

Brandt, SD, Kavanagh, PV, Westphal, F, Stratford, A, Elliott, SP, Dowling, G, Wallach, J and Halberstadt, AL

Return of the lysergamides. Part V: Analytical and behavioural characterization of 1-butanoyl-d-lysergic acid diethylamide (1B-LSD)

<http://researchonline.ljmu.ac.uk/id/eprint/10652/>

Article

Citation (please note it is advisable to refer to the publisher's version if you intend to cite from this work)

Brandt, SD, Kavanagh, PV, Westphal, F, Stratford, A, Elliott, SP, Dowling, G, Wallach, J and Halberstadt, AL (2019) Return of the lysergamides. Part V: Analytical and behavioural characterization of 1-butanoyl-d-lysergic acid diethylamide (1B-LSD). Drug Testing and Analysis. 11 (8). pp. 1122-1133.

LJMU has developed [LJMU Research Online](http://researchonline.ljmu.ac.uk) for users to access the research output of the University more effectively. Copyright © and Moral Rights for the papers on this site are retained by the individual authors and/or other copyright owners. Users may download and/or print one copy of any article(s) in LJMU Research Online to facilitate their private study or for non-commercial research. You may not engage in further distribution of the material or use it for any profit-making activities or any commercial gain.

The version presented here may differ from the published version or from the version of the record. Please see the repository URL above for details on accessing the published version and note that access may require a subscription.

For more information please contact researchonline@ljmu.ac.uk

<http://researchonline.ljmu.ac.uk/>

Return of the lysergamides. Part V: Analytical and behavioural characterization of 1-butanoyl-*d*-lysergic acid diethylamide (1B-LSD)

Simon D. Brandt,^{a,*} Pierce V. Kavanagh,^b Folker Westphal,^c Alexander Stratford,^d Simon P. Elliott,^e Geraldine Dowling,^{b,f} Jason Wallach,^g Adam L. Halberstadt,^h

^a School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK

^b Department of Pharmacology and Therapeutics, School of Medicine, Trinity Centre for Health Sciences, St. James Hospital, Dublin 8, Ireland

^c State Bureau of Criminal Investigation Schleswig-Holstein, Section Narcotics/Toxicology, Mühlenweg 166, D-24116 Kiel, Germany

^d Synex Synthetics BV, Karveelweg 20, 6222NH, Maastricht, The Netherlands

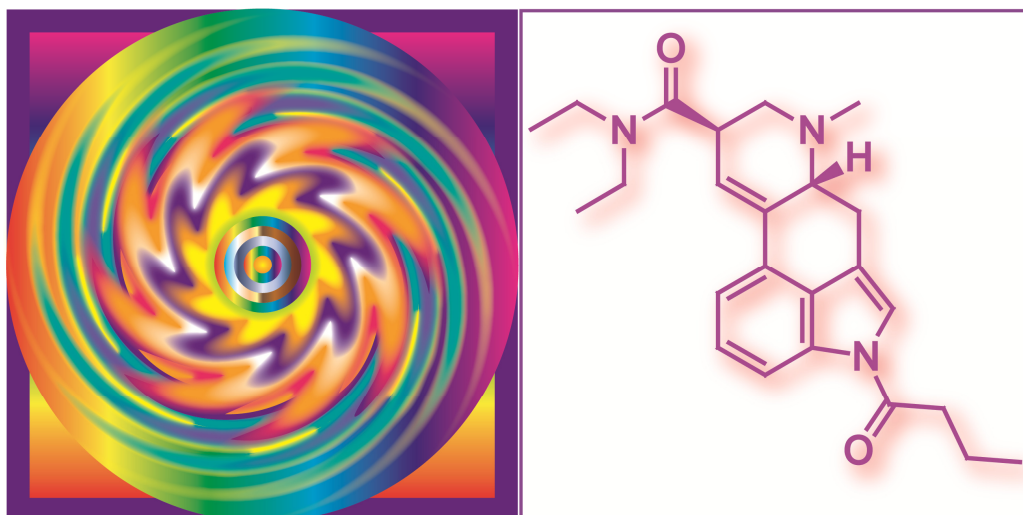
^e Elliott Forensic Consulting, Birmingham, UK

^f Department of Life Sciences, School of Science, Sligo Institute of Technology, Ash Lane, Sligo, F91YW50, Ireland

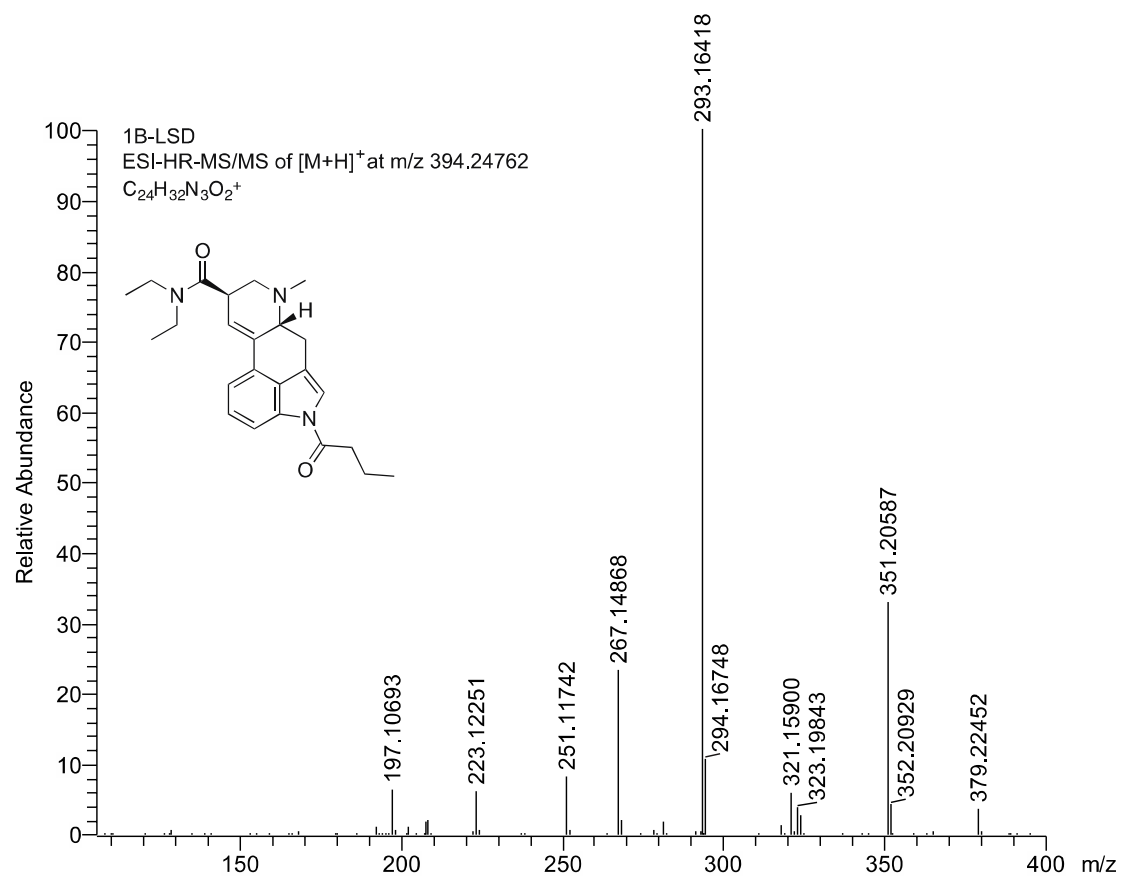
^g Department of Pharmaceutical Sciences, Philadelphia College of Pharmacy, University of the Sciences, Philadelphia, PA 19104, USA

^h Department of Psychiatry, University of California San Diego, La Jolla, CA 92093-0804, USA

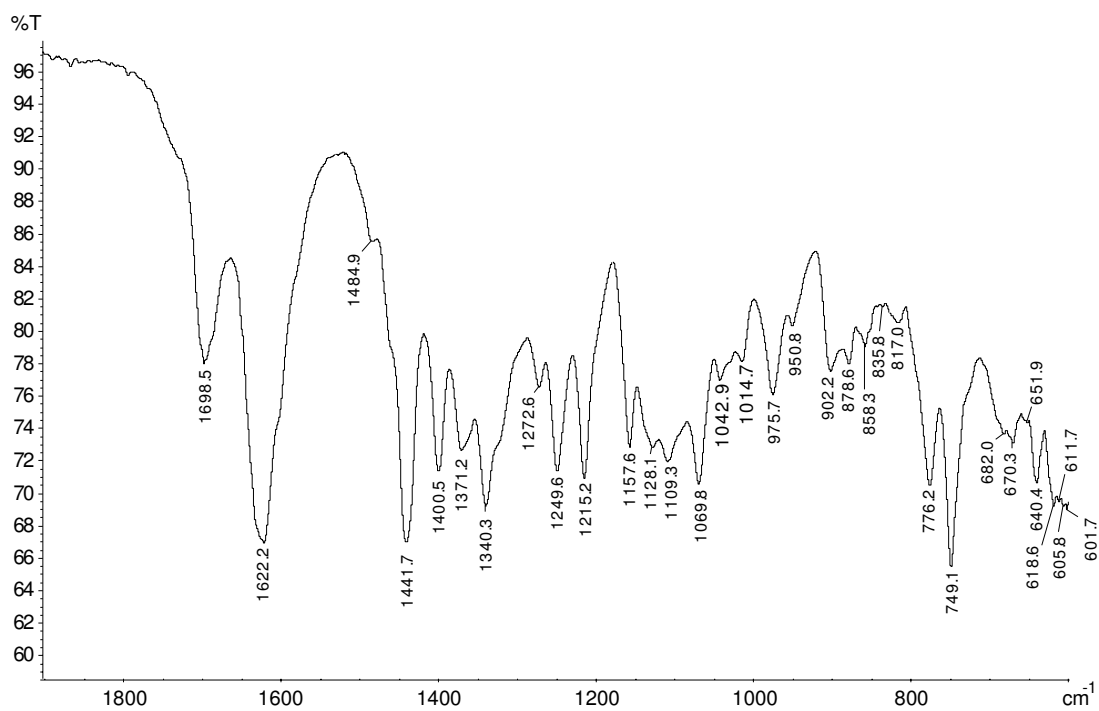
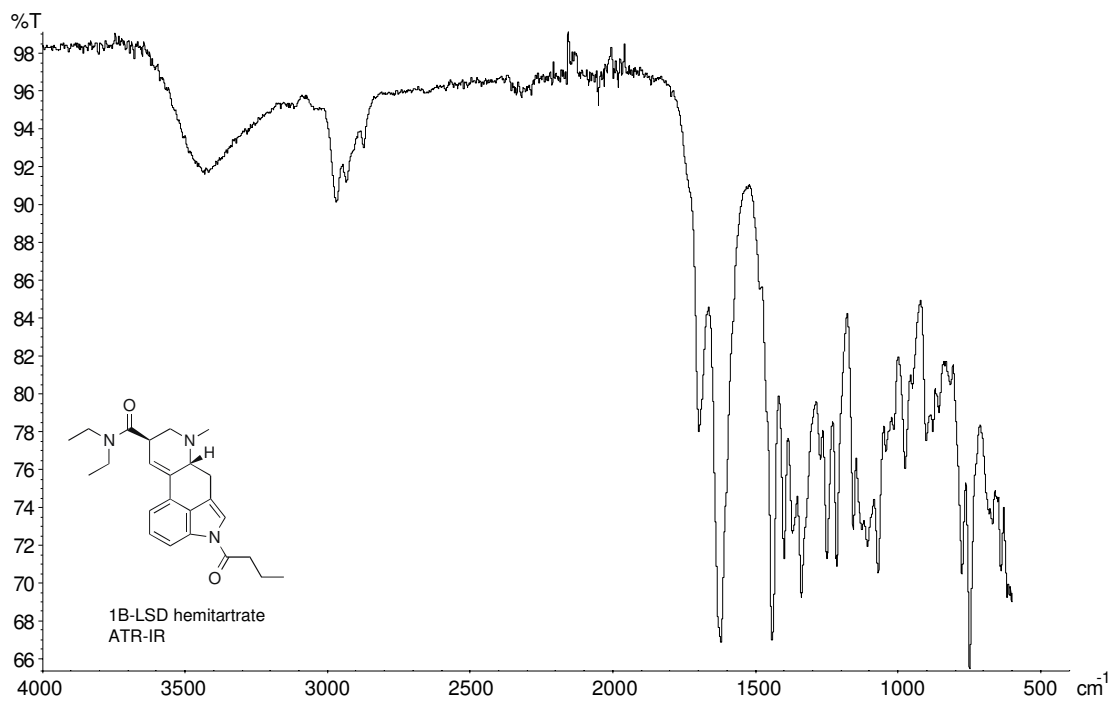
* Correspondence to: Simon D. Brandt, School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool, L3 3AF, UK. E-Mail: s.brandt@ljmu.ac.uk



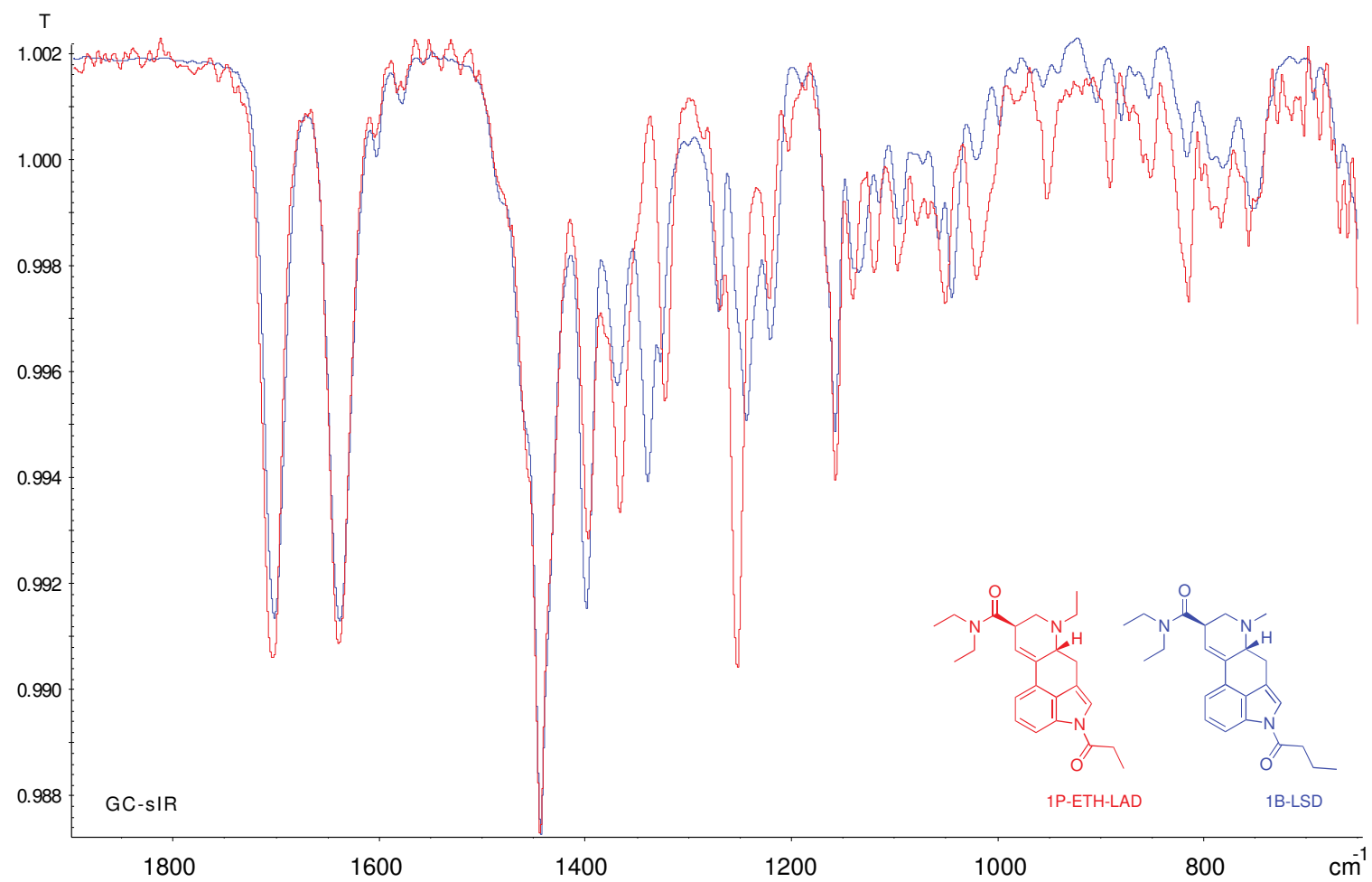
Supporting Information – Drug Testing and Analysis



Supporting Information – Drug Testing and Analysis

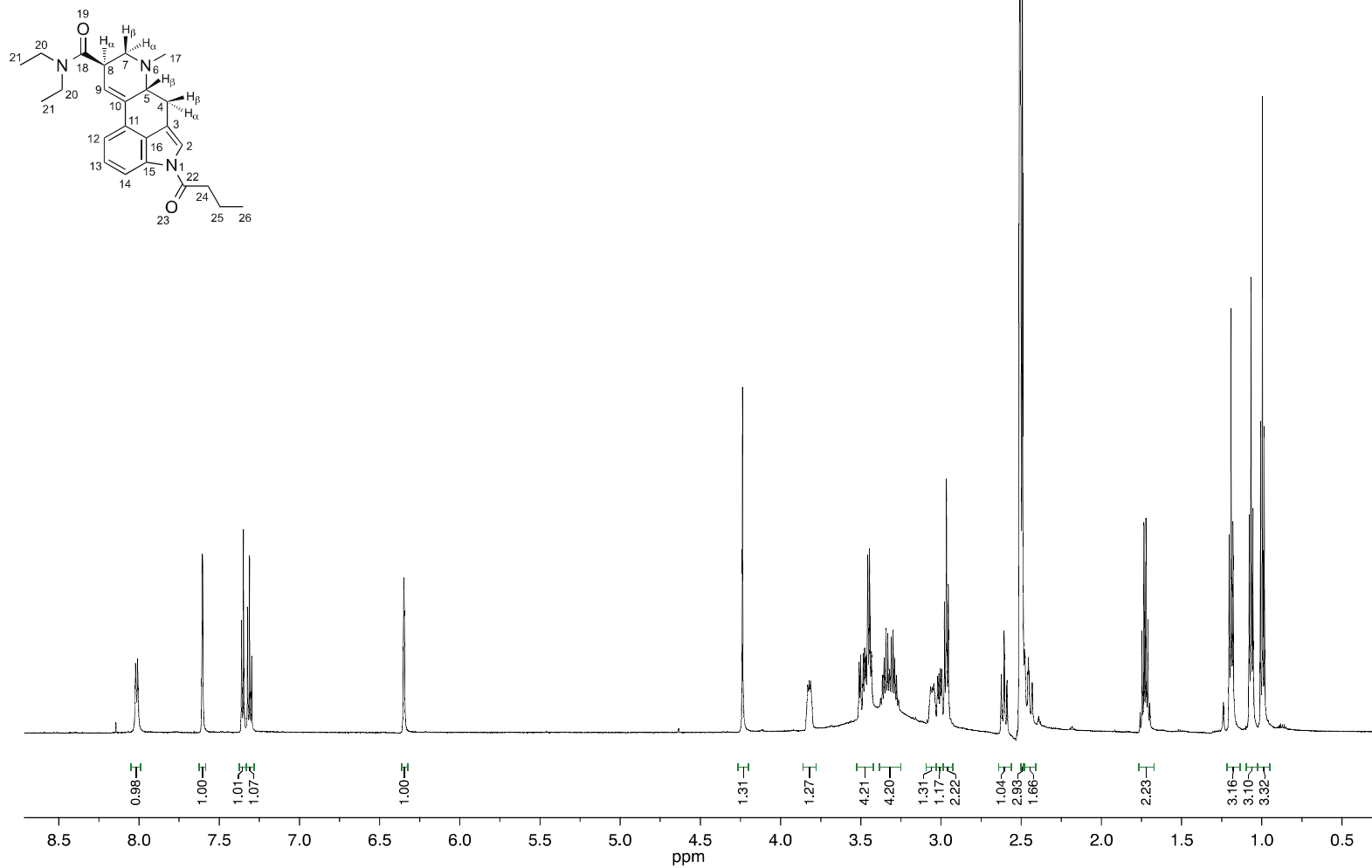


Supporting Information – Drug Testing and Analysis



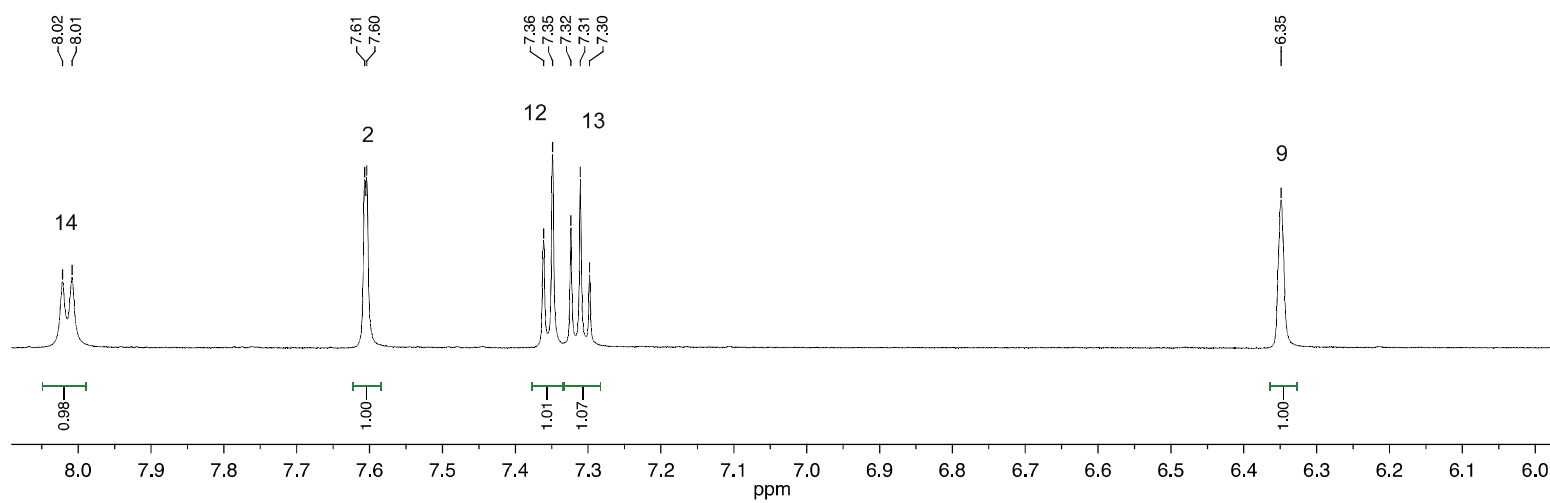
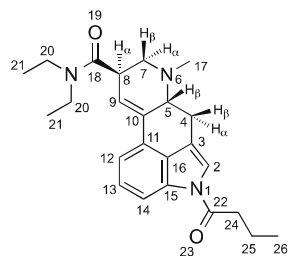
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
¹H-NMR (600 MHz)
d₆-DMSO



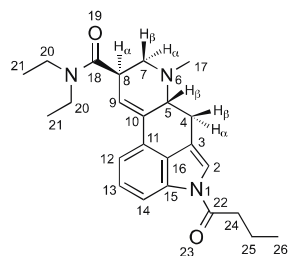
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
¹H-NMR (600 MHz)
d₆-DMSO

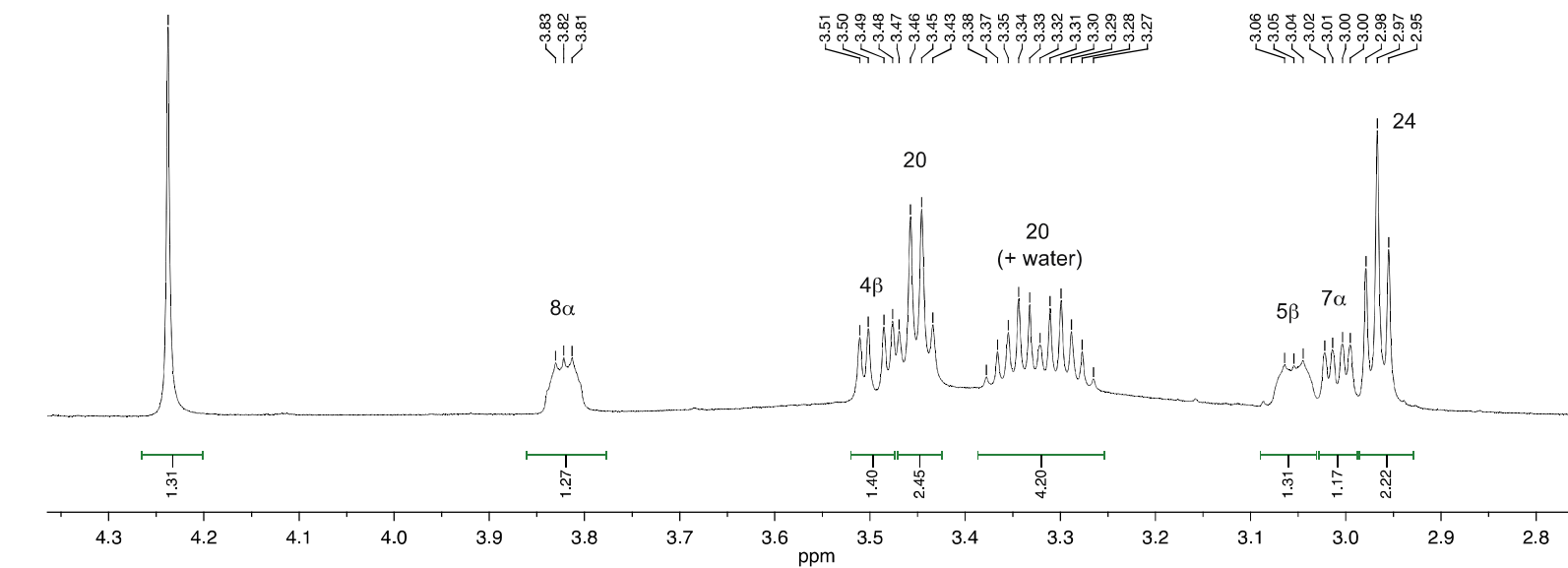


Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
¹H-NMR (600 MHz)
d₆-DMSO

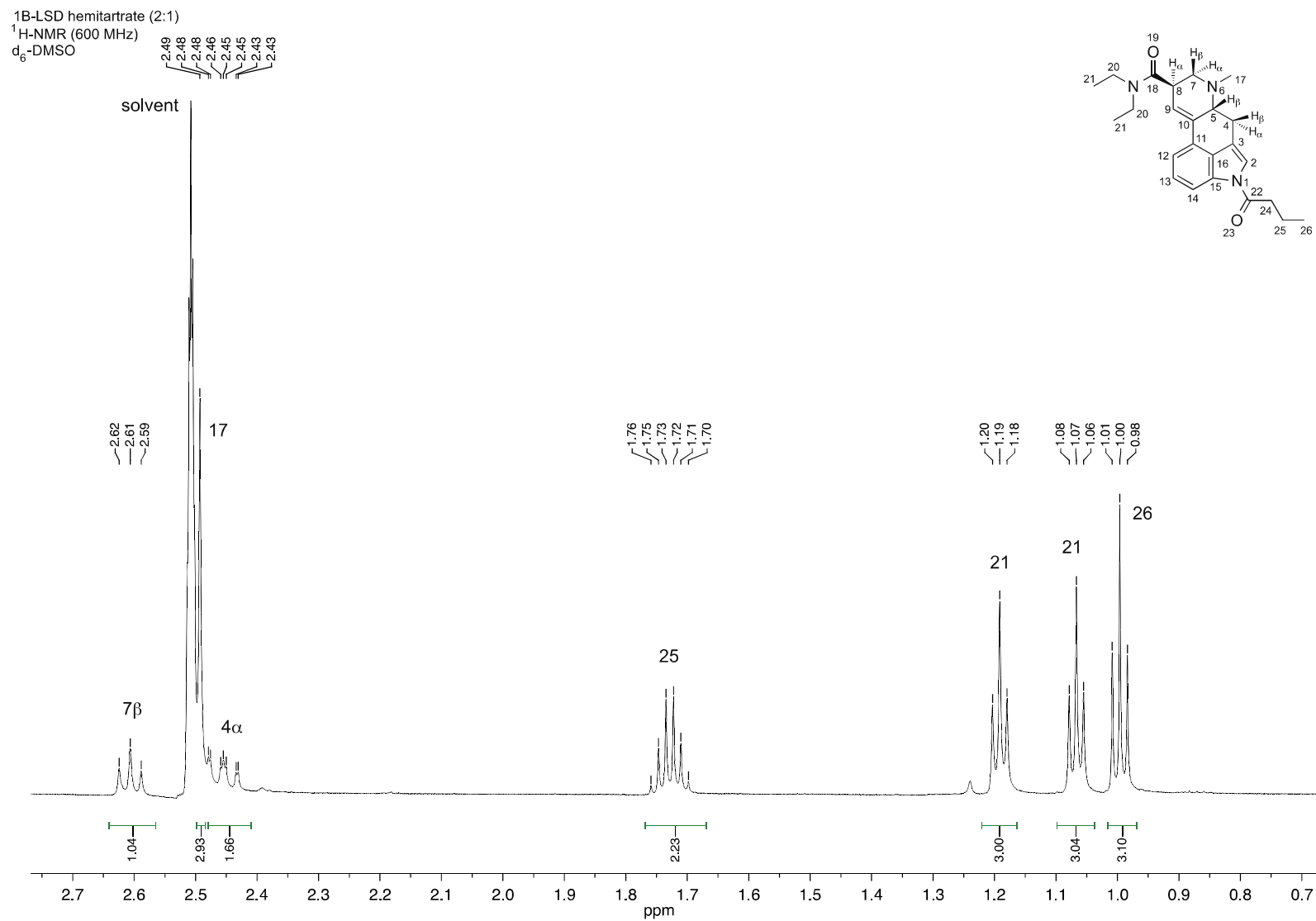


—4.24
TA



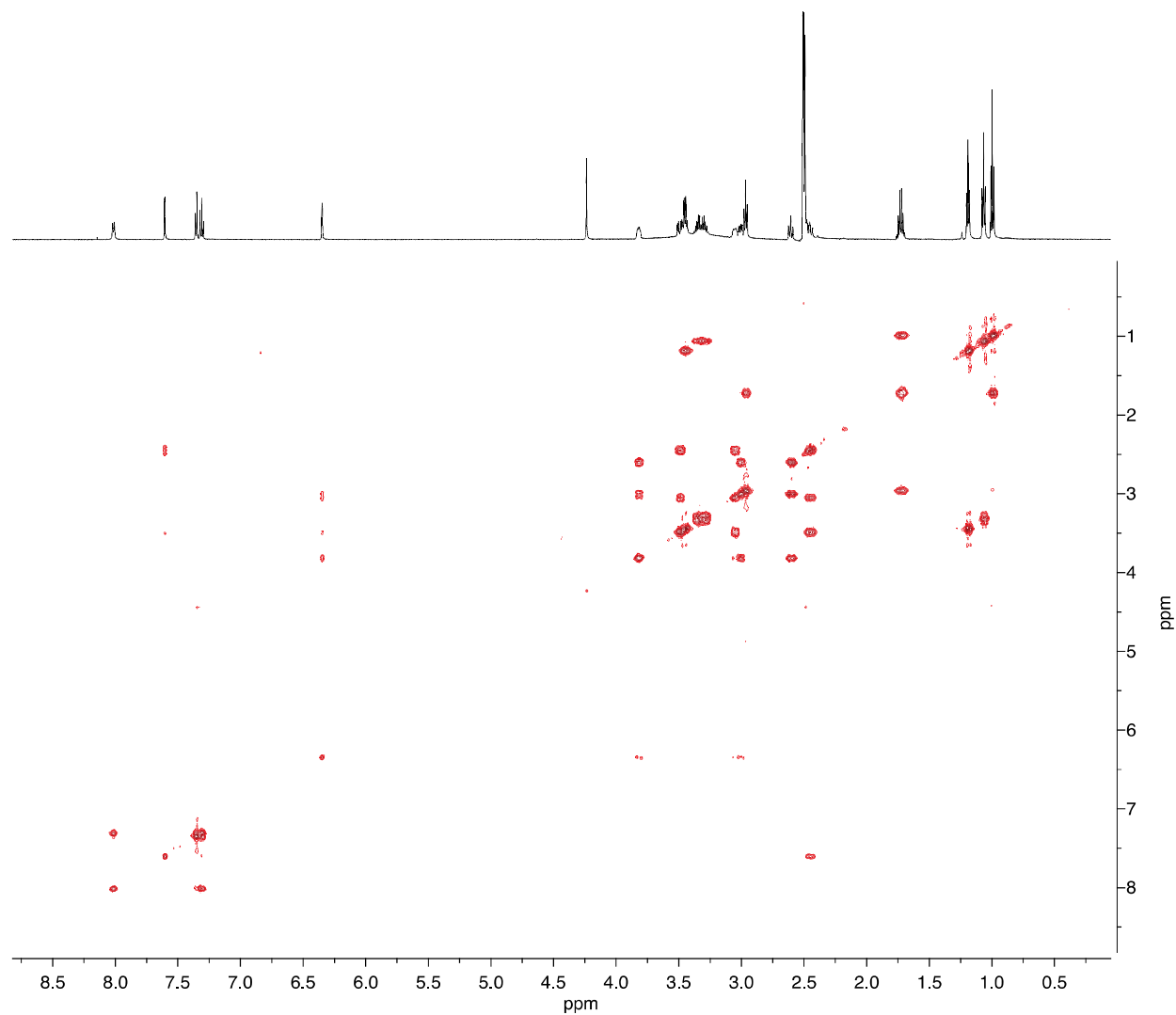
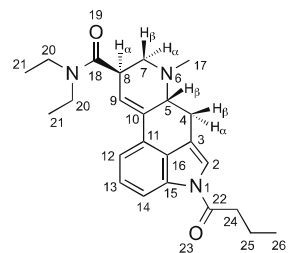
TA = Tartaric acid

Supporting Information – Drug Testing and Analysis



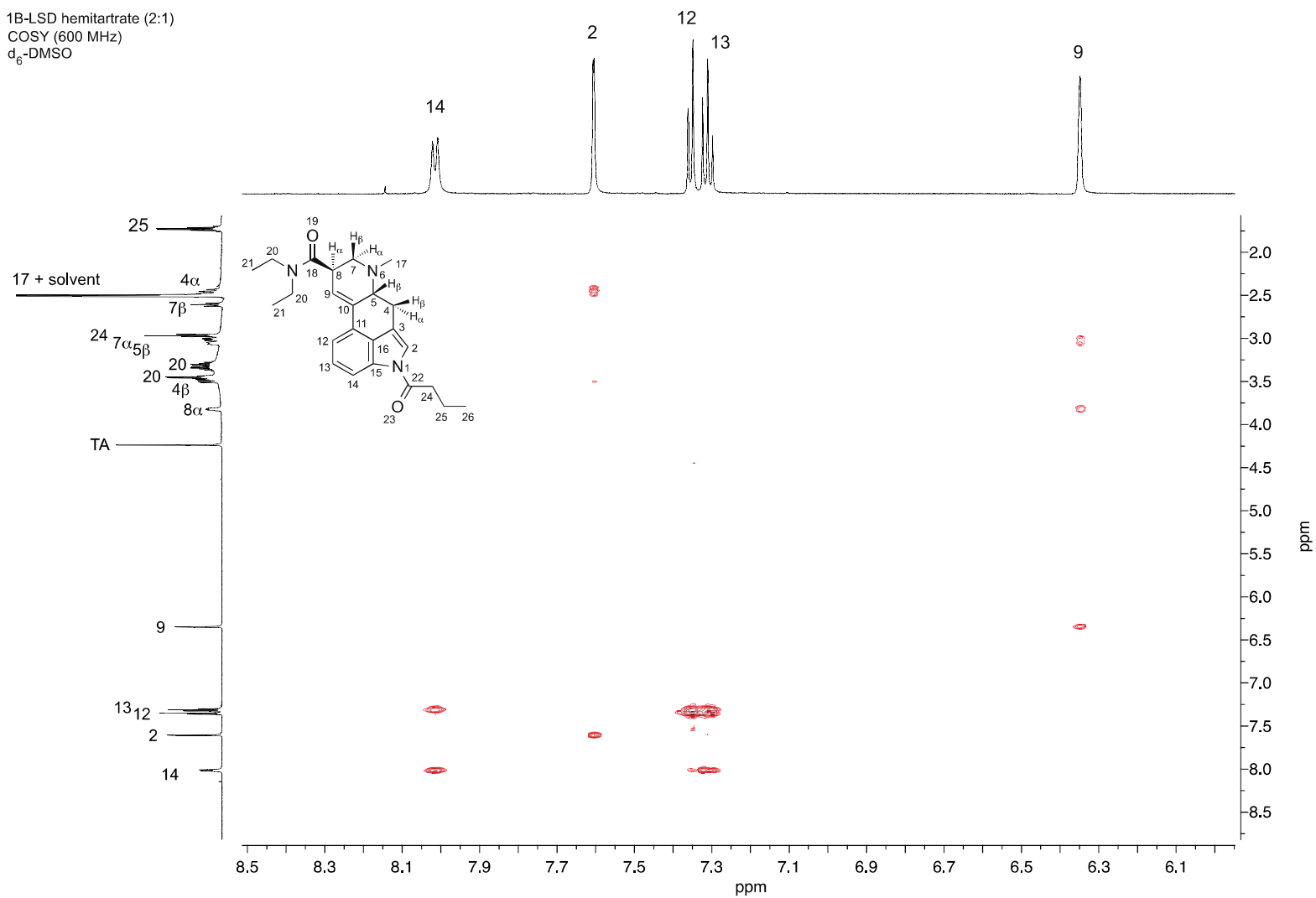
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
COSY (600 MHz)
d₆-DMSO



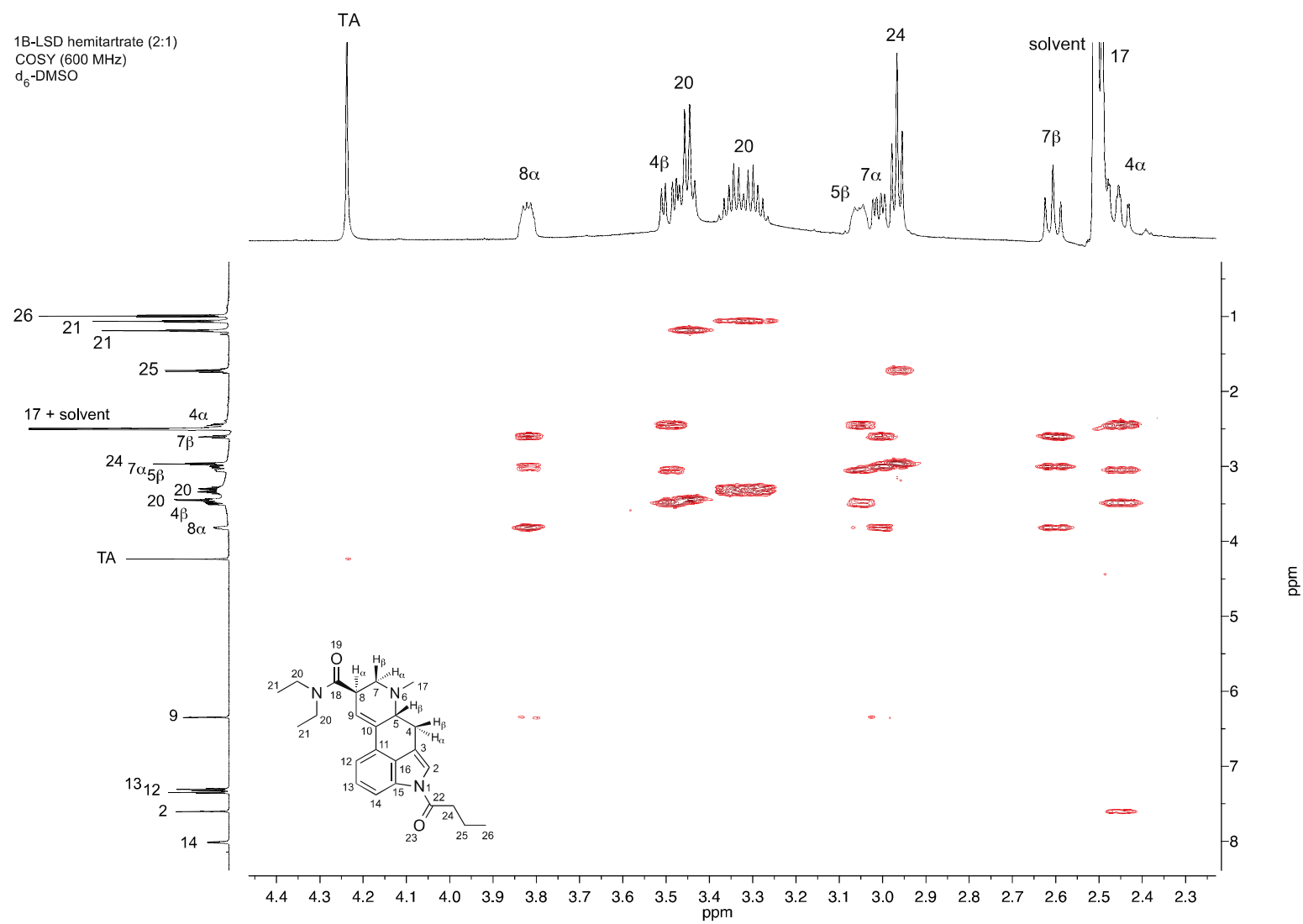
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
COSY (600 MHz)
d₆-DMSO

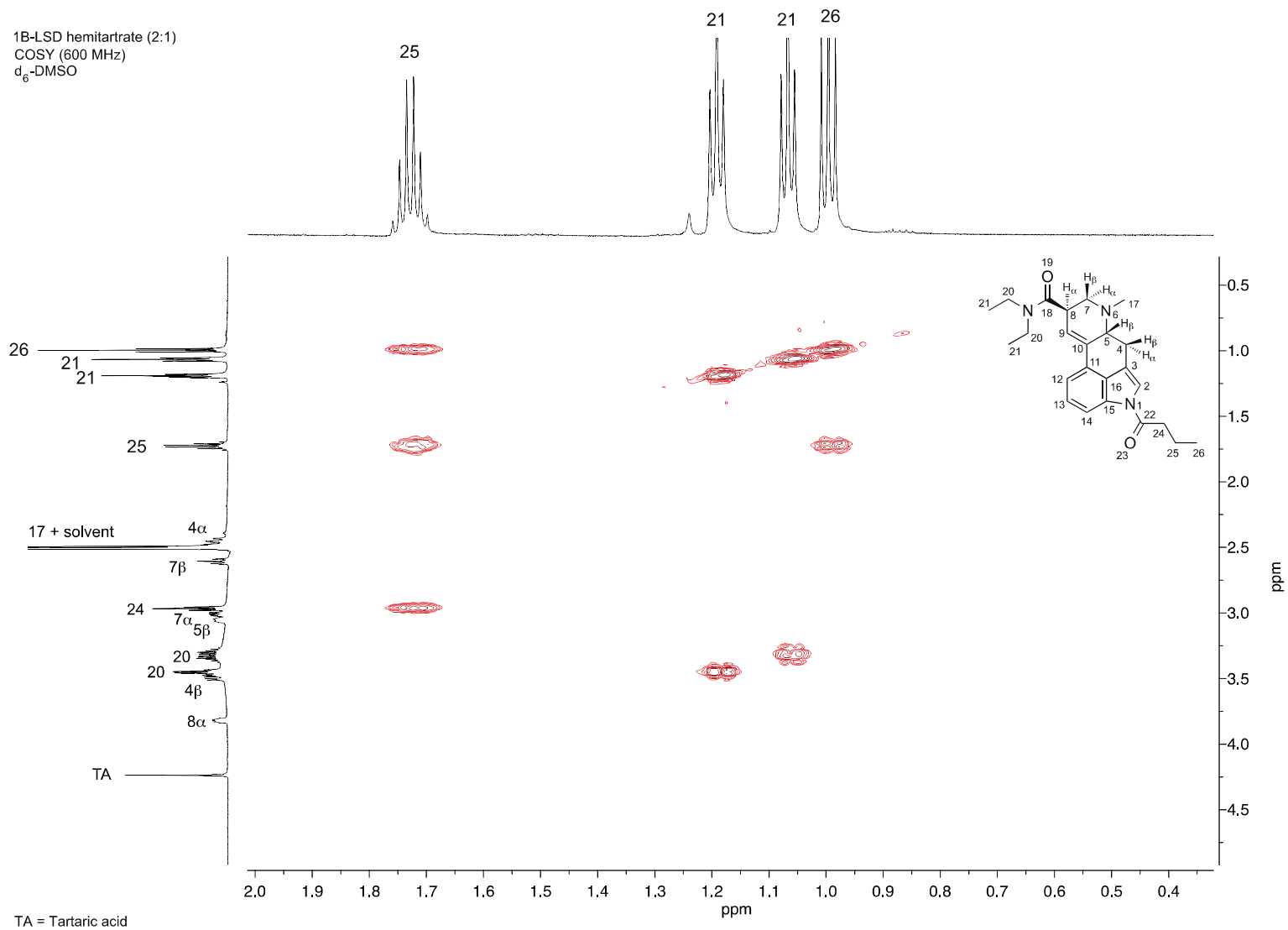


TA = Tartaric acid

Supporting Information – Drug Testing and Analysis

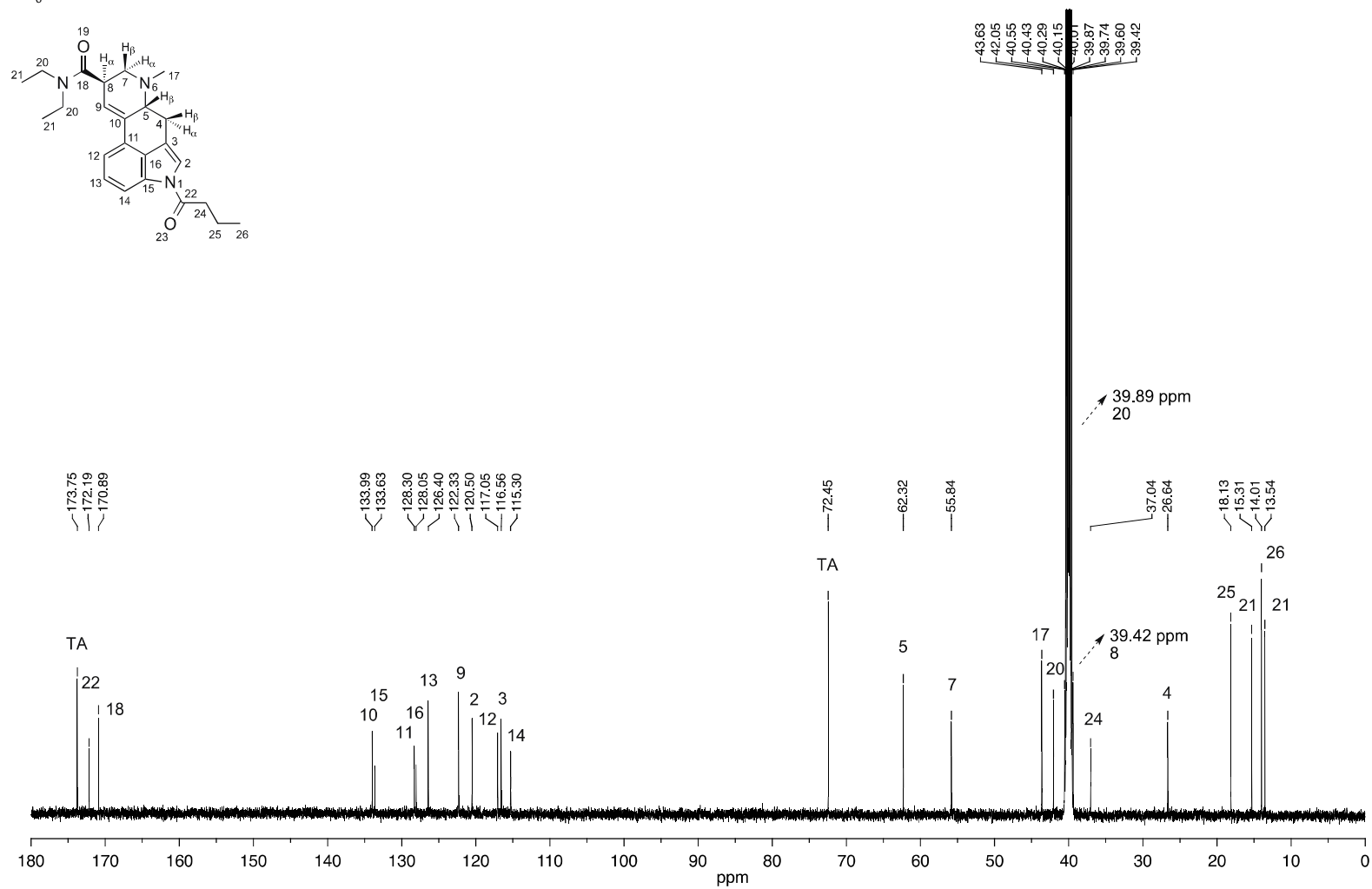


Supporting Information – Drug Testing and Analysis



Supporting Information – Drug Testing and Analysis

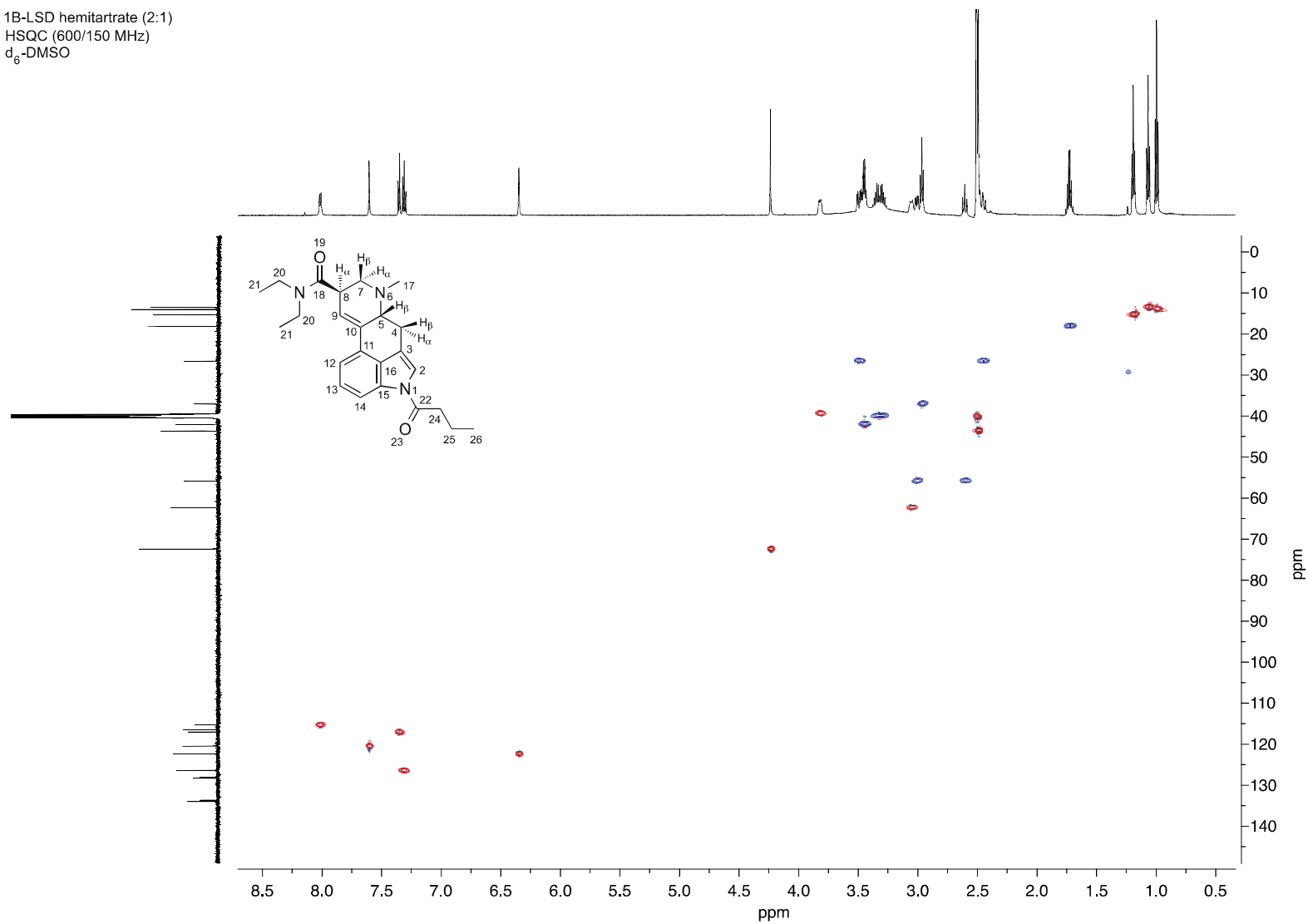
1B-LSD hemitartrate (2:1)

¹³C-NMR (150 MHz)d₆-DMSO

TA = Tartaric acid

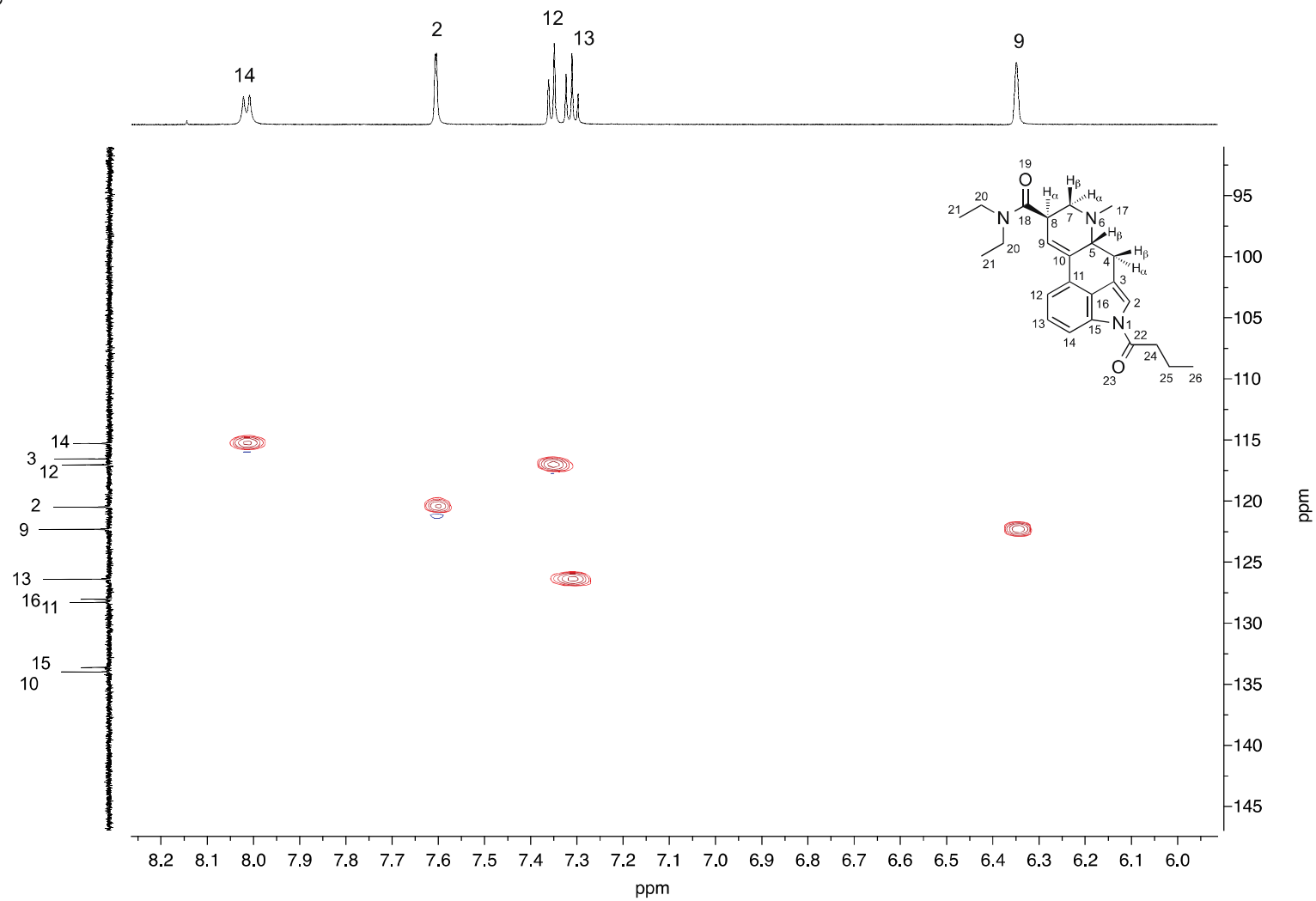
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
HSQC (600/150 MHz)
d₆-DMSO



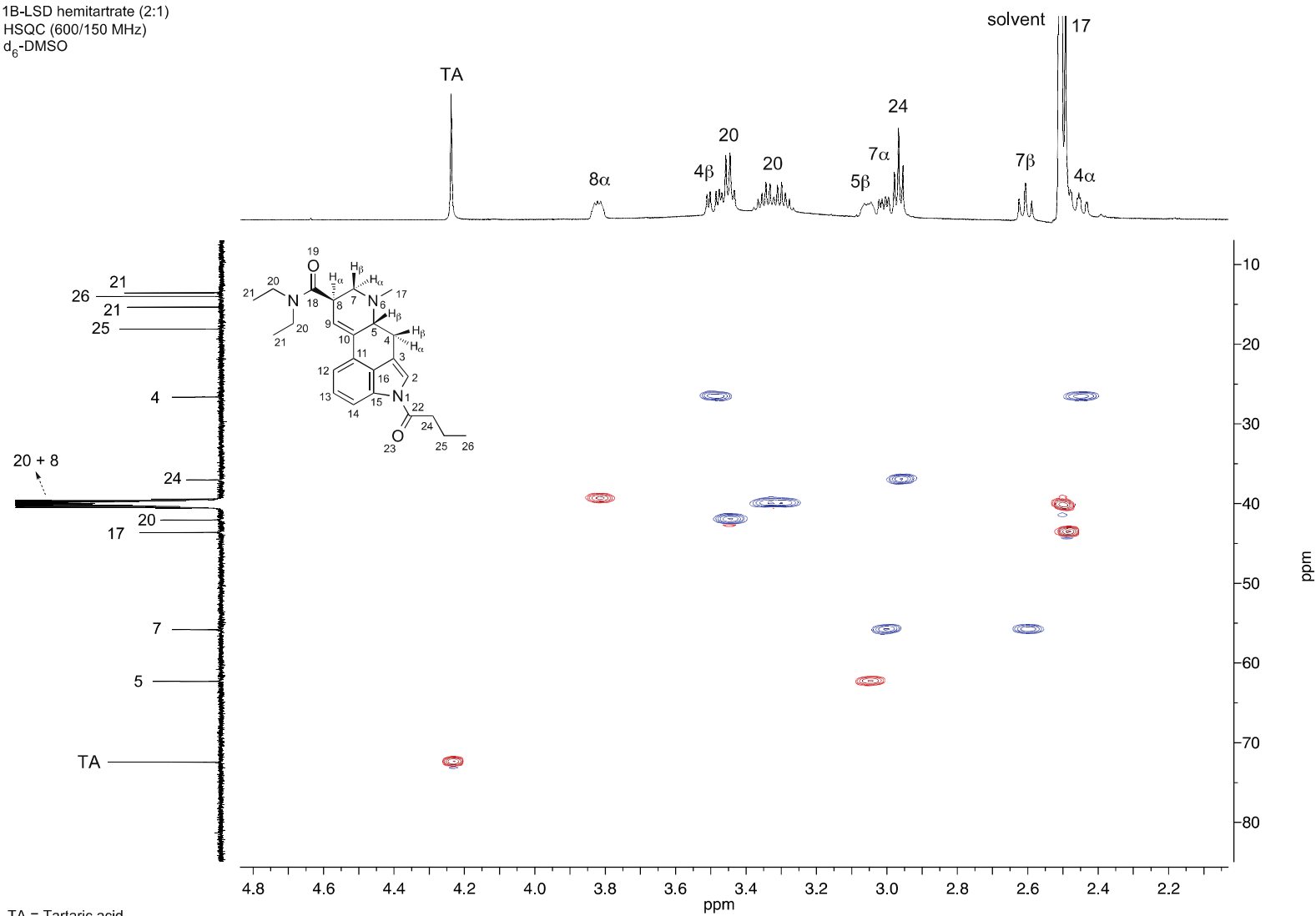
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
HSQC (600/150 MHz)
d₆-DMSO



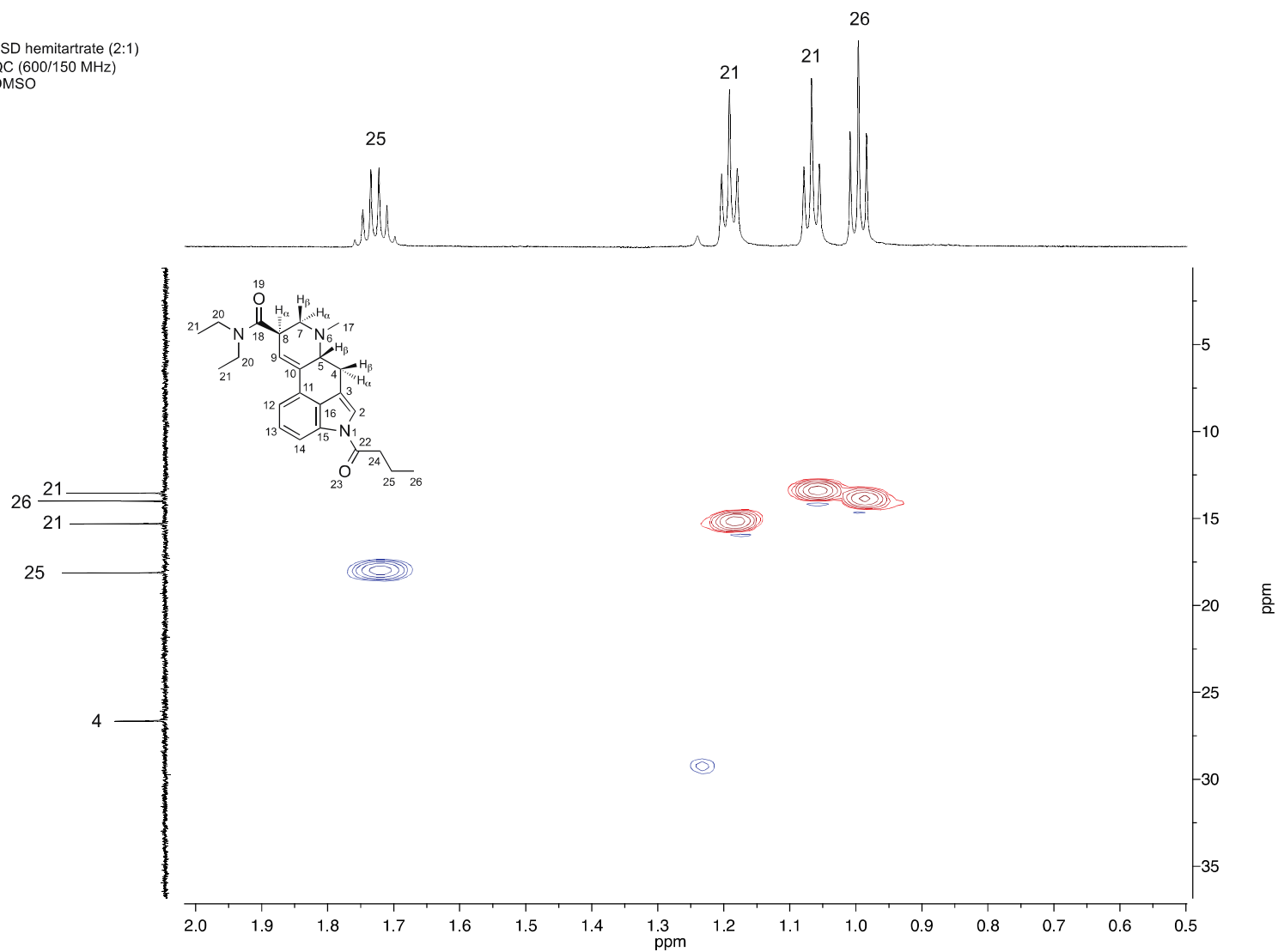
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
HSQC (600/150 MHz)
d₆-DMSO



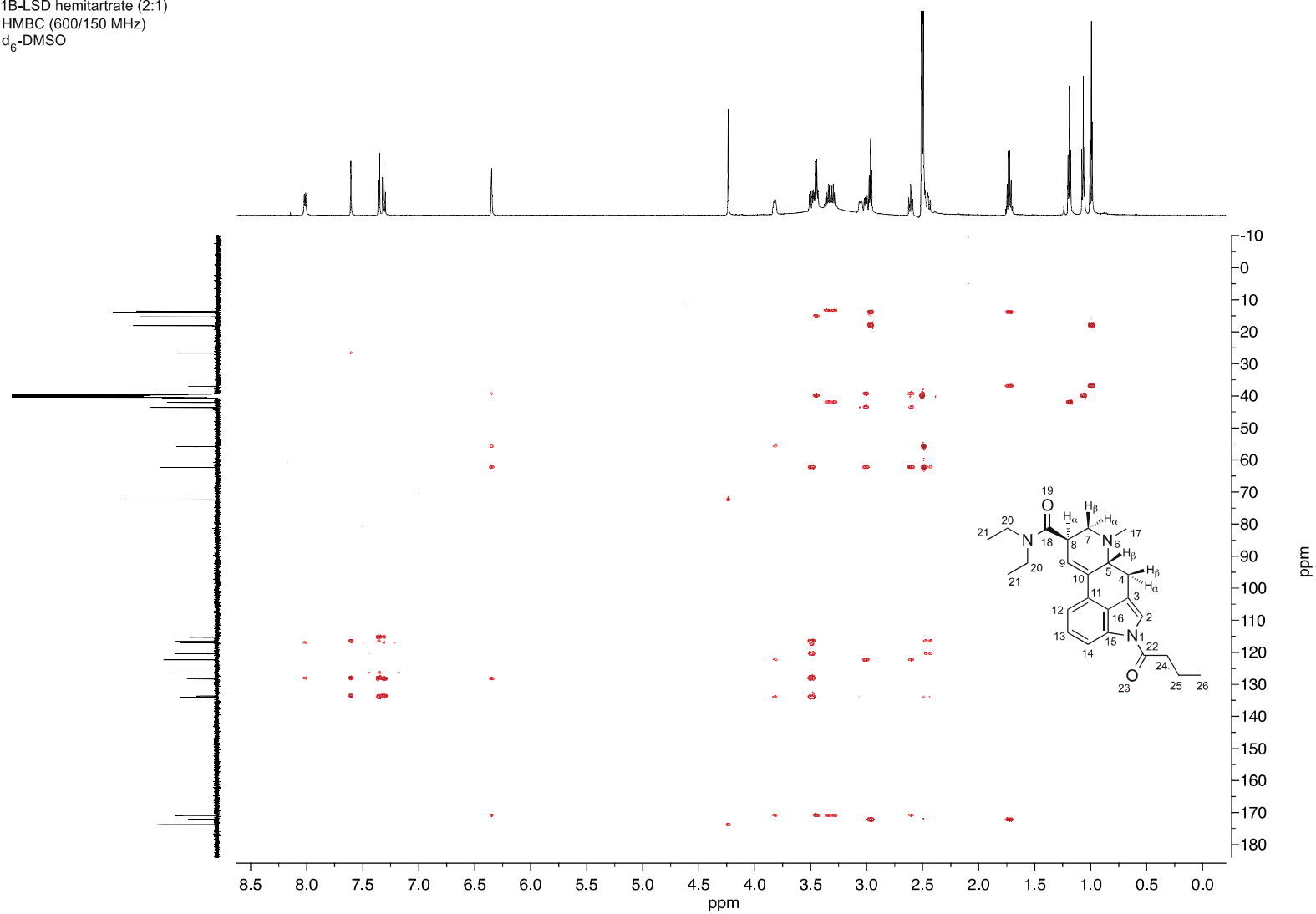
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
HSQC (600/150 MHz)
d₆-DMSO



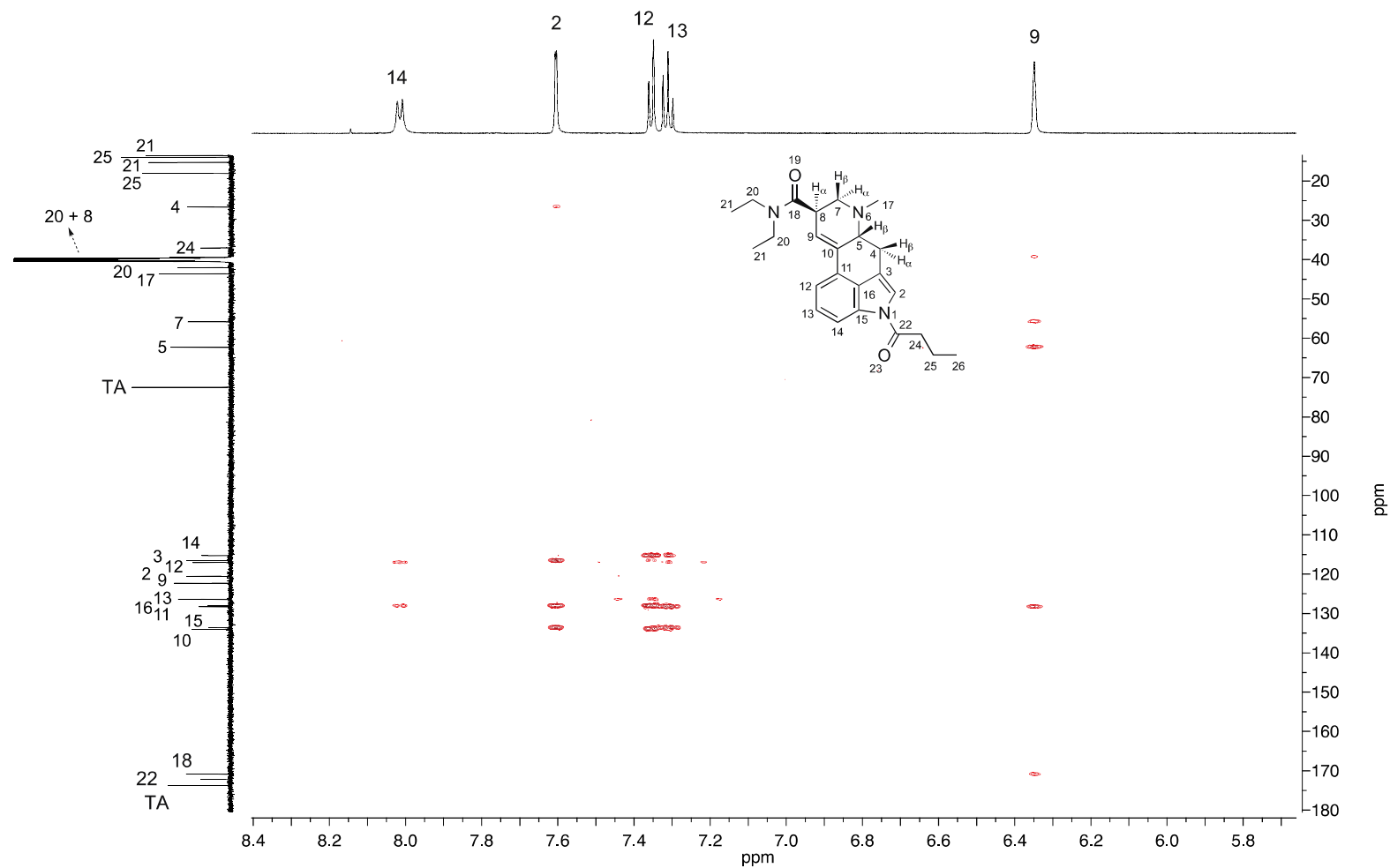
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
HMBC (600/150 MHz)
d₆-DMSO



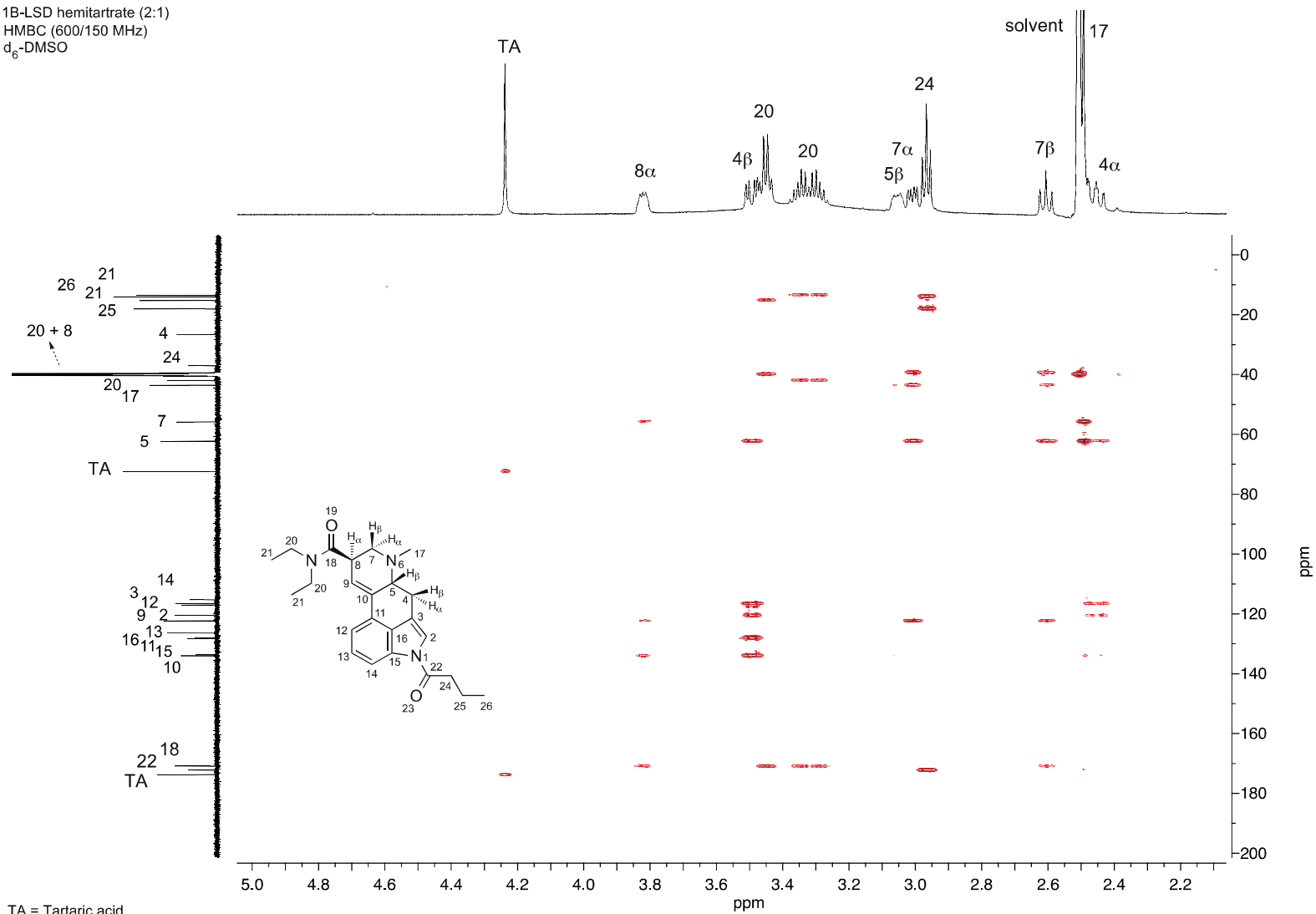
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
HMBC (600/150 MHz)
d₆-DMSO



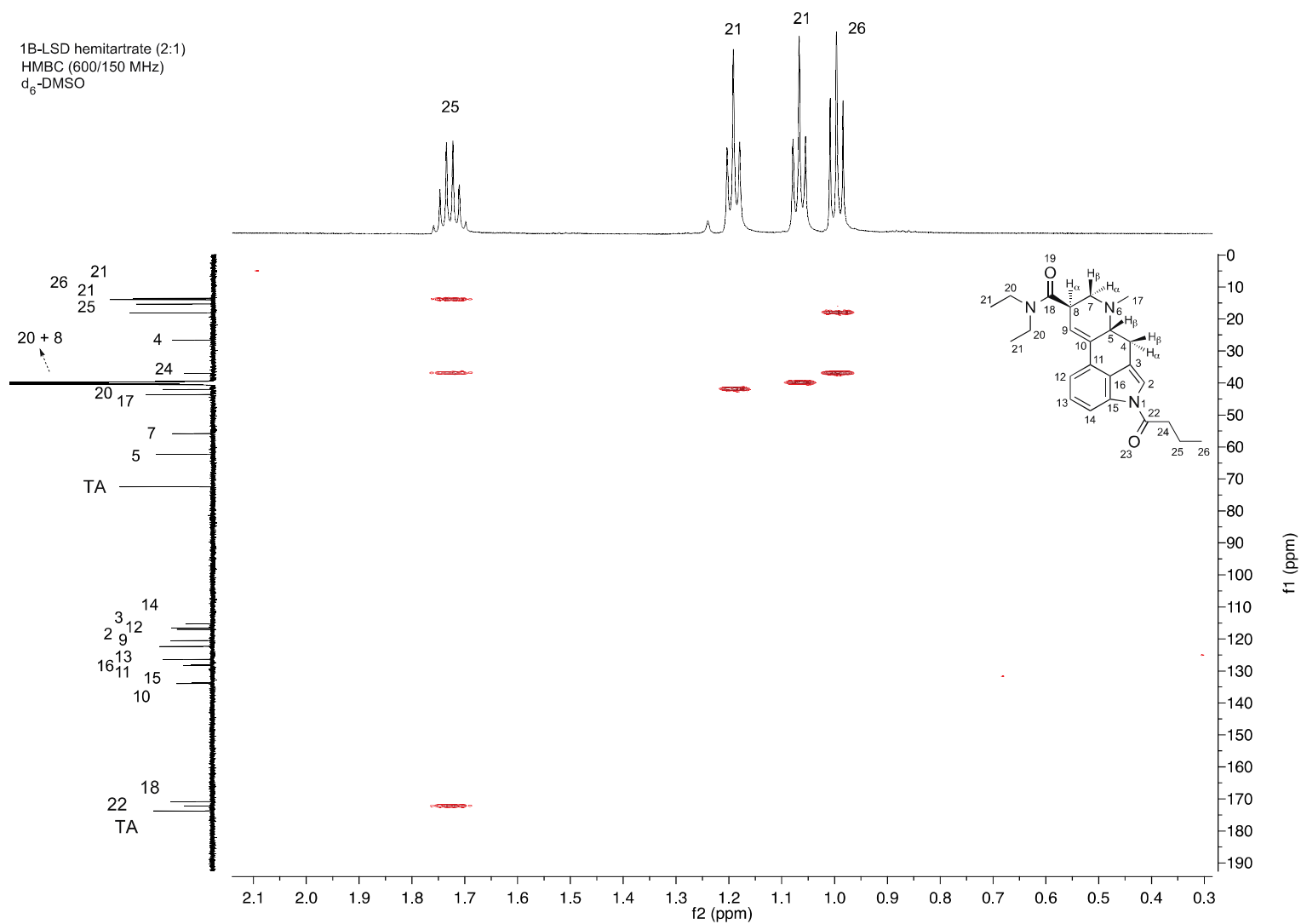
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
HMBC (600/150 MHz)
d₆-DMSO



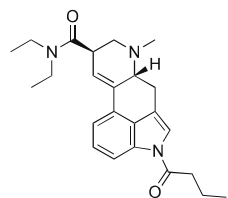
Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
HMBC (600/150 MHz)
d₆-DMSO

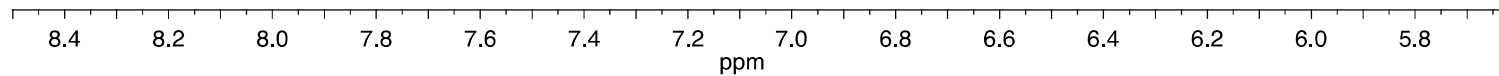
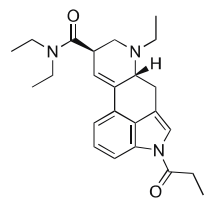


Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
¹H-NMR (600 MHz)
d₆-DMSO

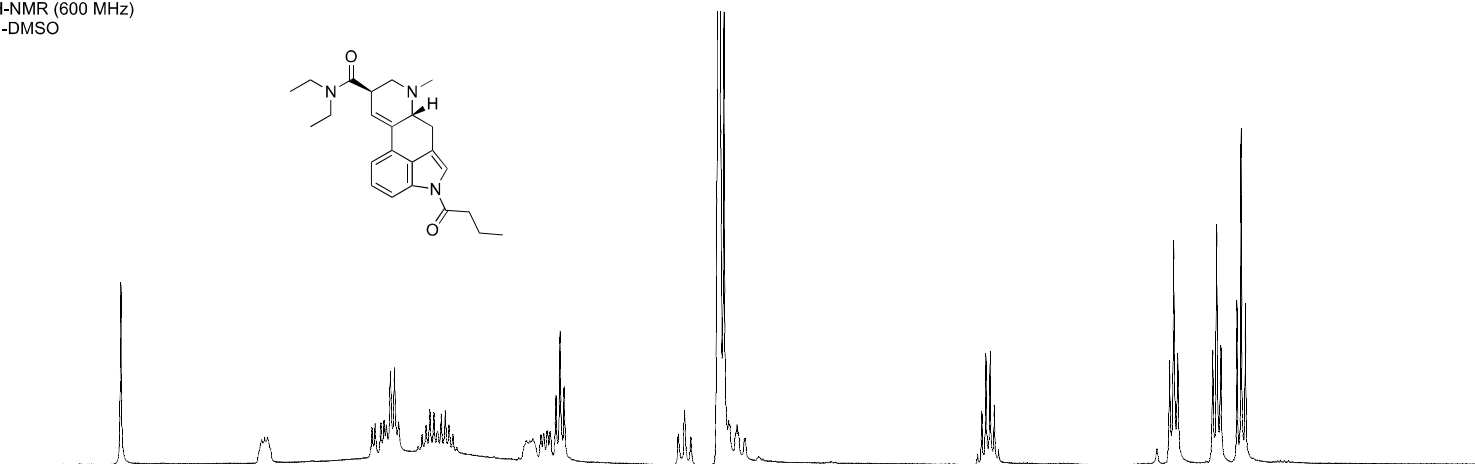
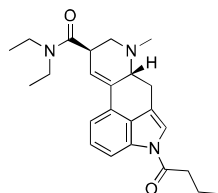


1P-ETH-LAD hemitartrate (2:1)
¹H-NMR (600 MHz)
d₆-DMSO

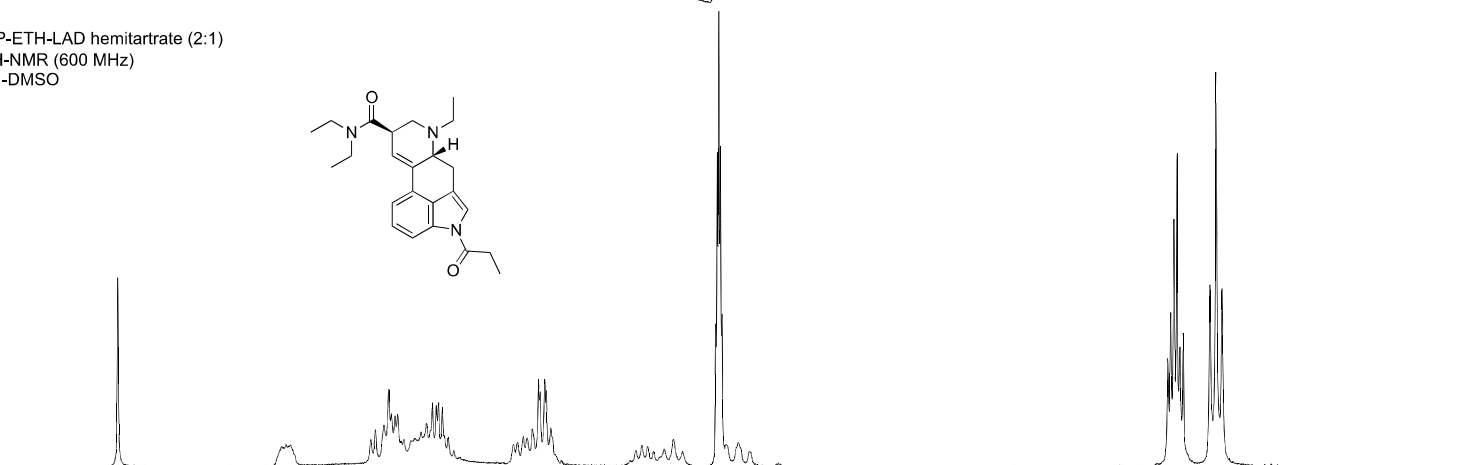
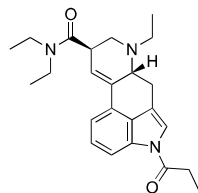


Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
¹H-NMR (600 MHz)
d₆-DMSO



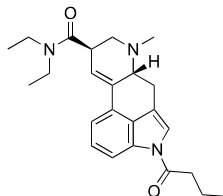
1P-ETH-LAD hemitartrate (2:1)
¹H-NMR (600 MHz)
d₆-DMSO



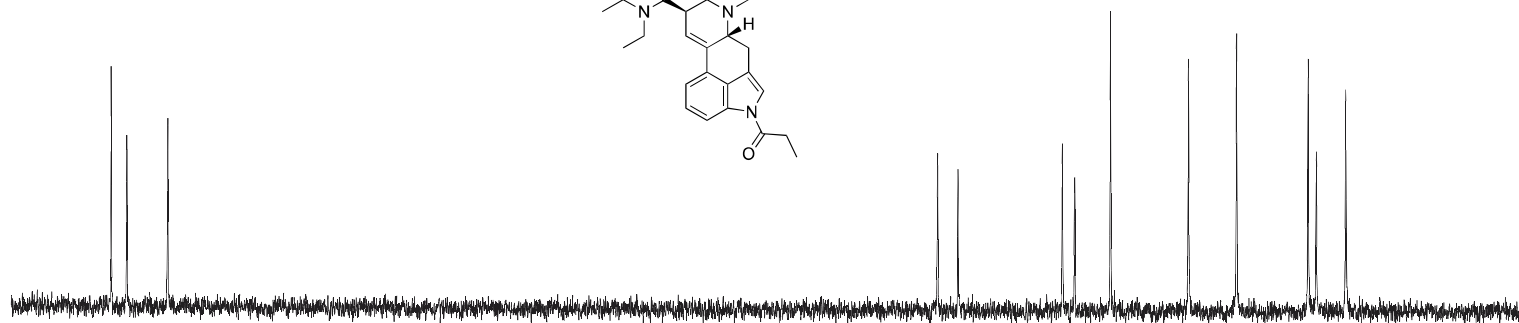
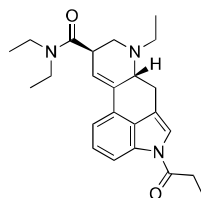
4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4
ppm

Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
¹³C-NMR (600 MHz)
d₆-DMSO



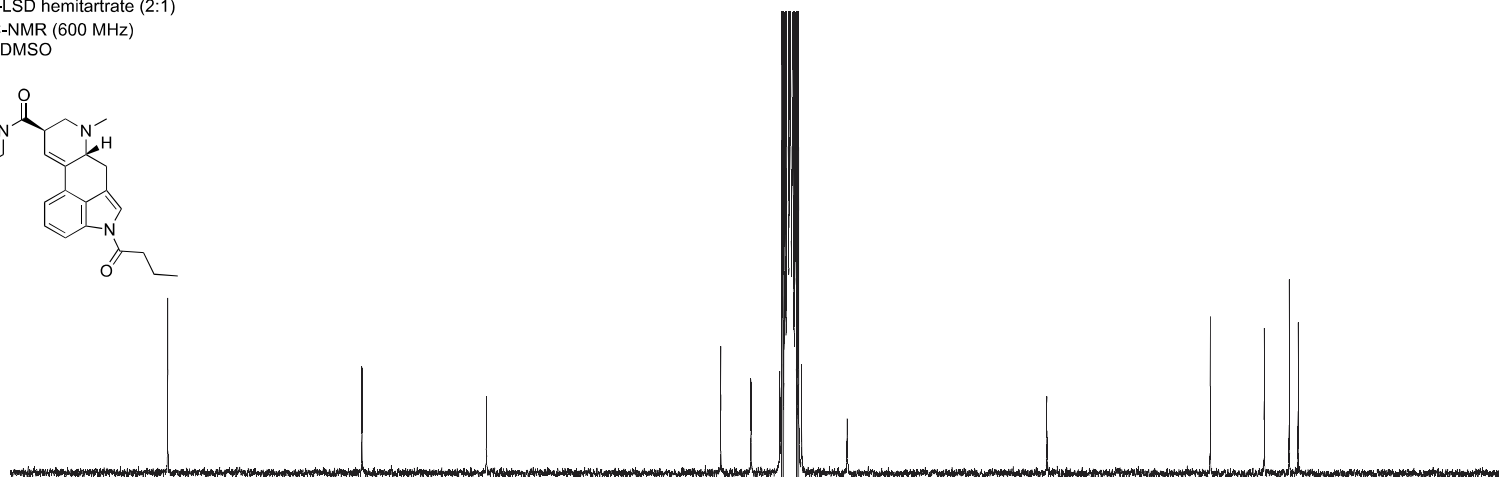
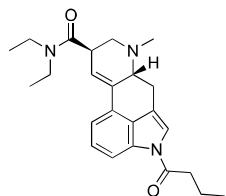
1P-ETH-LAD hemitartrate (2:1)
¹³C-NMR (600 MHz)
d₆-DMSO



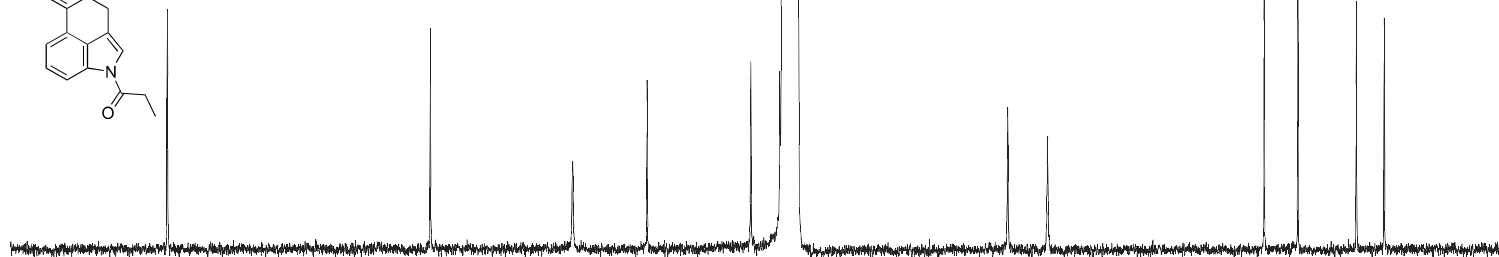
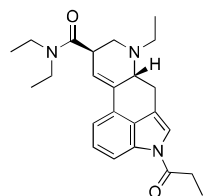
175 170 165 160 155 150 145 140 135 130 125 120 115 110
ppm

Supporting Information – Drug Testing and Analysis

1B-LSD hemitartrate (2:1)
 ^{13}C -NMR (600 MHz)
 d_6 -DMSO



1P-ETH-LAD hemitartrate (2:1)
 ^{13}C -NMR (600 MHz)
 d_6 -DMSO



80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
ppm