

Supporting Information

Identification of Novel Thiazolo[5,4-b]Pyridine Derivatives as Potent Phosphoinositide 3-Kinase Inhibitors

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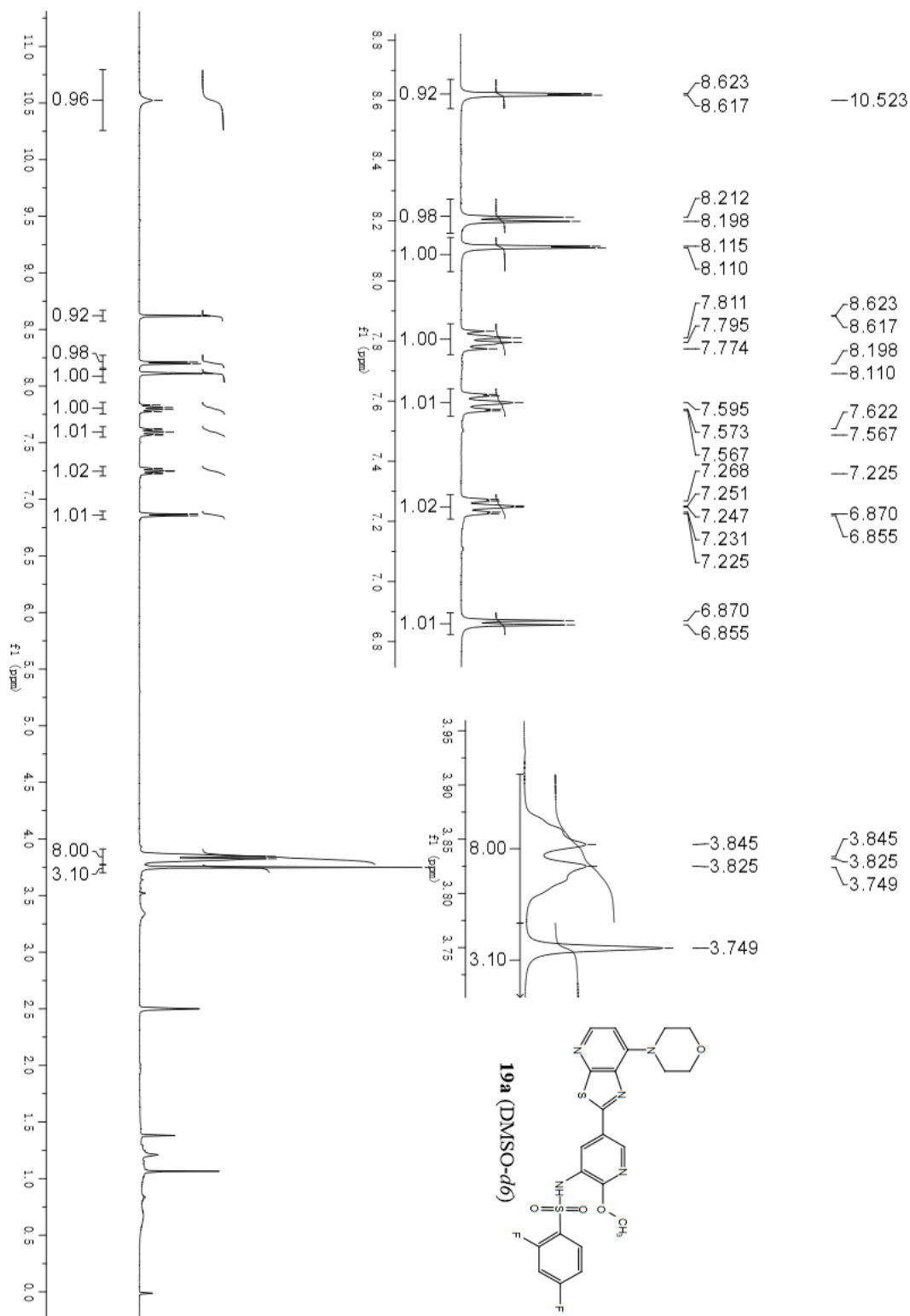
² Beijing Key Laboratory of Active Substances Discovery and Druggability Evaluation, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, China

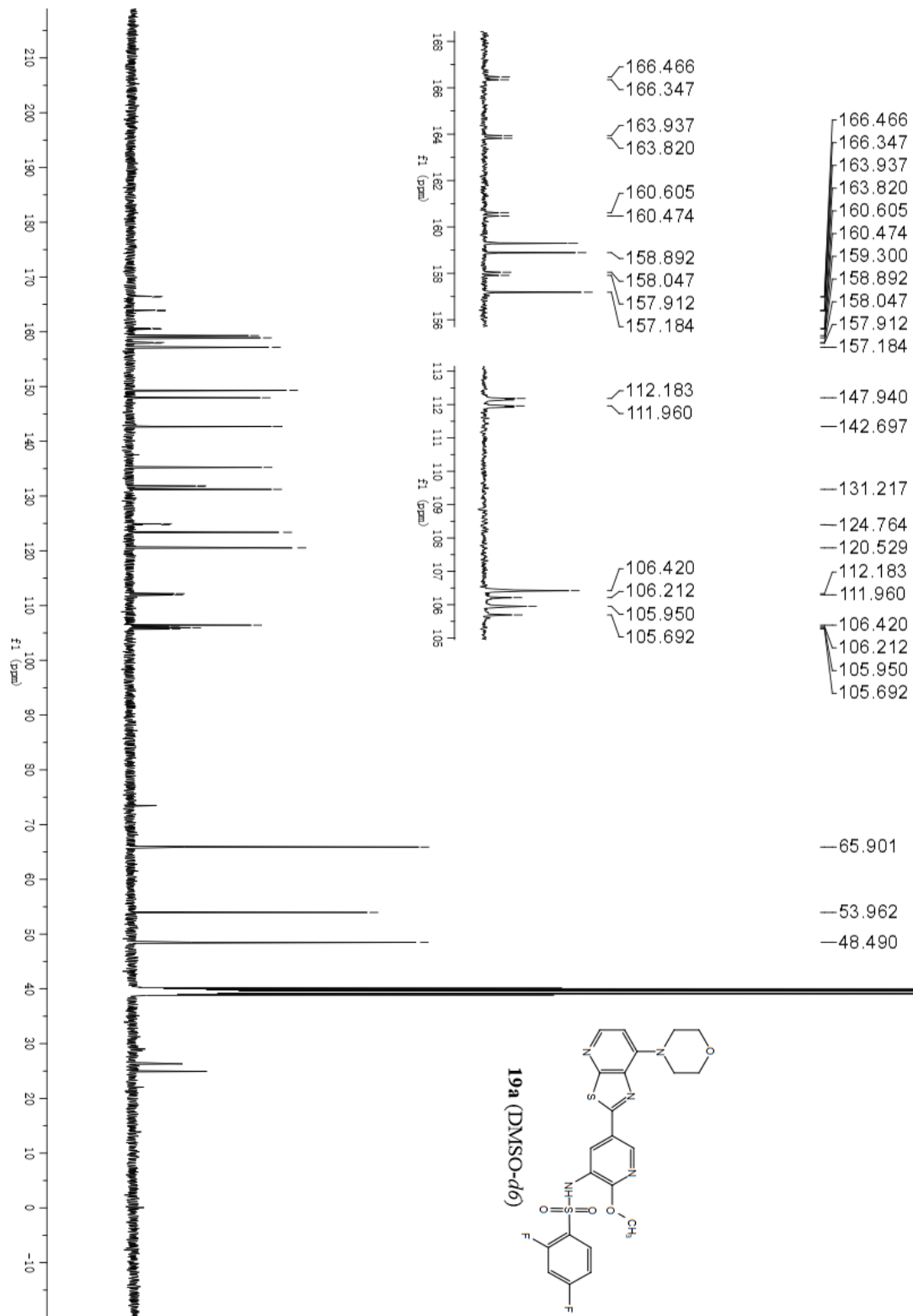
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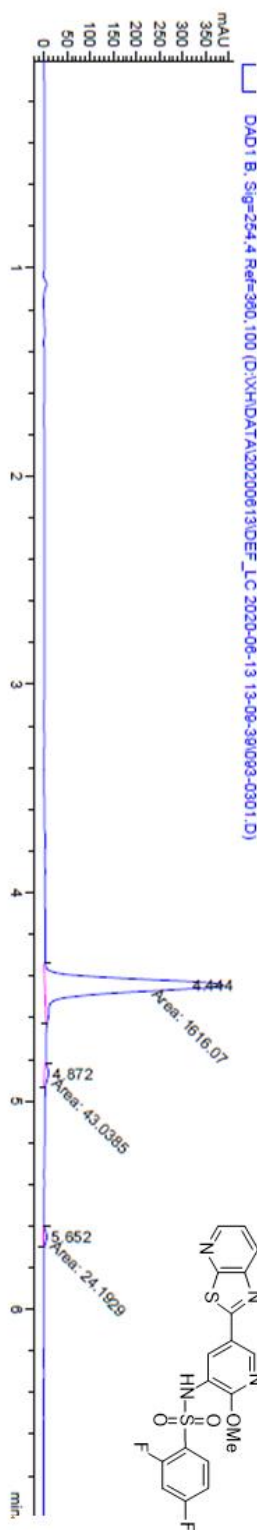
| | |
|--|---------|
| <i>¹H NMR, ¹³C NMR, HPLC spectrum of 2,4-difluoro-N-(2-methoxy-5-(7-morpholinothiazolo[5,4-b]pyridin-2-yl)pyridin-3-yl)benzenesulfonamide (19a)</i> | S1-S3 |
| <i>¹H NMR, ¹³C NMR, HPLC spectrum of 2-chloro-4-fluoro-N-(2-methoxy-5-(7-morpholinothiazolo[5,4-b]pyridin-2-yl)pyridin-3-yl)benzenesulfonamide (19b)</i> | S4- S6 |
| <i>¹H NMR, ¹³C NMR, HPLC spectrum of (5-chloro-N-(2-methoxy-5-(7-morpholinothiazolo[5,4-b]pyridin-2-yl)pyridin-3-yl)thiophene-2-sulfonamide (19c)</i> | S7-S9 |
| <i>¹H NMR, ¹³C NMR, HPLC spectrum of 4-(2-(6-methoxypyridin-3-yl)thiazolo[5,4-b]pyridin-7-yl)Morpholine (19d)</i> | S10-S12 |
| <i>¹H NMR, ¹³C NMR, HPLC spectrum of 2,4-difluoro-N-(2-methoxy-5-(7-morpholinothiazolo[5,4-b]pyridin-2-yl)phenyl)benzenesulfonamide (19e)</i> | S13-S15 |
| <i>¹H NMR, ¹³C NMR, HPLC spectrum of 2,4-difluoro-N-(5-(7-morpholinothiazolo[5,4-b]pyridin-2-yl)pyridin-3-yl)benzenesulfonamide (19f)</i> | S16-S18 |

¹H NMR spectrum of **19a**



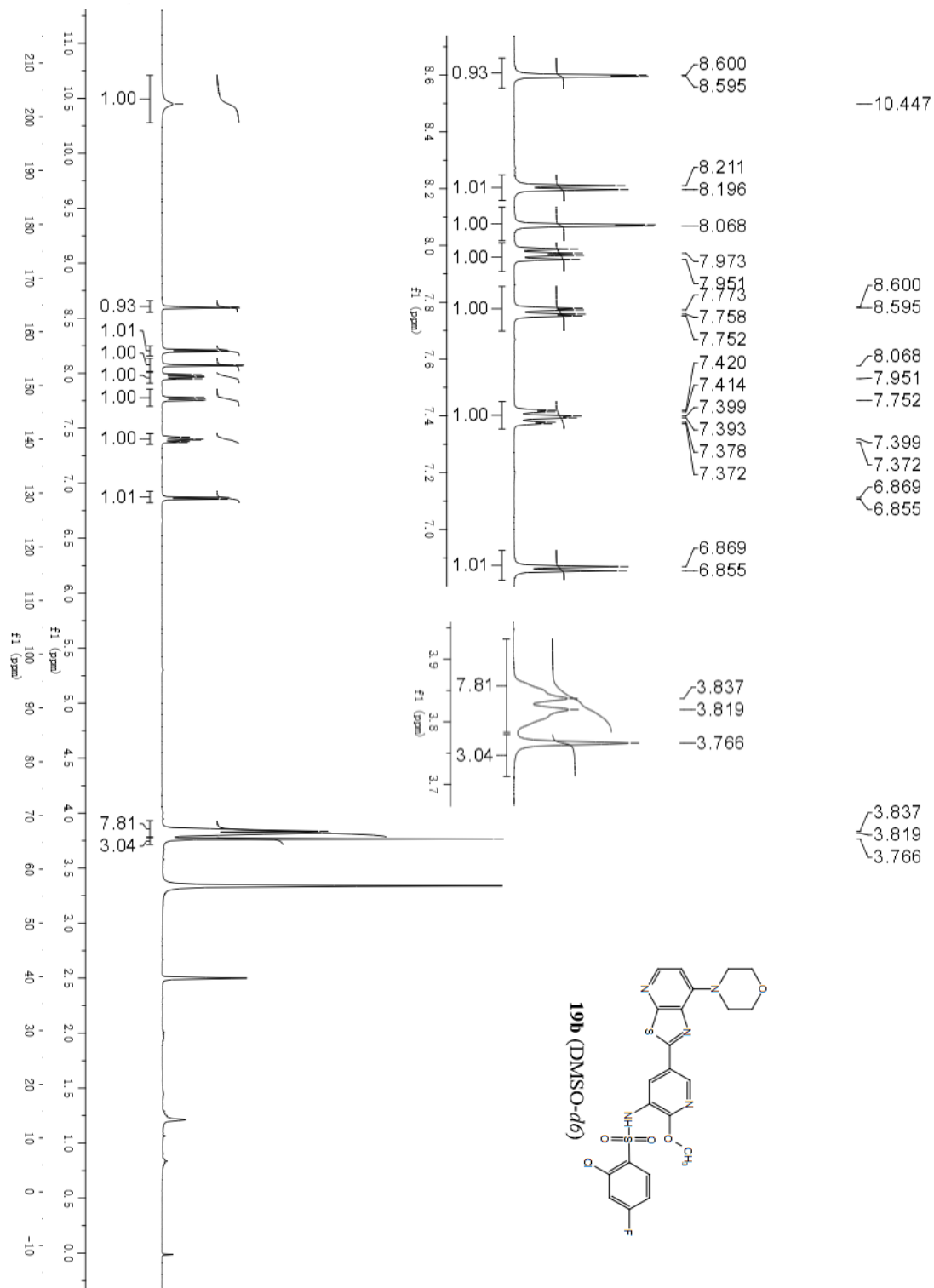


HPLC spectrum of 19a

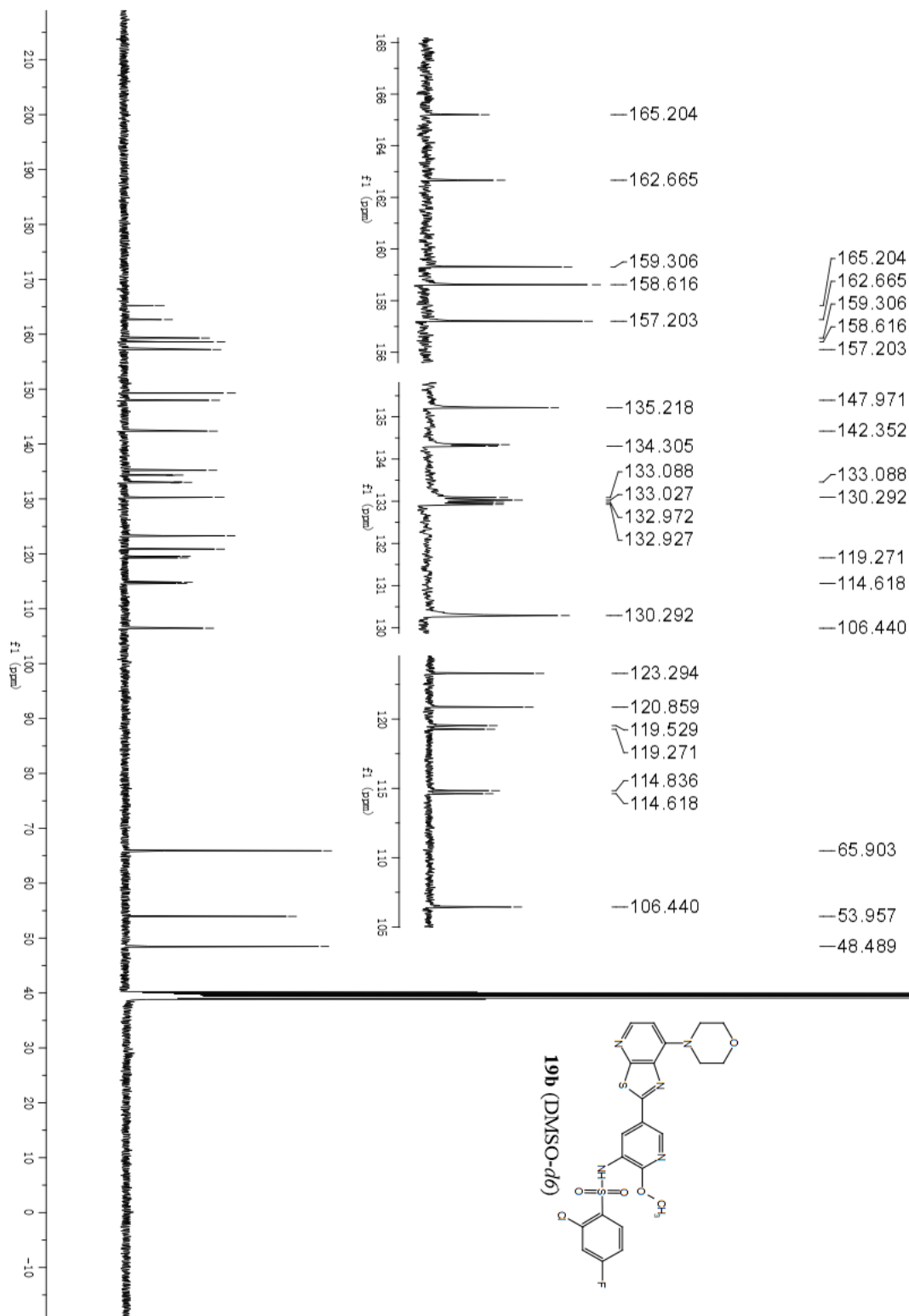


Signal 2: DAD1 B, Sig=254,4 Ref=360,100

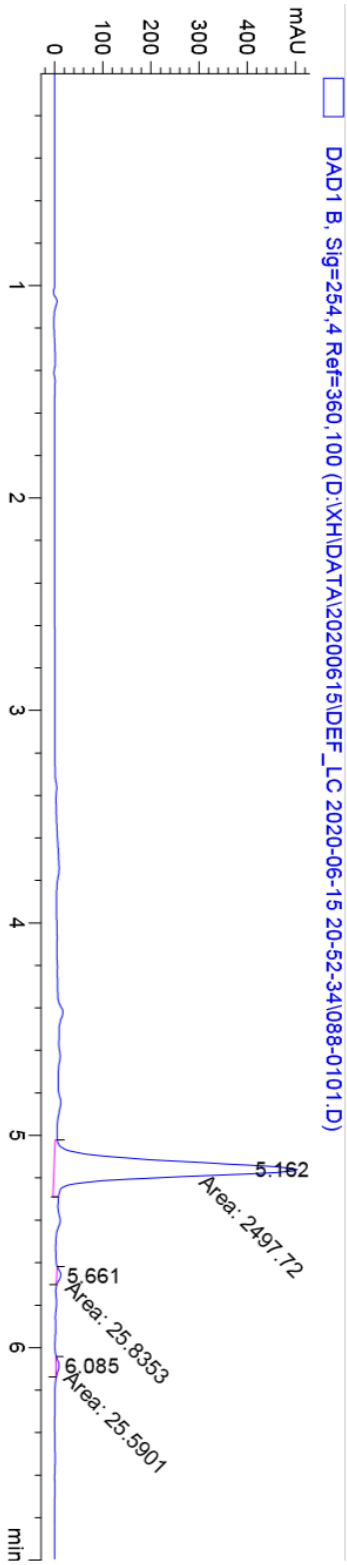
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.444 | MM | 0.0692 | 1616.07092 | 388.99686 | 96.0060 |
| 2 | 4.872 | MM | 0.0801 | 43.03851 | 8.95479 | 2.5568 |
| 3 | 5.652 | MM | 0.0630 | 24.19288 | 6.39731 | 1.4372 |

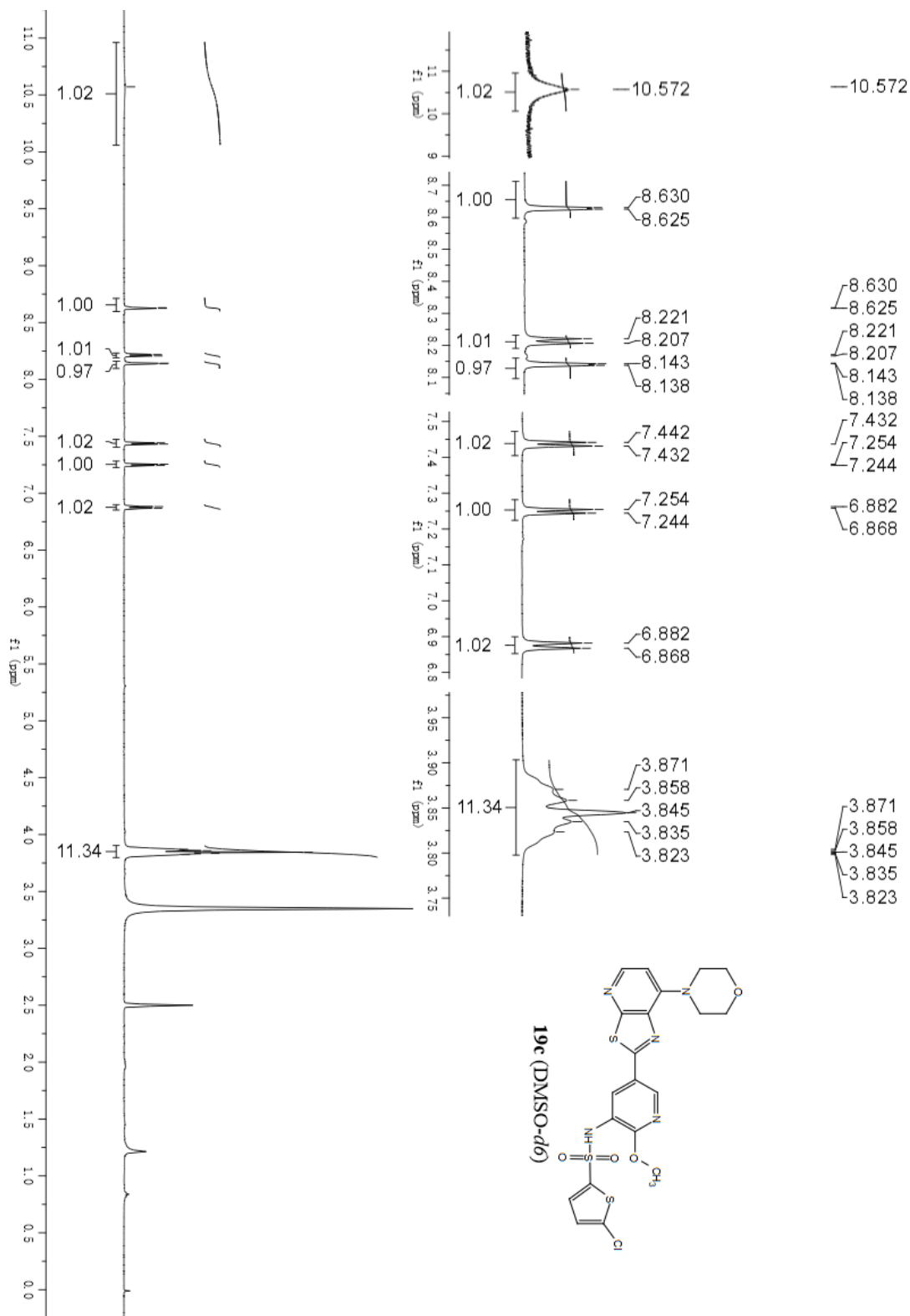


¹³C NMR spectrum of **19b**

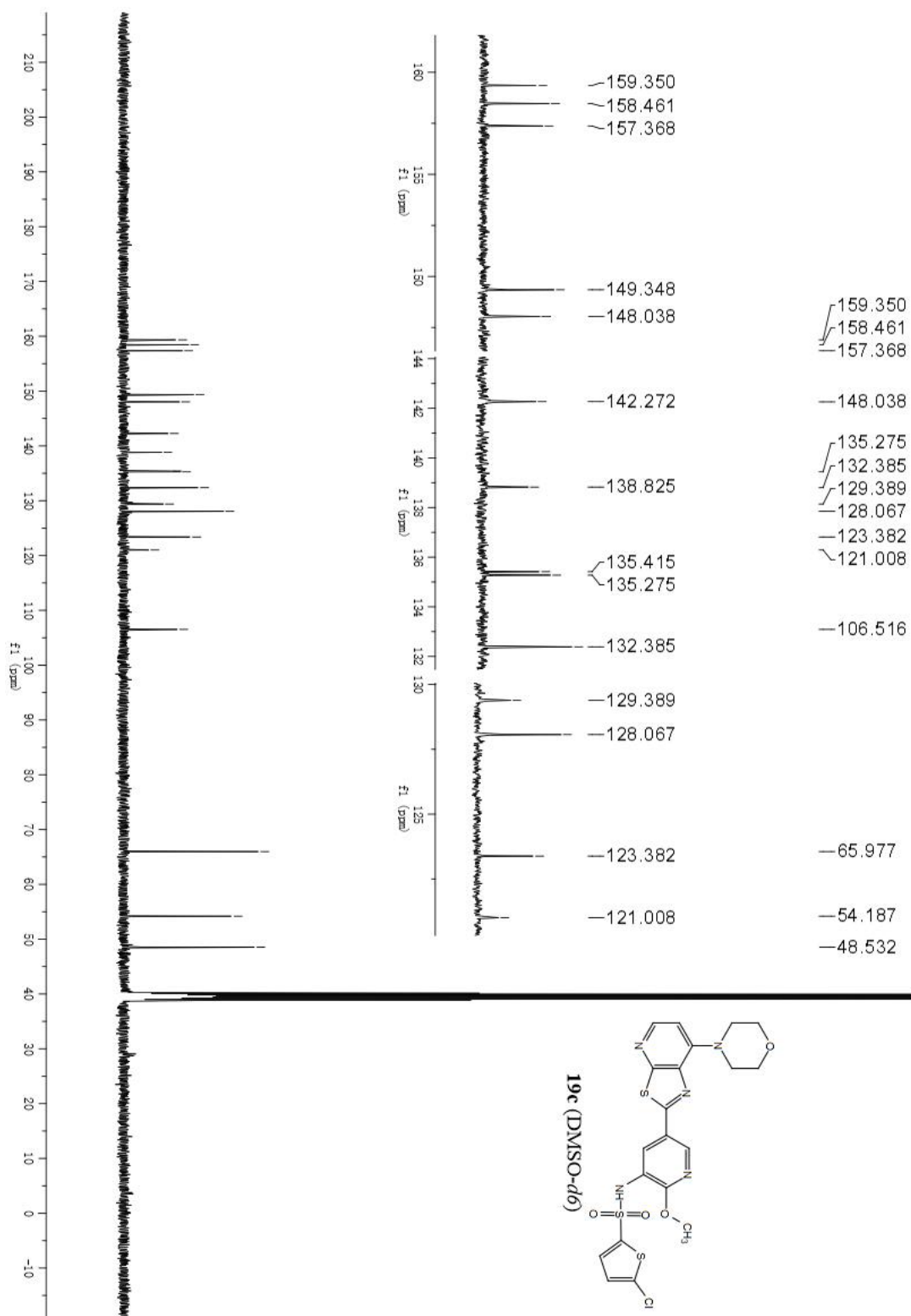
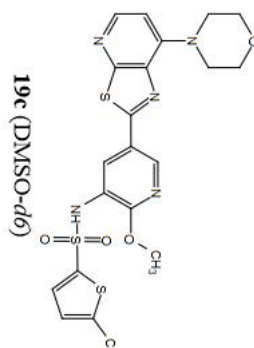


HPLC spectrum of 19b

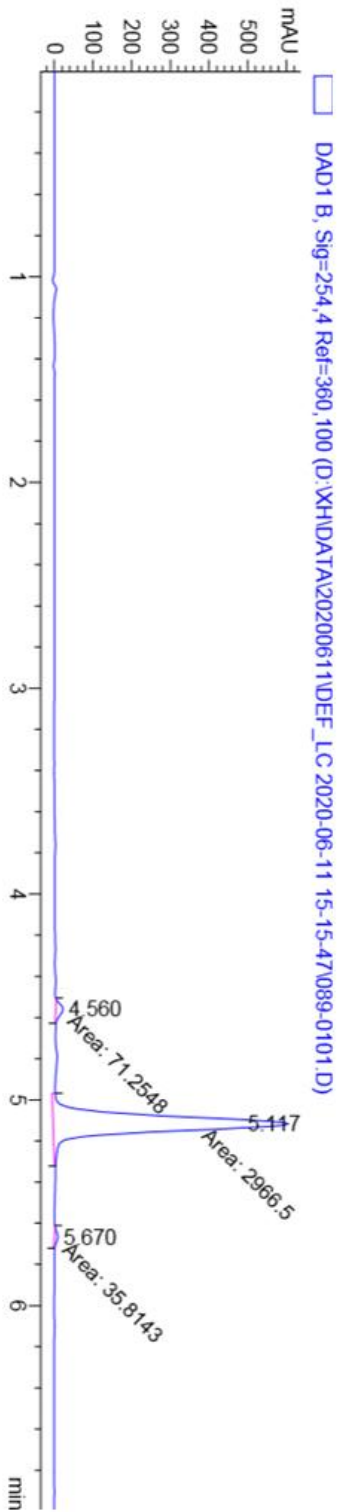




¹³C NMR spectrum of 19c

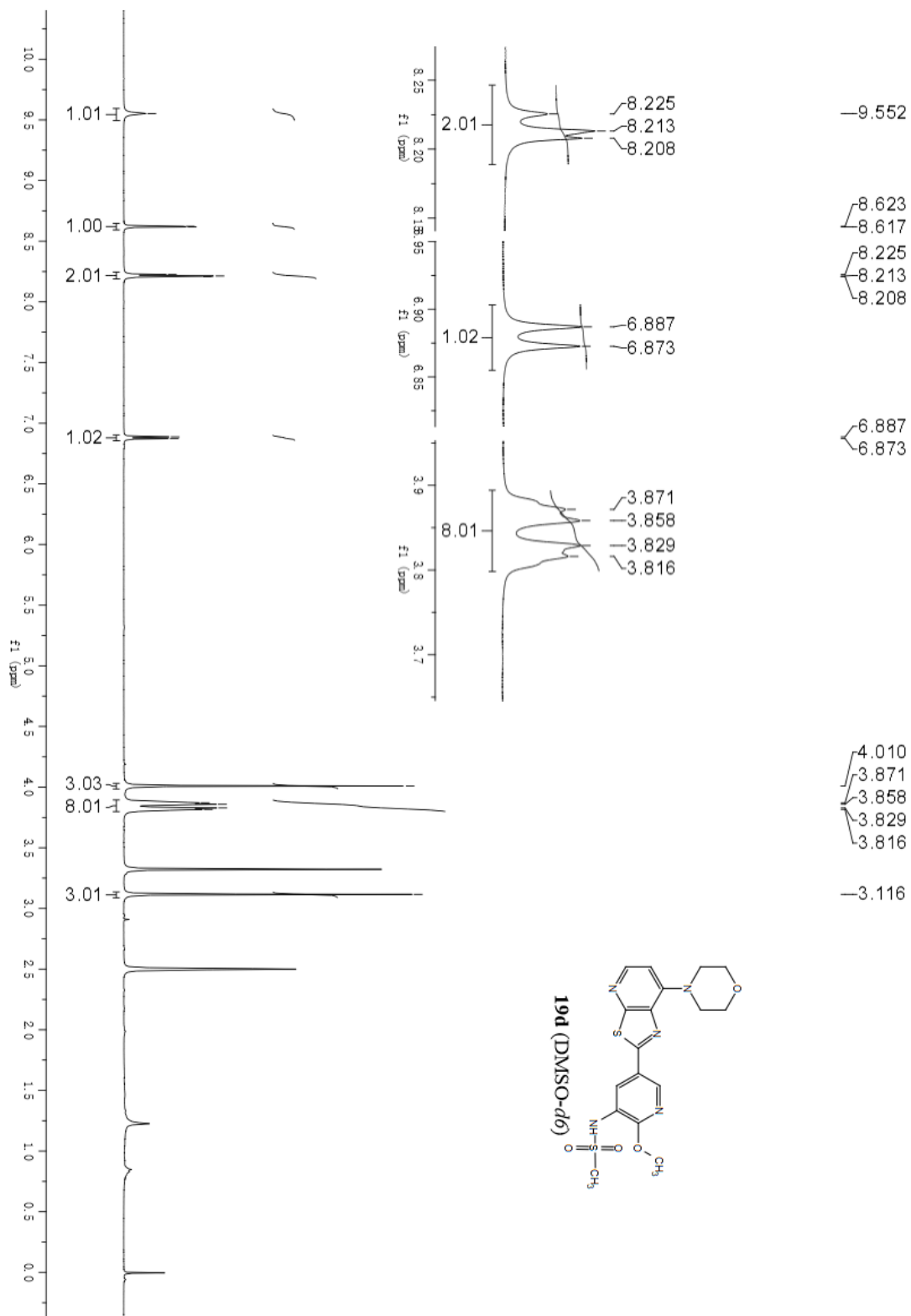


HPLC spectrum of 19c

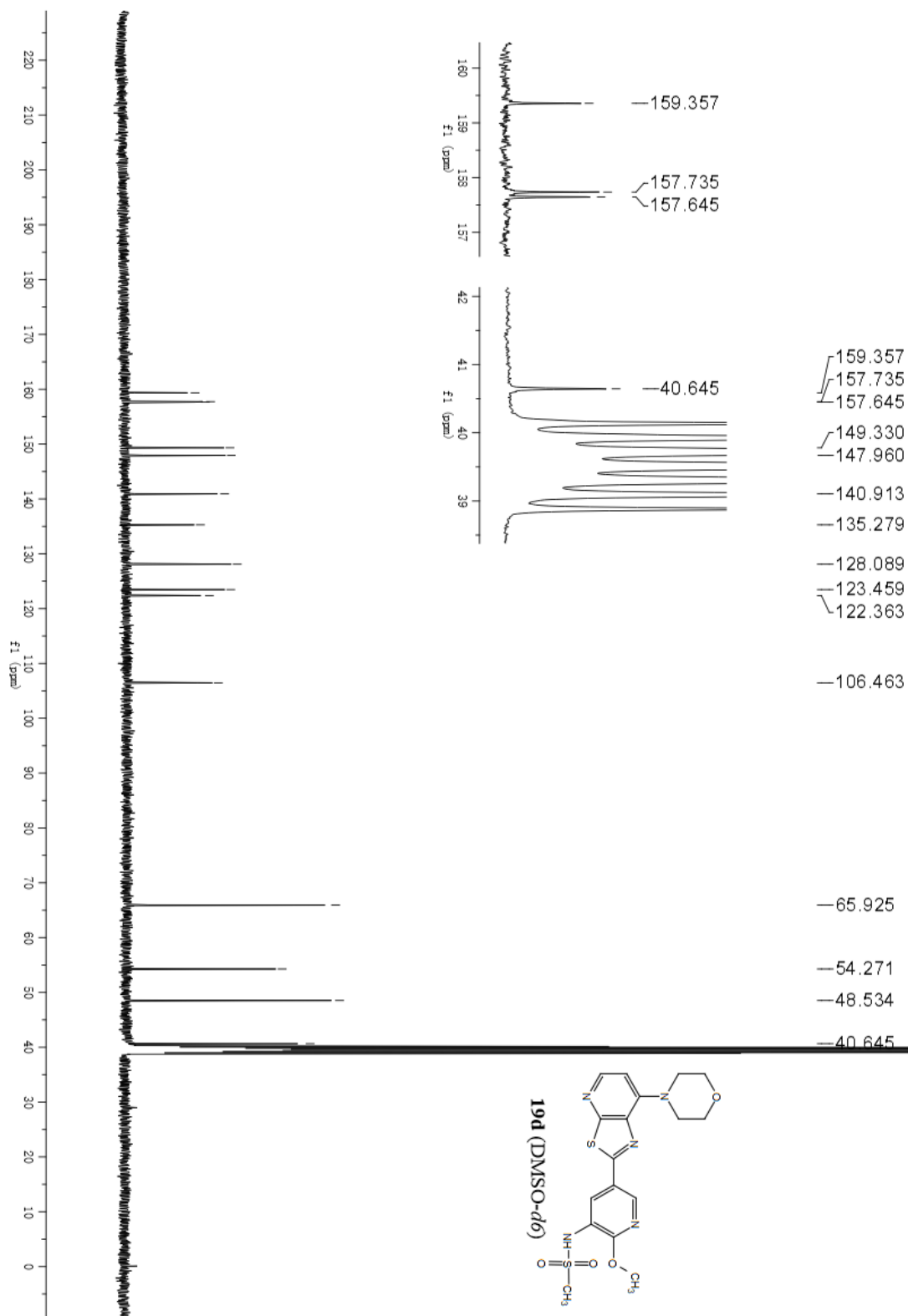


Signal 2: DAD1 B, Sig=254, 4 Ref=360, 100

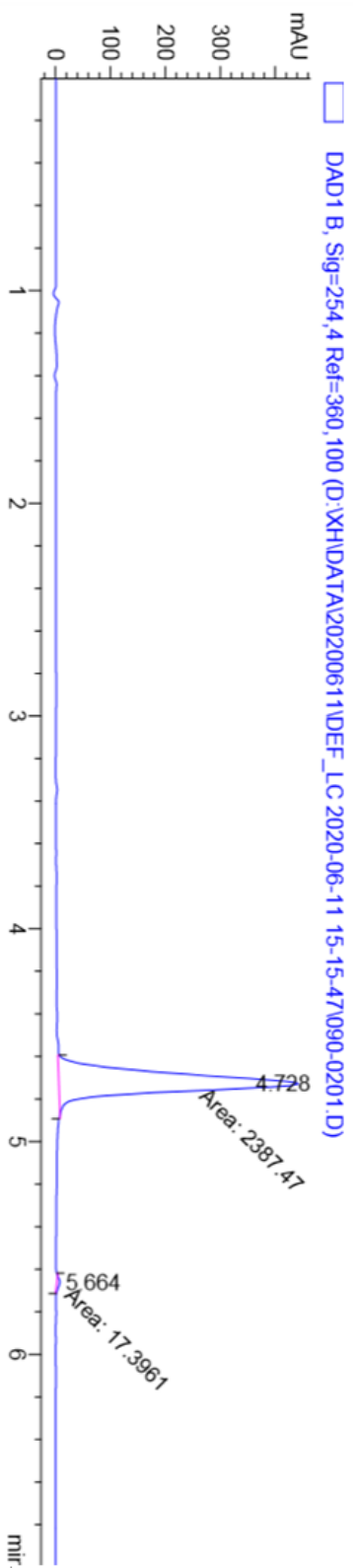
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|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.560 | MM | 0.0651 | 71.25484 | 18.23404 | 2.3183 |
| 2 | 5.117 | MM | 0.0810 | 2966.49585 | 610.17664 | 96.5165 |
| 3 | 5.670 | MM | 0.0655 | 35.81426 | 9.11627 | 1.1652 |



¹³C NMR spectrum of **19d**

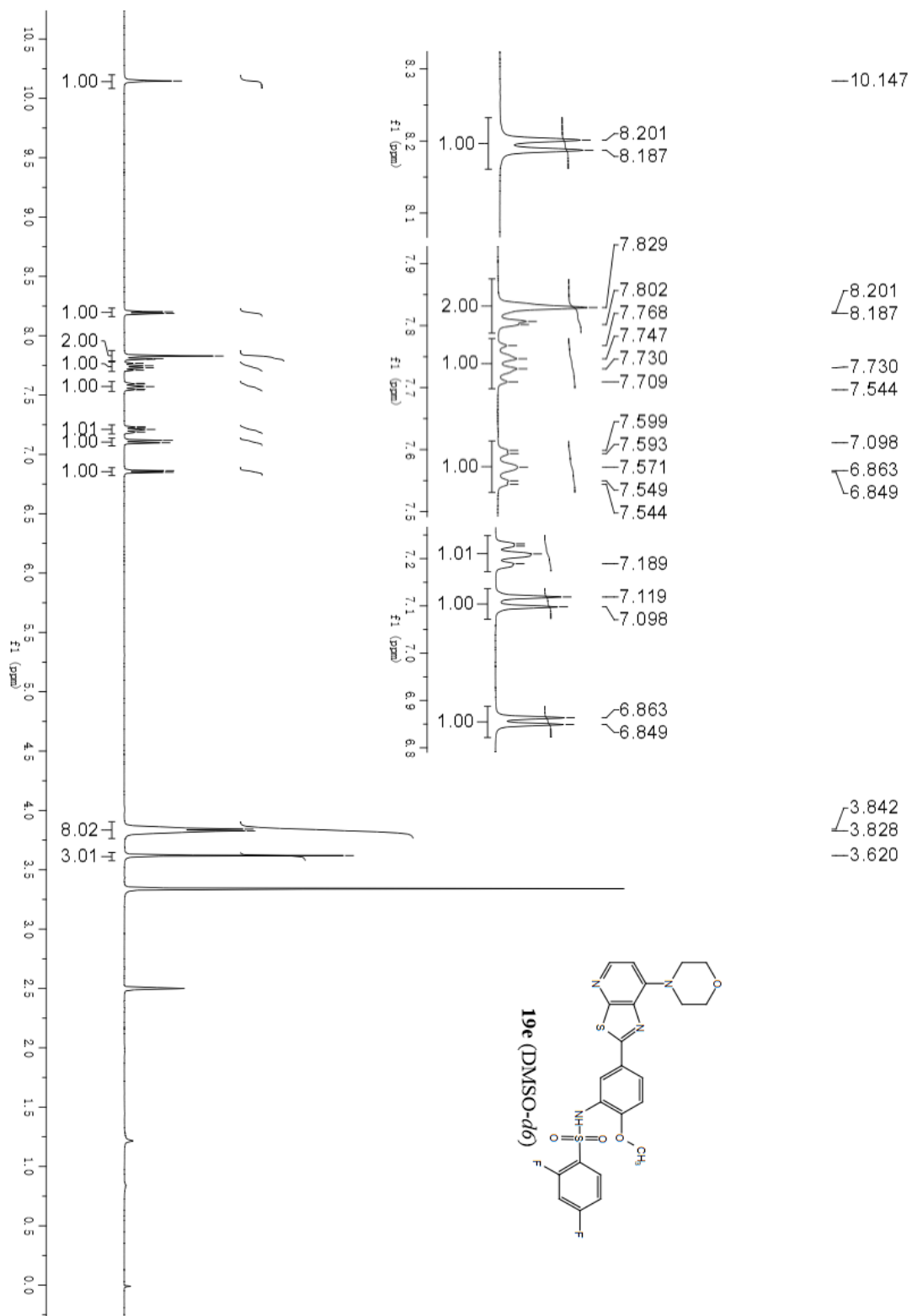


HPLC spectrum of 19d

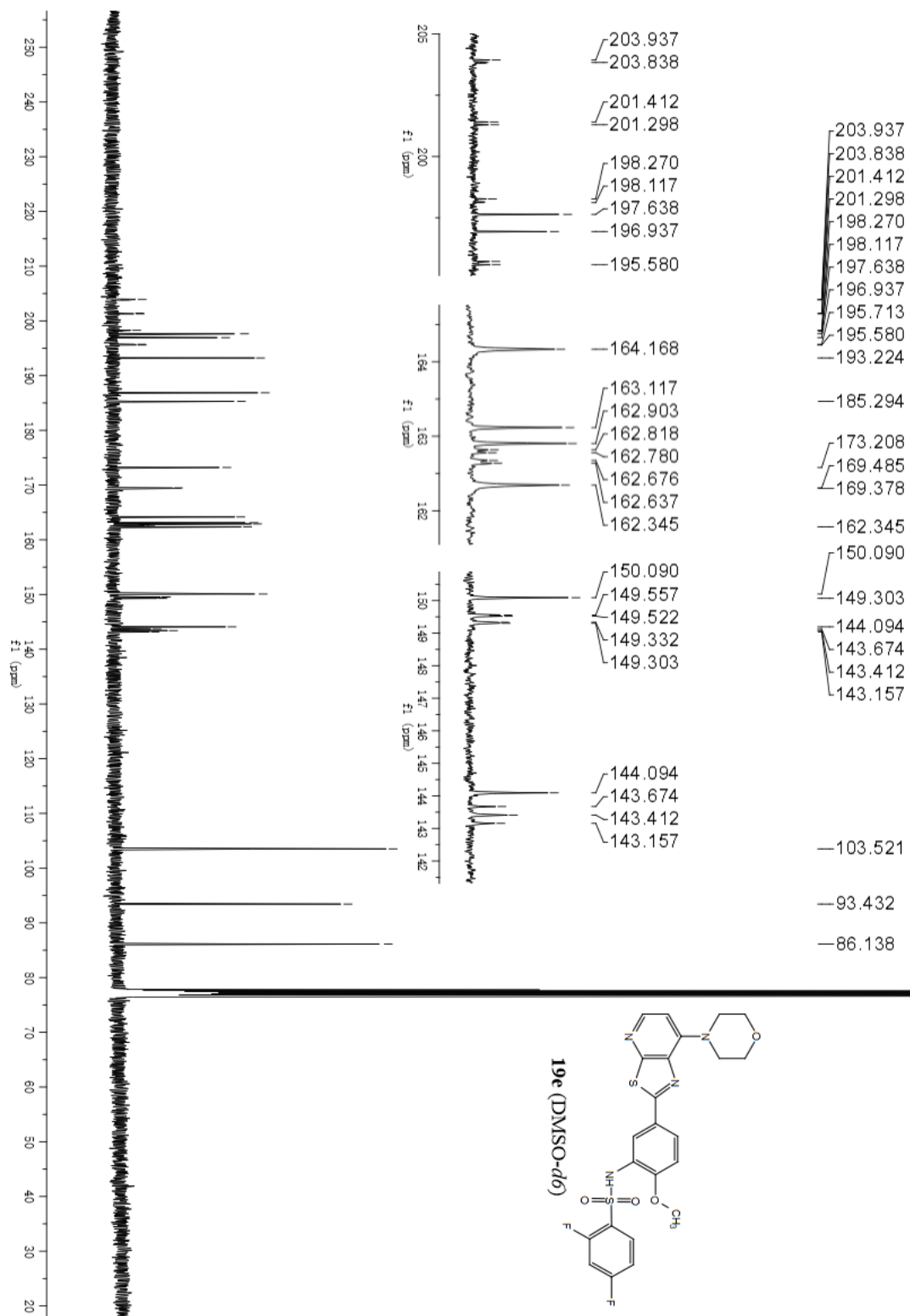


Signal 2: DAD1 B, Sig=254, 4 Ref=360, 100

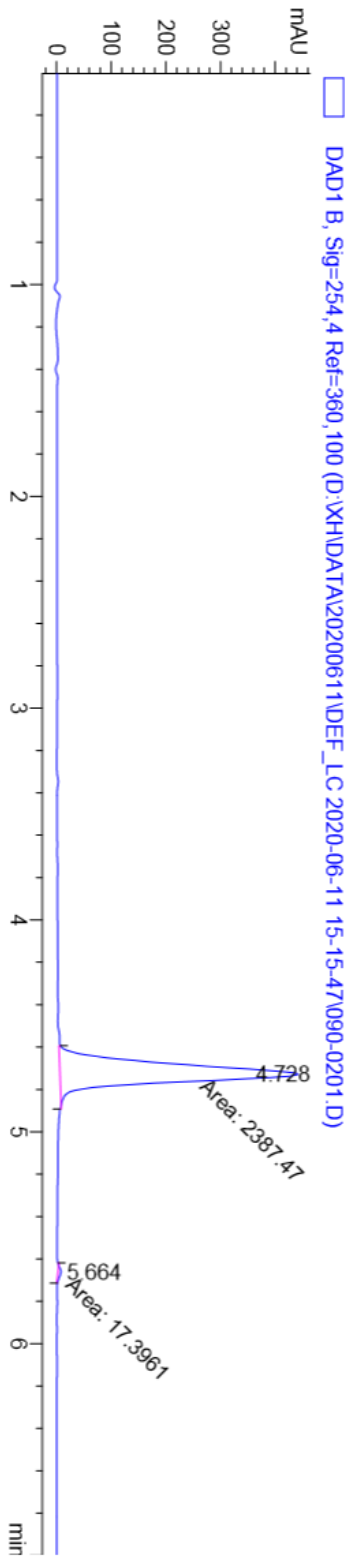
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.728 | MM | 0.0910 | 2387.46973 | 437.42035 | 99.2766 |
| 2 | 5.664 | MM | 0.0545 | 17.39607 | 5.31610 | 0.7234 |



¹³C NMR spectrum of **19e**



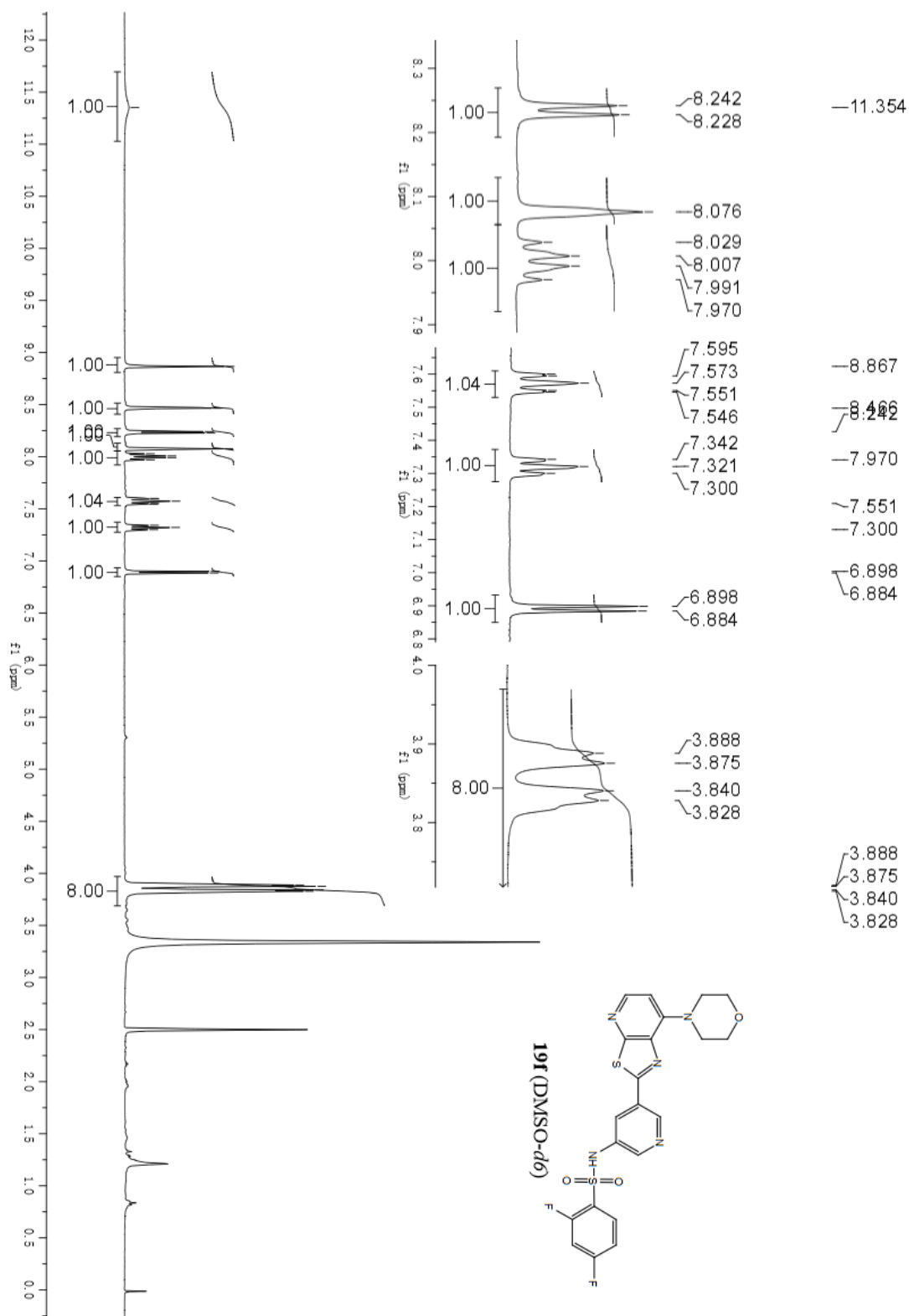
HPLC spectrum of 19e



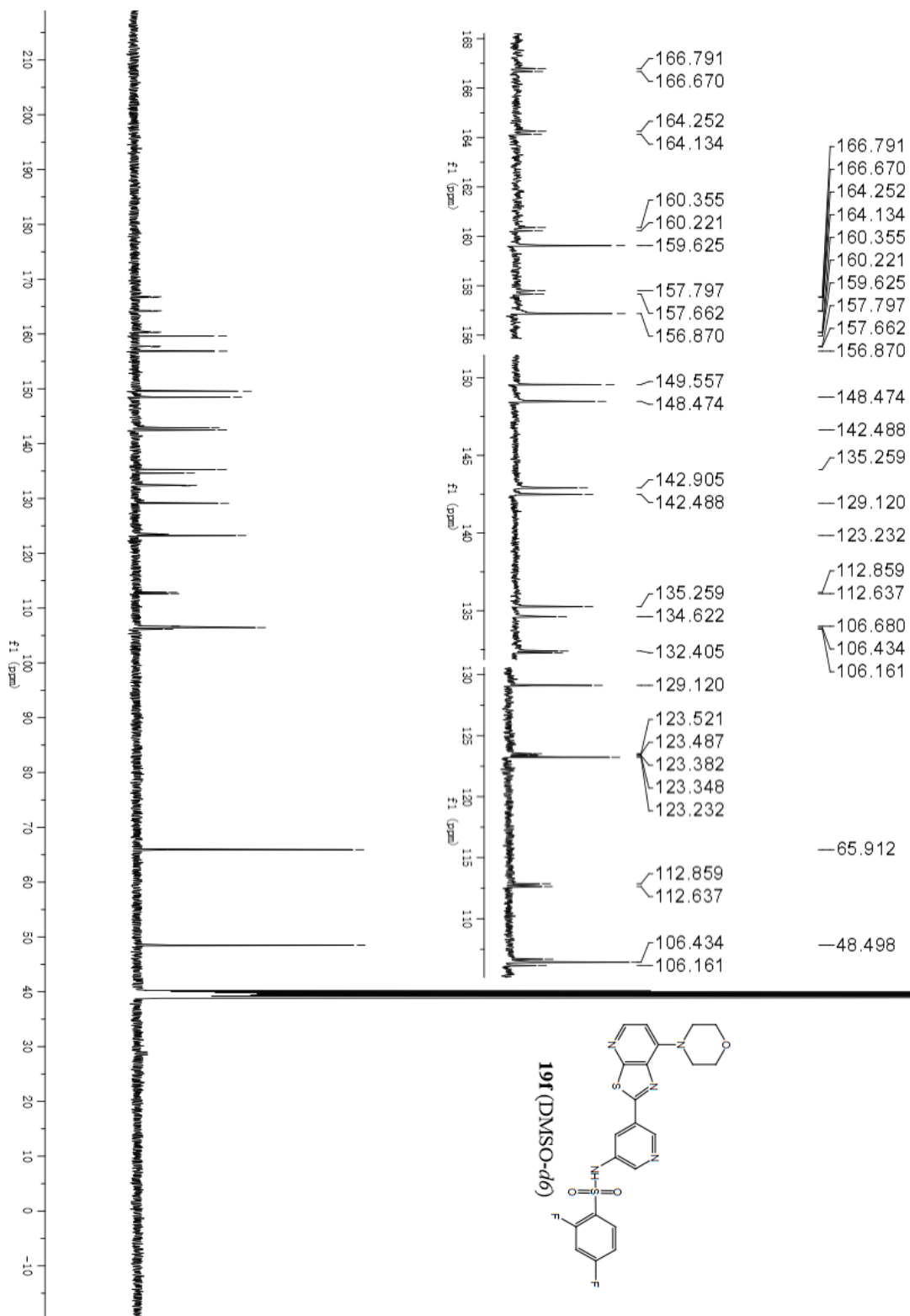
Signal 2: DAD1 B, Sig=254,4 Ref=360,100

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.728 | NM | 0.0910 | 2387.46973 | 437.42035 | 99.2766 |
| 2 | 5.664 | NM | 0.0545 | 17.39607 | 5.31610 | 0.7234 |

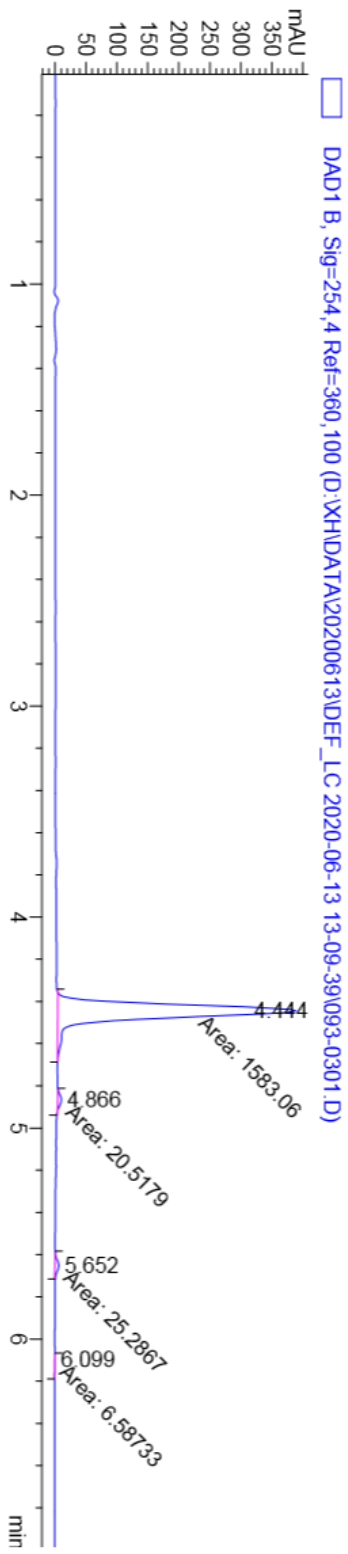
¹H NMR spectrum of **19f**



¹³C NMR spectrum of **19f**



HPLC spectrum of 19f



Signal 2: DAD1 B, Sig=254, 4 Ref=360, 100

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.444 | MM | 0.0684 | 1583.05725 | 385.95856 | 96.7965 |
| 2 | 4.866 | MM | 0.0591 | 20.51789 | 5.78970 | 1.2546 |
| 3 | 5.652 | MM | 0.0668 | 25.28674 | 6.31196 | 1.5462 |
| 4 | 6.099 | MM | 0.1068 | 6.58733 | 1.02797 | 0.4028 |