

# Practical Catalytic Enantioselective Synthesis of 2,3-Dihydroquinazolinones by Chiral Brønsted Acid Catalysis

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## Supporting Information

### Table of Contents

1. DFT calculations on the reaction mechanism.....	2
2. Experimental Section and compound characterization.....	2
3. NMR and HRM spectrum of 2,3-Dihydroquinazolinones <b>3</b> .....	41
4. HPLC of 2,3-Dihydroquinazolinones <b>3</b> .....	86

#### 1. DFT calculations on the reaction mechanism

DFT calculations were performed using the Gaussian 16 package (M. J. Frisch, M. J. et al. Gaussian,

Inc., Wallingford CT, 2016). All the structures were optimized using the M06-2X functional with the basis set 6-311G\*\* and 6-31+G\* for the H and O atoms respectively involved in the hydrogen bonding interactions and 6-31G\* for other atoms. A correction of  $-2.6$  kcal/mol was made for two-to-one (or  $2.6$  kcal/mol for one-to-two) transformations. Vibrational analyses were performed to ensure intermediates to have no imaginary frequencies and the transition state structures to have only one imaginary frequency. Transition state structures were confirmed to connect appropriate reactants or products by intrinsic reaction coordinate (IRC) calculations. Solvent effects were considered using the SMD mode at the M06-2X/6-311++G\*\* level.

**Table S1. The energies of calculated structures.**

	E	G	E <sub>sol</sub>	G <sub>sol</sub>
<b>Cat.11</b>	-1996.4836	-1995.9254	-1996.9810	-1996.4228
<b>1a</b>	-456.1282	-456.0147	-456.2699	-456.1564
<b>2a</b>	-231.1138	-231.0494	-231.1923	-231.1279
<b>TS1</b>	-2683.7745	-2682.9898	-2684.4710	-2683.6863
<b>1a-I</b>	-2683.7840	-2682.9913	-2684.4818	-2683.6892
<b>1a-II</b>	-2683.7930	-2683.0039	-2684.4869	-2683.6978
<b>TS2</b>	-2683.7648	-2682.9760	-2684.4668	-2683.6780
<b>1a-III</b>	-2607.3707	-2606.6120	-2608.0457	-2607.2870
<b>H2O</b>	-76.3852	-76.3811	-76.4252	-76.4211
<b>TS3</b>	-2607.3563	-2606.5919	-2608.0290	-2607.2646
<b>3aa+Ccat.11</b>	-2607.3893	-2606.6235	-2608.0577	-2607.2920
<b>TS3'</b>	-2607.3459	-2606.5821	-2608.0197	-2607.2559
<b>TScat.14(Re)</b>	-3078.8736	-3077.7791	-3079.6808	-3078.5862
<b>TScat.14(Si)</b>	-3078.8704	-3077.7753	-3079.6776	-3078.5825

### Cartesian coordinates

#### Cat.11

P	0.00627800	-0.77378900	-0.23503500
O	-0.60461900	-1.56258300	-1.30847400
O	0.72942500	-1.54069200	0.95618400
H	1.21930700	4.44183900	2.82089400
H	1.53296000	5.16125200	1.24200700
H	3.80301400	3.26954100	2.49607800
C	1.17716800	4.25287700	1.74438500
C	3.25405100	2.66042800	1.78394600
H	-0.87788400	4.71726500	1.05090600
C	-0.23048000	3.86062200	1.26018000
C	1.99914400	3.05165800	1.33729400
H	-0.72183900	3.23929200	2.01720600
C	3.79197700	1.46042600	1.32445300
H	4.77101300	1.13690600	1.66593900
H	0.87606100	4.77321800	-1.00301500

H	-1.53910900	5.18822800	-1.15284000
C	1.29535700	2.27746000	0.40873600
C	0.02145800	2.99079600	-0.00545500
C	0.24196900	3.91279600	-1.23739700
C	-1.18104200	4.29787000	-1.68491200
C	3.08403900	0.62829700	0.45162700
C	1.82975000	1.06465600	0.00115700
C	-1.24187800	2.26500100	-0.43250000
C	-1.98199300	3.07430500	-1.30028100
H	0.73309000	3.33075400	-2.02497100
O	-0.94583600	0.15532800	0.67077100
H	-1.24310600	4.51593500	-2.75496600
C	-1.75405000	1.02954700	-0.06456400
C	3.79138000	-1.70688500	1.03133100
C	3.61371000	-0.70773000	0.05345100
C	-3.25201300	2.69368100	-1.71136900
O	1.09708800	0.24925000	-0.85418900
C	-3.86366200	-0.90681200	1.35016200
C	-3.03357300	0.61517300	-0.45340900
H	-3.83006600	3.32538700	-2.37962300
C	-3.77568700	1.48343000	-1.26147000
C	4.22915200	-2.97299900	0.63277700
H	-4.62038300	-2.28805100	2.80523900
C	3.91435500	-0.98033200	-1.29412300
H	4.35326500	-3.74674700	1.38766000
C	-4.41157300	-2.12558300	1.74975500
C	-3.59574700	-0.69368000	-0.01255100
H	-4.77528500	1.17936700	-1.55779900
C	4.51688900	-3.26712000	-0.69931700
C	4.36534700	-2.25268000	-1.64330700
C	-4.69633000	-3.13545400	0.83419400
C	-3.87945300	-1.69661000	-0.95699500
H	4.60011000	-2.45786300	-2.68571100
C	-4.42094800	-2.90155400	-0.51211200
H	-4.62530800	-3.68412400	-1.24001100
C	-3.59013400	-1.50469800	-2.42531900
H	-2.57572300	-1.12573100	-2.57132900
H	-3.67735700	-2.45726000	-2.95408000
H	-4.28987000	-0.80093800	-2.88917300
C	-5.30939100	-4.43878900	1.27949100
H	-6.39610000	-4.43050800	1.13763100
H	-4.91074200	-5.27964200	0.70456900
H	-5.11561600	-4.62695600	2.33896500
C	-3.57782100	0.15670100	2.38191900

H	-2.50111200	0.25449400	2.55801100
H	-3.94872700	1.13526000	2.06057500
H	-4.05334100	-0.09425300	3.33351400
C	3.76546200	0.07740900	-2.35832900
H	2.71285900	0.21086700	-2.62797300
H	4.14337600	1.04421100	-2.01257200
H	4.31436500	-0.20566200	-3.25982400
C	4.96152300	-4.64601800	-1.11430400
H	4.12489800	-5.21507600	-1.53425400
H	5.74028200	-4.59561100	-1.88064100
H	5.35382500	-5.20983500	-0.26403200
C	3.50483200	-1.45269000	2.49394600
H	3.38039300	-2.39933000	3.02665700
H	4.32804600	-0.91162700	2.97281400
H	2.59835800	-0.85703300	2.62953800
H	1.44299300	-2.12213700	0.64926300

**1a**

C	-1.69529300	-0.18415500	-0.05389900
C	-0.20682500	-0.22613200	-0.03507400
C	0.53347100	0.97769800	0.06106500
C	1.93941000	0.88855700	0.09581900
C	2.58509200	-0.33063700	0.01006500
C	1.85738900	-1.51706600	-0.11814500
C	0.47468200	-1.44653900	-0.13853600
N	-0.07642600	2.19933400	0.17816600
N	-2.33836700	-1.35022900	0.27247800
O	-2.33955500	0.81201900	-0.36471800
H	0.49926900	3.00524400	0.00067700
H	-1.03444900	2.24256300	-0.13939700
H	-3.33742900	-1.25958800	0.37289500
H	-1.88101600	-2.01775400	0.87027000
H	2.51446000	1.80617900	0.18819300
H	3.67049300	-0.35843800	0.03121300
H	2.36263100	-2.47164800	-0.21035200
H	-0.10152000	-2.35680700	-0.27803900

**2a**

C	-1.04316500	-0.00006700	0.32749700
O	-2.15978100	0.00002900	-0.12754800
H	-0.87229100	-0.00005900	1.42905100
C	0.19821700	-0.00000600	-0.47505600
C	1.38705600	0.74264900	0.09660600
C	1.38709800	-0.74262000	0.09657000

H	0.05173100	0.00001400	-1.54782500
H	1.24369300	1.25364200	1.04393200
H	2.01802500	1.26700200	-0.61114000
H	2.01809400	-1.26690300	-0.61120500
H	1.24376600	-1.25366900	1.04387000

**TS1**

P	-0.61355900	-0.03144800	-0.13020500
O	0.32810200	-0.20471800	-1.26385200
O	-0.22371600	0.89267100	1.03610000
H	-5.47321300	-1.09827900	3.28777000
H	-6.47278100	-1.02052000	1.83806400
H	-5.43633500	1.76790400	3.05365200
C	-5.43582000	-1.01652400	2.19743500
C	-4.76697700	1.52011800	2.23476900
H	-5.18777100	-3.05826700	1.36348000
C	-4.61316800	-2.14417300	1.54251200
C	-4.70534200	0.22551400	1.73655100
H	-3.75867800	-2.39667000	2.18004600
C	-3.94615500	2.50068800	1.67749000
H	-3.98818300	3.52069000	2.04964700
H	-6.17120500	-1.35710500	-0.47864200
H	-5.64191000	-3.72258400	-0.89150500
C	-3.84458600	-0.08925000	0.68106200
C	-4.07638200	-1.51763600	0.22510900
C	-5.17594500	-1.58221700	-0.87416900
C	-5.05015200	-2.99772100	-1.46525400
C	-3.02768700	2.20093300	0.66649300
C	-2.98400900	0.88202300	0.19304100
C	-2.99634800	-2.36801400	-0.42202900
C	-3.57066100	-3.27115100	-1.32087400
H	-4.93916100	-0.83956000	-1.64430100
O	-1.05993400	-1.41186700	0.59680100
H	-5.38800200	-3.05587800	-2.50414200
C	-1.62048700	-2.37901700	-0.22775500
C	-1.14394200	3.85169100	0.91864200
C	-2.11994900	3.24659500	0.10927800
C	-2.79074800	-4.22206700	-1.96438600
O	-2.02258300	0.52473800	-0.73855800
C	1.20367900	-3.79063800	0.56558300
C	-0.80274700	-3.32305100	-0.86783400
H	-3.23697900	-4.92757100	-2.65949100
C	-1.42036700	-4.24874500	-1.71711600
C	-0.32150200	4.83759700	0.36699900

H	2.98566400	-4.17699600	1.69132700
C	-2.25558100	3.63643200	-1.23763500
H	0.44309800	5.29226100	0.99442300
C	2.58570900	-3.85841800	0.73003400
C	0.67753700	-3.37052100	-0.66658400
H	-0.79455800	-4.99039600	-2.20580500
C	-0.46125600	5.26011000	-0.95217600
C	-1.42848300	4.63808500	-1.74250100
C	3.46371900	-3.47760400	-0.28187800
C	1.54237000	-3.02696300	-1.71937600
H	-1.55139100	4.94935400	-2.77824100
C	2.92125000	-3.07132600	-1.50019800
H	3.59152500	-2.78893000	-2.31172000
C	1.01344400	-2.60061400	-3.06649900
H	0.23596900	-1.84200900	-2.95139800
H	1.81954000	-2.17952200	-3.67557700
H	0.59000000	-3.44638300	-3.61945200
C	4.95488600	-3.49069400	-0.05493800
H	5.49744600	-3.23693100	-0.97025400
H	5.24195300	-2.76320700	0.71410200
H	5.29736300	-4.47528000	0.28074700
C	0.29576500	-4.10024700	1.72635900
H	-0.11058100	-3.16519600	2.12907500
H	-0.54776700	-4.73070300	1.42850300
H	0.84363100	-4.60742300	2.52502400
C	-3.28842700	3.00099500	-2.13462100
H	-2.99610800	1.97948600	-2.39925700
H	-4.26398400	2.94647600	-1.64143100
H	-3.40099300	3.57434900	-3.05844700
C	0.37061100	6.39365800	-1.49953700
H	0.64675700	6.22350300	-2.54517600
H	-0.18606300	7.33680900	-1.46001600
H	1.28854700	6.52867400	-0.91984800
C	-0.95761400	3.47899600	2.36967500
H	0.09362500	3.59652700	2.65118600
H	-1.55179400	4.12960000	3.02286900
H	-1.24930100	2.44495100	2.55598300
C	2.55691700	-0.42843900	1.94798600
C	3.94159600	-0.19568600	1.42698300
C	4.13857800	0.01418900	0.05128200
C	5.43484500	0.16800700	-0.44213500
C	6.52891500	0.08062600	0.41203600
C	6.34049700	-0.13928200	1.77444400
C	5.04785500	-0.27006400	2.27351500

N	3.02958200	0.21265400	-0.79725300
N	2.27752900	0.08343100	3.18605500
O	1.75070300	-1.08575100	1.31330700
H	3.27310500	0.15693200	-1.78051400
H	2.23365100	-0.41048900	-0.61681800
H	1.28638000	0.07723800	3.39091300
H	2.75711900	0.93643300	3.43266800
H	5.57867000	0.35159100	-1.50406100
H	7.53146400	0.18360400	0.00943300
H	7.19265800	-0.21387500	2.44127300
H	4.88407400	-0.45851100	3.33061700
C	2.25506700	1.99246400	-0.43351500
O	1.91725500	1.96379200	0.79305600
H	1.48171400	1.83534600	-1.19700100
H	0.79337100	1.40945600	0.93542700
C	3.38471700	2.86516300	-0.83585800
C	3.74833400	2.95403700	-2.29077700
C	3.00633500	4.08093900	-1.64499700
H	4.16726500	2.96692600	-0.09266600
H	3.19378600	2.32979200	-2.98727400
H	4.79403400	3.09659500	-2.53949500
H	3.53520300	5.00429700	-1.43719200
H	1.95438100	4.19887100	-1.88771700

**1a-I**

P	-0.59411200	-0.02145100	-0.00492300
O	0.36725300	-0.26528500	-1.12819900
O	-0.20094500	0.89583000	1.12520000
H	-5.60799100	-1.03651100	3.16169900
H	-6.54909100	-0.96240000	1.67338000
H	-5.55345900	1.83252100	2.89919500
C	-5.52692200	-0.96245100	2.07309100
C	-4.84719200	1.57181100	2.11602600
H	-5.26145000	-3.01089800	1.26074900
C	-4.68676400	-2.10062600	1.45883300
C	-4.76963400	0.27180900	1.63409100
H	-3.86139900	-2.35635700	2.13228000
C	-3.99313600	2.54058600	1.58929200
H	-4.04733300	3.56463100	1.94860700
H	-6.15682300	-1.29995400	-0.61816900
H	-5.63213700	-3.67115000	-1.01384500
C	-3.86405800	-0.05684400	0.62180400
C	-4.09112200	-1.48481100	0.16247300
C	-5.15012600	-1.53546200	-0.97704700

C	-5.01727700	-2.94968100	-1.56744500
C	-3.02714400	2.22400100	0.62866900
C	-2.97074900	0.90133000	0.16549900
C	-2.99598400	-2.34485400	-0.44685400
C	-3.54530700	-3.23305800	-1.37592800
H	-4.87648000	-0.79355900	-1.73561100
O	-1.09635800	-1.42556700	0.66634700
H	-5.32225100	-3.00372500	-2.61675900
C	-1.62690000	-2.36480200	-0.20168900
C	-1.14470300	3.85155000	0.99104900
C	-2.07388200	3.25342500	0.12049700
C	-2.75119800	-4.17844500	-2.00953900
O	-1.97220200	0.52506900	-0.71267900
C	1.19640600	-3.79876600	0.60299000
C	-0.79511200	-3.29837200	-0.84304100
H	-3.17903200	-4.87231700	-2.72756600
C	-1.38857400	-4.20892600	-1.72511300
C	-0.26668000	4.81223900	0.48886800
H	2.96657000	-4.20888100	1.73978500
C	-2.10678600	3.62806400	-1.23468000
H	0.46201700	5.25955900	1.16231900
C	2.57729800	-3.86583400	0.78261800
C	0.68261600	-3.34888400	-0.62275900
H	-0.74892800	-4.94101500	-2.21073500
C	-0.29741200	5.21375700	-0.84528100
C	-1.21987900	4.60344200	-1.69362100
C	3.46520500	-3.45196000	-0.20598200
C	1.55957600	-2.97697500	-1.65701100
H	-1.26158700	4.90152200	-2.73982200
C	2.93609900	-3.01405500	-1.42060300
H	3.61624400	-2.71881400	-2.22055600
C	1.04468900	-2.53274500	-3.00369100
H	0.24453500	-1.79939700	-2.88400300
H	1.85042200	-2.07751000	-3.58966800
H	0.65593200	-3.37730600	-3.58322600
C	4.95280100	-3.46412700	0.04119800
H	5.50839100	-3.18214600	-0.85825100
H	5.22386700	-2.75845600	0.83602100
H	5.29623100	-4.45579700	0.35388200
C	0.27504300	-4.13866600	1.74382800
H	-0.14070500	-3.21348000	2.15917800
H	-0.56148200	-4.76475900	1.41870900
H	0.81378600	-4.66131400	2.53874800
C	-3.08906900	3.00507800	-2.19496200



H	-2.79757800	1.97723700	-2.43451600
H	-4.09521500	2.96913500	-1.76569900
H	-3.13218200	3.57589500	-3.12637300
C	0.60962200	6.31291800	-1.34035800
H	0.80677700	6.21944100	-2.41289200
H	0.15559500	7.29681200	-1.17584100
H	1.56837400	6.30250900	-0.81259900
C	-1.06717500	3.47574800	2.45070800
H	-0.06813100	3.69626200	2.84039800
H	-1.78828400	4.04458000	3.04964700
H	-1.26665700	2.41173700	2.58753000
C	2.44280100	-0.34905300	2.04166200
C	3.84211300	-0.14111900	1.53389300
C	4.04842200	0.03765500	0.16320600
C	5.32992600	0.11487700	-0.36404000
C	6.43054800	-0.00298300	0.48280300
C	6.24095600	-0.17065900	1.85080400
C	4.94976000	-0.23628600	2.37255200
N	2.90955700	0.27045300	-0.70329300
N	2.07062900	0.34823900	3.15129400
O	1.72104200	-1.14718300	1.47395400
H	3.15131100	0.06585000	-1.67363500
H	2.07843200	-0.33604300	-0.50411600
H	1.06083300	0.37452700	3.25047500
H	2.52805700	1.23890800	3.28332500
H	5.46668800	0.27587000	-1.43055100
H	7.43255600	0.04247700	0.06993700
H	7.09654300	-0.25919700	2.51186700
H	4.79084000	-0.38451600	3.43643800
C	2.37105300	1.75919100	-0.63726400
O	2.05604700	2.04115500	0.65182600
H	1.50375600	1.70428400	-1.30257600
H	1.13376300	1.67721800	0.85896200
C	3.42869300	2.66811800	-1.17819000
C	3.65676600	2.68460100	-2.66641100
C	2.96472600	3.83511200	-1.99529100
H	4.28162500	2.81550500	-0.52479100
H	3.04515600	2.03168000	-3.28489600
H	4.66979500	2.82847100	-3.02541000
H	3.50453400	4.76933400	-1.89170000
H	1.89323200	3.93910900	-2.14100100
<b>1a-II</b>			
P	0.58521100	-0.02432800	-0.07831600

O	-0.39967100	-0.39202700	1.07240200
O	0.14875500	0.88543000	-1.15630700
H	6.05489600	-1.24146700	-2.39522400
H	6.69505200	-1.23303300	-0.75305000
H	6.09197700	1.62153900	-2.06074400
C	5.76996000	-1.18000900	-1.34089000
C	5.23432800	1.38477600	-1.43770700
H	5.26358100	-3.22440600	-0.64299000
C	4.77944600	-2.28486400	-0.92613100
C	4.99743100	0.08073400	-1.02416900
H	4.08966000	-2.49222200	-1.75193200
C	4.35510000	2.39065500	-1.04171300
H	4.54093400	3.42061600	-1.33258400
H	5.84137500	-1.59379400	1.43101100
H	5.18312400	-3.95292900	1.61283300
C	3.90121200	-0.21762500	-0.21018800
C	3.97124100	-1.66115200	0.24745100
C	4.77599000	-1.79976600	1.57110700
C	4.48129100	-3.23262500	2.05191900
C	3.20871400	2.11379500	-0.28769500
C	2.99772300	0.78620700	0.10249900
C	2.74731600	-2.49120100	0.58637300
C	3.07820700	-3.46211500	1.53754400
H	4.38138100	-1.07780100	2.29480500
O	1.08008800	-1.41304800	-0.76098700
H	4.54943500	-3.33804300	3.13853100
C	1.45751800	-2.45675300	0.07731100
C	1.54047900	3.91170900	-0.84477700
C	2.27501600	3.20300900	0.12080500
C	2.16171800	-4.43807600	1.90366600
O	1.84301700	0.45375300	0.80876800
C	-0.97290800	-3.71388900	-1.58539200
C	0.51568300	-3.43948000	0.40909800
H	2.42124500	-5.19446900	2.63860400
C	0.89897100	-4.43419500	1.31445100
C	0.71329400	4.95414300	-0.42602500
H	-2.34599000	-4.01971900	-3.20625600
C	2.16903700	3.54316900	1.48165700
H	0.15248400	5.51086700	-1.17399800
C	-2.24966000	-3.79737500	-2.14482300
C	-0.84251100	-3.45655100	-0.20730800
H	0.17716700	-5.20504200	1.56903500
C	0.57760600	5.29629700	0.91664900
C	1.31885500	4.58205200	1.85602400

C	-3.40413400	-3.61382200	-1.38109800
C	-1.99045200	-3.28812000	0.58690700
H	1.23940100	4.84398800	2.90939500
C	-3.24883200	-3.36106800	-0.01850400
H	-4.13564800	-3.23082800	0.60173300
C	-1.89959900	-3.04684600	2.07445300
H	-1.05071700	-2.40509100	2.32219900
H	-2.81288300	-2.56567500	2.43524100
H	-1.77624700	-3.99055100	2.61830500
C	-4.76903200	-3.65213600	-2.01314200
H	-5.51281300	-4.06252800	-1.32409900
H	-5.07264800	-2.63343200	-2.27584100
H	-4.76886300	-4.26094800	-2.92141800
C	0.23949400	-3.91989200	-2.45913700
H	0.78188100	-2.97910900	-2.60360800
H	0.93705200	-4.63221000	-2.00743200
H	-0.05328400	-4.29924800	-3.44127900
C	2.96529000	2.81389900	2.53580000
H	2.56978100	1.80552200	2.69849100
H	4.01548500	2.71221000	2.24389300
H	2.92440400	3.35042800	3.48717200
C	-0.36829800	6.38741900	1.34812700
H	0.04400200	6.97040600	2.17702200
H	-0.58624300	7.07350600	0.52430600
H	-1.32044200	5.96288000	1.68851200
C	1.59154100	3.53891000	-2.30537100
H	0.95513000	4.20748800	-2.89159200
H	2.60346800	3.59629000	-2.71638800
H	1.23273300	2.51237000	-2.43330000
C	-3.20989400	0.17479700	-1.94000700
C	-3.07646500	1.63004100	-1.61240100
C	-3.70844600	2.15193500	-0.47020200
C	-3.48361400	3.48185400	-0.11427700
C	-2.67618800	4.29917000	-0.89676900
C	-2.08875700	3.79494300	-2.05459200
C	-2.27891600	2.46407100	-2.39981100
N	-4.56578500	1.36794500	0.36055800
N	-2.10237400	-0.40540400	-2.44531800
O	-4.25236700	-0.45828000	-1.73284600
H	-5.08565200	0.72193100	-0.22761300
H	-1.39638600	-0.30123000	0.91289300
H	-2.13413800	-1.41091900	-2.55368400
H	-1.20135400	0.04006200	-2.29689900
H	-3.97868100	3.86256100	0.77399400

H	-2.51950800	5.33598400	-0.61306500
H	-1.47789200	4.43403400	-2.68364200
H	-1.80173800	2.05999700	-3.28765600
C	-3.89261200	0.61783900	1.38689300
O	-2.91395000	-0.30659200	0.86293900
H	-3.33462700	-0.91666200	0.23457400
C	-4.88511500	-0.13199700	2.23256000
C	-4.48124700	-0.55796300	3.61240800
C	-5.47957600	0.54952500	3.42566700
H	-5.52825300	-0.80083900	1.66500500
H	-3.47943500	-0.29499200	3.93976600
H	-4.83710200	-1.51470100	3.97874300
H	-6.51919200	0.35257100	3.66031100
H	-5.15778000	1.56677400	3.62635900
H	-3.30338700	1.30254900	2.00445200

**TS2**

P	-0.56067700	0.05815200	-0.09110500
O	0.47636900	0.45428700	0.92012600
O	-0.23549100	-0.80687800	-1.26609700
H	-6.22799500	0.93059900	-2.21250500
H	-6.80333000	0.86793400	-0.54750000
H	-6.08603000	-1.92865800	-1.90070500
C	-5.89948400	0.87825000	-1.17013000
C	-5.21743500	-1.64571000	-1.31288400
H	-5.49506200	2.94420400	-0.46909100
C	-4.96514400	2.03839700	-0.77976500
C	-5.03727100	-0.33358700	-0.89716000
H	-4.31916900	2.29434000	-1.62709200
C	-4.26534000	-2.59824400	-0.95847300
H	-4.40396800	-3.63739300	-1.24451800
H	-5.89488600	1.24373800	1.60301600
H	-5.40428600	3.64263500	1.78722200
C	-3.92821900	0.02412600	-0.12557000
C	-4.07628600	1.45513600	0.35530000
C	-4.84246100	1.52538900	1.70685300
C	-4.63468100	2.97266300	2.19154900
C	-3.10650400	-2.25581100	-0.25187300
C	-2.94453900	-0.92013200	0.14128200
C	-2.90371600	2.36587600	0.66259800
C	-3.27200900	3.30748600	1.62786400
H	-4.37013100	0.82850100	2.40826800
O	-1.23265900	1.41501200	-0.75530300
H	-4.66913700	3.06441300	3.28130400

C	-1.63357200	2.41549600	0.10305100
C	-1.41739700	-4.00465600	-0.88937200
C	-2.11680700	-3.31115600	0.11254300
C	-2.42083400	4.35257900	1.95964900
O	-1.79835200	-0.53282600	0.80605400
C	0.67310700	3.83141700	-1.61360800
C	-0.75914900	3.46832500	0.41033300
H	-2.71020300	5.09184500	2.70109200
C	-1.18364400	4.43791800	1.32487600
C	-0.57471900	-5.05410000	-0.51902100
H	2.00109800	4.19029100	-3.26388600
C	-1.94520400	-3.66287000	1.46400000
H	-0.05427100	-5.61116400	-1.29678900
C	1.93563000	3.97677300	-2.19838700
C	0.58084800	3.57583800	-0.23465300
H	-0.51353600	5.26281600	1.55104400
C	-0.38104800	-5.41134100	0.81235400
C	-1.07498100	-4.70183100	1.79050900
C	3.10947800	3.85550600	-1.45437500
C	1.75029400	3.47840700	0.54184500
H	-0.94722800	-4.97203400	2.83724800
C	2.99140300	3.60974300	-0.08530400
H	3.89542000	3.52823100	0.51833800
C	1.68078600	3.23089700	2.02858200
H	0.96839100	2.43042800	2.24686100
H	2.66132100	2.93686800	2.41091500
H	1.35920200	4.12996600	2.56517400
C	4.46256500	3.94205700	-2.10934700
H	5.17850200	4.46909000	-1.47130500
H	4.84649800	2.93182300	-2.28859200
H	4.40762500	4.46610400	-3.06744400
C	-0.56478400	3.95771300	-2.46545400
H	-1.05577100	2.98515300	-2.57935200
H	-1.29059100	4.63702300	-2.00748200
H	-0.31389900	4.33712900	-3.45934700
C	-2.69540600	-2.94571100	2.55842200
H	-2.31047400	-1.92907400	2.68911300
H	-3.76125600	-2.86499400	2.32165800
H	-2.59298100	-3.47748000	3.50809600
C	0.57211500	-6.51664100	1.19075400
H	0.16099200	-7.14561700	1.98626000
H	0.79637900	-7.15878200	0.33354400
H	1.52105200	-6.10767700	1.55899300
C	-1.52383400	-3.59901300	-2.33833700

H	-0.90791100	-4.24960200	-2.96709900
H	-2.54920000	-3.65317900	-2.71391800
H	-1.18406100	-2.56216000	-2.44510900
C	3.14427500	0.02918100	-1.84383700
C	3.03845900	-1.44757700	-1.58712200
C	3.82742900	-2.03173900	-0.59052500
C	3.71698800	-3.37811000	-0.26853300
C	2.81512000	-4.17183700	-0.97143100
C	2.05051900	-3.61551900	-1.99173700
C	2.15145100	-2.26154300	-2.28910800
N	4.75211400	-1.20793400	0.12721200
N	2.01477800	0.62387200	-2.23417900
O	4.22100000	0.62632300	-1.68258500
H	5.24876600	-0.54780500	-0.47328000
H	1.97594100	0.45285400	1.03927900
H	2.02960800	1.63352000	-2.31873200
H	1.11724700	0.14884600	-2.09259900
H	4.34773500	-3.79498300	0.51085900
H	2.71669500	-5.22500800	-0.72732200
H	1.35724800	-4.23266500	-2.55066700
H	1.52379800	-1.82820600	-3.06005500
C	4.52561400	-0.83114400	1.35997200
O	2.97844900	0.58681300	1.14611000
H	3.22386000	1.19960000	0.43777000
C	5.47366800	0.02416800	2.06506300
C	5.01859100	0.70983900	3.32484700
C	5.93024500	-0.45692500	3.43742900
H	6.20277400	0.52571800	1.43890800
H	3.97096000	0.58996400	3.57665800
H	5.42092200	1.70140300	3.49698300
H	6.97472400	-0.29312500	3.67565700
H	5.52506000	-1.39776500	3.79500000
H	3.81622500	-1.42125900	1.93201700

**1a-III**

P	0.09981200	0.32181000	0.00648300
O	0.52597600	-0.48944600	1.22488000
O	-0.70610400	-0.34739200	-1.05141500
H	0.47761000	5.30249500	-3.36887500
H	0.25872600	6.28185500	-1.92001600
H	-2.37288200	4.92499400	-3.09772700
C	0.40049600	5.25446100	-2.27867400
C	-2.02939700	4.27452300	-2.29858800
H	2.45047300	5.29336100	-1.43046200

C	1.62913300	4.59606000	-1.62218200
C	-0.72899600	4.35879300	-1.82135500
H	2.00605100	3.79158700	-2.26342800
C	-2.89189000	3.33965500	-1.73223300
H	-3.92284800	3.27997300	-2.06933900
H	0.58673700	6.00454800	0.39657400
H	3.00214800	5.85265200	0.82250000
C	-0.29893000	3.52991400	-0.78176800
C	1.07499000	3.96420600	-0.31489300
C	0.96244900	5.05474100	0.78906800
C	2.37770900	5.14672600	1.38491000
C	-2.46644400	2.44268800	-0.74485400
C	-1.14339300	2.54232600	-0.29334000
C	2.07468400	3.02393700	0.32930500
C	2.88238900	3.73146500	1.22384000
H	0.26190700	4.70124200	1.55405800
O	1.42824300	0.96250400	-0.69621900
H	2.37983400	5.47547900	2.42834400
C	2.30248000	1.66914300	0.11552700
C	-4.02691200	0.49637600	-1.02323200
C	-3.43674000	1.45819700	-0.18492600
C	3.96266100	3.11712900	1.84076300
O	-0.65223400	1.63287000	0.63271100
C	4.21391600	-0.80718400	-0.78480400
C	3.39035500	1.02336200	0.72006200
H	4.59832500	3.66699900	2.52873500
C	4.21735400	1.77834600	1.56217400
C	-5.02084600	-0.33649100	-0.50070100
H	5.09685600	-2.39994300	-1.91882300
C	-3.83474000	1.55821400	1.16173600
H	-5.49799000	-1.06230100	-1.15975400
C	4.72244800	-2.09955600	-0.94174500
C	3.75305300	-0.40457100	0.47956200
H	5.07266200	1.28387300	2.01421700
C	-5.43194700	-0.25404700	0.82787700
C	-4.82124500	0.69831900	1.64389200
C	4.77830500	-3.00244900	0.11696200
C	3.77418500	-1.31024300	1.55897700
H	-5.13461700	0.78747900	2.68331200
C	4.28973600	-2.59044800	1.35846800
H	4.30570700	-3.28797400	2.19419800
C	3.24353100	-0.92164800	2.91767000
H	2.30529100	-0.37006100	2.81441300
H	3.06281200	-1.81510600	3.52232800

H	3.94979400	-0.28913800	3.46589800
C	5.29298800	-4.40609200	-0.07708000
H	5.84871800	-4.49942700	-1.01438500
H	5.95363200	-4.70524600	0.74222500
H	4.46442300	-5.12438100	-0.10663000
C	4.19677400	0.13899000	-1.95824300
H	3.16897500	0.34164200	-2.27625600
H	4.65453500	1.09903400	-1.69819800
H	4.74232800	-0.28480900	-2.80507400
C	-3.23236300	2.59205100	2.07987900
H	-2.19129400	2.34719400	2.31415800
H	-3.23726200	3.58298300	1.61457600
H	-3.79287100	2.64963200	3.01656200
C	-6.52341700	-1.14572200	1.36417700
H	-6.31239600	-1.46071800	2.39136400
H	-7.48672800	-0.62378500	1.37590200
H	-6.64207000	-2.04322300	0.75040100
C	-3.59187600	0.33164300	-2.46002800
H	-3.96832500	-0.61064400	-2.86849600
H	-3.96787000	1.14041000	-3.09484900
H	-2.49948900	0.32969700	-2.52856900
C	-2.23506700	-3.75571800	-1.30418000
C	-0.73944100	-3.93581200	-1.42052000
C	0.18577000	-3.42455000	-0.50154200
C	1.55317500	-3.47892900	-0.75284200
C	2.01240400	-4.11324700	-1.90131800
C	1.10826400	-4.69783300	-2.78613200
C	-0.25843400	-4.60625100	-2.54367500
N	-0.22910100	-2.80958700	0.71391600
N	-2.63385600	-2.49320200	-1.03942800
O	-2.99706000	-4.70133100	-1.44504000
H	0.21066200	-1.77440900	0.98297700
H	-3.62509400	-2.31897100	-0.98852400
H	-1.99427800	-1.69496300	-1.05624600
H	2.24121500	-3.03255200	-0.04142100
H	3.07965200	-4.14730800	-2.09716600
H	1.46606000	-5.20593500	-3.67558200
H	-0.98056000	-5.03014100	-3.23408600
C	-1.22704600	-3.22464600	1.40341700
C	-1.76174100	-2.47915300	2.52616700
C	-3.28535300	-2.42579300	2.58829600
C	-2.54290200	-3.23513900	3.58300100
H	-1.21794500	-1.58444400	2.80485700
H	-3.82868400	-2.93360600	1.79693000



H	-3.69495400	-1.46423300	2.87471000
H	-2.44649900	-2.86137800	4.59560900
H	-2.57775600	-4.31639200	3.49709600
H	-1.72054800	-4.15575900	1.11270800

**H<sub>2</sub>O**

O	0.00000000	0.00000000	0.11831700
H	0.00000000	0.75681600	-0.47326700
H	0.00000000	-0.75681600	-0.47326700

**TS3**

P	0.11340400	0.30266500	0.14241500
O	0.56103100	-0.43445900	1.37524500
O	-0.69061000	-0.41697700	-0.90001900
H	0.31070900	5.16861600	-3.47042600
H	0.04446000	6.18273900	-2.05331200
H	-2.50854500	4.65446100	-3.22096100
C	0.23080500	5.15151300	-2.37946500
C	-2.14835200	4.05711300	-2.38838500
H	2.27581600	5.30068400	-1.53175400
C	1.48166200	4.56625400	-1.69770900
C	-0.86160900	4.22466500	-1.89612400
H	1.88999600	3.75350700	-2.30868300
C	-2.97373300	3.10561900	-1.79539400
H	-3.99358900	2.97815300	-2.14760300
H	0.40171700	6.00566800	0.28424400
H	2.82317900	5.95197900	0.69182600
C	-0.40725000	3.46126100	-0.81738700
C	0.95114500	3.96106700	-0.36746500
C	0.81239200	5.08140000	0.70225000
C	2.23043700	5.23972500	1.28001400
C	-2.52375000	2.27860300	-0.75900900
C	-1.21428700	2.46086700	-0.29111900
C	1.98868800	3.07646900	0.29575200
C	2.78512300	3.83917000	1.15370000
H	0.13165800	4.72910600	1.48539400
O	1.39089700	0.96157000	-0.64074400
H	2.23036800	5.59794900	2.31376400
C	2.25930600	1.72454200	0.12116400
C	-4.00863600	0.26523500	-0.97653100
C	-3.46412200	1.28065400	-0.17115000
C	3.89805400	3.28148800	1.76726400
O	-0.69856800	1.62459900	0.68364500
C	4.21492000	-0.70676100	-0.76173400

C	3.38155200	1.13593800	0.72043300
H	4.52577000	3.87366900	2.42692500
C	4.19740200	1.94460100	1.52213800
C	-4.99203000	-0.57346600	-0.44002200
H	5.08887400	-2.30950000	-1.88966300
C	-3.89108300	1.42170200	1.16416200
H	-5.42569100	-1.34557000	-1.07632800
C	4.73619700	-1.99531000	-0.90886400
C	3.77798500	-0.28725400	0.50526800
H	5.07889900	1.49541400	1.97129200
C	-5.43503100	-0.44475200	0.87491800
C	-4.86275300	0.55434800	1.66294800
C	4.83354400	-2.87500300	0.16536300
C	3.83610900	-1.17220400	1.60022700
H	-5.19729700	0.67641000	2.69219000
C	4.36763200	-2.44736800	1.41062300
H	4.41750400	-3.12746100	2.25953700
C	3.32578300	-0.76649200	2.96118400
H	2.34750300	-0.28711000	2.86577500
H	3.22696100	-1.64498000	3.60523100
H	4.00292500	-0.06436800	3.45872800
C	5.37336800	-4.27207300	-0.01156100
H	5.86956400	-4.38647600	-0.97960000
H	6.09557900	-4.52240300	0.77161900
H	4.56802900	-5.01570200	0.04184800
C	4.15659900	0.21739700	-1.95155000
H	3.11872000	0.39990500	-2.24860300
H	4.60652100	1.18840200	-1.72005100
H	4.68807700	-0.21442500	-2.80340000
C	-3.33744100	2.50923500	2.04991700
H	-2.29237700	2.30872800	2.30656200
H	-3.36801300	3.48014800	1.54511400
H	-3.91390300	2.58399900	2.97555400
C	-6.52191900	-1.33567500	1.42176900
H	-6.35931000	-1.56221000	2.48032700
H	-7.50176000	-0.85224900	1.33959800
H	-6.57577300	-2.28109100	0.87390500
C	-3.53144300	0.03611900	-2.39108900
H	-3.79542800	-0.97379000	-2.72242400
H	-3.98715800	0.74188100	-3.09384000
H	-2.44539400	0.15237400	-2.45090900
C	-2.06387800	-3.49561300	-1.38747200
C	-0.60402000	-3.81809100	-1.48324000
C	0.31746700	-3.50922600	-0.46748000

C	1.67846400	-3.70210800	-0.67159700
C	2.12544000	-4.23771800	-1.87455600
C	1.21716900	-4.60642500	-2.86607300
C	-0.14165200	-4.39411400	-2.66673400
N	-0.11492200	-2.95202600	0.76262100
N	-2.37061000	-2.46933700	-0.48061400
O	-2.91818600	-4.10278100	-1.99405100
H	0.31894200	-2.03886500	1.04857500
H	-3.36750000	-2.28200900	-0.42171200
H	-1.79749900	-1.59689600	-0.61808200
H	2.37431100	-3.41894100	0.11198600
H	3.19253700	-4.36657500	-2.03104200
H	1.56824700	-5.03752300	-3.79739600
H	-0.87036400	-4.63935400	-3.43264800
C	-1.35995700	-3.14489200	1.17306400
C	-1.89040900	-2.35697800	2.28722200
C	-3.33606700	-2.54282800	2.66384000
C	-2.28320000	-3.13287600	3.53377300
H	-1.43701100	-1.38008200	2.41409200
H	-3.93021100	-3.21194300	2.04646700
H	-3.85529100	-1.65205700	2.99657800
H	-2.05422000	-2.65808800	4.48051000
H	-2.14505300	-4.20908000	3.51912800
H	-1.78205000	-4.13763200	1.01706400

**3aa+Cat.11**

P	0.23190200	0.32522700	0.26240700
O	0.45056300	-0.53188300	1.44497700
O	-0.72760700	-0.19242400	-0.86288600
H	1.40016300	5.12344700	-3.34764000
H	1.37712000	6.11607500	-1.89077300
H	-1.45013200	5.19877100	-3.08295500
C	1.33166400	5.08254000	-2.25676900
C	-1.22306400	4.51466100	-2.27059600
H	3.37163600	4.74922400	-1.45162000
C	2.43229500	4.21447400	-1.62099200
C	0.07127300	4.39555800	-1.78406800
H	2.64167800	3.35297300	-2.26485600
C	-2.22747800	3.73136800	-1.70993300
H	-3.24790300	3.81577300	-2.07208700
H	1.73275200	5.78808200	0.43135600
H	4.09407300	5.19425400	0.75054100
C	0.35961800	3.52315800	-0.73033700
C	1.80207900	3.69815400	-0.29582300

C	1.94179500	4.78277100	0.80925600
C	3.37727900	4.60708000	1.33830600
C	-1.96112800	2.79758100	-0.70103900
C	-0.64558600	2.70890100	-0.22728100
C	2.63420100	2.58352800	0.30863400
C	3.60853200	3.12475200	1.15238800
H	1.22357200	4.56147800	1.60654500
O	1.53539300	0.66594800	-0.62096900
H	3.48557400	4.91764500	2.38154700
C	2.59950100	1.21125800	0.10387600
C	-3.76012400	1.09186400	-1.06418800
C	-3.06941900	1.94478800	-0.18214700
C	4.59012300	2.31588100	1.70745700
O	-0.32584600	1.76481800	0.74672300
C	3.86528000	-1.59021100	-0.89669300
C	3.57554600	0.36553800	0.64432600
H	5.35441100	2.73528600	2.35524600
C	4.57904300	0.95274200	1.42503300
C	-4.86156000	0.37356400	-0.58978900
H	4.23747200	-3.33551800	-2.08746800
C	-3.47488500	2.04590800	1.16280100
H	-5.37545600	-0.30000100	-1.27375900
C	4.02992500	-2.96454900	-1.08573900
C	3.60980200	-1.10579900	0.39651900
H	5.35250200	0.30770900	1.83165800
C	-5.28008500	0.45995800	0.73826200
C	-4.56791400	1.29597300	1.59810200
C	3.95009700	-3.86489300	-0.02796700
C	3.49417400	-2.00107500	1.47812800
H	-4.88385300	1.38365600	2.63608000
C	3.67086700	-3.36374800	1.24489500
H	3.58571500	-4.05505500	2.08169500
C	3.17854500	-1.51667000	2.87259400
H	2.36287000	-0.78931300	2.85000100
H	2.87556700	-2.35669200	3.50349300
H	4.04472400	-1.04230400	3.34621300
C	4.11420600	-5.34781800	-0.24634200
H	4.49087300	-5.56175300	-1.25051200
H	4.81136200	-5.78113200	0.47754100
H	3.15771000	-5.87231300	-0.12811800
C	3.99032600	-0.65540800	-2.07365100
H	3.01468900	-0.24028900	-2.34734600
H	4.65360800	0.18533900	-1.84589100
H	4.39034600	-1.18246200	-2.94332700

C	-2.77473000	2.96651100	2.13122900
H	-1.80963000	2.55308900	2.44058600
H	-2.58095500	3.94372600	1.67798700
H	-3.38455300	3.11814300	3.02541400
C	-6.47811500	-0.31705200	1.22326300
H	-6.45209700	-0.45075500	2.30850200
H	-7.40913700	0.20456800	0.97511100
H	-6.52548900	-1.30597000	0.75636600
C	-3.33207600	0.89909700	-2.49996500
H	-3.65170700	-0.08535200	-2.85168200
H	-3.77711400	1.65478800	-3.15738300
H	-2.24621600	0.96727600	-2.60218300
C	-2.74526300	-2.64705000	-1.28784800
C	-1.56750700	-3.52987700	-1.44407000
C	-0.59622900	-3.58823400	-0.42471100
C	0.64485200	-4.17543300	-0.70738200
C	0.87978700	-4.73326300	-1.95192000
C	-0.11176100	-4.74014400	-2.94342200
C	-1.32436500	-4.12607200	-2.68761000
N	-0.86280900	-3.08147000	0.84118800
N	-2.72288200	-1.91504900	-0.08615800
O	-3.59322900	-2.45745000	-2.13843400
H	-0.14918200	-2.47704400	1.24156000
H	-3.59169500	-1.41177300	0.07900700
H	-1.49113600	-0.75178200	-0.52473800
H	1.40650400	-4.18019700	0.06551100
H	1.85093300	-5.17753500	-2.15520900
H	0.08209100	-5.19488400	-3.90867000
H	-2.09732200	-4.05070400	-3.44598500
C	-2.22050600	-2.66361000	1.08349200
C	-2.35950100	-1.82436800	2.31962200
C	-3.67534900	-1.84902200	3.04425400
C	-2.47347700	-2.52268300	3.64121400
H	-1.81489400	-0.88613800	2.29357900
H	-4.46457800	-2.48018000	2.64366700
H	-4.02045200	-0.92051500	3.48490200
H	-1.99409800	-2.05991300	4.49576200
H	-2.44394800	-3.60780400	3.63603000
H	-2.83340000	-3.57256000	1.19950200
<b>TS3'</b>			
P	0.48262400	-0.12388000	-0.07920300
O	-0.53578000	-0.26805600	1.00799000
O	0.23983300	0.84653900	-1.20493800

H	5.55759100	-2.09520800	-2.83997600
H	6.33779300	-2.11765600	-1.25890400
H	5.94446900	0.73210900	-2.67184900
C	5.37730800	-1.96751400	-1.76851100
C	5.13620300	0.63077000	-1.95333000
H	4.68601200	-3.91179100	-0.95332300
C	4.30067500	-2.92421600	-1.22518200
C	4.79411300	-0.61208900	-1.43957100
H	3.51402600	-3.05900500	-1.97579100
C	4.41588300	1.74849600	-1.54042000
H	4.67568600	2.73316000	-1.91908600
H	5.65837400	-2.32793300	1.00429800
H	4.71723300	-4.57548300	1.31583800
C	3.75845100	-0.74187400	-0.50913800
C	3.69337300	-2.17217400	-0.00710100
C	4.59212400	-2.38856700	1.24333100
C	4.15889200	-3.76053300	1.79404000
C	3.33225700	1.64149800	-0.66205400
C	3.00668000	0.37360200	-0.16001400
C	2.41024200	-2.82568800	0.46516200
C	2.69541300	-3.80898600	1.41623400
H	4.36100500	-1.60678700	1.97550300
O	0.81666100	-1.56206500	-0.78691100
H	4.31512900	-3.85346400	2.87293300
C	1.09751700	-2.61342000	0.06741300
C	1.85318900	3.58894300	-1.23860200
C	2.57843800	2.86707700	-0.27069000
C	1.69182900	-4.63794500	1.89845400
O	1.90586500	0.22221000	0.66640100
C	-1.72227600	-3.38933600	-1.22145000
C	0.06080900	-3.42844400	0.54518600
H	1.91240500	-5.41214700	2.62780900
C	0.38948100	-4.45332600	1.43956000
C	1.22611100	4.77645400	-0.86274700
H	-3.33476200	-3.33184200	-2.63313500
C	2.65678800	3.33971800	1.04999300
H	0.66014900	5.32965500	-1.61020000
C	-3.05371300	-3.19707000	-1.59047400
C	-1.35306000	-3.21579900	0.12427800
H	-0.40734500	-5.10124900	1.79415300
C	1.32038800	5.28291700	0.43338600
C	2.03313600	4.54704600	1.37752100
C	-4.03118700	-2.84769600	-0.66144900
C	-2.32268800	-2.86223000	1.07951600

H	2.12194300	4.92604400	2.39482900
C	-3.64515500	-2.69349900	0.66883100
H	-4.39804400	-2.43043300	1.41073200
C	-1.95694100	-2.61788400	2.52378500
H	-1.09080500	-1.95198900	2.58364600
H	-2.79820200	-2.15562800	3.05266400
H	-1.71131400	-3.54358800	3.05383800
C	-5.45835700	-2.62655300	-1.09043700
H	-6.13591900	-2.62507200	-0.23173900
H	-5.56758800	-1.66207800	-1.59957300
H	-5.78762300	-3.40464600	-1.78614500
C	-0.71063100	-3.78750000	-2.26660200
H	-0.06663400	-2.94046500	-2.52366700
H	-0.06518900	-4.59480800	-1.90668300
H	-1.21168200	-4.12585700	-3.17715800
C	3.42128500	2.58020100	2.10540700
H	2.91574400	1.63985600	2.34984300
H	4.42805600	2.32663800	1.75828100
H	3.51175900	3.17279000	3.01974000
C	0.66134400	6.59180800	0.79064100
H	-0.41419500	6.56340100	0.58192600
H	0.79557400	6.83068800	1.84993600
H	1.08233200	7.41696600	0.20682500
C	1.74515300	3.10686500	-2.66382900
H	0.91892400	3.61149500	-3.17227000
H	2.66118400	3.31790900	-3.22690900
H	1.56235800	2.03075000	-2.69178100
C	-3.12936500	1.53374500	-1.57206600
C	-4.35789700	1.10143500	-0.83288100
C	-4.31285400	0.60990400	0.48634000
C	-5.50648000	0.24774100	1.11163600
C	-6.71991900	0.35939100	0.44019800
C	-6.76255600	0.82228300	-0.87356000
C	-5.57843600	1.18262900	-1.50453300
N	-3.08548600	0.60352900	1.19460700
N	-2.05329800	1.98788700	-0.77364100
O	-3.02795000	1.47869900	-2.77094400
H	-3.20487000	0.38707000	2.17906600
H	-2.30553300	0.01885800	0.84539000
H	-1.07501300	1.63370700	-1.05648700
H	-5.47709200	-0.13011300	2.13040200
H	-7.63614000	0.07325200	0.94706800
H	-7.70793400	0.89647900	-1.39953800
H	-5.57028100	1.54167800	-2.52897800

C	-2.25110600	2.36819900	0.48825300
H	-3.21441600	2.81918500	0.71733600
C	-1.10613300	2.76627400	1.30314800
C	-1.30210400	3.98304600	2.19780300
C	-1.19231200	2.63449700	2.80416600
H	-0.12940500	2.61910500	0.85315600
H	-2.27784300	4.45909900	2.17902200
H	-0.45881000	4.65776700	2.26704700
H	-0.26511900	2.34707000	3.28650700
H	-2.08636800	2.17900000	3.21604900

**TScat.14(Re)**

P	0.02687100	0.57137600	0.14646700
O	0.67119700	-0.05197400	1.35676600
O	-0.69433900	-0.29485700	-0.84066100
H	-0.77689500	5.69924700	-3.15157400
H	-1.08324700	6.53079500	-1.62757400
H	-3.46350700	4.73447000	-2.78997300
C	-0.77345600	5.57307400	-2.06487200
C	-2.95492100	4.12452300	-2.04905600
H	1.28791100	5.95139800	-1.33709700
C	0.59446900	5.12476700	-1.51870700
C	-1.67822900	4.44969300	-1.61327900
H	1.06575200	4.43266900	-2.22555400
C	-3.56974900	2.98769600	-1.53226100
H	-4.56896600	2.71714500	-1.86154300
H	-0.55688300	6.21497500	0.64226800
H	1.86894400	6.53783600	0.85087900
C	-1.04218500	3.67646200	-0.63825900
C	0.25414000	4.34188300	-0.21812100
C	0.03268600	5.34534600	0.94818200
C	1.45464600	5.69736900	1.42207600
C	-2.92135500	2.13823300	-0.62677200
C	-1.64587200	2.51368700	-0.17792000
C	1.46331200	3.58510100	0.30200200
C	2.21076900	4.41916700	1.13925600
H	-0.50815800	4.83006700	1.74985800
O	1.11693900	1.44293100	-0.70613500
H	1.49302900	5.97722900	2.47904100
C	1.91776100	2.30032500	0.02828800
C	-3.99665900	-0.06640900	-1.17774800
C	-3.60019800	0.87695000	-0.19927300
C	3.45603500	4.02118000	1.60254000
O	-0.96909100	1.73122900	0.73800900



C	4.11368400	0.15254600	-1.10286600
C	3.16672900	1.86342300	0.49272700
H	4.05137000	4.67470400	2.23367800
C	3.93225000	2.76299300	1.24487500
C	-4.76264500	-1.16586000	-0.78564100
H	5.17612900	-1.26906700	-2.31339400
C	-3.92326500	0.65317100	1.15441000
H	-5.08519700	-1.87331500	-1.54805000
C	4.87172000	-1.00655000	-1.30125000
C	3.74703600	0.51274000	0.20810200
H	4.91861000	2.44633200	1.56866100
C	-5.10186800	-1.40275300	0.54818500
C	-4.64912900	-0.49240500	1.49971500
C	5.27223700	-1.82334300	-0.24934200
C	4.07264300	-0.34648100	1.28487500
H	-4.91443200	-0.65338000	2.54370700
C	4.84153600	-1.48390100	1.03467900
H	5.11521500	-2.12346900	1.87188200
C	3.61206000	-0.08485300	2.71409300
H	2.88319800	0.72954300	2.68925100
C	6.14816700	-3.03886700	-0.48870600
H	6.28041700	-3.13742000	-1.57470300
C	3.73317900	0.97345700	-2.32495400
H	3.21283700	1.87441100	-1.99244000
C	-3.59641500	1.65013100	2.25772200
H	-3.06161100	2.49392100	1.81706900
C	-5.96667100	-2.58831200	0.93927900
H	-6.01517900	-2.60970900	2.03635000
C	-3.62845100	0.04908200	-2.65336000
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**TScat.14(Si)**

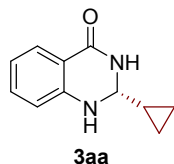
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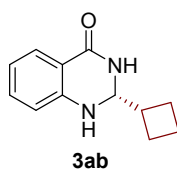
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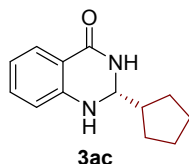
## 2. Compound characterization



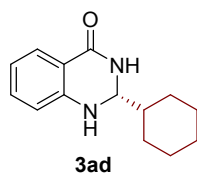
**(R)-2-cyclopropyl-2,3-dihydroquinazolin-4(1H)-one (3aa).** White solid, yield 90%; m.p. 205-206 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.88 (d, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.2 Hz, 1H), 6.85 (t, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 8.0 Hz, 1H), 6.16 (s, 1H), 4.01 (d, *J* = 8.8 Hz, 1H), 1.38 - 1.27 (m, 1H), 0.69 (d, *J* = 4.5 Hz, 2H), 0.38 (d, *J* = 4.5 Hz, 2H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.1, 147.4, 133.9, 128.6, 119.3, 115.7, 114.4, 71.2, 15.8, 2.3, 1.6. HRMS (m/z) calcd for C<sub>11</sub>H<sub>13</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 189.1028, found 189.1039; [α]<sub>D</sub><sup>25</sup> = - 265 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak AD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 70/30, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 4.9min, t<sub>R</sub> (major) = 6.3 min), 92% *ee*.



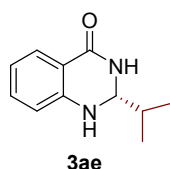
**(R)-2-cyclobutyl-2,3-dihydroquinazolin-4(1H)-one (3ab).** White solid, yield 98%; m.p. 149~151 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.87 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.36 - 7.25 (m, 1H), 6.94 - 6.76 (m, 1H), 6.65 (d, *J* = 8.1 Hz, 1H), 6.29 (s, 1H), 4.86 - 4.74 (m, 1H), 4.17 (s, 1H), 2.83 - 2.64 (m, 1H), 2.21 - 2.06 (m, 2H), 2.07 - 1.95 (m, 1H), 1.94 - 1.81 (m, 3H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.2, 147.3, 133.8, 128.5, 119.2, 115.8, 114.6, 69.3, 39.1, 23.2, 23.0, 17.9. HRMS (m/z) calcd for C<sub>12</sub>H<sub>15</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 203.1184, found 203.1184; [α]<sub>D</sub><sup>25</sup> = - 185 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 65/35, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 5.7 min, t<sub>R</sub> (major) = 6.3 min), 93% *ee*.



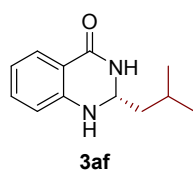
**(R)-2-cyclopentyl-2,3-dihydroquinazolin-4(1H)-one (3ac).** White solid, yield 98%; m.p. 181~182 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.87 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.30 (ddd, *J* = 8.1, 7.3, 1.6 Hz, 1H), 6.85 (td, *J* = 7.8, 0.6Hz, 1H), 6.67 (dd, *J* = 7.8, 0.6 Hz, 1H), 6.16 (s, 1H), 4.65 (d, *J* = 7.7 Hz, 1H), 2.39 - 2.21 (m, 1H), 1.97 - 1.82 (m, 2H), 1.76 - 1.58 (m, 4H), 1.42 - 1.29 (m, 2H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.3, 147.4, 133.9, 128.6, 119.3, 115.7, 114.6, 69.8, 44.6, 28.1, 27.8, 25.5 (2). HRMS (m/z) calcd for C<sub>13</sub>H<sub>17</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 217.1341, found 217.1321; [α]<sub>D</sub><sup>25</sup> = - 180 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 65/35, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 7.8 min, t<sub>R</sub> (major) = 9.3 min), 94% *ee*.



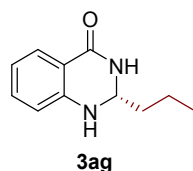
**(R)-2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-one (3ad).** White solid, **yield 98% (small-scale), yield 97% (Gram-scale)**; m.p. 180~182 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.86 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.30 (ddd, *J* = 8.1, 7.3, 1.6 Hz, 1H), 6.90 - 6.76 (m, 1H), 6.65 (dd, *J* = 8.1, 0.4 Hz, 1H), 6.24 (s, 1H), 4.66 (dd, *J* = 5.2, 1.1 Hz, 2H), 1.89 - 1.77 (m, 4H), 1.75 - 1.62 (m, 2H), 1.41 - 0.92 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.3, 147.4, 134.1, 128.5, 119.1, 115.3, 114.5, 69.6, 42.6, 27.6, 27.5, 26.1, 25.7, 25.6. HRMS (m/z) calcd for C<sub>14</sub>H<sub>19</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 231.14974, found 231.1493; [α]<sub>D</sub><sup>25</sup> = -126 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 60/40, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 7.1 min, t<sub>R</sub> (major) = 8.4 min), 96% *ee*.



**(R)-2-isopropyl-2,3-dihydroquinazolin-4(1H)-one (3ae).** White solid, **yield 98% (small-scale), yield 95% (Gram-scale)**; m.p. 172~174 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.87 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.31 (ddd, *J* = 8.1, 7.3, 1.6 Hz, 1H), 6.91 - 6.80 (m, 1H), 6.71 - 6.59 (m, 1H), 6.26 (s, 1H), 4.71 (d, *J* = 4.8 Hz, 1H), 2.05 - 1.91 (m, 1H), 1.06 (d, *J* = 6.6 Hz, 3H), 1.06 (d, *J* = 6.6 Hz, 3H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.4, 147.4, 134.2, 128.5, 119.2, 115.1, 114.5, 70.2, 32.8, 17.0, 16.8. HRMS (m/z) calcd for C<sub>11</sub>H<sub>15</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 191.1184, found 191.1189; [α]<sub>D</sub><sup>25</sup> = -197 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 75/25, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 7.6 min, t<sub>R</sub> (major) = 9.1 min), 91% *ee*.



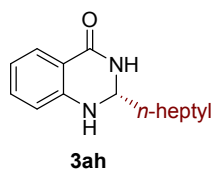
**(R)-2-isobutyl-2,3-dihydroquinazolin-4(1H)-one (3af).** White solid, **yield 99%**; m.p. 174~176 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.88 (d, *J* = 7.7 Hz, 1H), 7.34 - 7.27 (m, 1H), 6.86 (t, *J* = 7.5 Hz, 1H), 6.68 (d, *J* = 8.1 Hz, 1H), 6.38 (s, 1H), 4.93 (t, *J* = 6.3 Hz, 1H), 4.17 (s, 1H), 1.90 - 1.75 (m, 1H), 1.73 - 1.59 (m, 2H), 0.99 (d, *J* = 2.1 Hz, 3H), 0.97 (d, *J* = 2.1 Hz, 3H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.4, 147.4, 133.8, 128.6, 119.4, 116.2, 114.9, 63.6, 44.4, 23.9, 22.6, 22.5. HRMS (m/z) calcd for C<sub>12</sub>H<sub>17</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 205.1341, found 205.1342; [α]<sub>D</sub><sup>25</sup> = -202 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 70/30, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 9.6 min, t<sub>R</sub> (major) = 11.0 min), 94% *ee*.



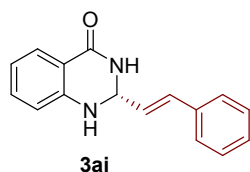
**(R)-2-propyl-2,3-dihydroquinazolin-4(1H)-one (3ag).** White solid, **yield 97% (small-scale), yield 95% (Gram-scale)**; m.p. 119~121 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.88 (d, *J* = 7.8 Hz, 1H), 7.30 (t, *J* = 7.7 Hz, 1H), 6.85 (t, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 8.1 Hz, 1H), 6.34 (s, 1H), 4.88 (t, *J* = 5.8 Hz, 1H), 4.22 (s, 1H), 1.78 (dd, *J* = 14.2, 7.1 Hz, 2H), 1.49 - 1.32 (m, 4H), 0.94 (t, *J* = 7.0 Hz, 3H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.4, 147.4, 133.8, 128.6, 119.4, 116.2, 114.9, 63.6, 44.4, 23.9, 22.6, 22.5.



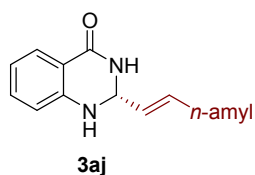
HRMS (m/z) calcd for C<sub>12</sub>H<sub>17</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 205.1341, found 205.1342; [ $\alpha$ ]<sub>D</sub><sup>25</sup> = - 195 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 65/35, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 7.6 min, t<sub>R</sub> (major) = 8.4 min), 91% *ee*.



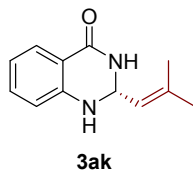
**(R)-2-heptyl-2,3-dihydroquinazolin-4(1H)-one (3ah).** White solid, yield 98%; m.p. 133~135 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): 7.88 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.31 (td, *J* = 8.2, 1.6 Hz, 1H), 6.90 - 6.82 (m, 1H), 6.68 (d, *J* = 8.0 Hz, 1H), 6.22 (s, 1H), 4.89 (t, *J* = 5.8 Hz, 1H), 1.78 (td, *J* = 7.9, 6.0 Hz, 2H), 1.51 - 1.39 (m, 2H), 1.40 - 1.20 (m, 8H), 0.89 (t, *J* = 7.0 Hz, 3H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>):  $\delta$  165.4, 147.4, 134.0, 128.6, 119.5, 115.7, 114.8, 65.4, 35.5, 31.7, 29.2, 29.1, 24.0, 22.6, 14.1. HRMS (m/z) calcd for C<sub>15</sub>H<sub>23</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 247.1810, found 247.1809; [ $\alpha$ ]<sub>D</sub><sup>25</sup> = - 165 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 50/50, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 8.6 min, t<sub>R</sub> (major) = 10.0 min), 92% *ee*.



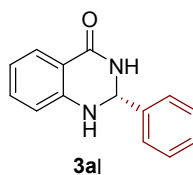
**(R,E)-2-styryl-2,3-dihydroquinazolin-4(1H)-one (3ai).** White solid, yield 98% (small-scale), yield 96% (Gram-scale); m.p. 155~156 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): 7.92 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.41 (d, *J* = 7.2 Hz, 2H), 7.36 - 7.30 (m, 4H), 6.88 (t, *J* = 7.5 Hz, 1H), 6.74 (d, *J* = 15.8 Hz, 1H), 6.68 (d, *J* = 8.0 Hz, 1H), 6.37 (dd, *J* = 15.8, 7.8 Hz, 1H), 6.07 (s, 1H), 5.48 (d, *J* = 7.8 Hz, 1H), 4.36 (s, 1H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>):  $\delta$  165.4, 146.9, 135.2, 135.0, 134.0, 128.9, 128.8 (2), 128.6, 127.0 (2), 126.0, 119.6, 115.5, 114.7, 67.9. HRMS (m/z) calcd for C<sub>16</sub>H<sub>15</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 251.1184, found 251.1186; [ $\alpha$ ]<sub>D</sub><sup>25</sup> = - 208 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 65/35, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 8.0 min, t<sub>R</sub> (major) = 8.6 min), 96% *ee*.



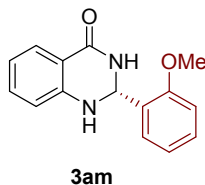
**(R,E)-2-(hept-1-en-1-yl)-2,3-dihydroquinazolin-4(1H)-one (3aj).** White solid, yield 95%; m.p. 116~118 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>):  $\delta$  7.88 (d, *J* = 7.8 Hz, 1H), 7.38 - 7.27 (m, 1H), 6.86 (t, *J* = 7.5 Hz, 1H), 6.65 (d, *J* = 8.1 Hz, 1H), 6.01 - 5.83 (m, 2H), 5.76 - 5.58 (m, 1H), 5.27 (d, *J* = 7.7 Hz, 1H), 4.21 (s, 1H), 2.08 (dd, *J* = 14.5, 7.1 Hz, 2H), 1.48 - 1.36 (m, 2H), 1.35 - 1.24 (m, 4H), 0.89 (t, *J* = 7.0 Hz, 3H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>):  $\delta$  164.9, 147.2, 138.2, 133.9, 128.6, 127.2, 119.4, 115.5, 114.6, 67.8, 31.9, 31.3, 28.3, 22.4, 14.0. HRMS (m/z) calcd for C<sub>15</sub>H<sub>21</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 245.1654, found 245.1651; [ $\alpha$ ]<sub>D</sub><sup>25</sup> = - 123 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 65/35, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 7.429 min, t<sub>R</sub> (major) = 8.985 min), 91% *ee*.



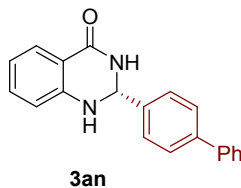
**(R)-2-(2-methylprop-1-en-1-yl)-2,3-dihydroquinazolin-4(1H)-one (3ak).** White solid, yield 95% (small-scale), yield 90% (Gram-scale); m.p. 146~148 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.89 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.42 - 7.27 (m, 1H), 6.86 (t, *J* = 7.5 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 1H), 5.76 (s, 1H), 5.59 (d, *J* = 8.4 Hz, 1H), 5.43 (dd, *J* = 8.3, 1.1 Hz, 1H), 4.16 (s, 1H), 1.80 (s, 3H), 1.75 (s, 3H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.3, 147.7, 140.9, 133.8, 128.6, 122.1, 119.4, 115.9, 114.7, 63.0, 25.8, 18.4. HRMS (m/z) calcd for C<sub>12</sub>H<sub>15</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 203.1184, found 203.1181; [α]<sub>D</sub><sup>25</sup> = - 256 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 70/30, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 7.9 min, t<sub>R</sub> (major) = 9.0 min), 87% *ee*.



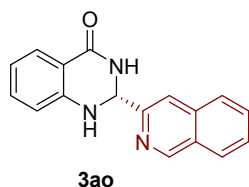
**(R)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3al).** White solid, yield 95%; m.p. 228~230 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.94 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.59 (dd, *J* = 6.6, 2.8 Hz, 2H), 7.46 - 7.44(m, 3H), 7.34 (td, *J* = 8.1, 1.4 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 8.0 Hz, 1H), 5.90 (s, 1H), 5.88 (s, 1H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 164.8, 147.2, 138.5, 134.0, 130.2, 129.1 (2), 128.7, 127.4 (2), 119.7, 115.6, 114.6, 69.1. HRMS (m/z) calcd for C<sub>14</sub>H<sub>13</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 225.1028, found 225.1021; [α]<sub>D</sub><sup>25</sup> = - 250 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 65/35, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 8.1 min, t<sub>R</sub> (major) = 8.9 min), 89% *ee*.



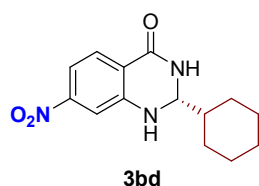
**(R)-2-(2-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3am).** White solid, yield 95%; m.p. 170~172 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.90 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.54 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.36 - 7.32 (m, 1H), 7.30 (ddd, *J* = 8.1, 7.3, 1.6 Hz, 1H), 6.98 (td, *J* = 7.5, 0.6 Hz, 1H), 6.93 (d, *J* = 8.3 Hz, 1H), 6.87 - 6.81 (m, 1H), 6.70 - 6.61 (m, 1H), 6.25 (d, *J* = 2.2 Hz, 1H), 6.15 (s, 1H), 3.89 (s, 3H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.0, 156.4, 147.1, 134.1, 130.3, 128.6, 127.7, 126.7, 121.0, 119.2, 114.6, 110.6, 62.5, 55.5. HRMS (m/z) calcd for C<sub>15</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>[M+H]<sup>+</sup> 255.1134, found 255.1126; [α]<sub>D</sub><sup>25</sup> = - 179 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 65/35, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 8.1 min, t<sub>R</sub> (major) = 8.9 min), 89% *ee*.



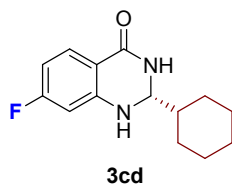
**(R)-2-([1,1'-biphenyl]-4-yl)-2,3-dihydroquinazolin-4(1H)-one (3an).** White solid, yield 90%; m.p. 178~180 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.96 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.66 (s, 4H), 7.60 (d, *J* = 7.9 Hz, 2H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.39 (dd, *J* = 10.9, 3.8 Hz, 1H), 7.35 (t, *J* = 7.7 Hz, 1H), 6.92 (s, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 5.96 (s, 2H), 3.91 (s, 1H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 164.8, 147.2, 143.2, 140.1, 137.3, 134.2, 134.1, 128.9, 128.7, 127.9, 127.8 (2), 127.2 (2), 119.7, 115.5, 114.6, 68.8. HRMS (m/z) calcd for C<sub>20</sub>H<sub>17</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 301.1341, found 301.1332; [α]<sub>D</sub><sup>25</sup> = -165 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 40/60, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 6.0 min, t<sub>R</sub> (major) = 8.4 min), 82% *ee*.



**(R)-2-(isoquinolin-3-yl)-2,3-dihydroquinazolin-4(1H)-one (3ao).** White solid, yield 87%; m.p. 155~156 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 8.35 - 8.25 (m, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.98 - 7.88 (m, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.84 - 7.73 (m, 2H), 7.62 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 7.33 (ddd, *J* = 8.1, 7.4, 1.6 Hz, 1H), 6.95 (s, 1H), 6.91 - 6.84 (m, 1H), 6.81 - 6.73 (m, 1H), 6.18 (d, *J* = 1.9 Hz, 1H), 5.36 (s, 1H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 164.5, 157.7, 146.4, 139.0, 134.2, 130.9, 128.6 (2), 128.0, 127.8 (2), 127.7, 119.9, 118.0, 116.1, 115.5, 68.0. HRMS (m/z) calcd for C<sub>17</sub>H<sub>14</sub>N<sub>3</sub>O[M+H]<sup>+</sup> 276.1137, found 276.1126; [α]<sub>D</sub><sup>25</sup> = -251 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 65/35, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 8.5 min, t<sub>R</sub> (major) = 9.0 min), 83% *ee*.

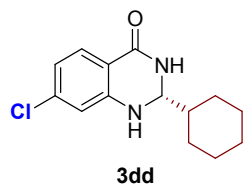


**(R)-2-cyclohexyl-7-nitro-2,3-dihydroquinazolin-4(1H)-one (3bd).** White solid, yield 70%; m.p. 226~227 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 8.01 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.51 (s, 1H), 6.36 (s, 1H), 4.74 (s, 1H), 1.93 - 1.63 (m, 6H), 1.22 - 1.04 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 163.1, 151.4, 147.6, 130.0, 119.7, 113.1, 109.3, 69.6, 43.1, 29.7, 27.4, 27.3, 26.0, 25.6. HRMS (m/z) calcd for C<sub>14</sub>H<sub>18</sub>N<sub>3</sub>O<sub>3</sub>[M+H]<sup>+</sup> 276.1348, found 276.1343; [α]<sub>D</sub><sup>25</sup> = -150 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 50/50, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 6.4 min, t<sub>R</sub> (major) = 7.0 min), 78% *ee*.

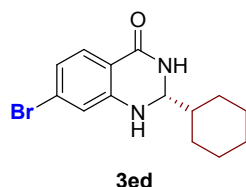


**(R)-2-cyclohexyl-7-fluoro-2,3-dihydroquinazolin-4(1H)-one (3cd).** White solid, yield 99%; m.p. 213~215 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.85 (dd, *J* = 8.6, 6.4 Hz, 1H), 6.50 (td, *J* = 8.6, 2.2 Hz, 1H), 6.39 (s, 1H), 6.33 (dd, *J* = 10.0, 2.3 Hz, 1H), 4.65 (d, *J* = 5.0 Hz, 1H), 4.41 (s, 1H), 1.89 - 1.57 (m, 6H), 1.32 - 1.01 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): 166.6 (d, *J* = 215.6 Hz), 164.5, 149.1 (d, *J* = 12.1 Hz), 131.1 (d, *J* = 11.3 Hz), 111.8, 106.5 (d, *J* = 22.7 Hz), 100.8 (d, *J* = 25.2 Hz), 69.6, 42.8, 27.4,

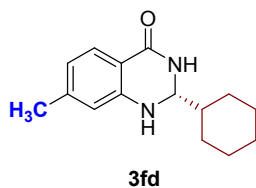
27.3, 26.1, 25.7, 25.6. HRMS (m/z) calcd for C<sub>14</sub>H<sub>18</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 249.1403, found 249.1409; [α]<sub>D</sub><sup>25</sup> = -108 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 60/40, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 8.4 min, t<sub>R</sub> (major) = 10.0 min), 92% *ee*.



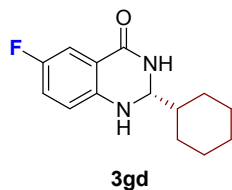
**(R)-7-chloro-2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-one (3dd).** White solid, yield 86%; m.p. 197~199 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.78 (d, *J* = 8.3 Hz, 1H), 6.77 (dd, *J* = 8.3, 1.8 Hz, 1H), 6.66 (d, *J* = 1.7 Hz, 1H), 6.40 (s, 1H), 4.64 (d, *J* = 5.0 Hz, 1H), 4.32 (s, 1H), 1.89 - 1.57 (m, 6H), 1.31 - 0.99 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 164.4, 148.1, 139.8, 129.9, 119.3, 114.1, 69.6, 42.9, 27.5, 27.4, 26.1, 25.7, 25.6. HRMS (m/z) calcd for C<sub>14</sub>H<sub>18</sub>ClN<sub>2</sub>O[M+H]<sup>+</sup> 265.1108, found 265.1116; [α]<sub>D</sub><sup>25</sup> = -100 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 50/50, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 6.7min, t<sub>R</sub> (major) = 8.1 min), 89% *ee*.



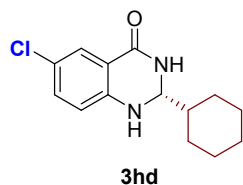
**(R)-7-bromo-2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-one (3ed).** White solid, yield 92%; m.p. 219~220 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.70 (d, *J* = 8.3 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 6.83 (s, 1H), 6.47 (s, 1H), 4.64 (d, *J* = 4.7 Hz, 1H), 4.37 (s, 1H), 1.86 - 1.57 (m, 6H), 1.28 - 1.04 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 164.5, 148.1, 130.0, 128.3, 122.1, 117.1, 69.6, 42.9, 27.4, 27.3, 26.1, 25.7, 25.6. HRMS (m/z) calcd for C<sub>14</sub>H<sub>18</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> 309.0603, found 309.0582; [α]<sub>D</sub><sup>25</sup> = -133 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 50/50, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 7.8 min, t<sub>R</sub> (major) = 9.4 min), 85% *ee*.



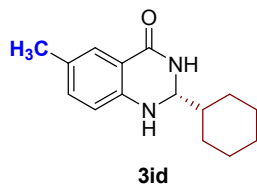
**(R)-2-cyclohexyl-7-methyl-2,3-dihydroquinazolin-4(1H)-one (3fd).** White solid, yield 99%; m.p. 190~192 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.75 (d, *J* = 7.9 Hz, 1H), 6.65 (dd, *J* = 7.9, 0.7 Hz, 1H), 6.46 (s, 1H), 6.13 (s, 1H), 4.68 - 4.54 (m, 1H), 4.19 (s, 1H), 2.29 (s, 3H), 1.89 - 1.59 (m, 6H), 1.33 - 1.03 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.4, 147.4, 144.8, 128.5, 120.4, 114.8, 113.2, 69.7, 42.6, 27.6, 27.5, 26.2, 25.8, 25.7, 21.8. HRMS (m/z) calcd for C<sub>15</sub>H<sub>21</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 245.1654, found 245.1666; [α]<sub>D</sub><sup>25</sup> = -90 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 50/50, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 5.3 min, t<sub>R</sub> (major) = 6.9 min), 82% *ee*.



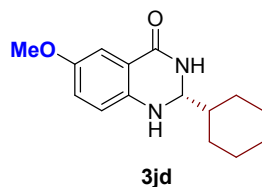
**(R)-2-cyclohexyl-6-fluoro-2,3-dihydroquinazolin-4(1H)-one (3gd).** White solid, yield 91%; m.p. 174~176 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.55 (dd, *J* = 8.7, 3.0 Hz, 1H), 7.02 (td, *J* = 8.5, 3.0 Hz, 1H), 6.74 (s, 1H), 6.63 (dd, *J* = 8.8, 4.2 Hz, 1H), 4.60 (d, *J* = 5.0 Hz, 1H), 4.19 (s, 1H), 1.87 - 1.58 (m, 6H), 1.32 - 1.04 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 164.5, 156.3 (d, *J* = 237.8 Hz), 143.7 (d, *J* = 1.4 Hz), 121.1 (d, *J* = 23.7 Hz), 116.9 (d, *J* = 7.0 Hz), 116.1 (d, *J* = 7.1 Hz), 114.1 (d, *J* = 23.6 Hz). 69.7, 42.4, 27.6, 27.5, 26.1, 25.7, 25.6. HRMS (m/z) calcd for C<sub>14</sub>H<sub>18</sub>FN<sub>2</sub>O[M+H]<sup>+</sup> 249.1403, found 249.1401; [α]<sub>D</sub><sup>25</sup> = - 138 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak AS-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 60/40, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 10.5 min, t<sub>R</sub> (major) = 13.2 min), 94% *ee*.



**(R)-6-chloro-2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-one (3hd).** White solid, yield 99%; m.p. 198~200 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.83 (s, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 6.60 (d, *J* = 8.4 Hz, 1H), 6.40 (s, 1H), 4.63 (d, *J* = 3.0 Hz, 1H), 4.28 (s, 1H), 1.84 - 1.64 (m, 6H), 1.27 - 1.07 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 164.1, 145.8, 133.7, 128.0, 124.0, 116.7, 115.9, 69.5, 42.7, 27.5, 27.4, 26.1, 24.7, 25.7. HRMS (m/z) calcd for C<sub>14</sub>H<sub>18</sub>ClN<sub>2</sub>O[M+H]<sup>+</sup> 265.1108, found 265.1109; [α]<sub>D</sub><sup>25</sup> = - 150 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 50/50, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 6.6 min, t<sub>R</sub> (major) = 7.6 min), 97% *ee*.

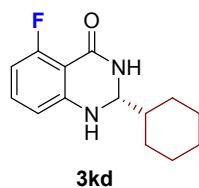


**(R)-2-cyclohexyl-6-methyl-2,3-dihydroquinazolin-4(1H)-one (3id).** White solid, yield 99%; m.p. 194~195 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.68 (d, *J* = 1.1 Hz, 1H), 7.11 (dd, *J* = 8.1, 1.7 Hz, 1H), 6.58 (d, *J* = 8.1 Hz, 1H), 6.32 (s, 1H), 4.59 (dd, *J* = 5.3, 1.4 Hz, 1H), 4.14 (s, 1H), 2.26 (s, 3H), 1.91 - 1.58 (m, 6H), 1.34 - 1.03 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.5, 145.2, 134.8, 128.5, 128.3, 115.6, 114.7, 69.7, 42.4, 27.6, 27.5, 26.2, 25.7, 25.6, 20.4. HRMS (m/z) calcd for C<sub>15</sub>H<sub>21</sub>N<sub>2</sub>O[M+H]<sup>+</sup> 245.1654, found 245.1660; [α]<sub>D</sub><sup>25</sup> = - 142 (c = 0.20, CHCl<sub>3</sub>); The *ee* was determined by HPLC analysis (Chiralpak OD-RH, CH<sub>3</sub>CN/H<sub>2</sub>O = 50/50, v/v, 1.0mL/min, 254nm, t<sub>R</sub> (minor) = 11.4 min, t<sub>R</sub> (major) = 13.1 min), 92% *ee*.

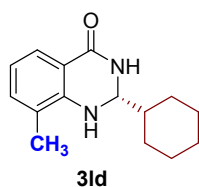


**(R)-2-cyclohexyl-6-methoxy-2,3-dihydroquinazolin-4(1H)-one (3jd).** White solid, yield 96%; m.p. 159~161 °C; <sup>1</sup>H NMR(600 MHz, CDCl<sub>3</sub>): δ 7.39 (d, *J* = 3.0 Hz, 1H), 6.94 (dd, *J* = 8.7, 3.0 Hz, 1H), 6.64 (d, *J* = 8.7 Hz, 1H), 6.35 (s, 1H), 4.57 (d, *J* = 5.0 Hz, 1H), 4.04 (s, 1H), 3.78 (s, 3H), 1.88 - 1.59 (m, 6H), 1.34 - 1.05 (m, 5H). <sup>13</sup>C NMR(150 MHz, CDCl<sub>3</sub>): δ 165.3, 153.2, 141.6, 122.5, 116.7, 116.6, 110.3, 69.9, 55.8, 42.2, 27.7, 27.6, 26.2, 25.8, 25.7. HRMS (m/z) calcd for C<sub>15</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub>[M+H]<sup>+</sup>

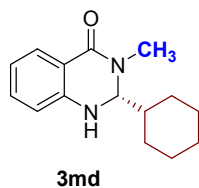
261.1603, found 261.1599;  $[\alpha]_D^{25} = -160$  ( $c = 0.20$ ,  $\text{CHCl}_3$ ); The *ee* was determined by HPLC analysis (Chiralpak OD-RH,  $\text{CH}_3\text{CN}/\text{H}_2\text{O} = 50/50$ , v/v, 1.0mL/min, 254nm,  $t_R$  (minor) = 7.5 min,  $t_R$  (major) = 8.7 min), 94% *ee*.



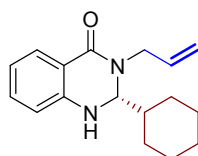
**(R)-2-cyclohexyl-5-fluoro-2,3-dihydroquinazolin-4(1H)-one (3kd).** White solid, yield 90%; m.p. 169~171 °C;  $^1\text{H}$  NMR(600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.20 (td,  $J = 8.2, 5.6$  Hz, 1H), 6.50 - 6.46 (m, 1H), 6.45 (d,  $J = 8.2$  Hz, 1H), 6.38 (d,  $J = 15.4$  Hz, 1H), 4.56 (dd,  $J = 5.3, 1.6$  Hz, 1H), 4.42 (s, 1H), 1.85-1.76 (m, 4H), 1.74 - 1.62 (m, 2H), 1.31 - 1.20 (m, 2H), 1.20 - 1.02 (m, 3H).  $^{13}\text{C}$  NMR(150 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.0, 162.4 (d,  $J = 41.4$  Hz), 149.5 (d,  $J = 3.8$  Hz), 134.3 (d,  $J = 11.6$  Hz), 110.3 (d,  $J = 3.6$  Hz), 106.7 (d,  $J = 21.8$  Hz), 104.8 (d,  $J = 9.5$  Hz), 69.1, 42.2, 27.6, 27.4, 26.1, 25.7, 25.6. HRMS ( $m/z$ ) calcd for  $\text{C}_{14}\text{H}_{18}\text{FN}_2\text{O}[\text{M}+\text{H}]^+$  249.1403, found 249.1398;  $[\alpha]_D^{25} = -135$  ( $c = 0.20$ ,  $\text{CHCl}_3$ ); The *ee* was determined by HPLC analysis (Chiralpak OD-RH,  $\text{CH}_3\text{CN}/\text{H}_2\text{O} = 60/40$ , v/v, 1.0mL/min, 254nm,  $t_R$  (minor) = 5.7 min,  $t_R$  (major) = 6.9 min), 96% *ee*.



**(R)-2-cyclohexyl-8-methyl-2,3-dihydroquinazolin-4(1H)-one (3ld).** White solid, yield 95%; m.p. 119~122 °C;  $^1\text{H}$  NMR(600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.77 (d,  $J = 7.7$  Hz, 1H), 7.18 (d,  $J = 7.3$  Hz, 1H), 6.76 (t,  $J = 7.6$  Hz, 1H), 6.50 (s, 1H), 4.63 (dd,  $J = 5.5, 1.4$  Hz, 1H), 4.12 (s, 1H), 2.16 (s, 3H), 1.93 - 1.63 (m, 6H), 1.34 - 1.04 (m, 5H).  $^{13}\text{C}$  NMR(150 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.6, 145.5, 134.7, 126.3, 121.8, 118.4, 115.2, 69.4, 42.6, 27.8, 27.5, 26.2, 25.7, 25.6, 16.6. HRMS ( $m/z$ ) calcd for  $\text{C}_{15}\text{H}_{21}\text{N}_2\text{O}[\text{M}+\text{H}]^+$  245.1654, found 245.1658;  $[\alpha]_D^{25} = -80$  ( $c = 0.20$ ,  $\text{CHCl}_3$ ); The *ee* was determined by HPLC analysis (Chiralpak OD-RH,  $\text{CH}_3\text{CN}/\text{H}_2\text{O} = 60/40$ , v/v, 1.0mL/min, 254nm,  $t_R$  (minor) = 10.1 min,  $t_R$  (major) = 11.6 min), 41% *ee*.

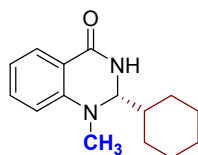


**(R)-2-cyclohexyl-3-methyl-2,3-dihydroquinazolin-4(1H)-one (3md).** White solid, yield 99%; m.p. 168~170 °C;  $^1\text{H}$  NMR(600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.86 (d,  $J = 7.6$  Hz, 1H), 7.24 (dd,  $J = 13.9, 6.0$  Hz, 1H), 6.79 (t,  $J = 7.5$  Hz, 1H), 6.59 (d,  $J = 8.0$  Hz, 1H), 4.36 (d,  $J = 6.1$  Hz, 1H), 3.14 (s, 3H), 1.91 - 1.57 (m, 6H), 1.28 - 0.88 (m, 5H).  $^{13}\text{C}$  NMR(150 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.9, 145.7, 133.1, 128.3, 118.5, 116.7, 113.9, 76.1, 42.9, 35.0, 29.0, 27.8, 26.0, 25.9, 25.6. HRMS ( $m/z$ ) calcd for  $\text{C}_{15}\text{H}_{21}\text{N}_2\text{O}[\text{M}+\text{H}]^+$  245.1654, found 265.1666;  $[\alpha]_D^{25} = -120$  ( $c = 0.20$ ,  $\text{CHCl}_3$ ); The *ee* was determined by HPLC analysis (Chiralpak OD-RH,  $\text{CH}_3\text{CN}/\text{H}_2\text{O} = 50/50$ , v/v, 1.0mL/min, 254nm,  $t_R$  (minor) = 5.2 min,  $t_R$  (major) = 7.5 min), 74% *ee*.



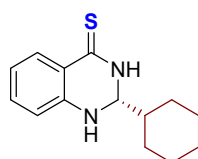
**3nd**

**(R)-3-allyl-2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-one (3nd).** White solid, yield 70%;  $^1\text{H}$  NMR(600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.88 (dd,  $J = 7.8, 1.4$  Hz, 1H), 7.29 - 7.15 (m, 1H), 6.89 - 6.75 (m, 1H), 6.60 (d,  $J = 8.0$  Hz, 1H), 5.92 - 5.77 (m, 1H), 5.34 - 5.22 (m, 1H), 5.19 (dd,  $J = 10.2, 1.3$  Hz, 1H), 5.05 - 4.90 (m, 1H), 4.34 (d,  $J = 6.7$  Hz, 1H), 3.46 - 3.36 (m, 1H), 3.50 - 3.32 (m, 1H), 1.91 - 1.55 (m, 6H), 1.28 - 0.82 (m, 5H).  $^{13}\text{C}$  NMR(150 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.5, 145.8, 133.2, 133.1, 128.6, 118.6, 117.0, 116.9, 114.1, 72.7, 48.6, 42.8, 29.1, 28.2, 26.0, 25.9, 25.6. HRMS ( $m/z$ ) calcd for  $\text{C}_{17}\text{H}_{23}\text{N}_2\text{O}[\text{M}+\text{H}]^+$  271.18104, found 271.1816;  $[\alpha]_{\text{D}}^{25} = -90$  ( $c = 0.20$ ,  $\text{CHCl}_3$ ); The *ee* was determined by HPLC analysis (Chiralpak OD-RH,  $\text{CH}_3\text{CN}/\text{H}_2\text{O} = 50/50$ , v/v, 1.0mL/min, 254nm,  $t_{\text{R}}$  (minor) = 6.3 min,  $t_{\text{R}}$  (major) = 8.2 min), 72% *ee*.



**3od**

**(R)-2-cyclohexyl-1-methyl-2,3-dihydroquinazolin-4(1H)-one (3od).** White solid, yield 70%; m.p. 147~148 °C;  $^1\text{H}$  NMR(600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.87 (d,  $J = 7.7$  Hz, 1H), 7.36 (dd,  $J = 8.1, 7.4$  Hz, 1H), 7.14 (s, 1H), 6.76 (t,  $J = 7.5$  Hz, 1H), 6.57 (d,  $J = 8.3$  Hz, 1H), 4.40 (t,  $J = 4.8$  Hz, 1H), 3.02 (s, 3H), 1.80-1.57 (m, 6H), 1.18 - 0.93 (m, 5H). 4.66 (dd,  $J = 5.2, 1.1$  Hz, 2H), 1.89 - 1.77 (m, 4H), 1.75 - 1.62 (m, 2H), 1.41 - 0.92 (m, 5H).  $^{13}\text{C}$  NMR(150 MHz,  $\text{CDCl}_3$ ):  $\delta$  163.4, 146.6, 133.2, 127.3, 116.1, 116.0, 110.6, 75.3, 42.8, 36.8, 27.3, 26.0, 25.0, 24.8, 24.6. HRMS ( $m/z$ ) calcd for  $\text{C}_{14}\text{H}_{21}\text{N}_2\text{O}[\text{M}+\text{H}]^+$  245.1654, found 245.1667;  $[\alpha]_{\text{D}}^{25} = -140$  ( $c = 0.20$ ,  $\text{CHCl}_3$ ); The *ee* was determined by HPLC analysis (Chiralpak OD-RH,  $\text{CH}_3\text{CN}/\text{H}_2\text{O} = 40/60$ , v/v, 1.0mL/min, 254nm,  $t_{\text{R}}$  (minor) = 6.6 min,  $t_{\text{R}}$  (major) = 10.3 min), 58% *ee*.



**3pd**

**(R)-2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-thione (3pd).** Yellow solid, yield 99% (small-scale), yield 90% (Gram-scale); m.p. 198~200 °C;  $^1\text{H}$  NMR(600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.29 (dd,  $J = 8.0, 0.9$  Hz, 1H), 8.13 (s, 1H), 7.33 - 7.27 (m, 1H), 6.82 (t,  $J = 7.6$  Hz, 1H), 6.62 (d,  $J = 8.1$  Hz, 1H), 4.53 (dd,  $J = 5.4, 2.1$  Hz, 1H), 4.41 (s, 1H), 1.87 - 1.70 (m, 6H), 1.27 - 1.10 (m, 5H).  $^{13}\text{C}$  NMR(150 MHz,  $\text{CDCl}_3$ ):  $\delta$  191.8, 143.2, 134.5, 132.6, 120.7, 119.5, 114.9, 69.7, 41.7, 27.7, 27.5, 26.0, 25.7, 25.6. HRMS ( $m/z$ ) calcd for  $\text{C}_{14}\text{H}_{19}\text{N}_2\text{S}[\text{M}+\text{H}]^+$  247.1269, found 247.1255;  $[\alpha]_{\text{D}}^{25} = -267$  ( $c = 0.20$ ,  $\text{CHCl}_3$ ); The *ee* was determined by HPLC analysis (Chiralpak OD-RH,  $\text{CH}_3\text{CN}/\text{H}_2\text{O} = 60/40$ , v/v, 1.0mL/min, 254nm,  $t_{\text{R}}$  (minor) = 7.7 min,  $t_{\text{R}}$  (major) = 9.3 min), 96% *ee*.

### 3. NMR and HRM spectrum of 2,3-Dihydroquinazolinones **3**



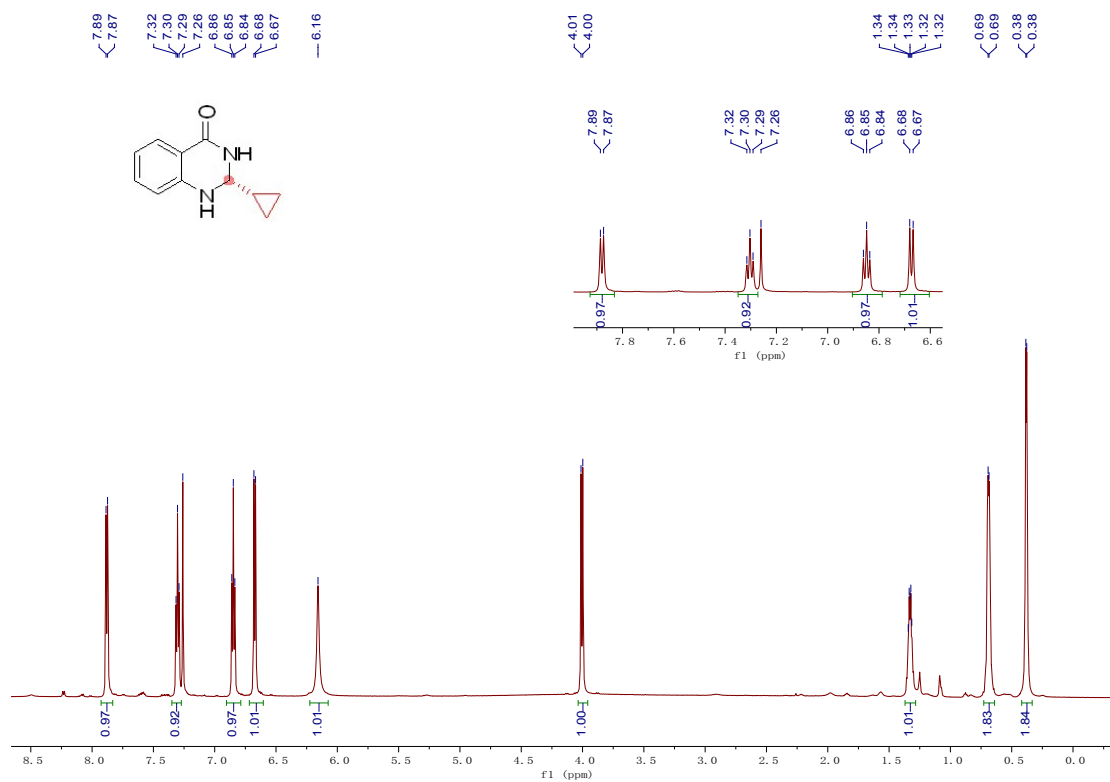


Fig.S 1 <sup>1</sup>H NMR of compound **3aa**

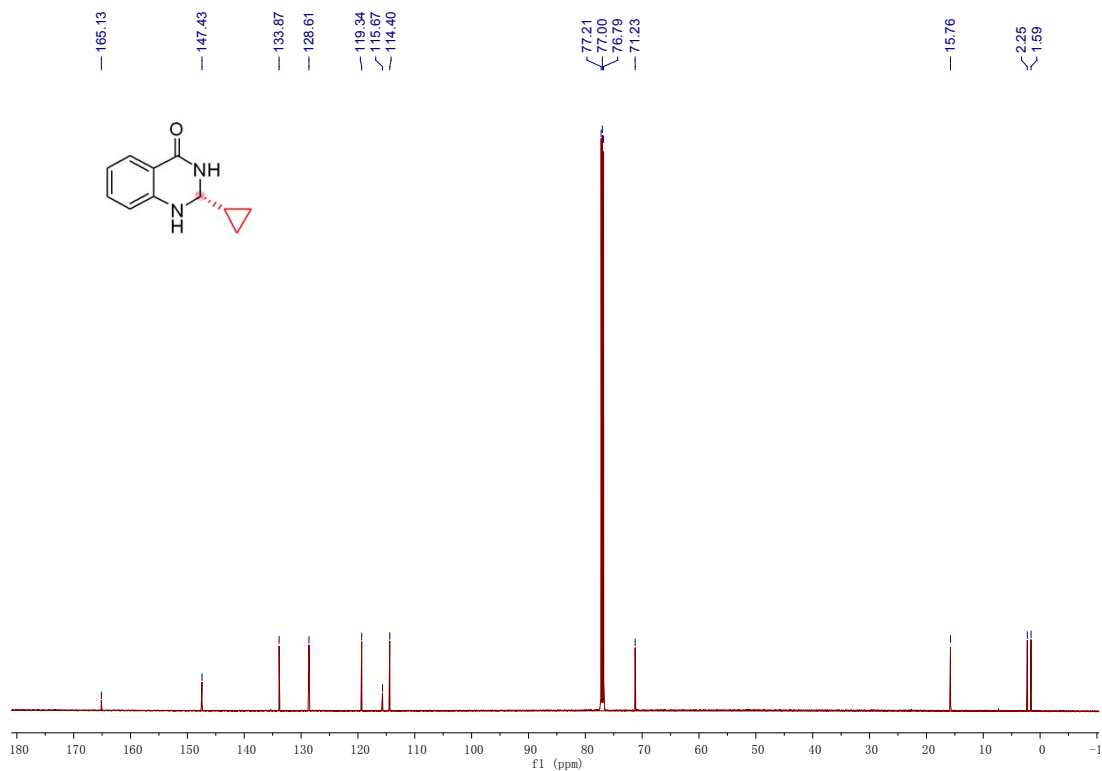


Fig.S 2 <sup>13</sup>C NMR of compound **3aa**

Sample Name 1-3aa-MS Position P1-A2 Instrument Name Instrument 1 User Name  
 Inj Vol 1 InjPosition SampleType Sample IRM Calibration Status All Ions Missed  
 Data Filename 1-3aa-MS.d ACQ Method LCC-FULLSCAN-L2A.m Comment Acquired Time 8/5/2020 2:59:07 AM

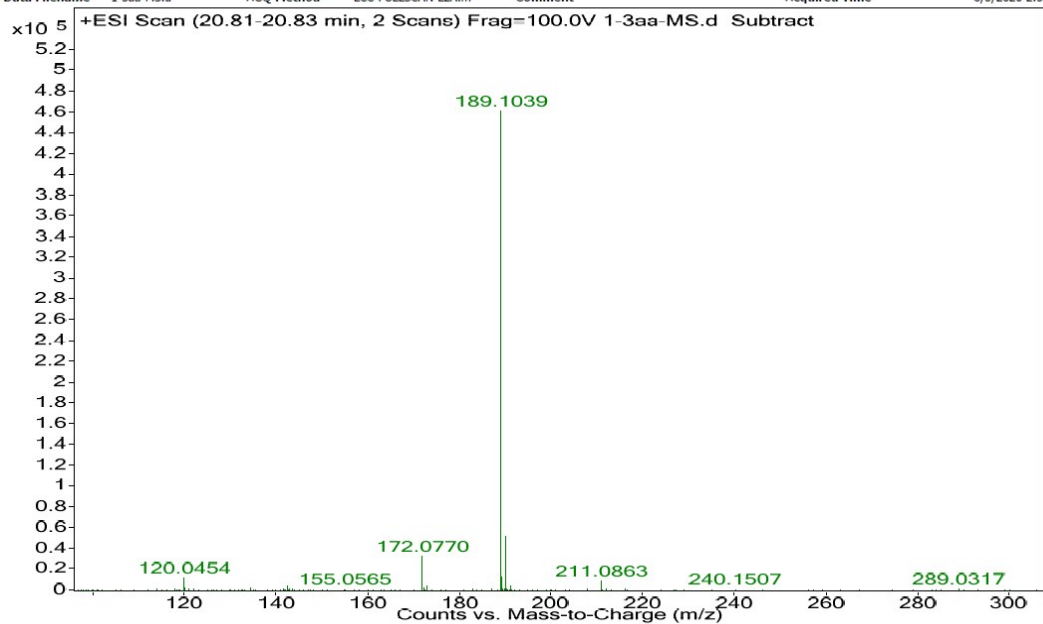


Fig.S 3 HR-MS of compound **3aa**

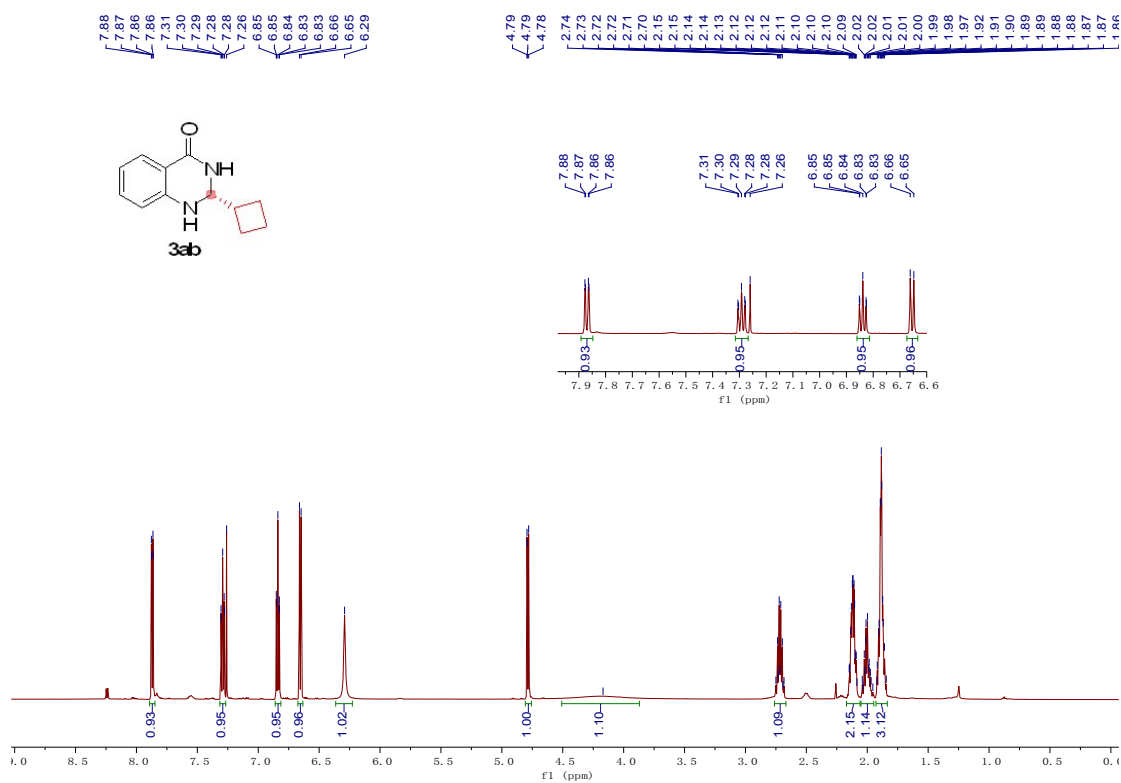


Fig.S 4 <sup>1</sup>H NMR of compound **3ab**

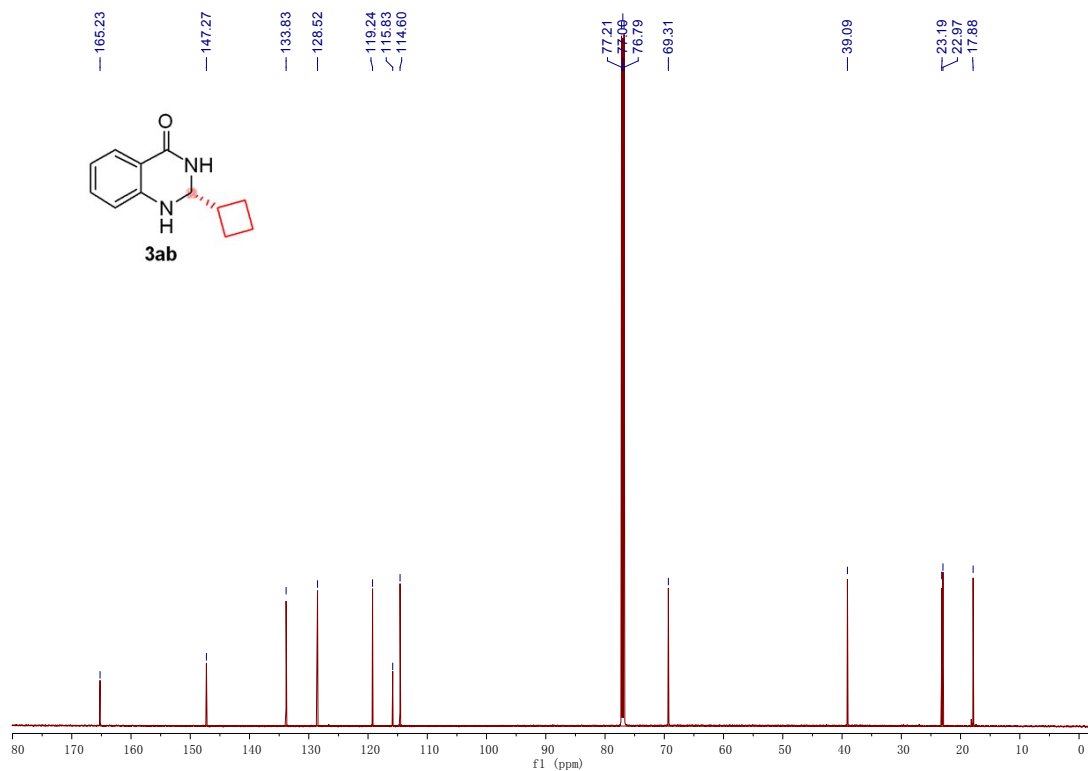


Fig.S 5 <sup>13</sup>C NMR of compound **3ab**

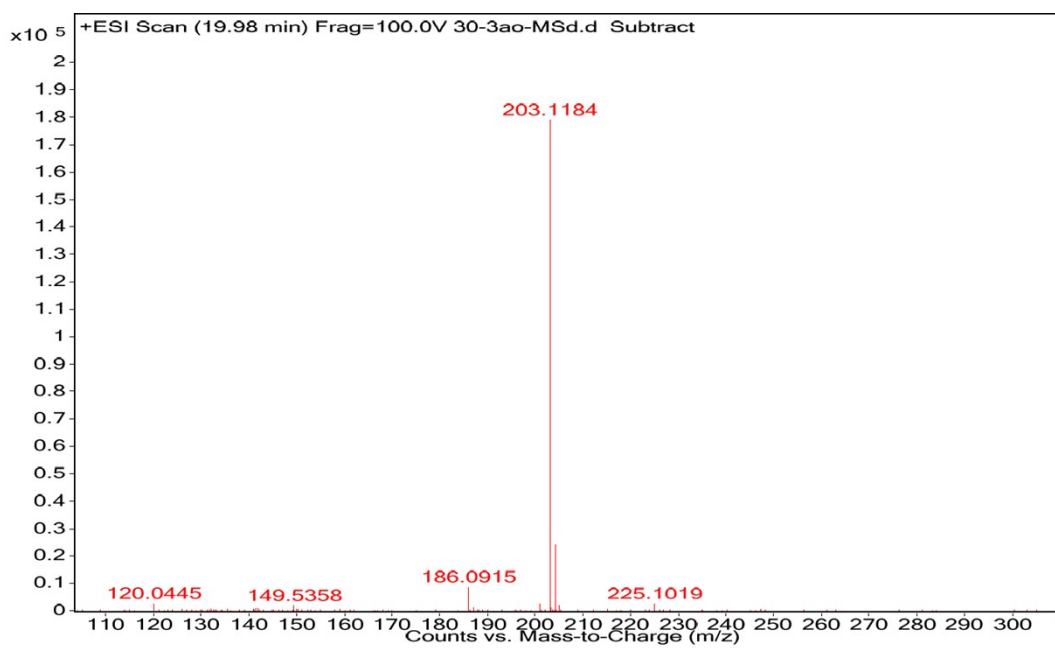


Fig.S 6 HR-MS of compound **3ab**

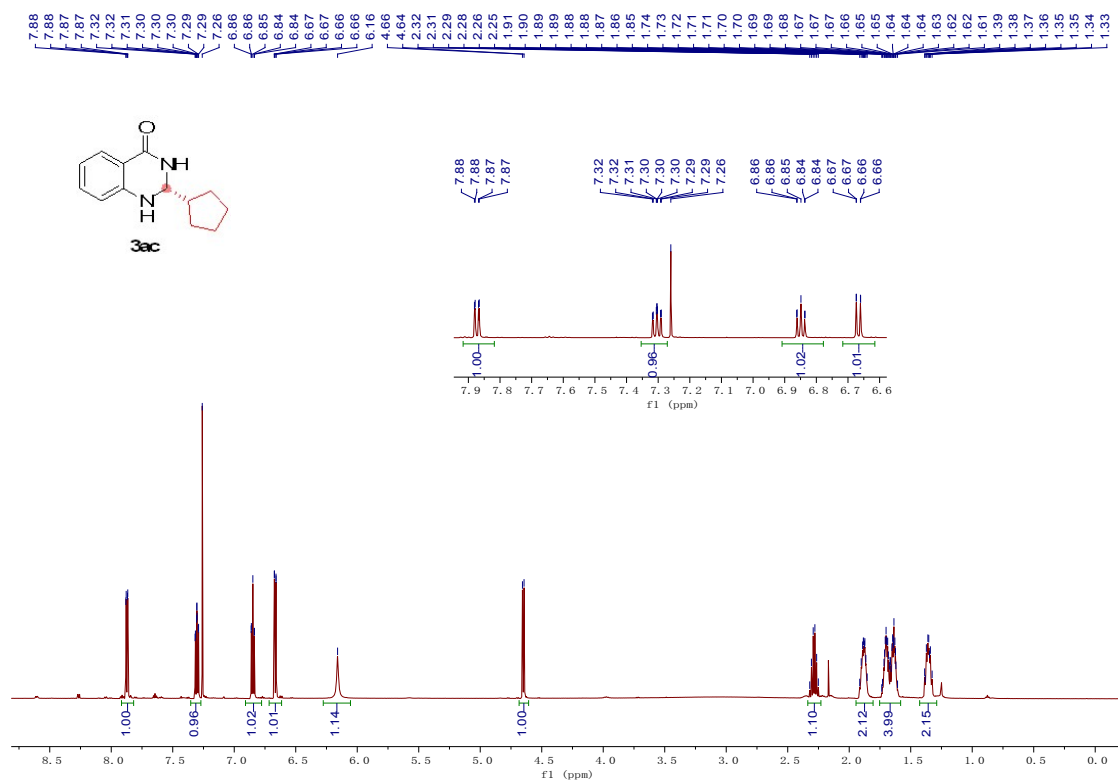


Fig.S 7 <sup>1</sup>H NMR of compound **3ac**

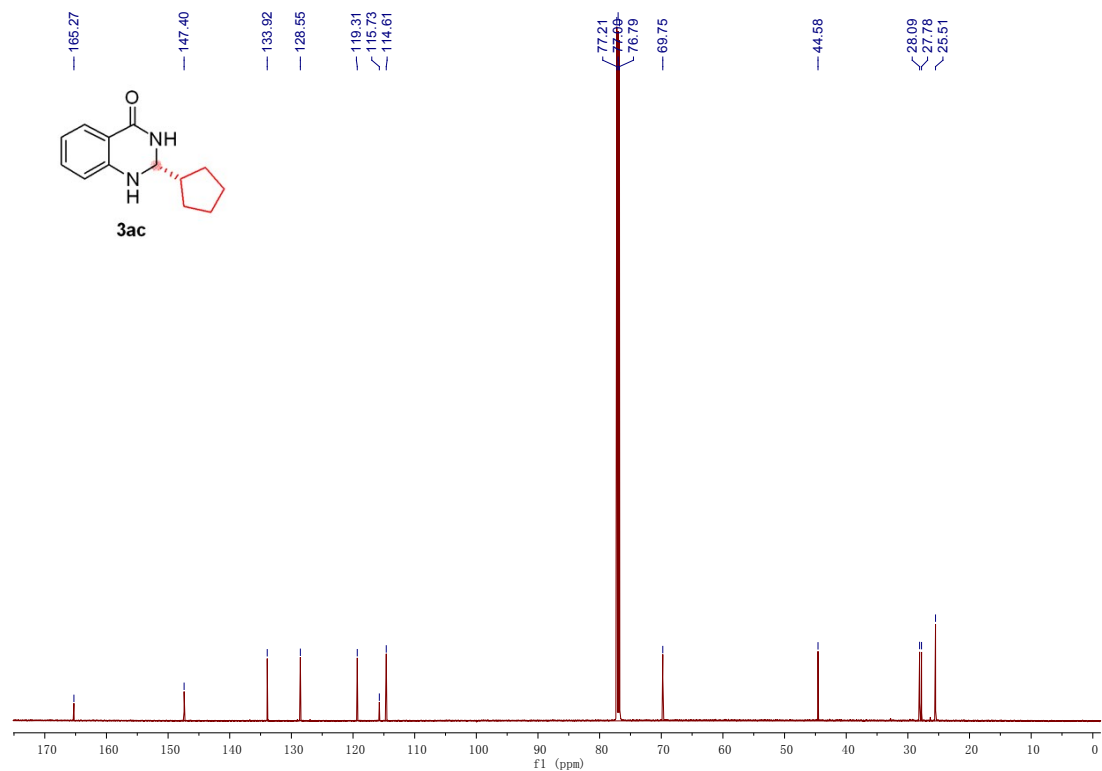


Fig.S 8 <sup>13</sup>C NMR of compound **3ac**

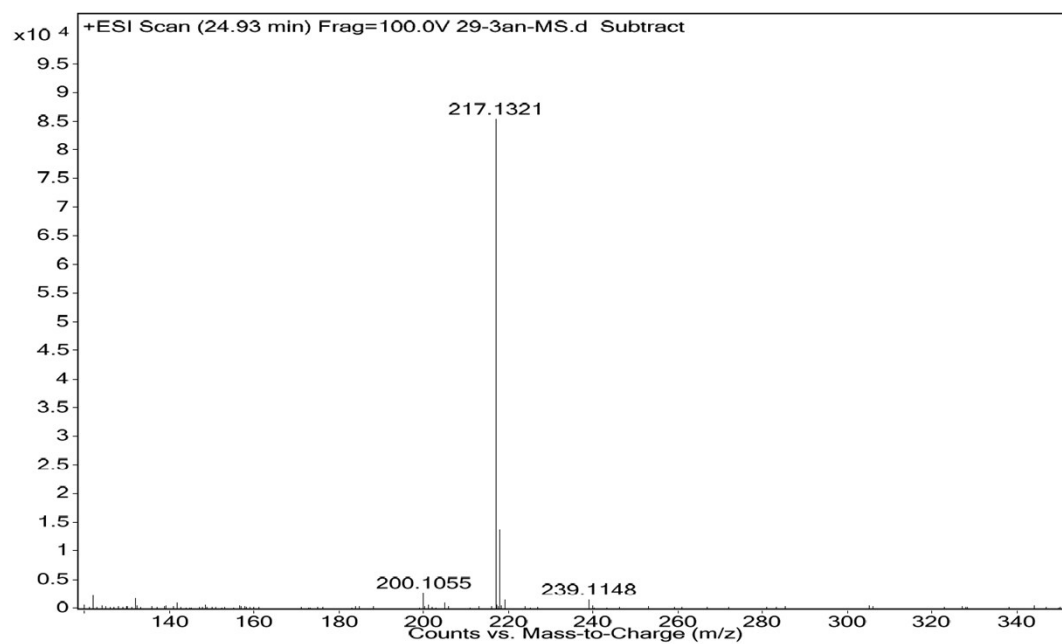


Fig.S 9 HR-MS of compound **3ac**

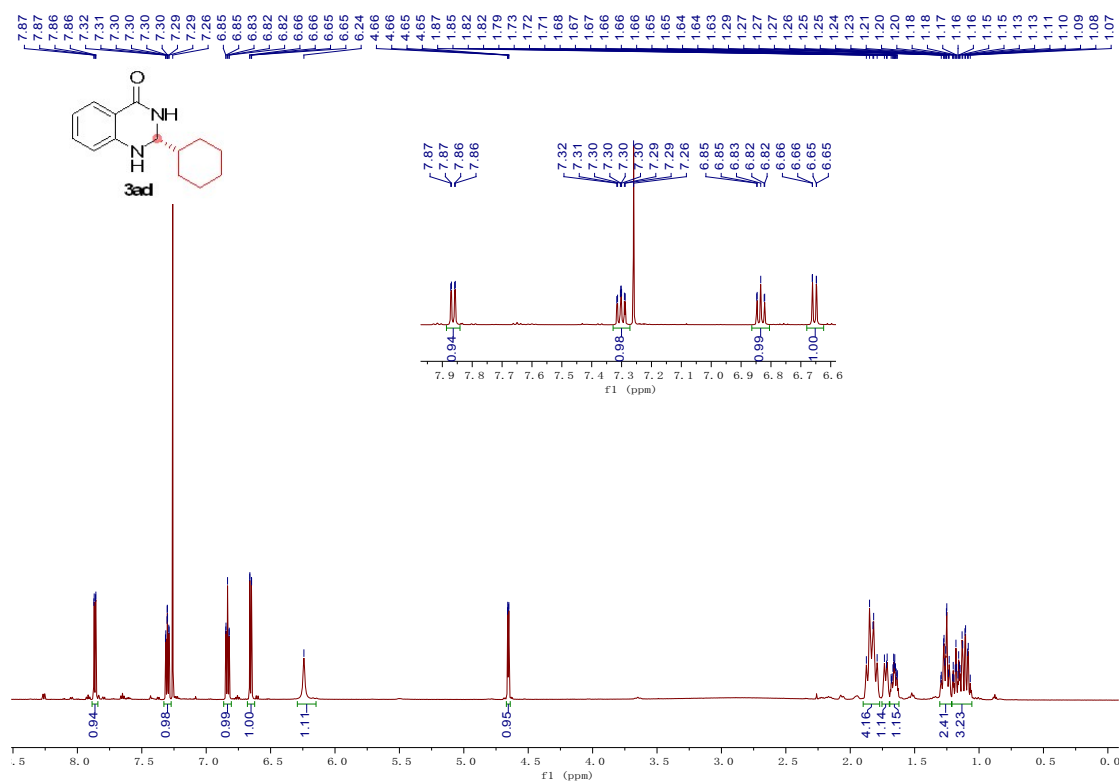


Fig.S 10 <sup>1</sup>H NMR of compound **3ad** (Gram-scale)

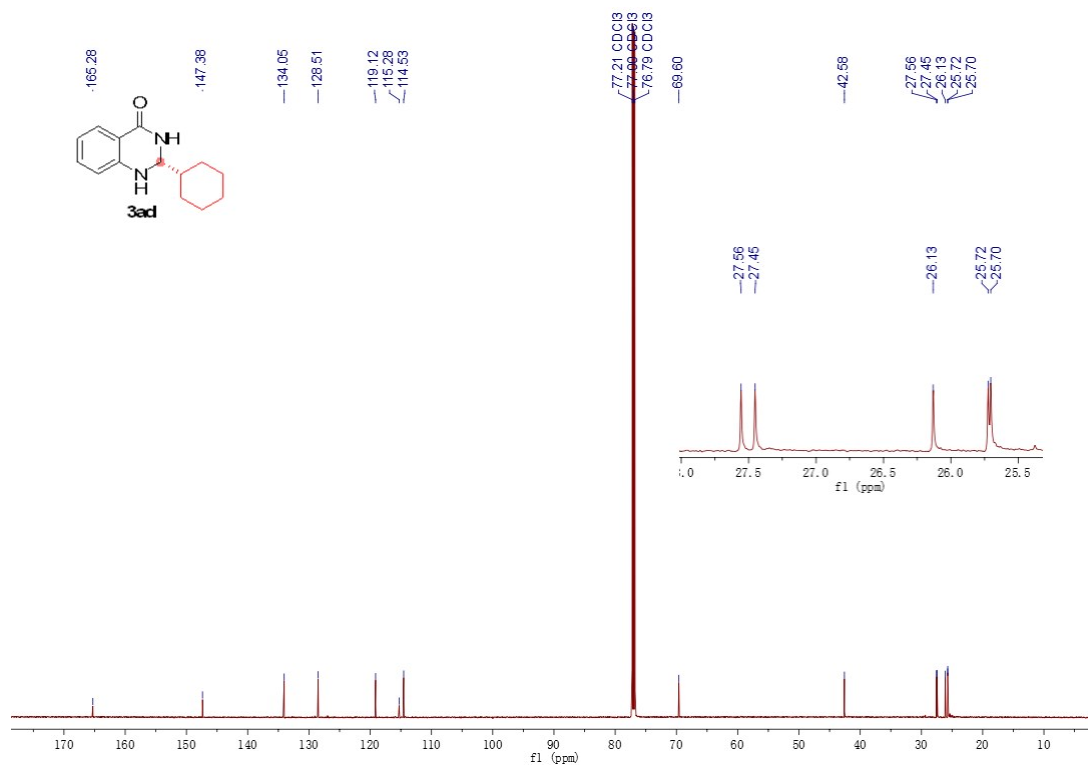


Fig.S 11 <sup>13</sup>C NMR of compound **3ad** (Gram-scale)

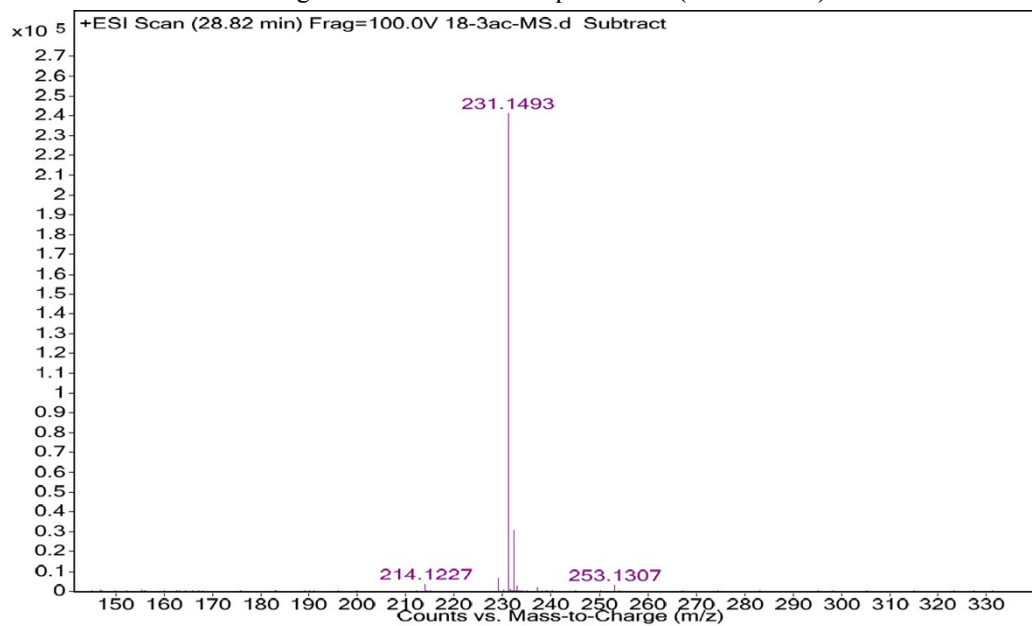


Fig.S 12 HR-MS of compound **3ad** (Gram-scale)

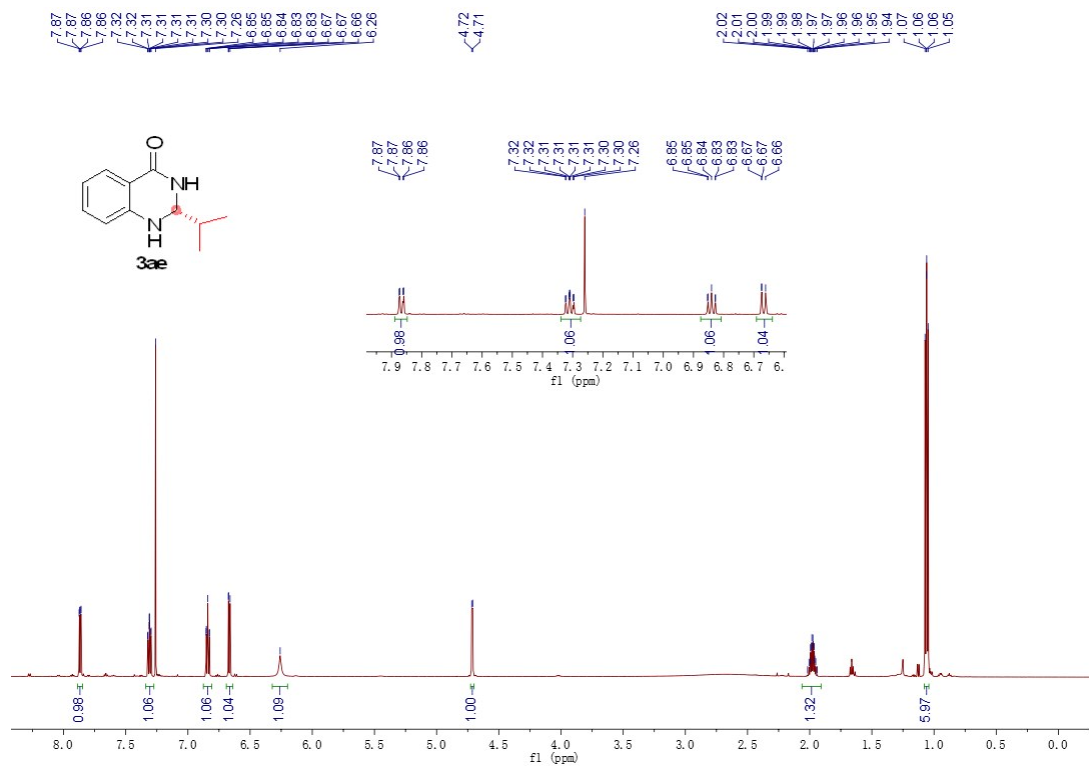


Fig.S 13 <sup>1</sup>H NMR of compound 3ae (Gram-scale)

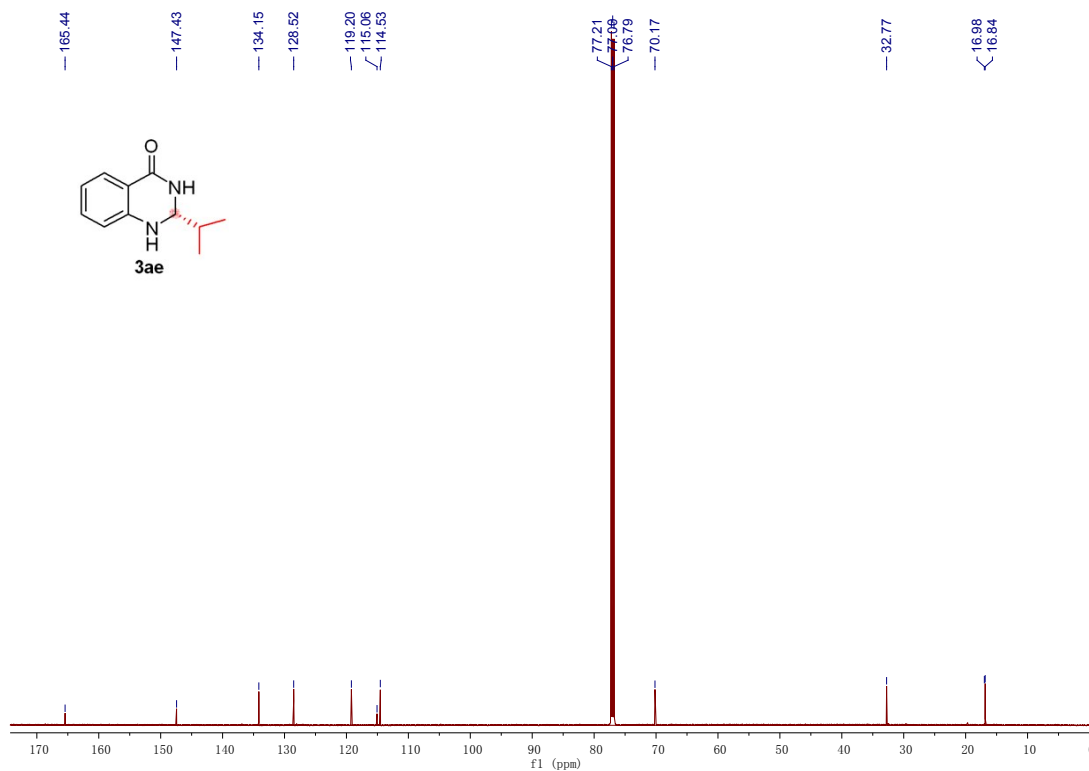


Fig.S 14 <sup>13</sup>C NMR of compound 3ae (Gram-scale)

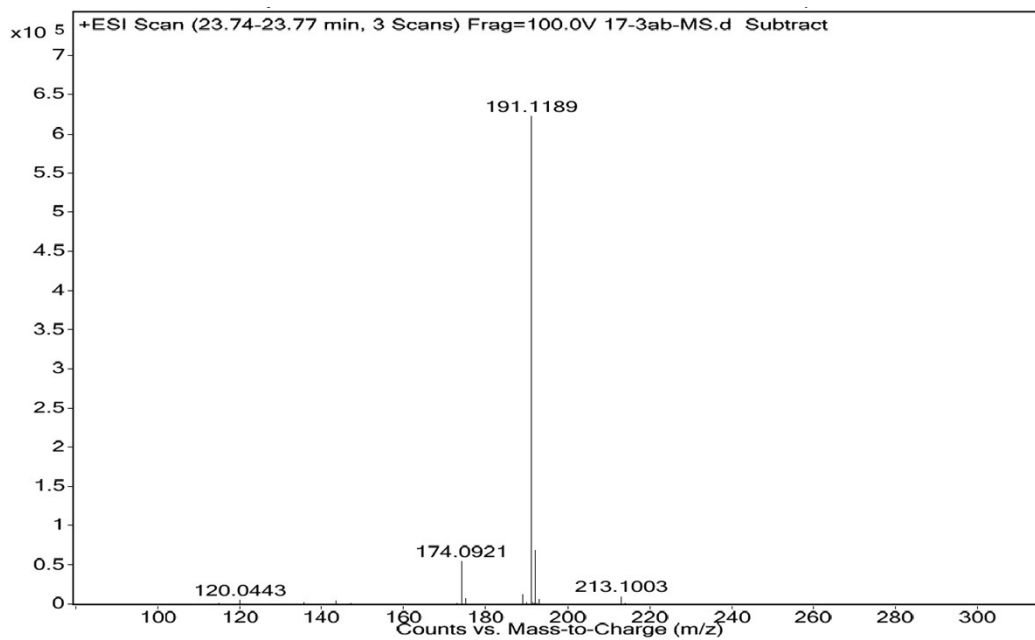


Fig.S 15 HR-MS of compound **3ae** (Gram-scale)

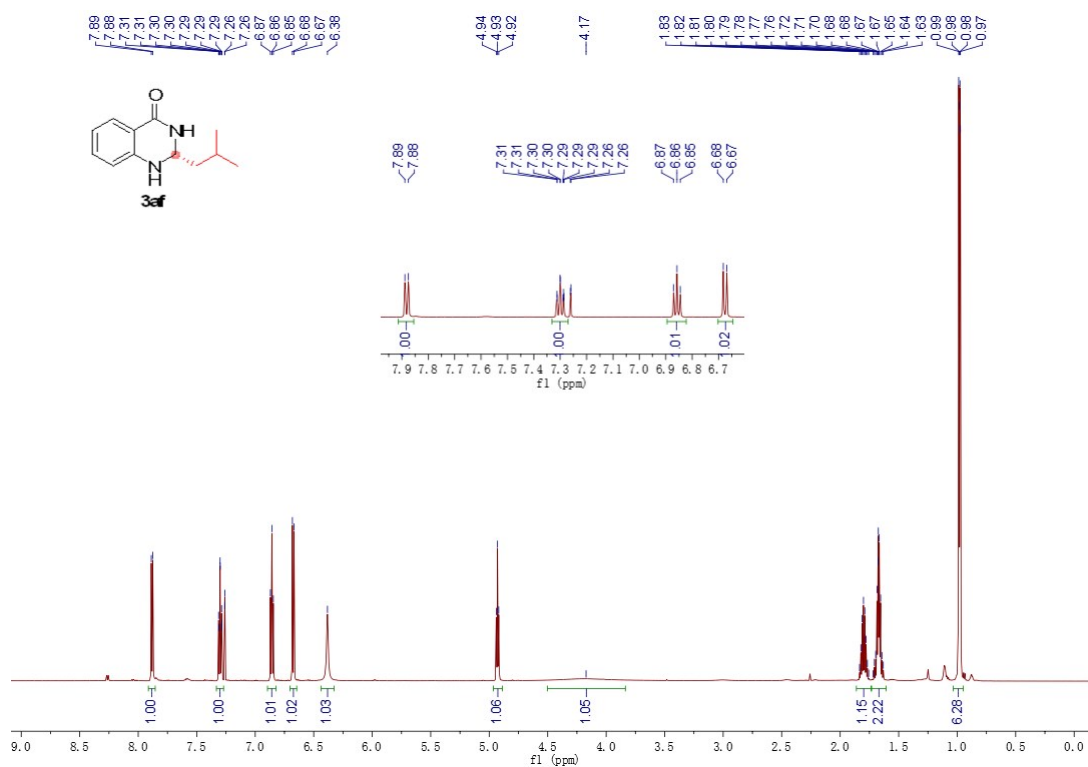


Fig.S 16 <sup>1</sup>H NMR of compound **3af**



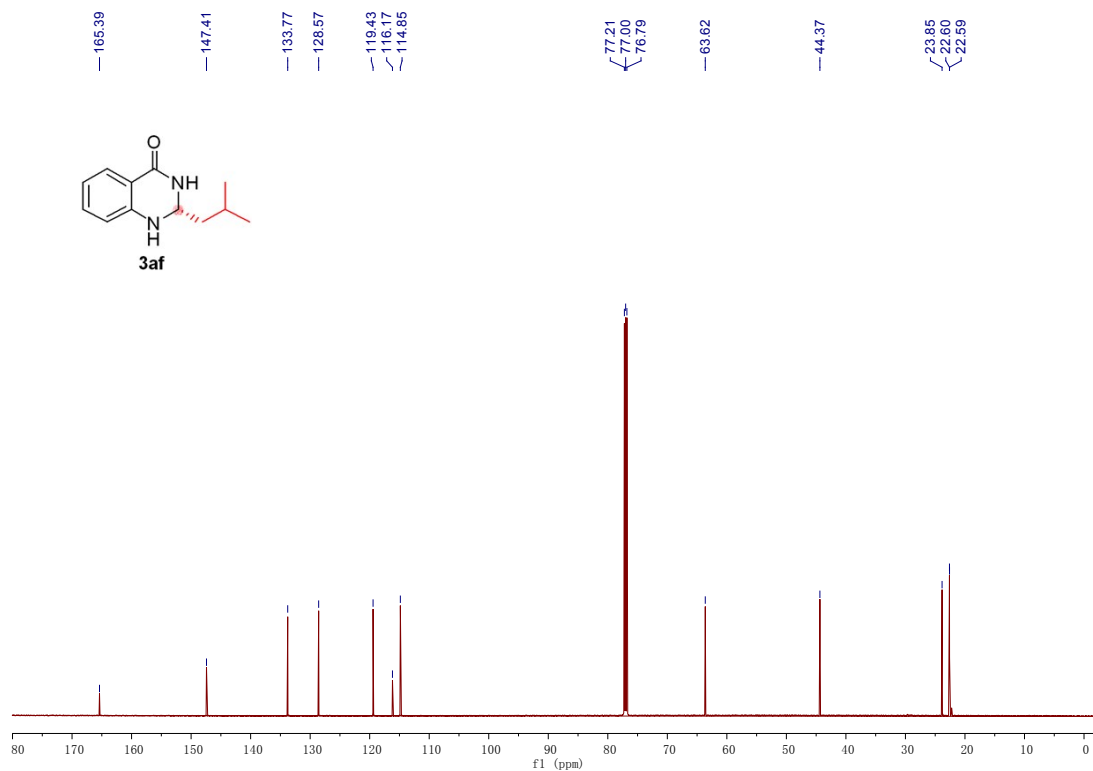


Fig.S 17  $^{13}\text{C}$  NMR of compound **3af**

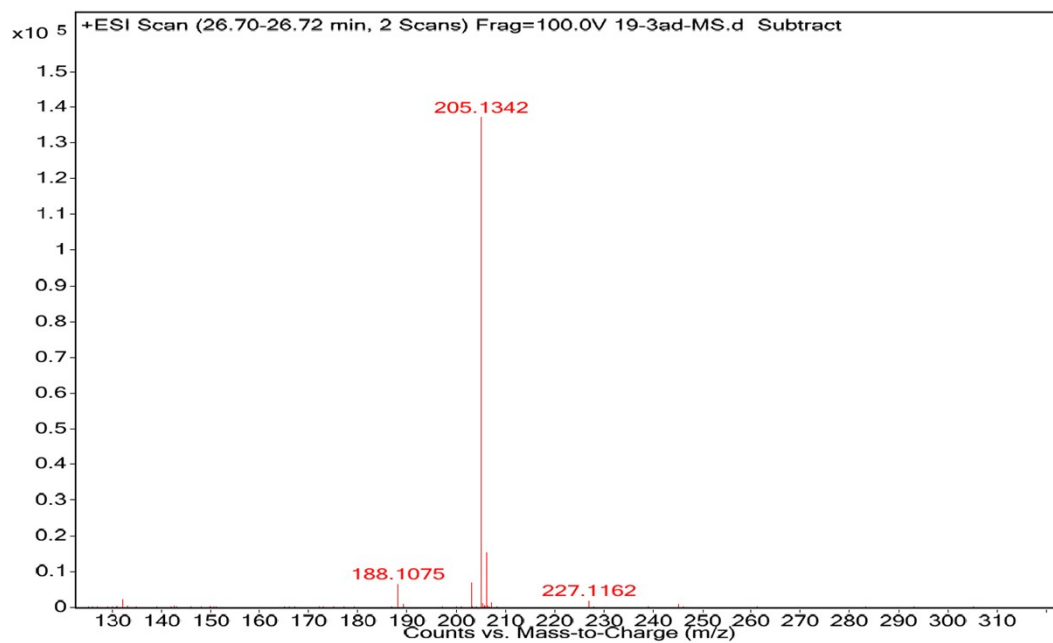


Fig.S 18 HR-MS of compound **3af**

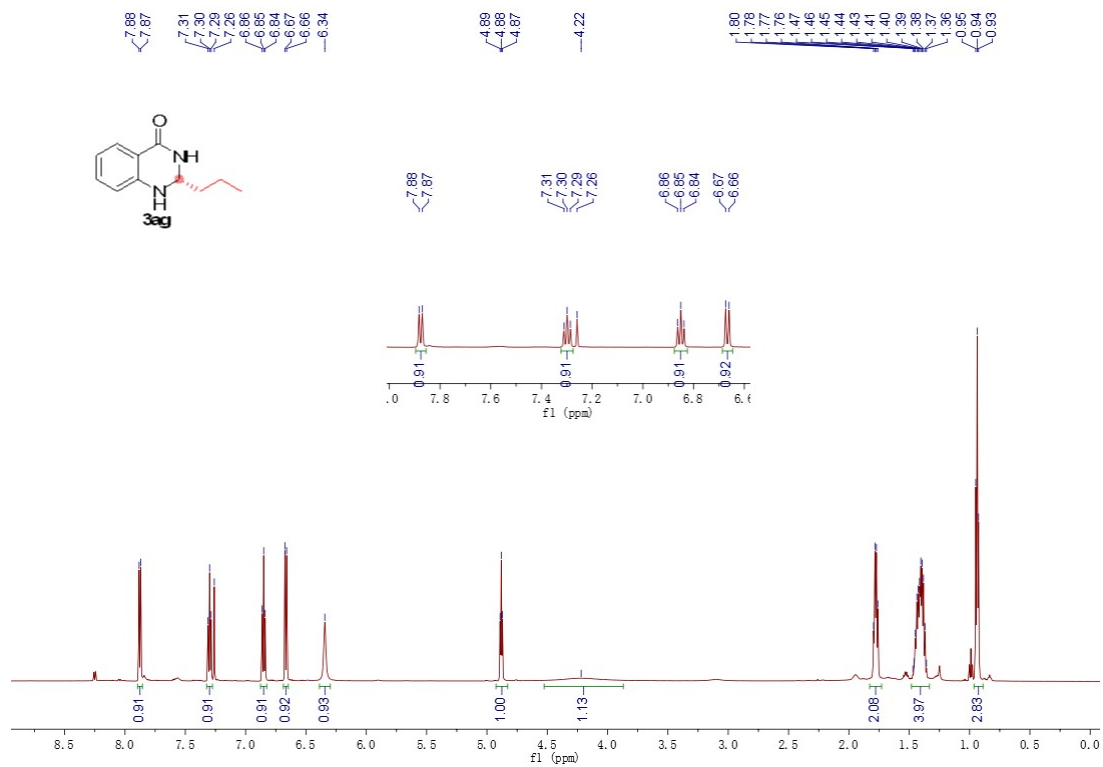


Fig.S 19 <sup>1</sup>H NMR of compound **3ag** (Gram-scale)

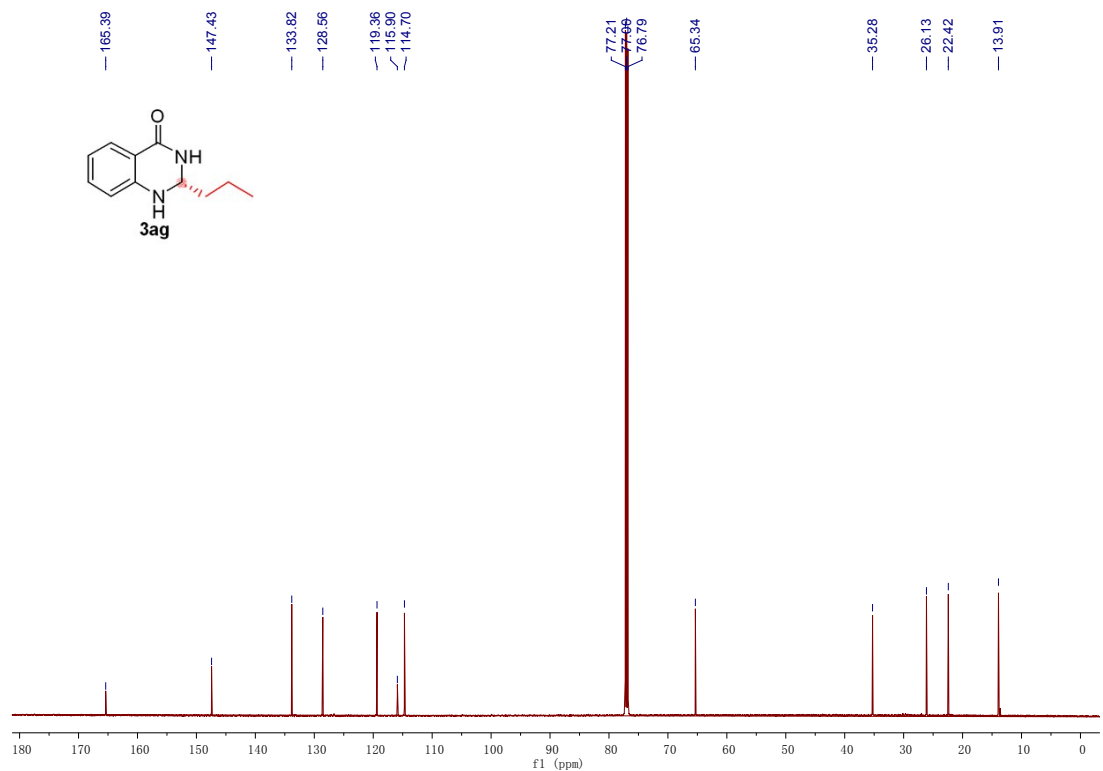


Fig.S 20 <sup>13</sup>C NMR of compound **3ag** (Gram-scale)



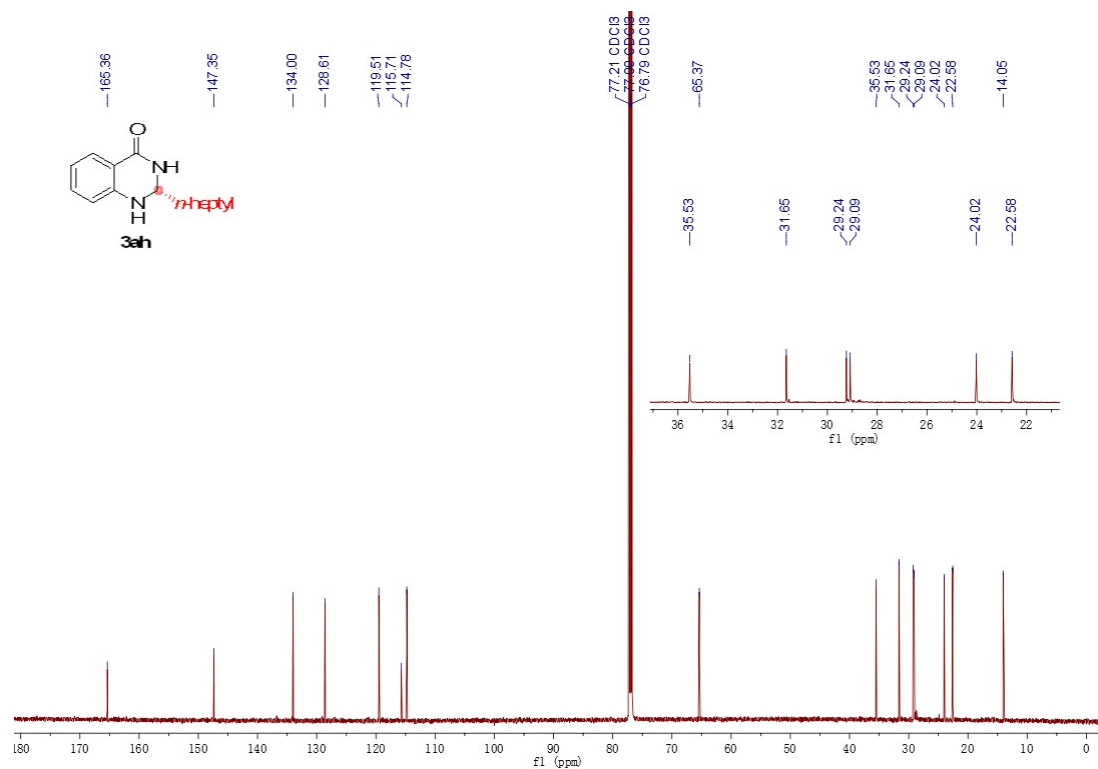


Fig.S 23 <sup>13</sup>C NMR of compound **3ah**

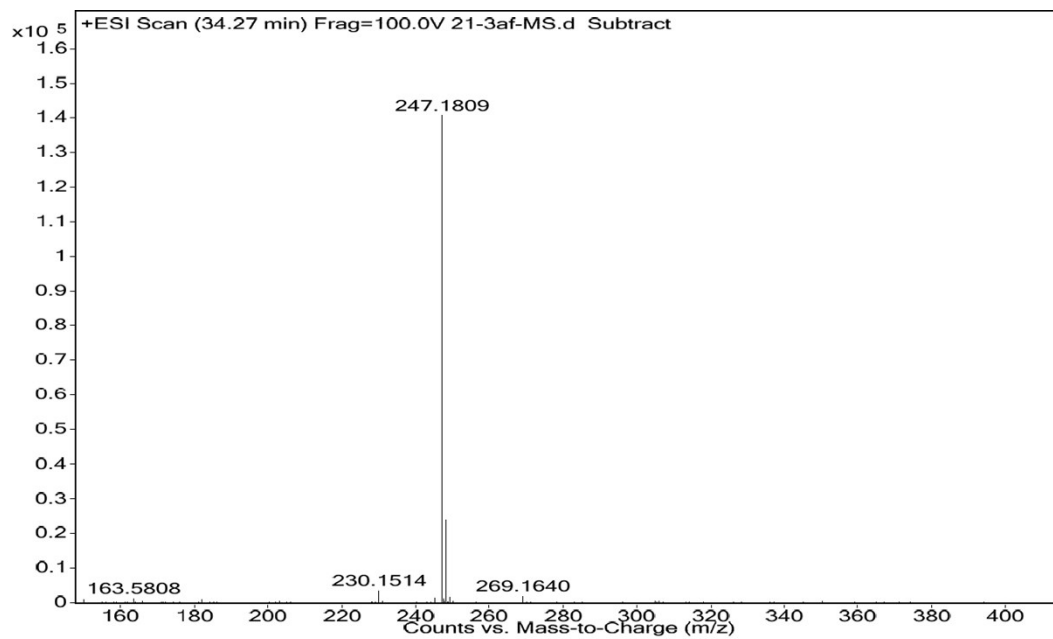


Fig.S 24 HR-MS of compound **3ah**

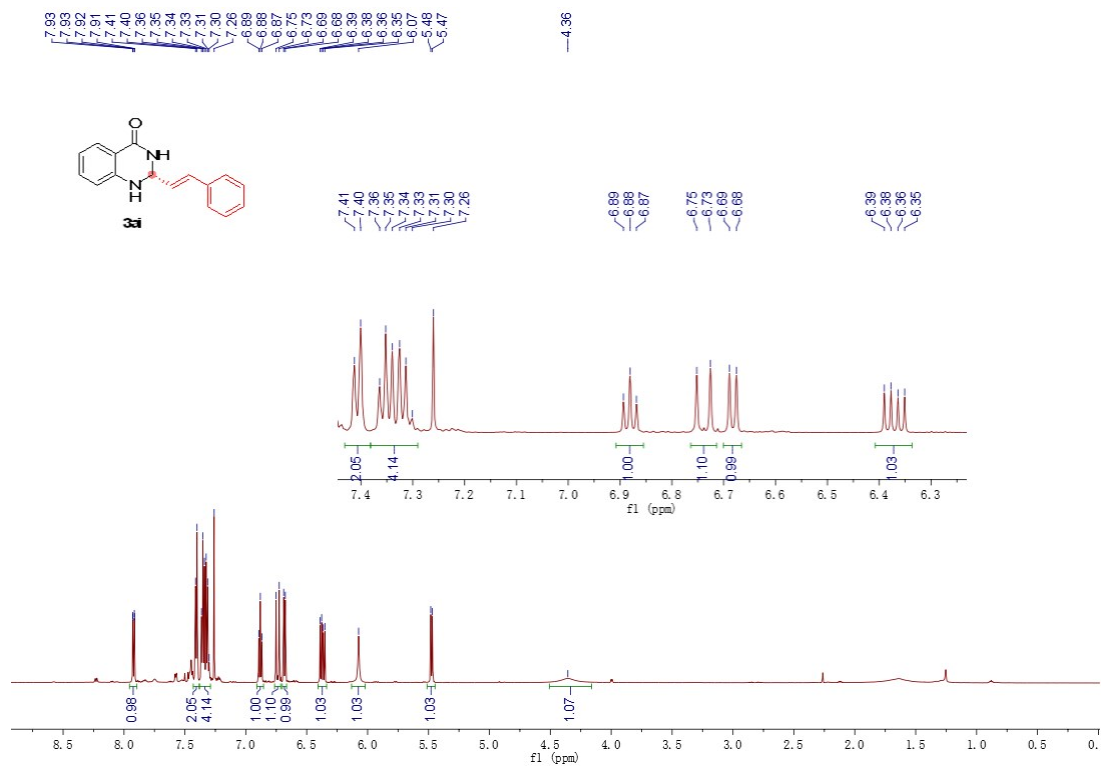


Fig.S 25 <sup>1</sup>H NMR of compound 3ai (Gram-scale)

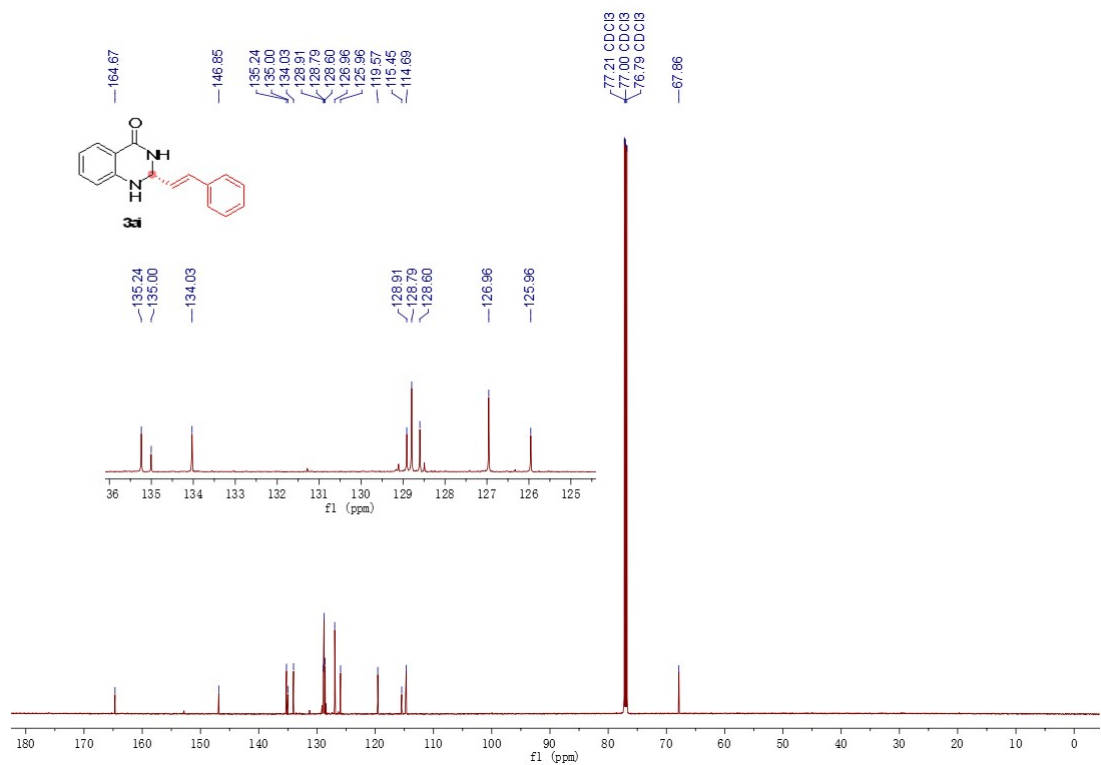


Fig.S 26 <sup>13</sup>C NMR of compound 3ai (Gram-scale)

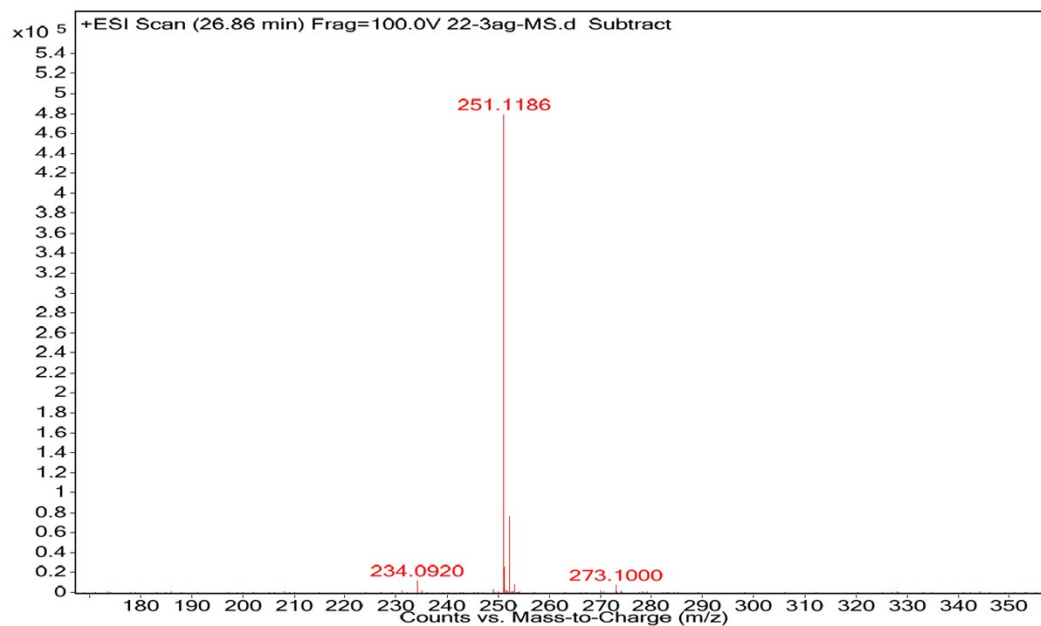


Fig.S 27 HR-MS of compound **3ai** (Gram-scale)

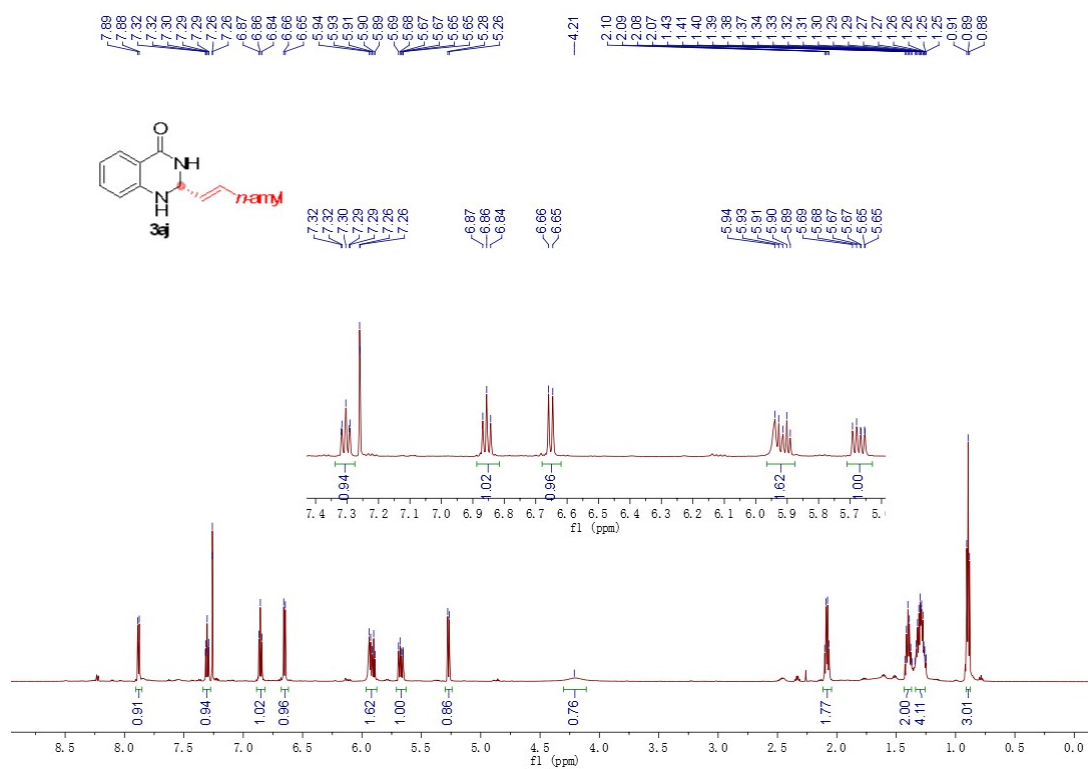


Fig.S 28 <sup>1</sup>H NMR of compound **3aj**

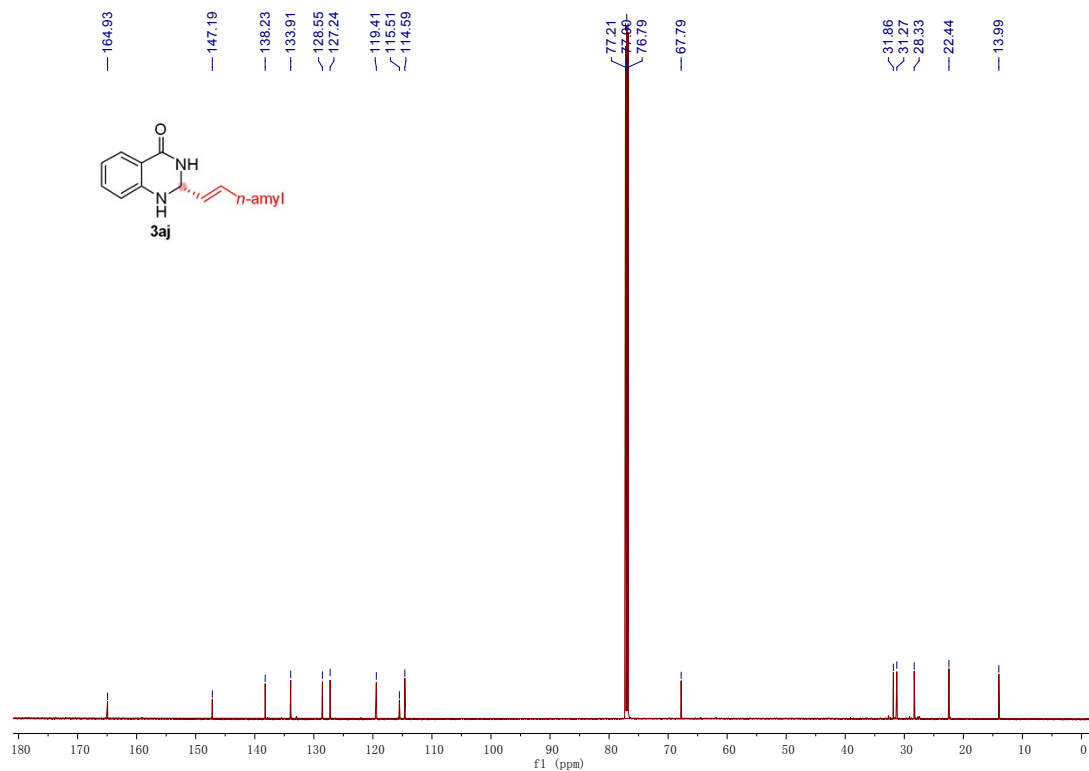


Fig.S 29 <sup>13</sup>C NMR of compound **3aj**

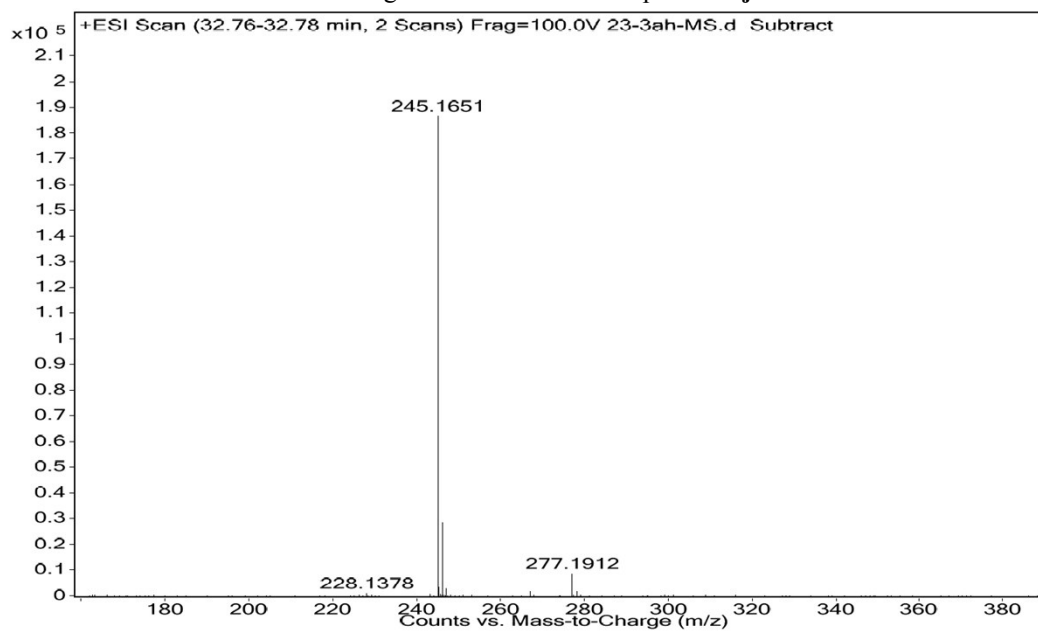


Fig.S 30 HR-MS of compound **3aj**

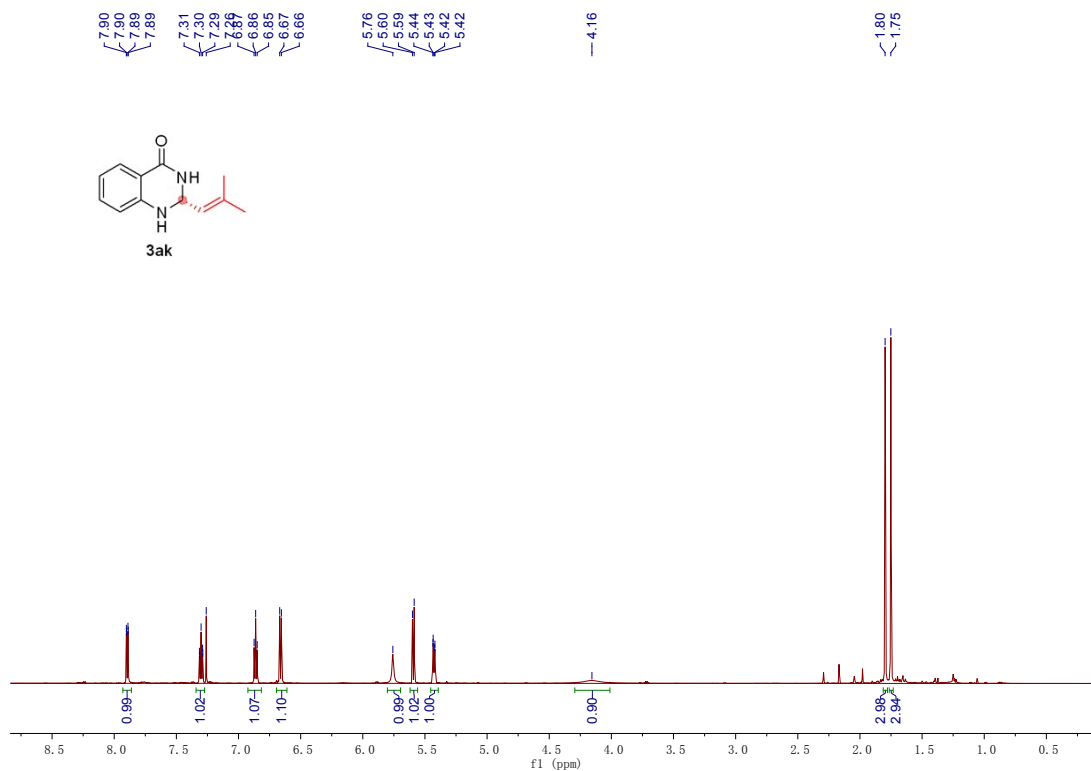


Fig.S 31 <sup>1</sup>H NMR of compound **3ak** (Gram-scale)

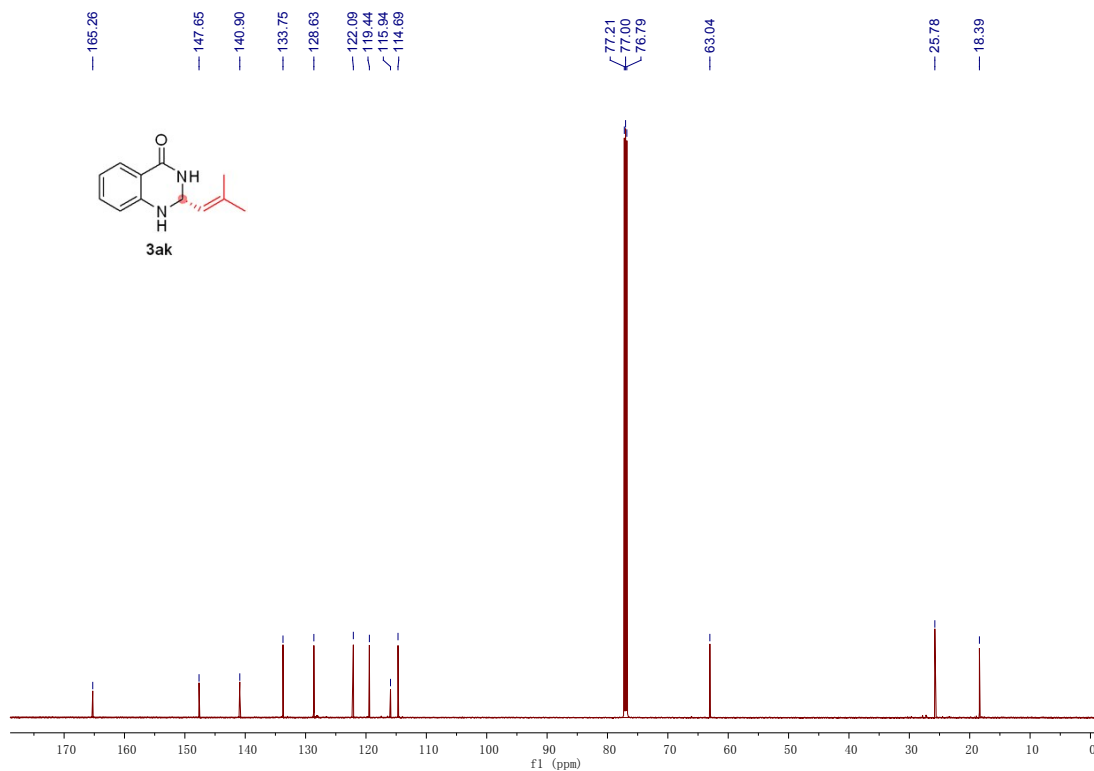


Fig.S 32 <sup>13</sup>C NMR of compound **3ak** (Gram-scale)



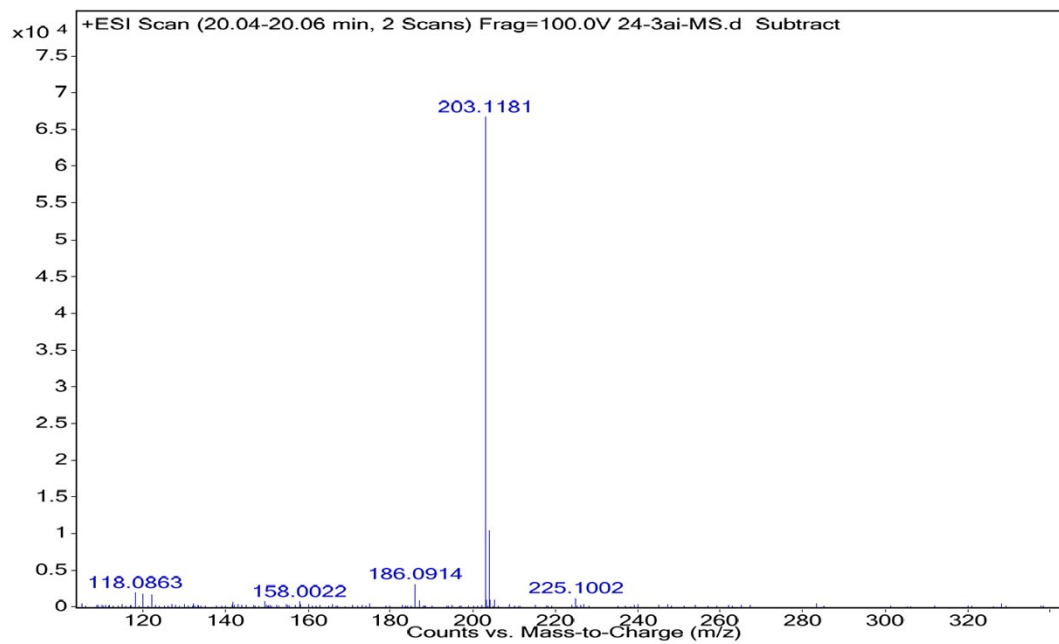


Fig.S 33 HR-MS of compound **3ak** (Gram-scale)

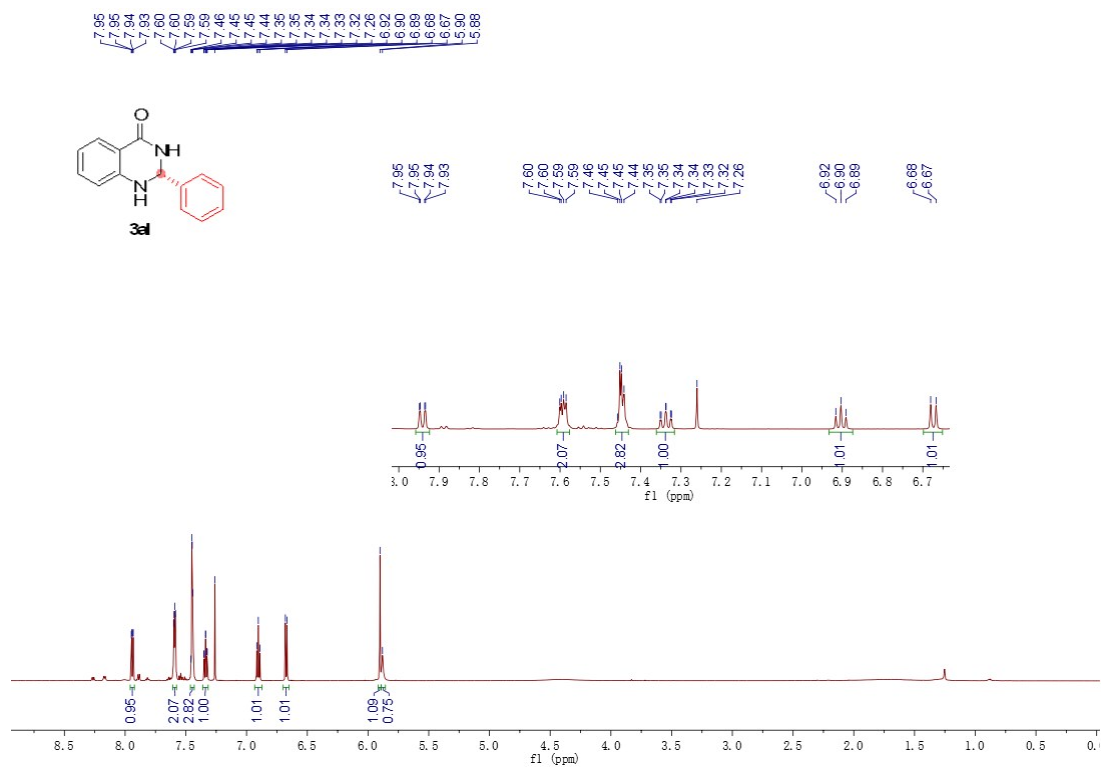


Fig.S 34 <sup>1</sup>H NMR of compound **3al**

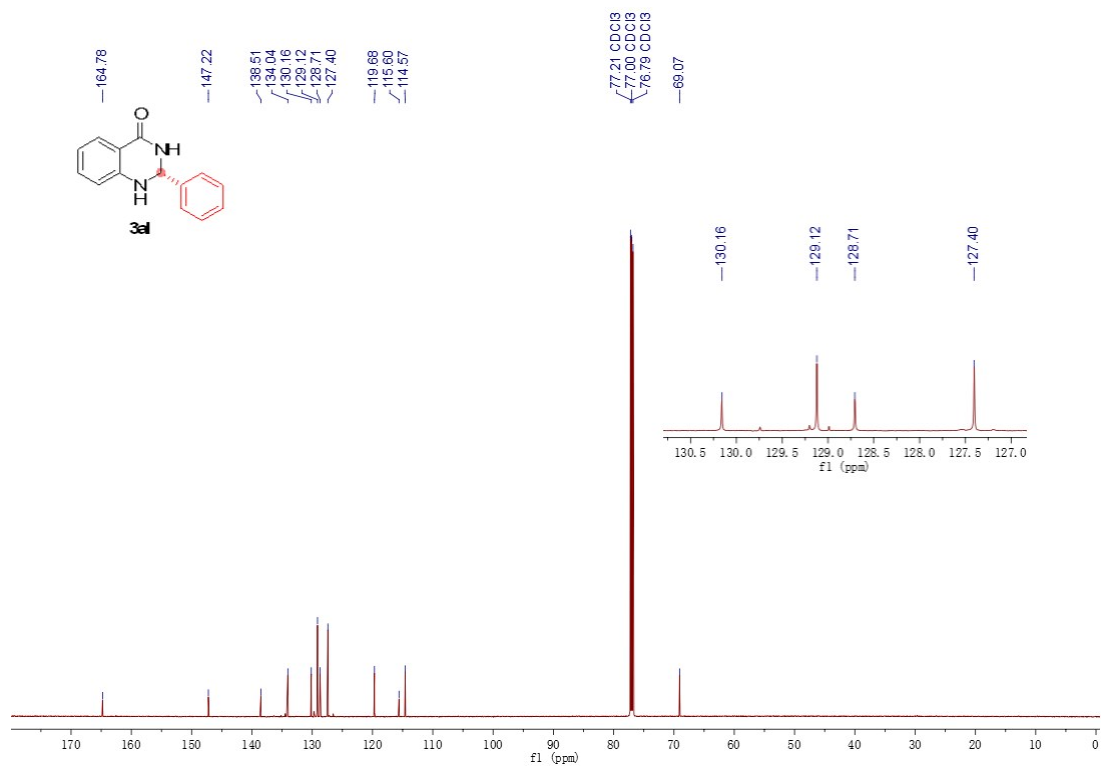


Fig.S 35  $^{13}\text{C}$  NMR of compound **3al**

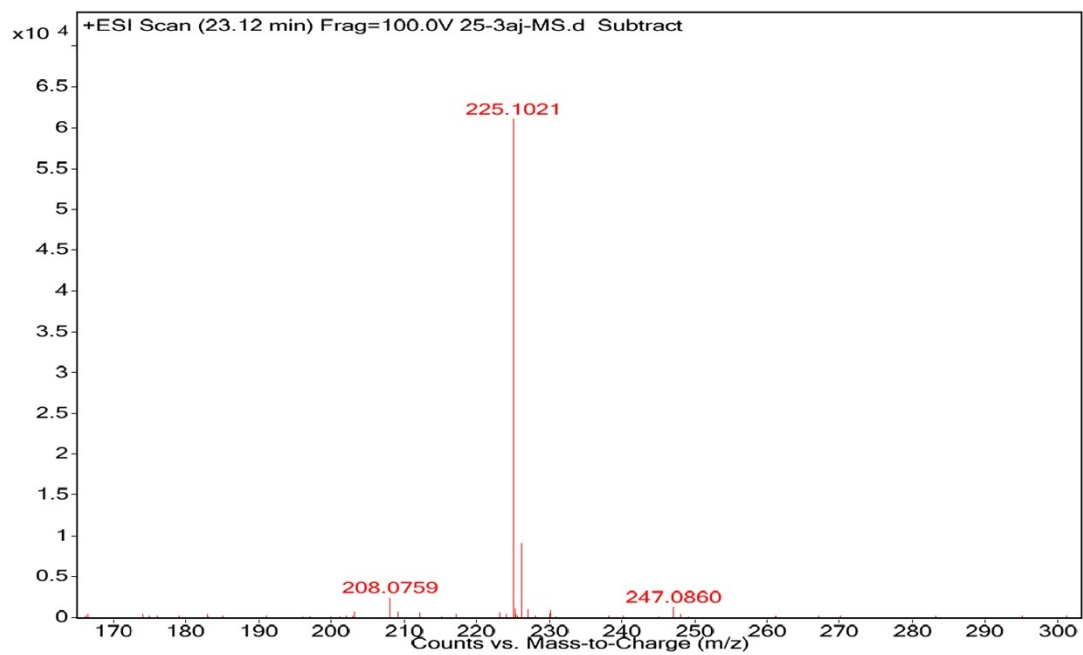


Fig.S 36 HR-MS of compound **3al**

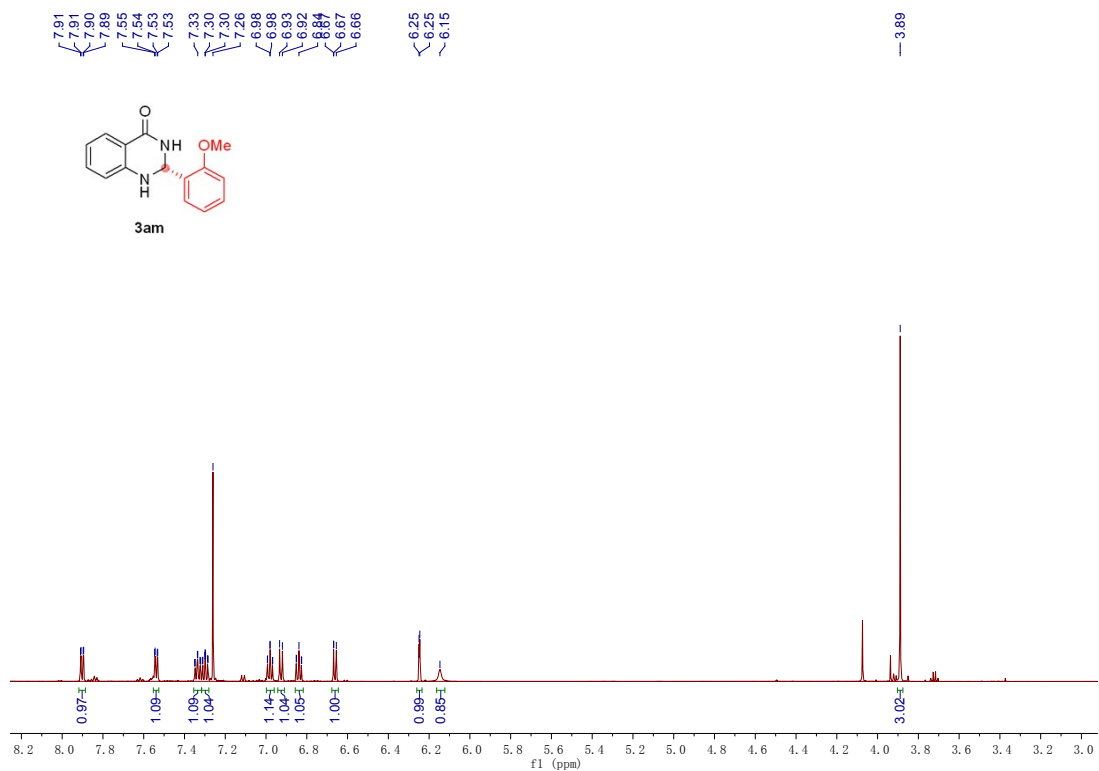


Fig.S 37 <sup>1</sup>H NMR of compound **3am**

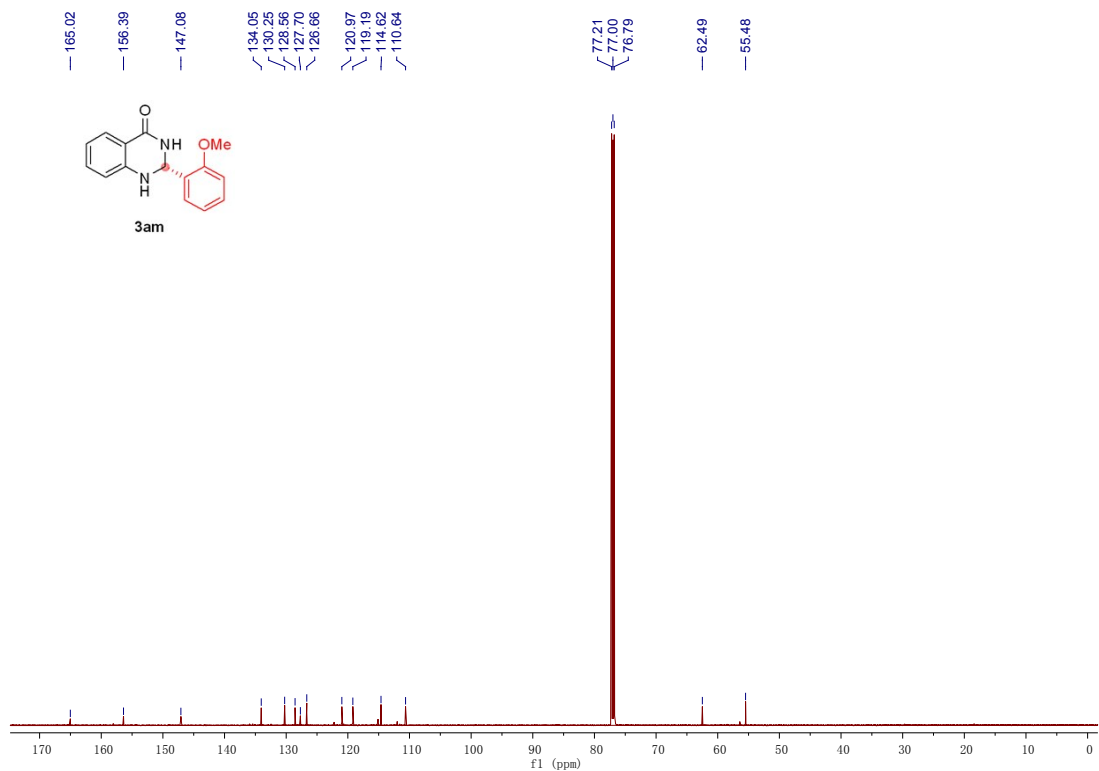


Fig.S 38 <sup>13</sup>C NMR of compound **3am**

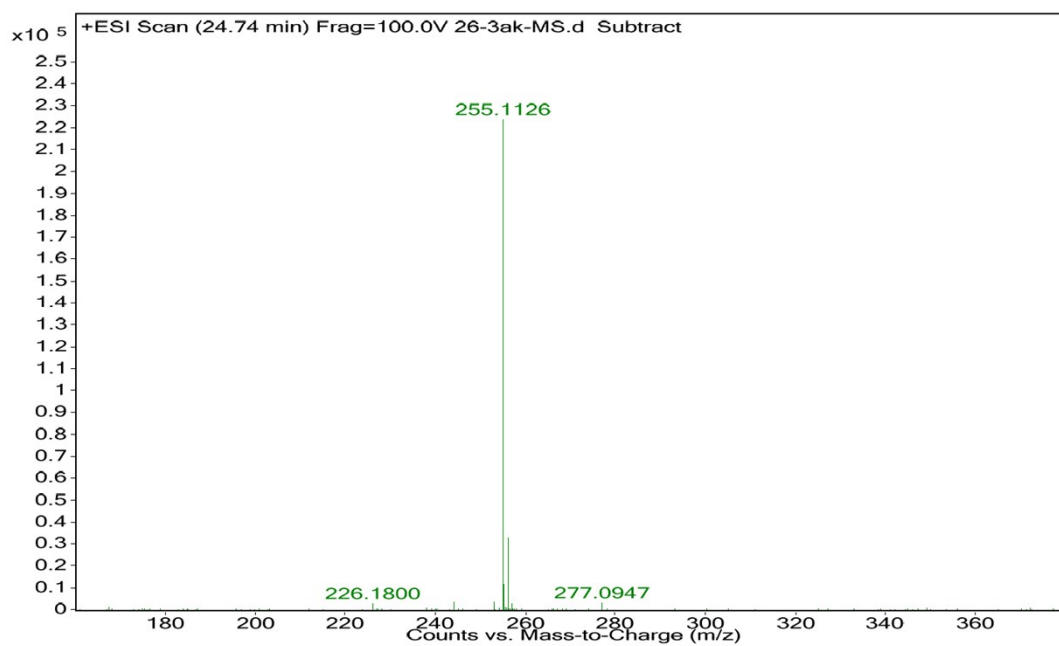


Fig.S 39 HR-MS of compound **3am**

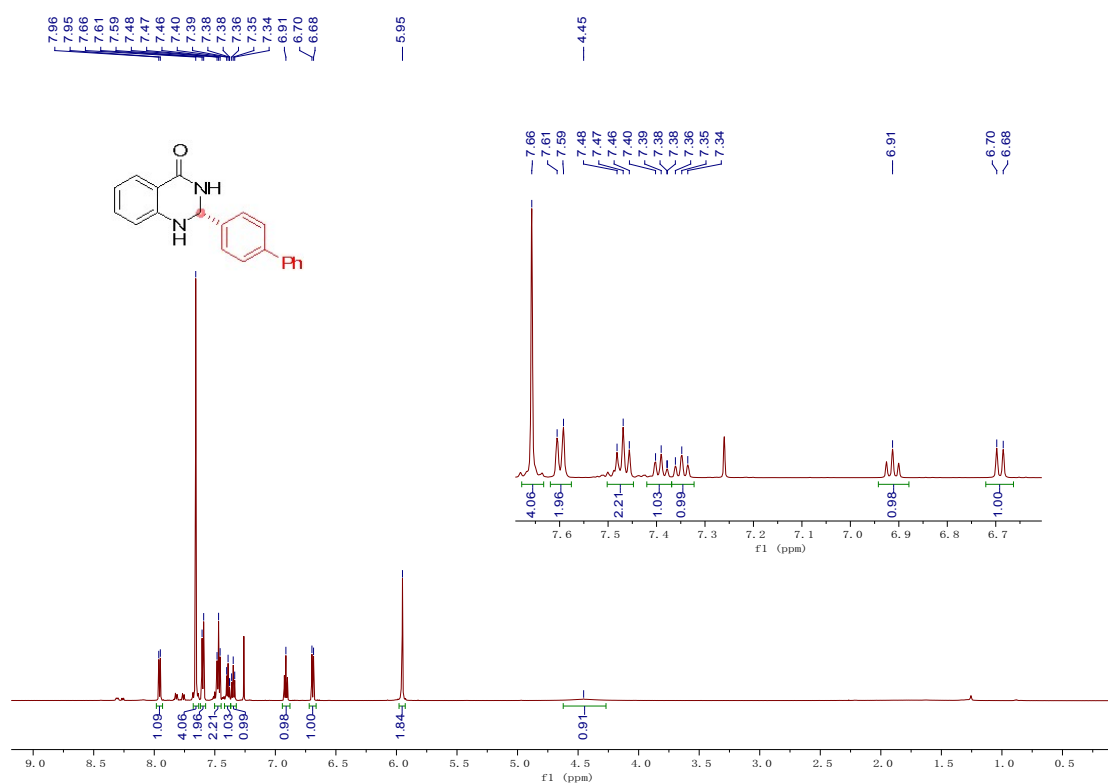


Fig.S 40 <sup>1</sup>H NMR of compound **3am**

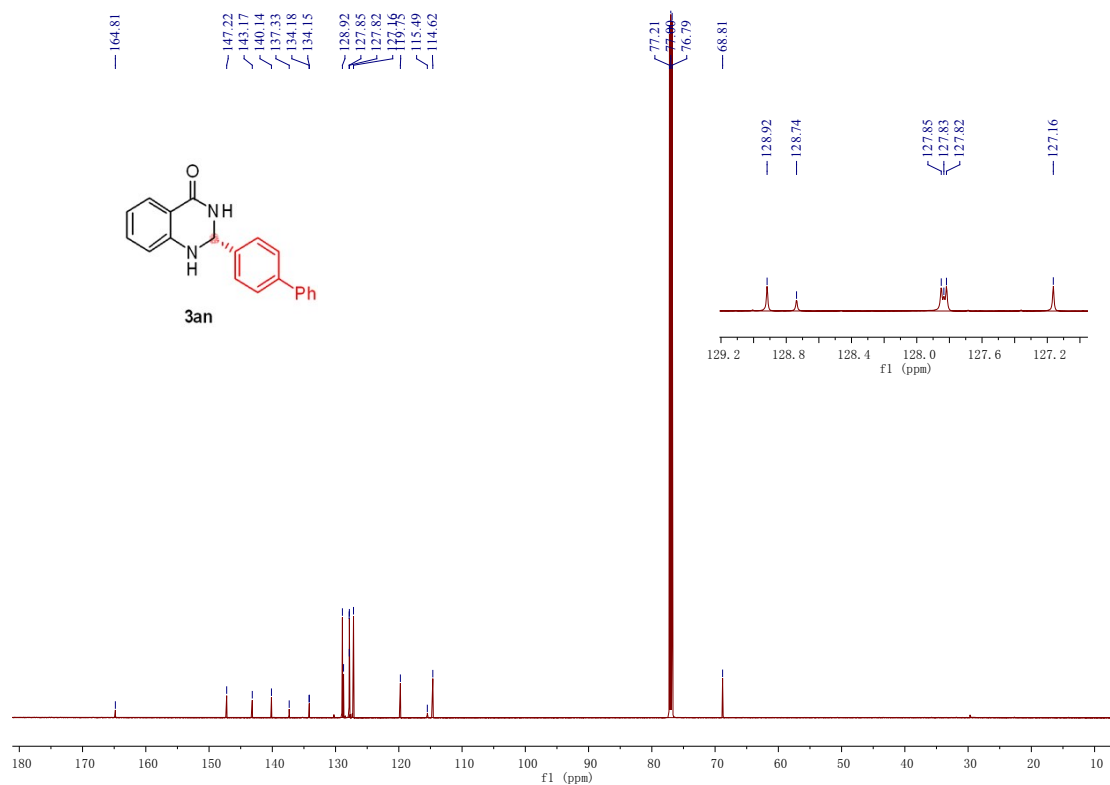


Fig.S 41 <sup>13</sup>C NMR of compound **3an**

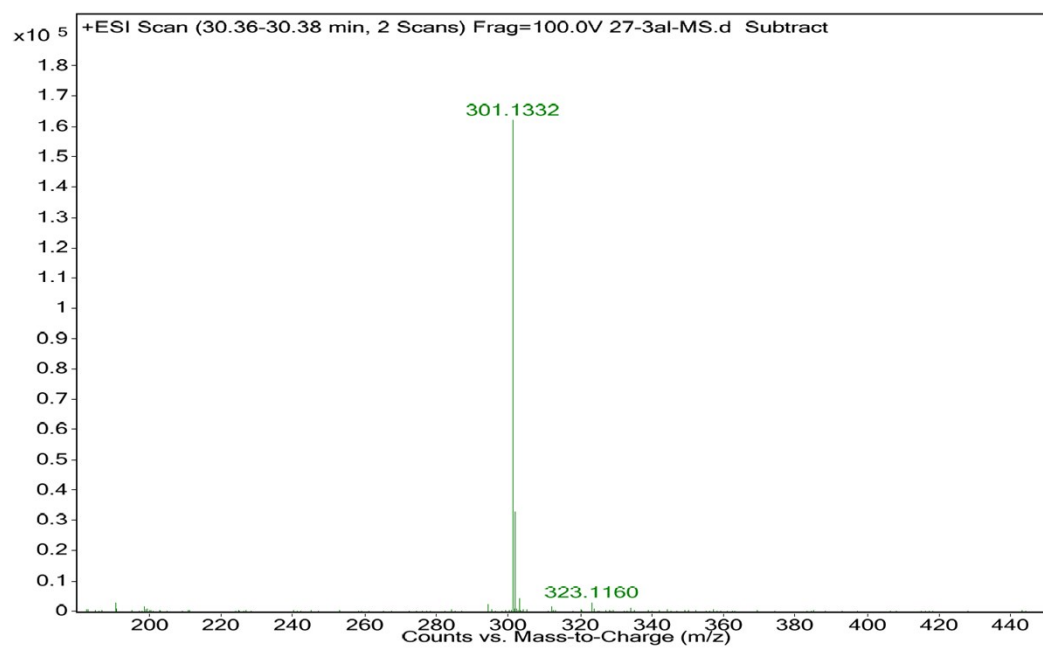


Fig.S 42 HR-MS of compound **3an**

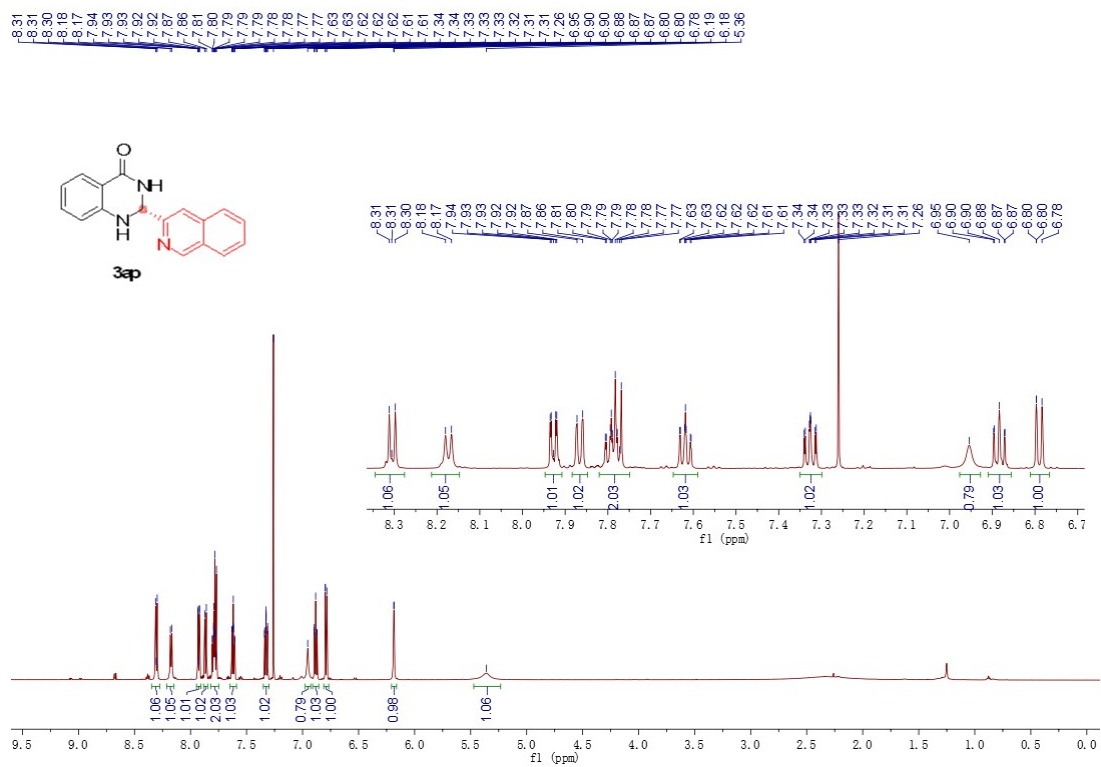


Fig.S 43 <sup>1</sup>H NMR of compound 3ao

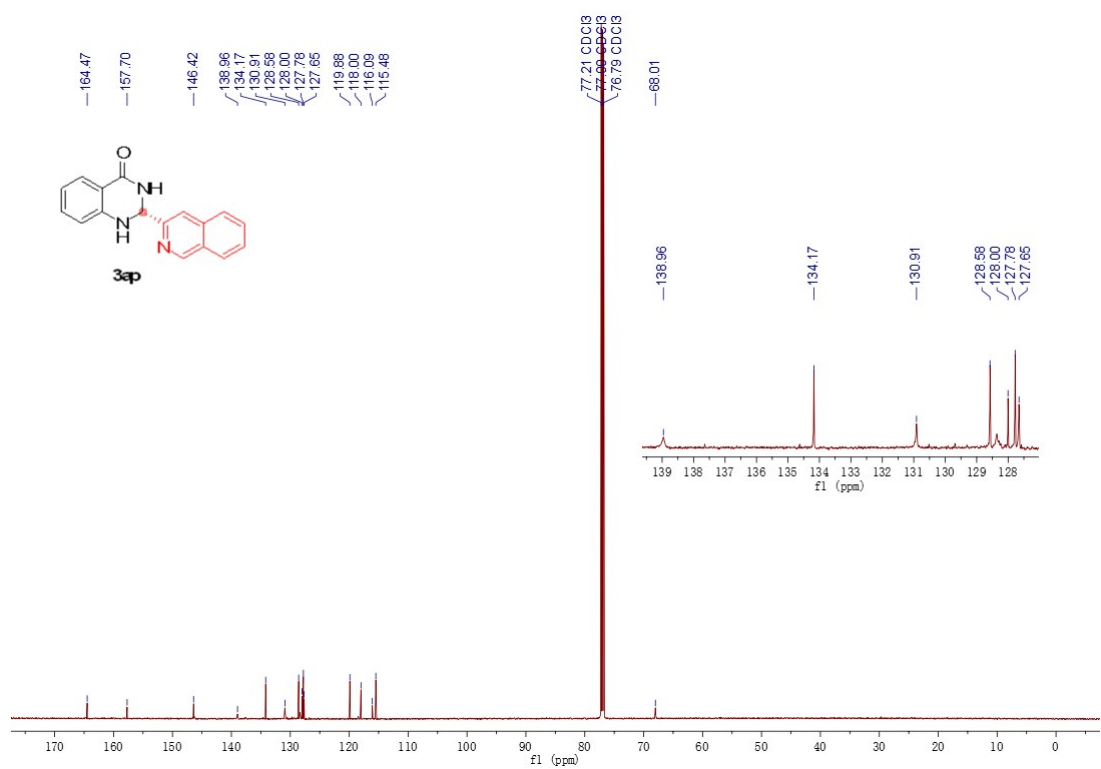


Fig.S 44 <sup>13</sup>C NMR of compound 3ao

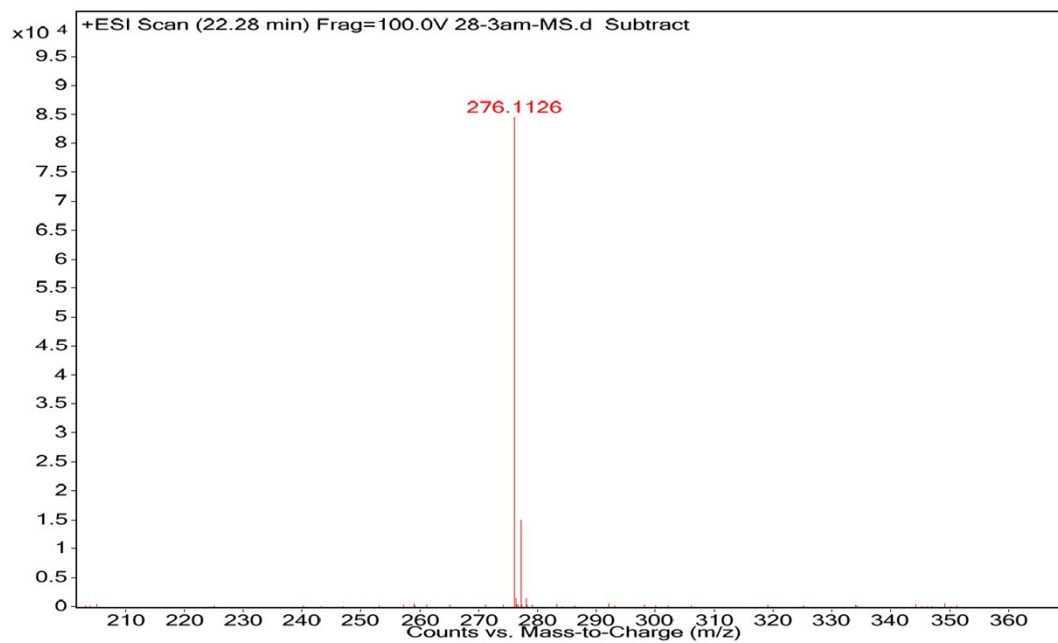


Fig.S 45 HR-MS of compound **3ao**

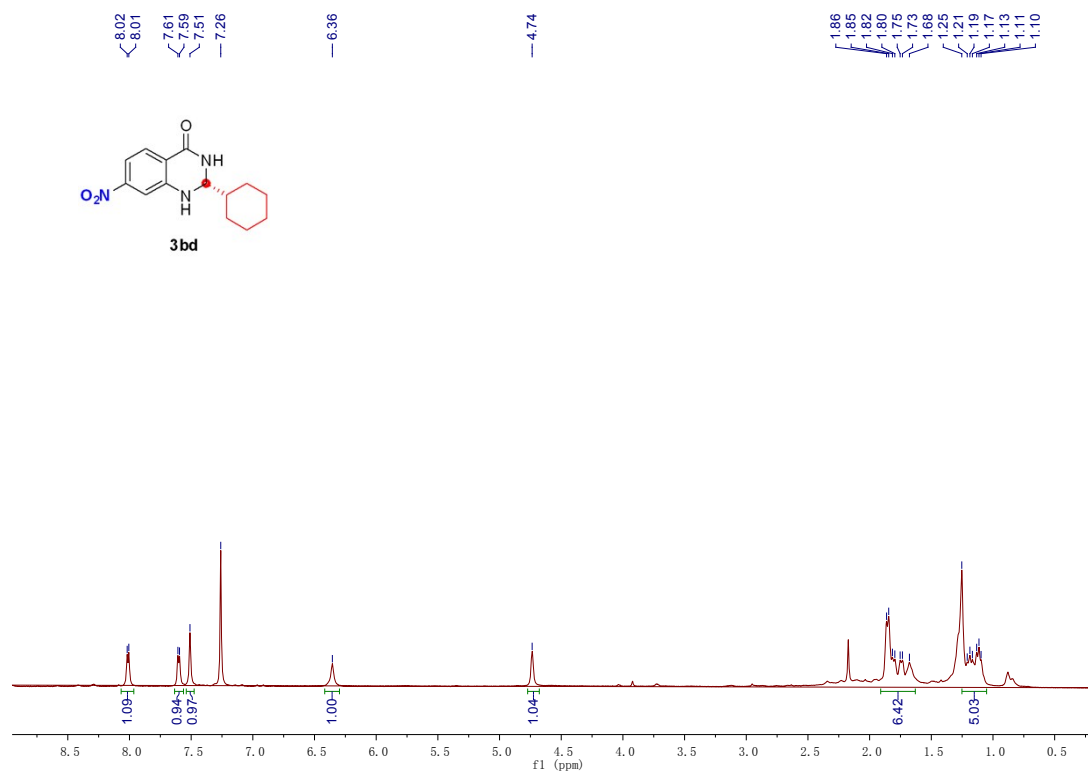


Fig.S 46  $^1\text{H}$  NMR of compound **3bd**

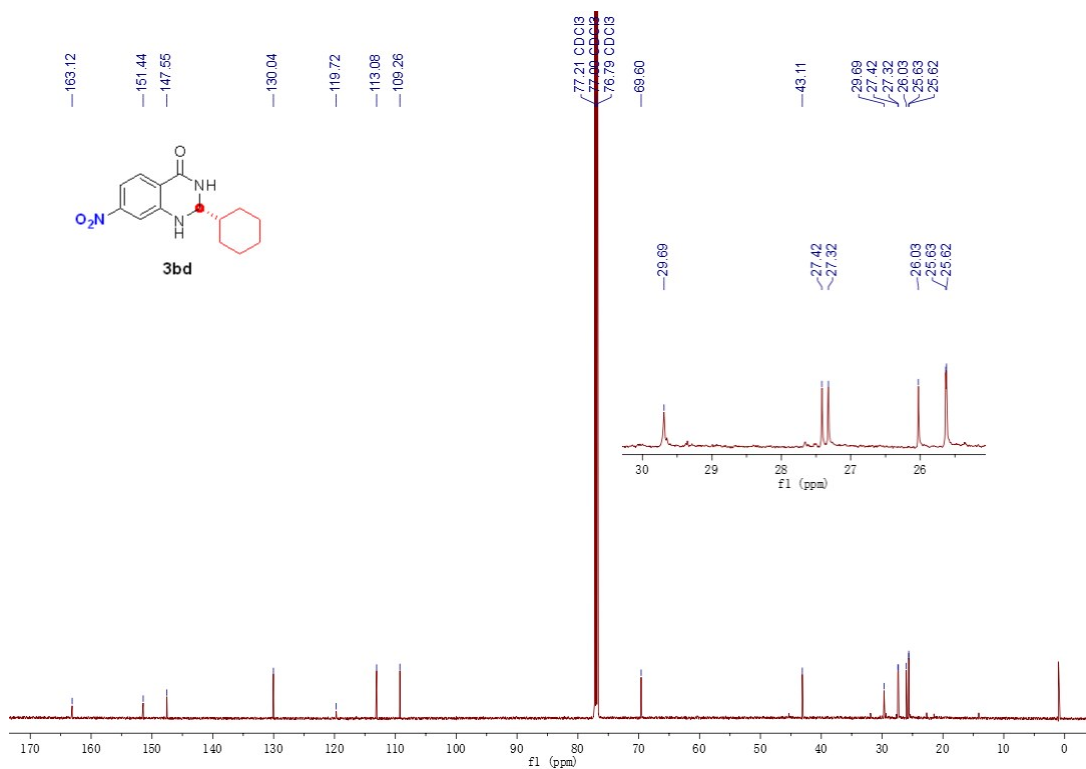


Fig.S 47 <sup>13</sup>C NMR of compound **3bd**

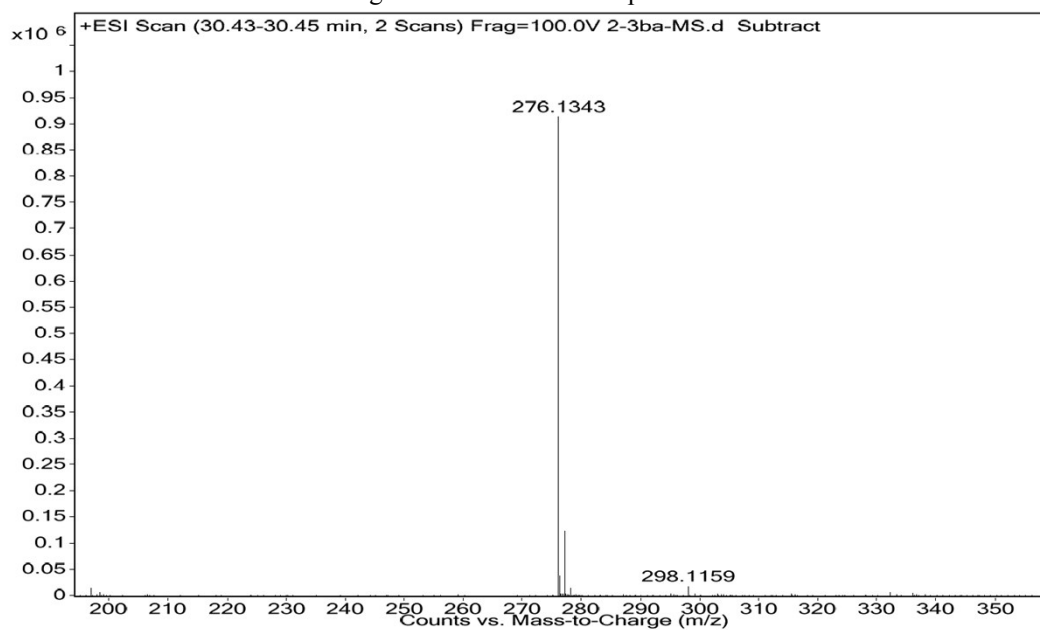


Fig.S 48 <sup>1</sup>H HRMS of compound **3bd**



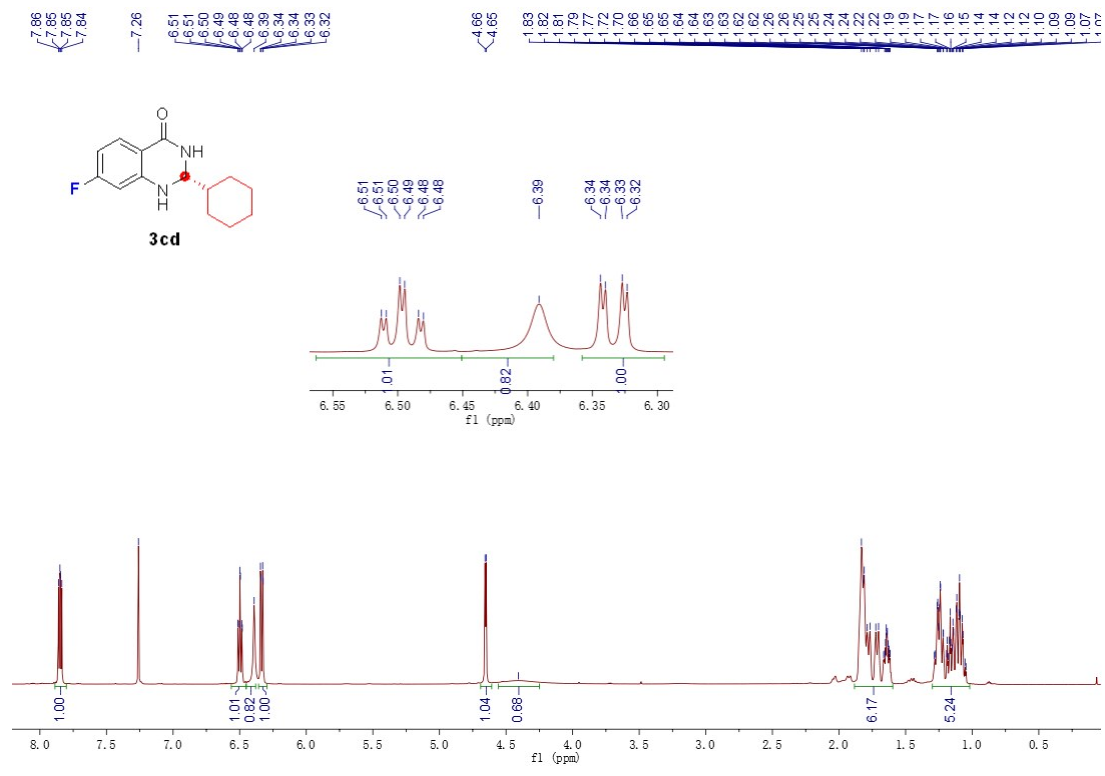


Fig.S 49 <sup>1</sup>H NMR of compound 3cd

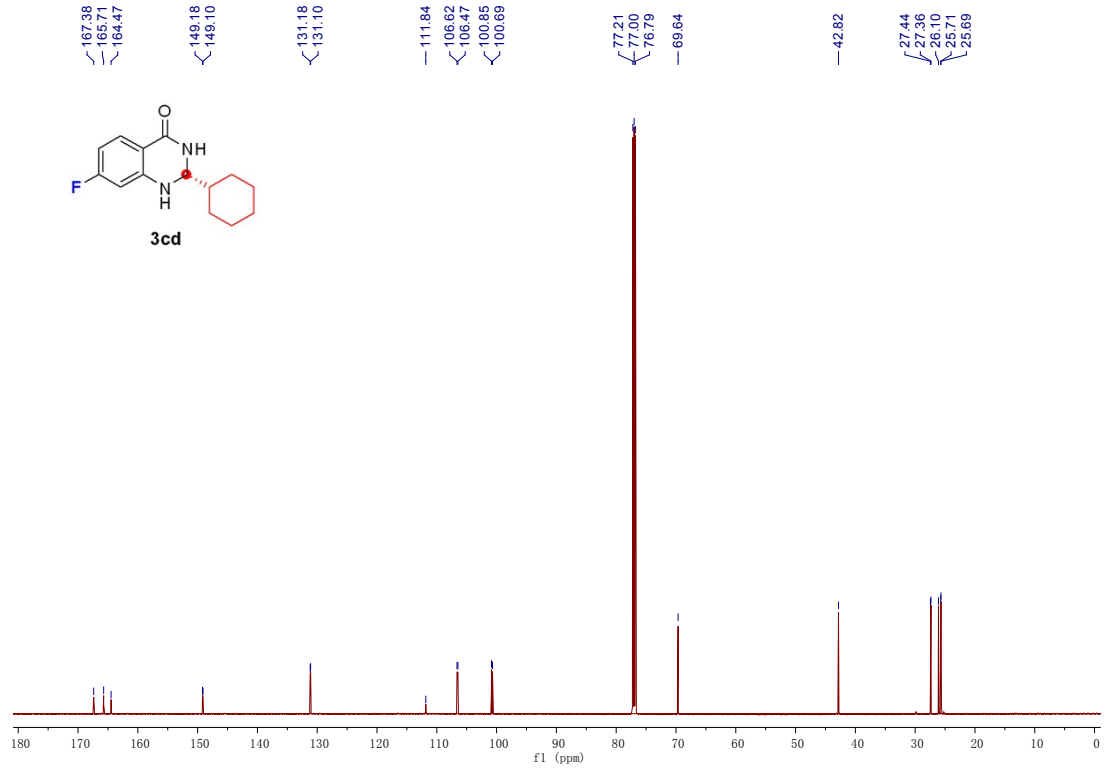


Fig.S 50 <sup>13</sup>C NMR of compound 3cd

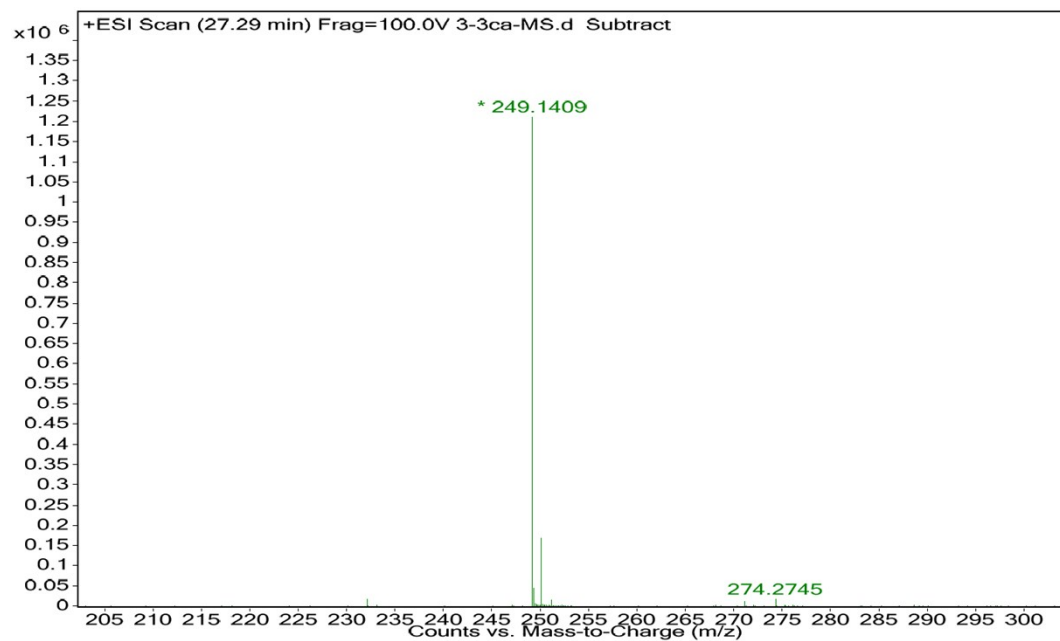


Fig.S 51 <sup>1</sup>H NMR of compound 3cd

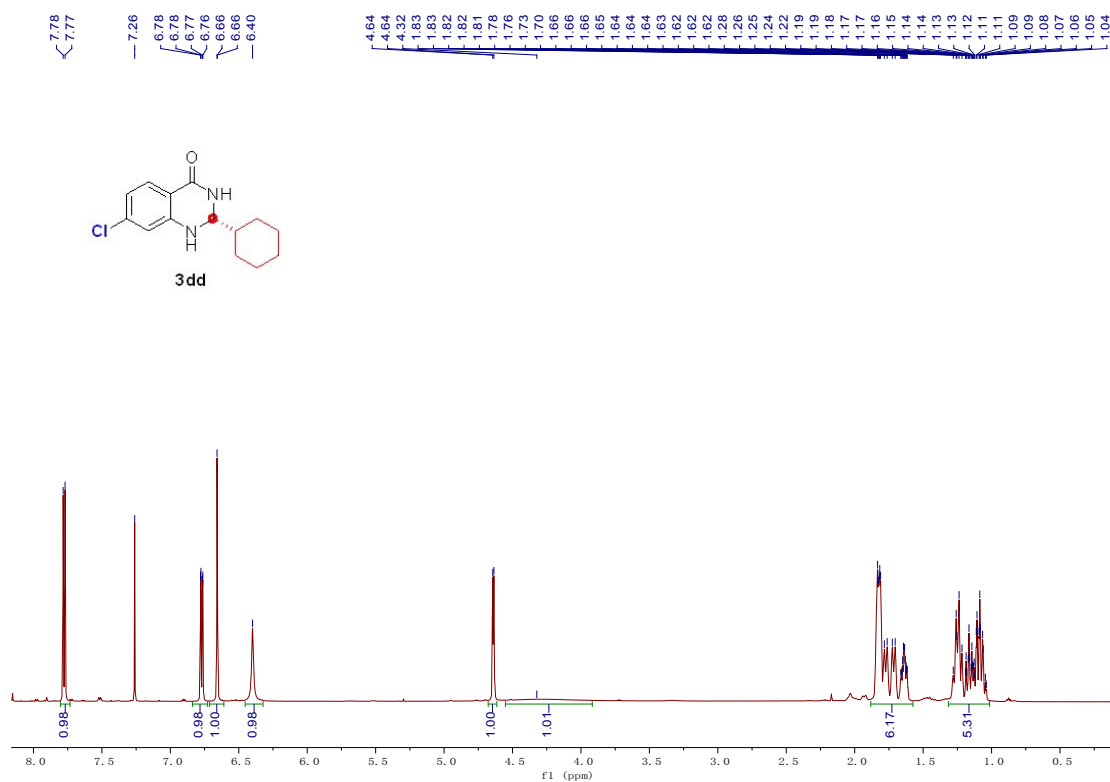


Fig.S 52 <sup>1</sup>H NMR of compound 3dd

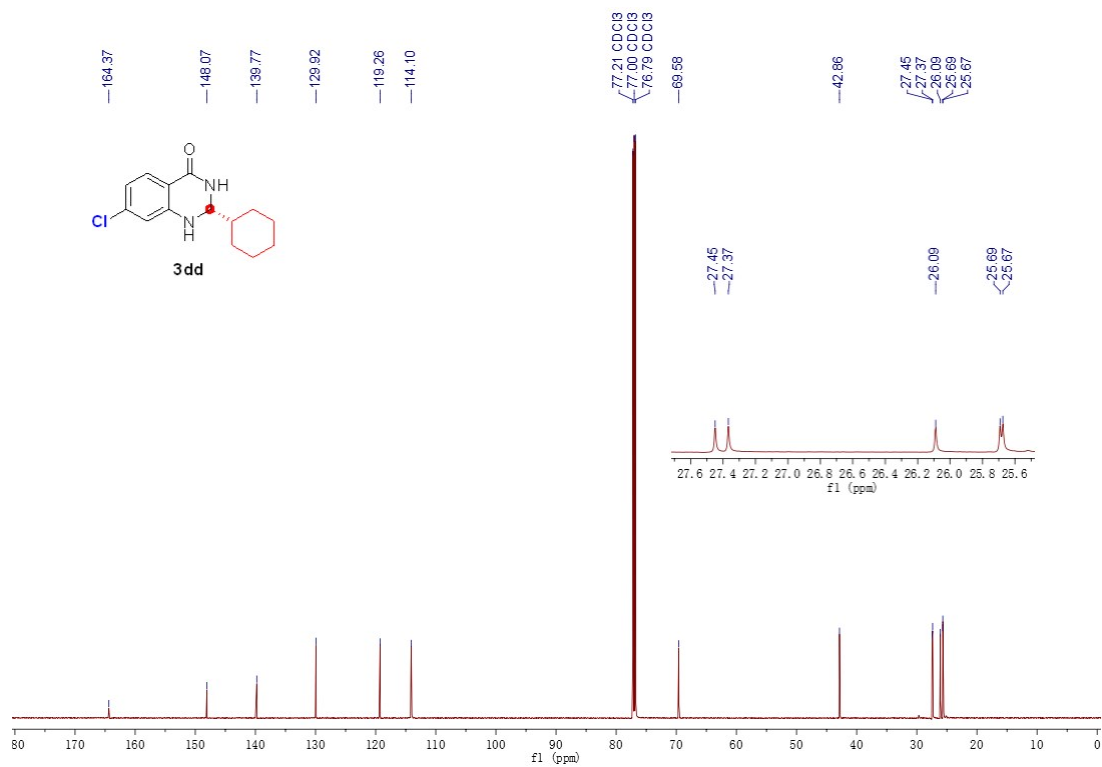


Fig.S 53 <sup>13</sup>C NMR of compound **3dd**

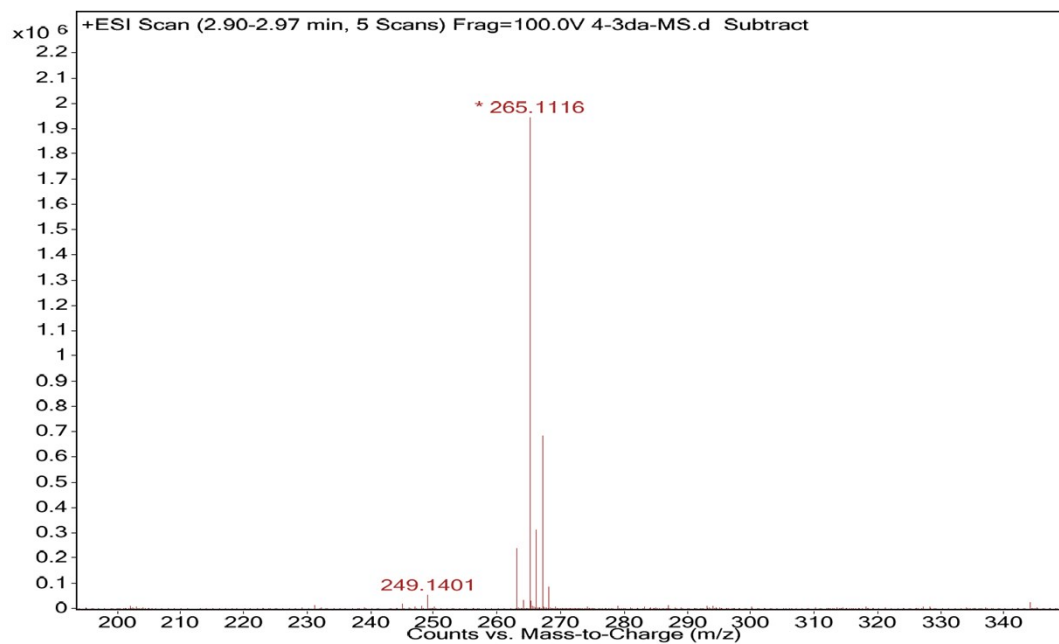


Fig.S 54 <sup>1</sup>H NMR of compound **3dd**



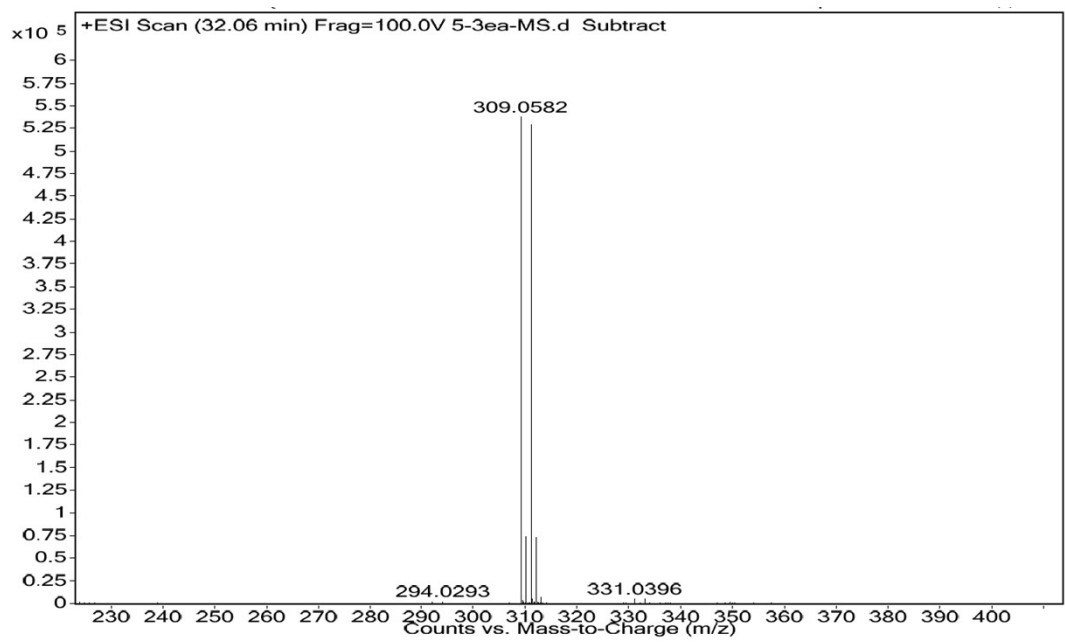


Fig.S 57 <sup>1</sup>H NMR of compound 3ed

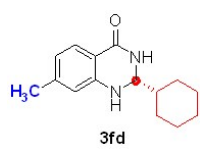
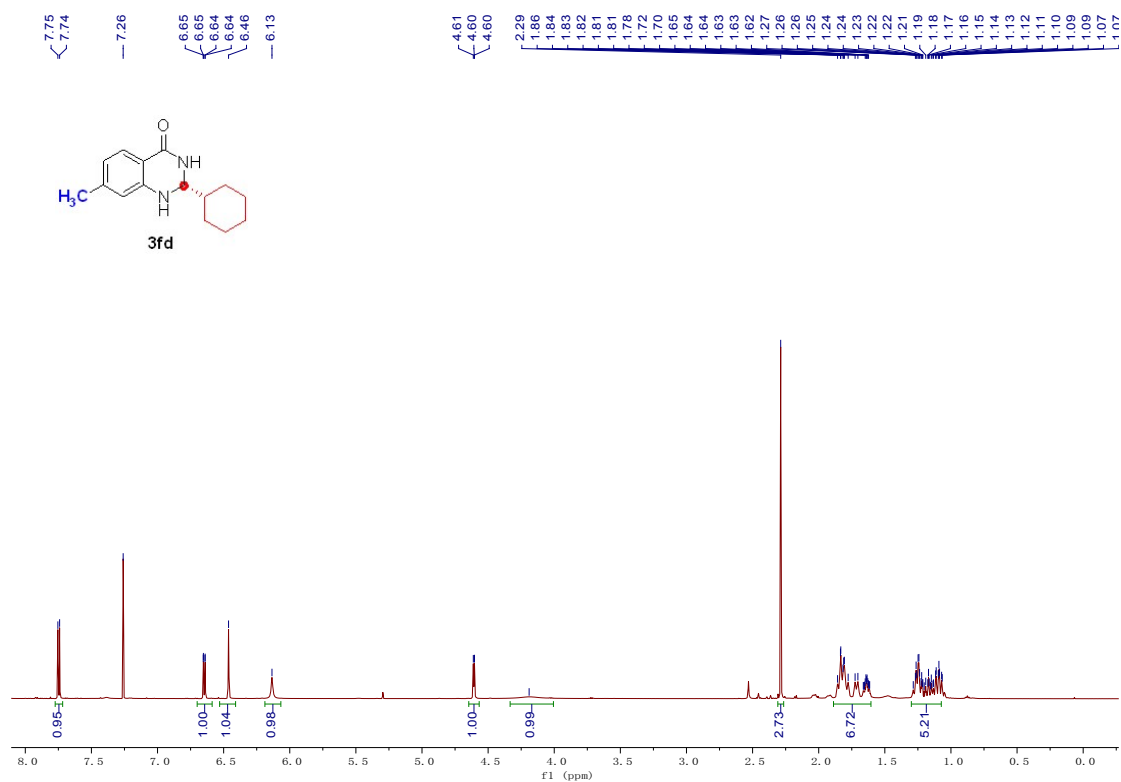


Fig.S 58 <sup>1</sup>H NMR of compound 3fd

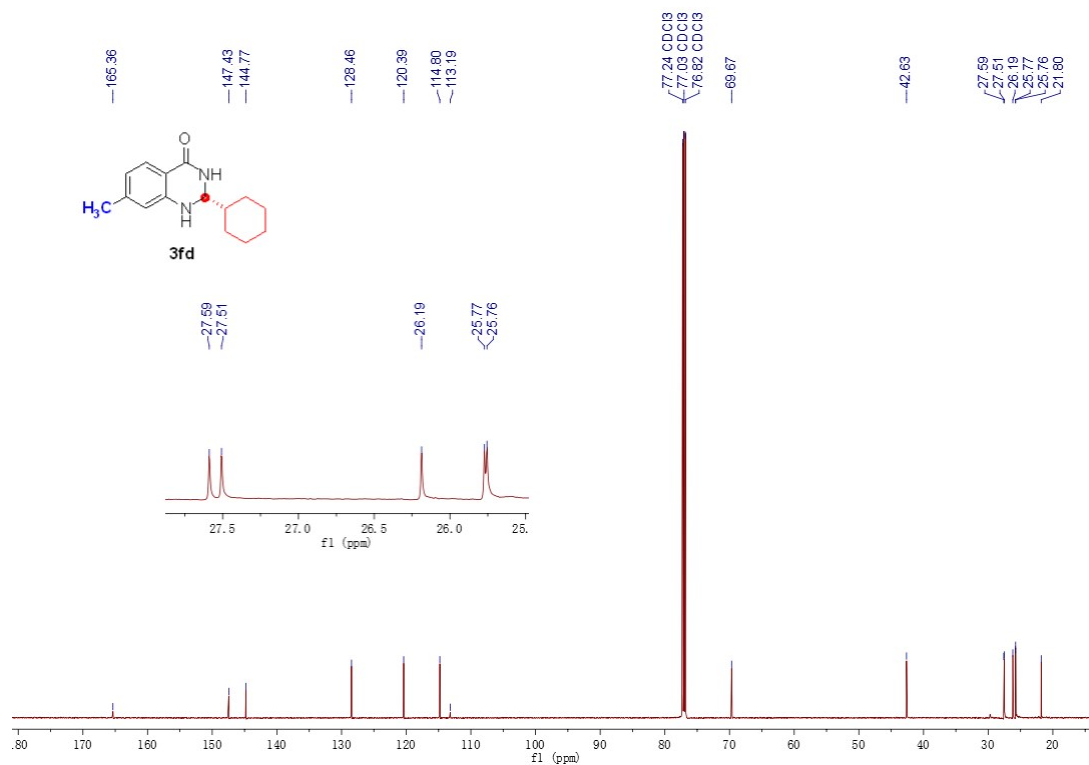


Fig.S 59 <sup>13</sup>C NMR of compound **3fd**

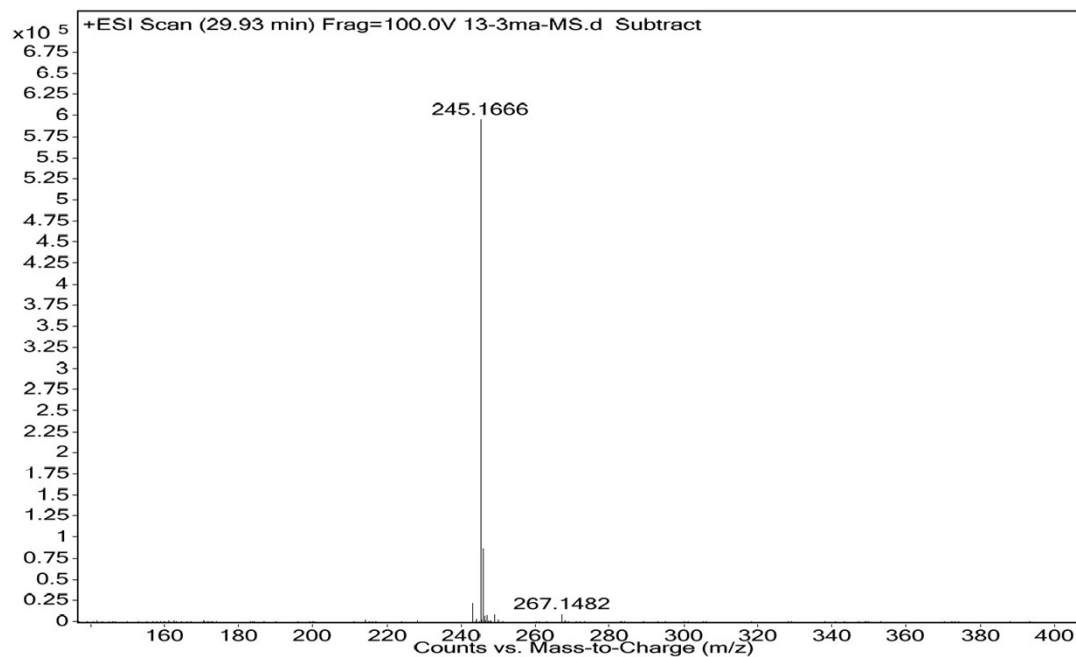


Fig.S 60 <sup>1</sup>H NMR of compound **3fd**

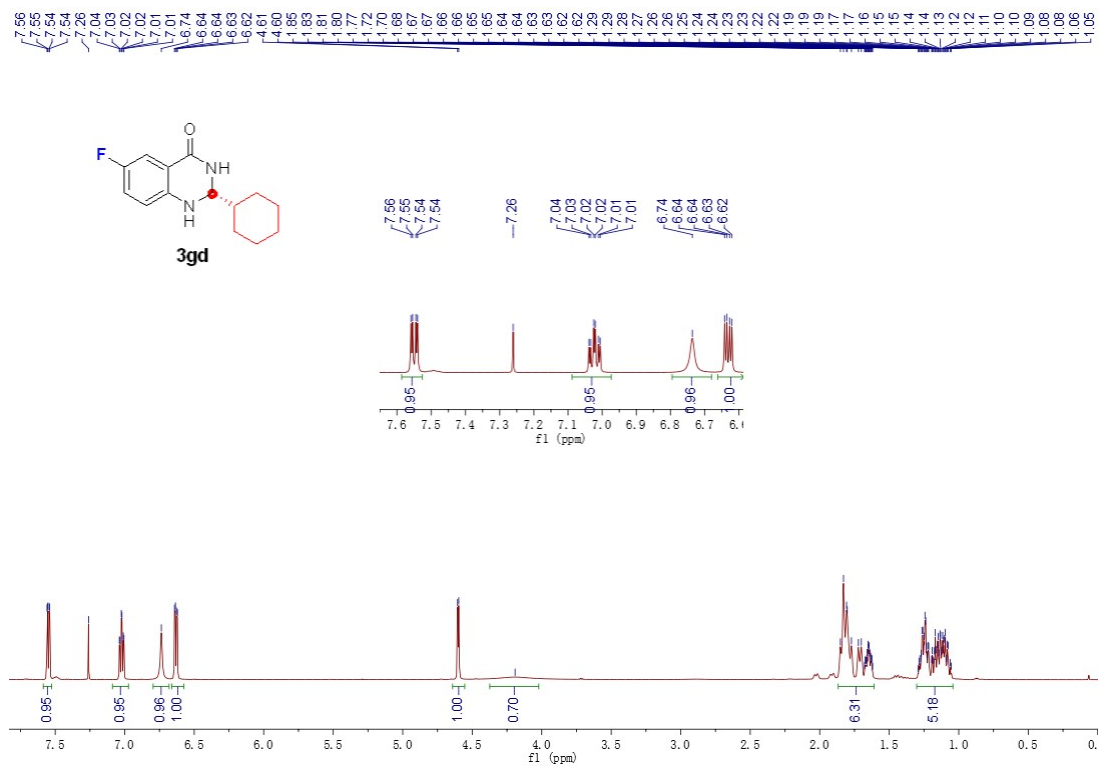


Fig.S 61 <sup>1</sup>H NMR of compound 3gd

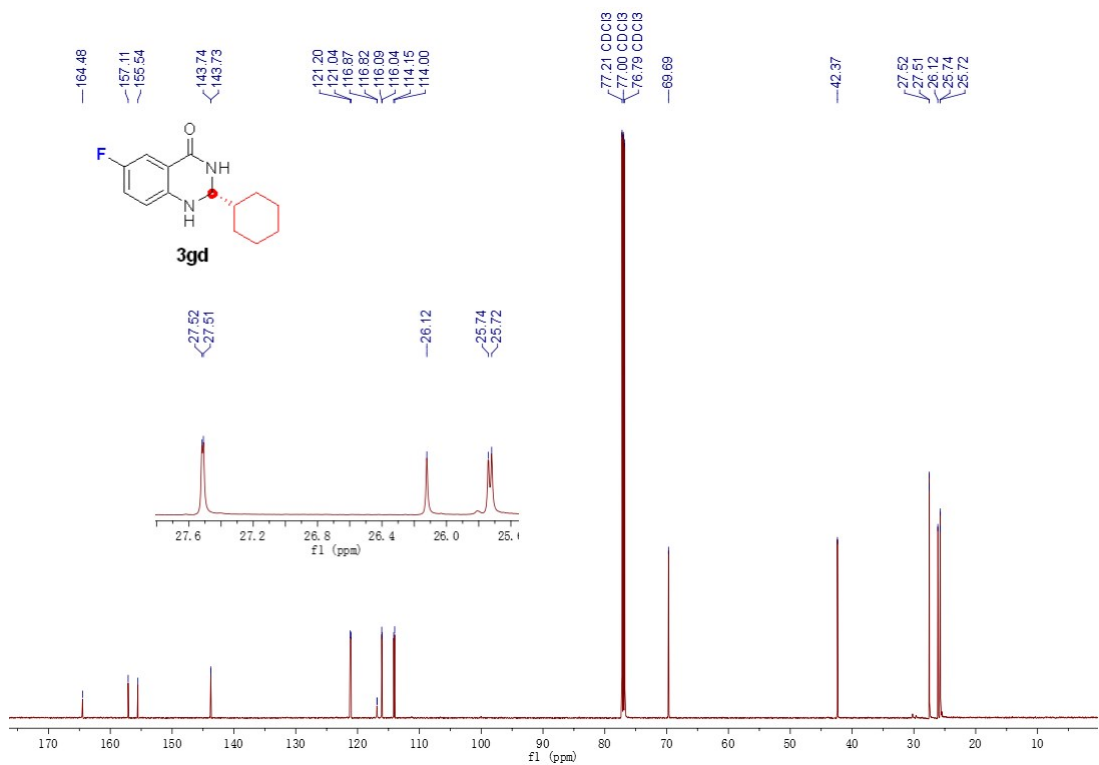


Fig.S 62 <sup>13</sup>C NMR of compound 3gd

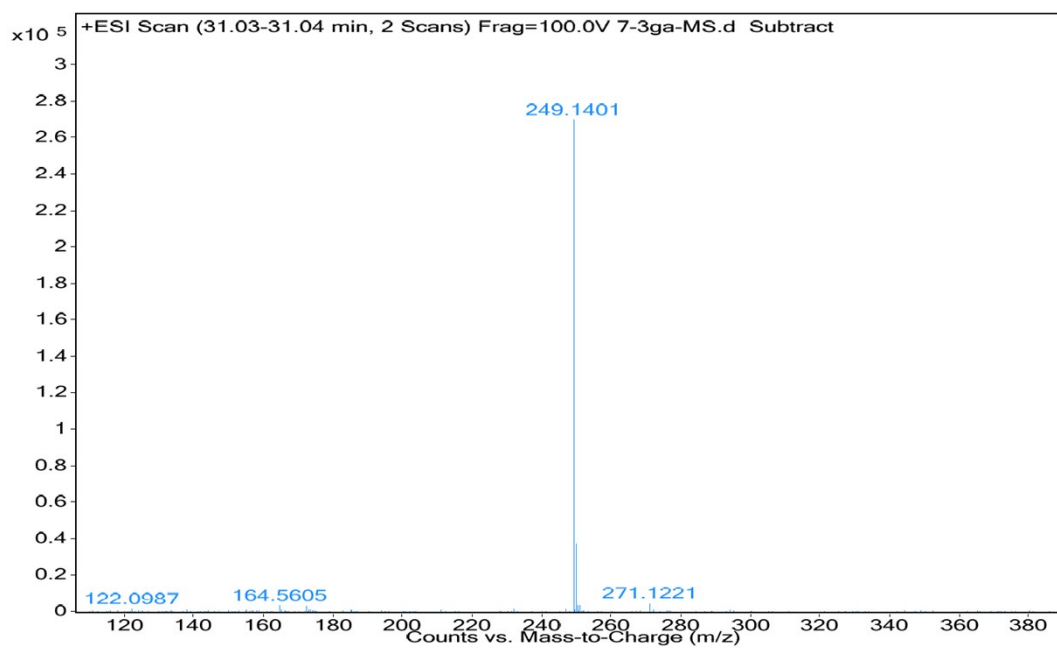


Fig.S 63 <sup>1</sup>H NMR of compound 3gd

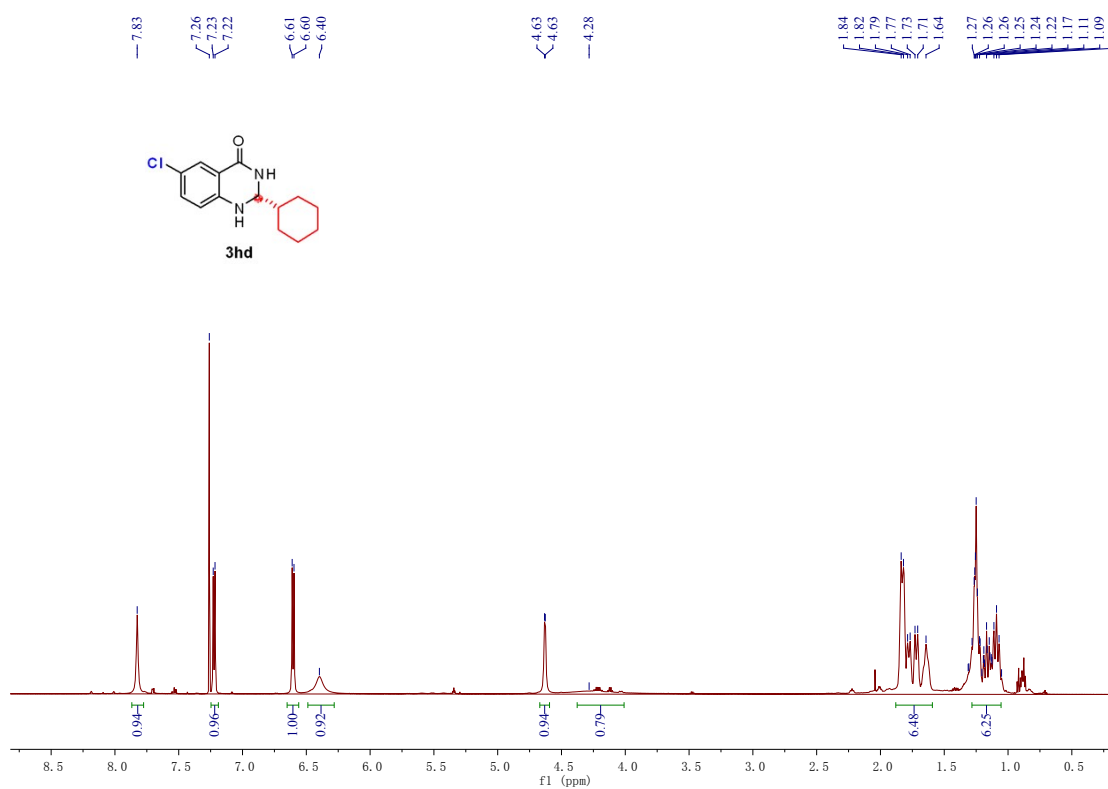


Fig.S 64 <sup>1</sup>H NMR of compound 3hd



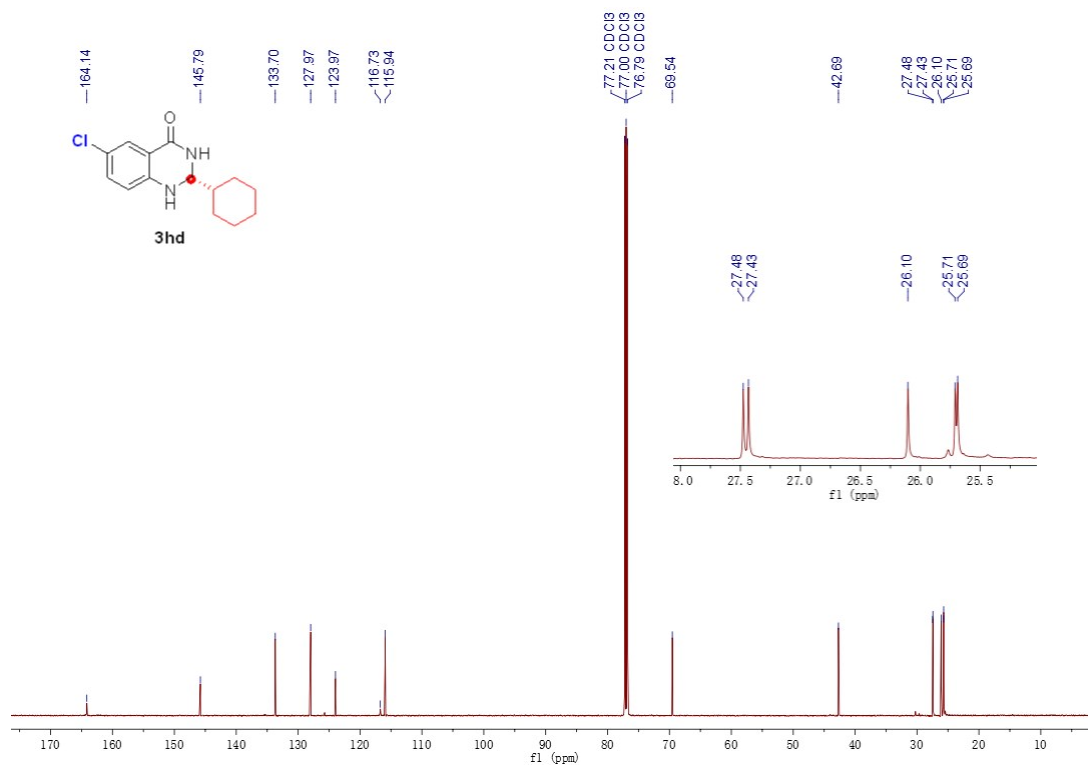


Fig.S 65 <sup>13</sup>C NMR of compound **3hd**

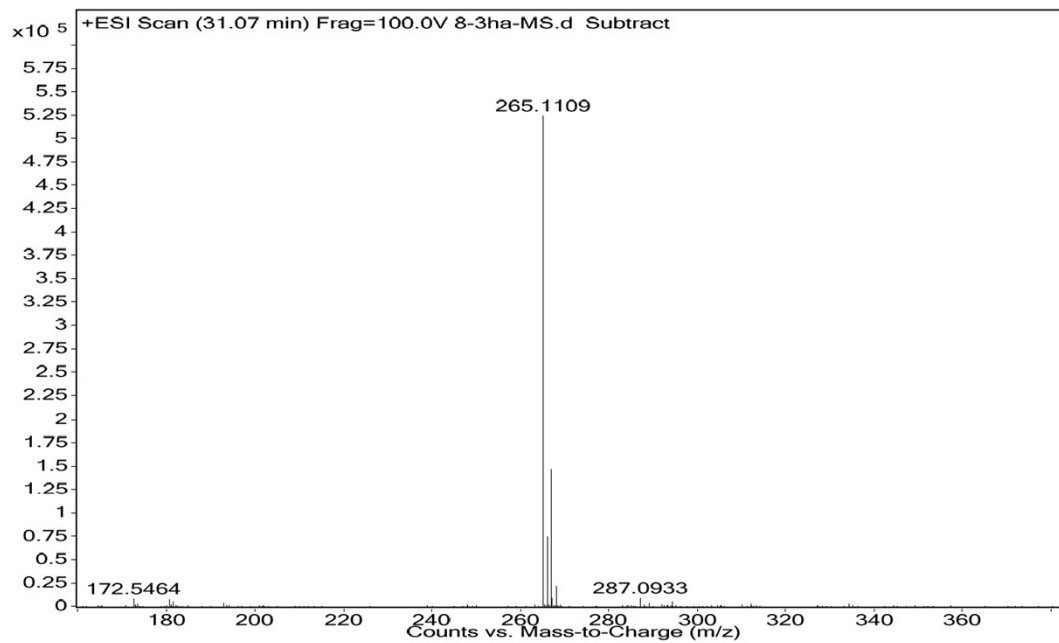


Fig.S 66 <sup>1</sup>H NMR of compound **3cd**

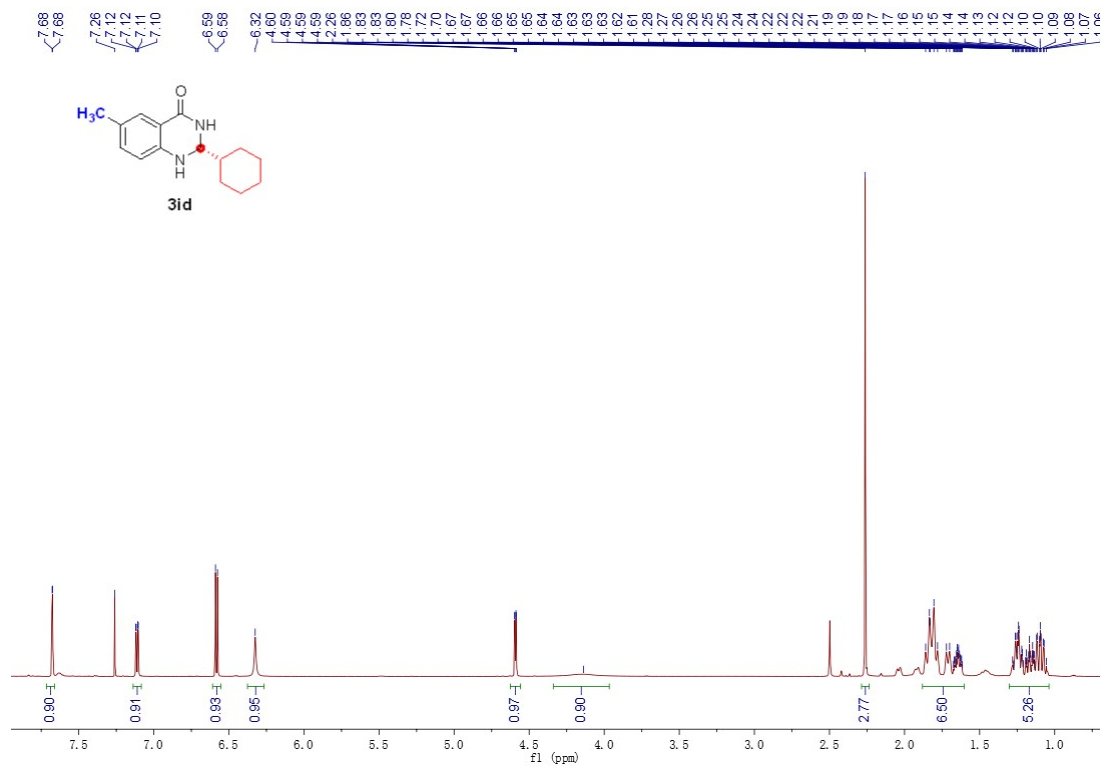


Fig.S 67 <sup>1</sup>H NMR of compound **3id**

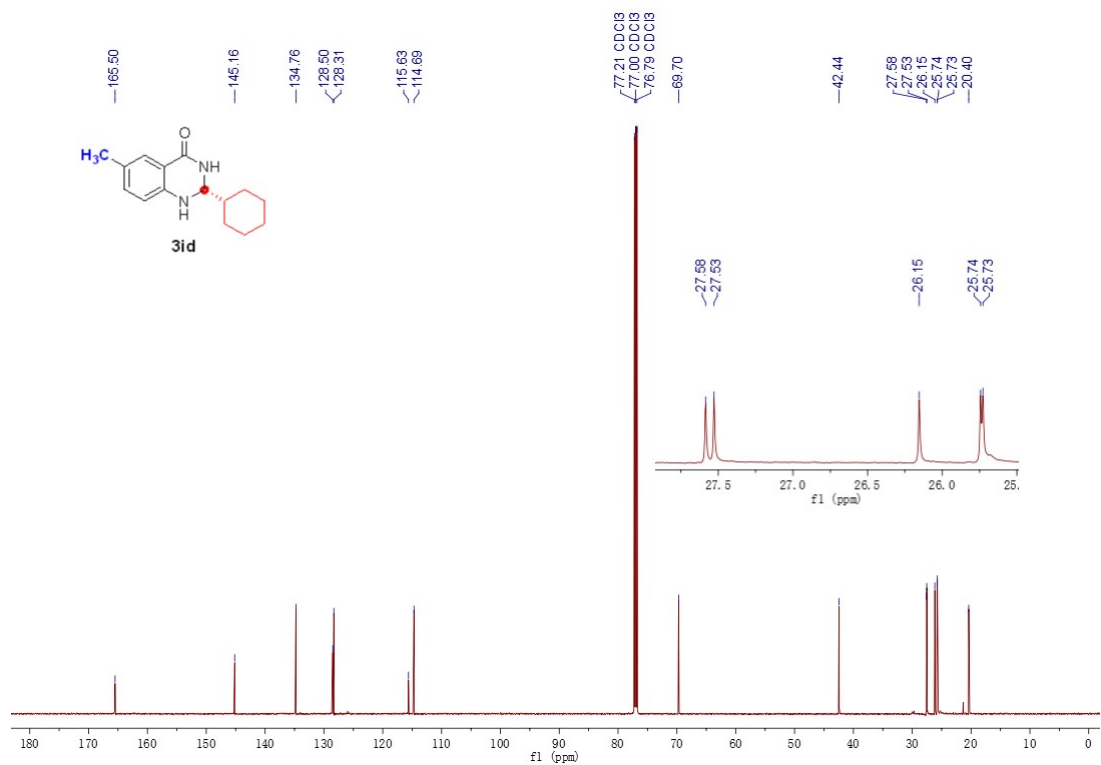


Fig.S 68 <sup>13</sup>C NMR of compound **3id**

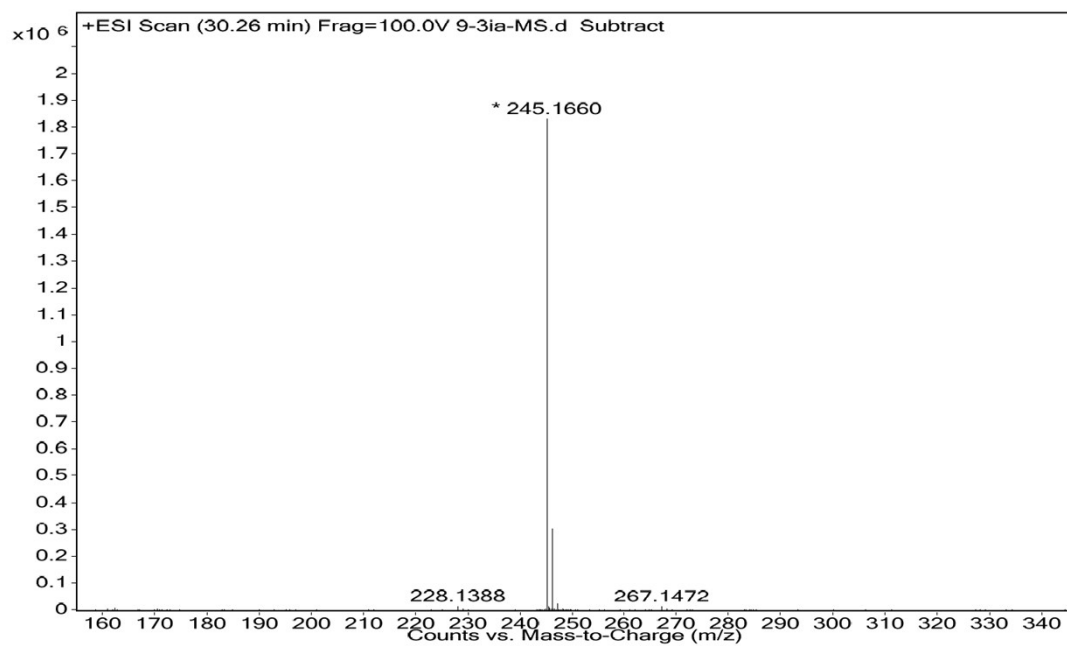


Fig.S 69 <sup>1</sup>H NMR of compound 3id

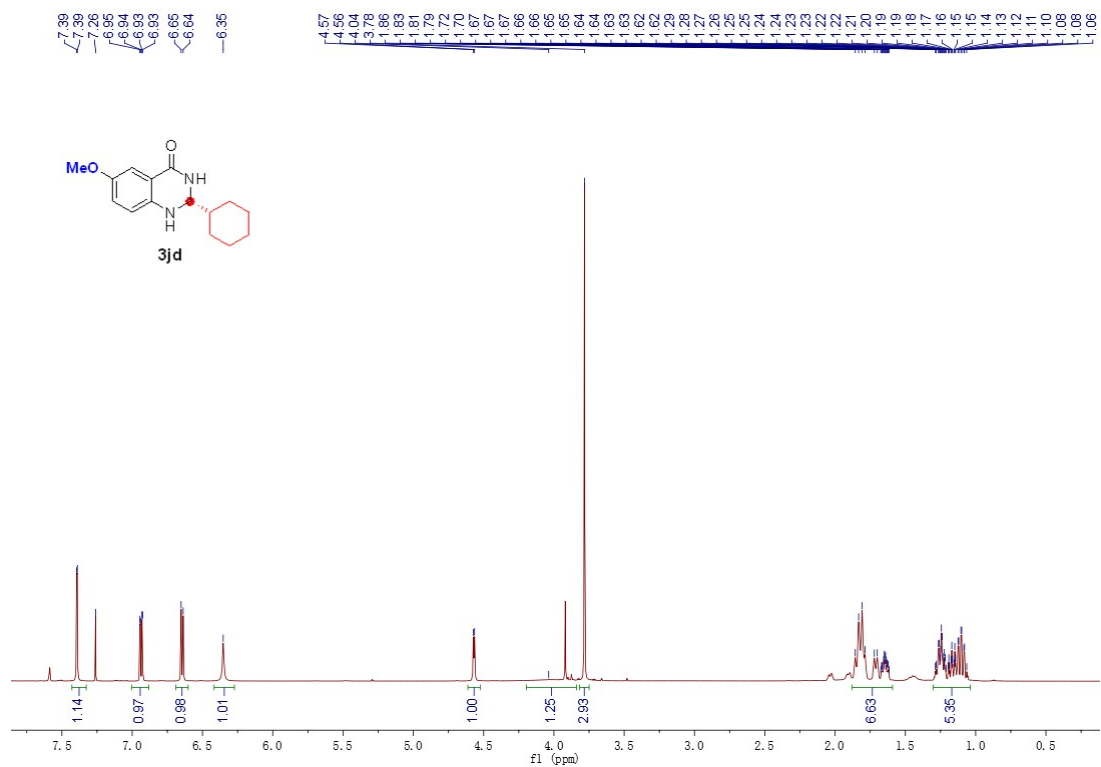


Fig.S 70 <sup>1</sup>H NMR of compound 3id

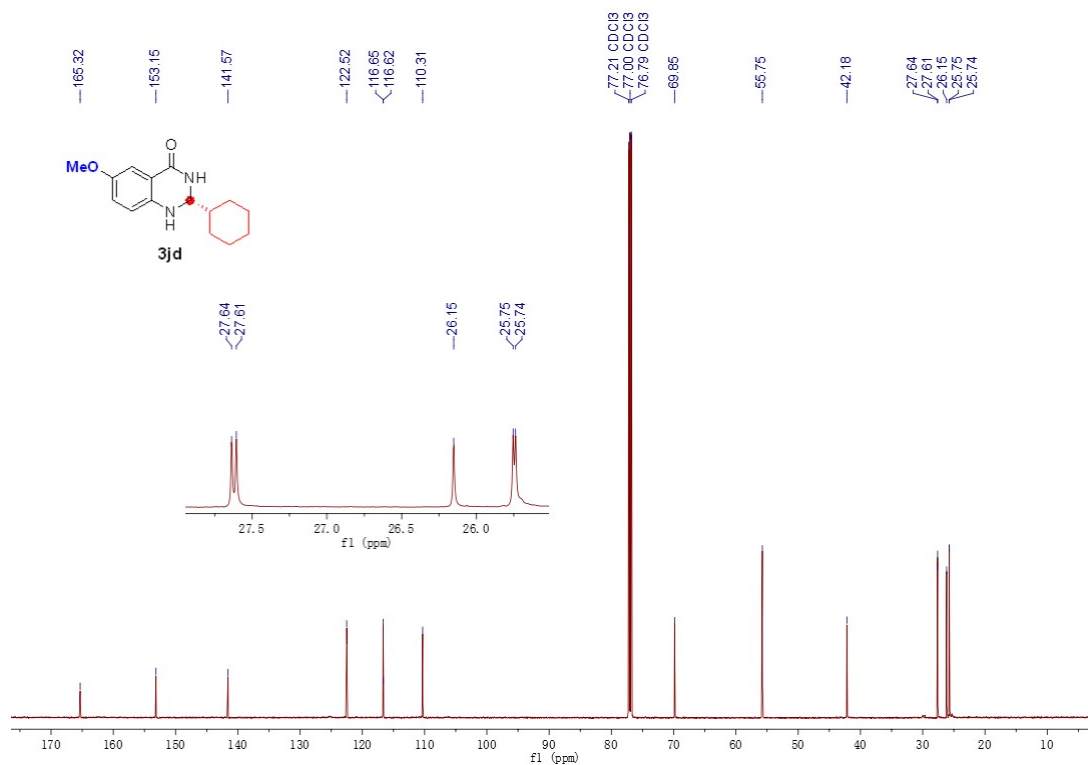


Fig.S 71 <sup>13</sup>C NMR of compound **3jd**

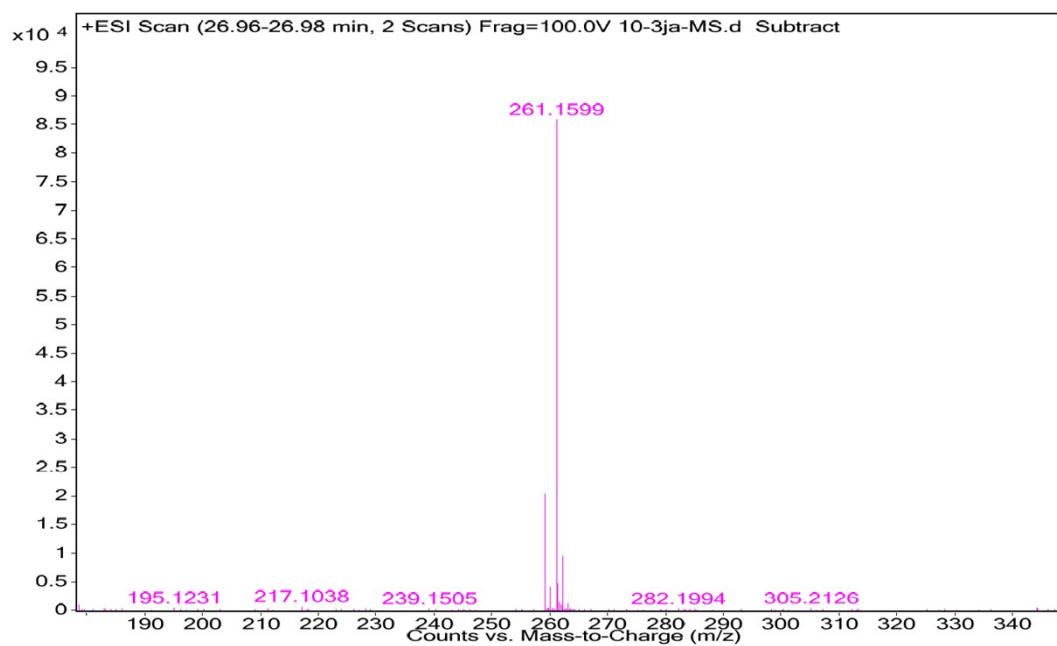


Fig.S 72 <sup>1</sup>H NMR of compound **3jd**

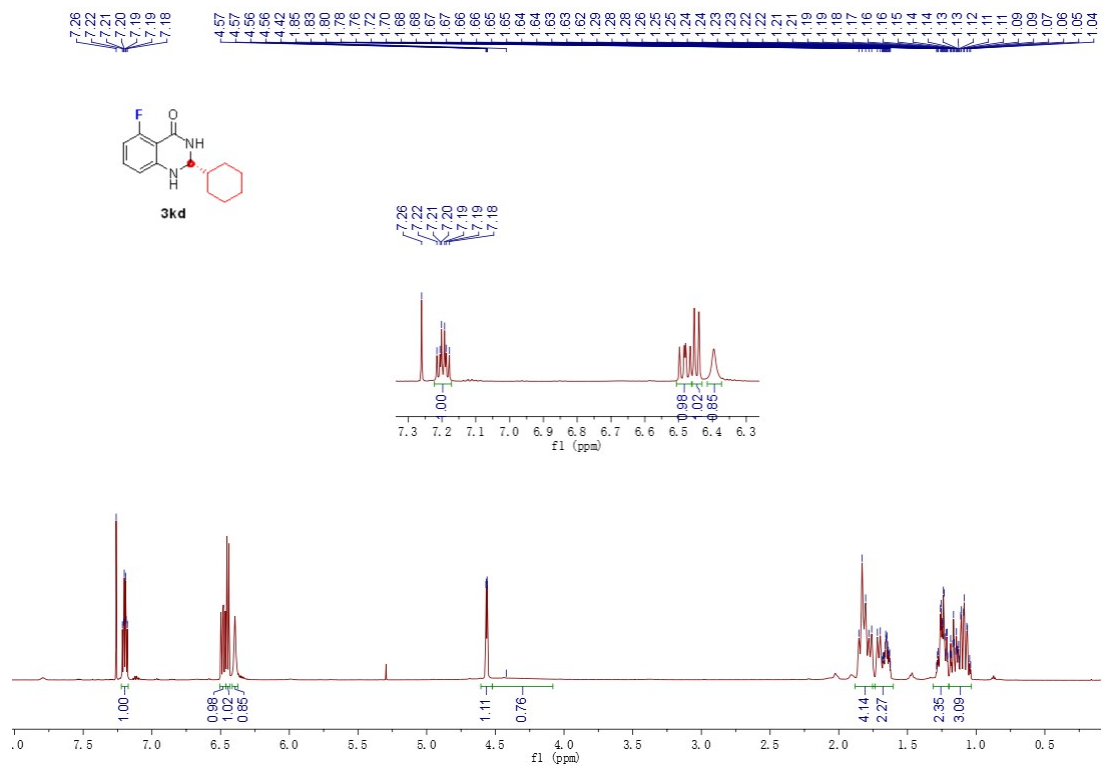


Fig.S 73 <sup>1</sup>H NMR of compound 3kd

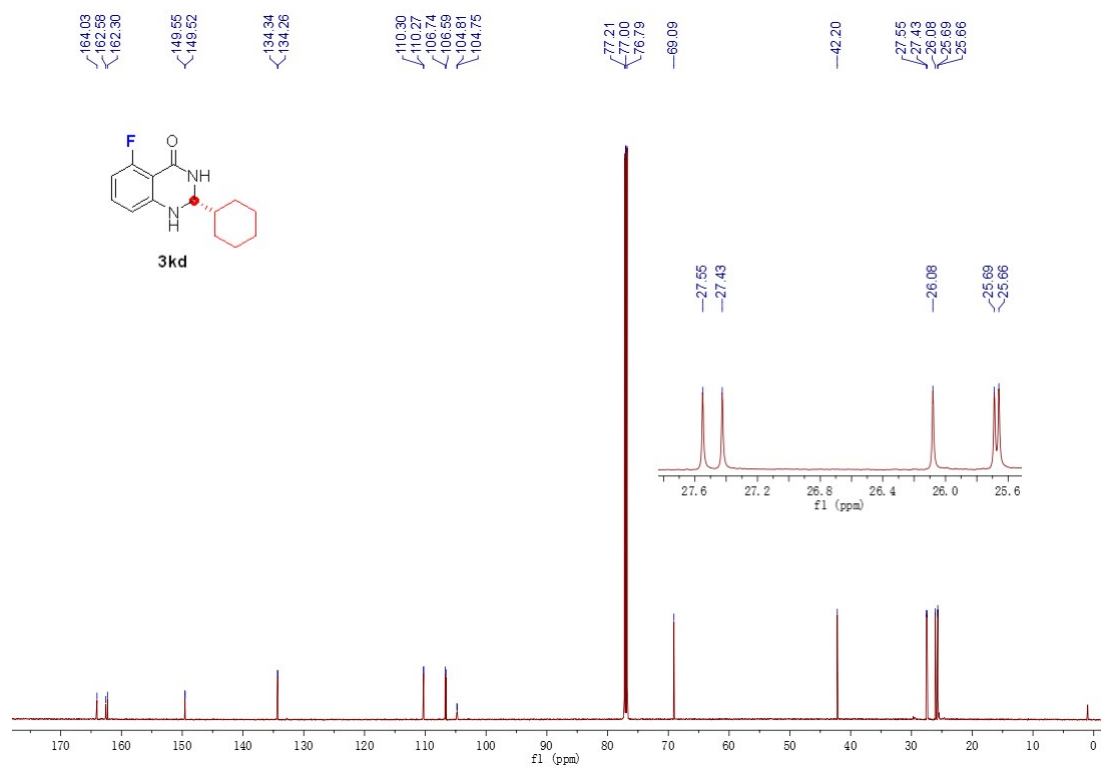


Fig.S 74 <sup>13</sup>C NMR of compound 3kd

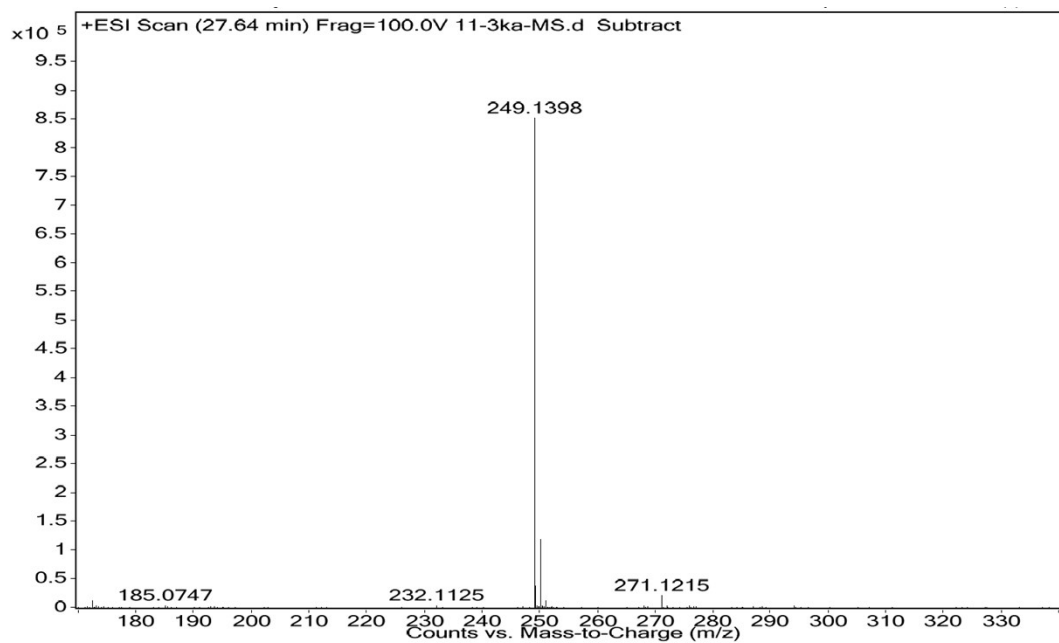


Fig.S 75 <sup>1</sup>H NMR of compound 3kd

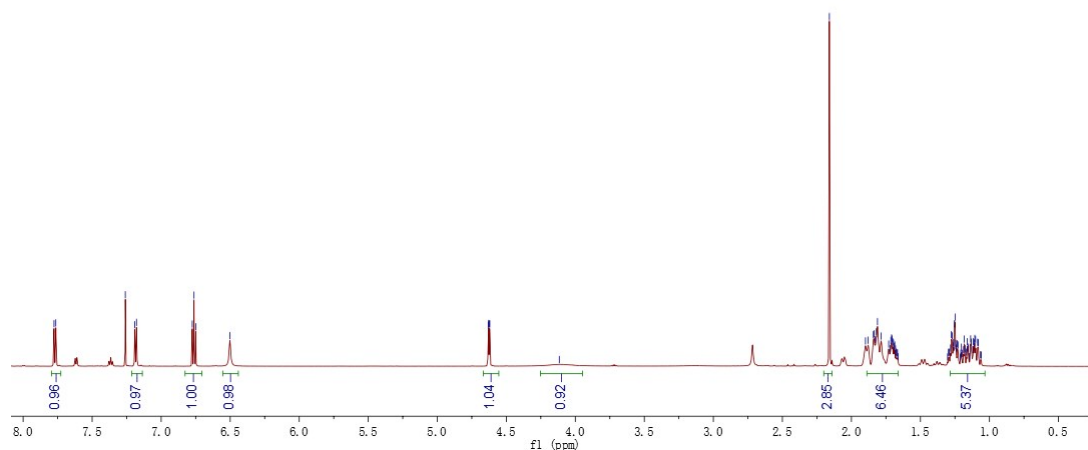
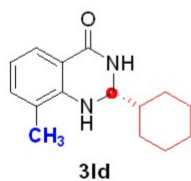


Fig.S 76 <sup>1</sup>H NMR of compound 3ld

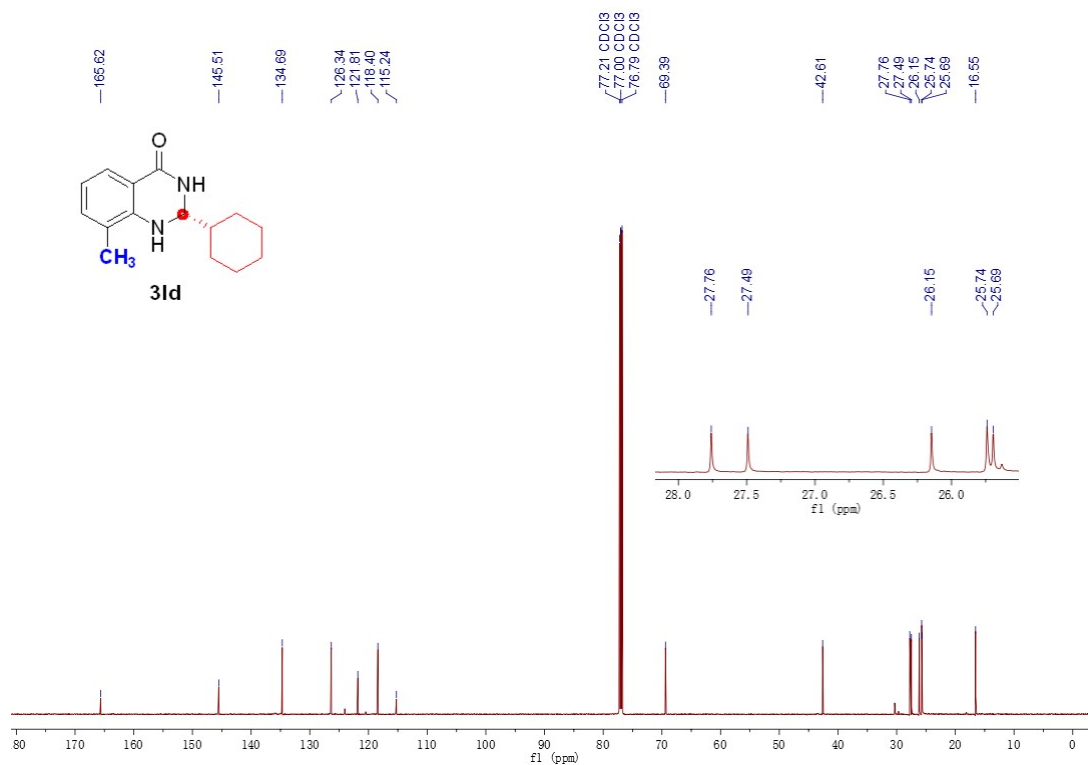


Fig.S 77 <sup>13</sup>C NMR of compound **31d**

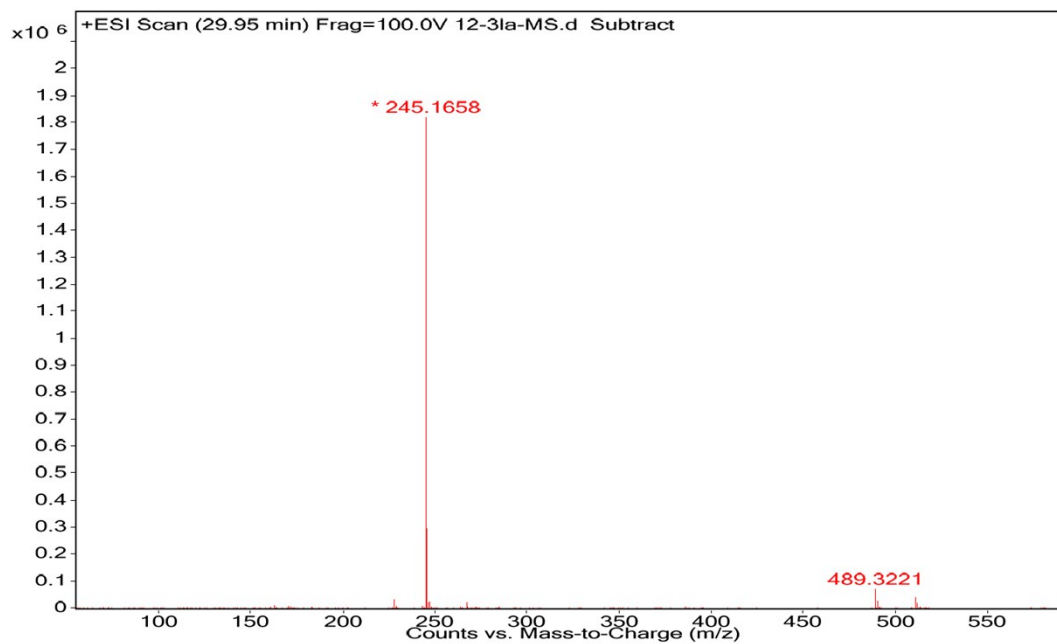


Fig.S 78 <sup>1</sup>H NMR of compound **31d**

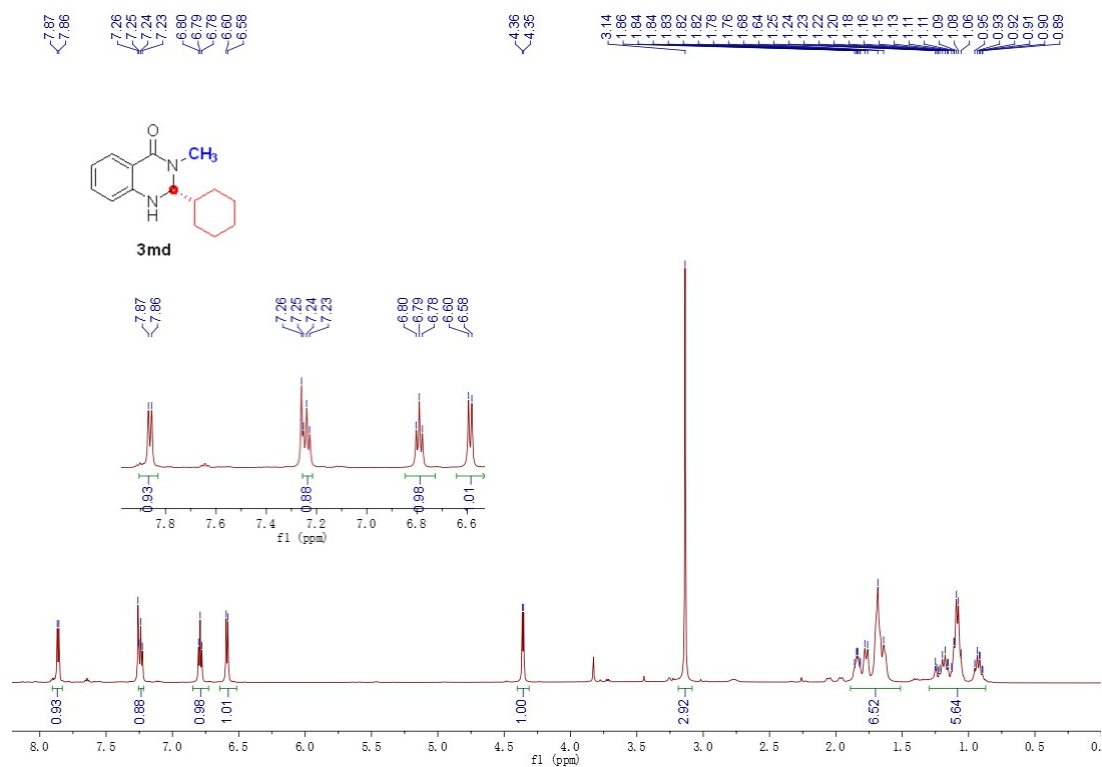


Fig.S 79 <sup>1</sup>H NMR of compound **3md**

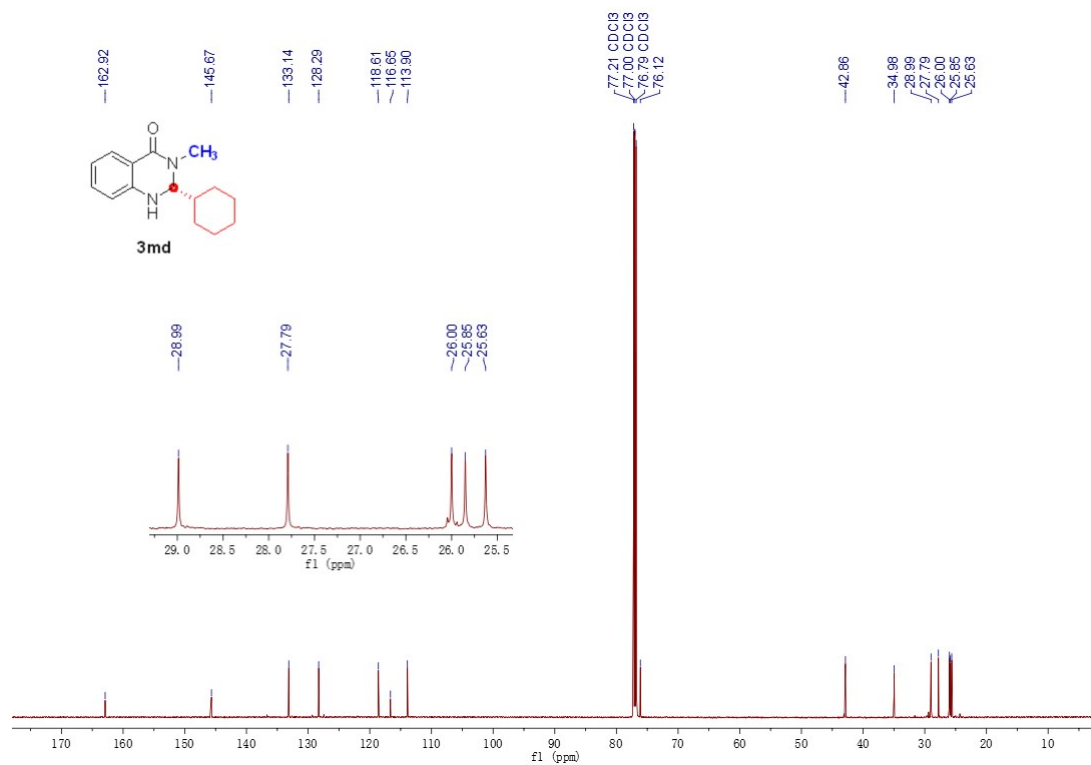


Fig.S 80 <sup>13</sup>C NMR of compound **3md**





Fig.S 81 <sup>1</sup>H NMR of compound **3md**

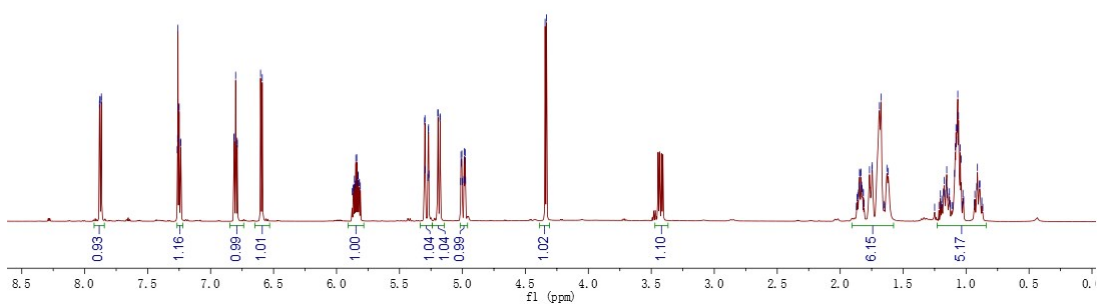
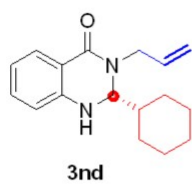


Fig.S 82 <sup>1</sup>H NMR of compound **3md**

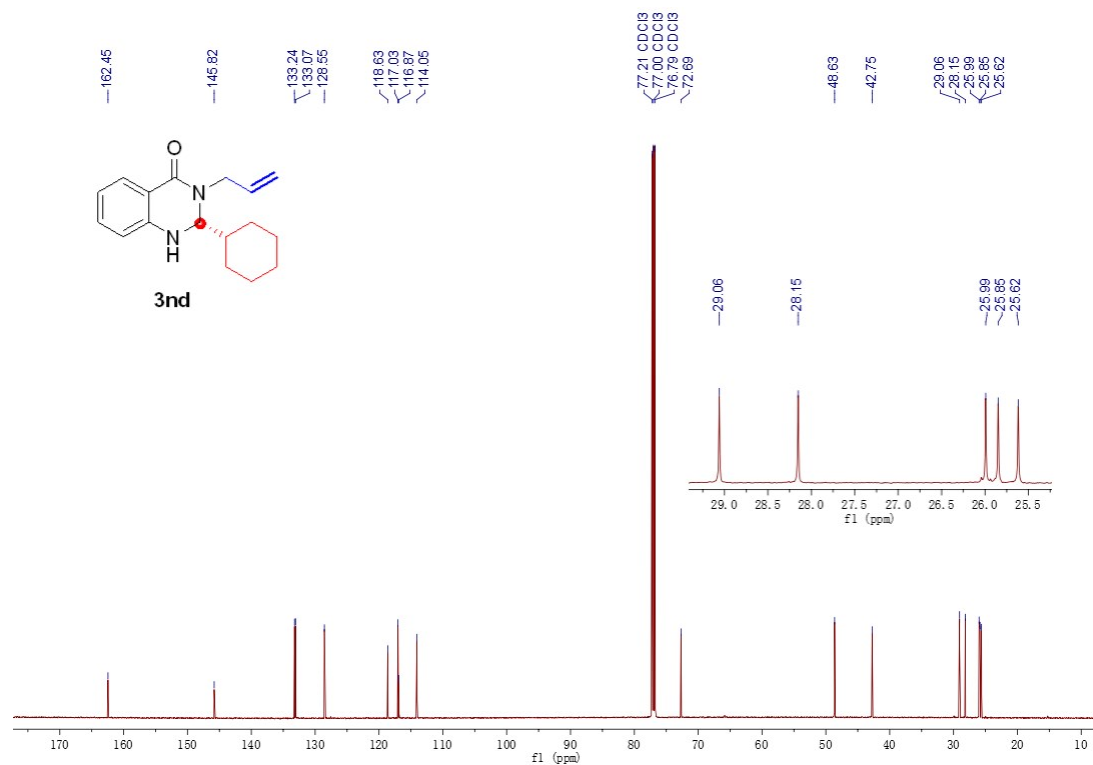


Fig.S 83 <sup>13</sup>C NMR of compound **3nd**

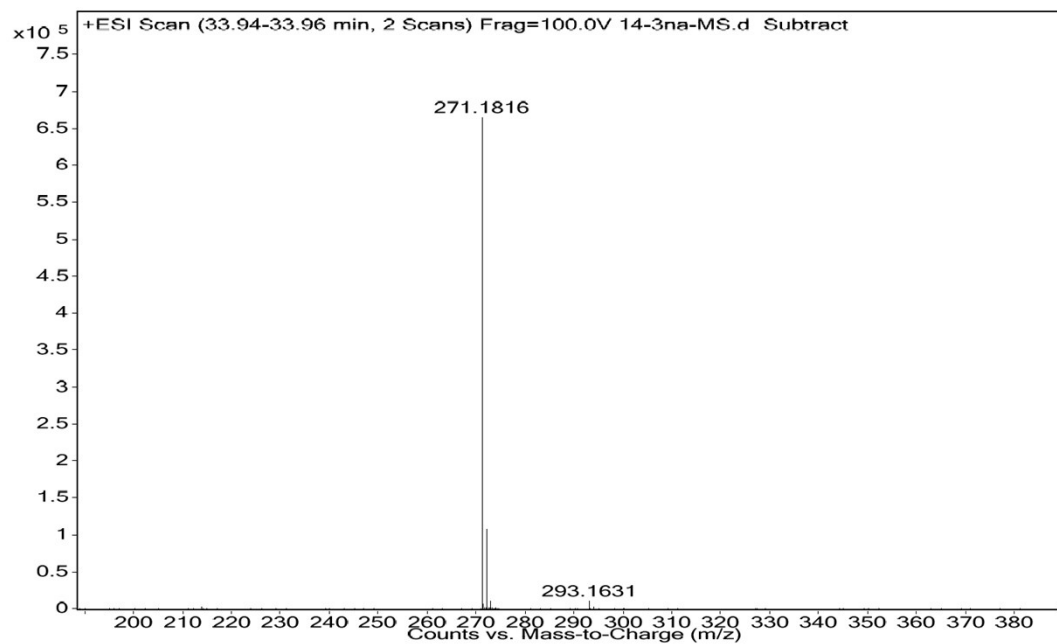


Fig.S 84 <sup>1</sup>H NMR of compound **3nd**



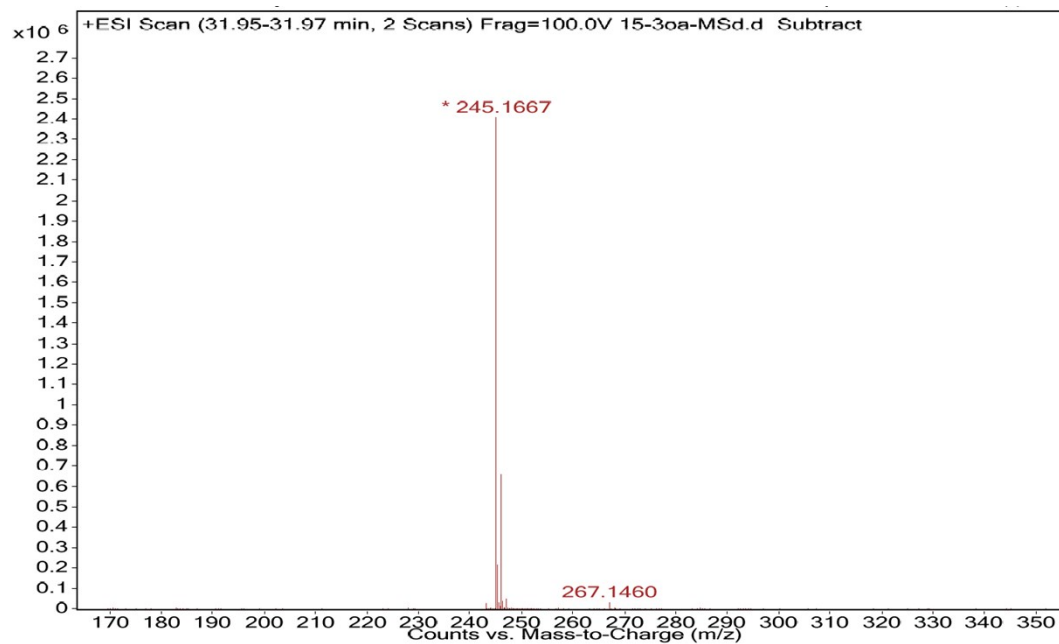


Fig.S 87 <sup>1</sup>H NMR of compound 30d

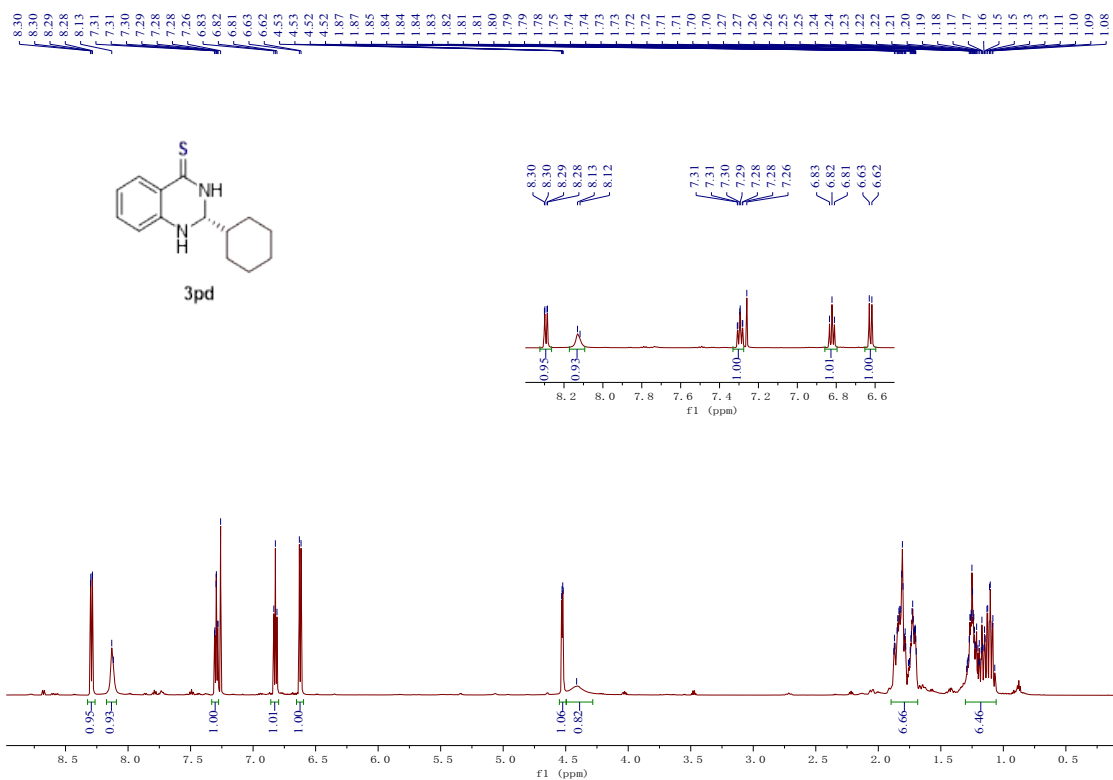


Fig.S 88 <sup>1</sup>H NMR of compound 3pd (Gram-scale)

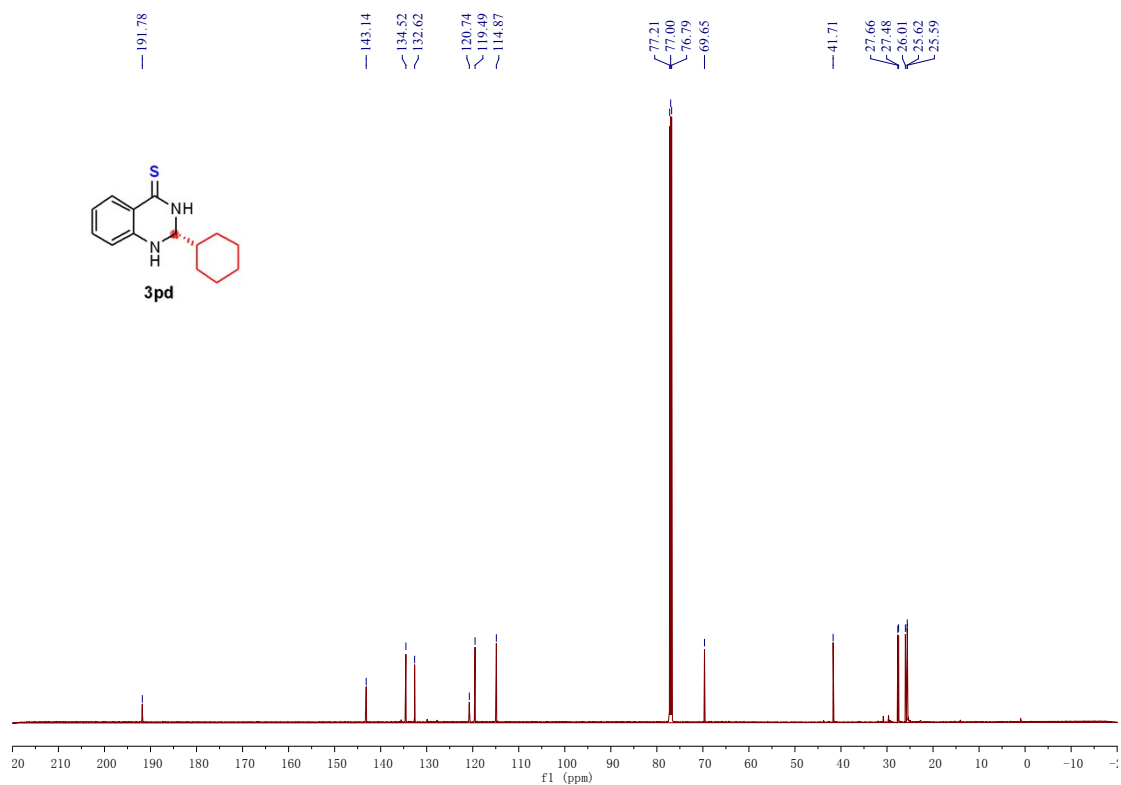


Fig.S 89 <sup>13</sup>C NMR of compound 3pd (Gram-scale)

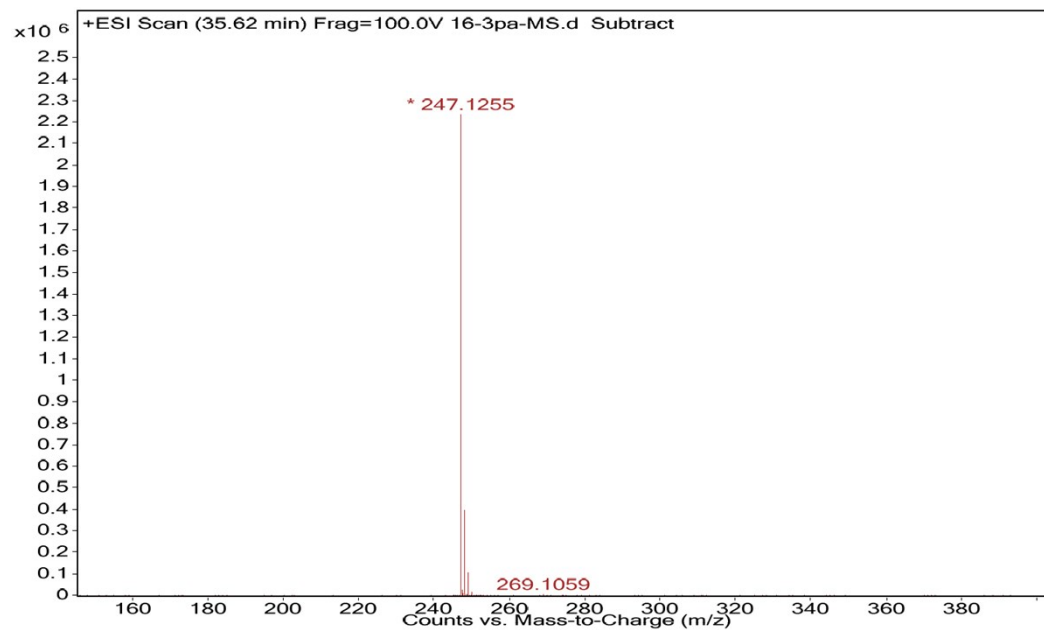
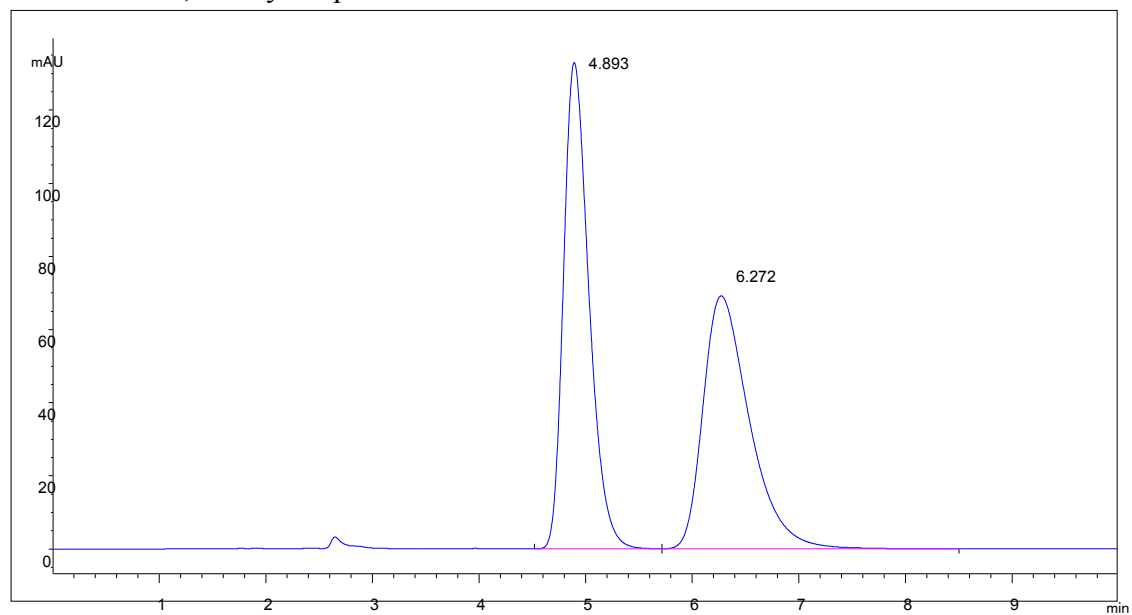


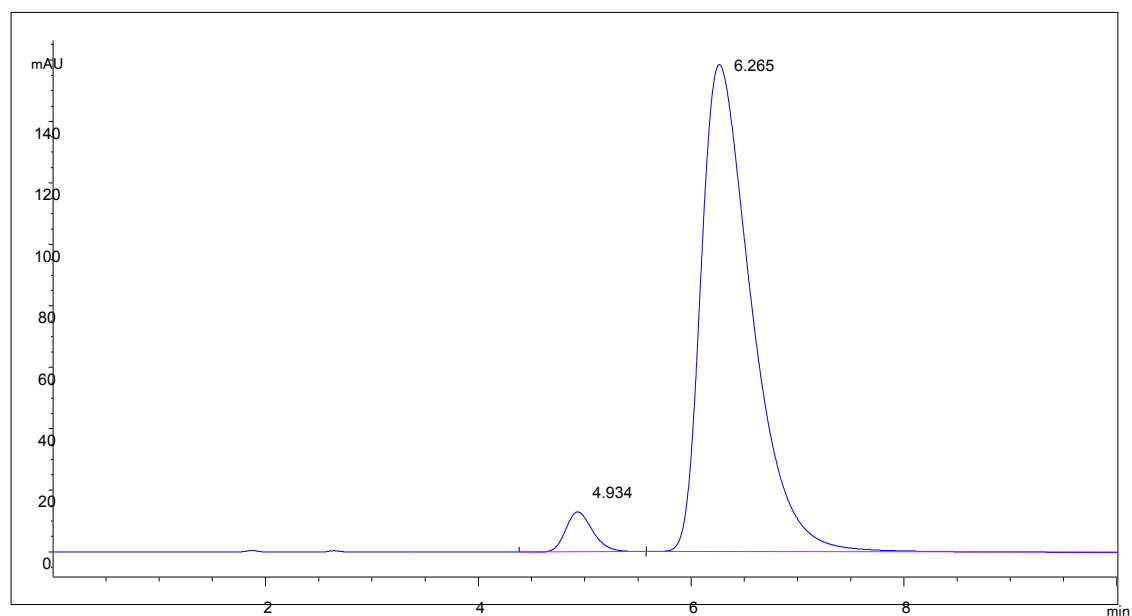
Fig.S 90 <sup>1</sup>H NMR of compound 3pd (Gram-scale)

#### 4. HPLC of 2,3-Dihydroquinazolinones **3**



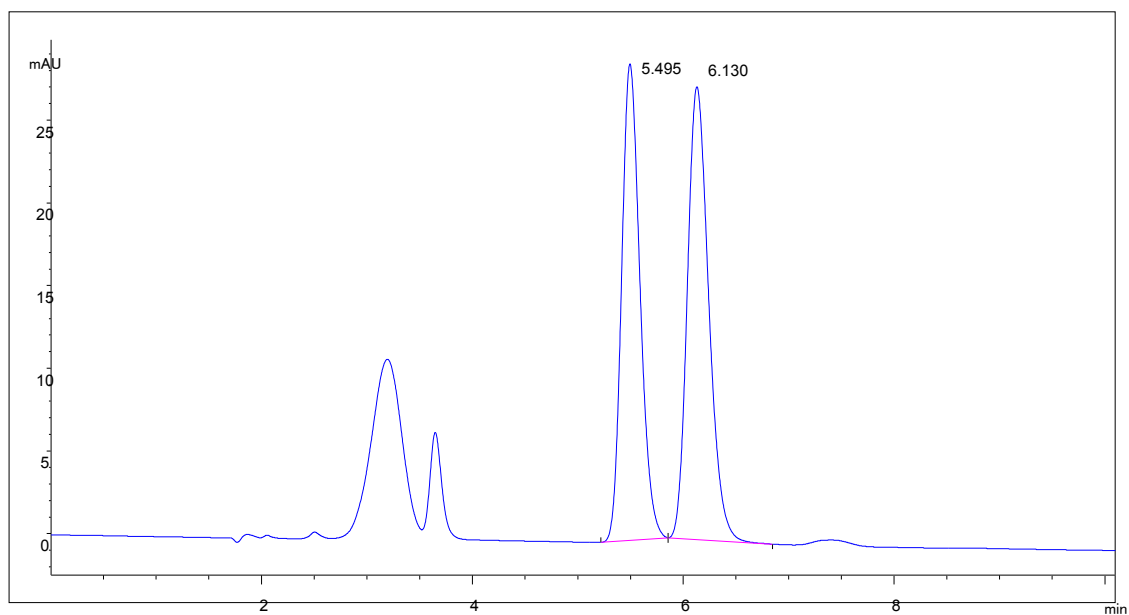
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	4.893	2201.5	132.9	51.265
2	6.272	2092.8	69.1	48.735

Fig.S 91 HPLC for racemic compound **3aa**



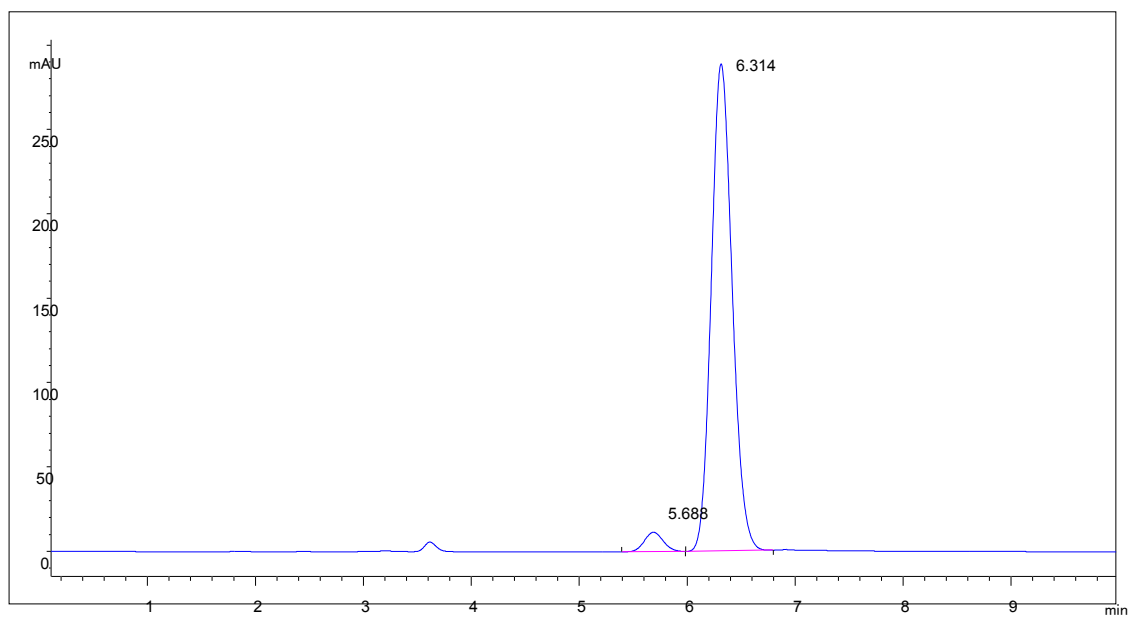
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	4.934	228.2	13	4.19
2	6.265	5218.8	158.5	95.810

Fig.S 92 HPLC for pure enantioenriched compound **3aa**



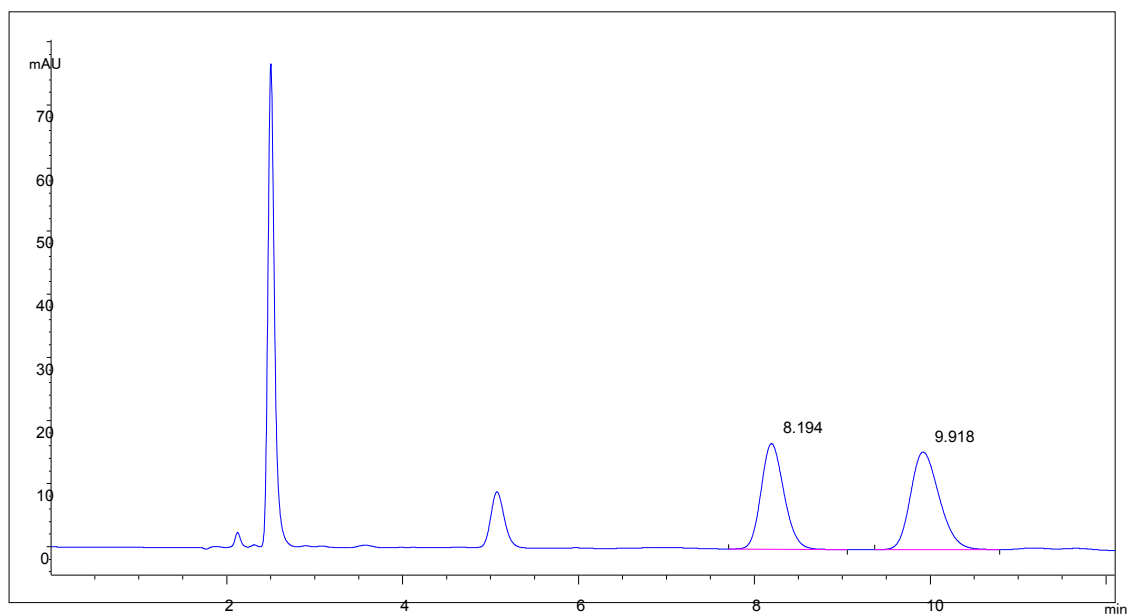
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	5.495	348.4	28.8	47.522
2	6.13	384.7	27.4	52.478

Fig.S 93 HPLC for racemic compound **3ab**



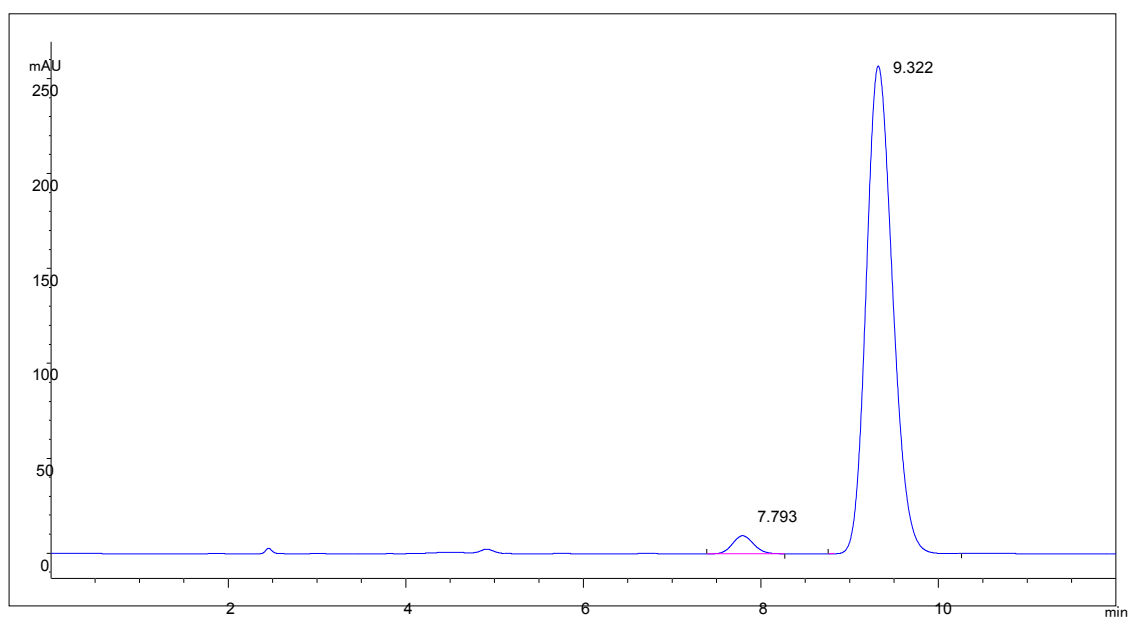
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	5.688	140	11.5	3.481
2	6.314	3883.3	288.5	96.519

Fig.S 94 HPLC for pure enantioenriched compound **3ab**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.194	302.7	16.8	46.268
2	9.918	351.6	15.5	53.732

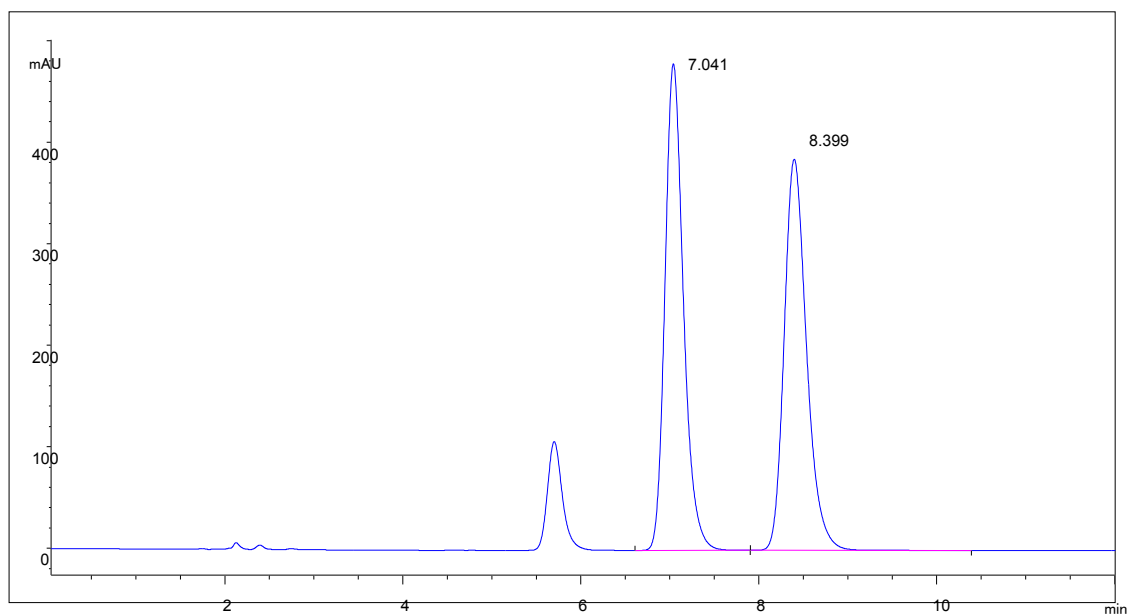
Fig.S 95 HPLC for racemic compound **3ac**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.793	156	9.5	2.862
2	9.322	5293.4	256.9	97.138

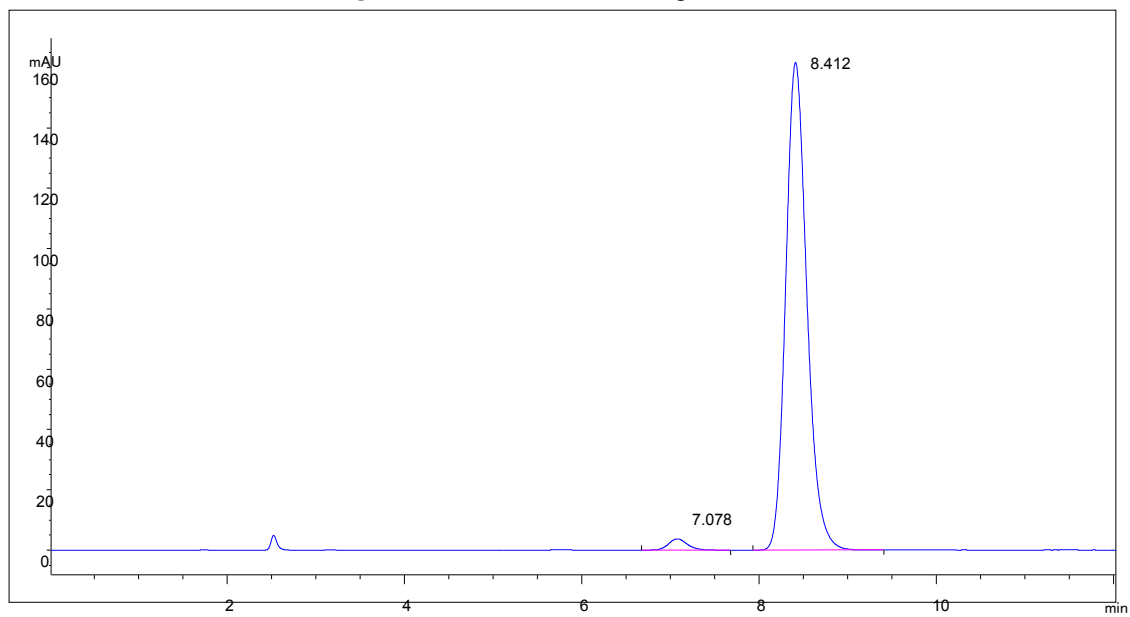
Fig.S 96 HPLC for pure enantioenriched compound **3ac**





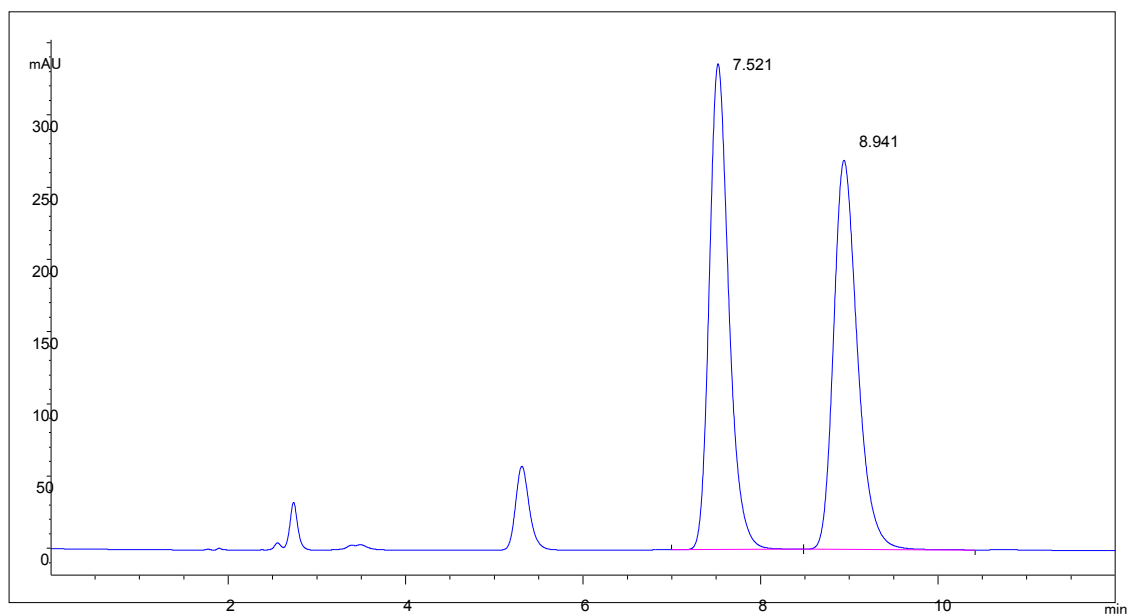
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.041	6897.2	479.2	50.648
2	8.399	6720.6	385.2	49.352

Fig.S 97 HPLC for racemic compound **3ad**



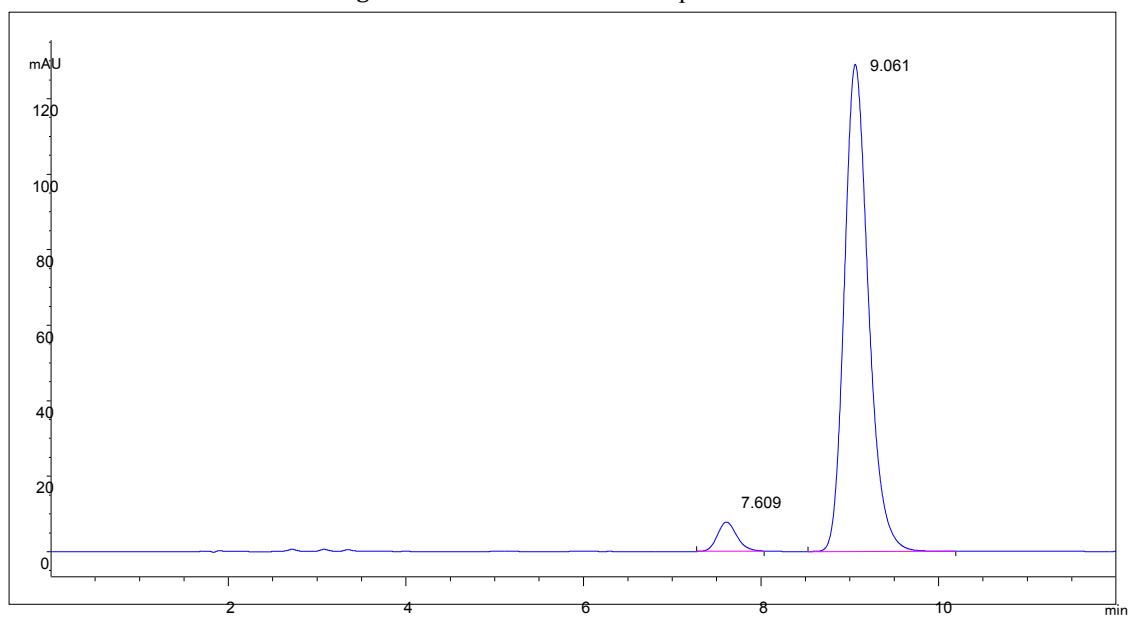
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.078	56.3	3.8	2.058
2	8.412	2680.4	161.7	97.942

Fig.S 98 HPLC for pure enantioenriched compound **3ad (Gram-scale)**



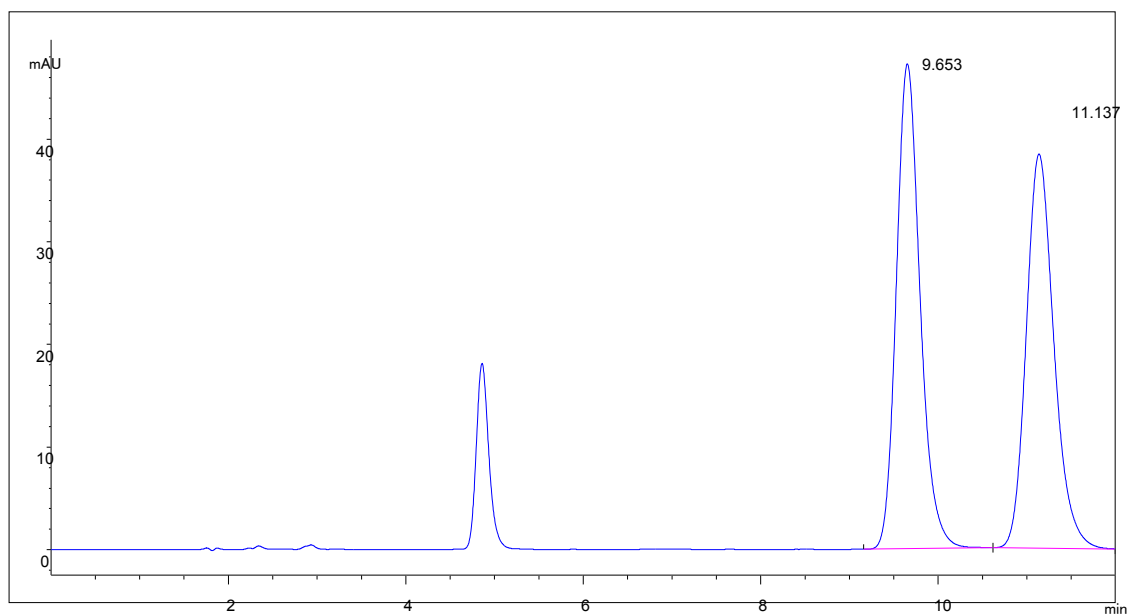
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.521	5147.8	336.3	50.575
2	8.941	5030.7	269.4	49.425

Fig.S 99 HPLC for racemic compound **3ae**



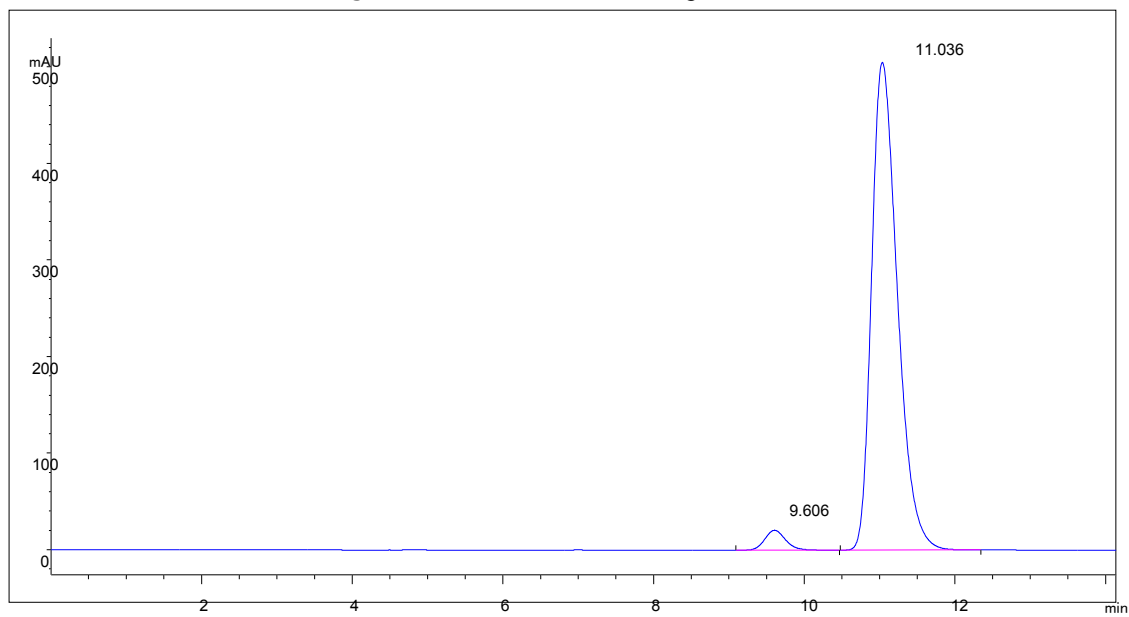
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.609	119.2	7.8	4.673
2	9.061	2431.7	129	95.327

Fig.S 100 HPLC for pure enantioenriched compound **3ae (Gram-scale)**



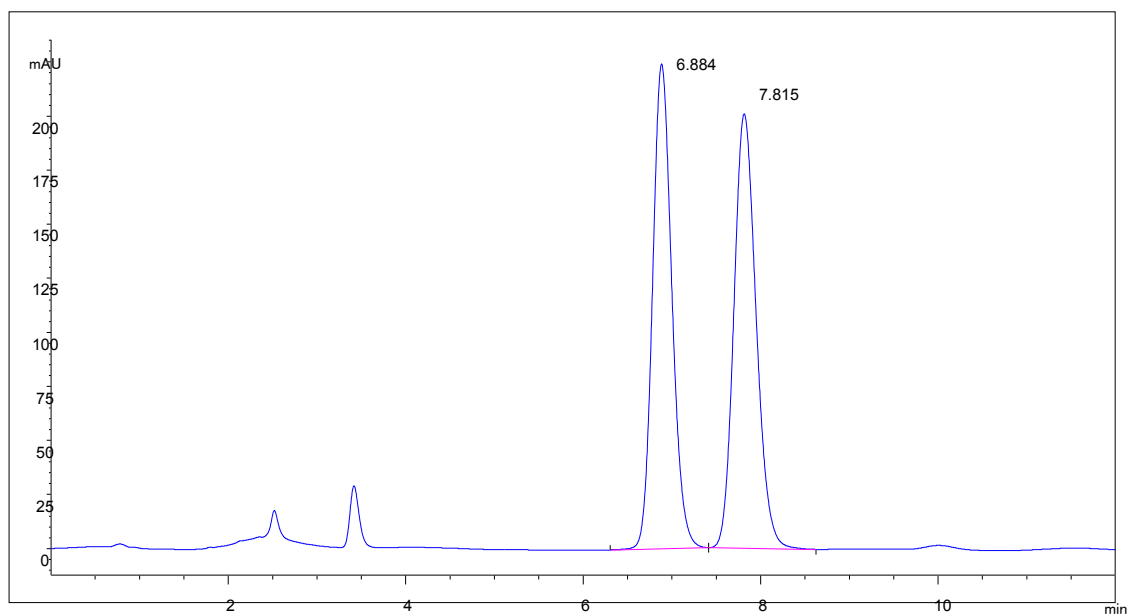
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	9.653	878.5	47.2	51.405
2	11.137	830.5	38.4	48.595

Fig.S 101 HPLC for racemic compound **3af**



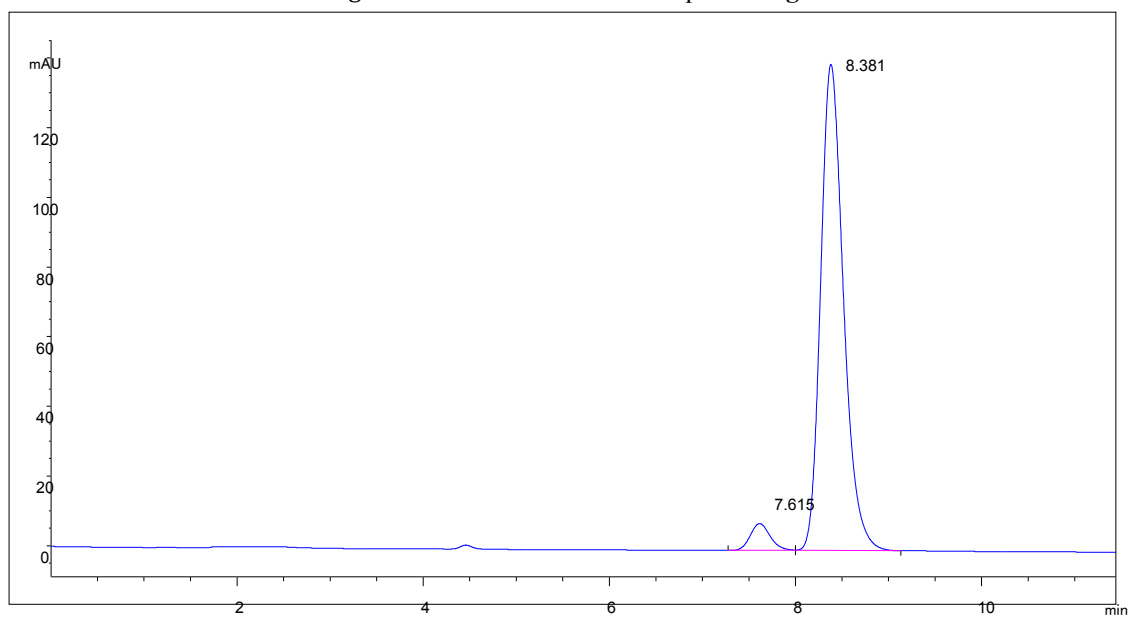
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	9.606	393.3	20.5	3.171
2	11.036	12010.6	505	96.829

Fig.S 102 HPLC for pure enantioenriched compound **3af**



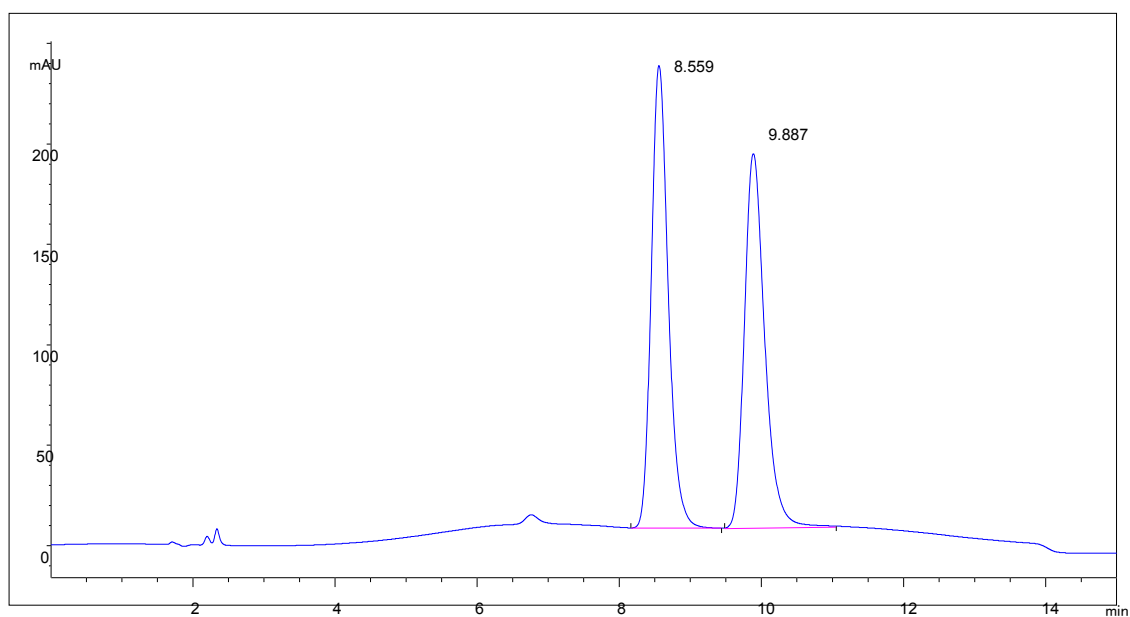
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.884	3376.1	224.3	49.188
2	7.815	3487.6	200.9	50.812

Fig.S 103 HPLC for racemic compound **3ag**



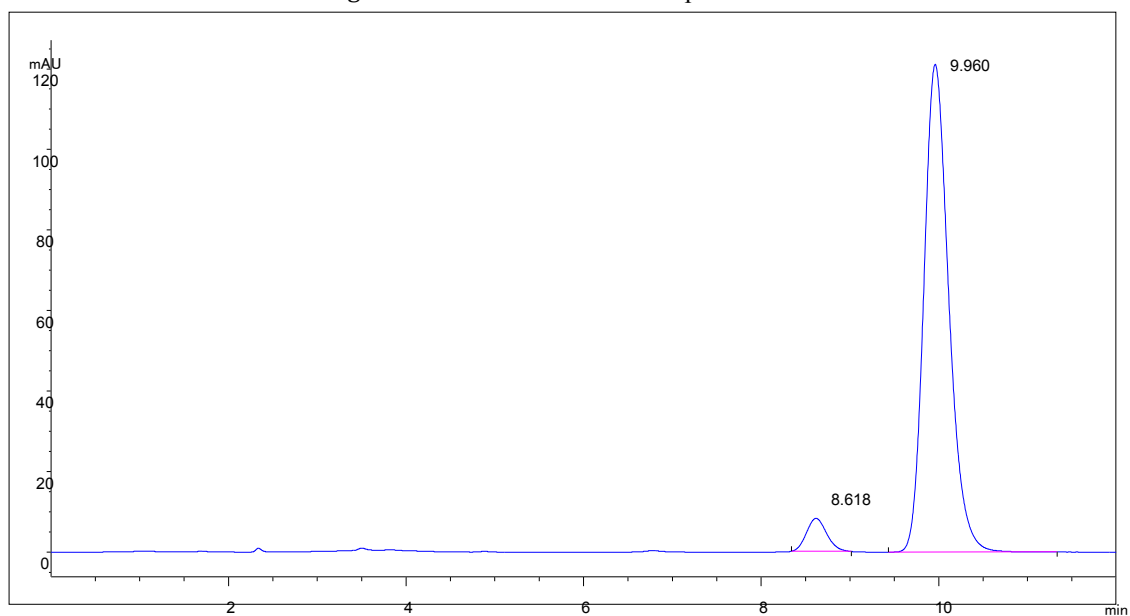
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.615	112.8	7.7	4.533
2	8.371	2376.4	139.6	95.467

Fig.S 104 HPLC for pure enantioenriched compound **3ag (Gram-scale)**



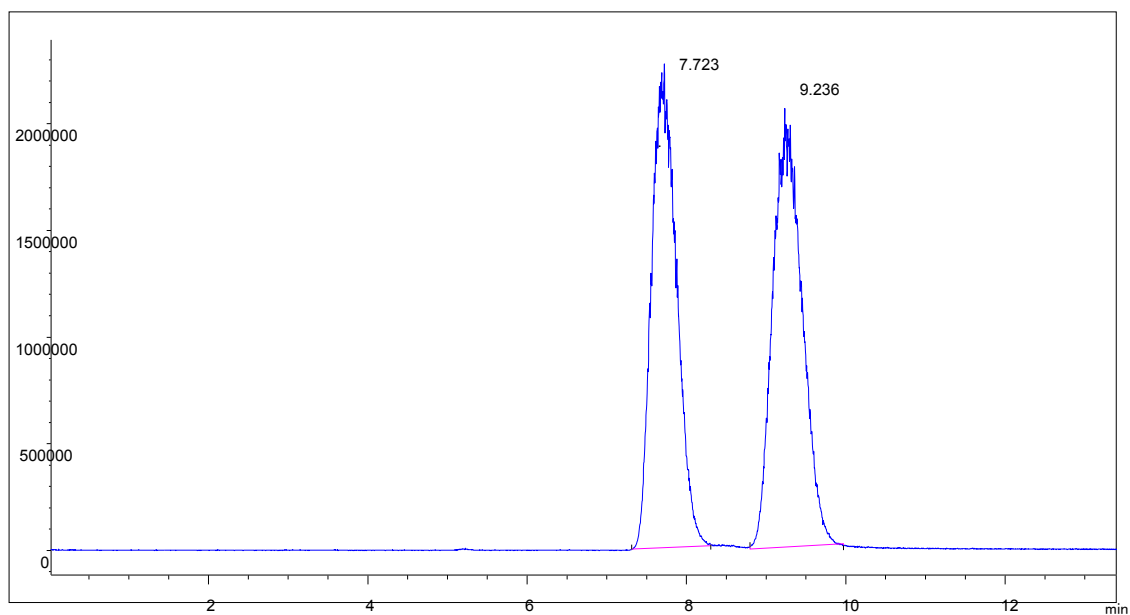
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.559	3823.2	230.2	50.743
2	9.887	3711.2	186.5	49.257

Fig.S 105 HPLC for racemic compound **3ah**



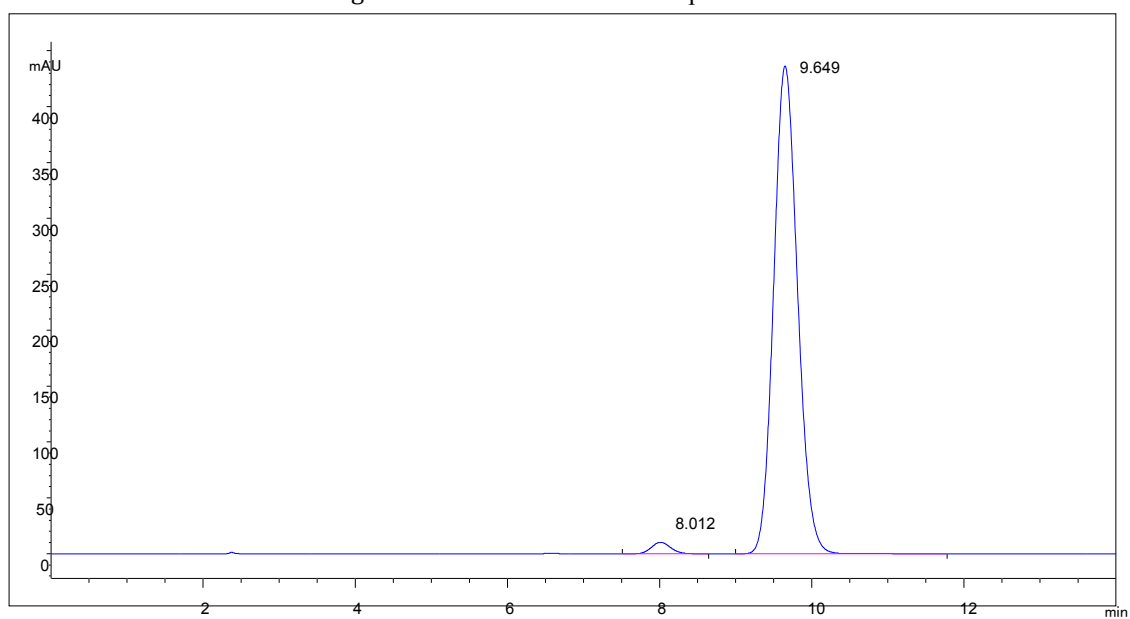
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.618	130.2	8.2	5.241
2	9.96	2354.4	121.1	94.759

Fig.S 106 HPLC for pure enantioenriched compound **3ah**



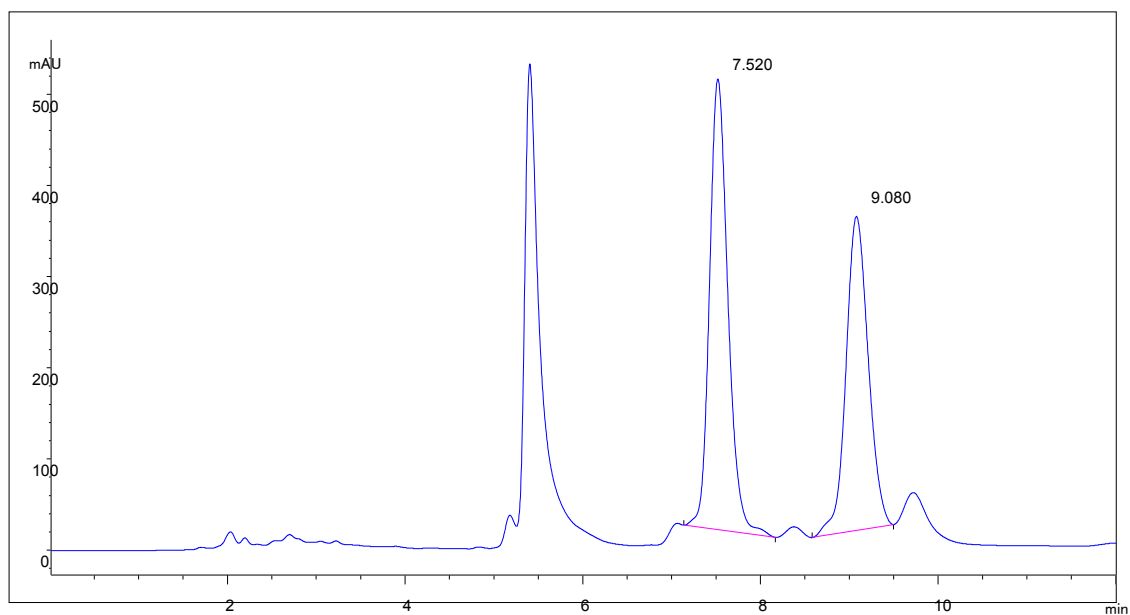
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.723	4862	227	48.642
2	9.236	5133	206	51.358

Fig.S 107 HPLC for racemic compound **3ai**



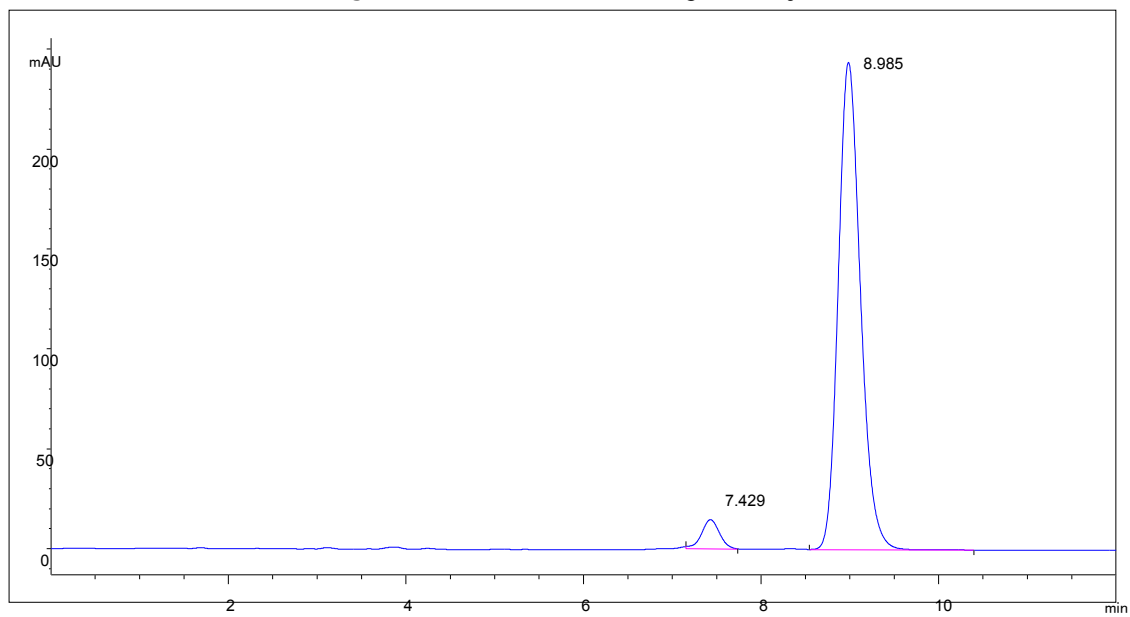
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.012	180.8	10.2	1.865
2	9.649	9511.2	436.4	98.135

Fig.S 108 HPLC for pure enantioenriched compound **3ai (Gram-scale)**



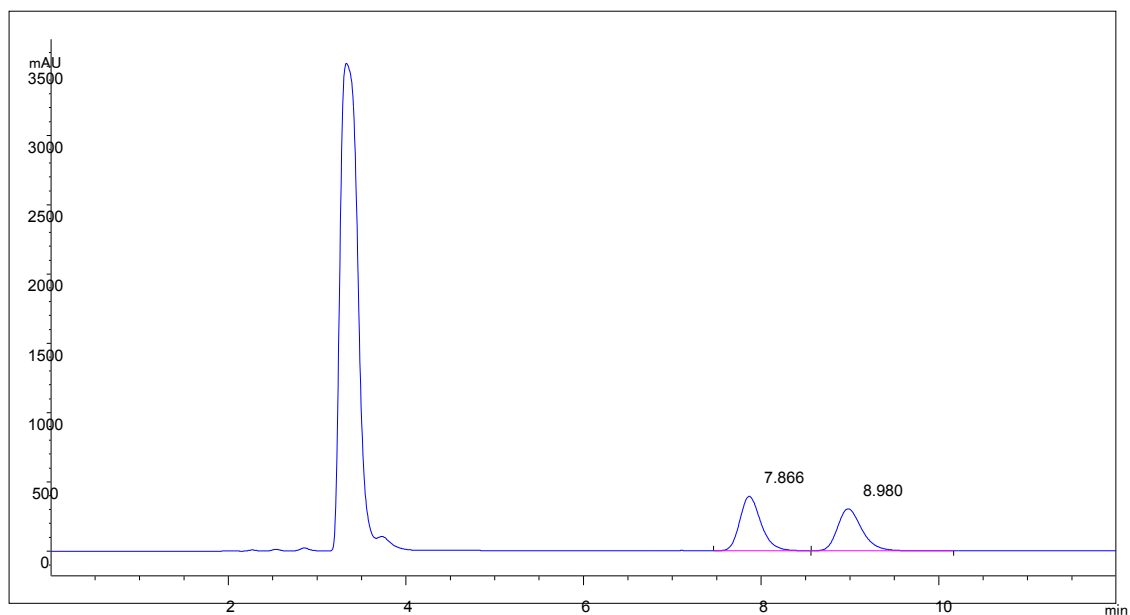
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.52	7142.8	494.4	54.334
2	9.08	6003.2	344.3	45.666

Fig.S 109 HPLC for racemic compound **3aj**



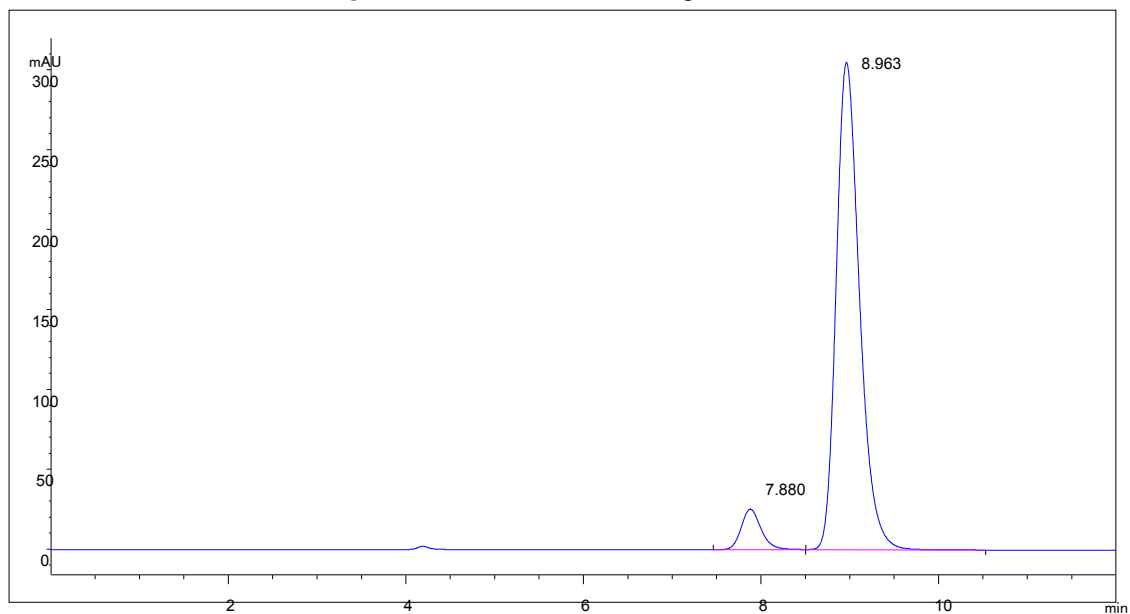
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.429	208.2	14.7	4.695
2	8.985	4227.6	243.8	95.305

Fig.S 110 HPLC for pure enantioenriched compound **3aj**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.866	6493.3	392.9	53.059
2	8.98	5744.5	303	46.941

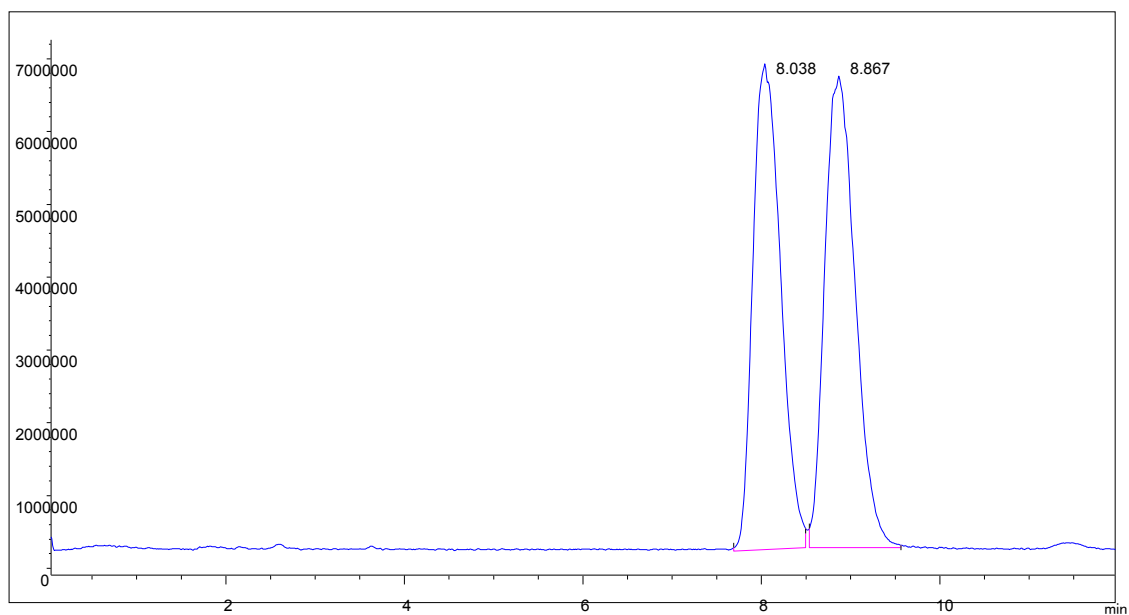
Fig.S 111 HPLC for racemic compound **3ak**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.88	381.5	25.3	6.582
2	8.963	5556.1	304.9	93.418

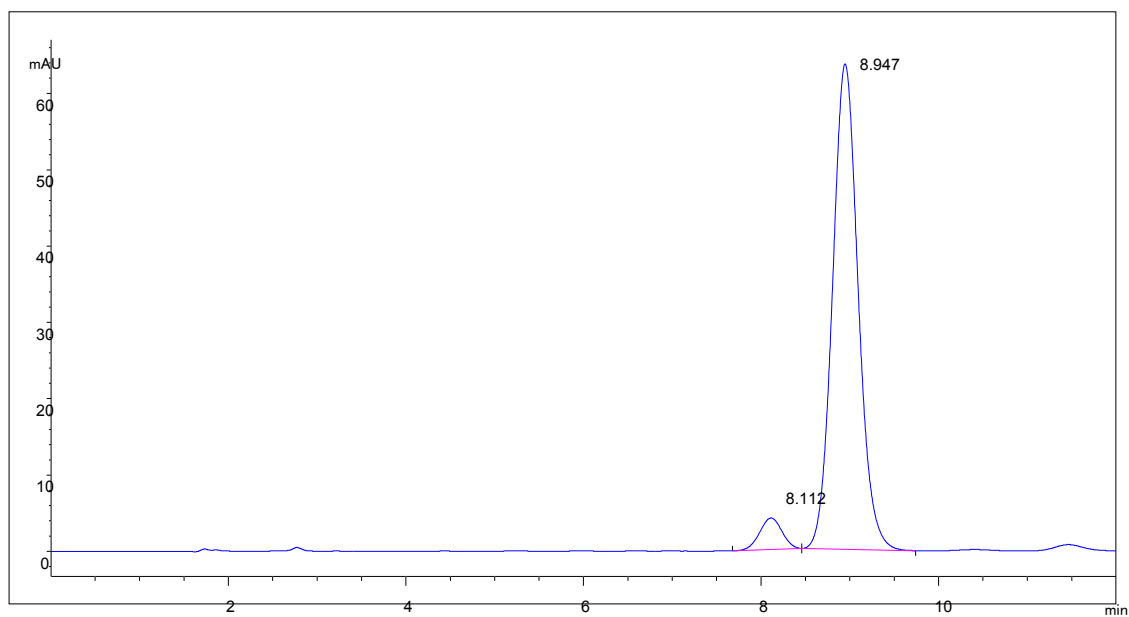
Fig.S 112 HPLC for pure enantioenriched compound **3ak (Gram-scale)**





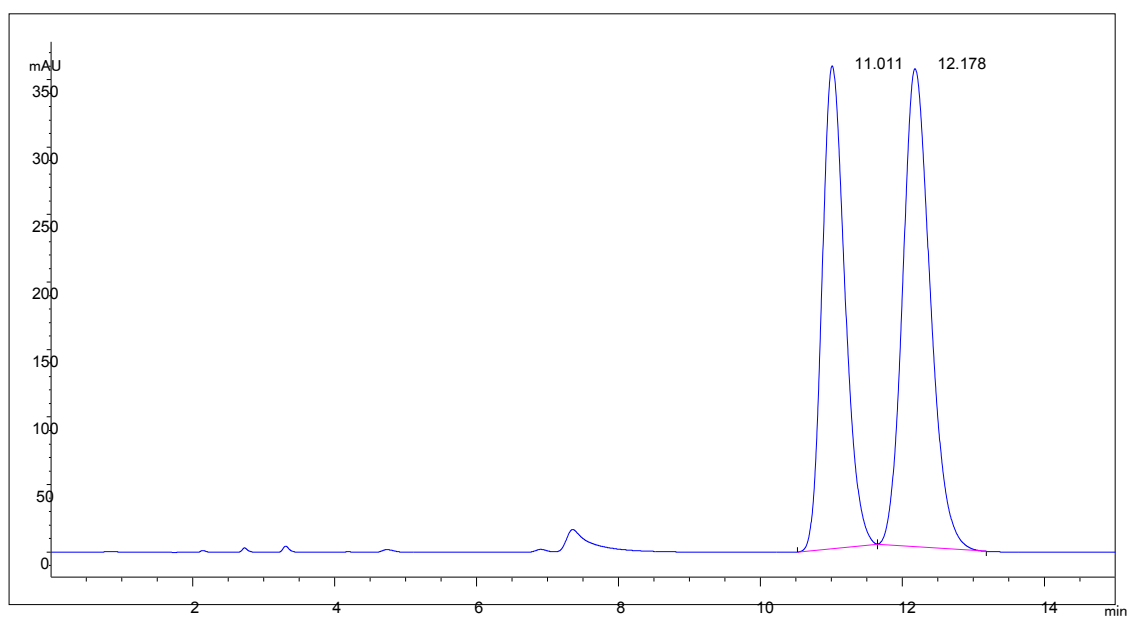
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.038	1444.1	667.8	48.466
2	8.867	1535.6	648.3	51.534

Fig.S 113 HPLC for racemic compound **3al**



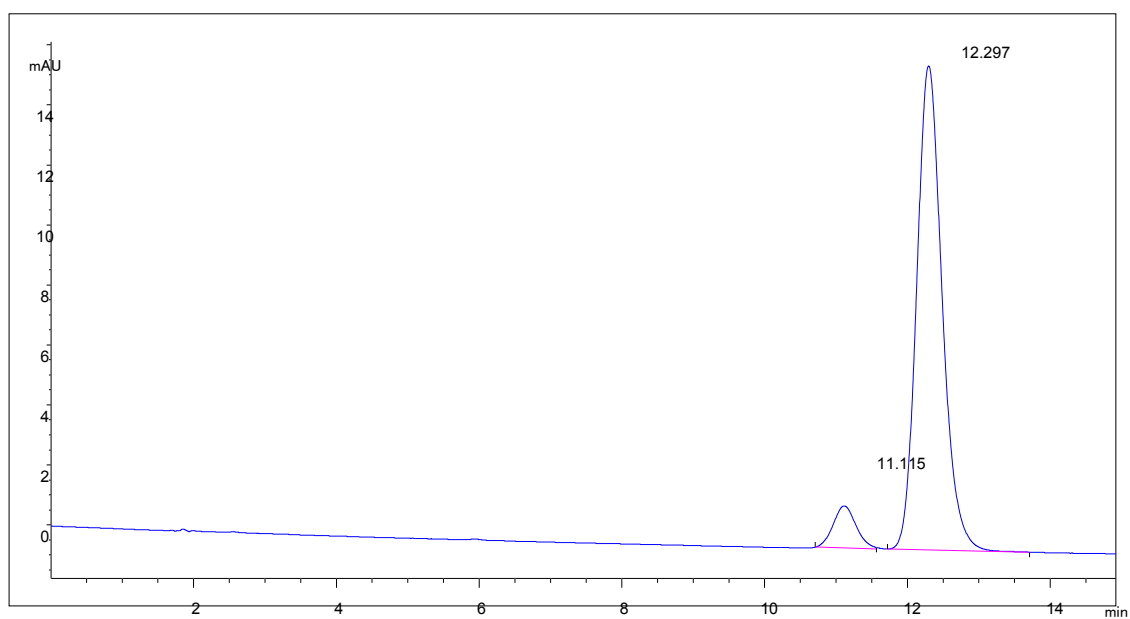
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.112	72.2	4.1	5.353
2	8.947	1276.7	63.6	94.647

Fig.S 114 HPLC for pure enantioenriched compound **3al**



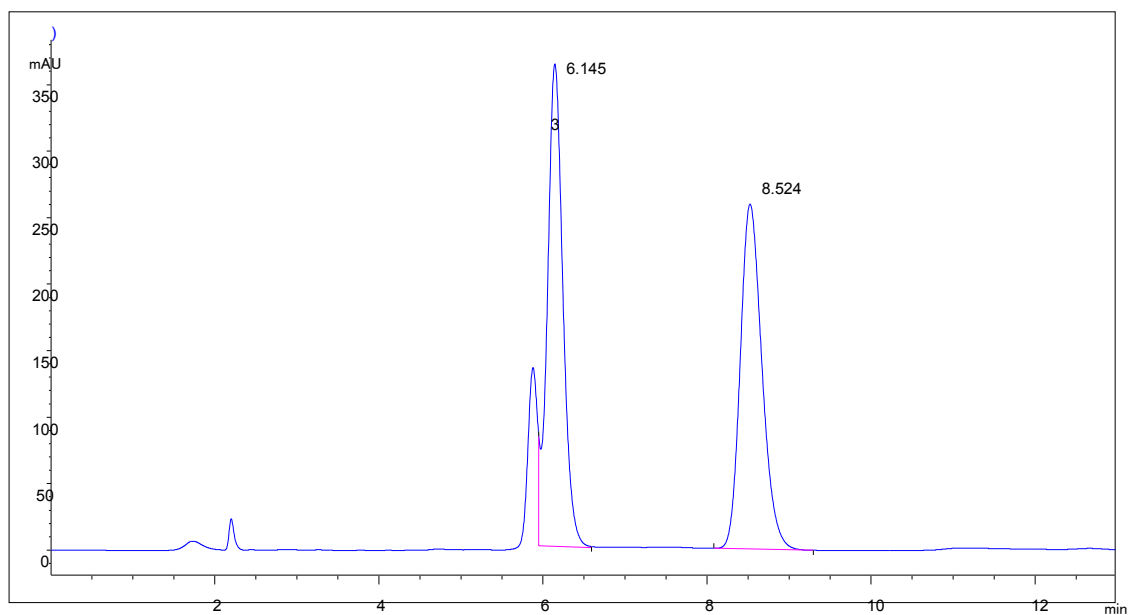
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	11.011	7982.8	357.7	45.541
2	12.178	9546.2	354.1	54.459

Fig.S 115 HPLC for racemic compound **3am**



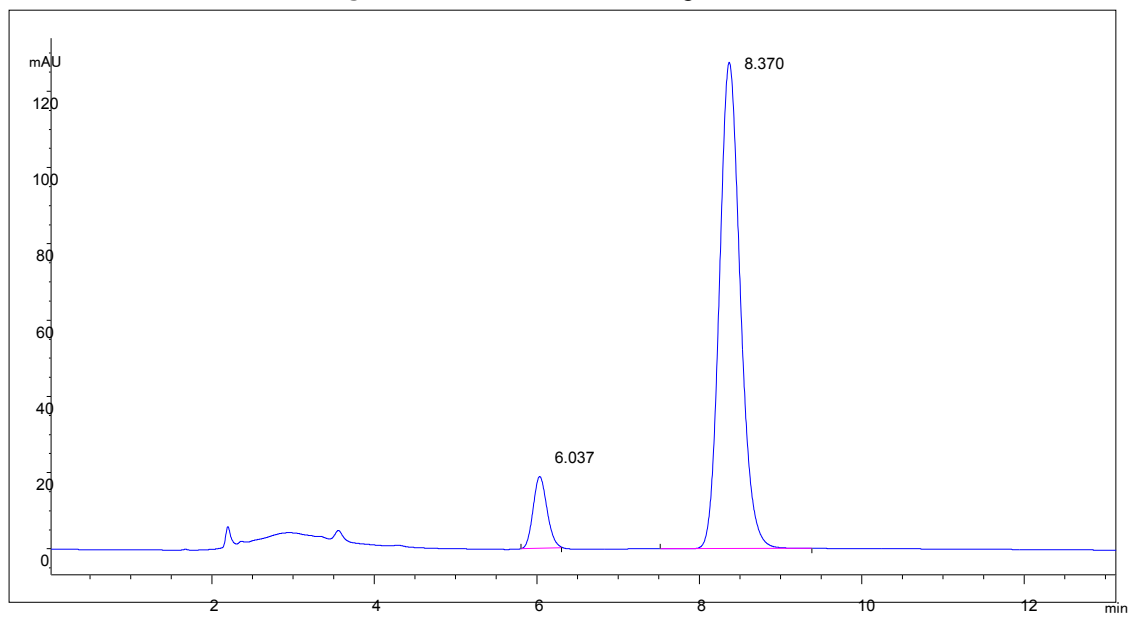
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	11.115	31.1	1.4	7.222
2	12.297	399	16.1	92.778

Fig.S 116 HPLC for pure enantioenriched compound **3am**



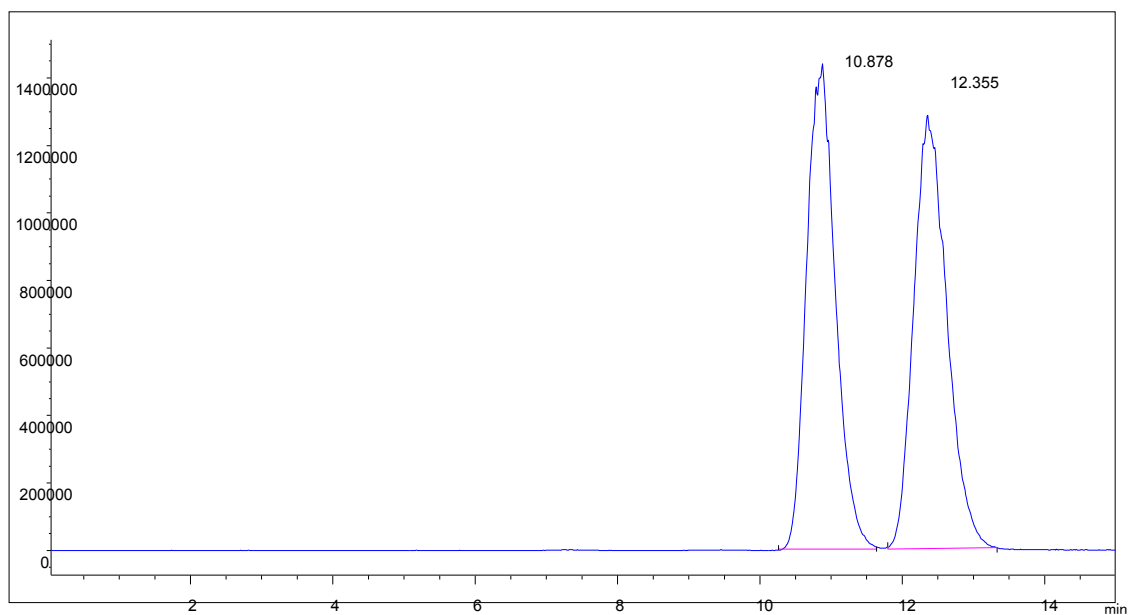
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.145	4775	362.8	50.115
2	8.524	4753.1	259.4	49.885

Fig.S 117 HPLC for racemic compound **3an**



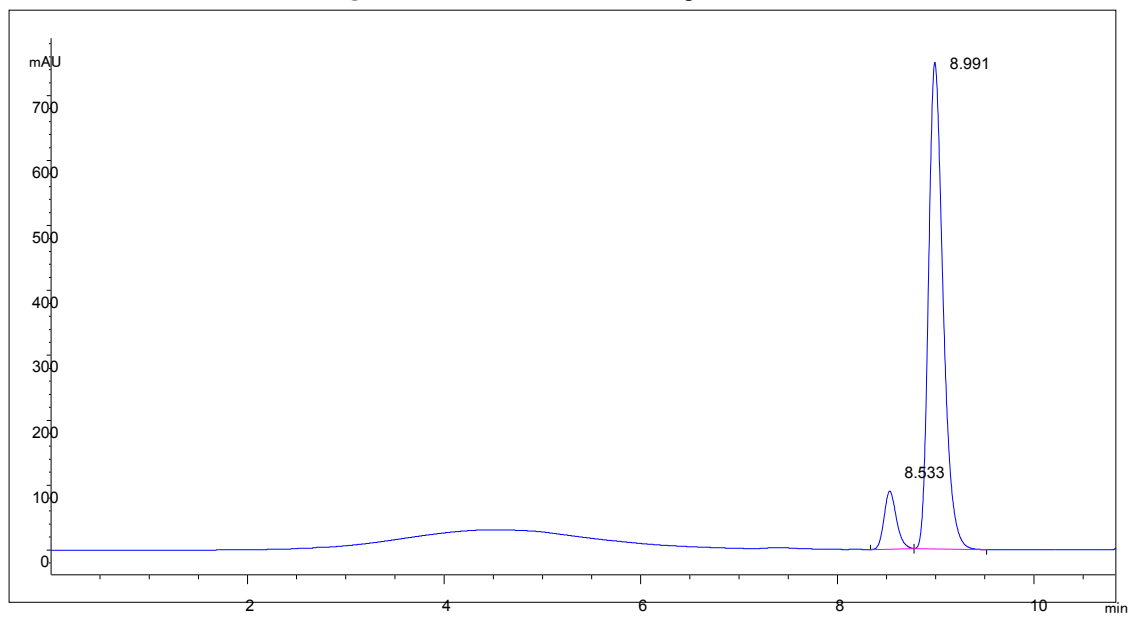
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.037	222.6	18.8	8.939
2	8.37	2268	127.5	91.061

Fig.S 118 HPLC for pure enantioenriched compound **3an**



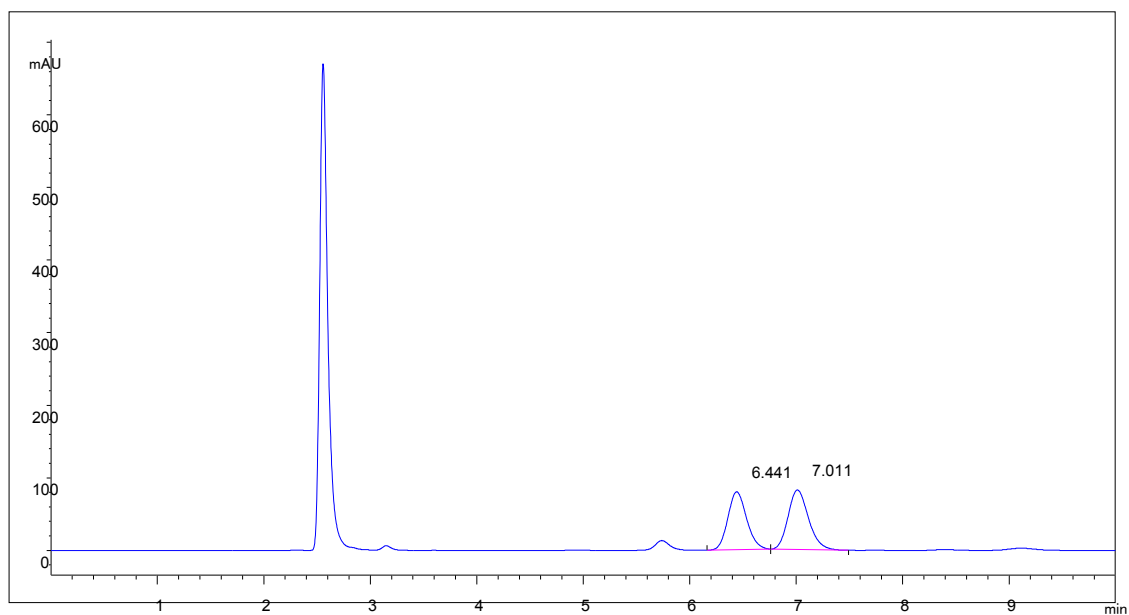
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	10.878	4068.6	144.3	49.389
2	12.355	4169.2	128.9	50.611

Fig.S 119 HPLC for racemic compound **3ao**



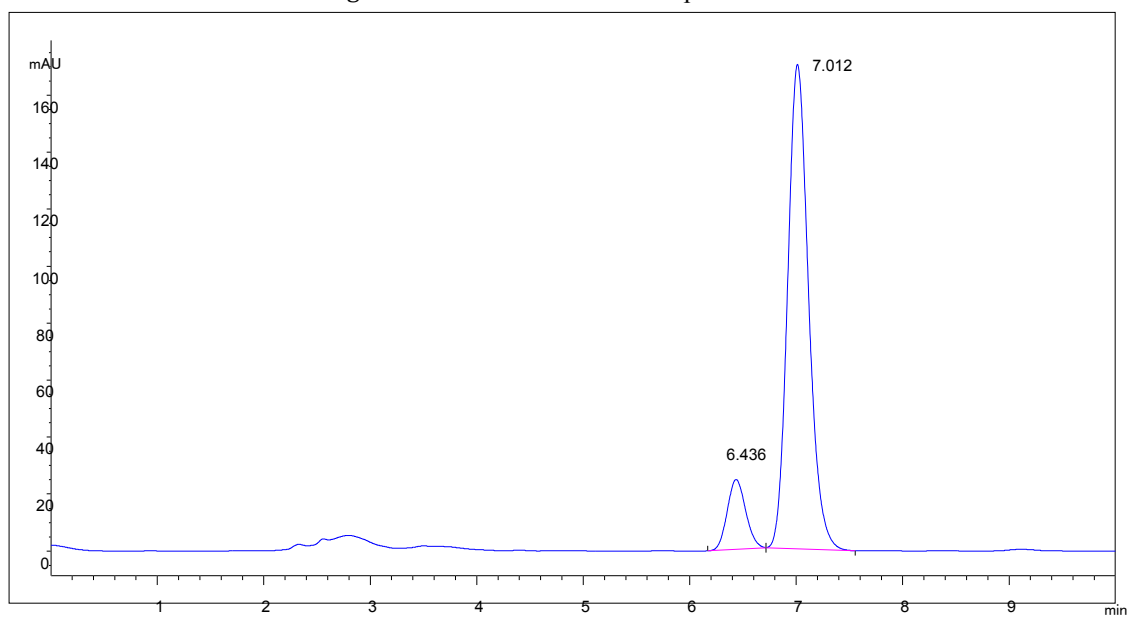
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.533	774.5	89.2	9.116
2	8.991	7721.7	749.5	90.884

Fig.S 120 HPLC for pure enantioenriched compound **3ao**



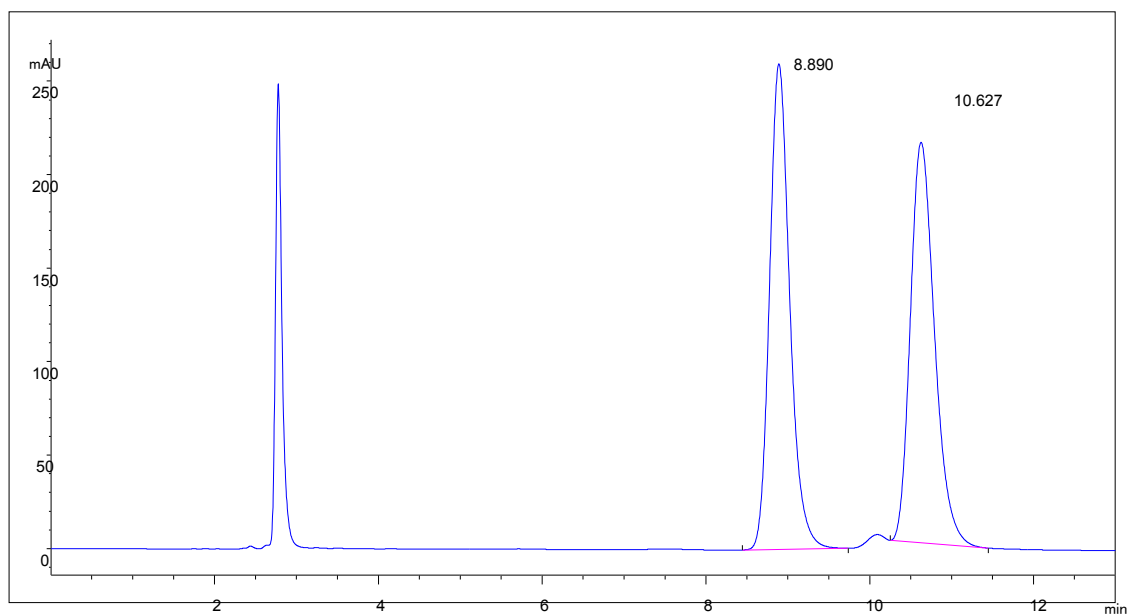
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.441	971.1	79.7	47.068
2	7.011	1092.1	82.1	52.932

Fig.S 121 HPLC for racemic compound **3bd**



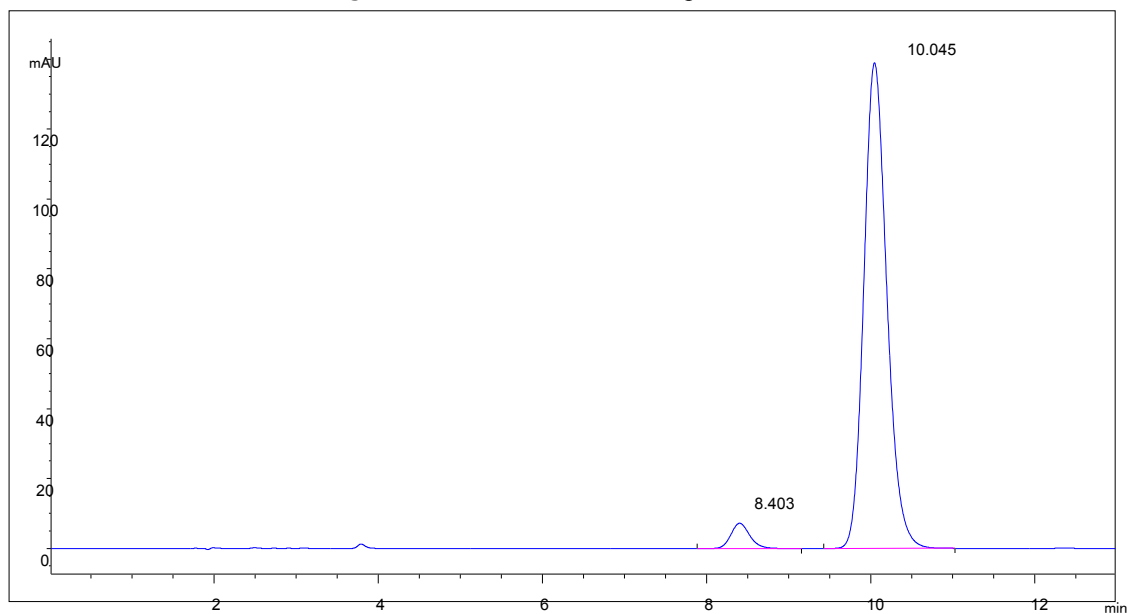
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.436	293.6	24.5	11.266
2	7.012	2312.1	170	88.734

Fig.S 122 HPLC for pure enantioenriched compound **3bd**



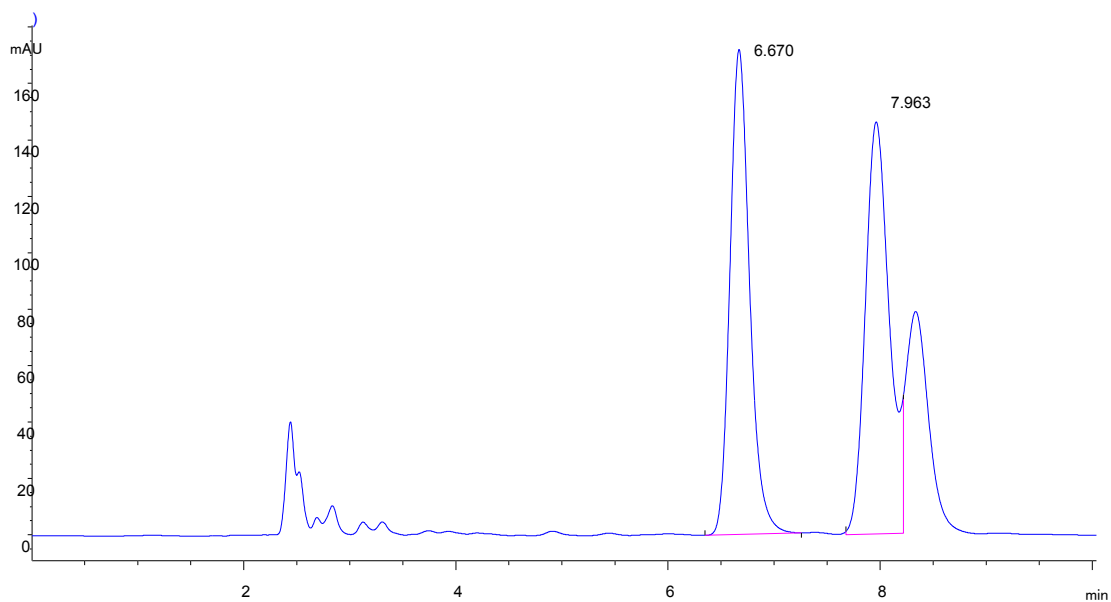
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.89	447.5	259.7	50.284
2	10.627	4397.3	214.2	49.716

Fig.S 123 HPLC for racemic compound **3cd**



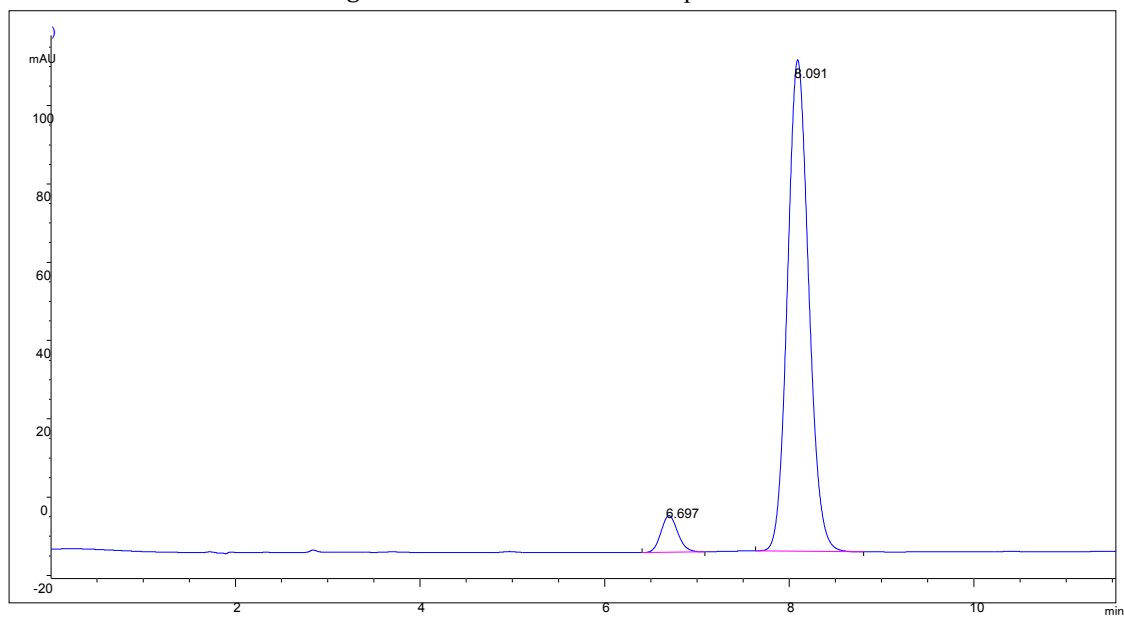
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.403	115.9	7.2	4.112
2	10.045	2703.2	139	95.888

Fig.S 124 HPLC for pure enantioenriched compound **3cd**



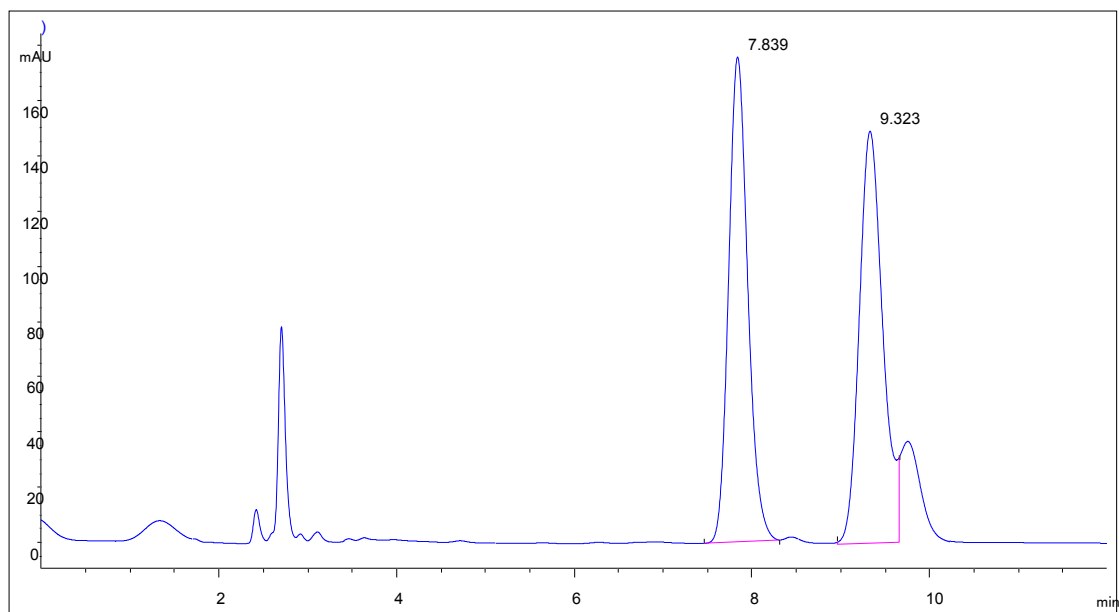
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.67	2217.1	171.9	48.829
2	7.963	2323.4	146.1	51.171

Fig.S 125 HPLC for racemic compound **3dd**



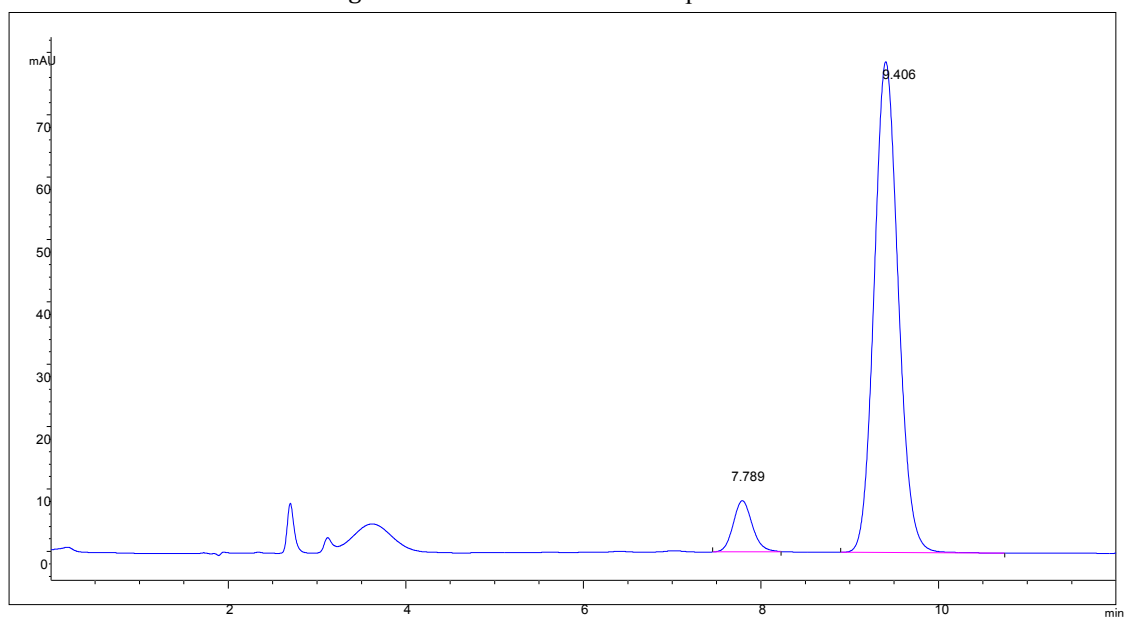
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.697	118.6	9.4	5.589
2	8.091	2003.5	125.5	94.411

Fig.S 126 HPLC for pure enantioenriched compound **3dd**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.839	2630	175.5	48.697
2	9.323	2770.7	149.2	51.303

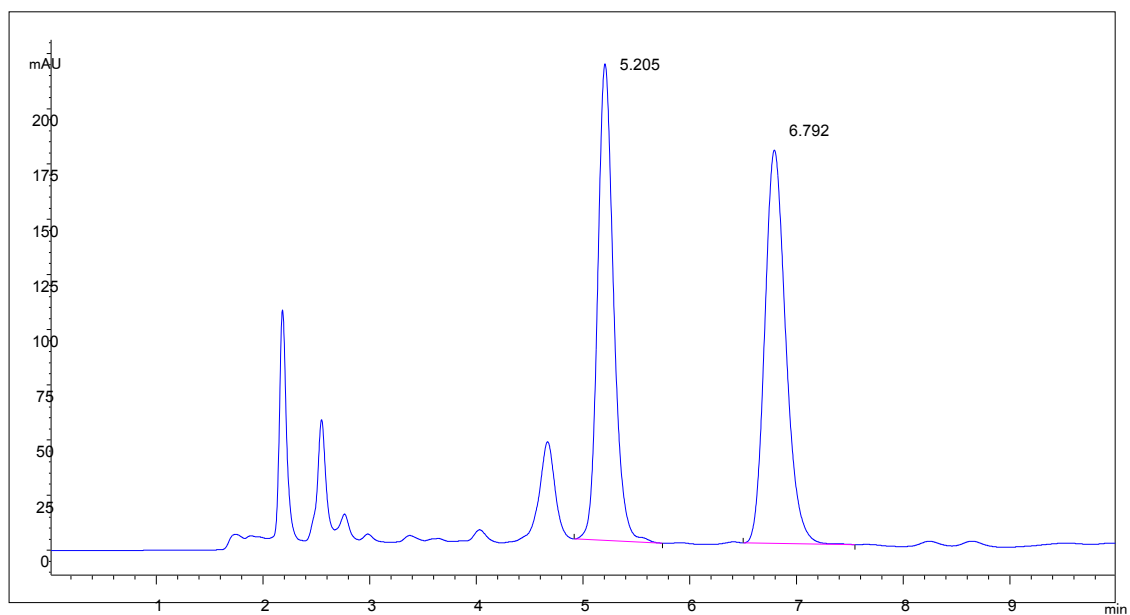
Fig.S 127 HPLC for racemic compound **3ed**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.789	122.4	8.2	7.637
2	9.406	1480.9	78.7	92.363

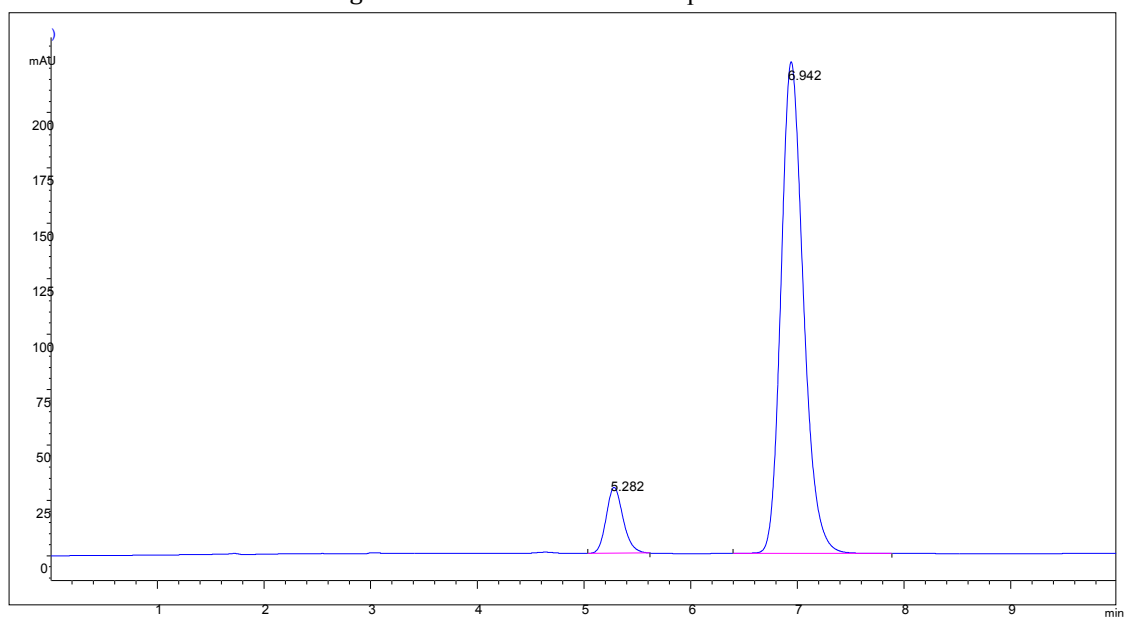
Fig.S 128 HPLC for pure enantioenriched compound **3ed**





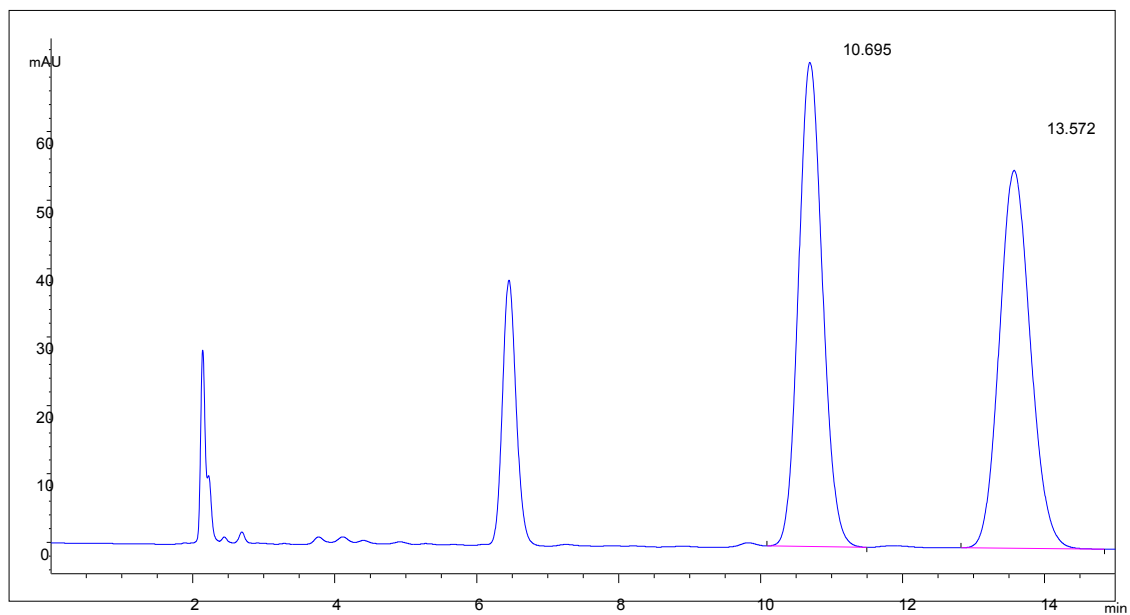
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	5.205	2244.9	216	47.987
2	6.798	2433.2	178.2	52.013

Fig.S 129 HPLC for racemic compound **3fd**



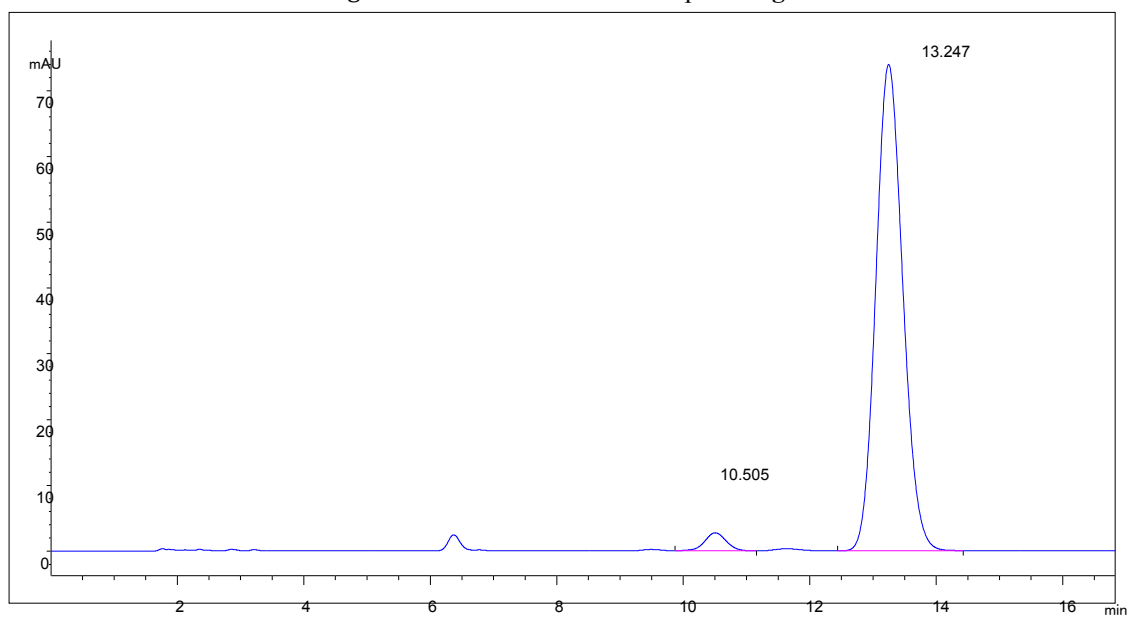
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	5.282	328.2	29.8	9.195
2	6.942	3240.7	221.8	90.805

Fig.S 130 HPLC for pure enantioenriched compound **3fd**



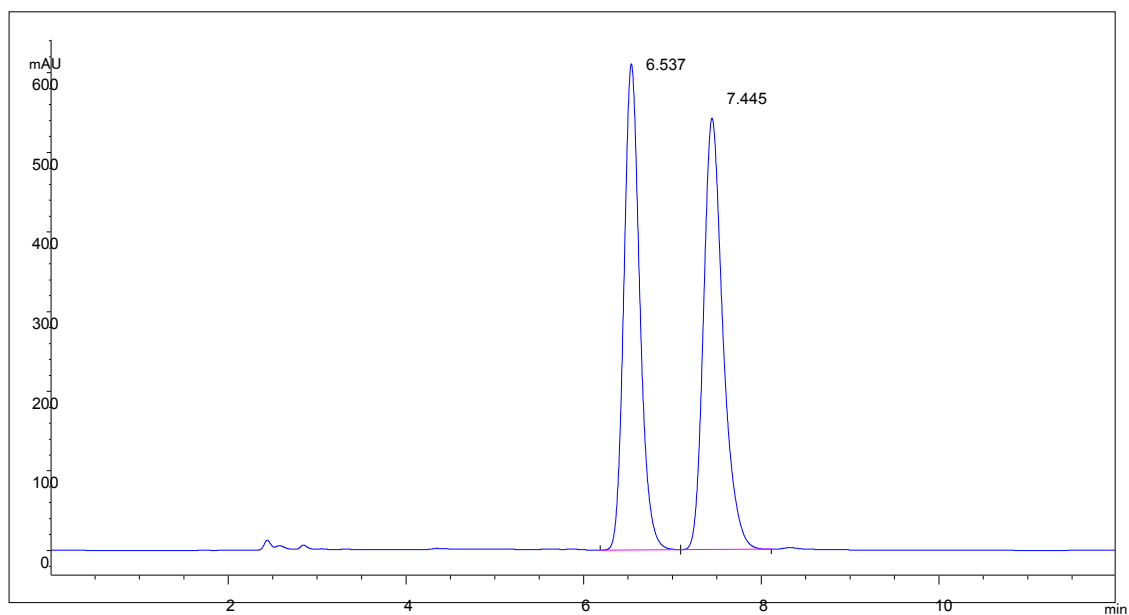
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	10.695	1664.3	70.7	49.753
2	13.572	1680.8	55.2	50.247

Fig.S 131 HPLC for racemic compound **3gd**



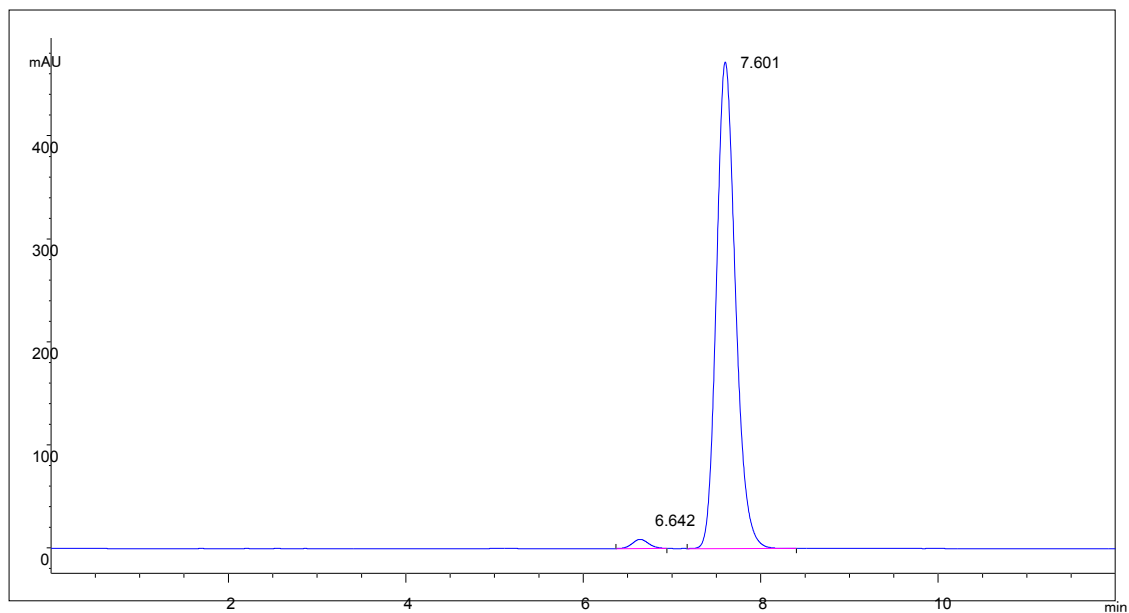
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	10.505	64.8	2.7	2.878
2	13.247	2188.7	73.9	97.122

Fig.S 132 HPLC for pure enantioenriched compound **3gd**



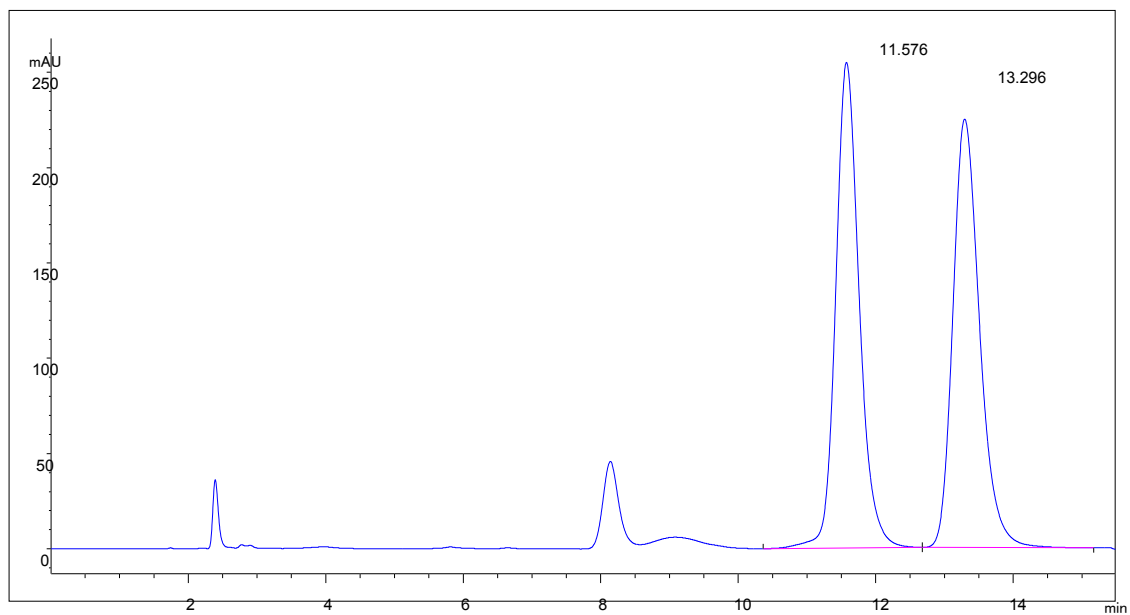
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.537	7584.7	610.5	47.964
2	7.445	8228.6	542	52.036

Fig.S 133 HPLC for racemic compound **3hd**



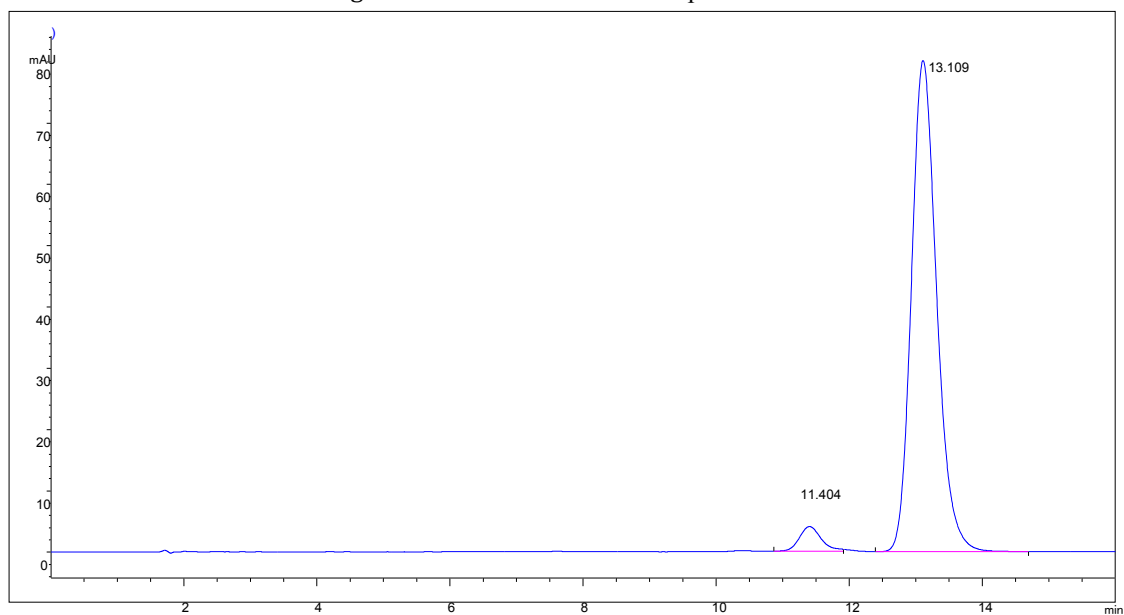
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.642	116.6	9	1.632
2	7.601	7028.4	472	98.369

Fig.S 134 HPLC for pure enantioenriched compound **3hd**



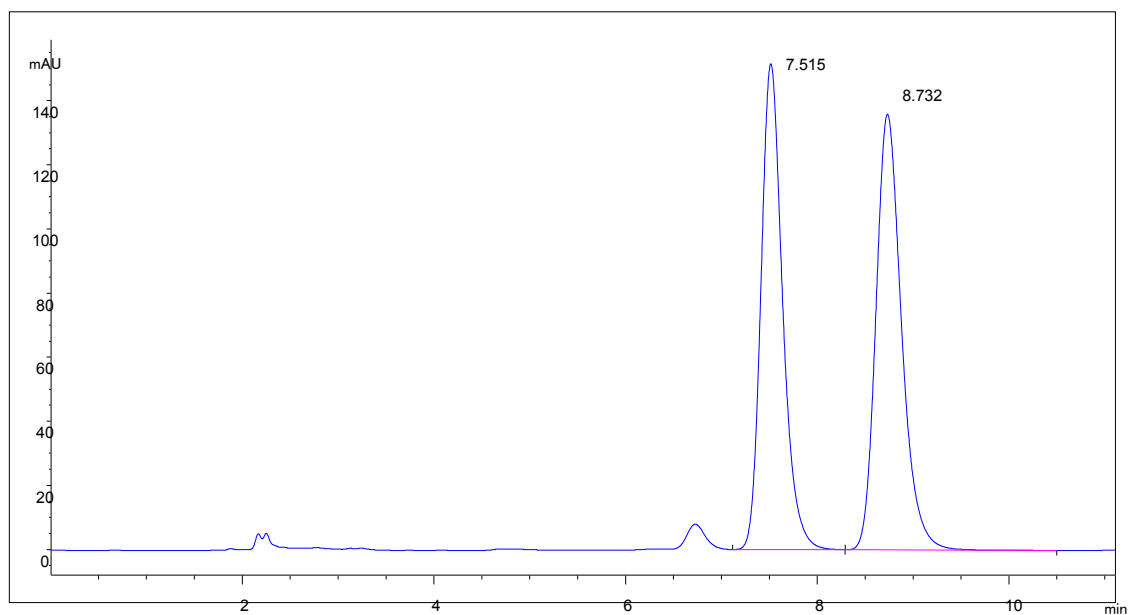
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	11.576	6066.3	254.7	49.999
2	13.296	6066.7	224.7	50.001

Fig.S 135 HPLC for racemic compound **3id**



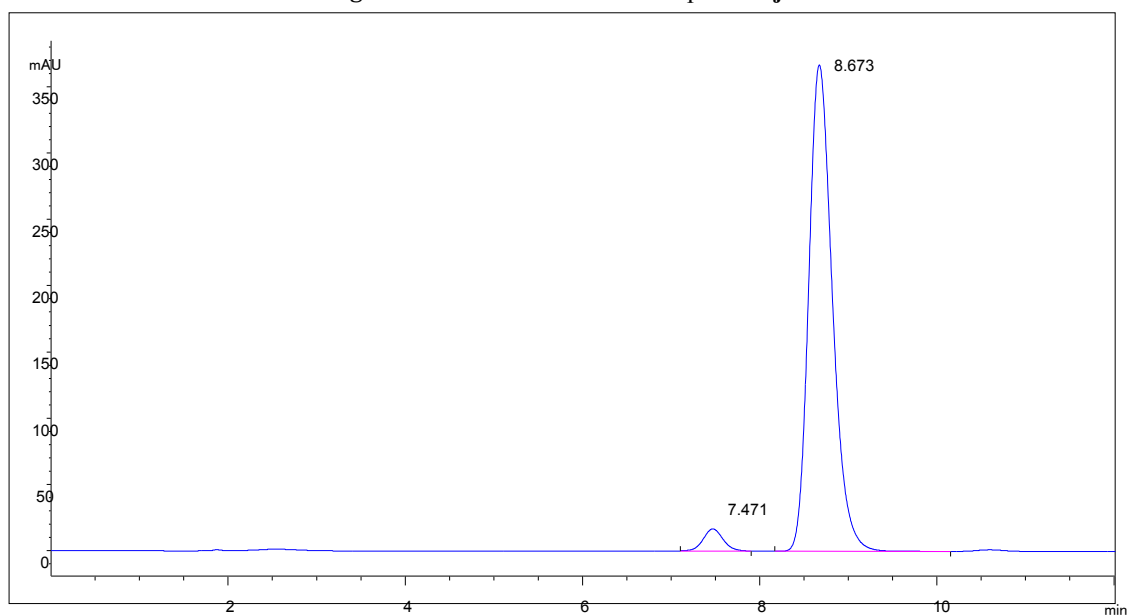
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	11.404	91	4	4.13
2	13.109	2111.7	80.1	95.87

Fig.S 136 HPLC for pure enantioenriched compound **3id**



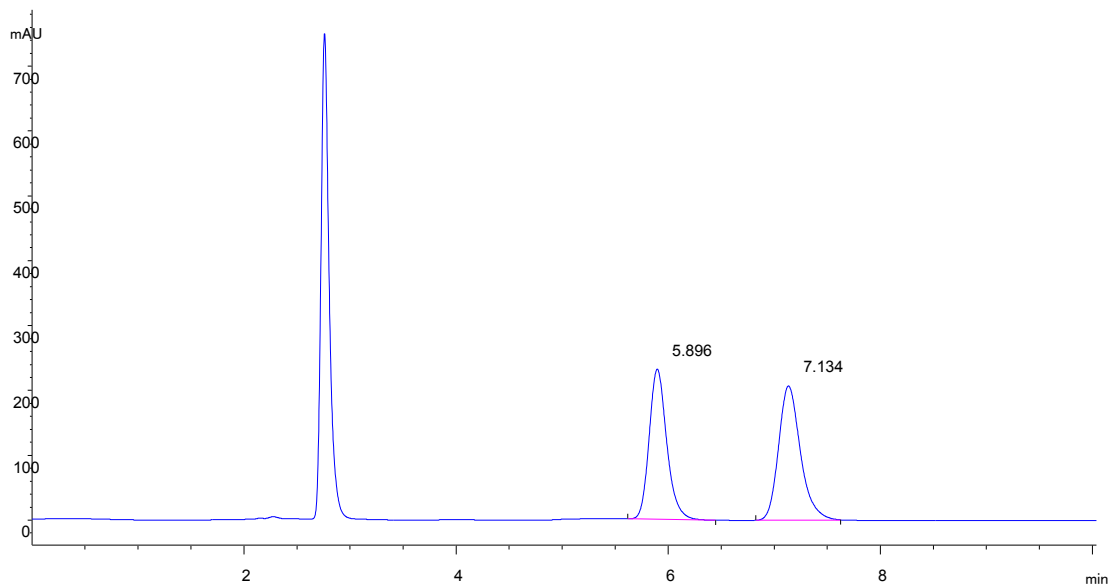
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.515	2374.6	151.6	48.5
2	8.732	2521.4	135.9	51.5

Fig.S 137 HPLC for racemic compound **3jd**



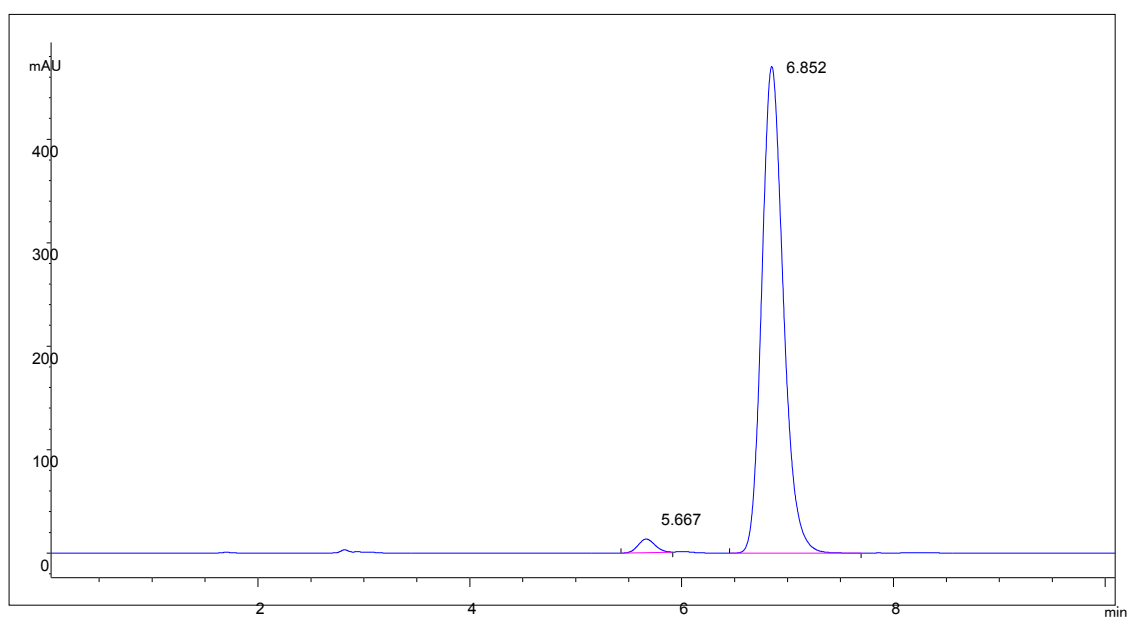
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.471	263.7	16.8	3.745
2	8.673	6778.4	367.2	96.255

Fig.S 138 HPLC for pure enantioenriched compound **3jd**



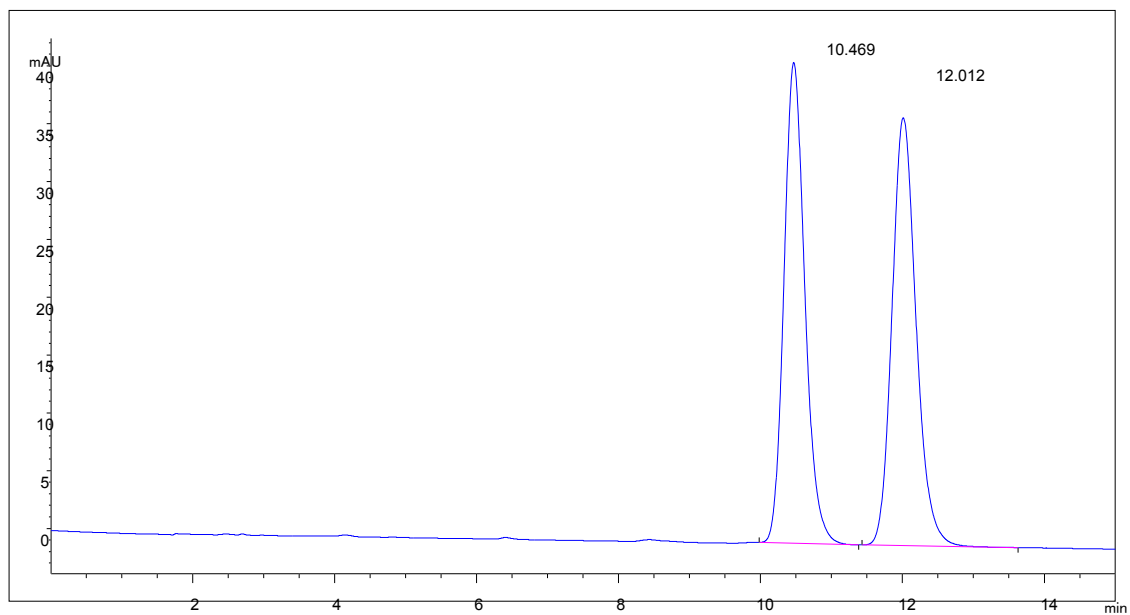
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	5.896	2671	231.6	47.419
2	7.134	2961.8	206.8	52.581

Fig.S 139 HPLC for racemic compound **3kd**



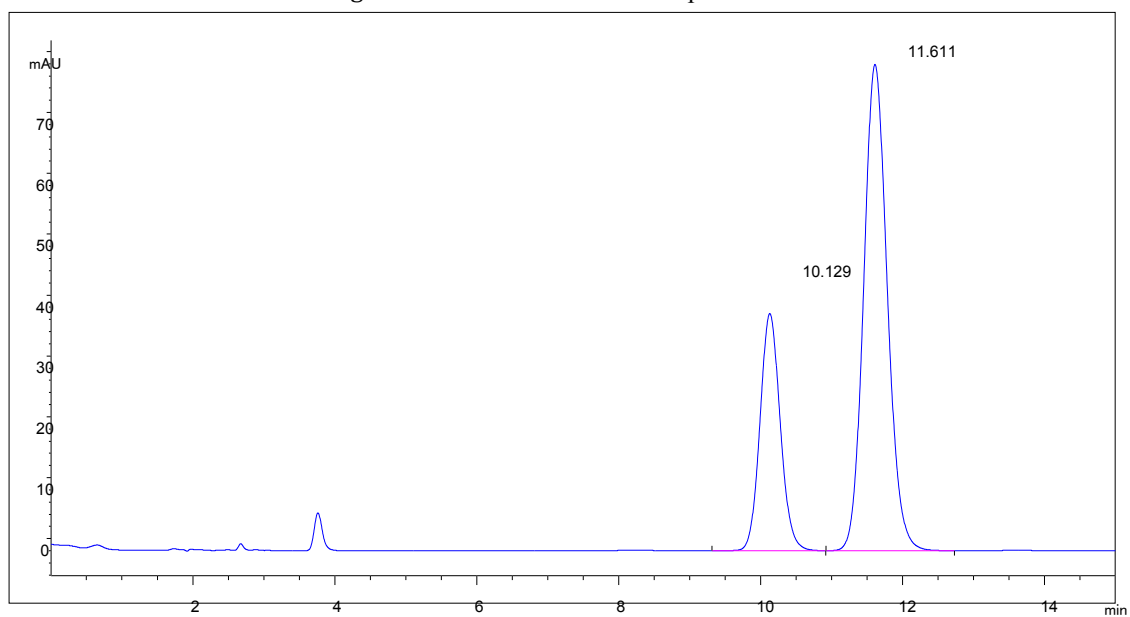
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	5.667	143.4	13	2.108
2	6.852	6658.1	470.3	97.892

Fig.S 140 HPLC for pure enantioenriched compound **3kd**



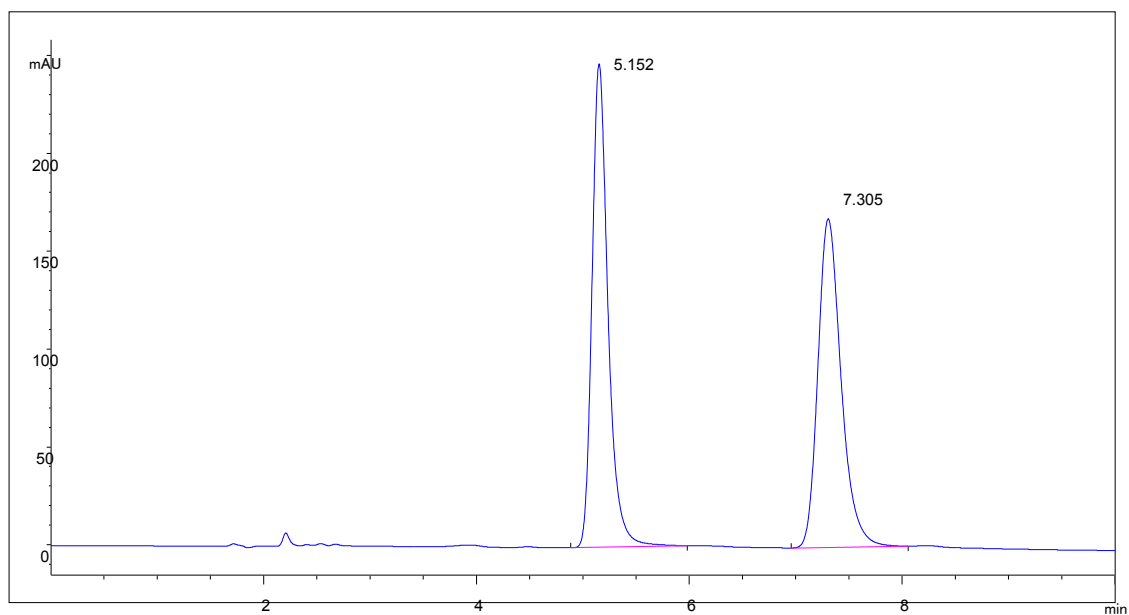
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	10.345	1320.5	63.6	49.026
2	11.882	1373	56.9	50.974

Fig.S 141 HPLC for racemic compound **3ld**



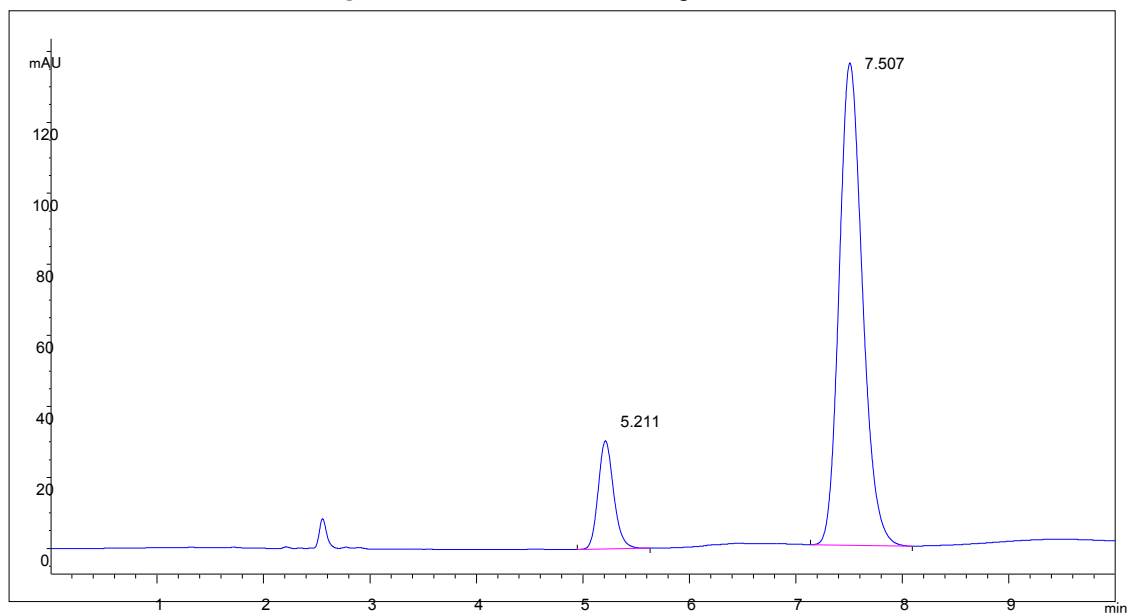
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	10.129	774.1	39	29.527
2	11.611	1847.6	79.9	70.473

Fig.S 142 HPLC for pure enantioenriched compound **3ld**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	5.152	2587.7	247	50.42
2	7.305	2544.5	167.9	49.58

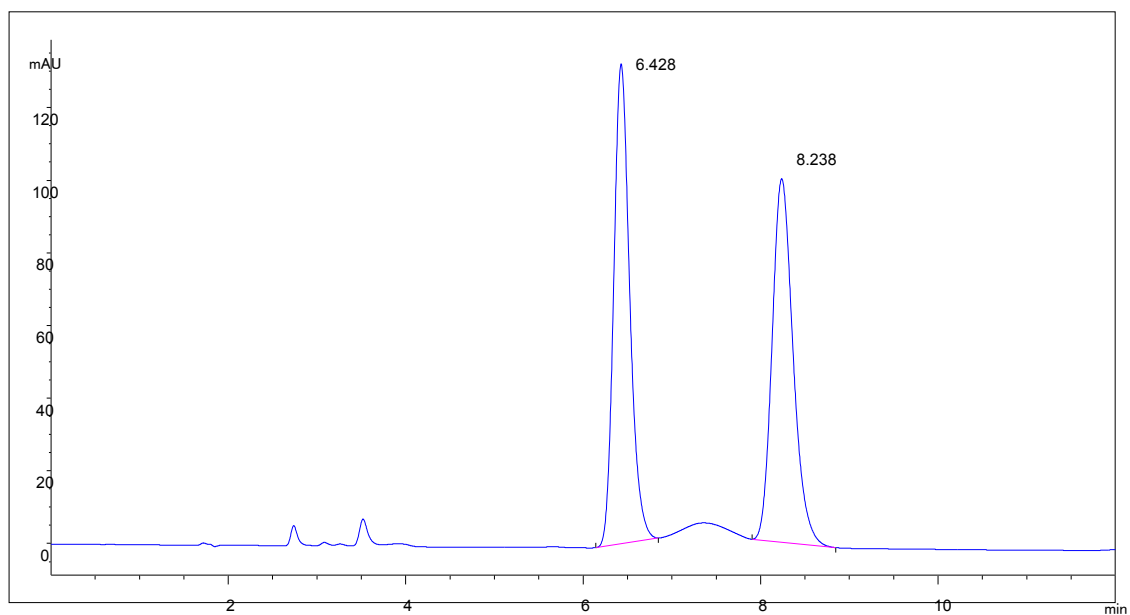
Fig.S 143 HPLC for racemic compound **3md**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	5.211	308.5	30.5	12.992
2	7.507	2066	135.9	87.008

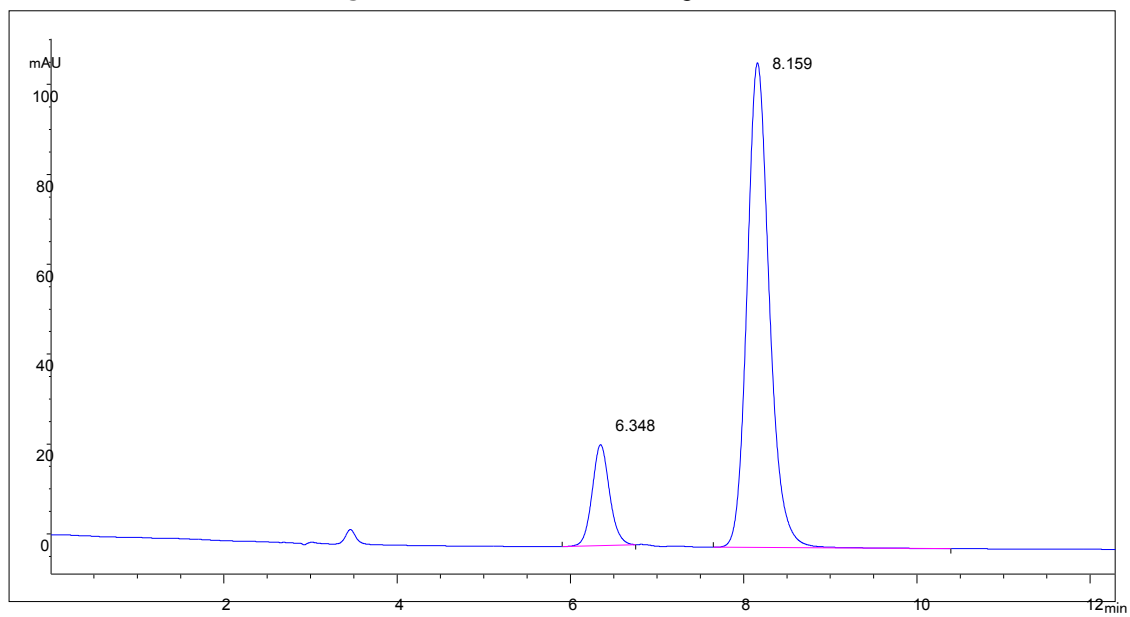
Fig.S 144 HPLC for pure enantioenriched compound **3md**





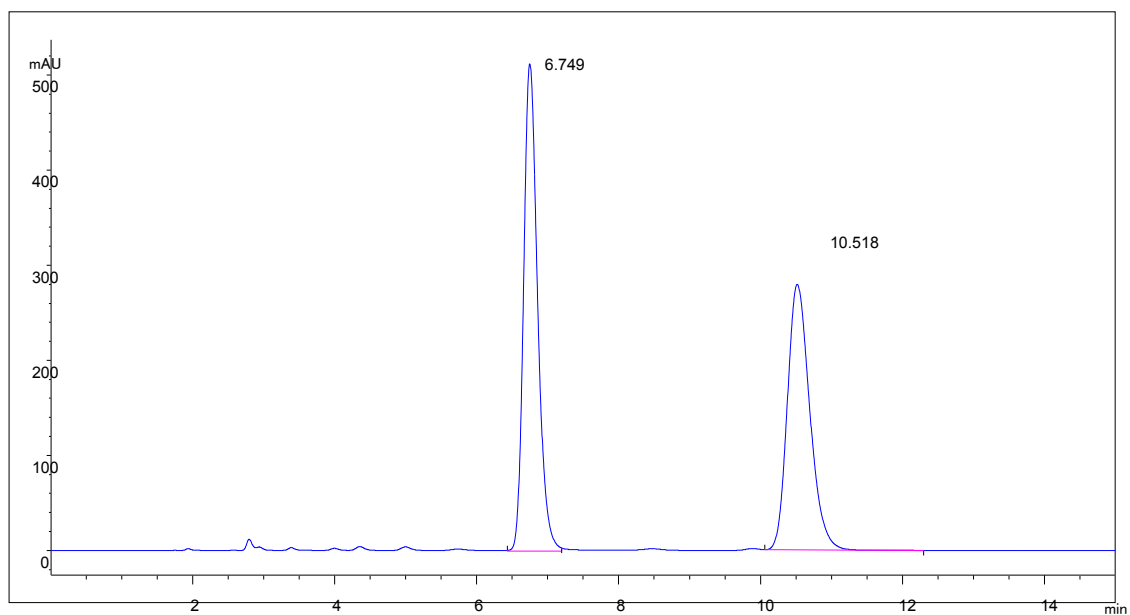
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.428	1650.4	132.1	50.127
2	8.238	1642.1	100.1	49.873

Fig.S 145 HPLC for racemic compound **3nd**



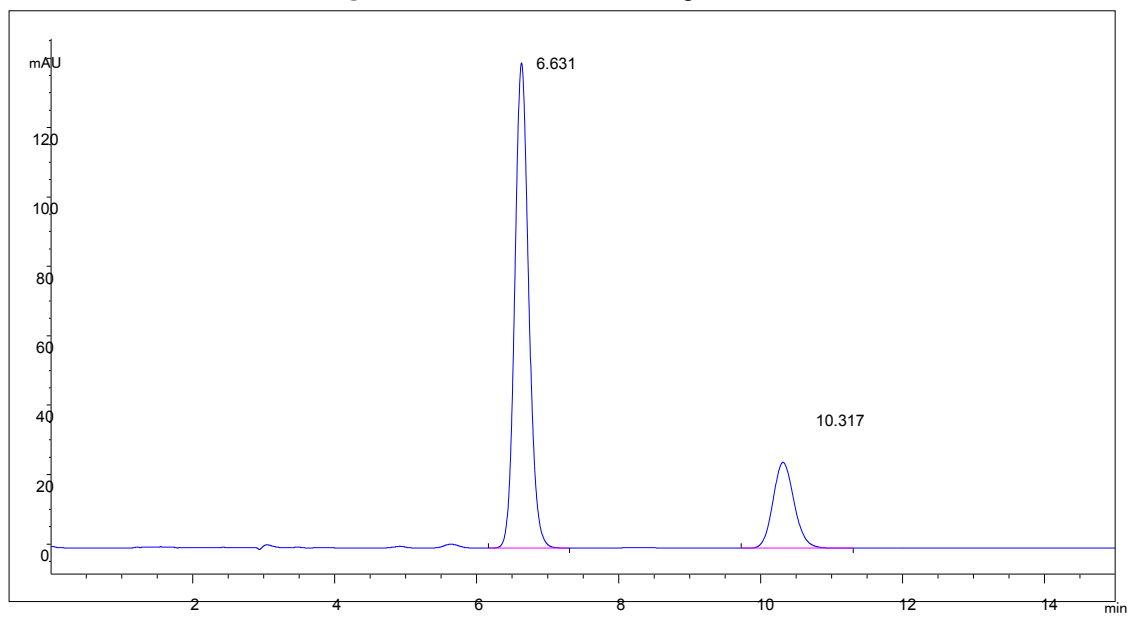
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.348	313.1	22.5	13.962
2	8.159	1929.4	107.9	86.038

Fig.S 146 HPLC for pure enantioenriched compound **3nd**



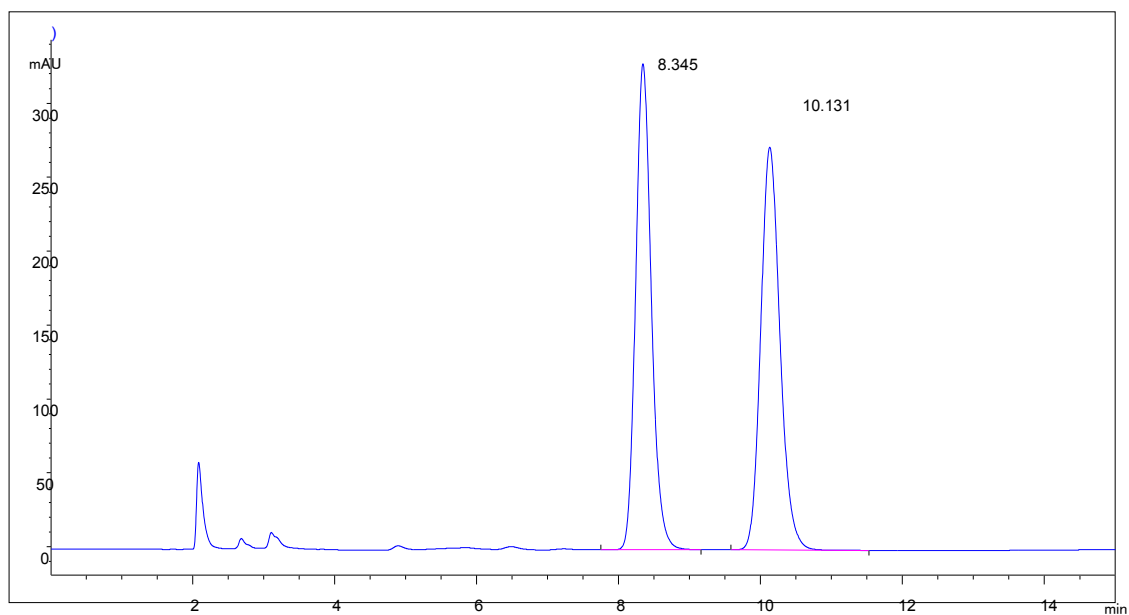
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.749	7001.9	512.5	53.359
2	10.518	612.3	279.2	46.641

Fig.S 147 HPLC for racemic compound **3od**



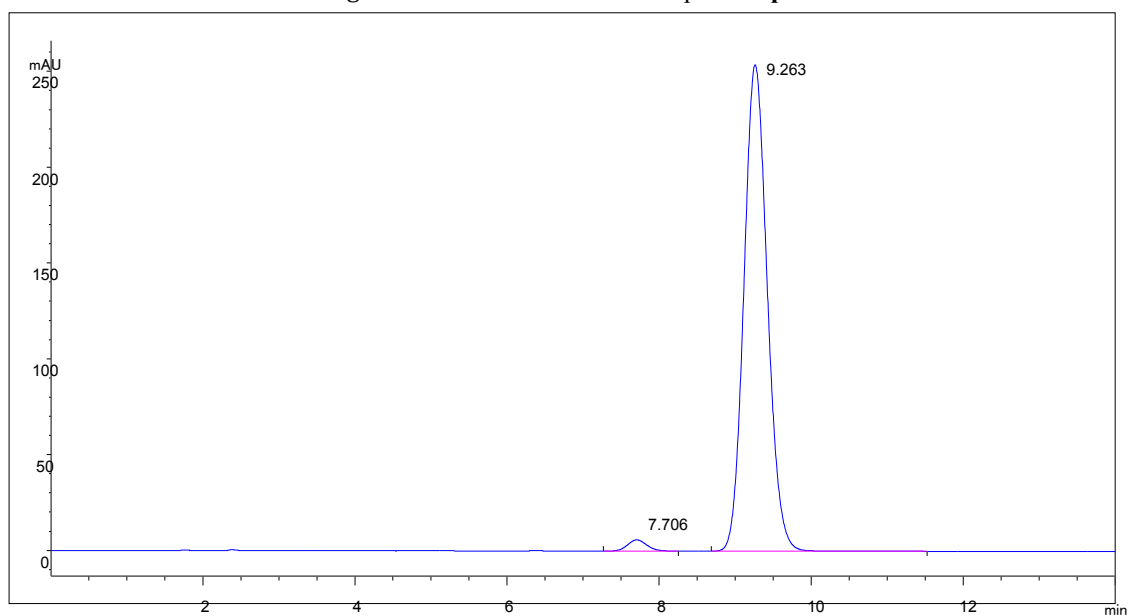
#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	6.631	1910.1	139.8	78.809
2	10.317	513.6	24.7	21.191

Fig.S 148 HPLC for pure enantioenriched compound **3od**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	8.345	5047	328.7	49.592
2	10.131	5130	272.5	50.408

Fig.S 149 HPLC for racemic compound **3pd**



#	Time (min)	Area (mAU*s)	Height (mAu)	Area %
1	7.706	102	5.8	1.883
2	9.263	5403.6	253.7	98.147

Fig.S 150 HPLC for pure enantioenriched compound **3pd (Gram-scale)**