

Supporting Information

Oleanane-type isomeric triterpenoids from *Barringtonia racemosa* Roxb.

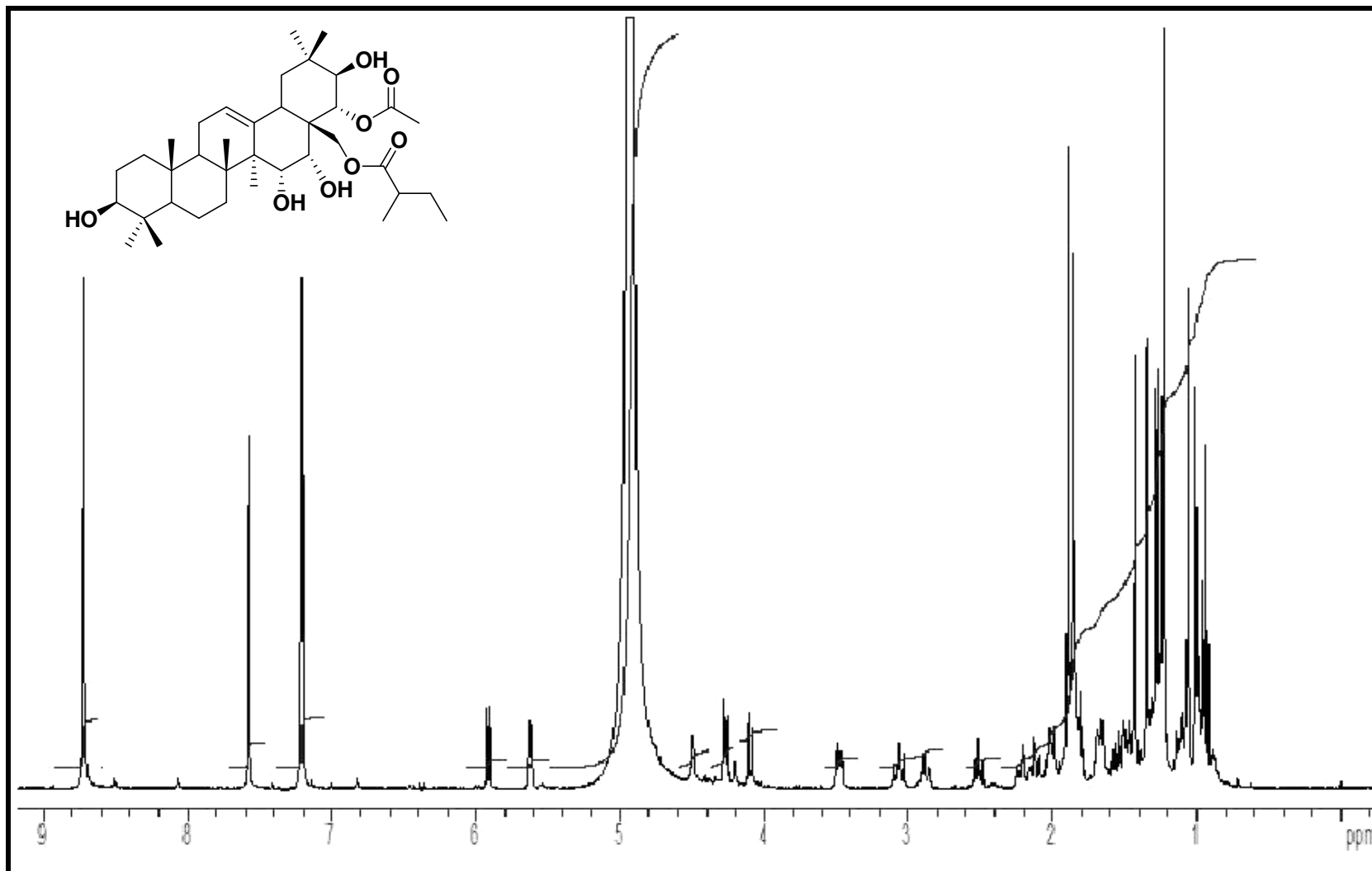
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Indian Institute of Chemical Technology, Hyderabad, India, 500 607

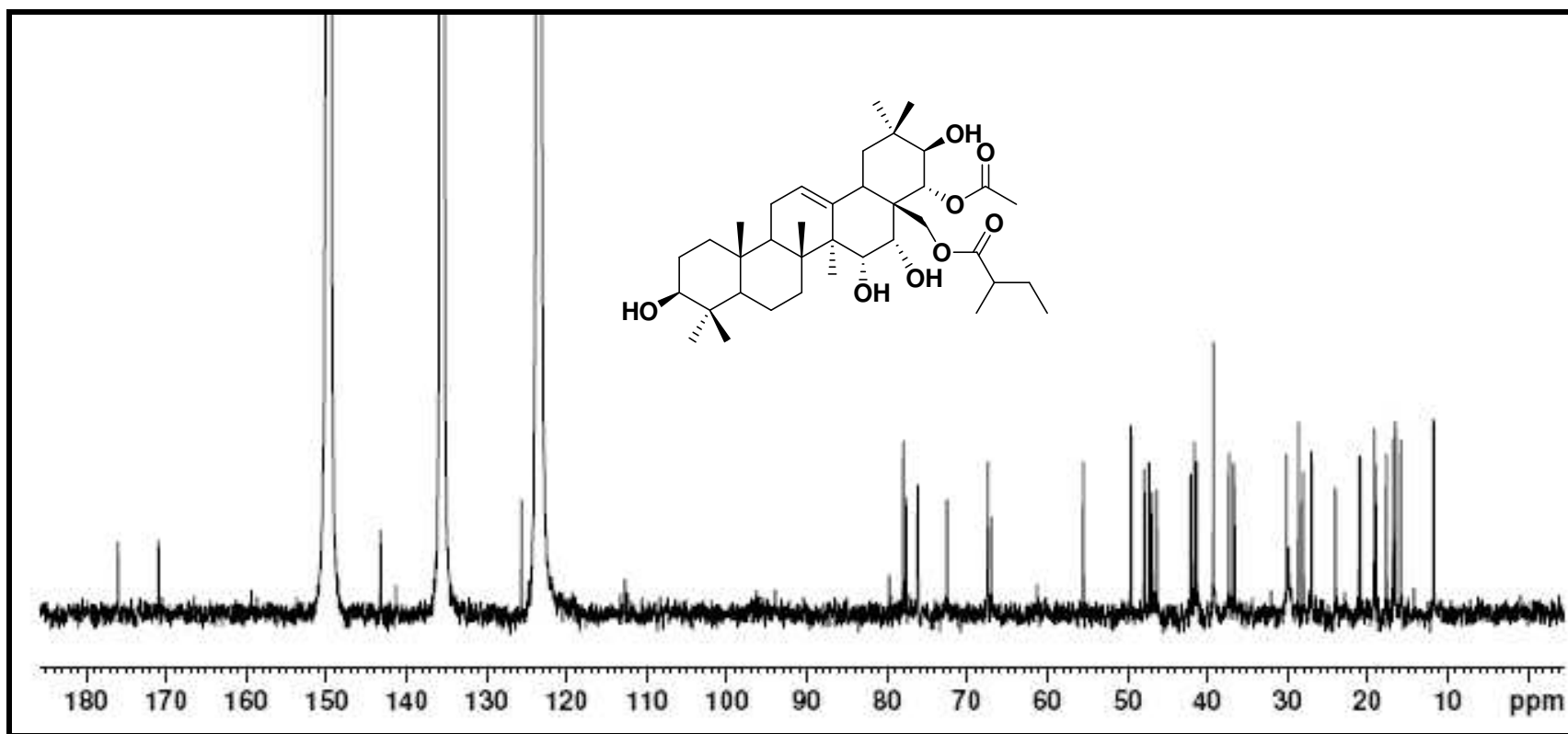
*Corresponding author: Tel/fax: +91-40-27160512.

E mail: mangala@iict.res.in,

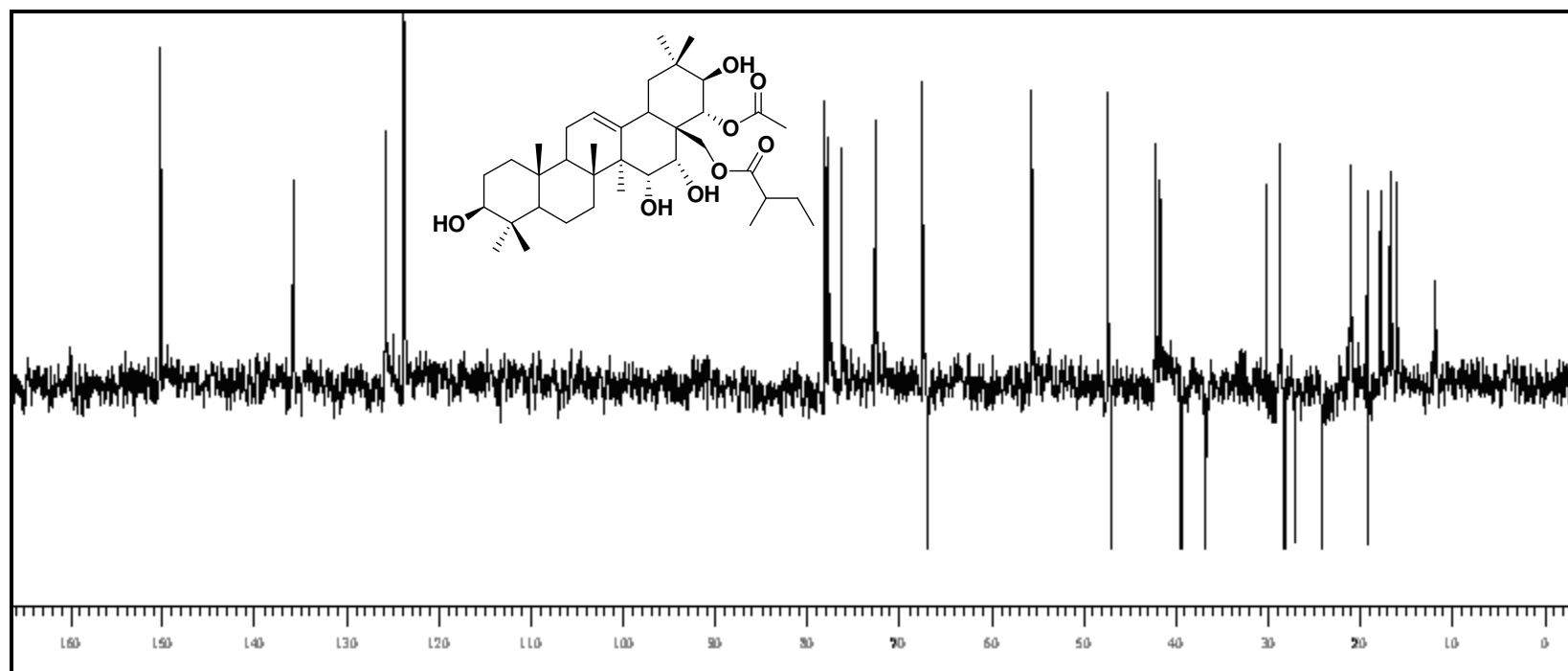
^a Natural Products Laboratory, ^b NMR Division



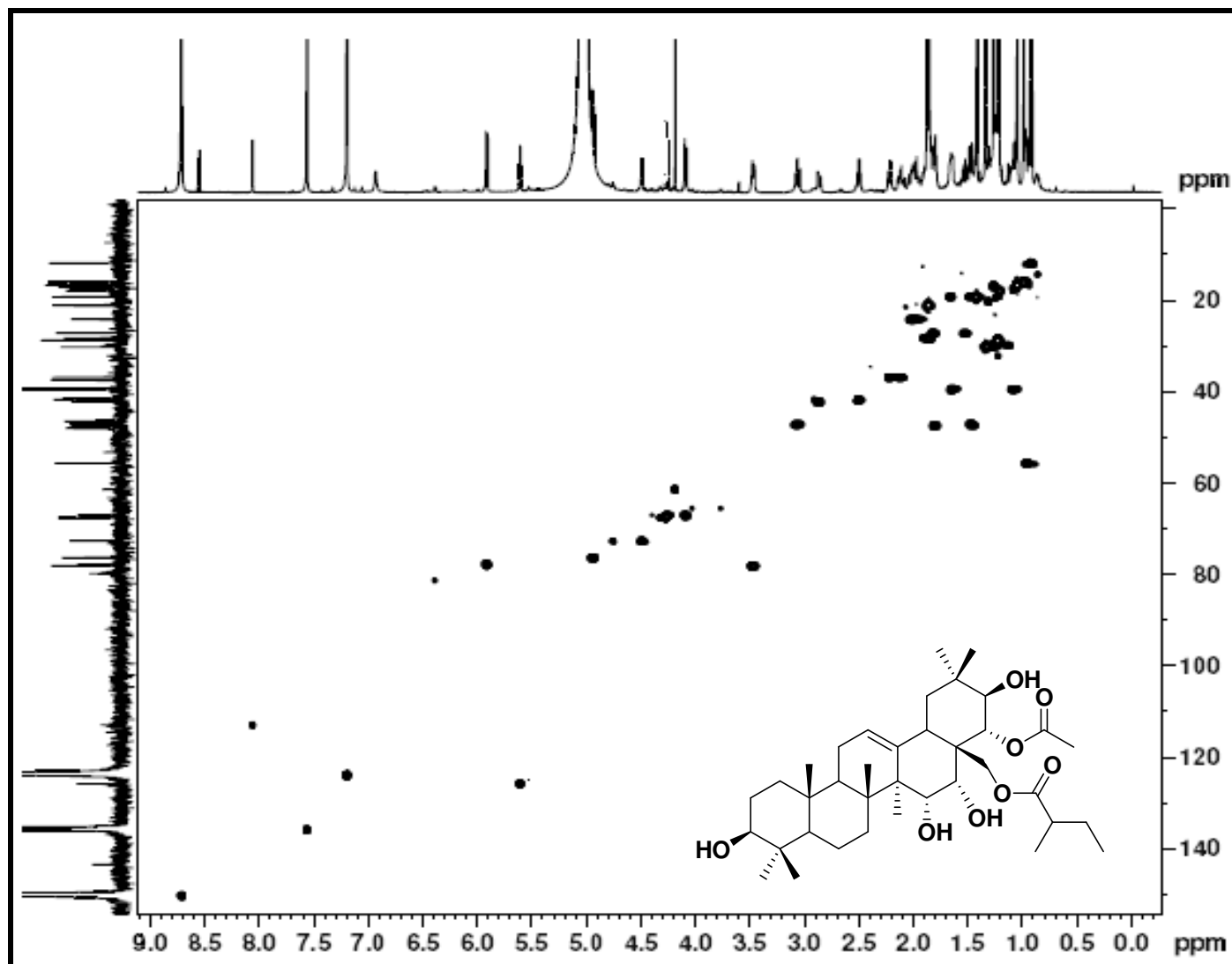
^1H NMR Spectrum of racemosol A (600MHz, $\text{C}_5\text{D}_5\text{N}$)



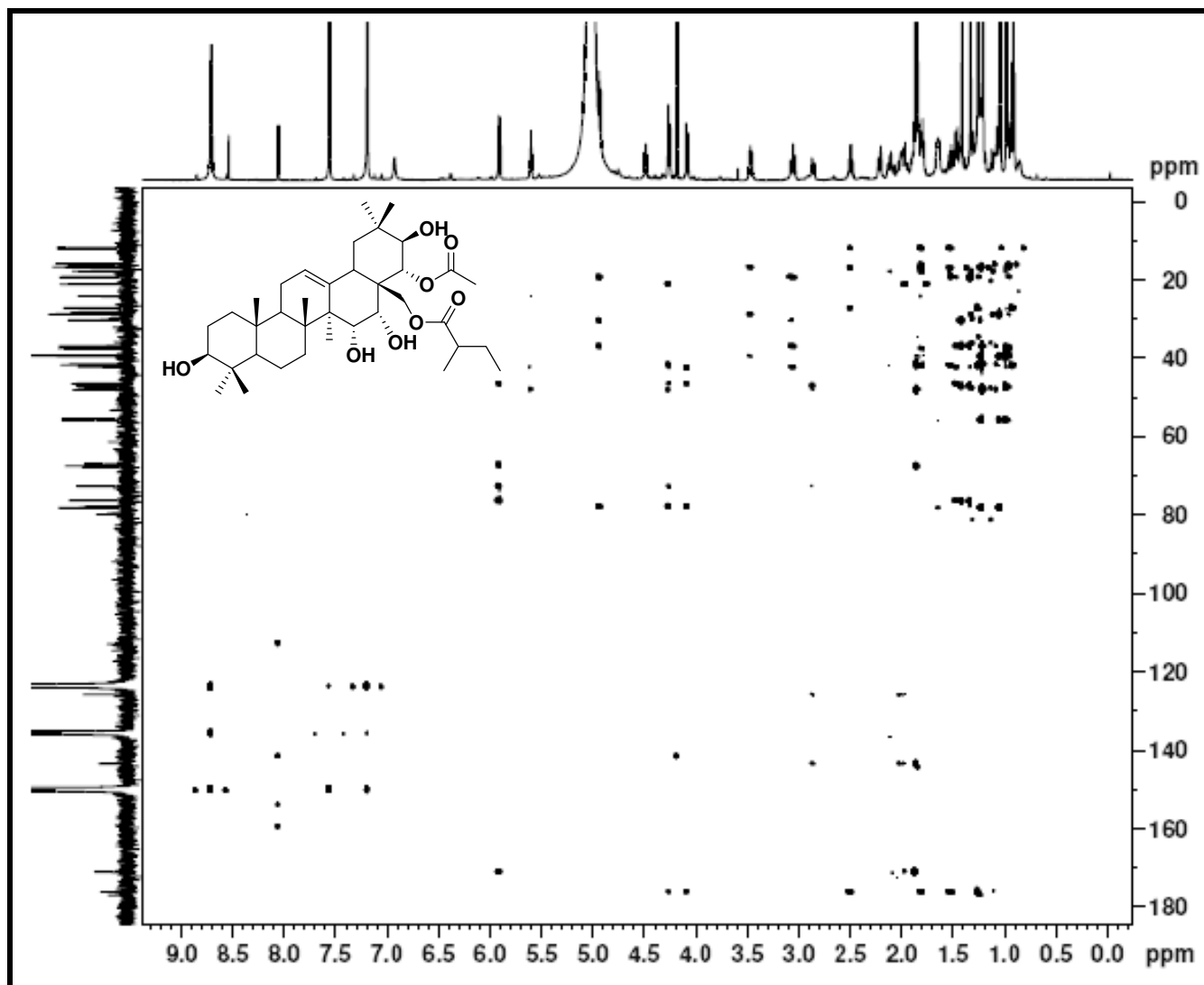
^{13}C NMR Spectrum of racemosol B (600MHz, $\text{C}_5\text{D}_5\text{N}$)



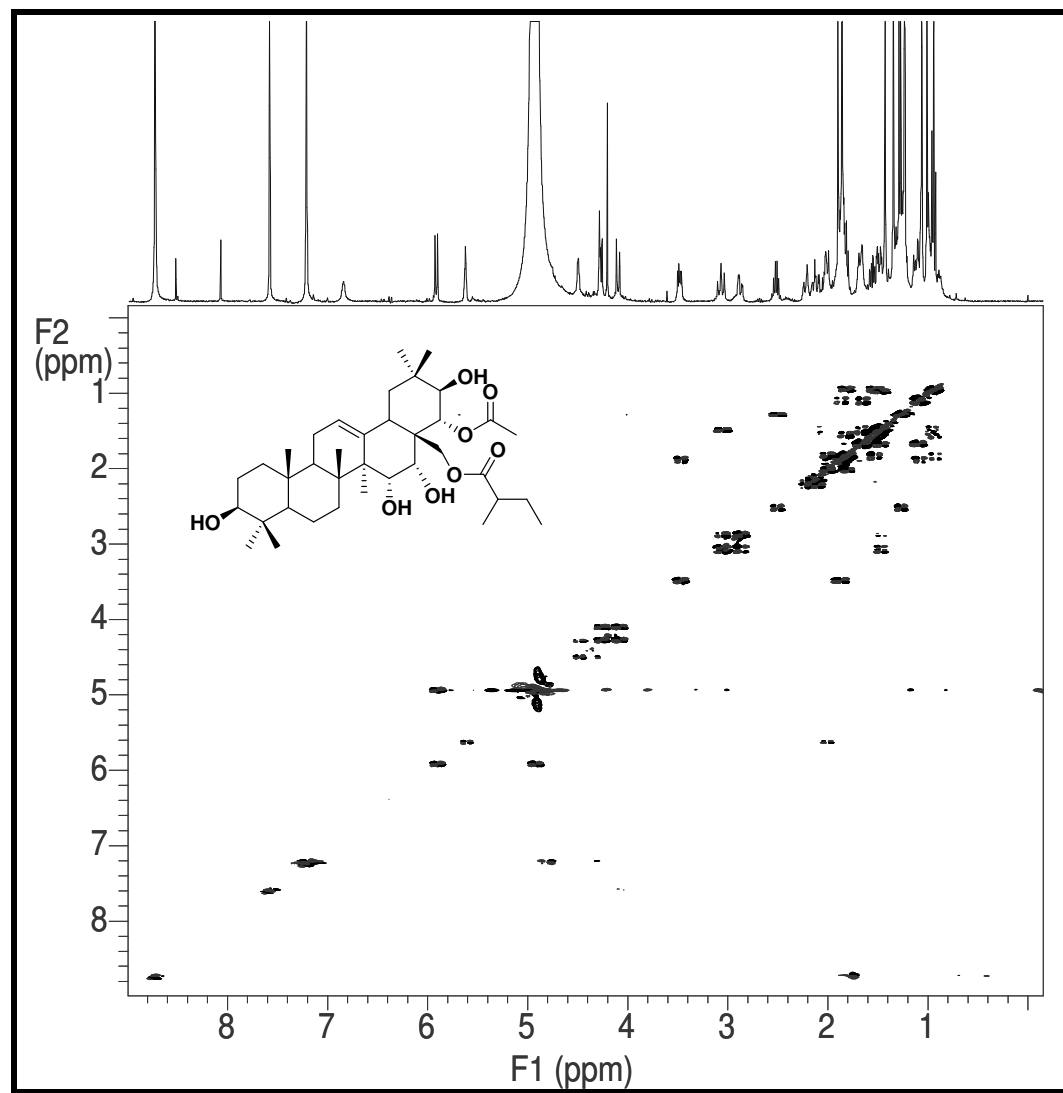
DEPT Spectrum of racemosol A (600MHz, C₅D₅N)

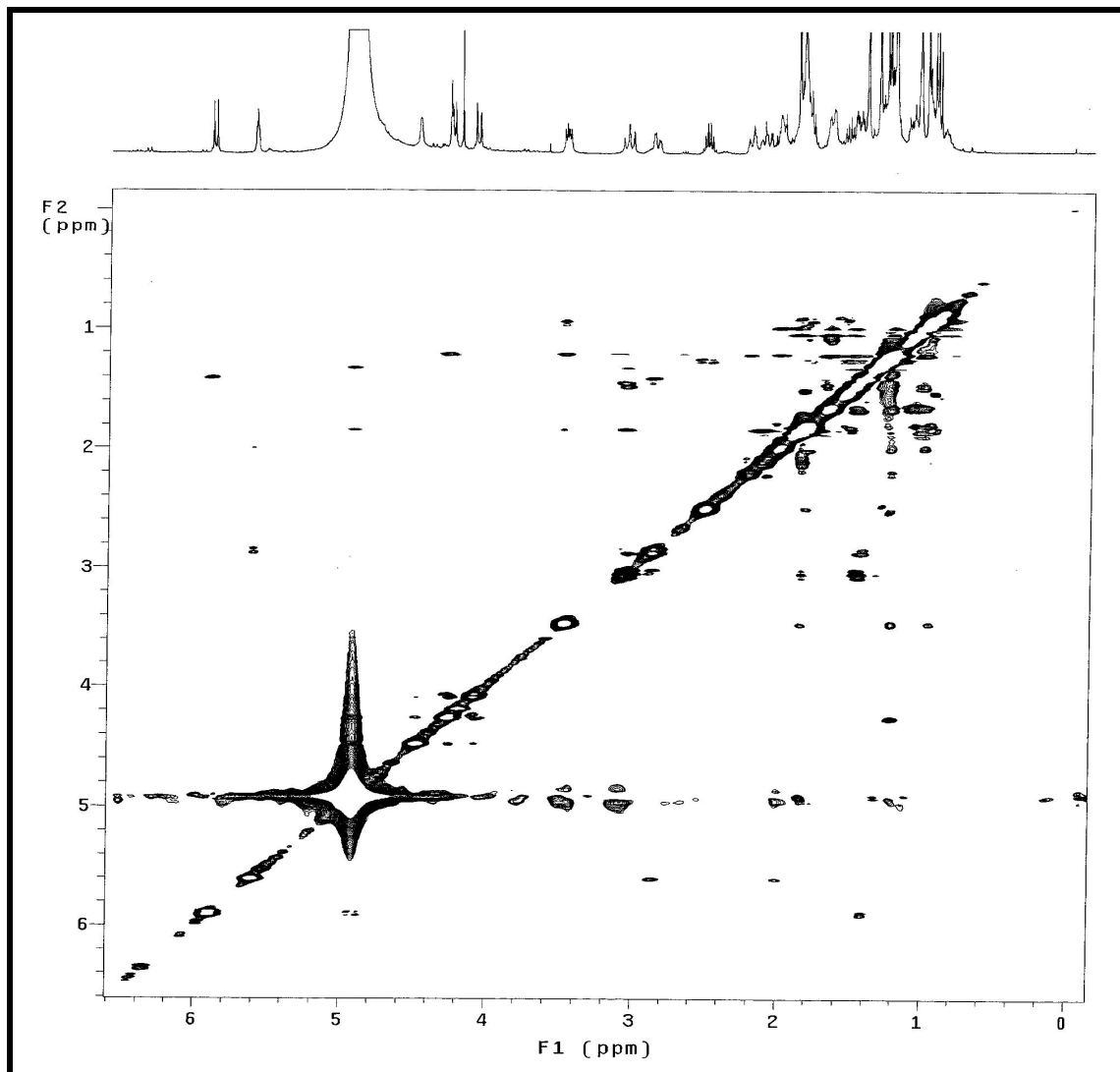


HSQC Spectrum of racemosol A (600MHz, C₅D₅N)

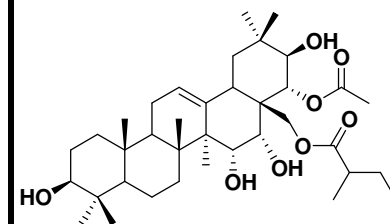


HMBC Spectrum of racemosol A (600MHz, C₅D₅N)

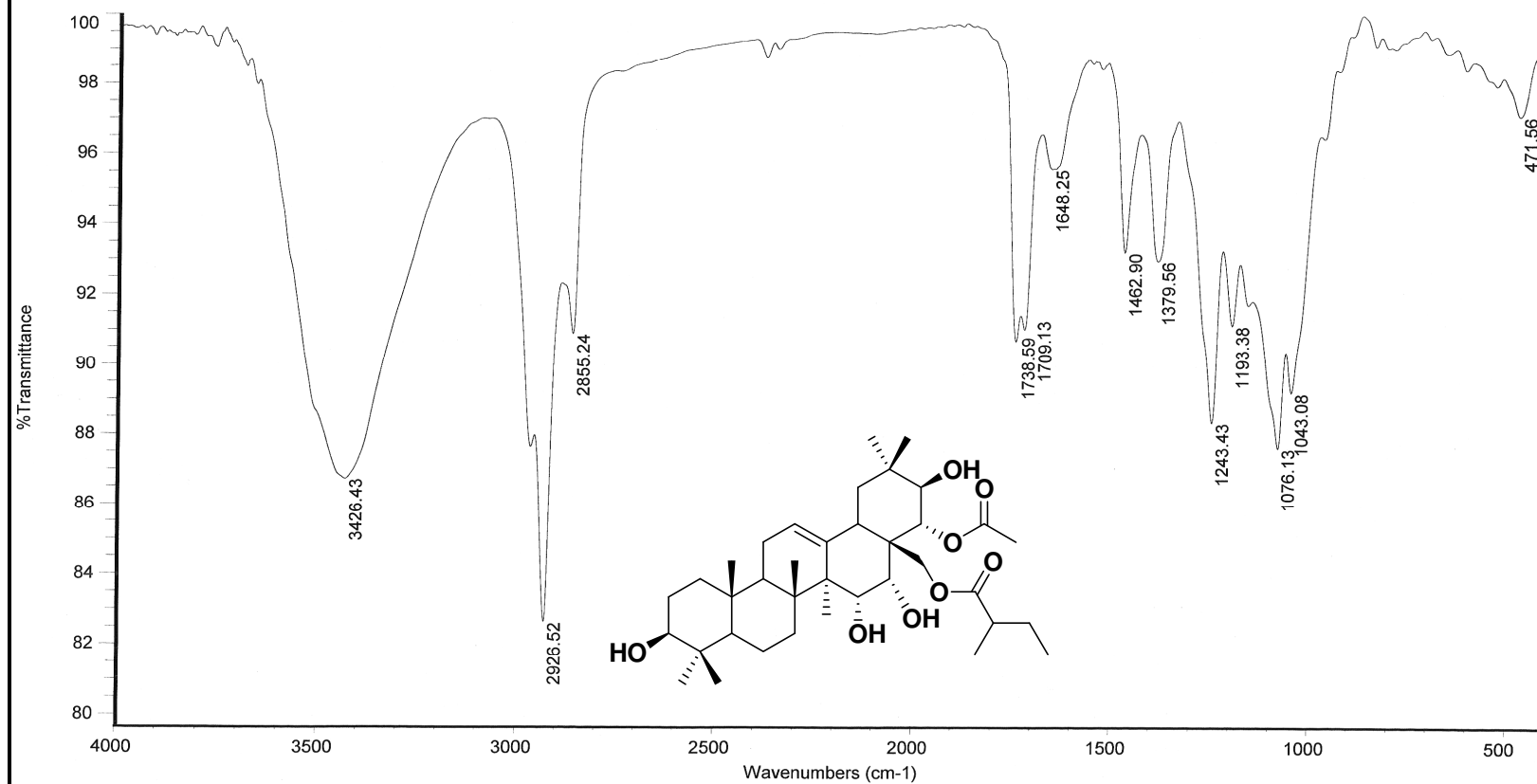




NOESY Spectrum of racemosol A (500MHz, C₅D₅N)



Indian Institute of Chemical Technology, Hyderabad
FTIR Analysis Report



Sample Name: JMR-BR3

Sample Preparation: KBr

Collection time: Thu May 01 11:14:23 2008 (GMT+05:30)

Bench: Thermo Nicolet Nexus 670 Spectrometer

Resolution: 4 cm⁻¹

Detector: DTGS KBr

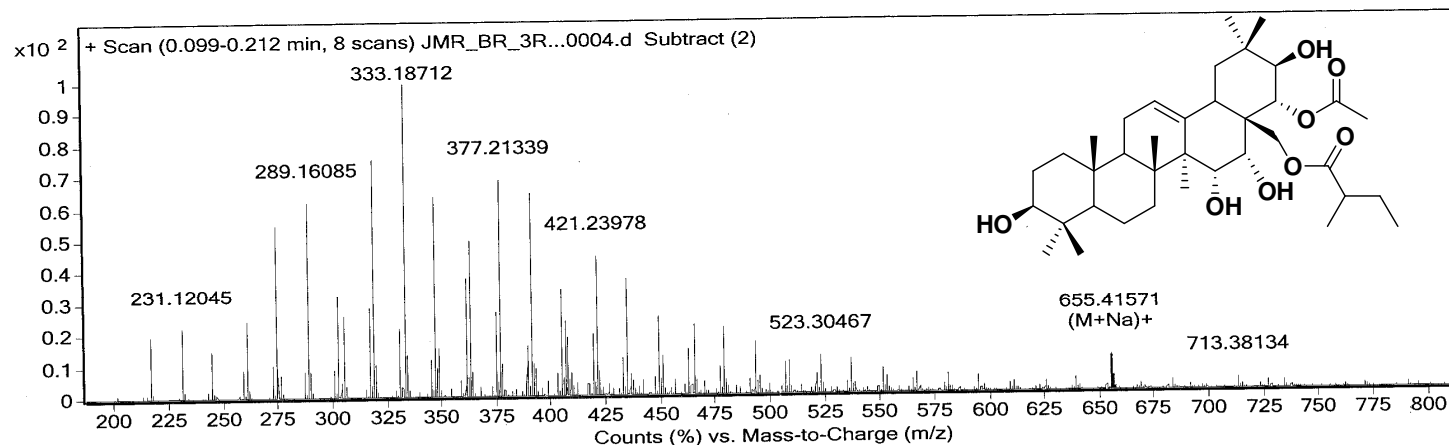
Beamsplitter: KBr

Source: IR

Analyst Name:

IR Spectrum of racemosol A

Plot Window Report



- End of Report ---

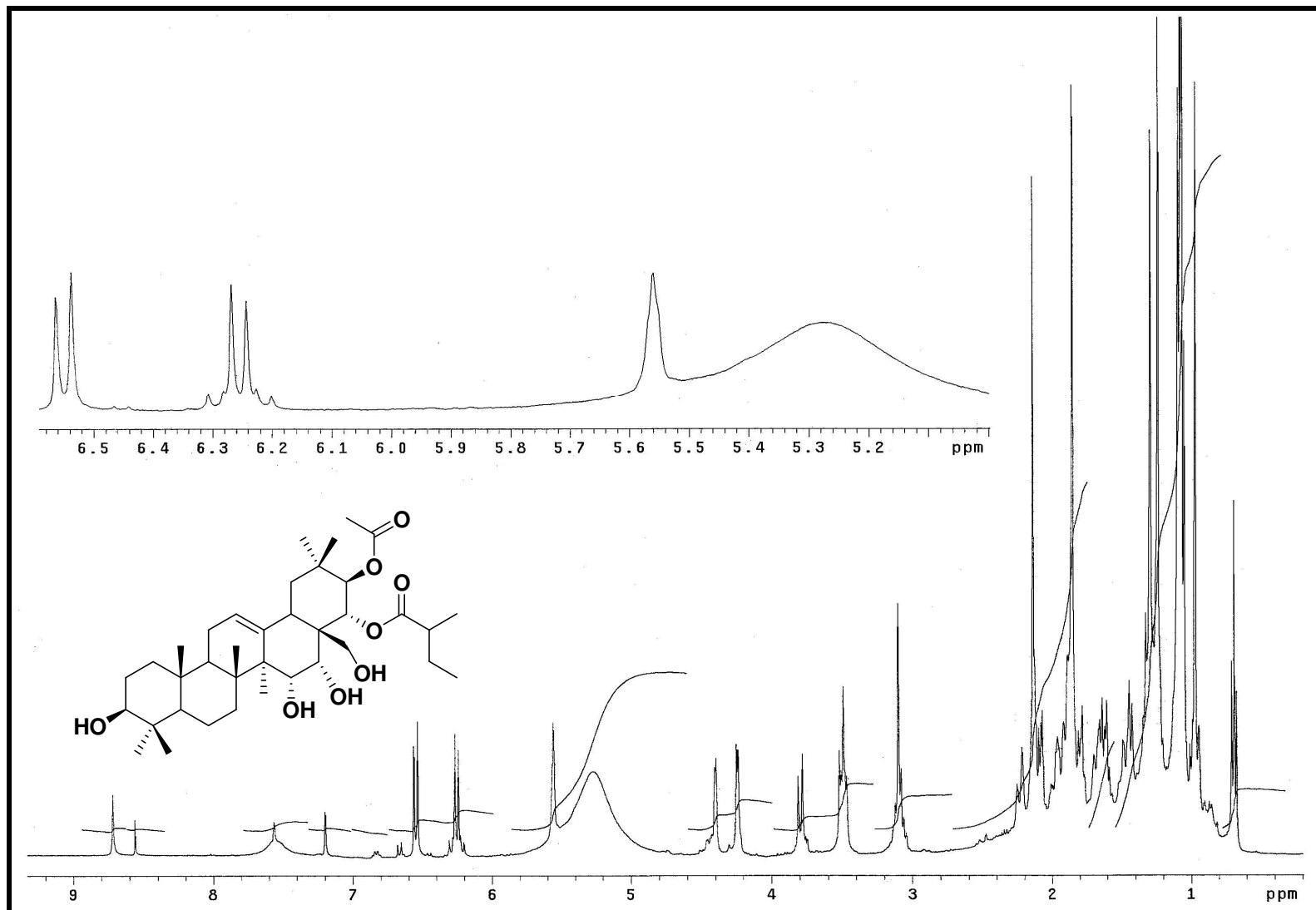
MS Formula Results: + Scan (0.099-0.212 min) Sub (2) (JMR_BR_3R...0004.d)

m/z	Ion	Formula	Abundance
655.41571	(M+Na)+	C37H60NaO8	7399.1

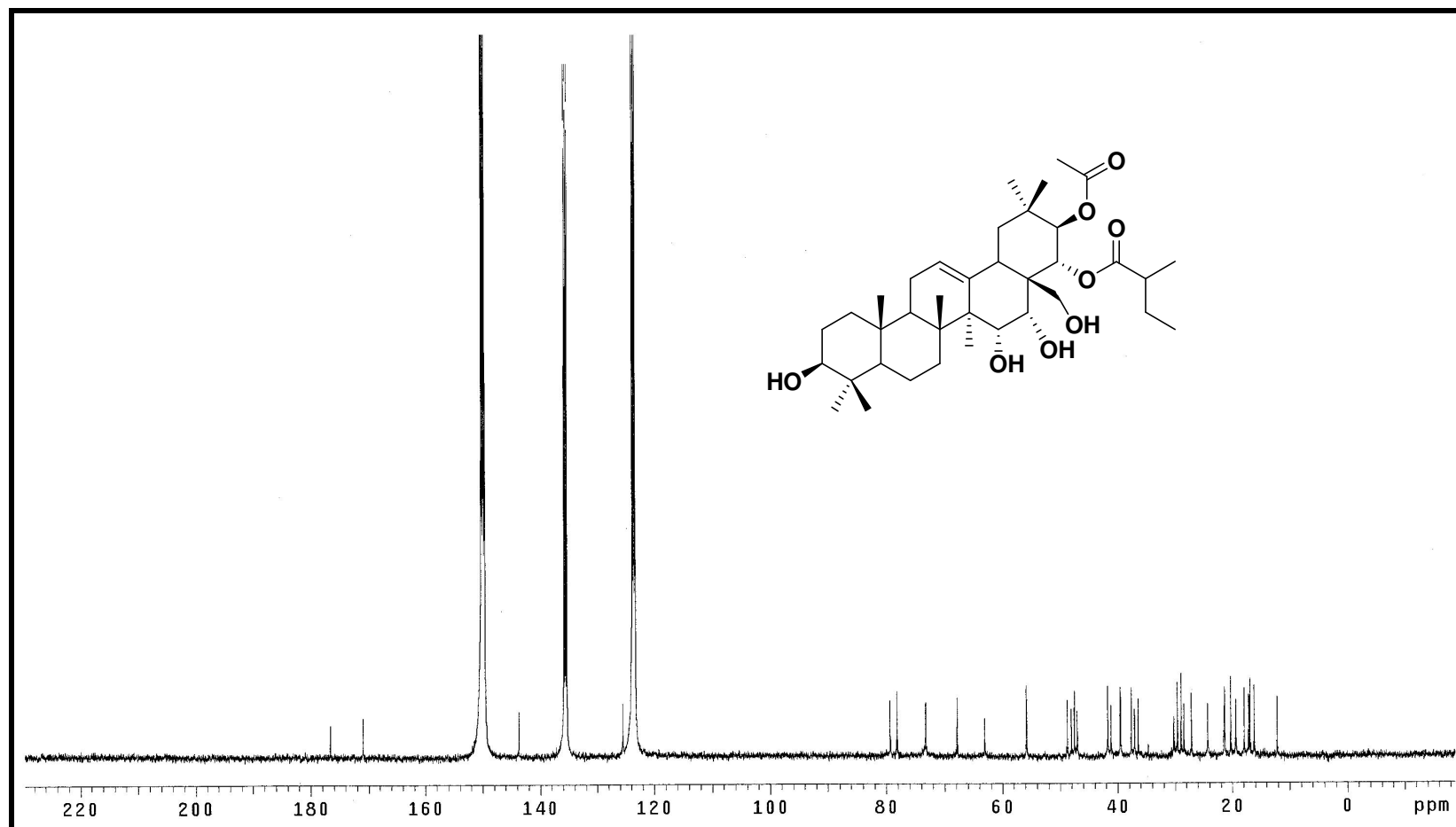
Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Difference (ppm)	Abs Diff (ppm)	DBE
✓	C37H60O8	C37H60NaO8	100		632.42649	632.42882	3.68	3.68	8

Isotope	Abund%	Calc Abund%	m/z	Calc m/z	Difference (ppm)
1	100	100	655.41571	655.41804	3.55
2	37.16	41.01	656.41879	656.42145	4.05
3	8.25	9.84	657.41684	657.42443	11.55
4	1.42	1.74	658.41984	658.42728	11.29

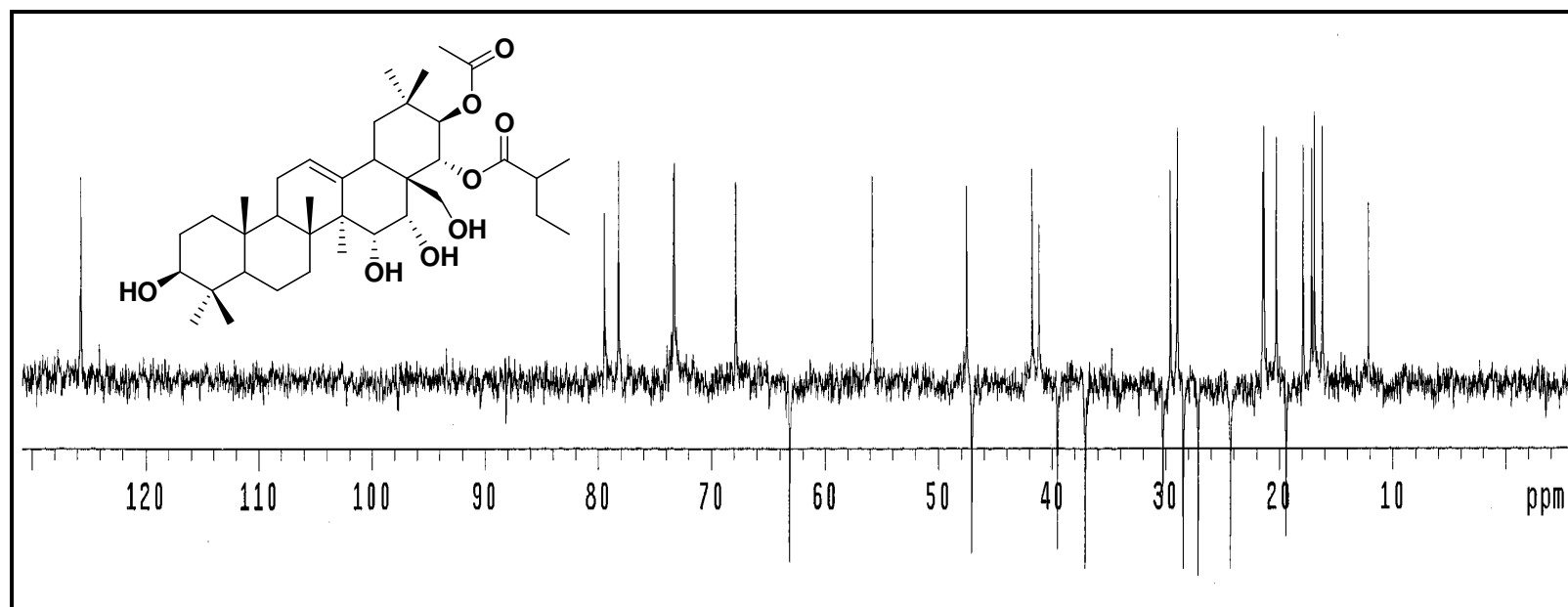
Mass Spectrum of racemosol A



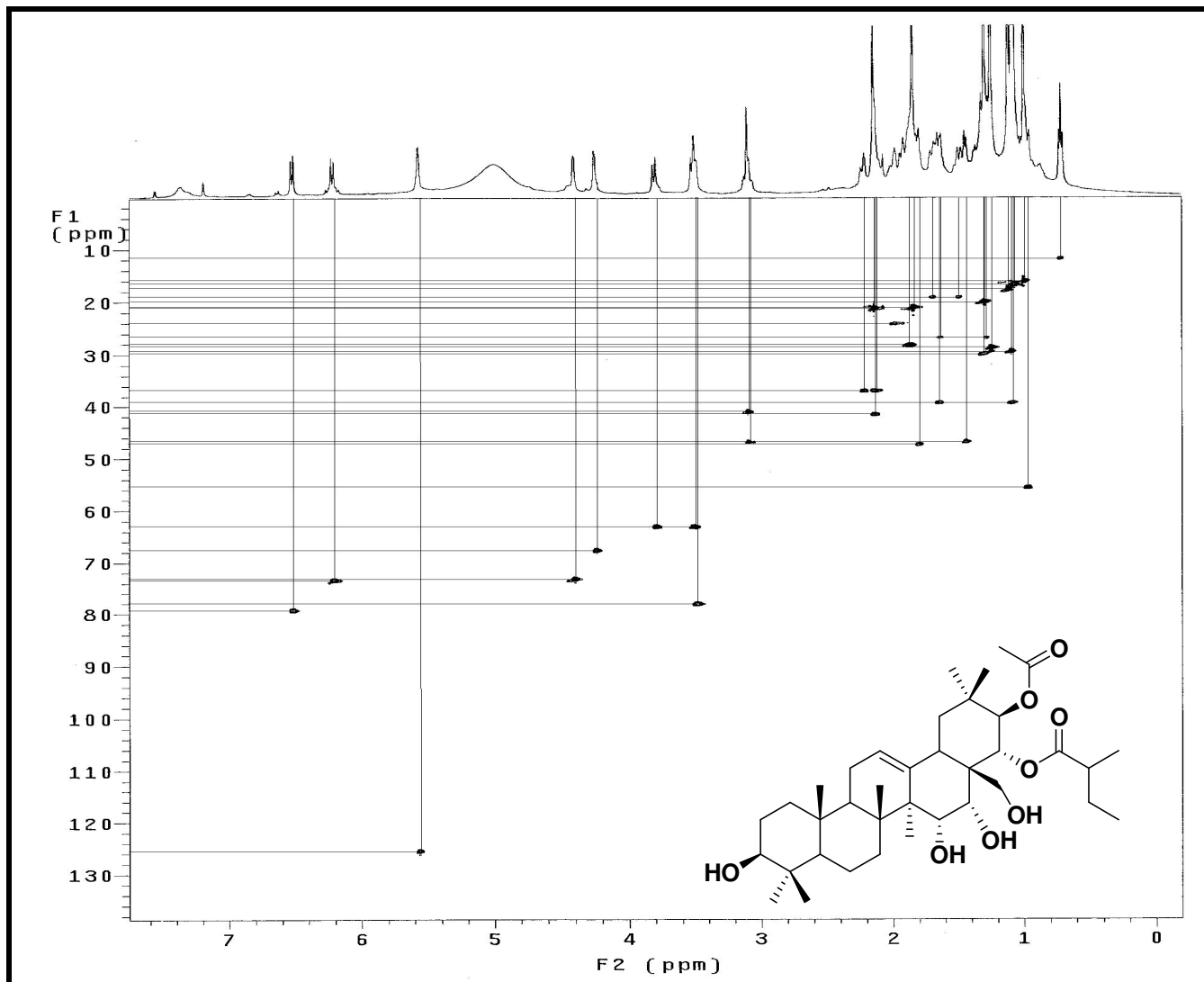
^1H NMR Spectrum of isoracemosol A (500MHz, $\text{C}_5\text{D}_5\text{N}$)



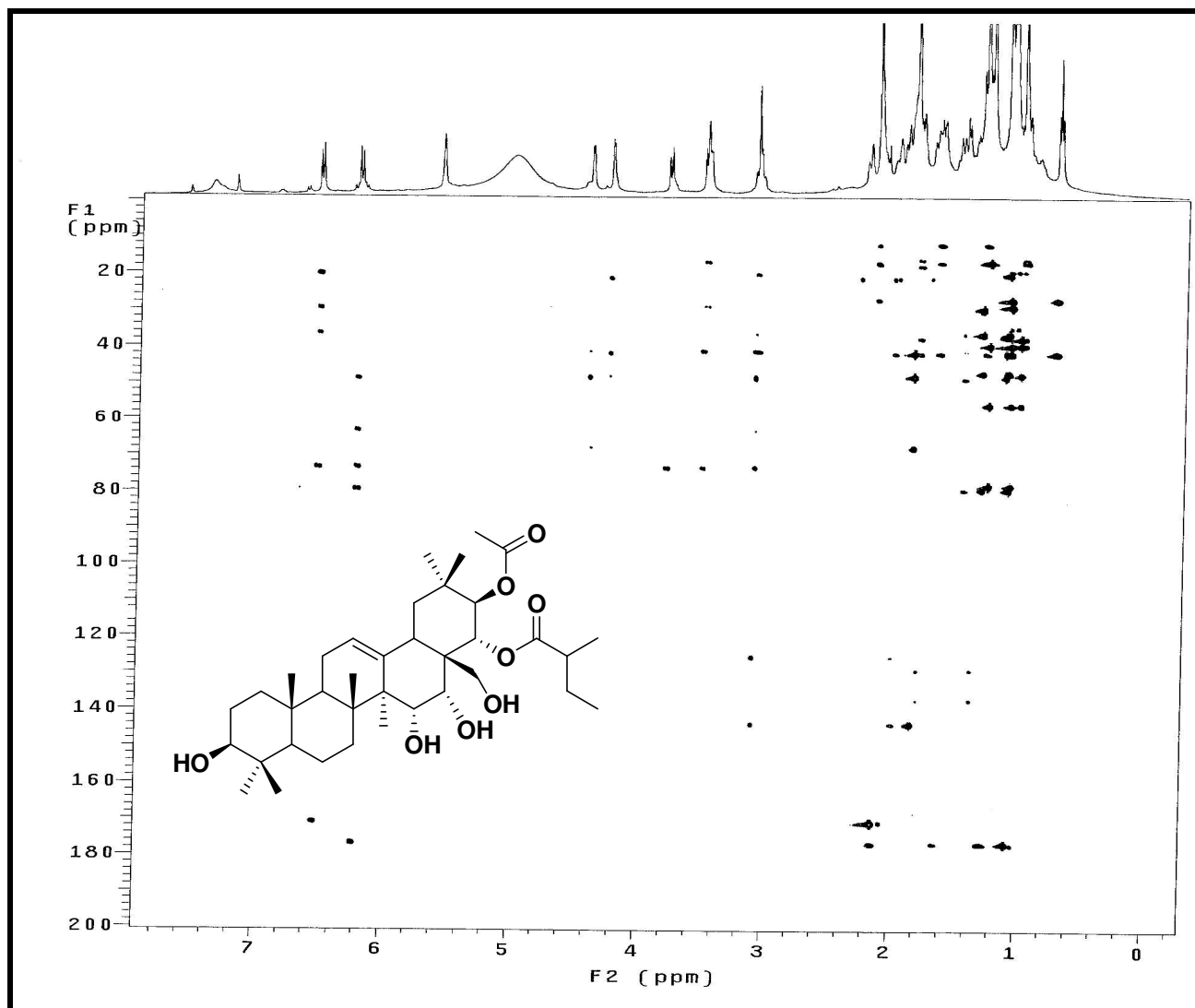
^{13}C NMR Spectrum of isoracemosol A (500MHz, $\text{C}_5\text{D}_5\text{N}$)



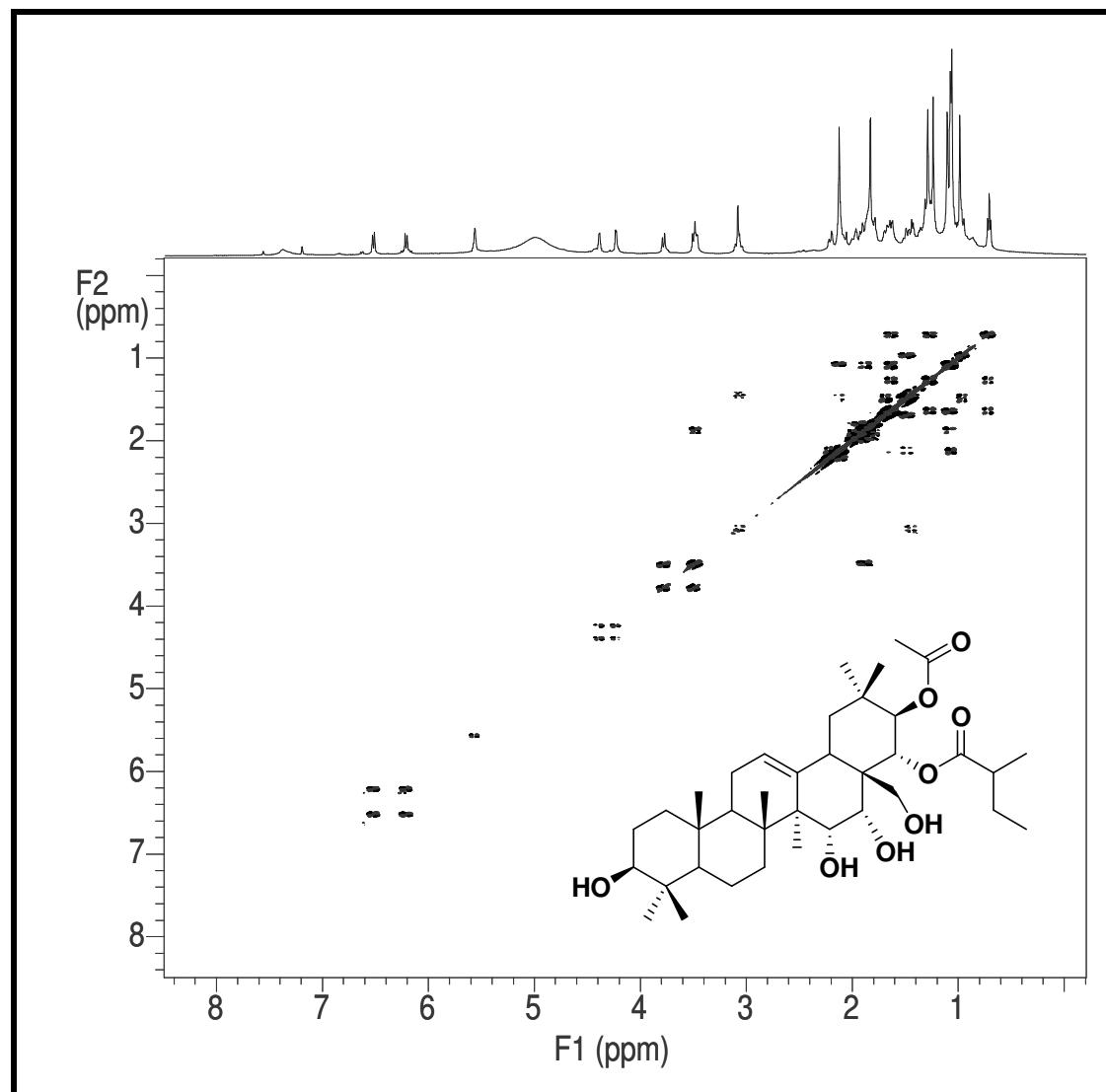
DEPT Spectrum of isoracemosol A (500MHz, C₅D₅N)



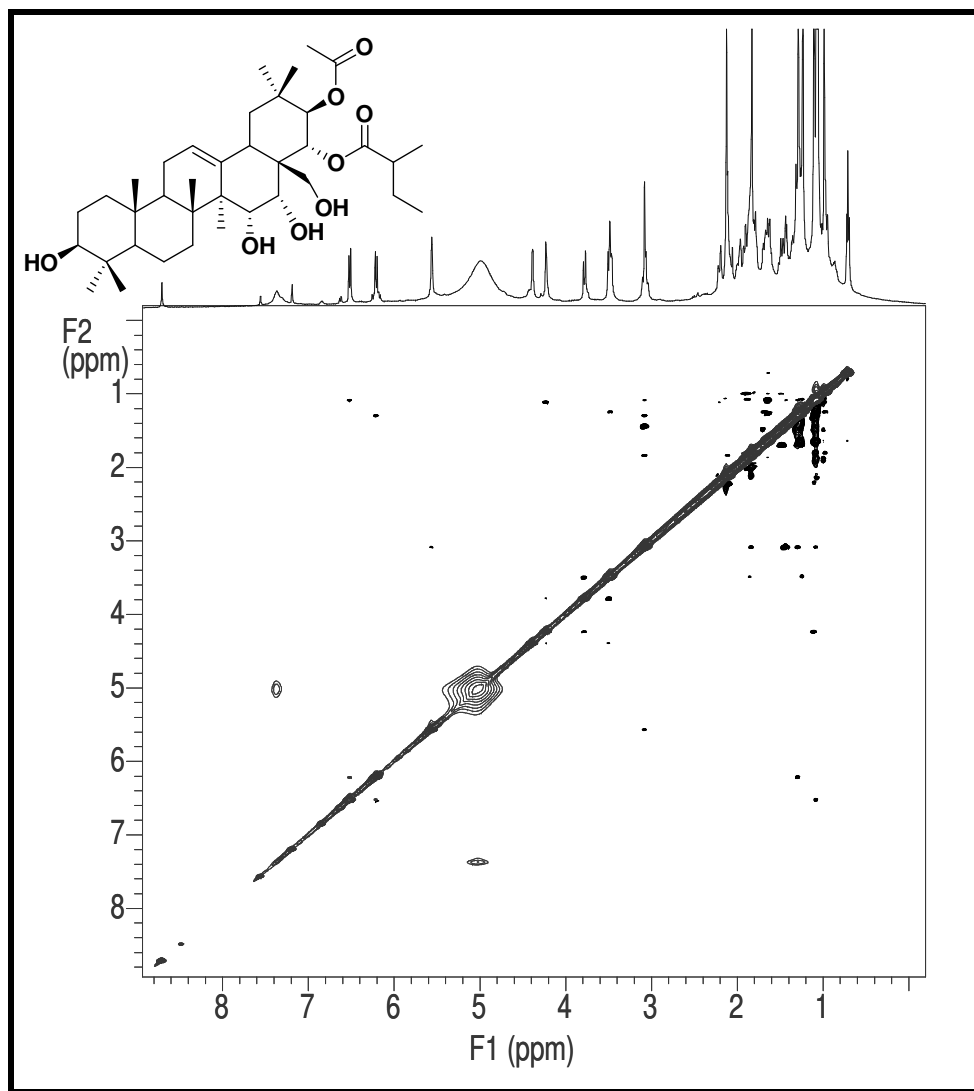
HSQC Spectrum of isoracemosol A (500MHz, C₅D₅N)



HMBC Spectrum of isoracemosol A (500MHz, C₅D₅N)

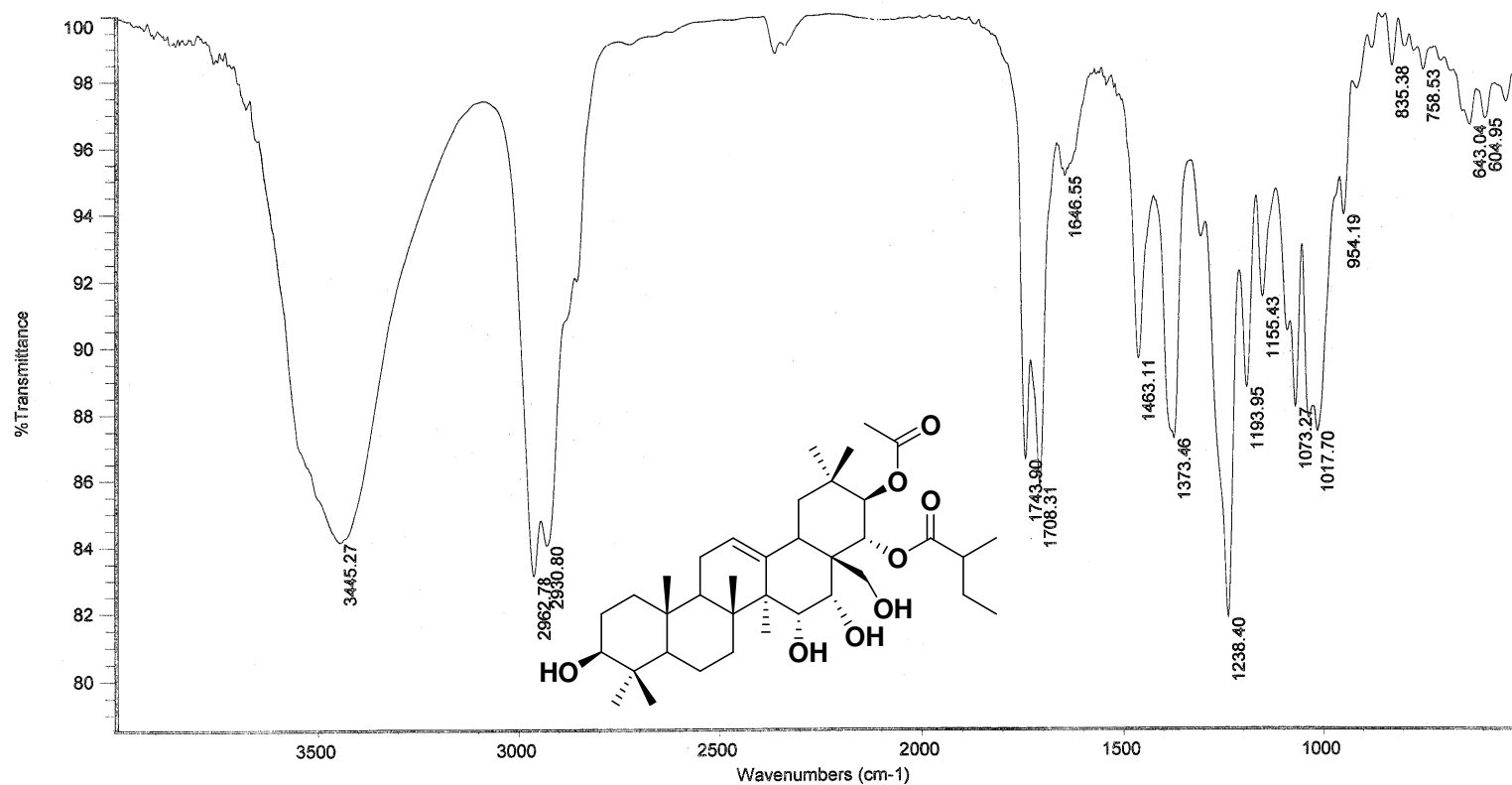


COSY Spectrum of isoracemosol A (500MHz, C₅D₅N)



HMBC Spectrum of isoracemosol A (500MHz, C₅D₅N)

Indian Institute of Chemical Technology, Hyderabad
FTIR Analysis Report



Sample Name: JMR-BR-13B

Sample Preparation: KBr

Collection time: Fri Sep 21 11:43:14 2007 (GMT+05:30)

Bench: Thermo Nicolet Nexus 670 Spectrometer

Resolution: 4 cm⁻¹

Detector: DTGS KBr

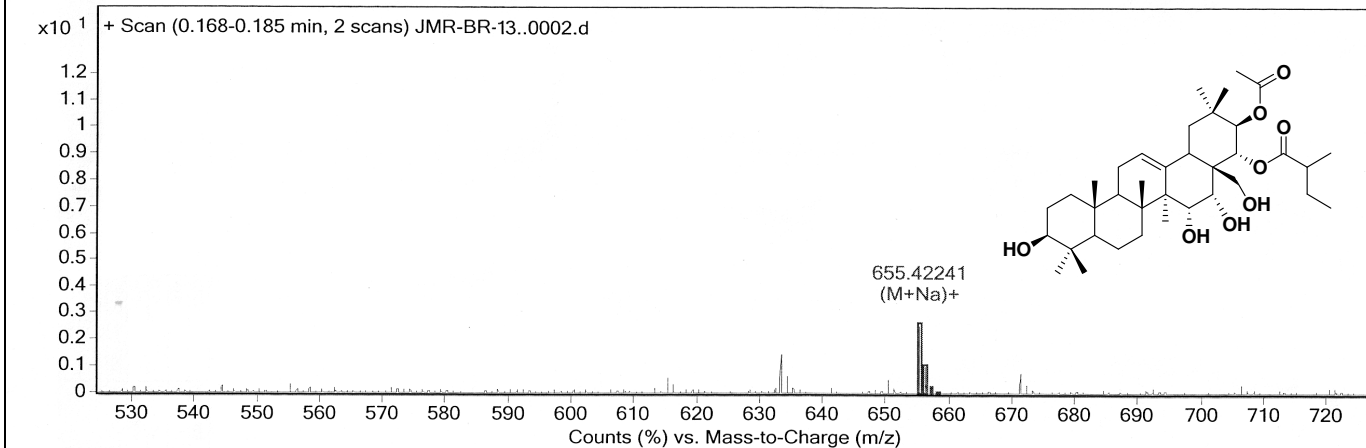
Beamsplitter: KBr

Source: IR

Analyst Name:

IR Spectrum of isoracemosol A

Plot Window Report



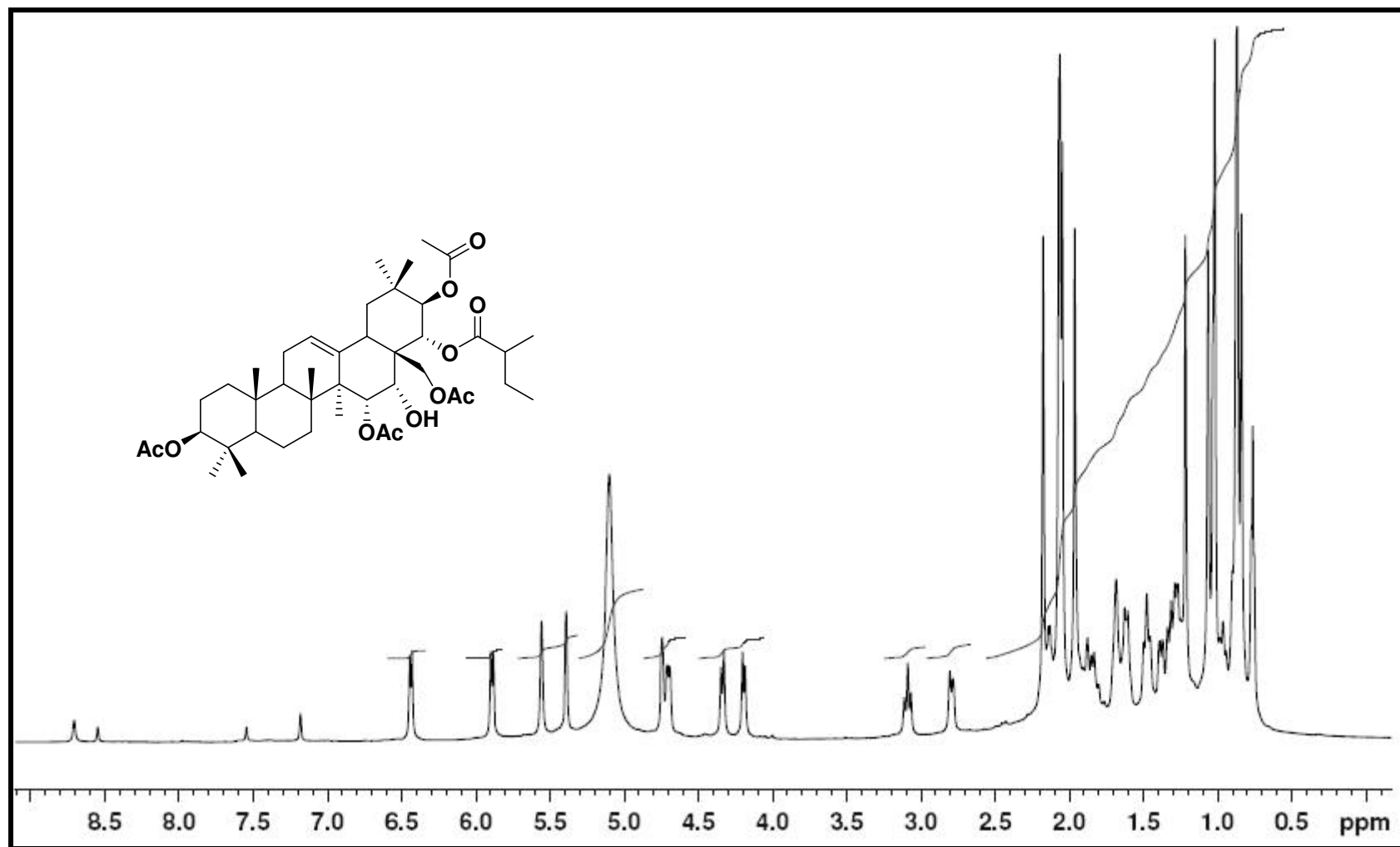
MS Formula Results: + Scan (0.168-0.185 min) (JMR-BR-3..0002.d)

m/z	Ion	Formula	Abundance
655.42241	(M+Na)+	C37H60NaO8	62403.2

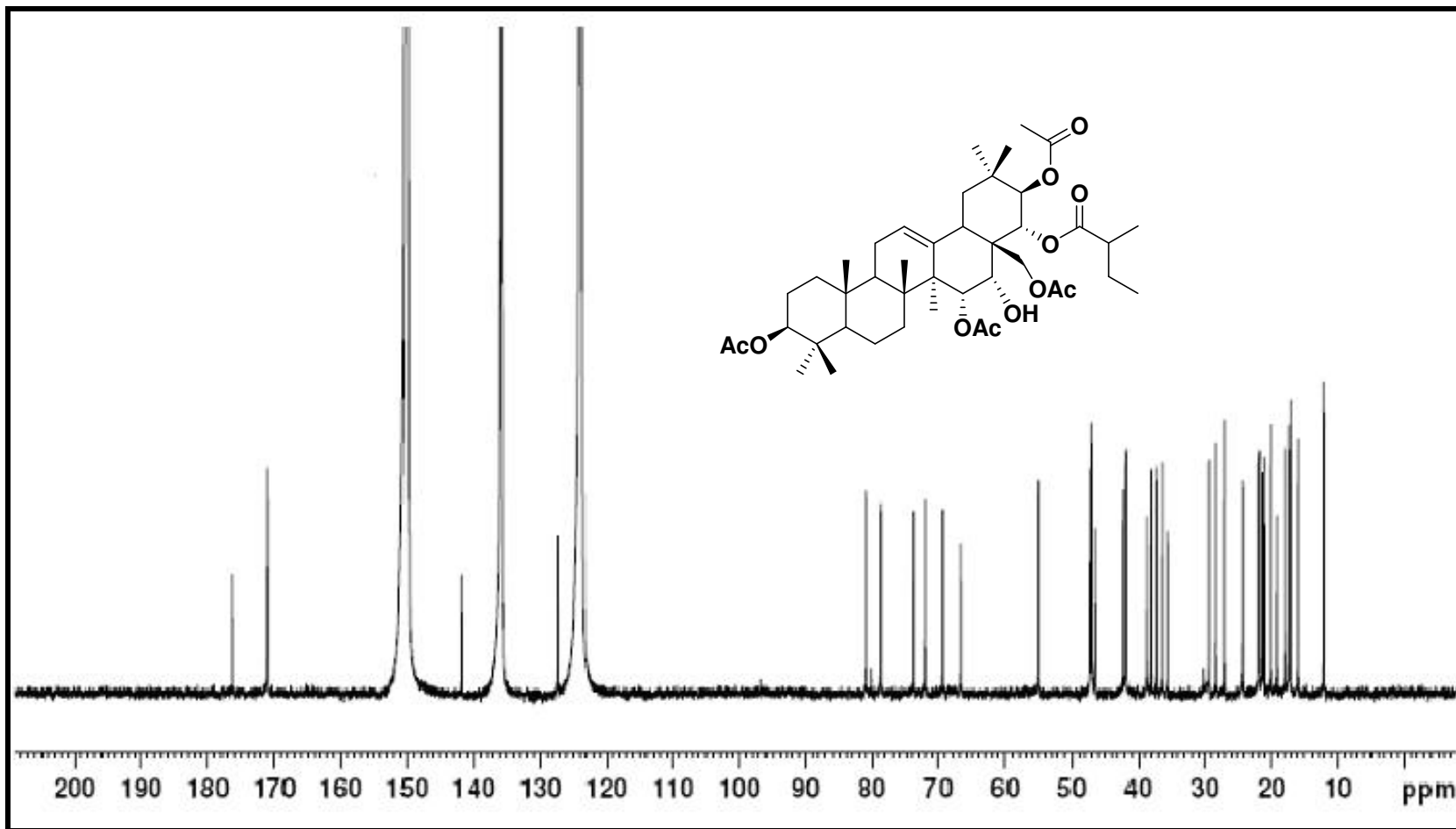
Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Difference (ppm)	Abs Diff (ppm)	DBE
✓	C37H60O8	C37H60NaO8	100		632.43319	632.42882	-6.91	6.91	8

Isotope	Abund%	Calc Abund%	m/z	Calc m/z	Difference (ppm)
1	100	100	655.42241	655.41804	-6.67
2	38.38	41.01	656.42626	656.42145	-7.33
3	9.39	9.84	657.4248	657.42443	-0.56
4	2.45	1.74	658.42015	658.42728	10.83

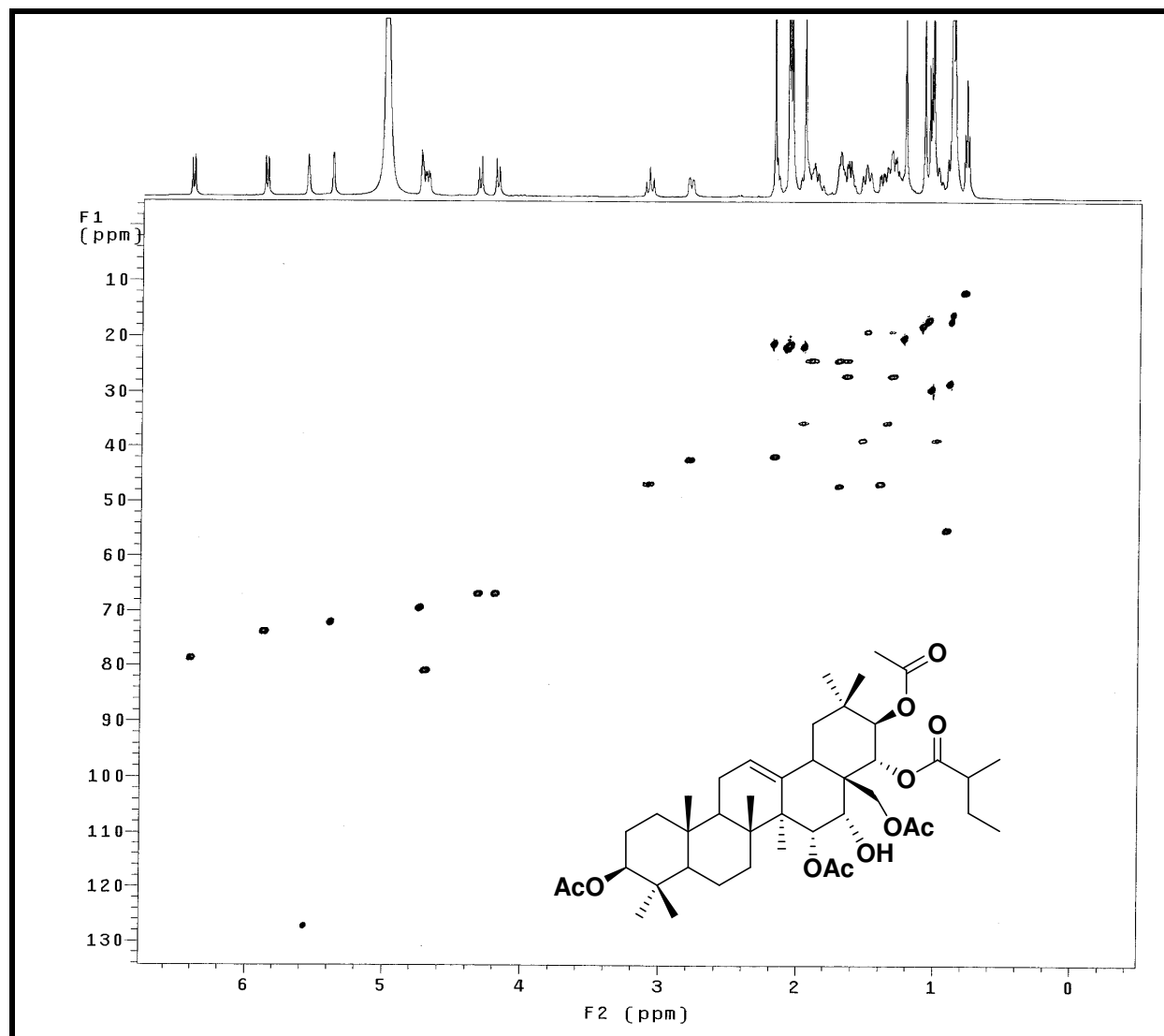
Mass Spectrum of isoracemosol A



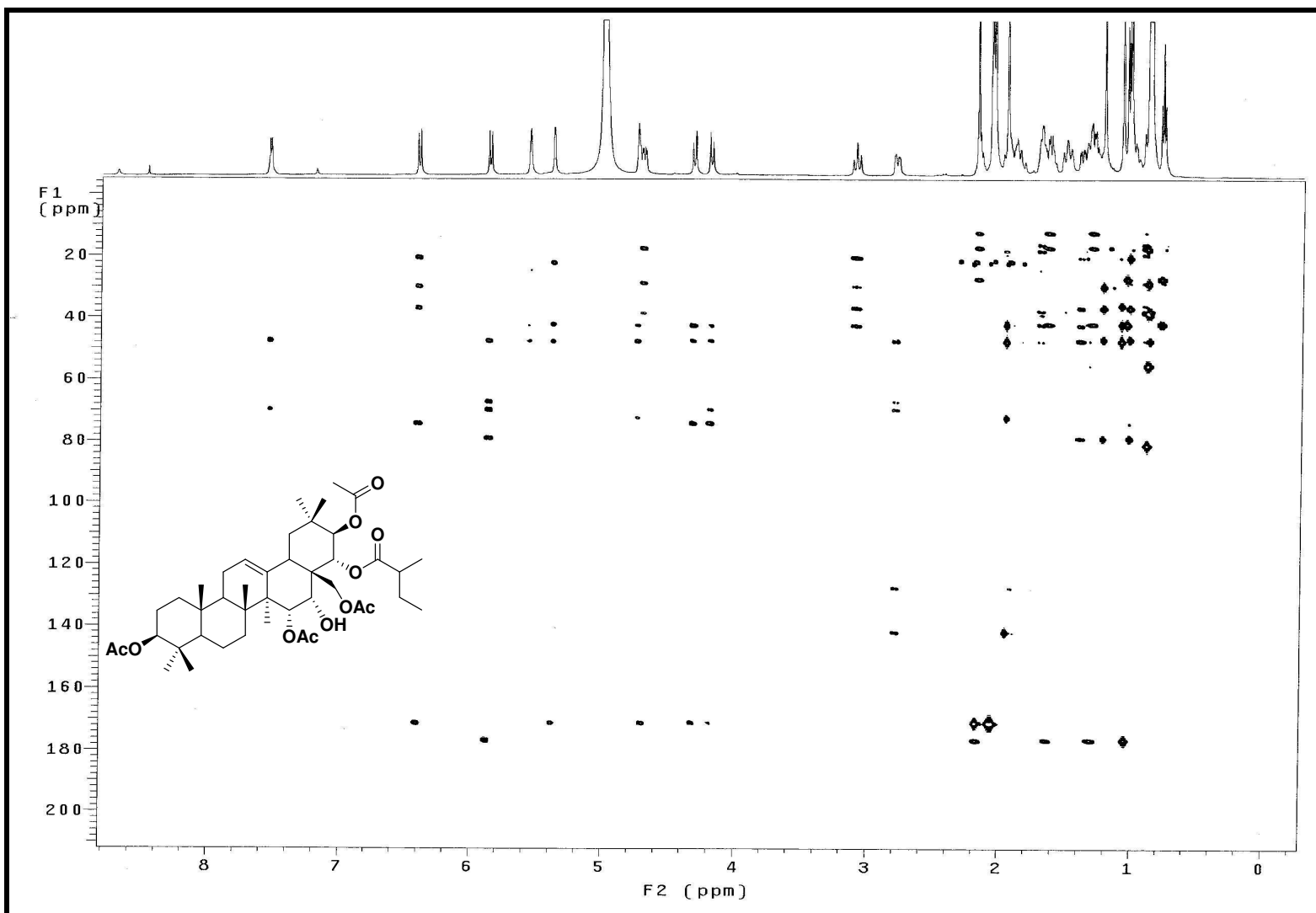
^1H NMR Spectrum of 3 β , 15 α , 21 α , 28-tetraacetoxy isoracemosol A (600MHz, $\text{C}_5\text{D}_5\text{N}$)



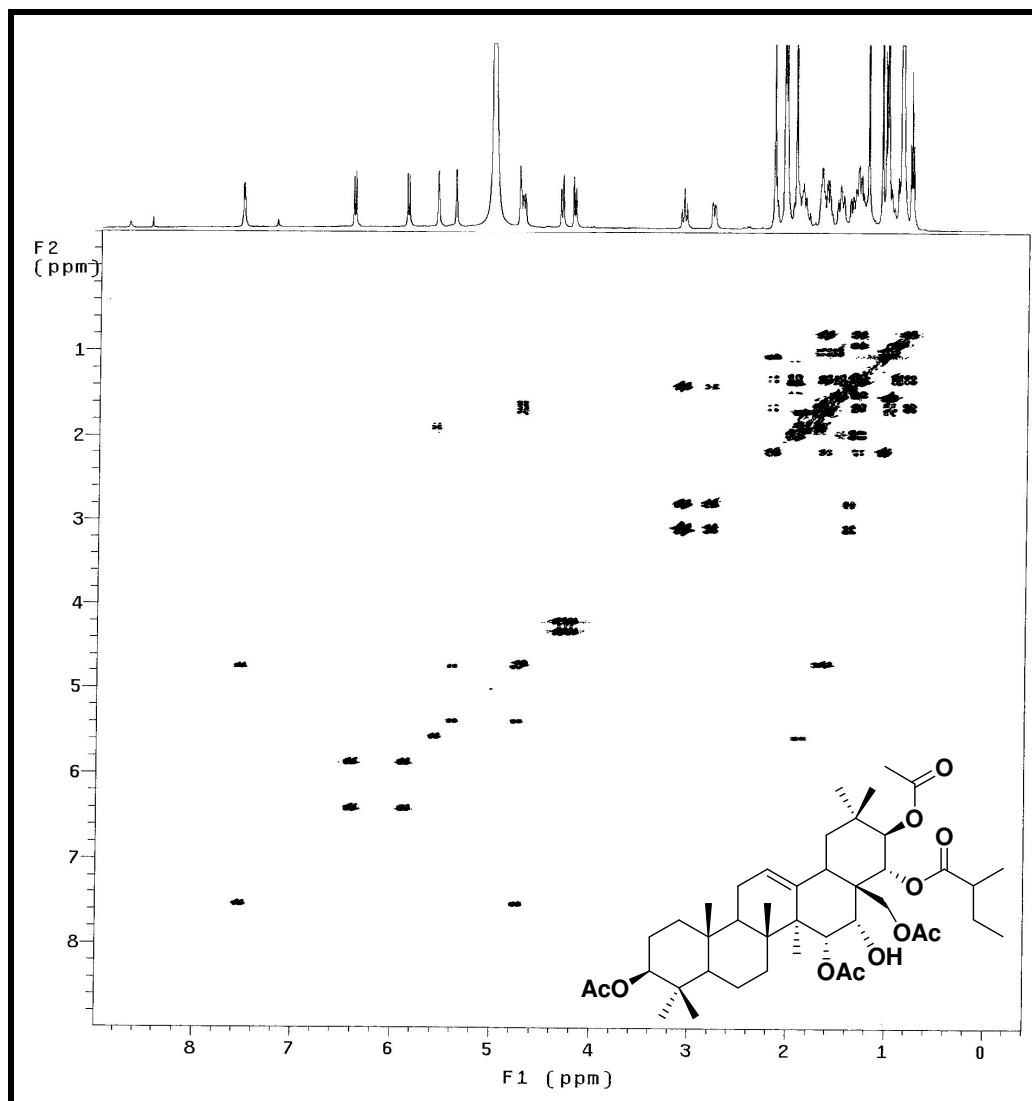
^{13}C NMR Spectrum of 3 β , 15 α , 21 α , 28-tetraacetoxy isoracemosol A (600MHz, $\text{C}_5\text{D}_5\text{N}$)



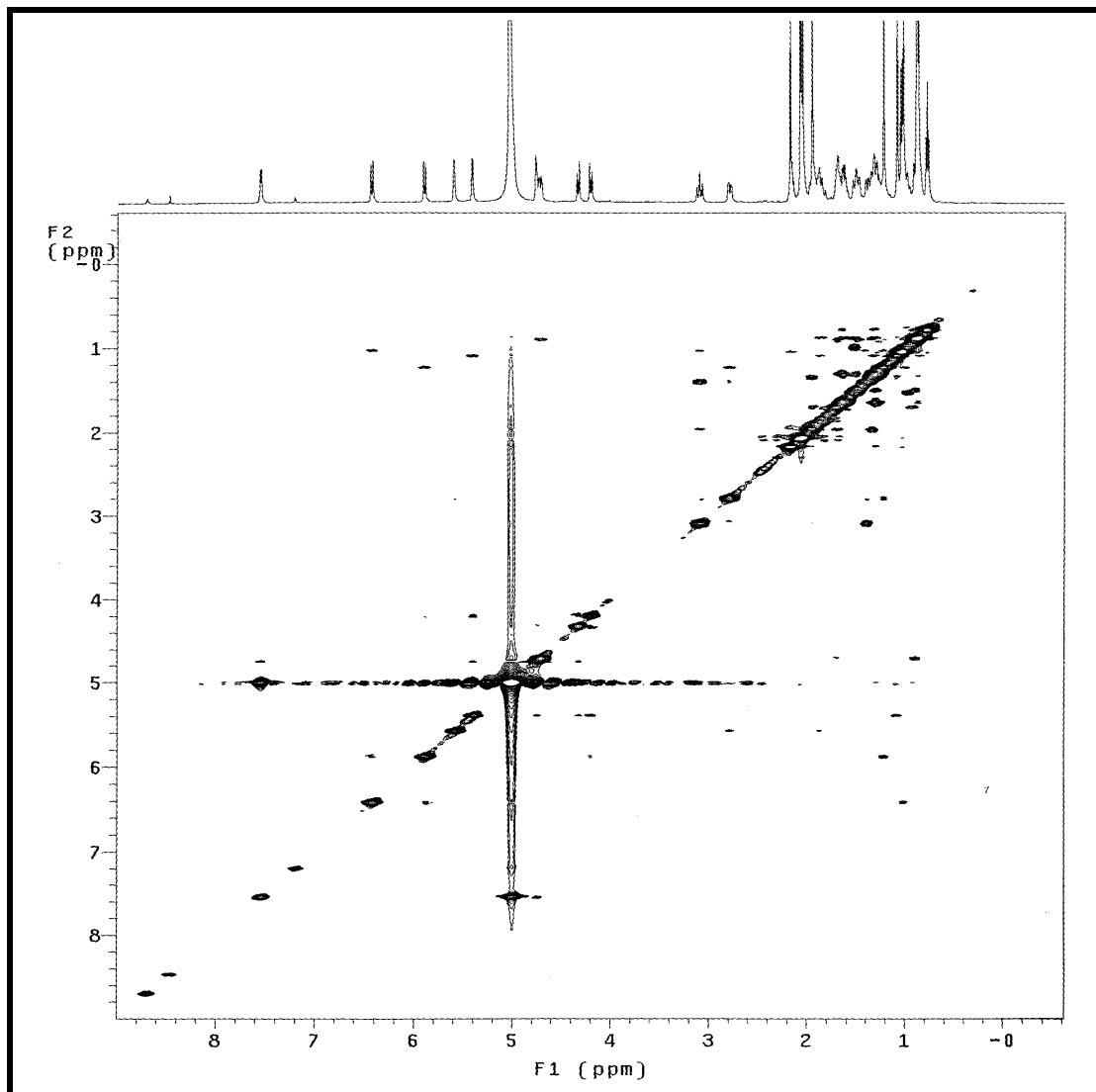
HSQC Spectrum of 3 β , 15 α , 21 α , 28-tetraacetoxy isoracemosol A (500MHz, $\text{C}_5\text{D}_5\text{N}$)



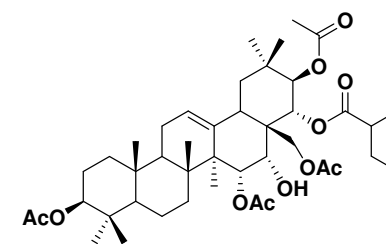
HMBC Spectrum of 3β, 15α, 21α, 28-tetraacetoxy isoracemosol A (500MHz, C₅D₅N)



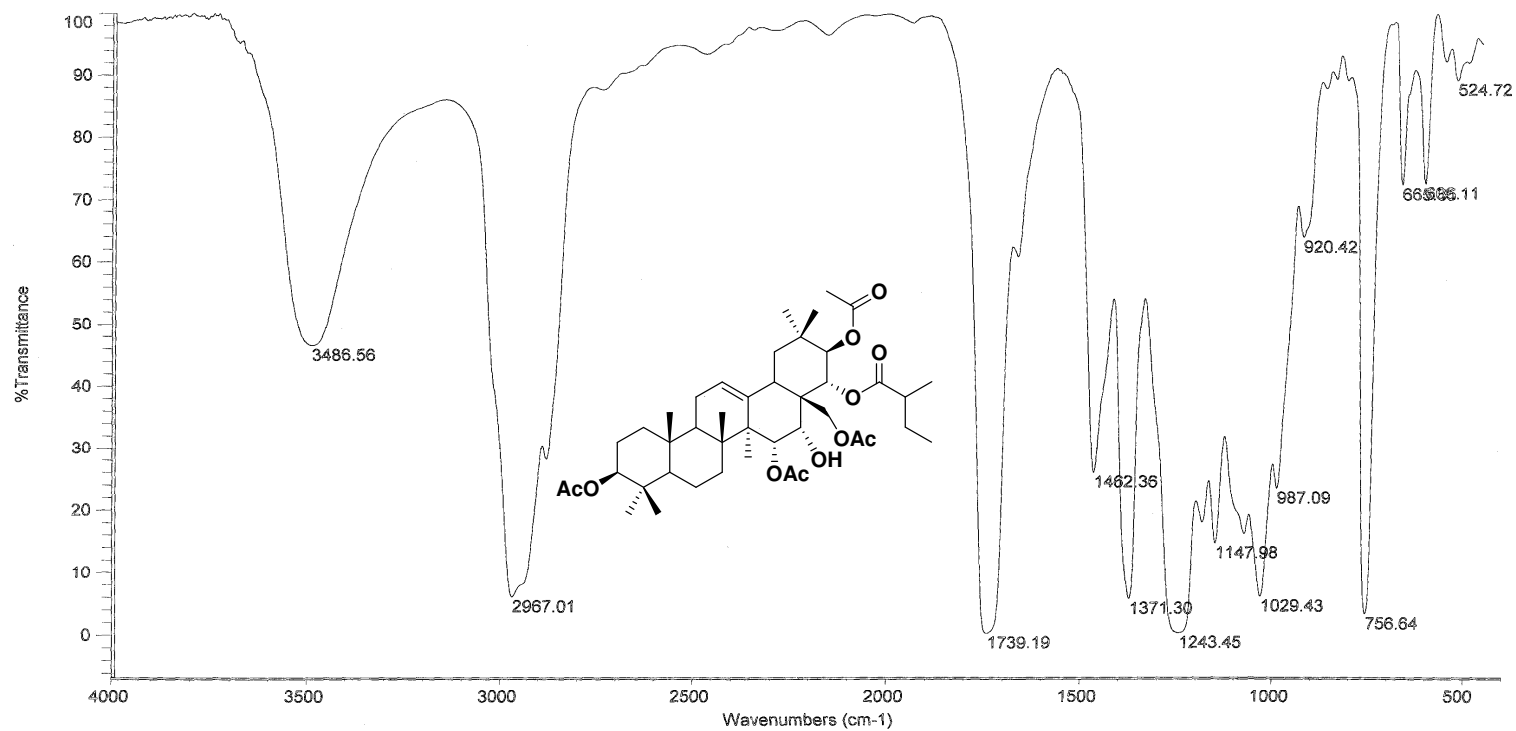
COSY Spectrum of 3 β , 15 α , 21 α , 28-tetraacetoxy isoracemosol A (500MHz, C₅D₅N)



NOESY Spectrum of 3 β , 15 α , 21 α , 28-tetraacetoxy isoracemosol A (500MHz, C₅D₅N)



Indian Institute of Chemical Technology, Hyderabad
FTIR Analysis Report



Sample Name: JMR-BR-13-AC

Sample Preparation: NEAT

Collection time: Tue Apr 29 15:10:13 2008 (GMT+05:30)

Bench: Thermo Nicolet Nexus 670 Spectrometer

Resolution: 4 cm⁻¹

Detector: DTGS KBr

Beamsplitter: KBr

Source: IR

Analyst Name:

IR Spectrum of 3β, 15α, 21α, 28-tetraacetoxy isoracemosol A