

Supplementary Material

Organocatalytic Synthesis of Enantiopure Spiro Acenaphthyl-pyrrolizidine/pyrrolidines: Justifying the Regioselectivity based on Distortion/interaction Model

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Table of Contents

General Information.....	S1
Computational details	S1
Tables, scheme and figures	S2
¹ H, ¹³ C NMR and HRMS spectra.....	S5
Z-Matrix data	S36

General Information

Optical rotations were measured with a Perkin–Elmer 341 polarimeter at 589 nm. ¹H and ¹³C NMR spectra were recorded BRUKER DRX-300 AVANCE spectrometer (at 300.13 MHz for Protons and 75.47 MHz for Carbon-13) and BRUKER DRX-400 AVANCE spectrometer (at 400.4 MHz for protons and 100.7 MHz for Carbon-13). IR spectra were recorded on a Bomen FT-IR-MB-series instrument. Enantiomeric excess (ee) of compound 7b and 9 were determined by HPLC analysis using a Daicel Chiralpak AD-H column. All reagents and starting materials were purchased from Aldrich, Merck, and Fluka. All solvents were reagent grade and were dried and distilled immediately before use as follows: methanol and ethanol from mg/I₂, methylene chloride from calcium hydride. Column chromatography was performed using silica gel 60 (230–400 mesh) eluting with ethyl acetate/n-hexane. TLC was performed using silica gel 60 F256 plates with visualization by UV.

Computational details

In this work, all geometries of the reactant (Re), transition states (TS) and products (Pr) have been fully optimized using B3LYP/6-31G(d,p) in gas phase at 298.15 K. Geometries of transition states have been verified to be correct structures by observation of a single imaginary frequency and intrinsic reaction coordinate (IRC) calculations. The electronic structures and Frontier orbital contributions are calculated by the natural bond orbital (NBO) method. Non-covalent interactions (NCI) have been plotted with using Multiwfn (version 3.3.8). All of the other calculations were carried out using the Gaussian 09 program. The optimized structures were shown using the CYLView software. Electronic chemical potential μ , chemical hardness η , global nucleophilicity N , global electrophilicity ω , softness S , Synchronicity S_y and Local Fukui functions were calculated based on the following formulas:

$$1) \quad \mu = (\epsilon_{\text{HOMO}} + \epsilon_{\text{LUMO}})/2$$

$$2) \quad \eta = \epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}}$$

$$3) \quad N = \epsilon_{\text{HOMO}} - \epsilon_{\text{HOMO(TCE)}}$$

$$4) \quad \omega = (\mu^2/2\eta)$$

$$5) \quad S = 1/(2\eta)$$

$$6) \quad S_y = 1 - (2n - 2)^{-1} \sum_{i=1}^n \frac{|\delta B_i - \delta B_{av}|}{\delta B_{av}}, \quad \delta B_i = \frac{B_i^{TS} - B_i^R}{B_i^P - B_i^R}, \quad \delta B_{av} = n^{-1} \sum_{i=1}^n \delta B_i$$

Here, n and δB_k correspond to the number of bonds directly involved in the reaction and the relative variation of the Wiberg bond indices.

$$7) \quad f_k^+ = q_k^N - q_k^{N+1}$$

$$8) \quad f_k^- = q_k^{N-1} - q_k^N$$

Where k , N and q , correspond to the index of the atom, the number of electrons and the net charge, respectively.

Tables, scheme and figures

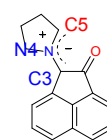
S1. The analysis of global properties.

	E_{Homo}	E_{Lumo}	μ	η	ω	s	N
Dipolaro-Phile	-6.75	-1.37	-4.06	5.39	1.53	0.09	2.37
Dipolar	-4.55	-1.38	-2.96	3.16	1.39	0.16	4.58

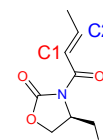
All data were reported in eV.

Table S2. Local properties analysis.

	f+	f-	ω_k	s+	s-
C1	0.020	0.026	0.030584	0.001857	0.002414
C2	0.070	0.032	0.107046	0.006499	0.002971
C3	0.012	0.114	0.016669	0.001897	0.018021
C5	0.069	0.091	0.095849	0.010907	0.014385



Dipolar 1



Dipolarophile 2

All data were reported in eV.

Table S3. Wiberg bond indices for reactants, transition structures and products

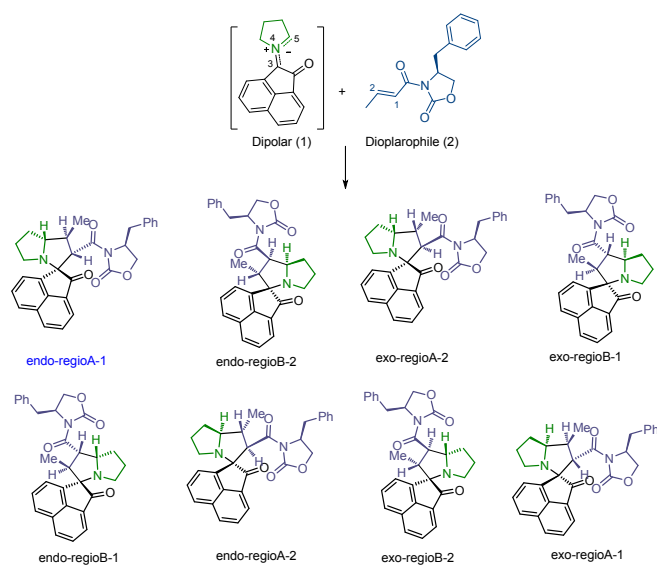
Structure's Name	B(1,2)	B(2,3)	B(3,4)	B(4,5)	B(1,5)	B(1,3)	B(2,5)
Dipolarophile 2	1.8284						
Dipolar 1			1.1267	1.4299			
TS-endo-regioA-2	1.4489		1.2191	1.2109		0.1121	0.4113
TS-exo-regioA-1	1.424		1.0041	0.9929		0.1352	0.4458
TS-exo-regioB-2	1.3698	0.3784	1.0933	1.2747	0.3391		
TS-endo-regioB-1	1.3547	0.4648	1.0477	1.3755	0.2096		
TS-endo-regioB-2	1.3523	0.4718	1.0487	1.3768	0.2058		
TS-exo-regioB-1	1.378	0.3797	1.0879	1.2819	0.3279		
TS-endo-regioA-1	1.4546		1.2067	1.2155		0.1236	0.4106
TS-exo-regioA-2	1.4277		1.1976	1.1879		0.1306	0.4419
Pr-endo-regioA-2	0.959		0.9779	0.948		0.9067	0.9736
Pr-exo-regioA-1	0.9582		0.972	0.9112		0.9183	0.9857
Pr-exo-regioB-2	0.9587	0.9288	0.9407	0.9418	0.946		
Pr-endo-regioB-1	0.9687	0.9357	0.9687	0.9484	0.9573		
Pr-endo-regioB-2	0.9599	0.9502	0.9414	0.9859	0.9187		
Pr-exo-regioB-1	0.9595	0.9207	0.9794	0.918	0.9793		
Pr-endo-regioA-1	0.9654		0.9681	0.9382		0.9256	0.9762
Pr-exo-regioA-2	0.9655		0.9444	0.9683		0.9465	0.9615

Table S4. Synchronicity of bond formation in 1,3-DC reaction

Structure's Name	Syn.
endo-regioA-2	-0.26177
exo-regioA-1	0.742837
exo-regioB-2	0.847305
endo-regioB-1	0.720736
endo-regioB-2	0.737395
exo-regioB-1	0.86008
endo-regioA-1	-0.00451
exo-regioA-2	0.238014

Table S5. Thermodynamic and Kinetic data (All data were reported in kcal mol⁻¹).

Structure's Name	E _a	ΔH	ΔG
endo-regioA-1	5.3	-21.1	-5.9
endo-regioA-2	6.0	-20.1	-4.2
endo-regioB-1	9.8	-20.4	-5.7
endo-regioB-2	9.4	-22.0	-6.4
exo-regioA-1	11.6	-17.0	-2.1
exo-regioA-2	11.4	-19.1	-4.2
exo-regioB-1	12.8	-20.9	-6.6
exo-regioB-2	13.1	-20.9	-6.2



Scheme S1. The possible Products of the 1,3-DC reaction.

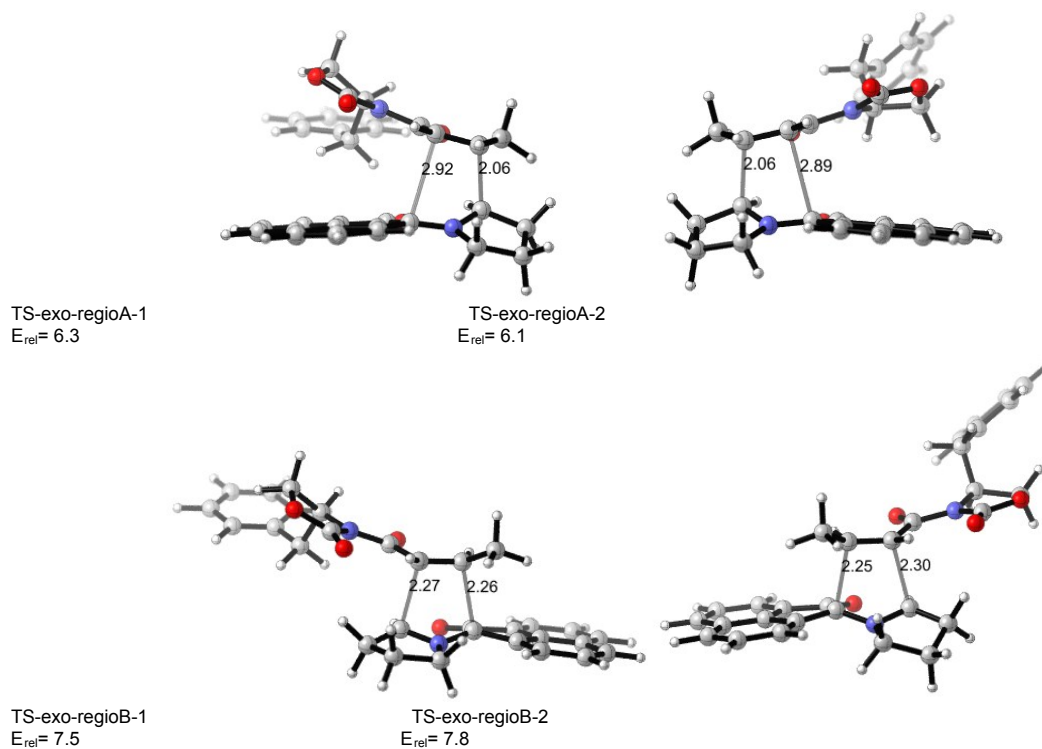


Figure S1. The transition state structures of endo products and relative electronic energies of these structures (in kcal mol⁻¹, Calculated with B3LYP/6-31G(d,p)).

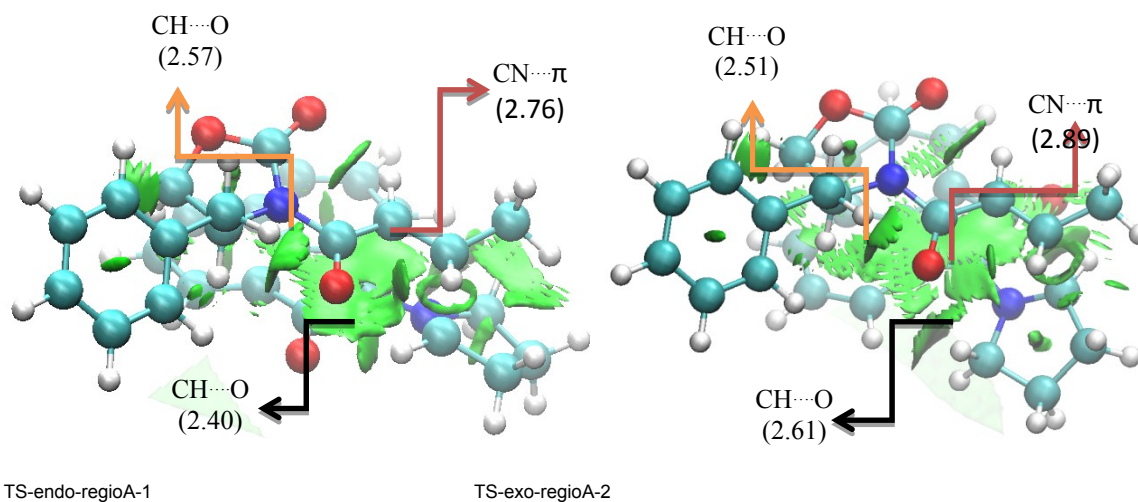
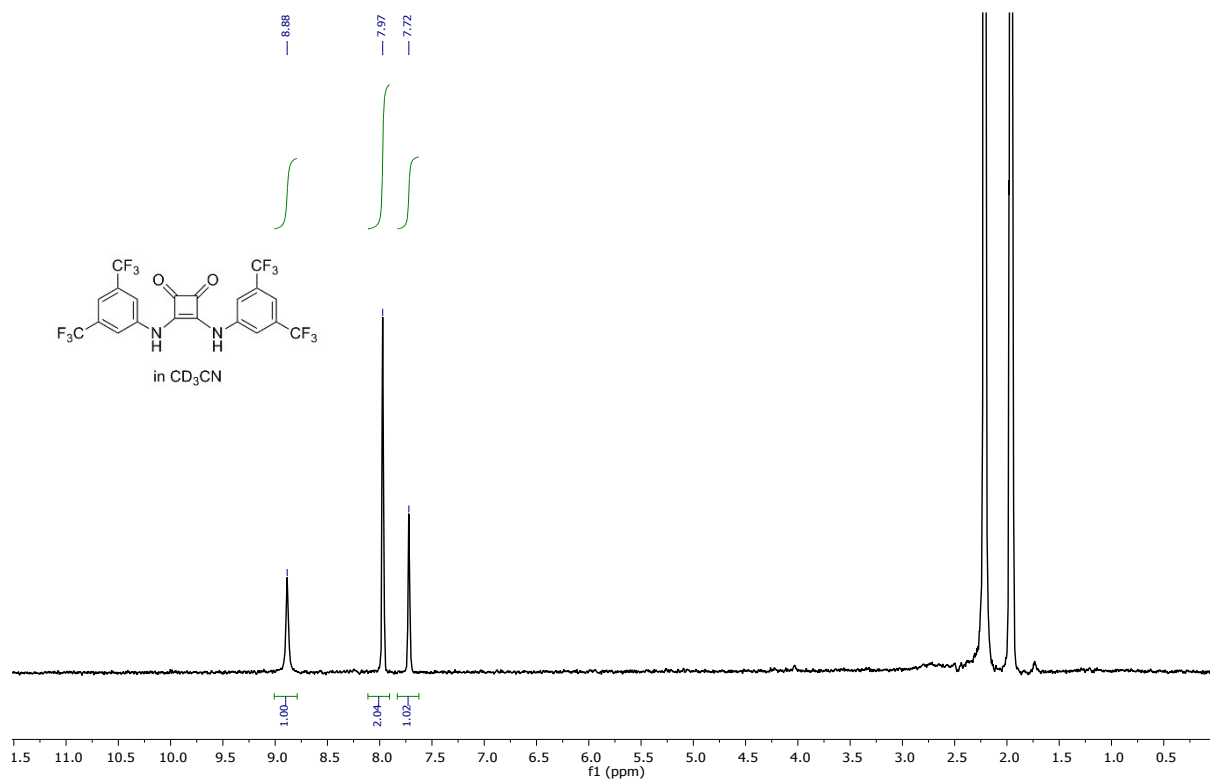
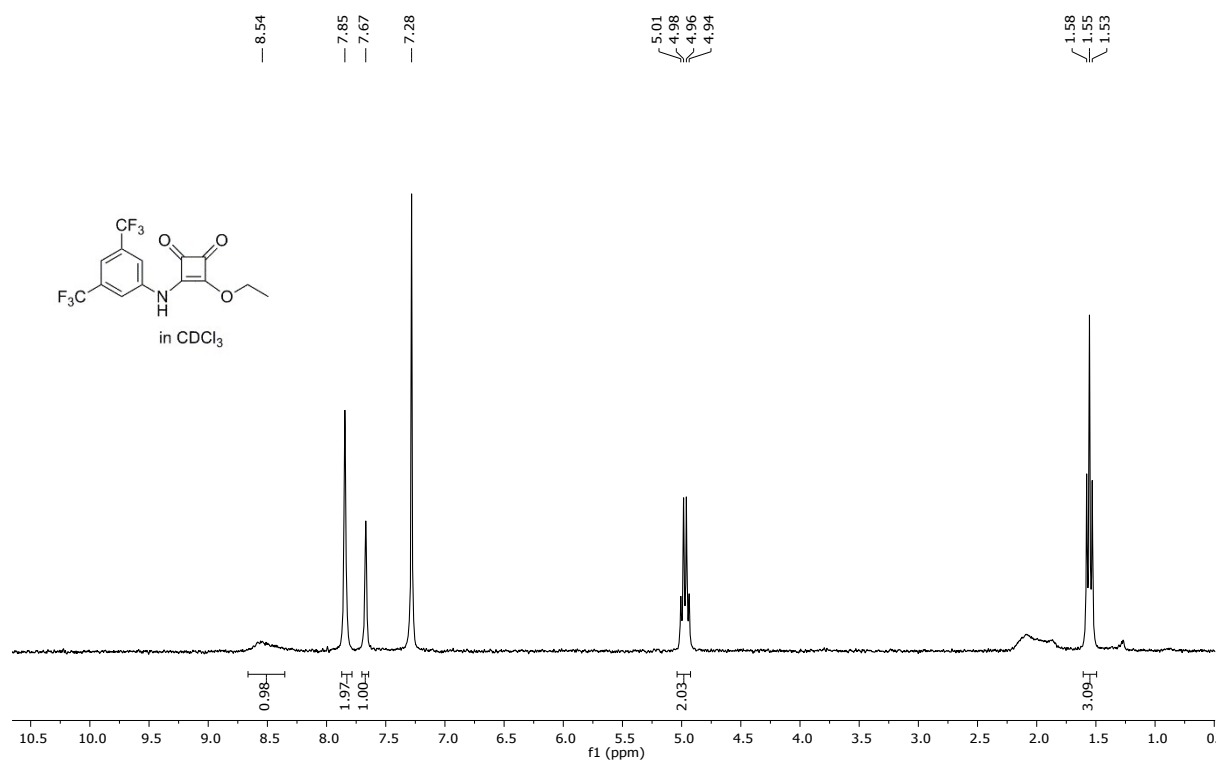


Figure S2. The NCI plots for the transition states TS-endo-regioA-1 and TS-exo-regioA-1 (Distances are given in parentheses (units in Å)).

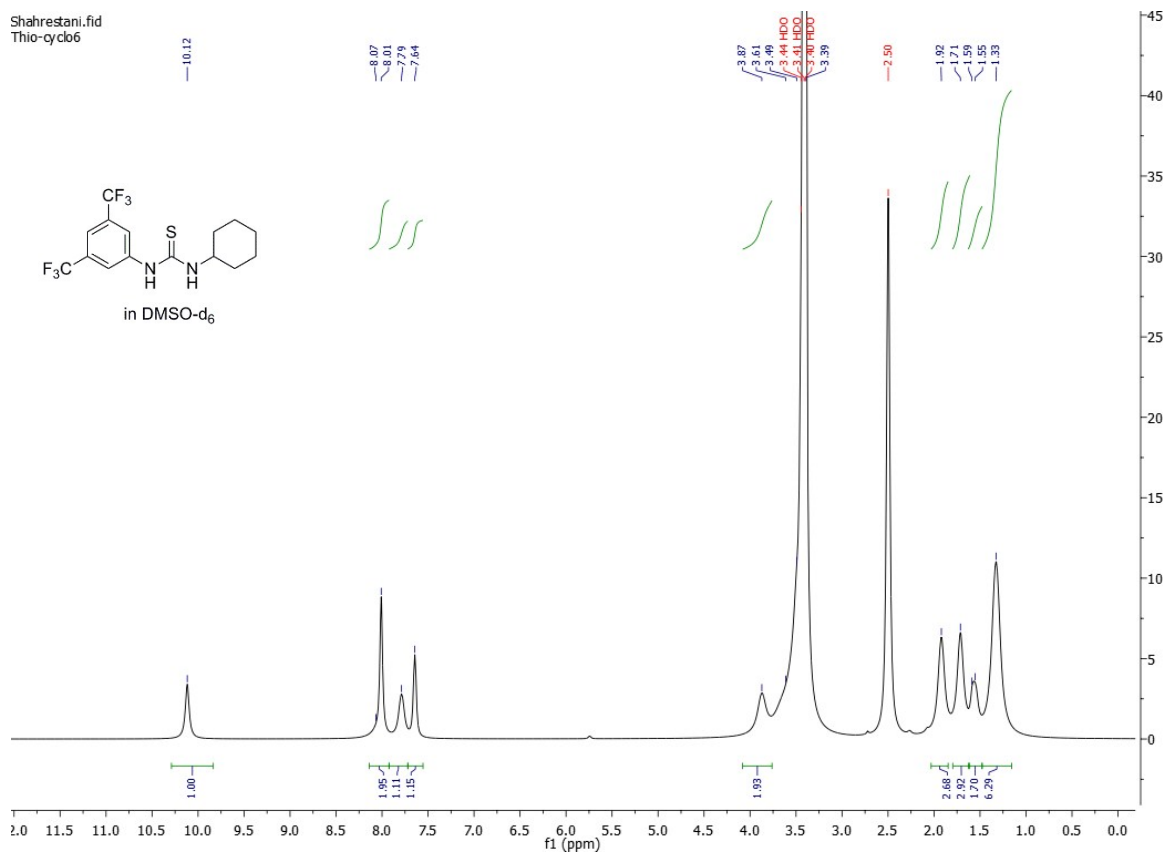
Table S6. single-point energy calculations using B3LYP/6-31+G(d,p) PCM (CH₂Cl₂) (All data were reported in kcal mol⁻¹).

Structure's Name	$\Delta\Delta E^\ddagger$	Structure's Name	$\Delta\Delta E^\ddagger$
endo-regioA-1	0.0	exo-regioA-1	3.8
endo-regioA-2	0.8	exo-regioA-2	4.2
endo-regioB-1	4.3	exo-regioB-1	6.9
endo-regioB-2	3.7	exo-regioB-1	7.2

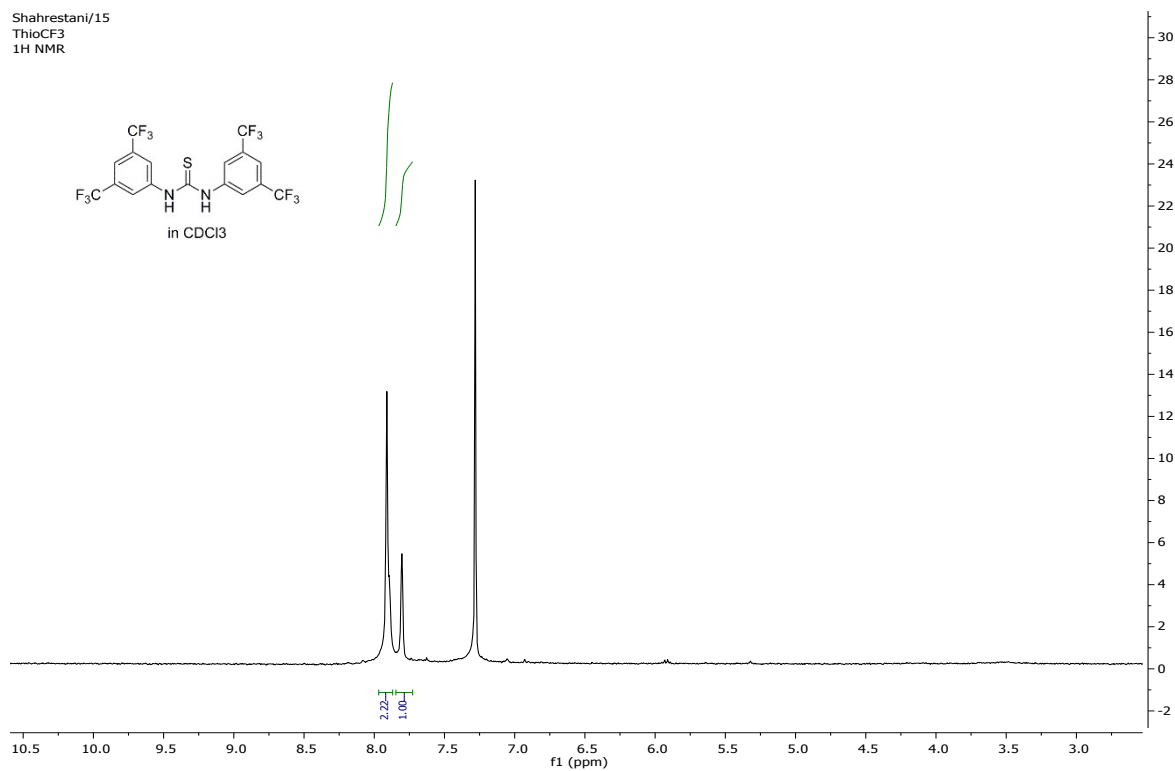
¹H, ¹³C NMR and HRMS spectra



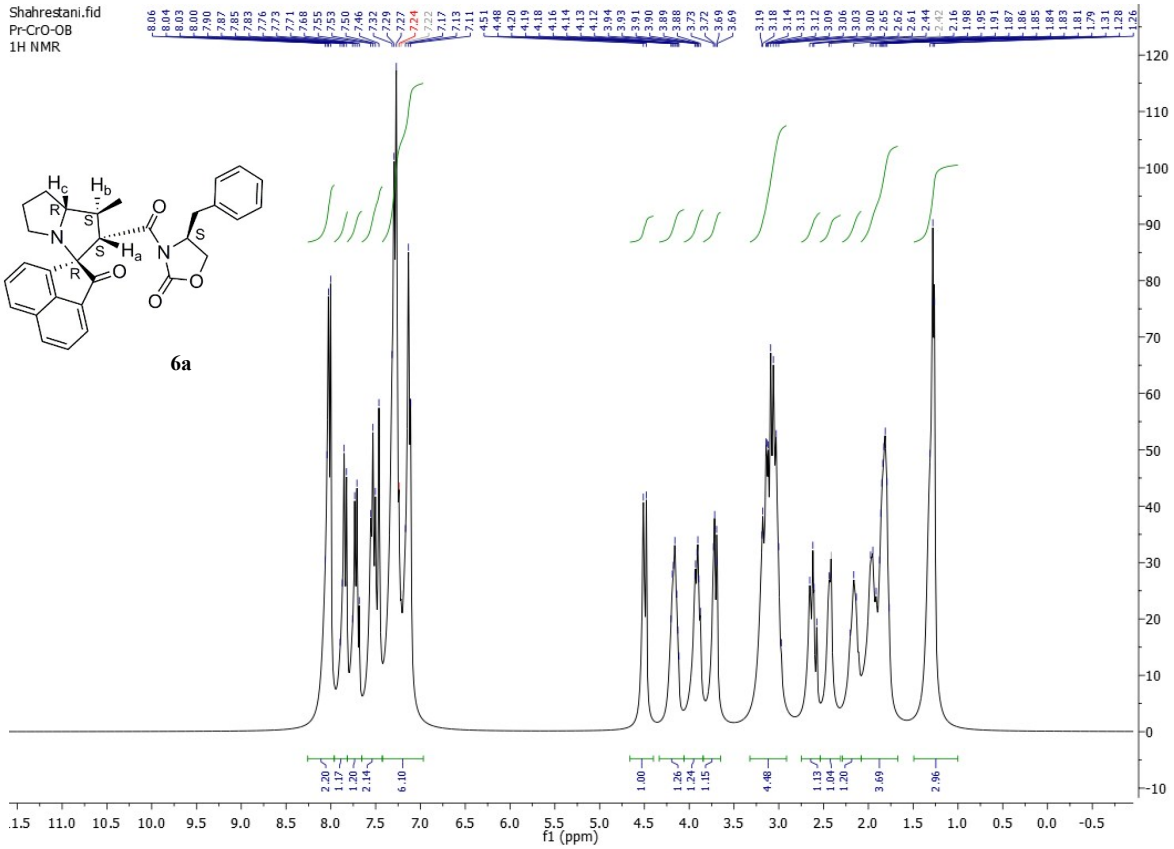
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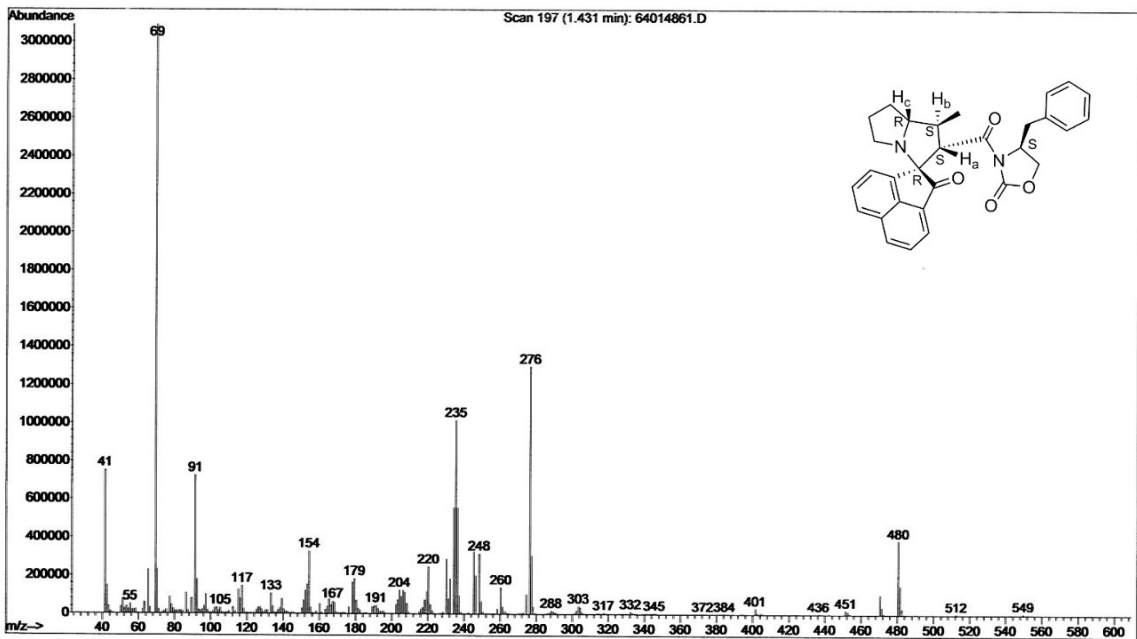
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1H NMR



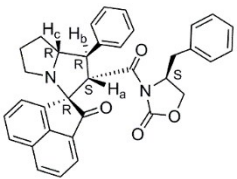
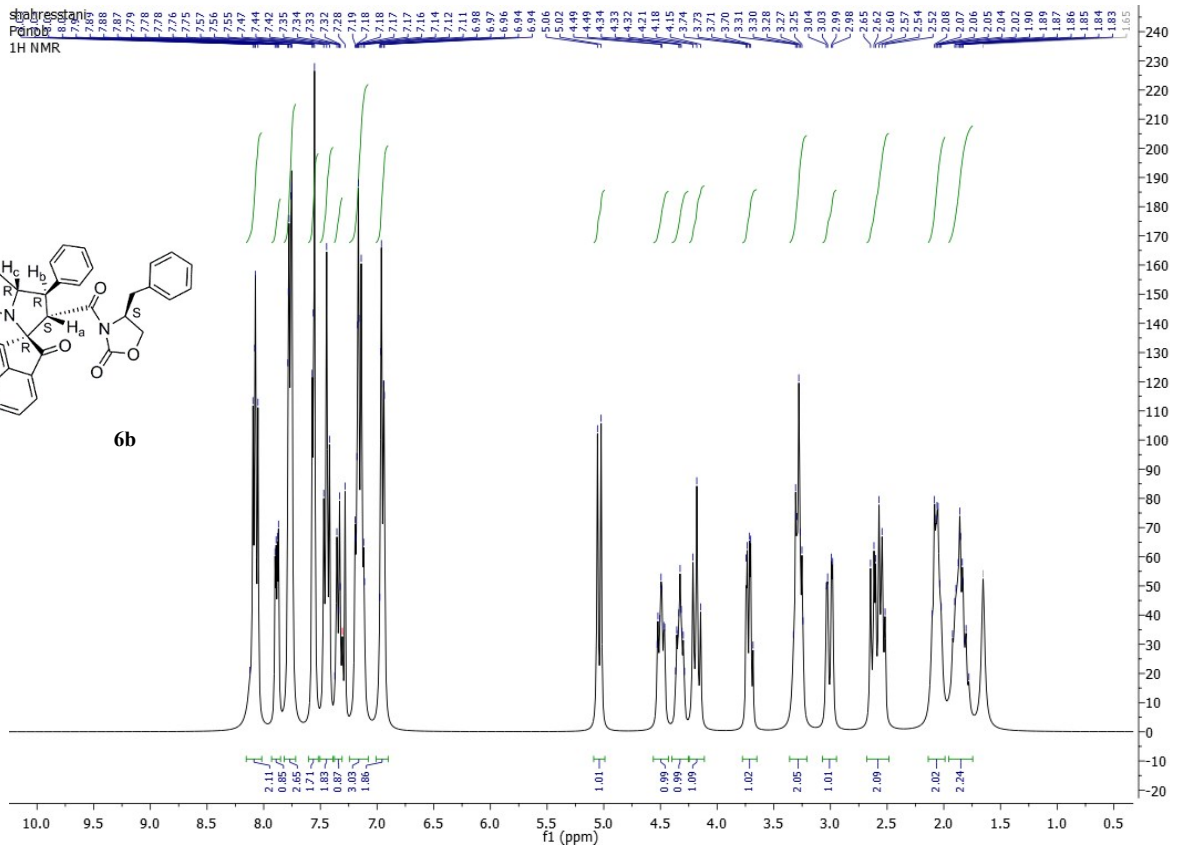
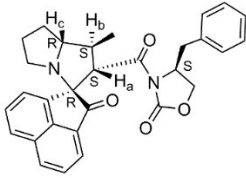
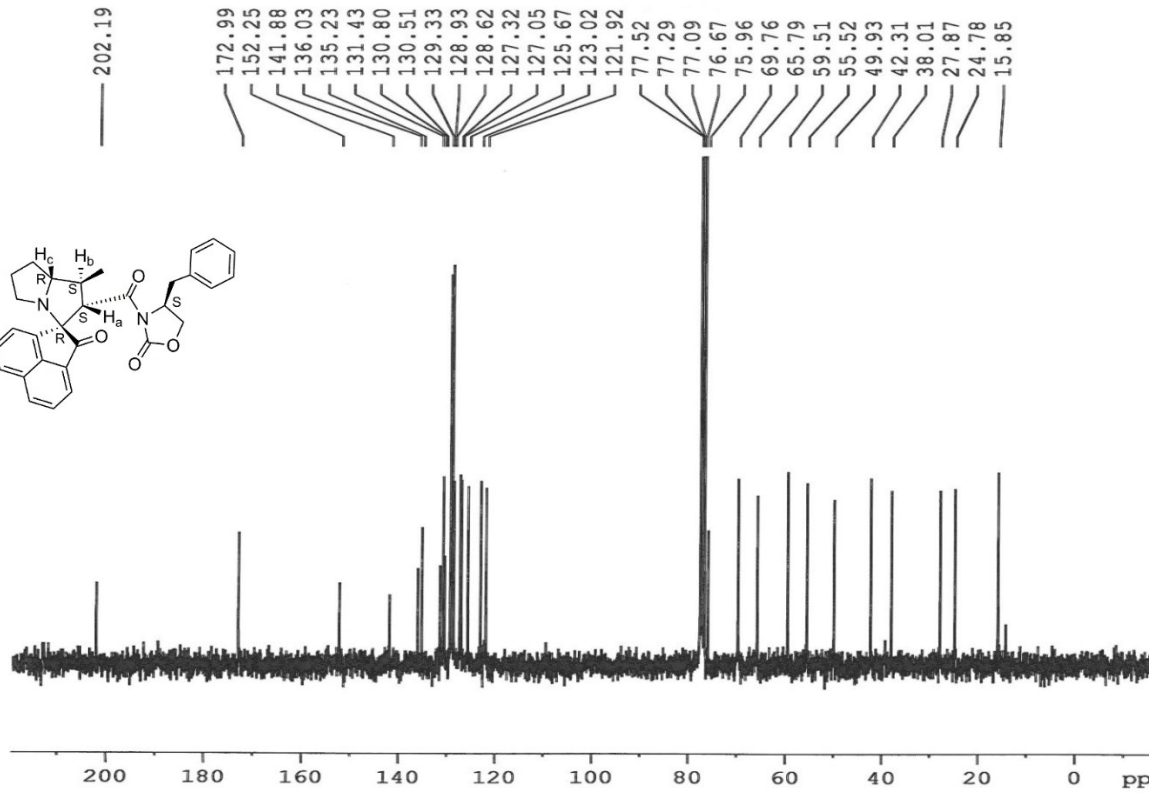
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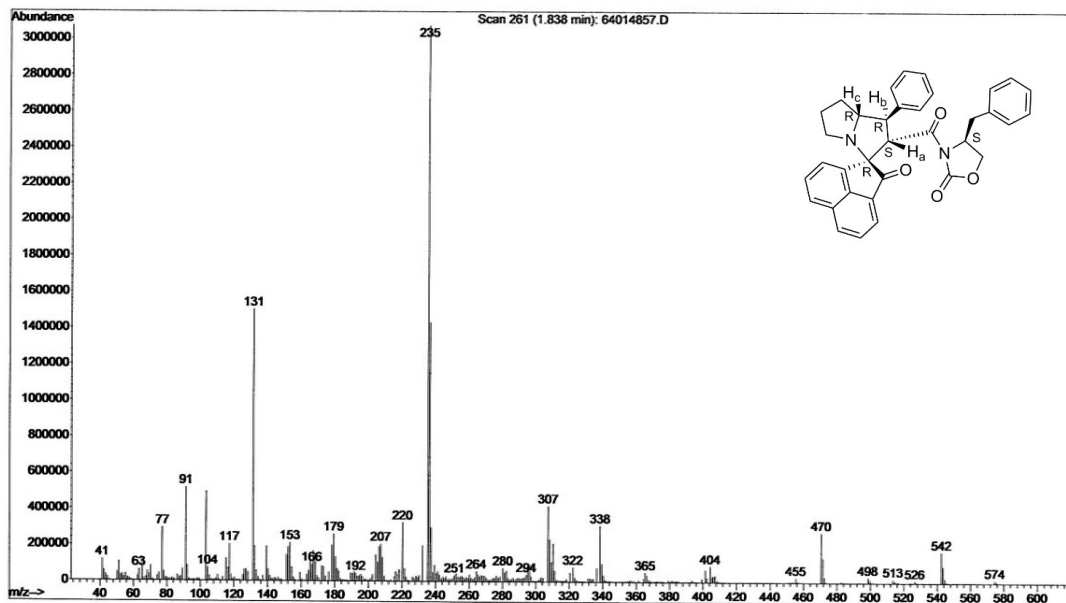


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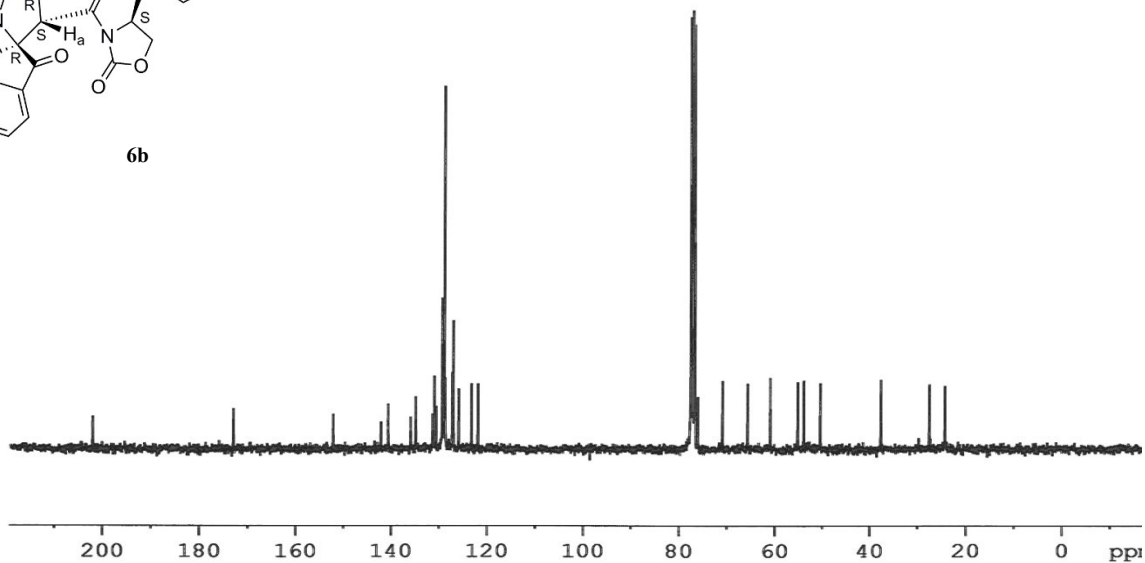
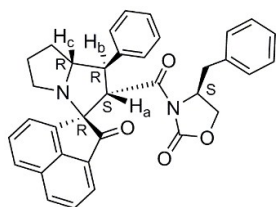
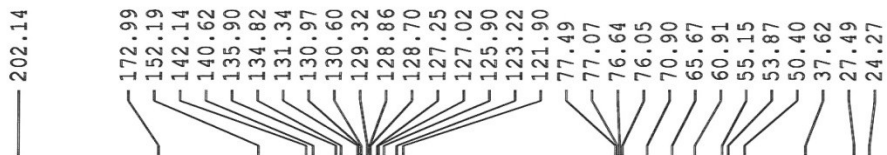


6b

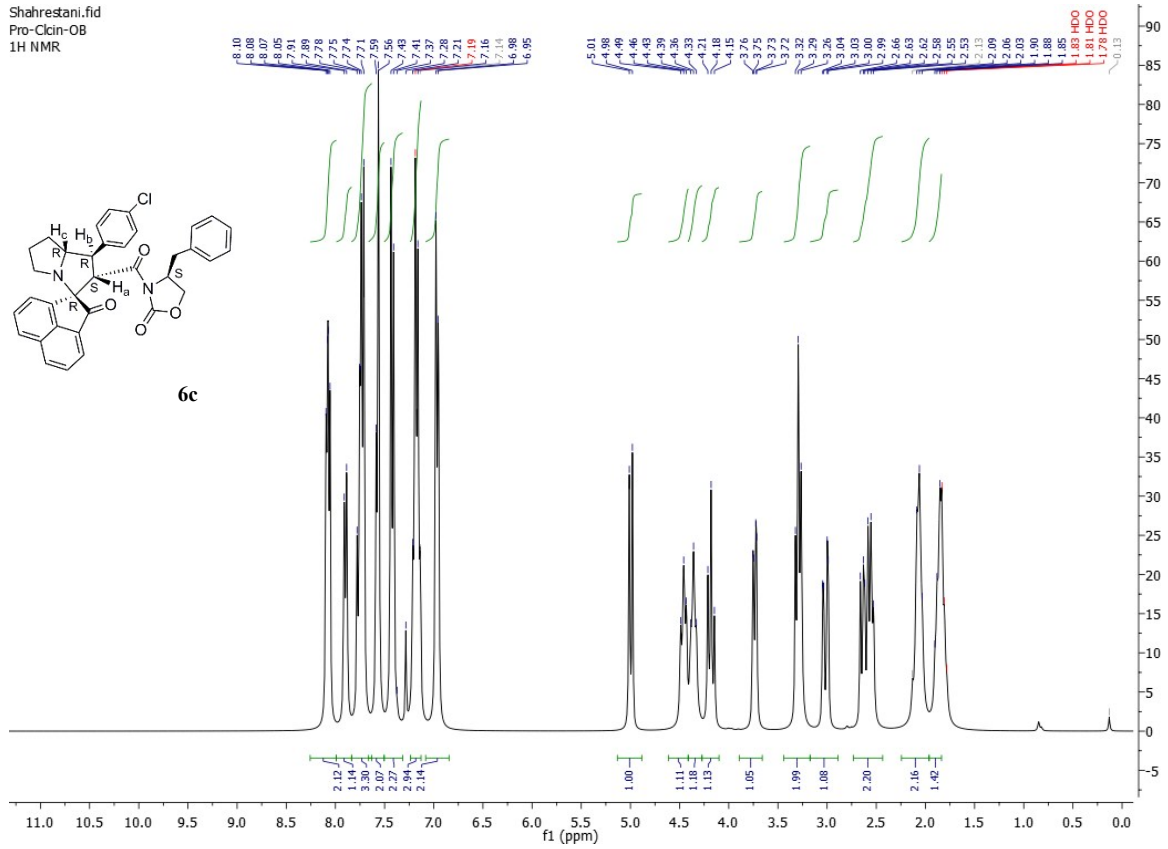
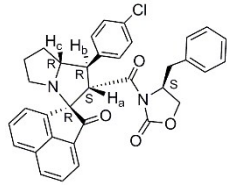
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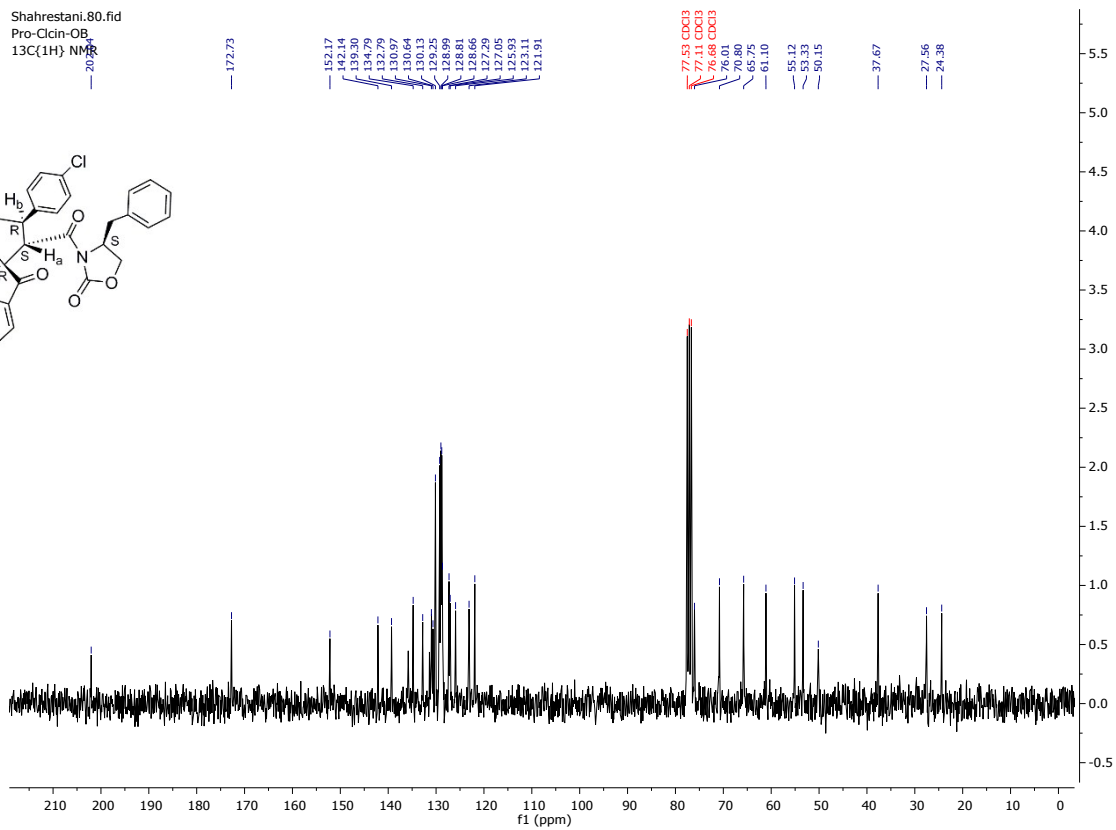
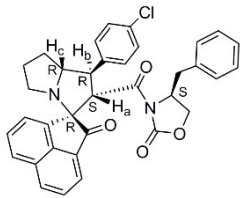
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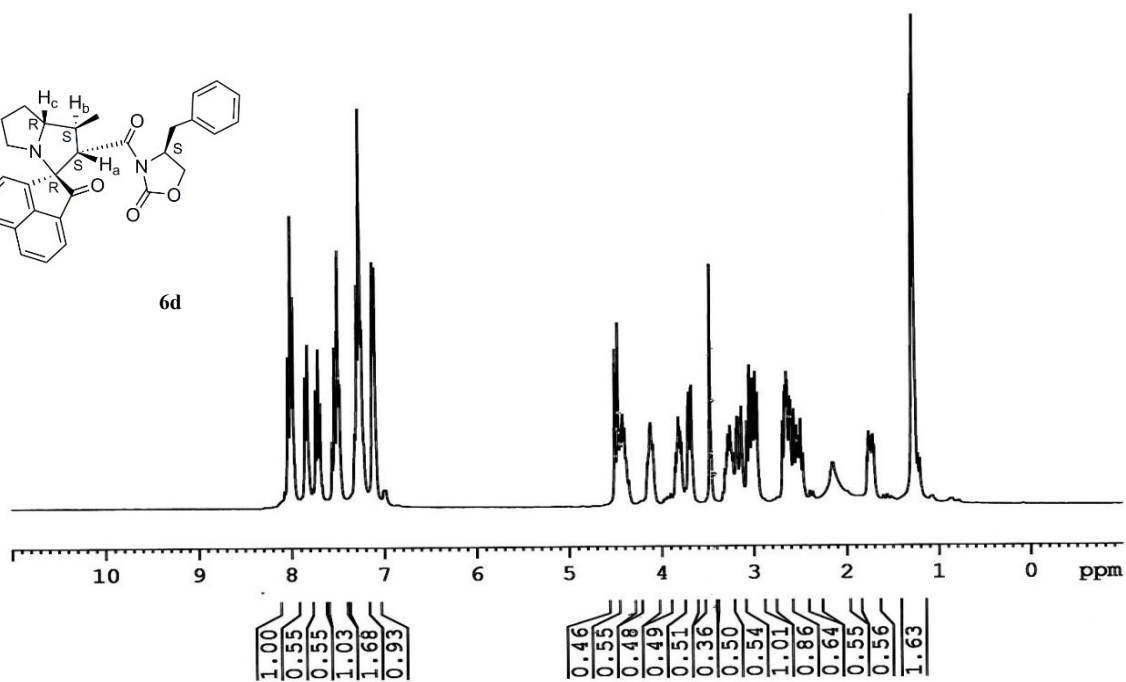
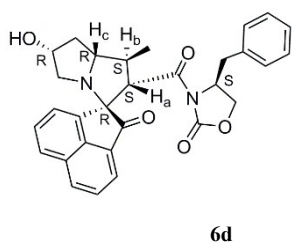
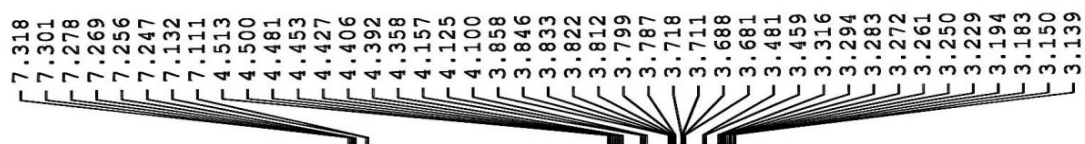
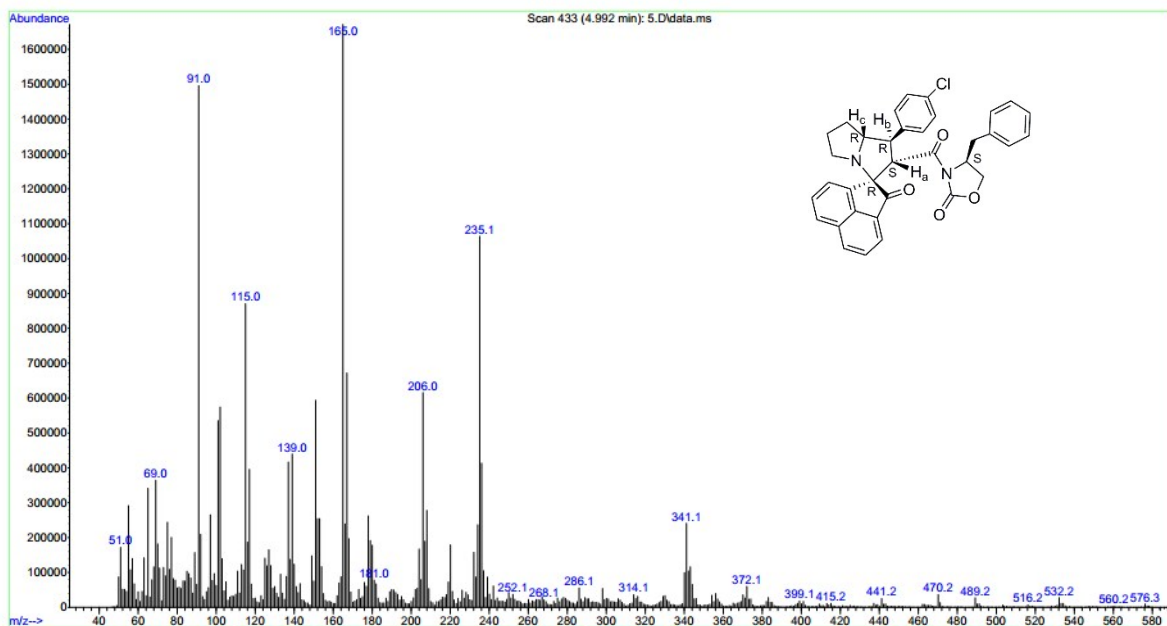


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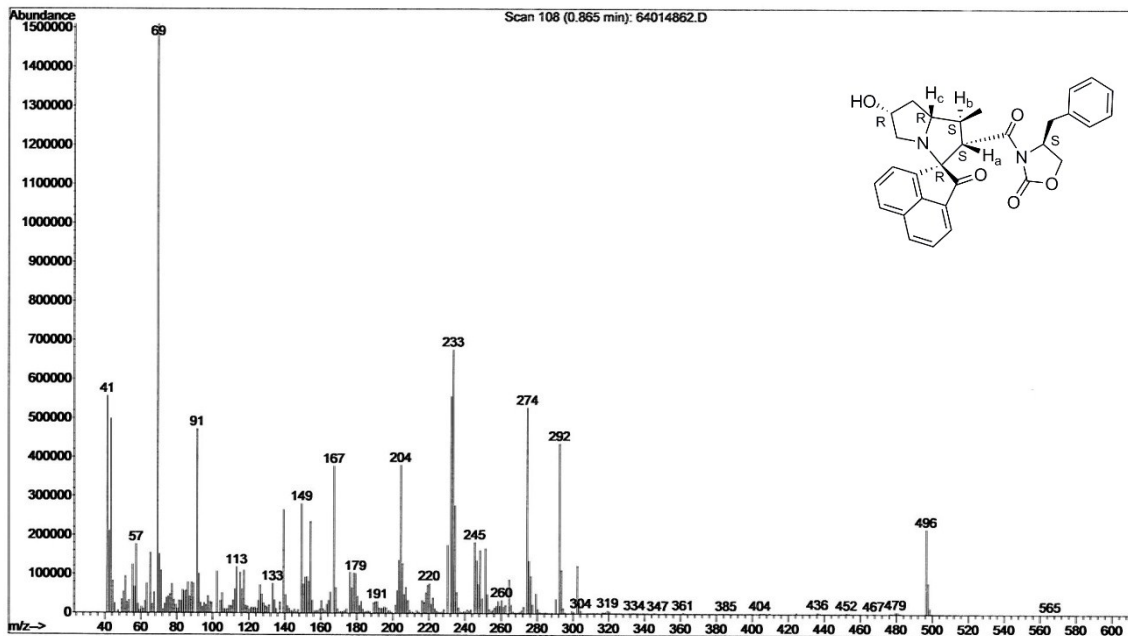


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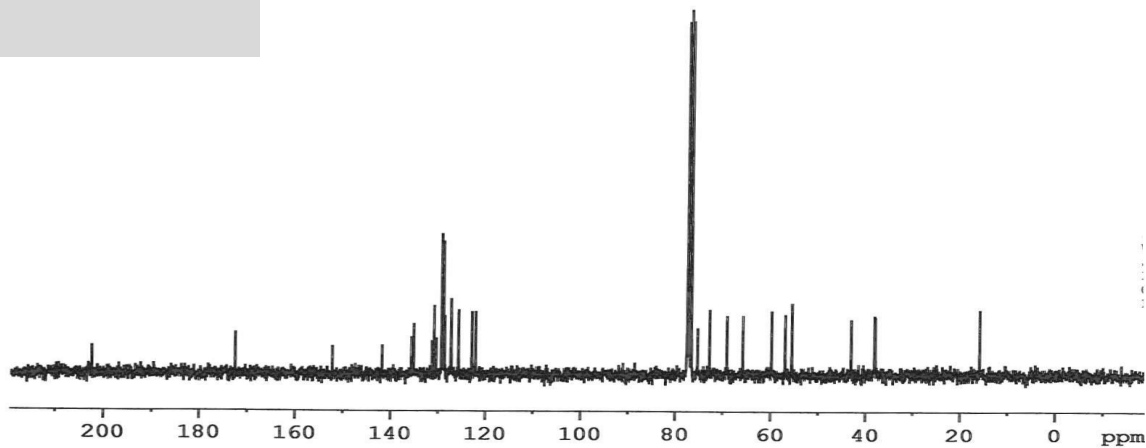


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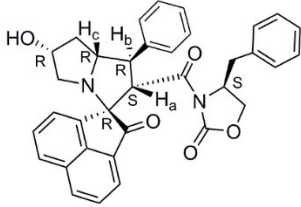


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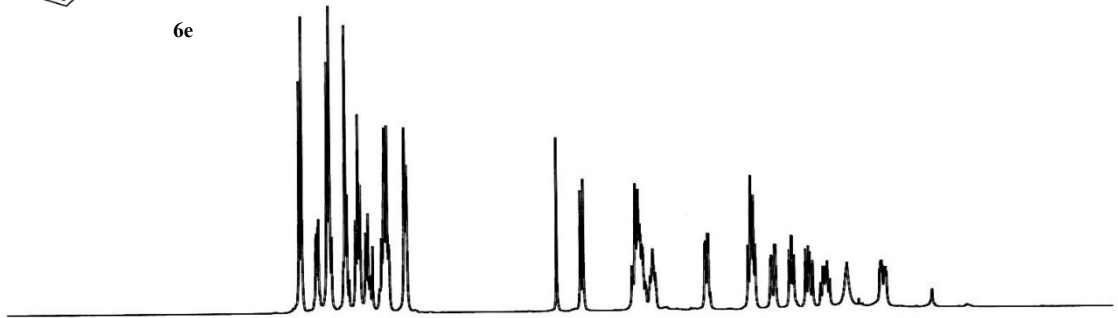
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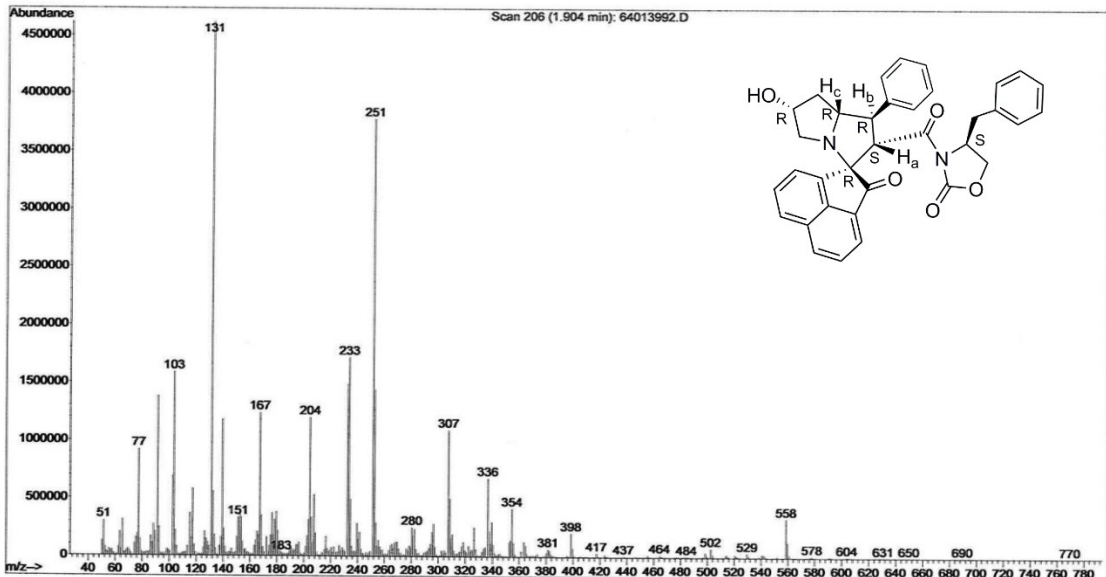
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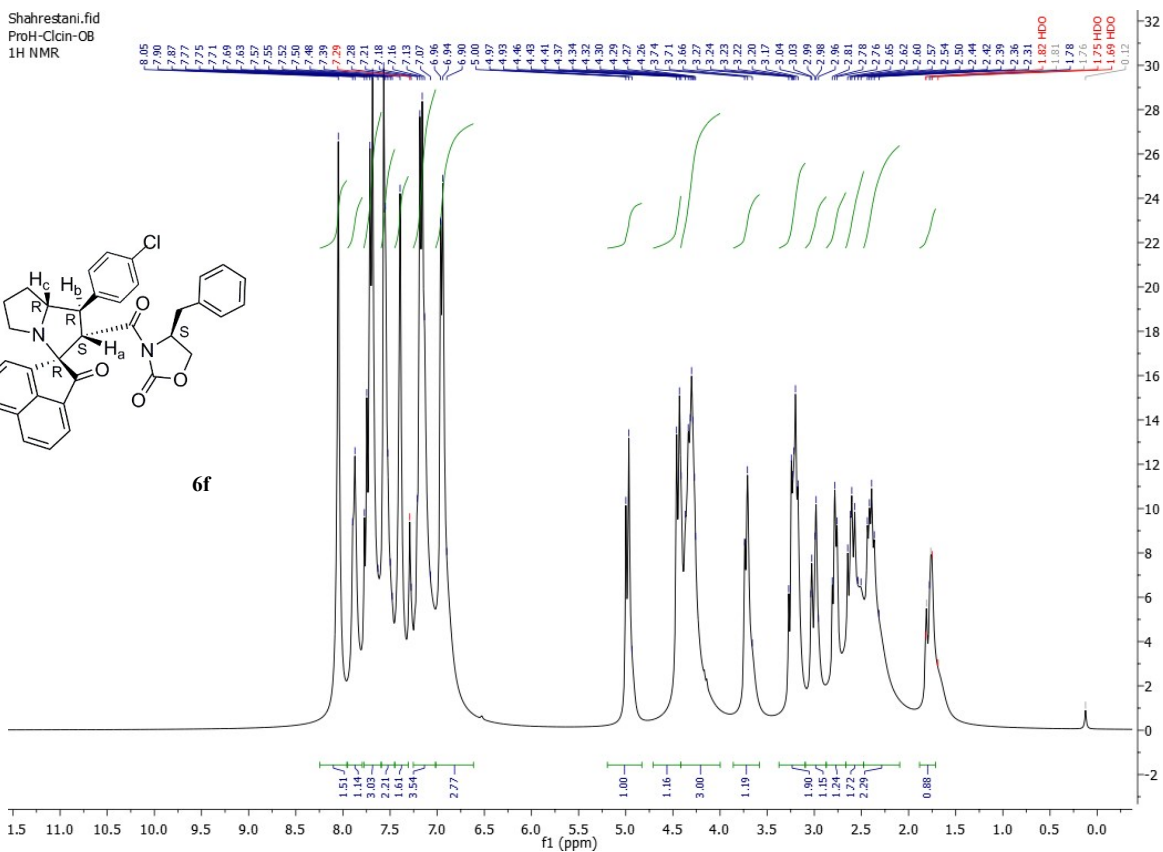
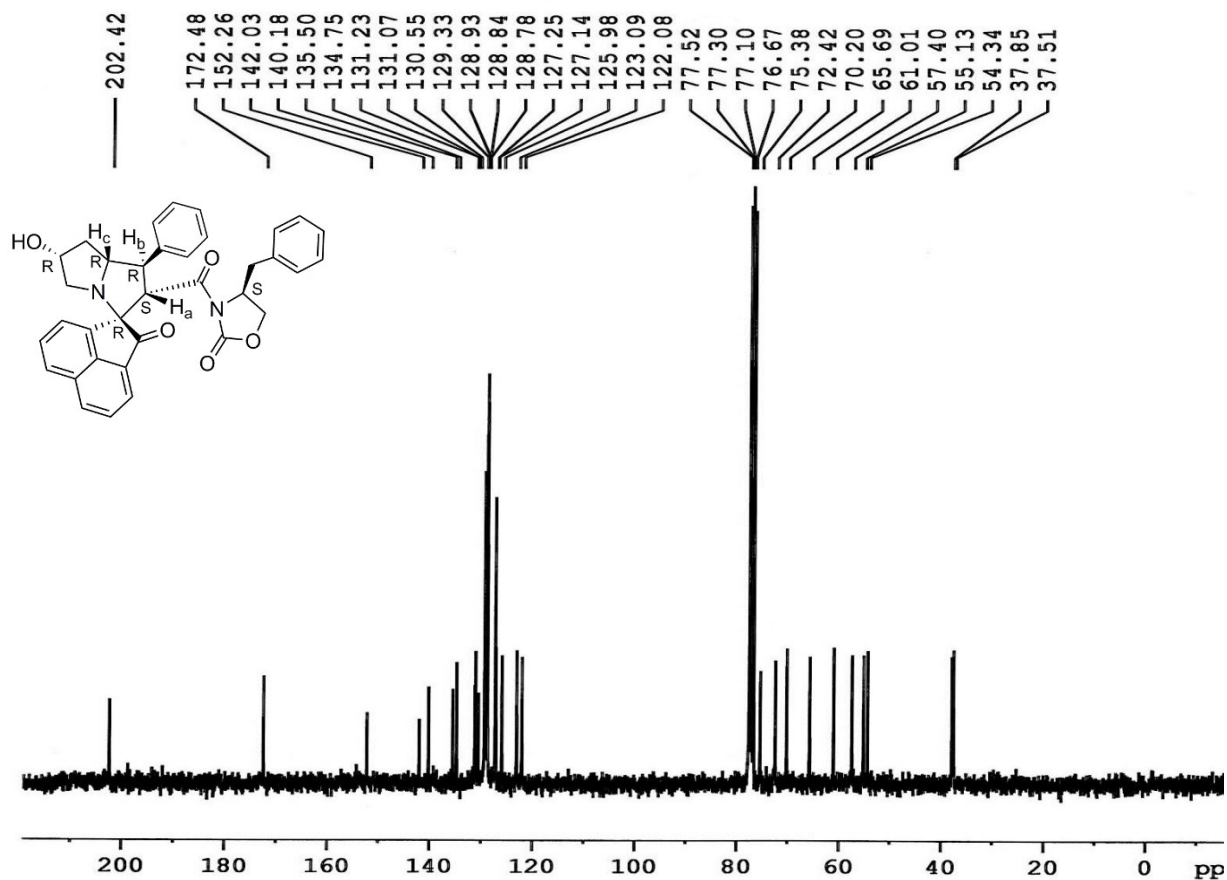
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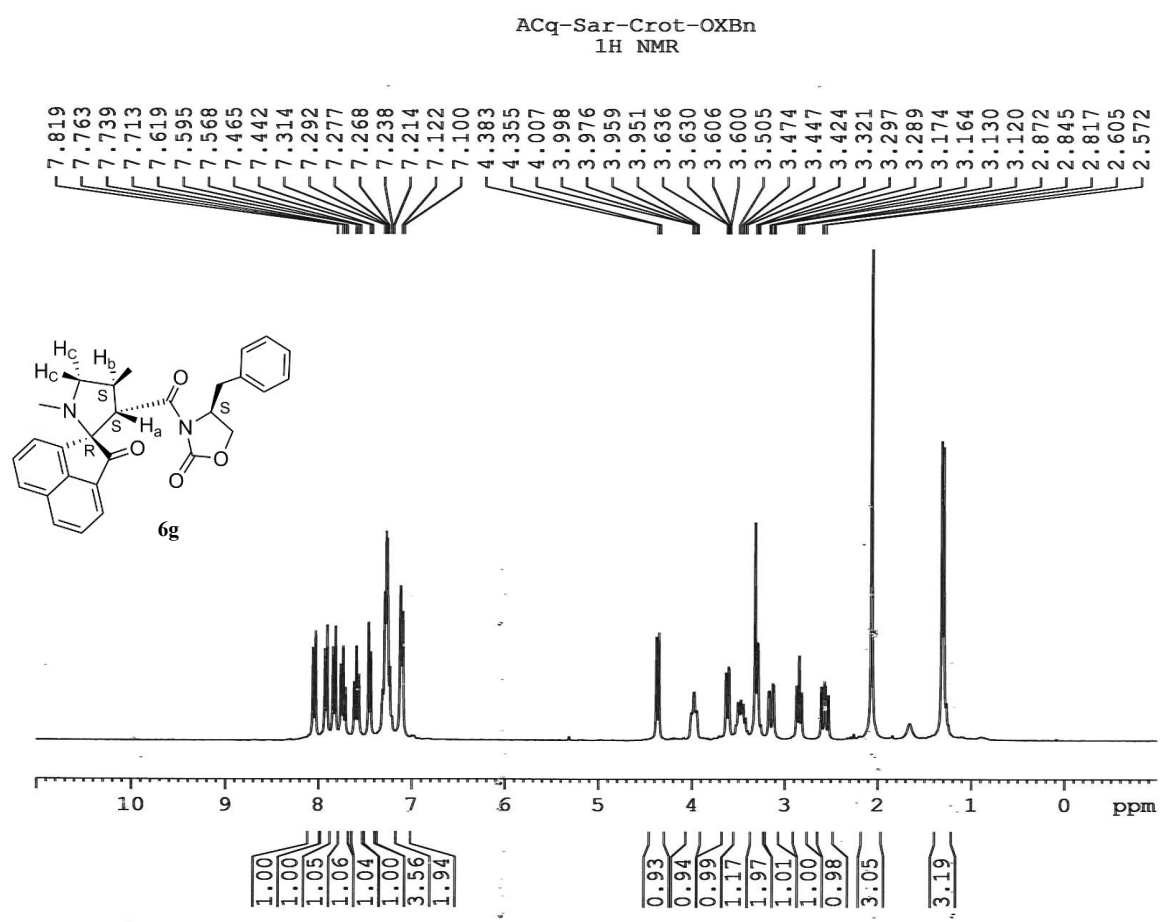
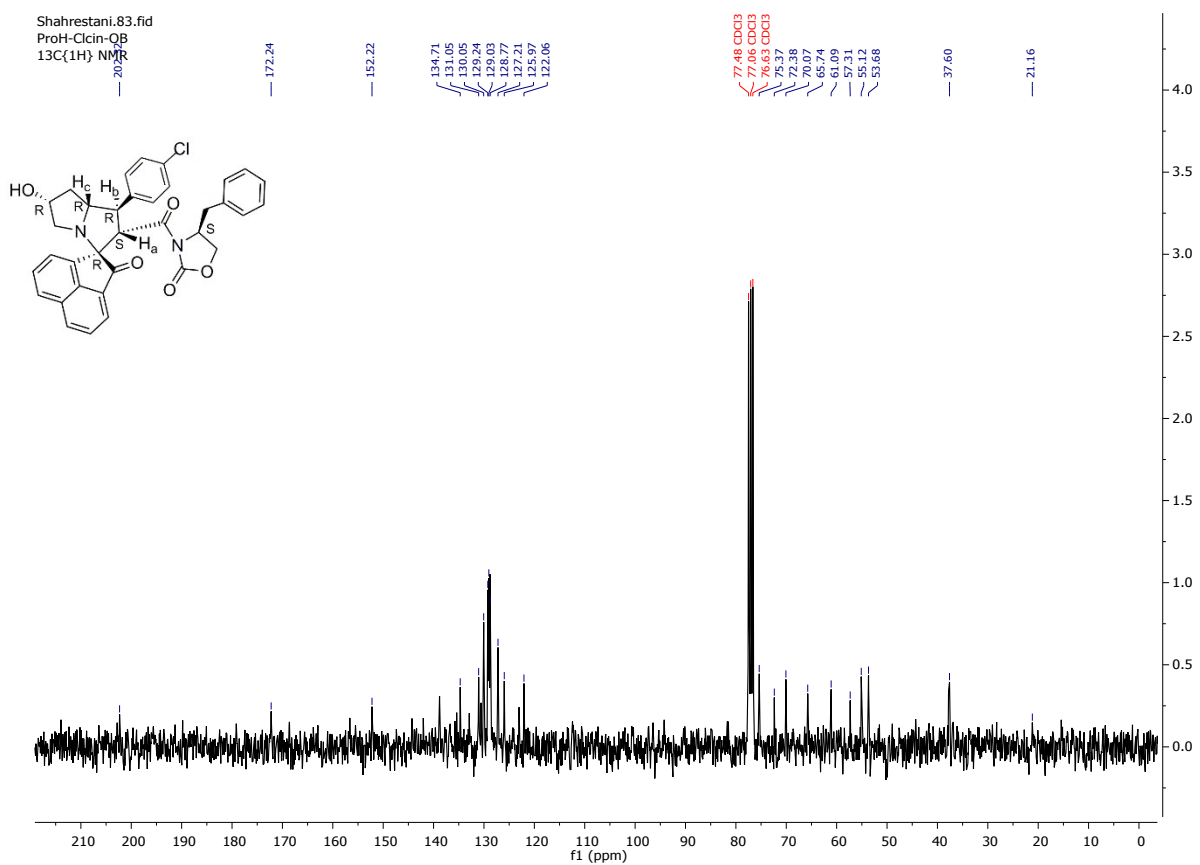
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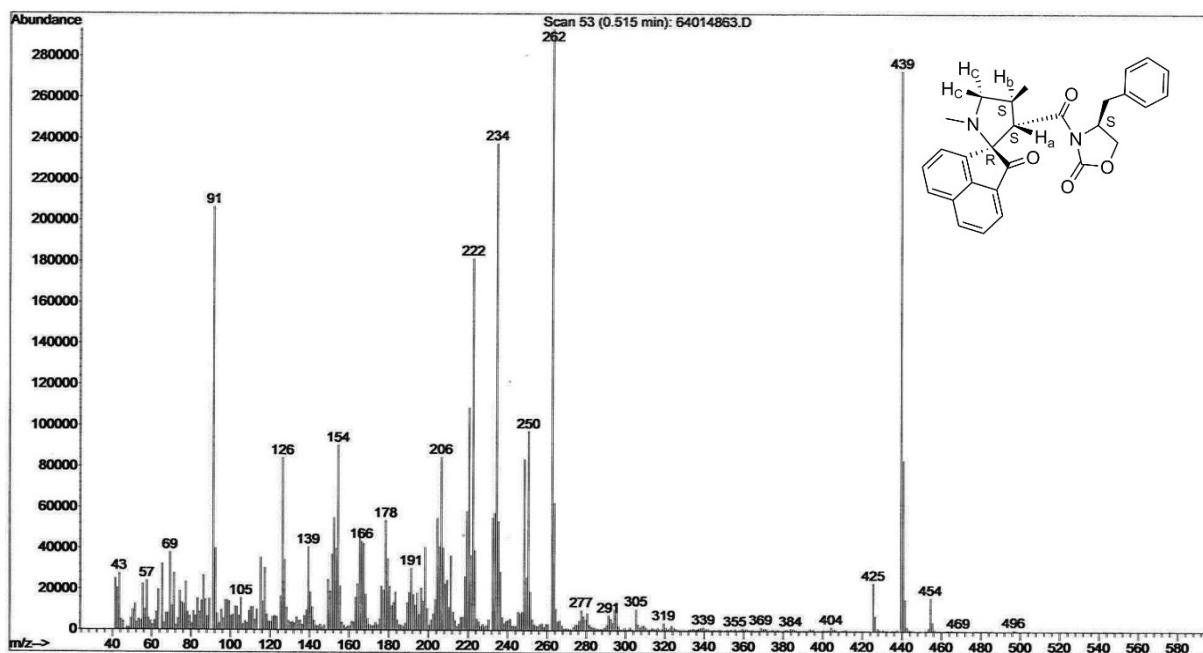


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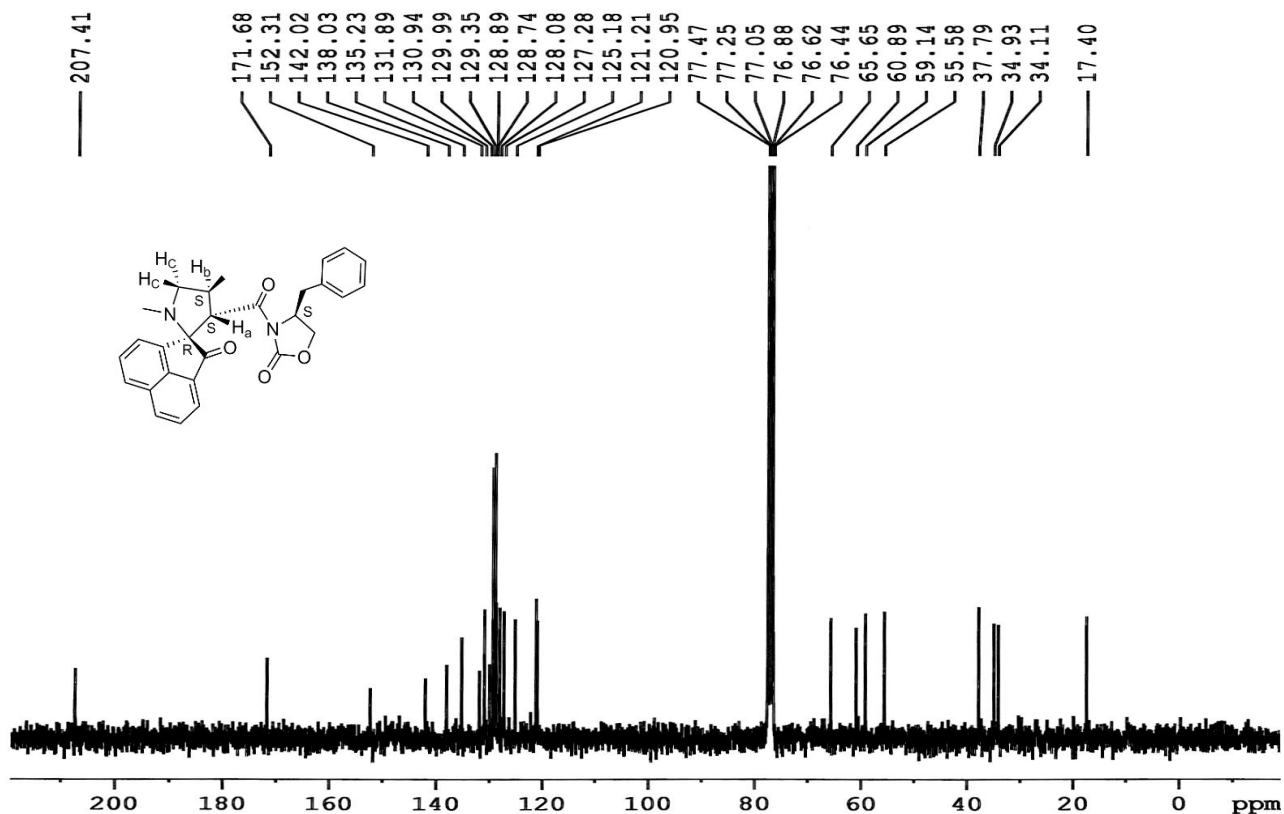


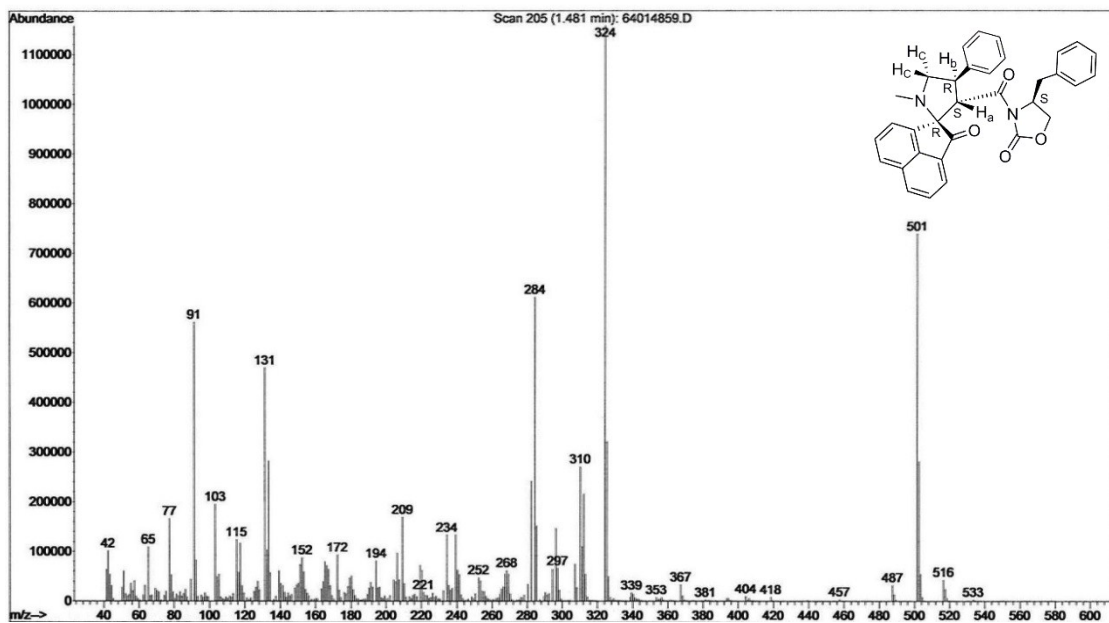
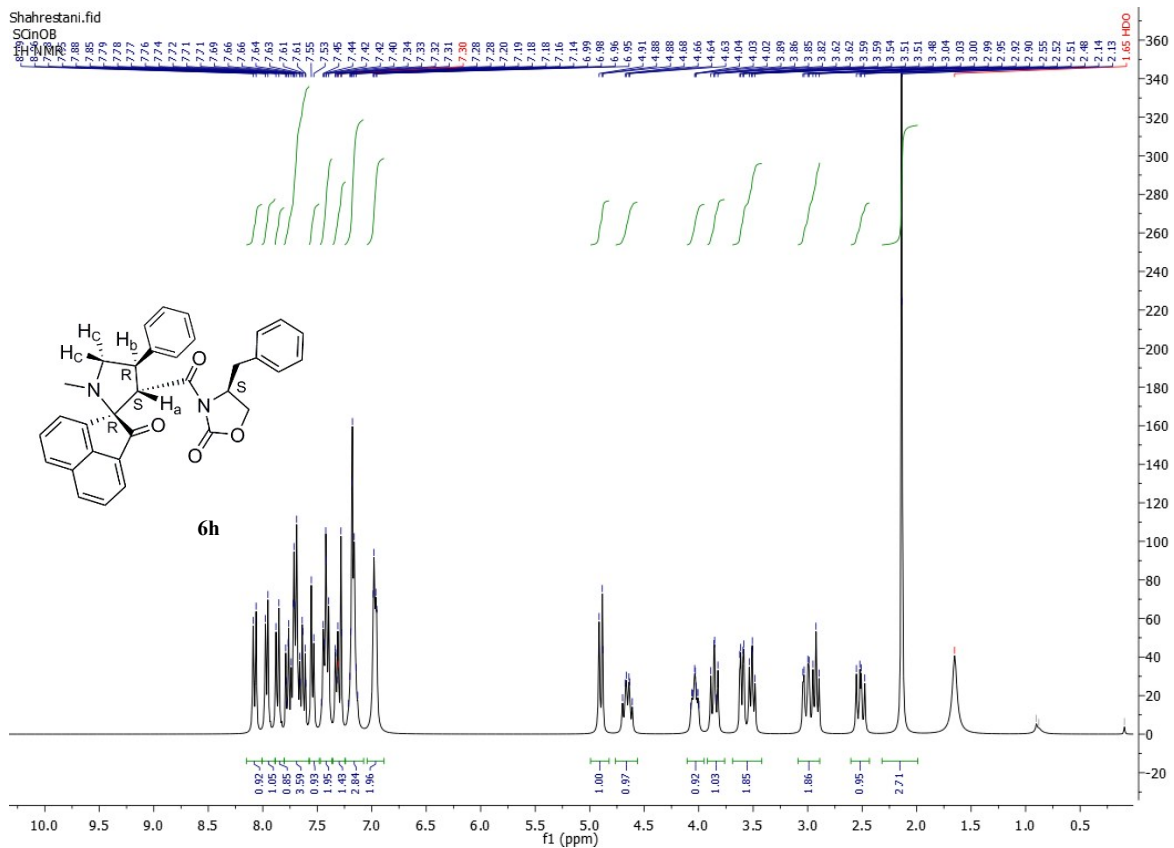


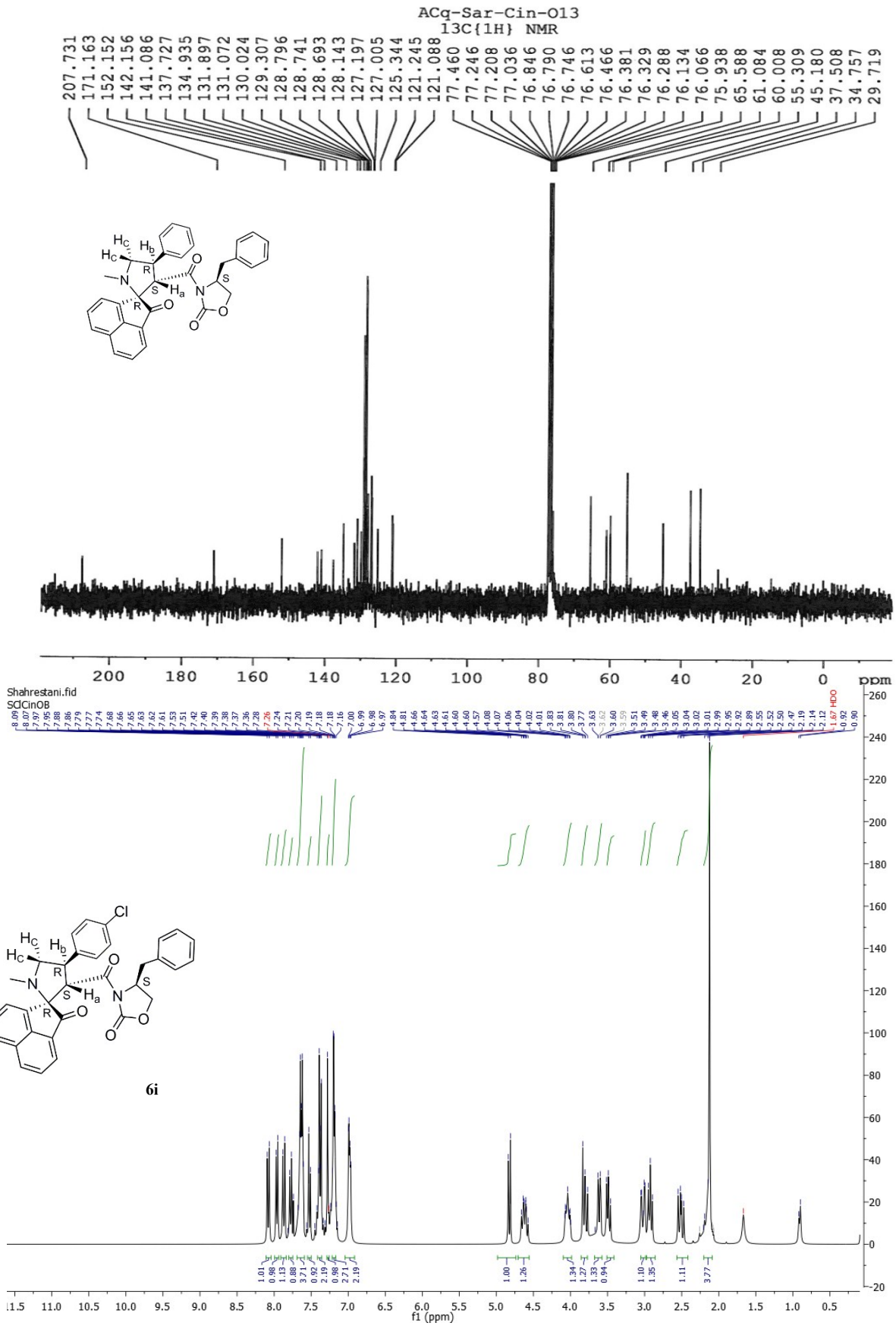
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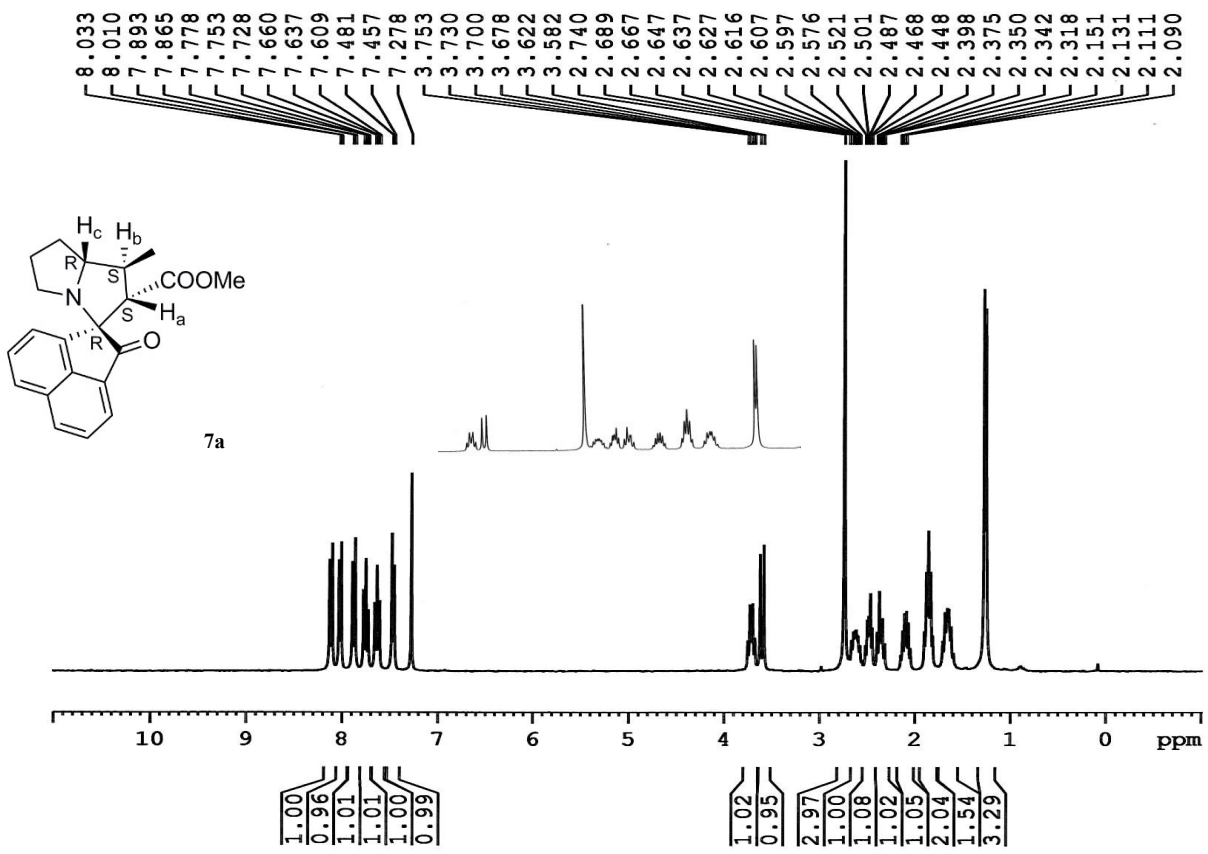
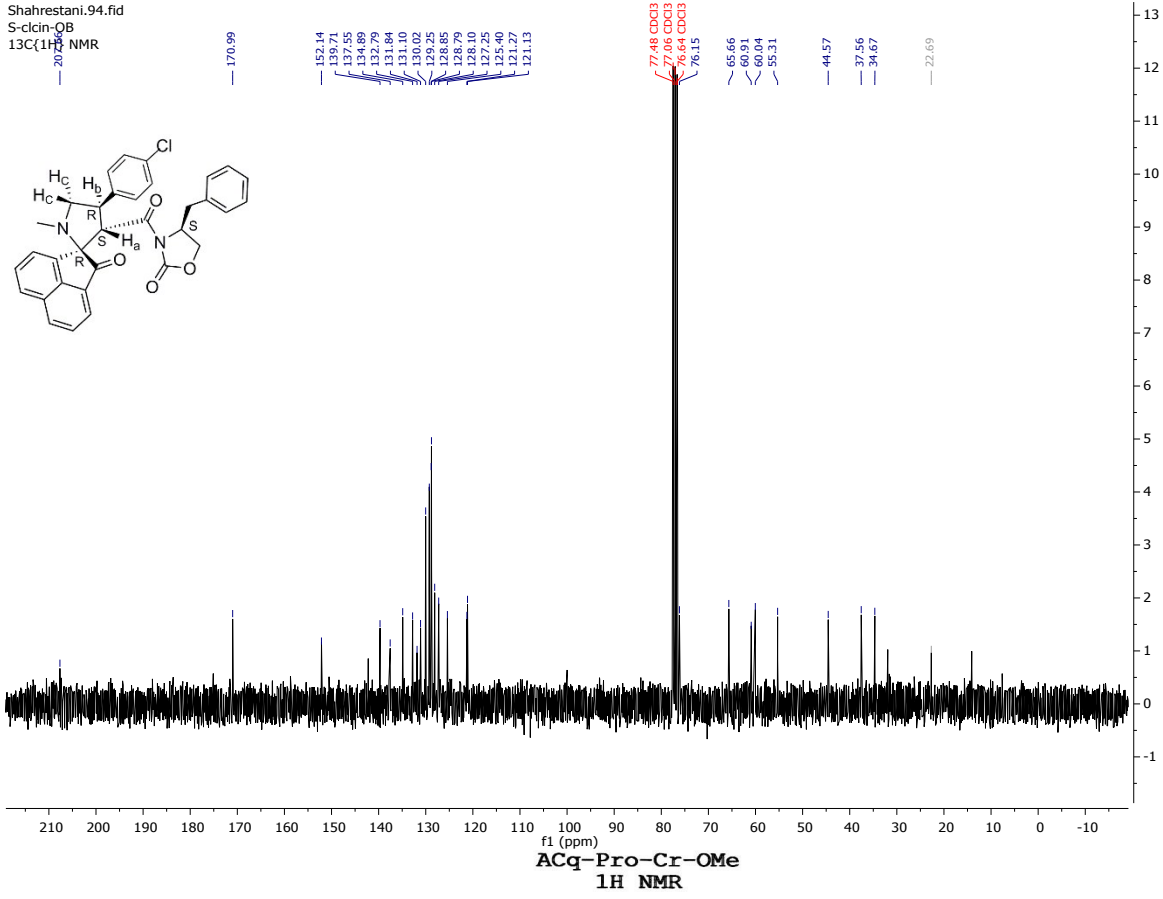
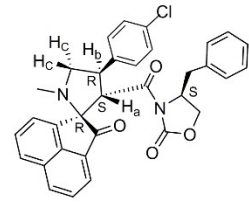
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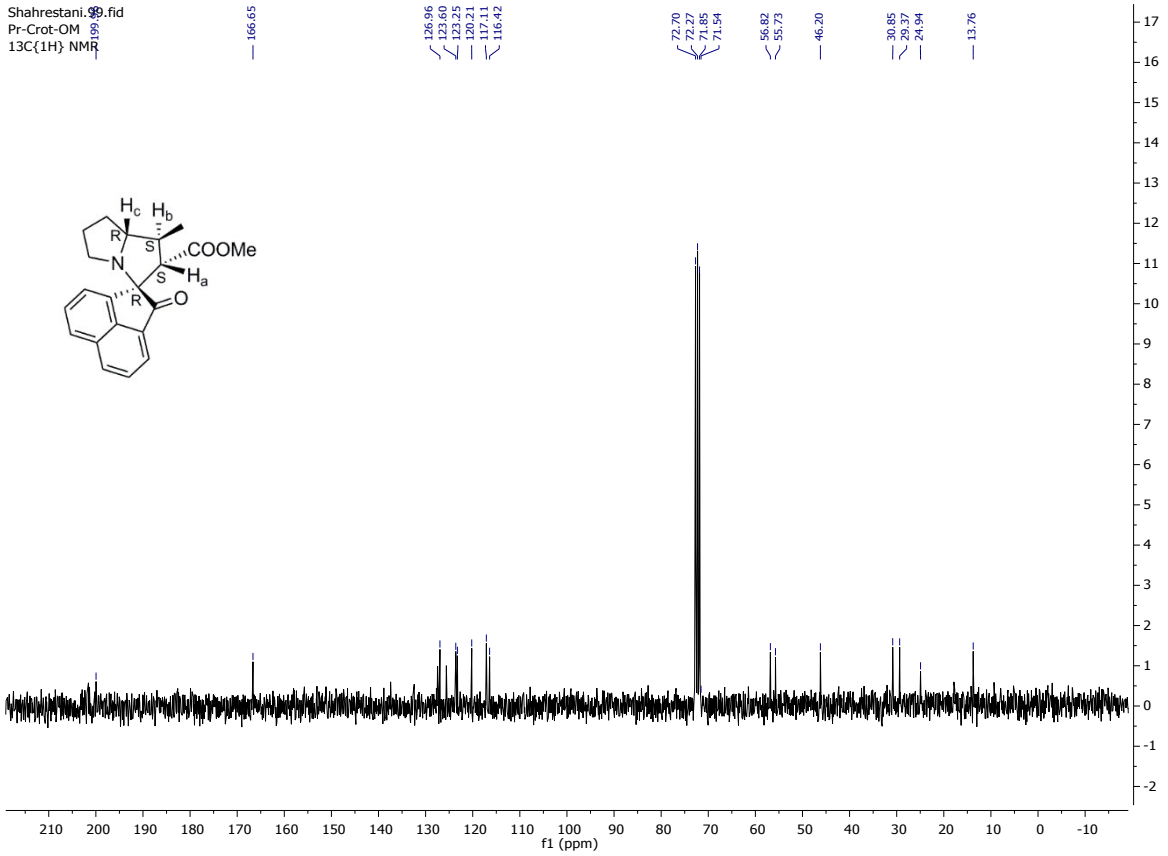




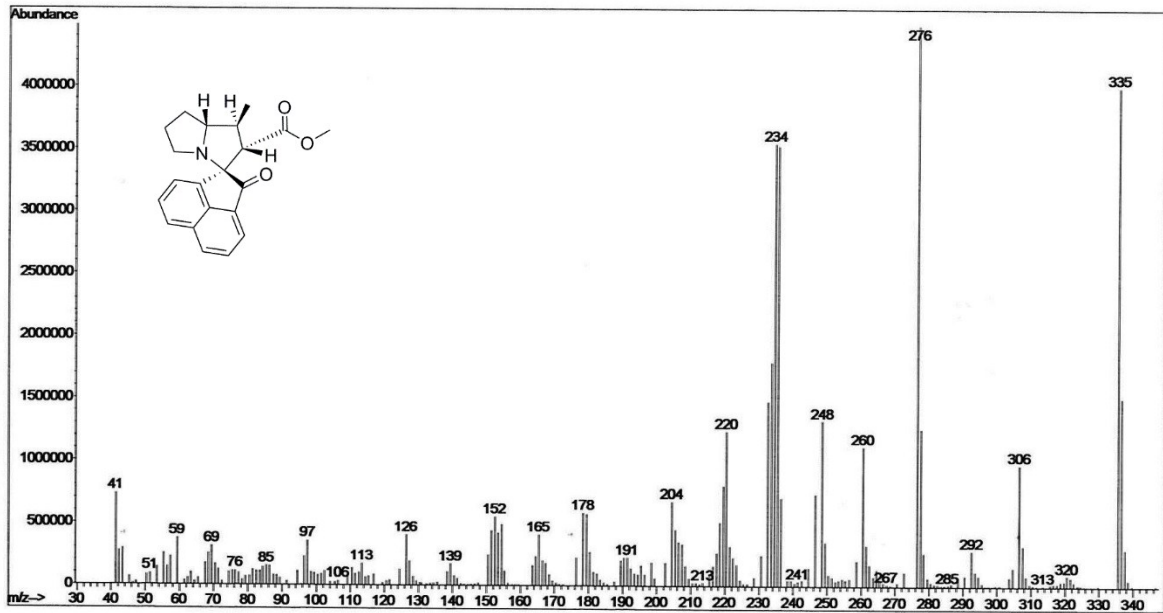
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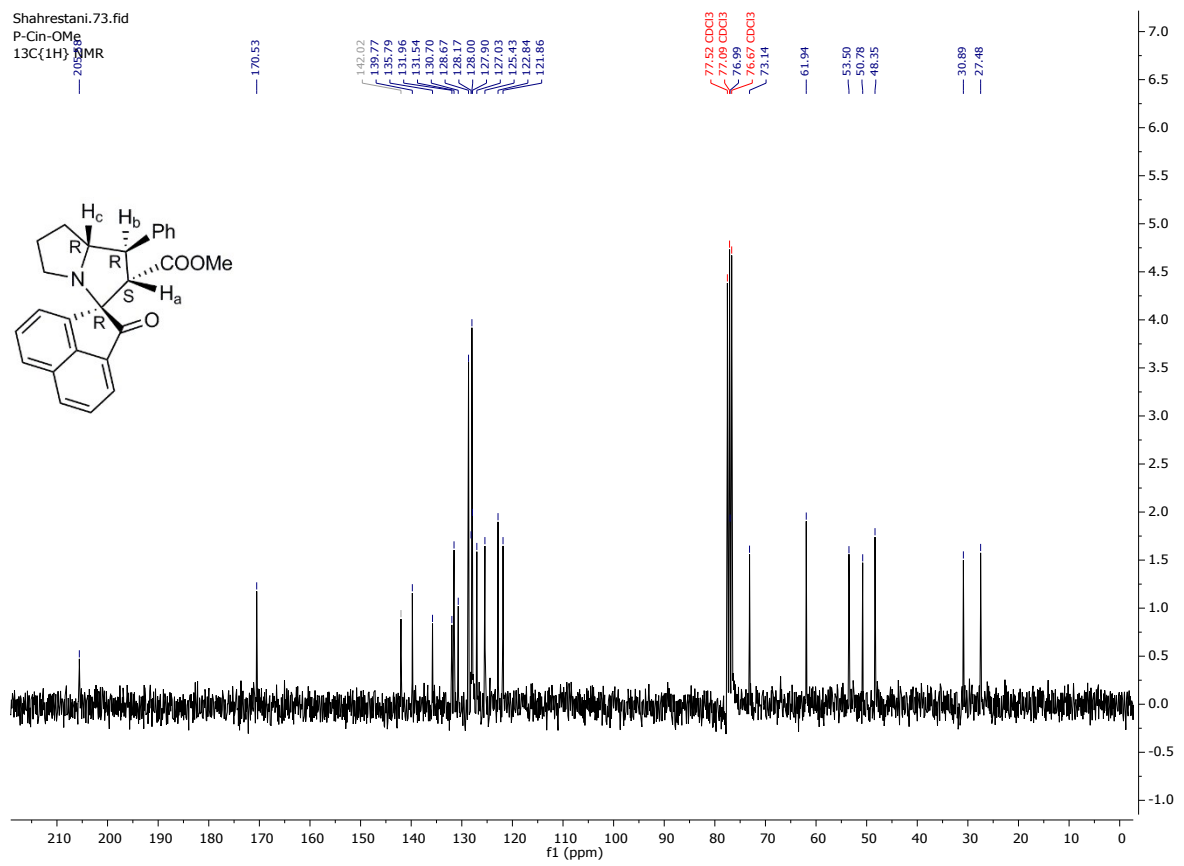
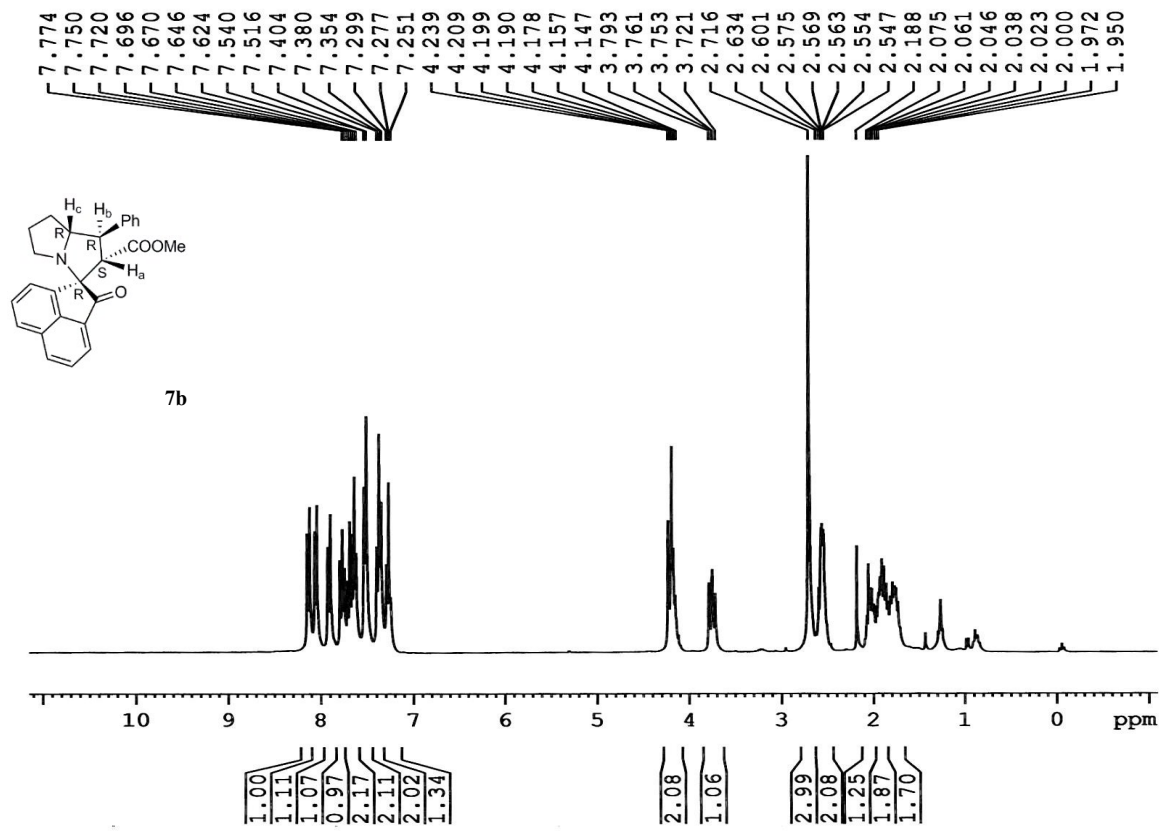


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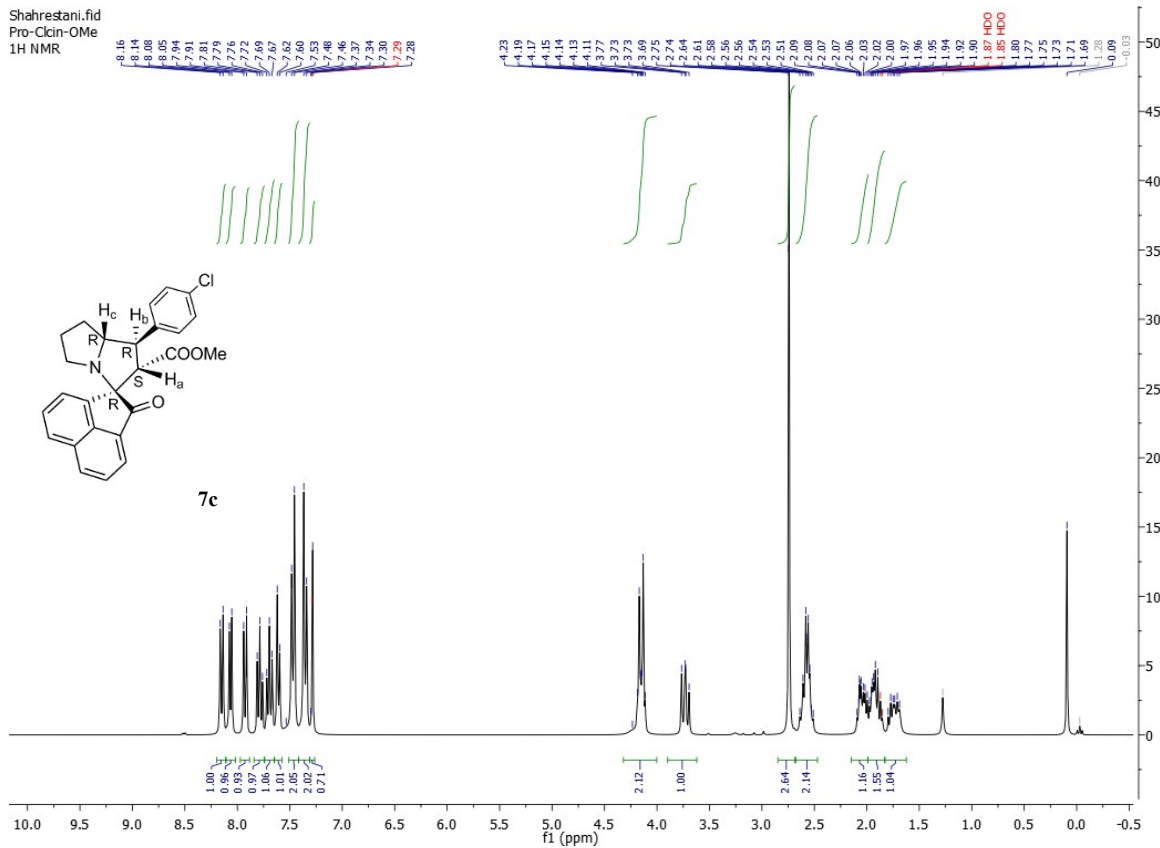
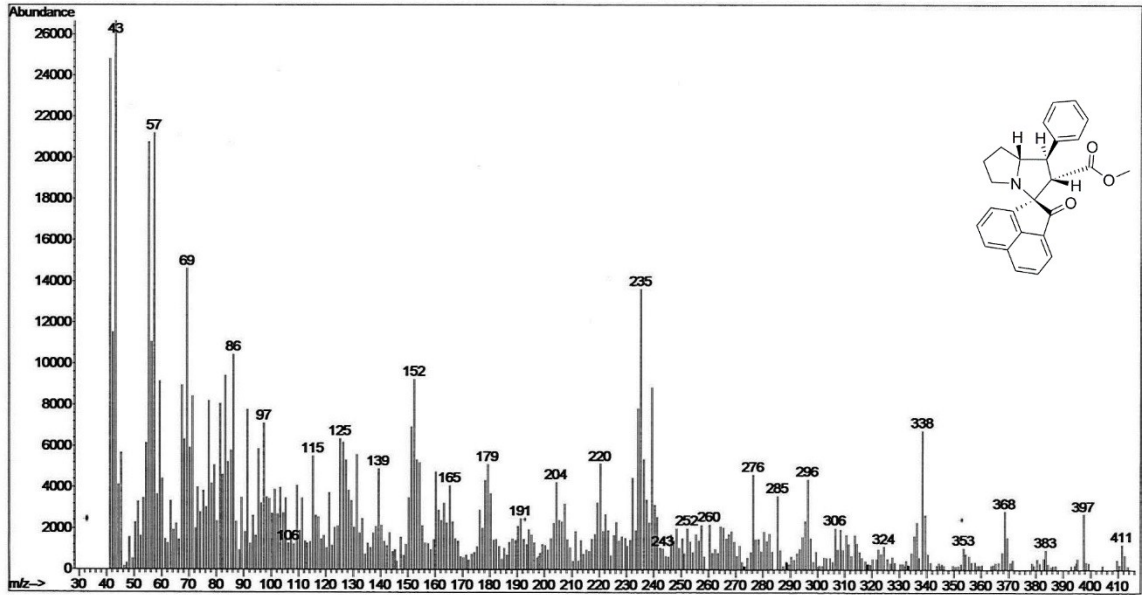


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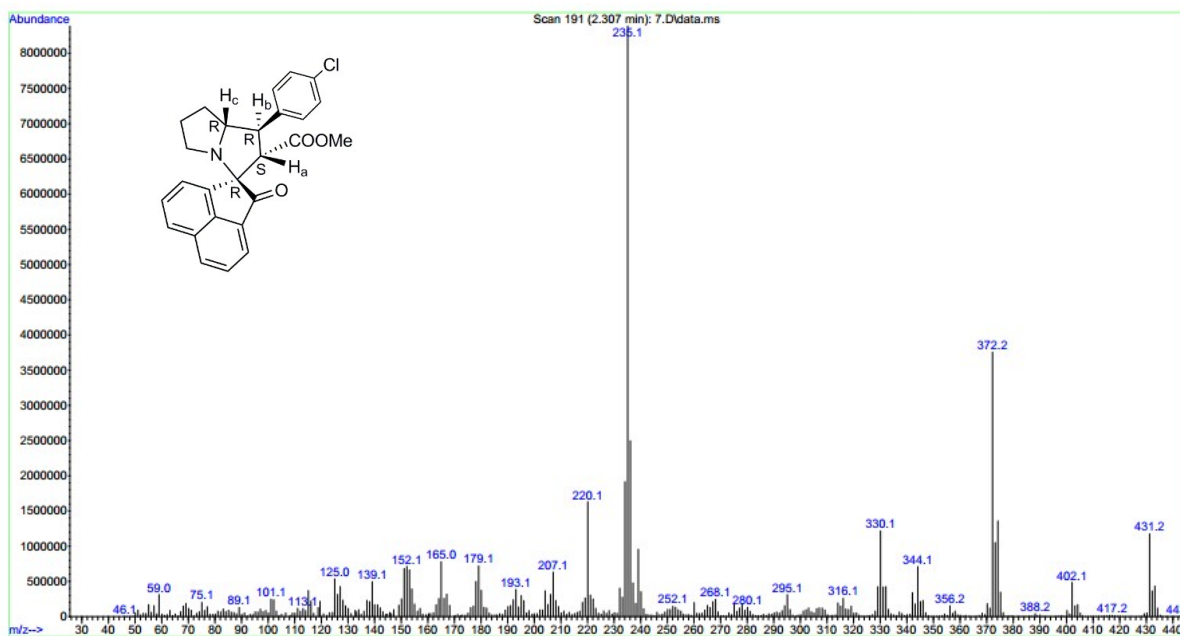
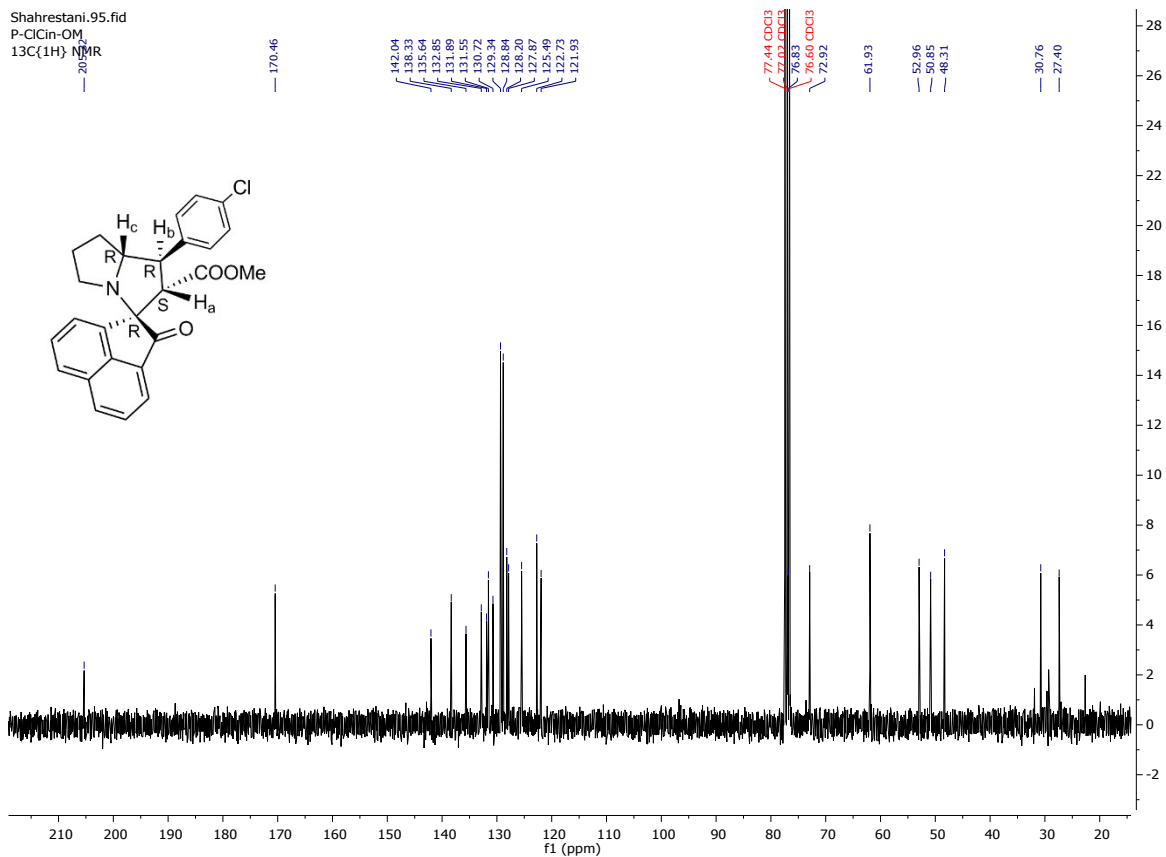


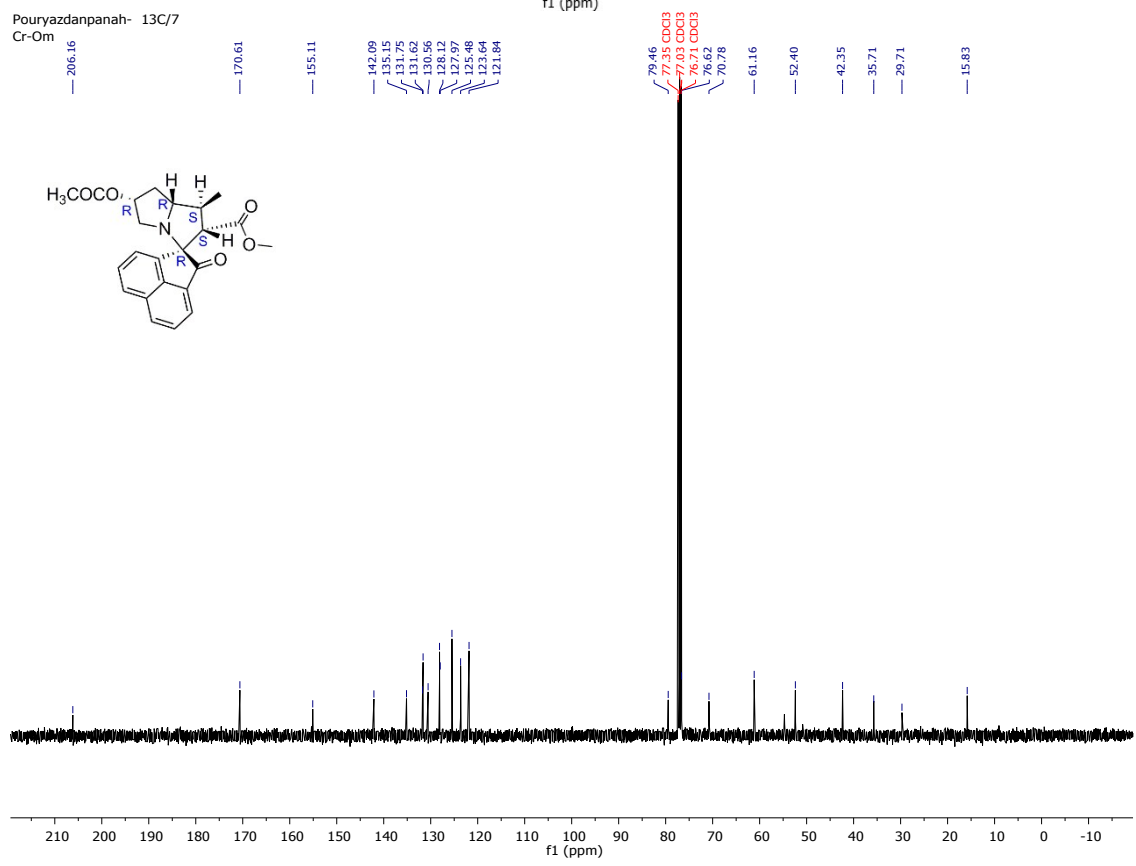
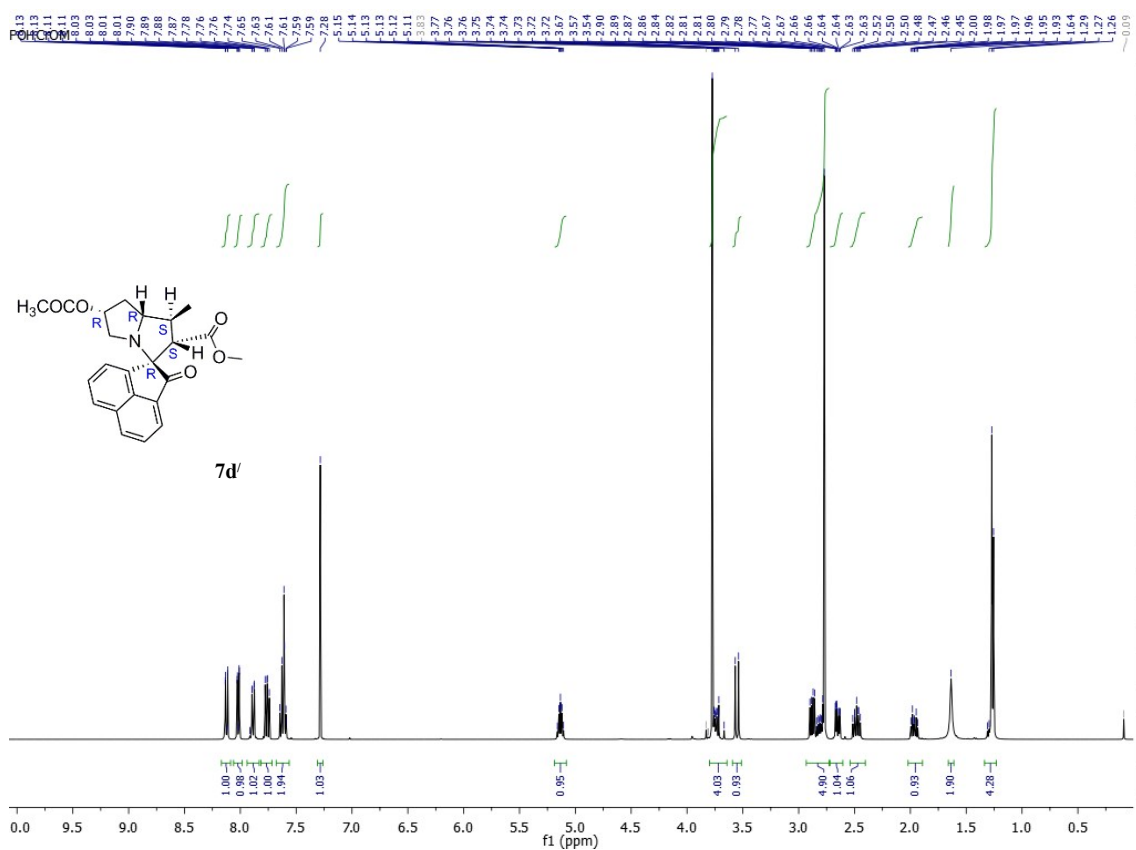


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 Operator :
 Acquired : 27 Nov 2014 8:26 using AcqMethod NORMAL
 Instrument : Instrumen
 Sample Name: B
 Misc Info :
 Vial Number: 1

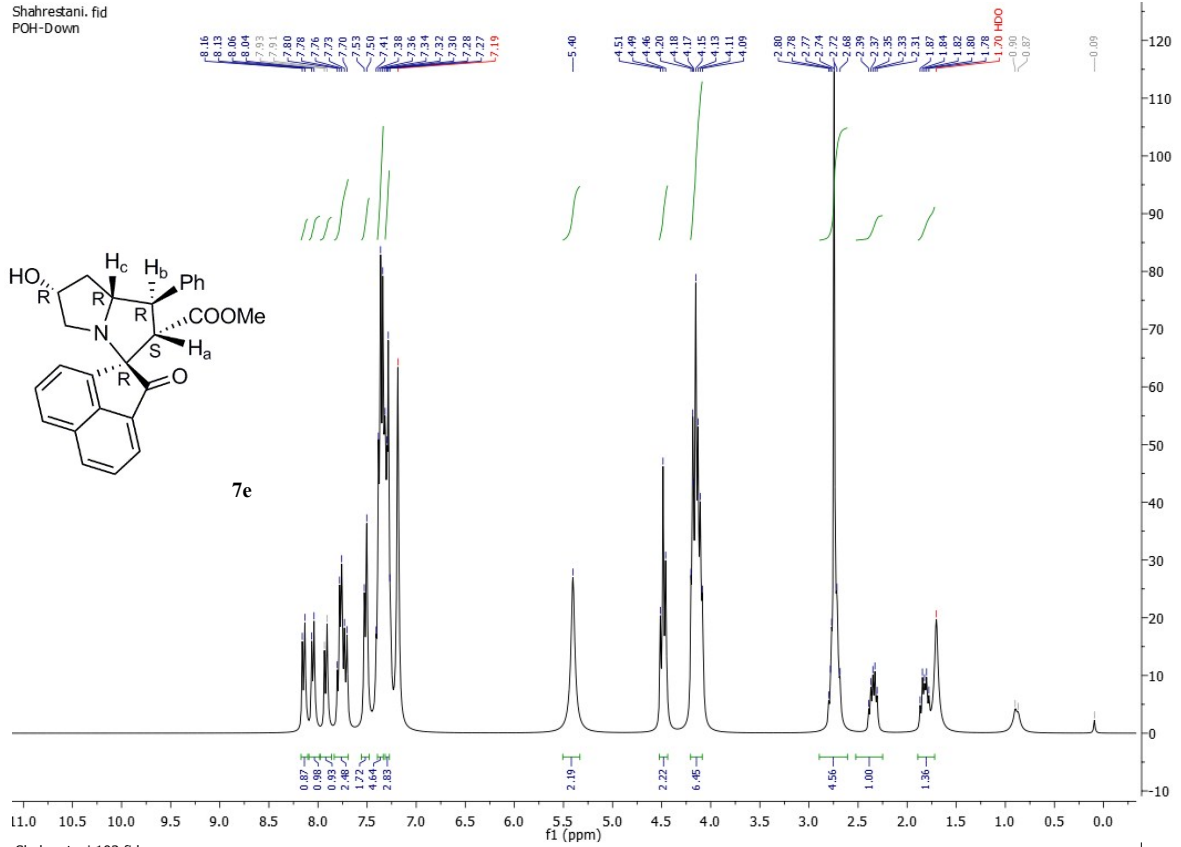


Shahrestani.95.fid
P-ClCin-OM
¹³C{¹H} NMR

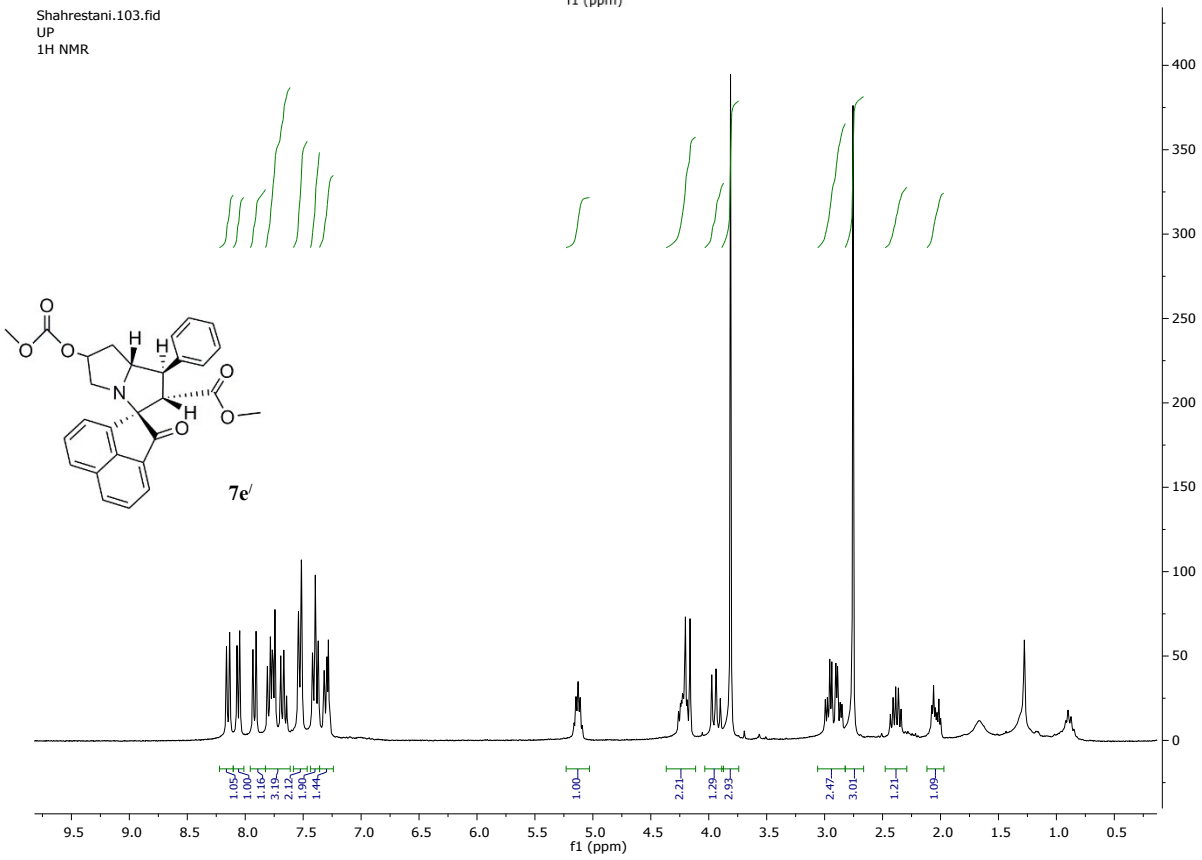


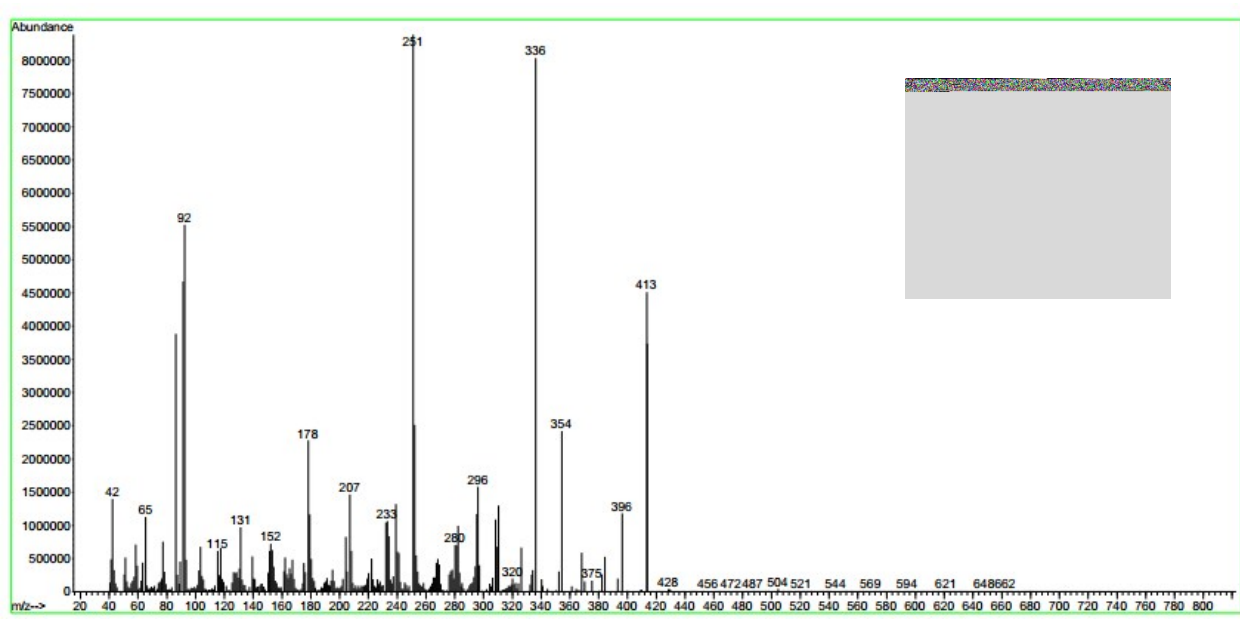
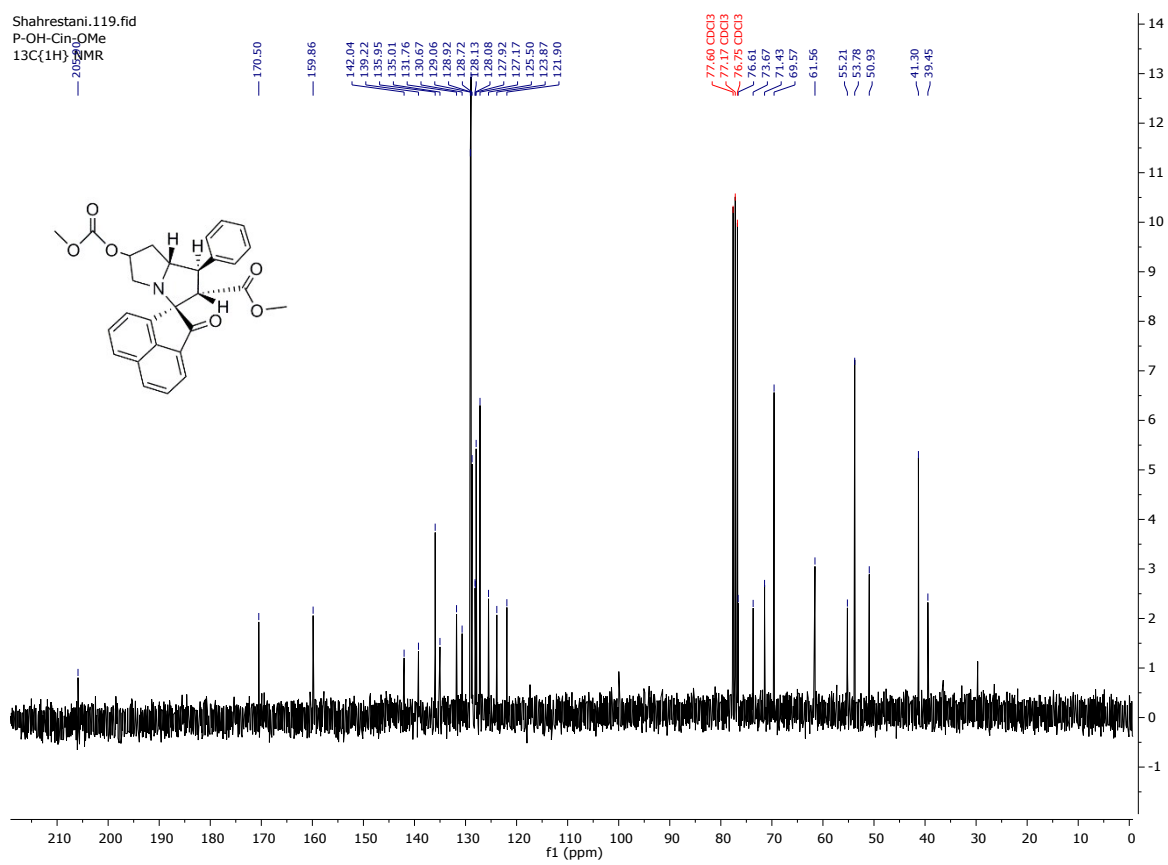


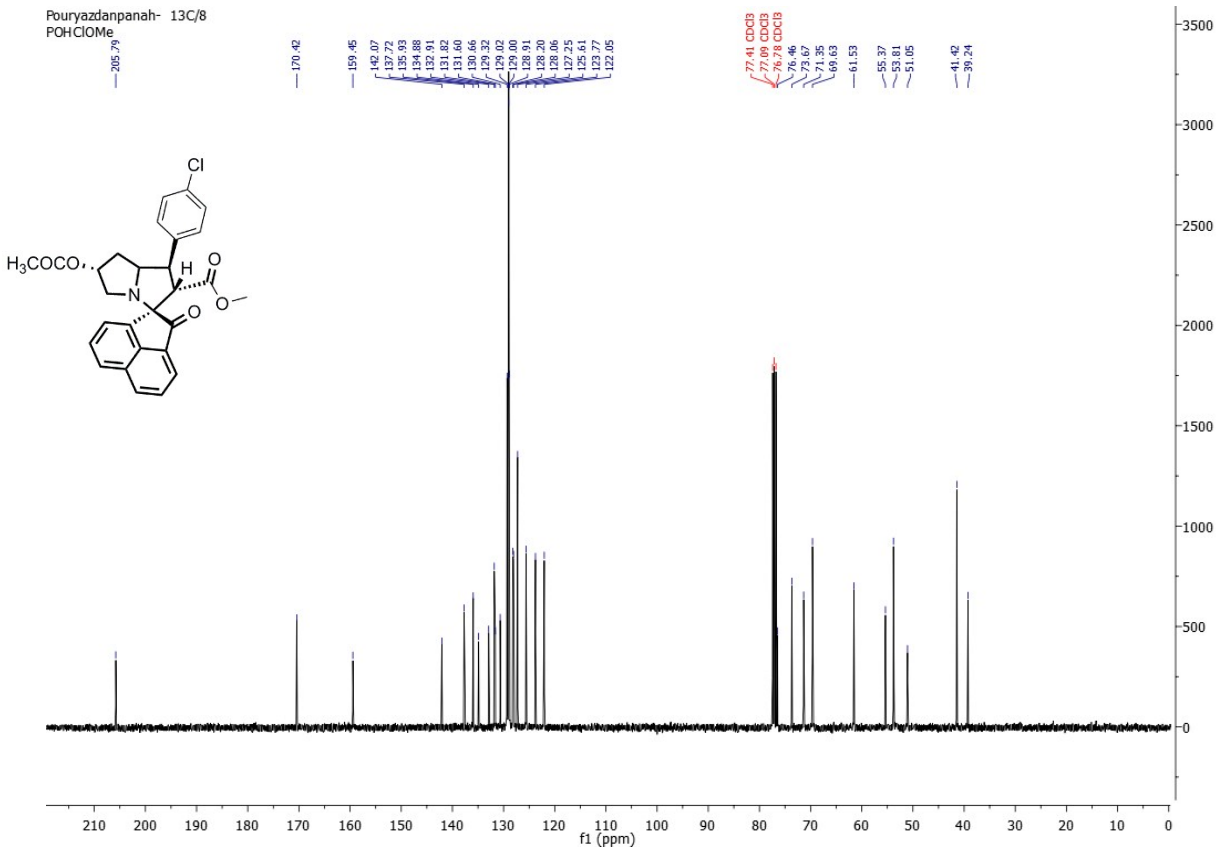
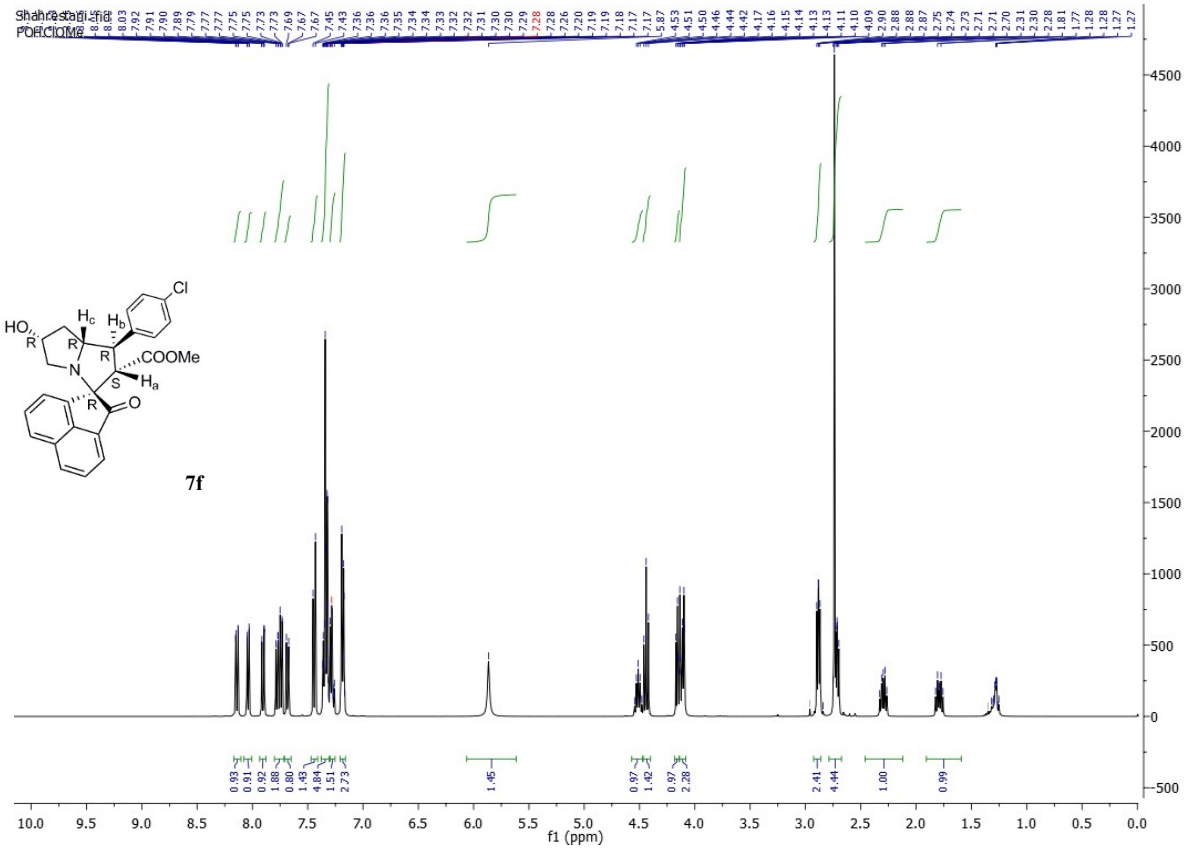
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POH-Down

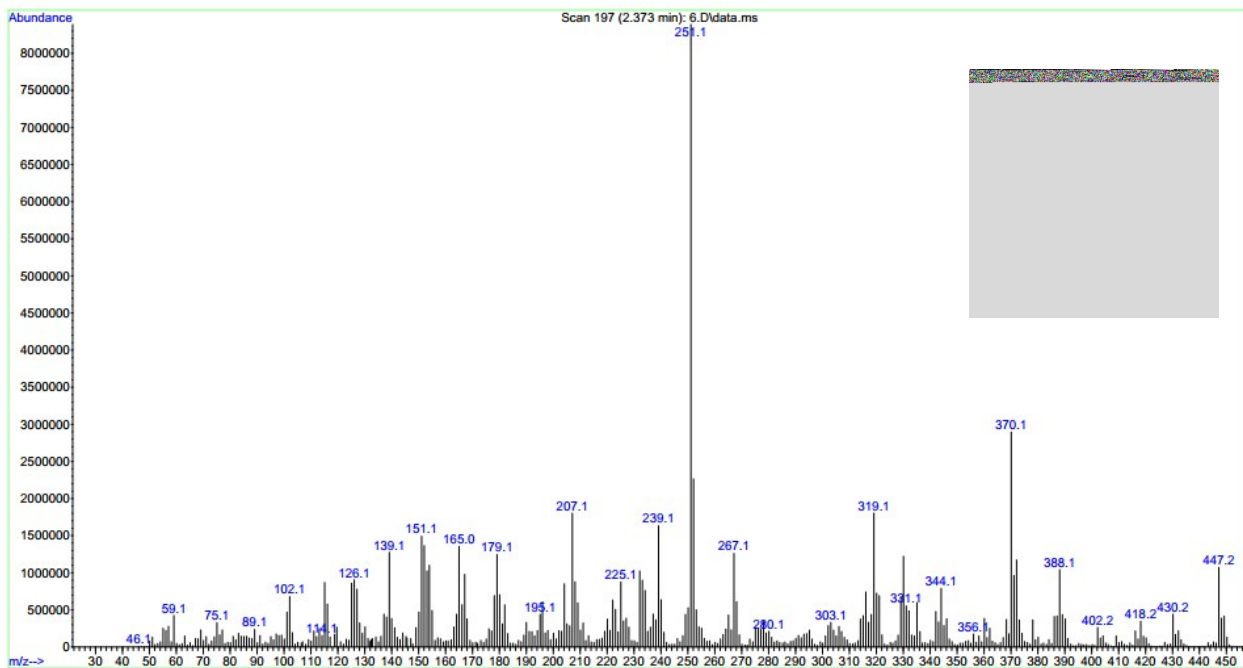


Shahrestani.103.fid
UP
1H NMR

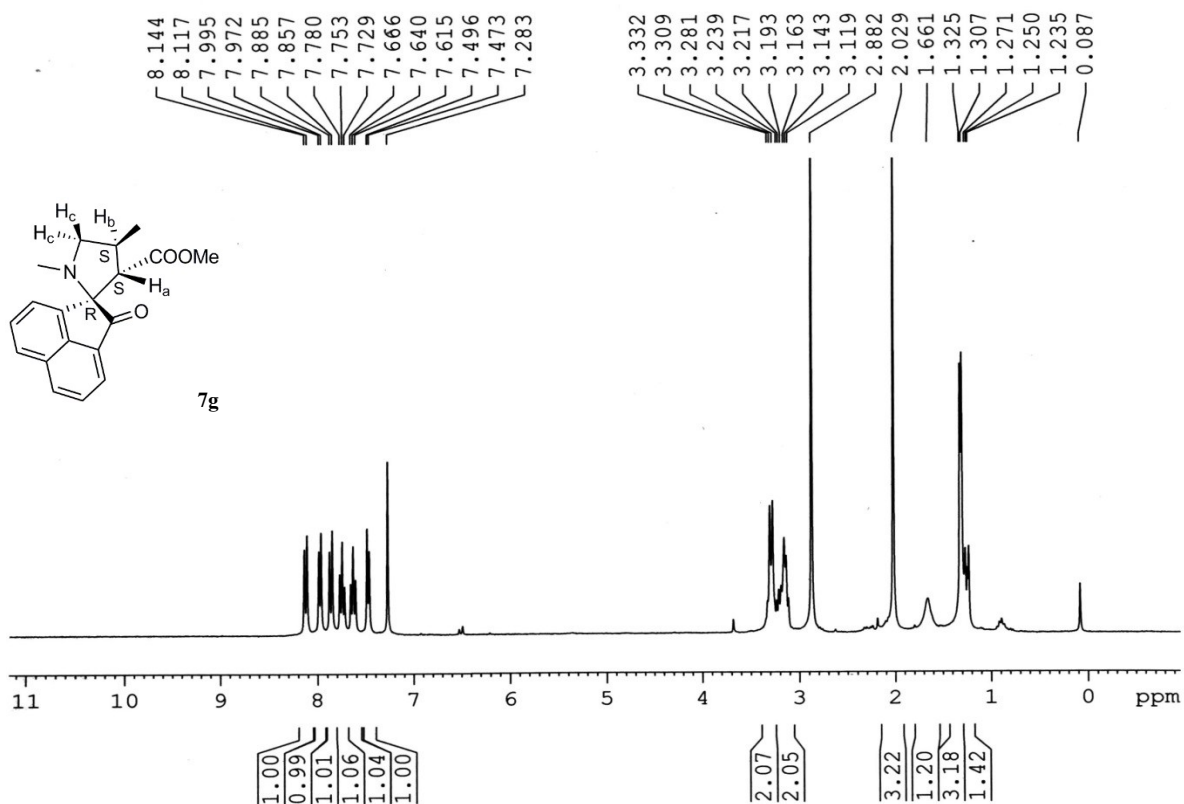


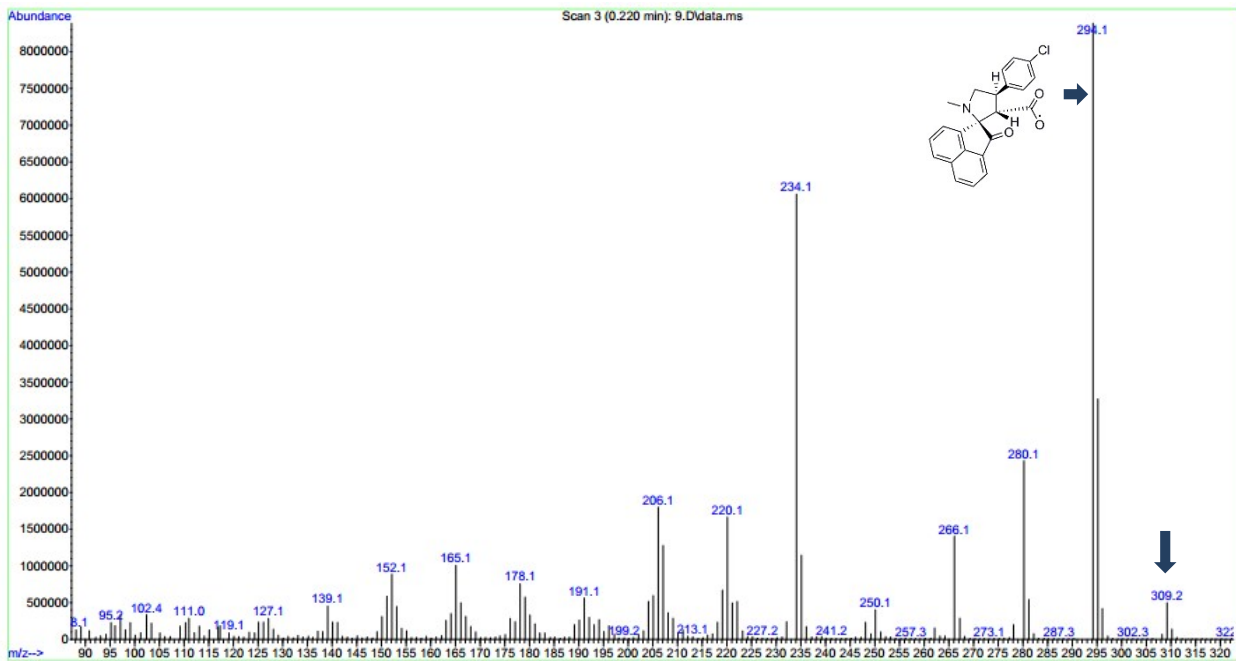
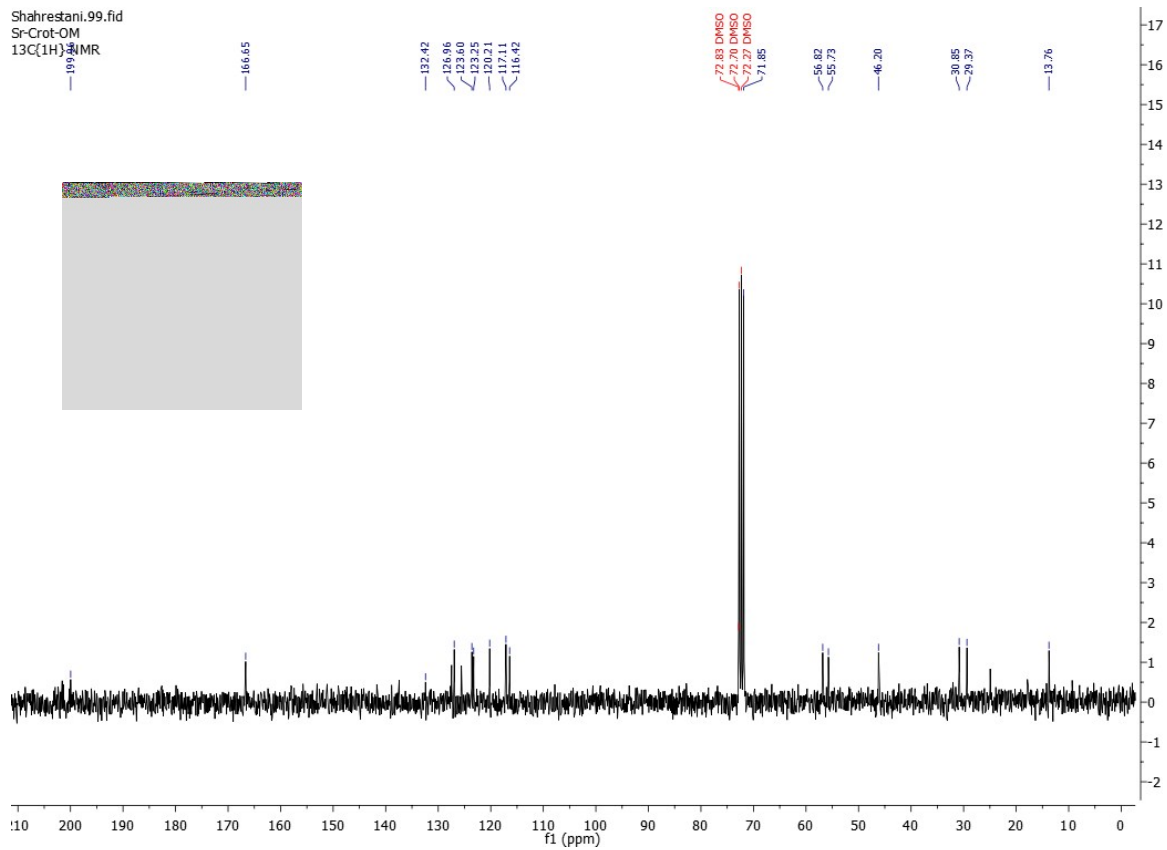


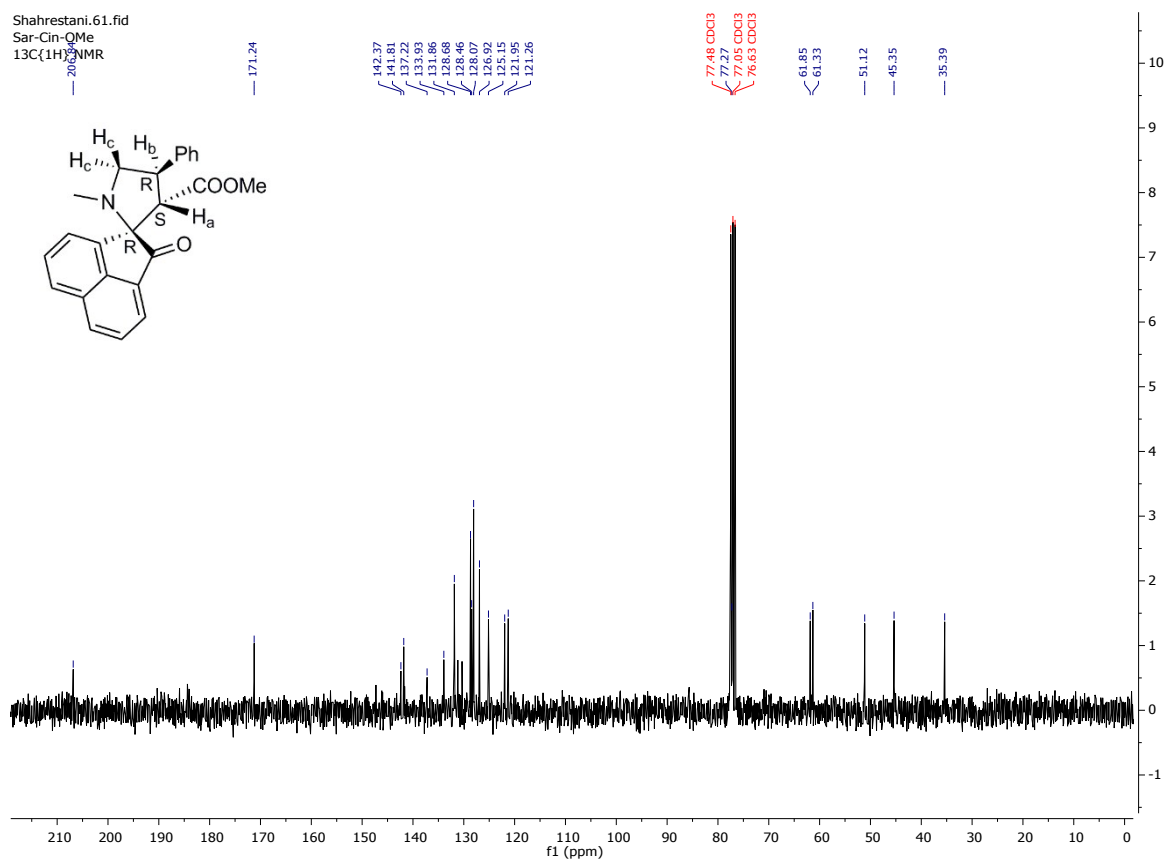
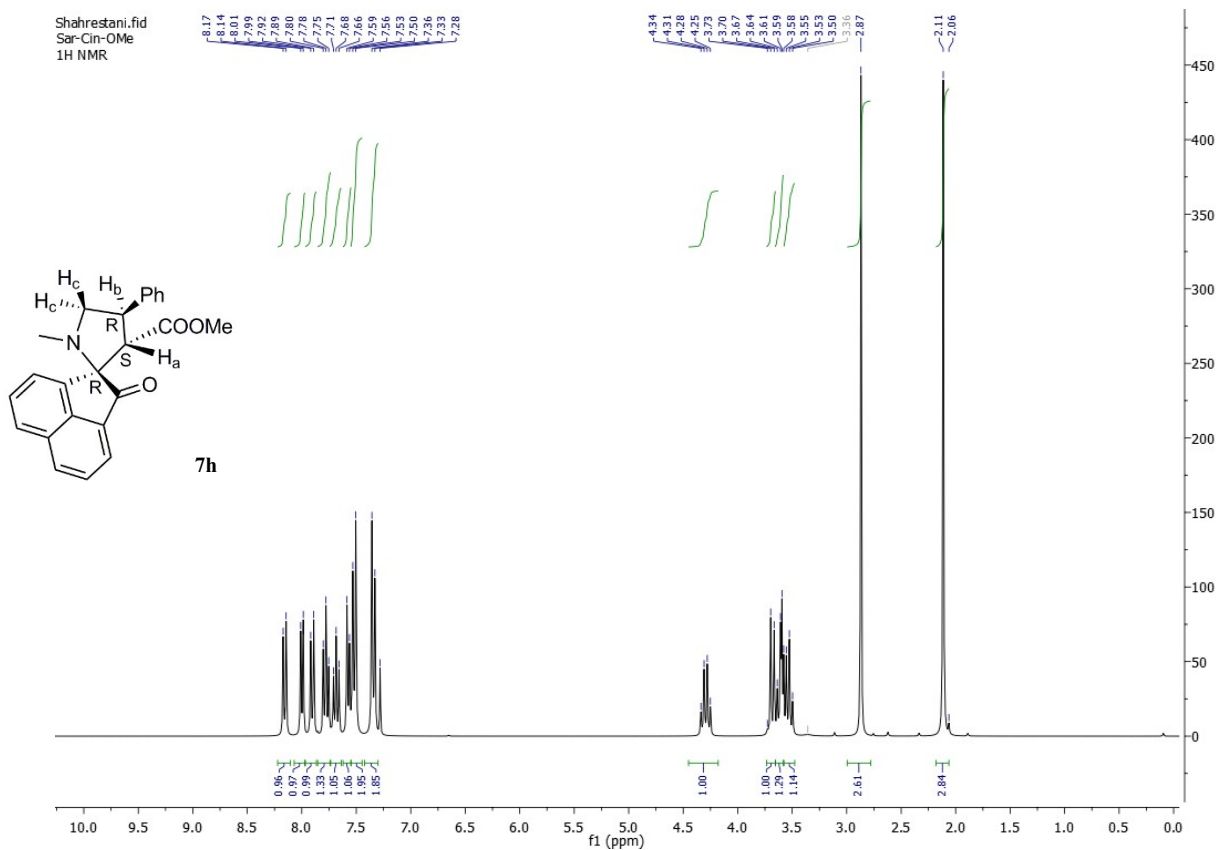




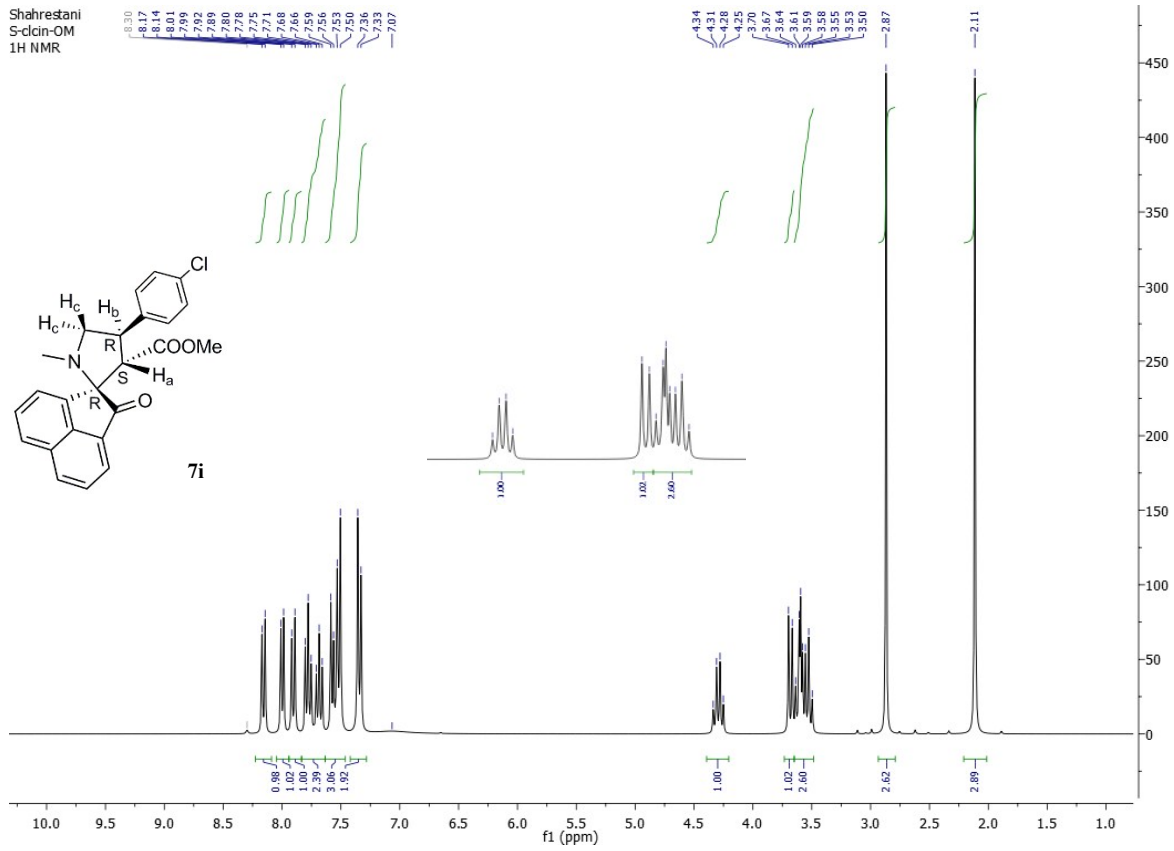
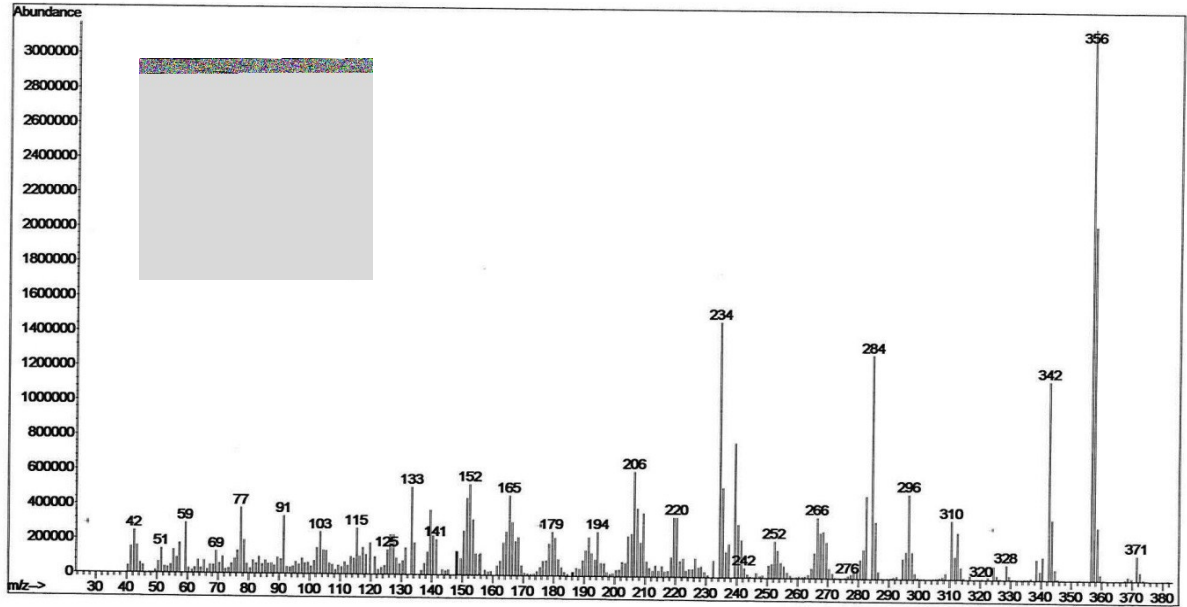
Sar-Crot-OMe
1H NMR



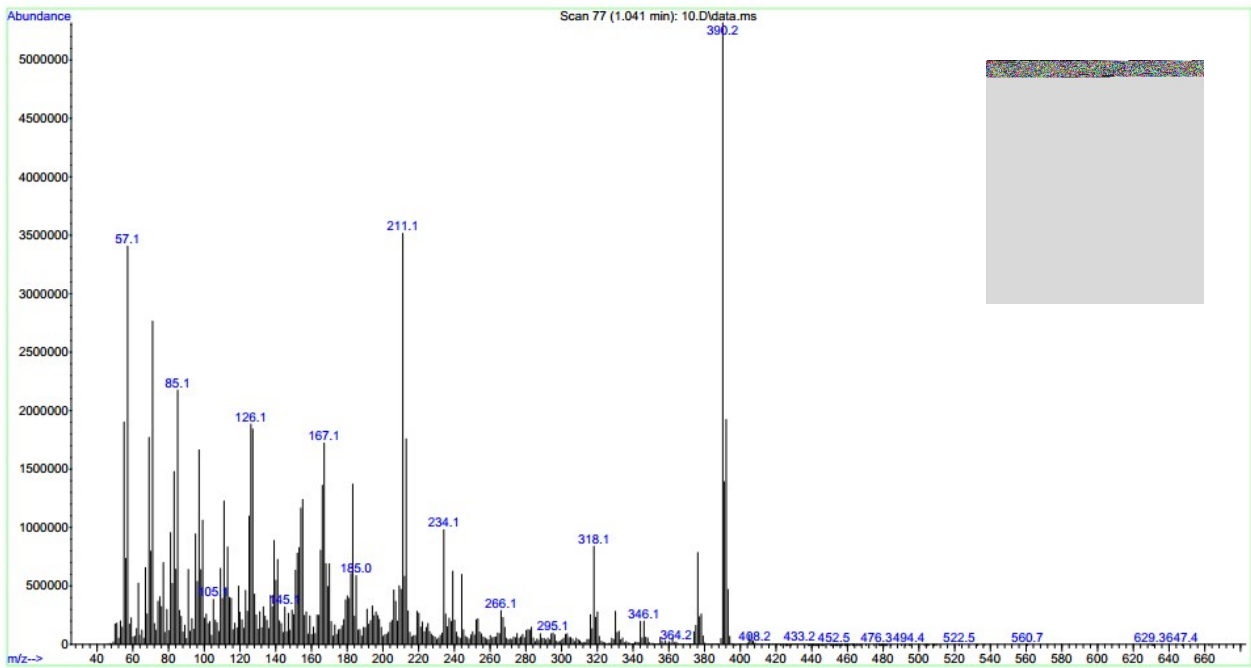
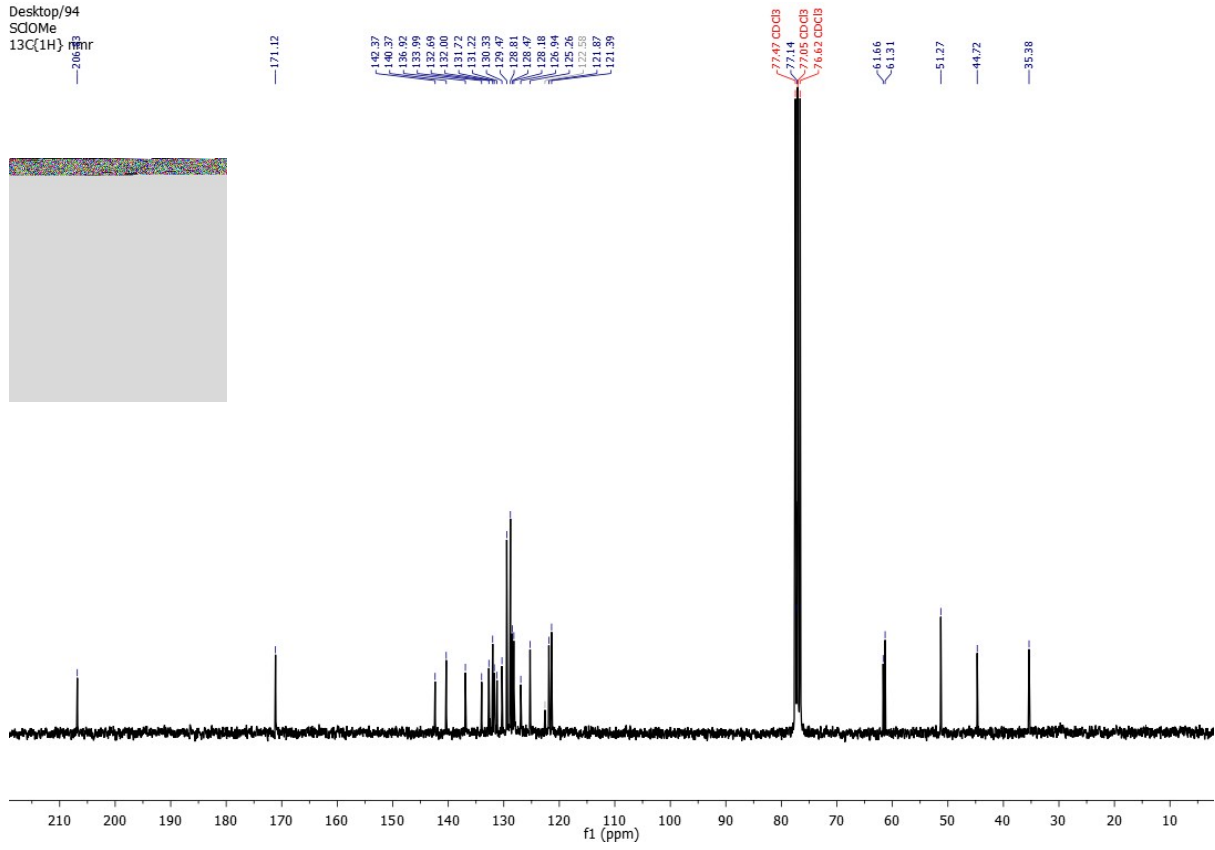


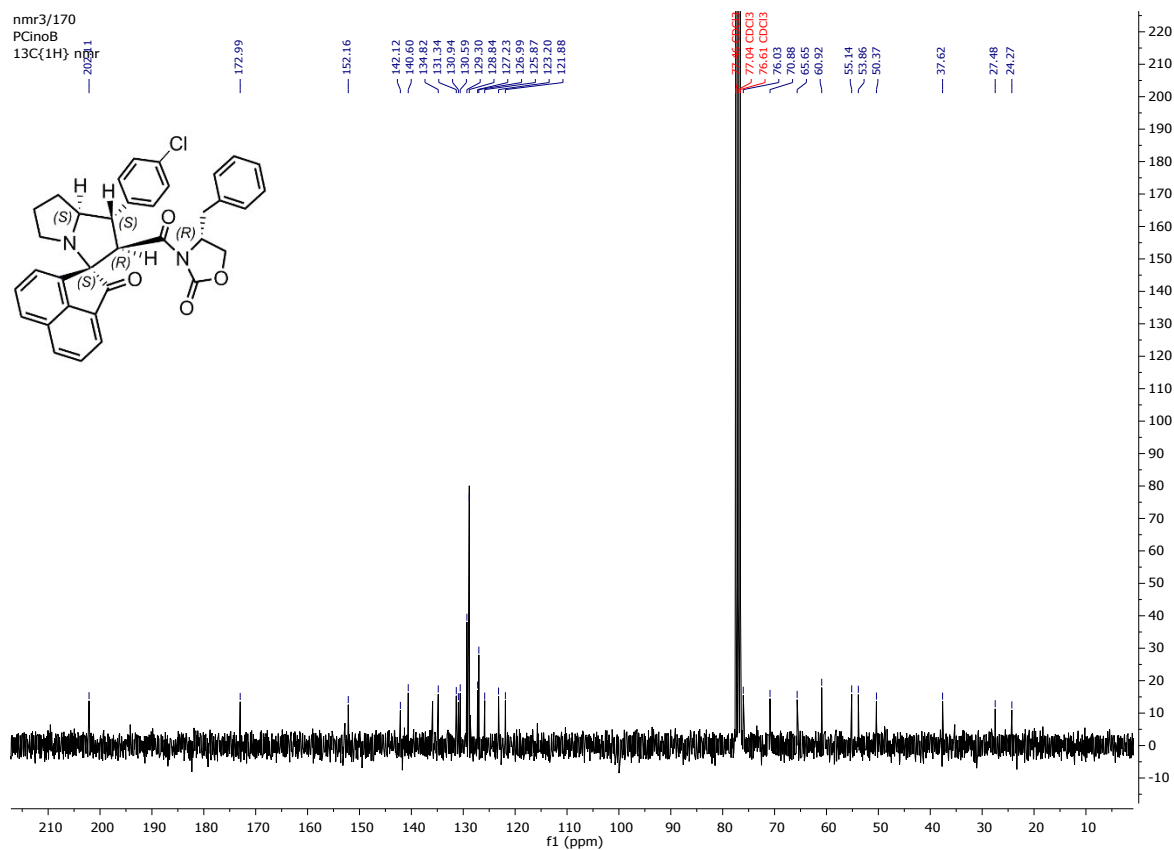
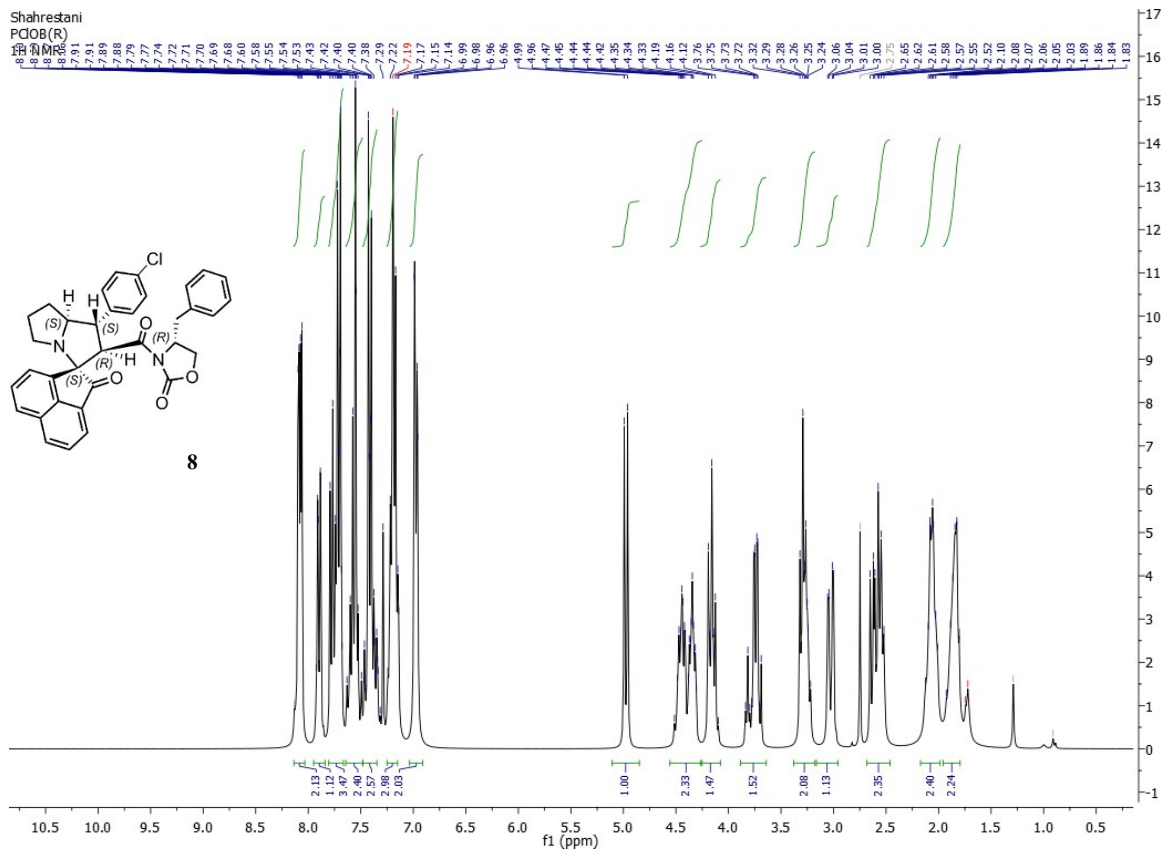


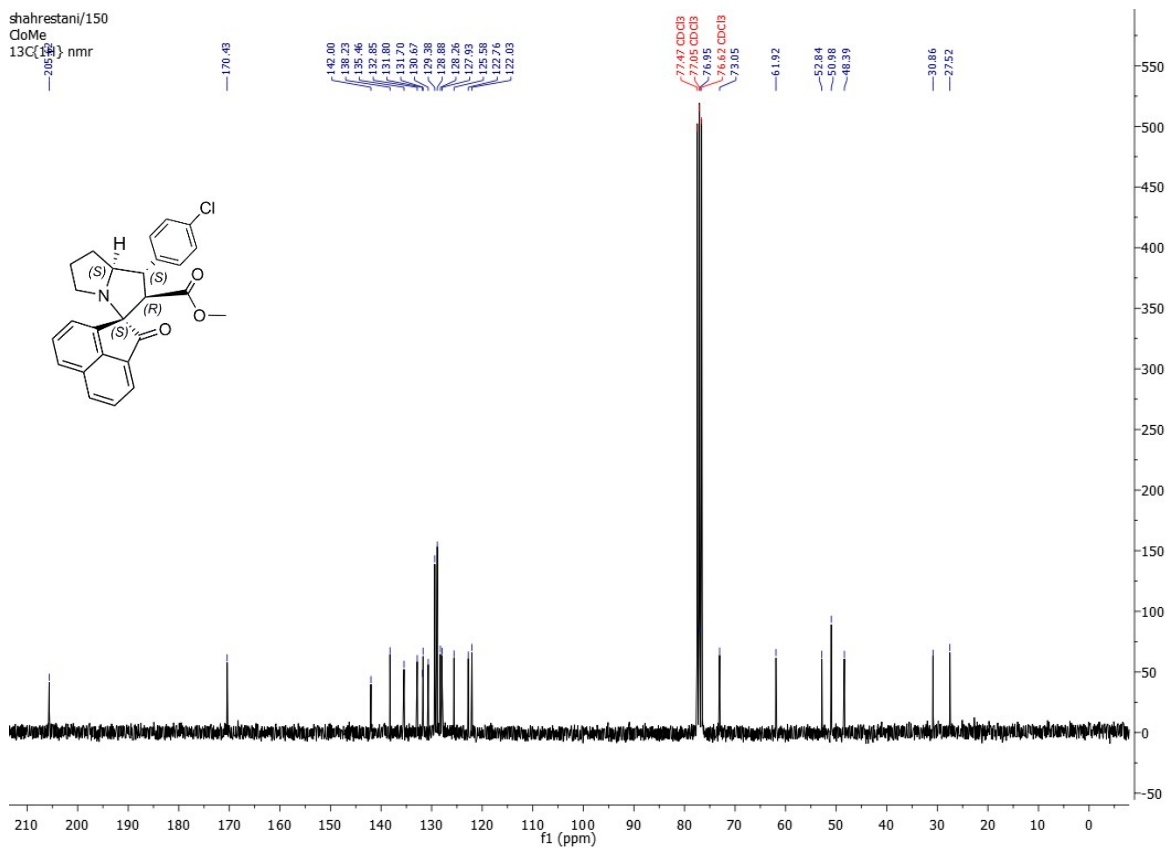
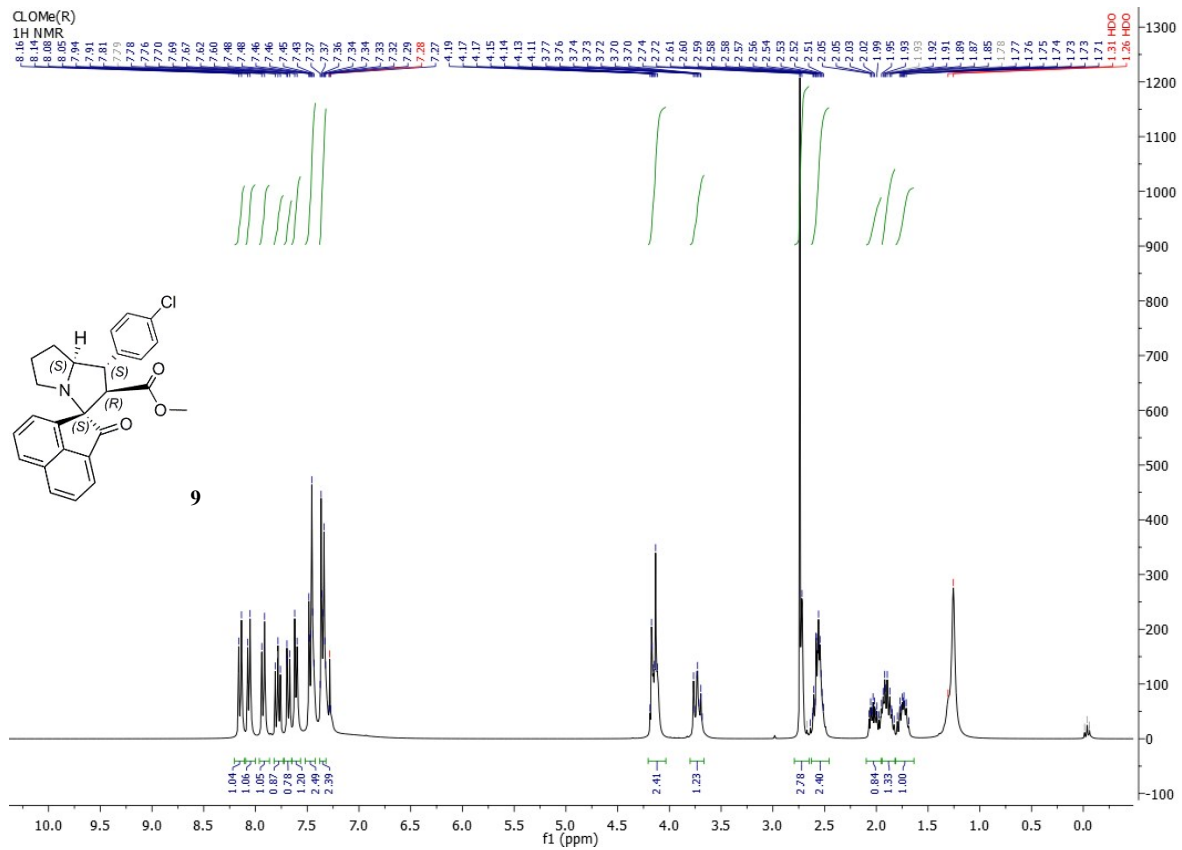
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 Operator :
 Acquired : 27 Nov 2014 8:29 using AcqMethod NORMAL
 Instrument : Instrumen
 Sample Name : C
 Misc Info :
 Vial Number : 1

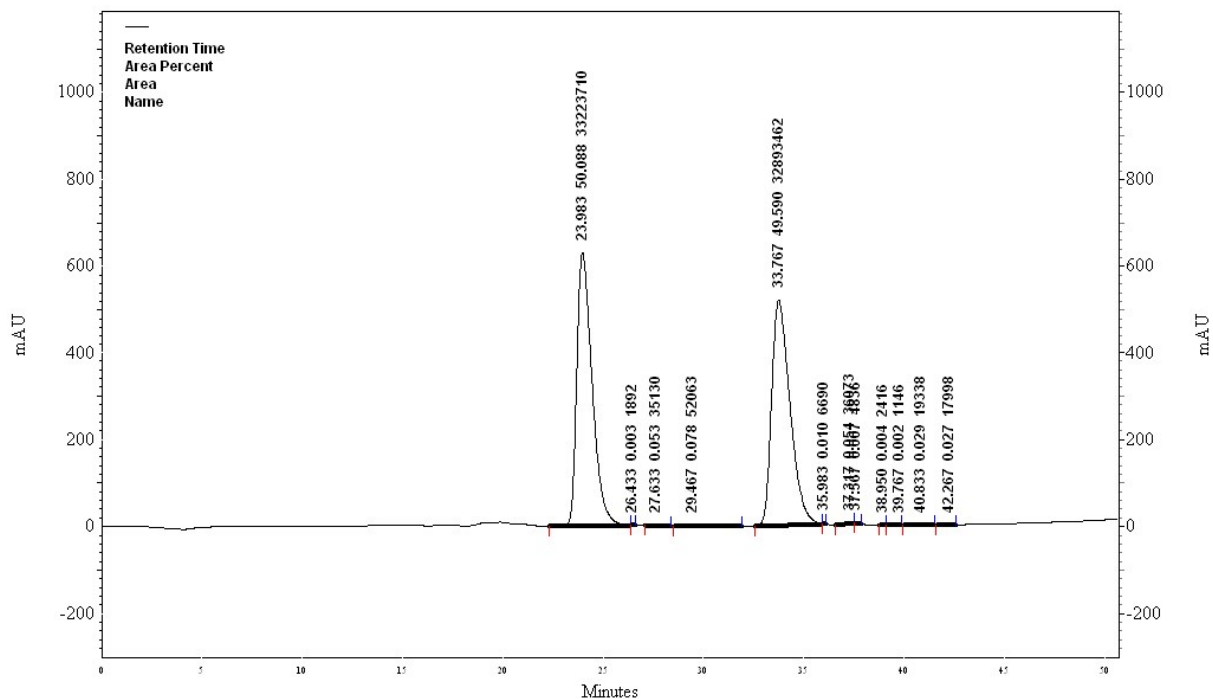


Desktop/94
SCIOME
13C(1H)

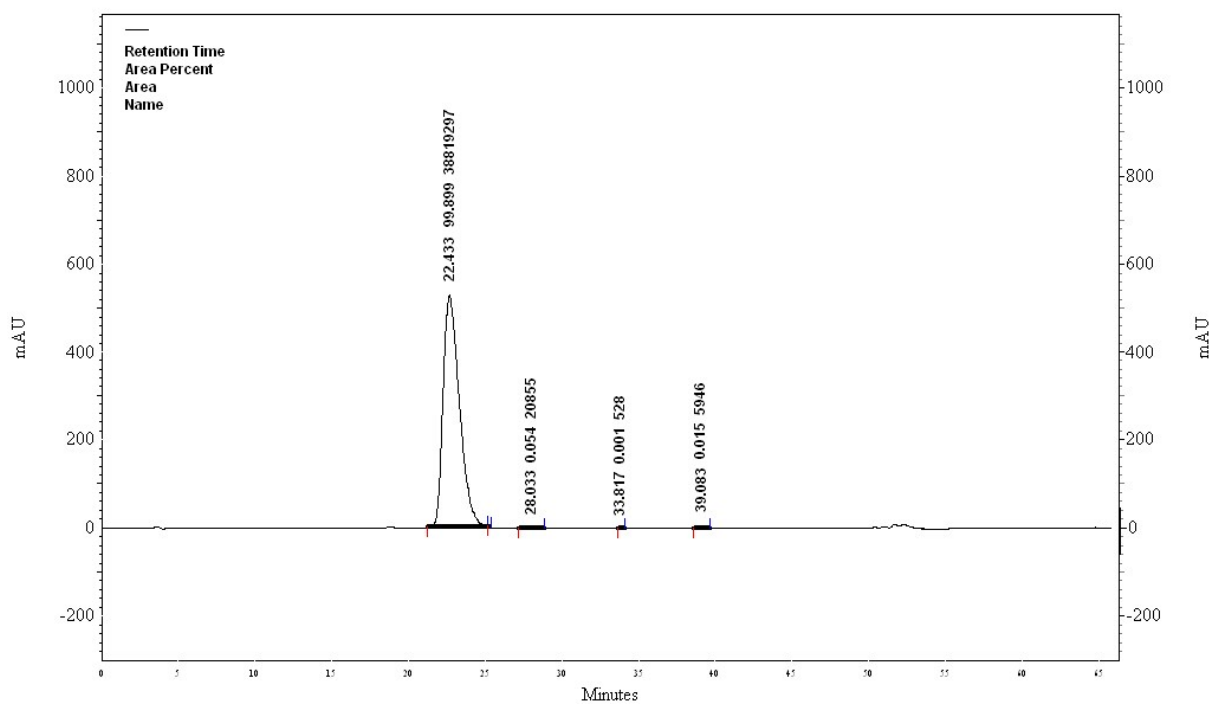




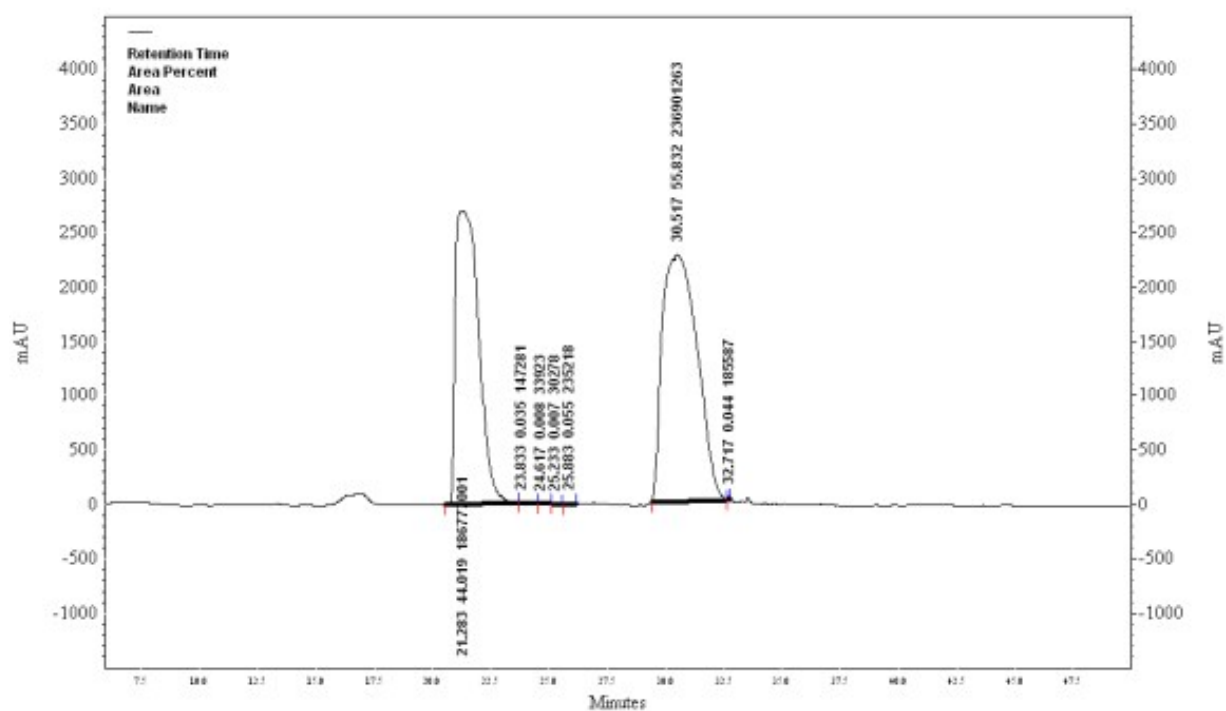




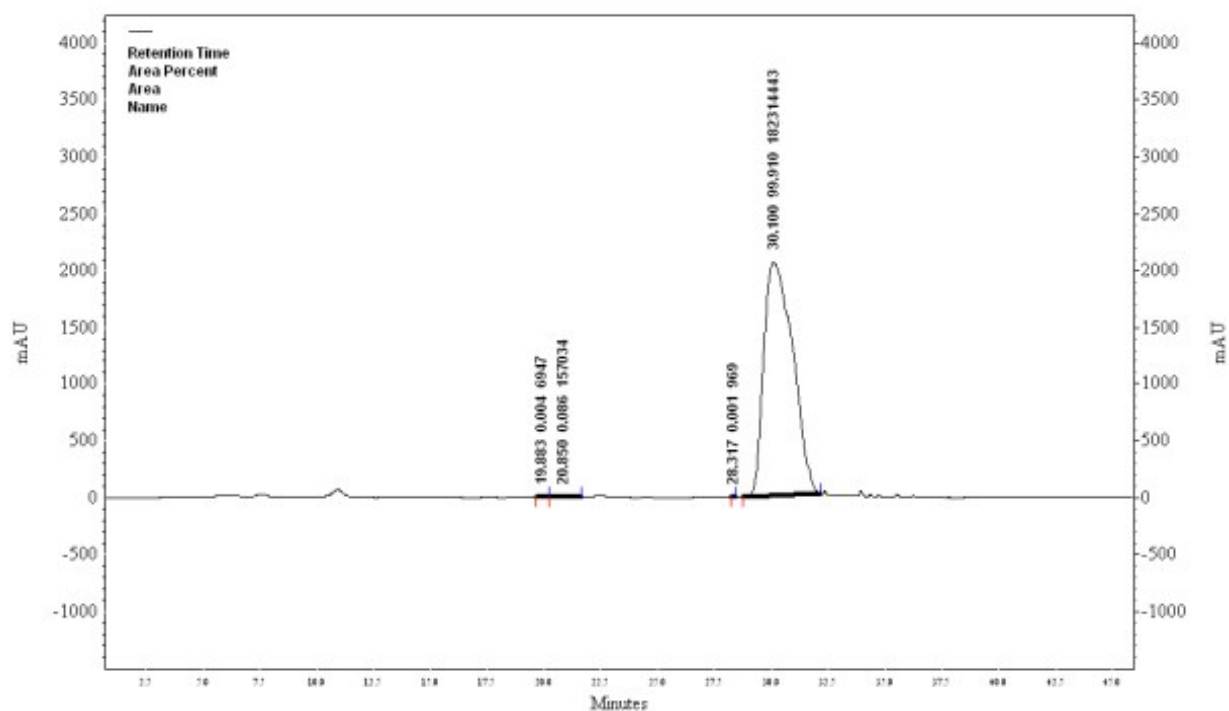
HPLC chromatogram of racemic product **7a**.



HPLC chromatogram of chiral product **7a**



HPLC chromatogram of racemic product **9**



HPLC chromatogram of chiral product **9**

Z-Matrix data

Dipolar 1

C	-2.42648000	-2.12521900	0.04676700
C	-1.32939300	-1.29246800	0.01369000
C	-1.50704500	0.10317700	0.00249300
C	-2.76831900	0.71935900	0.01532400
C	-3.88916300	-0.15630800	0.05325400
C	-3.71548800	-1.53201600	0.06906100
H	-2.30899000	-3.20469700	0.05409200
C	-0.25351600	0.80052700	-0.03649600
C	-2.78764200	2.14573600	-0.01513800
H	-4.89269400	0.26152200	0.06797800
H	-4.59059800	-2.17515500	0.09674900
C	-1.59194500	2.83186900	-0.06426100
C	-0.32115300	2.18626300	-0.07972300
H	-3.73283000	2.68075800	-0.00475400
H	-1.60721600	3.91815700	-0.09496200
H	0.56210200	2.81238800	-0.13538600
C	0.14512700	-1.55461600	-0.02340400
C	0.76877600	-0.23846800	-0.04043500
O	0.70287000	-2.66288100	-0.03130600
N	2.13665100	-0.09893300	-0.03975100
C	2.77346300	1.24883700	0.00006000
C	4.24789000	0.95854000	0.31274200
C	3.05081800	-1.05363000	-0.09334100
H	2.27632300	1.85115900	0.76033000
C	4.44286900	-0.51505500	-0.11201100
H	4.42682800	1.06466000	1.38626000
H	4.91714200	1.64719000	-0.20716200
H	2.62154100	1.72168000	-0.97517800
H	2.72051000	-2.08145900	-0.15293400
H	5.11229600	-1.06305900	0.56037200
H	4.88327900	-0.59672300	-1.11819600

Dipolarophile 2

C	5.72414400	-1.52780200	0.37059200
H	5.97029500	-2.13831500	1.24859700
H	6.09728200	-0.51403700	0.53686100
H	6.27255400	-1.96729400	-0.47226000
C	4.25292400	-1.55021700	0.11028700
H	3.78937000	-2.51972800	-0.06633100
C	3.46318100	-0.46692200	0.07878400
H	3.84409000	0.53181000	0.25071900
C	2.01891800	-0.63301400	-0.18956600
O	1.47771500	-1.71637300	-0.38217000
N	1.21333000	0.52274900	-0.24382400
C	1.56379900	1.86681100	-0.03836400
O	0.47772100	2.63482600	-0.31859100
C	-0.22791300	0.39206000	-0.50085700
H	-0.38417400	-0.32086500	-1.31191700
C	-0.55362300	1.82968800	-0.92691700
H	-1.52105400	2.17909600	-0.56467300
H	-0.50239500	1.96360200	-2.01263700
O	2.61457600	2.32845700	0.33104200
C	-0.99529900	-0.08348800	0.75439800
H	-0.89244500	0.67438800	1.53960500
H	-0.50624300	-0.99565800	1.10683000
C	-2.45586900	-0.35443100	0.46761700
C	-2.82984100	-1.50425400	-0.24450000
C	-3.45887600	0.53281300	0.87841600
C	-4.16846700	-1.75629000	-0.54068200
H	-2.06295400	-2.20870300	-0.55785300
C	-4.80103000	0.28258700	0.58404400
H	-3.18872000	1.42025000	1.44599500
C	-5.15901600	-0.86178400	-0.12820500
H	-4.43995900	-2.65409000	-1.08851600
H	-5.56494300	0.97992100	0.91572900
H	-6.20230300	-1.05943700	-0.35590000

TS-endo-regioA-1

C	-3.01618100	-2.84777600	-2.57581400
H	-2.48641400	-3.25578500	-3.44498900
H	-3.58501200	-1.97502300	-2.90872100

H	-3.72522300	-3.61242800	-2.24141000
C	-2.02855700	-2.46987200	-1.49124100
H	-1.49860000	-3.29441400	-1.01648700
C	-1.30464800	-1.28462600	-1.59548800
H	-1.59190600	-0.51442300	-2.29755800
C	-0.04288100	-1.15101600	-0.89206300
O	0.37478800	-1.94922600	-0.04092000
N	0.79212400	-0.04589000	-1.19165800
C	0.59855800	0.98571000	-2.11645200
O	1.62247900	1.87557800	-1.98318500
C	2.09945900	0.07853900	-0.53607400
H	1.98990600	-0.12932100	0.52854500
C	2.38940400	1.56086200	-0.80275700
H	3.44048800	1.76592300	-1.01078000
H	2.04444000	2.19900000	0.01709100
O	-0.28395200	1.12552900	-2.92730900
C	3.14043700	-0.88812400	-1.14804000
H	3.29660800	-0.61856000	-2.19904900
H	2.70244600	-1.88960200	-1.12233900
C	4.45413800	-0.87693700	-0.39889300
C	4.55575200	-1.50516700	0.85192000
C	5.58564600	-0.23124200	-0.91363000
C	5.75196800	-1.48478900	1.56741700
H	3.68872000	-2.02154700	1.25709500
C	6.78609700	-0.20961400	-0.20013400
H	5.53001600	0.24723800	-1.88852800
C	6.87217500	-0.83488600	1.04352300
H	5.81302300	-1.98173500	2.53157900
H	7.65365500	0.29197800	-0.61943000
H	7.80562900	-0.82178900	1.59851600
C	-3.01472200	3.25245300	-0.67390700
C	-2.67929100	2.06006200	-0.07109200
C	-1.66241600	2.02521100	0.90071300
C	-0.94012000	3.16332300	1.30082600
C	-1.30489400	4.38633500	0.67203700
C	-2.30951100	4.41992700	-0.28291800
H	-3.79211800	3.29745900	-1.42993500
C	-1.44668500	0.70804300	1.41073900
C	0.06769800	2.96168900	2.28882200
H	-0.78594900	5.30218100	0.94244700
H	-2.56185300	5.36695100	-0.75050900
C	0.29569300	1.68978600	2.78080200
C	-0.44007800	0.54878000	2.35069200
H	0.65006400	3.80365500	2.65251400
H	1.06994400	1.54442300	3.52901700
H	-0.18088500	-0.41946500	2.76019100
C	-3.20439500	0.67006200	-0.22307500
C	-2.37531800	-0.16592100	0.69511700
O	-4.15732200	0.31792300	-0.91716100
N	-2.69678900	-1.44813000	0.98687600
C	-2.08462100	-2.22999400	2.09286800
C	-3.00163000	-3.45615100	2.19271700
C	-3.36842500	-2.26303900	0.12534100
H	-2.07488600	-1.62249400	2.99915200
C	-3.59684500	-3.61289100	0.77146000
H	-3.80159400	-3.26524400	2.91431100
H	-2.45577100	-4.34161900	2.52634200
H	-1.06126900	-2.48647600	1.80756500
H	-4.10427800	-1.77828100	-0.50151300
H	-4.65874900	-3.87697700	0.79998600
H	-3.09057500	-4.40632800	0.20845100

Pr-endo-regioA-1

C	1.09422700	3.61917300	-1.99871700
H	0.03702800	3.63409700	-2.28460200
H	1.66506400	3.18657800	-2.82764100
H	1.41408400	4.66008900	-1.87623400
C	1.32023000	2.82498600	-0.71107800
H	0.71942400	3.26532800	0.09158200
C	0.92659500	1.33317000	-0.82323100
H	0.95114000	1.00256900	-1.86127700
C	-0.45196900	1.06192100	-0.25475200
O	-0.97669000	1.75203000	0.61131300
N	-1.16925600	-0.04870600	-0.72402400

C	-0.76787500	-1.03472000	-1.64211600
O	-1.70810900	-2.01323100	-1.65156700
C	-2.50877100	-0.33803300	-0.19242000
H	-2.50419300	-0.18474900	0.88780700
C	-2.63056300	-1.82415700	-0.55798400
H	-3.62808400	-2.10471000	-0.89748500
H	-2.32629400	-2.47893600	0.26487700
O	0.21865700	-1.06125800	-2.33360700
C	-3.58620700	0.56470400	-0.83421400
H	-3.61650500	0.36658100	-1.91181400
H	-3.26534400	1.60133000	-0.69721800
C	-4.95332900	0.35784400	-0.21952800
C	-5.23577200	0.86810300	1.05665400
C	-5.95383300	-0.35825100	-0.88907400
C	-6.48167500	0.66336400	1.64755300
H	-4.47402400	1.43880400	1.58262700
C	-7.20347700	-0.56404700	-0.30033600
H	-5.75808900	-0.74608200	-1.88605700
C	-7.46980600	-0.05544000	0.97062400
H	-6.68431200	1.07005200	2.63416500
H	-7.96813800	-1.11746600	-0.83773200
H	-8.44168100	-0.21216500	1.42910900
C	4.04212700	-2.55473100	-1.17973600
C	3.26968100	-1.53475100	-0.66617500
C	2.47064100	-1.75311200	0.47299900
C	2.40924900	-3.00059400	1.13388500
C	3.21975700	-4.03591200	0.59327200
C	4.00870000	-3.81147800	-0.52506000
H	4.65278100	-2.40064700	-2.06362300
C	1.73468100	-0.60992300	0.87023500
C	1.54330600	-3.07999900	2.25882100
H	3.21594400	-5.01630500	1.06252600
H	4.61370900	-4.62443500	-0.91558700
C	0.81643000	-1.97087300	2.64668400
C	0.90105800	-0.72376500	1.96330200
H	1.45503800	-4.01274300	2.80929800
H	0.15864800	-2.04317200	3.50832900
H	0.30642600	0.11352700	2.31219500
C	3.03017200	-0.14287100	-1.11812300
C	2.08930400	0.55151100	-0.05395100
O	3.46851400	0.39973700	-2.11177200
N	2.93425800	1.57802100	0.57586200
C	2.67376700	1.98703700	1.96709800
C	3.45712800	3.30037800	2.05666200
C	2.80311900	2.79823200	-0.25071300
H	3.02919400	1.22735100	2.66799300
C	3.23213300	3.96143700	0.67359400
H	4.51964700	3.08062000	2.19934400
H	3.12738400	3.92568100	2.89123200
H	1.60485800	2.16608400	2.17179500
H	3.44771300	2.70383200	-1.13002200
H	4.13613300	4.45943200	0.31340700
H	2.44427200	4.72080400	0.72014200

TS-endo-regioA-2

C	-3.84628300	-2.46015900	2.09757700
H	-4.58665000	-3.10184200	1.60808600
H	-4.30652900	-1.48642700	2.28343100
H	-3.61157600	-2.91859000	3.06582300
C	-2.58487500	-2.31180700	1.27165200
H	-2.12012700	-3.23924500	0.94121500
C	-1.69785400	-1.27328800	1.54952800
H	-1.98903600	-0.43802900	2.17008600
C	-0.31653800	-1.39278800	1.13253400
O	0.10797600	-2.25885800	0.35321000
N	0.64289200	-0.51150900	1.69818100
C	0.43712200	0.58948900	2.53373900
O	1.65228800	1.02175300	2.97962500
C	2.07393700	-0.71747100	1.44504200
H	2.29815600	-1.78410200	1.50449700
C	2.66688700	0.06126700	2.62815300
H	3.58059300	0.60078000	2.37547000
H	2.85419700	-0.58209200	3.49509000
O	-0.59745900	1.12841700	2.84167600

C	2.50965700	-0.18293300	0.06270700
H	2.32431100	0.89598800	0.02414500
H	1.85937900	-0.65147600	-0.67908100
C	3.95943500	-0.48452200	-0.24539800
C	4.35484300	-1.79075500	-0.57326400
C	4.94090500	0.51394600	-0.19323000
C	5.69094700	-2.08913600	-0.83660000
H	3.60344700	-2.57501300	-0.62849500
C	6.28020900	0.21920800	-0.45784700
H	4.65100400	1.53454000	0.04509900
C	6.65938600	-1.08402600	-0.77866900
H	5.97682800	-3.10567000	-1.09184800
H	7.02482400	1.00907900	-0.41600900
H	7.69999800	-1.31536800	-0.98631700
C	-2.68315800	3.41262000	0.57915400
C	-2.38239900	2.23505600	-0.06859400
C	-1.27789200	2.17014100	-0.93620300
C	-0.44587400	3.27155300	-1.20379500
C	-0.76708200	4.47740200	-0.52095000
C	-1.84964300	4.53576900	0.34300300
H	-3.53199000	3.47902300	1.25206400
C	-1.12443800	0.87479800	-1.52256000
C	0.60638900	3.06214300	-2.14128100
H	-0.15720100	5.36213400	-0.68390600
H	-2.06976900	5.46955000	0.85180500
C	0.75295300	1.82310500	-2.73402000
C	-0.09707200	0.71920800	-2.44168200
H	1.27937800	3.87606900	-2.39576700
H	1.55007000	1.67343000	-3.45666000
H	0.08455700	-0.21502100	-2.95799100
C	-3.04736500	0.90011300	-0.08674100
C	-2.18027200	0.03918500	-0.94624300
O	-4.12078200	0.61106900	0.44304200
N	-2.52060200	-1.22319300	-1.29013400
C	-1.75208200	-2.04230600	-2.26570300
C	-2.24902000	-3.47485700	-2.02256600
C	-3.44295600	-1.96834200	-0.61667600
H	-0.68767500	-1.94083100	-2.06639300
C	-3.60908600	-3.29182300	-1.31969100
H	-1.54675200	-3.98305400	-1.35773300
H	-2.32016100	-4.04638000	-2.95061900
H	-1.97950100	-1.67304100	-3.27209700
H	-4.26939500	-1.41580900	-0.19044600
H	-3.83977200	-4.10538900	-0.62544600
H	-4.43551700	-3.24409400	-2.04300500

Pr-endo-regioA-2

C	-1.95408600	-3.72530500	1.64424800
H	-2.45905700	-4.65914300	1.37340900
H	-2.47514400	-3.30102800	2.50977300
H	-0.93586800	-3.98433700	1.95357700
C	-1.95302100	-2.74473700	0.47046400
H	-1.39901400	-3.18423200	-0.36616900
C	-1.29442000	-1.38574400	0.79763800
H	-1.42502900	-1.15011400	1.85460500
C	0.18565500	-1.39592000	0.46416200
O	0.67302700	-2.09254900	-0.41802300
N	1.05750200	-0.61013800	1.23127800
C	0.74102900	0.36189900	2.19385200
O	1.89552500	0.76777700	2.78214100
C	2.51268500	-0.68332100	1.02836600
H	2.80782400	-1.72952300	0.93012500
C	2.98756400	-0.07472700	2.35588300
H	3.87855800	0.54522500	2.25267000
H	3.15966400	-0.83554900	3.12449300
O	-0.34068500	0.81064600	2.47662500
C	2.97310200	0.10084900	-0.22088800
H	2.71266900	1.15728100	-0.09163600
H	2.39940300	-0.27679600	-1.07073200
C	4.45595300	-0.05224700	-0.48032400
C	4.96193000	-1.25769700	-0.99031300
C	5.35587600	0.98459000	-0.20202500
C	6.32871500	-1.42254900	-1.20995100
H	4.27453900	-2.06716300	-1.22469900

C	6.72552600	0.82332600	-0.42249700
H	4.97954900	1.93130800	0.17828400
C	7.21575700	-0.38174700	-0.92499800
H	6.70163400	-2.36141100	-1.60911300
H	7.40669100	1.64092000	-0.20487800
H	8.28016600	-0.50854800	-1.09892800
C	-3.28364800	3.19730600	1.04683700
C	-2.77190500	2.01078200	0.56711400
C	-1.85242800	2.01560300	-0.50055800
C	-1.40717800	3.20524500	-1.11975900
C	-1.95400400	4.41648000	-0.61486400
C	-2.86339100	4.40367800	0.43205200
H	-3.98273800	3.20722800	1.87699300
C	-1.41554500	0.72081200	-0.87362700
C	-0.46310000	3.05712500	-2.17302100
H	-1.65137200	5.36303100	-1.05521300
H	-3.26057500	5.34632600	0.79719100
C	-0.02863300	1.79724800	-2.53725800
C	-0.49759500	0.61371800	-1.89740700
H	-0.08529500	3.93624100	-2.68812600
H	0.69314600	1.69767400	-3.34299300
H	-0.12046400	-0.35193100	-2.21805700
C	-2.93788000	0.60153600	1.00340000
C	-2.14411400	-0.30971900	-0.01806900
O	-3.58023300	0.18226500	1.94369600
N	-3.19124700	-1.06935200	-0.71546000
C	-3.29316400	-1.23087800	-2.17715900
C	-3.34533400	-2.75126300	-2.41206000
C	-3.36448700	-2.36158300	-0.03314000
H	-2.46504900	-0.75599100	-2.70678700
C	-3.95368700	-3.28976000	-1.10527400
H	-2.33307600	-3.14686000	-2.55155300
H	-3.92843500	-3.01854700	-3.29824500
H	-4.21659100	-0.75527400	-2.53856100
H	-4.03626000	-2.24879600	0.82726000
H	-3.71675400	-4.34197200	-0.91914300
H	-5.04501600	-3.19469100	-1.12475100

TS-endo-regioB-1

C	2.14383800	-1.00558700	-2.50144500
H	1.62140600	-0.91732000	-3.46156300
H	2.41238100	-2.05682000	-2.36388500
H	3.06572100	-0.42203700	-2.57820000
C	1.24766300	-0.50816300	-1.38742400
H	1.07511100	0.56487400	-1.38713100
C	0.12579900	-1.28505000	-1.02357100
H	0.00288900	-2.29680100	-1.38390500
C	-0.99324400	-0.61533600	-0.42026200
O	-0.97205000	0.54972900	0.01219700
N	-2.23894100	-1.30854100	-0.29247900
C	-2.53865600	-2.63392700	-0.59891900
O	-3.85327200	-2.86004900	-0.29975000
C	-3.44758000	-0.56872200	0.08799200
H	-3.23921500	0.05324600	0.95967200
C	-4.38377700	-1.73700600	0.42828300
H	-5.41389500	-1.57120300	0.10967300
H	-4.37363900	-1.97829000	1.49754600
O	-1.81886200	-3.49711500	-1.04115900
C	-3.95750500	0.33169100	-1.06197300
H	-4.23685500	-0.30464300	-1.90970000
H	-3.11739200	0.95677600	-1.37657000
C	-5.12275200	1.19986900	-0.64291200
C	-4.90629800	2.32018700	0.17420100
C	-6.43543600	0.90134200	-1.03041300
C	-5.97189600	3.11457100	0.59466200
H	-3.89085500	2.57162000	0.47131600
C	-7.50527000	1.69568700	-0.61202700
H	-6.62018900	0.04676800	-1.67704300
C	-7.27649800	2.80338500	0.20388700
H	-5.78453800	3.98084600	1.22288900
H	-8.51520100	1.45018900	-0.92782200
H	-8.10659800	3.42383200	0.52865200
C	6.12807100	-0.63313700	-0.55473200
C	4.81884400	-0.36627200	-0.21165300

C	4.38704600	0.96660300	-0.06405700
C	5.22905100	2.07758600	-0.26823300
C	6.57666300	1.77980000	-0.61093100
C	7.00332600	0.46616900	-0.74659300
H	6.47881600	-1.65330700	-0.67609900
C	3.01178600	1.05722600	0.28114500
C	4.63350600	3.36138700	-0.10971200
H	7.27967900	2.59313800	-0.77124600
H	8.03847000	0.27300500	-1.01244700
C	3.29023600	3.45874800	0.19929700
C	2.45619700	2.31793200	0.38210400
H	5.23168300	4.25812000	-0.24476300
H	2.84103500	4.44299300	0.29689900
H	1.39541000	2.45700400	0.56421700
C	3.64594200	-1.24628500	0.05590000
C	2.46440600	-0.32531700	0.30163900
O	3.63278600	-2.47035100	0.09225400
N	1.58446700	-0.75700600	1.30050100
C	1.07958600	0.06225600	2.43223900
C	-0.12366600	-0.74099500	2.95574900
C	0.99177700	-1.94117600	1.22978900
H	0.79925700	1.05368000	2.08658100
C	0.08409100	-2.16844800	2.39701400
H	-1.04001700	-0.31040700	2.54855900
H	-0.18512000	-0.71835600	4.04575900
H	1.88487900	0.15634100	3.16933100
H	1.41491900	-2.71334600	0.60877800
H	-0.84701200	-2.65822400	2.09752100
H	0.56987400	-2.83467300	3.12421800

Pr-endo-regioB-1

C	1.59236600	-0.31058300	-2.60245800
H	0.72568000	-0.12457600	-3.24528200
H	1.95110900	-1.32439300	-2.79874700
H	2.37754500	0.39273800	-2.90114700
C	1.20938500	-0.11701400	-1.13315700
H	0.80757200	0.88994200	-1.00722400
C	0.11749900	-1.12144800	-0.64085800
H	-0.13819500	-1.85069300	-1.40898500
C	-1.14991300	-0.39296000	-0.22168100
O	-1.19352800	0.79113600	0.07892800
N	-2.34942600	-1.12425100	-0.16133600
C	-2.56934100	-2.48496400	-0.43153700
O	-3.85863200	-2.77647600	-0.11878000
C	-3.60273600	-0.45211000	0.21321400
H	-3.41932500	0.19390000	1.07321100
C	-4.46198800	-1.66984200	0.58358300
H	-5.49879000	-1.58053600	0.25750200
H	-4.43722900	-1.88703800	1.65652500
O	-1.79740600	-3.30055100	-0.86915000
C	-4.17426200	0.39233700	-0.94852400
H	-4.41924800	-0.27494300	-1.78293800
H	-3.38035200	1.06543300	-1.28357800
C	-5.39090400	1.19031400	-0.53327300
C	-5.24275700	2.32910500	0.27305100
C	-6.68224600	0.80653100	-0.91680100
C	-6.35534700	3.05941500	0.68774900
H	-4.24531200	2.64711600	0.56720100
C	-7.79885100	1.53696500	-0.50409100
H	-6.81435800	-0.06326500	-1.55604000
C	-7.63823500	2.66401000	0.30139400
H	-6.22139300	3.94103400	1.30794000
H	-8.79179300	1.22659400	-0.81632000
H	-8.50492900	3.23459200	0.62167300
C	6.13754200	-0.38653700	-0.99912400
C	4.82344100	-0.18706000	-0.62662800
C	4.42052100	1.06180800	-0.10679500
C	5.30726000	2.14778900	0.06883000
C	6.65309400	1.91866600	-0.32775000
C	7.04533000	0.69149700	-0.84513300
H	6.46768400	-1.34136600	-1.39659400
C	3.05179100	1.10293200	0.23478700
C	4.75009100	3.33055800	0.62941800
H	7.38526900	2.71496500	-0.22043500

H	8.08213600	0.55082500	-1.13659800
C	3.41084700	3.36739000	0.97456900
C	2.54120600	2.25551200	0.78508300
H	5.37948200	4.20184700	0.78901700
H	3.00275100	4.27735000	1.40552900
H	1.49477100	2.32058700	1.06848600
C	3.62645400	-1.06933200	-0.64063300
C	2.40128800	-0.23054400	-0.10219600
O	3.58373100	-2.24598300	-0.95716000
N	1.73799300	-0.85018700	1.03197000
C	2.41222700	-1.40713300	2.19752000
C	1.27780100	-2.23467900	2.87775300
C	0.79803200	-1.85395900	0.55015900
H	2.80633800	-0.61071800	2.83704100
C	0.10239400	-2.25933600	1.85347700
H	0.96482200	-1.78790400	3.82498600
H	1.62959800	-3.24616700	3.09848000
H	3.24983400	-2.07150300	1.92711500
H	1.31235700	-2.73419500	0.13190300
H	-0.64685200	-1.51240600	2.13376100
H	-0.38438100	-3.23510800	1.78869100

TS-endo-regioB-2

C	-2.41882500	-1.38861200	-2.21023900
H	-3.36925500	-0.85237000	-2.28200800
H	-2.61418200	-2.38986000	-1.81535800
H	-2.03304200	-1.50365200	-3.23015400
C	-1.40368000	-0.64629200	-1.36504500
H	-1.24883000	0.39070800	-1.65618400
C	-0.22711100	-1.32201600	-0.97460500
H	-0.18101600	-2.40239100	-0.99260000
C	0.99648500	-0.57935000	-0.84358000
O	1.10204000	0.65716900	-0.88392500
N	2.22028400	-1.30936900	-0.70914100
C	2.40438300	-2.65630800	-0.40636000
O	3.72979900	-2.95392300	-0.55241700
C	3.51083600	-0.62981600	-0.86887900
H	3.45432600	0.06084300	-1.71218500
C	4.40526300	-1.84054800	-1.17161300
H	5.40424000	-1.76044500	-0.74078400
H	4.48801800	-2.03470500	-2.24671500
O	1.59022100	-3.46954700	-0.03819900
C	3.92591200	0.15217800	0.39924500
H	4.04346600	-0.55823600	1.22653300
H	3.09387100	0.81899500	0.63939800
C	5.19671800	0.94944800	0.20717300
C	5.17634200	2.13639600	-0.54143400
C	6.41798800	0.52001900	0.74266600
C	6.34391500	2.86857400	-0.75161000
H	4.23360100	2.48791700	-0.95394000
C	7.58926300	1.25165200	0.53505100
H	6.45011600	-0.38946400	1.33806500
C	7.55559500	2.42741600	-0.21438300
H	6.30801300	3.78677400	-1.33100200
H	8.52543600	0.90390800	0.96239300
H	8.46482400	2.99907500	-0.37547900
C	-6.03378800	-1.16883100	0.20319500
C	-4.76613400	-0.62704700	0.24800800
C	-4.56941600	0.73436200	-0.05356200
C	-5.61774900	1.60172000	-0.41924800
C	-6.91700600	1.02459100	-0.45512200
C	-7.10943800	-0.31604300	-0.15268300
H	-6.20400600	-2.21604300	0.43302500
C	-3.20480100	1.12052300	0.04446600
C	-5.25603200	2.95004000	-0.70017600
H	-7.76941000	1.64369100	-0.72257400
H	-8.11447000	-0.72588700	-0.19025100
C	-3.93122700	3.33268500	-0.61885400
C	-2.88806100	2.43058700	-0.25996600
H	-6.01895100	3.67019300	-0.98200200
H	-3.66354700	4.36079600	-0.84533600
H	-1.86444700	2.78957300	-0.24693100
C	-3.43384100	-1.20743600	0.57504400
C	-2.41532100	-0.10224600	0.35640500

O	-3.20017700	-2.34647900	0.95852500
N	-1.36569900	-0.08008200	1.28309500
C	-0.71144000	1.15870000	1.78310400
C	0.24561200	0.62450800	2.86047400
C	-0.61923400	-1.15302200	1.51802400
H	-1.46943800	1.84272200	2.16761500
C	0.51718600	-0.84132000	2.44223000
H	-0.24127900	0.64937700	3.83981900
H	1.15623700	1.22381500	2.92349000
H	-0.17853700	1.62515800	0.95149100
H	-1.00311900	-2.13471100	1.29615600
H	0.54700200	-1.53057000	3.29238600
H	1.47285900	-0.95388300	1.91723100

Pr-endo-regioB-2

C	1.44494400	-0.02104800	-2.36343100
H	2.23857400	-0.67072500	-2.74729300
H	1.72073000	1.01724700	-2.57177600
H	0.53293800	-0.25229600	-2.92242500
C	1.22533500	-0.25037300	-0.86744700
H	0.89963600	-1.28724600	-0.72092300
C	0.16349500	0.66551200	-0.22418500
H	0.25345300	1.67761600	-0.62105900
C	-1.23790000	0.15053200	-0.48130800
O	-1.48578000	-1.00618900	-0.79880500
N	-2.31643700	1.04216600	-0.37363500
C	-2.30779900	2.38015600	0.05420000
O	-3.55084200	2.89398800	-0.13992100
C	-3.68527800	0.59989100	-0.67780900
H	-3.67448900	0.00241600	-1.59103800
C	-4.35902100	1.96348700	-0.89073300
H	-5.37820800	2.00552800	-0.50545700
H	-4.35467500	2.26960100	-1.94211200
O	-1.39946900	3.00669400	0.53624100
C	-4.29613400	-0.23291200	0.47221000
H	-4.34951400	0.39211600	1.37112300
H	-3.60525600	-1.05455300	0.67911700
C	-5.66485000	-0.77753400	0.12629400
C	-5.79081500	-1.84946000	-0.77048900
C	-6.83020800	-0.21886300	0.66678800
C	-7.04650400	-2.34349100	-1.12055900
H	-4.89501500	-2.30374900	-1.18730500
C	-8.08954500	-0.71257200	0.31937800
H	-6.75100900	0.60119900	1.37660700
C	-8.20098600	-1.77486900	-0.57732400
H	-7.12438800	-3.17675100	-1.81299300
H	-8.98106700	-0.26905900	0.75326400
H	-9.17912300	-2.16175400	-0.84725000
C	5.79237500	1.79968000	-0.47036500
C	4.67844300	1.00312800	-0.30183400
C	4.81141600	-0.39904900	-0.25074500
C	6.05507000	-1.05558700	-0.38827500
C	7.19032800	-0.21490300	-0.54579900
C	7.05516400	1.16576200	-0.58033700
H	5.70291600	2.88024100	-0.52291200
C	3.57503300	-1.07016400	-0.09031700
C	6.02483900	-2.47746100	-0.37028600
H	8.17570400	-0.66210900	-0.64842500
H	7.94263800	1.77907400	-0.70628600
C	4.81829100	-3.13823500	-0.24256400
C	3.57959300	-2.44765900	-0.10686800
H	6.94915600	-3.04005800	-0.46906500
H	4.80666000	-4.22438600	-0.24522000
H	2.66190000	-3.02087000	-0.01950500
C	3.22723200	1.31290100	-0.22802400
C	2.46209200	-0.04030300	0.04328100
O	2.70209000	2.40367900	-0.34890600
N	1.91082000	0.10765000	1.40530400
C	1.84636200	-1.05021800	2.30704300
C	0.72865000	-0.65339400	3.27384000
C	0.56417400	0.73364400	1.30230300
H	2.80925700	-1.21279000	2.80175700
C	-0.30578500	-0.03028300	2.32338300
H	1.09682300	0.09248000	3.98643200

H	0.33905100	-1.50501200	3.83912900
H	1.57327900	-1.98986000	1.79693800
H	0.62436600	1.78987900	1.56918000
H	-1.02313900	0.62471600	2.82504900
H	-0.86793100	-0.83288000	1.83176400

TS-exo-regioA-1

C	2.60588400	-3.21295800	2.00113800
H	2.17925300	-3.65932900	2.90757700
H	3.20757500	-2.35650900	2.32159100
H	3.27110700	-3.96423800	1.56497500
C	1.48800400	-2.79343400	1.06958200
H	0.84769400	-3.60027400	0.71510000
C	0.83860200	-1.57817100	1.29991500
H	1.23611200	-0.83629300	1.97810300
C	-0.47515000	-1.38037600	0.71807200
O	-0.99658900	-2.17069400	-0.07362400
N	-1.20070300	-0.20615400	1.03923700
C	-0.91153500	0.76977800	1.99418000
O	-1.84559300	1.75760500	1.89196300
C	-2.48699100	0.05941800	0.38483400
H	-2.38431400	-0.12392500	-0.68607600
C	-2.63940000	1.55340000	0.70495200
H	-3.66750100	1.84509100	0.92392000
H	-2.23929900	2.18984200	-0.09090700
O	-0.02141500	0.79455200	2.80967600
C	-3.62347900	-0.82061700	0.95569900
H	-3.75578700	-0.58009100	2.01710300
H	-3.28941300	-1.85890500	0.88688800
C	-4.92585800	-0.64057100	0.20783000
C	-5.07772600	-1.17692800	-1.08030500
C	-5.99478100	0.07537200	0.76208400
C	-6.26237400	-0.99799000	-1.79294500
H	-4.26066000	-1.74479200	-1.51874300
C	-7.18354800	0.25520500	0.05137200
H	-5.89969400	0.48512100	1.76493700
C	-7.31984200	-0.27969200	-1.22936000
H	-6.36295700	-1.42382600	-2.78728600
H	-8.00247400	0.80953400	0.50110900
H	-8.24402000	-0.14316600	-1.78335400
C	0.26255400	2.55615600	-1.78208200
C	1.16605800	1.63236900	-1.30125400
C	2.27537400	2.06214800	-0.55107200
C	2.51789000	3.41010100	-0.23467800
C	1.56823000	4.34659800	-0.72831700
C	0.48090300	3.92543000	-1.47932000
H	-0.58732000	2.24640700	-2.38322200
C	3.11909300	0.97539600	-0.16640600
C	3.69153400	3.68431800	0.52553800
H	1.70123200	5.40436900	-0.51747400
H	-0.22326700	4.66496800	-1.84935100
C	4.51425100	2.64249000	0.90728400
C	4.24815700	1.28434300	0.57522700
H	3.93548300	4.70613700	0.80125400
H	5.40494500	2.85958900	1.48994300
H	4.93770500	0.52406900	0.92385000
C	1.26332000	0.14548100	-1.44050300
C	2.48026300	-0.23978100	-0.67126500
O	0.53276400	-0.57641000	-2.11614800
N	3.02188300	-1.47904600	-0.75616600
C	4.44394800	-1.78193300	-0.49074900
C	4.61598500	-3.23182300	-0.98640500
C	2.27284100	-2.62106800	-0.83017000
H	4.64620200	-1.68630200	0.58076500
C	3.17418400	-3.78699600	-1.16103500
H	5.20420200	-3.81995900	-0.27841000
H	5.14847700	-3.24499900	-1.94043600
H	5.06790100	-1.06019100	-1.02211400
H	1.29418200	-2.51706400	-1.28418900
H	2.97386900	-4.64741300	-0.51448400
H	3.00082100	-4.12584300	-2.18854300

Pr-exo-regioA-1

C	-2.47294500	-3.02483100	-2.23291300
H	-1.92104300	-2.79646000	-3.15085700
H	-3.37602200	-2.40652700	-2.21726900
H	-2.78318500	-4.07323400	-2.28956900
C	-1.60167700	-2.77137000	-0.99867000
H	-0.75476000	-3.46059600	-1.00111000
C	-1.06029400	-1.30605400	-0.96033300
H	-1.16080700	-0.81356700	-1.92868100
C	0.41708800	-1.27879600	-0.57518900
O	1.00167300	-2.22496300	-0.07744500
N	1.12288800	-0.07622300	-0.75188100
C	0.81606100	1.01188700	-1.58794200
O	1.73884000	1.98279800	-1.36969700
C	2.45943800	0.09786900	-0.15929300
H	2.43825300	-0.26031600	0.87150400
C	2.56512900	1.62611000	-0.23839700
H	3.57738200	1.98288300	-0.42929700
H	2.16111300	2.11654600	0.65312900
O	-0.07293600	1.11142000	-2.39576300
C	3.55847300	-0.64604400	-0.95287400
H	3.59200400	-0.24170400	-1.97127600
H	3.25561900	-1.69384700	-1.02015900
C	4.91762600	-0.53323500	-0.29750400
C	5.20832000	-1.27698300	0.85638400
C	5.90349200	0.32264300	-0.80571200
C	6.44716900	-1.16330600	1.48558500
H	4.45870900	-1.95579800	1.25595300
C	7.14601600	0.43761900	-0.17868500
H	5.70176000	0.89404400	-1.70868400
C	7.42021900	-0.30365100	0.97038400
H	6.65564600	-1.75027600	2.37543700
H	7.89900100	1.10277500	-0.59157500
H	8.38649800	-0.21758700	1.45853100
C	-0.92864700	2.46262600	2.28617500
C	-1.38930500	1.49874500	1.41049400
C	-2.23276700	1.86013300	0.33882700
C	-2.65606400	3.18902800	0.10984200
C	-2.16036500	4.16389800	1.01735700
C	-1.32313700	3.80567900	2.06560400
H	-0.29104300	2.19752800	3.12421400
C	-2.62826700	0.75993400	-0.45181800
C	-3.53667100	3.38945000	-0.98799500
H	-2.44647100	5.20486300	0.89084700
H	-0.96708100	4.57693600	2.74236100
C	-3.93966200	2.31005200	-1.75226200
C	-3.49823800	0.98196700	-1.49258700
H	-3.89393600	4.38870900	-1.22065200
H	-4.61681000	2.47694500	-2.58501100
H	-3.84684000	0.16674400	-2.11909300
C	-1.19226000	0.02924100	1.34754900
C	-1.98479700	-0.51402100	0.08578500
O	-0.58559400	-0.66738900	2.14226200
N	-2.96343700	-1.53450700	0.42438100
C	-3.82540400	-1.50289000	1.59920400
C	-4.38670000	-2.95716000	1.64431500
C	-2.35189600	-2.85864400	0.34182100
H	-4.60892800	-0.74540900	1.48924100
C	-3.55912900	-3.76457200	0.59654200
H	-5.45370900	-2.98407000	1.40772600
H	-4.26972800	-3.37359500	2.64869200
H	-3.27021500	-1.28458700	2.52613800
H	-1.60791700	-3.01208500	1.14277500
H	-4.13917400	-3.89514200	-0.32070200
H	-3.27518700	-4.75491900	0.96286200

TS-exo-regioA-2

C	-3.04172400	-2.98979600	1.89466900
H	-3.70575300	-3.68693600	1.37474700
H	-3.59040900	-2.06332900	2.09118900
H	-2.81504000	-3.43939400	2.86904900
C	-1.75229200	-2.72594400	1.14626500
H	-1.15670200	-3.60791700	0.91415500
C	-1.02013200	-1.57600200	1.44898300
H	-1.43837800	-0.76048900	2.02194100

C	0.38722200	-1.55310900	1.09549400
O	0.93766700	-2.43180300	0.42587400
N	1.20042300	-0.48980300	1.56218400
C	0.84637800	0.61770100	2.33288300
O	1.98884500	1.27467200	2.68686800
C	2.63435900	-0.48346200	1.25236400
H	3.03035900	-1.49294100	1.37423300
C	3.13596400	0.46947200	2.34669300
H	3.93448500	1.13224300	2.01019500
H	3.46420900	-0.06490700	3.24520800
O	-0.25187200	0.99571700	2.66228300
C	2.91824400	0.00673200	-0.18632200
H	2.64702400	1.06679600	-0.25142900
H	2.25466100	-0.54212200	-0.85987700
C	4.36358400	-0.19510700	-0.58260500
C	4.82853000	-1.48045600	-0.90157800
C	5.27238600	0.87016100	-0.61947800
C	6.16350700	-1.69310700	-1.24150400
H	4.12955200	-2.31321900	-0.88889600
C	6.61058100	0.66097900	-0.96076300
H	4.92625300	1.87557600	-0.39083400
C	7.06031500	-0.62215300	-1.27084800
H	6.50405100	-2.69440500	-1.48987400
H	7.29856000	1.50138300	-0.98771600
H	8.09988400	-0.78710600	-1.53877900
C	0.19648900	2.50535400	-1.48655200
C	-0.81928300	1.63323100	-1.15807700
C	-2.01305600	2.12846800	-0.60250700
C	-2.23412700	3.49012000	-0.33461300
C	-1.16893200	4.37178400	-0.66688100
C	0.00296500	3.88701500	-1.22718500
H	1.11737300	2.14786400	-1.93643400
C	-2.96481500	1.09227600	-0.35954600
C	-3.50126300	3.83258000	0.21974000
H	-1.27933600	5.43716500	-0.48273600
H	0.79722800	4.58461000	-1.47636300
C	-4.42962900	2.83926600	0.46393100
C	-4.18350600	1.46583900	0.18426600
H	-3.73350200	4.86889800	0.44757300
H	-5.39175500	3.10875100	0.89021900
H	-4.95971100	0.74506900	0.41530000
C	-0.96967500	0.15159800	-1.30348100
C	-2.31653300	-0.15870400	-0.74963600
O	-0.17987100	-0.62049400	-1.84699000
N	-2.90202900	-1.36930900	-0.91026600
C	-4.36489700	-1.58954900	-0.89198300
C	-4.52691800	-3.01953900	-1.44108900
C	-2.21866400	-2.55318300	-0.85717000
H	-4.84838500	-0.82683300	-1.50560500
C	-3.12526400	-3.67632400	-1.30561800
H	-4.82937000	-2.98511200	-2.49076100
H	-5.30060500	-3.56648400	-0.89727900
H	-4.73838600	-1.49363400	0.13228700
H	-1.17713200	-2.51494500	-1.15371600
H	-2.78527900	-4.09107400	-2.26077900
H	-3.11969900	-4.50532000	-0.58981700

Pr-exo-regioA-2

C	-1.93131500	-3.52134100	-1.43418000
H	-2.58432000	-4.03041200	-2.15106400
H	-2.09606600	-3.97003600	-0.44958500
H	-0.89890200	-3.74001200	-1.72810800
C	-2.18466300	-2.01218200	-1.43813300
H	-1.88800600	-1.60972500	-2.40925200
C	-1.40399800	-1.22711000	-0.35777700
H	-1.54814000	-1.70555600	0.61201700
C	0.07243600	-1.08532600	-0.63963800
O	0.50750700	-0.53060700	-1.63780100
N	1.00291400	-1.62245700	0.27200300
C	0.79574800	-2.24537000	1.51477200
O	1.99192000	-2.70034800	1.96559300
C	2.44306500	-1.49350500	-0.00731200
H	2.62491200	-1.73270300	-1.05610100
C	2.99372500	-2.57202200	0.93379400

H	3.93694400	-2.29335600	1.40455300
H	3.10581500	-3.54210300	0.43850000
O	-0.22846100	-2.37899900	2.13980200
C	2.96533600	-0.07007700	0.29401100
H	2.83914200	0.13349800	1.36363700
H	2.33255500	0.63276500	-0.25405400
C	4.41228200	0.10578100	-0.11216600
C	4.75162500	0.22491100	-1.46858000
C	5.44068600	0.13007100	0.83855400
C	6.08235700	0.35768100	-1.86201600
H	3.96269100	0.22339800	-2.21694900
C	6.77472100	0.26462600	0.44756200
H	5.19453700	0.05686400	1.89533200
C	7.09910700	0.37609100	-0.90420100
H	6.32596800	0.45306900	-2.91622000
H	7.55772600	0.28640600	1.20006800
H	8.13558000	0.48277100	-1.21027000
C	-1.29339700	3.58918600	-1.72591900
C	-1.57488600	2.40584700	-1.07549400
C	-1.47282700	2.32639500	0.32719500
C	-1.06176900	3.41705200	1.12679300
C	-0.78444000	4.62824800	0.43666800
C	-0.90193800	4.70426800	-0.94376200
H	-1.36332700	3.66010200	-2.80678800
C	-1.78516000	1.04410200	0.83970800
C	-0.95613300	3.17286700	2.52374000
H	-0.46992600	5.50320200	0.99974800
H	-0.67869200	5.64378400	-1.44092500
C	-1.22680800	1.91392100	3.02442100
C	-1.63450800	0.83087000	2.19357900
H	-0.64933100	3.97347500	3.19138400
H	-1.12367400	1.73425300	4.09069200
H	-1.79463000	-0.14529200	2.63848200
C	-1.97318700	1.06594000	-1.57823300
C	-2.17698300	0.12815000	-0.31222400
O	-2.19647700	0.75744400	-2.73072900
N	-3.58686300	-0.29017300	-0.38383700
C	-4.38096600	-0.43224100	0.84578300
C	-5.42194400	-1.48656000	0.45992600
C	-3.65735000	-1.55609900	-1.17774700
H	-4.82327500	0.52606800	1.13814700
C	-4.57803200	-2.47823400	-0.35480200
H	-6.20019800	-1.03719800	-0.16699400
H	-5.90409900	-1.93827600	1.33163100
H	-3.79382400	-0.79843400	1.70343000
H	-4.12320900	-1.34375500	-2.14736000
H	-5.17255200	-3.14639100	-0.98448600
H	-3.99666300	-3.10355600	0.33251700

TS-exo-regioB-1

C	-1.94838200	-0.55500900	2.46211300
H	-1.38313500	-0.32044200	3.37445600
H	-2.14297400	-1.63288100	2.47484300
H	-2.90608200	-0.03487800	2.53237100
C	-1.14413600	-0.13756500	1.25563700
H	-0.98887700	0.93286600	1.14804900
C	-0.08669900	-0.94967300	0.79654500
H	0.01380700	-1.95563400	1.18528300
C	1.13900300	-0.29640000	0.34345100
O	1.24163800	0.89216800	0.05410800
N	2.32363700	-1.08589800	0.20757100
C	2.53952100	-2.43180200	0.49060200
O	3.81939400	-2.74778800	0.14695600
C	3.57765700	-0.42699100	-0.18488100
H	3.38600100	0.23423100	-1.03092400
C	4.40879700	-1.65251400	-0.58494700
H	5.45930700	-1.57426400	-0.30220400
H	4.33712100	-1.87357900	-1.65554600
O	1.77734000	-3.24985200	0.95597900
C	4.19100900	0.39214000	0.97464600
H	4.46415500	-0.29290800	1.78588600
H	3.40884600	1.05778900	1.34821200
C	5.39259900	1.19857800	0.53437800
C	5.21520800	2.34892100	-0.24987400

C	6.69688800	0.81434400	0.87069200
C	6.31177600	3.08960700	-0.68803400
H	4.20735400	2.66554300	-0.50751100
C	7.79759700	1.55538500	0.43451300
H	6.85180200	-0.06513200	1.49140400
C	7.60782200	2.69395800	-0.34808500
H	6.15514400	3.97972700	-1.29067600
H	8.80111000	1.24405500	0.71035700
H	8.46203900	3.27284600	-0.68682500
C	-3.59881000	3.25184700	-0.96162800
C	-3.40784500	1.90851800	-0.71783200
C	-4.38424300	1.16972100	-0.02558300
C	-5.58590500	1.73511600	0.44274600
C	-5.76363100	3.12219700	0.18511400
C	-4.79578400	3.84981000	-0.49197700
H	-2.85688500	3.83331500	-1.49998600
C	-4.01789200	-0.19984400	0.13115600
C	-6.48960400	0.85347700	1.10199100
H	-6.67250700	3.61512400	0.52037600
H	-4.96172800	4.90768800	-0.67358400
C	-6.15149500	-0.47643700	1.25398200
C	-4.92027100	-1.02019400	0.78655300
H	-7.43727200	1.22680000	1.47954900
H	-6.84422600	-1.14353900	1.75925100
H	-4.71767900	-2.06840100	0.97388700
C	-2.31708200	0.96142700	-1.09342000
C	-2.64763300	-0.34069000	-0.40853900
O	-1.37415700	1.19299400	-1.83867500
N	-2.13176700	-1.51145500	-0.94418100
C	-2.69927800	-2.85177800	-0.68490000
C	-1.82290000	-3.76688700	-1.55062500
C	-0.82870100	-1.60162100	-1.27740800
H	-3.75478800	-2.86658000	-0.96054700
C	-0.46858000	-3.02186200	-1.63454100
H	-2.26403300	-3.86287400	-2.54717700
H	-1.73343300	-4.76803900	-1.12357800
H	-2.61053000	-3.08810300	0.38342400
H	-0.36264300	-0.72317600	-1.69936900
H	-0.01815500	-3.08978800	-2.63051500
H	0.25741900	-3.42313300	-0.92066100

Pr-exo-regioB-1

C	1.06646700	-1.29091300	1.52841100
H	0.08463500	-1.74364000	1.70157800
H	1.26514800	-0.58323900	2.33839800
H	1.81156000	-2.09016500	1.59324000
C	1.09015600	-0.61847500	0.15742100
H	0.81560700	-1.36156000	-0.59741300
C	0.07864700	0.55125700	0.00050300
H	0.10095800	1.21987000	0.86129900
C	-1.33151300	0.05691500	-0.24782100
O	-1.58283600	-1.00523100	-0.79707600
N	-2.41223500	0.88134800	0.11456900
C	-2.41254700	2.10275200	0.81155200
O	-3.68086300	2.58739700	0.81317000
C	-3.78926000	0.45314400	-0.18076200
H	-3.82891400	0.05193100	-1.19463700
C	-4.51405200	1.79992500	-0.06428400
H	-5.50488800	1.72032300	0.38377400
H	-4.58931800	2.31744400	-1.02633000
O	-1.49429500	2.66920900	1.34975200
C	-4.28817400	-0.61759000	0.81637700
H	-4.29287100	-0.18610500	1.82411500
H	-3.56140100	-1.43442100	0.80821400
C	-5.66314500	-1.13849900	0.45875100
C	-5.82461700	-2.01427400	-0.62557900
C	-6.80066100	-0.74573000	1.17571300
C	-7.08896500	-2.47817500	-0.98558800
H	-4.94928800	-2.33965400	-1.18279800
C	-8.06839700	-1.21001000	0.81847300
H	-6.69187500	-0.08107800	2.02961300
C	-8.21593600	-2.07578700	-0.26484300
H	-7.19454900	-3.15879400	-1.82545100
H	-8.93781100	-0.89789900	1.38987800

H	-9.20050500	-2.43970000	-0.54317500
C	5.41054100	-2.29865300	-1.28368300
C	4.44726200	-1.42988100	-0.81185400
C	4.64419900	-0.75231900	0.41092100
C	5.81539400	-0.89634100	1.18902100
C	6.78677600	-1.80512100	0.68775400
C	6.58081500	-2.48339400	-0.50573900
H	5.27859200	-2.82125800	-2.22605000
C	3.57699000	0.11126700	0.74628800
C	5.89262700	-0.10104800	2.36577200
H	7.70717900	-1.96375900	1.24392400
H	7.34556200	-3.16811200	-0.86072700
C	4.86284800	0.76665600	2.68026300
C	3.69535400	0.89044700	1.87385500
H	6.76603900	-0.16915800	3.00855900
H	4.94218000	1.37766900	3.57500500
H	2.91784700	1.59614700	2.15062200
C	3.14050300	-0.98357000	-1.35937800
C	2.48102700	-0.00727700	-0.30705300
O	2.64681700	-1.27019100	-2.43454100
N	2.08348300	1.27768200	-0.85258100
C	2.82301100	2.08194200	-1.81246300
C	1.79120700	3.19326600	-2.18321600
C	0.67662200	1.29159300	-1.21427400
H	3.11307100	1.51250700	-2.71070800
C	0.45337500	2.77866000	-1.49740000
H	1.67527600	3.24981600	-3.26931500
H	2.11894100	4.17870900	-1.84238300
H	3.73645200	2.48357000	-1.35987200
H	0.46633200	0.69791900	-2.12386000
H	-0.41485000	2.96828000	-2.13547700
H	0.31222500	3.31708500	-0.55720100

TS-exo-regioB-2

C	-2.31396100	-1.15385700	-2.27768000
H	-3.29460700	-0.67355000	-2.30861900
H	-2.45513800	-2.19873100	-1.98061300
H	-1.92437200	-1.16276800	-3.30505400
C	-1.34114900	-0.43544500	-1.37553200
H	-1.22884000	0.62884800	-1.56557600
C	-0.17815300	-1.09599200	-0.92197900
H	-0.09890000	-2.16758600	-1.05884200
C	1.07532800	-0.34591800	-0.88902600
O	1.16903600	0.87774700	-0.90174300
N	2.30251900	-1.07785300	-0.85628600
C	2.52528300	-2.45203400	-0.83158700
O	3.85602300	-2.68040400	-1.00378900
C	3.57333700	-0.34069500	-0.88081600
H	3.49983600	0.47444500	-1.60205900
C	4.52050800	-1.44965100	-1.35991700
H	5.49388000	-1.42982000	-0.86799100
H	4.66331200	-1.43536300	-2.44570000
O	1.73315800	-3.35309300	-0.66513100
C	3.92883600	0.24188700	0.50622300
H	4.06730600	-0.58516500	1.21277800
H	3.06596800	0.82578100	0.83771700
C	5.16332700	1.11496700	0.46500300
C	5.09562500	2.39912100	-0.09706200
C	6.39608700	0.66445700	0.95425400
C	6.22999400	3.20585700	-0.17144000
H	4.14185600	2.76684100	-0.46782900
C	7.53415800	1.47092100	0.88242200
H	6.46305000	-0.32156400	1.40818300
C	7.45439600	2.74320400	0.31689600
H	6.15770500	4.19914100	-0.60522500
H	8.47997300	1.10537700	1.27209900
H	8.33739900	3.37312400	0.26193300
C	-3.59619900	3.34635900	0.27096600
C	-3.37169300	1.98948300	0.36402300
C	-4.40406800	1.07865600	0.07845800
C	-5.69986300	1.48372200	-0.29638300
C	-5.91133100	2.88639100	-0.39423200
C	-4.88708900	3.78151800	-0.12200100
H	-2.80953500	4.05947900	0.49680500

C	-3.98914000	-0.27810000	0.23450900
C	-6.65336600	0.44825000	-0.51172400
H	-6.89158000	3.25910700	-0.67994600
H	-5.08138200	4.84698200	-0.20357600
C	-6.27242600	-0.86789500	-0.34585000
C	-4.94988200	-1.25182300	0.01931300
H	-7.67197600	0.69531500	-0.79700900
H	-7.00453100	-1.65452500	-0.50539400
H	-4.73593200	-2.30949300	0.11287200
C	-2.18099000	1.19542100	0.78424600
C	-2.53845500	-0.24852100	0.53274600
O	-1.14603800	1.63934100	1.26458100
N	-1.84808800	-1.23454800	1.21974200
C	-2.34861000	-2.61792300	1.39493500
C	-1.09530200	-3.44622400	1.75351800
C	-0.50563300	-1.17433200	1.32300900
H	-2.80510700	-2.96716100	0.46617900
C	0.01956300	-2.40609500	2.00000600
H	-0.81630200	-4.08746000	0.91441900
H	-1.26947800	-4.08770400	2.61996000
H	-3.11571500	-2.62157300	2.17560800
H	-0.06354300	-0.19342300	1.42835600
H	0.97711400	-2.72835800	1.58834500
H	0.16628800	-2.20637500	3.07084400

Pr-exo-regioB-2

C	-1.40458300	0.12813800	-2.18012600
H	-2.20720100	0.75413700	-2.58267100
H	-1.65964800	-0.91509700	-2.38722600
H	-0.49093500	0.37327200	-2.73221500
C	-1.19444300	0.38312300	-0.68921200
H	-0.87613200	1.42130600	-0.55409400
C	-0.08679400	-0.49665700	-0.03948800
H	-0.18062300	-1.54017100	-0.33860100
C	1.29974800	0.03274300	-0.33874300
O	1.55483200	1.22644400	-0.40063100
N	2.35344100	-0.87594300	-0.54215800
C	2.34727000	-2.28103000	-0.49472000
O	3.56712800	-2.72265300	-0.89604600
C	3.71079000	-0.37097700	-0.80418200
H	3.65534900	0.45183700	-1.51845600
C	4.34626000	-1.62530200	-1.41805800
H	5.38579200	-1.77175500	-1.12318500
H	4.27260400	-1.63765900	-2.51052500
O	1.46062600	-3.02422600	-0.15554900
C	4.40091200	0.11823500	0.48935800
H	4.50680800	-0.73013800	1.17530100
H	3.73184200	0.84434900	0.95920200
C	5.74822700	0.75104900	0.21790900
C	5.82112600	2.03299500	-0.34793500
C	6.94257700	0.07451100	0.49688600
C	7.05402600	2.61852800	-0.63134900
H	4.90238300	2.57608800	-0.55648700
C	8.17932200	0.65908500	0.21514100
H	6.90508600	-0.91255600	0.95188800
C	8.23797900	1.93172200	-0.35222300
H	7.09143400	3.61386600	-1.06456800
H	9.09470600	0.12091200	0.44369300
H	9.19861700	2.38897400	-0.56991500
C	-5.39578800	2.66766000	0.14721300
C	-4.44278800	1.66937400	0.12630900
C	-4.75157500	0.40885000	-0.42925700
C	-6.02445300	0.09253800	-0.95600500
C	-6.98466500	1.14053700	-0.93331300
C	-6.67076600	2.38453300	-0.40349600
H	-5.17733200	3.63985700	0.57813800
C	-3.67779300	-0.50739800	-0.36025100
C	-6.20016200	-1.23894600	-1.42444100
H	-7.98100300	0.96092600	-1.32916900
H	-7.42958100	3.16162500	-0.39947700
C	-5.16039800	-2.14580100	-1.33044300
C	-3.88884900	-1.79646200	-0.79220700
H	-7.15506700	-1.54334300	-1.84419400
H	-5.31395100	-3.16302200	-1.67954300

H	-3.10567900	-2.54548200	-0.72242100
C	-3.04425600	1.60364600	0.62281500
C	-2.46191100	0.18373000	0.24739400
O	-2.43254000	2.45681800	1.23872100
N	-1.90123400	-0.54874100	1.36816300
C	-2.44123500	-0.62596400	2.71562700
C	-1.29736200	-1.35178700	3.49126700
C	-0.46135500	-0.37450900	1.45196100
H	-3.38355900	-1.18485000	2.72529700
C	-0.08995200	-1.42064700	2.50496100
H	-1.59998300	-2.35246900	3.81022000
H	-1.03953600	-0.78977000	4.39339900
H	-2.63227900	0.36734500	3.15428100
H	-0.17473900	0.63496700	1.80034100
H	-0.01957900	-2.40556700	2.03765600
H	0.86174300	-1.20895700	3.00100000

Catalyst

C	4.33154200	-0.77791300	-0.88761400
C	3.39731700	1.25764300	0.74992300
C	5.24133600	-0.04171600	-0.12734700
C	2.96586400	-0.50386600	-0.85037000
C	2.49158700	0.51568500	-0.01527900
C	4.76273100	0.98313800	0.68515600
H	6.30067500	-0.26064300	-0.17090700
H	2.28063900	-1.07325700	-1.46121400
H	3.04016400	2.04325800	1.40871500
C	4.82957600	-1.92290100	-1.73482100
C	5.72136800	1.84437700	1.46620000
F	5.19057800	2.22969000	2.64846800
F	6.87860200	1.20353400	1.72393600
F	6.03135400	2.97432400	0.78982700
F	4.84985200	-3.07866600	-1.03716100
F	4.04662900	-2.12238200	-2.81582200
F	6.08779400	-1.70290100	-2.17493800
N	1.13113200	0.88805200	0.03997500
C	0.00216800	0.08879000	-0.00150500
N	-1.12781200	0.88552400	-0.05521200
H	-0.97817600	1.81972300	-0.41548200
S	0.00421100	-1.57455400	0.01088400
H	0.98104300	1.82651700	0.38880300
C	-4.32827400	-0.77301000	0.88729200
C	-3.39477700	1.25343400	-0.76244200
C	-5.23753400	-0.04265700	0.12229900
C	-2.96191900	-0.49933500	0.84757400
C	-2.48818600	0.51421800	0.00596600
C	-4.75918200	0.97888500	-0.69606500
H	-6.29683000	-0.26268000	0.16676500
H	-2.27660800	-1.06502300	1.46171300
H	-3.03864900	2.03675000	-1.42408100
C	-4.82473600	-1.91206500	1.74346300
C	-5.72845900	1.83192900	-1.47316000
F	-5.15873800	2.35260900	-2.58278800
F	-6.81335300	1.13021800	-1.85842000
F	-6.17097100	2.87304500	-0.73176000
F	-4.82545200	-3.07686400	1.06085900
F	-4.05163800	-2.08960700	2.83544800
F	-6.08970200	-1.69907200	2.16707900

Complex A

C	3.39213700	3.29951500	-0.38692600
C	2.52095300	0.85292900	-1.33693100
C	4.29164400	2.47877400	-1.06917800
C	2.07392300	2.90909900	-0.14914400
C	1.62619700	1.66878300	-0.62791300
C	3.84109900	1.24636900	-1.53679800
H	5.31563900	2.79097100	-1.22718500
H	1.40181200	3.55220600	0.39945400
H	2.17532700	-0.09267800	-1.74277300
C	3.83898200	4.66365400	0.07896100
C	4.77248200	0.28325900	-2.22096600
F	4.21506400	-0.25099400	-3.33015200
F	5.93683600	0.85305900	-2.57608300

F	5.07293200	-0.76684100	-1.40468100
F	3.54331000	5.61603900	-0.83146400
F	3.23947200	5.01807200	1.23506700
F	5.17453100	4.70860800	0.28201000
N	0.35593800	1.11861000	-0.39545700
C	-0.87524200	1.70237600	-0.17491400
N	-1.82284600	0.71308800	-0.02169100
H	-1.45444500	-0.23543800	-0.04878500
S	-1.15103100	3.35092100	-0.11507400
H	0.34324600	0.10701300	-0.50631600
C	-5.41720000	1.73862300	0.16960700
C	-3.81881700	-0.51096400	0.37008600
C	-6.01821000	0.49991500	0.38645500
C	-4.03495300	1.87433400	0.03568900
C	-3.21782800	0.73802000	0.13306200
C	-5.20034400	-0.62524700	0.48320200
H	-7.09338100	0.41213800	0.47633100
H	-3.59254800	2.84217900	-0.14646500
H	-3.20016500	-1.39759700	0.46765700
C	-6.28060200	2.97579000	0.12706700
C	-5.80957700	-1.99311400	0.63553300
F	-5.02921400	-2.81491700	1.37088300
F	-7.02342400	-1.94787700	1.21608600
F	-5.97416500	-2.59627200	-0.57325400
F	-6.46986200	3.48628400	1.36450000
F	-5.73132100	3.94890200	-0.62659900
F	-7.50511000	2.70727900	-0.37952800
C	-3.25029500	-3.77085800	-2.66720500
H	-4.18321200	-3.59747900	-2.11707400
H	-3.08677500	-4.84673100	-2.76169400
H	-3.39999000	-3.34706800	-3.66813300
C	-2.12137200	-3.08589800	-1.97332900
H	-2.22119500	-2.01176600	-1.82779900
C	-1.00969600	-3.68949300	-1.51971300
H	-0.83078600	-4.74610900	-1.66881400
C	0.01441700	-2.90975700	-0.80857600
O	-0.17058600	-1.74402200	-0.41647900
N	1.24789100	-3.48962100	-0.54282400
C	1.72639700	-4.76386200	-0.94566700
O	3.02703100	-4.85021400	-0.59617500
C	2.25495300	-2.80639900	0.29166600
H	2.32276700	-1.75631500	0.00818600
C	3.51533400	-3.57136200	-0.13132100
H	4.20613800	-3.74959000	0.69257000
H	4.04294600	-3.07731200	-0.95165800
O	1.12098500	-5.64800800	-1.49285300
C	1.91184700	-2.92142200	1.79462000
H	1.89944200	-3.98204800	2.07049600
H	0.89687800	-2.53622400	1.93238900
C	2.88211800	-2.16007200	2.67201200
C	2.81153500	-0.76183200	2.75779300
C	3.87678300	-2.82638700	3.39927400
C	3.71466900	-0.04896900	3.54480300
H	2.03640300	-0.22854400	2.21260200
C	4.78199200	-2.11527400	4.18965800
H	3.93424500	-3.91163200	3.35958800
C	4.70421900	-0.72468800	4.26242600
H	3.64249900	1.03299900	3.60224600
H	5.54299100	-2.64935400	4.75090000
H	5.40564500	-0.17005000	4.87826500

Complex B

C	5.81768000	0.96966000	-0.06270400
C	3.78056900	-0.87021000	0.30488700
C	6.14539400	-0.36302800	0.18431700
C	4.49184500	1.39826300	-0.13698800
C	3.45676000	0.47181300	0.05161500
C	5.10962600	-1.27875500	0.36354400
H	7.17955200	-0.67580200	0.24752700
H	4.26274000	2.43756200	-0.32015200
H	2.98587000	-1.58982900	0.46904600
C	6.91599500	1.96993900	-0.32536700
C	5.40454100	-2.73802800	0.58082800
F	5.24997300	-3.45329200	-0.56330700

F	6.66157600	-2.95040900	1.01419100
F	4.55923500	-3.29111700	1.48514800
F	7.15288500	2.10280600	-1.65134000
F	6.60287800	3.19417400	0.14400400
F	8.08144400	1.59651700	0.24759700
N	2.08446400	0.76151900	-0.04681300
C	1.38421900	1.93261800	0.12118600
N	0.03932100	1.70625300	-0.09719600
H	-0.22626000	0.74325100	-0.27267200
S	2.03985200	3.40690600	0.56246800
H	1.51955700	-0.07907600	-0.15920400
C	-2.25008100	4.65971700	-0.15156700
C	-2.29073400	1.93732000	0.34373100
C	-3.46620400	4.04434800	0.15192700
C	-1.06099800	3.93560300	-0.23156000
C	-1.07572700	2.55560600	0.02189400
C	-3.47229700	2.67291200	0.39213400
H	-4.38289600	4.61830600	0.19141500
H	-0.13575700	4.42932400	-0.48858000
H	-2.30905500	0.87376200	0.55153000
C	-2.21363500	6.15281600	-0.36555800
C	-4.75061900	1.93300900	0.67071100
F	-5.07023000	1.09443900	-0.35425900
F	-4.64422000	1.14560200	1.77135500
F	-5.79938700	2.75260000	0.85529600
F	-2.00304200	6.81288700	0.79423200
F	-1.23056600	6.51503000	-1.21495700
F	-3.38099500	6.60948900	-0.87304700
C	2.74663500	-6.18699900	0.03001500
H	2.91872500	-6.74842200	0.95699800
H	3.34254200	-5.27299900	0.06086400
H	3.11925100	-6.82225600	-0.78361300
C	1.28919300	-5.92026700	-0.14896800
H	0.62206600	-6.78062700	-0.17924600
C	0.73794500	-4.70217800	-0.27551100
H	1.33556600	-3.80106900	-0.25032700
C	-0.71997000	-4.58514200	-0.45095500
O	-1.49293600	-5.52978000	-0.50900700
N	-1.28177500	-3.28185300	-0.58833700
C	-0.67345600	-2.04528300	-0.51904000
O	-1.57603200	-1.08716700	-0.84242300
C	-2.74037300	-3.13268700	-0.78233200
H	-3.07475200	-3.87167900	-1.51115800
C	-2.79346800	-1.70689100	-1.34625700
H	-3.64039600	-1.11919000	-0.99370100
H	-2.75241400	-1.68053200	-2.43883900
O	0.46941400	-1.75514100	-0.21279400
C	-3.52114500	-3.31870500	0.53760000
H	-3.23089500	-2.52719100	1.23852700
H	-3.20908000	-4.27365100	0.96844300
C	-5.01882300	-3.30824200	0.31646200
C	-5.65139000	-4.43272900	-0.23489800
C	-5.79414300	-2.18368100	0.62632400
C	-7.02456200	-4.43068700	-0.47432400
H	-5.06206300	-5.31686500	-0.46691700
C	-7.17008100	-2.18060400	0.38639200
H	-5.32705800	-1.30679200	1.06535600
C	-7.78805300	-3.30237100	-0.16536500
H	-7.50003400	-5.31121800	-0.89647500
H	-7.75604100	-1.30053100	0.63408300
H	-8.85823600	-3.30103500	-0.34943300

TS-Mode A

C	-2.06482300	-3.65265800	-2.06450200
H	-2.85642400	-3.78717800	-1.31897700
H	-1.54909200	-4.60969400	-2.18135300
H	-2.55010100	-3.40226700	-3.01291300
C	-1.10458100	-2.57368100	-1.61297900
H	-1.49054200	-1.55623400	-1.62858800
C	-0.14435000	-2.85995300	-0.64593900
H	0.10857500	-3.88468300	-0.41619000
C	0.44168000	-1.82279100	0.16111700
O	0.18564100	-0.59612100	0.02431200
N	1.33385500	-2.16466300	1.18898800

C	1.73099300	-3.45571700	1.59412000
O	2.68551400	-3.32874300	2.54719100
C	1.95672600	-1.14027200	2.04549900
H	2.33279000	-0.32864500	1.42217200
C	3.11521600	-1.95566000	2.63947300
H	3.30586000	-1.72663300	3.68809900
H	4.03661600	-1.84105900	2.06127400
O	1.32045900	-4.52287300	1.21398600
C	0.98195700	-0.58340400	3.10744100
H	0.57362000	-1.42258800	3.68178700
H	0.14637500	-0.11510900	2.57855000
C	1.64369700	0.40730000	4.04418600
C	2.16806600	1.61602800	3.56195200
C	1.76656400	0.12825400	5.41172200
C	2.79746600	2.51634100	4.42033200
H	2.08723800	1.86291300	2.50751300
C	2.39037100	1.03073100	6.27555000
H	1.36249000	-0.80134000	5.80495200
C	2.90974400	2.22717300	5.78172600
H	3.19880300	3.44402200	4.02313000
H	2.46932900	0.79682600	7.33322000
H	3.39659900	2.92981900	6.45134200
C	4.10880200	-5.34323800	-1.42541100
C	3.46713200	-4.16215000	-1.72840800
C	4.04868800	-2.93134400	-1.37042900
C	5.28009600	-2.83055400	-0.69759100
C	5.93012900	-4.06020400	-0.39826300
C	5.35611500	-5.27125200	-0.75382200
H	3.67116800	-6.30084200	-1.68821000
C	3.24844000	-1.81414400	-1.76352300
C	5.73591900	-1.51359800	-0.39899900
H	6.88705700	-4.04693400	0.11650500
H	5.87338800	-6.19339300	-0.50722600
C	4.96689100	-0.42378300	-0.76356000
C	3.72094200	-0.55033900	-1.44069800
H	6.68536400	-1.36857300	0.10863700
H	5.31296800	0.57764600	-0.53134400
H	3.18291900	0.35639900	-1.68679900
C	2.18073900	-3.86632500	-2.41979500
C	2.05318800	-2.37411500	-2.39339100
O	1.42165200	-4.67545000	-2.94829200
N	1.10780800	-1.72638900	-3.10817600
C	1.10846900	-0.25654900	-3.33134900
C	0.08076100	-0.07247500	-4.45519300
C	-0.07845200	-2.27743200	-3.48586600
H	2.11385900	0.06510000	-3.60478300
C	-0.86171900	-1.29466600	-4.32686300
H	0.58686400	-0.08949200	-5.42447800
H	-0.44323500	0.88171000	-4.36974600
H	0.81275400	0.23264000	-2.39989600
H	-0.06965200	-3.34392000	-3.66178500
H	-1.12108200	-1.71441500	-5.30377000
H	-1.80804100	-1.02636700	-3.84172300
C	0.60541100	5.47712000	-0.92112700
C	1.38389300	2.90069500	-0.28606500
C	1.96334300	5.20365500	-0.75900400
C	-0.37002300	4.49112200	-0.77151000
C	0.01542800	3.18164400	-0.44099600
C	2.33962300	3.90019400	-0.44090400
H	2.70524200	5.98187800	-0.88021400
H	-1.41524900	4.72722800	-0.90400800
H	1.69304500	1.88944200	-0.03957500
C	0.16905600	6.89301600	-1.20944800
C	3.78890100	3.53099300	-0.29028300
F	4.22136900	2.77581500	-1.33803700
F	4.59400500	4.60468700	-0.21786000
F	4.00204700	2.78158500	0.82100400
F	-0.95176900	6.93145900	-1.95798100
F	-0.08863900	7.56956900	-0.06863500
F	1.12629800	7.58260300	-1.87023300
N	-0.83970800	2.08417600	-0.27720100
C	-2.20749000	1.97725600	-0.12985000
N	-2.53898000	0.65142500	0.05413600
H	-1.74066900	0.01791400	0.11634200
S	-3.28897100	3.25432300	-0.14880300

H	-0.33071200	1.20992900	-0.15397000
C	-6.17593600	-0.21968600	0.14734200
C	-3.70749200	-1.27672600	0.82501700
C	-6.11529000	-1.49978100	0.69530100
C	-5.02621700	0.53774500	-0.07754500
C	-3.77287900	0.01167100	0.26909400
C	-4.86563700	-2.02193900	1.02588600
H	-7.01662100	-2.07705900	0.85779700
H	-5.09881800	1.52289100	-0.51214800
H	-2.74728900	-1.69945600	1.10202300
C	-7.52295700	0.38392800	-0.16424600
C	-4.74940100	-3.42988200	1.54656200
F	-3.71869200	-3.56422600	2.40821900
F	-5.87047100	-3.82895900	2.17950200
F	-4.53273500	-4.31221000	0.53691300
F	-8.03862300	1.02009200	0.91077100
F	-7.45276800	1.28573600	-1.16512100
F	-8.41802200	-0.56162500	-0.52911600

TS-Mode B

C	-0.74326500	-3.15518800	-3.84012800
H	-0.71387500	-2.29634700	-4.52143600
H	-1.62647600	-3.05648400	-3.20338800
H	-0.86669600	-4.05055100	-4.45774000
C	0.52544900	-3.20531300	-3.01562400
H	1.44167800	-3.42895900	-3.55863400
C	0.67879000	-2.35155800	-1.92386300
H	-0.16200100	-1.80775300	-1.52062600
C	1.99507000	-2.12061500	-1.38821300
O	3.01301900	-2.74036000	-1.72135000
N	2.16921500	-1.11500000	-0.38058200
C	1.26088700	-0.21685600	0.12244300
O	1.82260500	0.47377100	1.14239000
C	3.50393400	-0.89355700	0.20928700
H	3.93996300	-1.85988200	0.46160600
C	3.11769600	-0.10006000	1.46556300
H	3.79804800	0.72145600	1.68852700
H	2.99184000	-0.73680400	2.34539900
O	0.11847200	0.01869200	-0.24734500
C	4.45053000	-0.12999900	-0.74476700
H	4.08100500	0.89279800	-0.88090800
H	4.41247900	-0.63400400	-1.71374300
C	5.87246600	-0.11252700	-0.22388700
C	6.65099100	-1.27880900	-0.28132300
C	6.43206400	1.04038900	0.34106700
C	7.95208500	-1.29371400	0.21834500
H	6.23189000	-2.17480700	-0.73346200
C	7.73612500	1.02702800	0.84182300
H	5.85118000	1.95719000	0.37200200
C	8.49841200	-0.13926000	0.78455700
H	8.54314300	-2.20334700	0.15992700
H	8.15604500	1.93190400	1.27154700
H	9.51326000	-0.14845400	1.17112700
C	-1.81986800	-2.92452200	2.29617000
C	-0.78795900	-3.47077600	1.56318900
C	0.49713600	-3.58498000	2.12396800
C	0.80528500	-3.15313500	3.42655600
C	-0.26694600	-2.57759400	4.16419400
C	-1.53386600	-2.47272800	3.61048300
H	-2.82095800	-2.85422100	1.88355800
C	1.42709300	-4.20417600	1.23068000
C	2.14564300	-3.35816600	3.86506300
H	-0.08952300	-2.22475100	5.17657900
H	-2.33363100	-2.03608300	4.20094600
C	3.05360800	-3.96430100	3.01696800
C	2.71795300	-4.39525300	1.70181800
H	2.44478200	-3.05492000	4.86432600
H	4.06987300	-4.13064000	3.36254100
H	3.48763300	-4.87465500	1.11047600
C	-0.73092900	-4.04714300	0.18961600
C	0.69268000	-4.45611200	-0.01157800
O	-1.67713400	-4.18620100	-0.58453500
N	1.09868700	-5.14605800	-1.10029600
C	2.44388300	-5.77376500	-1.23154000

C	2.56322800	-6.08314700	-2.73057900
C	0.40629400	-5.17780000	-2.27549200
H	2.45687400	-6.67171400	-0.60368700
C	1.10550400	-6.11008400	-3.23151700
H	3.09590300	-7.01878900	-2.91306100
H	3.11383600	-5.27384700	-3.21568200
H	3.20729200	-5.07579500	-0.89894300
H	-0.67043700	-5.11691300	-2.18915100
H	0.67283300	-7.11826700	-3.16753000
H	1.00838400	-5.78793000	-4.27245700
C	-6.23431200	0.54278100	0.50166400
C	-3.88411500	-0.62121200	-0.39388500
C	-6.25679200	-0.78122300	0.06612200
C	-5.05906200	1.29348100	0.50280400
C	-3.86822900	0.71463700	0.03922300
C	-5.06647300	-1.35691500	-0.37507400
H	-7.17659400	-1.35162400	0.07454000
H	-5.06352300	2.31413100	0.85359600
H	-2.97161200	-1.08821200	-0.75138300
C	-7.52117500	1.19702200	0.93769200
C	-5.03643700	-2.80605400	-0.78494400
F	-4.63784600	-3.59899700	0.24054500
F	-6.25488200	-3.24660300	-1.16656400
F	-4.18667300	-3.02218600	-1.81065200
F	-8.15458500	1.78599500	-0.10098500
F	-8.38275600	0.29672100	1.46423900
F	-7.31233700	2.15151100	1.86831500
N	-2.61912100	1.35871400	0.02565800
C	-2.28176500	2.69588600	-0.03965200
N	-0.91174900	2.82309000	-0.03440000
H	-0.40427800	1.94497800	0.06130300
S	-3.37237100	3.96475200	-0.11307900
H	-1.83846600	0.71219500	-0.04940200
C	0.54859700	6.21282500	-0.65559400
C	1.27987600	3.69420700	0.22648800
C	1.88052100	5.97709400	-0.31526600
C	-0.42146400	5.21321700	-0.57493000
C	-0.05795600	3.93330600	-0.12733500
C	2.23291100	4.70223200	0.12388800
H	2.61801600	6.76675000	-0.37926600
H	-1.44738800	5.42164800	-0.83919800
H	1.56970100	2.71907300	0.60252400
C	0.16200200	7.56683000	-1.19681700
C	3.66295700	4.36876200	0.44477500
F	4.25227500	3.67933500	-0.57174800
F	4.41402000	5.46295000	0.66497000
F	3.76832100	3.57247900	1.53937100
F	0.34912700	7.63177900	-2.53578100
F	-1.13228400	7.85774400	-0.96238100
F	0.90967200	8.55218800	-0.64956500