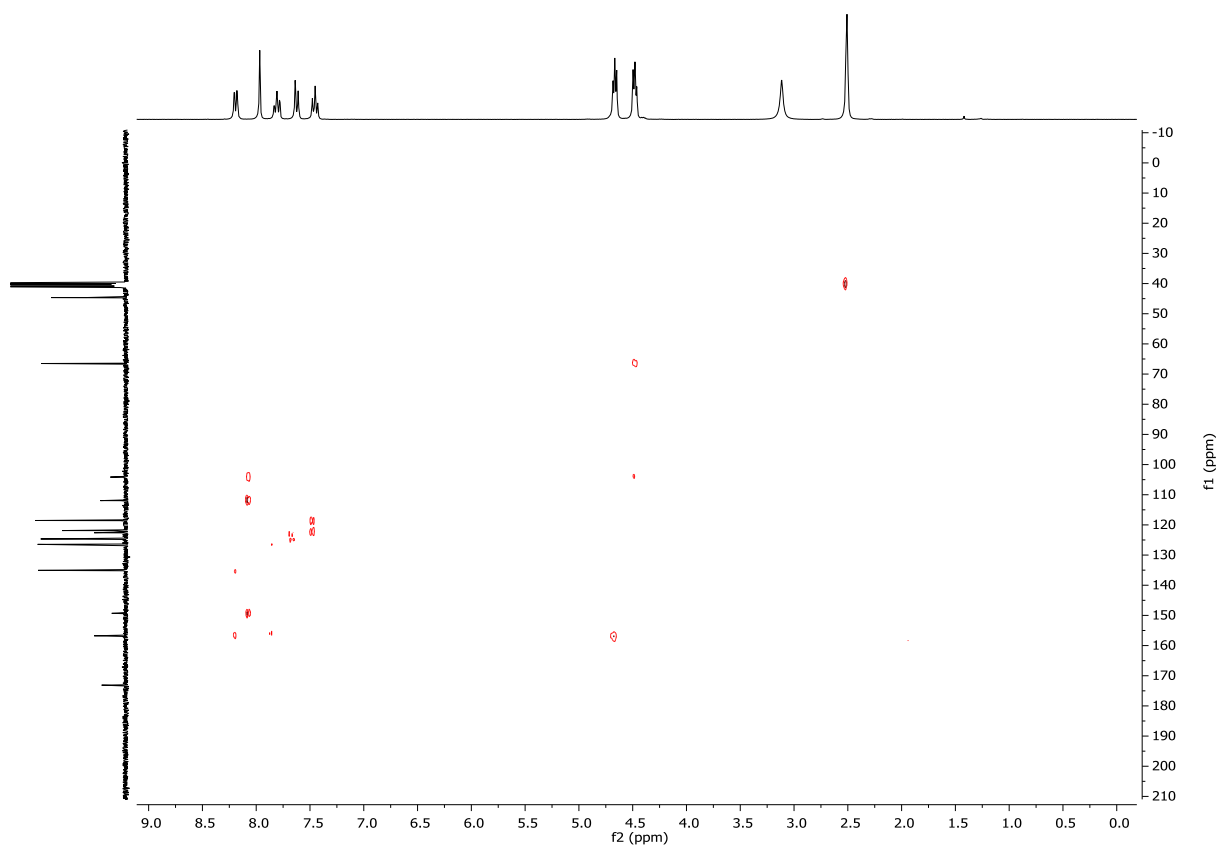
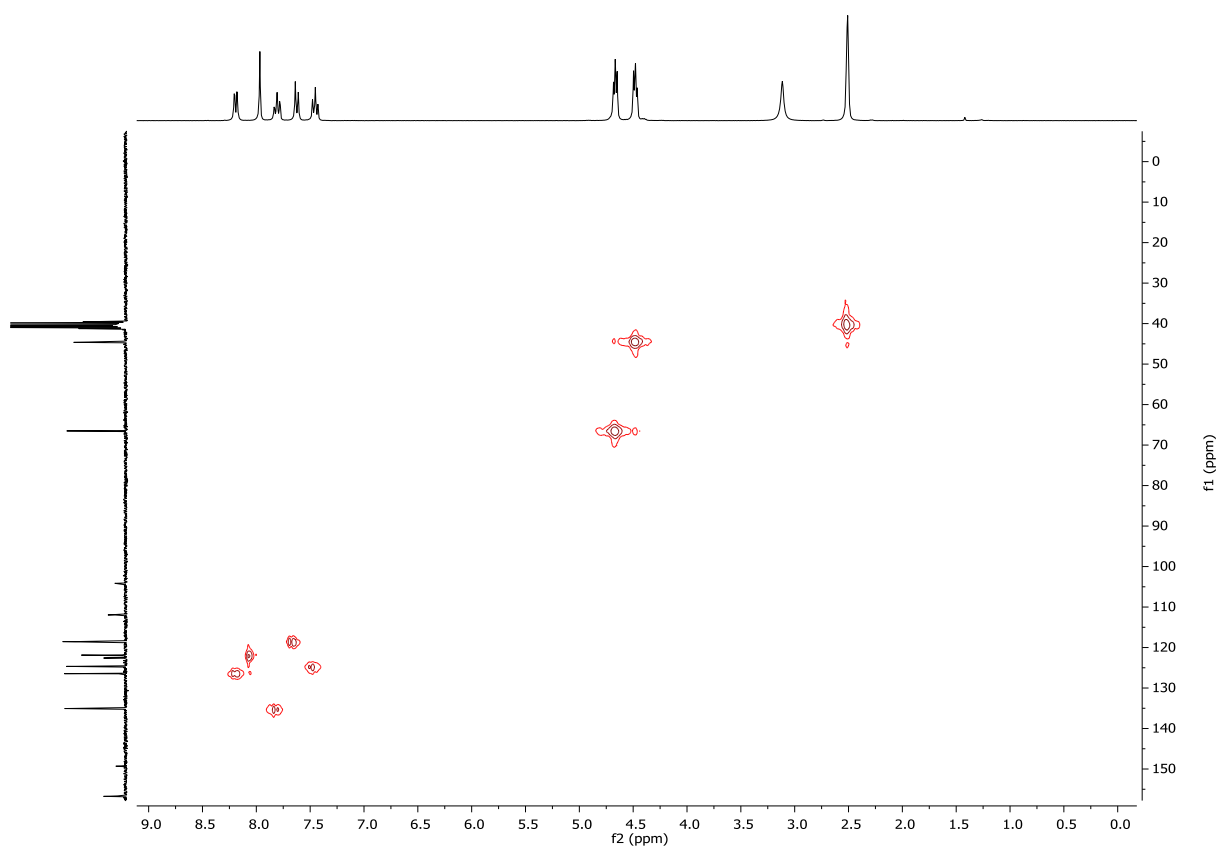
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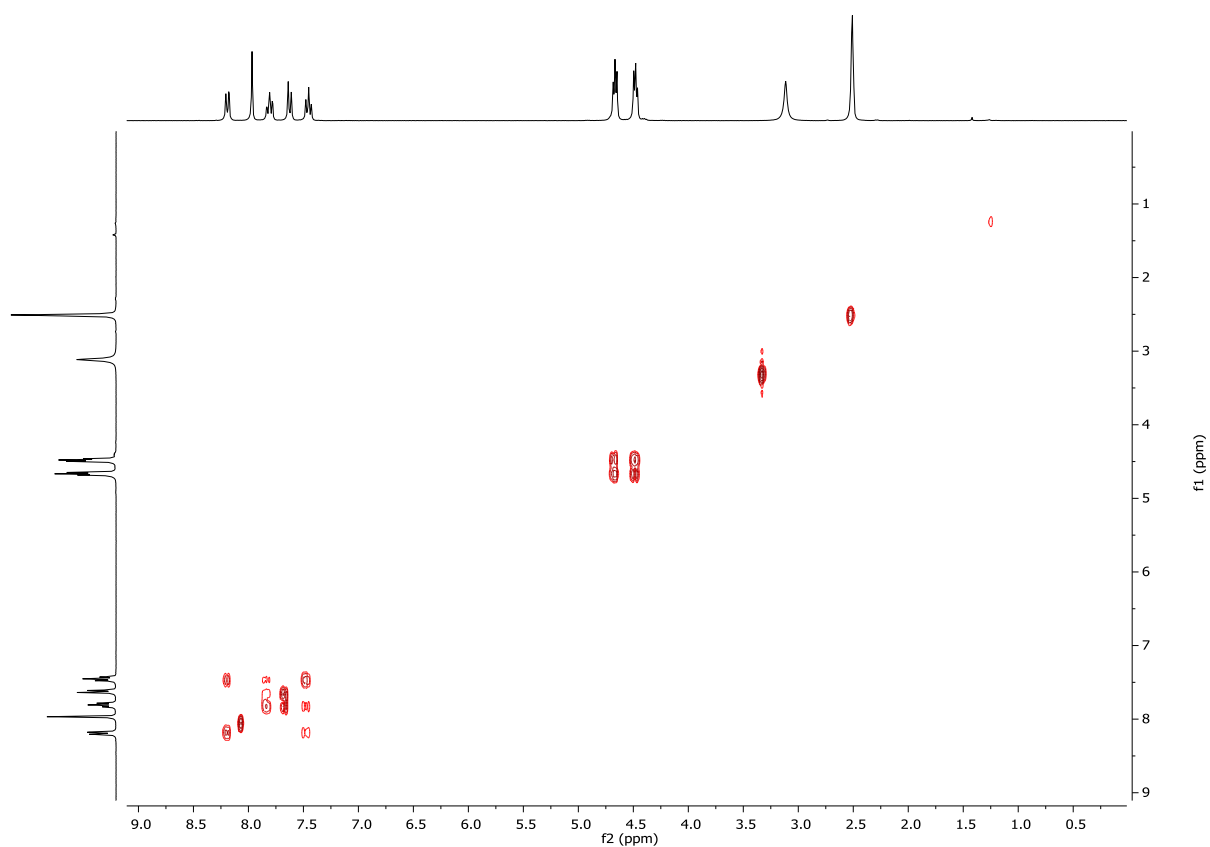


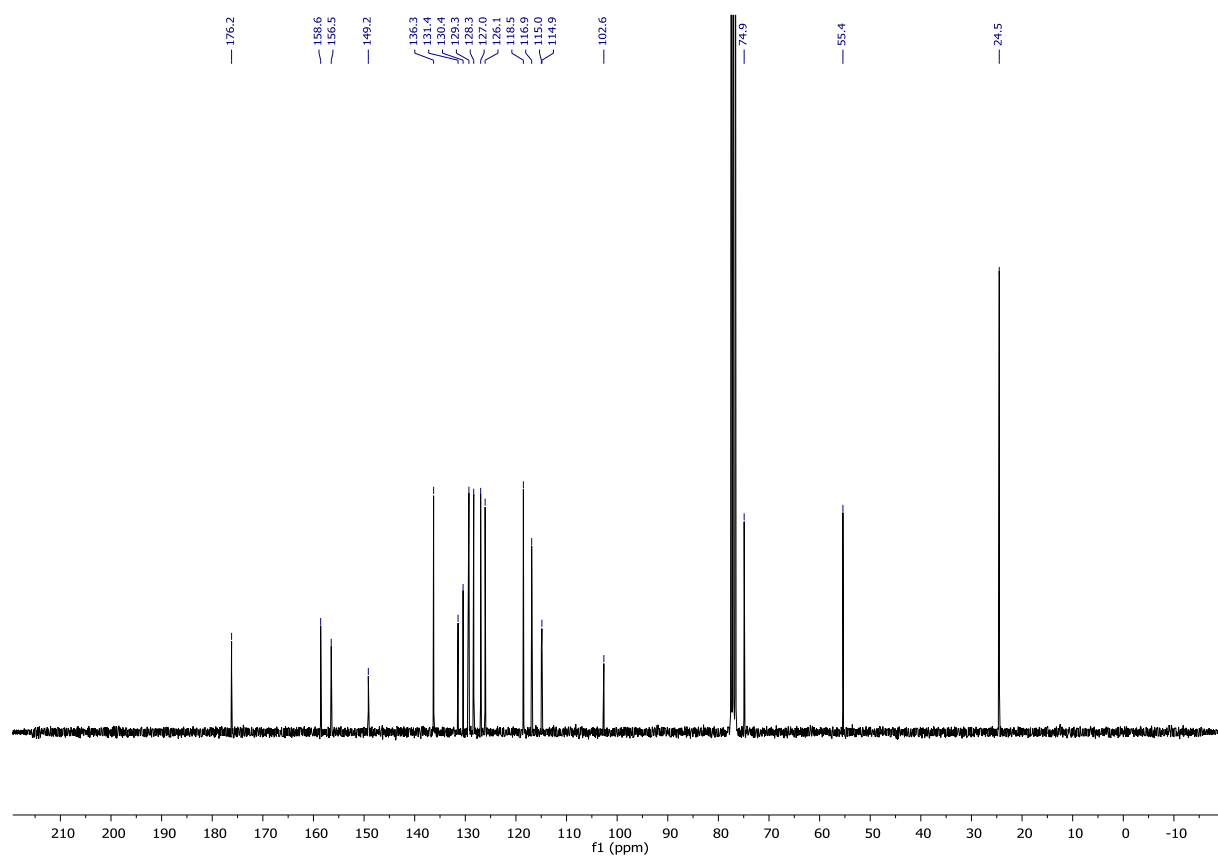
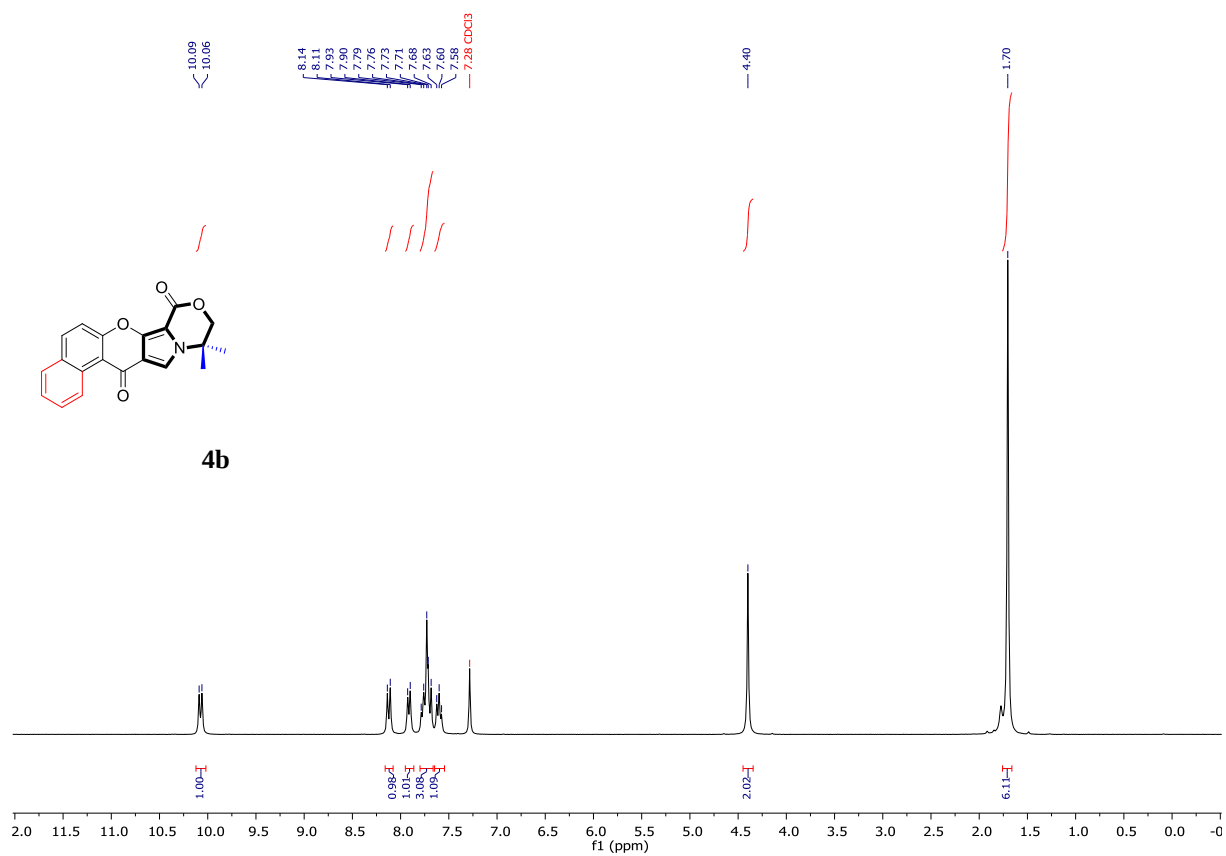


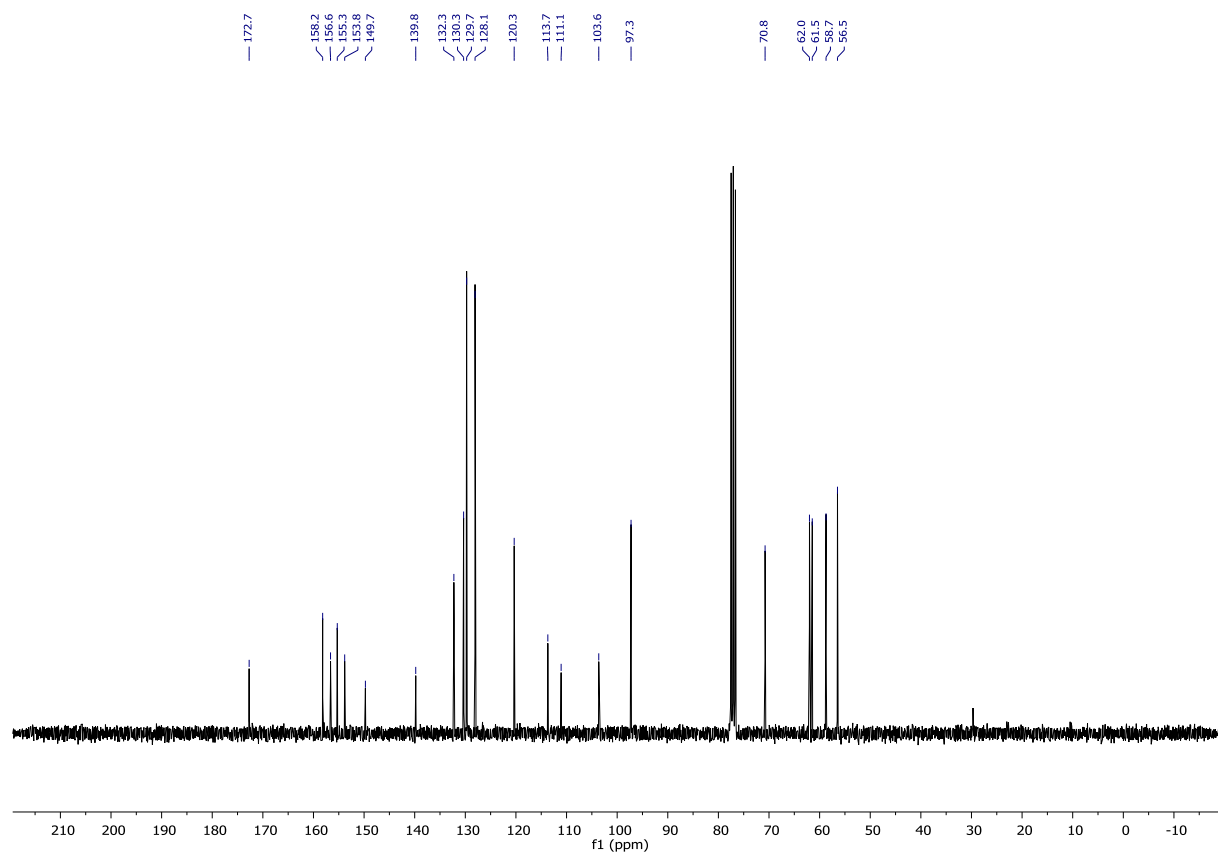
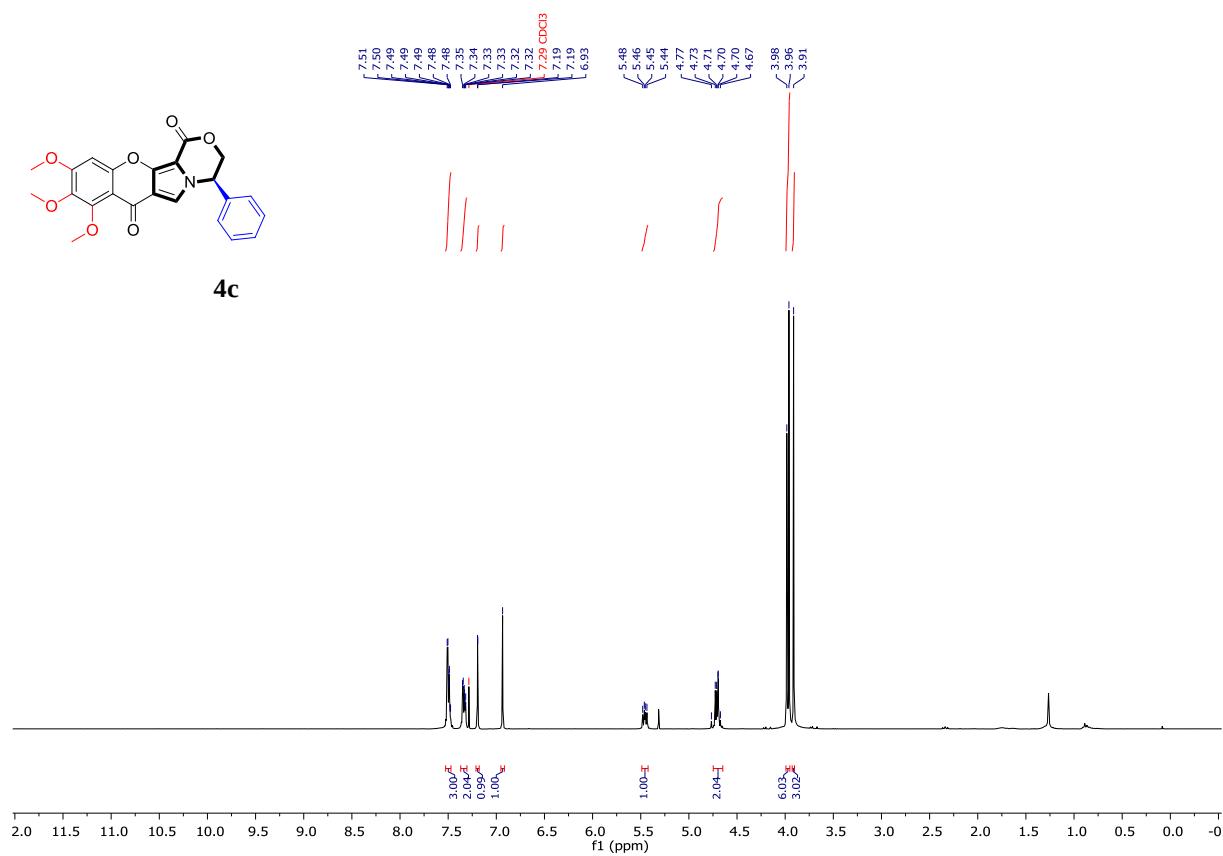


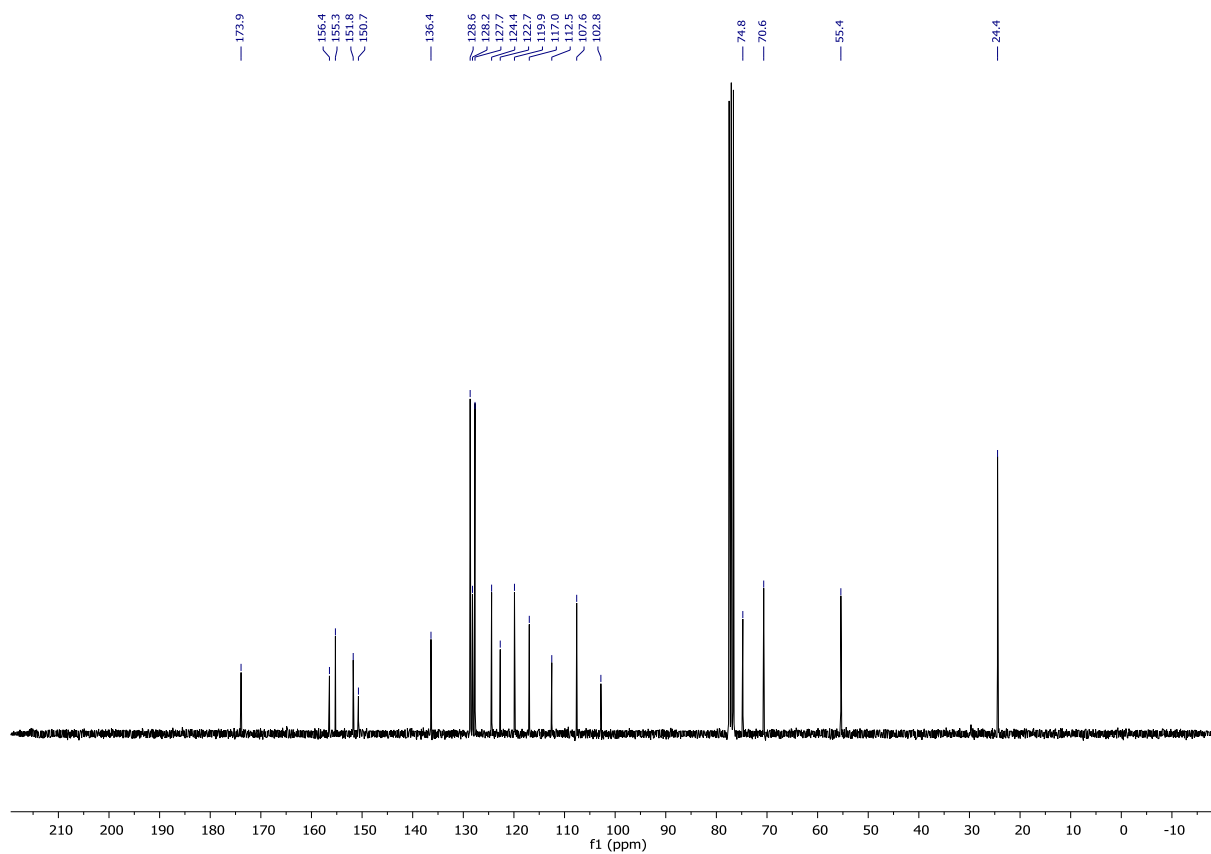
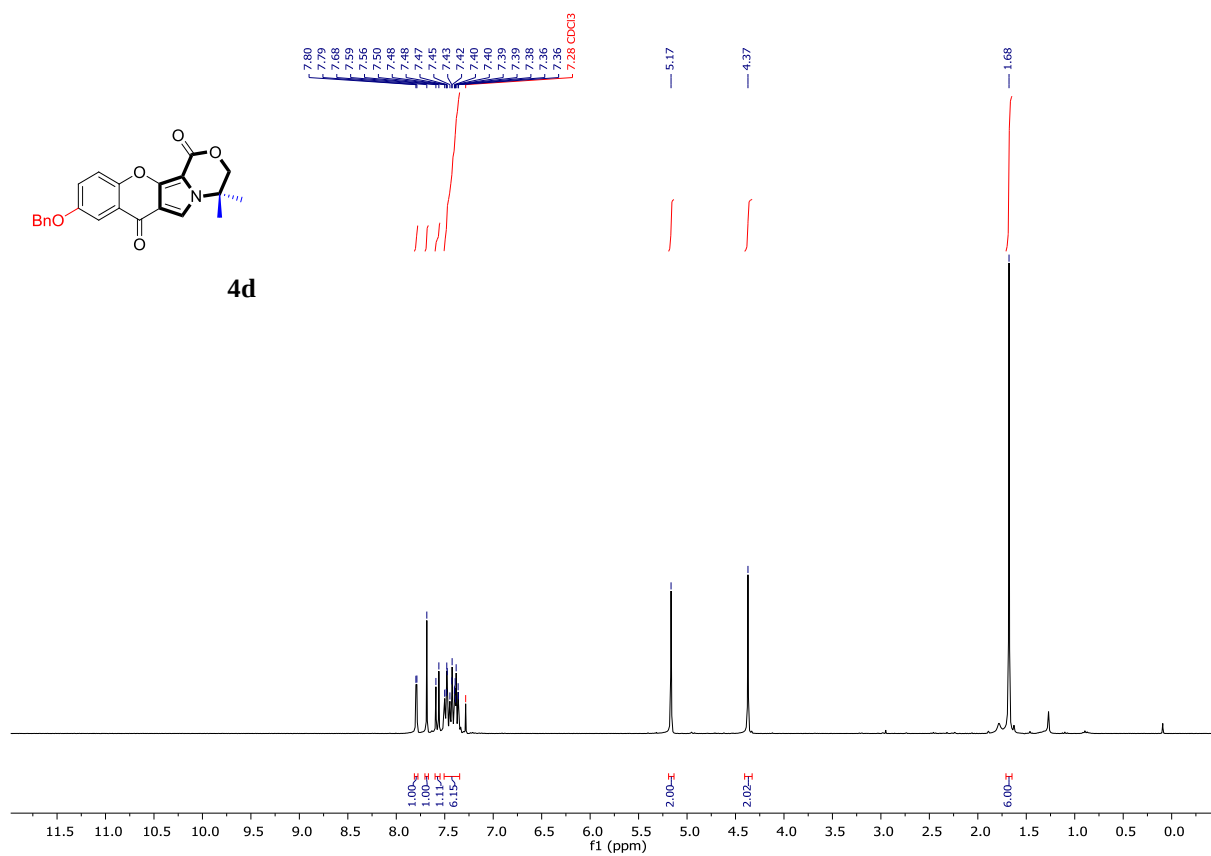


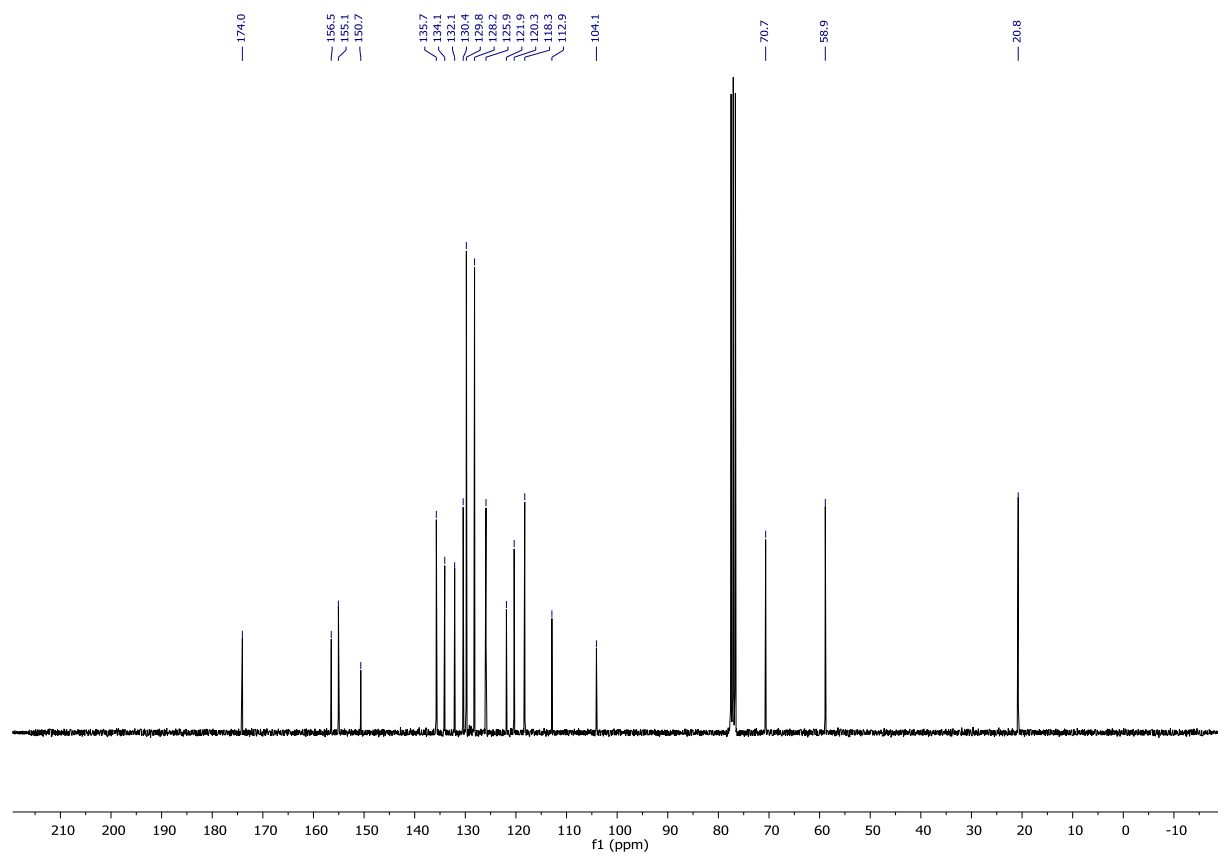
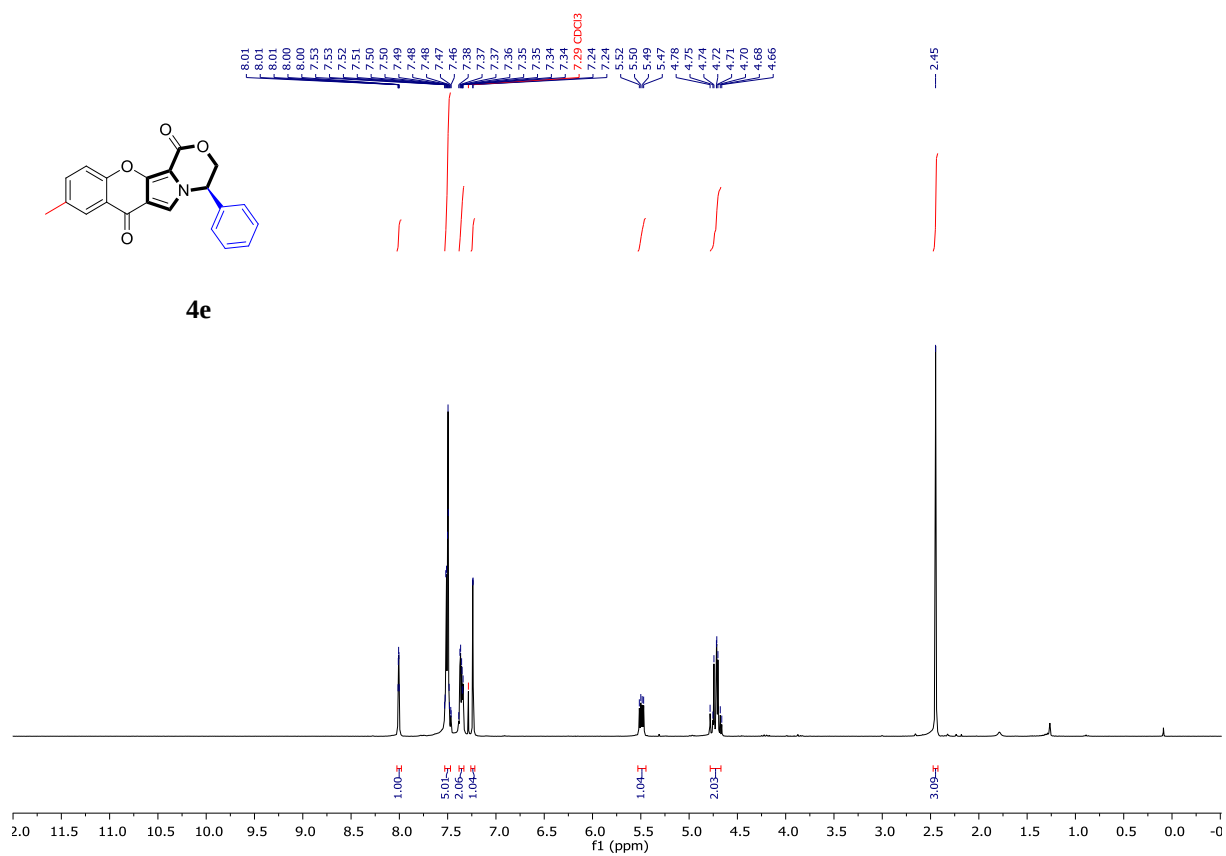
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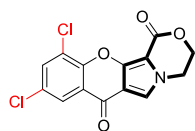




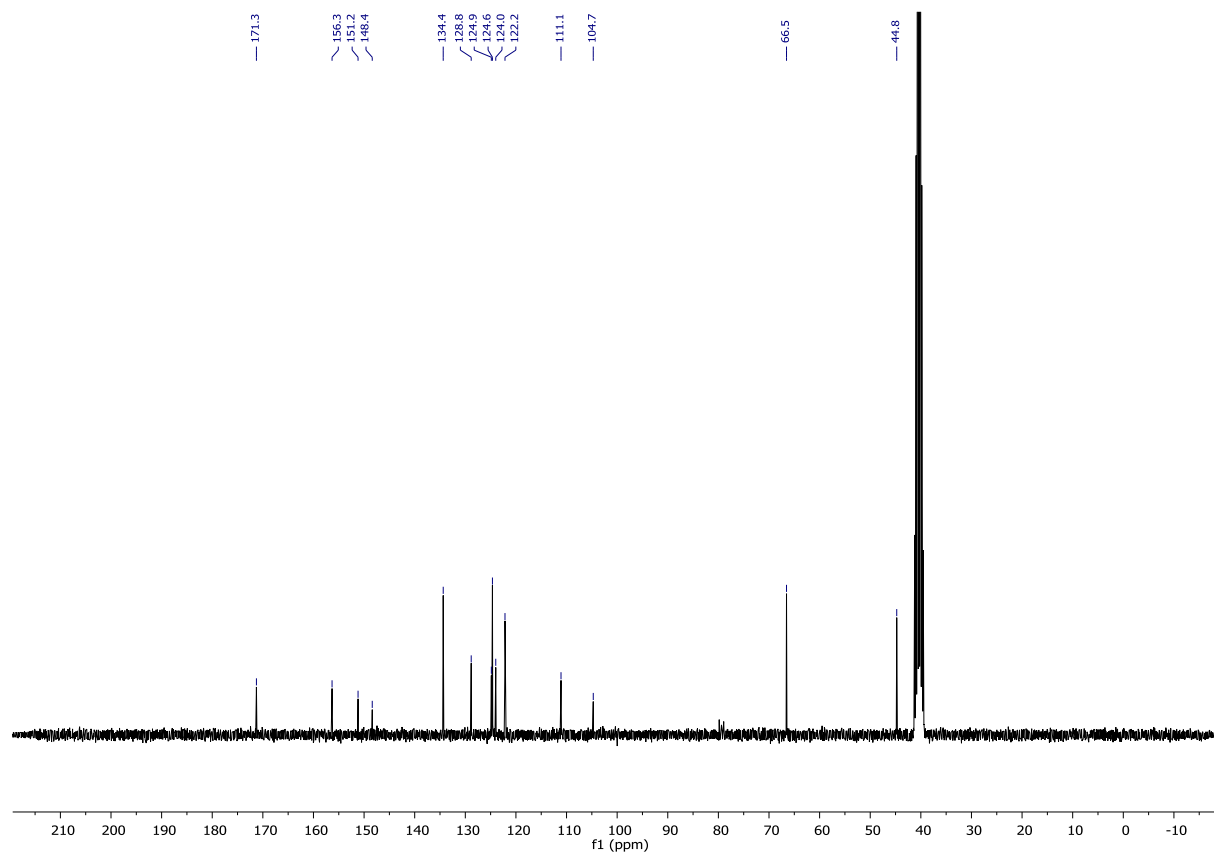
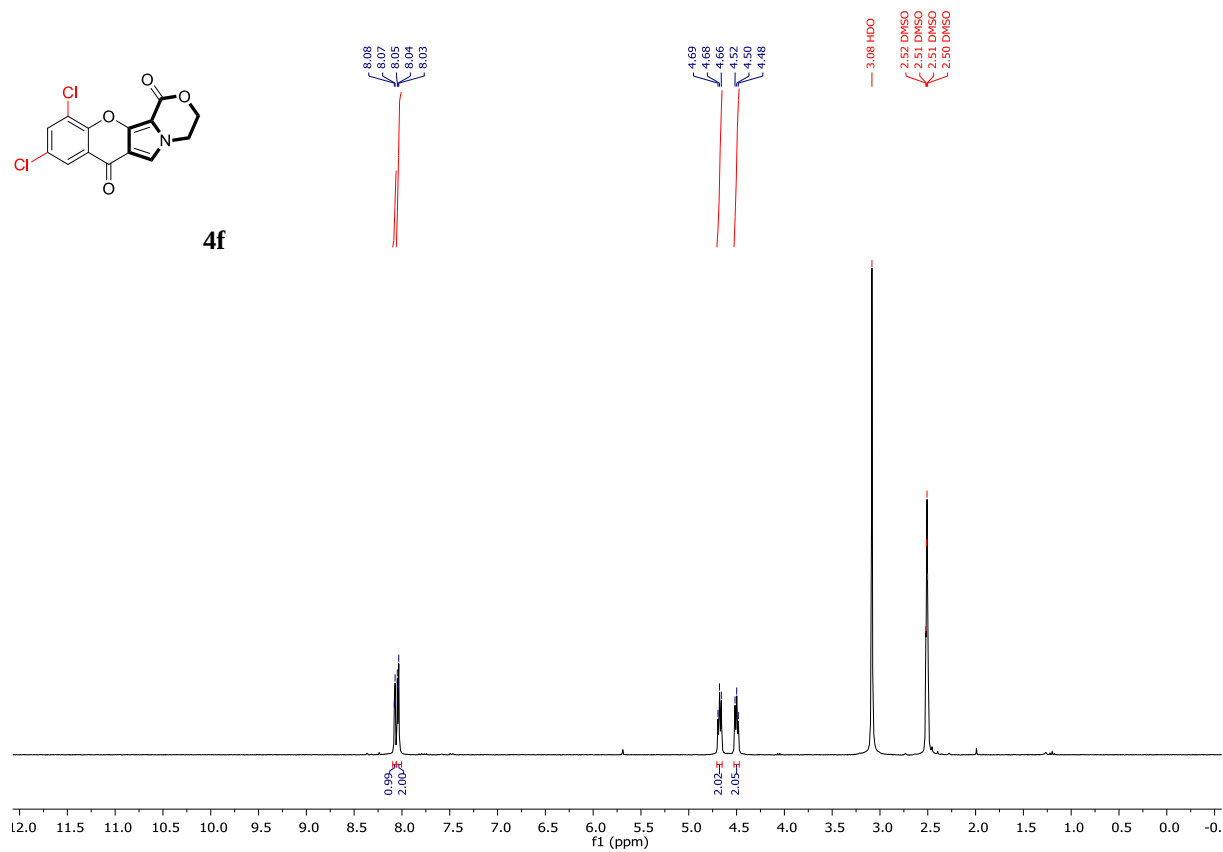


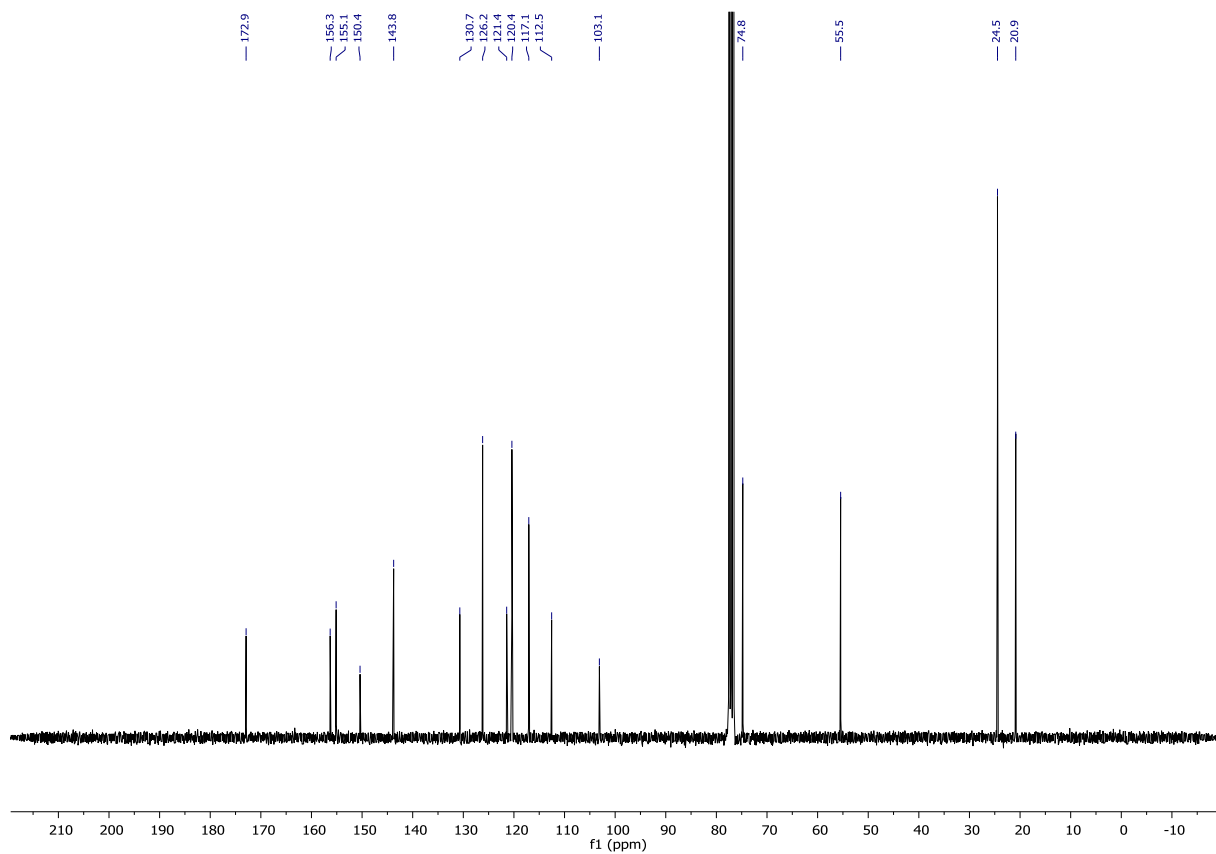
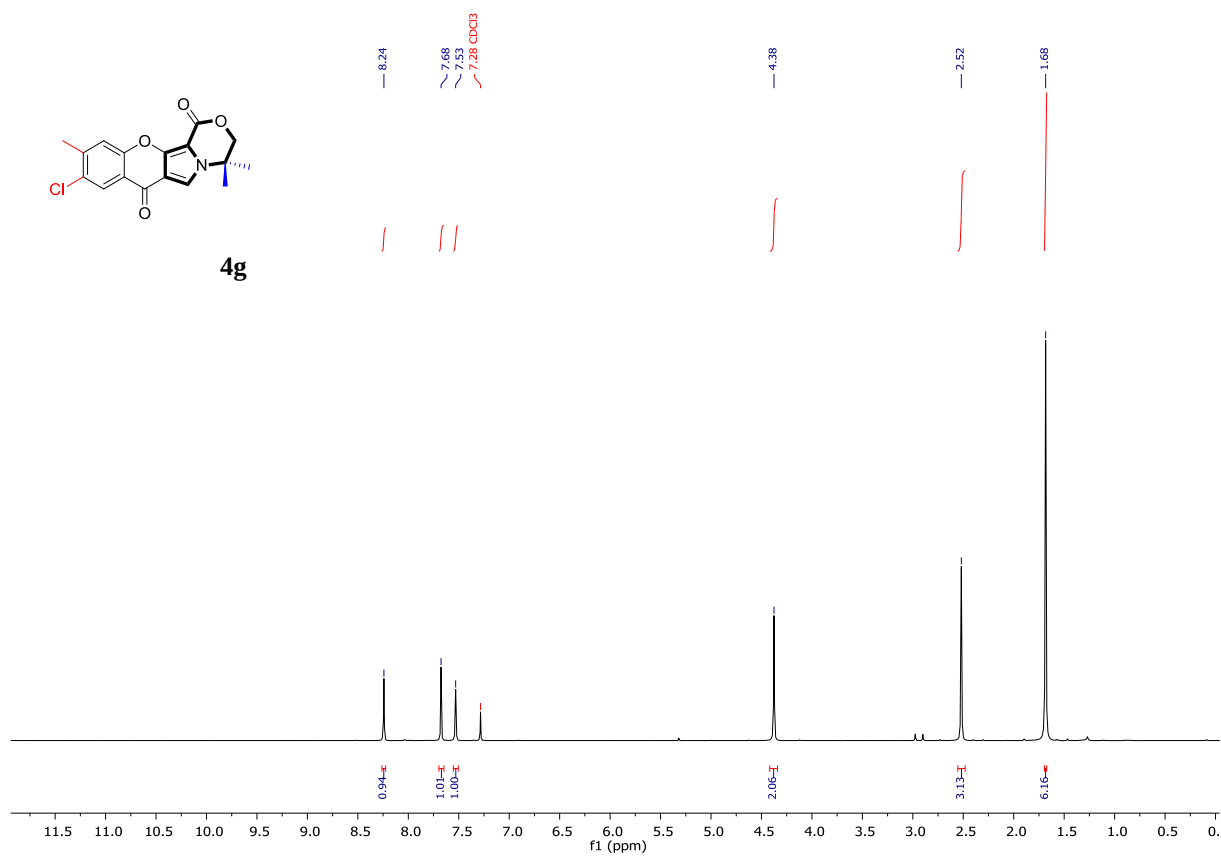


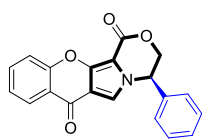




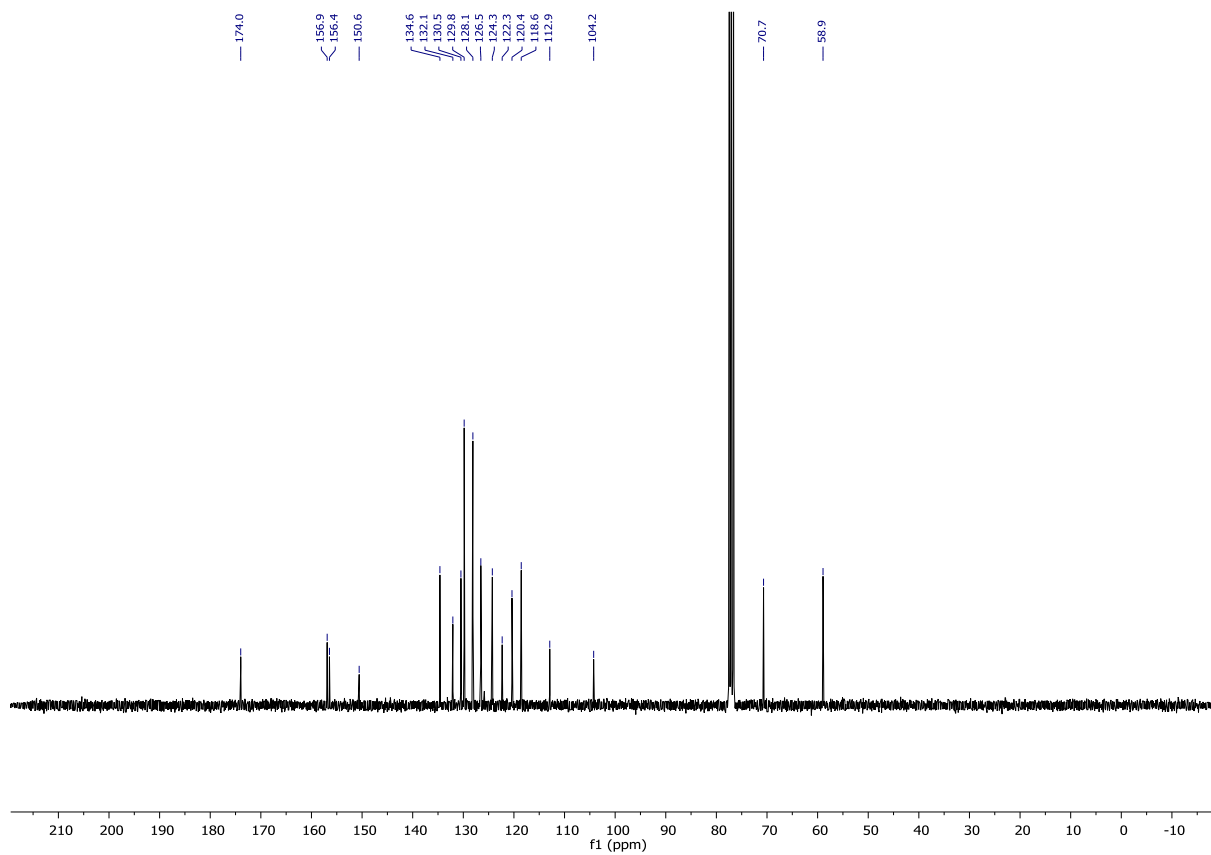
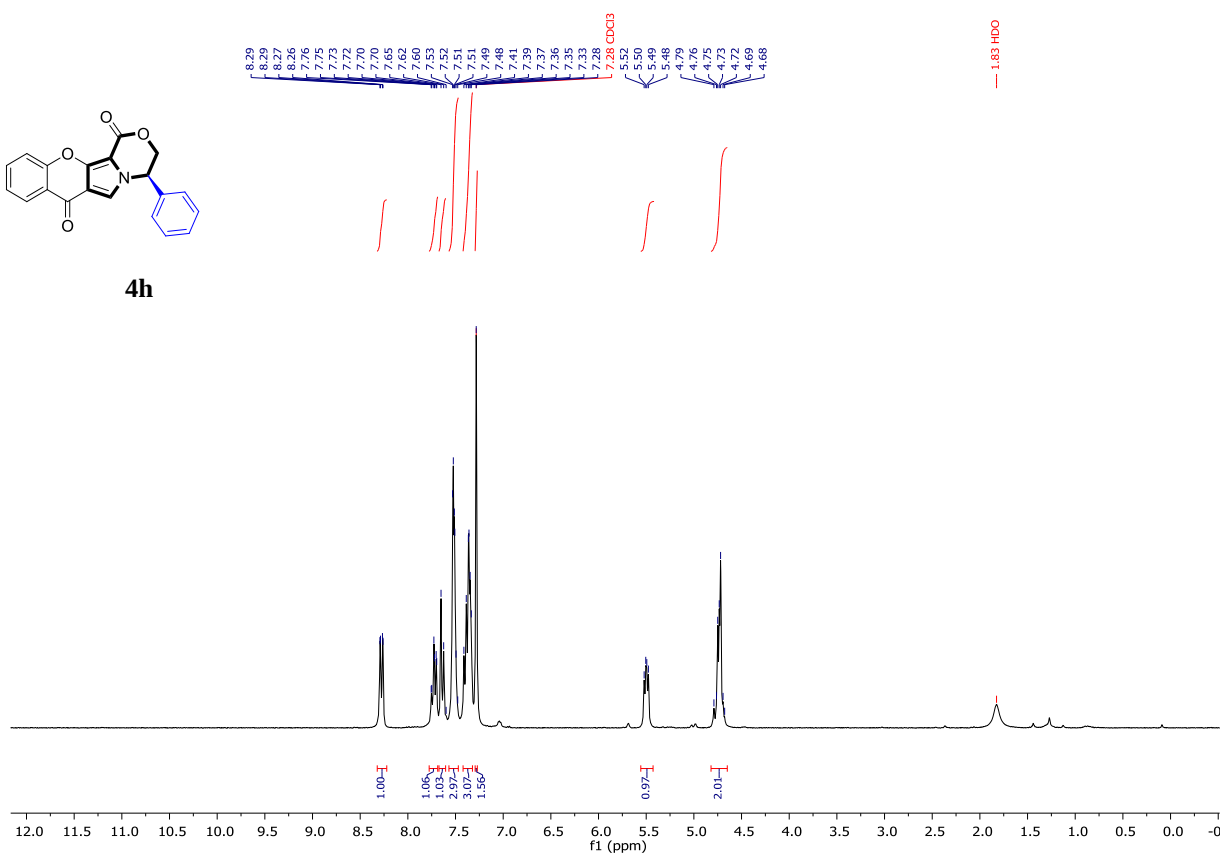
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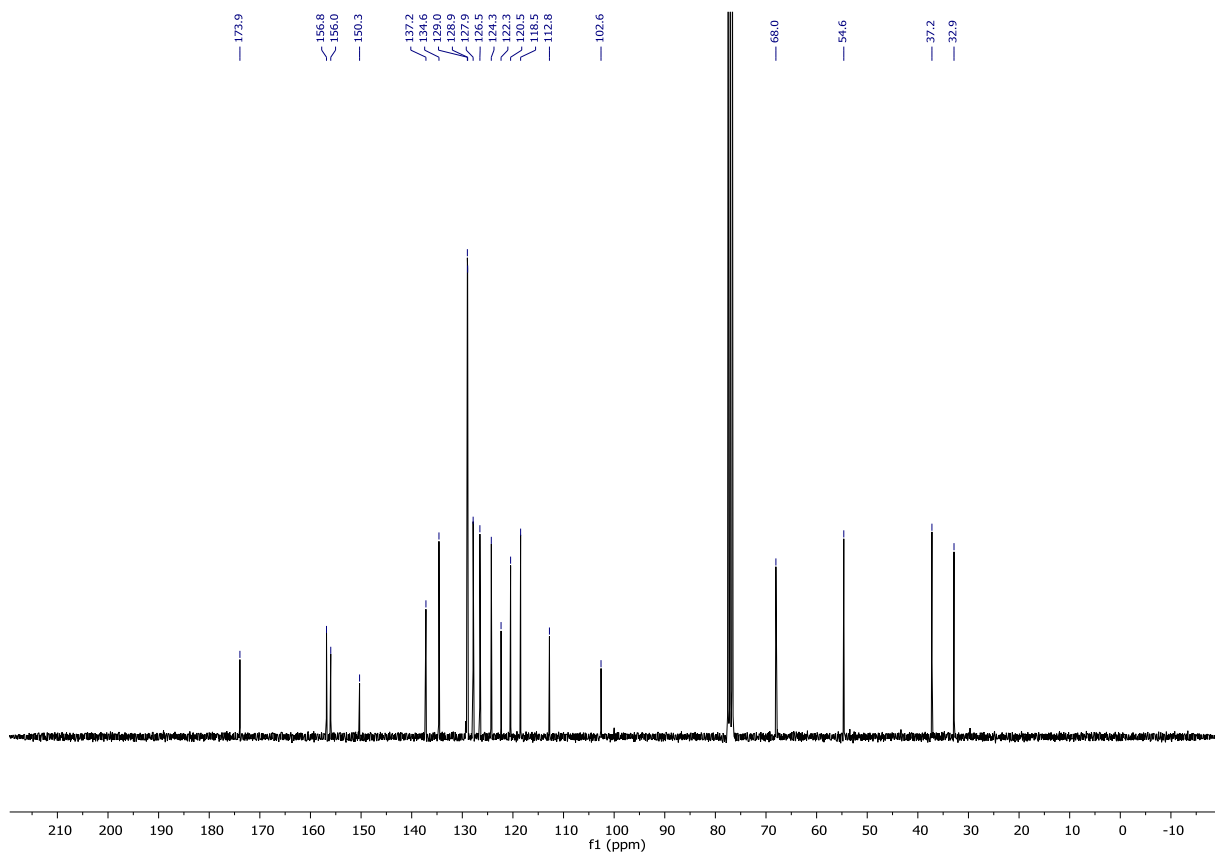
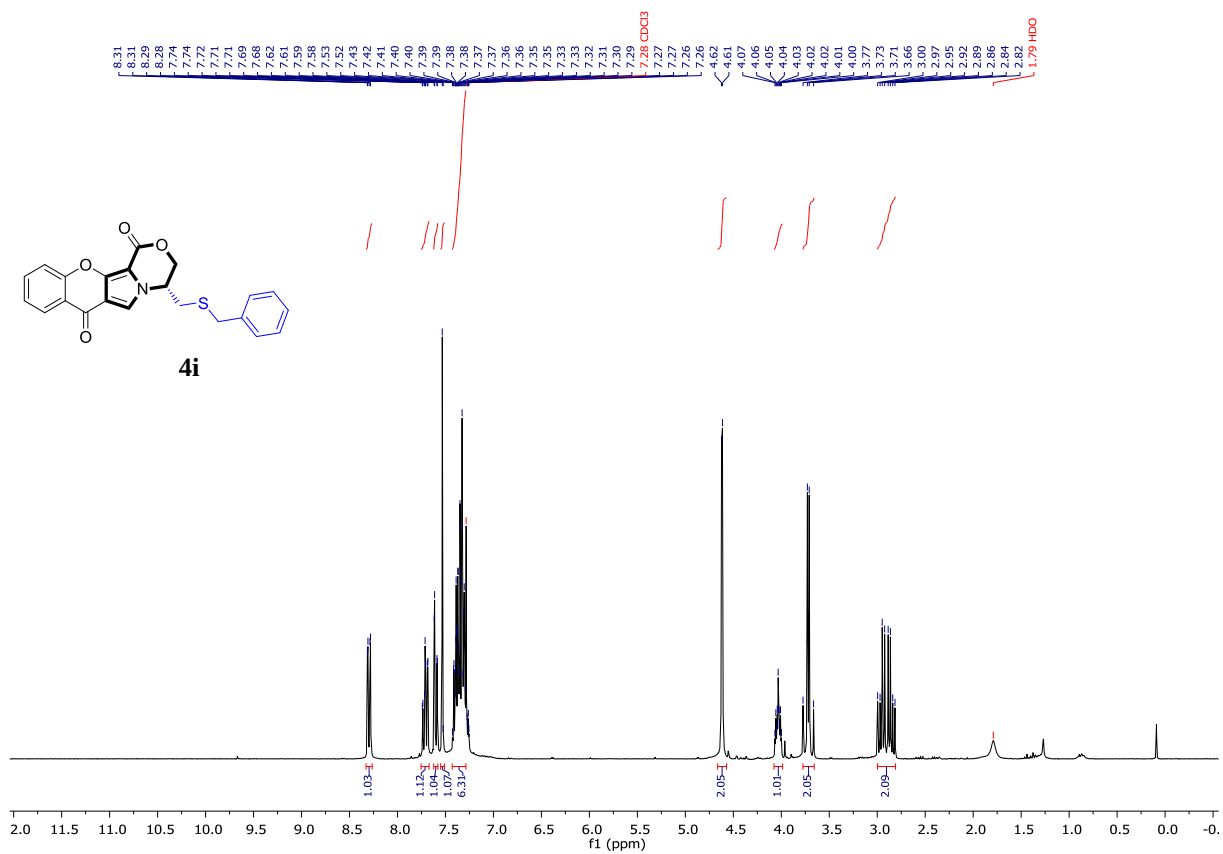


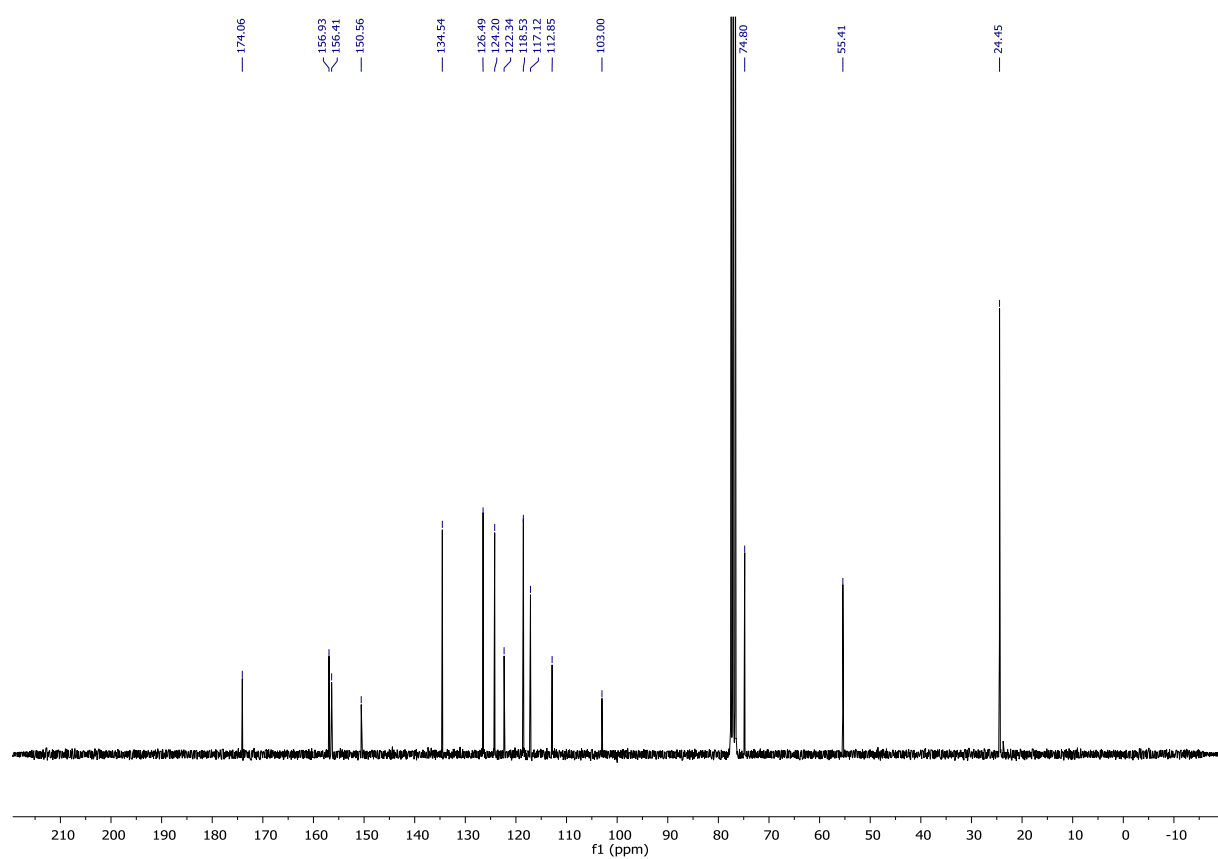
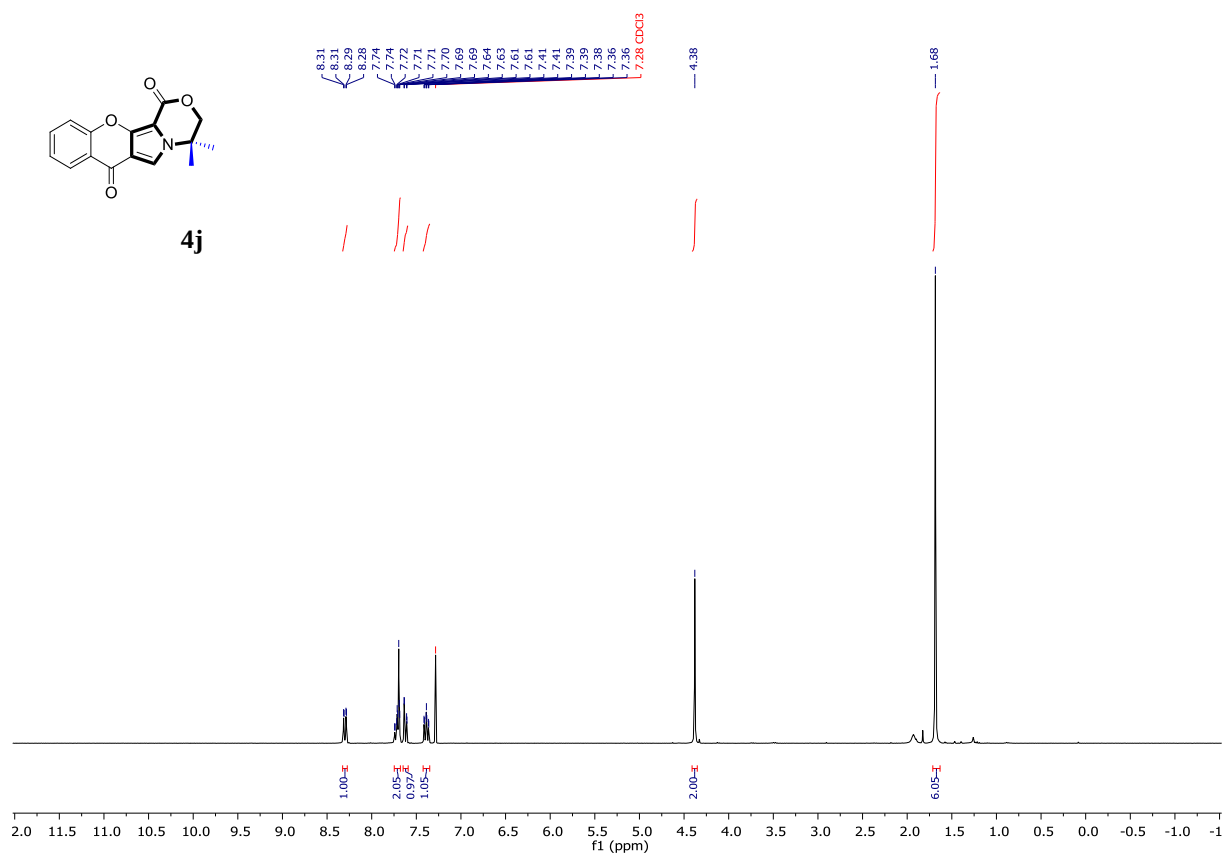


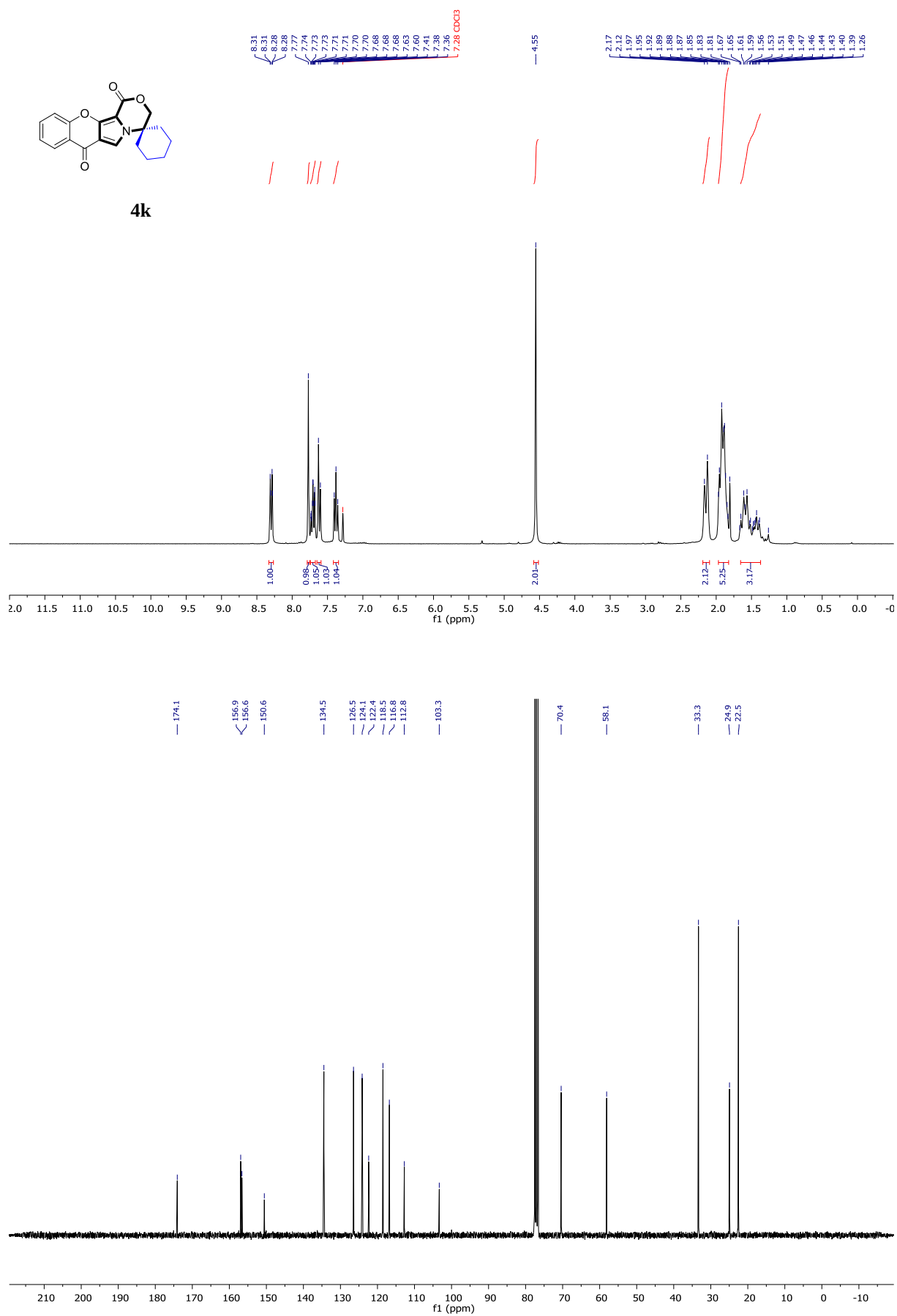


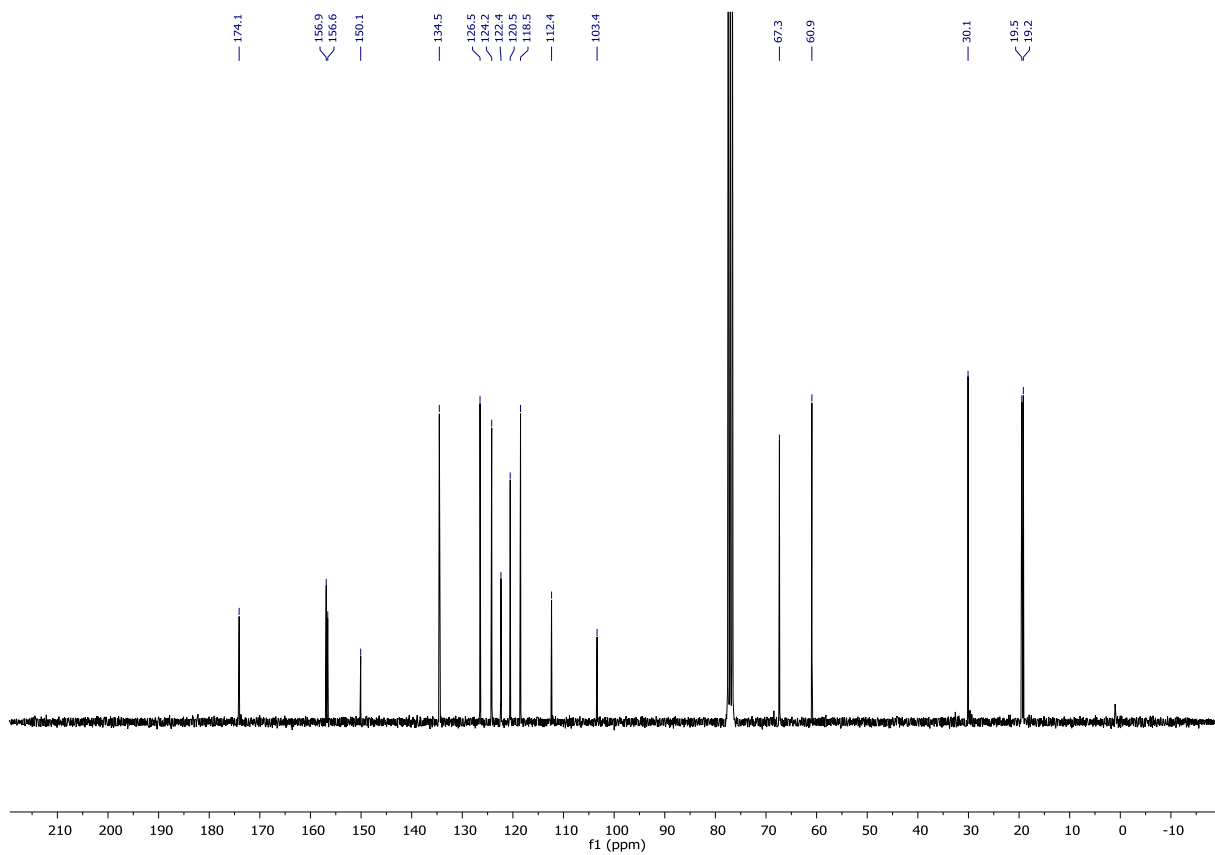
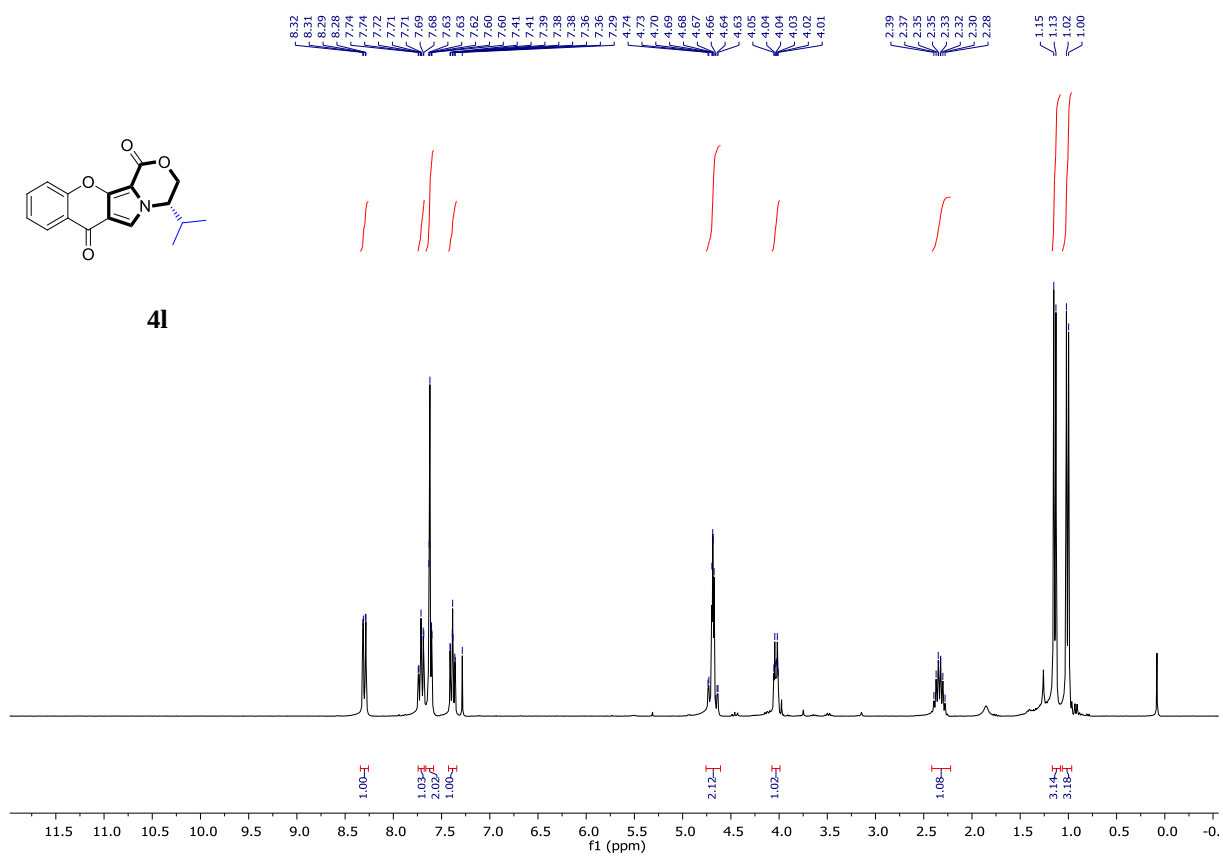
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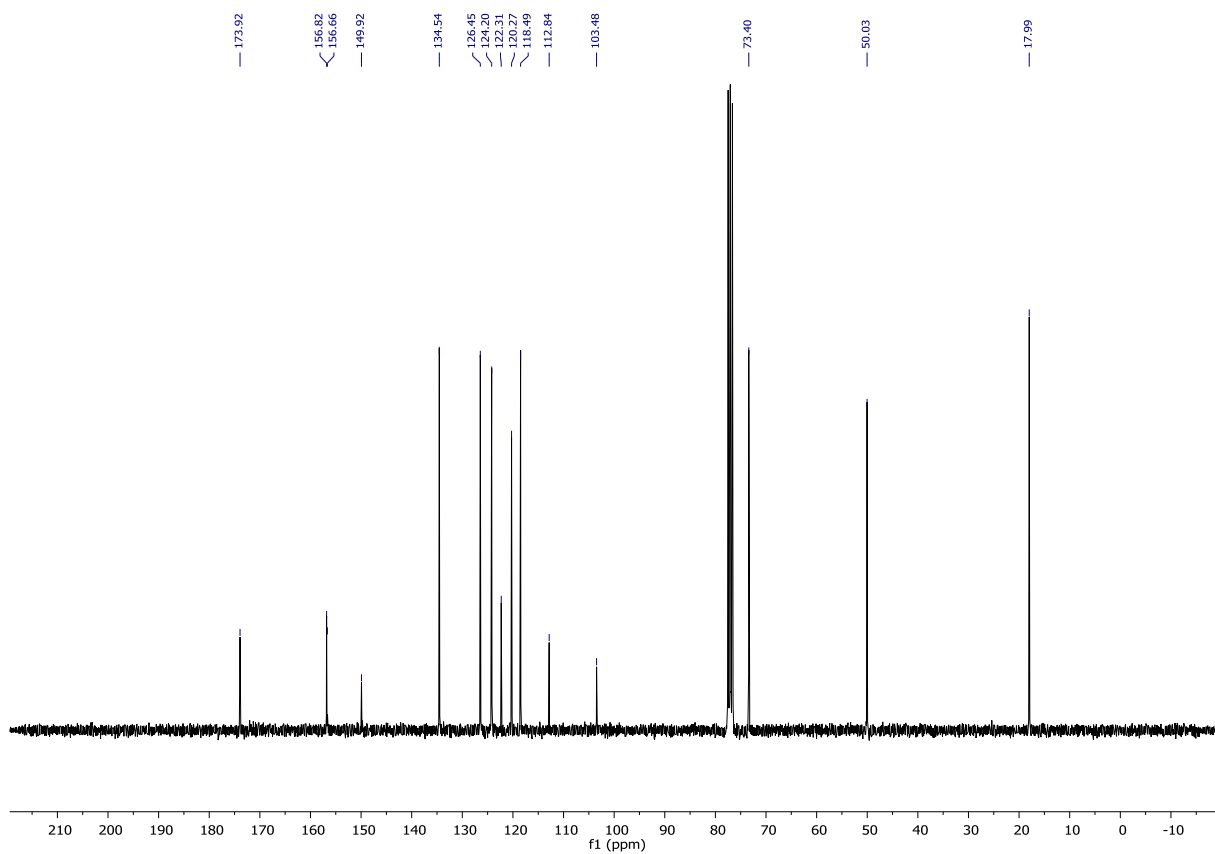
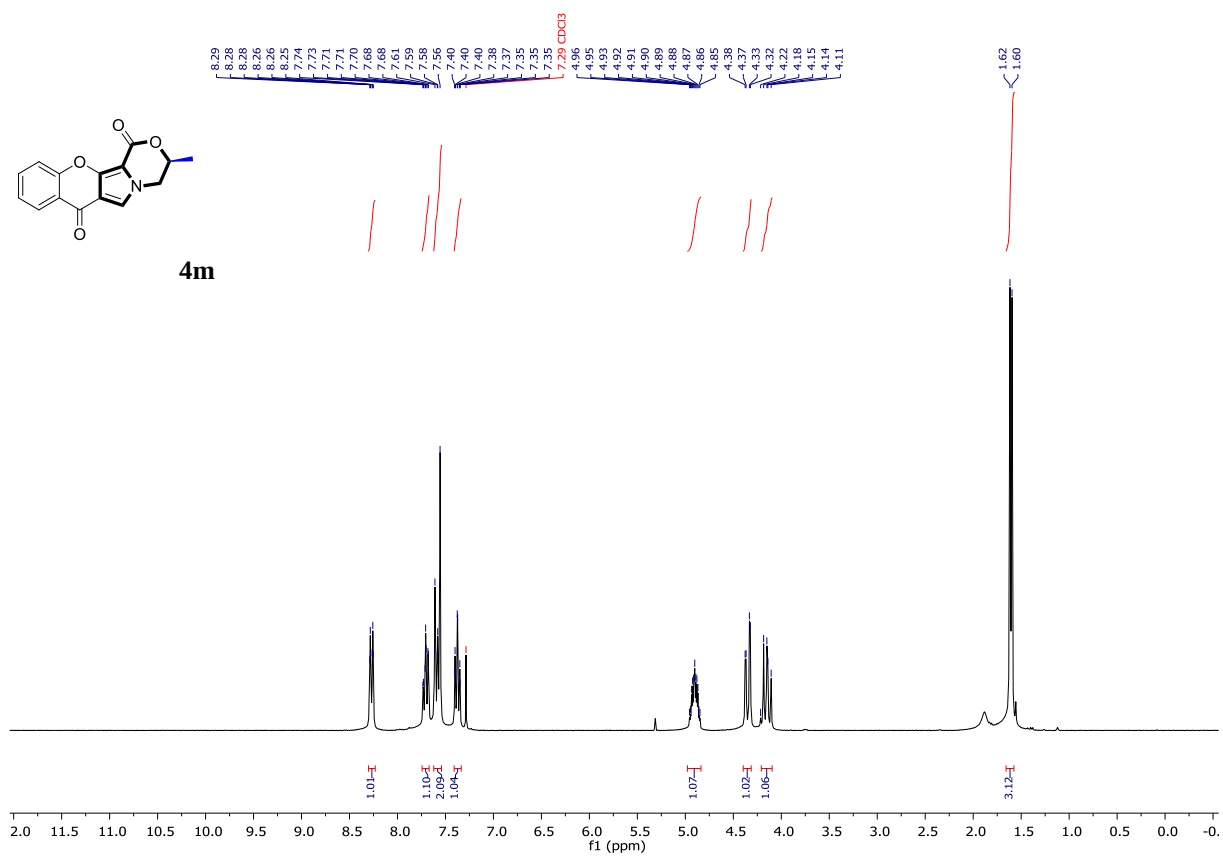




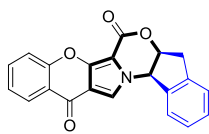




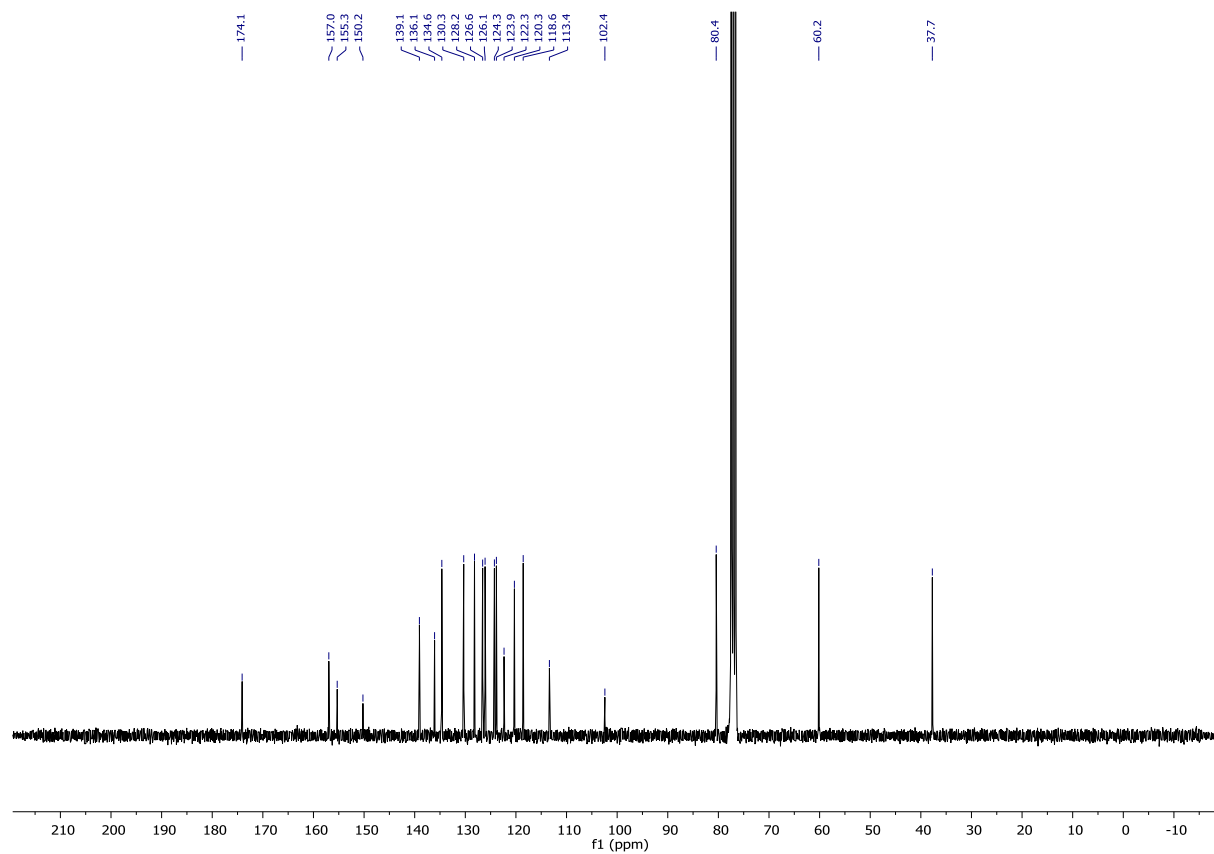
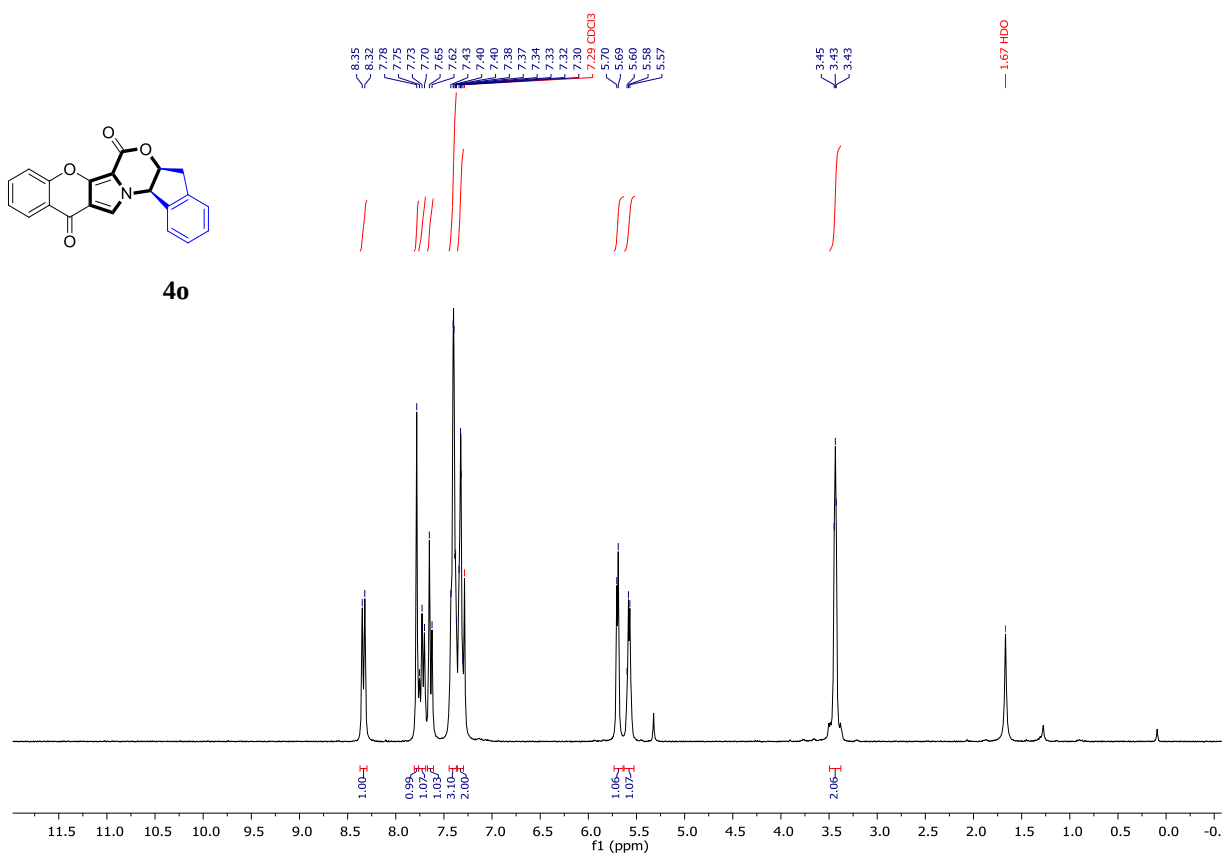


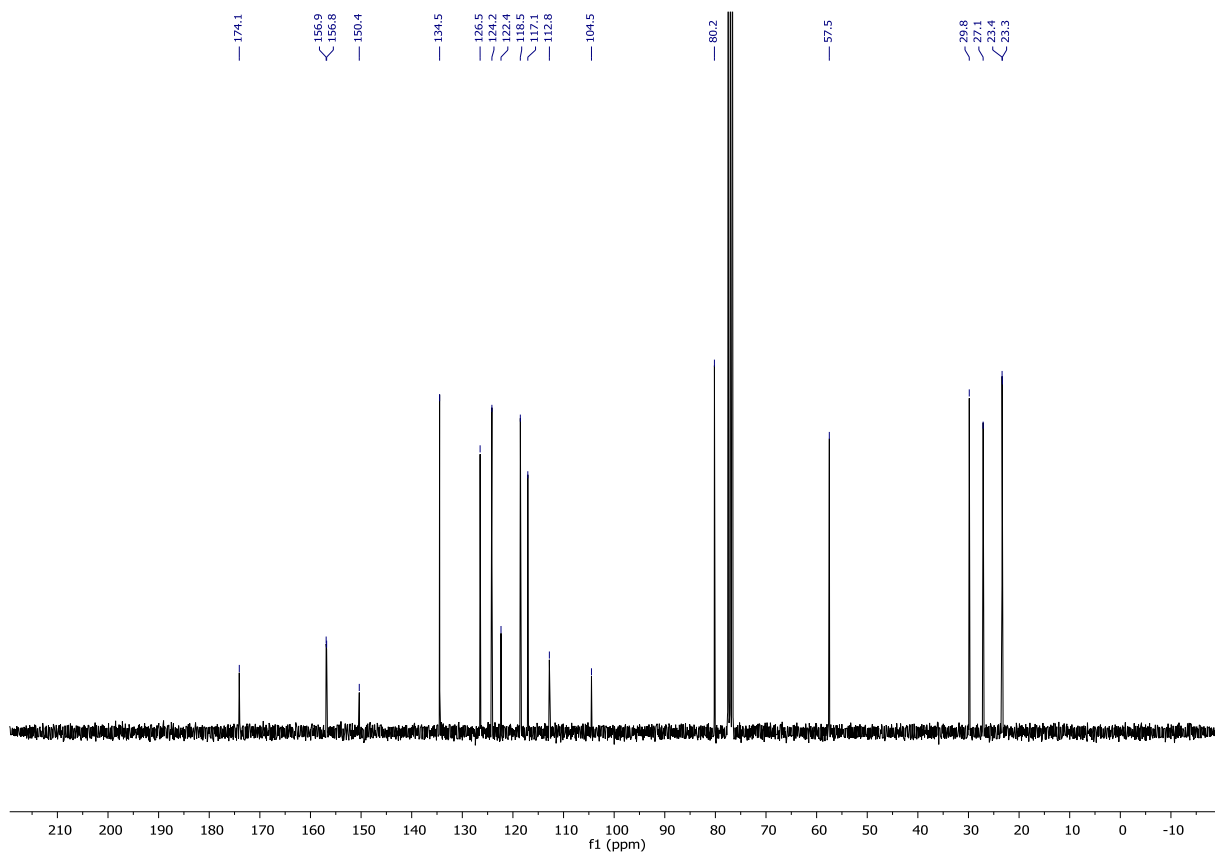
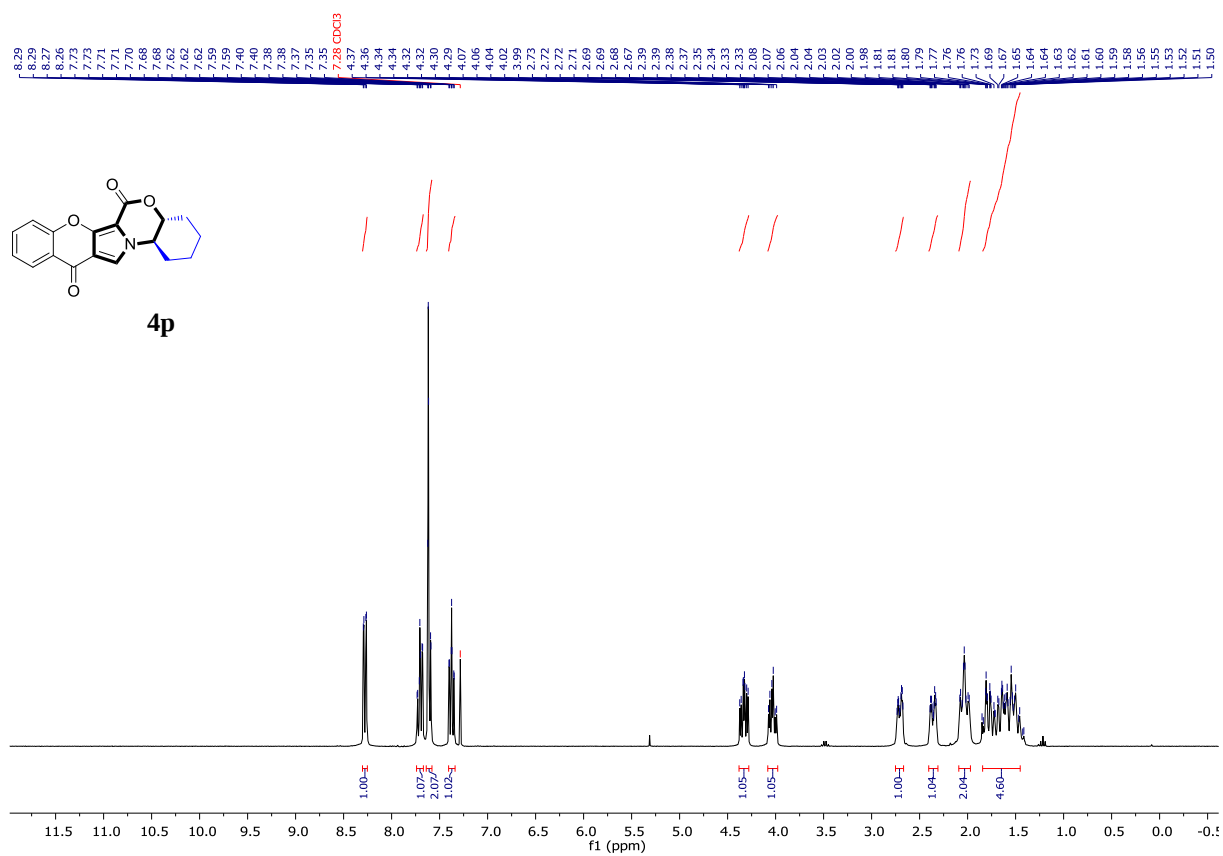






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II. X-ray crystal structure determination of compound 2a

Data collection and cell refinement of crystals were made by Stoe StadiVari diffractometer at 100 K using Dectris PILATUS3R 300K HPAD detector and microfocus source Xenocs Genix3D Cu HF with CuK α . The diffraction intensities were corrected for Lorentz and polarization factors. The structures were solved using programs SUPERFLIP³ or SHELXT⁴ and refined by the full-matrix least-squares procedure with SHELXL (version 2016/6).⁵ Geometrical analyses were performed with SHELXL. The structure was drawn with OLEX2 package.⁶

Table SI1. Crystal data and structure refinement for compound **2a**

CCDC Number	1552693
Identification code	05tlp113 (compound 2a)
Empirical formula	C ₁₆ H ₁₉ NO ₅
Formula weight	305.32
Temperature/K	100
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	5.0386(3)
b/Å	24.2827(13)
c/Å	12.1901(6)
α /°	90
β /°	94.863(4)
γ /°	90
Volume/Å ³	1486.10(14)
Z	4
ρ_{calc} /g/cm ³	1.365
μ /mm ⁻¹	0.846
F(000)	648.0
Crystal size/mm ³	0.48 × 0.35 × 0.25
Radiation	CuK α (λ = 1.54186)
2 Θ range for data collection/°	7.282 to 142.578
Index ranges	-5 ≤ h ≤ 2, -28 ≤ k ≤ 29, -14 ≤ l ≤ 14
Reflections collected	21185
Independent reflections	2801 [R_{int} = 0.0250, R_{sigma} = 0.0173]
Data/restraints/parameters	2801/175/213
Goodness-of-fit on F ²	1.041
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0457, wR_2 = 0.1189
Final R indexes [all data]	R_1 = 0.0533, wR_2 = 0.1226
Largest diff. peak/hole / e Å ⁻³	0.68/-0.35

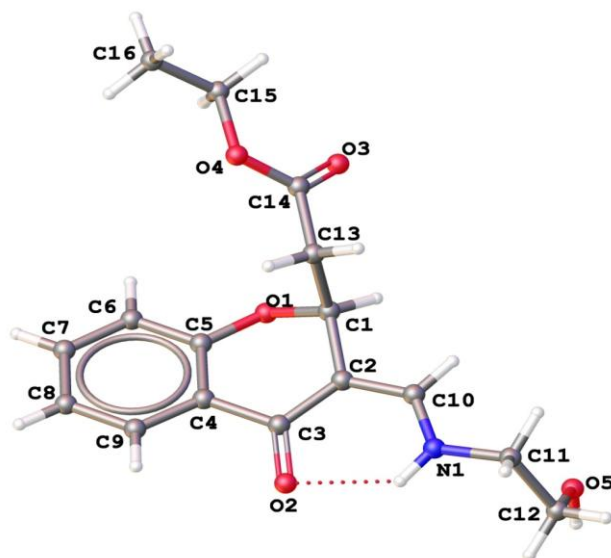


Figure SI1. Molecular structure of 05tlp113 (compound **2a**)

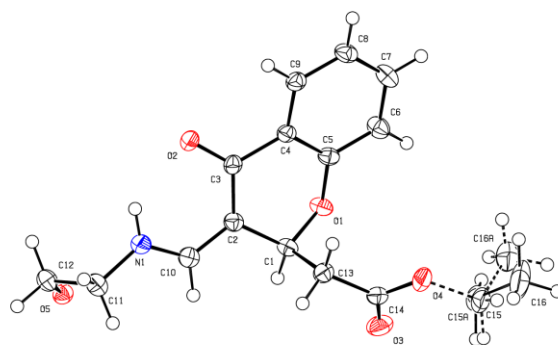


Figure SI2. X-ray structure of **2a** (Thermal ellipsoid representation with 50% of probability)

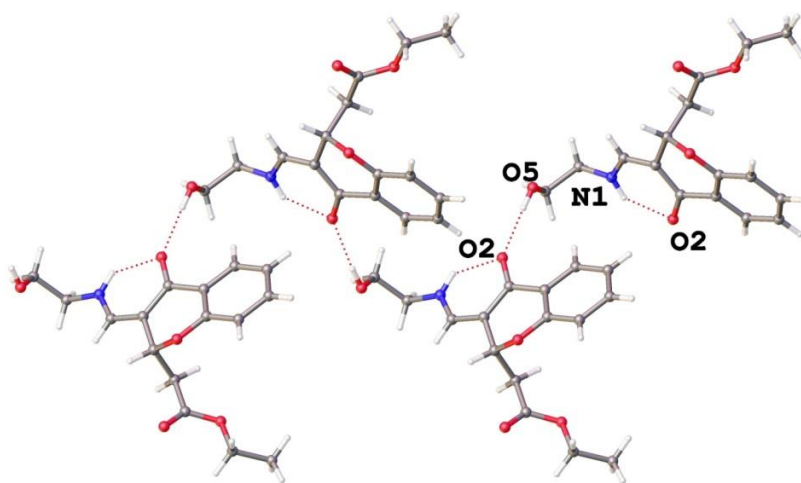


Figure SI3. Supramolecular chains from connecting molecules of 05tlp113 (compound **2a**) through O–H···O hydrogen bonds

III. Quantum chemical calculation details

All structures were fully optimized with the DFT method at the M06-2X⁷ level with a 6-31G(d,p) basis set for all atoms. The nature of all extrema as minimum or transition state was characterized with analytical calculations of frequencies, and the transition states were connected to reactants and products with IRC calculations. Transition states were located using Synchronous Transit-Guided Quasi-Newton method (STQN)⁸ and fully optimized using Berny algorithm. The effect of solvent (dichloromethane) was taken in account using the PCM formalism during optimization and frequency calculations. All calculations were done with the Gaussian09 revision A.02 program packages. The non-covalent interaction analysis was performed using NCIPLOT version 3.0 with standard parameters.⁹

Full reference of Gaussian09 software

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Complete thermodynamic parameters

A) Thermodynamic parameters (Thermodynamic vs. Kinetic pathway) using ethanol-amine

Table SI2. Thermodynamic parameters describing pathway using ethanolamine to reach intermediate **4a** calculated at the PCM/M06-2X/6-31G(d,p) level of theory (energies relative to the anionic adduct **1**).

	<i>TS1</i>	<i>2</i>	<i>3a</i>	<i>4a</i>
ΔH^{oa}	14.59	10.63	13.45	9.17
ΔG^{oa}	14.59	9.24	13.44	9.16
ΔS^{ob}	-0.03	4.64	0.05	0.02

^a: kcal/mol, ^b: cal/mol.K

Table SI3. Thermodynamic parameters describing thermodynamic pathway using ethanolamine to reach final product **Thermo** calculated at the PCM/M06-2X/6-31G(d,p) level of theory (energies relative to the anionic adduct **1**).

	<i>TS2a</i>	<i>5a</i>	<i>6a</i>	<i>Thermo</i>
ΔH^{oa}	11.36	9.69	-11.91	-18.35
ΔG^{oa}	12.58	11.17	-12.24	-31.95
ΔS^{ob}	-4.10	-4.96	1.10	45.62

^a: kcal/mol, ^b: cal/mol.K

Table SI4. Thermodynamic parameters describing kinetic pathway using ethanolamine to reach final product **Kinect** calculated at the PCM/M06-2X/6-31G(d,p) level of theory (energies relative to the anionic adduct **1**).

	3b	TS2b	4b	Kinect
ΔH^{oa}	16.31	21.31	12.32	-29.49
ΔG^{oa}	15.13	21.17	13.39	-30.28
ΔS^{ob}	3.97	0.47	-3.60	2.64

^a: kcal/mol, ^b: cal/mol.K

B) Thermodynamic parameters (Thermodynamic vs. Kinetic pathway) using 2,2-dimethylethanolamine

Table SI5. Thermodynamic parameters describing pathway using 2,2-dimethylethanolamine to reach intermediate **t-4a** calculated at the PCM/M06-2X/6-31G(d,p) level of theory (energies relative to the anionic adduct **t-1**).

	t-TS1	t-2	t-3a	t-4a
ΔH^{oa}	14.01	8.44	13.51	9.28
ΔG^{oa}	15.05	7.43	13.53	9.51
ΔS^{ob}	-3.50	3.37	-0.06	-0.78

^a: kcal/mol, ^b: cal/mol.K

Table SI6. Thermodynamic parameters describing thermodynamic pathway using 2,2-dimethylethanolamine to reach final product **t-Thermo** calculated at the PCM/M06-2X/6-31G(d,p) level of theory (energies relative to the anionic adduct **t-1**).

	t-TS2a	t-5a	t-6a	t-Thermo
ΔH^{oa}	20.33	15.24	-5.15	-14.65
ΔG^{oa}	22.58	17.48	-5.40	-27.14
ΔS^{ob}	-7.54	-7.54	0.86	41.88

^a: kcal/mol, ^b: cal/mol.K

Table SI7. Thermodynamic parameters describing kinetic pathway using 2,2-dimethylethanolamine to reach final product **t-Kinect** calculated at the PCM/M06-2X/6-31G(d,p) level of theory (energies relative to the anionic adduct **t-1**).

	t-3b	t-TS2b	t-4b	t-Kinect
ΔH^{oa}	14.52	19.45	11.54	-30.17
ΔG^{oa}	13.86	19.73	13.07	-31.11
ΔS^{ob}	2.23	-0.94	-5.15	3.18

^a: kcal/mol, ^b: cal/mol.K

C) Complete comparison of pathways using ethanolamine and 2,2-dimethylethanolamine

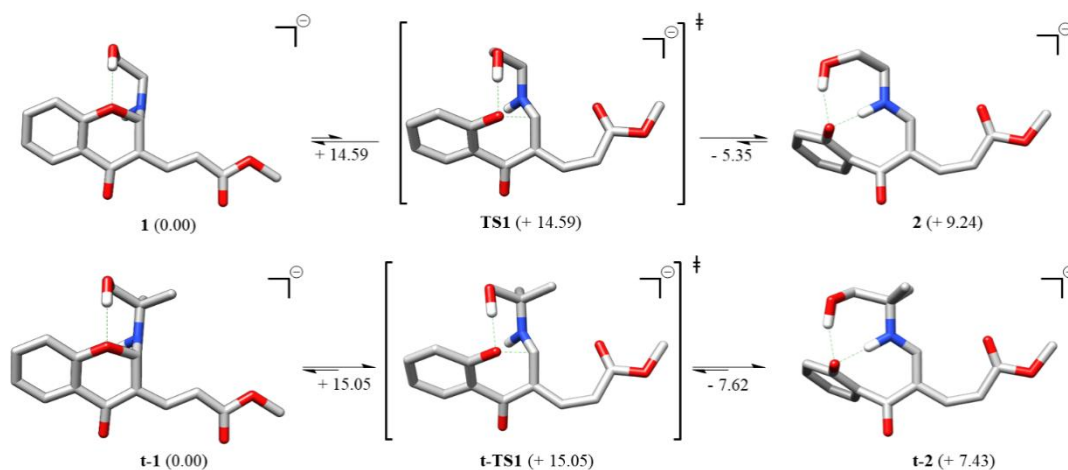


Figure SI4. Comparison of retro Michael reaction leading to **2** and **t-2** intermediates calculated at the PCM/M06-2X/6-31G(d,p) level of theory

C) 1. Thermodynamic pathway

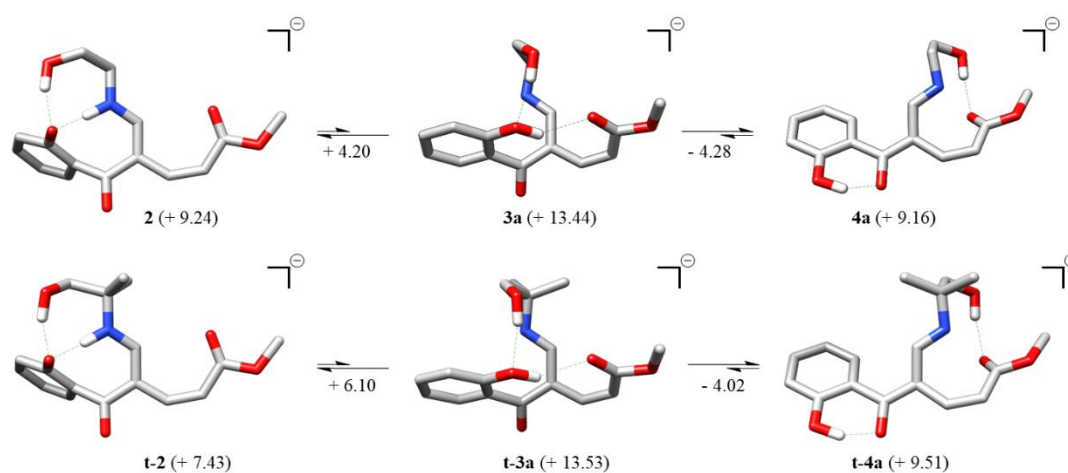


Figure SI5. Comparison of proton exchange and conformational changes leading to **4a** and **t-4a** intermediates calculated at the PCM/M06-2X/6-31G(d,p) level of theory

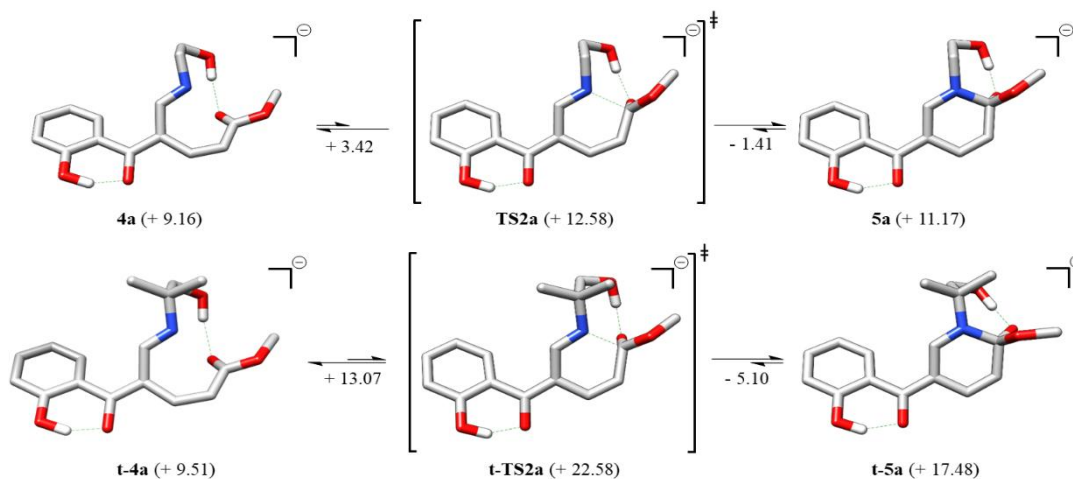


Figure SI6. Comparison of cyclisation step leading to tetrahedral intermediates **5a** and **t-5a** calculated at the PCM/M06-2X/6-31G(d,p) level of theory

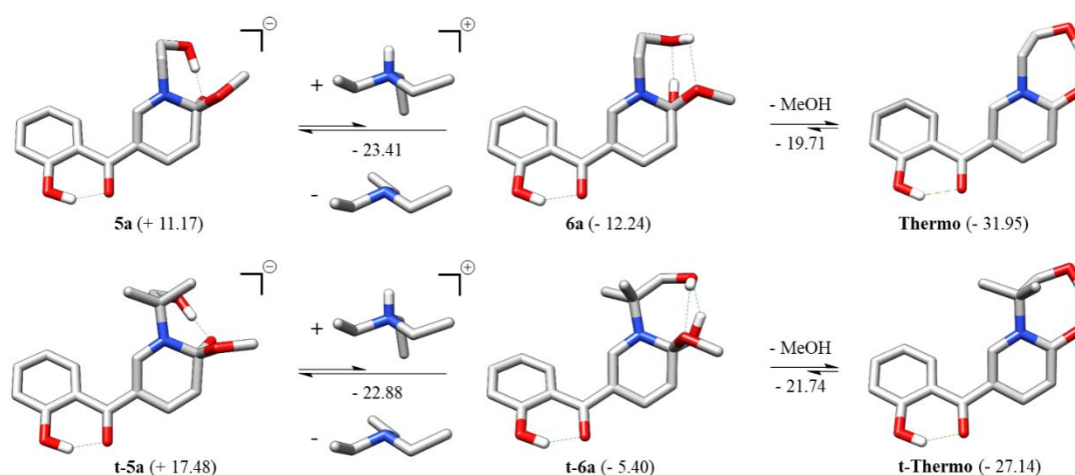


Figure SI7. Comparison of proton transfer and methanol extrusion steps leading to final products **Thermo** and **t-Thermo** calculated at the PCM/M06-2X/6-31G(d,p) level of theory

C) 2. Kinetic pathway

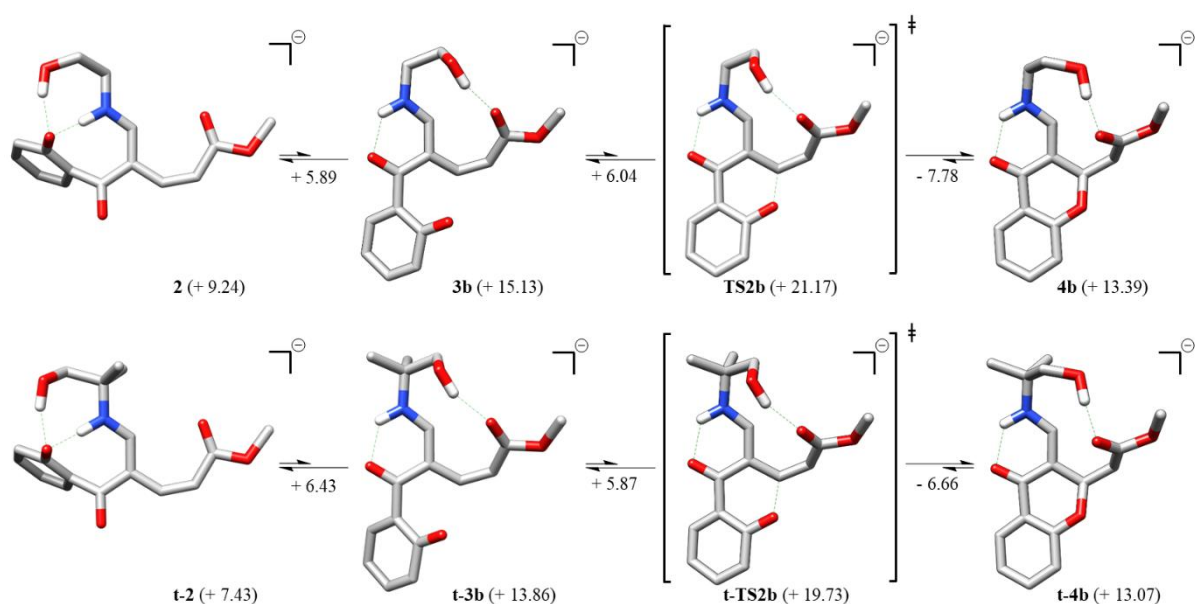


Figure SI8. Comparison of conformational changes and cyclisation steps leading to intermediates **4b** and **t-4b** calculated at the PCM/M06-2X/6-31G(d,p) level of theory

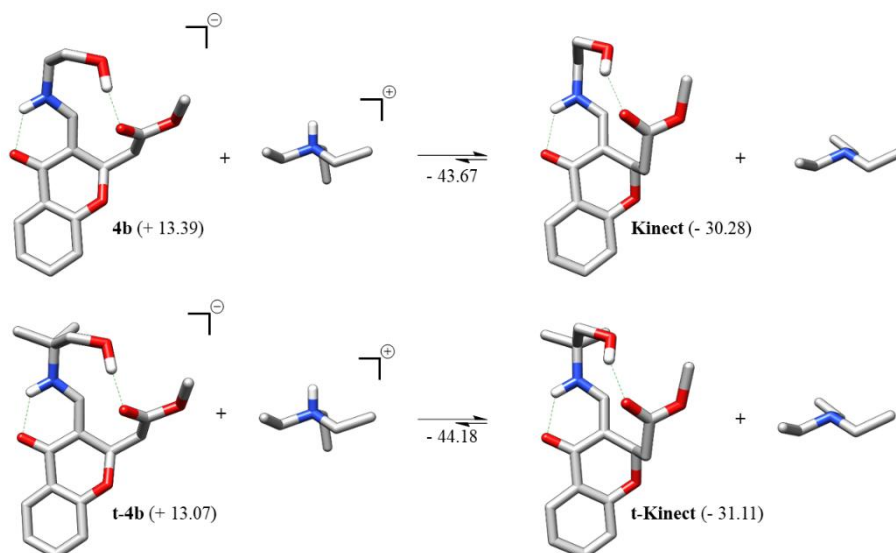


Figure SI9. Comparison of proton transfer between trimethylamine salt and intermediates **4b** and **t-4b** leading to kinetic products **Kinect** and **t-Kinect** calculated at the PCM/M06-2X/6-31G(d,p) level of theory

D) Study of the stabilization of the kinetic product induced by the presence of one or two esters modelled by isodesmic reaction with triethylamine

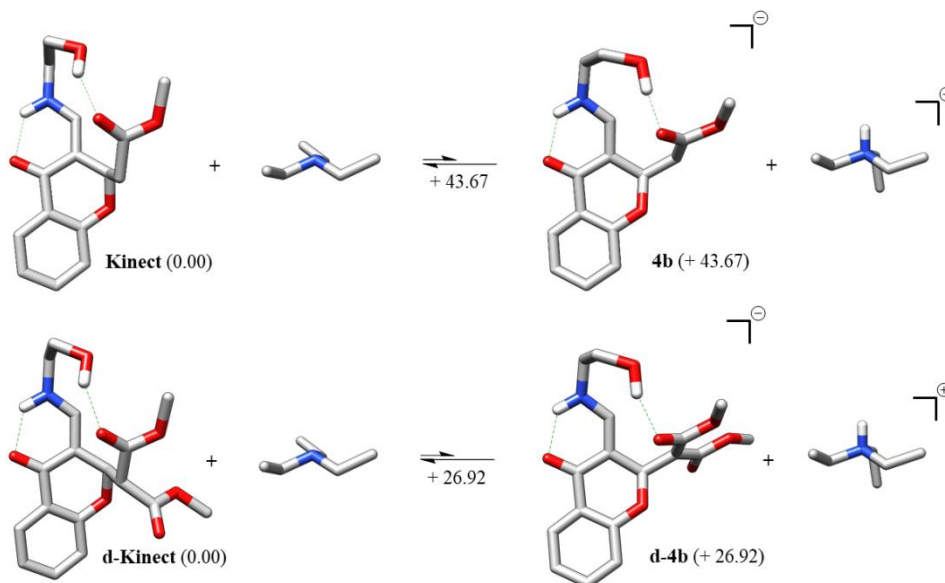


Figure SI10. Isodesmic reactions of trimethylamine mediated deprotonation of mono and disubstituted kinetic products calculated at the PCM/M06-2X/6-31G(d,p) level of theory

Table SI8. Thermodynamic parameters describing trimethylamine mediated deprotonation process calculated at the PCM/M06-2X/6-31G(d,p) level of theory (energies relative to neutral reactants **kinect** and **d-Kinect** energies).

	4b	d-4b
$\Delta H^{\circ a}$	41.81	24.83
$\Delta G^{\circ a}$	43.67	26.92
$\Delta S^{\circ b}$	-6.24	-7.01

^a: kcal/mol, ^b: cal/mol.K

E) Geometrical and non-covalent interaction analysis of involved transition states calculated at the PCM/M06-2X/6-31G(d,p) level of theory

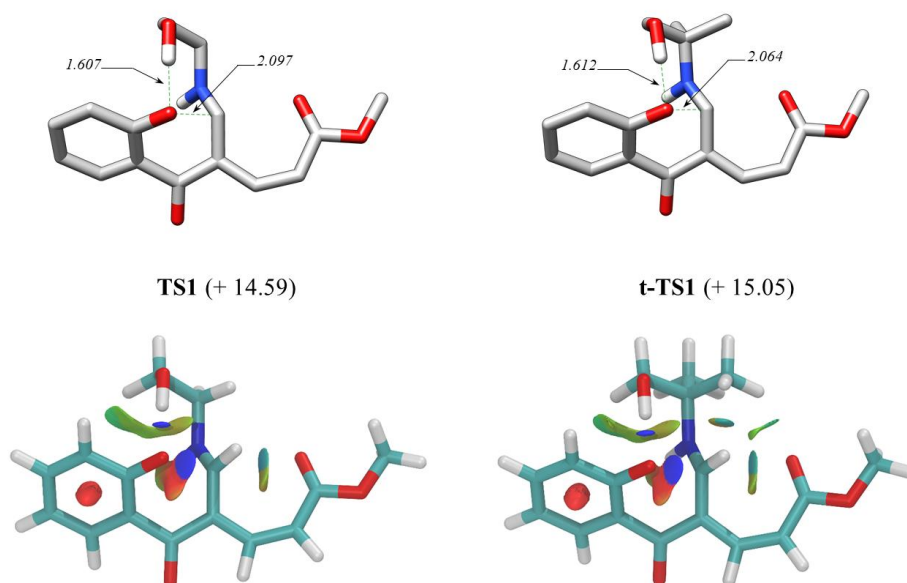


Figure SI11. Geometrical and non-covalent interaction analysis of located transition state **TS1** and **t-TS1**

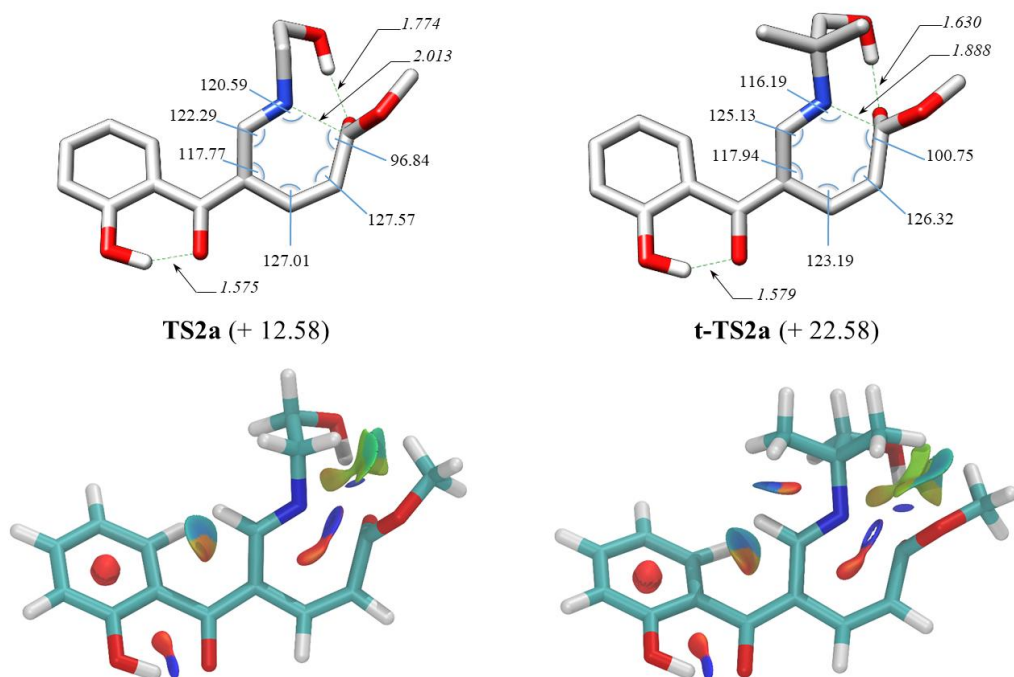


Figure SI12. Geometrical and non-covalent interaction analysis of located transition state TS2a and t-TS2a

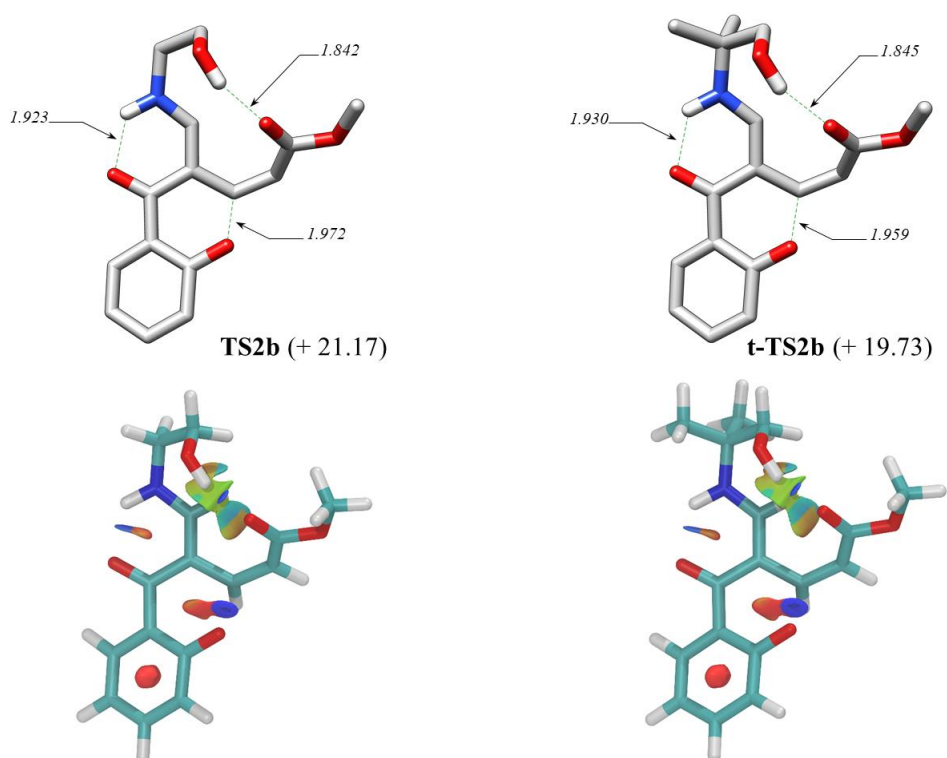


Figure SI13. Geometrical and non-covalent interaction analysis of located transition state TS2b and t-TS2b

Cartesian coordinates of reactants, intermediates and respective transition states calculated at the PCM/M06-2X/6-31G(d,p) level of theory

A. Common reactants, intermediates and transition states

Triethylamine

N	0.000407000	-0.000208000	-0.178114000
C	1.373721000	-0.208423000	0.282853000
H	1.973281000	0.633917000	-0.070818000
H	1.422939000	-0.191832000	1.390328000
C	-0.506712000	1.293494000	0.281581000
H	-1.535193000	1.391585000	-0.074128000
H	-0.547942000	1.327984000	1.389001000
C	-0.867205000	-1.086025000	0.280914000
H	-0.439033000	-2.026196000	-0.075345000
H	-0.876036000	-1.139740000	1.388274000
C	2.010428000	-1.491034000	-0.242509000
H	3.088621000	-1.466004000	-0.066117000
H	1.620322000	-2.387360000	0.244542000
H	1.839736000	-1.580451000	-1.319338000
C	-2.297405000	-0.993981000	-0.241625000
H	-2.814958000	-1.940390000	-0.066415000
H	-2.877296000	-0.209005000	0.248604000
H	-2.292295000	-0.799033000	-1.317957000
C	0.287122000	2.486170000	-0.242164000
H	-0.274528000	3.407288000	-0.067619000
H	1.256797000	2.596758000	0.247957000
H	0.453032000	2.382737000	-1.318468000

SCF Done: E(RM062X) = -292.272200605

of imaginary frequency = none

Triethylamonium salt

N	0.173895000	-0.008140000	0.450561000
C	-0.946074000	-0.994796000	0.695456000
H	-0.521395000	-1.769964000	1.335497000
H	-1.707734000	-0.465404000	1.268714000
C	-0.225493000	1.156169000	-0.420460000
H	0.615452000	1.848772000	-0.402814000
H	-0.328203000	0.765720000	-1.435139000
C	1.417299000	-0.695987000	-0.058174000
H	1.590750000	-1.535719000	0.617285000
H	1.178355000	-1.087140000	-1.047981000
C	-1.521916000	-1.583385000	-0.578805000
H	-2.303167000	-2.289515000	-0.291869000
H	-1.981072000	-0.824353000	-1.215394000
H	-0.777891000	-2.133165000	-1.157528000
C	2.624635000	0.224073000	-0.098911000
H	3.505456000	-0.384317000	-0.310777000
H	2.548943000	0.978220000	-0.883031000
H	2.785196000	0.718680000	0.863128000
C	-1.486818000	1.847890000	0.063145000
H	-1.622912000	2.755296000	-0.527631000
H	-2.378960000	1.231857000	-0.062311000
H	-1.402039000	2.143428000	1.112561000
H	0.412162000	0.380796000	1.369852000

SCF Done: E(RM062X) = -292.730350146

of imaginary frequency = none

Anionic adduct 1

C	2.894308000	-2.380237000	0.419055000
---	-------------	--------------	-------------

C	4.246776000	-2.074546000	0.318580000
C	4.637079000	-0.840436000	-0.206267000
C	3.683481000	0.081024000	-0.627427000
H	2.550848000	-3.331536000	0.813001000
H	4.995535000	-2.787948000	0.646922000
H	5.690728000	-0.590073000	-0.282262000
H	3.963076000	1.053316000	-1.022967000
C	2.331001000	-0.243545000	-0.525605000
C	1.920661000	-1.470656000	0.006035000
C	-0.421310000	-0.707552000	-0.103993000
C	0.130514000	0.680193000	-0.269466000
O	1.411954000	0.649682000	-0.992145000
C	-1.809498000	-0.901166000	-0.046814000
N	0.217669000	1.376959000	0.972865000
H	-0.491017000	1.278449000	-0.946682000
C	0.461531000	-1.806850000	0.086631000
O	0.127655000	-2.987011000	0.316784000
C	-2.803304000	0.043306000	-0.115763000
C	-4.187542000	-0.353708000	-0.079414000
O	-4.642824000	-1.487668000	0.008479000
O	-5.022984000	0.726586000	-0.154375000
C	-6.408410000	0.416847000	-0.120894000
H	-6.672281000	-0.102713000	0.803811000
H	-6.933904000	1.369860000	-0.178342000
H	-6.689456000	-0.217438000	-0.965718000
H	0.686371000	0.814605000	1.677148000
C	0.648068000	2.769362000	0.985390000
H	0.006800000	3.332582000	0.294772000
H	0.451179000	3.154965000	1.991938000
C	2.110028000	3.075907000	0.629560000
H	2.383097000	4.040351000	1.071054000
H	2.757880000	2.307743000	1.084298000
O	2.354579000	3.196972000	-0.757991000
H	2.069371000	2.355885000	-1.150788000
H	-2.126710000	-1.938292000	0.062525000
H	-2.592526000	1.105375000	-0.172429000

SCF Done: E(RM062X) = -1011.82968069

of imaginary frequency = none

Anionic adduct t-1

C	2.916064000	-2.635901000	0.598351000
C	4.266523000	-2.335236000	0.461776000
C	4.648875000	-1.173963000	-0.213463000
C	3.689219000	-0.320286000	-0.748489000
H	2.580263000	-3.532812000	1.109490000
H	5.019496000	-2.997327000	0.876416000
H	5.700821000	-0.927805000	-0.320436000
H	3.962776000	0.594571000	-1.266017000
C	2.338748000	-0.639078000	-0.608243000
C	1.936504000	-1.792806000	0.073200000
C	-0.409921000	-1.065926000	-0.133965000
C	0.128456000	0.295649000	-0.477344000
O	1.414348000	0.180248000	-1.187037000
C	-1.796180000	-1.258370000	-0.044164000
N	0.198967000	1.136994000	0.671895000
H	-0.499252000	0.780202000	-1.232152000
C	0.479761000	-2.125431000	0.195884000
O	0.152141000	-3.267827000	0.577013000
C	-2.794025000	-0.329839000	-0.210265000
C	-4.176284000	-0.723129000	-0.114652000
O	-4.627265000	-1.844679000	0.085326000

O	-5.015875000	0.344856000	-0.275664000
C	-6.399627000	0.039761000	-0.182005000
H	-6.639077000	-0.400384000	0.789425000
H	-6.927706000	0.984939000	-0.306142000
H	-6.701507000	-0.663281000	-0.962955000
H	0.656378000	0.653557000	1.440649000
C	0.599768000	2.552919000	0.600882000
C	2.070514000	2.784547000	0.176420000
H	2.368679000	3.788548000	0.500527000
H	2.701654000	2.059445000	0.718180000
O	2.313251000	2.739113000	-1.212779000
H	2.044533000	1.851014000	-1.501042000
H	-2.107244000	-2.277019000	0.188152000
H	-2.585623000	0.720568000	-0.381549000
C	0.444443000	3.093852000	2.025193000
H	0.631501000	4.170617000	2.056148000
H	-0.567195000	2.898926000	2.388970000
H	1.153657000	2.606399000	2.704716000
C	-0.337854000	3.303056000	-0.343773000
H	-1.376603000	3.159099000	-0.032724000
H	-0.106493000	4.372264000	-0.323196000
H	-0.224529000	2.966916000	-1.376658000

SCF Done: E(RM062X) = -1090.42727735

of imaginary frequency = none

Transition state TS1

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C	4.552001000	0.096659000	-0.244442000
C	4.457370000	-1.068783000	0.525397000
C	3.217987000	-1.680538000	0.654427000
H	3.503212000	1.537532000	-1.461473000
H	5.512333000	0.594029000	-0.355919000
H	5.335200000	-1.486312000	1.007136000
H	3.104721000	-2.596136000	1.229258000
C	2.070326000	-1.153435000	0.054811000
C	-0.458310000	-1.187566000	0.006799000
C	-0.453871000	0.260035000	0.027832000
O	1.111904000	0.537558000	-1.339375000
C	2.159783000	0.021148000	-0.748740000
C	0.785683000	-1.911192000	0.183079000
O	0.823061000	-3.137491000	0.378035000
C	-1.606039000	-1.925839000	-0.335957000
C	-2.937381000	-1.605488000	-0.497423000
C	-3.596313000	-0.389260000	-0.092907000
O	-3.125336000	0.602157000	0.454967000
O	-4.936749000	-0.454828000	-0.351381000
C	-5.684745000	0.679494000	0.063162000
H	-6.717761000	0.481147000	-0.221205000
H	-5.613348000	0.821753000	1.144576000
H	-5.325657000	1.586956000	-0.429001000
N	-0.002687000	0.933188000	1.071247000
C	-0.013515000	2.386404000	1.174106000
H	-0.941305000	2.740530000	0.713285000
H	-0.040198000	2.638052000	2.237994000
C	1.178489000	3.072341000	0.500526000
H	1.202653000	4.111837000	0.848934000
H	2.105680000	2.586406000	0.847404000
O	1.086007000	3.090035000	-0.897384000
H	-1.113866000	0.814991000	-0.626848000
H	-1.368281000	-2.977269000	-0.503556000
H	-3.603243000	-2.380804000	-0.857298000

H 0.542341000 0.416206000 1.751038000
H 1.125872000 2.138793000 -1.197390000
SCF Done: E(RM062X) = -1011.80382130
of imaginary frequency = one (-255.9054)

Transition state t-TS1

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C 4.605173000 -0.227577000 -0.493525000
C 4.537491000 -1.224809000 0.487057000
C 3.302679000 -1.785498000 0.778340000
H 3.515382000 0.973098000 -1.914107000
H 5.561882000 0.228273000 -0.736328000
H 5.432893000 -1.553420000 1.004216000
H 3.207544000 -2.577199000 1.516588000
C 2.132432000 -1.366440000 0.136858000
C -0.396785000 -1.437265000 0.124119000
C -0.412111000 -0.006577000 -0.129296000
O 1.123515000 0.053336000 -1.507682000
C 2.193590000 -0.364041000 -0.873073000
C 0.858873000 -2.090590000 0.439048000
O 0.916648000 -3.250028000 0.882174000
C -1.513985000 -2.265715000 -0.086885000
C -2.853064000 -2.042179000 -0.329169000
C -3.566468000 -0.804512000 -0.160562000
O -3.143660000 0.279318000 0.228610000
O -4.894649000 -0.960089000 -0.444474000
C -5.690971000 0.198899000 -0.245477000
H -6.707252000 -0.081110000 -0.521174000
H -5.661062000 0.520834000 0.798699000
H -5.345367000 1.024709000 -0.872455000
N 0.022643000 0.845362000 0.786239000
C 0.057179000 2.318533000 0.691263000
C 1.341414000 2.791188000 -0.028245000
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H 2.198931000 2.266941000 0.428155000
O 1.317079000 2.638535000 -1.418889000
H -1.095890000 0.396040000 -0.863999000
H -1.234707000 -3.319606000 -0.048396000
H -3.475893000 -2.899406000 -0.556042000
H 0.577259000 0.442145000 1.534839000
H 1.249190000 1.658456000 -1.595980000
C -1.177144000 2.829267000 -0.044130000
H -1.135442000 2.570608000 -1.103971000
H -2.087555000 2.413173000 0.390964000
H -1.198672000 3.920665000 0.025421000
C 0.078781000 2.829471000 2.132003000
H 0.976944000 2.484124000 2.656902000
H 0.078102000 3.921869000 2.145213000
H -0.799864000 2.472376000 2.675418000
SCF Done: E(RM062X) = -1090.40256999
of imaginary frequency = one (-271.9772)

Intermediate 2

C 4.058655000 -0.048990000 0.019161000
C 4.536444000 -0.954815000 0.953155000
C 3.737226000 -2.017610000 1.381227000
C 2.461509000 -2.150421000 0.844746000
H 4.675263000 0.779255000 -0.320168000
H 5.539301000 -0.833133000 1.354515000
H 4.106280000 -2.733321000 2.108265000
H 1.833715000 -2.985832000 1.145689000

C	1.947975000	-1.231707000	-0.077111000
C	-0.653762000	-0.856634000	-0.294247000
C	-0.673924000	0.457646000	0.203229000
C	2.759862000	-0.159038000	-0.533463000
C	0.586087000	-1.591731000	-0.643000000
O	0.525440000	-2.658821000	-1.257076000
C	-1.856554000	-1.624199000	-0.449563000
C	-3.200546000	-1.447491000	-0.271198000
O	-5.292169000	-0.525141000	0.023298000
C	-6.145006000	0.538860000	0.431169000
H	-5.960940000	1.434608000	-0.166763000
H	-5.984302000	0.782412000	1.484047000
H	-7.162767000	0.183909000	0.276034000
C	0.311695000	2.653818000	0.644652000
H	-0.716788000	3.025398000	0.723881000
H	0.752833000	2.640535000	1.648833000
C	1.156659000	3.564307000	-0.244798000
H	1.108436000	4.583713000	0.151771000
H	0.718801000	3.578569000	-1.254786000
H	-1.583193000	0.811425000	0.684174000
C	-3.962008000	-0.286964000	0.161608000
O	-3.569598000	0.784147000	0.602313000
H	-1.619163000	-2.615472000	-0.831583000
H	-3.830847000	-2.291559000	-0.527810000
O	2.312787000	0.719664000	-1.405314000
O	2.509188000	3.175842000	-0.269069000
H	2.578789000	2.332337000	-0.777608000
N	0.309271000	1.314060000	0.083574000
H	1.108635000	1.073028000	-0.590133000

SCF Done: E(RM062X) = -1011.81085219

of imaginary frequency = none

Intermediate t-2

C	4.047197000	-0.304684000	0.047746000
C	4.467993000	-1.102416000	1.101783000
C	3.652995000	-2.129163000	1.583463000
C	2.414728000	-2.335224000	0.983261000
H	4.676292000	0.495130000	-0.334822000
H	5.440187000	-0.923869000	1.554385000
H	3.978771000	-2.759863000	2.403833000
H	1.771215000	-3.139438000	1.332970000
C	1.959572000	-1.524314000	-0.059781000
C	-0.618142000	-1.171288000	-0.396803000
C	-0.647603000	0.179862000	-0.014794000
C	2.790893000	-0.496256000	-0.577094000
C	0.627567000	-1.930177000	-0.662041000
O	0.584995000	-3.034555000	-1.205921000
C	-1.819165000	-1.950063000	-0.484369000
C	-3.159608000	-1.763450000	-0.284703000
O	-5.246821000	-0.856050000	0.064358000
C	-6.098161000	0.212681000	0.462683000
H	-5.966502000	1.078069000	-0.190950000
H	-5.884823000	0.514683000	1.490811000
H	-7.114999000	-0.168914000	0.383578000
C	0.321184000	2.434720000	0.246631000
C	1.793486000	2.892906000	0.224902000
H	2.357165000	2.256312000	0.926400000
H	1.830024000	3.922156000	0.602492000
H	-1.565346000	0.556613000	0.427383000
C	-3.916384000	-0.587930000	0.115080000
O	-3.524295000	0.515848000	0.470167000

H	-1.586424000	-2.963426000	-0.807364000
H	-3.793228000	-2.622930000	-0.472828000
O	2.390507000	0.266058000	-1.569213000
O	2.370097000	2.885236000	-1.055148000
H	2.543688000	1.943437000	-1.307503000
N	0.331240000	1.032052000	-0.194850000
H	1.121478000	0.742911000	-0.846702000
C	-0.514746000	3.267208000	-0.727405000
H	-0.084907000	3.207249000	-1.729220000
H	-1.543491000	2.894006000	-0.753657000
H	-0.531589000	4.316152000	-0.415043000
C	-0.218615000	2.549994000	1.670989000
H	-0.133908000	3.584890000	2.014456000
H	-1.274585000	2.269092000	1.723188000
H	0.347288000	1.906635000	2.351295000

SCF Done: E(RM062X) = -1090.41201390

of imaginary frequency = none

B. Common intermediates and transition states describing thermodynamic pathway

Intermediate 3a

C	2.833191000	0.862179000	-1.534487000
C	4.151917000	0.584401000	-1.197634000
C	4.448991000	-0.469631000	-0.334331000
C	3.406253000	-1.227492000	0.183878000
H	2.582966000	1.667894000	-2.217333000
H	4.949217000	1.189841000	-1.618240000
H	5.477379000	-0.698437000	-0.075445000
H	3.604208000	-2.067438000	0.843028000
C	2.069869000	-0.945080000	-0.107300000
C	-0.282241000	-1.312980000	0.792146000
C	-0.476922000	0.020661000	1.325042000
C	1.786531000	0.106759000	-0.999527000
C	1.016010000	-1.864922000	0.457140000
O	1.285043000	-3.072921000	0.515926000
C	-1.399247000	-2.188437000	0.698168000
C	-2.692716000	-1.850030000	0.392208000
O	-4.388874000	-0.554803000	-0.519585000
C	-4.815317000	0.557063000	-1.298521000
H	-4.372454000	0.525488000	-2.297060000
H	-4.530621000	1.498009000	-0.821763000
H	-5.899826000	0.479595000	-1.365191000
C	0.000104000	2.173073000	2.062710000
C	0.261530000	3.237123000	0.997409000
H	1.343152000	3.270600000	0.794314000
H	-0.043676000	4.221709000	1.367833000
H	-1.518412000	0.235638000	1.607525000
C	-3.047121000	-0.631887000	-0.307331000
O	-2.297771000	0.227171000	-0.763442000
H	-1.184141000	-3.247468000	0.848285000
H	-3.479310000	-2.592453000	0.461886000
O	0.540954000	0.450476000	-1.422122000
O	-0.472563000	2.989690000	-0.180872000
H	-0.221362000	2.105142000	-0.494695000
N	0.436039000	0.893807000	1.550878000
H	-0.156584000	-0.083251000	-0.991031000
H	0.571167000	2.433689000	2.964219000
H	-1.073270000	2.183084000	2.320852000

SCF Done: E(RM062X) = -1011.80667581

of imaginary frequency = none

Intermediate t-3a

C	-2.841453000	-0.138305000	1.905584000
C	-4.155767000	-0.286333000	1.480786000
C	-4.436680000	-0.941029000	0.282073000
C	-3.383010000	-1.435425000	-0.476837000
H	-2.602572000	0.357998000	2.840890000
H	-4.962184000	0.106681000	2.092601000
H	-5.461262000	-1.067307000	-0.051289000
H	-3.568077000	-1.966078000	-1.405941000
C	-2.051362000	-1.266874000	-0.091963000
C	0.315375000	-1.251988000	-1.039176000
C	0.506975000	0.188501000	-1.047735000
C	-1.784586000	-0.624377000	1.131802000
C	-0.982806000	-1.895862000	-0.950719000
O	-1.239988000	-2.992543000	-1.466020000
C	1.435848000	-2.097089000	-1.246176000
C	2.731897000	-1.878612000	-0.844790000
O	4.433179000	-0.992319000	0.458963000
C	4.864570000	-0.211676000	1.566722000
H	4.400973000	-0.558593000	2.493388000
H	4.610111000	0.841607000	1.424068000
H	5.945911000	-0.333591000	1.618526000
C	-0.096720000	2.492174000	-0.932019000
C	-0.643452000	3.024975000	0.405225000
H	-1.726860000	2.827569000	0.428449000
H	-0.490507000	4.109879000	0.461663000
H	1.544642000	0.476542000	-1.244990000
C	3.090472000	-0.976425000	0.227106000
O	2.347628000	-0.312479000	0.946660000
H	1.224828000	-3.045137000	-1.743110000
H	3.516558000	-2.555246000	-1.162578000
O	-0.544058000	-0.444917000	1.659741000
O	0.002331000	2.457584000	1.521684000
H	-0.102655000	1.492886000	1.452521000
N	-0.416926000	1.065961000	-0.914322000
H	0.162464000	-0.747412000	1.054243000
C	1.387160000	2.848197000	-1.050004000
H	1.809276000	2.499871000	-1.998040000
H	1.507197000	3.935134000	-1.008468000
H	1.954317000	2.404051000	-0.227590000
C	-0.887172000	3.140630000	-2.072025000
H	-0.780312000	4.230587000	-2.052989000
H	-0.523637000	2.774801000	-3.036954000
H	-1.948206000	2.888538000	-1.989485000

SCF Done: E(RM062X) = -1090.40406016

of imaginary frequency = none

Intermediate 4a

C	-4.881054000	0.555262000	0.038349000
C	-4.551268000	1.776745000	-0.532012000
C	-3.251250000	2.021334000	-0.978374000
C	-2.278082000	1.044611000	-0.804411000
H	-5.894951000	0.331138000	0.353342000
H	-5.319698000	2.534338000	-0.653880000
H	-3.002517000	2.958706000	-1.463743000
H	-1.270972000	1.216576000	-1.171661000
C	-2.566567000	-0.177086000	-0.183609000
C	-0.163144000	-0.986008000	0.182585000
C	0.265235000	0.290970000	0.707739000
C	-3.907753000	-0.440464000	0.182657000
C	-1.551599000	-1.266408000	0.011839000

O	-2.008194000	-2.451657000	-0.015125000
C	0.709478000	-2.132702000	0.132549000
C	2.050607000	-2.228775000	-0.033364000
O	4.186513000	-1.316721000	0.031770000
C	5.152284000	-0.357034000	-0.393072000
H	6.098819000	-0.669351000	0.046264000
H	4.878506000	0.639981000	-0.039330000
H	5.226919000	-0.340315000	-1.482912000
N	1.471290000	0.605743000	1.025384000
C	1.664768000	1.945677000	1.545362000
H	0.761492000	2.361578000	2.024317000
H	2.467640000	1.928144000	2.292310000
C	2.072313000	2.873026000	0.399209000
H	2.346039000	3.860382000	0.787527000
H	1.200076000	3.002603000	-0.263093000
O	3.180089000	2.380130000	-0.321069000
H	0.186627000	-3.075000000	0.293787000
H	2.532207000	-3.188077000	0.131396000
H	-0.545745000	1.001804000	0.924713000
O	-4.272921000	-1.638896000	0.668942000
H	2.942918000	1.482741000	-0.620642000
H	-3.474799000	-2.223588000	0.473308000
C	2.948405000	-1.167264000	-0.488715000
O	2.701285000	-0.294501000	-1.305741000

SCF Done: E(RM062X) = -1011.81312237

of imaginary frequency = none

Intermediate t-4a

C	-5.024382000	0.596223000	-0.093730000
C	-4.652652000	1.656220000	-0.908509000
C	-3.359460000	1.727534000	-1.430286000
C	-2.433926000	0.749294000	-1.088490000
H	-6.035082000	0.501863000	0.289737000
H	-5.383576000	2.419517000	-1.158946000
H	-3.079336000	2.532547000	-2.100883000
H	-1.434110000	0.785488000	-1.510656000
C	-2.761822000	-0.303446000	-0.223888000
C	-0.394179000	-1.155134000	0.245425000
C	0.114191000	0.184592000	0.456082000
C	-4.100377000	-0.406282000	0.224145000
C	-1.798480000	-1.384383000	0.175597000
O	-2.317223000	-2.519772000	0.420128000
C	0.418550000	-2.328806000	0.446042000
C	1.745804000	-2.527182000	0.262582000
O	3.911447000	-1.724229000	-0.014843000
C	4.888381000	-0.997724000	-0.758806000
H	5.842015000	-1.191750000	-0.269432000
H	4.663285000	0.071253000	-0.746281000
H	4.917199000	-1.343872000	-1.794934000
N	1.351261000	0.490445000	0.621842000
C	1.722740000	1.886295000	0.868936000
C	2.054600000	2.497564000	-0.506453000
H	2.456951000	3.509764000	-0.373109000
H	1.110387000	2.582155000	-1.071775000
O	3.010982000	1.759919000	-1.228999000
H	-0.136866000	-3.174033000	0.852144000
H	2.201055000	-3.437074000	0.642496000
H	-0.664475000	0.946387000	0.564372000
O	-4.508726000	-1.456778000	0.954500000
H	2.685533000	0.841140000	-1.280046000
H	-3.741841000	-2.110330000	0.870012000

C	2.649695000	-1.659503000	-0.493256000
O	2.381591000	-1.023985000	-1.501191000
C	0.656756000	2.760358000	1.539241000
H	-0.204244000	2.944157000	0.888420000
H	0.295500000	2.286642000	2.457526000
H	1.084031000	3.733264000	1.800820000
C	2.983484000	1.851544000	1.735597000
H	3.380363000	2.859320000	1.897761000
H	2.759743000	1.403020000	2.708261000
H	3.746522000	1.243198000	1.243501000

SCF Done: E(RM062X) = -1090.41032363

of imaginary frequency = none

Transition state TS2a

C	-4.897172000	0.690410000	0.356959000
C	-4.552741000	1.960033000	-0.085527000
C	-3.286215000	2.205212000	-0.619200000
C	-2.356346000	1.173695000	-0.662102000
H	-5.889079000	0.472519000	0.739251000
H	-5.286619000	2.759079000	-0.037191000
H	-3.031300000	3.185863000	-1.005707000
H	-1.380920000	1.347503000	-1.105567000
C	-3.970954000	-0.356181000	0.283427000
C	-2.655379000	-0.105016000	-0.174232000
C	-0.279202000	-1.031366000	-0.098639000
C	0.282133000	0.152495000	0.448682000
C	0.603773000	-2.156733000	-0.319373000
C	1.948163000	-2.142475000	-0.321274000
H	0.103282000	-3.112030000	-0.456271000
O	-4.356739000	-1.588764000	0.652824000
C	-1.683258000	-1.245634000	-0.186849000
O	-2.178259000	-2.407920000	-0.284915000
C	2.848122000	-0.946635000	-0.322244000
N	1.561473000	0.322560000	0.564641000
H	-0.390516000	0.911138000	0.865338000
H	-3.608876000	-2.181085000	0.334137000
C	2.058271000	1.523576000	1.204310000
H	1.336490000	1.908974000	1.940219000
H	2.982297000	1.276284000	1.740332000
O	3.164935000	-0.364360000	-1.378797000
C	2.339281000	2.622643000	0.180218000
H	1.396760000	2.840582000	-0.349379000
H	2.642970000	3.535936000	0.704303000
O	3.370881000	2.294876000	-0.721265000
H	3.231221000	1.376089000	-1.041806000
H	2.491842000	-3.078287000	-0.433937000
O	3.768468000	-1.045102000	0.698076000
C	4.996462000	-0.352674000	0.492962000
H	5.587697000	-0.526722000	1.392729000
H	5.523598000	-0.749773000	-0.378993000
H	4.836931000	0.718072000	0.349971000

SCF Done: E(RM062X) = -1011.80802821

of imaginary frequency = one (-204.7140)

Transition state t-TS2a

C	-5.031041000	0.790596000	0.218788000
C	-4.643807000	1.935638000	-0.462733000
C	-3.392929000	2.003475000	-1.079290000
C	-2.519457000	0.928871000	-0.964656000
H	-6.013717000	0.702729000	0.670191000
H	-5.333014000	2.771446000	-0.537053000

H	-3.107110000	2.879489000	-1.651085000
H	-1.558025000	0.963919000	-1.468191000
C	-4.163326000	-0.303720000	0.307558000
C	-2.859659000	-0.219467000	-0.236081000
C	-0.532038000	-1.255138000	-0.035843000
C	0.088681000	-0.020139000	0.260152000
C	0.294485000	-2.439581000	-0.059347000
C	1.631820000	-2.399194000	-0.113550000
H	-0.219824000	-3.394546000	0.007759000
O	-4.594701000	-1.421703000	0.915289000
C	-1.948079000	-1.397180000	-0.060080000
O	-2.503530000	-2.527864000	0.069499000
C	2.475816000	-1.182572000	-0.370077000
N	1.377000000	0.168470000	0.359717000
H	-0.576059000	0.805376000	0.495772000
H	-3.895968000	-2.105784000	0.684005000
C	1.877657000	1.527280000	0.695941000
O	2.705380000	-0.833356000	-1.558730000
C	2.332329000	2.223520000	-0.606316000
H	1.457883000	2.251476000	-1.279893000
H	2.590537000	3.261757000	-0.359190000
O	3.446901000	1.652381000	-1.228882000
H	3.206370000	0.714724000	-1.466888000
H	2.216628000	-3.315464000	-0.078119000
O	3.546020000	-1.215436000	0.528540000
C	4.827039000	-0.965457000	-0.030074000
H	5.543387000	-1.170504000	0.767976000
H	5.020967000	-1.629103000	-0.878080000
H	4.936103000	0.069806000	-0.363819000
C	0.801114000	2.427233000	1.324200000
H	0.010563000	2.700292000	0.617611000
H	0.341145000	1.946608000	2.192771000
H	1.271447000	3.354624000	1.659389000
C	3.042633000	1.432937000	1.686514000
H	2.753793000	0.836645000	2.556510000
H	3.920003000	0.982987000	1.230915000
H	3.307902000	2.439452000	2.025036000

SCF Done: E(RM062X) = -1090.39183924

of imaginary frequency = one (-249.2374)

Intermediate 5a

C	-4.865472000	0.752869000	0.426913000
C	-4.498712000	2.018898000	-0.005930000
C	-3.240321000	2.239601000	-0.570020000
C	-2.339879000	1.186059000	-0.653478000
H	-5.851385000	0.555735000	0.834545000
H	-5.209658000	2.835703000	0.073787000
H	-2.969704000	3.219153000	-0.947935000
H	-1.372840000	1.341739000	-1.120614000
C	-3.970802000	-0.316715000	0.312333000
C	-2.662555000	-0.093237000	-0.178721000
C	-0.295313000	-1.068908000	-0.187937000
C	0.300139000	0.059862000	0.365278000
C	0.588345000	-2.172292000	-0.523090000
C	1.919251000	-2.033245000	-0.471996000
H	0.126350000	-3.112740000	-0.808150000
O	-4.386598000	-1.540497000	0.680401000
C	-1.718603000	-1.251237000	-0.230119000
O	-2.215370000	-2.403008000	-0.309489000
C	2.625581000	-0.724480000	-0.197106000
N	1.608867000	0.203880000	0.503367000

H	-0.308504000	0.855225000	0.790216000
H	-3.677724000	-2.159162000	0.352757000
C	2.135513000	1.421498000	1.116299000
H	1.392769000	1.789291000	1.831875000
H	3.038117000	1.152014000	1.669604000
O	3.136629000	-0.165461000	-1.261433000
C	2.457509000	2.526620000	0.104573000
H	1.546650000	2.701365000	-0.498816000
H	2.644841000	3.447785000	0.672709000
O	3.575325000	2.255202000	-0.685408000
H	3.456121000	1.287667000	-1.004275000
H	2.587956000	-2.852282000	-0.721933000
O	3.579896000	-0.998211000	0.863517000
C	4.903949000	-0.583334000	0.596653000
H	5.485911000	-0.843304000	1.485048000
H	5.327545000	-1.096667000	-0.273389000
H	4.970645000	0.495357000	0.418386000

SCF Done: E(RM062X) = -1011.81193685

of imaginary frequency = none

Intermediate t-5a

C	-4.988847000	0.657153000	0.462814000
C	-4.649865000	1.880921000	-0.095567000
C	-3.429317000	2.047317000	-0.753983000
C	-2.536311000	0.985752000	-0.804838000
H	-5.948438000	0.498861000	0.943465000
H	-5.354487000	2.705190000	-0.040714000
H	-3.183541000	2.989852000	-1.230263000
H	-1.600841000	1.095302000	-1.344237000
C	-4.102349000	-0.422431000	0.383550000
C	-2.827450000	-0.247246000	-0.203352000
C	-0.460402000	-1.229638000	-0.262552000
C	0.149061000	-0.064648000	0.176635000
C	0.406804000	-2.330913000	-0.636862000
C	1.733548000	-2.167310000	-0.638872000
H	-0.056724000	-3.265700000	-0.937809000
O	-4.494954000	-1.609524000	0.878166000
C	-1.886354000	-1.409774000	-0.218958000
O	-2.383818000	-2.561967000	-0.191023000
C	2.463762000	-0.890757000	-0.273463000
N	1.462141000	0.130094000	0.272767000
H	-0.473494000	0.752037000	0.518790000
H	-3.814501000	-2.258833000	0.557449000
C	1.936854000	1.518507000	0.592046000
O	3.187883000	-0.411492000	-1.252963000
C	1.808943000	2.375610000	-0.686232000
H	0.754392000	2.300686000	-1.020776000
H	1.972442000	3.425620000	-0.397681000
O	2.709483000	2.030882000	-1.688736000
H	2.896284000	1.029140000	-1.591602000
H	2.401792000	-2.963181000	-0.957730000
O	3.228079000	-1.217940000	0.932497000
C	4.546420000	-1.629089000	0.667915000
H	5.003675000	-1.860693000	1.633946000
H	4.583476000	-2.530995000	0.040101000
H	5.128543000	-0.849038000	0.166747000
C	1.061232000	2.139356000	1.690462000
H	0.083162000	2.468303000	1.325291000
H	0.910999000	1.429813000	2.508603000
H	1.566365000	3.022267000	2.089014000
C	3.390688000	1.545123000	1.073317000

H	3.501004000	1.016597000	2.021145000
H	4.057011000	1.101485000	0.336862000
H	3.666010000	2.595364000	1.214136000

SCF Done: E(RM062X) = -1090.40042917
of imaginary frequency = none

Intermediate 6a

C	4.911839000	0.752139000	-0.275819000
C	4.536380000	1.976847000	0.253193000
C	3.259613000	2.159395000	0.792292000
C	2.353190000	1.111494000	0.755908000
H	5.908462000	0.584769000	-0.669512000
H	5.252577000	2.792547000	0.268045000
H	2.982103000	3.105601000	1.242607000
H	1.371239000	1.235698000	1.200129000
C	4.010363000	-0.317978000	-0.283003000
C	2.690199000	-0.128682000	0.189399000
C	0.294860000	-1.038668000	0.078726000
C	-0.258854000	0.106710000	-0.441558000
C	-0.610487000	-2.143653000	0.323672000
C	-1.935834000	-1.958724000	0.301073000
H	-0.176871000	-3.125190000	0.484051000
O	4.440615000	-1.499013000	-0.756799000
C	1.733863000	-1.265071000	0.109004000
O	2.174977000	-2.427507000	0.052280000
C	-2.515356000	-0.577467000	0.177152000
N	-1.584954000	0.285737000	-0.572835000
H	0.360397000	0.895544000	-0.857950000
H	3.739460000	-2.155782000	-0.534997000
C	-2.089891000	1.446630000	-1.310452000
H	-1.272068000	1.820706000	-1.930545000
H	-2.883210000	1.112399000	-1.982282000
O	-2.720570000	-0.088288000	1.465598000
C	-2.588522000	2.583767000	-0.426659000
H	-1.803725000	2.889022000	0.271466000
H	-2.829685000	3.438920000	-1.069617000
H	-3.136043000	0.792865000	1.363908000
H	-2.633274000	-2.773192000	0.455680000
O	-3.710093000	-0.526744000	-0.569625000
C	-4.787977000	-1.286296000	-0.037020000
H	-5.696038000	-0.901290000	-0.501750000
H	-4.686286000	-2.347094000	-0.286640000
H	-4.852062000	-1.166520000	1.047402000
O	-3.712011000	2.228358000	0.368337000
H	-4.353958000	1.783721000	-0.203916000

SCF Done: E(RM062X) = -1012.30377914
of imaginary frequency = none

Intermediate t-6a

C	-5.043456000	0.671464000	0.563464000
C	-4.778403000	1.858884000	-0.099764000
C	-3.611577000	2.008147000	-0.855337000
C	-2.697426000	0.967653000	-0.901013000
H	-5.960152000	0.526254000	1.124681000
H	-5.498744000	2.669355000	-0.048067000
H	-3.425996000	2.921833000	-1.408318000
H	-1.807943000	1.063145000	-1.515551000
C	-4.136875000	-0.392645000	0.492823000
C	-2.915275000	-0.231071000	-0.201489000
C	-0.515308000	-1.136865000	-0.405402000
C	0.098264000	0.050372000	-0.109480000

C	0.328541000	-2.227727000	-0.836861000
C	1.653597000	-2.065691000	-0.891428000
H	-0.140687000	-3.154106000	-1.151674000
O	-4.467759000	-1.540543000	1.107487000
C	-1.943263000	-1.358262000	-0.205695000
O	-2.356409000	-2.516674000	-0.023007000
C	2.361118000	-0.824611000	-0.423041000
N	1.423079000	0.294973000	-0.216969000
H	-0.496272000	0.875405000	0.256142000
H	-3.809063000	-2.211695000	0.815872000
C	1.878903000	1.650917000	0.258537000
O	3.333236000	-0.548861000	-1.376022000
C	3.287955000	2.046075000	-0.224802000
H	3.313073000	2.036102000	-1.319037000
H	3.435013000	3.078532000	0.109273000
H	4.015920000	0.004663000	-0.946215000
H	2.315430000	-2.834811000	-1.273148000
O	2.970374000	-0.999970000	0.859329000
C	3.829705000	-2.130530000	0.971789000
H	4.363094000	-2.017990000	1.915569000
H	3.252753000	-3.059654000	0.993120000
H	4.548429000	-2.165214000	0.147105000
O	4.382080000	1.264626000	0.235189000
H	4.101536000	0.749017000	1.006273000
C	0.962355000	2.726106000	-0.357135000
H	0.865077000	2.575288000	-1.435658000
H	-0.034004000	2.740271000	0.088436000
H	1.394155000	3.713681000	-0.180637000
C	1.805571000	1.713903000	1.790454000
H	0.783807000	1.517758000	2.127266000
H	2.452698000	0.970641000	2.260267000
H	2.091595000	2.711377000	2.135560000

SCF Done: E(RM062X) = -1090.89017158

of imaginary frequency = none

Methanol

C	0.661048000	-0.019427000	0.000003000
H	1.087025000	0.986066000	-0.001125000
H	1.025786000	-0.545254000	0.891098000
H	1.025590000	-0.547139000	-0.890045000
O	-0.746745000	0.122939000	0.000007000
H	-1.130731000	-0.760624000	0.000001000

SCF Done: E(RM062X) = -115.667708336

of imaginary frequency = none

Final thermodynamic product Thermo

C	-4.418123000	1.021882000	0.307353000
C	-3.960651000	2.208859000	-0.238749000
C	-2.679728000	2.294323000	-0.795985000
C	-1.852001000	1.186180000	-0.760746000
H	-5.417761000	0.931382000	0.717545000
H	-4.613892000	3.075501000	-0.250500000
H	-2.340051000	3.215161000	-1.255548000
H	-0.869311000	1.238494000	-1.217296000
C	-3.598016000	-0.113049000	0.313753000
C	-2.275067000	-0.024331000	-0.181762000
C	0.070774000	-1.099401000	-0.152146000
C	0.744820000	-0.020576000	0.357871000
C	0.842357000	-2.218424000	-0.585778000
C	2.198257000	-2.177391000	-0.555898000
H	0.316482000	-3.097670000	-0.943870000

O	-4.113281000	-1.246782000	0.811929000
C	-1.405350000	-1.217033000	-0.104568000
O	-1.892086000	-2.345232000	0.025794000
C	2.906740000	-1.017756000	-0.069642000
N	2.097347000	0.022950000	0.412358000
H	0.231867000	0.836548000	0.779549000
H	-3.475799000	-1.967038000	0.619766000
C	2.771693000	1.187986000	1.013706000
H	1.993007000	1.777253000	1.499144000
H	3.463302000	0.824675000	1.778135000
O	4.135076000	-0.902619000	-0.044893000
C	3.550152000	2.047901000	0.006489000
H	3.047753000	1.984363000	-0.971182000
H	3.493285000	3.089491000	0.335342000
O	4.914472000	1.722392000	-0.071723000
H	4.949294000	0.756775000	-0.174876000
H	2.811808000	-3.002664000	-0.894969000

SCF Done: E(RM062X) = -896.643588261

of imaginary frequency = none

Final thermodynamic product t-Thermo

C	4.641366000	-1.128217000	0.284742000
C	4.169736000	-2.208038000	-0.441841000
C	2.934787000	-2.146341000	-1.097307000
C	2.163088000	-1.004034000	-0.977930000
H	5.608897000	-1.150439000	0.774040000
H	4.778105000	-3.103813000	-0.517163000
H	2.588398000	-2.979821000	-1.697162000
H	1.219254000	-0.938346000	-1.509149000
C	3.880489000	0.043345000	0.379542000
C	2.597374000	0.095945000	-0.215525000
C	0.309995000	1.292512000	-0.190307000
C	-0.438080000	0.185294000	0.117648000
C	-0.379026000	2.496831000	-0.509646000
C	-1.732820000	2.502920000	-0.562271000
H	0.199099000	3.392039000	-0.714096000
O	4.409198000	1.074278000	1.055719000
C	1.782635000	1.318650000	-0.041253000
O	2.317160000	2.392192000	0.258620000
C	-2.516565000	1.322903000	-0.279268000
N	-1.793710000	0.169064000	0.086781000
H	0.045413000	-0.726294000	0.432336000
H	3.824460000	1.848704000	0.909626000
C	-2.570450000	-1.070144000	0.482326000
O	-3.748856000	1.310895000	-0.345378000
C	-3.560492000	-1.461601000	-0.661614000
H	-3.159067000	-1.075894000	-1.610439000
H	-3.564202000	-2.552906000	-0.731058000
O	-4.893760000	-1.085616000	-0.456033000
H	-4.870345000	-0.115376000	-0.424925000
H	-2.302291000	3.387138000	-0.820085000
C	-1.621412000	-2.253608000	0.684338000
H	-1.072961000	-2.504361000	-0.229892000
H	-0.913467000	-2.095444000	1.501536000
H	-2.232374000	-3.116634000	0.953929000
C	-3.299125000	-0.786237000	1.796136000
H	-3.888421000	-1.663110000	2.073496000
H	-2.568953000	-0.587069000	2.585198000
H	-3.974526000	0.063096000	1.706273000

SCF Done: E(RM062X) = -975.235663474

of imaginary frequency = none

C. Common intermediates and transition states describing kinetic pathway

Intermediate 3b

C	4.144880000	1.512175000	0.621092000
C	5.226975000	0.834491000	0.107885000
C	5.087615000	-0.456966000	-0.438145000
C	3.824550000	-1.021227000	-0.451354000
H	4.264095000	2.500002000	1.059633000
H	6.209168000	1.303950000	0.130572000
H	5.943971000	-0.989248000	-0.838273000
H	3.675944000	-2.020366000	-0.855121000
C	2.688520000	-0.343765000	0.020672000
C	0.147147000	-0.427008000	-0.385613000
C	-1.016454000	-1.174847000	-0.500627000
C	2.806552000	0.964065000	0.636893000
C	1.413004000	-1.092462000	-0.040345000
O	1.843913000	1.583064000	1.172407000
C	0.123734000	0.949722000	-0.818703000
C	-0.884362000	1.861572000	-0.903637000
O	-2.764350000	0.913336000	0.312611000
C	-4.139101000	3.094700000	0.101939000
H	-4.081023000	2.971607000	1.185543000
H	-2.422623000	-3.962425000	0.454934000
H	-4.505273000	4.089336000	-0.146730000
N	-1.187347000	-2.452688000	-0.194193000
H	-0.353097000	-2.926166000	0.144139000
C	-2.466870000	-3.143141000	-0.266530000
H	-3.822140000	-1.495299000	-0.702332000
H	-2.622995000	-3.582468000	-1.260257000
C	-3.652093000	-2.241378000	0.085017000
H	-0.649310000	2.823560000	-1.343811000
H	-4.545225000	-2.874612000	0.117783000
H	-4.805600000	2.330729000	-0.304361000
O	1.425207000	-2.328189000	0.140463000
C	-2.211964000	1.815994000	-0.307337000
O	-2.843905000	2.997992000	-0.484908000
H	-1.891351000	-0.674175000	-0.896533000
H	1.083744000	1.312749000	-1.177605000
O	-3.491667000	-1.624532000	1.339172000
H	-3.073234000	-0.763292000	1.186570000

SCF Done: E(RM062X) = -1011.80309272

of imaginary frequency = none

Intermediate t-3b

C	-4.701814000	0.962562000	-0.510468000
C	-5.605029000	0.032172000	-0.050363000
C	-5.182277000	-1.233734000	0.401109000
C	-3.826825000	-1.509796000	0.377736000
H	-5.038171000	1.929851000	-0.875718000
H	-6.665551000	0.278536000	-0.040308000
H	-5.897078000	-1.966107000	0.760968000
H	-3.460951000	-2.478868000	0.709883000
C	-2.869316000	-0.570974000	-0.041388000
C	-0.364721000	-0.128281000	0.353191000
C	0.933178000	-0.613107000	0.433146000
C	-3.276774000	0.719821000	-0.564964000
C	-1.461542000	-1.029494000	-0.029346000
O	-2.481243000	1.569262000	-1.057320000
C	-0.623781000	1.198728000	0.858127000
C	0.181401000	2.291405000	0.956368000
O	2.120603000	1.802252000	-0.426185000

C	3.063084000	4.194936000	-0.138928000
H	2.957322000	4.116441000	-1.222979000
H	3.243254000	5.229048000	0.150011000
N	1.377604000	-1.801468000	0.051083000
H	0.664301000	-2.426036000	-0.321063000
C	2.779144000	-2.229340000	0.133860000
H	3.724690000	-0.306404000	0.549459000
C	3.714119000	-1.063569000	-0.247683000
H	-0.216513000	3.164991000	1.459169000
H	4.729329000	-1.473705000	-0.309664000
H	3.892580000	3.560169000	0.180664000
O	-1.208655000	-2.225365000	-0.285706000
C	1.451613000	2.540954000	0.288052000
O	1.855022000	3.811860000	0.512688000
H	1.680490000	0.041068000	0.867982000
H	-1.622460000	1.333611000	1.267085000
O	3.392724000	-0.488789000	-1.488260000
H	2.773595000	0.238118000	-1.317144000
C	3.108189000	-2.698511000	1.552720000
H	2.488529000	-3.557270000	1.824083000
H	4.159766000	-2.993467000	1.624992000
H	2.922928000	-1.897727000	2.275411000
C	2.949507000	-3.363947000	-0.873893000
H	3.960552000	-3.774242000	-0.808731000
H	2.239730000	-4.171974000	-0.670712000
H	2.783889000	-2.988479000	-1.886351000

SCF Done: E(RM062X) = -1090.40318959

of imaginary frequency = none

Transition state TS2b

C	-3.814886000	-1.618813000	0.552858000
C	-5.008914000	-0.925716000	0.543250000
C	-5.050783000	0.446128000	0.240690000
C	-3.860621000	1.095831000	-0.037737000
H	-3.783250000	-2.677814000	0.792222000
H	-5.931675000	-1.453565000	0.773221000
H	-5.993493000	0.982761000	0.234522000
H	-3.842397000	2.161851000	-0.248385000
C	-1.391907000	1.193284000	-0.250455000
C	-0.175434000	0.489923000	-0.626241000
C	-2.635163000	0.415980000	-0.053181000
C	1.022249000	1.164865000	-0.696756000
C	-0.209851000	-0.917584000	-1.070289000
C	0.891802000	-1.764060000	-1.130426000
H	4.479734000	-3.827075000	0.111000000
O	-1.401474000	2.430302000	-0.077200000
C	-2.575790000	-0.979304000	0.249656000
O	-1.465729000	-1.641719000	0.266288000
C	1.992692000	-1.766432000	-0.220773000
O	2.279697000	-0.977237000	0.685654000
O	2.808347000	-2.844838000	-0.438228000
N	1.256826000	2.437432000	-0.373601000
H	0.448509000	2.956173000	-0.045473000
H	4.564290000	-2.055752000	0.352179000
C	2.594276000	3.004004000	-0.293455000
H	3.613220000	-3.050210000	1.469202000
H	2.527410000	3.880452000	0.355157000
C	3.928658000	-2.941914000	0.428261000
H	2.942425000	3.346505000	-1.277283000
H	4.554425000	2.581421000	0.442557000
H	3.835762000	1.222047000	-0.416790000

H	1.886516000	0.610675000	-1.047718000
C	3.618964000	2.029259000	0.296355000
H	-0.975947000	-1.130265000	-1.816801000
H	0.820047000	-2.646417000	-1.754701000
O	3.202715000	1.508300000	1.532798000
H	2.716433000	0.686022000	1.347252000

SCF Done: E(RM062X) = -1011.79359307

of imaginary frequency = one (-268.3327)

Transition state t-TS2b

C	-4.441159000	1.024080000	-0.468778000
C	-5.447996000	0.079104000	-0.441656000
C	-5.170828000	-1.270783000	-0.166931000
C	-3.856459000	-1.640414000	0.061175000
H	-4.655962000	2.066724000	-0.684816000
H	-6.472727000	0.388321000	-0.634906000
H	-5.968828000	-2.005307000	-0.143719000
H	-3.592341000	-2.677847000	0.248661000
C	-1.422362000	-1.180781000	0.191751000
C	-0.389966000	-0.227783000	0.564410000
C	-2.815958000	-0.702202000	0.054866000
C	0.931313000	-0.613599000	0.597619000
C	-0.737224000	1.126078000	1.043566000
C	0.150920000	2.196748000	1.114758000
H	3.200544000	5.019084000	-0.071433000
O	-1.156173000	-2.381198000	-0.026434000
C	-3.082276000	0.675007000	-0.212763000
O	-2.149138000	1.571716000	-0.240017000
C	1.207223000	2.470214000	0.195405000
O	1.641729000	1.795645000	-0.745165000
O	1.776861000	3.690946000	0.446351000
N	1.444110000	-1.787545000	0.227995000
H	0.770150000	-2.468699000	-0.110606000
H	3.639965000	3.315767000	-0.401211000
C	2.883519000	-2.050018000	0.126699000
H	2.483330000	4.146123000	-1.457444000
C	2.835429000	4.055617000	-0.426571000
H	4.640252000	-1.135593000	-0.691642000
H	3.643532000	-0.008208000	0.229842000
H	1.652723000	0.112368000	0.959714000
C	3.603468000	-0.834136000	-0.495477000
H	-1.509815000	1.140594000	1.813596000
H	-0.103312000	3.021921000	1.768817000
O	3.022213000	-0.416371000	-1.702371000
H	2.363740000	0.264651000	-1.478262000
C	3.473837000	-2.333355000	1.509601000
H	3.022696000	-3.231308000	1.940364000
H	4.555839000	-2.485831000	1.442732000
H	3.285216000	-1.494614000	2.187212000
C	3.044031000	-3.254623000	-0.796854000
H	4.095613000	-3.547593000	-0.855080000
H	2.471447000	-4.109014000	-0.422165000
H	2.692170000	-2.999543000	-1.799443000

SCF Done: E(RM062X) = -1090.39374107

of imaginary frequency = one (-269.9279)

Intermediate 4b

C	3.679356000	-1.632773000	-0.389434000
C	4.890696000	-0.983919000	-0.585002000
C	4.987106000	0.407127000	-0.466786000
C	3.847554000	1.140606000	-0.169333000

H	3.592742000	-2.710704000	-0.477525000
H	5.773353000	-1.567848000	-0.828729000
H	5.939442000	0.903896000	-0.618225000
H	3.871917000	2.224184000	-0.101109000
C	1.372880000	1.290869000	0.233448000
C	0.230868000	0.538780000	0.665140000
C	2.620491000	0.505655000	0.037181000
C	-1.006244000	1.132430000	0.742505000
C	0.405958000	-0.920831000	1.045667000
C	-0.819903000	-1.741963000	1.121014000
H	-4.356799000	-1.692703000	-0.642986000
O	1.366585000	2.516141000	-0.008093000
C	2.534104000	-0.892766000	-0.065807000
O	1.369323000	-1.548107000	0.095554000
C	-1.781350000	-1.749500000	0.132024000
O	-1.856472000	-1.041978000	-0.914388000
O	-2.811547000	-2.658808000	0.370873000
N	-1.300996000	2.396665000	0.421100000
H	-0.529083000	2.945181000	0.053191000
H	-3.467586000	-2.895037000	-1.593550000
C	-2.675416000	2.841621000	0.263693000
H	-4.552529000	-3.430630000	-0.279207000
H	-2.656834000	3.916878000	0.068698000
C	-3.845813000	-2.660006000	-0.593896000
H	-3.222420000	2.677536000	1.199453000
H	-2.822258000	2.169918000	-1.780188000
H	-4.360493000	2.652667000	-1.044175000
H	-1.844226000	0.535728000	1.091042000
C	-3.421740000	2.114328000	-0.859982000
H	0.933973000	-0.982452000	2.010943000
H	-0.893940000	-2.483125000	1.906488000
O	-3.743865000	0.789307000	-0.522200000
H	-3.001745000	0.169455000	-0.748385000

SCF Done: E(RM062X) = -1011.80938608

of imaginary frequency = none

Intermediate t-4b

C	-4.308551000	1.116030000	-0.284954000
C	-5.367932000	0.236062000	-0.457504000
C	-5.171252000	-1.147032000	-0.376784000
C	-3.894384000	-1.635438000	-0.139842000
H	-4.448021000	2.190398000	-0.343733000
H	-6.360737000	0.631148000	-0.652172000
H	-6.005507000	-1.827555000	-0.509422000
H	-3.692889000	-2.701814000	-0.104067000
C	-1.426199000	-1.281424000	0.169905000
C	-0.445747000	-0.317900000	0.575568000
C	-2.816304000	-0.766319000	0.042933000
C	0.891358000	-0.640713000	0.592987000
C	-0.905433000	1.060603000	1.014518000
C	0.118906000	2.123054000	1.087027000
H	3.543775000	2.914484000	-0.704448000
O	-1.179331000	-2.474340000	-0.106058000
C	-3.024257000	0.621345000	-0.021844000
O	-2.014907000	1.500130000	0.121754000
C	1.035103000	2.370217000	0.086055000
O	1.259843000	1.721219000	-0.978521000
O	1.830299000	3.487868000	0.337186000
N	1.427826000	-1.808830000	0.229144000
H	0.765373000	-2.501702000	-0.111797000
H	2.406058000	3.919363000	-1.618939000

C	2.868011000	-2.003545000	0.017473000
H	3.355175000	4.641468000	-0.289868000
C	2.832687000	3.743774000	-0.626692000
H	2.763505000	-1.114244000	-1.944459000
H	4.409680000	-1.342238000	-1.321830000
H	1.593023000	0.116333000	0.926291000
C	3.395704000	-1.016877000	-1.049385000
H	-1.397495000	0.979838000	1.997449000
H	0.041756000	2.848098000	1.887531000
O	3.470879000	0.312435000	-0.607087000
H	2.630033000	0.799291000	-0.820190000
C	3.047052000	-3.430203000	-0.495776000
H	4.107828000	-3.654498000	-0.630987000
H	2.631915000	-4.146863000	0.218803000
H	2.540729000	-3.565781000	-1.457397000
C	3.625615000	-1.804569000	1.329859000
H	3.259829000	-2.501882000	2.088425000
H	4.694326000	-1.980922000	1.173946000
H	3.506339000	-0.781991000	1.693402000

SCF Done: E(RM062X) = -1090.40810646

of imaginary frequency = none

Intermediate d-4b

C	-3.405087000	-1.887898000	1.159498000
C	-4.768696000	-1.646710000	1.071885000
C	-5.258407000	-0.539936000	0.369099000
C	-4.360682000	0.331853000	-0.228788000
H	-3.012813000	-2.743923000	1.698311000
H	-5.461383000	-2.332101000	1.551332000
H	-6.326451000	-0.362652000	0.303227000
H	-4.696431000	1.220513000	-0.754652000
C	-2.013768000	1.102918000	-0.677330000
C	-0.643738000	0.669589000	-0.719627000
C	-2.983901000	0.103563000	-0.157630000
C	0.361076000	1.563313000	-0.983378000
C	-0.337047000	-0.791609000	-0.445390000
C	1.083386000	-1.136569000	-0.135343000
H	3.614003000	0.998053000	2.101286000
O	-2.404883000	2.243361000	-0.995223000
C	-2.501812000	-1.019368000	0.533621000
O	-1.185662000	-1.276135000	0.655223000
C	1.691766000	-0.448875000	0.951560000
O	1.142451000	0.455004000	1.609731000
O	2.968504000	-0.801971000	1.274725000
N	0.217317000	2.872954000	-1.237950000
H	-0.735708000	3.220656000	-1.176230000
H	2.950609000	-0.170720000	3.260521000
C	1.339082000	3.786211000	-1.116425000
H	4.535981000	-0.485055000	2.493975000
H	1.034717000	4.756404000	-1.517518000
C	3.540599000	-0.064873000	2.346501000
H	2.171880000	3.413967000	-1.723562000
H	0.979016000	4.235290000	0.964102000
H	2.564962000	4.747471000	0.359970000
H	1.388773000	1.205615000	-0.984800000
C	1.824587000	3.939801000	0.327751000
H	-0.637407000	-1.395523000	-1.309573000
O	2.456677000	2.774348000	0.804257000
H	1.807725000	2.110824000	1.111153000
C	1.635948000	-2.209515000	-0.911783000
O	1.045015000	-2.818476000	-1.807631000

O	2.927212000	-2.548822000	-0.626841000
C	3.449586000	-3.605245000	-1.416056000
H	3.450920000	-3.345480000	-2.477979000
H	4.471300000	-3.760828000	-1.068313000
H	2.867215000	-4.521569000	-1.288513000

SCF Done: E(RM062X) = -1239.62702364
of imaginary frequency = none

Final kinetic product Kinect

C	4.018898000	1.010414000	-0.489771000
C	4.988106000	0.320726000	0.226565000
C	4.674041000	-0.863979000	0.900384000
C	3.380526000	-1.359488000	0.838067000
H	4.245599000	1.931559000	-1.015110000
H	5.999197000	0.713515000	0.265542000
H	5.438501000	-1.392138000	1.459312000
H	3.102665000	-2.286898000	1.328911000
C	1.025837000	-1.255057000	-0.020364000
C	0.065022000	-0.398260000	-0.665863000
C	2.388976000	-0.679490000	0.124911000
C	-1.214437000	-0.828732000	-0.932007000
C	0.436408000	1.043959000	-0.888296000
C	0.179273000	1.912090000	0.368304000
H	-3.817282000	1.661802000	-0.165618000
O	0.786669000	-2.413796000	0.356461000
C	2.715677000	0.513635000	-0.533888000
O	1.803872000	1.209205000	-1.268391000
C	-1.289463000	1.866622000	0.691166000
O	-1.796452000	1.150518000	1.531095000
O	-1.989393000	2.657499000	-0.122194000
H	0.489014000	2.939559000	0.164154000
H	-3.659466000	2.918542000	1.088333000
C	-3.102863000	-2.380160000	-0.789766000
H	-3.800303000	3.395907000	-0.632919000
H	-3.187222000	-3.461386000	-0.923736000
C	-3.414345000	2.650973000	0.059126000
H	-3.492761000	-1.893704000	-1.689337000
H	-3.546125000	-2.407150000	1.326225000
H	-4.962728000	-2.242871000	0.273648000
H	-1.920110000	-0.152503000	-1.418995000
C	-3.924380000	-1.926222000	0.415649000
H	-0.138853000	1.465863000	-1.717715000
H	0.735477000	1.508994000	1.217653000
O	-3.921525000	-0.519636000	0.534713000
H	-3.139511000	-0.219992000	1.022995000
N	-1.701099000	-2.037040000	-0.645987000
H	-1.067408000	-2.652322000	-0.140196000

SCF Done: E(RM062X) = -1012.33279784
of imaginary frequency = none

Final kinetic product t-Kinect

C	-4.471315000	0.458183000	0.689962000
C	-5.351212000	-0.337423000	-0.031787000
C	-4.879349000	-1.384985000	-0.829263000
C	-3.517041000	-1.637619000	-0.884552000
H	-4.819465000	1.276685000	1.310365000
H	-6.416251000	-0.135418000	0.022548000
H	-5.574060000	-1.997614000	-1.393048000
H	-3.114831000	-2.455758000	-1.473566000
C	-1.164139000	-1.177381000	-0.145827000
C	-0.327327000	-0.217697000	0.524149000

C	-2.613867000	-0.848188000	-0.167205000
C	1.025250000	-0.427675000	0.684309000
C	-0.929781000	1.109652000	0.903498000
C	-0.908244000	2.119593000	-0.270562000
H	3.099460000	2.508086000	0.047018000
O	-0.752779000	-2.240616000	-0.639879000
C	-3.100662000	0.206718000	0.616301000
O	-2.278103000	0.994245000	1.362858000
C	0.522553000	2.360078000	-0.667287000
O	1.086619000	1.825533000	-1.600871000
O	1.132902000	3.177341000	0.191107000
H	-1.372816000	3.054358000	0.051525000
H	2.657724000	3.832299000	-1.061358000
C	3.148546000	-1.671653000	0.289214000
H	2.825669000	4.162036000	0.691591000
C	2.525058000	3.430761000	-0.055360000
H	3.352283000	-1.388464000	-1.847520000
H	4.834960000	-1.087699000	-0.919624000
H	1.620943000	0.329090000	1.195107000
C	3.748702000	-0.940470000	-0.927130000
H	-0.385082000	1.552879000	1.742422000
H	-1.443197000	1.704524000	-1.127500000
O	3.508652000	0.447714000	-0.884248000
H	2.655456000	0.658360000	-1.293335000
N	1.691444000	-1.503159000	0.265640000
H	1.126980000	-2.172224000	-0.256980000
C	3.432825000	-3.167279000	0.174589000
H	4.510491000	-3.342683000	0.128803000
H	3.030221000	-3.699155000	1.040419000
H	2.980921000	-3.583852000	-0.731568000
C	3.743077000	-1.108736000	1.578950000
H	3.231413000	-1.523627000	2.451476000
H	4.800530000	-1.380126000	1.633213000
H	3.681778000	-0.018611000	1.606794000

SCF Done: E(RM062X) = -1090.93087840

of imaginary frequency = none

Final kinetic product **d-Kinect**

C	3.824318000	-0.626764000	-0.395781000
C	4.575117000	-1.564149000	0.301756000
C	3.962232000	-2.667060000	0.904700000
C	2.589496000	-2.829788000	0.794063000
H	4.282044000	0.237678000	-0.864077000
H	5.649058000	-1.430021000	0.383082000
H	4.557479000	-3.390140000	1.451116000
H	2.081557000	-3.681974000	1.234316000
C	0.354181000	-2.104914000	-0.089624000
C	-0.347660000	-1.000617000	-0.691168000
C	1.814639000	-1.896836000	0.099565000
C	-1.687184000	-1.079680000	-0.997897000
C	0.378834000	0.304809000	-0.837100000
C	0.368924000	1.142800000	0.478393000
H	-3.568954000	2.049426000	0.165484000
O	-0.176323000	-3.184383000	0.216218000
C	2.443385000	-0.792881000	-0.491747000
O	1.747061000	0.138275000	-1.208532000
C	-1.066274000	1.433703000	0.866885000
O	-1.717333000	0.710795000	1.591153000
O	-1.543938000	2.518629000	0.271177000
H	-3.063674000	2.941342000	1.626269000
C	-3.908533000	-2.097300000	-0.967623000

H	-3.105711000	3.780886000	0.043223000
H	-4.267414000	-3.110492000	-1.163577000
C	-2.918876000	2.837228000	0.549901000
H	-4.135020000	-1.478920000	-1.841556000
H	-4.405536000	-2.126903000	1.136487000
H	-5.690824000	-1.516117000	0.079709000
H	-2.187272000	-0.222908000	-1.452966000
C	-4.610349000	-1.507162000	0.254853000
H	-0.060544000	0.918235000	-1.628010000
H	0.800984000	0.548088000	1.287118000
O	-4.222295000	-0.166062000	0.466013000
H	-3.407018000	-0.131777000	0.988817000
N	-2.469224000	-2.137460000	-0.789355000
H	-2.026877000	-2.920412000	-0.312857000
C	1.218452000	2.394606000	0.331732000
O	1.978971000	2.788192000	1.183160000
O	1.041091000	2.995347000	-0.844485000
C	1.829514000	4.172242000	-1.054080000
H	2.891598000	3.924301000	-1.011987000
H	1.559573000	4.537393000	-2.042275000
H	1.601933000	4.918783000	-0.291443000

SCF Done: E(RM062X) = -1240.12254843

of imaginary frequency = none

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