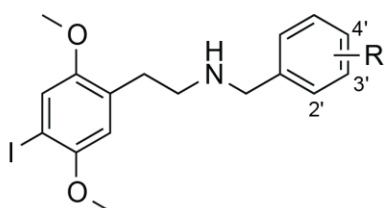
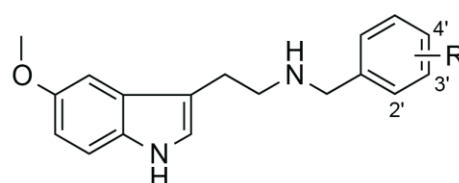


SUPPORTING INFORMATION

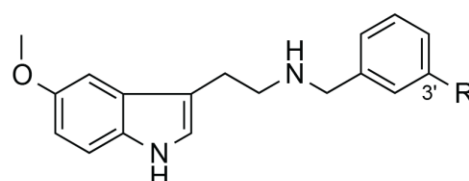
Analytical characterization of bioactive *N*-benzyl-substituted phenethylamines and 5-methoxytryptamines



- (1a): R = 2'-OCH₃ (25I-NB2OMe) - manuscript
(1b): R = 3'-OCH₃ (25I-NB3OMe) - manuscript
(1c): R = 4'-OCH₃ (25I-NB4OMe) - manuscript
(1d): R = 2'-Br (25I-NB2B) - suppl. information
(1e): R = 3'-Br (25I-NB3B) - suppl. information
(1f): R = 4'-Br (25I-NB4B) - suppl. information



- (2a): R = 2'-OCH₃ (5MT-NB2OMe) - manuscript
(2b): R = 3'-OCH₃ (5MT-NB3OMe) - manuscript
(2c): R = 4'-OCH₃ (5MT-NB4OMe) - manuscript
(2d): R = 2'-Br (5MT-NB2B) - suppl. information
(2e): R = 3'-Br (5MT-NB3B) - suppl. information
(2f): R = 4'-Br (5MT-NB4B) - suppl. information



- (3a): R = CF₃ (5MT-NB3TFM) - suppl. information
(3b): R = F (5MT-NB3F) - suppl. information
(3c): R = CH₃ (5MT-NB3Me) - suppl. information
(3d): R = Cl (5MT-NB3Cl) - suppl. information
(3e): R = I (5MT-NB3I) - suppl. information
(3f): R = SCH₃ (5MT-NB3SMe) - suppl. information

Page 3: GC/MS retention times, EI- and CI ion trap mass spectra of *N*-(methoxybenzyl)-substituted isomers (1d)–(1f) and (2d)–(2f).

Page 4: GC/MS retention times, EI- and CI ion trap mass spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (3d)–(3f).

Page 5: GC/MS chromatograms of *N*-(methoxybenzyl)-substituted phenethylamines (1a)–(1f).

Page 6: GC/MS chromatograms of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (2a)–(2f).

Page 7: GC/MS chromatograms of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3a**)–(**3f**).

Page 8: QTOF-MS accurate mass spectra and tandem mass spectra of *N*-(methoxybenzyl)-substituted phenethylamines (**1d**)–(**1f**).

Page 9: QTOF-MS accurate mass spectra and tandem mass spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**2d**)–(**2f**).

Page 10: QTOF-MS accurate mass spectra and tandem mass spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3a**)–(**3c**).

Page 11: QTOF-MS accurate mass spectra and tandem mass spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3d**)–(**3f**).

Page 12: QqQ-MS/MS of *N*-(methoxybenzyl)-substituted phenethylamines (**1d**)–(**1f**).

Page 13: QqQ-MS/MS of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**2d**)–(**2f**).

Page 14: QqQ-MS/MS of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3a**)–(**3c**).

Page 15: QqQ-MS/MS of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3d**)–(**3f**).

Page 16: LC-UV retention times and diode array full scan spectra of *N*-(methoxybenzyl)-substituted phenethylamines (**1d**)–(**1f**).

Page 17: LC-UV retention times and diode array full scan spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**2d**)–(**2f**).

Page 18: LC-UV retention times and diode array full scan spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3a**)–(**3c**).

Page 19: LC-UV retention times and diode array full scan spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3d**)–(**3f**).

Page 20: ATR-FT/IR spectra of *N*-(methoxybenzyl)-substituted phenethylamines (**1a**)–(**1c**).

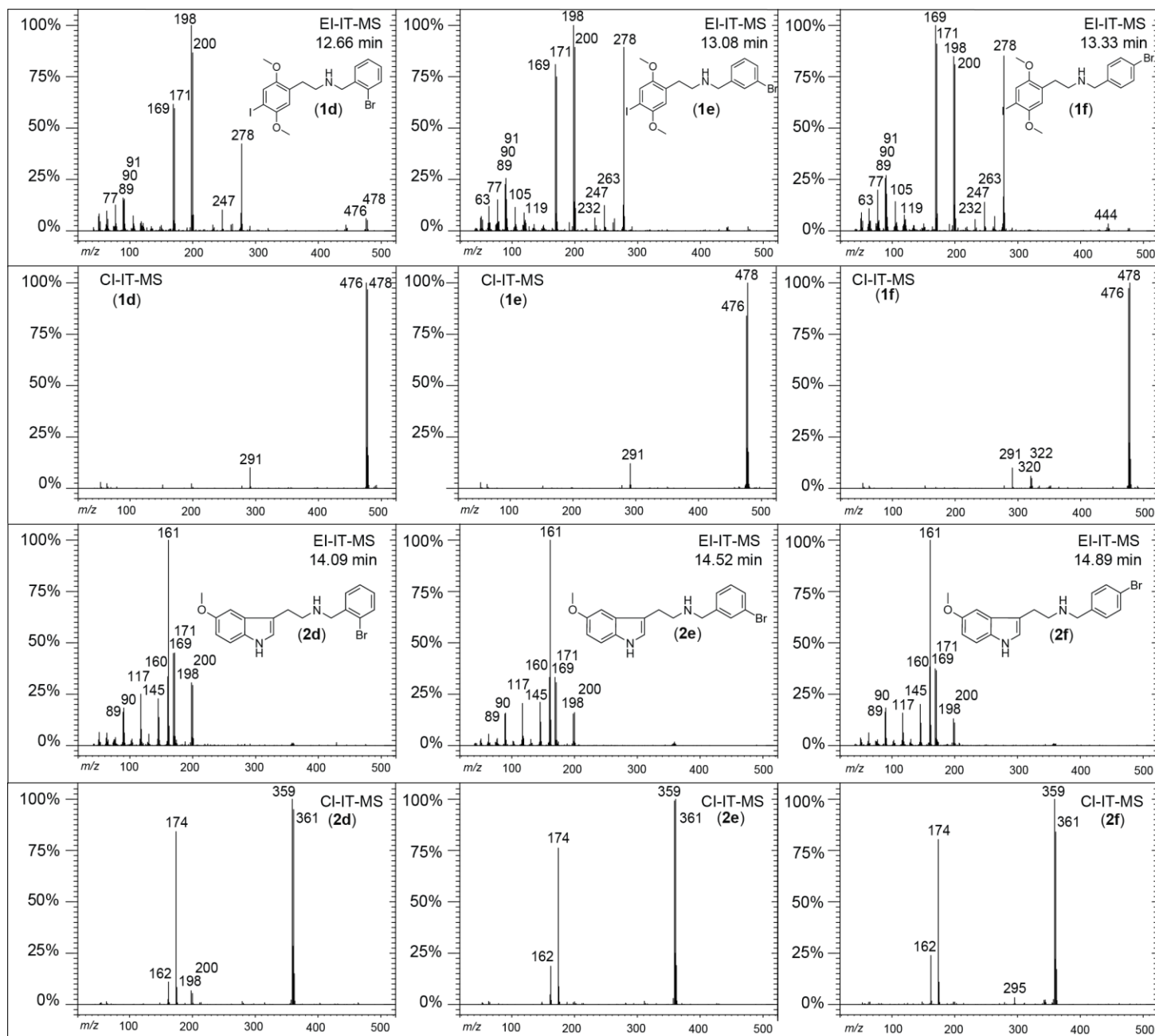
Page 21: ATR-FT/IR spectra of *N*-(methoxybenzyl)-substituted phenethylamines (**1d**)–(**1f**).

Page 22: ATR-FT/IR spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**2a**)–(**2c**).

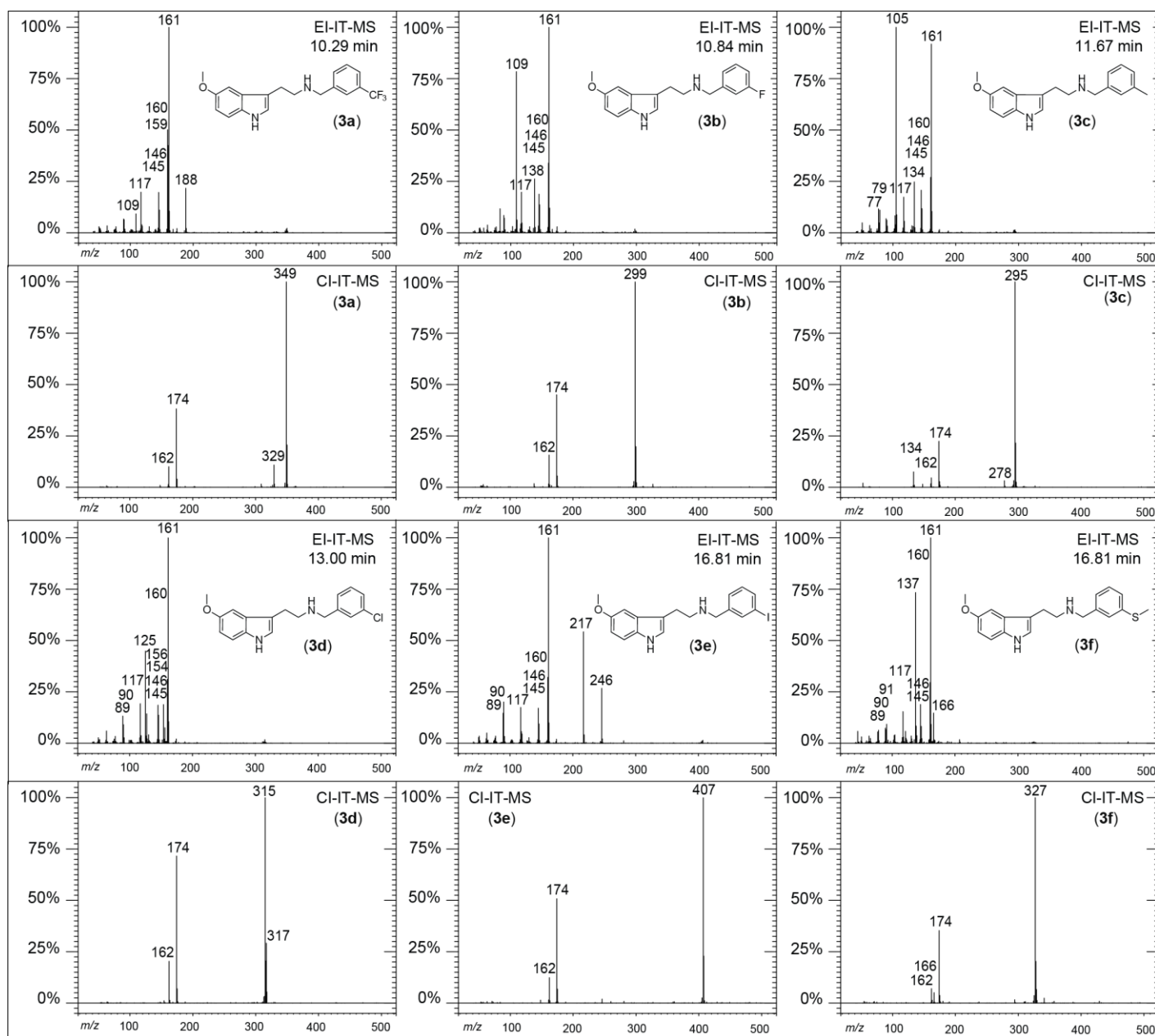
Page 23: ATR-FT/IR spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**2d**)–(**2f**).

Page 24: ATR-FT/IR spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3a**)–(**3c**).

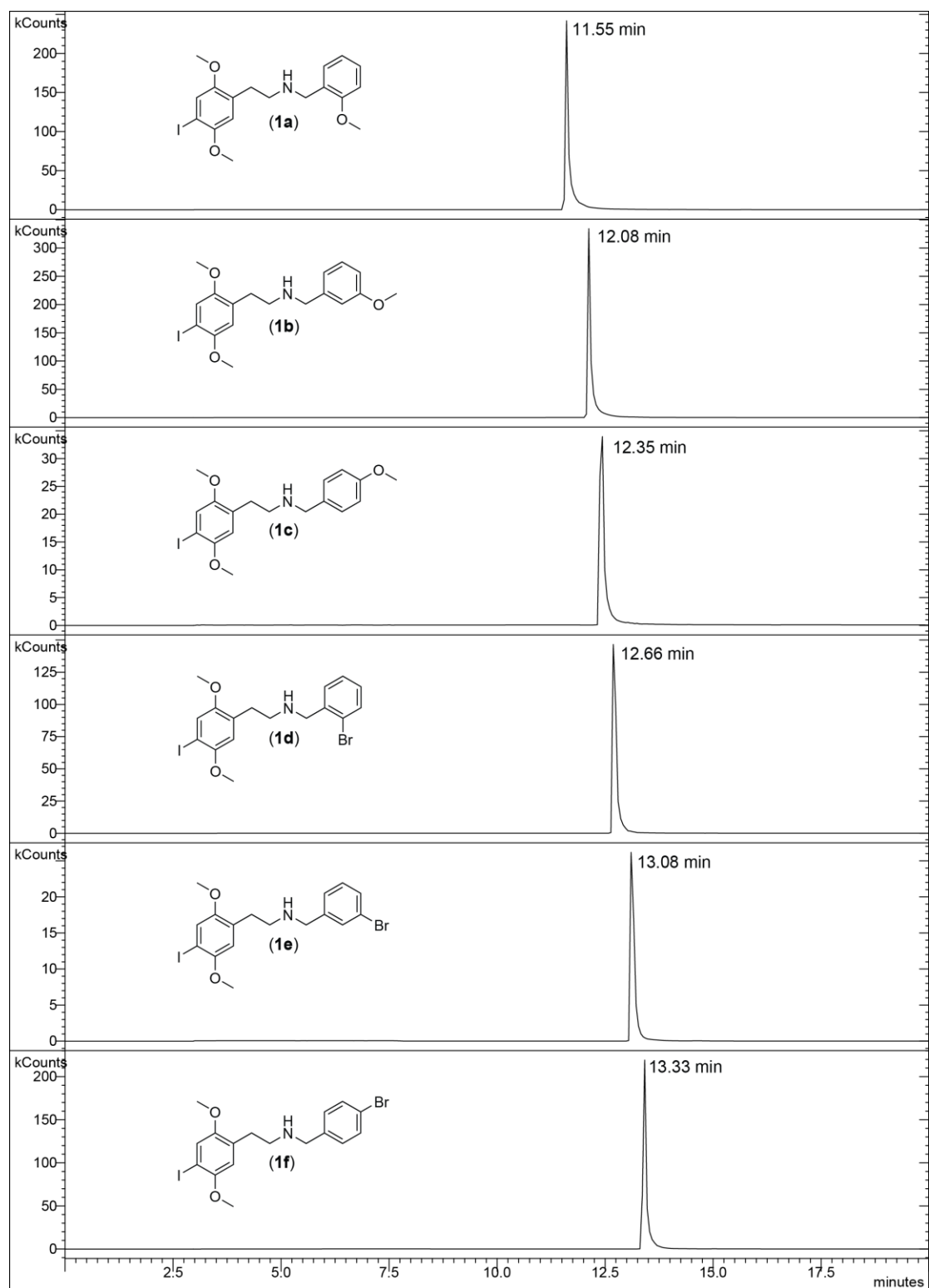
Page 23: ATR-FT/IR spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3d**)–(**3f**).



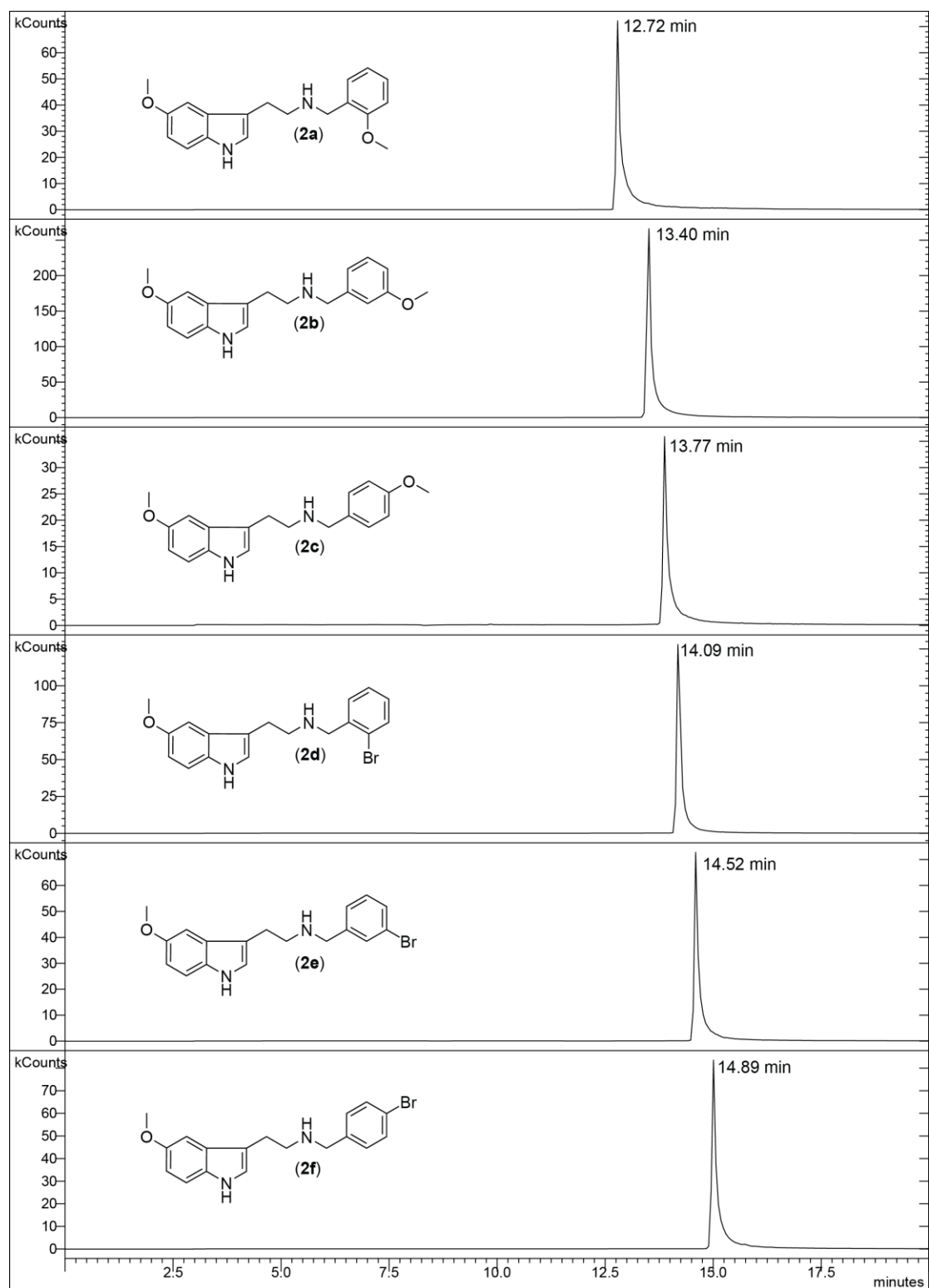
GC/MS retention times, EI- and CI ion trap mass spectra



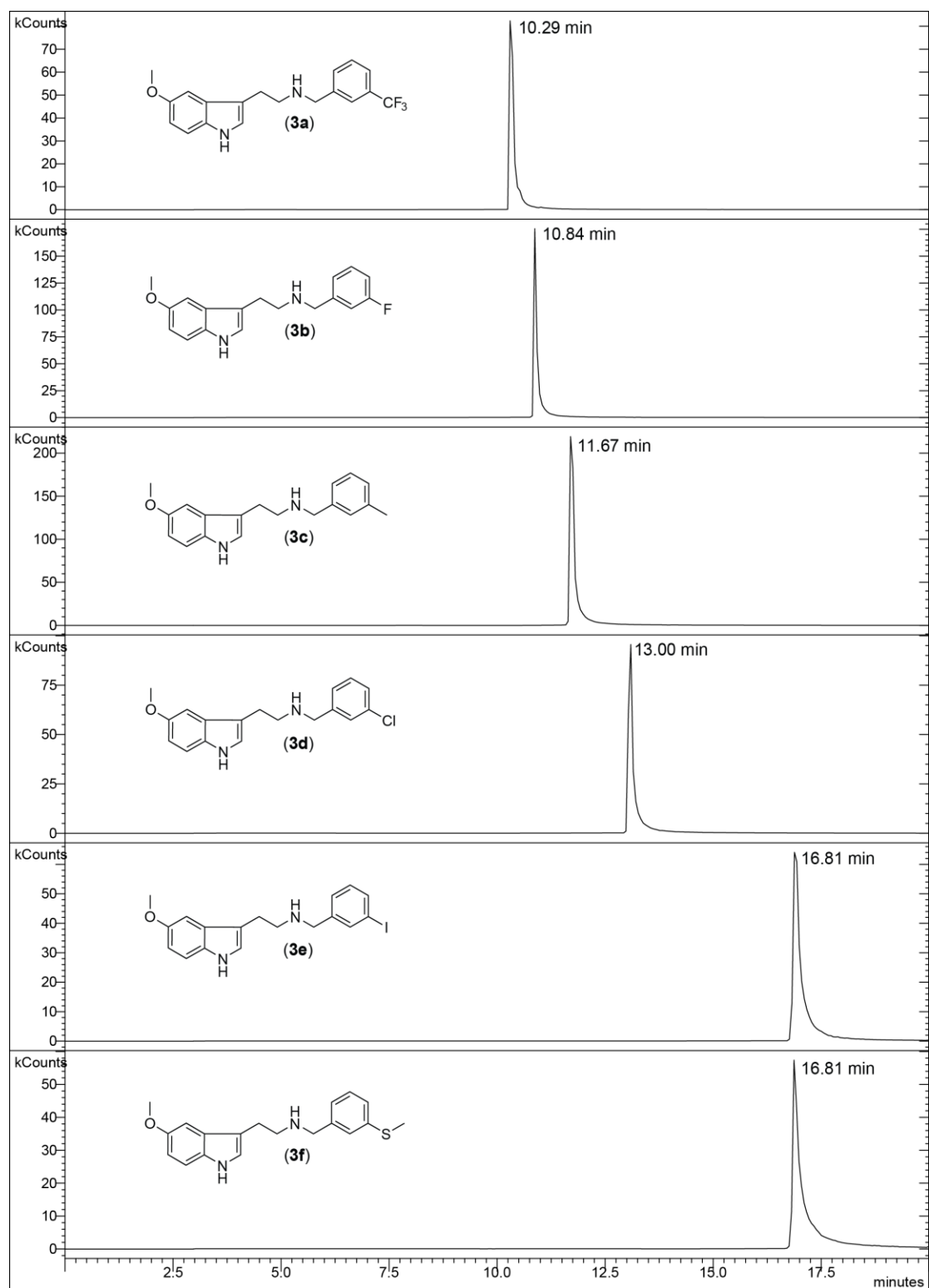
GC/MS retention times, EI- and CI ion trap mass spectra



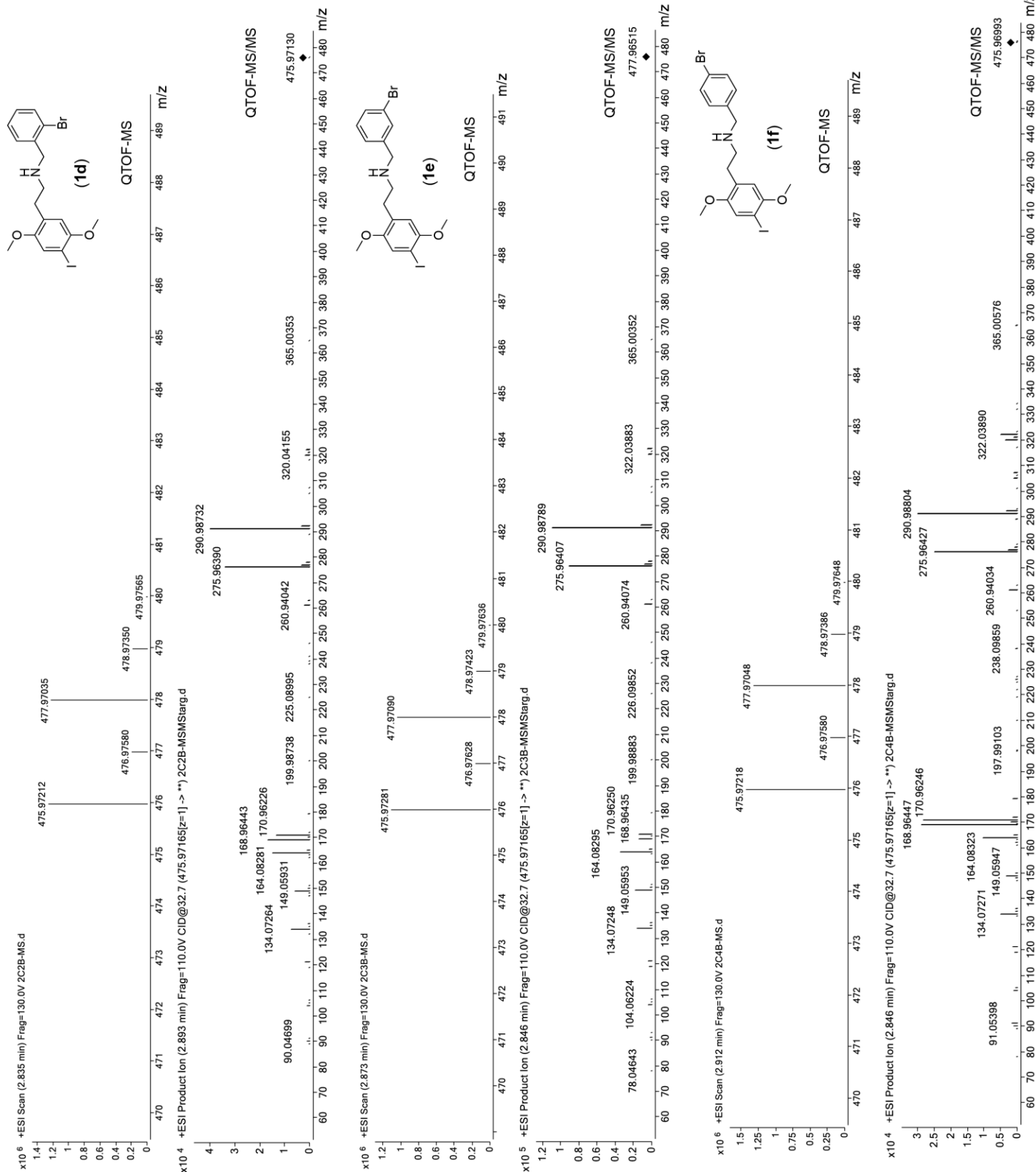
GC/MS chromatograms

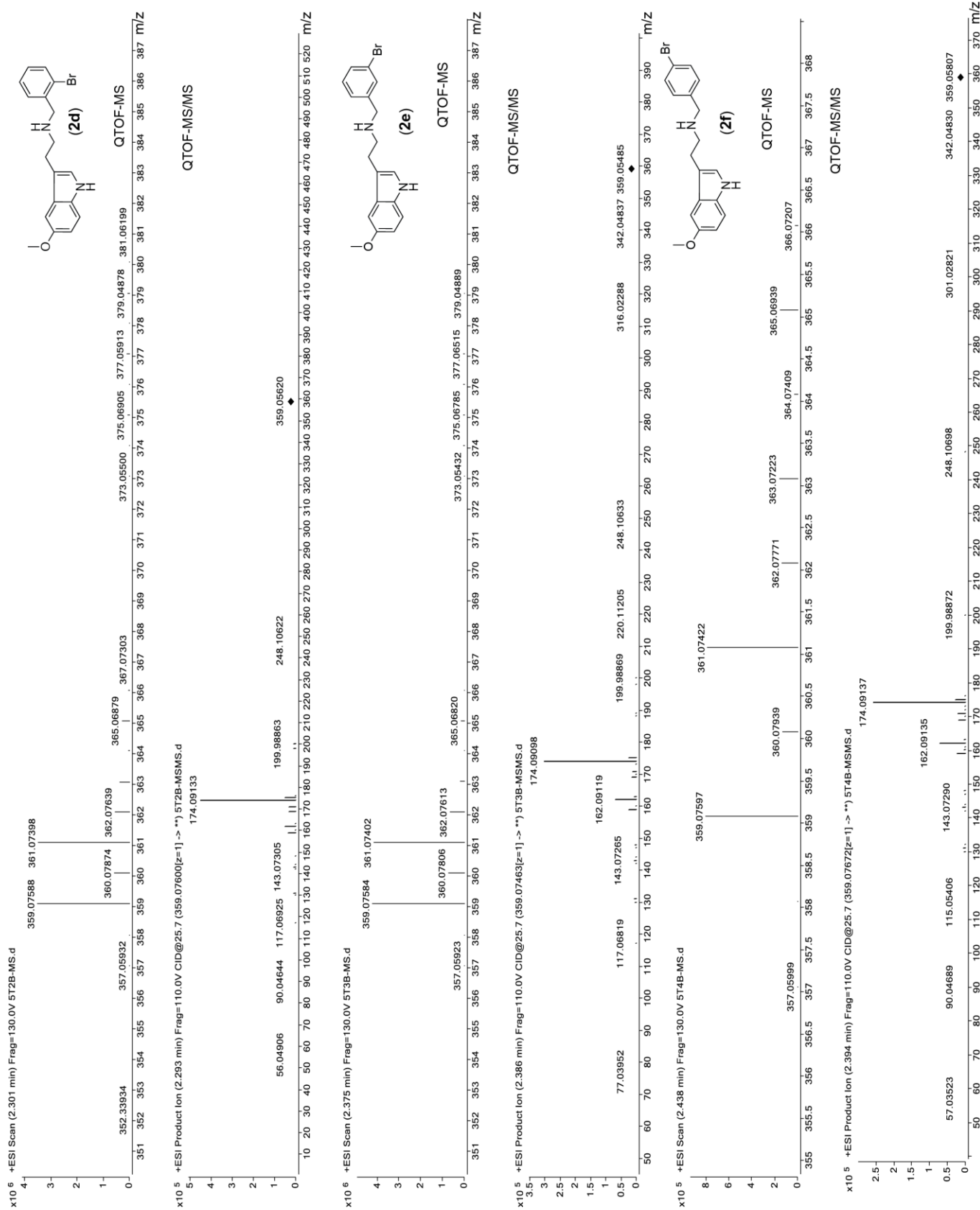


GC/MS chromatograms

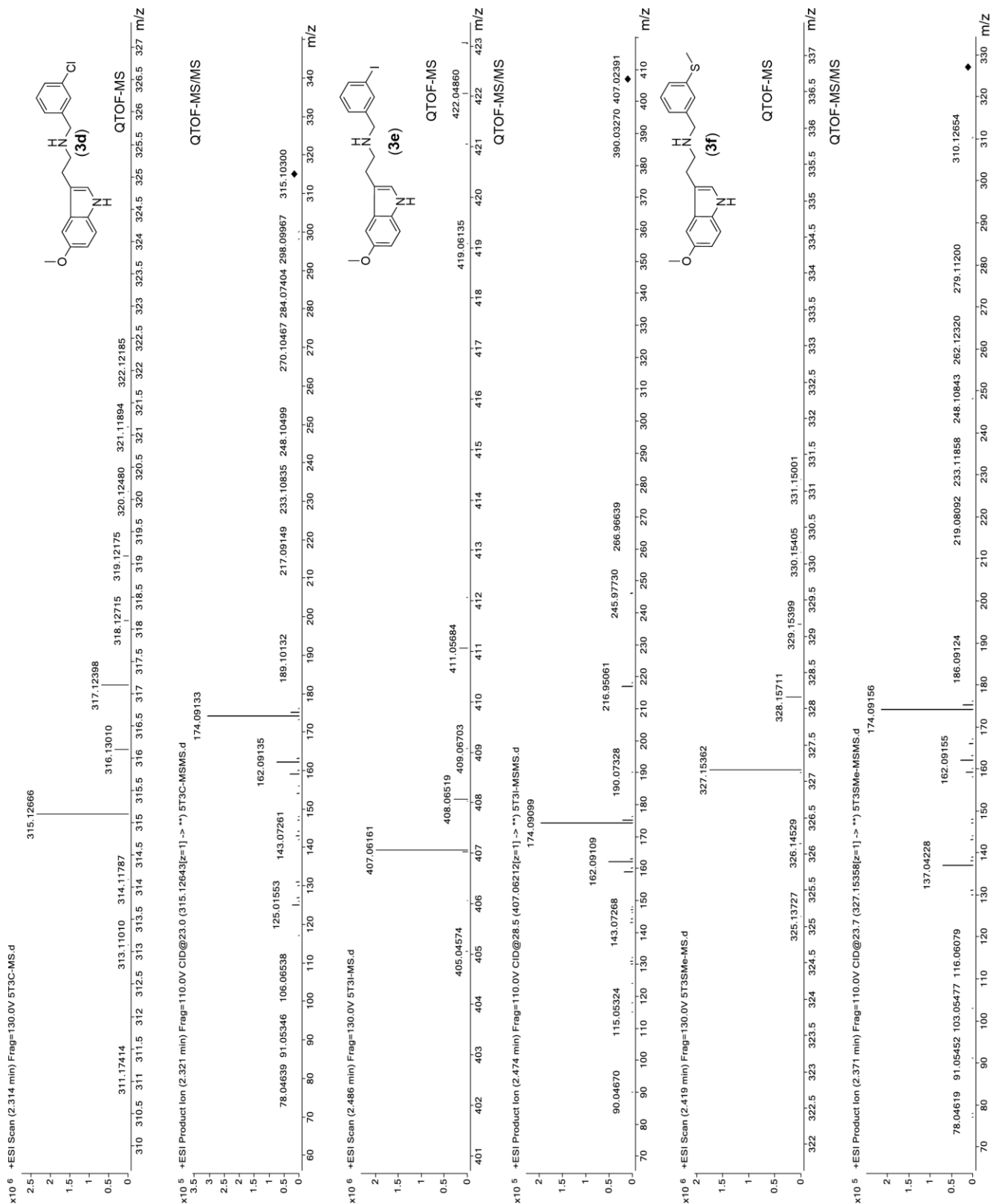


GC/MS chromatograms



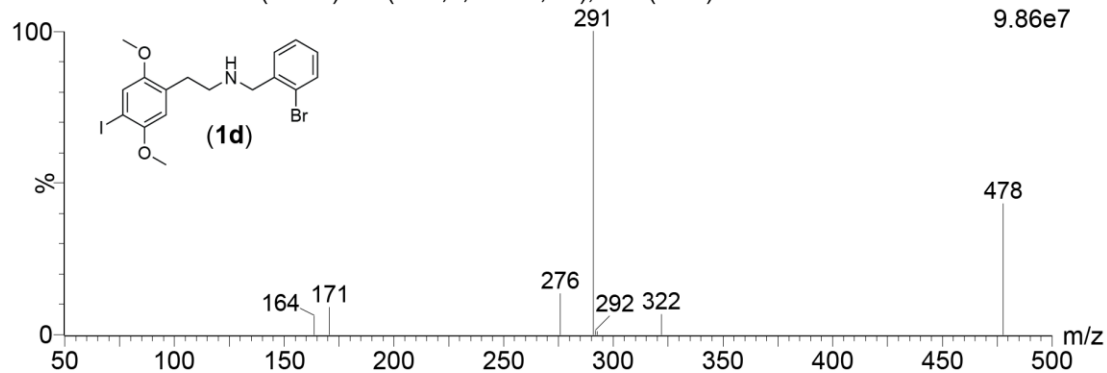


QTOF-MS and QTOF-MS/MS

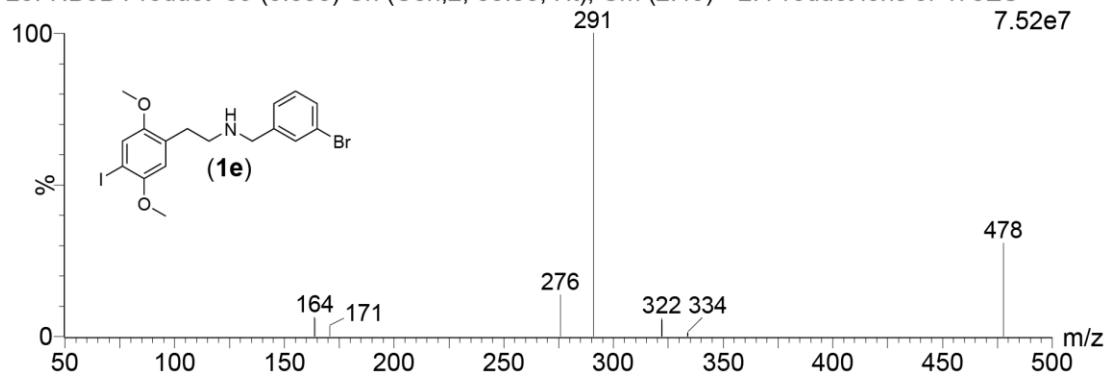


QTOF-MS and QTOF-MS/MS

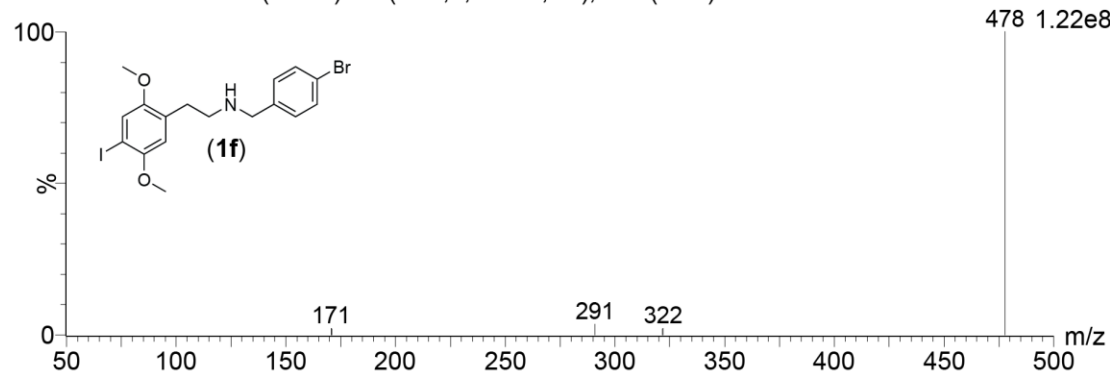
25I-NB2B Product 12 (0.626) Cn (Cen,2, 80.00, Ht); Cm (1:50) 2: Product ions of 478ES+ 9.86e7



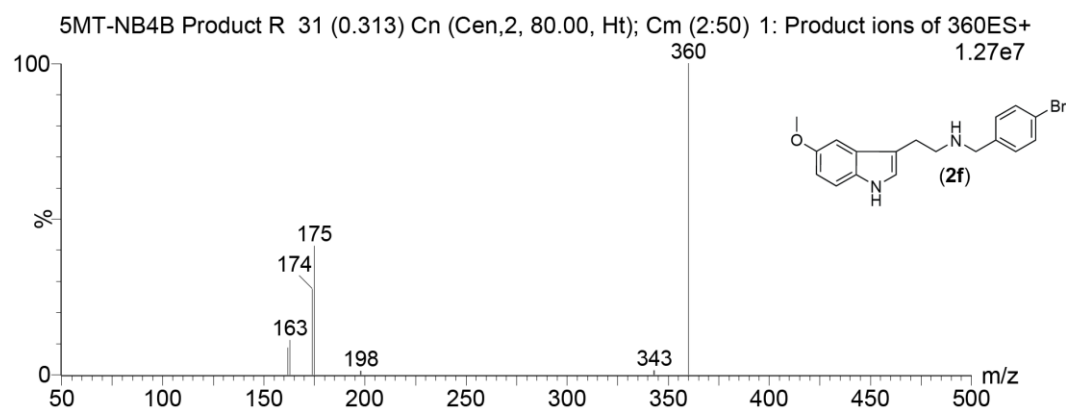
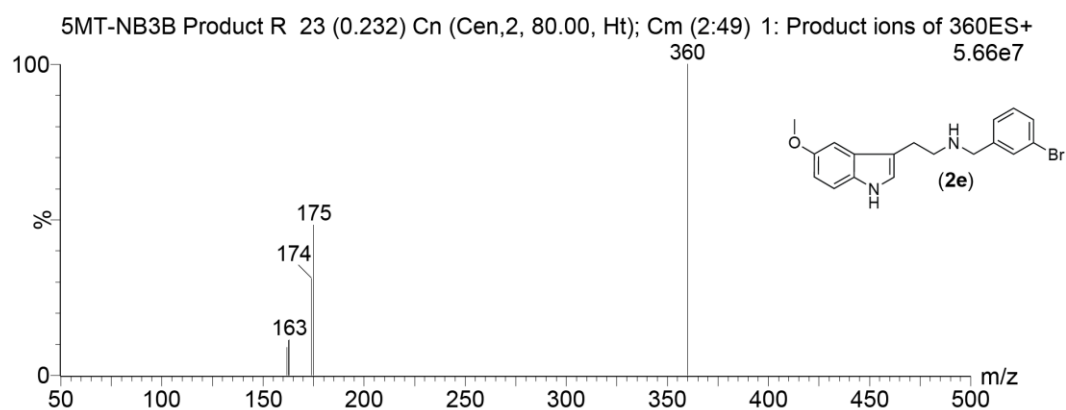
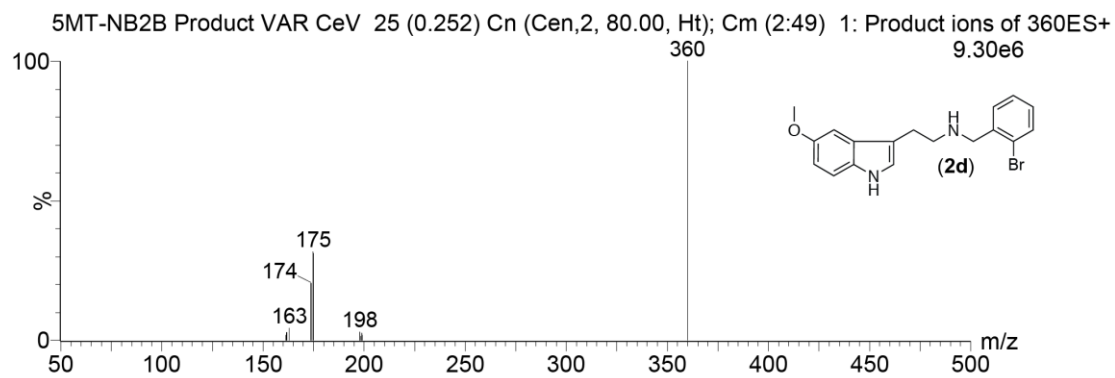
25I-NB3B Product 39 (0.898) Cn (Cen,2, 80.00, Ht); Cm (2:49) 2: Product ions of 478ES+ 7.52e7



25I-NB4B Product 47 (0.474) Cn (Cen,2, 80.00, Ht); Cm (1:49) 1: Product ions of 478ES+ 1.22e8

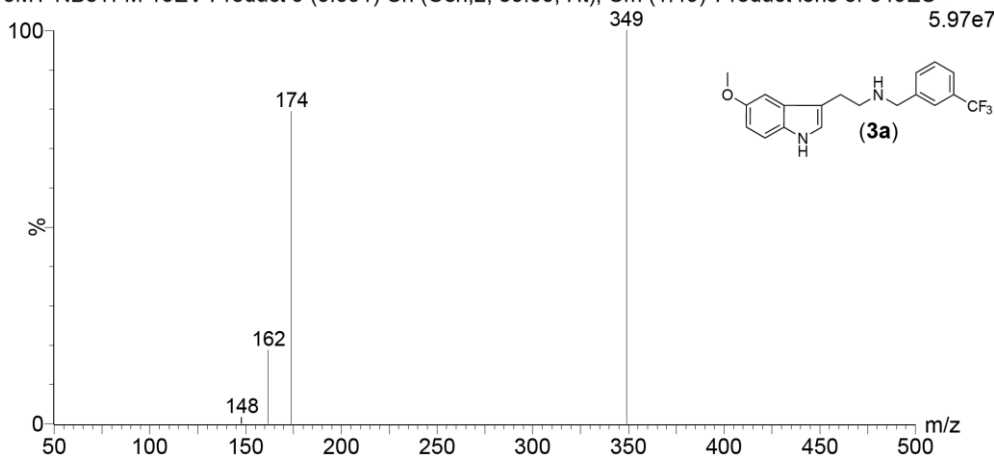


ESI-QqQ-MS/MS

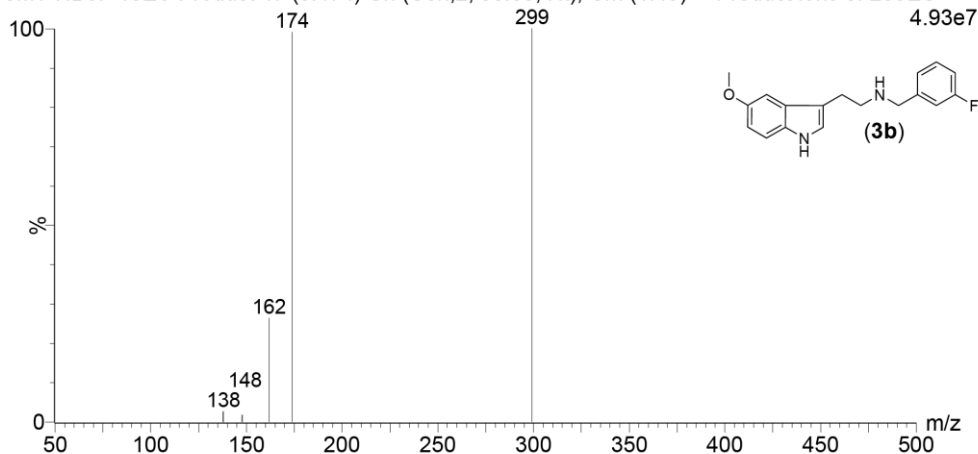


ESI-QqQ-MS/MS

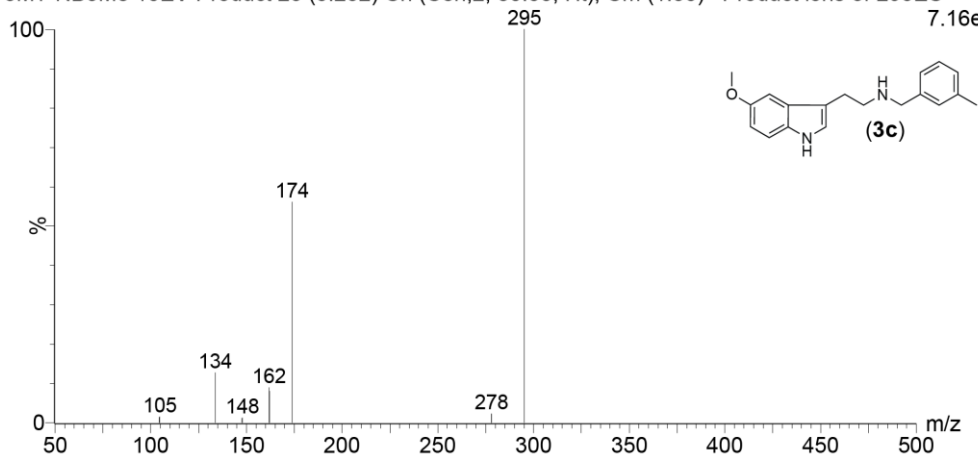
5MT-NB3TFM 10EV Product 9 (0.091) Cn (Cen,2, 80.00, Ht); Cm (1:49) Product ions of 349ES+ 5.97e7



5MT-NB3F 10EV Product 47 (0.474) Cn (Cen,2, 80.00, Ht); Cm (1:49) Product ions of 299ES+ 4.93e7

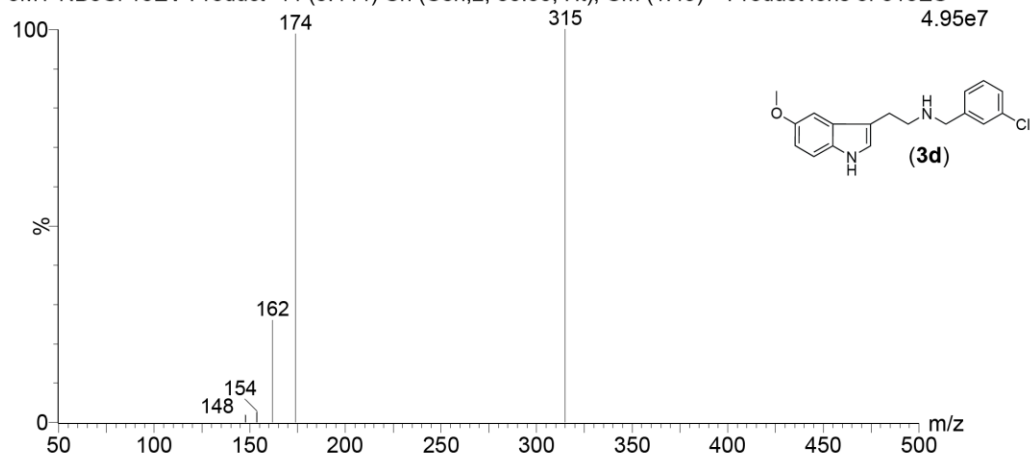


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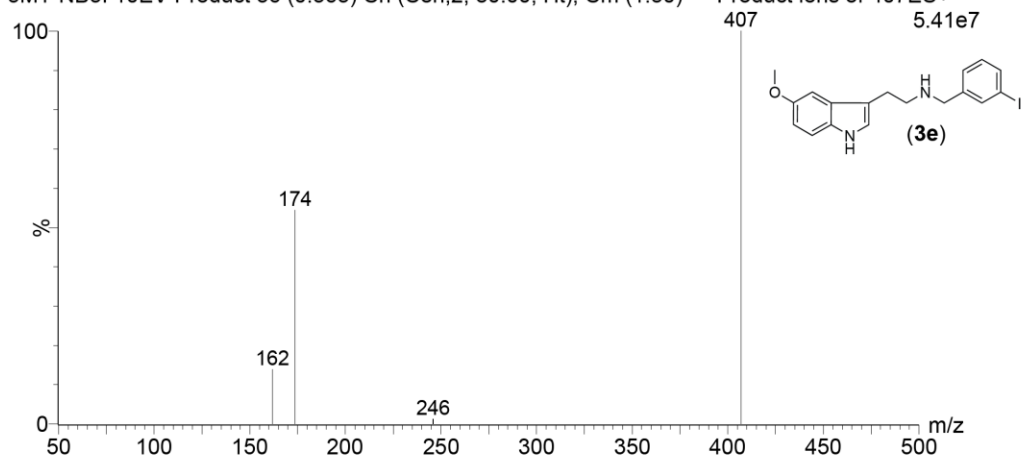


ESI-QqQ-MS/MS

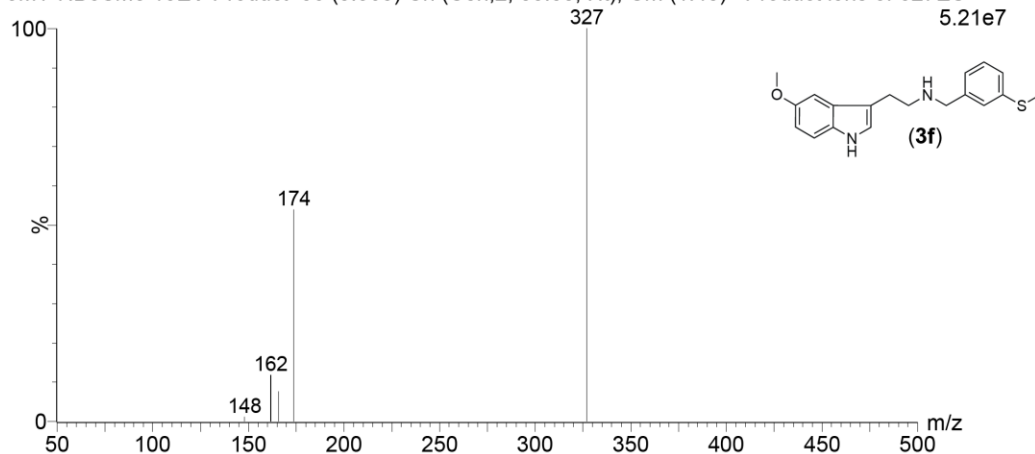
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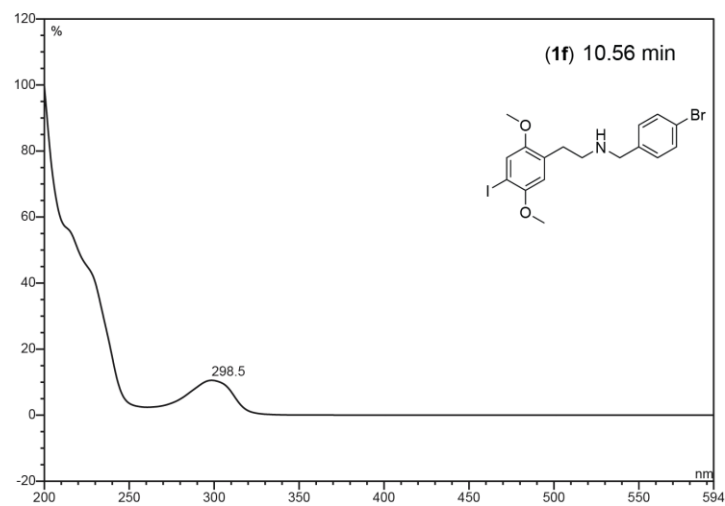
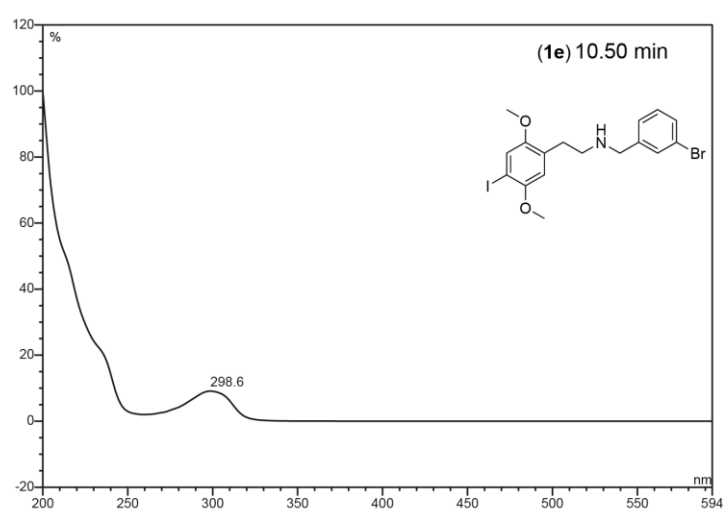
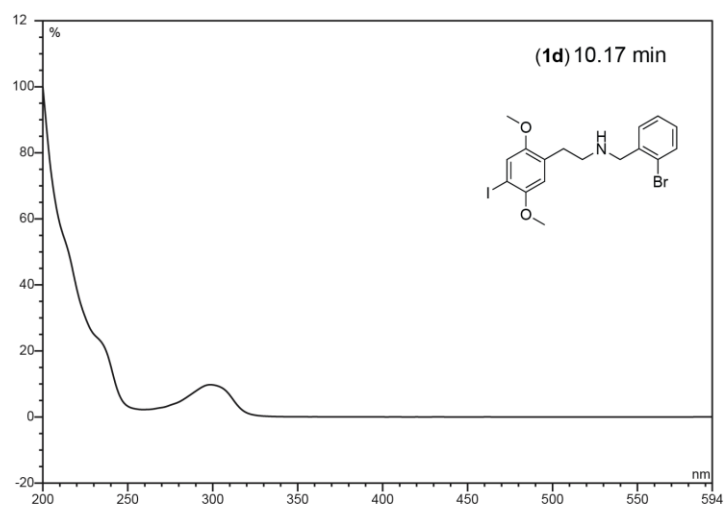
5MT-NB3I 10EV Product 36 (0.363) Cn (Cen,2, 80.00, Ht); Cm (1:50) Product ions of 407ES+ 5.41e7



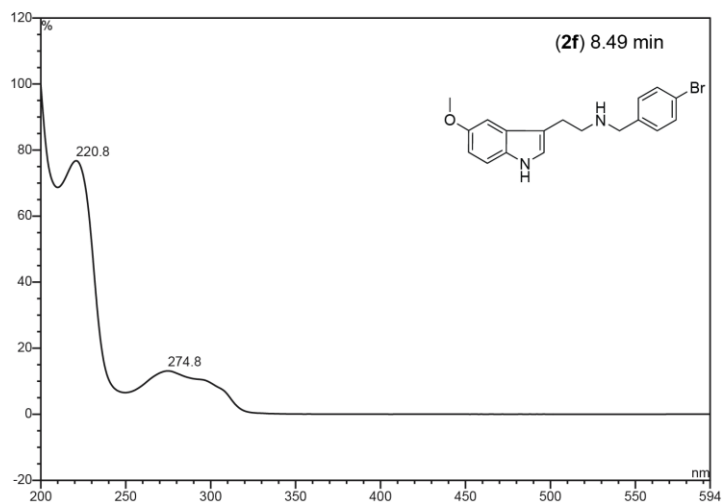
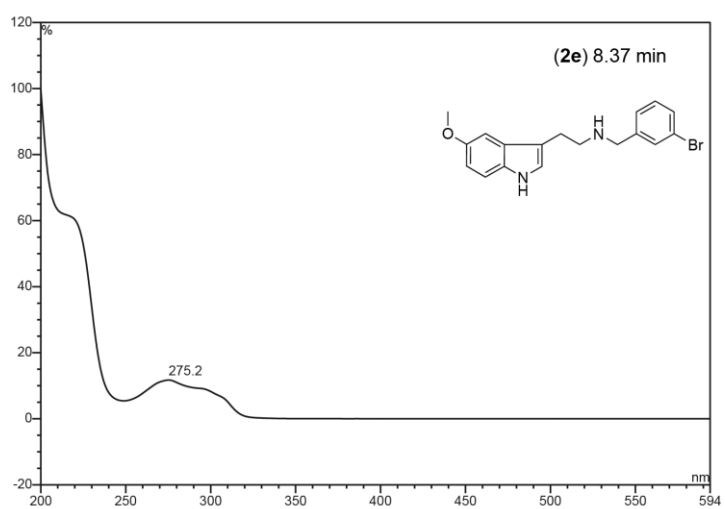
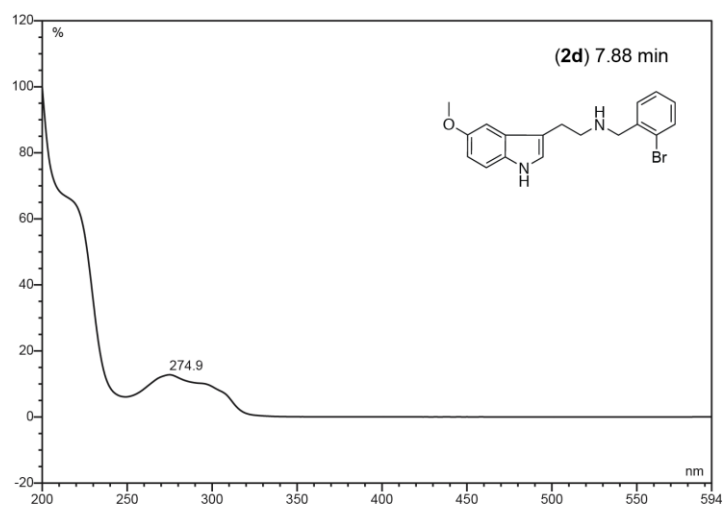
5MT-NB3SMe 10EV Product 36 (0.363) Cn (Cen,2, 80.00, Ht); Cm (1:48) Product ions of 327ES+ 5.21e7



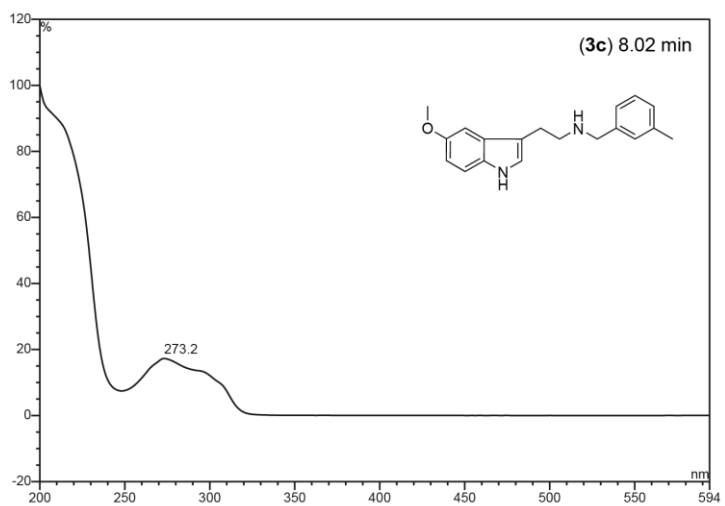
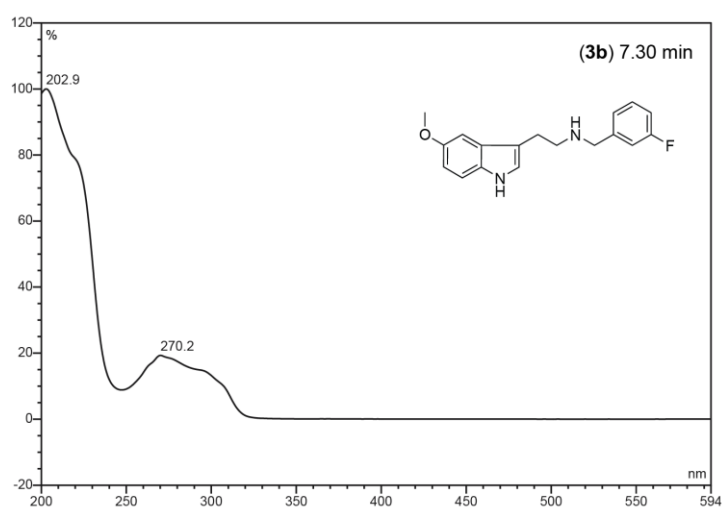
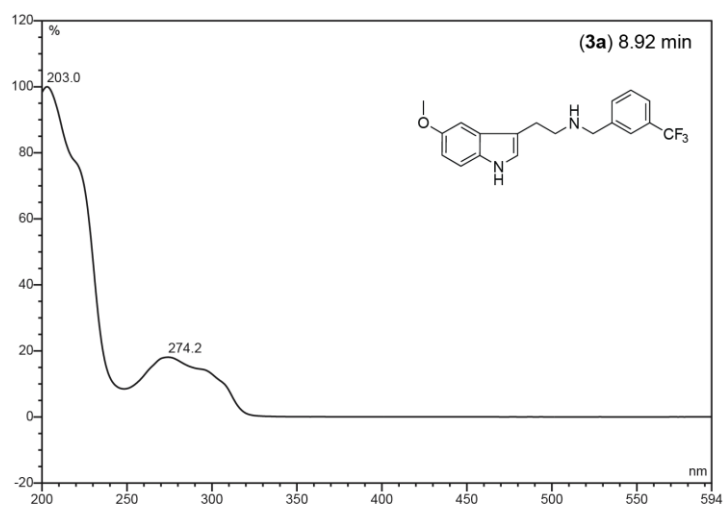
ESI-QqQ-MS/MS



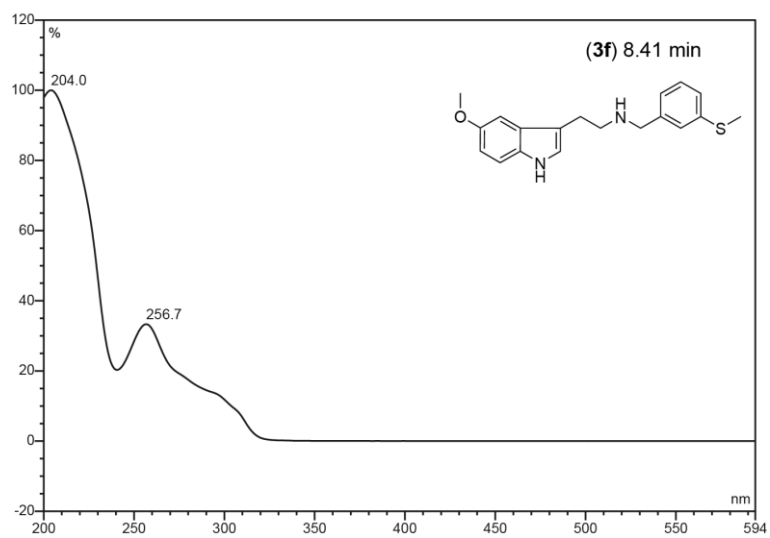
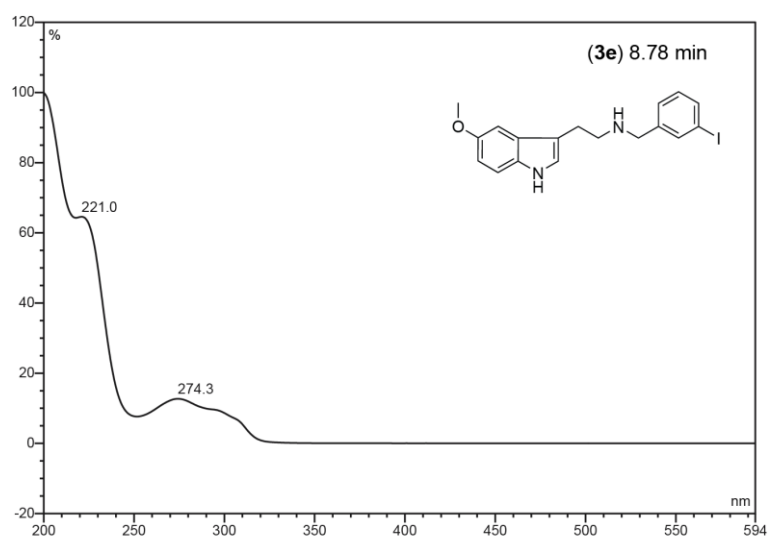
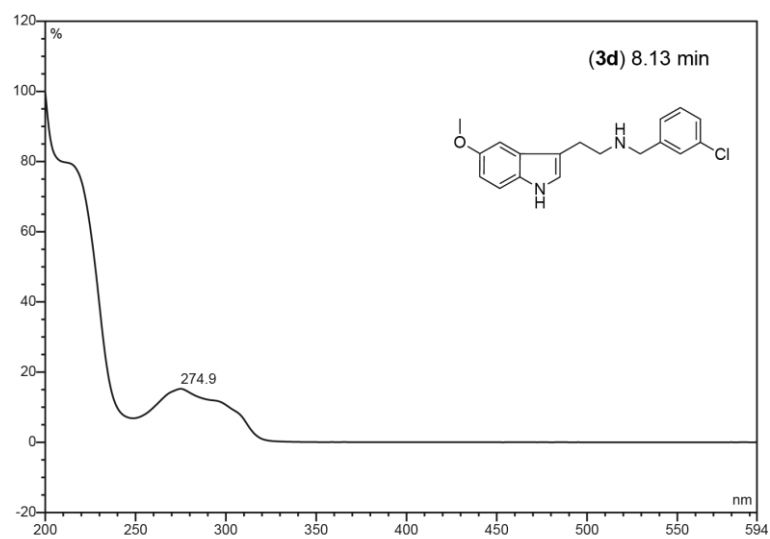
LC/UV retention times and diode array full scan spectra



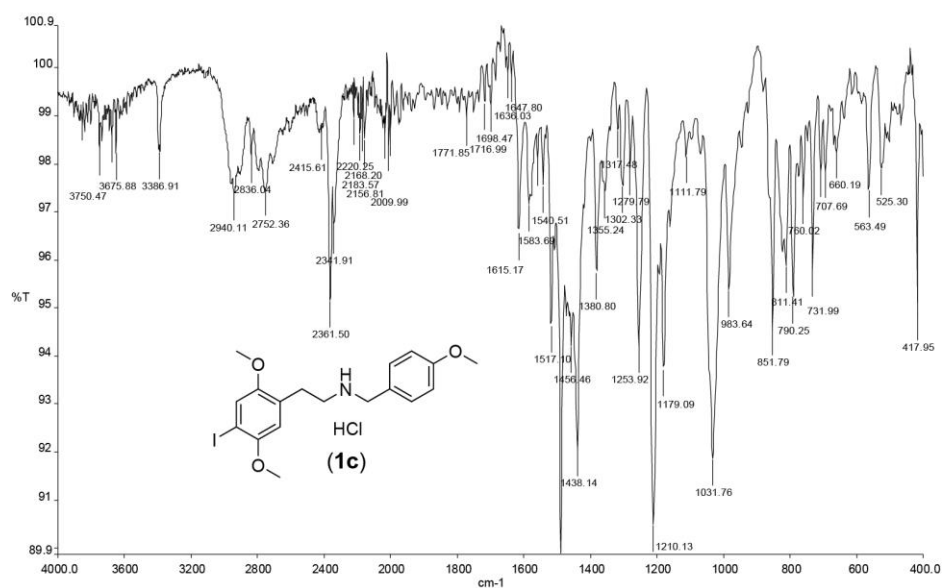
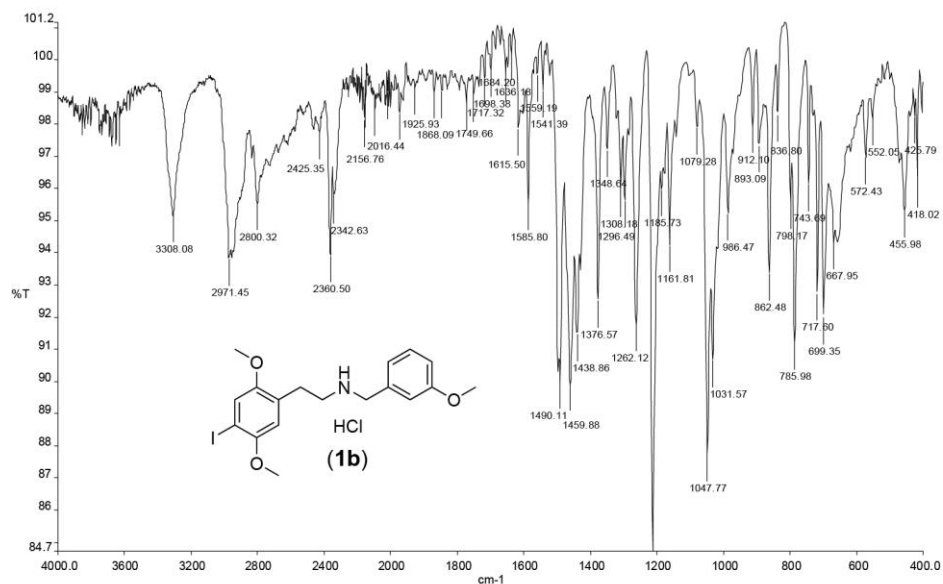
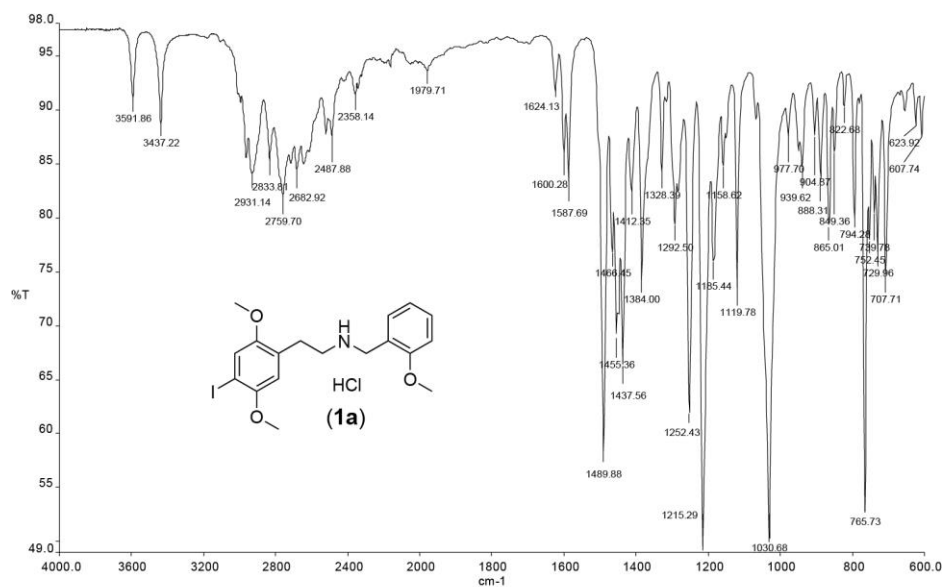
LC/UV retention times and diode array full scan spectra



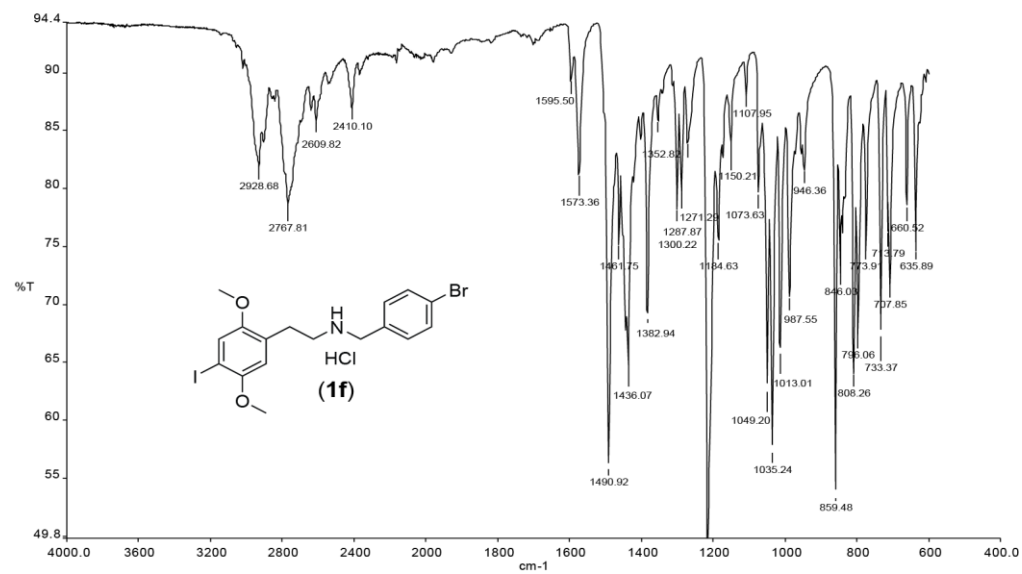
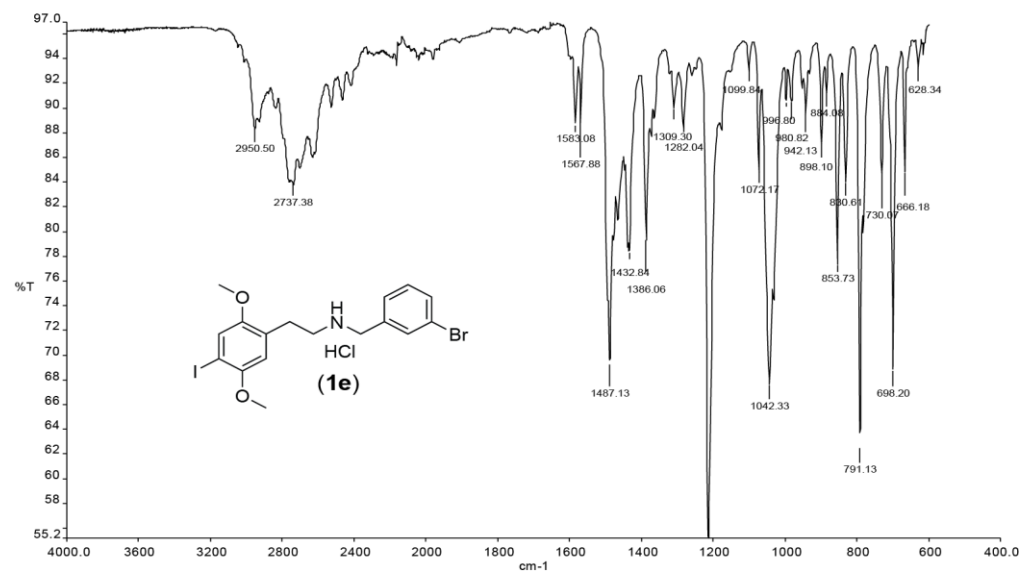
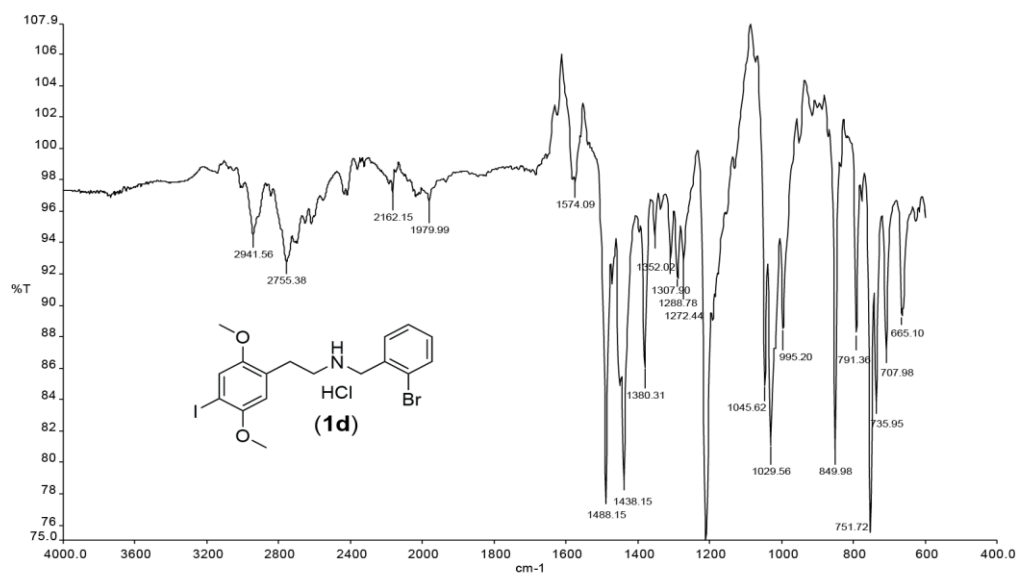
LC/UV retention times and diode array full scan spectra



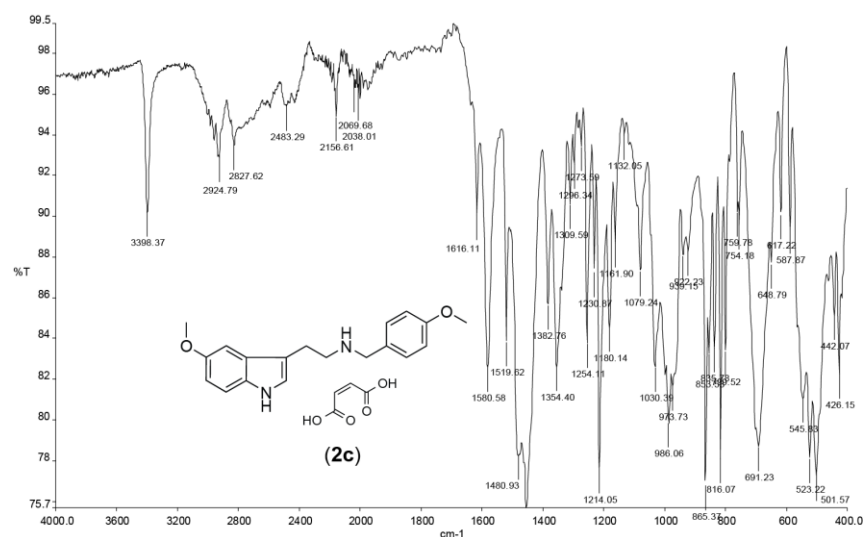
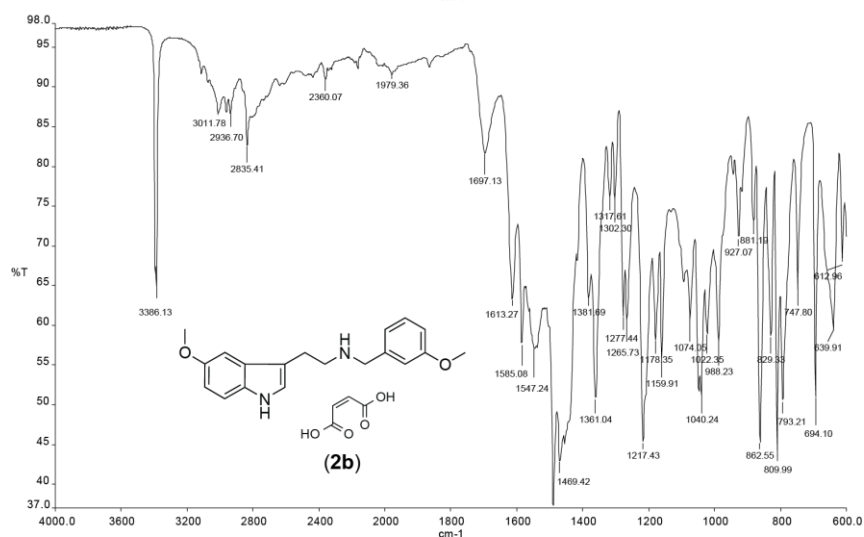
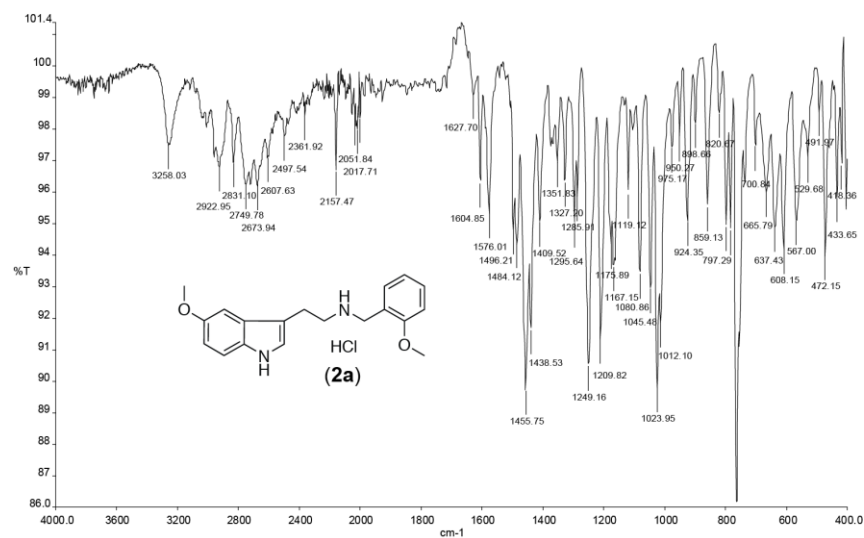
LC/UV retention times and diode array full scan spectra



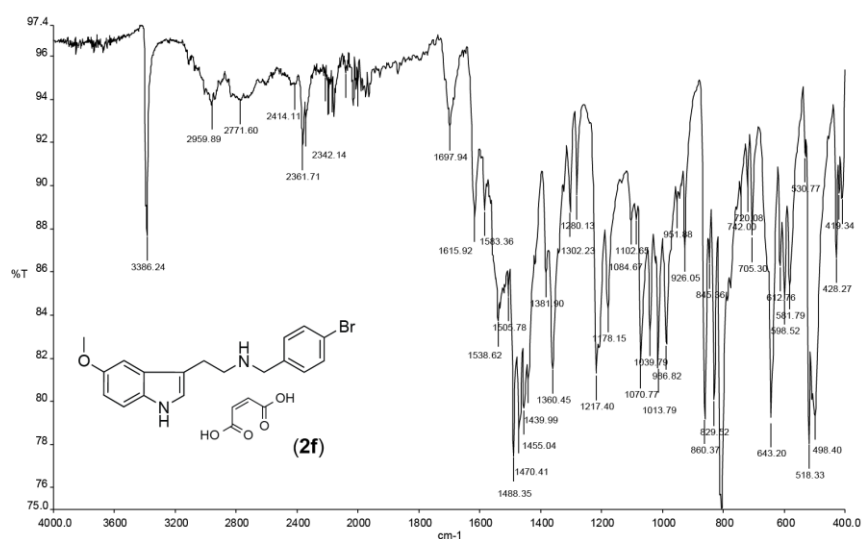
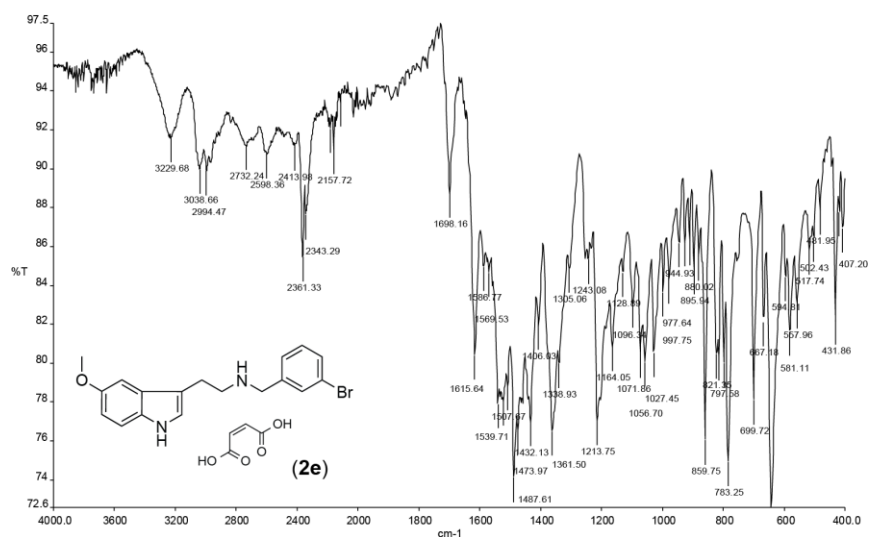
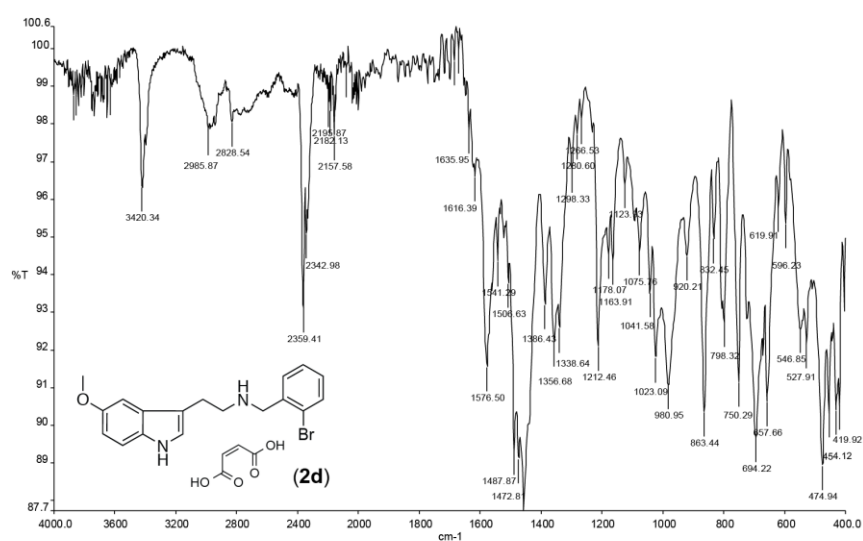
ATR-FTIR spectra



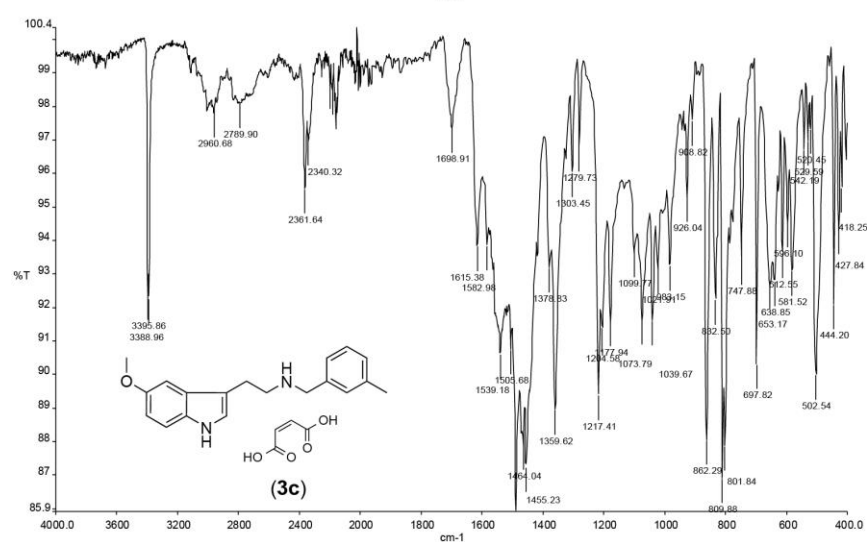
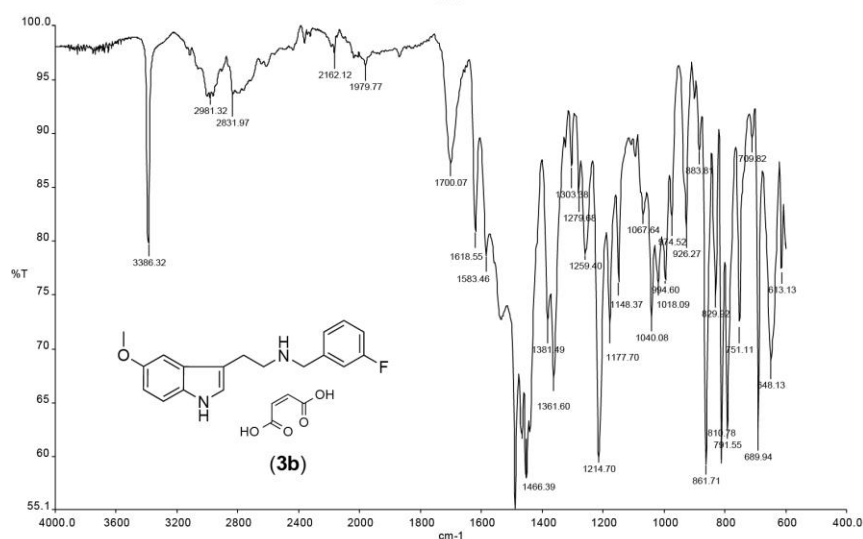
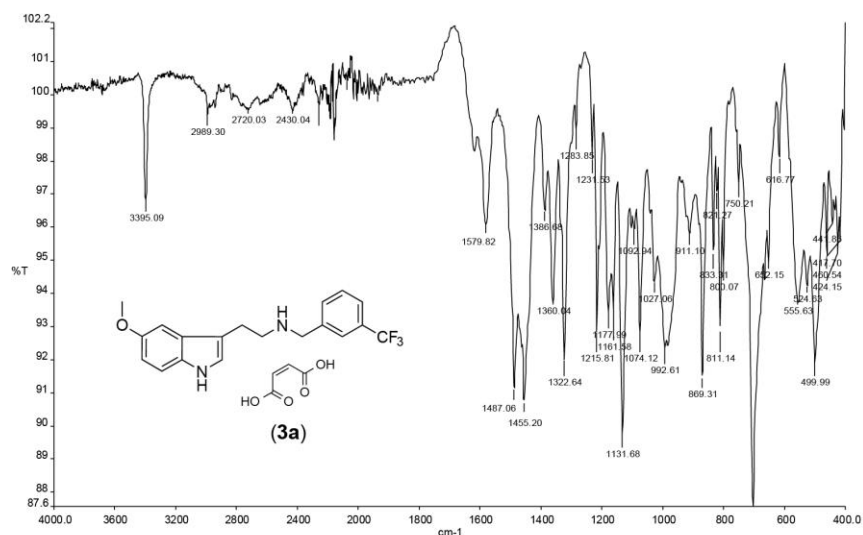
ATR-FTIR spectra



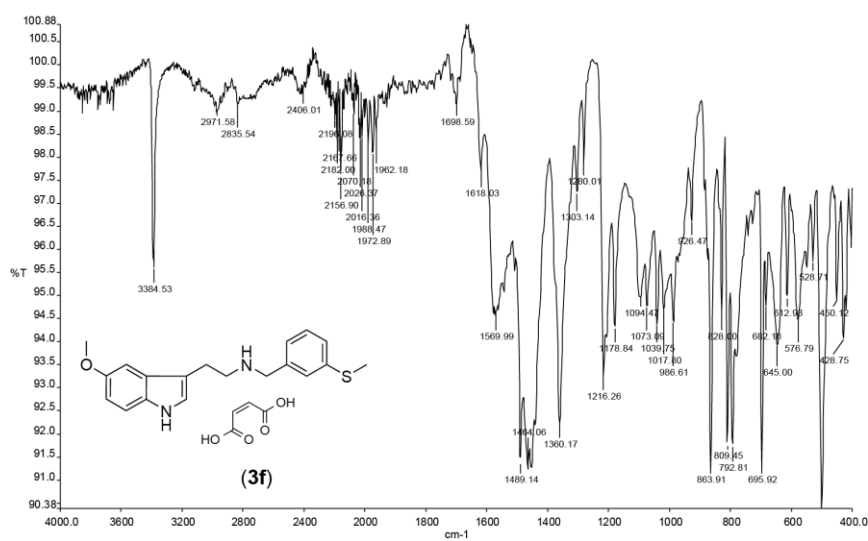
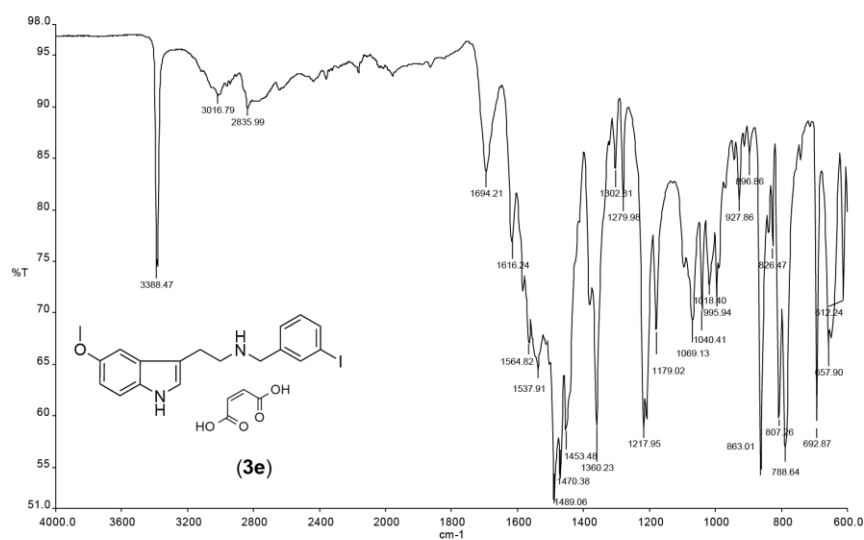
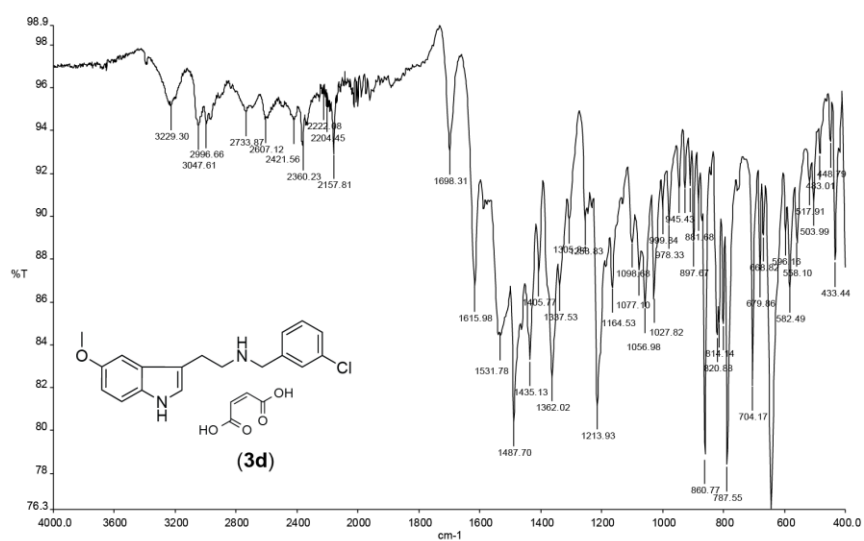
ATR-FTIR spectra



ATR-FTIR spectra



ATR-FTIR spectra



ATR-FTIR spectra