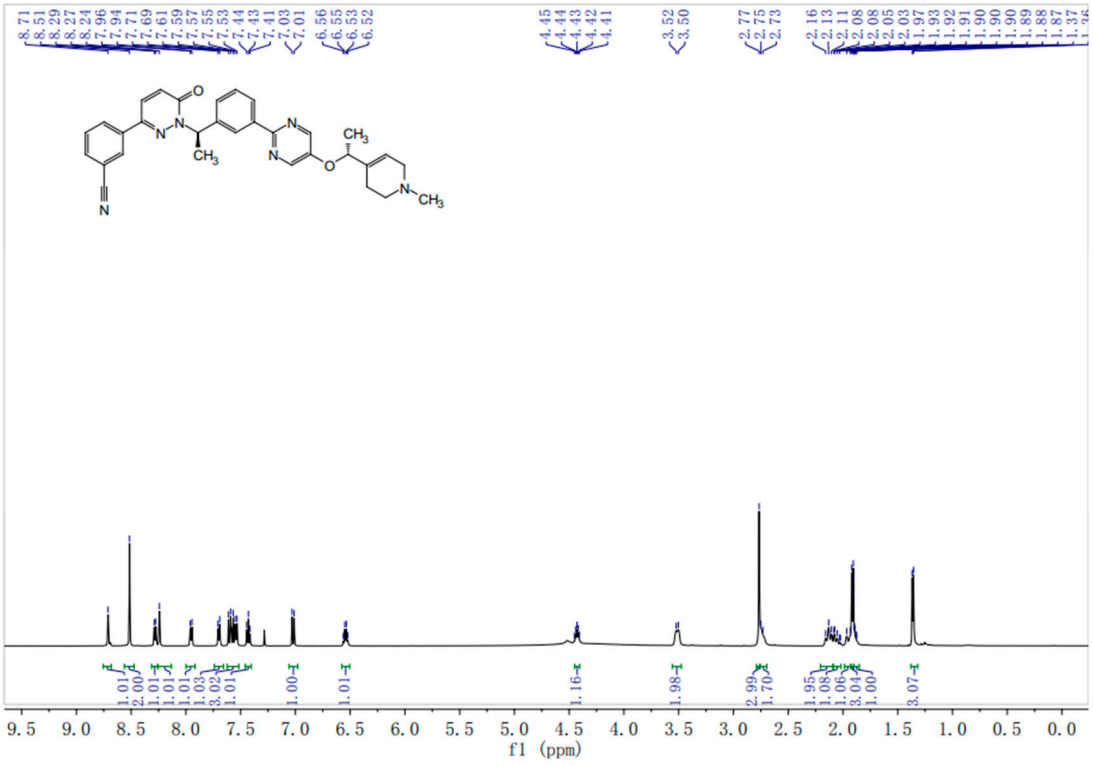
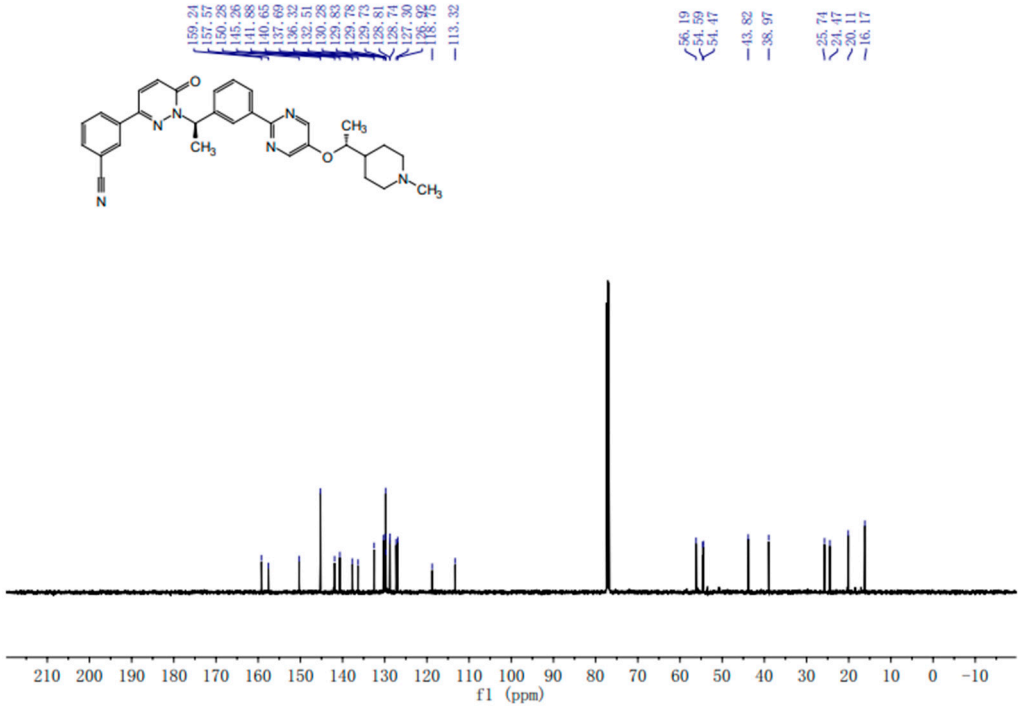
Supplementary Material

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HPLC Spectra	**10-13**
HPLC Spectra of Chiral Purity	**13-19**
HRMS Spectra	**20-27**
X-ray diffraction data	**28-42**

NMR Spectra
Compound (*R, R*)-12a
H^1 NMR

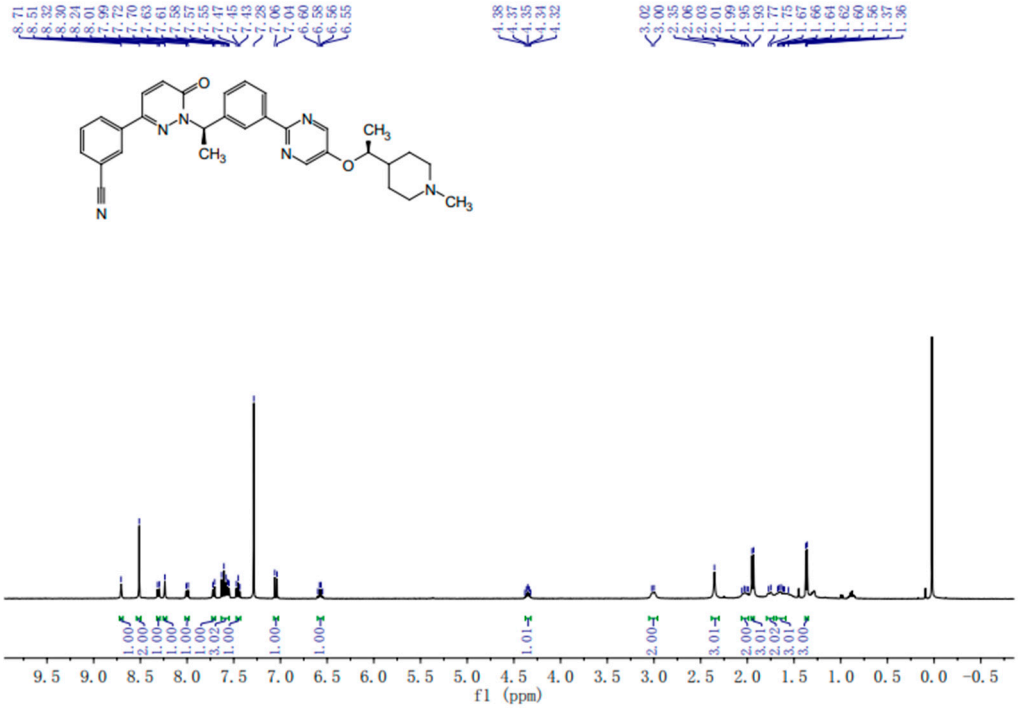


C^{13} NMR

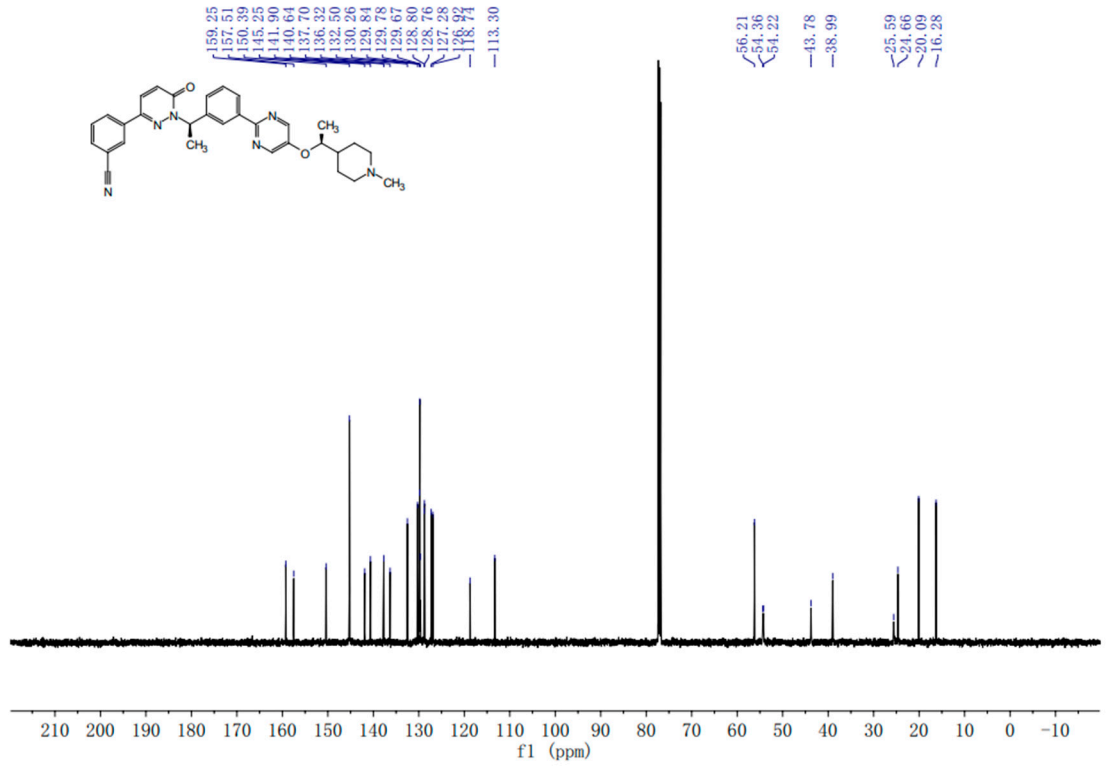


Compound (*R, S*)-12a

H^1 NMR

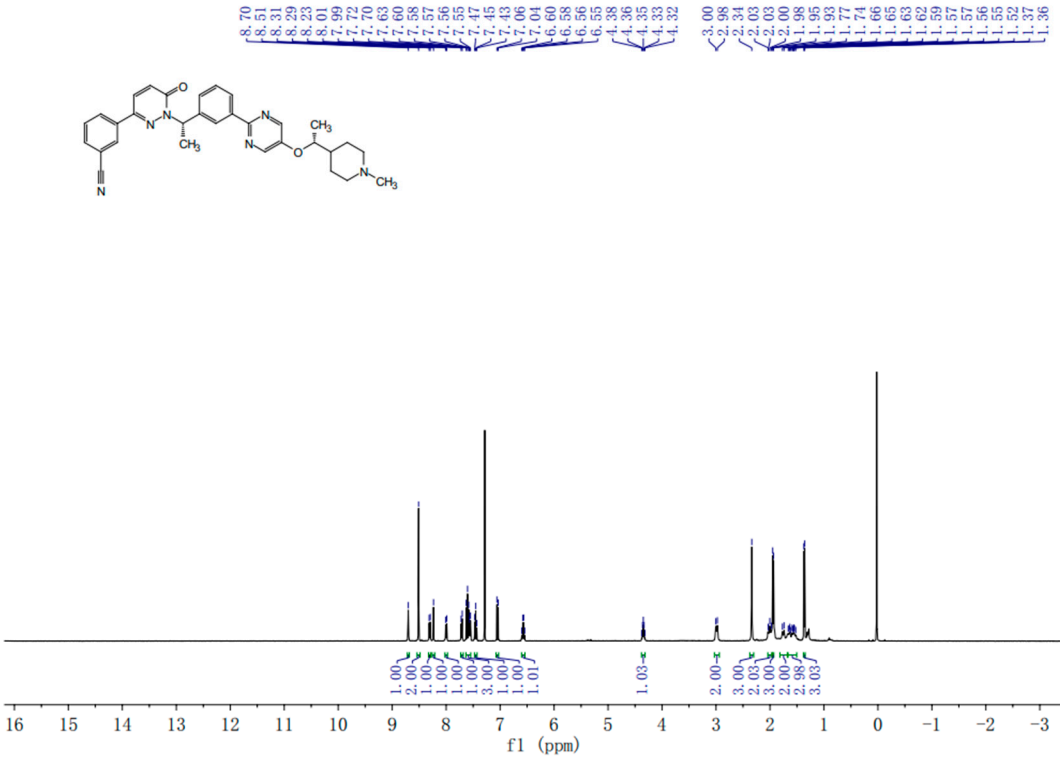


C^{13} NMR

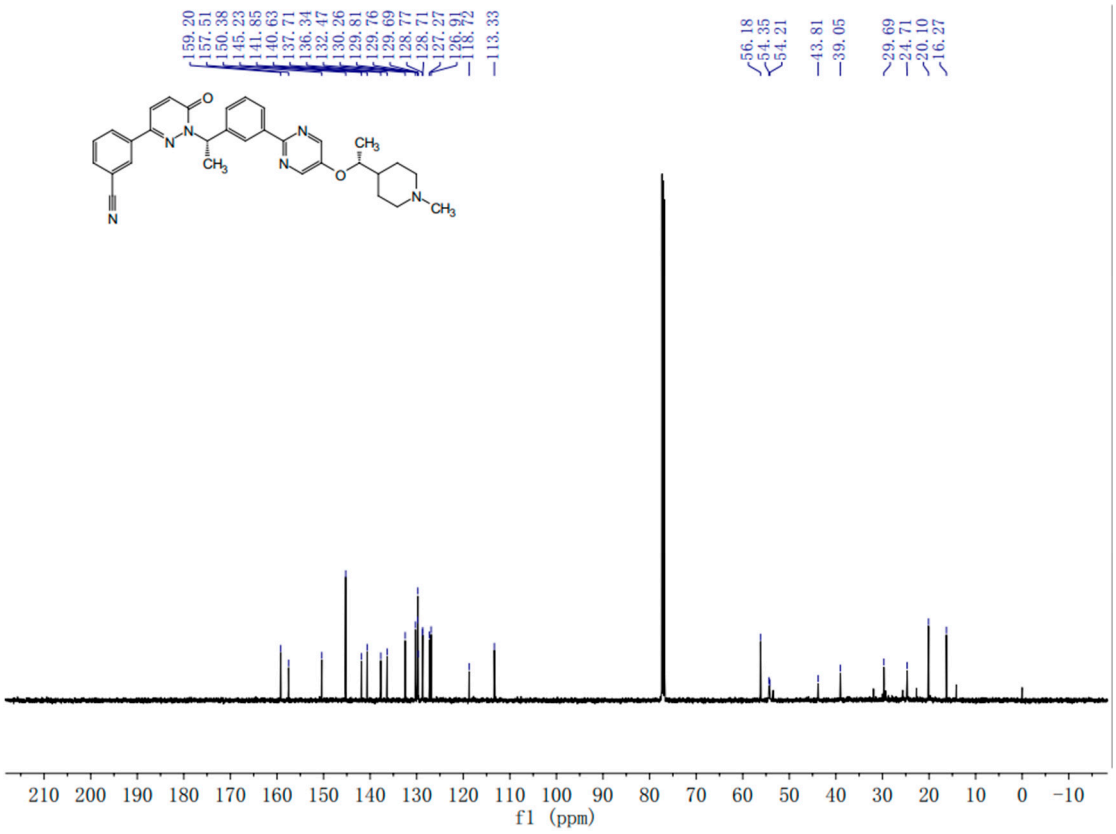


Compound (*S, R*)-12a

H^1 NMR

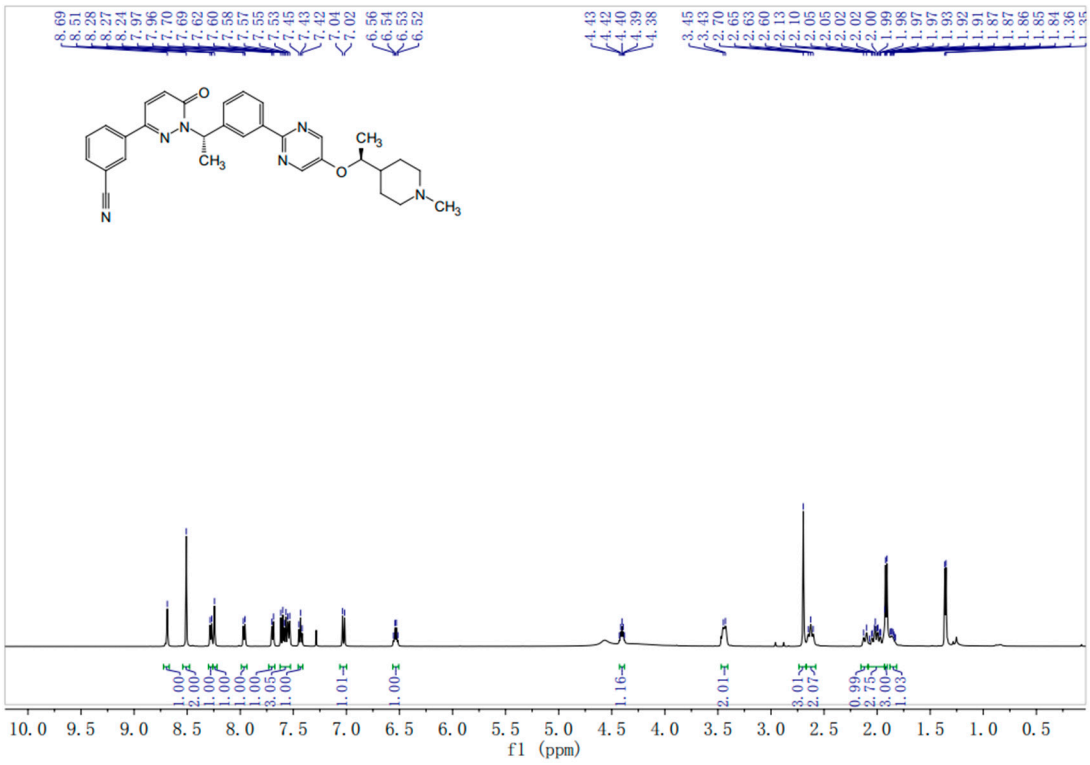


C^{13} NMR

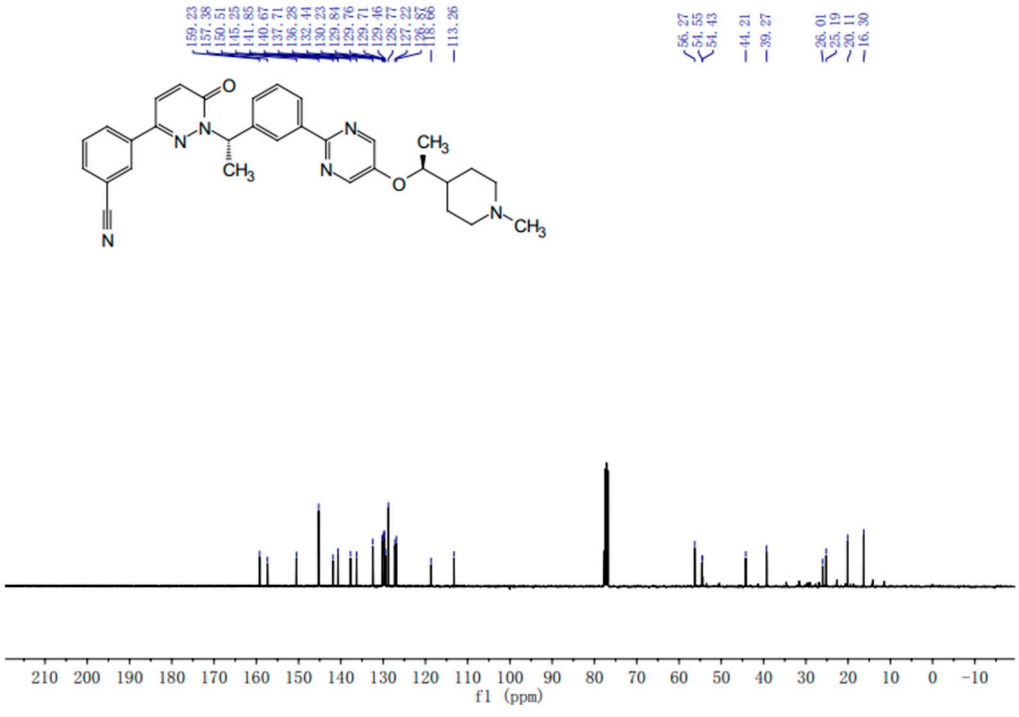


Compound (*S, S*)-12a

H^1 NMR

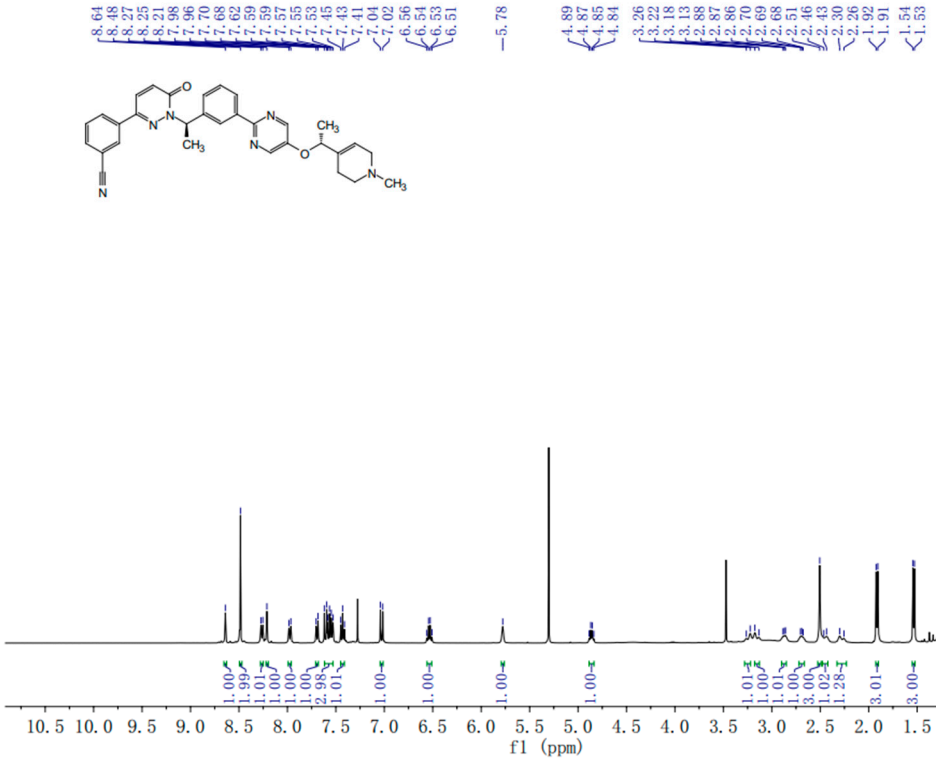


C^{13} NMR

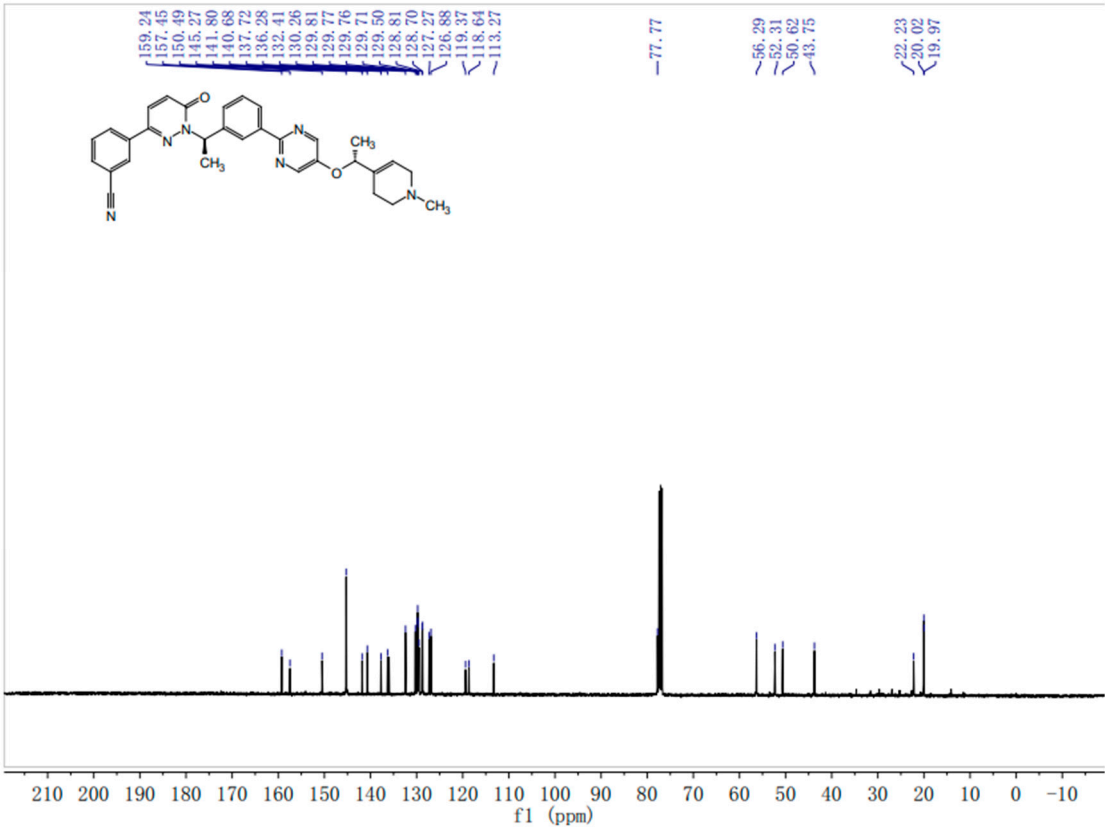


Compound (*R, R*)-12b

H^1 NMR

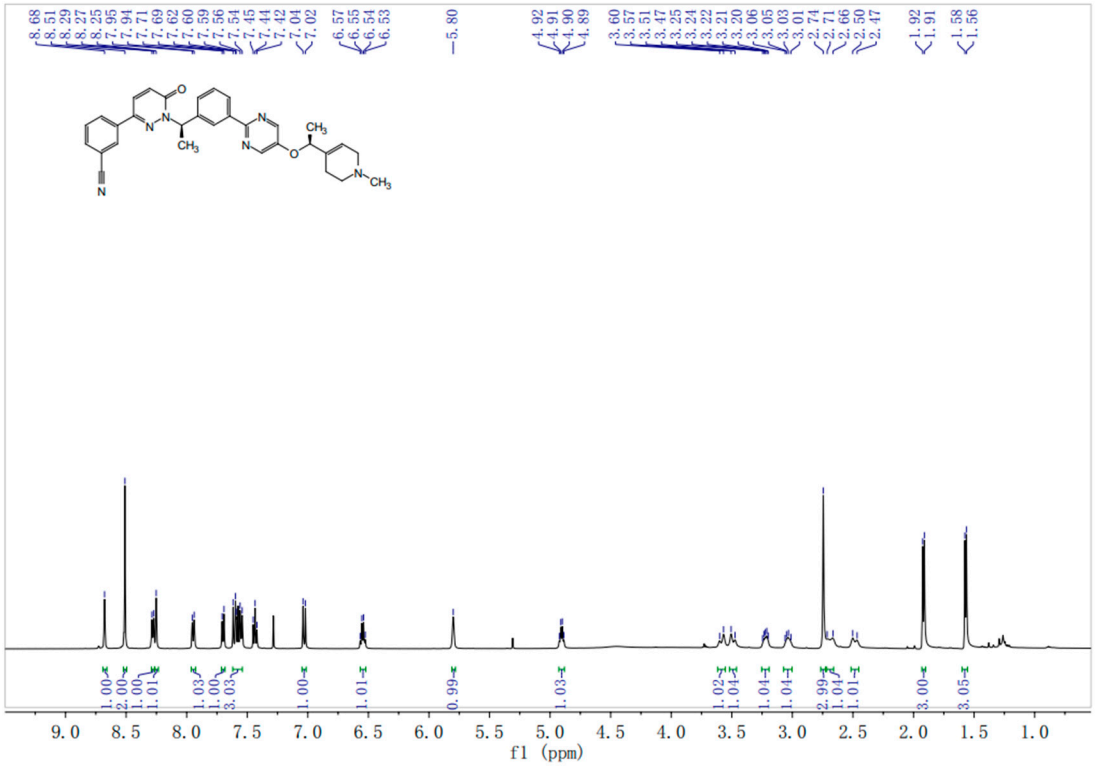


C^{13} NMR

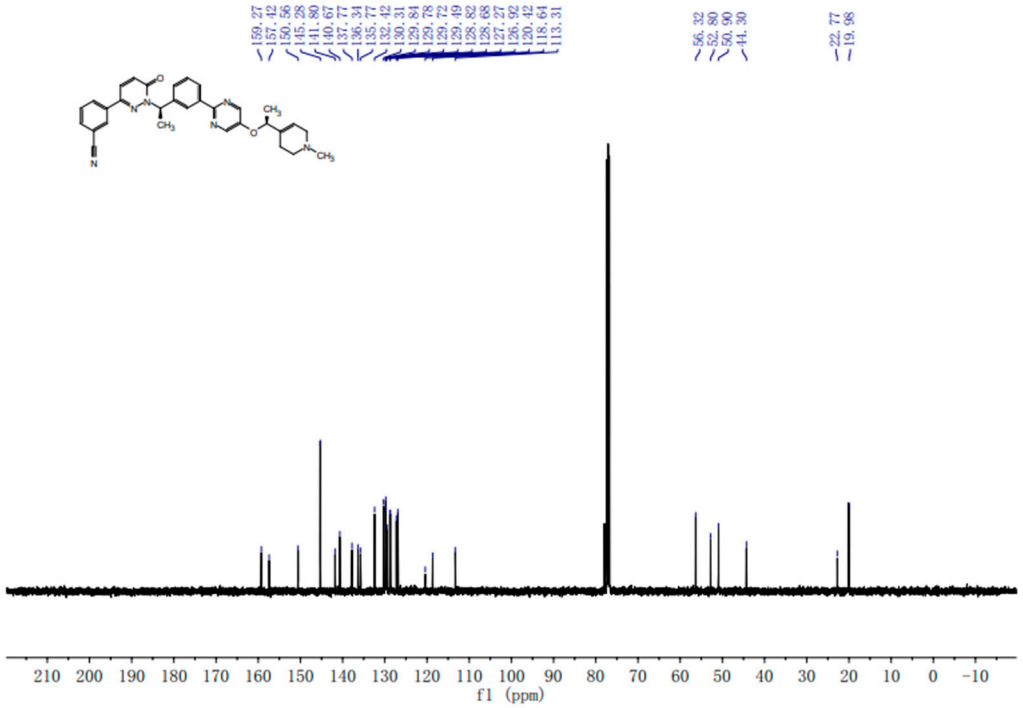


Compound (*R, S*)-12b

H^1 NMR

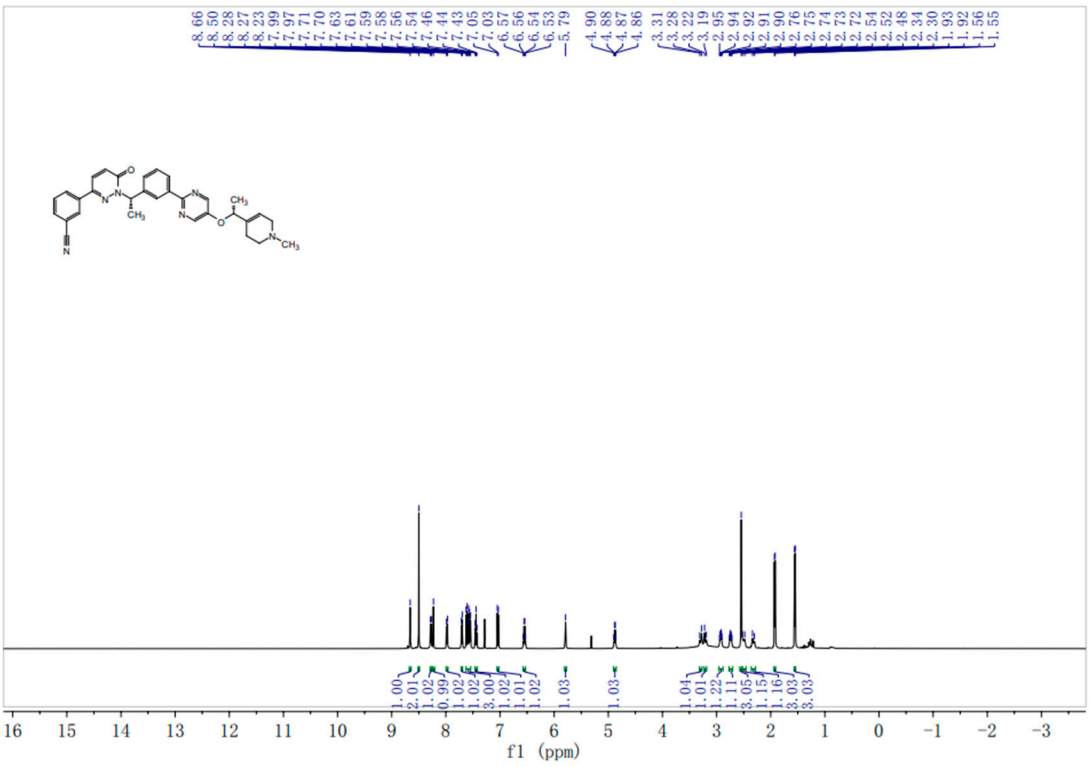


C^{13} NMR

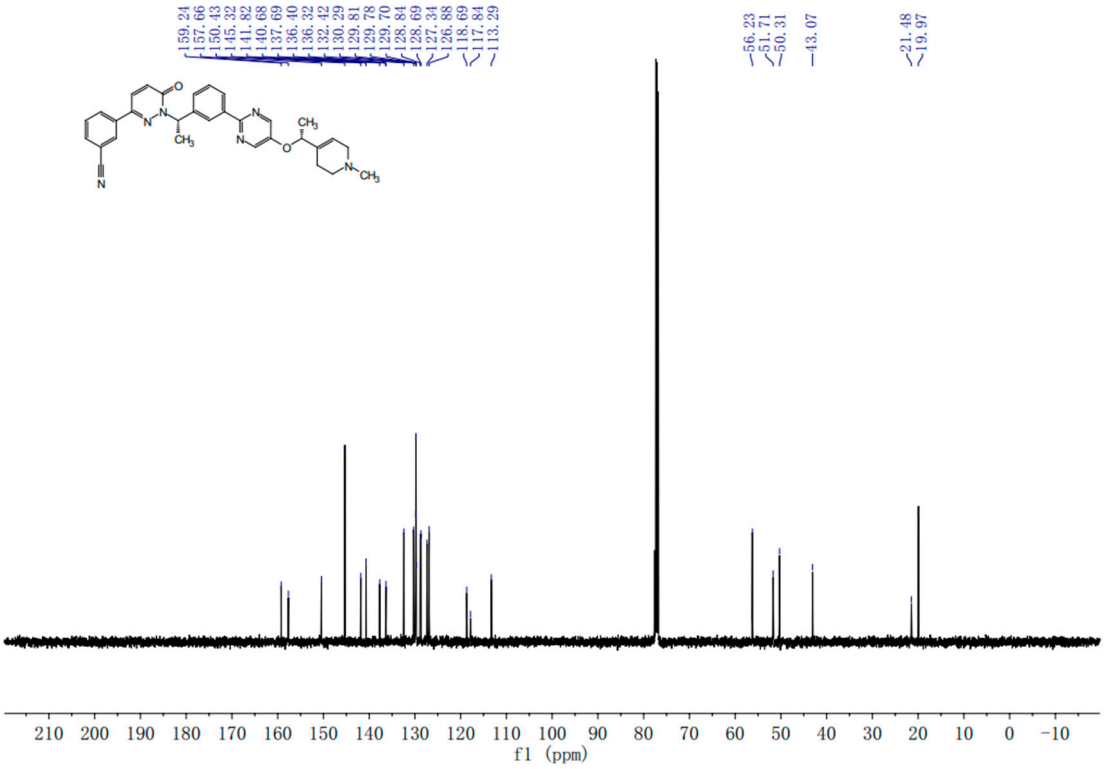


Compound (*S, R*)-12b

H^1 NMR

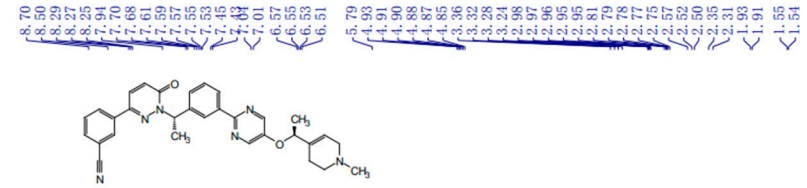


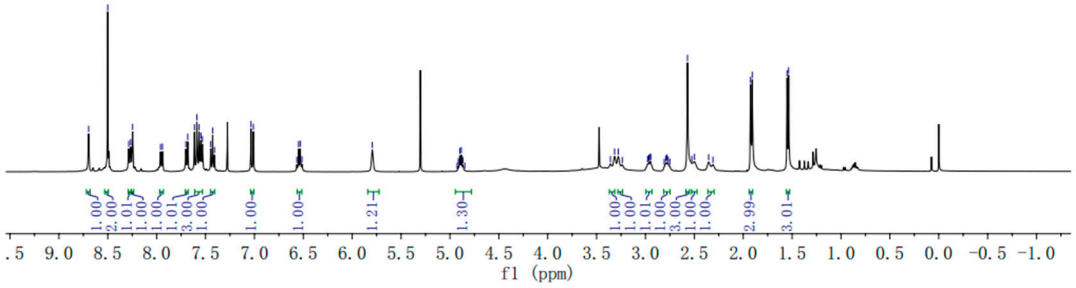
C^{13} NMR



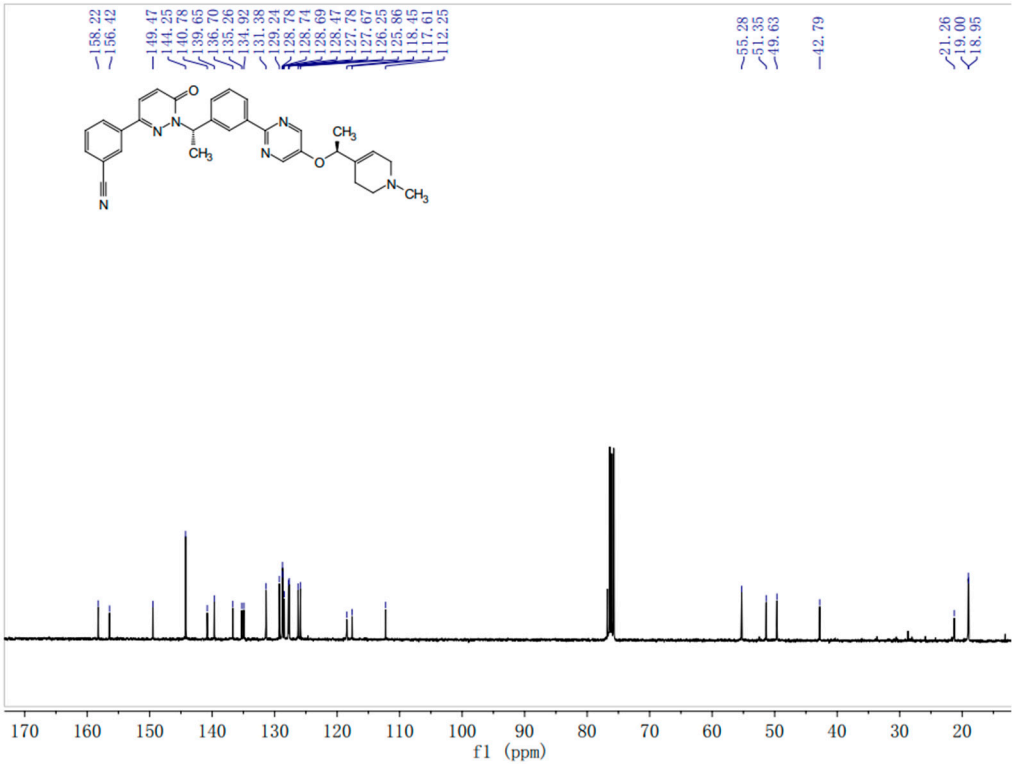
Compound (*S, S*)-12b

H[1] NMR



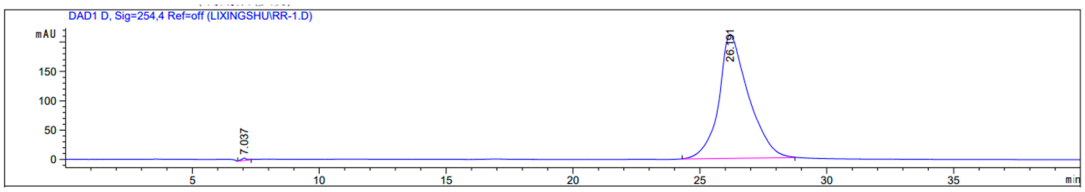


C[13] NMR



HPLC spectra of compounds

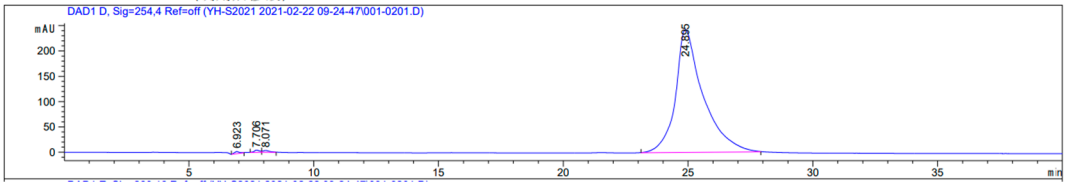
Compound (*R, R*)-12a



Signal 1: DAD1 D, Sig=254,4 Ref=off

Peak #	Ret.Time [min]	Type	width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.037	BB	0.1861	59.63461	4.24042	0.3464
2	26.191	BB	1.1411	1.71540e4	211.31198	99.6536
Total :				1.72136e4	215.55240	

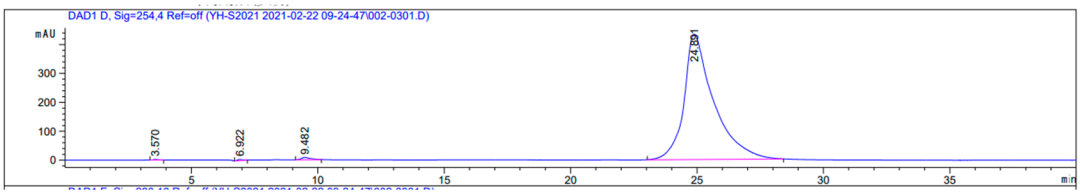
Compound (*R, S*)-12a



Signal 1: DAD1 D, Sig=254,4 Ref=off

Peak #	Ret.Time [min]	Type	width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.923	BB	0.1994	64.00987	4.30612	0.3380
2	7.706	BV	0.2265	70.79807	4.52691	0.3739
3	8.071	VB	0.2785	73.02588	3.72826	0.3856
4	24.895	BB	1.0696	1.87291e4	242.89191	98.9025
Total :				1.89369e4	255.45320	

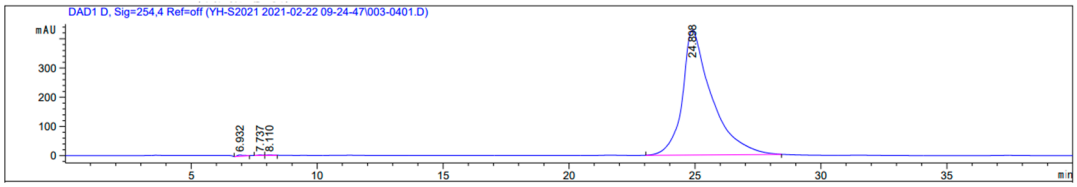
Compound (*S, R*)-12a



Signal 1: DAD1 D, Sig=254,4 Ref=off

Peak #	Ret.Time [min]	Type	width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.570	BB	0.2051	27.78988	1.87248	0.0778
2	6.922	BB	0.2073	65.20597	4.24351	0.1826
3	9.482	BB	0.3592	204.64351	8.03437	0.5729
4	24.891	BB	1.1350	3.54210e4	433.63293	99.1667
Total :				3.57187e4	447.78330	

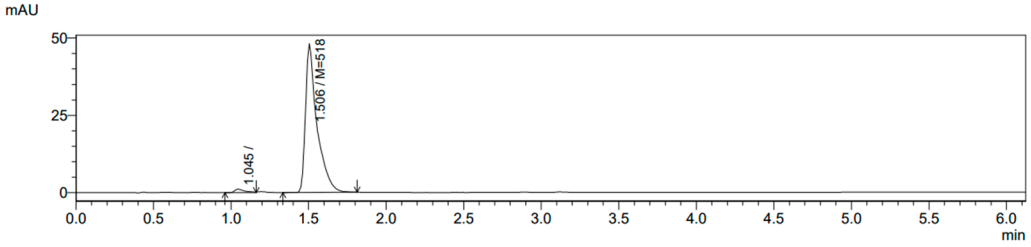
Compound (*S, S*)-12a



Signal 1: DAD1 D, Sig=254,4 Ref=off

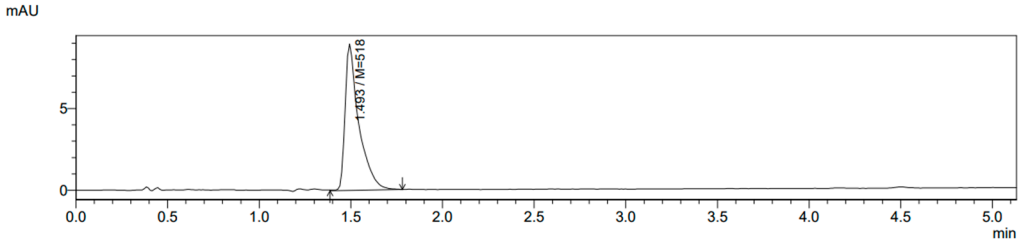
Peak #	Ret.Time [min]	Type	width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.037	BB	0.1861	59.63461	4.24042	0.3464
2	26.191	BB	1.1411	1.71540e4	211.31198	99.6536
Total :				1.72136e4	215.55240	

Compound (*R, R*)-12b



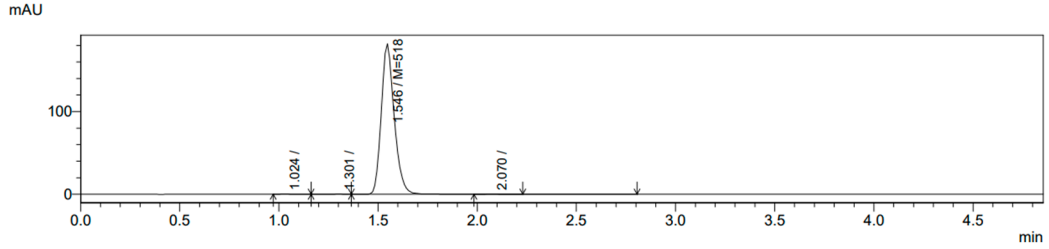
Ret.Time	Compounds	Width(Height 50%)	Height	Area	Area%	N(USP)	T	R(USP)
1.045		0.059	1140	5031	2.004	1304	--	--
1.506	M=518	0.069	48161	246057	97.996	1849	1.886	3.602
			49301	251088	100.000			

Compound (*R, S*)-12b



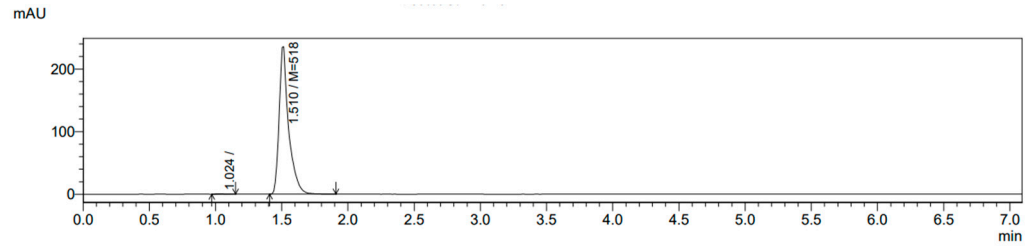
Ret.Time	Compounds	Width(Height 50%)	Height	Area	Area%	N(USP)	T	R(USP)
1.493	M=518	0.070	8975	46527	100.000	1772	1.977	--
			8975	46527	100.000			

Compound (*S, R*)-12b



Ret.Time	Compounds	Width(Height 50%)	Height	Area	Area%	N(USP)	T	R(USP)
1.024		0.074	356	1801	0.217	816	1.822	--
1.301		0.072	271	1510	0.182	1122	--	1.856
1.546	M=518	0.068	182115	823796	99.435	2064	1.218	1.675
2.070		0.087	237	1368	0.165	2443	1.470	3.452
			182979	828474	100.000			

Compound (*S, S*)-12b

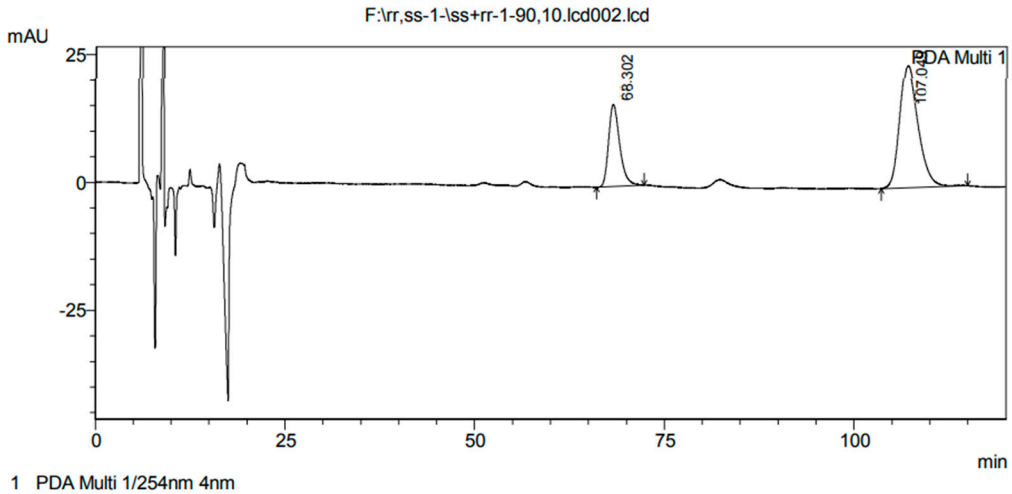


Ret.Time	Compounds	Width(Height 50%)	Height	Area	Area%	N(USP)	T	R(USP)
1.024		0.055	796	3168	0.270	1451	1.774	--
1.510	M=518	0.068	235375	1168377	99.730	2185	1.509	4.100
			236171	1171545	100.000			

HPLC Spectra of Chiral Purity

Mixture of enantiomer (*R, R*)-12a and (*S, S*)-12a

<Chromatogram>



1 PDA Multi 1/254nm 4nm

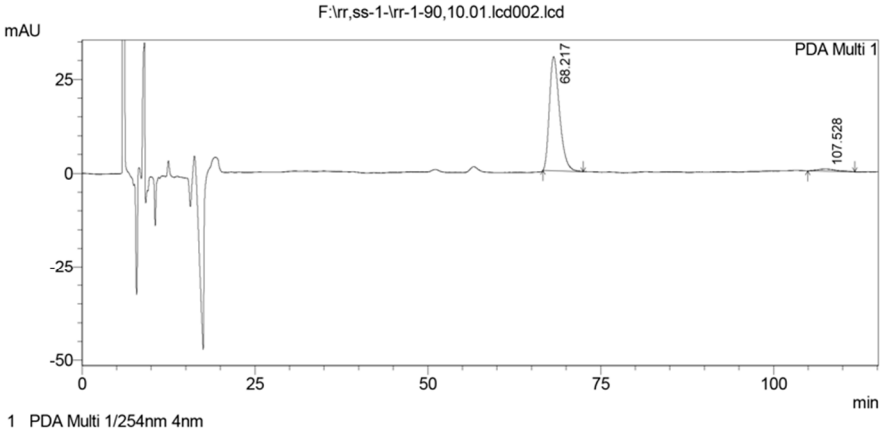
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	68.302	1629872	16034	28.806	40.228
2	107.049	4028229	23824	71.194	59.772
Total		5658101	39858	100.000	100.000

Compound (*R, R*)-12a

<Chromatogram>



1 PDA Multi 1/254nm 4nm

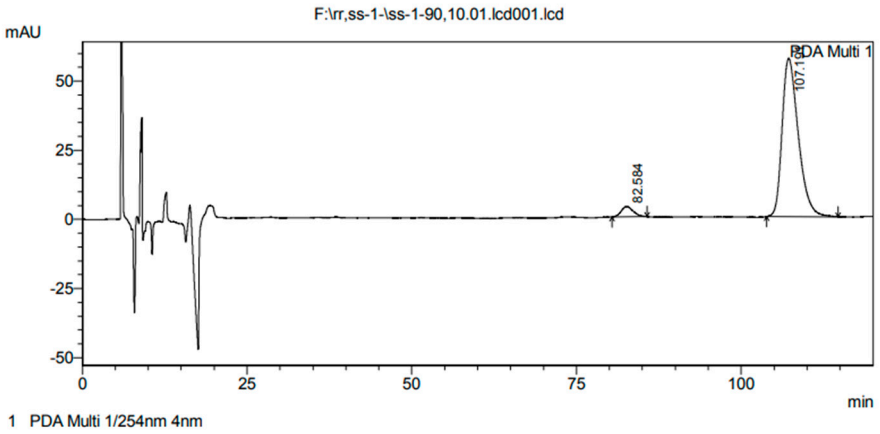
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	68.217	3104143	30404	96.562	97.955
2	107.528	110508	635	3.438	2.045
Total		3214651	31039	100.000	100.000

Compound (*S, S*)-12a

<Chromatogram>



1 PDA Multi 1/254nm 4nm

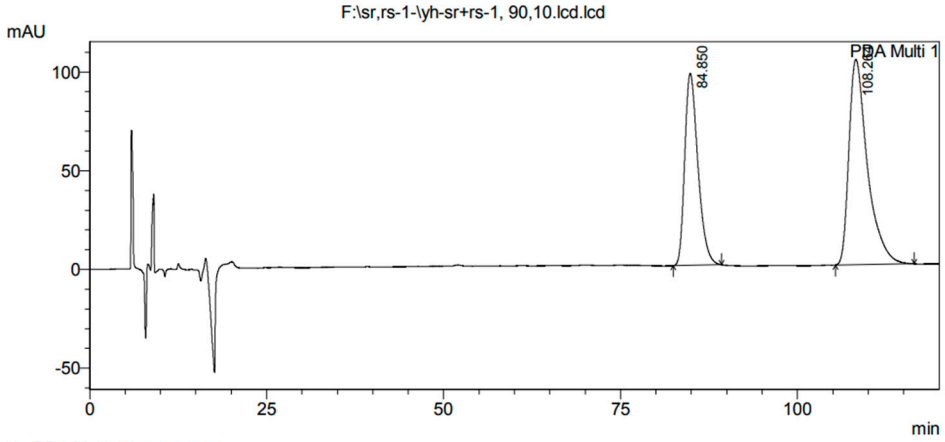
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	82.584	462538	3712	4.508	6.087
2	107.191	9798552	57264	95.492	93.913
Total		10261090	60975	100.000	100.000

Mixture of enantiomer (*R, S*)-12a and (*S, R*)-12a

<Chromatogram>



1 PDA Multi 1/254nm 4nm

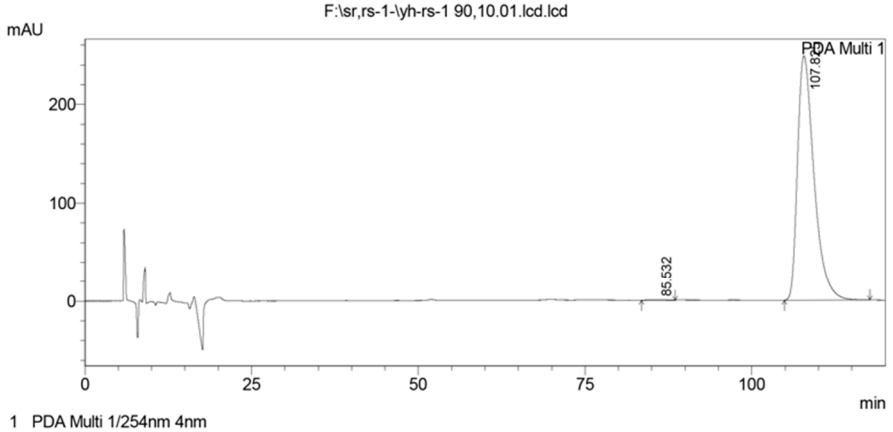
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	84.850	12578785	97205	39.941	48.307
2	108.264	18914975	104017	60.059	51.693
Total		31493760	201222	100.000	100.000

Compound (*R, S*)-12a

<Chromatogram>



1 PDA Multi 1/254nm 4nm

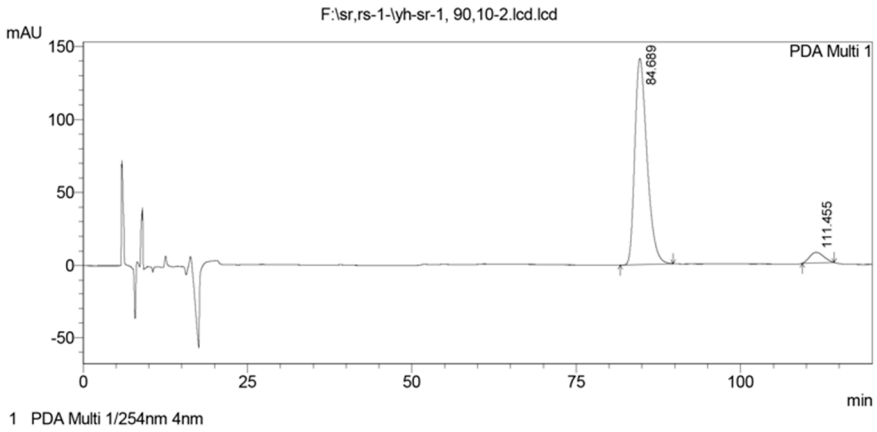
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	85.532	57750	506	0.135	0.203
2	107.825	42804480	248374	99.865	99.797
Total		42862230	248880	100.000	100.000

Compound (*S, R*)-12a

<Chromatogram>



1 PDA Multi 1/254nm 4nm

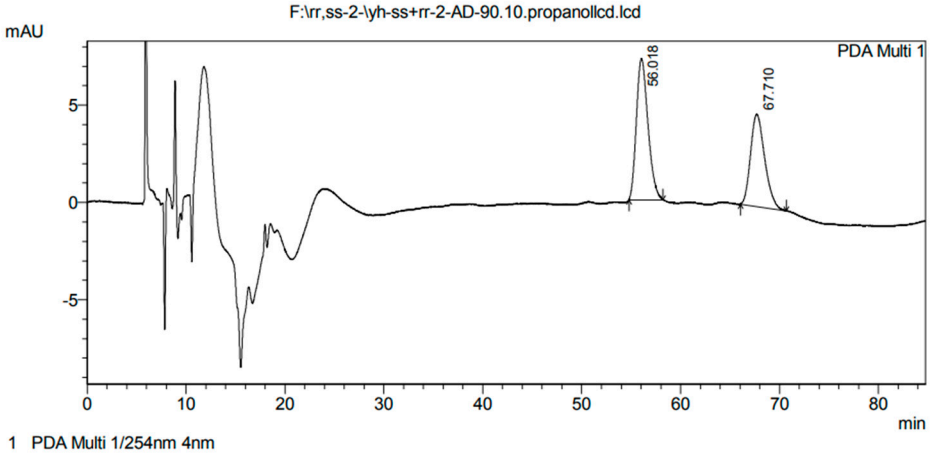
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	84.689	18236735	141137	94.462	95.116
2	111.455	1069150	7247	5.538	4.884
Total		19305885	148384	100.000	100.000

Mixture of enantiomer (*R, R*)-12b and (*S, S*)-12b

<Chromatogram>



1 PDA Multi 1/254nm 4nm

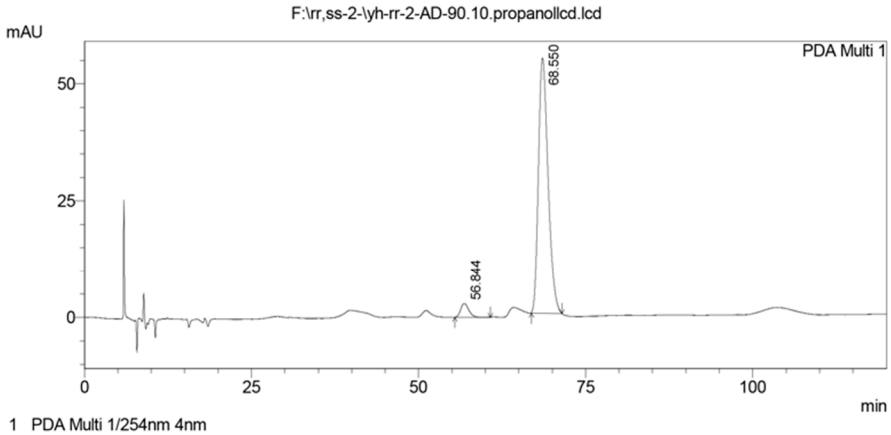
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	56.018	593148	7266	55.474	60.335
2	67.710	476097	4777	44.526	39.665
Total		1069245	12043	100.000	100.000

Compound (*R, R*)-12b

<Chromatogram>



1 PDA Multi 1/254nm 4nm

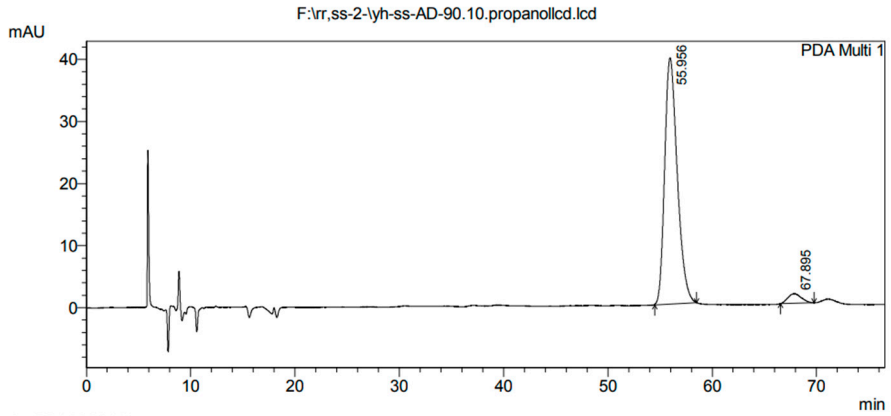
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	56.844	239685	2951	4.190	5.129
2	68.550	5480131	54587	95.810	94.871
Total		5719816	57538	100.000	100.000

Compound (*S, S*)-12b

<Chromatogram>



1 PDA Multi 1/254nm 4nm

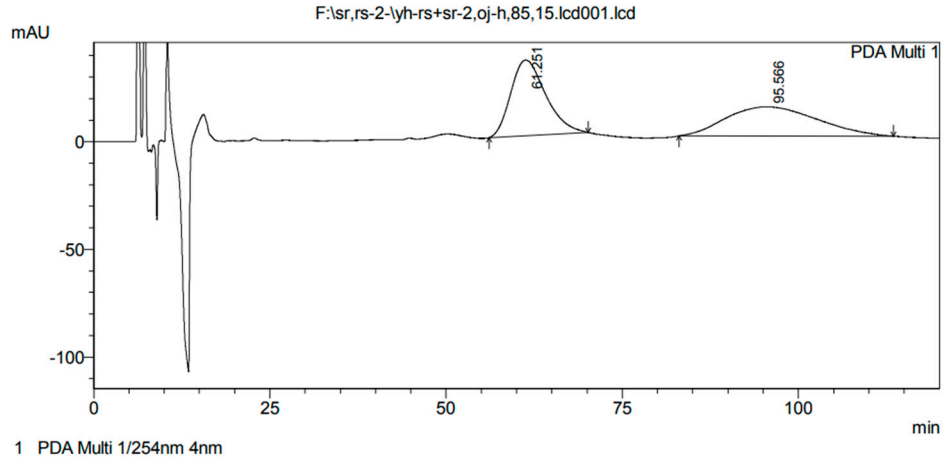
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	55.956	3326783	39683	96.087	96.272
2	67.895	135469	1537	3.913	3.728
Total		3462252	41220	100.000	100.000

Mixture of enantiomer (*R, S*)-12b and (*S, R*)-12b

<Chromatogram>



1 PDA Multi 1/254nm 4nm

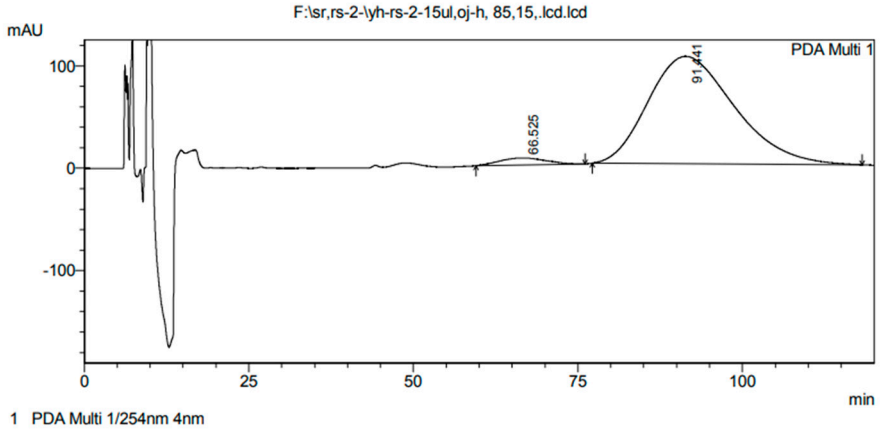
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	61.251	12117155	35183	49.740	72.071
2	95.566	12243921	13634	50.260	27.929
Total		24361076	48816	100.000	100.000

Compound (*R, S*)-12b

<Chromatogram>



1 PDA Multi 1/254nm 4nm

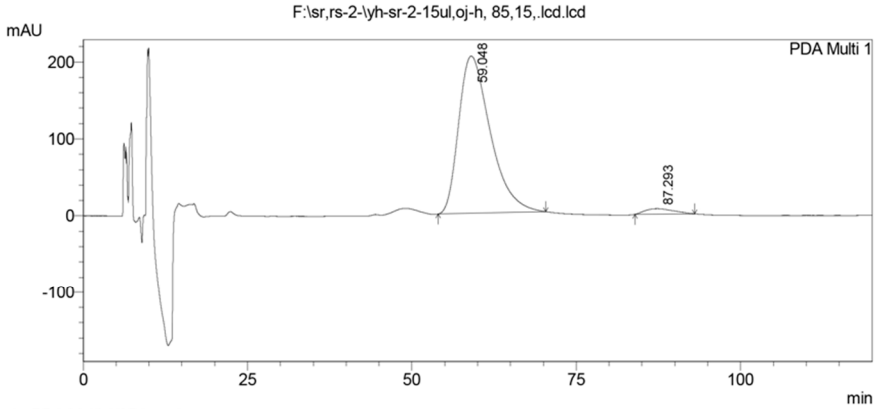
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	66.525	3328016	6867	3.352	6.142
2	91.441	95963580	104929	96.648	93.858
Total		99291596	111796	100.000	100.000

Compound (*S, R*)-12b

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	59.048	68532370	204360	97.011	96.669
2	87.293	2111818	7042	2.989	3.331
Total		70644188	211403	100.000	100.000

Compound (*R, R*)-**12a**

Formula Predictor Report - RR-1.lcd

Data File: \\Deep-20160624ld\data1\黎星术\YH\RR-1.lcd

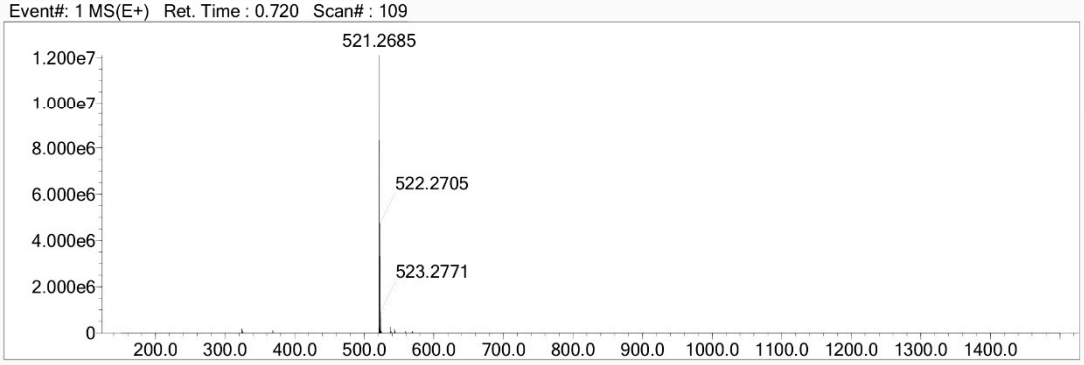
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	32	32	P	3	0	0	Se	2	0	0	H
B	3	0	0	S	2	0	0	Br	1	0	0	Na
C	4	31	31	Cl	1	0	10	Ru	2	0	0	NH4
N	3	6	6	Fe	2	0	4	Sb	3	0	0	K
O	2	2	2	Ni	2	0	0	I	3	0	0	
F	1	0	0	Cu	2	0	0	Ir	3	0	0	
Si	4	0	0	Zn	2	0	0	Pt	2	0	0	

Error Margin (mDa): 20.0
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

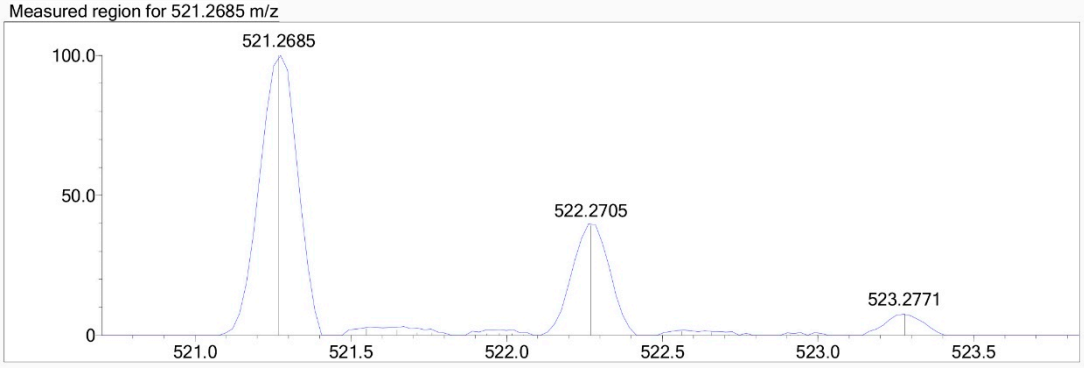
DBE Range: not fixed
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 429

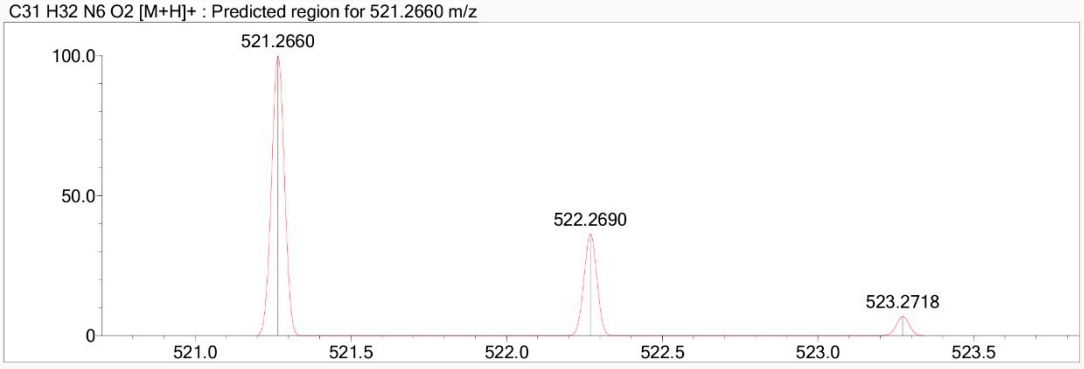
Event#: 1 MS(E+) Ret. Time : 0.720 Scan# : 109



Measured region for 521.2685 m/z



C31 H32 N6 O2 [M+H]+ : Predicted region for 521.2660 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	66.62	C31 H32 N6 O2	[M+H]+	521.2685	521.2660	2.5	4.80	73.62	19.0

Compound (*R, S*)-12a

Formula Predictor Report - RS-1.lcd

Data File: \\Deep-20160624ld\data1\黎星术\YH\RS-1.lcd

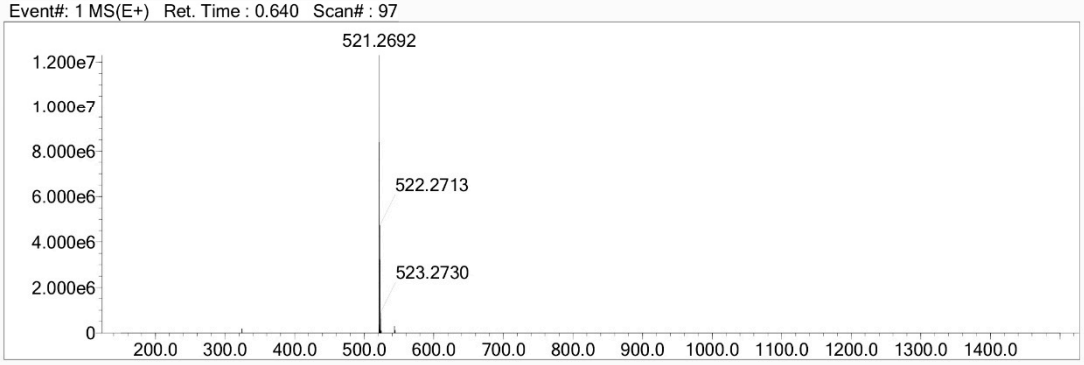
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	32	32	P	3	0	0	Se	2	0	0	H
B	3	0	0	S	2	0	0	Br	1	0	0	Na
C	4	31	31	Cl	1	0	10	Ru	2	0	0	NH4
N	3	6	6	Fe	2	0	4	Sb	3	0	0	K
O	2	2	2	Ni	2	0	0	I	3	0	0	
F	1	0	0	Cu	2	0	0	Ir	3	0	0	
Si	4	0	0	Zn	2	0	0	Pt	2	0	0	

Error Margin (mDa): 20.0
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

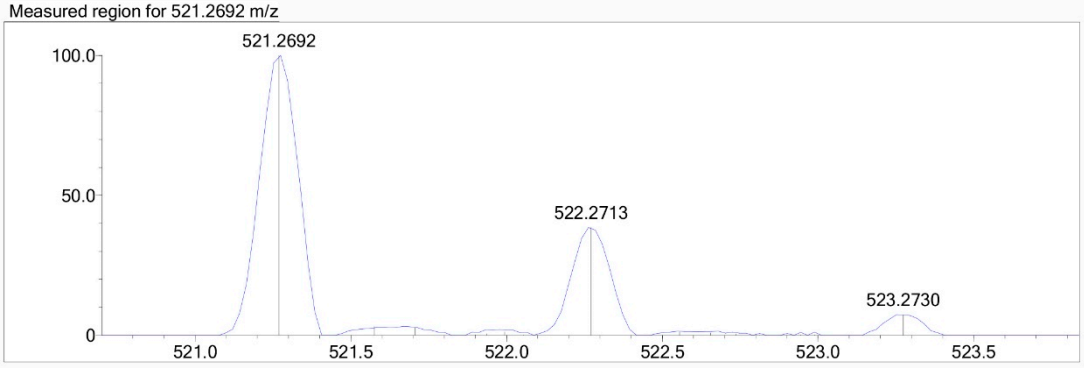
DBE Range: not fixed
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 429

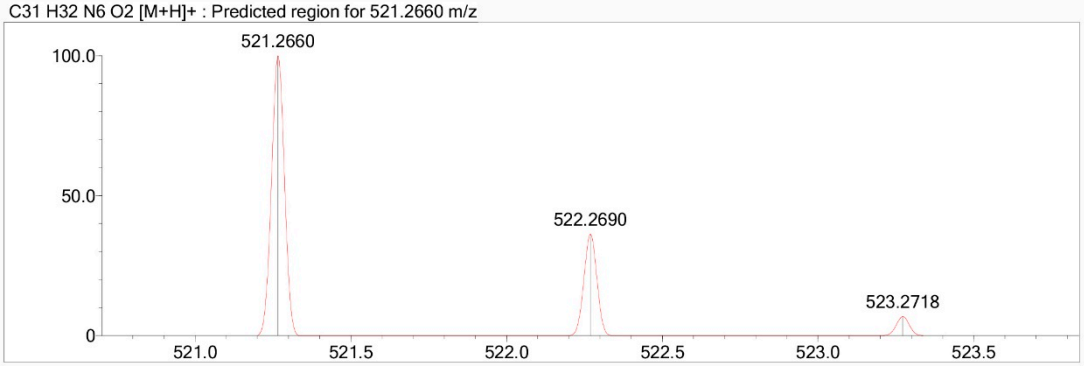
Event#: 1 MS(E+) Ret. Time : 0.640 Scan# : 97



Measured region for 521.2692 m/z



C31 H32 N6 O2 [M+H]+ : Predicted region for 521.2660 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	58.42	C31 H32 N6 O2	[M+H]+	521.2692	521.2660	3.2	6.14	74.32	19.0

Compound(*S, R*)-**12a**

Formula Predictor Report - SR-1.lcd

Data File: \\Deep-20160624ld\data1\黎星术\YH\SR-1.lcd

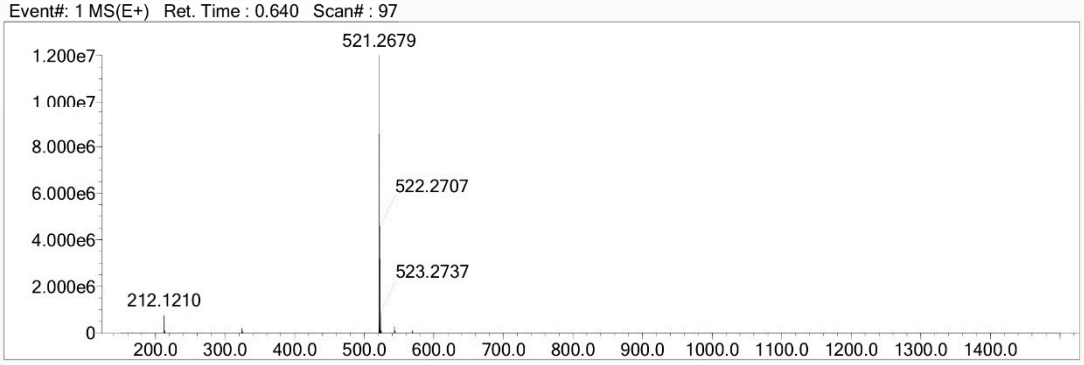
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	32	32	P	3	0	0	Se	2	0	0	H
B	3	0	0	S	2	0	0	Br	1	0	0	Na
C	4	31	31	Cl	1	0	10	Ru	2	0	0	NH4
N	3	6	6	Fe	2	0	4	Sb	3	0	0	K
O	2	2	2	Ni	2	0	0	I	3	0	0	
F	1	0	0	Cu	2	0	0	Ir	3	0	0	
Si	4	0	0	Zn	2	0	0	Pt	2	0	0	

Error Margin (mDa): 20.0
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

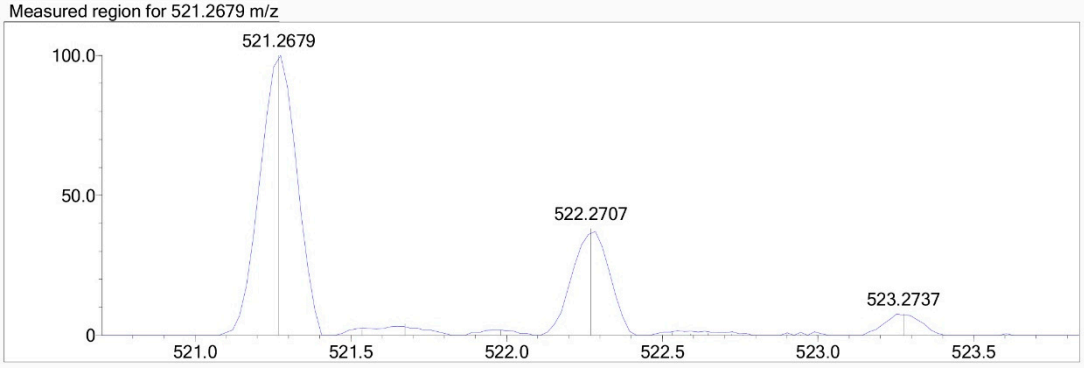
DBE Range: not fixed
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 429

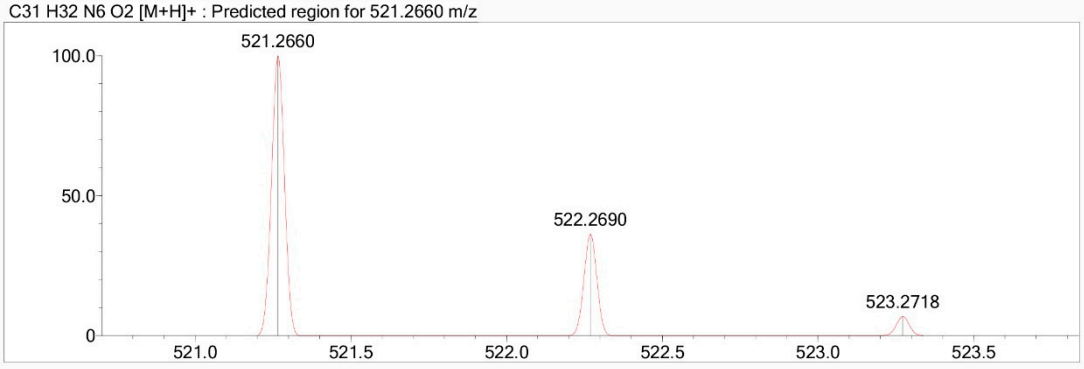
Event#: 1 MS(E+) Ret. Time : 0.640 Scan# : 97



Measured region for 521.2679 m/z



C31 H32 N6 O2 [M+H]+ : Predicted region for 521.2660 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	69.73	C31 H32 N6 O2	[M+H]+	521.2679	521.2660	1.9	3.64	74.65	19.0

Compound(*S, S*)-12a

Formula Predictor Report - SS-1.lcd

Data File: \\Deep-20160624ld\data1\黎星术\YH\SS-1.lcd

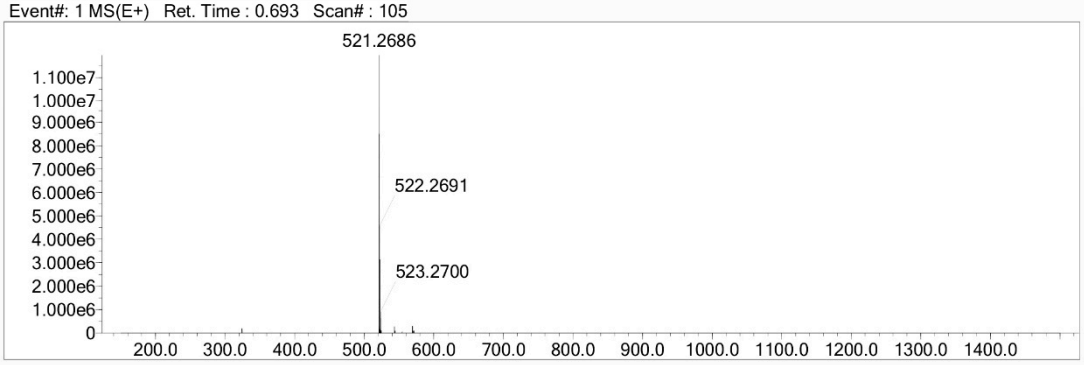
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	32	32	P	3	0	0	Se	2	0	0	H
B	3	0	0	S	2	0	0	Br	1	0	0	Na
C	4	31	31	Cl	1	0	10	Ru	2	0	0	NH4
N	3	6	6	Fe	2	0	4	Sb	3	0	0	K
O	2	2	2	Ni	2	0	0	I	3	0	0	
F	1	0	0	Cu	2	0	0	Ir	3	0	0	
Si	4	0	0	Zn	2	0	0	Pt	2	0	0	

Error Margin (mDa): 20.0
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

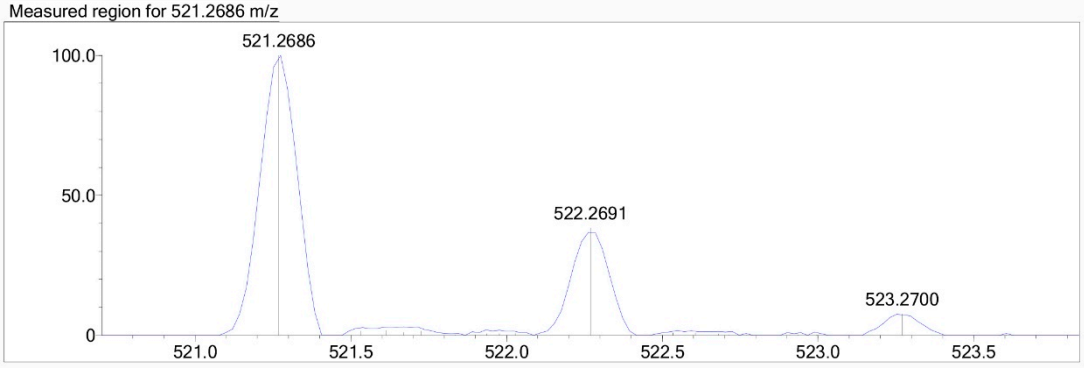
DBE Range: not fixed
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 429

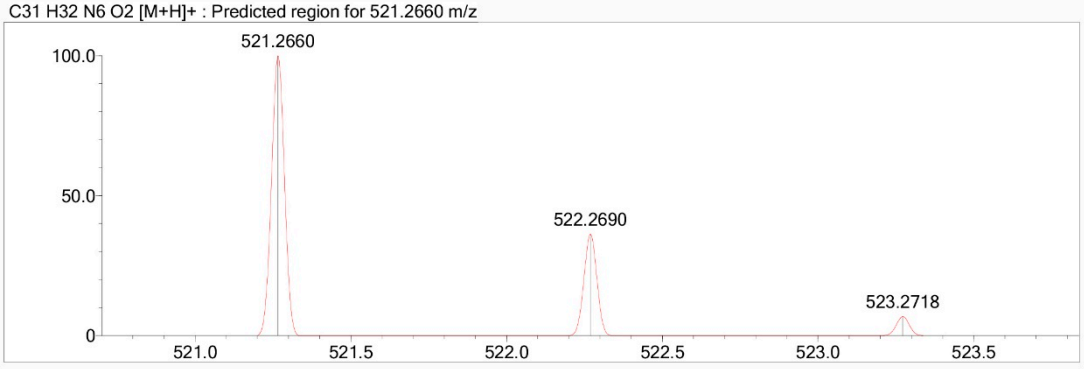
Event#: 1 MS(E+) Ret. Time : 0.693 Scan# : 105



Measured region for 521.2686 m/z



C31 H32 N6 O2 [M+H]+ : Predicted region for 521.2660 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	66.72	C31 H32 N6 O2	[M+H]+	521.2686	521.2660	2.6	4.99	74.12	19.0

Compound(*R, R*)-**12b**

Formula Predictor Report - RR-2.lcd

Data File: \\Deep-20160624ld\data1\黎星术\YH\RR-2.lcd

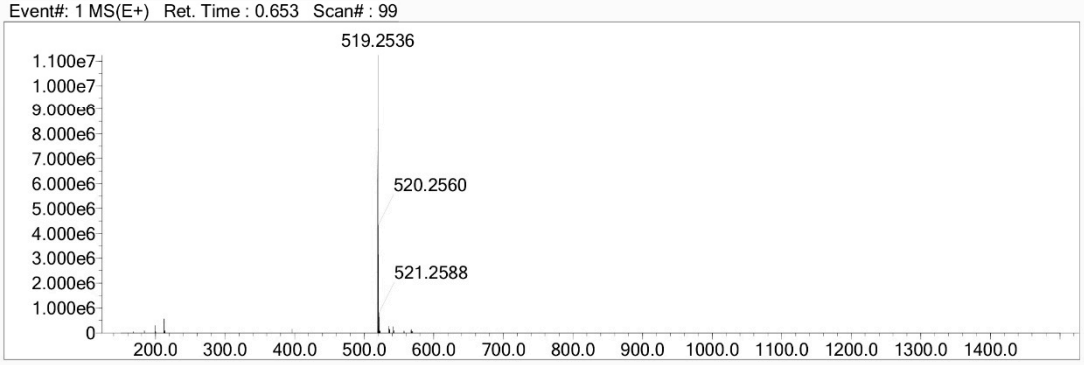
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	30	30	P	3	0	0	Se	2	0	0	H
B	3	0	0	S	2	0	0	Br	1	0	0	Na
C	4	31	31	Cl	1	0	10	Ru	2	0	0	NH4
N	3	6	6	Fe	2	0	4	Sb	3	0	0	K
O	2	2	2	Ni	2	0	0	I	3	0	0	
F	1	0	0	Cu	2	0	0	Ir	3	0	0	
Si	4	0	0	Zn	2	0	0	Pt	2	0	0	

Error Margin (mDa): 20.0
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

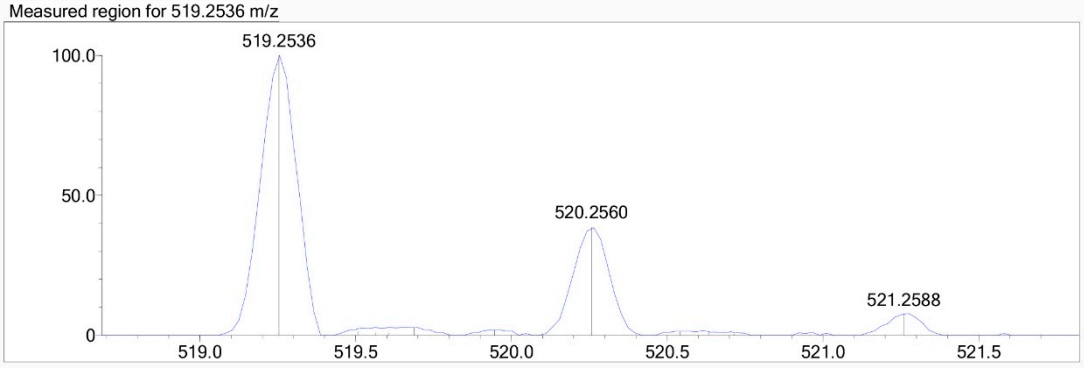
DBE Range: not fixed
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 429

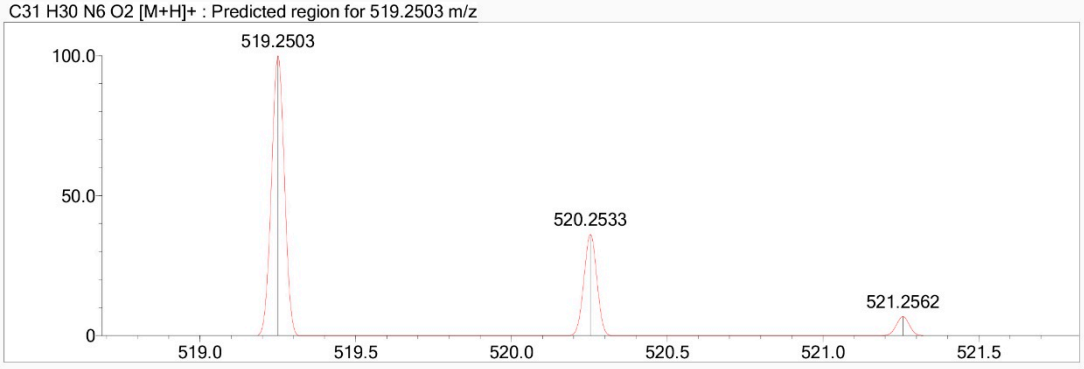
Event#: 1 MS(E+) Ret. Time : 0.653 Scan# : 99



Measured region for 519.2536 m/z



C31 H30 N6 O2 [M+H]+ : Predicted region for 519.2503 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	60.91	C31 H30 N6 O2	[M+H]+	519.2536	519.2503	3.3	6.36	79.73	20.0

Compound(*R, S*)-**12b**

Formula Predictor Report - RS-2.lcd

Data File: \\Deep-20160624ld\data1\黎星术\YH\RS-2.lcd

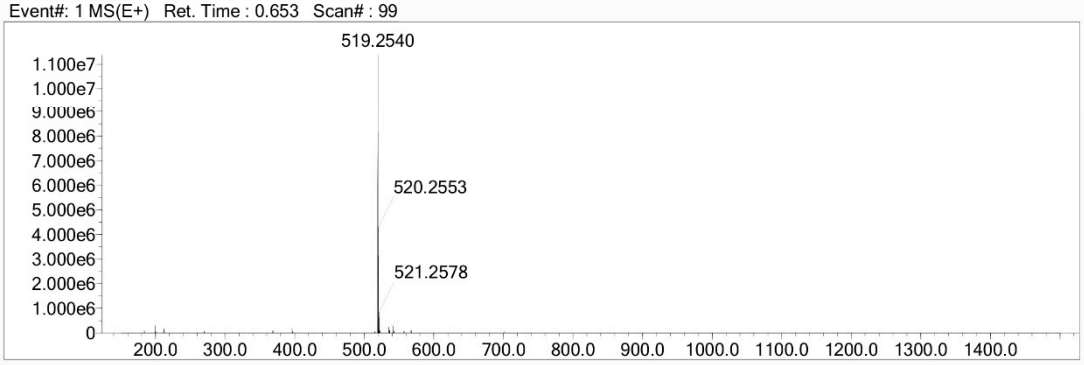
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	30	30	P	3	0	0	Se	2	0	0	H
B	3	0	0	S	2	0	0	Br	1	0	0	Na
C	4	31	31	Cl	1	0	10	Ru	2	0	0	NH4
N	3	6	6	Fe	2	0	4	Sb	3	0	0	K
O	2	2	2	Ni	2	0	0	I	3	0	0	
F	1	0	0	Cu	2	0	0	Ir	3	0	0	
Si	4	0	0	Zn	2	0	0	Pt	2	0	0	

Error Margin (mDa): 20.0
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

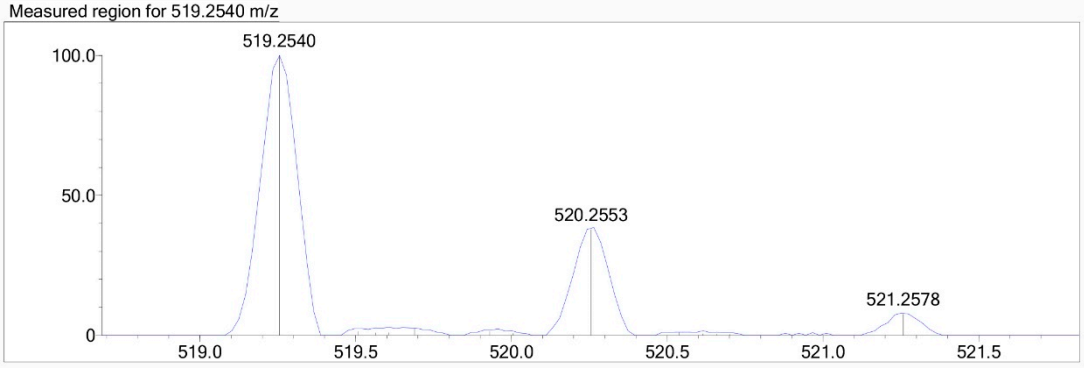
DBE Range: not fixed
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 429

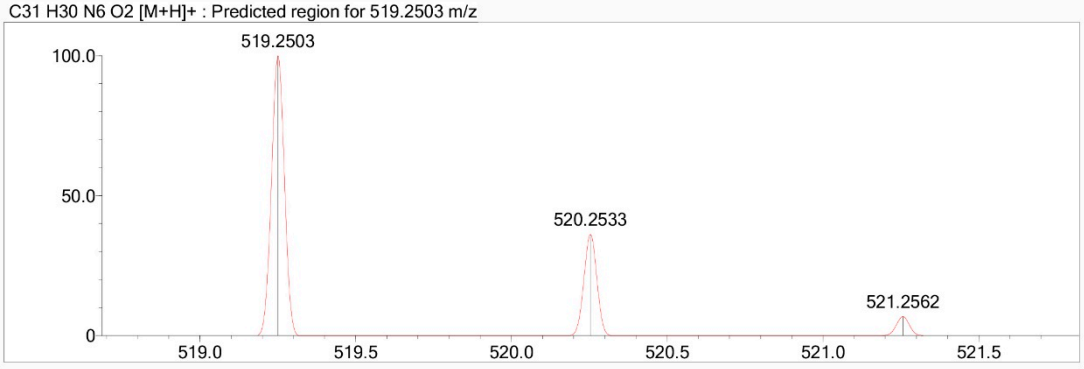
Event#: 1 MS(E+) Ret. Time : 0.653 Scan# : 99



Measured region for 519.2540 m/z



C31 H30 N6 O2 [M+H]+ : Predicted region for 519.2503 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	55.41	C31 H30 N6 O2	[M+H]+	519.2540	519.2503	3.7	7.13	80.65	20.0

Compound(*S, R*)-**12b**

Formula Predictor Report - SR-2.lcd

Data File: \\Deep-20160624ld\data1\黎星术\YH\SR-2.lcd

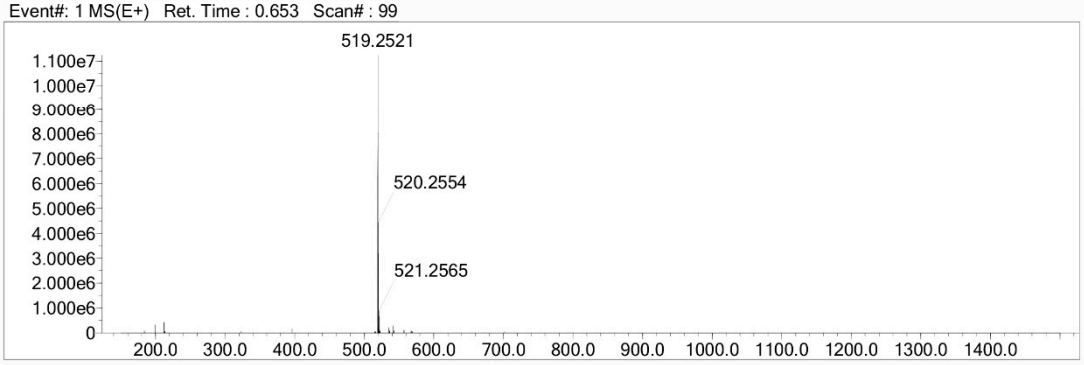
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	30	30	P	3	0	0	Se	2	0	0	H
B	3	0	0	S	2	0	0	Br	1	0	0	Na
C	4	31	31	Cl	1	0	10	Ru	2	0	0	NH4
N	3	6	6	Fe	2	0	4	Sb	3	0	0	K
O	2	2	2	Ni	2	0	0	I	3	0	0	
F	1	0	0	Cu	2	0	0	Ir	3	0	0	
Si	4	0	0	Zn	2	0	0	Pt	2	0	0	

Error Margin (mDa): 20.0
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

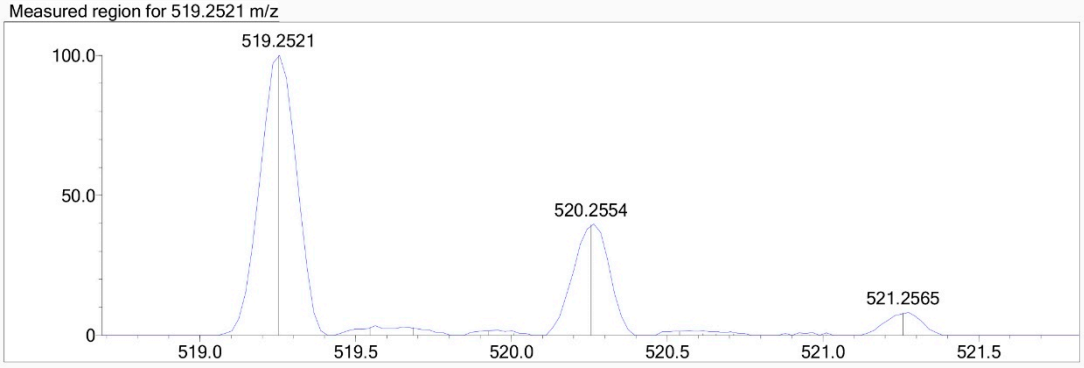
DBE Range: not fixed
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 429

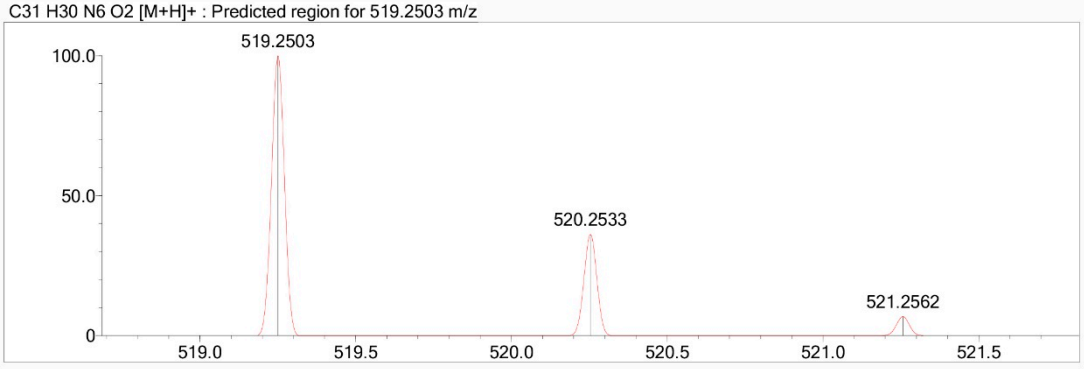
Event#: 1 MS(E+) Ret. Time : 0.653 Scan# : 99



Measured region for 519.2521 m/z



C31 H30 N6 O2 [M+H]+ : Predicted region for 519.2503 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	75.56	C31 H30 N6 O2	[M+H]+	519.2521	519.2503	1.8	3.47	80.53	20.0

Compound(*S, S*)-**12b**

Formula Predictor Report - SS-2.lcd

Data File: \\Deep-20160624ld\data1\黎星术\YH\SS-2.lcd

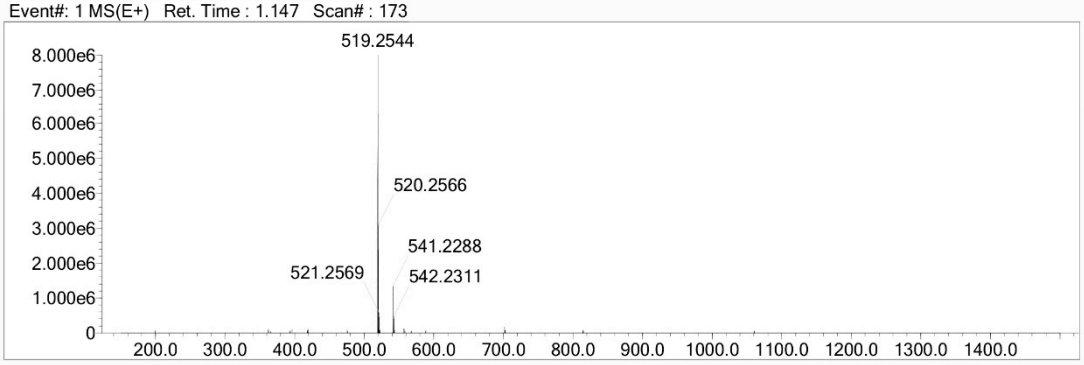
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	30	30	P	3	0	0	Se	2	0	0	H
B	3	0	0	S	2	0	0	Br	1	0	0	Na
C	4	31	31	Cl	1	0	10	Ru	2	0	0	NH4
N	3	6	6	Fe	2	0	4	Sb	3	0	0	K
O	2	2	2	Ni	2	0	0	I	3	0	0	
F	1	0	0	Cu	2	0	0	Ir	3	0	0	
Si	4	0	0	Zn	2	0	0	Pt	2	0	0	

Error Margin (mDa): 20.0
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

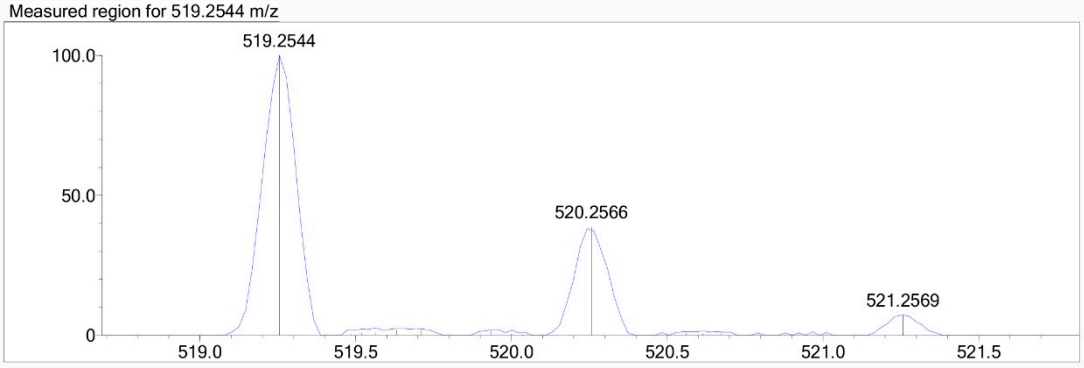
DBE Range: not fixed
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 429

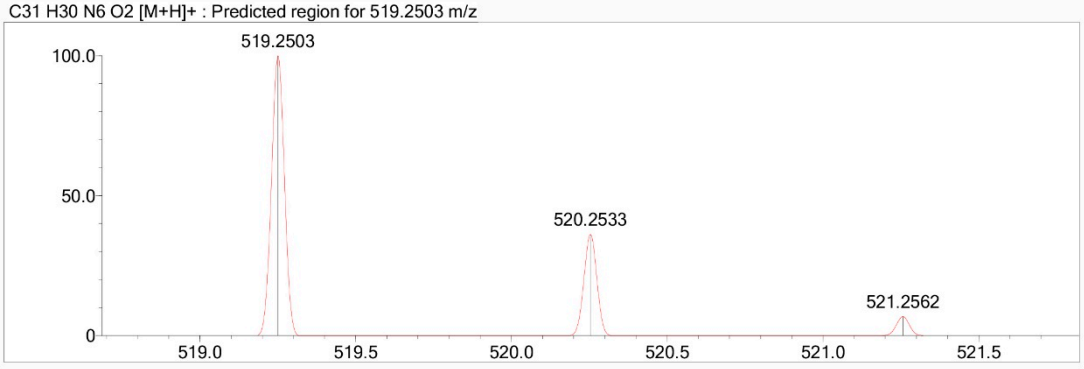
Event#: 1 MS(E+) Ret. Time : 1.147 Scan# : 173



Measured region for 519.2544 m/z



C31 H30 N6 O2 [M+H]+ : Predicted region for 519.2503 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	51.23	C31 H30 N6 O2	[M+H]+	519.2544	519.2503	4.1	7.90	83.98	20.0

Hy0102 representing compound **R-5b**

Table S1 Crystal data and structure refinement for hy0102.

Identification code	hy0102
Empirical formula	$C_{30}H_{31}ClN_6O_2$
Formula weight	543.06
Temperature/K	169.99(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	13.7983(8)
b/Å	7.3771(3)
c/Å	14.3578(7)
α/°	90
β/°	101.730(5)
γ/°	90
Volume/Å^3	1430.97(12)
Z	2
ρ_{calc}g/cm^3	1.260
μ/mm^{-1}	1.482
F(000)	572.0
Crystal size/mm^3	0.15 × 0.11 × 0.09

Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.288 to 133.078
Index ranges	-16 ≤ h ≤ 14, -5 ≤ k ≤ 8, -17 ≤ l ≤ 16
Reflections collected	5010
Independent reflections	3735 [R_{int} = 0.0499, R_{sigma} = 0.0818]
Data/restraints/parameters	3735/1/354
Goodness-of-fit on F^2	1.018
Final R indexes [I>=2σ (I)]	R_1 = 0.0529, wR_2 = 0.1253
Final R indexes [all data]	R_1 = 0.0592, wR_2 = 0.1330
Largest diff. peak/hole / e $Å^{-3}$	0.30/-0.34
Flack parameter	0.02(3)

Crystal structure determination of [hy0102]

Crystal Data for $C_{30}H_{31}ClN_6O_2$ (*M* =543.06 g/mol): monoclinic, space group $P2_1$ (no. 4), *a* = 13.7983(8) Å, *b* = 7.3771(3) Å, *c* = 14.3578(7) Å, *β* = 101.730(5)°, *V* = 1430.97(12) $Å^3$, *Z* = 2, *T* = 169.99(10) K, μ(Cu Kα) = 1.482 mm^{-1}, *Dcalc* = 1.260 g/cm^3, 5010 reflections measured (6.288° ≤ 2Θ ≤ 133.078°), 3735 unique (R_{int} = 0.0499, R_{sigma} = 0.0818) which were used in all calculations. The final R_1 was 0.0529 (I > 2σ(I)) and wR_2 was 0.1330 (all data).

Refinement model description

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for hy0102. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	9110.0(9)	-255.3(16)	1009.5(8)	32.6(3)
O1	5324(3)	5668(6)	9674(2)	43.5(10)
O2	7510(2)	5542(5)	3237(2)	30.0(8)
N1	4192(6)	8460(8)	3222(4)	73(2)
N2	4389(3)	7162(5)	7318(3)	25.1(9)
N3	4901(3)	7052(5)	8223(3)	23.5(8)
N4	6661(3)	6914(6)	5333(3)	25.6(9)
N5	8371(3)	6173(6)	5796(3)	28.8(9)
N6	8297(3)	3325(6)	79(3)	27.0(9)
C1	3176(4)	6144(7)	6012(4)	32.5(12)
C2	3692(4)	6829(7)	5351(4)	32.7(12)
C3	3207(4)	7062(8)	4410(4)	41.0(14)
C4	2215(5)	6614(9)	4114(4)	50.3(16)
C5	1717(5)	5922(8)	4768(5)	52.0(17)
C6	2179(4)	5685(8)	5722(4)	41.4(14)
C7	3748(5)	7843(9)	3742(4)	50.4(16)

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for hy0102. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C8	3690(4)	5959(7)	7020(3)	27.6(11)
C9	3473(4)	4569(8)	7634(4)	36.3(12)
C10	4008(4)	4440(7)	8529(4)	38.0(13)
C11	4781(4)	5694(7)	8871(3)	32.3(12)
C12	5636(3)	8498(7)	8518(3)	26.0(10)
C13	5211(4)	10328(7)	8173(4)	31.7(11)
C14	6591(3)	8105(6)	8193(3)	24.6(10)
C15	7487(3)	8343(7)	8836(3)	27.4(11)
C16	8366(4)	8069(7)	8552(3)	30.3(11)
C17	8395(4)	7564(7)	7627(3)	30.4(11)
C18	7498(3)	7322(6)	6969(3)	22.5(10)
C19	6613(4)	7621(7)	7257(3)	26.1(10)
C20	7522(3)	6757(7)	5984(3)	26.1(10)
C22	8395(4)	5727(7)	4894(3)	30.6(11)
C23	7551(3)	5896(7)	4176(3)	25.3(10)
C24	6695(4)	6463(7)	4443(3)	27.4(11)

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for hy0102. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C26	8430(3)	5167(7)	2954(3)	28.4(12)
C27	8217(3)	5128(6)	1873(3)	26.0(11)
C28	9182(3)	4896(7)	1532(3)	25.6(10)
C29	8979(3)	4845(7)	448(3)	26.2(10)
C30	7333(4)	3508(8)	390(3)	34.4(12)
C31	7512(4)	3605(8)	1476(3)	31.4(11)
C32	8139(4)	3198(8)	-988(3)	40.0(13)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for hy0102. The Anisotropic displacement factor exponent takes the form: -$2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	44.5(7)	28.5(6)	23.4(5)	-1.5(5)	3.7(4)	2.2(6)
O1	56(2)	45(2)	29.1(19)	13.6(18)	7.1(17)	9.9(19)
O2	30.8(18)	43(2)	16.9(15)	-3.6(15)	7.2(13)	6.8(16)
N1	138(6)	45(3)	41(3)	3(3)	30(4)	22(4)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for hy0102. The Anisotropic displacement factor exponent takes the form: -

$2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N2	32(2)	22(2)	21.0(19)	-1.9(16)	5.5(16)	0.0(17)
N3	32(2)	22(2)	18.9(18)	1.7(17)	10.3(16)	0.9(17)
N4	28(2)	32(2)	16.8(19)	-2.1(18)	5.8(16)	1.3(18)
N5	28(2)	37(3)	22(2)	-2.0(18)	6.7(16)	3.1(18)
N6	37(2)	25(2)	19.5(19)	-1.3(17)	6.0(16)	1.5(18)
C1	33(3)	25(3)	38(3)	-9(2)	4(2)	3(2)
C2	40(3)	27(3)	29(3)	-5(2)	2(2)	4(2)
C3	56(4)	33(3)	32(3)	-6(3)	5(3)	8(3)
C4	60(4)	45(4)	39(3)	-7(3)	-6(3)	5(3)
C5	43(3)	41(4)	61(4)	-16(3)	-16(3)	0(3)
C6	38(3)	32(3)	52(3)	-6(3)	5(3)	-6(2)
C7	77(5)	43(4)	29(3)	-7(3)	7(3)	15(3)
C8	28(2)	22(2)	33(3)	0(2)	8(2)	-1(2)
C9	47(3)	28(3)	39(3)	-4(3)	19(2)	-10(2)
C10	58(3)	25(3)	37(3)	4(2)	24(3)	-2(2)
C11	44(3)	29(3)	28(3)	8(2)	17(2)	8(2)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for hy0102. The Anisotropic displacement factor exponent takes the form: -

$2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	28(3)	28(2)	21(2)	-4(2)	4.1(19)	-1(2)
C13	35(3)	22(3)	38(3)	-3(2)	8(2)	4(2)
C14	27(2)	26(3)	21(2)	-0.6(19)	6.2(19)	0(2)
C15	37(3)	25(3)	20(2)	-1(2)	5(2)	-4(2)
C16	29(3)	38(3)	21(2)	-2(2)	-2.7(19)	-6(2)
C17	27(2)	38(3)	27(2)	-3(2)	7(2)	-6(2)
C18	25(2)	27(2)	14(2)	-0.3(18)	0.7(17)	-4(2)
C19	30(2)	27(3)	20(2)	-2(2)	3.8(19)	0(2)
C20	29(2)	30(3)	18(2)	0(2)	1.1(18)	-5(2)
C22	30(3)	36(3)	27(2)	0(2)	6(2)	9(2)
C23	32(3)	28(3)	16(2)	1(2)	4.0(18)	3(2)
C24	28(2)	34(3)	21(2)	1(2)	6.4(19)	-2(2)
C26	32(3)	33(3)	21(2)	-1(2)	7.7(19)	3(2)
C27	32(2)	27(3)	19(2)	1.1(19)	7.0(19)	3(2)
C28	29(2)	27(2)	20(2)	-1(2)	3.3(18)	3(2)
C29	31(2)	27(2)	22(2)	-1(2)	8.2(18)	0(2)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for hy0102. The Anisotropic displacement factor exponent takes the form: -$2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C30	30(3)	46(3)	28(3)	-6(2)	5(2)	-1(2)
C31	31(3)	38(3)	27(2)	-7(2)	12(2)	-4(2)
C32	60(4)	39(3)	22(3)	-4(2)	10(2)	-3(3)

Table S4 Bond Lengths for hy0102.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C11	1.240(6)	C4	C5	1.370(9)
O2	C23	1.363(5)	C5	C6	1.398(8)
O2	C26	1.436(5)	C8	C9	1.423(7)
N1	C7	1.152(8)	C9	C10	1.349(7)
N2	N3	1.350(5)	C10	C11	1.422(7)
N2	C8	1.316(6)	C12	C13	1.515(7)
N3	C11	1.400(6)	C12	C14	1.513(6)
N3	C12	1.474(6)	C14	C15	1.395(6)
N4	C20	1.358(6)	C14	C19	1.397(6)
N4	C24	1.331(6)	C15	C16	1.372(7)

Table S4 Bond Lengths for hy0102.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N5	C20	1.327(6)	C16	C17	1.387(7)
N5	C22	1.342(6)	C17	C18	1.407(6)
N6	C29	1.490(6)	C18	C19	1.385(6)
N6	C30	1.494(6)	C18	C20	1.481(6)
N6	C32	1.505(6)	C22	C23	1.395(6)
C1	C2	1.393(7)	C23	C24	1.379(7)
C1	C6	1.396(7)	C26	C27	1.520(6)
C1	C8	1.483(7)	C27	C28	1.519(6)
C2	C3	1.391(7)	C27	C31	1.519(6)
C3	C4	1.388(8)	C28	C29	1.525(5)
C3	C7	1.448(9)	C30	C31	1.530(6)

Table S5 Bond Angles for hy0102.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C23	O2	C26	117.1(3)	N3	C12	C13	110.7(4)
C8	N2	N3	118.5(4)	N3	C12	C14	111.4(4)
N2	N3	C11	125.0(4)	C14	C12	C13	111.9(4)

Table S5 Bond Angles for hy0102.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	N3	C12	115.4(4)	C15	C14	C12	118.8(4)
C11	N3	C12	119.6(4)	C15	C14	C19	118.7(4)
C24	N4	C20	116.3(4)	C19	C14	C12	122.4(4)
C20	N5	C22	118.1(4)	C16	C15	C14	120.2(4)
C29	N6	C30	111.2(4)	C15	C16	C17	121.6(4)
C29	N6	C32	111.1(4)	C16	C17	C18	119.0(5)
C30	N6	C32	110.9(4)	C17	C18	C20	119.4(4)
C2	C1	C6	119.5(5)	C19	C18	C17	119.2(4)
C2	C1	C8	119.3(5)	C19	C18	C20	121.5(4)
C6	C1	C8	121.1(5)	C18	C19	C14	121.4(4)
C3	C2	C1	119.7(5)	N4	C20	C18	116.6(4)
C2	C3	C7	118.8(5)	N5	C20	N4	124.9(4)
C4	C3	C2	121.2(6)	N5	C20	C18	118.5(4)
C4	C3	C7	120.1(5)	N5	C22	C23	120.7(4)
C5	C4	C3	118.7(5)	O2	C23	C22	125.0(4)
C4	C5	C6	121.7(6)	O2	C23	C24	117.8(4)
C1	C6	C5	119.2(6)	C24	C23	C22	117.1(4)
N1	C7	C3	178.8(7)	N4	C24	C23	122.8(4)

Table S5 Bond Angles for hy0102.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	C8	C1	115.4(4)	O2	C26	C27	107.1(4)
N2	C8	C9	121.2(4)	C28	C27	C26	109.3(4)
C9	C8	C1	123.5(5)	C31	C27	C26	111.9(4)
C10	C9	C8	119.8(5)	C31	C27	C28	109.4(4)
C9	C10	C11	120.7(5)	C27	C28	C29	109.9(4)
O1	C11	N3	119.9(5)	N6	C29	C28	110.7(4)
O1	C11	C10	125.5(5)	N6	C30	C31	109.9(4)
N3	C11	C10	114.7(4)	C27	C31	C30	112.0(4)

Table S6 Torsion Angles for hy0102.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O2	C23	C24	N4	-177.3(5)	C12	N3	C11	O1	-3.2(7)
O2	C26	C27	C28	175.2(4)	C12	N3	C11	C10	176.1(4)
O2	C26	C27	C31	-63.5(5)	C12	C14	C15	C16	-177.4(5)
N2	N3	C11	O1	176.5(4)	C12	C14	C19	C18	178.0(5)
N2	N3	C11	C10	-4.2(7)	C13	C12	C14	C15	101.1(5)
N2	N3	C12	C13	43.7(5)	C13	C12	C14	C19	-74.9(6)

Table S6 Torsion Angles for hy0102.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N2	N3	C12	C14	-81.5(5)	C14	C15	C16	C17	0.4(8)
N2	C8	C9	C10	-2.0(8)	C15	C14	C19	C18	2.0(7)
N3	N2	C8	C1	-178.7(4)	C15	C16	C17	C18	-0.3(8)
N3	N2	C8	C9	0.1(7)	C16	C17	C18	C19	1.0(7)
N3	C12	C14	C15	-134.4(4)	C16	C17	C18	C20	-179.1(5)
N3	C12	C14	C19	49.6(6)	C17	C18	C19	C14	-1.9(7)
N5	C22	C23	O2	177.5(5)	C17	C18	C20	N4	-166.5(5)
N5	C22	C23	C24	-2.6(8)	C17	C18	C20	N5	12.3(7)
N6	C30	C31	C27	55.8(6)	C19	C14	C15	C16	-1.3(7)
C1	C2	C3	C4	-0.4(8)	C19	C18	C20	N4	13.3(7)
C1	C2	C3	C7	177.6(5)	C19	C18	C20	N5	-167.9(5)
C1	C8	C9	C10	176.7(5)	C20	N4	C24	C23	-1.1(7)
C2	C1	C6	C5	0.0(8)	C20	N5	C22	C23	0.8(8)
C2	C1	C8	N2	31.1(7)	C20	C18	C19	C14	178.2(5)
C2	C1	C8	C9	-147.8(5)	C22	N5	C20	N4	1.1(8)
C2	C3	C4	C5	-0.3(9)	C22	N5	C20	C18	-177.6(4)
C3	C4	C5	C6	0.9(10)	C22	C23	C24	N4	2.8(8)
C4	C5	C6	C1	-0.8(9)	C23	O2	C26	C27	-170.9(4)

Table S6 Torsion Angles for hy0102.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C6	C1	C2	C3	0.5(8)	C24	N4	C20	N5	-1.0(8)
C6	C1	C8	N2	-147.4(5)	C24	N4	C20	C18	177.8(4)
C6	C1	C8	C9	33.8(8)	C26	O2	C23	C22	-7.5(7)
C7	C3	C4	C5	-178.3(6)	C26	O2	C23	C24	172.6(4)
C8	N2	N3	C11	3.2(7)	C26	C27	C28	C29	179.7(4)
C8	N2	N3	C12	-177.2(4)	C26	C27	C31	C30	-177.4(4)
C8	C1	C2	C3	-177.9(5)	C27	C28	C29	N6	-59.0(5)
C8	C1	C6	C5	178.5(5)	C28	C27	C31	C30	-56.1(5)
C8	C9	C10	C11	0.8(8)	C29	N6	C30	C31	-56.8(5)
C9	C10	C11	O1	-178.7(5)	C30	N6	C29	C28	59.3(5)
C9	C10	C11	N3	2.1(7)	C31	C27	C28	C29	56.9(5)
C11	N3	C12	C13	-136.6(4)	C32	N6	C29	C28	-176.8(4)
C11	N3	C12	C14	98.2(5)	C32	N6	C30	C31	179.1(4)

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for hy0102.

Atom	*x*	*y*	*z*	U(eq)
H6	8609	2194.44	346	32
H2	4357.95	7128.57	5536.79	39
H4	1894.45	6779.72	3484.62	60
H5	1054.89	5602.33	4573.4	62
H6A	1826.11	5227.06	6156.49	50
H9	2962.73	3752.61	7418.51	44
H10	3869.38	3521.16	8925.88	46
H12	5787.47	8528.87	9214.87	31
H13A	5670.46	11264.81	8432.01	47
H13B	4597.56	10512.89	8376.31	47
H13C	5096.14	10367.48	7490.62	47
H15	7487.52	8688.84	9459.11	33
H16	8957.61	8224.96	8989.15	36
H17	8997.55	7387.75	7444.56	37
H19	6020.04	7497.44	6818.06	31
H22	8979.64	5300.52	4746.57	37
H24	6116.24	6534.55	3980.49	33

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for hy0102.

Atom	*x*	*y*	*z*	U(eq)
H26A	8692.05	4007.86	3207.44	34
H26B	8911.9	6101.11	3189.73	34
H27	7916.61	6285.2	1634.06	31
H28A	9501.7	3779.5	1785.16	31
H28B	9623.01	5895.69	1760.57	31
H29A	8685.18	5984.1	196.81	31
H29B	9597.72	4694.3	235	31
H30A	6913.67	2476.7	166.07	41
H30B	6996.12	4597.72	118.18	41
H31A	6885.6	3788.9	1669.59	38
H31B	7785.29	2460.39	1741.43	38
H32A	7798.14	4260.65	-1268.2	60
H32B	7750.59	2142.41	-1202.37	60
H32C	8768.24	3109.05	-1172.5	60

Table S8 Solvent masks information for hy0102.

Number	X	Y	Z	Volume	Electron count	Content
1	-0.006	-0.078	0.340	39.5	10.0	?
2	0.006	0.422	0.660	39.5	10.2	?

Experimental

Single crystals of $C_{30}H_{31}ClN_6O_2$ **[hy0102]**.A suitable crystal was selected and operated on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. The crystal was kept at 169.99(10) K during data collection.