Supplementary Information

A highly efficient route for synthesis of N-hydroxymethyl sumatriptan and sumatriptan dimer: Impurity C and H of anti-migraine drug sumatriptan

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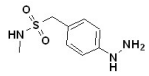
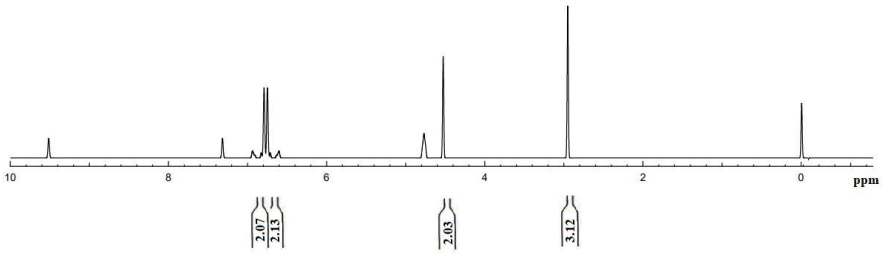
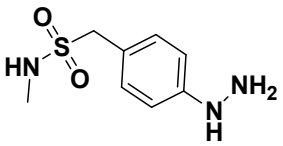
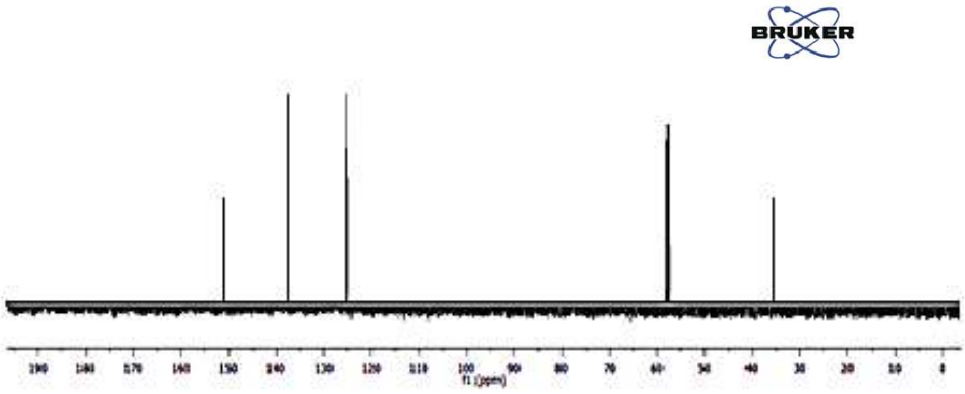
^{1}H NMR data for compound 2:



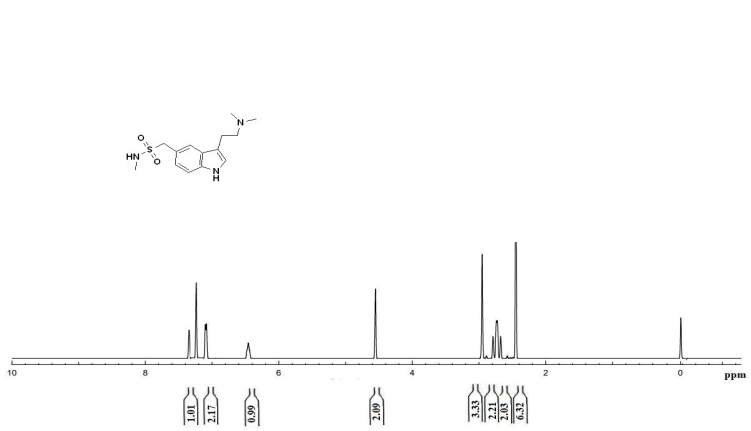


^{13}C NMR data for compound 2:

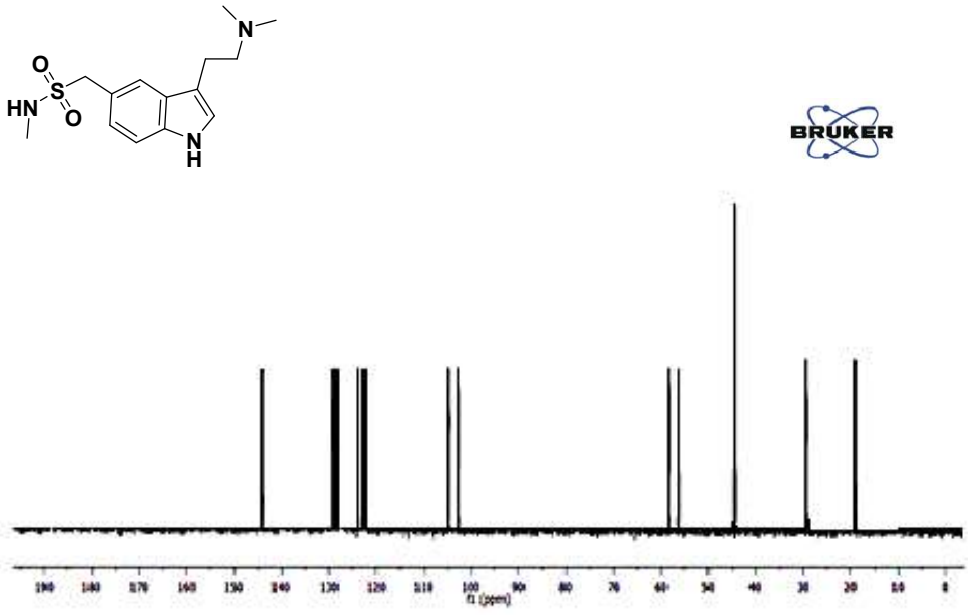




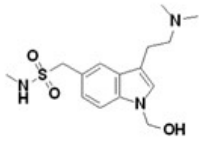
^{1}H NMR data for compound 6:



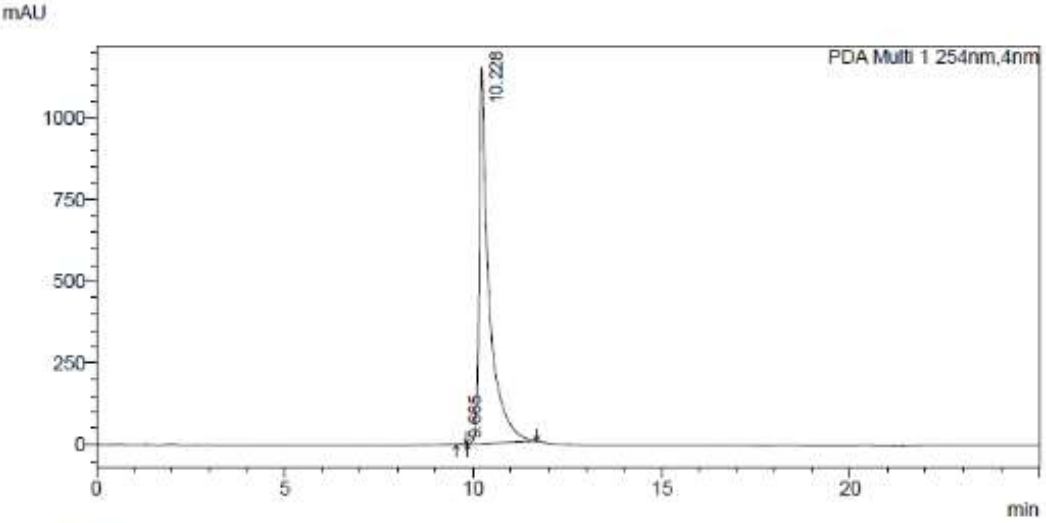
^{13}C NMR data for compound 6:



HPLC data for Sumatriptan Impurity C (7):



Mobile phase -A : OPA
Mobile phase-B : Acetonitrile
Flow rate :1.0ml/min
Temperture : 30° C
Column : C18 250*4.6 5um
Gradient program(T/M.P-B) : 0/20,3/20,8/80,18/80,20/20,25/20.
Sample preparation :1 mg of sample dissolved in1 ml Methanol

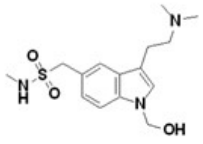


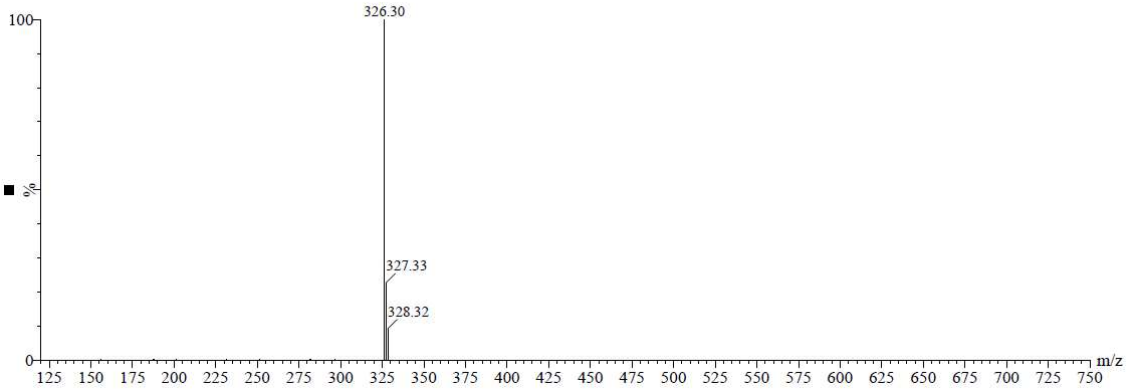
<Peak Table>

PDA Ch1 254nm

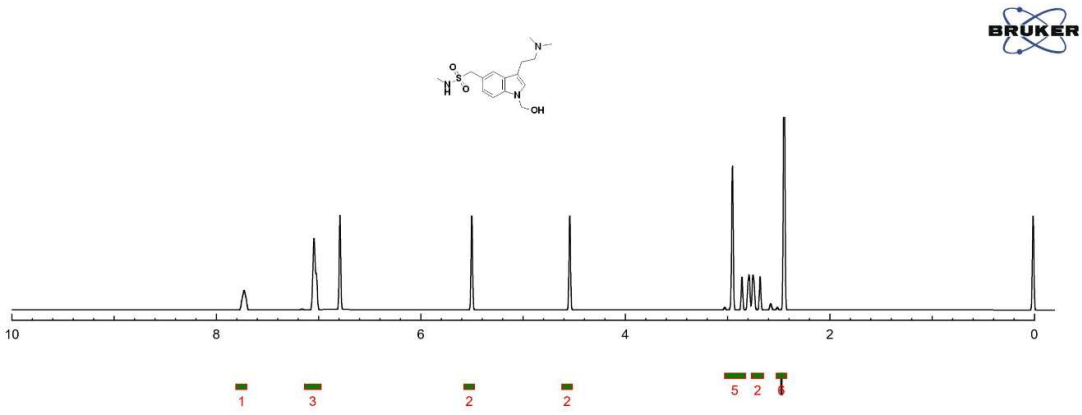
Peak#	Ret. Time	Area	Height	Area%
1	9.665	16062	2146	0.076
2	10.228	20988741	1153215	99.924
Total		21004803	1155361	100.000

Mass spectrum for Sumatriptan Impurity C (7):

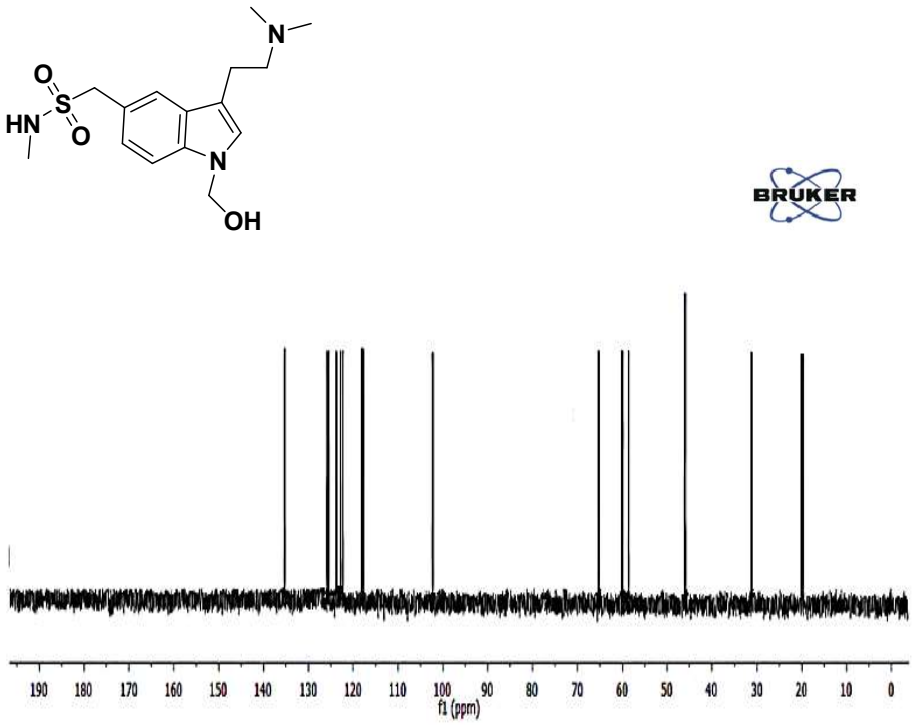




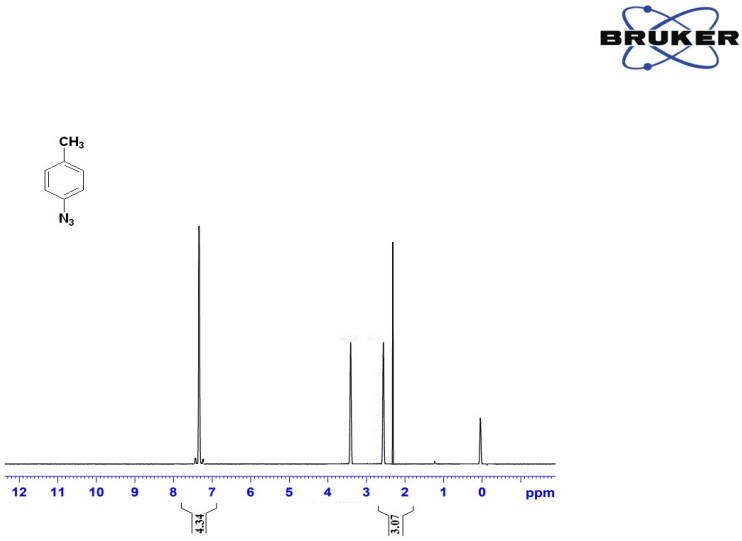
^{1}H NMR data for Sumatriptan Impurity C (7):



^{13}C NMR data for Sumatriptan Impurity C (7):



^{1}H NMR data for compound 9:



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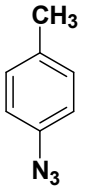
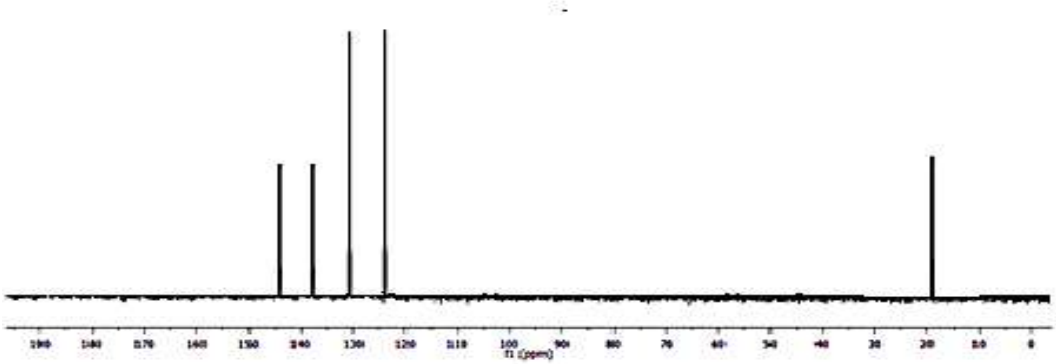
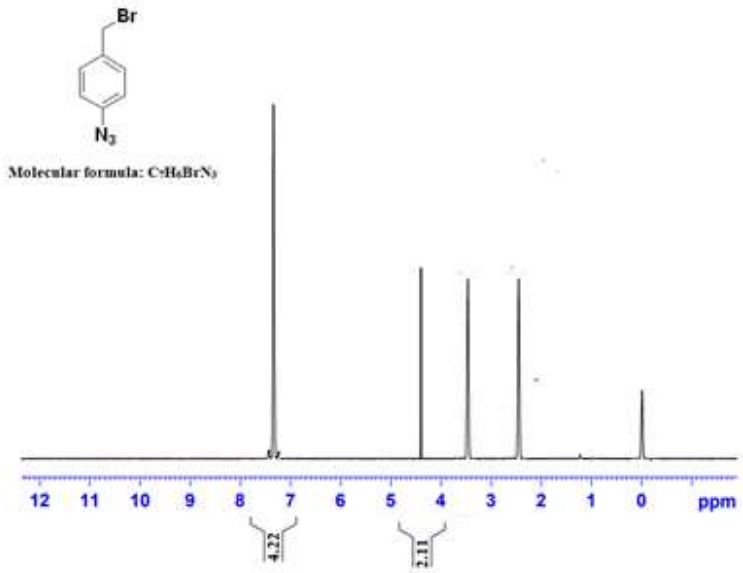




^{1}H NMR data for compound 10:



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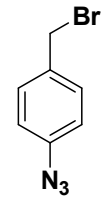
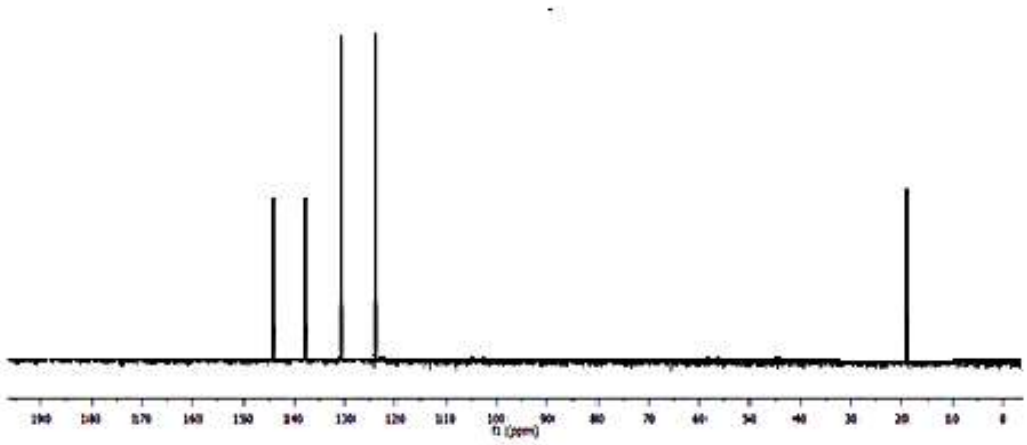
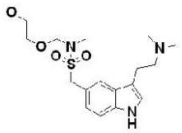
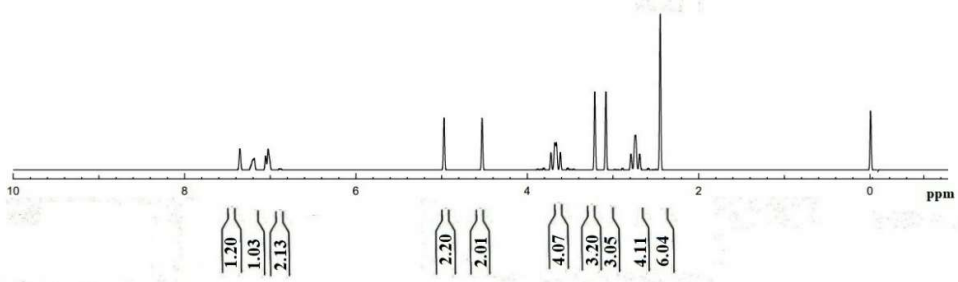




^{1}H NMR data for compound 11:





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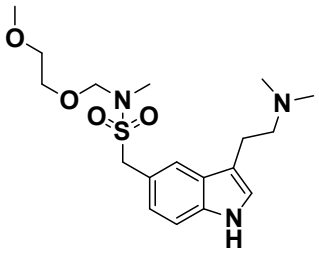
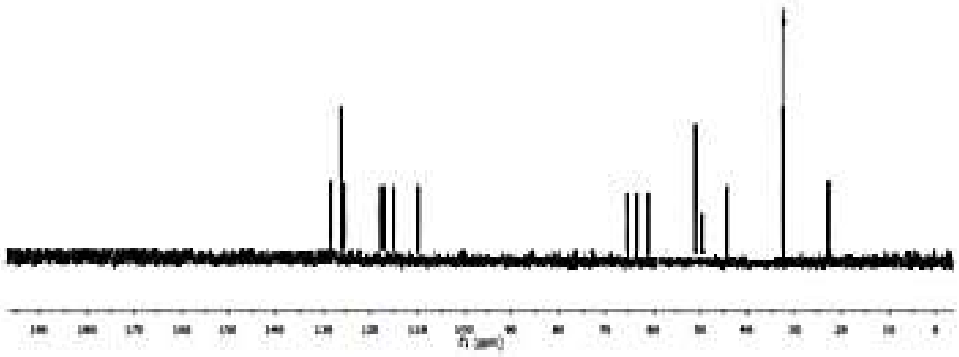
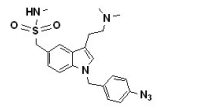
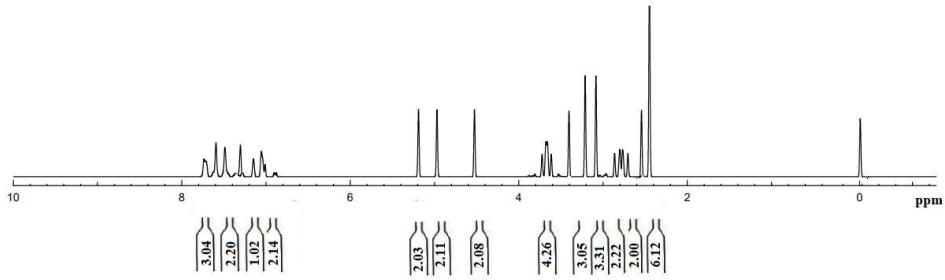




^{1}H NMR data for compound 12:



Molecular formula:$C_{25}H_{34}N_6O_4S$



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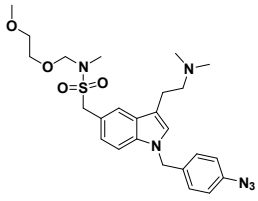
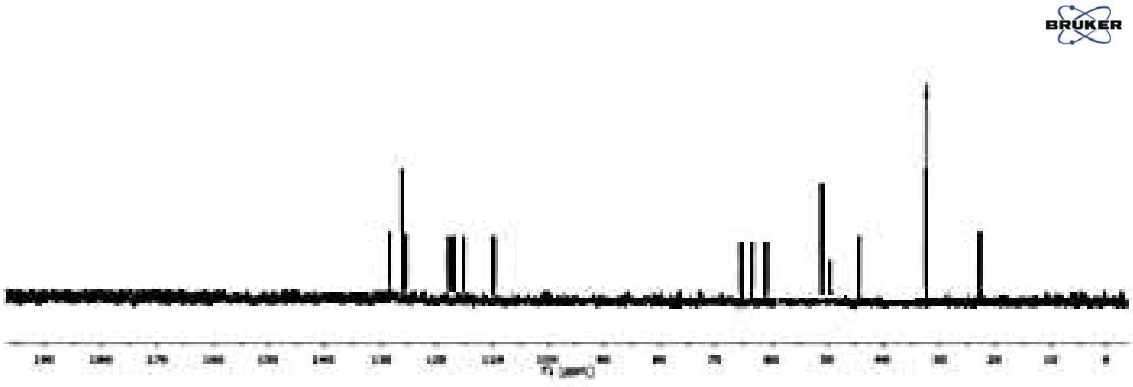
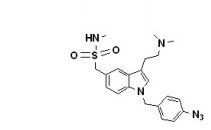
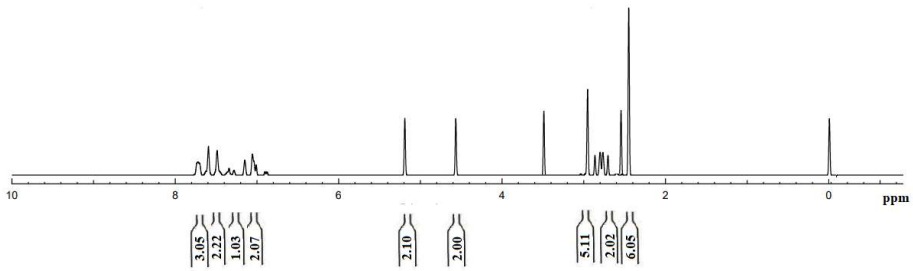




^{1}H NMR data for compound 13:





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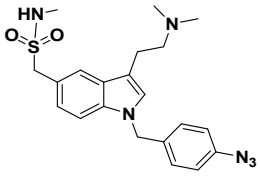
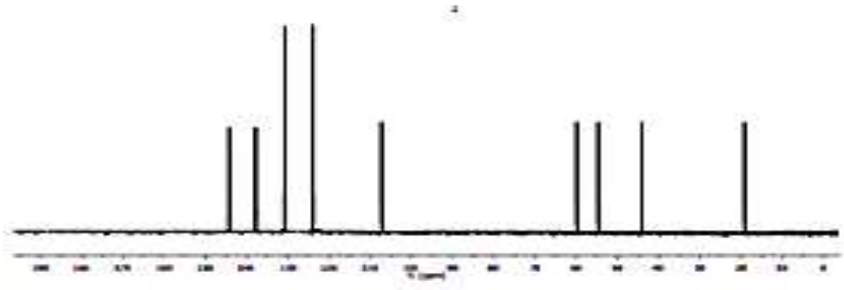
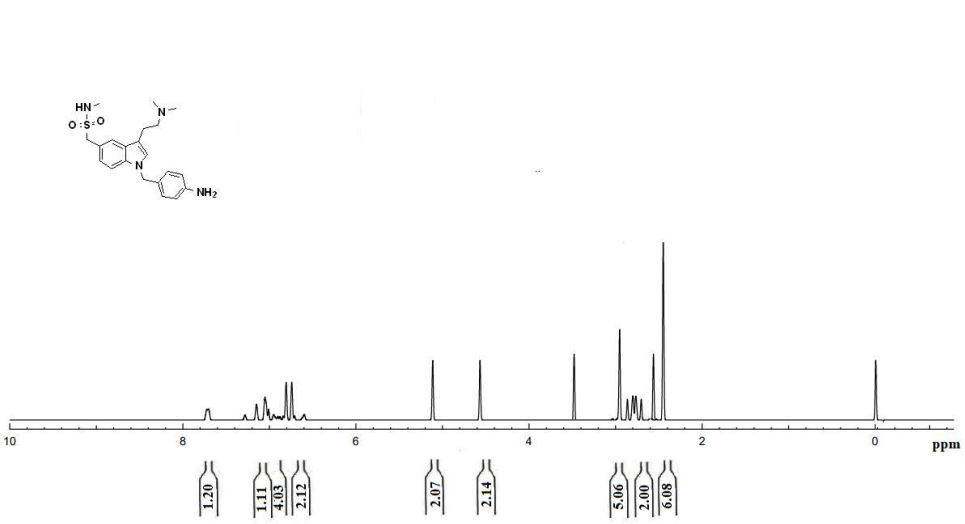
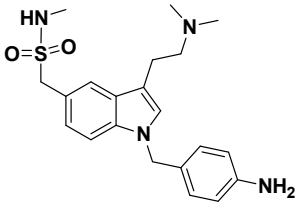


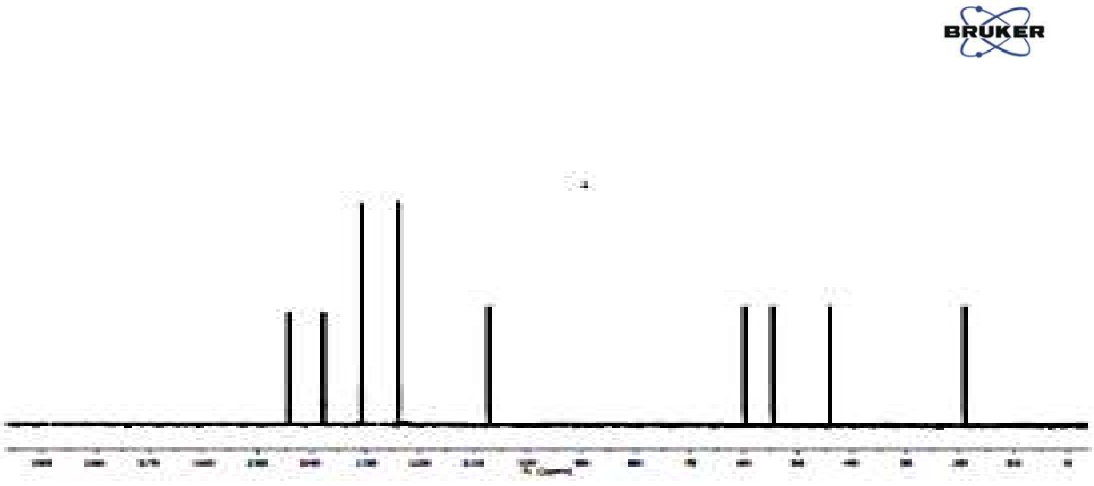


^{1}H NMR data for compound 14:



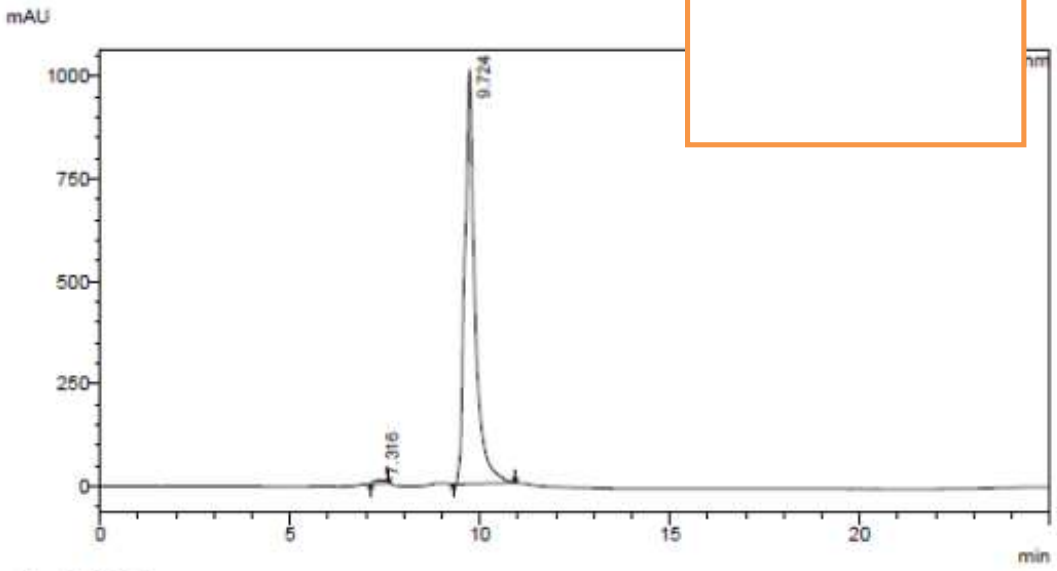
^{13}C NMR data for compound 14:





HPLC data for Sumatriptan Impurity H: (17)

Mobile phase -A :0.1%OPA
Mobile phase-B : Acetonitrile
Flow rate :1.0ml/min
Temperture : 30° C
Column : C18 150*4.6 5um
Gradient program(T/M.P-B) : 0/20,3/20,8/80,18/80,20/20,25/20.
Sample preparation :10 mg of sample dissolved in10 ml Methan

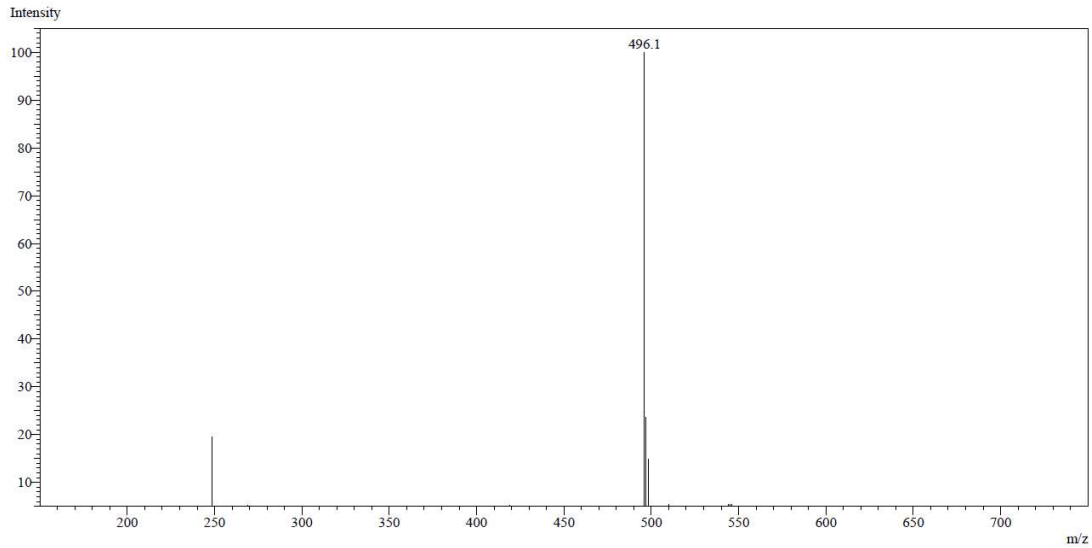


<Peak Table>

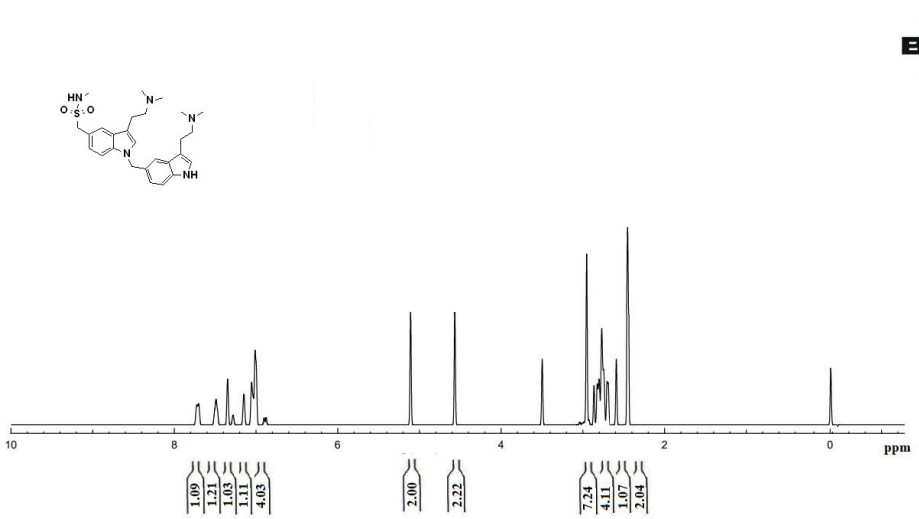
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%
1	7.316	176170	8405	0.923
2	9.724	18908148	1002575	99.077
Total		19084318	1010980	100.000

Mass spectrum for Sumatriptan Impurity H: (17)



^{1}H NMR data for Sumatriptan Impurity H (17):



^{13}C NMR data for Sumatriptan Impurity H (17):