

Supporting Information

Organocatalytic Diastereo- and Enantioselective Conjugate Addition of Pyrazol-3-ones to 3-Trifluoroethylidene Oxindoles with A Newly Developed Squaramide Catalyst

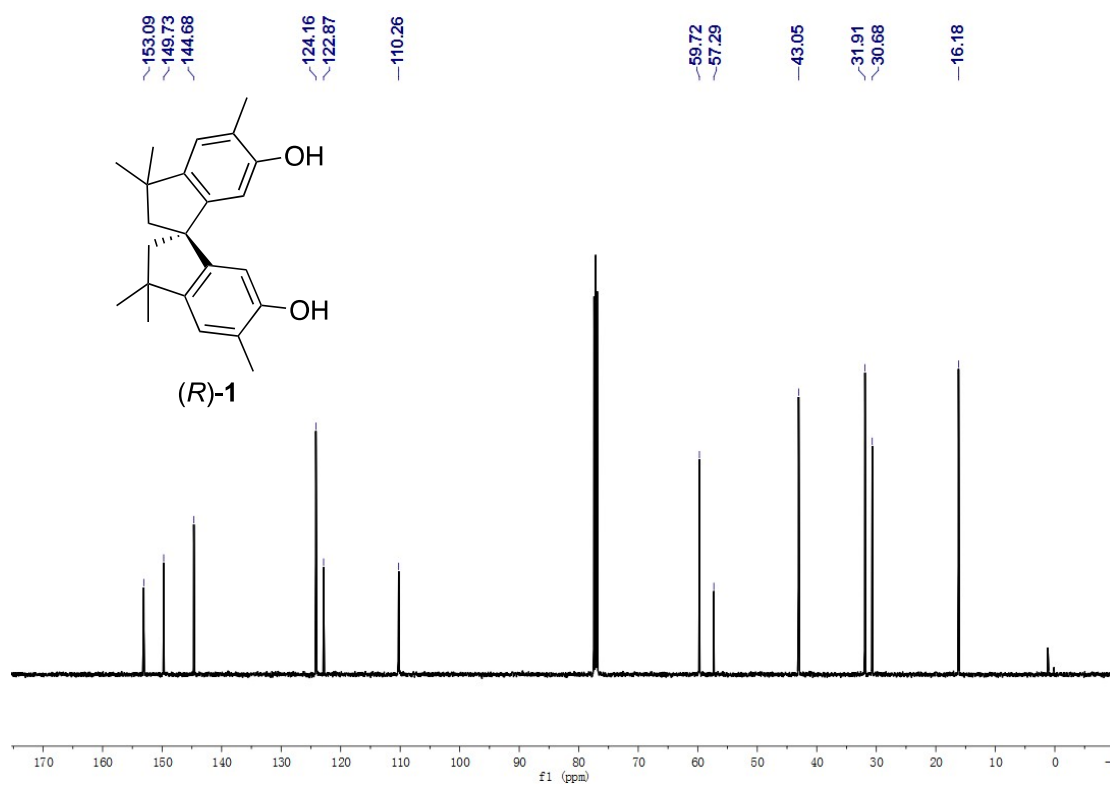
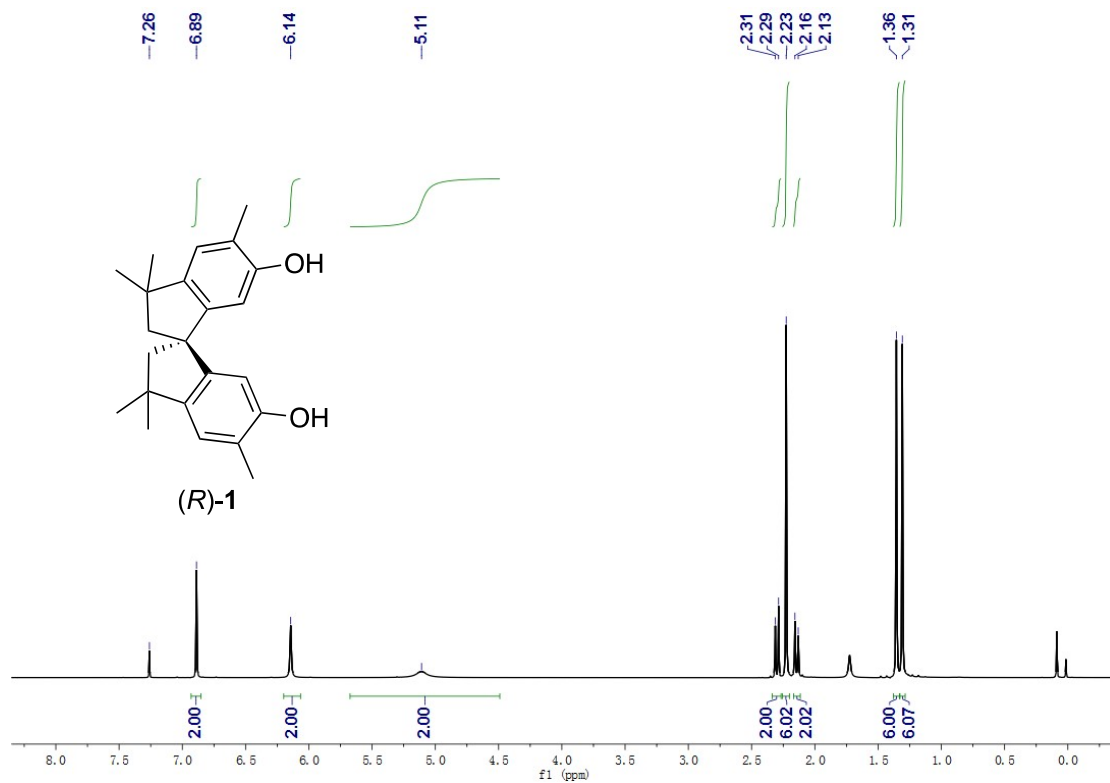
Zhao Han, Jiaping Jin, Alemayehu Gashaw Woldegiorgis and Xufeng Lin*
Department of Chemistry, Zhejiang University, Hangzhou 310027, P. R of China; E-mail:
lxfok@zju.edu.cn

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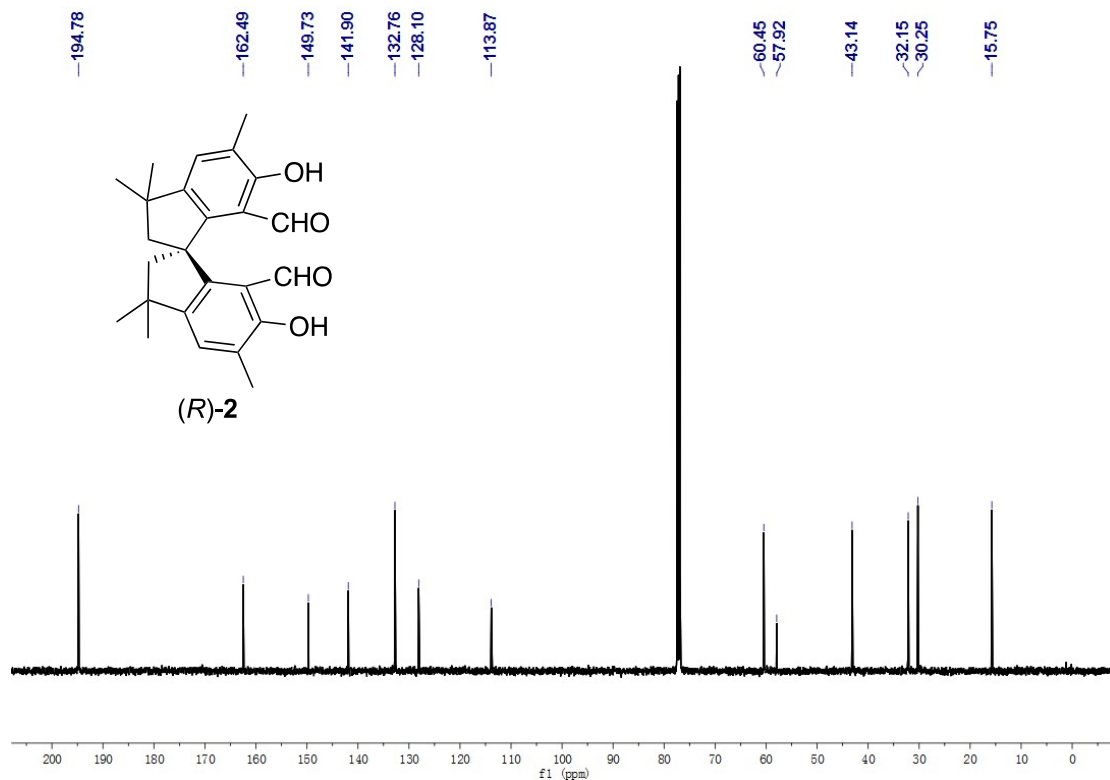
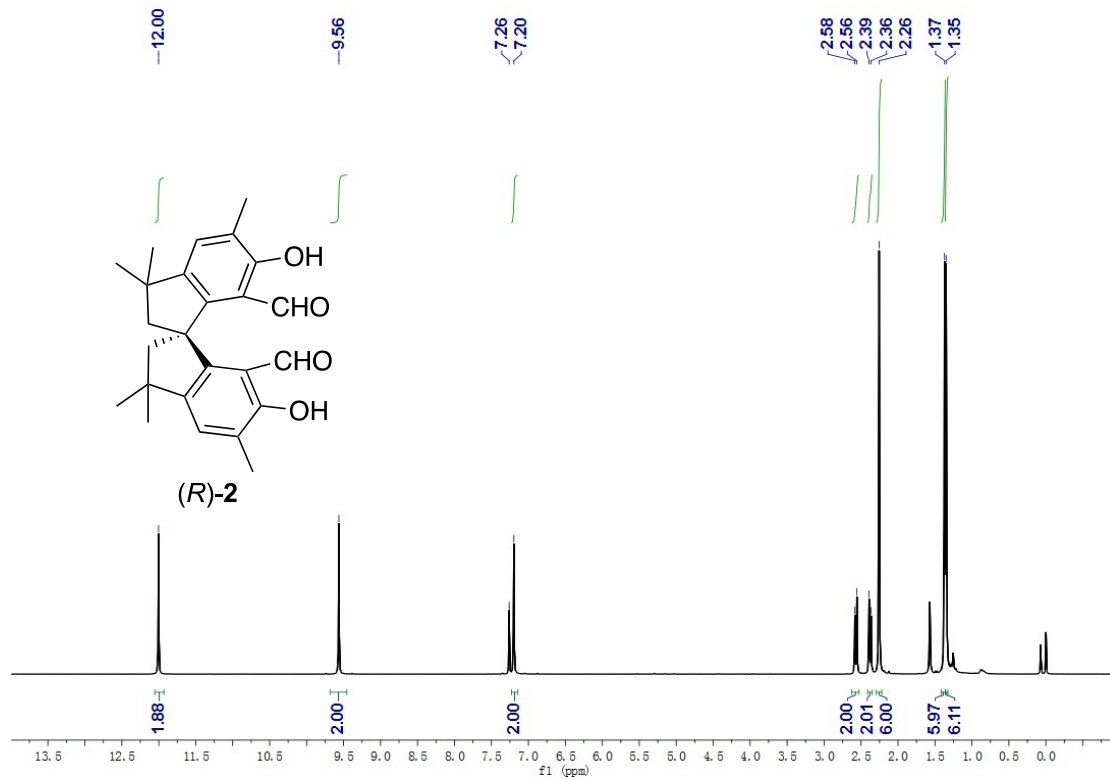
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1 Copies of NMR spectra

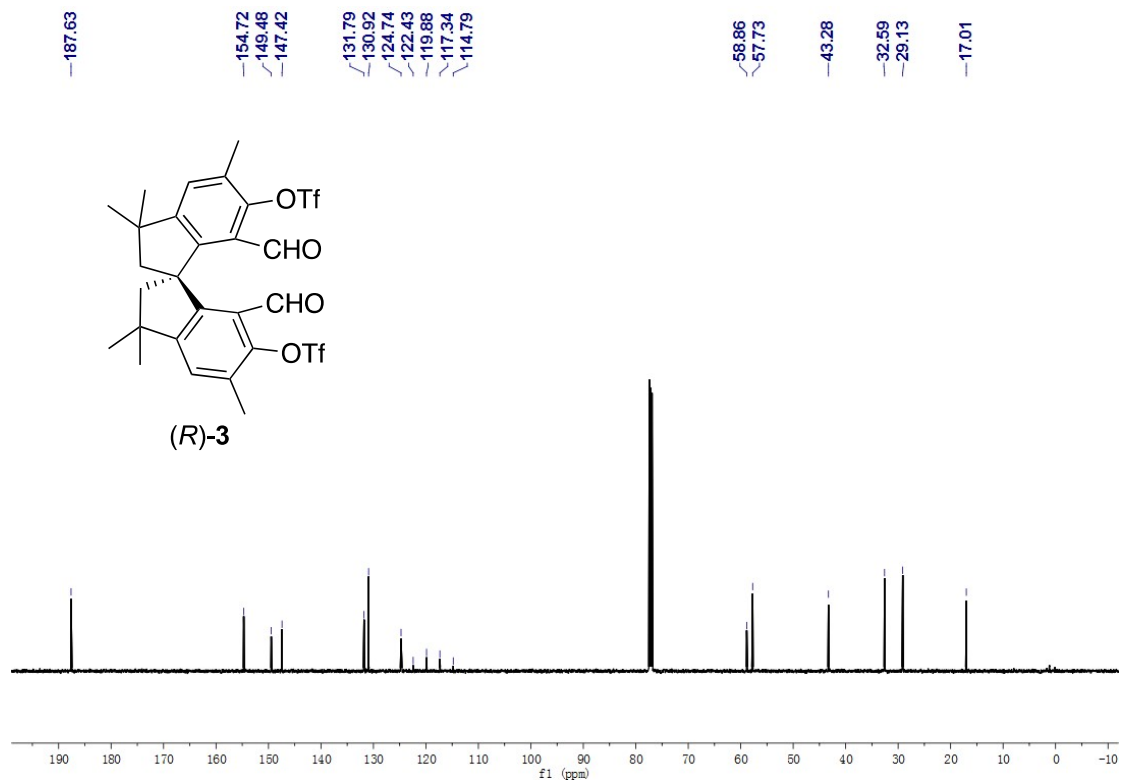
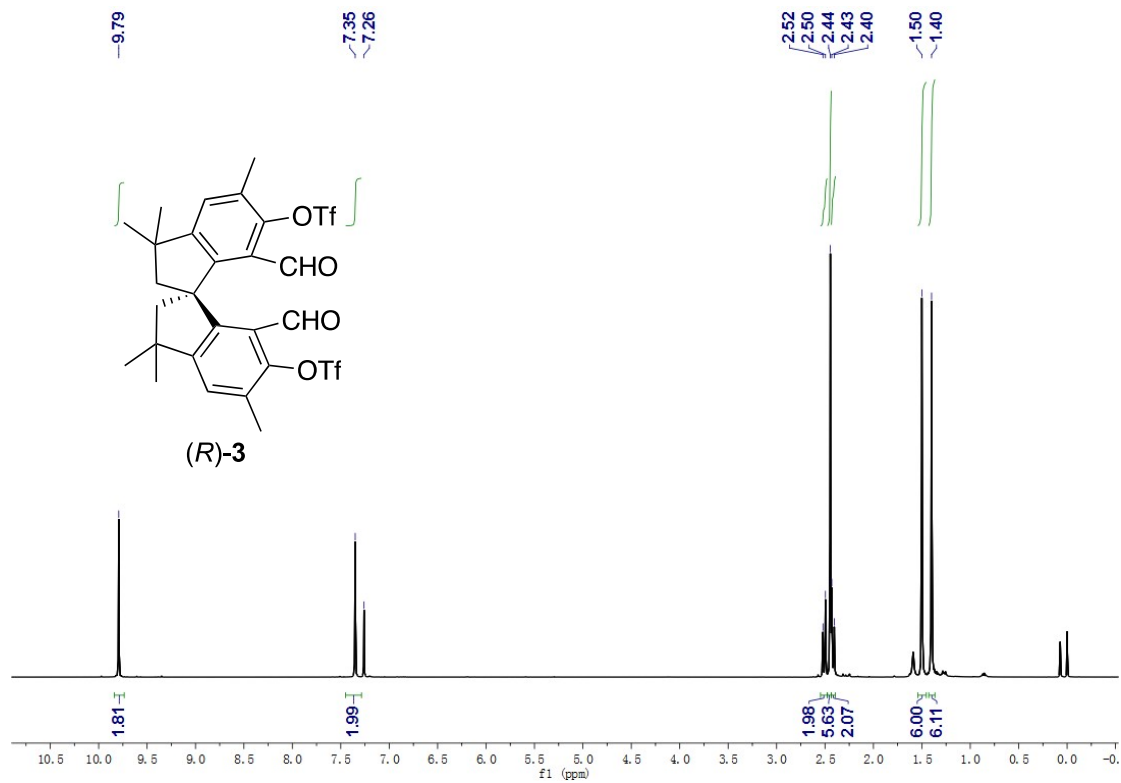
(R)-3,3,3',3',5,5'-hexamethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-6,6'-diol [*(R)*-1]



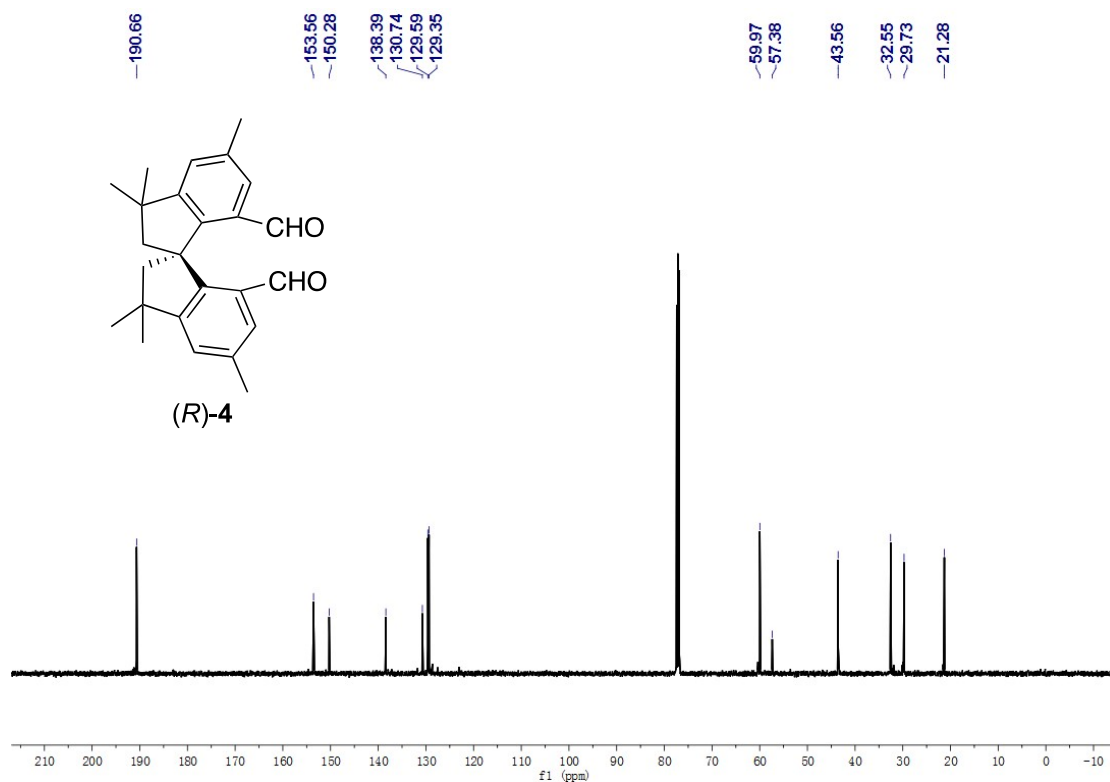
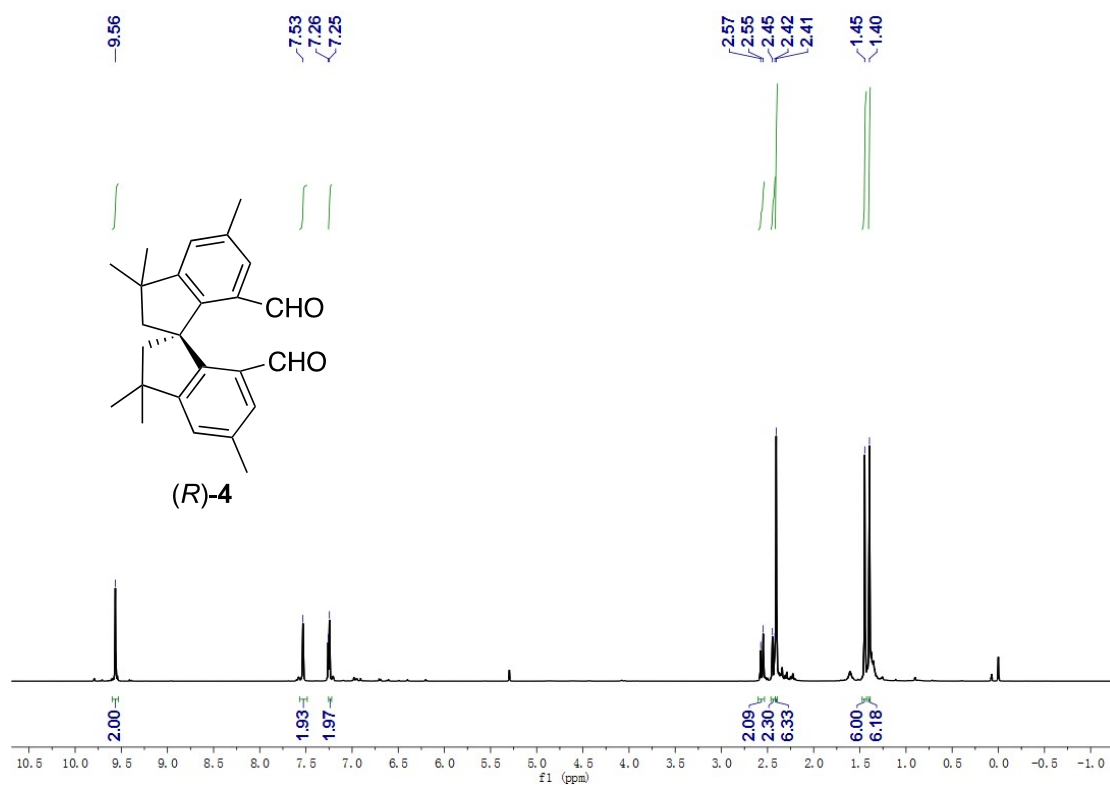
(R)-6,6'-dihydroxy-3,3,3',3',5,5'-hexamethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-dicarbaldehyde [(R)-2]



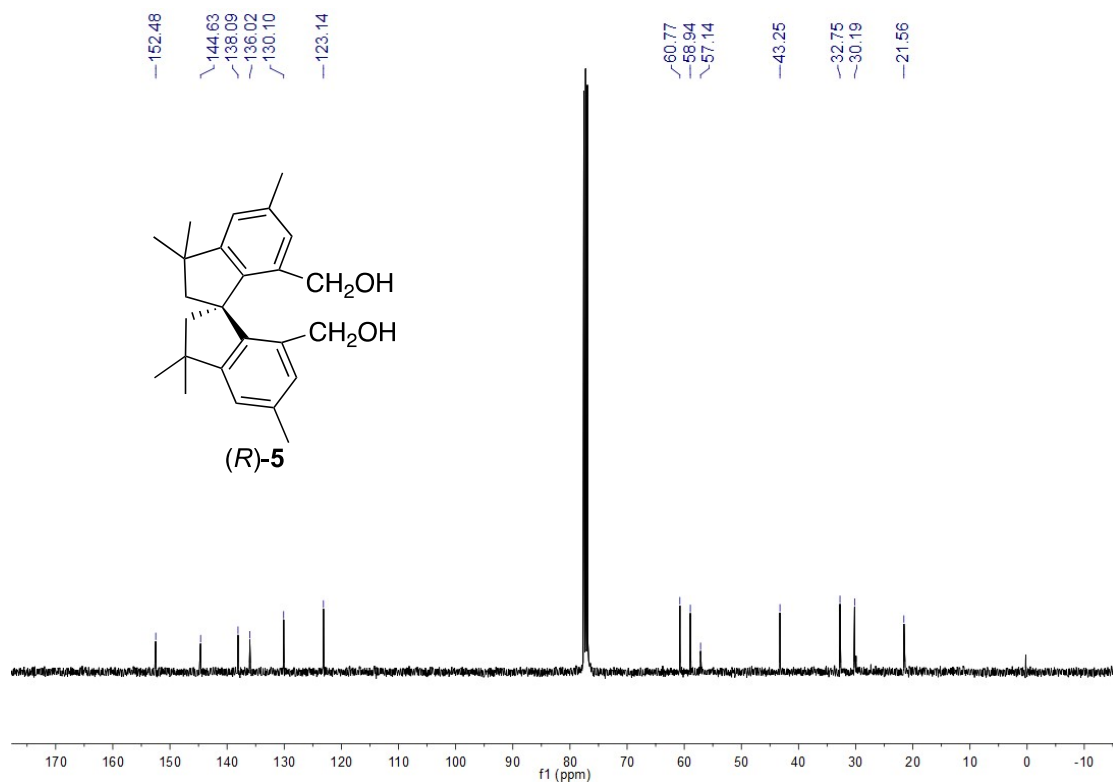
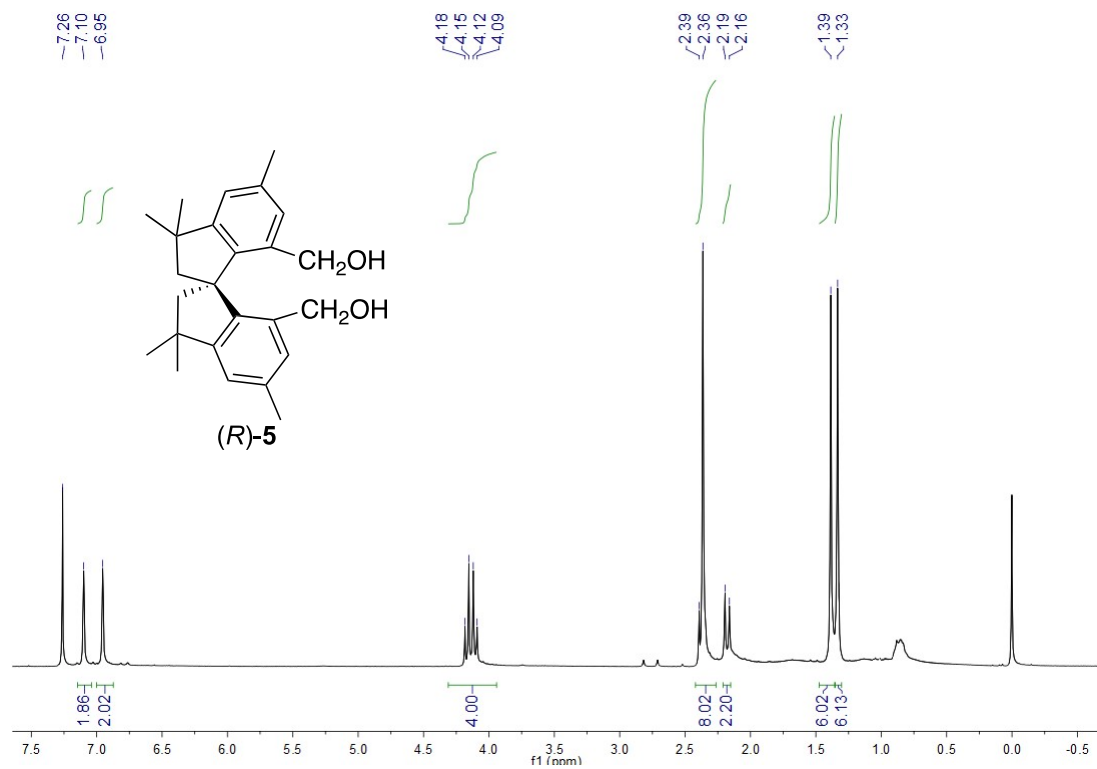
(R)-7,7'-diformyl-3,3,3',3',5,5'-hexamethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-6,6'-diyl bis(trifluoromethanesulfonate) [(R)-3]



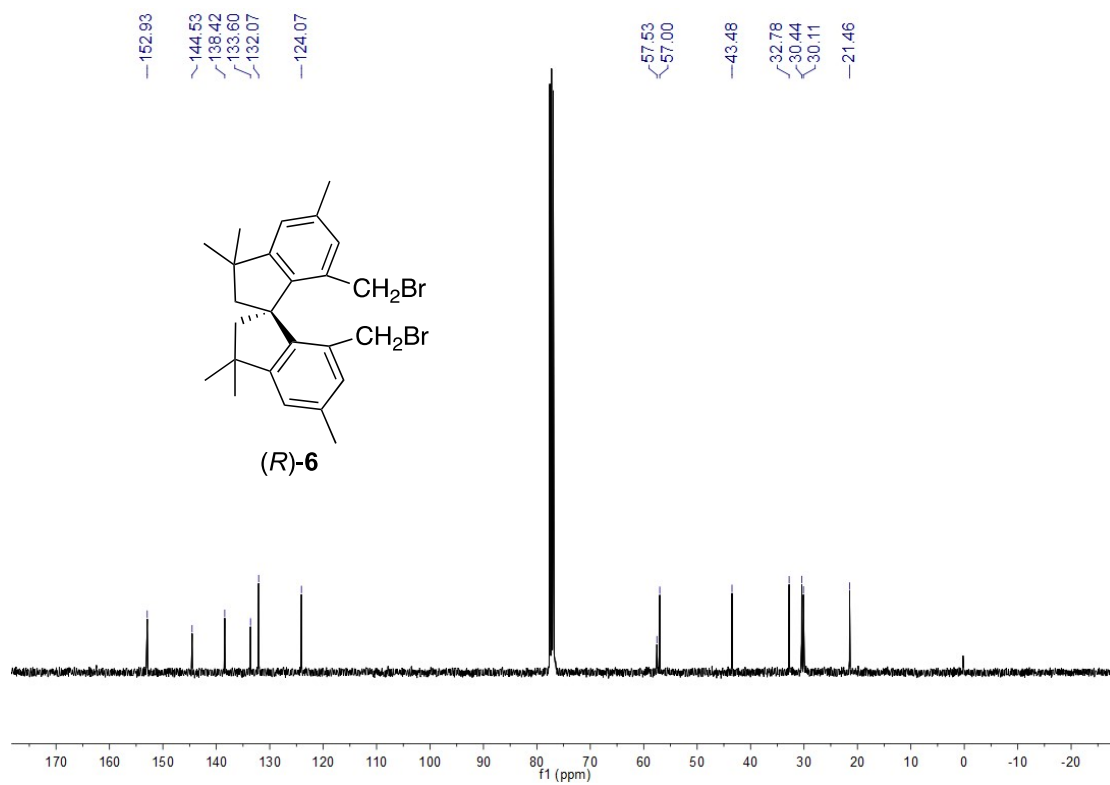
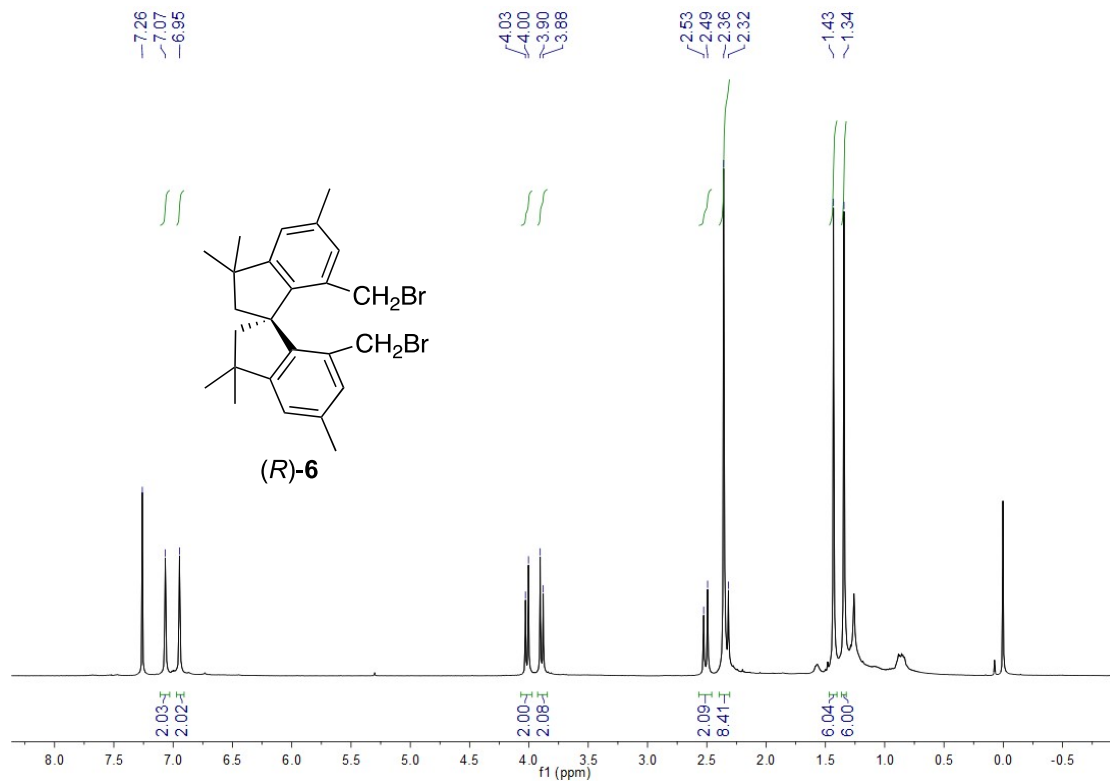
(R)-3,3,3',3',5,5'-hexamethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-dicarbaldehyde
[(R)-4]



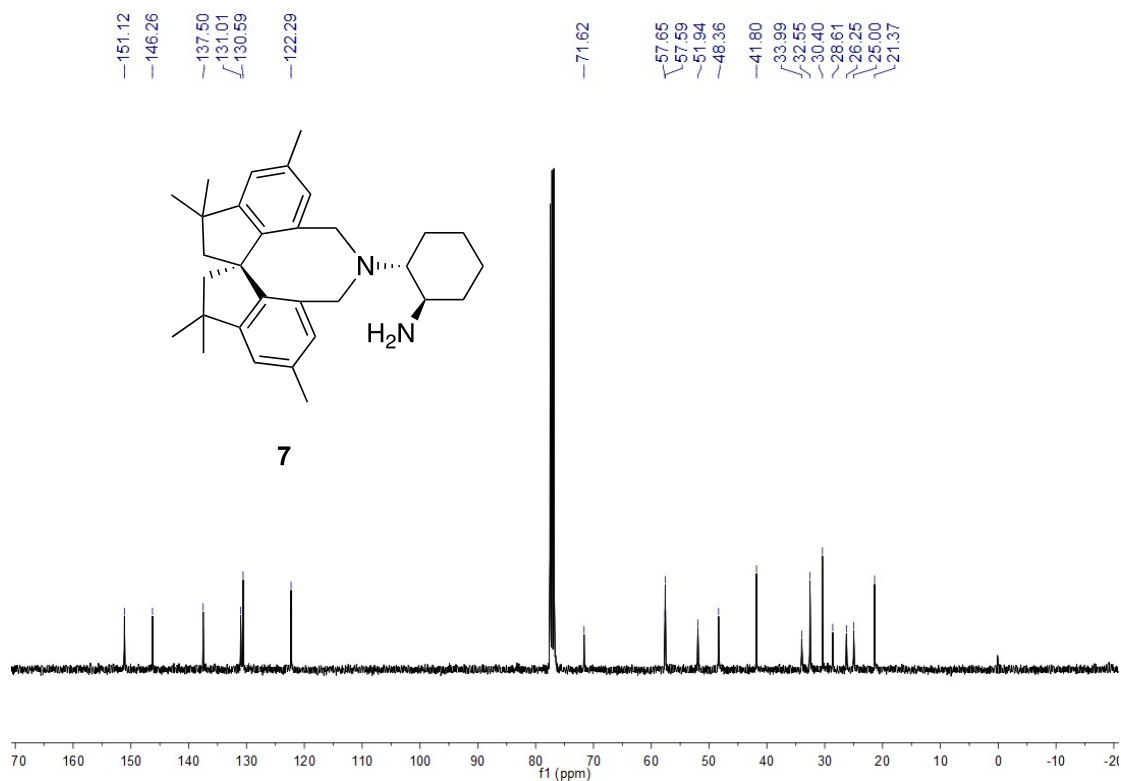
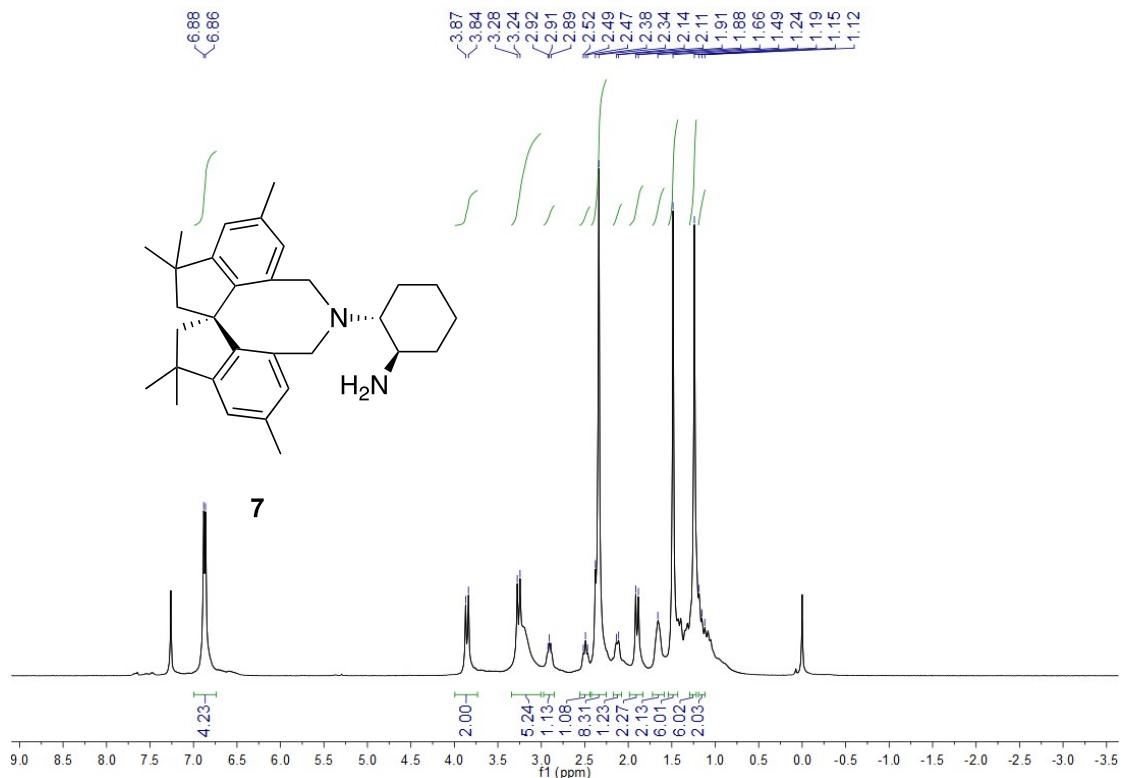
(R)-(3,3,3',3',5,5'-hexamethyl-2,2',3,3'-tetrahydro-1,1'-spiro[indene]-7,7'-diyl)dimethanol
[(R)-5]



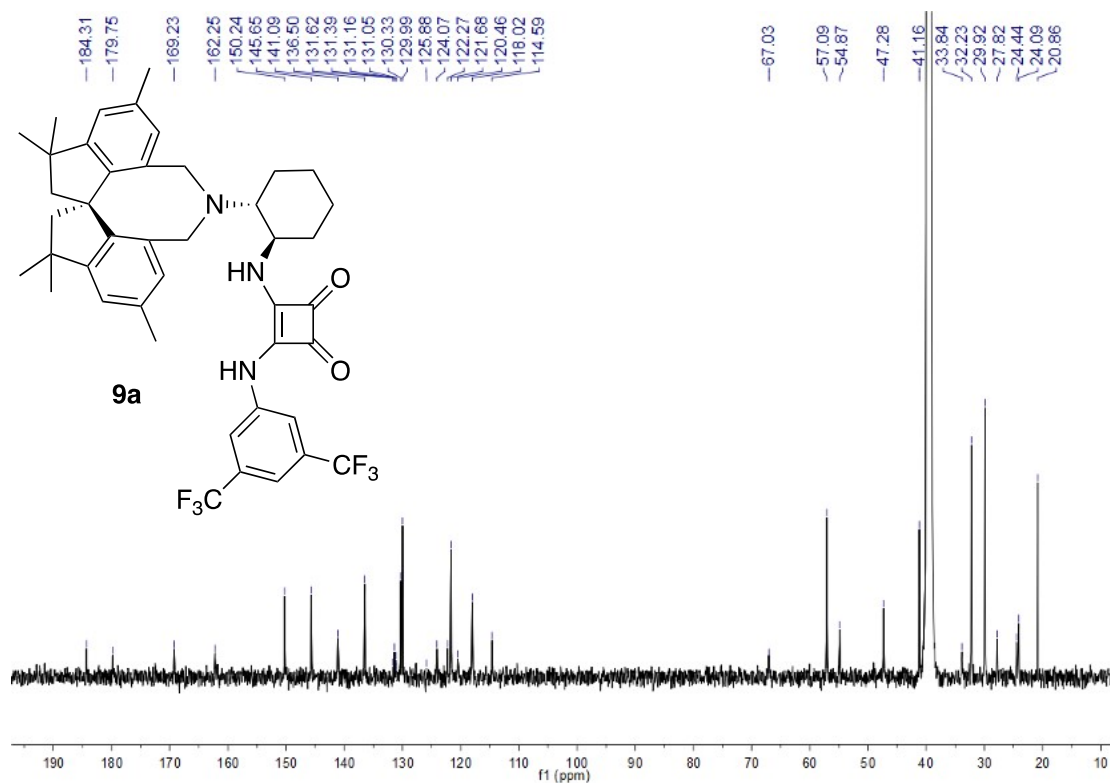
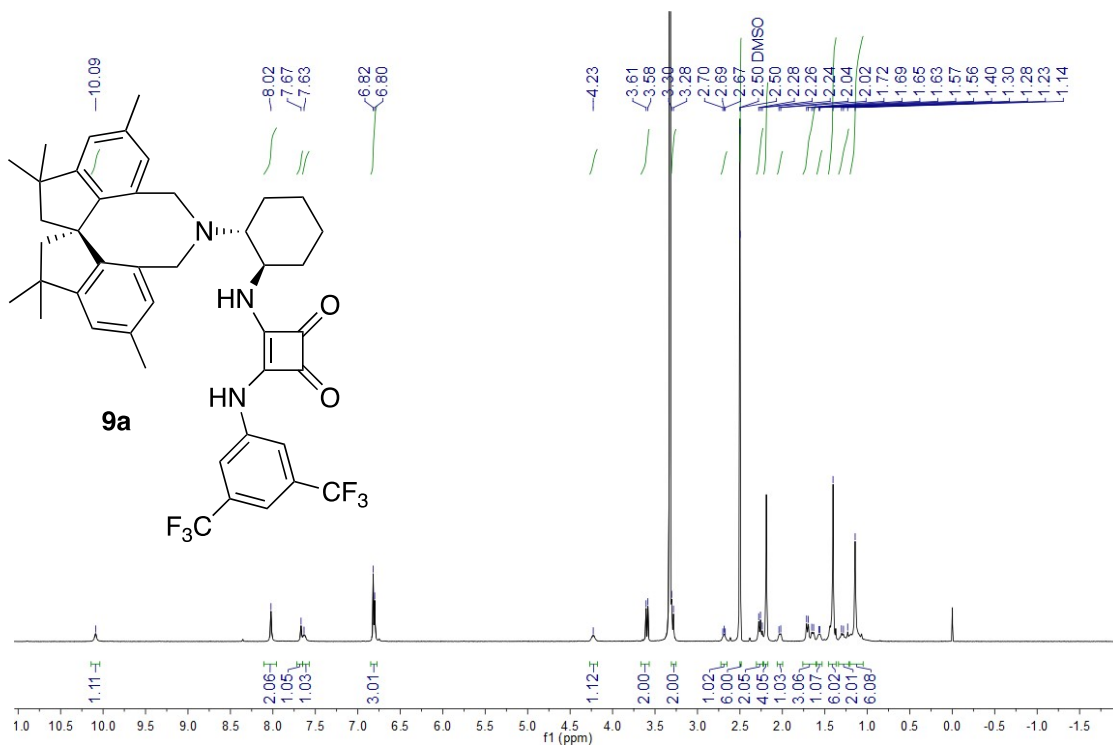
(R)-7,7'-bis(bromomethyl)-3,3,3',3',5-pentamethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]
[(R)-6]

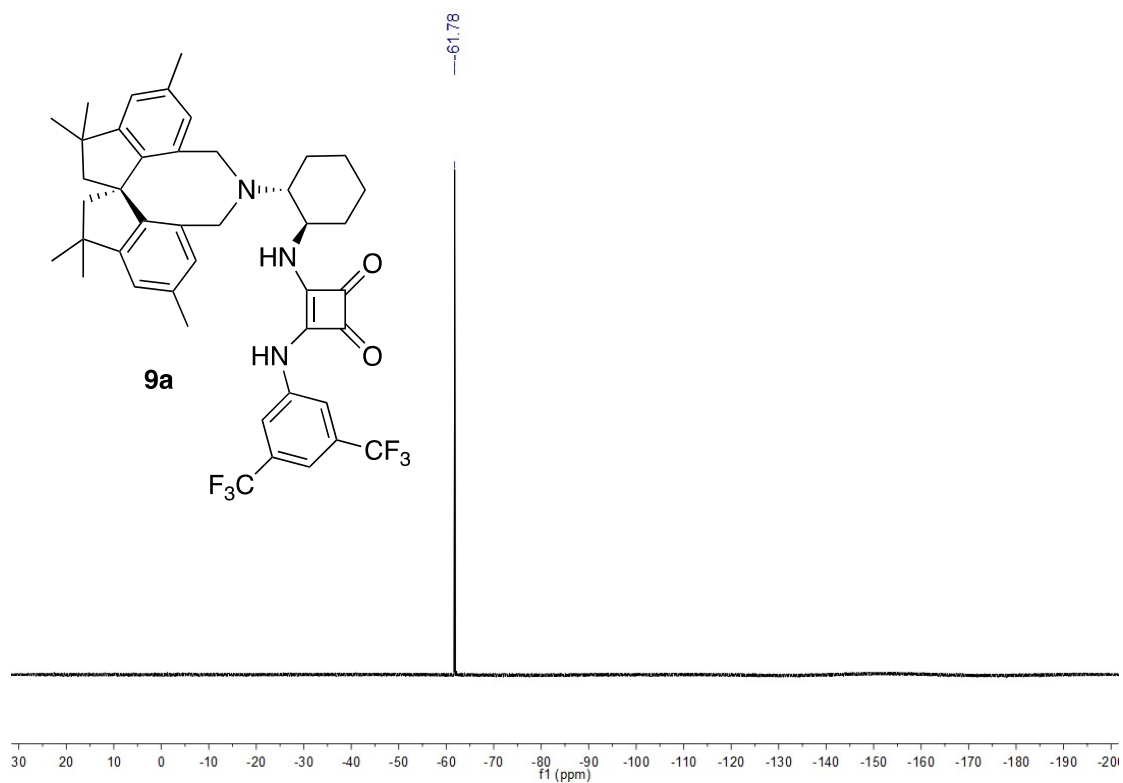


(1R,2R)-2-(2,4,4,7,7,9-hexamethyl-4,5,6,7-tetrahydro-11H-diindeno[7,1-cd:1',7'-ef]azocin-12(13H)-yl)cyclohexan-1-amine (7)

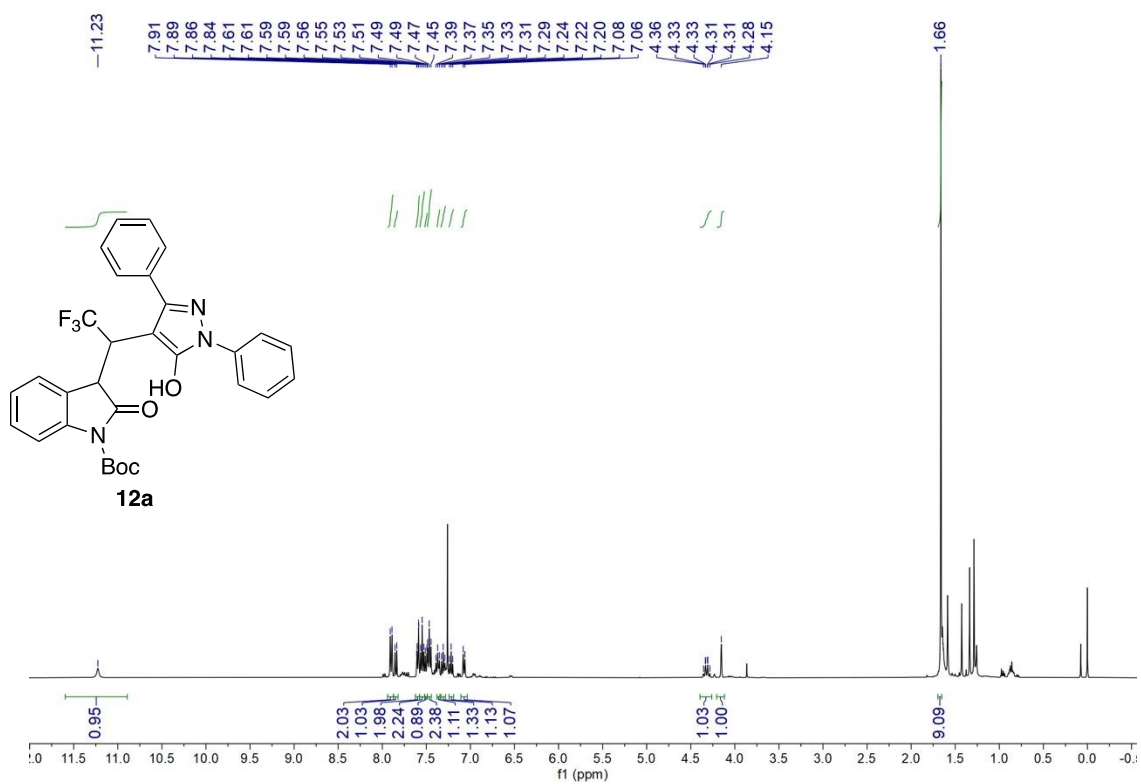


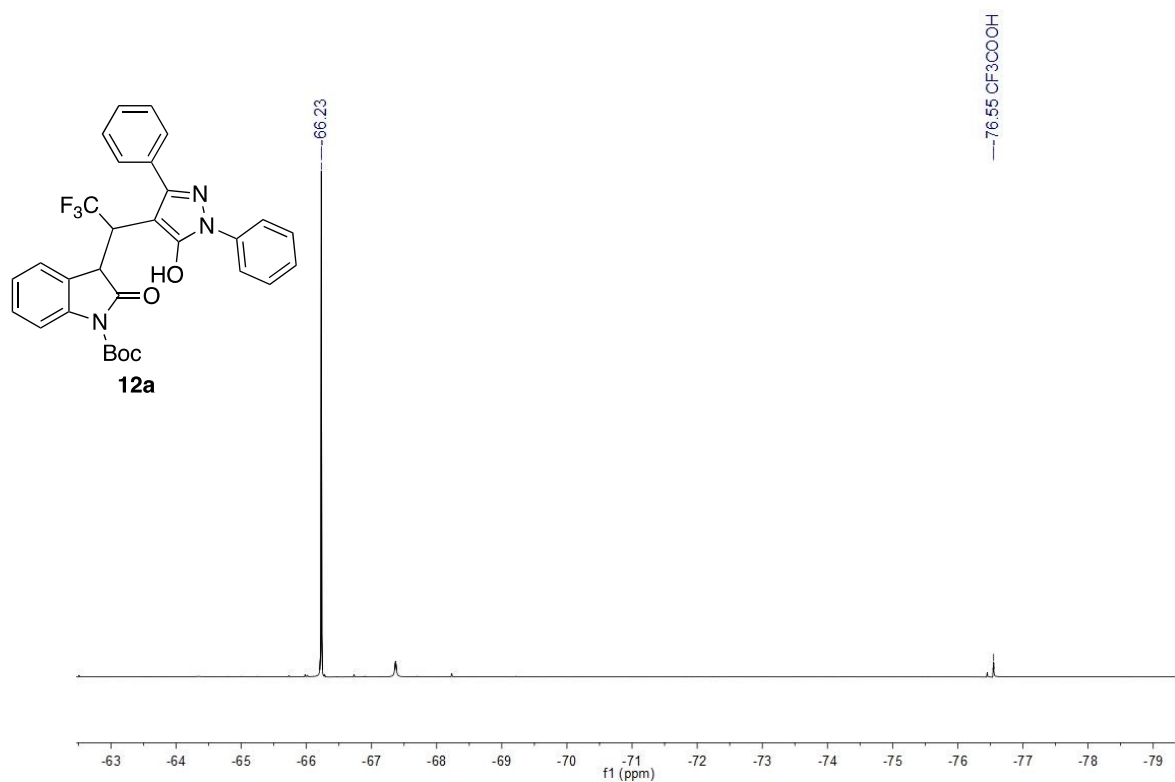
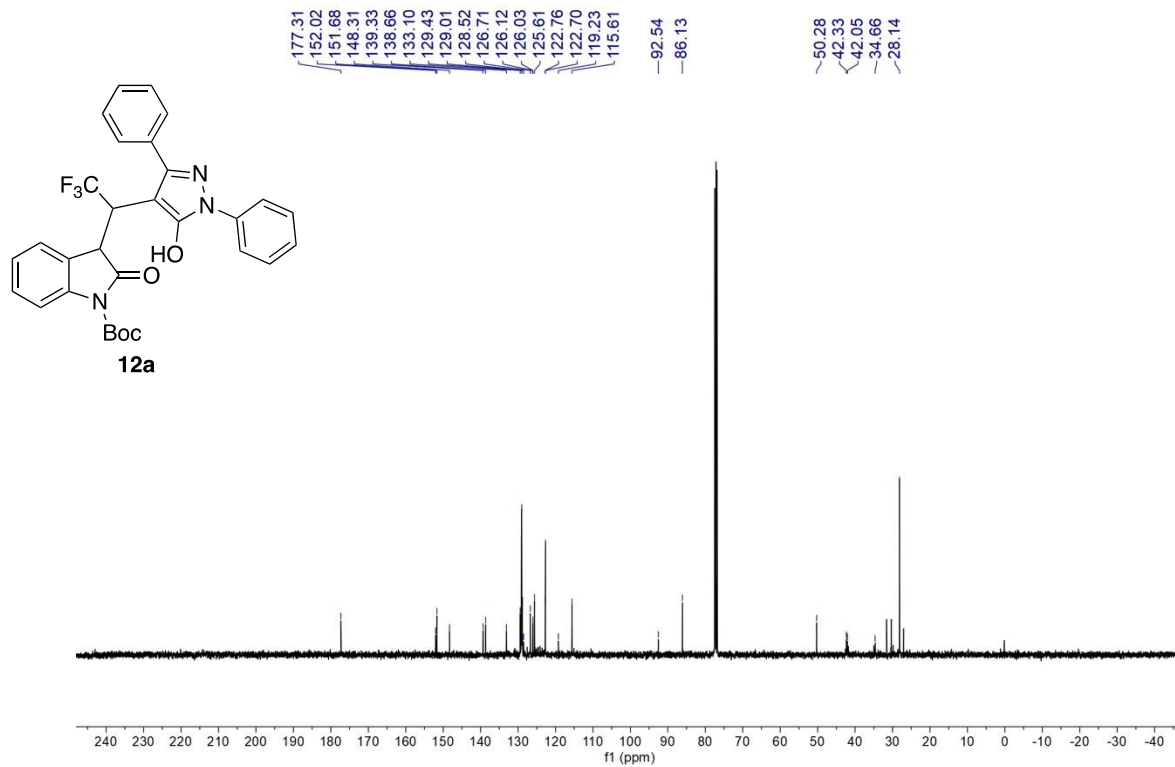
3-((3,5-bis(trifluoromethyl)phenyl)amino)-4-(((1R,2R)-2-(2,4,4,7,7,9-hexamethyl-4,5,6,7-tetrahydro-11H-diindeno[7,1-cd:1',7'-ef]azocin-12(13H)-yl)cyclohexyl)amino)cyclobut-3-ene-1,2-dione (9a)



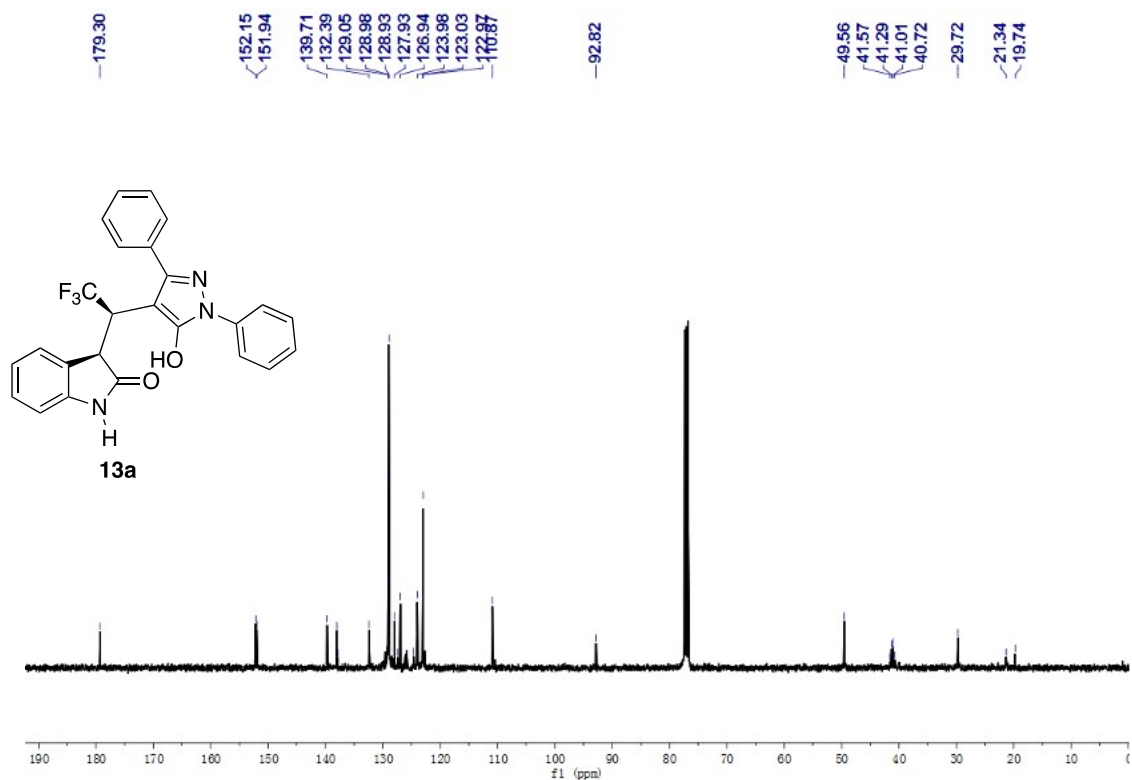
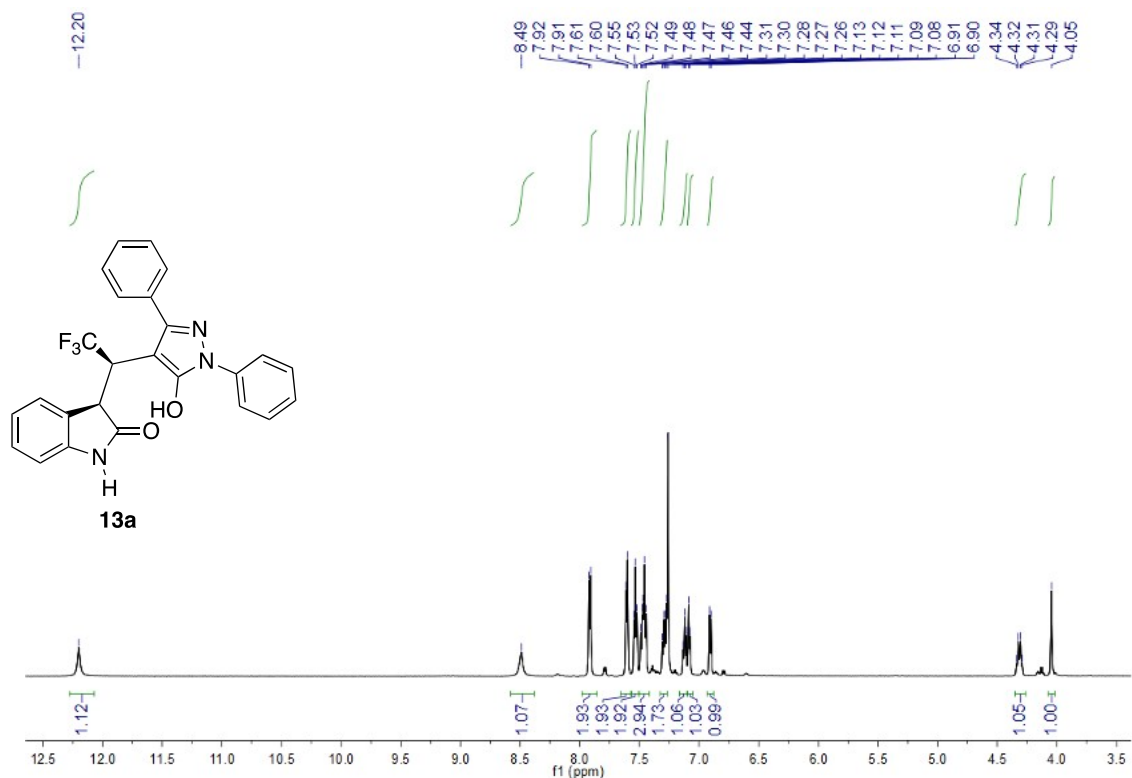


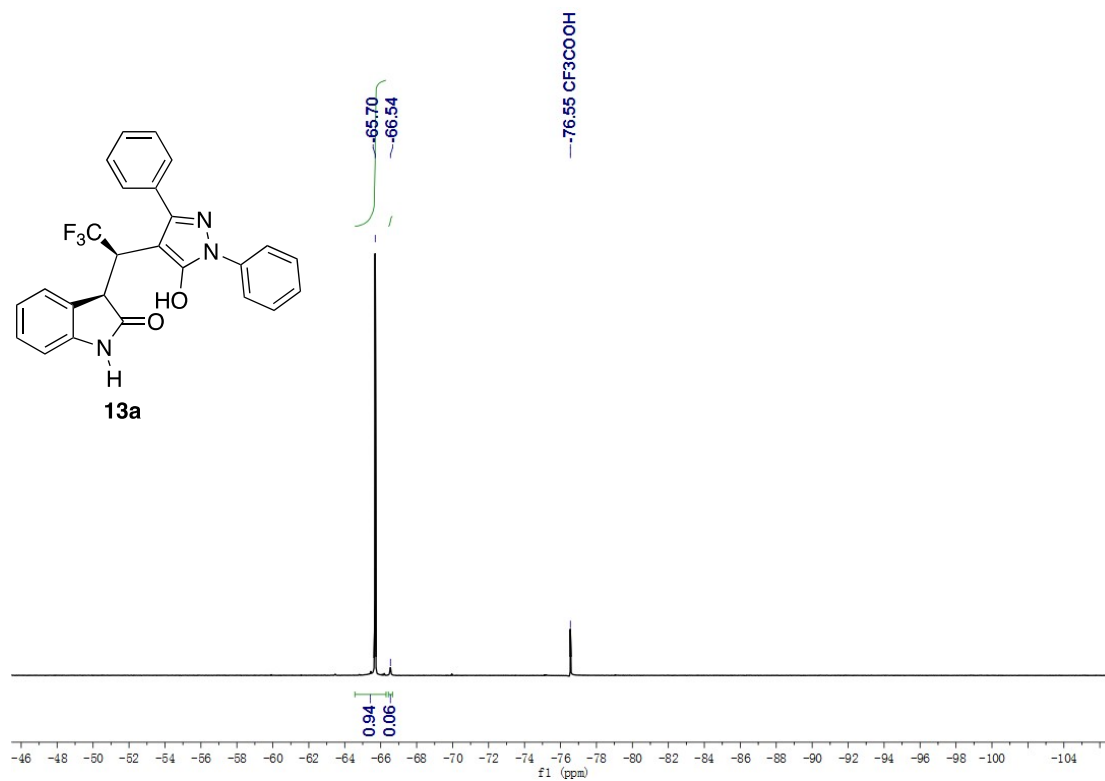
Tert-butyl 2-oxo-3-(2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indoline-1-carboxylate (12a)



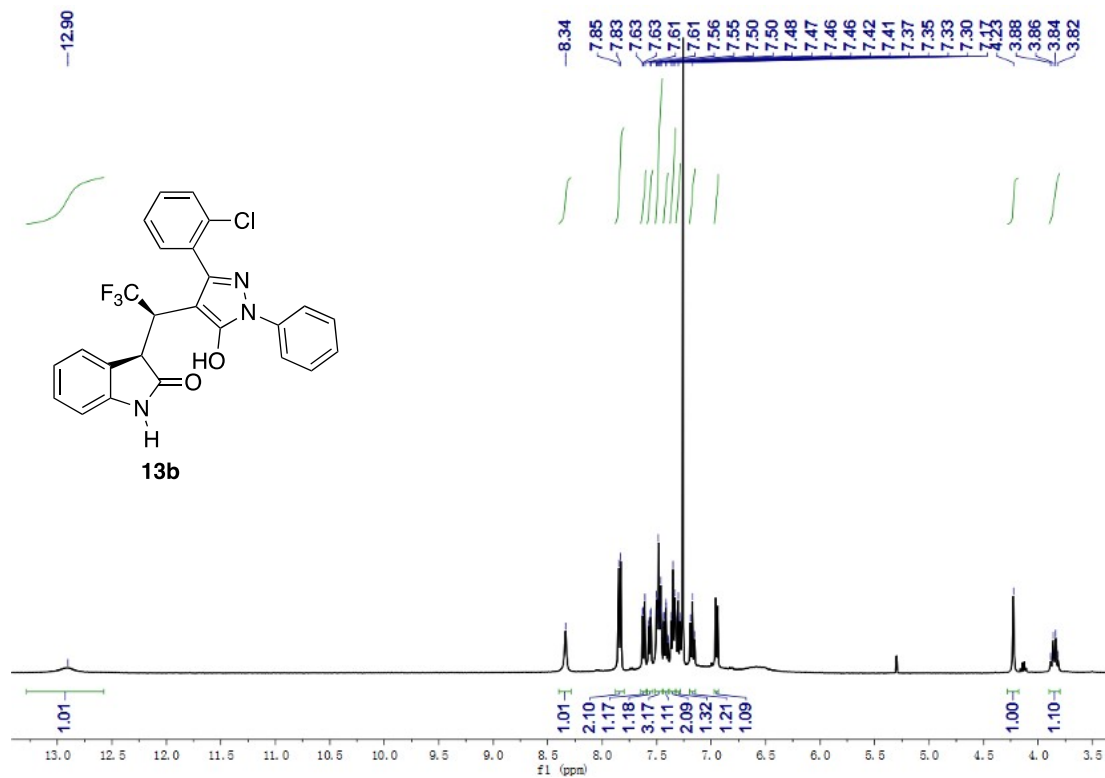


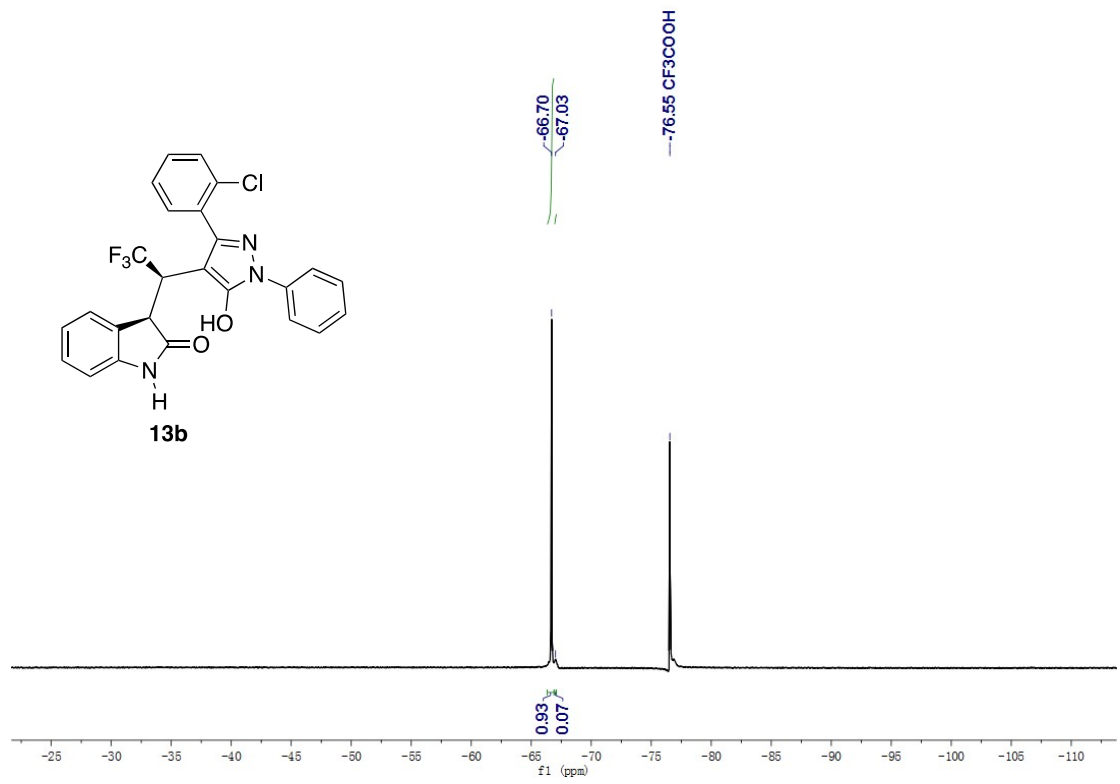
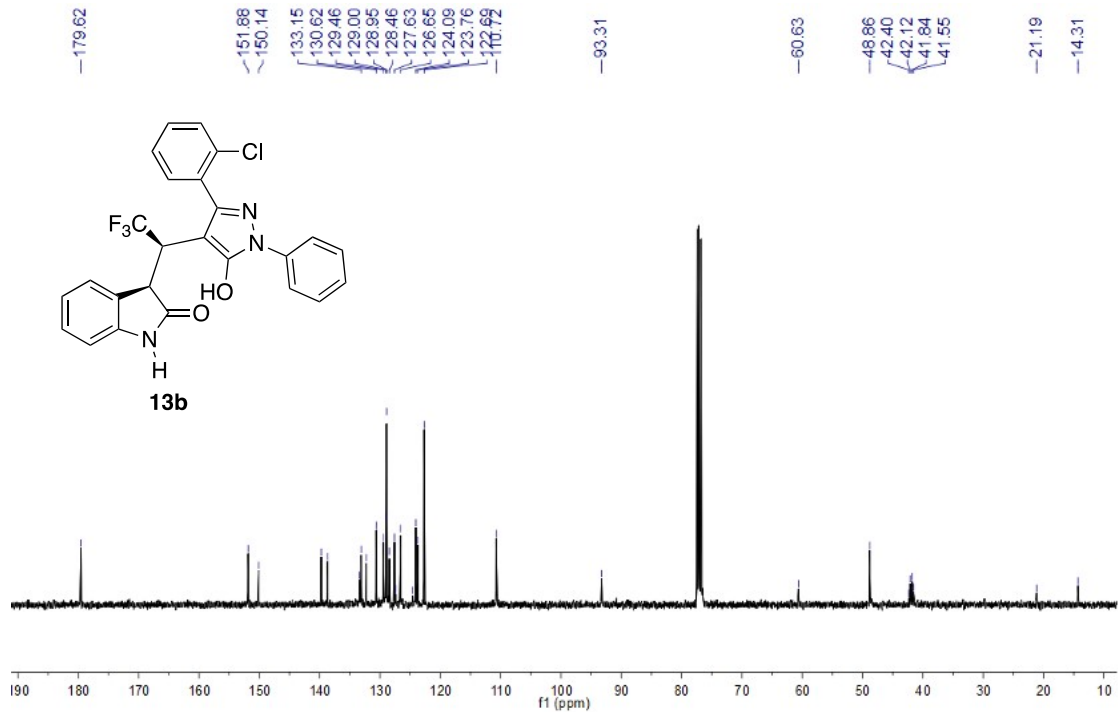
(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13a).



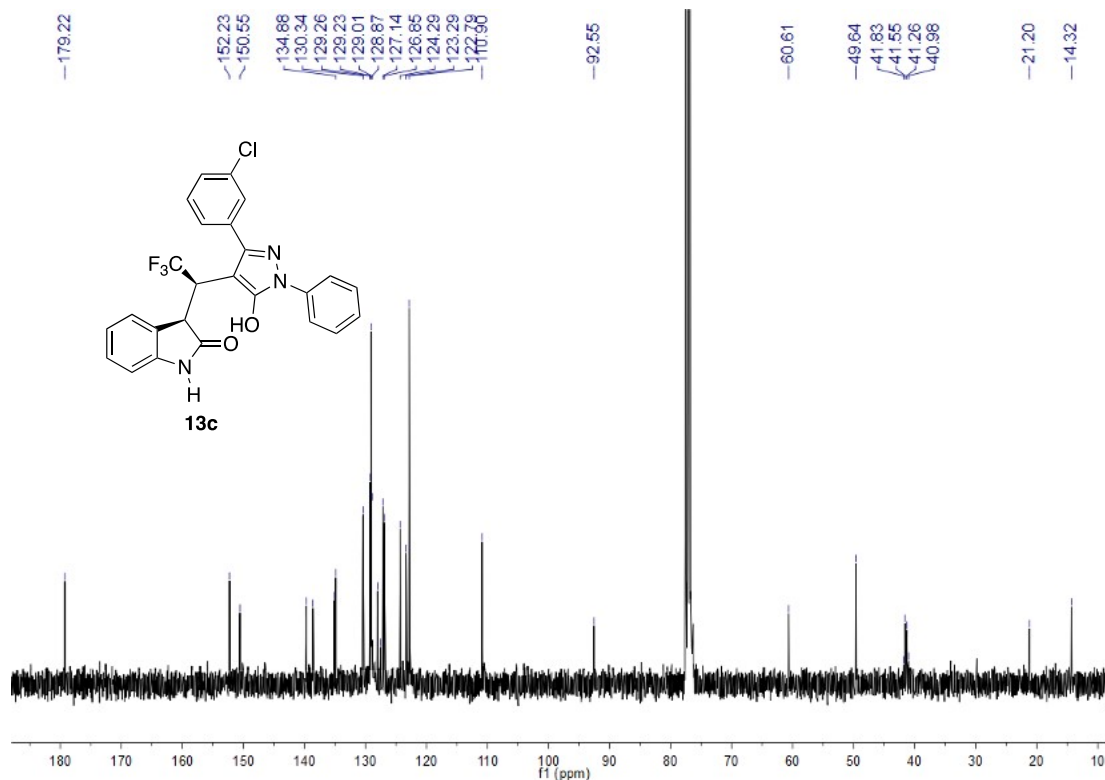
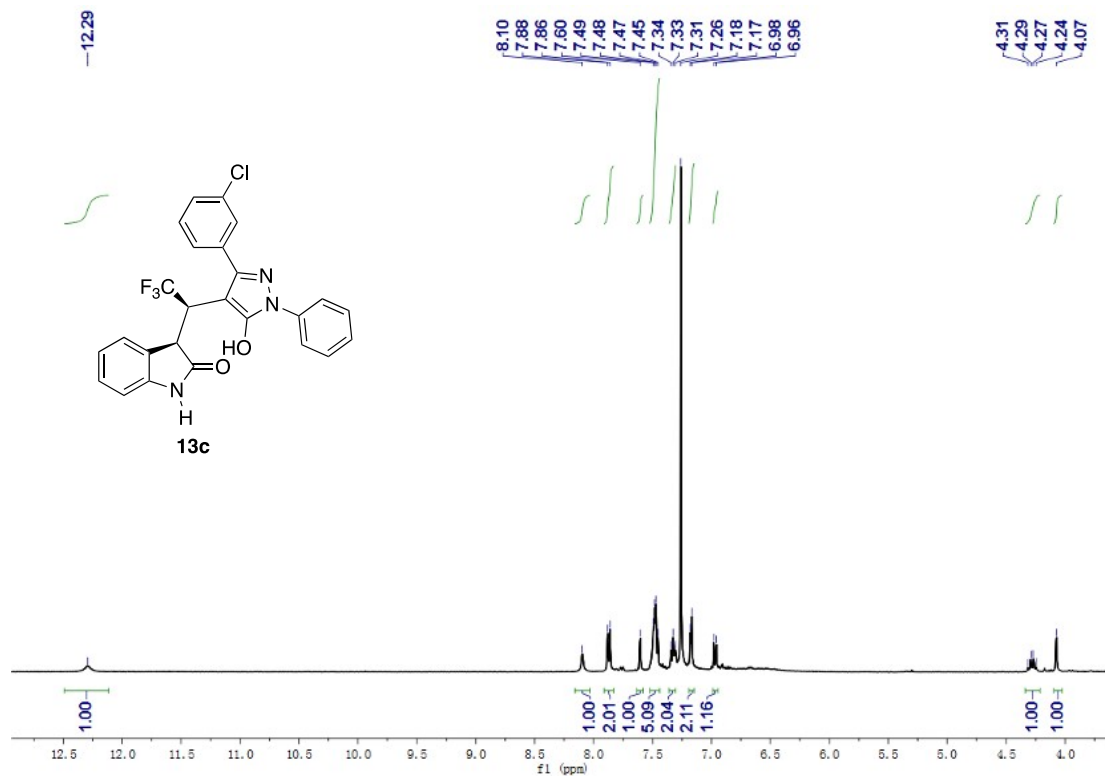


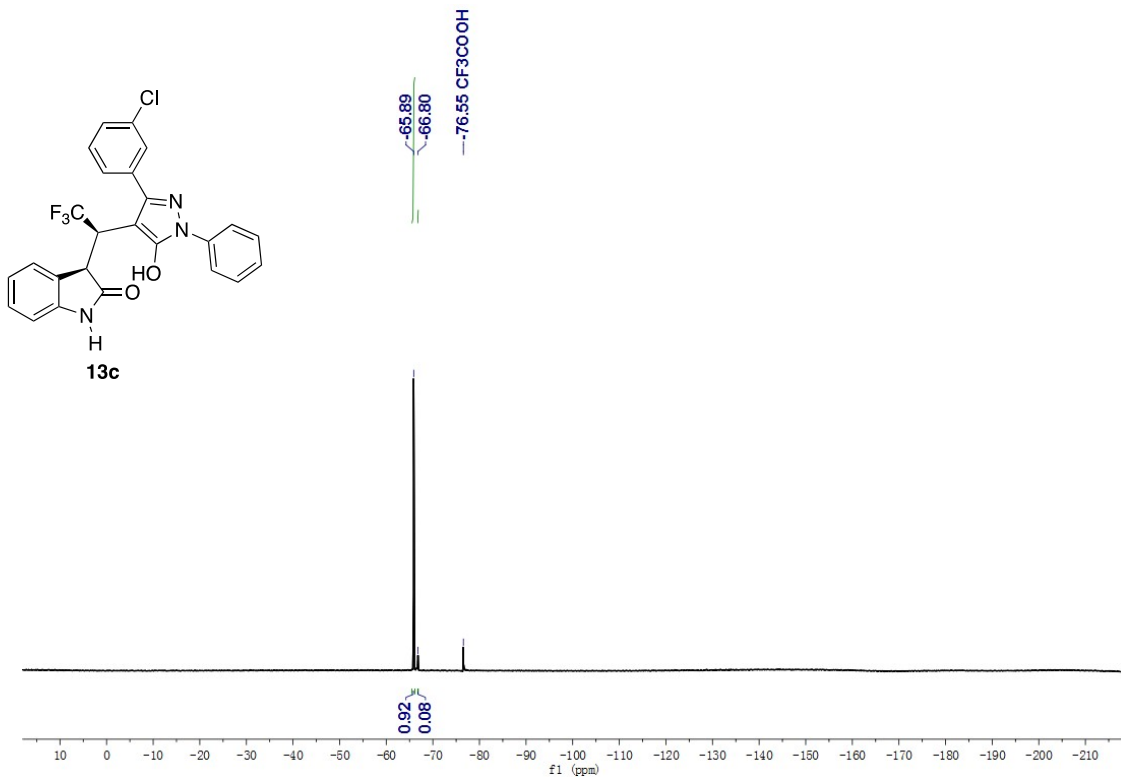
(R)-3-((R)-1-(3-(2-chlorophenyl)-5-hydroxy-1-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13b)



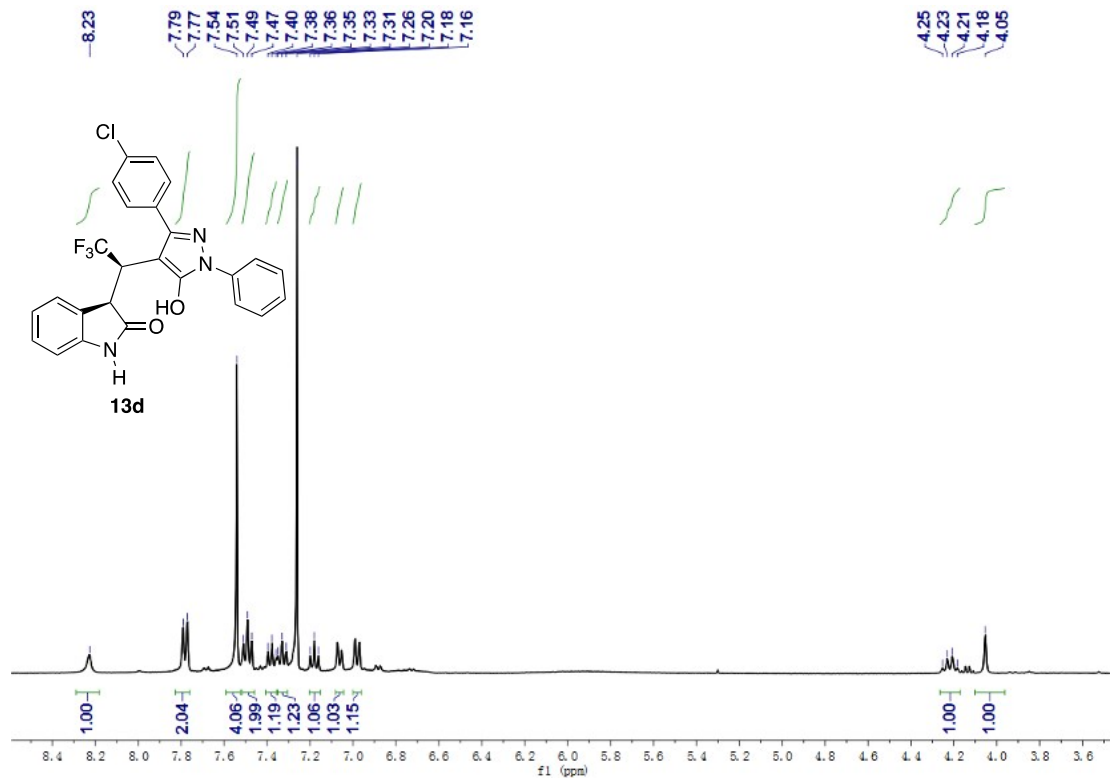


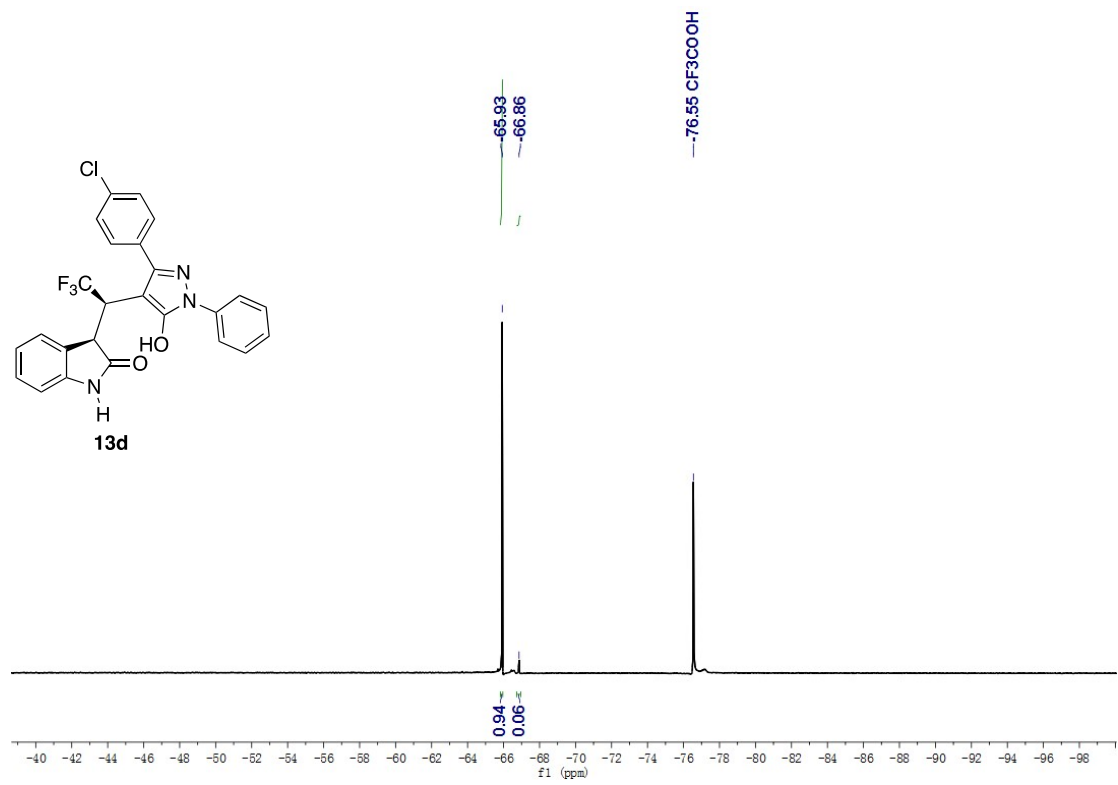
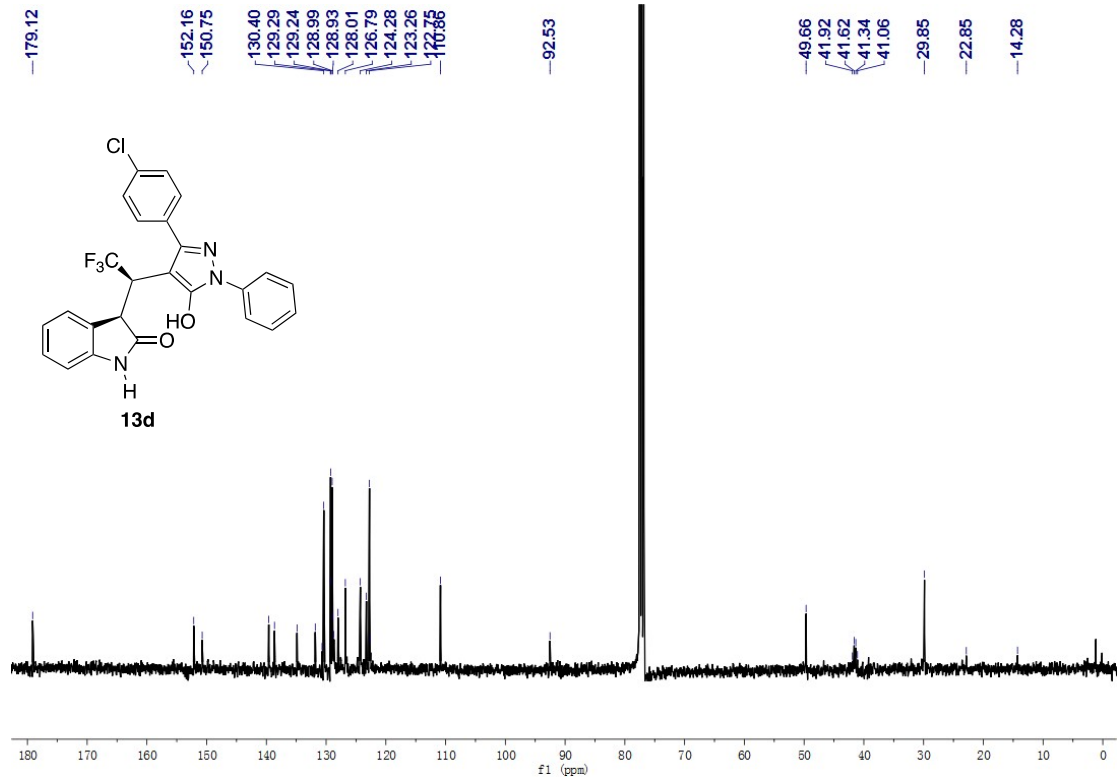
(R)-3-((R)-1-(3-(3-chlorophenyl)-5-hydroxy-1-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13c)



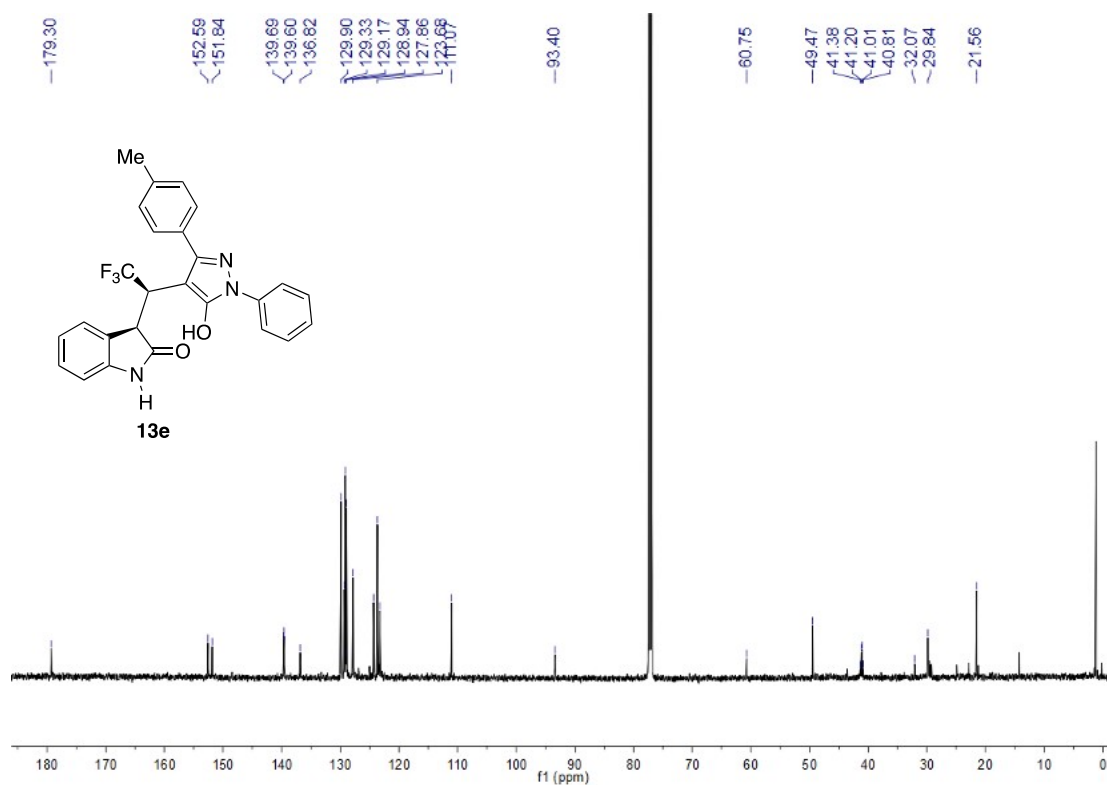
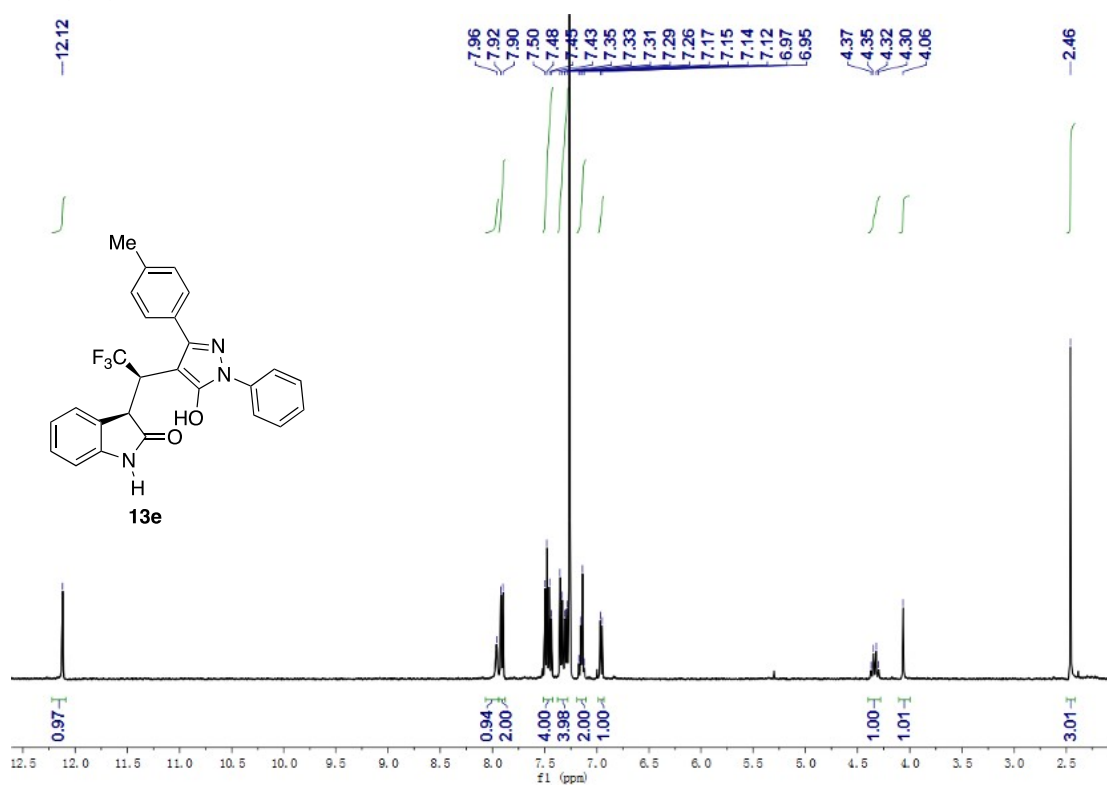


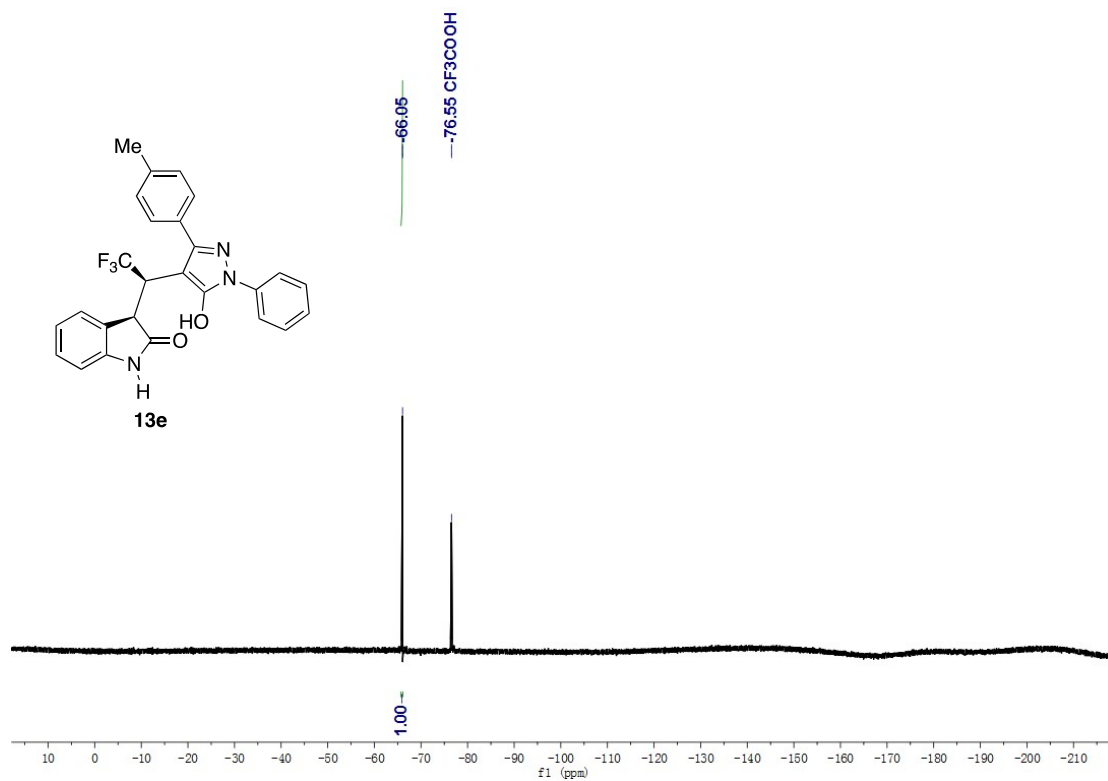
(R)-3-((R)-1-(3-(4-chlorophenyl)-5-hydroxy-1-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13d)



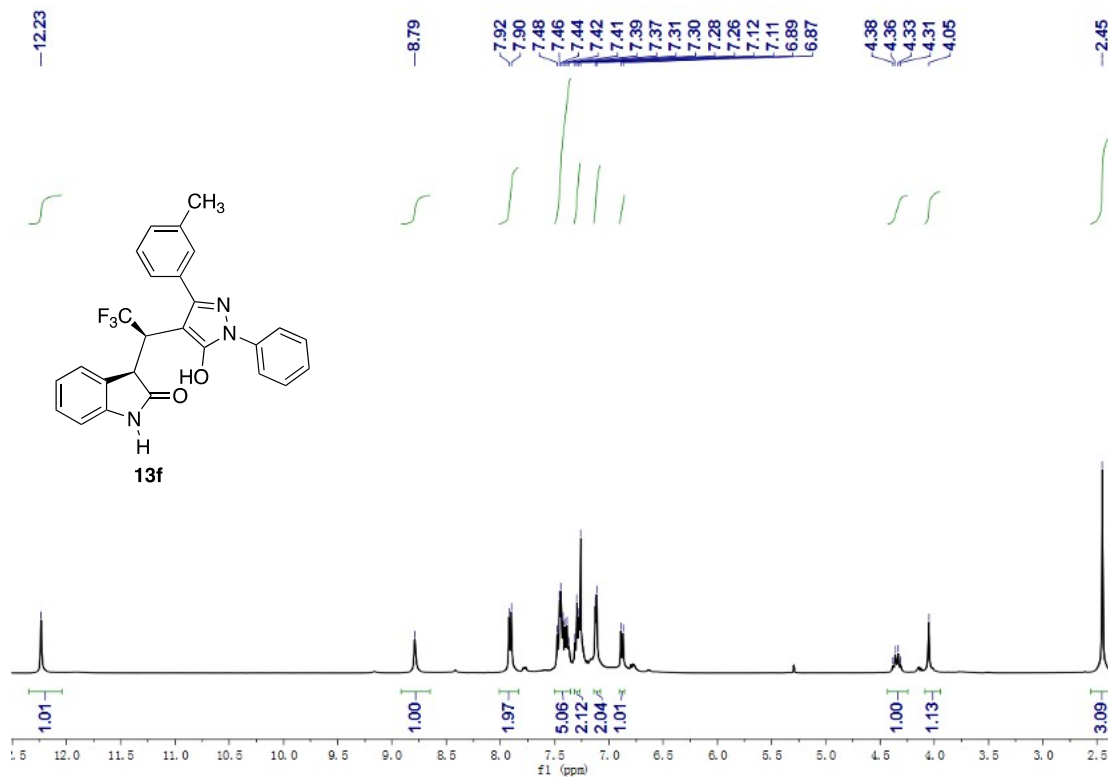


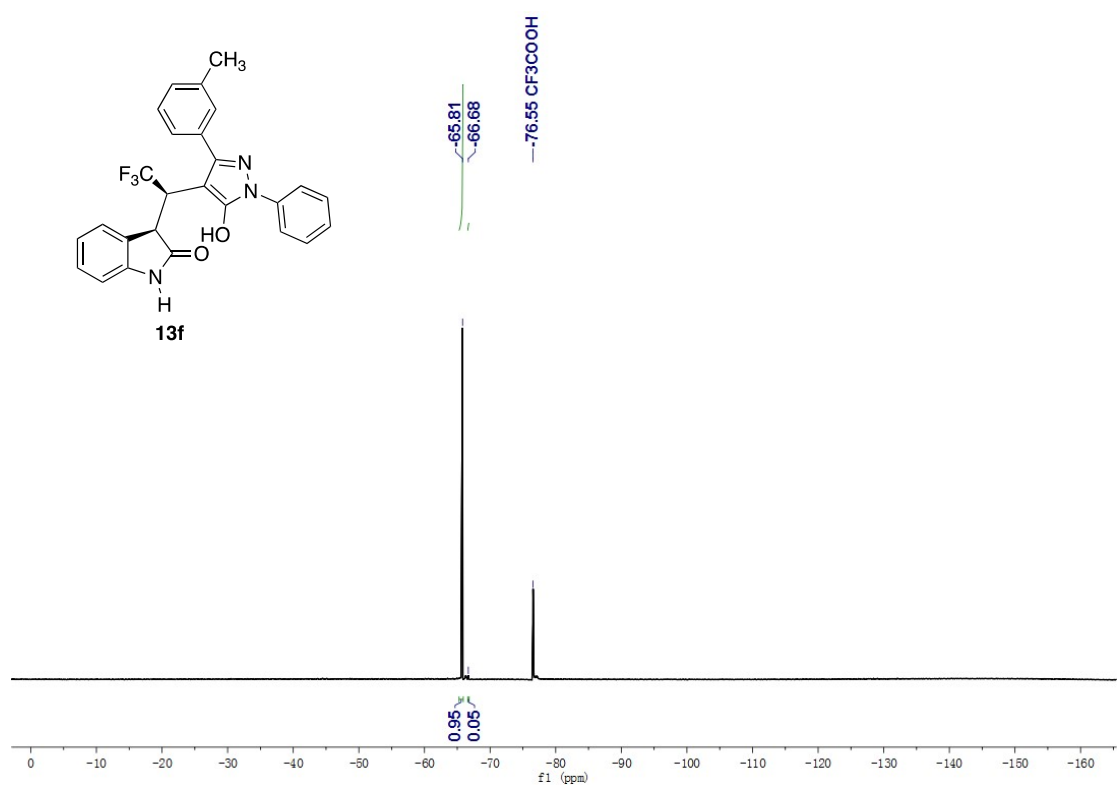
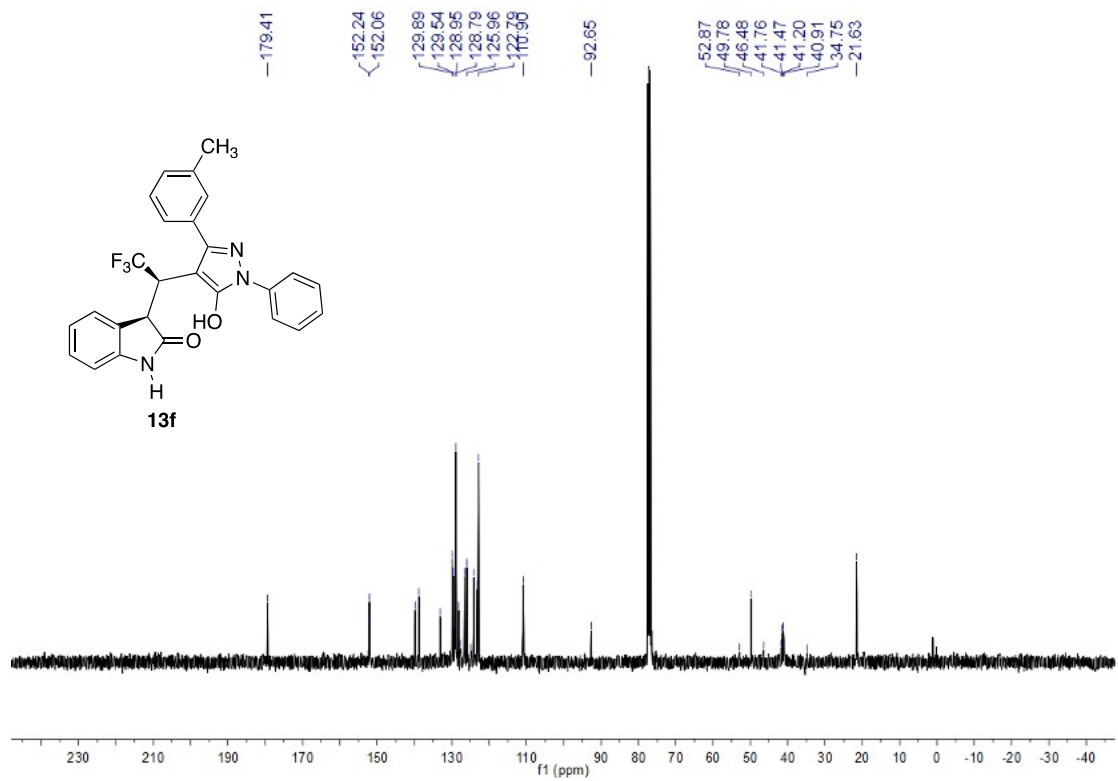
(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-phenyl-3-(*p*-tolyl)-1*H*-pyrazol-4-yl)ethyl)indolin-2-one (13e)



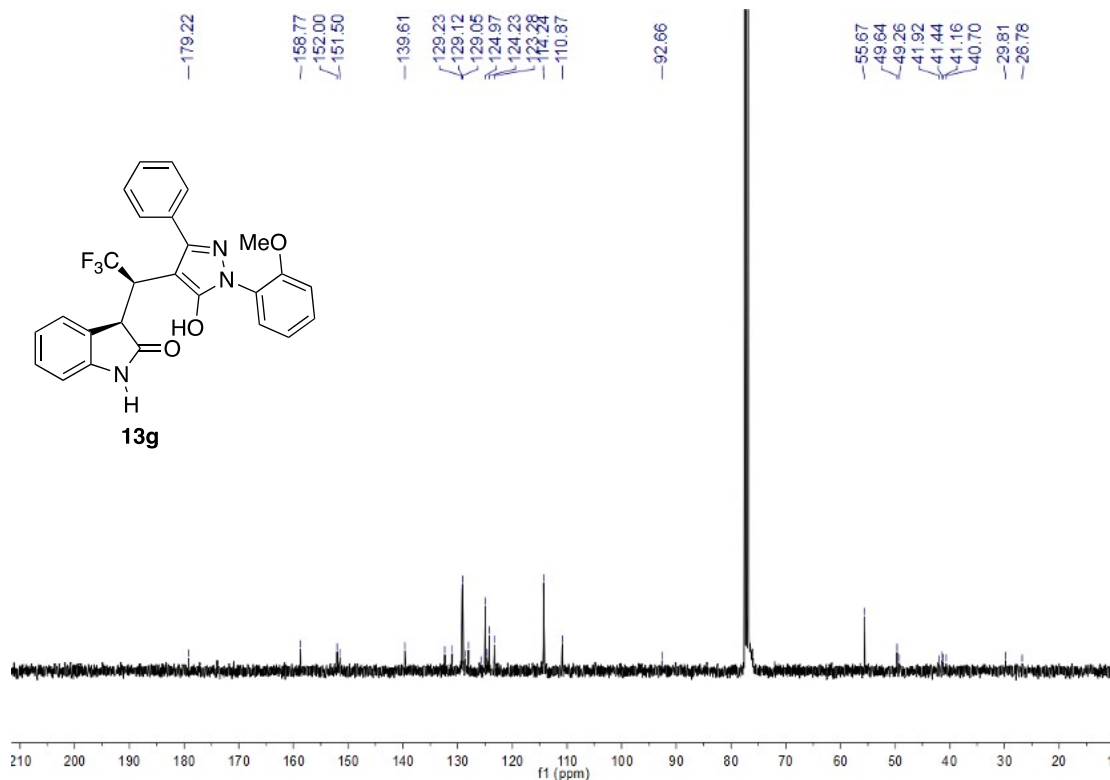
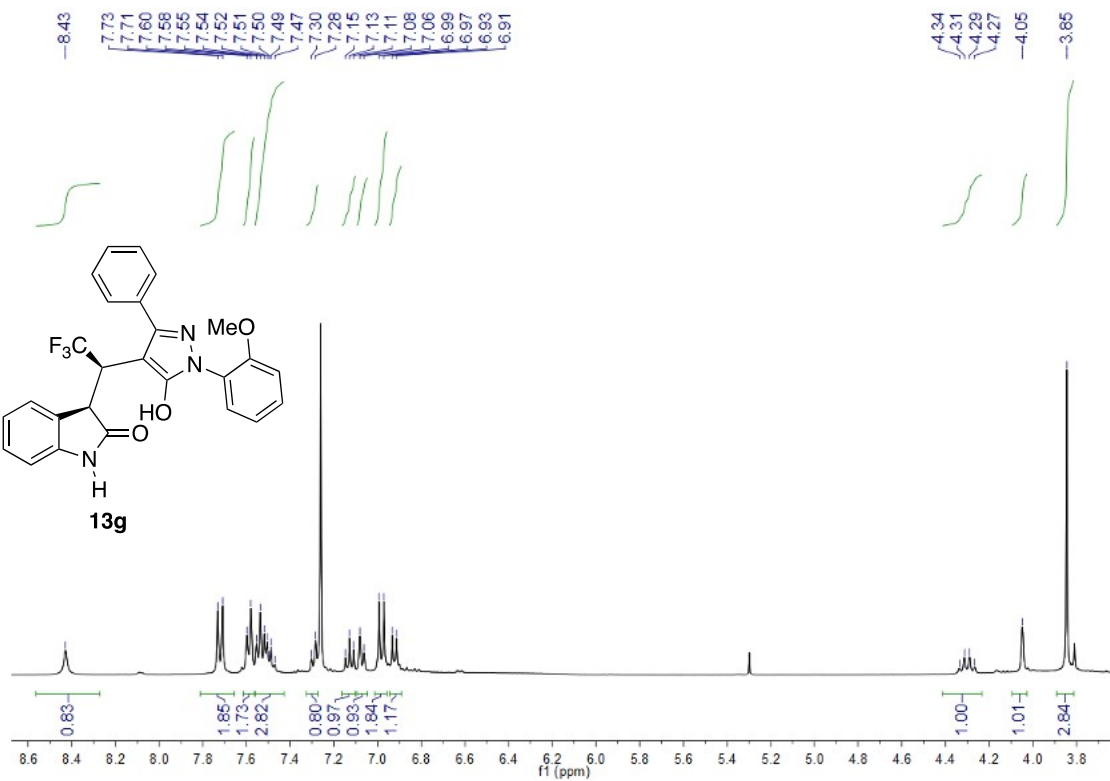


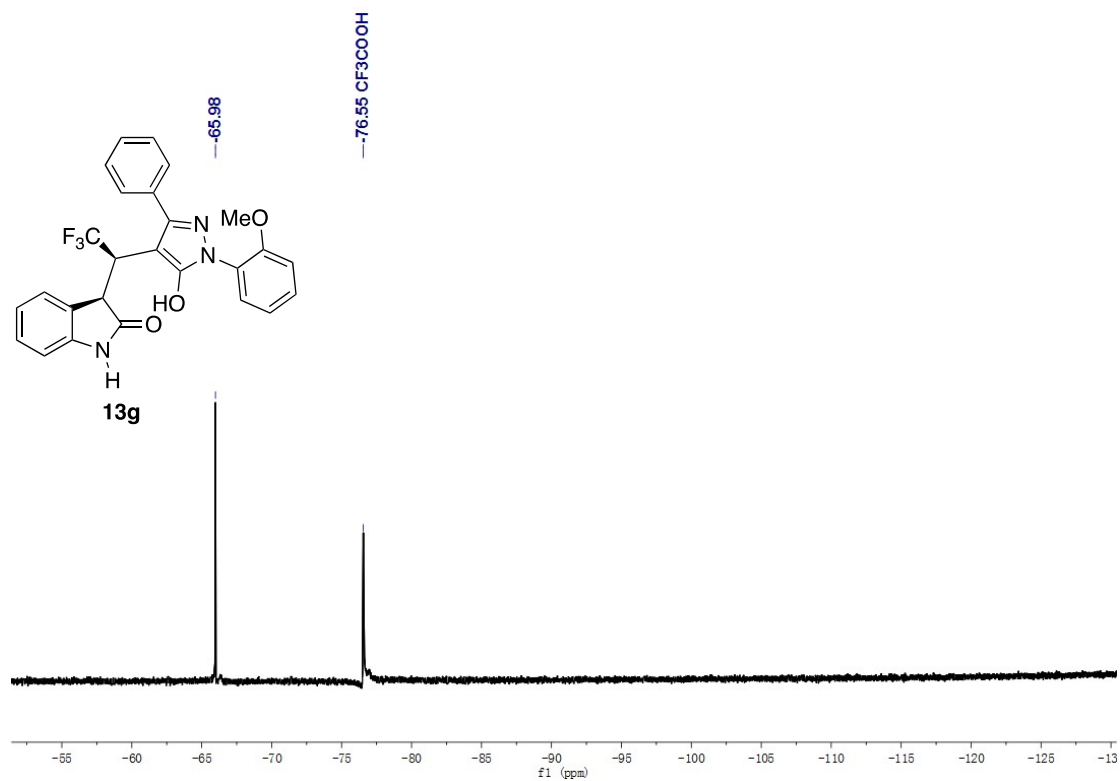
(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-phenyl-3-(*m*-tolyl)-1*H*-pyrazol-4-yl)ethyl)indolin-2-one (13f)



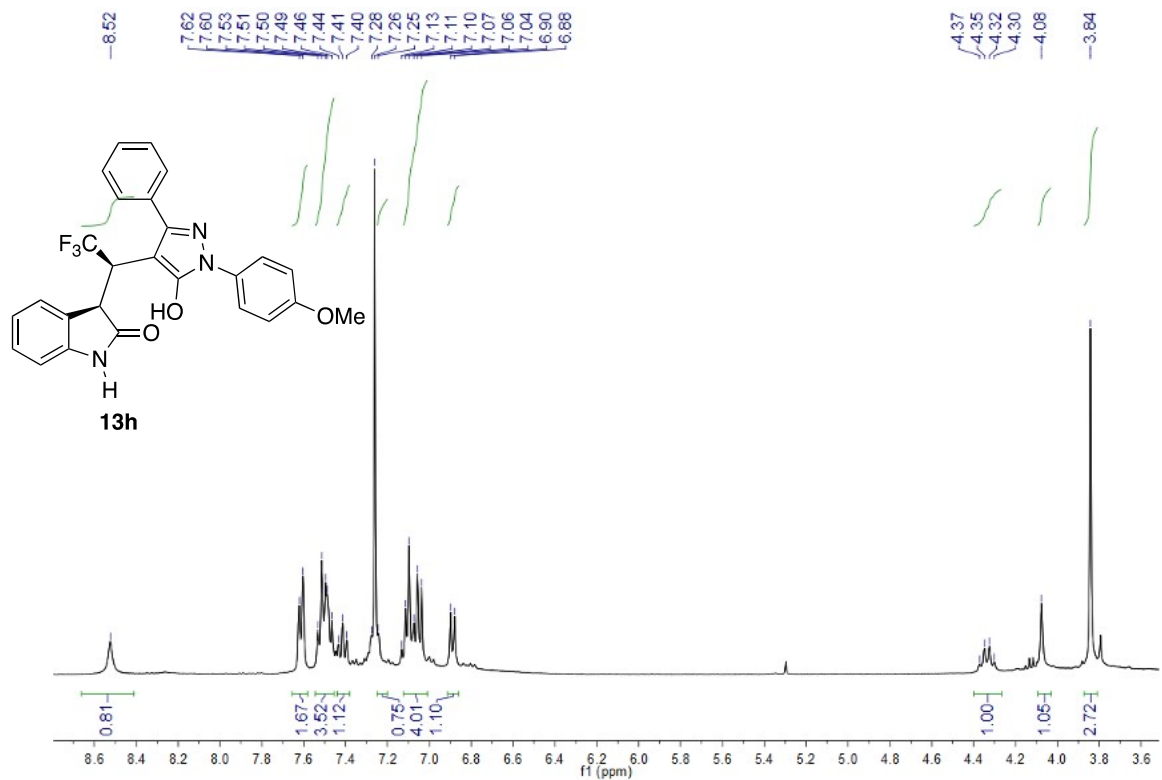


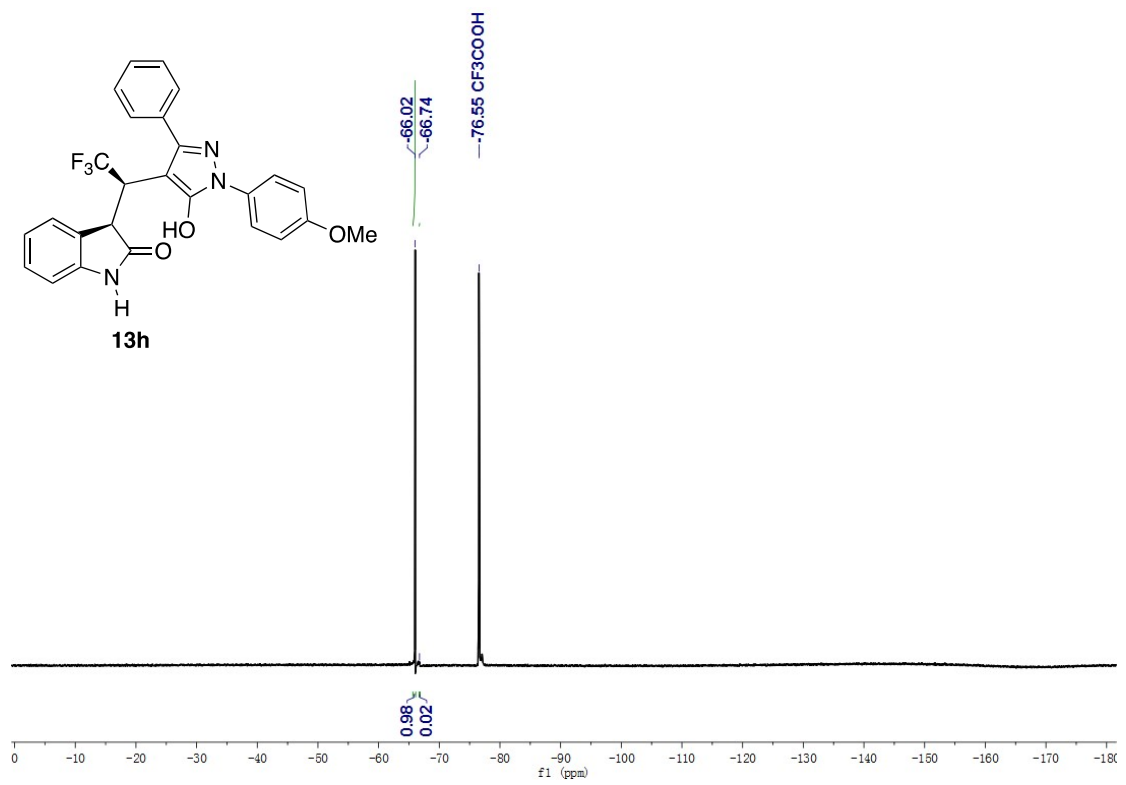
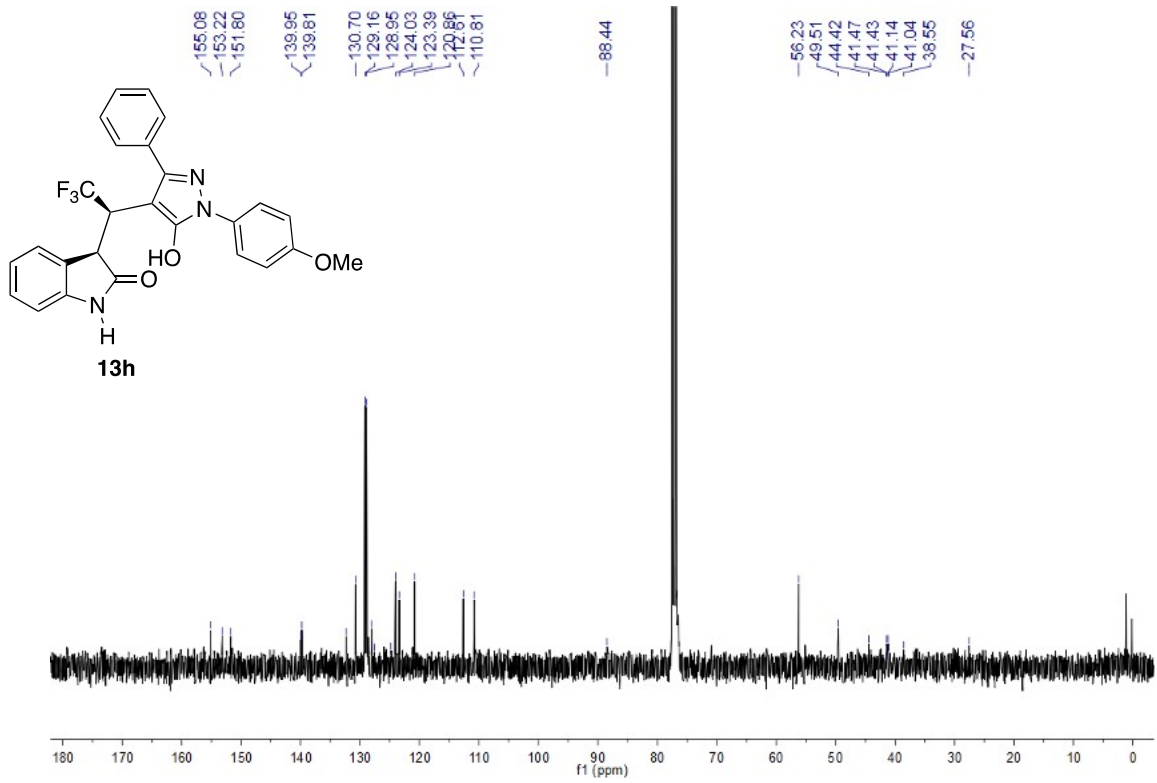
(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-(2-methoxyphenyl)-3-phenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13g)



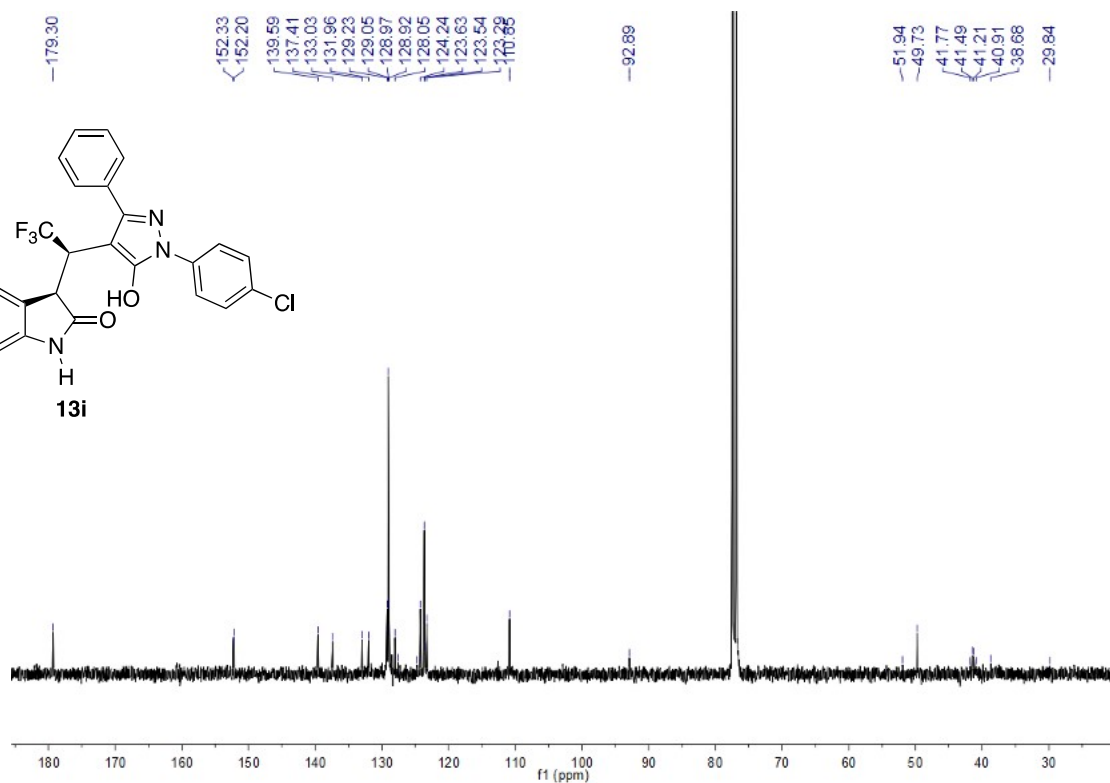
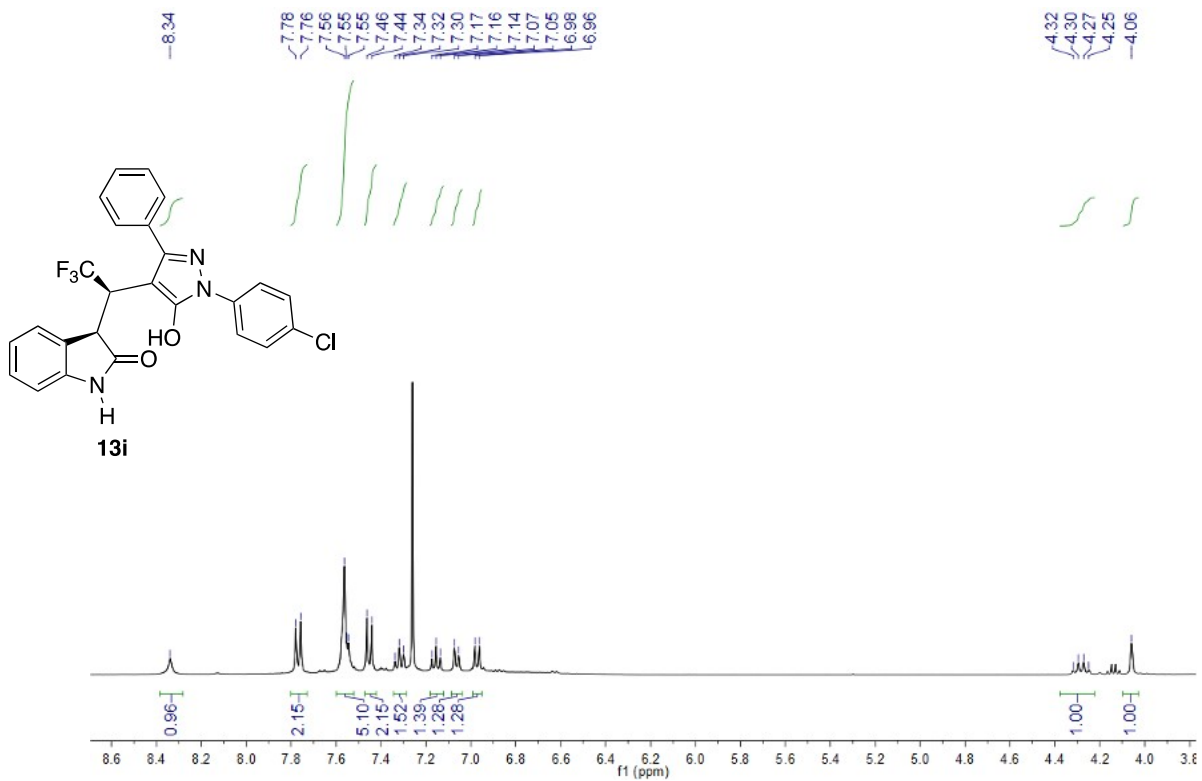


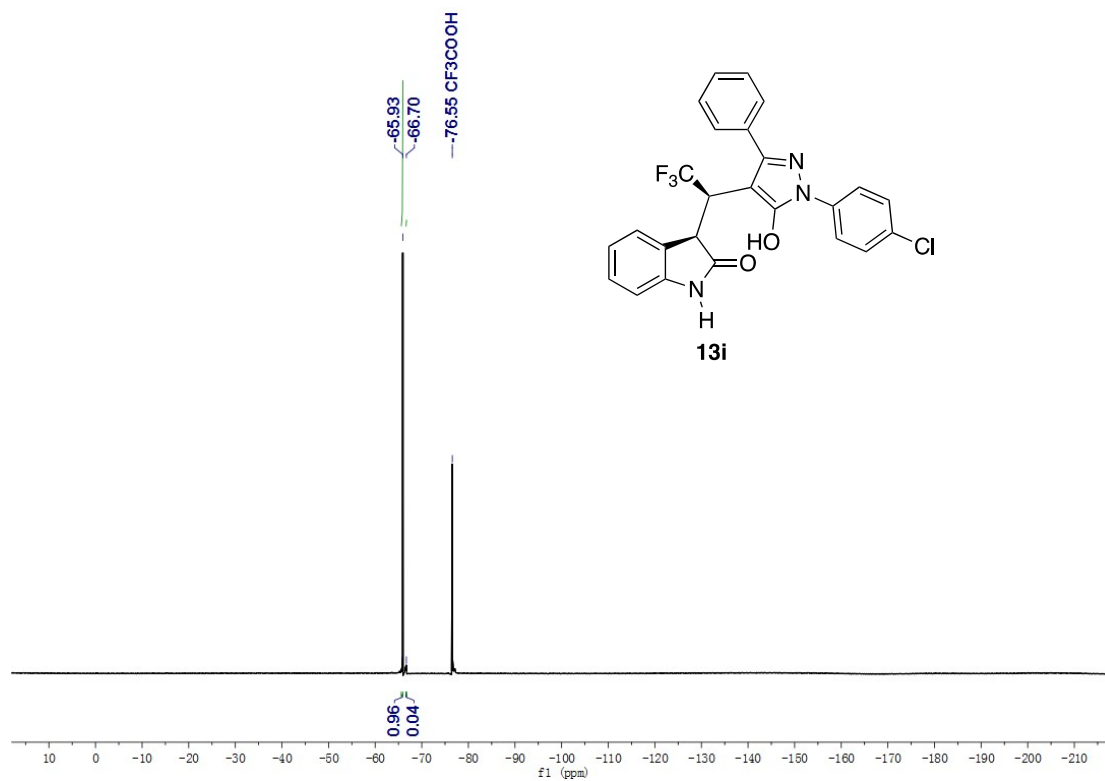
(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-(4-methoxyphenyl)-3-phenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13h)



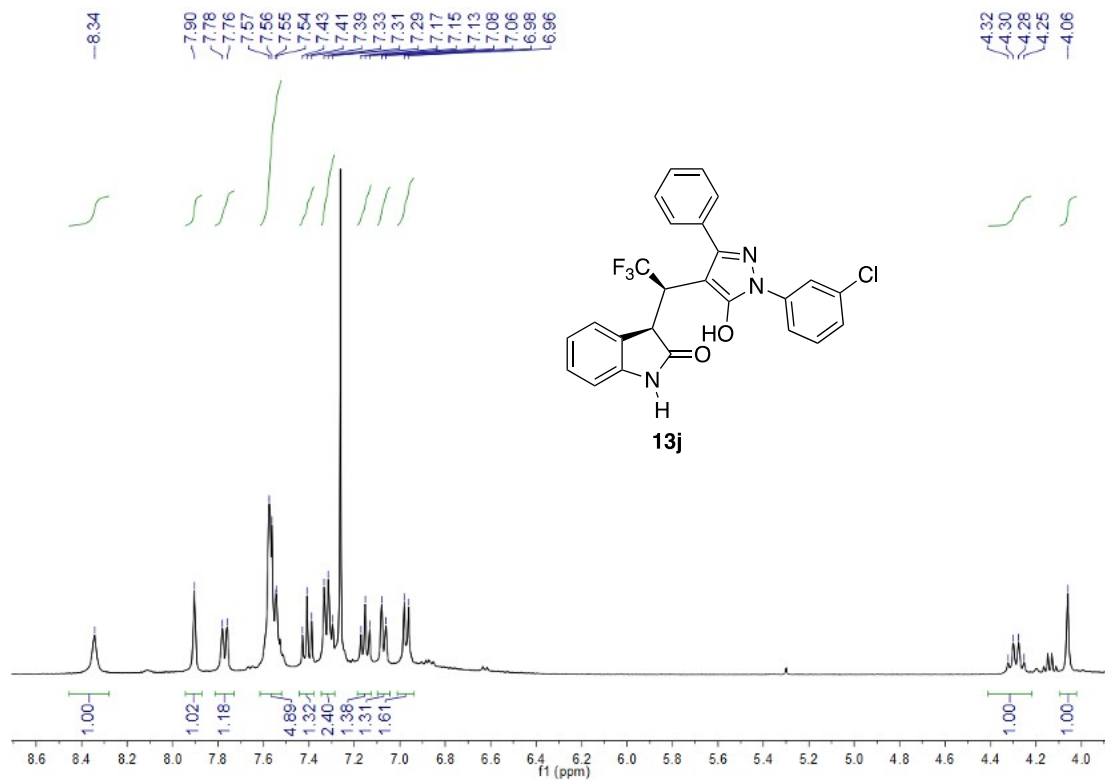


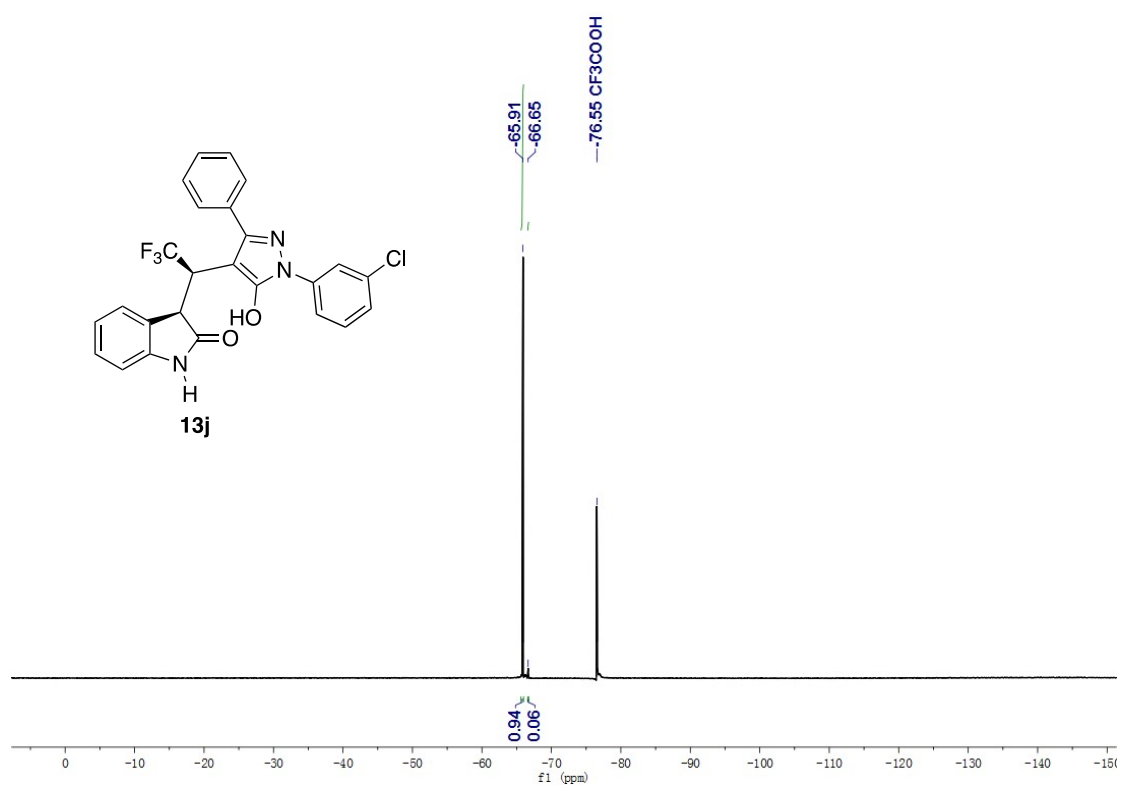
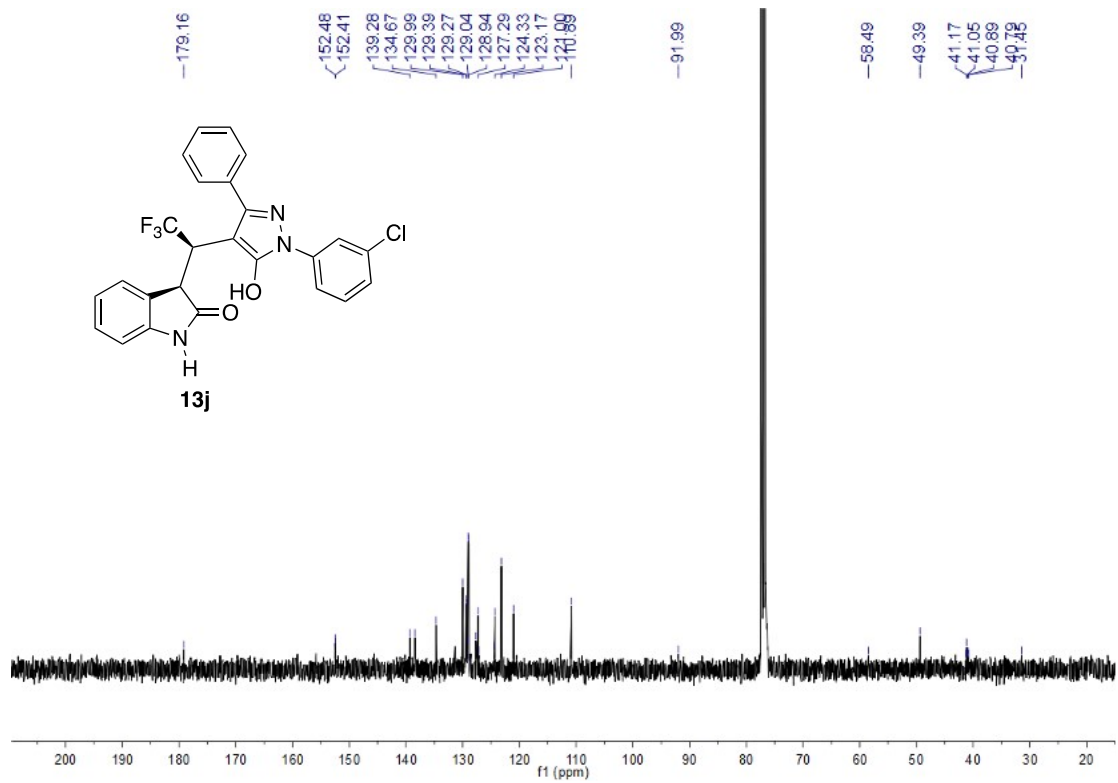
(R)-3-((R)-1-(1-(4-chlorophenyl)-5-hydroxy-3-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13i)



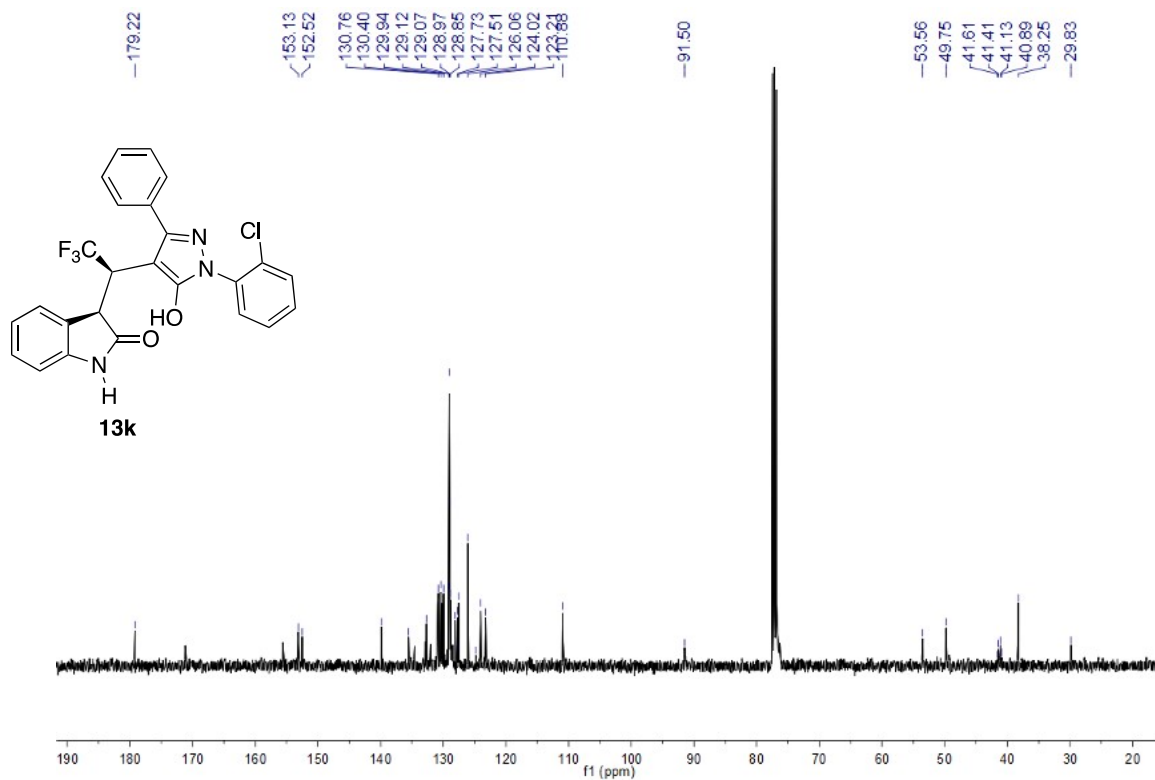
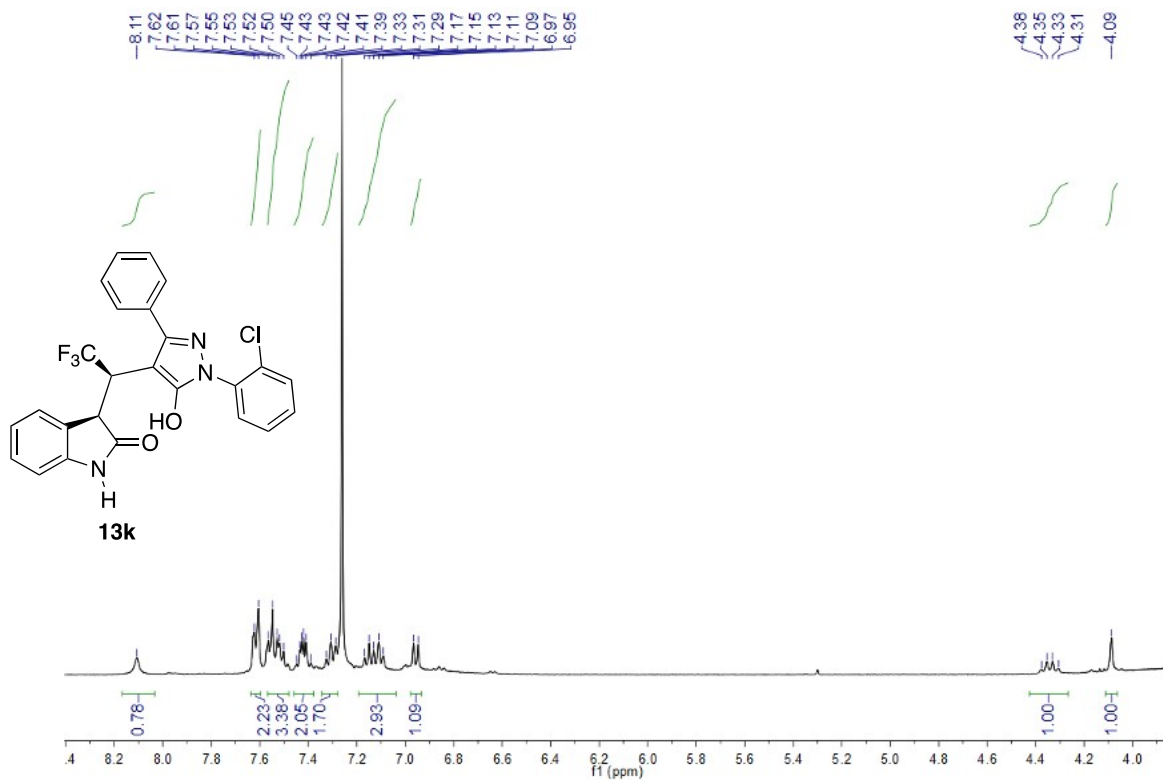


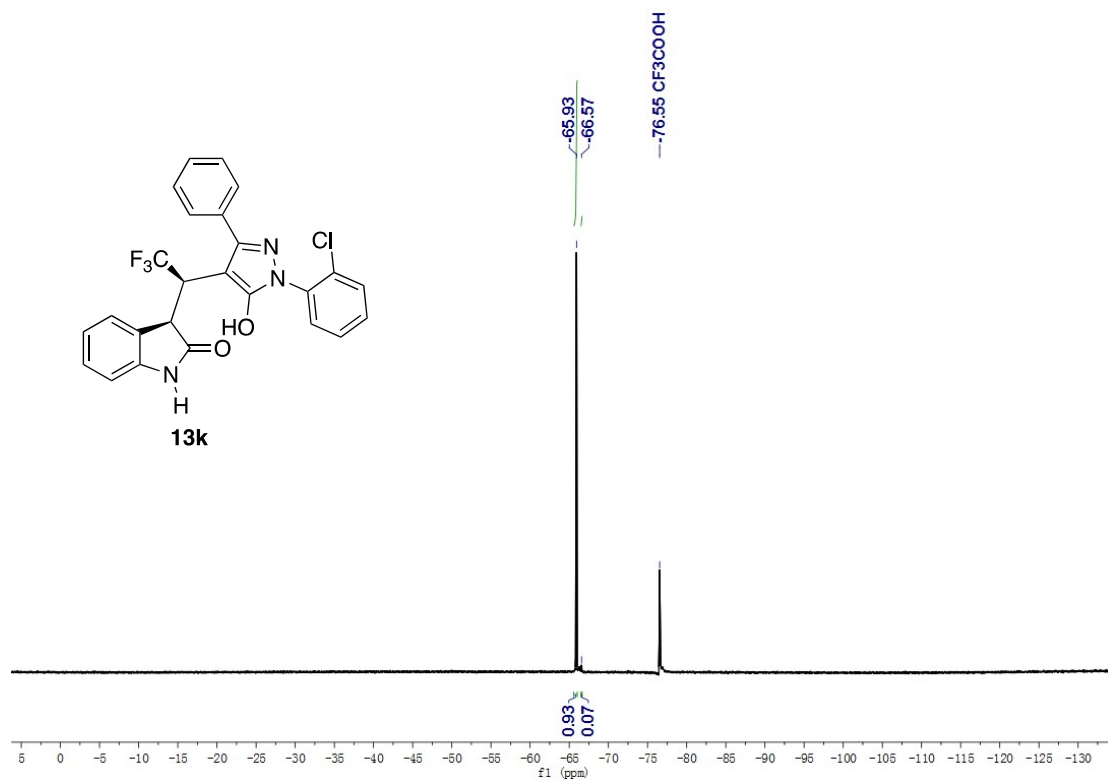
(R)-3-((R)-1-(1-(3-chlorophenyl)-5-hydroxy-3-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13j)



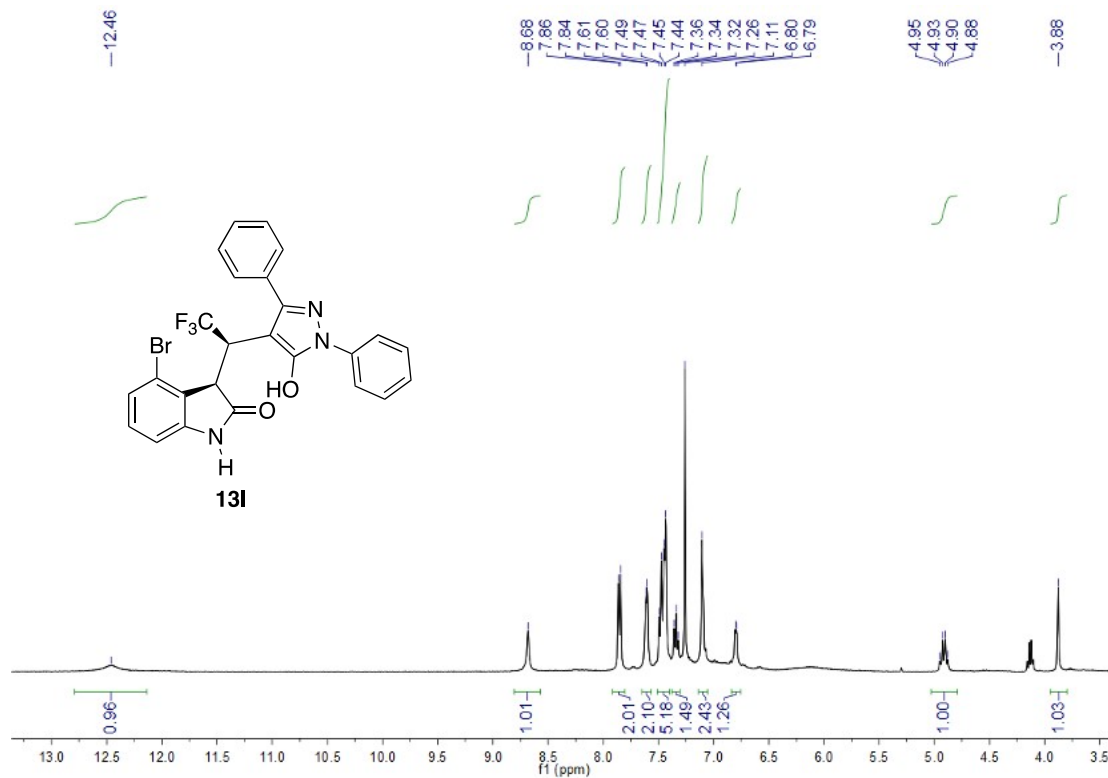


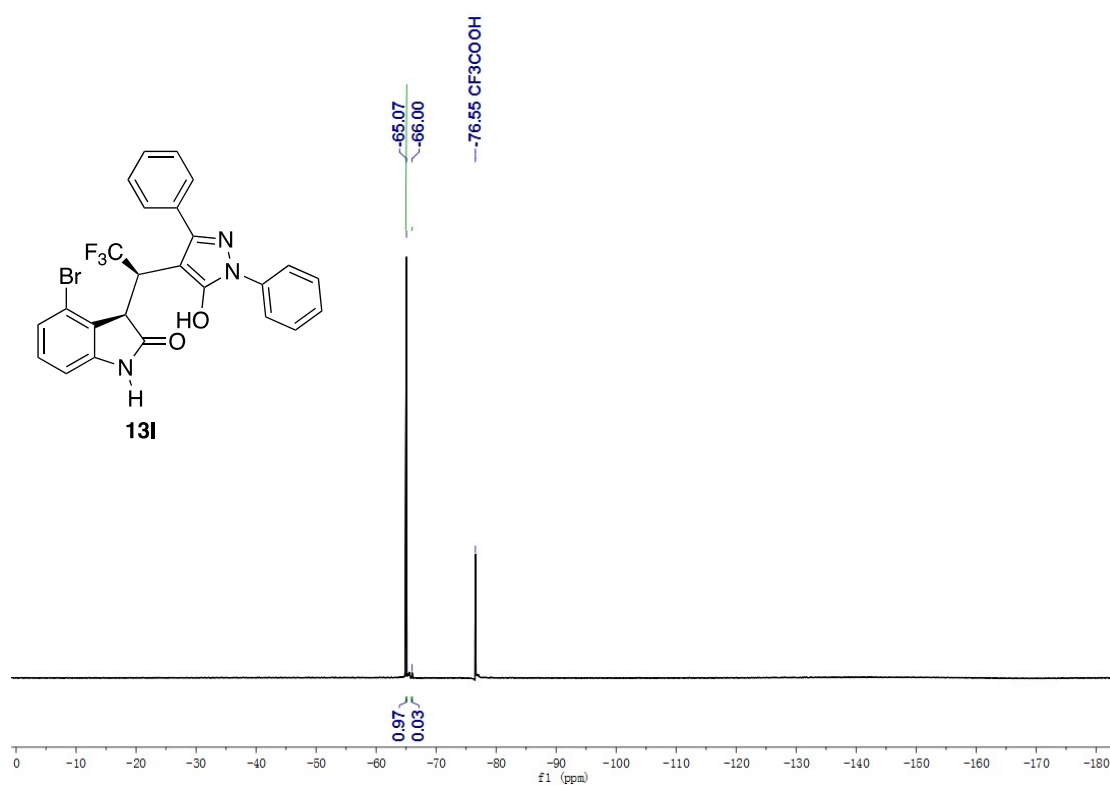
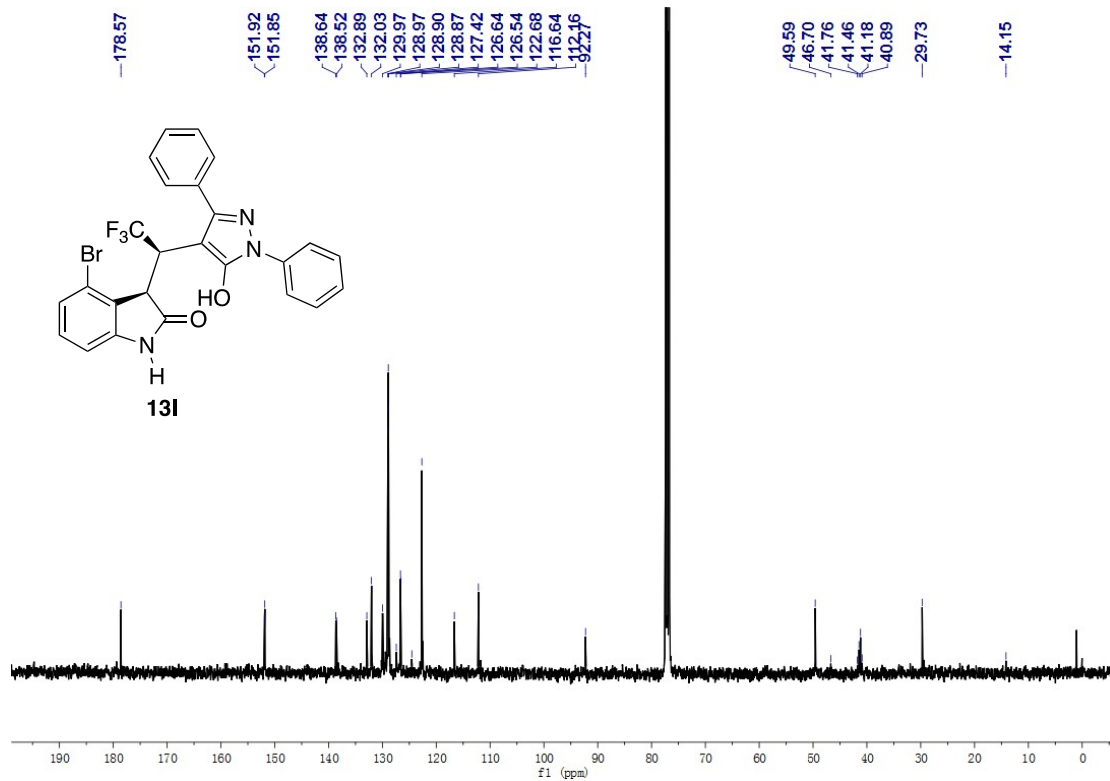
(R)-3-((R)-1-(1-(2-chlorophenyl)-5-hydroxy-3-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13k)



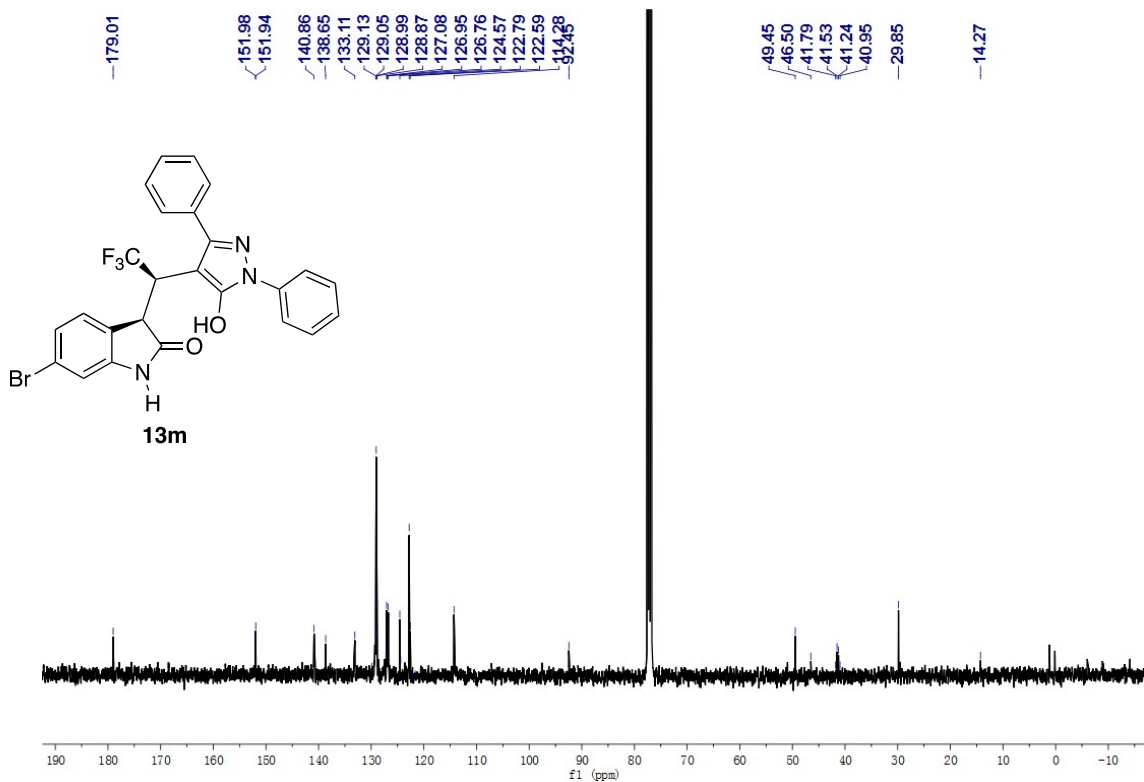
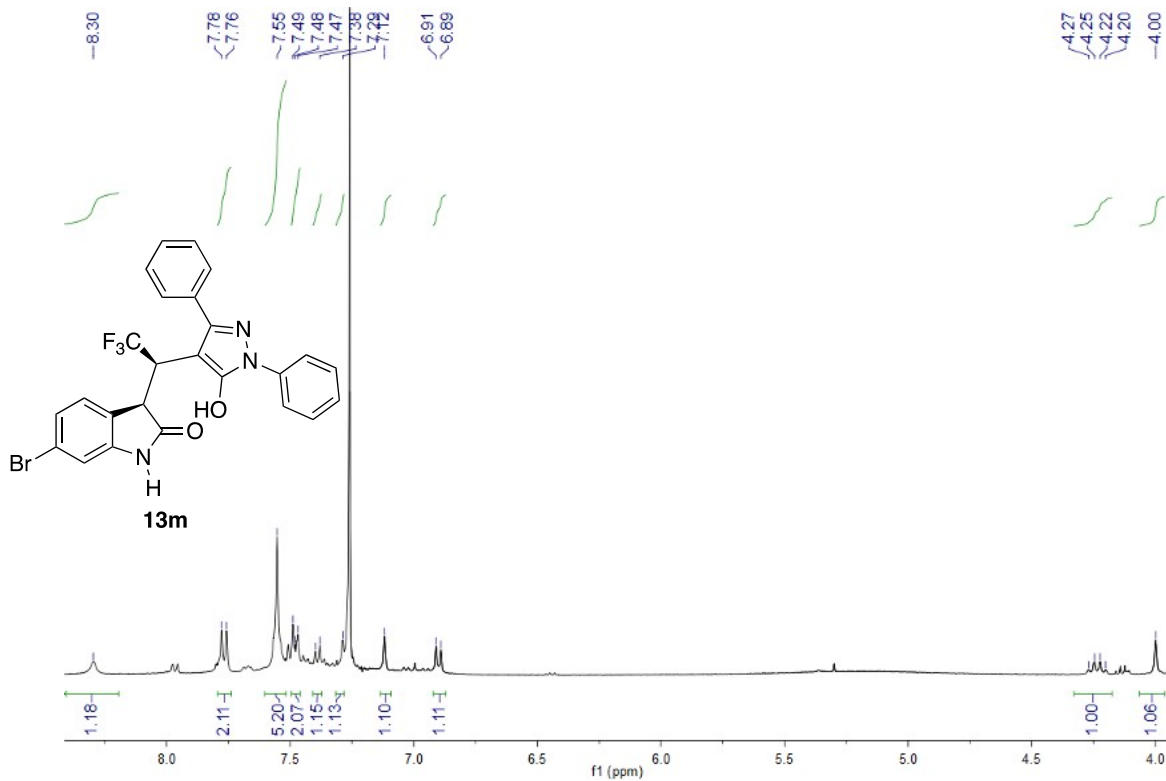


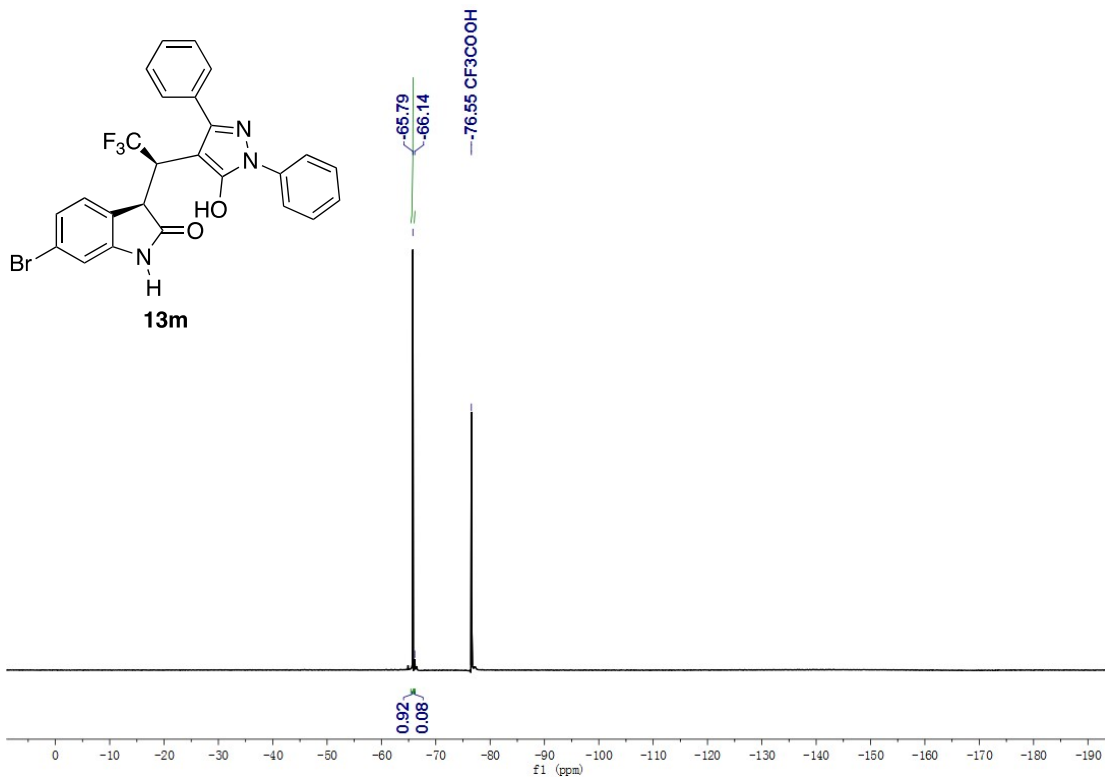
(R)-4-bromo-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13l)



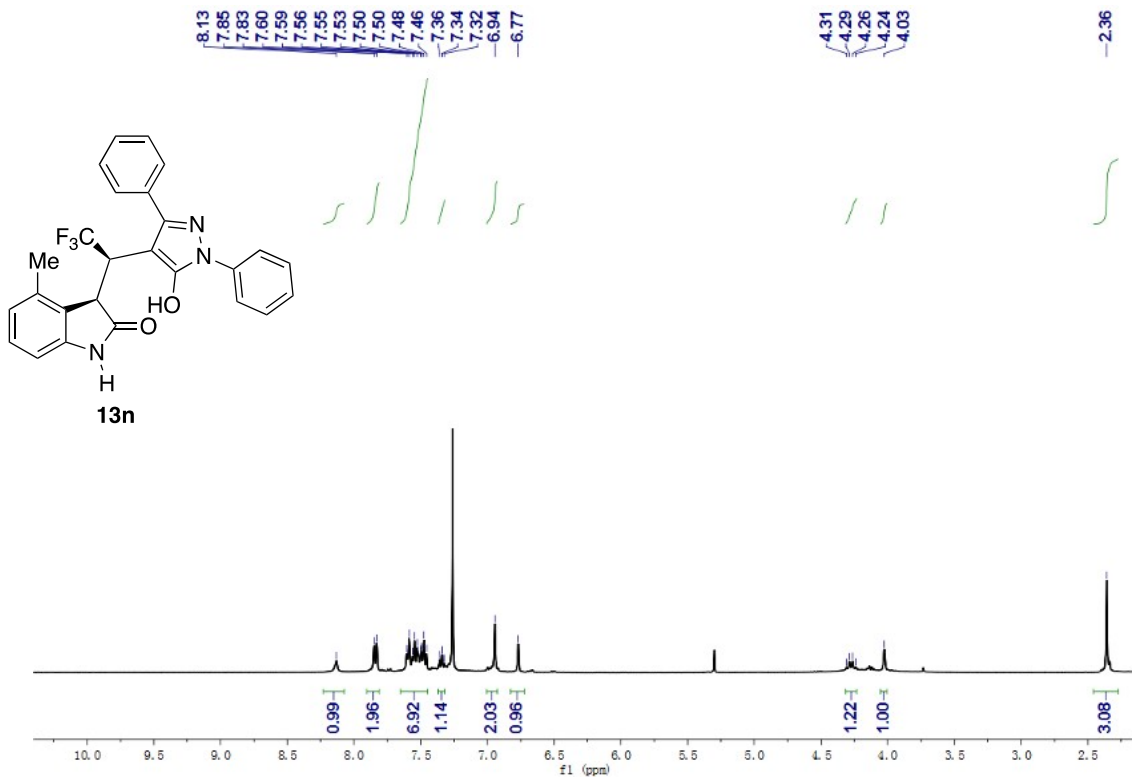


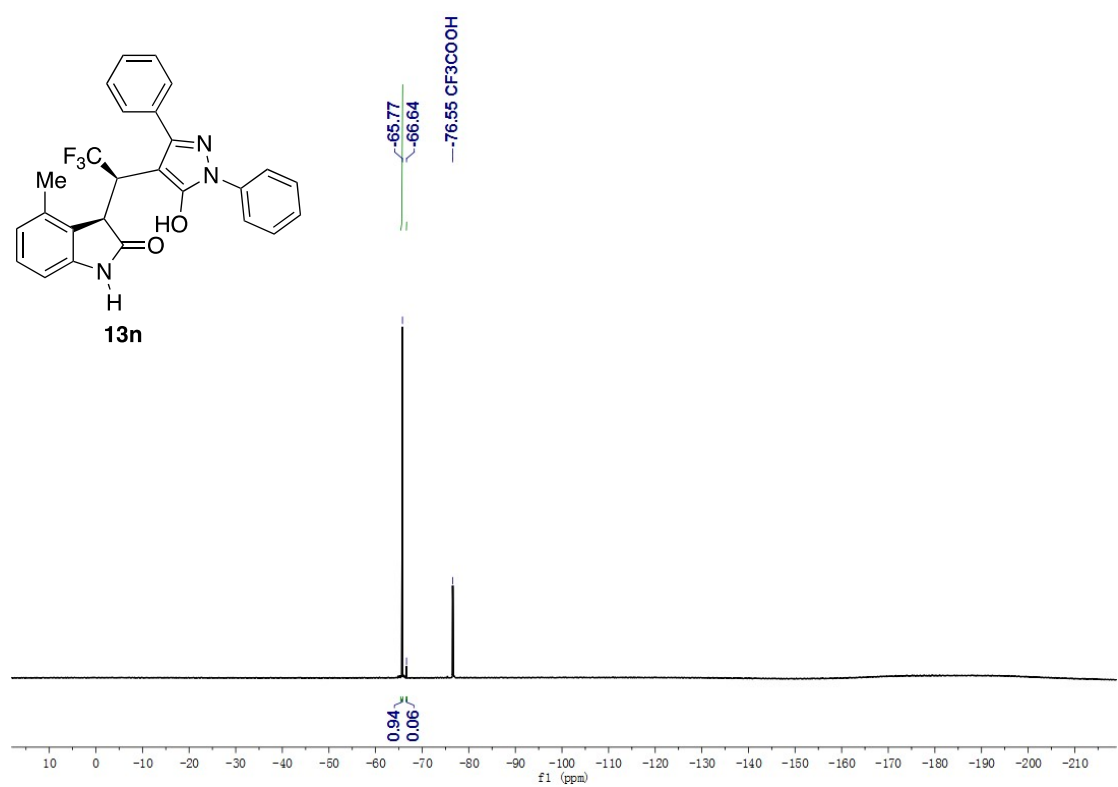
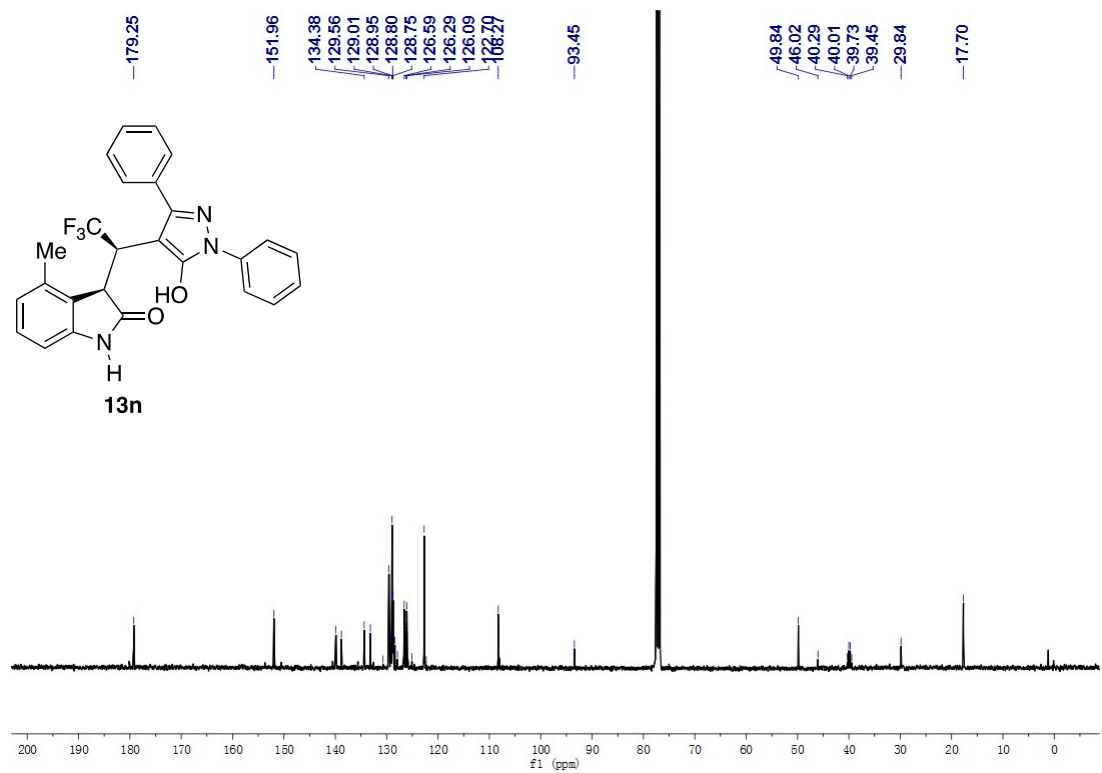
(R)-6-bromo-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13m)



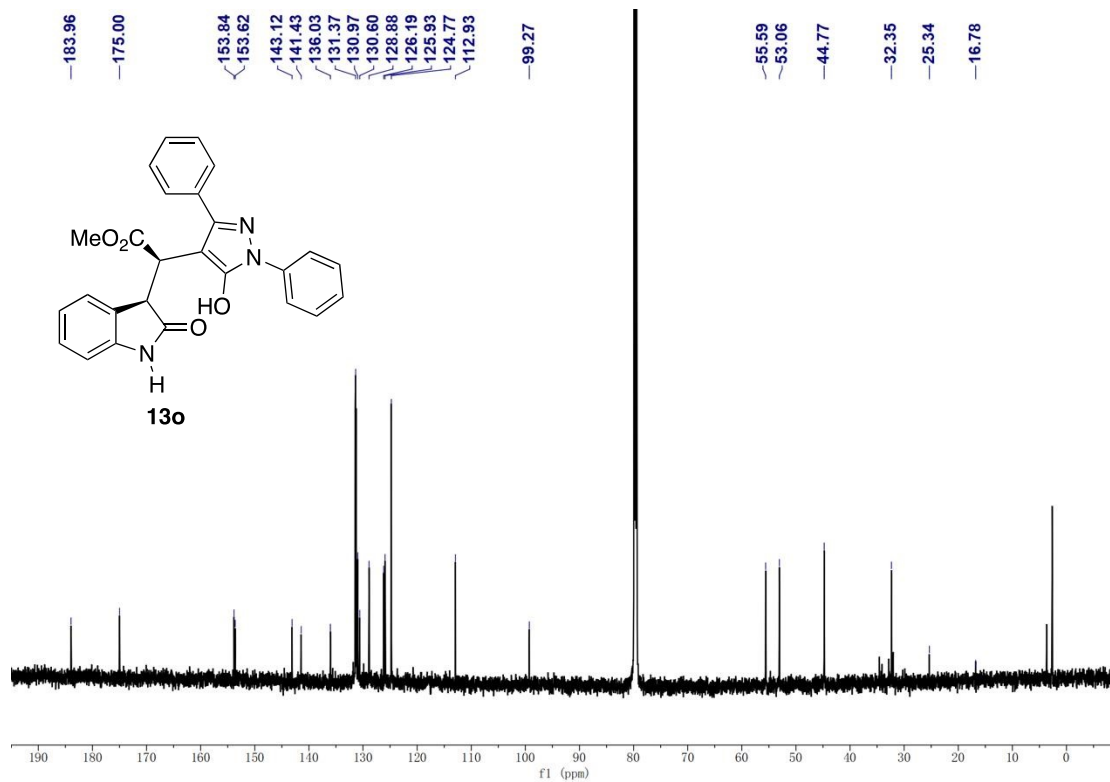
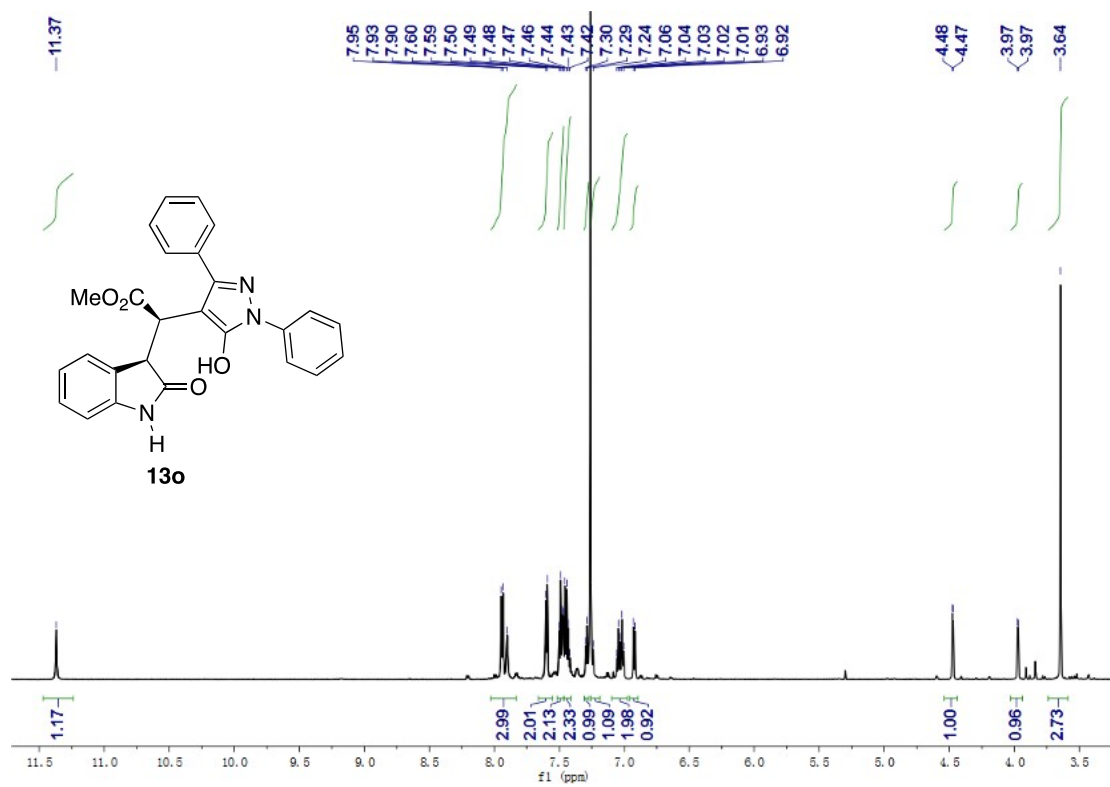


(R)-4-methyl-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13n)

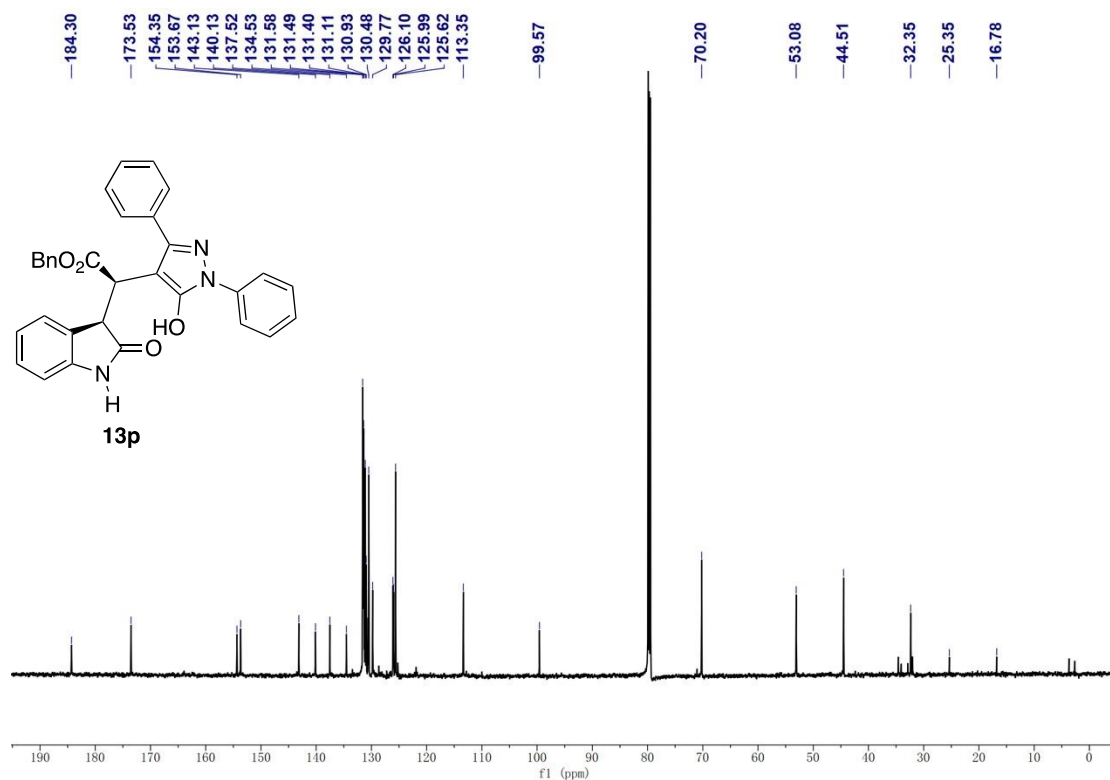
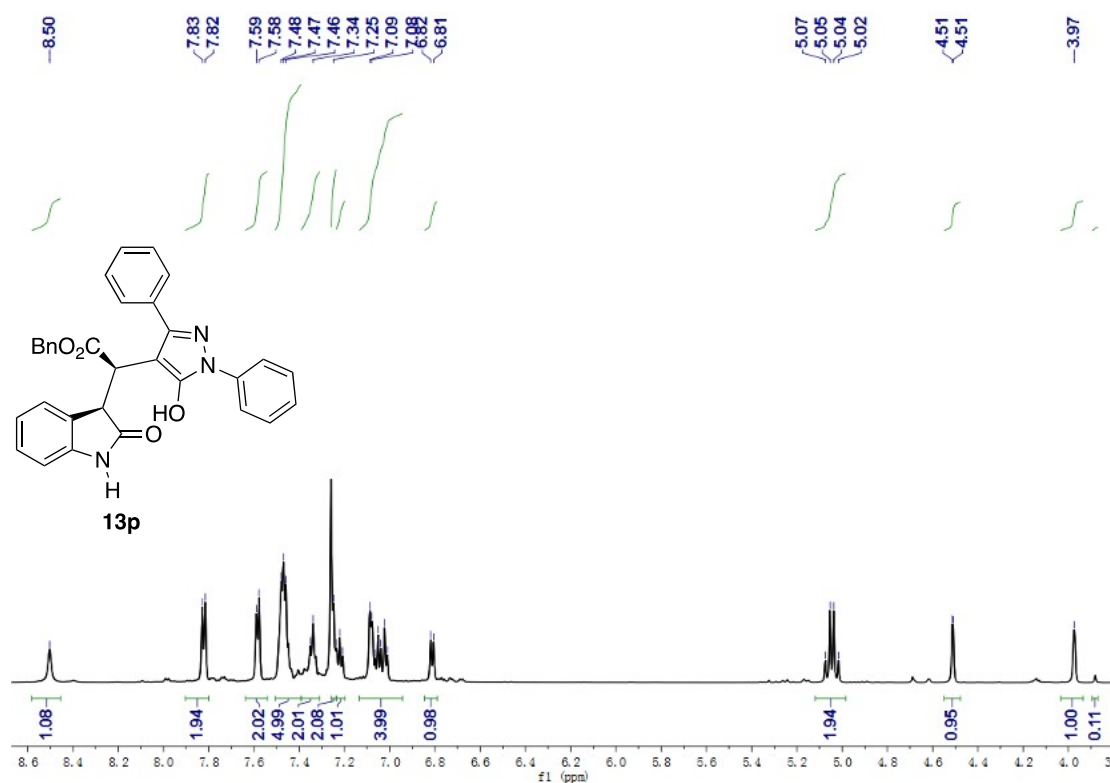




Methyl (*R*)-2-(5-hydroxy-1,3-diphenyl-1*H*-pyrazol-4-yl)-2-((*R*)-2-oxoindolin-3-yl)acetate (**13o**)

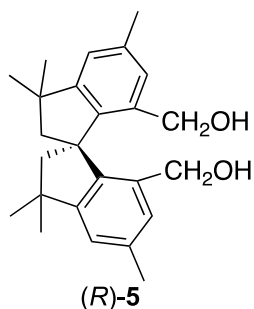


Benzyl (*R*)-2-(5-hydroxy-1,3-diphenyl-1*H*-pyrazol-4-yl)-2-((*R*)-2-oxoindolin-3-yl)acetate (13p**)**

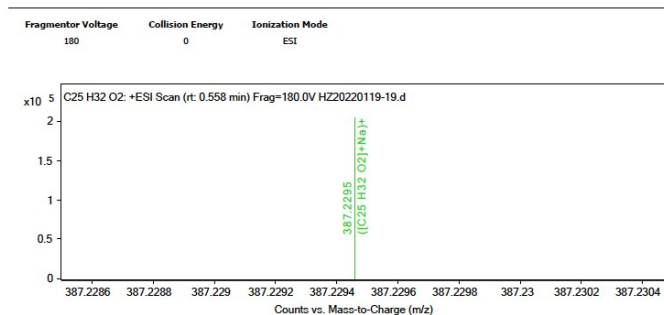


2 Copies of HRMS Spectra

(R)-(3,3,3',3',5,5'-hexamethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-diyl)dimethanol [(R)-5]



Spectra



Formula Calculator Element Limits

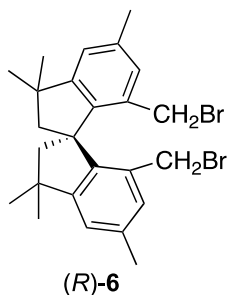
Element	Min	Max
C	0	100
H	0	200
O	0	10

Formula Calculator Results

Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C25 H32 Na O2	True	387.2295	387.2295	0.03	100

--- End Of Report ---

(R)-7,7'-bis(bromomethyl)-3,3,3',3',5-pentamethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene] [(R)-6]



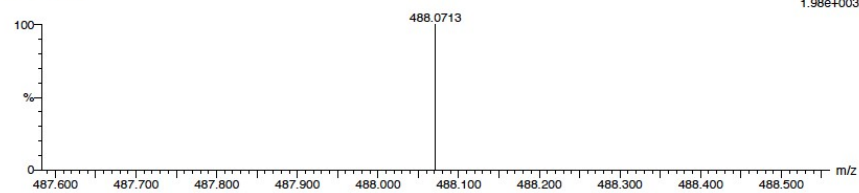
Elemental Composition Report

Page 1

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

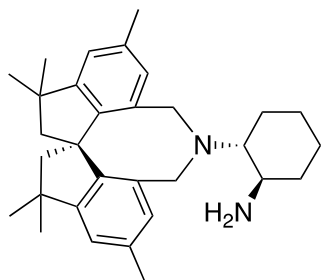
Monoisotopic Mass, Odd and Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 70 closest results for each mass)
Elements Used:
C: 0-100 H: 0-200 Br: 0-2

HZ0120-20 1126 (6.083)
TOF MS EI+



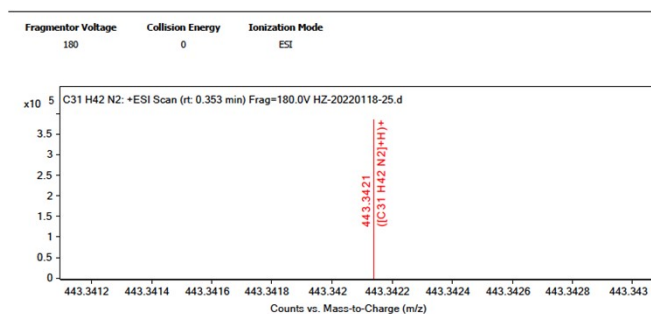
Minimum:						
Maximum:	5.0	10.0		-1.5		50.0
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
488.0713	488.0714	-0.1	-0.2	10.0	5547013.5	C25 H30 Br2

(1R,2R)-2-(2,4,4,7,7,9-hexamethyl-4,5,6,7-tetrahydro-11H-diindeno[7,1-cd:1',7'-ef]azocin-12(13H)-yl)cyclohexan-1-amine (7)



7

Spectra

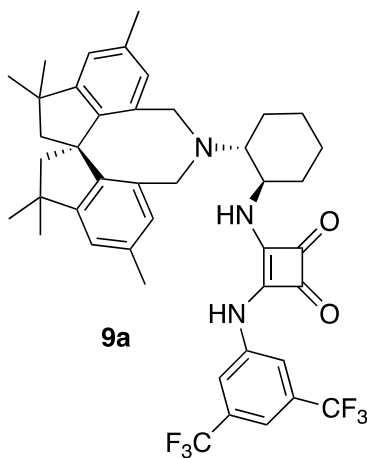


Formula Calculator Element Limits		
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10

Formula Calculator Results					
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C31 H43 N2	True	443.3421	443.3421	0.13	99.98

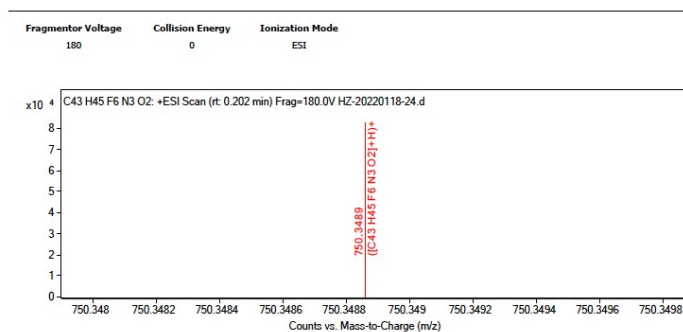
--- End Of Report ---

3-((3,5-bis(trifluoromethyl)phenyl)amino)-4-(((1R,2R)-2-(2,4,4,7,7,9-hexamethyl-4,5,6,7-tetrahydro-11H-diindeno[7,1-cd:1',7'-ef]azocin-12(13H)-yl)cyclohexyl)amino)cyclobut-3-ene-1,2-dione (9a)



9a

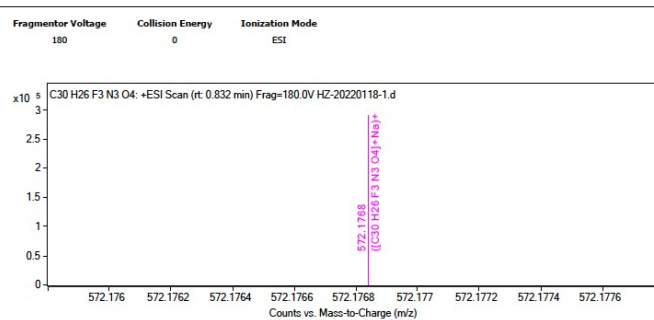
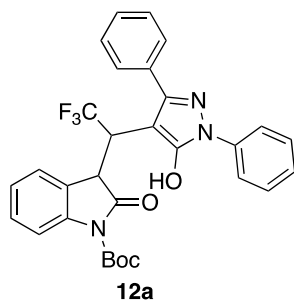
Spectra



Formula Calculator Element Limits		
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	6

Formula Calculator Results					
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C43 H46 F6 N3 O2	True	750.3489	750.3489	0.06	99.99

2-oxo-3-(2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indoline-1-carboxylate (12a)



Formula Calculator Element Limits

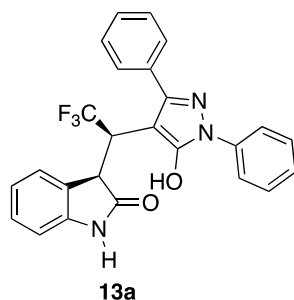
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	3	3

Formula Calculator Results

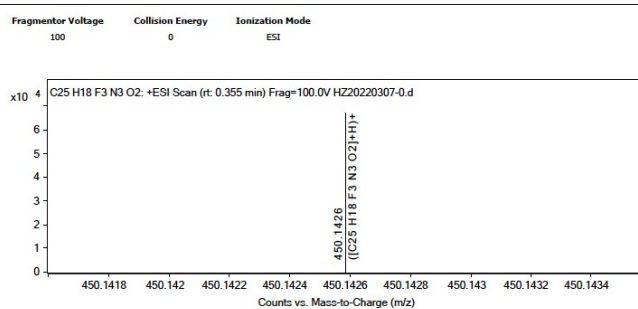
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C30 H26 F3 N3 Na O4	True	572.1768	572.1768	0.02	100

-- End Of Report --

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13a)



Spectra



Formula Calculator Element Limits

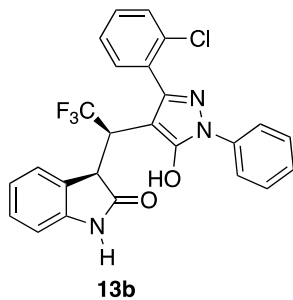
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3

Formula Calculator Results

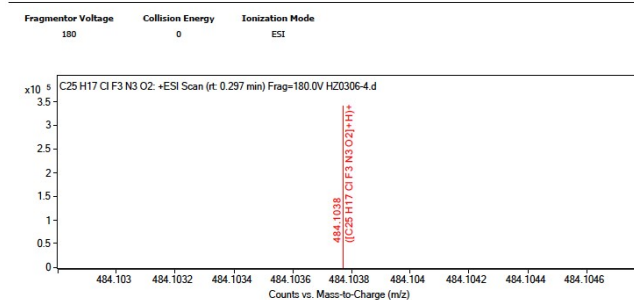
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C25 H19 F3 N3 O2	True	450.1426	450.1424	-0.81	99.35

-- End Of Report --

(R)-3-((R)-1-(3-(2-chlorophenyl)-5-hydroxy-1-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13b)



Spectra

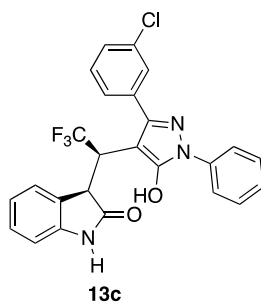


Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3
Cl	0	1

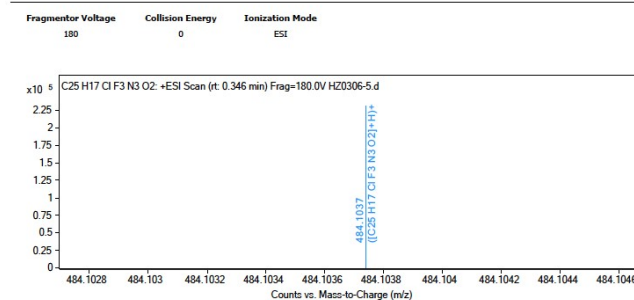
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C25 H18 Cl F3 N3 O2	True	484.1038	484.1034	-0.14	99.98

--- End Of Report ---

(R)-3-((R)-1-(3-(3-chlorophenyl)-5-hydroxy-1-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13c)



Spectra

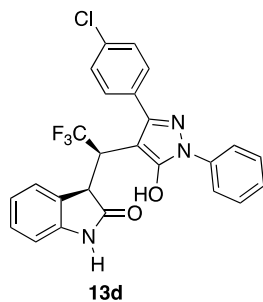


Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3
Cl	0	1

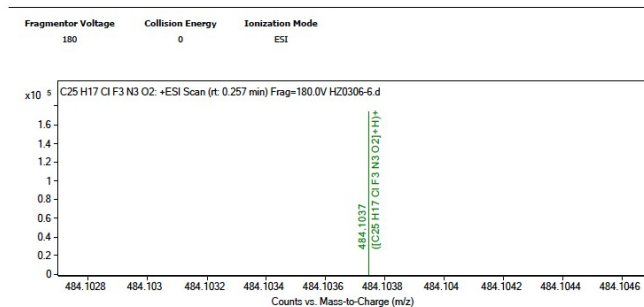
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C25 H18 Cl F3 N3 O2	True	484.1037	484.1034	-0.2	99.96

--- End Of Report ---

(R)-3-((R)-1-(3-(4-chlorophenyl)-5-hydroxy-1-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13d)



Spectra



Formula Calculator Element Limits

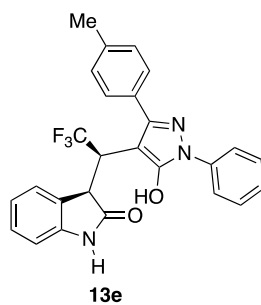
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3
Cl	0	1

Formula Calculator Results

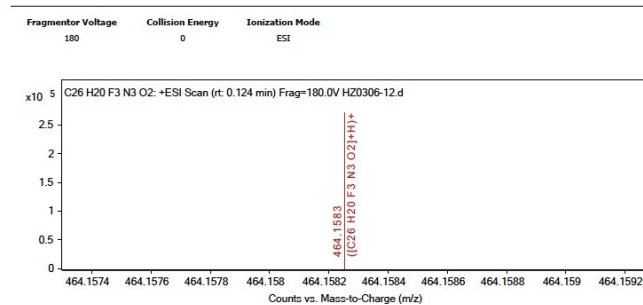
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C25 H18 Cl F3 N3 O2	True	484.1037	484.1034	-0.57	99.66

--- End Of Report ---

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-phenyl-3-(p-tolyl)-1H-pyrazol-4-yl)ethyl)indolin-2-one (13e)



Spectra



Formula Calculator Element Limits

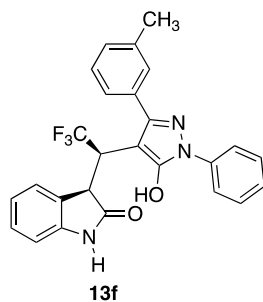
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3

Formula Calculator Results

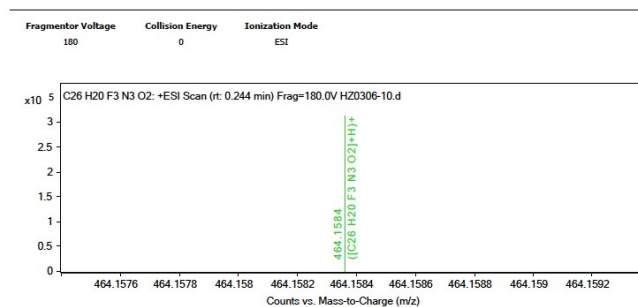
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C26 H21 F3 N3 O2	True	464.1583	464.158	-0.11	99.99

--- End Of Report ---

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-phenyl-3-(*m*-tolyl)-1*H*-pyrazol-4-yl)ethyl)indolin-2-one (13f)



Spectra



Formula Calculator Element Limits

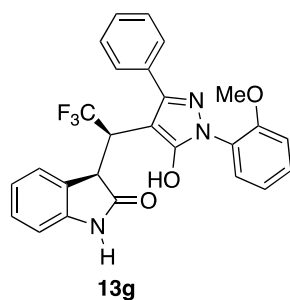
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3

Formula Calculator Results

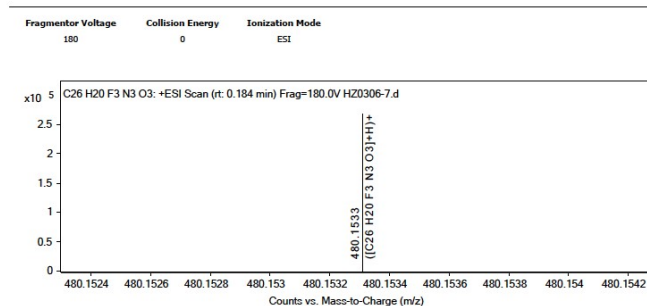
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C26 H21 F3 N3 O2	True	464.1584	464.158	-0.51	99.74

--- End Of Report ---

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-(2-methoxyphenyl)-3-phenyl-1*H*-pyrazol-4-yl)ethyl)indolin-2-one (13g)



Spectra



Formula Calculator Element Limits

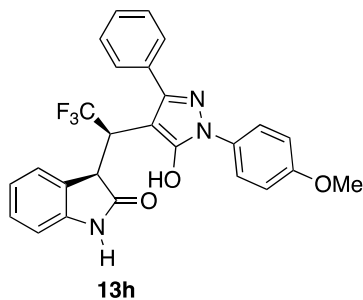
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3

Formula Calculator Results

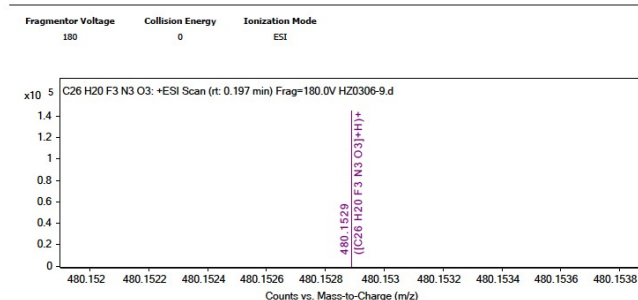
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C26 H21 F3 N3 O3	True	480.1533	480.153	-0.46	99.77

--- End Of Report ---

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-(4-methoxyphenyl)-3-phenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13h)



Spectra



Formula Calculator Element Limits

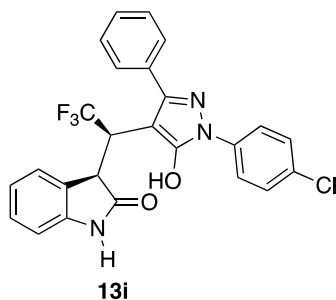
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3

Formula Calculator Results

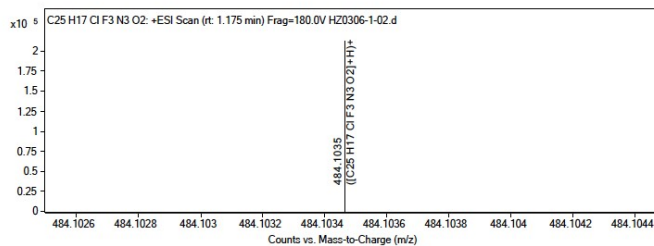
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C26 H21 F3 N3 O3	True	480.1529	480.153	0.19	99.96

-- End Of Report --

(R)-3-((R)-1-(1-(4-chlorophenyl)-5-hydroxy-3-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13i)



Fragmentor Voltage	Collision Energy	Ionization Mode
180	0	ESI



Formula Calculator Element Limits

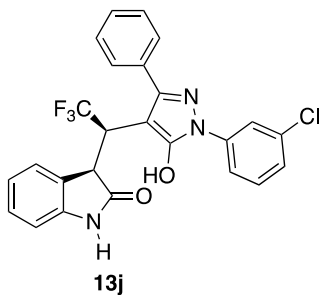
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3
Cl	0	1

Formula Calculator Results

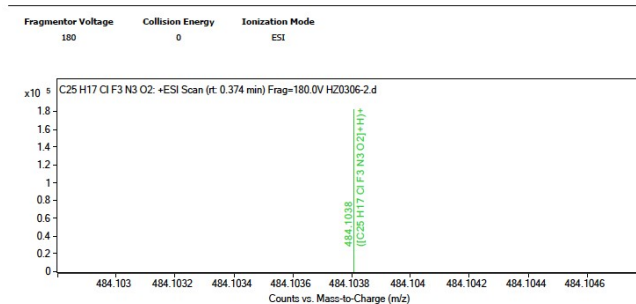
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C25 H18 Cl F3 N3 O2	True	484.1035	484.1034	0.42	99.81

-- End Of Report --

(R)-3-((R)-1-(1-(3-chlorophenyl)-5-hydroxy-3-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13j)



Spectra



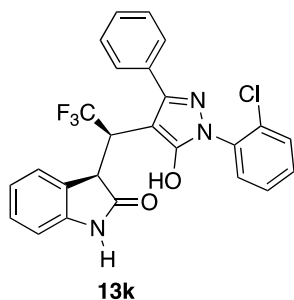
Formula Calculator Element Limits		
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3
Cl	0	1

Formula Calculator Results

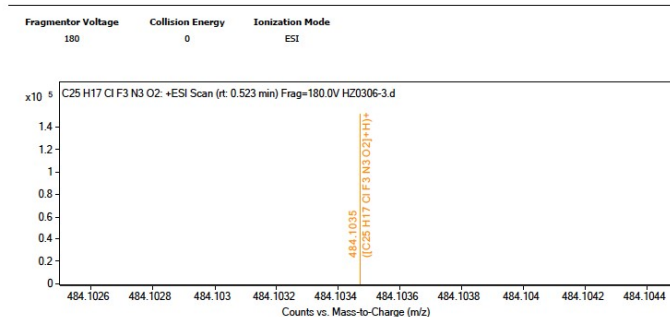
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C25 H18 Cl F3 N3 O2	True	484.1038	484.1034	-0.55	99.68

--- End Of Report ---

(R)-3-((R)-1-(1-(2-chlorophenyl)-5-hydroxy-3-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13k)



Spectra

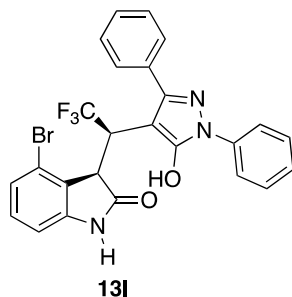


Formula Calculator Element Limits		
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3
Cl	0	1

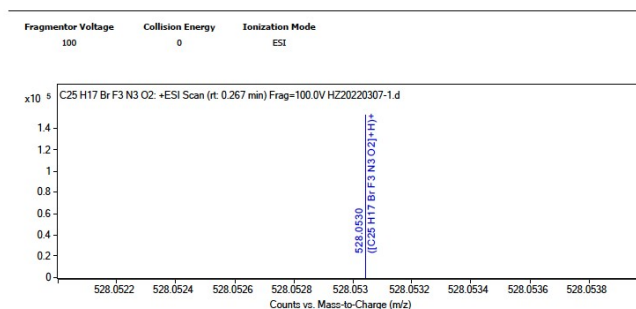
Formula Calculator Results

Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C25 H18 Cl F3 N3 O2	True	484.1035	484.1034	0.05	100

(R)-4-bromo-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13l)



Spectra



Formula Calculator Element Limits

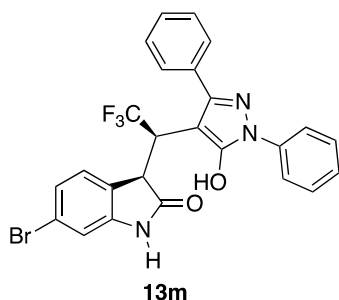
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	3	3
Br	1	1

Formula Calculator Results

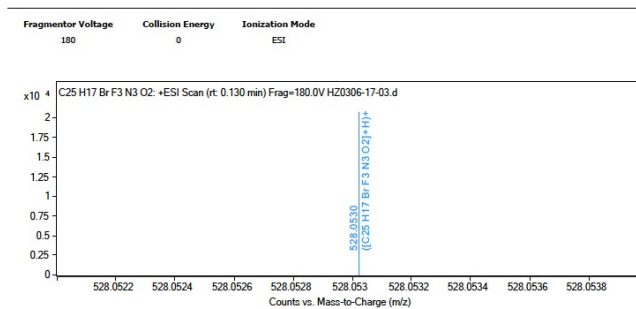
Formula	Best	Measured Mass	Tag Mass	Diff (ppm)	Score
C25 H17 Br F3 N3 O2	True	528.053	528.0529	-0.11	99.99

--- End Of Report ---

(R)-6-bromo-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13m)



Spectra



Formula Calculator Element Limits

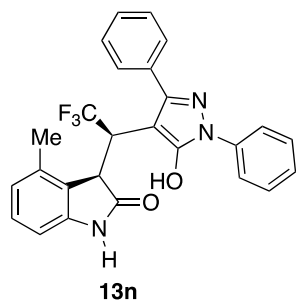
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3
Br	0	1

Formula Calculator Results

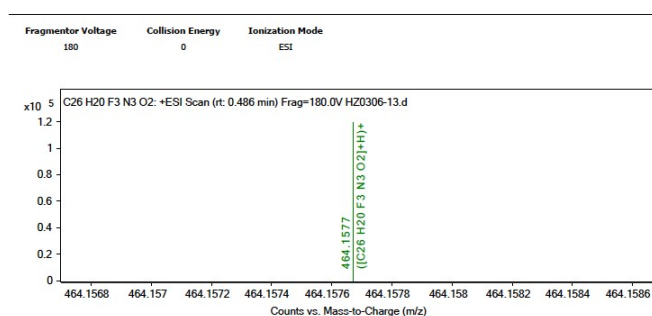
Formula	Best	Measured Mass	Tag Mass	Diff (ppm)	Score
C25 H17 Br F3 N3 O2	True	528.053	528.0529	0.56	99.65

--- End Of Report ---

(R)-4-methyl-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13n)



Spectra



Formula Calculator Element Limits

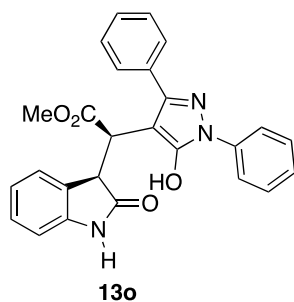
Element	Min	Max
C	0	50
H	0	100
O	0	50
N	0	10
F	0	3

Formula Calculator Results

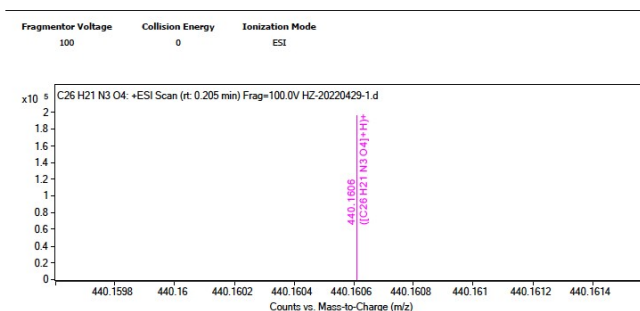
Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C26 H21 F3 N3 O2	True	464.1577	464.158	0.87	99.23

--- End Of Report ---

Methyl (R)-2-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)-2-((R)-2-oxindolin-3-yl)acetate (13o)



Spectra



Formula Calculator Element Limits

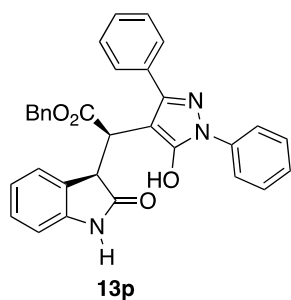
Element	Min	Max
C	0	100
H	0	150
O	0	10
N	0	5

Formula Calculator Results

Formula	Best	Measured Mass	Tgt Mass	Diff (ppm)	Score
C26 H22 N3 O4	True	440.1606	440.1605	-0.3	99.91

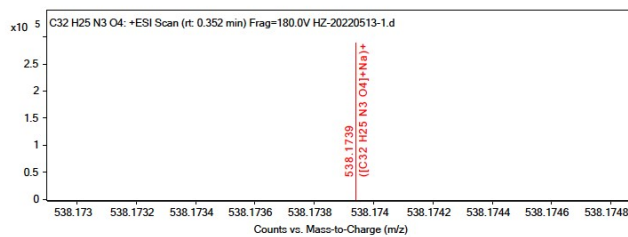
--- End Of Report ---

Benzyl (*R*)-2-(5-hydroxy-1,3-diphenyl-1*H*-pyrazol-4-yl)-2-((*R*)-2-oxoindolin-3-yl)acetate (13p)



Spectra

Fragmentor Voltage: 180
Collision Energy: 0
Ionization Mode: ESI



Formula Calculator Element Limits

Element	Min	Max
C	0	100
H	0	150
O	0	10
N	0	5

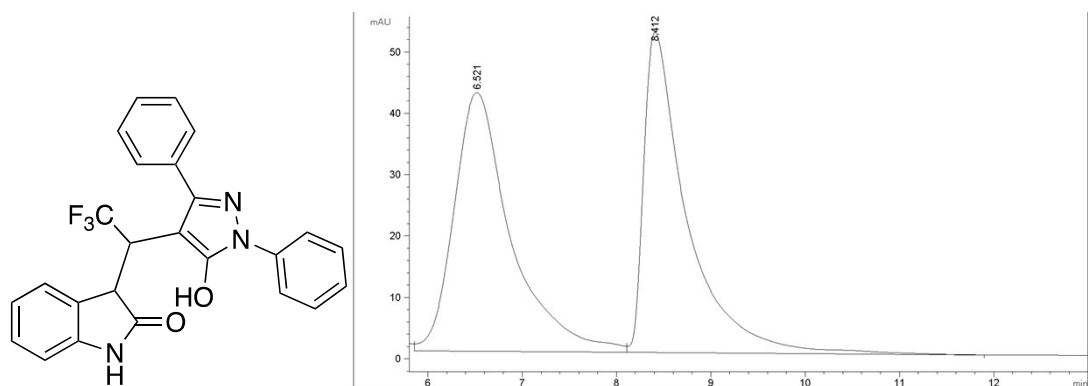
Formula Calculator Results

Formula	Best	Measured Mass	Igt Mass	Diff (ppm)	Score
C32 H25 N3 Na O4	True	538.1739	538.1737	-0.24	99.94

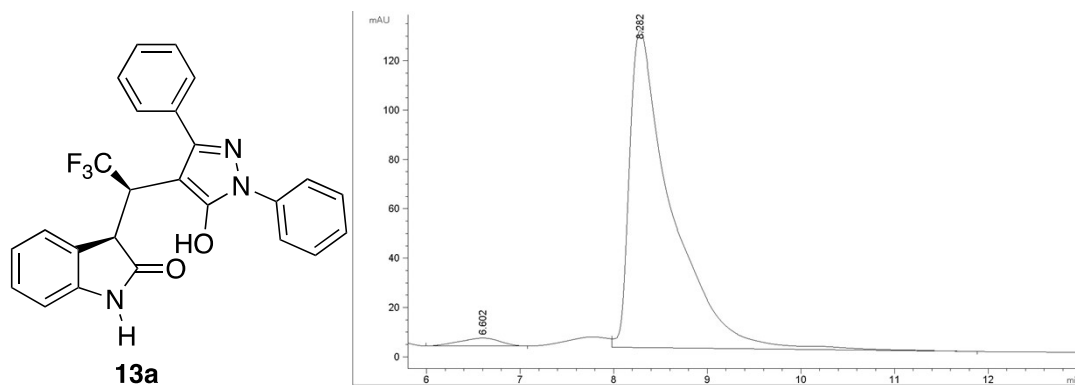
--- End Of Report ---

3 Copies of HPLC spectra

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13a)

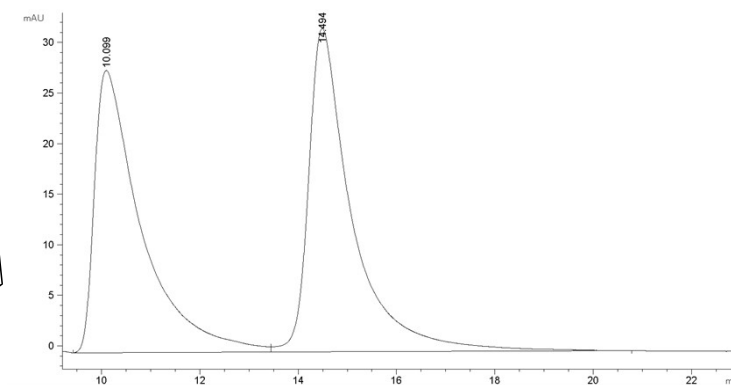
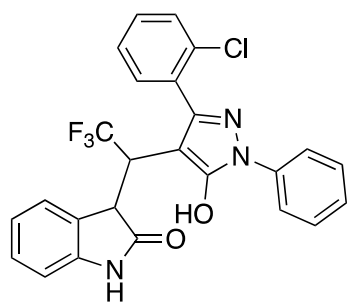


#	[min]		[min]	mAU	*s	[mAU]	%
1	6.521	VV	0.6124	1769.34705	42.12235	51.5210	
2	8.412	VB	0.4539	1664.87561	52.16689	48.4790	

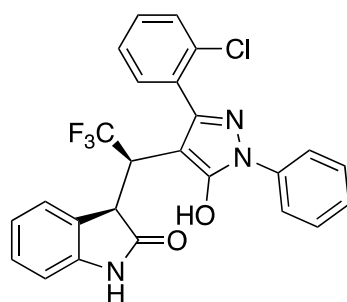


#	[min]		[min]	mAU	*s	[mAU]	%
1	6.602	BB	0.4521	95.53866	3.20929	2.3195	
2	8.282	VB	0.4350	4023.36890	128.54436	97.6805	

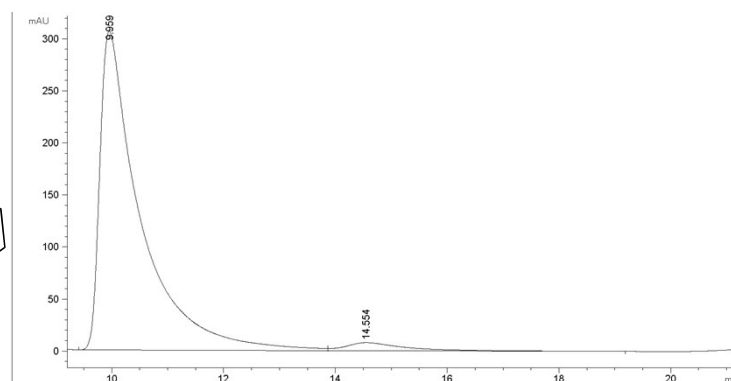
(*R*)-3-((*R*)-1-(3-(2-chlorophenyl)-5-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (**13b**)



#	[min]		[min]	mAU	*s	[mAU]	%
1	10.099	BV	0.9570	1842.83875		27.89900	48.3119
2	14.494	VB	0.8650	1971.62390		31.97630	51.6881

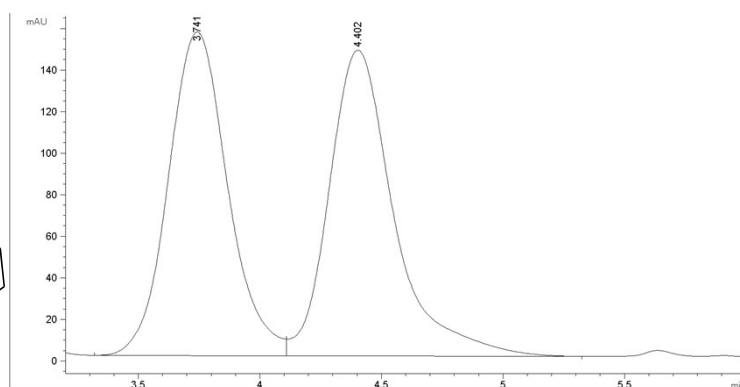
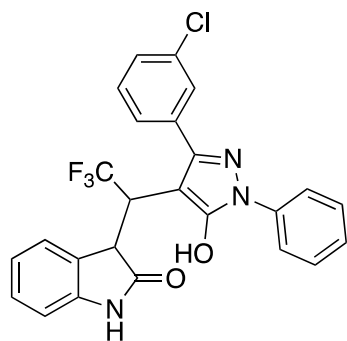


13b

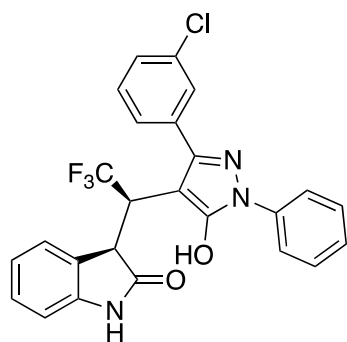


#	[min]		[min]	mAU	*s	[mAU]	%
1	9.959	BV	0.6946	1.54457e4		306.31384	96.3269
2	14.554	VB	1.0500	588.97430		7.79876	3.6731

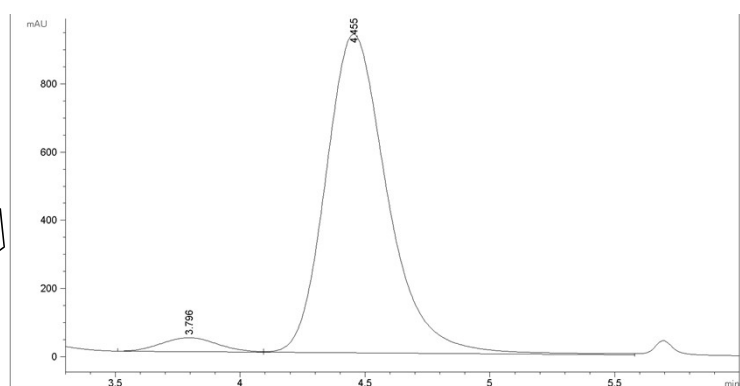
(R)-3-((R)-1-(3-(3-chlorophenyl)-5-hydroxy-1-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13c)



#	[min]		[min]	mAU	*s	[mAU]	%
1	3.741	BV	0.2633	2639.13940	155.66644	49.2635	
2	4.402	VB	0.2810	2718.05298	147.13158	50.7365	

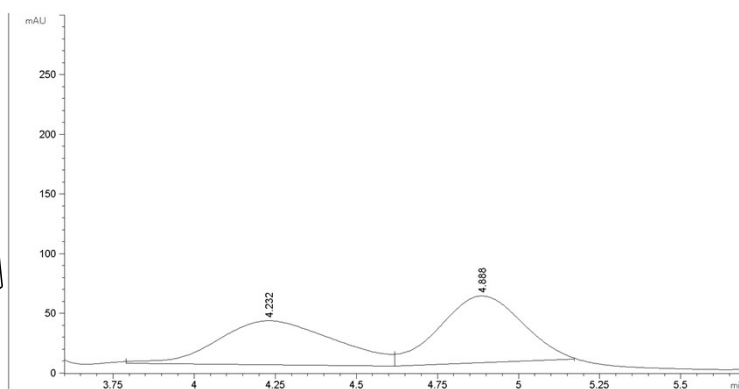
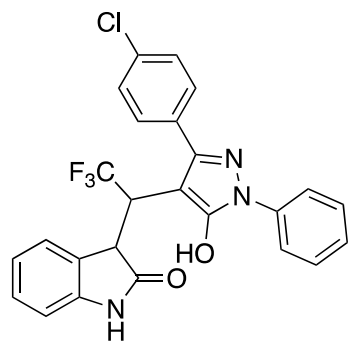


13c

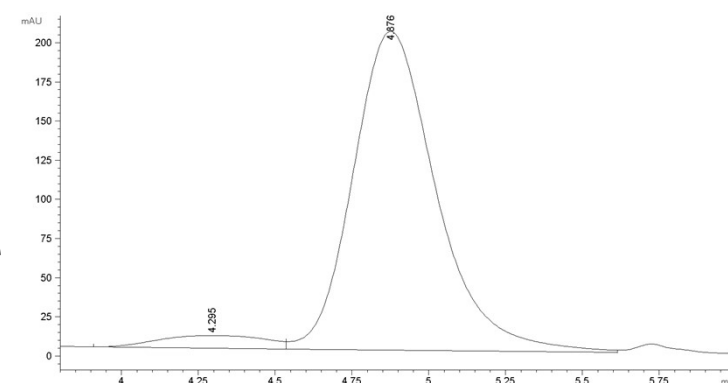
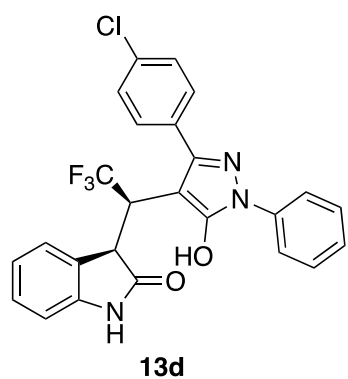


#	[min]		[min]	mAU	*s	[mAU]	%
1	3.796	BV	0.2479	632.25885	40.77148	3.7987	
2	4.455	VV	0.2640	1.60117e4	934.18903	96.2013	

(R)-3-((R)-1-(3-(4-chlorophenyl)-5-hydroxy-1-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13d)

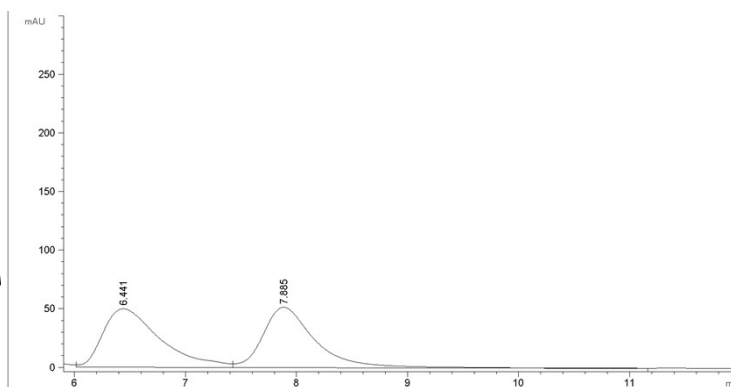
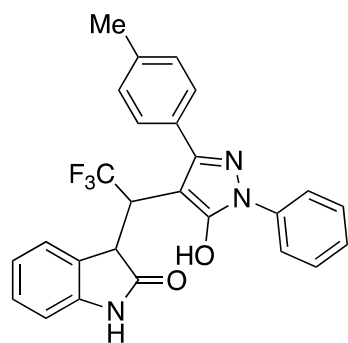


#	[min]		[min]	mAU	*s	[mAU]	%
1	4.232	MM	0.4204	931.25403	36.91518	48.3801	
2	4.888	MM	0.2959	993.61511	55.97254	51.6199	

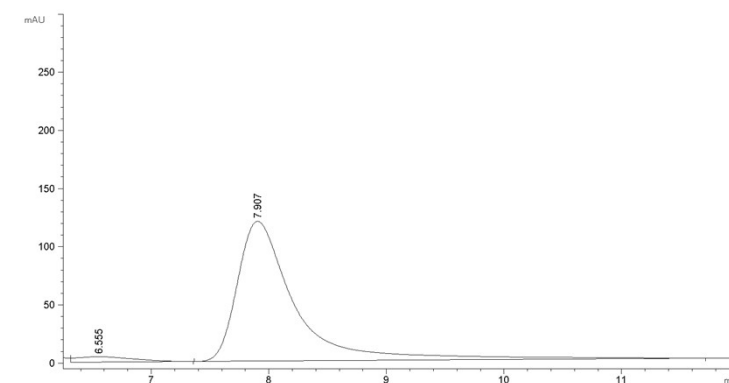
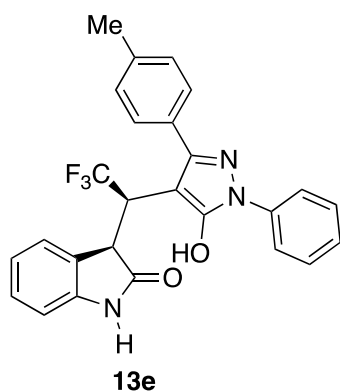


#	[min]		[min]	mAU	*s	[mAU]	%
1	4.295	BV	0.3997	194.55821	7.93374	4.8360	
2	4.876	VV	0.2895	3828.57129	203.42377	95.1640	

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-phenyl-3-(p-tolyl)-1H-pyrazol-4-yl)ethyl)indolin-2-one (13e)

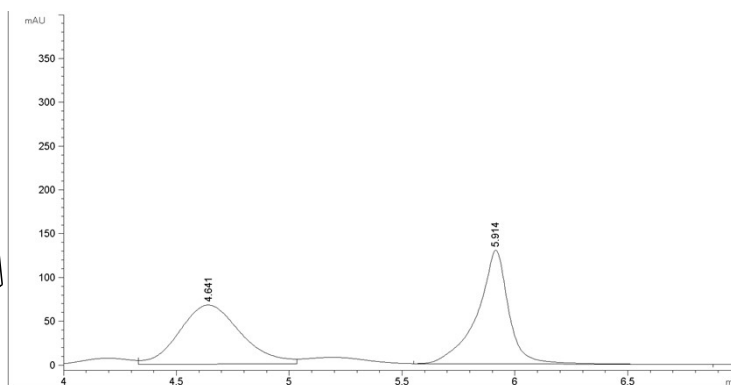
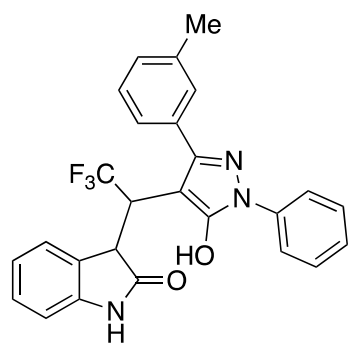


#	[min]		[min]	mAU	*s	[mAU]	%
1	6.441	VV	0.5422	1787.05835	49.99774	51.5116	
2	7.885	VB	0.4799	1682.17859	51.52204	48.4884	

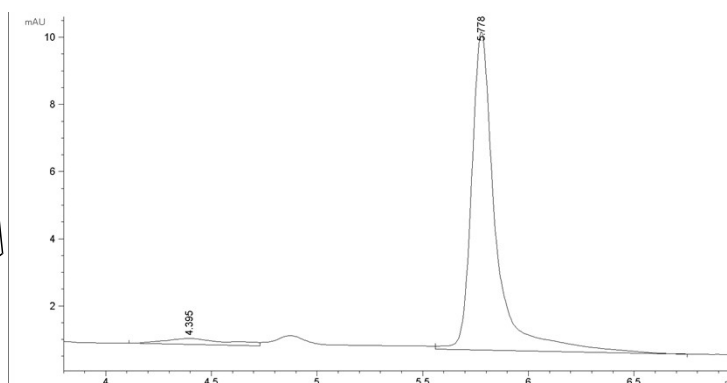
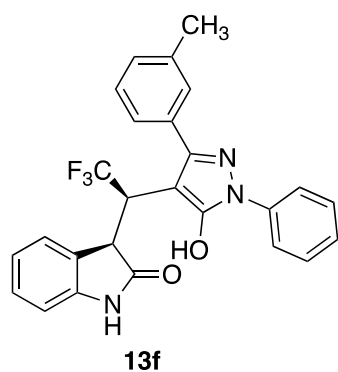


#	[min]		[min]	mAU	*s	[mAU]	%
1	6.555	VB	0.4809	155.30009	4.63789	3.6008	
2	7.907	BB	0.5053	4157.59180	120.23469	96.3992	

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-phenyl-3-(*m*-tolyl)-1*H*-pyrazol-4-yl)ethyl)indolin-2-one (13f)

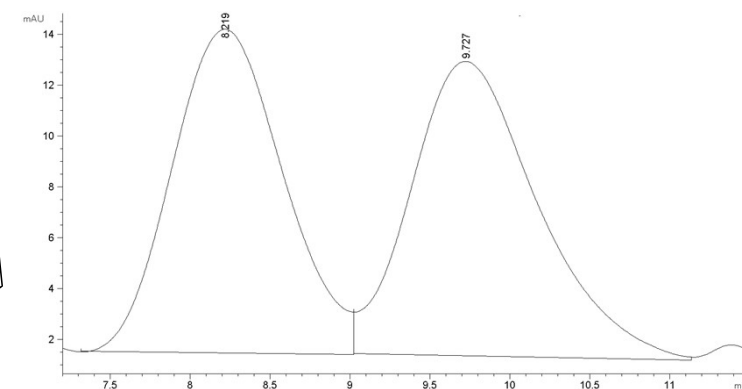
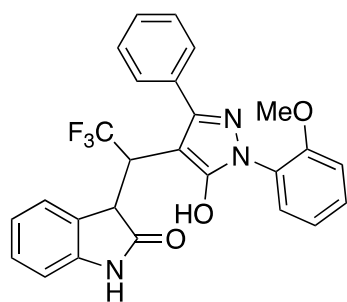


#	[min]		[min]	mAU	*s	[mAU]	%
1	4.641	VV	0.2948	1285.96606		67.56731	50.6817
2	5.914	BB	0.1387	1251.37170		129.80740	49.3183

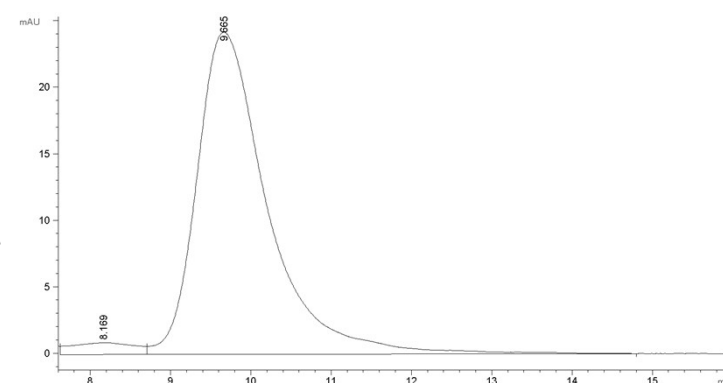
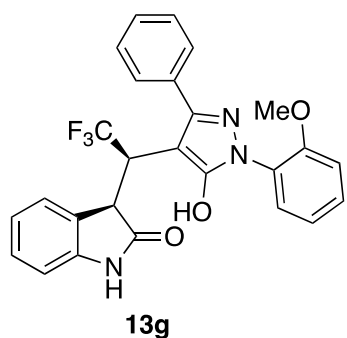


#	[min]		[min]	mAU	*s	[mAU]	%
1	4.395	BV	0.2749	3.78966		1.77762e-1	4.7981
2	5.778	VB	0.1173	75.19232		9.47867	95.2019

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-(2-methoxyphenyl)-3-phenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13g)

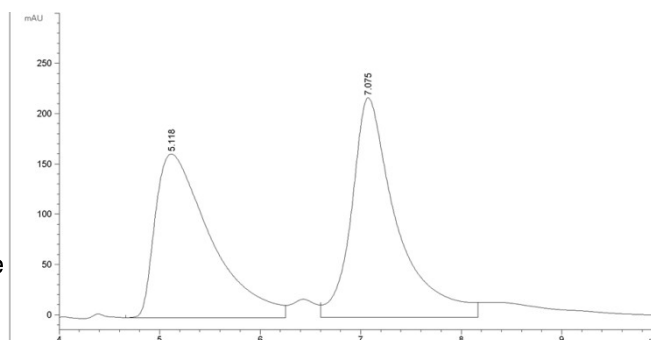
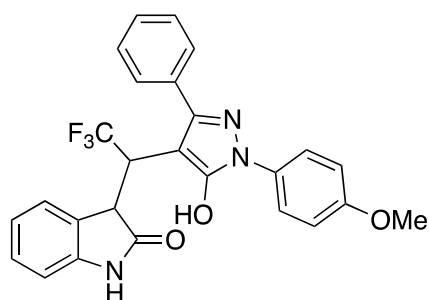


#	[min]	[min]	mAU	*s	[mAU]	%
1	8.219 MM	0.8033	614.25244	12.74394	49.0322	
2	9.727 MM	0.9188	638.50165	11.58276	50.9678	

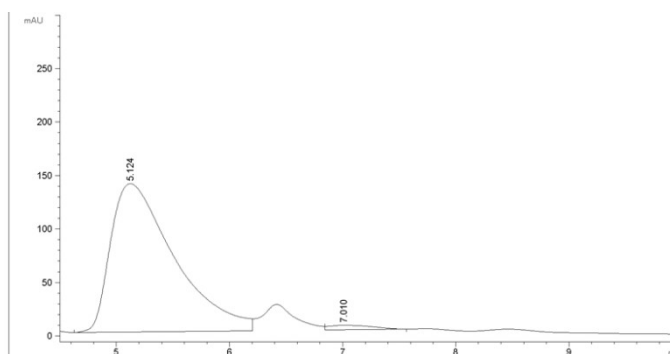
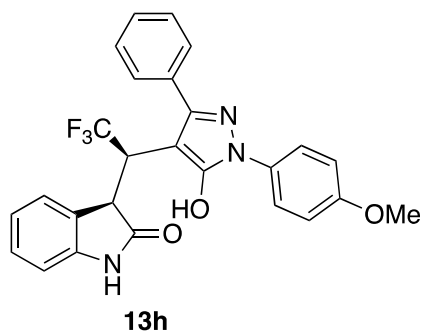


#	[min]	[min]	mAU	*s	[mAU]	%
1	8.169 VV	0.6559	48.38693	8.76238e-1	3.1562	
2	9.665 VB	0.9134	1484.71106	24.21462	96.8438	

(R)-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1-(4-methoxyphenyl)-3-phenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13h)

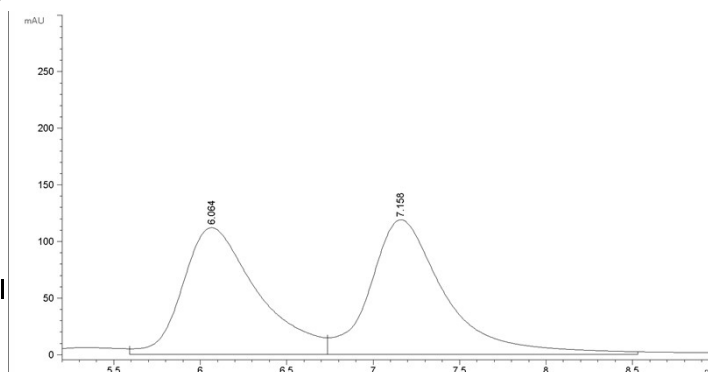
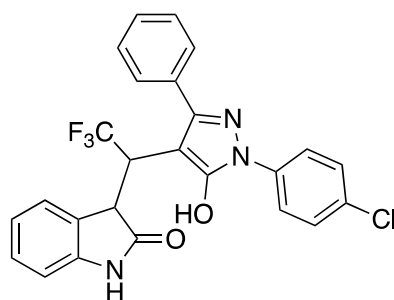


#	[min]		[min]	mAU	*s	[mAU]	%
1	5.118	BV	0.5911	6213.99121		162.72942	47.7116
2	7.075	VV	0.4396	6810.06982		218.36449	52.2884

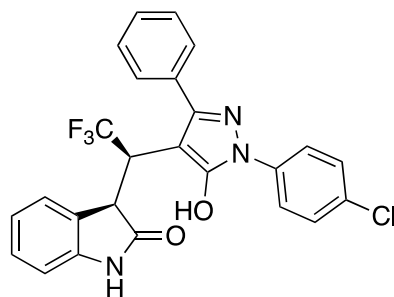


#	[min]		[min]	mAU	*s	[mAU]	%
1	5.124	BV	0.5853	5435.19189		138.71611	98.0074
2	7.010	VB	0.4295	110.50494		4.19622	1.9926

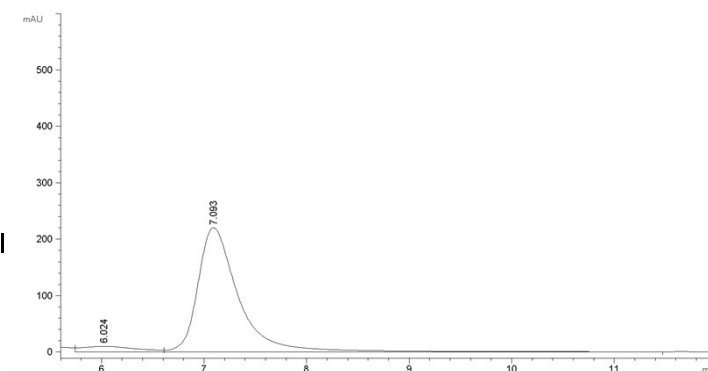
(R)-3-((R)-1-(1-(4-chlorophenyl)-5-hydroxy-3-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (13i)



#	[min]		[min]	mAU	*s	[mAU]	%
1	6.064	VV	0.4471	3365.99268	111.87138	48.4691	
2	7.158	MF	0.5018	3578.62402	118.85399	51.5309	

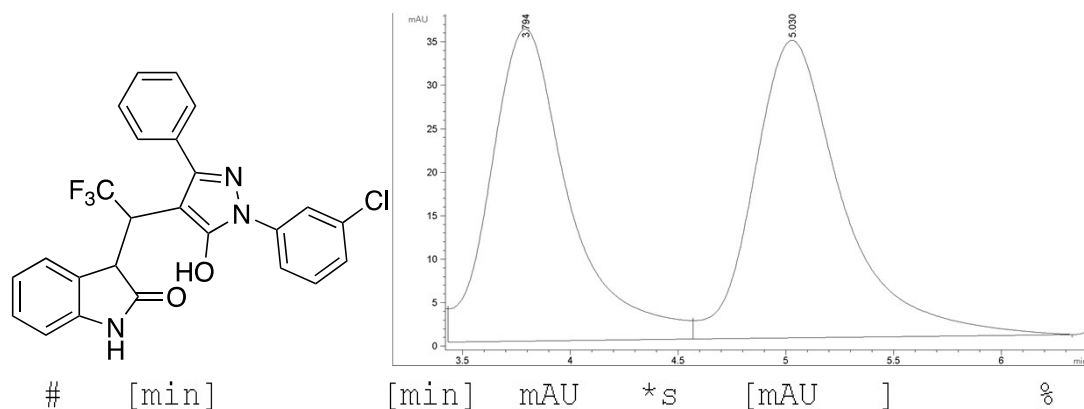


13i

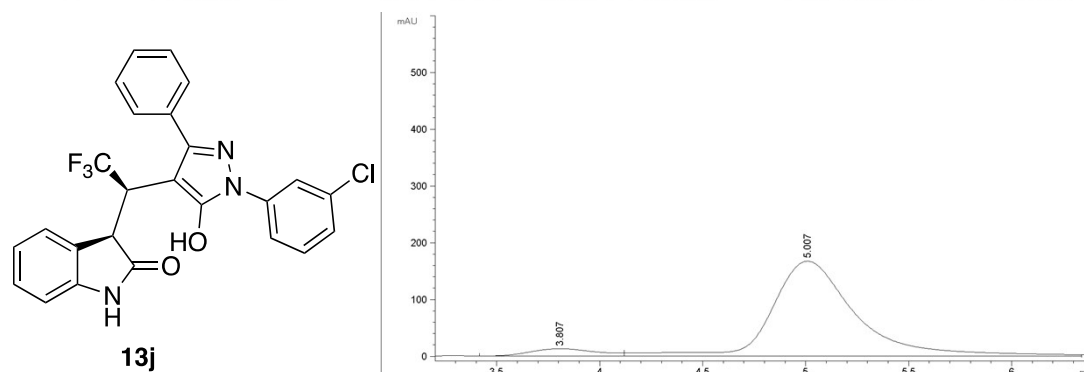


#	[min]		[min]	mAU	*s	[mAU]	%
1	6.024	VV	0.5247	364.63638	9.99376	5.6476	
2	7.093	VB	0.4104	6091.85791	220.03296	94.3524	

(*R*)-3-((*R*)-1-(1-(3-chlorophenyl)-5-hydroxy-3-phenyl-1*H*-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (**13j**)

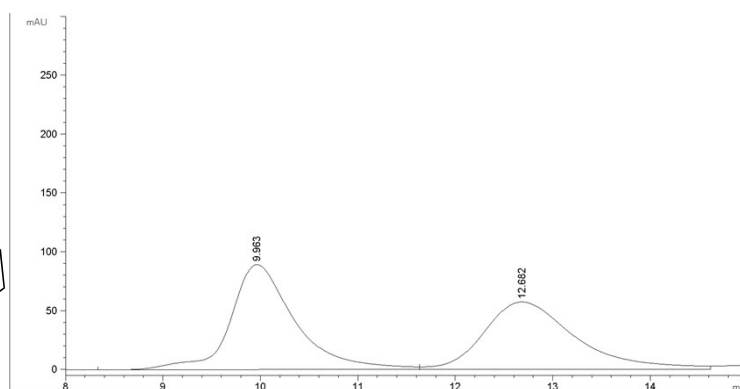
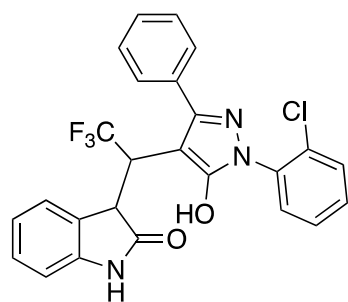


#	[min]	[min]	mAU	*s	[mAU]	%
1	3.794	VV	0.3810	912.50159	35.89902	48.0653
2	5.030	VB	0.4321	985.96039	34.23189	51.9347

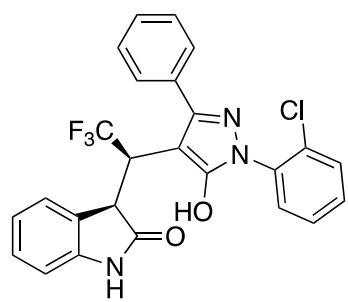


#	[min]	[min]	mAU	*s	[mAU]	%
1	3.807	BV	0.3353	280.82233	12.76337	5.6598
2	5.007	VV	0.4176	4680.89990	166.84137	94.3402

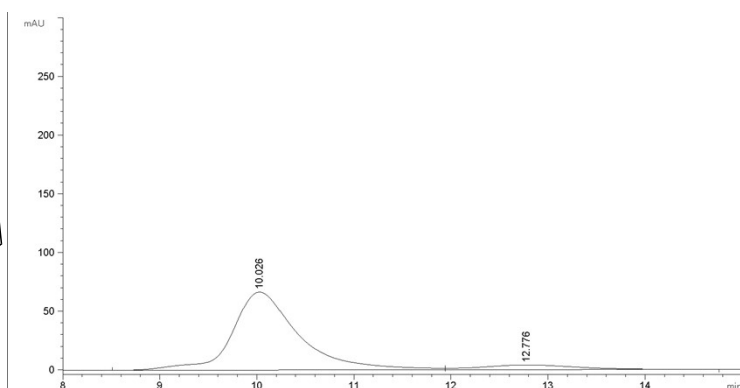
(R)-3-((R)-1-(1-(2-chlorophenyl)-5-hydroxy-3-phenyl-1H-pyrazol-4-yl)-2,2,2-trifluoroethyl)indolin-2-one (10k)



#	[min]		[min]	mAU	*s	[mAU]	%
1	9.963	BV	0.6788	4125.13037	89.27793	52.4944	
2	12.682	VV	0.9818	3733.10474	57.26619	47.5056	

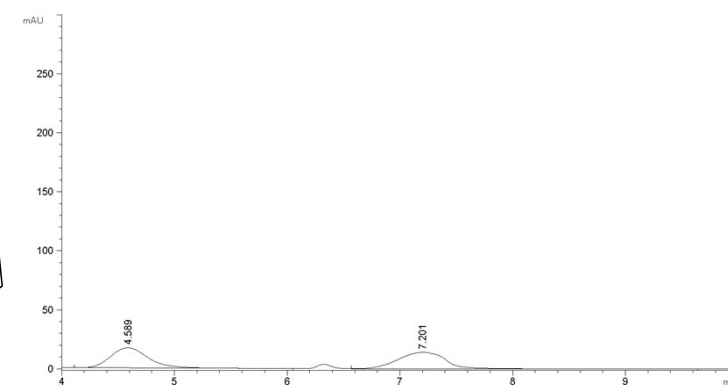
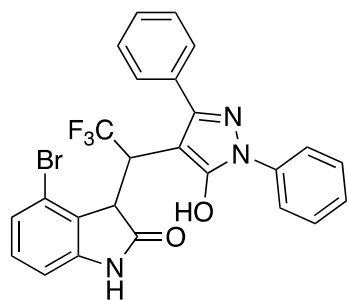


13k

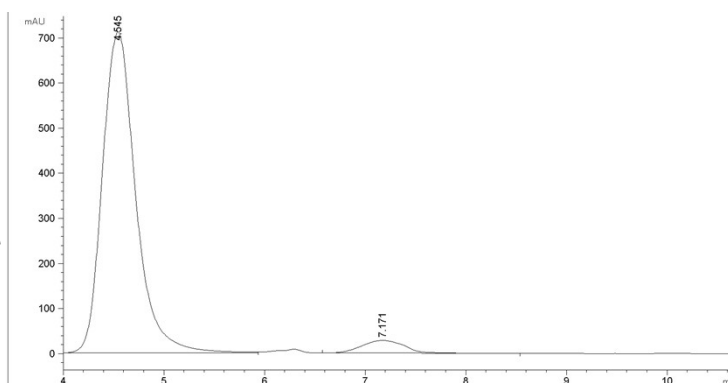
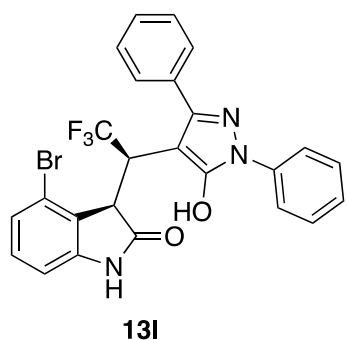


#	[min]		[min]	mAU	*s	[mAU]	%
1	10.026	BV	0.6996	3171.24829	66.42992	91.7772	
2	12.776	VB	1.0644	284.12689	4.07219	8.2228	

(R)-4-bromo-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13I)

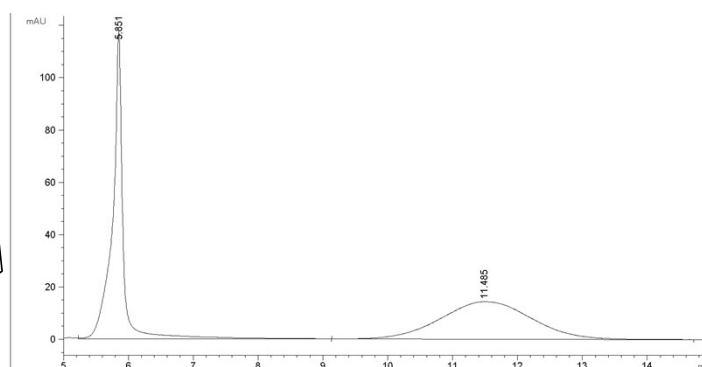
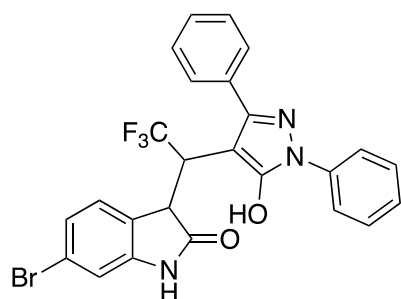


#	[min]		[min]	mAU	*s	[mAU]	%
1	4.589	BB	0.3633	404.10199	17.08638	49.6677	
2	7.201	VB	0.4680	409.50961	13.93612	50.3323	

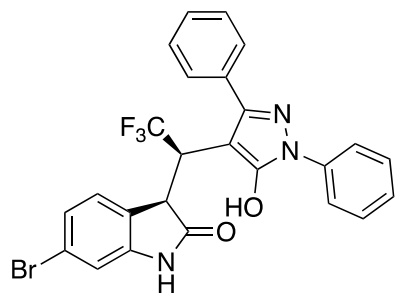


#	[min]		[min]	mAU	*s	[mAU]	%
1	4.545	BV	0.3572	1.63941e4	712.64734	95.1277	
2	7.171	BB	0.4820	839.67566	28.26545	4.8723	

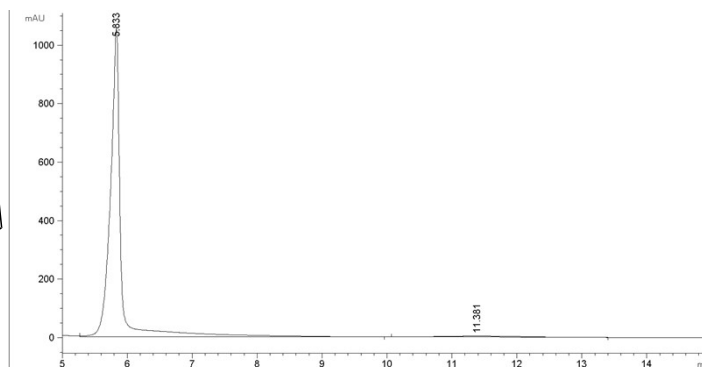
(R)-6-bromo-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13m)



#	[min]	[min]	mAU	*s	[mAU]	%
1	5.851	VB	0.1485	1322.33154	117.71284	48.6907
2	11.485	BB	1.3716	1393.44824	14.27794	51.3093

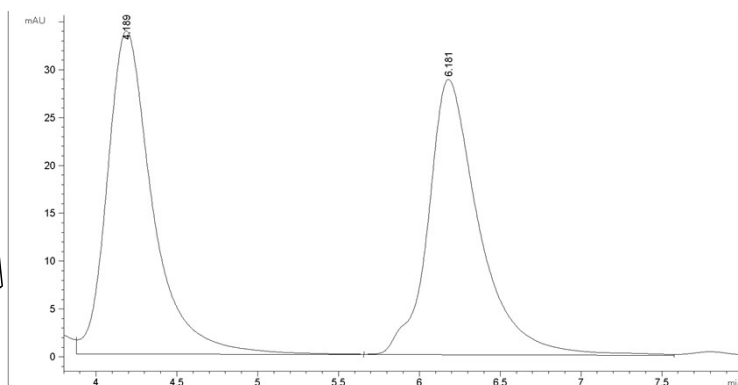
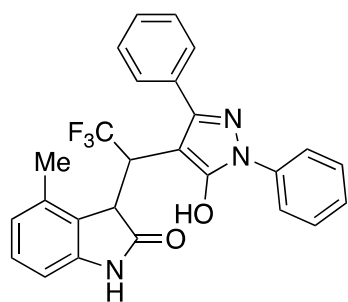


13m

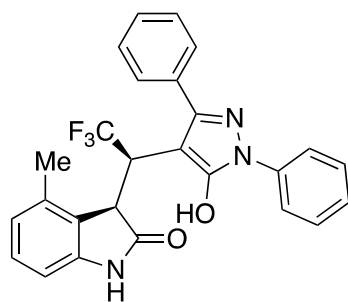


#	[min]	[min]	mAU	*s	[mAU]	%
1	5.833	VB	0.1512	1.18392e4	1055.59583	97.4132
2	11.381	BB	1.0417	314.39594	3.64340	2.5868

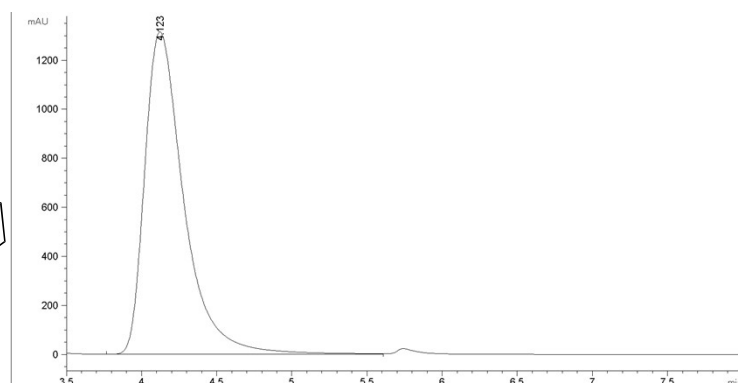
(R)-4-methyl-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13n)



#	[min]		[min]	mAU	*s	[mAU]	%
1	4.189	VB	0.2913	656.98907	33.73678	51.0095	
2	6.181	BV	0.3232	630.98529	28.73274	48.9905	

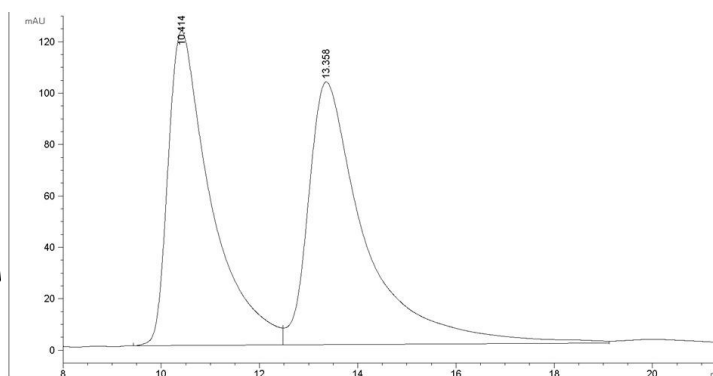
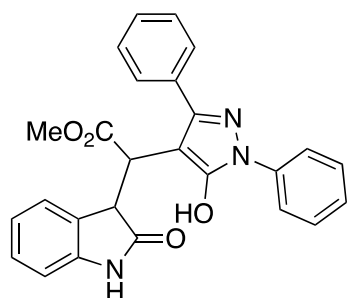


13n

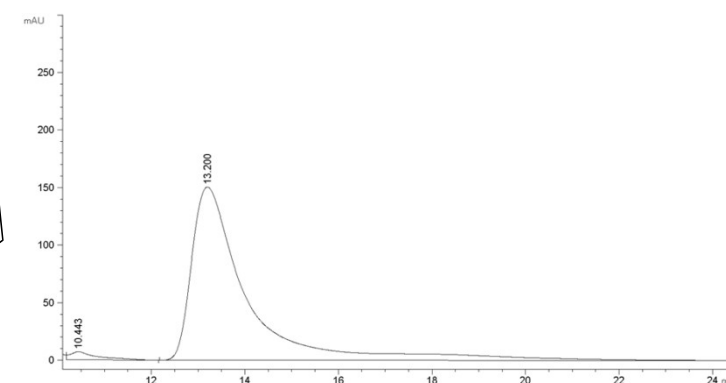
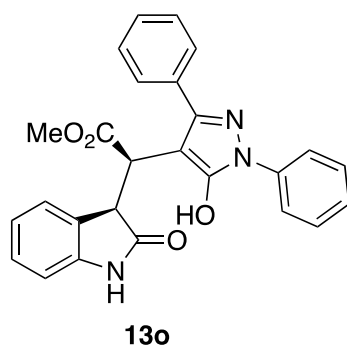


#	[min]		[min]	mAU	*s	[mAU]	%
1	4.123	BV	0.2760	2.38877e4	1314.96423	100.0000	

(*R*)-4-methyl-3-((*R*)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1*H*-pyrazol-4-yl)ethyl)indolin-2-one (**13o**)

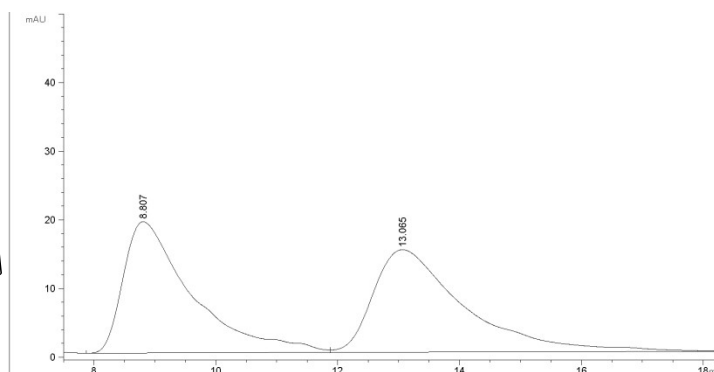
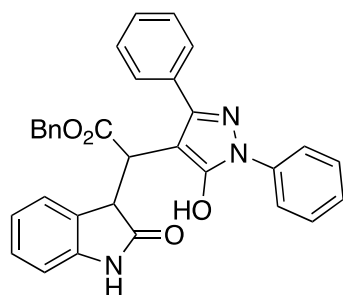


#	[min]	[min]	mAU	*s	[mAU]	%
1	10.414 BV	0.8656	7423.72754	122.27828	47.4450	
2	13.358 VV	1.1541	8223.28613	102.21088	52.5550	

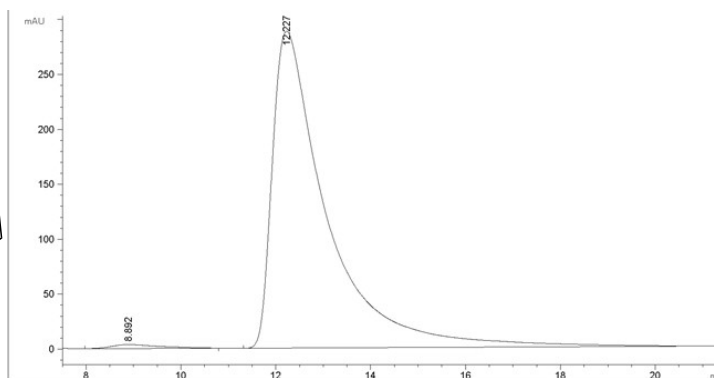
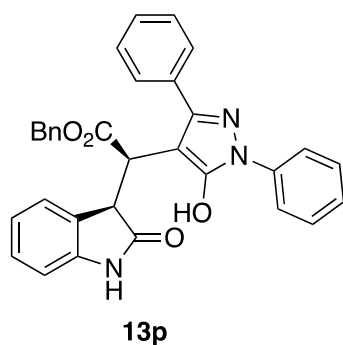


#	[min]	[min]	mAU	*s	[mAU]	%
1	10.443 VB	0.5463	292.71744	7.12405	2.2981	
2	13.200 BBA	1.1825	1.24448e4	150.59853	97.7019	

(R)-4-methyl-3-((R)-2,2,2-trifluoro-1-(5-hydroxy-1,3-diphenyl-1H-pyrazol-4-yl)ethyl)indolin-2-one (13p)

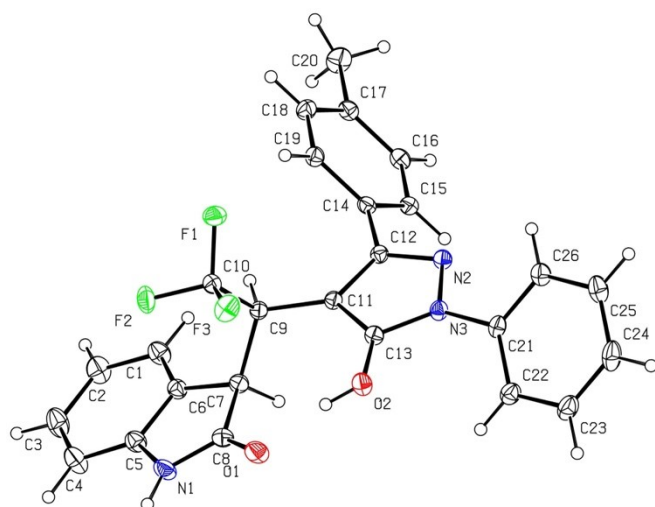


#	[min]		[min]	mAU	*s	[mAU]	%
1	8.807	BV	1.1321	1488.20984		19.12426	49.1189
2	13.065	VBA	1.5108	1541.59973		14.92546	50.8811



#	[min]		[min]	mAU	*s	[mAU]	%
1	8.882	BV	1.0126	258.28604		3.55922	1.1024
2	12.227	BBA	1.1355	2.31704e4		288.34030	98.8976

4 X-ray data for compound 13e



Data block: mo_220425_hz_1_0m

Bond precision: C-C = 0.0031 Å

Wavelength=1.54178

Cell: a=11.5944(5)

b=7.9944(4)

c=11.8474(5)

alpha=90

beta=101.879(2)

gamma=90

Temperature:

170 K

	Calculated	Reported
Volume Space	1074.62(8)	1074.62(8)
group Hall	P 21	P 1 21 1
group	P 2yb	P 2yb
Moiety formula	C26 H20 F3 N3 O2	C26 H20 F3 N3 O2
Sum formula	C26 H20 F3 N3 O2	C26 H20 F3 N3 O2
Mr	463.45	463.45
Dx,g cm-3	1.432	1.432
Z	2	2
Mu (mm-1)	0.925	0.925
F000	480.0	480.0
F000'	481.68	
h,k,lmax	13,9,14	13,9,14
Nref	3940[2122]	3929
Tmin,Tmax	0.957,0.973	0.661,0.753
Tmin'	0.744	

Correction method= # Reported T Limits: Tmin=0.661 Tmax=0.753

AbsCorr = MULTI-SCAN

Data completeness= 1.85/1.00

Theta(max)= 68.525

R(reflections)= 0.0307(3728)

wR2(reflections)= 0.0734(3929)

S = 1.067

Npar= 309