Mechanism of Palladium/Amine Cocatalyzed Carbocyclization of Aldehydes with Alkynes and its Merging with "Pd Oxidase Catalysis"

Stefano Santoro,[a] *Luca Deiana,*[a,b] *Gui-Ling Zhao,*[a,b] *Shuangzheng Lin,*[a,b] *Fahmi Himo*,*[a] *and Armando Córdova**[a-c]

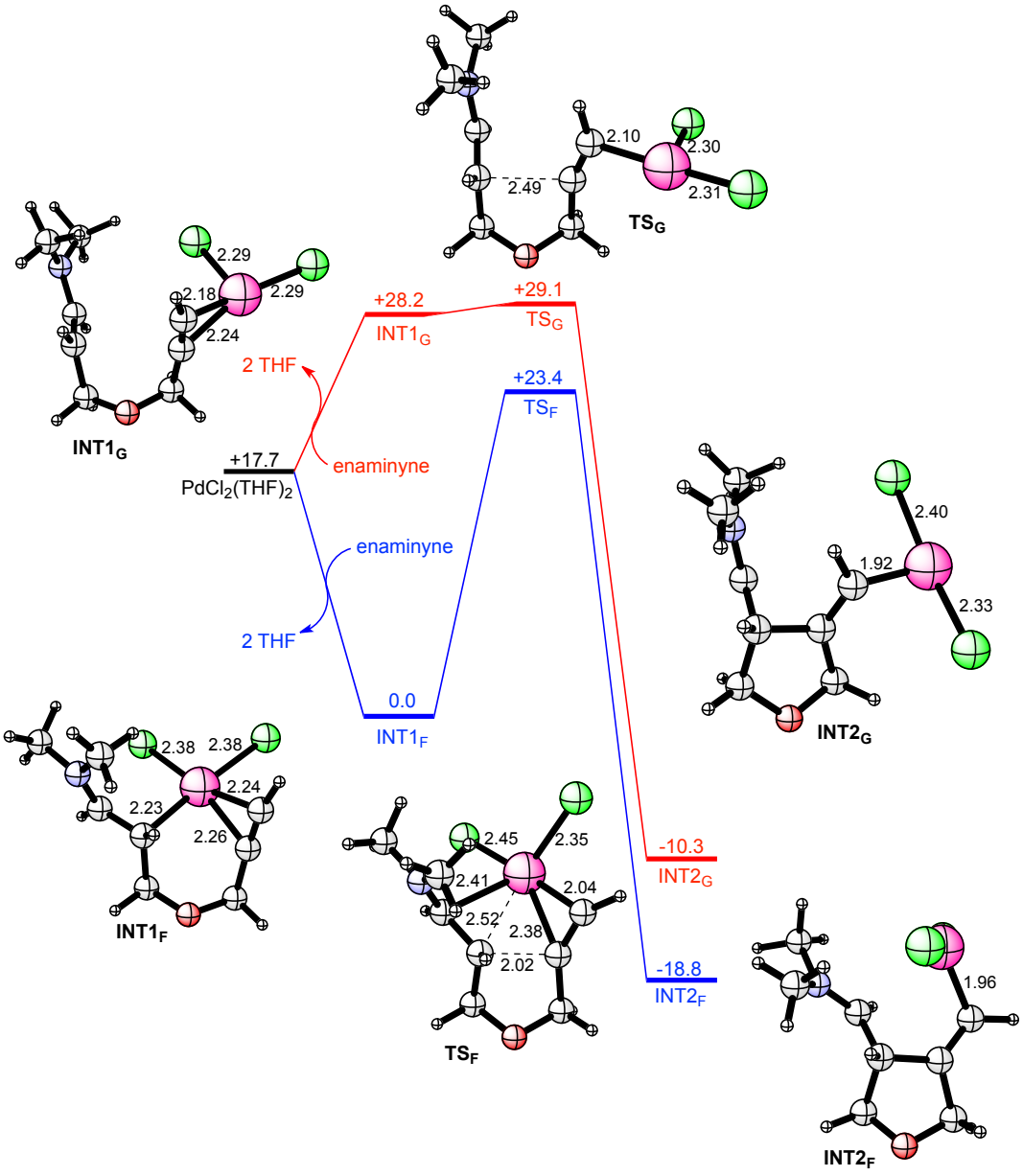
a) Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, SE-106 91 Stockholm, Sweden
b) Berzelii Center EXSELENT on Porous Materials, Arrhenius Laboratory, Stockholm University, SE-106 91 Stockholm, Sweden
c) Department of Natural Sciences, Engineering and Mathematics, Mid Sweden University, SE-851 70 Sundsvall, Sweden

acordova@organ.su.se, armando.cordova@miun.se, himo@organ.su.se

SUPPORTING INFORMATION

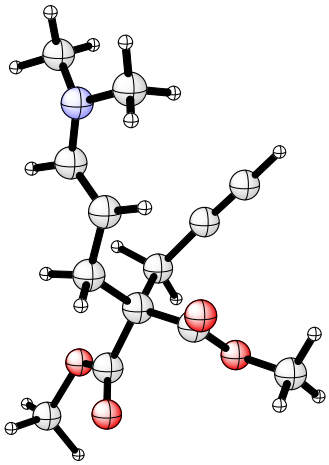
SUPPORTING INFORMATION, PART A

1. Free energy profile for the Pd(II)-catalyzed carbocyclization of the enaminyne obtained from 3-(prop-2-yn-1-yloxy)propanal.



2. Optimized structures and Cartesian coordinates of stationary points.

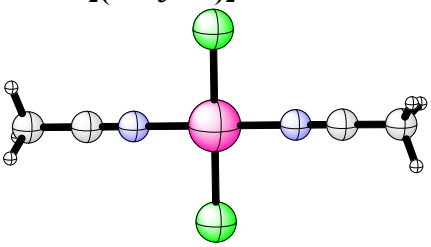
- A



B3LYP/6-311+G(2d,2p) energy: -862.661391735 a.u.
ZPE: 0.305789 a.u.
Thermal correction to Gibbs Free Energy: 0.254146 a.u.
Solvation energy: -4.67 kcal/mol
Dispersion correction: -42.60 kcal/mol

C	4.26827900	0.80563200	-0.73739400
H	5.35320200	0.92799500	-0.79846600
H	3.83672500	1.08549000	-1.70266400
H	3.87874500	1.49991700	0.02522200
N	3.95954400	-0.58233200	-0.44695000
C	4.79729900	-1.20542400	0.56581600
H	4.56409800	-2.27232800	0.62973300
H	5.85117900	-1.10595900	0.28653200
H	4.66528900	-0.76746300	1.56964500
C	2.62487500	-0.96832500	-0.47958300
H	2.47983300	-2.01010700	-0.19374500
C	1.56371700	-0.23568900	-0.86485100
H	1.66701800	0.80818700	-1.13685500
C	0.18969800	-0.82648300	-0.98397600
H	-0.18681600	-0.73472200	-2.00950400
H	0.23057600	-1.89748100	-0.75009400
C	-0.48160600	-0.15905000	1.44335200
H	-1.38269600	-0.11371300	2.06229100
H	0.01510100	-1.10501500	1.68263100
C	0.38117000	0.96358500	1.81153100
C	1.04635900	1.90685100	2.16769400
H	1.64934400	2.73363100	2.46355200
C	-0.90710600	-0.19812400	-0.05892900
C	-2.15556400	-1.06525000	-0.25997600
C	-1.27344700	1.21293600	-0.54454300
O	-2.93914900	-0.92507900	-1.17316000
O	-0.77916300	1.78550700	-1.48778100
O	-2.24108800	-2.06010700	0.64890200
O	-2.23245100	1.74471600	0.23984400
C	-3.34733300	-2.96305900	0.46652300
H	-3.26769600	-3.69072300	1.27353600
H	-4.29483800	-2.42295900	0.52581300
H	-3.28197300	-3.45615900	-0.50604500
C	-2.65181700	3.07296100	-0.11527500
H	-3.42457100	3.33963100	0.60513900
H	-1.81052600	3.76697700	-0.05099900
H	-3.05114100	3.08746100	-1.13185000

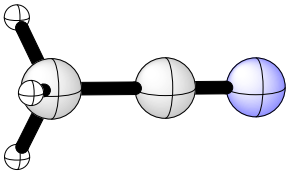
- $PdCl_2(CH_3CN)_2$



B3LYP/BS2 energy: -1312.89965167 a.u.
ZPE: 0.096895 a.u.
Thermal correction to Gibbs Free Energy: 0.050632 a.u.
Solvation energy: -10.53 kcal/mol
Dispersion correction: -17.25 kcal/mol

Pd	-0.00206600	0.00224900	0.01344100
Cl	-0.00928900	-2.36618000	0.01046200
Cl	0.00506300	2.37050600	0.01616000
N	-2.00316800	0.00661400	0.01398700
N	1.99894100	-0.00308800	0.01233800
C	3.15172200	-0.00559200	0.01065900
C	-3.15595500	0.00506400	0.01323800
C	-4.61139900	0.00089600	0.01199500
H	-4.98163200	0.56036300	-0.85140100
H	-4.97771100	-1.02787700	-0.04066000
H	-4.98294100	0.46944300	0.92738300
C	4.60712900	-0.00699900	0.00838700
H	4.97725300	0.98754300	-0.25475300
H	4.97767200	-0.27751400	1.00092900
H	4.97491100	-0.73413600	-0.72066000

- CH_3CN

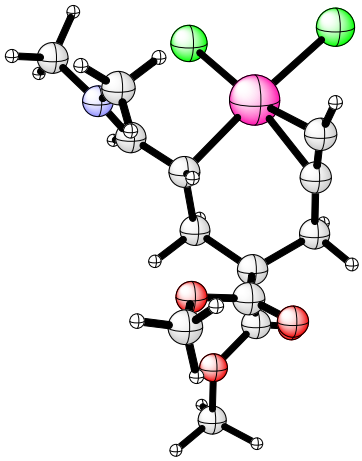


B3LYP/6-311+G(2d,2p) energy: -132.800199277 a.u.
ZPE: 0.045437 a.u.
Thermal correction to Gibbs Free Energy: 0.022457 a.u.
Solvation energy: -3.64 kcal/mol
Dispersion correction: -2.99 kcal/mol

C	0.00000000	0.00000000	0.27993300
N	0.00000000	0.00000000	1.44021100
C	0.00000000	0.00000000	-1.18053300
H	0.00000000	1.02588700	-1.55929000

H	0.88844500	-0.51294400	-1.55929000
H	-0.88844500	-0.51294400	-1.55929000

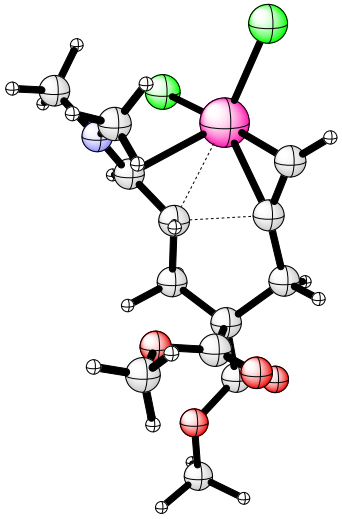
- INT1$_A$



B3LYP/BS2 energy: -1909.95299730 a.u.
ZPE: 0.311247 a.u.
Thermal correction to Gibbs Free Energy: 0.252627 a.u.
Solvation energy: -15.81 kcal/mol
Dispersion correction: -60.76 kcal/mol

C	1.98947400	2.88912500	1.21786900
H	2.50658200	3.81940800	1.45666800
H	1.02295700	2.88479500	1.72562900
H	2.58565300	2.03954900	1.57472400
N	1.80710300	2.80461300	-0.22905200
C	2.83695000	3.45434700	-1.04420800
H	2.57504900	3.37373000	-2.09915800
H	2.91059000	4.50912500	-0.76563200
H	3.80069100	2.95788100	-0.89243200
C	1.01530000	1.88755900	-0.76899800
H	1.03304800	1.86031300	-1.85316500
C	0.17434300	0.97350200	-0.08810100
H	-0.02389900	1.21488700	0.95299600
C	-1.06119900	0.51282900	-0.86781200
H	-1.66402200	1.38011400	-1.15820800
H	-0.74828400	0.01428000	-1.79307400
C	-1.33613200	-1.77148200	0.34259600
H	-2.06876700	-2.35783500	0.90655000
H	-1.06063500	-2.35054400	-0.54233500
C	-0.16493000	-1.55225700	1.19148800
C	0.71503800	-1.39712800	2.03938800
H	1.33823200	-1.44760500	2.90599300
Pd	1.63356000	-0.68974200	0.13533900
Cl	3.02707000	0.00896900	-1.67551700
Cl	3.08991900	-2.52247200	0.55550800
C	-2.01432200	-0.45132900	-0.10703500
C	-2.70065000	0.18207700	1.12081300
C	-3.13865800	-0.83859600	-1.09404700
O	-3.29139900	-0.47052600	1.95347900
O	-3.20291900	-1.89047300	-1.68615900
O	-2.60066300	1.52256800	1.15870600
O	-4.02209200	0.16615700	-1.23960800
C	-3.30328100	2.15641200	2.24529200
H	-4.37346500	1.94967400	2.17476200
H	-2.93395900	1.79022100	3.20576500
H	-3.11008800	3.22315300	2.13614100
C	-5.10085800	-0.08621600	-2.16297400
H	-5.71328000	0.81448900	-2.14883300
H	-4.70804100	-0.27139300	-3.16513800
H	-5.68050700	-0.95370200	-1.84028300

- TS$_A$

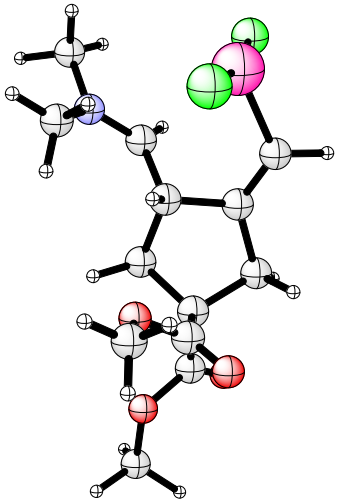


B3LYP/BS2 energy: -1909.91104649 a.u.
ZPE: 0.310172 a.u.
Thermal correction to Gibbs Free Energy: 0.250853 a.u.
Solvation energy: -16.32 kcal/mol
Dispersion correction: -59.88 kcal/mol

C	-1.78192400	2.92206200	-0.25795800
H	-1.97871600	3.96382900	0.00629800
H	-0.85410100	2.87495100	-0.82743600
H	-2.60036100	2.54482900	-0.88111400
N	-1.68734300	2.13760900	0.97375000
C	-2.77040700	2.38078800	1.93442500
H	-2.61605000	1.77986800	2.82861700
H	-2.78854500	3.44446600	2.18846900
H	-3.72818300	2.08616700	1.49281700
C	-0.94540700	1.03481200	1.09798800
H	-1.05604800	0.52417600	2.04926700
C	0.14169000	0.62427300	0.22866400
H	0.40352400	1.40119700	-0.48412800
C	1.35947300	0.02701400	0.91063400
H	1.83846600	0.75865900	1.56626900
H	1.06504400	-0.83728800	1.51563900
C	1.50827500	-1.20086900	-1.22587600
H	2.00505800	-1.20157600	-2.20088600
H	1.43248300	-2.23961000	-0.88823900
C	0.13261600	-0.64192600	-1.36918600
C	-0.96981300	-0.69660600	-2.01681700
H	-1.39769000	-0.96332200	-2.96944100
Pd	-1.99461800	-0.58423400	-0.26713000
Cl	-2.92623500	-1.08725400	1.94331200
Cl	-4.01924800	-0.82524300	-1.43945400
C	2.34407600	-0.42108300	-0.19529900
C	3.07423400	0.74019200	-0.89743700
C	3.41843600	-1.33926200	0.41682100

O	3.67086700	0.60137500	-1.94207800
O	3.39409800	-2.54721000	0.38430200
O	2.98831400	1.90752800	-0.23396100
O	4.36490600	-0.61449800	1.03857300
C	3.72105000	3.00241900	-0.82074700
H	4.78864700	2.77306600	-0.83852300
H	3.37976600	3.18750700	-1.84150900
H	3.52279000	3.86236300	-0.18201700
C	5.41177400	-1.37571100	1.67698100
H	6.07929200	-0.63774400	2.11980900
H	4.99132300	-2.02847300	2.44489600
H	5.94041900	-1.98328200	0.93952100

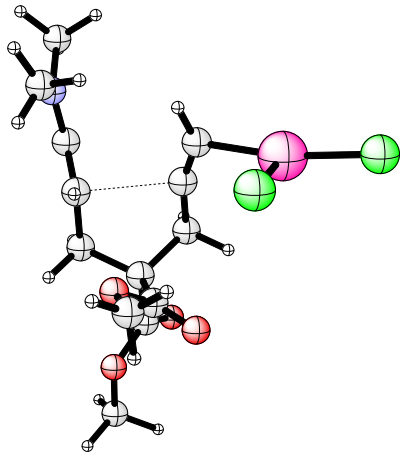
- INT2$_A$



B3LYP/BS2 energy: -1909.98816005 a.u.
ZPE: 0.314090 a.u.
Thermal correction to Gibbs Free Energy: 0.255468 a.u.
Solvation energy: -12.82 kcal/mol
Dispersion correction: -60.65 kcal/mol

C	-1.19167100	1.72269400	2.52586000
H	-1.63576000	2.02499200	3.47402500
H	-0.11527700	1.89372600	2.56797800
H	-1.62848800	2.29857200	1.69981900
N	-1.47750600	0.29483000	2.31064000
C	-2.59459000	-0.26927500	3.08048900
H	-2.82307500	-1.27091900	2.71641800
H	-2.33304900	-0.29276800	4.14189900
H	-3.47599000	0.36328900	2.93945900
C	-0.95774200	-0.38104000	1.31687900
H	-1.26048200	-1.42169700	1.23399200
C	0.19352200	0.07948600	0.47979900
H	0.19201500	1.17011700	0.40134900
C	1.57021100	-0.40551800	1.00952600
H	1.98023800	0.22093800	1.80229000
H	1.49028100	-1.43455100	1.37889800
C	1.50384100	-0.95351000	-1.36875600
H	1.78386900	-0.57527000	-2.35442200
H	1.59143700	-2.04442900	-1.39377000
C	0.11434600	-0.51725400	-0.92105700
C	-1.03655700	-0.63727200	-1.57000300
H	-1.18248000	-1.04999300	-2.56438100
Pd	-2.70941100	-0.08567500	-0.70274900
Cl	-3.35945400	-2.28952900	-0.16018800
Cl	-2.33008400	2.23228700	-0.88626600
C	2.45622800	-0.41269700	-0.26936900
C	2.97721500	0.97374800	-0.68253500
C	3.66654000	-1.33271600	-0.05944000
O	3.57146000	1.16614000	-1.71895300
O	3.74075200	-2.48174100	-0.42898400
O	2.69559100	1.94262000	0.21073700
O	4.62311500	-0.70651300	0.65384000
C	3.15696000	3.25991800	-0.15281800
H	4.24326200	3.26216500	-0.26456000
H	2.69898700	3.57574700	-1.09240000
H	2.85093700	3.91299100	0.66386500
C	5.80497100	-1.48496500	0.92375200
H	6.46383200	-0.82931800	1.49198800
H	5.55174900	-2.37560600	1.50365800
H	6.27858900	-1.79129600	-0.01148400

- TS$_B$

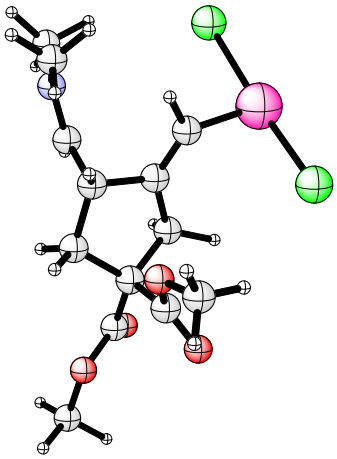


B3LYP/BS2 energy: -1909.90669615 a.u.
ZPE: 0.308686 a.u.
Thermal correction to Gibbs Free Energy: 0.246393 a.u.
Solvation energy: -15.03 kcal/mol
Dispersion correction: -55.53 kcal/mol

C	-0.62429200	4.37396400	1.24094300
H	-0.55281200	5.45201900	1.40876800
H	-1.33647300	3.95910000	1.95880600
H	0.36152200	3.93272300	1.43658300
N	-1.09691800	4.13702800	-0.11484600
C	-0.67709500	5.08105500	-1.13973500
H	-1.22275400	4.88687100	-2.06584200
H	-0.89162500	6.10635200	-0.81954300
H	0.39812100	5.00624900	-1.35423600
C	-1.72380500	2.97877300	-0.45654000
H	-2.12102100	2.98251000	-1.47065700
C	-1.90708900	1.87024800	0.32183200
H	-1.51055000	1.83091900	1.32924900
C	-2.82553600	0.75485300	-0.08520800
H	-3.61502500	0.60361600	0.65780000
H	-3.32009800	1.01184200	-1.03003000
C	-0.83672300	-0.36410300	-1.17322600
H	-0.30338800	-1.31421900	-1.29264500

H	-1.15123700	-0.04856300	-2.17367200
C	0.08981000	0.60749700	-0.58702500
C	1.15296500	1.15572400	-0.20045300
H	1.48325500	2.07311700	0.25387800
Pd	2.64721700	-0.29128100	-0.45946100
Cl	2.59144500	-0.60186900	1.82382900
Cl	4.47306900	-1.59126200	-1.02364200
C	-2.09179500	-0.60458300	-0.30282700
C	-1.63912300	-1.33356800	0.97450700
C	-3.03643300	-1.54309700	-1.06711000
O	-1.16357300	-2.44616800	0.93825100
O	-2.95366400	-1.79537600	-2.24843200
O	-1.78733700	-0.60565100	2.09057100
O	-4.01307900	-1.99138200	-0.26122400
C	-1.25411800	-1.21654500	3.28947600
H	-0.17628300	-1.35558400	3.18225300
H	-1.47998200	-0.51789300	4.09421700
H	-1.73346400	-2.18127100	3.46577200
C	-4.96951800	-2.87844000	-0.87464300
H	-4.46698000	-3.77192300	-1.25108400
H	-5.67465000	-3.13715400	-0.08582300
H	-5.47910000	-2.37779000	-1.70112000

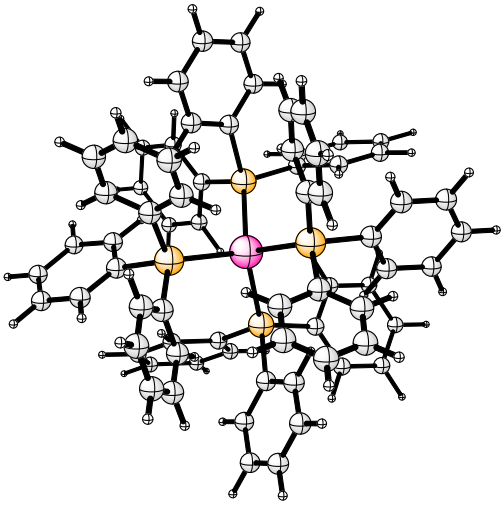
- INT1$_B$



B3LYP/BS2 energy: -1909.96841569 a.u.
ZPE: 0.313805 a.u.
Thermal correction to Gibbs Free Energy: 0.253810 a.u.
Solvation energy: -19.07 kcal/mol
Dispersion correction: -57.92 kcal/mol

C	1.85745700	3.22450000	2.02300100
H	2.10028400	4.24834900	2.31798800
H	1.10951600	2.82364000	2.70304000
H	2.76558100	2.61476100	2.07089900
N	1.35880700	3.23916100	0.64422700
C	2.30191900	3.80448100	-0.33963800
H	1.77875900	4.00605200	-1.27495300
H	2.71839900	4.73363300	0.05370300
H	3.09440800	3.06709000	-0.52214600
C	0.31126000	2.57345000	0.22862600
H	0.09440400	2.68970800	-0.83083000
C	-0.52845400	1.59377400	0.95025900
H	-0.38137800	1.57326800	2.02884500
C	-2.02496000	1.59431000	0.54406200
H	-2.67306500	1.73415400	1.40942300
H	-2.23568000	2.41097400	-0.15477100
C	-0.90574000	-0.14648200	-0.77816600
H	-0.78013900	-1.21935300	-0.94209900
H	-0.81707700	0.34220200	-1.75653500
C	0.09018300	0.36666200	0.22937500
C	1.33886800	-0.03265000	0.51406100
H	1.90442700	0.46588200	1.30004200
Pd	2.42660900	-1.30862700	-0.40880100
Cl	1.07223700	-3.15565000	0.06018200
Cl	3.92270100	0.47517500	-0.96688700
C	-2.28522100	0.23012700	-0.16946900
C	-2.70318900	-0.89403100	0.78356600
C	-3.36716300	0.38816600	-1.23987400
O	-3.35368200	-1.85510900	0.44432600
O	-3.18300900	0.33251200	-2.43426800
O	-2.19078100	-0.72119500	2.01862600
O	-4.55414900	0.67130500	-0.67046500
C	-2.34703700	-1.84860900	2.90802000
H	-1.80190700	-2.70793900	2.51188500
H	-1.92319900	-1.53048400	3.86003800
H	-3.40304900	-2.10282100	3.01769800
C	-5.66012100	0.81069800	-1.58140900
H	-5.81349500	-0.11949100	-2.13285000
H	-6.52599000	1.03435700	-0.95902900
H	-5.47425900	1.62031700	-2.29135900

- Pd(Ph$_3$P)$_4$



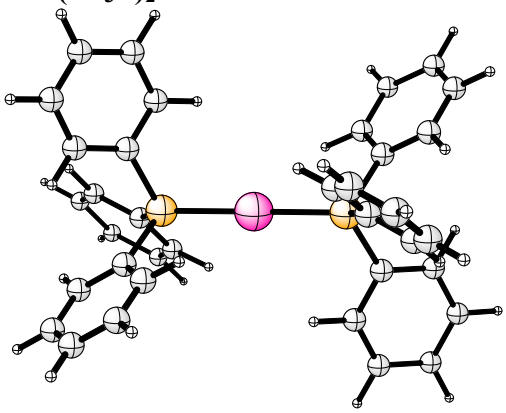
B3LYP/BS2 energy: -4272.9181816 a.u.
ZPE: 1.101443 a.u.
Thermal correction to Gibbs Free Energy: 0.98274 a.u.
Solvation energy: -2.65 kcal/mol
Dispersion correction: -306.81 kcal/mol

Pd	0.00227000	0.01360900	-0.01381400
P	1.46638300	-1.49558200	-1.47799400
P	1.51031300	1.47442700	1.45692200
P	-1.47512600	1.49090900	-1.48423200
P	-1.46613700	-1.45208600	1.49655300
C	-0.65775300	4.54802000	4.24703200
C	-1.12990700	4.27355800	2.96187800
C	-0.47466700	3.33608300	2.16259400

C	0.67243900	2.66977500	2.61964800
C	1.13950100	2.95705000	3.91305100
C	0.47531400	3.88351100	4.72079700
H	-1.16994300	5.27115300	4.87600300
H	-2.01695400	4.77103800	2.58131600
H	-0.86911200	3.10844800	1.17949700
H	2.02468000	2.45985900	4.29427700
H	0.85038900	4.08924500	5.71991300
C	4.57336700	4.25493400	-0.74414100
C	3.76217800	4.79472000	0.25479900
C	2.84162600	3.98846300	0.93098900
C	2.70774400	2.62808000	0.61027400
C	3.52356200	2.10226300	-0.40561800
C	4.45269400	2.90199600	-1.07017400
H	5.29145600	4.88228300	-1.26510000
H	3.84843400	5.84534200	0.51961100
H	2.23069700	4.42561500	1.71273200
H	3.43065700	1.05938800	-0.68717700
H	5.06738800	2.46700400	-1.85246300
C	4.27883400	-0.71437400	4.53922200
C	4.81935800	0.29630200	3.74306200
C	4.02003700	0.96799700	2.81307300
C	2.66627000	0.63047100	2.65513600
C	2.13970900	-0.39515000	3.45732400
C	2.93199400	-1.05610600	4.39512700
H	4.90121200	-1.23201900	5.26404900
H	5.86512300	0.57323600	3.84805200
H	4.45732800	1.75843300	2.21346000
H	1.10280400	-0.68965700	3.34307300
H	2.49610600	-1.84740500	4.99752500
C	4.23771600	0.67549500	-4.56665700
C	4.71624600	-0.45694600	-3.90445300
C	3.91411400	-1.12190400	-2.97370000
C	2.62168600	-0.65626300	-2.67974300
C	2.15988400	0.49019100	-3.34380400
C	2.95349500	1.14622400	-4.28557700
H	4.86231700	1.18828100	-5.29315000
H	5.71470800	-0.83089300	-4.11535300
H	4.29890000	-2.00663700	-2.47845000
H	1.17762900	0.88354600	-3.11088400
H	2.56930800	2.03273000	-4.78122600
C	4.57065200	-4.24631500	0.70229500
C	4.41315400	-2.90265000	1.05084500
C	3.46849600	-2.11624900	0.39254300
C	2.67287200	-2.64527500	-0.63690800
C	2.84388200	-3.99587000	-0.98074600
C	3.78076200	-4.78944500	-0.31196700
H	5.30087000	-4.86435500	1.21758100
H	5.01013400	-2.46476800	1.84519900
H	3.34297600	-1.08227700	0.69246100
H	2.24883400	-4.43501600	-1.77360100
H	3.89565400	-5.83294000	-0.59341500
C	-0.73343400	-4.57197500	-4.24521300
C	-1.04729500	-4.45818300	-2.88879700
C	-0.38361400	-3.52546100	-2.09254800
C	0.61964000	-2.69870400	-2.62579900
C	0.92823400	-2.82576700	-3.98966200
C	0.25272800	-3.75012000	-4.79217500
H	-1.25385000	-5.29306100	-4.86956800
H	-1.81953300	-5.08136900	-2.44800100
H	-0.65592800	-3.43957000	-1.04659100
H	1.70019400	-2.20662400	-4.43257500
H	0.50829300	-3.83091500	-5.84552000
C	-4.65545100	4.14323000	0.70674800
C	-4.47812100	2.79681800	1.03458300
C	-3.51443100	2.03745100	0.37173100
C	-2.71930700	2.59753400	-0.64165900
C	-2.91172800	3.95010300	-0.96591900
C	-3.86749200	4.71628400	-0.29250000
H	-5.40008800	4.74022800	1.22622100
H	-5.07401100	2.33571400	1.81647900
H	-3.37606100	1.00011100	0.65376100
H	-2.31787600	4.41191300	-1.74672400
H	-3.99810700	5.76213000	-0.55778200
C	0.71271700	4.67348300	-4.13602300
C	1.04513200	4.49197500	-2.79129100
C	0.38328000	3.52740100	-2.03213500
C	-0.63367600	2.73580000	-2.59073700
C	-0.96238300	2.93222800	-3.94163200
C	-0.28994000	3.88878000	-4.70766400
H	1.23137700	5.41877700	-4.73290700
H	1.82977400	5.08525400	-2.33146400
H	0.66869600	3.38529400	-0.99621000
H	-1.74585200	2.34087400	-4.40217700
H	-0.55858600	4.02260600	-5.75224400
C	-4.12878000	-0.69757600	-4.66476000
C	-2.78627900	-1.03588100	-4.47794700
C	-2.02669700	-0.37373200	-3.51385300
C	-2.58258200	0.64913700	-2.72813900
C	-3.93128000	0.98381500	-2.92995700
C	-4.69777800	0.31122400	-3.88596400
H	-4.72611200	-1.21641900	-5.40957500
H	-2.32855300	-1.82531200	-5.06649800
H	-0.99281100	-0.66396900	-3.36701400
H	-4.38972300	1.77185500	-2.34304000
H	-5.74066000	0.58432800	-4.02394600
C	0.71361700	-4.52664900	4.27924000
C	1.10465900	-4.33821100	2.95155300
C	0.44656800	-3.40094700	2.15575600
C	-0.62440500	-2.64543700	2.65911400
C	-1.01043500	-2.84666100	3.99429900
C	-0.34223300	-3.77524300	4.79769200
H	1.22858200	-5.25068000	4.90481900
H	1.93170400	-4.90447800	2.53392700
H	0.78015100	-3.24655300	1.13632700
H	-1.83557400	-2.28147300	4.41309500
H	-0.65597800	-3.91418600	5.82898600
C	-4.25560800	0.74312700	4.55551700
C	-2.90034800	1.06333000	4.44500300
C	-2.09819900	0.40106400	3.51647800
C	-2.62421100	-0.60650200	2.69045800
C	-3.98689900	-0.92133500	2.81389400
C	-4.79542700	-0.24755300	3.73437200
H	-4.88459700	1.26217100	5.27356700
H	-2.46529700	1.83922700	5.06770000
H	-1.05323600	0.67792500	3.43224300
H	-4.42400000	-1.69711300	2.19536700
H	-5.84774200	-0.50806100	3.81280400
C	-4.52639000	-4.24972300	-0.68096300
C	-3.85521800	-4.72621200	0.44692800

C	-2.93307000	-3.91602100	1.11436100
C	-2.65690300	-2.61732500	0.65568900
C	-3.32905400	-2.15779700	-0.48719400
C	-4.26238800	-2.95945400	-1.14524000
H	-5.24632400	-4.88045300	-1.19548800
H	-4.05240100	-5.72940100	0.81569000
H	-2.43092200	-4.29960400	1.99567900
H	-3.10925300	-1.17076900	-0.87633700
H	-4.76473000	-2.57681900	-2.02864400

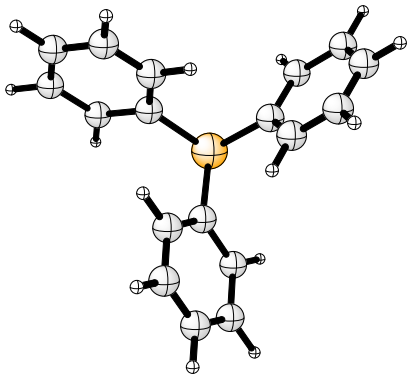
- $Pd(Ph_3P)_2$



B3LYP/BS2 energy: -2199.87509097 a.u.
ZPE: 0.550063 a.u.
Thermal correction to Gibbs Free Energy: 0.472296 a.u.
Solvation energy: -3.41 kcal/mol
Dispersion correction: -125.35 kcal/mol

Pd	0.00165900	0.00388200	0.00147200
P	2.32890100	-0.00355700	0.00310300
P	-2.32521200	0.00595400	-0.00087200
C	-3.11104100	1.67532200	0.14643700
C	-2.42533600	2.76375200	-0.41707100
C	-4.33852300	1.90654700	0.78574400
C	-2.96516400	4.04874600	-0.36342300
H	-1.45854500	2.59344400	-0.88425900
C	-4.87336600	3.19543800	0.84684500
H	-4.87499100	1.08196500	1.24485500
C	-4.19102000	4.26745700	0.26930000
H	-2.42313300	4.88029400	-0.80512900
H	-5.82273300	3.36063500	1.34897300
H	-4.60779200	5.26949800	0.31998800
C	-3.11404400	-0.95613300	1.36995900
C	-4.30757500	-1.68024800	1.23055100
C	-2.46484900	-0.95405800	2.61572500
C	-4.84397200	-2.37695300	2.31622700
H	-4.81663300	-1.70821100	0.27225500
C	-3.00710100	-1.64145400	3.70114600
H	-1.52412500	-0.41955500	2.72075300
C	-4.19831400	-2.35598900	3.55326300
H	-5.76626500	-2.93800700	2.19244700
H	-2.49353200	-1.62905000	4.65846300
H	-4.61619000	-2.90041000	4.39549000
C	-3.10583100	-0.70057900	-1.52374600
C	-4.32465400	-0.25336000	-2.05546000
C	-2.42317500	-1.74044200	-2.17607200
C	-4.85378800	-0.84216400	-3.20631300
H	-4.85850000	0.56154700	-1.57675300
C	-2.95757200	-2.33404400	-3.31955100
H	-1.46263300	-2.06751900	-1.78590000
C	-4.17461400	-1.88537900	-3.83768900
H	-5.79627300	-0.48245600	-3.61011200
H	-2.41795400	-3.13811500	-3.81214700
H	-4.58695000	-2.34047300	-4.73393400
C	3.10971500	-1.64266200	-0.35719000
C	2.44378800	-2.78949400	0.10596700
C	4.31251600	-1.79772200	-1.06265300
C	2.97915100	-4.05885800	-0.11097200
H	1.49571600	-2.67582700	0.62556000
C	4.84191900	-3.07064300	-1.28849000
H	4.83437300	-0.92589800	-1.44458300
C	4.17991300	-4.20232600	-0.81012400
H	2.45303600	-4.93592700	0.25555800
H	5.77166000	-3.17604600	-1.84093200
H	4.59273100	-5.19134400	-0.98841200
C	3.11628700	1.12583900	-1.23395700
C	4.33743900	1.78438500	-1.02493700
C	2.43556500	1.33027000	-2.44538700
C	4.87064600	2.61757300	-2.01121200
H	4.86998700	1.65593800	-0.08773200
C	2.97389200	2.15495800	-3.43306100
H	1.47361100	0.84712200	-2.59795200
C	4.19333300	2.80121200	-3.21768600
H	5.81474400	3.12535300	-1.83358000
H	2.43581600	2.30161800	-4.36546100
H	4.60880400	3.45155600	-3.98240200
C	3.11299700	0.50078500	1.60203700
C	4.32893500	-0.01631800	2.07445200
C	2.43562500	1.45484400	2.37915700
C	4.85988900	0.42162100	3.29000200
H	4.85952900	-0.76872600	1.49924100
C	2.97179800	1.89802800	3.58799700
H	1.47752800	1.83408500	2.03234600
C	4.18583000	1.38145500	4.04661000
H	5.79998800	0.00906000	3.64600700
H	2.43624000	2.63762600	4.17670100
H	4.59981500	1.71860700	4.99282300

- Ph_3P

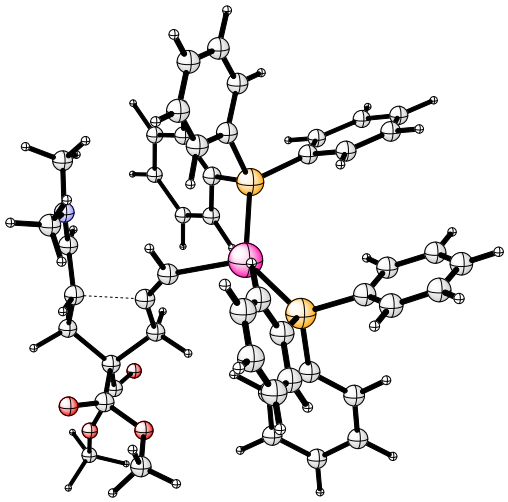


B3LYP/6-311+G(2d,2p) energy: -1036.5280313 a.u.
ZPE: 0.273823 a.u.
Thermal correction to Gibbs Free Energy: 0.227275 a.u.
Solvation energy: -1.75 kcal/mol

Dispersion correction: -53.17 kcal/mol

P	-2.31340900	-0.00404500	-0.00222500
C	-3.11202400	1.66078300	0.16665500
C	-2.46909400	2.74078600	-0.46118000
C	-4.28378000	1.91148300	0.89686200
C	-2.99294200	4.03063400	-0.38051700
H	-1.54830500	2.56839000	-1.01275400
C	-4.80235700	3.20477300	0.98699300
H	-4.79072300	1.09478700	1.40085300
C	-4.16146400	4.26606100	0.34641300
H	-2.48361100	4.85253700	-0.87567000
H	-5.70923100	3.38181500	1.55861900
H	-4.56594100	5.27157000	0.41860700
C	-3.12368700	-0.97598900	1.35307300
C	-4.28172400	-1.75210000	1.19440000
C	-2.50415900	-0.94520500	2.61384600
C	-4.80948300	-2.46938200	2.27004300
H	-4.77100300	-1.79886800	0.22681700
C	-3.03764600	-1.65201600	3.69084500
H	-1.59439500	-0.36570600	2.74935700
C	-4.19208300	-2.41867600	3.52043200
H	-5.70562600	-3.06748100	2.12956000
H	-2.54688200	-1.61280900	4.65920200
H	-4.60395500	-2.97798600	4.35553700
C	-3.12150800	-0.68761700	-1.52480200
C	-4.27236600	-0.15364100	-2.12350600
C	-2.50609500	-1.79835500	-2.12639800
C	-4.79777100	-0.72164700	-3.28595500
H	-4.75815000	0.71082700	-1.68256600
C	-3.03745100	-2.37302600	-3.28034800
H	-1.60127800	-2.21184100	-1.68796900
C	-4.18507000	-1.83362600	-3.86486100
H	-5.68829900	-0.29404200	-3.73832200
H	-2.54989200	-3.23401400	-3.72878300
H	-4.59495200	-2.27356900	-4.76946400

- TS_C

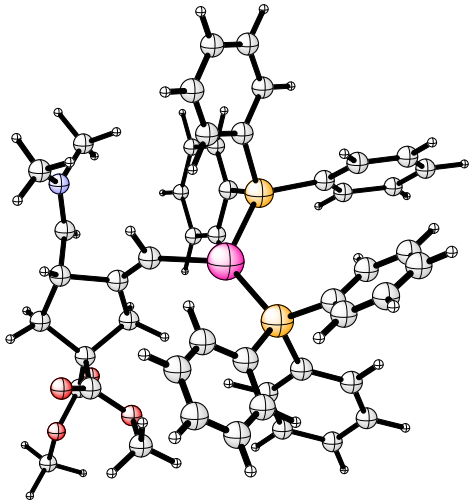


B3LYP/BS2 energy: -3062.49789227 a.u.
ZPE: 0.856677 a.u.
Thermal correction to Gibbs Free Energy: 0.751055 a.u.
Solvation energy: -7.05 kcal/mol
Dispersion correction: -190.45 kcal/mol

C	2.47442400	-2.68510300	3.82889700
H	3.21203200	-3.16688800	4.48756600
H	2.70201200	-1.62369100	3.75758100
H	1.48518500	-2.79109700	4.28173300
N	2.46504900	-3.30790400	2.50922400
C	1.81874300	-4.61368100	2.44488000
H	1.79901800	-4.96548300	1.41272300
H	2.34453500	-5.35004000	3.06914100
H	0.78542000	-4.53284400	2.79643700
C	3.24603100	-2.88451700	1.49267900
H	3.25156400	-3.54588800	0.62996500
C	3.83079100	-1.62419300	1.37565700
H	3.98314800	-1.04174000	2.27845500
C	4.89842400	-1.39566000	0.32216000
H	5.89547300	-1.33700700	0.76628200
H	4.89106200	-2.20664700	-0.41410200
C	3.04815200	-0.17379900	-0.70040300
H	2.63357200	0.77496400	-1.04510300
H	2.91726000	-0.89863600	-1.51175300
C	2.35171500	-0.61856300	0.54794400
C	1.17510400	-0.57278200	1.08390500
H	0.93455800	-1.13931400	1.98357800
Pd	-0.72295800	0.11293600	0.24362800
P	-1.67321500	-1.96197900	-0.38709000
P	-1.43139900	2.37706500	0.20465100
C	4.56165600	-0.07245500	-0.42109600
C	4.88619200	1.11877900	0.49029400
C	5.35842100	-0.00037600	-1.72296300
O	5.44646700	1.04328100	1.56285500
O	5.02277600	-0.51966700	-2.76570000
O	4.45196300	2.28133300	-0.03713100
O	6.52589400	0.65570200	-1.55997800
C	4.70183100	3.44934500	0.76730700
H	5.77701000	3.62099600	0.86189600
H	4.22204700	4.27487900	0.24339900
H	4.27056300	3.32484000	1.76261400
C	7.36549300	0.72713700	-2.72555100
H	6.85032600	1.24778500	-3.53632100
H	8.25156400	1.28021100	-2.41517300
H	7.63626600	-0.27560800	-3.06484200
C	-0.39275100	3.47269900	-0.87916500
C	0.99026800	3.22586100	-0.90714700
C	-0.90778300	4.49146300	-1.69475200
C	1.83369900	3.97287100	-1.72921100
H	1.39556700	2.43366600	-0.28414900
C	-0.06207000	5.24091600	-2.51771000
H	-1.97302600	4.69816000	-1.69576900
C	1.30871100	4.98306900	-2.53981500
H	2.89580900	3.74612200	-1.74991900
H	-0.47985700	6.02330200	-3.14587000
H	1.96247200	5.55904400	-3.18922000
C	-3.14657300	2.82186100	-0.36463900
C	-3.66681300	2.10148200	-1.45200800
C	-3.94345800	3.81587900	0.22426700
C	-4.93678700	2.38311300	-1.95510400
H	-3.07272200	1.30435200	-1.89054600
C	-5.22320800	4.08575300	-0.26826900
H	-3.56763500	4.38181200	1.07052000
C	-5.72078600	3.37590000	-1.36190200
H	-5.31756800	1.81478400	-2.79908300

H	-5.82949400	4.85455800	0.20370300
H	-6.71526900	3.58906700	-1.74454400
C	-1.34158000	3.23552100	1.84769300
C	-0.95922300	4.57564500	2.01131700
C	-1.66238200	2.48406800	2.99010400
C	-0.90568400	5.14988100	3.28399300
H	-0.69841100	5.17263700	1.14267900
C	-1.62056600	3.06049300	4.25938500
H	-1.93475900	1.43809800	2.87372700
C	-1.23921500	4.39603100	4.41010000
H	-0.60349300	6.18814200	3.39371500
H	-1.87606400	2.46492400	5.13180100
H	-1.19687700	4.84400300	5.39914800
C	-3.09358100	-2.11196700	-1.58074500
C	-4.26191700	-1.38513400	-1.29032100
C	-3.05273600	-2.86514800	-2.76383100
C	-5.36311400	-1.43070900	-2.14313100
H	-4.30218600	-0.77097700	-0.39475900
C	-4.15125800	-2.89550000	-3.62802800
H	-2.16306600	-3.43287100	-3.01501500
C	-5.31077900	-2.18497100	-3.31927400
H	-6.25821300	-0.86737400	-1.89405800
H	-4.09839300	-3.48218800	-4.54141200
H	-6.16516200	-2.21330500	-3.98985500
C	-0.42914400	-3.12245800	-1.14335500
C	-0.34719200	-4.49734700	-0.87602600
C	0.51438600	-2.55584300	-2.01718400
C	0.64890300	-5.28194800	-1.46640700
H	-1.06039700	-4.96329300	-0.20375300
C	1.50019600	-3.33903000	-2.61915700
H	0.48065400	-1.48635100	-2.20732000
C	1.57380200	-4.70653300	-2.34025700
H	0.69302200	-6.34670500	-1.25057500
H	2.21802500	-2.87849800	-3.29269100
H	2.34391400	-5.31821400	-2.80237900
C	-2.33569000	-2.94811500	1.04407000
C	-3.24520900	-4.00904300	0.90259200
C	-1.90863600	-2.60095900	2.33590500
C	-3.69478800	-4.71735800	2.01891700
H	-3.61040100	-4.27650400	-0.08440100
C	-2.35661800	-3.30975600	3.45309500
H	-1.24301800	-1.75048600	2.45331300
C	-3.24824800	-4.37321900	3.29652400
H	-4.39911600	-5.53493300	1.89047300
H	-2.02462100	-3.01956900	4.44671700
H	-3.60410700	-4.92101600	4.16478600

- INT1$_C$

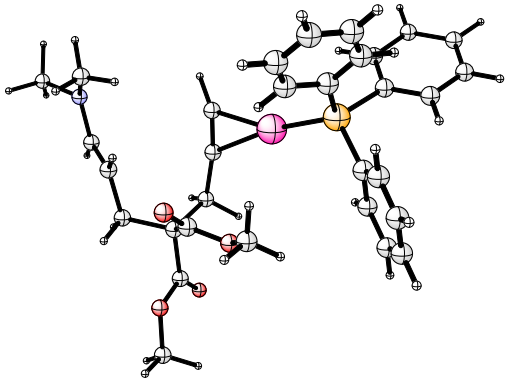


B3LYP/BS2 energy: -3062.5045755 a.u.
ZPE: 0.859284 a.u.
Thermal correction to Gibbs Free Energy: 0.757034 a.u.
Solvation energy: -7.75 kcal/mol
Dispersion correction: -192.64 kcal/mol

C	-1.85477000	-4.11829000	-3.44178000
H	-1.79938100	-5.10737600	-3.90778700
H	-2.76346500	-3.62536000	-3.78320100
H	-0.98588800	-3.53207500	-3.76400900
N	-1.87167500	-4.28184000	-1.99240800
C	-0.79137100	-5.10769000	-1.45344900
H	-0.91751300	-5.23209900	-0.37741800
H	-0.79821100	-6.08972400	-1.93704500
H	0.17860700	-4.62758300	-1.63099400
C	-2.60059300	-3.52059700	-1.16773200
H	-2.58696300	-3.83311900	-0.12851700
C	-3.35555200	-2.31428600	-1.49130500
H	-3.46251200	-2.09328000	-2.55180400
C	-4.65433700	-2.08739000	-0.67854500
H	-5.49794800	-1.85502700	-1.32930500
H	-4.90340700	-2.97116700	-0.08356600
C	-2.82819000	-1.08303300	0.56261000
H	-2.34581000	-0.18327700	0.94437300
H	-2.72841600	-1.86330200	1.32749900
C	-2.24928900	-1.46837800	-0.78339800
C	-1.06777200	-1.04963400	-1.33238600
H	-0.91591800	-1.49789900	-2.32817100
Pd	0.46824200	0.07170200	-0.52301100
P	2.14375400	-1.43000100	0.30276500
P	0.69267100	2.44102400	-0.31869900
C	-4.34027200	-0.89869500	0.27688100
C	-4.58774300	0.42617900	-0.45767400
C	-5.18879600	-0.99954400	1.54217900
O	-5.05396700	0.52790400	-1.57228100
O	-4.89367200	-1.65104300	2.52138600
O	-4.19427500	1.47399200	0.28890400
O	-6.35074300	-0.32492200	1.42097300
C	-4.34364500	2.76828700	-0.32824600
H	-5.39994000	2.97505500	-0.51837000
H	-3.93138700	3.47998200	0.38573300
H	-3.78941000	2.80799100	-1.26737600

C	-7.23180200	-0.39719800	2.55485900
H	-6.74540000	0.01169700	3.44372900
H	-8.10454300	0.19761500	2.28667400
H	-7.51777200	-1.43306100	2.75346700
C	0.20654600	3.10325000	1.34869600
C	-1.03328300	2.68856200	1.86911000
C	1.00364500	3.95706900	2.12401700
C	-1.46376400	3.12274700	3.12180200
H	-1.66674200	2.02725200	1.28491100
C	0.57489800	4.38354500	3.38475000
H	1.96427500	4.29168500	1.74698300
C	-0.65834800	3.97060300	3.88752300
H	-2.42624500	2.79185500	3.50317900
H	1.20906300	5.04360800	3.97079100
H	-0.98962500	4.30321900	4.86741200
C	2.32855400	3.26827800	-0.62866500
C	3.44871700	2.74825600	0.04306200
C	2.52212800	4.33183700	-1.52284200
C	4.71646100	3.29558100	-0.14787400
H	3.32566800	1.90464800	0.71539200
C	3.79705100	4.86581200	-1.73049500
H	1.67872800	4.74752200	-2.06288500
C	4.89623200	4.35621000	-1.03978500
H	5.56344700	2.88170800	0.39222300
H	3.92661800	5.68556300	-2.43232100
H	5.88569100	4.77606100	-1.19935800
C	-0.44632500	3.42789100	-1.41479000
C	-0.83775400	4.74658900	-1.12895800
C	-0.94056400	2.81682500	-2.57559200
C	-1.69527200	5.43686600	-1.98786300
H	-0.47551600	5.23462300	-0.22876900
C	-1.78995300	3.50996300	-3.44173300
H	-0.67181400	1.78215400	-2.77272700
C	-2.17044700	4.82137200	-3.14900400
H	-1.99193000	6.45530100	-1.75070900
H	-2.16339100	3.02110000	-4.33754200
H	-2.83801800	5.35896000	-3.81705600
C	3.64085400	-1.06865100	1.35270500
C	4.77231300	-0.47687400	0.75977200
C	3.63964400	-1.24004500	2.74664600
C	5.86991500	-0.09482400	1.53066100
H	4.79775000	-0.31939500	-0.31488500
C	4.73371200	-0.84406300	3.51937900
H	2.78235700	-1.69170600	3.23539800
C	5.85553000	-0.27466300	2.91655700
H	6.73929100	0.34256000	1.04639500
H	4.70914000	-0.99036100	4.59605200
H	6.70878800	0.02647100	3.51767300
C	1.31476900	-2.74682100	1.33036500
C	1.69904400	-4.09605600	1.36183600
C	0.21696600	-2.34840400	2.11052500
C	1.00308700	-5.01952500	2.14722900
H	2.54003100	-4.43630400	0.76676200
C	-0.47031500	-3.26546200	2.90858600
H	-0.10577700	-1.31180100	2.06928500
C	-0.08174300	-4.60743500	2.92461100
H	1.31603000	-6.06064000	2.15721500
H	-1.31410600	-2.93299000	3.50729400
H	-0.61822200	-5.32495300	3.53962400
C	2.92467500	-2.40539800	-1.07829600
C	4.06758300	-3.20941500	-0.92545700
C	2.33218000	-2.32313500	-2.34904100
C	4.58698000	-3.92654200	-2.00493000
H	4.56500500	-3.26269700	0.03804300
C	2.85249600	-3.03989900	-3.42964100
H	1.47167500	-1.67167900	-2.47631000
C	3.97848000	-3.84735400	-3.25954900
H	5.47151700	-4.54259000	-1.86645500
H	2.38778800	-2.95329400	-4.40856800
H	4.38791200	-4.40059300	-4.10042900

- INT1$_D$

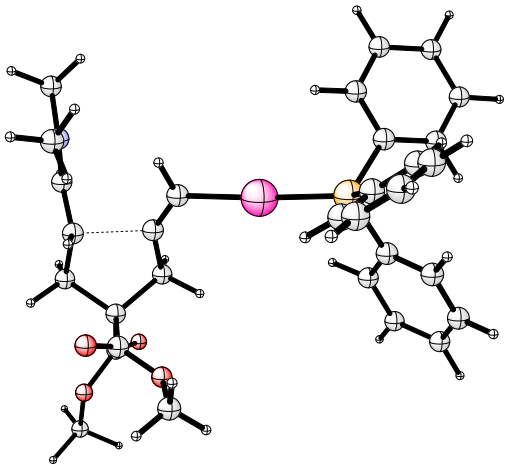


B3LYP/BS2 energy: -2025.99427477 a.u.
ZPE: 0.58180 a.u.
Thermal correction to Gibbs Free Energy: 0.498999 a.u.
Solvation energy: -6.15 kcal/mol
Dispersion correction: -114.32 kcal/mol

C	4.21147000	-4.03426600	1.11838200
H	4.77859300	-3.81646800	2.03971500
H	3.25472600	-3.50841000	1.17891400
H	4.01248300	-5.10905800	1.08118200
N	4.91699900	-3.63586500	-0.08632100
C	5.99301200	-4.52783300	-0.49134800
H	6.39155200	-4.20715700	-1.45843100
H	6.82901800	-4.55727500	0.22848500
H	5.60684300	-5.54600500	-0.60492000
C	5.12943700	-2.27433000	-0.28707500
H	5.72847300	-2.06586400	-1.17366600
C	4.64844600	-1.25374500	0.44578100
H	4.07015500	-1.42729500	1.34544500
C	4.88653300	0.18215000	0.07957600
H	5.37892600	0.70475600	0.90742000
H	5.56530100	0.23375400	-0.78172100
C	2.78839500	0.42970500	-1.45497200
H	2.16135500	1.22145800	-1.86861800
H	3.48956500	0.14567200	-2.24880100
C	1.95294300	-0.73895300	-1.12467800
C	1.48290900	-1.87824700	-0.98470100
H	1.45614500	-2.94745300	-0.92524200
Pd	-0.22335800	-0.65287100	-0.59889500
P	-2.44959300	-0.19146200	-0.10629900
C	3.62394500	1.03438700	-0.28590900
C	2.74471700	1.25755000	0.95386500
C	4.14110300	2.40107400	-0.76316900
O	2.89222700	0.72374500	2.03034900
O	4.12603200	2.79945200	-1.90716600

O	1.77125100	2.14998200	0.68375500
O	4.67949300	3.09657400	0.26070100
C	0.84982700	2.40941300	1.75917300
H	1.38607500	2.77045200	2.64002500
H	0.16257000	3.16470900	1.38092000
H	0.30627000	1.49586900	2.00883800
C	5.22840600	4.37985200	-0.08354900
H	4.45573400	5.02460800	-0.50919700
H	5.60601500	4.79708600	0.84961900
H	6.03680100	4.26921800	-0.81048800
C	-3.09750300	-1.04508600	1.40189500
C	-4.44020200	-1.41819600	1.56773600
C	-2.18294100	-1.33155900	2.42841600
C	-4.85899400	-2.05195800	2.73952300
H	-5.15952100	-1.22308900	0.77875900
C	-2.60496200	-1.95590300	3.60248000
H	-1.13583200	-1.07475900	2.28904200
C	-3.94438300	-2.31819300	3.76011400
H	-5.90051400	-2.34021600	2.85239600
H	-1.88530500	-2.16969300	4.38769900
H	-4.27217600	-2.81374400	4.66969500
C	-3.69359600	-0.60970600	-1.41013200
C	-3.41289700	-1.69572300	-2.25399100
C	-4.89042400	0.10025900	-1.59412600
C	-4.31764300	-2.07749300	-3.24476100
H	-2.47225700	-2.22732500	-2.13621600
C	-5.79105400	-0.27770700	-2.59223000
H	-5.11636800	0.95562100	-0.96451800
C	-5.50866500	-1.36878100	-3.41614600
H	-4.08659800	-2.92016400	-3.89033700
H	-6.71162500	0.28345600	-2.72732100
H	-6.20918400	-1.65946700	-4.19400200
C	-2.78428900	1.59941600	0.22331700
C	-3.56208700	2.06223400	1.29432800
C	-2.20020200	2.53845200	-0.64449800
C	-3.75374900	3.43286500	1.49070800
H	-4.01580600	1.35435100	1.98044000
C	-2.40212400	3.90480400	-0.45419700
H	-1.57804600	2.19157400	-1.46540800
C	-3.17789900	4.35618100	0.61757600
H	-4.35521400	3.77621500	2.32798100
H	-1.94729300	4.61683700	-1.13711700
H	-3.32867400	5.42088200	0.77187900

- TS_D

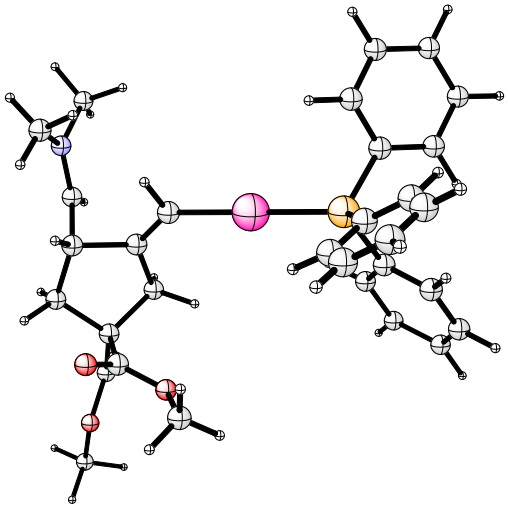


B3LYP/BS2 energy: -2025.96558317 a.u.
ZPE: 0.581634 a.u.
Thermal correction to Gibbs Free Energy: 0.496748 a.u.
Solvation energy: -10.71 kcal/mol
Dispersion correction: -111.51 kcal/mol

C	-3.38426600	4.37872200	1.44914000
H	-4.21302000	4.96712800	1.86774600
H	-3.27858100	3.45733200	2.01696300
H	-2.46064000	4.95384500	1.56062000
N	-3.61277400	4.09817600	0.03469700
C	-3.47015600	5.24577100	-0.85126300
H	-3.67621400	4.94996400	-1.88088200
H	-4.16254300	6.05014500	-0.56870500
H	-2.44823000	5.63736200	-0.80148900
C	-4.14415500	2.94345800	-0.41712900
H	-4.39008100	2.95349700	-1.47649200
C	-4.24591600	1.74559000	0.27613700
H	-4.16972500	1.75313900	1.35747500
C	-5.09879000	0.62259100	-0.27227400
H	-6.01455600	0.49376500	0.31062600
H	-5.37980900	0.82884400	-1.31177900
C	-2.87356100	-0.29301200	-0.78446400
H	-2.13629500	-1.07572500	-0.60208700
H	-2.95742100	-0.17497500	-1.87130200
C	-2.41811200	0.97650900	-0.13732400
C	-1.35391800	1.63161200	0.18103200
H	-1.34999500	2.66837800	0.51488700
Pd	0.54610300	0.77706000	0.08631500
P	2.67694700	-0.05488600	-0.03755300
C	-4.26402000	-0.68735200	-0.24770500
C	-4.15632600	-1.21232700	1.18987300
C	-4.92450400	-1.73706400	-1.14186200
O	-4.63134100	-0.68048100	2.17032400
O	-4.61113000	-1.98052800	-2.28593600
O	-3.43334700	-2.34645200	1.22774200
O	-5.96509900	-2.32121600	-0.51075800
C	-3.22680100	-2.91107600	2.53478100
H	-4.18437000	-3.16145800	2.99794600
H	-2.62899000	-3.80771100	2.37483500
H	-2.69345800	-2.20382400	3.17384100
C	-6.68522200	-3.30108000	-1.27894500
H	-6.02497300	-4.12396500	-1.56318600
H	-7.48290500	-3.65645800	-0.62720500
H	-7.09892100	-2.85049900	-2.18436000
C	3.71032500	0.13715600	1.49317100
C	5.09573200	0.36031000	1.48785300
C	3.04584700	0.06046900	2.72835100
C	5.79951000	0.49139900	2.68774800
H	5.62793600	0.44149300	0.54521400
C	3.75046900	0.18069800	3.92604100
H	1.96754100	-0.07818000	2.73556400
C	5.13037100	0.39763400	3.90885300
H	6.87144600	0.66949400	2.66607600
H	3.22050800	0.11702200	4.87266500
H	5.67889200	0.50164500	4.84111700
C	3.74954600	0.70637800	-1.34789600
C	3.51034400	2.05172600	-1.67207100
C	4.76652000	0.02057100	-2.02986200

C	4.28211900	2.70150100	-2.63530600
H	2.69961900	2.57452300	-1.17025500
C	5.53250200	0.66887700	-3.00182300
H	4.95714000	-1.02529000	-1.80945100
C	5.29559500	2.01079800	-3.30371400
H	4.08442600	3.74339400	-2.87275800
H	6.31295800	0.12250900	-3.52484500
H	5.89104600	2.51261700	-4.06159700
C	2.83277600	-1.86923600	-0.40127900
C	3.83587900	-2.69706100	0.12513500
C	1.86989400	-2.43662400	-1.25205300
C	3.88012400	-4.05523600	-0.20047100
H	4.58192900	-2.28446000	0.79718300
C	1.92076800	-3.78979000	-1.58570900
H	1.07282500	-1.80544400	-1.63724200
C	2.92651200	-4.60394500	-1.05893700
H	4.66090700	-4.68379700	0.21971000
H	1.16903000	-4.21079900	-2.24796400
H	2.96182700	-5.66058700	-1.31006800

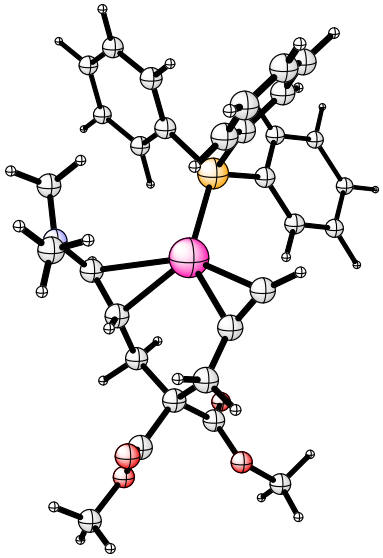
- INT2$_D$



B3LYP/BS2 energy: -2025.97161739 a.u.
ZPE: 0.584353 a.u.
Thermal correction to Gibbs Free Energy: 0.502091 a.u.
Solvation energy: -12.95 kcal/mol
Dispersion correction: -111.93 kcal/mol

C	-3.40565500	4.64058200	1.33122400
H	-3.80245100	5.66047300	1.32992700
H	-3.98965000	4.04058900	2.02635000
H	-2.36387400	4.66818500	1.67036000
N	-3.50320000	4.09763900	-0.02196700
C	-2.86991700	4.90808400	-1.06174200
H	-3.16831300	4.54595800	-2.04707600
H	-3.17663100	5.95211700	-0.95666800
H	-1.77715300	4.84026900	-0.98055400
C	-3.83853700	2.83541700	-0.29468800
H	-3.95416600	2.61318800	-1.35151400
C	-4.00466700	1.72874700	0.63514200
H	-4.02091900	1.99224200	1.69060500
C	-5.05764100	0.66398200	0.24724400
H	-5.74989300	0.47247800	1.06804300
H	-5.63083200	0.97956800	-0.62935600
C	-2.94439400	-0.03125300	-0.72559000
H	-2.11413900	-0.73744600	-0.73873500
H	-3.16403400	0.25226700	-1.76328000
C	-2.61788800	1.14877900	0.16686000
C	-1.39686200	1.57060500	0.59331200
H	-1.46936200	2.48150800	1.20575000
Pd	0.46104700	0.80439800	0.26283400
P	2.58694400	-0.06147400	-0.04067500
C	-4.24561200	-0.61380100	-0.11386800
C	-3.92116500	-1.39442300	1.16611000
C	-5.03050200	-1.46036600	-1.11458300
O	-4.31999600	-1.10780000	2.27536900
O	-5.08887500	-1.23232800	-2.30390500
O	-3.10189100	-2.42659000	0.90555500
O	-5.71170100	-2.45511600	-0.51230400
C	-2.68518000	-3.19400200	2.04790000
H	-3.55088000	-3.63589000	2.54777000
H	-2.02859900	-3.96962800	1.65504500
H	-2.14692800	-2.55910900	2.75514900
C	-6.50829500	-3.27768200	-1.38285100
H	-5.87839900	-3.75951800	-2.13418100
H	-6.97453500	-4.02158800	-0.73745300
H	-7.26749100	-2.67688300	-1.88969600
C	3.50180000	-0.47457800	1.52000100
C	4.89600100	-0.39875600	1.66107300
C	2.73312200	-0.87877700	2.62359700
C	5.50681500	-0.73551100	2.87143600
H	5.50790100	-0.06632300	0.82794100
C	3.34449500	-1.22348700	3.82918900
H	1.65034900	-0.89868900	2.52682700
C	4.73374400	-1.15305600	3.95606000
H	6.58739200	-0.66782000	2.96647600
H	2.73530800	-1.53495700	4.67350100
H	5.21029200	-1.41259400	4.89756900
C	3.78274100	1.04505200	-0.93035600
C	3.63994400	2.42897400	-0.73617200
C	4.80071000	0.58640200	-1.78022500
C	4.50705900	3.32874700	-1.35570400
H	2.83033900	2.78836100	-0.10599600
C	5.66286000	1.48897200	-2.40817800
H	4.91791600	-0.47771000	-1.96059700
C	5.52150300	2.86076000	-2.19426300
H	4.38423300	4.39618800	-1.19270400
H	6.44393700	1.11783800	-3.06651600
H	6.19211900	3.56125300	-2.68460000
C	2.70232600	-1.64025200	-1.01082300
C	3.65652800	-2.64329600	-0.78245700
C	1.75697100	-1.82996000	-2.03209900
C	3.67281800	-3.80021500	-1.56579200
H	4.38474100	-2.52702000	0.01434500
C	1.77984900	-2.98036900	-2.82041200
H	0.99474300	-1.07051500	-2.18741800
C	2.73856600	-3.96953300	-2.58876100
H	4.41557800	-4.57000100	-1.37328600
H	1.04219600	-3.10981900	-3.60784800
H	2.75175900	-4.87069500	-3.19586700

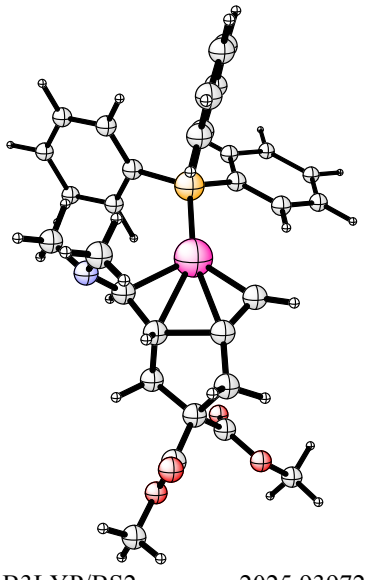
- INT1$_E$



B3LYP/BS2 energy: -2025.99244994 a.u.
ZPE: 0.582564 a.u.
Thermal correction to Gibbs Free Energy: 0.504261 a.u.
Solvation energy: -5.31 kcal/mol
Dispersion correction: -120.78 kcal/mol

C	0.61999000	-4.12552200	0.78032800
H	0.15963600	-5.11529600	0.83804400
H	1.70233800	-4.25085100	0.87779400
H	0.26354000	-3.52187200	1.63329500
N	0.28972500	-3.52559200	-0.49918100
C	-1.08714500	-3.74123200	-0.91580900
H	-1.24713700	-3.32009900	-1.91067700
H	-1.29252000	-4.81594700	-0.95809400
H	-1.81212500	-3.27024600	-0.23361000
C	0.85388000	-2.28987500	-0.80984200
H	0.55188500	-1.90997900	-1.78261300
C	1.91445300	-1.70208500	-0.14607600
H	2.31819000	-2.22235800	0.71757700
C	2.85199700	-0.71986500	-0.82377600
H	3.49821700	-1.23540800	-1.54721600
H	2.28851000	0.01608700	-1.40136100
C	3.24282700	0.22596800	1.60631500
H	3.36687000	-0.73844100	2.10734600
H	3.89151800	0.93073500	2.13777200
C	1.83723600	0.64396600	1.68965100
C	0.78625300	1.23604800	2.01861500
H	0.20575600	1.96549300	2.54844200
Pd	0.20035100	-0.28930600	0.57487700
P	-2.03947400	0.25497700	0.01906100
C	-3.04241200	-0.70646500	-1.21638300
C	-4.19982300	-1.42454400	-0.88466700
C	-2.57394300	-0.76545800	-2.54135700
C	-4.86931800	-2.18310100	-1.85013500
H	-4.58503900	-1.39237800	0.12928800
C	-3.24875600	-1.51131900	-3.50606600
H	-1.67883900	-0.21482600	-2.82005900
C	-4.39902000	-2.22826400	-3.16208300
H	-5.76449300	-2.73346200	-1.57300100
H	-2.87648300	-1.53532800	-4.52667700
H	-4.92269600	-2.81446200	-3.91182700
C	-3.14779600	0.27583000	1.50765200
C	-4.24846200	1.13217600	1.66249400
C	-2.84833200	-0.62794500	2.54004900
C	-5.03294800	1.07900500	2.81634600
H	-4.49097500	1.85184900	0.88777900
C	-3.63946400	-0.68927500	3.68818100
H	-1.97847000	-1.27177900	2.44049000
C	-4.73390200	0.16590100	3.82935100
H	-5.87761800	1.75410200	2.92384800
H	-3.39318000	-1.39584800	4.47600000
H	-5.34537700	0.12694300	4.72662500
C	-2.21148000	1.96422900	-0.69211900
C	-3.34838400	2.37445200	-1.41043400
C	-1.16571400	2.88180000	-0.51262000
C	-3.44312000	3.67178400	-1.91564200
H	-4.15822000	1.67402200	-1.58947400
C	-1.26093300	4.17965600	-1.01916500
H	-0.26985000	2.56625000	0.01247300
C	-2.39994600	4.57919400	-1.71872200
H	-4.32953800	3.97078700	-2.46854100
H	-0.43767700	4.87376700	-0.87511600
H	-2.47170000	5.58742600	-2.11723900
C	3.79527600	0.06028000	0.15312200
C	5.11927700	-0.71537300	0.26112100
C	4.08683400	1.45383200	-0.43320900
O	5.45241400	-1.40997600	1.19667900
O	3.52845900	1.96208500	-1.37831400
O	5.85761500	-0.57632300	-0.85927700
O	5.05319600	2.07611300	0.27906900
C	7.09441200	-1.30869800	-0.88218700
H	7.74633200	-0.98494500	-0.06719900
H	6.90740600	-2.38059000	-0.78157700
H	7.54825400	-1.08763400	-1.84793300
C	5.40082200	3.39503300	-0.17286200
H	6.18837100	3.73774600	0.49810000
H	5.76021800	3.36331800	-1.20430300
H	4.53517300	4.05981000	-0.12006800

- TS$_E$



B3LYP/BS2 energy: -2025.93972247 a.u.
ZPE: 0.582931 a.u.

Thermal correction to Gibbs Free Energy: 0.506731 a.u.
Solvation energy: -6.28 kcal/mol
Dispersion correction: -119.59 kcal/mol

C	-0.14789100	-3.56188800	-1.17142400
H	-0.14283500	-4.65672000	-1.18904400
H	-0.92878200	-3.21546000	-1.85098600
H	0.82129700	-3.20351900	-1.55721200
N	-0.39436400	-3.10504800	0.18787100
C	0.59961200	-3.60770400	1.12414100
H	0.34855300	-3.29550300	2.14074500
H	0.60632600	-4.70233500	1.09091300
H	1.61523700	-3.24737200	0.89636900
C	-0.80693900	-1.77093600	0.39331400
H	-0.79824400	-1.52529800	1.45426400
C	-2.00554400	-1.25674300	-0.34693900
H	-2.35557900	-2.02012600	-1.04384600
C	-3.12973600	-0.80644900	0.59004100
H	-3.59228000	-1.67783400	1.06537000
H	-2.73492100	-0.16959300	1.38526600
C	-3.59561900	0.15814900	-1.64794900
H	-3.95144400	-0.69898200	-2.23171100
H	-3.94203100	1.06507500	-2.14734800
C	-2.09253700	0.15970500	-1.52756700
C	-1.14486800	0.93367700	-2.00937600
H	-1.35281100	1.75699500	-2.68910200
Pd	0.08798300	-0.15170000	-0.66386000
P	2.20893900	0.22339100	-0.00308900
C	2.84808600	-0.61111200	1.52584700
C	4.00303100	-1.40503100	1.56097900
C	2.08774600	-0.47675000	2.70140200
C	4.38620000	-2.05051300	2.74087900
H	4.60744700	-1.52494300	0.66817200
C	2.47837900	-1.10876300	3.88004500
H	1.18301200	0.12598400	2.68890500
C	3.62877800	-1.90362700	3.90234600
H	5.28203600	-2.66551700	2.74857000
H	1.88291100	-0.98591300	4.78057100
H	3.92957600	-2.40355800	4.81864000
C	3.48248400	-0.14783500	-1.29221800
C	4.78507400	0.37448200	-1.24147700
C	3.12184900	-0.96305900	-2.37430600
C	5.70930900	0.06864400	-2.24105500
H	5.07666300	1.03016900	-0.42677100
C	4.04730400	-1.27004100	-3.37333900
H	2.10171400	-1.33147200	-2.43578600
C	5.34338300	-0.75710000	-3.30674400
H	6.71318600	0.48111400	-2.19092400
H	3.75175800	-1.90089500	-4.20687500
H	6.06326100	-0.99035200	-4.08627800
C	2.51010200	2.01190200	0.38554100
C	3.44685100	2.43564500	1.34165300
C	1.78798900	2.97710800	-0.33346000
C	3.66257500	3.79685100	1.56621300
H	4.00319800	1.70582000	1.92144300
C	2.00973100	4.33625500	-0.10917900
H	1.04427900	2.64878900	-1.05462700
C	2.94661000	4.74976700	0.84002000
H	4.38786000	4.11047900	2.31209200
H	1.44248900	5.07271700	-0.67156100
H	3.11323300	5.80855000	1.01805400
C	-4.18023800	0.02025600	-0.22028600
C	-5.51818800	-0.72300300	-0.24343200
C	-4.37900400	1.40497800	0.41377500
O	-5.92540600	-1.41640100	-1.14926900
O	-3.78305100	1.84623700	1.37043800
O	-6.17764300	-0.56090500	0.92378100
O	-5.31511100	2.10307600	-0.26517300
C	-7.43033300	-1.25820000	1.03027600
H	-8.12582900	-0.91612500	0.25994100
H	-7.28097600	-2.33492300	0.91877300
H	-7.81272400	-1.02460100	2.02367100
C	-5.58529000	3.42241600	0.23663200
H	-6.35300900	3.83442500	-0.41816800
H	-5.94442000	3.37364200	1.26763700
H	-4.68262600	4.03741400	0.20531600

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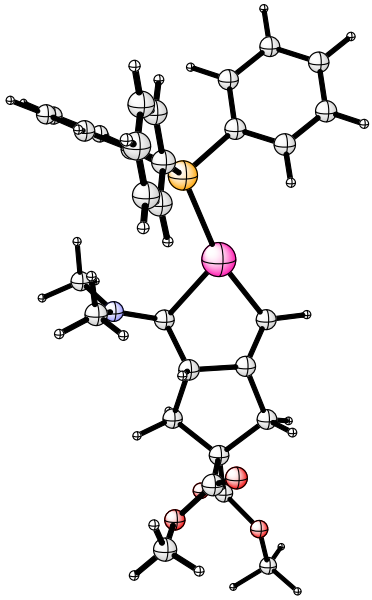
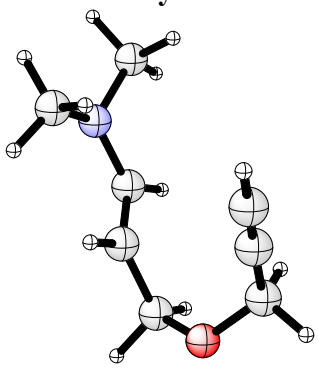


B3LYP/BS2 energy: -2026.0016779 a.u.
ZPE: 0.584921 a.u.
Thermal correction to Gibbs Free Energy: 0.505177 a.u.
Solvation energy: -8.01 kcal/mol
Dispersion correction: -117.96 kcal/mol

C	-0.57976500	-2.75399700	0.42834900
H	-0.97381300	-3.66084500	0.90458900
H	-1.12474400	-2.58732700	-0.50017300
H	0.47640200	-2.93724700	0.17921700
N	-0.72859800	-1.61700300	1.31928100
C	0.03713100	-1.73309800	2.54860800
H	-0.12976500	-0.85459900	3.17423300
H	-0.28967300	-2.62130400	3.10487400
H	1.11538800	-1.82782200	2.36301000
C	-1.13229900	-0.36243800	0.86254500
H	-1.17898300	0.33219300	1.70240000
C	-2.43254500	-0.29681900	0.05373900
H	-2.42896500	-1.05035400	-0.74567900
C	-3.73966400	-0.43790500	0.86552800

H	-4.03982700	-1.46592700	1.08225800
H	-3.66211700	0.09369300	1.81923000
C	-3.99685100	1.45490600	-0.72196200
H	-4.30669600	1.51419900	-1.76908300
H	-4.21293200	2.42431700	-0.25914600
C	-2.53394900	1.07655300	-0.55675500
C	-1.39736800	1.75765300	-0.74152700
H	-1.40991100	2.77752700	-1.13924600
Pd	0.33245000	0.79476600	-0.27167700
P	2.66811900	0.09204200	-0.07485600
C	3.36075800	-0.34745500	1.58158600
C	4.02811700	-1.54823200	1.86202800
C	3.12173500	0.55332800	2.63591300
C	4.45535400	-1.83632100	3.16216900
H	4.21513300	-2.26460800	1.06935300
C	3.55994700	0.27014500	3.92759600
H	2.58493000	1.47807900	2.44103400
C	4.22740100	-0.92867400	4.19583600
H	4.96911500	-2.77268100	3.36186600
H	3.37298700	0.98102500	4.72747400
H	4.56235200	-1.15341500	5.20439400
C	3.29070700	-1.21945500	-1.22089300
C	4.65780300	-1.46510900	-1.43524300
C	2.34766900	-1.96258700	-1.94561200
C	5.06741400	-2.44961100	-2.33352800
H	5.40356500	-0.87839000	-0.90705300
C	2.75901600	-2.94757600	-2.84742600
H	1.29184200	-1.74600100	-1.81254800
C	4.11800200	-3.19538200	-3.03844500
H	6.12722700	-2.62996500	-2.49028400
H	2.01720400	-3.51268100	-3.40450000
H	4.43964100	-3.95884700	-3.74114300
C	3.68710700	1.55569400	-0.57597900
C	4.91197300	1.89484100	0.01719800
C	3.19424900	2.35758200	-1.61903400
C	5.62984600	3.00686600	-0.42824500
H	5.30334600	1.29867800	0.83528200
C	3.91494100	3.46501800	-2.06563900
H	2.24011900	2.11379500	-2.08133200
C	5.13495300	3.79257400	-1.47026800
H	6.57618100	3.25925900	0.04222000
H	3.51946200	4.07497100	-2.87267300
H	5.69396500	4.65863500	-1.81302500
C	-4.79484300	0.30908200	-0.00787700
C	-5.37687500	-0.66567600	-1.03843500
C	-5.92781800	0.88346000	0.84079100
O	-5.13418300	-0.68383700	-2.22452000
O	-5.93756500	0.97434200	2.04831800
O	-6.18404000	-1.56979700	-0.43510200
O	-6.92342400	1.34686500	0.05133700
C	-6.77346000	-2.54736300	-1.30632000
H	-7.38850200	-2.06161500	-2.06803300
H	-5.99983400	-3.13800700	-1.80365200
H	-7.38659200	-3.18143200	-0.66583500
C	-8.02623400	1.95535900	0.74162300
H	-8.72157500	2.27221600	-0.03568700
H	-8.50252700	1.23686400	1.41360200
H	-7.68770400	2.81402700	1.32686000

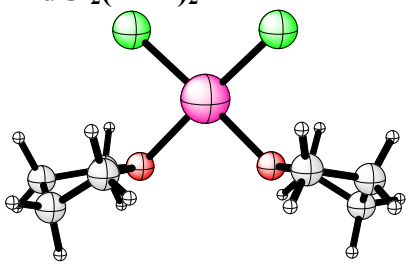
- O-enaminyne



B3LYP/6-311+G(2d,2p) energy: -442.676673236 a.u.
ZPE: 0.196547 a.u.
Thermal correction to Gibbs Free Energy: 0.157702 a.u.
Solvation energy: -2.57 kcal/mol
Dispersion correction: -21.44 kcal/mol

C	2.47220200	0.58154400	-1.19934400
H	3.51771500	0.88546900	-1.29792900
H	2.21354900	-0.03938600	-2.06201000
H	1.84010500	1.48385400	-1.22472500
N	2.30979600	-0.18455400	0.02234500
C	3.03355500	0.31597400	1.18060400
H	2.94101000	-0.39513100	2.00638800
H	4.09625600	0.41660800	0.93801500
H	2.66709900	1.29500800	1.53098300
C	1.09076100	-0.79936400	0.25022600
H	1.03821800	-1.29020000	1.22192200
C	0.03926200	-0.89635900	-0.58656200
H	0.03265600	-0.39784100	-1.55074200
C	-1.17022400	-1.70835800	-0.24533800
H	-1.34022000	-2.50682400	-0.97755700
H	-1.03446900	-2.18784200	0.73897400
O	-2.41094700	-0.98369700	-0.26348600
C	-2.50641500	0.05735900	0.69597400
H	-3.56212200	0.10631900	0.99056700
H	-1.92817800	-0.18586500	1.60082700
C	-2.10010500	1.38004900	0.19771300
C	-1.82486500	2.48869300	-0.19560300
H	-1.56763300	3.46006100	-0.54925400

- $PdCl_2(THF)_2$

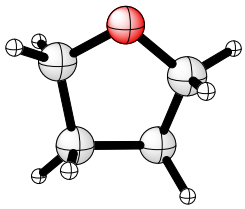


B3LYP/BS2 energy: -1512.34133645 a.u.
ZPE: 0.241005 a.u.
Thermal correction to Gibbs Free Energy: 0.193443 a.u.
Solvation energy: -7.54 kcal/mol

Dispersion correction: -37.82 kcal/mol

Pd	0.00017100	0.58003300	0.00023400
C	-2.28370200	-1.11670000	1.19796800
C	-2.38983200	-1.02920500	-1.19166500
C	-3.52412900	-1.88058700	0.75149600
H	-2.53135700	-0.12374600	1.58543800
H	-1.64995300	-1.64882100	1.91095900
C	-3.79515100	-1.26072000	-0.62975100
H	-2.03142800	-1.86603000	-1.79981100
H	-2.30027400	-0.09531000	-1.74733900
H	-3.30822700	-2.95107600	0.66570300
H	-4.35712100	-1.75179100	1.44746200
H	-4.39479900	-1.90390700	-1.27893500
H	-4.31337400	-0.30388200	-0.51816500
O	-1.50377400	-0.95765200	-0.02456500
Cl	-1.68153200	2.15990500	-0.02557900
C	2.28154700	-1.11925900	-1.19772200
C	2.38968100	-1.03046500	1.19193600
C	3.52331500	-1.88119000	-0.75158200
H	2.52782000	-0.12671800	-1.58709200
H	1.64747700	-1.65315400	-1.90911100
C	3.79479700	-1.25965700	0.62881500
H	2.03289100	-1.86841800	1.79951500
H	2.29922600	-0.09728900	1.74864800
H	3.30888900	-2.95187800	-0.66455800
H	4.35549100	-1.75198700	-1.44845300
H	4.39639900	-1.90111500	1.27789900
H	4.31092300	-0.30185200	0.51581000
Cl	1.68319000	2.15856700	0.02480500
O	1.50280200	-0.95882800	0.02549600

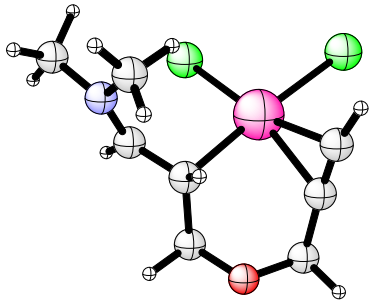
- THF



B3LYP/6-311+G(2d,2p) energy: -232.527888361 a.u.
ZPE: 0.116912 a.u.
Thermal correction to Gibbs Free Energy: 0.088273 a.u.
Solvation energy: -1.37 kcal/mol
Dispersion correction: -9.71 kcal/mol

C	1.16570000	-0.43025400	-0.13180800
O	0.00006900	-1.25196200	-0.00023100
C	-1.16555600	-0.43042700	0.13209800
C	-0.73347200	0.99620800	-0.22731900
C	0.73324900	0.99640500	0.22718800
H	1.95013300	-0.82124000	0.52626200
H	1.53626400	-0.48109700	-1.16720200
H	-1.95036000	-0.82162100	-0.52540000
H	-1.53546600	-0.48112500	1.16775000
H	-0.79601300	1.15372100	-1.31002100
H	-1.34378300	1.76049800	0.26186200
H	1.34341300	1.76068000	-0.26219700
H	0.79573800	1.15427800	1.30984200

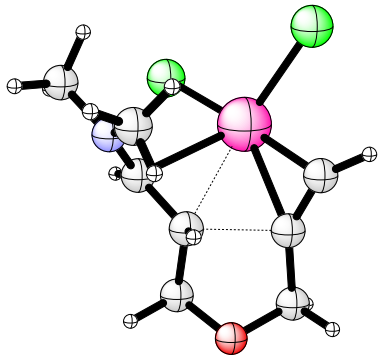
- INT1$_F$



B3LYP/BS2 energy: -1489.96569563 a.u.
ZPE: 0.201831 a.u.
Thermal correction to Gibbs Free Energy: 0.156295 a.u.
Solvation energy: -12.13 kcal/mol
Dispersion correction: -39.14 kcal/mol

C	2.66669200	0.39558900	1.89478000
H	3.62830600	0.21695800	2.37723000
H	2.25536700	1.33503200	2.26888600
H	1.97794100	-0.42224900	2.14113100
N	2.86612400	0.46310600	0.44847200
C	3.98224300	-0.32322400	-0.08337300
H	4.05617900	-0.17402200	-1.16045200
H	4.91293900	-0.00506500	0.39432100
H	3.80986200	-1.38752400	0.10471800
C	1.90294300	0.88289800	-0.35767900
H	2.13031300	0.79448700	-1.41519800
C	0.64856100	1.42493600	0.01508300
H	0.55926500	1.76187500	1.04693800
C	0.03010000	2.41710300	-0.97594500
H	0.69918400	3.27160700	-1.13389700
H	-0.13879400	1.93682700	-1.95262500
O	-1.16452600	3.01519700	-0.48907500
C	-2.28881300	2.15705000	-0.43300300
H	-3.14027500	2.78832700	-0.15683600
H	-2.50008300	1.70536300	-1.41344200
C	-2.13298700	1.09302400	0.57718300
C	-2.04582300	0.33371900	1.54264700
H	-2.19718700	-0.23979200	2.43167500
Pd	-0.56770800	-0.44460300	0.05036200
Cl	0.97920800	-1.70336800	-1.25674800
Cl	-1.99465400	-2.34251200	0.18886700

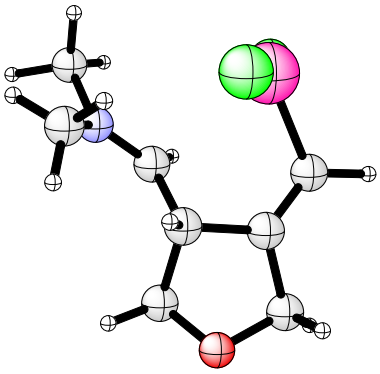
- TS$_F$



B3LYP/BS2 energy: -1489.9258355 a.u.
ZPE: 0.201107 a.u.
Thermal correction to Gibbs Free Energy: 0.15560 a.u.
Solvation energy: -13.52 kcal/mol
Dispersion correction: -38.88 kcal/mol

C	-0.16120000	2.25813300	-2.09518400
H	-0.41676300	3.23054600	-2.52180900
H	0.85223100	2.00024400	-2.40277100
H	-0.85580400	1.50343500	-2.47950000
N	-0.26706800	2.34832800	-0.63863500
C	-1.42771200	3.10470600	-0.15378200
H	-1.48751100	3.03813100	0.93048700
H	-1.33684200	4.14676900	-0.47608500
H	-2.34570900	2.67300200	-0.56484300
C	0.42960600	1.58965800	0.20772000
H	0.19344500	1.74514700	1.25563000
C	1.59017600	0.79317200	-0.12422400
H	1.94007900	0.94948900	-1.14184800
C	2.74120400	0.82012800	0.87145900
H	3.21619500	1.80580300	0.90075500
H	2.38784100	0.56528700	1.88276800
O	3.72808300	-0.07935500	0.40259600
C	3.12199600	-1.33061700	0.16327600
H	3.78392400	-1.90778800	-0.48952500
H	2.98313400	-1.88380800	1.10585000
C	1.77289500	-1.18206300	-0.48103200
C	0.79455400	-1.78629900	-1.03653600
H	0.50633800	-2.66068900	-1.59547700
Pd	-0.48052300	-0.63538300	0.06188600
Cl	-1.77696200	0.35902500	1.88281800
Cl	-2.24896800	-1.96975000	-0.71287000

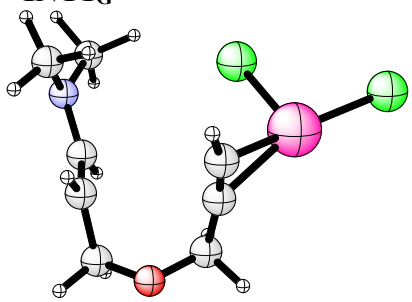
- INT2$_F$



B3LYP/BS2 energy: -1490.00106558 a.u.
ZPE: 0.204823 a.u.
Thermal correction to Gibbs Free Energy: 0.159774 a.u.
Solvation energy: -10.15 kcal/mol
Dispersion correction: -39.95 kcal/mol

C	-0.42279400	2.97680600	0.76386700
H	-0.03485900	3.98872500	0.64975200
H	-1.49099000	3.02962500	0.97544700
H	0.09581200	2.45726500	1.57994200
N	-0.17979100	2.24012600	-0.48858900
C	0.87556700	2.77655300	-1.36145500
H	1.10796700	2.05343800	-2.14331000
H	0.54343700	3.72434700	-1.79412700
H	1.77422100	2.94917800	-0.76241700
C	-0.67832500	1.05466700	-0.71877500
H	-0.38736200	0.58506500	-1.65530300
C	-1.75723000	0.40205200	0.07415000
H	-1.81069000	0.80054600	1.09115200
C	-3.16102500	0.47695300	-0.59759000
H	-3.71987800	1.38236200	-0.34684100
H	-3.06604300	0.40826300	-1.69423800
O	-3.85220900	-0.63302900	-0.06104800
C	-2.94094000	-1.73594500	0.00044200
H	-3.22082800	-2.34776000	0.86336200
H	-3.01637000	-2.35321100	-0.90725500
C	-1.55791000	-1.10500700	0.12515700
C	-0.37037800	-1.69126000	0.19893600
H	-0.19223700	-2.76356600	0.21921600
Pd	1.27621300	-0.63239600	0.22812800
Cl	1.72391200	-0.94747600	-2.07166900
Cl	1.03293700	0.10220400	2.44995400

- INT1$_G$

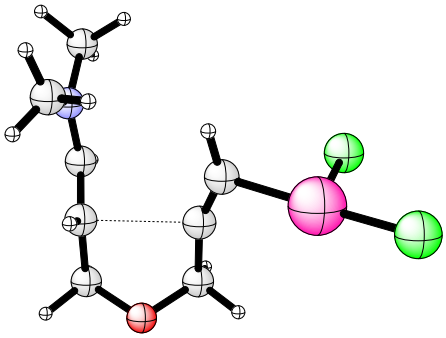


B3LYP/BS2 energy: -1489.93213775 a.u.
ZPE: 0.199756 a.u.
Thermal correction to Gibbs Free Energy: 0.150484 a.u.
Solvation energy: -6.71 kcal/mol
Dispersion correction: -33.73 kcal/mol

C	3.27151800	-1.72473000	1.36850400
H	3.63158100	-2.73123300	1.59559800
H	3.94220600	-1.00534400	1.84711500
H	2.26402500	-1.60845900	1.79663300
N	3.27853500	-1.52838500	-0.07008100
C	2.85919600	-2.66870300	-0.86918600
H	3.01307400	-2.45338100	-1.92971800
H	3.45682800	-3.54693600	-0.60555800
H	1.79418900	-2.91034700	-0.71969500
C	3.07291700	-0.26791300	-0.57239800
H	3.01097600	-0.24707300	-1.65983800
C	2.99572300	0.90139300	0.10564500
H	3.03179300	0.93094700	1.19014500
C	2.89592100	2.20850100	-0.60670300
H	3.69060000	2.90288200	-0.31297100
H	2.96864100	2.05708600	-1.69484300
O	1.69460700	2.97075100	-0.32021000
C	0.49121600	2.33712200	-0.67455600
H	-0.20266500	3.11435700	-1.01663200
H	0.61496900	1.61566400	-1.49311500
C	-0.12847400	1.64484600	0.48715000

C	-0.48416400	1.23793900	1.60126400
H	-0.54749400	1.01963400	2.64758600
Pd	-1.82347800	0.19806800	0.22913700
Cl	-3.72878100	-0.73430600	-0.63837400
Cl	-0.57348200	-1.69669300	-0.07757100

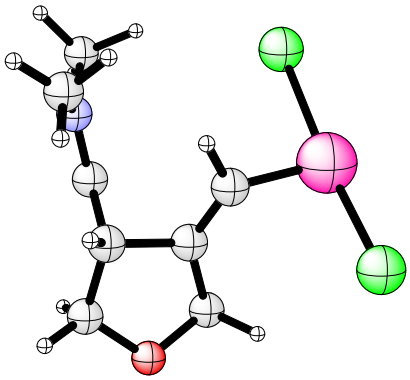
- TS_G



B3LYP/BS2 energy: -1489.92183837 a.u.
ZPE: 0.199617 a.u.
Thermal correction to Gibbs Free Energy: 0.149869 a.u.
Solvation energy: -11.76 kcal/mol
Dispersion correction: -33.84 kcal/mol

C	-3.88870800	-1.43044500	-1.59957300
H	-4.48349800	-2.32728800	-1.78581700
H	-4.39585600	-0.57714700	-2.05890000
H	-2.91253000	-1.55574200	-2.08429100
N	-3.77454300	-1.22560100	-0.16186200
C	-3.88665000	-2.40001500	0.69452600
H	-3.86770700	-2.09440300	1.74213300
H	-4.82888700	-2.92398600	0.50010500
H	-3.05926000	-3.10131500	0.52842600
C	-3.42346800	-0.02284100	0.34713600
H	-3.44071400	0.01758800	1.43489100
C	-3.05287000	1.10115800	-0.34366800
H	-3.02330400	1.10376200	-1.42860400
C	-2.87885700	2.41967700	0.34458800
H	-3.52106900	3.19500200	-0.08440600
H	-3.12213600	2.32862300	1.41605900
O	-1.54759100	2.93118400	0.19102100
C	-0.60115600	2.00851400	0.67275100
H	0.38399200	2.46713800	0.54773700
H	-0.74366300	1.80070000	1.74620700
C	-0.61226900	0.71422400	-0.05718800
C	-0.19129400	-0.36703800	-0.54056300
H	-0.54244800	-1.29825800	-0.95009400
Pd	1.88191200	-0.12974100	-0.34888600
Cl	1.76955600	-1.09074600	1.73492400
Cl	4.17181300	0.02743700	-0.61597500

- $INT2_G$



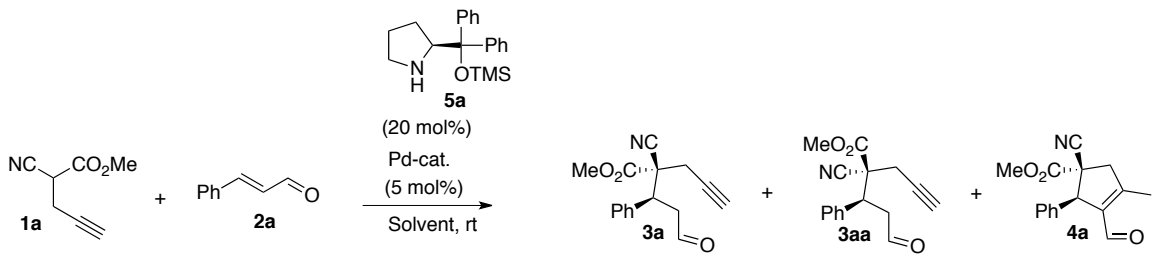
B3LYP/BS2 energy: -1489.98168967 a.u.
ZPE: 0.204763 a.u.
Thermal correction to Gibbs Free Energy: 0.158806 a.u.
Solvation energy: -16.27 kcal/mol
Dispersion correction: -36.82 kcal/mol

C	3.12841400	-1.34062400	1.59643900
H	4.09609500	-1.82744400	1.74223200
H	3.08815800	-0.43210400	2.19228600
H	2.33448600	-2.02340000	1.91445200
N	2.96127300	-1.04339200	0.16924000
C	2.96400100	-2.23098300	-0.70760200
H	3.11637700	-1.92209300	-1.74214000
H	3.77032800	-2.90030900	-0.40281700
H	1.98774100	-2.72546000	-0.62029800
C	2.59339100	0.11491200	-0.30988600
H	2.50285300	0.14904800	-1.39310900
C	2.15689200	1.33060700	0.40478900
H	2.41104700	1.36502200	1.46463100
C	2.47542800	2.66128500	-0.34082900
H	3.15367600	3.30312000	0.22648900
H	2.93985700	2.44774000	-1.31966000
O	1.24370800	3.32878900	-0.49233900
C	0.25370700	2.33301800	-0.76575400
H	-0.73336400	2.71939500	-0.50558300
H	0.26007800	2.06312900	-1.83549900
C	0.64070000	1.17086700	0.12088600
C	-0.05317200	0.10986400	0.55441800
H	0.41781900	-0.61551400	1.21413800
Pd	-1.78020600	-0.51915800	0.00245900
Cl	-2.97514000	1.42052100	0.49720400
Cl	-0.73606100	-2.59346800	-0.59184900

SUPPORTING INFORMATION, PART B

General methods: Chemicals and solvents were either purchased *puriss p. A.* from commercial suppliers or purified by standards techniques. The pyrrolidine catalysts **5a** was synthesized according to literature procedures.[1] $Pd(PPh_3)_2O_2$ was prepared according to literature procedures.[2] For thin-layer chromatography (TLC), silica gel plates Merck 60 F254 were used and compounds were visualized by irradiation with UV light and/or by treatment with a solution of ammoniummolybdate (100 g), $Ce(SO_4)_2$ (2 g) and 10% H_2SO_4 (1 L) followed by heating or by treatment with a solution of potassium permanganate (3 g), K_2CO_3 (20 g), 5% aq. NaOH (5 mL) and water (300 mL) followed by heating. Flash chromatography was performed using silica gel Merck 60 (particle size 0.040-0.063 mm), ^{1}H NMR, ^{13}C NMR and ^{31}P NMR spectra were recorded on Bruker AM400 or Varian AS400. Chemical shifts are given in δ relative to tetramethylsilane (TMS), the coupling constants *J* are given in Hz. The spectra were recorded in $CDCl_3$ as solvent at room temperature, TMS served as internal standard (δ = 0 ppm) for ^{1}H NMR and $CDCl_3$ was used as internal standard (δ = 77.16 ppm) for ^{13}C NMR. HPLC was carried out using a Waters 2690 Millenium with photodiode array detector. Optical rotations were recorded on a Perkin Elmer 241 Polarimeter (d = 589 nm, 1 dm cell). High-resolution mass spectra (ESI) were obtained with a Bruker MicroTOF spectrometer.

Monitoring the reaction progress:



Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $Pd(PPh_3)_4$ and chiral amine 5a: To a stirred solution of propargyl malonate **1a** (0.375 mmol, 1 equiv) in CH_3CN (0.6 mL) was added the $Pd(PPh_3)_4$ (5 mol%). After stirring for 5 minutes, the chiral pyrrolidine catalyst **5a** (20 mol%) and cinnamic aldehyde **2a** (0.25 mmol, 1 equiv) were added sequentially. The reaction was stirred at room temperature and the formations of **3a**, **3aa** and **4a** were measured by taking aliquots (5 μL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^1H NMR analysis was performed (Figure S1).

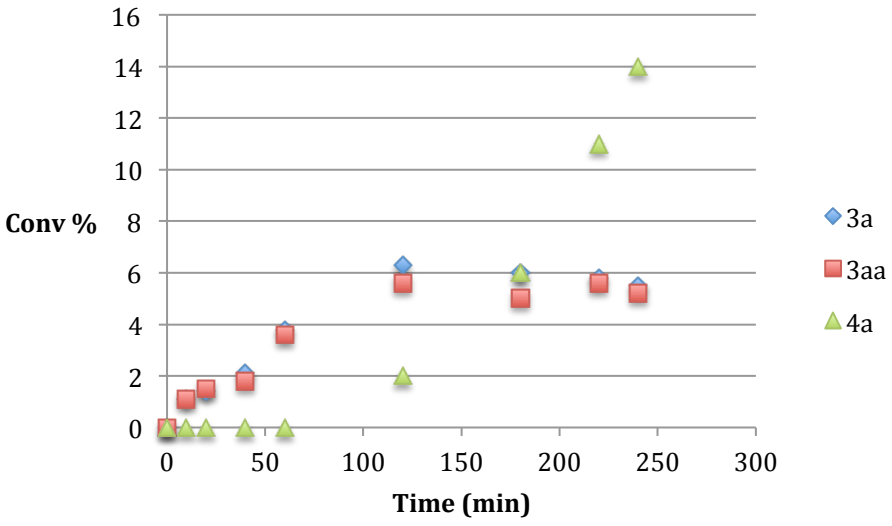


Figure S1. $Pd(PPh_3)_4$/chiral amine **5a**-co-catalyzed reaction.

Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $Pd(PPh_3)_4$ and chiral amine 5a under inert atmosphere: To a solution of propargyl malonate **1a** (0.375 mmol, 1 equiv) in degassed CH_3CN (0.6 mL) was added $Pd(PPh_3)_4$ (5 mol%) in a glove box. Next, the chiral pyrrolidine catalyst **5a** (20 mol%) and cinnamic aldehyde **2a** (0.25 mmol, 1 equiv) were added sequentially. The reaction was stirred at room temperature under inert atmosphere and the formations of **3a**, **3aa** and **4a** were measured by taking aliquots (5 μL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^1H NMR analysis was performed (Figure S2).

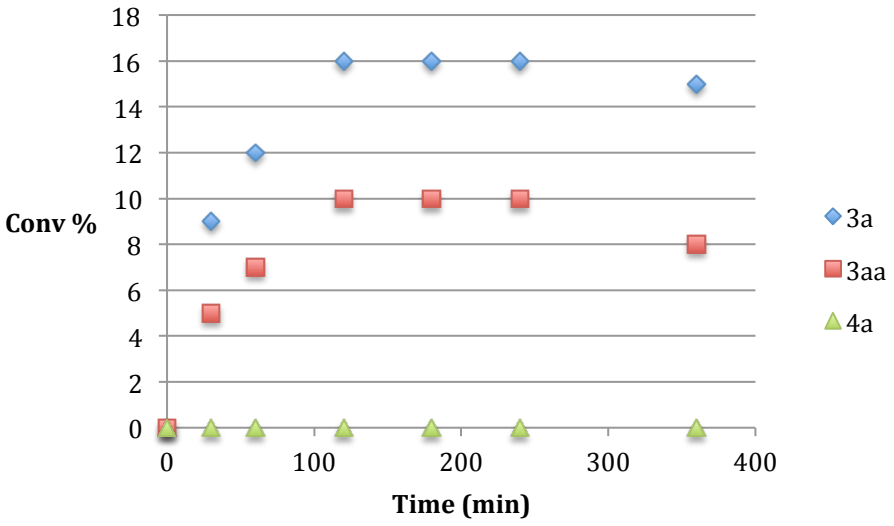


Figure S2. $Pd(PPh_3)_4$/chiral amine **5a**-co-catalyzed reaction under inert atmosphere in glove-box.

Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $Pd(PPh_3)_4$, which has been pre-stirred in solution for 2h under oxygen atmosphere, and chiral amine 5a: A solution mixture of $Pd(PPh_3)_4$ in CH_3CN (0.6 mL) was stirred for 2h in the presence of molecular oxygen. Next, the oxygen balloon was removed and propargyl malonate **1a** (0.375 mmol, 1 equiv), the chiral pyrrolidine catalyst **5a** (20 mol%) as well as cinnamic aldehyde **2a** (0.25 mmol, 1 equiv) were added sequentially. The reaction was stirred at room temperature and the formations

of **3a**, **3aa** and **4a** were measured by taking aliquots (5 μL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^1H NMR analysis was performed (Figure S3).

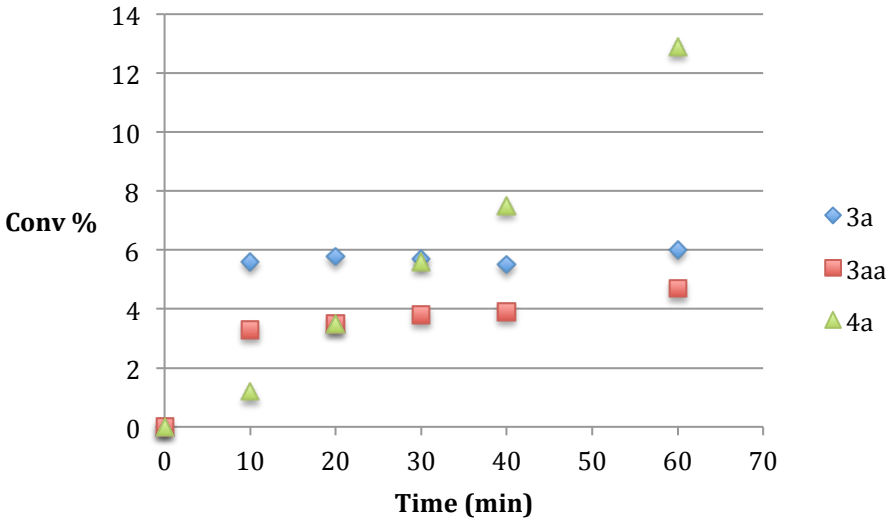


Figure 3S. $Pd(PPh_3)_4$/chiral amine **5a**-co-catalyzed reaction were the Pd-catalyst was first pre-stirred for 2h under O_2 atmosphere.

Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $Pd(PPh_3)_2O_2$ and chiral amine 5a: To a stirred solution of propargyl malonate **1a** (0.375 mmol, 1 equiv) in CH_3CN (0.6 mL) was added $Pd(PPh_3)_4O_2$ (5 mol%). After stirring for 5 minutes, the chiral pyrrolidine catalyst **5a** (20 mol%) and cinnamic aldehyde **2a** (0.25 mmol, 1 eq) were added sequentially. The reaction was stirred at room temperature and the formations of **3a**, **3aa** and **4a** were measured by taking aliquots (5 μL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^1H NMR analysis was performed (Figure S4).

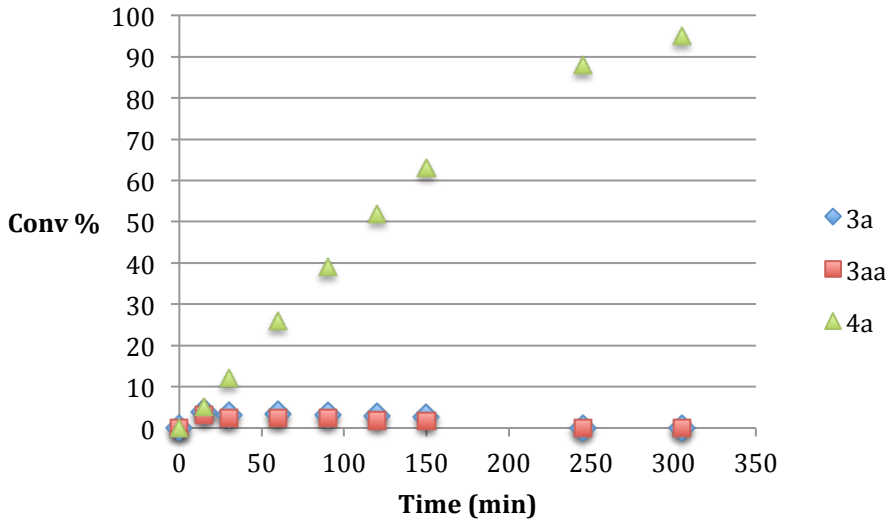


Figure S4. $Pd(PPh_3)_2O_2$/chiral amine **5a**-co-catalyzed reaction.

Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $PdCl_2$ and chiral amine 5a: A solution mixture of $PdCl_2$ in CH_2Cl_2 (0.6 mL) was stirred for 5 min. Next, the propargyl malonate **1a** (0.375 mmol, 1 equiv), the chiral pyrrolidine catalyst **5a** (20 mol%) as well as cinnamic aldehyde **2a** (0.25 mmol, 1 eq) were added sequentially. The reaction was stirred at room temperature and the formations of **3a**, **3aa** and **4a** were measured by taking aliquots (5 μL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^{1}H NMR analysis was performed (Figure S5).

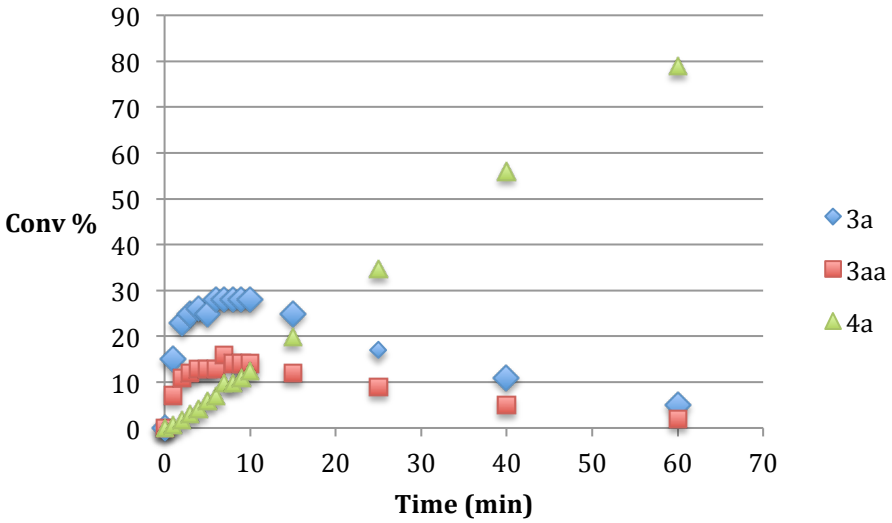


Figure S5. $PdCl_2$/chiral amine **5a**-co-catalyzed reaction.

Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $PdCl_2$ and chiral amine 5a in CH_3CN: A solution mixture of $PdCl_2$ in CH_3CN (0.6 mL) was stirred for 5 min. Next, the propargyl malonate **1a** (0.375 mmol, 1 equiv), the chiral pyrrolidine catalyst **5a** (20 mol%) as well as cinnamic aldehyde **2a** (0.25 mmol, 1 eq) were added sequentially. The reaction was stirred at room temperature and the formations of **3a**, **3aa** and **4a** were measured by taking aliquots (5 μL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^1H NMR analysis was performed (Figure S6).

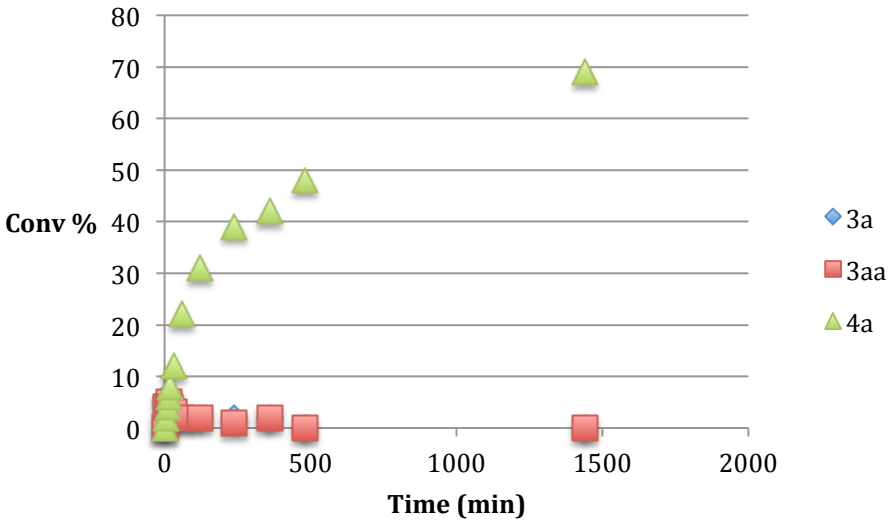


Figure S6. $PdCl_2$/chiral amine **5a**-co-catalyzed reaction in CH_3CN.

Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $Pd(PPh_3)_2O_2$ and chiral amine 5a under inert atmosphere: To a solution of propargyl malonate **1a** (0.375 mmol, 1 equiv) in degassed CH_3CN (0.6 mL) was added $Pd(PPh_3)_2O_2$ (5 mol%) in a glove box. Next, the chiral pyrrolidine catalyst **5a** (20 mol%) and cinnamic aldehyde **2a** (0.25 mmol, 1 equiv) were added sequentially. The reaction was stirred at room temperature under inert atmosphere and the formations of **3a**, **3aa** and **4a** were measured by taking aliquots (5 μL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^1H NMR analysis was performed (Figure S7).

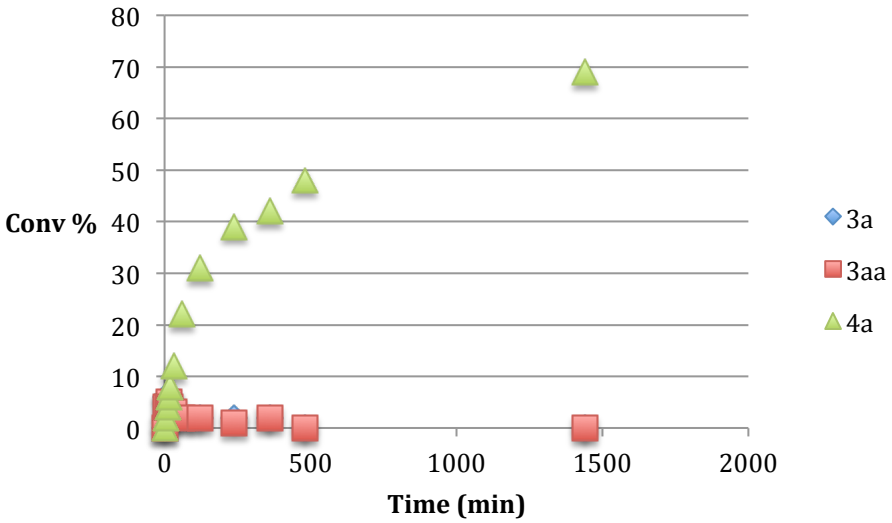


Figure S7. $Pd(PPh_3)_2O_2$/chiral amine 5a-co-catalyzed reaction under inert atmosphere in glove-box.

Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $PdCl_2$ and chiral amine 5a under inert atmosphere: To a solution of propargyl malonate **1a** (0.375 mmol, 1 equiv) in degassed CH_3CN (0.6 mL) was added $PdCl_2$ (5 mol%) in a glove box. Next, the chiral pyrrolidine catalyst **5a** (20 mol%) and cinnamic aldehyde **2a** (0.25 mmol, 1 equiv) were added sequentially. The reaction was stirred at room temperature under inert atmosphere and the formations of **3a**, **3aa** and **4a** were measured by taking aliquots (5 μL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^1H NMR analysis was performed (Figure S8).

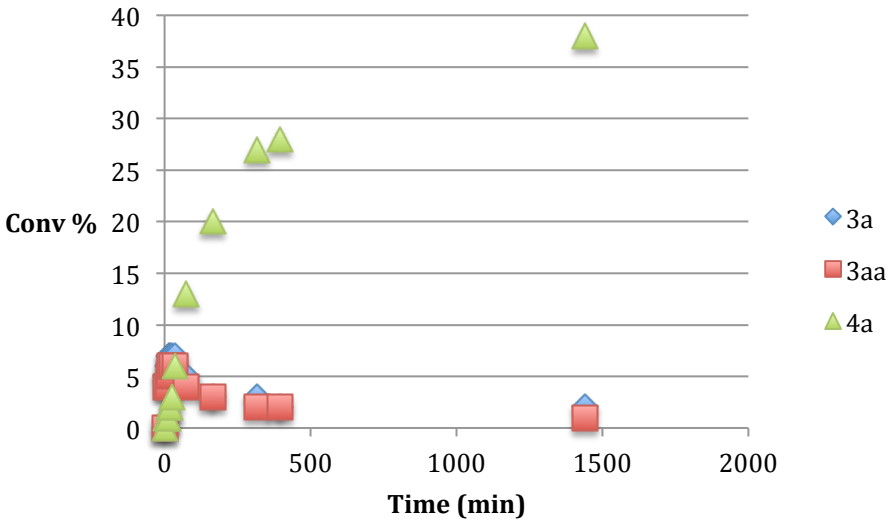


Figure S8. $PdCl_2$/chiral amine **5a**-co-catalyzed reaction under inert atmosphere in glove-box.

Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $Pd^0[P(o\text{-tolyl})_3]_2$ and chiral amine 5a: To a stirred solution of propargyl malonate **1a** (0.375 mmol, 1 equiv) in CH_3CN (0.6 mL) was added $Pd^0[P(o\text{-tolyl})_3]_2$ (5 mol%). After stirring for 5 minutes, the chiral pyrrolidine catalyst **5a** (20 mol%) and cinnamic aldehyde **2a** (0.25 mmol, 1 eq) were added sequentially. The reaction was stirred at room temperature and the formations of **3a**, **3aa** and **4a** were measured by taking aliquots (5 mL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^1H NMR analysis was performed (Figure S9).

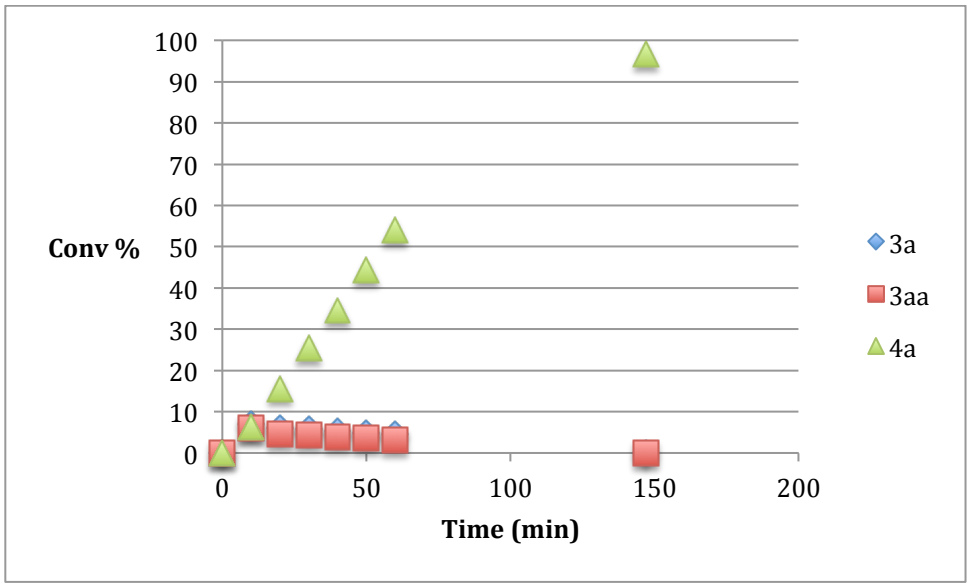


Figure S9. $Pd^0[P(o\text{-tolyl})_3]_2$/chiral amine **5a**-co-catalyzed reaction on CH_3CN.

Carbocyclization between cinnamic aldehyde and methyl 2-cyanopent-4-ynoate in the presence of $Pd^0[P(o\text{-tolyl})_3]_2$ and chiral amine 5a under inert atmosphere: To a solution of propargyl malonate **1a** (0.375 mmol, 1 equiv) in degassed CH_3CN (0.6 mL) was added $Pd^0[P(o\text{-tolyl})_3]_2$ (5 mol%) in a glove box. Next, the chiral pyrrolidine catalyst **5a** (20 mol%) and cinnamic aldehyde **2a** (0.25 mmol, 1 equiv) were added sequentially. The reaction was stirred at room temperature under inert atmosphere and the formations of **3a**, **3aa** and **4a** were measured by taking aliquots (5 mL) of the reaction mixture to NMR vials with $CDCl_3$ (0.6 mL) followed by freezing with liquid nitrogen. Next, ^1H NMR analysis was performed (Figure S10).

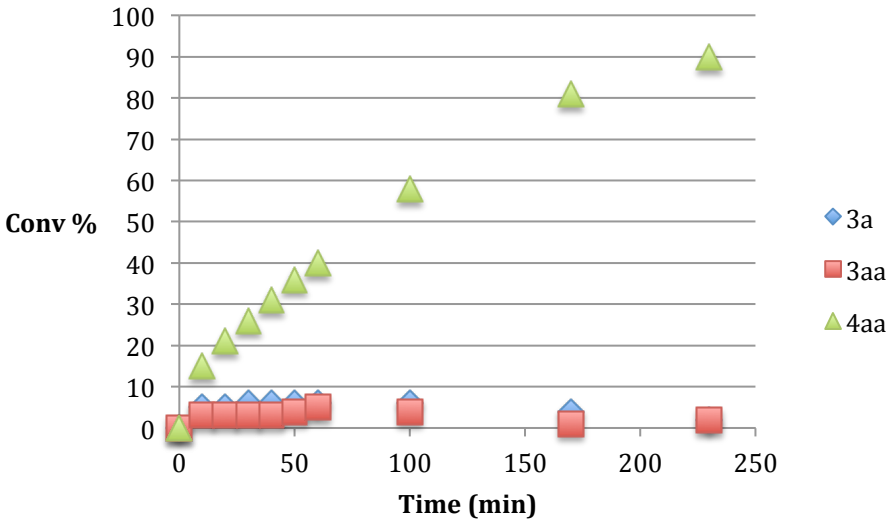
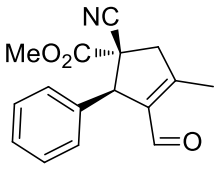


Figure S10. $Pd^0[P(o\text{-tolyl})_3]_2$/chiral amine **5a**-co-catalyzed reaction under inert atmosphere in glove-box.

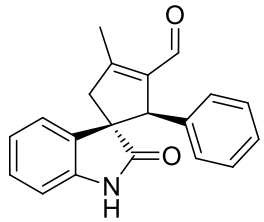
Aerobic allylic alcohol oxidation/Michael/carbocyclization catalytic relay to 4a: Cinnamic alcohol (0.24 mmol, 1.2 equiv) and $Pd(PPh_3)_4$ (5 mol% to **1a**, 11.5 mg) was weighed into a microwave vial and was suspended in toluene (0.5 mL). The vial was capped, evacuated and an oxygen balloon was connected to the reaction vessel. The reaction was stirred at 70 °C for 6 hours. Next, the reaction mixture was cooled to room temperature and propargylcyanomalonate **1a** (0.2 mmol, 1 equiv) as well as catalyst **5a** (20 mol%, 13 mg) were sequentially added. After stirring vigorously for 16 h, the crude reaction mixture was directly loaded on a silica-gel column and next chromatograph (pentane/EtOAc mixtures-3:1) afforded the corresponding product **5a** (34 mg, 62% yield).



(1*R*,2*R*)-methyl 1-cyano-3-formyl-4-methyl-2-phenylcyclopent-3-enecarboxylate: oil. **^{1}H NMR (400MHz, $CDCl_3$):** δ 9.92 (s, 1H), 7.38-7.32 (m, 3H), 7.17-7.15 (m, 2H), 4.72 (bs, 1H), 3.88 (s, 3H), 3.41 (d, J = 14.8 Hz, 1H), 3.26 (d, J = 14.8 Hz, 1H), 2.33 (s, 3H);

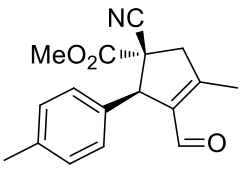
^{13}C NMR (100MHz, $CDCl_3$): 186.2, 168.8, 157.9, 136.8, 136.6, 129.0, 128.7, 128.0, 117.4, 58.4, 54.4, 51.7, 47.8, 14.3; **HRMS (ESI)** : calcd for [M+Na] ($C_{16}H_{15}NO_3$) requires m/z 292.0944, found 292.0944; $[\alpha]_D^{25}$ = - 5.2 (*c* 1.0, $CHCl_3$).The enantiomeric excess was determined by HPLC analysis in comparison with authentic racemic material (ODH-column, *n*-hexane/*i*-PrOH = 85/15, λ = 210 nm, 1.0 ml/min) t_r (major enantiomer) = 17.0 min, t_r (minor enantiomer) = 27.0 min.

Aerobic allylic alcohol oxidation/Michael/carbocyclization catalytic relay to 4b: Cinnamic alcohol (0.24 mmol, 1.0 equiv) and $Pd(PPh_3)_4$ (5 mmol%, 14 mg) was weighed into a microwave vial and was suspended in toluene (0.5 mL). The vial was capped, evacuated and an oxygen balloon was connected to the reaction vessel. The reaction was stirred at 70 °C for 6 hours. Then the reaction was cooled to room temperature and toluene (0.5 mL), Propargyl-2-oxindole **1b** (0.4 mmol, 1.7 equiv), catalyst **5a** (17 mol%, 13 mg) as well as benzoic acid (17 mol%, 5 mg) were sequentially added. After vigorous stirring for 20 hours, the crude reaction mixture was directly loaded on a silica-gel column and immediate chromatograph (pentane/EtOAc) afforded the corresponding product **4b** (55 mg, 76% yield).

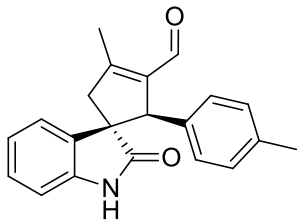


(1*R*,2*R*)-4-methyl-2'-oxo-2-phenylspiro[cyclopent[3]ene-1,3'-indoline]-3-carbaldehyde: oil. **^{1}H NMR (400MHz, $CDCl_3$):** δ 10.08 (s, 1H), 8.26 (bs, 1H), 7.11-7.10 (m, 3H), 7.03-6.99 (m, 1H), 6.84-6.82 (m, 2H,), 6.73 (d, *J* = 8.0 Hz, 1H), 6.63 (t, *J* = 0.8 Hz, 1H), 6.24 (d, *J* = 7.6 Hz, 1H), 4.63 (bs, 1H), 3.0 (dd, *J* = 18.8 Hz, *J′* = 18.4 Hz, 2H), 2.42 (d, *J* = 1.2 Hz, 3H); **^{13}C NMR (100MHz, $CDCl_3$):** 187.3, 182.7, 160.9, 140.3, 138.1, 137.8, 130.6, 128.2, 128.0, 127.3, 125.1, 122.0, 109.4, 58.4, 56.6, 49.0, 14.9; **HRMS (ESI)** : calcd for [M+Na] ($C_{20}H_{17}NO_2$) requires m/z 326.1151, found 326.1154; $[\alpha]_D^{25}$ = -70.3 (*c*=1, $CHCl_3$).The enantiomeric excess was determined by HPLC analysis in comparison with authentic racemic material (ODH-column, *n*-hexane/*i*-

PrOH = 80/20, λ = 254 nm, 1.0 ml/min) t_r (major enantiomer) = 29.5 min, t_r (minor enantiomer) = 20.8 min.

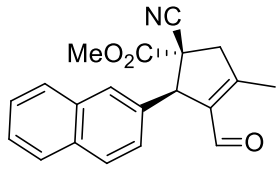


(1*R*,*2*R)-methyl 1-cyano-3-formyl-4-methyl-2-(p-tolyl)cyclopent-3-enecarboxylate: oil. **^{1}H NMR (400MHz, $CDCl_3$):** δ 9.91 (s, 1H), 7.16 (d, *J* = 6.4 Hz, 2H), 7.04 (d, *J* = 6.4 Hz, 2H), 4.68 (bs, 1H), 3.88 (s, 3H), 3.39 (d, *J* = 14.8 Hz, 1H), 3.25 (d, *J* = 14.8 Hz, 1H), 2.32 (s, 3H); **^{13}C NMR (100MHz, $CDCl_3$):** 186.3, 168.9, 157.7, 138.4, 136.8, 133.6, 129.8, 127.9, 117.6, 58.2, 54.4, 51.8, 47.8, 21.4, 14.3; **HRMS (ESI)** : calcd for [M+Na] ($C_{17}H_{17}NO_3$) requires m/z 306.1101, found 306.1104; $[\alpha]_D^{25}$ = -81.6 (*c*=1.30$CHCl_3$). The enantiomeric excess was determined by HPLC analysis in comparison with authentic racemic material (ODH-column, *n*-hexane/*i*-PrOH = 90/10, λ = 250 nm, 1.0 ml/min) t_r (major enantiomer) = 23.9 min, t_r (minor enantiomer) =32.9 min.



(1R,2R)-4-methyl-2'-oxo-2-(p-tolyl)spiro[cyclopent[3]ene-1,3'-indoline]-3-carbaldehyde: δ 10.06 (s, 1H), 8.10 (bs, 1H), 7.04 (t, *J* = 1.2 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.75-6.70 (m, 3H), 6.63 (t, *J* = 7.6 Hz, 1H) , 6.43 (d, *J* = 7.6 Hz, 1H), 4.59 (bs, 1H), 2.98 (q, *J* = 18.4 Hz, *J′*= 15.2 Hz, 2H), 2.41 (d, *J* =1.6 Hz, 3H), 2.22 (s, 3H); **^{13}C NMR (100MHz, $CDCl_3$):**187.4, 182.6, 160.6, 140.3, 138.0, 136.8, 135.0, 130.7, 128.9, 128.1, 128.0, 125.2, 122.0, 109.4, 58.0, 56.6, 49.0, 21.2, 15.0; **HRMS (ESI)** : calcd for [M+Na] ($C_{21}H_{19}NO_2$) requires m/z 340.1308, found 340.1310; $[\alpha]_D^{25}$ = -120.4

(*c*=1, $CHCl_3$).The enantiomeric excess was determined by HPLC analysis in comparison with authentic racemic material (ODH-column, *n*-hexane/*i*-PrOH = 80/20, λ = 250 nm, 1.0 ml/min) t_r (major enantiomer) = 39.2 min, t_r (minor enantiomer) = 19.5 min.



(1R,2R)-methyl 1-cyano-3-formyl-4-methyl-2-(naphthalen-2-yl)cyclopent-3-enecarboxylate: oil. **^{1}H NMR (400MHz, $CDCl_3$):** δ 9.95 (s, 1H), 7.87-7.80 (m, 3h), 7.16 (d, *J* = 1.2 Hz, 1H), 7.50-7.45 (m, 2H), 7.28 (dd, *J* = 2.0 Hz, *J′* = 6.4 Hz, 1H), 4.90 (bs, 1H), 3.90 (s, 3H), 3.38 (q, *J* = 18.8 Hz, *J′* = 26.0 Hz, 2H), 2.36 (s, 3H); **^{13}C NMR (100MHz, $CDCl_3$):** 186.2, 168.9, 158.0, 136.8, 134.1, 133.5, 133.5, 128.9, 128.2, 127.9, 127.3, 126.4, 126.4, 125.7, 117.4, 58.5, 54.5, 51.7, 48.0, 14.4; **HRMS (ESI)** : calcd for [M+Na] ($C_{20}H_{17}NO_3$) requires m/z 342.1101, found 342.1098; $[\alpha]_D^{25}$ = -127.5 (*c*=1.0, $CHCl_3$). The enantiomeric excess was determined by HPLC analysis in comparison with authentic racemic material (ODH-column, *n*-hexane/*i*-PrOH = 70/30, λ = 230 nm, 1.0 ml/min) t_r (major enantiomer) = 13.2 min, t_r (minor enantiomer) =30.9 min.

Typical aerobic allylic alcohol oxidation of cinnamic alcohol with H_2O_2: Cinnamic alcohol (0.24 mmol, 1.0 equiv) and $Pd(PPh_3)_4$ (5 mol%) was weighed into a microwave vial and was suspended in toluene (0.5 mL). The vial was capped, evacuated and hydrogen peroxide (1, 2 or 4 equiv) was added. The reaction was stirred at 70 °C and the reaction was monitored by ^{1}H NMR by taking aliquots (5 μL) of the reaction mixture (Figure S11).

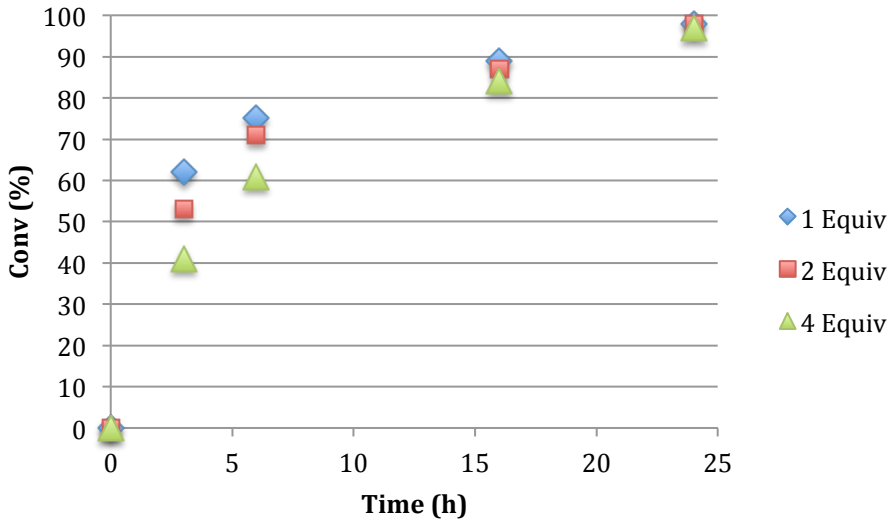


Figure S11. Conversion of cinnamic alcohol to cinnamic aldehyde as a function of time using different equiv. of H_2O_2 and $Pd(PPh_3)_4$ as the catalyst.

Non-linear effect study: To a stirred solution of propargyl malonate **1a** (0.375 mmol, 1 equiv) in CH_3CN (0.6 mL) was added the $Pd(PPh_3)_4$ (5 mol%). After stirring for 5 minutes, the chiral pyrrolidine catalyst **5a** (20 mol%, with a specific ee) and cinnamic aldehyde **2a** (0.25 mmol, 1 equiv) were added sequentially. After 16h, the mixture was diluted with CH_2Cl_2 and loaded upon a silica-gel column and immediate chromatography (pentane:EtOAc-mixture) furnished the corresponding product **4a**. Plotting the ee of catalyst **5a** as a function of **4a** is shown in Figure S12.

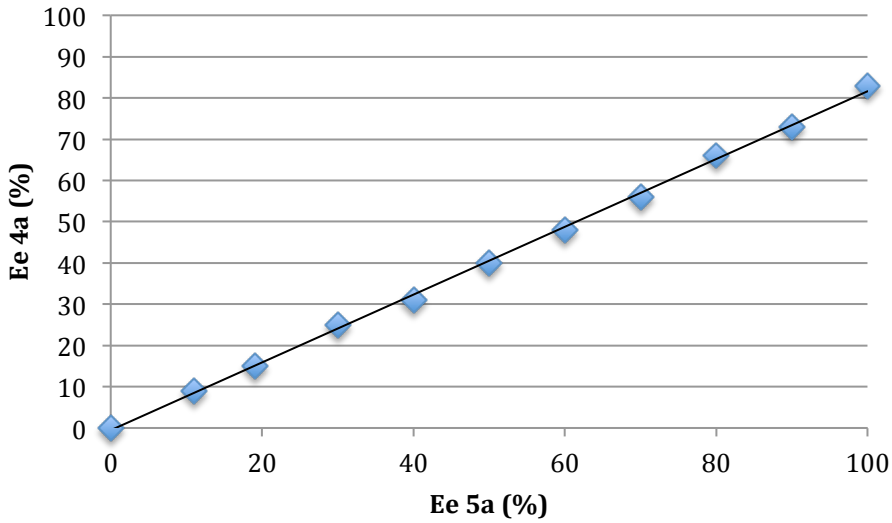


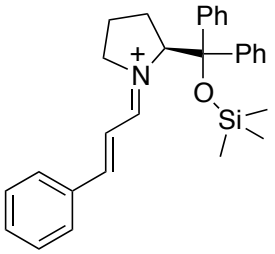
Figure S12. The ee of **4a** as a function the ee of catalyst 5a.

Table 1

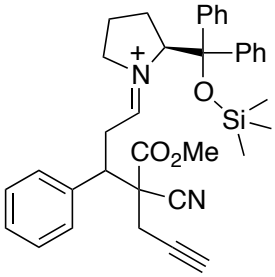
Ee of **5a** (%)	Ee of **4a** (%)[a]
0	0
11	9
19	15
30	25
40	31
50	40
60	48
70	56
80	66
90	73
100	83

[a] Determined by chiral-phase HPLC analysis.

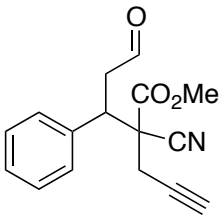
HRMS spectra analysis on the crude reaction mixture: To a stirred solution of propargyl malonate **1a** (0.375 mmol, 1 equiv) in CH_3CN (0.6 mL) was added the $Pd(PPh_3)_4$ (5 mol%). After stirring for 5 minutes, the chiral pyrrolidine catalyst **5a** (20 mol%) and cinnamic aldehyde **2a** (0.25 mmol, 1 eq) were added sequentially. The reaction was stirred at room temperature and the reaction intermediates were monitored by HRMS by taking aliquots (5 μL) of the reaction mixture that were directly injected to the mass spectrometer.



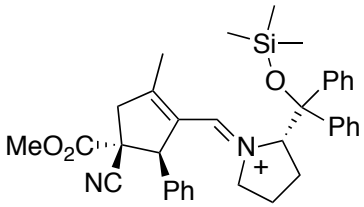
HRMS (ESI) : calcd for [M] ($C_{29}H_{34}NOSi$) requires m/z 440.2410, found 440.2409.



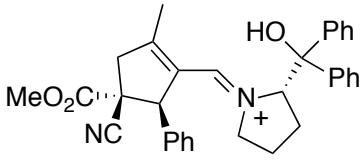
HRMS (ESI) : calcd for [M+Na] ($C_{36}H_{41}N_2O_3Si$) requires m/z 600.2784, found 600.2728.



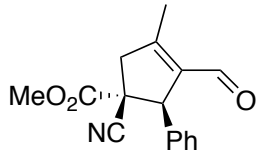
HRMS (ESI) : calcd for [M+Na] ($C_{16}H_{15}NNaO_3$) requires m/z 292.0950, found 292.0951.



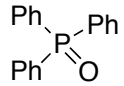
HRMS (ESI) : calcd for [M] ($C_{36}H_{41}N_2O_3Si$) requires m/z 577.2886, found 577.2879.



HRMS (ESI) : calcd for [M] ($C_{33}H_{33}N_2O_3$) requires m/z 505.2491, found 505.2480.



HRMS (ESI) : calcd for [M+Na] ($C_{16}H_{15}NO_3$) requires m/z 292.0950, found 292.0939.



HRMS (ESI) : calcd for [M+Na] ($C_{18}H_{15}OP$) requires m/z 301.0758, found 301.0750.

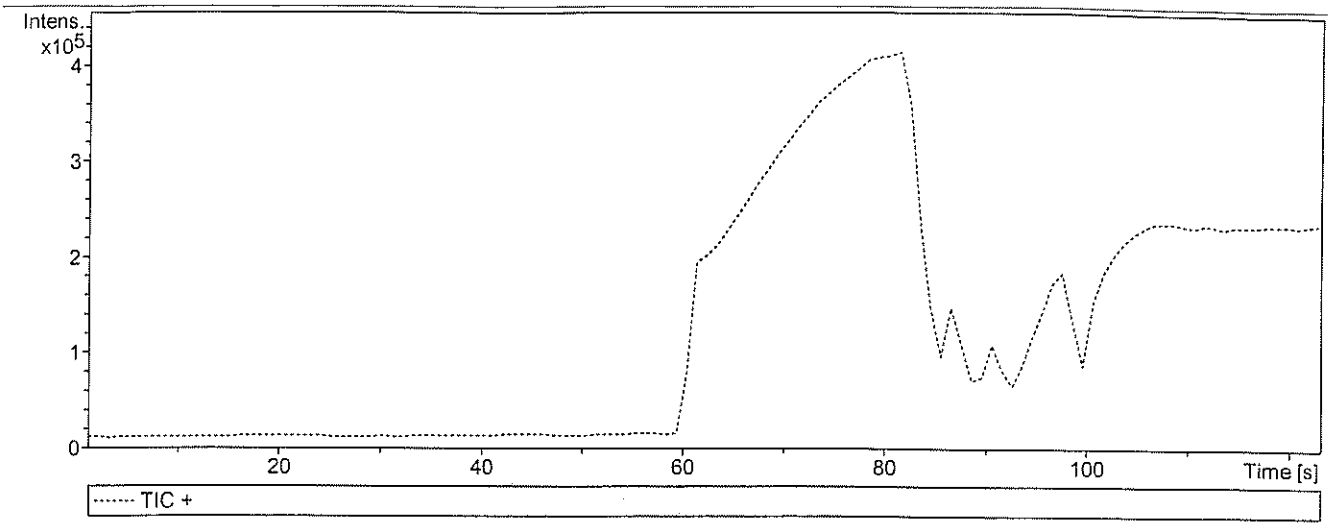
(1) (a) Marigo, M.; Wabnitz, T. C.; Fielenbach, D.; Jørgensen, K. A. *Angew. Chem. Int. Ed.* **2005**, *44*, 794. (b) Hayashi, Y.; Gotoh, H.; Hayashi, T.; Shoji, M. *Angew. Chem. Int. Ed*. **2005**, *44*, 4212. (c) Marigo, M.; Franzén, J.; Poulsen, T. B.; Zhuang, W.; Jørgensen, K. A. *J. Am. Chem. Soc.* **2005**, *127*, 6964. (d) Sundén, H. Ibrahem, I.; Córdova, A.; *Tetrahedron Lett.* **2006**, *47*, 99. (e) Ibrahem, I.; Córdova, A. *Chem. Commun.* **2006**, 1760.

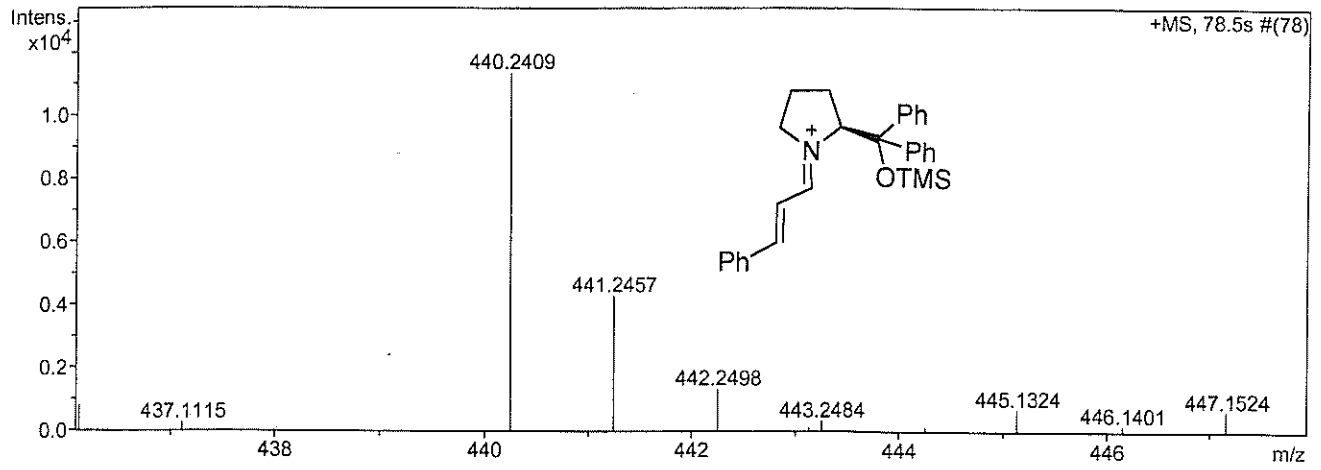
(2) (a) Nyman, C. J.; Wymore, C. E.; Wilkinson, G. *J. Chem. Soc. (A),* **1968**, 561. (b) Aboelell, N. W.; York, J. T.; Reynolds, A. M.; Fujita, K.; Kinsinger, C. R.; Cramer, C. J.; Riordan, C. G.; Tolman, W. B. *Chem. Commun.,* **2004**, 1716.

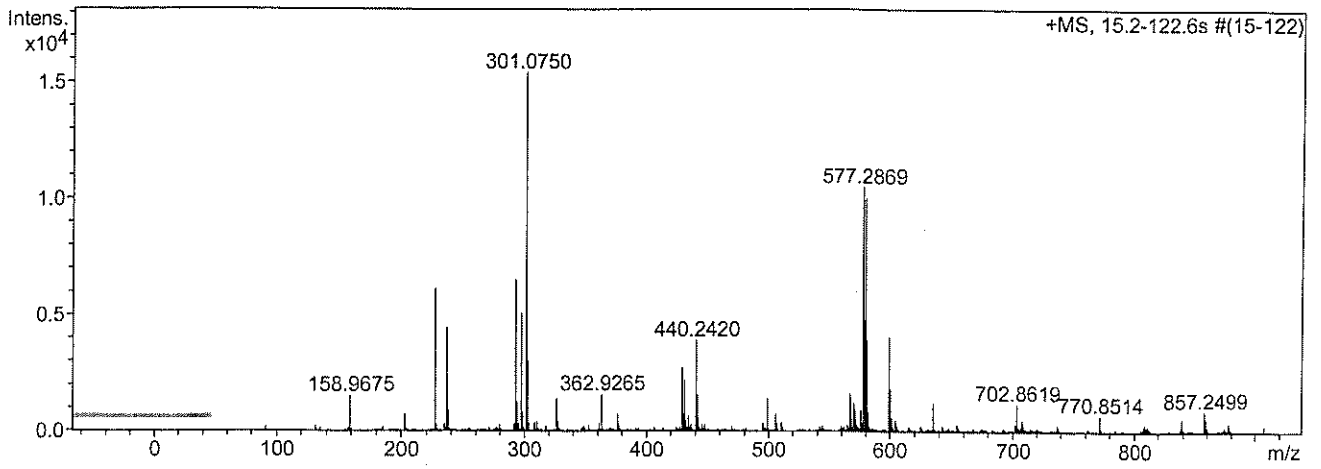
Display Report

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



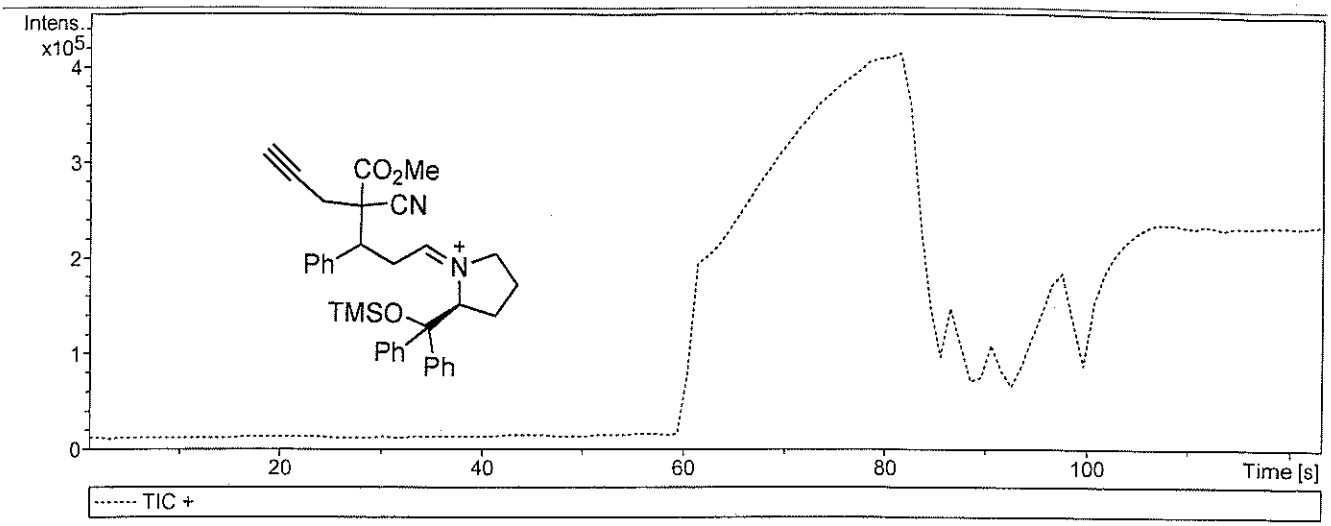


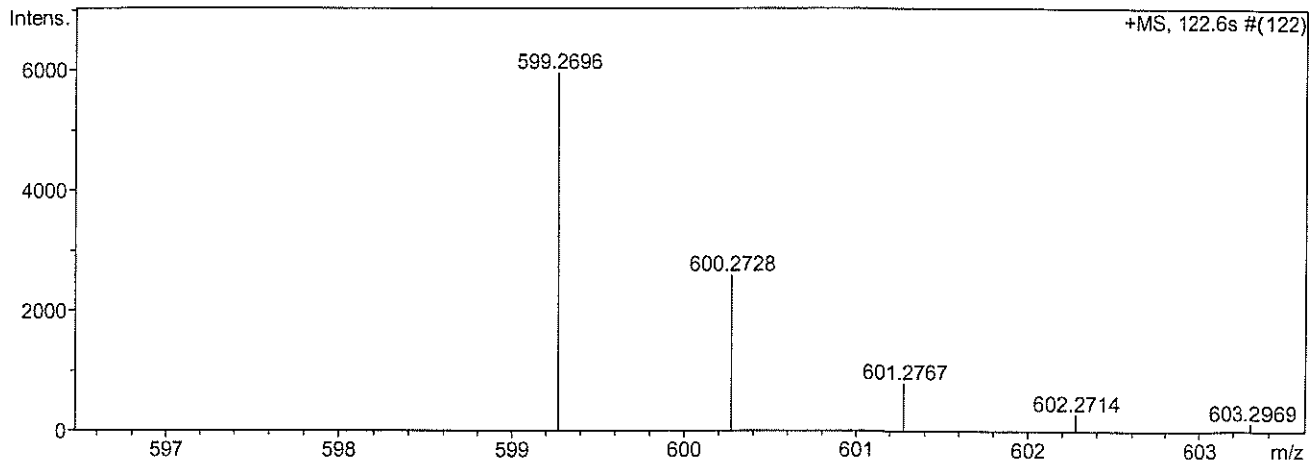


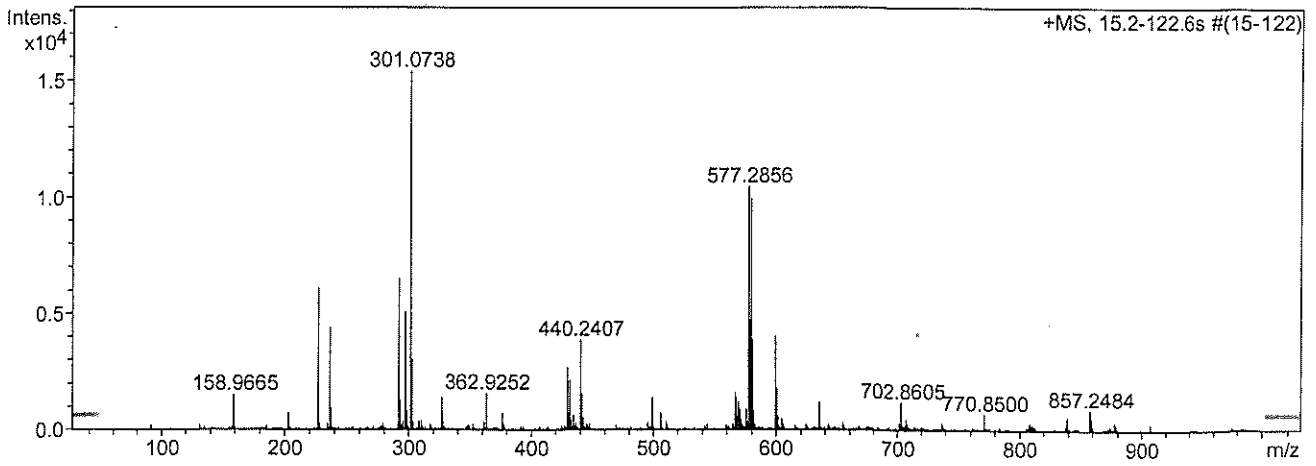
Display Report

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



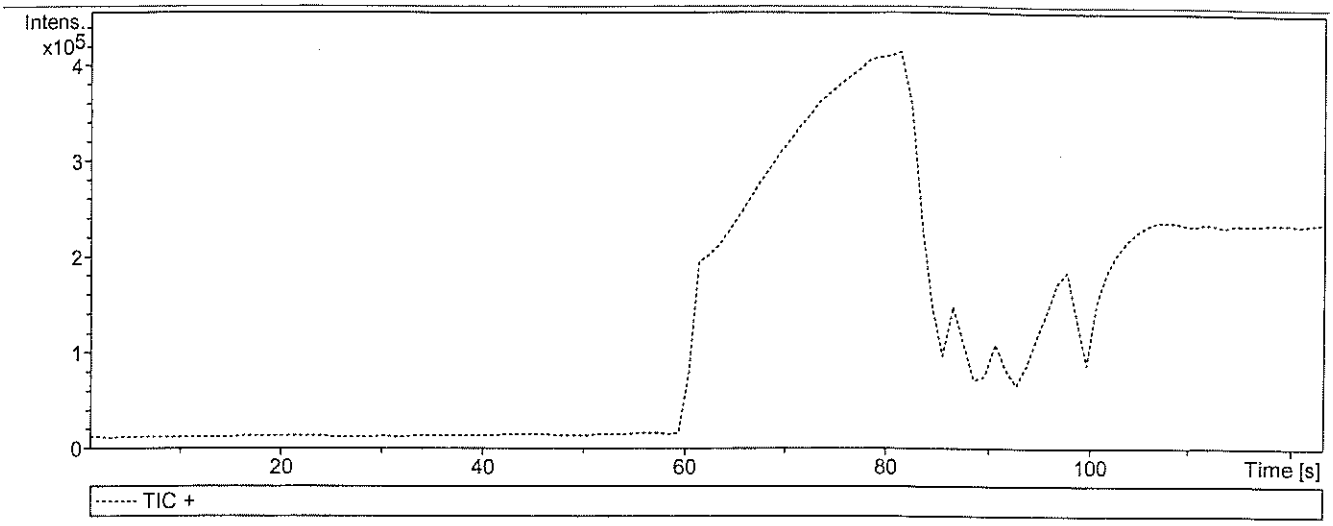


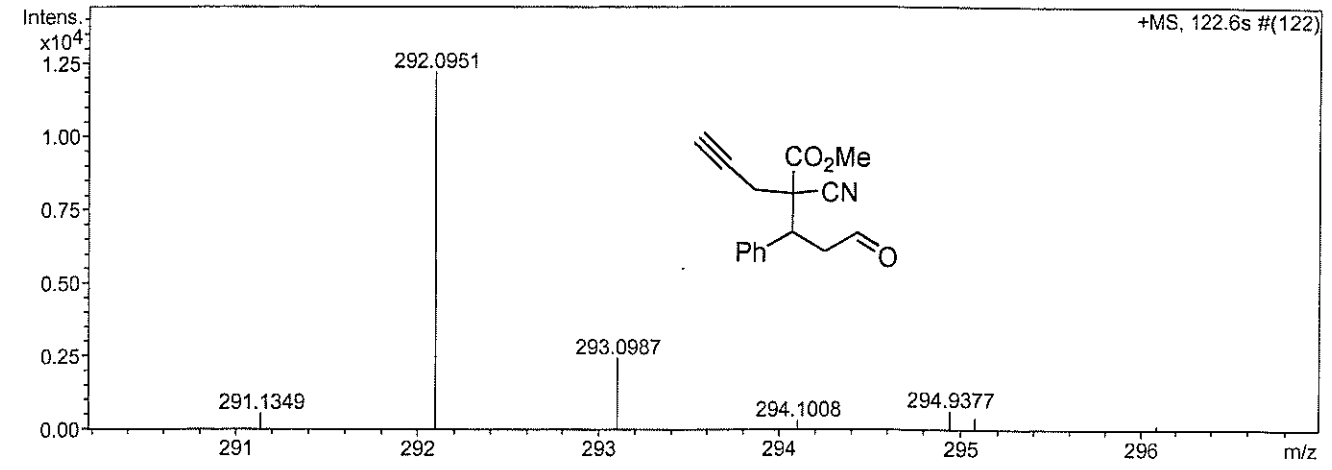


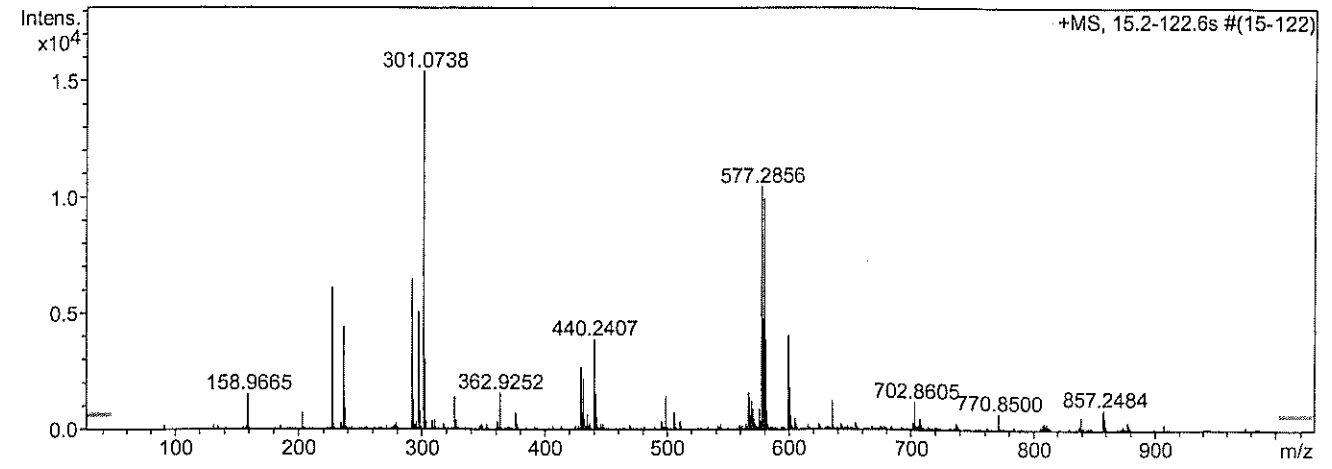
Display Report

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



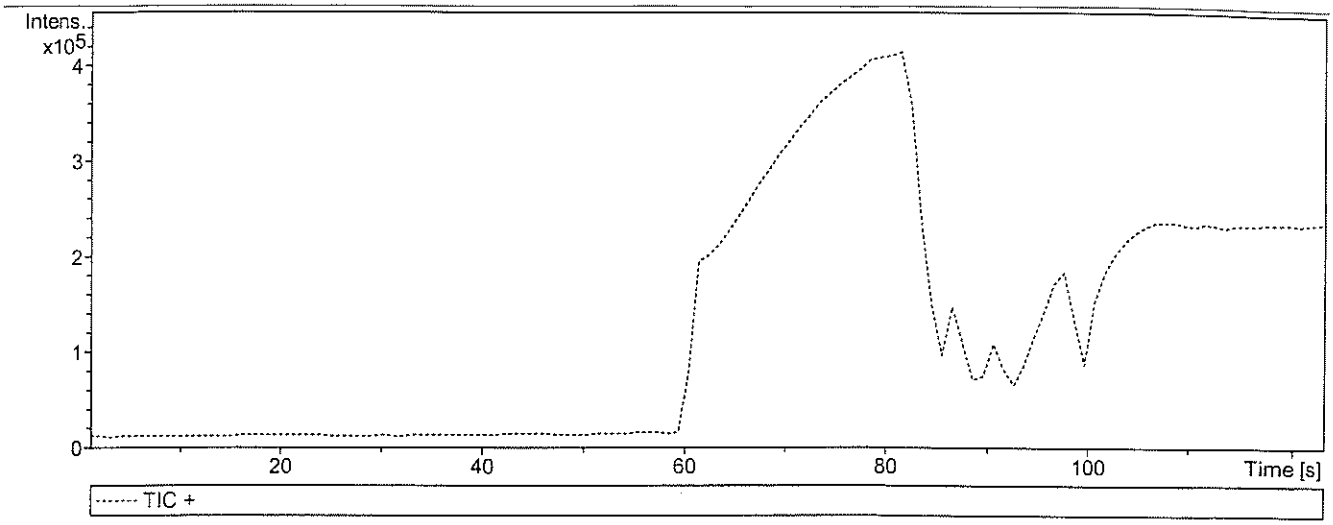


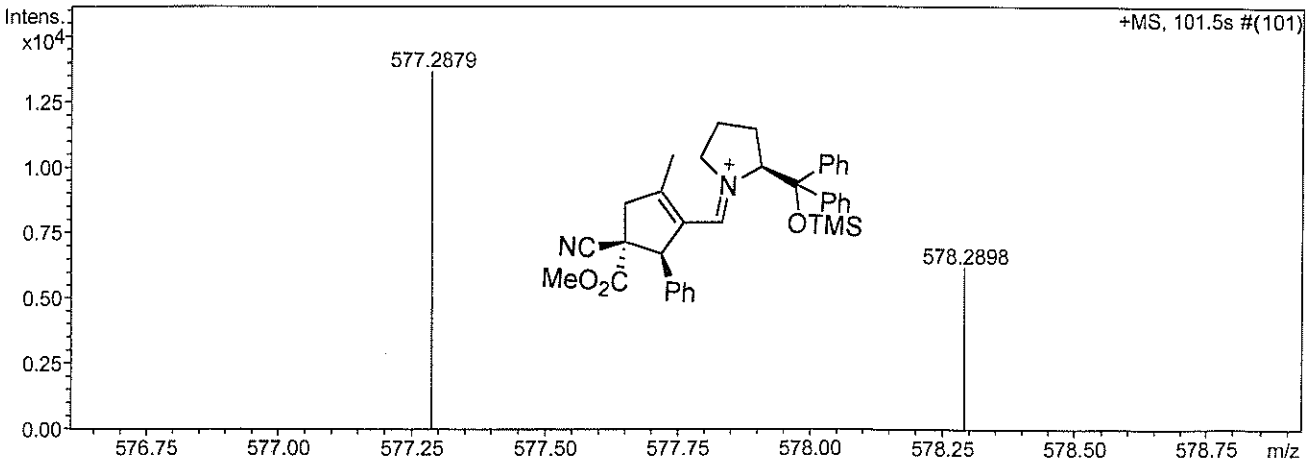


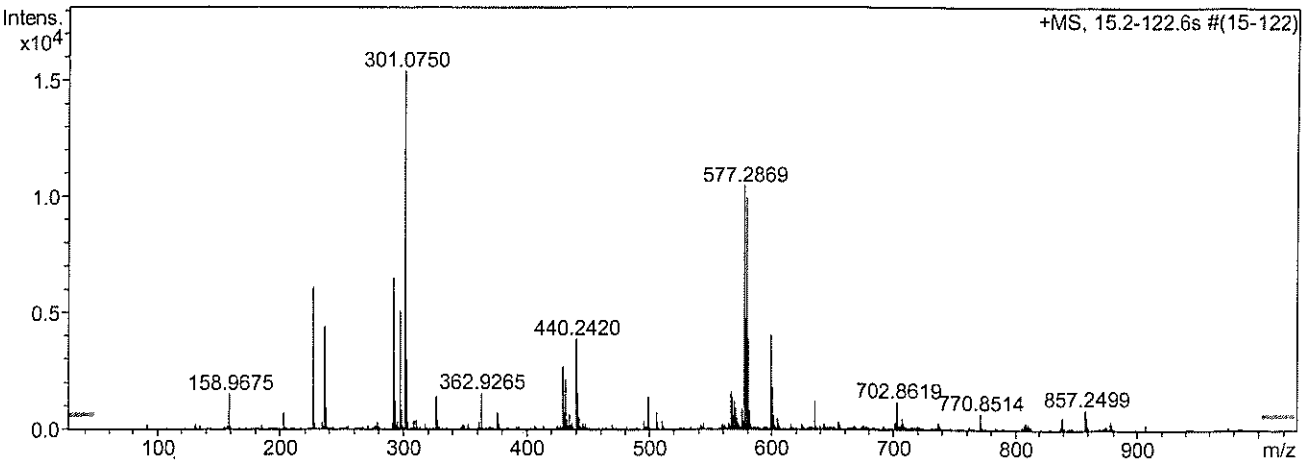
Display Report

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



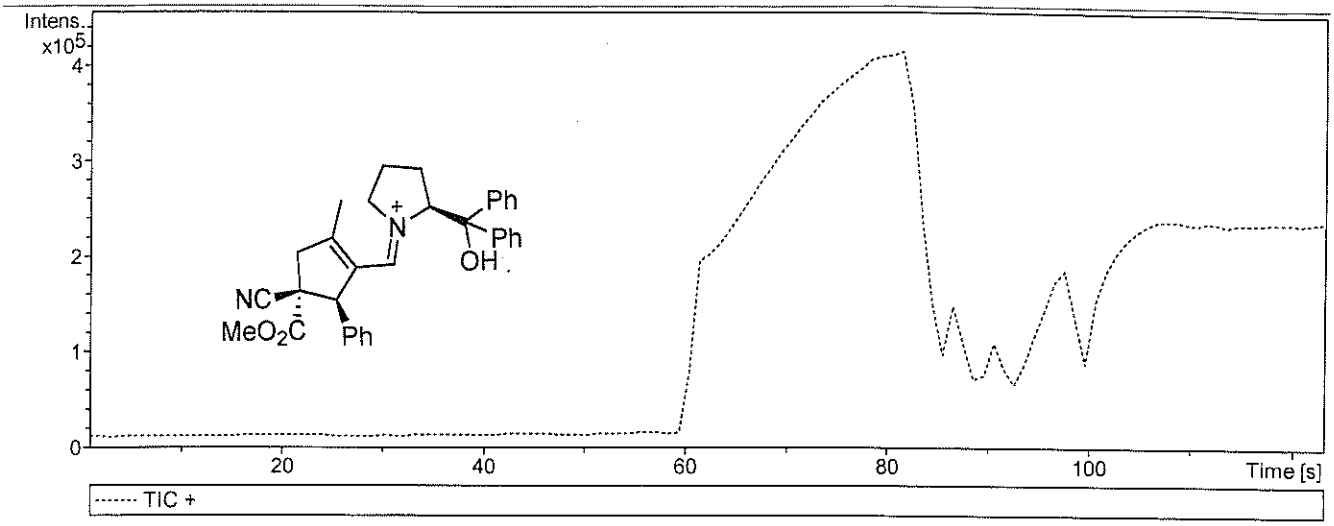


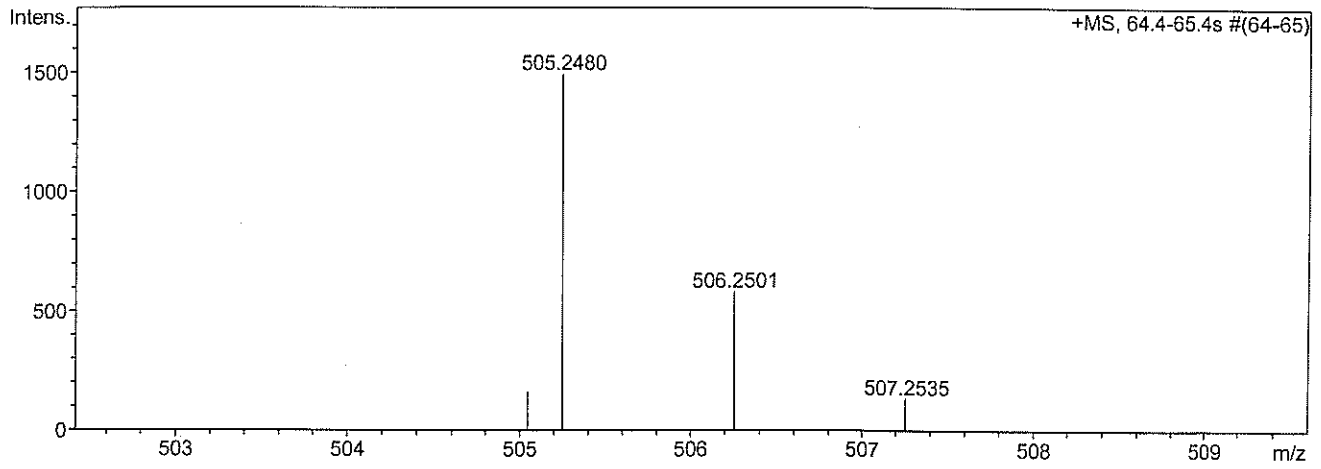


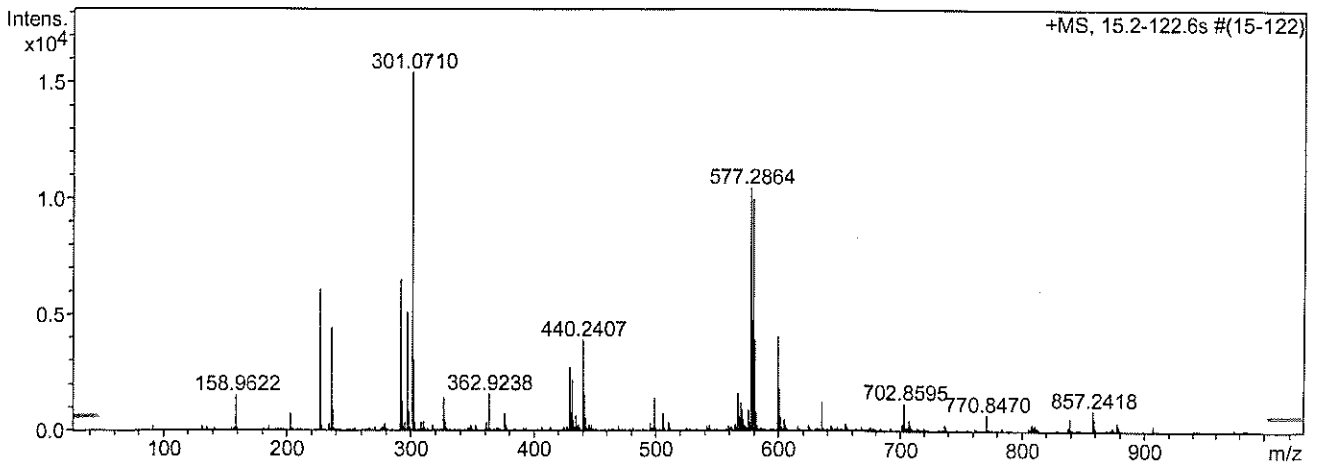
Display Report

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



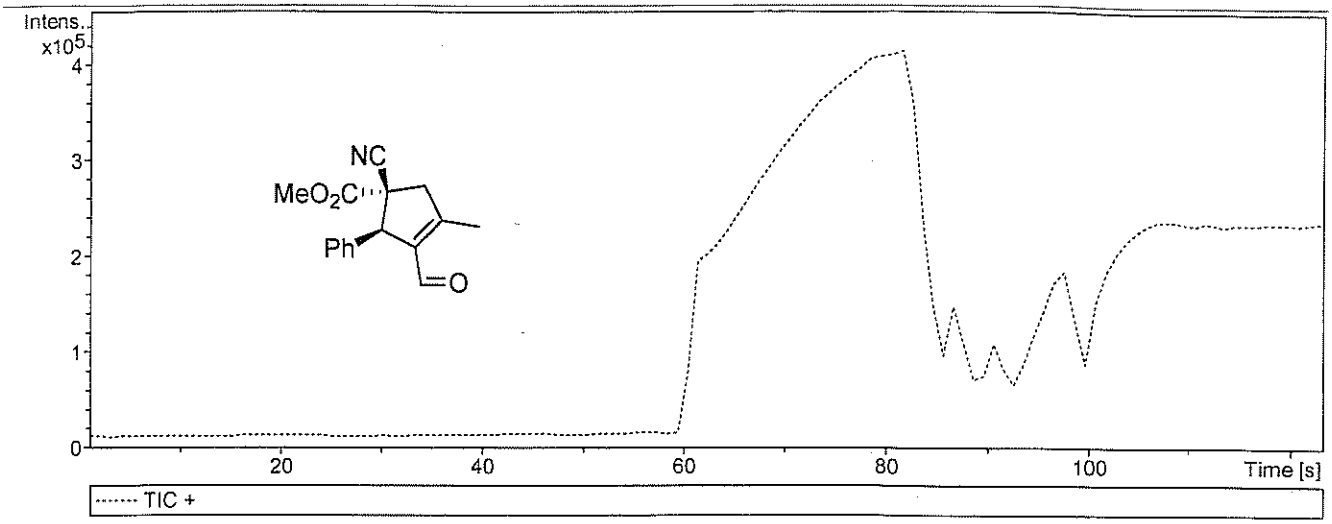


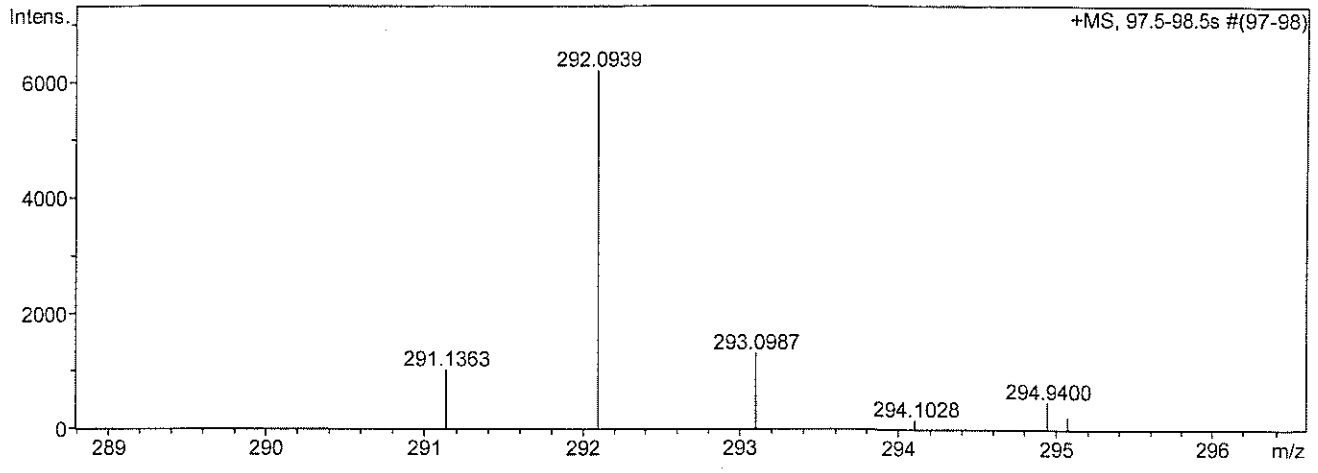


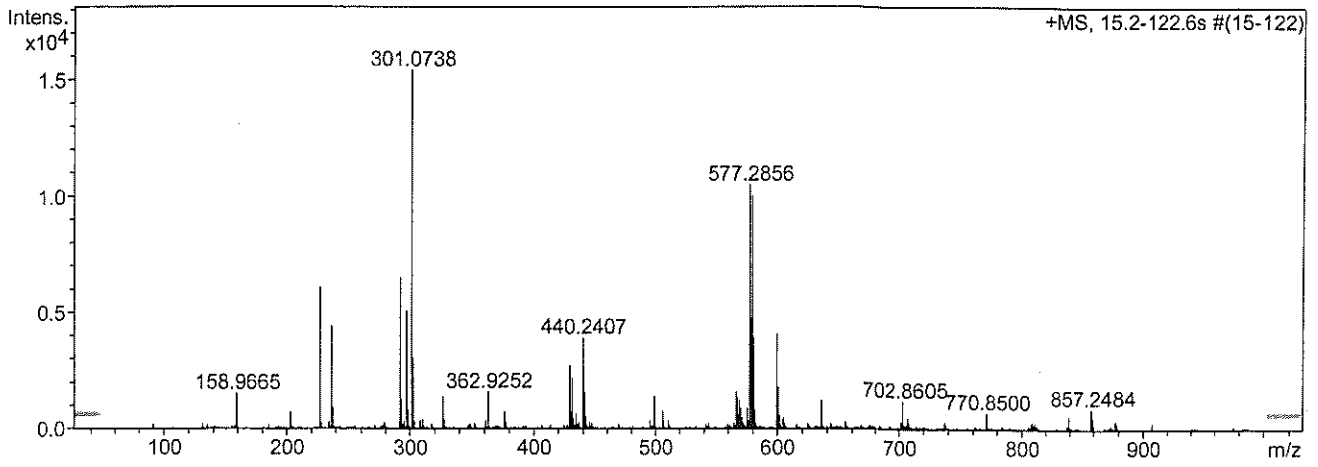
Display Report

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



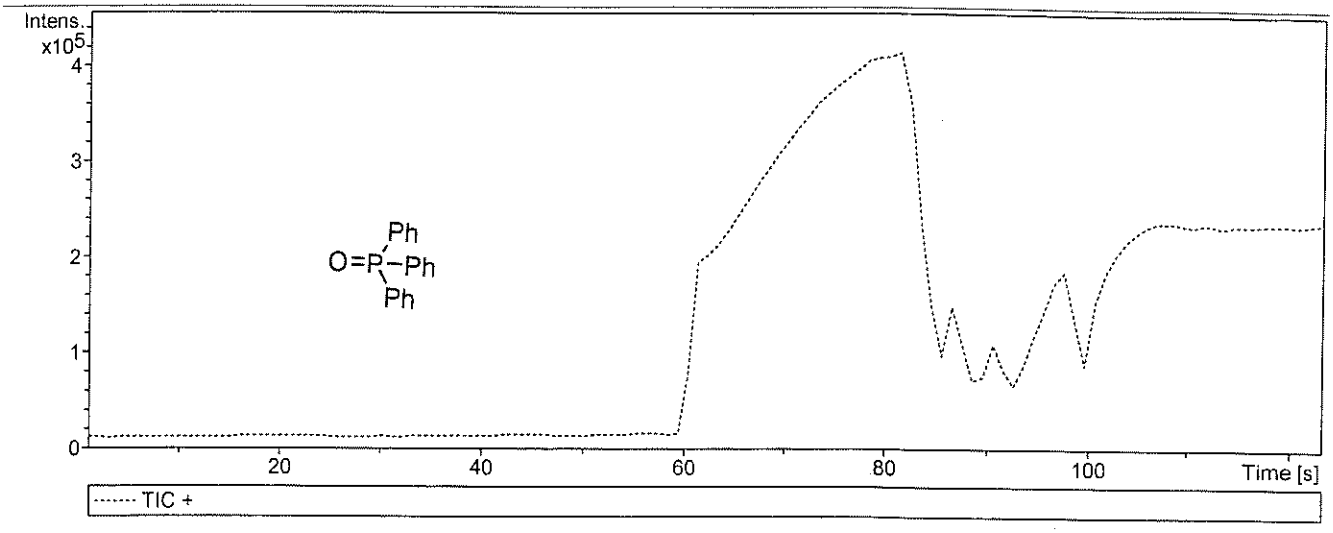


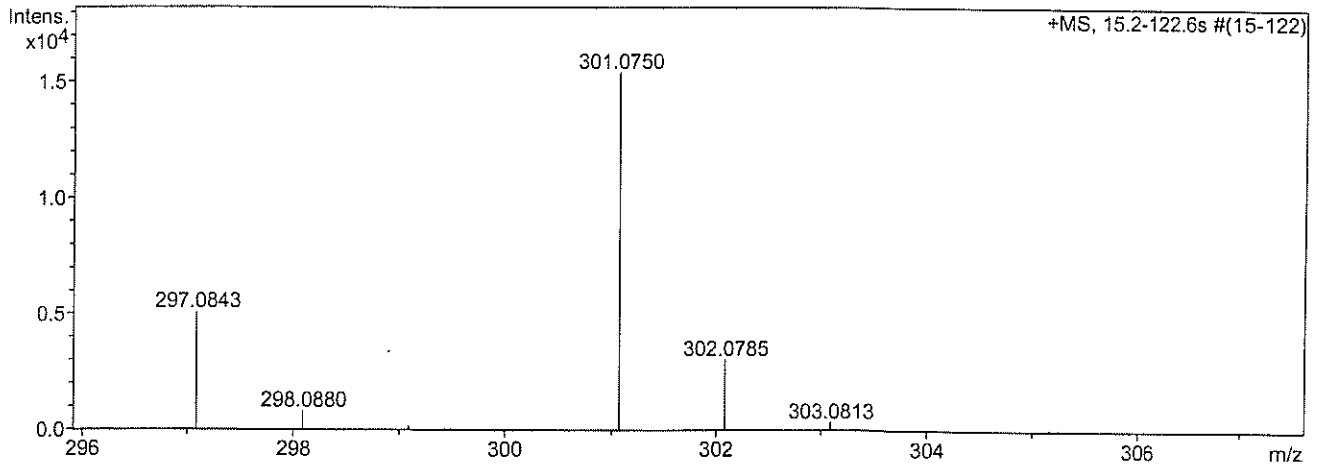


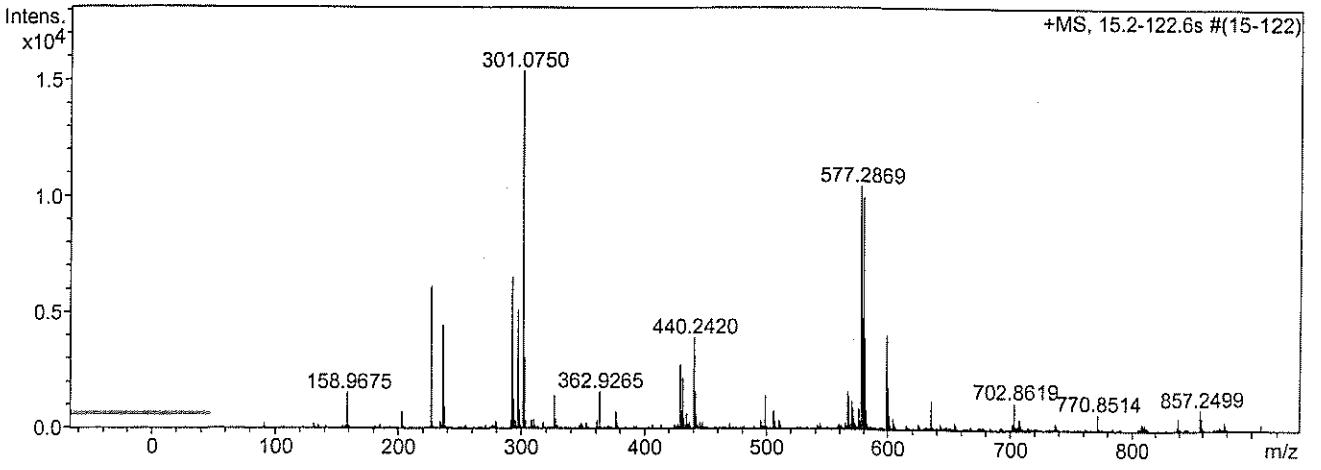
Display Report

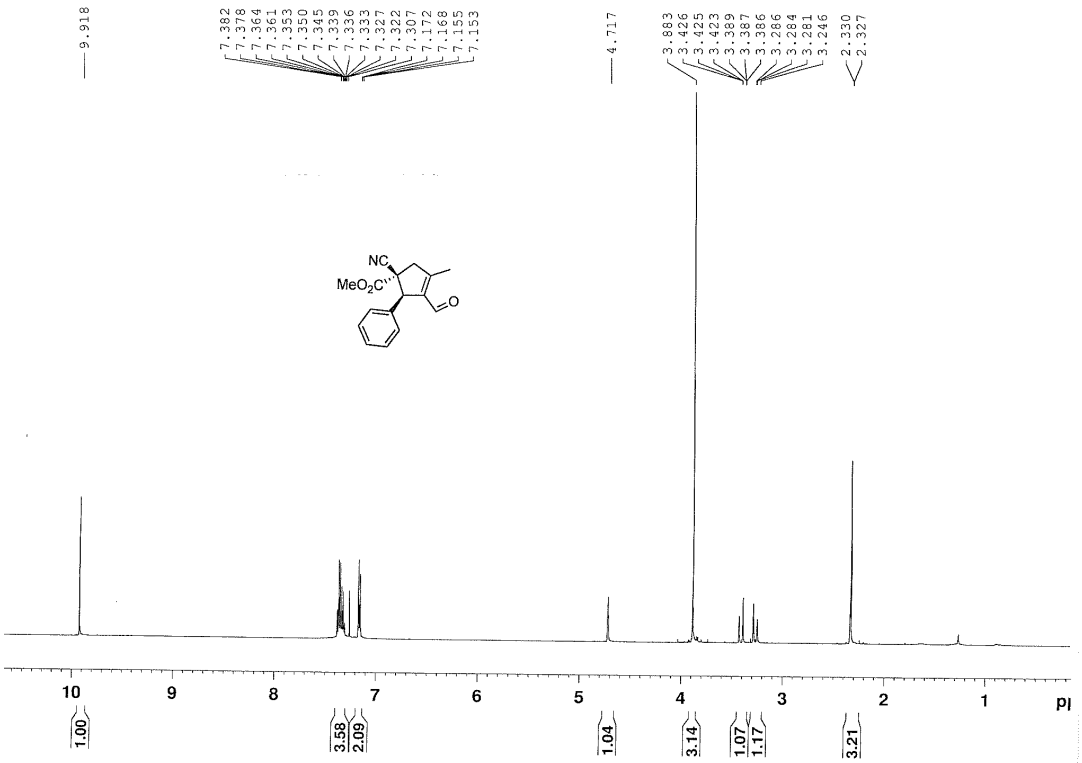
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source





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7.353
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7.345
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7.336
7.333
7.327
7.322
7.307
7.172
7.168
7.155
7.153
4.717
3.883
3.426
3.425
3.423
3.389
3.387
3.386
3.286
3.284
3.281
3.246
2.330
2.327
NC
MeO2C
O
10
9
8
7
6
5
4
3
2
1
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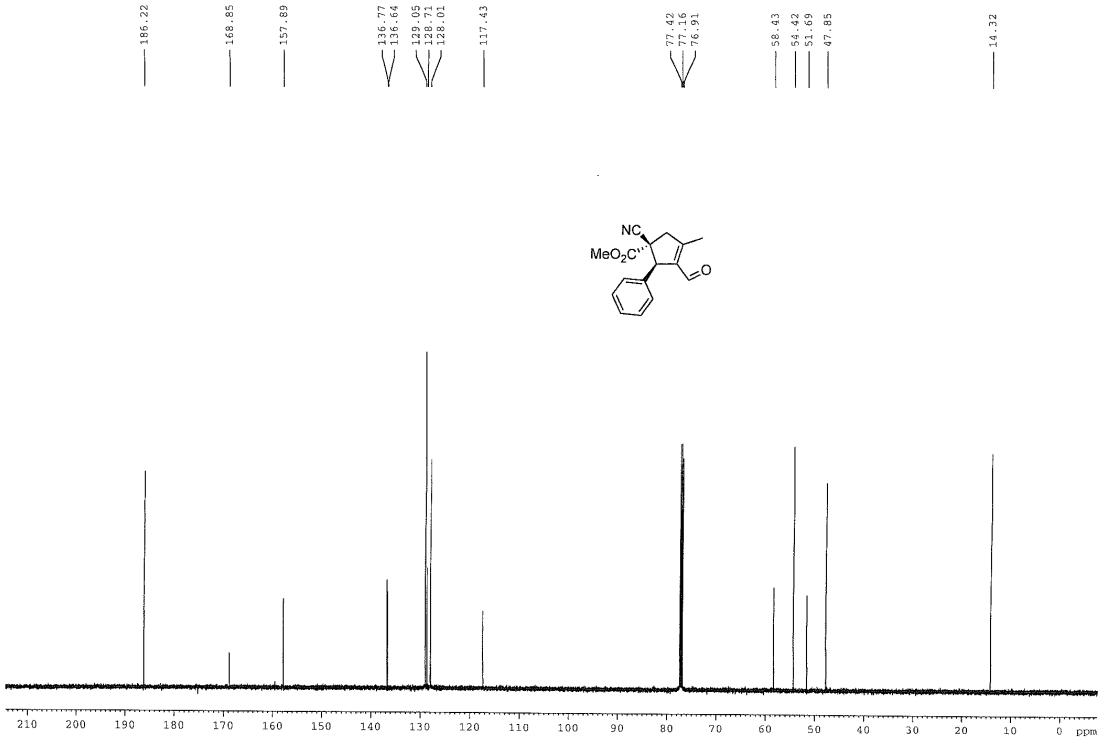
3.58
2.09
1.04
3.14
1.07
1.17
3.21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77.42
77.16
76.91
58.43
54.42
51.69
47.85
14.32
NC
MeO2C
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

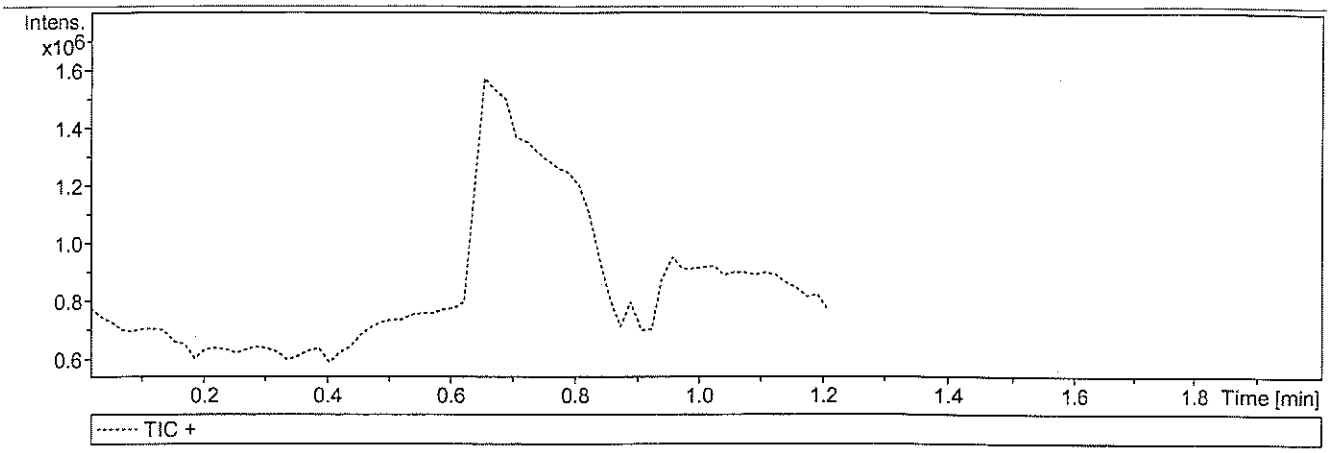
Display Report

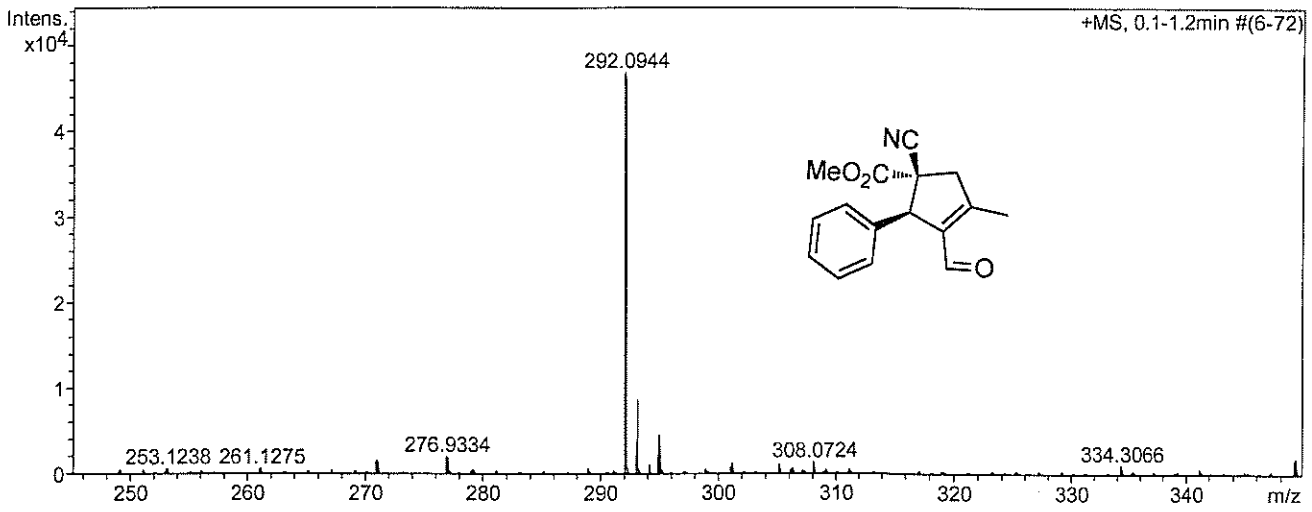
Analysis Info

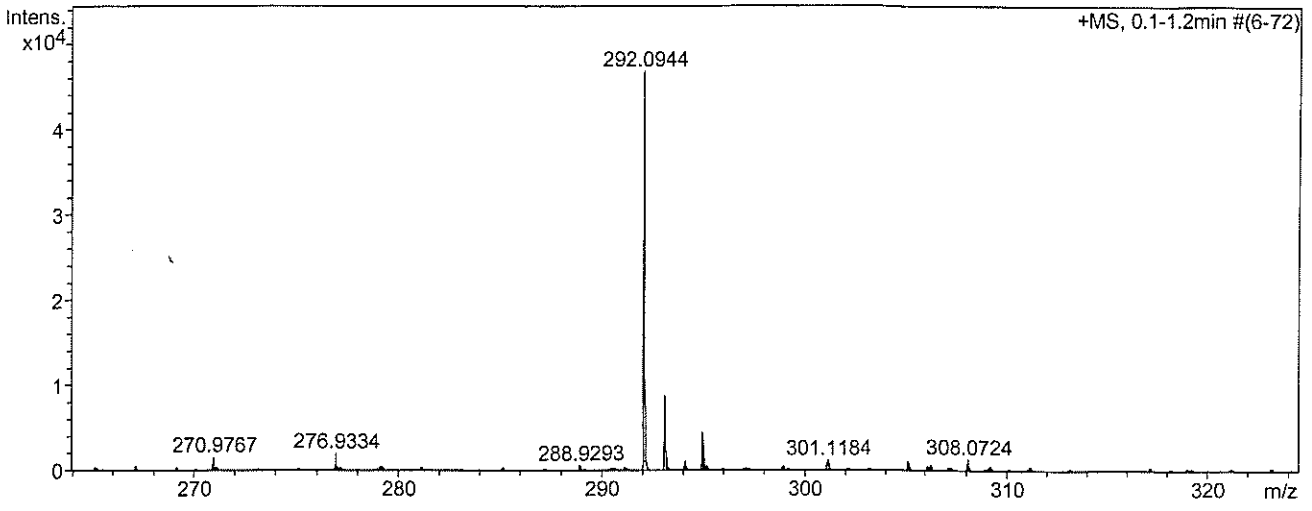
Analysis Name	E:\Data2\Luca\ld1256000001.d	Acquisition Date	2012-11-21 16:19:46
Method	Tune_low_pos.m	Operator	Carin Larsson
Sample Name	ld1256	Instrument / Ser#	micrOTOF 125
Comment			

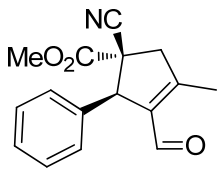
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source





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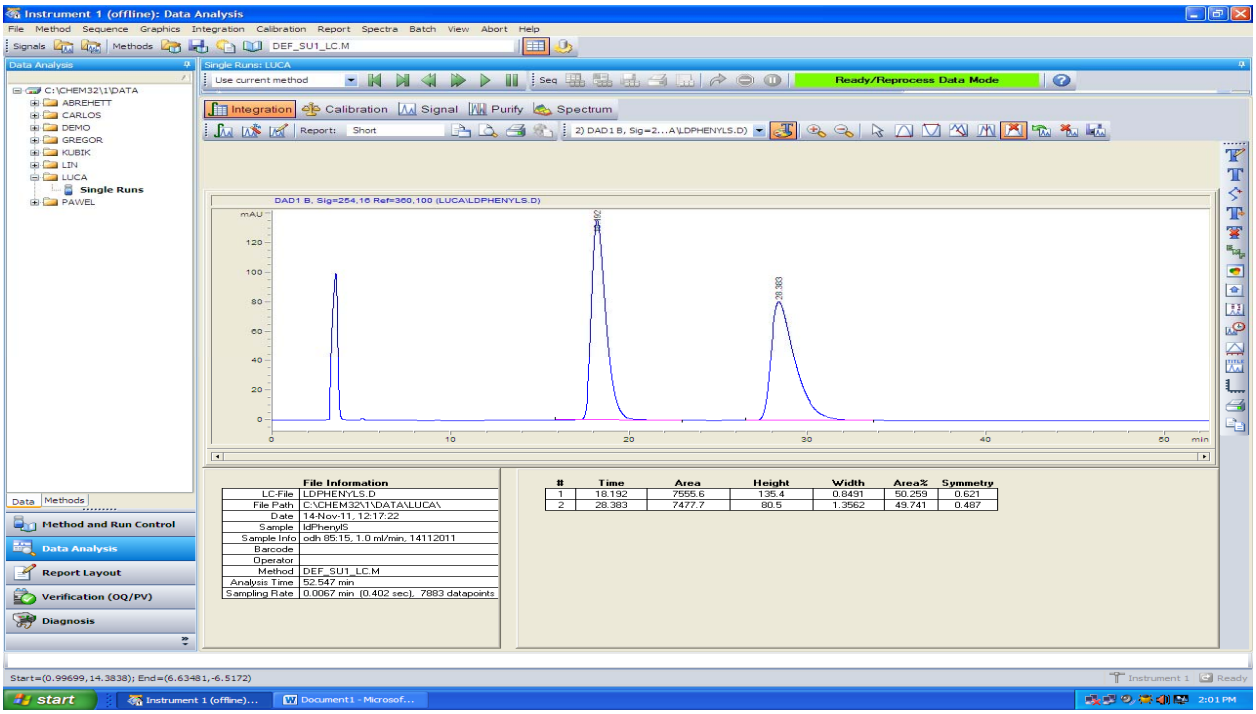
MeO2C
O


Instrument 1 (offline): Data Analysis
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File Information
LC-File LDPHENYLS.D
File Path C:\CHEM32\1\DATA\LUCA\
Date 14-Nov-11, 12:17:22
Sample ldPhenylS
Sample Info odh 85:15, 1.0 ml/min, 14112011
Method DEF_SU1_LC.M
Analysis Time 52.547 min
Sampling Rate 0.0067 min (0.402 sec), 7883 datapoints
Time Area Height Width Area% Symmetry
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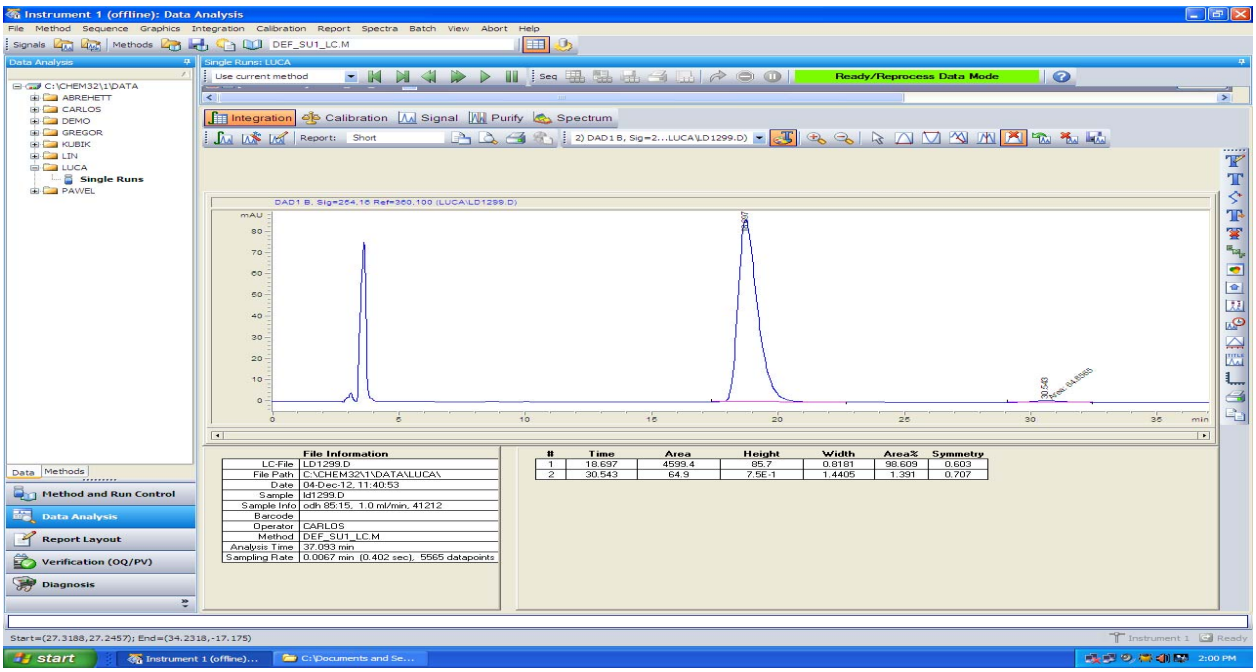
2 28.383 7477.7 80.5 1.3562 49.741 0.487


Instrument 1 (offline): Data Analysis
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Date 04-Dec-12, 11:40:53
Sample ld1299.D
Sample Info odh 85:15, 1.0 ml/min, 41212
Barcode
Operator CARLOS
Method DEF_SU1_LC.M
Analysis Time 37.093 min
Sampling Rate 0.0067 min (0.402 sec), 5565 datapoints
Time Area Height Width Area% Symmetry
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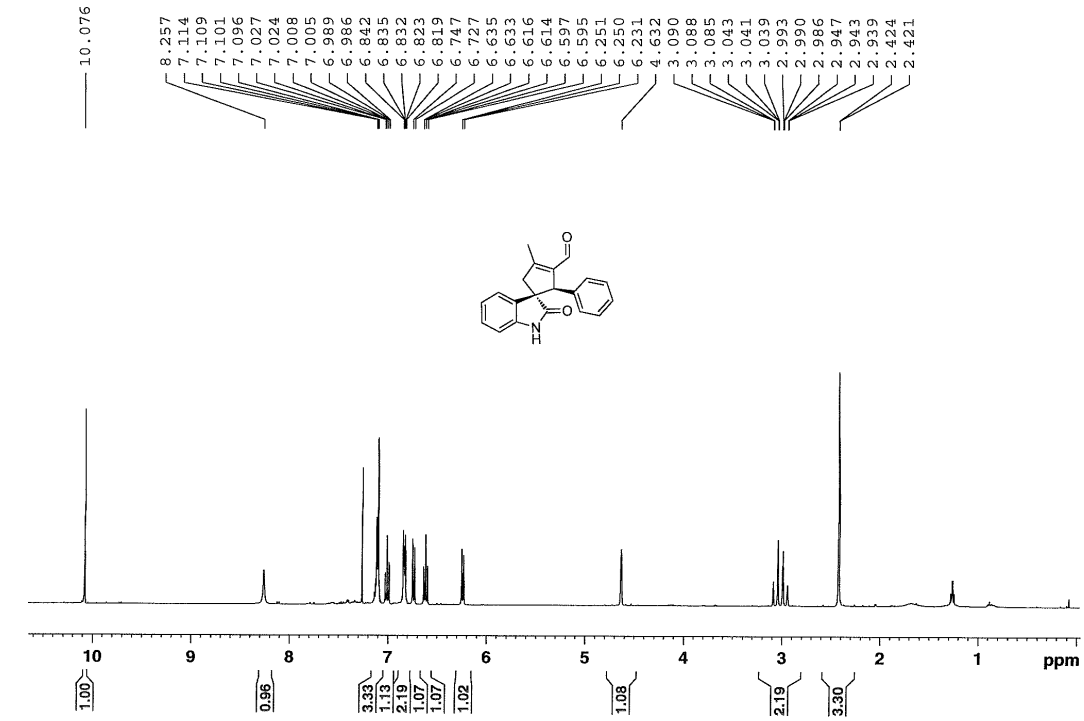
2 30.543 64.9 7.5E-1 1.4405 1.391 0.707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6.835
6.832
6.823
6.819
6.747
6.727
6.635
6.633
6.616
6.614
6.597
6.595
6.251
6.250
6.231
4.632
3.090
3.088
3.085
3.043
3.041
3.039
2.993
2.990
2.986
2.947
2.943
2.939
2.424
2.421
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H
10
9
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7
6
5
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3
2
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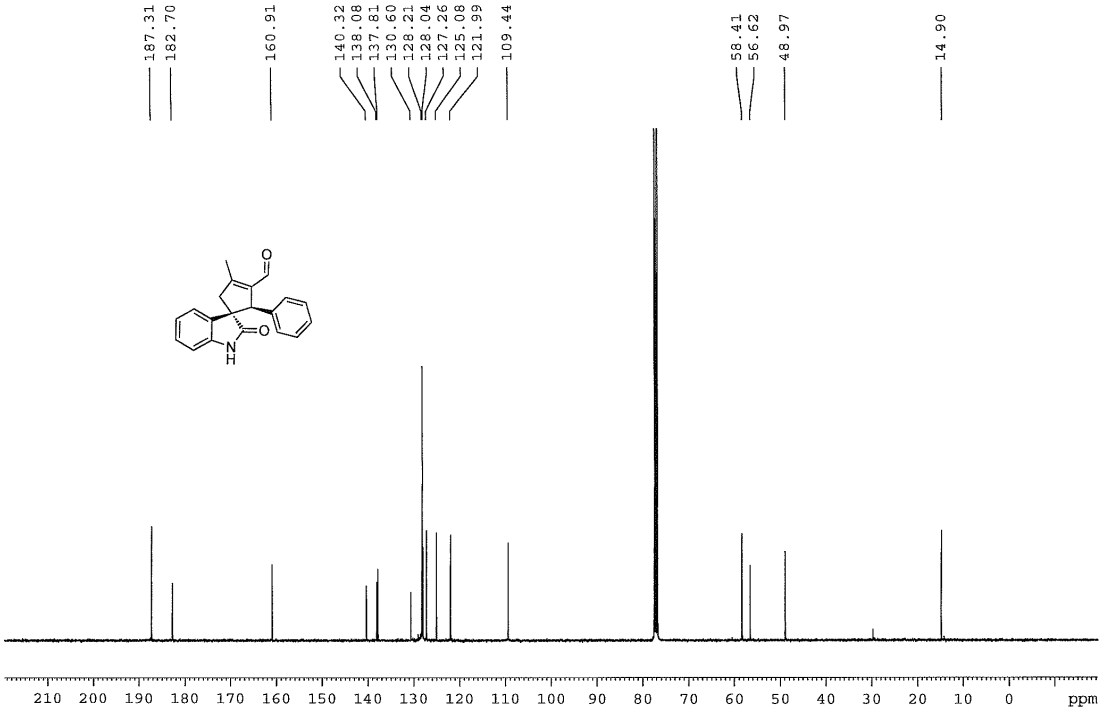
1.07
1.07
1.02
1.08
2.19
3.30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137.81
130.60
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128.04
127.26
125.08
121.99
109.44
58.41
56.62
48.97
14.90
O
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

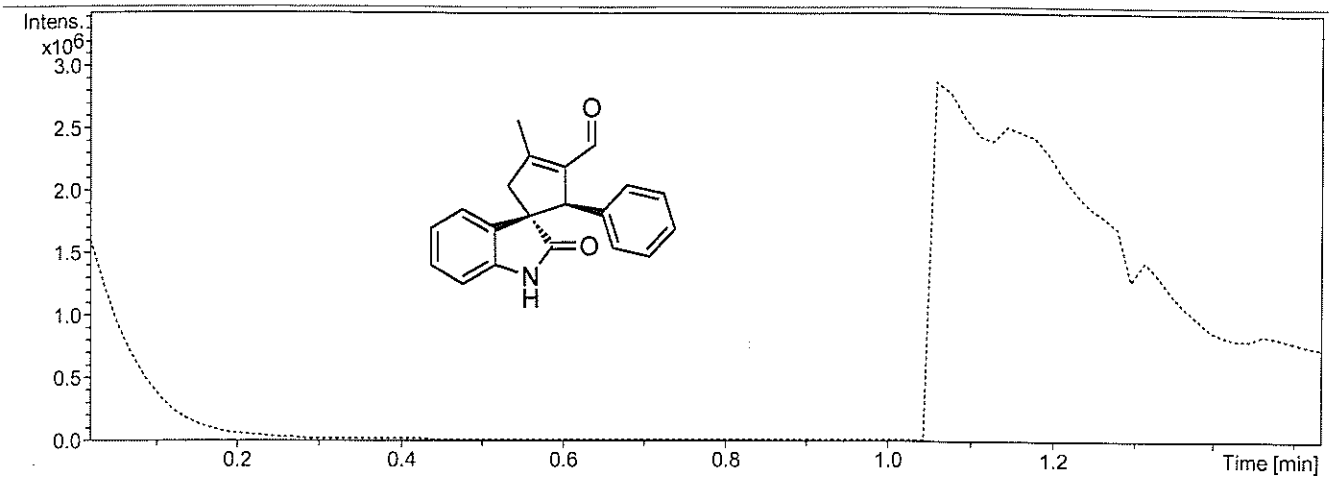
Display Report

Analysis Info

Analysis Name	H:\Data2\Luca\ld1226000001.d	Acquisition Date	2012-10-10 15:26:34
Method	tune_wide_dirk.m	Operator	pia
Sample Name	ld1226	Instrument / Ser#	micrOTOF 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



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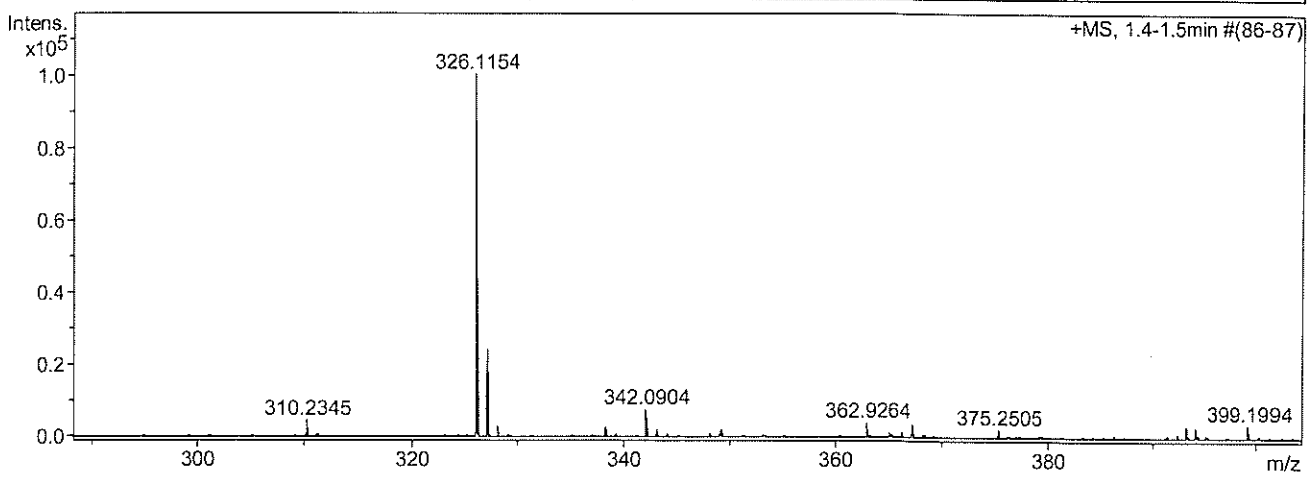

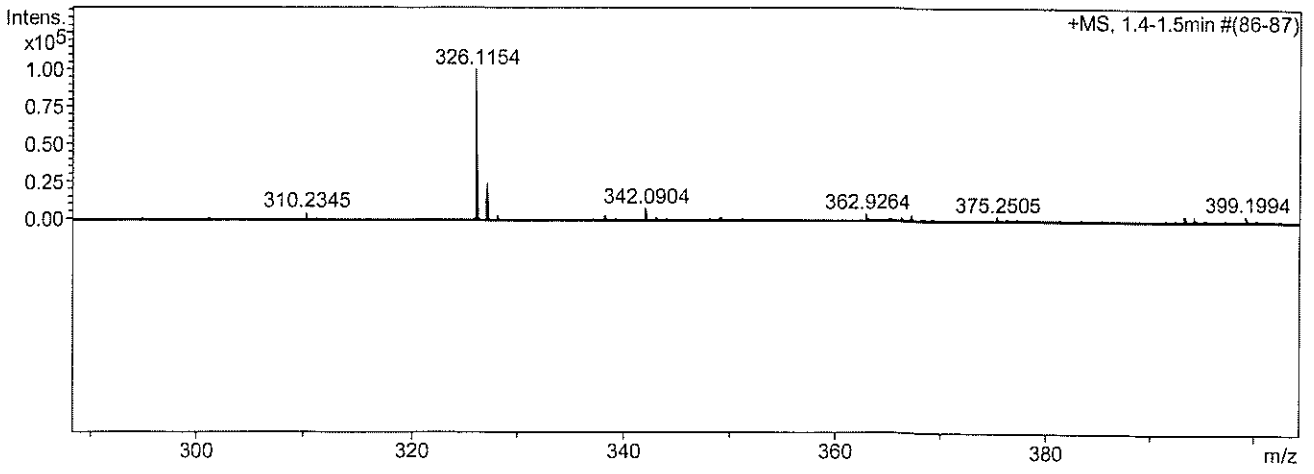

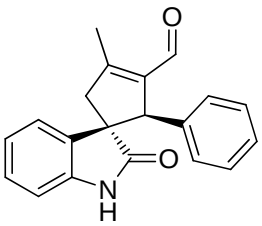
O
O
N
H


Instrument 1 (offline): Data Analysis
DAD1 B, Sig=254,16 Ref=360,100 (LUCA\LD1226.D)
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min
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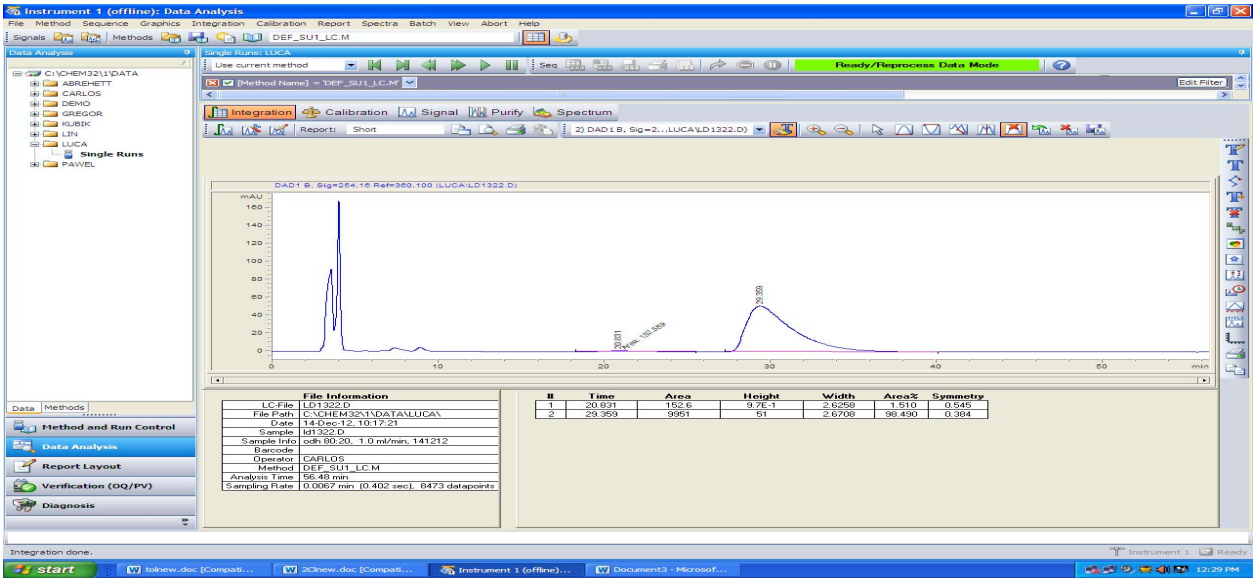
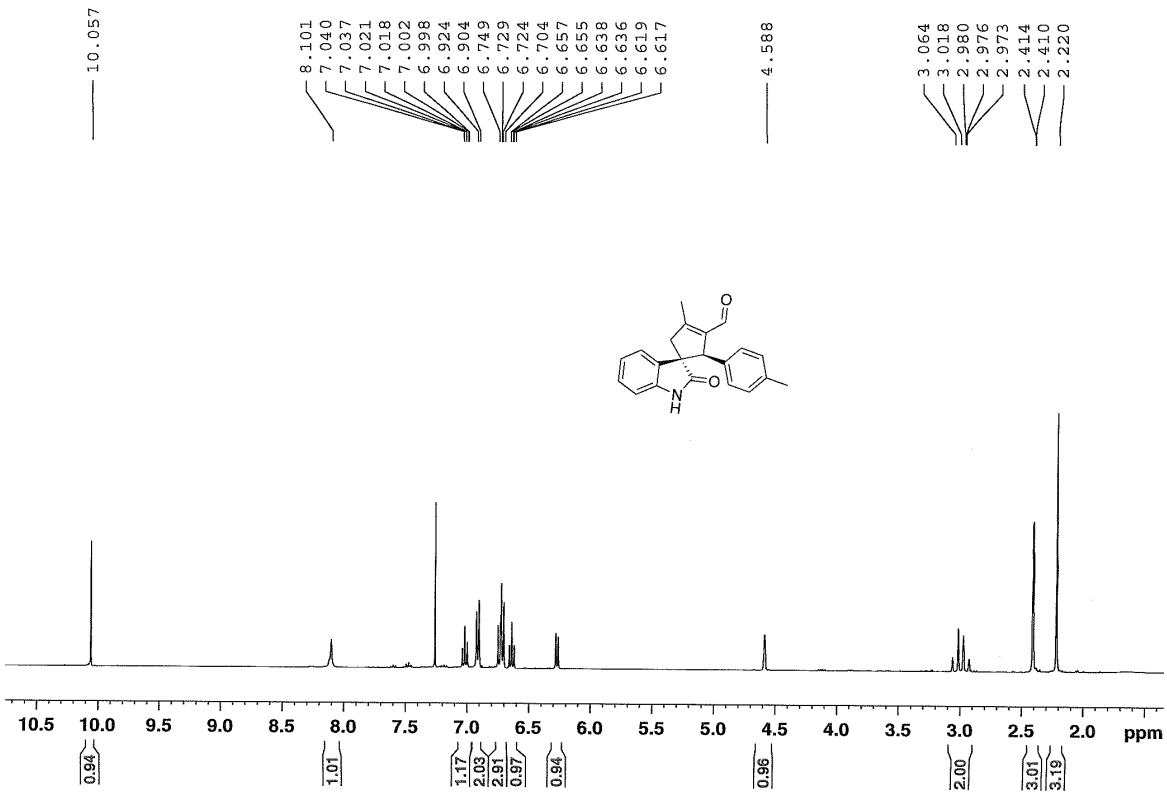
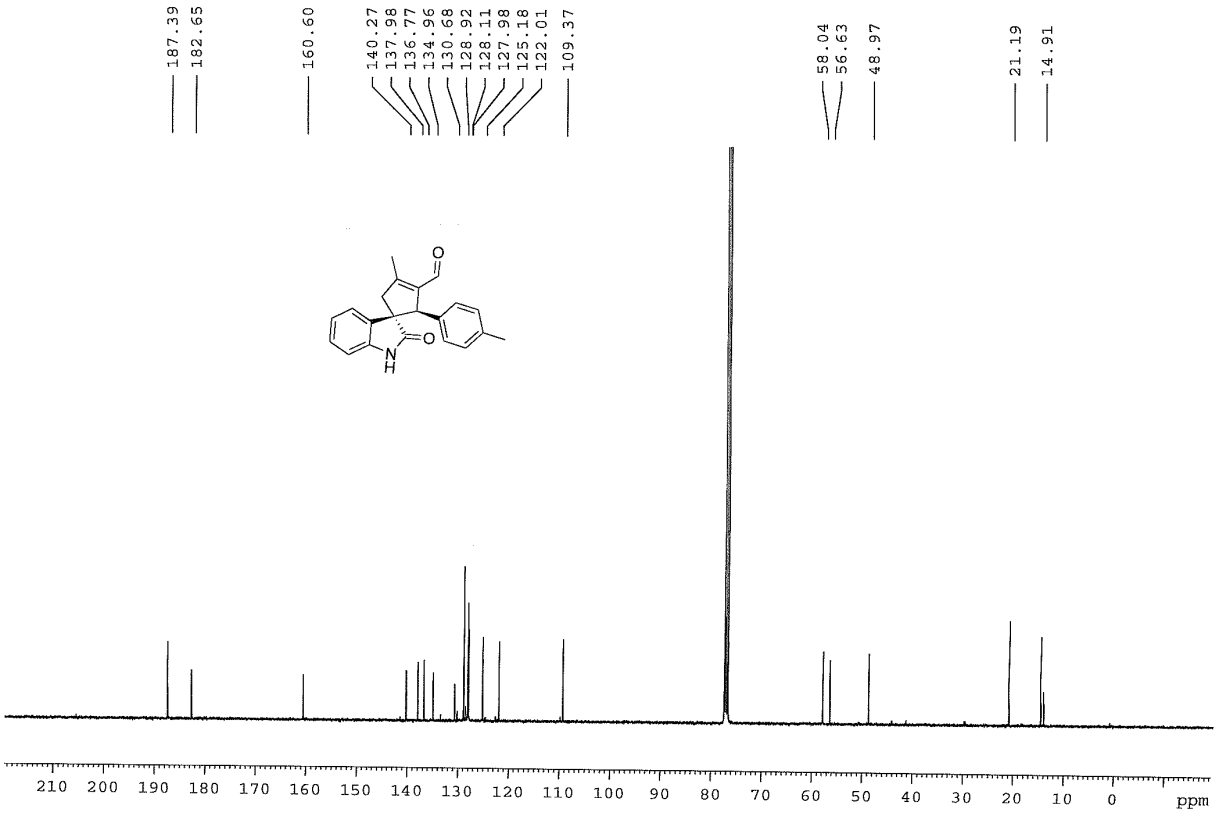
29.636
File Information
LC-File LD1226.D
File Path C:\CHEM32\1\DATA\LUCA\
Date 10-Oct-12, 11:46:45
Sample ld1226.D
Sample Info odh 80:20, 1 ml/min, 101012
Barcode
Operator CARLOS
Method DEF_SU1_LC.M
Analysis Time 61.24 min
Sampling Rate 0.0067 min (0.402 sec), 9187 datapoints
Time Area Height Width Area% Symmetry
1 19.351 5027.1 41.6 1.704 49.662 0.427
2 29.636 5095.5 27.9 2.2402 50.338 0.42


Instrument 1 (offline): Data Analysis
DAD1 B, Sig=254,16 Ref=360,100 (LUCA\LD1322.D)
mAU
min
20.831
29.359
File Information
LC-File LD1322.D
File Path C:\CHEM32\1\DATA\LUCA\
Date 14-Dec-12, 10:17:21
Sample ld1322.D
Sample Info odh 80:20, 1.0 ml/min, 141212
Barcode
Operator CARLOS
Method DEF_SU1_LC.M
Analysis Time 56.48 min
Sampling Rate 0.0067 min (0.402 sec), 8473 datapoints
Time Area Height Width Area% Symmetry
1 20.831 152.6 9.7E-1 2.6258 1.510 0.545
2 29.359 9951 51 2.6708 98.490 0.384


10.057
8.101
7.040
7.037
7.021
7.018
7.002
6.998
6.924
6.904
6.749
6.729
6.724
6.704
6.657
6.655
6.638
6.636
6.619
6.617
4.588
3.064
3.018
2.980
2.976
2.973
2.414
2.410
2.220
O
O
N
H
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
0.94
1.01
1.17
2.03
2.91
0.97
0.94
0.96
2.00
3.01
3.19


187.39
182.65
160.60
140.27
137.98
136.77
134.96
130.68
128.92
128.11
127.98
125.18
122.01
109.37
58.04
56.63
48.97
21.19
14.91
O
O
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

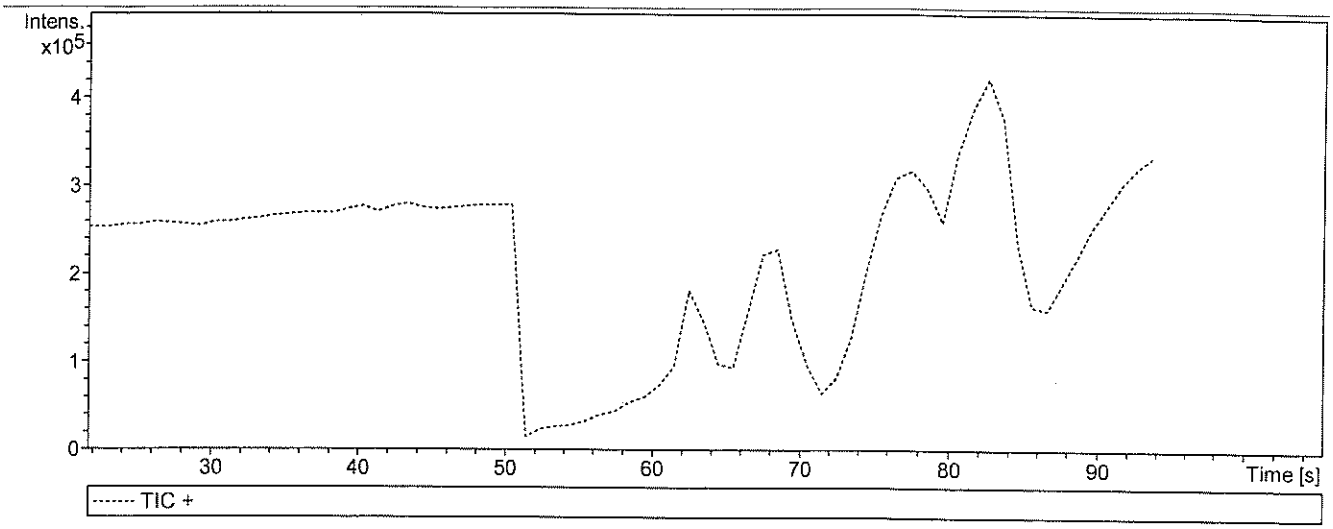
Display Report

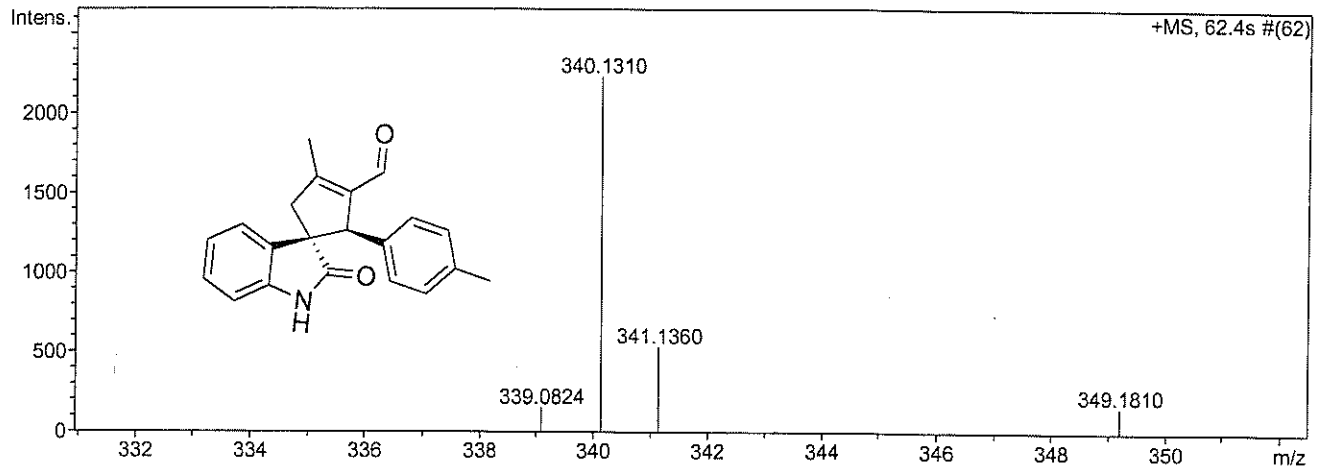
Analysis Info

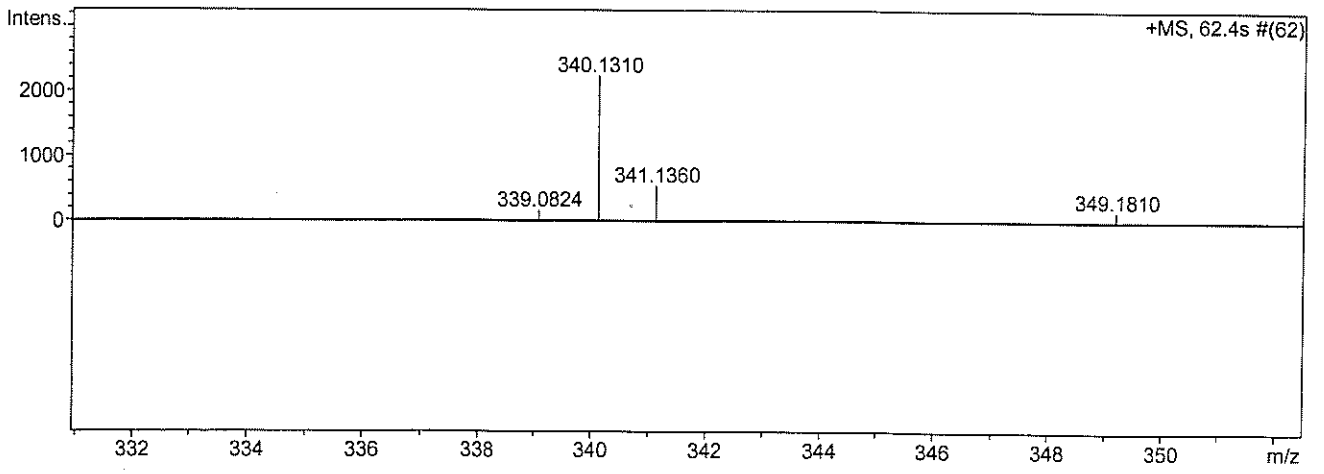
Analysis Name	E:\Data2\Luca\ld1384000001.d	Acquisition Date	2013-03-01 12:11:40
Method	Tune_low_pos.m	Operator	Carin Larsson
Sample Name	ld1384	Instrument / Ser#	micrOTOF 125
Comment			

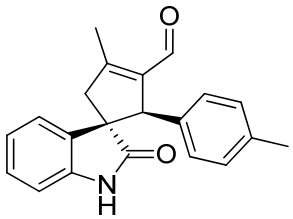
Acquisition Parameter

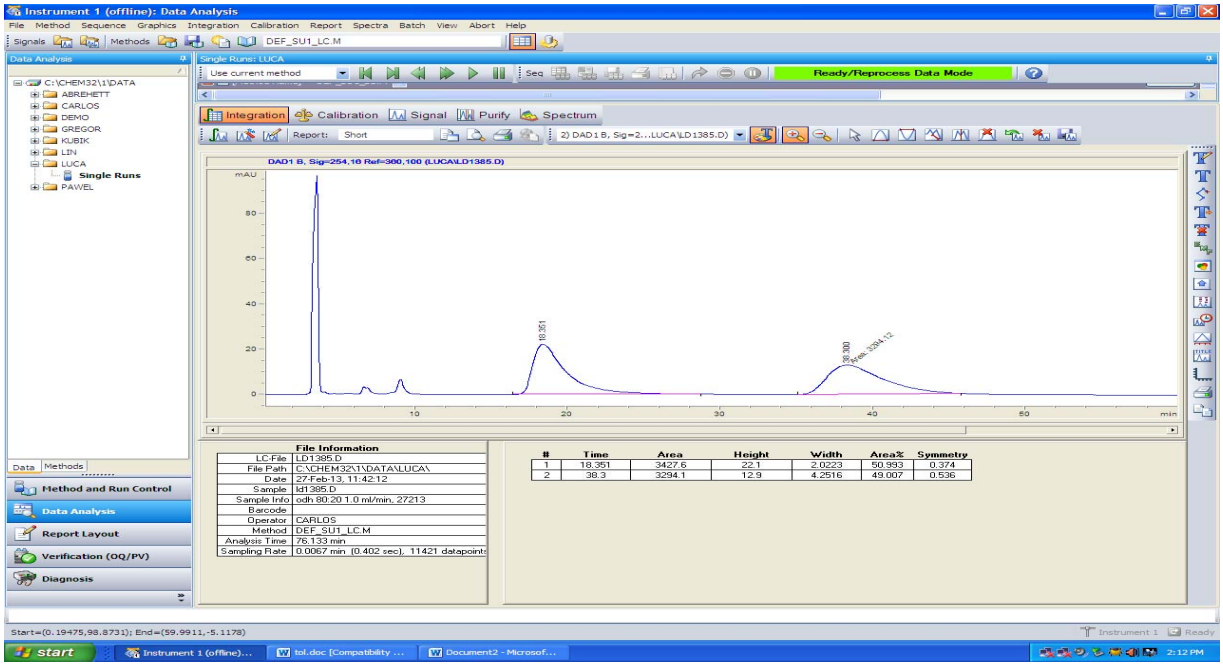
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

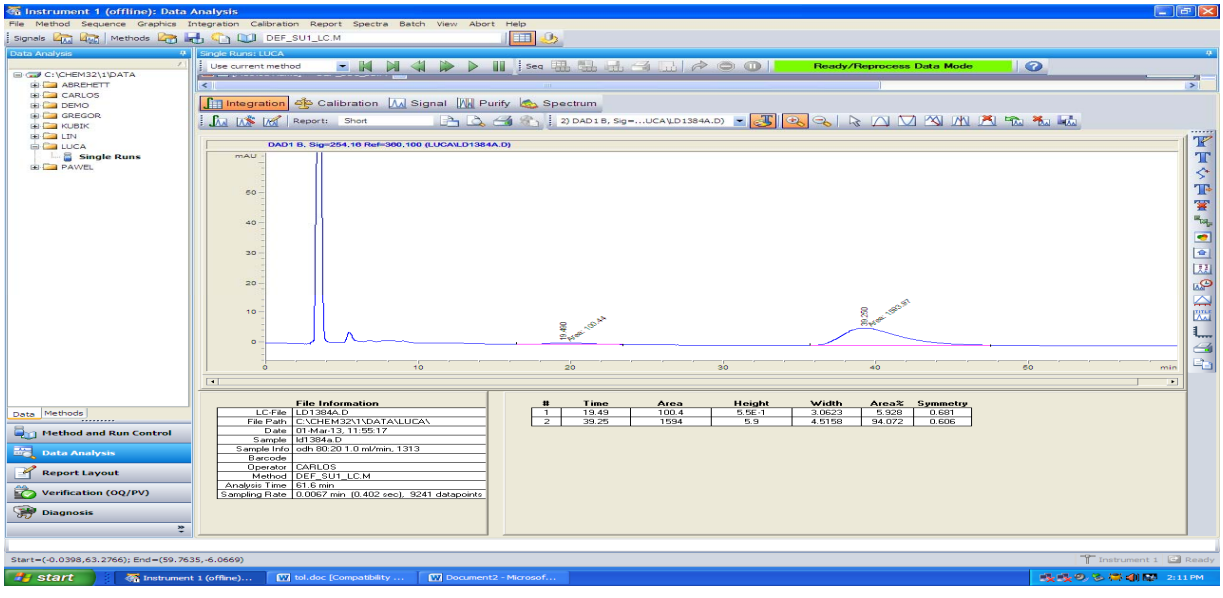


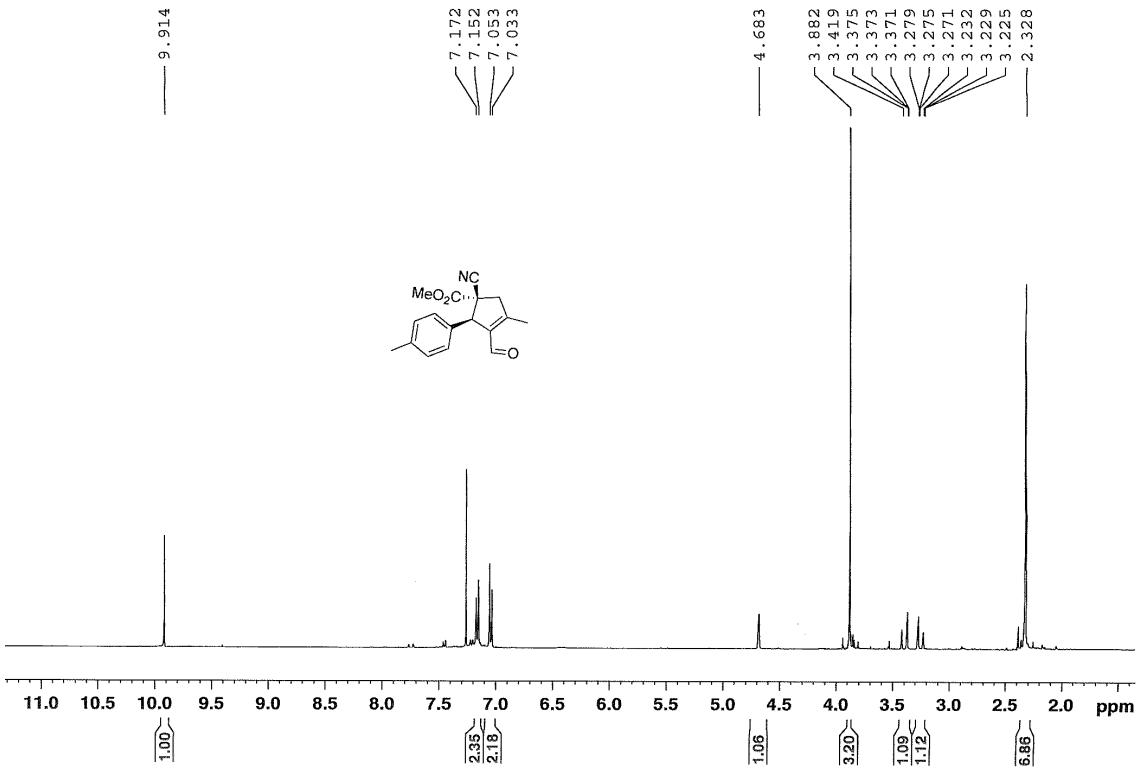


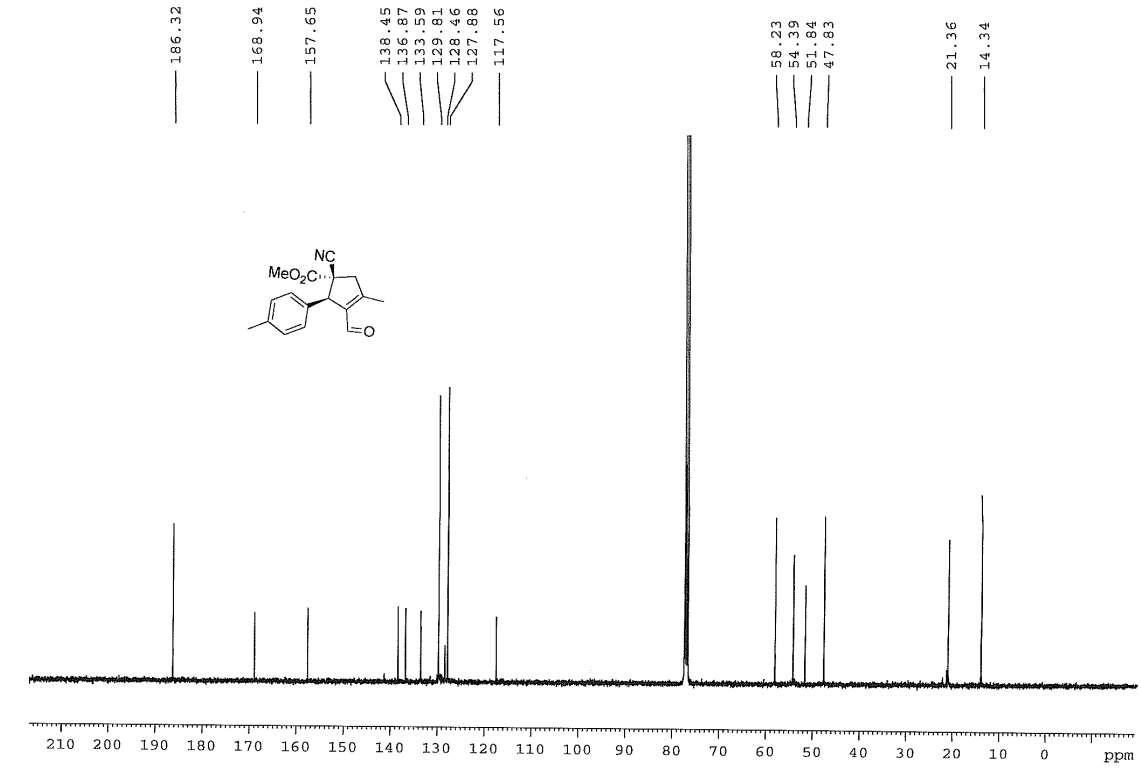



O
O
N
H


Instrument 1 (offline): Data Analysis
DAD1 B, Sig=254,16 Ref=360,100 (LUCA\LD1385.D)
mAU
min
18.351
49.300
File Information
LC File LD1385.D
File Path C:\CHEM32\1\DATA\LUCA\
Date 27-Feb-13, 11:42:12
Sample ld1385.D
Sample Info odh 80:20 1.0 ml/min, 27213
Barcode
Operator CARLOS
Method DEF_SU1_LC.M
Analysis Time 76.133 min
Sampling Rate 0.0067 min (0.402 sec), 11421 datapoints
Time Area Height Width Area% Symmetry
1 18.351 3427.6 22.1 2.0223 50.993 0.374
2 38.3 3294.1 12.9 4.2516 49.007 0.536


Instrument 1 (offline): Data Analysis
DAD1 B, Sig=254,16 Ref=360,100 (LUCA\LD1384A.D)
mAU
min
19.449
39.250
File Information
LC File LD1384A.D
File Path C:\CHEM32\1\DATA\LUCA\
Date 01-Mar-13, 11:55:17
Sample ld1384a.D
Sample Info odh 80:20 1.0 ml/min, 1313
Barcode
Operator CARLOS
Method DEF_SU1_LC.M
Analysis Time 61.6 min
Sampling Rate 0.0067 min (0.402 sec), 9241 datapoints
Time Area Height Width Area% Symmetry
1 19.49 100.4 5.5E-1 3.0623 5.928 0.681
2 39.25 1594 5.9 4.5158 94.072 0.606


9.914
7.172
7.152
7.053
7.033
4.683
3.882
3.419
3.375
3.373
3.371
3.279
3.275
3.271
3.232
3.229
3.225
2.328
NC
MeO2C
O
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
1.00
2.35
2.18
1.06
3.20
1.09
1.12
6.86


186.32
168.94
157.65
138.45
136.87
133.59
129.81
128.46
127.88
117.56
58.23
54.39
51.84
47.83
21.36
14.34
NC
MeO2C
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

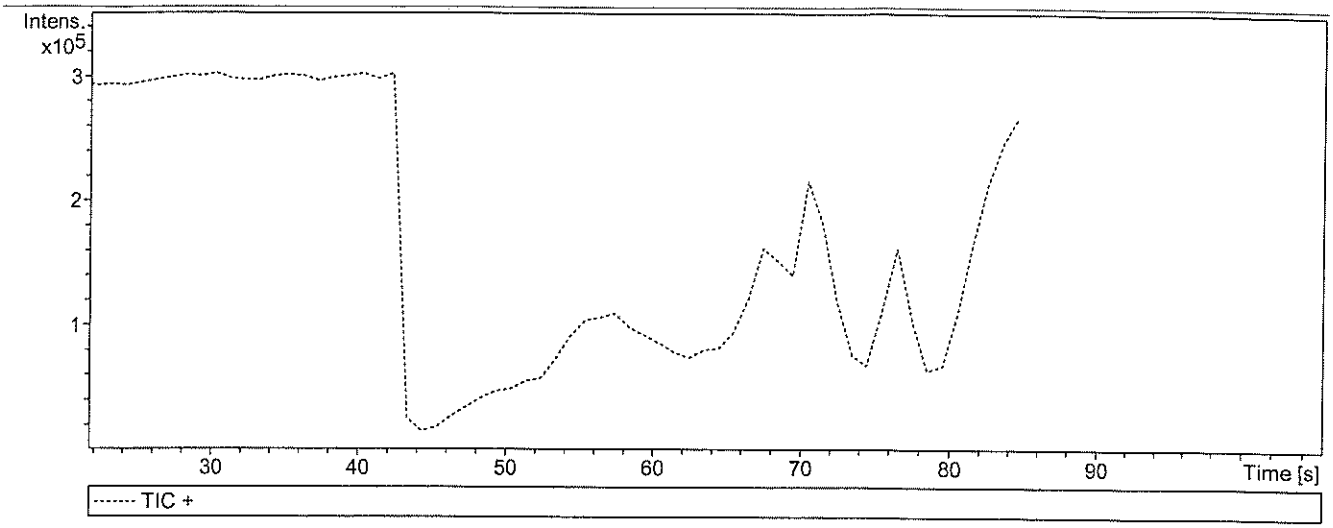
Display Report

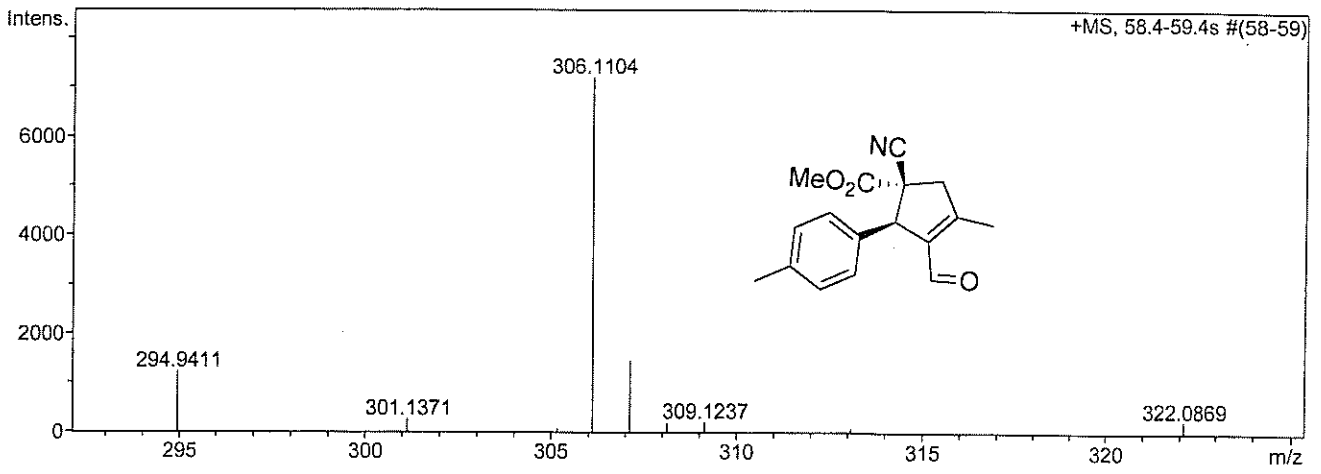
Analysis Info

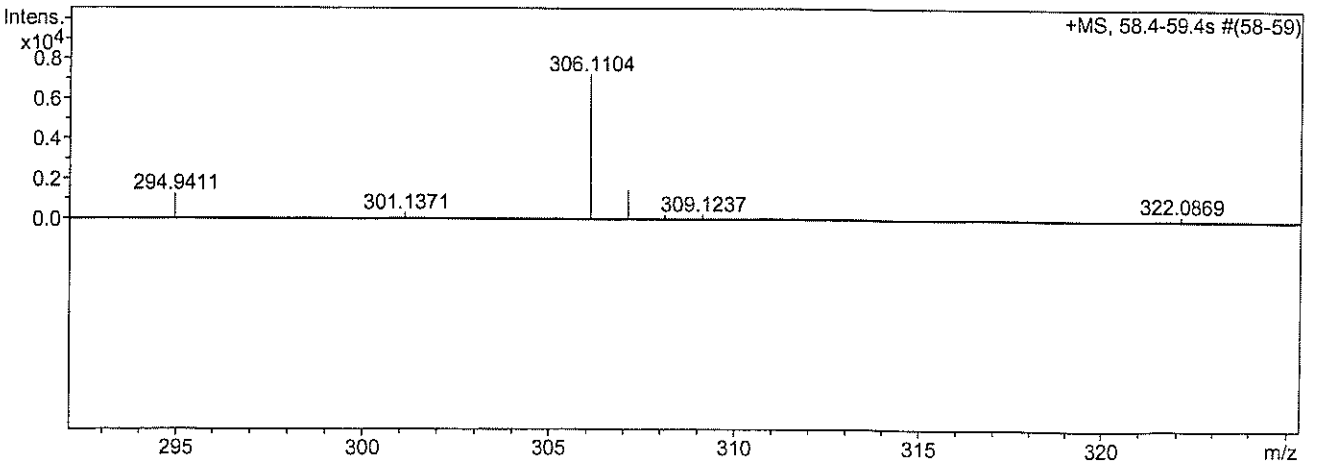
Analysis Name	E:\Data2\Luca\ld1382000001.d	Acquisition Date	2013-03-01 12:01:49
Method	Tune_low_pos.m	Operator	Carin Larsson
Sample Name	ld1382	Instrument / Ser#	micrOTOF 125
Comment			

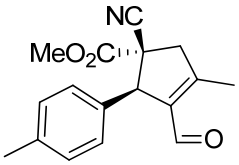
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

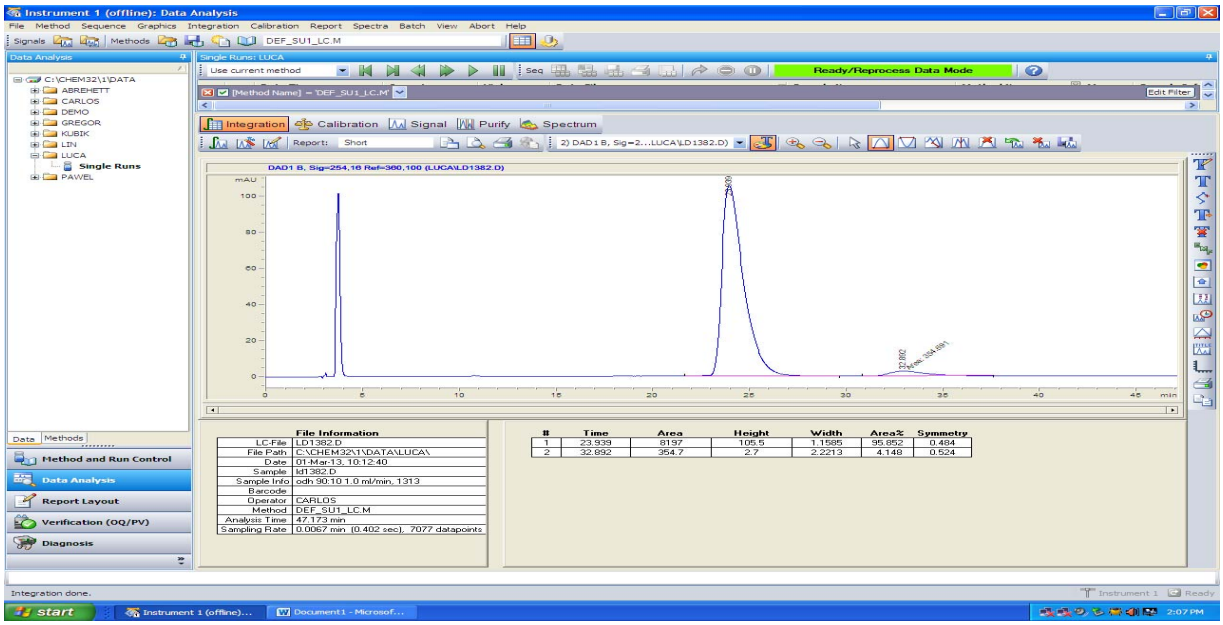


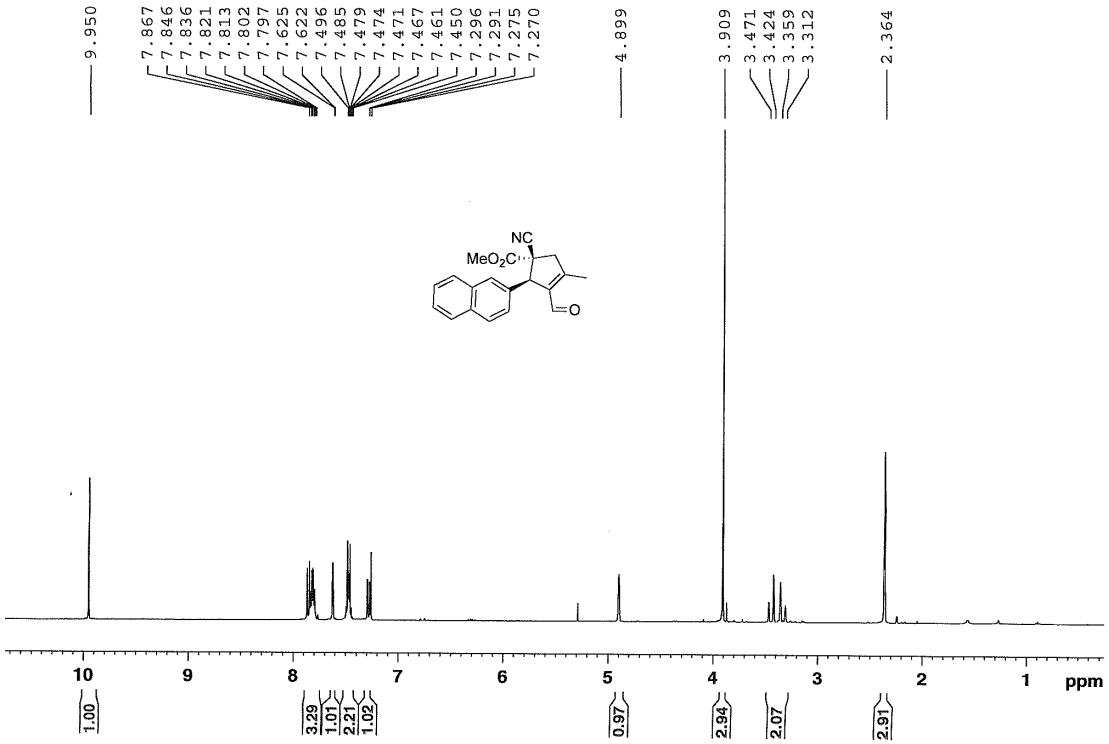


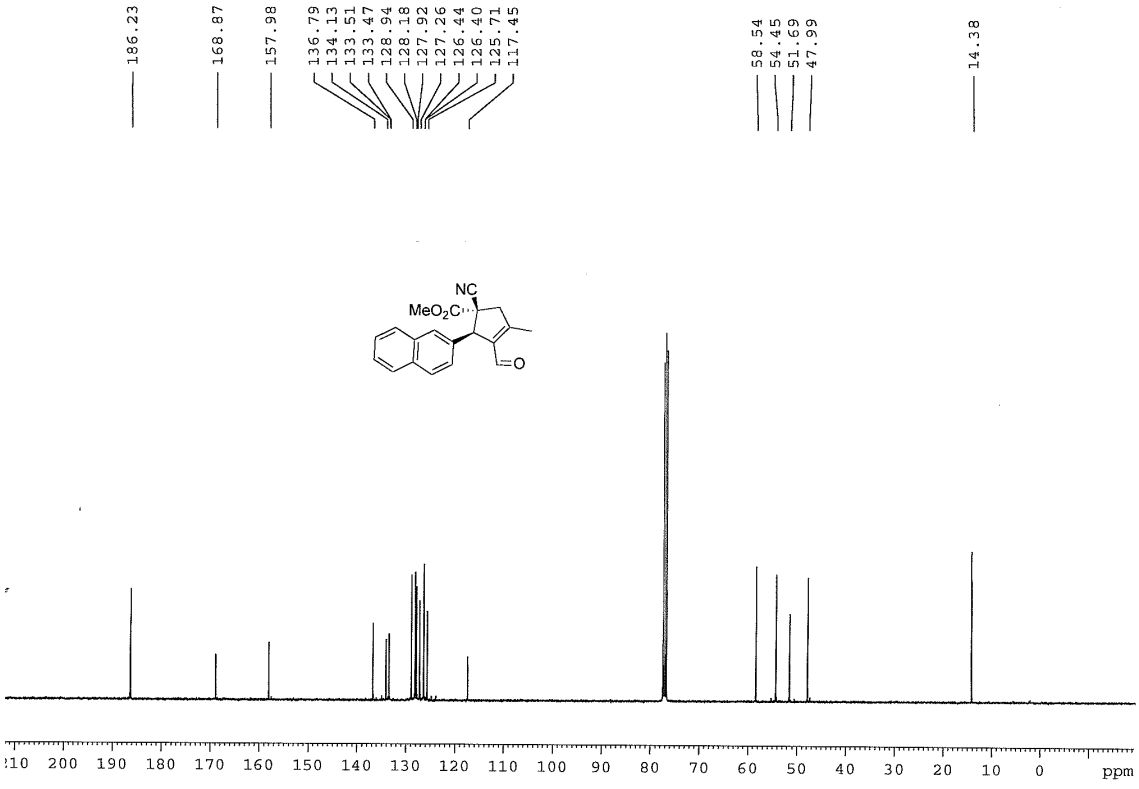



NC
MeO2C
O


Instrument 1 (offline): Data Analysis
DAD1 B, Sig=254,16 Ref=360,100 (LUCA\LD1382RAC.D)
24.359
31.756
File Information
LC-File LD1382RAC.D
File Path C:\CHEM32\1\DATA\LUCA\
Date 01-Mar-13, 11:02:21
Sample ld1382rac.D
Sample Info odh 90:10 1.0 ml/min, 1313
Barcode
Operator CARLOS
Method DEF_SU1_LC.M
Analysis Time 45.607 min
Sampling Rate 0.0067 min (0.402 sec), 6842 datapoints
Time Area Height Width Area% Symmetry
1 24.359 3328.8 31.8 1.4813 50.654 0.947
2 31.756 3242.8 23.6 1.8439 49.346 0.473


Instrument 1 (offline): Data Analysis
DAD1 B, Sig=254,16 Ref=360,100 (LUCA\LD1382.D)
23.939
32.892
File Information
LC-File LD1382.D
File Path C:\CHEM32\1\DATA\LUCA\
Date 01-Mar-13, 10:12:40
Sample ld1382.D
Sample Info odh 90:10 1.0 ml/min, 1313
Barcode
Operator CARLOS
Method DEF_SU1_LC.M
Analysis Time 47.173 min
Sampling Rate 0.0067 min (0.402 sec), 7027 datapoints
Time Area Height Width Area% Symmetry
1 23.939 8197 105.5 1.1585 95.852 0.484
2 32.892 354.7 2.7 2.2213 4.148 0.524


9.950
7.867
7.846
7.836
7.821
7.813
7.802
7.797
7.625
7.622
7.496
7.485
7.479
7.474
7.471
7.467
7.461
7.450
7.296
7.291
7.275
7.270
4.899
3.909
3.471
3.424
3.359
3.312
2.364
NC
MeO2C
O
10
9
8
7
6
5
4
3
2
1
ppm
1.00
3.29
1.01
2.21
1.02
0.97
2.94
2.07
2.91


186.23
168.87
157.98
136.79
134.13
133.51
133.47
128.94
128.18
127.92
127.26
126.44
126.40
125.71
117.45
58.54
54.45
51.69
47.99
14.38
NC
MeO2C
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

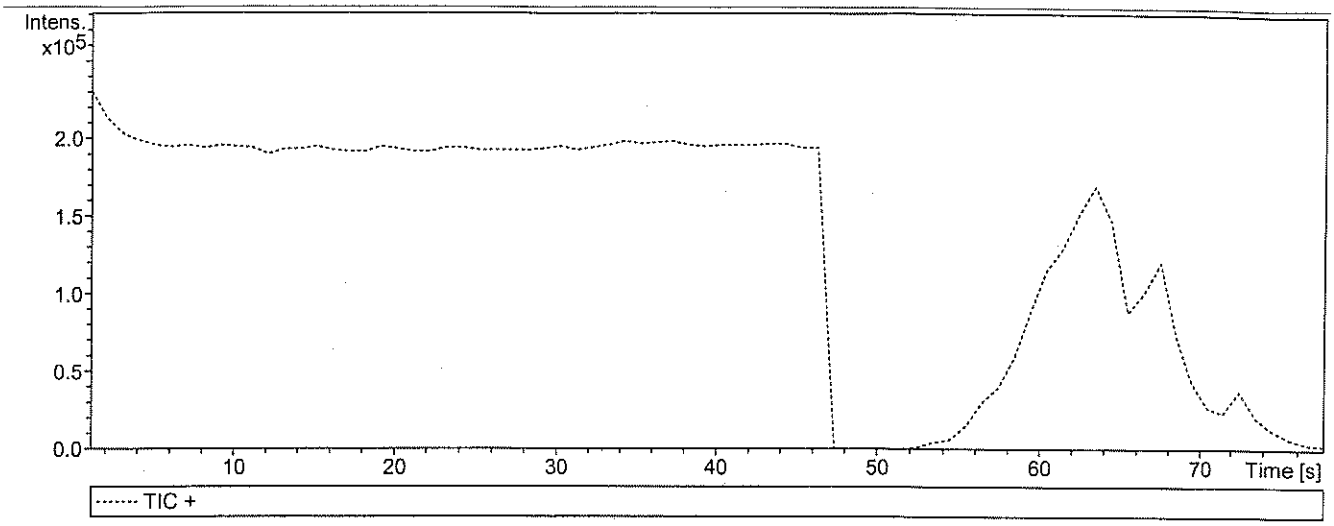
Display Report

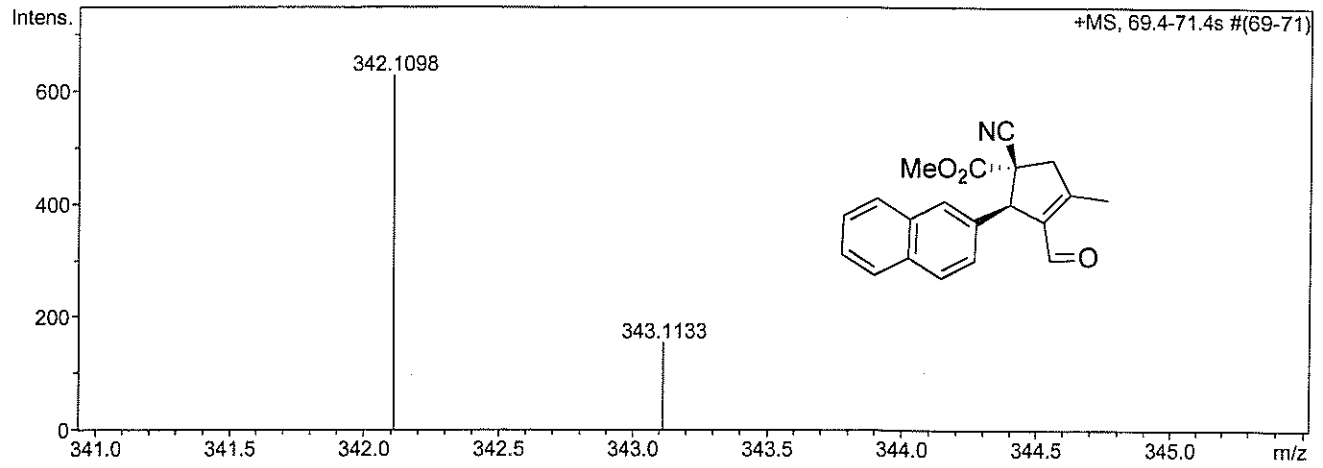
Analysis Info

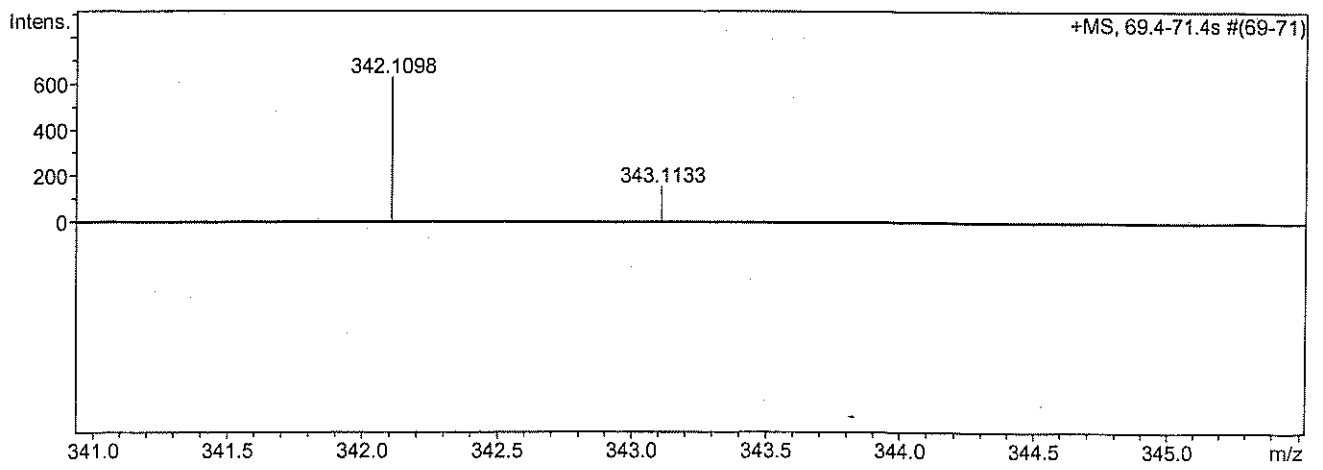
Analysis Name	E:\Data2\Luca\ld1396000001.d	Acquisition Date	2013-03-21 12:27:36
Method	Tune_low_pos.m	Operator	Carin Larsson
Sample Name	ld1396	Instrument / Ser#	micrOTOF 125
Comment			

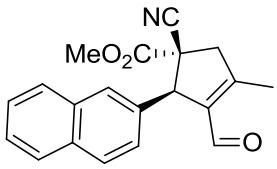
Acquisition Parameter

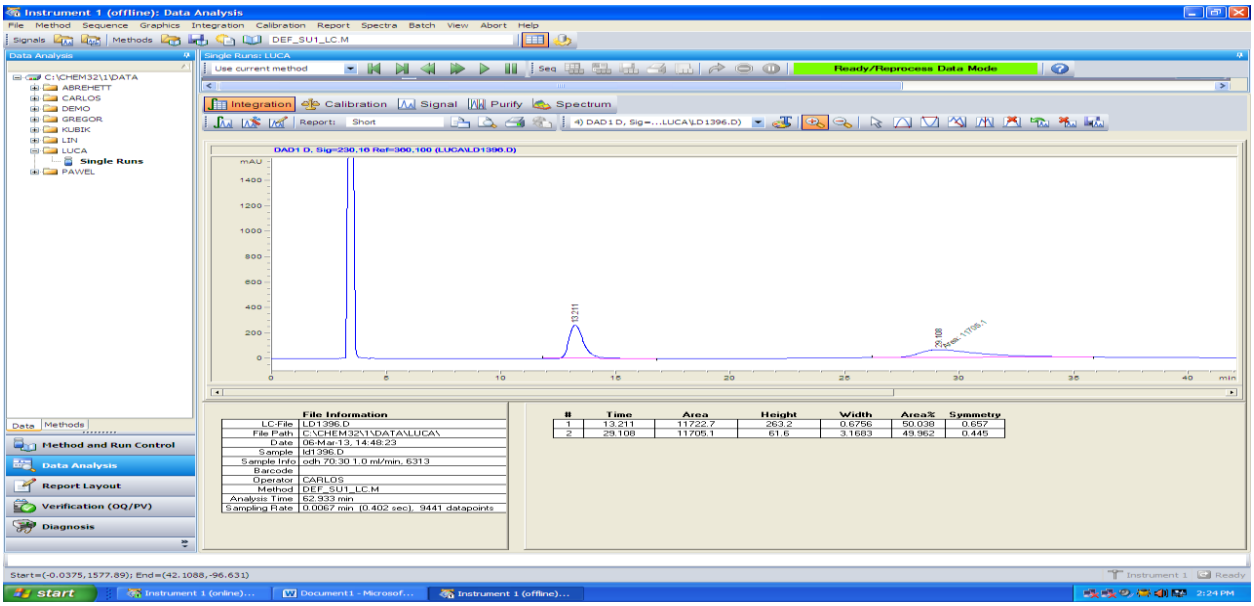
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

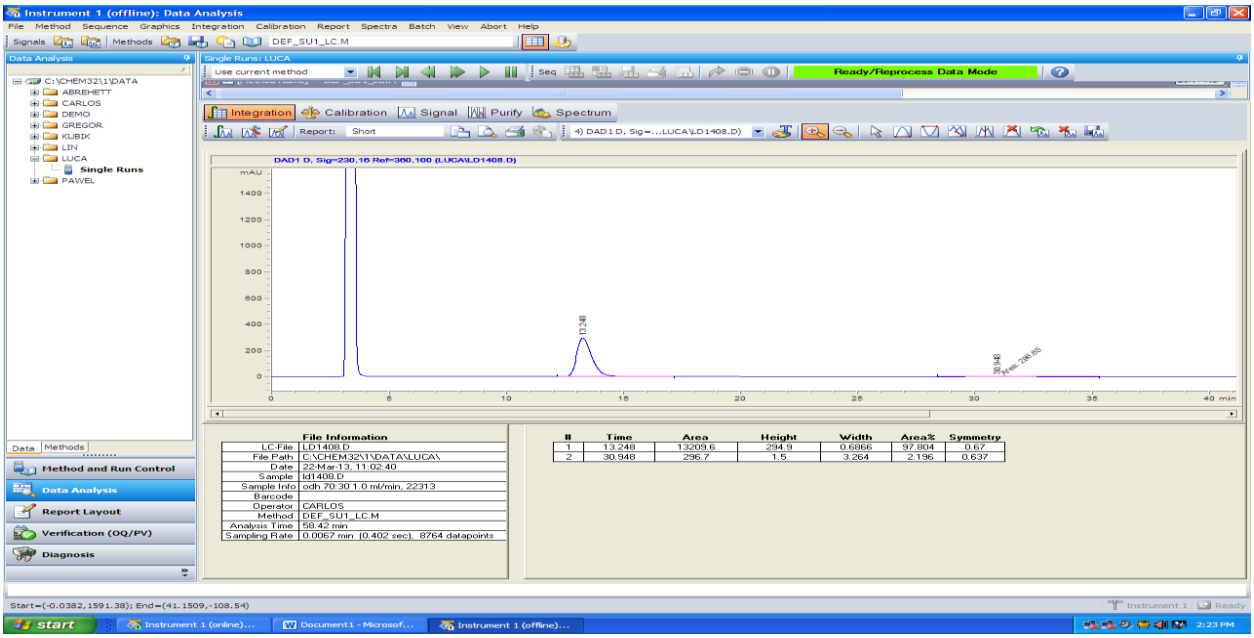







NC
MeO2C
O


Instrument 1 (offline): Data Analysis
DAD1 D, Sig=230,16 Ref=360,100 (LUCA\LD1396.D)
13.211
29.108
Area: 11705.1
File Information
LC-File LD1396.D
File Path C:\CHEM32\1\DATA\LUCA\
Date 06-Mar-13, 14:48:23
Sample ld1396.D
Sample Info odh 70:30 1.0 ml/min, 6313
Barcode
Operator CARLOS
Method DEF_SU1_LC.M
Analysis Time 62.933 min
Sampling Rate 0.0067 min (0.402 sec), 9441 datapoints
Time Area Height Width Area% Symmetry
1 13.211 11722.7 263.2 0.6756 50.036 0.657
2 29.108 11705.1 61.6 3.1683 49.962 0.445


Instrument 1 (offline): Data Analysis
DAD1 D, Sig=230,16 Ref=360,100 (LUCA\LD1408.D)
13.248
30.948
Area: 296.65
File Information
LC-File LD1408.D
File Path C:\CHEM32\1\DATA\LUCA\
Date 22-Mar-13, 11:02:40
Sample ld1408.D
Sample Info odh 70:30 1.0 ml/min, 22313
Barcode
Operator CARLOS
Method DEF_SU1_LC.M
Analysis Time 58.42 min
Sampling Rate 0.0067 min (0.402 sec), 8764 datapoints
Time Area Height Width Area% Symmetry
1 13.248 1320.6 294.9 0.6868 97.804 0.67
2 30.948 29.7 1.5 3.264 2.196 0.637