Identification of Gallic acid based Glycoconjugates as a novel anti-tumor agents targeting tubulin polymerization

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Supporting Information

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2D spectra and complete chemical shifts value for compound 4d and 4d' S72-S79

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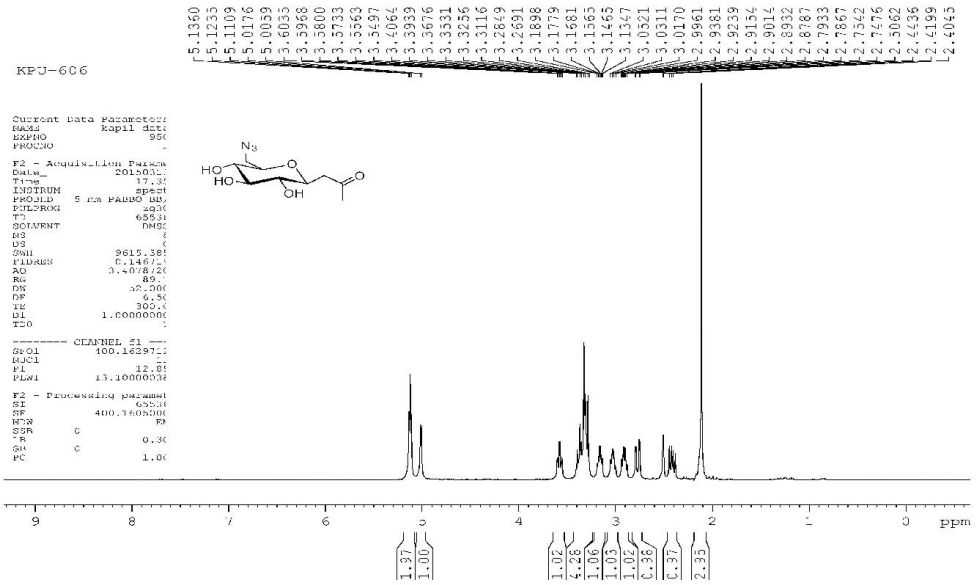
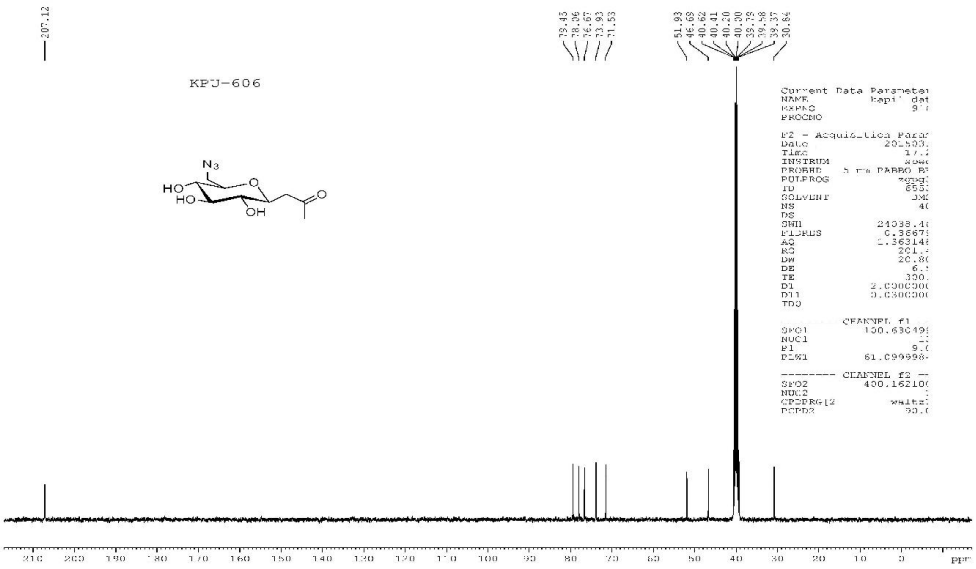
^{1}H NMR spectrum of compound **b'**



^{13}C NMR spectrum of compound **b'**



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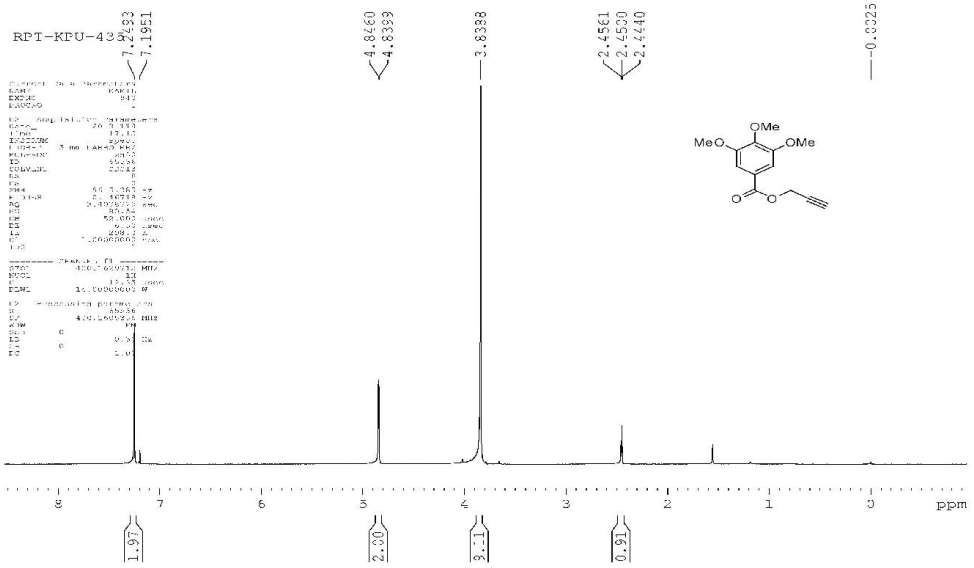

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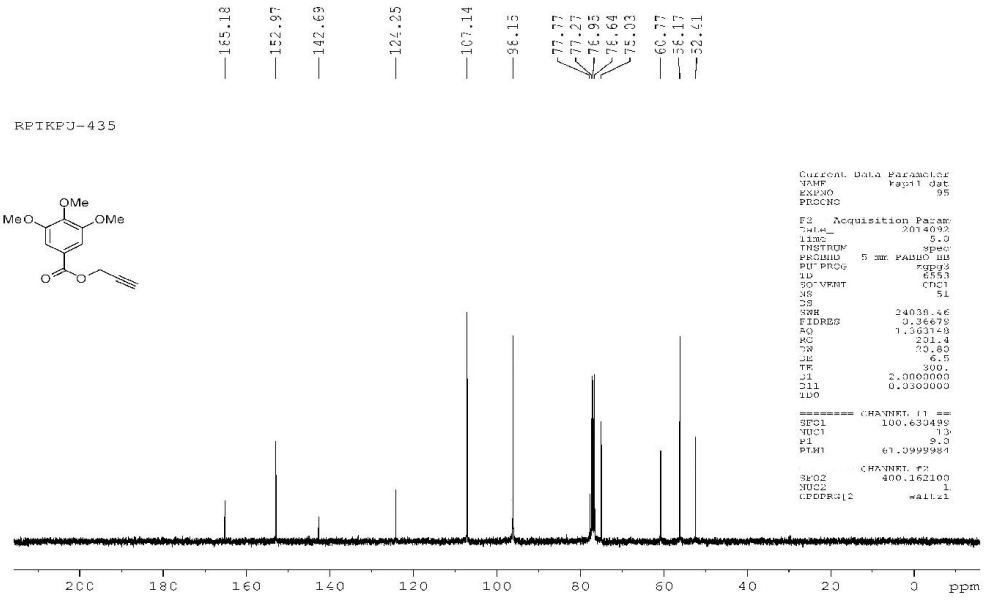
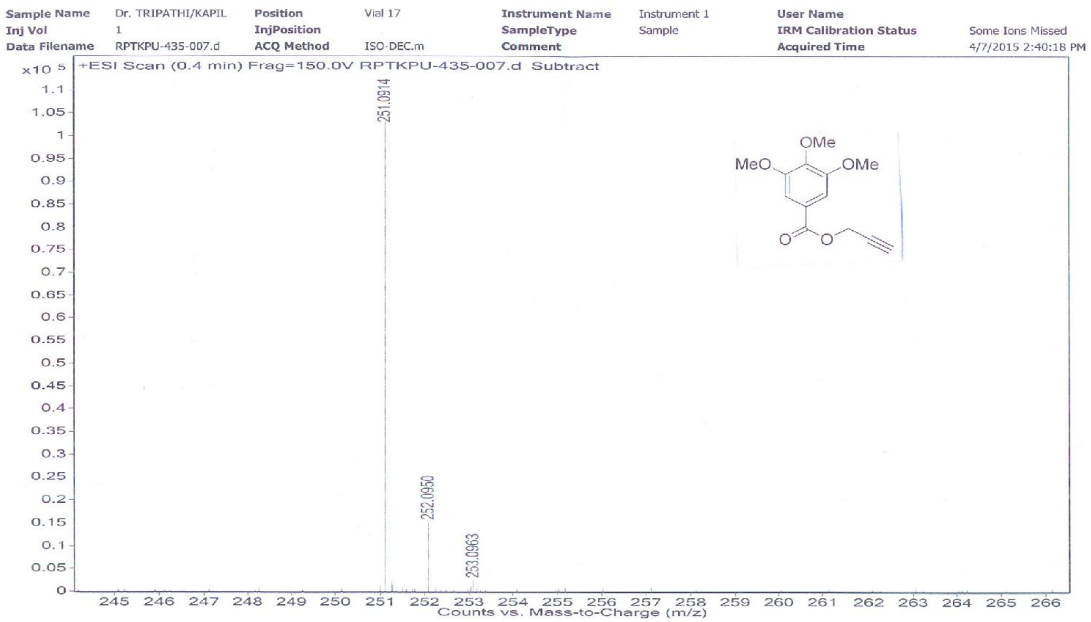


HRMS spectrum of compound **2**



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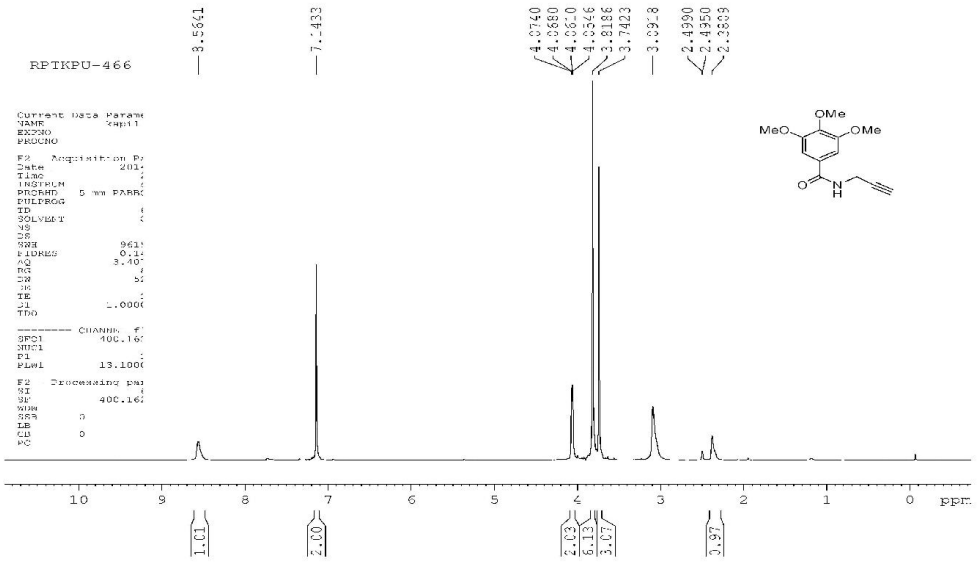
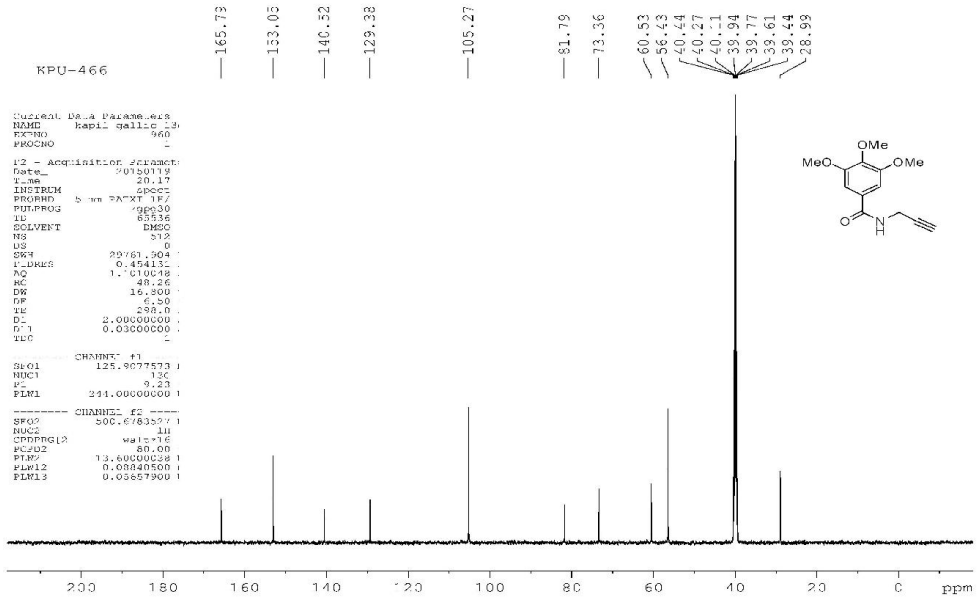
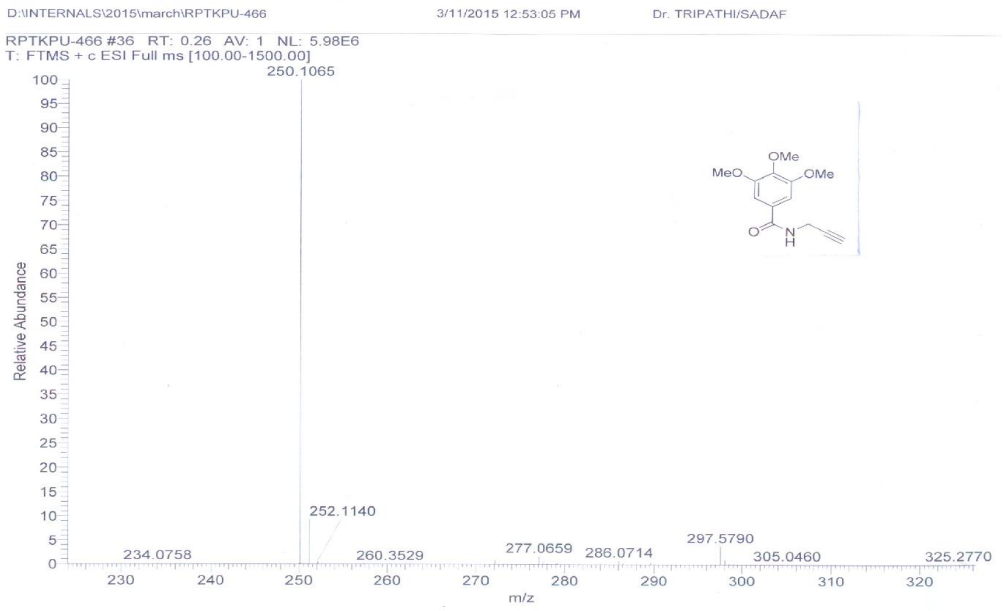


^{13}C NMR spectrum of compound **4**



HRMS spectrum of compound **4**



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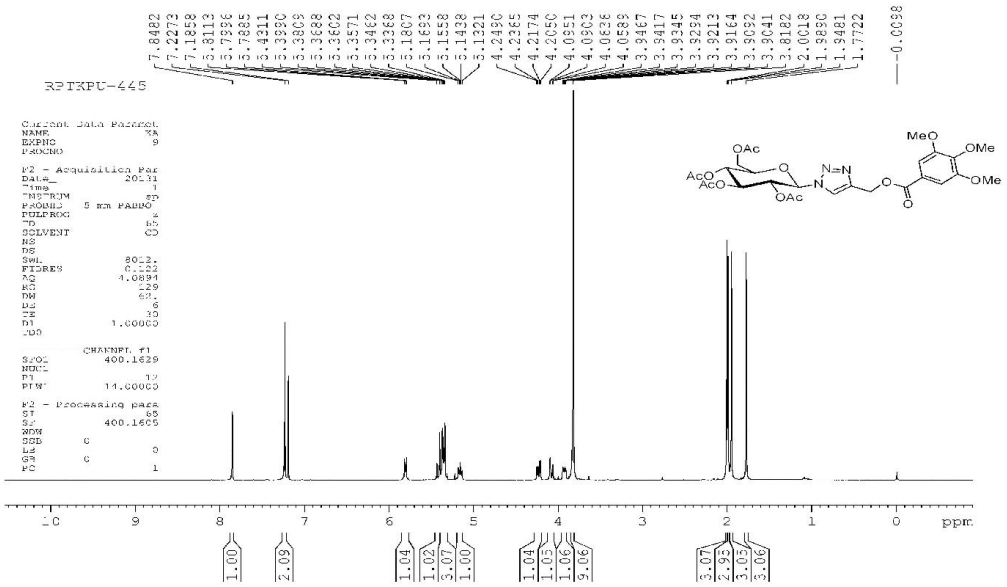

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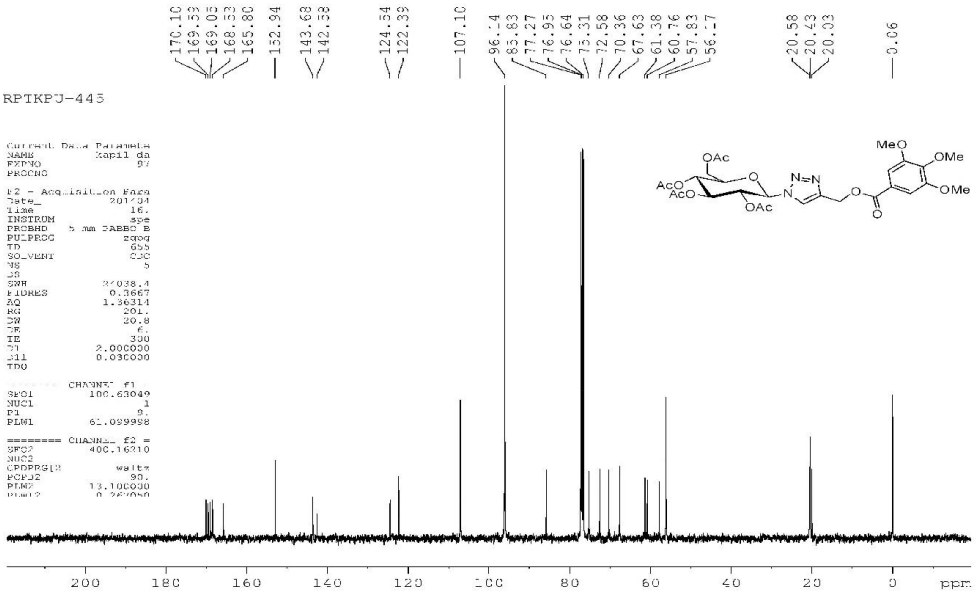
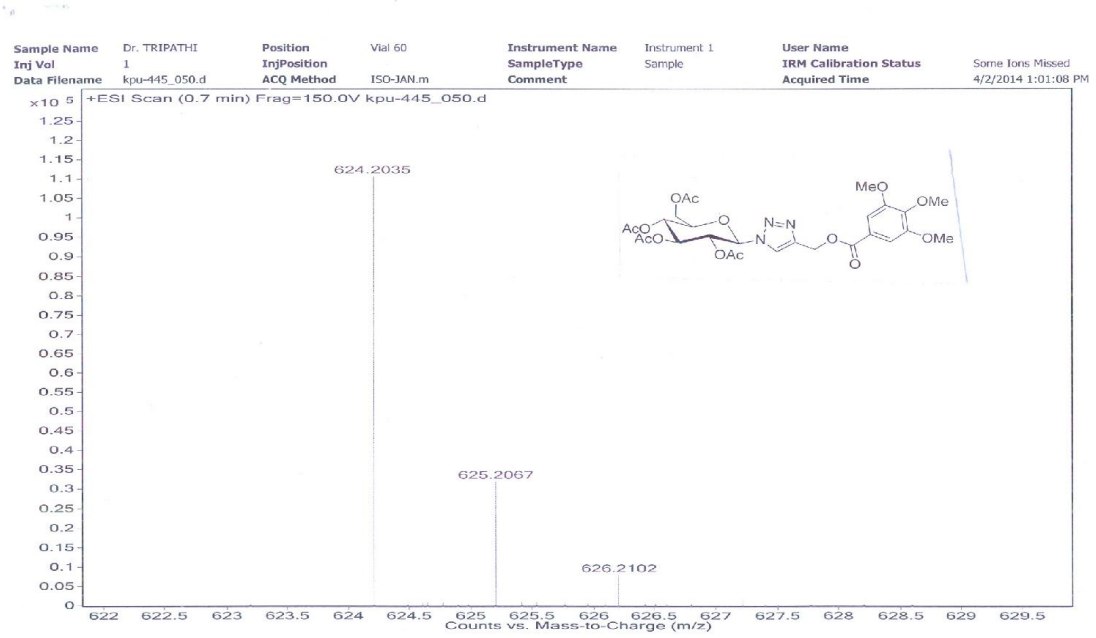


HRMS spectrum of compound **2a**



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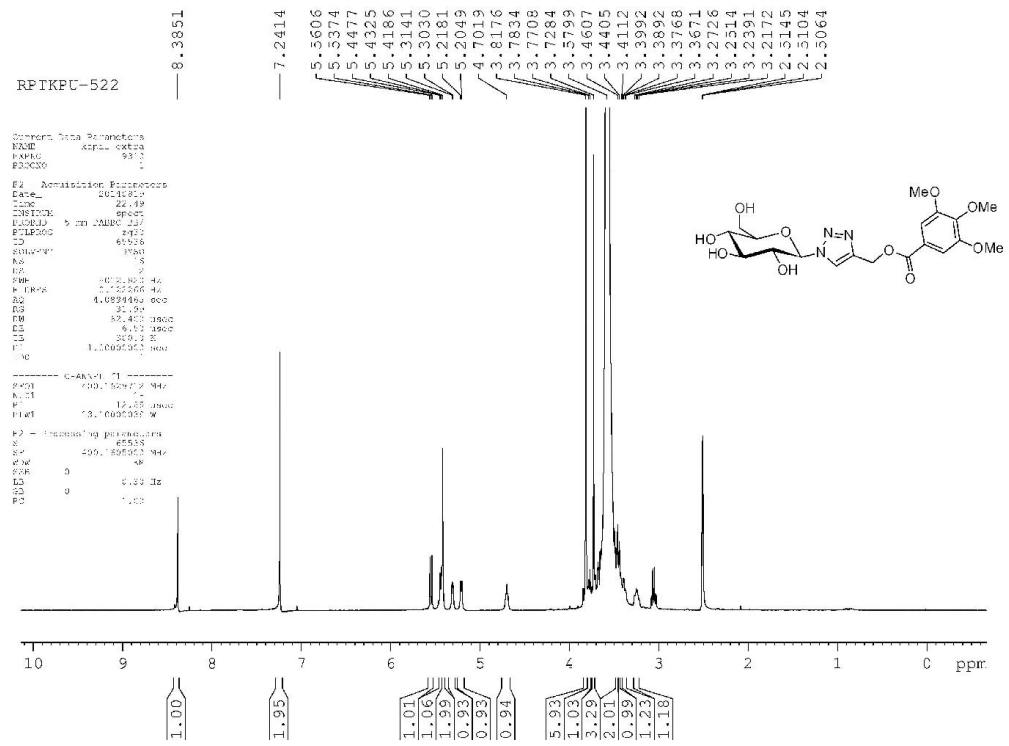

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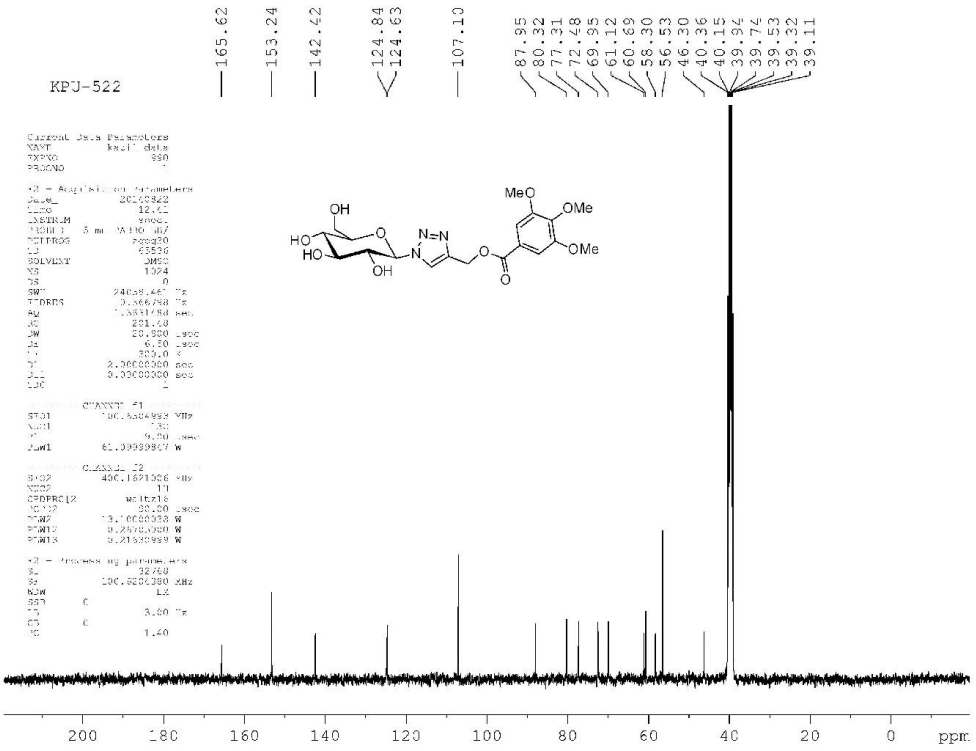

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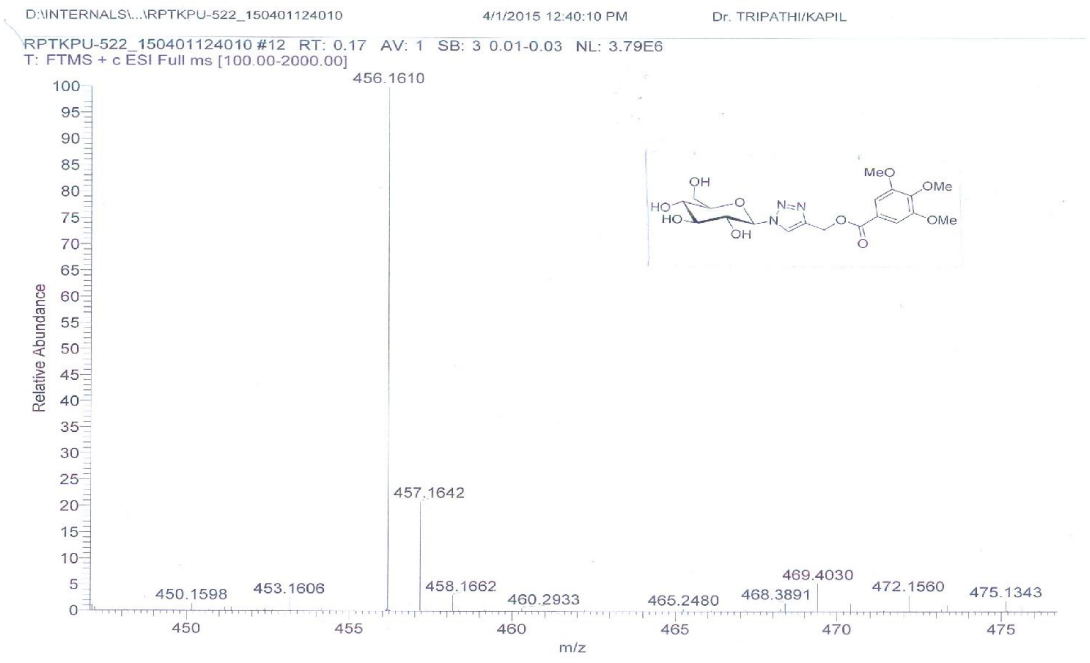

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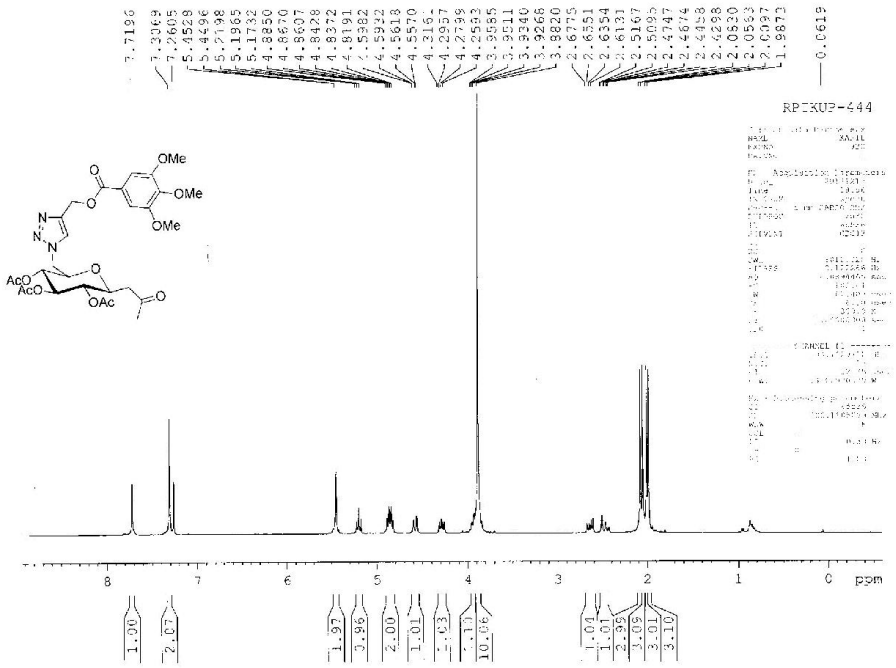

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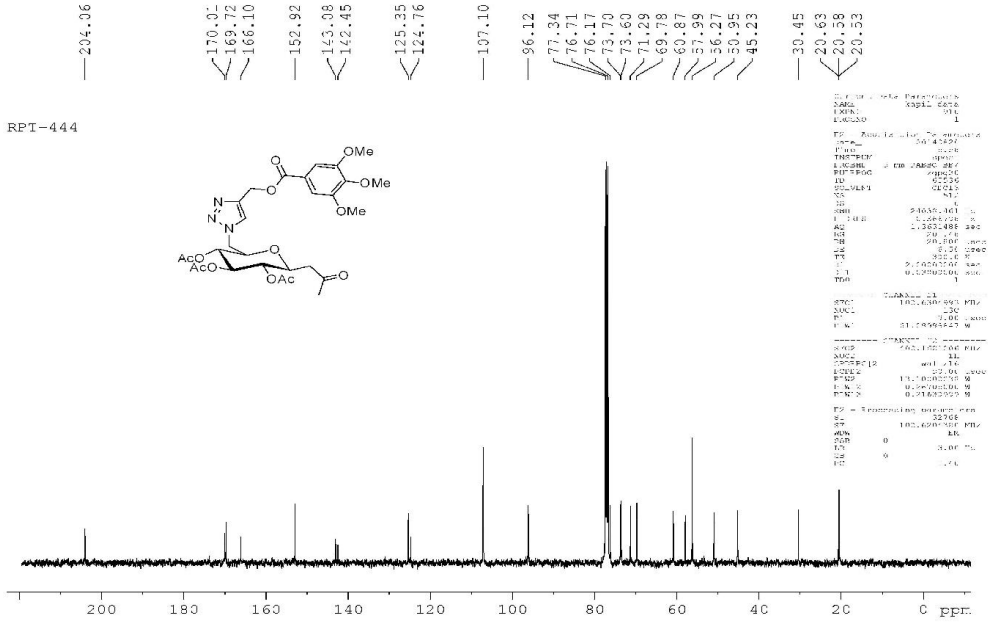

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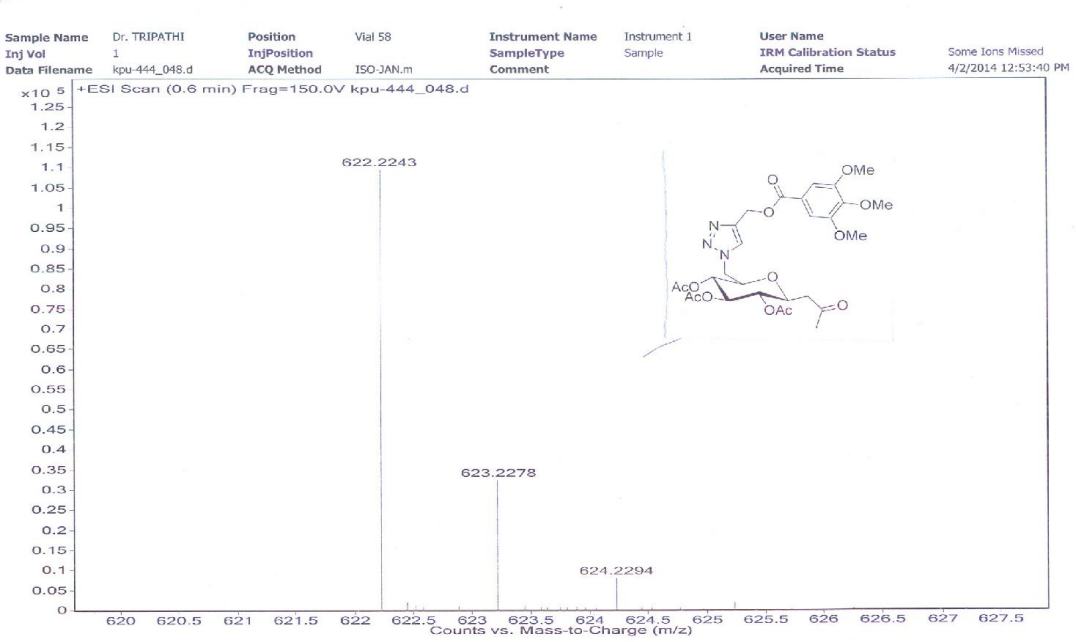
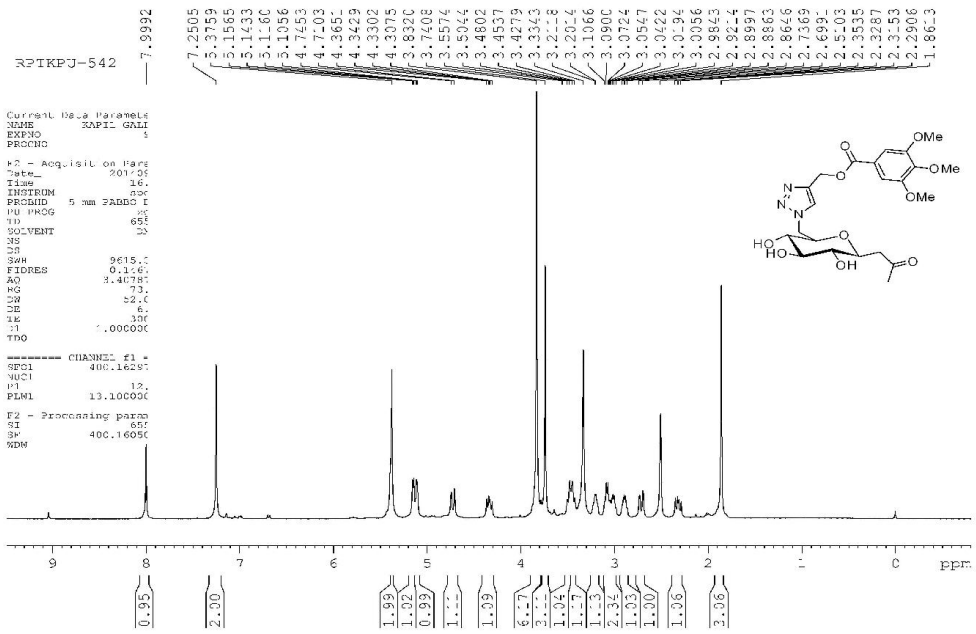


^{1}H NMR spectrum of compound **2b'**



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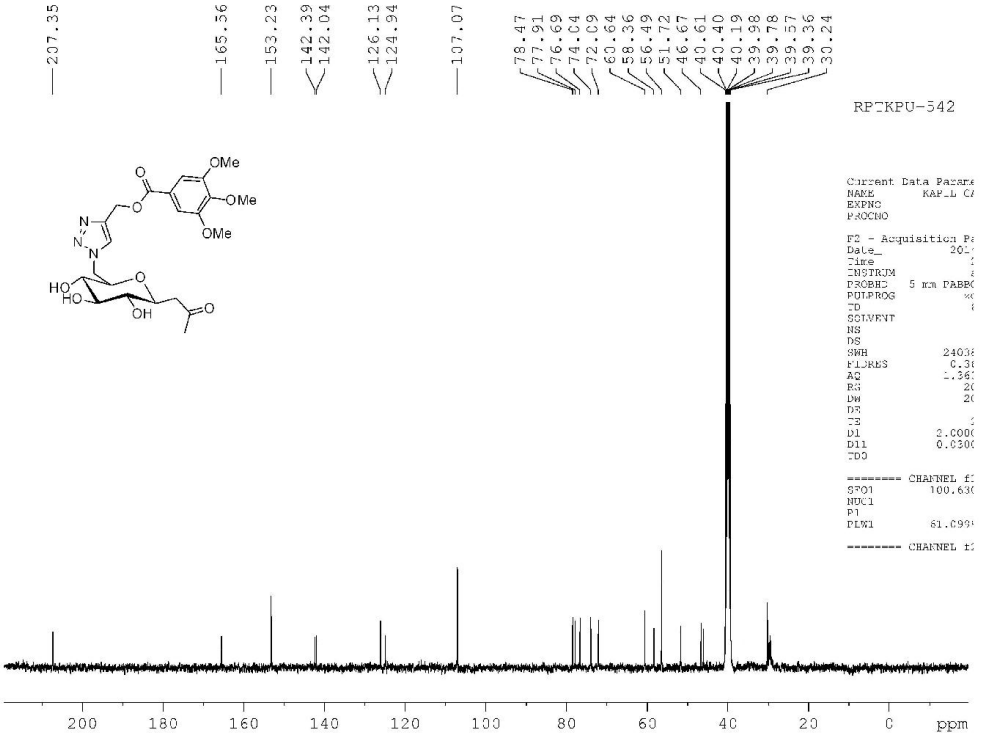

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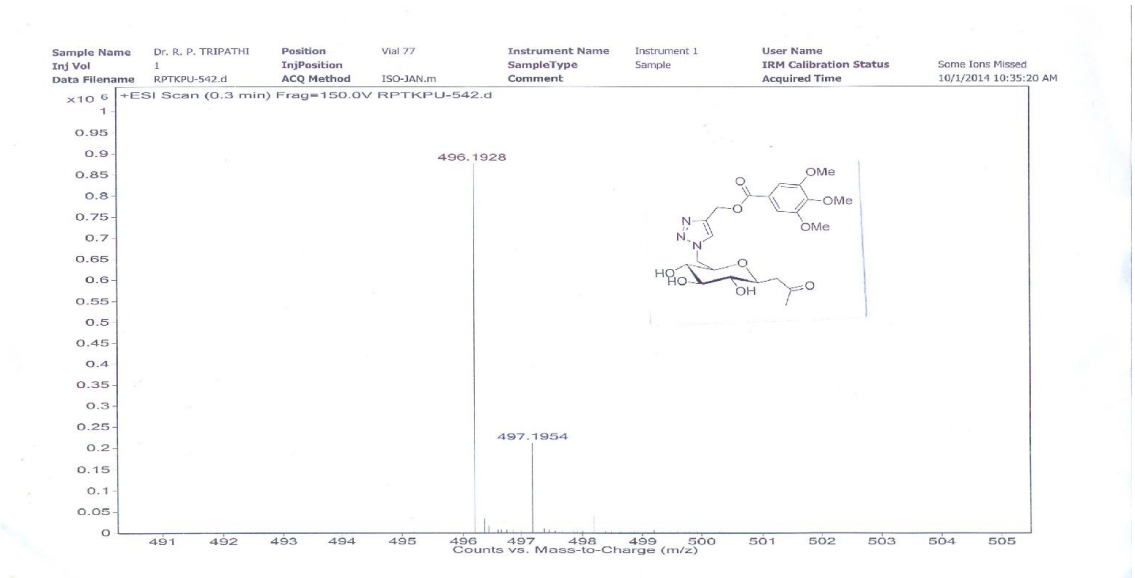
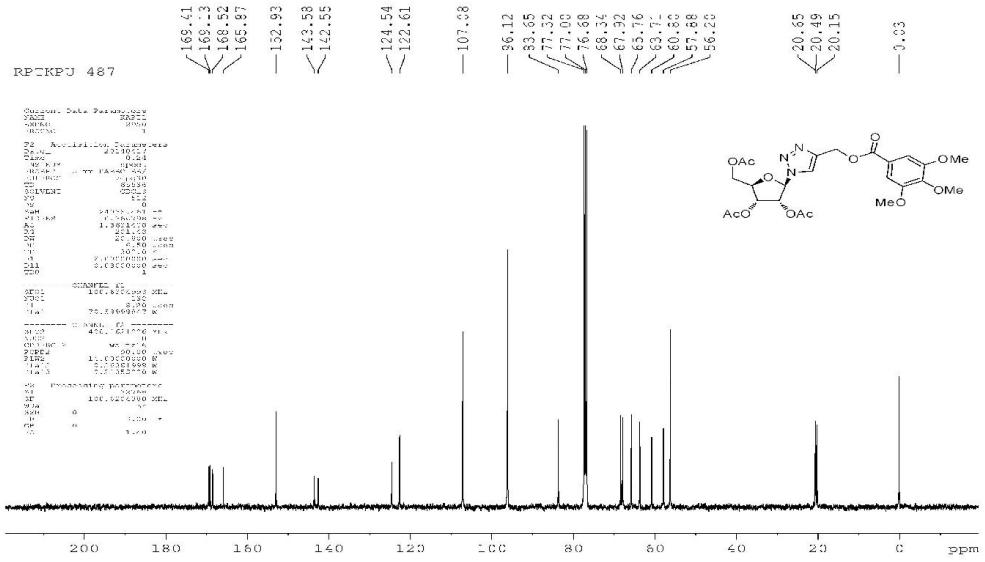
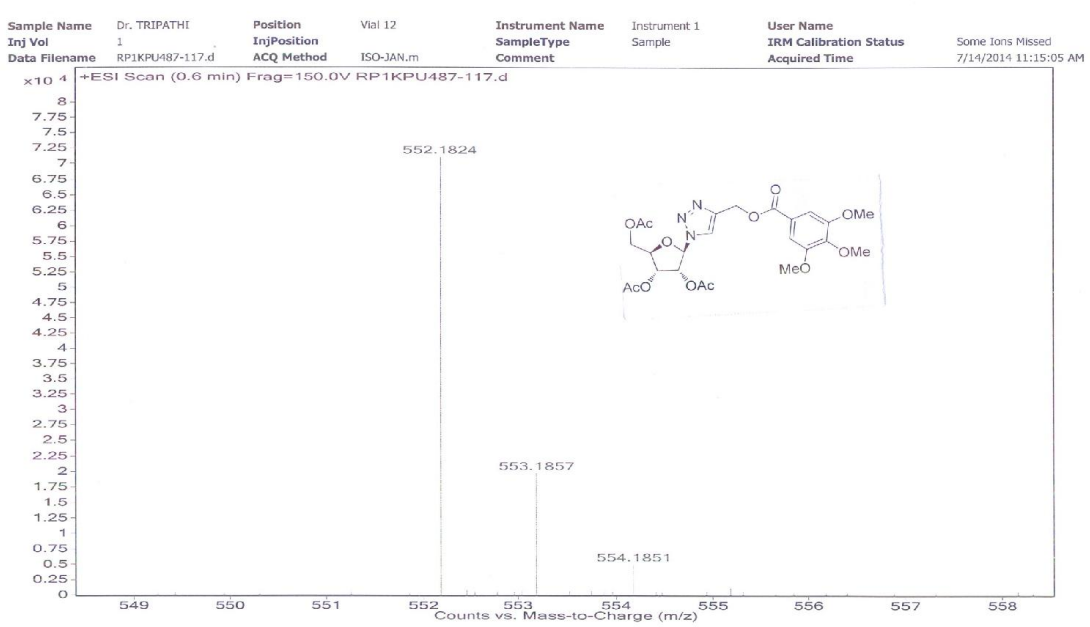


^{1}H NMR spectrum of compound **2c**

^{13}C NMR spectrum of compound **2c**



HRMS spectrum of compound **2c**



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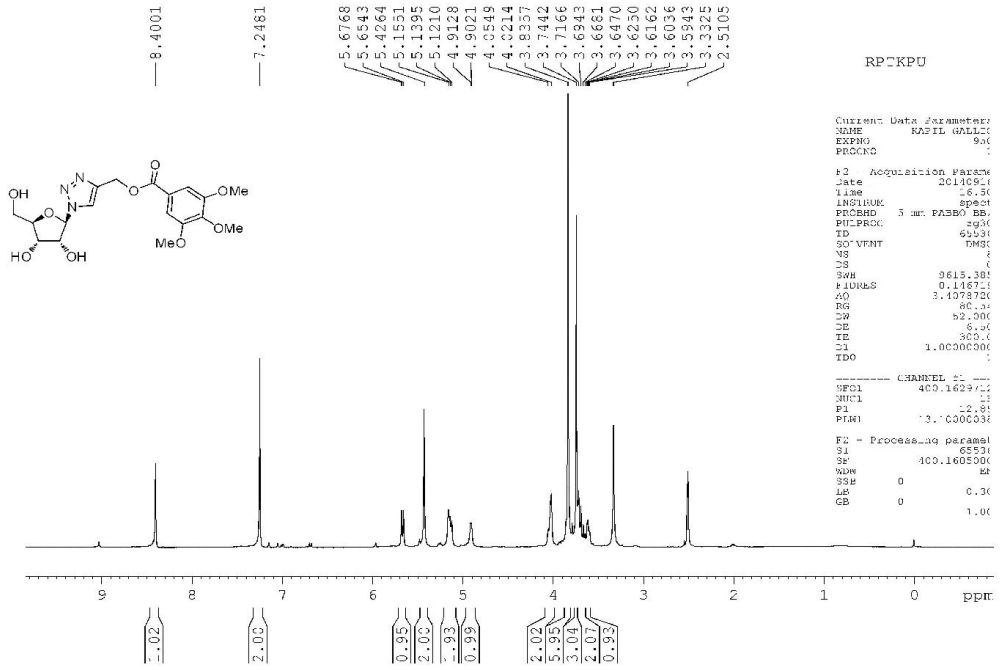

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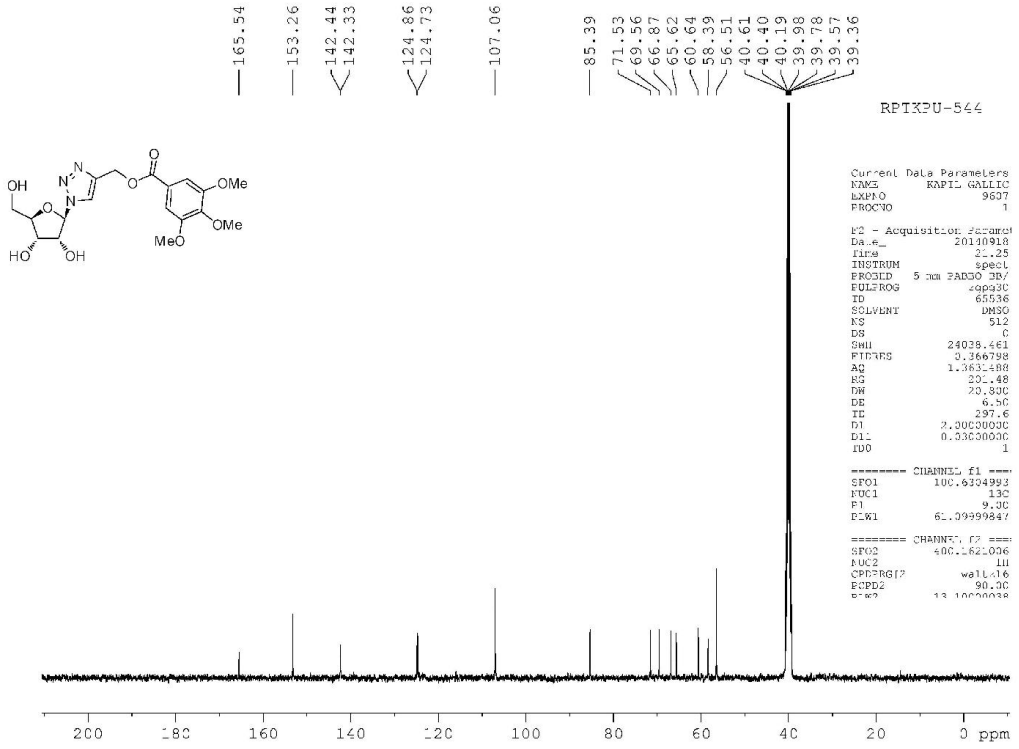

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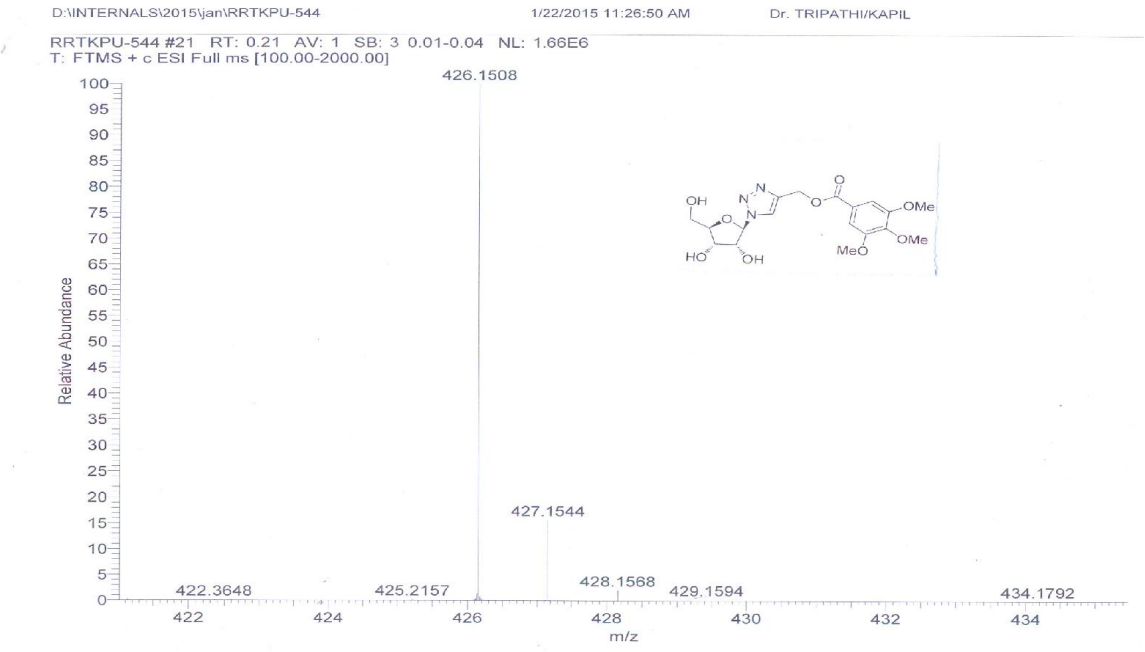

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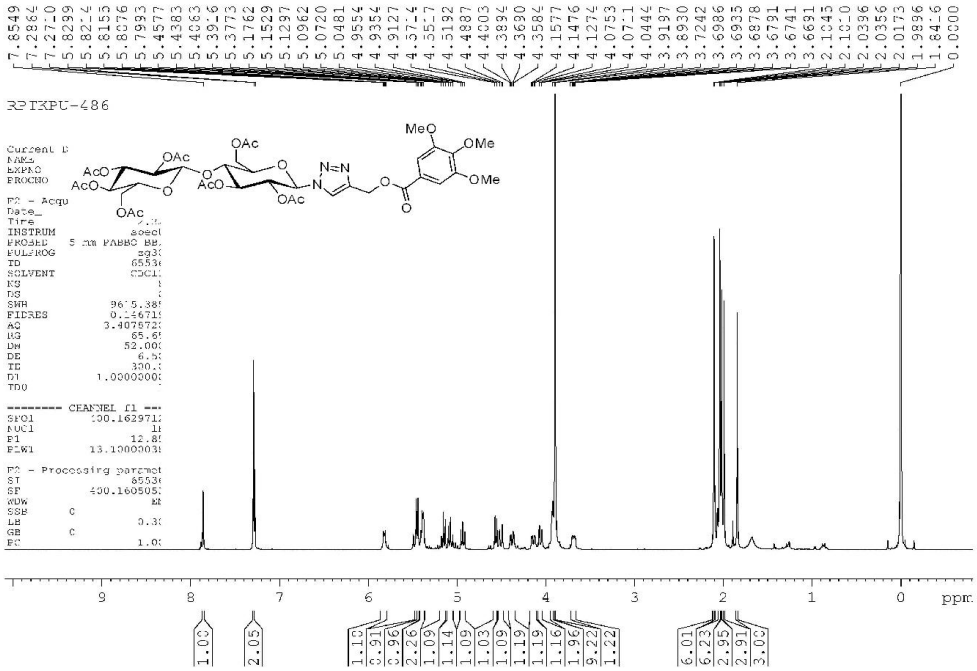

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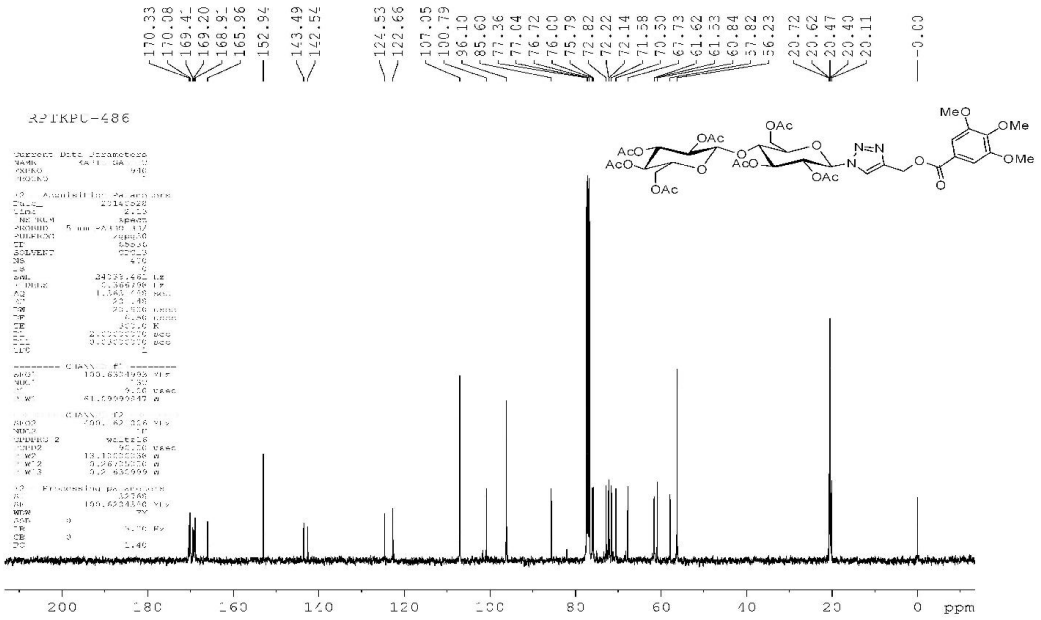

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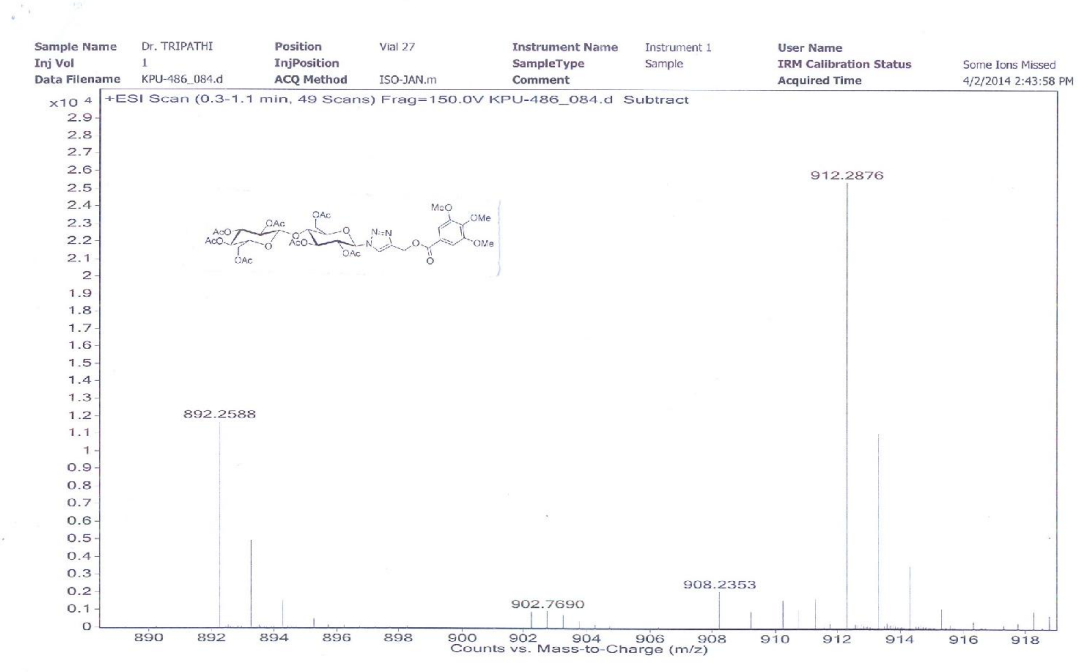

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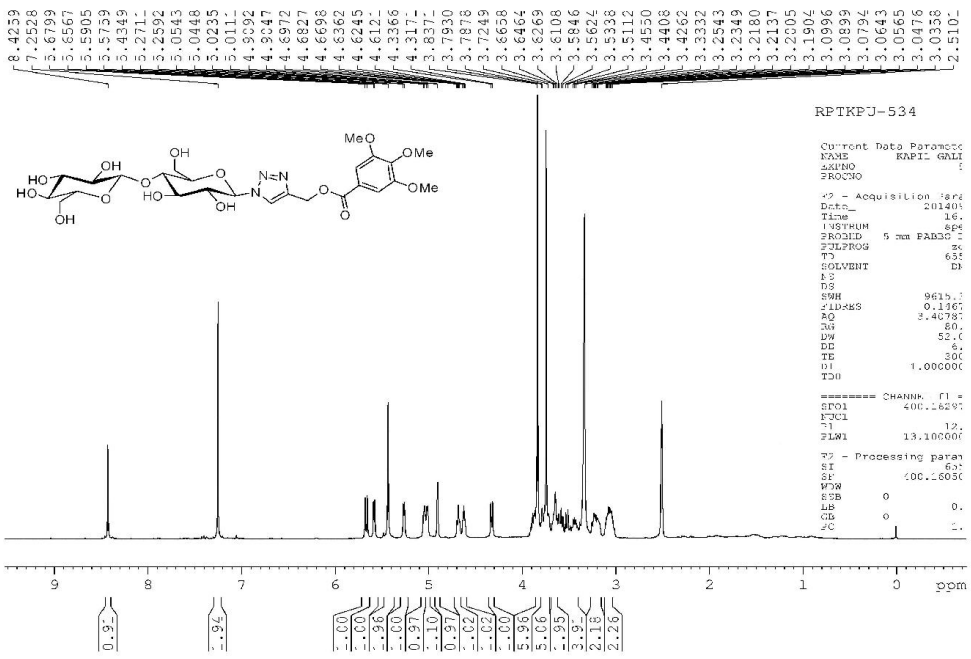

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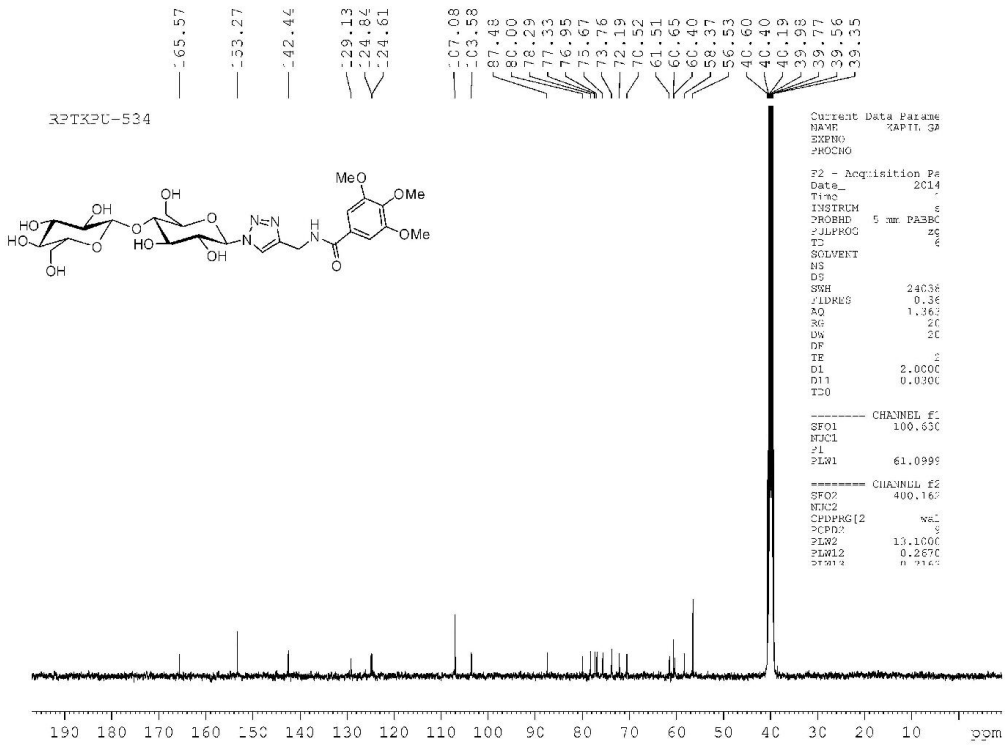

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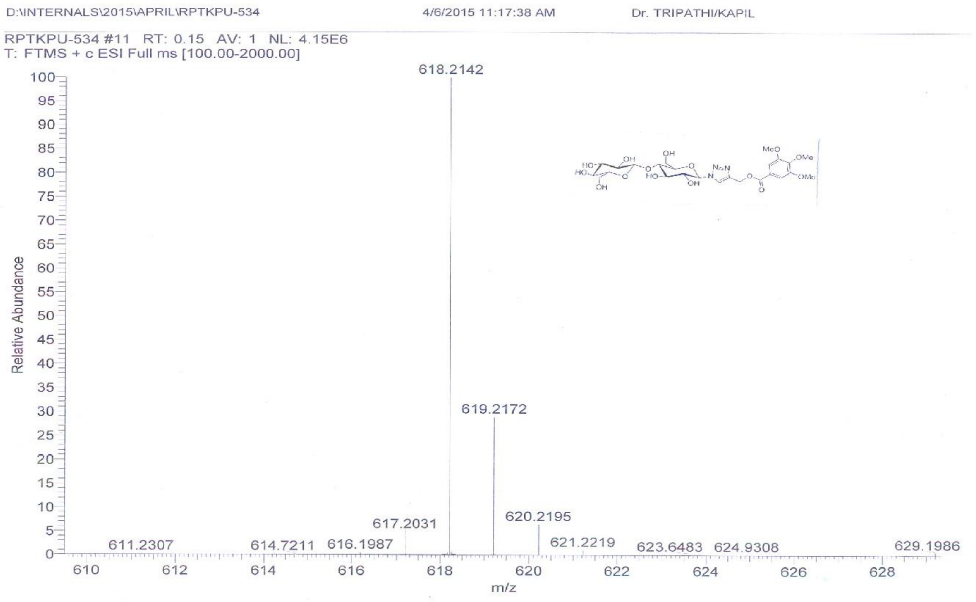

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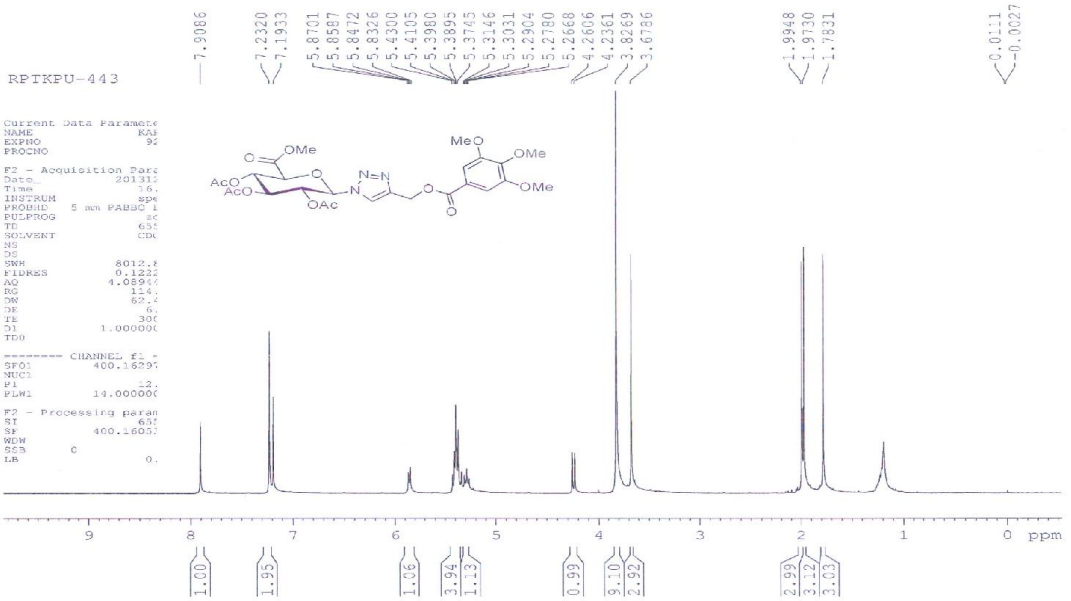

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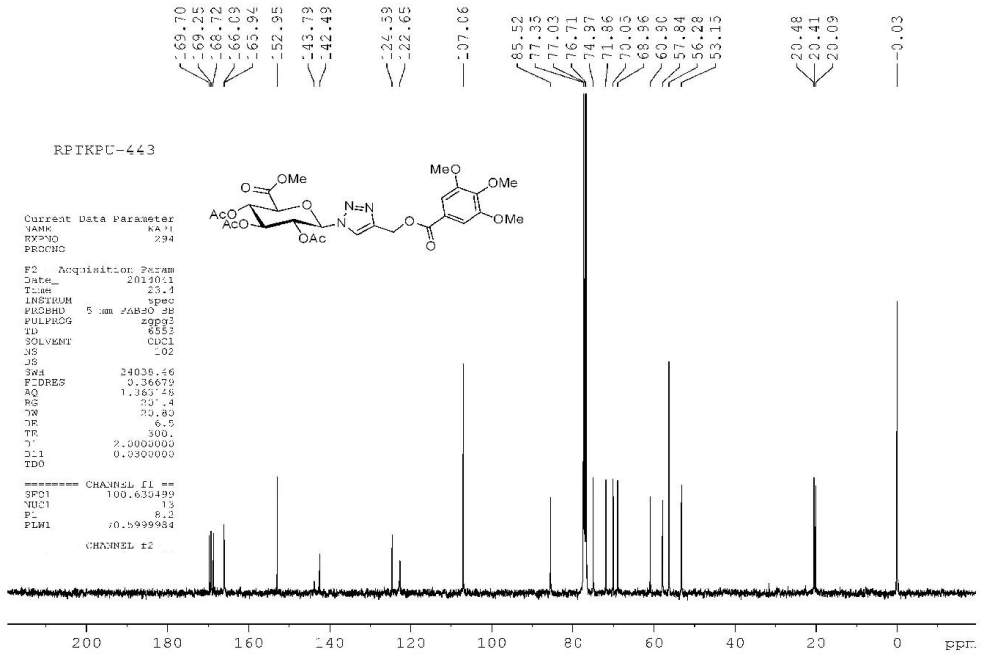
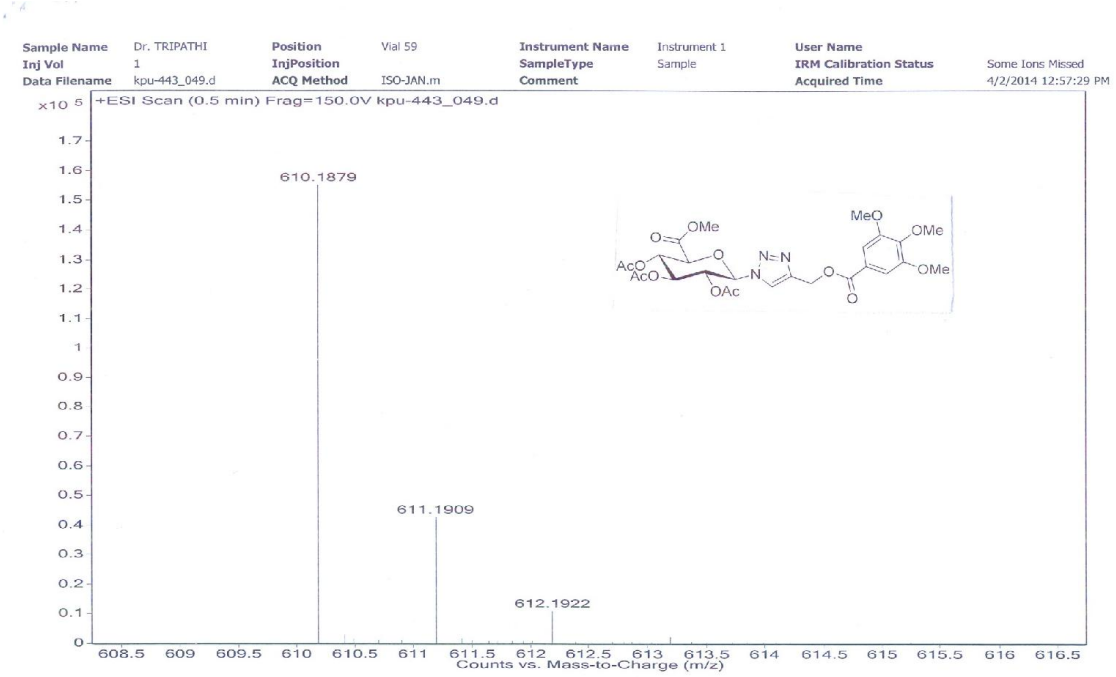


HRMS spectrum of compound **2e**



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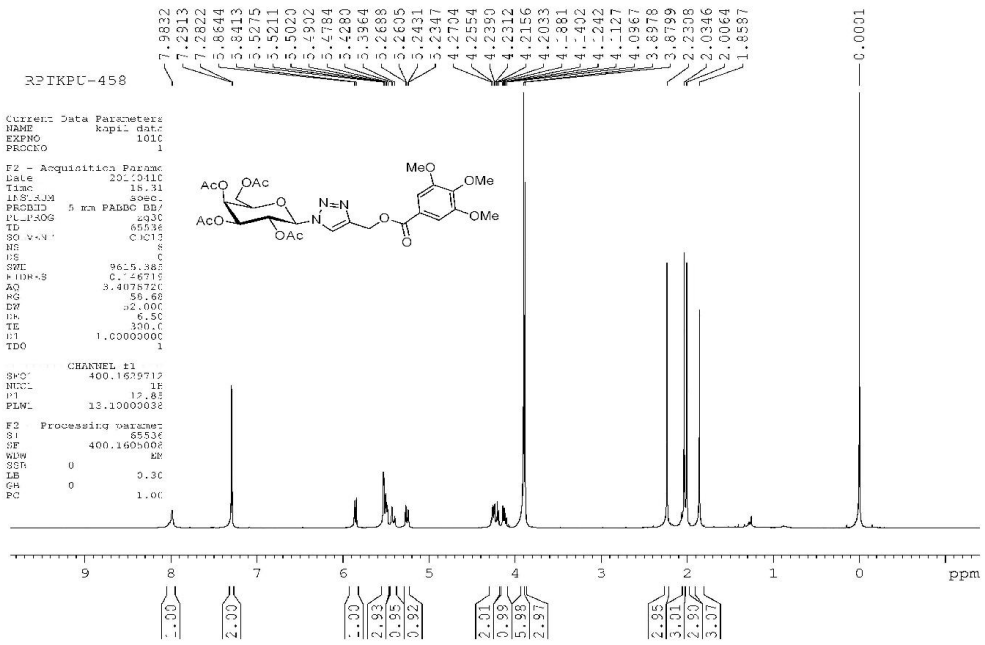

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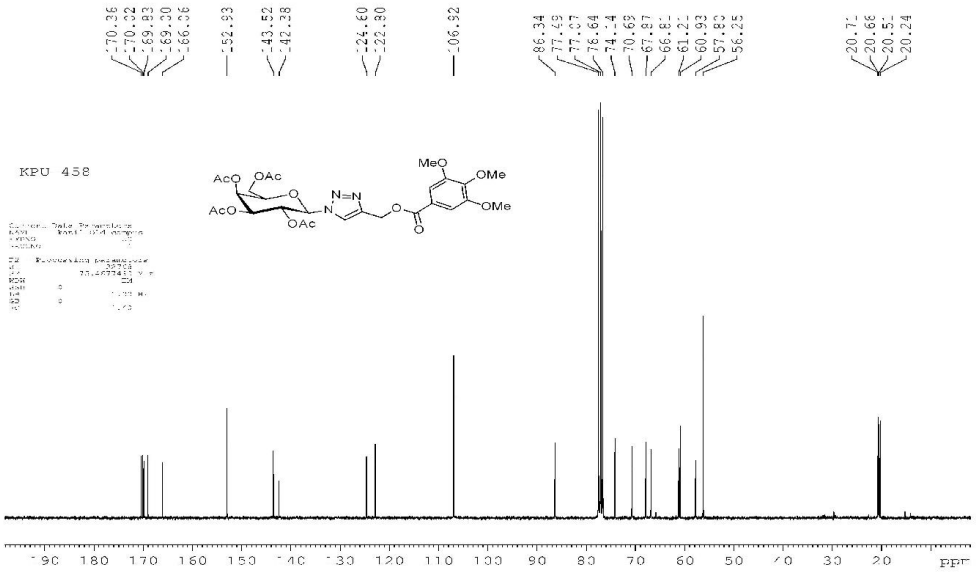

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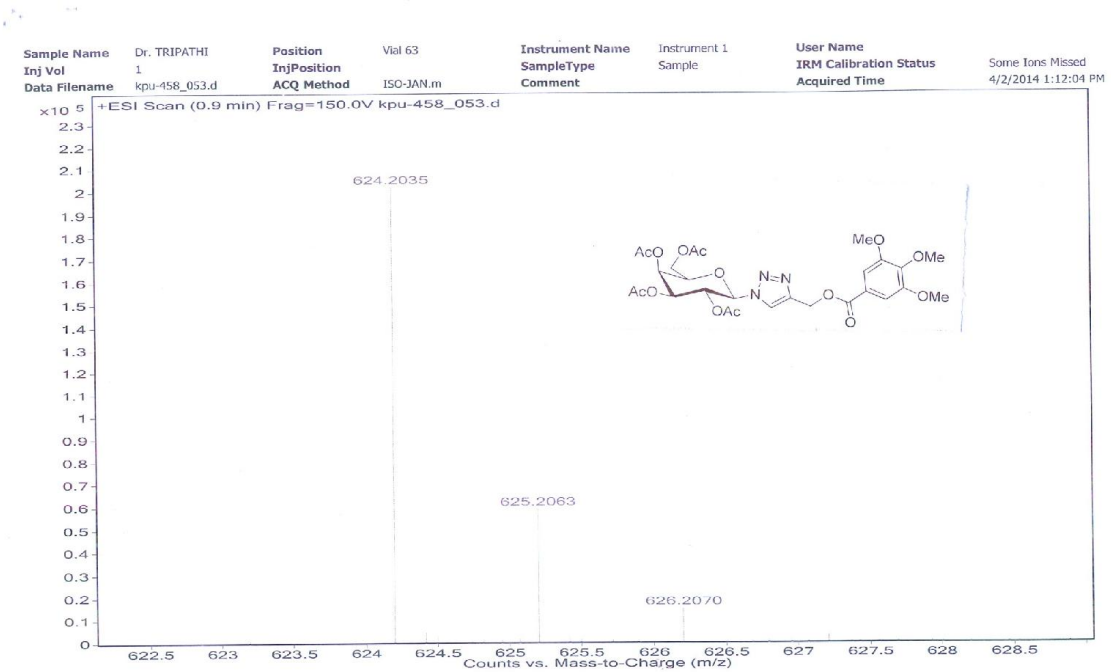

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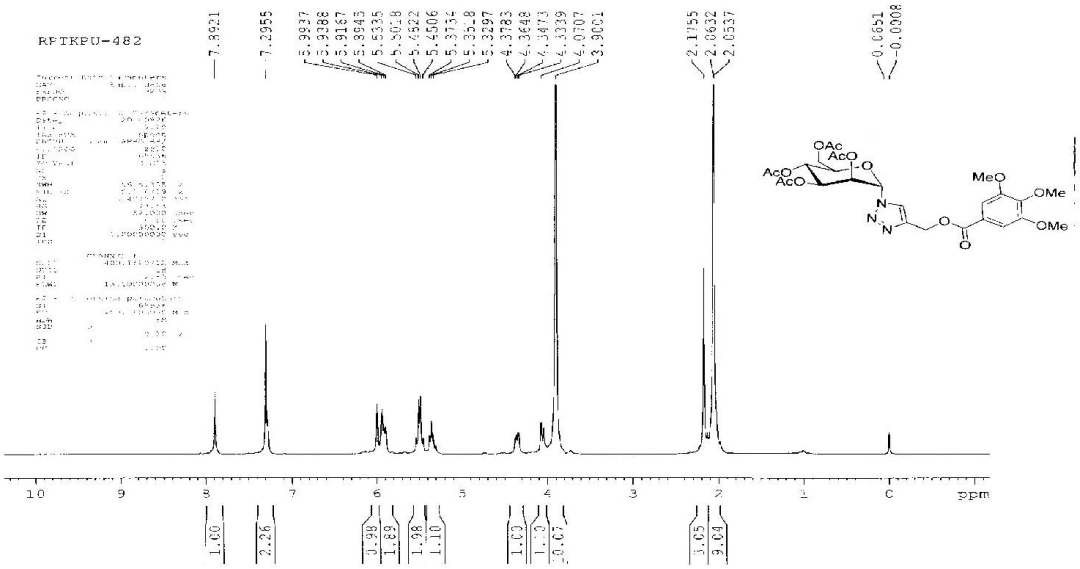

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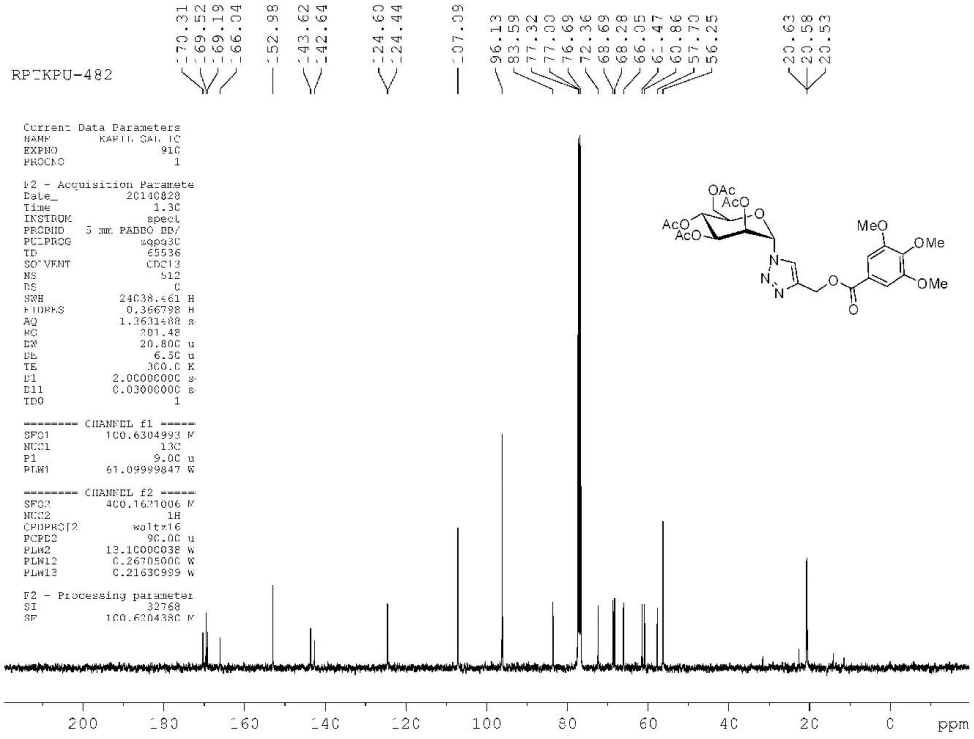

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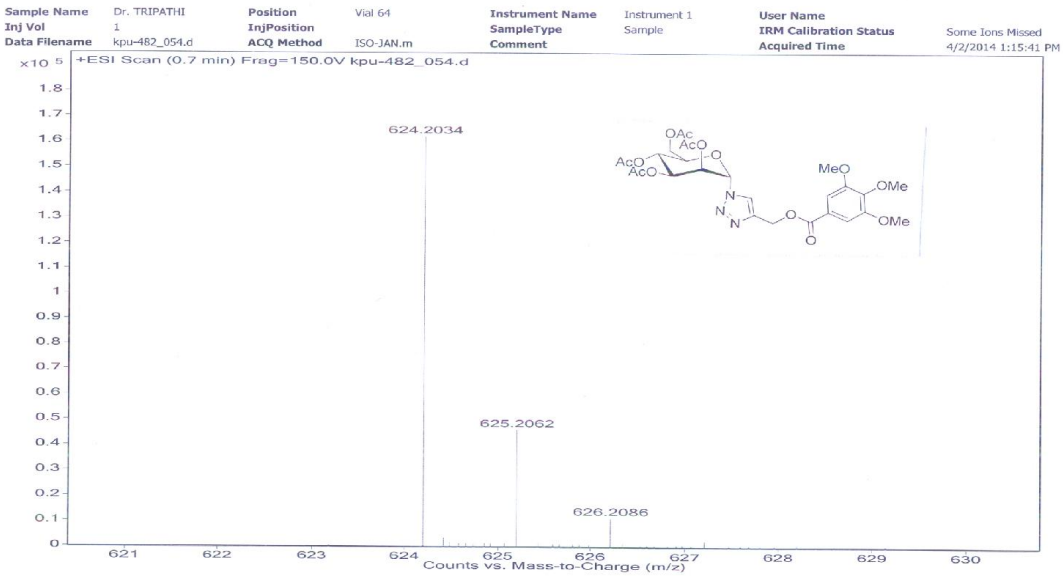

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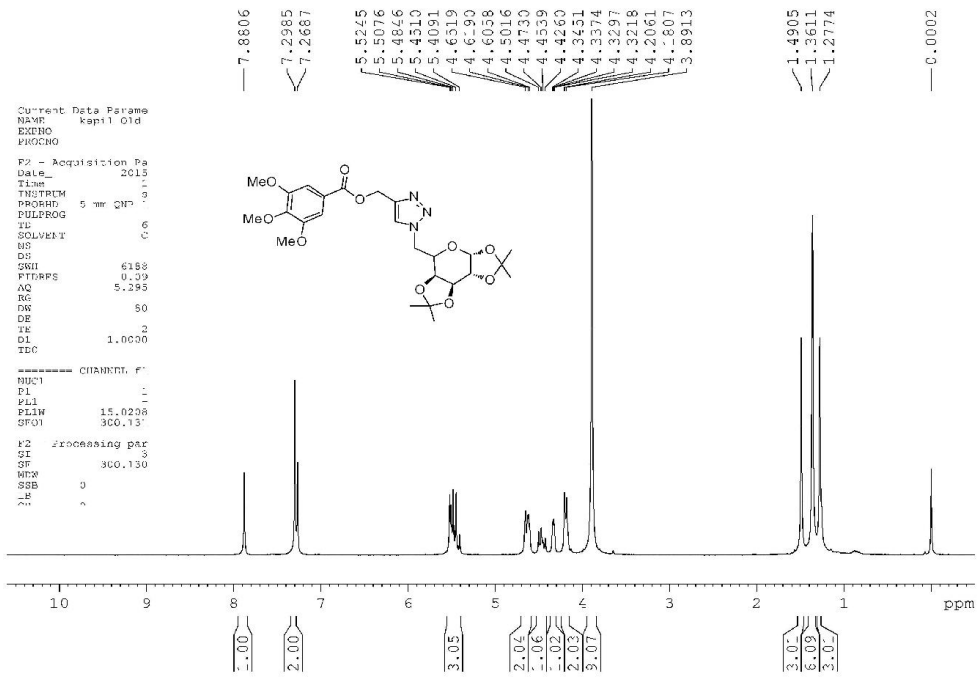
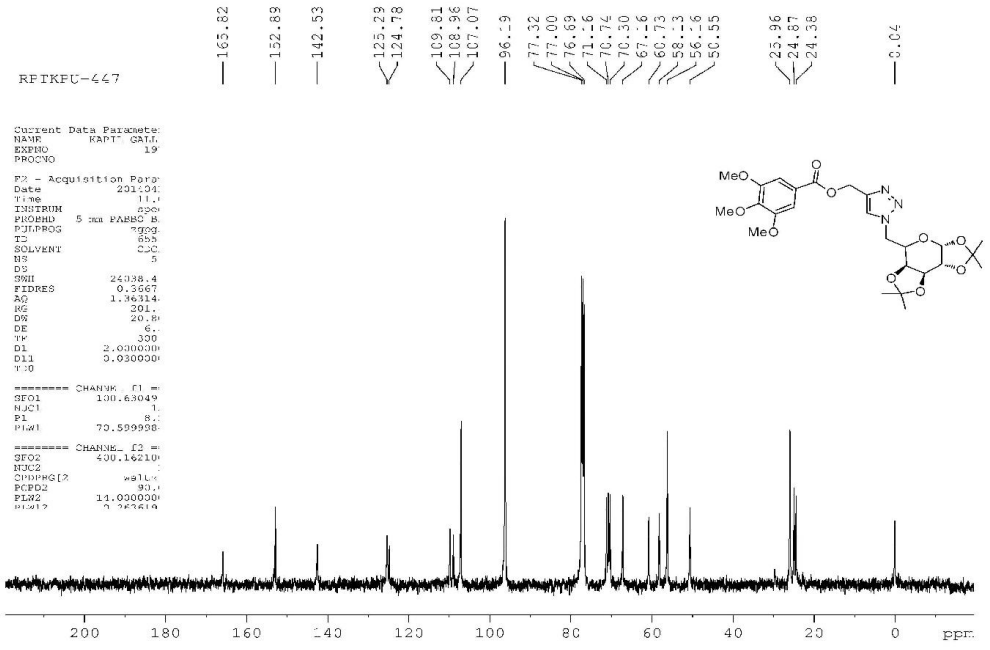


^{13}C NMR spectrum of compound **2h**



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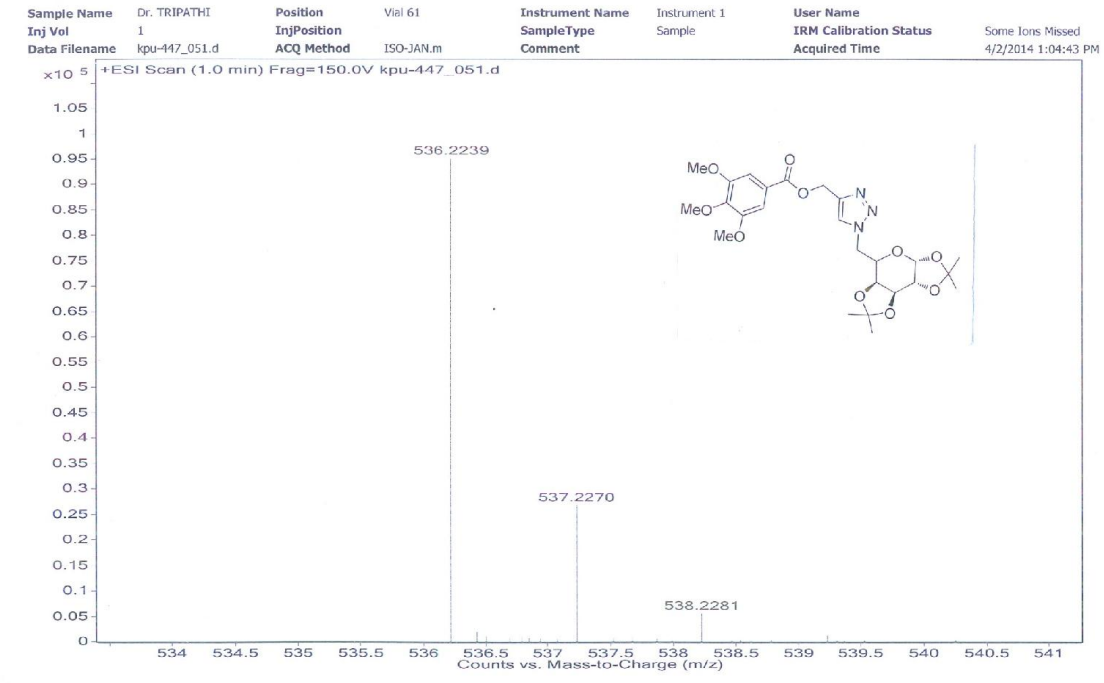

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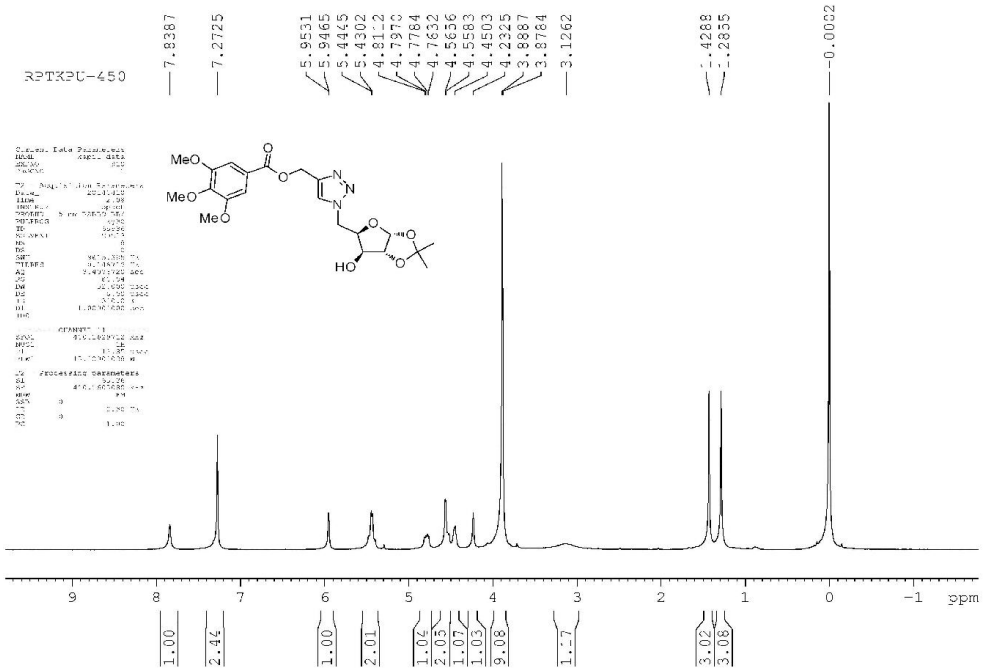
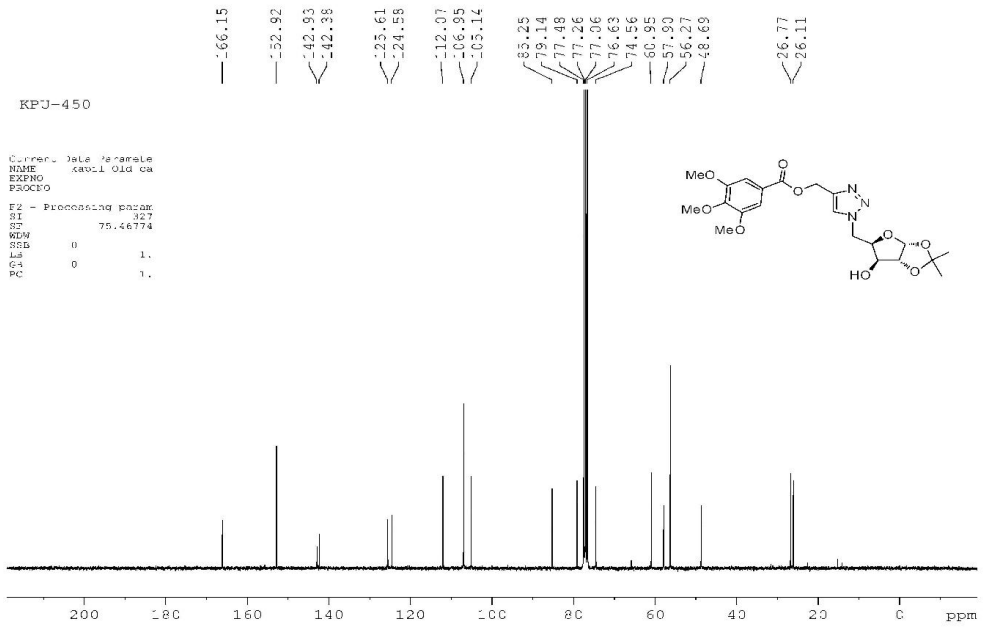
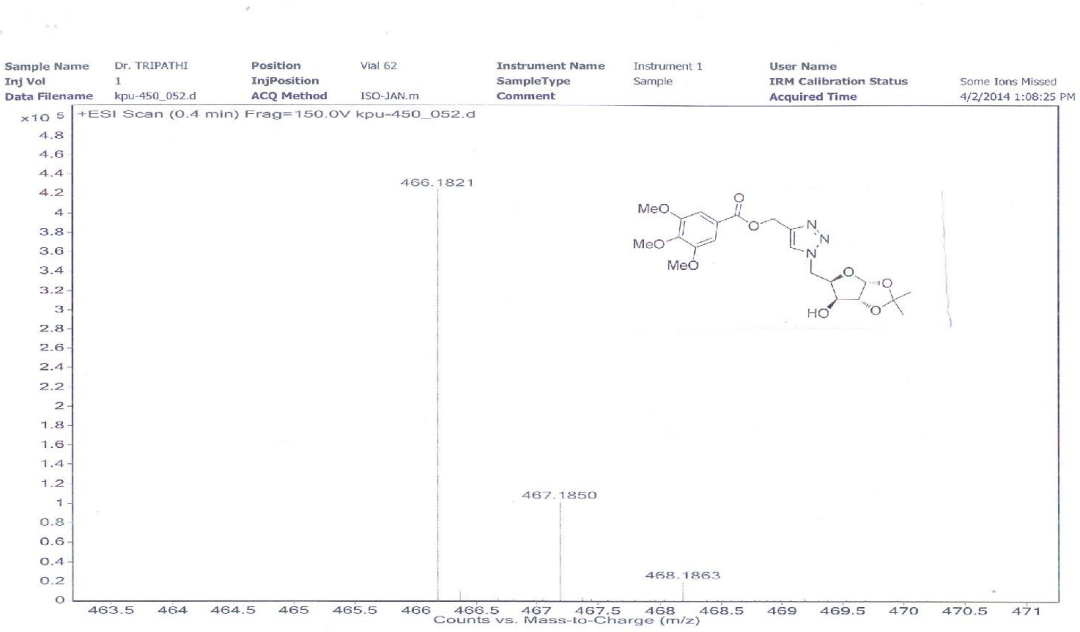


^{13}C NMR spectrum of compound **2i**



HRMS spectrum of compound **2i**



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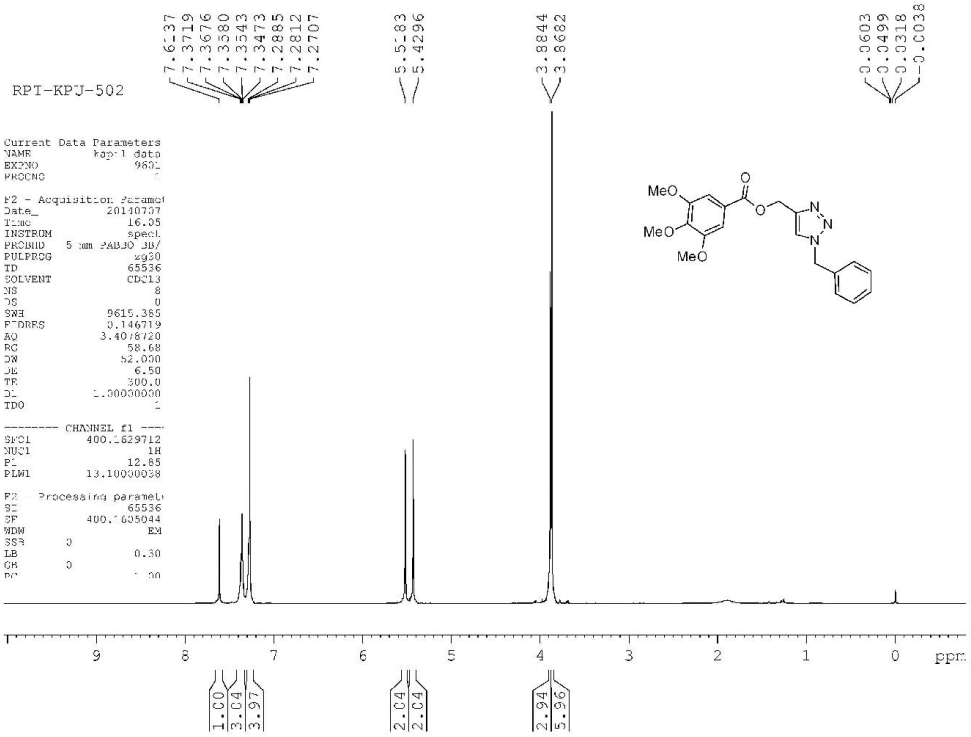

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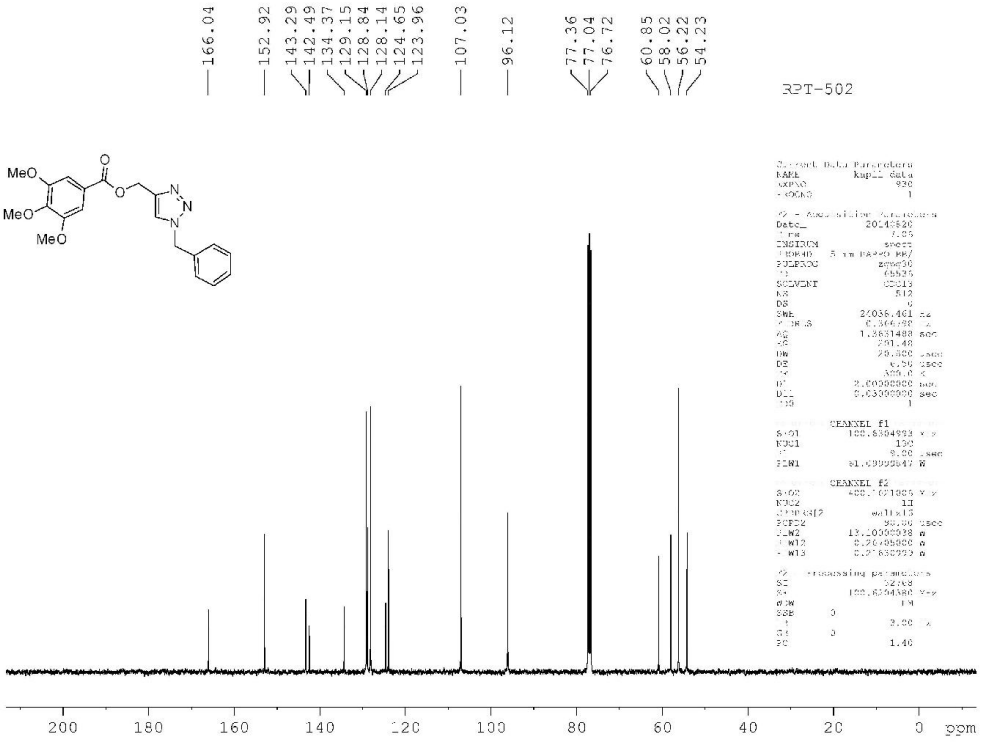

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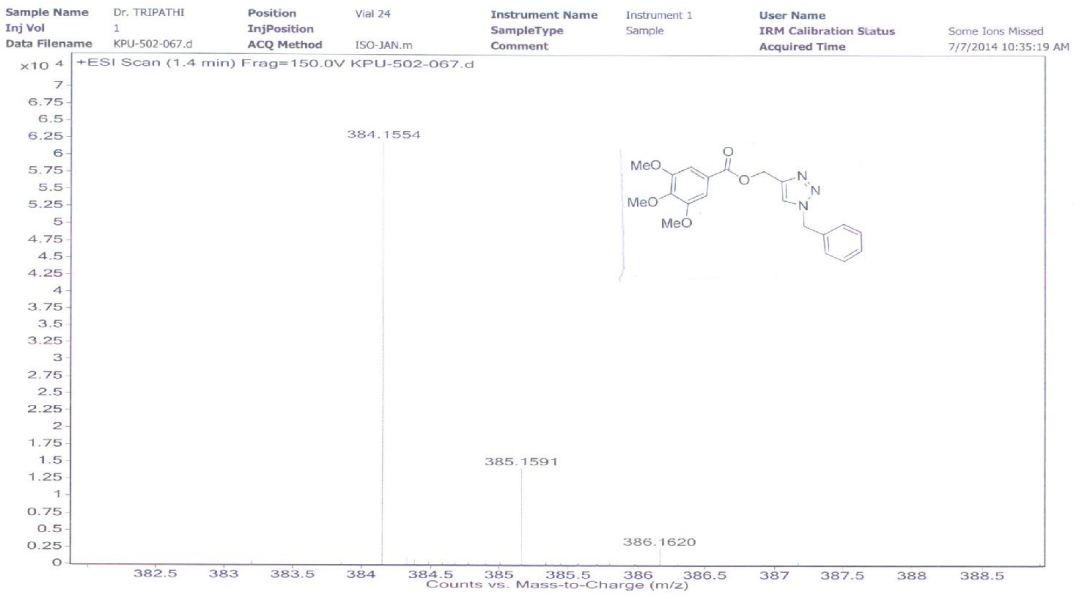
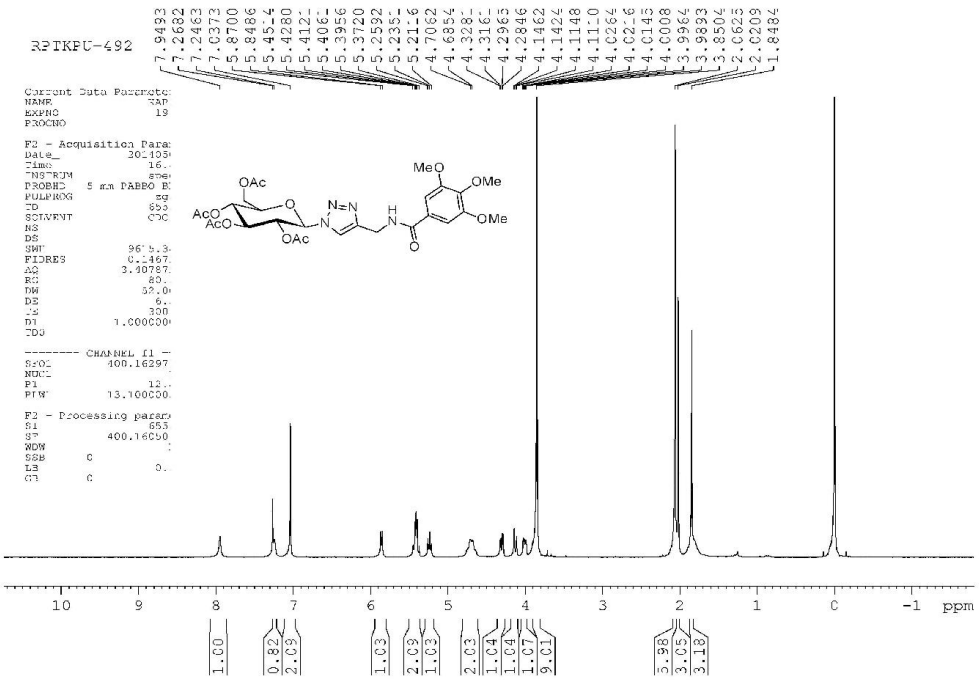
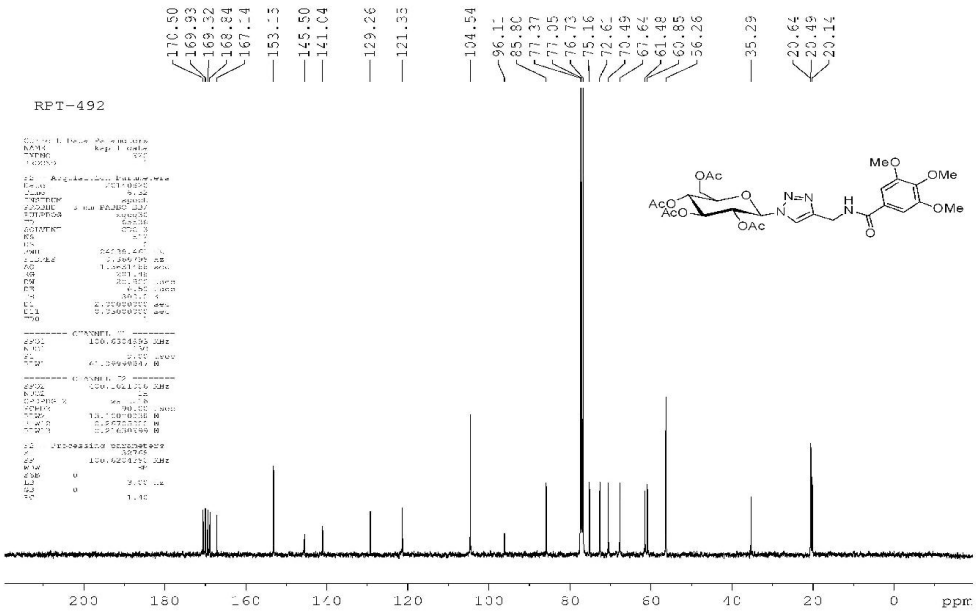


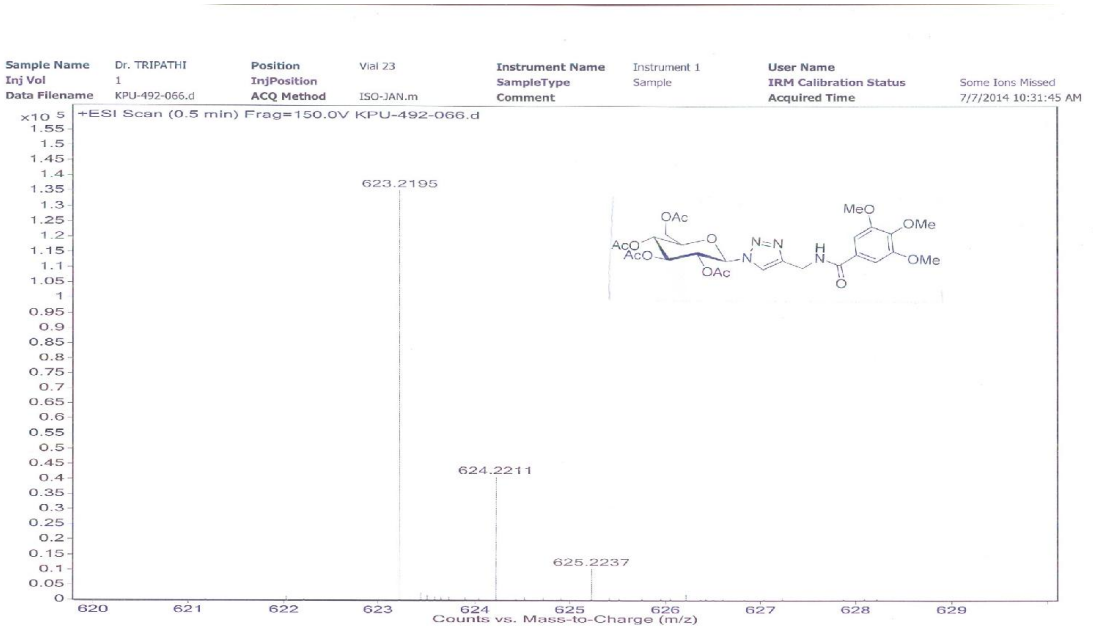
^{1}H NMR spectrum of compound **4a**



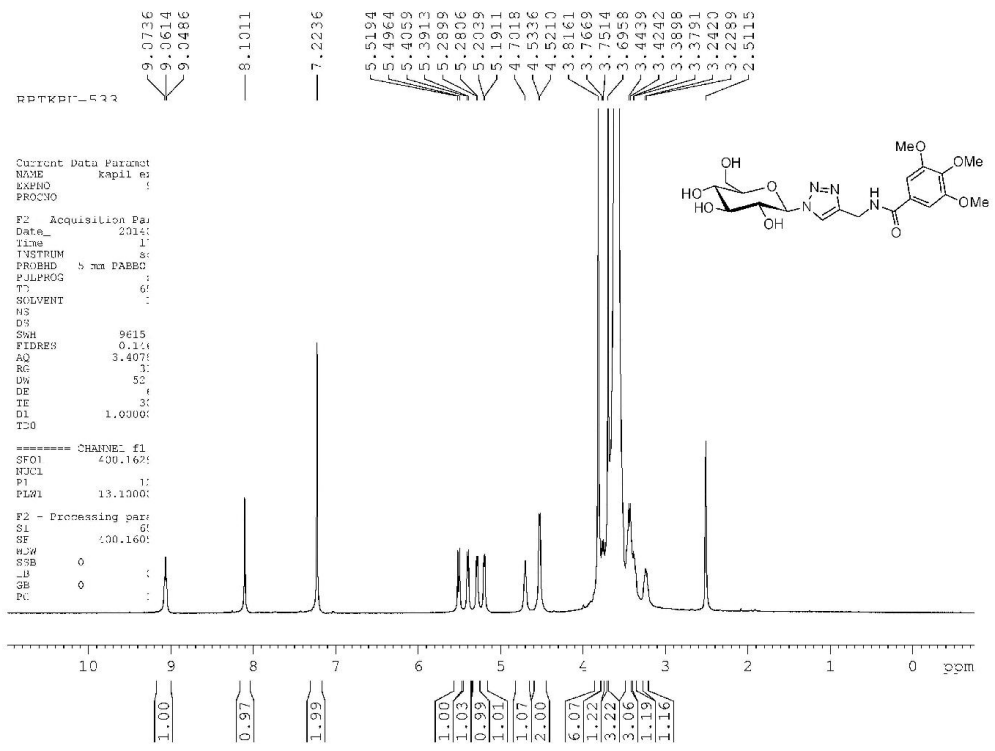
^{13}C NMR spectrum of compound **4a**



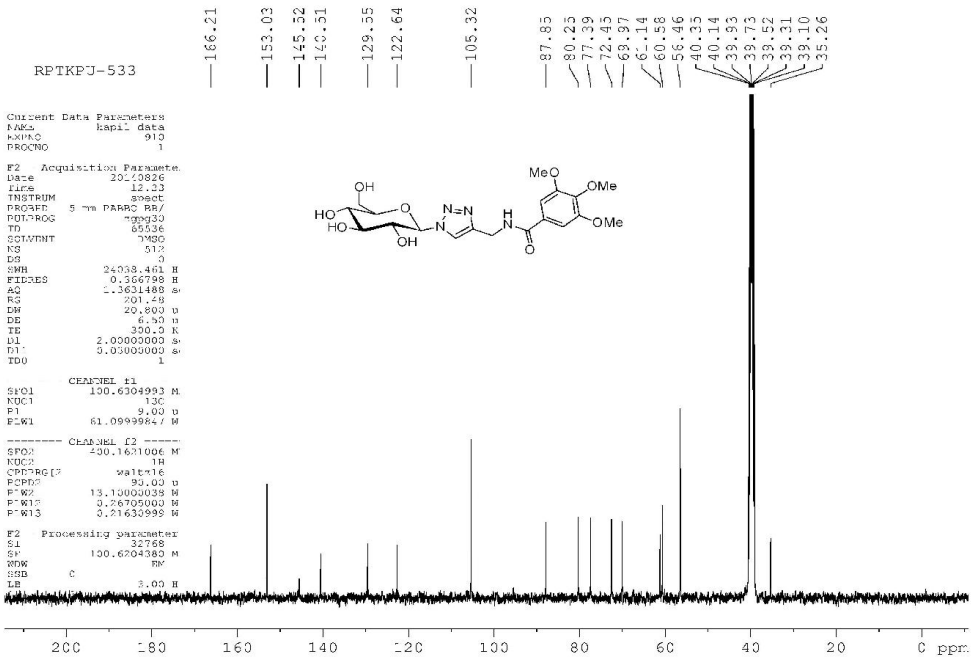
HRMS spectrum of compound **4a**



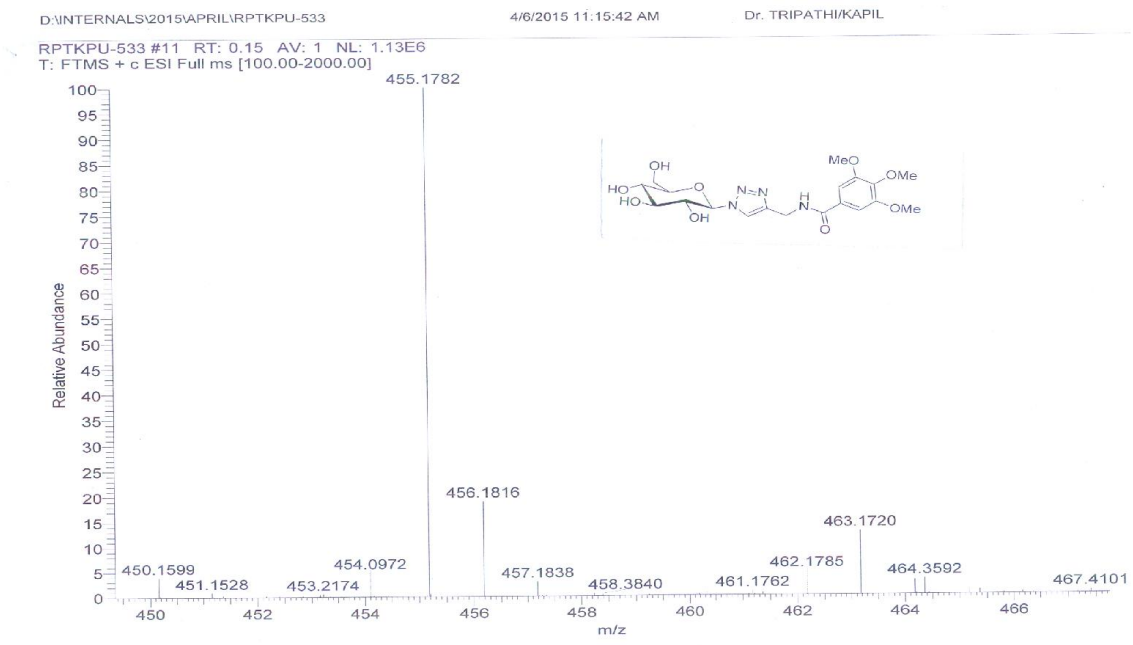
^{1}H NMR spectrum of compound **4a'**



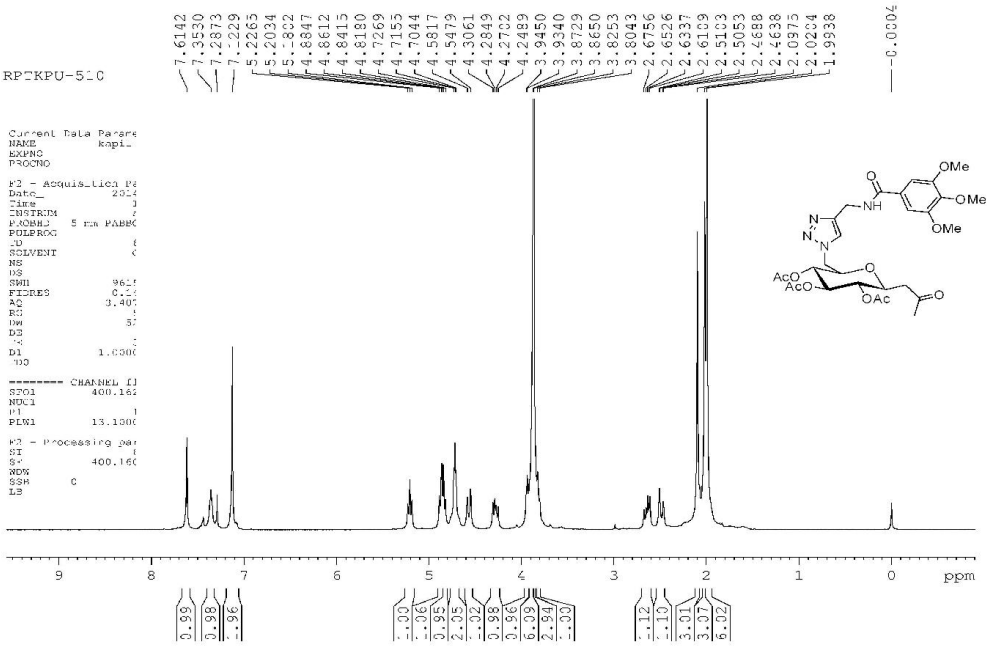
^{13}C NMR spectrum of compound **4a'**



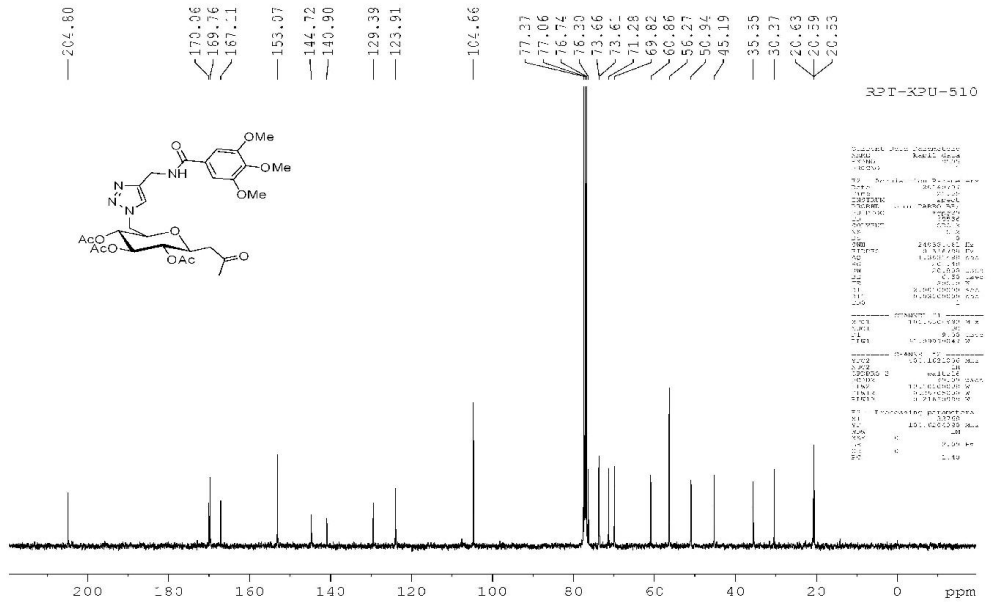
HRMS spectrum of compound **4a'**



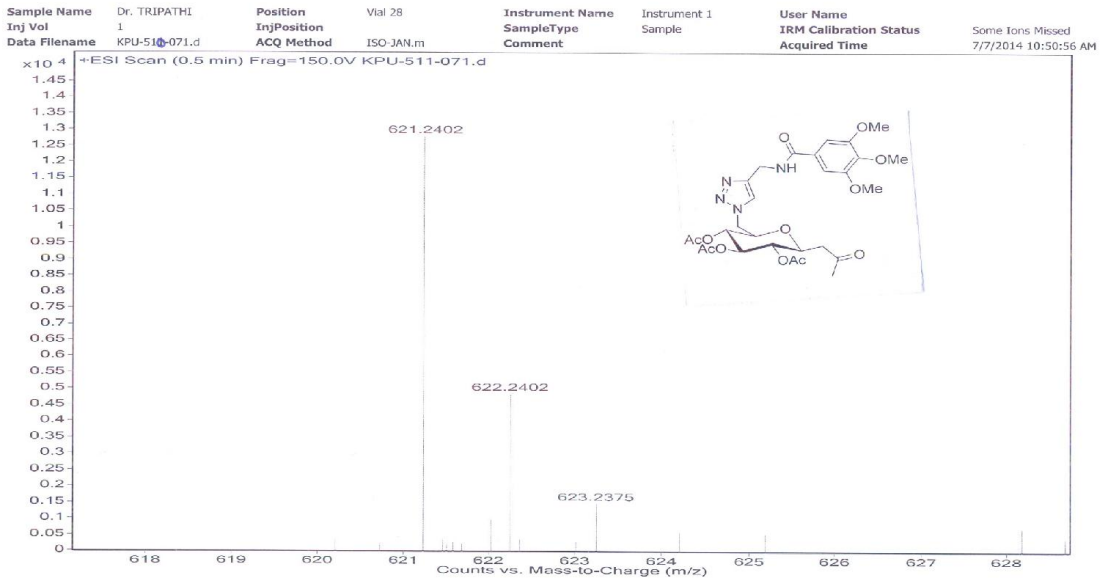
^{1}H NMR spectrum of compound **4b**



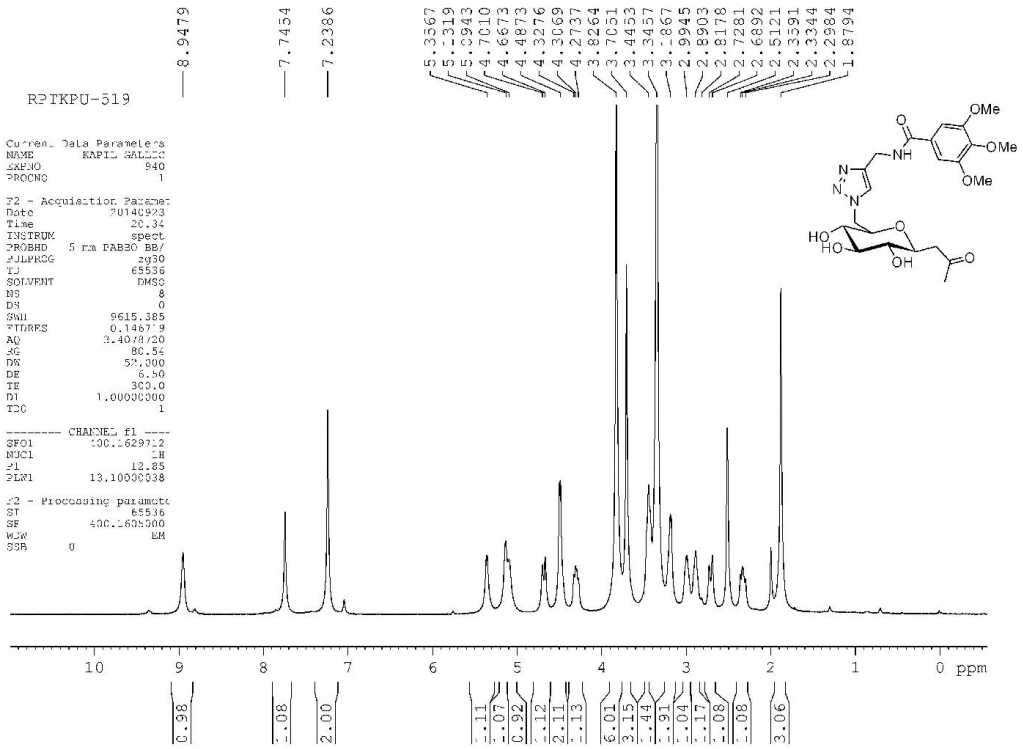
^{13}C NMR spectrum of compound **4b**



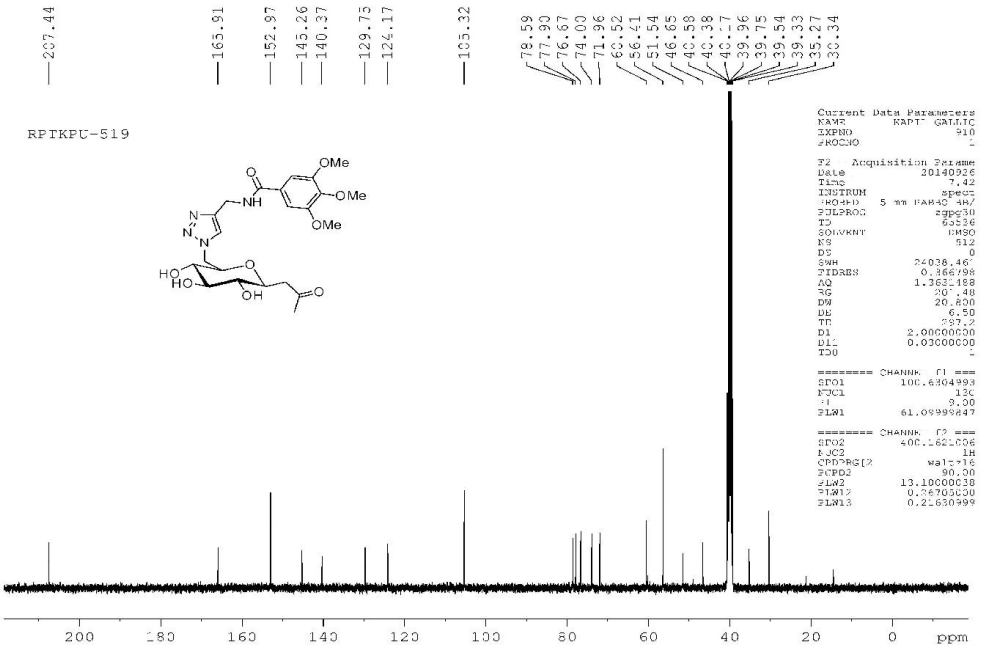
HRMS spectrum of compound **4b**



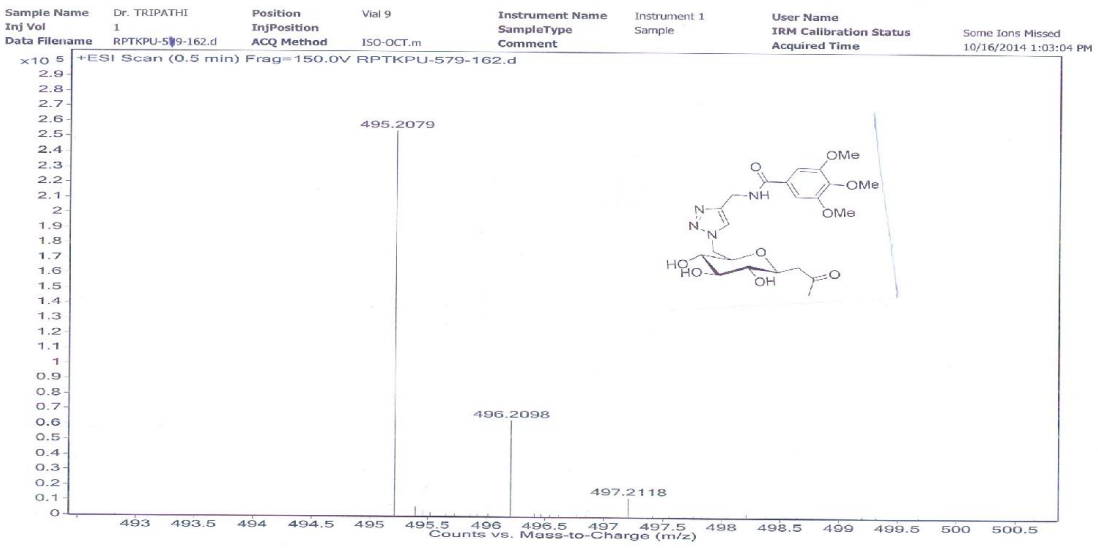
^{1}H NMR spectrum of compound **4b'**



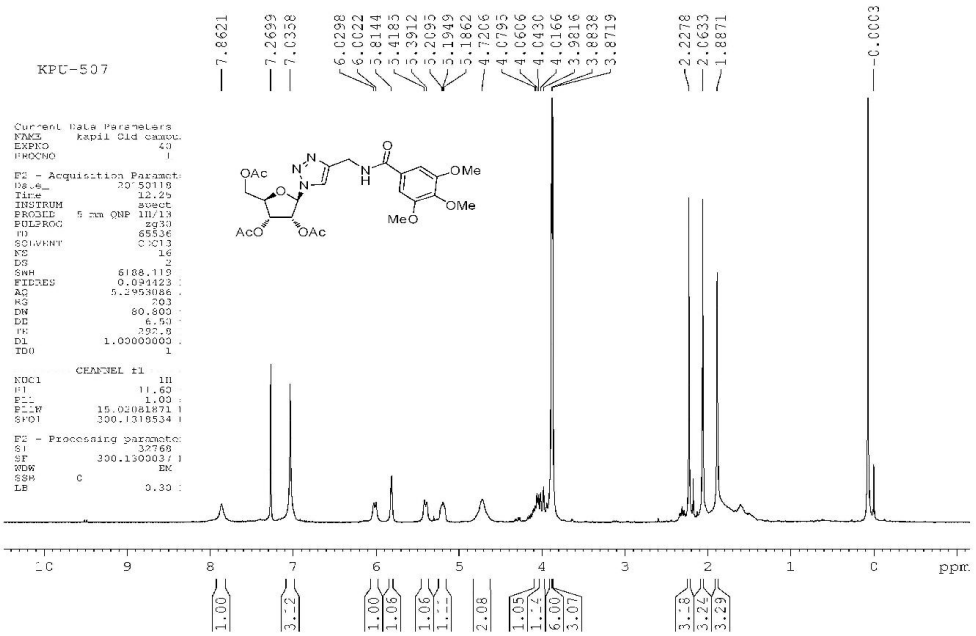
^{13}C NMR spectrum of compound **4b'**



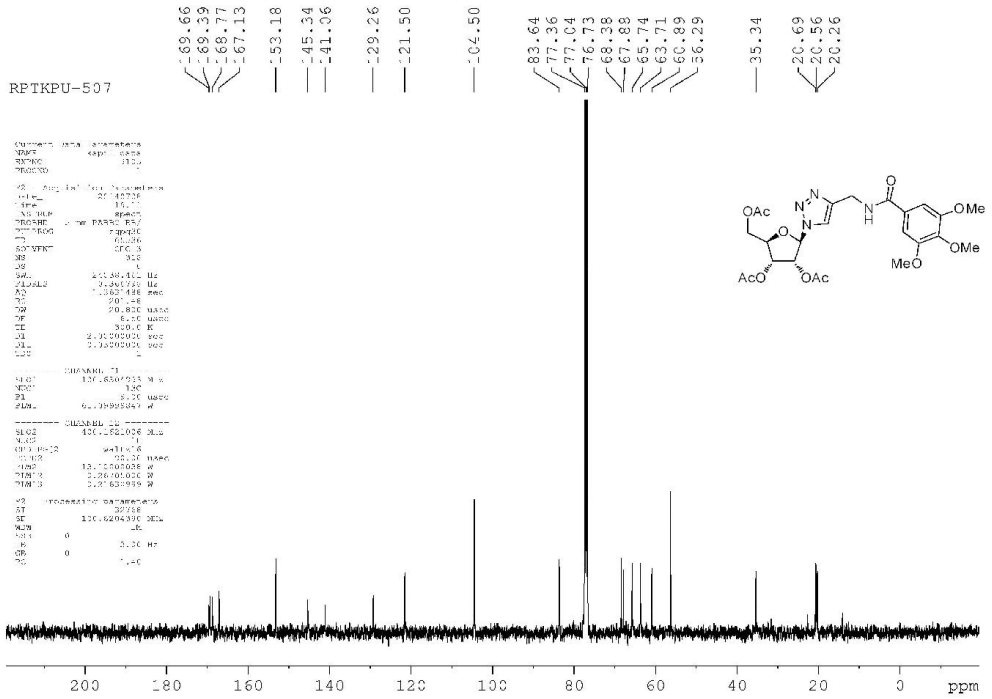
HRMS spectrum of compound **4b'**



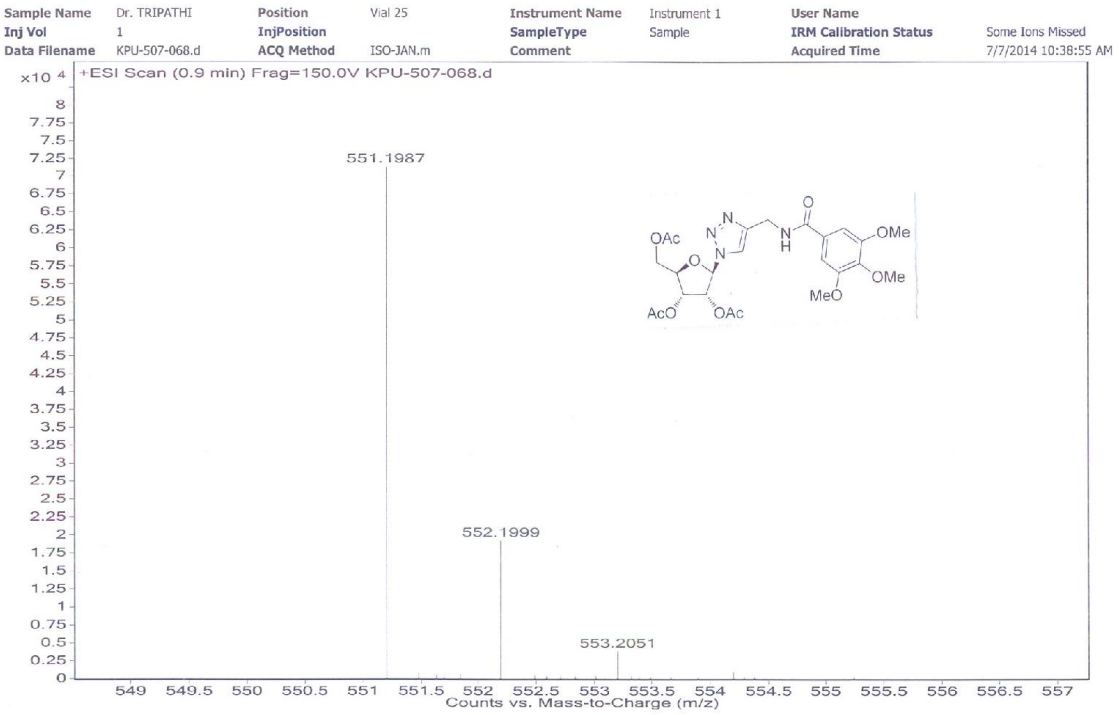
^{1}H NMR spectrum of compound **4c**



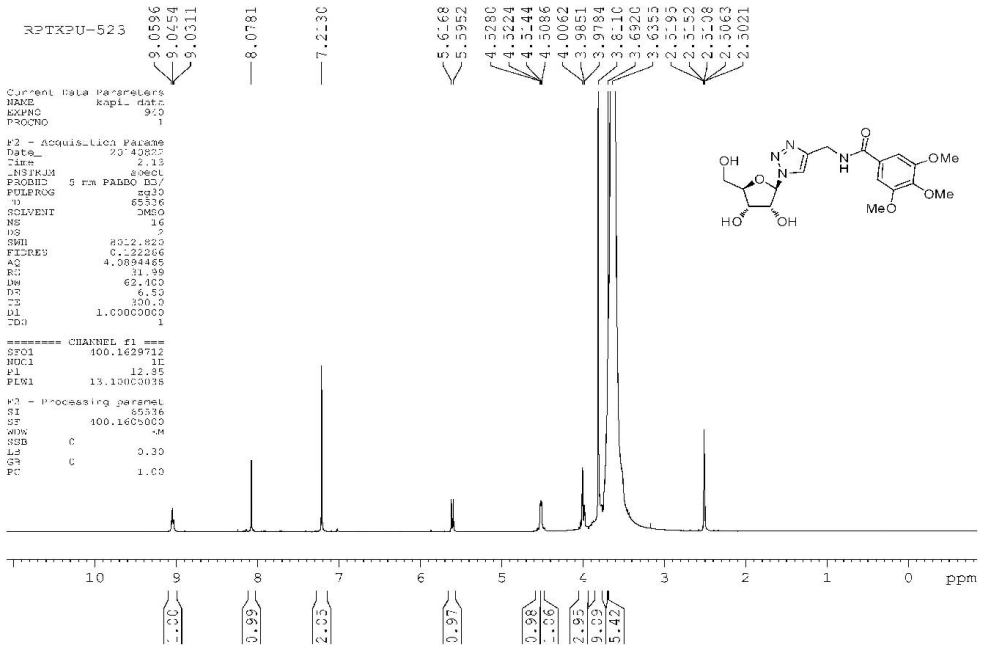
^{13}C NMR spectrum of compound **4c**



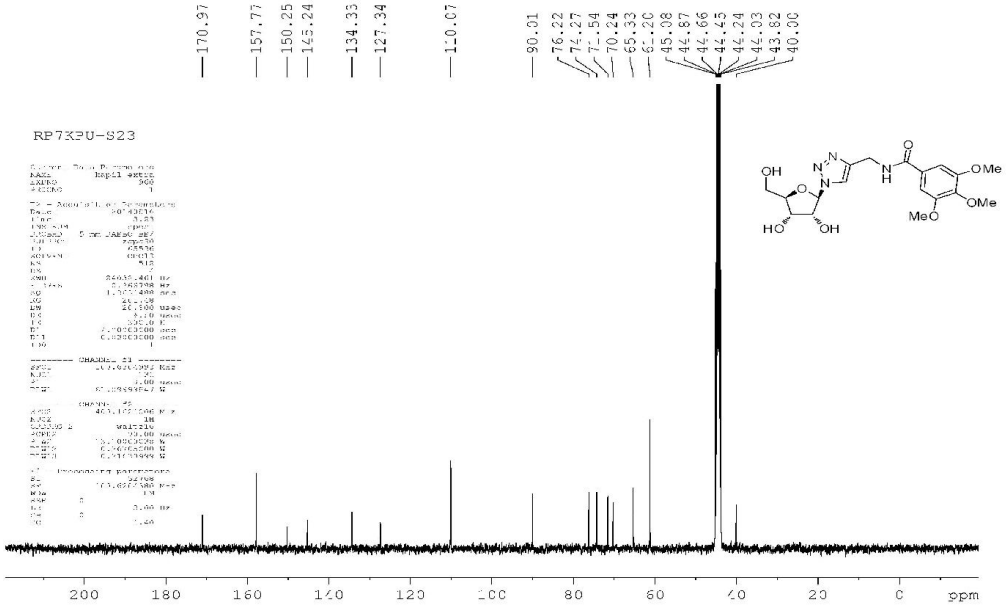
HRMS spectrum of compound **4c**



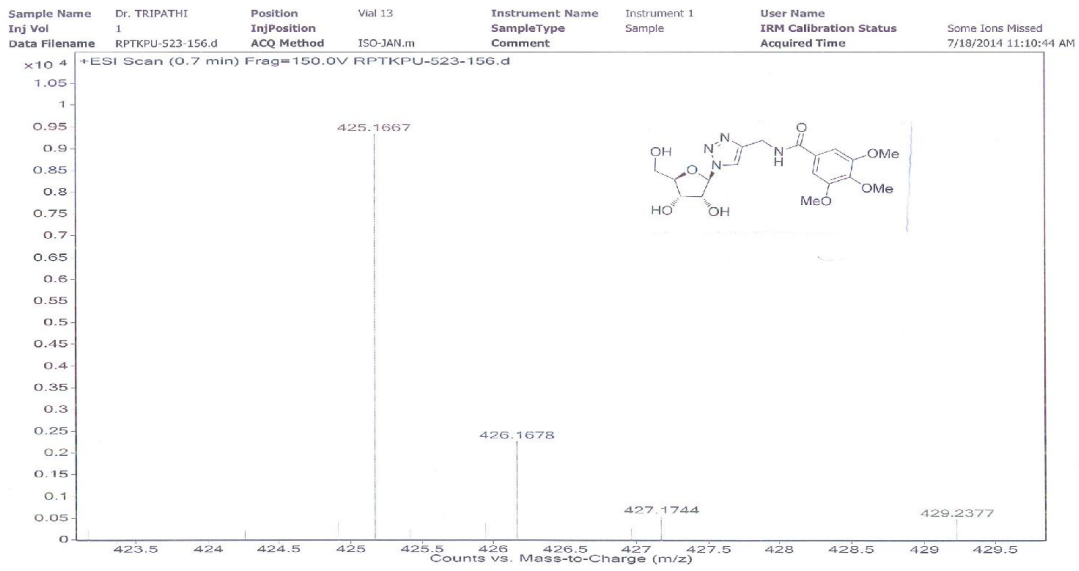
^{1}H NMR spectrum of compound **4c'**



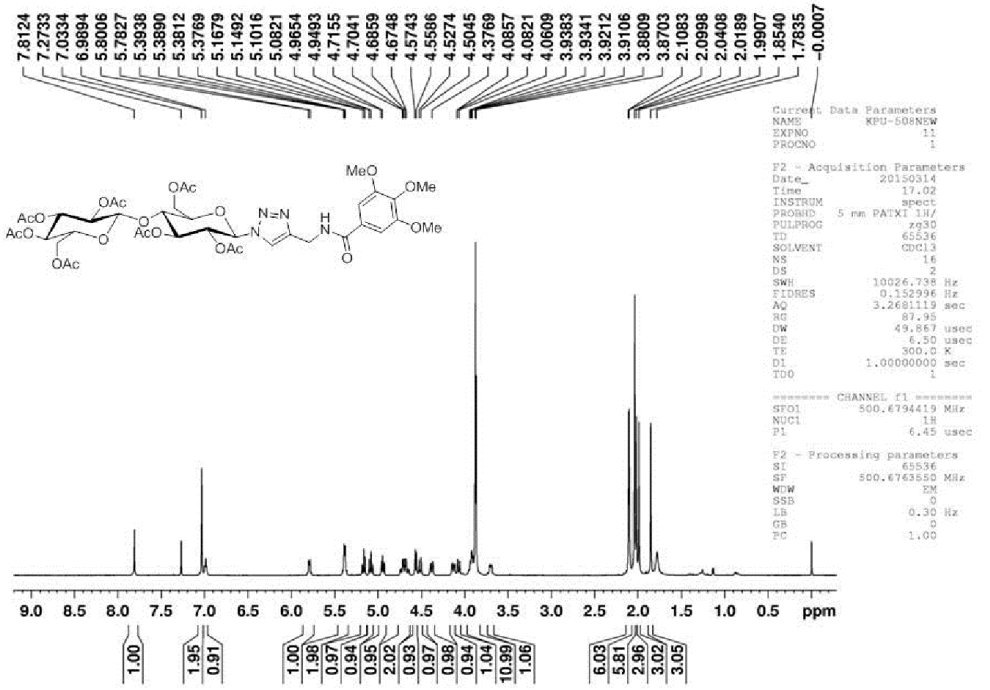
^{13}CNMR spectrum of compound **4c'**



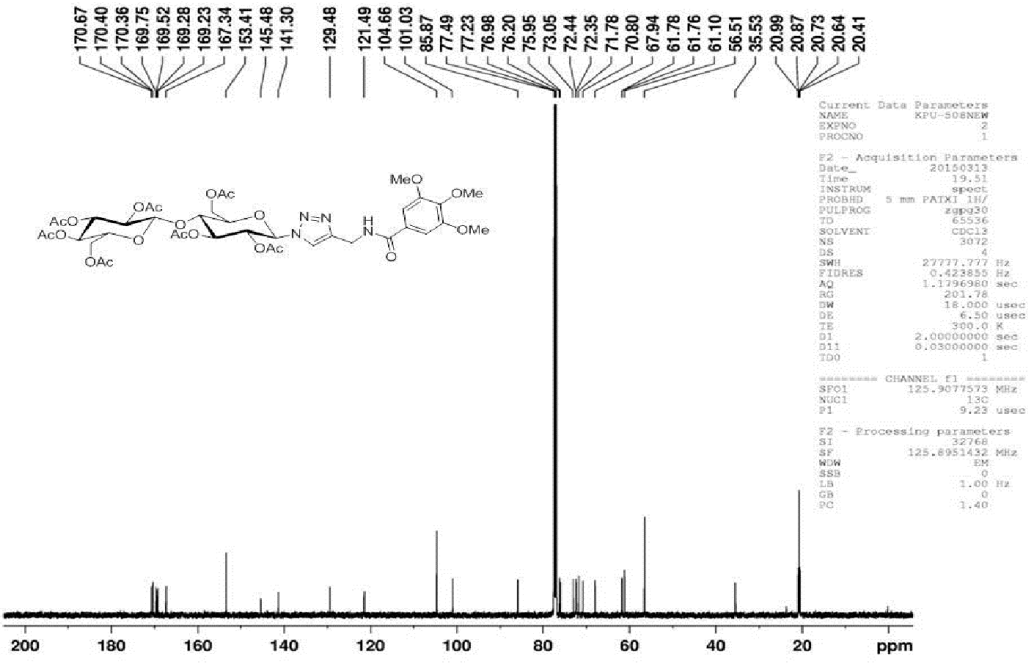
HRMS spectrum of compound **4c'**



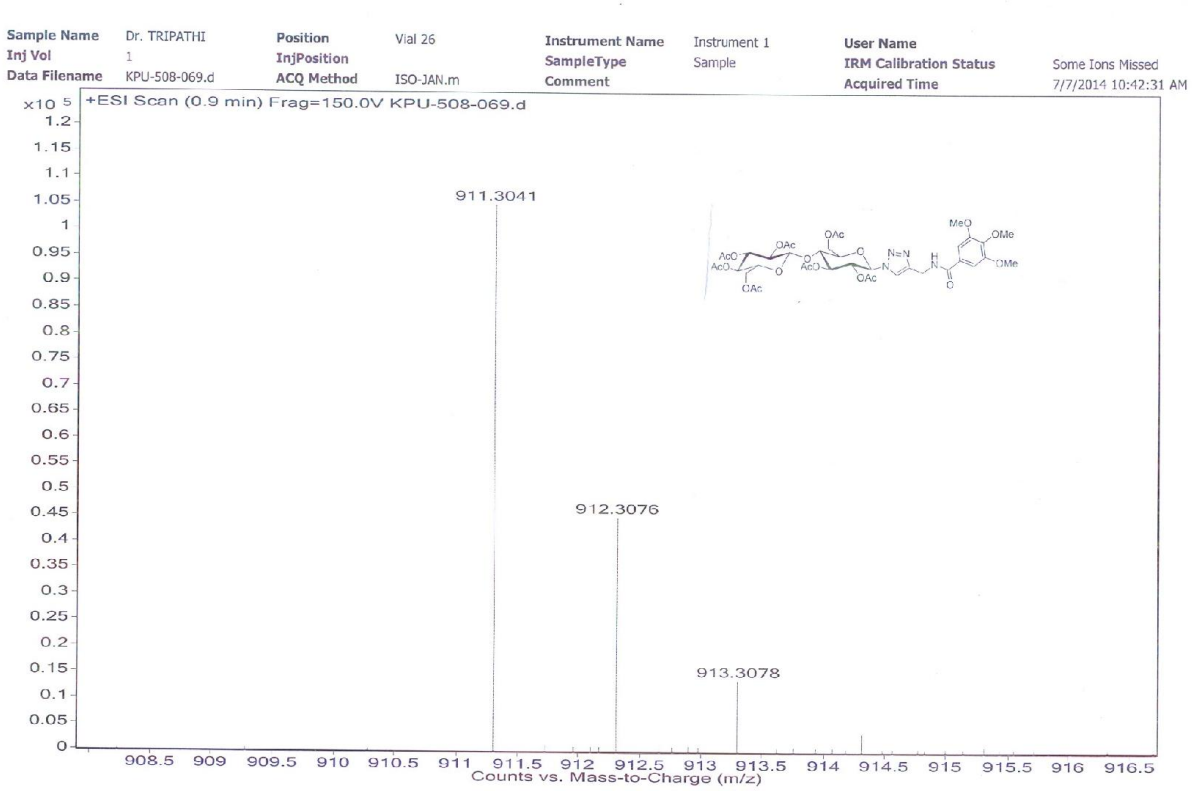
^{1}H NMR spectrum of compound **4d**



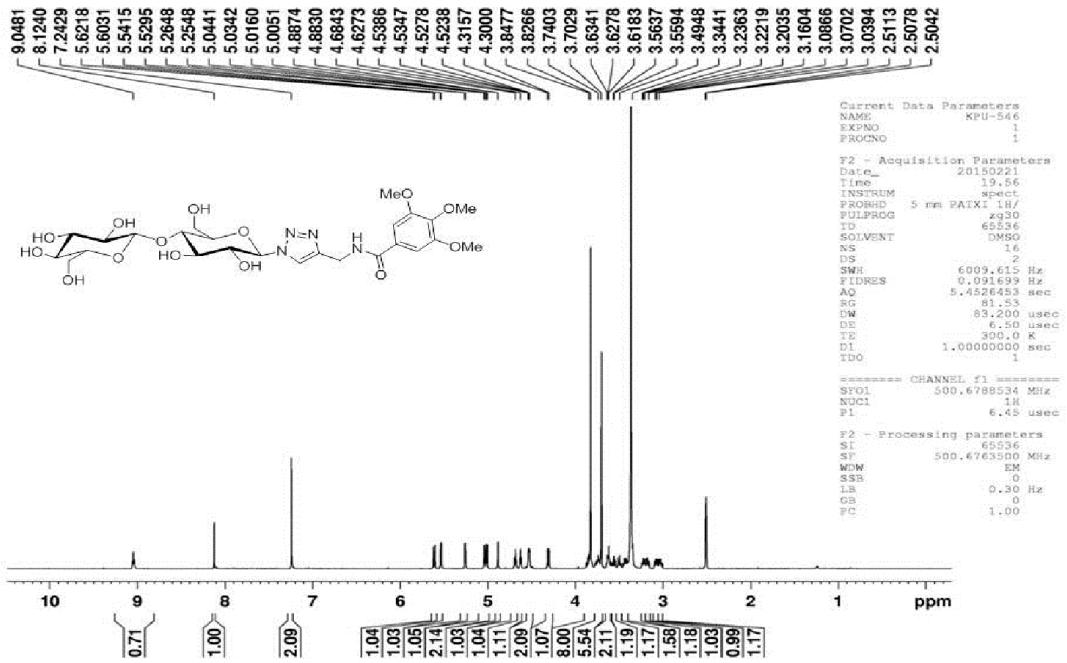
^{13}C NMR spectrum of compound **4d**



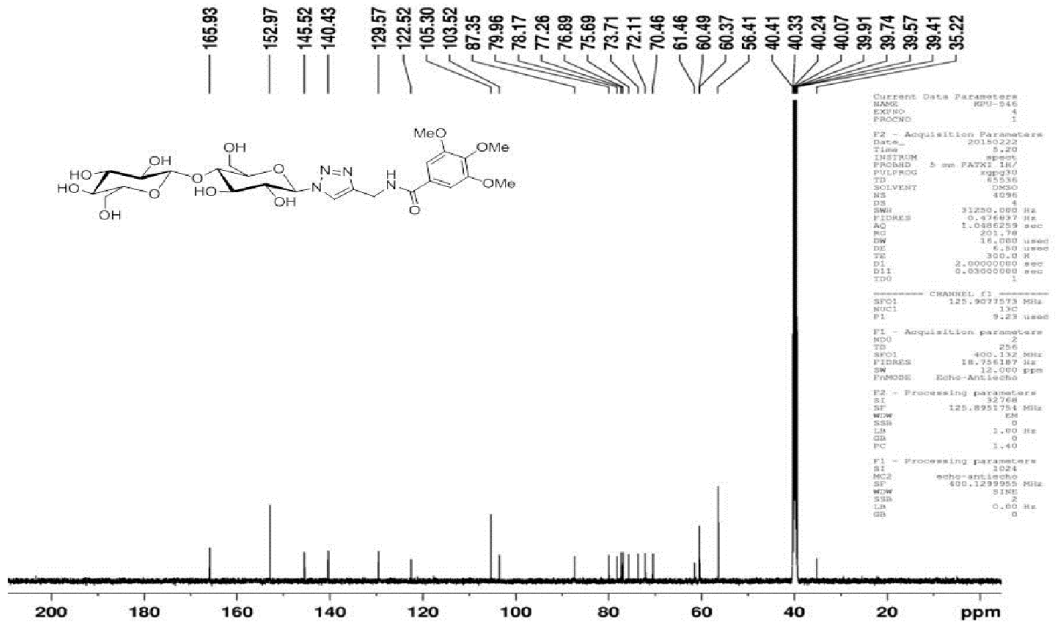
HRMS spectrum of compound **4d**



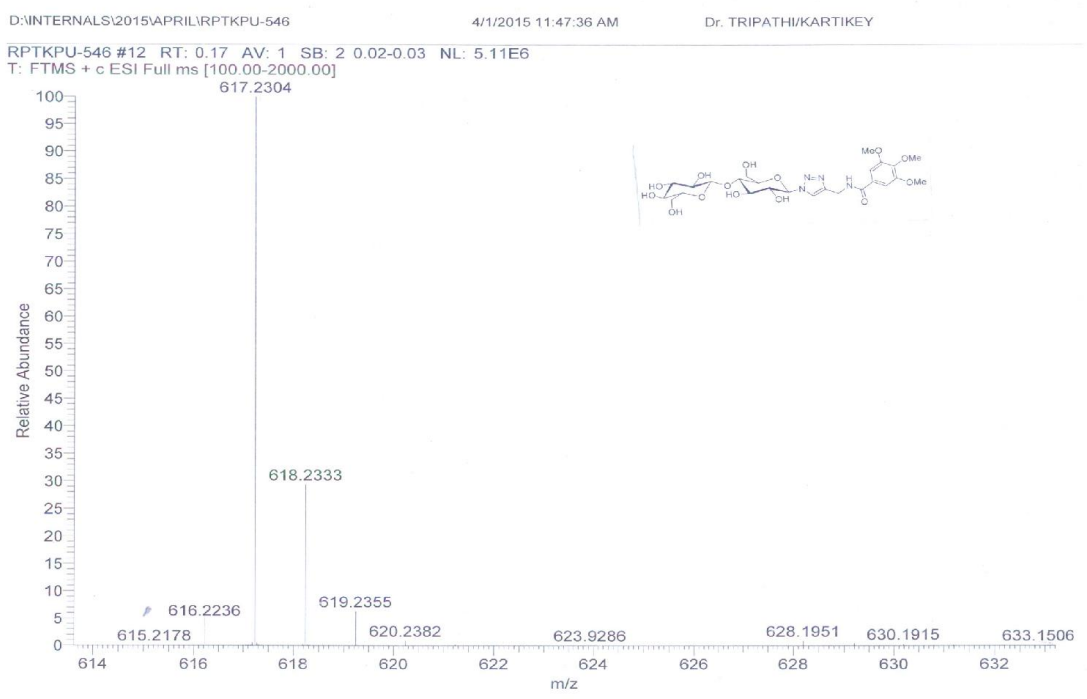
^{1}H NMR spectrum of compound **4d'**



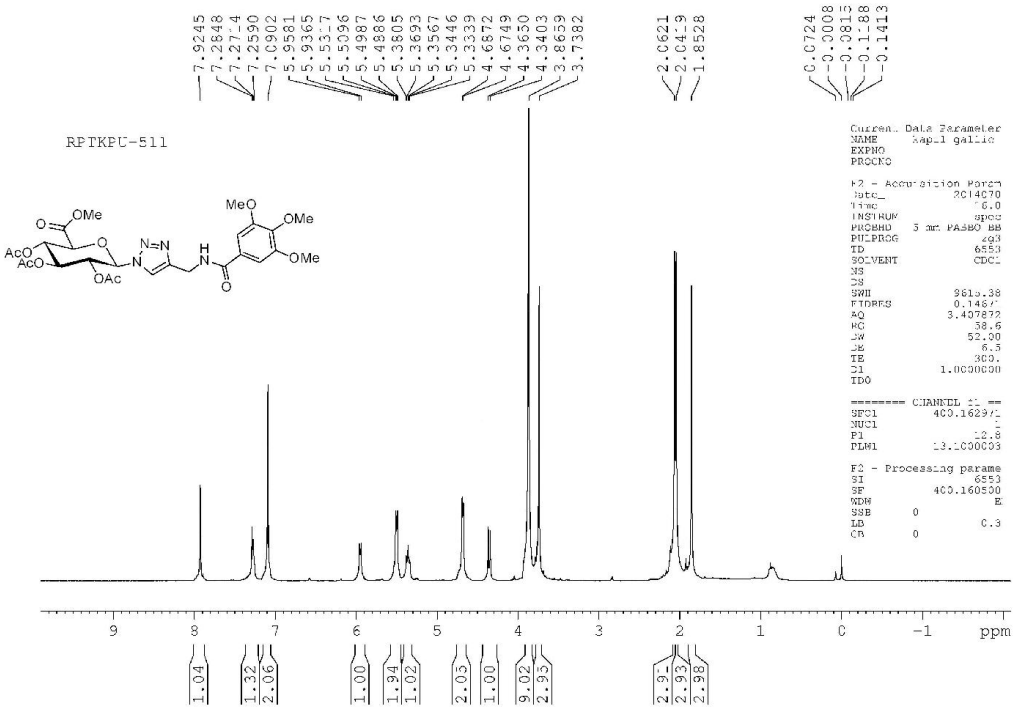
^{13}C NMR spectrum of compound **4d'**



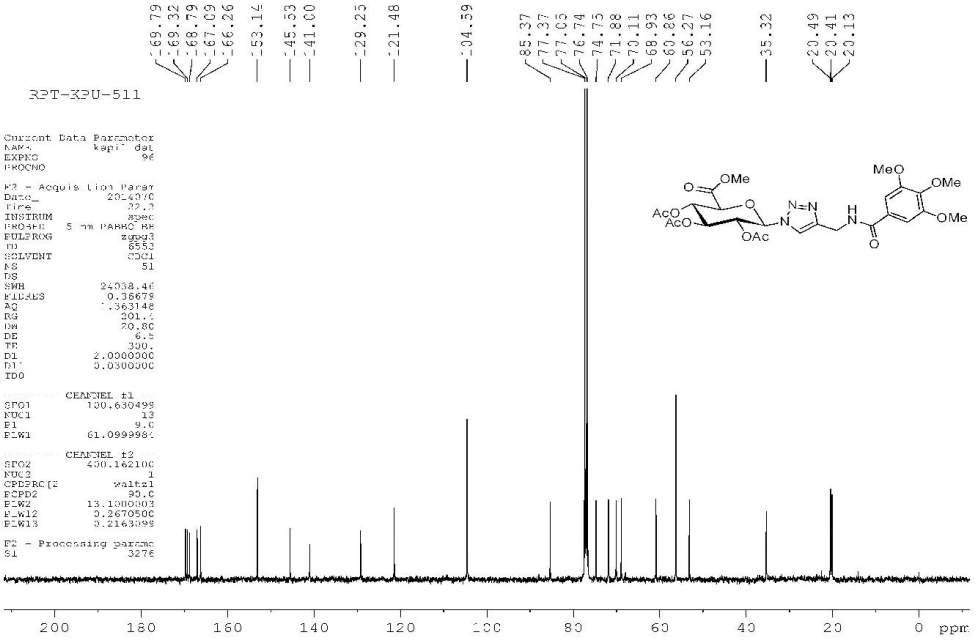
HRMS spectrum of compound **4d'**



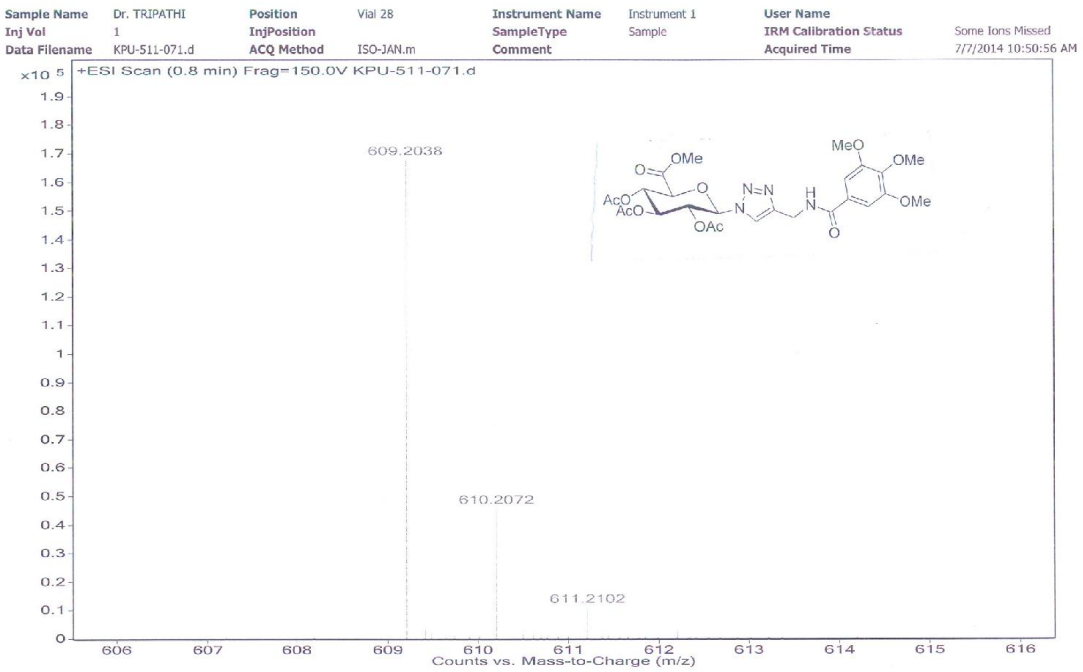
^{1}H NMR spectrum of compound **4e**



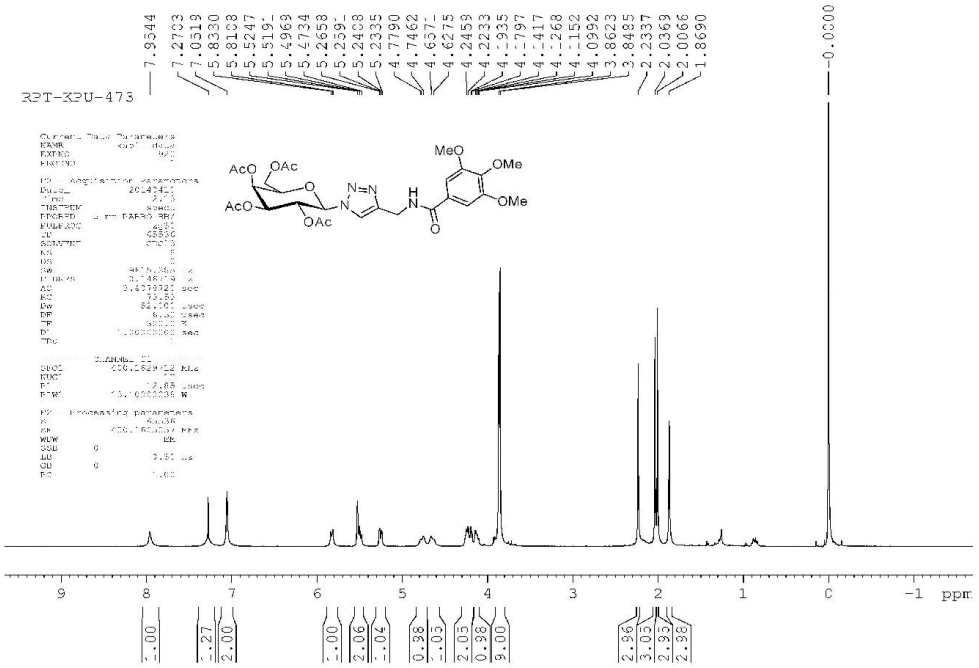
^{13}C NMR spectrum of compound **4e**



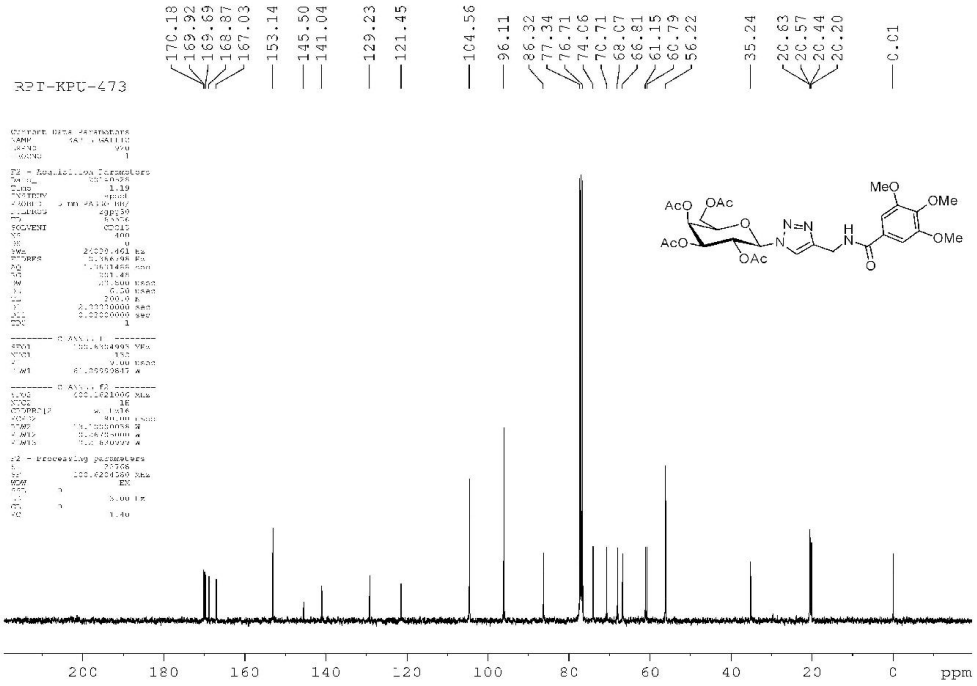
HRMS spectrum of compound **4e**



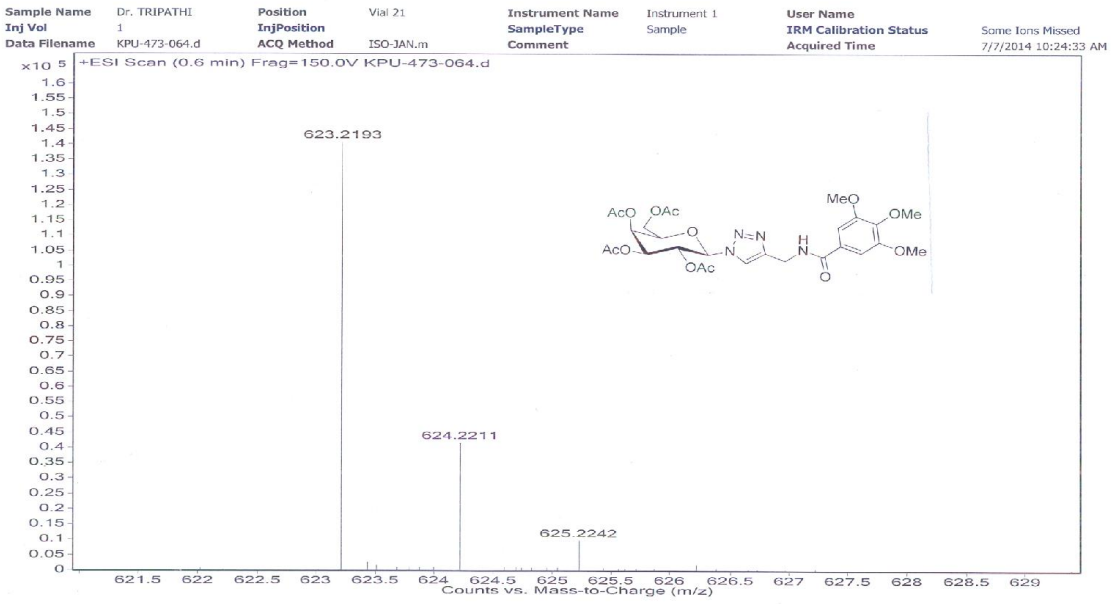
^{1}H NMR spectrum of compound **4f**



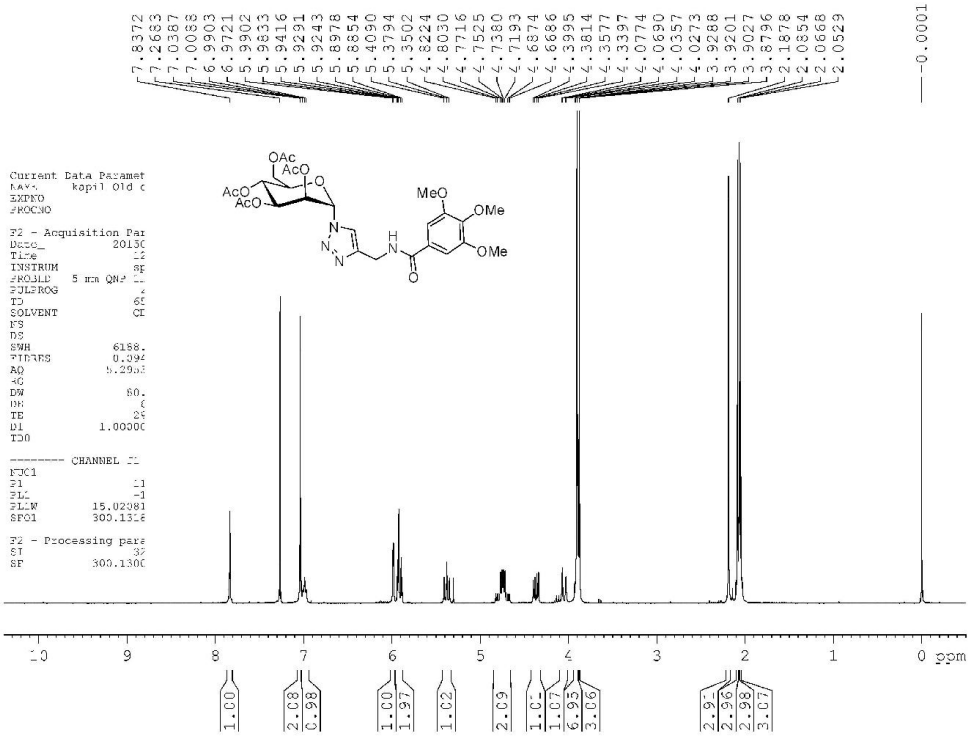
^{13}C NMR spectrum of compound **4f**



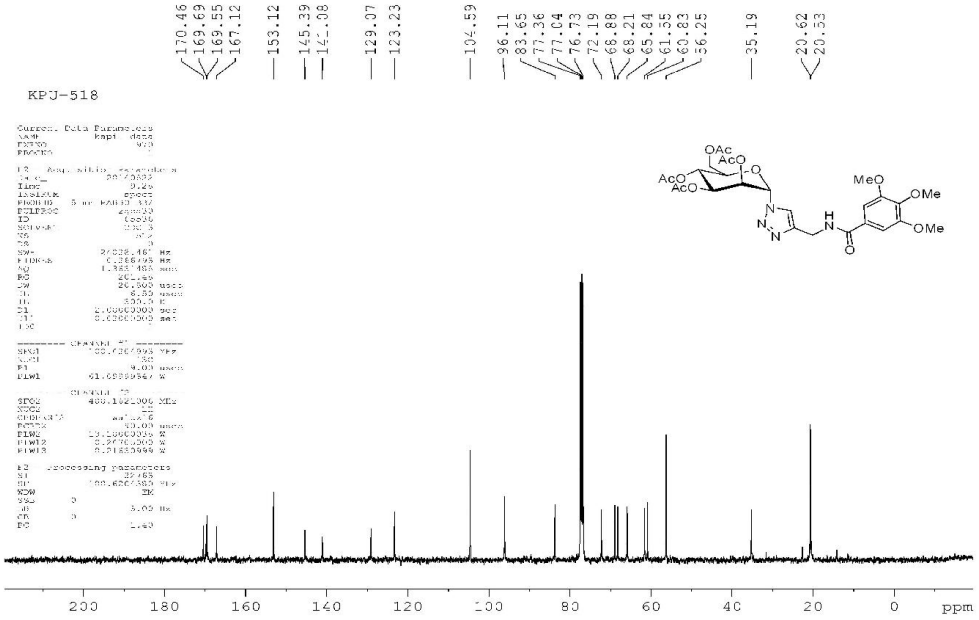
HRMS spectrum of compound **4f**



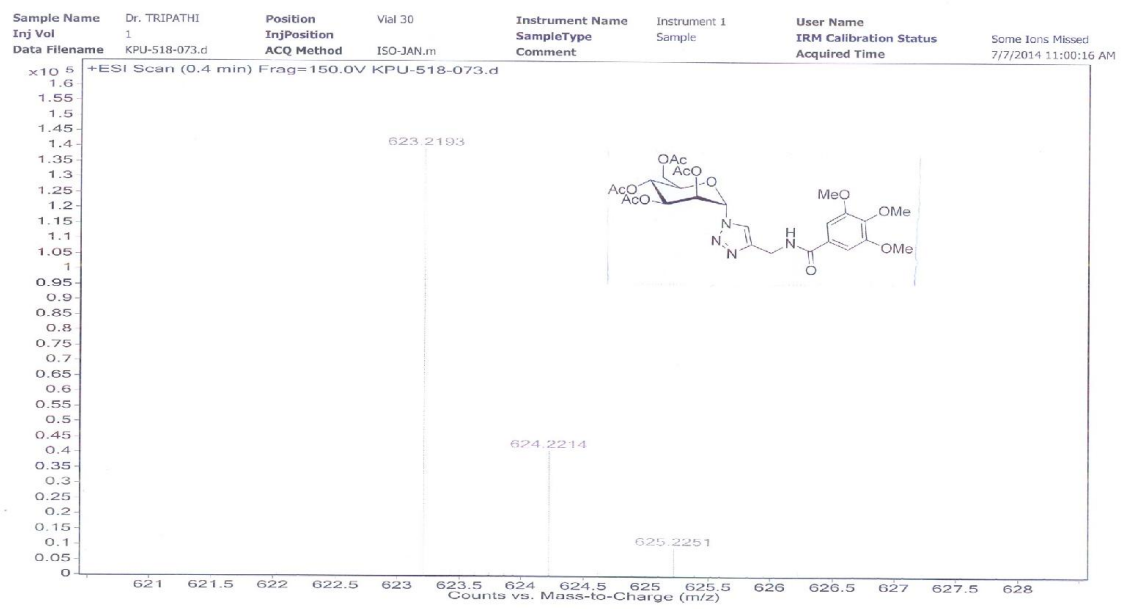
^{1}H NMR spectrum of compound **4g**



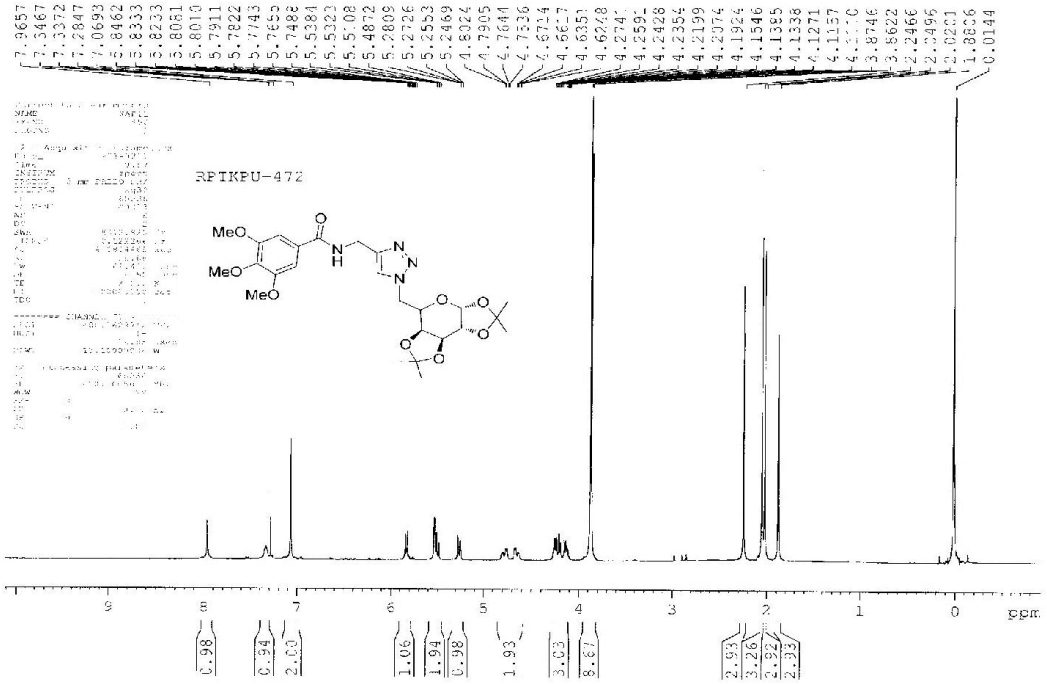
^{13}C NMR spectrum of compound **4g**



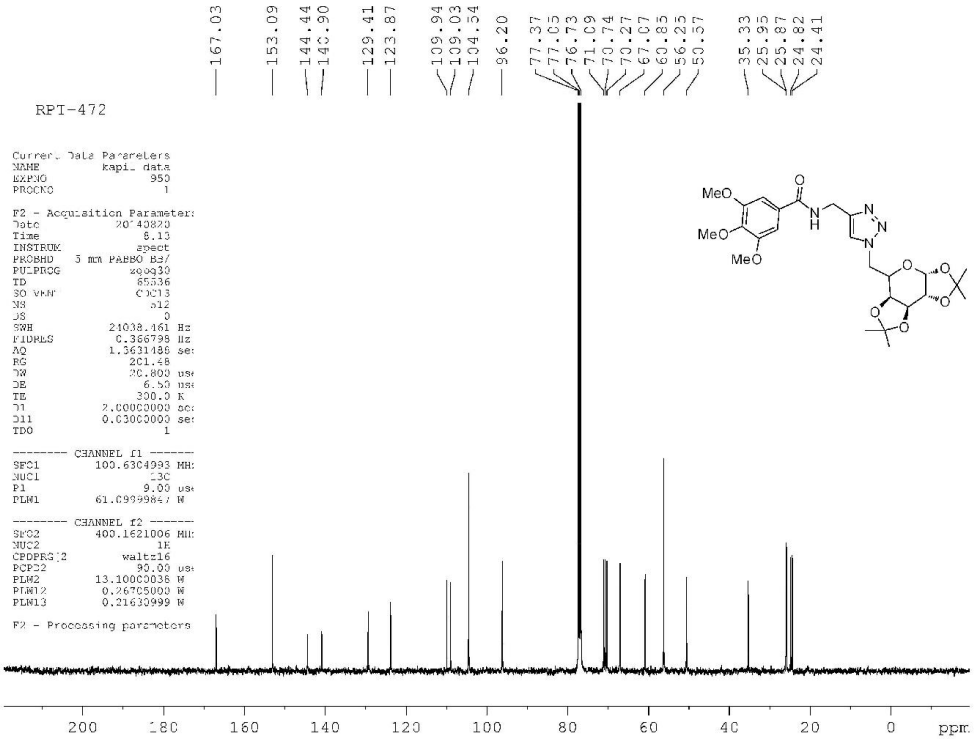
HRMS spectrum of compound **4g**



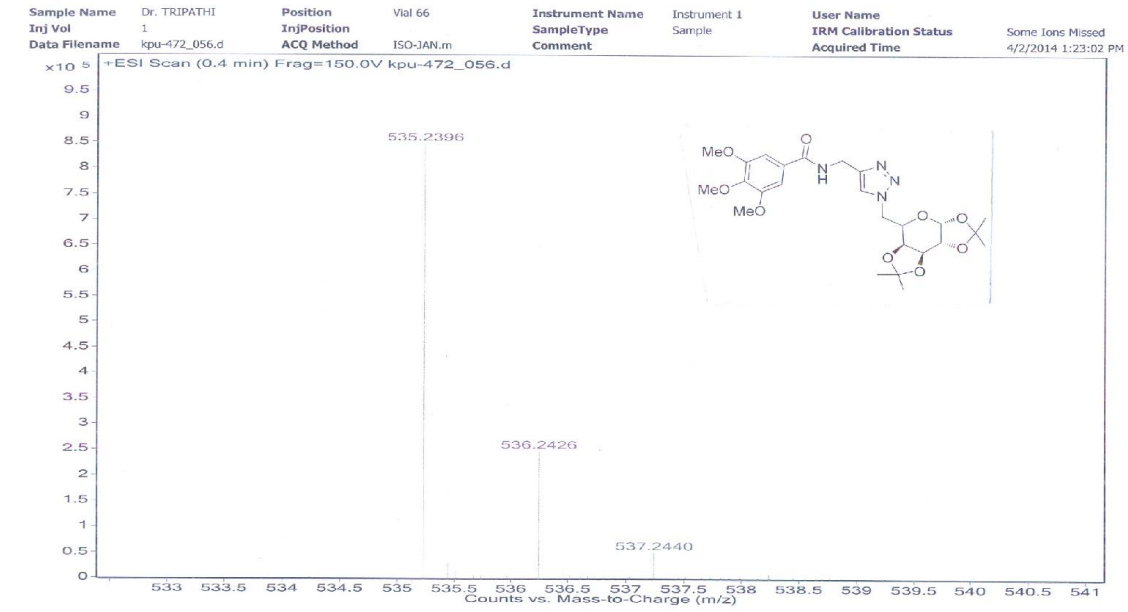
^{1}H NMR spectrum of compound **4h**



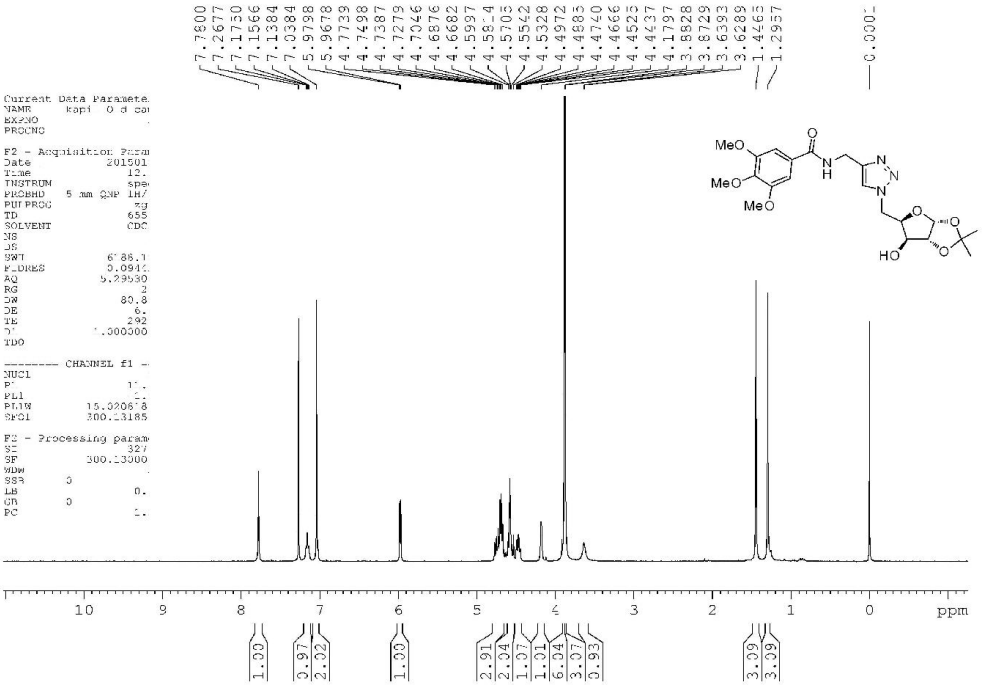
^{13}C NMR spectrum of compound **4h**



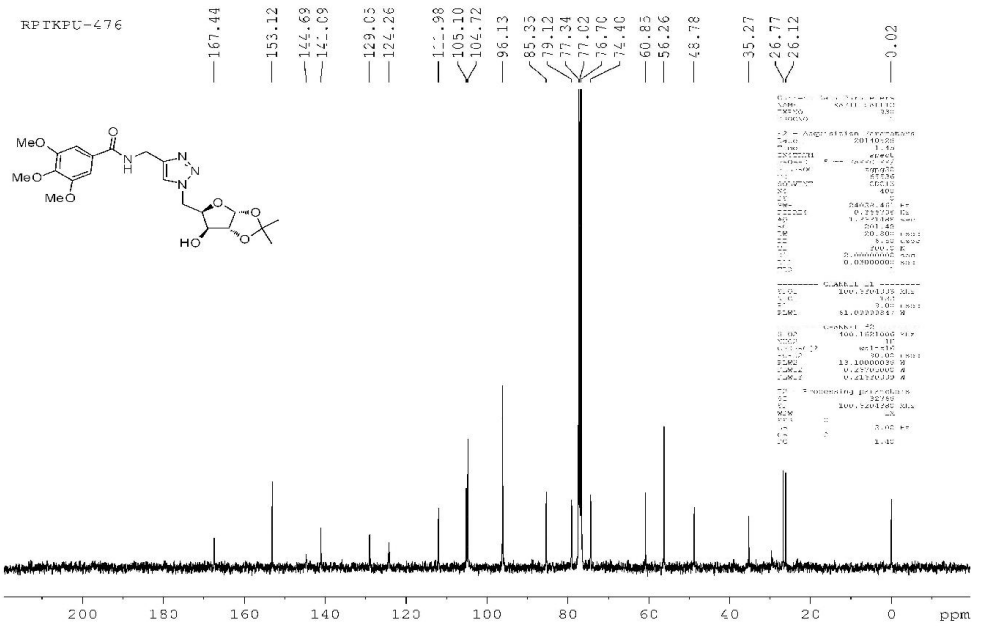
HRMS spectrum of compound **4h**



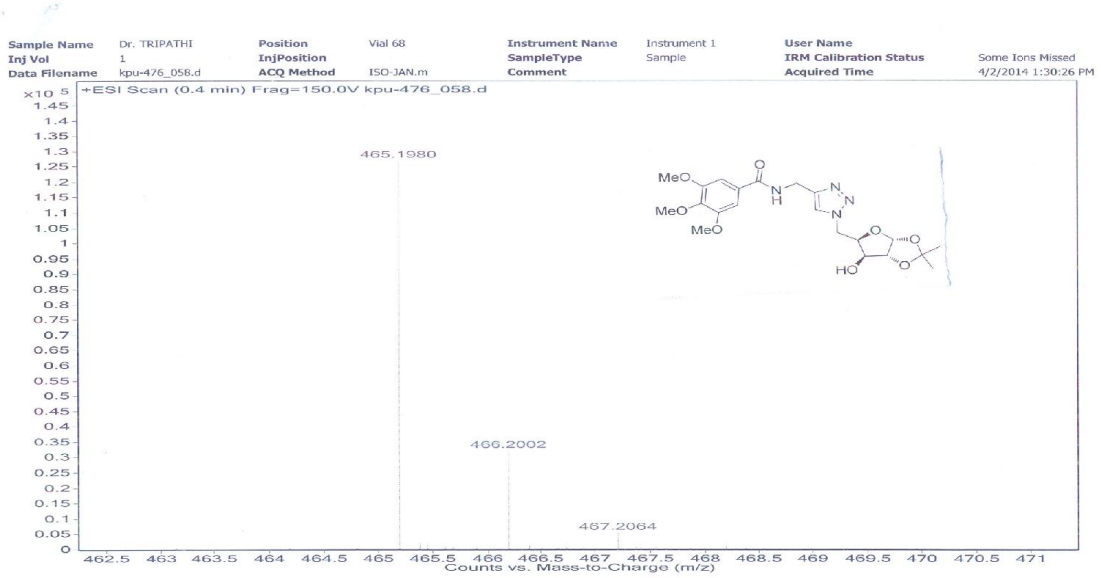
^{1}H NMR spectrum of compound **4i**



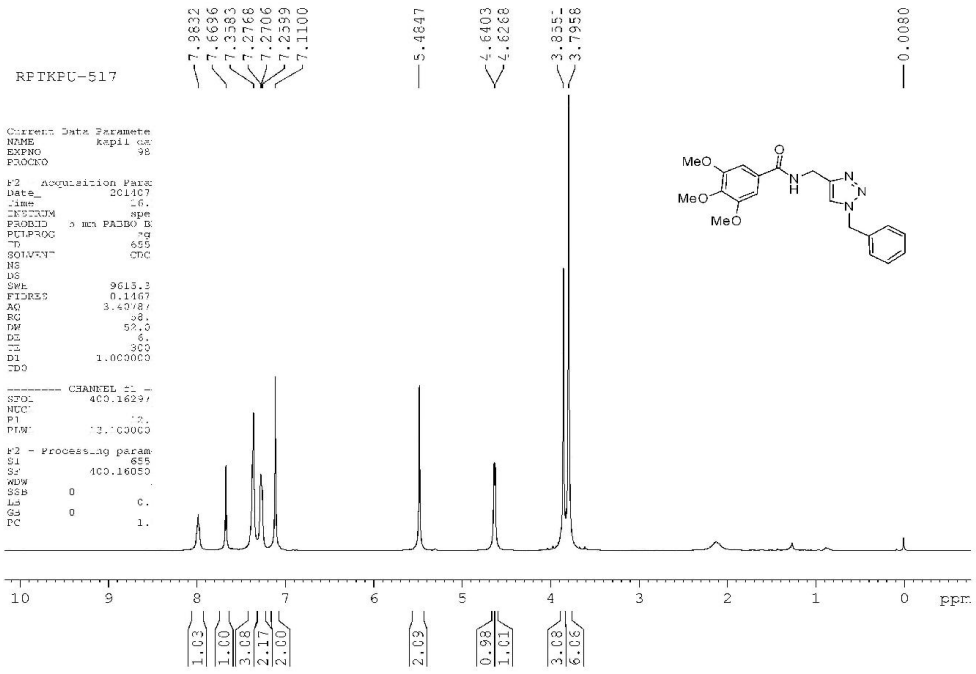
^{13}C NMR spectrum of compound **4i**



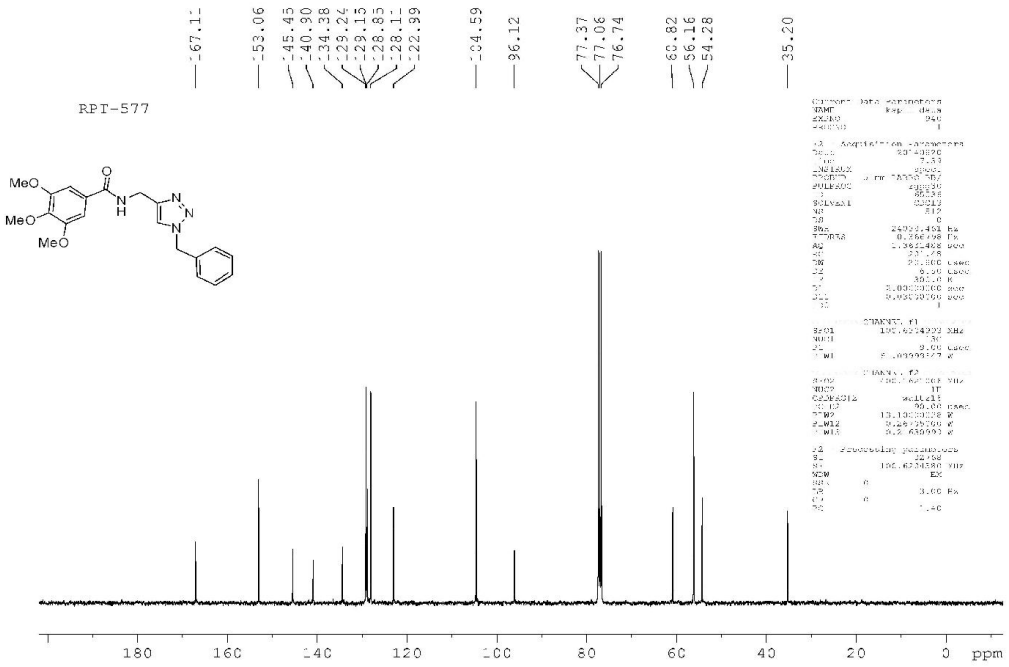
HRMS spectrum of compound **4i**



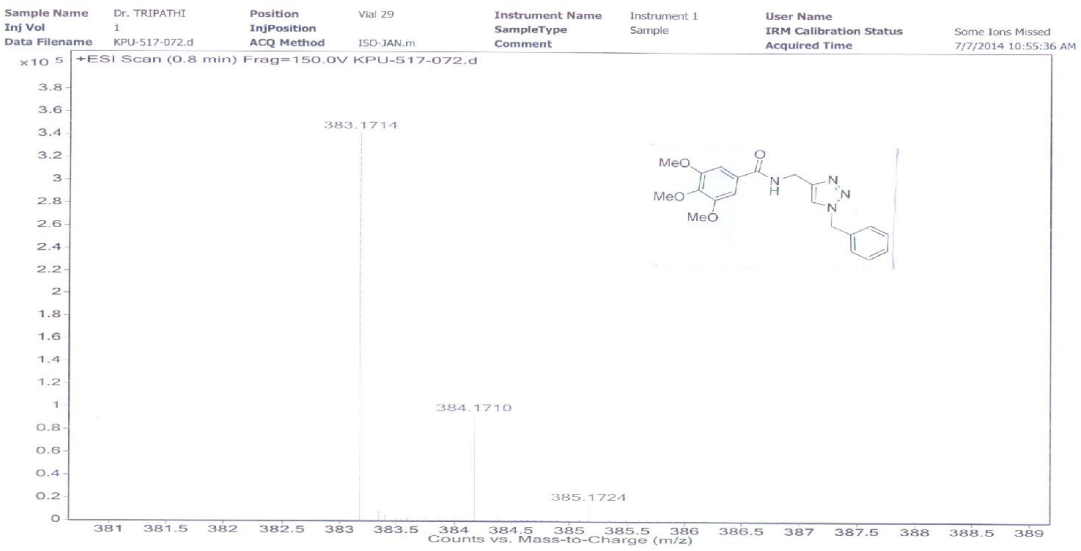
^{1}H NMR spectrum of compound **4j**



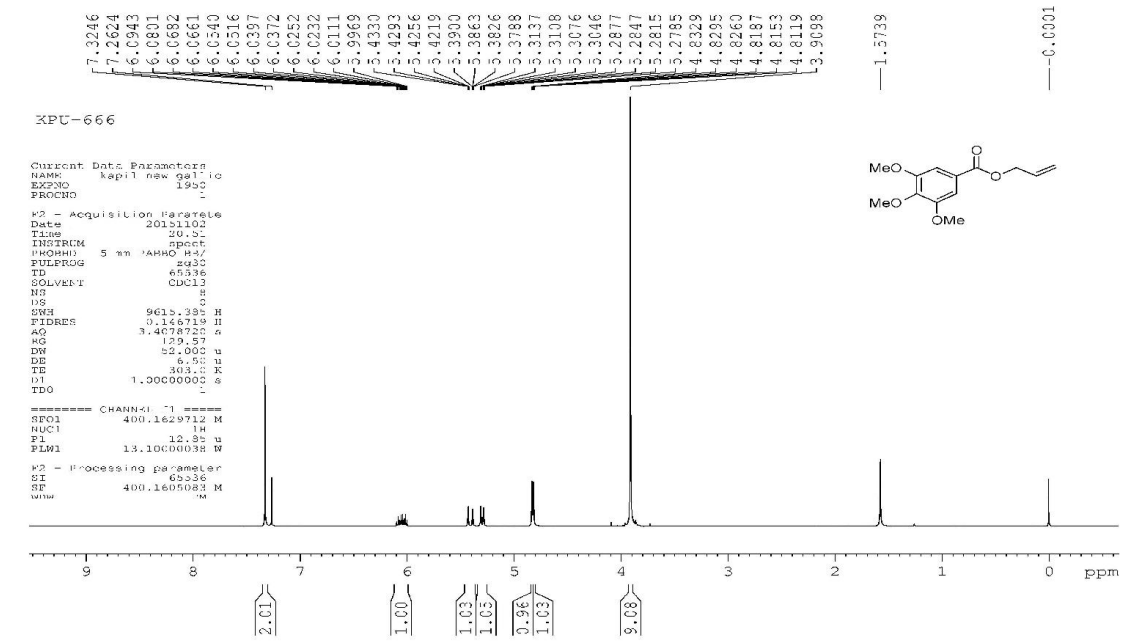
^{13}C NMR spectrum of compound **4j**



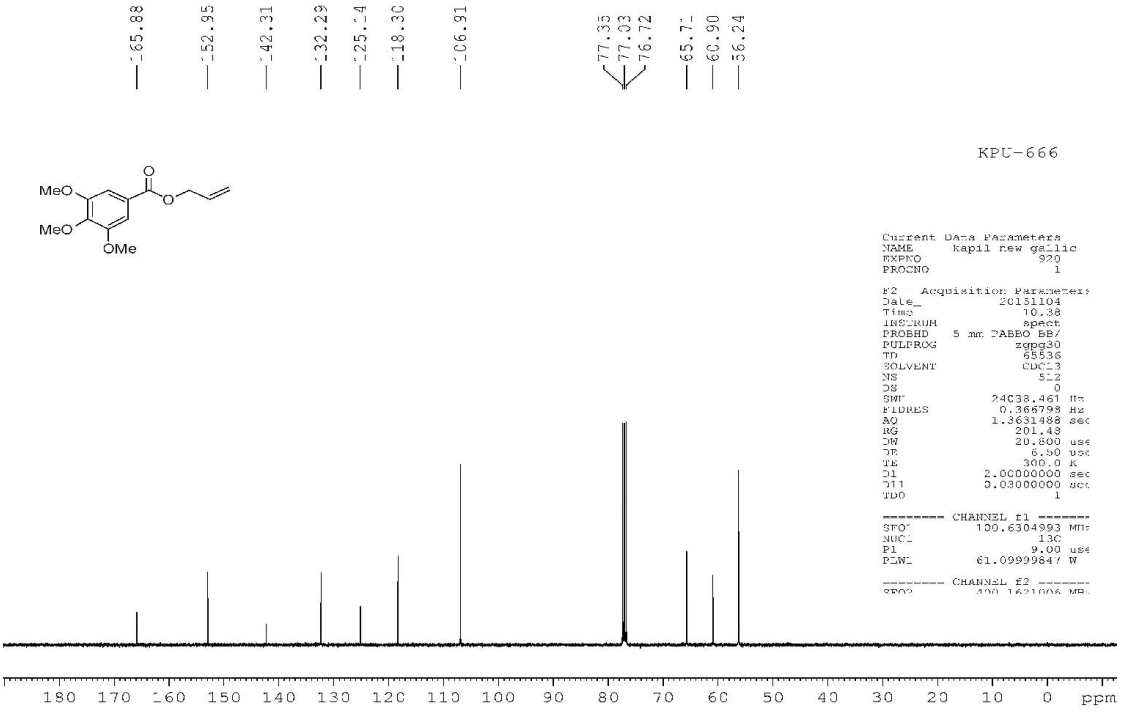
HRMS spectrum of compound **4j**



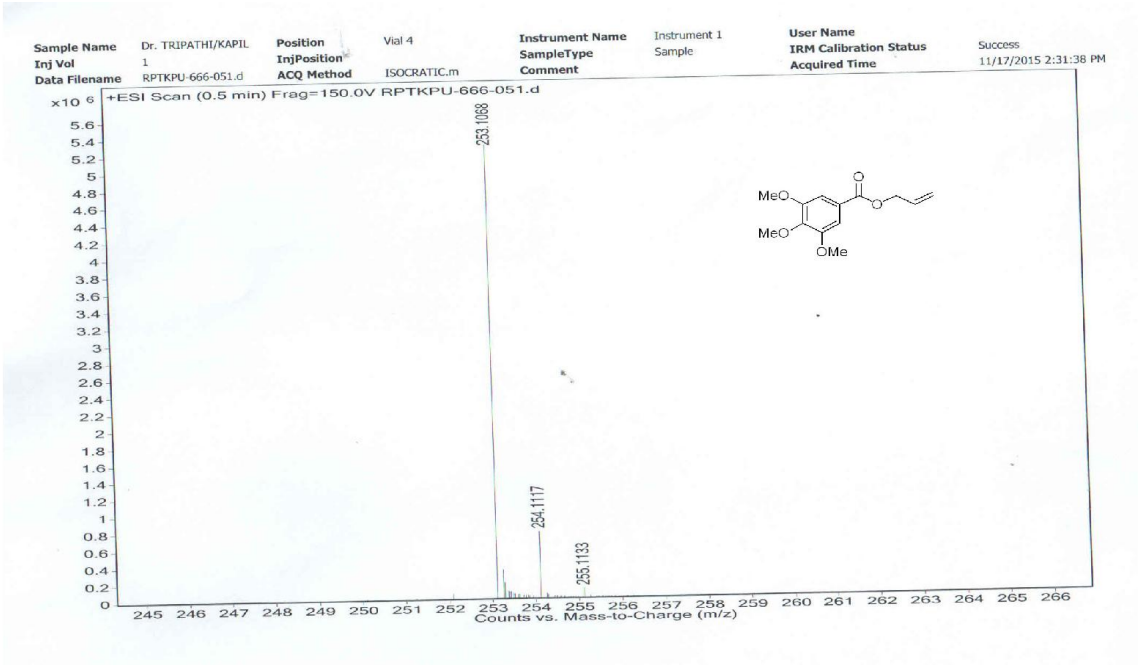
^{1}H NMR spectrum of compound **5**



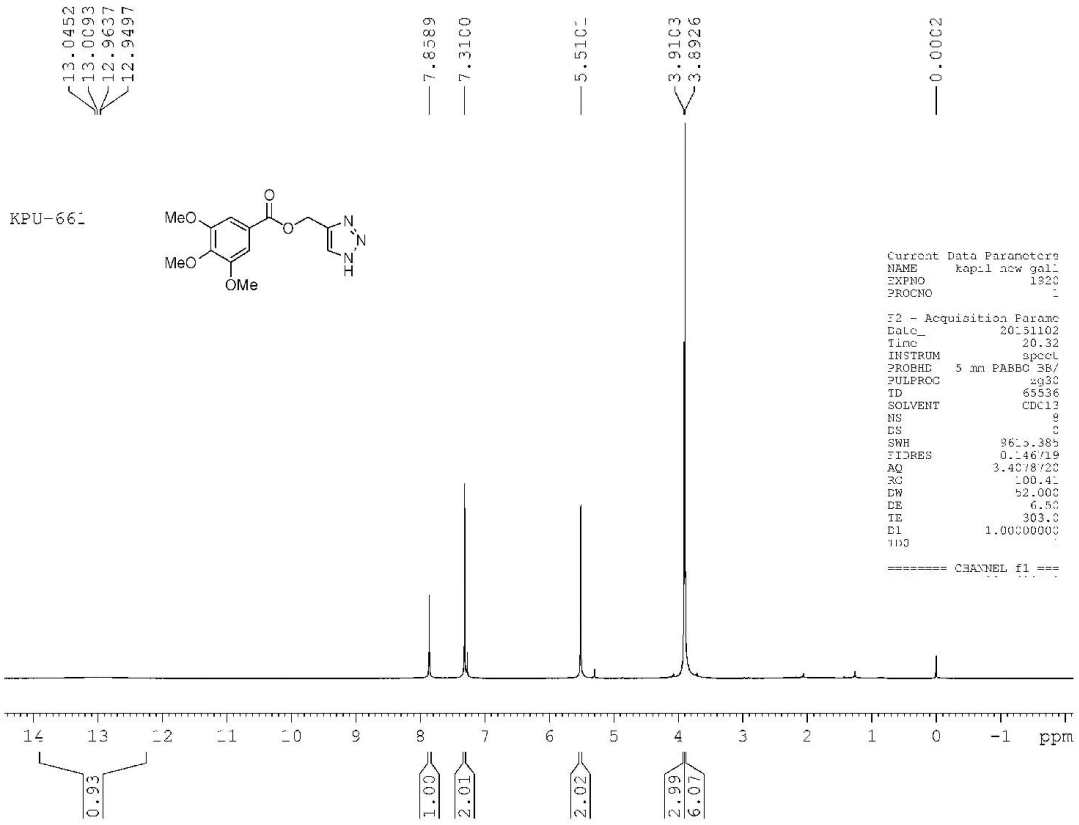
^{13}C NMR spectrum of compound **5**



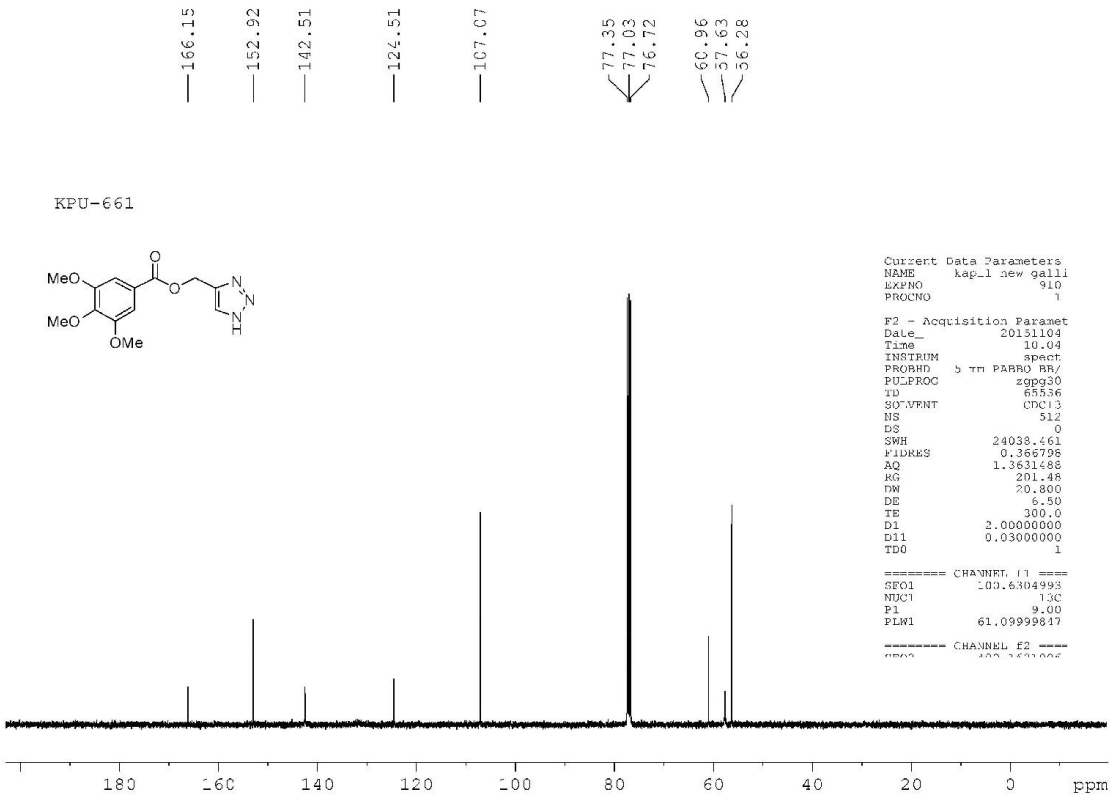
HRMS spectrum of compound **5**



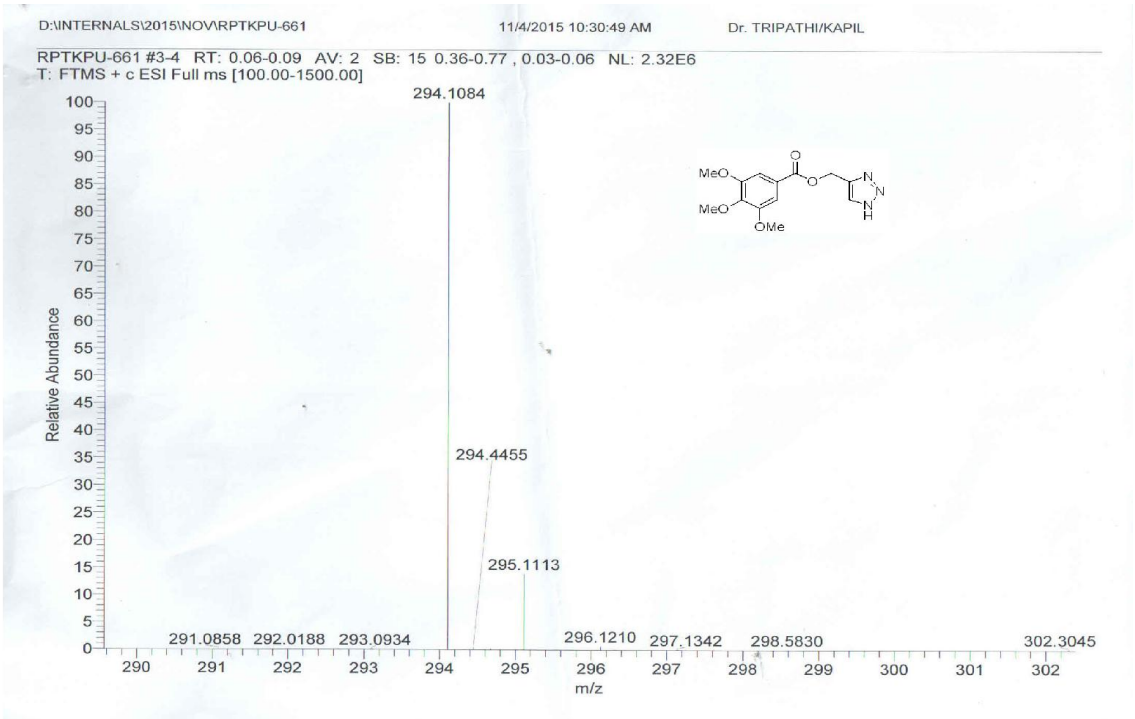
^{1}H NMR spectrum of compound **6**



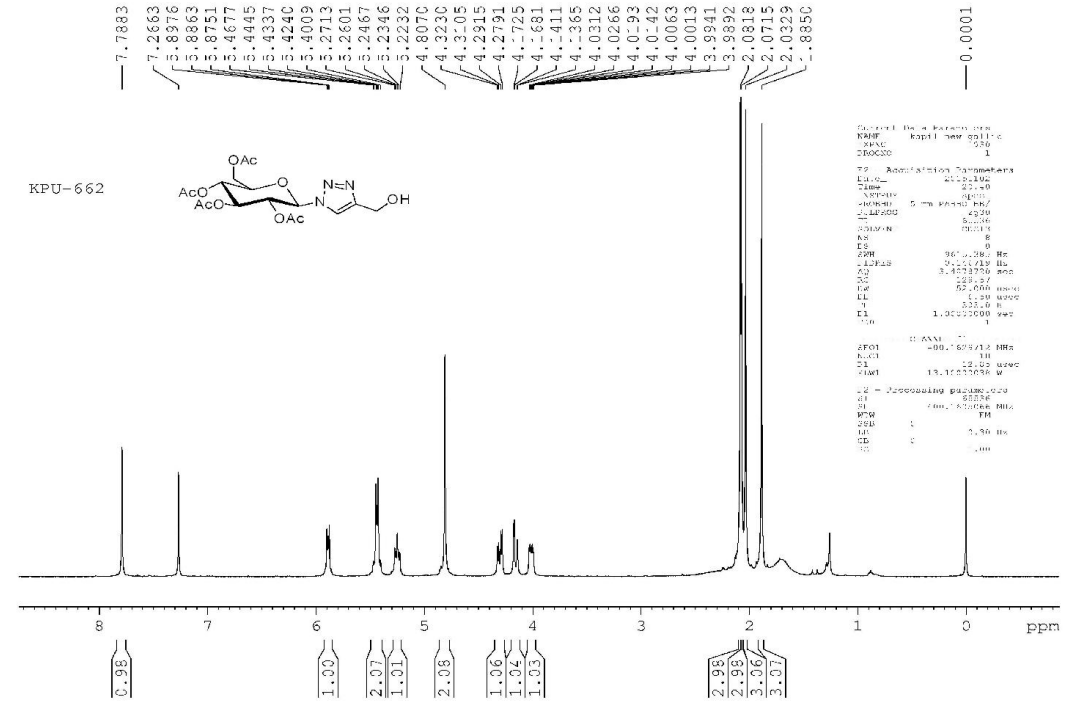
^{13}C NMR spectrum of compound **6**



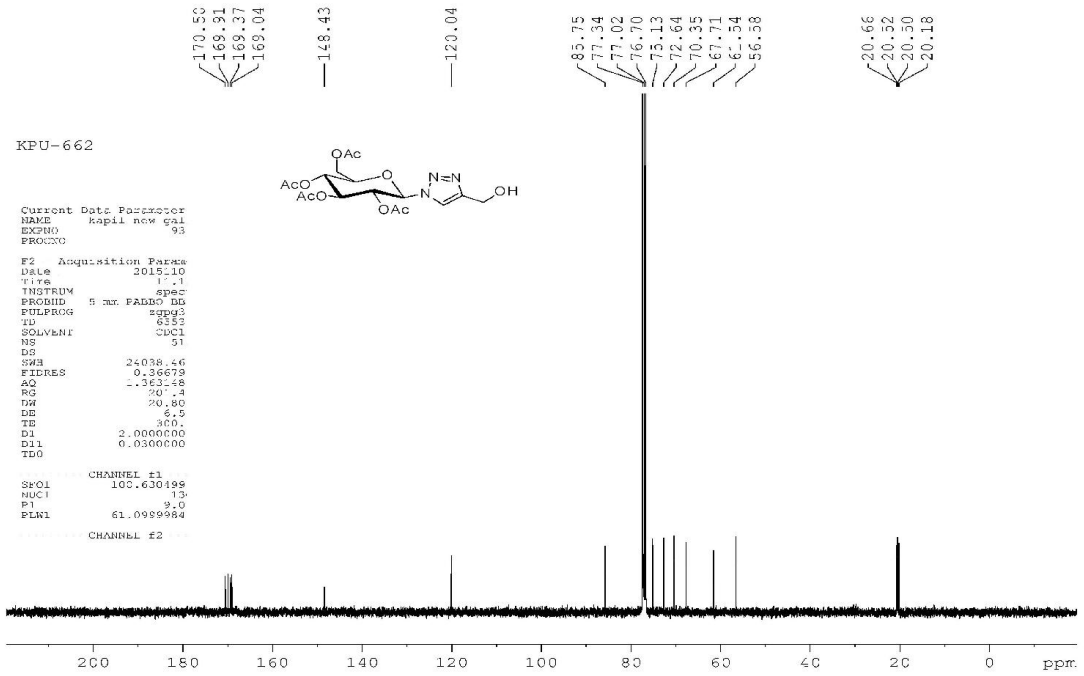
HRMS spectrum of compound **6**



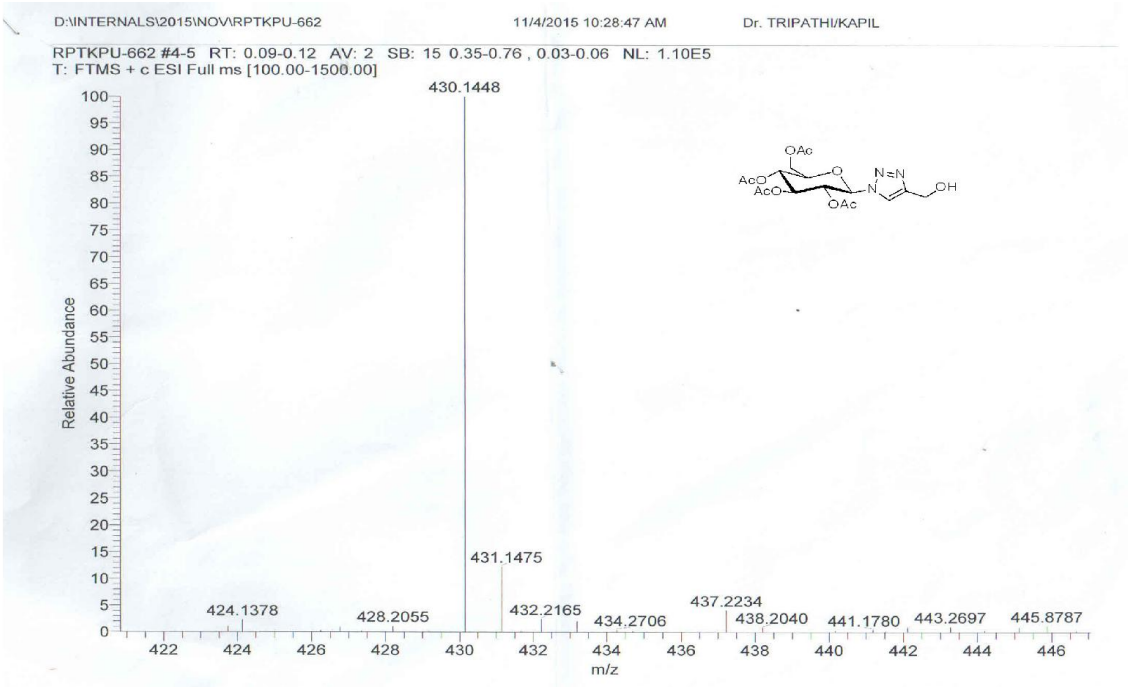
^{1}H NMR spectrum of compound **7a**



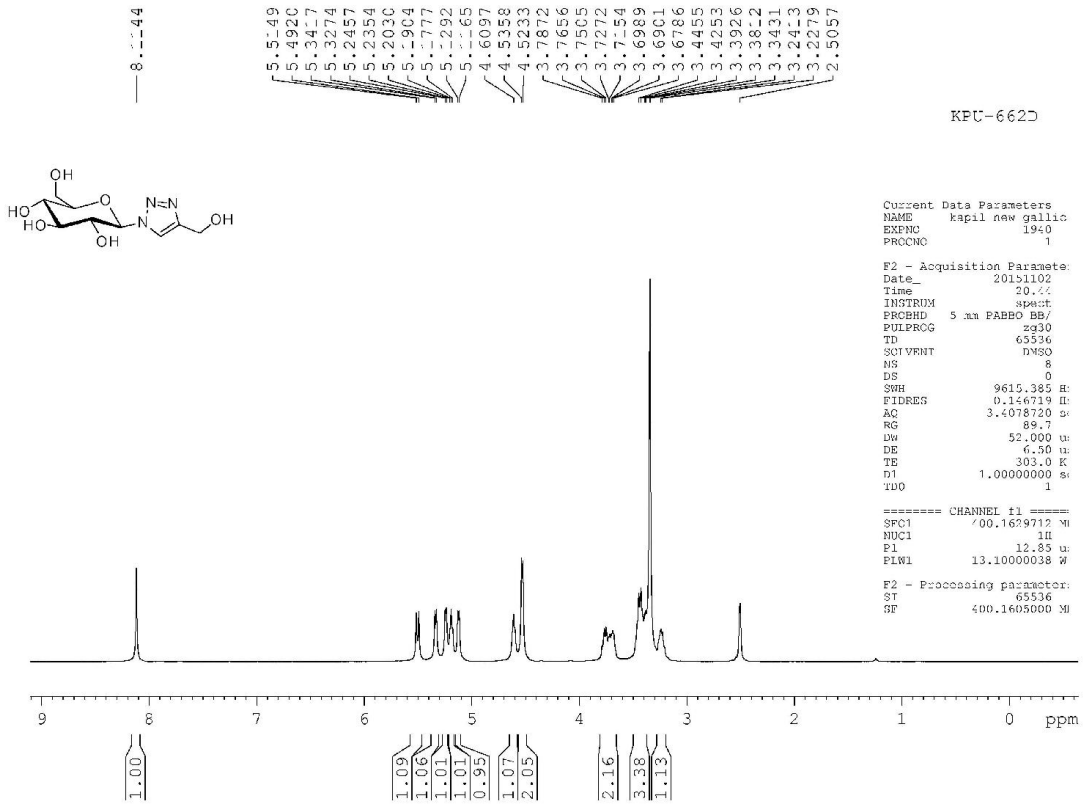
^{13}C NMR spectrum of compound **7a**



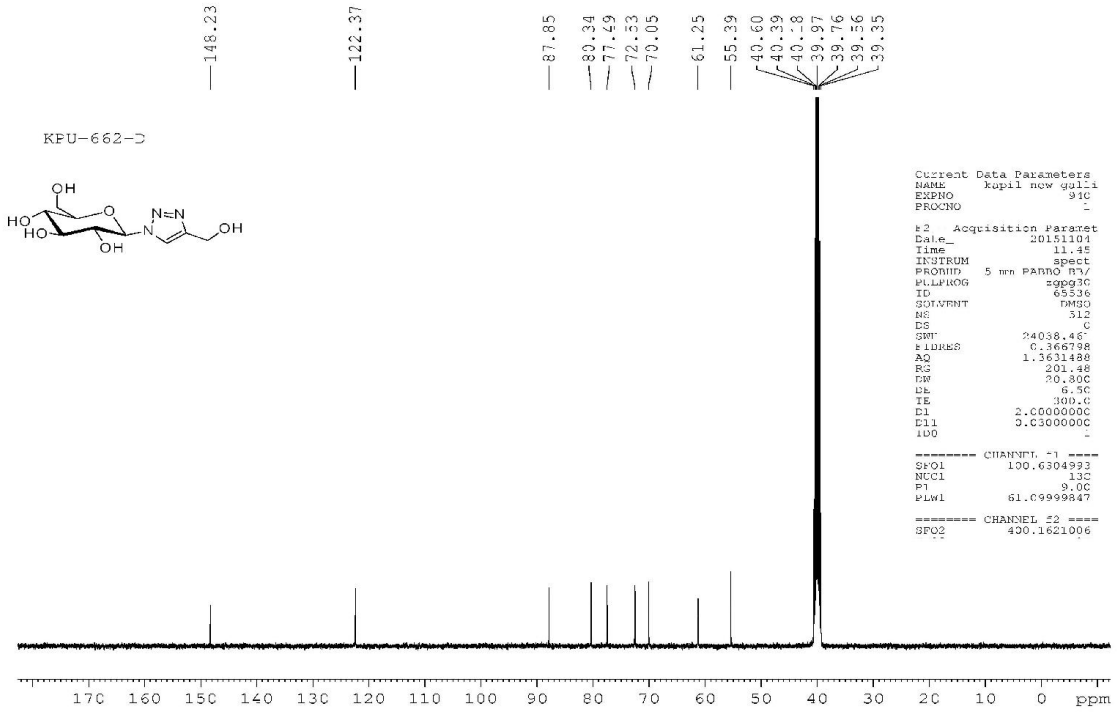
HRMS spectrum of compound **7a**



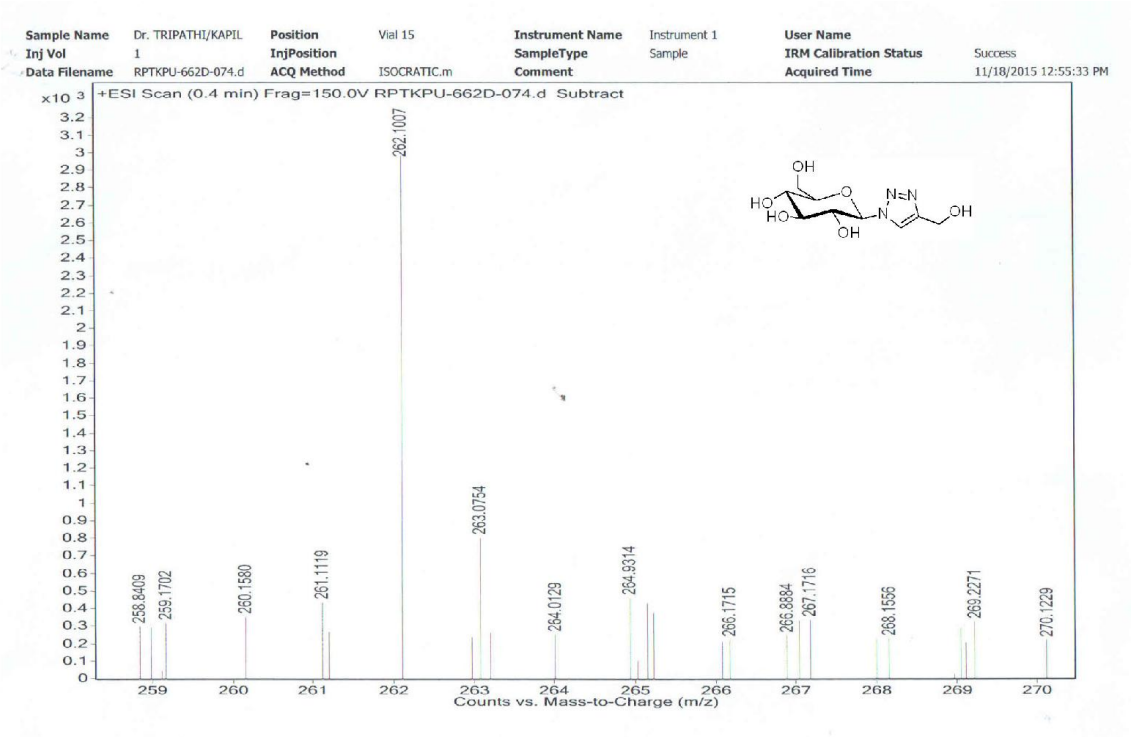
^{1}H NMR spectrum of compound **7a'**



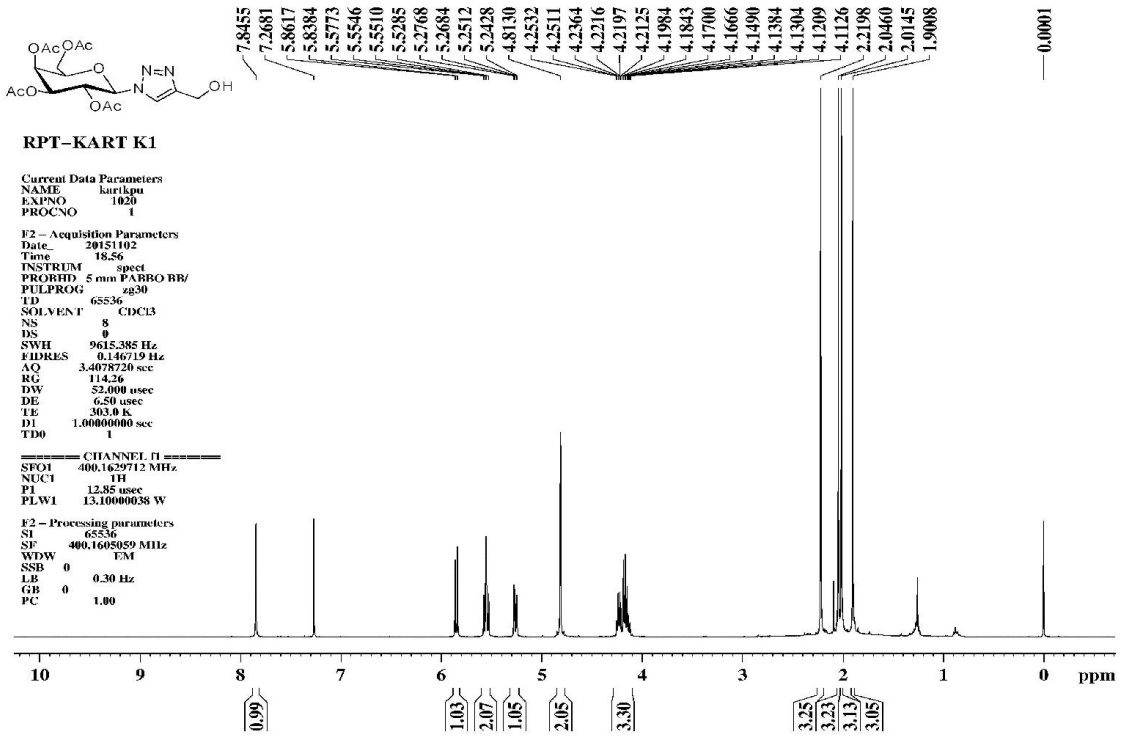
^{13}C NMR spectrum of compound **7a'**



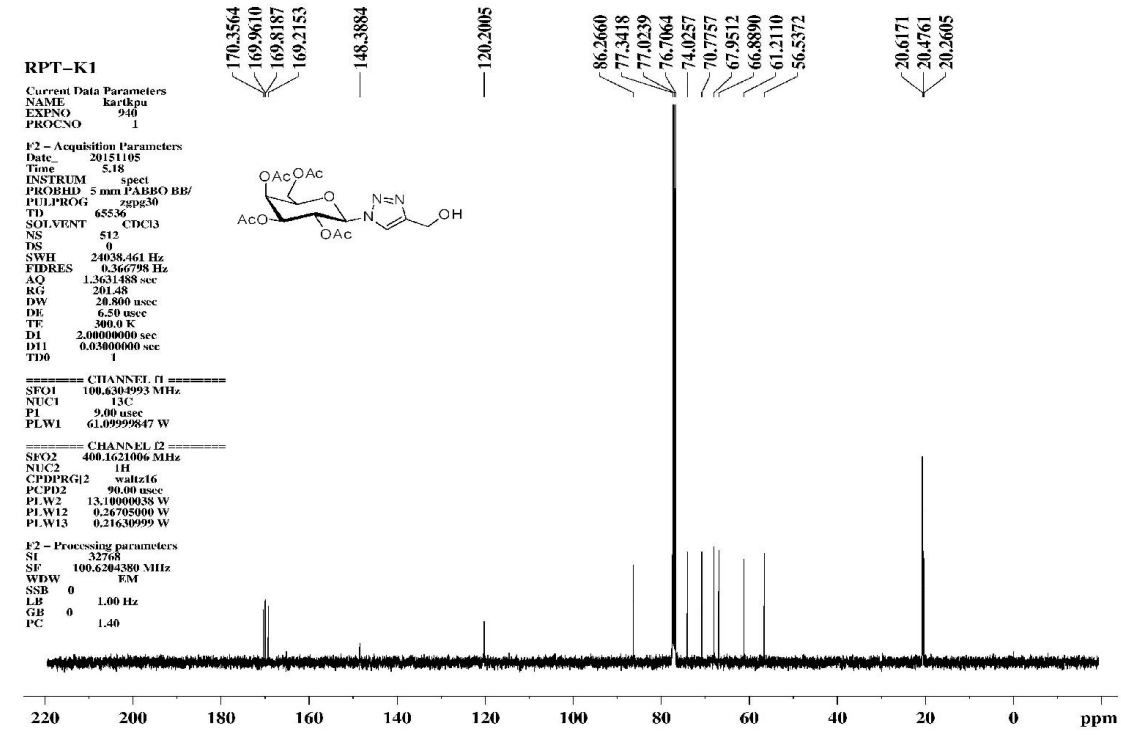
HRMS spectrum of compound **7a'**



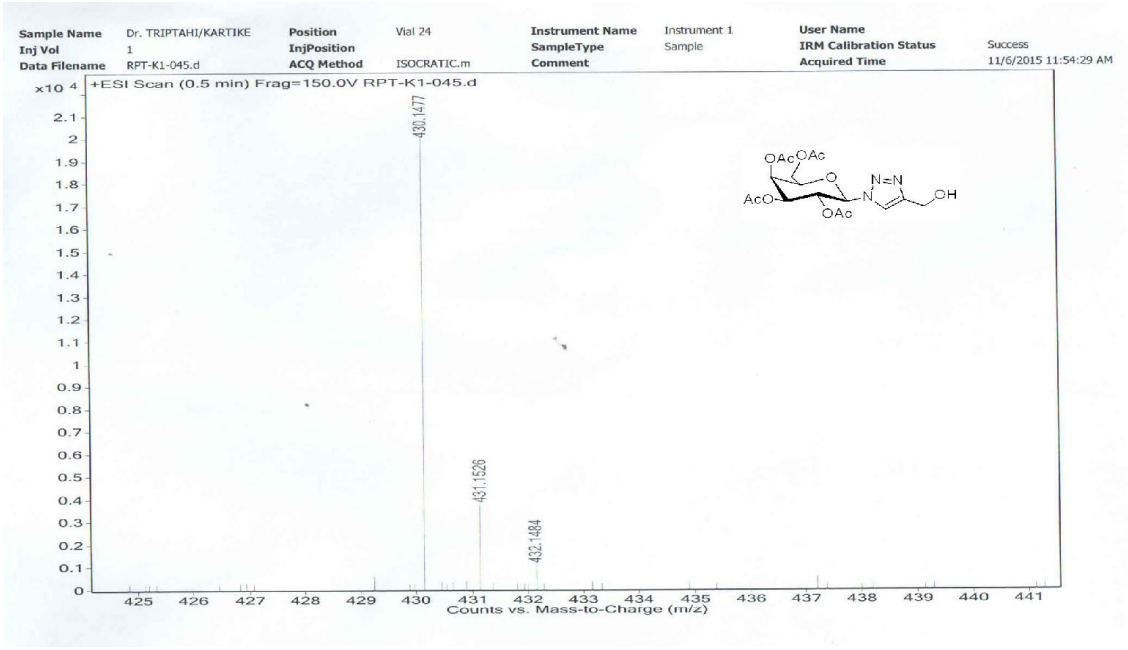
^{1}H NMR spectrum of compound **7f**



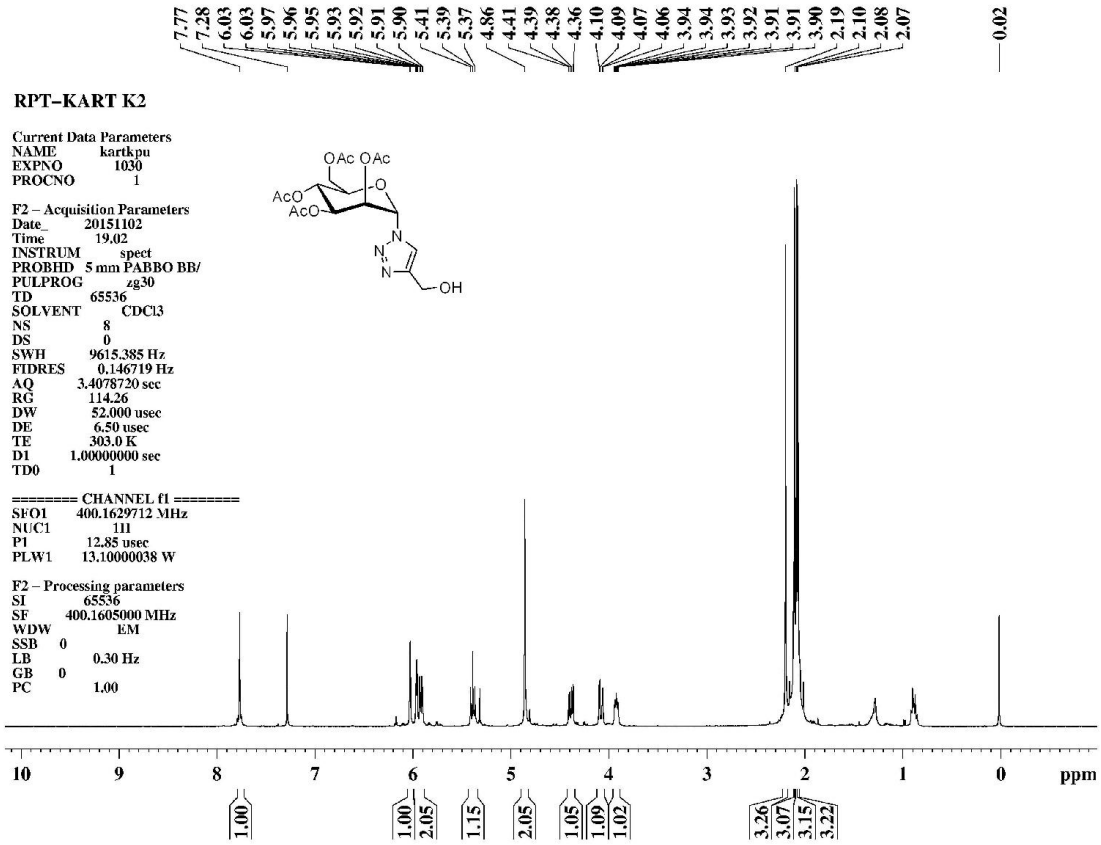
^{13}C NMR spectrum of compound **7f**



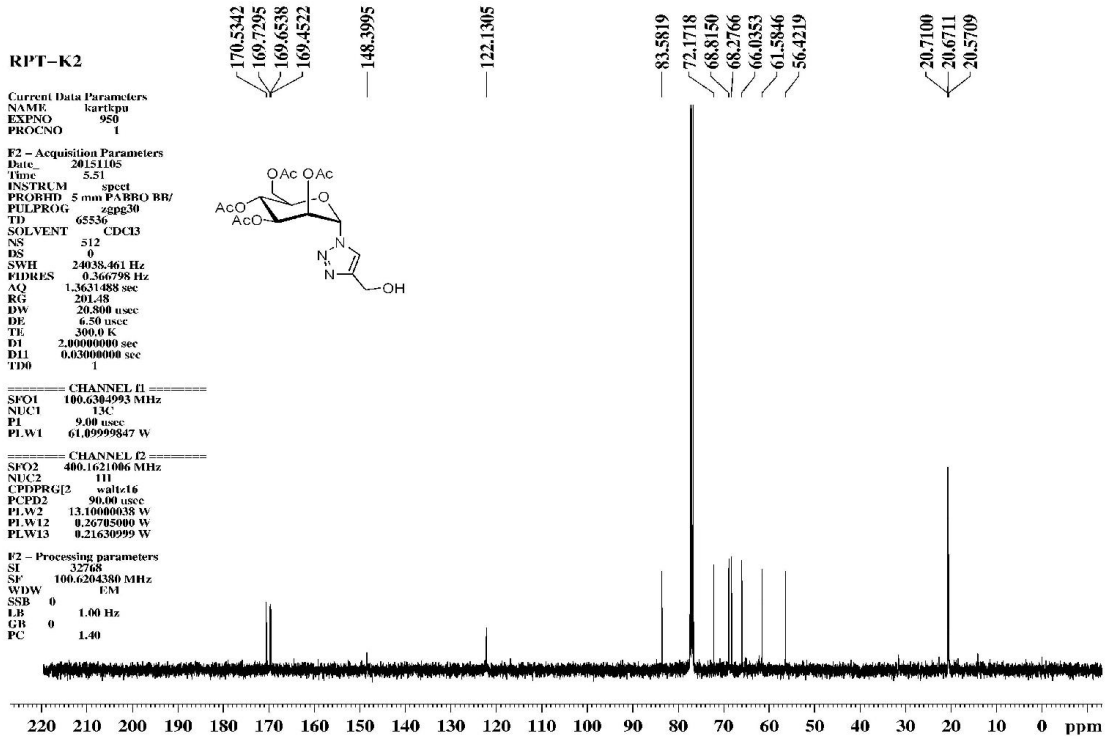
HRMS spectrum of compound **7f**



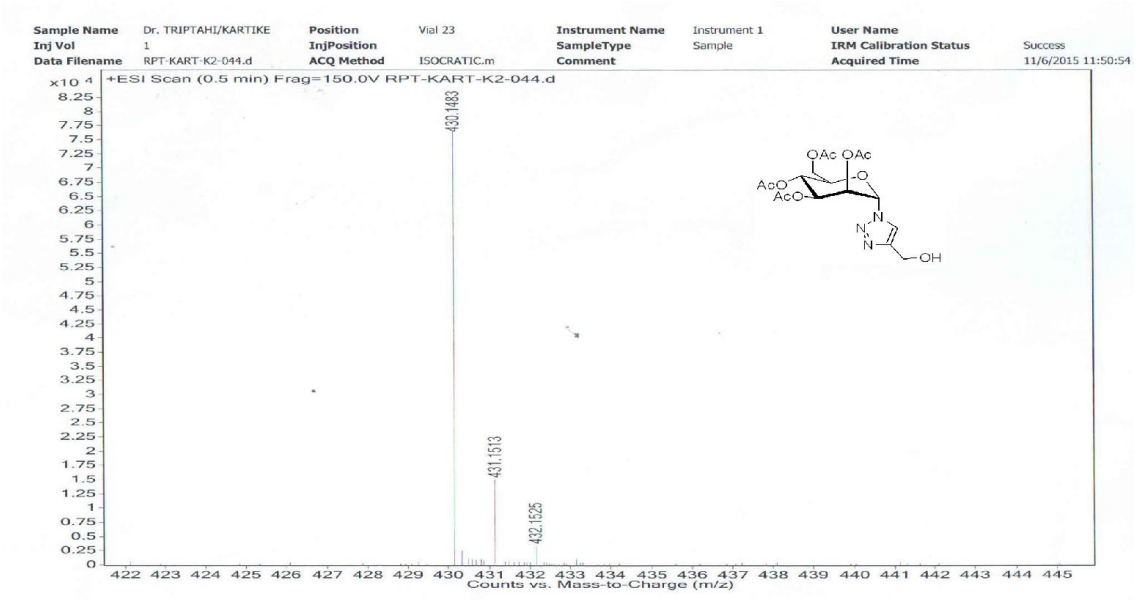
^{1}H NMR spectrum of compound **7g**



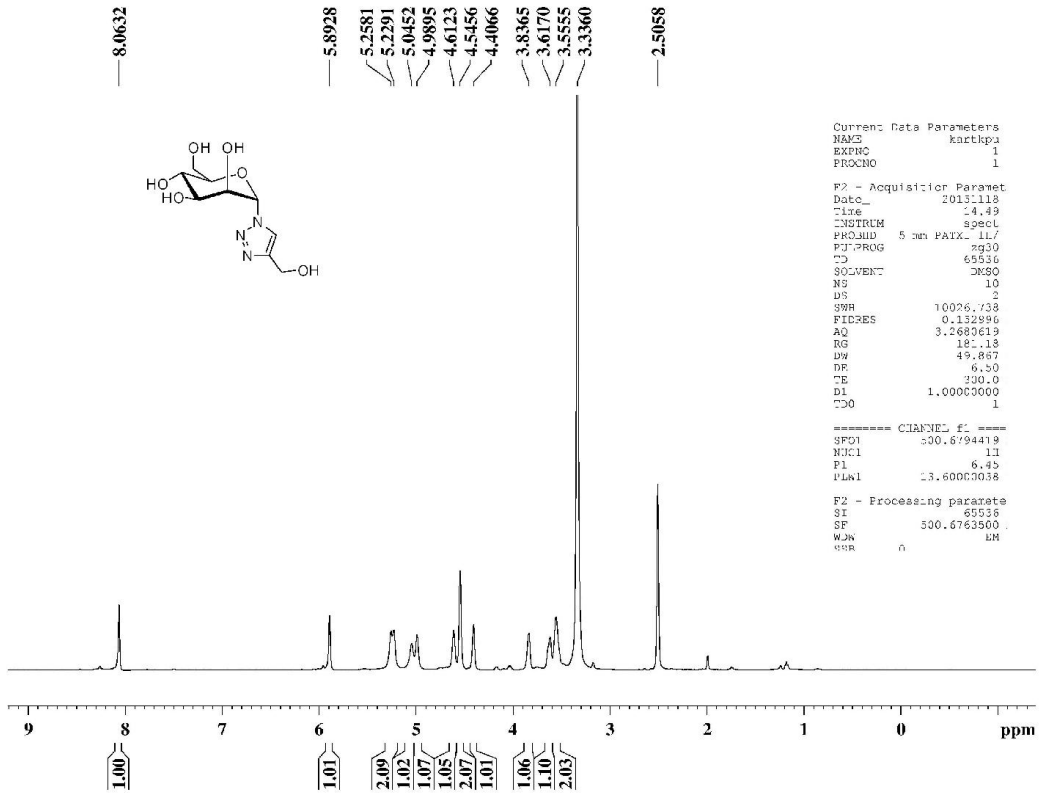
^{13}C NMR spectrum of compound **7g**



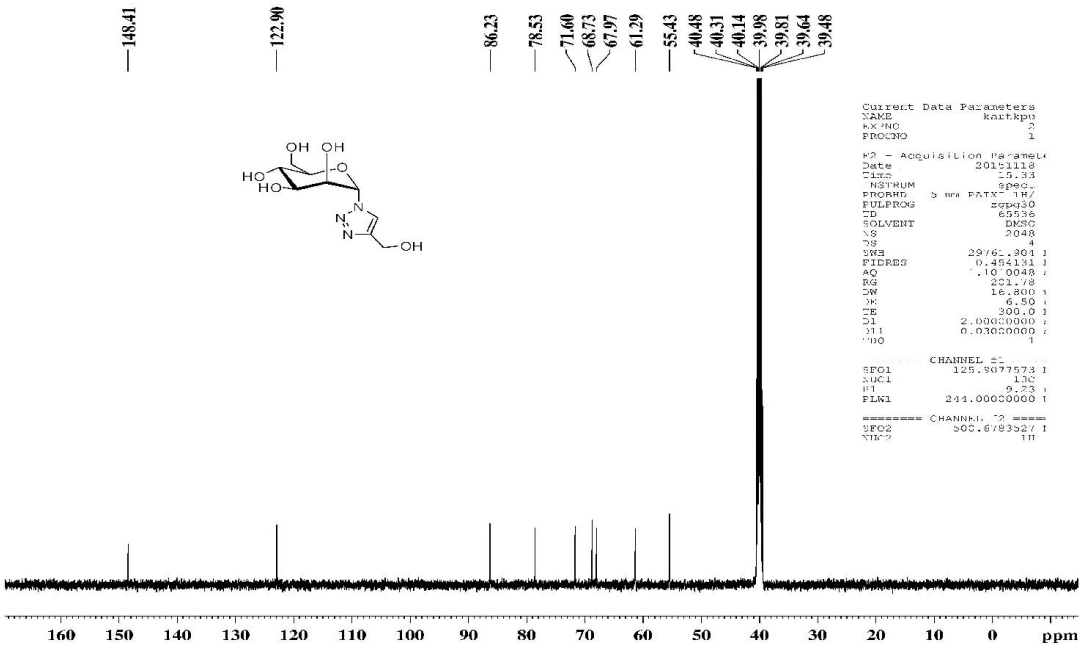
HRMS spectrum of compound **7g**



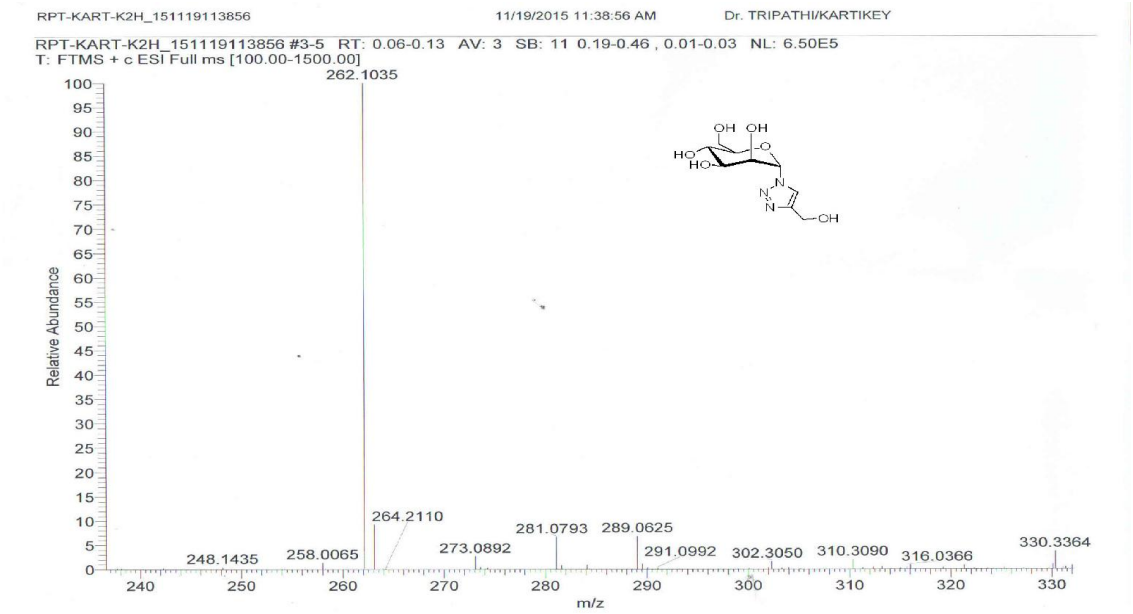
^{1}H NMR spectrum of compound **7g'**



^{13}C NMR spectrum of compound **7g'**



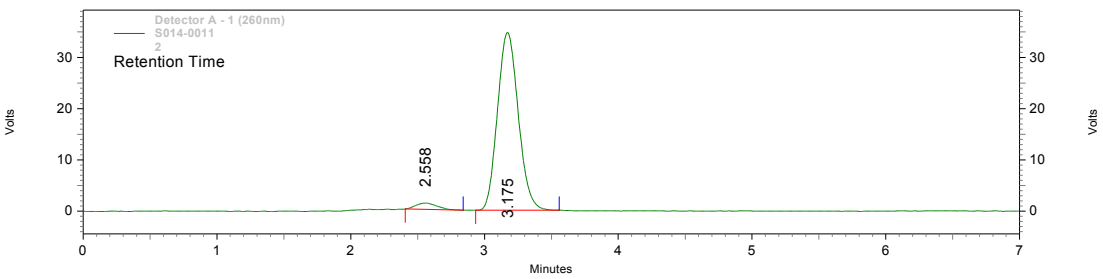
HRMS spectrum of compound **7g'**



HPLC Purity Determination Assay

The purity of the compounds was determined by using reversed phase HPLC method on a Discovery HS C-18 (Supelco, Bellefonte, USA) column (5 µm, 100 x 4.6 mm id) preceded with a C-18 guard column (5 µm, 20 x 4.0 mm, id) packed with the same material under isocratic condition at ambient temperature using mobile phase [acetonitrile:ammonium acetate buffer (10 mM, pH 3.5), 70:30, %v/v] at a flow rate of 0.9 mL/min. The HPLC system consisted of a pump (LC-10AT VP with FCV-10AL VP), degasser (DGU-14A) and auto-injector (SIL-HTc, fixed with a 100 µl loop) (Shimadzu, Japan). Eluents were monitored at 260 nm with UV-Vis multiple wavelength detector and chromatograms were integrated using Class-VP (version 6.12 SP5) software (Shimadzu, Japan).

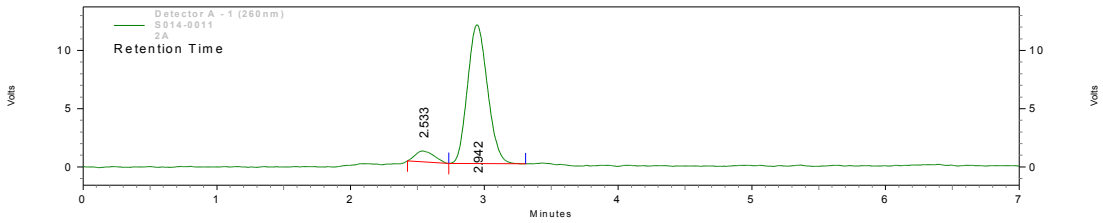
HPLC chromatogram of compound **2**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.558	13762	3.549	1253	3.487
2	3.175	373988	96.451	34680	96.513
Totals		387750	100.000	35933	100.000

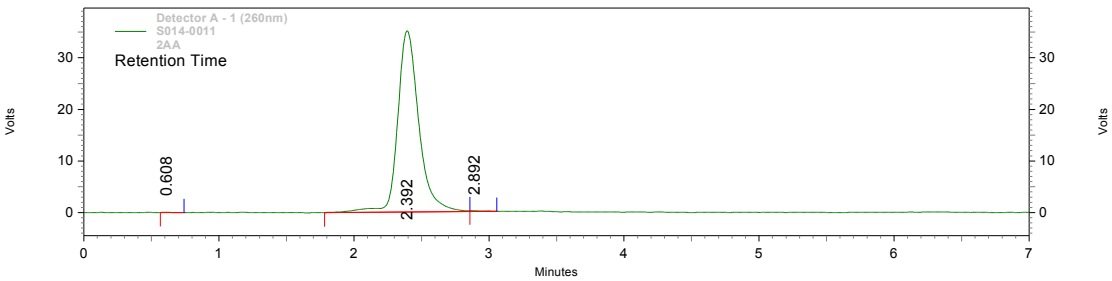
HPLC chromatogram of compound **2a**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.533	3576	2.924	508	4.143
2	2.942	118738	97.076	11754	95.857
Totals		122314	100.000	12262	100.000

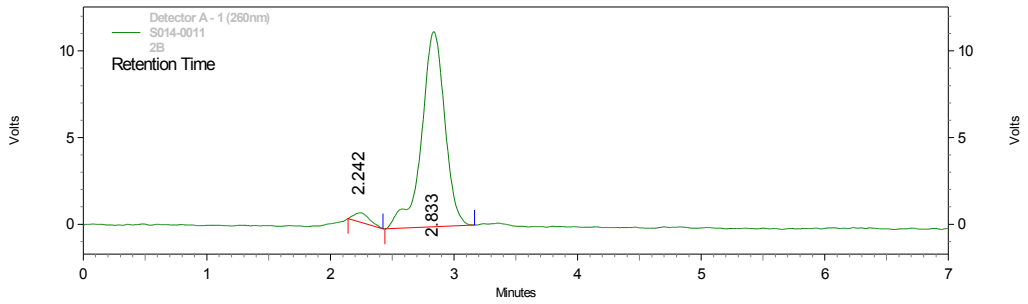
HPLC chromatogram of compound **2a'**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	0.608	256	0.067	46	0.130
2	2.392	381332	99.671	35105	99.450
3	2.892	1001	0.262	148	0.419
Totals		382589	100.000	35299	100.000

HPLC chromatogram of compound **2b**

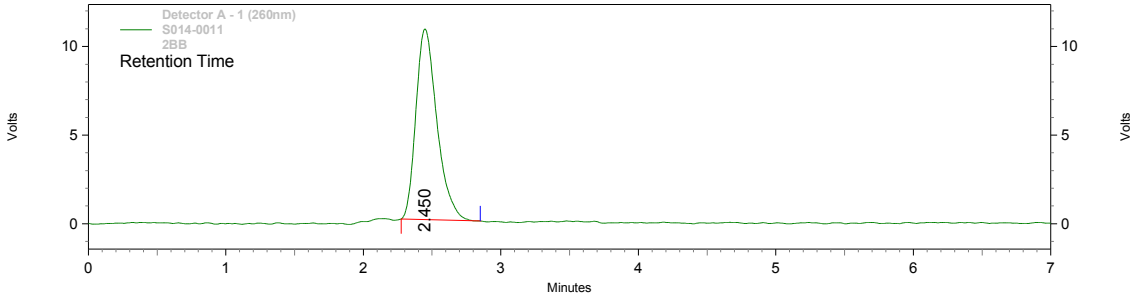


Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.242	4781	3.144	545	4.615
2	2.833	147278	96.856	11264	95.385

Totals		152059	100.000	11809	100.000

HPLC chromatogram of compound **2b'**

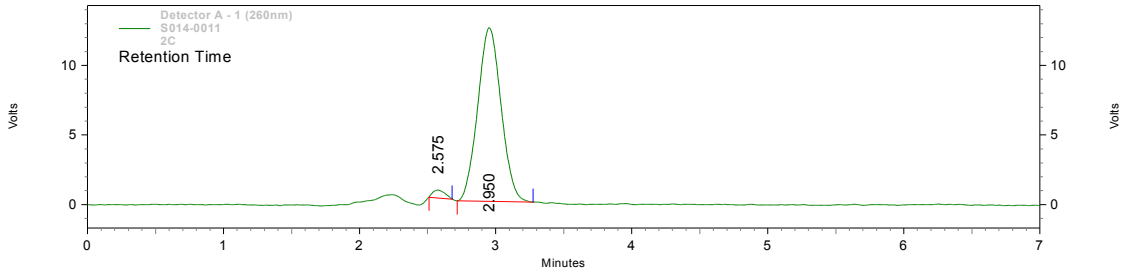


Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.450	114346	100.000	10753	100.000

Totals		114346	100.000	10753	100.000

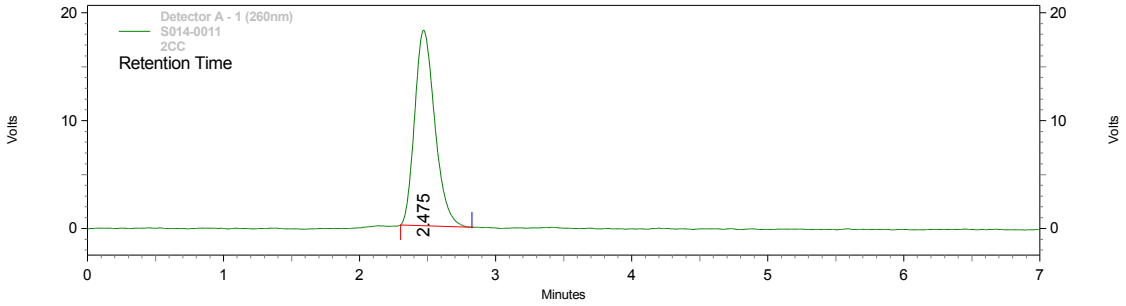
HPLC chromatogram of compound **2c**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.575	3577	2.350	567	4.349
2	2.950	148618	97.650	12471	95.651
Totals		152195	100.000	13038	100.000

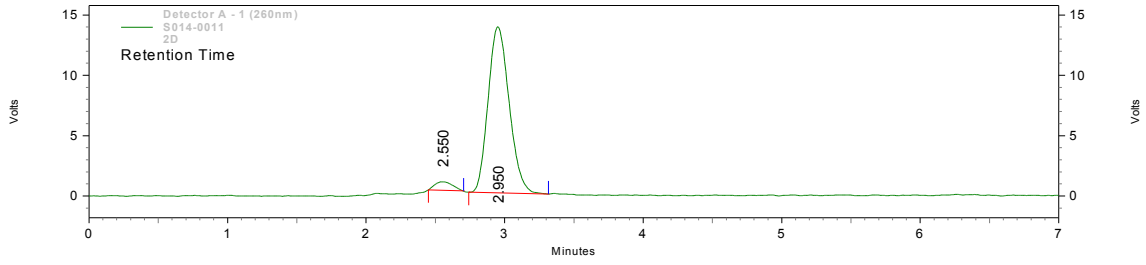
HPLC chromatogram of compound **2c'**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.475	186721	100.000	18113	100.000
Totals		186721	100.000	18113	100.000

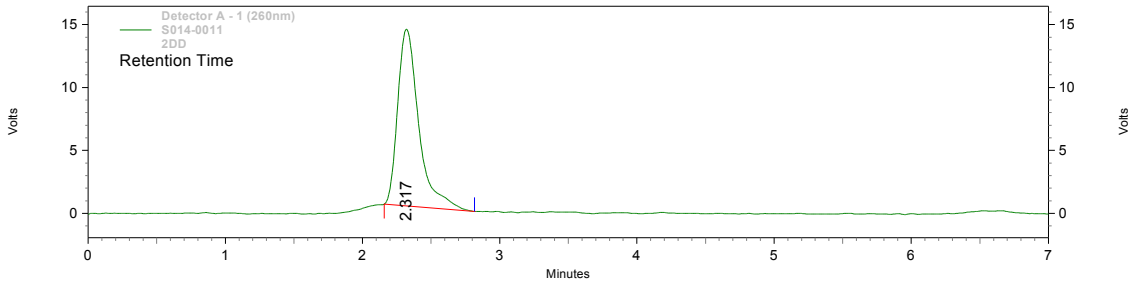
HPLC chromatogram of compound **2d**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.550	6326	4.169	705	4.867
2	2.950	145421	95.831	13781	95.133
Totals		151747	100.000	14486	100.000

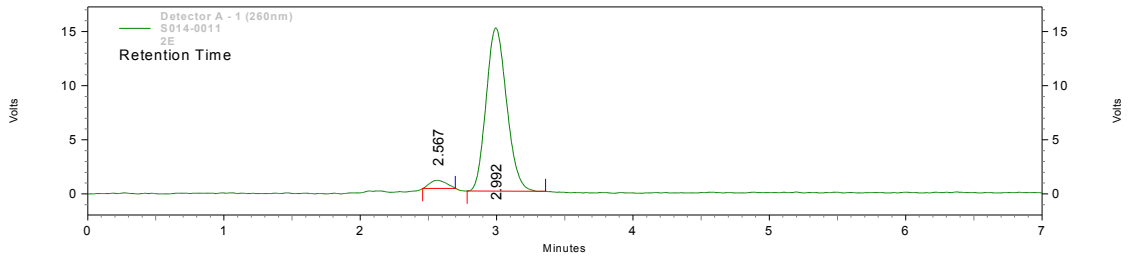
HPLC chromatogram of compound **2d'**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.317	150094	100.000	14035	100.000
Totals		150094	100.000	14035	100.000

HPLC chromatogram of compound **2e**



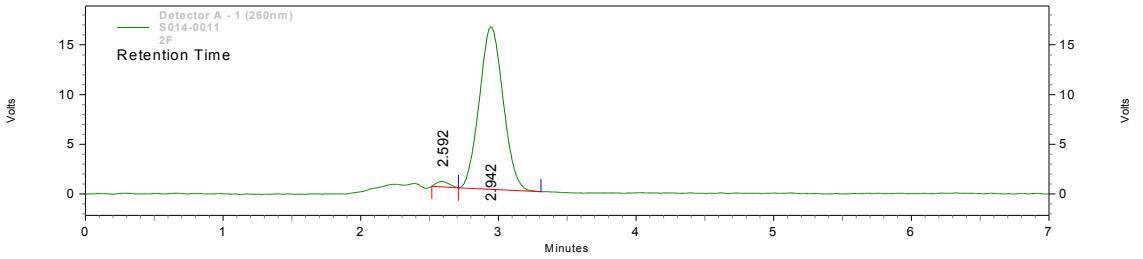
Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %

1	2.567	6386	3.882	755	4.760
2	2.992	158114	96.118	15105	95.240

Totals		164500	100.000	15860	100.000

HPLC chromatogram of compound **2f**

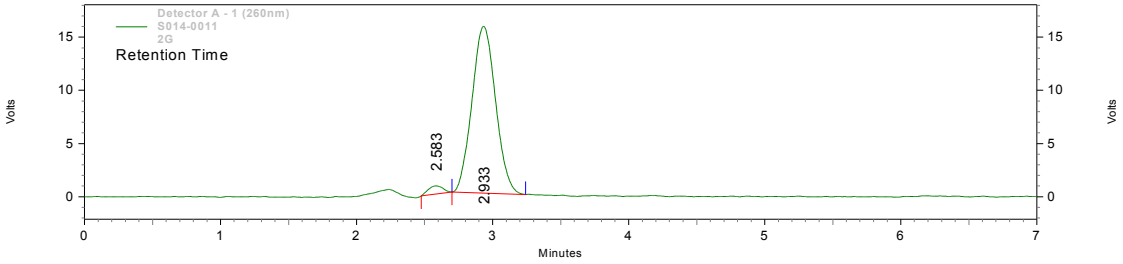


Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.592	3417	1.713	531	3.147
2	2.942	196044	98.287	16340	96.853

Totals		199461	100.000	16871	100.000

HPLC chromatogram of compound **2g**

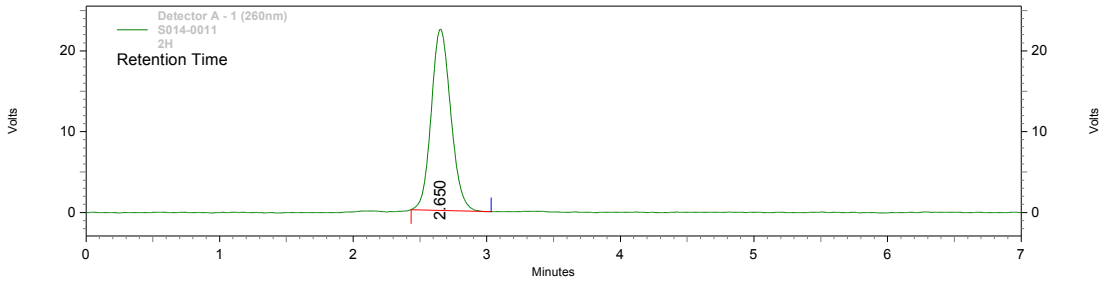


Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.583	5892	3.021	779	4.724
2	2.933	189160	96.979	15711	95.276

Totals		195052	100.000	16490	100.000

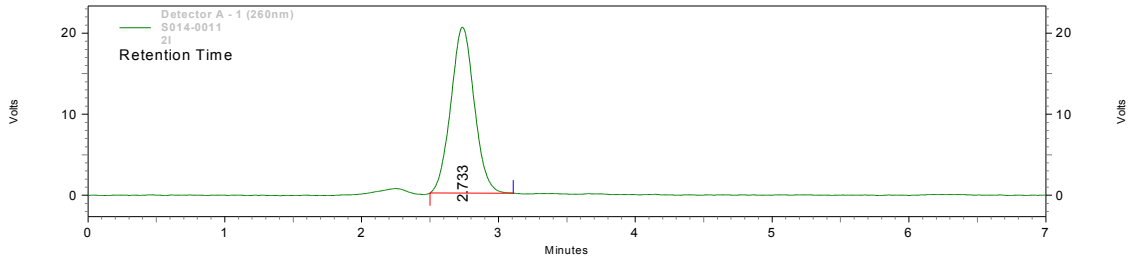
HPLC chromatogram of compound **2h**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.650	228136	100.000	22451	100.000
Totals		228136	100.000	22451	100.000

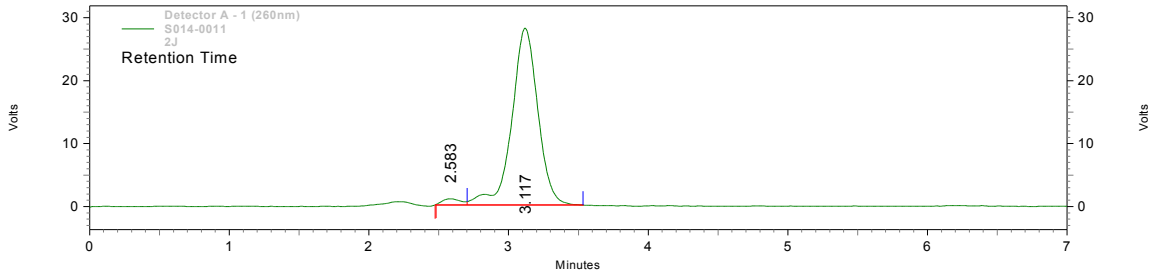
HPLC chromatogram of compound **2i**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.733	243767	100.000	20451	100.000
Totals		243767	100.000	20451	100.000

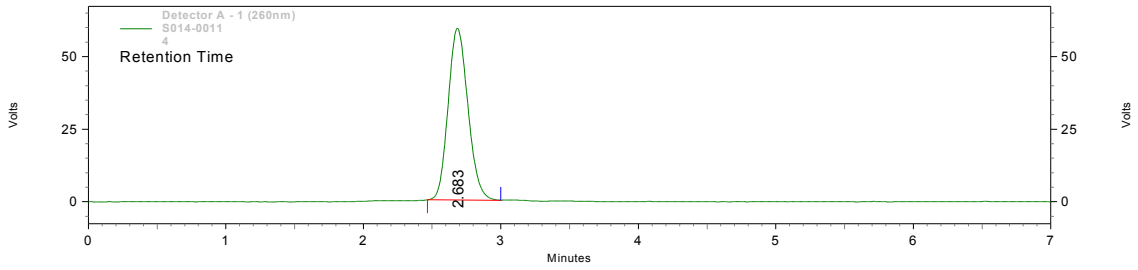
HPLC chromatogram of compound **2j**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.583	8971	2.340	983	3.380
2	3.117	374454	97.660	28102	96.620
Totals		383425	100.000	29085	100.000

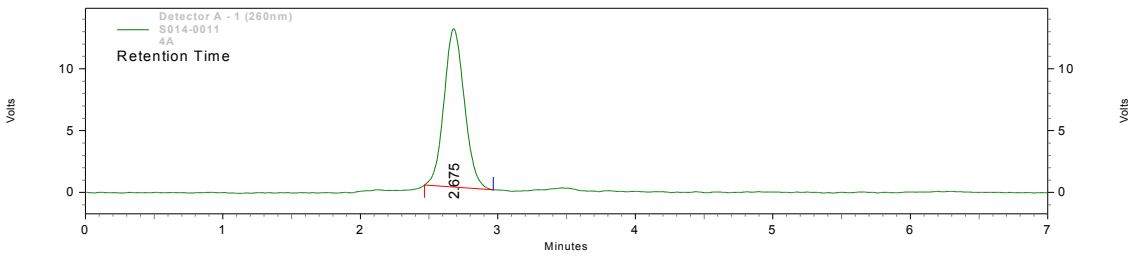
HPLC chromatogram of compound **4**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.683	591966	100.000	59251	100.000
Totals		591966	100.000	59251	100.000

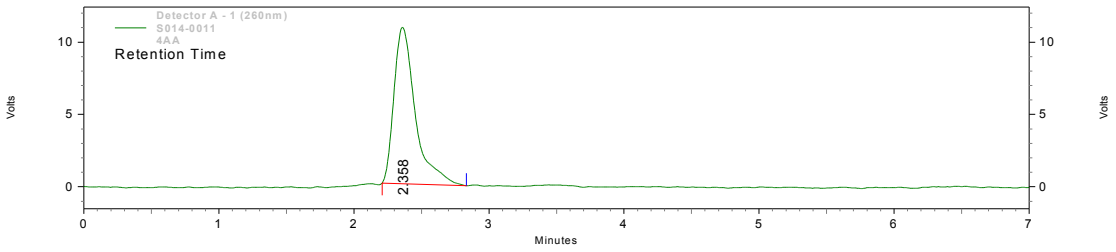
HPLC chromatogram of compound **4a**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.675	131474	100.000	12781	100.000
Totals		131474	100.000	12781	100.000

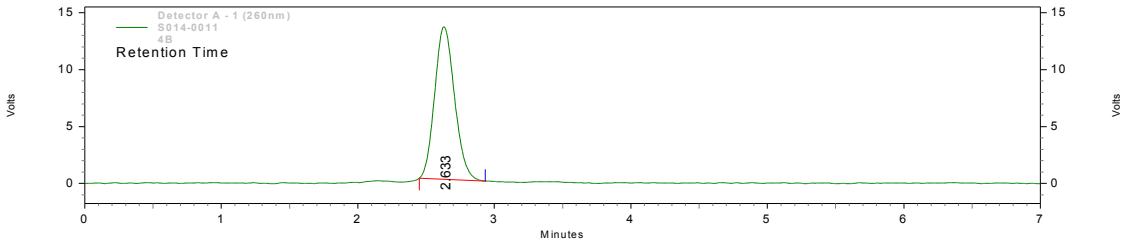
HPLC chromatogram of compound **4a'**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.358	118706	100.000	10831	100.000
Totals		118706	100.000	10831	100.000

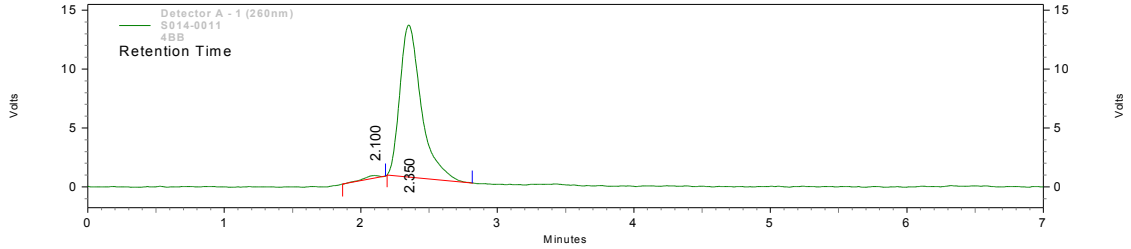
HPLC chromatogram of compound **4b**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.633	135982	100.000	13414	100.000
Totals		135982	100.000	13414	100.000

HPLC chromatogram of compound **4b'**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.100	1709	1.205	214	1.629
2	2.350	140173	98.795	12923	98.371
Totals		141882	100.000	13137	100.000

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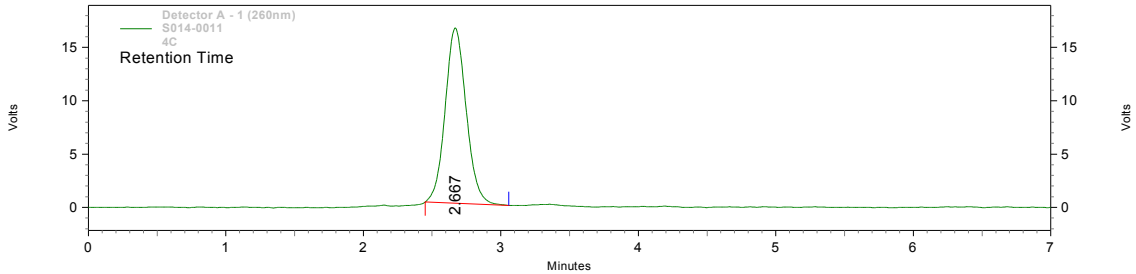
HPLC chromatogram of compound **4c**

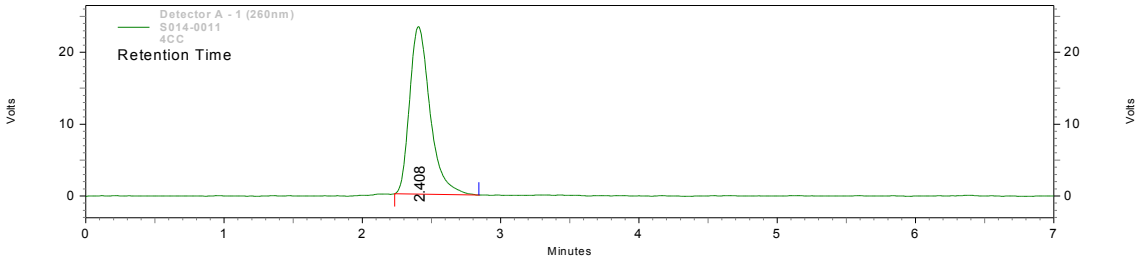


Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.667	174489	100.000	16442	100.000

Totals		174489	100.000	16442	100.000

HPLC chromatogram of compound **4c'**

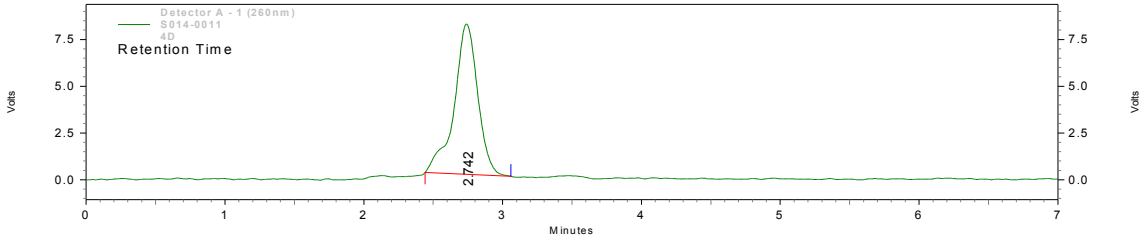


Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.408	239832	100.000	23299	100.000

Totals		239832	100.000	23299	100.000

HPLC chromatogram of compound **4d**

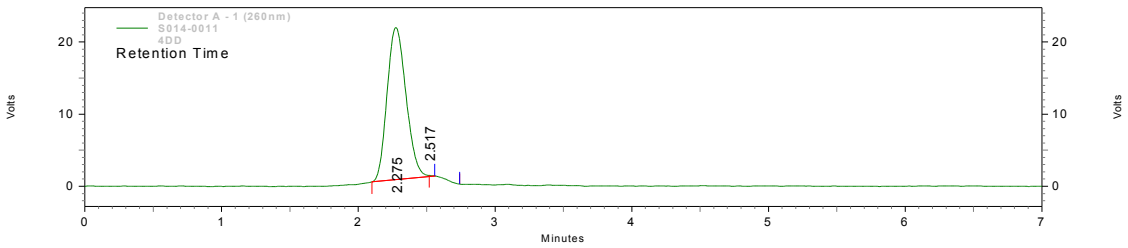


Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.742	94773	100.000	8041	100.000

Totals		94773	100.000	8041	100.000

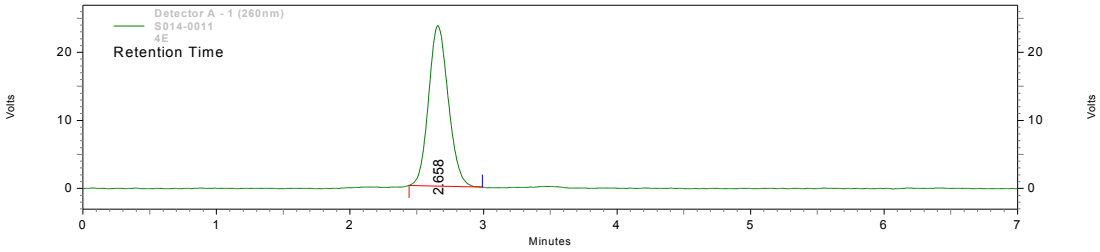
HPLC chromatogram of compound **4d'**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.275	203233	96.277	21102	99.327
2	2.517	7860	3.723	143	0.673
Totals		211093	100.000	21245	100.000

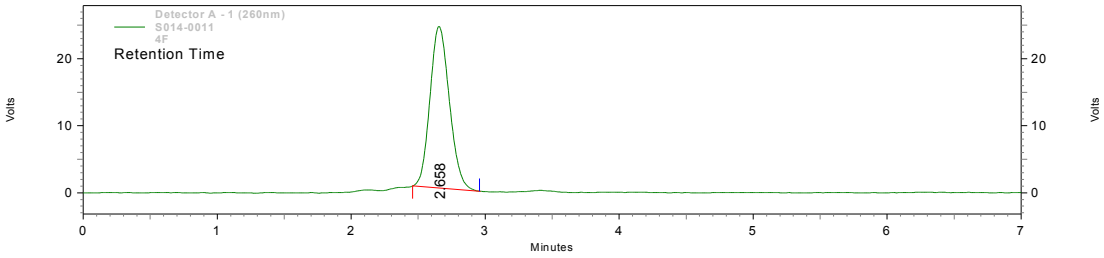
HPLC chromatogram of compound **4e**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.658	242093	100.000	23600	100.000
Totals		242093	100.000	23600	100.000

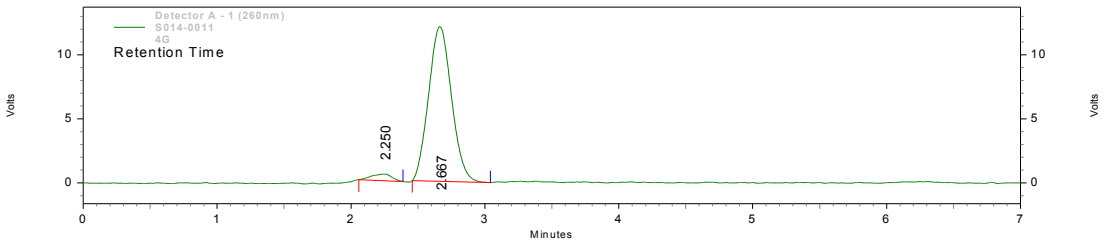
HPLC chromatogram of compound **4f**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.658	242992	100.000	24122	100.000
Totals		242992	100.000	24122	100.000

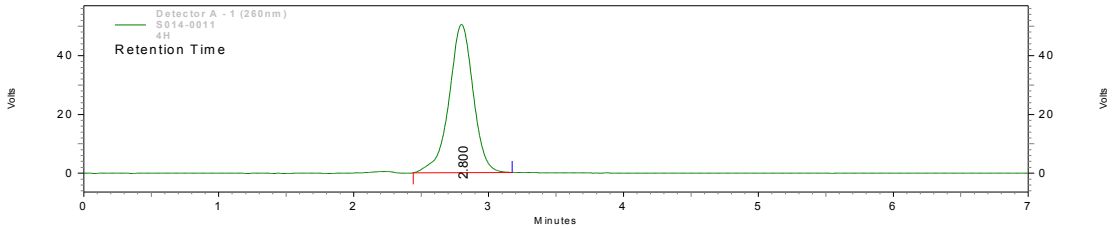
HPLC chromatogram of compound **4g**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.250	5363	3.599	515	4.091
2	2.667	143661	96.401	12074	95.909
Totals		149024	100.000	12589	100.000

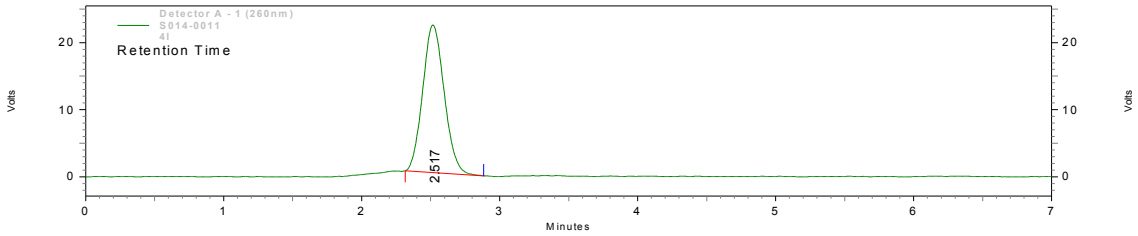
HPLC chromatogram of compound **4h**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.800	625507	100.000	50418	100.000
Totals		625507	100.000	50418	100.000

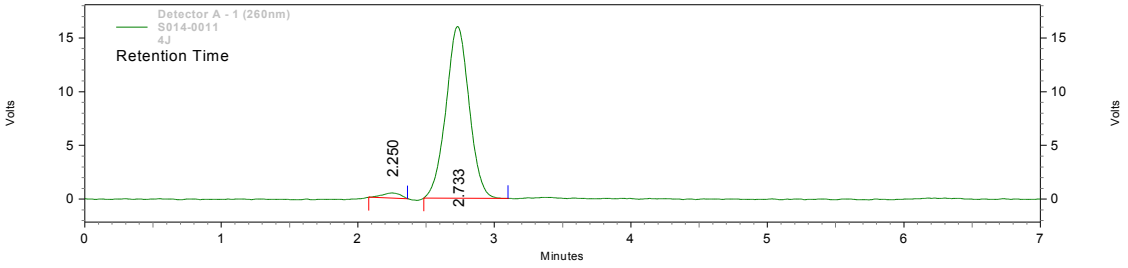
HPLC chromatogram of compound **4i**



Detector A - 1 (260nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.517	237636	100.000	21976	100.000
Totals		237636	100.000	21976	100.000

HPLC chromatogram of compound **4j**

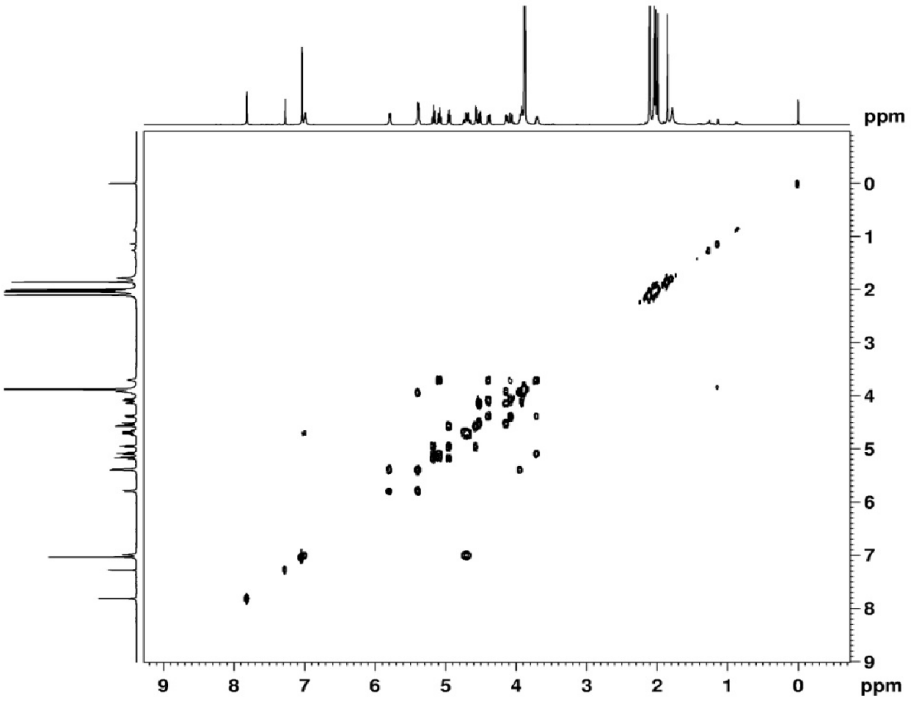


Detector A - 1 (260nm)

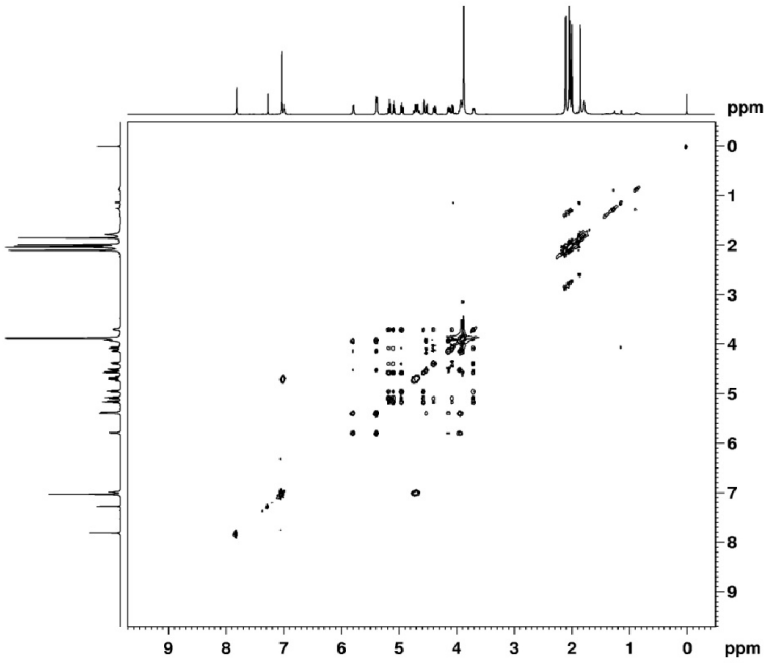
Pk #	Retention Time	Area	Area %	Height	Height %
1	2.250	4486	2.326	485	2.946

2	2.733	188350	97.674	15979	97.054
Totals		192836	100.000	16464	100.000

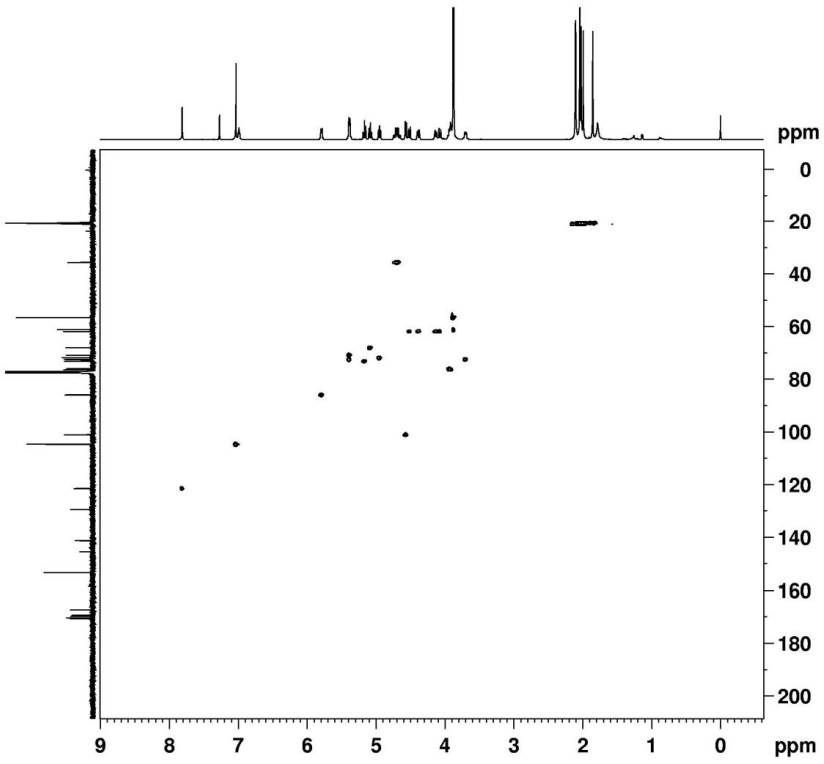
COSY spectrum of **4d**



TOCSY spectrum of **4d**



HSQC spectrum of **4d**



HMBC spectrum of **4d**

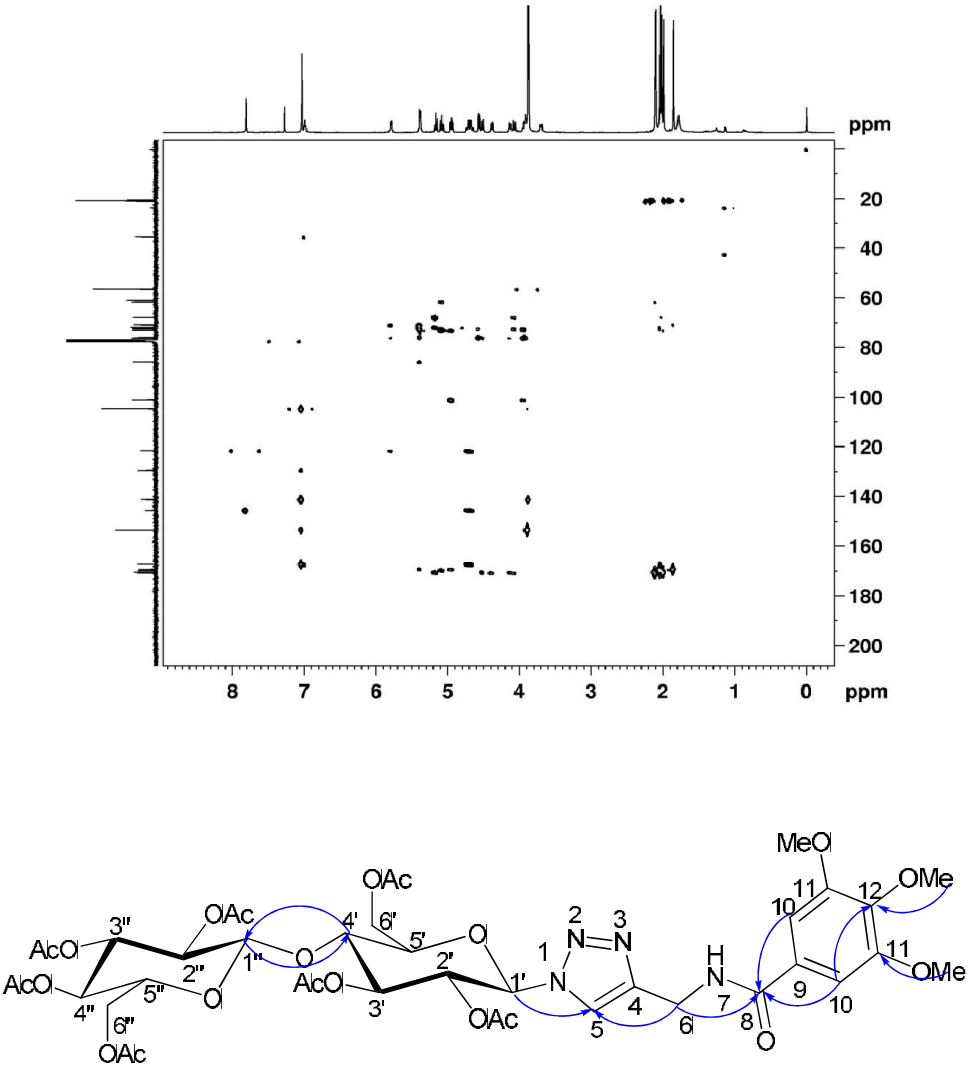
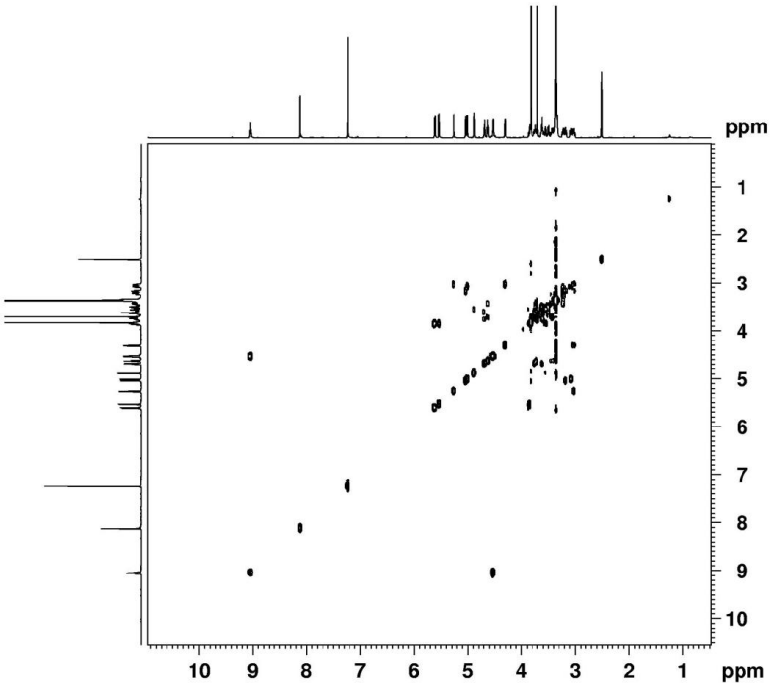


Figure 1. Important HMBC correlation of compound **4d**

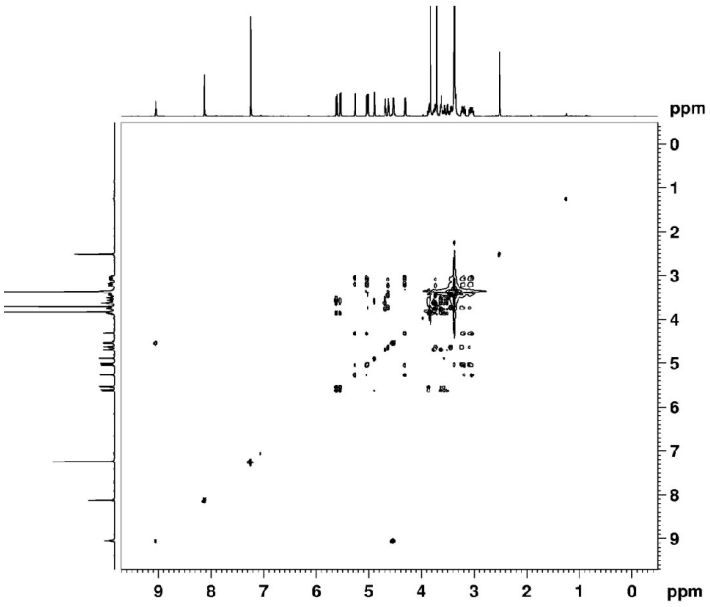
Complete ^{1}H and ^{13}C signal assignments of compound **4d**

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (s, 1H, H-5), 7.03 (s, 2H, H-10), 6.98 (t, *J* = 5.52 Hz, 1H, H-7), 5.79 (dd, J_1 = 6.15 Hz, J_2 = 2.60 Hz, 1H, H-1′), 5.39 (m, 2H, H-2′,H-3′), 5.14 (t, *J* = 9.80 Hz, 1H, H-3′′), 5.08 (t, *J* = 9.58 Hz, 1H, H-4′′), 4.96 (t, *J* = 8.20 Hz, 1H, H-2′′), 4.70 (m, 2H, H-6), 4.55 (d, *J* = 8.42 Hz, 1H, H-1′′), 4.50 (d, *J* = 12.33 Hz, 1H, H_b-6′), 4.36 (dd, J_1 = 12.6 Hz, J_2 = 4.28 Hz, 1H, H_b-6′′), 4.12 (dd, J_1 = 12.33 Hz, J_2 = 4.78 Hz, 1H, H_a-6′), 4.07 (dd, J_1 = 12.60 Hz, J_2 = 2.00 Hz, 1H, H_a-6′′), 3.93 (m, 2H, H-4′,H-5′), 3.88 (s, 6H, OMe-11), 3.87 (s, 3H, OMe-12), 3.69 (m, 1H, H-5′′), 2.10 (s, 3H, OAc-6′), 2.09 (s, 3H, OAc-6′′), 2.04 (s, 6H, OAc-3′, OAc-2′′), 2.01 (s, 3H, OAc-4′′), 1.99 (s, 3H, OAc-3′′), 1.85 (s, 3H, OAc -2′); ^{13}C NMR (125 MHz) δ 170.6 (C-6′′-C=O), 170.4 & 170.3 (C-6′-C=O & C-3′′-C=O), 169.7 (C-4′′-C=O), 169.5 (C-2′′-C=O), 169.2 (2C, C-2′-C=O & C-3′- C=O), 167.3 (C-8), 153.4 (2C, C-11), 145.4 (C-4), 141.3 (C-12), 129.4 (C-9), 121.4 (C-5), 104.6 (2C, C-10), 101.0 (C-1′′), 85.8 (C-1′), 76.2 & 75.9 (C-4′ & C-5′), 73.0 (C-3′′), 72.4 & 72.3 (C-3′ & C-5′′), 71.7 (C-2′′), 70.8 (C-2′), 67.9 (C-4′′), 61.7 (2C, C-6′, C-6′′), 61.1 (C-12-OMe), 56.5 (2C, C-11-OMe), 35.5 (C-6), [20.9, 20.8, 20.7, 20.6 & 20.4 (total 7C for 2′, 3′, 6′, 2′′, 3′′, 4′′ & 6′′-OAc)]

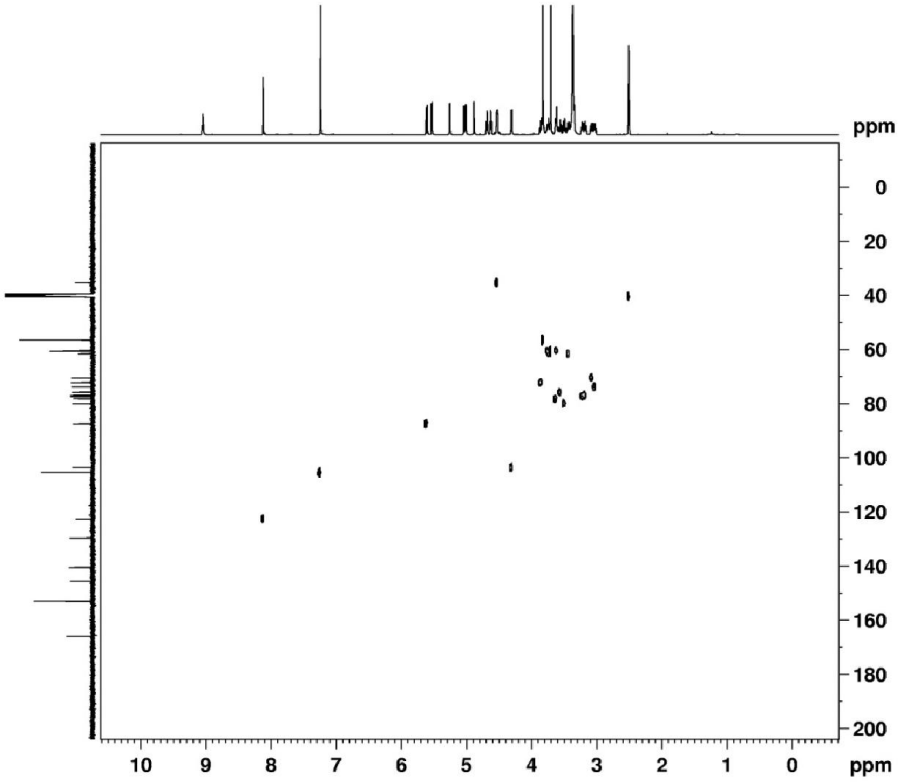
COSY spectrum of **4d'**



TOCSY spectrum of **4d'**



HSQC spectrum of **4d'**



HMBC spectrum of **4d'**

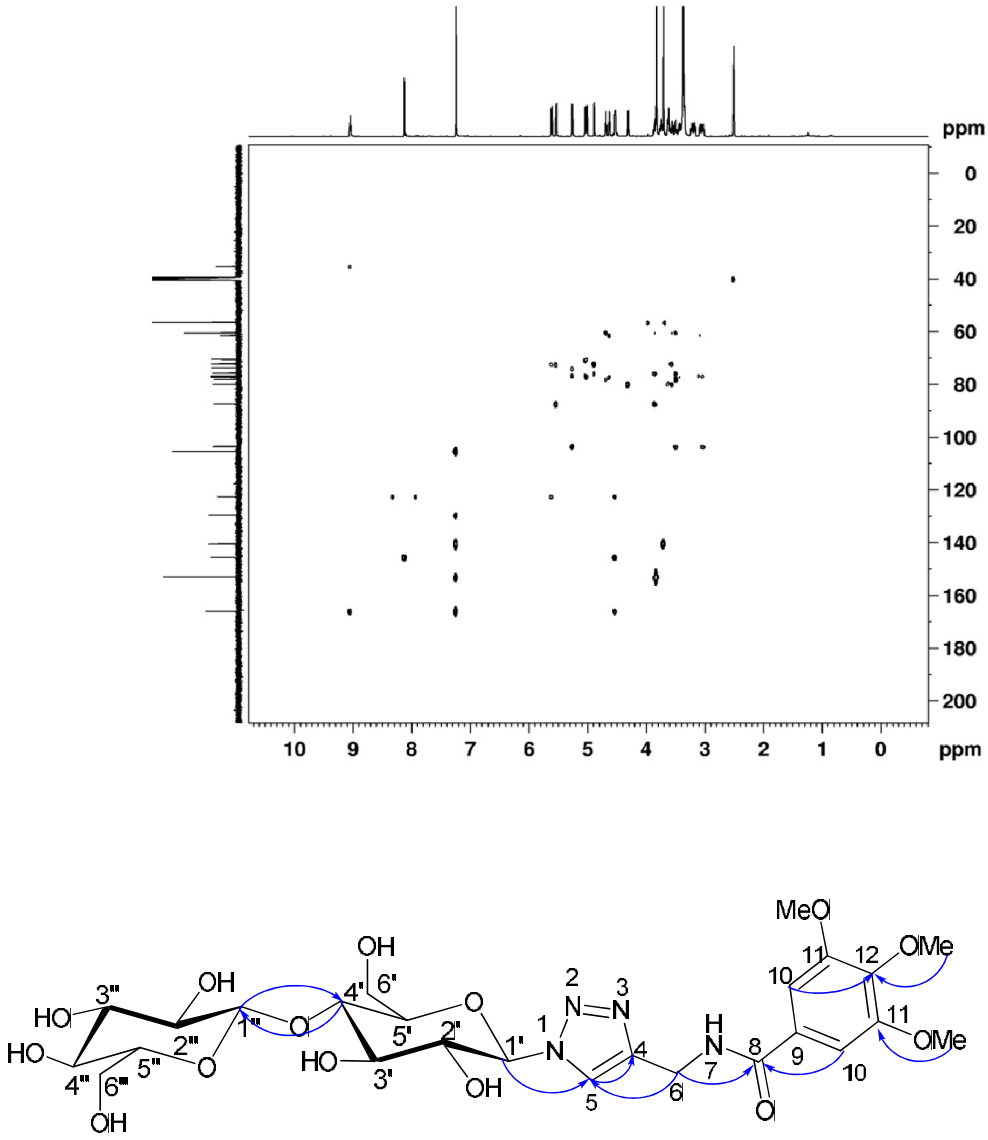


Figure 2. Important HMBC correlation of compound **4d'**

Complete ^{1}H and ^{13}C signal assignments of compound **4d'**

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.04 (t, *J* = 5.75 Hz, 1H, H-7), 8.12 (s, 1H, H-5), 7.24 (s, 2H, H-10), 5.60 (d, *J* = 9.55 Hz, 1H, H-1´), 5.52 (d, *J* = 6.15 Hz, OH-2´), 5.25 (d, *J* = 5.01 Hz, OH-2´´), 5.03 (d, *J* = 5.10 Hz, OH-3´´), 5.00 (d, *J* = 5.47 Hz, OH-4´´), 4.88 (d, *J* = 2.30 Hz, OH-3´), 4.68 (t, *J* = 4.90 Hz, OH-6´), 4.62 (t, *J* = 5.36 Hz, OH-6´´), 4.53 (dd, J_1 = 5.75 Hz, J_2 = 2.60 Hz, 2H, H-6),

4.30 (d, *J* = 7.80 Hz, 1H, H-1´´), 3.85 (m, 1H, H-2´), 3.82 (s, 6H, OMe-11), 3.74 (m, 1H, H_b-6´), 3.71 (m, 1H, H_b-6´´), 3.70 (s, 3H, OMe-12), 3.63 (m, 1H, H-5´), 3.60 (m, 1H, H_a-6´), 3.55 (m, 1H, H-3´), 3.50 (t, *J* = 7.80 Hz, 1H, H-4´), 3.40 (m, 1H, H_a-6´´), 3.23 (m, 1H, H-5´´), 3.16 (m, 1H, H-3´´), 3.07 (m, 1H, H-4´´), 3.01 (m, 1H, H-2´´); ^{13}C NMR (125 MHz) δ 165.9 (C-8), 152.9 (2C, C-11)), 145.5 (C-4), 140.4 (C-12), 129.5 (C-9), 122.5 (C-5), 105.3 (2C, C-10), 103.5 (C-1´´), 87.3 (C-1´), 79.9 (C-4´), 78.1 (C-5´), 77.2 (C-5´´), 76.8 (C-3´´), 75.6 (C-3´), 73.7 (C-2´´), 72.1 (C-2´), 70.4 (C-4´´), 61.4 (C-6´´), 60.4 (OMe-12), 60.3 (C-6´), 56.4 (2C, OMe-11), 35.2 (C-6).