Supporting Information Part 2

Significantly improved Radiochemical Yields in gaseous Tritium Reactions by Iridium(I)-catalyzed Hydrogen Isotope Exchange

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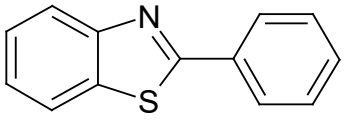
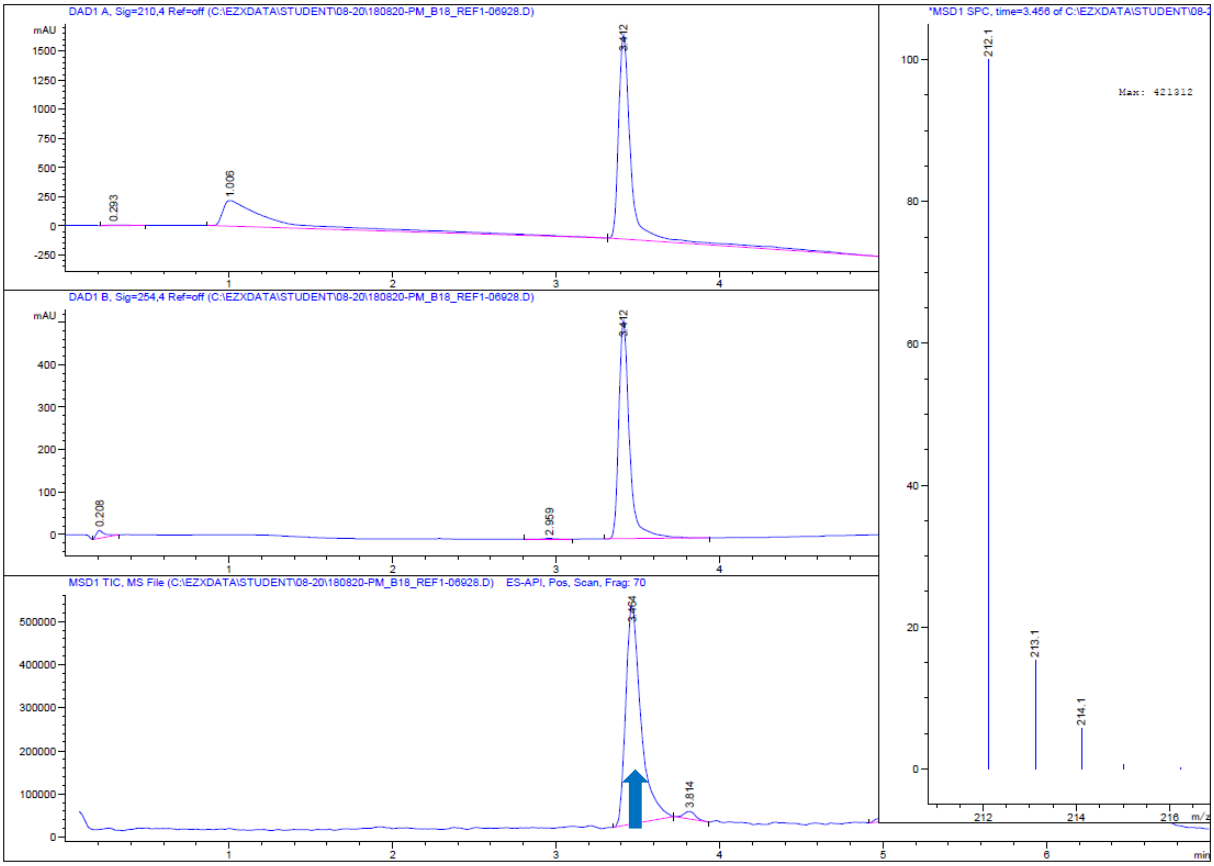
Table of content

Data for 2-phenylbenzothiazole **13**



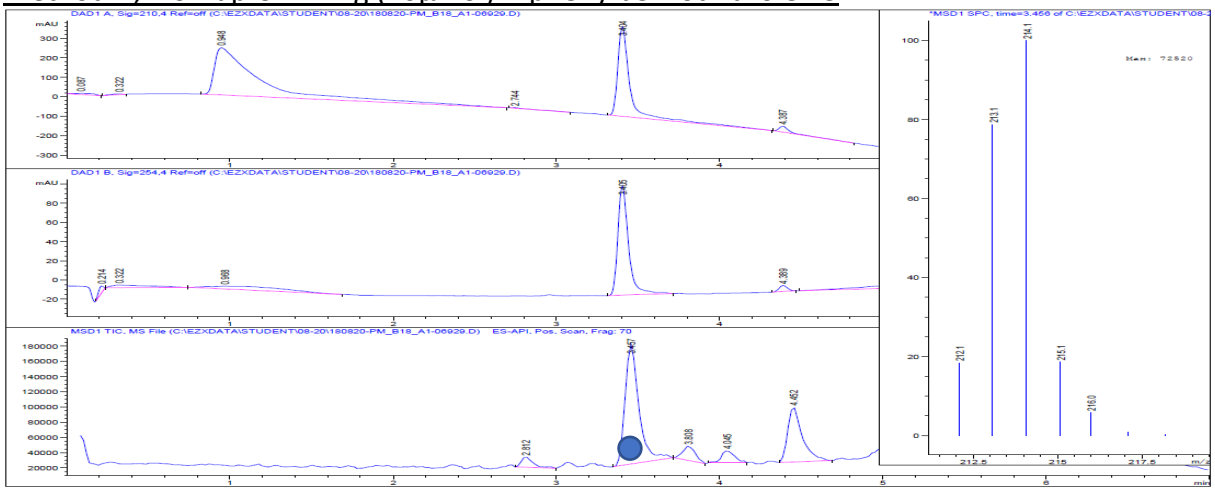
13



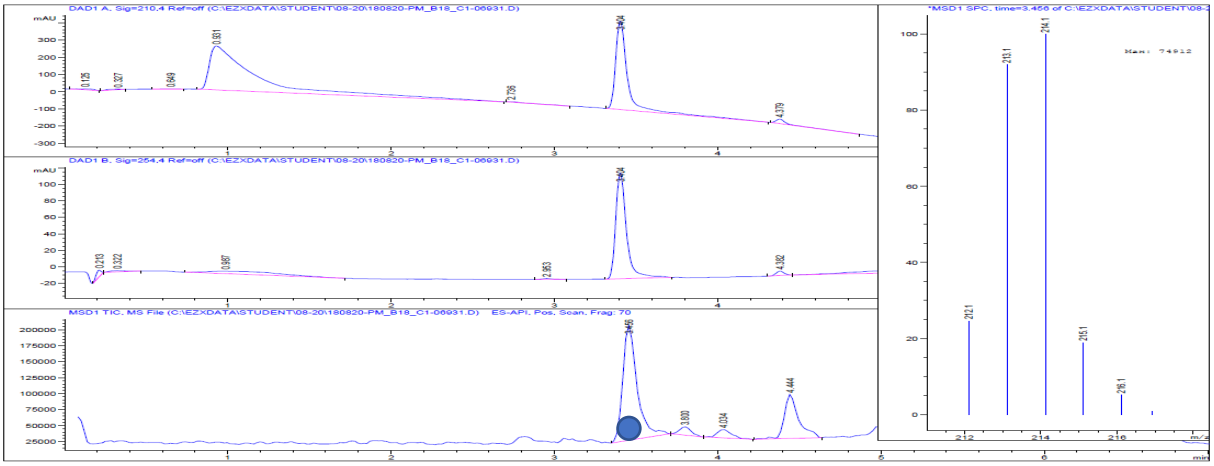
LC-MS (positive ESI): m/z 212.1 $[M+H]^+$ (100), 213.1 $[M+1+H]^+$ (15.3), 214.1 $[M+2+H]^+$ (5.7)

experiments with 2-phenylbenzothiazole **13**

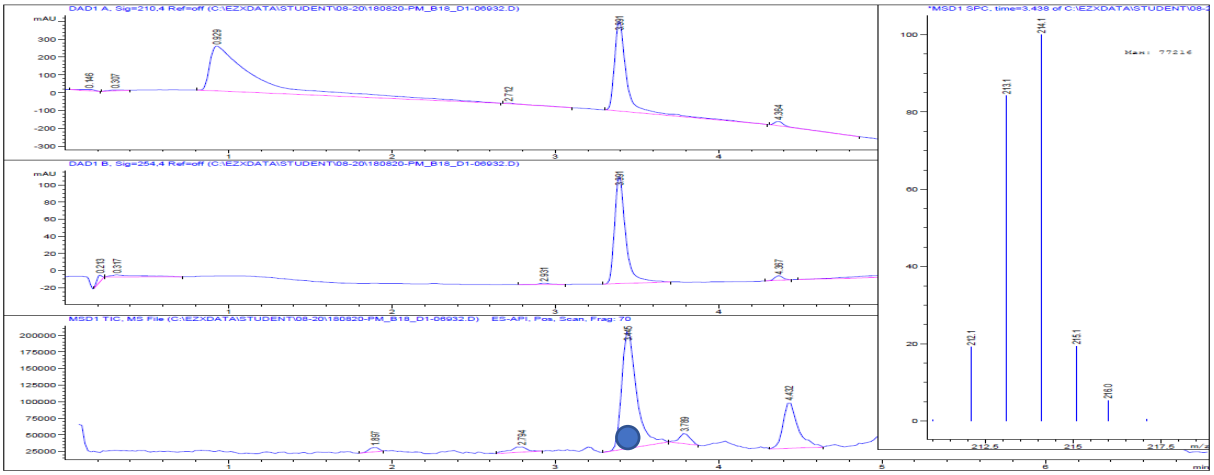
Method A, workup C: 2.2mg (10µmol) 2-phenylbenzothiazole **13**



LC-MS (positive ESI): m/z 212.1 $[M+H]^+$ (18.4), 213.1 $[M(1D)+H]^+$ (78.7), 214.1 $[M(2D)+H]^+$ (100), 215.1 $[M(3D)+H]^+$ (18.6), 216.0 $[M(4D)+H]^+$ (5.9) : 69% D



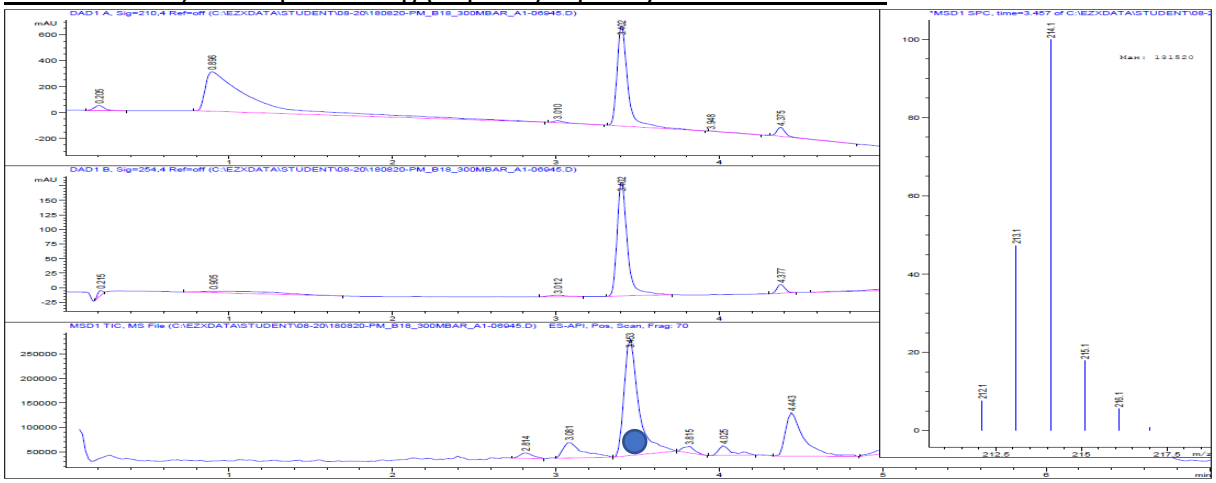
LC-MS (positive ESI): m/z 212.1 $[M+H]^+$ (24.6), 213.1 $[M(1D)+H]^+$ (92.0), 214.1 $[M(2D)+H]^+$ (100), 215.1 $[M(3D)+H]^+$ (18.9), 216.1 $[M(4D)+H]^+$ (5.1) : 65% D



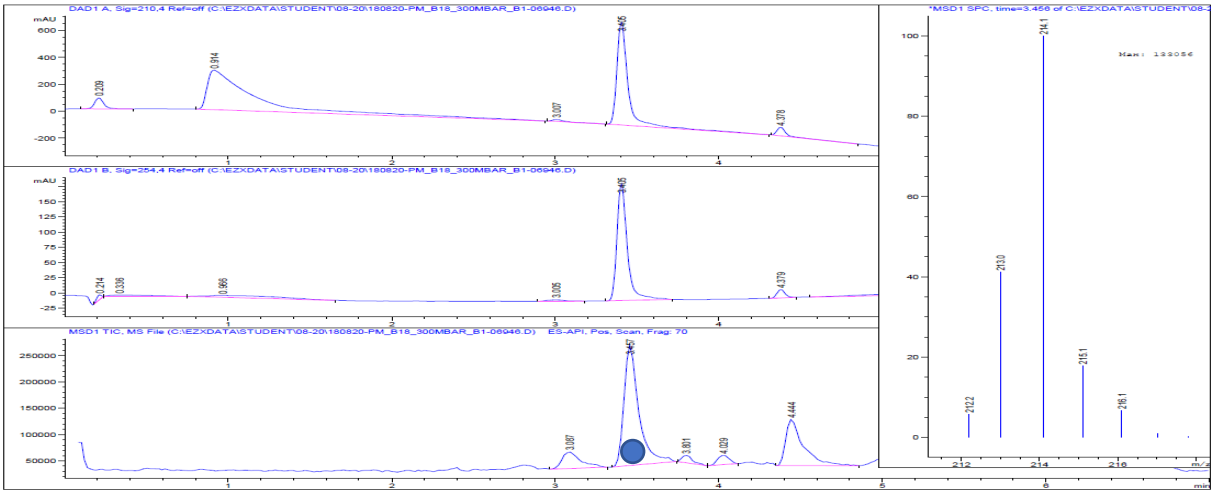
LC-MS (positive ESI): m/z 212.1 $[M+H]^+$ (19.2), 213.1 $[M(1D)+H]^+$ (84.3), 214.1 $[M(2D)+H]^+$ (100), 215.1 $[M(3D)+H]^+$ (19.4), 216.0 $[M(4D)+H]^+$ (5.3) : 68% D

Average of three reactions: 67% D, Yield: 96%, DCY: 64%

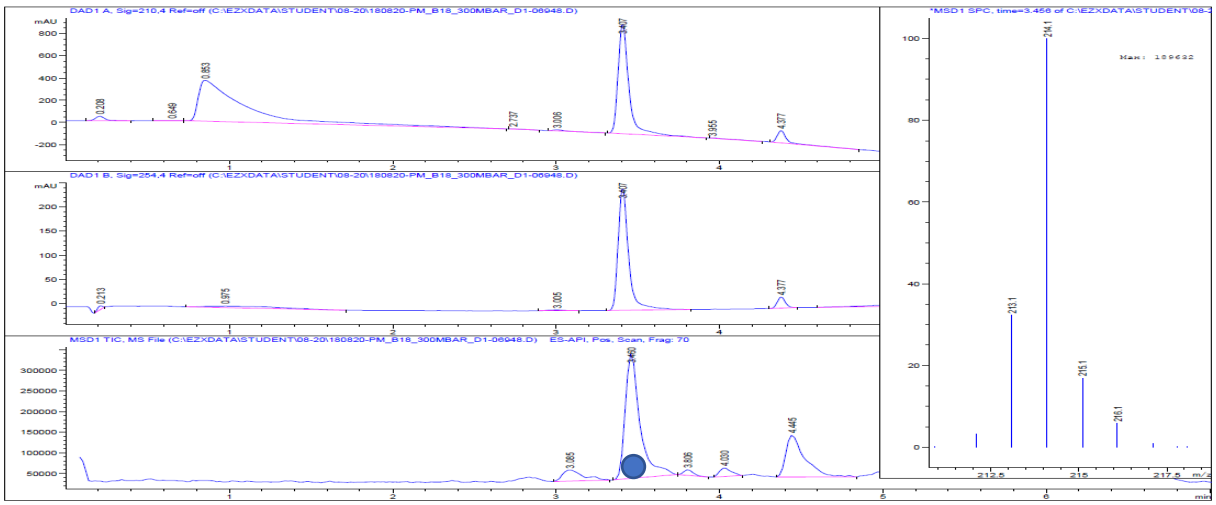
13: Method B, workup C: 2.7mg (13µmol) 2-phenylbenzothiazole **13**



LC-MS (positive ESI): m/z 212.1 $[M+H]^+$ (7.6), 213.1 $[M(1D)+H]^+$ (47.3), 214.1 $[M(2D)+H]^+$ (100), 215.1 $[M(3D)+H]^+$ (17.9), 216.1 $[M(4D)+H]^+$ (5.6) : 80% D



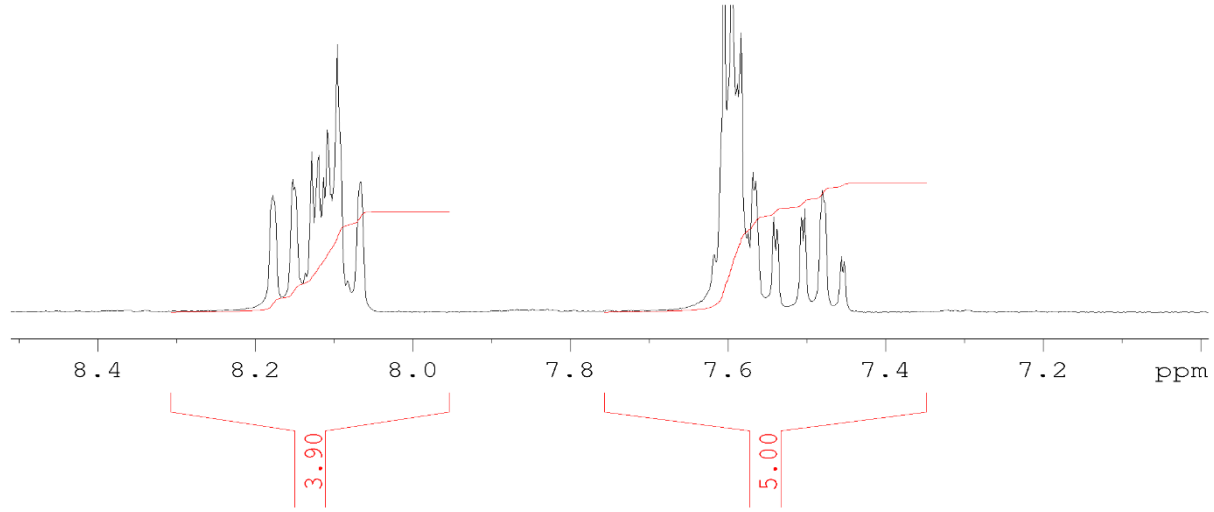
LC-MS (positive ESI): m/z 212.2 $[M+H]^+$ (5.8), 213.0 $[M(1D)+H]^+$ (41.1), 214.1 $[M(2D)+H]^+$ (100), 215.1 $[M(3D)+H]^+$ (17.8), 216.1 $[M(4D)+H]^+$ (6.6) : 82% D



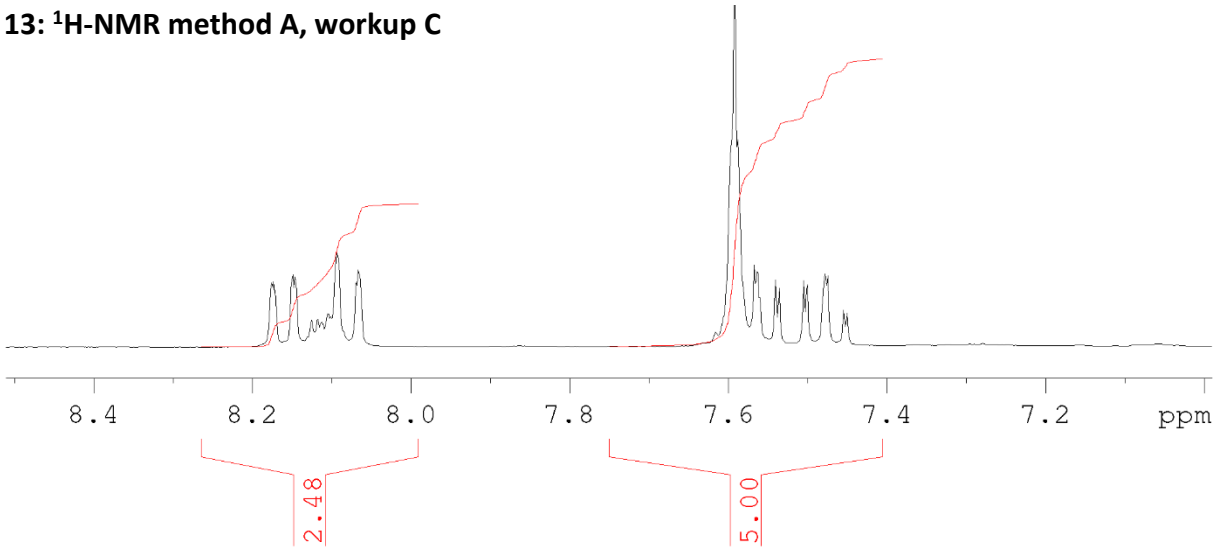
LC-MS (positive ESI): m/z 212.2 $[M+H]^+$ (3.2), 213.0 $[M(1D)+H]^+$ (32.3), 214.1 $[M(2D)+H]^+$ (100), 215.1 $[M(3D)+H]^+$ (16.9), 216.1 $[M(4D)+H]^+$ (5.8) : 85% D

Average of three reactions: 82% D, Yield: 96%, DCY: 8%

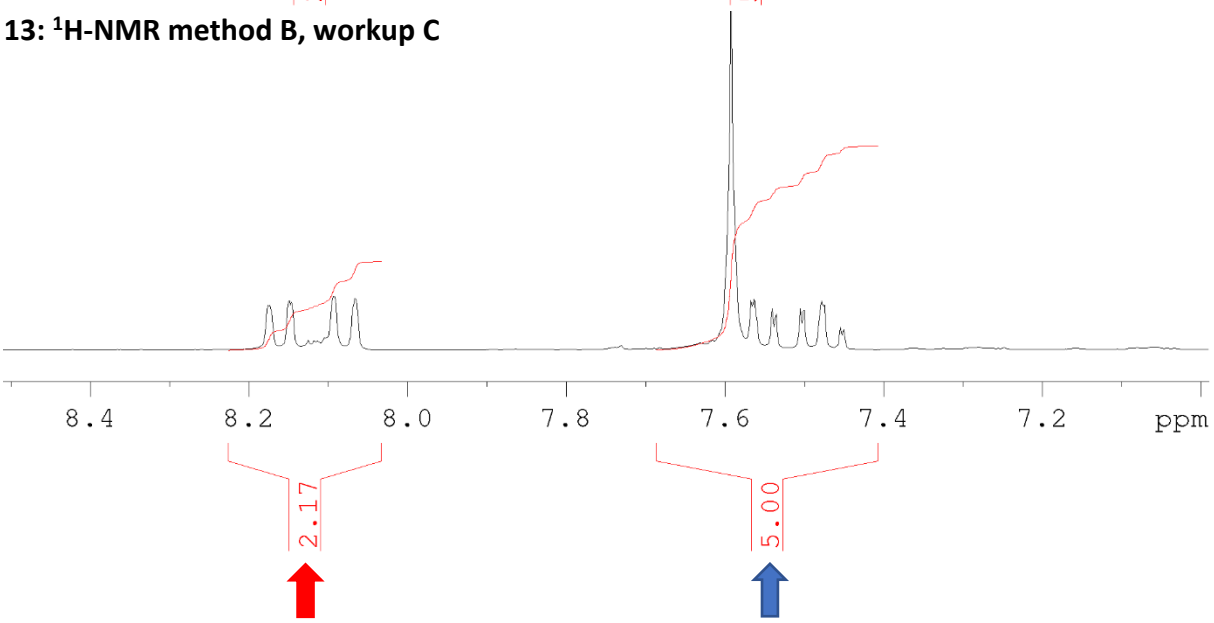
13: ^{1}H-NMR reference



13: ^{1}H-NMR method A, workup C

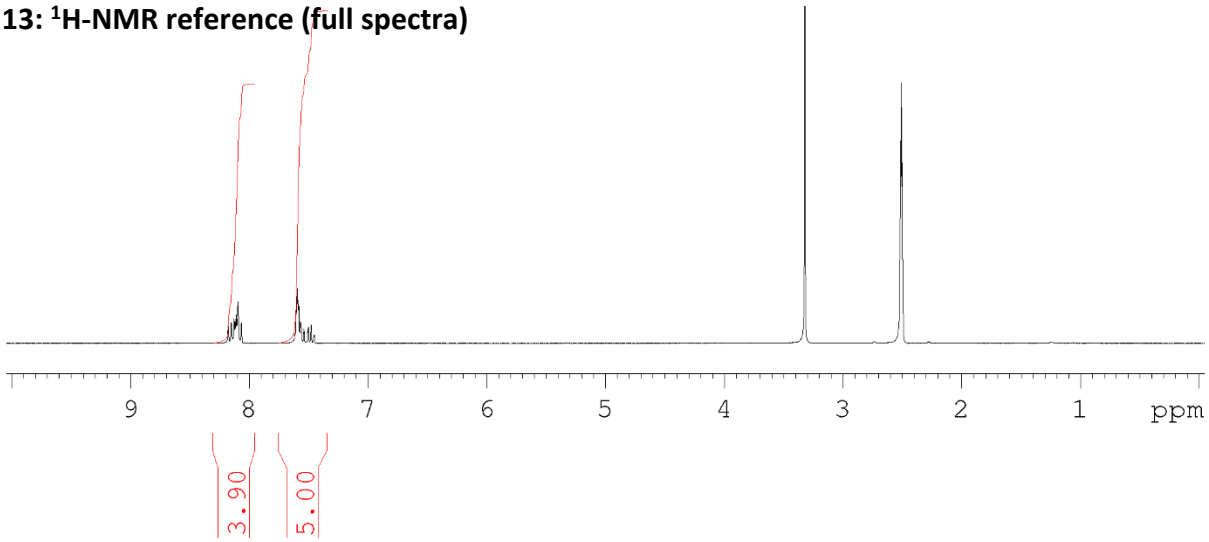


13: ^{1}H-NMR method B, workup C

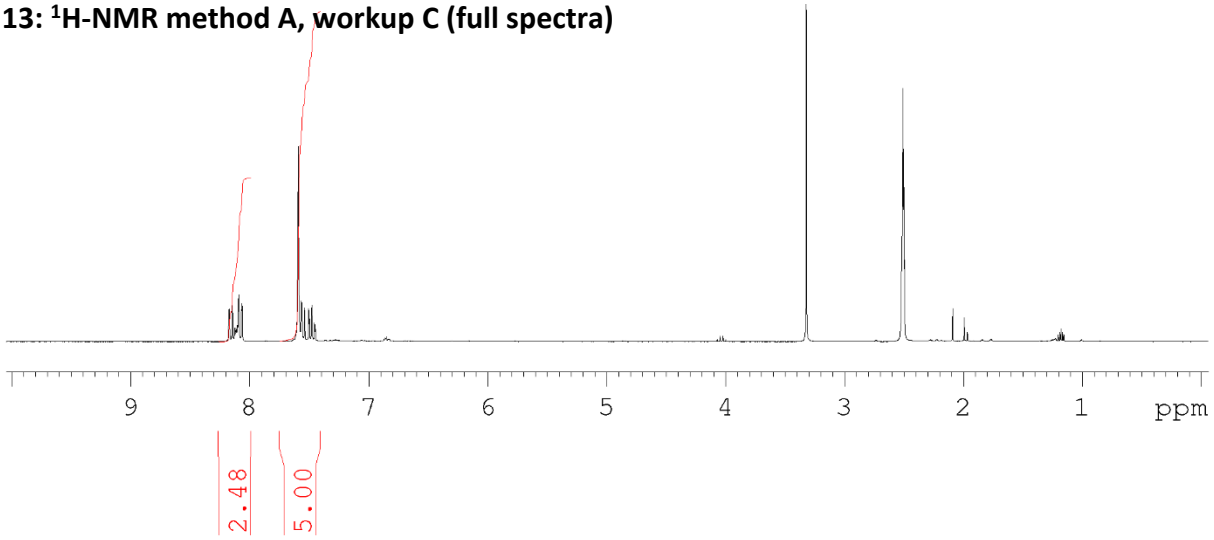


Deuterium incorporation: red arrow. Reference-integral: blue arrow.

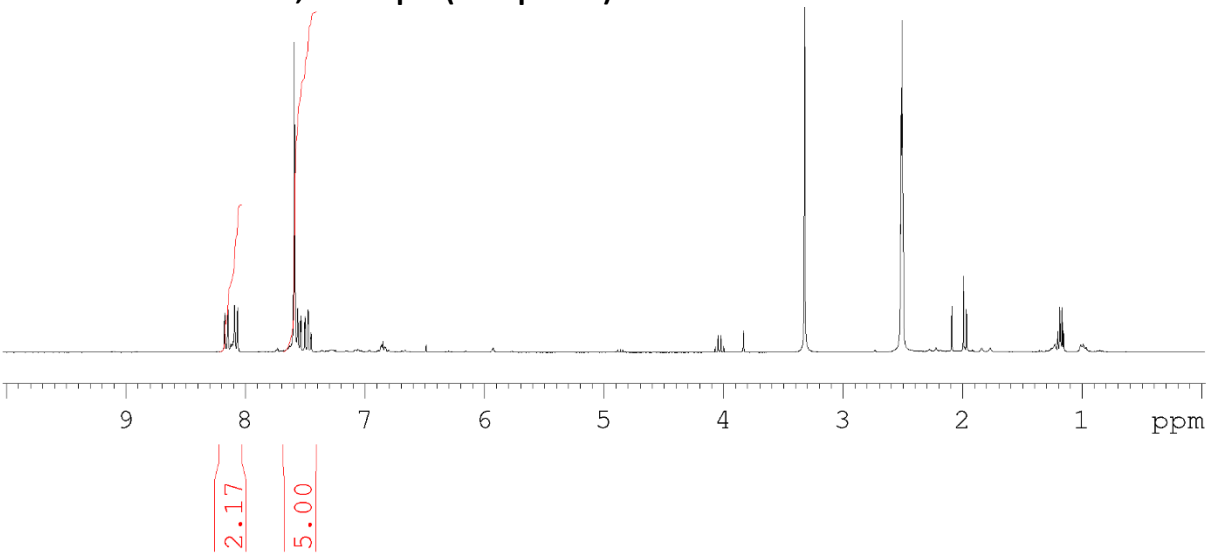
13: ^{1}H-NMR reference (full spectra)



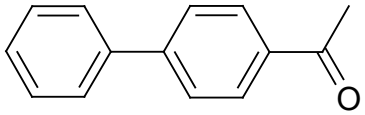
13: ^{1}H-NMR method A, workup C (full spectra)



13: ^{1}H-NMR method B, workup C (full spectra)



Data for 4-acetylbiphenyl **14**



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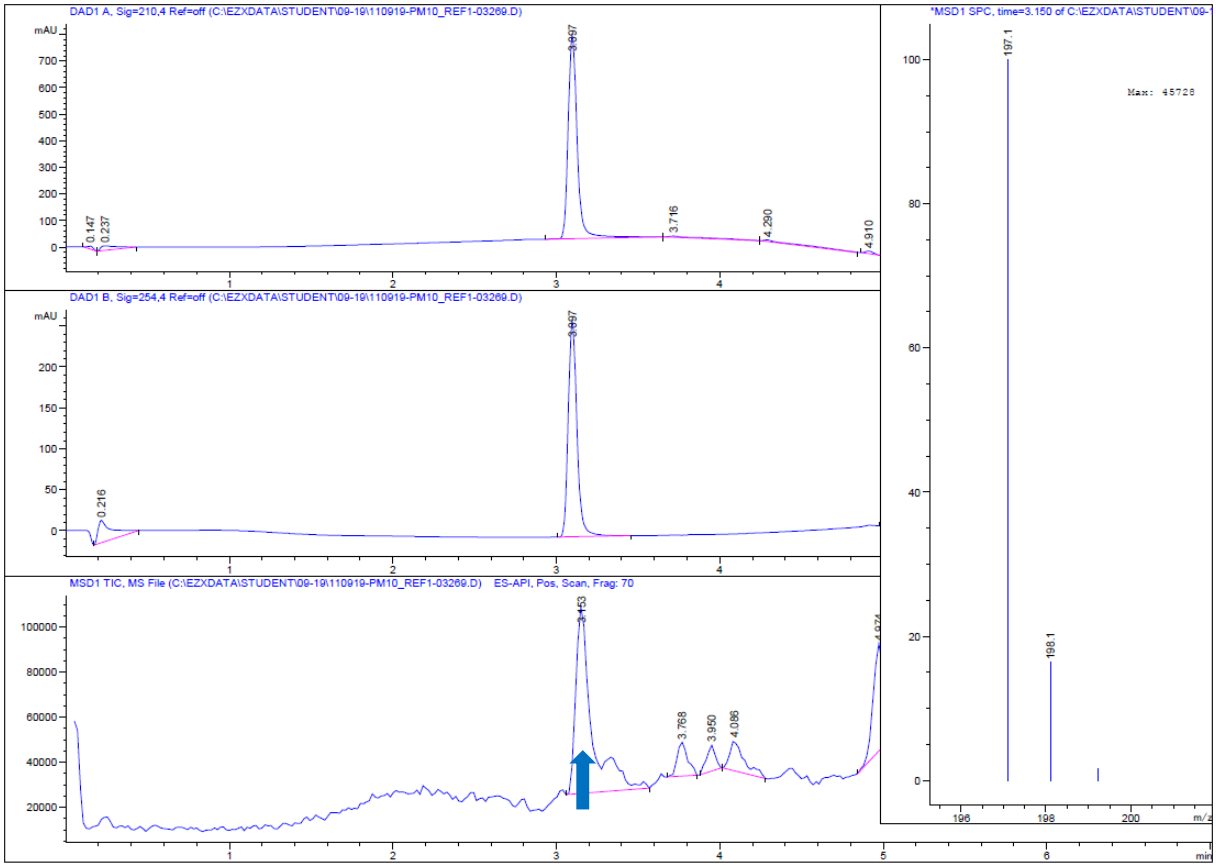
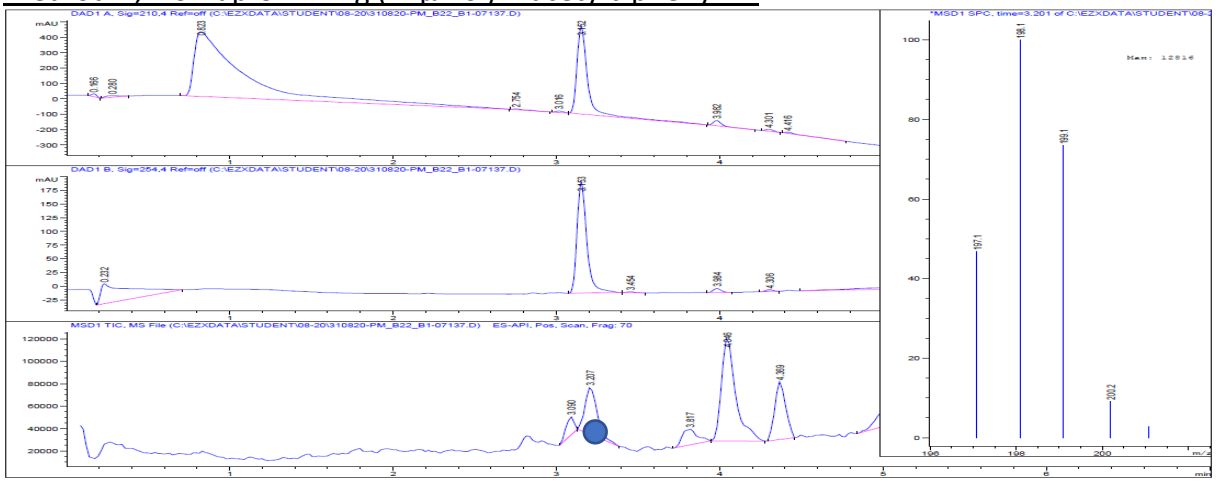


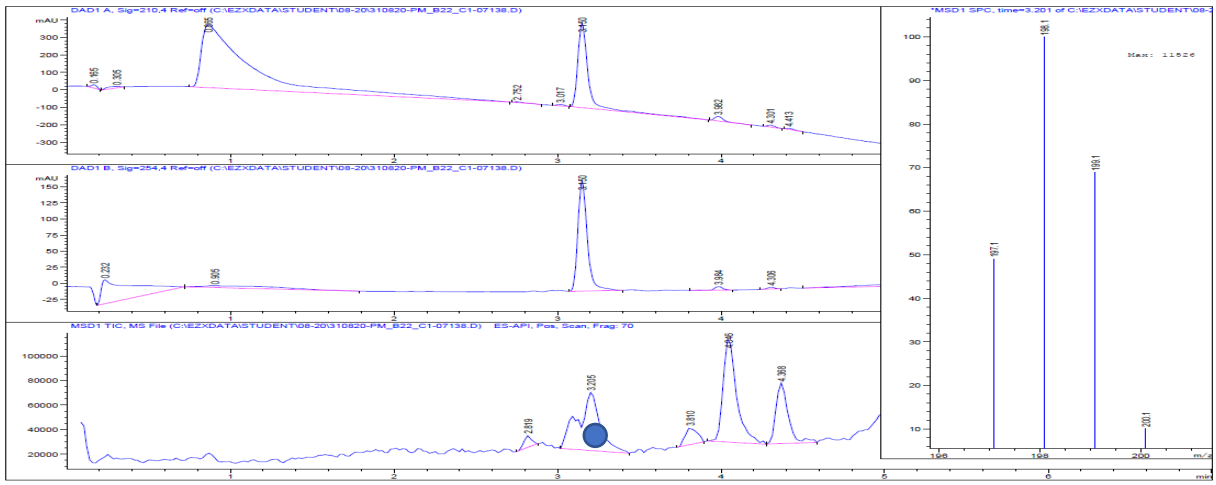
LC-MS (positive ESI): m/z 197.1 $[M+H]^+$ (100), 198.1 $[M+1+H]^+$ (16.4), 199.1 $[M+2+H]^+$ (1.6)

Deuterium experiments with 4-acetylbiphenyl **14**

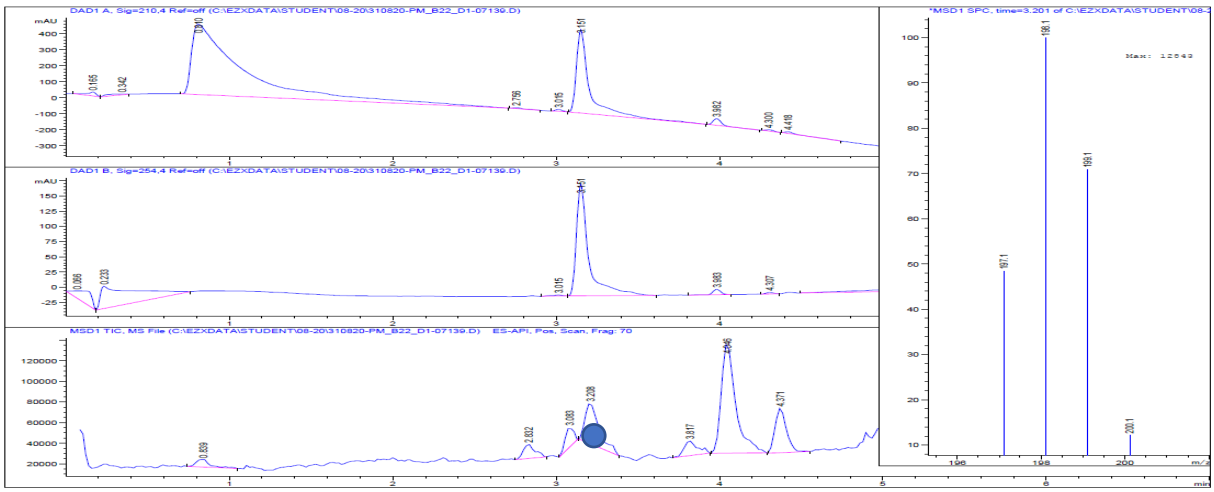
Method A, workup C: 2.1mg (11µmol) 4-acetylbiphenyl **14**



LC-MS (positive ESI): m/z 197.1 $[M+H]^+$ (46.8), 198.1 $[M(1D)+H]^+$ (100), 199.1 $[M(2D)+H]^+$ (73.4), 200.1 $[M(3D)+H]^+$ (9.2) : 52% D



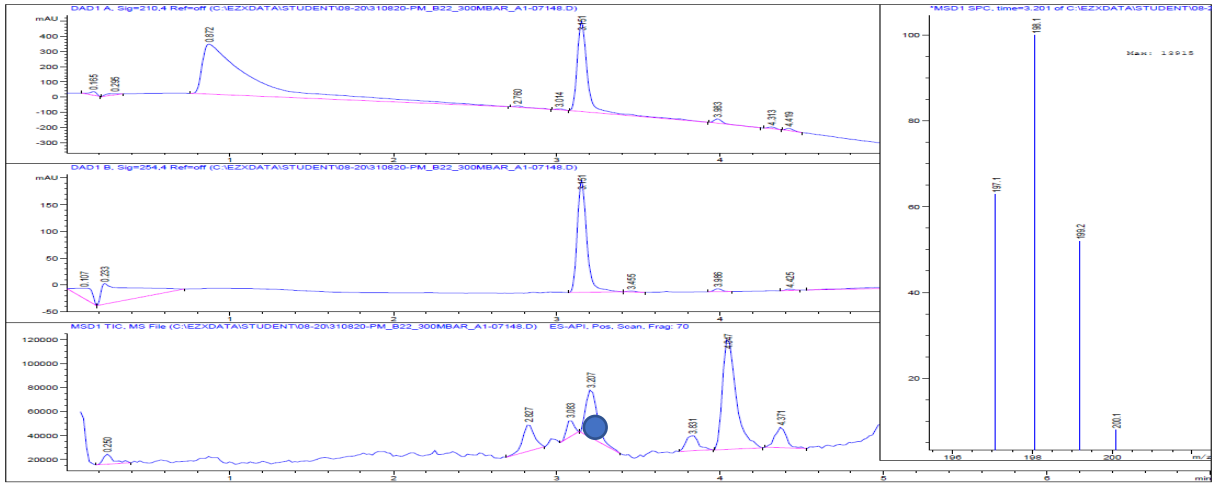
LC-MS (positive ESI): m/z 197.1 $[M+H]^+$ (49.1), 198.1 $[M(1D)+H]^+$ (100), 199.1 $[M(2D)+H]^+$ (68.9), 200.1 $[M(3D)+H]^+$ (10.1) : 51% D



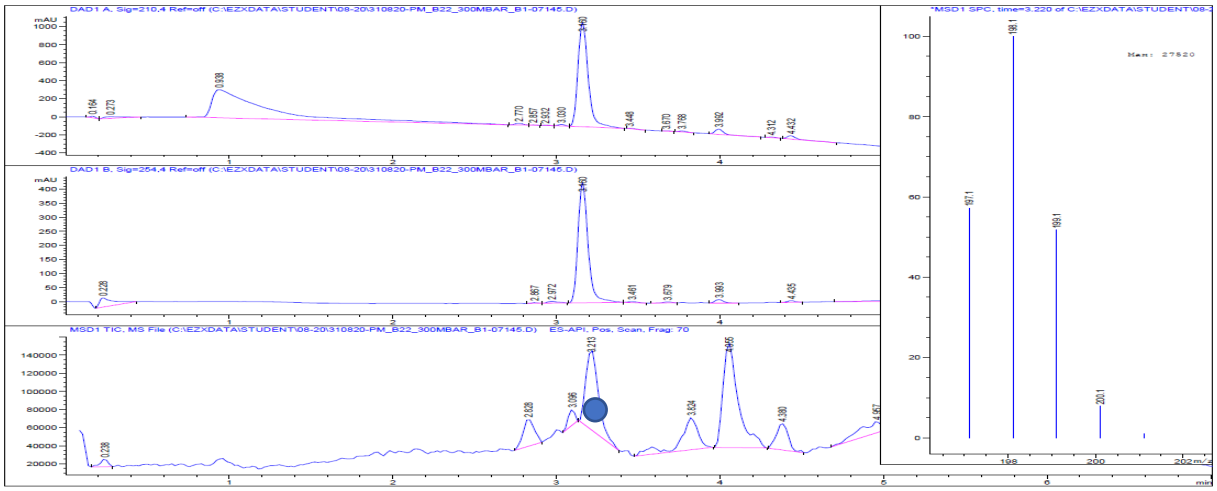
LC-MS (positive ESI): m/z 197.1 $[M+H]^+$ (48.4), 198.1 $[M(1D)+H]^+$ (100), 199.1 $[M(2D)+H]^+$ (70.9), 200.1 $[M(3D)+H]^+$ (12.1) : 51% D

Average of three reactions: 51% D, Yield: 96%, DCY: 49%

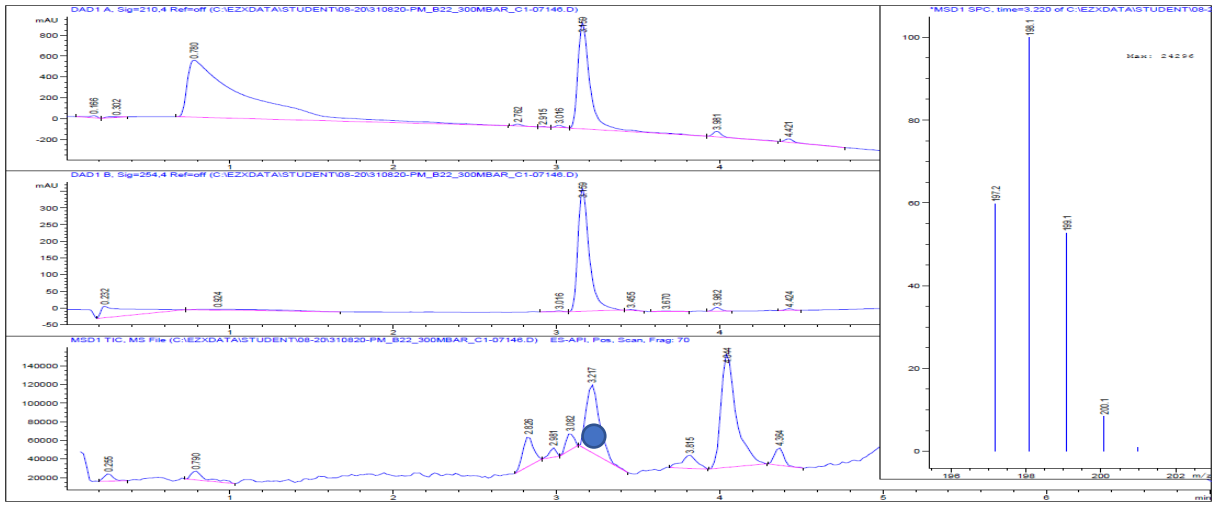
14: Method B, workup C: 2.5mg (13µmol) 4-acetylbiphenyl **14**



LC-MS (positive ESI): m/z 197.1 $[M+H]^+$ (62.9), 198.1 $[M(1D)+H]^+$ (100), 199.2 $[M(2D)+H]^+$ (51.9), 200.1 $[M(3D)+H]^+$ (7.9) : 43% D



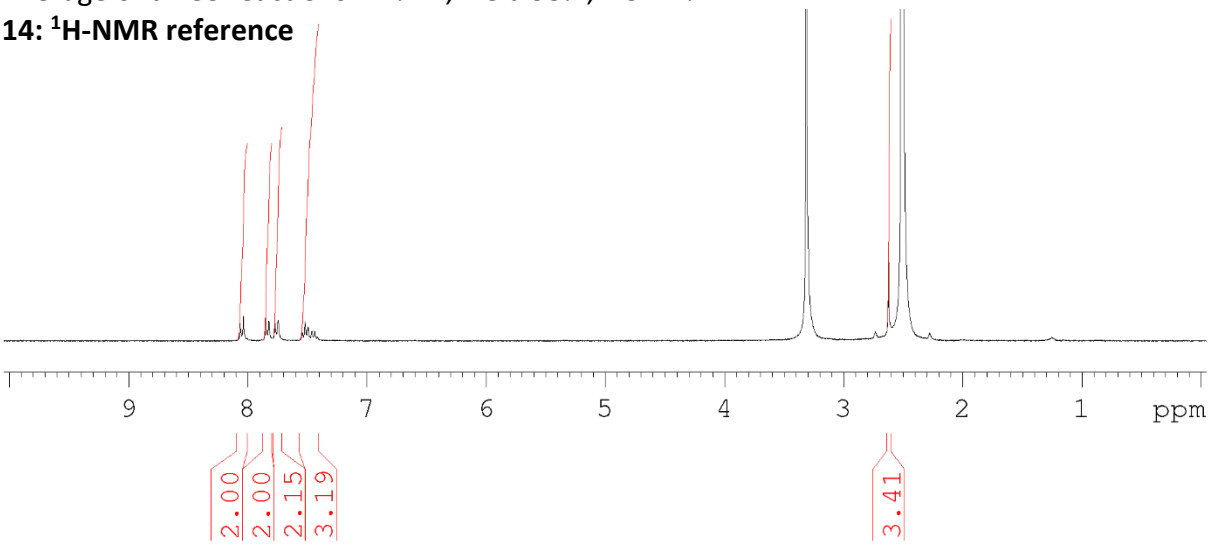
LC-MS (positive ESI): m/z 197.1 $[M+H]^+$ (57.2), 198.1 $[M(1D)+H]^+$ (100), 199.1 $[M(2D)+H]^+$ (51.8), 200.1 $[M(3D)+H]^+$ (7.9) : 45% D



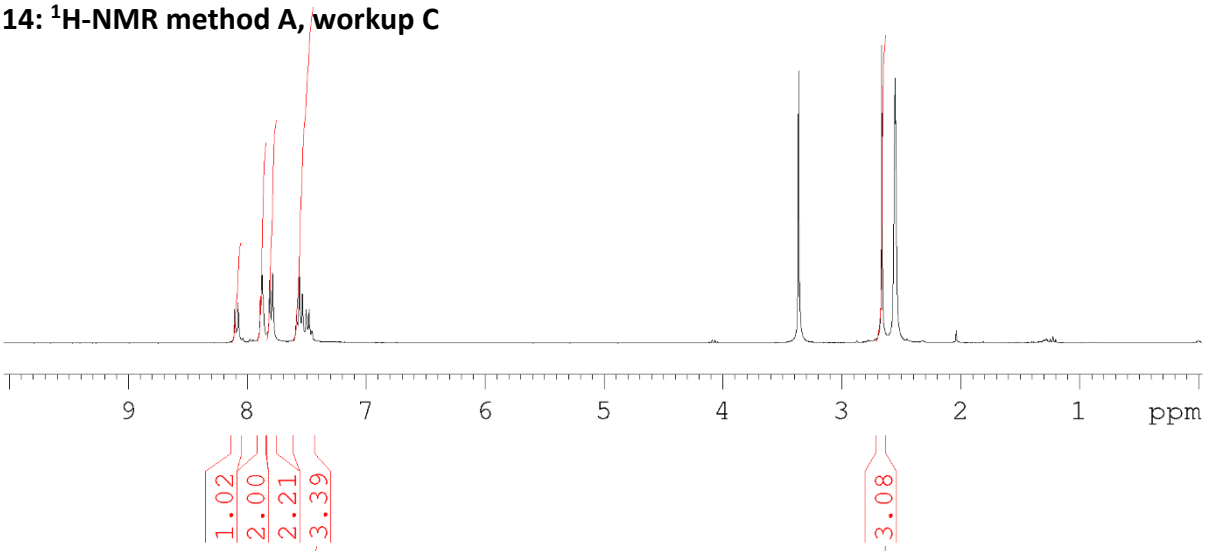
LC-MS (positive ESI): m/z 197.1 $[M+H]^+$ (59.8), 198.1 $[M(1D)+H]^+$ (100), 199.1 $[M(2D)+H]^+$ (52.7), 200.1 $[M(3D)+H]^+$ (8.4) : 44% D

Average of three reactions: 44% D, Yield 95%, DCY: 4%

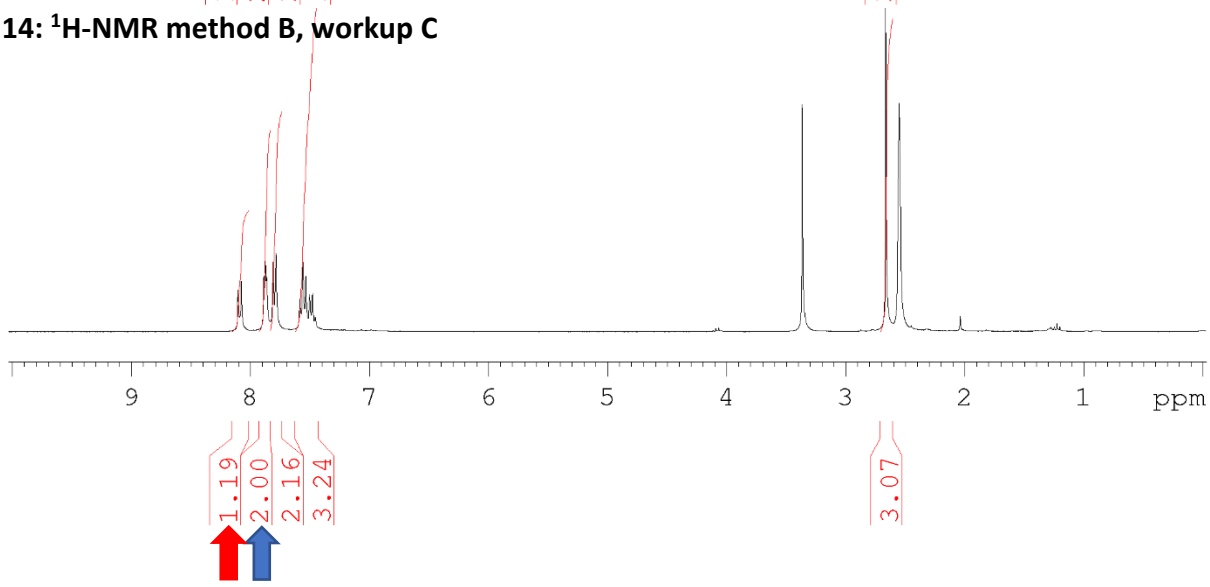
14: ^{1}H-NMR reference



14: ^{1}H-NMR method A, workup C

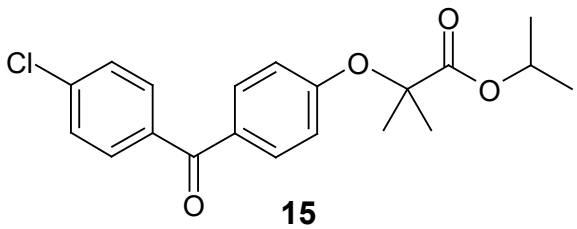


14: ^{1}H-NMR method B, workup C



Deuterium incorporation: red arrow. Reference-integral: blue arrow.

Data for Fenofibrate **15**



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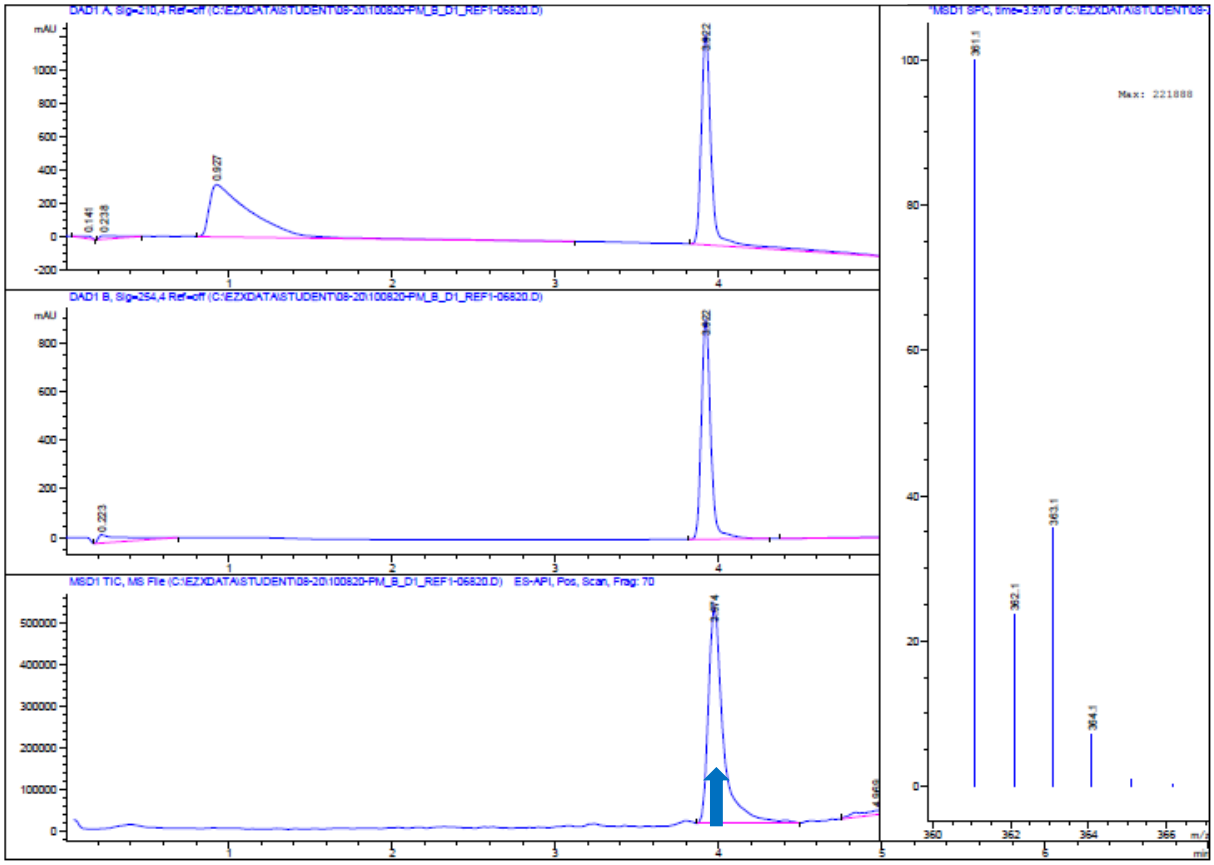
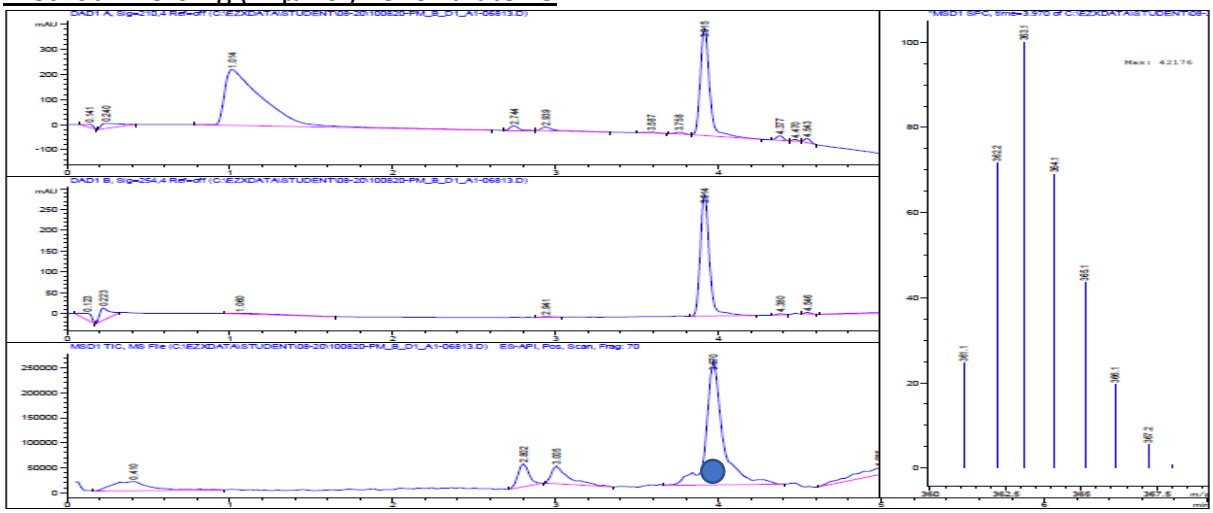


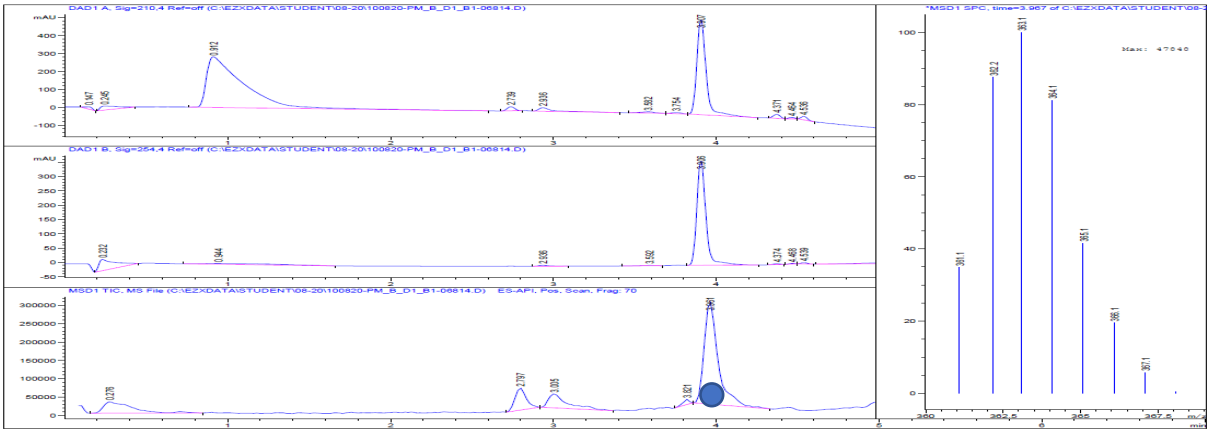
LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (100), 362.1 $[M+1+H]^+$ (23.7), 363.1 $[M+2+H]^+$ (35.6), 364.1 $[M+3+H]^+$ (7.2)

Deuterium experiments with Fenofibrate **15**

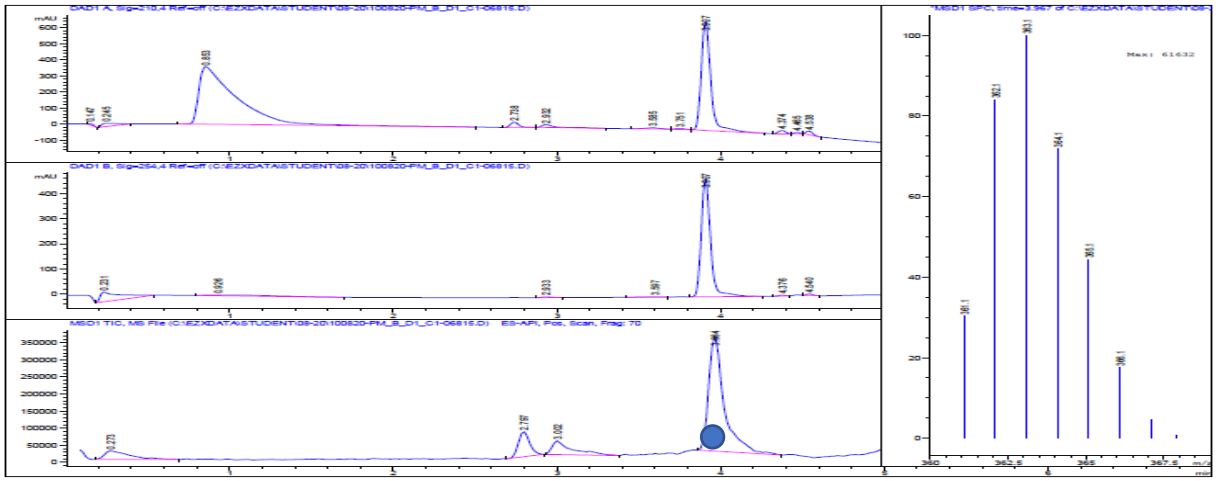
Method D: 5.0mg (14µmol) Fenofibrate **15**



LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (24.6), 362.2 $[M(1D)+H]^+$ (71.7), 363.1 $[M(2D)+H]^+$ (100), 364.1 $[M(3D)+H]^+$ (69), 365.1 $[M(4D)+H]^+$ (43.6), 366.1 $[M(5D)+H]^+$ (19.6) : 40% D



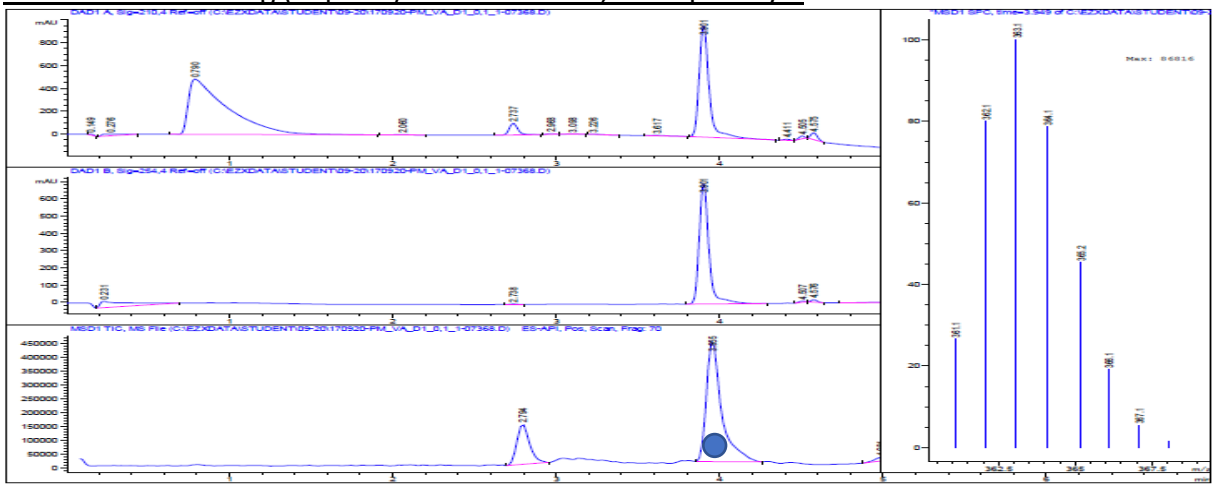
LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (34.9), 362.2 $[M(1D)+H]^+$ (87.6), 363.1 $[M(2D)+H]^+$ (100), 364.1 $[M(3D)+H]^+$ (88.2), 365.1 $[M(4D)+H]^+$ (41.6), 366.1 $[M(5D)+H]^+$ (19.5) : 37% D



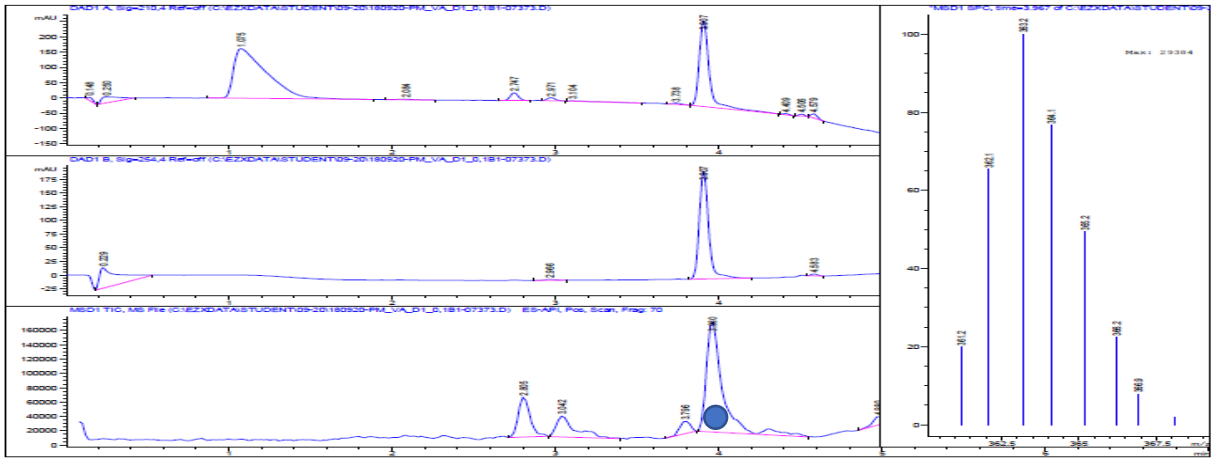
LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (30.3), 362.1 $[M(1D)+H]^+$ (84.1), 363.1 $[M(2D)+H]^+$ (100), 364.1 $[M(3D)+H]^+$ (71.9), 365.1 $[M(4D)+H]^+$ (44.4), 366.1 $[M(5D)+H]^+$ (17.5) : 37% D

Average of three reactions: 38% D, Yield: 94%, DCY: 71%

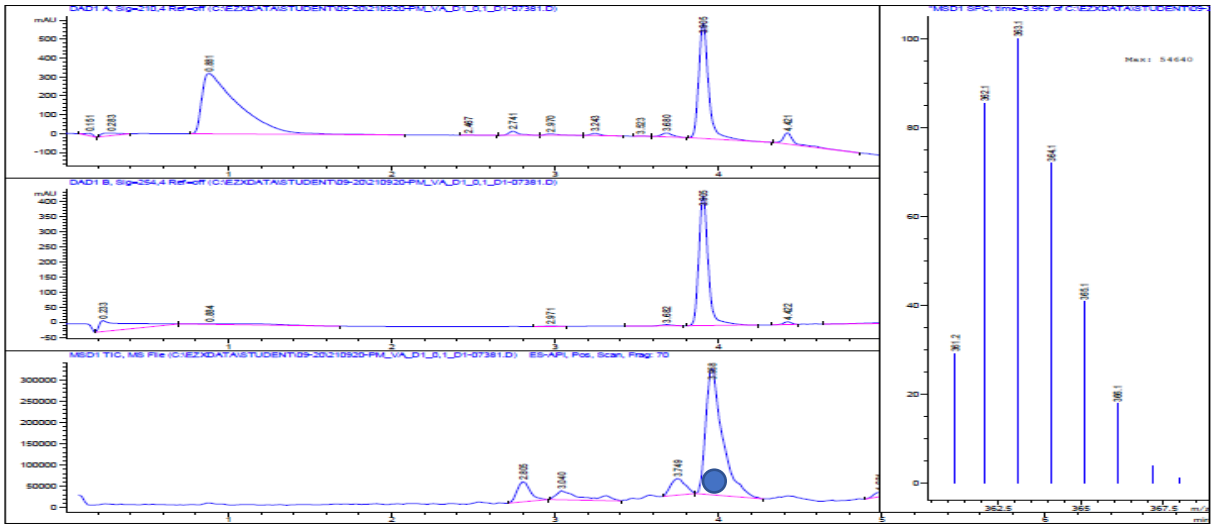
15: Method E: 5.0mg (14µmol) Fenofibrate **15**, 0.1 eq catalyst



LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (26.6), 362.1 $[M(1D)+H]^+$ (80.0), 363.1 $[M(2D)+H]^+$ (100), 364.1 $[M(3D)+H]^+$ (78.7), 365.1 $[M(4D)+H]^+$ (45.4), 366.1 $[M(5D)+H]^+$ (19.1) : 39% D



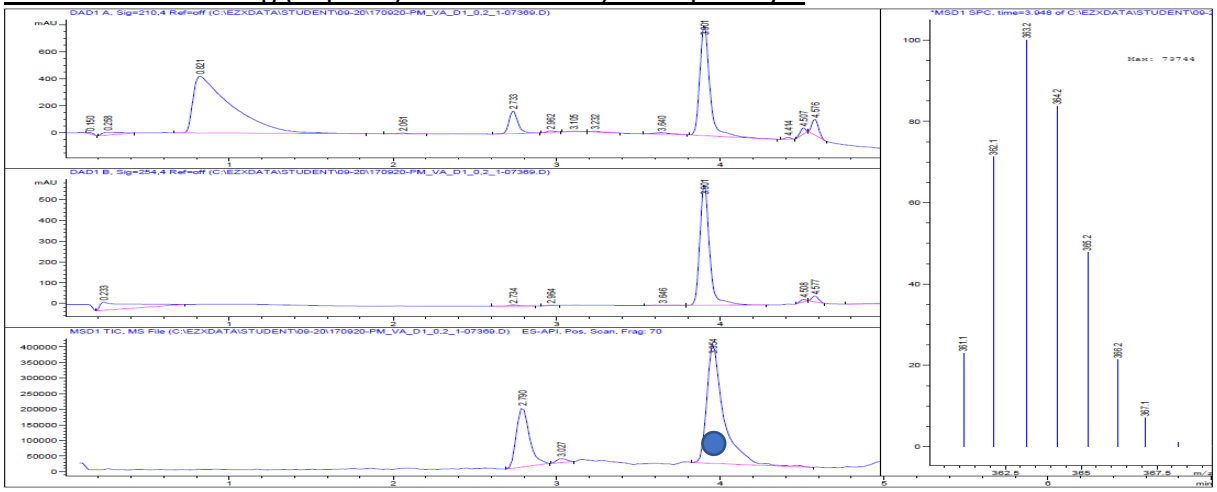
LC-MS (positive ESI): m/z 361.2 $[M+H]^+$ (20.0), 362.1 $[M(1D)+H]^+$ (65.5), 363.1 $[M(2D)+H]^+$ (100), 364.1 $[M(3D)+H]^+$ (76.7), 365.2 $[M(4D)+H]^+$ (49.4), 366.2 $[M(5D)+H]^+$ (22.4) : 44% D



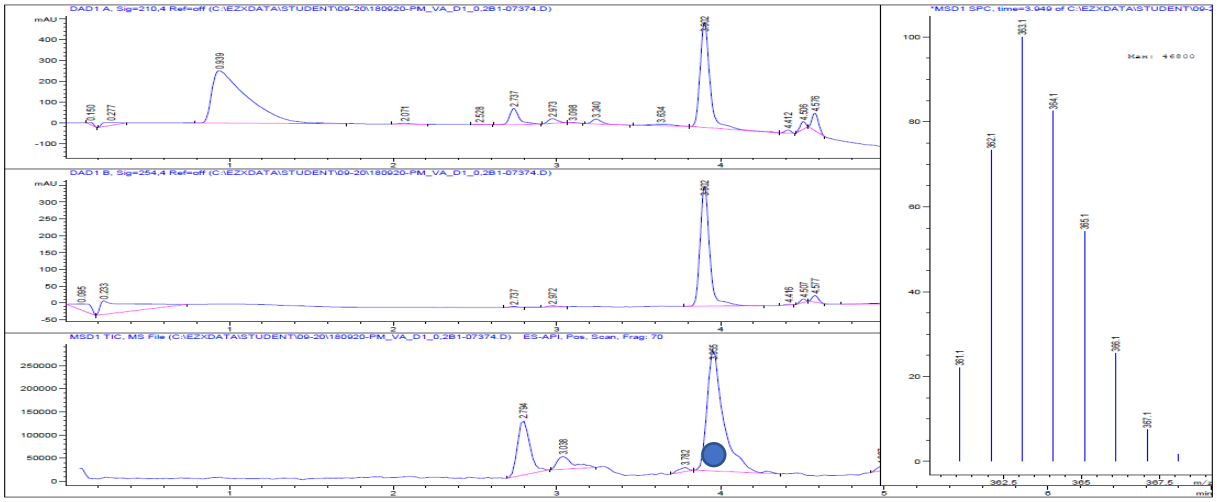
LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (26.3), 362.1 $[M(1D)+H]^+$ (74.8), 363.1 $[M(2D)+H]^+$ (100), 364.2 $[M(3D)+H]^+$ (75.7), 365.1 $[M(4D)+H]^+$ (43.8), 366.2 $[M(5D)+H]^+$ (19.4) : 41% D

Average of three reactions: 40% D, Yield: 76%, DCY: 61%

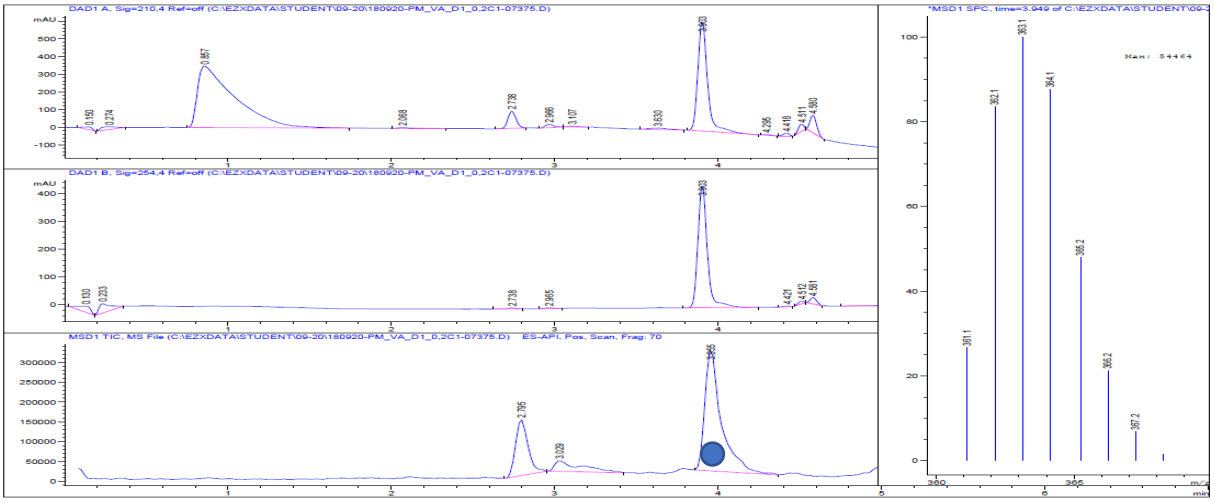
15: Method E: 5.0mg (14µmol) Fenofibrate **15**, 0.2 eq catalyst



LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (23.0), 362.1 $[M(1D)+H]^+$ (71.3), 363.2 $[M(2D)+H]^+$ (100), 364.2 $[M(3D)+H]^+$ (83.7), 365.2 $[M(4D)+H]^+$ (47.8), 366.2 $[M(5D)+H]^+$ (21.3) : 43% D



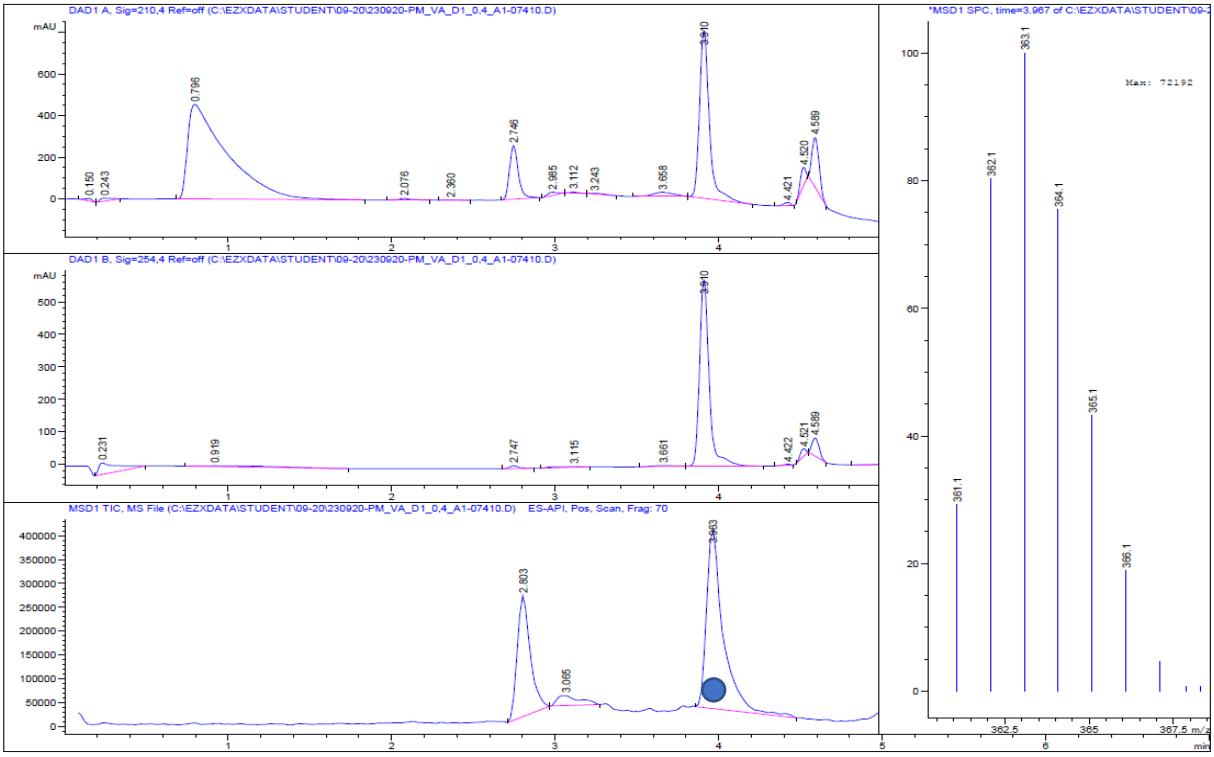
LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (22.1), 362.1 $[M(1D)+H]^+$ (73.3), 363.1 $[M(2D)+H]^+$ (100), 364.1 $[M(3D)+H]^+$ (82.6), 365.1 $[M(4D)+H]^+$ (54.3), 366.1 $[M(5D)+H]^+$ (25.4) : 45% D



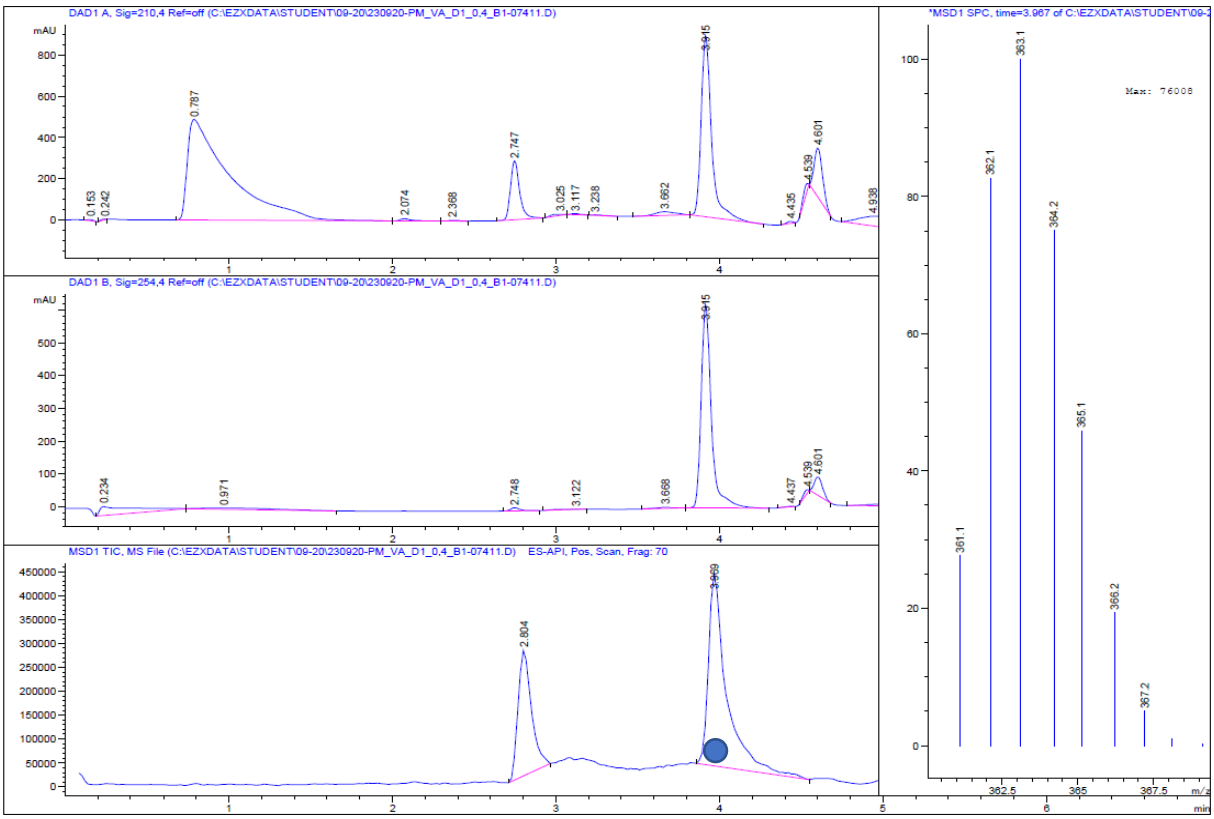
LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (26.7), 362.1 $[M(1D)+H]^+$ (83.5), 363.1 $[M(2D)+H]^+$ (100), 364.1 $[M(3D)+H]^+$ (87.7), 365.2 $[M(4D)+H]^+$ (48.0), 366.2 $[M(5D)+H]^+$ (21.3) : 41% D

Average of three reactions: 43% D, Yield: 75%, DCY: 65%

15: Method E: 5.0mg (14µmol) Fenofibrate **15**, 0.4 eq catalyst



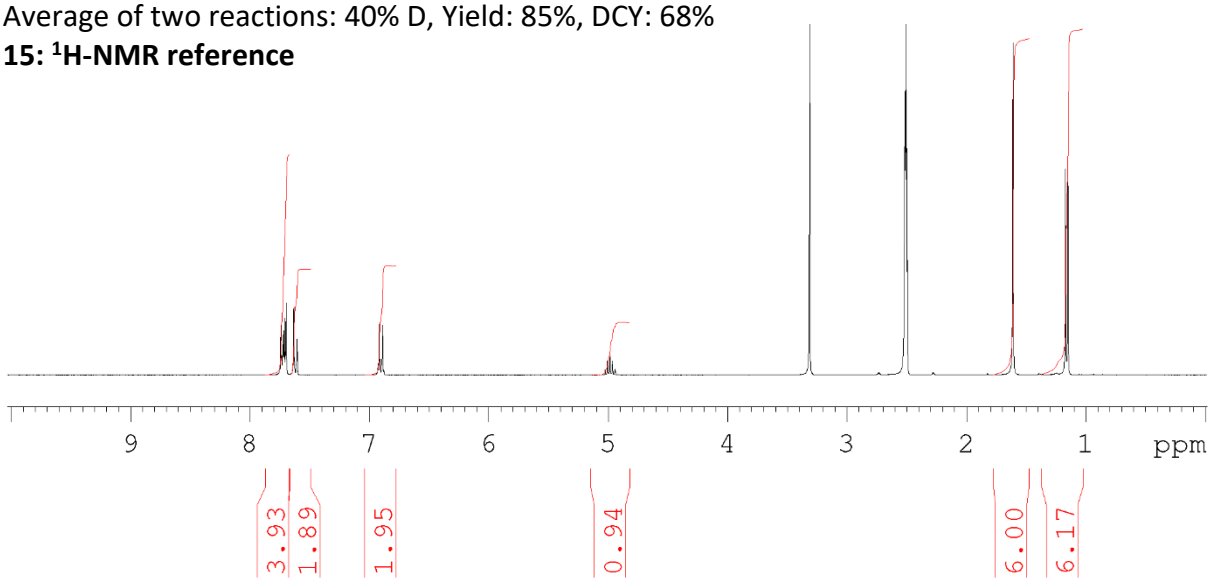
LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (29.3), 362.1 $[M(1D)+H]^+$ (80.3), 363.1 $[M(2D)+H]^+$ (100), 364.1 $[M(3D)+H]^+$ (75.5), 365.1 $[M(4D)+H]^+$ (43.2), 366.1 $[M(5D)+H]^+$ (18.9) : 39% D



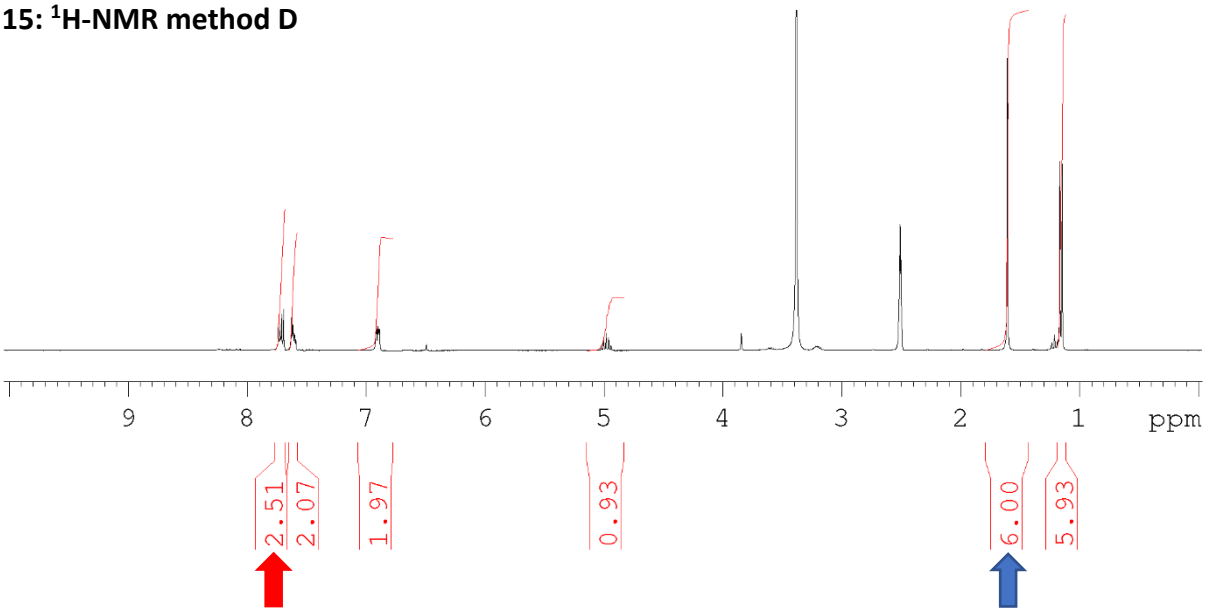
LC-MS (positive ESI): m/z 361.1 $[M+H]^+$ (27.7), 362.1 $[M(1D)+H]^+$ (82.7), 363.1 $[M(2D)+H]^+$ (100), 364.2 $[M(3D)+H]^+$ (75.0), 365.1 $[M(4D)+H]^+$ (45.9), 366.2 $[M(5D)+H]^+$ (19.4) : 40% D

Average of two reactions: 40% D, Yield: 85%, DCY: 68%

15: ^{1}H-NMR reference

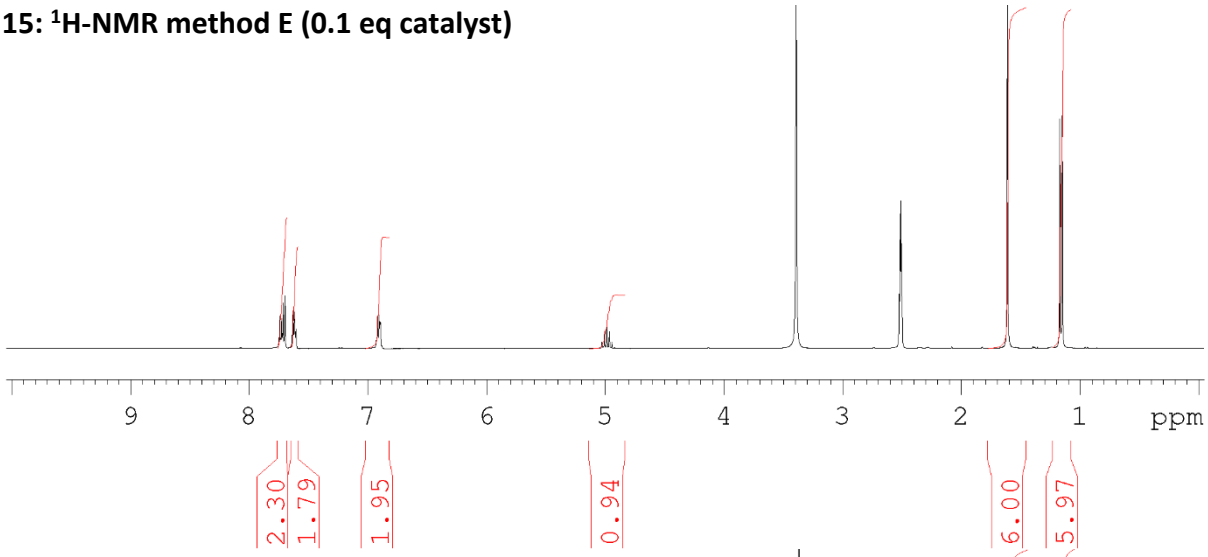


15: ^{1}H-NMR method D

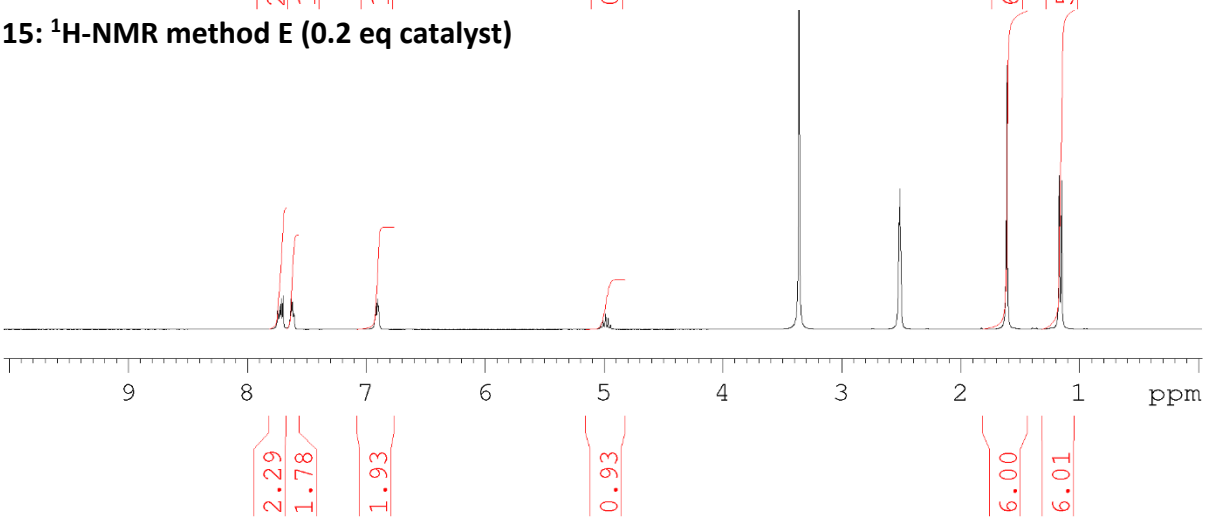


Deuterium incorporation: red arrow. Reference-integral: blue arrow.

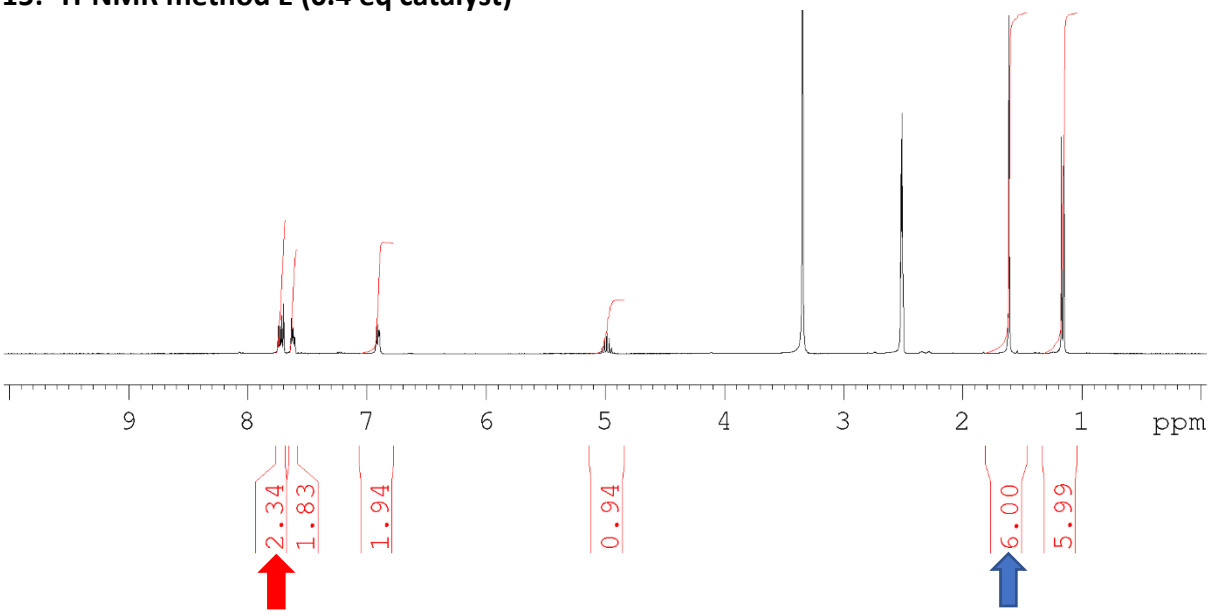
15: ^{1}H-NMR method E (0.1 eq catalyst)



15: ^{1}H-NMR method E (0.2 eq catalyst)

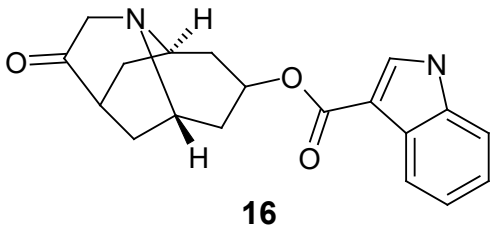


15: ^{1}H-NMR method E (0.4 eq catalyst)

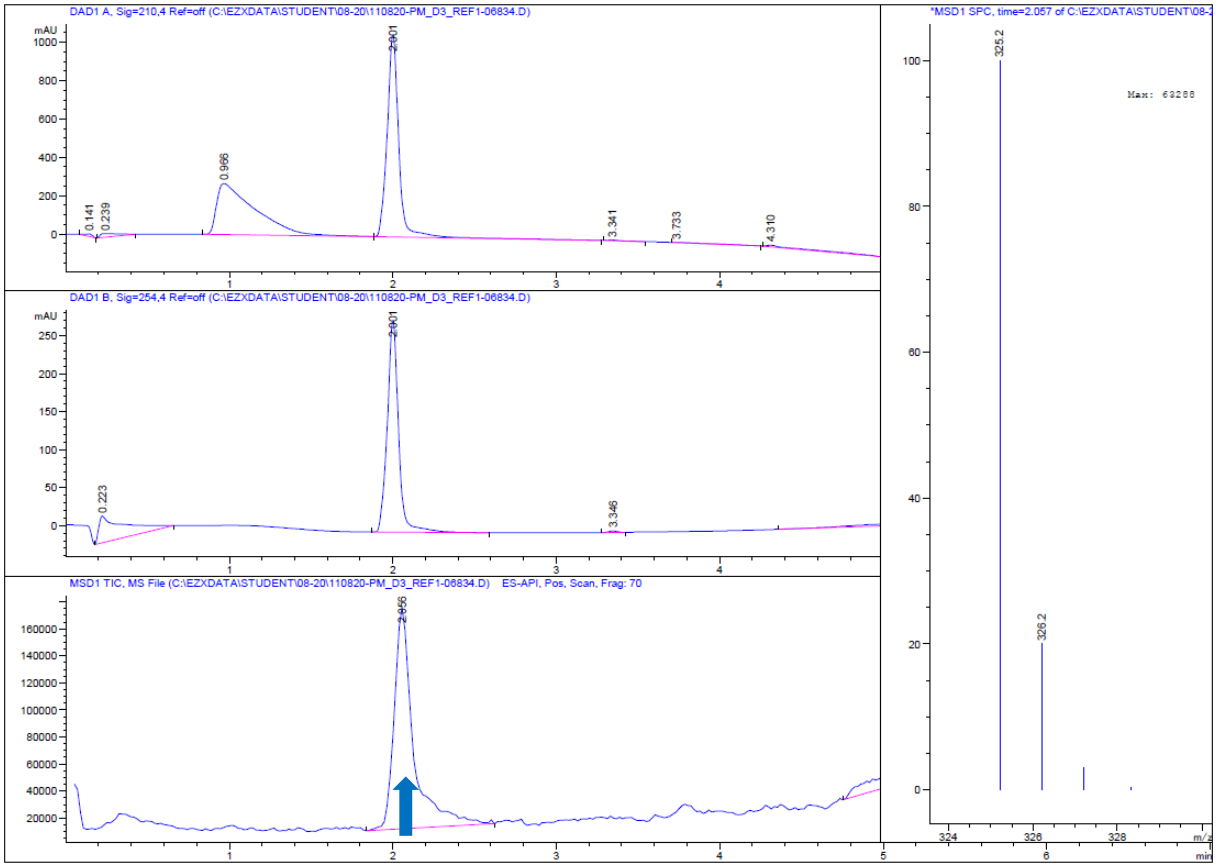


Deuterium incorporation: red arrow. Reference-integral: blue arrow.

Data for Dolasetron **16**



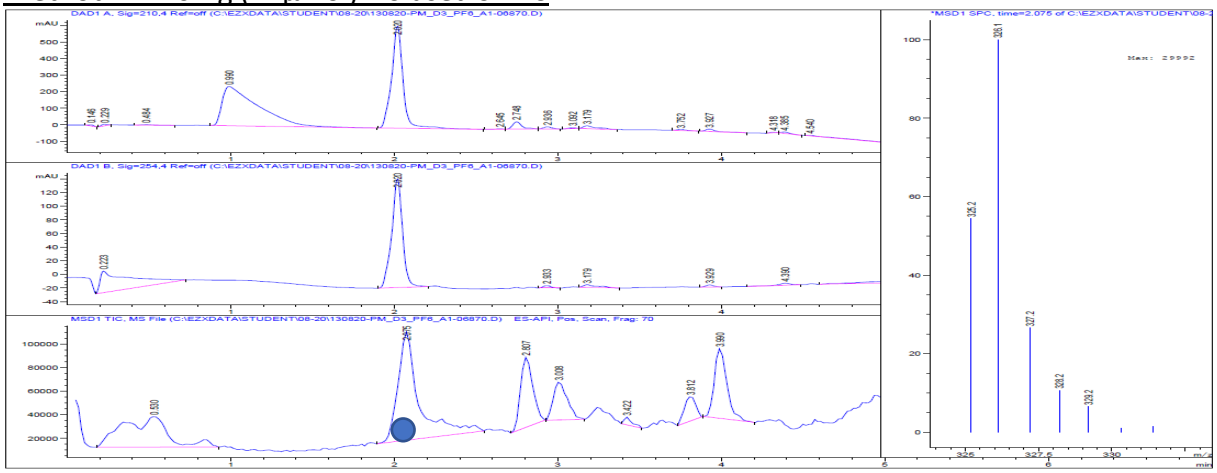
16



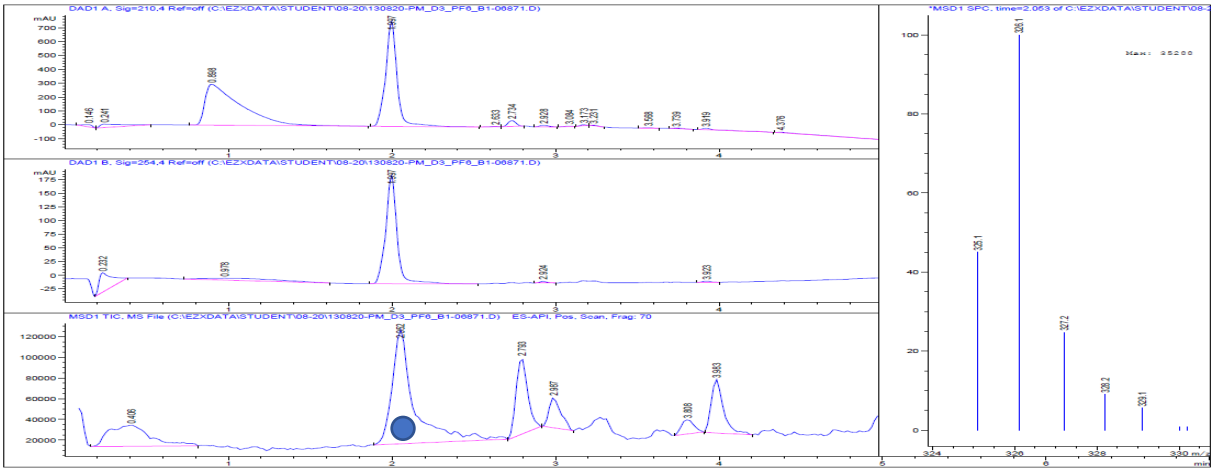
LC-MS (positive ESI): m/z 325.2 $[M+H]^+$ (100), 326.2 $[M+1+H]^+$ (20.0), 327.2 $[M+2+H]^+$ (3.0)

Deuterium experiments with Dolasetron **16**

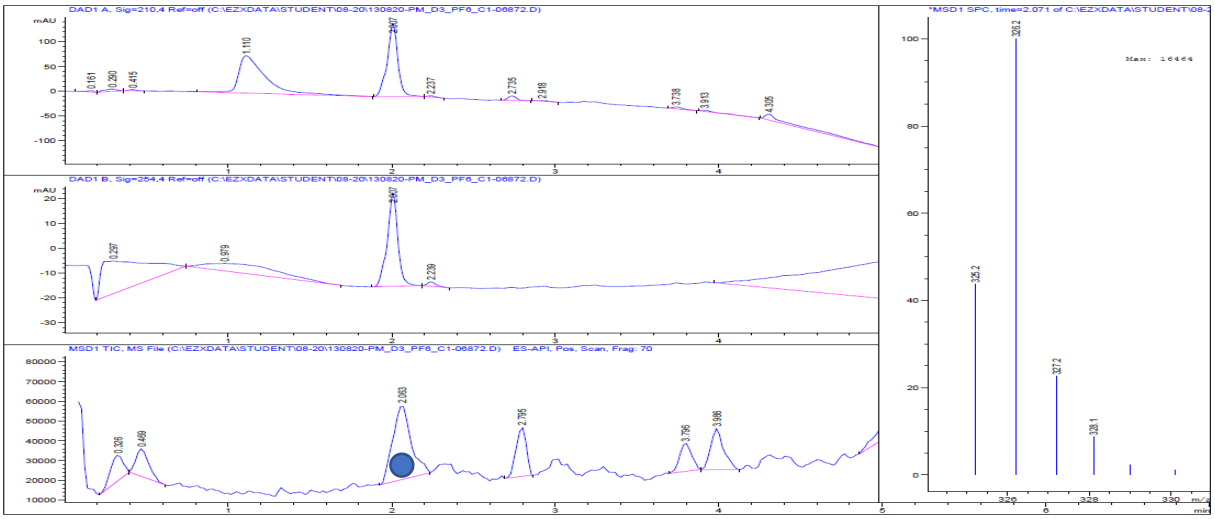
Method D: 4.6mg (14µmol) Dolasetron **16**



LC-MS (positive ESI): m/z 325.2 $[M+H]^+$ (54.4), 326.1 $[M(1D)+H]^+$ (100), 327.2 $[M(2D)+H]^+$ (26.6), 328.2 $[M(3D)+H]^+$ (10.7), 329.2 $[M(4D)+H]^+$ (6.6) : 43% D



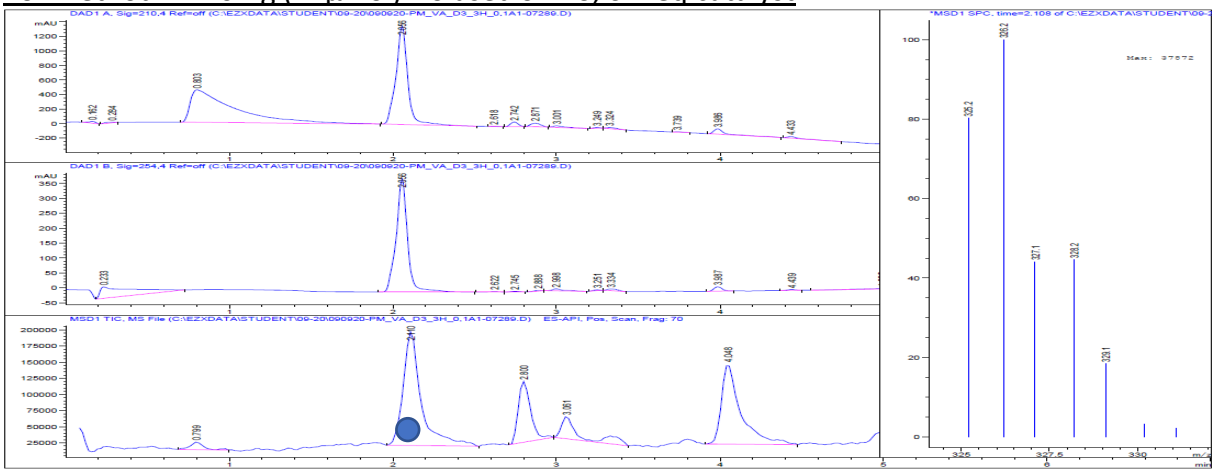
LC-MS (positive ESI): m/z 325.1 $[M+H]^+$ (45.1), 326.1 $[M(1D)+H]^+$ (100), 327.2 $[M(2D)+H]^+$ (24.8), 328.2 $[M(3D)+H]^+$ (9.1), 329.2 $[M(4D)+H]^+$ (5.6) : 45% D



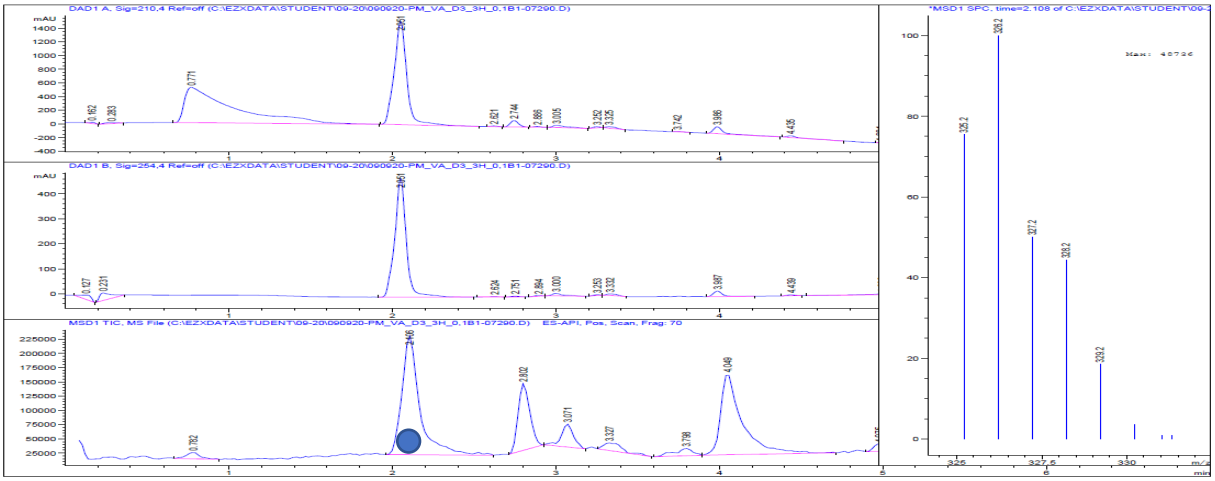
LC-MS (positive ESI): m/z 325.2 $[M+H]^+$ (43.8), 326.2 $[M(1D)+H]^+$ (100), 327.2 $[M(2D)+H]^+$ (22.6), 328.1 $[M(3D)+H]^+$ (8.7), 329.0 $[M(4D)+H]^+$ (2.3) : 42% D

Average of three reactions: 43% D, Yield: 94%, DCY: 40%

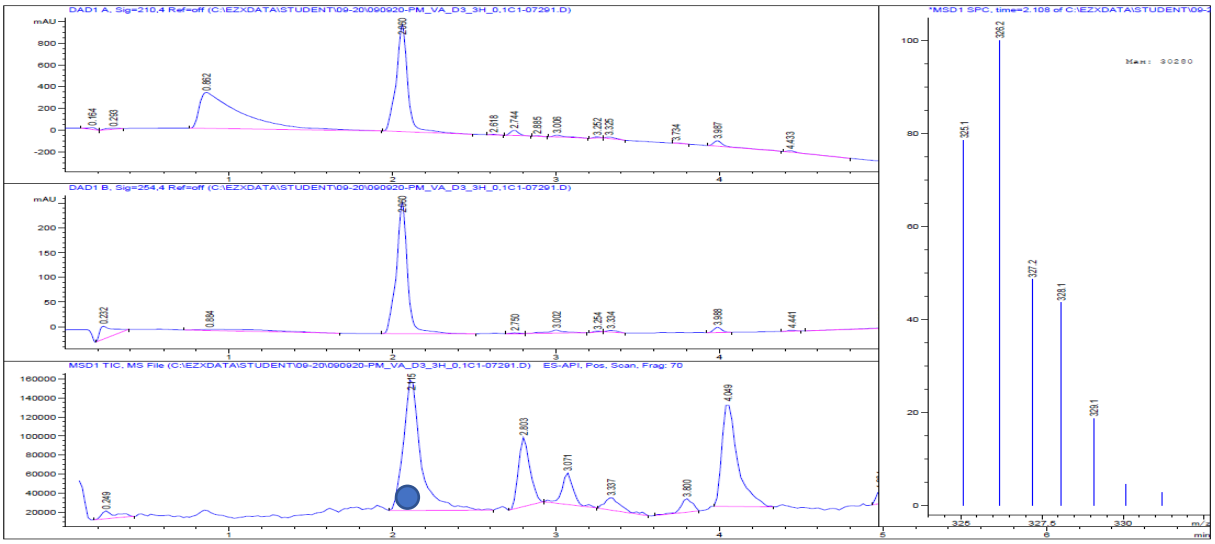
16: Method E: 4.6mg (14µmol) Dolasetron **16**, 0.1 eq catalyst



LC-MS (positive ESI): m/z 325.2 $[M+H]^+$ (80.3), 326.2 $[M(1D)+H]^+$ (100), 327.1 $[M(2D)+H]^+$ (44.1), 328.2 $[M(3D)+H]^+$ (44.7), 329.1 $[M(4D)+H]^+$ (18.5) : 61% D



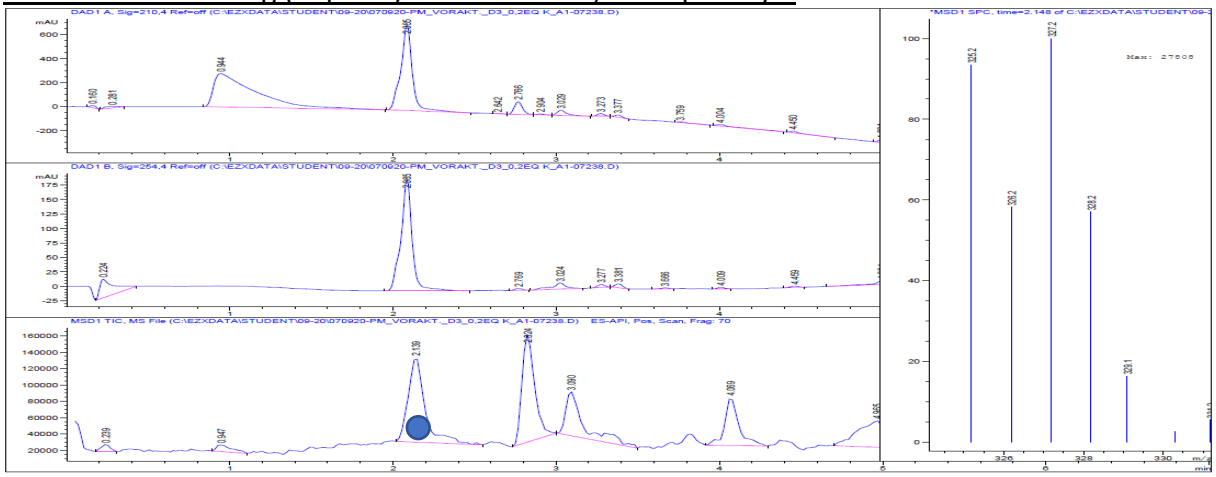
LC-MS (positive ESI): m/z 325.2 $[M+H]^+$ (75.5), 326.2 $[M(1D)+H]^+$ (100), 327.2 $[M(2D)+H]^+$ (50.1), 328.2 $[M(3D)+H]^+$ (44.4), 329.2 $[M(4D)+H]^+$ (18.7) : 62% D



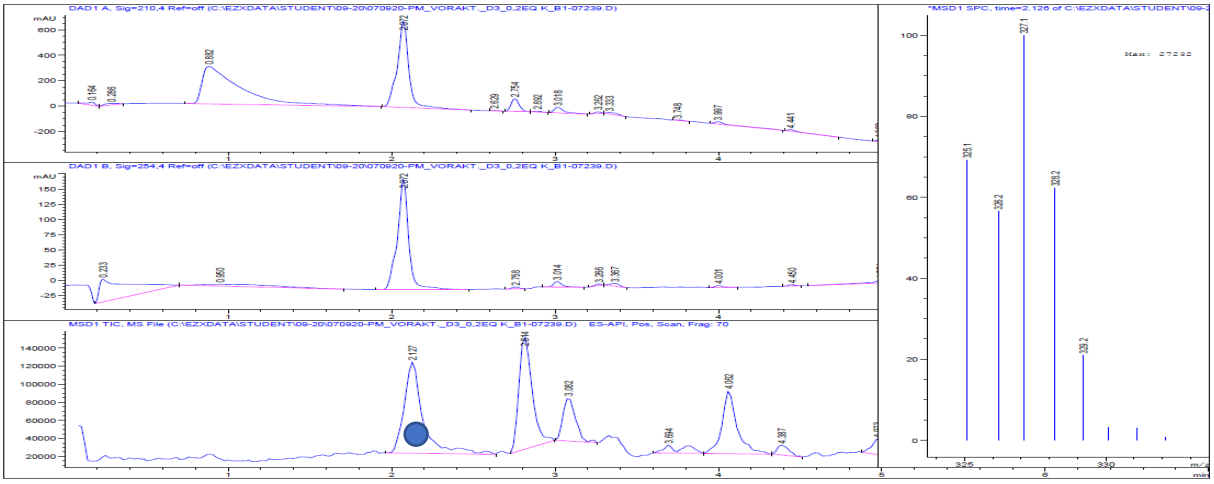
LC-MS (positive ESI): m/z 325.1 $[M+H]^+$ (78.5), 326.2 $[M(1D)+H]^+$ (100), 327.2 $[M(2D)+H]^+$ (48.6), 328.1 $[M(3D)+H]^+$ (43.7), 329.1 $[M(4D)+H]^+$ (18.7) : 62% D

Average of three reactions: 62% D, Yield: 95%, DCY: 59%

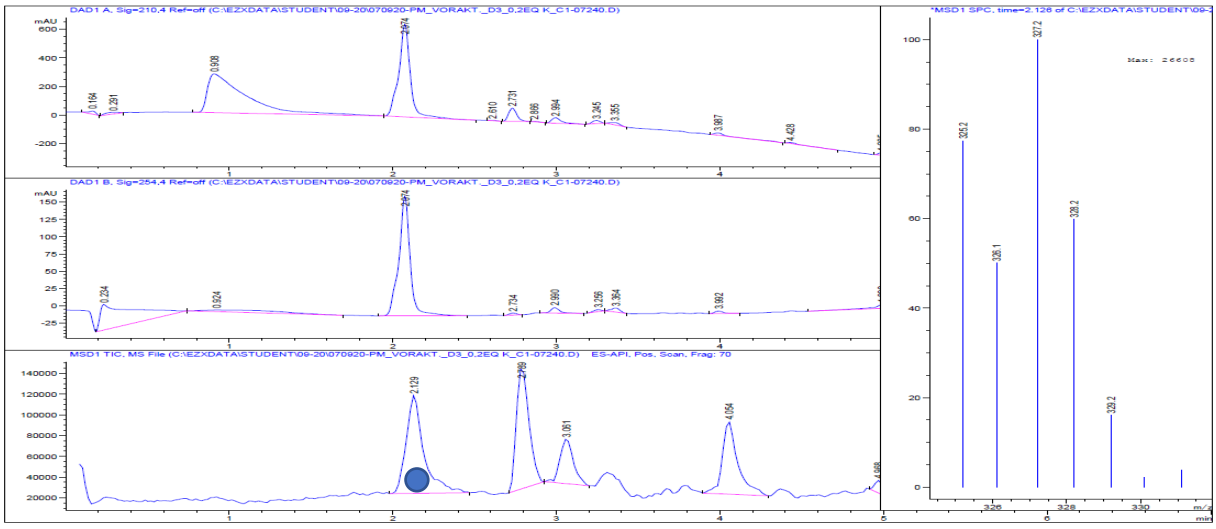
16: Method E: 4.6mg (14µmol) Dolasetron **16**, 0.2 eq catalyst



LC-MS (positive ESI): m/z 325.2 $[M+H]^+$ (93.5), 326.2 $[M(1D)+H]^+$ (58.2), 327.2 $[M(2D)+H]^+$ (100), 328.2 $[M(3D)+H]^+$ (57.0), 329.1 $[M(4D)+H]^+$ (16.3) : 68% D



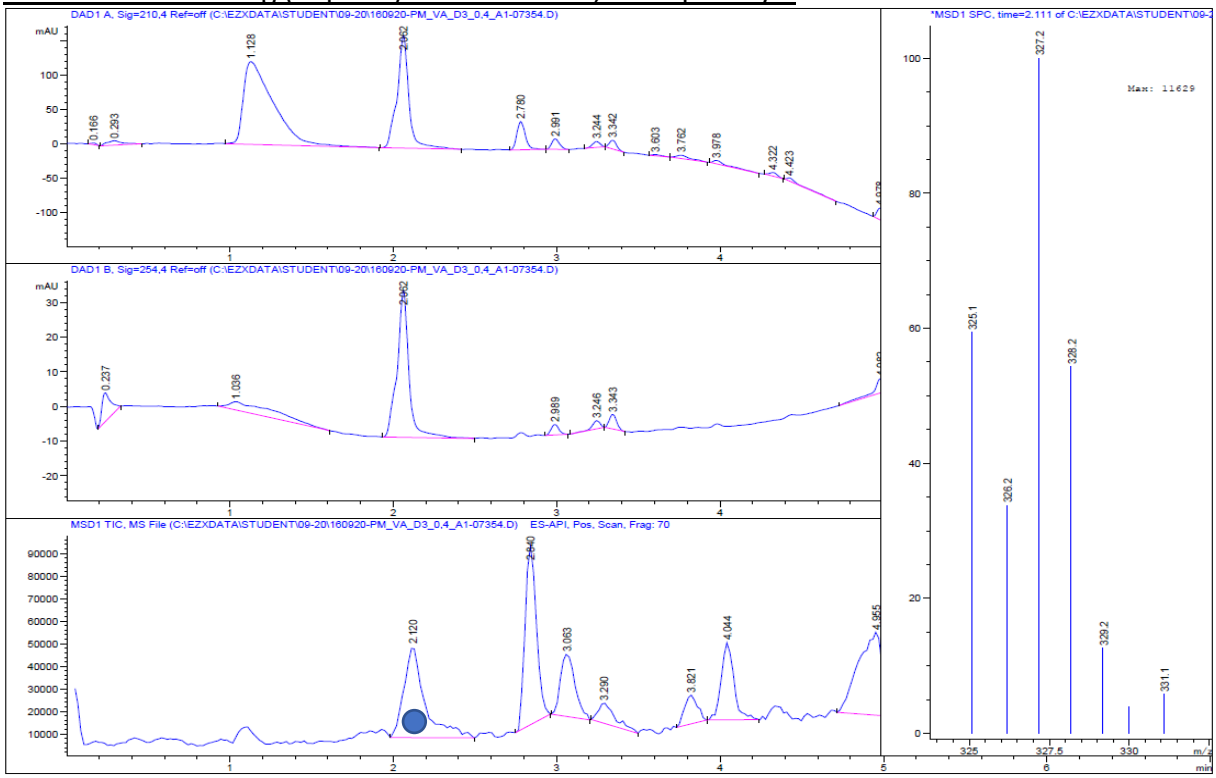
LC-MS (positive ESI): m/z 325.1 $[M+H]^+$ (69.3), 326.2 $[M(1D)+H]^+$ (56.6), 327.1 $[M(2D)+H]^+$ (100), 328.2 $[M(3D)+H]^+$ (62.4), 329.2 $[M(4D)+H]^+$ (21.0) : 77% D



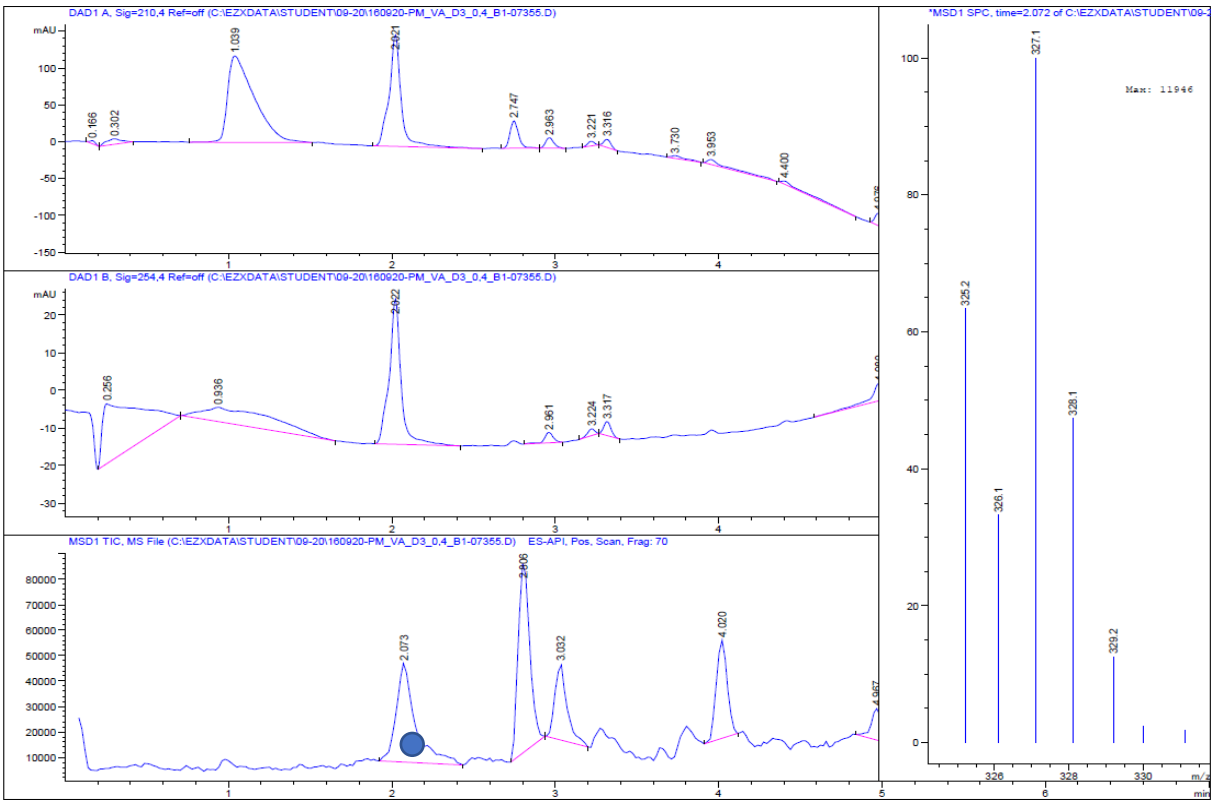
LC-MS (positive ESI): m/z 325.2 $[M+H]^+$ (72.4), 326.1 $[M(1D)+H]^+$ (50.1), 327.2 $[M(2D)+H]^+$ (100), 328.2 $[M(3D)+H]^+$ (59.9), 329.2 $[M(4D)+H]^+$ (16.1) : 73% D

Average of three reactions: 73% D, Yield: 93%, DCY: 68%

16: Method E: 4.6mg (14µmol) Dolasetron **16**, 0.4 eq catalyst



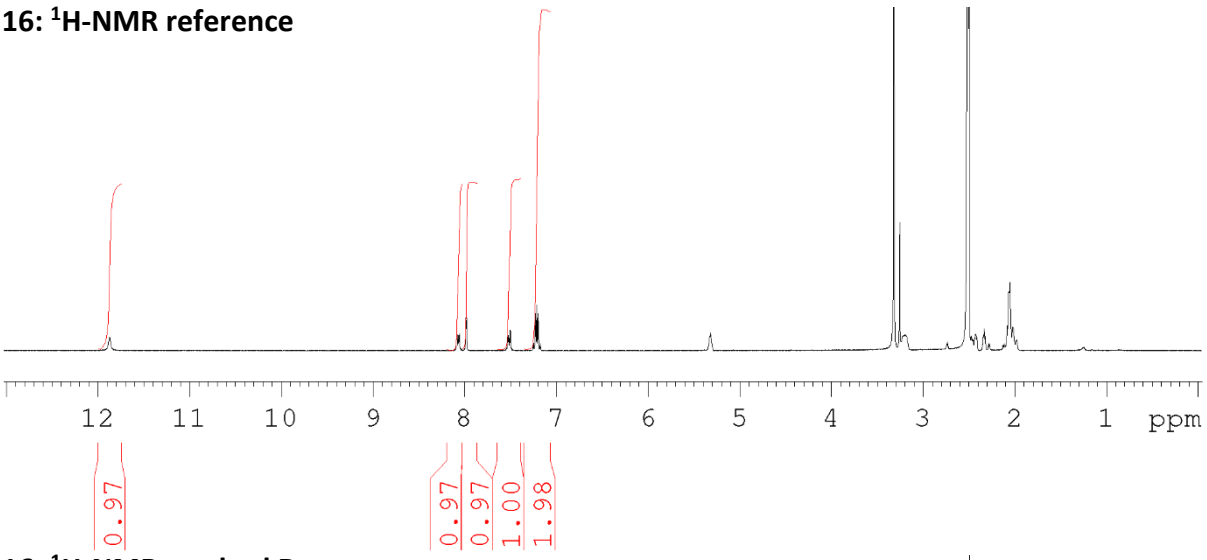
LC-MS (positive ESI): m/z 325.1 $[M+H]^+$ (59.3), 326.2 $[M(1D)+H]^+$ (33.8), 327.2 $[M(2D)+H]^+$ (100), 328.2 $[M(3D)+H]^+$ (54.3), 329.2 $[M(4D)+H]^+$ (12.6) : 80% D



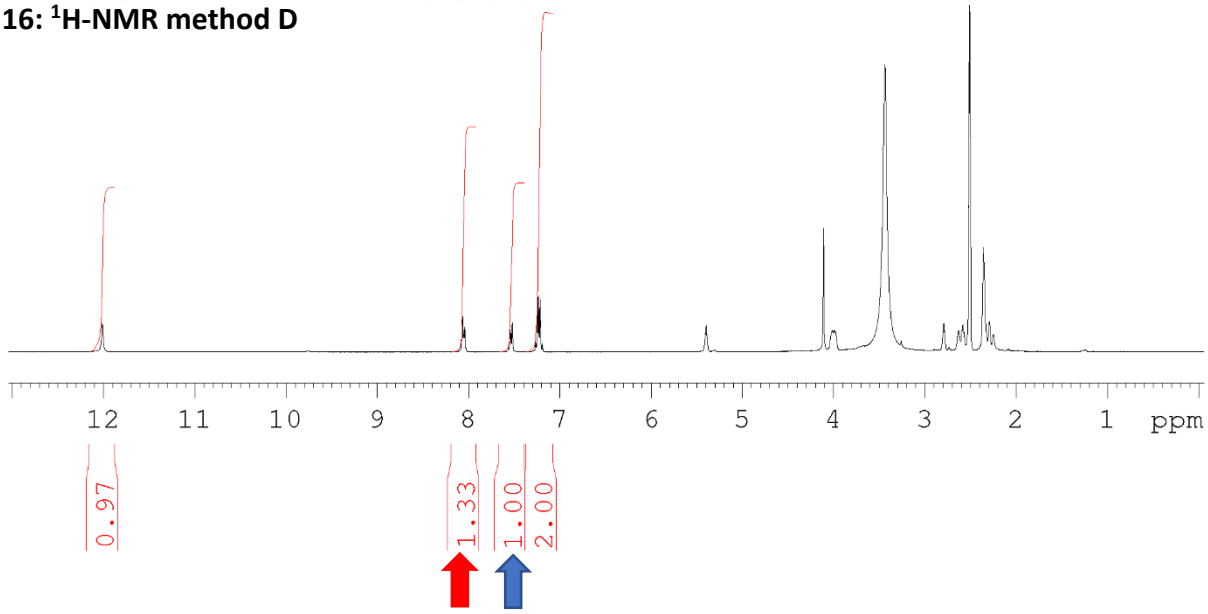
LC-MS (positive ESI): m/z 325.2 $[M+H]^+$ (63.4), 326.1 $[M(1D)+H]^+$ (33.2), 327.1 $[M(2D)+H]^+$ (100), 328.1 $[M(3D)+H]^+$ (47.4), 329.2 $[M(4D)+H]^+$ (12.5) : 74% D

Average of two reactions: 77% D, Yield: 90%, DCY: 69%

16: ^{1}H-NMR reference

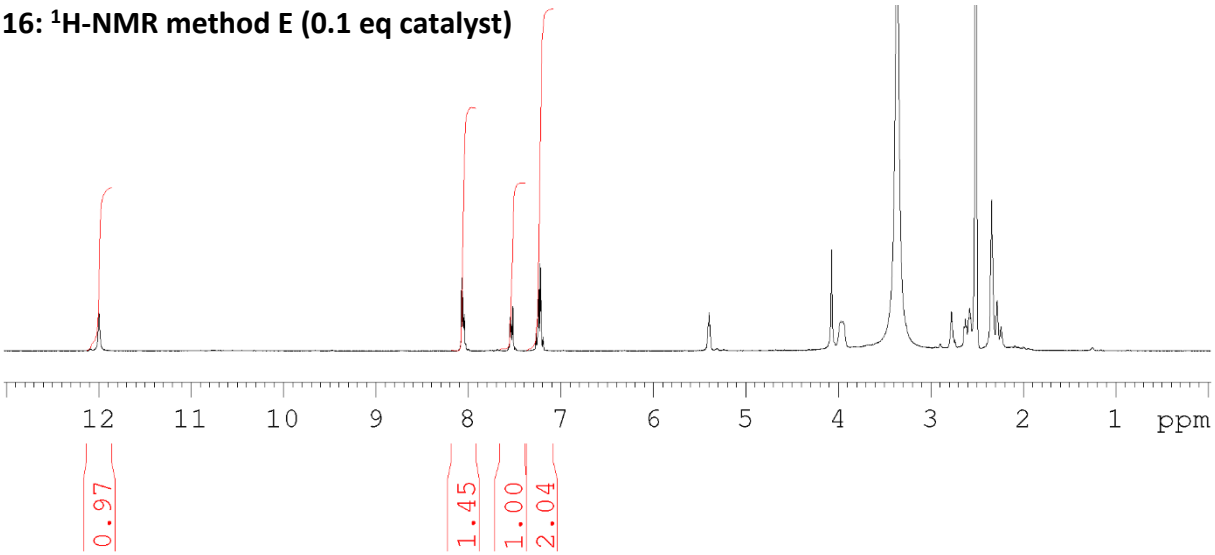


16: ^{1}H-NMR method D

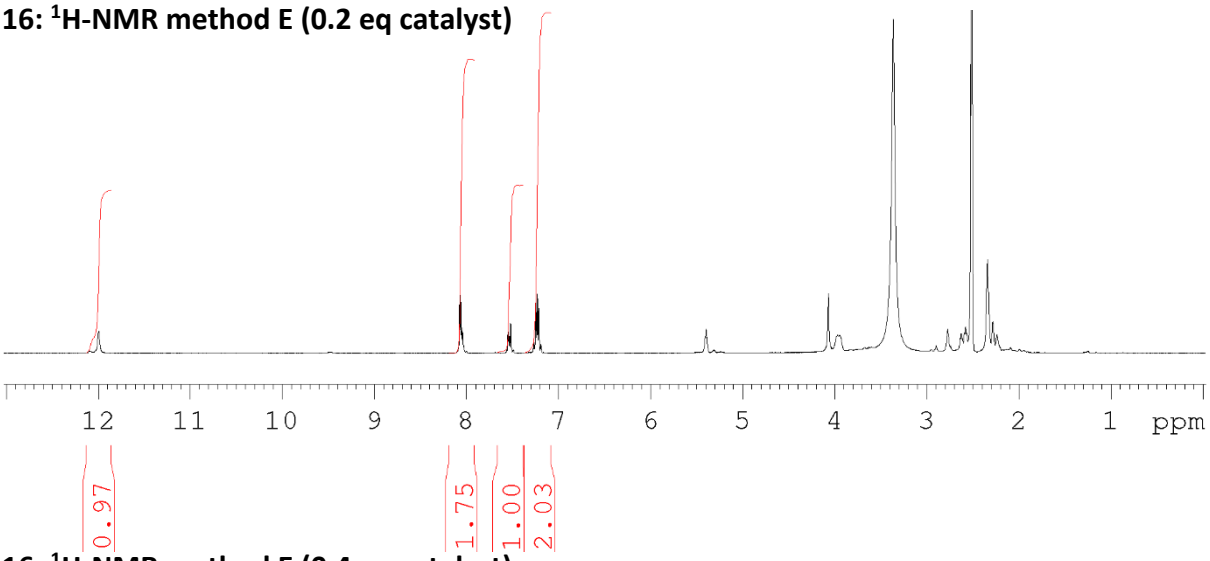


Deuterium incorporation: red arrow. Reference-integral: blue arrow.

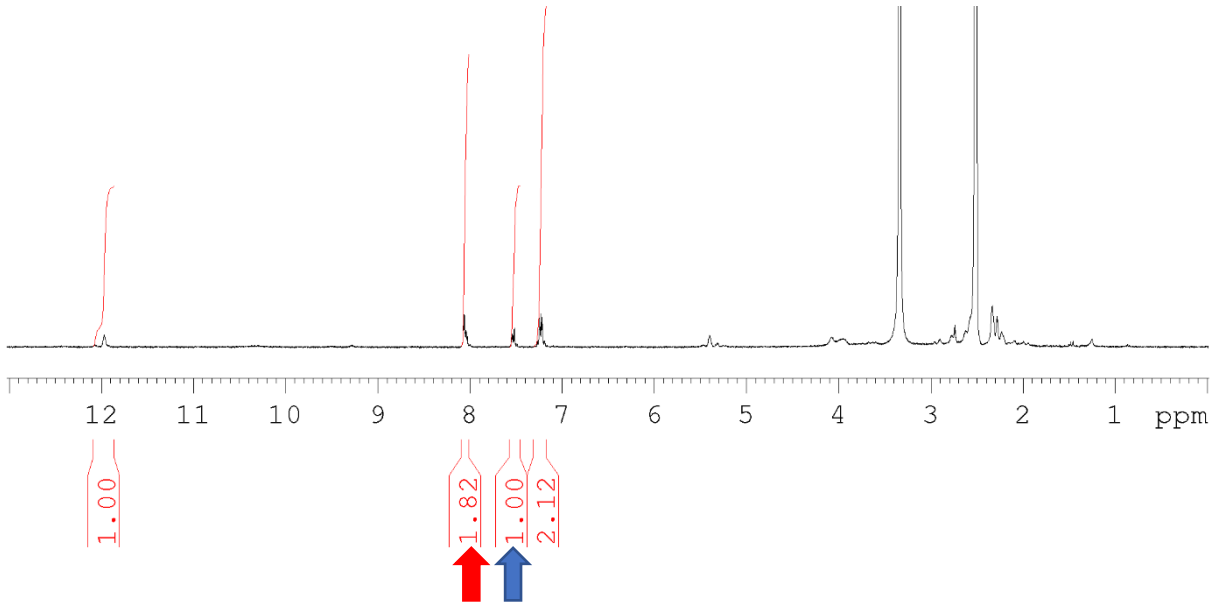
16: ^{1}H-NMR method E (0.1 eq catalyst)



16: ^{1}H-NMR method E (0.2 eq catalyst)

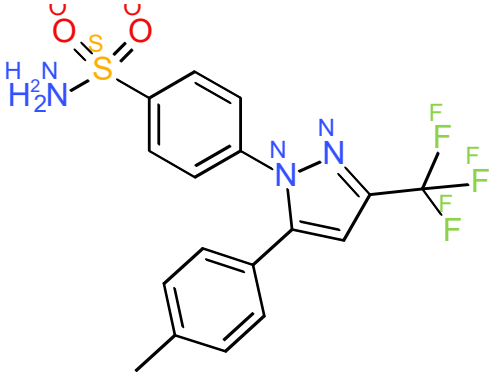


16: ^{1}H-NMR method E (0.4 eq catalyst)

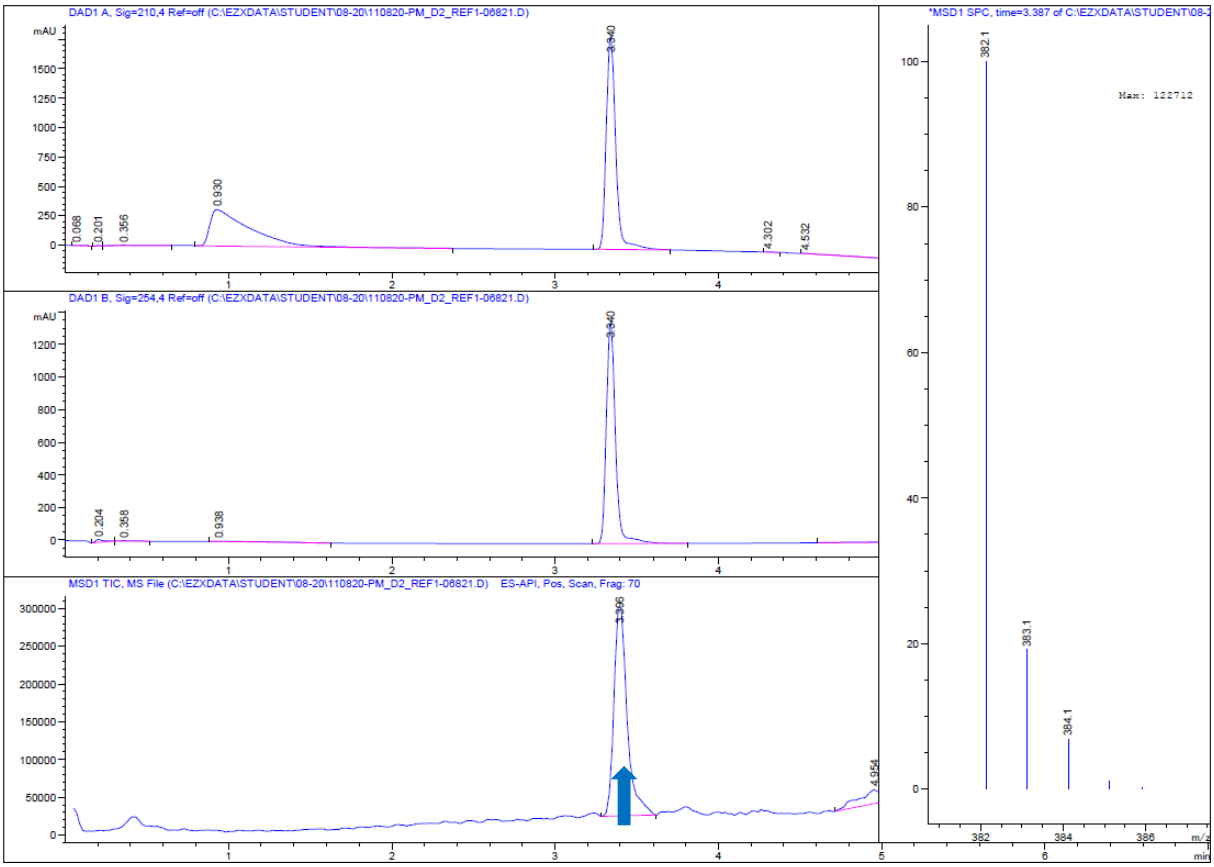


Deuterium incorporation: red arrow. Reference-integral: blue arrow.

Data for Celecoxib **17**



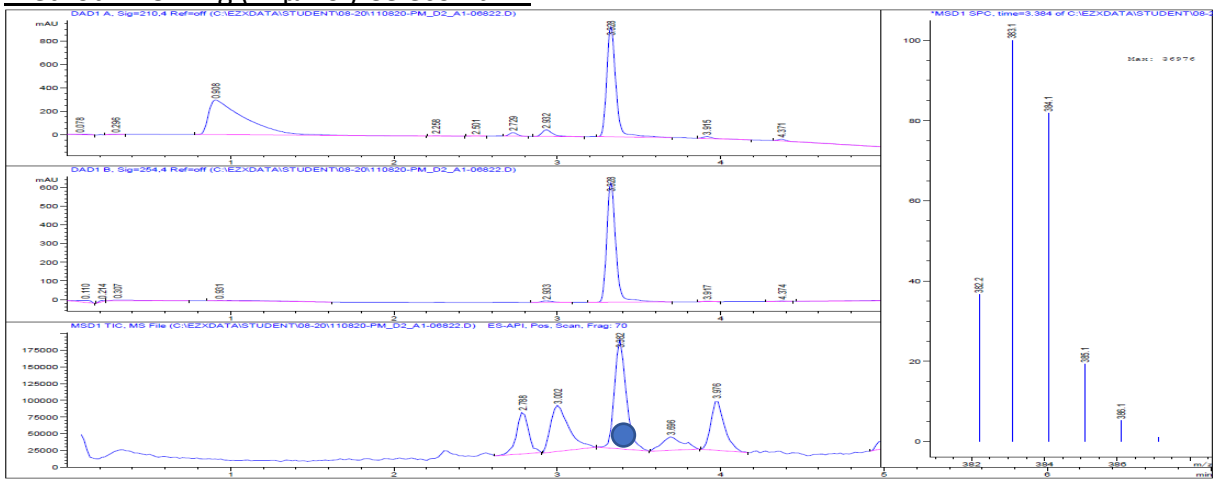
17



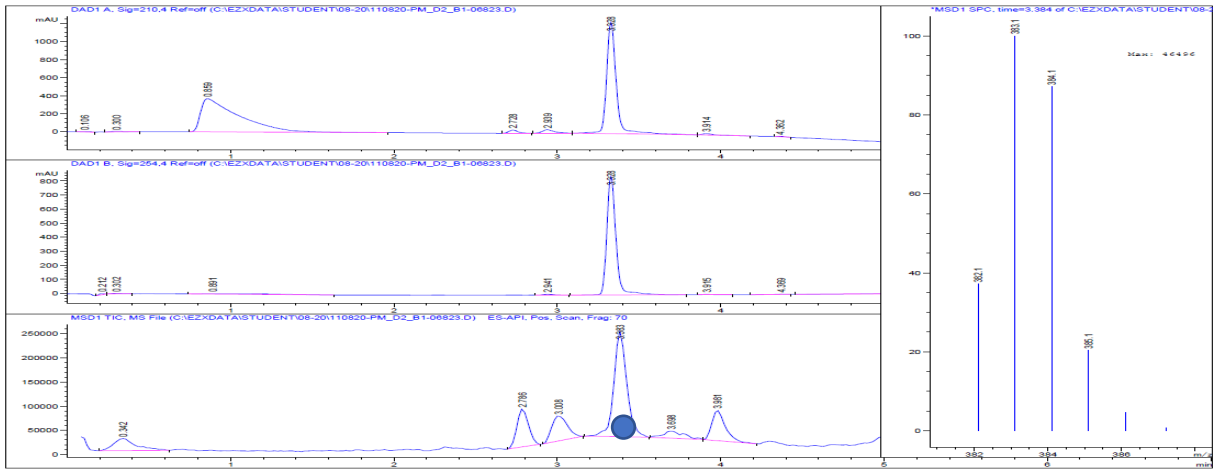
LC-MS (positive ESI): m/z 382.1 $[M+H]^+$ (100), 383.1 $[M+1+H]^+$ (19.1), 384.1 $[M+2+H]^+$ (6.9), 385.1 $[M+3+H]^+$ (1.0)

Deuterium experiments with Celecoxib **17**

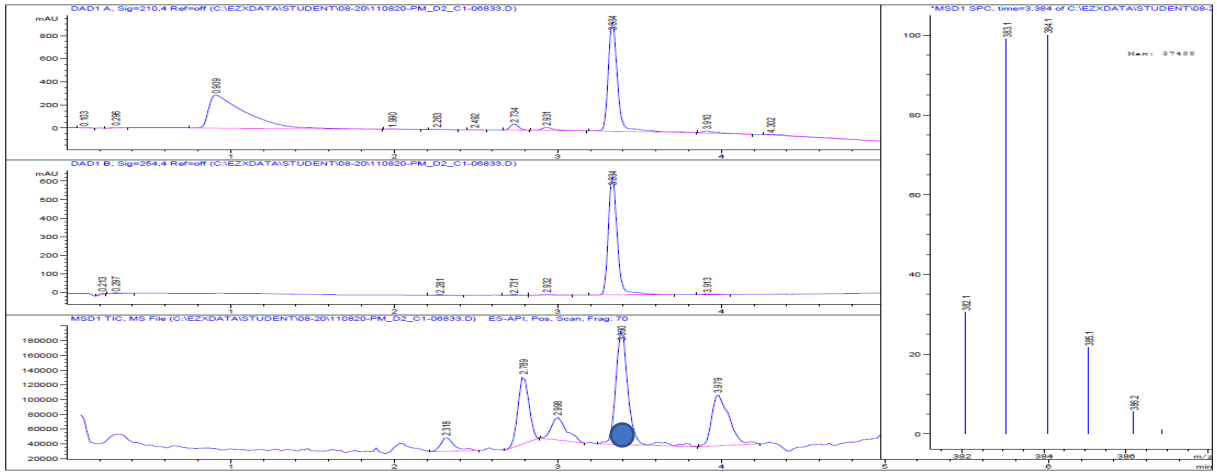
Method D: 5.4mg (14µmol) Celecoxib **17**



LC-MS (positive ESI): m/z 382.2 $[M+H]^+$ (36.7), 383.1 $[M(1D)+H]^+$ (100), 384.1 $[M(2D)+H]^+$ (81.8), 385.1 $[M(3D)+H]^+$ (19.3), 386.1 $[M(4D)+H]^+$ (5.3) : 57% D



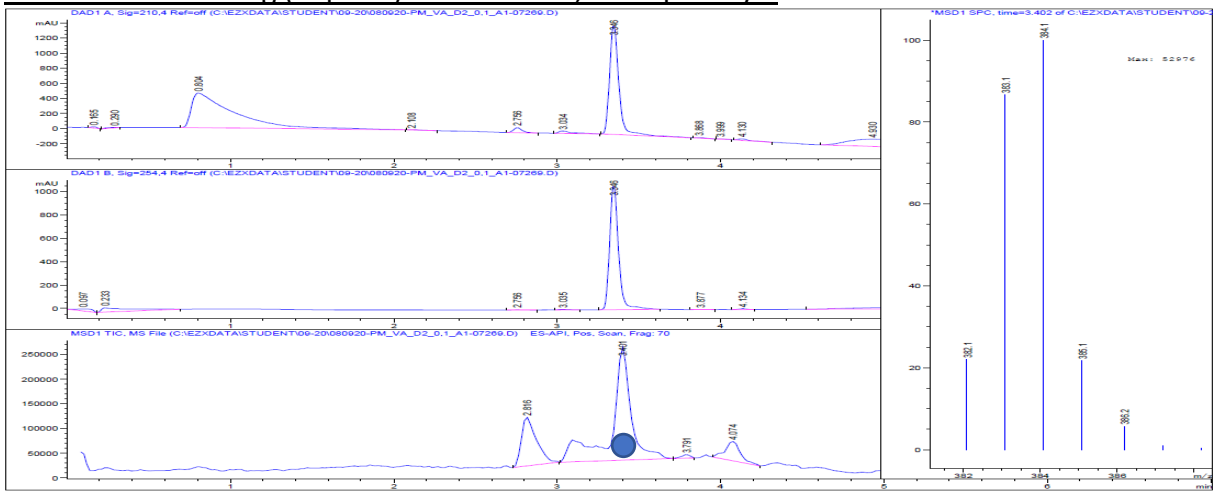
LC-MS (positive ESI): m/z 382.1 $[M+H]^+$ (37.1), 383.1 $[M(1D)+H]^+$ (100), 384.1 $[M(2D)+H]^+$ (87.2), 385.1 $[M(3D)+H]^+$ (20.4), 386.1 $[M(4D)+H]^+$ (4.6) : 58% D



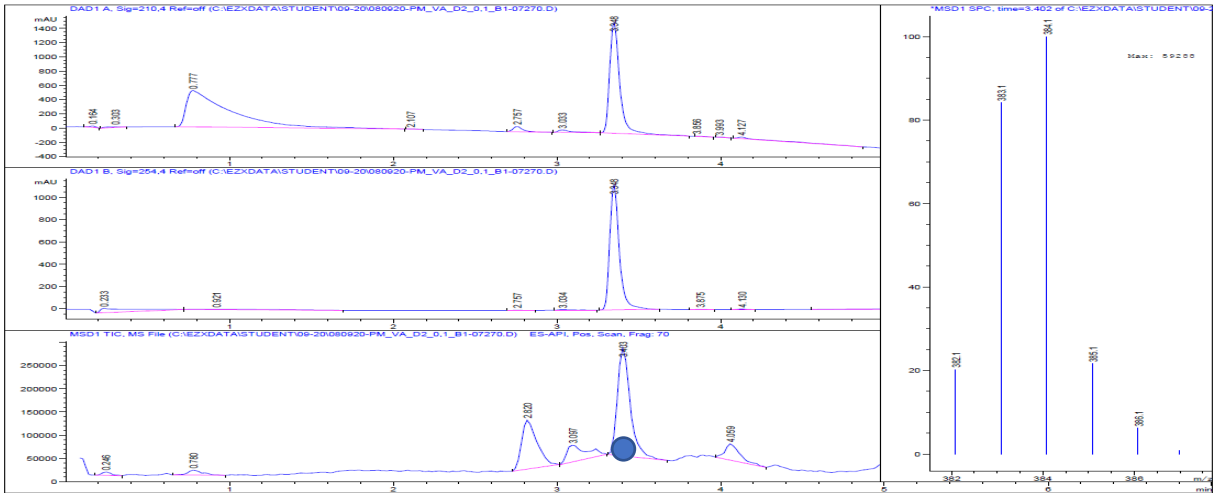
LC-MS (positive ESI): m/z 382.1 $[M+H]^+$ (30.6), 383.1 $[M(1D)+H]^+$ (99.1), 384.1 $[M(2D)+H]^+$ (100), 385.1 $[M(3D)+H]^+$ (21.7), 386.1 $[M(4D)+H]^+$ (5.6) : 62% D

Average of three reactions: 59% D, Yield 80%, DCY: 47%

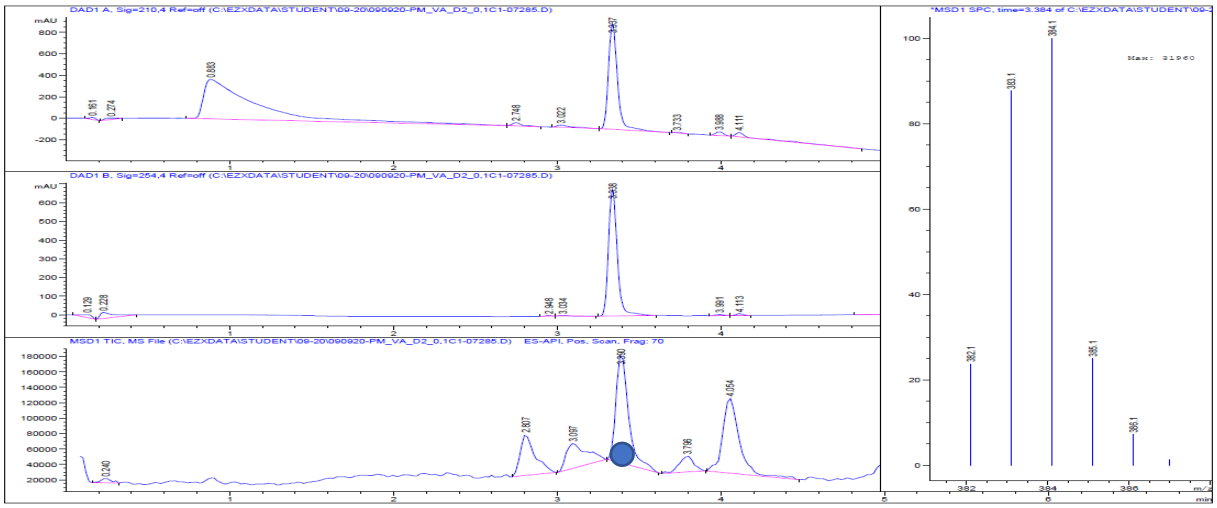
17: Method E: 4.1mg (10µmol) Celecoxib **18**, 0.1 eq catalyst



LC-MS (positive ESI): m/z 382.1 $[M+H]^+$ (22.1), 383.1 $[M(1D)+H]^+$ (86.7), 384.1 $[M(2D)+H]^+$ (100), 385.1 $[M(3D)+H]^+$ (21.8), 386.2 $[M(4D)+H]^+$ (5.7) : 68% D



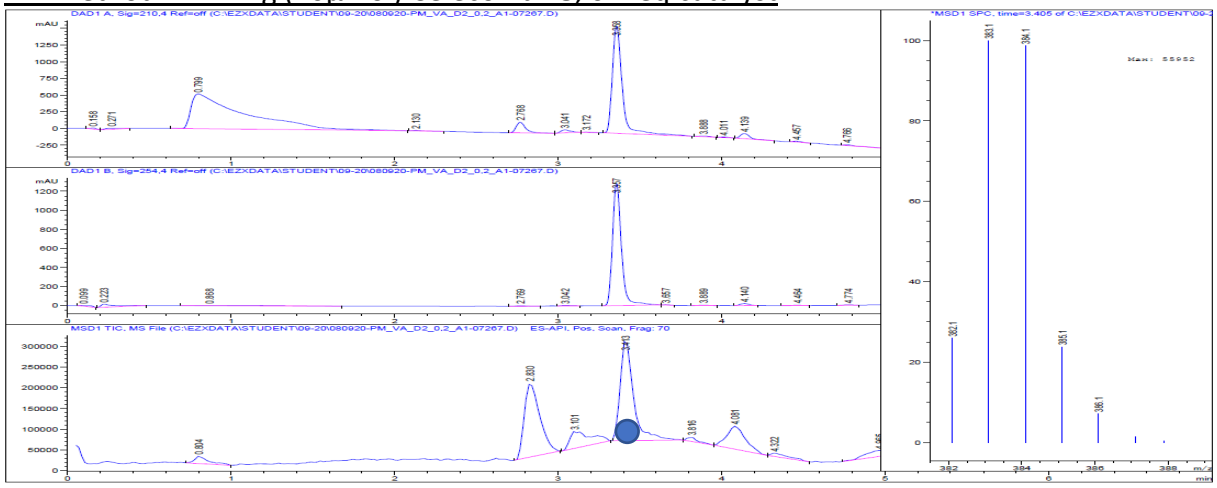
LC-MS (positive ESI): m/z 382.1 $[M+H]^+$ (20.2), 383.1 $[M(1D)+H]^+$ (84.2), 384.1 $[M(2D)+H]^+$ (100), 385.1 $[M(3D)+H]^+$ (21.6), 386.1 $[M(4D)+H]^+$ (6.1) : 67% D



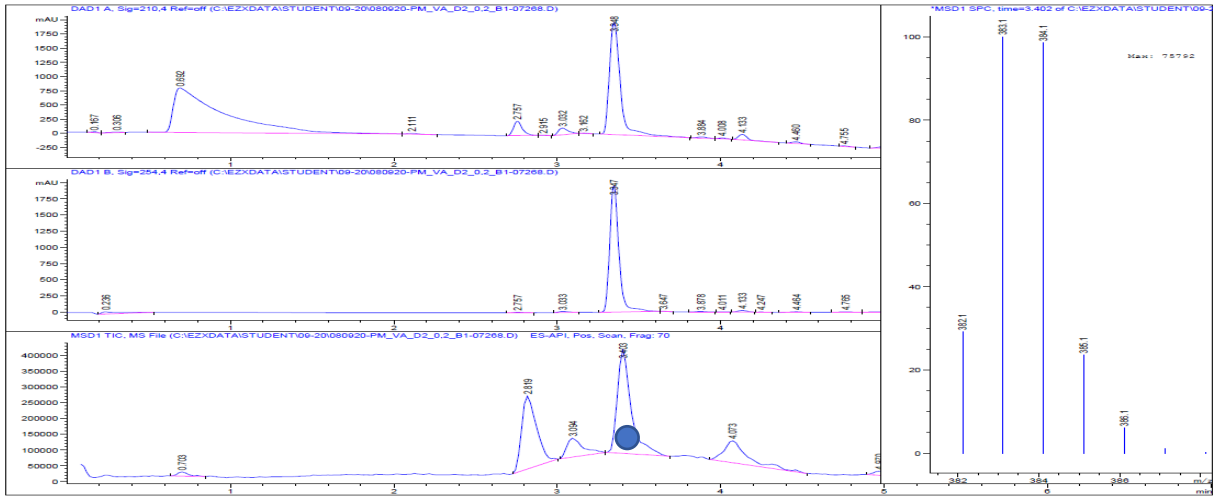
LC-MS (positive ESI): m/z 382.1 $[M+H]^+$ (23.8), 383.1 $[M(1D)+H]^+$ (87.7), 384.1 $[M(2D)+H]^+$ (100), 385.1 $[M(3D)+H]^+$ (25.0), 386.1 $[M(4D)+H]^+$ (7.2) : 67% D

Average of three reactions: 67% D, Yield: 81%, DCY: 54%

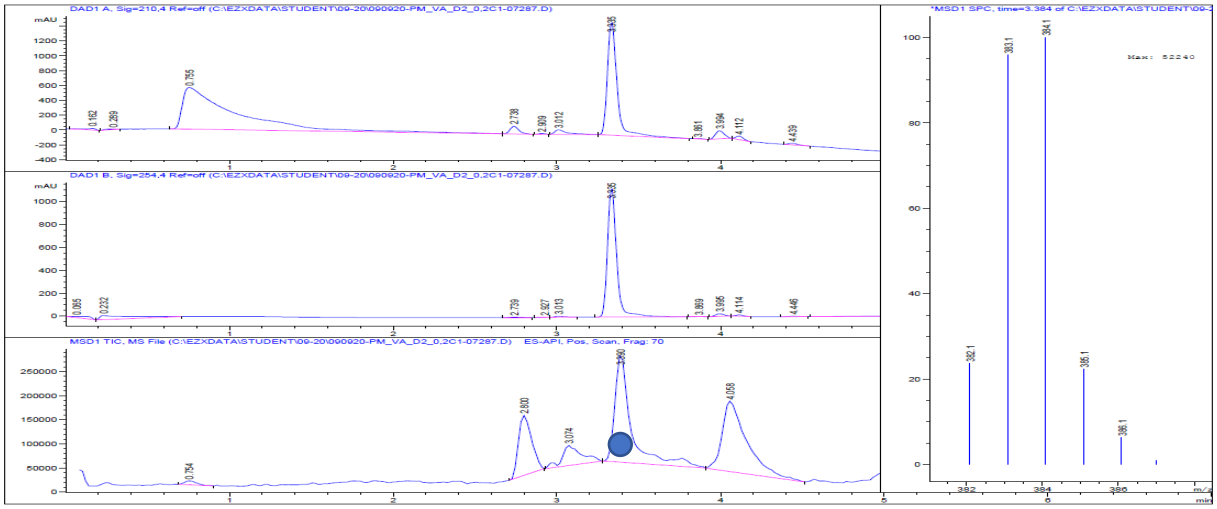
17: Method E: 4.1mg (10µmol) Celecoxib **18**, 0.2 eq catalyst



LC-MS (positive ESI): m/z 382.1 $[M+H]^+$ (25.9), 383.1 $[M(1D)+H]^+$ (100), 384.1 $[M(2D)+H]^+$ (98.7), 385.1 $[M(3D)+H]^+$ (23.8), 386.1 $[M(4D)+H]^+$ (7.1) : 64% D



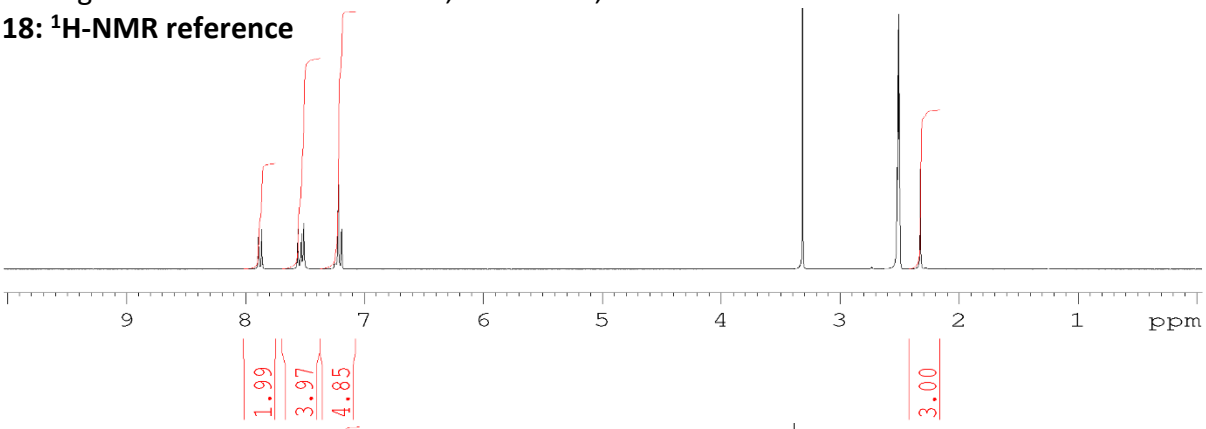
LC-MS (positive ESI): m/z 382.1 $[M+H]^+$ (29.2), 383.1 $[M(1D)+H]^+$ (100), 384.1 $[M(2D)+H]^+$ (98.6), 385.1 $[M(3D)+H]^+$ (23.6), 386.1 $[M(4D)+H]^+$ (6.1) : 63% D



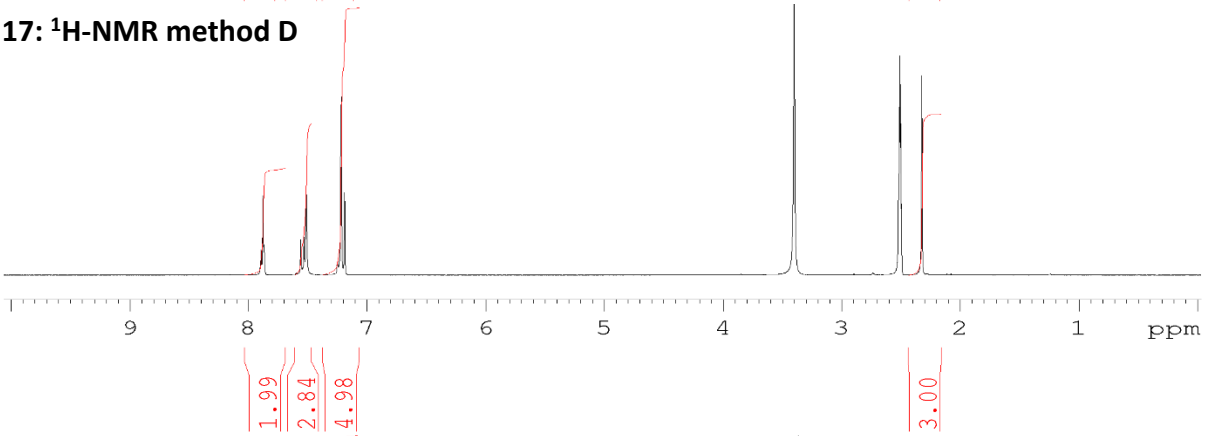
LC-MS (positive ESI): m/z 382.1 $[M+H]^+$ (23.7), 383.1 $[M(1D)+H]^+$ (95.8), 384.1 $[M(2D)+H]^+$ (100), 385.1 $[M(3D)+H]^+$ (22.3), 386.1 $[M(4D)+H]^+$ (6.3) : 65% D

Average of three reactions: 64% D, Yield: 80%, DCY: 51%

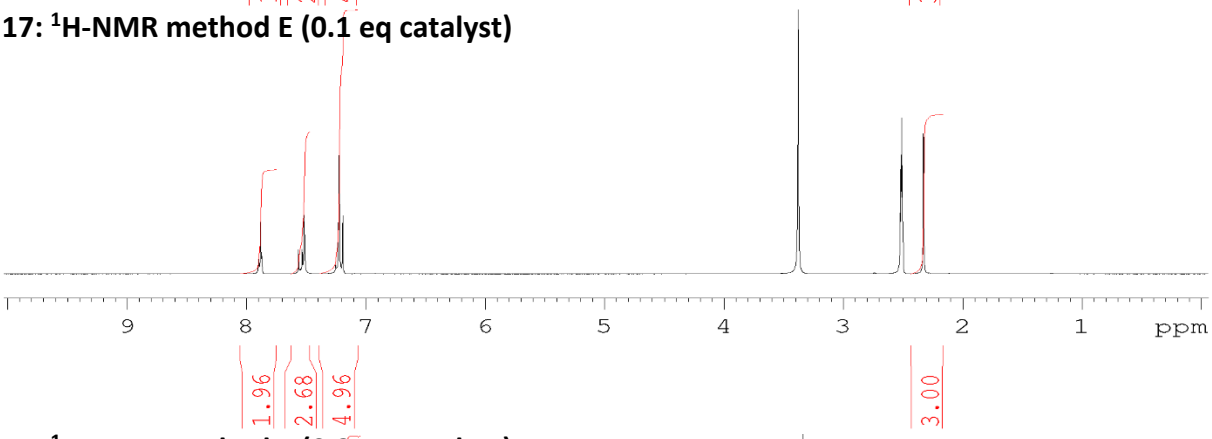
18: ^{1}H-NMR reference



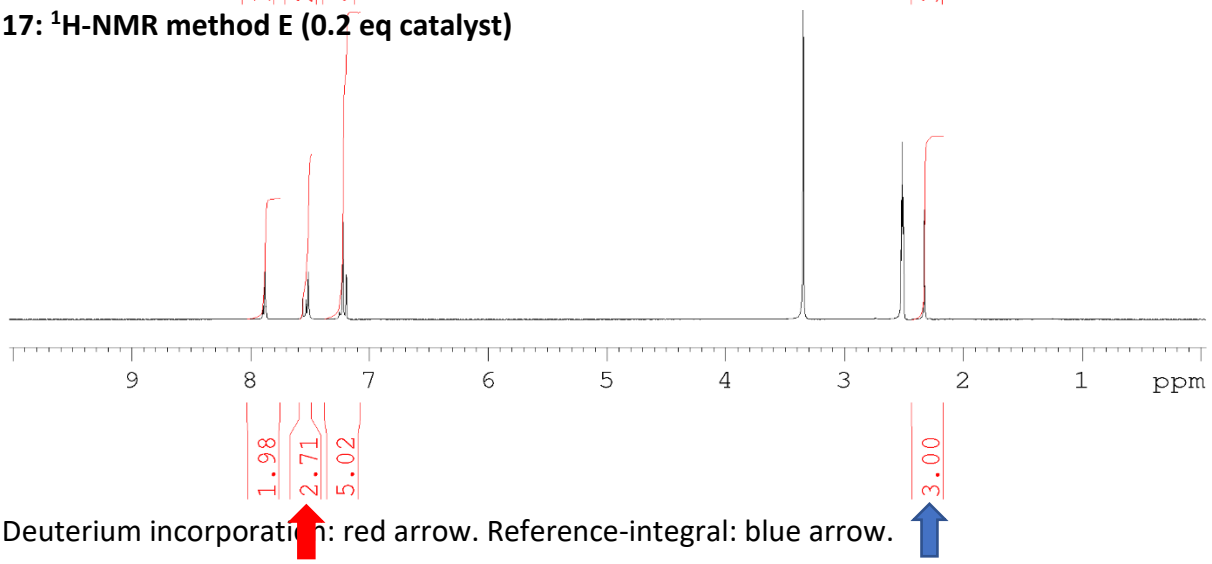
17: ^{1}H-NMR method D



17: ^{1}H-NMR method E (0.1 eq catalyst)

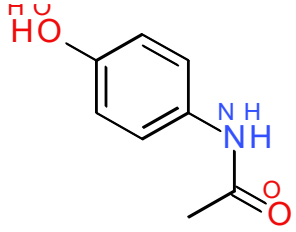


17: ^{1}H-NMR method E (0.2 eq catalyst)

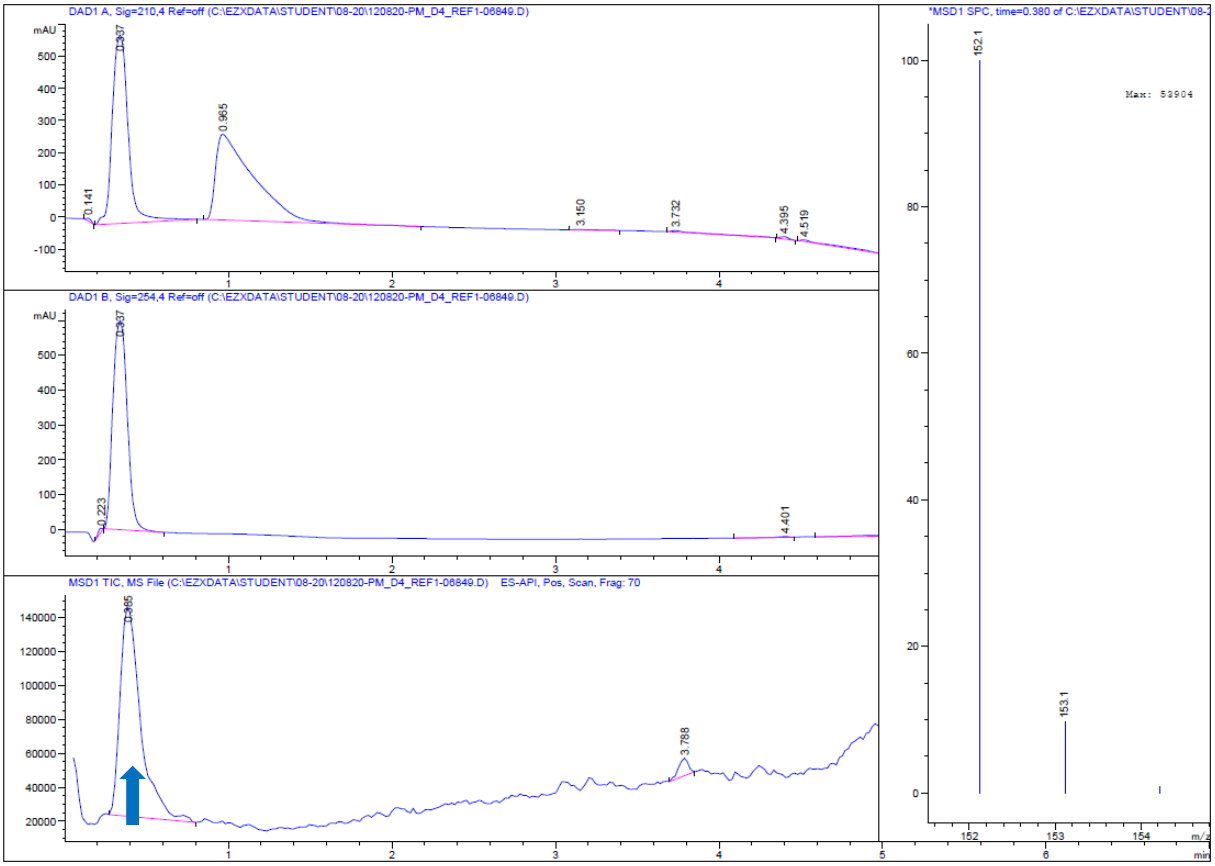


Deuterium incorporation: red arrow. Reference-integral: blue arrow.

Data for Paracetamol **18**



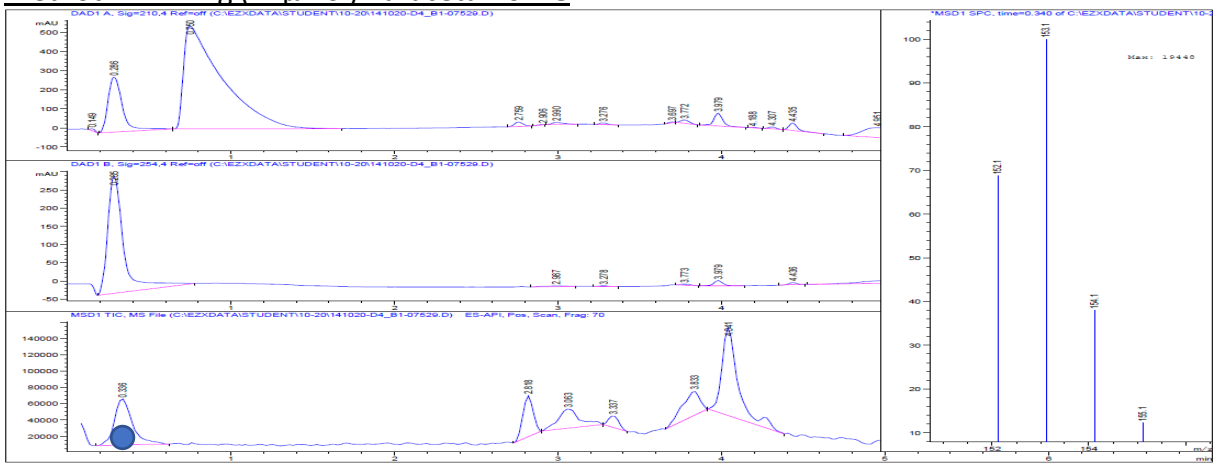
18



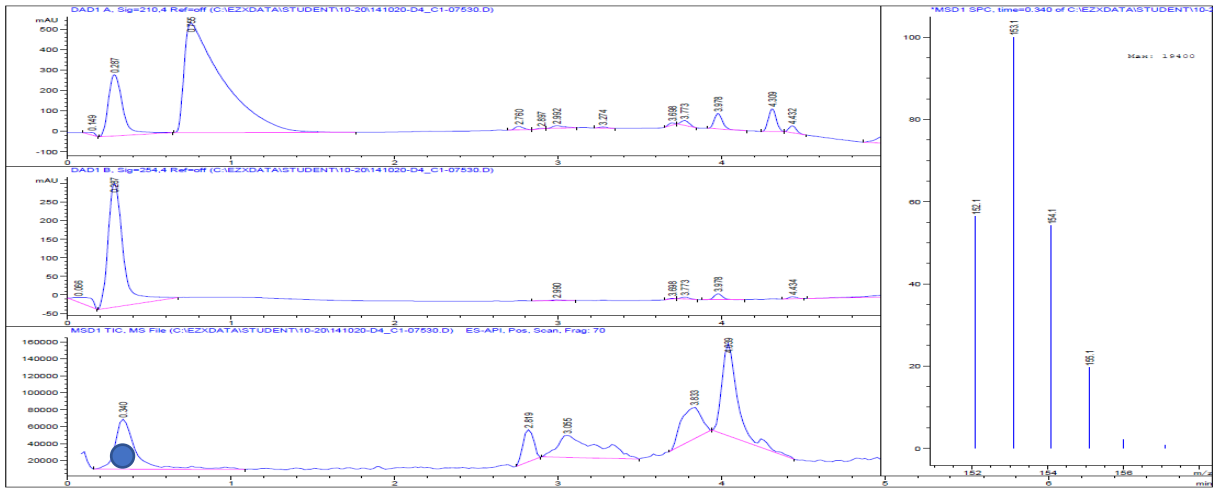
LC-MS (positive ESI): m/z 152.1 $[M+H]^+$ (100), 153.1 $[M+1+H]^+$ (9.7), 154.2 $[M+2+H]^+$ (0.8)

Deuterium experiments with Paracetamol **18**

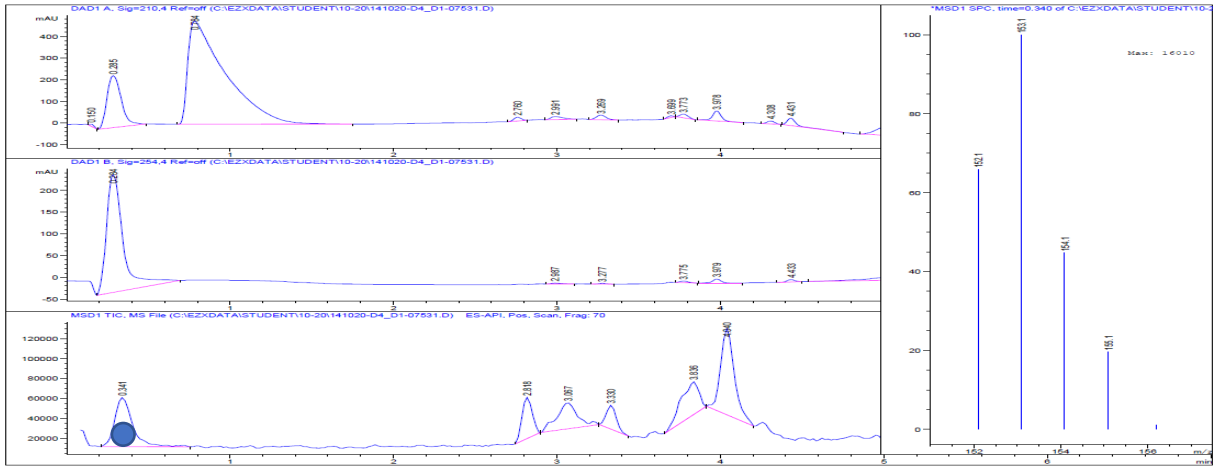
Method D: 2.1mg (11µmol) Paracetamol **18**



LC-MS (positive ESI): m/z 152.1 $[M+H]^+$ (68.7), 153.1 $[M(1D)+H]^+$ (100), 154.1 $[M(2D)+H]^+$ (38.0), 155.1 $[M(3D)+H]^+$ (12.3) : 44% D



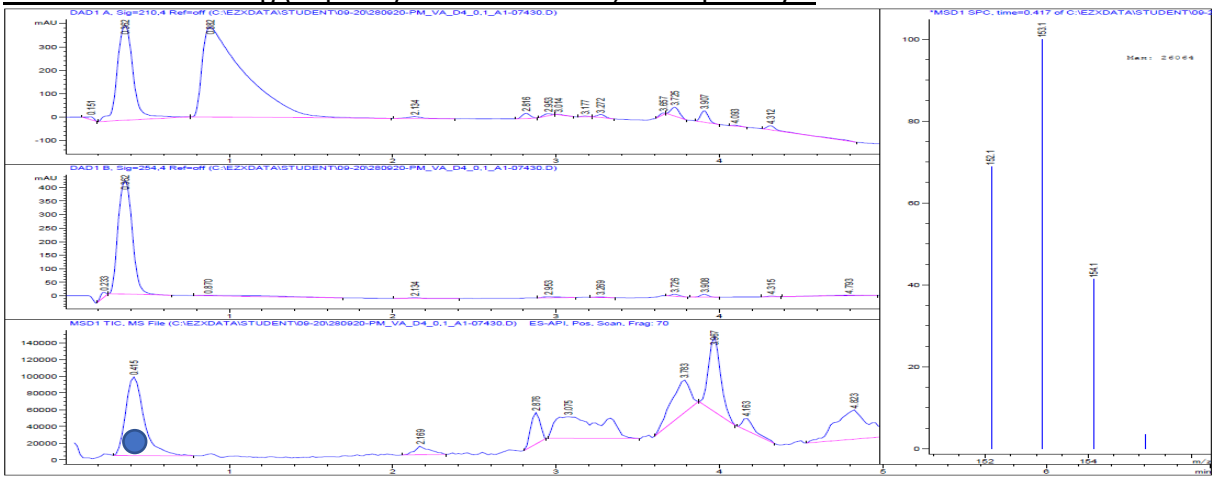
LC-MS (positive ESI): m/z 152.1 $[M+H]^+$ (56.4), 153.1 $[M(1D)+H]^+$ (100), 154.1 $[M(2D)+H]^+$ (54.1), 155.1 $[M(3D)+H]^+$ (19.7) : 54% D



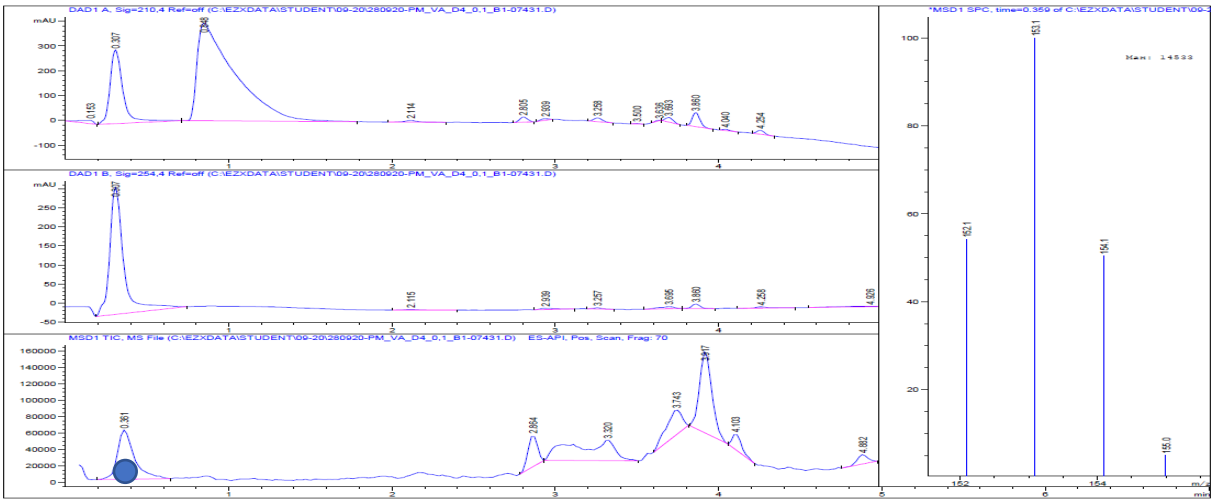
LC-MS (positive ESI): m/z 152.1 $[M+H]^+$ (65.9), 153.1 $[M(1D)+H]^+$ (100), 154.1 $[M(2D)+H]^+$ (44.7), 155.1 $[M(3D)+H]^+$ (19.6) : 49% D

Average of three reactions: 49% D, Yield: 85%, DCY: 42%

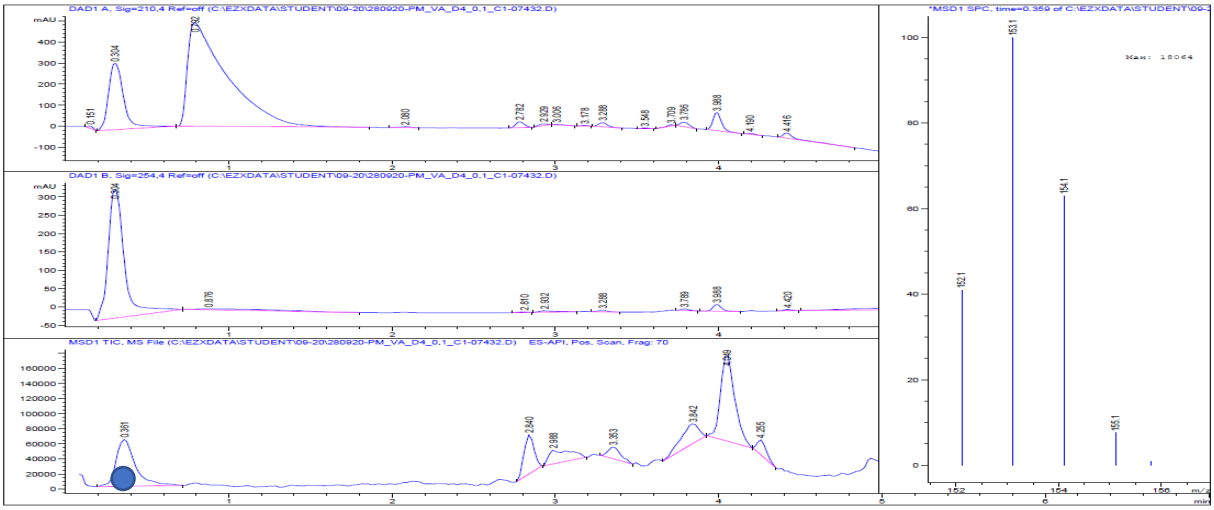
18: Method E: 2.1mg (14µmol) Paracetamol **18**, 0.1 eq catalyst



LC-MS (positive ESI): m/z 152.1 $[M+H]^+$ (68.8), 153.1 $[M(1D)+H]^+$ (100), 154.1 $[M(2D)+H]^+$ (41.4), 155.1 $[M(3D)+H]^+$ (3.5) : 40% D



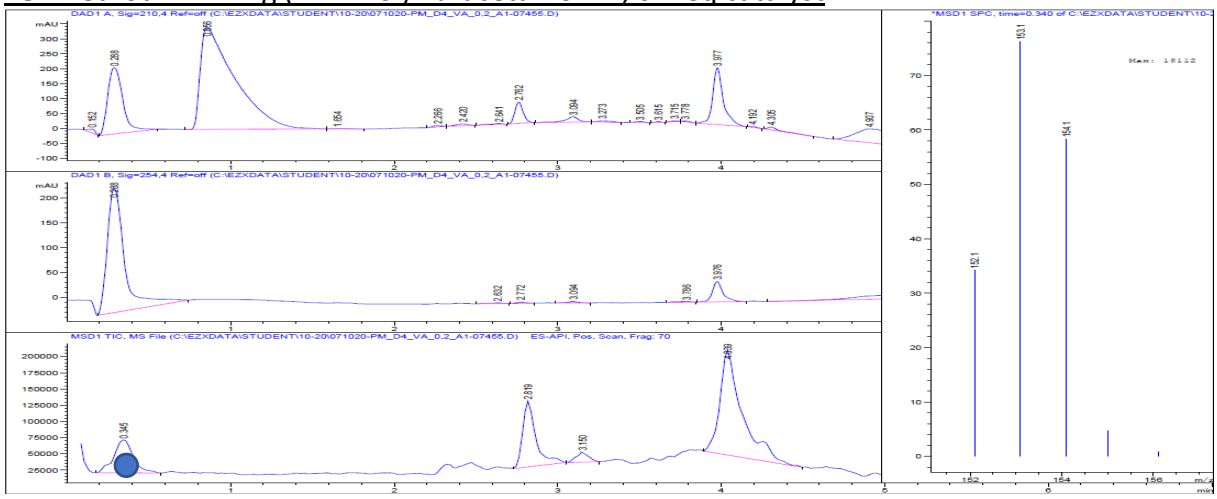
LC-MS (positive ESI): m/z 152.1 $[M+H]^+$ (54.2), 153.1 $[M(1D)+H]^+$ (100), 154.1 $[M(2D)+H]^+$ (50.4), 155.1 $[M(3D)+H]^+$ (5.1) : 46% D



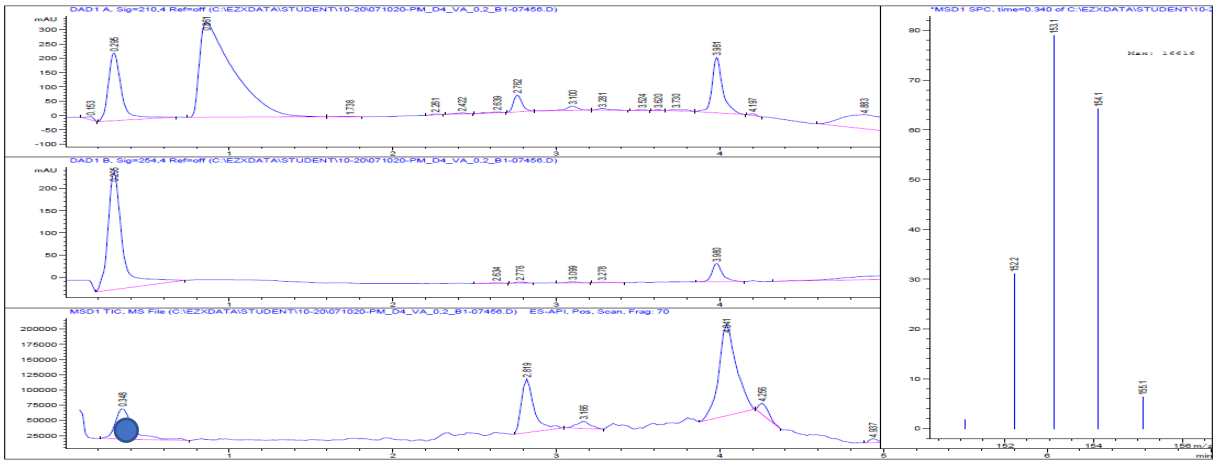
LC-MS (positive ESI): m/z 152.1 $[M+H]^+$ (41.0), 153.1 $[M(1D)+H]^+$ (100), 154.1 $[M(2D)+H]^+$ (63.0), 155.1 $[M(3D)+H]^+$ (7.6) : 54% D

Average of three reactions: 47% D, Yield: 86%, DCY: 40%

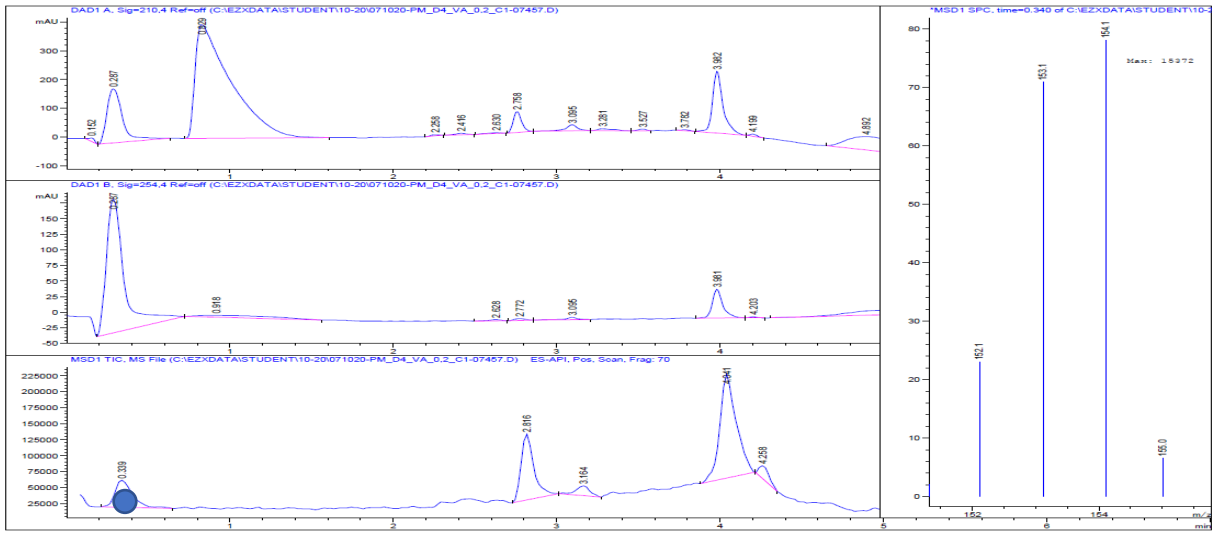
18: Method E: 2.1mg (14mmol) Paracetamol **17**, 0.2 eq catalyst



LC-MS (positive ESI): m/z 152.1 $[M+H]^+$ (34.2), 153.1 $[M(1D)+H]^+$ (100), 154.1 $[M(2D)+H]^+$ (58.4), 155.1 $[M(3D)+H]^+$ (4.7) : 55% D



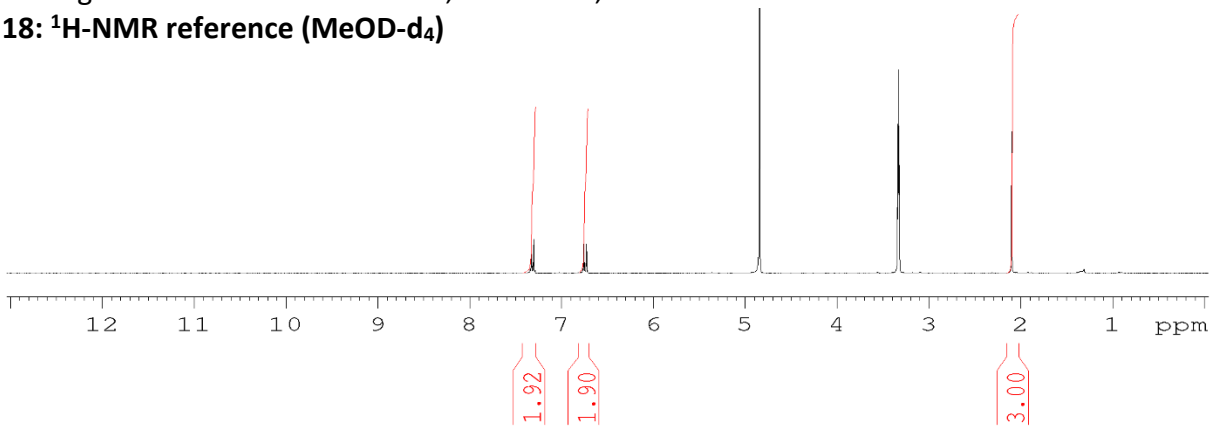
LC-MS (positive ESI): m/z 152.2 $[M+H]^+$ (31.1), 153.1 $[M(1D)+H]^+$ (100), 154.1 $[M(2D)+H]^+$ (64.3), 155.1 $[M(3D)+H]^+$ (6.4) : 58% D



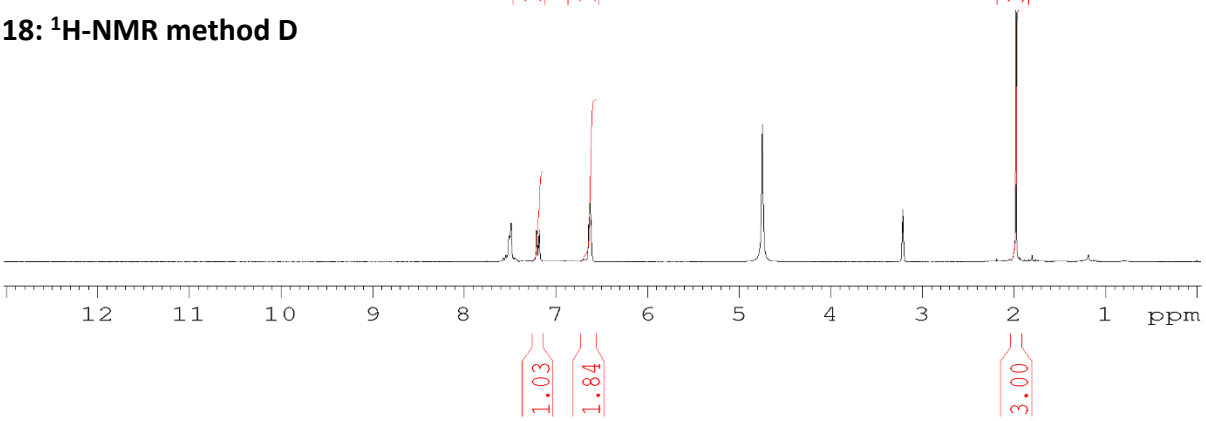
LC-MS (positive ESI): m/z 152.1 $[M+H]^+$ (23.0), 153.1 $[M(1D)+H]^+$ (70.9), 154.1 $[M(2D)+H]^+$ (100), 155.0 $[M(3D)+H]^+$ (6.6) : 66% D

Average of three reactions: 60% D, Yield: 80%, DCY: 48%

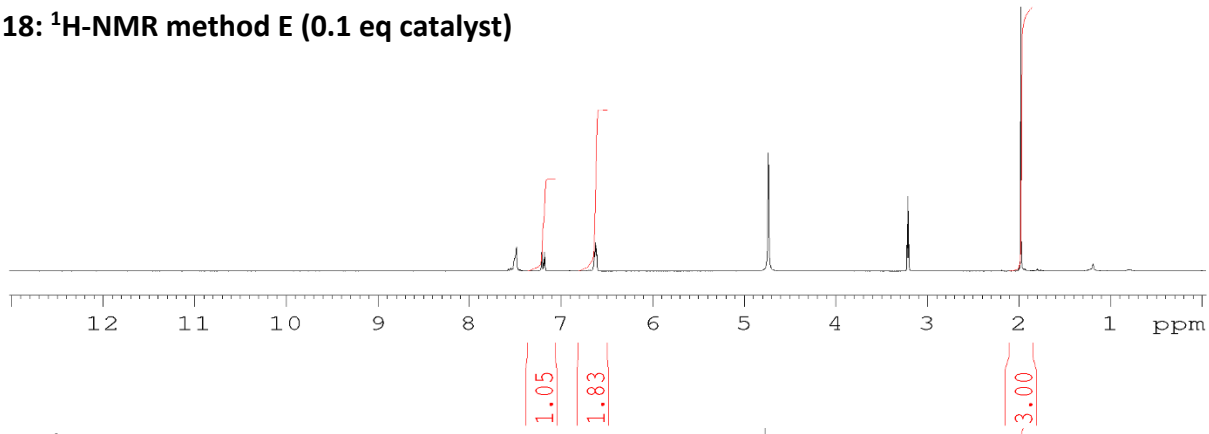
18: ^{1}H-NMR reference (MeOD-d_4)



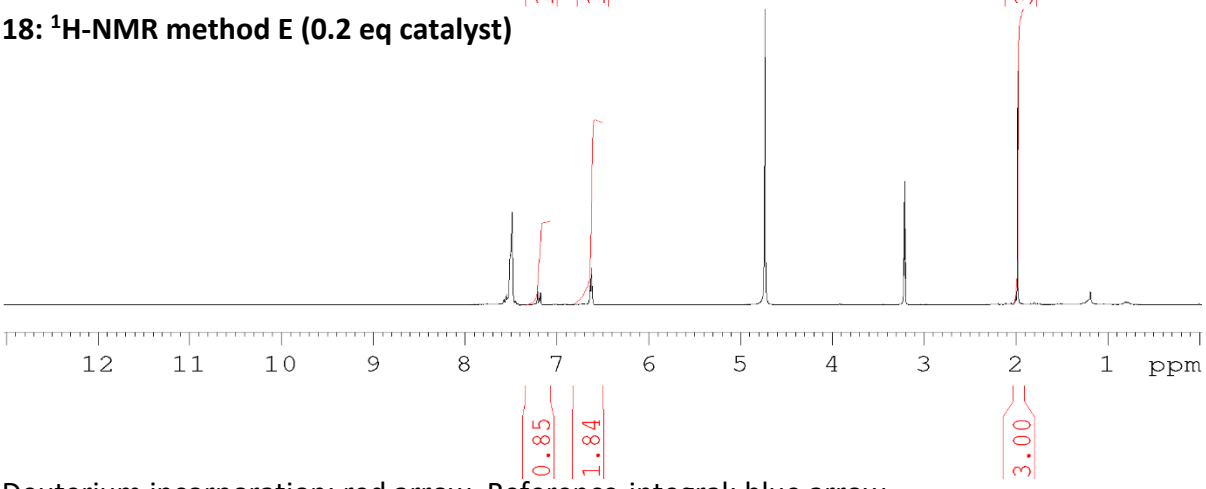
18: ^{1}H-NMR method D



18: ^{1}H-NMR method E (0.1 eq catalyst)

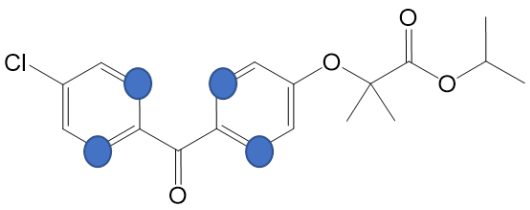


18: ^{1}H-NMR method E (0.2 eq catalyst)



Deuterium incorporation: red arrow. Reference-integral: blue arrow.

Summary pre-activation of catalyst with H_2 gas:



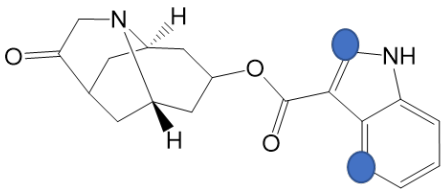
Fenofibrat **15**

94% , 77% D

0,1Eq 92% , 79% D

0,2Eq 89% , 86% D

0,4Eq 90% , 79% D



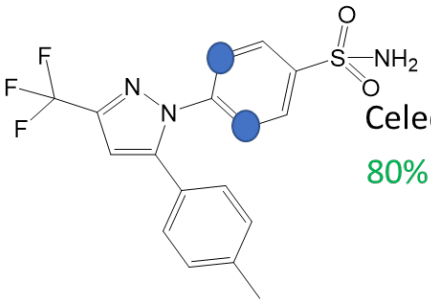
Dolasetron **16**

94% , 43% D

0,1Eq 95% , 63% D

0,2Eq 93% , 73% D

0,4Eq 92% , 77% D



Celecoxib **17**

80% , 59% D

0,1Eq 81% , 67% D

0,2Eq 80% , 64% D

1 Eq.D_2 @ 25 mbar,0.1 eq. Kerr catalyst,2 h rt, isopropylacetate

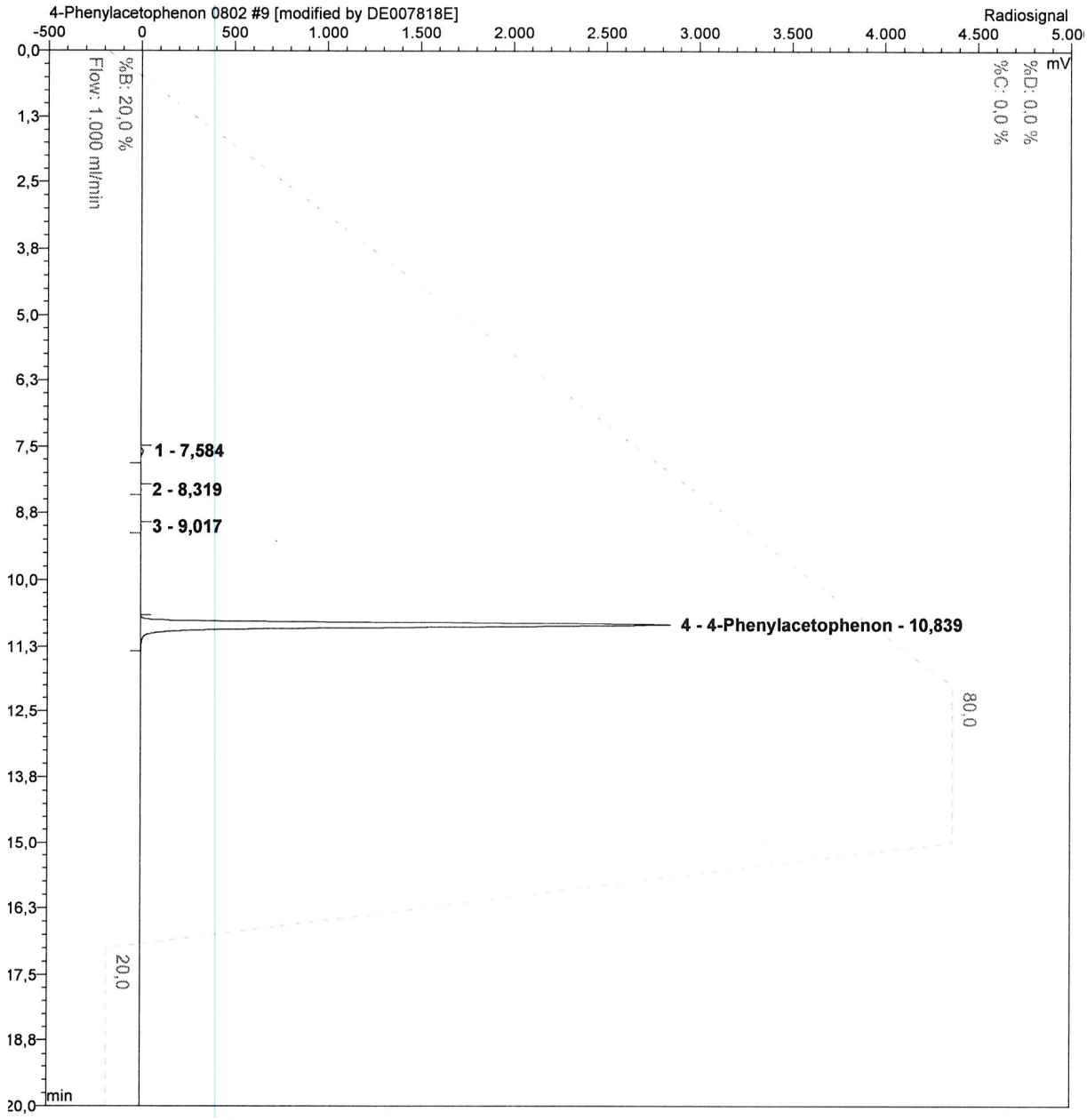
Eq cat preactivation 1h with H2, 100mbar

1 Eq.D_2 @ 25 mbar, Kerr catalyst,3 h rt, isopropylacetate

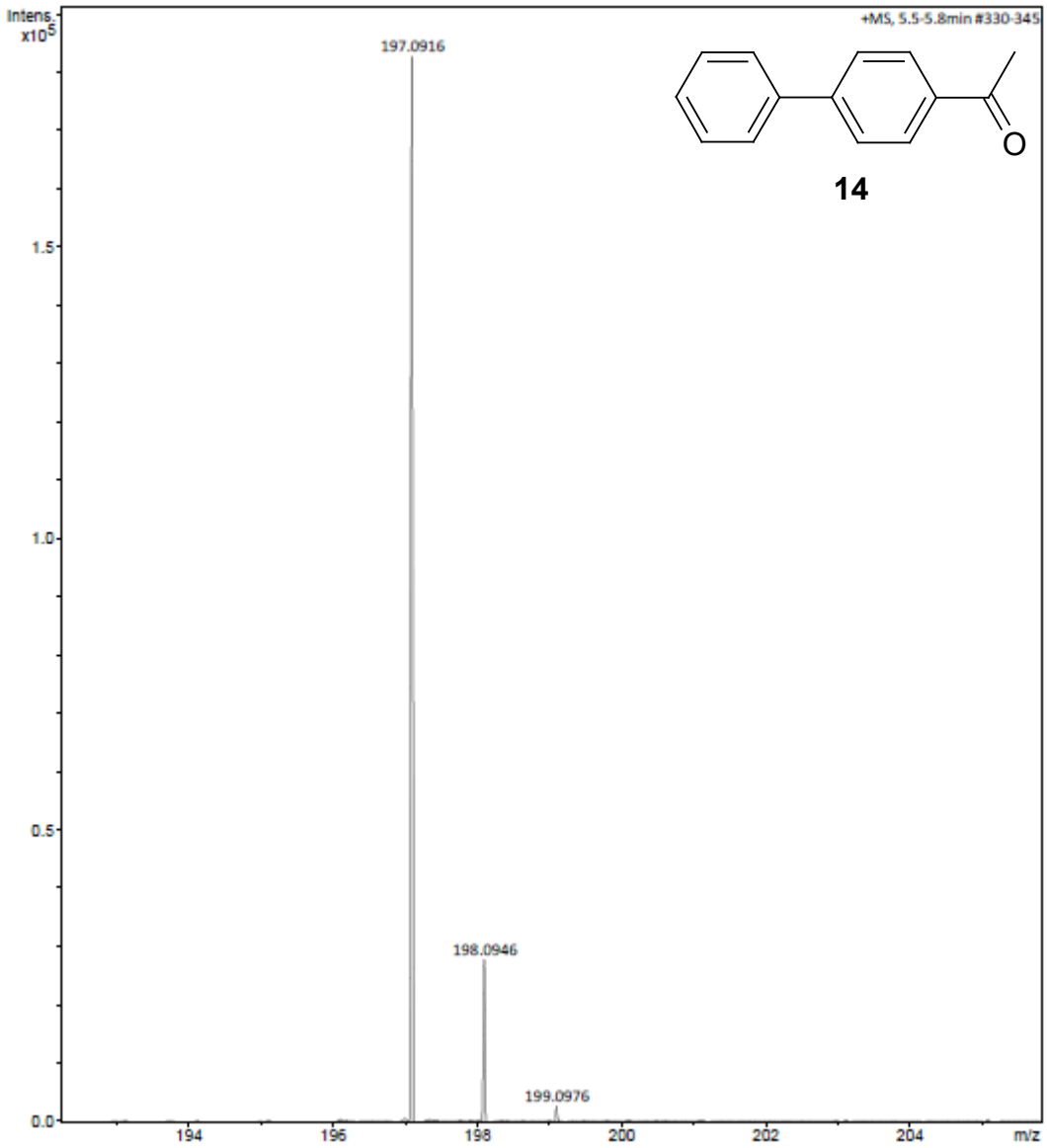
2.Tritium experiments

Tritium experiment 4-Acetylbiphenyl **14**

5.3 mg (27.0 ⍰mol) 4-Acetylbiphenyl **14** and 1.2 mg Kerr PF_6 (cas1019852-99-3) (4,4 mol%) were placed in a 1 mL reaction flask and dissolved in 0.7 mL dry DCM. The 1 mL reaction flask was adapted to a tritium manifold and the solution was frozen in liquid nitrogen. The flask was evacuated, charged with tritium (48100 MBq, 21.7 µmol, 0,9 eq). (pressure 52 mbar) The reaction mixture was then allowed to warm to room temperature before stirring at rt for 5 hours. After removal of solvent in vacuo the labile tritium was exchanged and removed by addition of methanol and a freeze-drying process (three times repeated). The solid residue was dissolved in 3 mL methanol. Purification and isolation *via* HPLC (Phenomenex Gemini NX C18 10x150 mm, 5 µm, 5 mL/min flow, ACN/water gradient program) give (5,2 mg, 30346 MBq, 63.1 % RCY, 1147 GBq/mmol (31 Ci/mmol).

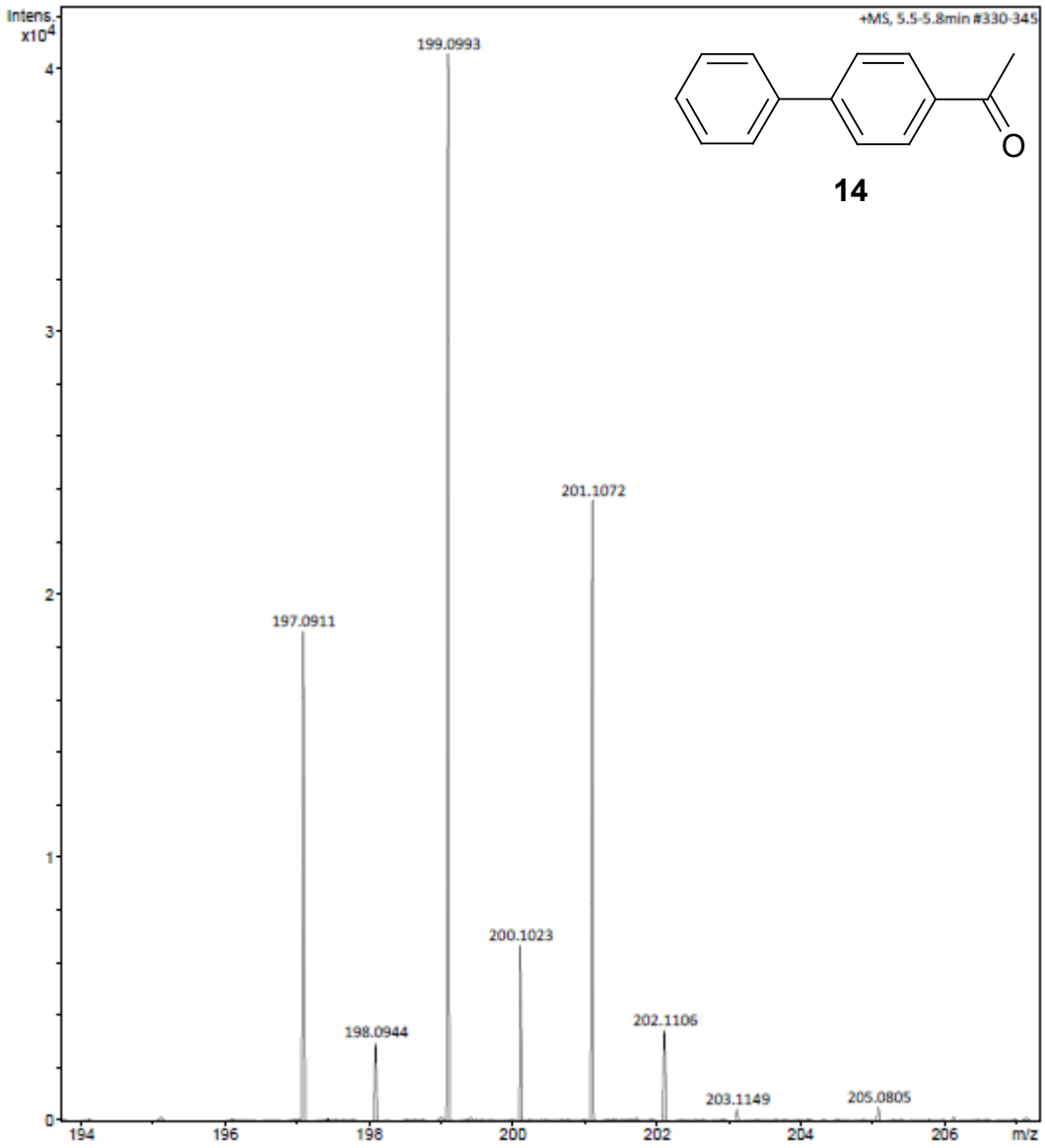

4-Phenylacetophenon 0802 #9 [modified by DE007818E]
Radiosignal
-500
0
500
1.000
1.500
2.000
2.500
3.000
3.500
4.000
4.500
5.000
mV
0,0
1,3
2,5
3,8
5,0
6,3
7,5
8,8
10,0
11,3
12,5
13,8
15,0
16,3
17,5
18,8
20,0
min
Flow: 1,000 ml/min
%B: 20,0 %
%C: 0,0 %
%D: 0,0 %
1 - 7,584
2 - 8,319
3 - 9,017
4 - 4-Phenylacetophenon - 10,839
80,0
20,0

4-Acetylbiphenyl – reference mass spectra



m/z 197.09 $[M+H]^+$ (100), 198.09 $[M+1+H]^+$ (15.1), 199.10 $[M+2+H]^+$ (1.4)

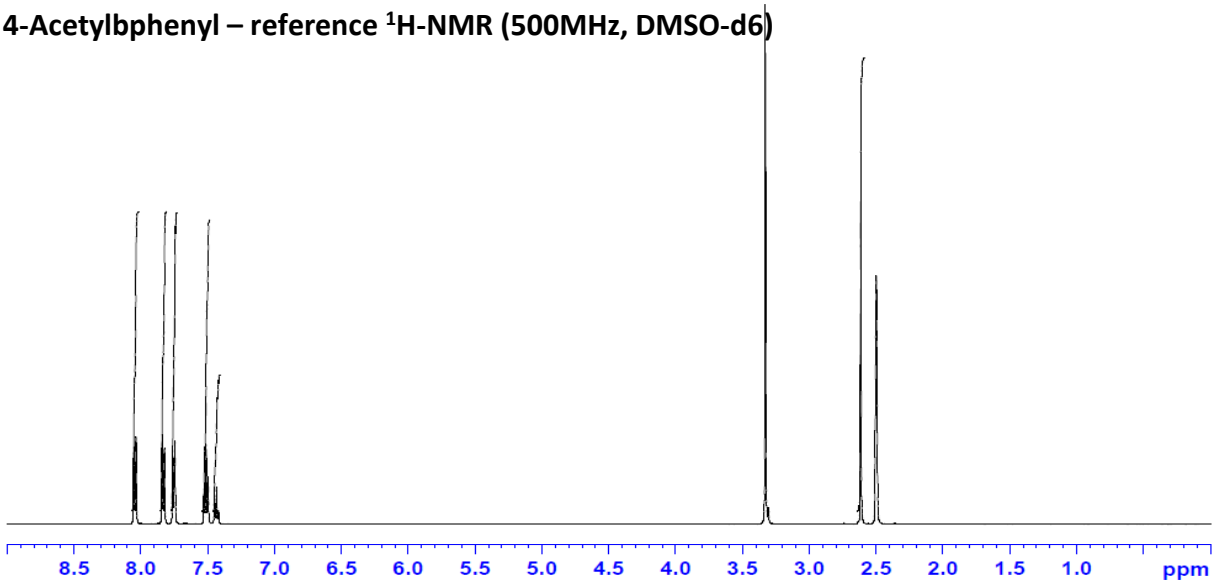
4-Acetylbiphenyl – mass spectra for tritium experiment



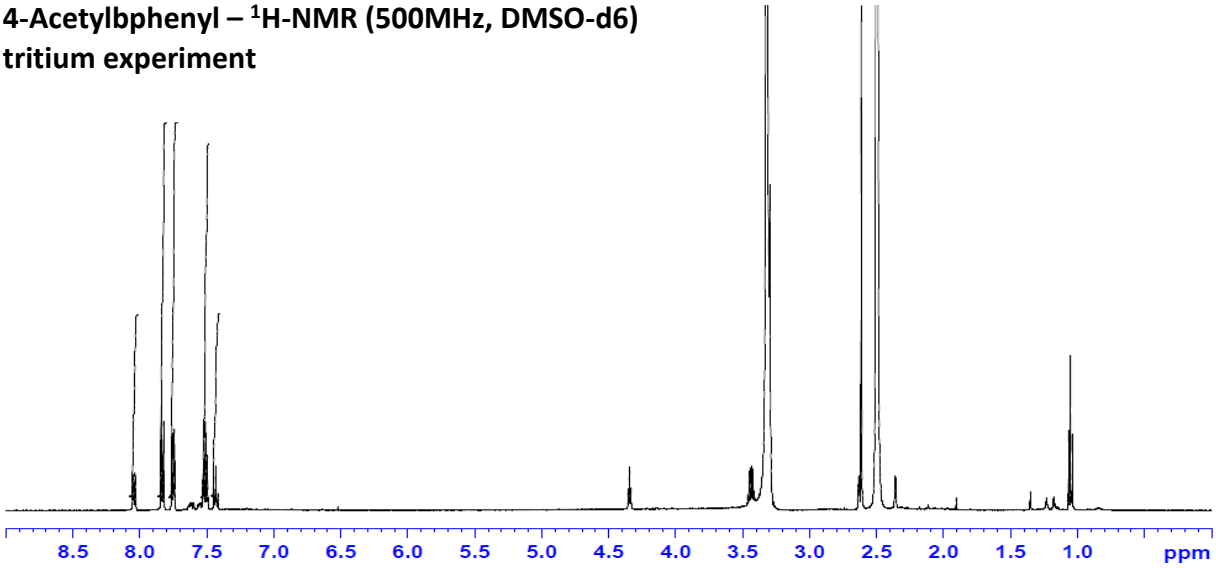
m/z 197.09 $[M+H]^+$ (45.9), 198.09 $[M+1+H]^+$ (7.2), 199.10 $[M+2+H]^+$ (100), 200.10 $[M+3+H]^+$ (16.4), 201.11 $[M+4+H]^+$ (58.1), 202.11 $[M+5+H]^+$ (8.5), 203.11 $[M+6+H]^+$ (1.1)

22,7 % T0
49,2 % T1 → x 29 Ci/mmol → **14,3 Ci/mmol**
28,1 % T2 → x 58 Ci/mmol → **16,3 Ci/mmol**
0,1 % T3 → x 87 Ci/mmol → **0,1 Ci/mmol**
100,0 % **30,6 Ci/mmol → 31 Ci/mmol**

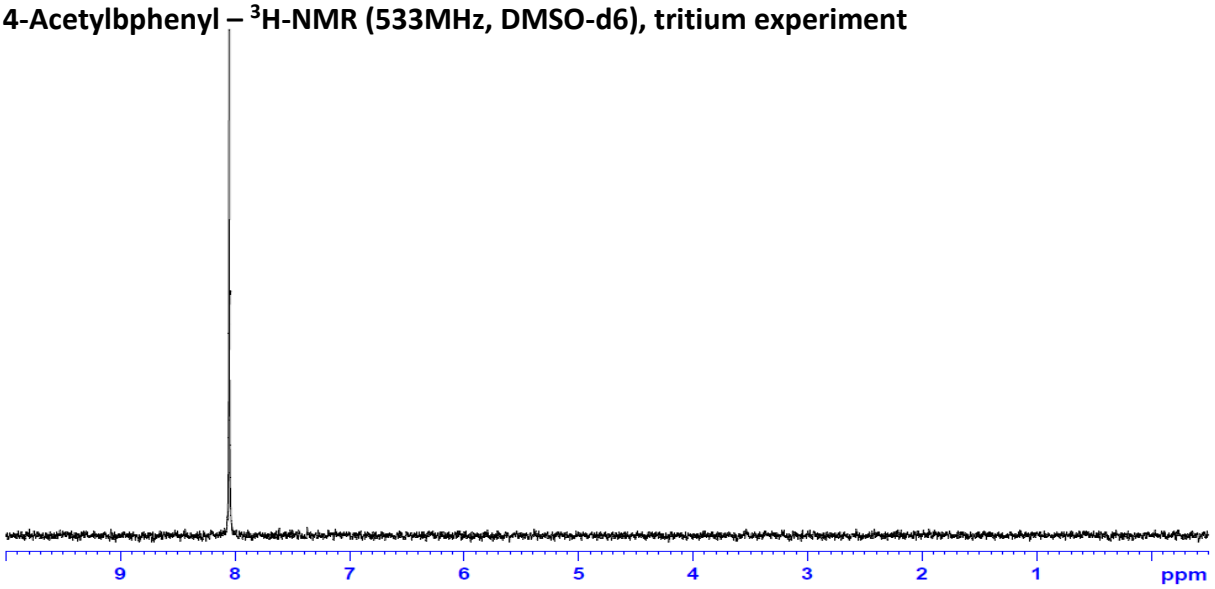
4-Acetylbphenyl – reference ^{1}H-NMR (500MHz, DMSO-d6)



4-Acetylbphenyl – ^{1}H-NMR (500MHz, DMSO-d6)
tritium experiment



4-Acetylbphenyl – ^{3}H-NMR (533MHz, DMSO-d6), tritium experiment



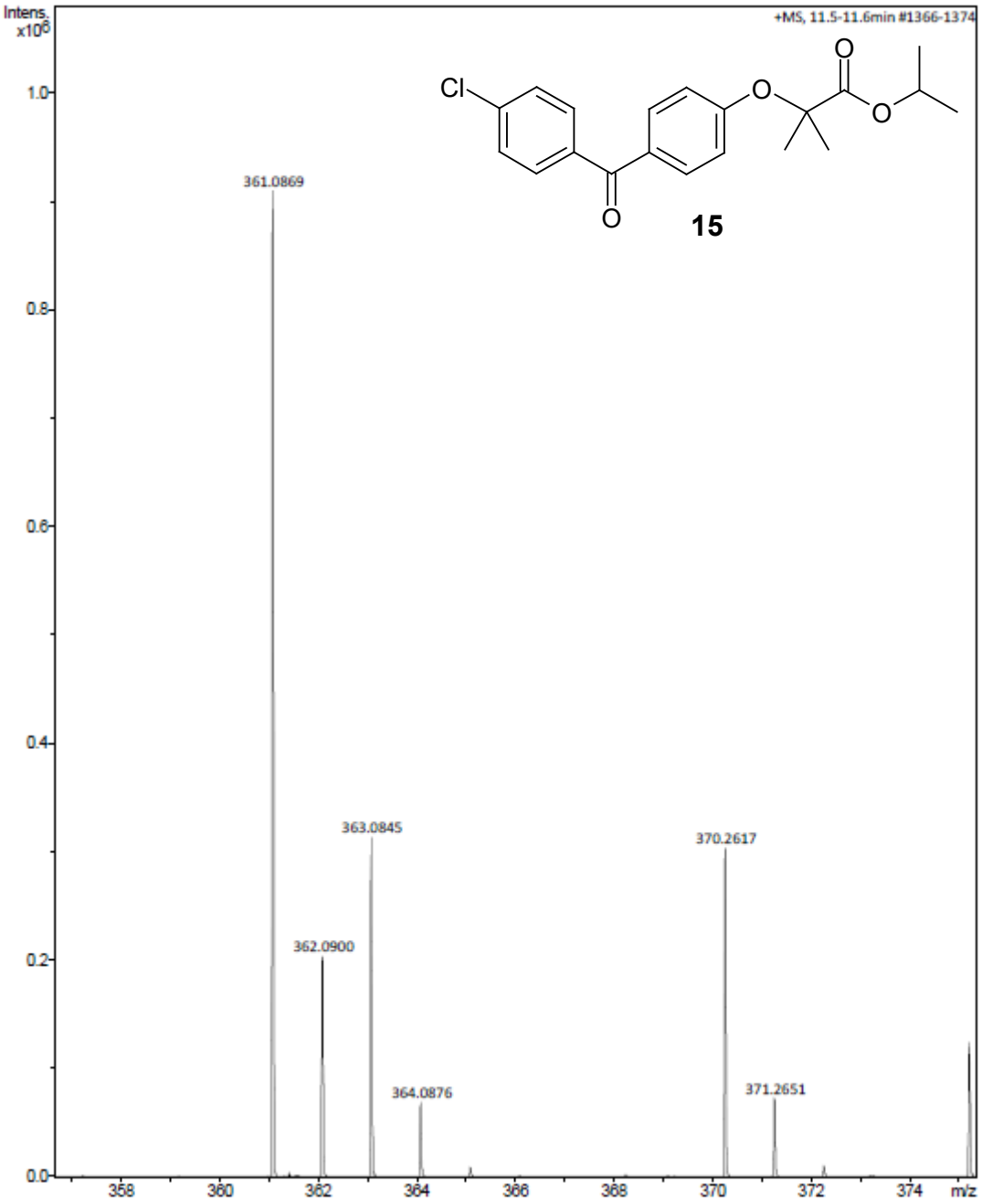
Tritium experiment fenofibrate **15**

4.60 mg (12.6 μmol) fenofibrate **15** and 2.2 mg Kerr BArF (cas 1628471-64-6) (10 mol%) were placed in a 1 mL reaction flask and dissolved in 0.7 mL dry isopropyl acetate. The reaction flask was adapted to a tritium manifold (TRITEC) and the solution was frozen in liquid nitrogen (-196°C). The flask was evacuated, charged with tritium (30010 MBq, 13.7 μmol T2, 1.1 eq, pressure 21 mbar. The reaction mixture was then allowed to warm to room temperature before stirring at rt for 5 hours. Then the valve between the reaction flask and a flask with 60.0 mg (264,3μmol) PtO_2 suspended in 1 ml methanol were opened for 18h to react the H/T-atmosphere to get THO. Then all volatile components were distilled into an ampule in vacuo at -196°C. The labile tritium was exchanged and removed by addition of methanol and a freeze-drying process (three times repeated).
The solid residue was dissolved in 3 mL methanol. Purification and isolation *via* HPLC (Phenomenex Gemini NX C18 10x150 mm, 5 μm, 5 mL/min flow, ACN/water gradient program) to give (4.6 mg, 13940 MBq , 46,5 % RCY, 1088 GBq/mmol (29.5 Ci/mmol). The waste ampule with all the volatile tritium species contained 14450 MBq (48 %). HPLC-waste: (555 MBq).

RCY = 13940 Mbq/30010 MBq = 46,5 %, purity >98% UV and RD.

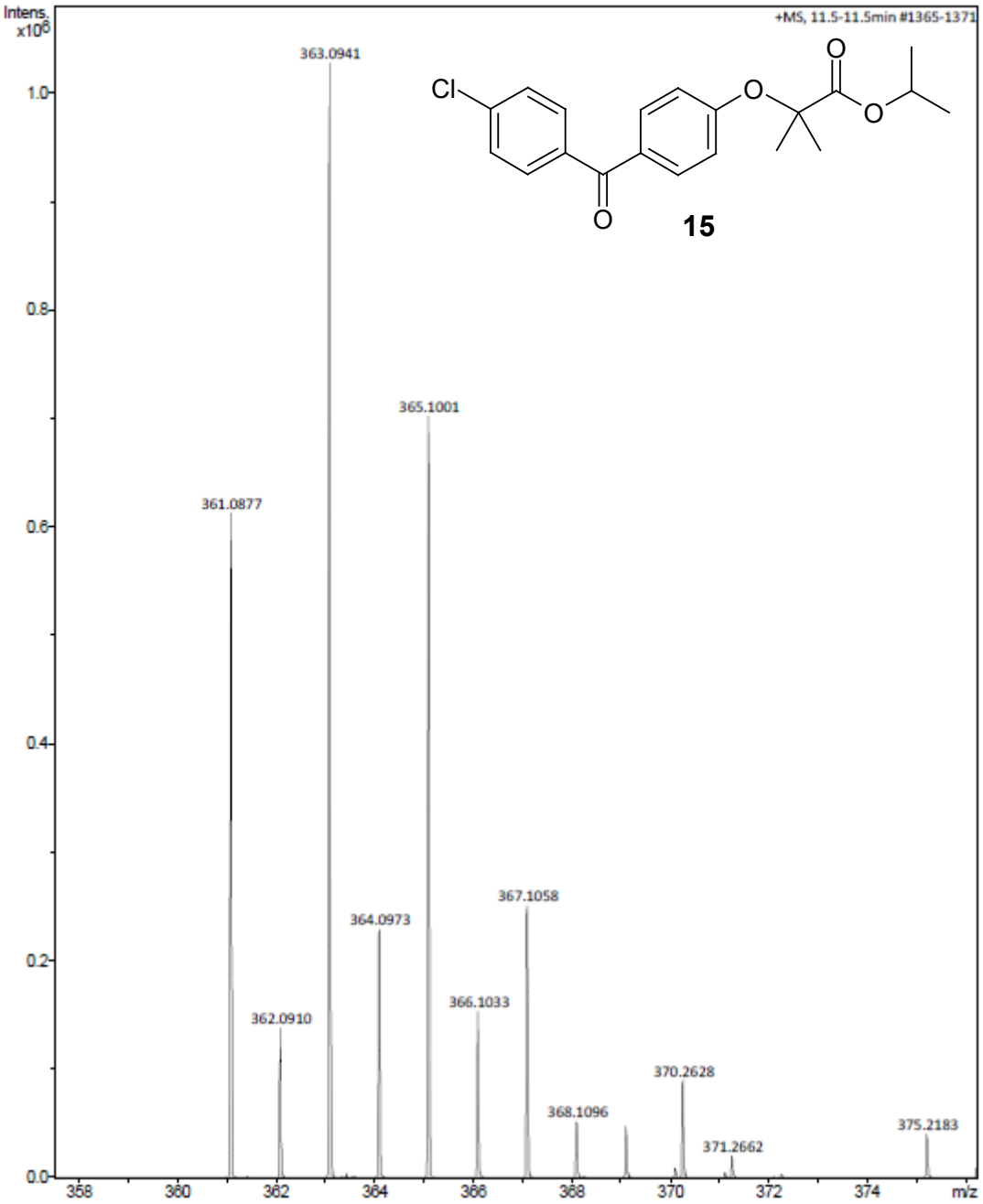
Activity recovery: 13940 MBq product + 15005 MBq (volatile waste/THO) = 96%

Fenofibrate – reference mass spectra



m/z 361.09 $[M+H]^+$ (100), 362.09 $[M+1+H]^+$ (22.4), 363.08 $[M+2+H]^+$ (34.4), 364.09 $[M+3+H]^+$ (7.4), 365.09 $[M+4+H]^+$ (1.0)

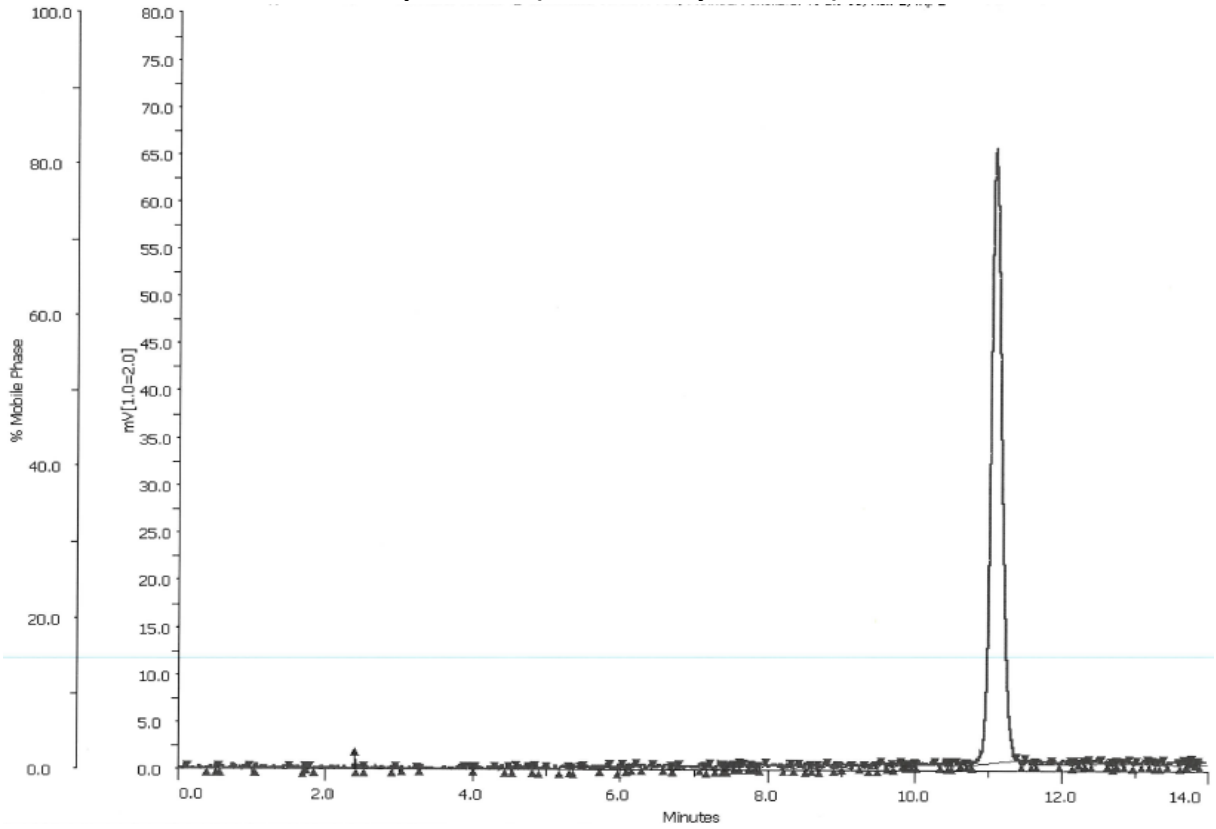
Fenofibrate – mass spectra for tritium experiment 1



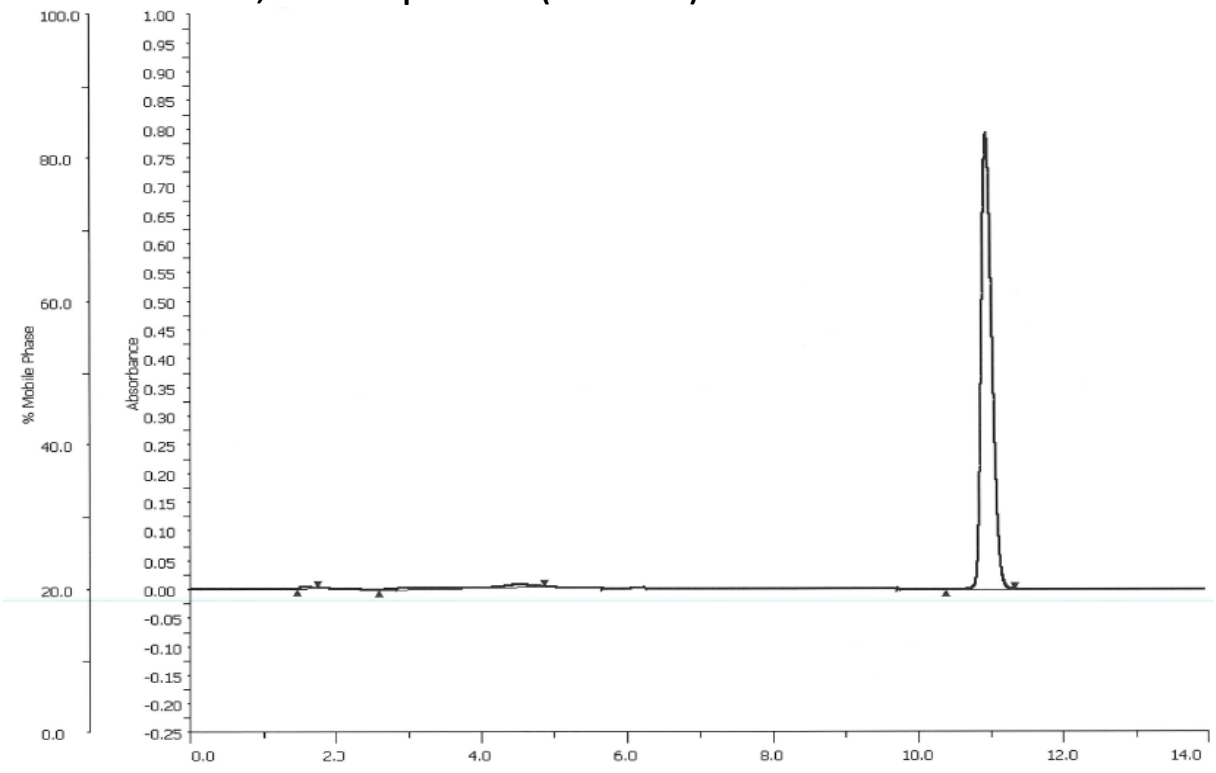
m/z 361.09 $[M+H]^+$ (59.6), 362.09 $[M+1+H]^+$ (13.5), 363.09 $[M+2+H]^+$ (100), 364.10 $[M+3+H]^+$ (22.3), 365.10 $[M+4+H]^+$ (68.3), 366.10 $[M+5+H]^+$ (14.9), 367.11 $[M+6+H]^+$ (24.4), 368.11 $[M+7+H]^+$ (5.0), 369.10 $[M+8+H]^+$ (4.6), 370.26 $[M+9+H]^+$ (8.6), 371.27 $[M+10+H]^+$ (2.0)

31,4 % T0
41.8 % T1 → **x** 29 Ci/mmol → **12.1 Ci/mmol**
21.2 % T2 → **x** 58 Ci/mmol → **12.3 Ci/mmol**
5.1 % T3 → **x** 87 Ci/mmol → **4.4 Ci/mmol**
0.5 % T4 → **x** 116 Ci/mmol → **0.5 Ci/mmol**
100,0 % **29.491 Ci/mmol → 29.5 Ci/mmol**

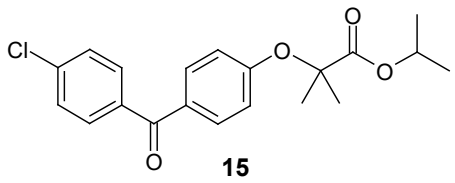
Fenofibrate – HPLC, tritium experiment (radioactivity detector)



Fenofibrate – HPLC, tritium experiment (UV 210nm)

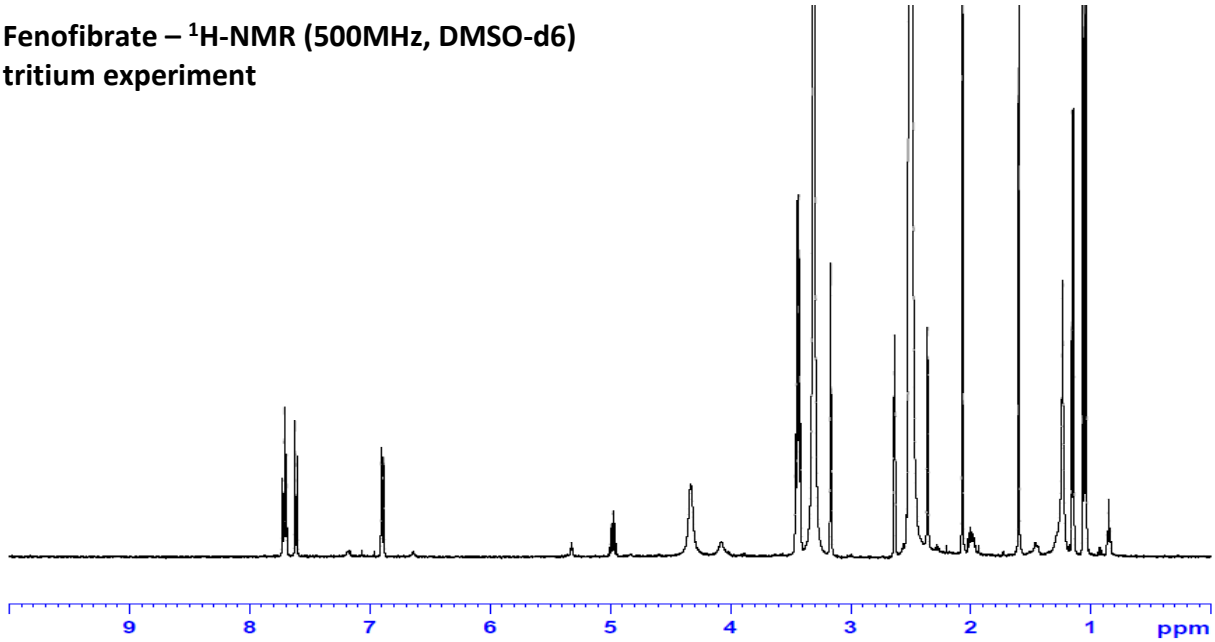


Fenofibrate – reference ^{1}H-NMR (500MHz, DMSO-d6)

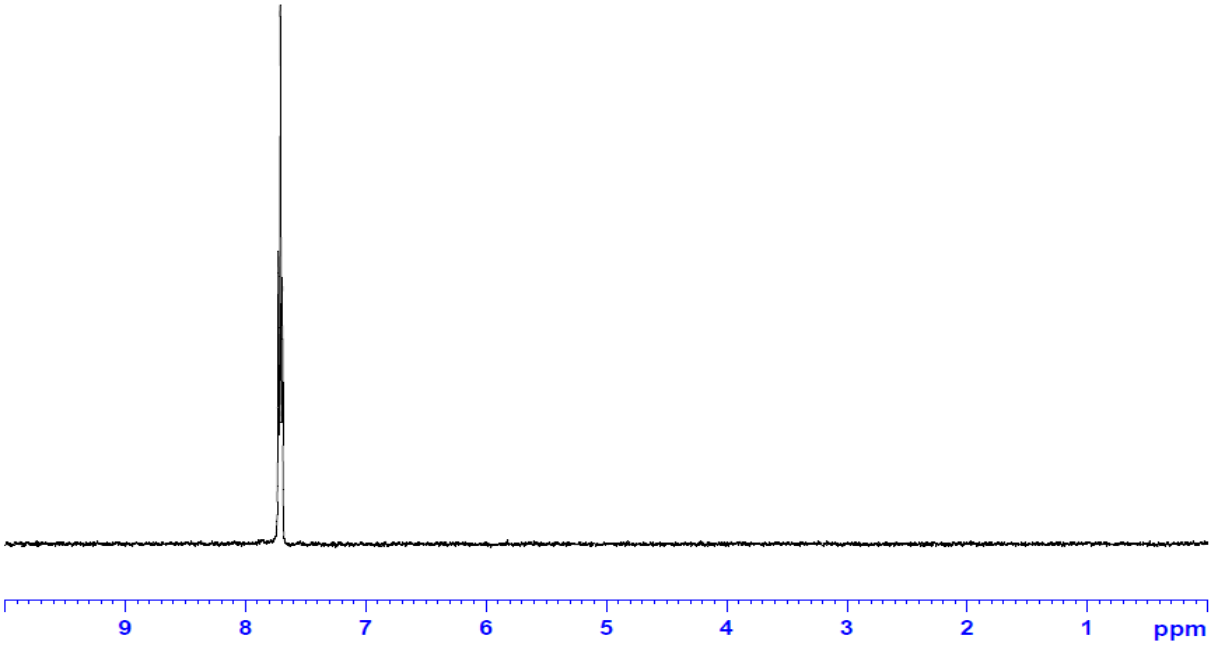


15

Fenofibrate – ^{1}H-NMR (500MHz, DMSO-d6)
tritium experiment



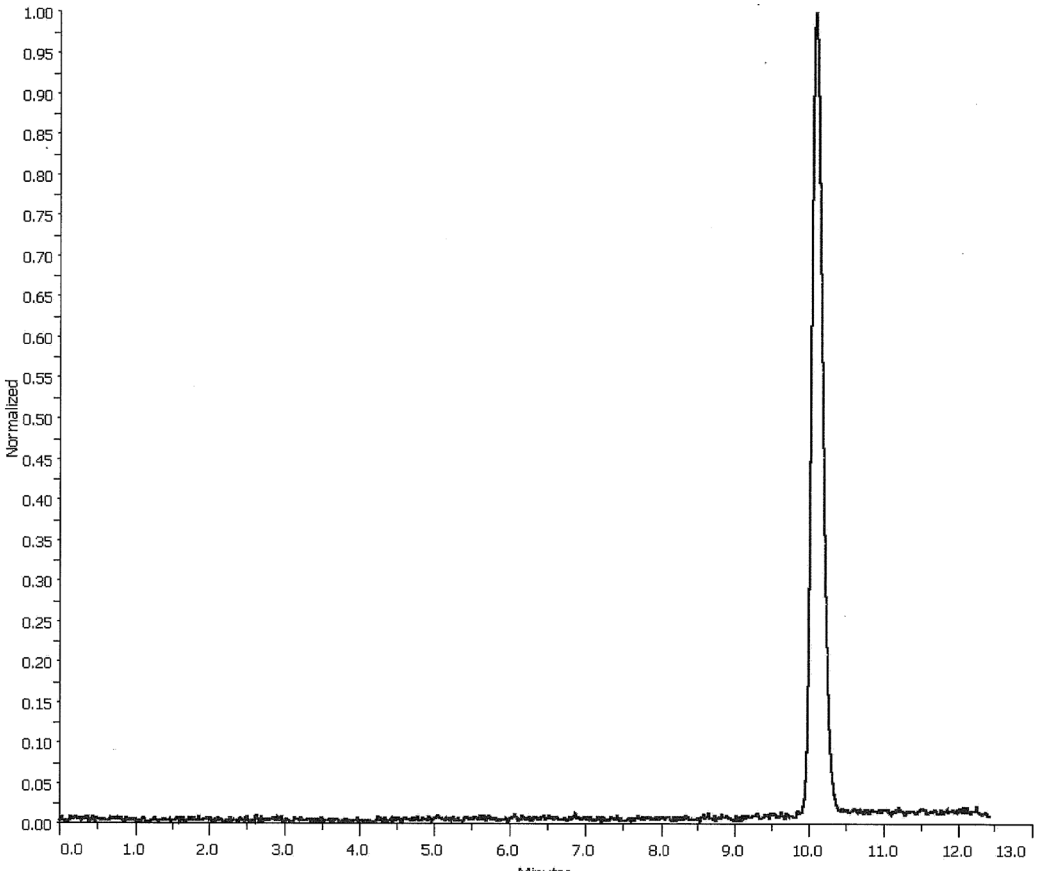
Fenofibrate – ^{3}H-NMR (533MHz, DMSO-d6), tritium experiment



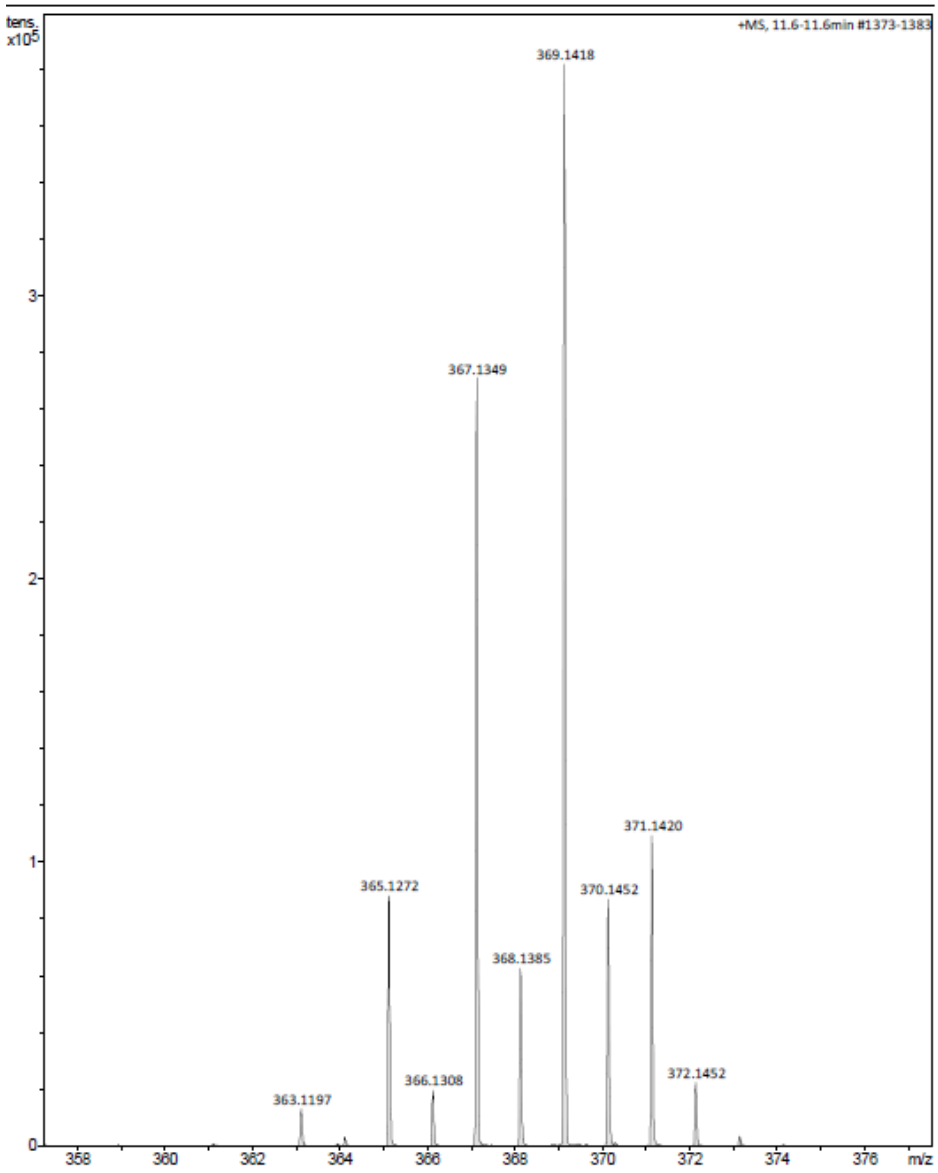
Tritium Experiment Fenofibrate 15 (10 eq. T_2)

1.40 mg (3.9 mmol) fenofibrate **15** and 0.67 mg Kerr BArF (cas 1628471-64-6) (10 mol%) were placed in a 1 mL reaction flask and dissolved in 0.7 mL dry isopropyl acetate. The reaction flask was adapted to a tritium manifold (TRITEC) and the solution was frozen in liquid nitrogen (-196°C). The flask was evacuated, charged with tritium (85220 MBq, 39.4 mmol T_2, 10.1 eq, pressure 74 mbar). The reaction mixture was then allowed to warm to room temperature before stirring at rt for 5 hours. Then all volatile components were distilled into an ampule in vacuo at -196°C. The labile tritium was exchanged and removed by addition of methanol and a freeze-drying process (three times repeated).
The solid residue was dissolved in 3 mL methanol. Purification and isolation *via* HPLC (Phenomenex Gemini NX C18 10x150 mm, 5 mm, 5 mL/min flow, ACN/water gradient program) to give **^{3}H-15** (1.10 mg, 9630 MBq, 11.3 % RCY, 3537 GBq/mmol (95 Ci/mmol).
RCY = 9630 Mbq/85220 MBq = 11.3 %

HPLC (RD), purity > 98%



MS-spectra:



0,1 % T0					
2,0 % T1	→	x	29 Ci/mmol	→	**0,6 Ci/mmol**
13,1 % T2	→	x	58 Ci/mmol	→	**7,6 Ci/mmol**
37,9 % T3	→	x	87 Ci/mmol	→	**32,9 Ci/mmol**
46,5 % T4	→	x	116 Ci/mmol	→	**53,9 Ci/mmol**
0,5 % T5	→	x	145 Ci/mmol	→	**0,7 Ci/mmol**
-0,2 % T6	→	x	174 Ci/mmol	→	**-0,3 Ci/mmol**
0,0 % T7	→	x	203 Ci/mmol	→	**0,1 Ci/mmol**
0,0 % T8	→	x	232 Ci/mmol	→	**0,0 Ci/mmol**
0,0 % T9	→	x	261 Ci/mmol	→	**0,0 Ci/mmol**
0,0 % T10	→	x	290 Ci/mmol	→	**0,0 Ci/mmol**

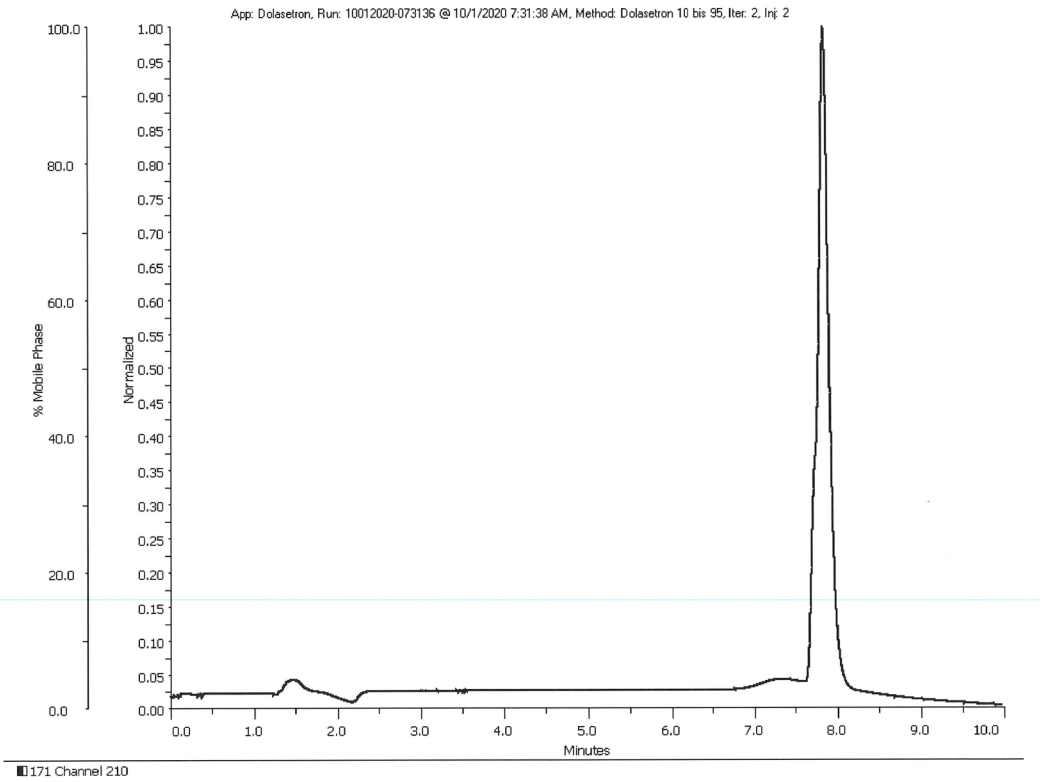
100,0 %	**95,564 Ci/mmol**

Tritium experiment dolasetron **16**

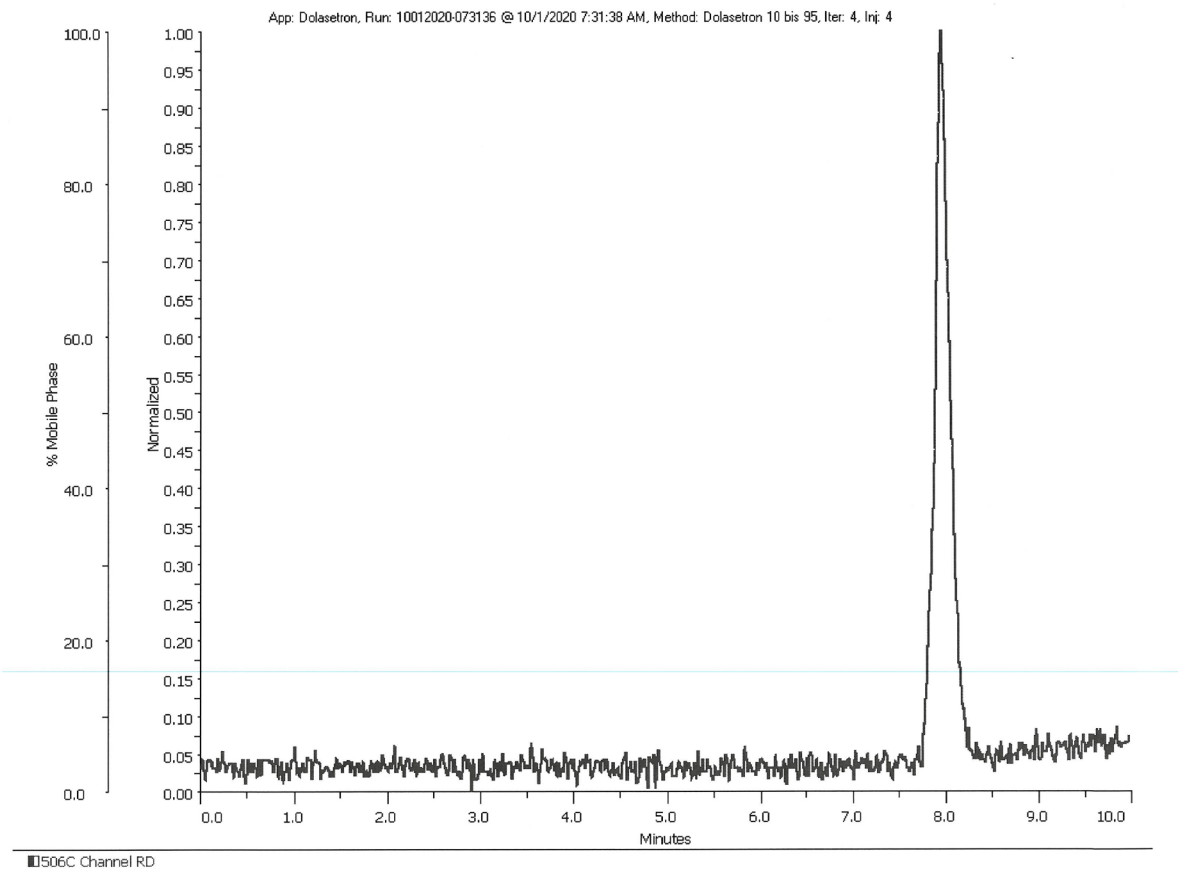
4.10 mg (12.6 mmol) dolasetron **16** and 1.3 mg Kerr PF_6 (cas 1019852-99-3) (10 mol%) were placed in a 1 mL reaction flask and dissolved in 0.7 mL dry isopropyl acetate. The reaction flask was adapted to a tritium manifold (TRITEC) and the solution was frozen in liquid nitrogen (-196°C). The flask was evacuated, charged with tritium (27605 MBq, 12.76 mmol T_2, 1 eq, pressure 25 mbar). The reaction mixture was then allowed to warm to room temperature before stirring at rt for 5 hours. Then all volatile components were distilled into an ampule in vacuo at -196°C. The labile tritium was exchanged and removed by addition of methanol and a freeze-drying process (three times repeated).
The solid residue was dissolved in 3 mL methanol. Purification and isolation *via* HPLC (Phenomenex Gemini NX C18 10x150 mm, 5 mm, 5 mL/min flow, ACN/water gradient program) to give 3.4 mg, 3471 MBq , 328 GBq/mmol (8,9 Ci/mmol) of **^{3}H-16**.

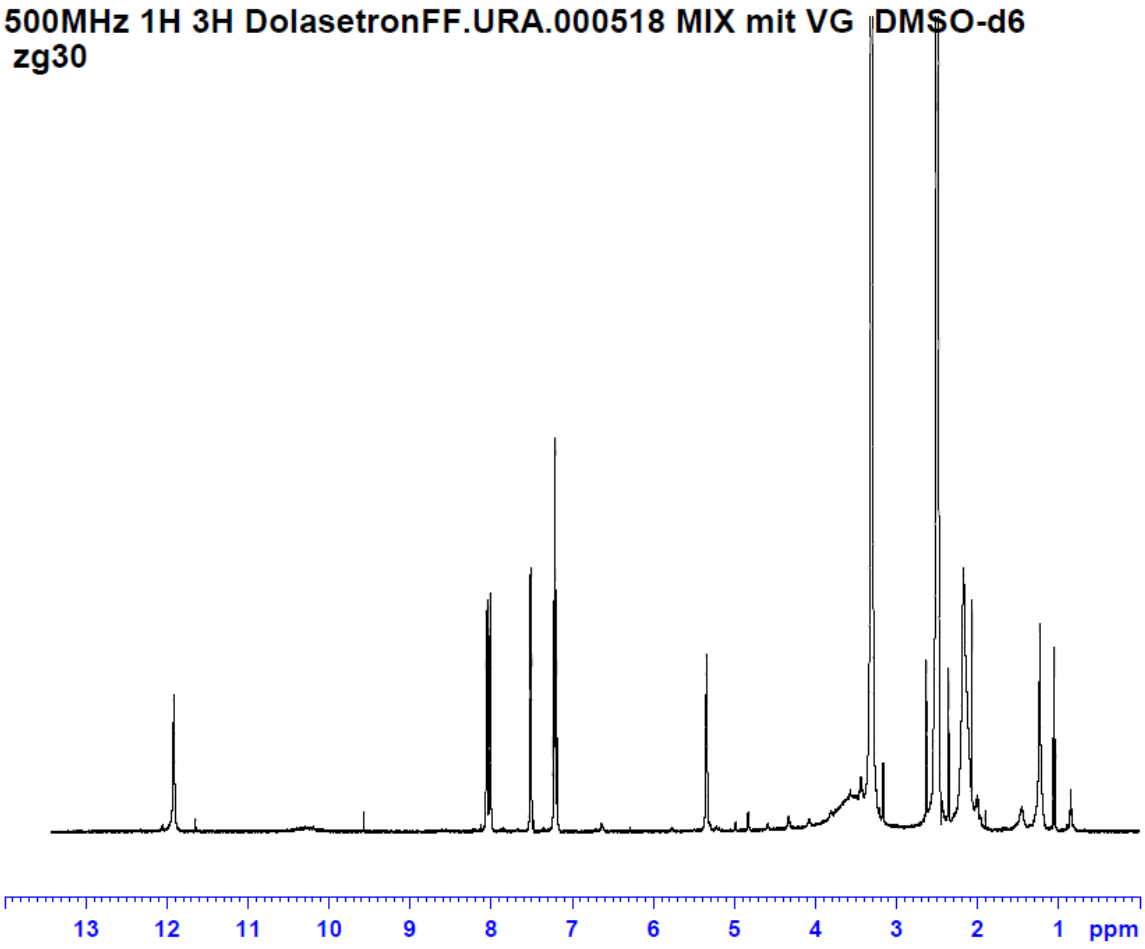
RCY = 3471 Mbq/27605 MBq = 12,6 % purity >98% RD.

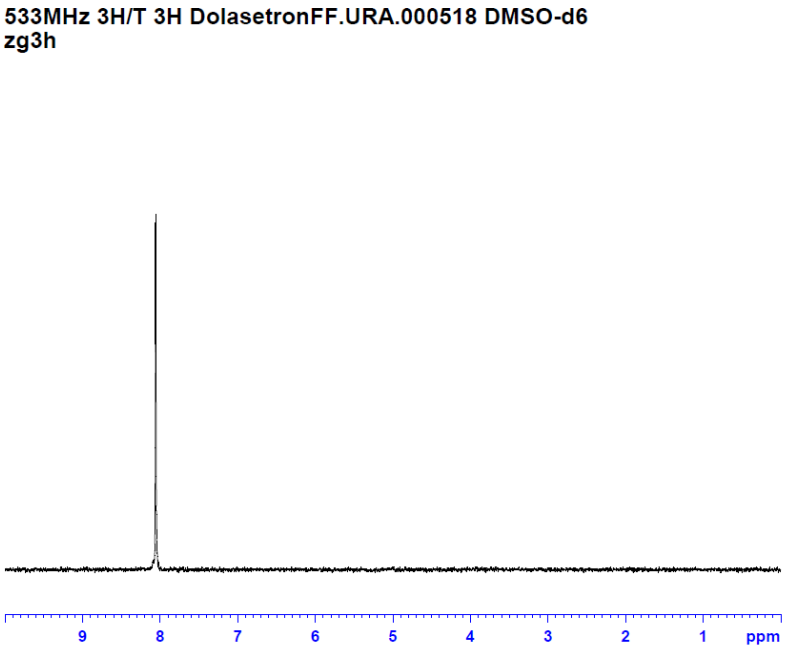
HPLC, tritium experiment (UV 210nm)

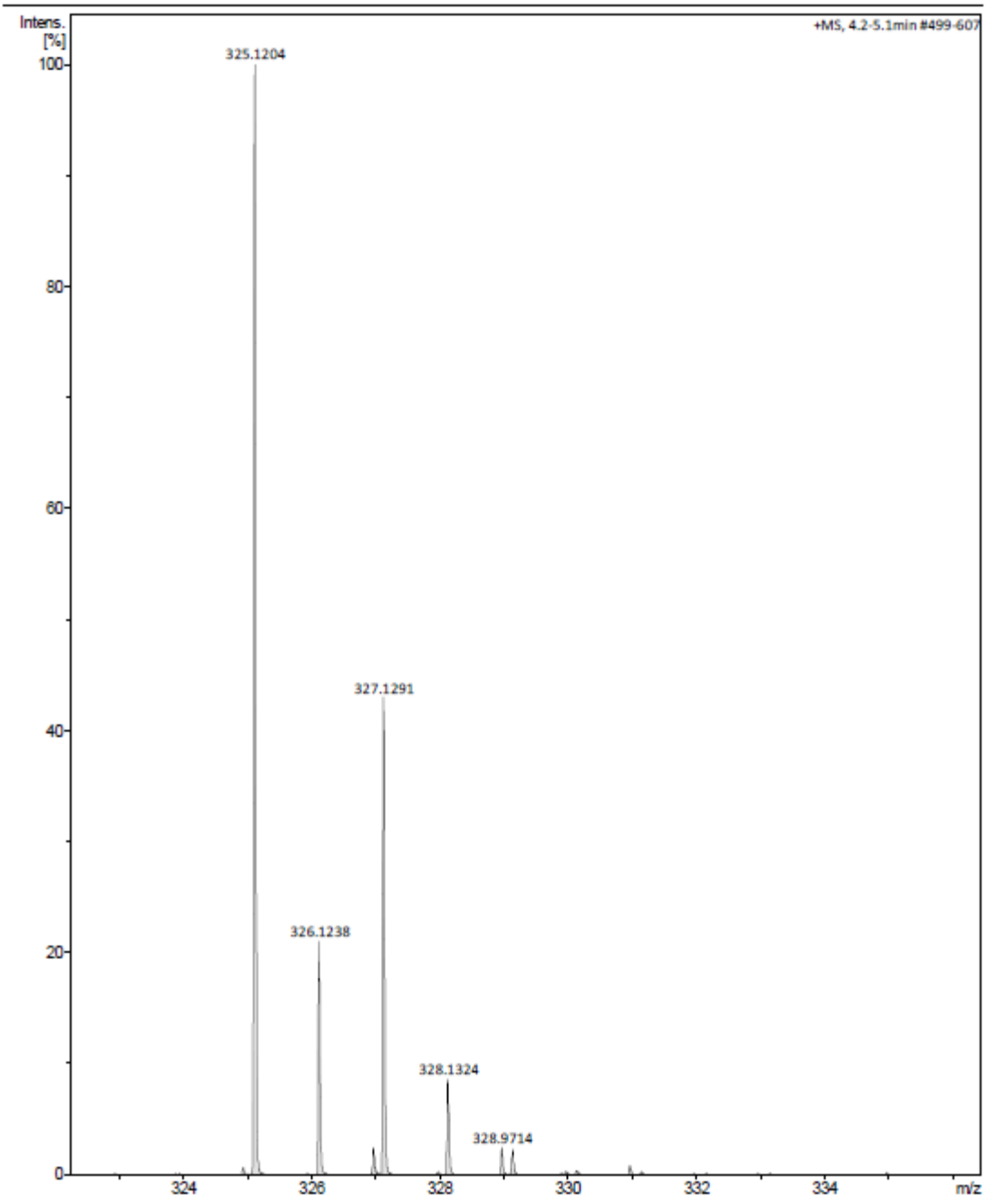


Dolasetron - HPLC, tritium experiment (radioactivity detector)




500MHz 1H 3H DolasetronFF.URA.000518 MIX mit VG DMSO-d6
zg30
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm


533MHz 3H/T 3H DolasetronFF.URA.000518 DMSO-d6
zg3h
9 8 7 6 5 4 3 2 1 ppm



70,6 % T0					
28,4 % T1	→	x	29 Ci/mmol	→	8,2 Ci/mmol
0,8 % T2	→	x	58 Ci/mmol	→	0,5 Ci/mmol
0,2 % T3	→	x	87 Ci/mmol	→	0,1 Ci/mmol
0,0 % T4	→	x	116 Ci/mmol	→	0,0 Ci/mmol
0,0 % T5	→	x	145 Ci/mmol	→	0,0 Ci/mmol
0,0 % T6	→	x	174 Ci/mmol	→	0,0 Ci/mmol
0,0 % T7	→	x	203 Ci/mmol	→	0,0 Ci/mmol
0,0 % T8	→	x	232 Ci/mmol	→	0,0 Ci/mmol
0,0 % T9	→	x	261 Ci/mmol	→	0,0 Ci/mmol
0,0 % T10	→	x	290 Ci/mmol	→	0,0 Ci/mmol

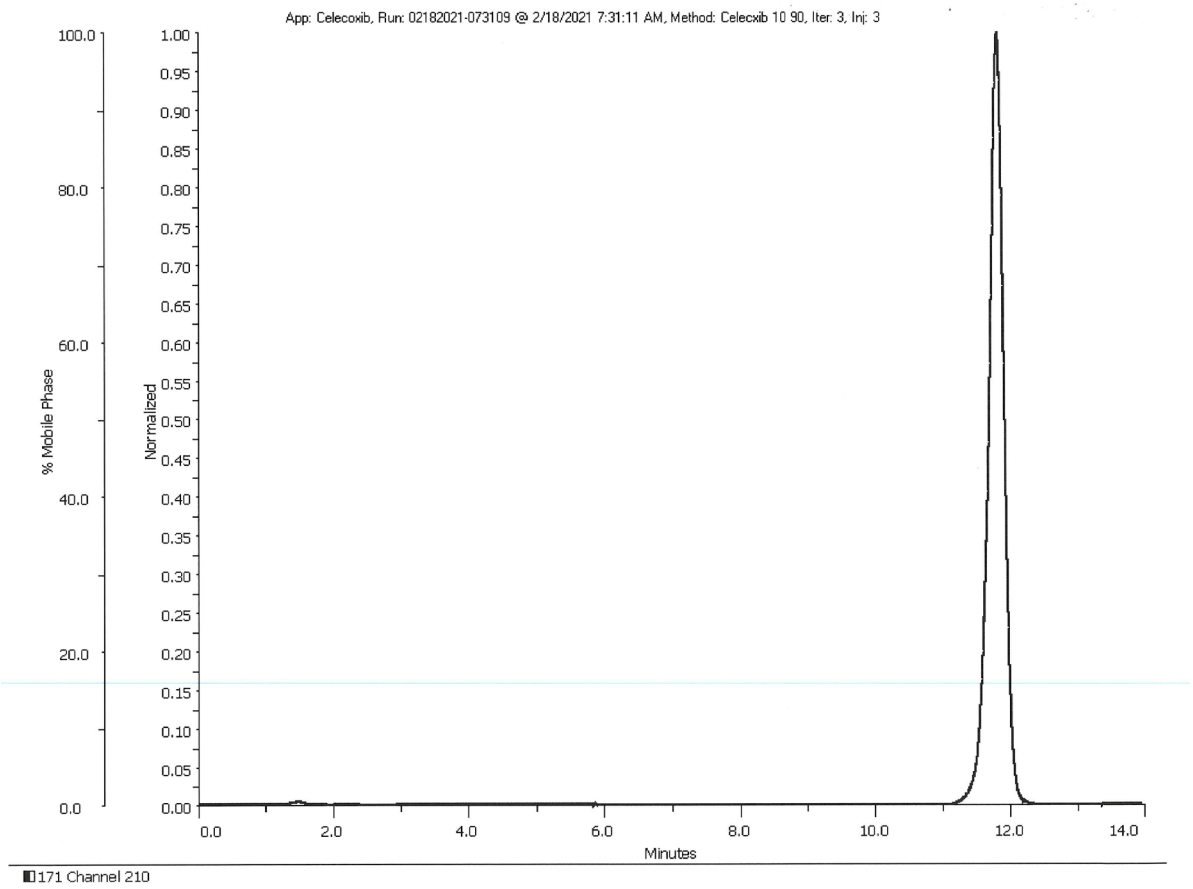
100,0 %	8,851 Ci/mmol →	8,9 Ci/mmol

Tritium experiment celecoxib **17**

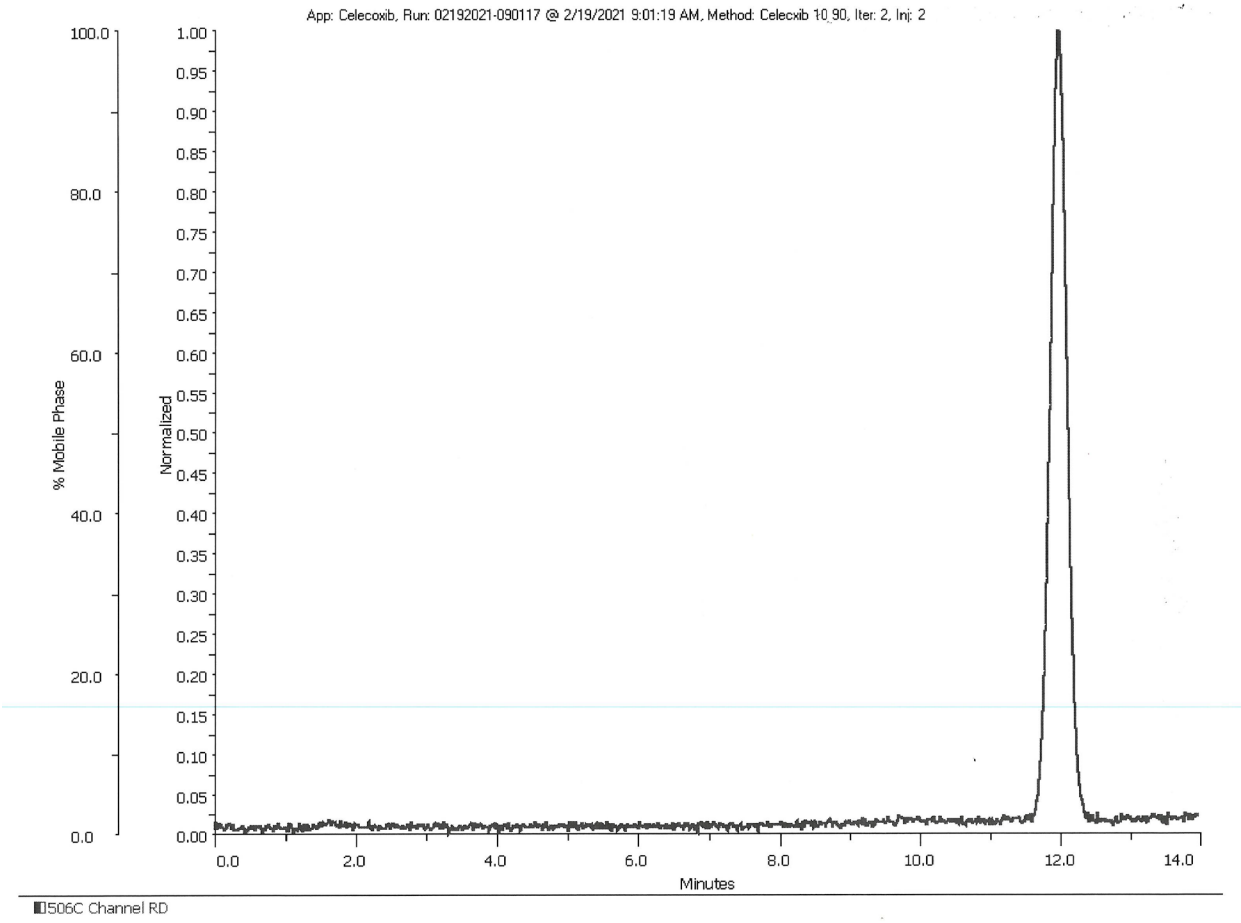
5.40 mg (14.17 mmol) Celecoxib **17** and 2.4 mg Kerr BArF (cas 1628471-64-6) (10 mol%) were placed in a 1 mL reaction flask and dissolved in 0.7 mL dry isopropyl acetate. The reaction flask was adapted to a tritium manifold (TRITEC) and the solution was frozen in liquid nitrogen (-196°C). The flask was evacuated, charged with tritium (30606 MBq, 14.16 mmol T_2, 1 eq, pressure 23 mbar). The reaction mixture was then allowed to warm to room temperature before stirring at rt for 5 hours. Then all volatile components were distilled into an ampule in vacuo at -196°C. The labile tritium was exchanged and removed by addition of methanol and a freeze-drying process (three times repeated).
The solid residue was dissolved in 3 mL methanol. Purification and isolation *via* HPLC (Phenomenex Gemini NX C18 10x150 mm, 5 mm, 5 mL/min flow, ACN/water gradient program) to give (4.9 mg, 9625 MBq, 752 GBq/mmol (20,3 Ci/mmol) of **^{3}H-17**.

RCY = 9625 Mbq/30606 MBq = 31,4 %, purity >98% UV and RD.

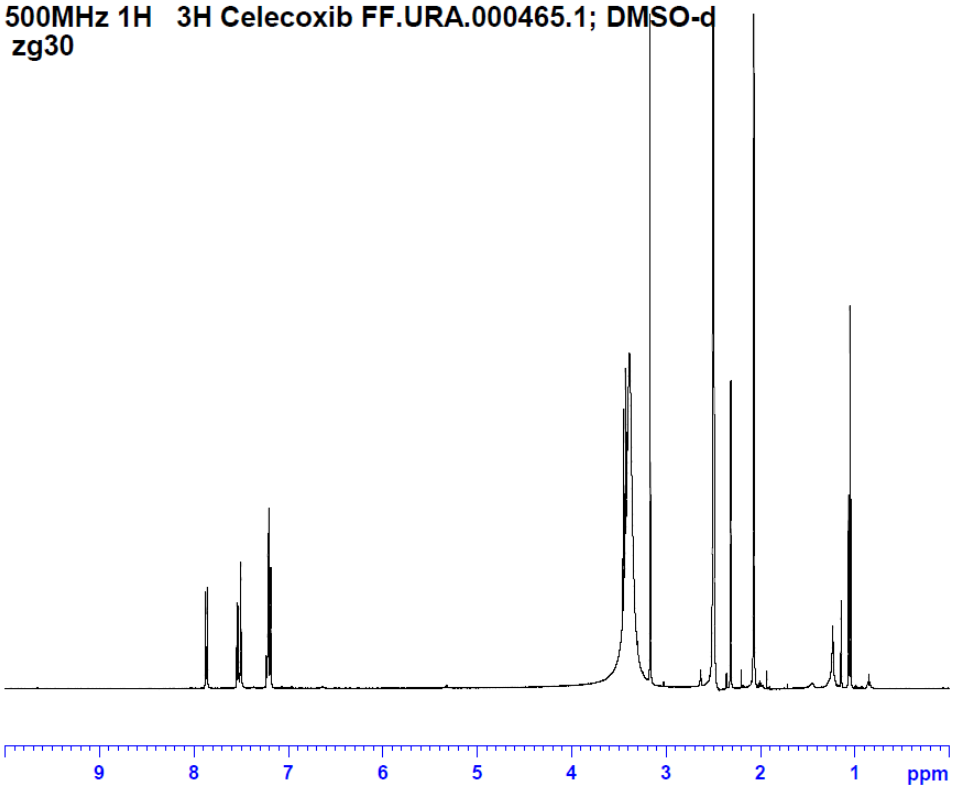
HPLC, tritium experiment (UV 210nm)



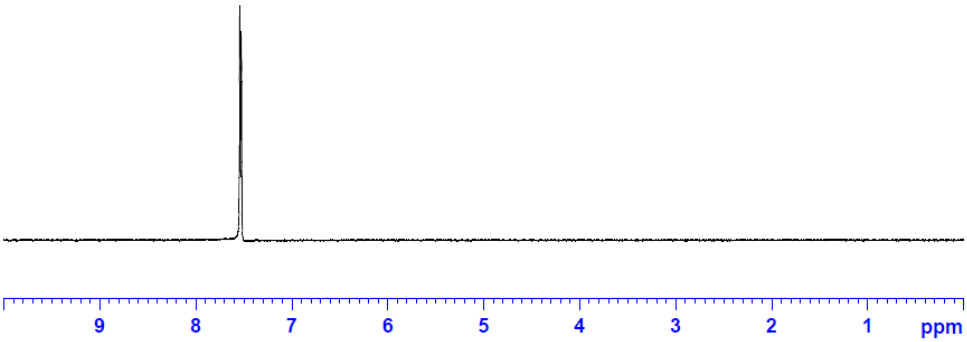
HPLC, tritium experiment (RD)

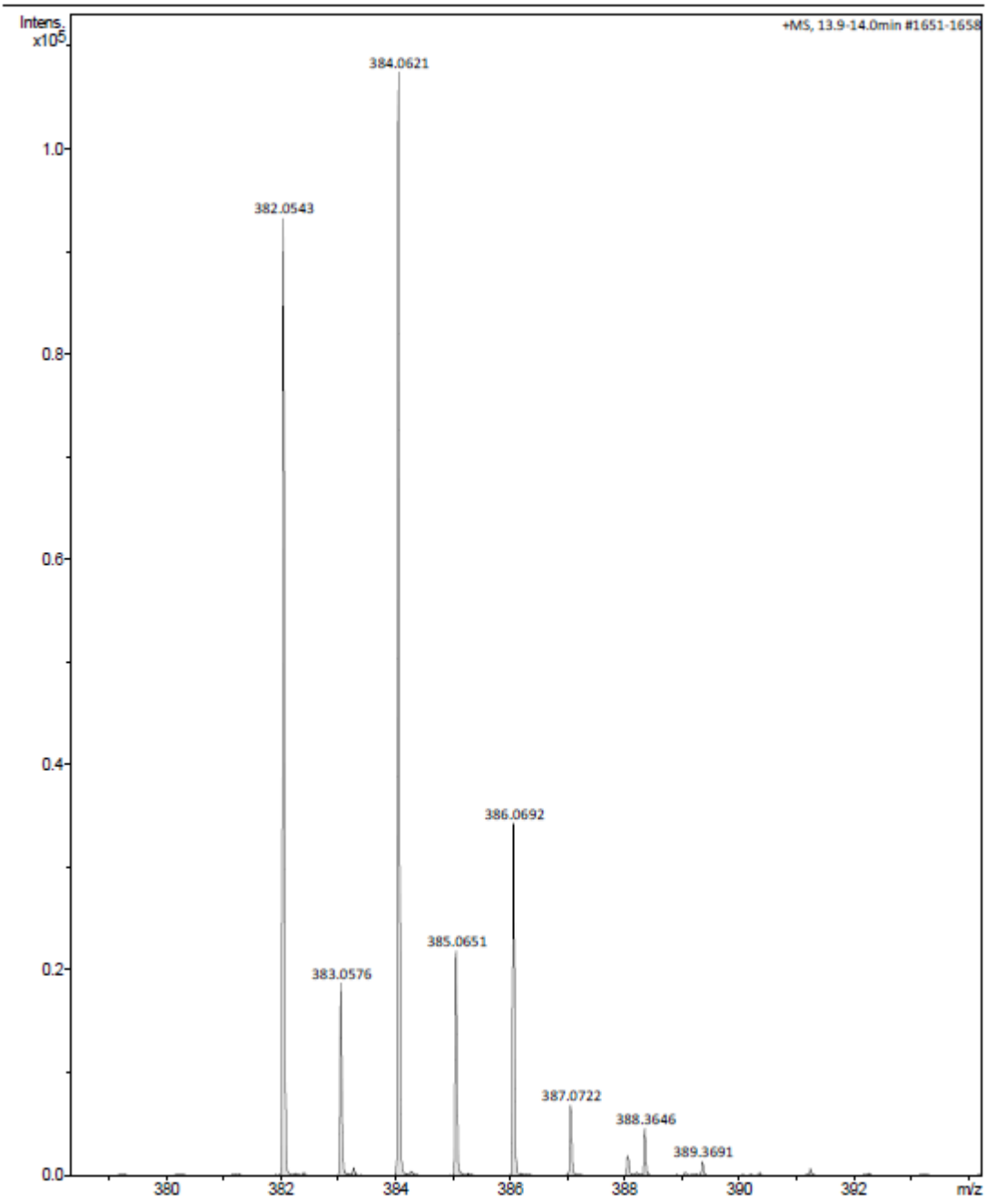


500MHz 1H 3H Celecoxib FF.URA.000465.1; DMSO-d
zg30



533MHz 3H/T 3H Celecoxib FF.URA.000465.1; DMSO-d
zg3h





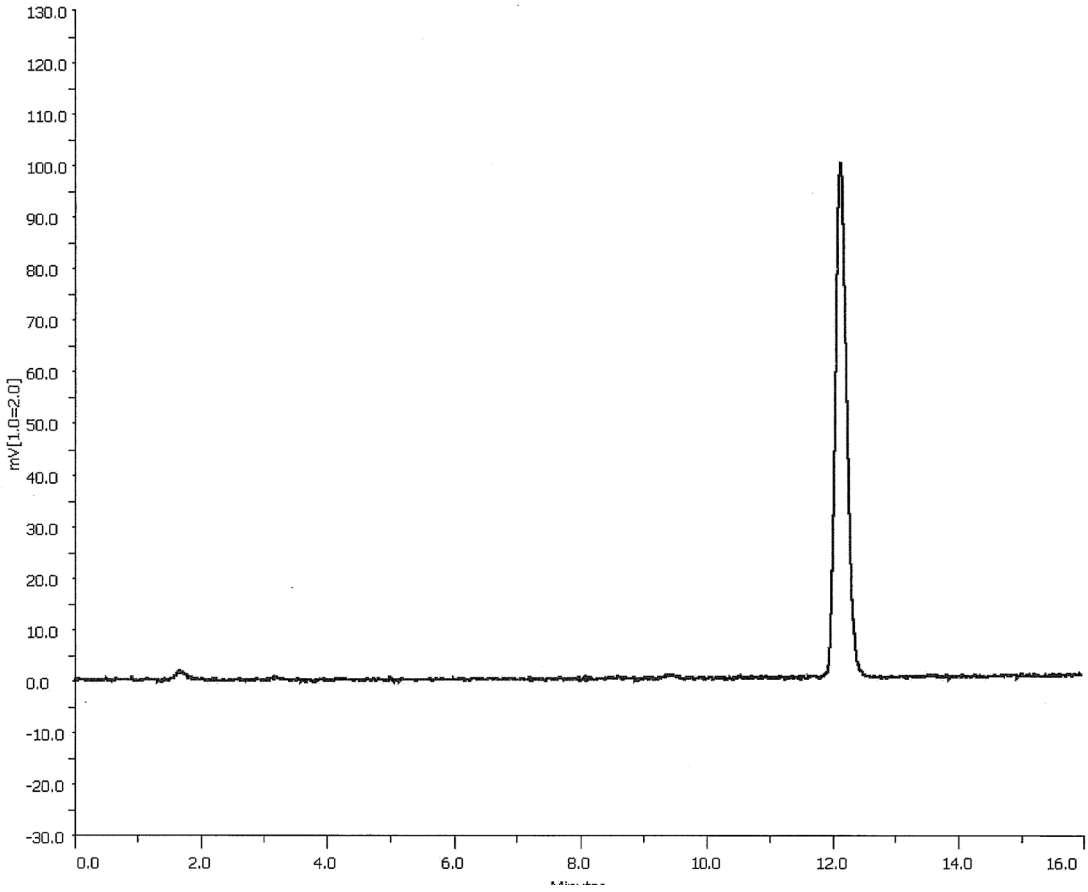
42,1 % T0						
45,6 % T1	→	x	29 Ci/mmol	→	**13,2 Ci/mmol**
12,3 % T2	→	x	58 Ci/mmol	→	**7,1 Ci/mmol**
0,0 % T3	→	x	87 Ci/mmol	→	**0,0 Ci/mmol**
0,0 % T4	→	x	116 Ci/mmol	→	**0,0 Ci/mmol**
0,0 % T5	→	x	145 Ci/mmol	→	**0,0 Ci/mmol**
0,0 % T6	→	x	174 Ci/mmol	→	**0,0 Ci/mmol**
0,0 % T7	→	x	203 Ci/mmol	→	**0,0 Ci/mmol**
0,0 % T8	→	x	232 Ci/mmol	→	**0,0 Ci/mmol**
0,0 % T9	→	x	261 Ci/mmol	→	**0,0 Ci/mmol**
0,0 % T10	→	x	290 Ci/mmol	→	**0,0 Ci/mmol**

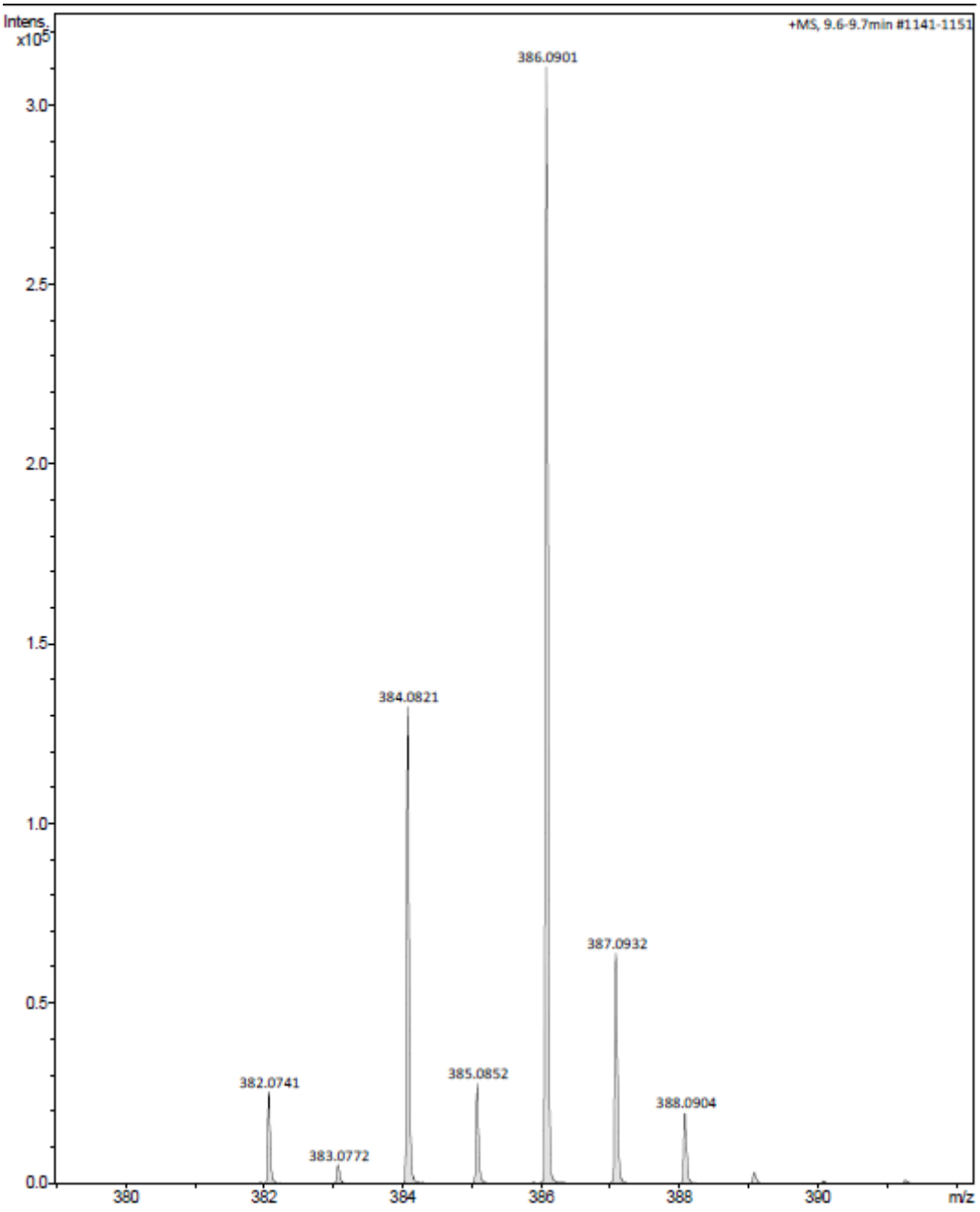
100,0 %	**20,325 Ci/mmol**	→	**20,3 Ci/mmol**

Tritium Experiment Celecoxib 17 (10 eq. T_2)

1.50 mg (3.93 mmol) Celecoxib **17** and 0.68 mg Kerr BArF (cas 1628471-64-6) (10 mol%) were placed in a 1 mL reaction flask and dissolved in 0.7 mL dry isopropyl acetate. The reaction flask was adapted to a tritium manifold (TRITEC) and the solution was frozen in liquid nitrogen (-196°C). The flask was evacuated, charged with tritium (81610 MBq, 37.77 mmol T_2, 9.6 eq, pressure 71 mbar). The reaction mixture was then allowed to warm to room temperature before stirring at rt for 5 hours. Then all volatile components were distilled into an ampule in vacuo at -196°C. The labile tritium was exchanged and removed by addition of methanol and a freeze-drying process (three times repeated).
The solid residue was dissolved in 3 mL methanol. Purification and isolation *via* HPLC (Phenomenex Gemini NX C18 10x150 mm, 5 mm, 5 mL/min flow, ACN/water gradient program) to give **^{3}H-17** (1.10 mg, 5125 MBq, 6.3% RCY, 1720 GBq/mmol (46 Ci/mmol).
RCY = 5125 Mbq/81610MBq = 6.3 %

HPLC (RD): >98% purity





5,6 % T0					
28,6 % T1	→	x	29 Ci/mmol	→	8,3 Ci/mmol
66,0 % T2	→	x	58 Ci/mmol	→	38,3 Ci/mmol
-0,1 % T3	→	x	87 Ci/mmol	→	-0,1 Ci/mmol
0,0 % T4	→	x	116 Ci/mmol	→	0,0 Ci/mmol
0,0 % T5	→	x	145 Ci/mmol	→	0,0 Ci/mmol
0,0 % T6	→	x	174 Ci/mmol	→	0,0 Ci/mmol
0,0 % T7	→	x	203 Ci/mmol	→	0,0 Ci/mmol
0,0 % T8	→	x	232 Ci/mmol	→	0,0 Ci/mmol
0,0 % T9	→	x	261 Ci/mmol	→	0,0 Ci/mmol
0,0 % T10	→	x	290 Ci/mmol	→	0,0 Ci/mmol

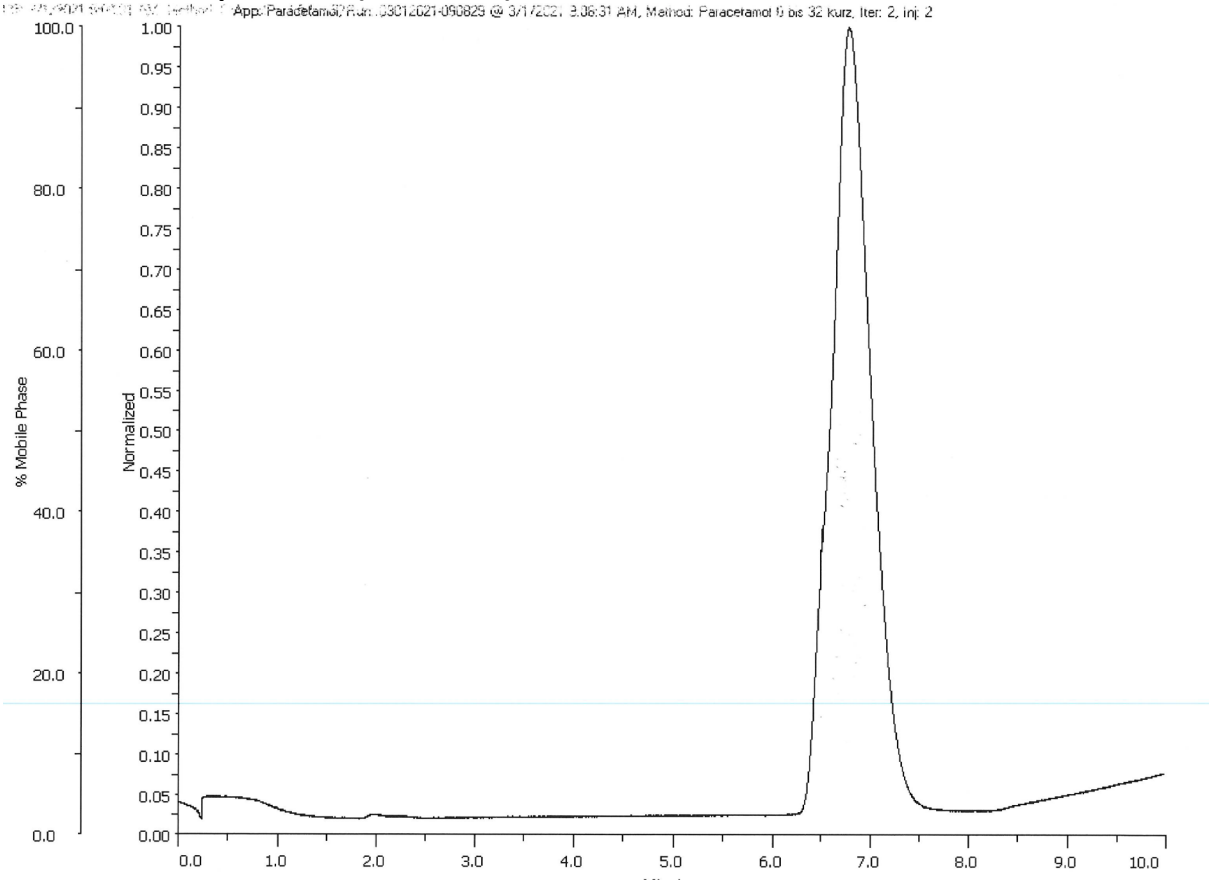
100,0 %	**46,461** Ci/mmol

Tritium experiment Paracetamol **18**

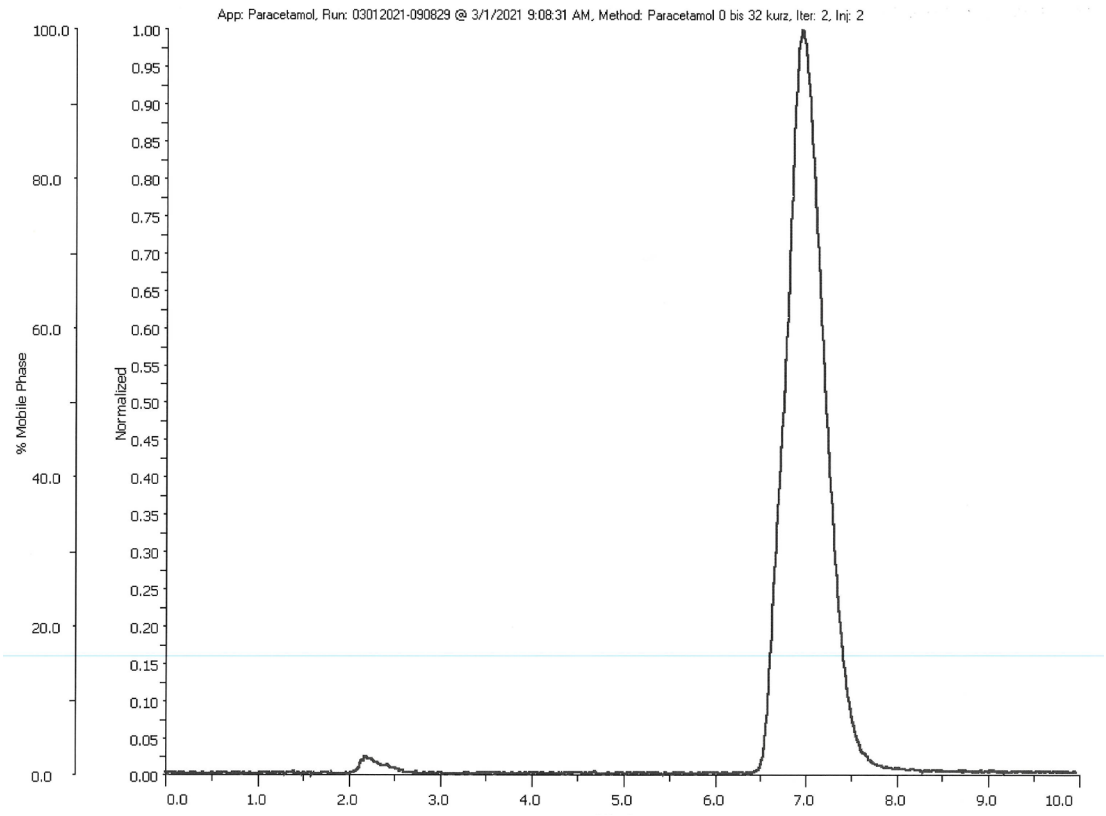
2.30 mg (15.2 mmol) Paracetamol **18** and 1.4 mg Kerr PF6 (cas1019852-99-3) (10 mol%) were placed in a 1 mL reaction flask and dissolved in 0.7 mL dry isopropyl acetate. The reaction flask was adapted to a tritium manifold (TRITEC) and the solution was frozen in liquid nitrogen (-196°C). The flask was evacuated, charged with tritium (30606 MBq, 14.16 mmol T_2, 0.93 eq, pressure 24 mbar. The reaction mixture was then allowed to warm to room temperature before stirring at rt for 5 hours. Then all volatile components were distilled into an ampule in vacuo at -196°C. The labile tritium was exchanged and removed by addition of methanol and a freeze-drying process (three times repeated). The solid residue was dissolved in 2 mL methanol/ water 1/1. Purification and isolation *via* HPLC (Phenomenex Synergi™ 4 µm Polar-RP 80 Å, LC Column 150 x 10 mm, 4 µm, 5 mL/min flow, ACN/water gradient program) to give (2.2 mg, 11125 MBq, 734 GBq/mmol (19,8 Ci/mmol).

RCY = 11125 Mbq/30606 MBq = 36,3 %

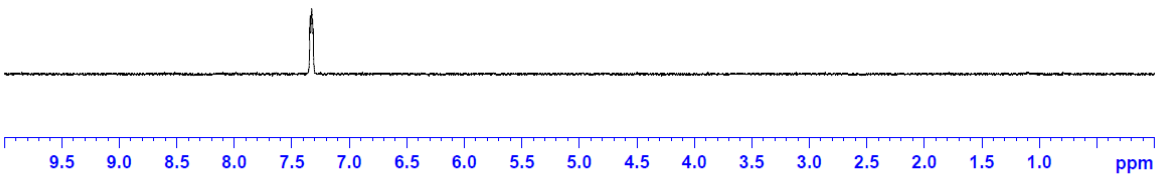
HPLC, tritium experiment (UV 210nm)



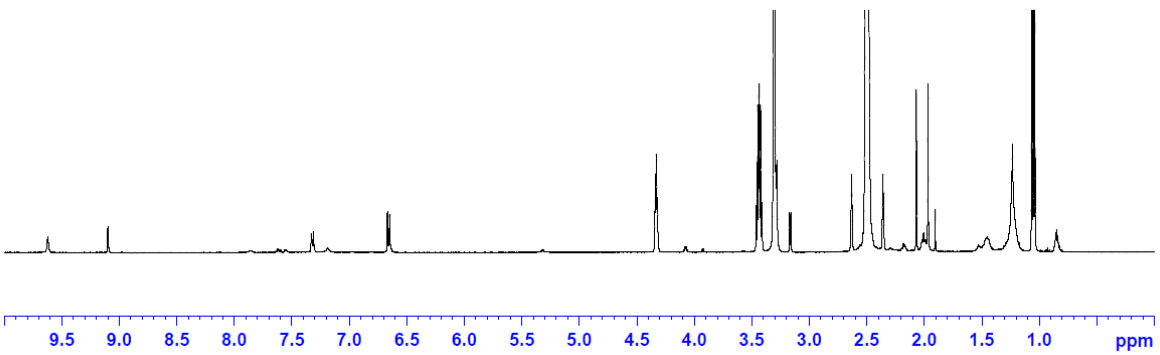
HPLC, tritium experiment (RD)

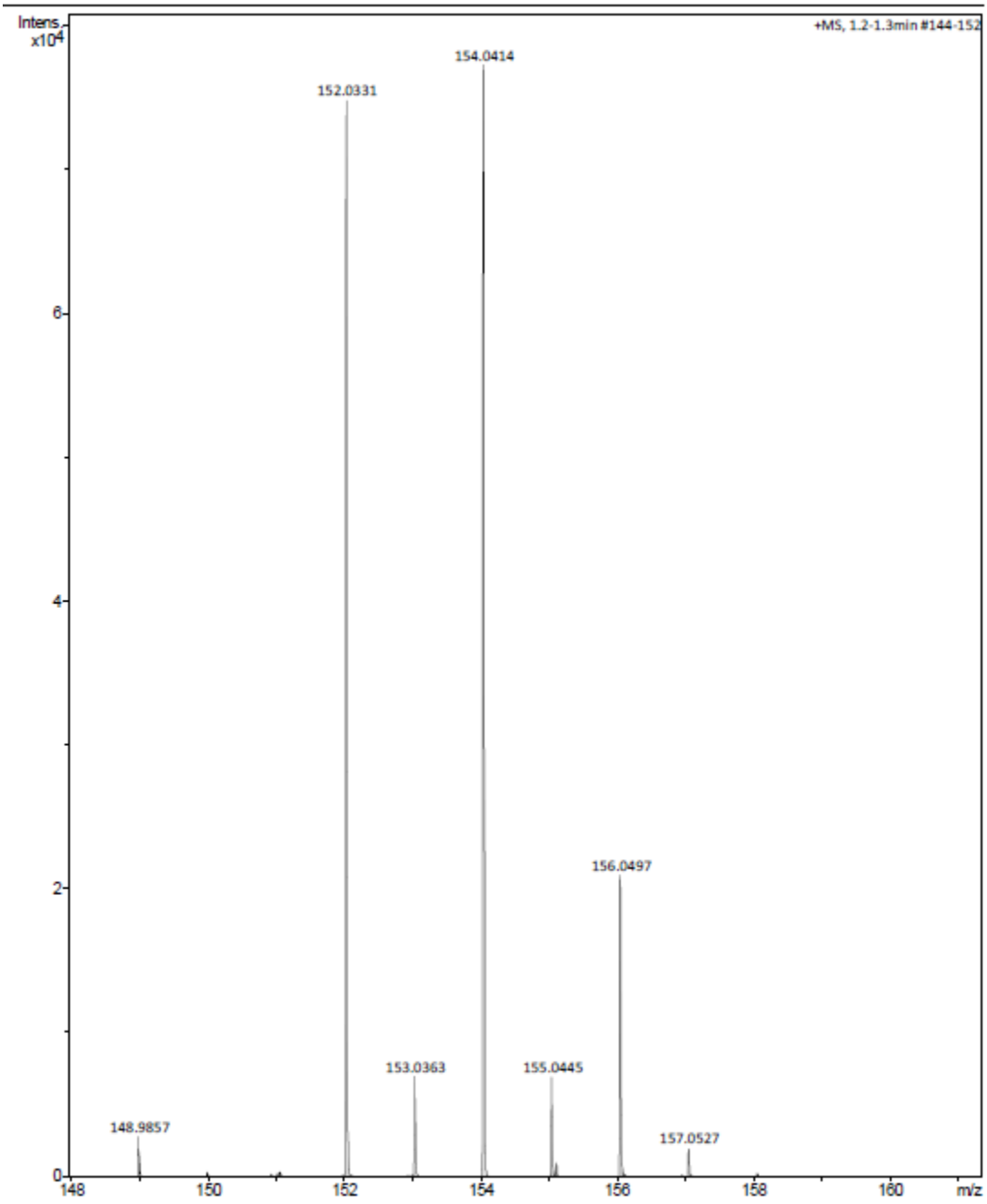


3H-NMR Paracetamol-3H FF.AURA.42 in DMSO-D6



1H-NMR Paracetamol-3H FF.AURA.42 in DMSO-D6 zg30





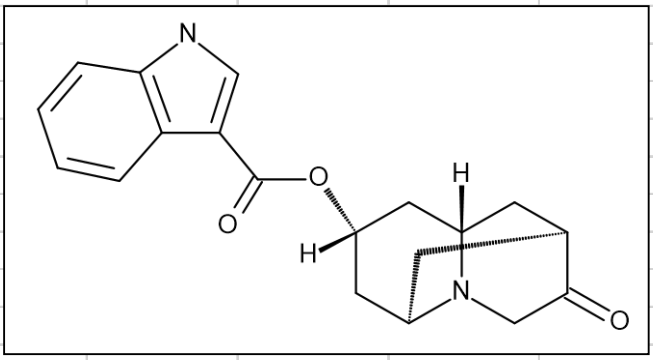
43,5 % T0						
44,6 % T1	→	x	29 Ci/mmol	→		**12,9 Ci/mmol**
11,9 % T2	→	x	58 Ci/mmol	→		**6,9 Ci/mmol**
0,0 % T3	→	x	87 Ci/mmol	→		**0,0 Ci/mmol**

Spec. Activity: 19.8 Ci/mmol

6. Influence of basic or acidic additives in the HIE reaction of dolasetron 16

Table S5: basic or acidic additives in the HIE reaction of dolasetron 16

Dolasetron HIE additive



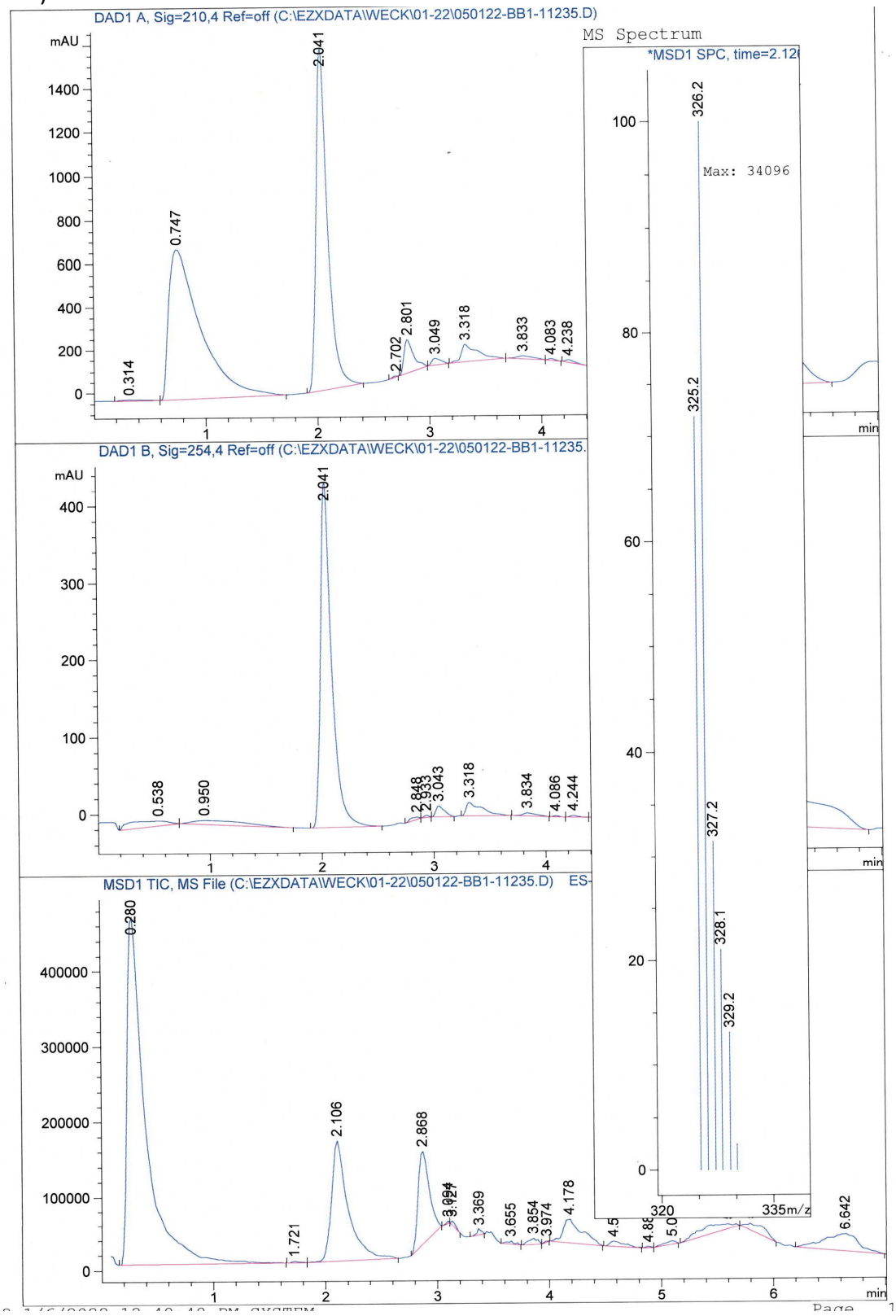
Entry	Additive	DCY
1	no	45%
2	1 eq. Et3N	20%
3	0,3 eq. TFA	9%
4	1 eq. TFA	5%
5	2 eq. TFA	4%
6	3 eq. TFA	3%
7	1 eq. HCO2H	2%
8	2 eq. HCL	1%

In conclusion especially acidic additives have a negative effect on the HIE reaction of dolasetron **16** with catalyst **2**.

Table S5, entry 2, General HIE protocol D:

3,9 mg Dolesatron, 10 mol% Kerr PF6, Isopropyl acetate, 1Eq D_2, 1Eq Et3N, 2h RT:

LC-MS Chromatogram: DAD1 = 210 nm; DAD2 =254 nm; MS-TIC and MS spectra (peak 2.120 min)

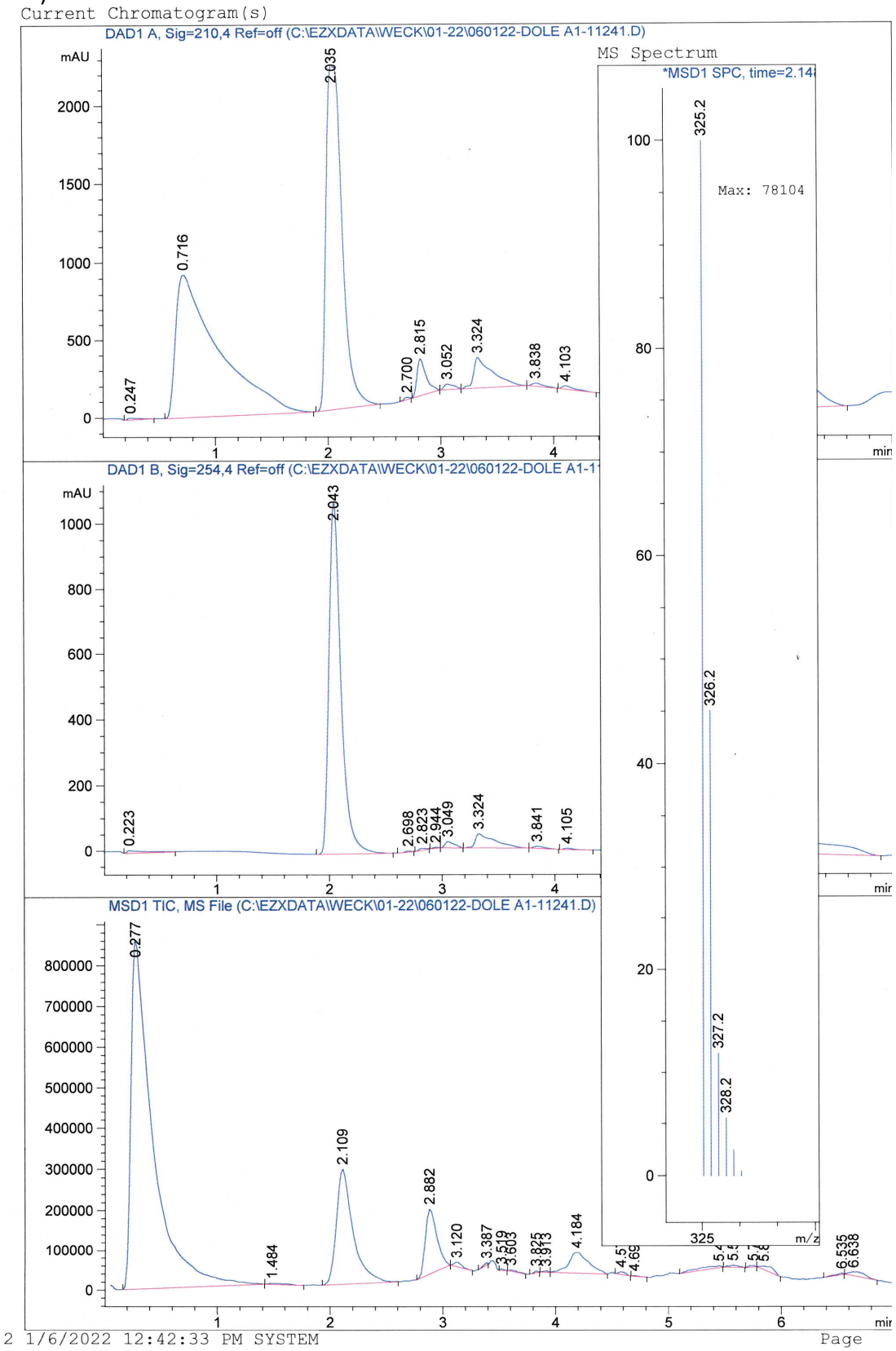


Result: 19,9% DCY

Table S5, entry 3, General HIE protocol D:

3,9 mg Dolesatron, 10 mol% Kerr PF6, Isopropyl acetate, 1Eq D_2, 0,3Eq TFA, 2h RT:

LC-MS Chromatogram: DAD1 = 210 nm; DAD2 =254 nm; MS-TIC and MS spectra (peak 2.120 min)

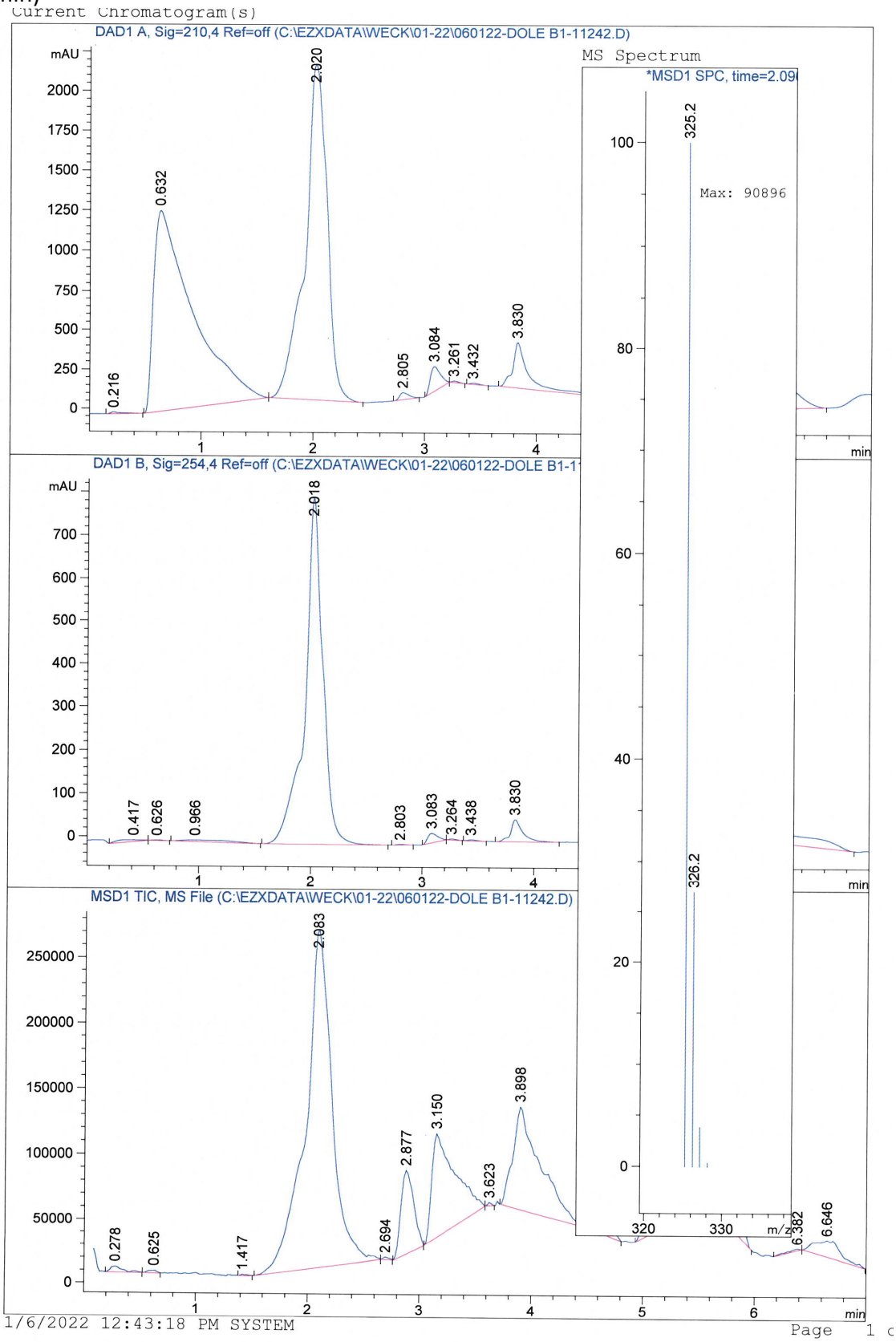


Result: 9,1% DCY

Table S5, entry 4, General HIE protocol D:

3,9 mg Dolesatron, 10 mol% Kerr PF6, Isopropyl acetate, 1Eq D_2, 1Eq TFA, 2h RT:

LC-MS Chromatogram: DAD1 = 210 nm; DAD2 =254 nm; MS-TIC and MS spectra (peak 2.120 min)

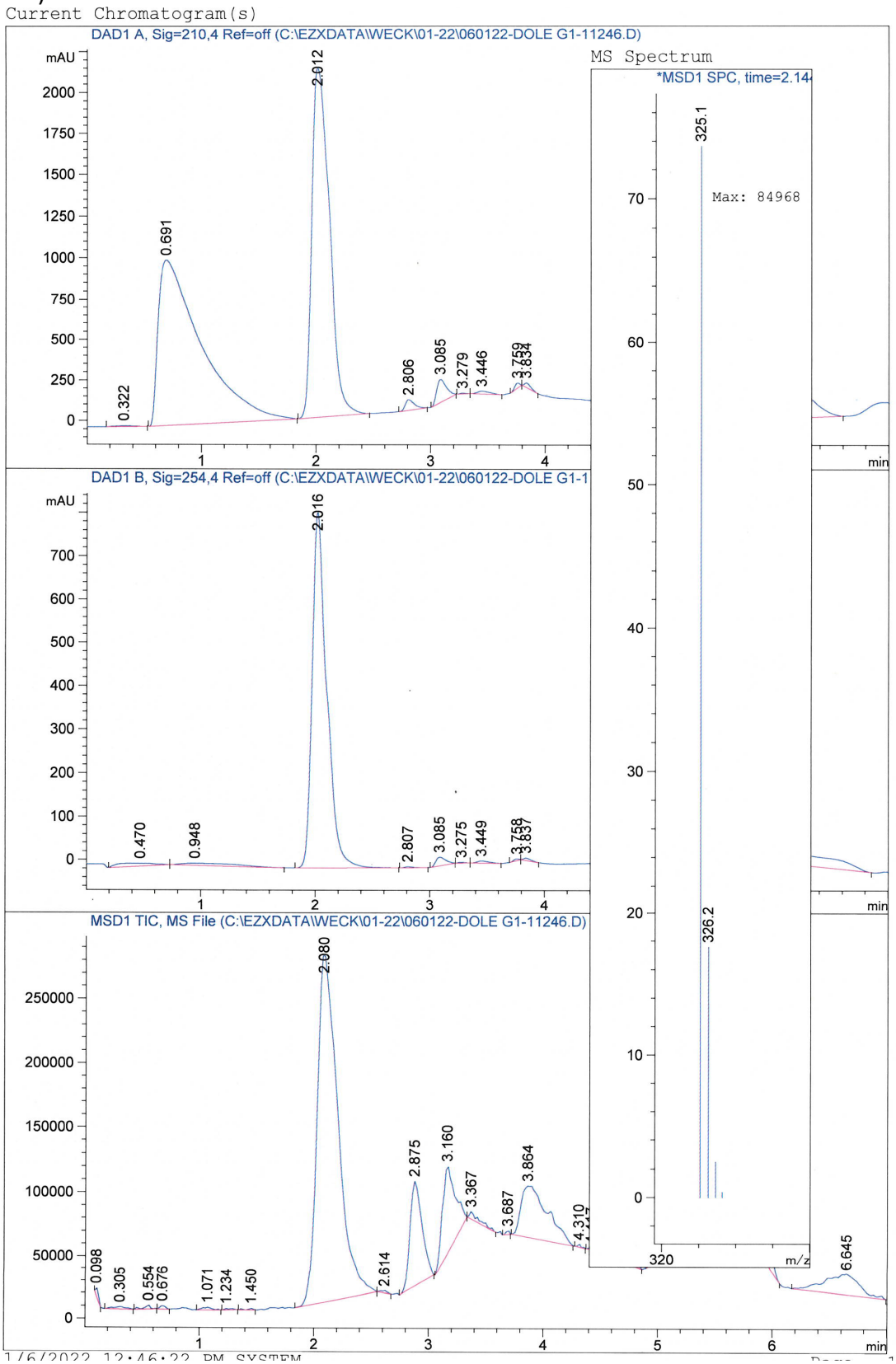


Result: 4,9% DCY

Table S5, entry 5, General HIE protocol D:

3,9 mg Dolesatron, 10 mol% Kerr PF6, Isopropyl acetate, 1Eq D_2, 2Eq TFA, 2h RT:

LC-MS Chromatogram: DAD1 = 210 nm; DAD2 =254 nm; MS-TIC and MS spectra (peak 2.120 min)

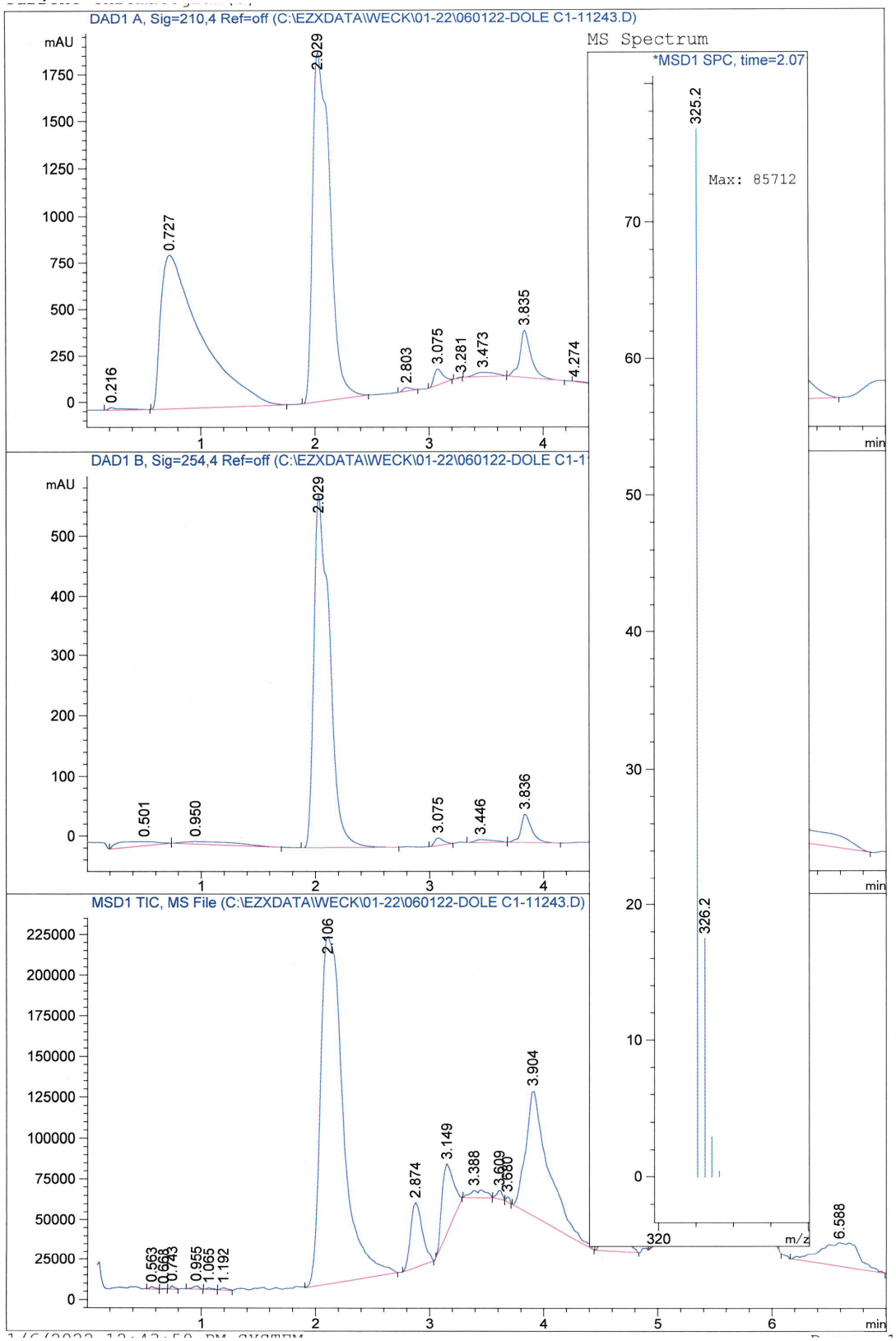


Result: 4,1% DCY

Table S5, entry 6, General HIE protocol D:

3,9 mg Dolesatron, 10 mol% Kerr PF6, Isopropyl acetate, 1Eq D_2, 3Eq TFA, 2h RT:

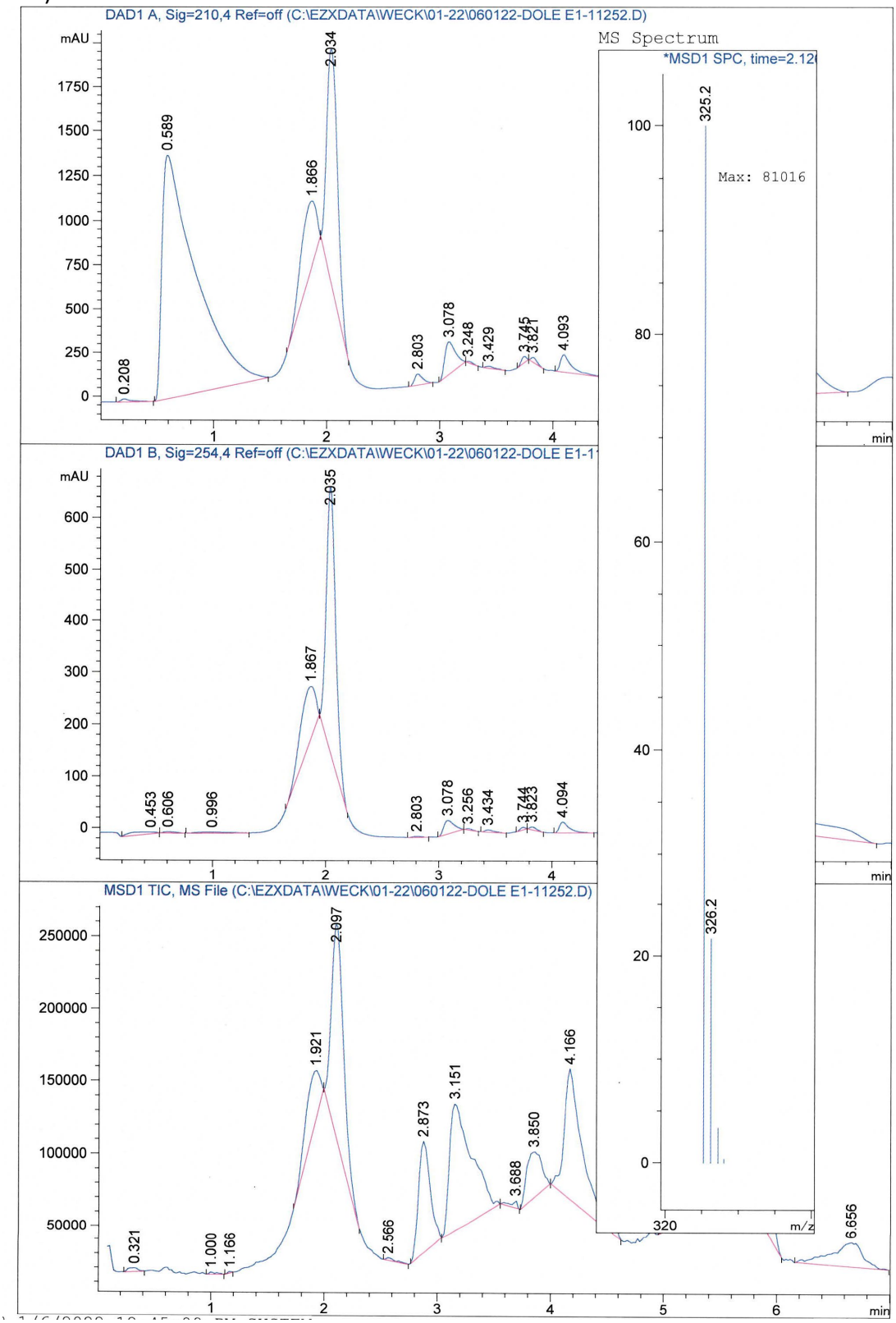
LC-MS Chromatogram: DAD1 = 210 nm; DAD2 =254 nm; MS-TIC and MS spectra (peak 2.120 min)



Result: 3,3% DCY

Table S5, entry 7, General HIE protocol D:

3,9 mg Dolesatron, 10 mol% Kerr PF6, Isopropyl acetate, 1Eq D_2, 1HCO2HEq TFA, 2h RT: LC-MS Chromatogram: DAD1 = 210 nm; DAD2 =254 nm; MS-TIC and MS spectra (peak 2.120 min)

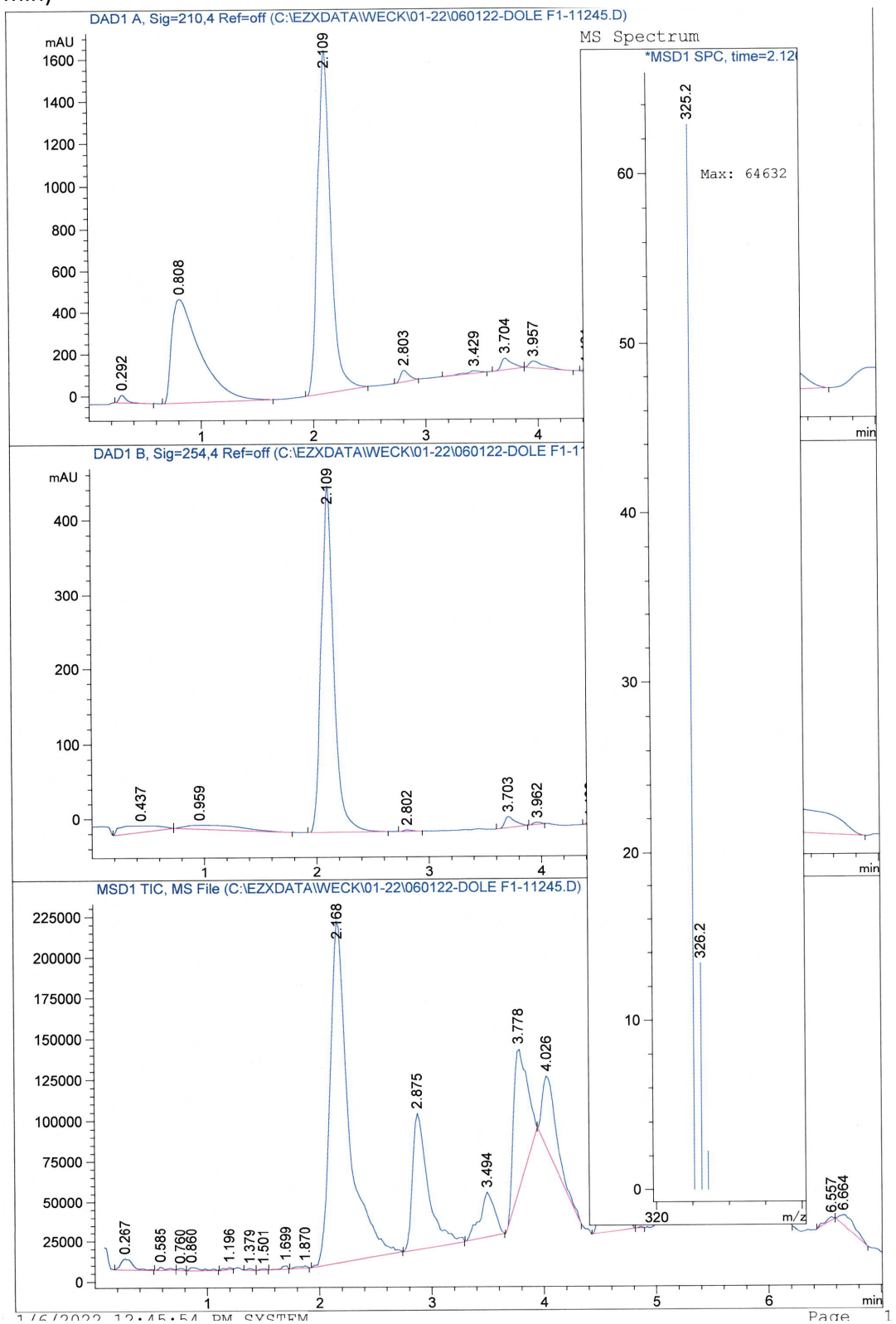


Result: 1,9% DCY

Table S5, entry 8, General HIE protocol D:

3,9 mg Dolesatron, 10 mol% Kerr PF6, Isopropyl acetate, 1Eq D_2, 1HCl Eq TFA, 2h RT:

LC-MS Chromatogram: DAD1 = 210 nm; DAD2 =254 nm; MS-TIC and MS spectra (peak 2.120 min)



Result: 1,3% DCY

The data for figure 1 is based on a literature search in SciFinder (CAS) based on the following search criteria :

Date: 2nd May 2020

SciFinder search research topic with the words "synthesis" and "tritium"; refined English only

SciFinder search research topic with the words "3H" and "tritium"; refined English only

SciFinder search research topic with the words "hydrogen isotope exchange"; refined English only

The year and month of the publication was converted in a metric scale e.g. 2020.4 to make the graphic easier to read.

Data of Figure 1 :

	Title	Citation	doi	year	RCY	Ci/T2	spec. Activity	Comment
1	Synthesis of Tritium-Labeled Deoxyglucose and Its Derivative	Sidorov, G. V.; Myasoedov, N. F. From Radiochemistry (Moscow, Russian Federation) (2020), 62(2), 260-263.	DOI:10.1134/s1066362220020150	2020,4	n/a	n/a	7,9	Br/T
2	Synthesis of Tritium-Labeled Non-Natural Analogs of Purine and Pyrimidine Nucleosides	Sidorov, G. V.; Myasoedov, N. F. From Radiochemistry (Moscow, Russian Federation) (2020), 62(2), 255-259.	doi.org/10.1134/S1066362220020149	2020,4	n/a	n/a	n/a	Br/T
3	Ruthenium(II)-Catalyzed Hydrogen Isotope Exchange of Pharmaceutical Drugs by C-H Deuteration and C-H Tritiation	Mueller, Valentin; Weck, Remo; Derdau, Volker; Ackermann, Lutz From ChemCatChem (2020), 12(1), 100-104.	DOI:10.1002/cctc.201902051	2020,3	0,3	2,3	5,5	HIE/Ru
4	An Agonist Radioligand for the Proinflammatory Lipid-Activated G Protein-Coupled Receptor GPR84 Providing Structural Insights	Koese, Meryem; Pillaiyar, Thanigaimalai; Namasivayam, Vigneshwaran; De Filippo, Elisabetta; Sylvester, Katharina; Ulven, Trond; von Kuegelgen, Ivar; Mueller, Christa E. From Journal of Medicinal Chemistry (2020), 63(5), 2391-2410.	DOI:10.1021/acs.jmedchem.9b01339	2020,3	n/a	n/a	60,0	DB/T2 - CRO

5	Hydrogen Isotope Exchange Catalyzed by Ru Nanocatalysts: Labelling of Complex Molecules Containing N-Heterocycles and Reaction Mechanism Insights	Pfeifer, Viktor; Certiat, Marie; Bouzouita, Donia; Palazzolo, Alberto; Garcia-Argote, Sebastien; Marcon, Elodie; Buisson, David-Alexandre; Lesot, Philippe; Maron, Laurent; Chaudret, Bruno; et al From Chemistry - A European Journal (2020), 26(22), 4988-4996.	DOI:10.1002/chem.201905651	2020,3	n/a	6,6	8,7	
			DOI:10.1002/chem.201905651	2020,3	n/a	11,1	24,7	HIE/Ru
			DOI:10.1002/chem.201905651	2020,3	n/a	12,4	23,7	
6	Synthesis of [3H] and [14C]genipin	Queen, Adele. E.; Hesk, David; Lindsay, David. M.; Kerr, William. J.; Rehder, Kenneth; Fennell, Tim; Mascarella, Wayne; Zhong, Desong; Runyon, Scott From Journal of Labelled Compounds and Radiopharmaceuticals (2020), 63(4), 196-202.	DOI:10.1002/jlcr.3832	2020,2	6	1,5	69,2	HIE/Ir
7	Recent advances in iridium(I) catalysis towards directed hydrogen isotope exchange	Kerr, William J.; Knox, Gary J.; Paterson, Laura C. From Journal of Labelled Compounds and Radiopharmaceuticals (2020), Ahead of Print.	DOI:10.1002/jlcr.3812	2020,2	n/a	n/a	n/a	review/no RCY
8	C-H Functionalization - Prediction of Selectivity in Iridium(I)- Catalyzed Hydrogen Isotope Exchange Com petition Reactions	Valero, Megane; Kruissink, Thomas; Blass, Jennifer; Weck, Remo; Guessregen, Stefan; Plowright, Alleyn T.; Derdau, Volker From Angewandte Chemie, International Edition (2020), 59(14), 5626-5631.	DOI:10.1002/anie.201914220	2020,1	7	2,9	32,3	HIE/Ir

9	NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines	Valero, Megane; Bouzouita, Donia; Palazzolo, Alberto; Atzrodt, Jens; Dugave, Christophe; Tricard, Simon; Feuillastre, Sophie; Pieters, Gregory; Chaudret, Bruno; Derdau, Volker From Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.	DOI:10.1002/anie.201914369	2020,1	0,4	10,0	26,0	HIE/Ir
10	High specific activity tritiation of various methylated histamine analogues	Filer, Crist N.; Andrews, Joseph R.; Do, Ernest; Peng, C. T. From Journal of Radioanalytical and Nuclear Chemistry (2019), 322(2), 1107-1113.	DOI:10.1007/s10967-019-06781-6	2019,8	n/a	n/a	n/a	Br/T
11	A convenient synthesis of the muscarinic cholinergic antagonist (R)-[N-methyl-3H] quinuclidinyl benzilate methiodide	Filer, Crist N.; Seguin, Richard J. From Journal of Labelled Compounds and Radiopharmaceuticals (2019), 62(9), 604-607.	DOI:10.1002/jlcr.3775	2019,6	n/a	4,1	n/a	MeI
12	Frustrated Lewis pairs: A real alternative to deuteride/tritide reductions	Doubkova, Sabina; Marek, Ales From Journal of Labelled Compounds and Radiopharmaceuticals (2019), 62(11), 729-742.	DOI:10.1002/jlcr.3774	2019,4	20	2,5	27,1	BF6/T2
13	Synthesis, 3H-labelling and in vitro evaluation of a substituted dipiperidine alcohol as a potential ligand for chemokine receptor 2	Artelsmair, Markus; Miranda-Azpiazu, Patricia; Kingston, Lee; Bergare, Jonas; Schou, Magnus; Varrone, Andrea; Elmore, Charles S. From Journal of Labelled Compounds and Radiopharmaceuticals (2019), 62(6), 265-279.	DOI:10.1002/jlcr.3731	2019,3	0.2	9,0	24,3	I/T
14	The synthesis of 3H-labelled 8-azido-N6-benzyladenine and related compounds for Photoaffinity labelling of cytokinin-binding proteins	Letham, David. S.; Zhang, Xue-Dong; Hocart, Charles H. From Molecules (2019), 24(2), 349/1-349/13.	DOI:10.3390/molecules24020349	2019,1	n/a	n/a	6,0	I/T
15	Radioactive gangliosides for biological studies	Mauri, Laura; Prioni, Simona; Ciampa, Maria Grazia; Sonnino, Sandro From Methods in Molecular Biology (New York, NY, United States) (2018), 1804(Gangliosides), 311-322.	DOI:10.1007/978-1-4939-8552-4_15	2018,9	8	0,1	2,0	NaBT4

16	Synthesis and Testing of Abscisic Acid with Predominant Replacement of Protium Atoms by Tritium in the Cyclohexene Moiety	Shevchenko, V. P.; Nagaev, I. Yu.; Shaposhnikov, A. I.; Shevchenko, K. V.; Belimov, A. A.; Batasheva, S. N.; Gogoleva, N. E.; Gogolev, Yu. V.; Myasoedov, N. F. From Doklady Chemistry (2018), 483(1), 268-271.	DOI:10.1134/s0012500818110113	2018,8	n/a	n/a	30,5	base/T2O
17	Synthesis of Deuterium- or Tritium-Labeled Norepinephrine and Evaluation of Its Biological Activity	Shevchenko, V. P.; Nagaev, I. Yu.; Pronina, T. S.; Shevchenko, K. V.; Murtazina, A. R.; Surkov, S. A.; Ugryumov, M. V.; Myasoedov, N. F. From Doklady Chemistry (2018), 480(2), 117-120.	DOI:10.1134/S0012500818006006X	2018,8	n/a	n/a	27,0	Br/T
18	Synthesis of tritium-labeled cyadox, a promising antimicrobial growth-promoting agent with high specific activity	Harnud, Sechenchogt; Zhang, Aiqun; Yuan, Zonghui From Applied Radiation and Isotopes (2018), 139, 244-250.	DOI:10.1016/j.apradiso.2018.05.018	2018,7	n/a	n/a	2,1	Br/T
19	Design of A Metabolically Stable Tritium-Tracer of the PI3Kδ-Inhibitor CDZ173 (Leniolisib) as a Tool to Study Liver Metabolites	Bauer, Carsten; Luu, Tong; Eggimann, Fabian; Bross, Patrick; Gertsch, Werner; Hu, Cheng; Ramstein, Philippe; Bourgailh, Julien; Glaenzel, Albrecht; Dix, Ina; et al From Helvetica Chimica Acta (2018), 101(6),	DOI:10.1002/hlca.201800044	2018,7	0,2	11,8	16,9	Cl/T
20	Potent and selective CC chemokine receptor 1 antagonists labeled with carbon-13, carbon-14, and tritium	Latli, Bachir; Hrapchak, Matt; Cheveliakov, Maxim; Reeves, Jonathan T.; Marsini, Maurice; Busacca, Carl A.; Senanayake, Chris H. From Journal of Labelled Compounds and Radiopharmaceuticals (2018), 61(10), 764-772.	DOI:10.1002/jlcr.3635	2018,6	n/a	n/a	42,1	CN/T2
21	The chemoenzymatic synthesis of labeled L-amino acids and some of their derivatives	Pajak, Malgorzata; Palka, Katarzyna; Winnicka, Elzbieta; Kanska, Marianna From Journal of Radioanalytical and Nuclear Chemistry (2018), 317(2), 643-666.	DOI:10.1007/s10967-018-5932-z	2018,5	n/a	n/a	n/a	enzyme/T2O

22	Tritium-labeled agonists as tools for studying adenosine A2B receptors	Hinz, Sonja; Alnouri, Wessam M.; Pleiss, Ulrich; Mueller, Christa E. From Purinergic Signalling (2018), 14(3), 223-233.	DOI:10.1007/s11302-018-9608-5	2018,4	n/a	n/a	15,9	CRO synthesis
	Synthesis and characterization of tritium-labelled substances	Filer, Crist N. From Applied Radiation and Isotopes (2018), 137, 261-272	DOI:10.1016/j.apradiso.2018.02.029	2018,4	n/a	n/a	n/a	review
23	Enzymatic synthesis of methyl derivatives of L-tryptophan selectively labeled with hydrogen isotopes	Winnicka, Elzbieta; Kanska, Marianna From Applied Radiation and Isotopes (2018), 137, 118-122.	DOI:10.1016/j.apradiso.2018.03.019	2018,3	n/a	6,1 Gbq	n/a	T2O
24	Synthesis of tritium-labeled PAM-43	Nagaev, Igor Yu.; Shevchenko, Konstantin V.; Shevchenko, Valeriy P.; Myasoedov, Nicolay F.; Grigoriev, Vladimir V.; Lavrov, Mstislav I.; Bondarenko, Ekaterina V.; Kalashnikova, Elena E. From Mendeleev Communications (2018), 28(1), 64-65.	DOI:10.1016/j.mencom.2018.01.021	2018,2	n/a	n/a	132,0	Pd/HIE
25	A General Strategy for Site-Selective Incorporation of Deuterium and Tritium into Pyridines, Diazines, and Pharmaceuticals	Koniarczyk, J. Luke; Hesk, David; Overgard, Alix; Davies, Ian W.; McNally, Andrew From Journal of the American Chemical Society (2018), 140(6), 1990-1993.	DOI:10.1021/jacs.7b11710	2018,1	1	1,0	n/a	P/T exchange
			DOI:10.1021/jacs.7b11710	2018,1	2,5	1,0	18,4	P/T exchange
			DOI:10.1021/jacs.7b11710	2018,1	2,7	1,0	1,7	P/T exchange
26	Synthesis of deuterium- or tritium-labeled acetylcholine	Shevchenko, V. P.; V'yunova, T. V.; Nagaev, I. Yu.; Shevchenko, K. V.; Myasoedov, N. F. From Radiochemistry (Moscow, Russian Federation) (2017), 59(5), 520-524.	DOI:10.1134/S1066362217050137	2017,9	n/a	n/a	20-40	Lindlar Cat/T2

27	Heterodimerization of Dibenzodiazepinone-Type Muscarinic Acetylcholine Receptor Ligands Leads to Increased M2R Affinity and Selectivity	She, Xueke; Pegoli, Andrea; Mayr, Judith; Huebner, Harald; Bernhardt, Guenther; Gmeiner, Peter; Keller, Max From ACS Omega (2017), 2(10), 6741-6754.	DOI:10.1021/acsomega.7b01085	2017,8	n/a	n/a	n/a	outsourced
28	Preparation of tritium-labeled PF-622, a novel fatty acid amide hydrolase inhibitor	Zhang, Yinsheng From Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(13), 608-615.	DOI:10.1002/jlcr.3559	2017,8	0,9	1,1	15,8	Crabtree/T2
			DOI:10.1002/jlcr.3559	2017,8	1,5	1,1	24,7	Bt/T2
29	Novel Radiolabeled Vanilloid with Enhanced Specificity for Human Transient Receptor Potential Vanilloid 1 (TRPV1)	Pearce, Larry V.; Ann, Jihyae; Jung, Aeran; Thorat, Shivaji A.; Herold, Brienna K. A.; Habtemichael, Amelework D.; Blumberg, Peter M.; Lee, Jeewoo From Journal of Medicinal Chemistry (2017), 60(19), 8246-8252.	DOI:10.1021/acs.jmedchem.7b00859	2017,7	n/a	n/a	78,0	DB/Pd/T2
30	A synthesis of tritium-labeled juvenile hormone and radiometric analysis of the enzymatic hydrolysis level	Romanova, I. V.; Alekseev, A. A.; Richter, V. A.; Gruntenko, N. E.; Agafontsev, A. M.; Karpova, E. K. From Russian Journal of Bioorganic Chemistry (2017), 43(2), 211-215.	DOI:10.1134/S1068162017020121	2017,6	n/a	n/a	2,2	HSCIE
31	Synthesis and In Vitro and In Vivo Evaluation of [3H]LRRK2-IN-1 as a Novel Radioligand for LRRK2	Malik, Noeen; Gifford, Andrew N.; Sandell, Johan; Tuchman, Daniel; Ding, Yu-Shin From Molecular Imaging and Biology (2017), 19(6), 837-845.	DOI:10.1007/s11307-017-1070-1	2017,5	n/a	n/a	41,0	Crabtree HIE
32	Enantiospecific tritium labeling of 28-homocastasterone	Elbert, Tomas; Patil, Mahadeo R.; Marek, Ales From Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(3), 176-182.	DOI:10.1002/jlcr.3488	2017,4	0,1	11,5	5,8	Cl/T2
33	Tritium-labelled alkaloids: Synthesis and applications	Filer, Crist N. From Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(2), 96-109.	DOI:10.1002/jlcr.3480	2017,3	n/a	n/a	n/a	review

34	Design, synthesis, in vitro characterization and preliminary imaging studies on fluorinated bile acid derivatives as PET tracers to study hepatic transporters	Testa, Andrea; Dall'Angelo, Sergio; Mingarelli, Marco; Augello, Andrea; Schweiger, Lutz; Welch, Andy; Elmore, Charles S.; Sharma, Pradeep; Zanda, Matteo From Bioorganic & Medicinal Chemistry (2017), 25(3), 963-976.	DOI:10.1016/j.bmc.2016.12.008	2017,3	n/a	n/a	20,0	I/T
35	The synthesis of a tritium, carbon-14, and stable isotope-labeled cathepsin C inhibitors	Allen, Paul; Bragg, Ryan A.; Caffrey, Moya; Ericsson, Cecilia; Hickey, Michael J.; Kingston, Lee P.; Elmore, Charles S. From Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(2), 124-129.	DOI:10.1002/jlcr.3483	2017,2	0,1	8,7	12,4	Cl/T
			DOI:10.1002/jlcr.3483	2017,2	7	2,3	13,3	HIE/T2
36	Synthetic Peptide TPLVTLFK, a Selective Agonist of Nonopioid β-Endorphin Receptor, Reduces the Corticotropin and Corticosterone Response	Navolotskaya, Elena V.; Sadovnikov, Vladimir B.; Lipkin, Valety M. From International Journal of Peptide Research and Therapeutics (2017), 23(1), 111-118.	DOI:10.1007/s10989-016-9543-7	2017,1	n/a	n/a	n/a	HSCIE
37	Iron-catalysed tritiation of pharmaceuticals	Pony Yu, Renyuan; Hesk, David; Rivera, Nelo; Pelczer, Istvan; Chirik, Paul J. From Nature (London, United Kingdom) (2016), 529(7585), 195-199.	DOI:10.1038/nature16464	2016,9	n/a	1,2	20,0	HIE/T2
38	A novel non-opioid binding site for endomorphin-1	Lengyel, I.; Toth, F.; Biyashev, D.; Szatmari, I.; Monory, K.; Tomboly, C.; Toth, G.; Benyhe, S.; Borsodi, A. J Physiol Pharmacol. 2016 Aug;67(4):605-616.	http://www.jpp.krakow.pl/journal/archive/08_16/pdf/605_08_16_article.pdf	2016,9	n/a	n/a	62,0	Hal/T
39	The LKEKK synthetic peptide as a ligand of rat intestinal epithelial cell membranes	Navolotskaya, E. V.; Sadovnikov, V. B.; Zinchenko, D. V.; Vladimirov, V. I.; Zolotarev, Y. A.; Kolobov, A. A. Russian Journal of Bioorganic Chemistry (2016), 42(5), 479-483.	DOI:10.1134/S1068162016050137	2016,8	n/a	n/a	28,0	HSCIE

40	The synthesis of tritium, carbon-14 and stable isotope labelled selective estrogen receptor degraders	Bragg, Ryan A.; Bushby, Nick; Ericsson, Cecilia; Kingston, Lee P.; Ji, Hailong; Elmore, Charles S.Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(11), 454-461.	DOI:10.1002/jlcr.3437	2016,8	0,02	6,2	n/a	DB/Pt/H2
41	Candidate PET Radioligand Development for Neurofibrillary Tangles: Two Distinct Radioligand Binding Sites Identified in Postmortem Alzheimer's Disease Brain	Cai, Lisheng; Qu, Baoxi; Hurtle, Bryan T.; Dadiboyena, Sureshbabu; Diaz-Arrastia, Ramon; Pike, Victor W. ACS Chemical Neuroscience (2016), 7(7), 897-911.	DOI:10.1021/acschemneuro.6b00051	2016,7	n/a	n/a	n/a	I/T
42	Binding of synthetic LKEKK peptide to human T-lymphocytes	Navolotskaya, E. V.; Zinchenko, D. V.; Zolotarev, Y. A.; Kolobov, A. A.; Lipkin, V. M. Biochemistry (Moscow) (2016), 81(8), 871-875.	DOI:10.1134/S0006297916080071	2016,7	n/a	n/a	28,0	HSCIE
43	Syntheses of halogen derivatives of L-tryptophan, L-tyrosine and L-phenylalanine labeled with hydrogen isotopes	Pajak, Malgorzata; Palka, Katarzyna; Winnicka, Elzbieta; Kanska, Marianna From Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(1), 4-8.	DOI:10.1002/jlcr.3357	2016,6	11	0,2	1,6	Ezymatic/THO
44	Carbon-13 and carbon-14 labeled dabigatran etexilate and tritium labeled dabigatran	Bachir Latli, Ralf Kiesling, Stefan Aßfalg, Max Chevliakov, Matt Hrapchak, Scot Campbell, Nina Gonnella, Carl A. Busacca and Chris H. Senanayake, JLCR 2016	DOI: 10.1002/jlcr.3402	2016,5	4,8	7,7	43,0	Crabtree
45	Iridium-catalysed ortho-H/D and -H/T Exchange under Basic Conditions: C-H Activation of Unprotected Tetrazoles	William J. Kerr,*a David M. Lindsay,a Marc Reid,a Jens Atzrodt,b Volker Derdau,b Patrick Rojahn,b and Remo Weckb, Chem. Commun., 2016,52, 6669-6672	DOI: 10.1039/C6CC02137A	2016,3	2	1,5	21,0	Kerr Valsartan
46	Influence of the conditions of deuterium and tritium labeling of His–Phe–Arg–Trp–Pro–Gly–Pro oligopeptide on the isotope exchange efficiency	Shevchenko, V. P.; Radilov, A. S.; Nagaev, I. Yu.; Shevchenko, K. V.; Rembovskii, V. R.; Myasoedov, N. F.	DOI:10.1134/S1066362215050161	2015,9				HSCIE, no RCY

47	Synthesis and Pharmacological Evaluation of [3H]HS665, a Novel, Highly Selective Radioligand for the Kappa Opioid Receptor	Elena Guerrieri†, Jayapal Reddy Mallareddy‡, Géza Tóth‡, Helmut Schmidhammer†, and Mariana Spetea*†, ACS Chem. Neurosci., 2015, 6 (3), pp 456–463	DOI: 10.1021/cn5002792	2015,6			31,0	Hal/T
48	Synthesis and characterization of tritium labeled N-((R)-1-((S)-4-(4-chlorophenyl)-4-hydroxy-3,3-dimethylpiperidin-1-yl)-3-methyl-1-oxobutan-2-yl)-3-sulfamoylbenzamide (pages 414–418)	Yang Hong, John Hynes, Yuan Tian, Balu Balasubramanian and Samuel Bonacorsi Jr., J. Label Compd. Radiopharm 2015, 58, 414–418	DOI: 10.1002/jlcr.3320	2015,6	2	1,0	49,1	Crabtree
49	Frustrated Lewis pairs-assisted reduction of carbonyl compounds	A. Marek, M.H.F. Pedersen	doi:10.1016/j.tet.2014.12.086	2015,3	4,3	9,0	24,0	Frustrated Ion pair FLP
50	Synthesis of 3H, 13C,2H3,15N and 14C-labelled SCH 466036, a histamine 3 receptor antagonist (pages 36–41)	D. Hesk, S. Borges, R. Dumpit, S. Hendershot, D. Koharski, C. Lavey, P. McNamara and K. Voronin	DOI: 10.1002/jlcr.3261	2015,2	5,8	0,5	0,4	Raney-Nickel HTO
51	Efficient tritiation of the translocator protein (18 kDa) selective ligand DPA-714	Annelaure Damont, Sébastien Garcia-Argote, David-Alexandre Buisson, Bernard Rousseau and Frédéric Dollé, J. Label Compd. Radiopharm 2015, 58 1–6	DOI: 10.1002/jlcr.3252	2015,1	n/a	n/a	n/a	
52	Synthesis of phenylsilocane tritium-labeled at the benzene ring	Avrorin, V. V.; Fominykh, G. E.; Ignat'ev, I. S.; Sinotova, E. N.; Kochina, T. A., Russian Journal of General Chemistry (2014), 84(11), 2125-2129.	DOI:10.1134/S1070363214110140	2014,9	7	2,5		Br/T
53	The Synthesis of Highly Active Iridium(I) Complexes and their Application in Catalytic Hydrogen Isotope Exchange	Brown, Jack A.; Cochrane, Alison R.; Irvine, Stephanie; Kerr, William J.; Mondal, Bhaskar; Parkinson, John A.; Paterson, Laura C.; Reid, Marc; Tuttle, Tell; Andersson, Shalini; et al From Advanced Synthesis & Catalysis (2014), 356(17), 3551-3562.	DOI:10.1002/adsc.201400730	2014,7	n/a	n/a	20-50	HIE

54	Synthesis of [3H], [13C3, 15N], and [14C]SCH 900567: an inhibitor of TNF-α (tumor necrosis factor alpha) converting enzyme (TACE) (pages 632–636)	Sumei Ren, David Hesk, Paul McNamara, David Koharski and Scott Borges, J. Label Compd. Radiopharm 2014, 57 632–636	DOI: 10.1002/jlcr.3229	2014,7	6	0,5 HTO		Pt/THO
55	Evaluation of the efficiency of Pd/H2-catalyzed benzylic H/D exchange of dehydroabietinal with D2O and synthesis of a tritium-labeled analogue (pages 53–56)	Robby A. Petros and Jyoti Shah, J. Label Compd. Radiopharm 2014, 57 53–56	DOI: 10.1002/jlcr.3117	2014,1	5	10,0	0,1	HTO/Pd/C
56	Syntheses of [3H2]T0901317 and a labeled structural isomer, and characterization of the dispersed labeled compounds via 19F NMR (pages 57–60)	Benjamin P. Fauber, Adam R. Johnson, Stephen Bowerman, Brenda Burton, Adam Colebrook, Annerley Flynn, Gareth Harrold, Steve Huhn, Gary Jones, Peter Lockey, Maxine Norman, Olivier René and Harvey Wong, J. Label Compd. Radiopharm 2014,5757–60	DOI: 10.1002/jlcr.3138	2014,1	n/a	2,0	54,0	Br/T
			DOI: 10.1002/jlcr.3138	2014,1	n/a	2,0	48,0	Br/T
57	Preparation of [3H]fluoroethyl tosylate and its use in the labelling of the dopamine transporter radioligand [3H]FE-PE2I (pages 447–450)	Alison R Cochrane, William John Kerr and Johan Sandell	DOI: 10.1002/jlcr.3012	2013,9	2	10,0		Kerr-catalyst
58	Synthesis of selectively labeled histidine and its methylderivatives with deuterium, tritium, and carbon-14 (pages 317–320)	J. Šamonina-Kosicka and M. Kańska, J. Label Compd. Radiopharm 2013, 56 317–320	DOI: 10.1002/jlcr.3027	2013,6	0,02	0,2	0,1	T2O/HCl
59	Synthesis of ximelagatran, melagatran, hydroxymelagatran, and ethylmelagatran in H-3 labeled form (pages 334–337)	Roger Simonsson, Gunnar Stenhagen, Cecilia Ericsson and Charles S. Elmore	DOI: 10.1002/jlcr.3028	2013,6	5,2	1,0	42,0	Kerr -catalyst
60	Synthesis of [15, 16-3H] beta-funaltrexamine (pages 310–311)	Crist N. Filer and Richard J. Seguin	DOI: 10.1002/jlcr.3050	2013,5			26,7	DB reduction noyield

61	Multiple labeling of a potent CX3CR1 antagonist for the treatment of multiple sclerosis (pages 387–392)	Jonas Malmquist and Peter Ström	DOI: 10.1002/jlcr.2958	2012,8	1	10,0		Br/T
62	Imaging agents for myeloperoxidase (pages 393–399)	Jonas Malmquist, Alexandra Bernlind, Maria Johansson, Anders Juréus and Maria Nilsson	DOI: 10.1002/jlcr.2961	2012,8	n/a			Br/T
63	Tritium labeling of full-length small interfering RNAs (pages 189–196)	Jesper Christensen, François Natt, Jürg Hunziker, Joel Krauser, Hendrik Andres and Piet Swart	DOI: 10.1002/jlcr.2919	2012,6	n/a			Br/T
64	Alternative efficient tritium labeling of repaglinide (pages 155–157)	Maarten Vliegen, Pieter Haspeslagh and Willy Verluyten	DOI: 10.1002/jlcr.2913	2012,3				Ir black
65	Tritium labeling of a γ-secretase inhibitor and two modulators as in vitro imaging agents (pages 80–83)	Jonas Malmquist, Alexandra Bernlind, Johan Sandell, Peter Ström and Magnus Waldman	DOI: 10.1002/jlcr.1955	2012,2	1,3	8,0		
66	Tritium labelling of PACAP-38 using a synthetic diiodinated precursor peptide(pages 1–4)	Martin Holst Friborg Pedersen and Michael Baun	DOI: 10.1002/jlcr.1941	2012,1	0,3	8,2		I/T
67	Synthesis of tritium-labeled levetiracetam ((2S)-2-(2-oxopyrrolidin-1-yl)butanamide) with high specific activity (pages 48–51)	Simone Hildenbrand, Younis Baqi and Christa E. Müller	DOI: 10.1002/jlcr.1942	2012,1	5	10,0	98,0	cl/T
68	Synthesis of 3H-labeled Tetrabenazine (TBZ) (pages 367–370)	Sung-Whi Rhee, Kenneth J. Ryan and Mary J. Tanga	DOI: 10.1002/jlcr.1881	2011,7	2,2	####		DB
69	Synthesis of the NK3 receptor antagonist AZD2624 in C-14-, H-3- and C-13-labeled forms (pages 239–246)	Charles S. Elmore, Peter N. Dorff, Mark E. Powell, James E. Hall and Thomas R. Simpson	DOI: 10.1002/jlcr.1858	2011,5	6	0,6	37,0	I/T
70	Synthesis of 3H-, 13C3-, and 14C-labeled Sch 727965 (pages 196–201)	C. Flader Lavey, D. Hesk, D. Koharski, V. Truong and P. McNamara	DOI: 10.1002/jlcr.1845	2011,4	8	0,5		T2O
71	Direct metal-catalyzed tritiation of organic compounds (pages 739–744)	Crist N. Filer	DOI: 10.1002/jlcr.1801	2010,9	2	####	33,0	T2O
				2010,9	0,9	60,0	30,0	Rh/Al2O3
				2010,9	0,04	####	78,0	Crabtree

72	The use of metal-catalysed hydrogen isotope exchange in the contract supply of tritiated compounds (pages 745–751)	Michael R. Chappelle and Calvin R. Hawes	DOI: 10.1002/jlcr.1821	2010,9	n/a	20,0		no RCY
73	Metal-catalysed isotopic exchange labelling: 30 years of experience in pharmaceutical R&D (pages 731–738)	Paul H. Allen, Michael J. Hickey, Lee P. Kingston and David J. Wilkinson	DOI: 10.1002/jlcr.1825	2010,9	n/a	3,0		Crabtree
			DOI: 10.1002/jlcr.1825	2010,9	0,6	3,5		Ir-Kat
			DOI: 10.1002/jlcr.1825	2010,9	7,2	1,8	41,0	Crabtree-Polymer
74	Asymmetric [3H]-labeling using ruthenium catalyzed transfer hydrogenation(pages 205–207)	Steve Arns, Anne Moreau and Robert N. Young	DOI: 10.1002/jlcr.1753	2010,1	1	0,1	0,1	Ru/T2O
75	Synthesis of [3-3H]20(S)-protopanaxadiol (pages 482–484)	Jian Meng, Lizhi Zhao, Youhong Hu, Xiaoyan Chen and Dafang Zhong	DOI: 10.1002/jlcr.1663	2009,9	7	0,1	5,0	NaBT4
76	Enzymatic synthesis of N-methylhistamine labeled with deuterium and tritium(pages 372–375)	J. Šamonina and M. Kańska	DOI: 10.1002/jlcr.1611	2009,8	0,1	0,2		enzyme/T2O
77	Preparation of high specific activity tritium labeled 6α,9,-difluoro-11β,21-dihydroxy-16α,17-[(1-methylethylidene)bis(oxy)]pregna-1,4-diene-3,20-one, fluocinolone acetonide (pages 103–109)	D. Zhong and Anita H. Lewin	DOI: 10.1002/jlcr.1575	2009,3	5	10,0		DB/Rh/T2
78	Synthesis of [3H]ABT-518, a matrix metalloproteinase inhibitor (MMPI) labeled in the phenyl rings (pages 98–102)	Shirish N. Raja, Bruce W. Surber, Jia Du and Jeffrey L. Cross	DOI: 10.1002/jlcr.1574	2009,2	11	3,7		I/T
79	Synthesis of tritium labelled thiorphan, an enkephalinase inhibitor (pages 23–28)	Shao-Yong Wu and Mohammad R. Masjedizadeh	DOI: 10.1002/jlcr.1566	2009,1	n/a			Br/T

80	Studies on Taxol® biosynthesis. Preparation and tritium labeling of biosynthetic intermediates by deoxygenation of a taxadiene tetra-acetate obtained from Japanese yew (pages 325–328)	Tohru Horiguchi, Christopher D. Rithner, Rodney Croteau and Robert M. Williams	DOI: 10.1002/jlcr.1529	2008,8	1	0,1		nBuSn3H
81	Syntheses of AZ12320927 labeled with H-3, C-14, and H-2 (pages 343–346)	Charles S. Elmore, Mark E. Powell and J. Richard Heys	DOI: 10.1002/jlcr.1534	2008,8	9	3,5	43,0	Crabtree
82	Enzymatic synthesis of phenylpyruvic acid labeled with deuterium, tritium, and carbon-14 (pages 321–324)	Katarzyna Skowera and Marianna Kańska	DOI: 10.1002/jlcr.1530	2008,7	2	0,3	0,0	T2O
83	Synthesis of herbicidal ZJ0273 labeled with tritium and carbon-14 (pages 182–186)	Zheng-Min Yang, Qing-Fu Ye and Long Lu	DOI: 10.1002/jlcr.1498	2008,4				precursor purchased no RCY
84	Synthesis of tritium-labeled bilirubin (pages 106–108)	Bachir Latli, Matt Hrapchak, Dhileepkumar Krishnamurthy and Chris H. Senanayake	DOI: 10.1002/jlcr.1489	2008,2	11,5	1,0	7,0	NaBT4
85	Synthesis of tritium- and deuterium-labeled budesonide (pages 64–67)	Bachir Latli, Dhileep Krishnamurthy and Chris Senanayake	DOI: 10.1002/jlcr.1480	2008,1	n/a	0,3	n/a	DB/Pd/T2
86	Synthesis of [3H]fenobam, a radioligand for the mGlu5 receptor (pages 77–79)	Thomas Hartung, Jens-Uwe Peters, Jürgen Wichmann, Christian Hubschwerlen and Georg Jaeschke	DOI: 10.1002/jlcr.1470	2008,1	n/a	n/a	n/a	precursor purchased no RCY
87	Synthesis of radiolabelled photolabile fusidic acid analogues (pages 1260–1261)	Søren Christian Schou, Ditte Riber and Gunnar Grue-Sørensen	DOI: 10.1002/jlcr.1458	2007,9	n/a	n/a	40,0	DB/T2
88	Synthesis of 13C6, 3H, and 14C labeled Sch 414319 and 35S labeling of an analog, Sch 225336 (pages 264–272)	Carolee Flader Lavey, David Hesk, Sharon Hendershot, David Koharski, Surinderjit Saluja and Paul Mc Namara	DOI: 10.1002/jlcr.1183	2007,5	3	0,5	1,0	n-BuLI/t2O
89	Tritium-labelling via an iridium-based solid-phase catalyst (pages 286–289)	Michael J. Hickey, Lee P. Kingston, William J. S. Lockley, Paul Allen, Andrew Mather and David. J. Wilkinson	DOI: 10.1002/jlcr.1233	2007,5	7	1,8	41,0	Ir/polymer
90	Synthesis of [3H]doxorubicin by isotope exchange with tritiated water (pages 416–417)	Valerii P. Shevchenko, Igor Yu. Nagaev, Nikolay F. Myasoedov and Alex B. Susan	DOI: 10.1002/jlcr.1167	2007,5	8	1,0	0,1	T2O

91	Synthesis of [3H,33P]-phosphoramide and -isophosphoramide mustards and metabolites [3H]-chloroethylaziridine and -aziridine for studies of DNA alkylation(pages 79–84)	James B. Springer, O. Michael Colvin and Susan M. Ludeman	DOI: 10.1002/jlcr.1157	2007,2	n/a	n/a	n/a	LiAlT4, no RCY
92	Enzymatic synthesis of isotopomers of tyramine labeled with deuterium and tritium(pages 85–89)	Edyta Panufnik and Marianna Kañska	DOI: 10.1002/jlcr.1160	2007,2	0,5	0,3	n/a	T2O
93	Synthesis of 3H, 14C and 2H4 labelled SCH 211803 (pages 131–137)	D. Hesk, K. Voronin, P. McNamara, P. Royster, D. Koharski, S. Hendershot, S. Saluja, V. Truong and T. M. Chan	DOI: 10.1002/jlcr.1206	2007,2	6	0,5	1,6	T2O
94	Synthesis of 3H- and 2H4-labelled versions of the hypoxia-activated pre-prodrug 2-[(2-bromoethyl)-2,4-dinitro-6- [[[2-(phosphonooxy)ethyl]amino]carbonyl]anilino]ethyl methanesulfonate (PR-104)(pages 7–12)	Graham J. Atwell and William A. Denny	DOI: 10.1002/jlcr.1147	2007,1	n/a	1,2	6,3	NaBT4
95	Synthesis of isotopomers of dopamine labeled with deuterium or tritium (pages 1061–1067)	M. Pająk and M. Kańska	DOI: 10.1002/jlcr.1123	2006,9	0,2	0,3	0,1	T2O
96	Preparation of tritium-labeled Silybin—a protectant for common liver diseases(pages 1125–1130)	D. Y. W. Lee, X. Zhang and X. S. Ji	DOI: 10.1002/jlcr.1132	2006,9	n/a	0,0	n/a	NaBT4
97	Synthesis of [3H]-labelled 4-[Ethyl[2,5,6-trimethyl-7-(2,4,6-trimethylphenyl)pyrrolo[2,3-d]pyrimidin-4-yl]amino]-2,3-[3H]-butan-1-ol: a high affinity radioligand for the corticotropin-releasing hormone type 1 receptor (pages 635–640)	Anne-Cécile Hiebel, John S. Partilla, Richard B. Rothman, Arthur E. Jacobson and Kenner C. Rice	DOI: 10.1002/jlcr.1082	2006,5	4,1	12,4	35,0	DB/T2/Pd/C
98	Synthesis of site-specifically deuterated arachidonic acid derivatives containing a remote tritium radiolabel (pages 545–558)	Chris M. McGinley and Wilfred A. van der Donk	DOI: 10.1002/jlcr.1073	2006,4	n/a	n/a		no RCY

99	Synthesis of tritium-labelled BIBN4096, an experimental h-CGRP-antagonist(pages 421–427)	V. P. Shevchenko, I. Yu. Nagaev, N. F. Myasoedov, A. B. Susan, K.-H. Switek and H. Braunger	DOI: 10.1002/jlcr.1061	2006,4	n/a	n/a	180,0	Pyr/T2
100	A novel asymmetric synthesis of tritium and carbon-14 labeled (R)-ibuprofen(pages 237–244)	Yinsheng Zhang, Yang Hong, Che C. Huang and Daniel Belmont	DOI: 10.1002/jlcr.1040	2006,3	1,8	0,6	54,0	DB/T2
101	High specific activity tritium labeling of vitamin D derivative RO275646 (pages 1013–1023)	Steve A. de Keczer, Tim S. Lane, Tatyana Voronin and Mohammad R. Masjedizadeh	DOI: 10.1002/jlcr.1014	2005,9	3	40,0	50,0	T2O
102	Preparation of tritiated fluorenone and fluorenol	Devika, K.; Chandrika, R.; Padmanabhan, D.; Unny, V. K. P.; Sivaprasad, N. Journal of Radioanalytical and Nuclear Chemistry volume 266, pages507–508(2005)	DOI:10.1007/s10967-005-0940-1	2005,8	n/a	n/a	17,0	I/T
103	High specific activity tritium labeling of anti-tumor agent CEP-2563	Egan, Judith A.; Filer, Crist N.; Hudkins, Robert L. J Label Compd Radiopharm 2005; 48: 997–1001	DOI:10.1002/jlcr.1010	2005,8	6	42,0		NaBT4
104	Synthesis of 2H- and 3H-labeled N-cyclopropylmethyl-7α-[(R)-1-hydroxy-1-methyl-3-(2-thienyl)propyl]-6,14-endoetheno-6,7,8,14-tetrahydronororipavine	Wu, Bo; Chen, Lanfu; Wang, Jingyan; Liu, Chunhe; Liu, He; Zhong, Bohua J Label Compd Radiopharm 2005; 48: 811–817.	DOI:10.1002/jlcr.1000	2005,7	n/a	n/a	18,0	Br/T
105	Design, Synthesis, and Biological Evaluation of Potent Discodermolide Fluorescent and Photoaffinity Molecular Probes	Smith, Amos B., III; Rucker, Paul V.; Brouard, Ignacio; Freeze, B. Scott; Xia, Shujun; Horwitz, Susan Band Org. Lett. 2005, 7, 23, 5199-5202	DOI:10.1021/ol0520166	2005,7	n/a	n/a	26,2	I/T
106	Efficient Synthesis of [3H]-Sanglifehrin A via Selective Oxidation/Reduction of Alcohols at C31 and C35	Wagner, Juergen; Andres, Hendrik; Rohrbach, Stefan; Wagner, Dieter; Oberer, Lukas; France, Julien J. Org. Chem. 2005, 70, 9588-9590	DOI:10.1021/jo051112h	2005,6	9	11,7	24,3	LiT

107	Synthesis of deramciclane labeled with tritium in various positions	Szammer, Janos; Simon-Trompler, Edit; Banka, Zoltan; Szunyog, Jozsef; Klebovich, Imre J Label Compd Radiopharm 2005; 48: 693–700	DOI:10.1002/jlcr.964	2005,6	11	0.1	0.2	NaBT4
108	A Synthesis of tritium-labeled Olanzapine	Shevchenko, V. P.; Nagaev, I. Yu.; Kuznetsov, Yu. V.; Polunin, E. V.; Zozulya, A. A.; Myasoedov, N. F. Russian Journal of Bioorganic Chemistry, Vol. 31, No. 4, 2005, pp. 378–382	DOI:10.1007/s11171-005-0052-2	2005,5	n/a	n/a	12,0	Pd/BaSO4/T2
109	Tritiation of the cannabinoid receptor antagonist SR144528 involving lithium aluminum tritide reduction; Assessment of the kinetic isotope effect by 3H-NMR	Seltzman, Herbert H.; Foster, Matthew C.; Wyrick, Christopher D.; Burgess, Jason P.; Carroll, F. Ivy J Label Compd Radiopharm 2005; 48: 589–596	DOI:10.1002/jlcr.952	2005,5	5,7	8,7		LiAlT4
110	Fast and efficient tritium labeling of the nonsteroidal anti-inflammatory drugs naproxen, tolmetin, and zomepirac J Label Compd Radiopharm 2005; 48: 569–576	Johansen, Steen K.; Sorensen, Lone; Martiny, Lars J Label Compd Radiopharm 2005; 48: 569–576	DOI:10.1002/jlcr.950	2005,4	0,2	8,7	26,0	Br/T
			DOI:10.1002/jlcr.950	2005,4	7	8,5	81,0	Crabtree
111	Tritium labeling of bromhexine via amide reduction with LiB3H4	Larsen, Uffe S.; Begtrup, Mikael; Martiny, Lars J Label Compd Radiopharm 2005; 48: 429–434	DOI:10.1002/jlcr.938	2005,4	6	5,0	54,0	LiBT4
112	Dopamine receptor stimulants N-0923 and (+/-)-threo-methylphenidate: Labeling with tritium	Laseter, A. G.; Seguin, R. J.; Filer, C. N. Journal of Radioanalytical and Nuclear Chemistry, Vol. 264, No. 3 (2005) 723ñ725	DOI:10.1007/s10967-005-0779-5	2005,3	2	60,0		DB/T2
113	Tritiation of CEP-1347 at high specific activity using several methods	Egan, Judith A.; Filer, Crist N.; Pounds, Scot; Connors, Thomas; Knight, Ernest, Jr.; Hudkins, Robert L. J Label Compd Radiopharm 2005; 48: 331–335	DOI:10.1002/jlcr.927	2005,3	8	21,0	27,4	NaBT4

114	Solid-phase catalytic reactions of tritium with carbohydrates: 1. Influence of temperature, catalysts, and solid phase composition on solid-phase catalytic hydrogenation of D-ribose with tritium	Baitov, A. A.; Sidorov, G. V.; Myasoedov, N. F. Radiochemistry, Vol. 47, No. 2, 2005, pp. 20120	DOI:10.1007/s11137-005-0074-x	2005,3	n/a	n/a	1.41 TBq/mmol	Pd/BaSO4
115	Enzymatic synthesis of tritium-labeled isotopomers of L-DOPA	Kozlowska, M.; Kanski, R.; Kanska, M.	DOI:10.1002/jlcr.919	2005,2	0.08	5.2 GBq	5.5MBq/mmol	HIE/enzymatic
116	Enzymatic synthesis of tritium-labeled isotopomers of histamine	Panufnik, E.; Kanski, R.; Kanska, M. J Label Compd Radiopharm 2005; 48: 45–50	DOI:10.1002/jlcr.894	2005,2	0.5	5.2 GBq	25MBq/mmol	HIE/enzymatic
117	The synthesis of a benzamidine-containing NR2B-selective NMDA receptor ligand labelled with tritium or fluorine-18	Hamill, Terence G.; McCauley, John A.; Burns, H. Donald	DOI:10.1002/jlcr.871	2005,1	0.06	5,0	11,0	Br/T
118	(2S,1'S,2'R,3'R)-2(2'-Carboxy-3'-hydroxymethylcyclopropyl)glycine-[3H], a potent and selective radioligand for labeling group 2 and 3 metabotropic glutamate receptors	Wheeler, William J.; Clodfelter, Dean K.; Kulanthaivel, Palaniappan; Pedregal, Concepcion; Stoddard, Eli A.; Wright, Rebecca A.; Schoepp, Darryle D.	DOI:10.1016/j.bmcl.2004.10.093	2005	n/a	5,0	14,0	NaBT4
119	Synthesis of [3H], [13C215N] and [14C]Sch 66336 (Sarasar™)	D. Hesk D. Cesarz C. Magatti K. Voronin C. Lavey P. McNamara D. Koharski S. Saluja S. Hendershot H. Pham V. Truong J Label Compd Radiopharm 2005; 48: 11–23	10.1002/jlcr.891	2005	14	0.5	1,4	Ru/T2O