Synthesis of pyrrolo[2,3-d]pyridazines and pyrrolo[2,3-c]pyridines (6-azaindoles). Experimental and theoretical study.

Ilya V. Efimov,*[a] Yana V. Sultanova[b], Alessandra Cicolella,[c] Giovanni Talarico[c,d] and Leonid G. Voskressensky[a]

[a] Research Centre: Molecular Design and Synthesis of Innovative Compounds for Medicine, Peoples' Friendship University of Russia (RUDN University), 117198, Russia, Moscow, Miklukho-Maklaya st, 6
[b] Department of Chemistry, Lomonosov Moscow State University,119991 Moscow, Russia
[c] Scuola Superiore Meridionale, Largo San Marcellino, 80138, Naples, Italy
[d] Dipartimento di Scienze Chimiche, Università degli Studi di napoli Federico II, Napoli, Italy

efimov_iv@rudn.ru

Supporting information

1. General information

Starting reagents were purchased from commercial sources and were used without any additional purification or were prepared according to literature procedures. ^{1}H and ^{13}C spectra were acquired on a Bruker Avance Neo 700 spectrometer (with operating frequencies of 700 and 176 respectively) and Jeol JNM-ECA 600 spectrometer (with operating frequencies of 600 and 150 respectively) at room temperature and referenced to the residual signals of the solvent. The solvents used for NMR was DMSO-d_6. Coupling constants are reported in Hertz (*J*/Hz). The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quadruplet; m, multiplet; dd, doublet of doublets and br s, broad singlet. The wavelengths are reported in reciprocal centimeters (ν_{max} /cm^{-1}). HRMS spectra were recorded on a tandem quadrupole time-of-flight (QTOF) accurate mass detector (Agilent 6545 Q-TOF LC/MS; Agilent Technologies, USA). The reaction progress was monitored by TLC and the spots were visualized under UV light (254 or 365 nm). Melting points (not corrected) were determined on a SMP-10 apparatus. Solvents were distilled and dried according to standard procedures. All microwave irradiation experiments were carried out using CEM-Discover, operating at a frequency of 2.45 GHz with continuous irradiation power from 0 to 300W. The reactions were carried out in 10 mL snap-cap glass vials. The temperature was measured with an IR sensor on the outer surface of the process vial. The reaction vessel is cooled rapidly (60-120s) to ambient temperature by gas jet cooling after the irradiation period.

2. General procedure for the synthesis of the starting materials

*General procedure for the synthesis of 4-aroylpyrroles **1a-j**.*

A 50 mL round-bottom flask equipped with a magnetic stirring bar was charged with mixture of enaminone (10 mmol) and of *tert*-BuOK (20 mmol) and 10 ml of anhydrous DMF. The mixture was stirred until all substrates to be completely dissolved on the ice-water bath. Than to the prepared mixture at 0 °C appropriate isocyanide (20 mmol) was added. After 1 min the mixture was quenched with 25 mL of 10% solution of HCl. After 2 hours the formed precipitate was filtered off and dried on air to give final product. The protocols for preparation of 4-aroylpyrroles were also reported previously.[S1] The structure of all used pyrroles are presented below (Figure 1).

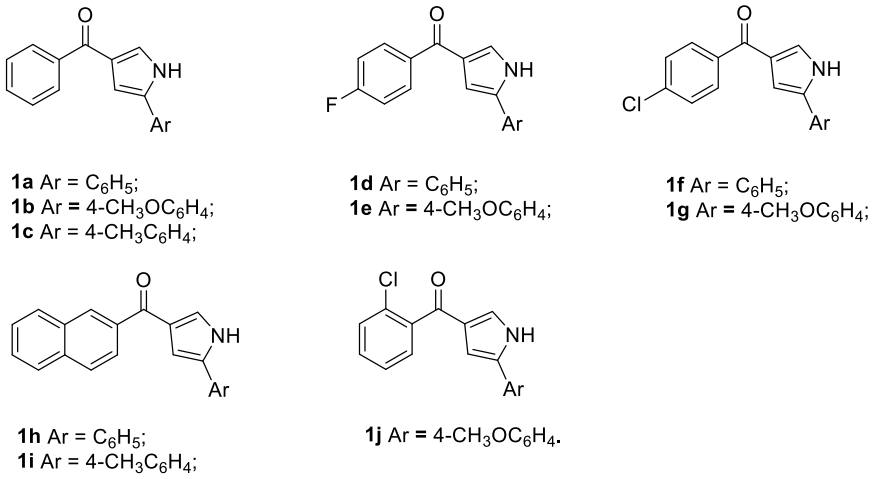
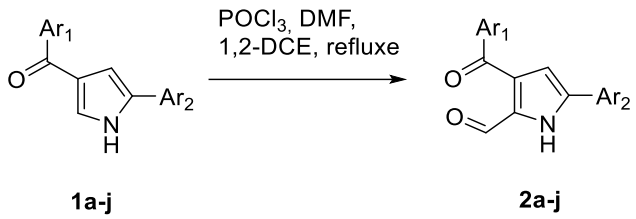


Figure 1. Scope of used pyrroles.

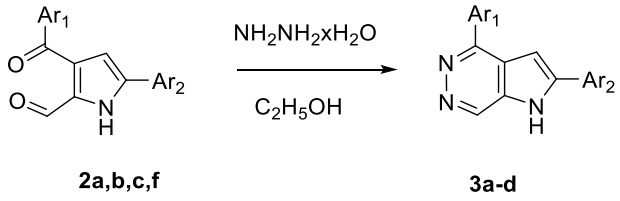
General procedure for formylation of 4-aroylpyrroles (GP1).



Scheme 1. Formylation of 4-aroylpyrroles

A 50 mL round-bottom flask equipped with a magnetic stirring bar was charged 10 mL of 1,2-DCE and pyrrole **1a** (247.3 mg, 1.0 mmol, 1 equiv). Then solution of *N*,*N*-dimethylformamide (109.6 mg, 1.5 mmol, 1.5 equiv), $POCl_3$ (230 mg, 1.5 mmol, 1.5 equiv) in 10 mL of 1,2-DCE was added dropwise, and the reaction mixture was refluxed until the reaction was judged to be completed by thin-layer chromatography (TLC; hexane/ethyl acetate = 5/1) analysis (around 1 hour). Then the reaction mixture was cooled to room temperature and all volatiles were evaporated. The product was purified by column chromatography (hexane/ethyl acetate = 10/1).

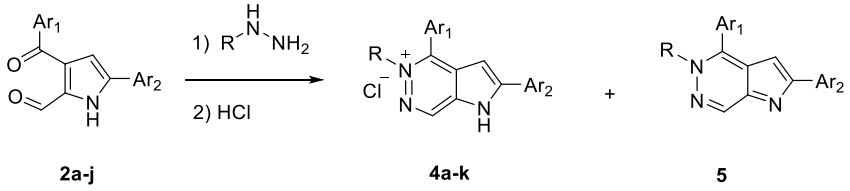
General procedure for the synthesis of pyrrolo[2,3-d]pyridazines (GP2).



Scheme 2. Preparation of pyrrolo[2,3-d]pyridazines

A 50 mL round-bottom flask equipped with a magnetic stirring bar was charged with 1*H*-pyrrole-2-carbaldehyde (275.3 mg, 1.0 mmol, 1 equiv), 10 mL of ethanol and hydrazine hydrate (100 mg, 2 mmol, 2 equiv.). The reaction mixture was stirred overnight and formed precipitate was filtered off and dried on air.

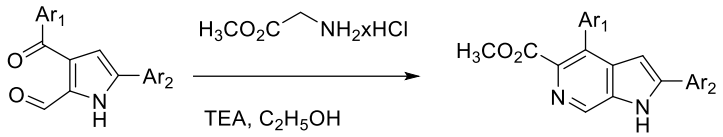
General procedure for the synthesis of pyrrolo[2,3-d]pyridazin-5-ium chlorides (GP3).



Scheme 3. Preparation of pyrrolo[2,3-d]pyridazin-5-ium chlorides

A 50 mL round-bottom flask equipped with a magnetic stirring bar was charged with 1*H*-pyrrole-2-carbaldehyde (275.3 mg, 1.0 mmol, 1 equiv), 10 mL of ethanol and phenyl hydrazine (108 mg, 1.1 mmol, 1.1 equiv.). The reaction mixture was stirred overnight. The reaction progress was monitored by TLC (hexane/ethyl acetate = 2/1). After completion 50 μL of HCl^{conc} was added and reaction mixture was refluxed until the reaction was judged to be completed by TLC (hexane/ethyl acetate = 5/1) analysis (around 1-6 hours). Then the reaction mixture was cooled to room temperature and all volatiles were evaporated. The product was purified by flash chromatography (hexane/ethyl acetate = 1/1).

General procedure for the synthesis of pyrrolo[2,3-d]pyridines (6-azaindoles) (GP4).



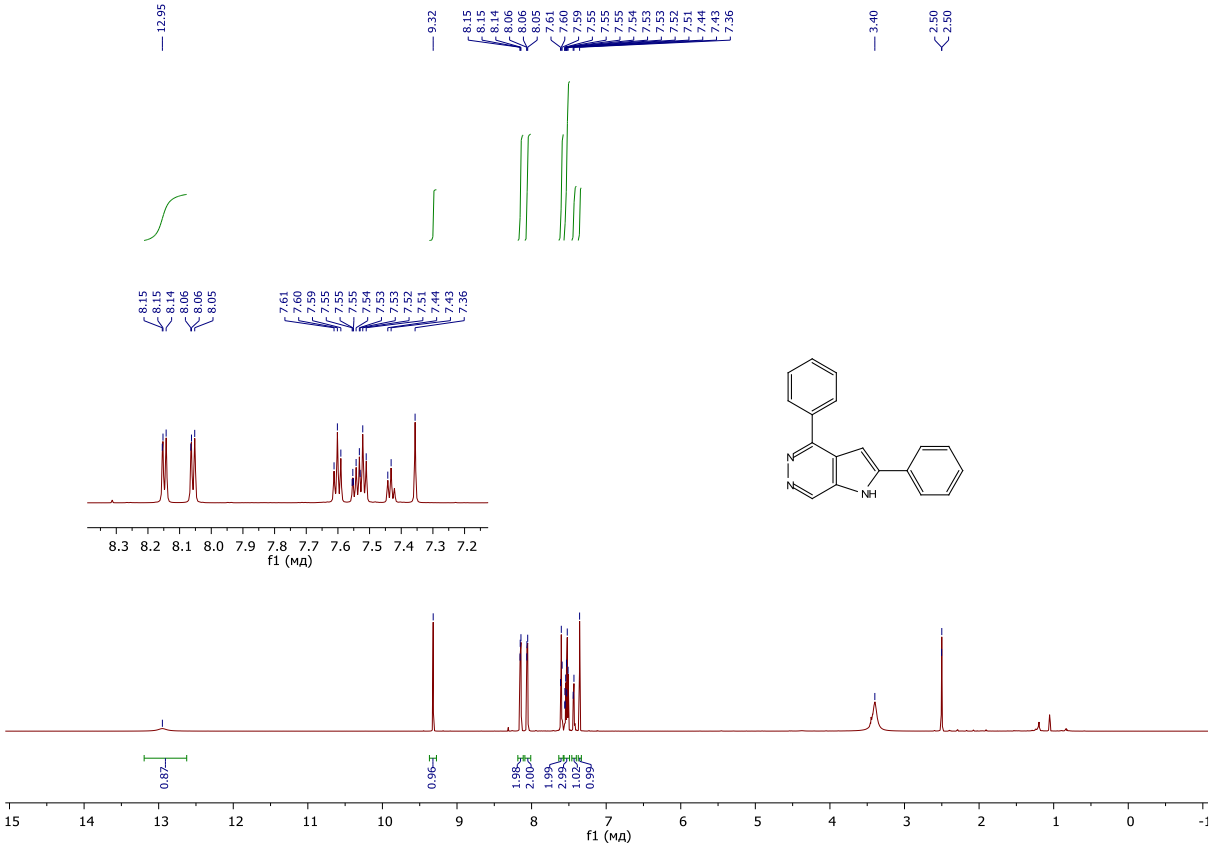
2b,e,f,h,i,j **6a-e**

Scheme 4. Preparation of *pyrrolo[2,3-d]pyridines (6-azaindoles)*

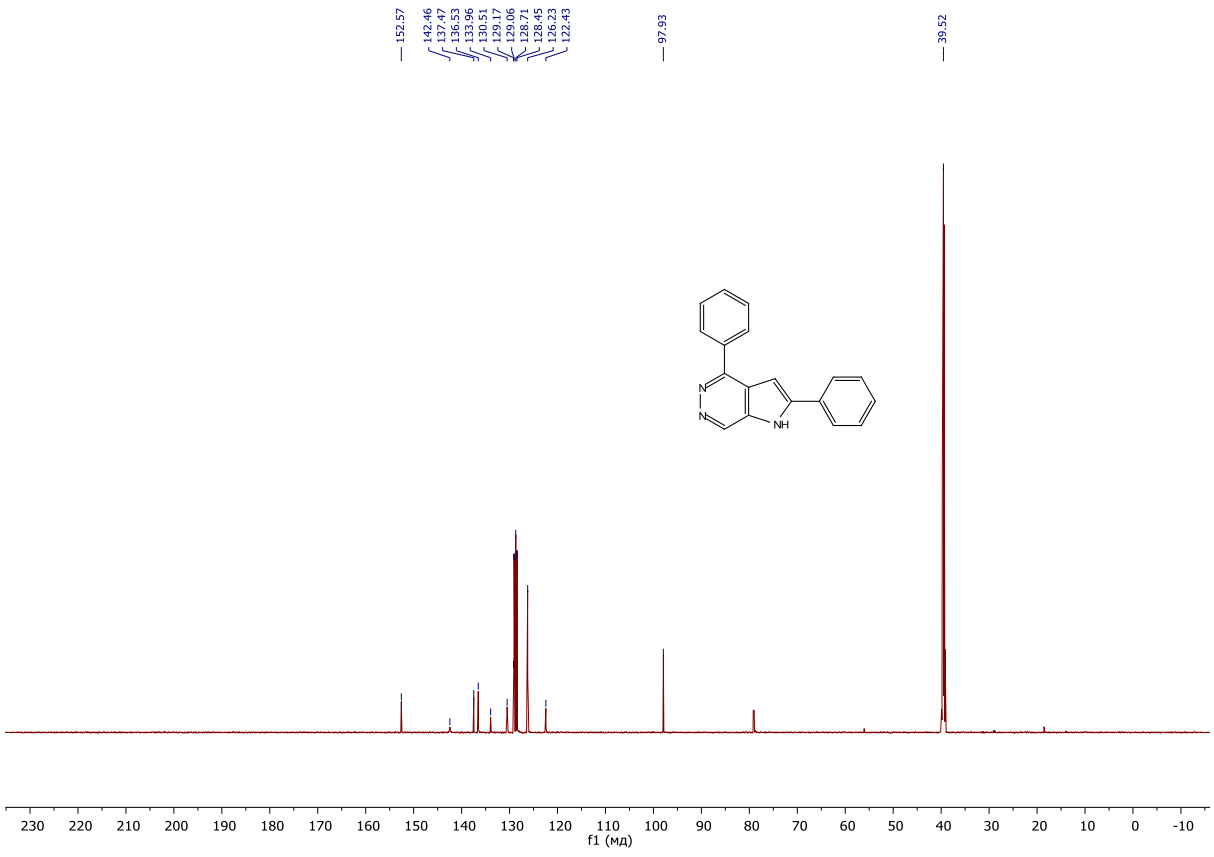
A 50 mL round-bottom flask equipped with a magnetic stirring bar was charged with 1*H*-pyrrole-2-carbaldehyde (275.3 mg, 1.0 mmol, 1 equiv), methyl 2-aminoacetate hydrochloride (138 mg, 1.1 mmol, 1.1 equiv.), trimethylamine (153 μL, 1.1 mmol, 1.1 equiv.) and 10 mL ethanol. The reaction mixture was refluxed until the reaction was judged to be completed by TLC (hexane/ethyl acetate = 3/2) analysis (around 6 hours). Then the reaction mixture was cooled to room temperature, all volatiles were evaporated and 10 mL of H_2O was added. The reaction mixture was stirred around 30 minutes and formed precipitate was filtered off and dried on air.

3. NMR

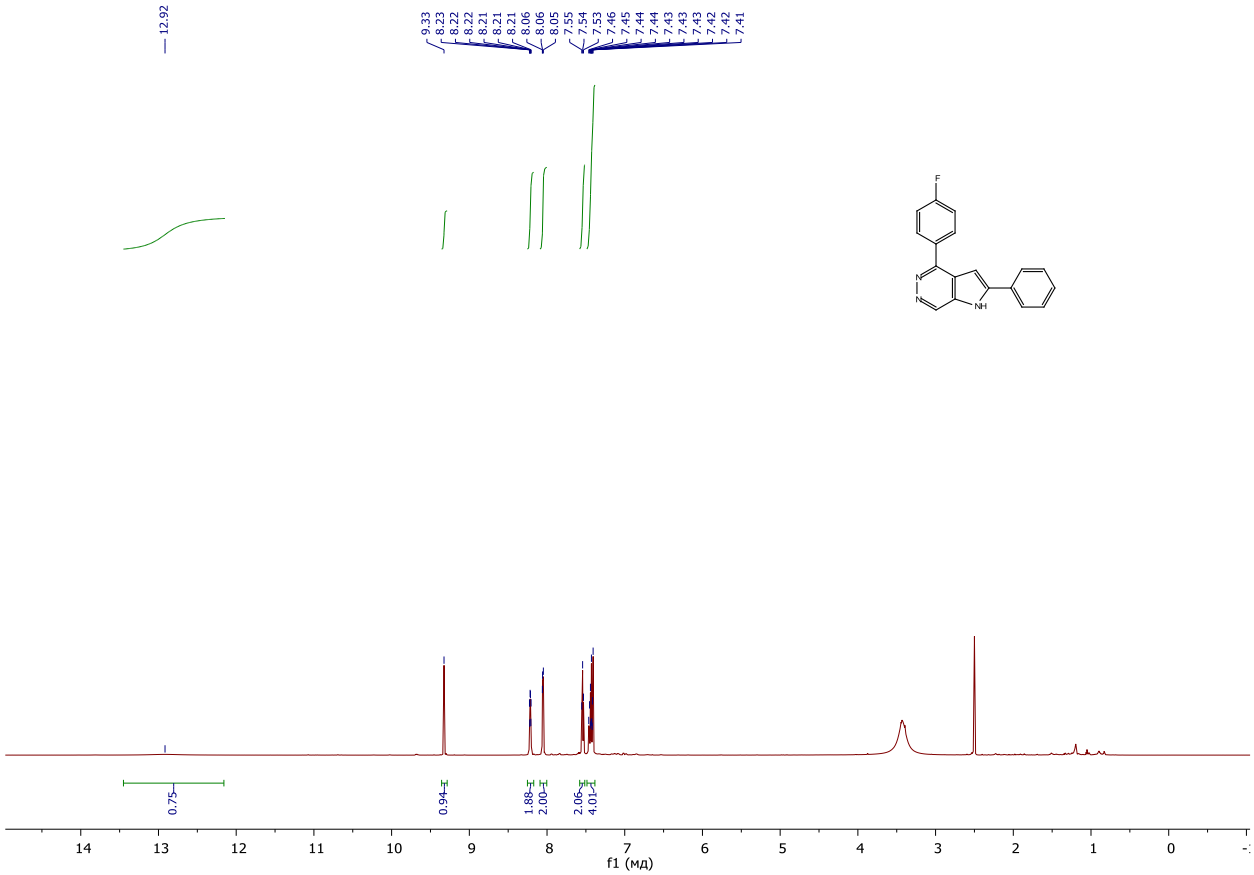
3a ^{1}H NMR



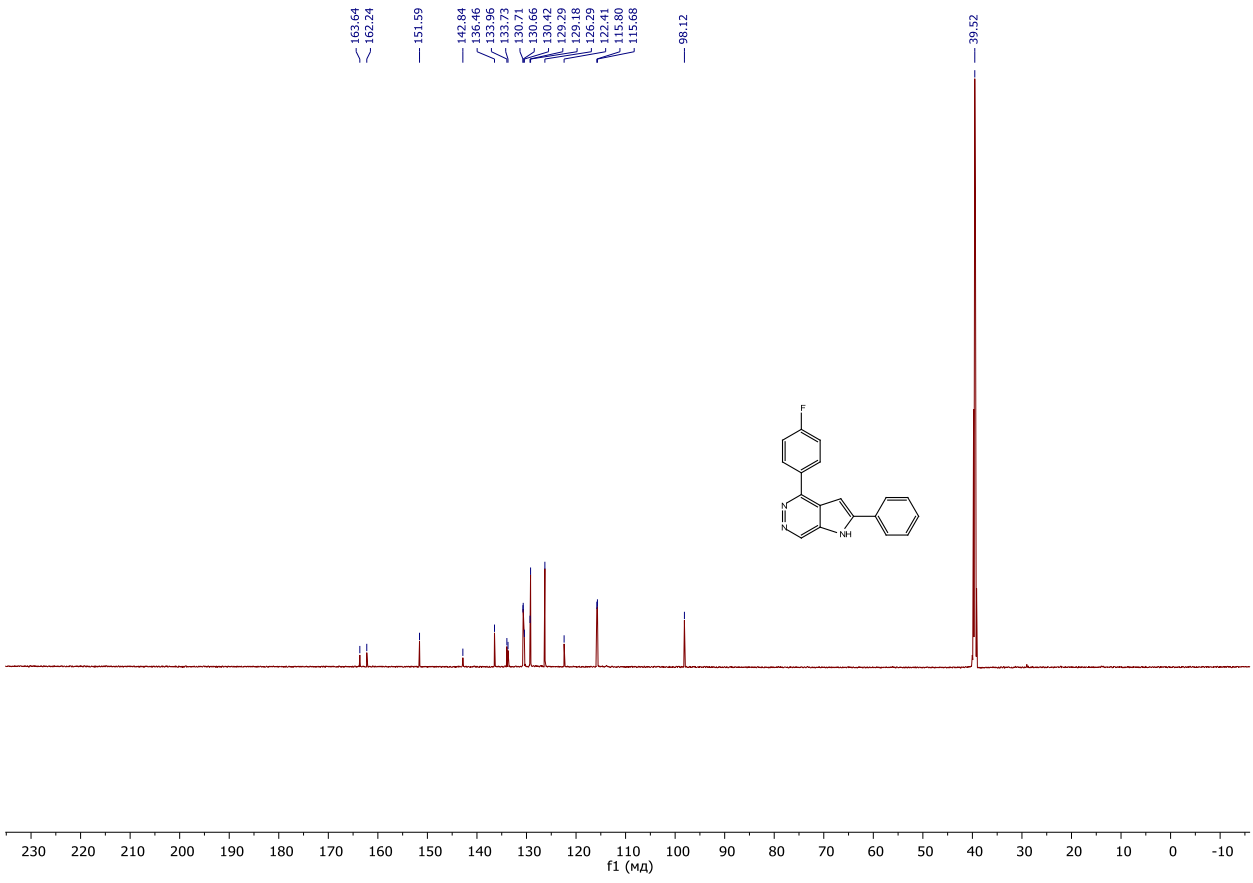
3a ^{13}C NMR



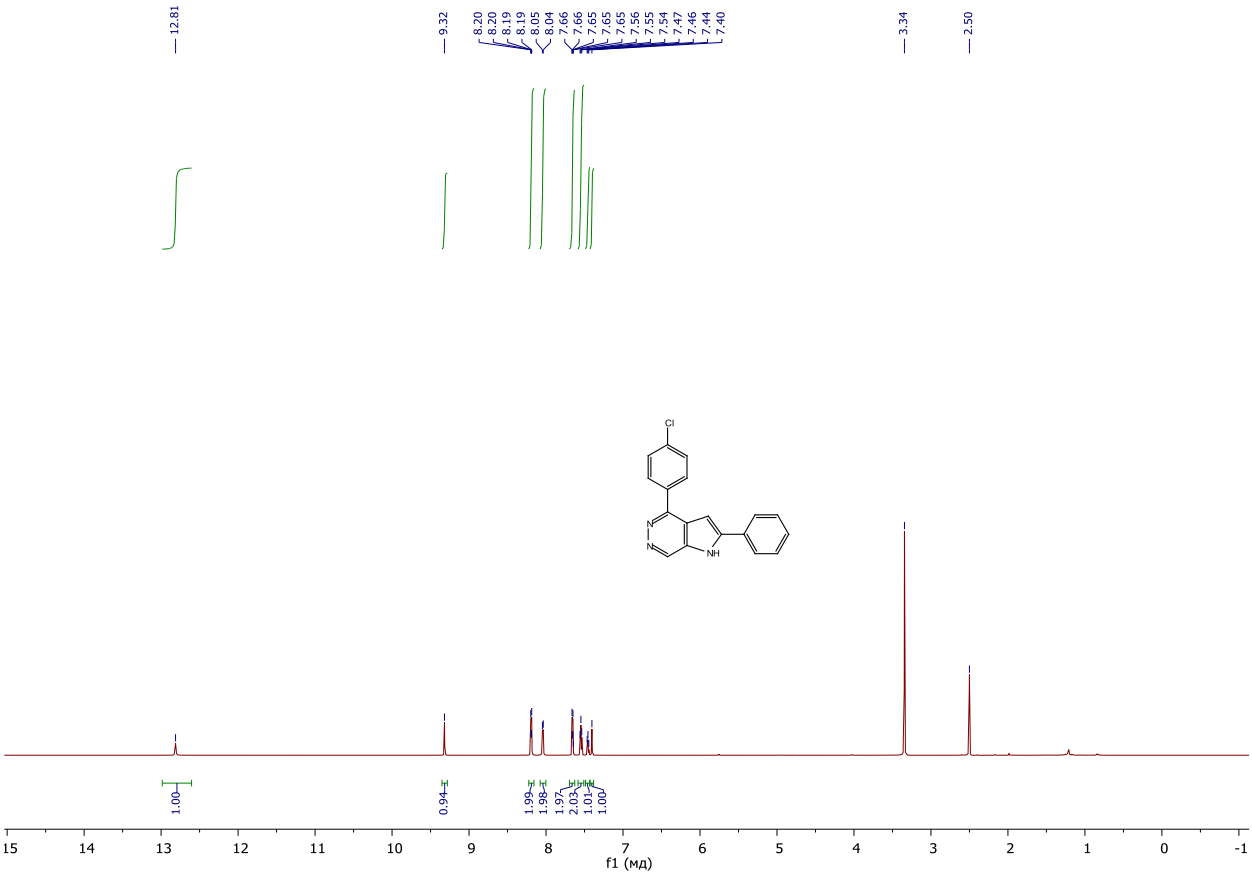
3b ^{1}H NMR



3b ^{13}C NMR



3c ^{1}H NMR



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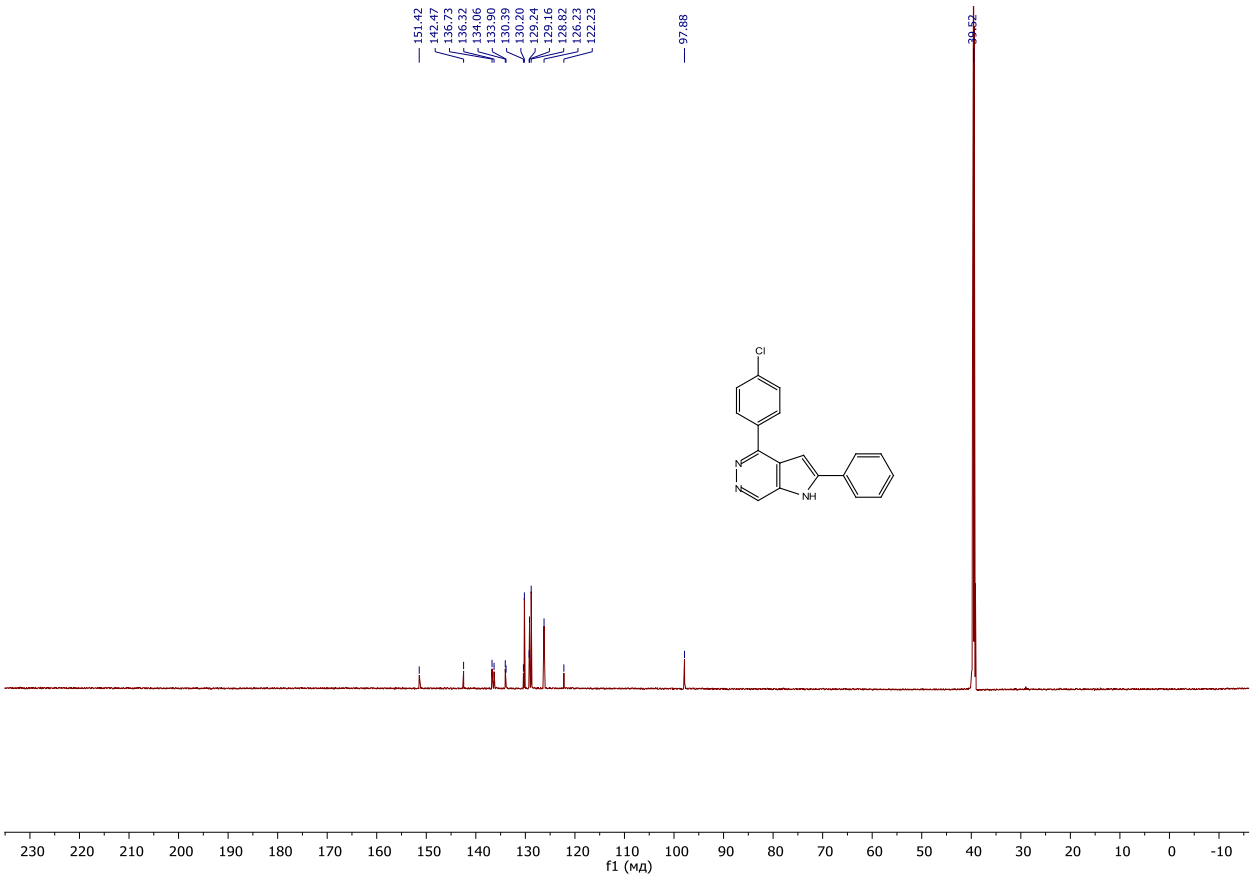
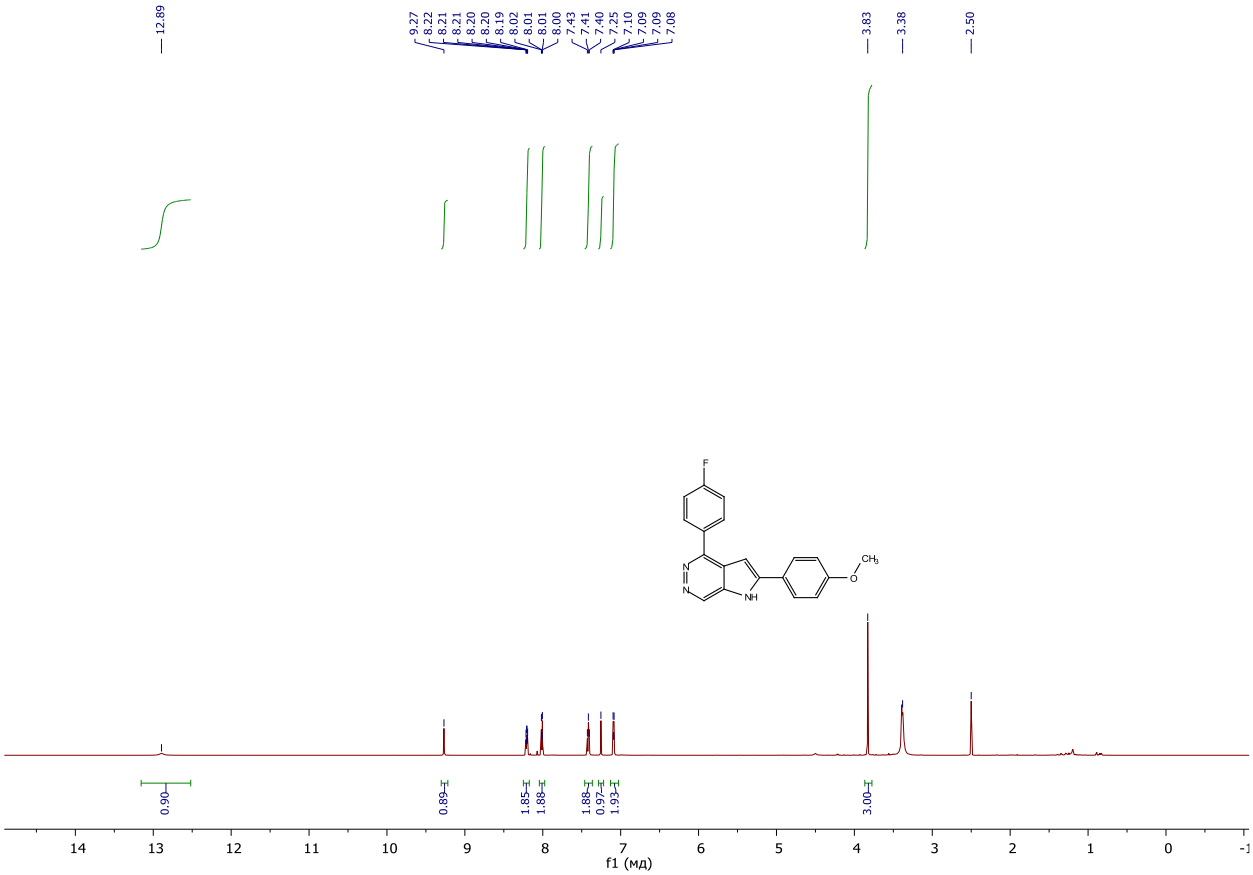


3d ^{1}H NMR



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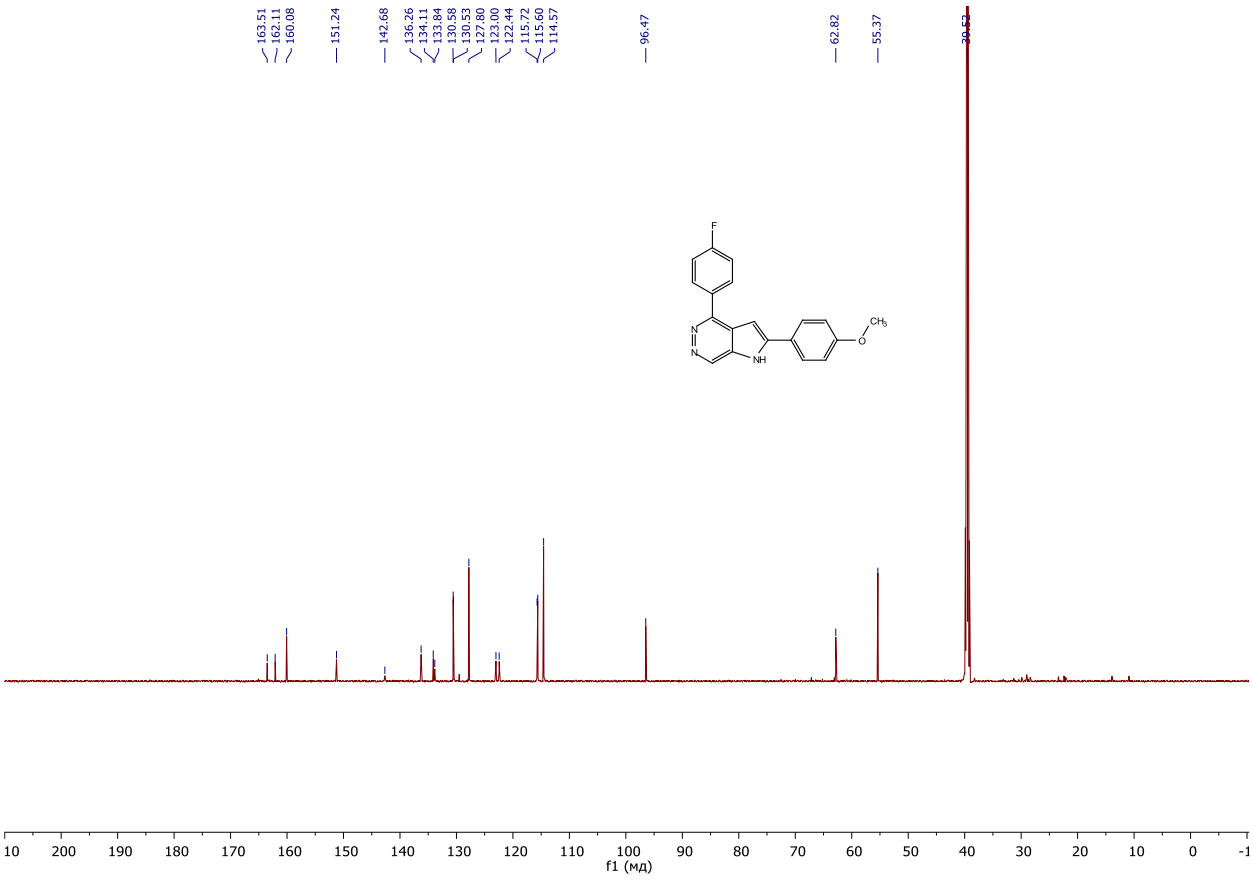
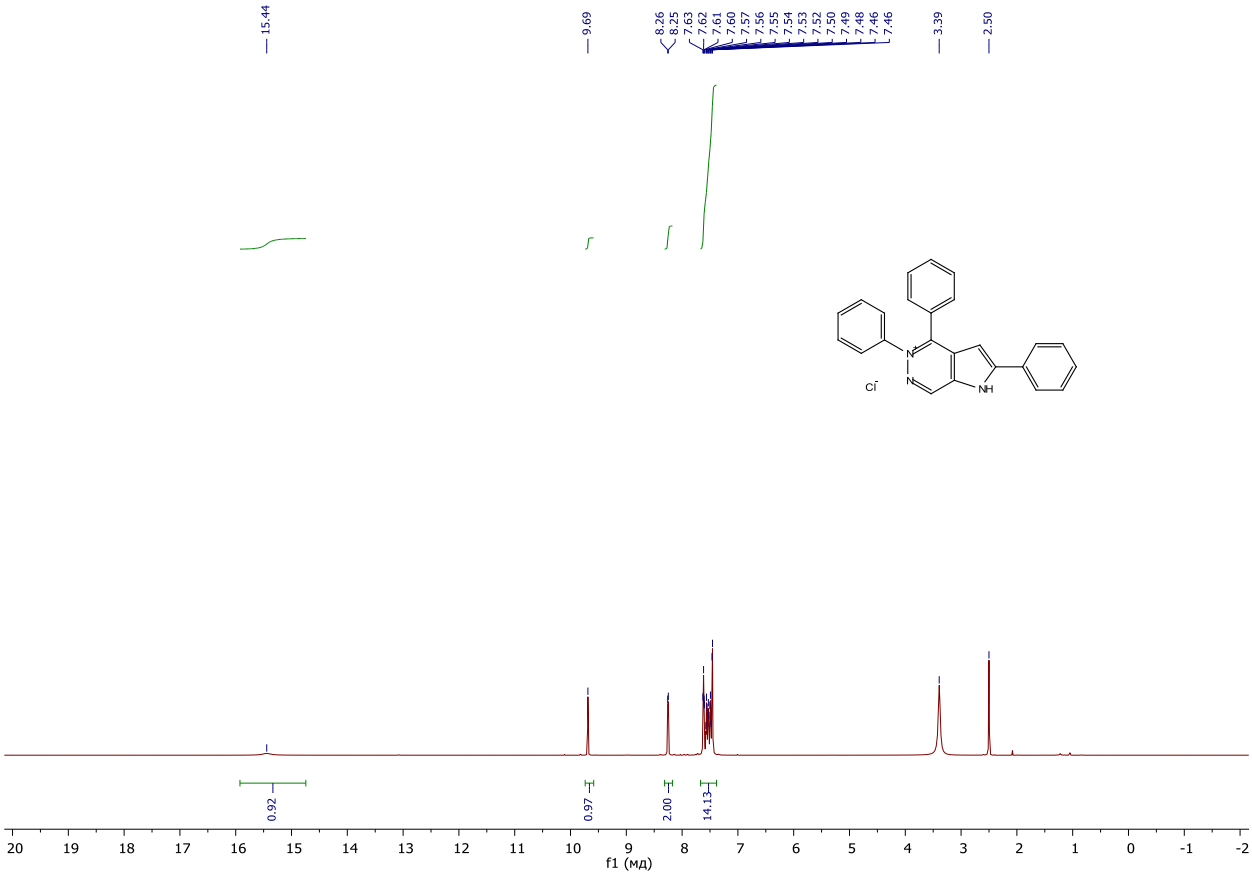


4a ^{1}H NMR



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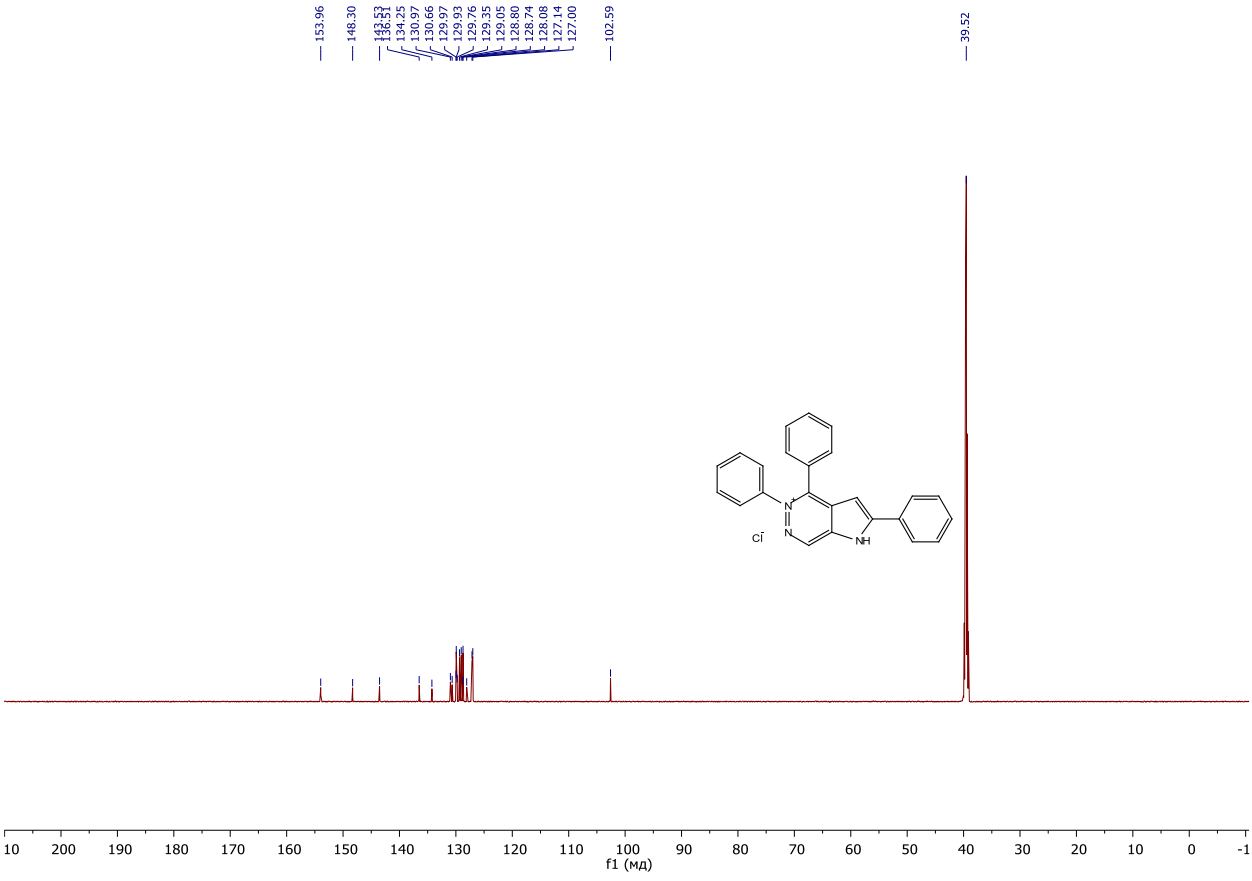

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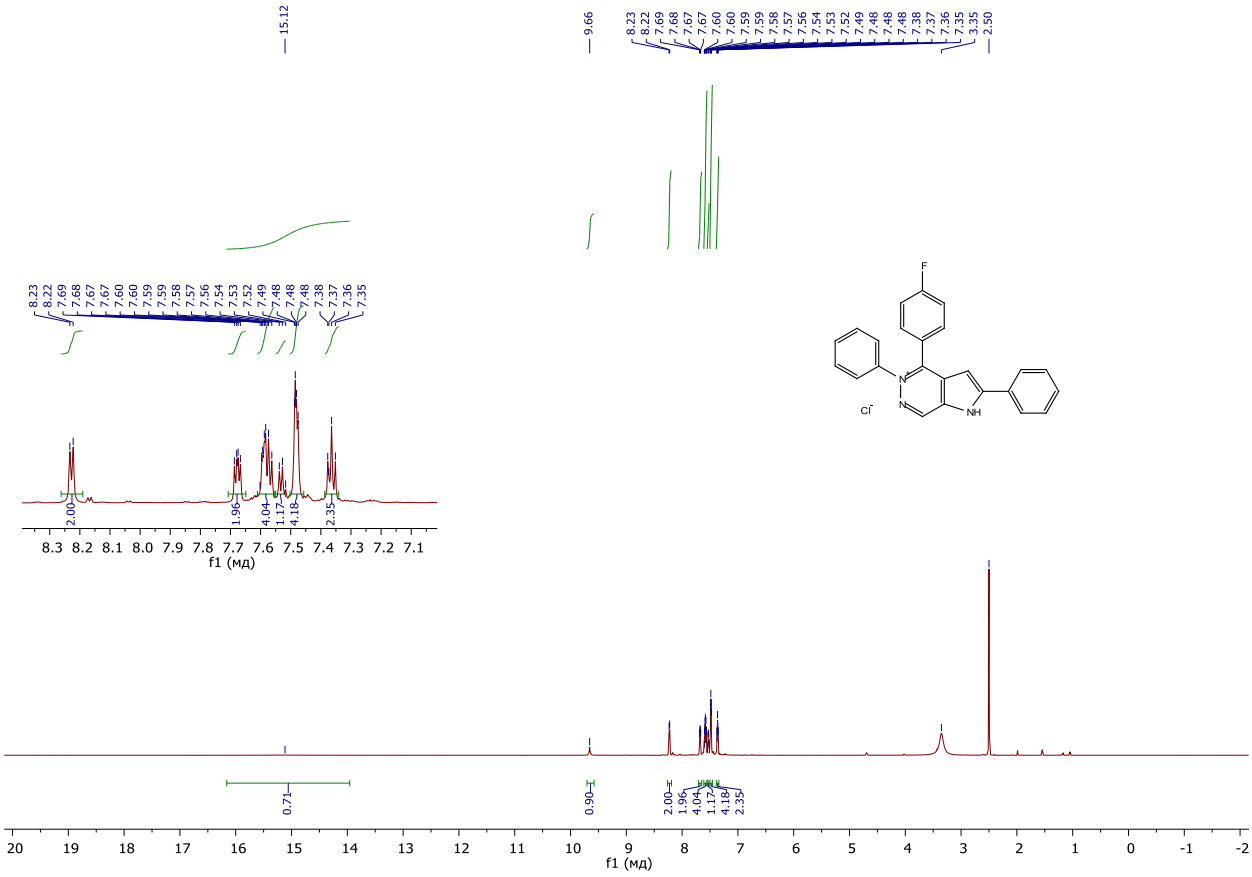

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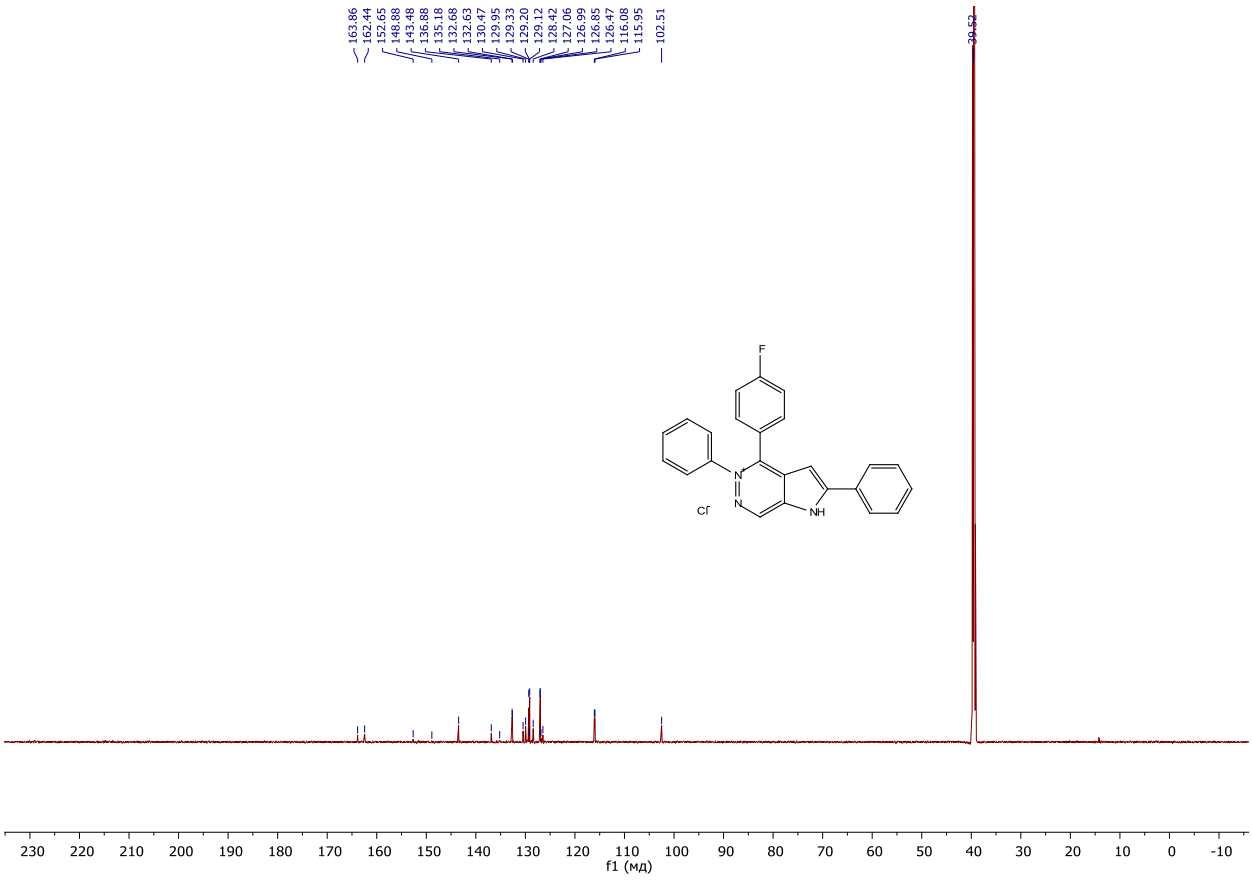

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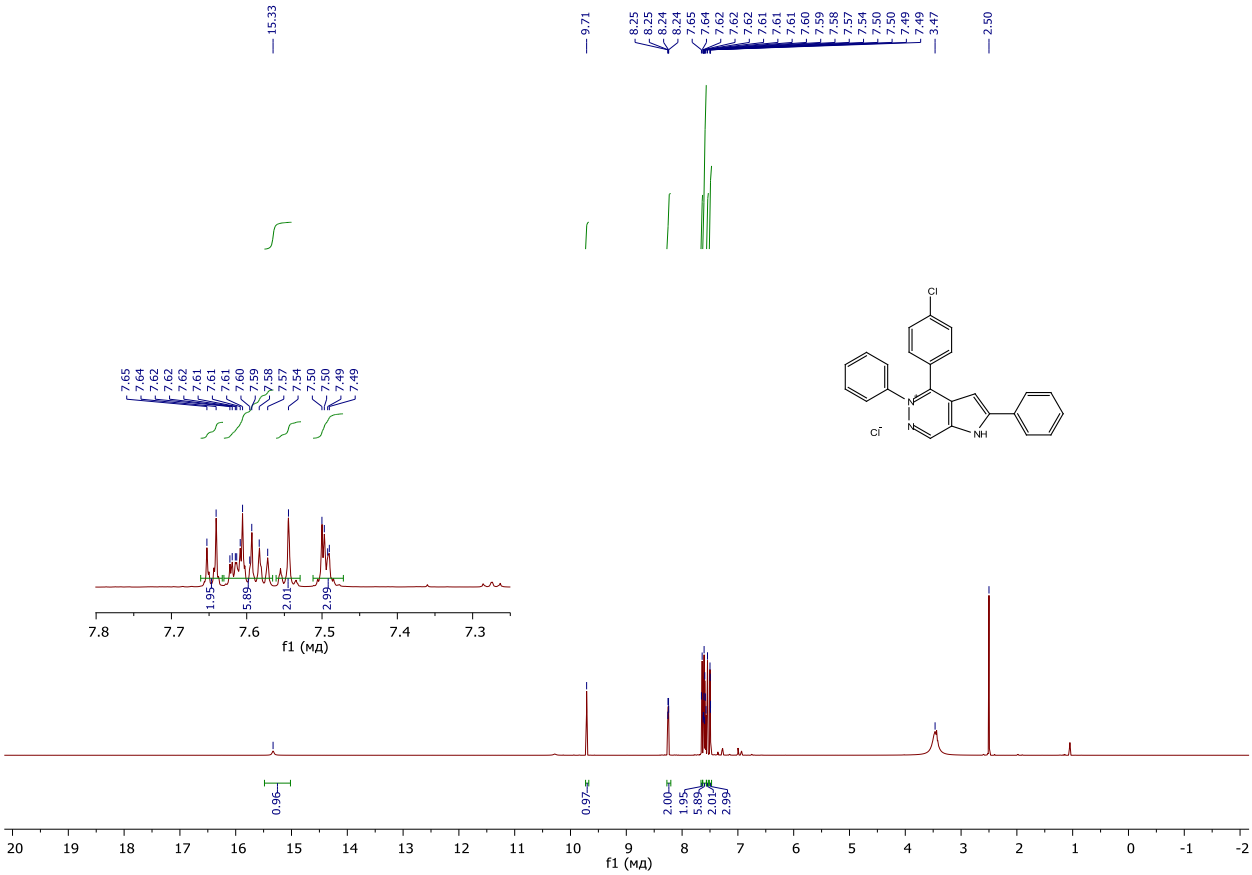

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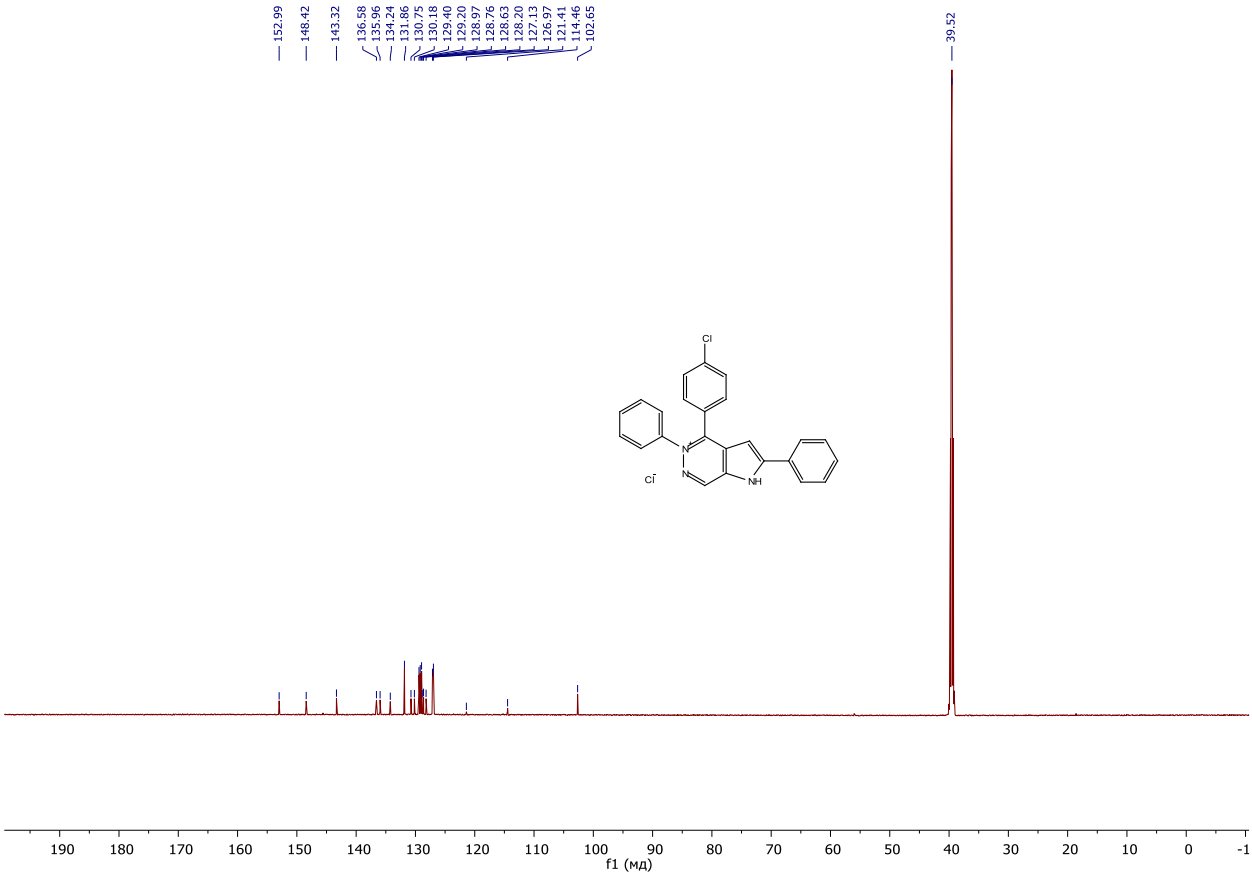

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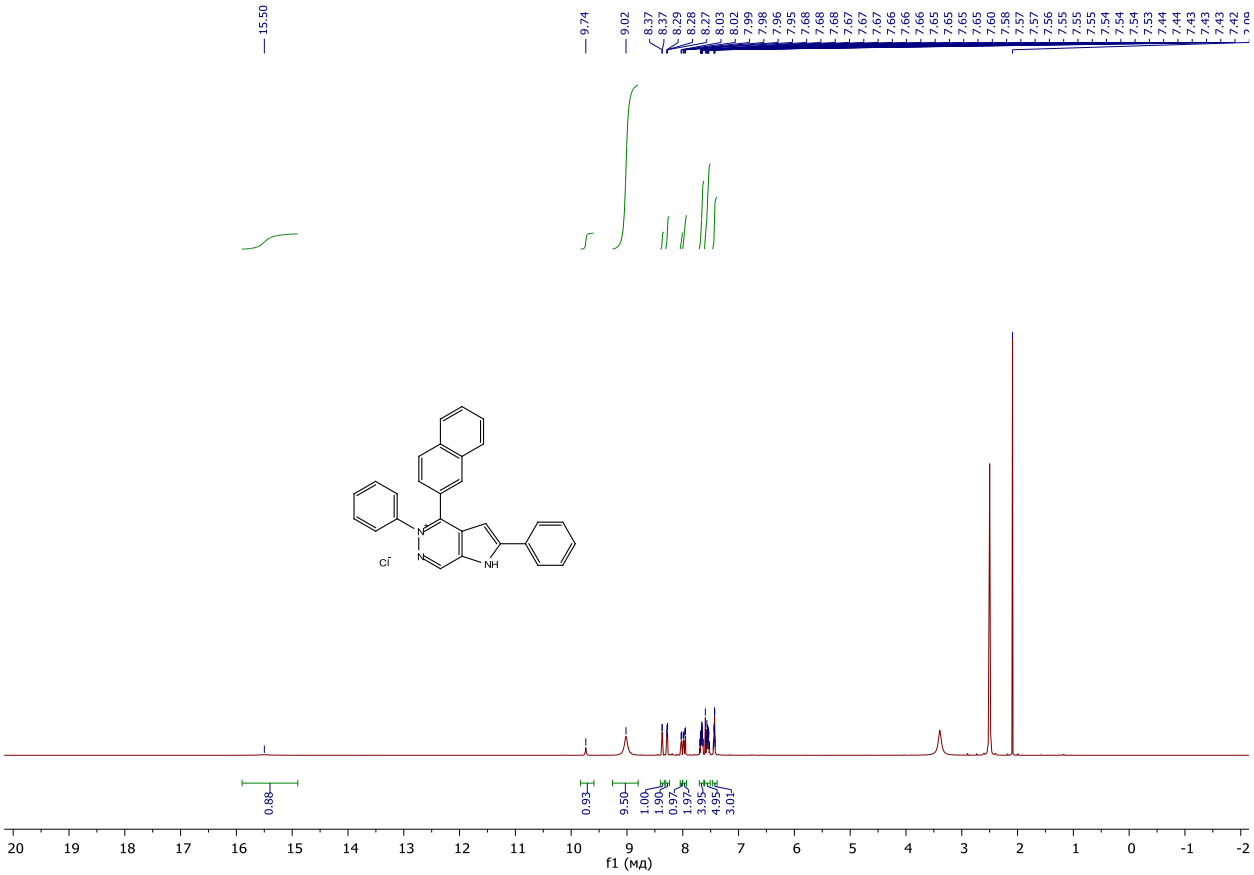

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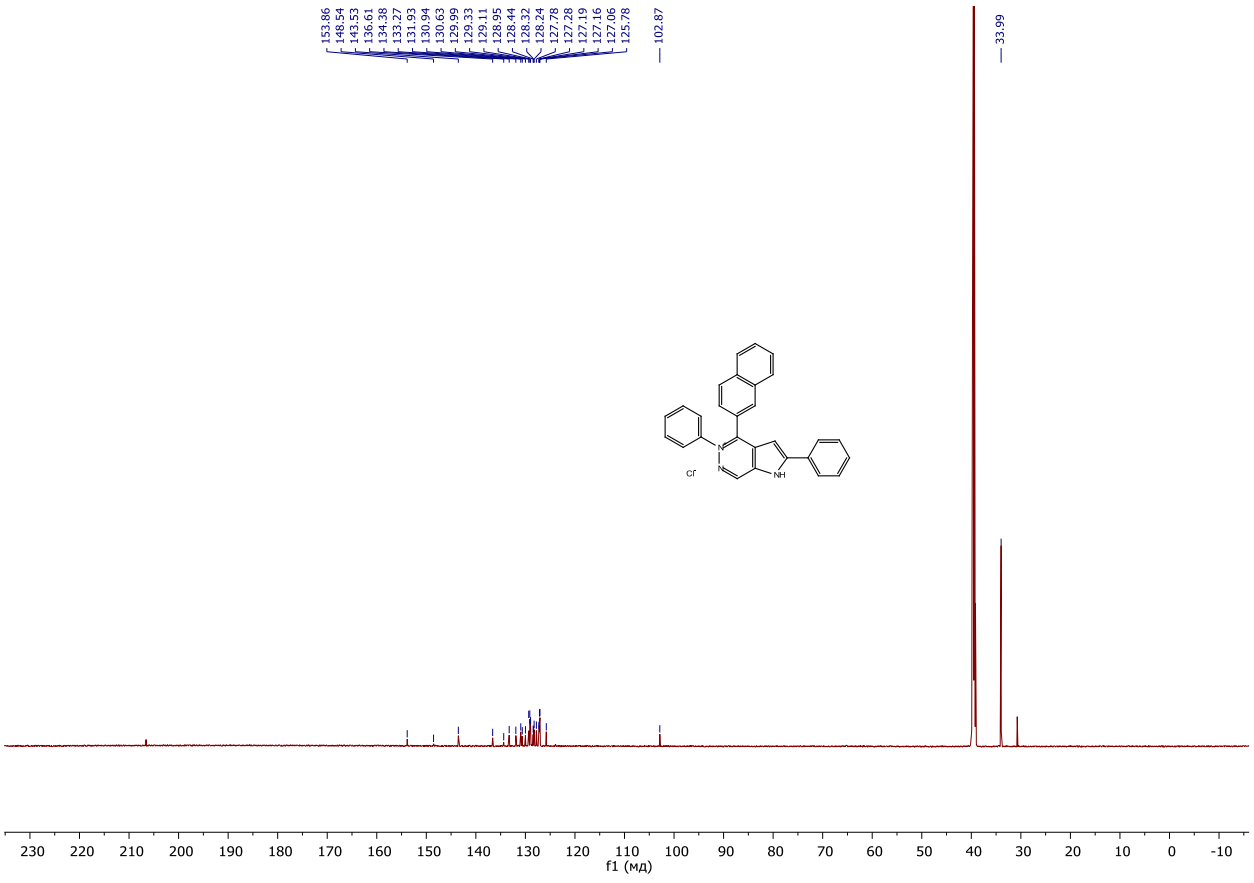

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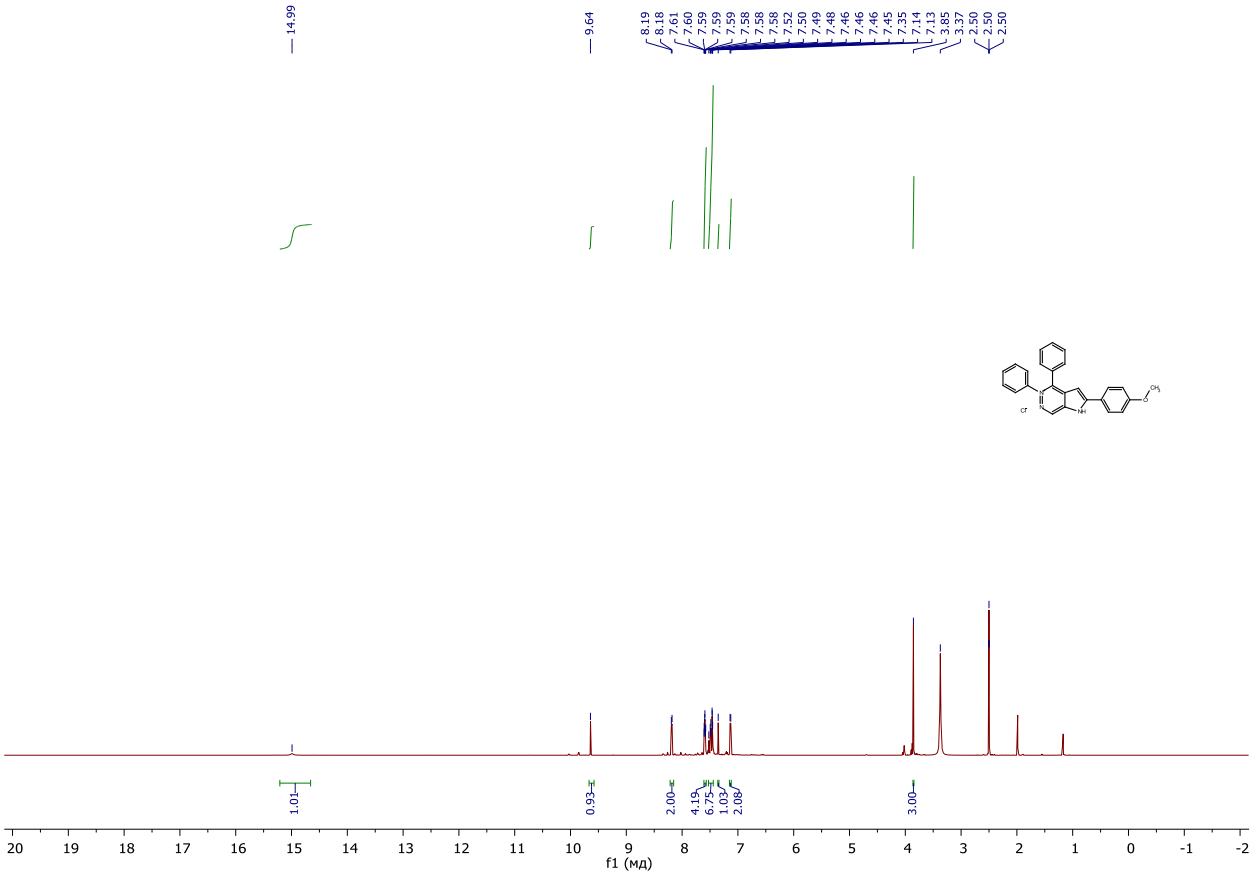

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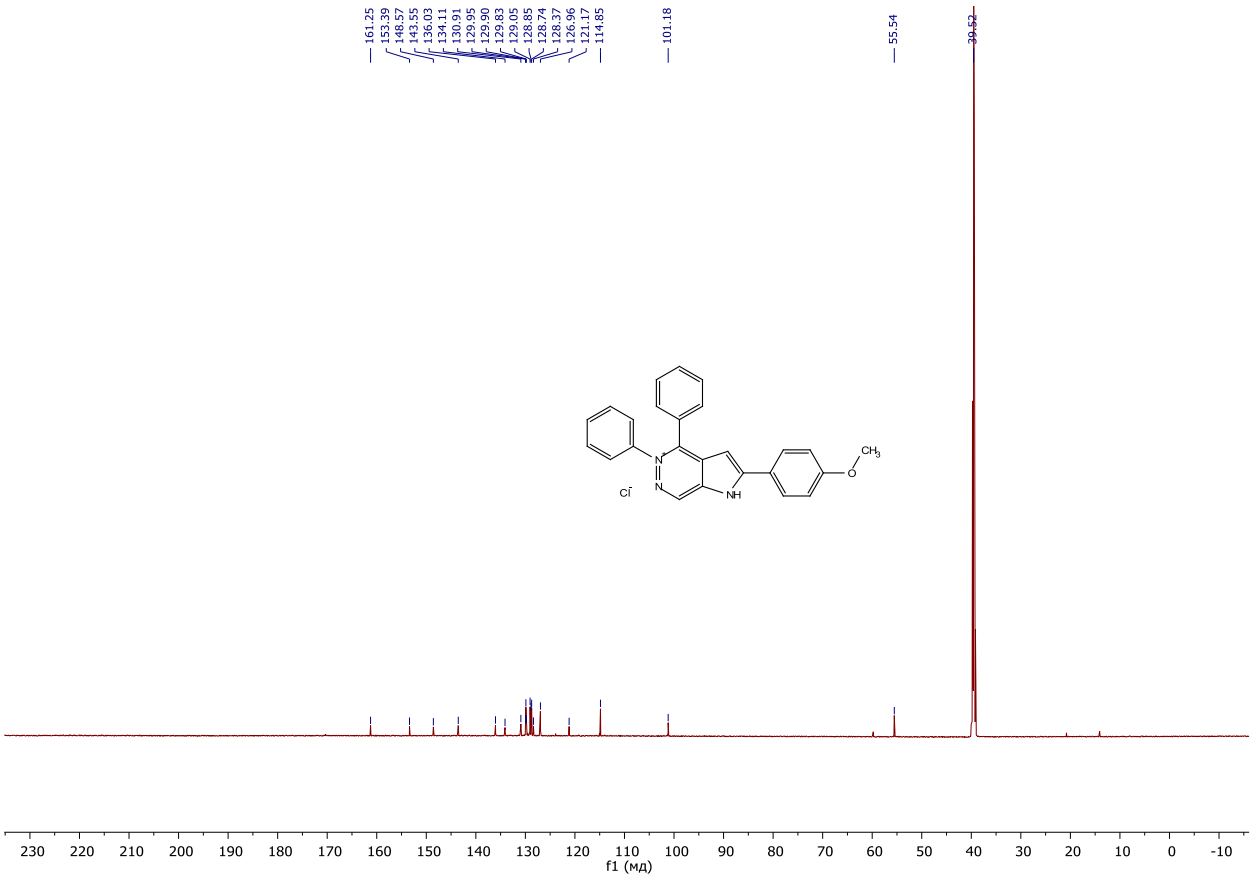
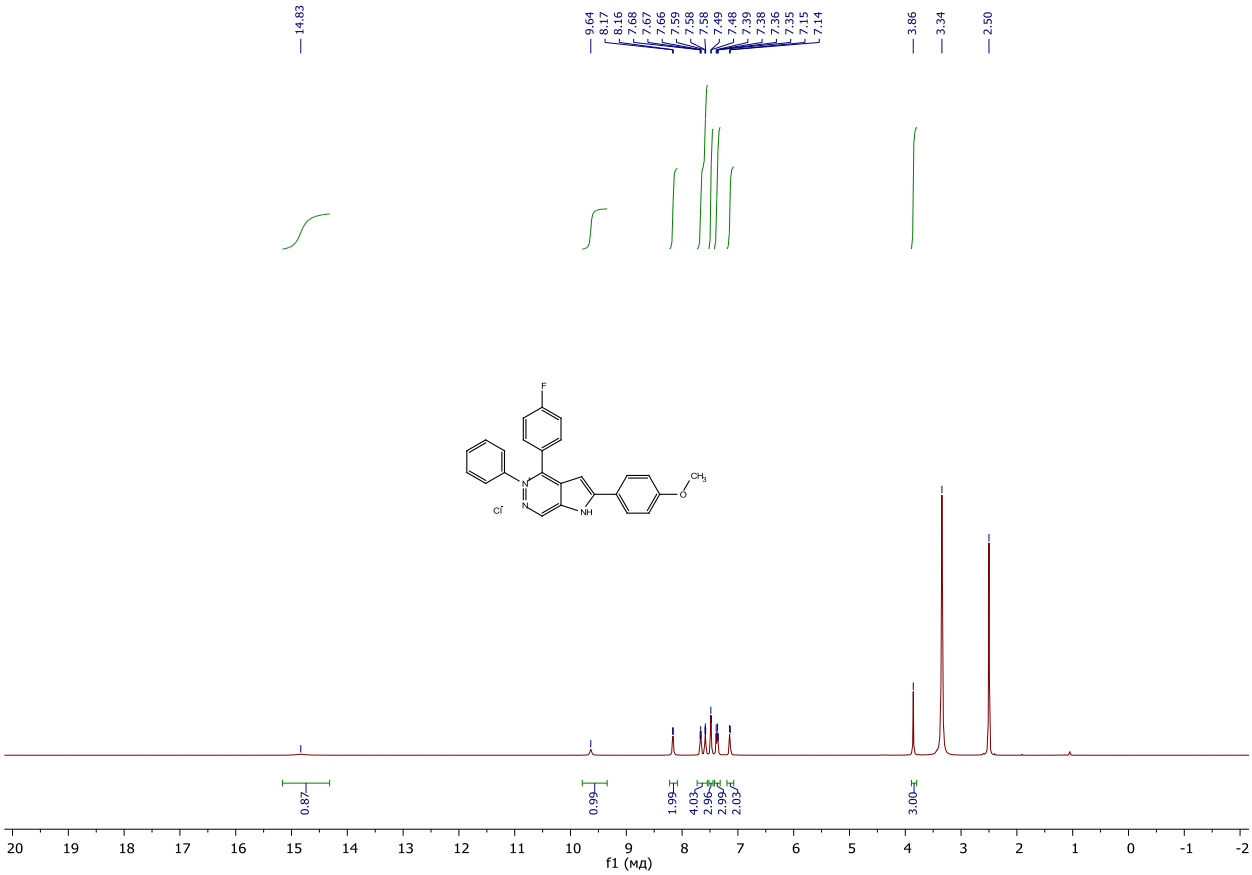
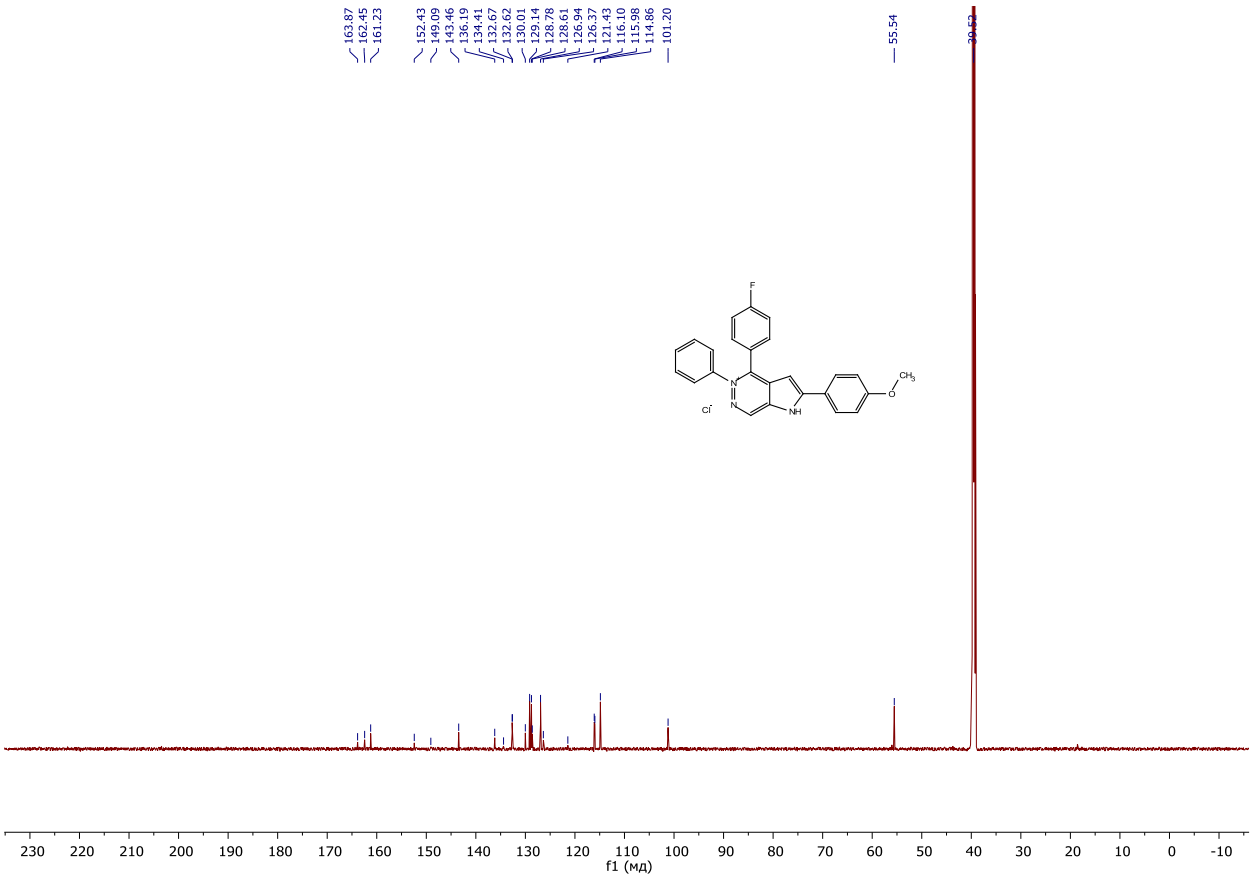


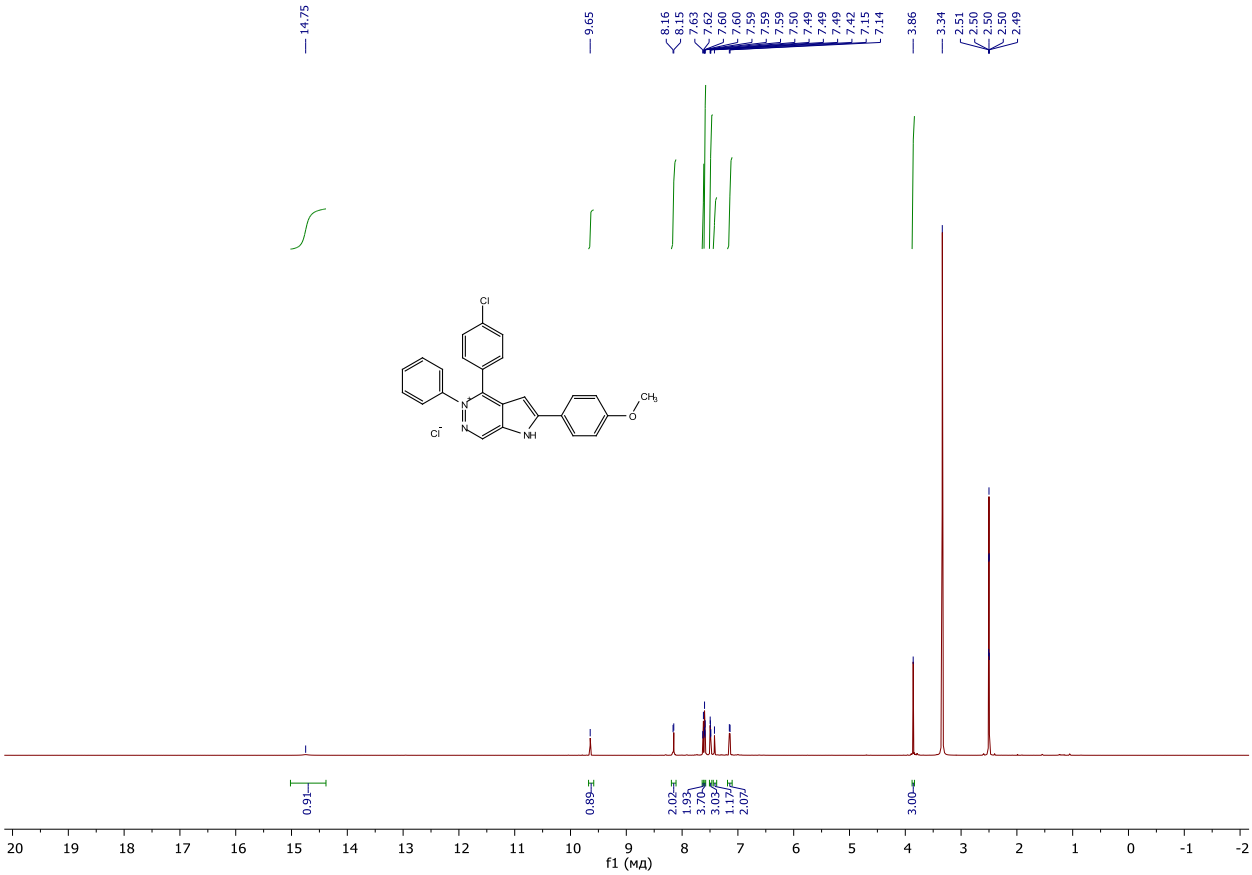
4f ^{1}H NMR



4f ^{13}C NMR



4g ^{1}H NMR



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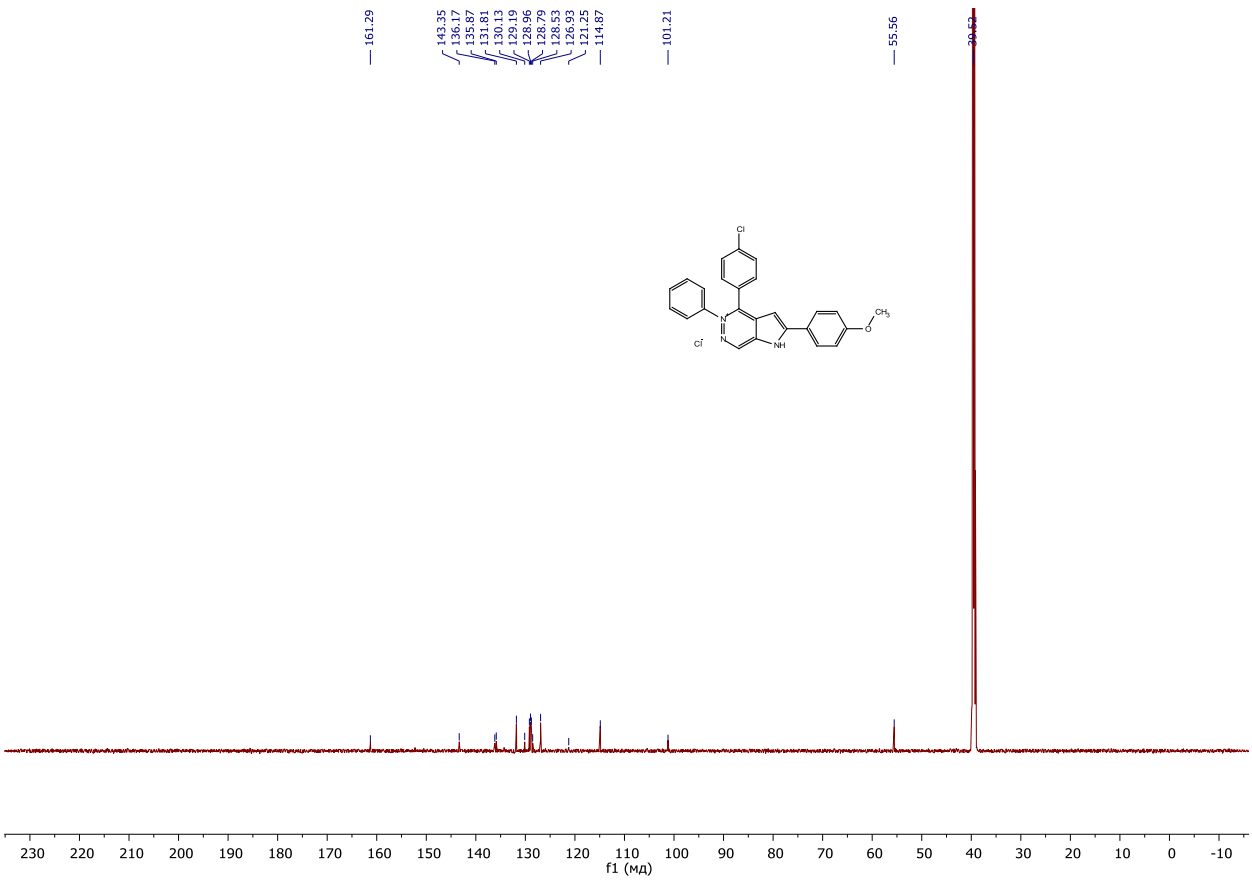

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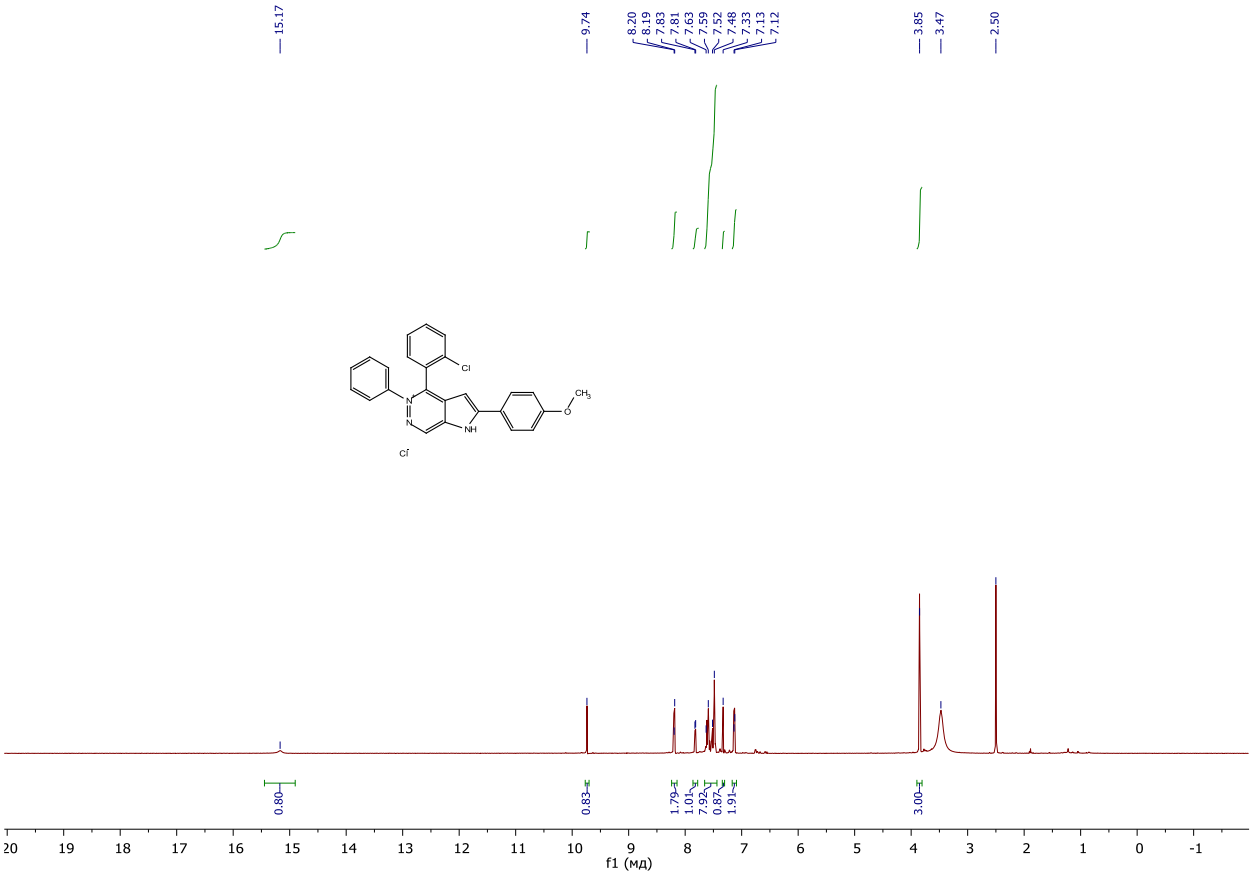

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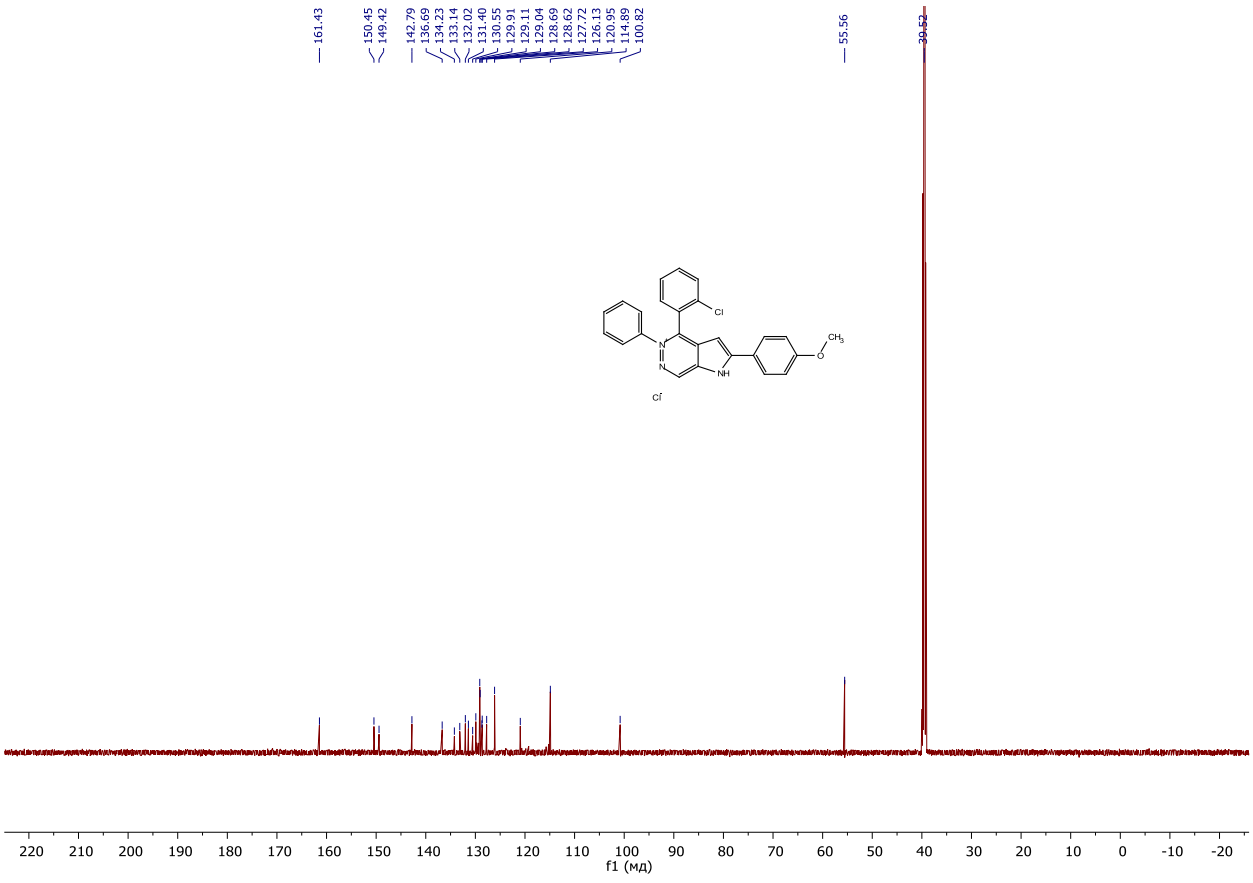

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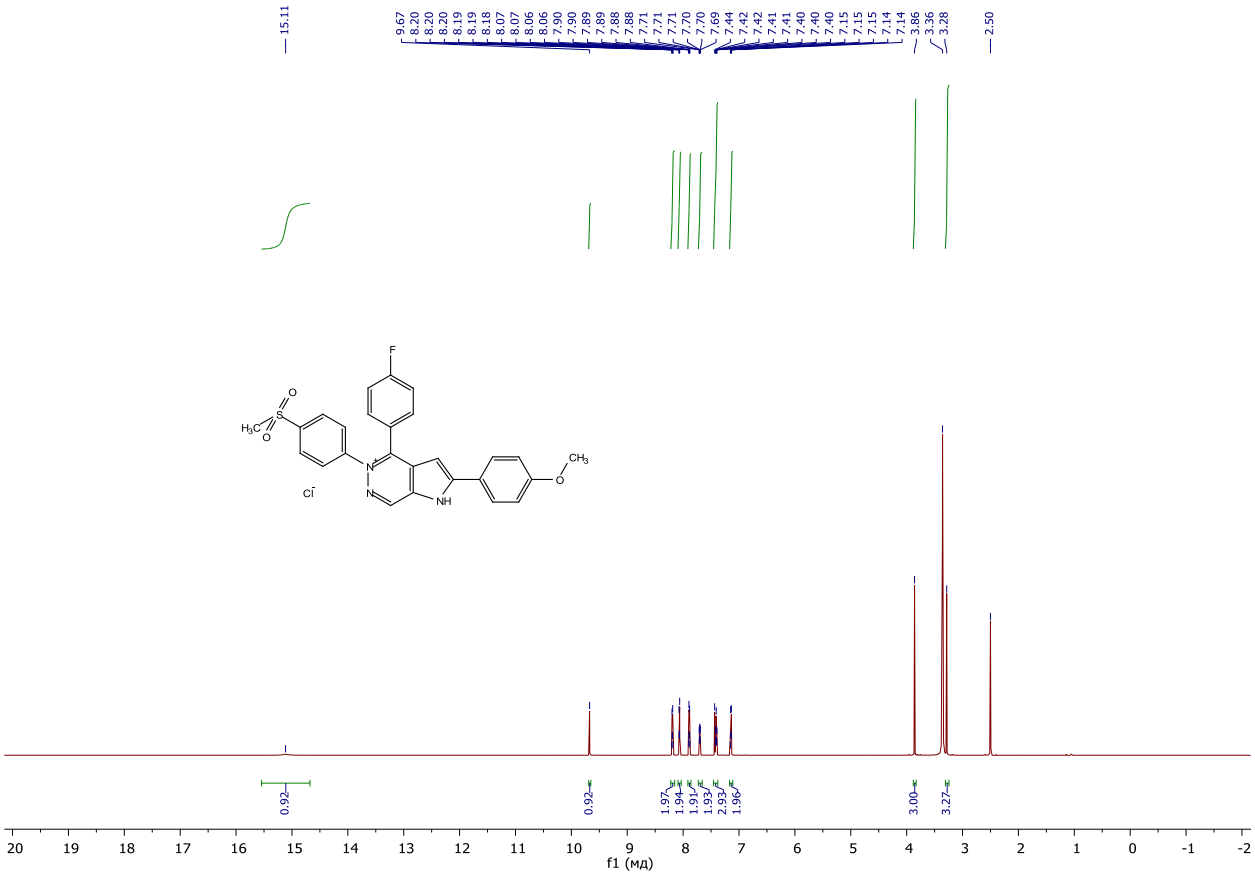

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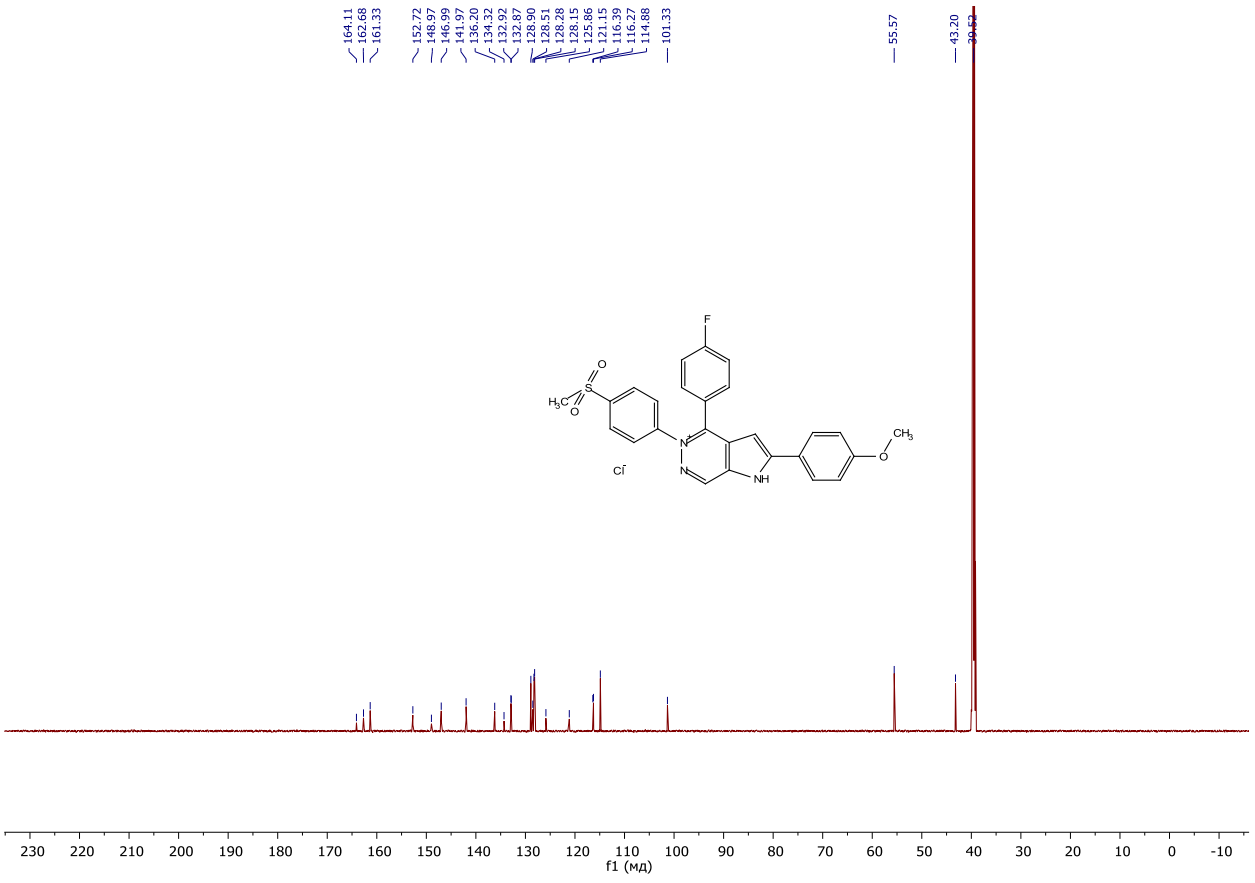

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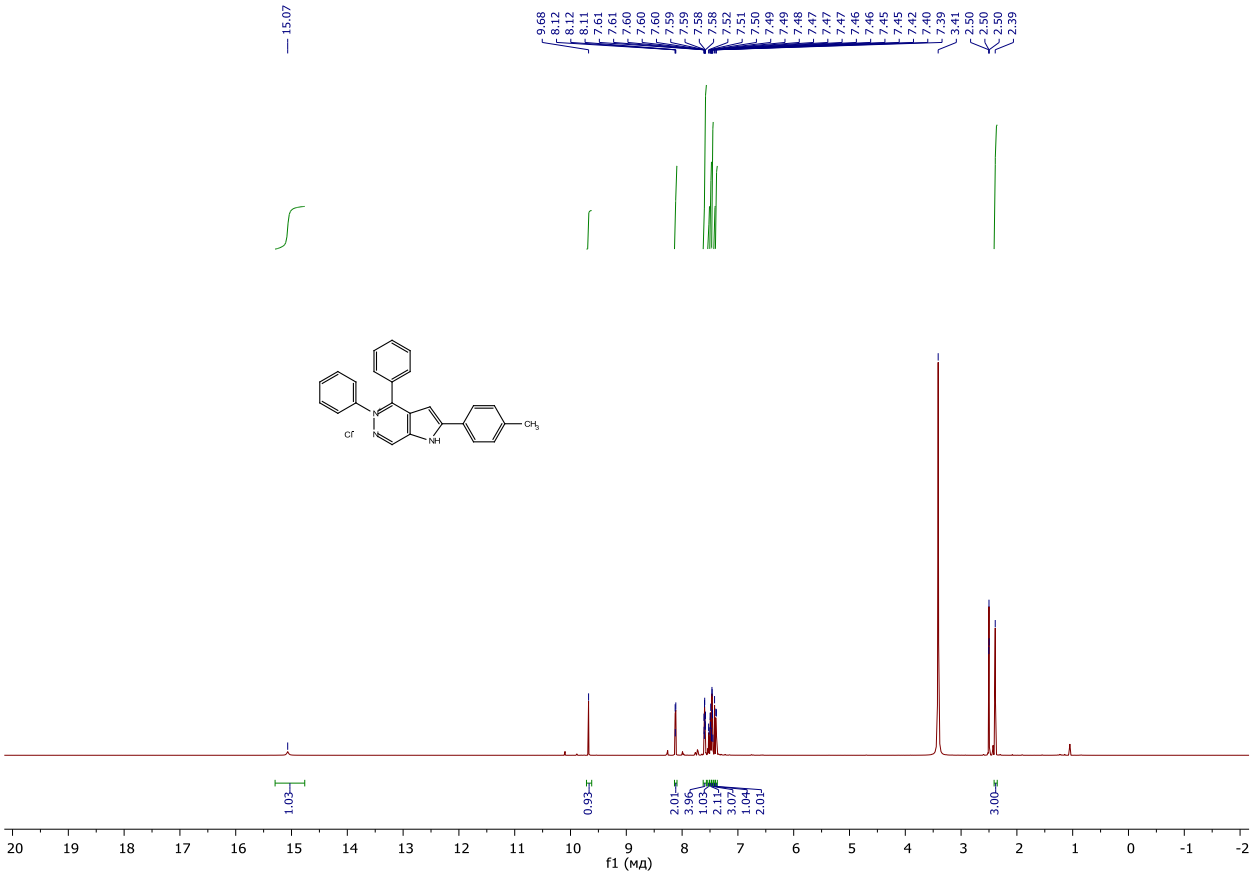

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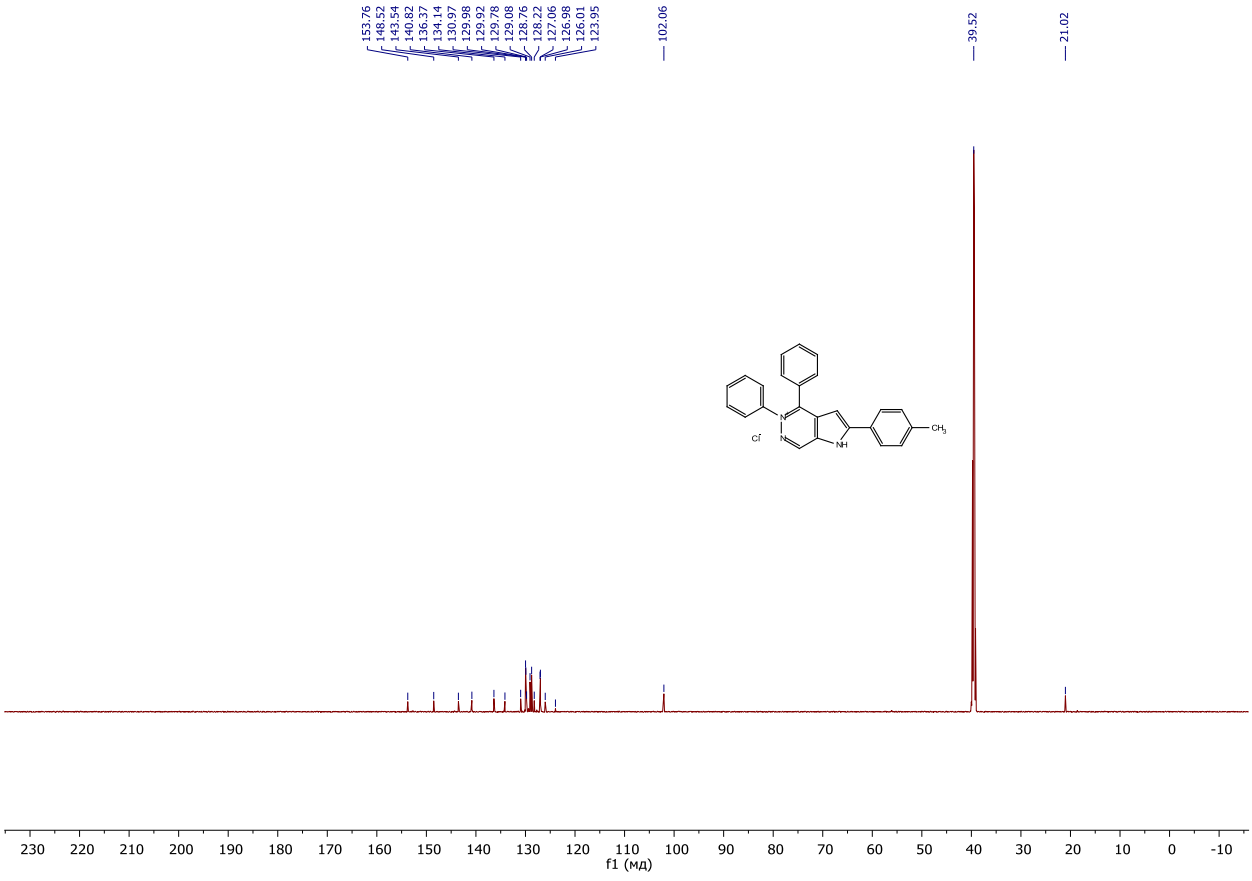

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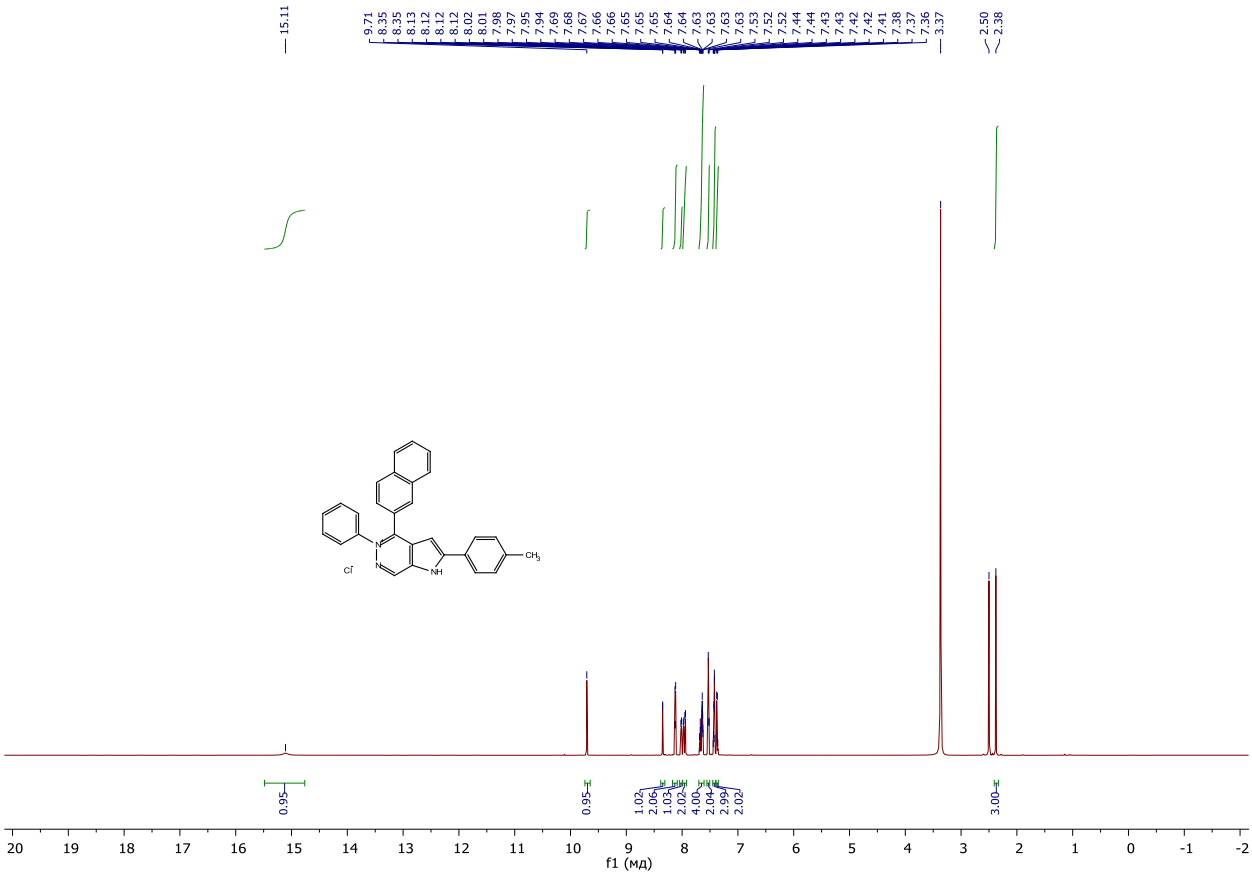

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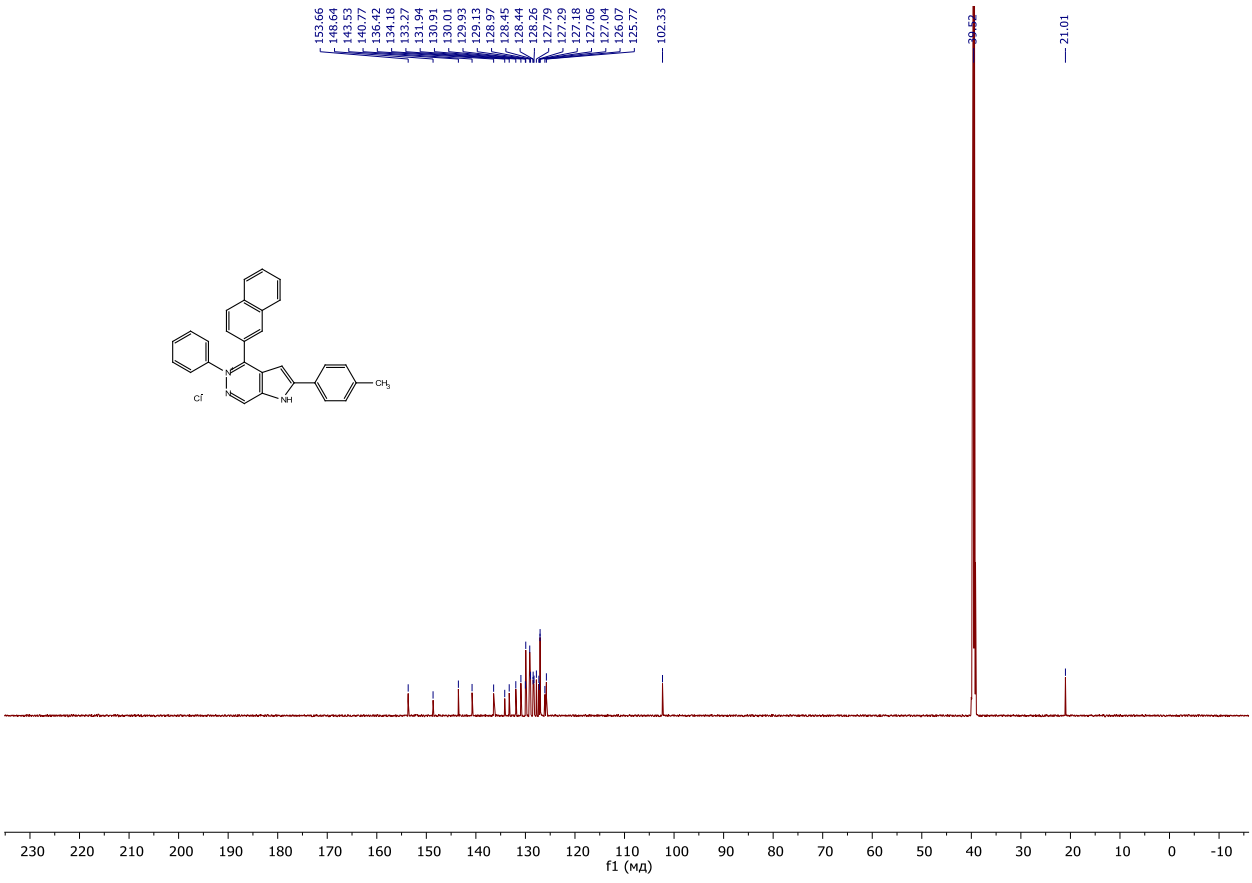
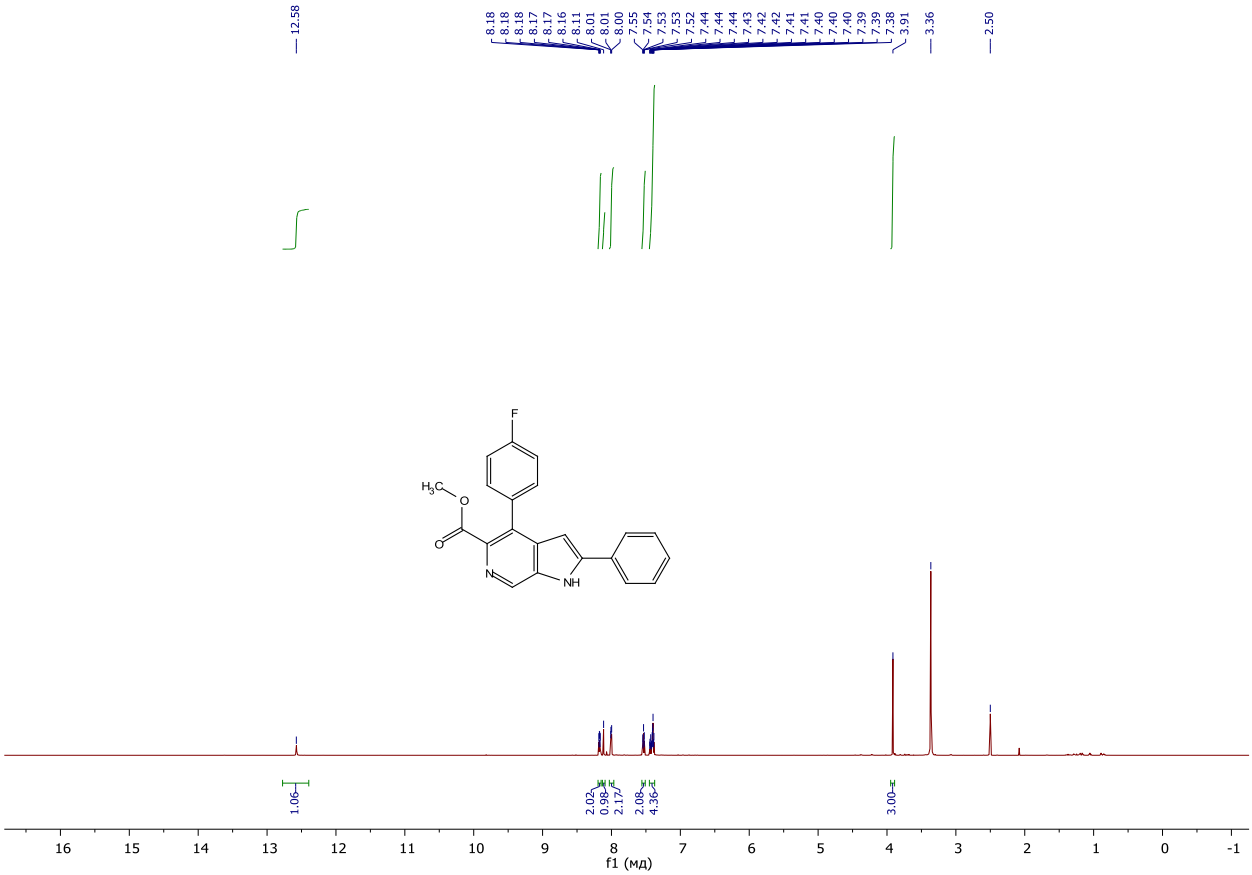


6a ^{1}H NMR



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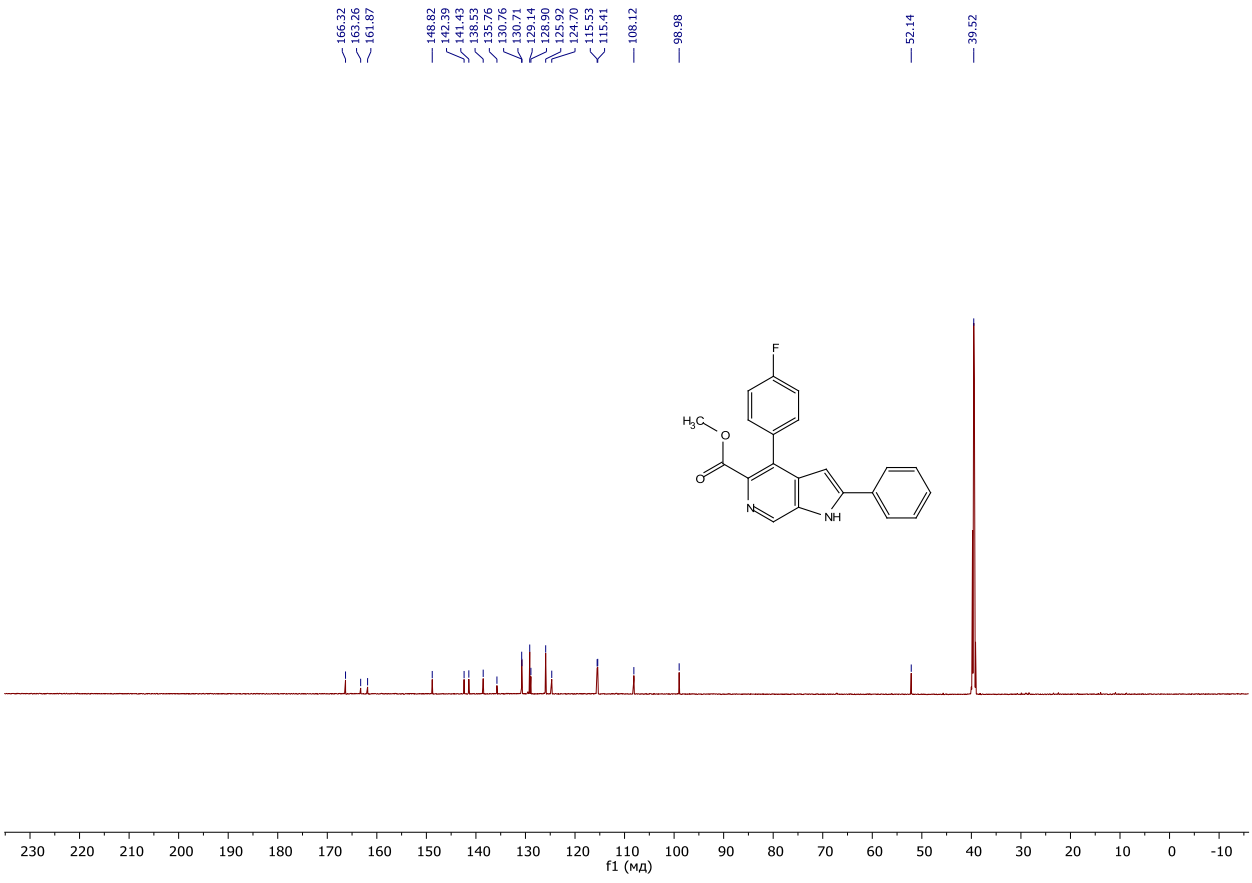

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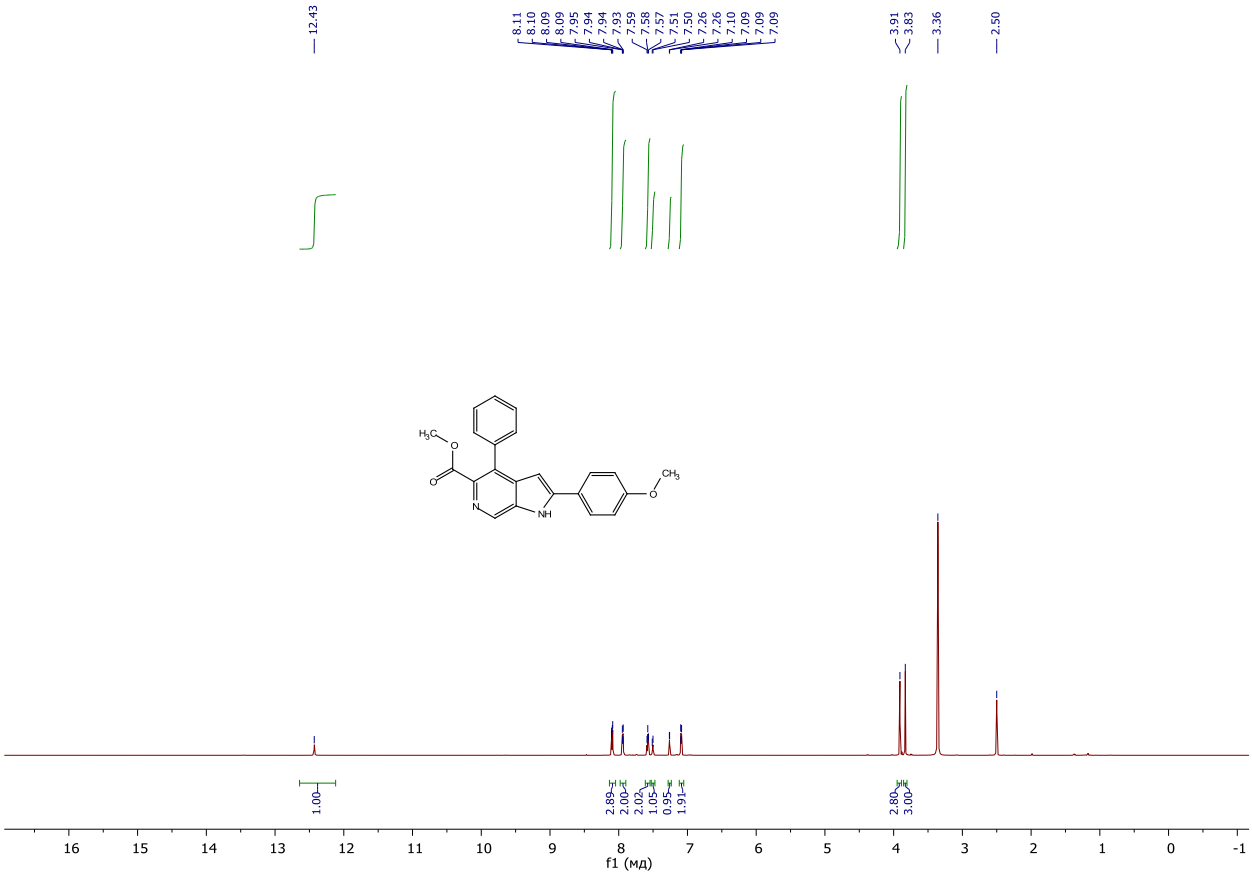

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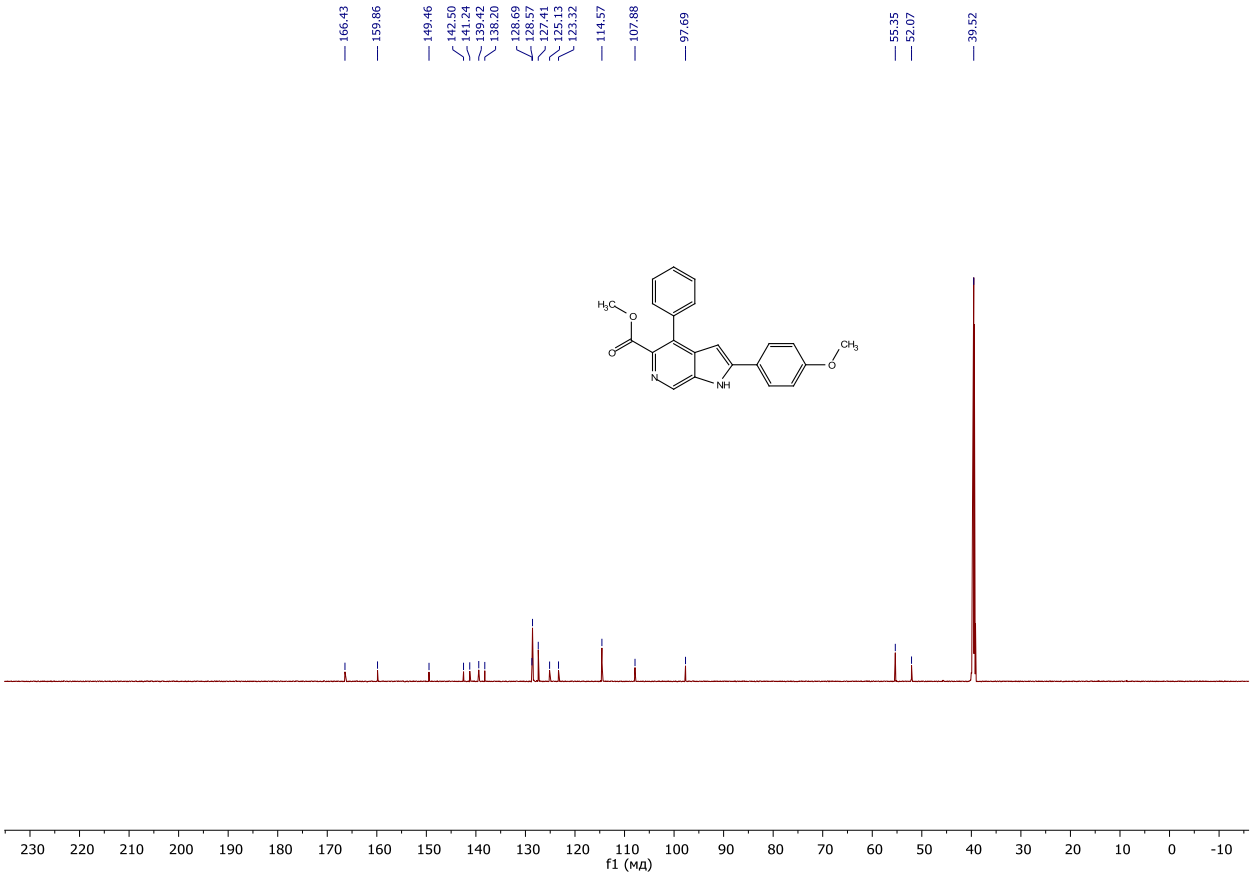

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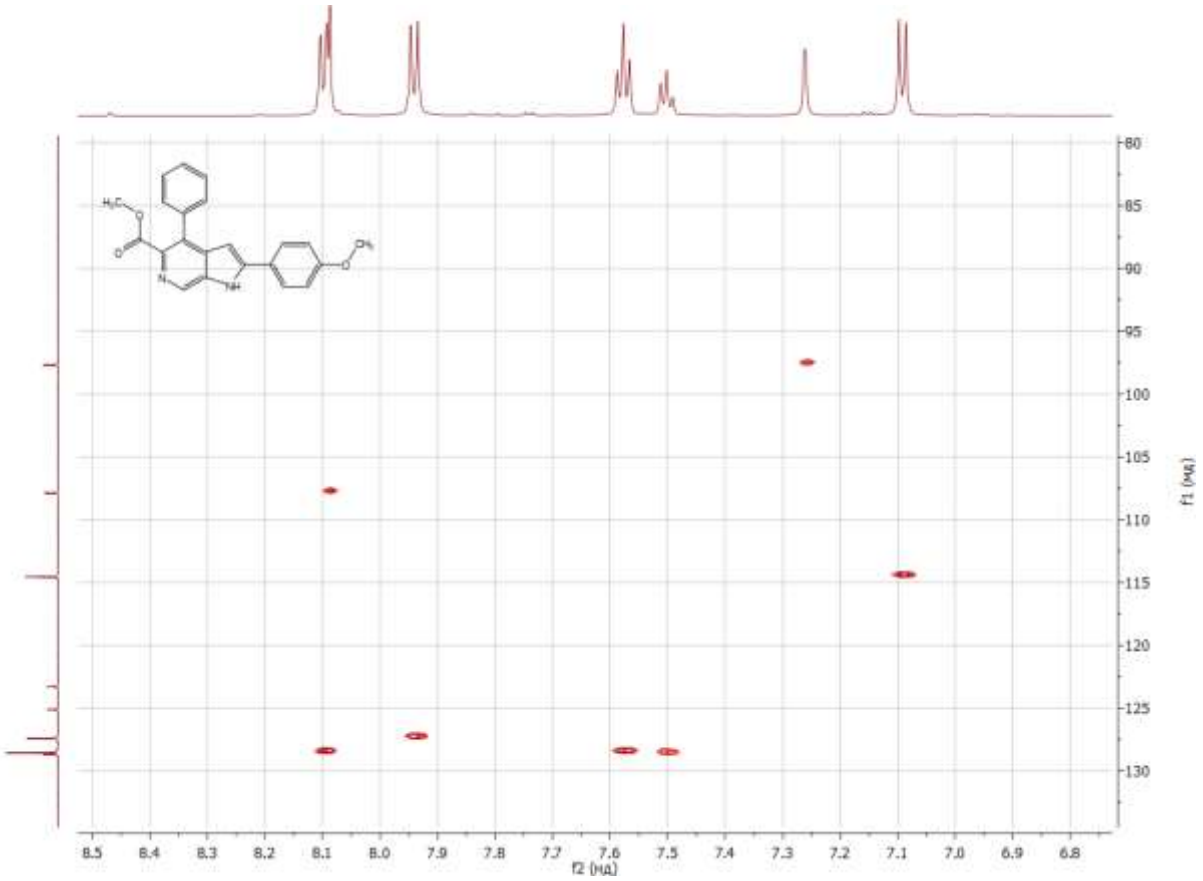

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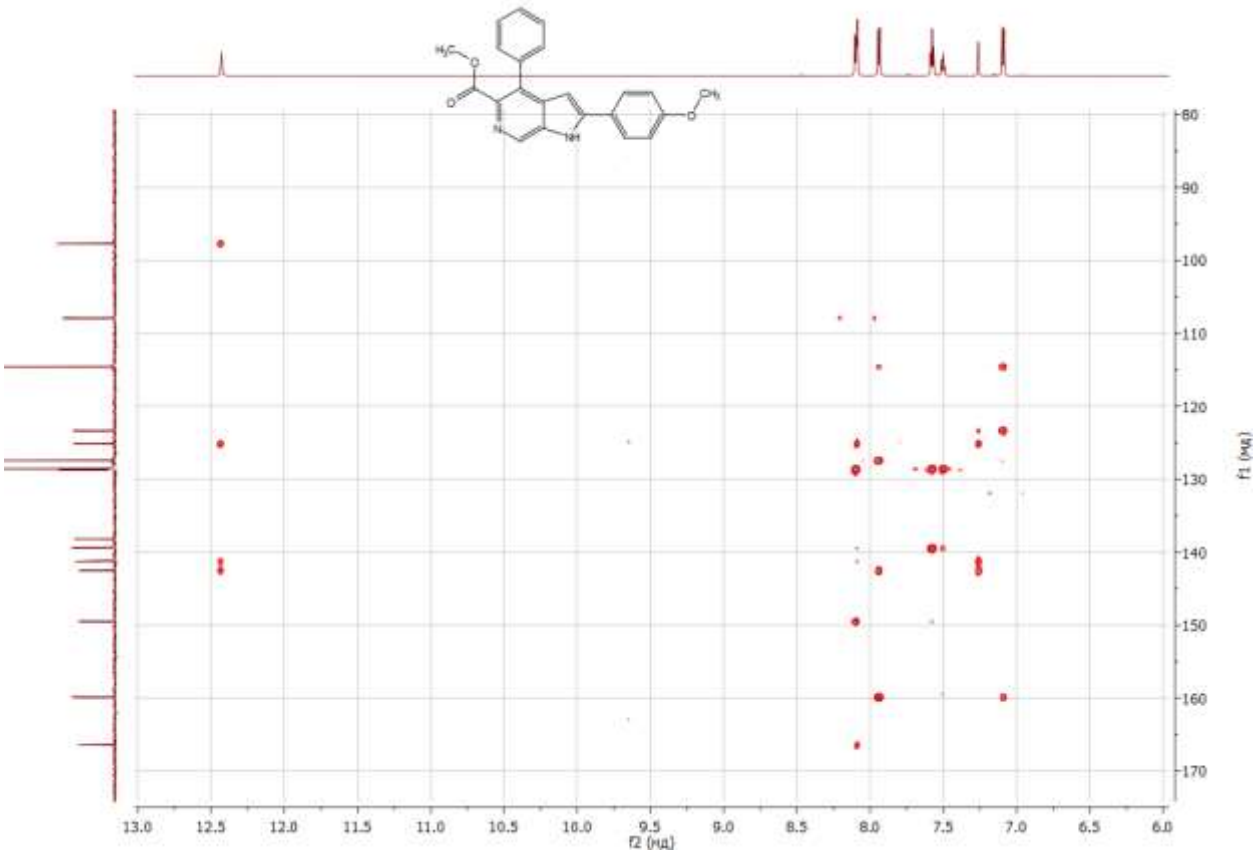

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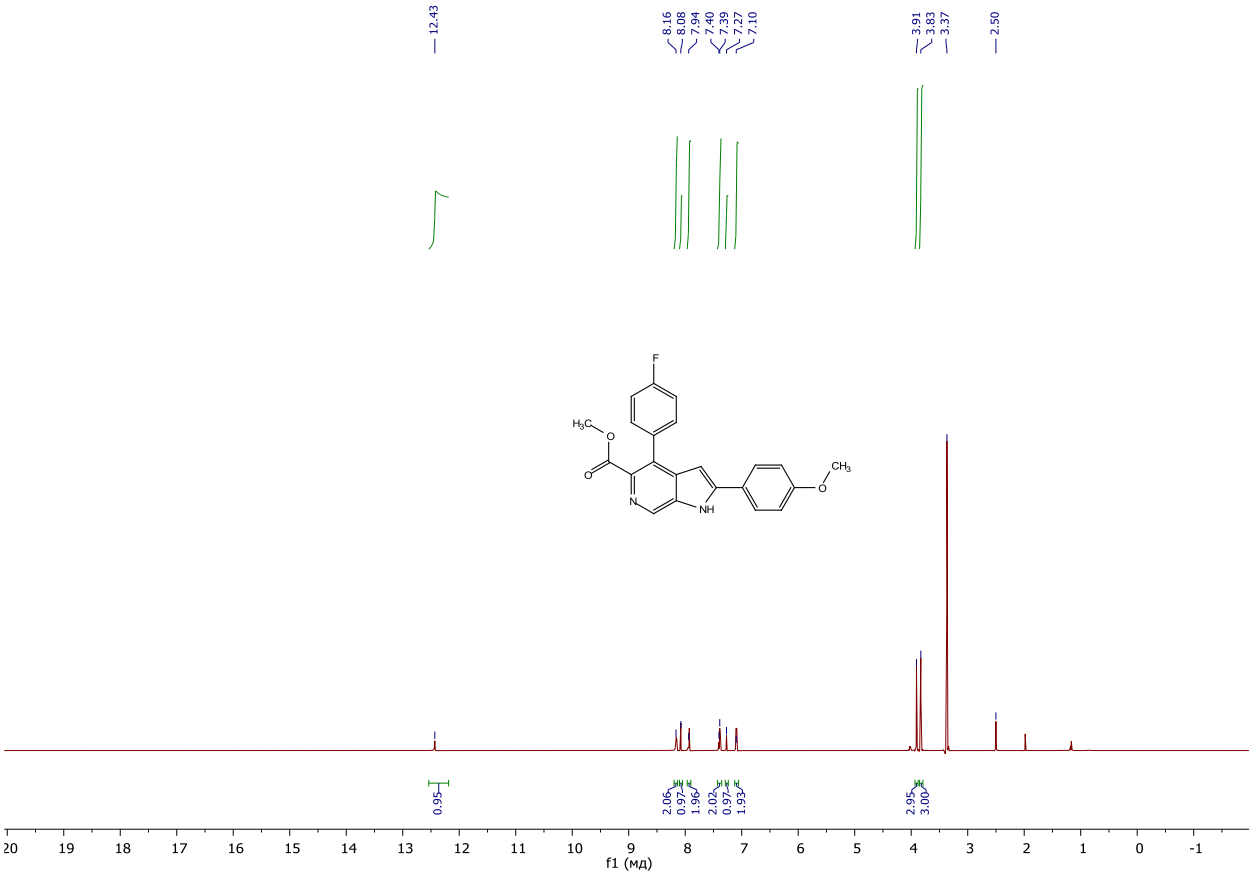
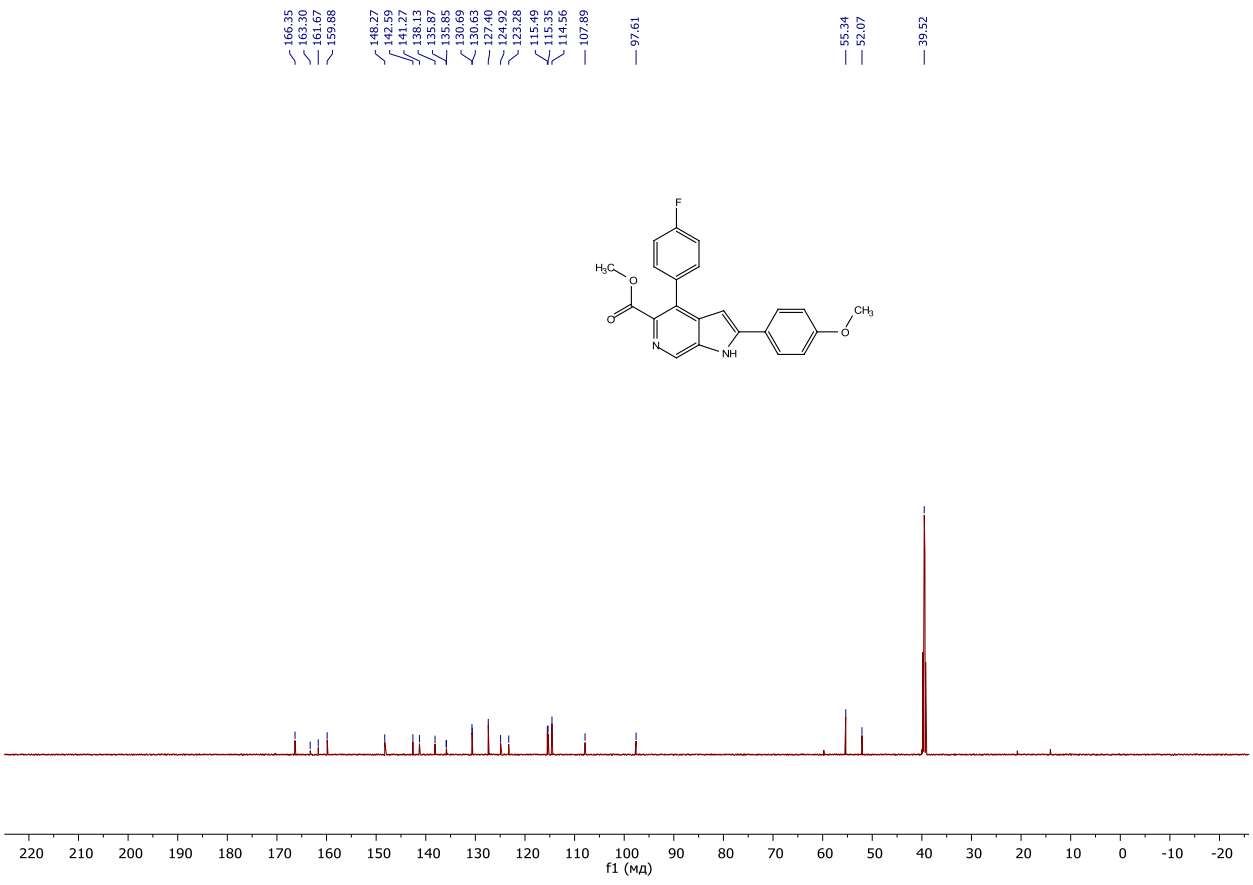
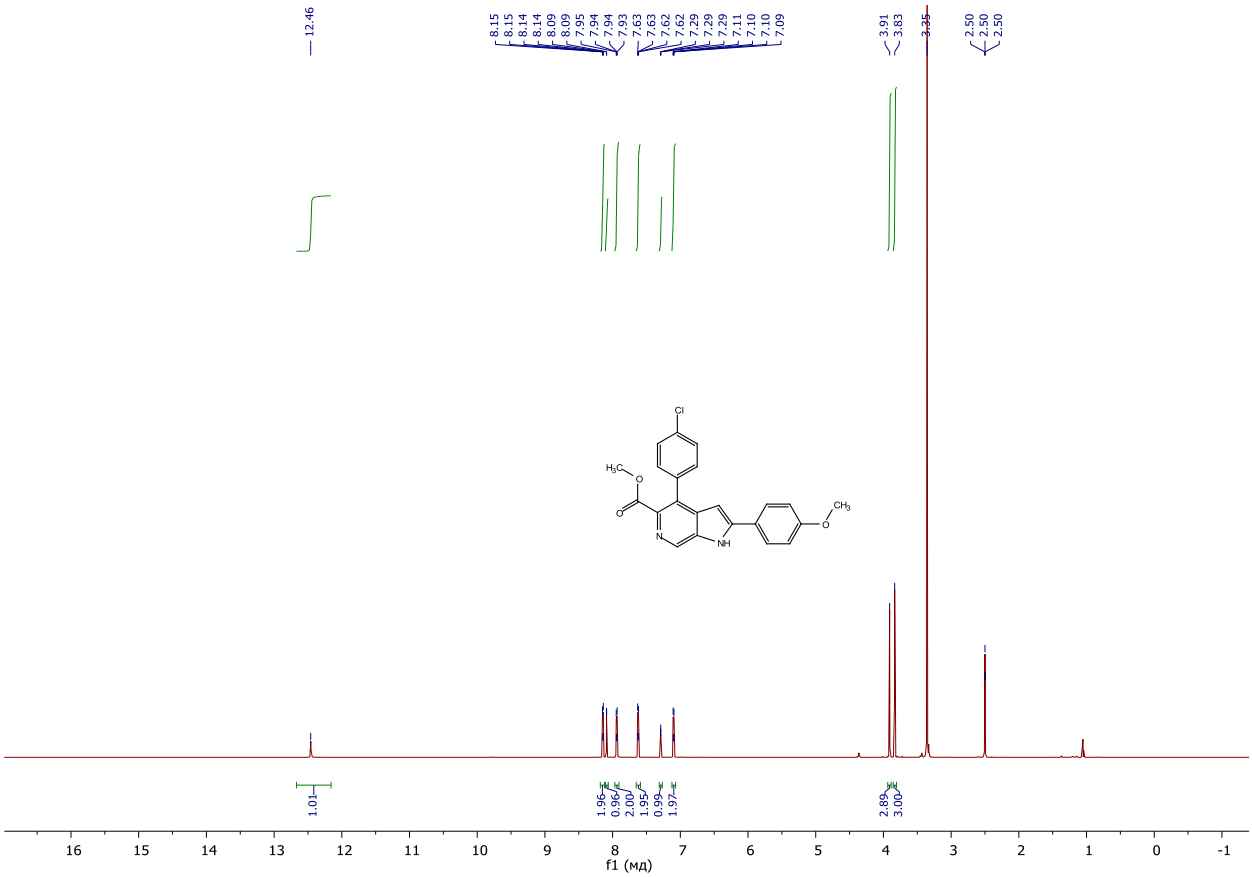


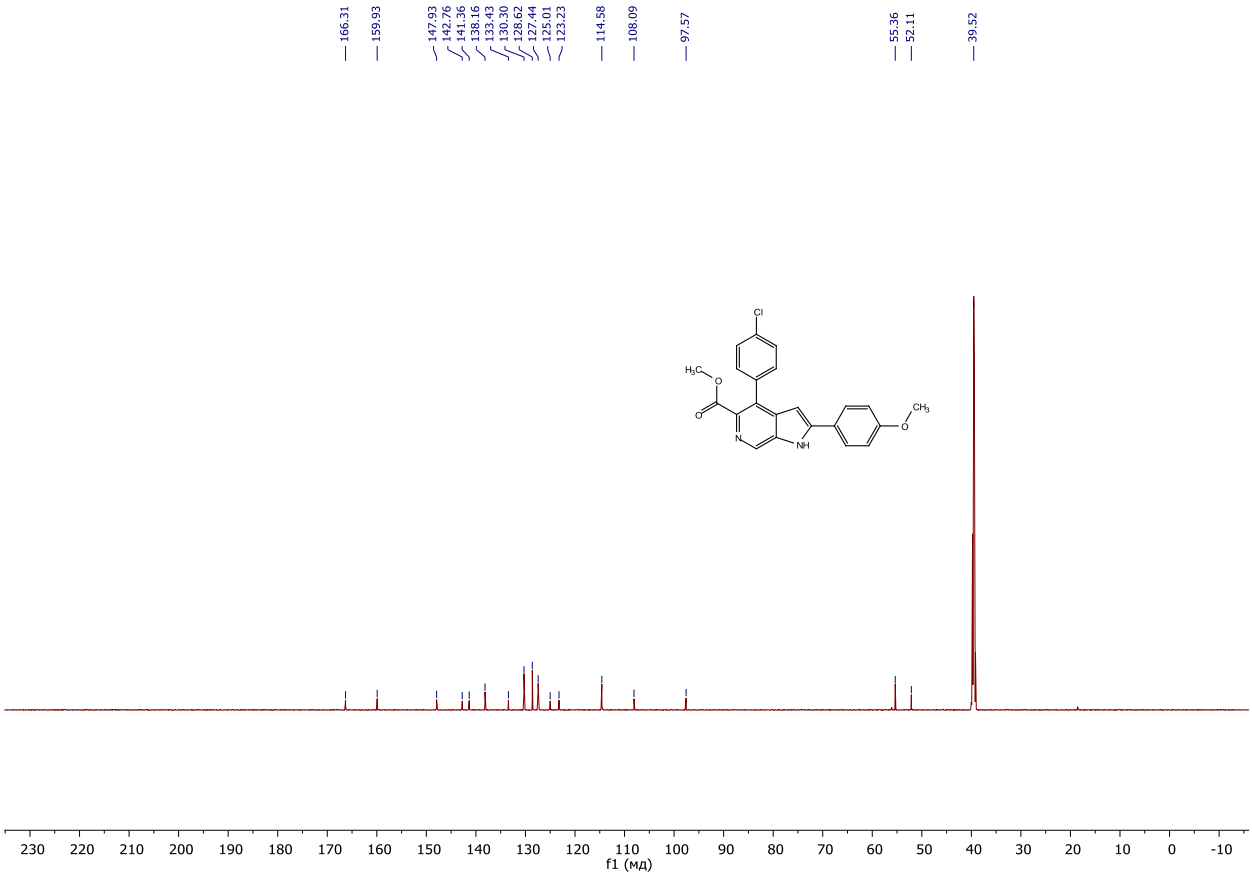
6c ^{13}C NMR



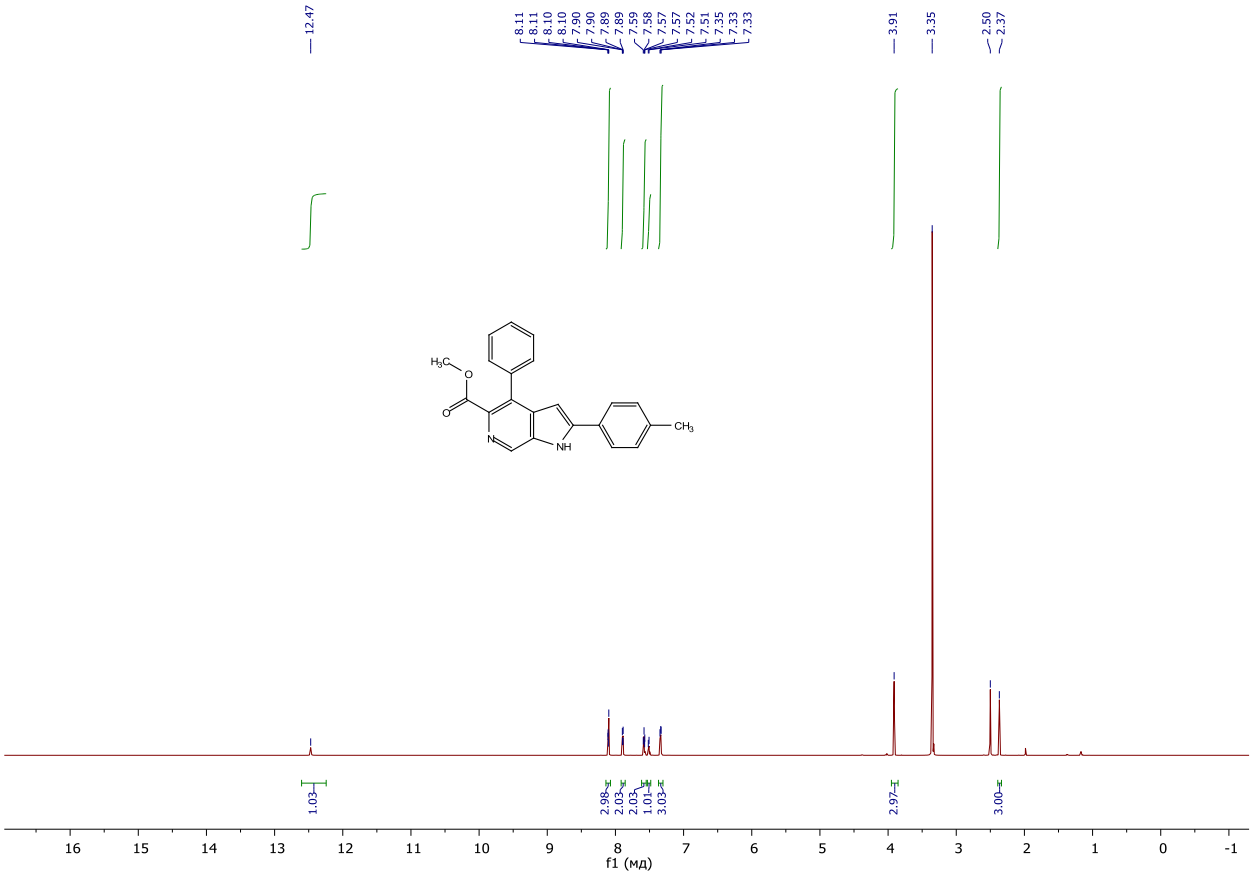
6d ^{1}H NMR



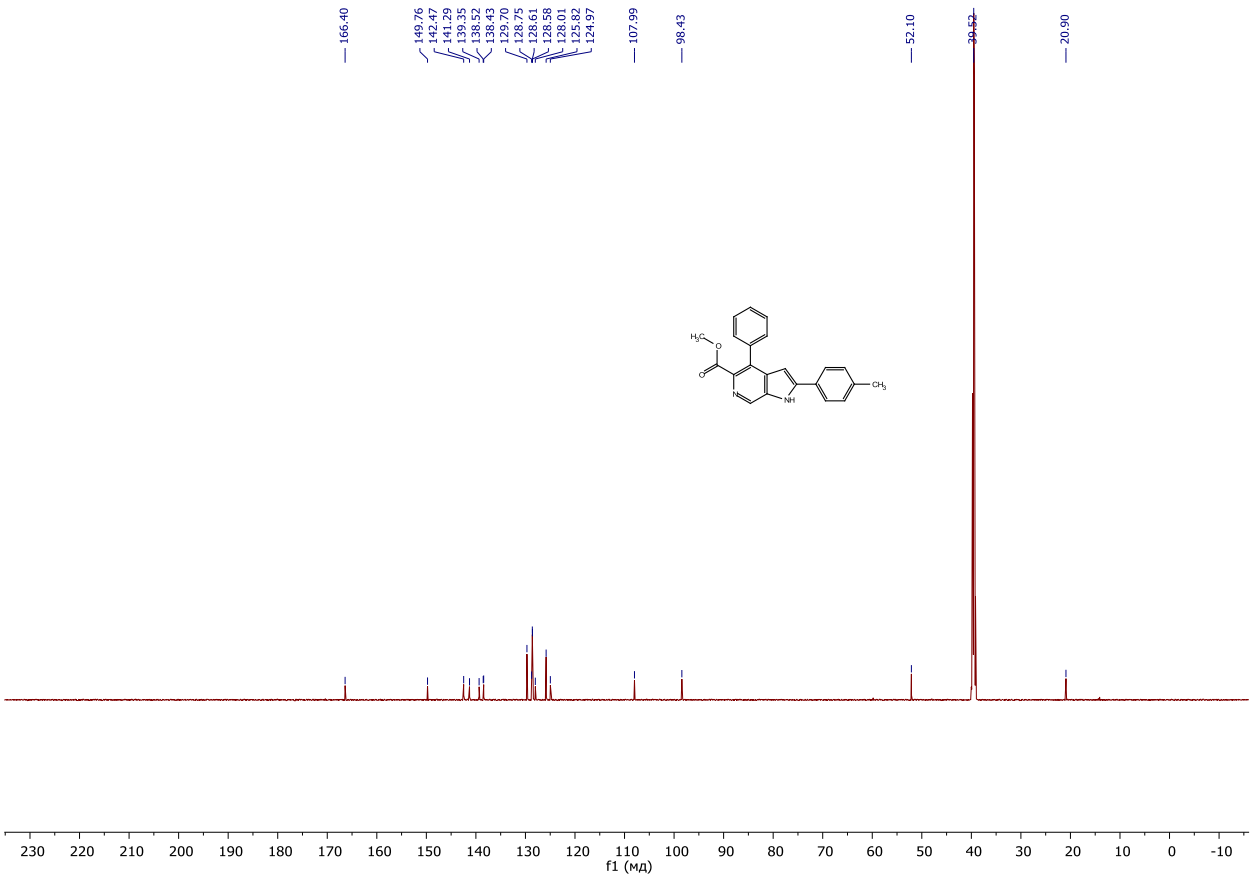
6d ^{13}C NMR



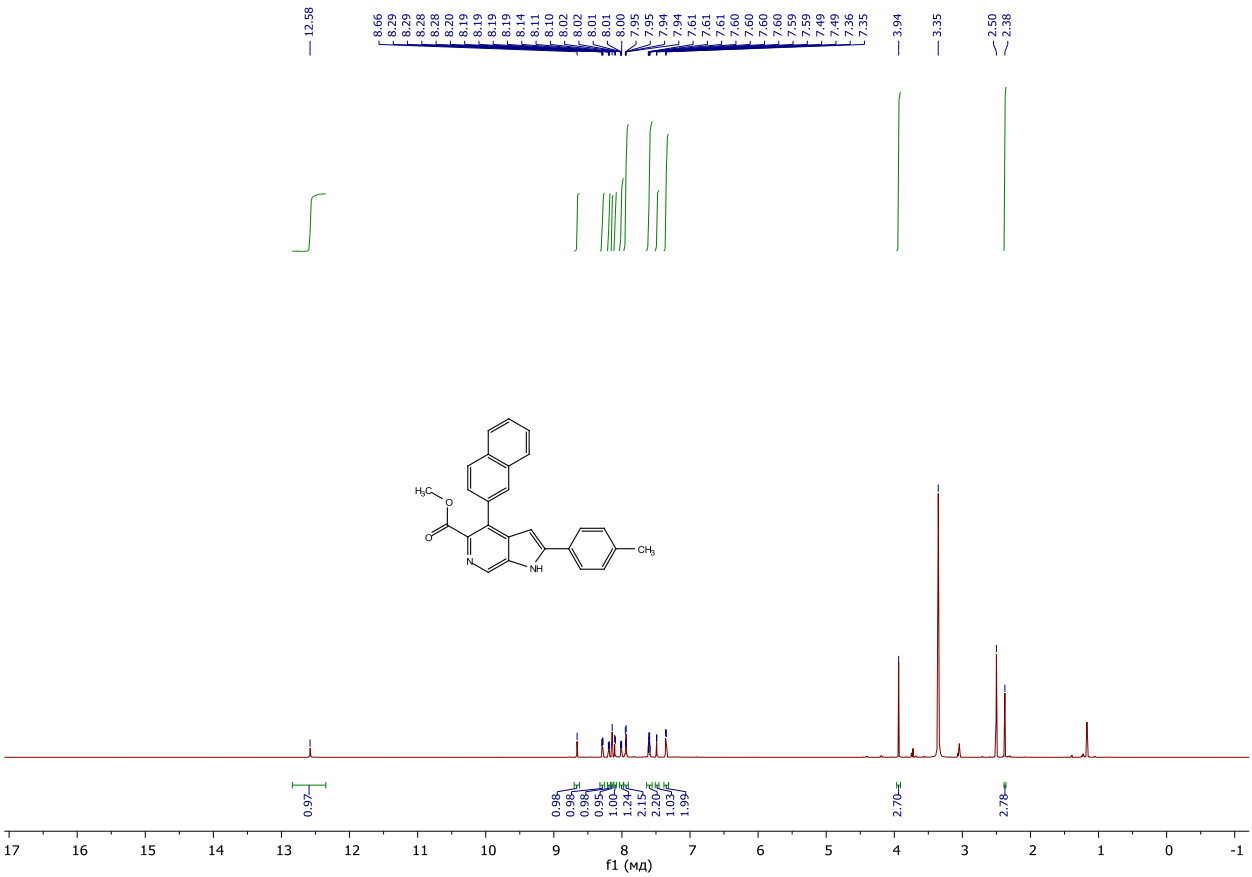
6e ^{1}H NMR



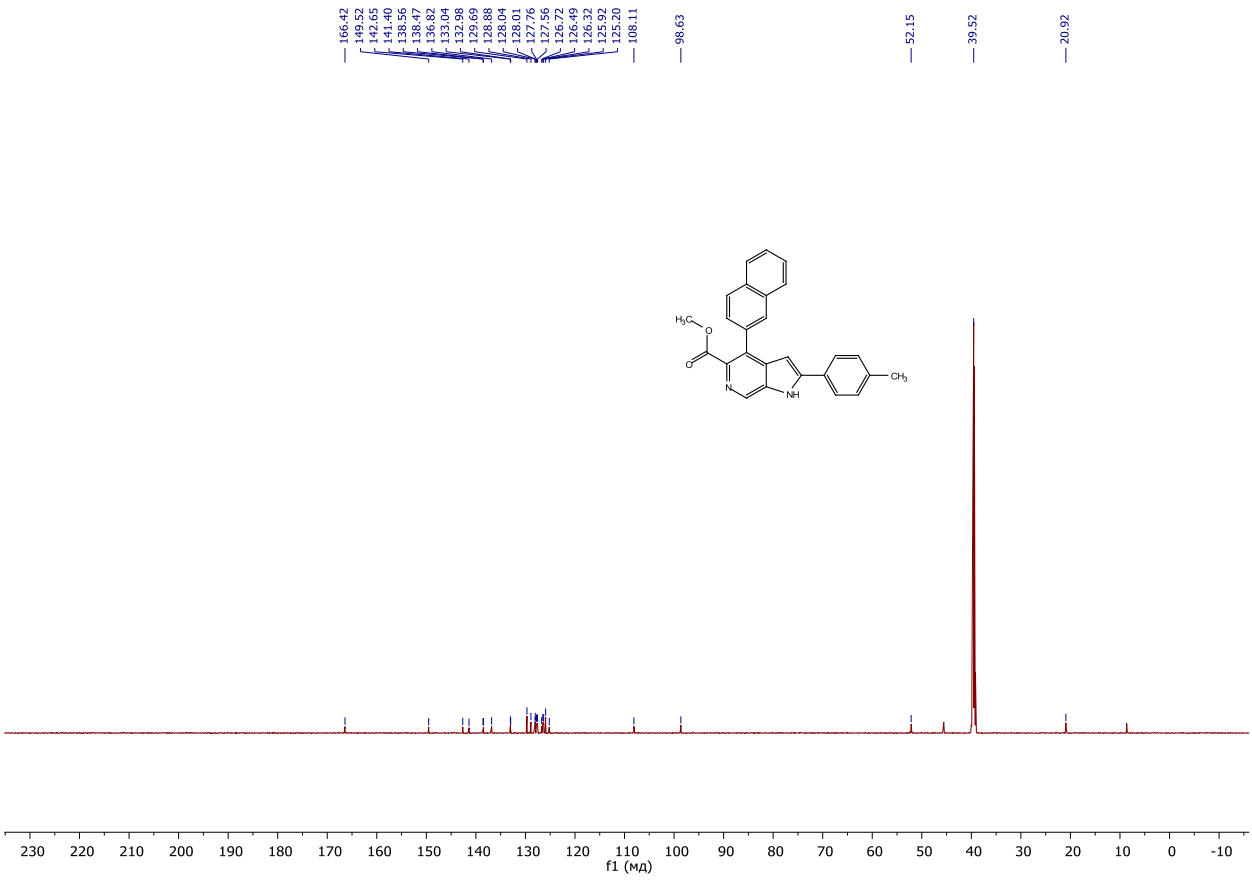
6e ^{13}C NMR



6f ^{1}H NMR



6f ^{13}C NMR



4. Computational Details

All DFT static calculations have been performed with Gaussian16 package,[S2] using the B3LYP functional of Becke and Perdew.[S3,S4] The split-valence basis set Def2-SVP from Ahlrichs and co-workers was used for all atoms.[S5] Stationary points were characterized using vibrational analysis, and this analysis has been also used to calculate zero-point energies and thermal (enthalpy and entropy) corrections (298.15 K, 1 bar). Improved electronic energies were obtained from single-point energy calculations using a Def2-TZVP[S6,S7] basis set on all the atoms, a solvation contribution (PCM model,[S8] ethanol) and the dispersion corrections through the Grimme D3BJ method.[S9] These energies added to the Def2-SVP-level thermal corrections are named ΔG.

5. Additional Figures

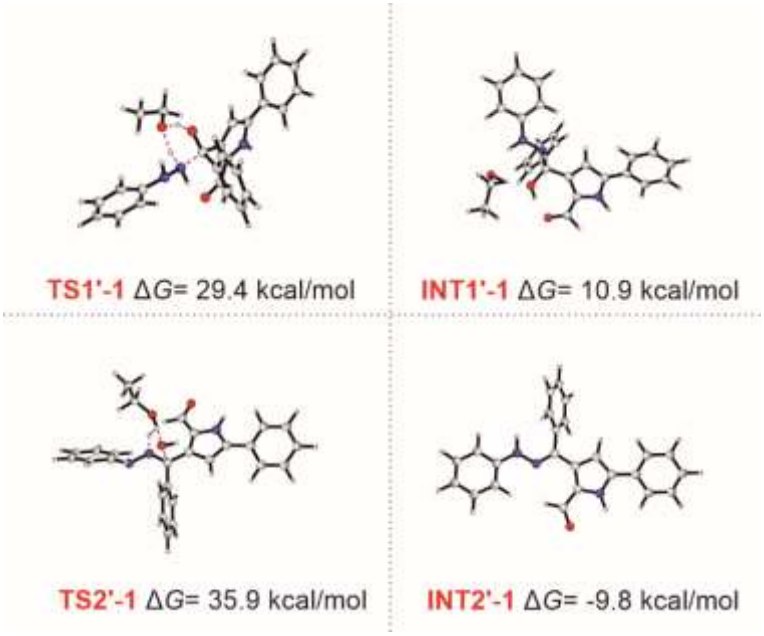


Figure S1. Optimized structures of transition states and intermediates leading to formation of hydrazone at ketone moiety of pyrrolo-2,3-dicarbonyl **2a** in the reaction with phenyl hydrazine.

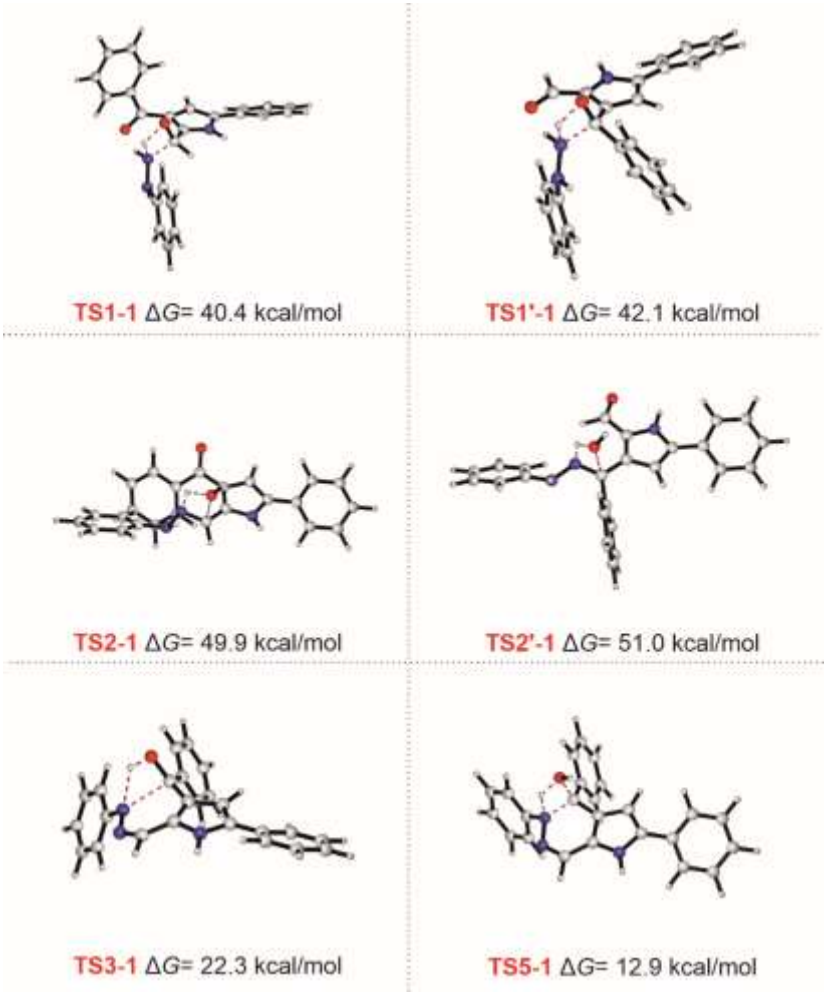


Figure S2. Optimized structures of the non-assisted transition states involved in the reaction between pyrrolo-2,3-dicarbonyl **2a** and phenyl hydrazine.

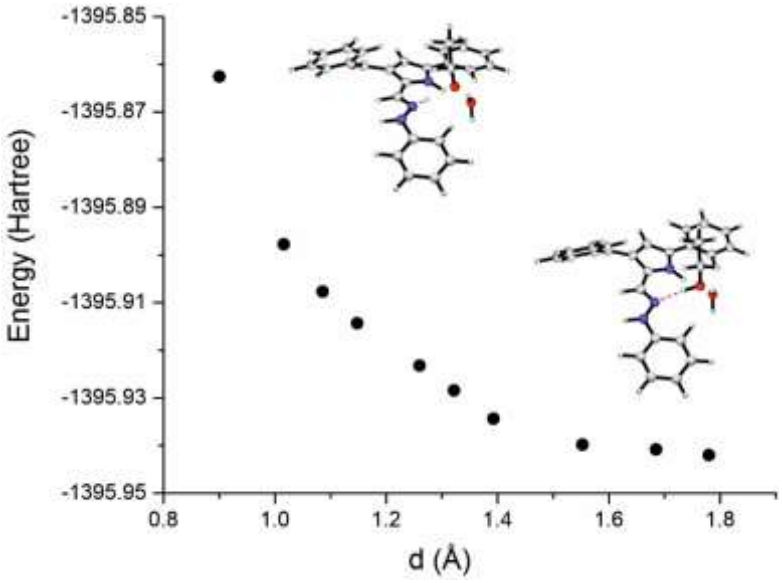


Figure S3. Deprotonation by ethoxide leading to **INT2-1**.

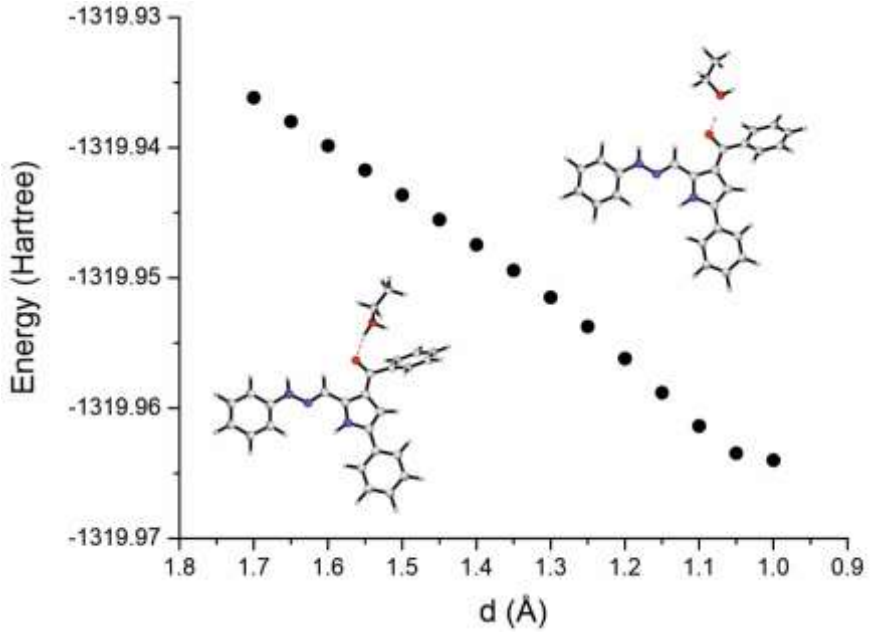


Figure S4. Protonation of **INT2-1** by $EtOH_2^+$ acid to generate **INT4-1**.

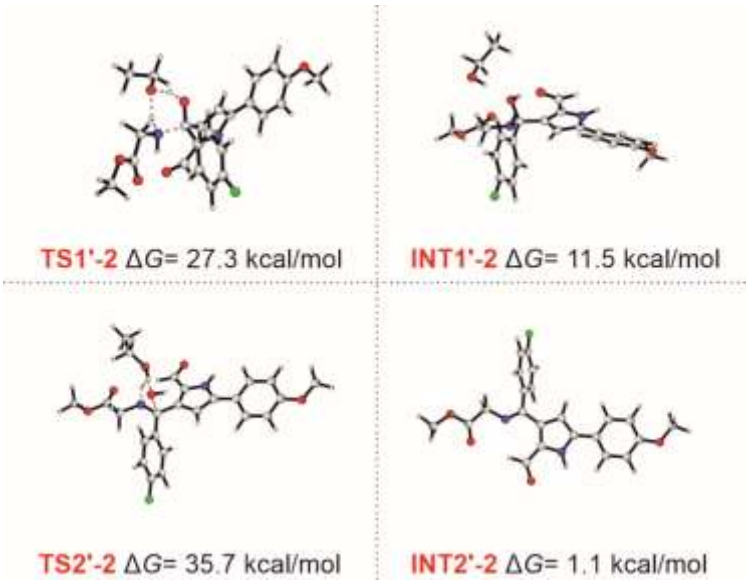


Figure S5. Optimized structures of transition states and intermediates leading to formation of hydrazone at ketone moiety of pyrrolo-2,3-dicarbonyl **2f** in the reaction with glycine methyl ester.

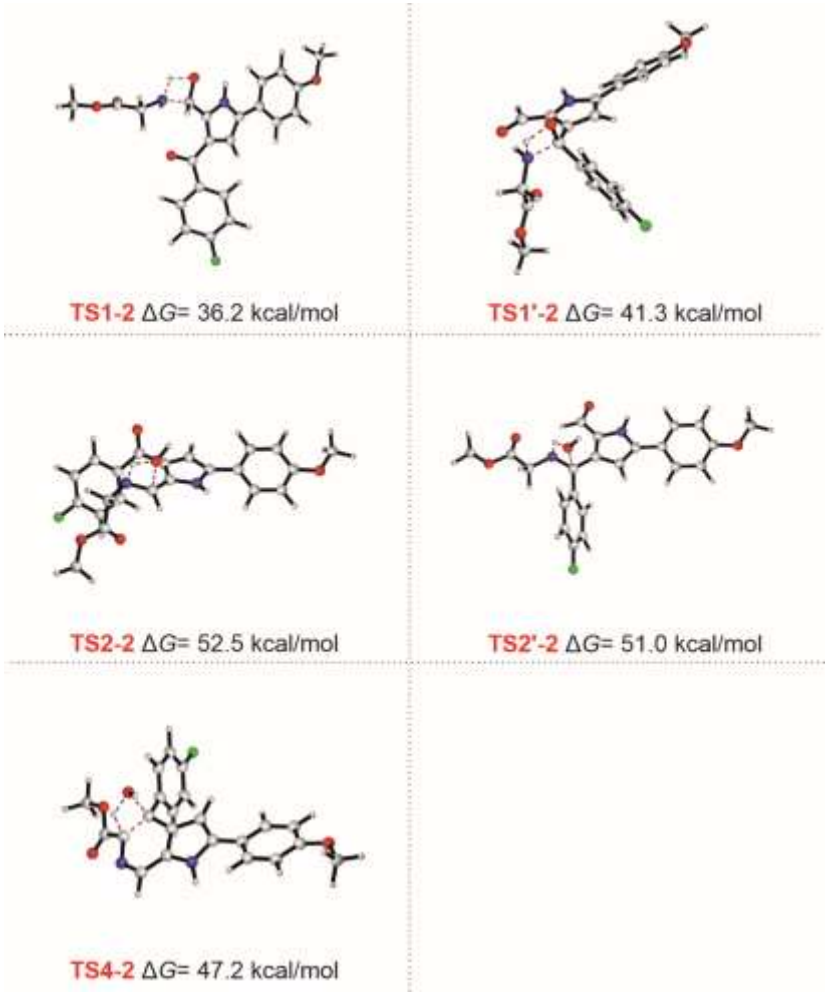


Figure S6. Optimized structures of the non-assisted transition states involved in the reaction between pyrrolo-2,3-dicarbonyl **2f** and glycine methyl ester.

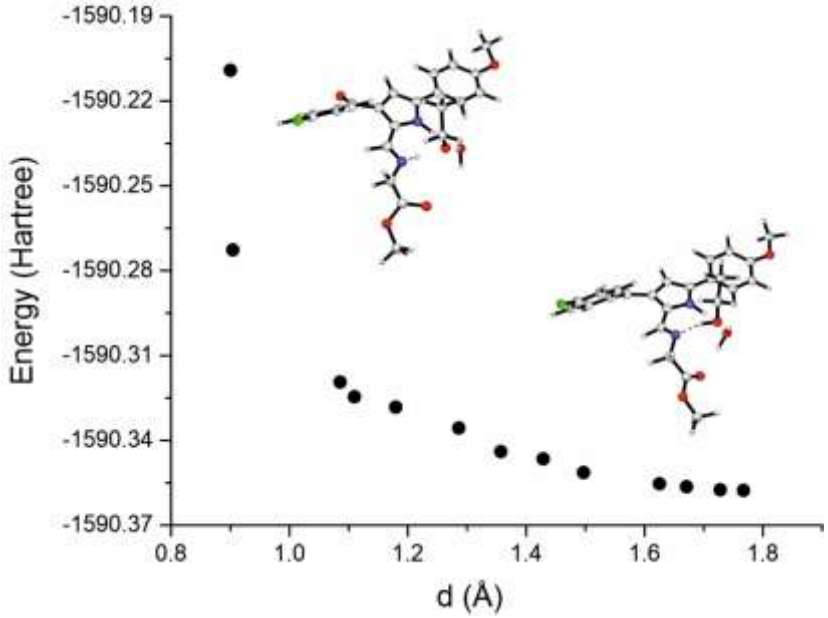


Figure S7. Deprotonation by ethoxide leading to **INT2-2.**

Figure S8. Optimized structures of the lowest energy intermediate, rate determining step and product of the reaction between pyrrolo-2,3-dicarbonyl **2a** and glycine methyl ester.

6. Cartesian Coordinates

Mechanism 1 (leading to product **4a**)

Pyrrolo-2,3-dicarbonyl 2a

E=-899,368558264

C	-0.11787600	1.06041200	-0.67770000
C	-0.39839300	-0.30182800	-0.46208600
C	0.83109300	-0.93119300	-0.16076600
H	1.73361100	2.09215500	-0.66298200
H	0.95507000	-1.98634500	0.07017300
C	3.27387600	-0.07839600	0.10710700
C	4.03529800	1.02869600	0.53118900
C	3.92616500	-1.31756400	-0.04812200
C	5.40310400	0.90364900	0.77950400
H	3.55199700	1.99503200	0.69916500
C	5.29112500	-1.44152800	0.20896300
H	3.35876200	-2.18481900	-0.39207700
C	6.03738700	-0.33180700	0.62032600
H	5.97398200	1.77462900	1.11101400
H	5.77859000	-2.41091600	0.07864000
H	7.10749400	-0.43037900	0.81786700
C	-1.68030800	-1.06996700	-0.59337200
C	-2.93476300	-0.59422500	0.07106600
C	-2.94019600	0.37871500	1.08303800
C	-4.14431300	-1.21112400	-0.29335100
C	-4.13387100	0.73332200	1.71423400
H	-2.00486500	0.85161100	1.38770700
C	-5.33788500	-0.84633900	0.32625400
H	-4.12003000	-1.97776000	-1.07006100
C	-5.33454400	0.12688100	1.33297900
H	-4.12825300	1.48757200	2.50511300
H	-6.27568200	-1.32220900	0.02834800
H	-6.26980500	0.41101100	1.82263700
O	-1.65701000	-2.12646200	-1.20228700
C	-0.92829300	2.17605500	-1.14896400
H	-0.35104600	3.13916100	-1.23373600
O	-2.10351000	2.13045100	-1.44195200
C	1.83753200	0.03909900	-0.16547700

N	1.23764600	1.22745700	-0.47954700

Phenyl hydrazine

E= -343,089432476

N	-2.83348600	0.31294400	0.11211100
H	-2.63953100	0.88907100	0.93708300
H	-2.93979900	0.93985100	-0.68643400
N	-1.81199100	-0.60068900	-0.12317600
H	-2.06099600	-1.55483900	0.11082300
C	-0.46480900	-0.27446400	-0.05134300
C	-0.02149000	1.06320500	-0.05330700
C	0.50259400	-1.30269600	-0.00404200
C	1.34515700	1.35380200	-0.01207400
H	-0.74895800	1.87530400	-0.09346700
C	1.86030600	-0.99761000	0.03597300
H	0.17405200	-2.34645200	-0.00053600
C	2.29756600	0.33366900	0.03262900
H	1.66486600	2.39967000	-0.01569100
H	2.58905100	-1.81211300	0.07323400
H	3.36371300	0.56828500	0.06542000

TS1-1 (non-assisted)

E=-1242,41491183

C	-0.12036300	0.22183600	-0.35137200
C	1.00296100	-0.55679800	-0.00400900
C	2.08389300	0.35682500	0.22296500
H	-0.32685400	2.29363500	-0.56971200
H	3.09194000	0.09319000	0.53095100
C	2.29494900	2.94159300	0.10224700
C	1.81330500	4.07536300	-0.58244500
C	3.46077200	3.08495200	0.88174100
C	2.46601700	5.30566100	-0.48375200
H	0.93316400	3.99673100	-1.22651900
C	4.11693600	4.31201200	0.97011300
H	3.84402700	2.22664100	1.43775300
C	3.62193400	5.43118900	0.29146700
H	2.07351800	6.16903900	-1.02706500
H	5.01789500	4.39837700	1.58299300
H	4.13442200	6.39330000	0.36600600
C	1.02268600	-2.01176000	0.19495800
C	2.31243000	-2.76617200	0.07257400
C	3.34772400	-2.36793800	-0.79114300
C	2.45010900	-3.96282000	0.79935000
C	4.50306900	-3.14470300	-0.91136300
H	3.23600700	-1.46547200	-1.39405300
C	3.61104300	-4.72639900	0.69183800
H	1.62775100	-4.27731700	1.44455200
C	4.64104900	-4.31805700	-0.16430300
H	5.29592400	-2.83486900	-1.59673100
H	3.71365800	-5.64759100	1.27098300
H	5.54864300	-4.92059600	-0.25493500
O	0.00324100	-2.64482000	0.49450800
C	-1.51341800	-0.09712200	-0.84338400

O	-1.61461000	-0.73132700	-2.01805400
H	-2.13128300	0.82959200	-0.70240900
N	-2.25037400	-1.21267100	-0.00326800
H	-2.37400500	-1.52894600	-1.16312700
H	-1.52185900	-1.85656000	0.37991800
N	-3.26209900	-0.98890000	0.92207900
H	-2.93772900	-0.78890900	1.86355400
C	-4.46115300	-0.38598900	0.52714000
C	-5.37768700	0.00446100	1.52330100
C	-4.79894500	-0.20166500	-0.82703200
C	-6.60826600	0.55523300	1.17101500
H	-5.12257800	-0.13843500	2.57756600
C	-6.04027100	0.34768800	-1.16093800
H	-4.09083300	-0.46450100	-1.61565200
C	-6.95296200	0.72855800	-0.17445600
H	-7.30669600	0.84972300	1.95887900
H	-6.28729100	0.48478400	-2.21705500
H	-7.91881400	1.15910900	-0.44777100
C	1.61911200	1.64361500	0.00885800
N	0.28710200	1.51883800	-0.34595200

TS1-1 (assisted by EtOH)

E= -1397,58286941

C	0.29893200	-0.43800700	-0.32409900
C	0.66924600	0.86038700	0.08652700
C	2.10107900	0.91477100	-0.00146100
H	1.36380000	-2.04184400	-1.01709500
H	2.72981500	1.74632800	0.30478700
C	3.91437800	-0.81116700	-0.69382300
C	4.18376000	-2.18895700	-0.81266300
C	4.99367800	0.08780500	-0.80912800
C	5.48183600	-2.64898500	-1.04152700
H	3.37725700	-2.91849000	-0.70578200
C	6.29036400	-0.37450000	-1.02947700
H	4.81017400	1.16211900	-0.73947700
C	6.54254100	-1.74562500	-1.14968100
H	5.66492500	-3.72301500	-1.12791000
H	7.11084000	0.34242000	-1.11666100
C	-0.25135800	1.88892500	0.57426600
C	0.15123100	3.33143400	0.57647700
C	1.03105200	3.88081800	-0.37296300
C	-0.43922500	4.17855400	1.53247200
C	1.32372800	5.24689100	-0.35503700
H	1.46348900	3.24463800	-1.14658100
C	-0.13112100	5.53746800	1.55991800
H	-1.14041800	3.74667900	2.24884100
C	0.75197600	6.07469900	0.61552500
H	1.99716200	5.66734700	-1.10605700
H	-0.58384300	6.18396500	2.31585600
O	-1.37579000	1.59457700	1.00851000
C	-1.00138600	-1.18644300	-0.58998500
N	-1.85904400	-1.09639900	0.69328900

H	-1.34386700	-1.85774400	1.34490100
C	2.55541100	-0.31506100	-0.45354400
N	1.43249100	-1.09764400	-0.64175500
O	-0.78799400	-2.48814300	-0.89390300
H	-1.57800900	-0.65998100	-1.37574300
H	-1.83968000	-0.11683600	1.05028300
H	-0.69551500	-3.02116400	0.14901900
O	-0.83422500	-3.21942800	1.38264000
C	0.22210900	-3.76311300	2.12146700
H	0.48742100	-4.76527100	1.72288000
H	1.14728200	-3.14808400	2.03564200
C	-0.14332800	-3.90469500	3.59510400
H	-1.04547600	-4.52778200	3.70480100
H	0.67522500	-4.37026700	4.16926300
H	-0.35790100	-2.91996600	4.04305700
N	-3.17318600	-1.60956100	0.57882500
H	7.55860900	-2.10638300	-1.32674400
H	0.98845000	7.14178300	0.63225700
C	-4.08488800	-1.02804800	-0.32066700
C	-5.02875300	-1.85833100	-0.95230400
C	-4.13812900	0.36057400	-0.54039600
C	-6.01064300	-1.31042800	-1.77694200
H	-4.98606700	-2.93919300	-0.79167800
C	-5.11831100	0.89331700	-1.38172700
H	-3.42605600	1.02750000	-0.05109200
C	-6.06117600	0.06916600	-2.00217600
H	-6.73616500	-1.97231100	-2.25702800
H	-5.14492600	1.97396000	-1.54486400
H	-6.82576800	0.49578700	-2.65525900
H	-3.10653200	-2.62368900	0.52496300

TS1'-1 (non-assisted)

E=-1242,41127049

C	-0.89230200	-1.35141700	1.36953200
C	-0.49657300	-0.03658700	1.01913900
C	-1.59370200	0.53868800	0.34733300
H	-2.73969000	-2.35990200	1.05653000
H	-1.62737200	1.54365600	-0.06413700
C	-3.97038600	-0.28987900	-0.31069200
C	-4.70039800	-1.43199300	-0.69569900
C	-4.55272300	0.97611100	-0.51876200
C	-5.97217600	-1.31288700	-1.25760400
H	-4.26273400	-2.42774600	-0.58391700
C	-5.82109100	1.09260100	-1.08655800
H	-4.01195400	1.87405900	-0.21342300
C	-6.53857800	-0.05019500	-1.45586300
H	-6.51918400	-2.21189000	-1.55243400
H	-6.25662300	2.08387200	-1.23476300
H	-7.53339600	0.04311600	-1.89803600
C	0.72550900	0.75751500	1.45882300
C	1.06329200	1.90550600	0.50571900
C	1.18940100	1.73398200	-0.88267300

C	1.28712900	3.17292700	1.05888600
C	1.53332400	2.81381500	-1.70091000
H	1.01799700	0.75133500	-1.32977700
C	1.62644900	4.25518700	0.24049100
H	1.17730300	3.27483000	2.14059400
C	1.75157800	4.07795800	-1.14079300
H	1.63133800	2.66784500	-2.77996300
H	1.79103900	5.24163900	0.68262100
H	2.01702800	4.92278500	-1.78203400
O	0.71168000	1.05736000	2.76491300
C	-0.25111100	-2.44859200	2.03952800
O	0.92235900	-2.51907100	2.39671100
H	-0.92317100	-3.32654400	2.21802600
N	2.12322200	-0.13693500	1.61266100
H	1.86410200	-1.11517700	1.85035100
H	1.92484300	0.47831900	2.64890100
N	3.24710900	-0.06696300	0.80069200
H	3.54751200	0.89347500	0.66991900
C	3.44115100	-0.90397100	-0.30771700
C	4.26408900	-0.45085800	-1.35799300
C	2.89932600	-2.19994500	-0.38122800
C	4.54165600	-1.27538200	-2.44684200
H	4.68445600	0.55793200	-1.31428300
C	3.17936600	-3.01157700	-1.48378400
H	2.28068100	-2.58759200	0.42870100
C	3.99877800	-2.56286200	-2.52274300
H	5.18416800	-0.90233300	-3.24895500
H	2.75161000	-4.01713900	-1.52112700
H	4.21373100	-3.20636500	-3.37872000
C	-2.63598000	-0.39836800	0.28795400
N	-2.19035500	-1.52226600	0.90774500

TS1'-1 (assisted by EtOH)

E= -1397,57237784

C	-1.12929700	-0.02634300	-1.49820600
C	-0.85316200	0.24285800	-0.13502100
C	-2.07125100	0.14036800	0.55423100
H	-2.96276900	-0.57626400	-2.43128100
H	-2.18876300	0.30308200	1.62176800
C	-4.51852200	-0.38632300	-0.15233300
C	-5.44811700	-0.23494700	-1.20025300
C	-4.99845000	-0.74367600	1.12302600
C	-6.81013100	-0.44661800	-0.98288400
H	-5.11229800	0.08162500	-2.19148700
C	-6.36084600	-0.94847400	1.33860200
H	-4.29300600	-0.87877800	1.94524500
C	-7.27241000	-0.80447300	0.28714700
H	-7.51559400	-0.31964500	-1.80775100
H	-6.71329500	-1.22960800	2.33401000
H	-8.33928200	-0.96734600	0.45779800
C	0.43258500	0.64817100	0.60703800

C	0.66191500	2.16517000	0.48943600
C	0.92196900	2.79332100	-0.73826800
C	0.57523000	2.94485800	1.64899000
C	1.09622200	4.17747200	-0.80018200
H	1.00779000	2.20588500	-1.65466900
C	0.74286400	4.33158900	1.58443100
H	0.37994600	2.44050800	2.59585800
C	1.00381100	4.95261200	0.36066200
H	1.30907400	4.65259400	-1.76141200
H	0.67181300	4.92851700	2.49770300
H	1.13852100	6.03627800	0.30978300
O	0.40453700	0.24373300	1.90094700
C	-0.32298800	-0.12124600	-2.68401700
O	0.89729200	0.01804300	-2.75797300
H	-0.90037900	-0.34676000	-3.61538800
N	1.59142400	-0.13623000	-0.06396400
H	1.57407000	-0.00529400	-1.09380400
H	1.34547500	-1.19852400	0.30889300
N	2.83832600	0.28314900	0.48272100
H	2.71053700	0.34353700	1.49330400
H	0.52803100	-0.92376200	1.83144300
O	0.91860600	-2.02891500	1.37345600
C	0.02188800	-3.09740000	1.27085300
H	-0.55401900	-3.20171300	2.21445500
H	-0.73838400	-2.92886600	0.47352000
C	0.75310400	-4.40705300	0.99245600
H	1.30057900	-4.35342800	0.03676900
H	0.05217500	-5.25765800	0.94107500
H	1.48975900	-4.60637900	1.78699200
C	3.98064000	-0.43349800	0.09097800
C	5.07461200	-0.48992500	0.97563100
C	4.09838700	-1.02971300	-1.17734400
C	6.25715500	-1.12116500	0.59615100
H	4.98829200	-0.03216300	1.96498000
C	5.28857400	-1.66617200	-1.54119500
H	3.27390600	-0.99334200	-1.89173700
C	6.37466500	-1.71723800	-0.66489400
H	7.09398600	-1.15461200	1.29884000
H	5.36144000	-2.12598200	-2.53037900
H	7.30104400	-2.21627700	-0.95787000
C	-3.08315600	-0.17612200	-0.36530700
N	-2.49601800	-0.26330400	-1.58825200

INT1-1

E=-1242,47101144

C	-0.27395700	-0.92688700	-0.31199500
C	-0.58815200	0.44396100	-0.41388200
C	-2.00866600	0.54689300	-0.24245900
H	-1.43663000	-2.58269900	0.09996600
H	-2.59564200	1.45682100	-0.33142300
C	-3.89403100	-1.19436400	0.15432900
C	-4.24456100	-2.54755700	-0.02334400

C	-4.91065600	-0.29138000	0.52613200
C	-5.55767000	-2.98130400	0.16833900
H	-3.49069900	-3.27422800	-0.33701900
C	-6.22304100	-0.72496400	0.70814000
H	-4.66357300	0.75992800	0.68831300
C	-6.55496800	-2.07314200	0.53348100
H	-5.80337300	-4.03630200	0.02239500
H	-6.99304300	-0.00523200	0.99772600
C	0.34273800	1.54430100	-0.71152500
C	-0.01246700	2.95033400	-0.31806700
C	-0.78591800	3.25953700	0.81435500
C	0.52807600	3.99999900	-1.08301900
C	-1.02453800	4.59153400	1.16376400
H	-1.17839400	2.45730500	1.44123700
C	0.27295000	5.32771300	-0.74408900
H	1.15125000	3.74840300	-1.94323700
C	-0.50491400	5.62652200	0.38108700
H	-1.61468400	4.82149800	2.05449500
H	0.68615900	6.13513700	-1.35389400
O	1.41215500	1.35260300	-1.29421800
C	0.99940300	-1.75835900	-0.26840500
N	1.87476600	-1.46265000	-1.38028200
C	-2.51880700	-0.72538800	-0.04095300
N	-1.43772300	-1.58385800	-0.08138500
O	0.66037700	-3.14165100	-0.29822000
H	1.49186100	-1.61637800	0.71461000
H	1.85029100	-0.47319400	-1.64423800
H	0.55436300	-3.34814600	-1.24180900
N	3.17816900	-1.95281400	-1.26565600
H	-7.58308600	-2.41227600	0.68113300
H	-0.69920000	6.66765700	0.65178300
C	4.05787000	-1.54995200	-0.25503300
C	5.08362100	-2.42538900	0.15655000
C	3.99503000	-0.26546300	0.32032500
C	6.01867400	-2.02639000	1.11023200
H	5.14131000	-3.42695500	-0.28087400
C	4.93251400	0.11617000	1.28320800
H	3.23155300	0.44055700	-0.00885100
C	5.94964700	-0.75335900	1.68743900
H	6.80544700	-2.72336900	1.41206100
H	4.86762800	1.11844000	1.71588600
H	6.67947000	-0.44448200	2.43924400
H	3.24318600	-2.93323400	-1.51437500

INT1‘-1

E=-1242,4690747

C	-1.74536600	-1.80568000	-0.90140100
C	-0.77837400	-0.79750700	-0.69319400
C	-1.47950500	0.36425200	-0.31872500
H	-3.86672000	-1.71445600	-0.77896500
H	-1.02924900	1.31693100	-0.05485500
C	-3.99597400	0.92581800	0.03652300

C	-5.21811100	0.38230500	0.48011500
C	-3.89029100	2.32588100	-0.08030500
C	-6.30026300	1.20940200	0.78356400
H	-5.32029500	-0.69714700	0.62094400
C	-4.97103800	3.15049500	0.23076600
H	-2.95718900	2.76759700	-0.43582200
C	-6.18186500	2.59703300	0.66054200
H	-7.23777200	0.76753800	1.13010100
H	-4.86975300	4.23388300	0.12974200
H	-7.02829300	3.24460000	0.90144800
C	0.74085400	-0.94900500	-0.77712500
C	1.27970900	-1.54686300	0.54111500
C	1.11265000	-0.85770900	1.75192000
C	1.92909100	-2.78626500	0.55294300
C	1.58563100	-1.39729400	2.94890700
H	0.61574900	0.11422800	1.75509400
C	2.39905700	-3.33082100	1.75319300
H	2.07828800	-3.32246200	-0.38415700
C	2.22938500	-2.63978200	2.95434200
H	1.45436700	-0.84381900	3.88252100
H	2.90577400	-4.29953800	1.74427600
H	2.59946200	-3.06374500	3.89154300
O	1.10999100	-1.72285000	-1.89867600
C	-1.65115500	-3.18556700	-1.30571500
H	-2.62528300	-3.73724200	-1.29969100
O	-0.63025900	-3.77399800	-1.64520500
C	-2.85214500	0.06926900	-0.29234000
N	-2.98295200	-1.24148400	-0.63276500
N	1.29421500	0.38529200	-0.96968700
N	2.67968700	0.36056800	-1.08239600
C	3.44695300	1.43346000	-0.65813100
C	2.92439700	2.46403700	0.14856600
C	4.80854900	1.49155700	-1.02699100
C	3.74842000	3.50700200	0.57595100
H	1.87330500	2.42940800	0.43365800
C	5.61742100	2.53921400	-0.59175200
H	5.22698800	0.70037300	-1.65635000
C	5.09792700	3.55902300	0.21445200
H	3.32246500	4.29503800	1.20388200
H	6.66947600	2.55921800	-0.88990100
H	5.73444700	4.37998800	0.55214900
H	0.62196700	-2.57645500	-1.88082700
H	0.86879900	0.77999400	-1.81642000
H	3.05322200	-0.22332800	-1.82671600

TS2-1 (non-assisted)

E=-1242,39603572

C	0.99430400	-0.45319900	-0.14796700
C	1.14106500	0.77947900	0.52140200
C	2.52967200	1.01627400	0.64252800
H	2.45704800	-1.84889200	-0.74384200
H	2.97644300	1.90200600	1.08713400
C	4.64983400	-0.27349100	-0.12812000

C	5.14750400	-1.10934600	-1.14790900
C	5.57203700	0.34123300	0.74236900
C	6.51855700	-1.33037100	-1.28546400
H	4.45971400	-1.57122900	-1.86114500
C	6.94172400	0.12493400	0.59690600
H	5.20681700	0.97763100	1.55108100
C	7.42209900	-0.71397300	-0.41477100
H	6.88369700	-1.97955500	-2.08523400
H	7.64015000	0.60792800	1.28481300
C	0.12494300	1.73611800	1.06548600
C	-0.99356800	2.23766700	0.20042100
C	-0.99873400	2.10070300	-1.19729000
C	-2.03737600	2.94386200	0.82396200
C	-2.03345000	2.65217700	-1.95656700
H	-0.18331500	1.57303200	-1.69513800
C	-3.07487000	3.48528400	0.06687100
H	-2.00894500	3.05625800	1.90936400
C	-3.07440600	3.34093200	-1.32635800
H	-2.02714100	2.54536300	-3.04410400
H	-3.88656500	4.02541700	0.56076300
O	0.27202700	2.16087400	2.19844300
C	-0.13007600	-1.28218800	-0.44145900
C	3.21290600	-0.03828600	0.03295700
N	2.26381400	-0.89638500	-0.45644600
H	-1.93247500	-2.96530100	0.19659000
H	-0.05782500	-2.00961900	-1.25754400
H	-1.06123200	-1.29141000	1.16600400
O	-0.09369400	-2.52583200	1.39820700
H	0.39827000	-3.04498400	2.05368900
H	-3.88545000	3.76864200	-1.92150100
H	8.49567800	-0.88501400	-0.52454100
N	-1.32799000	-1.09969700	0.11821300
N	-2.24175100	-2.10380600	-0.26553800
C	-3.60669700	-1.81987900	-0.11981000
C	-4.11038000	-0.50903600	-0.18239700
C	-4.50665200	-2.89176900	0.03529400
C	-5.48622600	-0.28634700	-0.09195000
H	-3.42073000	0.32700500	-0.29857900
C	-5.87827000	-2.65491300	0.11707100
H	-4.12025900	-3.91366300	0.08872000
C	-6.38095000	-1.35041400	0.05528700
H	-5.86039100	0.74007500	-0.13812800
H	-6.56091100	-3.50052100	0.23769400
H	-7.45570000	-1.16699700	0.12413500

TS2-1 (assisted by EtOH)

E=-1397,57051773

C	1.22209300	-0.34834800	-0.26970600
C	1.43890600	0.91171900	0.32238900
C	2.84210600	1.09283700	0.40213200
H	2.62248200	-1.81393700	-0.88581300
H	3.32960900	1.98003100	0.79793100
C	4.89056100	-0.31988000	-0.34947300

C	5.32305500	-1.23868900	-1.32653600
C	5.86537000	0.31603400	0.44525900
C	6.67993500	-1.52019400	-1.49453300
H	4.59652700	-1.72034800	-1.98671100
C	7.22058100	0.03966900	0.26899300
H	5.55213600	1.01937800	1.21962500
C	7.63548800	-0.88224700	-0.69852400
H	6.99261900	-2.23385600	-2.26097800
H	7.95947100	0.54184600	0.89851600
C	0.51100700	1.94755900	0.88156500
C	-0.67038000	2.42826900	0.09177300
C	-0.76443500	2.26789400	-1.29920100
C	-1.65968500	3.16474700	0.76652400
C	-1.82887400	2.83627600	-2.00460500
H	0.00667600	1.71134500	-1.83500200
C	-2.73264200	3.71292800	0.06610500
H	-1.55835400	3.29853700	1.84516100
C	-2.81627600	3.55430500	-1.32321000
H	-1.88724500	2.71852900	-3.08957800
H	-3.50383000	4.27439700	0.59962300
O	0.79825000	2.47434300	1.94150700
C	0.08576200	-1.21406600	-0.49925700
C	3.46911100	-0.02000100	-0.15405900
N	2.47022300	-0.87038600	-0.55041400
H	-1.83708400	-2.72282000	-0.00890500
H	0.28230500	-2.10507400	-1.10447000
H	-1.32895700	-0.41147300	0.73913800
O	0.15254700	-2.36963800	1.25294000
H	-0.39556200	-1.47346500	1.83298300
H	1.03927700	-2.45948400	1.62829800
O	-1.05926400	-0.42506500	2.01592800
C	-2.02689900	-0.33189100	3.03433300
H	-1.51825900	-0.10126900	3.99094700
H	-2.69047200	0.52837800	2.82347500
C	-2.86205100	-1.60049500	3.19403900
H	-2.21501800	-2.46958800	3.39880600
H	-3.57362100	-1.50002600	4.03054900
H	-3.44295300	-1.81493500	2.28213100
H	-3.65081400	3.99493400	-1.87511800
H	8.69779000	-1.10012000	-0.83233600
N	-1.17699400	-0.86000000	-0.36346400
N	-2.04739700	-1.92806300	-0.61443900
C	-3.40275700	-1.65950100	-0.81239000
C	-3.85845800	-0.39962500	-1.24021300
C	-4.33780300	-2.69748000	-0.62417500
C	-5.22037700	-0.19426200	-1.47219900
H	-3.14424900	0.41049500	-1.38627800
C	-5.69280900	-2.47802900	-0.86690800
H	-3.99151300	-3.67948600	-0.28891500
C	-6.14782900	-1.22451700	-1.29213900
H	-5.55754400	0.79287500	-1.80029300
H	-6.40192900	-3.29645600	-0.71582200
H	-7.21078400	-1.05448100	-1.47764700

TS2‘-1 (non-assisted)

E=-1242,39338382

C	-0.92758300	-1.67021300	0.03959400
C	-0.64124100	-0.29193800	0.18239900
C	-1.89003700	0.38552900	0.14309300
H	-2.71360900	-2.69488300	-0.21312400
H	-2.03155300	1.45706000	0.25306900
C	-4.35670200	-0.40323800	-0.07595500
C	-5.22877800	-1.48610900	0.15074400
C	-4.91759600	0.85374800	-0.37650800
C	-6.61211500	-1.31880500	0.07344300
H	-4.82946200	-2.46899500	0.41333500
C	-6.30022900	1.01948500	-0.44725900
H	-4.26191800	1.70464200	-0.57210400
C	-7.15485700	-0.06570100	-0.22505300
H	-7.26972500	-2.17228700	0.25605800
H	-6.71424400	2.00260800	-0.68478100
C	0.65347900	0.35785100	0.32109400
C	0.76077900	1.81208000	0.00169500
C	0.64542500	2.23749400	-1.33130100
C	0.96855700	2.75810000	1.01849900
C	0.76019500	3.59417400	-1.64557200
H	0.47581100	1.50511600	-2.12412100
C	1.07061900	4.11333800	0.69730700
H	1.03159800	2.38830700	2.04392200
C	0.97198000	4.53419600	-0.63289400
H	0.68040300	3.91662000	-2.68677400
H	1.22613700	4.84614300	1.49334300
O	0.83275300	0.06996800	2.50107500
C	-0.13936600	-2.89607700	-0.06921000
O	-0.67647200	-3.98207300	-0.21780800
H	0.96341600	-2.78656600	-0.01675200
C	-2.90108300	-0.56615000	-0.00022800
N	-2.28584100	-1.78676200	-0.05725800
N	1.74824700	-0.41933500	0.45968200
H	3.07975400	0.74203300	1.40425200
H	0.28189500	0.02264900	3.29806400
N	2.97713400	0.25280400	0.51603300
C	4.11219500	-0.44995600	0.09935900
C	4.04688800	-1.45569200	-0.88239000
C	5.36821000	-0.10142800	0.63315100
C	5.21322700	-2.09377300	-1.30983300
H	3.08003800	-1.72618600	-1.30835500
C	6.52570200	-0.74003300	0.19028000
H	5.42913600	0.67686700	1.39946800
C	6.45971000	-1.74367100	-0.78266600
H	5.14261800	-2.87533400	-2.07133900
H	7.49044600	-0.45416700	0.61812700
H	7.36771400	-2.24621200	-1.12342000
H	1.05514100	5.59561700	-0.88026400
H	-8.23805200	0.06523700	-0.28344700

H	1.50314700	-0.82764900	1.45877100

TS2'-1 (assisted by EtOH)

E= -1397,55710332

C	1.08085400	1.35974400	-0.65830000
C	0.85409700	0.05754800	-0.16143000
C	2.13558900	-0.51580600	0.06701100
H	2.82274100	2.40518800	-1.06431500
H	2.32197900	-1.50717500	0.47100100
C	4.56900600	0.35509300	-0.20868200
C	5.36331700	1.51845900	-0.22354800
C	5.21619500	-0.89385200	-0.12933200
C	6.75527200	1.43489400	-0.16708500
H	4.89391000	2.50491200	-0.25648900
C	6.60684100	-0.97413100	-0.06650800
H	4.62284800	-1.81052500	-0.13388100
C	7.38405900	0.18901300	-0.08738000
H	7.35135700	2.35078000	-0.17686800
H	7.08858000	-1.95339200	-0.00836500
C	-0.40680100	-0.63127100	0.11642400
C	-0.39112400	-2.13386700	0.12923400
C	-0.28170000	-2.78305400	-1.11240800
C	-0.47612800	-2.89680200	1.30219200
C	-0.27192900	-4.17781300	-1.17902800
H	-0.20834100	-2.19349200	-2.02953600
C	-0.45801400	-4.29284000	1.22830300
H	-0.55549300	-2.36559400	2.25123900
C	-0.35874700	-4.93682900	-0.00792100
H	-0.19368200	-4.67211600	-2.15063800
H	-0.52406000	-4.88040000	2.14774400
O	-0.42097000	-0.16320300	2.31578300
C	0.25207400	2.46140800	-1.15580300
O	0.75833000	3.50264200	-1.53558300
H	-0.84232200	2.29764800	-1.19644800
C	3.10551700	0.42925600	-0.26936800
N	2.43351200	1.54096000	-0.69837000
N	-1.55489500	0.01529900	-0.06326500
H	-2.73557000	-0.88601200	1.28406900
O	-1.14330600	1.97912400	1.48701200
H	-0.75133600	1.01156100	2.02259400
C	-2.10490600	2.69487400	2.21938600
H	-1.65754000	3.06265000	3.16625500
H	-2.95888400	2.04750700	2.51890000
C	-2.63104300	3.88377300	1.42540200
H	-3.14097600	3.55039800	0.50626300
H	-3.35193100	4.47044400	2.01871300
H	-1.80098700	4.54616100	1.13160100
H	0.50097600	-0.14185700	2.60733500
N	-2.71745800	-0.66080900	0.28986700
C	-3.92373100	-0.22292900	-0.26363900
C	-3.97299000	0.42446700	-1.51153100
C	-5.12697400	-0.48041900	0.42108900

C	-5.20299300	0.80717000	-2.05164700
H	-3.04726700	0.61569600	-2.05623400
C	-6.34769000	-0.10154900	-0.13517800
H	-5.09710400	-0.98069100	1.39324900
C	-6.39745200	0.54788000	-1.37389700
H	-5.22340800	1.31187800	-3.02128200
H	-7.27109900	-0.31024900	0.41155600
H	-7.35551200	0.84835700	-1.80371800
H	-0.34744400	-6.02855500	-0.06022400
H	8.47380100	0.12431400	-0.04100700
H	-1.51739400	1.03141900	0.35503400

INT2-1

E= -1166,00789672

C	0.01129300	-0.38176700	-0.14239000
C	-1.37933500	-0.62962700	-0.18847700
C	-2.01782400	0.64862900	-0.17121100
H	1.09429900	1.39511700	0.00102500
H	-3.08396500	0.83600400	-0.25899600
C	-1.14095800	3.08951100	-0.10344700
C	-0.04906500	3.91158600	-0.44898300
C	-2.35408400	3.71560900	0.25018100
C	-0.16395100	5.30269000	-0.43480900
H	0.89875800	3.46411100	-0.75916700
C	-2.46892000	5.10477800	0.25457500
H	-3.21021200	3.10303300	0.54051700
C	-1.37402100	5.90786400	-0.08449800
H	0.69708500	5.91733200	-0.70971900
H	-3.41959200	5.56604500	0.53433500
H	-1.46437100	6.99673900	-0.07594300
C	-1.97785800	-1.97305000	-0.30034100
C	-3.44948600	-2.16384200	-0.03899700
C	-4.16482500	-1.42911600	0.92168500
C	-4.10796700	-3.19003600	-0.73937700
C	-5.51395100	-1.70526700	1.16306300
H	-3.65865500	-0.65976600	1.50709800
C	-5.45871000	-3.45083900	-0.51297000
H	-3.53460900	-3.77680600	-1.45975900
C	-6.16597800	-2.70771400	0.43971600
H	-6.05639300	-1.13772000	1.92367400
H	-5.96315900	-4.24112500	-1.07497700
H	-7.22317500	-2.91645000	0.62360700
O	-1.30266300	-2.94865200	-0.61634000
C	1.13455900	-1.28854700	-0.12465500
H	0.90344300	-2.35884800	-0.21389900
N	2.33902100	-0.82590200	-0.02533100
N	3.35572900	-1.68582900	-0.02000000
H	3.16029100	-2.68507200	-0.09709900
C	4.68633500	-1.28877800	0.08154400
C	5.05395000	0.06462200	0.19600400
C	5.69021600	-2.27613800	0.06939400
C	6.40188600	0.40970900	0.29476000

H	4.27605300	0.82701900	0.20656400
C	7.03291800	-1.91383500	0.16941000
H	5.41205800	-3.33061100	-0.01943800
C	7.40154500	-0.56922400	0.28272400
H	6.67421300	1.46495900	0.38335400
H	7.79872700	-2.69381800	0.15818100
H	8.45402200	-0.28812800	0.36089500
C	-1.03417800	1.62872500	-0.11257300
N	0.17909800	0.97052500	-0.09202600

INT2‘-1

E= -1166,00322868

C	-0.84900800	-1.62418800	0.35558200
C	-0.57559100	-0.25913400	0.11052900
C	-1.83199700	0.35996100	-0.12620700
H	-2.62320100	-2.71038600	0.37530300
H	-1.99334000	1.41458000	-0.33336600
C	-4.28591900	-0.49855600	-0.19217000
C	-5.15807400	-1.50831800	0.26132800
C	-4.84922900	0.63946100	-0.80358800
C	-6.53937300	-1.38686200	0.10461900
H	-4.75999900	-2.39445100	0.76189500
C	-6.23011000	0.76139600	-0.95385700
H	-4.19518300	1.42904200	-1.17881100
C	-7.08342300	-0.25139700	-0.50278700
H	-7.19506000	-2.18274900	0.46673900
H	-6.64373600	1.65187000	-1.43409200
C	0.72583900	0.41745200	0.08078900
C	0.75223200	1.91553700	0.17573900
C	1.23829800	2.69389200	-0.89168500
C	0.29539200	2.57025400	1.33350500
C	1.26685700	4.08857300	-0.80164900
H	1.58356500	2.20032900	-1.80408600
C	0.32759800	3.96426500	1.42349500
H	-0.08963400	1.97761500	2.16698200
C	0.81316000	4.72698600	0.35658700
H	1.63935500	4.67870400	-1.64294300
H	-0.02926700	4.45735100	2.33139700
C	-0.04737200	-2.78395000	0.71342400
O	-0.54768300	-3.88911800	0.87052100
H	1.04016900	-2.60311000	0.84354200
C	-2.83262500	-0.61539500	-0.03473500
N	-2.20826400	-1.79177300	0.25685200
N	1.80000700	-0.30583500	-0.02774200
H	3.09398100	1.25830600	0.18427600
N	3.00643900	0.25784500	0.00518700
C	4.17730700	-0.48264000	-0.15120700
C	4.15713000	-1.85061000	-0.47966700
C	5.41470500	0.16771900	0.01673800
C	5.35875500	-2.54459300	-0.62453700
H	3.19943300	-2.34958100	-0.62381600
C	6.60662900	-0.53972900	-0.13704100

H	5.43710600	1.23116400	0.27325500
C	6.59000500	-1.90147900	-0.45630700
H	5.32928600	-3.60762000	-0.87850900
H	7.55842500	-0.01917600	-0.00190000
H	7.52479100	-2.45398800	-0.57428500
H	0.83553700	5.81744200	0.42672200
H	-8.16516900	-0.15593100	-0.62392200

TS3-1 (non-assisted)

E=-1165,95331551

C	-0.94397600	-1.60276300	-0.56823300
C	-0.58824100	-0.22994800	-0.65364700
C	-1.75874800	0.52006100	-0.30763100
H	-2.78293800	-2.49313400	-0.02944400
H	-1.84776700	1.60339400	-0.32760200
C	-4.22088200	-0.13040100	0.15425900
C	-5.20696500	-1.07627900	-0.19186100
C	-4.63590900	1.06655400	0.77279800
C	-6.55560800	-0.83776400	0.07893100
H	-4.92219100	-1.99766700	-0.70657800
C	-5.98437700	1.30629300	1.03284000
H	-3.88729200	1.80519000	1.06742100
C	-6.95201500	0.35441700	0.69133500
H	-7.30280000	-1.58446200	-0.20199800
H	-6.28291500	2.24048000	1.51545400
H	-8.00792900	0.54207500	0.90059200
C	0.68333400	0.28399600	-1.10700500
C	1.21169000	1.53288500	-0.54351900
C	0.96379000	1.89384000	0.79924400
C	2.01216000	2.38553800	-1.33362200
C	1.48350300	3.07489400	1.32442200
H	0.37723600	1.22729100	1.43389100
C	2.52375300	3.57019600	-0.80518800
H	2.20478500	2.10627800	-2.36980700
C	2.26144700	3.92025000	0.52351800
H	1.29068800	3.33511400	2.36825400
H	3.13173800	4.22611800	-1.43357600
H	2.66827600	4.84623900	0.93801600
O	1.11532100	-0.00338700	-2.36643200
C	-0.08429900	-2.71944600	-0.37733900
H	-0.52961300	-3.70033600	-0.17551100
N	1.21784100	-2.64684900	-0.20828600
N	1.87478300	-1.56855100	-0.55954700
C	3.11580000	-1.39784500	0.08567100
C	4.05109800	-0.52351400	-0.50275200
C	3.45147100	-2.04582800	1.29155900
C	5.28938900	-0.30485600	0.09972800
H	3.79498100	-0.03408300	-1.44349600
C	4.69551000	-1.82714000	1.88220800
H	2.72385400	-2.72158500	1.74244700
C	5.61984200	-0.95544900	1.29390700
H	6.00595600	0.37354000	-0.37083800
H	4.94665300	-2.33876000	2.81559700

H	6.59203200	-0.78505300	1.76321200
H	1.52161600	-0.89309000	-2.27064300
C	-2.80122400	-0.37262500	-0.11636500
N	-2.29265100	-1.64757800	-0.29266400

TS3-1 (assisted by EtOH)

E= -1321,09275894

C	0.97302600	0.45649000	1.01778600
C	0.74077700	-0.15868200	-0.21937700
C	2.00308200	-0.54093600	-0.74827600
H	2.79597900	0.90326500	1.98928400
H	2.17026200	-1.07085000	-1.68333400
C	4.44664600	-0.27480400	0.09297300
C	5.24296300	-0.21531100	1.25558000
C	5.09633300	-0.47300500	-1.14329500
C	6.63141300	-0.33840400	1.18332000
H	4.77397600	-0.10011100	2.23660100
C	6.48231200	-0.60603700	-1.21114000
H	4.50577600	-0.50449100	-2.06134900
C	7.25980000	-0.53566700	-0.04954500
H	7.22517000	-0.29140300	2.09986400
H	6.96198800	-0.75642500	-2.18175400
H	8.34642100	-0.63521900	-0.10547200
C	-0.55526200	-0.46746300	-0.89427900
C	-1.25242900	-1.73109500	-0.61569600
C	-0.85143600	-2.57509900	0.43989200
C	-2.35633500	-2.10279500	-1.41122300
C	-1.53514900	-3.76366500	0.68857500
H	-0.00113000	-2.29150700	1.06203400
C	-3.03762800	-3.29055100	-1.15532400
H	-2.66134700	-1.44501900	-2.22492000
C	-2.62884600	-4.12397700	-0.10757000
H	-1.21660500	-4.41287700	1.50777400
H	-3.89448100	-3.56927700	-1.77345600
H	-3.16538900	-5.05541800	0.09116800
O	-0.86159200	0.16391800	-1.96497700
C	0.05287600	0.93504300	2.02621900
H	0.44155700	1.10143200	3.03864400
N	-1.21796000	1.13009000	1.86334800
N	-1.71446000	1.03875200	0.61191200
C	-3.10358300	0.86169500	0.54815400
C	-3.77323200	1.13280900	-0.66658800
C	-3.86174400	0.38369500	1.63977700
C	-5.14977100	0.93157000	-0.77773600
H	-3.20832200	1.52509100	-1.51301700
C	-5.23774400	0.19725800	1.51771300
H	-3.34863300	0.17454200	2.57852200
C	-5.89446000	0.46483600	0.31039000
H	-5.64768300	1.15521400	-1.72558700
H	-5.80681000	-0.16733200	2.37799700
H	-6.97317000	0.31433500	0.22058400
H	-1.17589500	1.97015000	-0.36850700
H	-0.66225900	1.30757700	-1.82053700

O	-0.80344900	2.43256900	-1.29884000
C	0.28939100	3.33566800	-1.15230800
H	1.13319300	2.83833200	-0.63960300
H	0.63268000	3.59915400	-2.16687200
C	-0.13673500	4.58373900	-0.39630500
H	0.70109400	5.29617400	-0.32591700
H	-0.97509500	5.08080700	-0.90837900
H	-0.45994900	4.33436600	0.62715400
C	2.99000600	-0.14515200	0.15441000
N	2.33576000	0.44353400	1.21372000

INT3-1

E= -1165,99272983

C	0.54749900	-0.43653400	0.28950900
C	0.90504600	-1.68885500	-0.19208900
C	-0.08684500	-2.66905600	-0.50581000
C	-0.87595100	-0.11299200	0.65257700
C	1.73791600	0.32274700	0.43075300
C	2.80032400	-0.48889300	0.03434800
H	0.15505000	-3.66824600	-0.88009700
H	1.82108200	1.33817900	0.81033300
H	2.79584400	-2.46364100	-0.76101100
C	4.23911100	-0.21629200	-0.00519900
C	5.18897000	-1.25769600	0.03122400
C	4.71348800	1.10983500	-0.07629400
C	6.55728300	-0.98458100	-0.01243800
H	4.85946500	-2.29606200	0.12463000
C	6.08075600	1.38023200	-0.10876000
H	3.99790900	1.93322500	-0.12612600
C	7.01152300	0.33541500	-0.08124600
H	7.27343800	-1.80977600	0.01992000
H	6.42373300	2.41648100	-0.16678200
H	8.08259000	0.54935400	-0.11217900
N	2.26944000	-1.71414700	-0.33135100
N	-1.34503600	-2.38741400	-0.36928400
N	-1.75413900	-1.18047200	0.07413400
C	-3.17690500	-1.02427900	0.07407900
C	-3.93316500	-1.66091400	-0.92635400
C	-3.84114200	-0.25682400	1.04528500
C	-5.32057800	-1.52486900	-0.95659500
H	-3.41717200	-2.26632200	-1.67097700
C	-5.23091600	-0.11688000	0.99571200
H	-3.27409400	0.20776800	1.84837500
C	-5.98066000	-0.74679000	0.00022900
H	-5.89007500	-2.02706400	-1.74335400
H	-5.73044600	0.48444600	1.76001700
H	-7.06753400	-0.63723100	-0.02836200
C	-1.26244500	1.27264600	0.11374300
C	-1.30491600	2.39141100	0.95528700
C	-1.49226700	1.44361500	-1.25893300
C	-1.58257000	3.65905700	0.43189400
H	-1.12474200	2.26051700	2.02229200
C	-1.77249500	2.70760700	-1.77978300

H	-1.45680400	0.57732500	-1.92329900
C	-1.81874800	3.82181000	-0.93488100
H	-1.61685700	4.52331800	1.10062800
H	-1.95678900	2.82338600	-2.85096300
H	-2.03888400	4.81205400	-1.34208400
O	-1.01147900	-0.06309200	2.07168900
H	-0.54963100	-0.83226200	2.43347700

INT4-1

E= -1321,57671196

C	0.38100100	0.17140700	-0.06013100
C	-1.01926100	0.51758800	-0.05688800
C	-1.07917200	1.96314000	-0.07937300
H	2.07179600	1.37198700	-0.03697500
H	-1.97966600	2.56455000	-0.15303200
C	0.72320300	3.81698900	-0.14711100
C	2.01033800	4.09486100	-0.64690900
C	-0.07317900	4.89054700	0.29728400
C	2.48652600	5.40587500	-0.69756900
H	2.64209700	3.28944900	-1.03103000
C	0.40310900	6.19929200	0.23944600
H	-1.06525200	4.69481100	0.70986100
C	1.68524700	6.46227600	-0.25562300
H	3.48531100	5.60357100	-1.09351500
H	-0.22608500	7.01986700	0.59197600
H	2.05828700	7.48817400	-0.29627500
C	-2.10003200	-0.38039100	-0.06916900
C	-3.50255500	0.05229500	0.09217500
C	-3.86835000	0.98560000	1.08337000
C	-4.49958400	-0.48777000	-0.74780400
C	-5.20189600	1.36794700	1.22866400
H	-3.11024800	1.38499900	1.75911000
C	-5.82694500	-0.08329200	-0.60993100
H	-4.22950600	-1.20649600	-1.52354900
C	-6.18092600	0.84204200	0.37871000
H	-5.47950000	2.07826400	2.01066000
H	-6.58872900	-0.48583500	-1.28152400
H	-7.22260800	1.15319600	0.48730000
O	-1.85535600	-1.65253700	-0.26541300
C	1.05212200	-1.09493100	-0.01632600
H	0.44876200	-2.00979400	-0.02804000
N	2.35638800	-1.10883800	0.02984600
N	2.99720400	-2.24569200	0.06440200
H	2.46821200	-3.12220600	0.05033800
C	4.39794000	-2.35047400	0.11928300
C	5.22473800	-1.21697200	0.16116600
C	4.96166700	-3.63678400	0.13289600
C	6.60826100	-1.38294300	0.21495600
H	4.78001500	-0.22252800	0.15291300
C	6.34727900	-3.78610000	0.18751800
H	4.31566700	-4.51912900	0.10001200
C	7.17739600	-2.66167700	0.22846700
H	7.25093700	-0.49997200	0.24795400

H	6.77945000	-4.78924800	0.19768900
H	8.26199000	-2.78037200	0.27124600
C	0.20737300	2.44553600	-0.09409400
N	1.05809000	1.33881100	-0.07840600
H	-2.64239300	-2.27092000	-0.11188600
O	-3.72511500	-3.40467300	0.08008600
C	-3.47161900	-4.81656600	-0.04750400
H	-2.62780600	-4.89413600	-0.74946900
H	-3.13570800	-5.22293000	0.92322000
C	-4.68254800	-5.56732000	-0.56840500
H	-4.44372500	-6.63547500	-0.68936100
H	-5.53102200	-5.49830200	0.13305100
H	-5.00347600	-5.17223500	-1.54428000
H	-4.47561000	-3.25264400	0.67275400

TS5-1 (not assisted)

E=-1166,36790832

C	-0.98050800	-1.69327300	-0.28881700
C	-0.59227200	-0.37098700	-0.52043800
C	-1.74485100	0.44696300	-0.40706900
H	-2.89492100	-2.50763700	0.12025100
H	-1.79360900	1.52891800	-0.49731900
C	-4.23809100	-0.08866700	0.08862300
C	-5.06716900	-0.93761100	0.84798900
C	-4.79410800	1.08115700	-0.46472400
C	-6.41433200	-0.62964200	1.03955200
H	-4.65866200	-1.83283000	1.32520000
C	-6.13961800	1.38848300	-0.26632700
H	-4.17420800	1.74393400	-1.07229400
C	-6.95472200	0.53377900	0.48335200
H	-7.04231300	-1.29569000	1.63552600
H	-6.55738900	2.29675900	-0.70647900
H	-8.00916300	0.77505800	0.63544600
C	0.81304400	-0.05832600	-0.81597700
C	1.34223400	1.25055400	-0.30448200
C	1.15314300	1.54552100	1.05774600
C	2.00305700	2.17576100	-1.12663000
C	1.62572700	2.74570700	1.58769100
H	0.63378900	0.83633200	1.70590600
C	2.46611200	3.38040400	-0.59056100
H	2.14710400	1.96512800	-2.18605600
C	2.28246800	3.66647100	0.76415800
H	1.47582600	2.96528400	2.64706400
H	2.97178600	4.09871400	-1.23963600
H	2.64717100	4.60880100	1.17935800
O	1.06418700	-0.13171200	-2.36317000
C	-0.03641000	-2.76120000	-0.17990200
H	-0.34900500	-3.78634800	0.04790100
N	1.23837000	-2.58294800	-0.28956700
N	1.73598400	-1.31762300	-0.62759600
C	3.05629900	-1.10743800	-0.03461300
C	4.10605200	-0.66893000	-0.84456000
C	3.25794100	-1.36969700	1.32317100

C	5.37119800	-0.47568500	-0.28330500
H	3.94890700	-0.49060100	-1.91092000
C	4.52562100	-1.17764800	1.87517200
H	2.43487400	-1.73723900	1.93832900
C	5.58134600	-0.72811800	1.07496100
H	6.19615300	-0.13883700	-0.91471800
H	4.69035000	-1.38592000	2.93461800
H	6.57277800	-0.58330800	1.50984700
H	1.66007500	-1.06334000	-1.99594100
H	0.23414500	-0.32897000	-2.84120400
C	-2.81983500	-0.39943000	-0.12093400
N	-2.32594500	-1.68562700	-0.05054900

TS5-1 (assisted by EtOH)

E= -1321,53566042

C	-1.07116500	-1.46483700	0.42893300
C	-0.80877900	-0.27837400	-0.24873300
C	-2.04292800	0.37847200	-0.46332800
H	-2.91455900	-2.30604700	1.07655700
H	-2.20321300	1.34295000	-0.93833700
C	-4.49288800	-0.22407200	0.16472400
C	-5.27441700	-0.84696700	1.15786700
C	-5.13408900	0.61765600	-0.76528000
C	-6.65359300	-0.64242700	1.21213000
H	-4.80480700	-1.47457400	1.92040000
C	-6.51160400	0.82515400	-0.70436700
H	-4.55166300	1.09769800	-1.55452300
C	-7.27732000	0.19417700	0.28176200
H	-7.24241800	-1.12986300	1.99260700
H	-6.99270600	1.47779600	-1.43656100
H	-8.35672100	0.35590800	0.32634100
C	0.59205000	0.00044300	-0.69344100
C	0.89234200	1.48914500	-0.83132100
C	0.54415700	2.36415500	0.21110700
C	1.49471900	2.00993900	-1.98471800
C	0.80415500	3.73059400	0.10341200
H	0.07034200	1.97635000	1.11495600
C	1.74958400	3.38102000	-2.09308600
H	1.76454600	1.34525600	-2.80591800
C	1.40787200	4.24359800	-1.04979500
H	0.53075400	4.39913800	0.92298000
H	2.21610000	3.77349800	-2.99968900
H	1.60680300	5.31446700	-1.13483100
O	0.78021200	-0.66926300	-2.00195700
C	-0.01367400	-2.31242500	0.87289500
H	-0.20095100	-3.28409600	1.34363100
N	1.23179800	-1.95810200	0.79776900
N	1.57242400	-0.73097600	0.19291900
C	2.54295600	-0.00362500	0.99517300
C	3.64115300	0.61009500	0.37854900
C	2.40550600	0.04343800	2.38783600
C	4.58328300	1.29011900	1.15352000
H	3.76054300	0.56684700	-0.70539800

C	3.35778600	0.71538500	3.15755200
H	1.55927800	-0.45126600	2.86633500
C	4.44503800	1.34411800	2.54354000
H	5.43430500	1.77176500	0.66668600
H	3.24709700	0.74800300	4.24390400
H	5.18697300	1.87082600	3.14787400
H	2.63594500	-1.64316400	-0.81958900
H	2.01805300	-1.60150000	-2.19396300
O	2.84295000	-2.01386600	-1.74874000
C	2.90549000	-3.49426900	-1.78881200
H	1.89969100	-3.87263100	-1.55658100
H	3.16118600	-3.73079400	-2.83023900
C	3.94610300	-3.97378600	-0.80762500
H	4.01206900	-5.07083500	-0.86740800
H	4.93759900	-3.55824300	-1.04062500
H	3.66708100	-3.70504400	0.22292000
H	-0.00948000	-0.53188700	-2.54716500
C	-3.04212300	-0.43036700	0.09464900
N	-2.42634400	-1.54144900	0.62536000

Product 4a

E= -1089,98846799

C	0.52499400	-0.38568500	-0.05142800
C	0.94312900	-1.74570900	-0.10337000
C	-0.01724800	-2.76642500	-0.10972700
C	-0.86009200	-0.11792800	-0.00651700
C	1.70234400	0.41235600	-0.00148900
C	2.78757500	-0.45604500	-0.03835300
H	0.23033000	-3.83152900	-0.12877900
H	1.75654700	1.49293500	0.08776600
H	2.88070000	-2.58503300	-0.17403300
C	4.22375900	-0.17259300	-0.01181100
C	5.15051500	-1.13573700	0.43524500
C	4.70026100	1.08597200	-0.42974500
C	6.51517000	-0.84903100	0.45752500
H	4.81156200	-2.10793800	0.80342000
C	6.06463700	1.36876900	-0.40389400
H	4.00040000	1.83844400	-0.79874600
C	6.97572200	0.40280100	0.03759300
H	7.22123400	-1.60245800	0.81344700
H	6.42126900	2.34579800	-0.73731500
H	8.04483300	0.62623600	0.05544300
N	2.29903100	-1.75762500	-0.09638000
N	-1.30073900	-2.47914500	-0.09582400
N	-1.69237600	-1.19724700	-0.06286600
C	-3.14329000	-1.06519600	-0.13285800
C	-3.92038400	-1.70198700	0.83746100
C	-3.72469600	-0.36828500	-1.19408500
C	-5.31126900	-1.61362300	0.75402900
H	-3.44083300	-2.26457000	1.64022800
C	-5.11727400	-0.29095300	-1.26784700
H	-3.10298700	0.10125000	-1.95787700

C	-5.90983000	-0.90719700	-0.29454100
H	-5.92874900	-2.10382800	1.50977100
H	-5.58289100	0.24681700	-2.09649500
H	-6.99838600	-0.84415800	-0.35803900
C	-1.37748100	1.26172300	0.13872500
C	-2.23372100	1.61012300	1.19994800
C	-0.95176600	2.25581200	-0.76241600
C	-2.65557200	2.93051000	1.35140900
H	-2.55922800	0.85278600	1.91514700
C	-1.39433000	3.57159100	-0.61496900
H	-0.29447100	1.99368800	-1.59468100
C	-2.24320100	3.91135500	0.44279300
H	-3.31038600	3.19543200	2.18444500
H	-1.07487700	4.33373400	-1.32925300
H	-2.58318600	4.94278900	0.56097400

Mechanism 2 (leading to product 6c)

Pyrrolo-2,3-dicarbonyl 2f

E=-1113,23007981

C	-0.61622200	1.13817200	-0.79588100
C	-0.81980000	-0.24484800	-0.62623000
C	0.44213100	-0.81463300	-0.34175400
H	1.17746700	2.26761300	-0.74408700
H	0.62350500	-1.86833900	-0.14477400
C	2.83420600	0.16168000	-0.04451700
C	3.54224900	1.29067600	0.42181600
C	3.56013500	-1.02533500	-0.24074500
C	4.90766000	1.23646200	0.66764000
H	3.01277000	2.22553800	0.62520100
C	4.93139400	-1.09593400	0.00997700
H	3.04735800	-1.91336400	-0.61644500
C	5.62033400	0.04053100	0.46482800
H	5.45244600	2.10855700	1.03428900
H	5.45316100	-2.03731000	-0.16201300
C	-2.05320000	-1.08206600	-0.78746400
C	-3.33945200	-0.69560000	-0.13020200
C	-3.42247400	0.26688500	0.88901400
C	-4.50340800	-1.38794300	-0.51027400
C	-4.63839800	0.54162400	1.51343300
H	-2.52582900	0.79986300	1.20877600
C	-5.72727300	-1.11444600	0.09320200
H	-4.42186100	-2.14564700	-1.29162300
C	-5.77592700	-0.14971800	1.10046700
H	-4.72179900	1.28262500	2.31053200
H	-6.64317100	-1.63302800	-0.19671600
O	-1.96399100	-2.12284100	-1.41830600
C	-1.48306300	2.22376700	-1.23061300
H	-0.95345800	3.21572200	-1.29110800
O	-2.65803200	2.13158800	-1.51753200
C	1.39472400	0.20903000	-0.31326700
N	0.73008000	1.37117600	-0.59092200
F	-6.94797800	0.11522000	1.69087700

O	6.94588500	0.08153400	0.73323500
C	7.72570200	-1.08300500	0.56518100
H	7.72001900	-1.43295600	-0.48264400
H	8.75282300	-0.81353200	0.84451800
H	7.38101200	-1.90500500	1.21779900

Glycine methylester

E=-323,893424611

C	0.03018200	0.09706100	0.04521900
O	0.08412900	1.30179600	0.08926500
C	-1.24986700	-0.70984200	0.14435300
H	-1.14478400	-1.60748800	-0.48787000
H	-1.27431300	-1.08399800	1.19448200
N	-2.38150300	0.09632800	-0.26264800
H	-3.25279100	-0.29311500	0.09120600
H	-2.28059100	1.03605300	0.12252400
O	1.11005800	-0.69659400	-0.04320000
C	2.37843500	-0.04043300	-0.06329500
H	2.52758300	0.55361200	0.85139800
H	3.13284500	-0.83412300	-0.12877000
H	2.45657700	0.63242900	-0.93062400

TS1-2 (non-assisted)

E=-1437,0864739

C	0.21979000	-0.87506600	0.81200000
C	0.34687100	0.44437200	0.34665200
C	-0.97408500	0.86176300	-0.02872100
H	-1.35369400	-2.13495800	1.09345200
H	-1.24506900	1.80524200	-0.49509800
C	-3.29351900	-0.31068400	0.00828800
C	-3.94590100	-1.55432300	0.03498200
C	-4.08724800	0.83139200	-0.23735500
C	-5.32446800	-1.66973000	-0.16890100
H	-3.37418300	-2.47036800	0.20258300
C	-5.45475600	0.73076600	-0.44862000
H	-3.62191800	1.81929900	-0.24962100
C	-6.09286900	-0.52299600	-0.41511600
H	-5.78210000	-2.65866000	-0.13988900
H	-6.06469800	1.61695700	-0.63528000
C	1.64237400	1.12349700	0.23292300
C	1.71473000	2.61716600	0.09616900
C	0.74379100	3.48924100	0.61873900
C	2.85251900	3.16469500	-0.52489600
C	0.89361500	4.87323600	0.51094400
H	-0.12424200	3.08715500	1.14252100
C	3.00717800	4.54221300	-0.65486900
H	3.61529100	2.48128200	-0.90221800
C	2.02011000	5.37974800	-0.13358800
H	0.15612400	5.56432000	0.92359000
H	3.87749100	4.98161400	-1.14628200
O	2.69164300	0.47506800	0.24066400
C	1.14113600	-1.90427800	1.41846700
N	2.11019600	-2.50983900	0.36208500

H	1.42631000	-3.42041900	0.76758200
C	-1.84845700	-0.19022900	0.22211000
N	-1.08347600	-1.21804000	0.73508700
C	3.54491300	-2.47872400	0.63601800
H	3.76308700	-3.02779600	1.56367600
H	3.87272600	-1.43351000	0.75986700
C	4.31016400	-3.07750800	-0.52702400
O	3.85266200	-3.22587600	-1.63397000
O	5.56402000	-3.37988100	-0.17714900
C	6.41113000	-3.88829700	-1.21289000
H	6.50193000	-3.16025200	-2.03273700
H	7.38819600	-4.06407500	-0.74741700
H	6.00589300	-4.82677400	-1.61953500
F	2.16433700	6.70572800	-0.24890600
O	-7.43276400	-0.52048400	-0.62776100
C	-8.13776100	-1.74059100	-0.60047900
H	-9.19194300	-1.49804400	-0.79074600
H	-7.78530000	-2.43780900	-1.38227200
H	-8.05797100	-2.24060000	0.38193800
O	0.50980100	-3.05900700	1.74266500
H	1.78010200	-1.43325000	2.19914300
H	1.92946300	-2.19829200	-0.59791000

TS1-2 (assisted by EtOH)

E=-1592,2515823

C	-0.23299900	-0.35439700	-0.84501000
C	-0.15281500	0.94908200	-0.31600900
C	1.22982700	1.16398800	0.01023400
H	1.17124300	-1.78503800	-1.26000400
H	1.64413900	2.03578600	0.50932400
C	3.35900800	-0.31145500	-0.18533300
C	3.81787500	-1.63839800	-0.22202200
C	4.32274000	0.70374800	0.00069800
C	5.17316700	-1.95407200	-0.08562200
H	3.10856700	-2.46168500	-0.33807600
C	5.66955200	0.40413200	0.14592400
H	4.00798200	1.74947000	0.01715300
C	6.11346100	-0.93070000	0.10217400
H	5.47816200	-3.00005900	-0.11766200
H	6.41229400	1.19195500	0.28660400
C	-1.30004500	1.83514300	-0.10297100
C	-1.10257300	3.31124800	0.06266200
C	-0.04613700	4.02079800	-0.53575500
C	-2.07177700	4.02478300	0.79300000
C	0.05252500	5.40611000	-0.39649100
H	0.69101800	3.49272000	-1.14177500
C	-1.97553700	5.40398800	0.95479700
H	-2.90386200	3.47097000	1.23121600
C	-0.90966900	6.07696500	0.35577000
H	0.85770100	5.97424600	-0.86612800
H	-2.71059000	5.96967300	1.53059700
O	-2.45447200	1.39089100	-0.04537100
C	-1.31492100	-1.21502200	-1.48649000

N	-2.48135000	-1.33457500	-0.50824800
H	-2.10773200	-2.18644100	0.17353200
C	1.93825100	0.02020100	-0.32760400
N	1.01632900	-0.86660900	-0.84884100
C	-3.71156200	-1.80797000	-1.14828100
H	-3.49592200	-2.74201100	-1.68629700
H	-4.08059100	-1.07504300	-1.88591200
C	-4.79266200	-2.04483400	-0.11034400
O	-4.70559300	-1.74596600	1.05326100
O	-5.86662700	-2.61208100	-0.67333900
C	-6.97360200	-2.87735000	0.19333100
H	-7.34311800	-1.94641300	0.64889500
H	-7.75012800	-3.33030900	-0.43460100
H	-6.67930400	-3.56865600	0.99696600
F	-0.81407400	7.40345200	0.50098300
O	7.44747400	-1.12396800	0.24804800
C	7.96364700	-2.43548700	0.21139400
H	9.05015800	-2.34840200	0.34579500
H	7.55249000	-3.06243100	1.02326100
H	7.76173900	-2.93038500	-0.75588200
O	-0.85624900	-2.45272900	-1.80417100
H	-1.70929700	-0.67925600	-2.37659800
H	-2.63112900	-0.41280100	-0.05333500
H	-1.00276200	-3.08081100	-0.81969900
O	-1.45077900	-3.42024200	0.30360700
C	-0.54337500	-3.69133100	1.33601800
H	0.17157600	-4.47811500	1.01457400
H	0.07796600	-2.80189100	1.58905800
C	-1.26641700	-4.16607800	2.59185800
H	-1.85898800	-5.06799700	2.36933400
H	-0.55537700	-4.40422900	3.40089000
H	-1.96023900	-3.39142700	2.95770800

TS1‘-2 (non-assisted)

E= -1437,07875287

C	-0.15345200	-2.04760700	0.64642900
C	0.29303000	-0.73137600	0.91981900
C	-0.83176400	0.10550400	0.78185000
H	-2.10312600	-2.75946000	0.17187900
H	-0.83315200	1.18499700	0.90798700
C	-3.32647900	-0.27619300	0.16000800
C	-4.18524700	-1.05786500	-0.63081000
C	-3.84308500	0.92496600	0.69395600
C	-5.50751700	-0.67917400	-0.87729900
H	-3.81703600	-1.97584200	-1.09716100
C	-5.15159700	1.31599300	0.45188200
H	-3.20815100	1.54980600	1.32530800
C	-6.00264000	0.51694200	-0.33493300
H	-6.13421900	-1.31542400	-1.50217700
H	-5.55193700	2.24140400	0.87044000
C	1.62785800	-0.18922600	1.43869100
C	1.98542300	1.14622700	0.75895600
C	1.87367200	1.36398500	-0.62393600

C	2.43260900	2.19171600	1.57661400
C	2.21664100	2.59794300	-1.18220100
H	1.51541700	0.56200500	-1.27241600
C	2.77823500	3.43219000	1.03346300
H	2.48361500	1.99720800	2.64996500
C	2.66671200	3.61612700	-0.34242700
H	2.13390700	2.78645200	-2.25471900
H	3.12327800	4.25869600	1.65851100
O	1.67569500	-0.16209900	2.79187100
C	0.45220100	-3.35167800	0.61643300
O	1.61546500	-3.65140600	0.87068400
H	-0.26011400	-4.16611500	0.32652100
N	2.82388800	-1.22211000	1.27315500
H	2.45881800	-2.18593500	1.11287400
H	2.73217800	-0.95500600	2.44623800
H	4.84545700	-1.60339200	0.89177100
C	-1.94177600	-0.67278600	0.42579500
N	-1.50854300	-1.95769400	0.34088700
C	4.02862100	-0.97863200	0.49477100
H	4.35593500	0.06685900	0.59773100
C	3.87203300	-1.29761100	-0.98347700
O	2.84951800	-1.64617500	-1.51863900
O	5.04133700	-1.14122900	-1.62085100
C	5.04213400	-1.40054000	-3.02684200
H	4.72822100	-2.43486800	-3.23246000
H	6.07231100	-1.23908300	-3.36652600
H	4.35691800	-0.71578700	-3.54892400
F	2.99311100	4.80498100	-0.87555800
O	-7.26262300	0.97920500	-0.51190700
C	-8.17497500	0.23065500	-1.28464300
H	-7.83045000	0.11353700	-2.32794700
H	-9.11924800	0.79113500	-1.28326800
H	-8.35298300	-0.77112000	-0.85373700

TS1‘-2 (assisted by EtOH)

E= -1592,2415655

C	0.42345500	0.38950800	-1.54013800
C	0.07518700	0.26602800	-0.17471900
C	1.27203000	0.05402800	0.53102400
H	2.34121100	0.37710600	-2.46234600
H	1.33367600	-0.08928700	1.60587600
C	3.77201100	-0.14793700	-0.15183100
C	4.63675400	-0.58768000	-1.16812600
C	4.33233000	0.10638700	1.11953200
C	6.00555500	-0.75818600	-0.94647100
H	4.24056300	-0.83574500	-2.15669000
C	5.68825000	-0.06418000	1.35460600
H	3.69105500	0.46057200	1.92909800
C	6.54403000	-0.49592500	0.32317000
H	6.63626600	-1.10790700	-1.76368100
H	6.12208400	0.13846500	2.33566600
C	-1.27085500	0.25993400	0.57337300
C	-1.89551300	-1.14494700	0.53786500

C	-2.28847300	-1.76287700	-0.66049300
C	-2.04538000	-1.84305000	1.74374000
C	-2.82252700	-3.05262900	-0.65466300
H	-2.20520700	-1.23267700	-1.61070400
C	-2.57318400	-3.13672400	1.76248000
H	-1.73801900	-1.34788800	2.66539400
C	-2.95373900	-3.72450400	0.55947100
H	-3.14168700	-3.54181800	-1.57698100
H	-2.69352300	-3.69344300	2.69412700
O	-1.11444100	0.69918200	1.84477700
C	-0.31763800	0.65458000	-2.74384400
O	-1.52400000	0.86087300	-2.83219200
H	0.30905400	0.66624200	-3.67272200
N	-2.20666700	1.29141800	-0.13449800
H	-2.25219500	1.14437000	-1.16437500
H	-1.66471500	2.23181600	0.15577600
H	-3.75990900	2.47117000	0.65681900
H	-0.94941500	1.84607700	1.72668000
O	-1.03814400	3.01153200	1.21769700
C	0.09932600	3.81731600	1.14749200
H	0.56521800	3.91182500	2.15210200
H	0.88709900	3.37605800	0.49371600
C	-0.24041900	5.21504900	0.63667700
H	-0.65456900	5.16890300	-0.38484200
H	0.64986900	5.86662000	0.61602800
H	-1.00003100	5.68148700	1.28476500
C	2.33804200	0.03890300	-0.38091800
N	1.80301500	0.23444500	-1.61614900
C	-3.53741000	1.40550800	0.48684900
H	-3.51147000	0.94159600	1.48243200
C	-4.64434200	0.81088300	-0.35764200
O	-4.52480400	0.43240200	-1.49570400
O	-5.79481100	0.79774400	0.32730000
C	-6.94067500	0.29281800	-0.36356500
H	-7.14555300	0.88804200	-1.26610000
H	-7.77783000	0.36627800	0.34095000
H	-6.78264000	-0.75421500	-0.66222700
F	-3.46361200	-4.96665000	0.56723200
O	7.85050300	-0.62969800	0.64741900
C	8.77088600	-1.05626500	-0.33352700
H	8.52894200	-2.06571600	-0.71179200
H	9.75469200	-1.08545500	0.15317600
H	8.81448000	-0.35617600	-1.18714600

INT1-2

E=-1437,13350052

C	0.35718100	-0.89403500	0.51905900
C	0.34355900	0.45326400	0.11263000
C	-1.02924700	0.78138500	-0.15055100
H	-1.16022800	-2.25083000	0.86547800
H	-1.39602200	1.72068900	-0.55546400
C	-3.24474800	-0.56874000	-0.02337200
C	-3.78866900	-1.86096800	-0.10736900

C	-4.14624000	0.51749500	-0.07142900
C	-5.16521700	-2.07709600	-0.22723900
H	-3.13115300	-2.73426600	-0.10340000
C	-5.51314400	0.31813700	-0.19973500
H	-3.76436200	1.53759100	0.00834400
C	-6.04192400	-0.98386400	-0.27648700
H	-5.53673100	-3.09984700	-0.29207500
H	-6.20664000	1.16080400	-0.23349300
C	1.52700200	1.31284900	-0.05277500
C	1.37779200	2.80826100	-0.02543200
C	0.38655100	3.47589900	0.71488000
C	2.33809800	3.57172100	-0.71522900
C	0.34186500	4.87092400	0.75431400
H	-0.34235100	2.90367600	1.29030700
C	2.29471600	4.96320000	-0.69963800
H	3.12227700	3.04587300	-1.26288400
C	1.29223700	5.59483700	0.03756300
H	-0.41227400	5.40497500	1.33555300
H	3.02373900	5.56893500	-1.24145900
O	2.65066100	0.84056900	-0.22488200
C	1.42101600	-1.84354000	1.04467200
N	2.50352400	-2.00837300	0.11574200
C	-1.80267800	-0.34009100	0.10436500
N	-0.92752100	-1.32668300	0.51633800
C	3.72373200	-2.51355600	0.70829900
H	3.53116900	-3.45570000	1.24489100
H	4.17745500	-1.82602500	1.45769400
C	4.78404200	-2.76728700	-0.34582700
O	4.76259300	-2.35357300	-1.47615500
O	5.79489300	-3.49552300	0.16697900
C	6.89663300	-3.74654600	-0.70487800
H	7.35383900	-2.80335600	-1.04133900
H	7.61954900	-4.33378300	-0.12503700
H	6.57347300	-4.31025000	-1.59337500
F	1.24770800	6.93262600	0.06318200
O	-7.38970300	-1.07803700	-0.39423100
C	-7.98880600	-2.35153600	-0.47247500
H	-9.07085400	-2.18424800	-0.55839400
H	-7.64346100	-2.91546100	-1.35801400
H	-7.79148400	-2.95571500	0.43171200
O	0.83344200	-3.11684000	1.31082600
H	1.75219700	-1.47703300	2.04153000
H	2.68411100	-1.13429700	-0.38528400
H	0.95875800	-3.60701500	0.48114000

INT1‘-2

E=-1437,1331573

C	-0.26350800	-1.58954400	-1.66683900
C	0.27329500	-0.49675600	-0.94973500
C	-0.80714600	0.14187000	-0.31462700
H	-2.28504000	-2.21275100	-1.89639900
H	-0.72894000	1.00544500	0.33994000
C	-3.37098500	-0.28974400	-0.23069300

C	-4.35339500	-1.30425500	-0.23869900
C	-3.76465800	0.99305400	0.18724200
C	-5.66324200	-1.04441600	0.13989600
H	-4.08530800	-2.32667500	-0.51860300
C	-5.07662800	1.26654500	0.57681200
H	-3.03404000	1.80459500	0.19240000
C	-6.04195300	0.24641300	0.55283800
H	-6.41992700	-1.83128700	0.13981600
H	-5.33650900	2.27829600	0.88791900
C	1.74931200	-0.10924700	-0.81713700
C	2.41474100	-1.01771500	0.24710200
C	2.01389900	-0.94216500	1.59094400
C	3.41926000	-1.92747400	-0.10384500
C	2.59510900	-1.75657900	2.56303600
H	1.24071000	-0.22728500	1.87875300
C	4.00894300	-2.75465400	0.85809100
H	3.75186500	-1.98550400	-1.13982800
C	3.58740200	-2.65837900	2.17979300
H	2.29395800	-1.70406400	3.61134200
H	4.79286500	-3.46752900	0.59447700
O	2.40797800	-0.20835900	-2.06220100
C	0.32916400	-2.58603200	-2.51746800
H	-0.38332700	-3.37095600	-2.87830700
O	1.50500600	-2.63587500	-2.86786400
C	-1.98775000	-0.55003300	-0.63382700
N	-1.63241000	-1.59139700	-1.43401200
N	1.79258300	1.26545800	-0.36209100
H	2.23512400	-1.09469000	-2.45020600
H	1.25253700	1.85256000	-0.99901800
H	3.79511400	1.58865200	-1.06278300
C	3.11683700	1.84018900	-0.22162200
H	3.61609100	1.49061800	0.69562300
C	3.02005700	3.34979800	-0.18278700
O	2.07935300	3.99322500	-0.58291300
O	4.13970300	3.89936600	0.31515900
C	4.19530900	5.32570100	0.32666700
H	5.17219800	5.59066000	0.74963300
H	4.09838200	5.73057100	-0.69236800
H	3.38639500	5.74436600	0.94459900
F	4.14914700	-3.44750700	3.11042900
O	-7.33830500	0.40458500	0.90545900
C	-7.79100700	1.66797700	1.34340600
H	-7.67604500	2.43888800	0.56057000
H	-8.85797600	1.55341500	1.57588300
H	-7.25989200	2.00095700	2.25300400

TS2-2 (non-assisted)

E=-1437,0559205

C	-0.12774300	0.58823700	0.59692900
C	-0.15538800	-0.80713500	0.76832300
C	-1.49322300	-1.22035600	0.55475300
H	-1.70583200	1.94523300	0.22755100
H	-1.84478900	-2.24873800	0.58390000

C	-3.67877300	0.02594500	-0.09651600
C	-4.17623400	1.10966700	-0.85288900
C	-4.60061300	-0.94468800	0.33146900
C	-5.52691400	1.22022200	-1.15530400
H	-3.49060600	1.86933600	-1.23769100
C	-5.95961100	-0.85002800	0.02729600
H	-4.25319100	-1.78709100	0.93349200
C	-6.43666800	0.24014200	-0.71888200
H	-5.90866900	2.05571200	-1.74528400
H	-6.63745600	-1.62482500	0.38550000
C	0.91958600	-1.78070400	1.15210800
C	2.16434700	-1.91832800	0.33048900
C	2.36882000	-1.24048900	-0.88183900
C	3.14574800	-2.81979200	0.78195500
C	3.52958800	-1.44841500	-1.62728200
H	1.62432600	-0.53457400	-1.24944300
C	4.31092500	-3.03453700	0.05131500
H	2.96723800	-3.34729500	1.72067600
C	4.48500900	-2.34216600	-1.14813700
H	3.70407200	-0.92279000	-2.56757300
H	5.08530400	-3.72648800	0.38839200
O	0.71087400	-2.52847400	2.09305800
C	0.89938900	1.56949800	0.81684500
N	2.07970200	1.22148000	1.37609000
C	-2.25738300	-0.09657100	0.23346700
N	-1.40706200	0.97764500	0.25492400
C	3.16317400	2.16873000	1.21931100
H	4.01220900	1.86566300	1.84832200
H	2.88501200	3.19480300	1.54321100
C	3.64562300	2.28922700	-0.21797100
O	2.98256100	2.04393300	-1.19799600
O	4.90032700	2.75904500	-0.26732700
C	5.44920500	2.98627200	-1.56707000
H	6.44815900	3.40985300	-1.40704800
H	5.52268400	2.04259100	-2.12826700
H	4.82284800	3.68668100	-2.13993100
O	-7.73222400	0.43021100	-1.06329400
C	-8.70132200	-0.51690600	-0.66986400
H	-8.77098000	-0.60095400	0.42957900
H	-9.66345900	-0.15992000	-1.06059000
H	-8.49289500	-1.51684400	-1.09100300
F	5.60396200	-2.54308600	-1.85844500
H	0.79269700	2.51926700	0.27469100
O	0.47411700	2.18316700	2.73523300
H	1.56606500	1.38226000	2.43020500
H	-0.29736800	1.82199200	3.20178500

TS2-2 (assisted by EtOH)

E=-1592,23653976

C	-0.32328200	-0.79982600	0.34332400
C	1.06750800	-1.05372300	0.37146600
C	1.69559100	0.20212300	0.15474500

H	-1.48961100	0.94549700	0.33227300
H	2.76439800	0.39177900	0.11848200
C	0.79614100	2.61733300	-0.17621300
C	-0.31735100	3.38633400	-0.58095200
C	2.01172700	3.29178700	0.02537300
C	-0.21544200	4.75804500	-0.77046700
H	-1.27790600	2.89915400	-0.76171400
C	2.12882000	4.67010300	-0.16677900
H	2.89154100	2.73504600	0.35526500
C	1.00996100	5.41770100	-0.56728900
H	-1.07689100	5.34993800	-1.08587300
H	3.09254000	5.14933100	0.00598900
C	1.67976700	-2.37632500	0.62899000
C	3.10904900	-2.63479800	0.24334000
C	3.74058500	-2.02035300	-0.85211100
C	3.81489400	-3.60886100	0.97393000
C	5.05065100	-2.35458100	-1.20119400
H	3.19713500	-1.29591400	-1.46000300
C	5.12787600	-3.93812700	0.64892700
H	3.30645700	-4.10457600	1.80290900
C	5.72930000	-3.30224200	-0.43816600
H	5.55050200	-1.89791100	-2.05753700
H	5.69340200	-4.68084900	1.21505000
O	1.04156000	-3.27085200	1.17631100
C	-1.41893800	-1.73790900	0.48052000
N	-2.52339800	-1.65820400	-0.25888400
C	0.69086800	1.16806200	0.02168300
N	-0.51521900	0.53060000	0.11272300
H	-1.13652300	-2.71828700	0.86584900
H	-2.84627200	-0.70428300	-0.47473400
O	-2.24241100	-1.08087400	2.26222100
H	-2.61601400	-0.12383100	1.76479700
H	-1.52720000	-0.83851600	2.86753200
O	-2.91545700	0.82769800	0.91737900
C	-3.87945800	1.77824100	1.25903500
H	-4.11587400	2.41224300	0.37846200
H	-4.83761700	1.28371200	1.53289500
C	-3.44850500	2.68197900	2.41599700
H	-2.52567800	3.22982700	2.16185200
H	-4.22917800	3.42213200	2.66266900
H	-3.24803400	2.08630400	3.32273400
C	-4.70353300	-2.38064200	-1.06254200
H	-4.03276900	-2.47836700	0.96827000
O	1.01322900	6.75659200	-0.77949700
C	2.20751100	7.48331900	-0.59833900
H	1.97370800	8.53191600	-0.82634400
H	2.57586700	7.41771200	0.44151100
H	3.00641900	7.13913000	-1.27997900
F	6.98921600	-3.61818900	-0.76124300
C	-3.60197400	-2.59886300	-0.04341300
H	-3.23630500	-3.63515200	-0.11212800
O	-4.78469800	-1.42523400	-1.79183300
O	-5.59326700	-3.38060900	-1.01702800

C	-6.72078500	-3.26918600	-1.89037400
H	-6.39681700	-3.23683500	-2.94136400
H	-7.33620900	-4.15827800	-1.70803700
H	-7.29322200	-2.35526500	-1.67187900

TS2‘-2 (non-assisted)

E=-1437,05931666

C	-0.15683900	-1.76876100	-0.22055400
C	0.22011600	-0.45533900	0.13747300
C	-0.98031000	0.29834000	0.24863300
H	-2.00982800	-2.62468700	-0.58740800
H	-1.04948700	1.34082100	0.54812000
C	-3.49666300	-0.29272100	-0.01128400
C	-4.43755900	-1.33340500	0.05887800
C	-3.99033700	1.02880400	-0.07535000
C	-5.81251500	-1.08413900	0.05919400
H	-4.10409900	-2.37129600	0.13741600
C	-5.35228000	1.29090100	-0.07032300
H	-3.29012200	1.86377500	-0.14529200
C	-6.28262200	0.23639500	-0.00506700
H	-6.50312200	-1.92520700	0.11947200
H	-5.73195100	2.31308100	-0.12425300
C	1.57613800	0.04477900	0.32516200
C	1.85439700	1.48521700	0.06044800
C	1.54637800	2.07149500	-1.17818900
C	2.44294200	2.26832700	1.07094000
C	1.84801200	3.41373100	-1.42119900
H	1.07569600	1.47350000	-1.96172800
C	2.73322200	3.61185500	0.84079600
H	2.60944400	1.79010000	2.03941500
C	2.43840300	4.16386300	-0.40642000
H	1.62774000	3.88651100	-2.38014800
H	3.17376900	4.24326000	1.61500500
O	1.63440500	-0.31412400	2.49551200
C	0.55243600	-2.99786000	-0.58347300
O	-0.06870900	-4.00508900	-0.88982100
H	1.66094800	-2.96264700	-0.57348300
C	-2.05489300	-0.55315900	-0.01406400
N	-1.52285300	-1.78416100	-0.29109500
N	2.56166700	-0.85897600	0.45953000
H	4.37391200	-0.15823200	1.32355500
H	2.26296200	-1.22768300	1.46051200
H	0.97816500	-0.39583900	3.20550300
C	3.96069600	-0.51906500	0.36548900
H	4.13977800	0.28275900	-0.36893500
C	4.77675300	-1.72937400	-0.06975900
O	4.33835800	-2.79851200	-0.40893600
O	6.08776600	-1.43401200	-0.03360200
C	6.98396400	-2.47197800	-0.43407000
H	6.87634500	-3.35318800	0.21630600
H	6.78746700	-2.78006600	-1.47224100
H	7.99456000	-2.05480900	-0.34546200
F	2.72009500	5.45378000	-0.63079900

O	-7.58953300	0.59021300	-0.00910200
C	-8.57989300	-0.41279800	0.05001500
H	-8.50909400	-1.00565800	0.97969400
H	-9.54896500	0.10329700	0.03066300
H	-8.52223300	-1.09830100	-0.81462200

TS2‘-2 (assisted by EtOH)

E=-1592,22408335

C	-0.32815100	-1.38977100	-0.78733900
C	-0.01910700	-0.13969700	-0.21368300
C	-1.25914500	0.48973300	0.08557600
H	-2.13456200	-2.30913600	-1.21455000
H	-1.38112000	1.45847400	0.56329200
C	-3.74243200	-0.22842300	-0.18014900
C	-4.60571600	-1.33475000	-0.24331000
C	-4.32651200	1.04511800	-0.00411800
C	-5.99226300	-1.19296100	-0.14368900
H	-4.19905300	-2.34359400	-0.35056800
C	-5.70081900	1.19955600	0.10221300
H	-3.68896600	1.93091200	0.03393600
C	-6.55307100	0.08133400	0.03155900
H	-6.62026800	-2.08236700	-0.19376700
H	-6.15089000	2.18548000	0.23374000
C	1.30244400	0.43057900	0.06001700
C	1.42577700	1.92613400	0.07945300
C	1.14823700	2.64159800	-1.09810800
C	1.84089900	2.62148600	1.22690300
C	1.29938300	4.02909700	-1.13999500
H	0.81278500	2.11042900	-1.99193000
C	1.98498500	4.00947800	1.19544300
H	2.00402700	2.04078800	2.13651900
C	1.71730600	4.69387600	0.01121500
H	1.09317300	4.60066300	-2.04686300
H	2.29581000	4.57015100	2.07932200
O	1.20681700	-0.01071000	2.26742300
C	0.43290600	-2.49628500	-1.37738600
O	-0.14117100	-3.48217100	-1.80864600
H	1.53349800	-2.38485900	-1.43984000
C	-2.28870200	-0.37670400	-0.28536500
N	-1.68996000	-1.49340200	-0.80382300
N	2.37175900	-0.32847100	-0.11930300
H	4.02024800	0.23493000	1.08321600
O	1.73778300	-2.21704100	1.45600300
H	1.43874500	-1.19553600	1.98279400
C	2.61747900	-3.01761800	2.19484800
H	2.13899400	-3.33138900	3.14729200
H	3.53541900	-2.45992200	2.49531400
C	3.02521600	-4.26060200	1.41170700
H	3.55767500	-3.98228800	0.48767000
H	3.68512700	-4.91145900	2.01011200
H	2.13248900	-4.83952700	1.12518500
H	0.28065000	0.03323800	2.54372700
H	2.22517900	-1.32704900	0.29803100

C	3.72609800	0.14941900	0.02067600
H	3.85485200	1.14977500	-0.41851600
C	4.69242800	-0.81084600	-0.65525500
O	4.39251000	-1.85422200	-1.17861500
O	5.94432300	-0.33917000	-0.57451400
C	6.97157300	-1.15513400	-1.14488600
H	7.01139400	-2.13499700	-0.64591000
H	6.79050800	-1.31584000	-2.21814500
H	7.91171500	-0.61135600	-0.99319300
F	1.85731200	6.02567100	-0.02076700
O	-7.87910000	0.33157800	0.14159300
C	-8.79494600	-0.73962000	0.07593800
H	-8.63396800	-1.46814000	0.89085900
H	-9.79620800	-0.30174000	0.18340300
H	-8.73813900	-1.26963500	-0.89187600

INT2-2

E=-1360,65849477

C	0.33383800	-1.06145600	0.22046300
C	-1.01088200	-0.74006900	-0.05159600
C	-1.07062700	0.68124100	-0.15810600
H	2.01865500	0.11228500	0.50715600
H	-1.94115300	1.27277800	-0.42702300
C	0.70839900	2.56704400	0.01546400
C	2.06967700	2.86081200	-0.17013500
C	-0.17772700	3.65664300	0.16432600
C	2.54186600	4.17597000	-0.20102800
H	2.79022700	2.05275900	-0.32029000
C	0.27639200	4.96686700	0.12827400
H	-1.24106100	3.46831900	0.32711700
C	1.64450100	5.24405800	-0.05246800
H	3.60673400	4.35238600	-0.35272600
H	-0.41028900	5.80722400	0.24778500
C	-2.08107800	-1.74300700	-0.24911200
C	-3.52469000	-1.33179700	-0.14920800
C	-3.98218900	-0.29344500	0.68037500
C	-4.46774400	-2.09083700	-0.86667200
C	-5.34508600	-0.00563800	0.78024300
H	-3.27340800	0.27890300	1.28025900
C	-5.82786300	-1.80312700	-0.79163800
H	-4.10689900	-2.91601700	-1.48341300
C	-6.24807300	-0.75925600	0.03373100
H	-5.71824700	0.78741800	1.43109500
H	-6.56997600	-2.37370400	-1.35351200
O	-1.81179100	-2.91091000	-0.50563500
C	1.02330700	-2.32095400	0.44448000
H	0.42303100	-3.23513000	0.30819400
N	2.26160900	-2.31556700	0.76580600
H	2.27348400	-4.45819000	0.81379900
C	0.21249900	1.18880000	0.04821500
N	1.02811300	0.11005900	0.28232700
C	2.92893700	-3.57251300	0.95600600
H	3.32831300	-3.64068800	1.98338900

C	4.11090900	-3.73304100	0.00570700
O	4.33689100	-3.06067400	-0.96515200
O	4.87258800	-4.77573700	0.39249400
C	5.98981600	-5.08414400	-0.44046100
H	6.68880400	-4.23519700	-0.48910300
H	6.48044400	-5.95415600	0.01340400
H	5.66256400	-5.32218300	-1.46423000
F	-7.55497000	-0.48048100	0.11677000
O	1.99325200	6.55320100	-0.06904800
C	3.34755600	6.90679200	-0.24186200
H	3.74397700	6.55494200	-1.21143600
H	3.39000900	8.00389400	-0.21795300
H	3.98352500	6.50654900	0.56836000

INT2‘-2

E=-1360,65131481

C	0.03472000	-1.95305200	0.01353900
C	0.35059400	-0.59213800	-0.17545400
C	-0.88417900	0.10838300	-0.21363000
H	-1.77720200	-2.94766000	0.19754500
H	-1.00865000	1.18128300	-0.33577600
C	-3.37314700	-0.62601000	-0.02629000
C	-4.24387400	-1.61570300	0.47995700
C	-3.95268400	0.56371300	-0.49888100
C	-5.61887600	-1.42528000	0.50714600
H	-3.84197500	-2.54986200	0.88026900
C	-5.33308000	0.77105600	-0.47233200
H	-3.31435600	1.34643900	-0.91401800
C	-6.18192400	-0.22755800	0.03151300
H	-6.28790900	-2.19171600	0.90312800
H	-5.73492600	1.70951900	-0.85446800
C	1.70375400	-0.01950600	-0.32434000
C	1.84488300	1.46093100	-0.09076000
C	2.36969700	2.30214800	-1.08663100
C	1.45522400	2.03138100	1.13412500
C	2.50665100	3.67520500	-0.87222200
H	2.66204300	1.88073500	-2.05122200
C	1.60044800	3.39958900	1.36878300
H	1.03752400	1.39378000	1.91655700
C	2.12328900	4.20446300	0.35809100
H	2.90407500	4.33936200	-1.64211700
H	1.31217500	3.85204000	2.31963000
C	0.81255000	-3.18103500	0.18399300
O	0.25320700	-4.25835300	0.33104900
H	1.91566800	-3.07091500	0.17936100
C	-1.92111300	-0.81968800	-0.05838700
N	-1.32958200	-2.04369900	0.07980000
N	2.66316500	-0.81047400	-0.63739300
H	4.27667600	0.56344600	-0.22335200
C	4.03336400	-0.39980300	-0.71390900
H	4.34349700	-0.28488500	-1.76916800
C	4.94942300	-1.46053000	-0.11067900
O	4.60724500	-2.45016400	0.48151300

O	6.23679700	-1.12087400	-0.31918500
C	7.21922000	-2.00848900	0.21490900
H	7.11700300	-3.01409800	-0.22068000
H	8.19467700	-1.57897100	-0.04512500
H	7.11905800	-2.09276500	1.30785700
F	2.25688800	5.51978900	0.57367600
O	-7.53157400	-0.13076500	0.09952900
C	-8.16589200	1.04407900	-0.35470500
H	-7.97993700	1.22280700	-1.42917800
H	-9.24324800	0.89748600	-0.20043200
H	-7.84095200	1.93341300	0.21498800

TS3-2

E=-1360,61139607

C	0.22741200	-1.67859800	-0.53987900
C	0.42039900	-0.25244100	-0.35817800
C	-0.89324300	0.30075800	-0.09676100
H	-1.55161400	-2.79578700	-0.53493000
H	-1.12688900	1.34720400	0.06552500
C	-3.27747600	-0.68807100	-0.02090600
C	-4.00325200	-1.83799300	0.35751000
C	-4.00481100	0.49379300	-0.24122300
C	-5.38425300	-1.80708300	0.50283100
H	-3.48085000	-2.77430700	0.57146400
C	-5.39167400	0.54128600	-0.09194000
H	-3.47934700	1.39767200	-0.55695200
C	-6.09675100	-0.61534600	0.28047400
H	-5.94197500	-2.69683000	0.80119700
H	-5.91274600	1.47999600	-0.28011300
C	1.59432800	0.48863200	-0.62865800
C	1.72381800	1.93702400	-0.34130000
C	1.12284500	2.55221500	0.77484700
C	2.54535300	2.72098600	-1.17798600
C	1.31175100	3.90911200	1.03521500
H	0.53289500	1.95726400	1.47300600
C	2.73192200	4.07903700	-0.93481000
H	3.03654500	2.24629500	-2.02850900
C	2.10716600	4.65804200	0.16967100
H	0.86499400	4.39208200	1.90629800
H	3.35542500	4.69723600	-1.58346700
O	2.63535000	-0.04213000	-1.21014700
C	1.06701200	-2.78735300	-0.87037700
H	0.53675400	-3.61159300	-1.37220400
N	2.34723800	-2.99433000	-0.66354500
C	-1.81857700	-0.71183500	-0.17158200
N	-1.12525100	-1.88289700	-0.43848400
C	3.12641000	-2.21781200	0.09659000
H	2.70195300	-1.59517400	0.90399200
H	2.98472600	-0.96323500	-0.79291800
C	4.54361500	-2.60376100	0.28377600
O	5.16529700	-3.43749600	-0.32940900
O	5.10179700	-1.83384400	1.25972800
C	6.48047000	-2.06418300	1.51624300

H	6.77180500	-1.35916500	2.30594400
H	6.65545400	-3.09913800	1.85082500
H	7.08751600	-1.89321900	0.61292000
O	-7.43839600	-0.67966100	0.44638900
C	-8.21988500	0.47840900	0.24711000
H	-8.13927900	0.85498300	-0.78840500
H	-9.26140000	0.18901400	0.43991100
H	-7.93864600	1.28824800	0.94402100
F	2.28476800	5.96168700	0.41112300

TS3'-2

E= -1515,67745547

C	-0.30607200	-1.23164700	1.06452100
C	0.08795300	-0.44705600	-0.01862700
C	-1.08394600	0.11589600	-0.57253200
H	-2.22771300	-1.53801800	1.92660000
H	-1.13660200	0.74950900	-1.45454900
C	-3.60006000	-0.01489000	0.06238900
C	-4.03066500	1.15137700	-0.60856800
C	-5.37864400	1.44772700	-0.74824400
H	-3.28850100	1.84376400	-1.01121900
C	-5.95313900	-0.57459100	0.45443200
H	-4.30880900	-1.79943800	1.07350800
C	-6.35863600	0.58973600	-0.21490800
H	-5.70813000	2.35251500	-1.26288700
H	-6.68421200	-1.26889000	0.86882000
C	1.51419600	-0.36570000	-0.53290000
C	2.01882300	1.09066700	-0.57441400
C	1.56386000	2.08536400	0.30483100
C	2.93823400	1.45065000	-1.57184700
C	2.02148900	3.40268700	0.20401800
H	0.84619300	1.83254400	1.08614300
C	3.40845900	2.75988800	-1.68406400
H	3.25920400	0.68165200	-2.27446200
C	2.94186200	3.72185200	-0.79069600
H	1.66817200	4.18333400	0.88078900
H	4.12033100	3.04934500	-2.46012500
O	1.64805900	-0.89890500	-1.78051900
C	0.55771500	-2.09738200	1.81281900
H	0.12087900	-2.75366000	2.58094400
N	1.82193800	-2.21741300	1.60067600
C	2.42763800	-1.27522900	0.65068800
C	3.07830000	-0.22808800	1.58816000
O	2.56206500	0.25477200	2.56021800
O	4.32851800	0.04724700	1.18180200
C	5.02552100	1.05738700	1.91634400
H	6.02230500	1.12786800	1.46439300
H	4.50119100	2.02068500	1.83450300
H	5.10200500	0.78147400	2.97847900
H	3.35336000	-1.67253000	0.19358300
C	-4.59154700	-0.86537100	0.58023800
C	-2.17235900	-0.31542700	0.19418900
N	-1.67874900	-1.14179700	1.17490800

H	2.22056400	-2.37140200	-0.10959300
O	1.95230500	-3.10877400	-0.85585400
H	1.63923200	-2.18176400	-1.57028800
C	3.12953200	-3.77541800	-1.32751600
H	3.82966700	-3.03276300	-1.75259700
H	3.61754200	-4.25100300	-0.46012400
C	2.74927500	-4.81207100	-2.36758700
H	2.27077100	-4.33936100	-3.23949500
H	3.64662400	-5.34640300	-2.71658300
H	2.04802200	-5.54692600	-1.94384600
F	3.38281200	4.98728300	-0.89675000
O	-7.64799700	0.96620200	-0.39647200
C	-8.68365200	0.15710500	0.11364900
H	-8.62325700	0.05550400	1.21248200
H	-9.62723800	0.65569800	-0.14546300
H	-8.67764800	-0.85195000	-0.33700500

INT3-2

E=-1360,62711462

C	0.25241300	-1.21580100	-0.06990800
C	-1.15760000	-0.79270400	-0.08800700
C	-1.13035100	0.66125000	-0.06145000
H	1.99990200	-0.10562300	0.05665200
H	-1.99101700	1.31698500	-0.14421200
C	0.74588100	2.41970900	-0.01806700
C	2.09432400	2.65607800	-0.33403500
C	-0.05315600	3.53876700	0.30648500
C	2.63565900	3.94469900	-0.33196800
H	2.74764200	1.82580000	-0.61149100
C	0.46960600	4.82251300	0.30832100
H	-1.10054500	3.39210000	0.57804400
C	1.82401800	5.04233600	-0.01014600
H	3.68690500	4.07696600	-0.58755200
H	-0.14801400	5.68565400	0.56434200
C	-2.25073300	-1.63012700	-0.14744600
C	-3.66080900	-1.21764900	-0.05929600
C	-4.09449700	-0.19976500	0.81765900
C	-4.63606300	-1.88817600	-0.83187900
C	-5.44097900	0.14516200	0.90922300
H	-3.36845300	0.30356600	1.45710700
C	-5.98603300	-1.55044700	-0.74693100
H	-4.32814200	-2.66448000	-1.53689600
C	-6.37266500	-0.53287700	0.12278500
H	-5.78481800	0.92299100	1.59386400
H	-6.74095100	-2.05485200	-1.35311900
O	-2.02709500	-2.95794600	-0.35432300
C	0.86297700	-2.46171500	-0.05569600
H	0.26373200	-3.37569500	-0.10604700
N	2.21613500	-2.48447800	0.02130700
C	0.18047100	1.06898600	-0.02634000
N	0.99098600	-0.05865700	-0.03371600
C	2.89468200	-3.58311900	0.04511100
H	2.42916900	-4.58300700	0.00633700

C	4.36980500	-3.53081600	0.12672800
O	5.06203700	-2.53963300	0.17331200
O	4.87905400	-4.79091900	0.14330300
C	6.29493600	-4.88724400	0.21972700
H	6.67644600	-4.41083900	1.13689300
H	6.53398200	-5.95867800	0.22342700
H	6.77355900	-4.39537900	-0.64207400
F	-7.66660200	-0.20274700	0.21079600
O	2.24455600	6.32920600	0.02389500
C	3.59151300	6.62564900	-0.27304100
H	3.86045400	6.32758200	-1.30241300
H	3.70025600	7.71430200	-0.17829200
H	4.28525100	6.13367200	0.43222400
H	-2.81458600	-3.45831000	-0.09757300

TS4-2 (non-assisted)

E= -1360,57188308

C	0.19923200	-2.03830400	-0.18301700
C	-0.30363900	-0.79999700	0.23879600
C	0.80429400	0.09409300	0.35111600
H	2.16977100	-2.61939400	-0.68295700
H	0.77214800	1.13026000	0.67844700
C	3.35345400	-0.20134300	-0.01797400
C	3.69757800	1.15837600	-0.18645900
C	5.02205200	1.56933300	-0.21257400
H	2.90691600	1.90022900	-0.31779400
C	5.74485900	-0.72294700	0.08739500
H	4.18798800	-2.18043300	0.29124800
C	6.06465200	0.63264400	-0.07938200
H	5.28543200	2.62015200	-0.34834000
H	6.52533200	-1.47473400	0.20499300
C	-1.73767400	-0.62787500	0.46043600
C	-2.24871500	0.77760200	0.25619000
C	-2.33788500	1.24379800	-1.06632600
C	-2.58188600	1.64630100	1.30305400
C	-2.75219900	2.54728200	-1.34206000
H	-2.08180700	0.57863000	-1.89466200
C	-2.99380800	2.95554000	1.04015600
H	-2.53057500	1.28045600	2.32761500
C	-3.07512100	3.38922800	-0.27980900
H	-2.82819400	2.91853700	-2.36588200
H	-3.25812800	3.64175000	1.84726600
O	-2.04025300	-0.95913800	2.16710900
C	-0.66027400	-3.13611200	-0.52027600
H	-0.24517300	-4.08641700	-0.88328700
N	-1.94461100	-3.00705300	-0.44906500
C	-2.54755200	-1.85516300	0.04084200
C	-3.98607400	-1.72933500	-0.36930200
O	-4.56144900	-2.43750000	-1.15687900
O	-4.60933300	-0.73502100	0.31066700
C	-5.97826300	-0.51652700	-0.01083500
H	-6.30836200	0.32683500	0.60898200
H	-6.10025300	-0.27331900	-1.07777100

H	-6.58205500	-1.41067500	0.20845900
C	4.40522700	-1.12220600	0.12192200
C	1.94874000	-0.61760800	0.01475000
N	1.55624400	-1.91295400	-0.29680800
H	-2.56460000	-1.84961300	1.43340400
F	-3.47355100	4.64484000	-0.53658500
O	7.32434700	1.12872300	-0.12423600
C	8.42030700	0.24920800	-0.00466900
H	8.43571400	-0.50094100	-0.81595300
H	9.32589600	0.86642200	-0.07422600
H	8.42079700	-0.27748300	0.96677300
H	-1.20064000	-1.30621200	2.51892200

TS4-2 (assisted by 2 EtOH)

E=-1670,86923630449

C	0.77422700	-0.76644800	-1.59844300
C	0.32072700	-0.19551200	-0.41369400
C	1.46367600	0.19932200	0.33212500
H	2.74215600	-1.00937500	-2.34910600
H	1.47091700	0.65578800	1.31884800
C	4.01629200	0.00117900	-0.09789200
C	4.45402500	0.97404200	0.82925000
C	5.79792500	1.12717500	1.13754800
H	3.72156300	1.63333200	1.29980700
C	6.35988800	-0.65327400	-0.40287500
H	4.71019000	-1.59566000	-1.39284400
C	6.77051000	0.31730400	0.52198400
H	6.13135500	1.88394900	1.85059100
H	7.08324200	-1.30604700	-0.89191500
C	-1.14957000	-0.01889400	-0.13040700
C	-1.48806100	1.47849900	-0.06583700
C	-1.79004100	2.16195300	-1.25441300
C	-1.40328700	2.21690600	1.12424400
C	-2.01367900	3.53925400	-1.26041900
H	-1.85225000	1.60828800	-2.19401000
C	-1.62890700	3.59608100	1.13525800
H	-1.17089400	1.71341700	2.06318300
C	-1.93088000	4.24084700	-0.06002900
H	-2.25359200	4.07535300	-2.18081000
H	-1.57603700	4.17485300	2.05954700
O	-1.35536100	-0.59713400	1.23463400
C	-0.12214800	-1.25765300	-2.61230500
H	0.25793600	-1.64402400	-3.56831900
N	-1.39682600	-1.25912100	-2.40334100
C	-1.95396300	-0.82791900	-1.19894900
C	-3.40201100	-0.62025300	-1.22057600
O	-4.07311900	-0.15515700	-0.29173700
O	-4.01230000	-1.02899100	-2.34630100
C	-5.42948800	-0.92453500	-2.37591000
H	-5.73838200	-1.27962700	-3.36773000
H	-5.89472600	-1.54600500	-1.59385100
H	-5.75805400	0.11562900	-2.22698600
C	5.00050800	-0.80474900	-0.69574300

C	2.59306800	-0.15046900	-0.40693600
N	2.14737000	-0.74216300	-1.57589200
H	-1.95886100	-2.19196400	-0.41499000
O	-1.78621800	-2.82542600	0.49385800
H	-1.50358000	-1.87416500	1.04348900
C	-0.72129000	-3.78643900	0.34251100
H	-1.01485700	-4.46109900	-0.47648100
H	0.20207200	-3.26406200	0.04095500
C	-0.52469100	-4.55150100	1.63691300
H	-1.45208600	-5.06461600	1.93456700
H	0.26606000	-5.30832600	1.51249500
H	-0.22218200	-3.87761800	2.45417900
F	-2.14891400	5.56629000	-0.05683100
O	8.05873500	0.54701100	0.88223300
C	9.08558000	-0.22021800	0.29759400
H	9.12178800	-0.09269000	-0.79979800
H	10.03006800	0.13937100	0.72774900
H	8.97714100	-1.29647100	0.52520700
H	-2.20488400	-0.26554900	1.67522900
H	-3.95435200	0.15968900	1.33669800
O	-3.64834800	0.09227900	2.27727800
C	-4.35501300	-0.97399700	2.89931400
H	-3.92756800	-1.08913200	3.90938400
H	-4.17683500	-1.92586100	2.36076000
C	-5.84795200	-0.69296200	2.98644000
H	-6.28265600	-0.59452200	1.97848800
H	-6.37163300	-1.51201800	3.50605700
H	-6.03442500	0.24442800	3.53348800

Product 6c

E=-1284,21024472

C	0.19241300	-2.06865900	-0.11885100
C	-0.34953800	-0.75418900	-0.06699000
C	0.76364100	0.14744000	-0.05471600
H	2.20953200	-2.71889600	-0.25346800
H	0.72442000	1.23149400	0.00265900
C	3.32541500	-0.19544700	-0.07388200
C	3.69759500	1.08229800	-0.54661000
C	5.02109100	1.49642900	-0.53592800
H	2.93255600	1.75086800	-0.94681400
C	5.68405500	-0.62992000	0.41955200
H	4.09863400	-2.01509500	0.81847300
C	6.03311900	0.64382700	-0.05455000
H	5.30884700	2.48175700	-0.90771300
H	6.43972700	-1.31138200	0.81017800
C	-1.75956300	-0.60740700	-0.06334200
C	-2.38442000	0.74224400	-0.05336900
C	-3.31997700	1.11222100	-1.03716100
C	-2.03945200	1.69051800	0.92684600
C	-3.89941400	2.38231100	-1.04297000
H	-3.59085700	0.39831400	-1.81859700
C	-2.61214900	2.96355700	0.93481500
H	-1.32651600	1.42014900	1.70877000

C	-3.53687000	3.29308700	-0.05356700
H	-4.62123600	2.67798500	-1.80691000
H	-2.35755700	3.70135000	1.69834900
C	-0.64800100	-3.18441300	-0.20147300
H	-0.24990000	-4.20509300	-0.26297000
N	-1.96287900	-3.03512000	-0.21109500
C	-2.50141700	-1.80228300	-0.12758400
C	-4.01143200	-1.81456300	-0.10737900
O	-4.70637000	-2.37327100	-0.91816400
O	-4.49931600	-1.14341500	0.95414200
C	-5.92028300	-1.07387800	1.05415800
H	-6.13621100	-0.52076700	1.97668600
H	-6.34760800	-0.54680600	0.18692900
H	-6.36050000	-2.08148800	1.09852400
C	4.34538100	-1.03188200	0.40900000
C	1.92083800	-0.61622100	-0.08330200
N	1.56277400	-1.95505200	-0.10862500
F	-4.08876500	4.51612800	-0.05320400
O	7.29402000	1.13432900	-0.08877400
C	8.36273500	0.33632800	0.37143500
H	8.46009700	-0.59611000	-0.21326500
H	9.27563700	0.93302900	0.24392500
H	8.25127700	0.07720700	1.43969000

Mechanism 3 (leading to product 6a)

INT2-3

E= -1246,08003089

C	0.69006500	-0.29738400	0.21381800
C	-0.69070400	-0.38469200	-0.05526700
C	-1.15963800	0.95576400	-0.18349700
H	1.96404200	1.31707000	0.46947100
H	-2.16500400	1.26500000	-0.45477500
C	-0.00369000	3.27948300	-0.05115500
C	1.22419300	3.94521100	-0.23831200
C	-1.17033000	4.06003800	0.07498400
C	1.28283300	5.33870500	-0.29099300
H	2.14539100	3.37205800	-0.36996500
C	-1.11000700	5.45169800	0.01401700
H	-2.13194100	3.56911100	0.23879100
C	0.11693500	6.09957000	-0.16636000
H	2.24650500	5.83218500	-0.44038600
H	-2.02775400	6.03642200	0.11645800
C	-1.42425700	-1.65849800	-0.23156600
C	-2.92467800	-1.68216600	-0.13170100
C	-3.66381900	-0.80824600	0.68423700
C	-3.60679800	-2.69317600	-0.83381300
C	-5.05159200	-0.92644700	0.78550600
H	-3.15188100	-0.04609400	1.27323300
C	-4.99188100	-2.81096700	-0.75735500
H	-3.02217100	-3.38776800	-1.43982100
C	-5.69700100	-1.92103700	0.05407300
H	-5.63890000	-0.26582200	1.42614100

H	-5.53648700	-3.58082600	-1.30751900
O	-0.82650700	-2.70124600	-0.47066500
C	1.71565000	-1.30036000	0.45404100
H	1.40649800	-2.35130400	0.33411700
N	2.89798700	-0.92977300	0.76984300
H	3.53209400	-2.97472500	0.86064500
C	-0.07843300	1.81629000	0.00686000
N	1.01584200	1.02445400	0.25181800
C	3.90360100	-1.93410200	0.97549100
H	4.31421100	-1.85805100	1.99759000
C	5.07128500	-1.76642000	0.00858800
O	5.07412500	-1.09323500	-0.98766200
O	6.11432600	-2.51734800	0.41310800
C	7.26458200	-2.50748700	-0.43243800
H	7.67666000	-1.49071200	-0.52132400
H	7.99744400	-3.17431300	0.03849800
H	7.01314100	-2.86887200	-1.44135800
F	-7.02836800	-2.03184200	0.13841100
H	0.16322000	7.19041500	-0.21032000

TS4-3 (assisted by 2 EtOH)

E= -1401,1468803

C	1.41212800	-0.73647500	-1.52123600
C	0.91119100	-0.17779300	-0.34878500
C	2.02280400	0.21995100	0.43938100
H	3.40582700	-0.96596900	-2.20101200
H	1.99058900	0.67054000	1.42825400
C	4.59062100	0.04137200	0.10235100
C	4.97820900	0.98893000	1.07307900
C	6.31669200	1.14385400	1.43025900
H	4.21880900	1.62297800	1.53540800
C	6.94220700	-0.57608600	-0.14301500
H	5.33784800	-1.51044900	-1.22522100
C	7.30877400	0.36573100	0.82238900
H	6.59045100	1.88780700	2.18299300
H	7.70494300	-1.19706900	-0.62021900
C	-0.57004900	-0.01550300	-0.11592300
C	-0.92375200	1.47869600	-0.05762100
C	-1.18932100	2.16509100	-1.25315900
C	-0.88835300	2.21195400	1.13815700
C	-1.42504400	3.54036600	-1.26090200
H	-1.21316400	1.61563300	-2.19697400
C	-1.12671500	3.58896500	1.14729900
H	-0.68561800	1.70599300	2.08263900
C	-1.39154900	4.23683300	-0.05513700
H	-1.63678200	4.07876700	-2.18683200
H	-1.11244000	4.16366500	2.07551400
O	-0.81803200	-0.60240800	1.23627100
C	0.55603400	-1.22841000	-2.56920900
H	0.97201500	-1.60492000	-3.51396200
N	-0.72499900	-1.24288100	-2.40292100
C	-1.32819500	-0.82543200	-1.21736300
C	-2.77728900	-0.63340500	-1.28782000

O	-3.48416800	-0.18031800	-0.38019800
O	-3.34357800	-1.04280000	-2.43568200
C	-4.76010200	-0.95268600	-2.51438500
H	-5.03045500	-1.30701800	-3.51761500
H	-5.24561900	-1.58189800	-1.75113400
H	-5.10414000	0.08354300	-2.37336400
C	5.60124000	-0.74098100	-0.49438900
C	3.18113900	-0.11656800	-0.26080300
N	2.78198500	-0.70338700	-1.44934300
H	-1.34594400	-2.19743000	-0.44183200
O	-1.19912500	-2.83248400	0.46872000
H	-0.94751400	-1.88650200	1.03327500
C	-0.11913500	-3.78268600	0.35225100
H	-0.37618900	-4.45513200	-0.48055500
H	0.80910200	-3.24919800	0.08770200
C	0.03665400	-4.55249400	1.64918700
H	-0.89597800	-5.07620800	1.90955300
H	0.83886500	-5.30088900	1.55011800
H	0.30226200	-3.88024700	2.48048200
F	-1.62153300	5.56006000	-0.05370000
H	-1.68491400	-0.27987800	1.64888100
H	-3.42654900	0.13233500	1.25394700
O	-3.15030400	0.06481000	2.20342000
C	-3.87058000	-1.00614900	2.80152900
H	-3.47322300	-1.12162200	3.82374200
H	-3.67181800	-1.95592500	2.26648300
C	-5.36670200	-0.73209600	2.84418400
H	-5.77152800	-0.63343900	1.82387500
H	-5.90193300	-1.55468800	3.34610500
H	-5.57387400	0.20317400	3.38736900
H	8.35805900	0.49310000	1.09937000

Product 6a

E= -1169,63136454

C	1.01602100	-1.95460400	-0.09680700
C	0.39920300	-0.67365000	-0.04853700
C	1.45896100	0.28988300	-0.02150800
H	3.06838200	-2.49016100	-0.20134900
H	1.35772600	1.36988000	0.03663700
C	4.03669300	0.09427100	-0.00621800
C	4.33579700	1.38659300	-0.48083300
C	5.64213300	1.87332100	-0.44839000
H	3.53701300	2.00390100	-0.89707900
C	6.39851900	-0.20489400	0.52493400
H	4.88479600	-1.68446700	0.90936000
C	6.68044400	1.07959100	0.05153700
H	5.85372200	2.87705700	-0.82542000
H	7.20030200	-0.82964800	0.92650200
C	-1.01697200	-0.60616500	-0.06205400
C	-1.71726800	0.70586700	-0.05555800
C	-2.65994600	1.02579100	-1.05003400
C	-1.43904600	1.66798300	0.93236800
C	-3.31041900	2.26093000	-1.05896700

H	-2.88011100	0.30080200	-1.83716900
C	-2.08331400	2.90631700	0.93727500
H	-0.72219600	1.43529700	1.72282000
C	-3.01269100	3.18677300	-0.06188600
H	-4.03825200	2.51823800	-1.83102300
H	-1.88098900	3.65415500	1.70663000
C	0.24078300	-3.11648100	-0.19319600
H	0.69651100	-4.11283700	-0.25245400
N	-1.07942900	-3.04076400	-0.21881400
C	-1.68867400	-1.84051800	-0.13885700
C	-3.19589100	-1.93856500	-0.13891300
O	-3.84665500	-2.52908900	-0.96353800
O	-3.73419200	-1.30487300	0.92073200
C	-5.15819900	-1.31726900	1.00348700
H	-5.41637400	-0.78351200	1.92651200
H	-5.60426500	-0.80980400	0.13406200
H	-5.54030500	-2.34870700	1.03654800
C	5.09036300	-0.69173600	0.50040600
C	2.65707400	-0.40718400	-0.03679900
N	2.37694000	-1.76400000	-0.06867000
F	-3.63303400	4.37623200	-0.06450800
H	7.70411400	1.46123100	0.07212800

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