NMR in the School of Chemistry: Departmental NMR Service (DS) & NMR Research (R) Units

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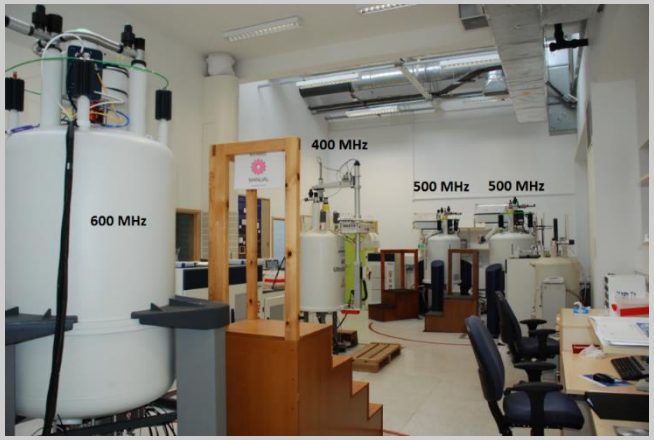

- 6 Bruker instruments with AV III (3x HD) consoles, 5 cryoprobes, 5 sample changers.
- 4 instruments in Departmental Service (24/7), 2 instruments in research units.
- 2.08 members of stuff (PI, NMR manager & technician).
- About 250 active users and 60,000 samples run on yearly basis.
- Most of the samples is synthetic chemistry. The rest are natural products and biochemistry.
- Departmental Service spectrometers operate predominantly in automation (about 85-90%).
- Data are archived in searchable format (string search) on NMR web based Server and on UoE managed Data Store. Processing/viewing: J-Viewer (Gary Sharman), Mnova - site lic., Topspin.
- We apply FEC charges per hour of sp. time (DS: £14.14 & R: £18.11) although majority of the grants is charged by flat fee of £2.20 (400 RT probe); £4.50 (500's & 600 cryoprobes) both in automation & manual. Running cost of £11.14 applies to 800.
- About 15-20% of income is coming from industrial users.

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Default setup (all probes are 5 mm z-gradient):

- **AVA800** - (R) Bruker AVIII 800, 4 channels, TCI CryoProbe, **- available to share**
- **AVA600** - (DS/R) Bruker AVIII-HD 600, 4 channels, TCI-atm CryoProbe, SampleXpress Lite
- **AVA500** - (DS) Bruker AVIII 500, DCH-atm CryoProbe, SampleXpress
- **PRO500** - (DS) Bruker AVIII-HD 500, BBO-atm CryoProbe Prodigy, SampleXpress, high VT
- **AVA400** - (DS) Bruker AVIII 400, BBFO$^+$-atm, BACS (60 positions), high/low VT,
- **GLJ400** - (R-GLJ) Bruker AVIII-HD 400, 2.5 channels, BBO-atm CryoProbe Prodigy, BCU-II, SampleXpress, high VT, CryoFit - flow conversion system
- **NMReady-60E** Nanalysis benchtop ^{1}H teaching & showcase spectrometer

Additional RT probes and CryoProbe (available to share):

- 5 mm z-gradient: 800: TXI, TBI, BBO; **600: TXI CryoProbe**, TXI, TXI-xyz-grad., BBO, HRMAS; 500: TXI, TBI, BBO, 10 mm BBO, 400: BBO

Unusual capabilities (available to share):

- AVA400 (ongoing upgrade): complete 3 channels system, two receivers, triple resonance (TBO-X,FH)-atm probe, nitrogen evaporator, shim gas cooling/heating.

Planned upgrades:

- Nomad (St-Andrew) - data archiving / searching - utilising Data Store.
- Helium Gas Recovery - CCC (Central Compressor Consultants Ltd) in collaboration with BOC

Scottish NMR User Group - SNUG

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SNUG – an association of Scottish NMR laboratories set up in 2015 to facilitate:

- access to NMR instrumentation for academic and industrial users
- sharing of resources - hardware & expertise
- application for funds to maintain our first-class instrumentation
- educational activities for academia and industry
- outreach and high school activities.

http://www.snug.ac.uk/ - under construction,

- will list of our resources and will consists of public and private pages.
- 1st SNUG meeting at Loch Tay, August, 2015
- 2nd SNUG meeting at Loch Tay, August 31st, 2016

SNUG NMR Facilities

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All NMR laboratories in Scotland

Beatson Institute Glasgow CRUK research: 600 - 1x, 400 -1x (Agilent); CP - 1x

Heriot-Watt University, Institute of Chemical Sciences: 400 - 2x, 300 - 1x

University of Aberdeen, Department of Chemistry, Marine Biodiscovery Centre:
600 -1x, 400 - 1x, 300 - 1x; CP - 1x

University of Dundee, Drug Discovery Unit: 500 - 2x, 400 - 1x, CP - 1x **500 CPQCI-F-atm**

University of Edinburgh, School of Chemistry, School of Biol. Sciences, School of Physics:
800 - 1x, 600 - 1x, 500 - 2x, 400 - 3x(1SS); CP - 5x: **500 CPDCH-atm** & **800 CPTCI-atm**

University of Glasgow, School of Chemistry, Institute of Molecular, Cell and Systems Biology:
600 - 2x, 500 - 1x, 400 - 3x; CP - 2x

University of St Andrews, School of Chemistry, School of Biology:
700 -1x, 600 - 1x(SS), 500 - 2x, 400 - 3x(1SS), 300 - 1x; CP - 2x; RT - **(TBO-X,FH)-atm**

University of Strathclyde, Department of Pure and Applied Chemistry:
600 - 1x, 500 - 1x, 400 - 3x; CP - 1x

Totalling 37 NMR spectrometers: 800-1x, 700-1x, 600-7x(1SS), 500-8x, 400-17x(2SS), 300-3x;
13 CryoProbes - 7 Helium cooled CP + 6 Prodigy CP.