BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Design, synthesis and biological evaluation of 2,5-diaryloxazolo[4,5-*d*]pyrimidin-7-ylamines as selective cytotoxic agents against HeLa cells

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Analytical and spectral data of compounds 1–9

2,5-Diphenyl-*N*-(2-piperidin-1-ylpropyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (1)

Yield 80%. White solid, mp 161–163 °C. IR (KBr, cm^{-1}) ν_{max}: 3336-2936 (NH, Ar-CH), 1647, 1553, 1483, 1381, 1367, 771, 702. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, 2H, J_{HH} = 8.0 Hz, ArH), 8.31 (d, 2H, J_{HH} = 8.0 Hz, ArH), 7.60-7.56 (m, 3H, ArH), 7.47-7.45 (m, 3H, ArH), 6.35 (br s, 1H, NH), 4.08-3.88 (m, 1H, CH), 3.44 (br s, 1H, CH), 3.00 (br s, 1H, CH), 2.69 (br s, 2H, CH_2), 2.46 (br s, 2H, CH_2), 1.80-1.66 (m, 4H, $2CH_2$), 1.53 (br s, 2H, CH_2), 1.13 (d, 3H, J_{HH} = 8.0 Hz, CH_3). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.0, 161.3, 148.2, 138.3, 132.3, 130.7, 129.9, 129.0, 128.4, 128.2, 128.1, 128.0, 126.6, 58.5, 49.1, 26.6, 26.5, 24.8, 11.1. LC-MS: *m/z* (%) 414.2 (96.7) $[M+1]^+$. Anal. Calcd for $C_{25}H_{27}N_5O$: C, 72.61; H, 6.58; N, 16.94. Found: C, 72.53; H, 6.52; N, 16.76.

***N*-(2-Morpholin-4-ylpropyl)-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (2)**

Yield 80%. White solid, mp 186-188 °C. IR (KBr, cm^{-1}) ν_{max}: 3307-2971 (NH, Ar-CH), 2807, 1645, 1581, 1512, 1480, 1449, 1368, 1311, 1265, 1217, 1144, 1114, 1024, 966, 923, 872, 773, 703. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50-8.49 (m, 2H, ArH), 8.23-8.22 (m, 2H, ArH), 7.55-7.43 (m, 6H, ArH), 6.05 (br s, 1H, NH), 4.02-3.78 (m, 5H, ArH), 3.44 (t, 1H, J_{HH} = 8 Hz, CH), 2.95 (br s, 1H, CH), 2.70 (br s, 2H, CH_2), 2.54 (br s, 2H, CH_2), 1.13 (d, 3H, J_{HH} = 8.0 Hz, CH_3). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.0, 161.1, 148.0, 138.2, 132.5, 132.4, 130.0, 129.9, 129.0, 128.3, 128.2, 128.0, 126.4, 67.4, 58.3, 48.4, 42.8, 11.5. LC-MS: *m/z* (%) 416.2 (93.2) $[M+1]^+$. Anal. Calcd for $C_{24}H_{25}N_5O_2$: C, 69.38; H, 6.06; N, 16.86. Found: C, 69.30; H, 6.00; N, 16.99.

***N*-[2-(4-Ethylpiperazin-1-yl)propyl]-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (3)**

Yield 76%. White solid, mp 145–147 °C. IR (KBr, cm^{-1}) ν_{max}: 3381-2966 (NH, Ar-CH), 2811, 1642, 1502, 1369, 702. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, 2H, J_{HH} = 4 Hz, ArH), 8.29 (d, 2H, J_{HH} = 8 Hz, ArH), 7.59-7.53 (m, 3H, ArH), 7.46-7.45 (m, 3H, ArH), 6.12 (br s, 1H, NH), 3.93-3.87 (m, 1H, CH), 3.51-3.45 (m, 1H, CH), 3.04-3.01 (m, 1H, CH), 2.79 (br s, 2H, CH_2), 2.61 (br s, 5H, $2CH_2$, CH), 2.52-2.47 (m, 3H, CH_2, CH), 1.16-1.12 (m, 6H, $2CH_3$). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.1, 161.3, 148.2, 138.2, 132.4, 129.9, 129.1, 129.0, 128.4, 128.2, 128.1, 128.0, 126.6, 57.9, 53.3, 52.4, 11.9, 11.6. LC-MS: *m/z* (%) 443.2 (100) $[M+1]^+$. Anal. Calcd for $C_{28}H_{23}N_5O_2$: C, 72.87; H, 5.02; N, 15.17. Found: C, 72.76; H, 5.09; N, 15.41.

***N*-[2-(4-Chlorophenyl)-2-piperidin-1-ylethyl]-5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (4)**

Yield 79%. White solid, mp 198–200 °C. IR (KBr, cm^{-1}) ν_{max}: 3326-2928 (NH, Ar-CH), 1680, 1636, 1552, 1481, 1366, 1159, 1093, 777, 690. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, 2H,

J_{HH} = 8 Hz, ArH), 8.26 (d, 2H, J_{HH} = 8 Hz, ArH), 7.61-7.52 (m, 3H, ArH), 7.37 (d, 2H, J_{HH} = 8 Hz, ArH), 7.27-7.25 (m, 4H, ArH), 5.95 (br s, 1H, NH), 4.13-4.01 (m, 2H, CH_2), 3.84-3.80 (m, 1H, CH), 2.57-2.53 (m, 2H, CH_2), 2.41-2.40 (m, 5H, CH_3, CH_2), 1.69-1.61 (m, 4H, $2CH_2$), 1.44 (dd, 2H, J_{HH} = 12, 8 Hz, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7, 161.3, 145.6, 140.1, 135.4, 135.3, 133.6, 132.4, 130.0, 129.0, 128.9, 128.5, 128.3, 128.0, 126.5, 125.3, 36.9, 26.5, 23.8, 21.5, 17.5. LC-MS: *m/z* (%) 525.2 (95.8) $[M+1]^+$. Anal. Calcd for $C_{31}H_{30}ClN_5O$: C, 71.05; H, 5.77; Cl, 6.76; N, 13.36. Found: C, 71.13; H, 5.80; Cl, 6.87; N, 13.56.

***N*-[2-(4-Chlorophenyl)-2-morpholin-4-ylethyl]-5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (5)**

Yield 76%. White solid, mp 225–227 °C. IR (KBr, cm^{-1}) ν_{max}: 3301-2821 (NH, Ar-CH), 1641, 1552, 1480, 1368, 1110. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, 2H, J_{HH} = 8 Hz, ArH), 8.21 (d, 2H, J_{HH} = 8 Hz, ArH), 7.57 (t, 1H, J_{HH} = 8 Hz, ArH), 7.52 (t, 2H, J_{HH} = 8 Hz, ArH), 7.37 (d, 2H, J_{HH} = 4 Hz, ArH), 7.28-7.23 (m, 4H, ArH), 5.60 (1H, NH), 4.24-4.19 (m, 1H, CH), 4.09-3.77 (m, 6H, CH, $2CH_2$), 2.57-2.54 (m, 4H, $2CH_2$), 2.40 (s, 3H, CH_3). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.2, 161.3, 147.8, 140.2, 135.3, 132.4, 130.0, 129.0, 128.8, 128.3, 128.1, 126.4, 68.2, 67.2, 50.5, 37.1, 21.4. LC-MS: *m/z* (%) 526.2 (95.6) $[M+1]^+$. Anal. Calcd for $C_{30}H_{28}ClN_5O_2$: C, 68.50; H, 5.37; Cl, 6.74; N, 13.31. Found: C, 68.45; H, 5.31; Cl, 6.89; N, 13.44.

11-(2,5-Diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (6)

Yield 75%. White solid, mp 225–227 °C. IR (KBr, cm^{-1}) ν_{max}: 3057, 2847, 1654, 1613, 1603 (C=O), 1545, 1475, 1373, 1067, 771, 698. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42-8.40 (m, 2H, ArH), 8.21 (d, 2H, J_{HH} = 8 Hz, ArH), 7.61-7.52 (m, 3H, ArH), 7.44-7.43 (m, 3H, ArH), 7.14 (t, J_{HH} = 8 Hz, 1H, ArH), 6.27 (t, J_{HH} = 8 Hz, 1H, ArH), 6.16 (t, J_{HH} = 8 Hz, 1H, ArH), 5.03 (dd, J_{HH} = 28, 12 Hz, 2H, CH_2), 4.21 (d, 1H, J_{HH} = 16 Hz, CH), 3.97 (dd, J_{HH} = 16, 8 Hz, 1H, CH), 3.46 (d, 2H, J_{HH} = 12 Hz, CH_2), 3.27 (br s, 1H, CH), 2.73 (br s, 1H, CH), 2.17 (br s, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 163.3, 162.5, 160.4, 148.6, 148.2, 138.6, 137.8, 132.6, 130.0, 129.1, 128.3, 128.2, 128.2, 128.0, 127.8, 126.1, 117.6, 105.3, 49.1, 34.9, 27.8, 26.4. LC-MS: *m/z* (%) 462.2 (97.2) $[M+1]^+$. Anal. Calcd for $C_{26}H_{30}N_6O$: C, 70.50; H, 6.75; N, 18.76. Found: C, 70.56; H, 6.83; N, 18.99.

11-[5-(4-Methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (7)

Yield 71%. White solid, mp 263–265 °C. IR (KBr, cm^{-1}) ν_{max}: 3057, 2946, 1817, 1652, 1601 (C=O), 1572, 1547, 1449, 1371, 1144, 810, 777, 712, 689. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, 2H, J_{HH} = 8 Hz, ArH), 8.19 (d, 2H, J_{HH} = 8 Hz, ArH), 7.59-7.50 (m, 3H, ArH), 7.23 (d, 2H, J_{HH} = 8 Hz, ArH), 7.13 (t, 1H, J_{HH} = 8 Hz, ArH), 6.26 (d, 2H, J_{HH} = 8 Hz, ArH), 6.15 (d, 2H,

J_{HH} = 8 Hz, ArH), 5.00 (q, 2H, J_{HH} = 12 Hz, CH_2), 4.19 (d, 2H, J_{HH} = 16 Hz, CH), 3.96 (dd, 1H, J_{HH} = 16, 8 Hz, CH), 3.43 (d, 2H, J_{HH} = 8 Hz, CH_2), 3.26 (br s, 1H, CH), 2.72 (br s, 1H, CH), 2.40 (s, 3H, CH_3), 2.15 (br s, 1H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 163.3, 162.4, 148.7, 148.1, 140.1, 138.6, 135.2, 132.5, 129.0, 128.9, 128.3, 127.9, 127.7, 126.1, 117.6, 105.3, 51.5, 49.1, 34.8, 27.8, 26.3, 21.5. LC-MS: *m/z* (%) 476.2 (100) $[M+1]^+$. Anal. Calcd for $C_{29}H_{25}N_5O_2$: C, 73.25; H, 5.30; N, 14.73. Found: C, 73.31; H, 5.38; N, 14.89.

11-[2,5-Bis(4-methylphenyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**8)**

Yield 70%. White solid, mp > 250 °C. IR (KBr, cm^{-1}) ν_{max}: 2921, 2242, 1610 (C=O), 1552, 1494, 1470, 1414, 1319, 1277, 1125, 1088, 1010, 822, 736. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, 2H, J_{HH} = 10 Hz, ArH), 8.07 (d, 2H, J_{HH} = 10 Hz, ArH), 7.41 (d, 2H, J_{HH} = 10 Hz, ArH), 7.31 (d, 2H, J_{HH} = 10 Hz, ArH), 7.13 (t, 1H, J_{HH} = 10 Hz, ArH), 6.27 (d, 1H, J_{HH} = 10 Hz, ArH), 6.16 (d, 1H, J_{HH} = 5 Hz, ArH), 5.02 (dd, J_{HH} = 35, 10 Hz, 2H, CH_2), 4.21 (d, J_{HH} = 15 Hz, 1H, CH), 3.97 (dd, J_{HH} = 15, 10 Hz, 1H, CH), 3.44 (d, J_{HH} = 10 Hz, 2H, CH_2), 3.27 (s, 1H, CH), 2.73 (s, 1H, CH), 2.47 (s, 3H, CH_3), 2.44 (s, 3H, CH_3), 2.16 (s, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2, 163.2, 148.7, 143.4, 138.6, 131.1, 130.0, 130.0, 129.8, 129.0, 128.6, 128.6, 128.3, 128.1, 127.9, 127.6, 123.2, 117.5, 49.1, 38.0, 34.8, 27.8, 26.3, 21.9. LC-MS: *m/z* (%) 490.2 (95.9) $[M+1]^+$. Anal. Calcd for $C_{30}H_{27}N_5O_2$: C, 73.60; H, 5.56; N, 14.30. Found: C, 73.67; H, 5.65; N, 14.57.

6-[(2,5-Diphenyl[1,3]oxazolo[4,5-*d*]pyrimidin-amino-7-yl)]-*N*-methyl-(2R,3R,4S,5S)-hexane-1,2,3,4,5-pentaol (9)

Yield 65%. White solid, mp 210–212 °C. IR (KBr, cm^{-1}) ν_{max}: 3396 (OH), 1631, 1550, 1389, 1110, 1092, 1071, 1022, 769, 703. ^{1}H NMR (500 MHz, $CF_3C(O)OD$) δ 7.58-7.50 (m, 4H, ArH), 7.13-7.04 (m, 2H, ArH), 7.00-6.96 (m, 4H, ArH), 4.35-4.00 (m, 3H, CH_2, CH), 3.85-3.80 (m, 1H, CH), 3.76-3.72 (m, 1H, CH), 3.64-3.37 (m, 3H, CH_2, CH), 3.26, 3.05 (s, 3H, CH_3). ^{13}C NMR (126 MHz, $CF_3C(O)OD$) δ 169.3, 154.2, 1495, 135.0, 134.0, 128.9, 128.7, 127.8, 127.7, 127.1, 126.8, 126.8, 121.3, 71.5, 70.8, 68.6, 66.8, 53.5, 52.5, 37.8. LC-MS: *m/z* (I_{rel}, %): 467.2 $[M+H]^+$ (100). Found, %: C 61.65; H 5.60; N 12.45. $C_{24}H_{26}N_4O_6$. Calculated, %: C 61.79; H 5.62; N 12.01.

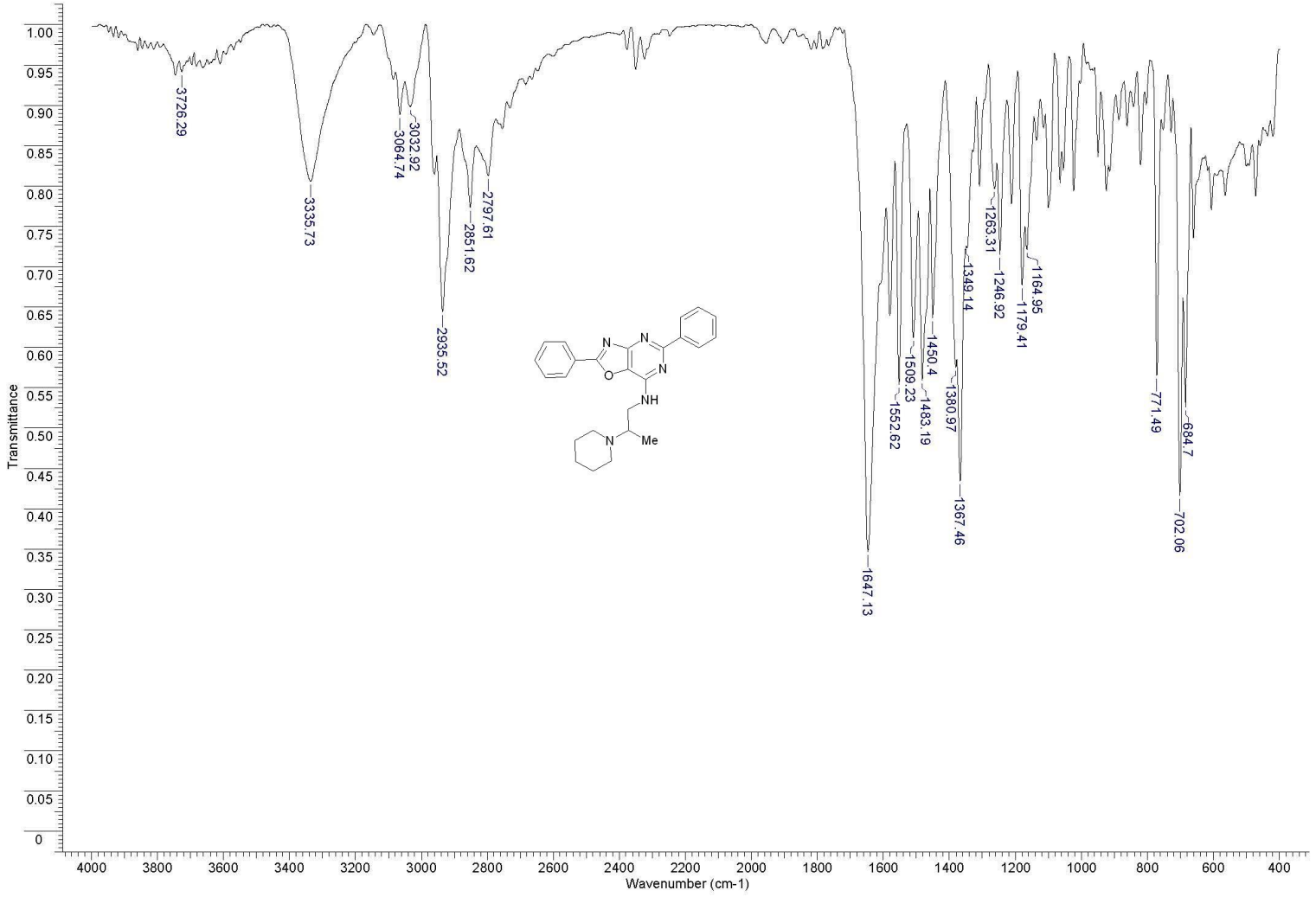


Figure S1. IR spectrum of 2,5-diphenyl-*N*-(2-piperidin-1-ylpropyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**1**)

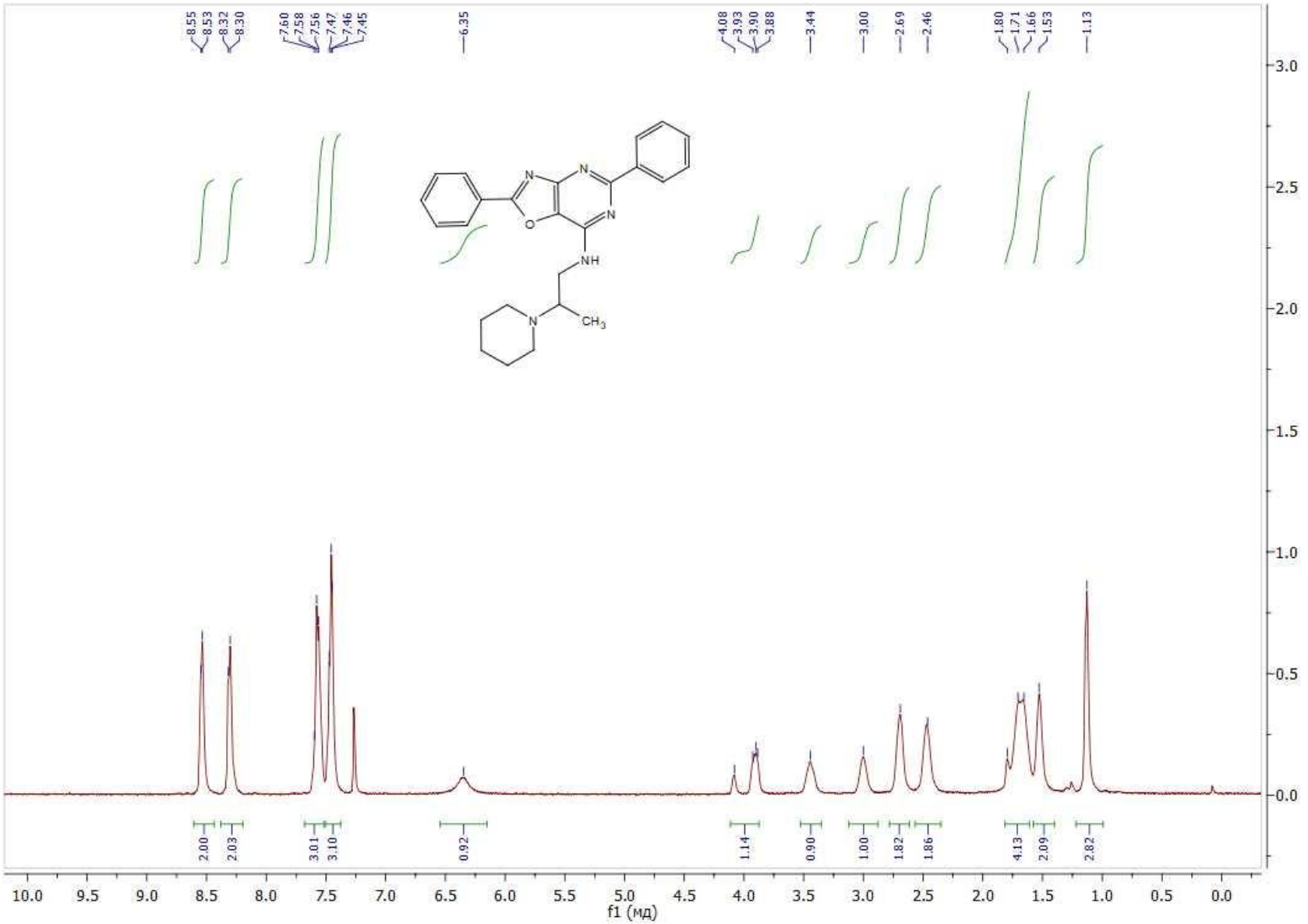


Figure S2. ^{1}H NMR spectrum of 2,5-diphenyl-*N*-(2-piperidin-1-ylpropyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**1**)

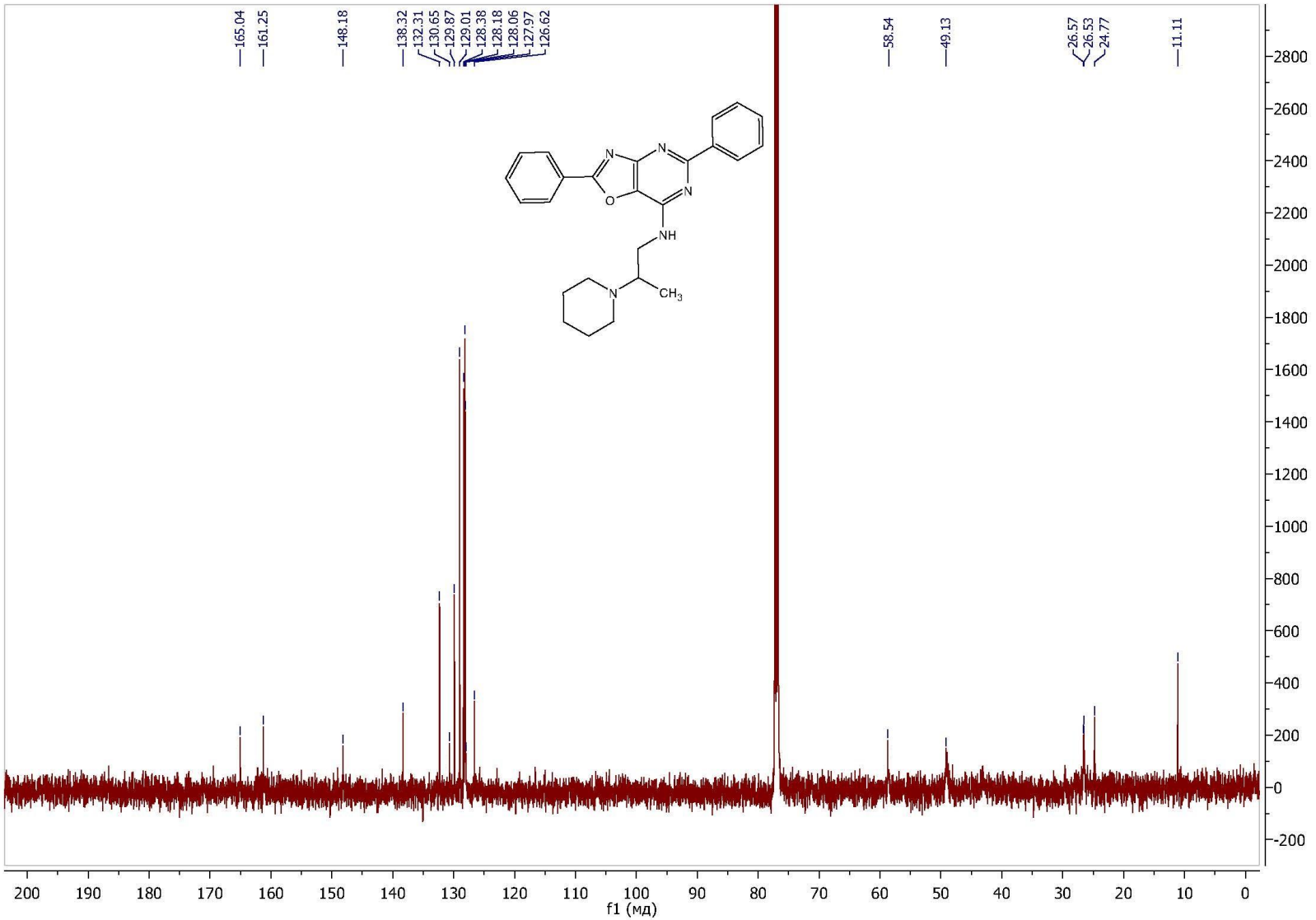
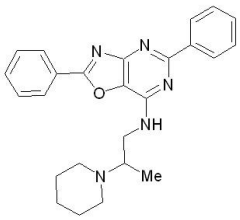


Figure S3. ^{13}C NMR spectrum of 2,5-diphenyl-*N*-(2-piperidin-1-ylpropyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**1**)



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2	1.249	3.3%	---	---	---	---	---	---	---	---	
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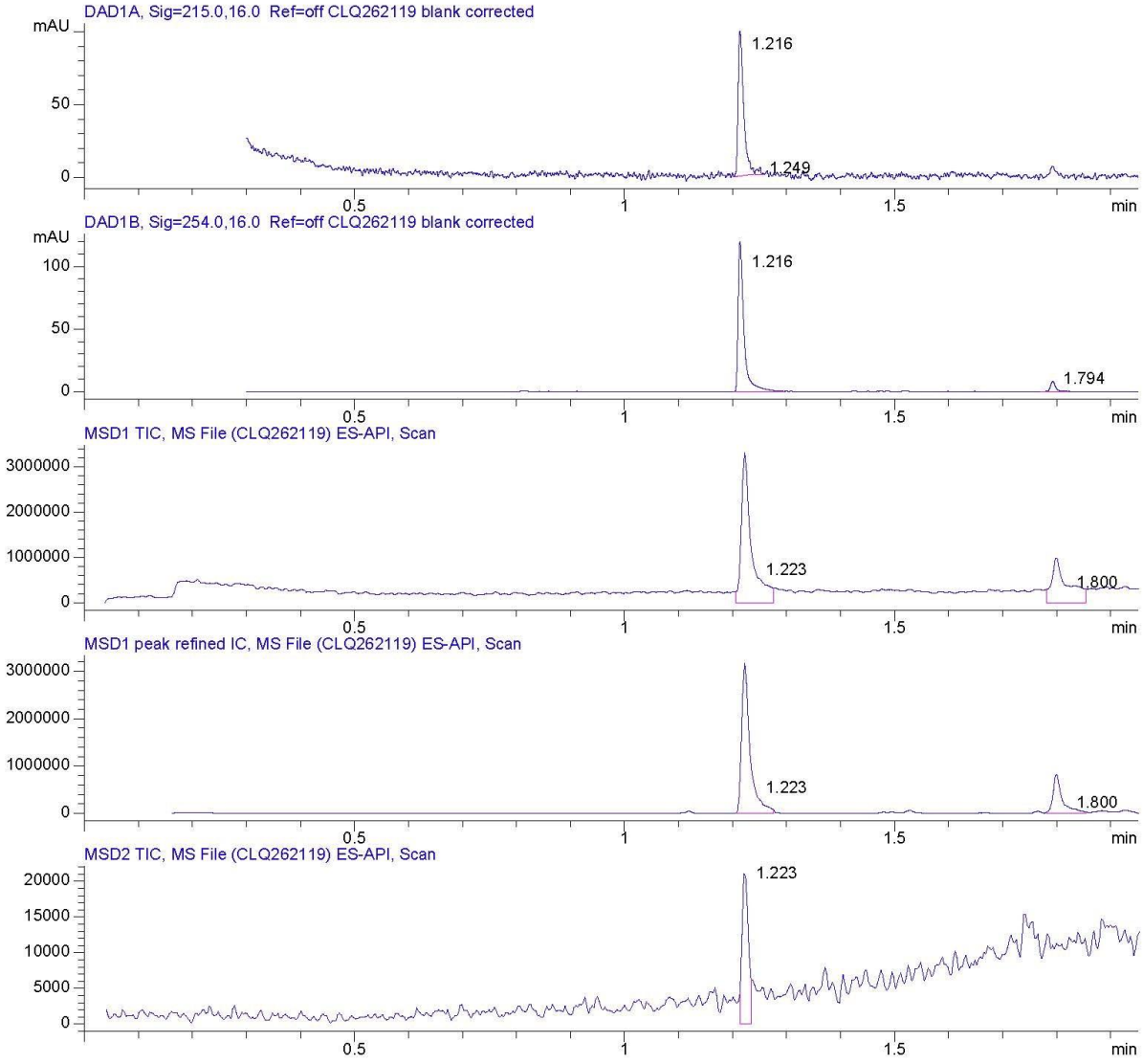


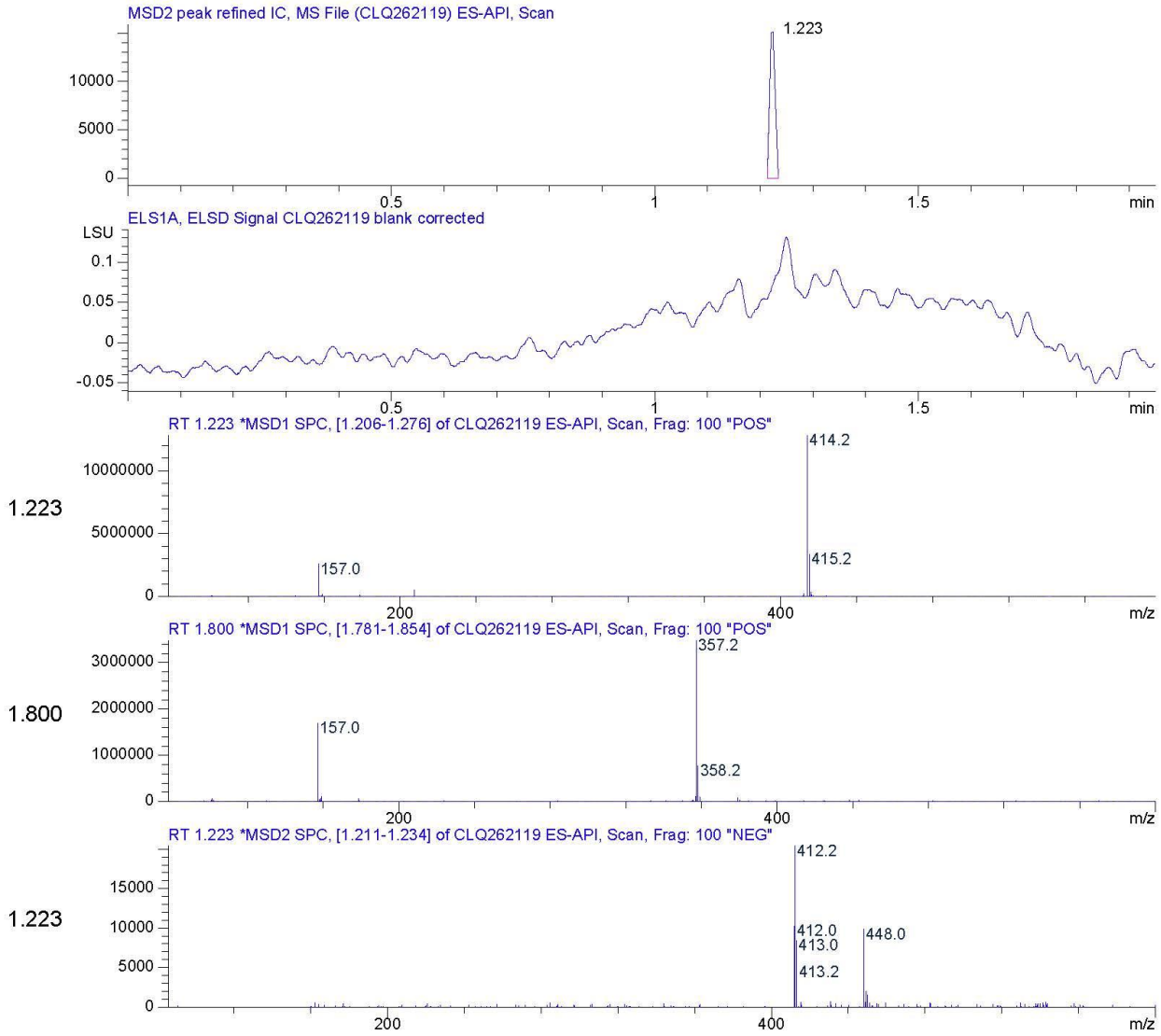


Figure S4. LC–MS spectrum of 2,5-diphenyl-*N*-(2-piperidin-1-ylpropyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**1**)

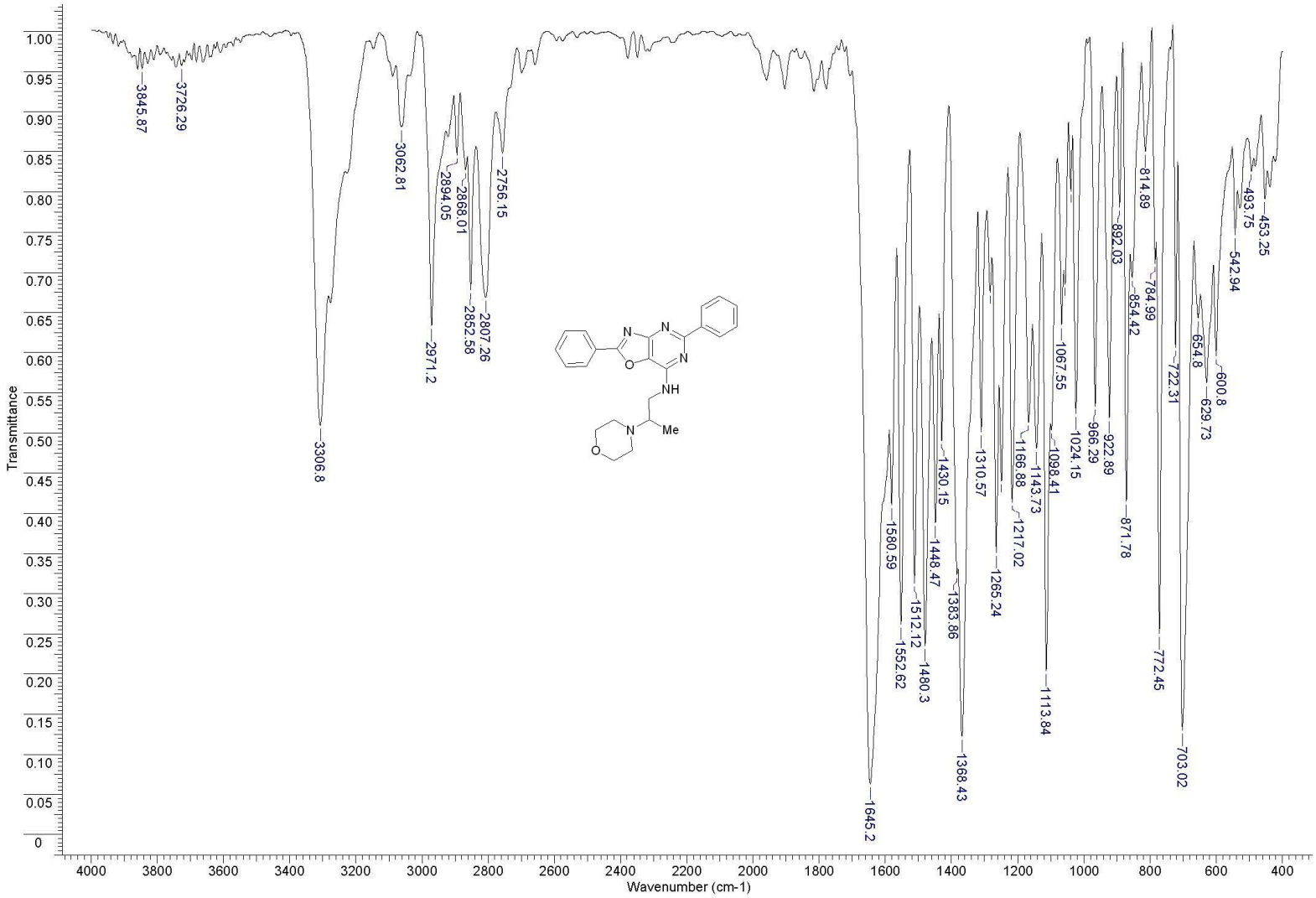


Figure S5. IR spectrum of *N*-(2-morpholin-4-ylpropyl)-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**2**)

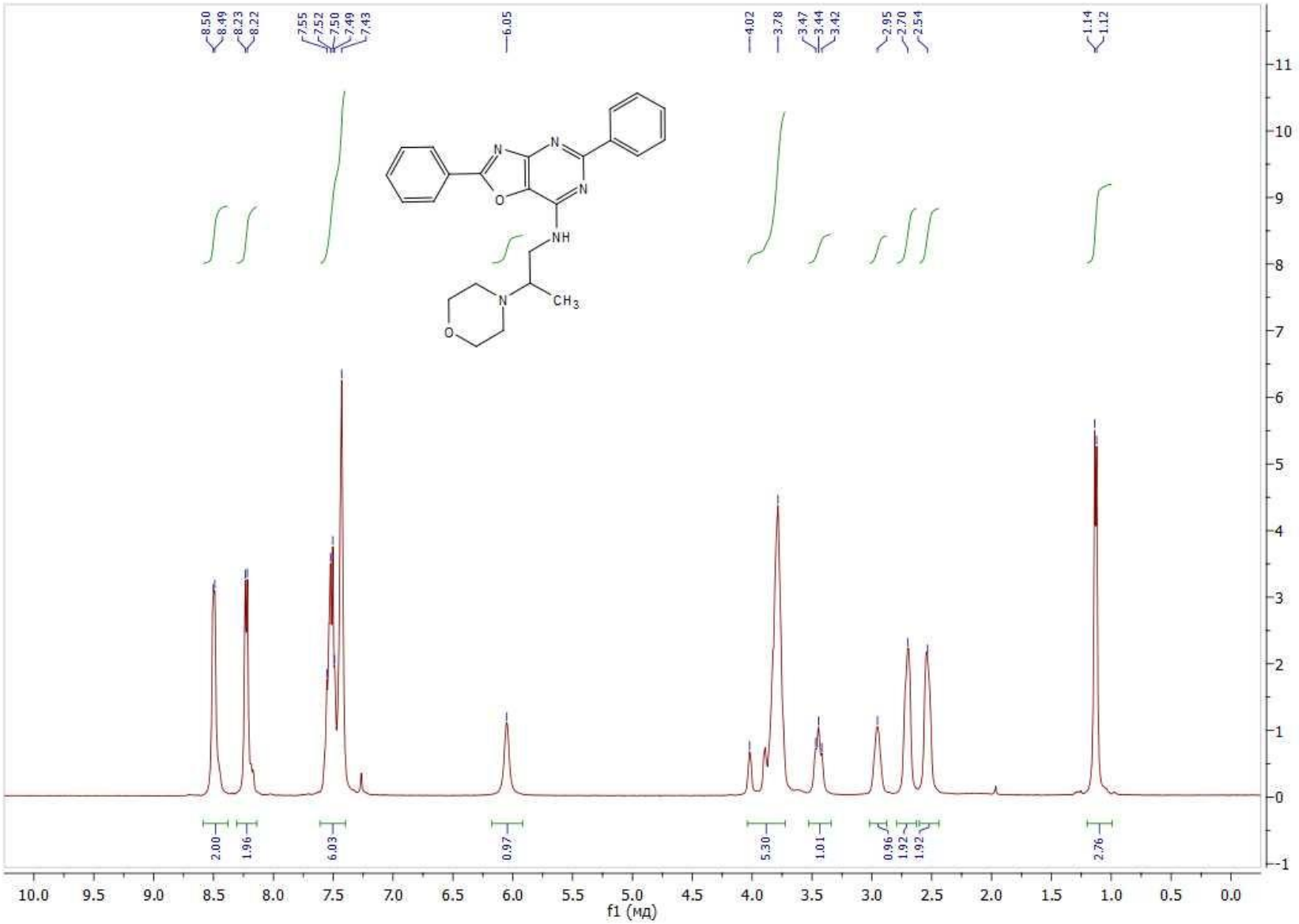


Figure S6. [1]H NMR spectrum of *N*-(2-morpholin-4-ylpropyl)-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**2**)

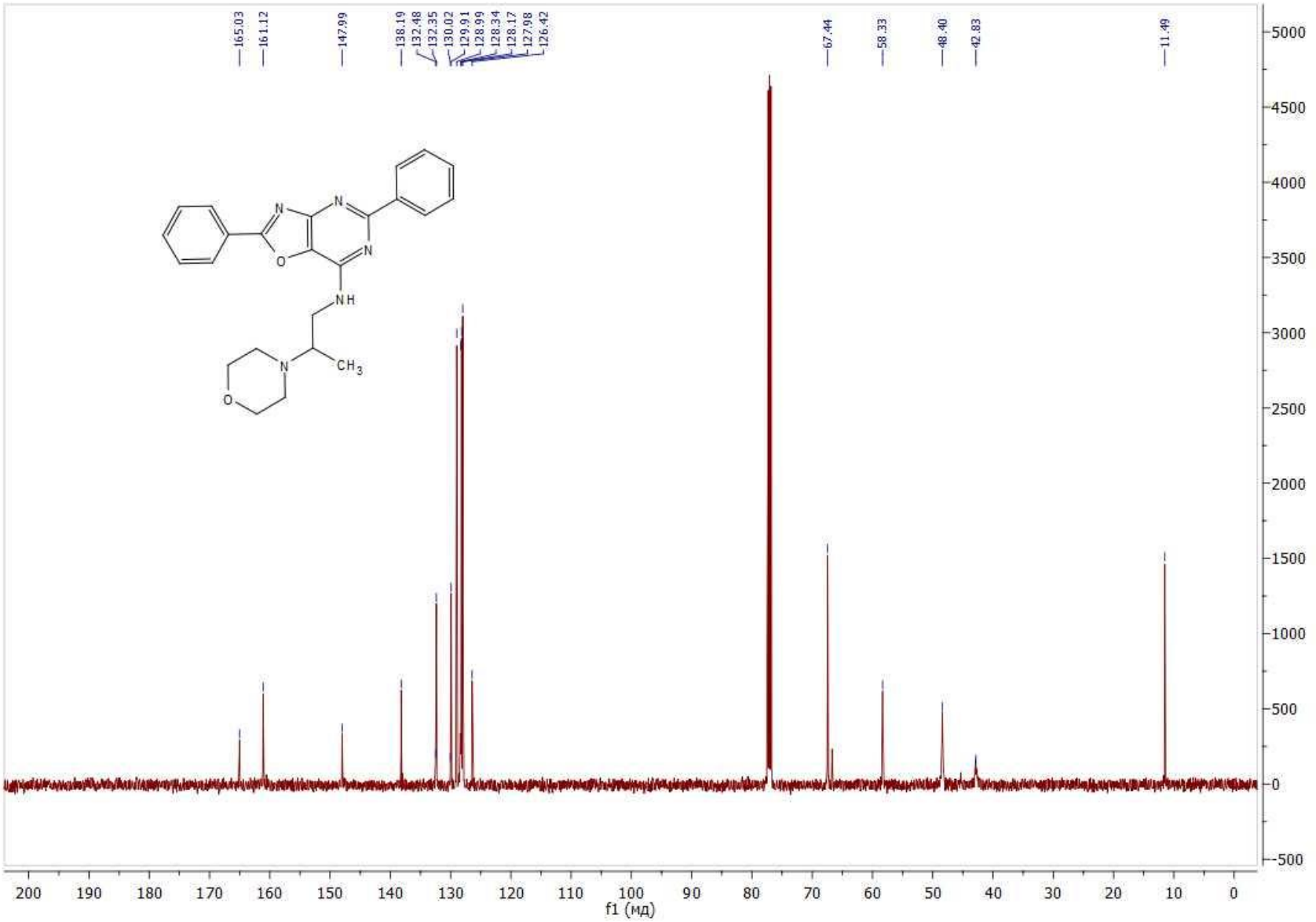
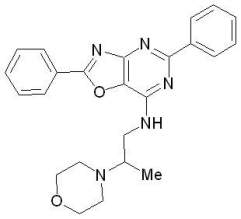


Figure S7. ^{13}C NMR spectrum of *N*-(2-morpholin-4-ylpropyl)-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**2**)



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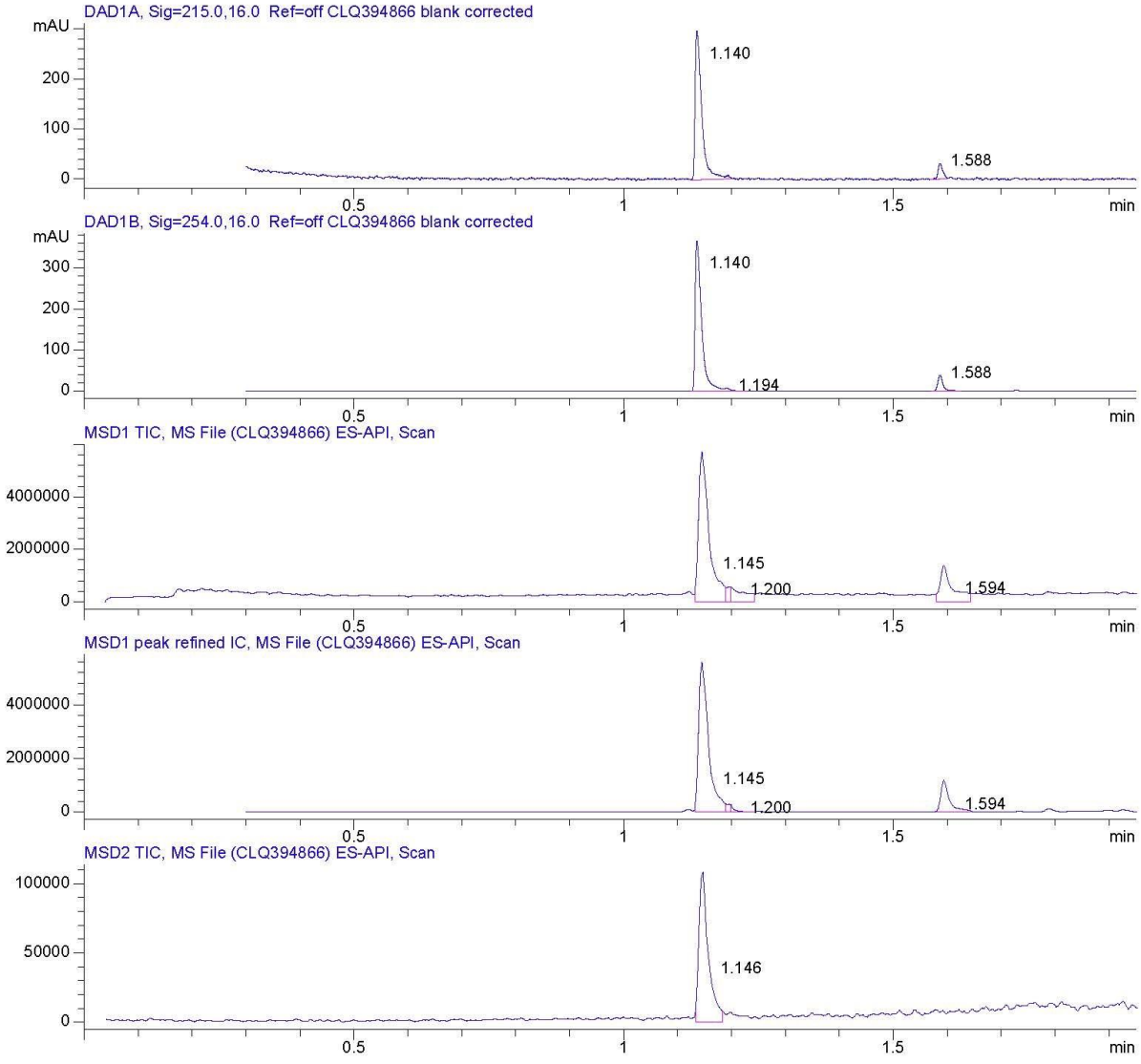
1	1.140	93.2%	90.5%	83.5%	100.0%	100.0%	416.2(98),208.6(2)	1.145	414.2(50),450.2(50)	1.146	
2	1.194	---	1.8%	1.7%	---	---	430.2(100)	1.200	---	---	
3	1.588	6.8%	7.7%	14.9%	---	---	359.2(100)	1.594	---	---	



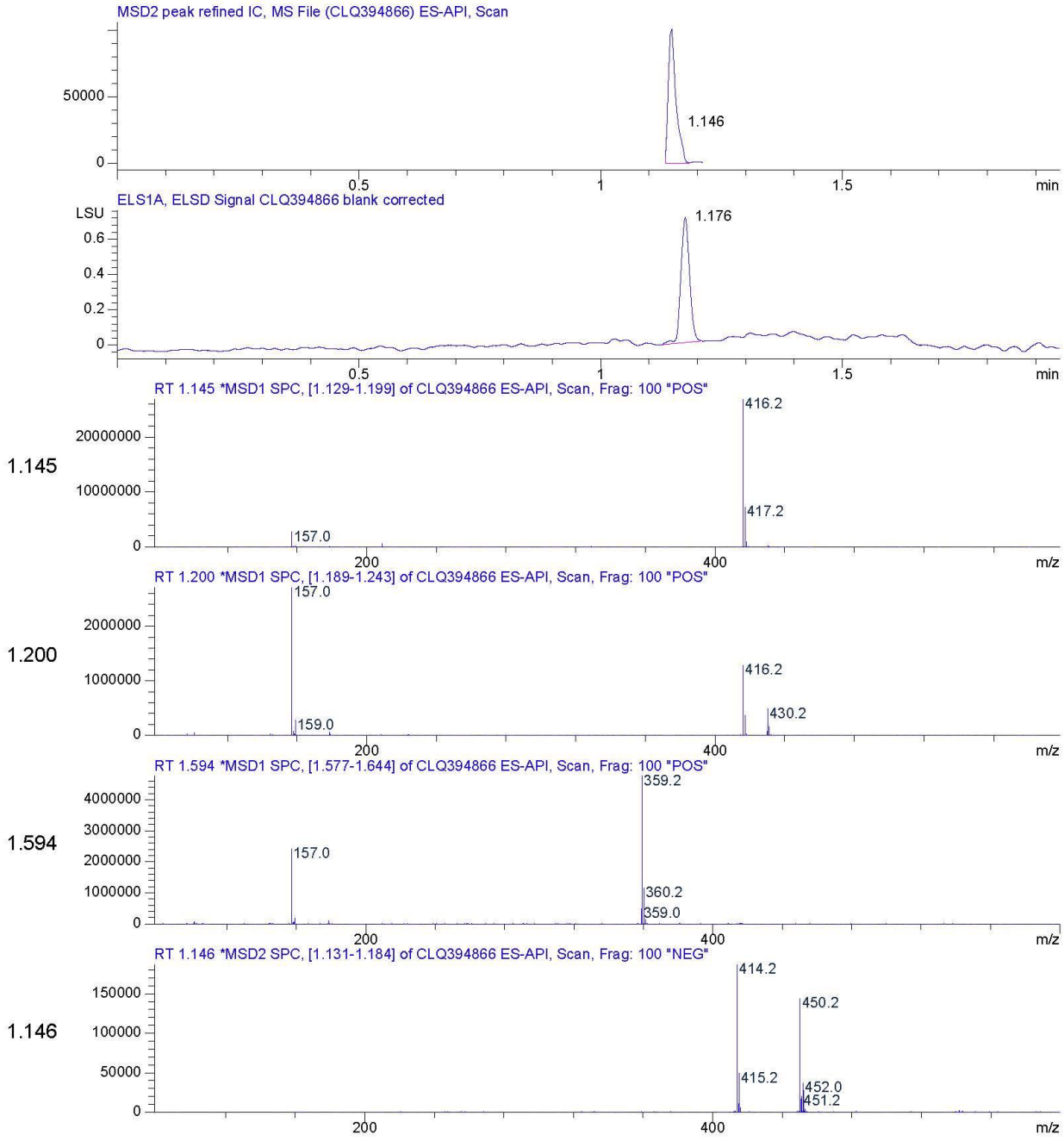


Figure S8. LC–MS spectrum of *N*-(2-morpholin-4-ylpropyl)-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**2**)

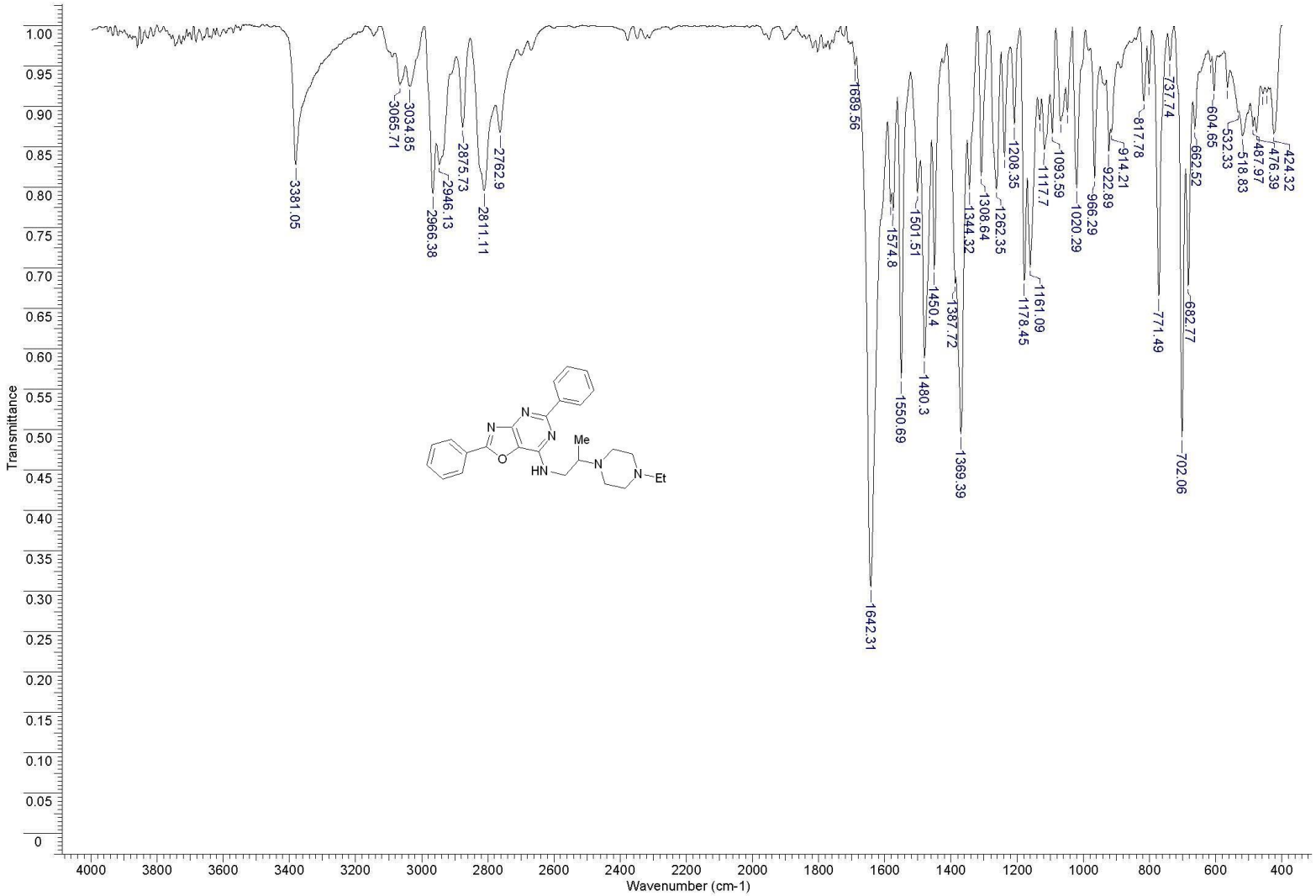


Figure S9. IR spectrum of *N*-[2-(4-ethylpiperazin-1-yl)propyl]-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**3**)

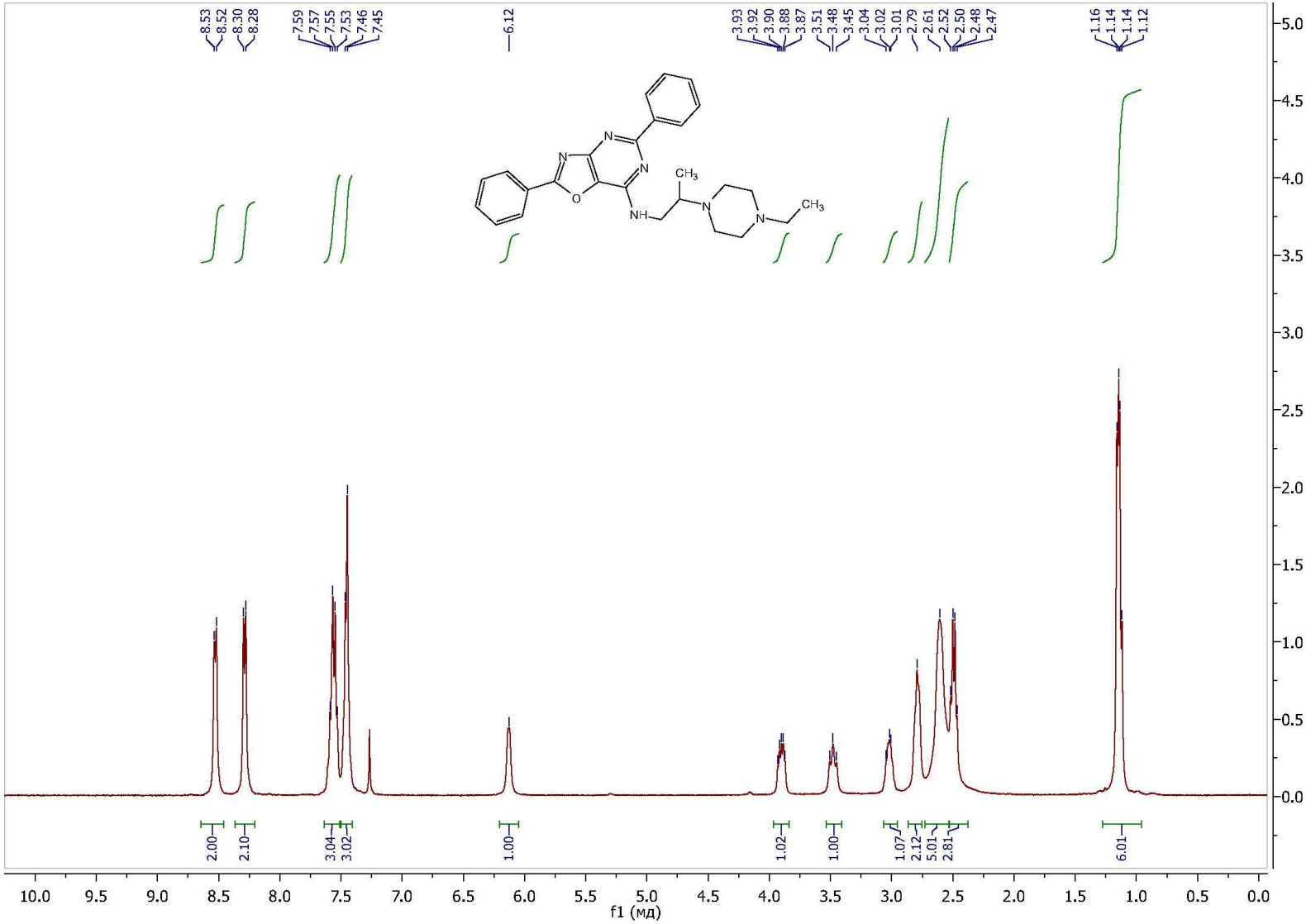


Figure S10. ^{1}H NMR spectrum of *N*-[2-(4-ethylpiperazin-1-yl)propyl]-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**3**)

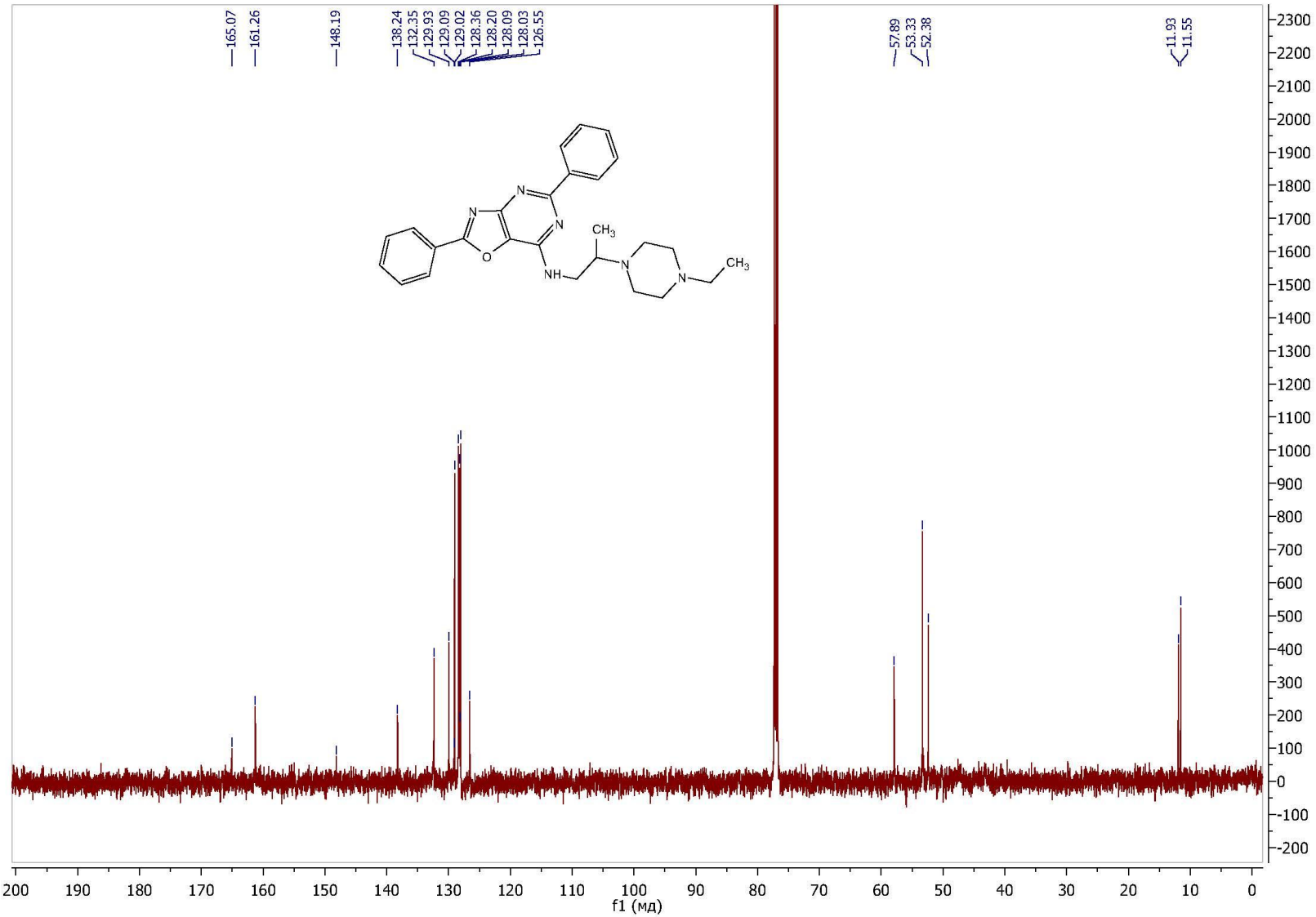
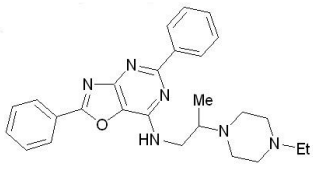


Figure S11. ^{13}C NMR spectrum of *N*-[2-(4-ethylpiperazin-1-yl)propyl]-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**3**)



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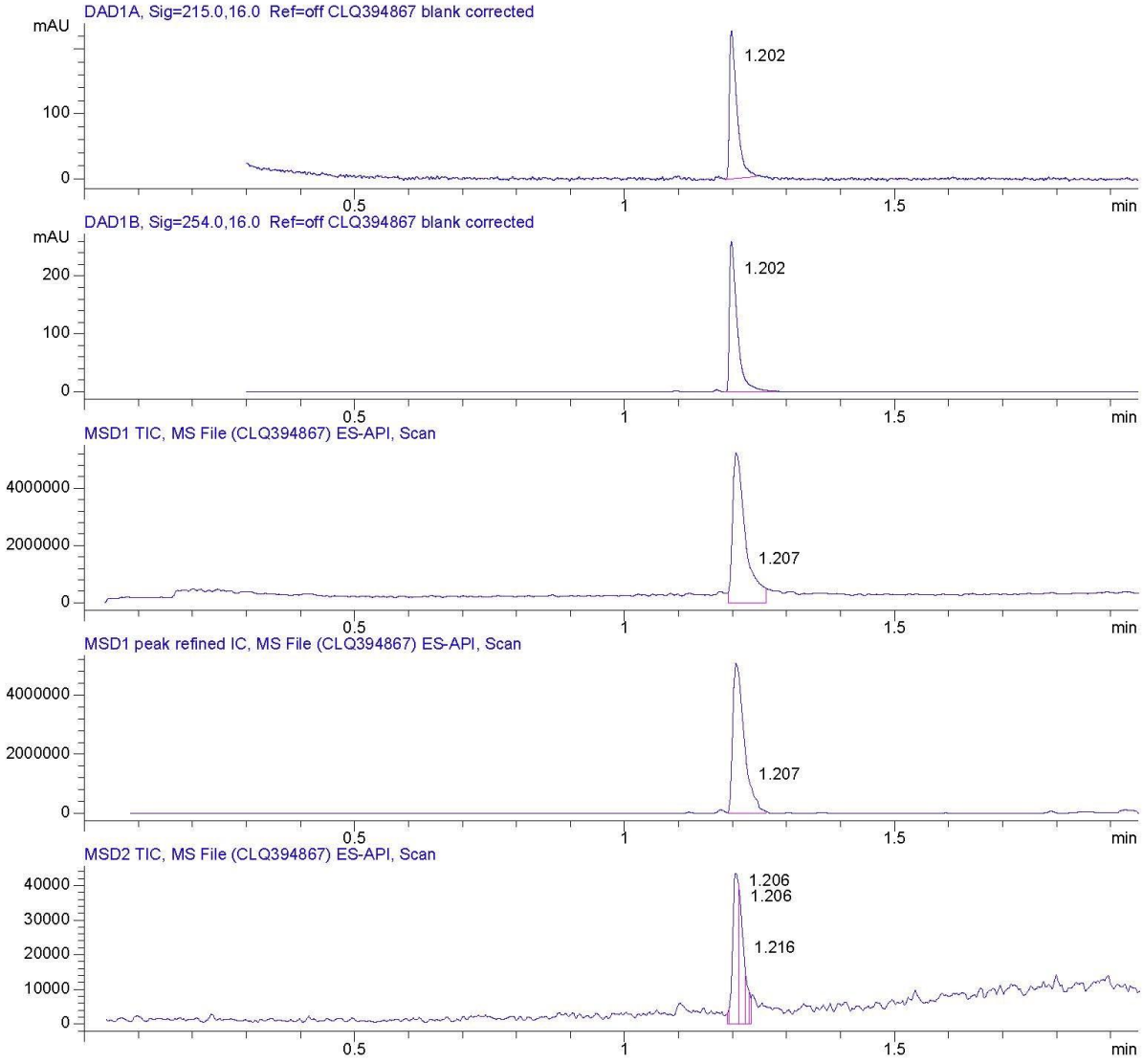
2	1.202	100.0%	100.0%	100.0%	71.8%	100.0%	443.2(66),222.2(34)	1.207	441.2(87),479.0(13)	1.206	
3	1.210	---	---	---	10.5%	---	---	---	442.2(56),478.0(44)	1.216	



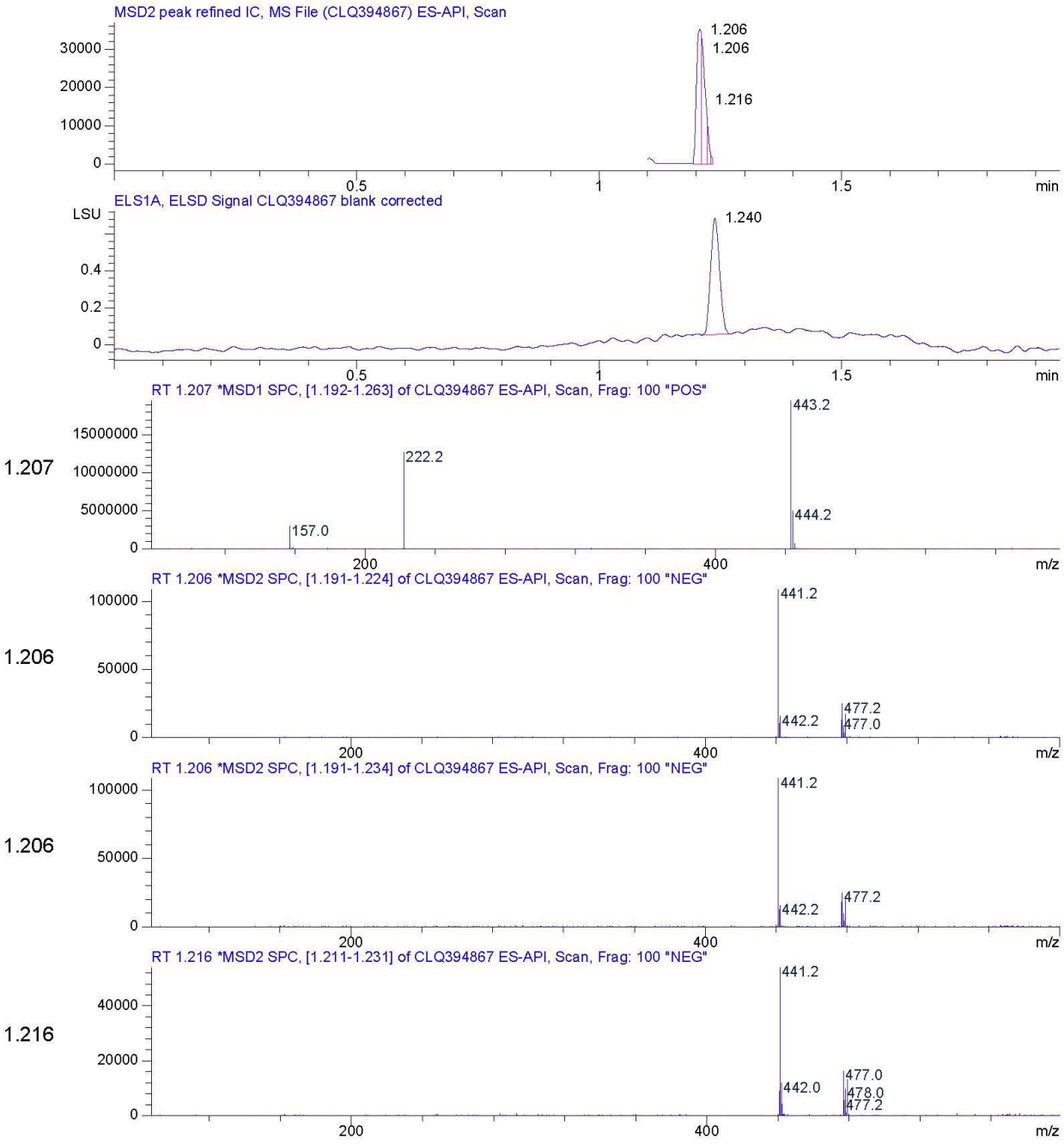


Figure S12. LC–MS spectrum of *N*-[2-(4-ethylpiperazin-1-yl)propyl]-2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**3**)

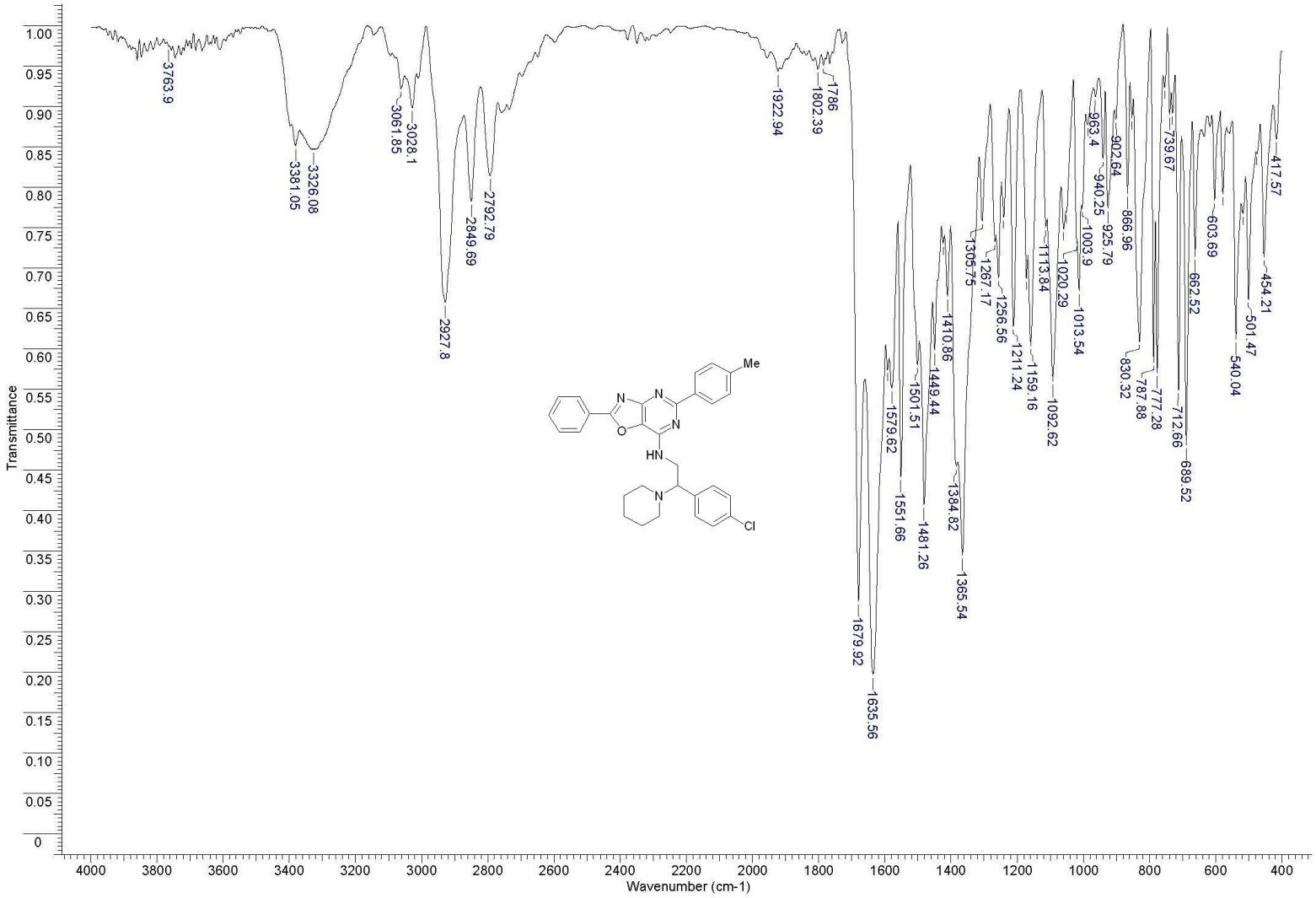


Figure S13. IR spectrum of *N*-[2-(4-chlorophenyl)-2-piperidin-1-ylethyl]-5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**4**)

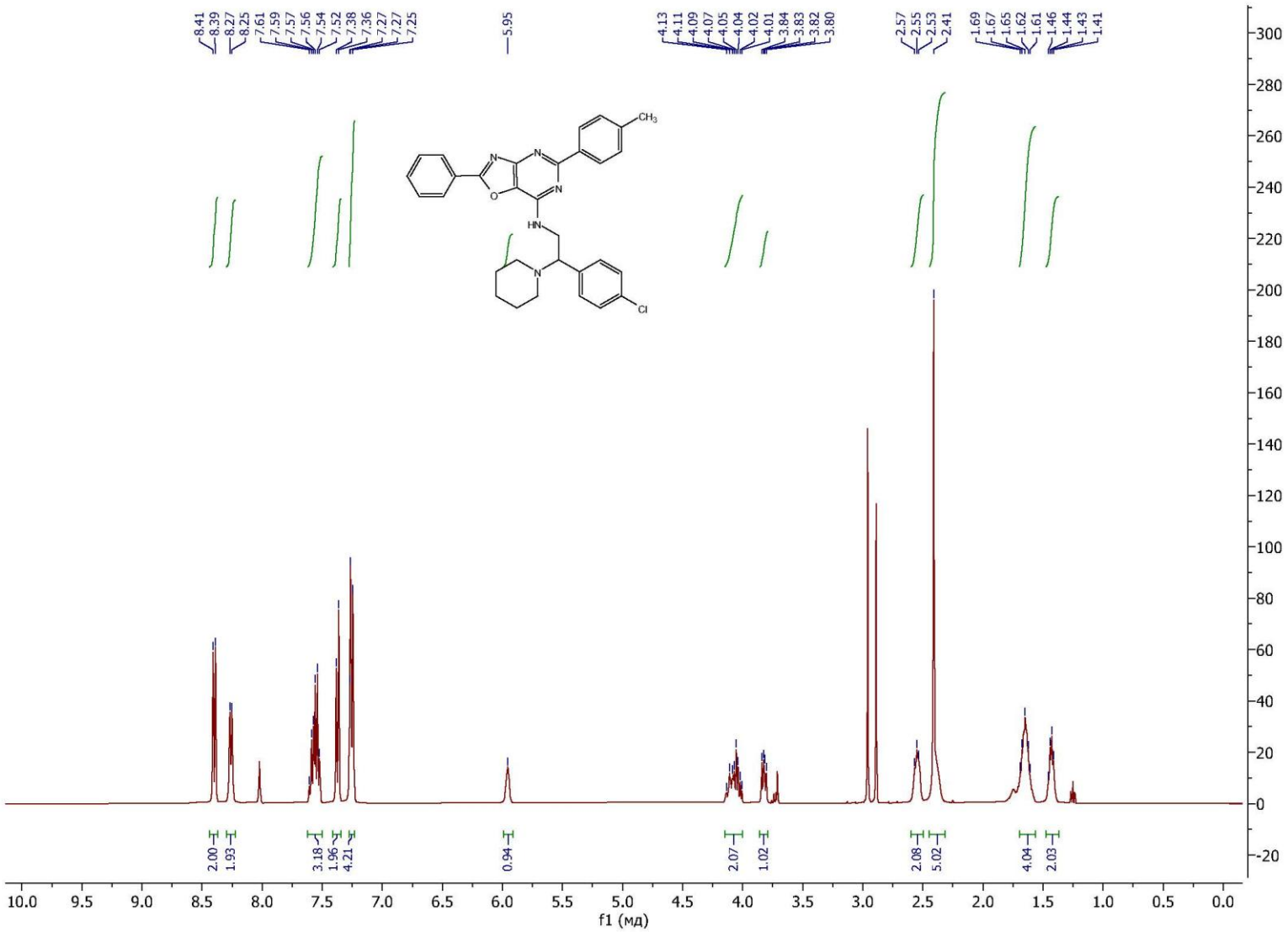


Figure S14. ^{1}H NMR spectrum of *N*-[2-(4-chlorophenyl)-2-piperidin-1-ylethyl]-5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**4**)

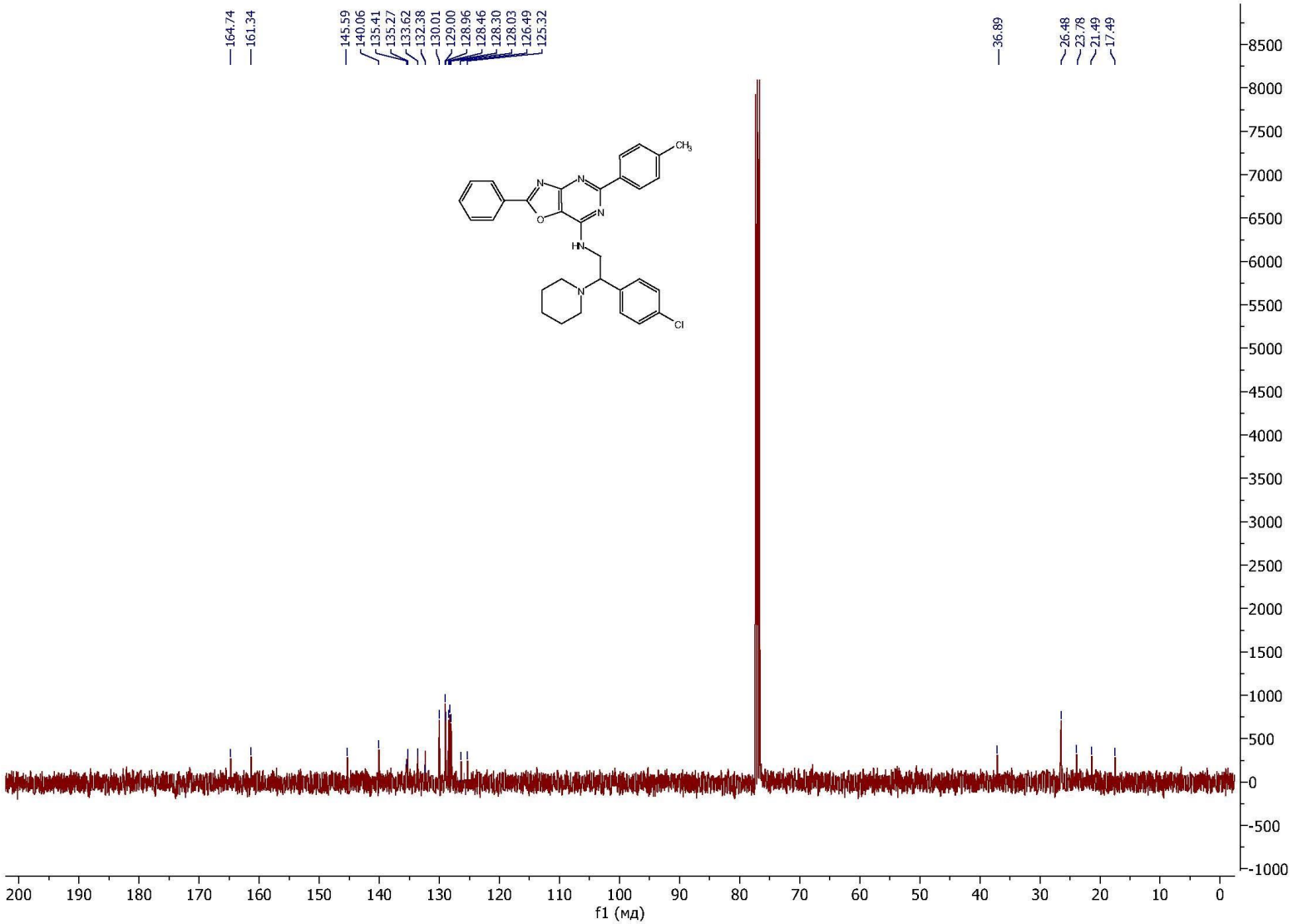
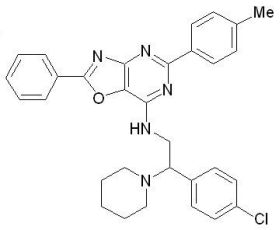


Figure S15. ^{13}C NMR spectrum of *N*-[2-(4-chlorophenyl)-2-piperidin-1-ylethyl]-5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**4**)



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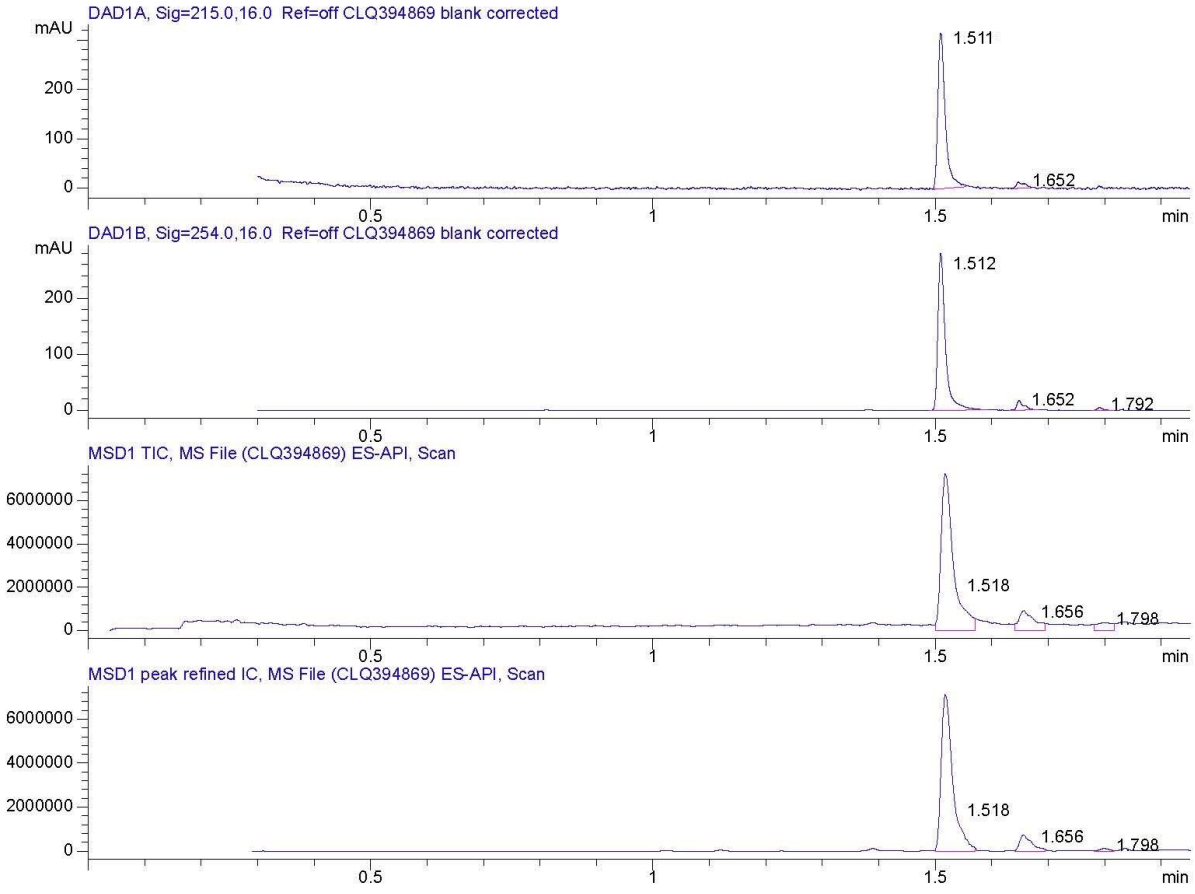
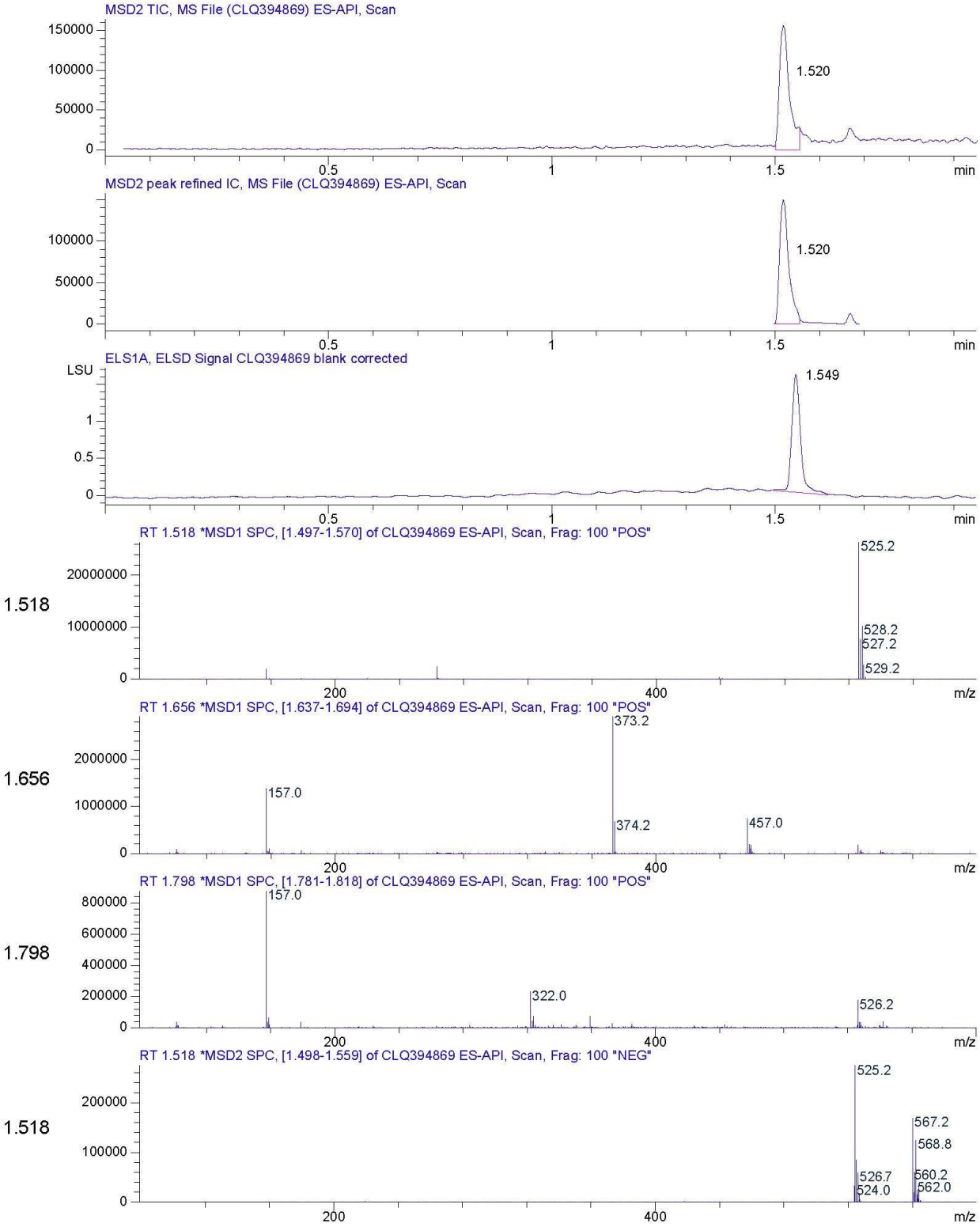
2	1.514	---	---	---	58.1%	---	---	---	524.2(100)	1.520	
3	1.652	4.4%	5.4%	7.2%	---	---	373.2(100)	1.656	---	---	
4	1.792	---	1.1%	0.7%	---	---	322.0(100)	1.798	---	---	

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ELS1A, ELSD Signal CLQ394869 blank corrected
1.549
min
LSU
1.518
RT 1.518 *MSD1 SPC, [1.497-1.570] of CLQ394869 ES-API, Scan, Frag: 100 "POS"
525.2
528.2
527.2
529.2
1.656
RT 1.656 *MSD1 SPC, [1.637-1.694] of CLQ394869 ES-API, Scan, Frag: 100 "POS"
373.2
157.0
374.2
457.0
1.798
RT 1.798 *MSD1 SPC, [1.781-1.818] of CLQ394869 ES-API, Scan, Frag: 100 "POS"
157.0
322.0
526.2
1.518
RT 1.518 *MSD2 SPC, [1.498-1.559] of CLQ394869 ES-API, Scan, Frag: 100 "NEG"
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567.2
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524.0
560.2
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m/z

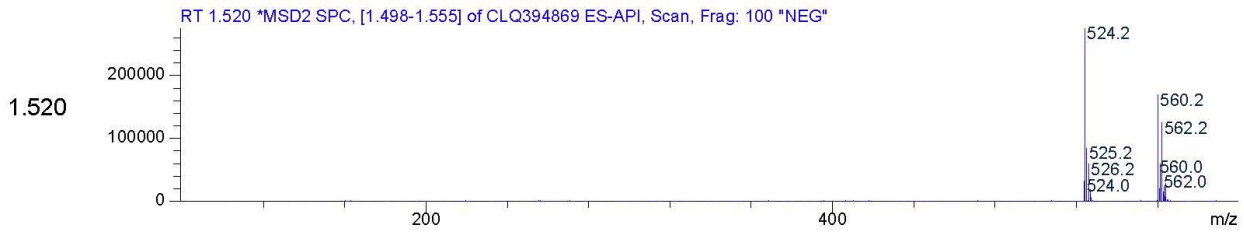


Figure S16. LC–MS spectrum of *N*-[2-(4-chlorophenyl)-2-piperidin-1-ylethyl]-5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**4**)

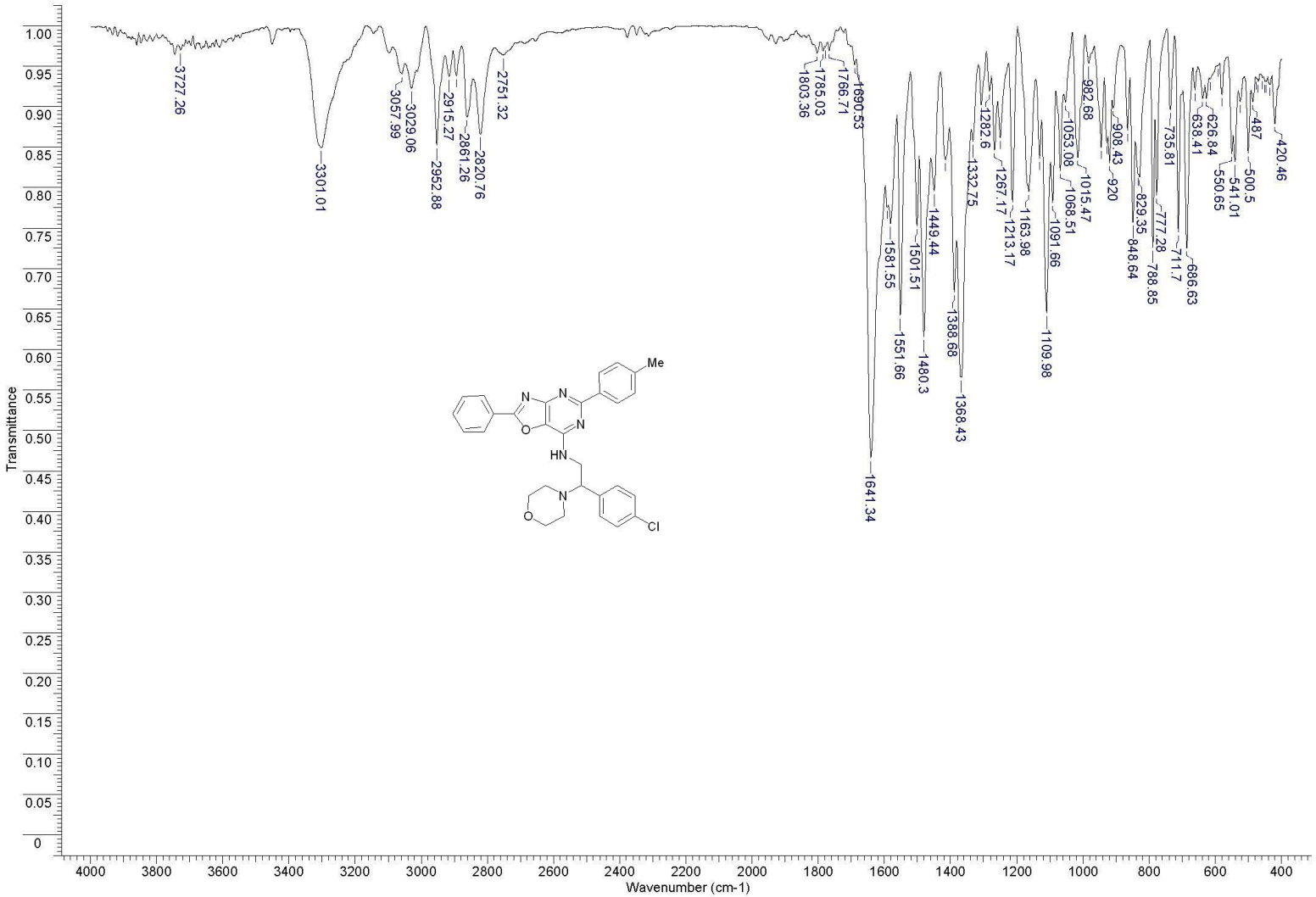


Figure S17. IR spectrum of *N*-[2-(4-chlorophenyl)-2-morpholin-4-ylethyl]-5-(4-methylphenyl)-2-phenyl[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**5**)

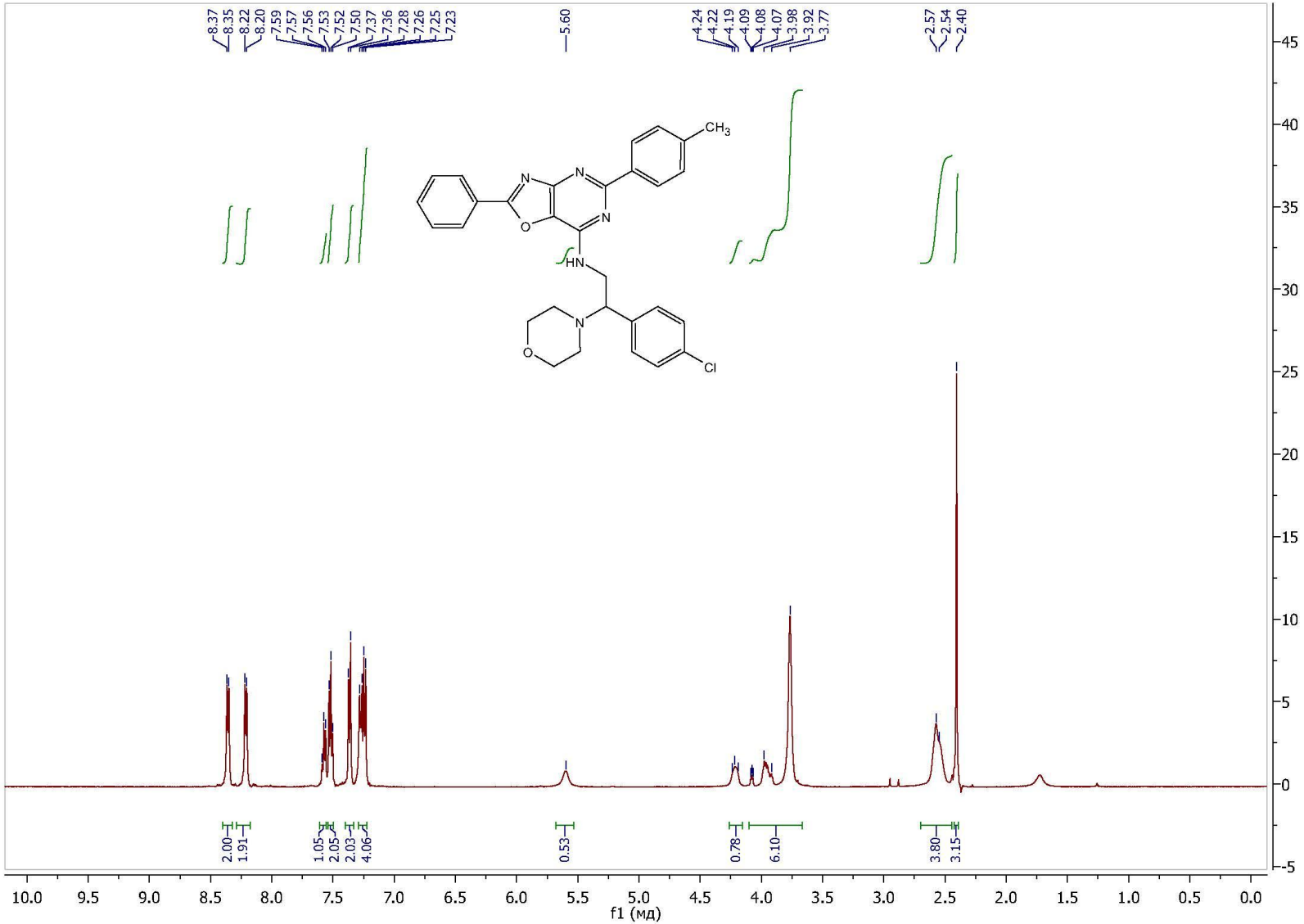


Figure S18. ^{1}H NMR spectrum of *N*-[2-(4-chlorophenyl)-2-morpholin-4-ylethyl]-5-(4-methylphenyl)-2-phenyl[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**5**)

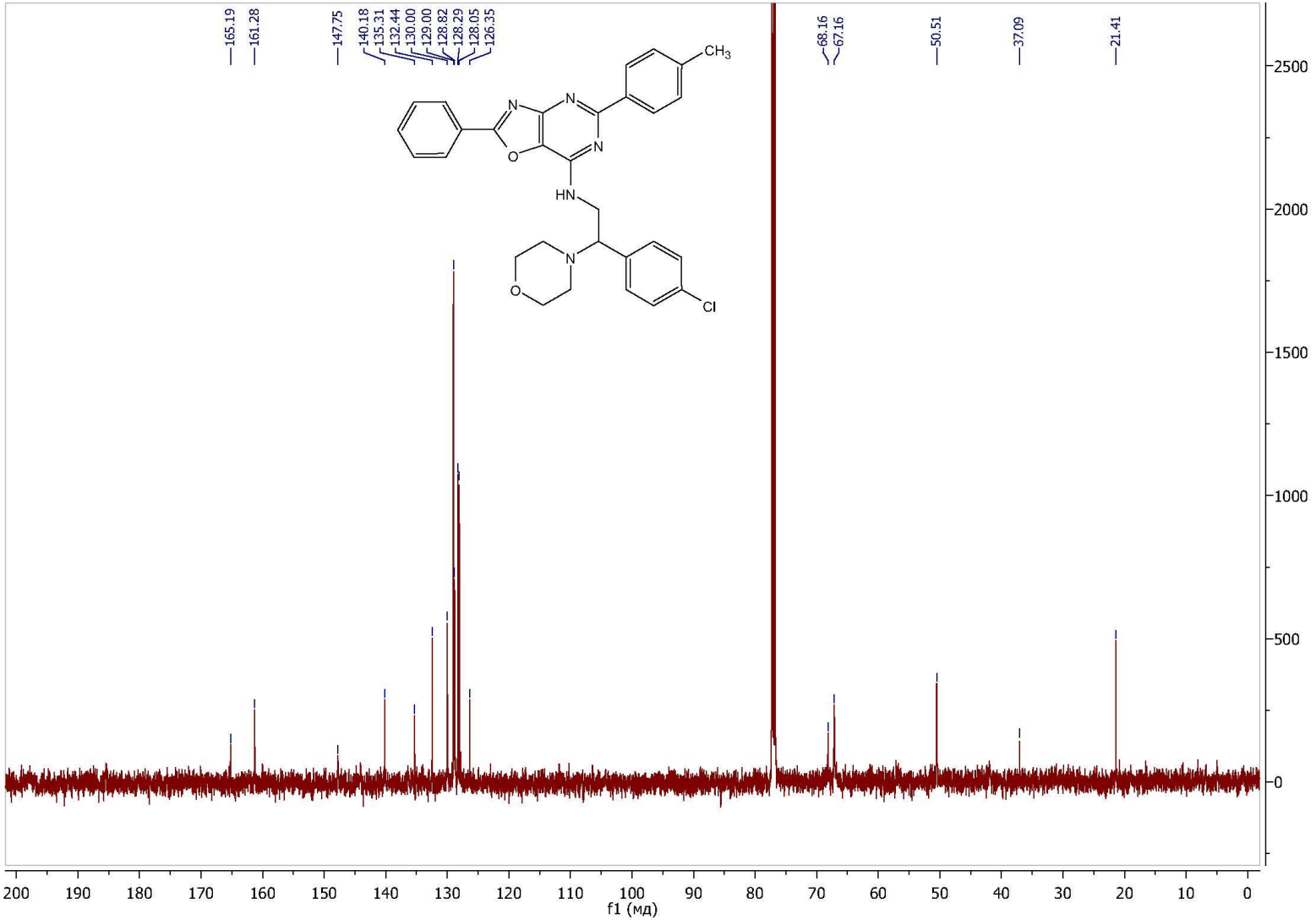
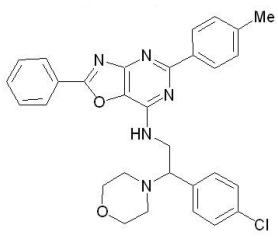


Figure S19. ^{13}C NMR spectrum of *N*-[2-(4-chlorophenyl)-2-morpholin-4-ylethyl]-5-(4-methylphenyl)-2-phenyl[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**5**)



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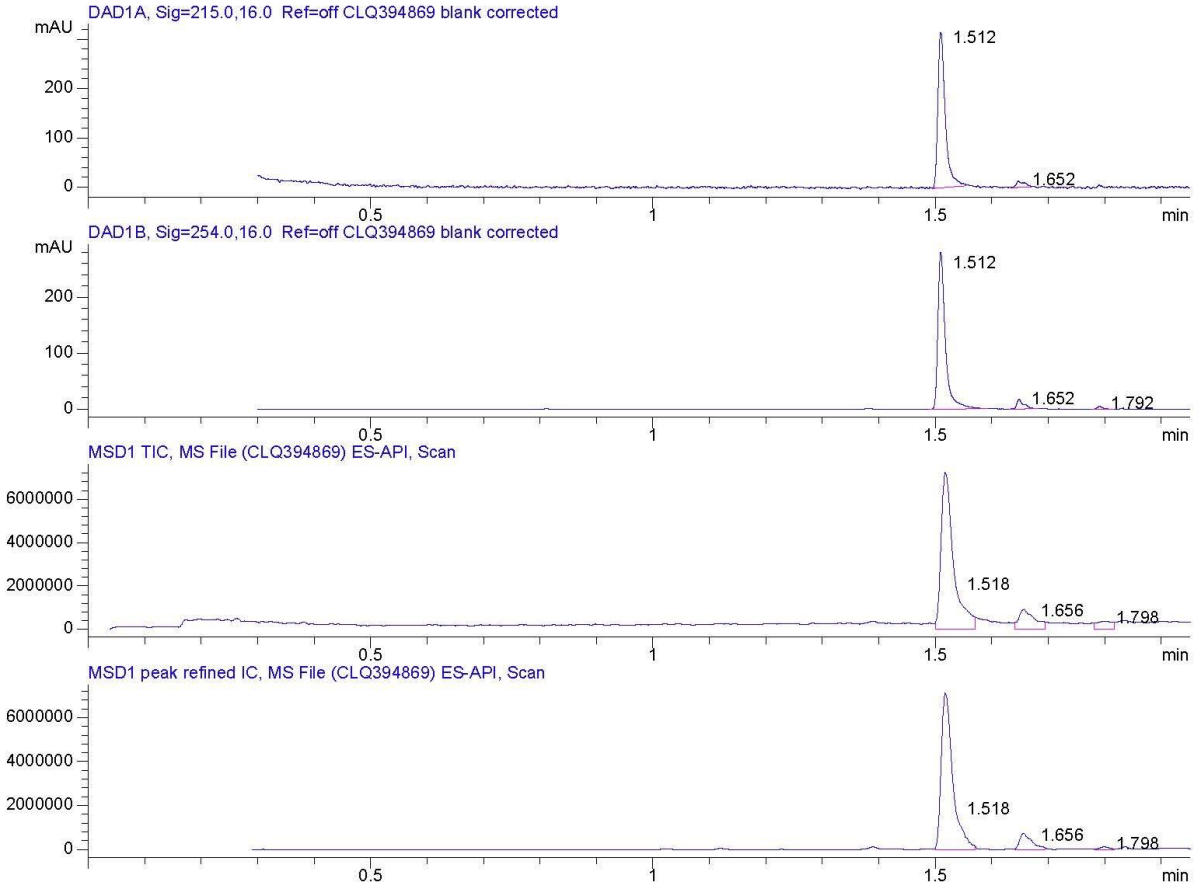
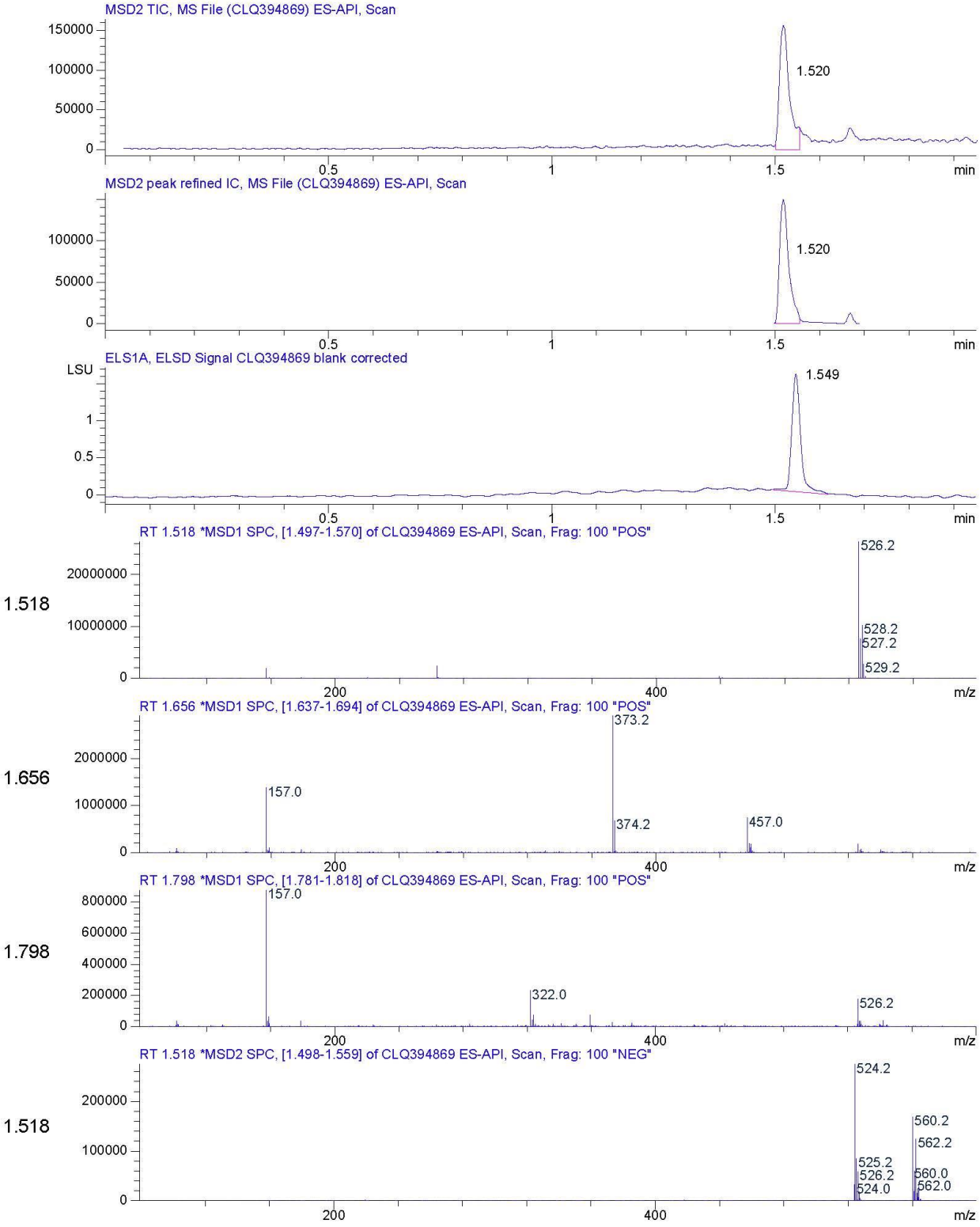
1	1.512	95.6%	93.4%	92.1%	41.9%	100.0%	526.2(88),529.2(7),263.6(5)	1.518	560.2(52),562.2(48)	1.518	
2	1.514	---	---	---	58.1%	---	---	---	524.2(100)	1.520	
3	1.652	4.4%	5.4%	7.2%	---	---	373.2(100)	1.656	---	---	
4	1.792	---	1.1%	0.7%	---	---	322.0(100)	1.798	---	---	

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MSD2 peak refined IC, MS File (CLQ394869) ES-API, Scan
1.520
ELS1A, ELSD Signal CLQ394869 blank corrected
1.549
LSU
min
1.518
RT 1.518 *MSD1 SPC, [1.497-1.570] of CLQ394869 ES-API, Scan, Frag: 100 "POS"
526.2
528.2
527.2
529.2
1.656
RT 1.656 *MSD1 SPC, [1.637-1.694] of CLQ394869 ES-API, Scan, Frag: 100 "POS"
373.2
157.0
374.2
457.0
1.798
RT 1.798 *MSD1 SPC, [1.781-1.818] of CLQ394869 ES-API, Scan, Frag: 100 "POS"
157.0
322.0
526.2
1.518
RT 1.518 *MSD2 SPC, [1.498-1.559] of CLQ394869 ES-API, Scan, Frag: 100 "NEG"
524.2
560.2
562.2
525.2
526.2
560.0
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m/z

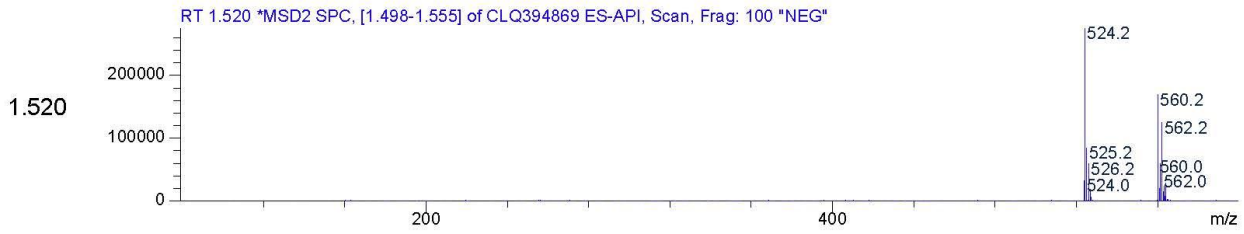


Figure S20. LC–MS spectrum of *N*-[2-(4-chlorophenyl)-2-morpholin-4-ylethyl]-5-(4-methylphenyl)-2-phenyl[1,3]oxazolo[4,5-*d*]pyrimidin-7-amine (**5**)

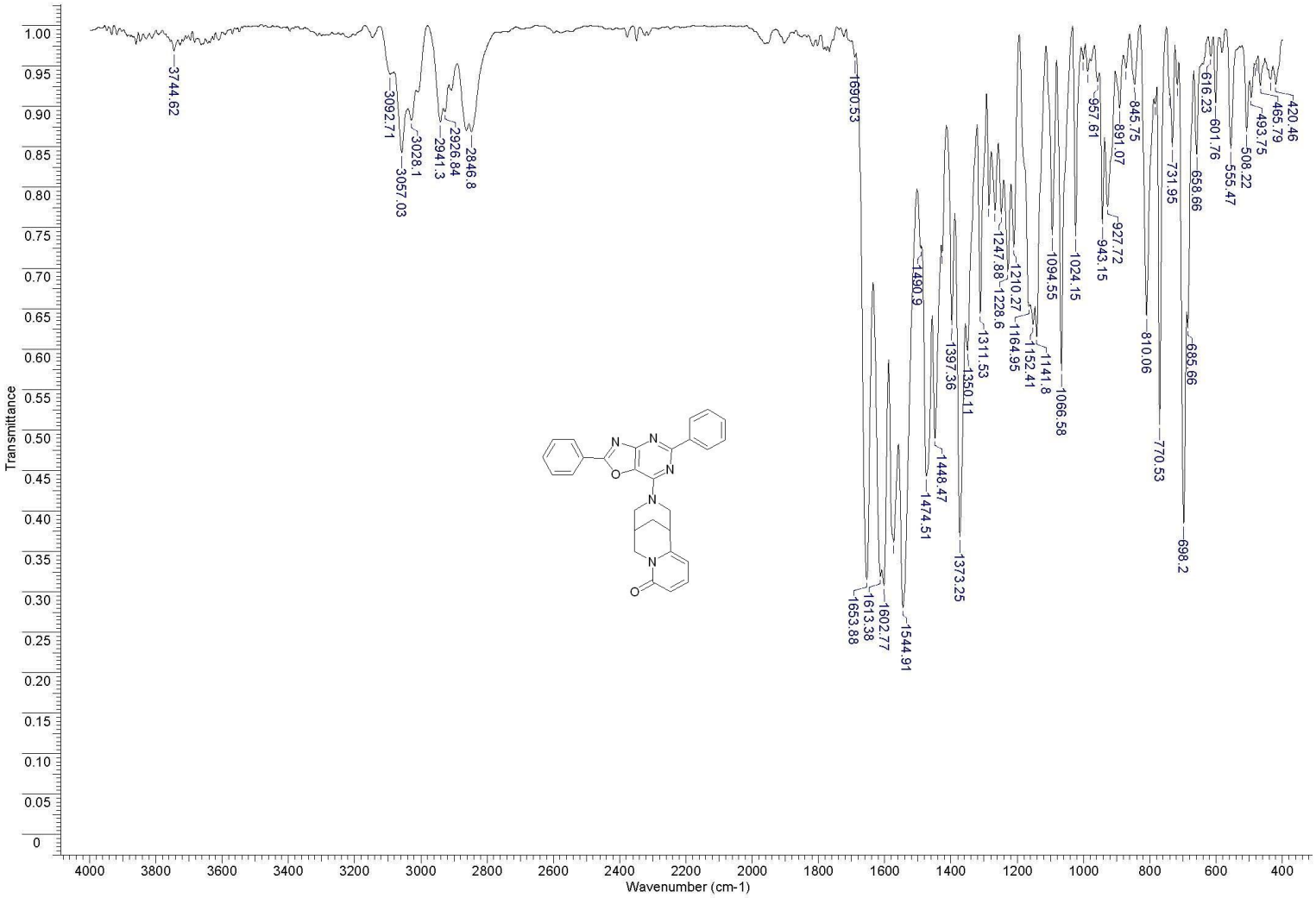


Figure S21. IR spectrum of 11-(2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**6**).

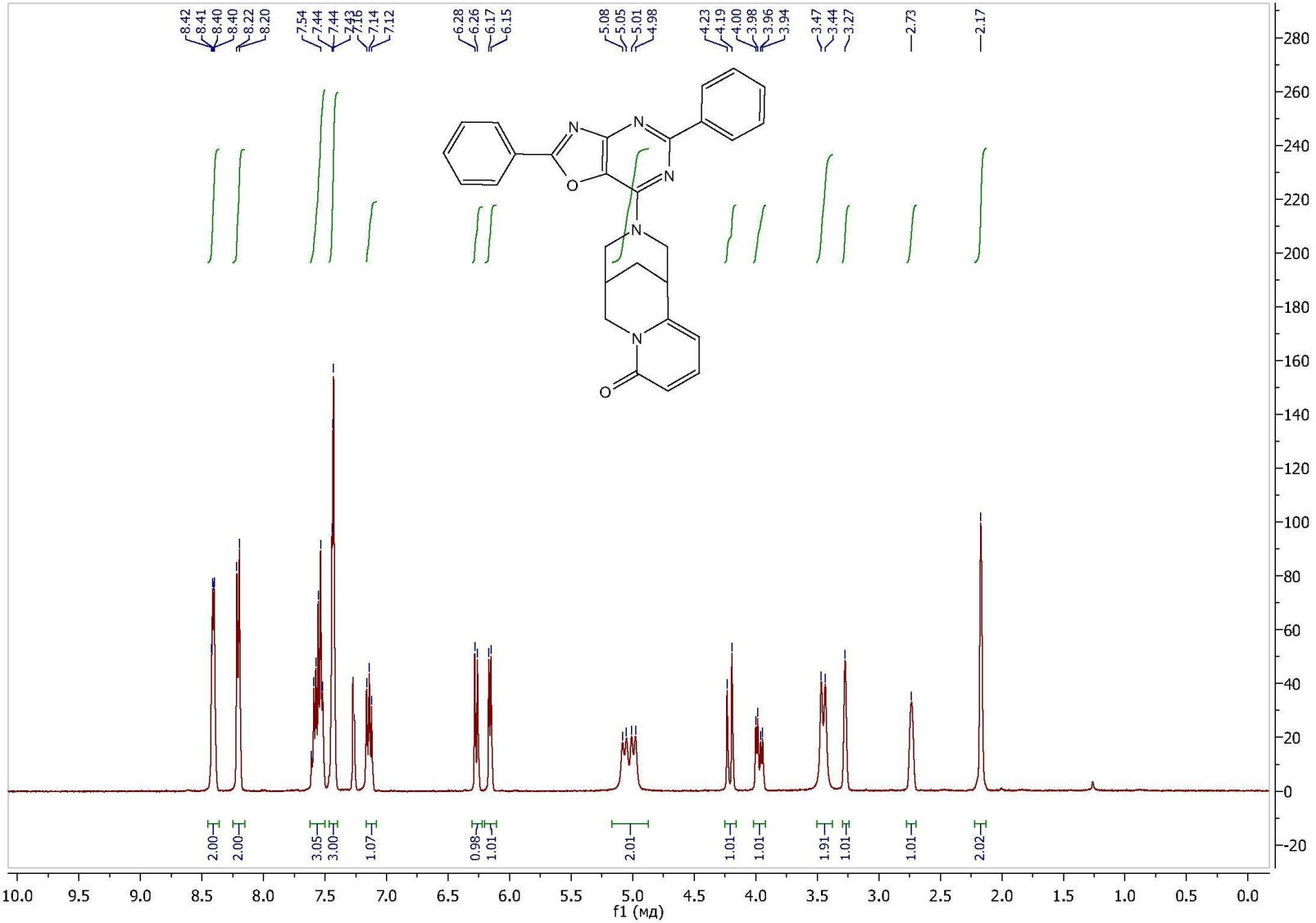


Figure S22. ^{1}H NMR spectrum of 11-(2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**6**)

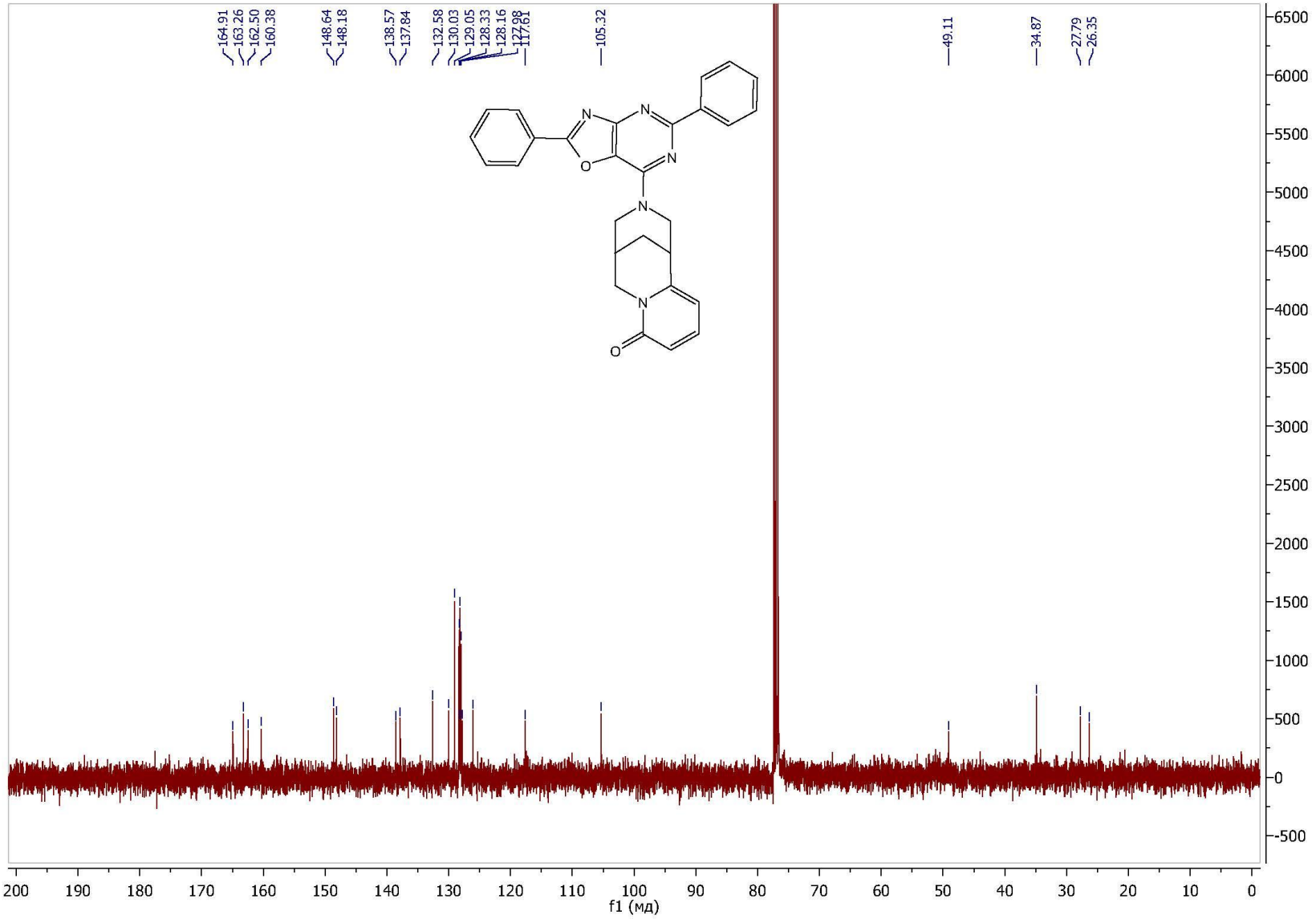
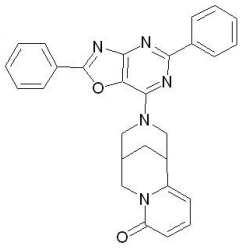


Figure S23. ^{13}C NMR spectrum of 11-(2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**6**)



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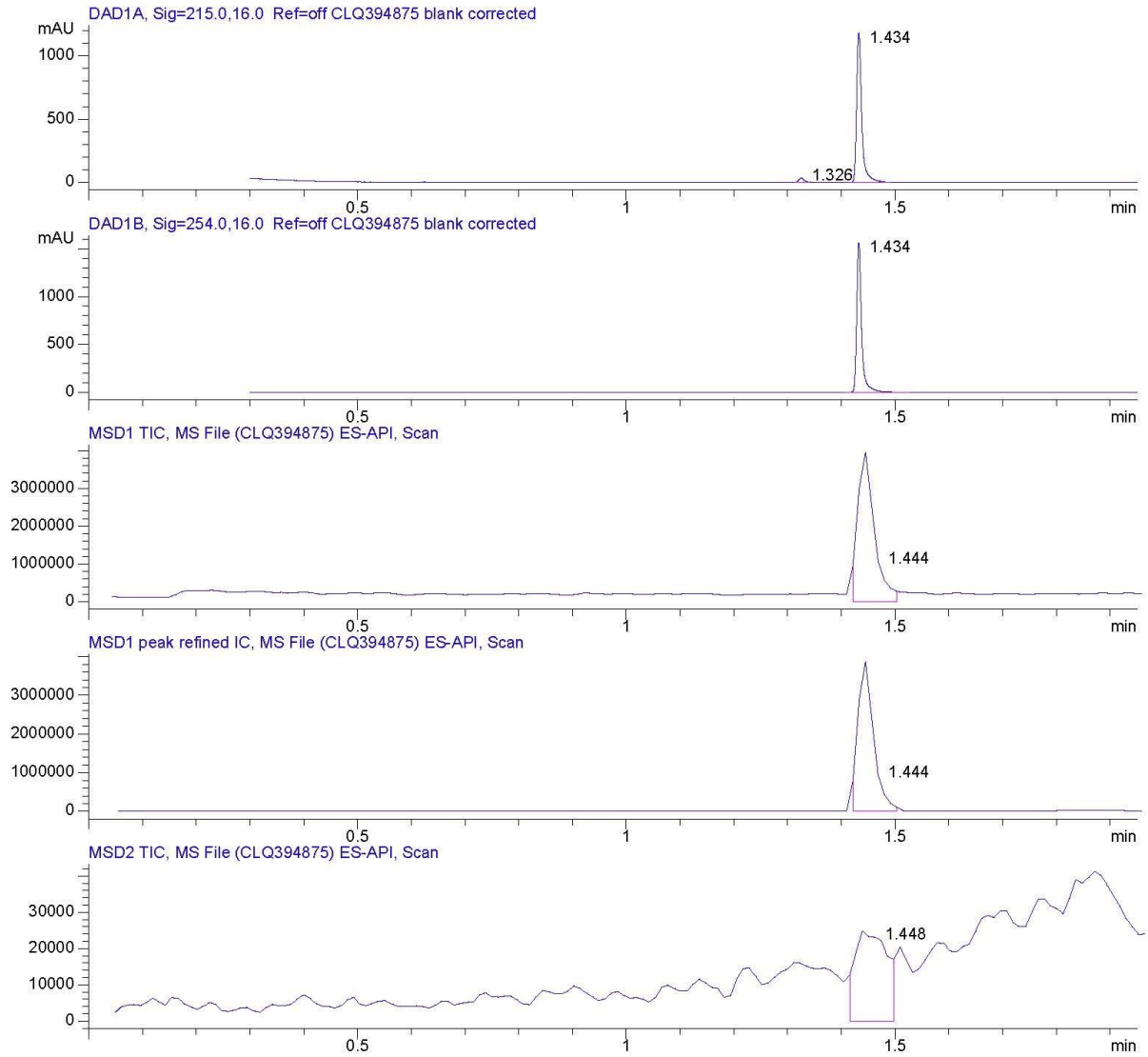
2	1.434	97.2%	100.0%	100.0%	100.0%	100.0%	462.2(100)	1.444	496.0(81),506.0(12),248.6(7)	1.448	



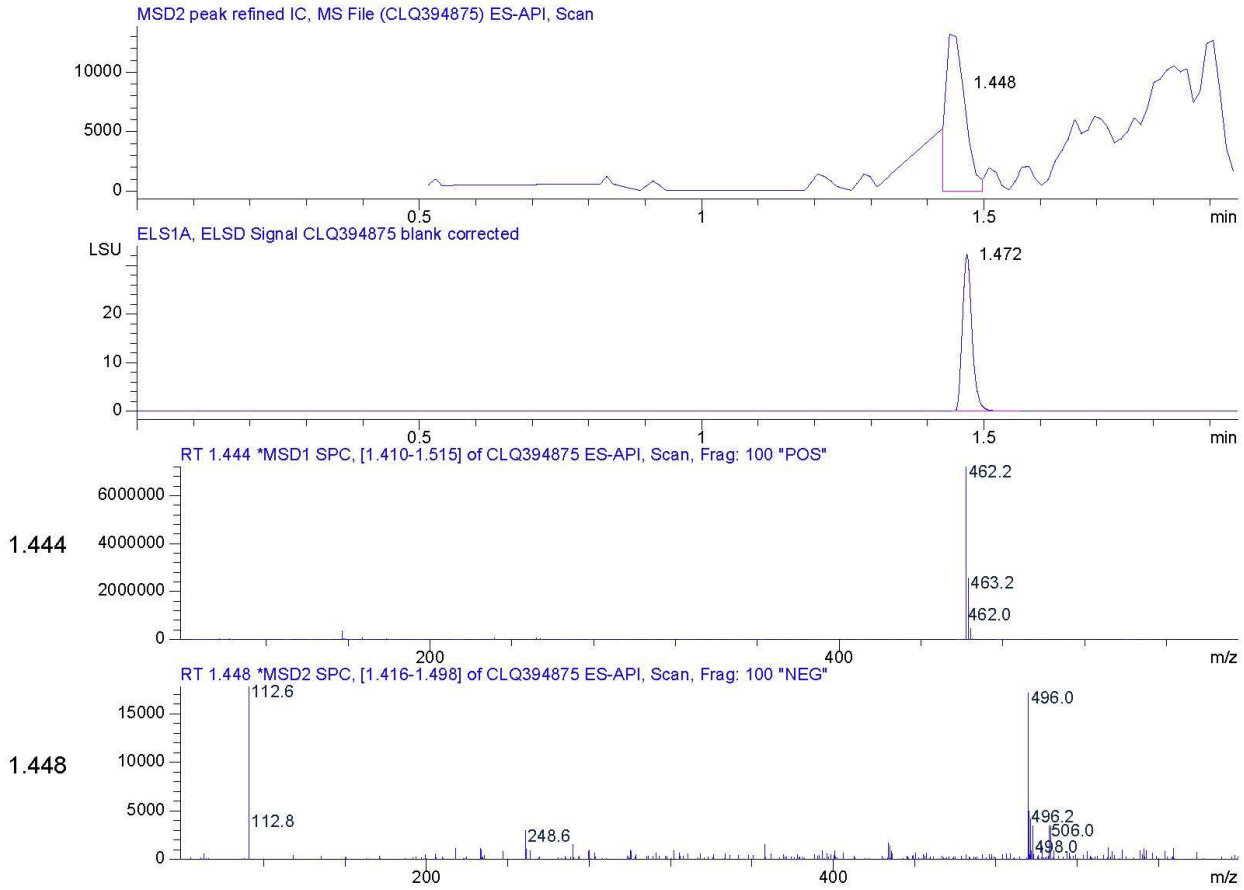


Figure S24. LC–MS spectrum of 11-(2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**6**)

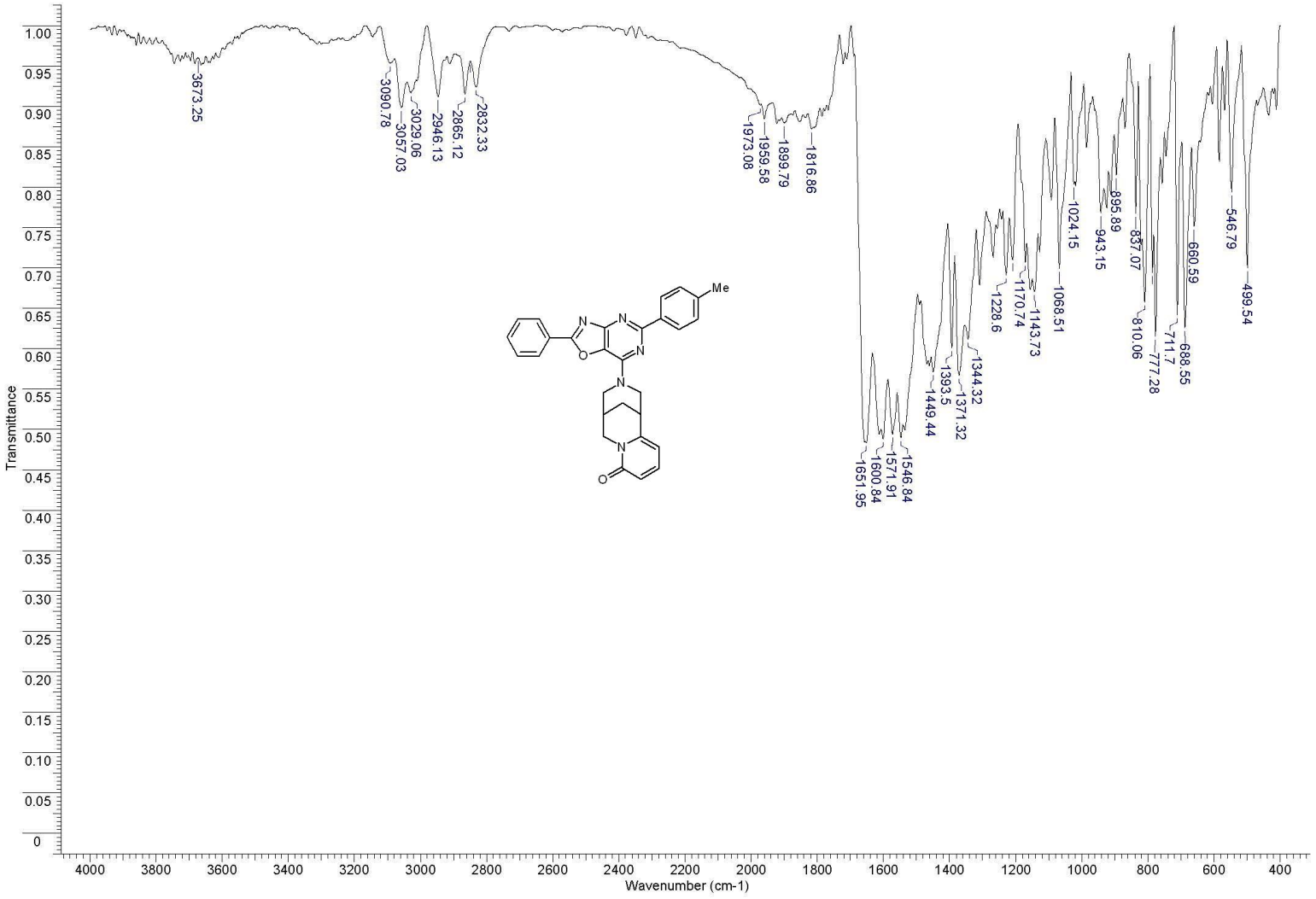


Figure S25. IR spectrum of 11-[5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**7**)

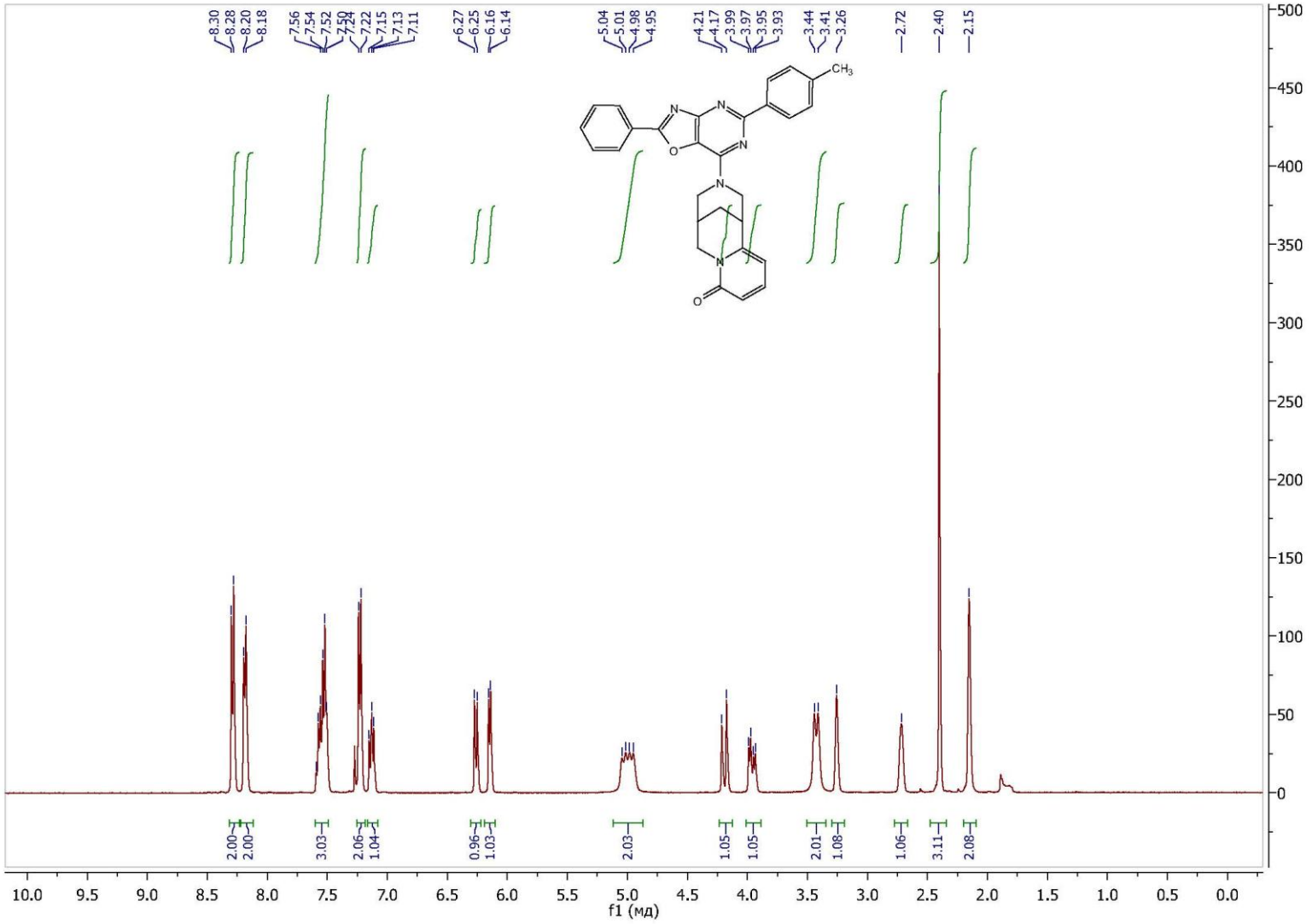


Figure S26. ^{1}H NMR spectrum of 11-[5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**7**)

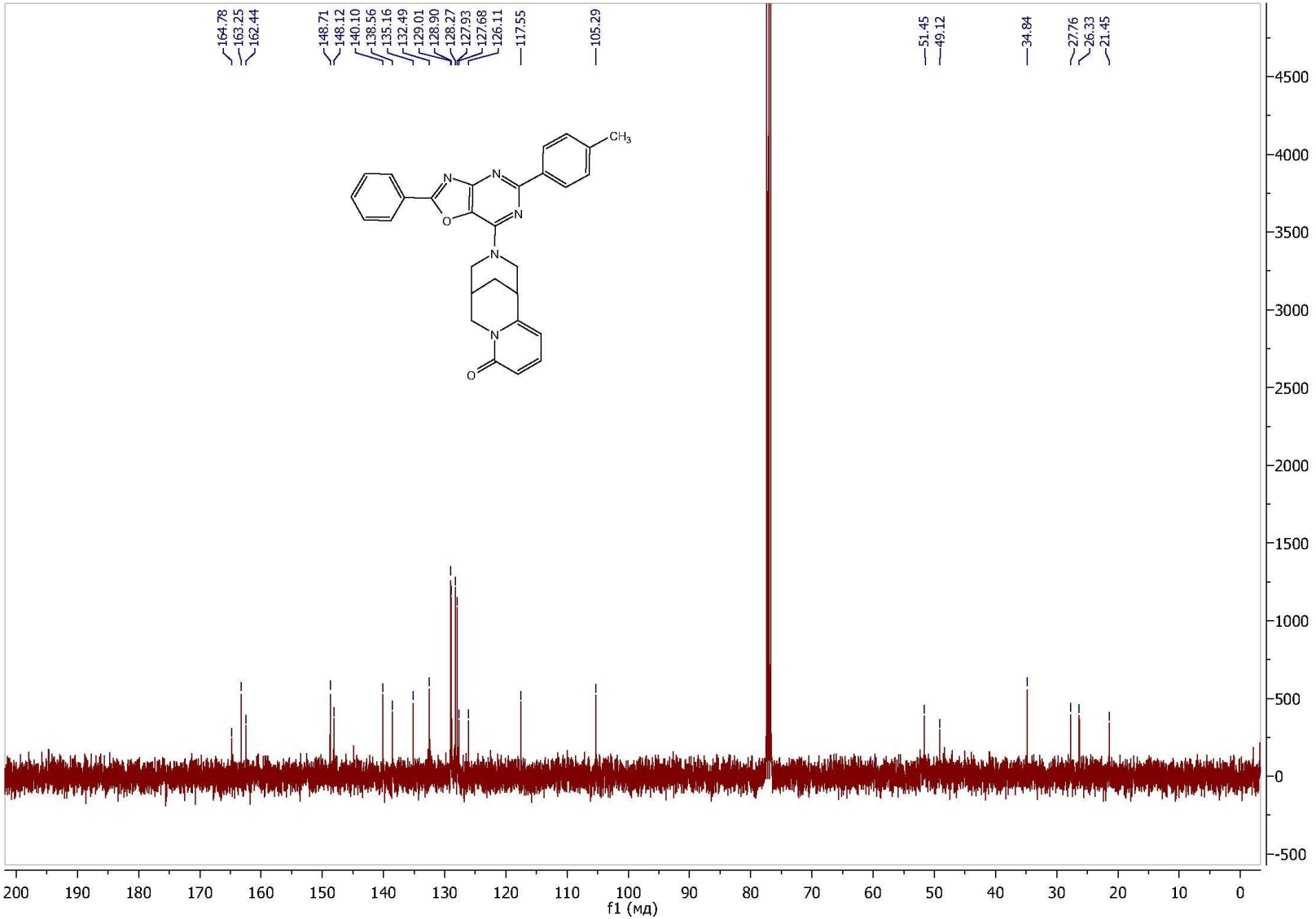
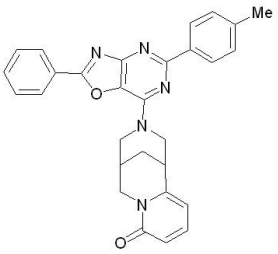


Figure S27. ^{13}C NMR spectrum of 11-[5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**7**)



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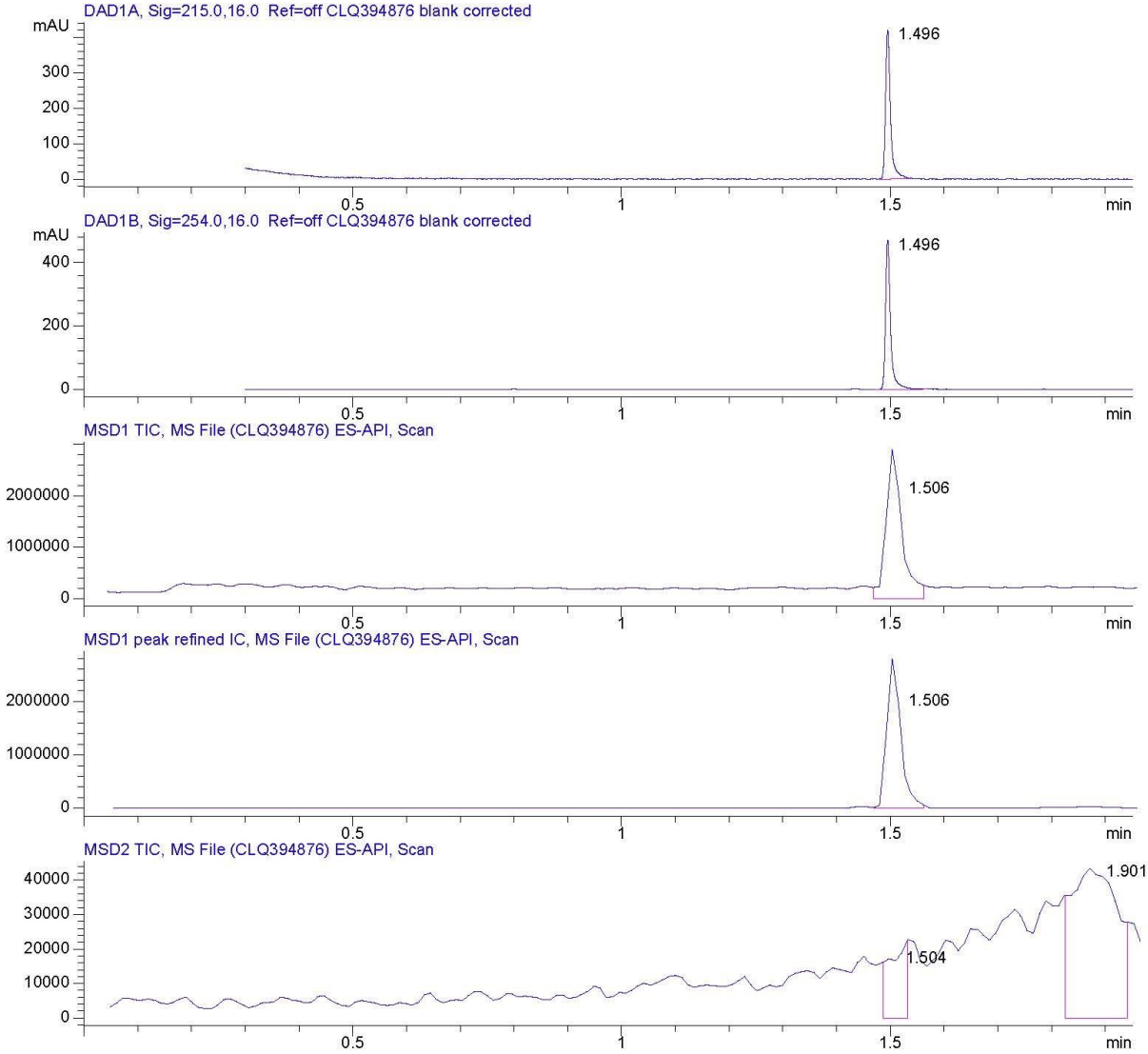
2	1.893	---	---	---	72.4%	---	---	---	489.2(58),461.2(10),536.0(8)	1.901	



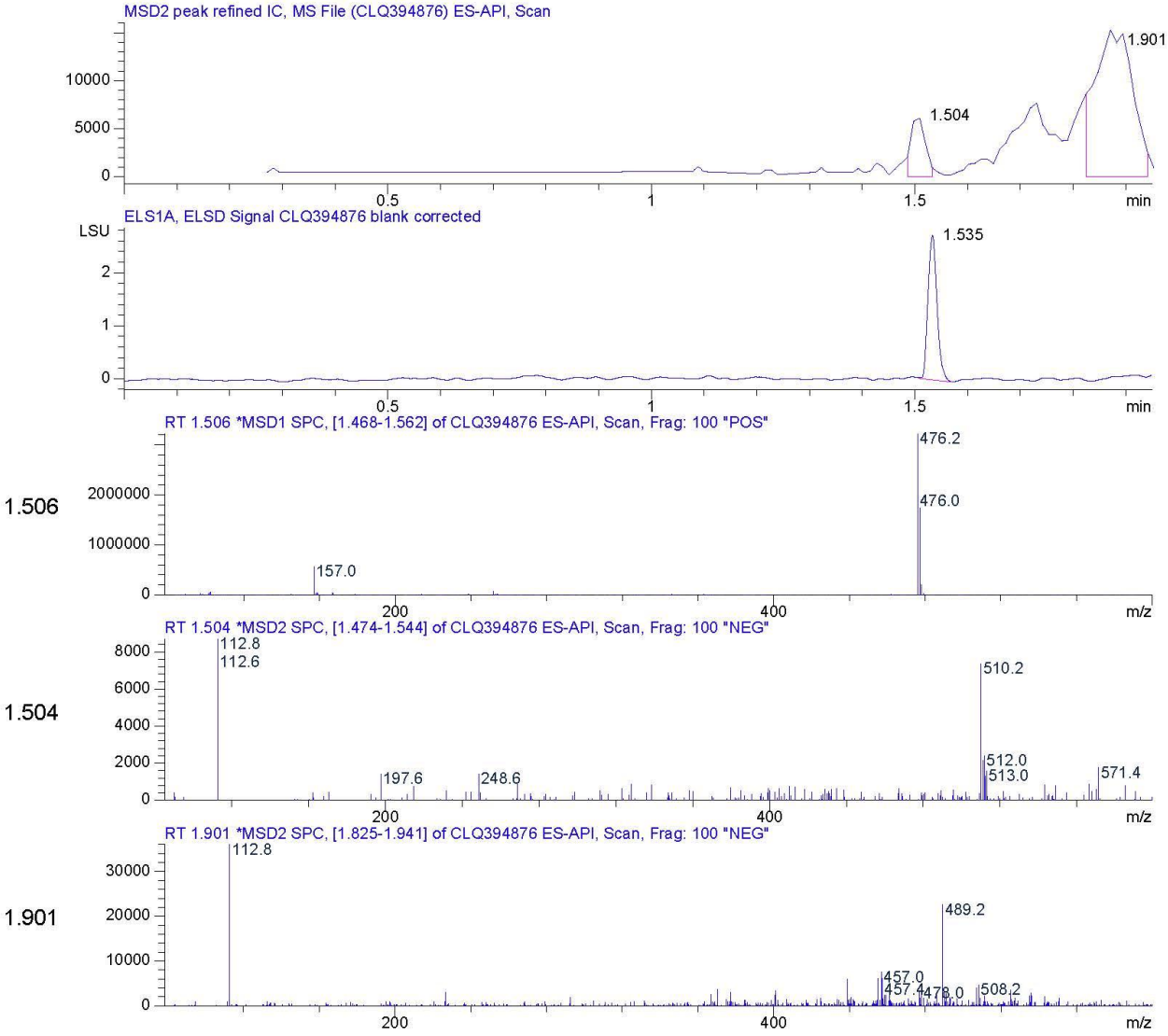


Figure S28. LC–MS spectrum of 11-[5-(4-methylphenyl)-2-phenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**7**)

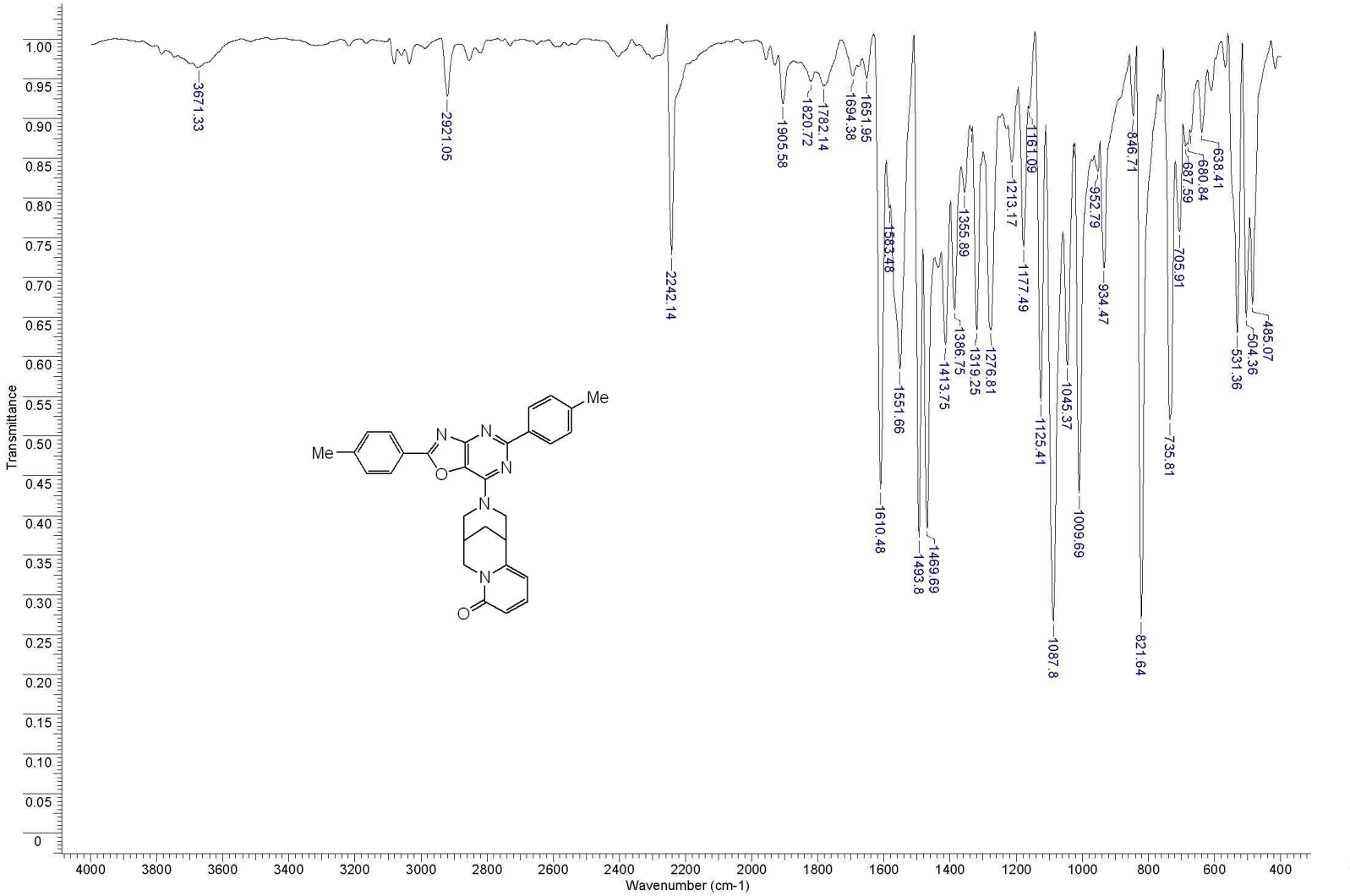


Figure S29. IR spectrum of 11-[2,5-bis(4-methylphenyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**8**)

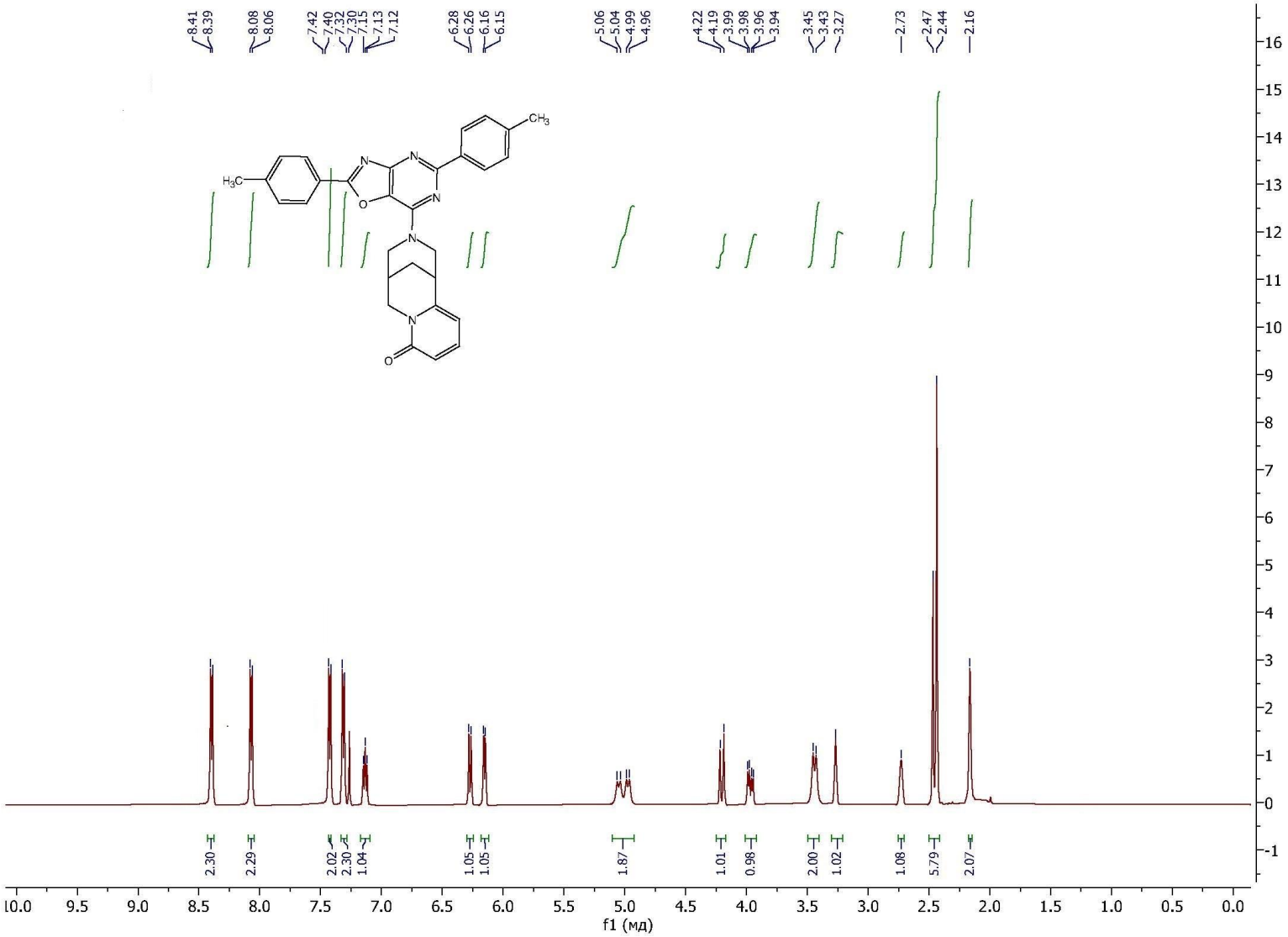


Figure S30. [1]H NMR spectrum of 11-[2,5-bis(4-methylphenyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**8**)

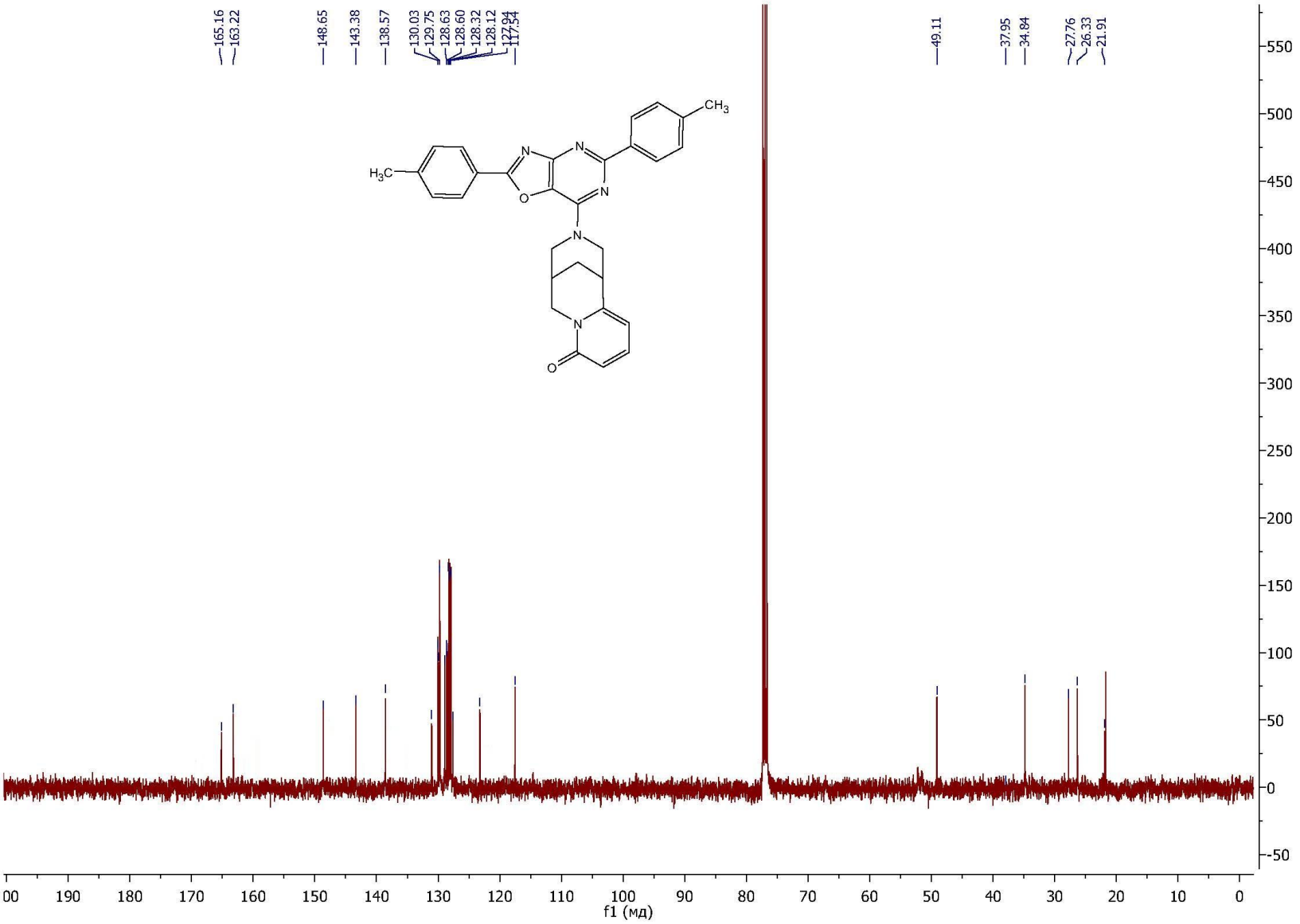
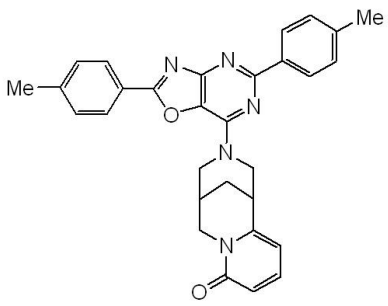


Figure S31. ^{13}C NMR spectrum of 11-[2,5-bis(4-methylphenyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**8**)



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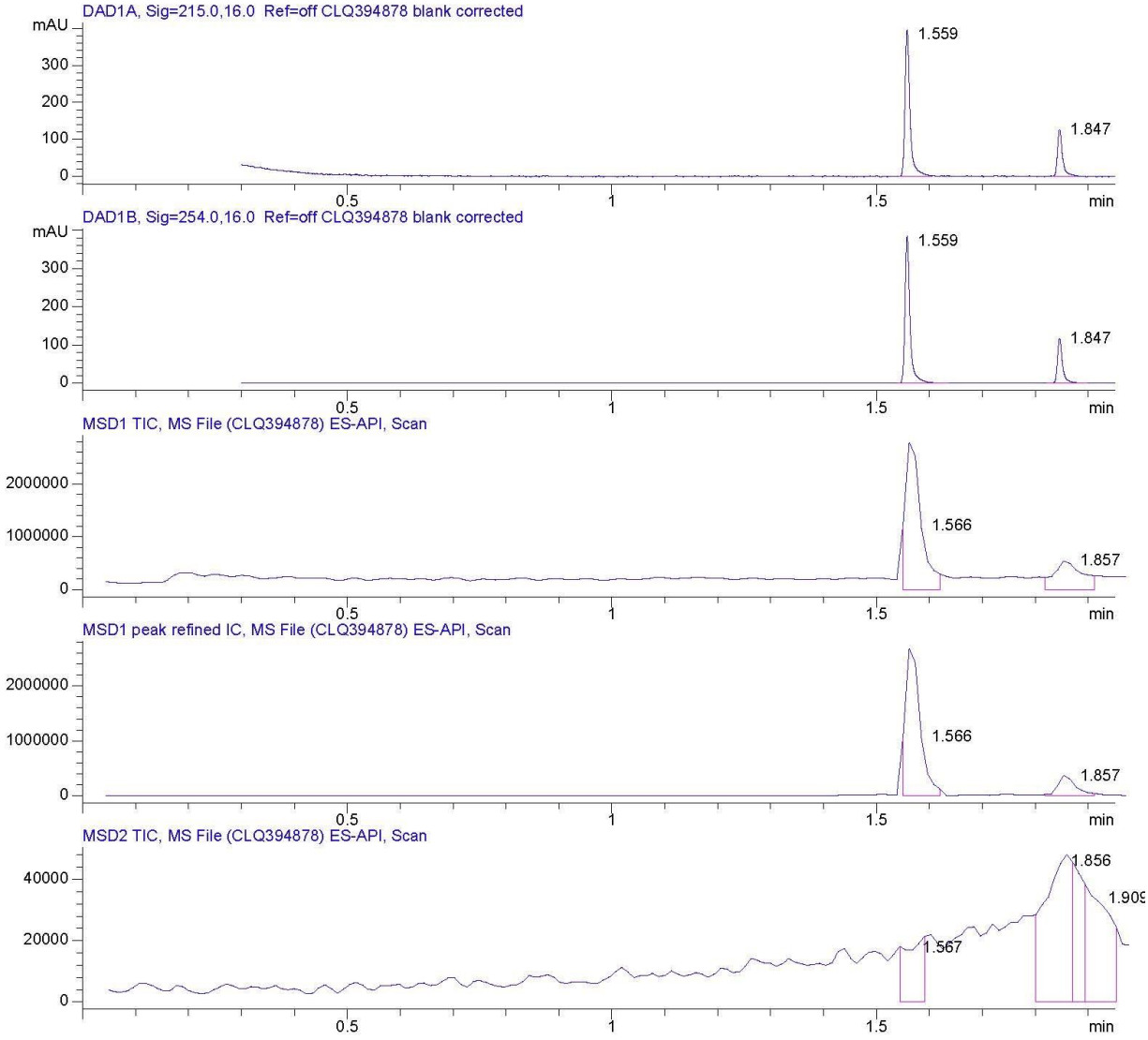
#	RT	DAD1A	DAD1B	MSD1	MSD2	ELSD	MSD1 ions	MSD1 rt	MSD2 ions	MSD2 rt	Info
1	1.559	95.9%	96.7%	89.2%	4.9%	89.6%	490.2(100)	1.566	248.6(57),526.0(43)	1.567	
2	1.847	4.1%	3.3%	10.8%	67.7%	10.4%	336.0(100)	1.857	457.2(29),489.0(12),455.2(8)	1.856	
3	1.901	---	---	---	27.4%	---	---	---	457.2(29),441.2(26),377.2(18)	1.909	



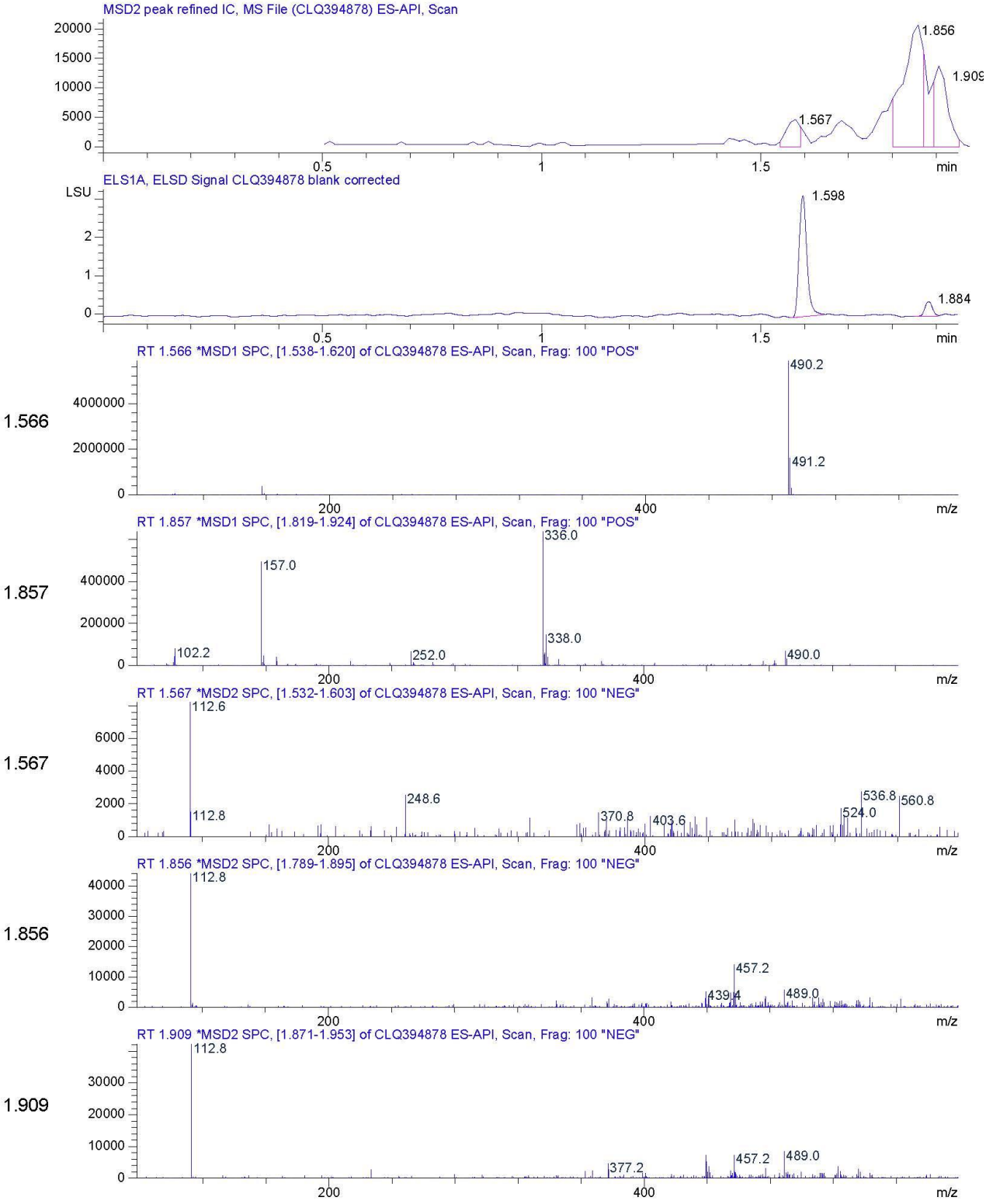


Figure S32. LC–MS spectrum of 11-[2,5-bis(4-methylphenyl)-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one (**8**)

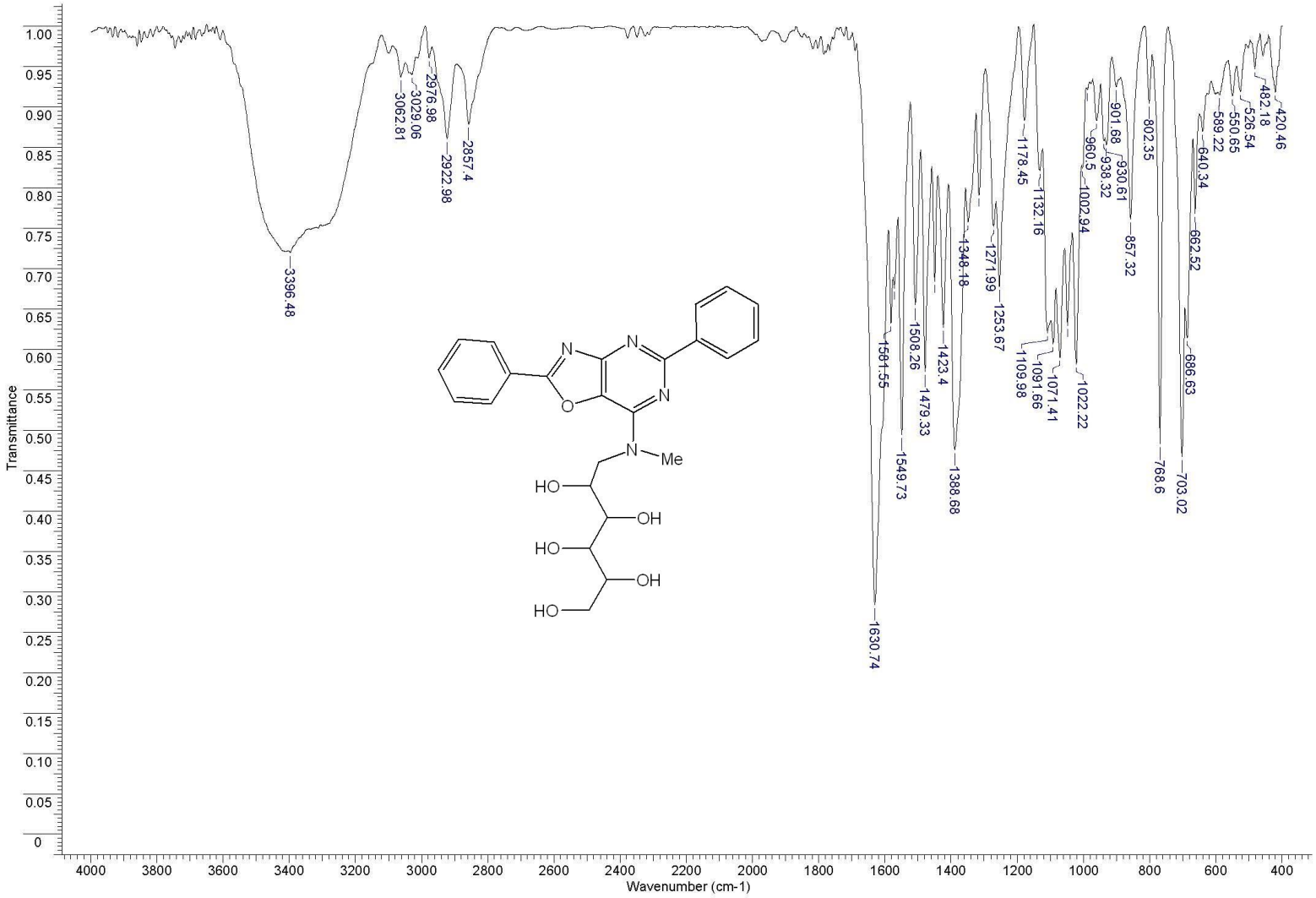


Figure S33. IR spectrum of 6-[(2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl)-methylamino]hexane-1,2,3,4,5-pentol (**9**)

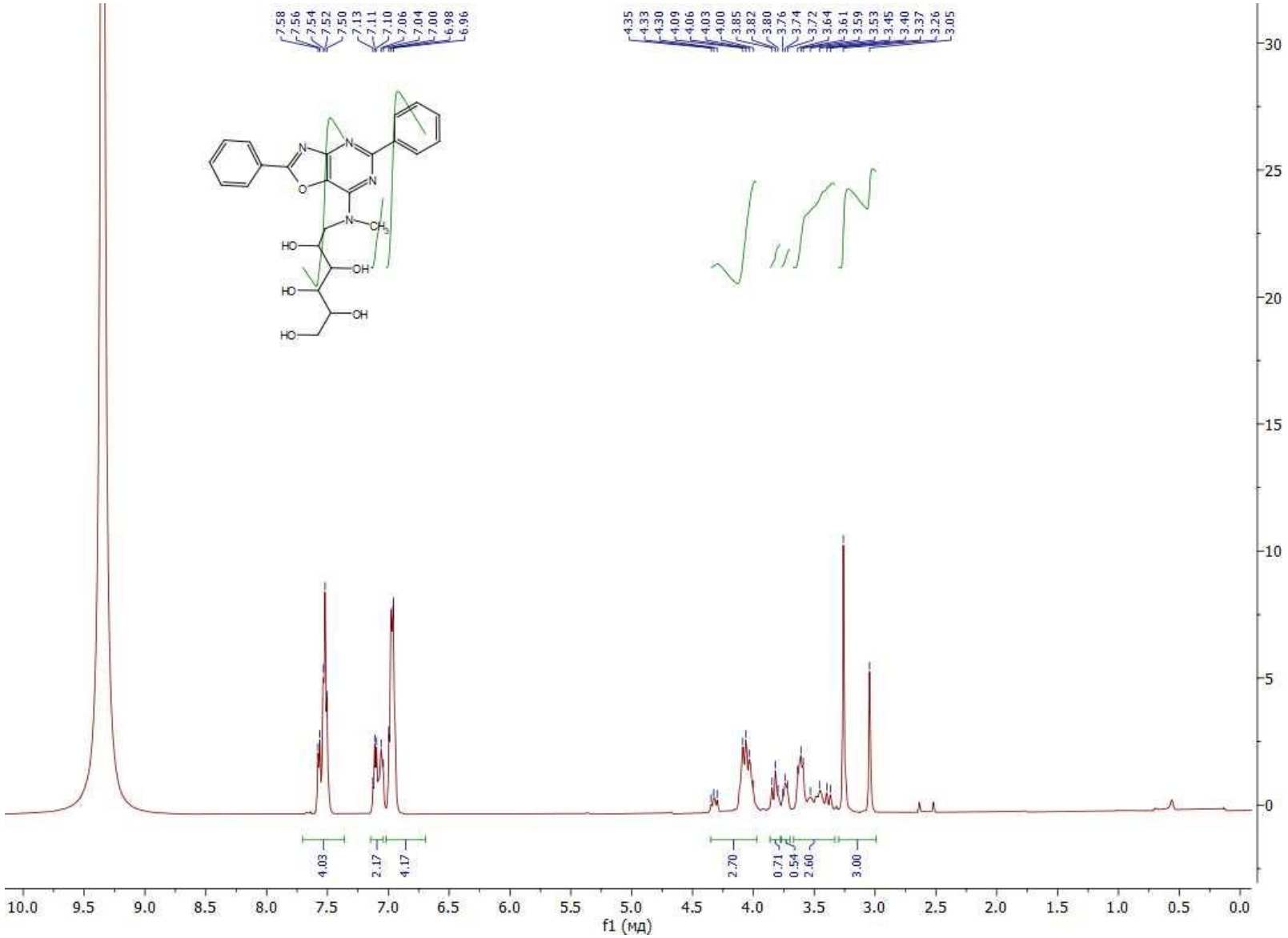


Figure S34. ^{1}H NMR spectrum of 6-[(2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl)-methylamino]hexane-1,2,3,4,5-pentol (**9**)

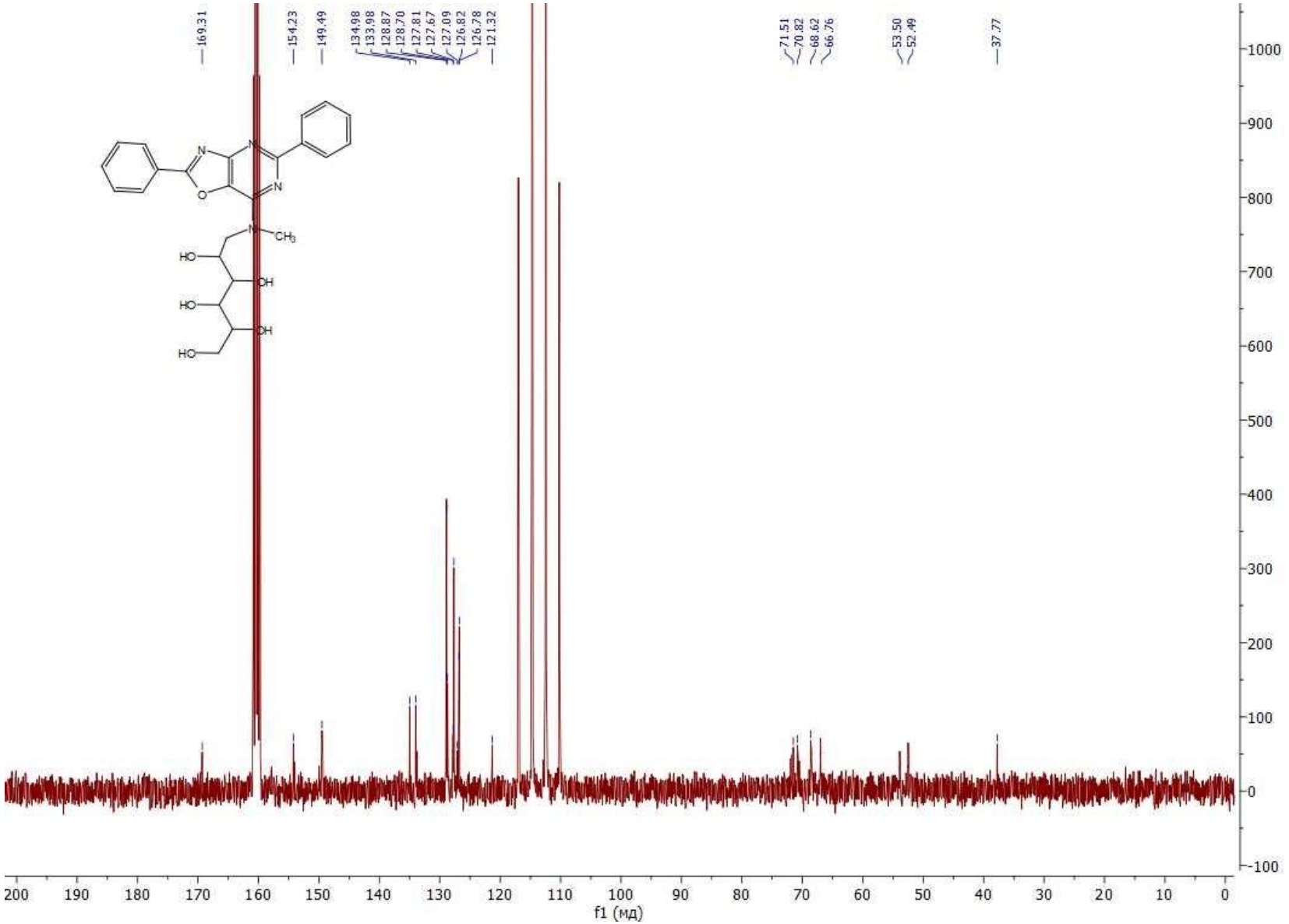
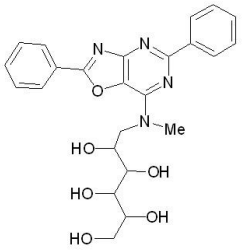


Figure S35. ^{13}C NMR spectrum of 6-[(2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl)-methylamino]hexane-1,2,3,4,5-pentol (**9**)



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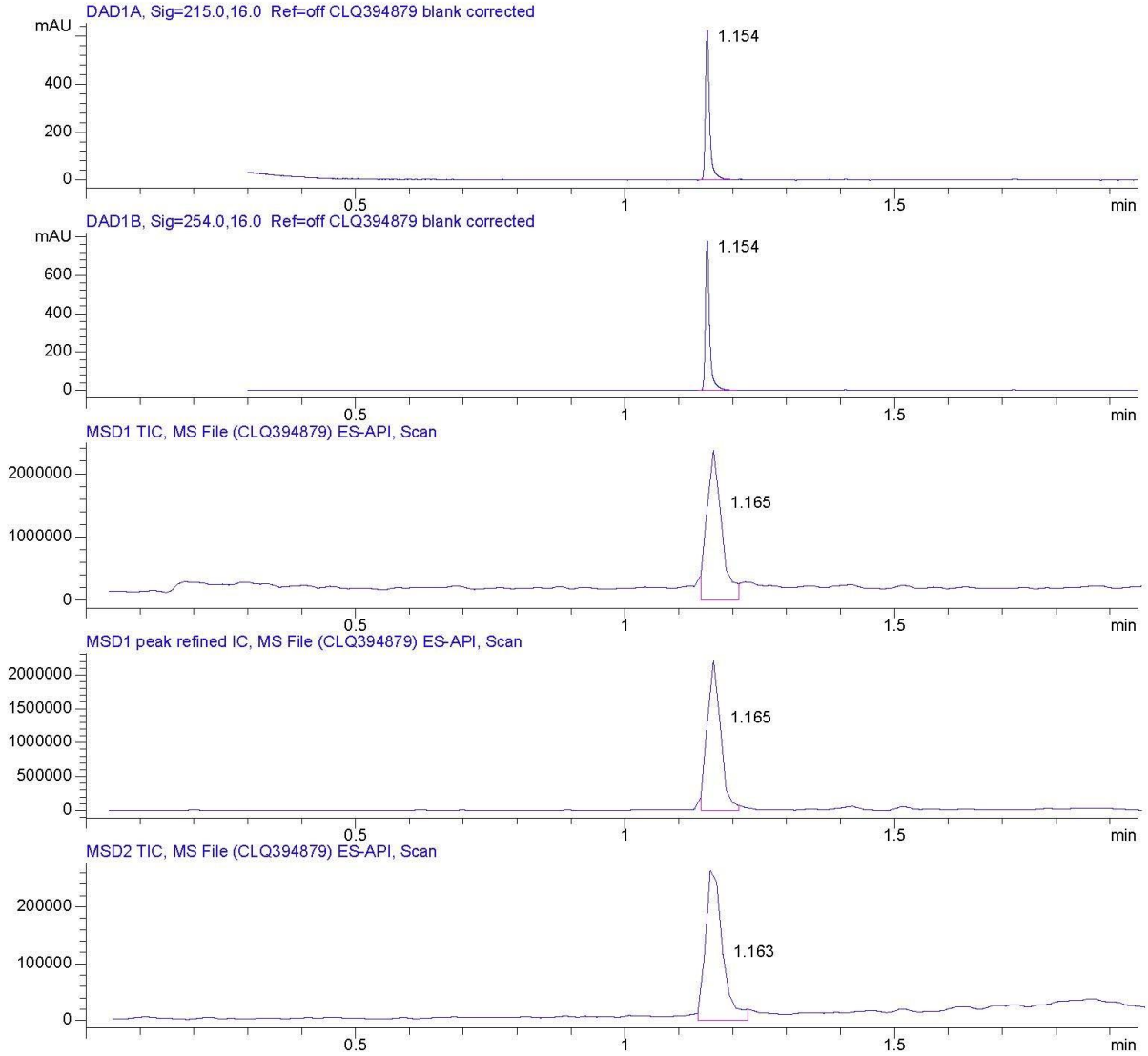
1	1.154	100.0%	100.0%	100.0%	100.0%	100.0%	467.2(100)	1.165	465.2(40),501.2(36),579.2(12)	1.163	



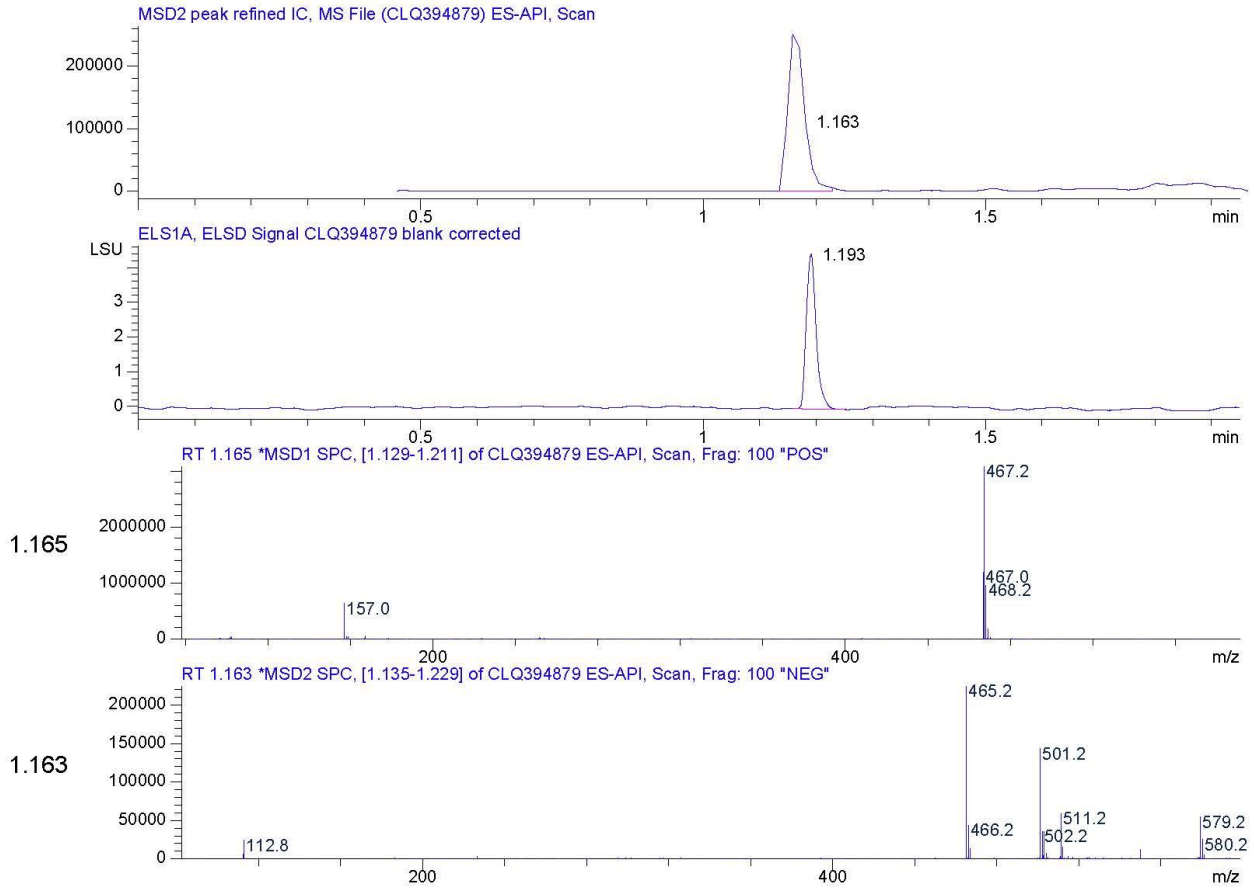


Figure S36. LC–MS spectrum of 6-[(2,5-diphenyl-[1,3]oxazolo[4,5-*d*]pyrimidin-7-yl)-methylamino]hexane-1,2,3,4,5-pentol (**9**)