

Supporting Information

Molecular Hybrids of Pyrazolo[3,4-*b*]pyridine and Triazole: Design, Synthesis and In Vitro Antibacterial Studies

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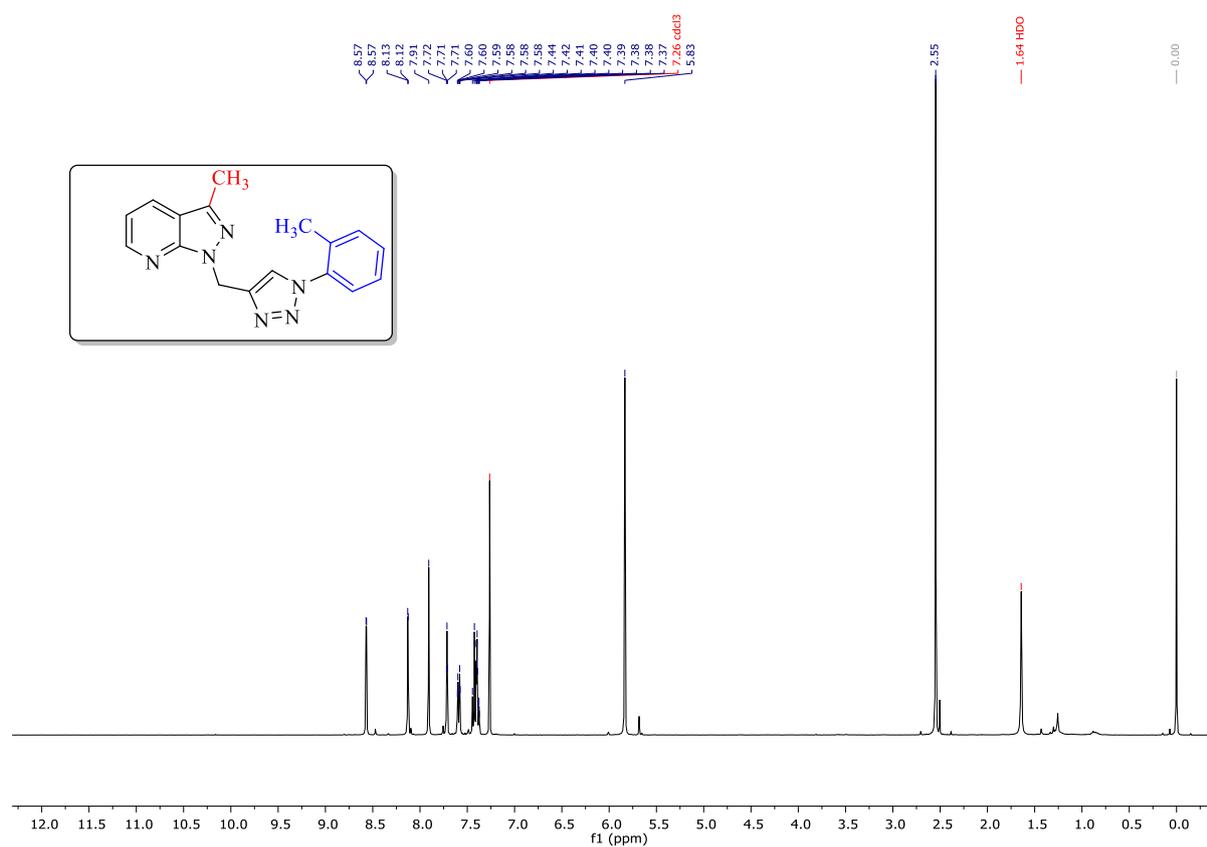
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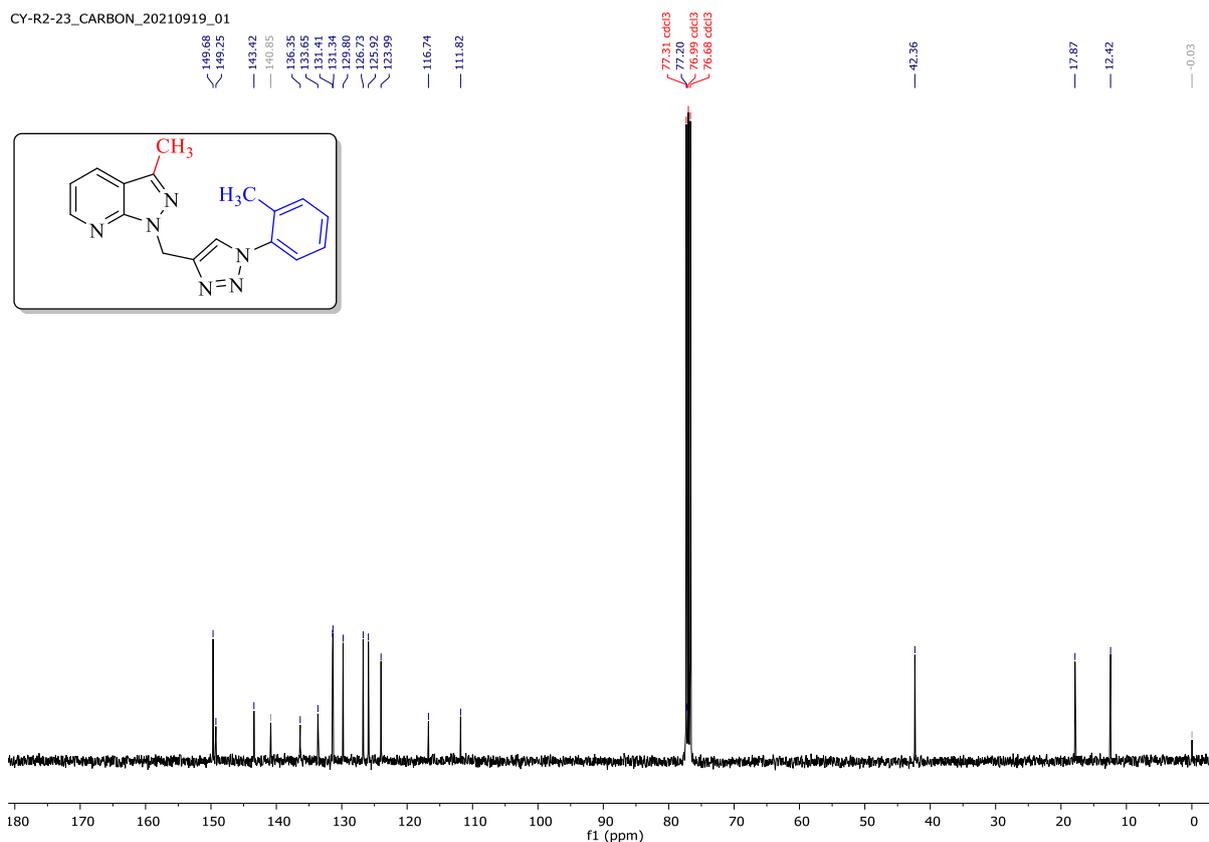
Spectra:

¹H NMR spectrum of 3-Methyl-1-((1-(*o*-tolyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine (14)

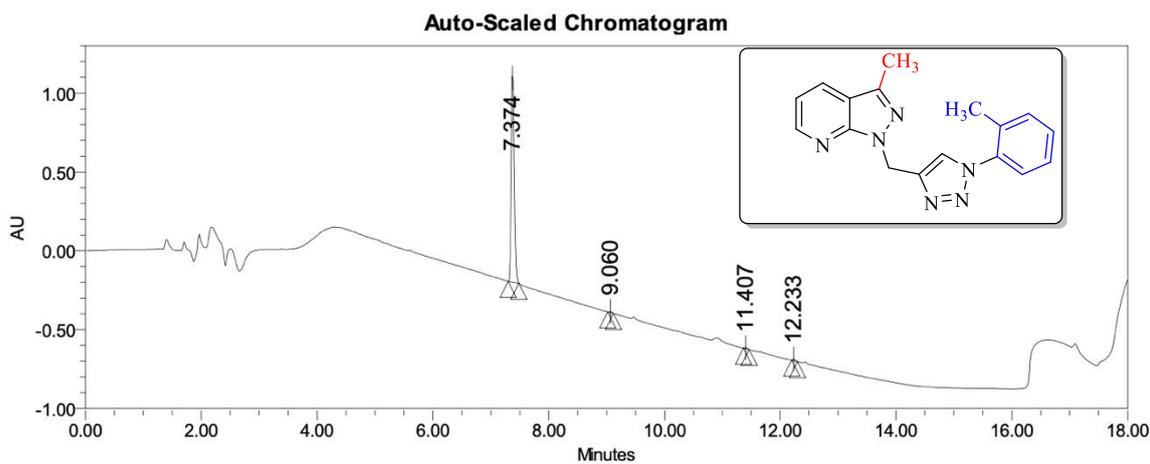


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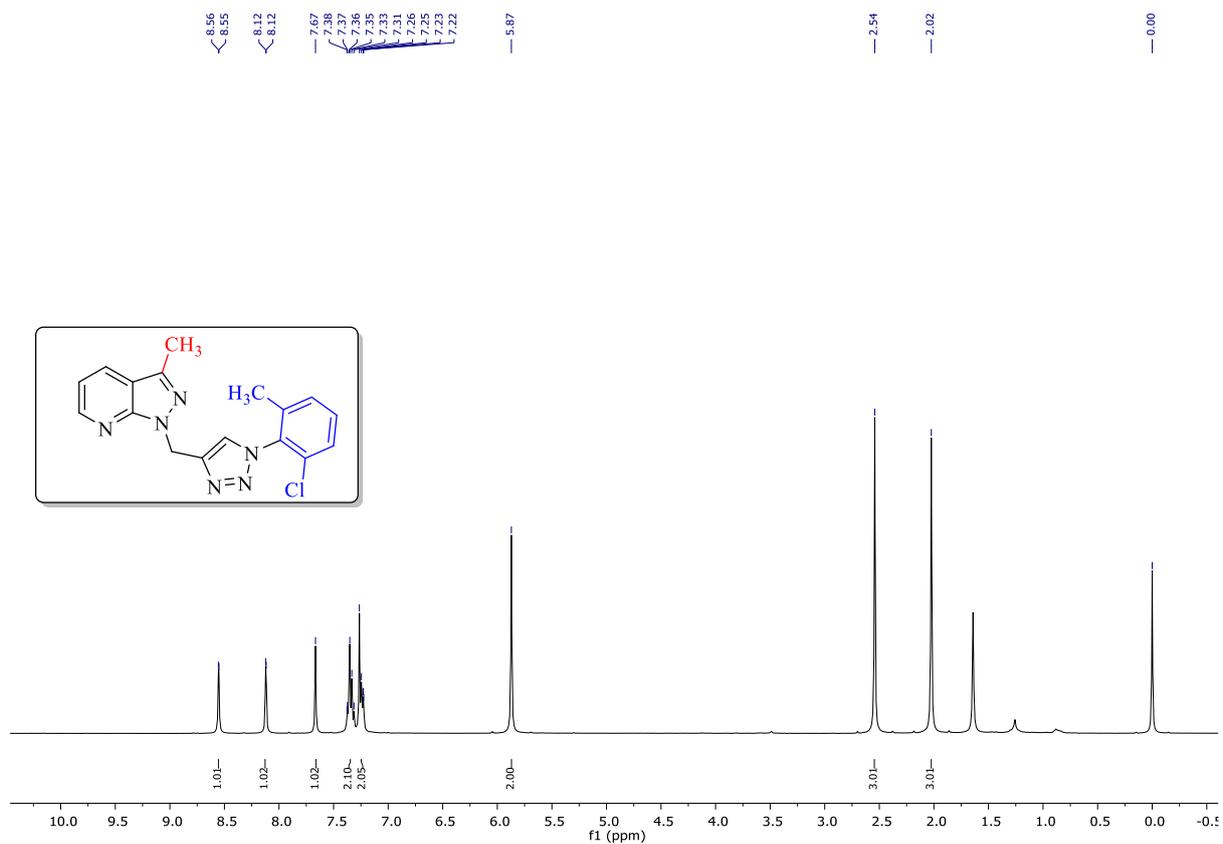
HPLC chromatogram of 3-Methyl-1-((1-(*o*-tolyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-*b*]pyridine (14)



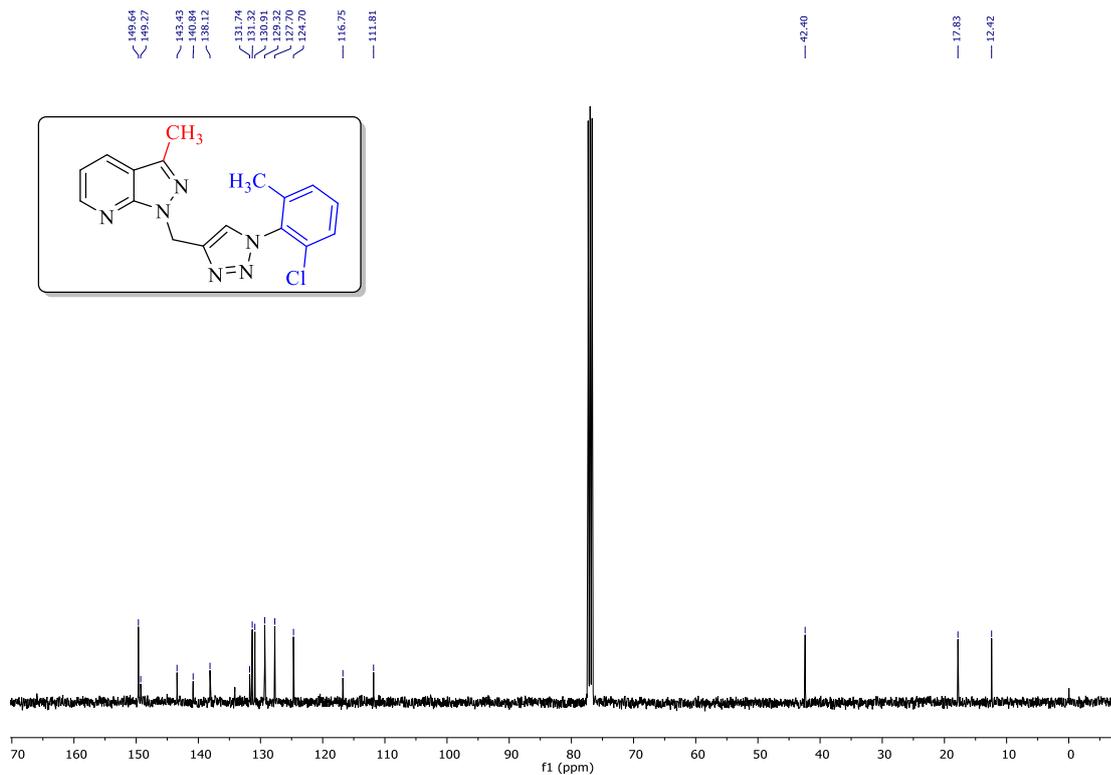
Peak Results

Name	RT	Area	% Area
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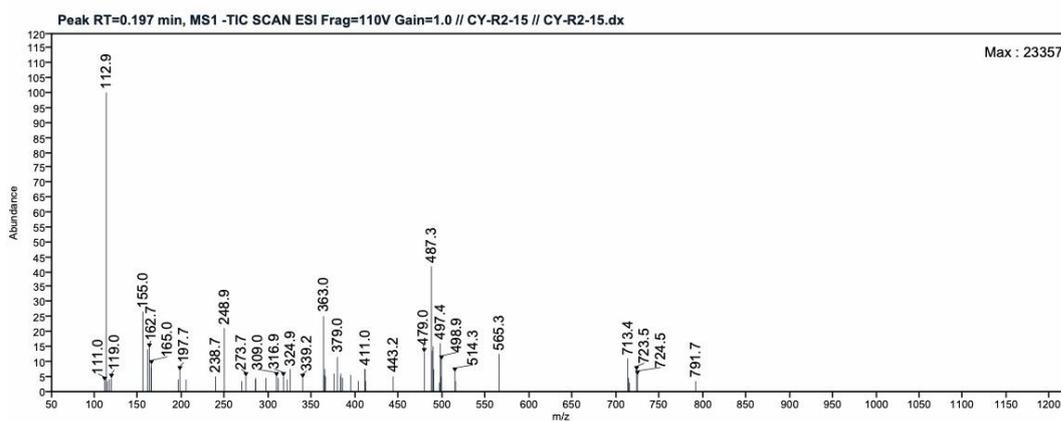
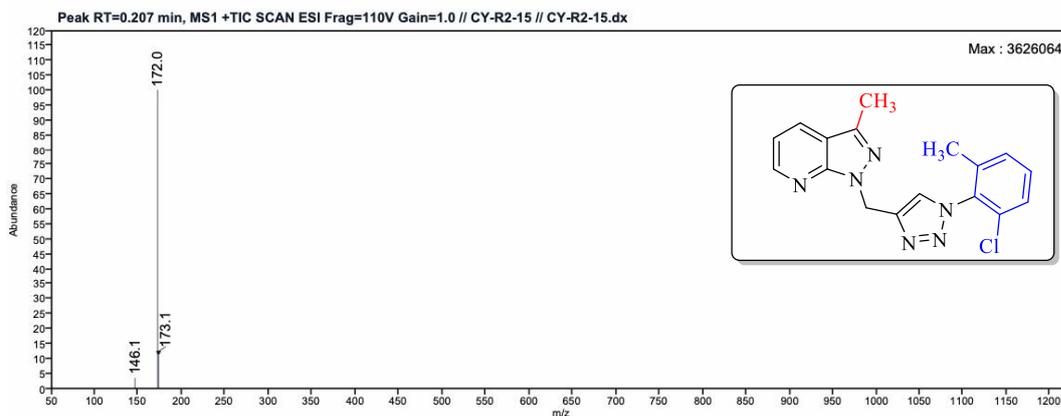
¹H NMR spectrum of 1-((1-(2-Chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-*b*]pyridine (15)



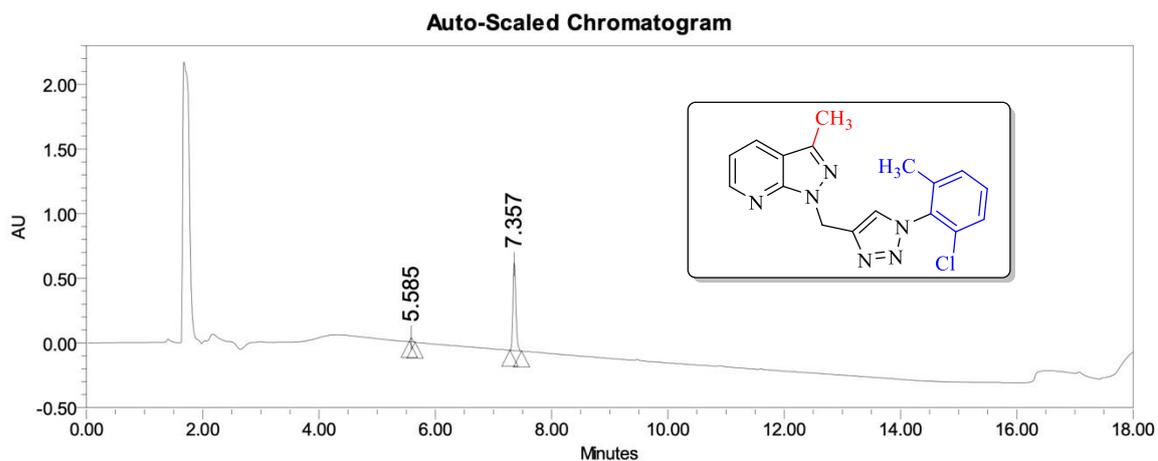
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Mass spectrum of 1-((1-(2-Chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (15)



HPLC chromatogram of 1-((1-(2-Chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (15)

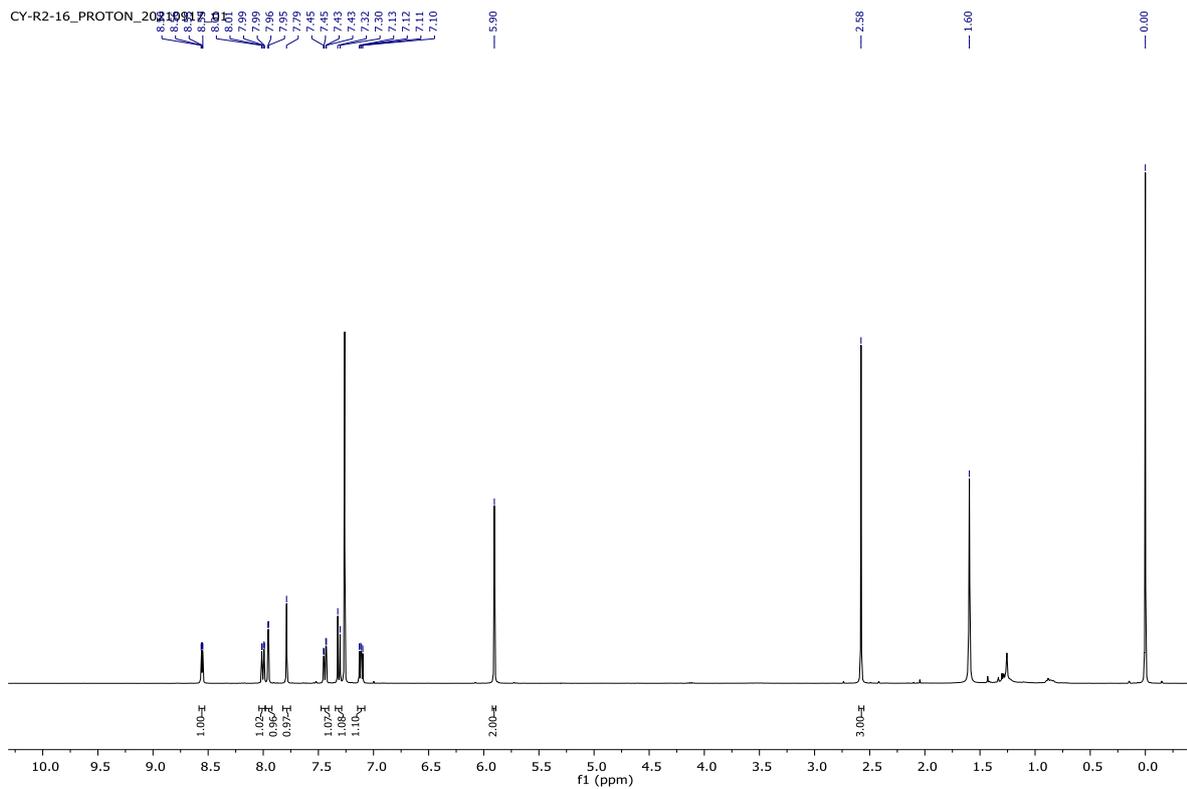


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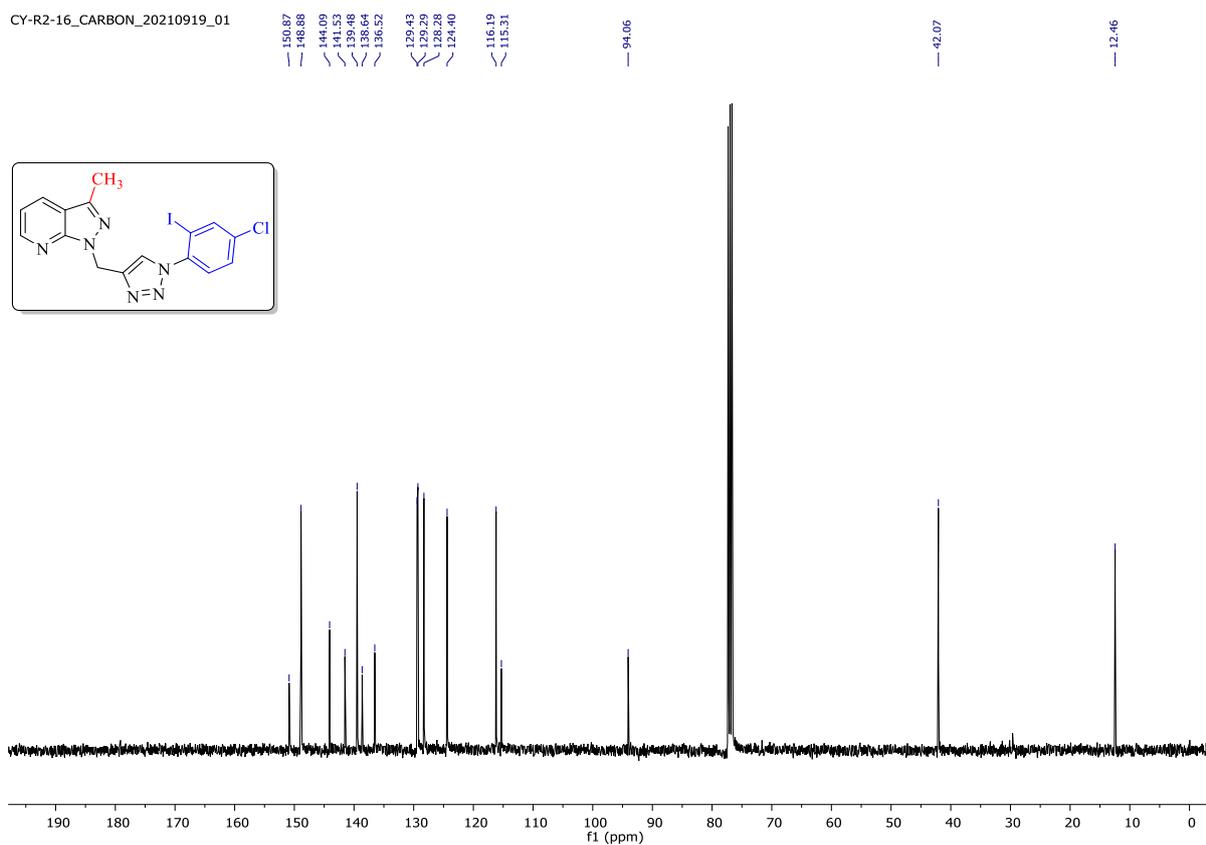
Name	RT	Area	% Area
1	5.585	82860	3.37
2	7.357	2373545	96.63

¹H NMR spectrum of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (16)

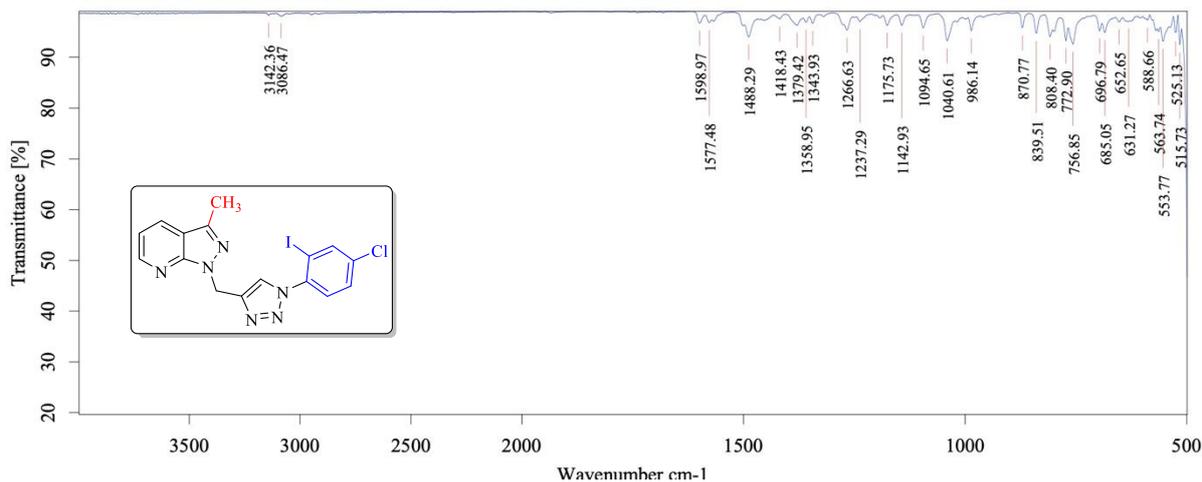




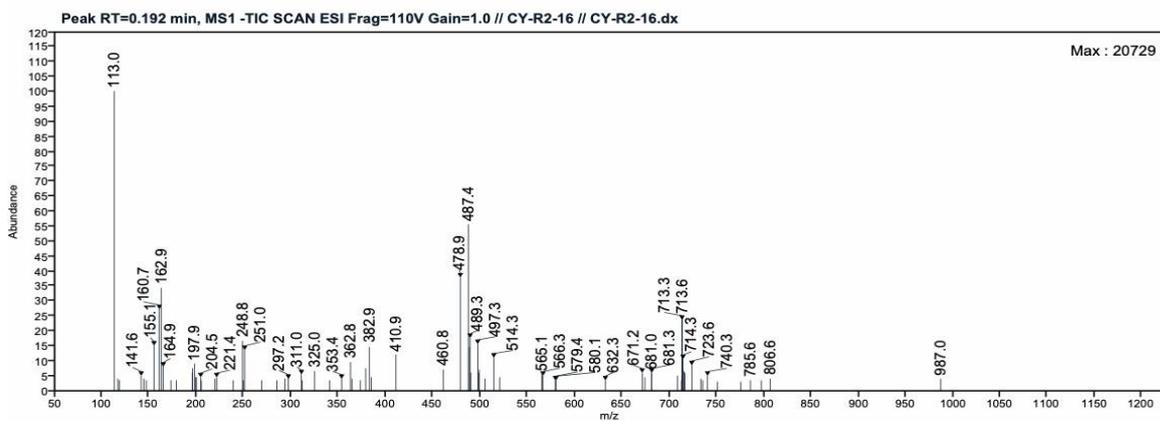
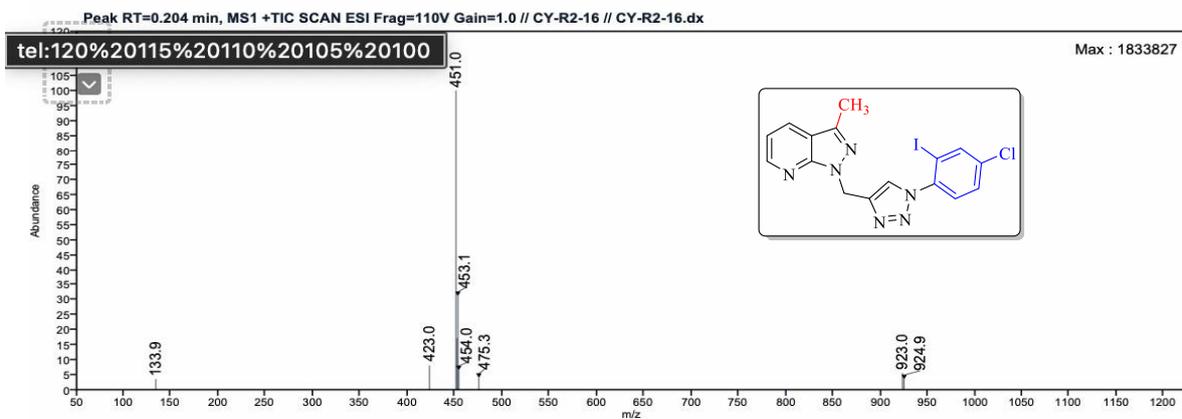
¹³C NMR spectrum of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (**16**)



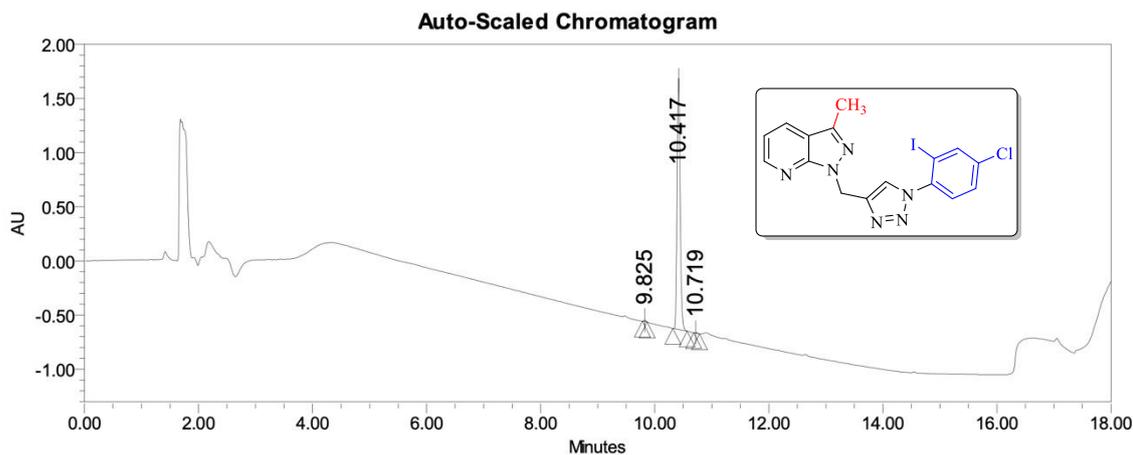
IR spectrum of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (**16**)



Mass spectrum of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (16)



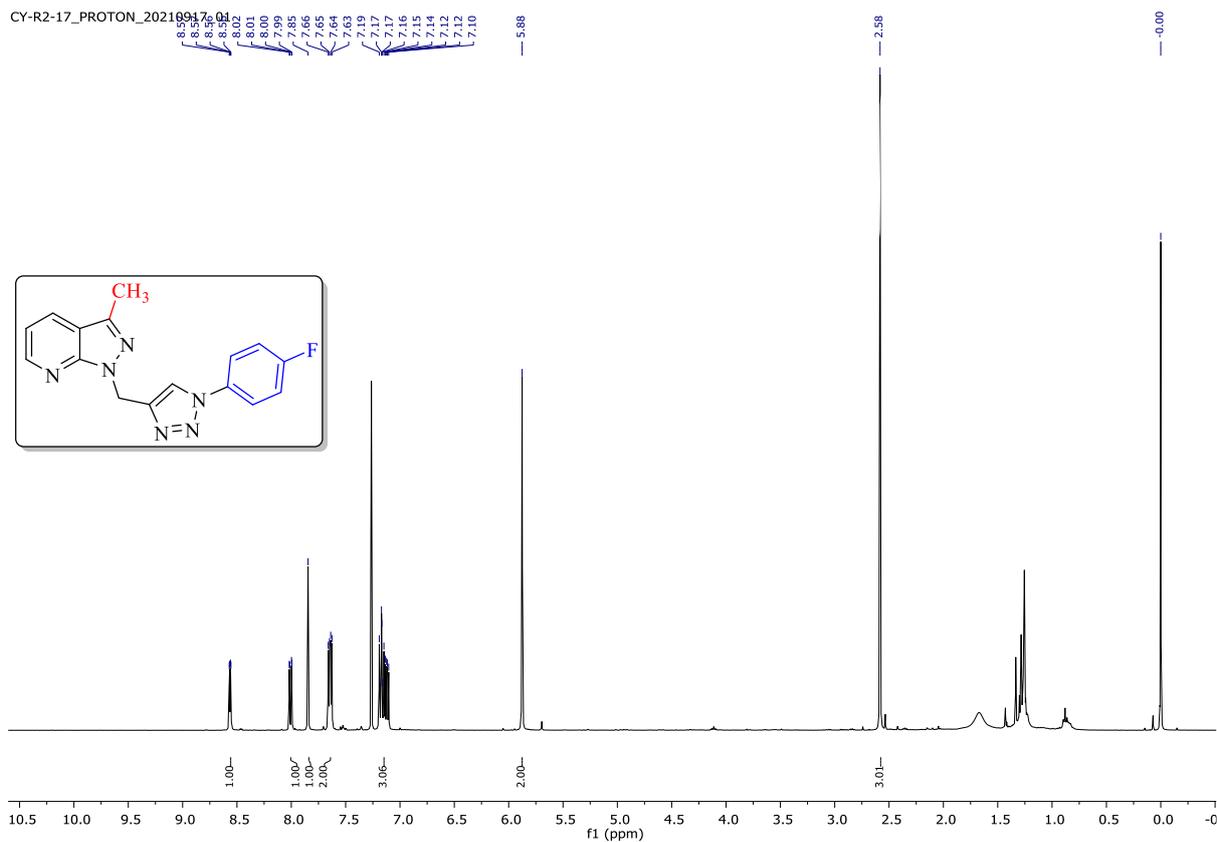
HPLC chromatogram of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (16)



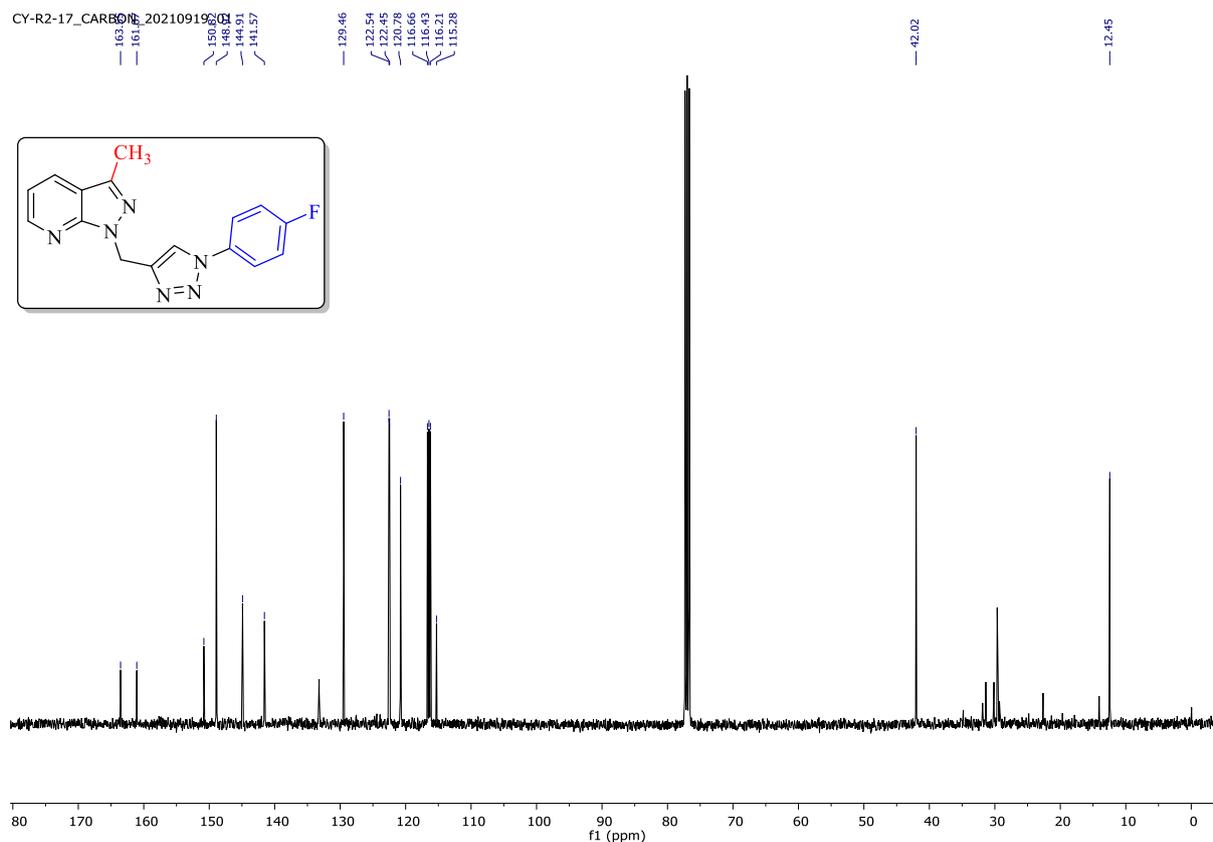
Peak Results

Name	RT	Area	% Area
1	9.825	39331	0.44
2	10.417	8898778	99.35
3	10.719	19338	0.22

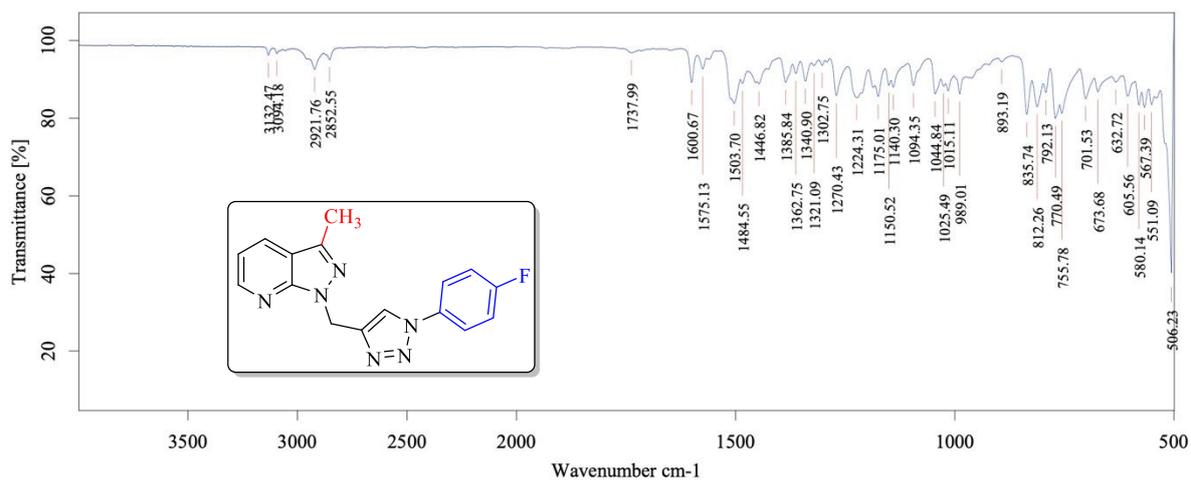
¹H NMR spectrum of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (17)



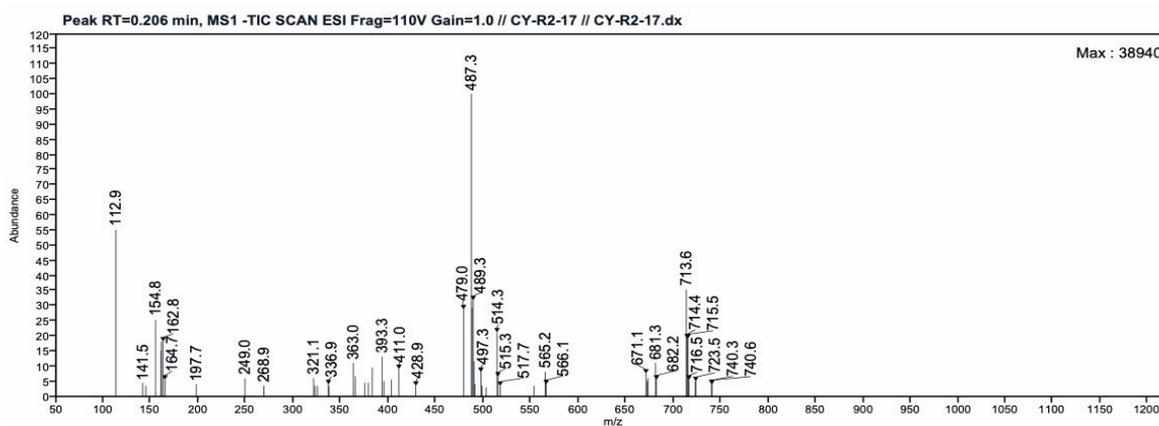
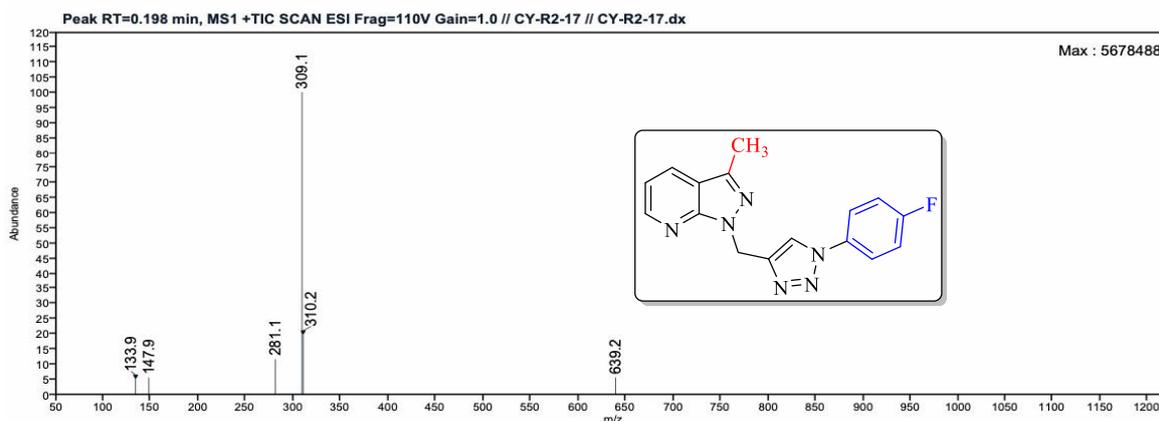
¹³C NMR spectrum of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (17)



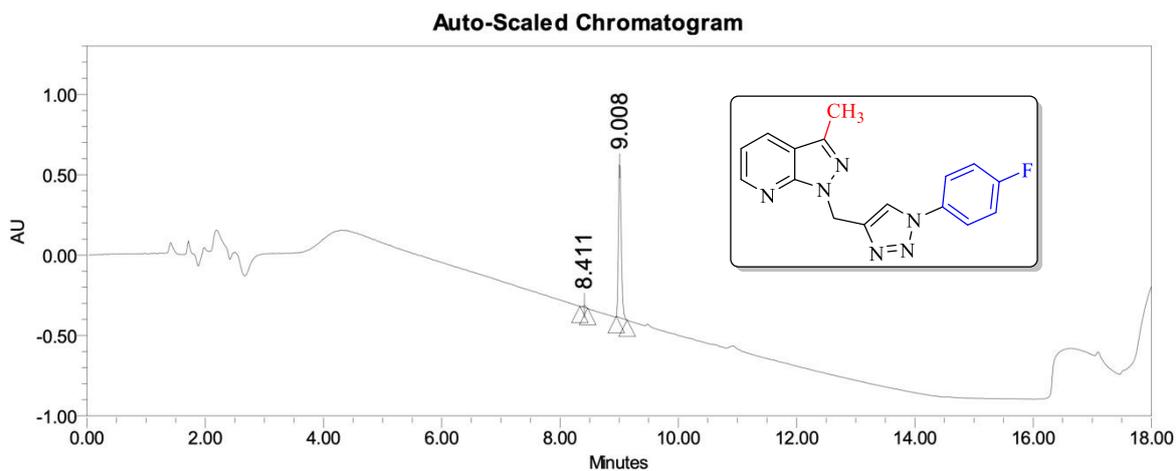
IR spectrum of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (17)



Mass spectrum of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (17)



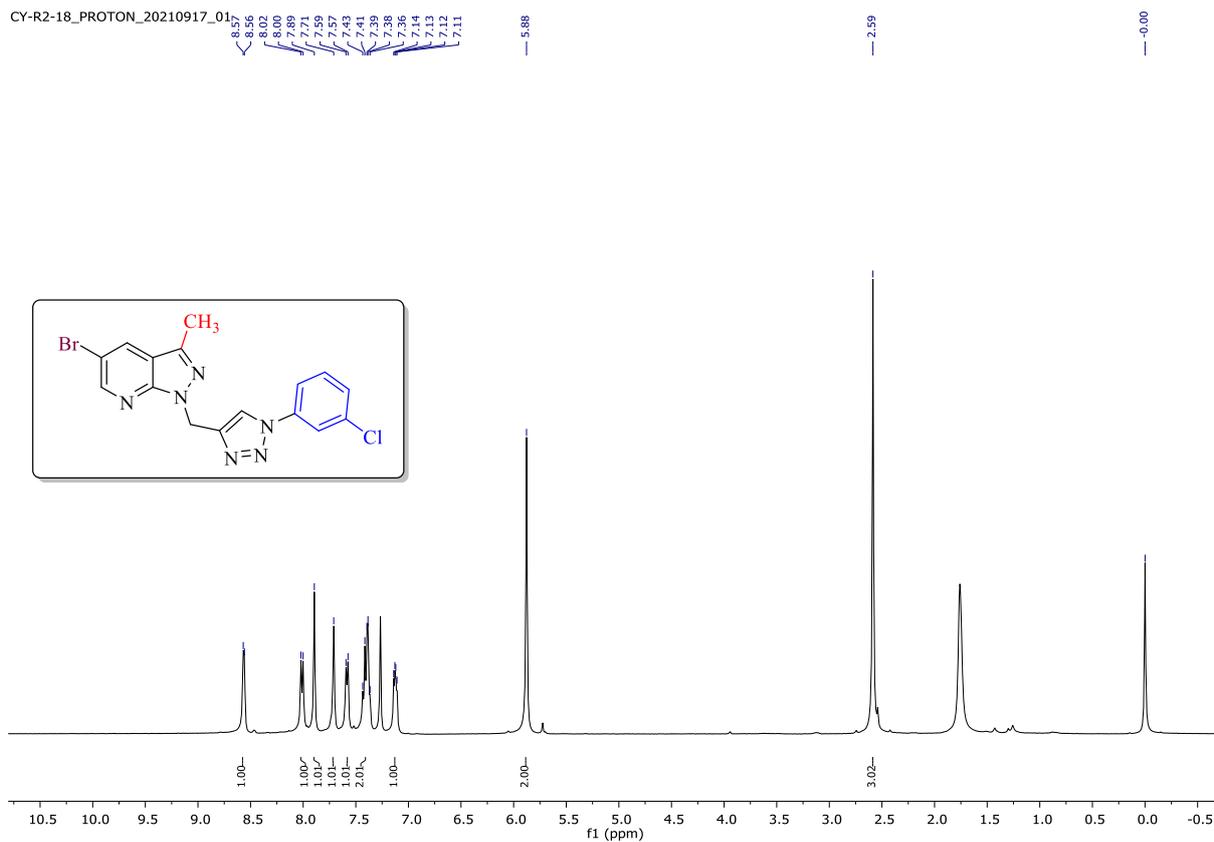
HPLC chromatogram of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (17)



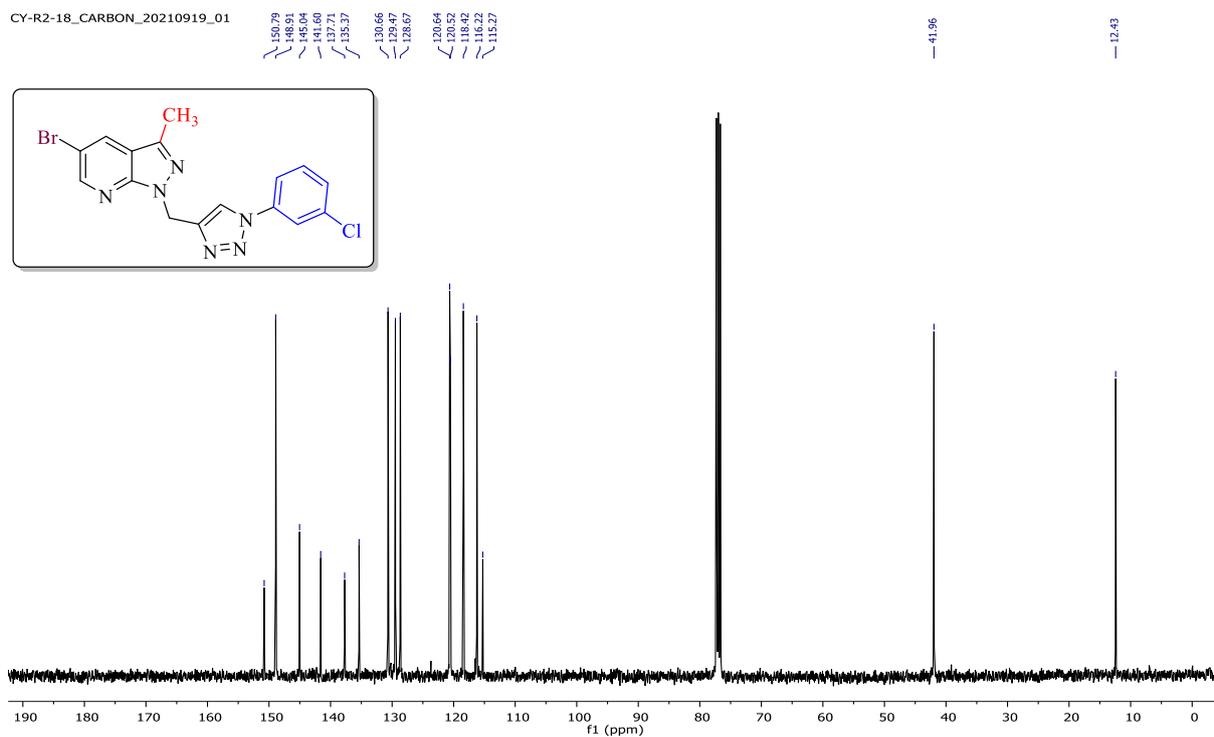
Peak Results

	Name	RT	Area	% Area
1		8.411	40037	1.20
2		9.008	3290473	98.80

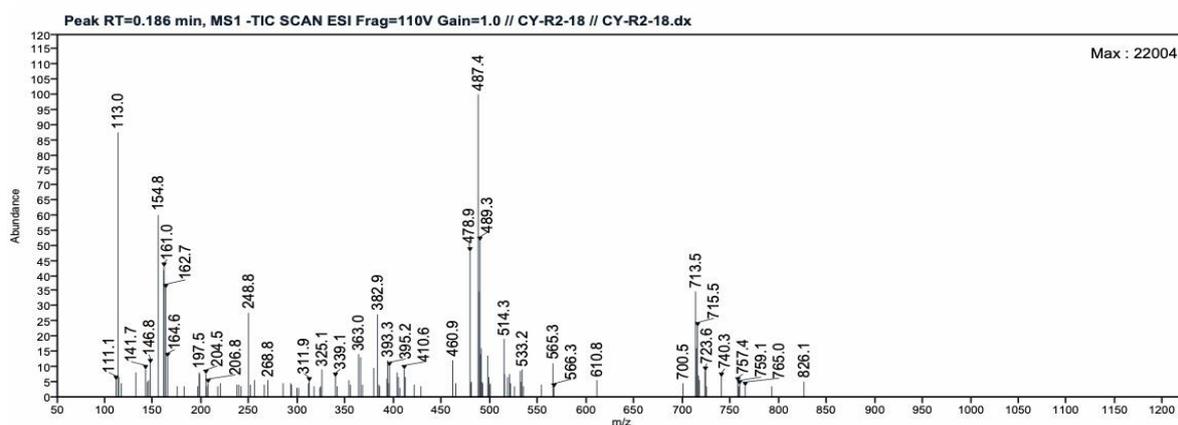
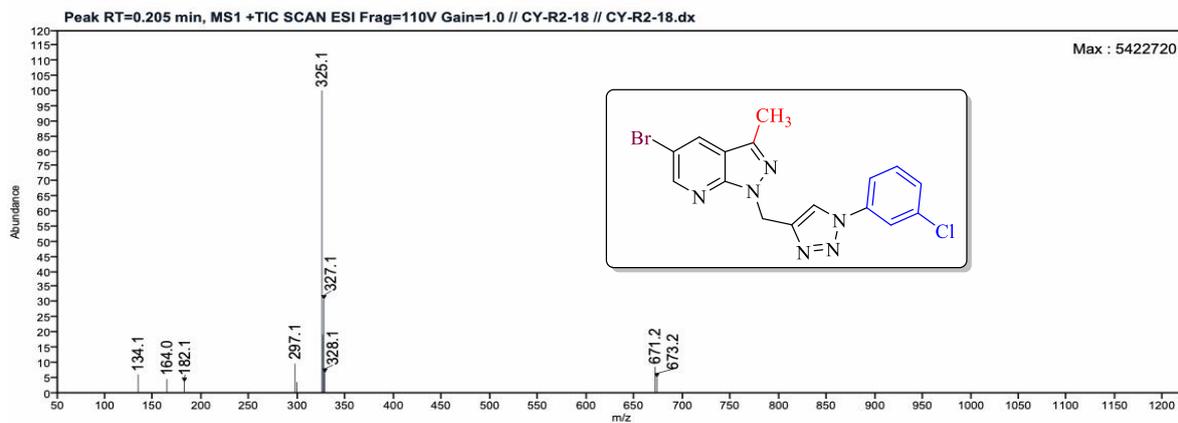
^1H NMR spectrum of 1-((1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (18)



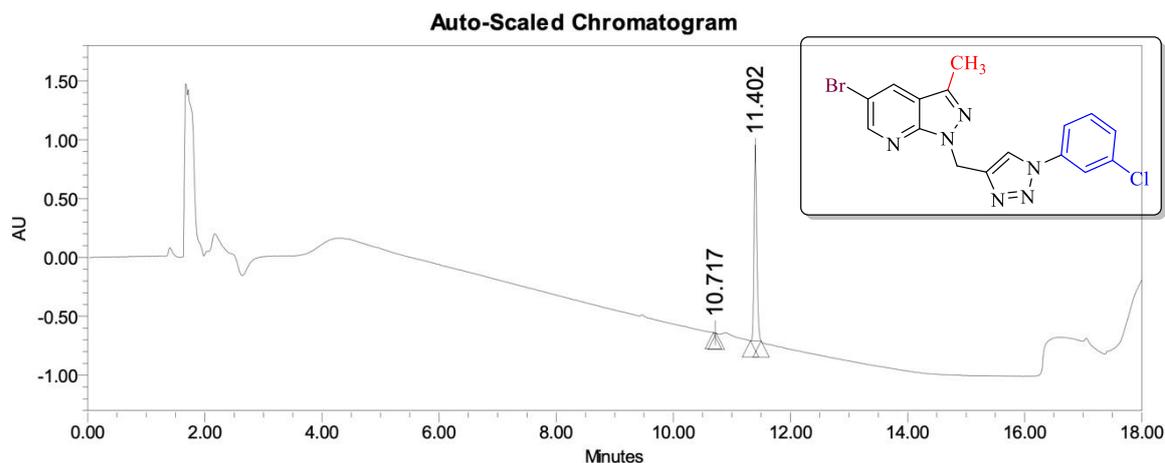
¹³C NMR spectrum of 1-((1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (18)



Mass spectrum of 1-((1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (18)



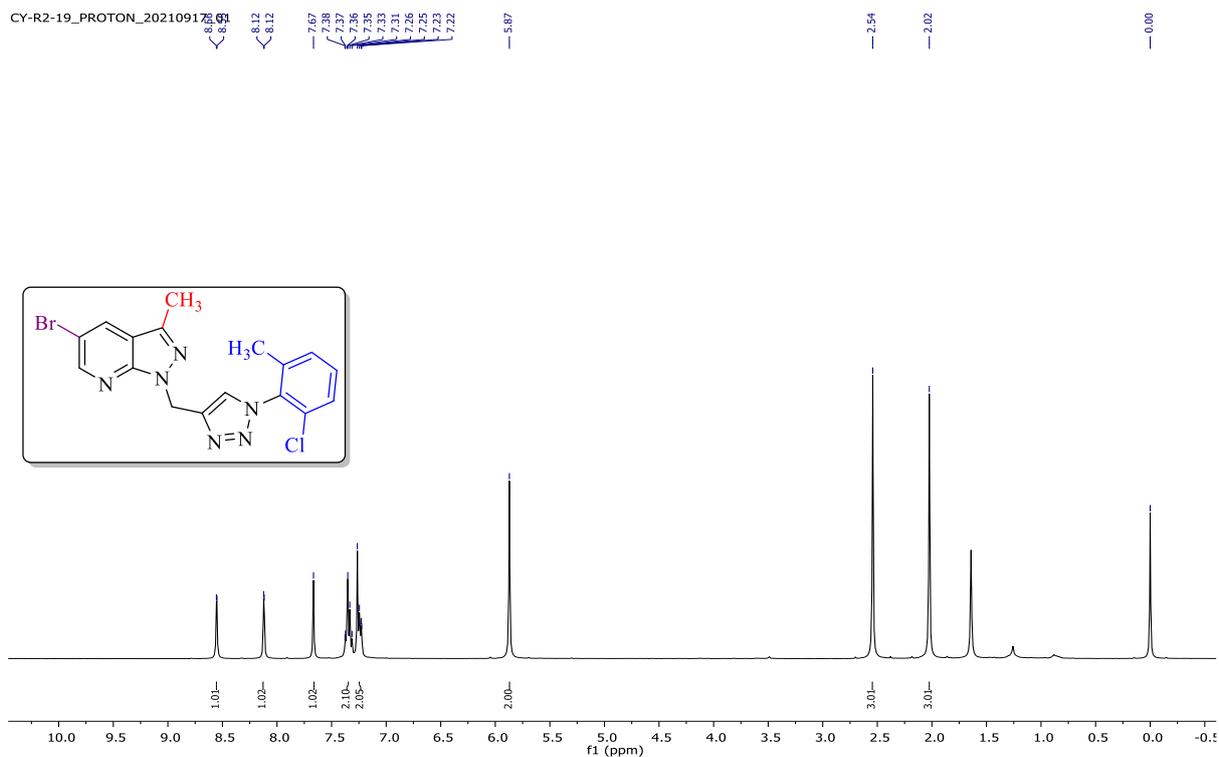
HPLC chromatogram of 1-((1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (18)



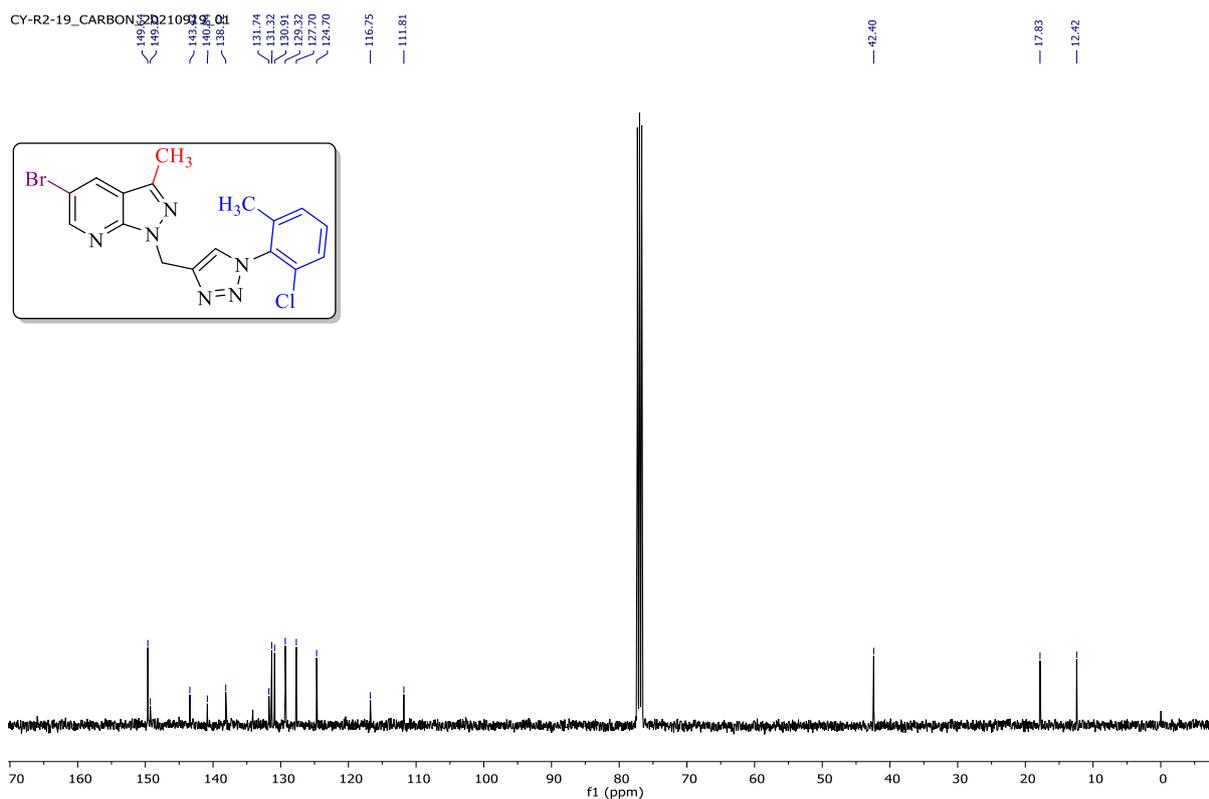
Peak Results

Name	RT	Area	% Area
1	10.717	4609	0.08
2	11.402	5474714	99.92

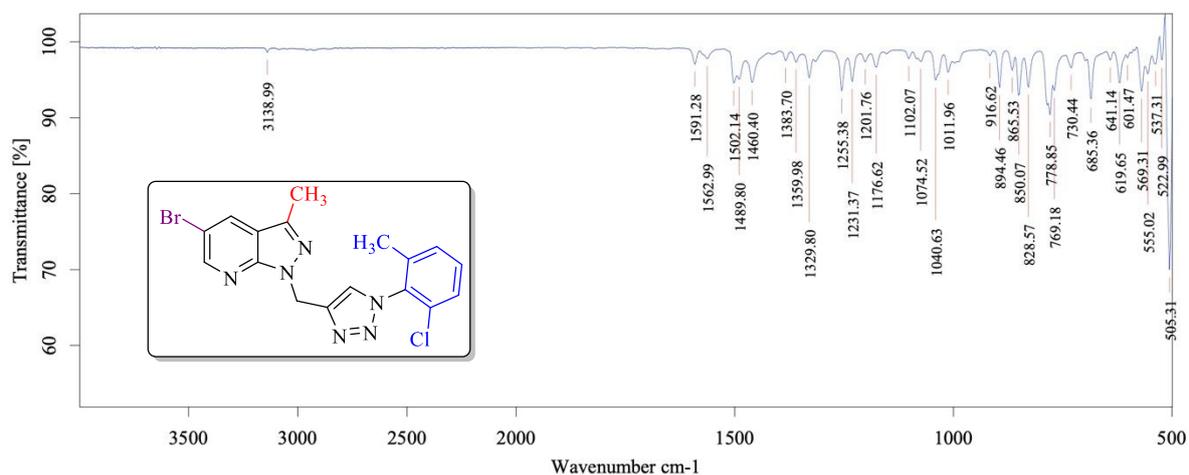
¹H NMR spectrum of 5-Bromo-1-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (19)



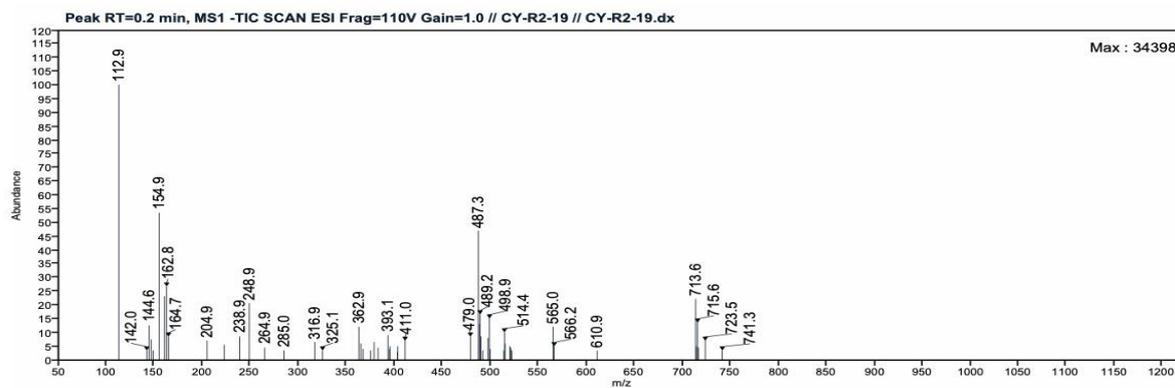
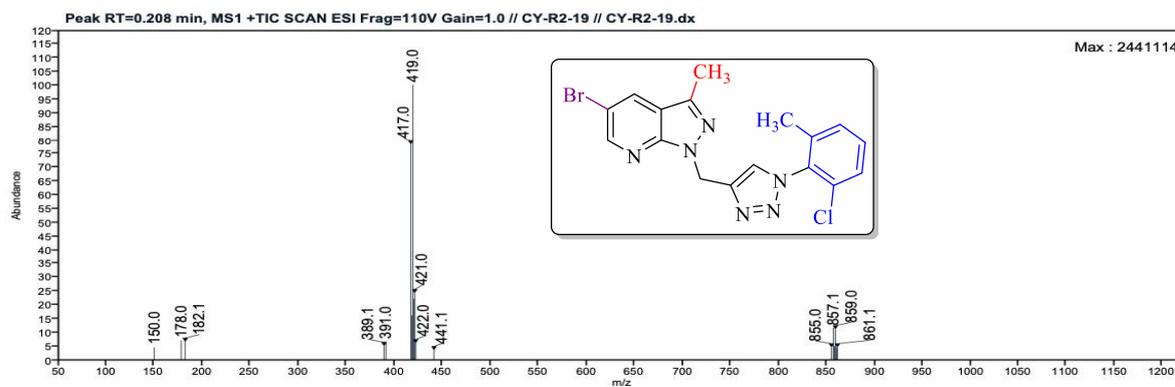
¹³C NMR spectrum of 5-Bromo-1-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (19)



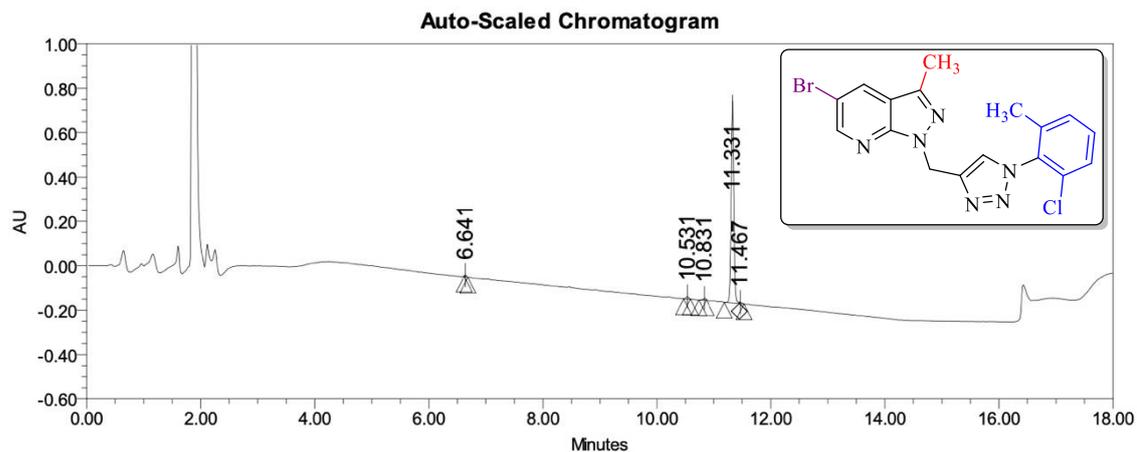
IR spectrum of 5-Bromo-1-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (19)



Mass spectrum of 5-Bromo-1-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (19)



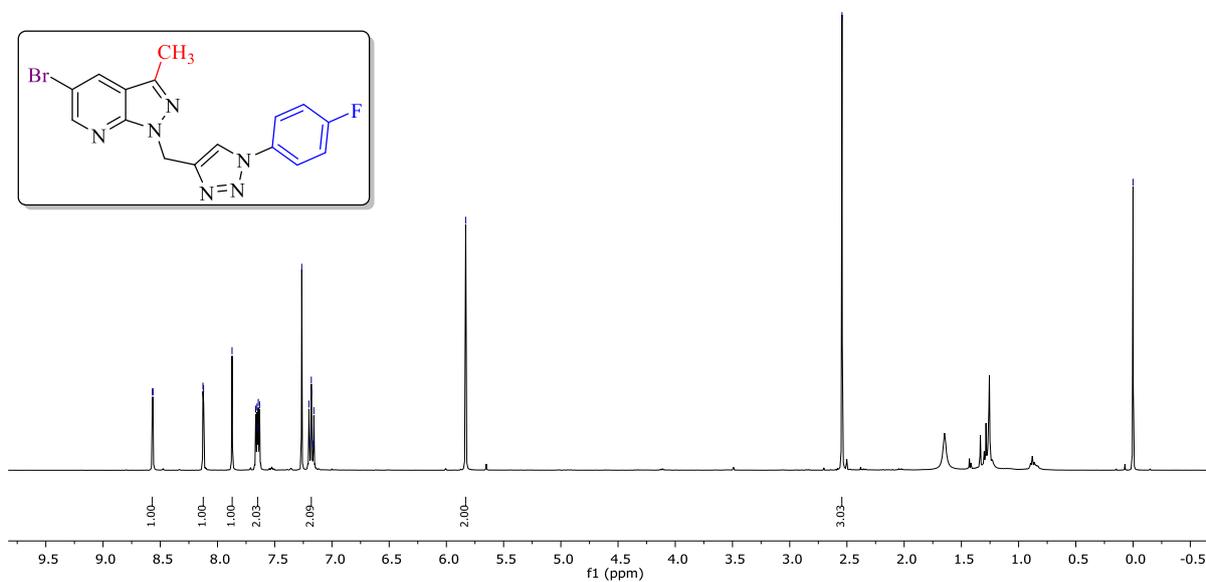
HPLC chromatogram of 5-Bromo-1-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (19)



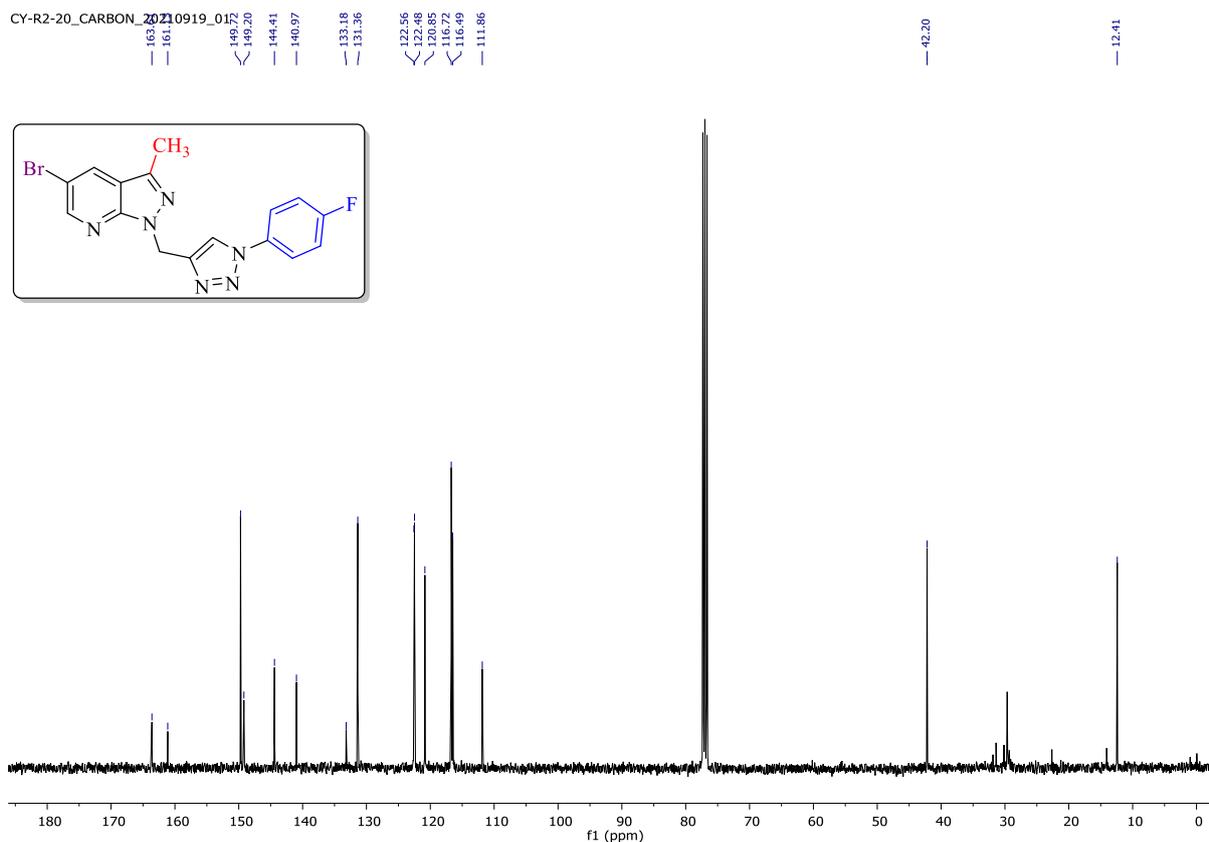
Peak Results

Name	RT	Area	% Area
1	6.641	14263	0.48
2	10.531	34427	1.16
3	10.831	22944	0.78
4	11.331	2869270	97.05
5	11.467	15584	0.53

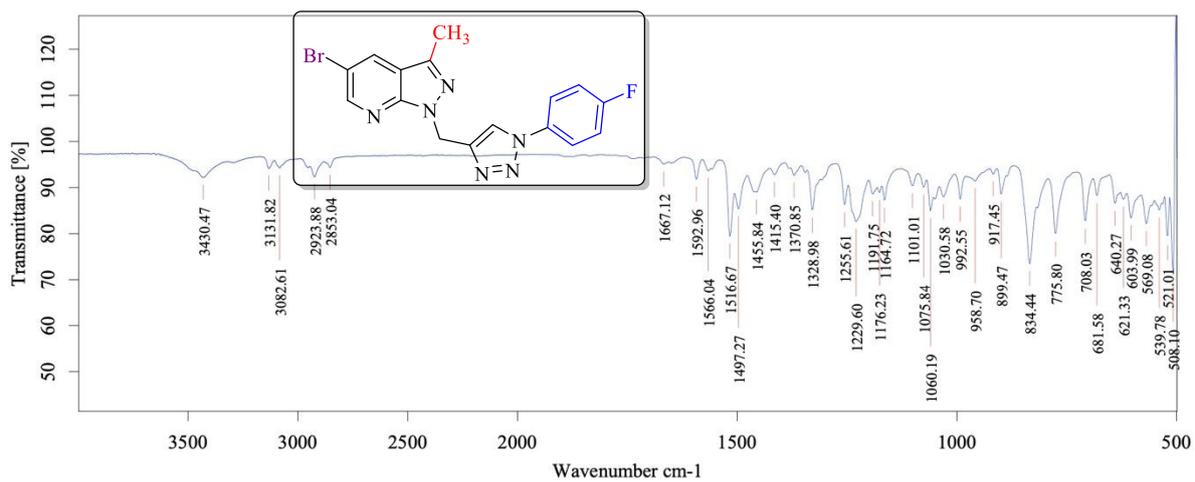
¹H NMR spectrum of 5-Bromo-1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (20)



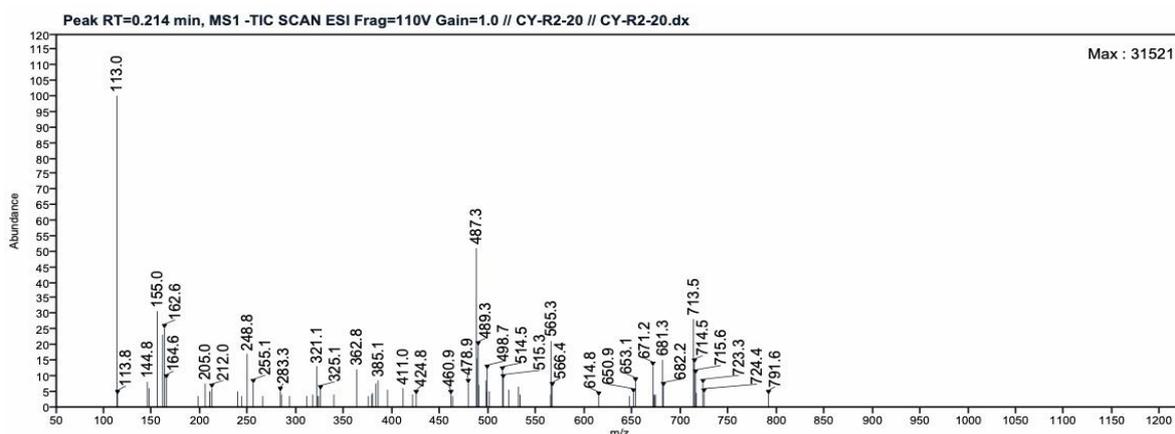
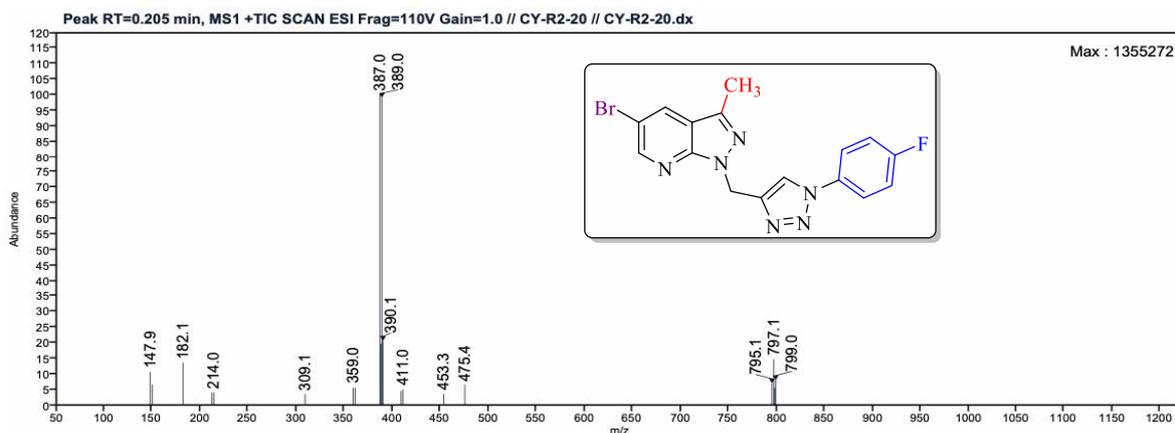
¹³C NMR spectrum of 5-Bromo-1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (20)



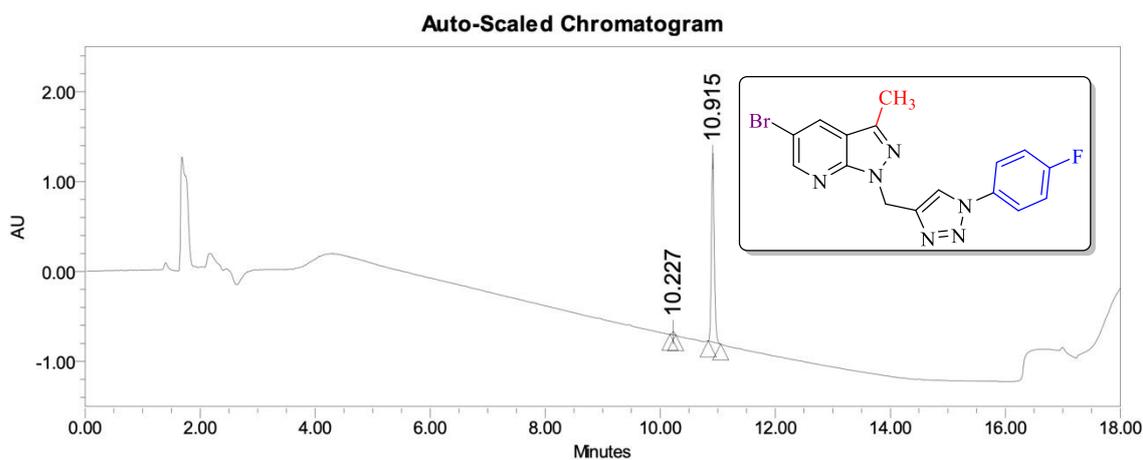
IR spectrum of 5-Bromo-1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (20)



Mass spectrum of 5-Bromo-1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (20)



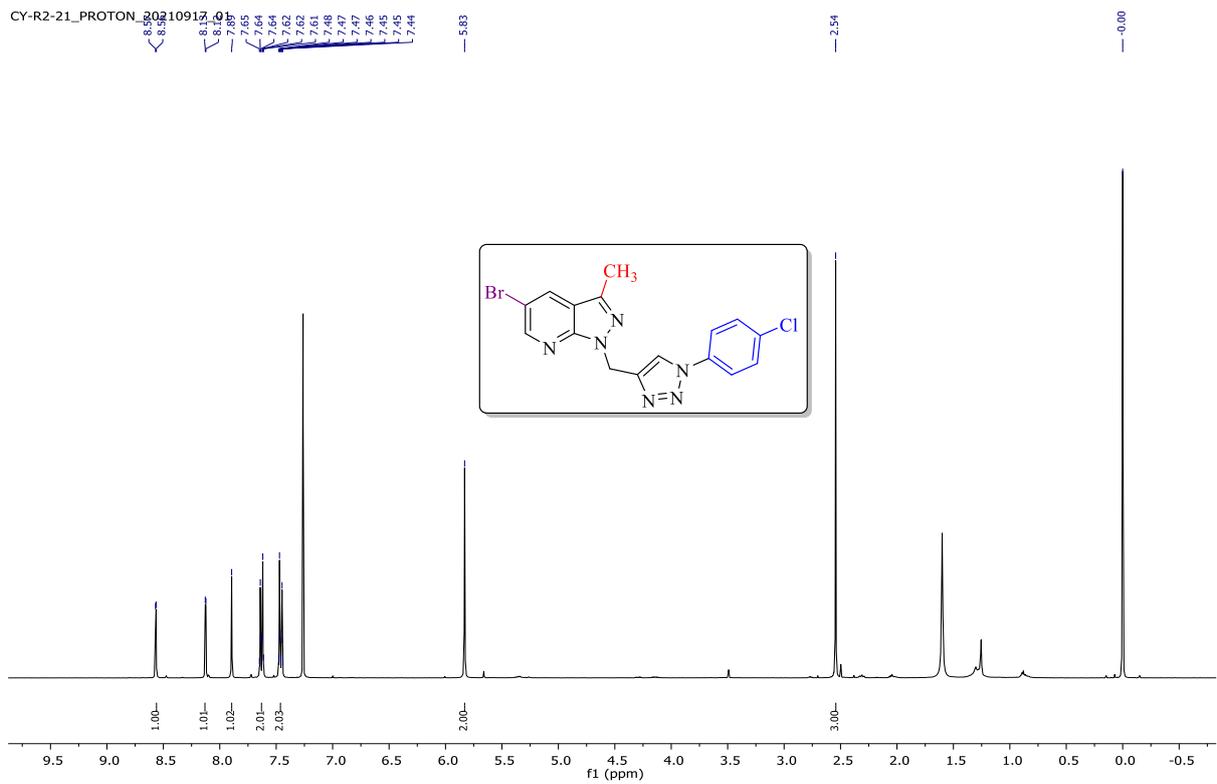
HPLC chromatogram of 5-Bromo-1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (20)



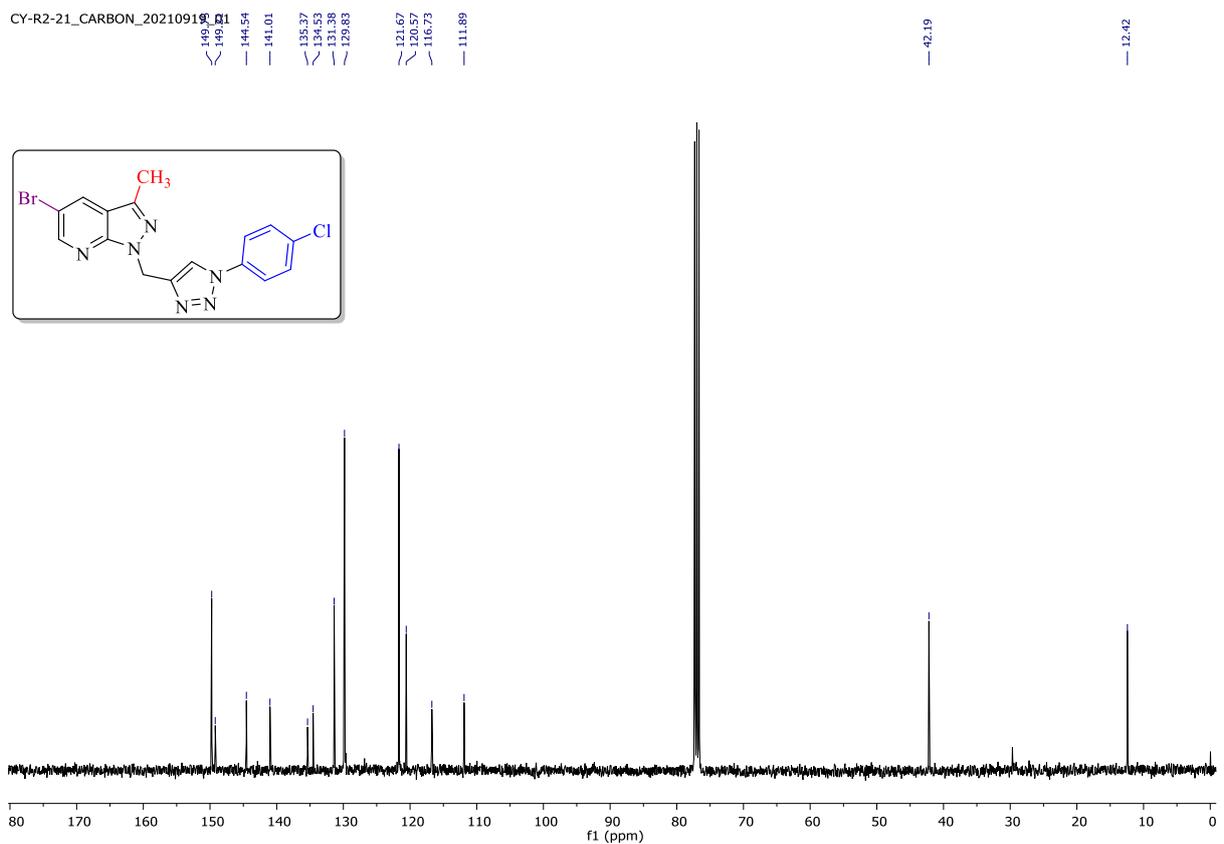
Peak Results

Name	RT	Area	% Area
1	10.227	90125	1.28
2	10.915	6944173	98.72

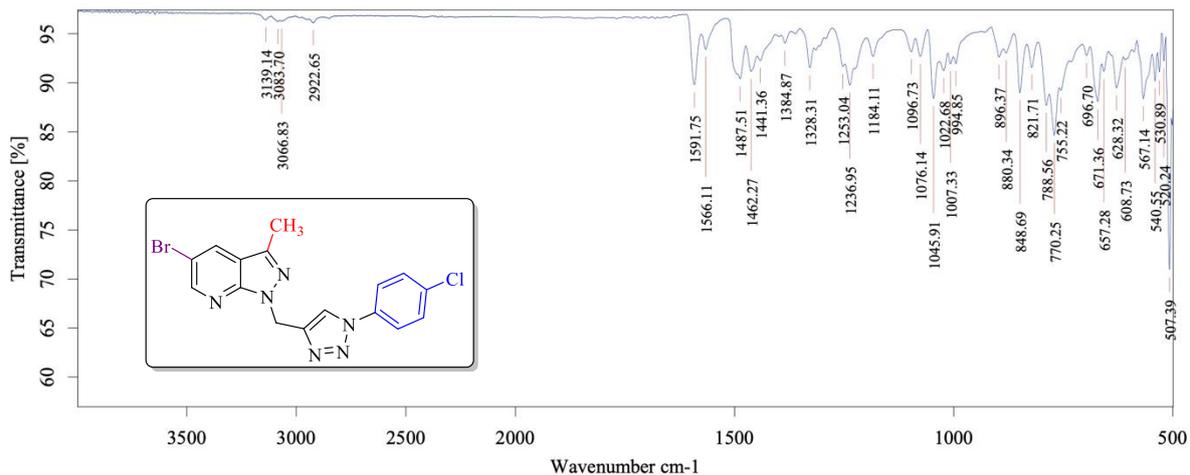
¹H NMR spectrum of 5-Bromo-1-((1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (21)



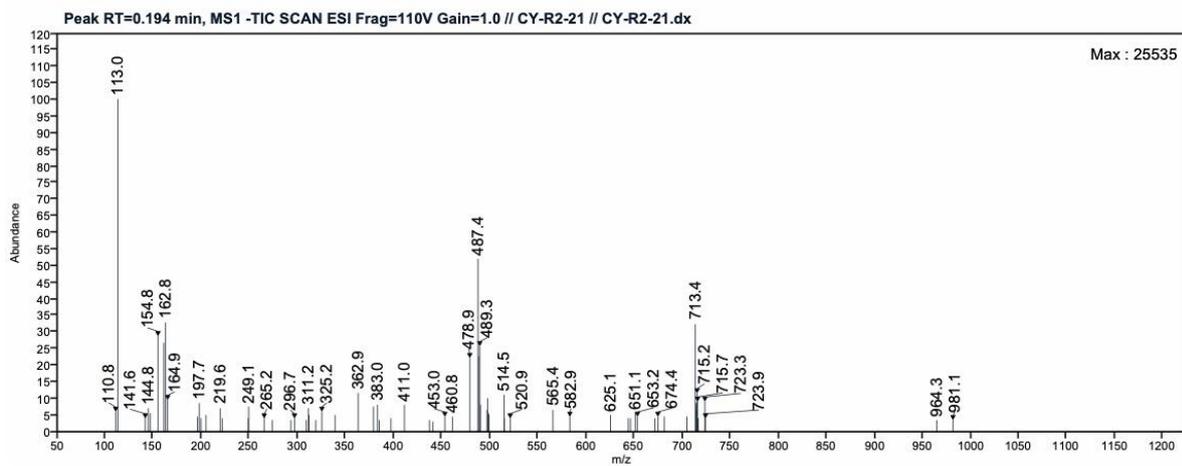
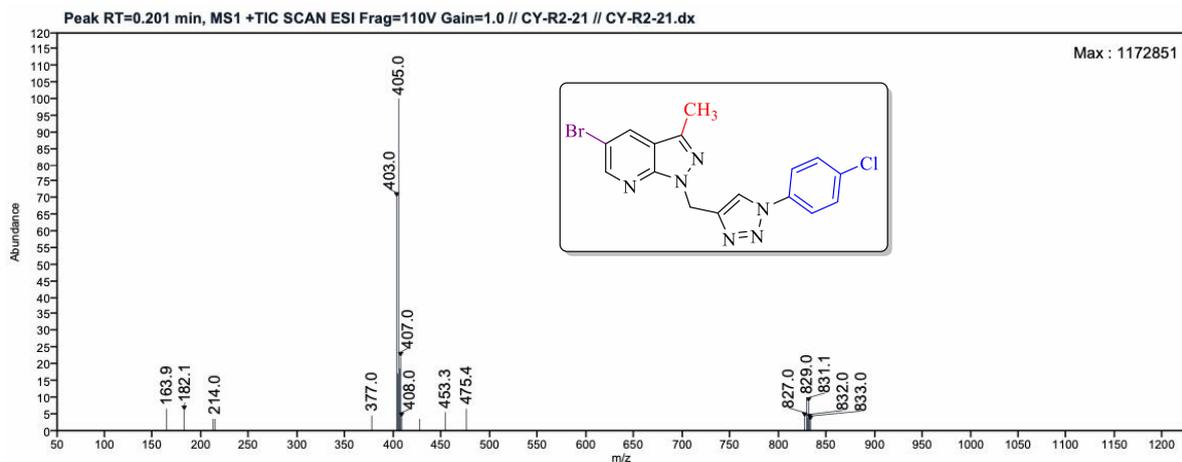
¹³C NMR spectrum of 5-Bromo-1-((1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (21)



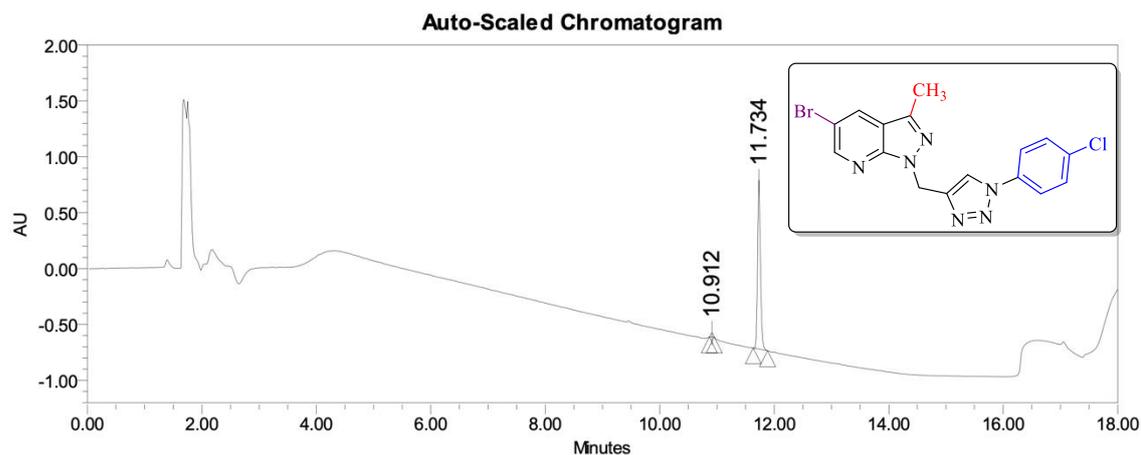
IR spectrum of 5-Bromo-1-((1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (21)



Mass spectrum of 5-Bromo-1-((1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (21)



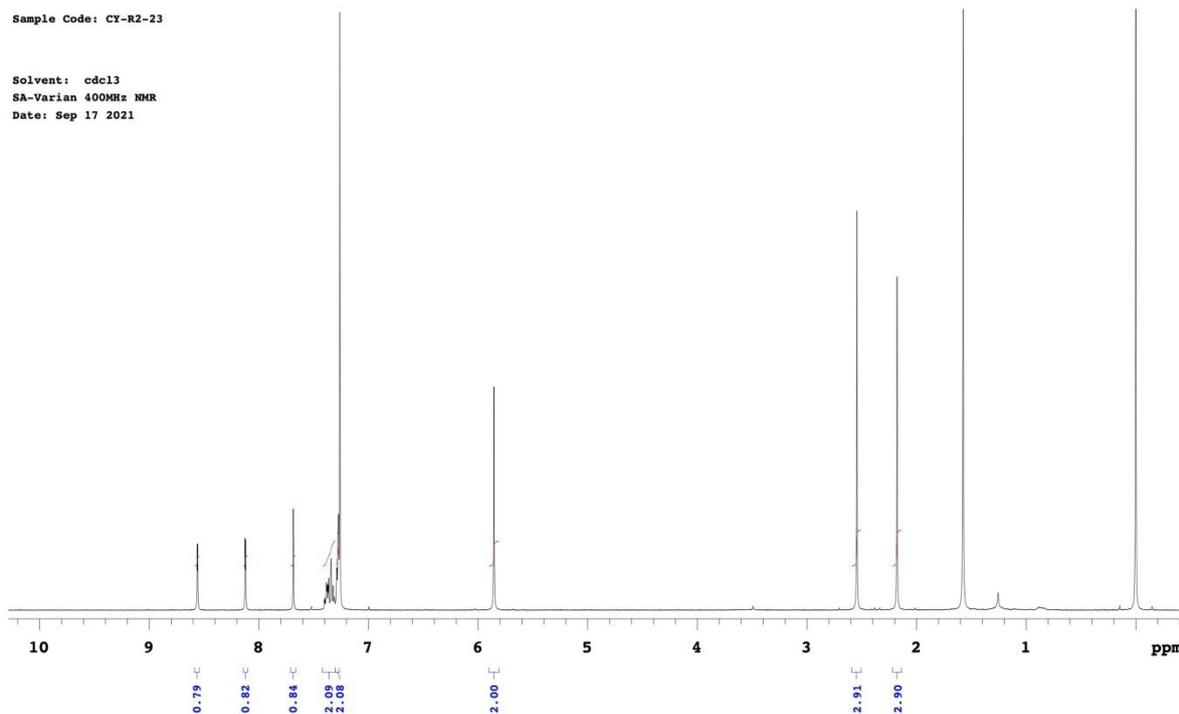
HPLC chromatogram of 5-Bromo-1-((1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (21)



Peak Results

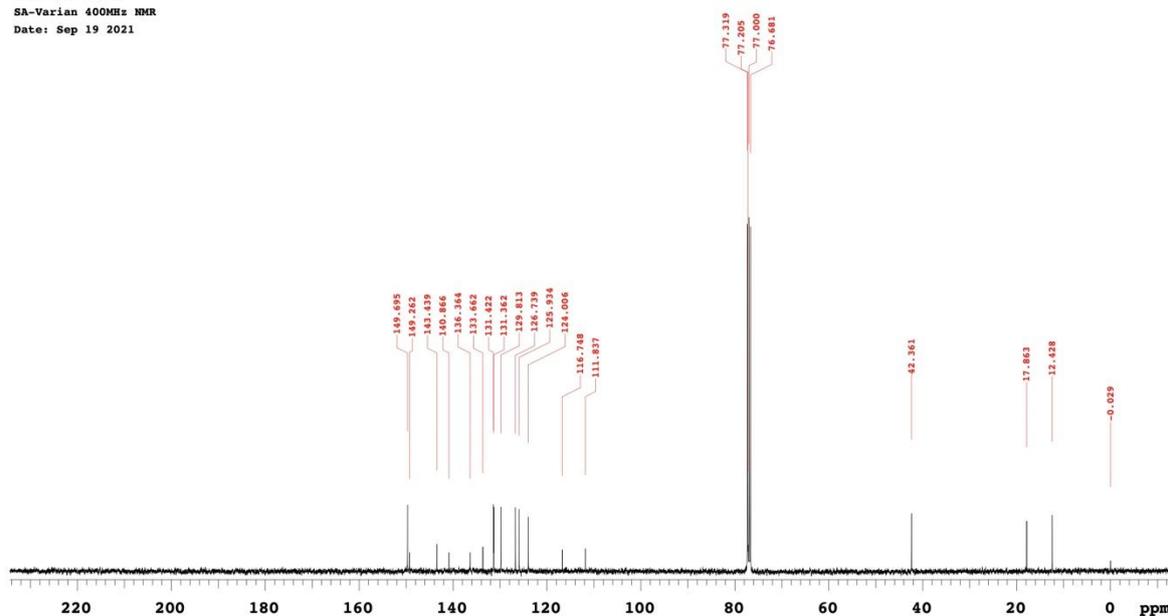
Name	RT	Area	% Area
1	10.912	101965	1.97
2	11.734	5085406	98.03

¹H NMR spectrum of 5-Bromo-1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (22)

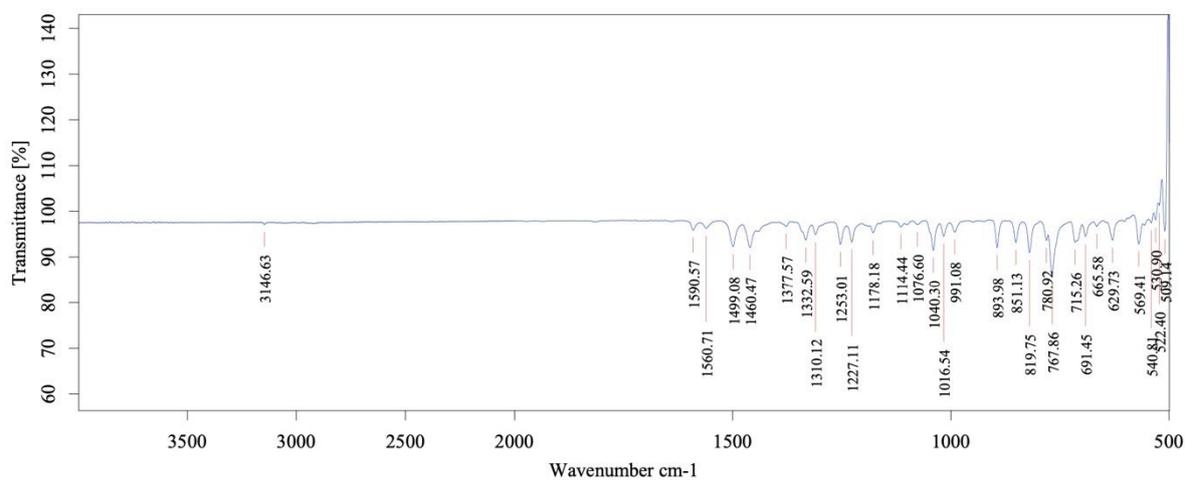


¹³C NMR spectrum of 5-Bromo-1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (22)

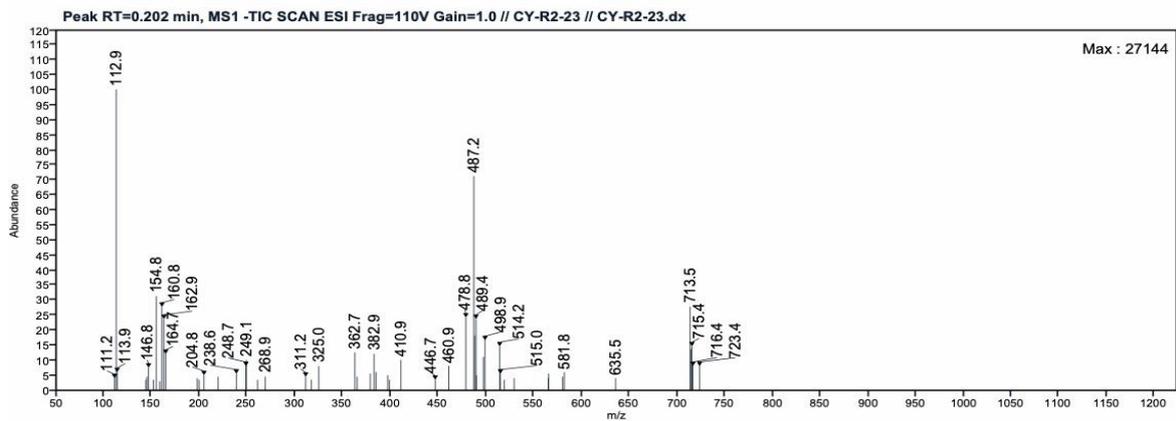
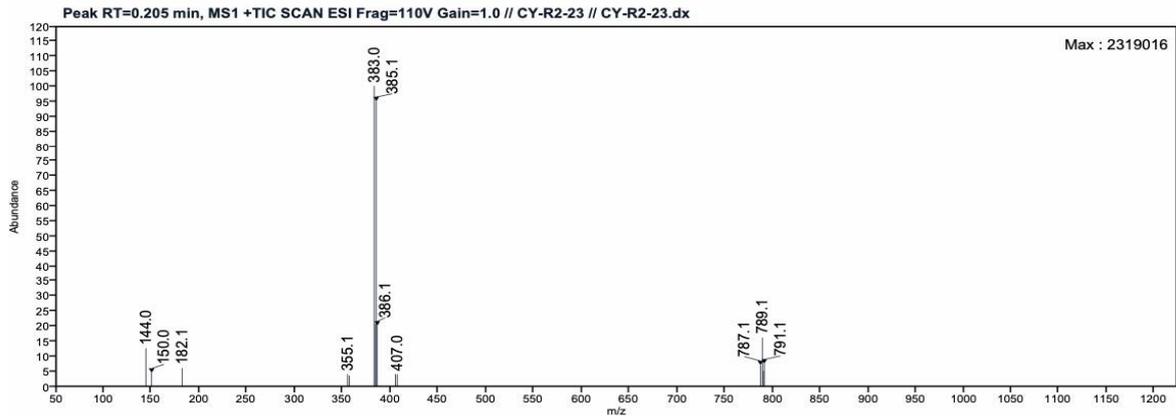
Solvent: cdcl3
SA-Varian 400MHz NMR
Date: Sep 19 2021



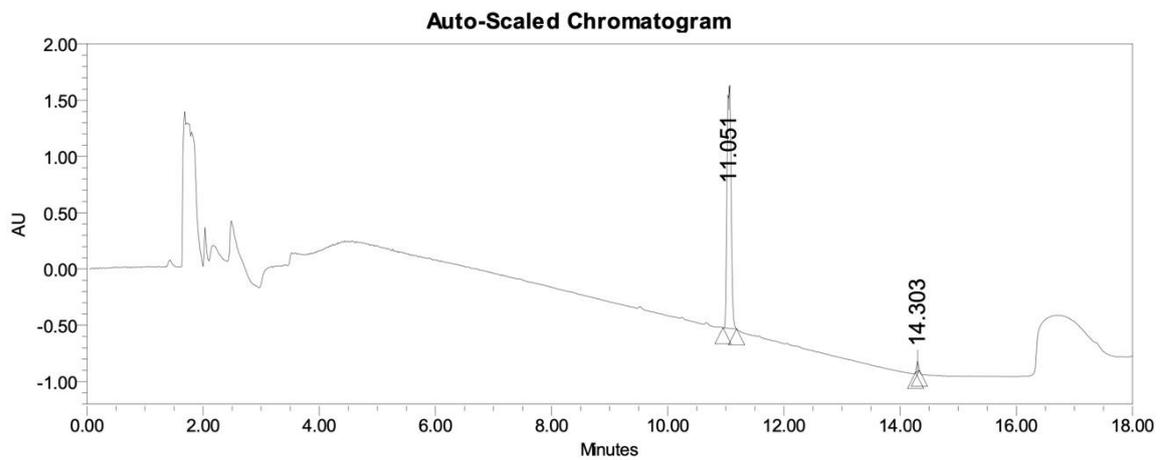
IR spectrum of 5-Bromo-1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (22)



Mass spectrum of 5-Bromo-1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (22)



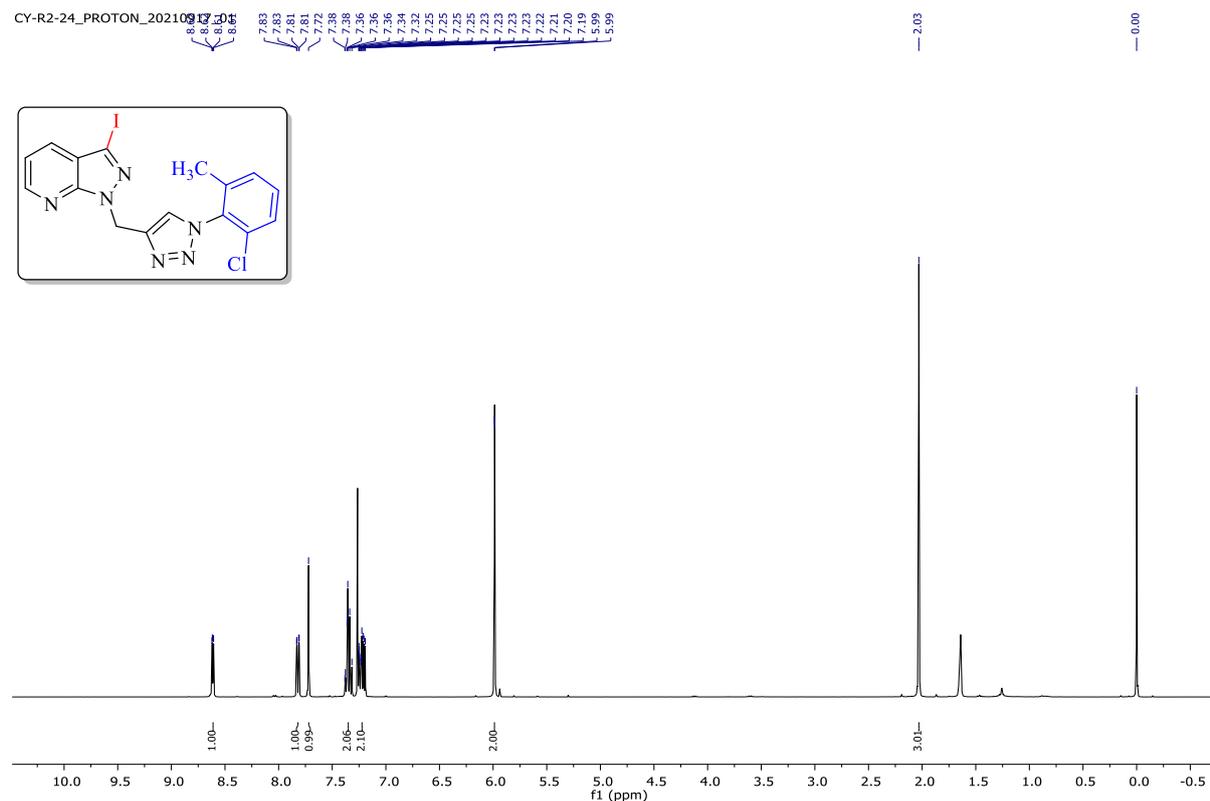
HPLC chromatogram of 5-Bromo-1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-methyl-1H-pyrazolo[3,4-b]pyridine (22)



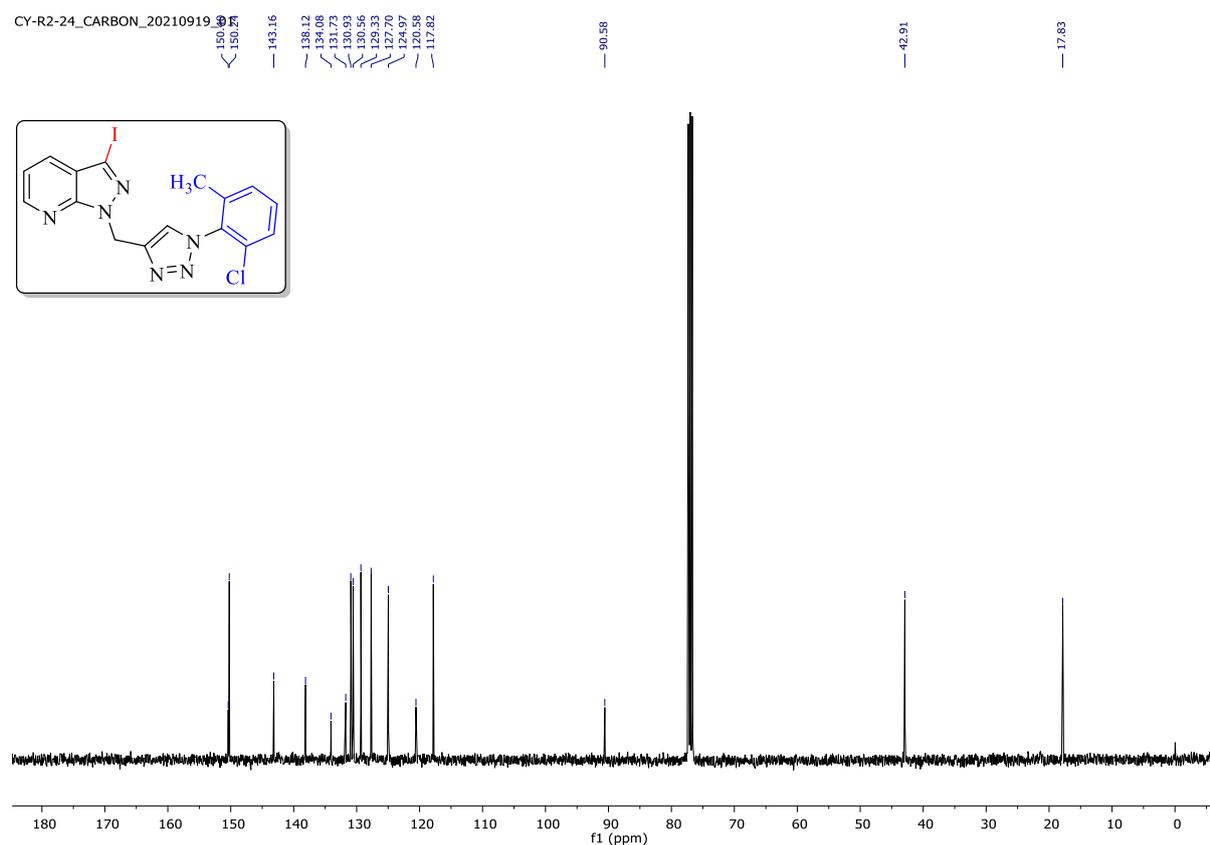
Peak Results

Name	RT	Area	% Area
1	11.051	10361708	98.19
2	14.303	191009	1.81

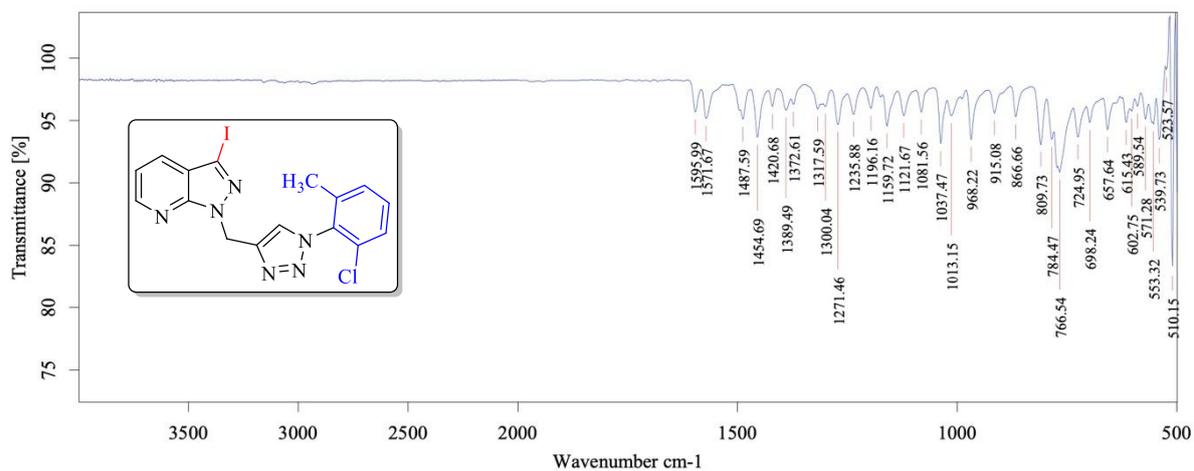
¹H NMR spectrum of 1-((1-(2-Chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (23)



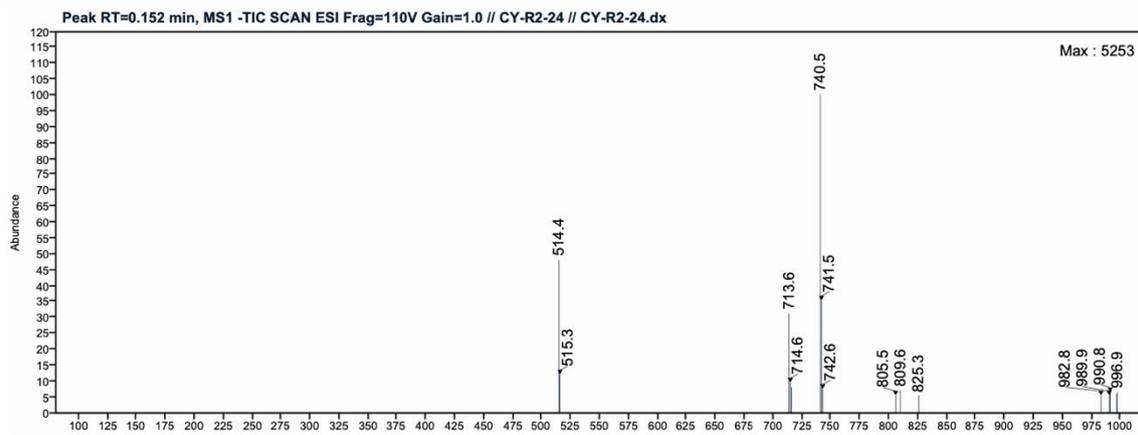
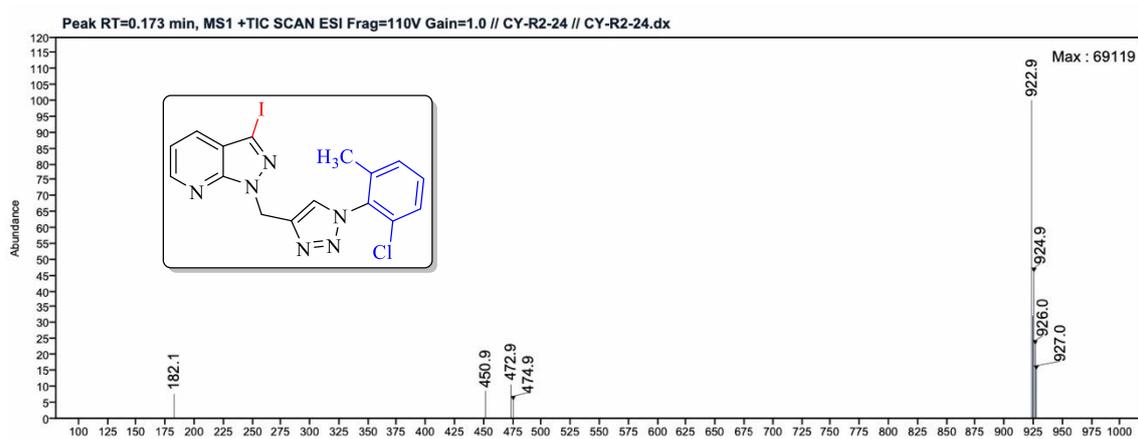
¹³C NMR spectrum of 1-((1-(2-Chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (23)



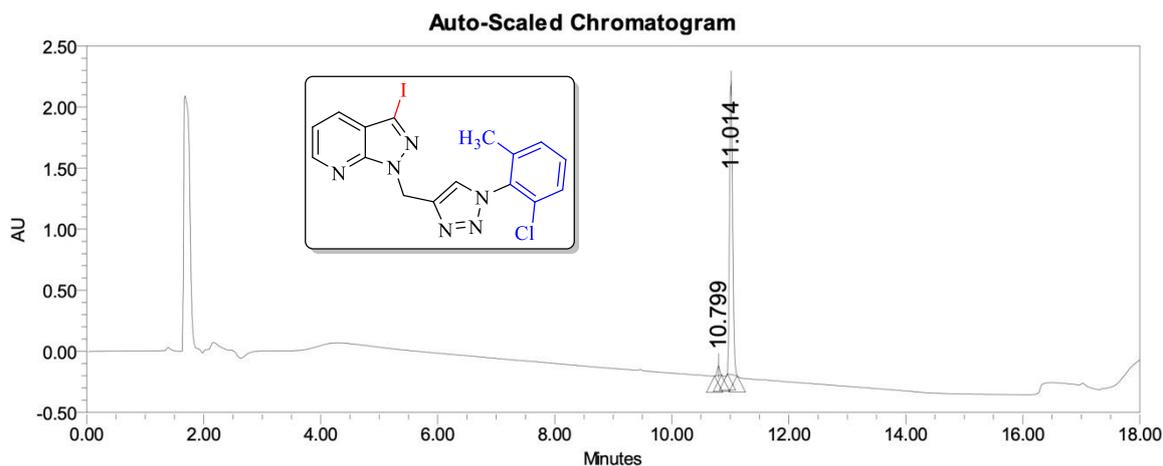
IR spectrum of 1-((1-(2-Chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (23)



Mass spectrum of 1-((1-(2-Chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (23)



HPLC chromatogram of 1-((1-(2-Chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (23)

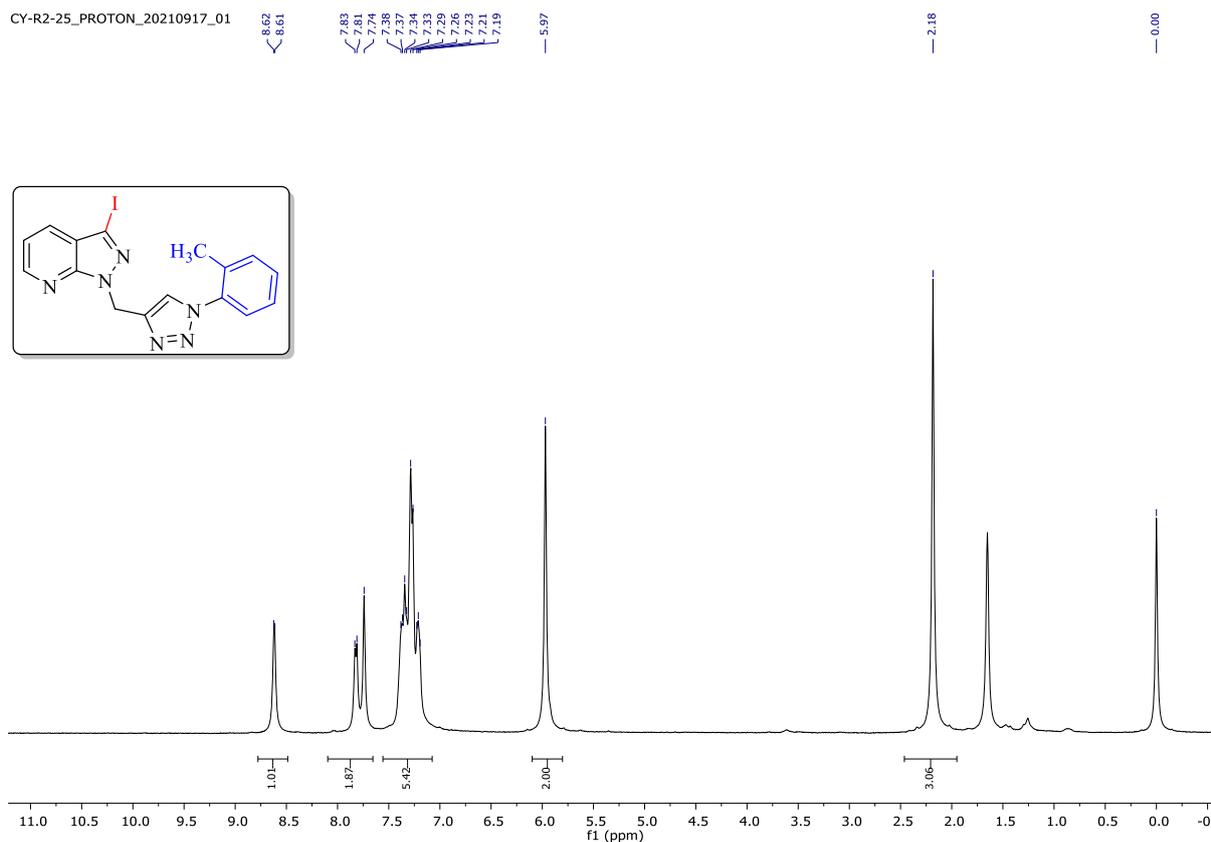


Peak Results

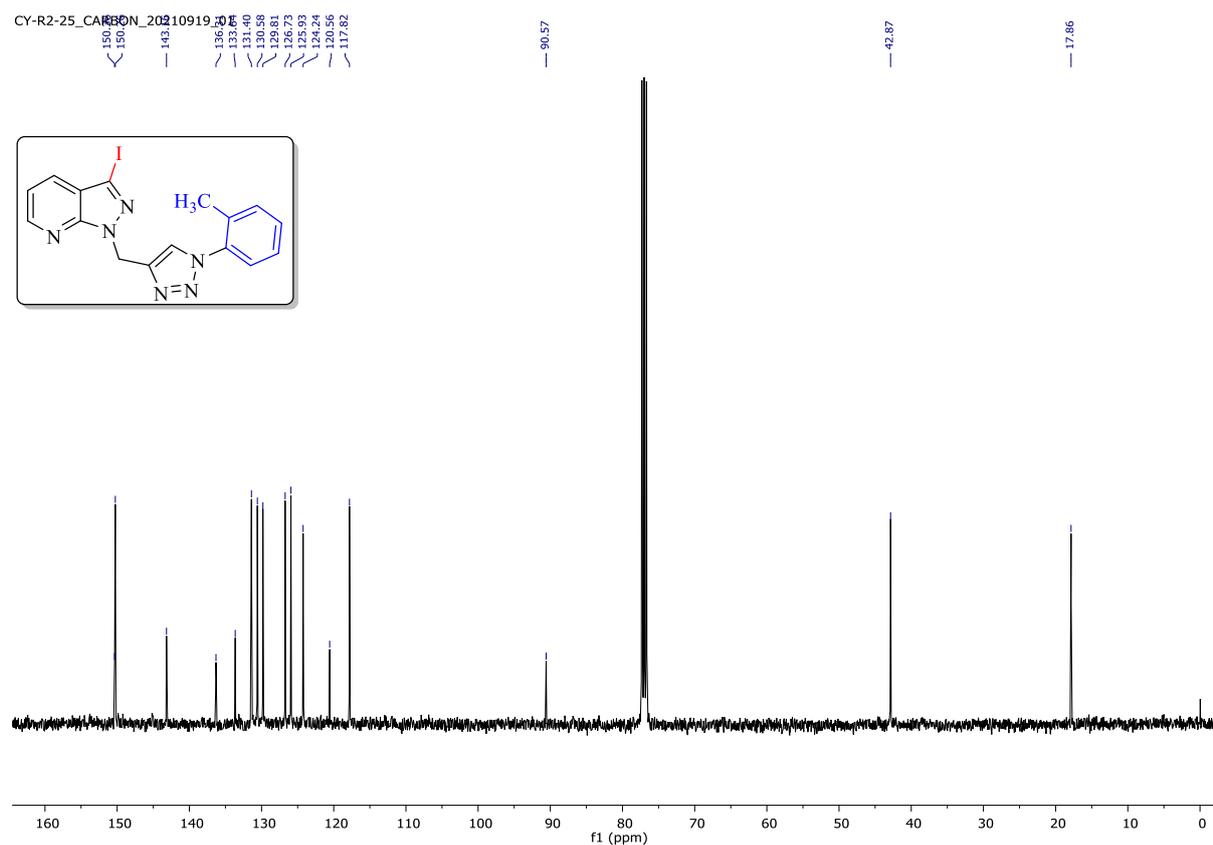
	Name	RT	Area	% Area
1		10.799	243648	2.67
2		11.014	8884521	97.33

¹H NMR spectrum of 3-Iodo-1-((1-(*o*-tolyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine (24)

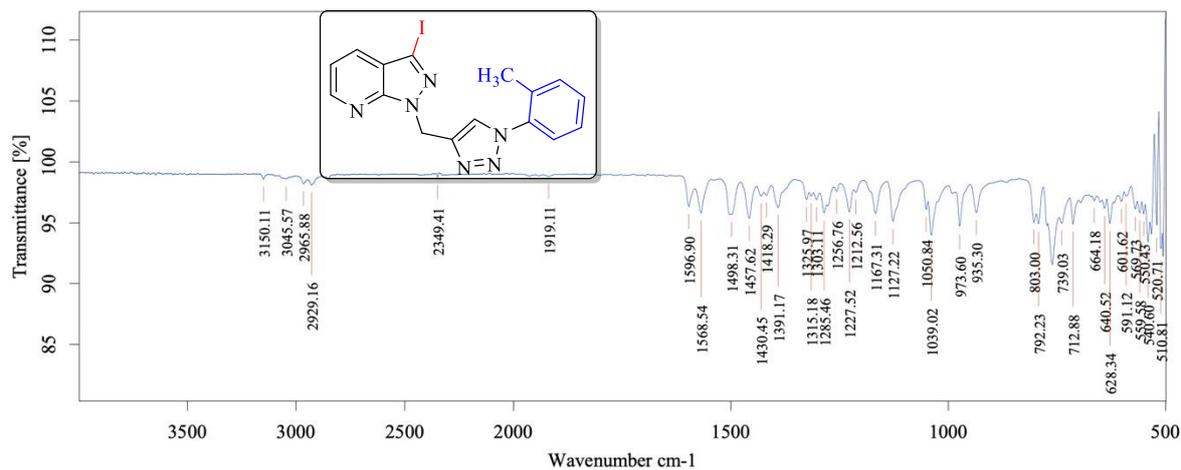
CY-R2-25_PROTON_20210917_01



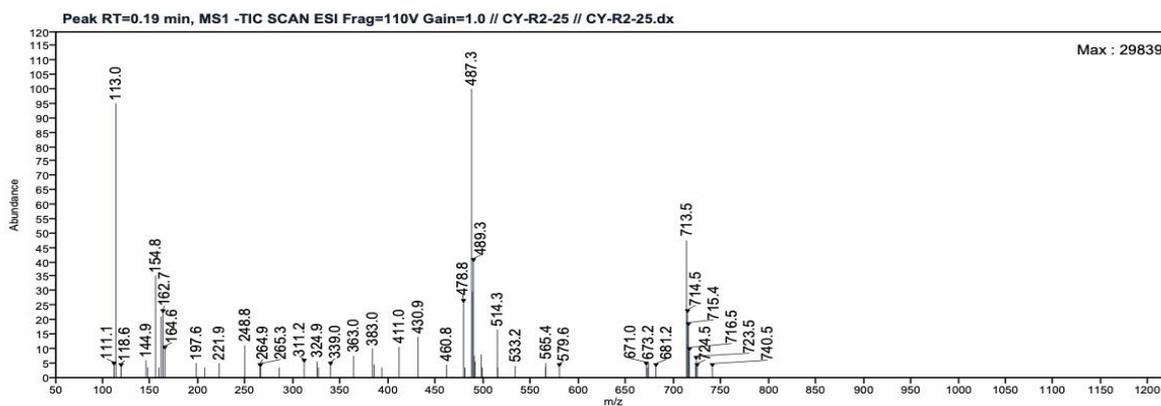
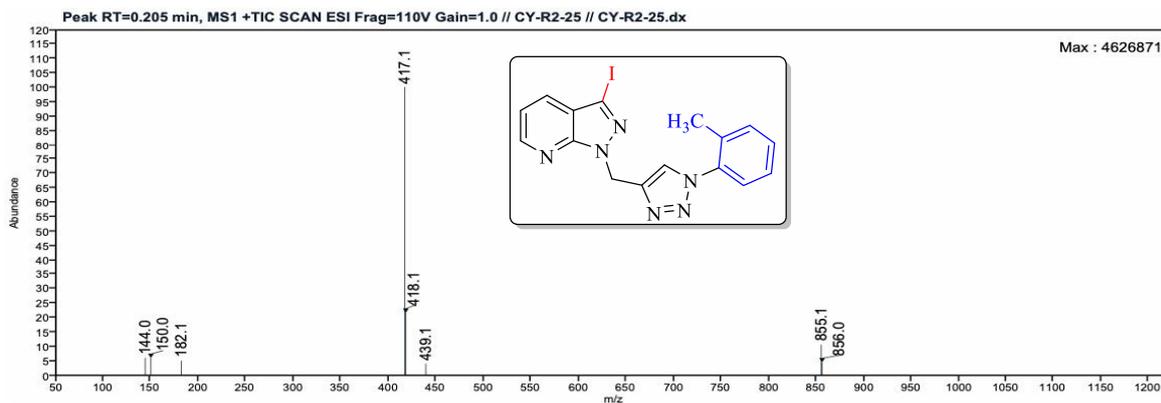
¹³C NMR spectrum of 3-Iodo-1-((1-(*o*-tolyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-*b*]pyridine (24)



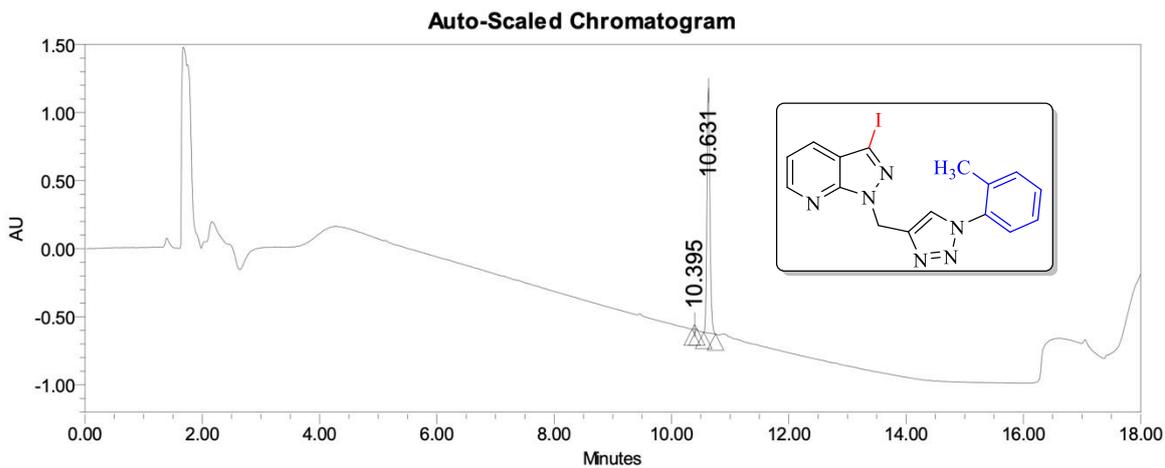
IR spectrum of 3-Iodo-1-((1-(*o*-tolyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-*b*]pyridine (24)



Mass spectrum of 3-Iodo-1-((1-(*o*-tolyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-*b*]pyridine (24)



HPLC chromatogram of 3-Iodo-1-((1-(*o*-tolyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-*b*]pyridine (24)

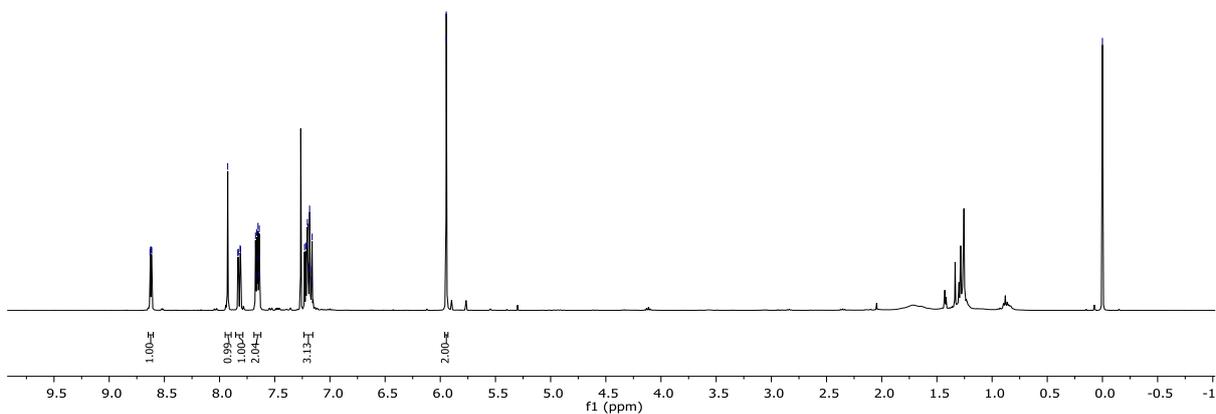
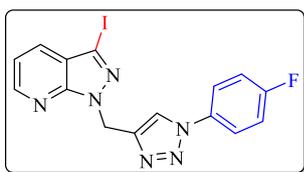


Peak Results

	Name	RT	Area	% Area
1		10.395	87247	1.33
2		10.631	6452798	98.67

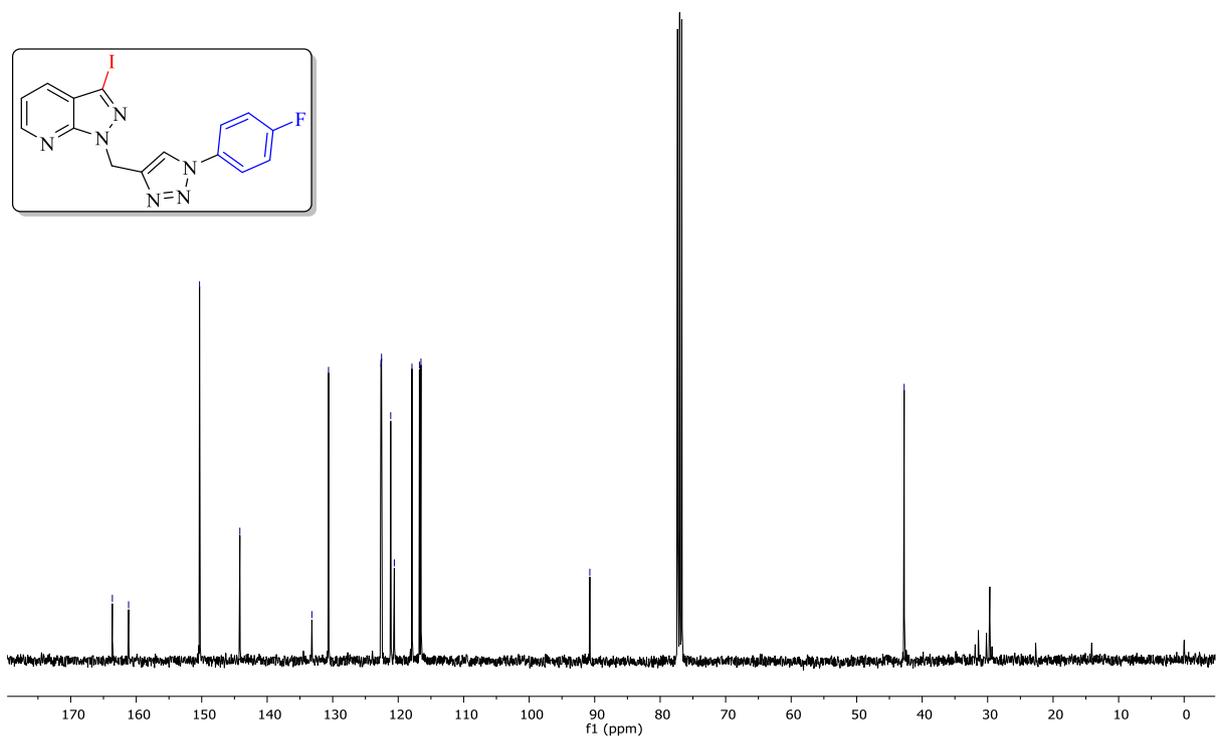
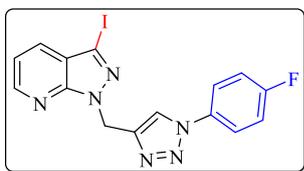
¹H NMR spectrum of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridin (25)

CY-R2-26_PROTON_20210919_01

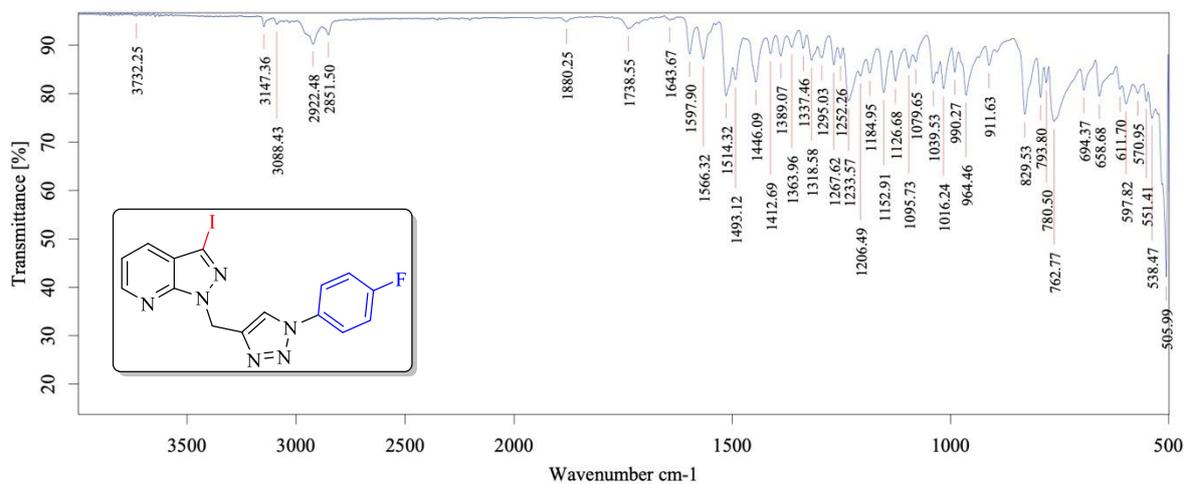


¹³C NMR spectrum of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridin (25)

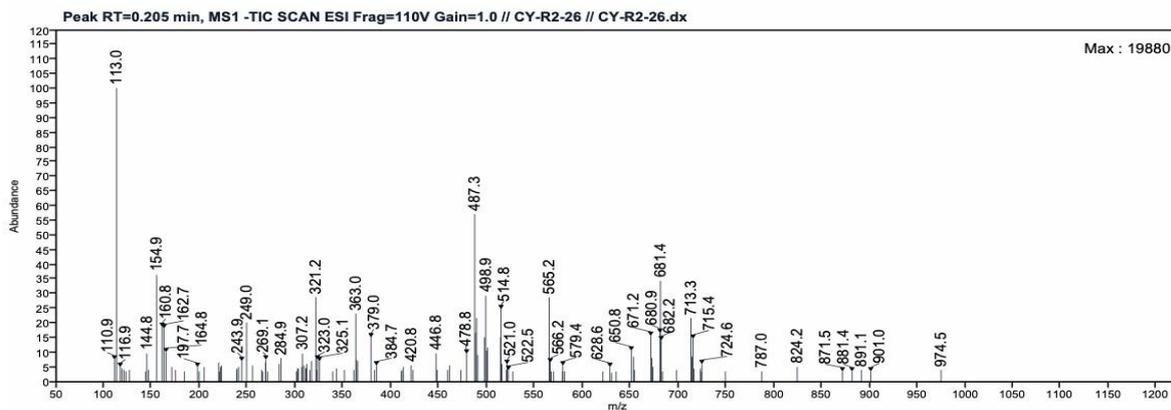
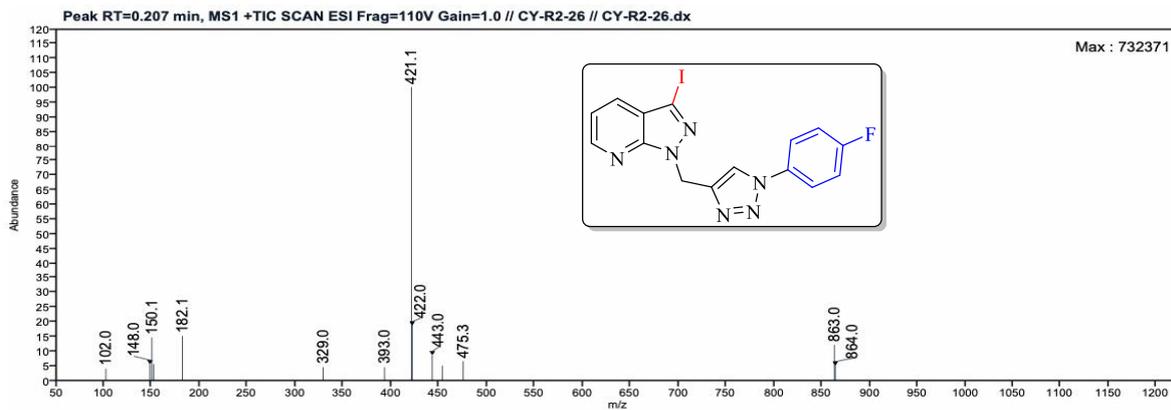
CY-R2-26_CARBON_20210919_01



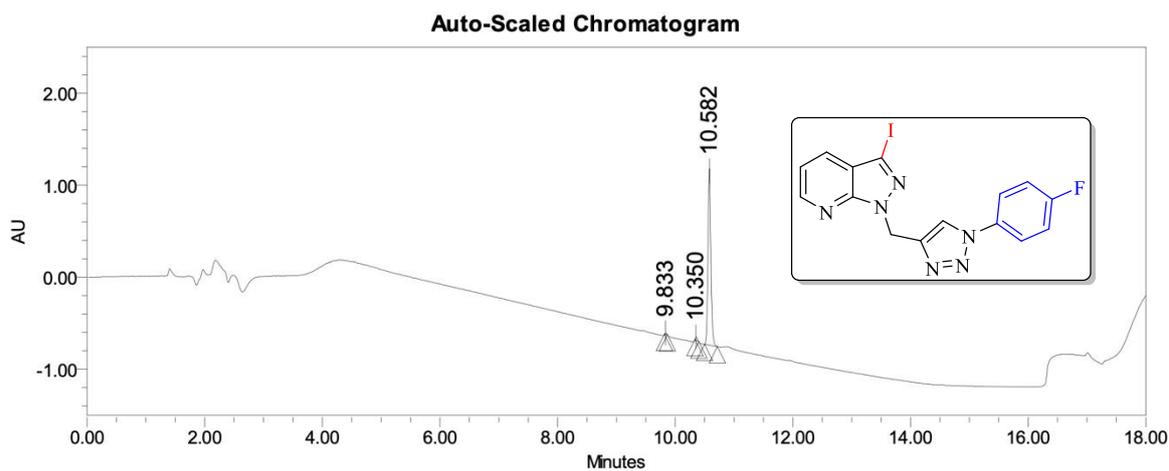
IR spectrum of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridin (25)



Mass spectrum of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridin (25)



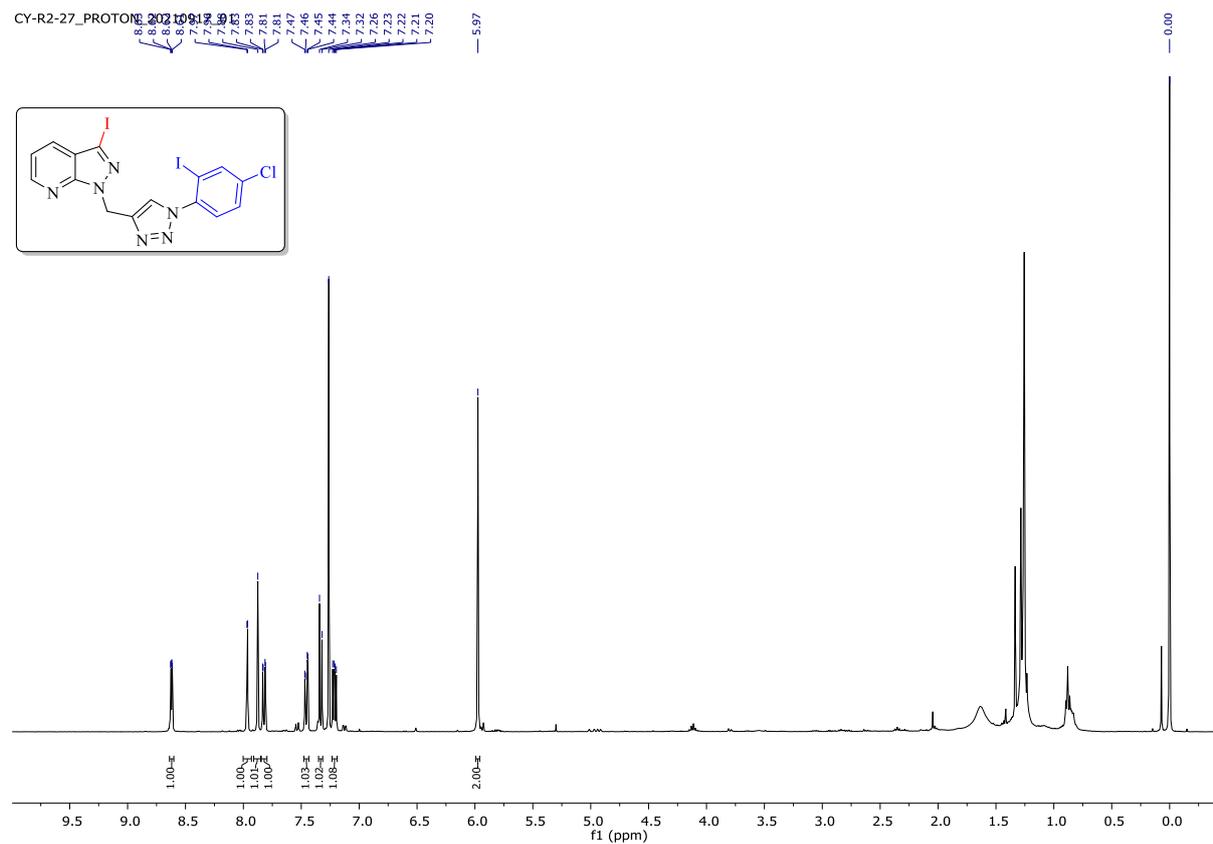
HPLC chromatogram of 1-((1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridin (25)



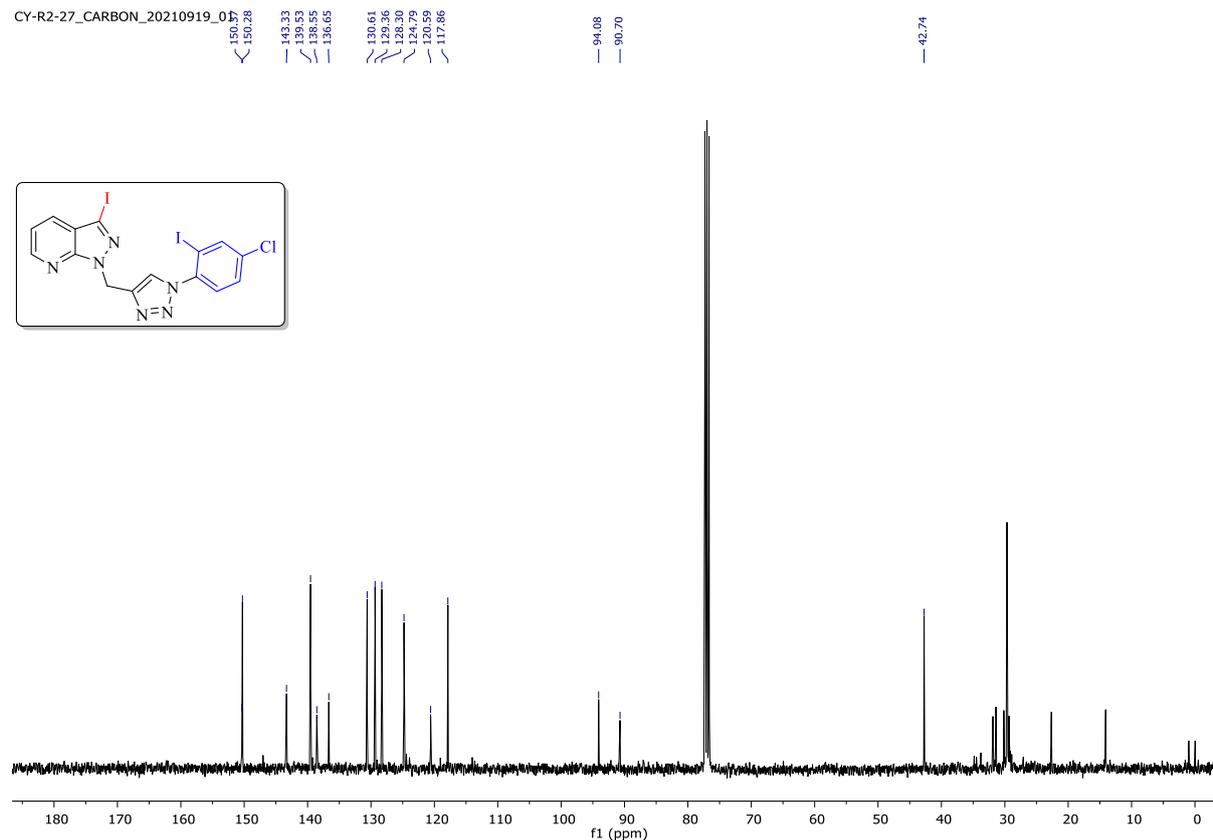
Peak Results

	Name	RT	Area	% Area
1		9.833	34621	0.53
2		10.350	77602	1.18
3		10.582	6481318	98.30

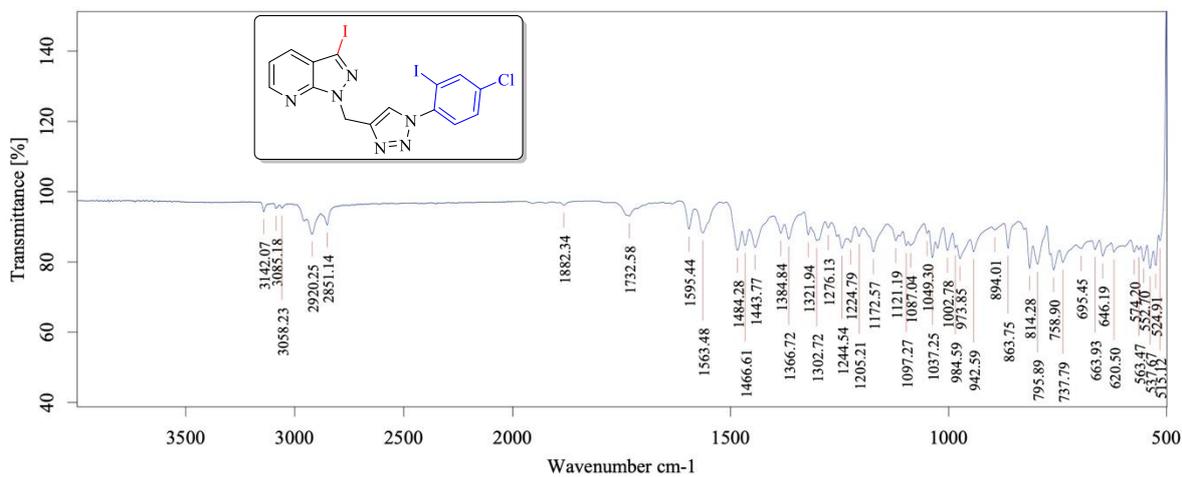
¹H NMR spectrum of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (26)



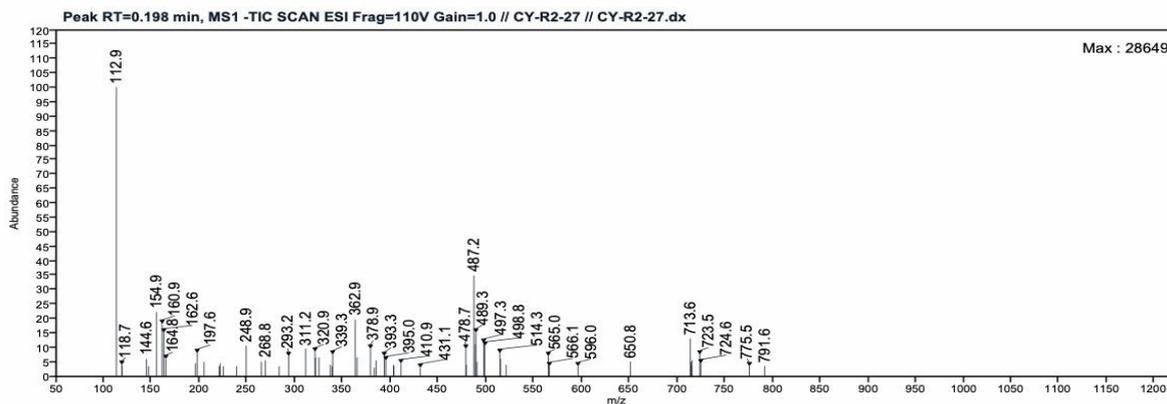
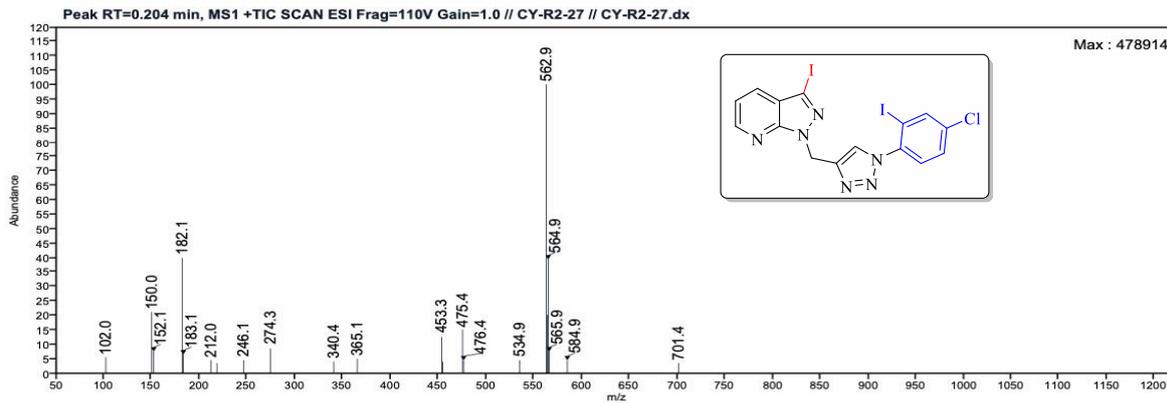
¹³C NMR spectrum of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (26)



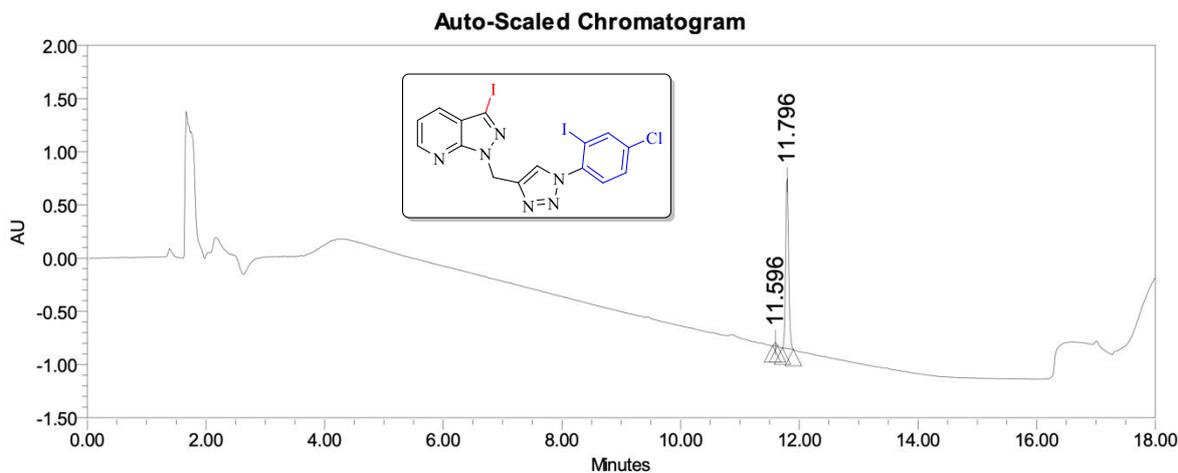
IR spectrum of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (26)



Mass spectrum of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (26)



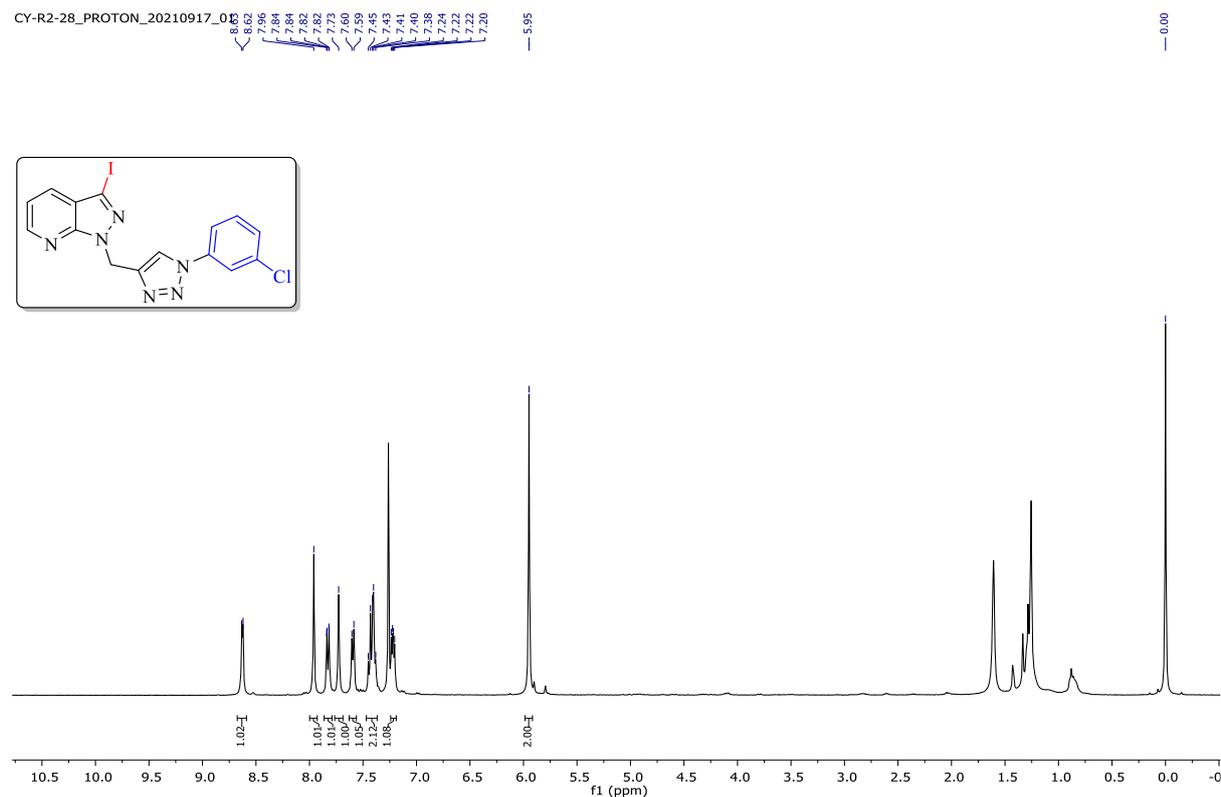
HPLC chromatogram of 1-((1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (26)



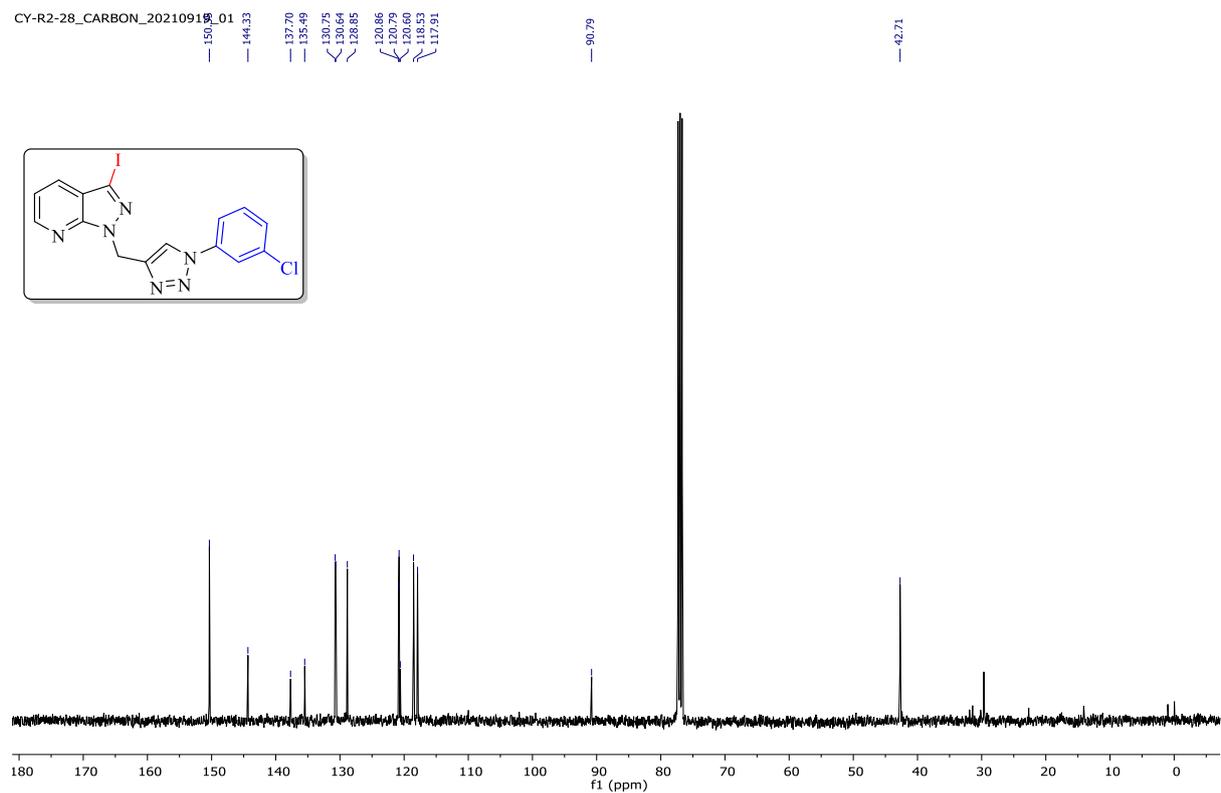
Peak Results

Name	RT	Area	% Area
1	11.596	80924	1.41
2	11.796	5672987	98.59

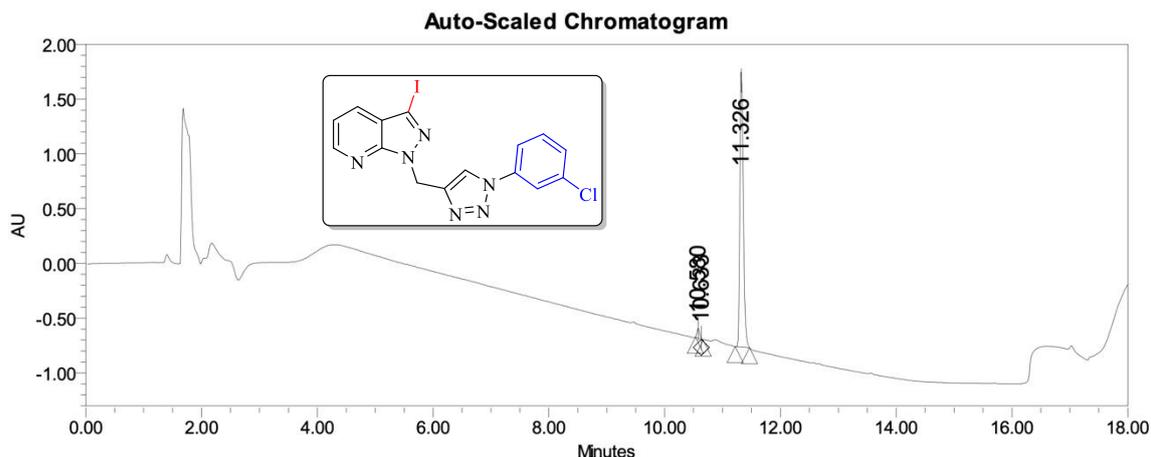
¹H NMR spectrum of 1-((1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (27)



¹³C NMR spectrum of 1-((1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (27)



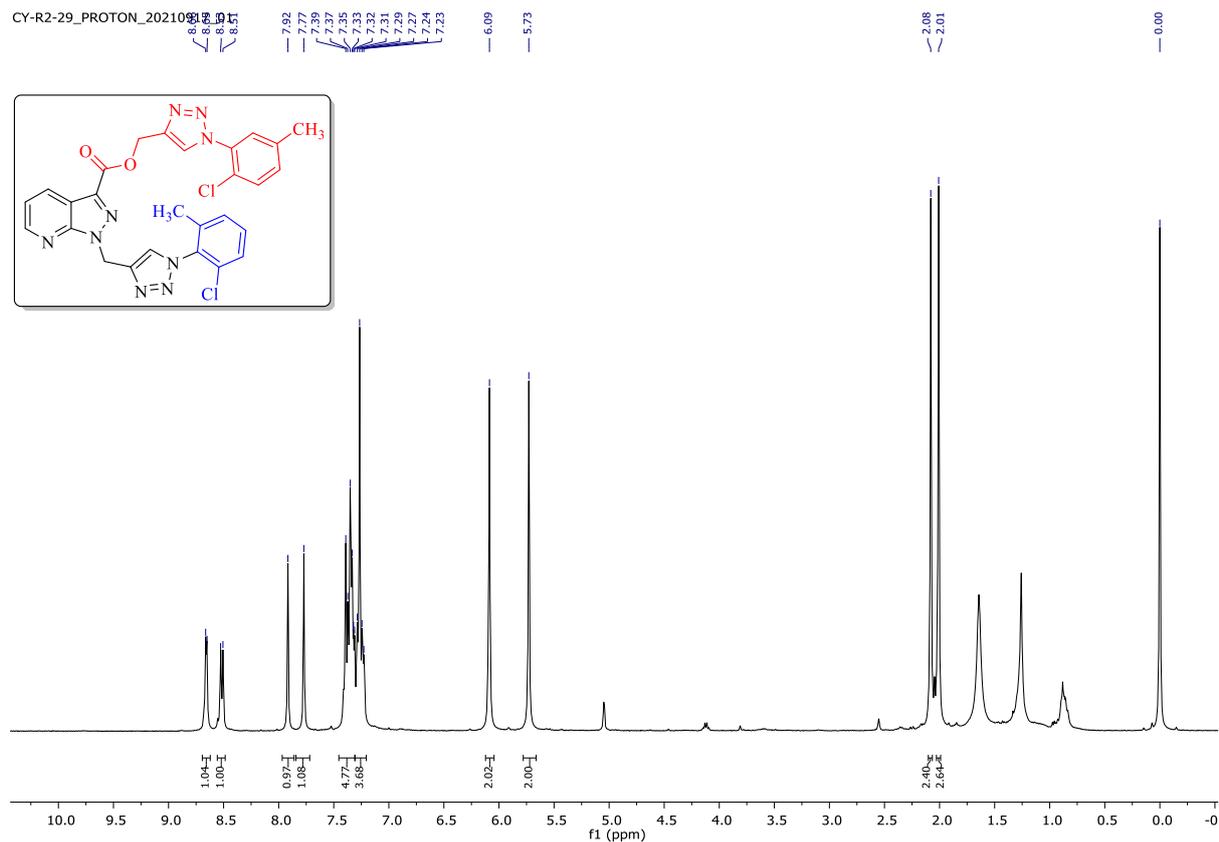
HPLC chromatogram of 1-((1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-iodo-1H-pyrazolo[3,4-b]pyridine (27)



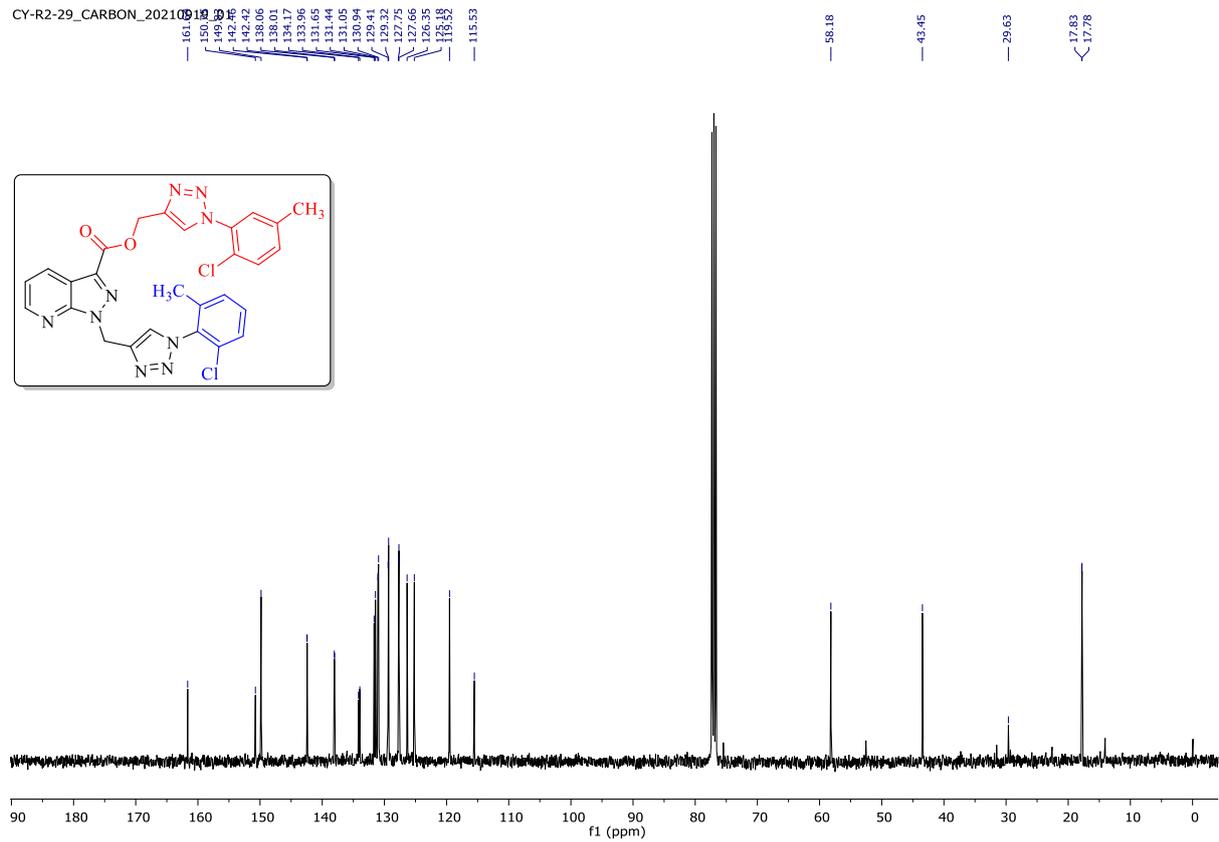
Peak Results

	Name	RT	Area	% Area
1		10.580	300138	2.84
2		10.633	16729	0.16
3		11.326	10261032	97.00

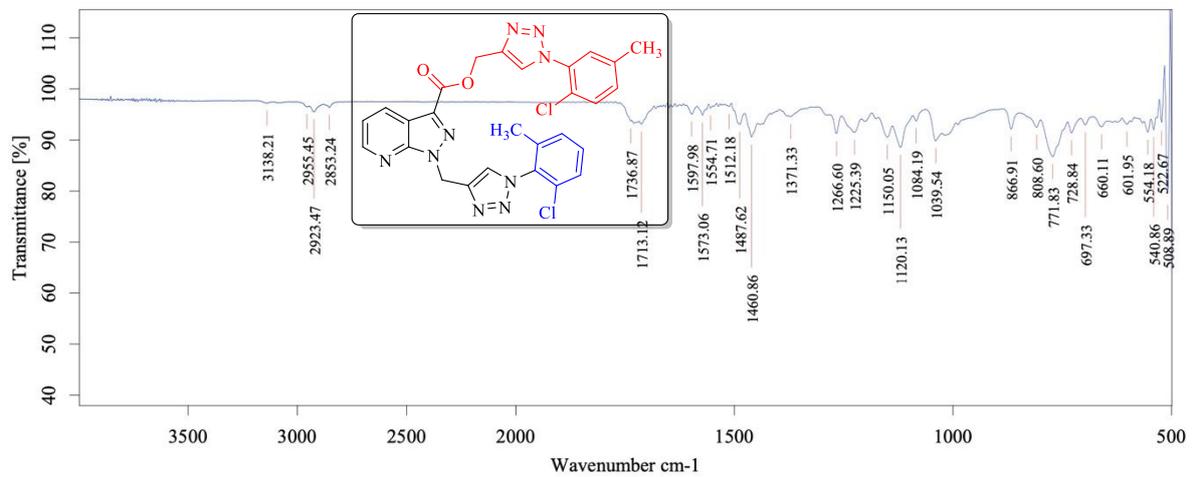
¹H NMR spectrum of (1-(2-Chloro-5-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl-1-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (28)



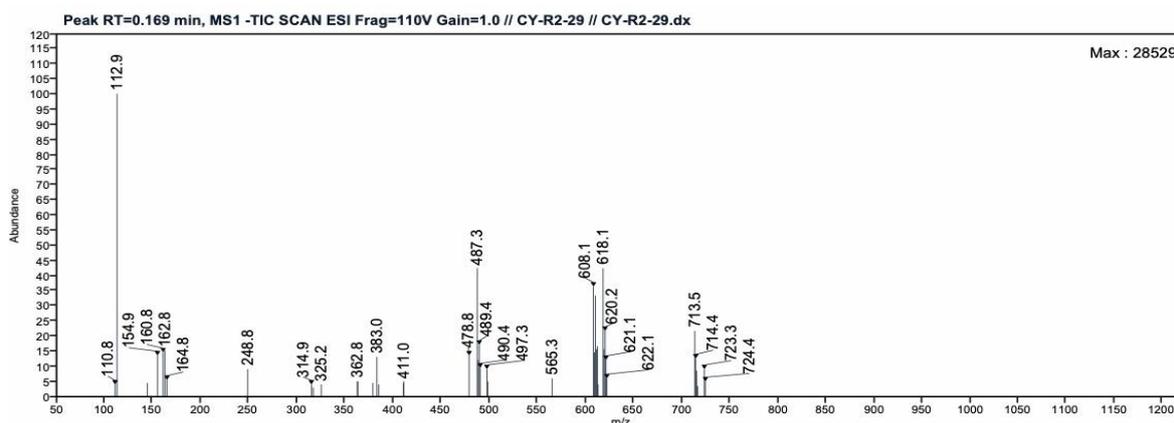
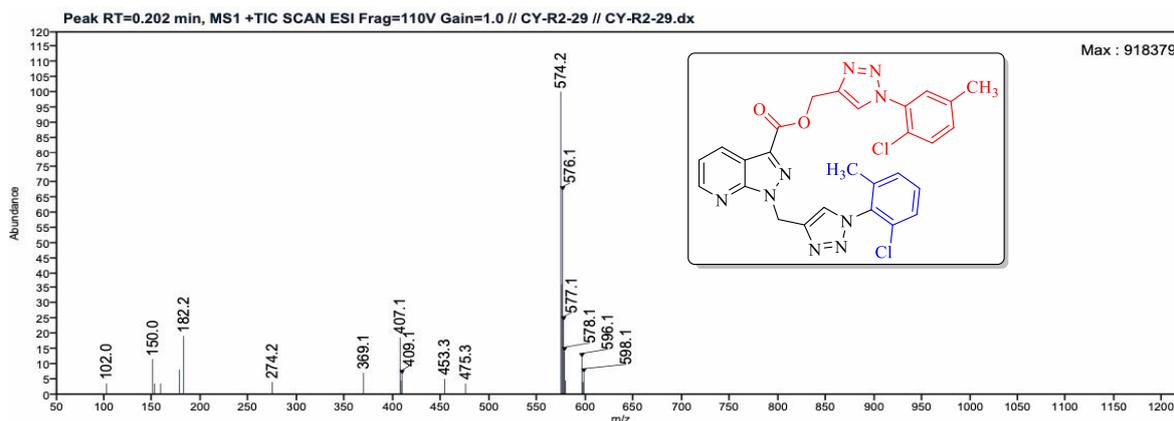
¹³C NMR spectrum of (1-(2-Chloro-5-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (28)



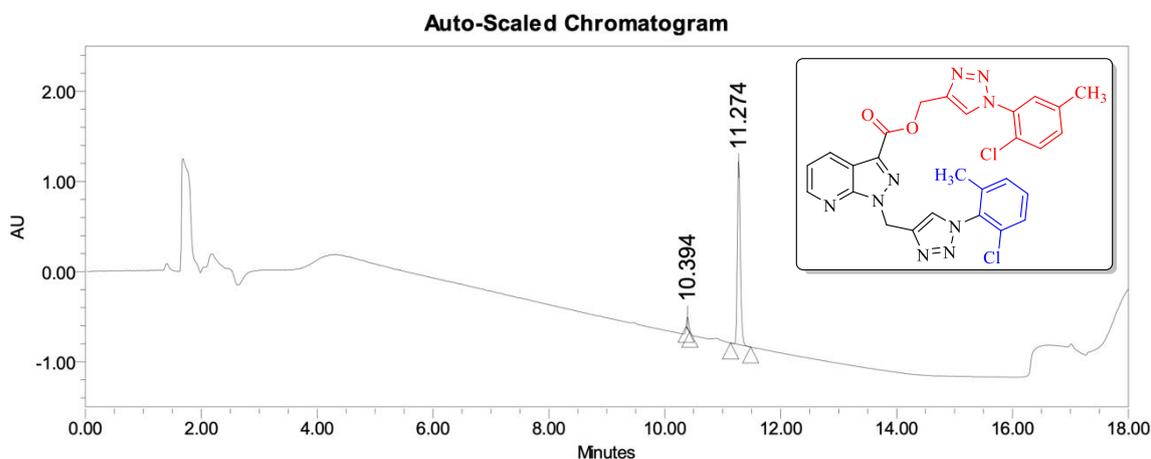
IR spectrum of (1-(2-Chloro-5-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (28)



Mass spectrum of (1-(2-Chloro-5-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (28)



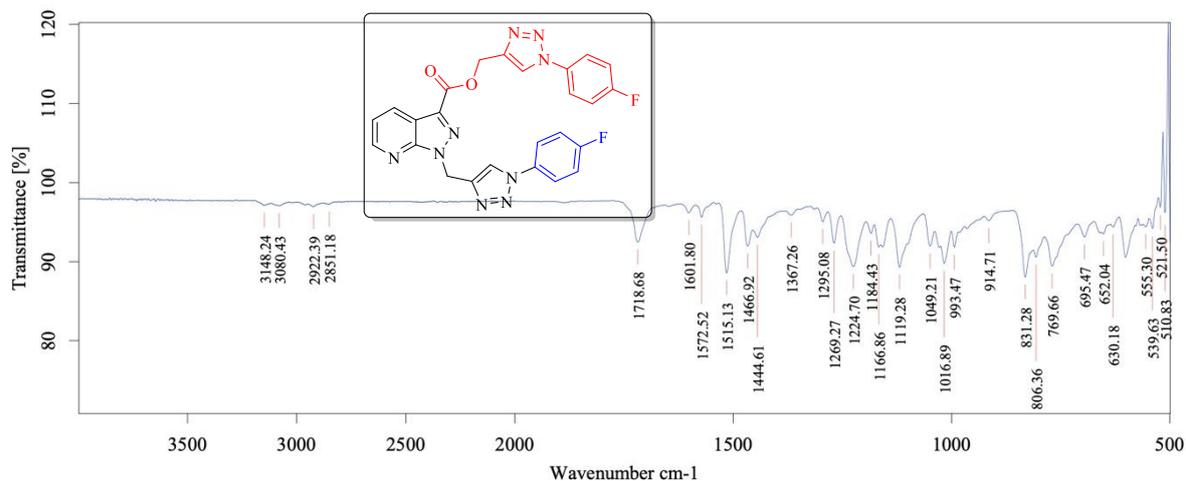
HPLC chromatogram of (1-(2-Chloro-5-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl-((1-(2-chloro-6-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (28)



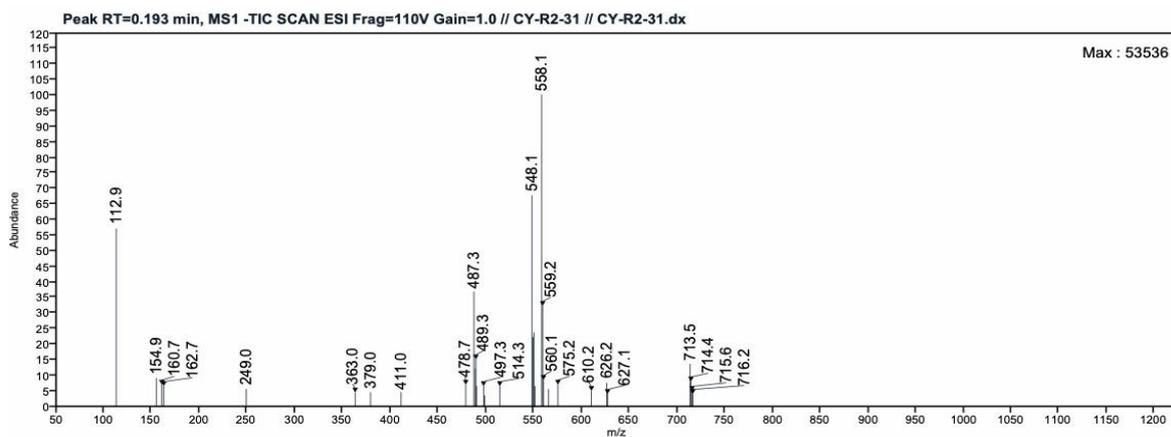
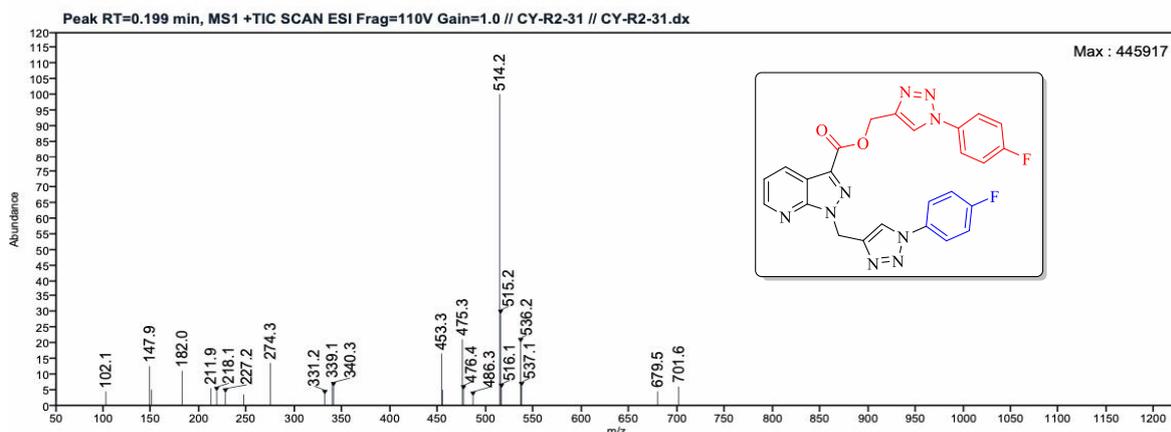
Peak Results

	Name	RT	Area	% Area
1		10.394	289952	3.86
2		11.274	7227763	96.14

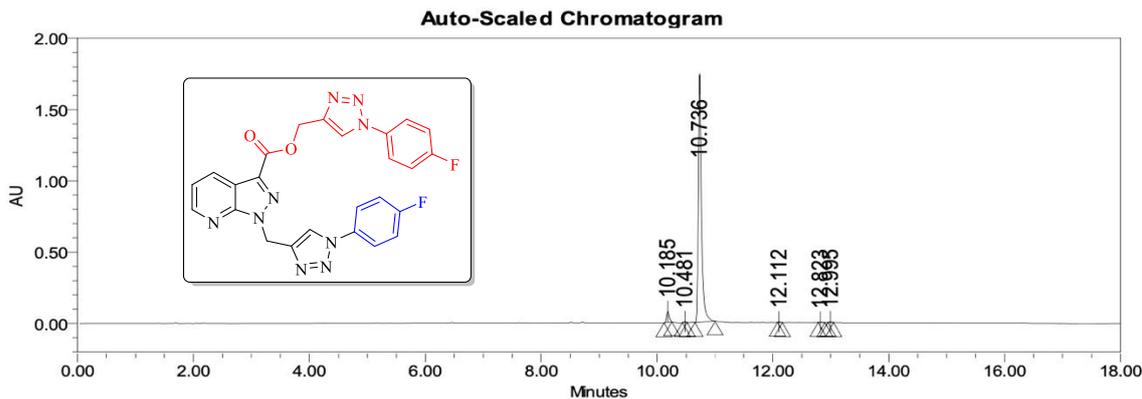
IR spectrum of (1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (29)



Mass spectrum of (1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (29)



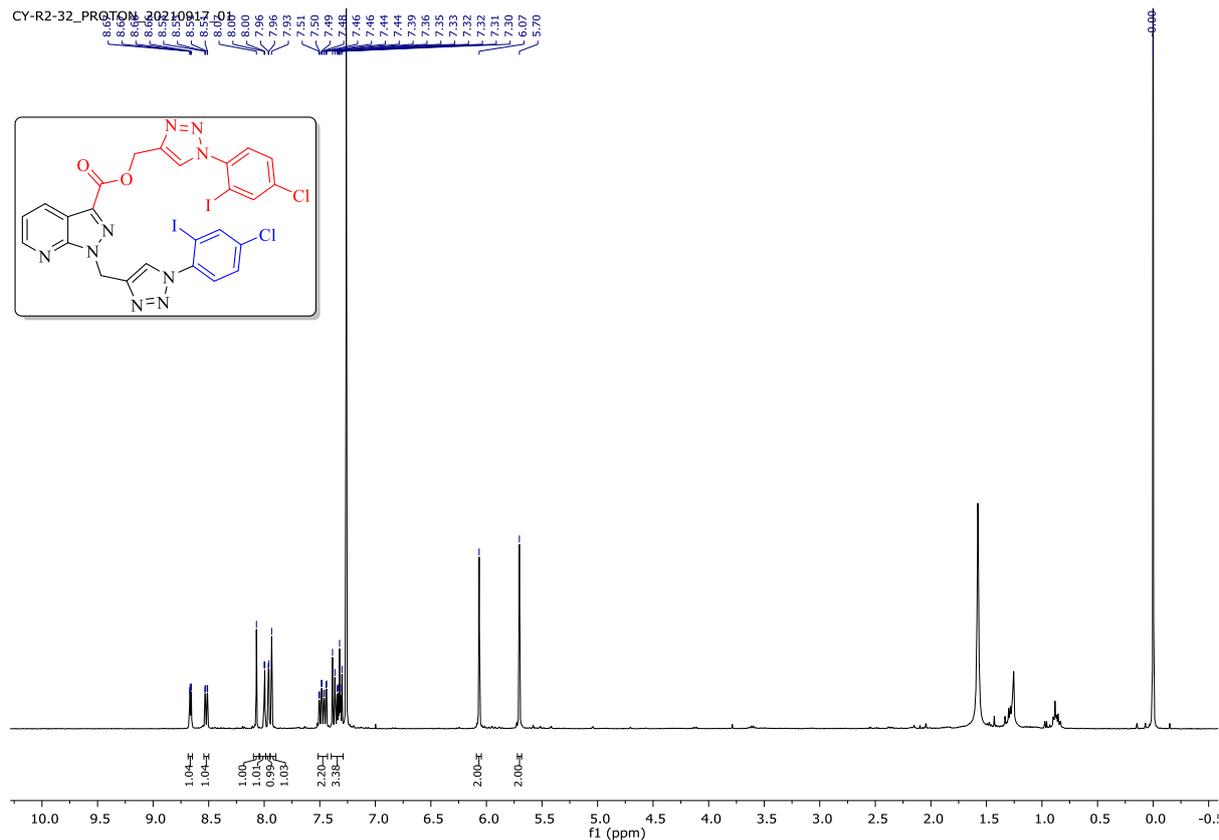
HPLC chromatogram of (1-(4-Fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (29)



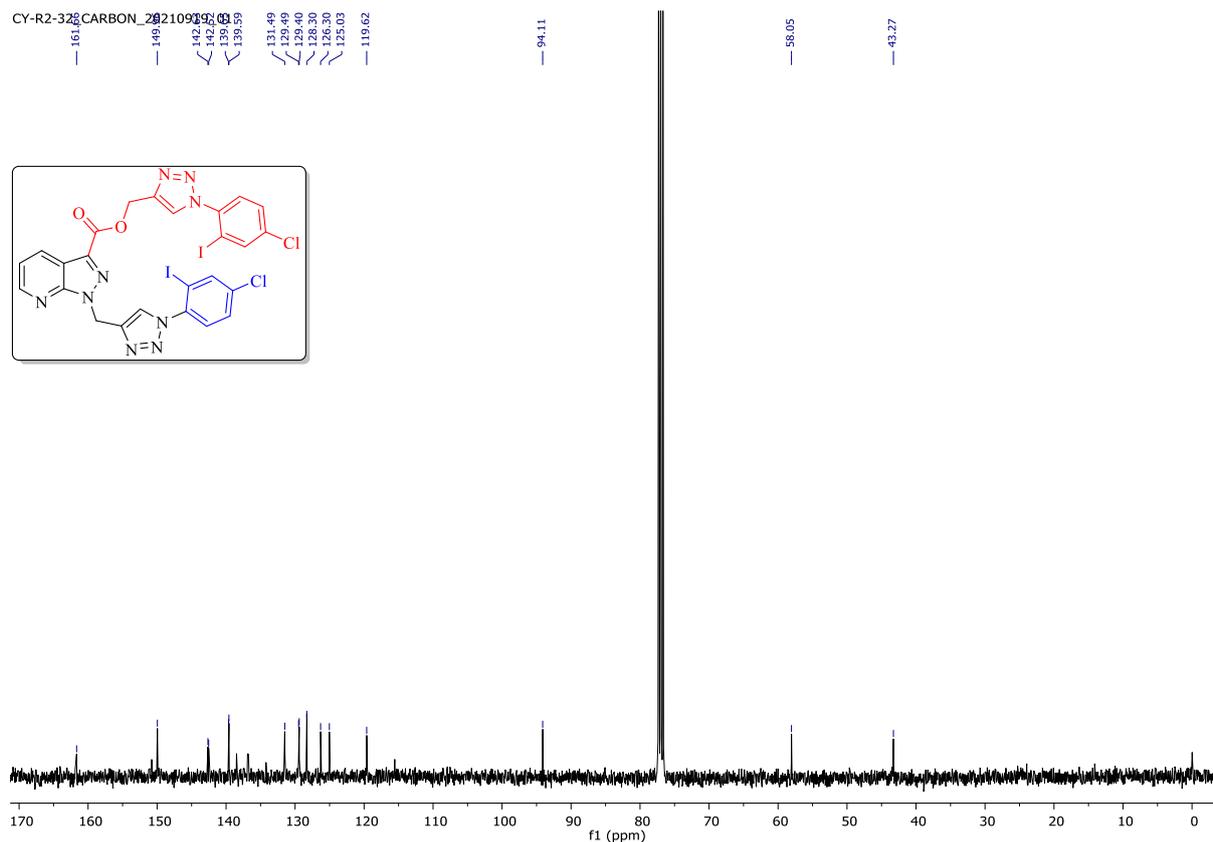
Peak Results

	Name	RT	Area	% Area
1		10.185	242899	3.66
2		10.481	20449	0.31
3		10.736	6330986	95.27
4		12.112	11445	0.17
5		12.823	15600	0.23

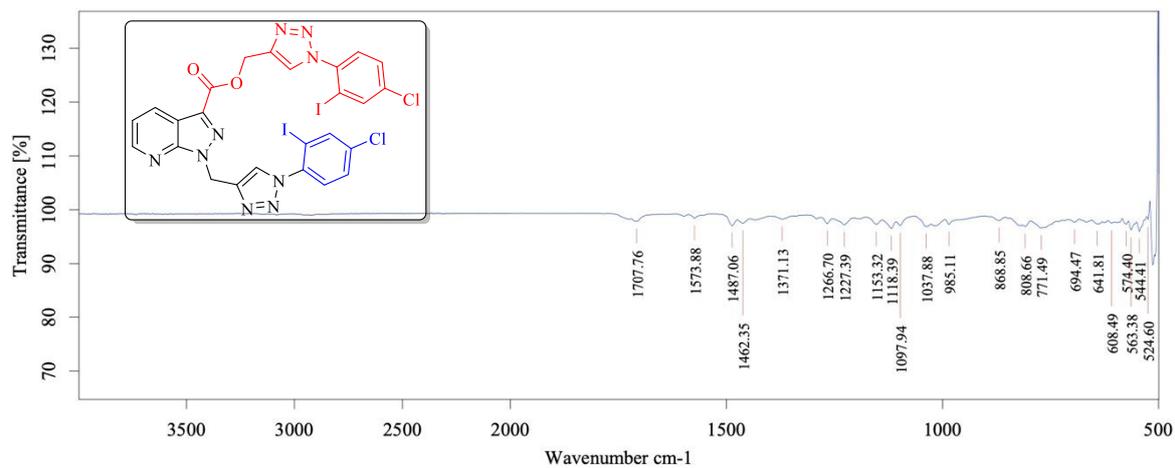
¹H NMR spectrum of (1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(4-chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (30)



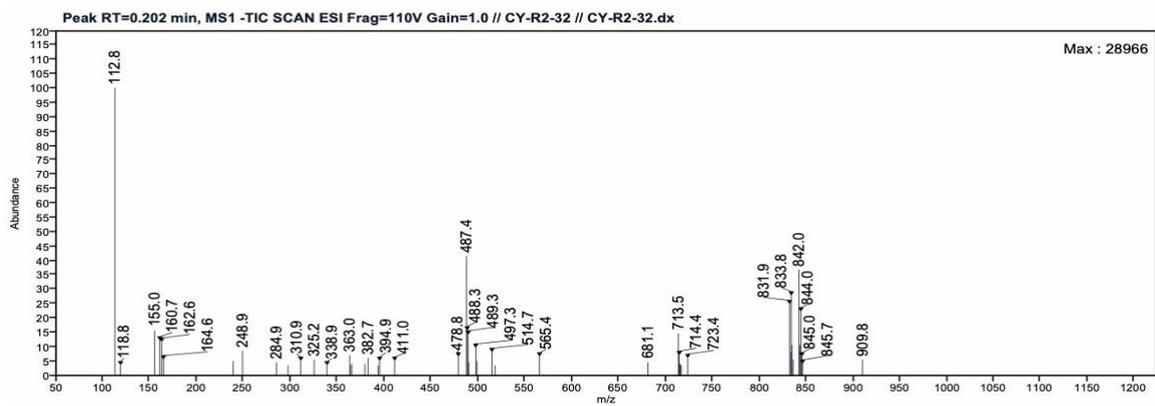
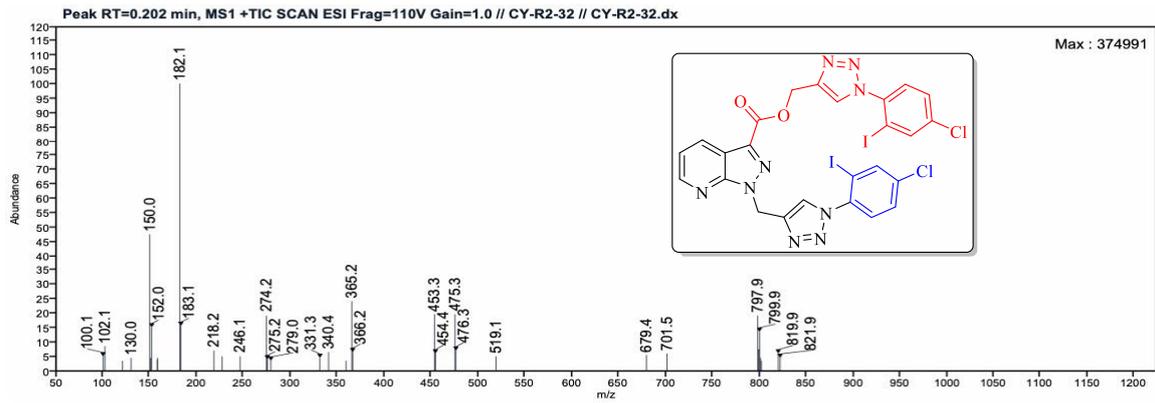
¹³C NMR spectrum of (1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(4-chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (30)



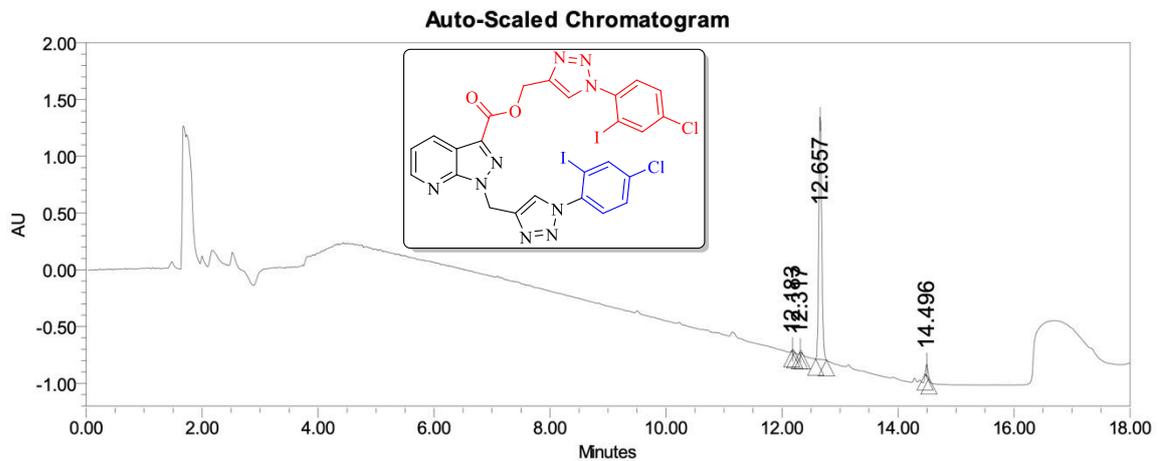
IR spectrum of (1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(4-chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (30)



Mass spectrum of (1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(4-chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (30)



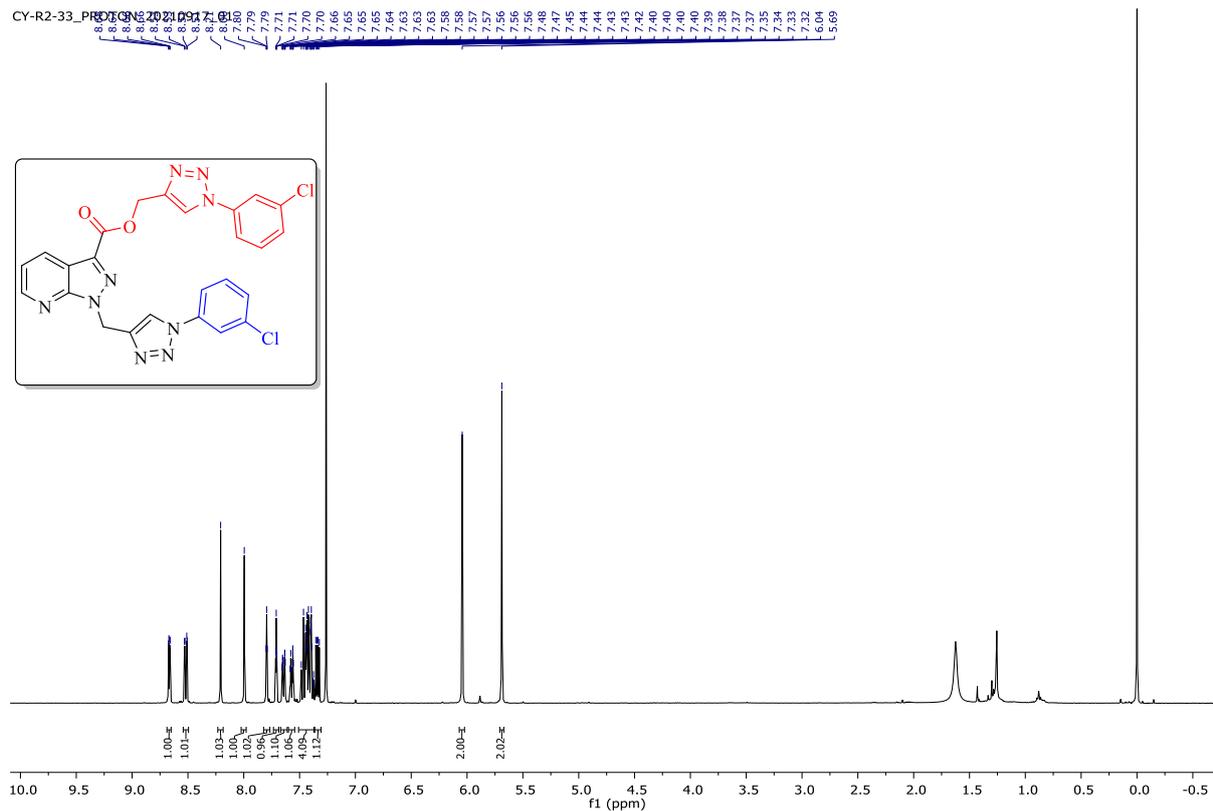
HPLC chromatogram of (1-(4-Chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(4-chloro-2-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (30)



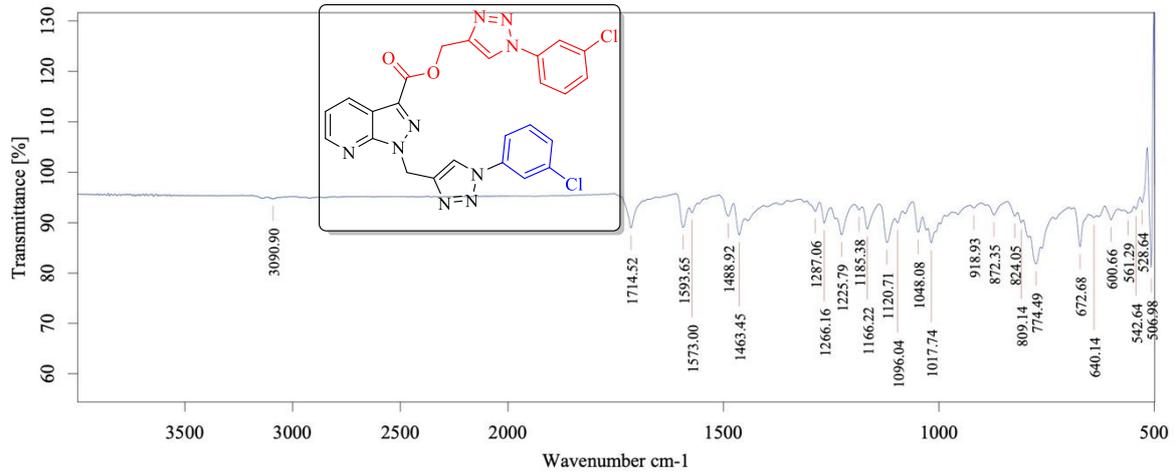
Peak Results

	Name	RT	Area	% Area
1		12.183	25667	0.32
2		12.317	40781	0.50
3		12.657	7807837	96.28
4		14.496	234849	2.90

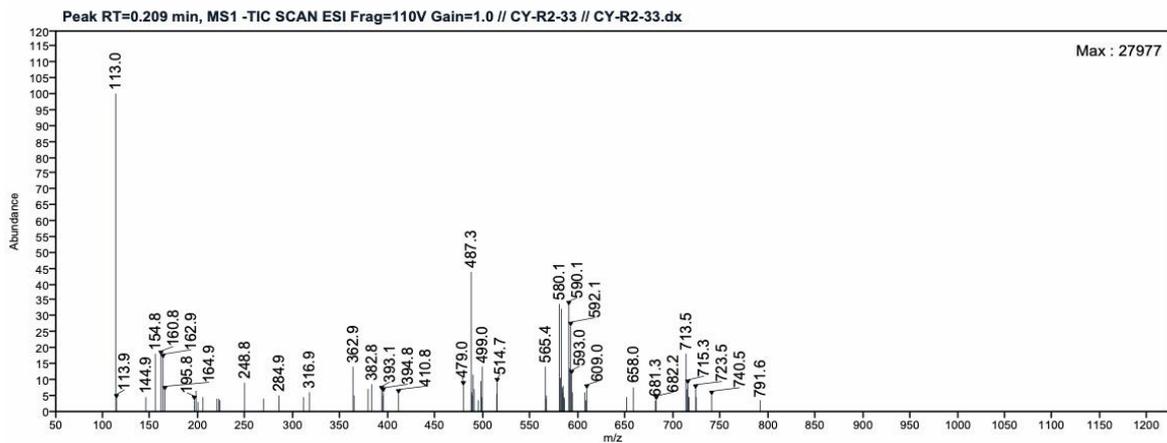
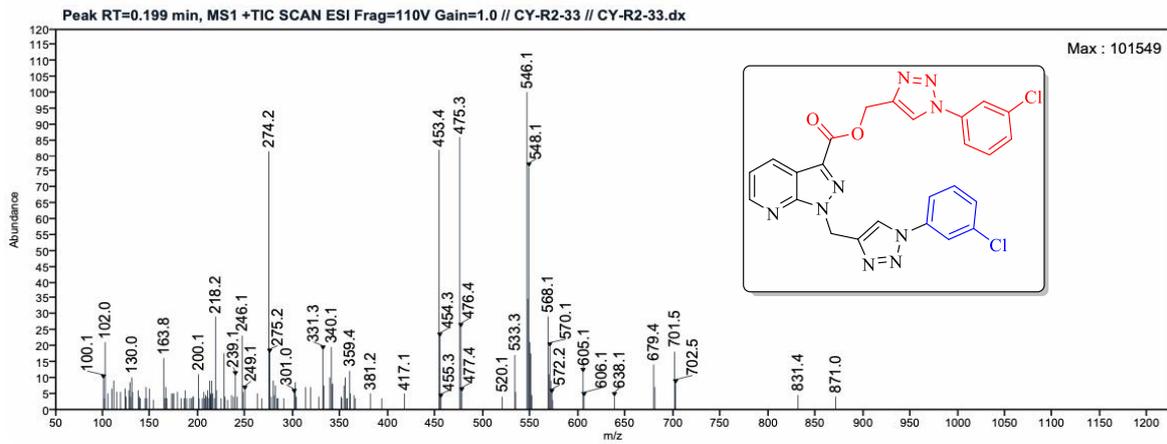
¹H NMR spectrum of (1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (31)



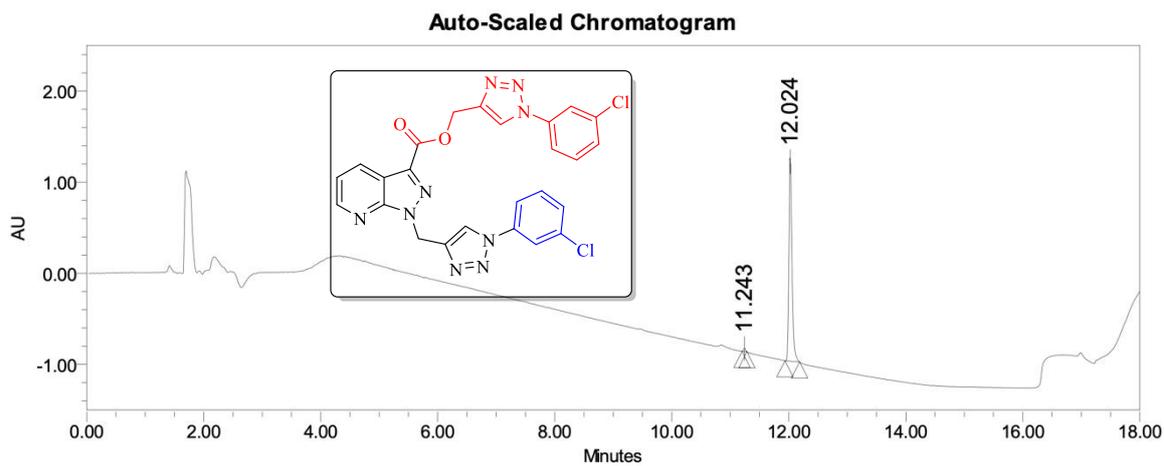
IR spectrum of (1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (31)



Mass spectrum of (1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (31)



HPLC chromatogram of (1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl 1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxylate (31)



Peak Results

	Name	RT	Area	% Area
1		11.243	94473	1.13
2		12.024	8264804	98.87