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A convenient synthesis of dihydropyridinone dicarboxylic derivatives by the recyclization of *N*-arylitaconimides with 3-aminocrotonates

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Materials and Methods

^{1}H and ^{13}C NMR spectra were registered on Bruker DRX-500 (500.13 and 125.76 MHz, respectively) spectrometer in DMSO-d_6, internal standard was TMS. Melting points were determined on Stuart SMP 30. Control of reagent and products individuality, qualitative analysis of reaction mass was performed by TLC on Merck TLC Silica gel 60 F_{254} chromatographic plate; eluents: methanol, chloroform and their mixtures in various ratios. The chromatograms were visualized by UV or iodine vapor.

Product purity was monitored by high performance liquid chromatography with high resolution mass spectrometric electrospray ionization detection (HPLC-HRMS-ESI) in combination with UV detection. The analyzes were performed on Agilent 1260 Infinity chromatograph (Agilent Technologies, CA, USA) and Agilent 6230 TOF LC/MS high-resolution time-of-flight mass detector. The ionization block was double electrospray; the signals were recorded in positive polarity; nebulizer N_2 20 psig; desiccant gas N_2, 6 ml min-1,325 °C; mass detection range is 50-2000 daltons. Capillary voltage 4.0 kV, fragmentator +191 V, skimmer +66 V, OctRF 750 V. Poroshell 120 EC-C18 column (4.6 x 50 mm; 2.7 μm) was used. Gradient elution: acetonitrile/water (0.1% formic acid); flow rate 0.4 ml min^{-1}. Software for processing research results - MassHunter Workstation/Data Acquisition V.06.00.

Experimental.

Synthesis of alkyl 6-alkyl-3-(2-(R-anilino)-2-oxo-ethyl)- 2-oxo-3,4-dihydro-1*H*-pyridine-5-carboxylates 3a-f. A solution of *N*-arylitaconimid **2a-j** (5 mmol) and 2,3-unsaturated 3-amino ester **1a-c** (5 mmol) is boiled in acetic acid (5 ml) for 2-5 hours. The precipitate that forms during cooling is recrystallized from 2-propanol.

Ethyl 3-(2-anilino-2-oxoethyl)-6-methyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3a.** Yield 55%, colorless powdery compound, m.p. 206-207 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 1.18 (3H, t , *J* = 7.1, CH_3); 2.20 (3H, s, CH_3); 2.31 (1H, t, *J* = 14.2, CH_2(4)); 2.39 (1H, dd, *J* = 16.9, *J* = 9.2, CH_2CO); 2.74 (1H, dd, *J* = 16.2, J = 6.7, CH_2(4)); 2.78-2.84 (2H, m, CH_2CO+CH(3)); 4.08 (2H, q, *J* = 7.0; OCH_2); 7.01-7.60 (5H, m, 5CH-Ar); 9.79 (1H, s, NH(1)); 9.97 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 14.18, 17.67, 26.75, 35.84, 35.97, 59.26, 101.83, 118.93, 122.94, 128.58, 139.14, 146.92, 166.49, 169.31, 172.23. IR, ν (cm^{-1}): 1607 (C=O, amide I); 1542 (C=O, amide II). HRMS: m/z calcd for $C_{17}H_{20}N_2O_4$, 317.1497; found, 317.1495

Ethyl 6-methyl-3-[2-(4-methylanilino)-2-oxoethyl]-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3b.** Yield 50%, colorless powdery compound, m.p. 184-185 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 1.18 (3H, t , *J* = 7.1, CH_3); 2.20 (3H, s, CH_3); 2.24 (3H, s, Ar-CH_3), 2.29 (1H, t, *J* = 13.8, CH_2(4)); 2.36 (1H, dd, *J* = 16.9, J = 9.2, CH_2CO); 2.73 (1H, dd, *J* = 15.9, *J* = 6.6, CH_2(4)); 2.77-2.83 (2H, m, CH_2CO + CH(3)); 4.07 (2H, q, *J* = 7.1; OCH_2); 7.08-7.48 (4H, m, 4CH-Ar); 9.79 (1H, s, NH(1)); 9.88 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 14.19, 17.67, 20.34, 26.75, 35.86, 35.92, 59.26, 101.82, 118.97, 128.95, 131.81, 136.65, 146.92, 166.49, 169.04, 172.25. IR, ν (cm^{-1}): 1611 (C=O, amide I); 1540 (C=O, amide II). HRMS: m/z calcd for $C_{12}H_{15}N_3O_2$, 234.1243; found, 234.1237.

Ethyl 3-[2-(4-chloroanilino)-6-methyl-2-oxoethyl]-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3c**. Yield 75%, colorless powdery compound, m.p. 204-205 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 1.18 (3H, t, *J* = 7.1 CH_3), 2.20 (3H, s, CH_3), 2.26-2.34 (1H, m, CH_2(4)), 2.40 (1H, dd, *J* = 8.9, *J* = 17.1, CH_2CO), 2.74 (1H, dd, *J* = 8.9, *J* = 15.9, CH_2(4)), 2.78-2.84 (2H, m, CH_2CO + CH(3)); 4.08 (2H, q, *J* = 7.1; OCH_2); 7.33-7.64 (4H, m, 4CH-Ar); 9.79 (1H, s, NH(1)); 10.12 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 14.64, 18.12, 27.21, 36.25, 36.43, 59.72, 102.31, 120.90, 126.92, 128.95, 138.55, 147.37, 166.93, 169.97, 172.63. IR, ν (cm^{-1}): 1599 (C=O, amide I); 1538 (C=O, amide II). HRMS: m/z calcd for $C_{17}H_{19}ClN_2O_4$, 353.1078; found, 353.1076.

Ethyl 3-[2-(3-chloroanilino)-2-oxoethyl]-6-methyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3d.** Yield 65%, colorless powdery compound, m.p. 193-194 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 1.18 (3H, t , *J* = 7.1 CH_3); 2.20 (3H, s, CH_3); 2.25-2.38 (1H, m, CH_2(4)); 2.42 (1H, dd, *J* = 8.9, *J* = 17.4, CH_2CO); 2.72-2.85 (3H, m, CH_2(4) + CH_2CO + CH(3)); 4.08 (2H, q, *J* = 7.1; OCH_2); 7.08-7.85 (4H, m, 4CH-Ar); 9.79 (1H, s, NH(1)); 10.18 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 14.64, 18.12, 27.19, 36.24, 36.47, 59.72, 102.32, 117.72, 118.84, 123.10, 130.76, 133.42, 141.01, 147.36, 166.93, 170.25, 172.59. IR, ν (cm^{-1}): 1611 (C=O, amide I); 1544 (C=O, amide II). HRMS: m/z calcd for $C_{17}H_{19}ClN_2O_4$, 353.1078; found, 353.1077.

Methyl 3-(2-anilino-2-oxoethyl)-6-methyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3e.** Yield 50%, colorless powdery compound, m.p. 211-212 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 2.17 (3H, s, CH_3); 2.26 (1H, t, *J* = 15.6, CH_2(4)); 2.34 (1H, dd, *J* = 16.7, *J* = 9.1, CH_2CO); 2.74 (1H, dd, *J* = 15.6, *J* = 6.6, CH_2(4)); 2.75-2.82 (2H, m, CH_2CO + CH(3)); 3.57 (3H, s, OCH_3), 6.95-7.60 (5H, m, 5CH-Ar); 9.80 (1H, s, NH(1)); 9.95 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 18.26, 27.33, 36.44, 36.60, 51.47, 102.19, 119.54, 123.58, 129.23, 139.77, 147.86, 167.51, 169.94, 172.84. IR, ν (cm^{-1}): 1606 (C=O, amide I); 1542 (C=O, amide II). HRMS: m/z calcd for $C_{16}H_{18}N_2O_4$, 303.1340; found, 303.1336.

Methyl 6-methyl-3-[2-(4-methylanilino)-2-oxoethyl]-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3f.** Yield 50%, colorless powdery compound, m.p. 191-192 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 2.19 (3H, s, CH_3), 2.24 (3H, s, CH_3-Ar), 2.28 (1H, t, *J* = 15.2, CH_2(4)); 2.35 (1H, dd, *J* = 16.8, *J* = 8.9, CH_2CO); 2.74 (1H, dd, *J* = 15.9, *J* = 6.3, CH_2(4)); 2.76-2.83 (2H, m, CH_2CO + CH(3)); 3.60 (3H, s, OCH3), 7.08-7.47 (4H, m, 4CH-Ar); 9.81 (1H, s, NH(1)); 9.88 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 18.19, 20.89, 27.26, 36.39, 36.48, 51.39, 102.11, 119.49, 129.52, 132.37, 137.20, 147.77, 167.43, 169.59, 172.78. IR, ν (cm^{-1}): 1601 (C=O, amide I); 1539 (C=O, amide II). HRMS: m/z calcd for $C_{17}H_{20}N_2O_4$, 317.1497; found: 317.1495.

Methyl 3-[2-(3,4-dimethylanilino)-2-oxoethyl]-6-methyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3g.** Yield 45%, colorless powdery compound, m.p. 217-218 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 2.12 (3H, s, CH_3), 2.14 (3H, s, CH_3), 2.16 (3H, s, CH_3), 2.25 (1H, t, *J* = 14.9, CH_2(4)); 2.31 (1H, dd, *J* = 16.6, *J* = 9.1, CH_2CO); 2.31 (1H, dd, *J* = 16.1, *J* = 9.3, CH_2(4)); 2,69 (1H, dd, *J* = 16.5, *J* = 6.8, CH_2(4)); 2.72-2.79 (2H, m, CH_2CO + CH(3)); 3.57 (3H, s, OCH_3), 6.96-7.36 (3H, m, 3CH-Ar); 9.78 (1H, s, NH(1)); 9.79 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 16.26, 19.30, 20.16, 27.31, 36.48, 36.53, 51.46,

102.16, 117.11, 120.81, 130.05, 131.24, 136.74, 137.52, 147.85, 167.51, 169.60, 172.86. IR, ν (cm^{-1}): 1579 (C=O, amide I); 1532 (C=O, amide II). HRMS: m/z calcd for $C_{18}H_{22}N_2O_4$, 331.1654; found, 311.1651.

Methyl 3-[2-(4-ethoxyanilino)-2-oxoethyl]-6-methyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3h.** Yield 40%, colorless powdery compound, m.p. 182-183 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 1.14 (3H, t, *J* =7.8, CH_3), 2.19 (3H, s, CH_3), 2.28 (1H, t, *J* = 14.9, CH_2(4)); 2.35 (1H, dd, *J* = 16.6, *J* = 9.1, CH_2CO); 2.54 (2H, q, *J* = 7.5, CH_2), 2.74 (1H, dd, *J* = 15.8, *J* = 6.2, CH_2(4)); 2.77-2.84 (2H, m, CH_2CO + CH(3)); 3.60 (3H, s, OCH_3), 7.11-7.49 (4H, m, 4CH-Ar); 9.81 (1H, s, NH(1)); 9.89 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 16.19, 18.19, 27.26, 28.05, 36.41, 36.49, 51.39, 102.10, 119.58, 128.32, 137.39, 138.88, 147.78, 167.43, 169.61, 172.78. IR, ν (cm^{-1}): 1587 (C=O, amide I); 1526 (C=O, amide II). HRMS: m/z calcd for $C_{18}H_{22}N_2O_5$, 347.1603; found, 347.1605.

Methyl 3-[2-(4-allyloxyanilino)-2-oxoethyl]-6-methyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3i.** Yield 65%, colorless powdery compound, m.p. 185-186 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 2.19 (3H, s, CH_3), 2.28 (1H, t, *J* = 14.1, CH_2(4)); 2.33 (1H, dd, *J* = 16.8, *J* = 9.3, CH_2CO); 2.73 (1H, dd, *J* = 15.8, *J* = 6.1, CH_2(4)); 2.76-2.84 (2H, m, CH_2CO + CH(3)); 3.60 (3H, s, OCH_3), 4.51 (2H, d, *J* = 5.2, OCH_2); 5.24 (1H, dd, *J* = 10.5, *J* = 1.5, =CH_2); 5.37 (1H, dd, *J* = 17.3, *J* = 1.7, =CH_2); 5.98-6.06 (1H, m, -CH=); 6.87-7.49 (4H, m, 4CH-Ar); 9.81 (1H, s, NH(1)); 9.83 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 18.19, 27.26, 36.40, 36.43, 51.39, 68.78, 102.10, 115.12, 117.77, 120.95, 133.03, 134.34, 147.77, 154.43, 167.43, 169.32, 172.79. IR, ν (cm^{-1}): 1593 (C=O, amide I); 1512 (C=O, amide II). HRMS: m/z calcd for $C_{19}H_{22}N_2O_5$, 359.1603; found, 359.1607.

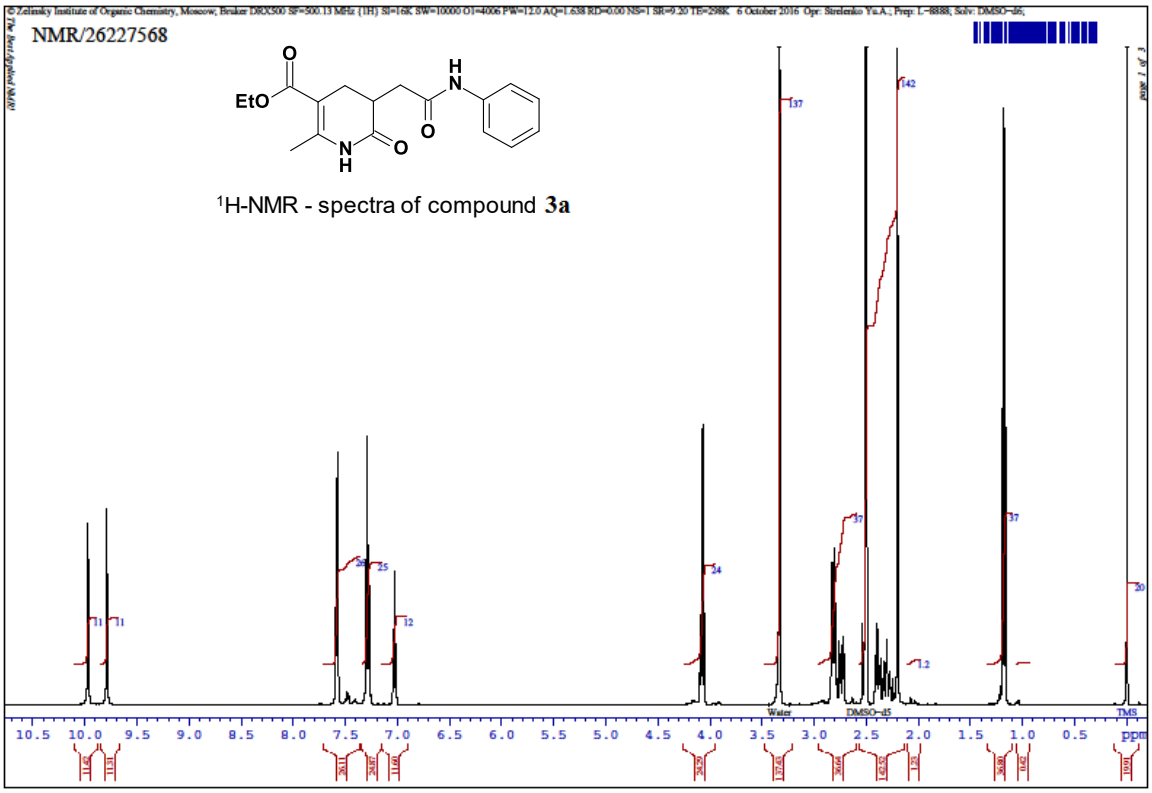
Methyl 3-[2-(3,4-dichloroanilino)-2-oxoethyl]-6-methyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3j.** Yield 65%, colorless powdery compound, m.p. 216-217 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 2.20 (3H, s, CH_3); 2.31 (1H, t, *J* = 13.6, CH_2(4)); 2.42 (1H, dd, *J* = 17.2, *J* = 8.8, CH_2CO); 2.75 (1H, dd, *J* = 15.8, *J* = 6.4, CH_2(4)); 2.79-2.86 (2H, m, CH_2CO + CH(3)); 3.61 (3H, s, OCH3), 7.46-8.01 (3H, m, 3CH-Ar); 9.82 (1H, s, NH(1)); 10.28 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 18.09, 27.17, 36.18, 36.47, 51.30, 102.08, 119.37, 120.52, 124.78, 131.01, 131.33, 139.64, 147.66, 167.30, 170.40, 172.52. IR, ν (cm^{-1}): 1631 (C=O, amide I); 1528 (C=O, amide II). HRMS: m/z calcd for $C_{16}H_{16}Cl_2N_2O_4$, 375.0502; found, 375.0505.

Methyl 3-[2-(3-chloro-2-methylanilino)-2-oxo-ethyl]-6-methyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3k.** Yield 70%, colorless powdery compound, m.p. 220-221 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 2.17 (3H, s, CH_3); 2.19 (3H, s, CH_3); 2.29 (1H, t, *J* = 14.0, CH_2(4)); 2.39 (1H, dd, *J* = 15.1, *J* = 7.3, CH_2CO); 2.70-2.82 (3H, m, CH_2(4) + CH_2CO + CH(3)); 3.58 (3H, s, OCH_3), 7.10-7.30 (3H, m, 3CH-Ar); 9.60 (1H, s, NH(1)); 9.81 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 15.62, 18.25, 27.30, 35.98, 36.67, 51.48, 59.89, 102.17, 125.16, 126.52, 127.30, 131.07, 134.27, 138.45, 147.85, 167.50, 170.17, 172.86. IR, ν (cm^{-1}): 1602 (C=O, amide I); 1521 (C=O, amide II). HRMS: m/z calcd for $C_{17}H_{19}ClN_2O_4$, 353.1078; found, 353.1081.

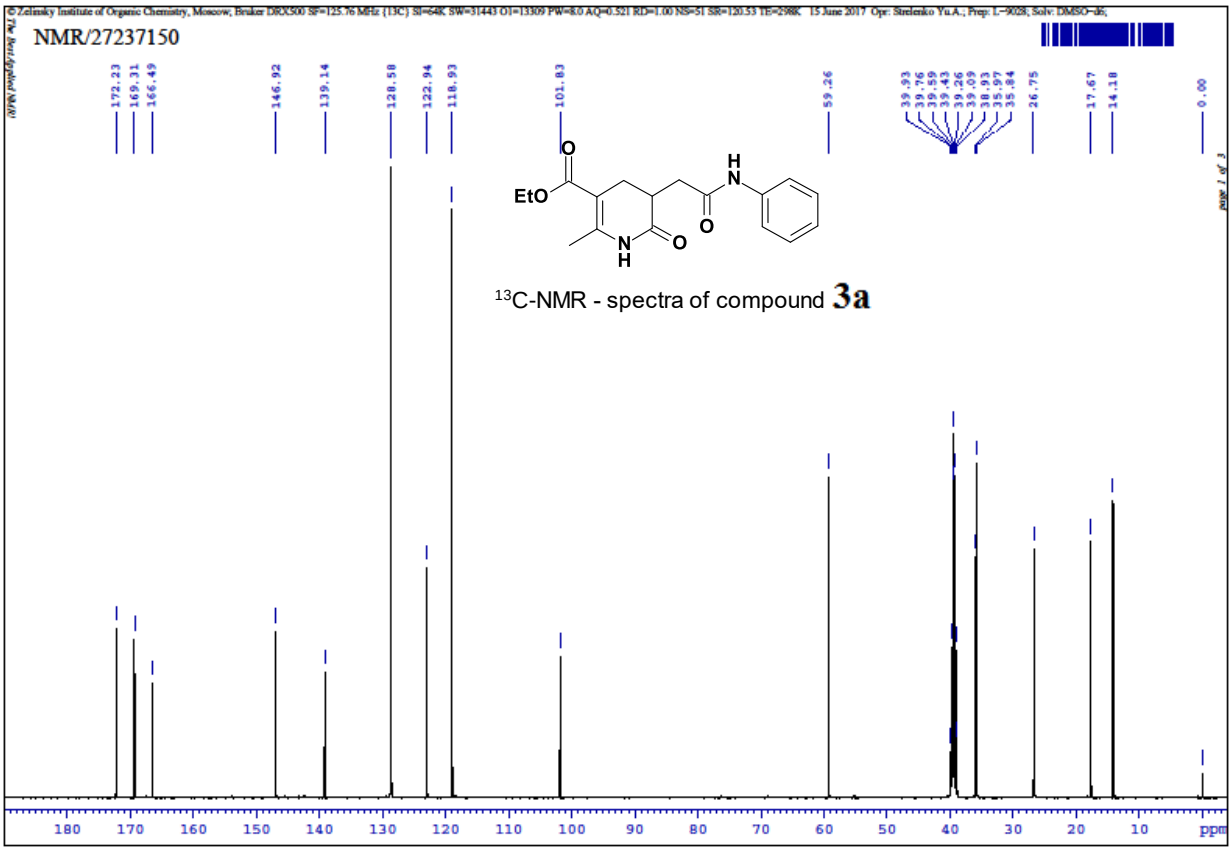
Methyl 3-[2-(4-ethylanilino)-2-oxoethyl]-6-isopropyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3l.** Yield 45%, colorless powdery compound, m.p. 146-147 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 1.08 (3H, s, CH_3), 1.10 (3H, s, CH_3), 1.15 (3H, t, *J* = 7.6, CH3); 2.28-2.39 (2H, m, CH_2(4) + CH_2CO); 2.54 (2H, q, *J* = 7.6, Ar-CH_2), 2.72-2.84 (3H, m, CH_2(4) + CH_2CO + CH(3)); 3.61 (3H, s, OCH3), 4.07 (1H, m, CH); 7.11-7.51 (4H, m, 4CH-Ar); 9.51 (1H, s, NH(1)); 9.89 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 15.59, 18.96, 19.03, 26.79, 26.98, 27.48, 35.80, 50.96, 101.87, 119.01, 127.73, 136.83, 138.30, 154.99,

166.88, 169.05, 172.78. IR, ν (cm^{-1}): 1579 (C=O, amide I); 1532 (C=O, amide II). HRMS: m/z calcd for $C_{20}H_{26}N_2O_4$, 359.1967; found, 359.1965.

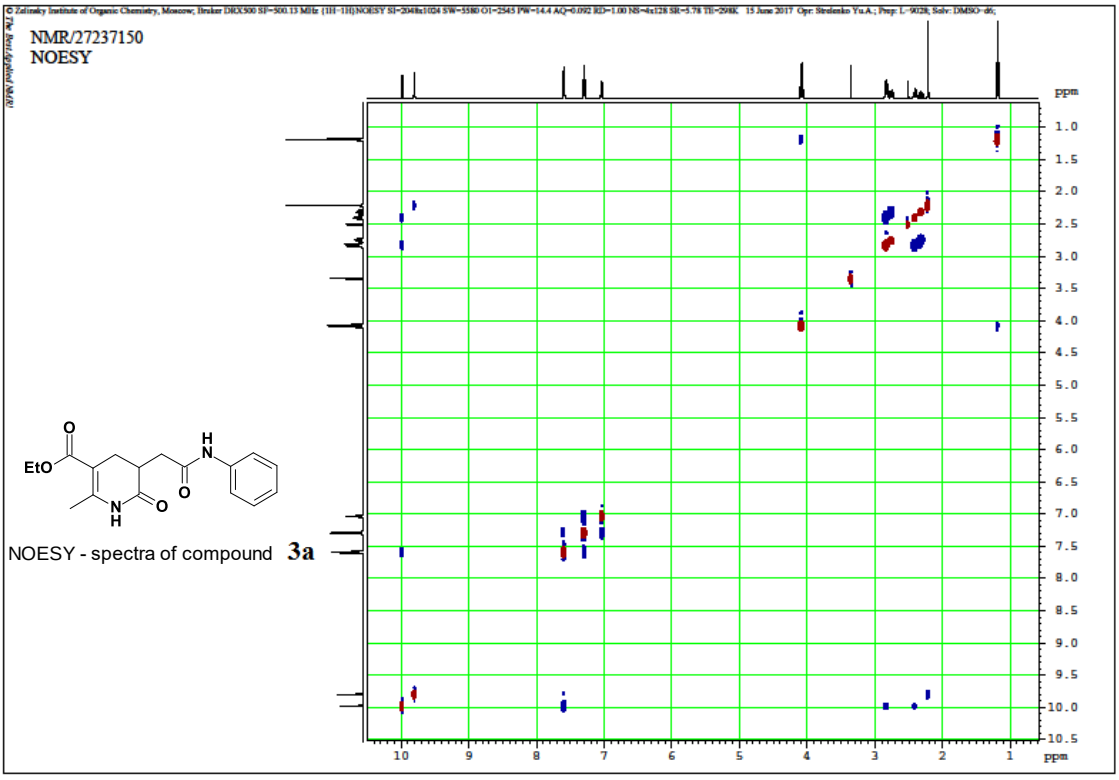
Methyl 3-[2-(4-chloroanilino)-2-oxoethyl]-6-isopropyl-2-oxo-3,4-dihydro-1H-pyridine-5-carboxylate **3m.** Yield 55%, colorless powdery compound, m.p. 206-207 °C. ^{1}H NMR, ((δ, ppm., *J*/Hz): 1.04 (3H, s, CH_3), 1.05 (3H, s, CH_3), 2.28 (1H, t, *J* = 15.3, CH_2(4)), 2.36 (1H, dd, *J* = 15.2, *J* = 6.8, CH_2CO), 2.68-2.82 (3H, m, CH_2(4) + CH_2CO + CH(3)), 4.03 (1H, m, CH); 7.29-7.50 (4H, m, 4CH-Ar); 9.50 (1H, s, NH(1)); 10.09 (1H, s, NHCO). ^{13}C NMR (δ, ppm): 19.59, 19.69, 27.42, 27.62, 36.35, 36.49, 51.63, 101.55, 121.06, 127.09, 129.13, 138.72, 155.65, 167.52, 170.18, 173.36. IR, ν (cm^{-1}): 1597 (C=O, amide I); 1544 (C=O, amide II). HRMS: m/z calcd for $C_{18}H_{21}ClN_2O_4$, 367.1234; found, 367.1230.



^{1}H-NMR - spectra of compound **3a**

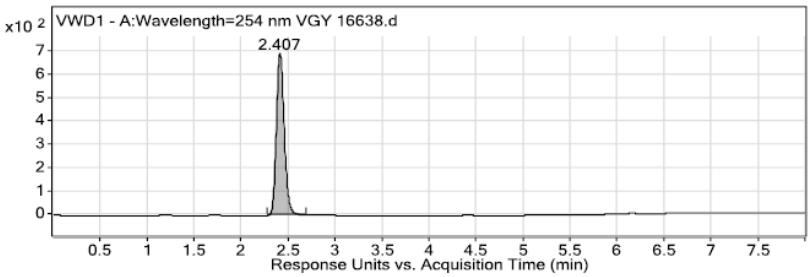


^{13}C-NMR - spectra of compound **3a**



NOESY - spectra of compound **3a**

User Chromatograms



Integration Peak List

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User Spectra

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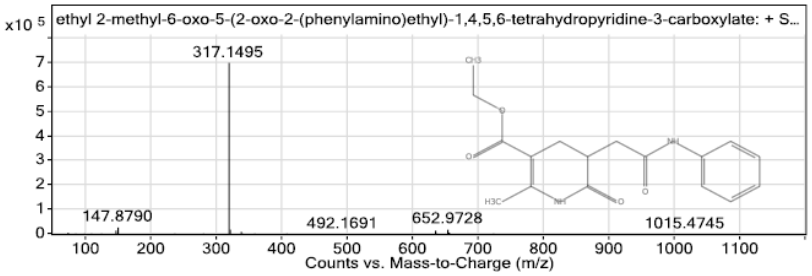

Peak List

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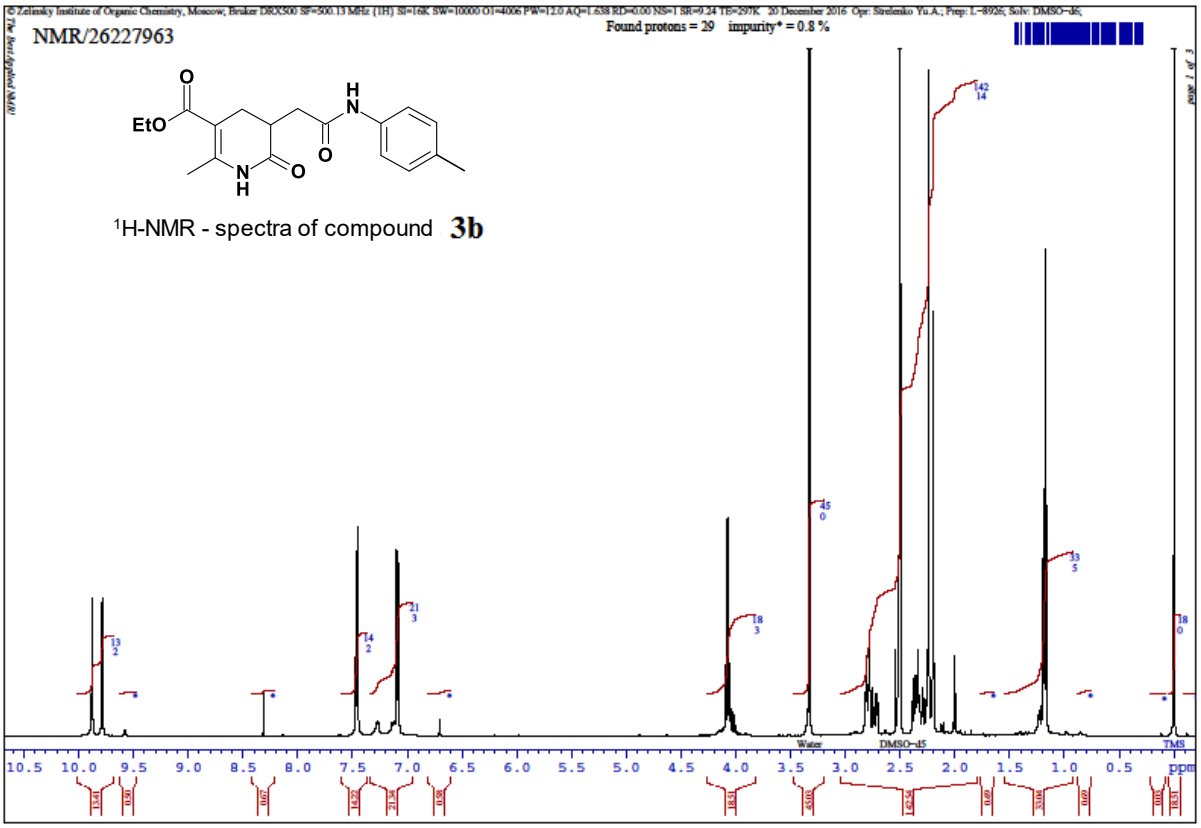
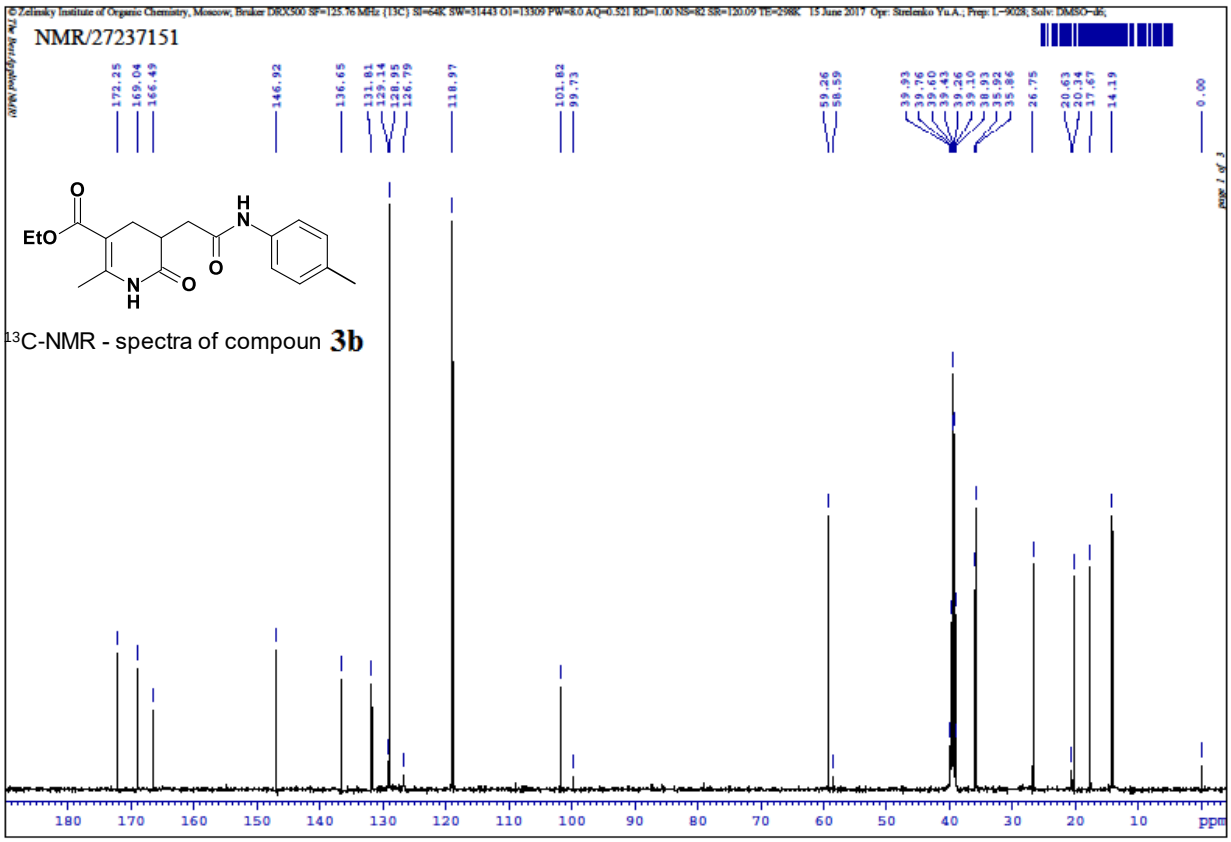
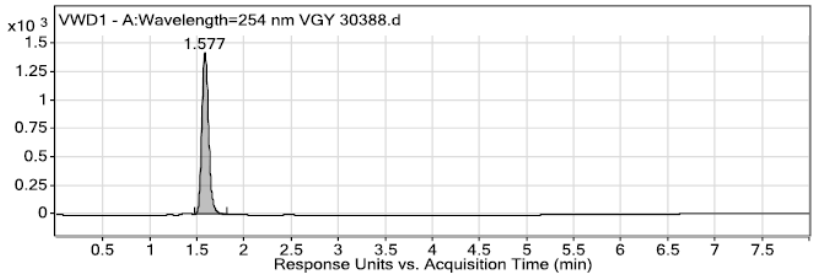


^{1}H-NMR - spectra of compound **3b**



^{13}C-NMR - spectra of compoun **3b**

User Chromatograms



Integration Peak List

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User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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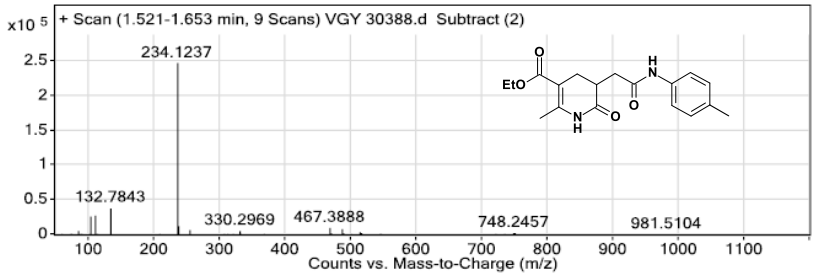

Peak List

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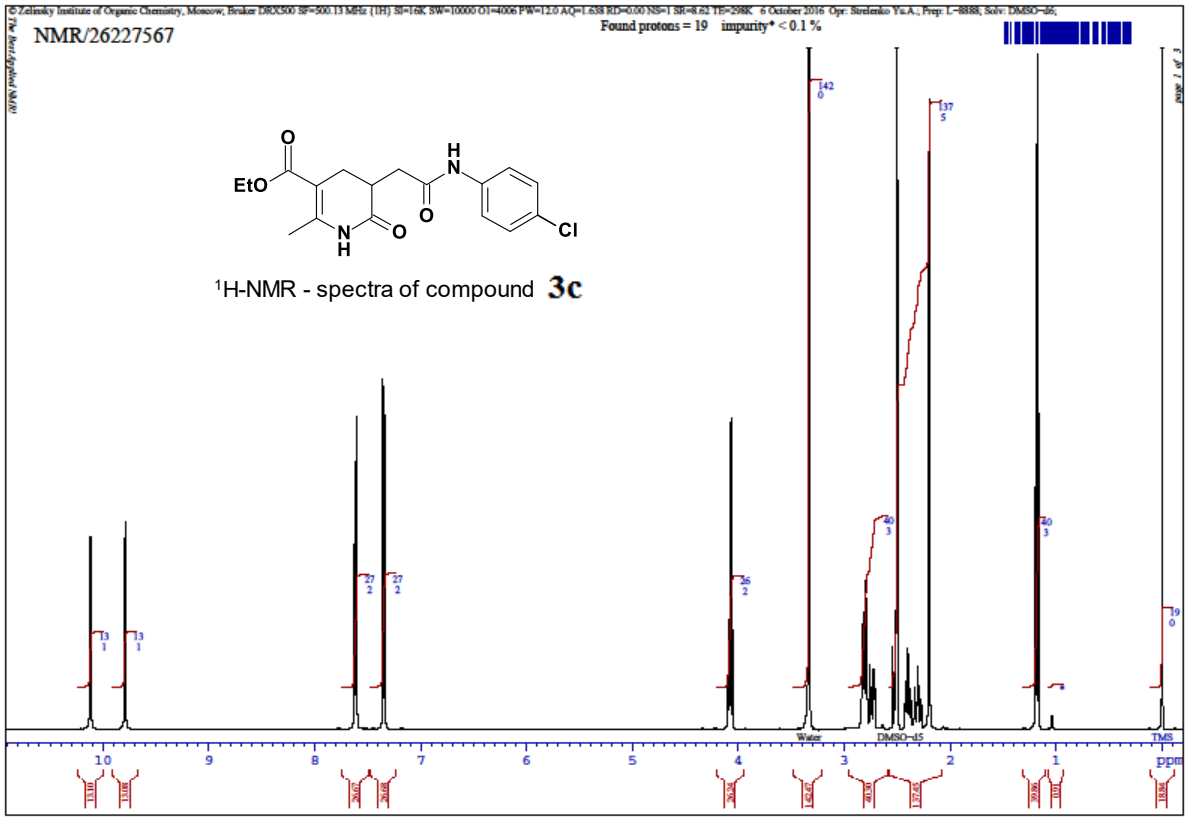
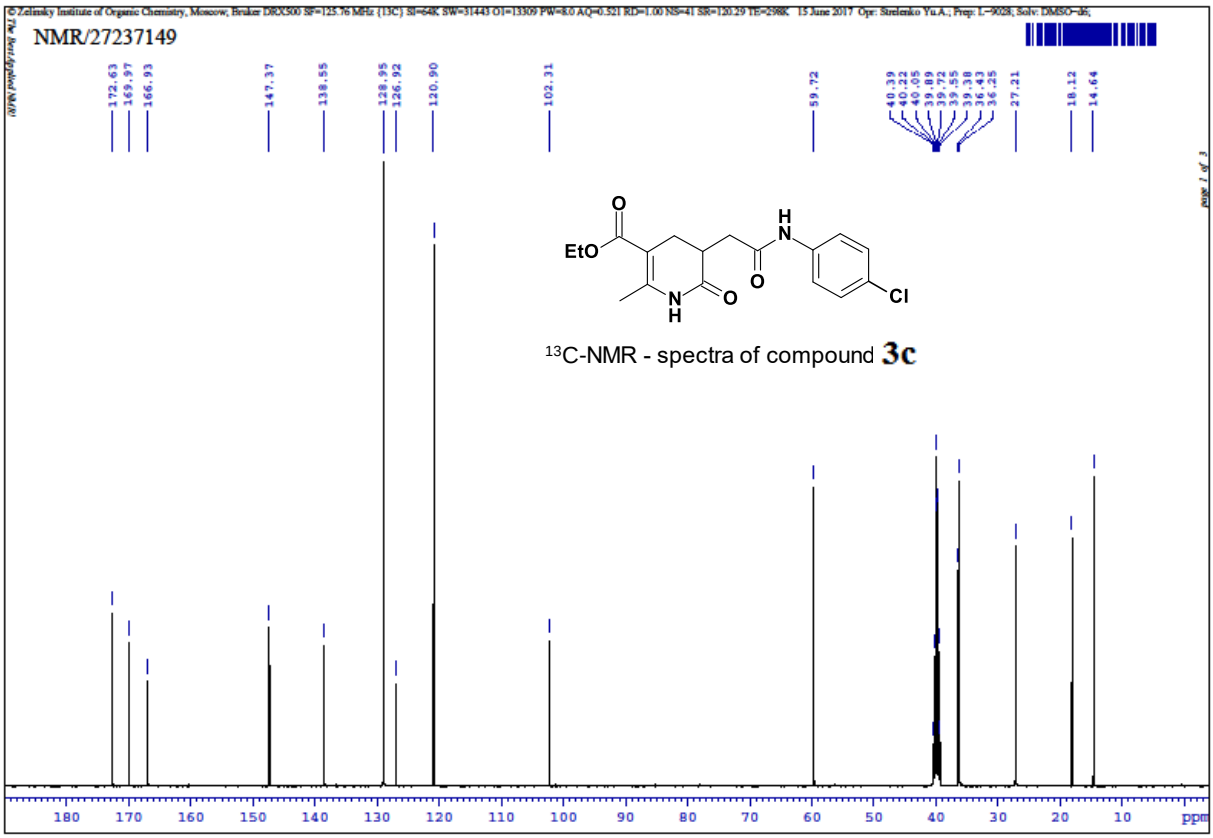
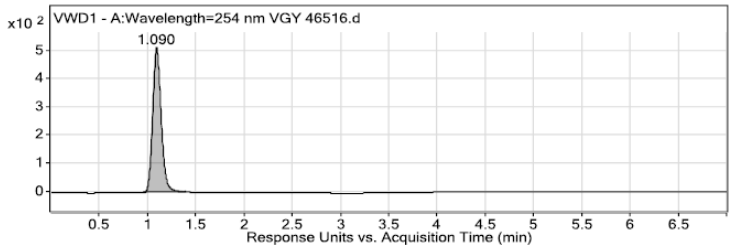




^{13}C-NMR - spectra of compound **3c**

User Chromatograms

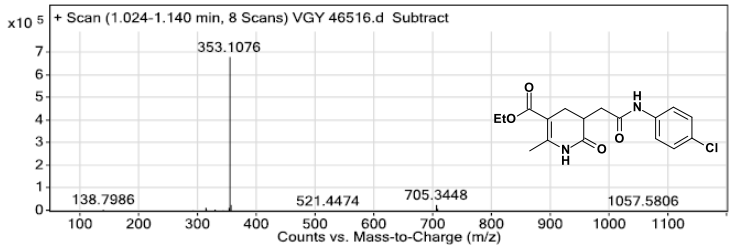


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.96	1.09	1.393	515.09	3186.13	100

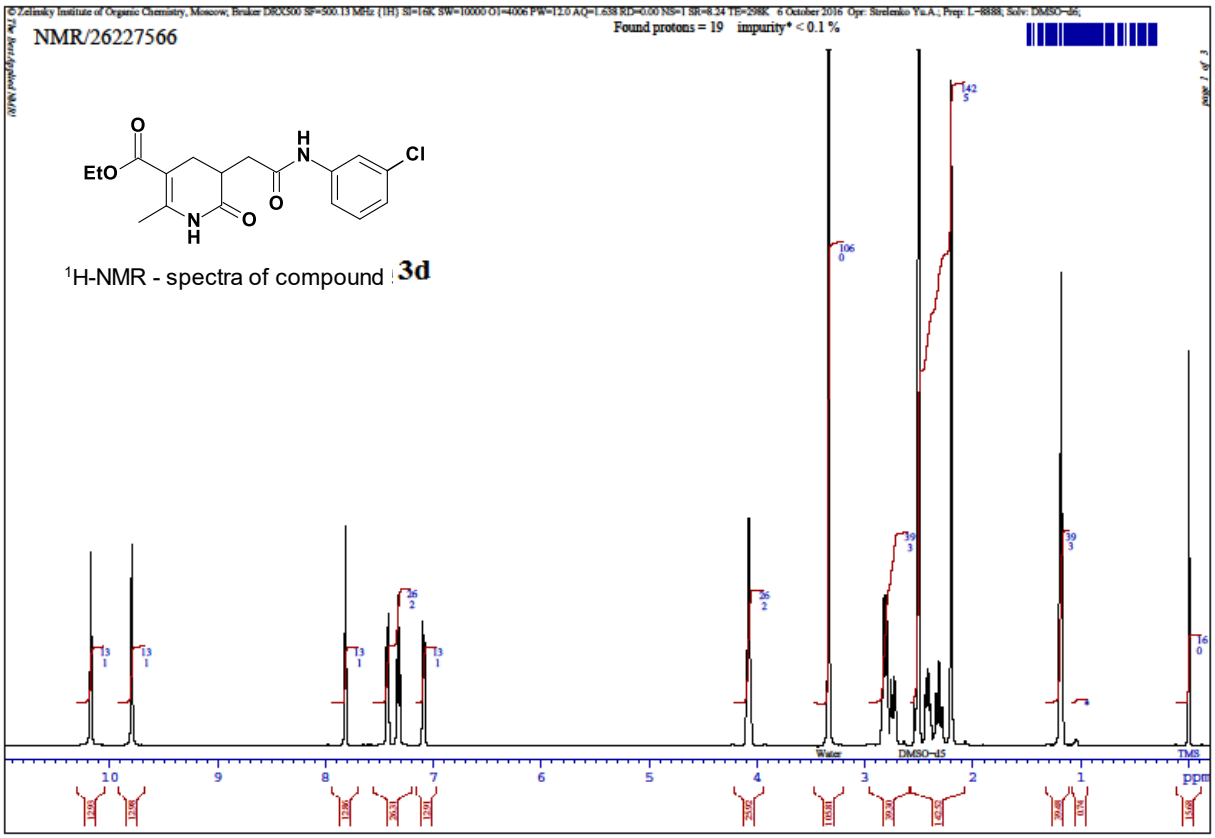
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
185	0	ESI

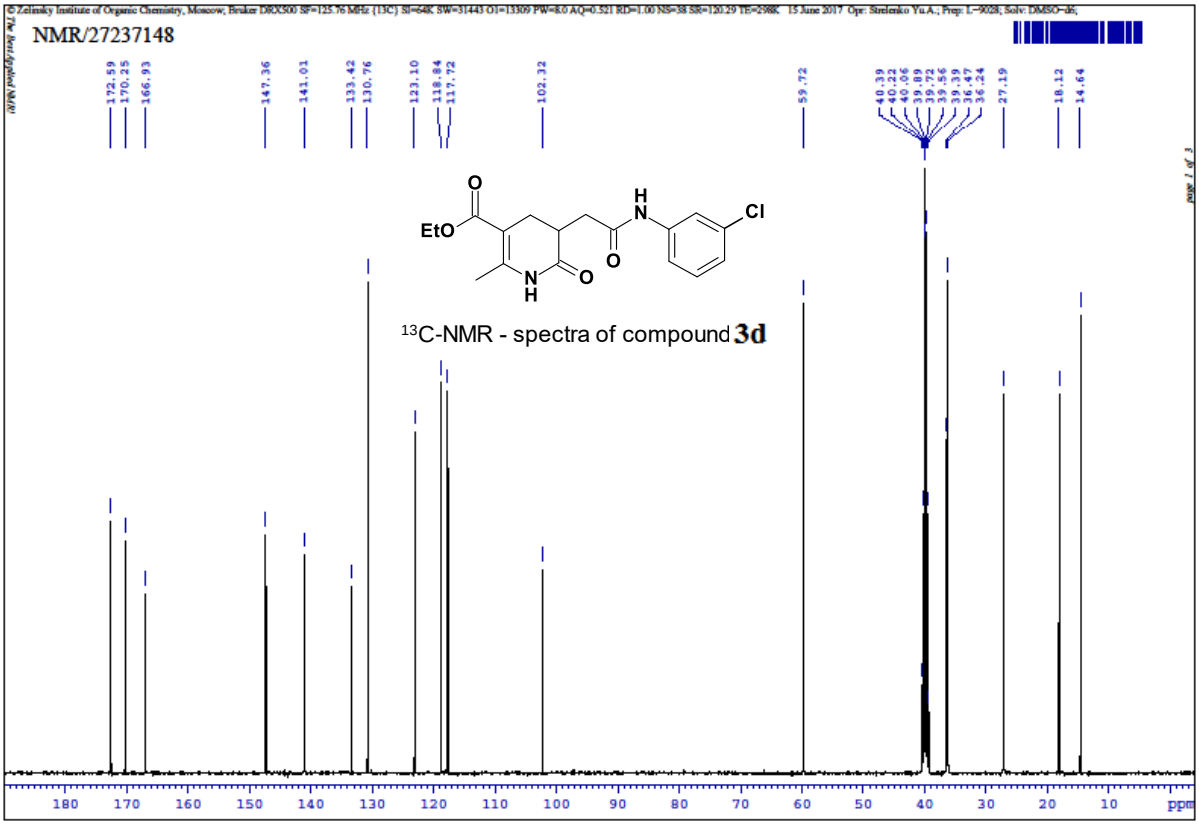


Peak List

m/z	Abund
138.7986	6911.35
290.6485	2126.38
313.1788	17489.34
314.0484	4049.19
328.7981	6388.22
340.9561	2125.51

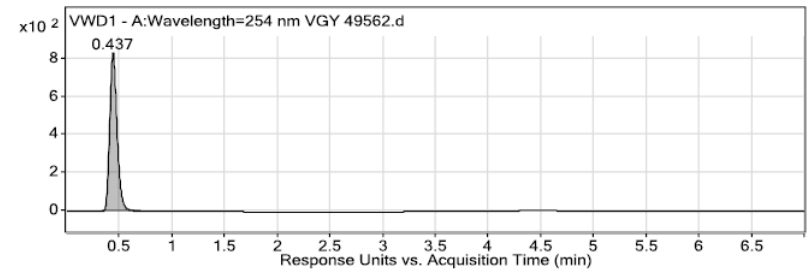


^{1}H-NMR - spectra of compound **3d**



^{13}C-NMR - spectra of compound **3d**

User Chromatograms

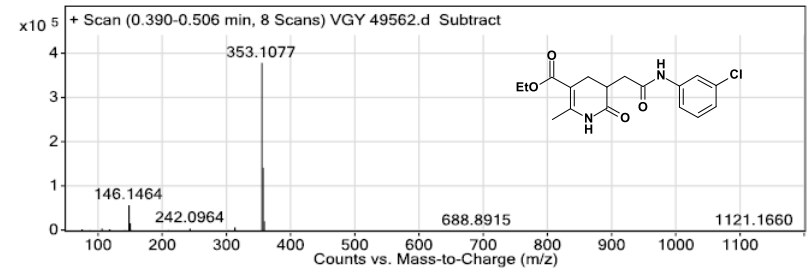


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.34	0.437	0.7	834.47	4077.9	100

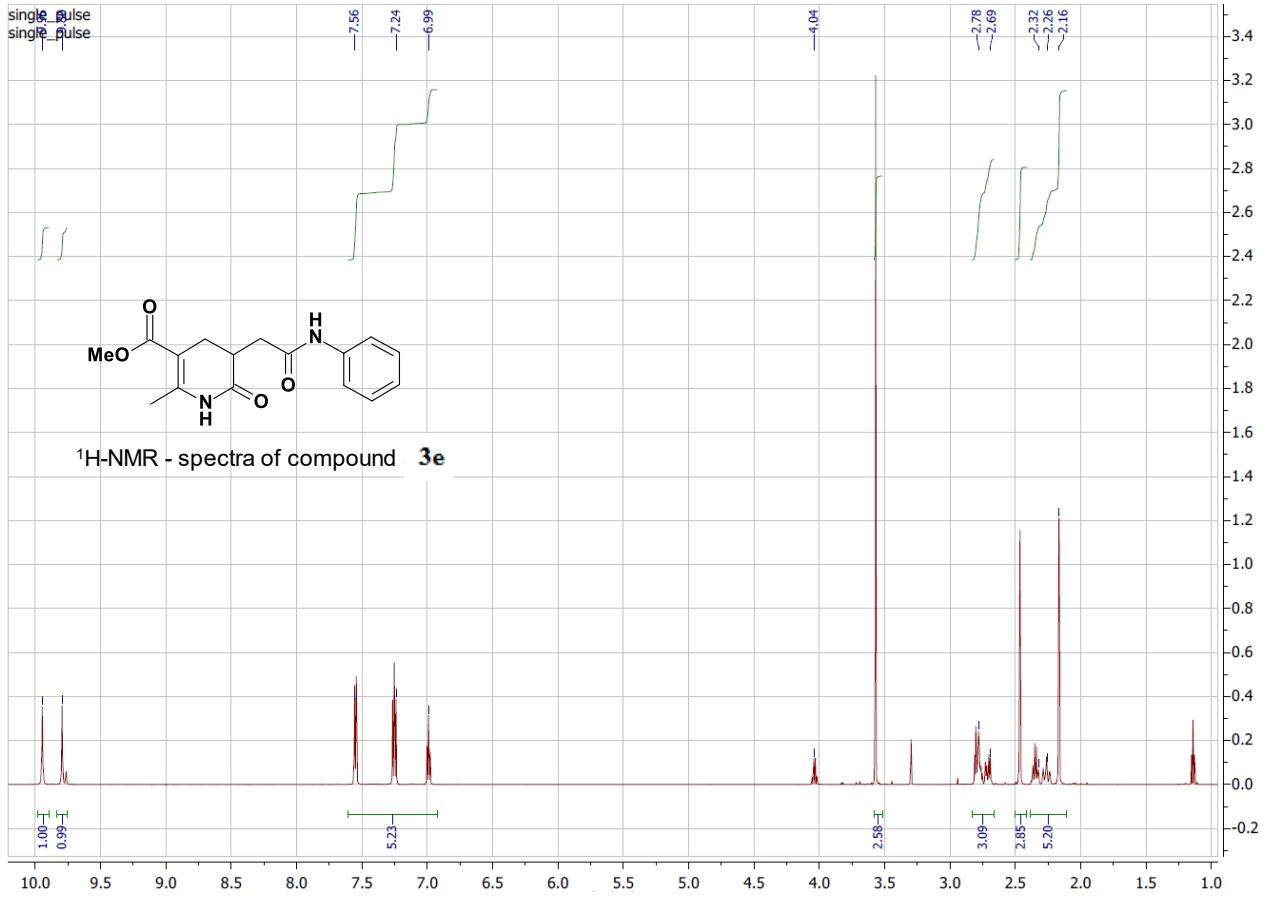
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
185	0	ESI

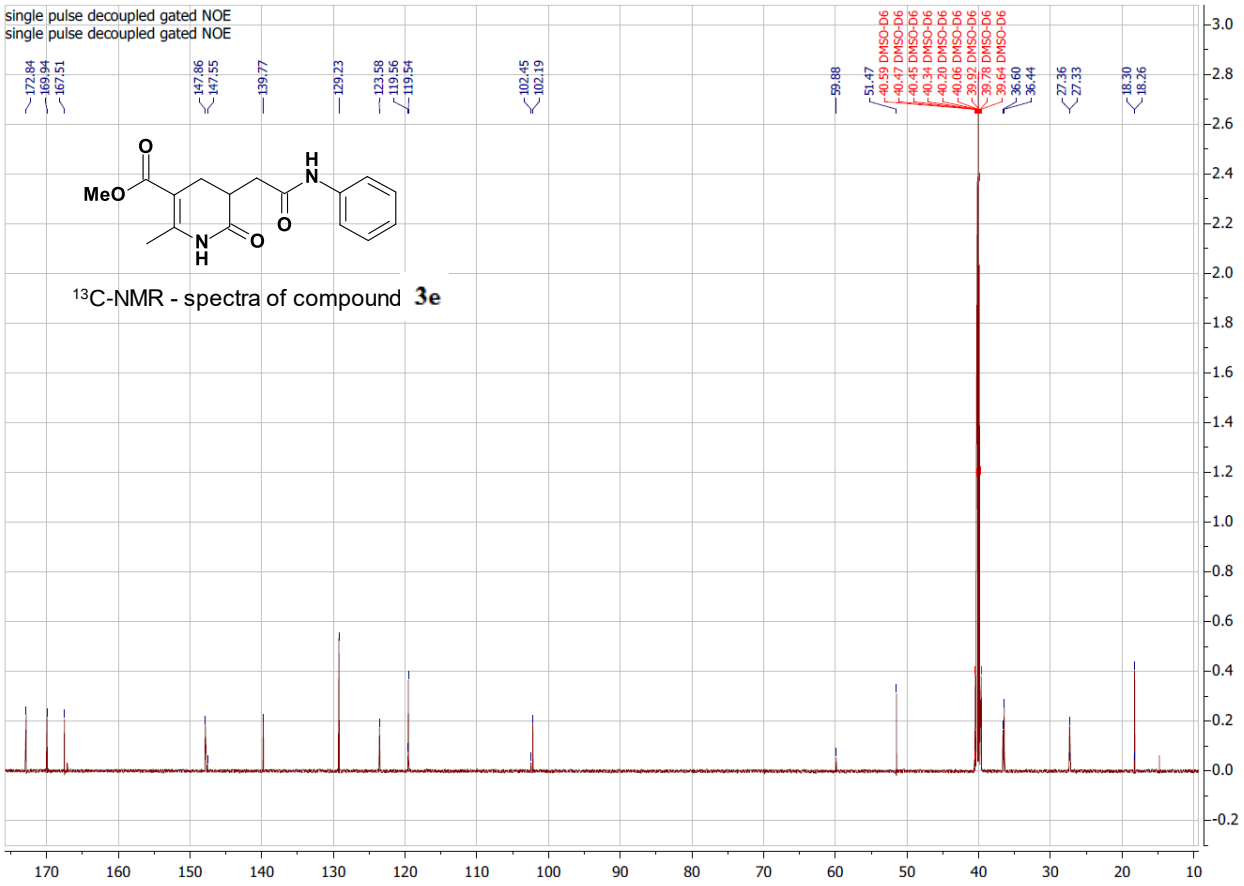


Peak List

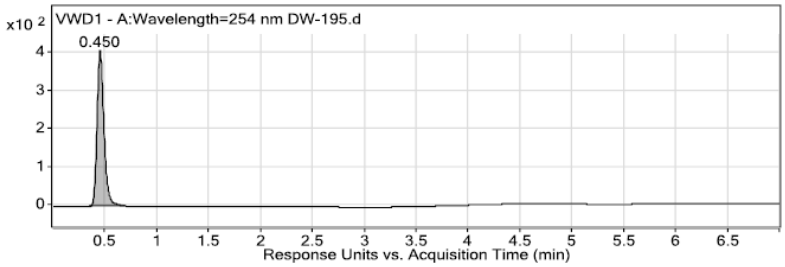
m/z	Abund
73.6757	4213.29
104.0912	6970.46
105.2662	3397.36
115.7328	4402.17
146.1464	59062.63
147.3193	4133.64



^{1}H-NMR - spectra of compound **3e**



User Chromatograms

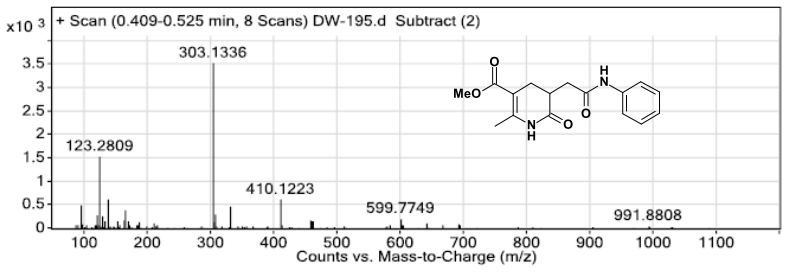


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.357	0.45	0.693	409.03	1918.38	100

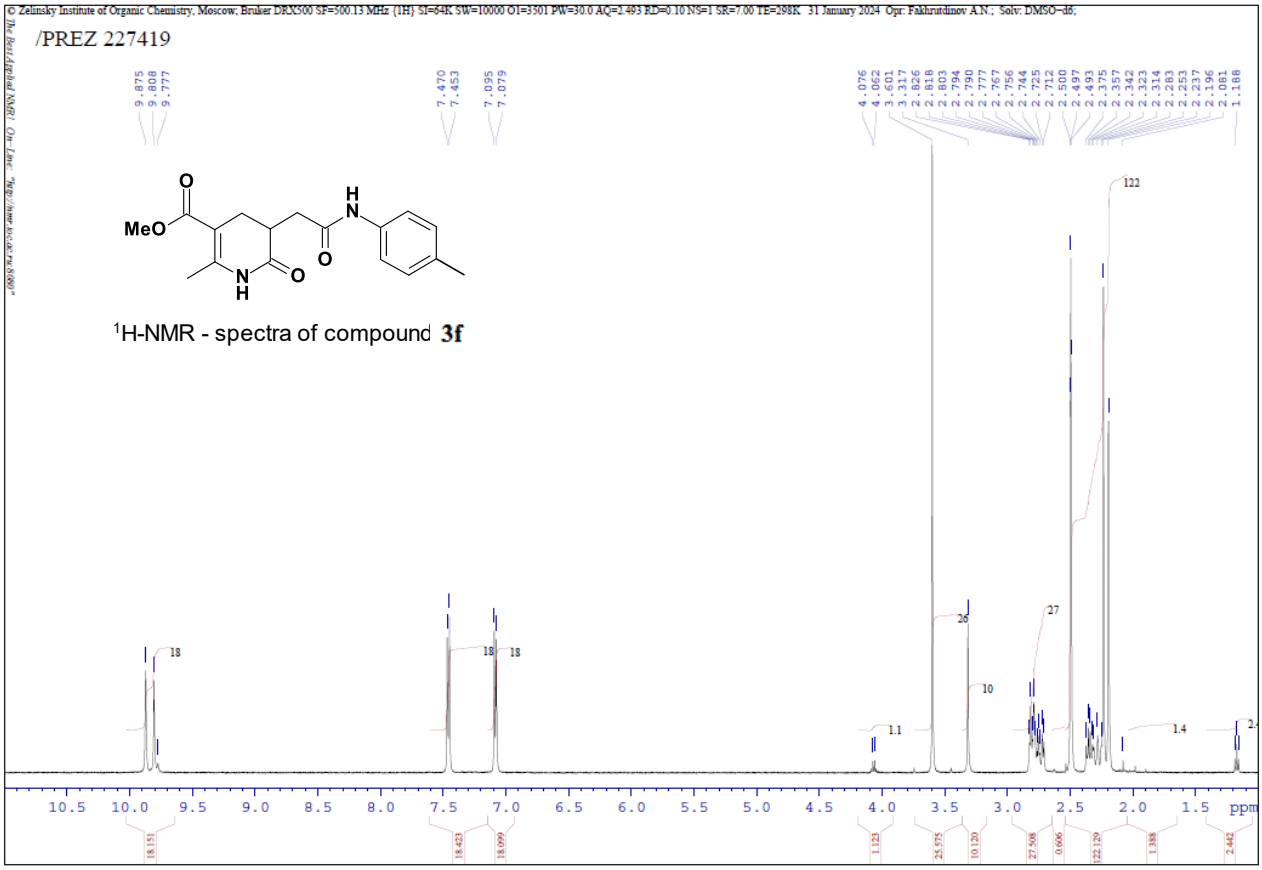
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
185	0	ESI

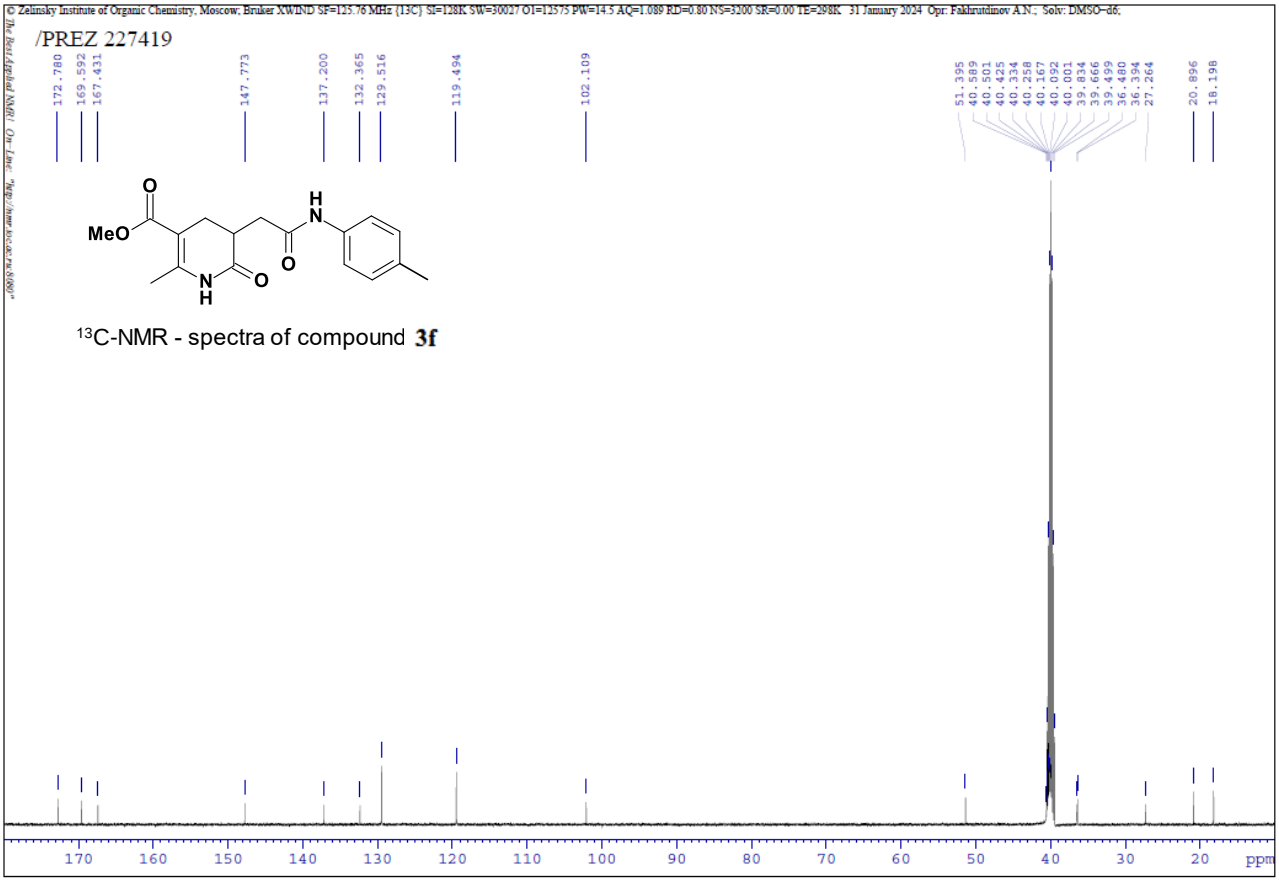


Peak List

m/z	Abund
94.0959	497.17
120.0745	293.53
123.2809	1543.96
127.2117	265.94
136.2155	634.31
152.4394	171.15

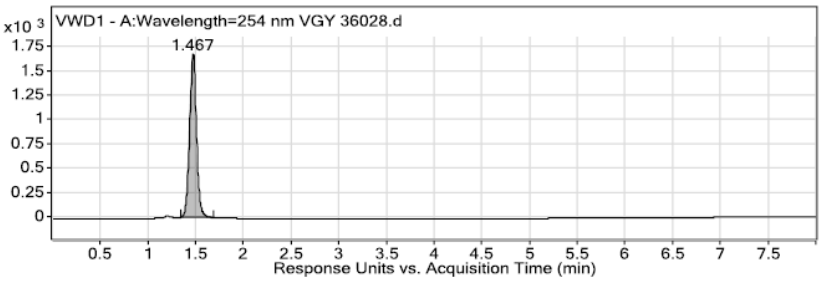


^{1}H-NMR - spectra of compound **3f**



^{13}C-NMR - spectra of compound **3f**

User Chromatograms

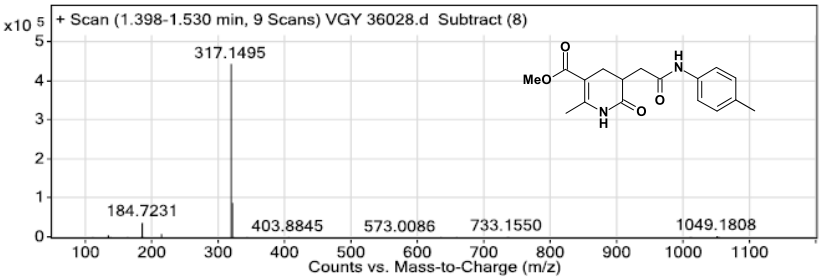


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	1.347	1.467	1.69	1682.2	8578.11	100

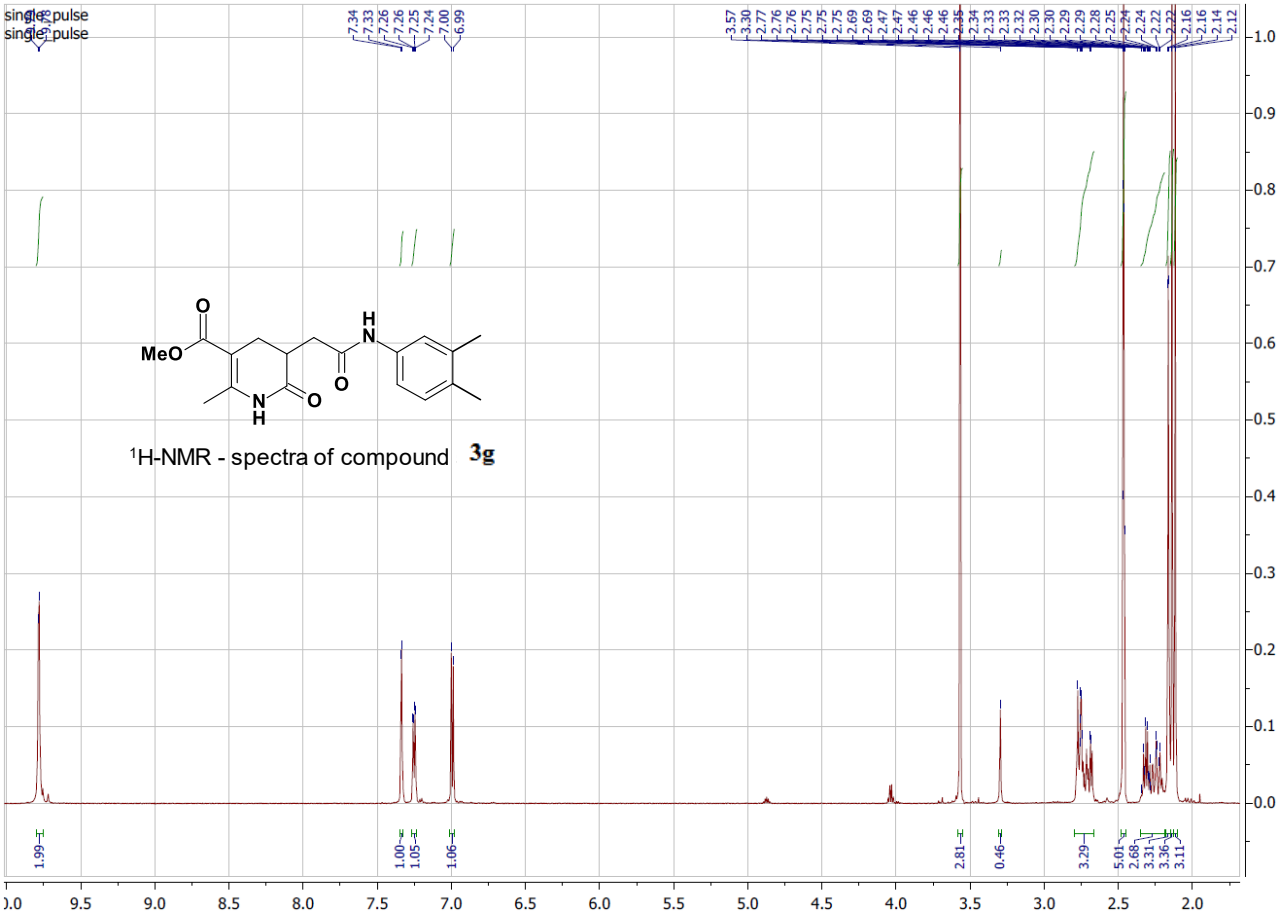
User Spectra

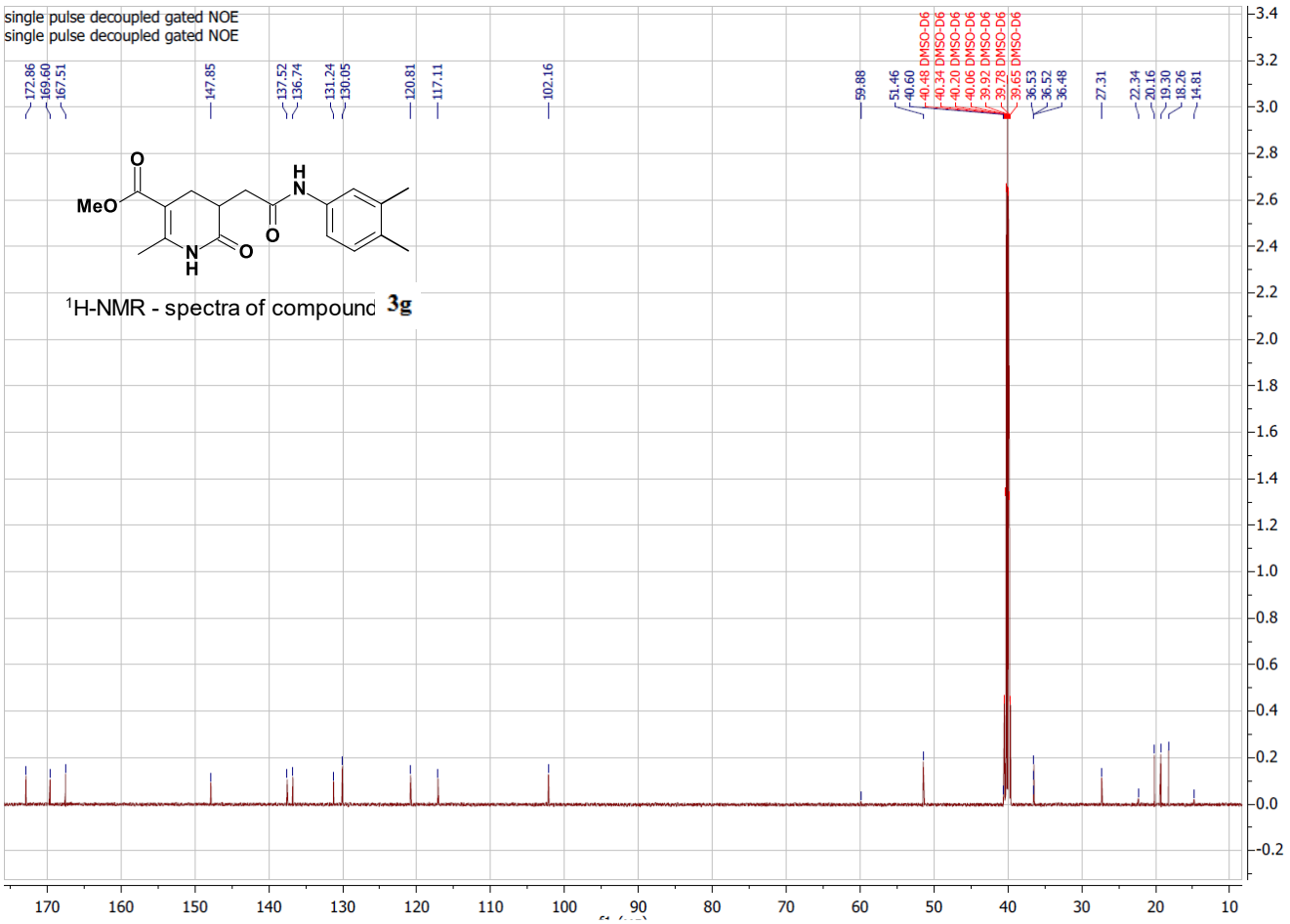
Fragmentor Voltage	Collision Energy	Ionization Mode
185	0	ESI



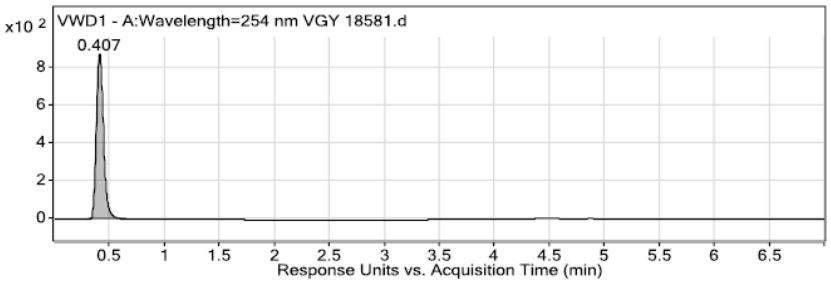
Peak List

m/z	Abund
133.5462	7561.82
184.7231	40702.13
185.8383	3589.03
213.6562	9897.22
317.1495	445238.09
318.2651	82006.85





User Chromatograms

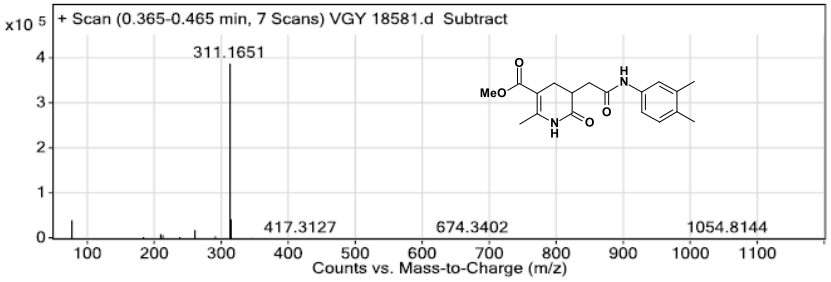


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.313	0.407	0.65	876.67	3956.2	100

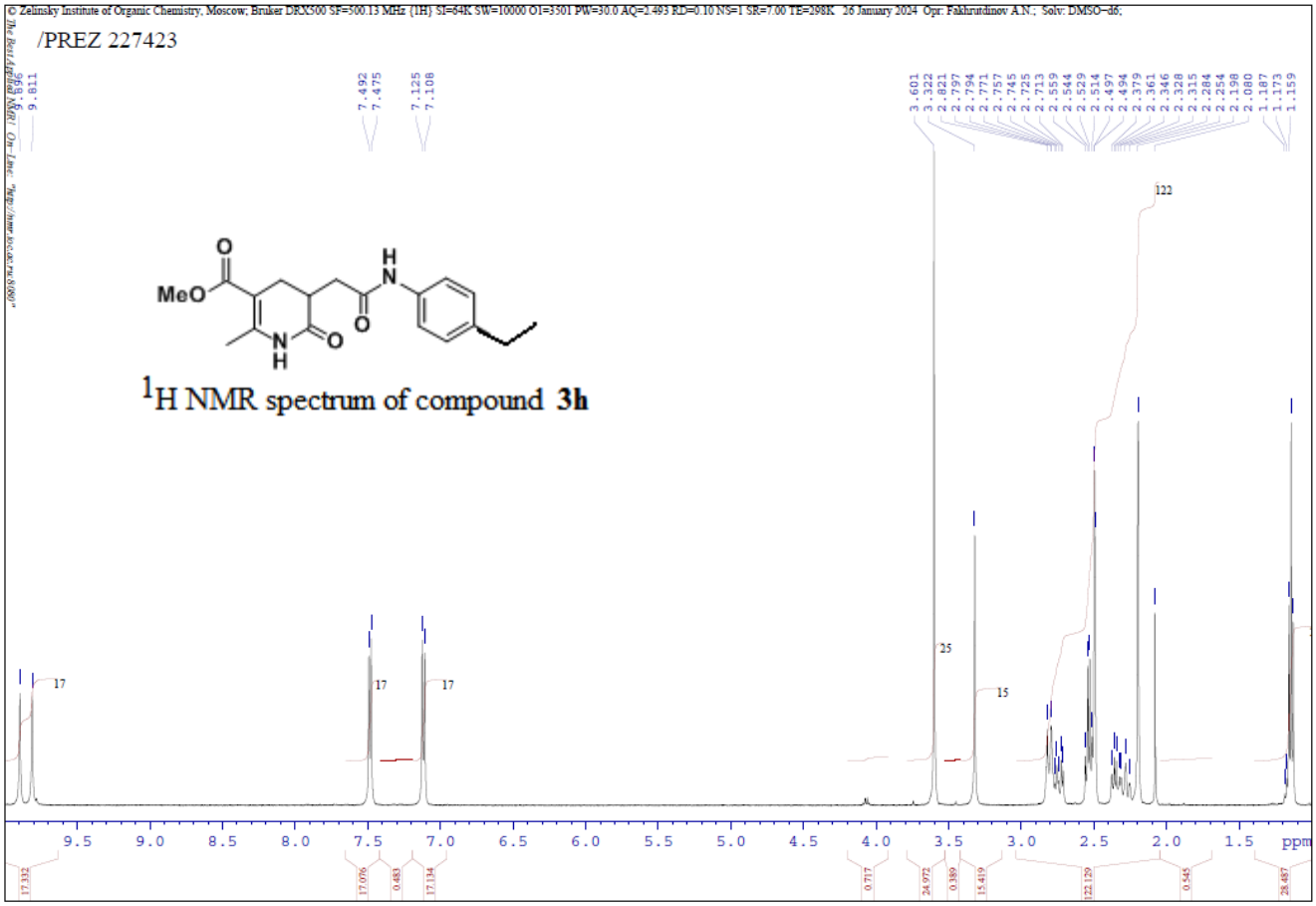
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
185	0	ESI

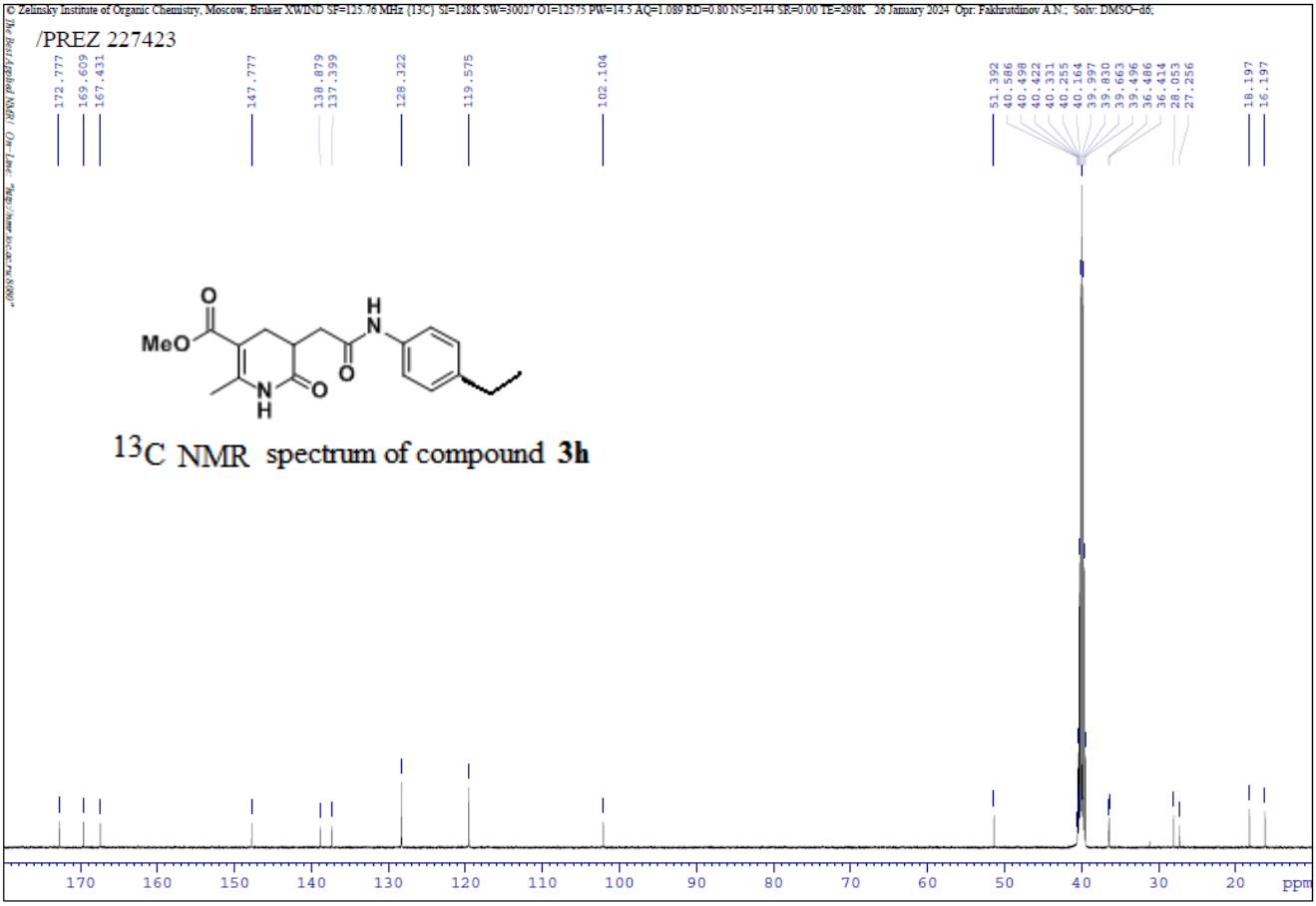


Peak List

m/z	Abund
75.9357	41548.94
77.2011	1092.92
182.1447	5663.89
185.9117	1084.31
207.4407	11842.31
208.7083	1213.26



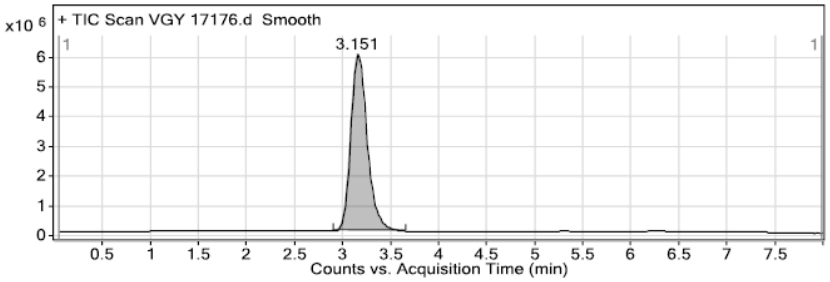
^{1}H NMR spectrum of compound **3h**



^{13}C NMR spectrum of compound **3h**

User Chromatograms

Fragmentor Voltage 185 Collision Energy 0 Ionization Mode ESI

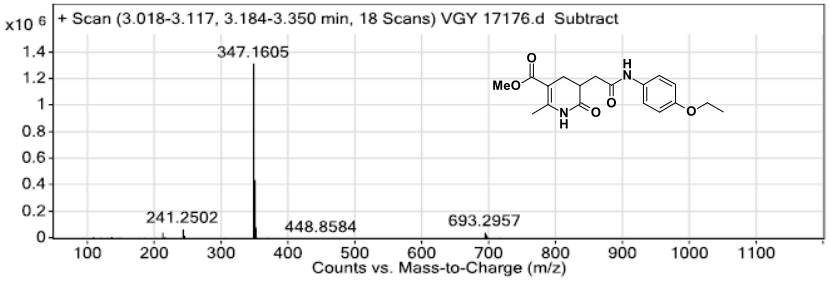


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	2.902	3.151	3.653	5928459.74	70493675.23	100

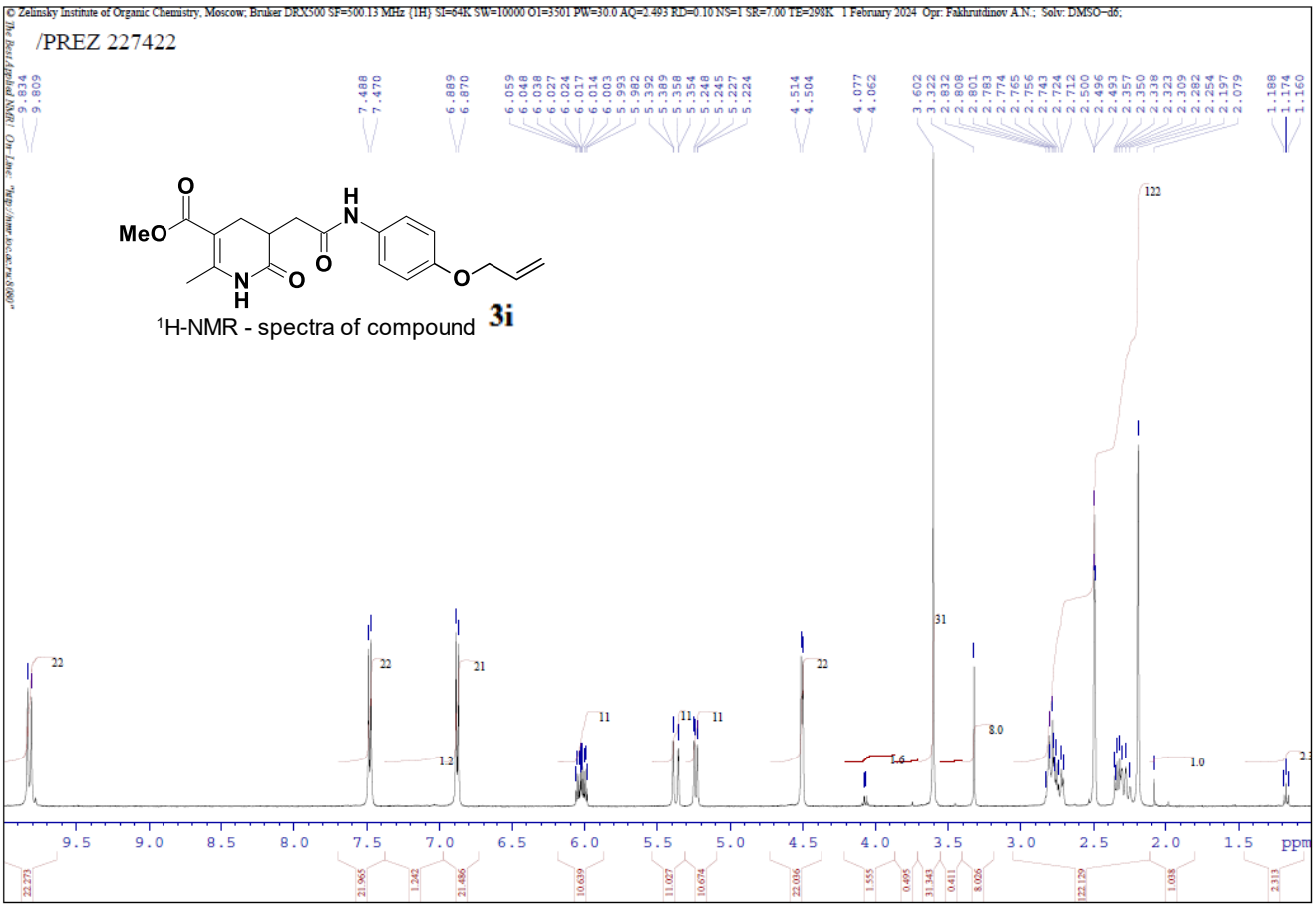
User Spectra

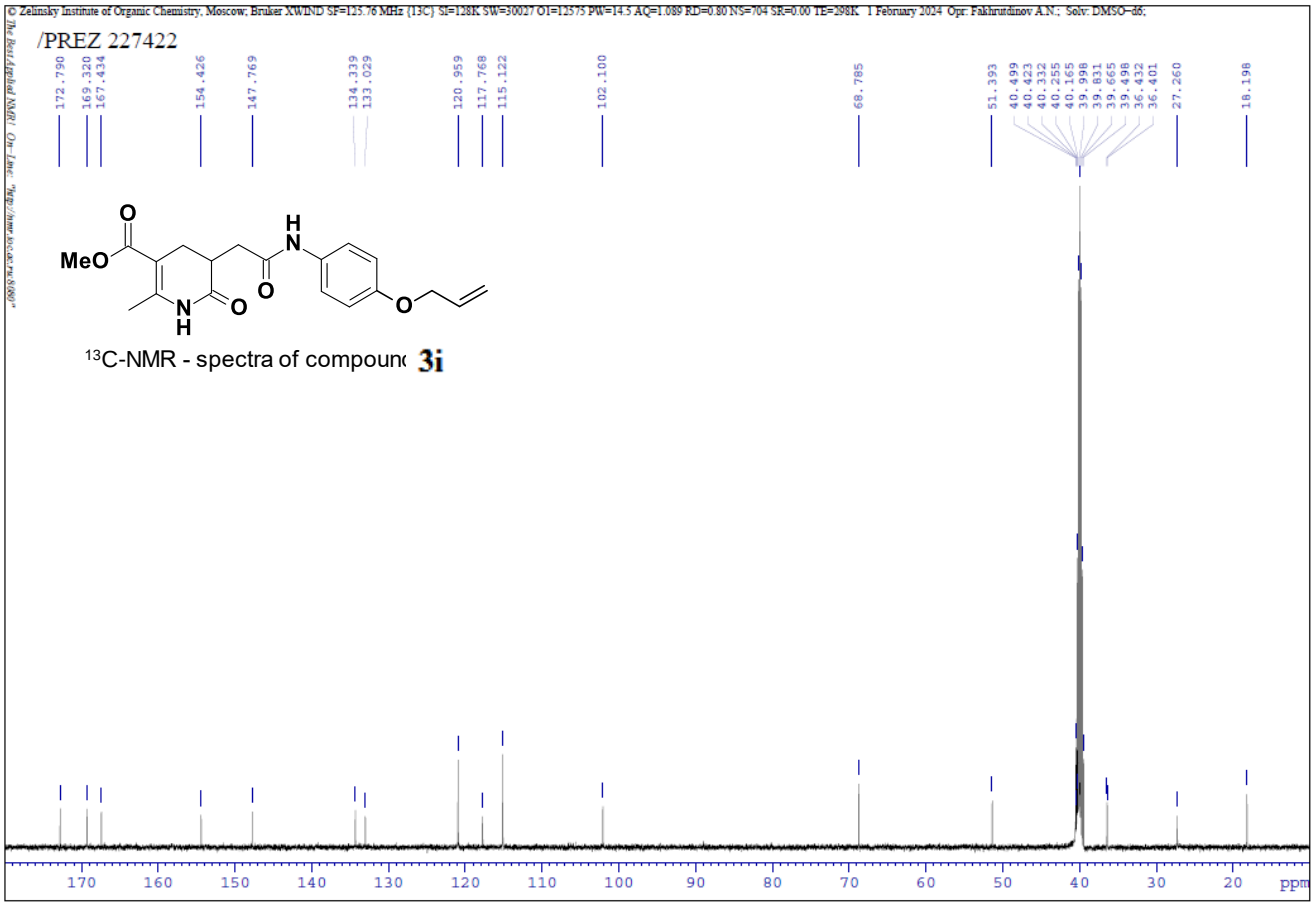
Fragmentor Voltage 185 Collision Energy 0 Ionization Mode ESI



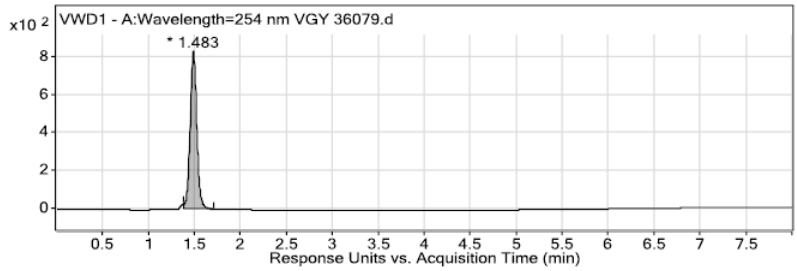
Peak List

m/z	z	Abund
106.9346		12262.53
135.4507		12564
183.2164		11310.36
211.7084		50422.05
213.7413		15757.6





User Chromatograms

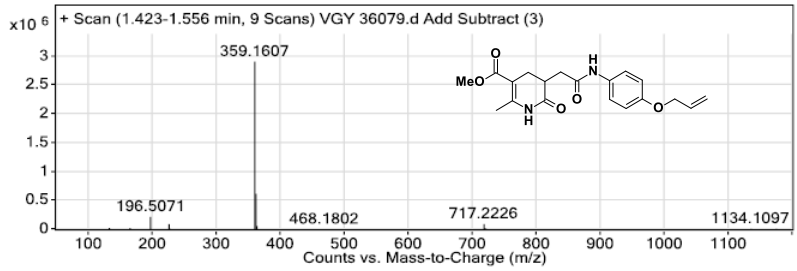


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	1.383	1.483	1.707	835.64	4227.63	100

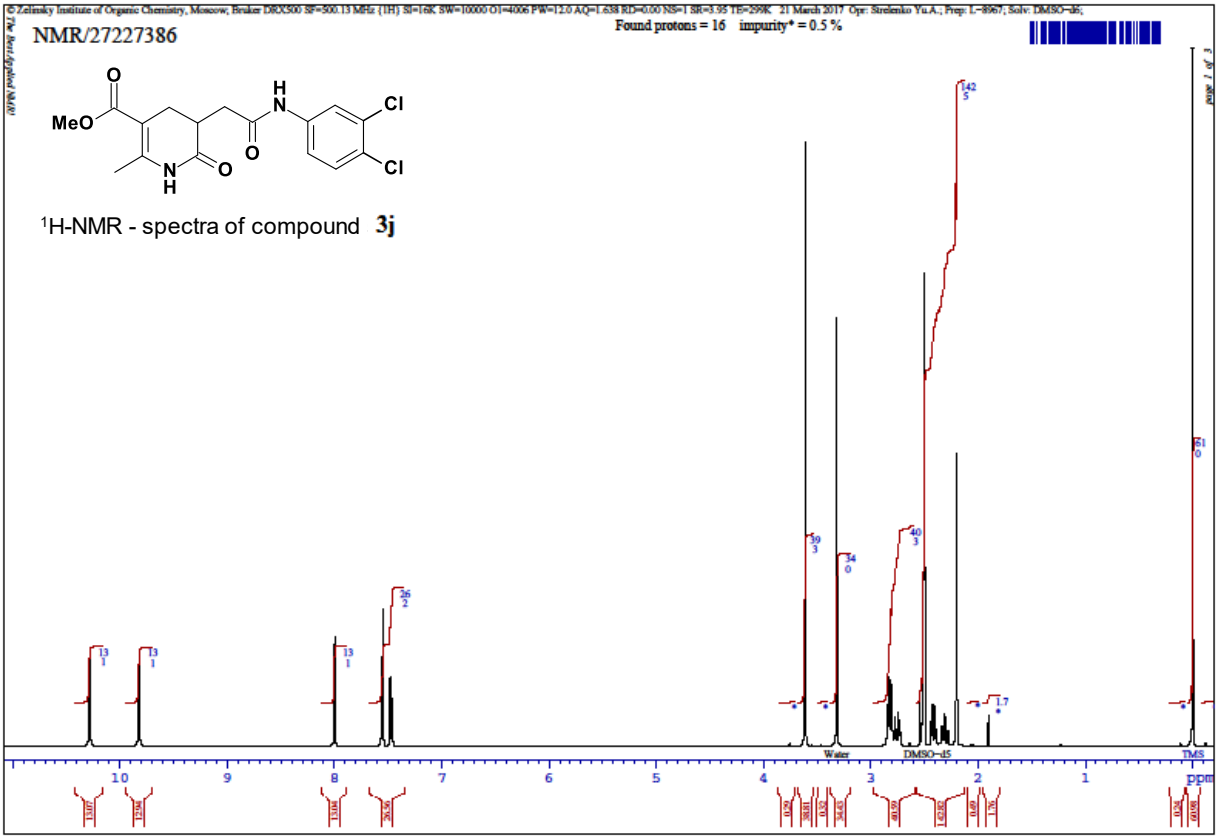
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
185	0	ESI

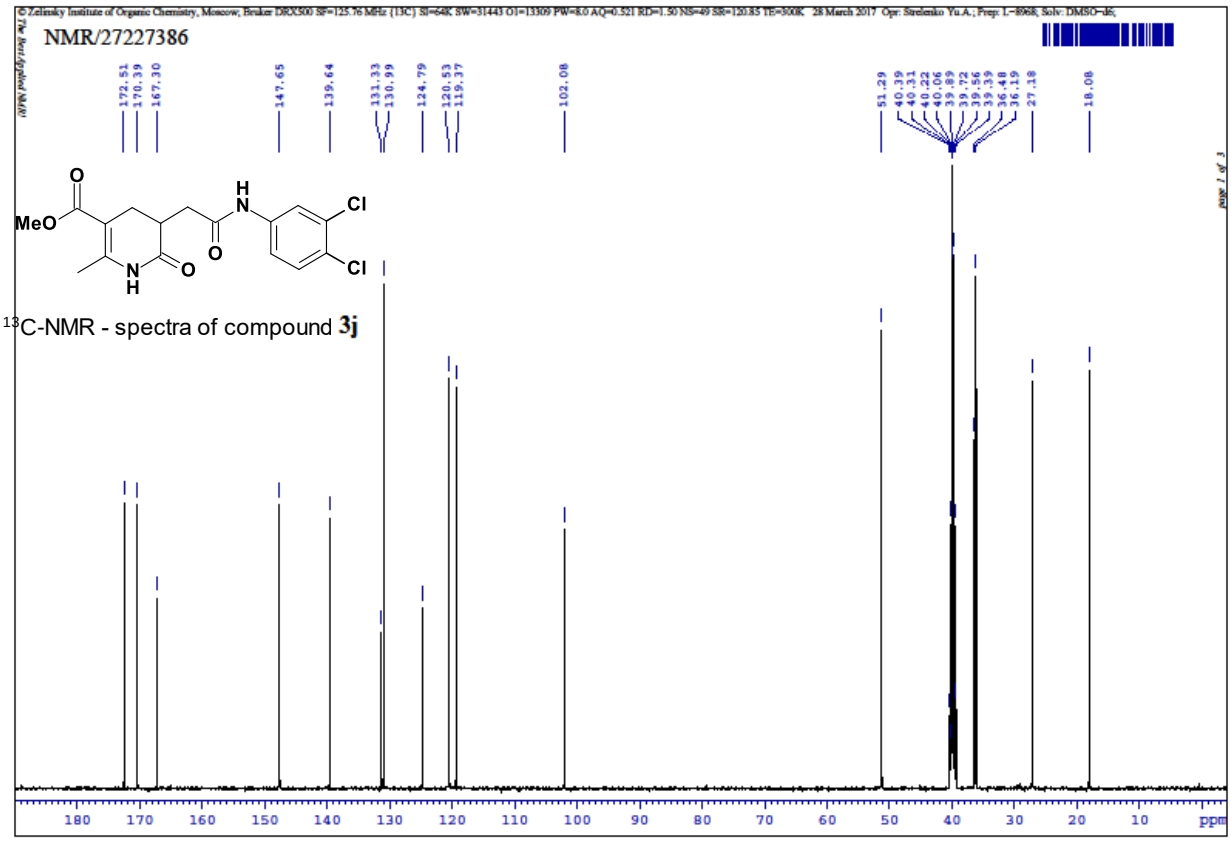


Peak List

m/z	Abund
130.9707	40780.58
163.7528	38552.06
196.5071	221756
197.601	22787.34
224.8907	98275.2
359.1607	2909324.75

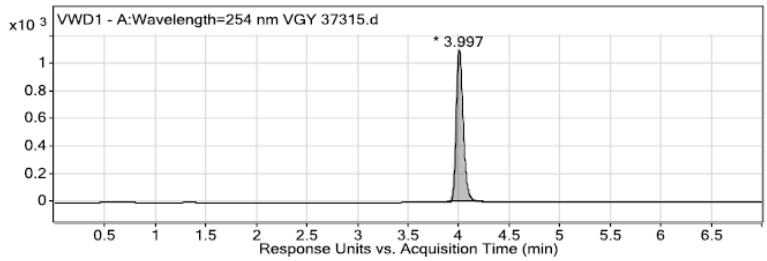


^{1}H-NMR - spectra of compound **3j**



^{13}C-NMR - spectra of compound **3j**

User Chromatograms

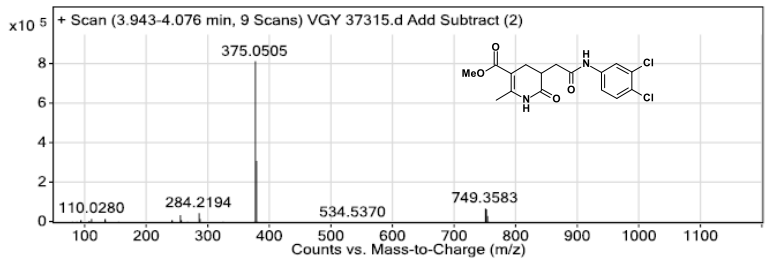


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.883	3.997	4.24	1101.25	5196.12	100

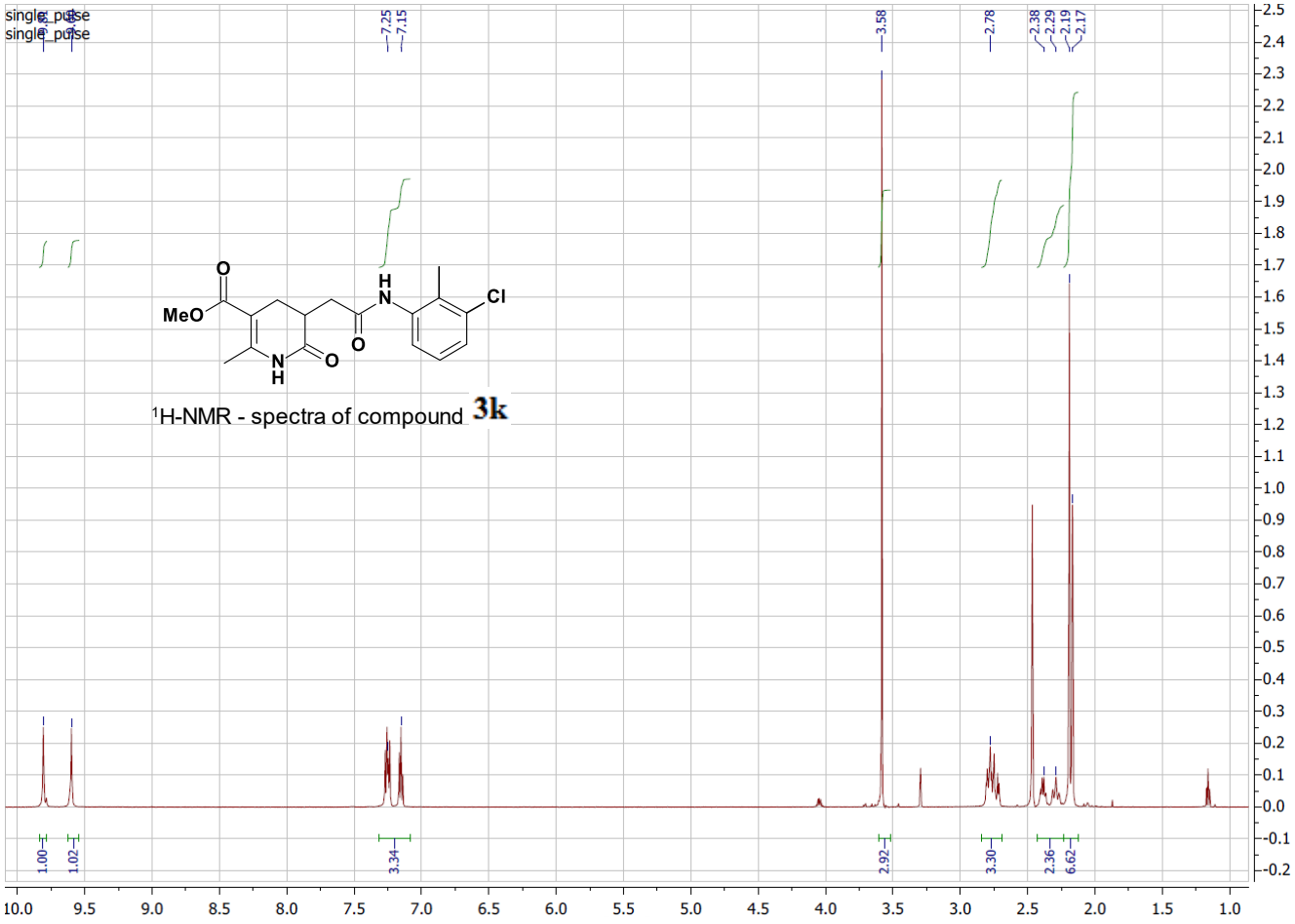
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
185	0	ESI

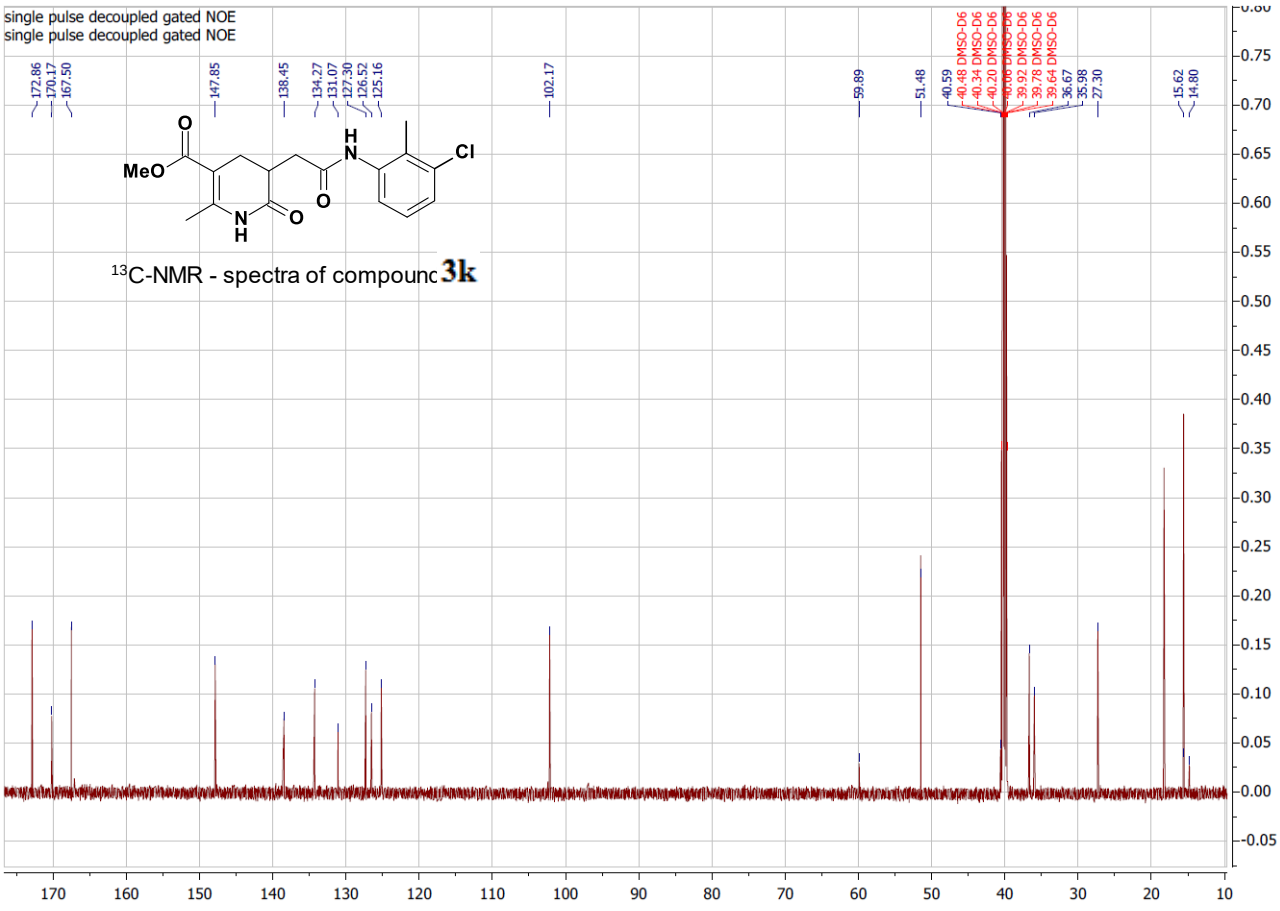


Peak List

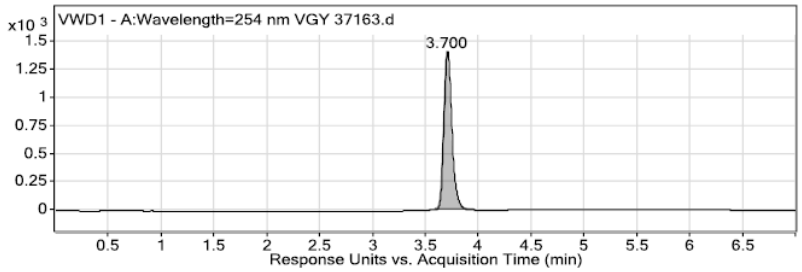
m/z	z	Abund
110.028		21162.63
131.4013		19889.23
253.2539		38138.89
284.2194		48430.89
285.6938		17551.68
375.0505		813028.56



^{1}H-NMR - spectra of compound **3k**



User Chromatograms

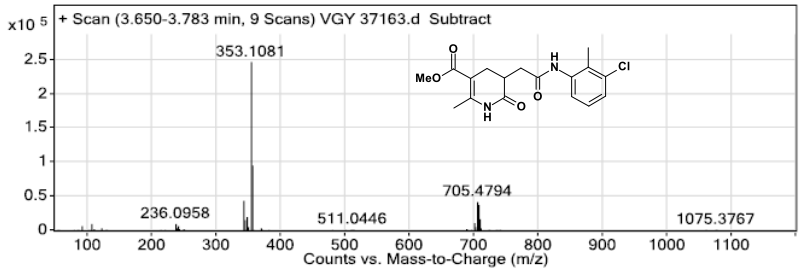


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.593	3.7	3.96	1409.29	7340.93	100

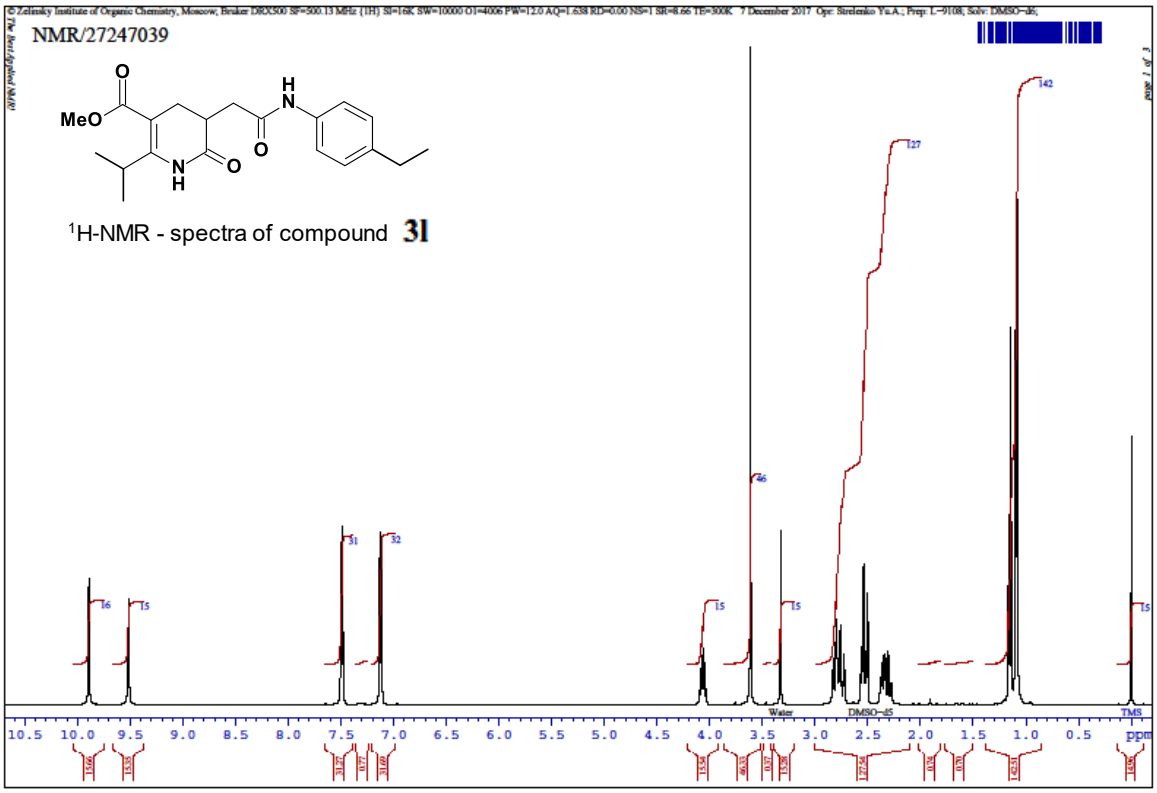
User Spectra

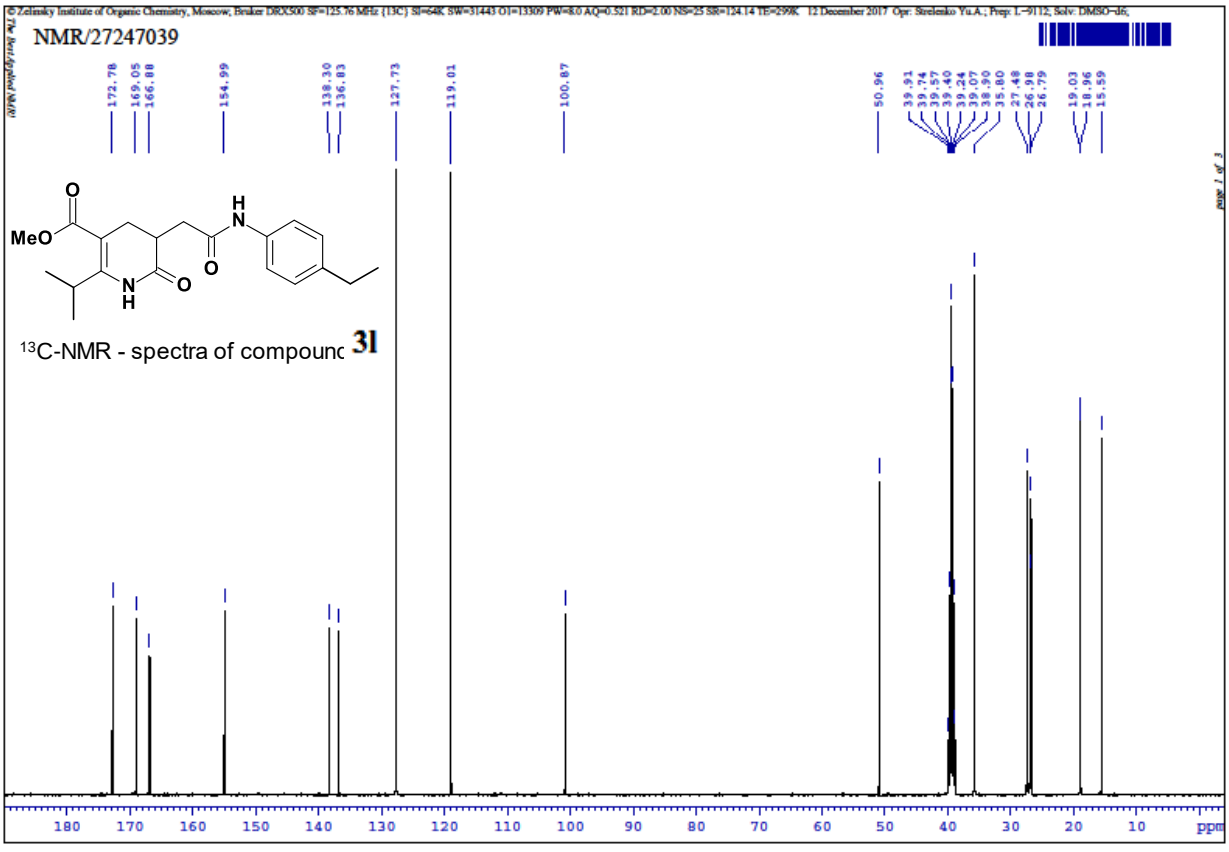
Fragmentor Voltage	Collision Energy	Ionization Mode
185	0	ESI



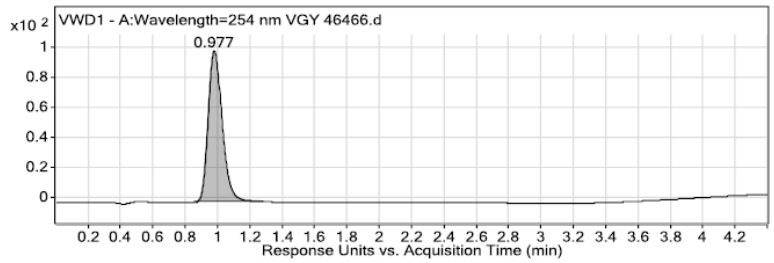
Peak List

m/z	Abund
43.1569	31182.45
341.4175	43928.8
342.1504	11616.72
342.8771	16754.58
347.2534	20017.43
353.1081	246961.44


NMR/27247039
MeO
O
N
H
O
H
N
O
1H-NMR - spectra of compound 3l


NMR/27247039
172.78
169.05
166.88
154.99
138.30
136.83
127.73
119.01
100.87
50.96
39.91
39.74
39.57
39.40
39.24
39.07
38.90
35.80
27.48
26.98
26.79
19.03
18.96
15.59
MeO
O
N
H
O
H
N
O
13C-NMR - spectra of compound 3l

User Chromatograms

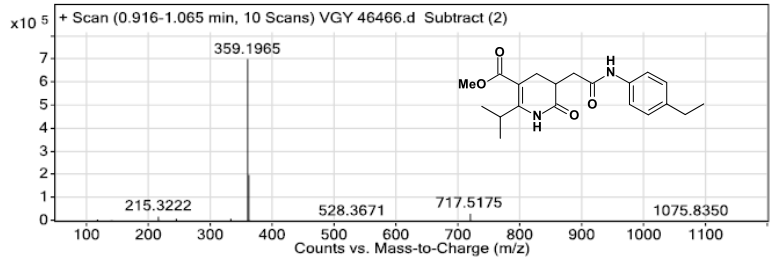


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.857	0.977	1.28	100.76	614.09	100

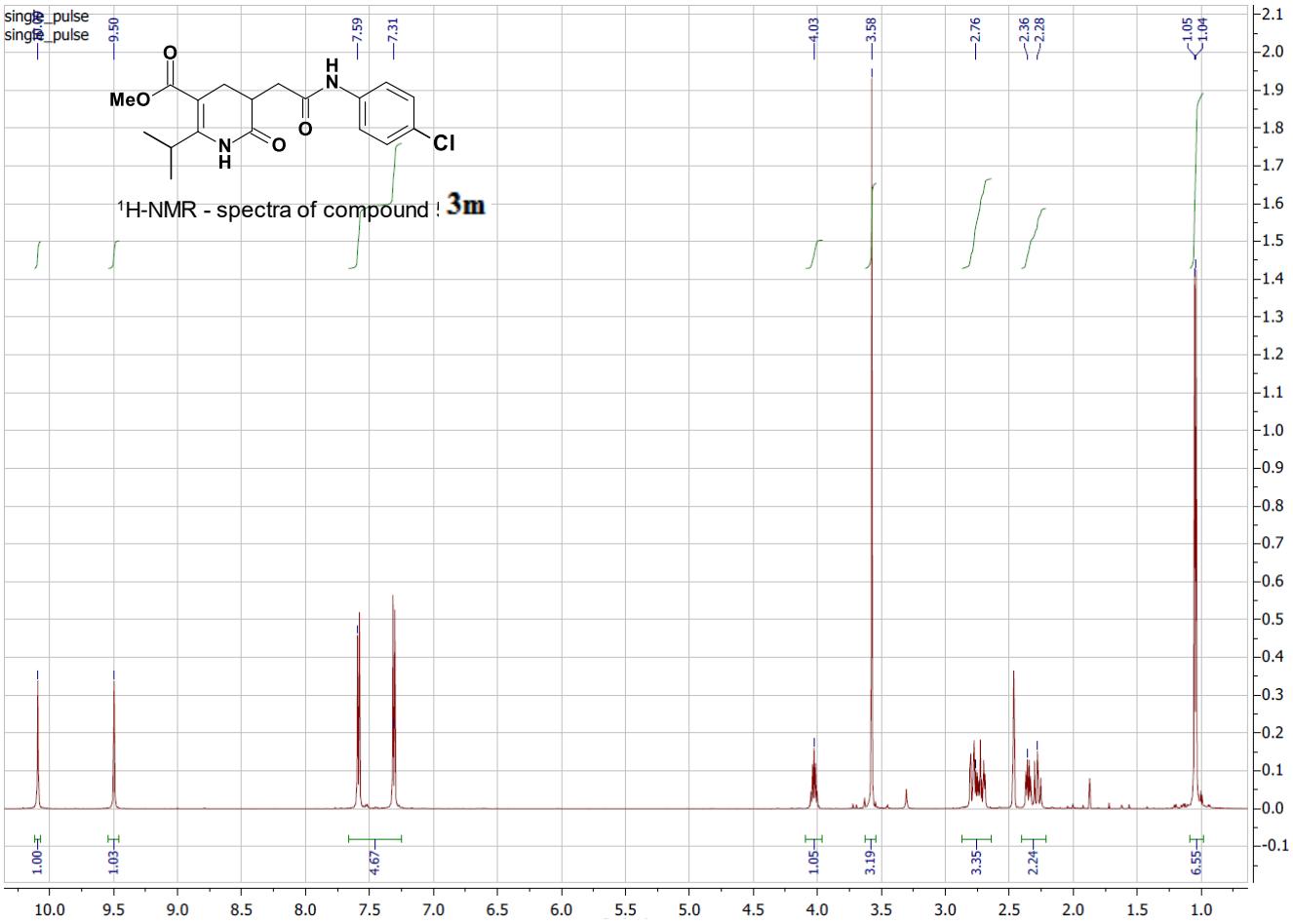
User Spectra

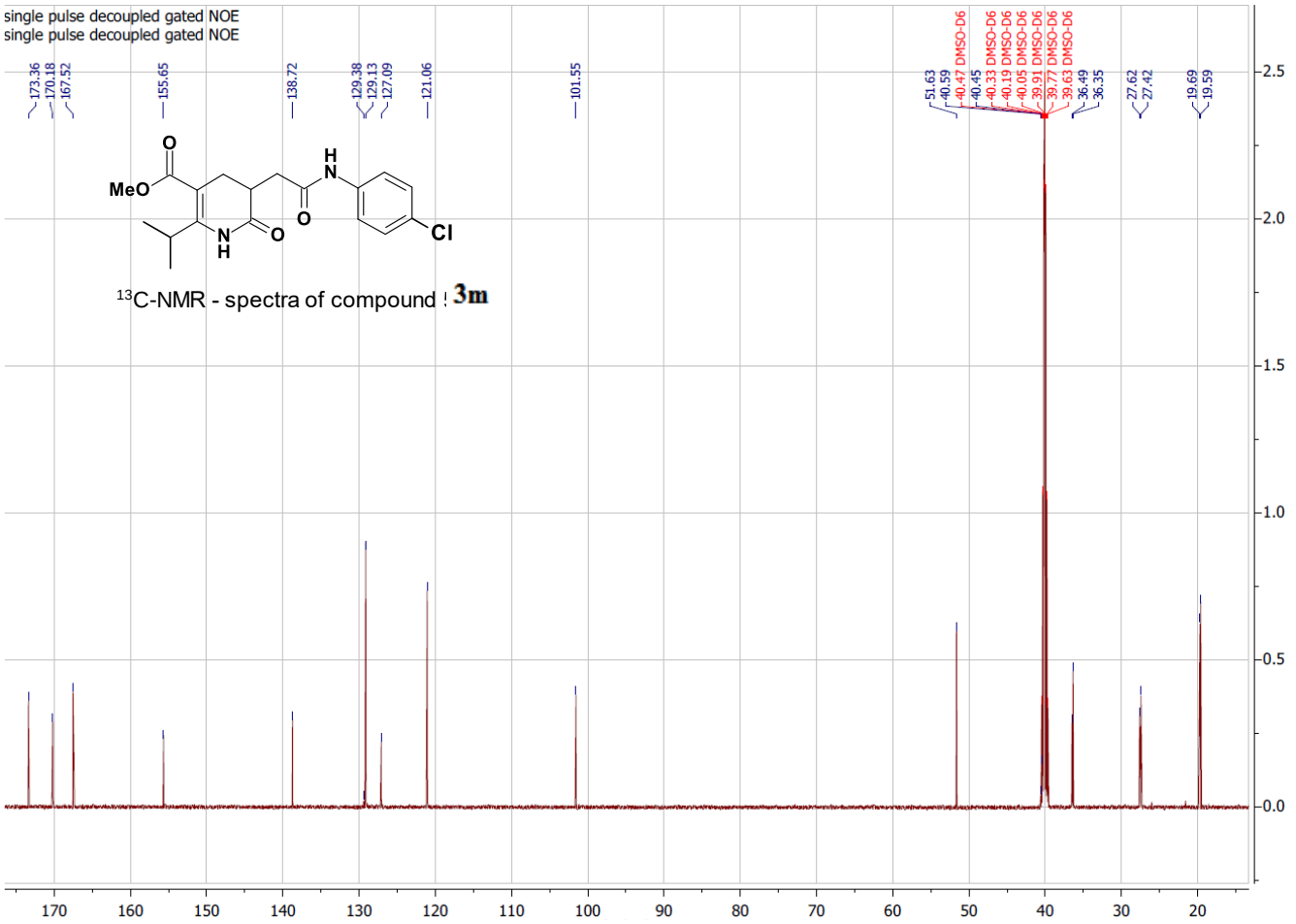
Fragmentor Voltage 185 | Collision Energy 0 | Ionization Mode ESI



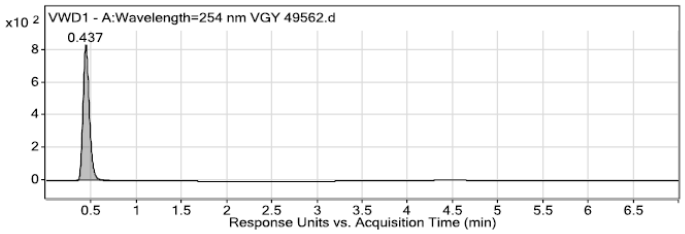
Peak List

m/z	Abund
116.8407	10472.52
137.7561	3363.14
215.3222	22332.99
216.1966	4019.49
243.2321	14632.22
244.107	2917.89





User Chromatograms

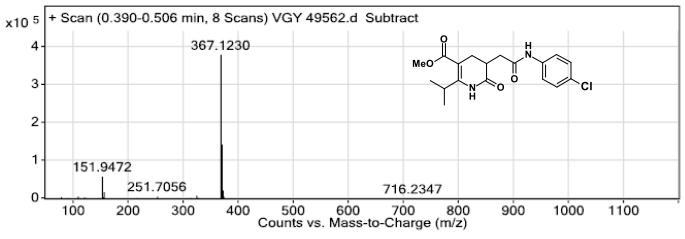


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.34	0.437	0.7	834.47	4077.9	100

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
185	0	ESI



Peak List

m/z	Abund
76.6	4213.29
108.2228	6970.46
109.4444	3397.36
120.3264	4402.17
151.9472	59062.63
153.1666	4133.64