

Certificate of analysis

IUPAC name: 4-(2-aminoethyl)benzenesulfonyl fluoride hydrochloride

Synonyms: AEBSF, AEBSF hydrochloride

Catalogue number: SF011

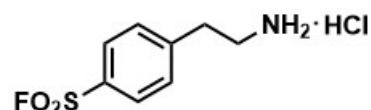
Lot number: CFTV05_41

CAS number: 30827-99-7

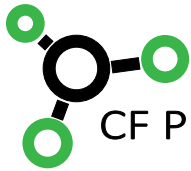
Chemical formula: C₈H₁₀FNO₂S.HCl

Molecular weight: 239.69 g/mol

Date of production: 19.02.2024



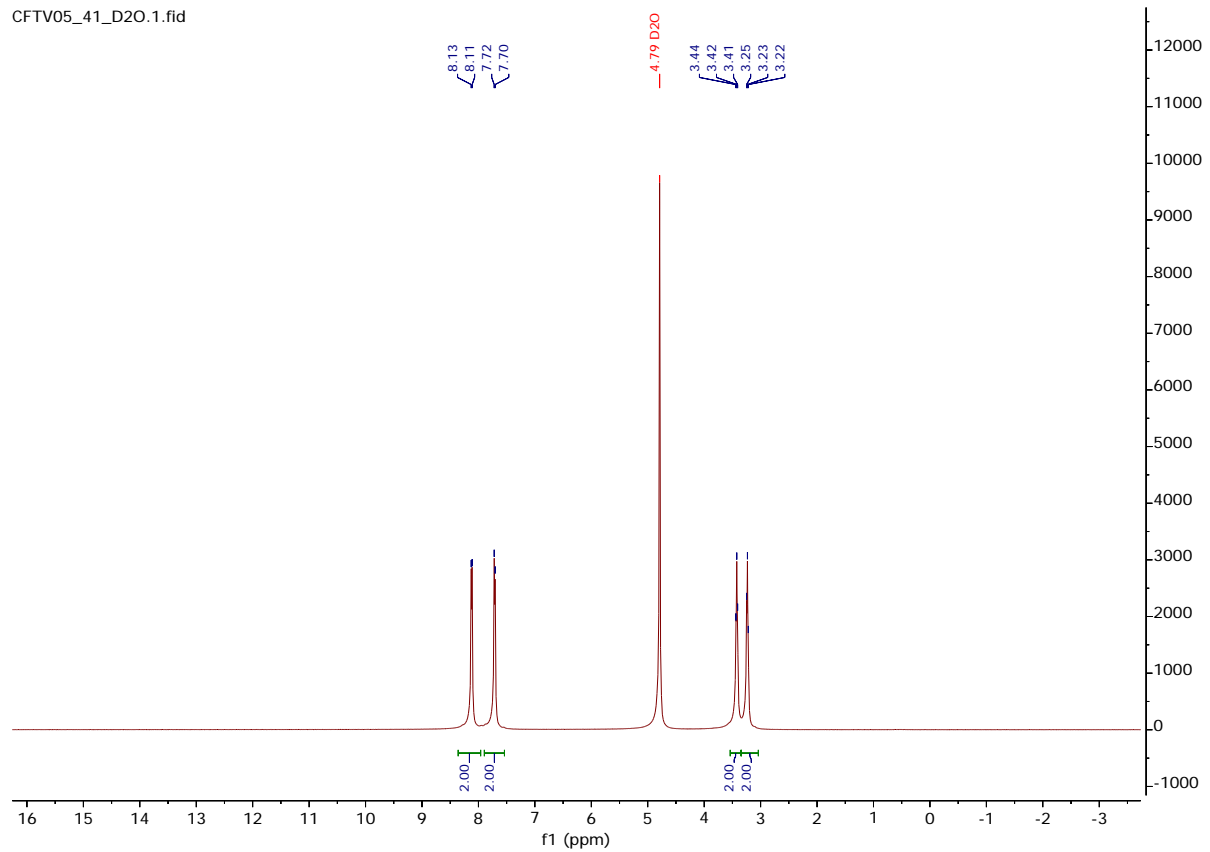
Test	Specification	Result
Appearance	White to off-white powder	White powder
NMR purity	98 % or higher	passes
HPLC	98 % or higher	98.93 %
Loss on drying	<1%	0.11%
TLC	R _f = 0.195 (DCM:MeOH 9:1)	R _f = 0.190
TLC purity	≤ 2 % impurities	passes
Melting point	180.0-190.0 °C	178-180 °C
Elemental analysis	C: 40.09 % ± 0.40 % H: 4.63 % ± 0.40 % N: 5.84 % ± 0.40 % S: 13.38 % ± 0.40 %	C: 40.06% H: 4.53 % N: 5.67 % S: N/A



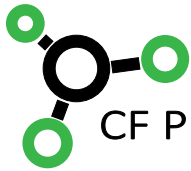
Attachment:

^1H NMR (500 MHz, D_2O) δ 8.12 (d, $J = 8.2$ Hz, 2H), 7.71 (d, $J = 8.2$ Hz, 2H), 3.42 (t, $J = 7.6$ Hz, 2H), 3.23 (t, $J = 7.7$ Hz, 2H).

CFTV05_41_D2O.1.fid



Impurities found in ^1H -NMR spectrum: None, or below 1 %.



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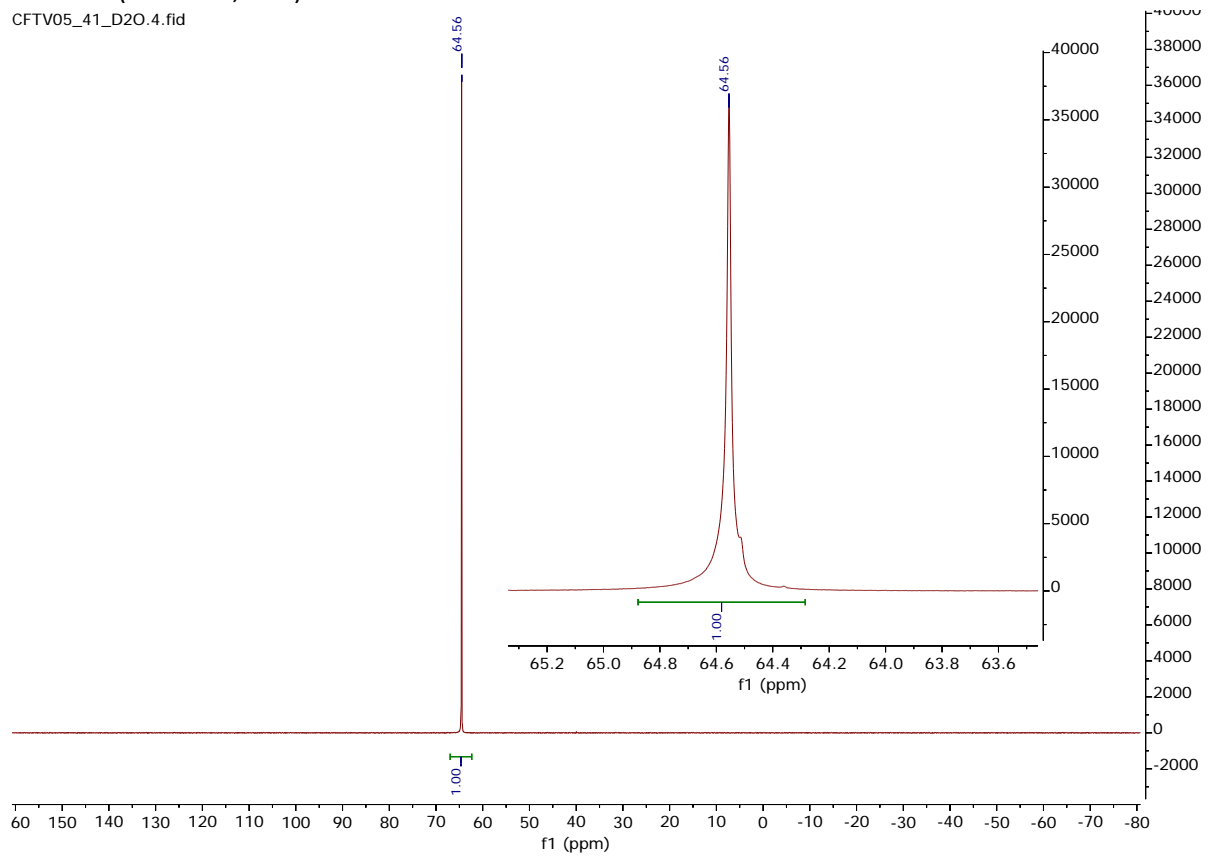
Czech Republic

Phone: +420770645920

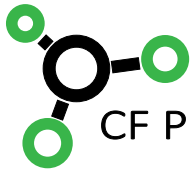
Email: sales@cfplus.cz

^{19}F NMR (471 MHz, D_2O) δ 64.56.

CFTV05_41_D2O.4.fid



Impurities found in ^{19}F -NMR spectrum: None, or below 1 %.



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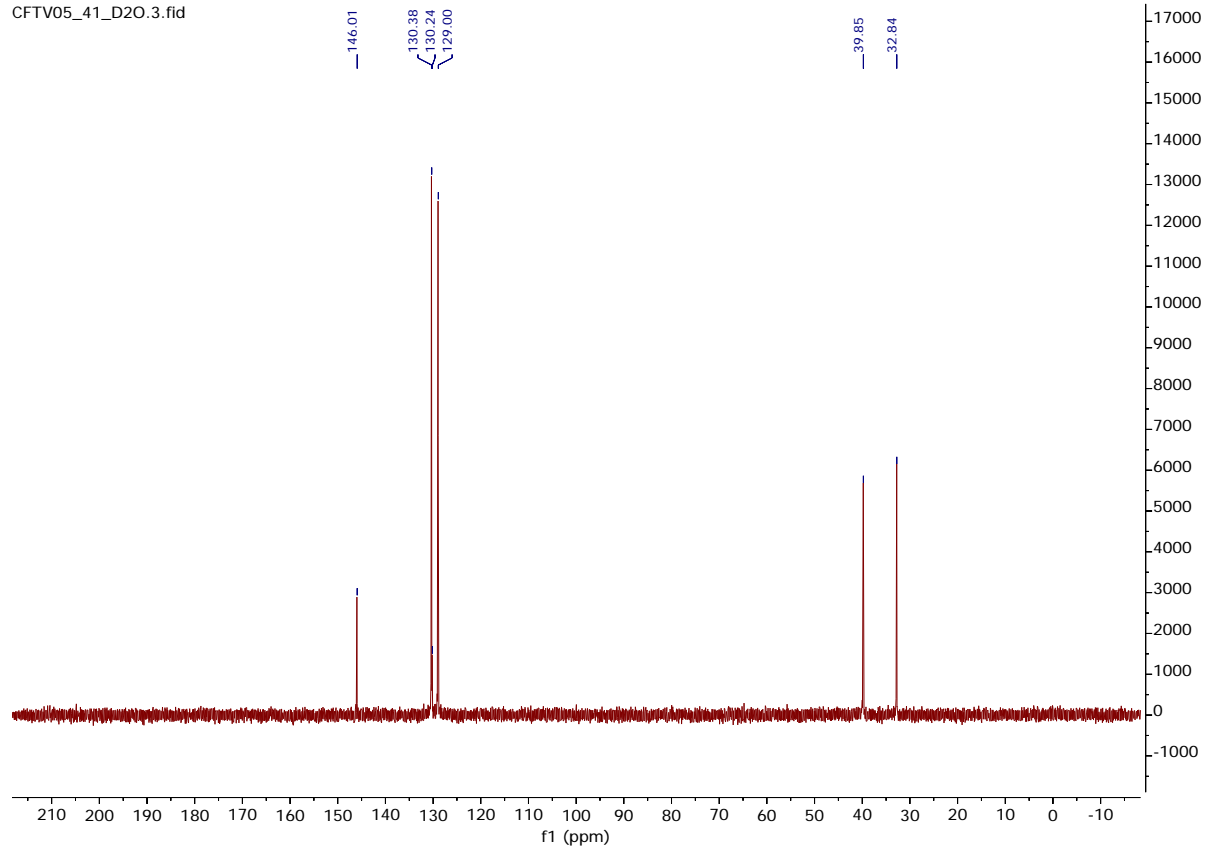
Czech Republic

Phone: +420770645920

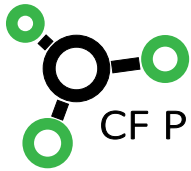
Email: sales@cfplus.cz

^{13}C NMR (126 MHz, D_2O) δ 146.01 , 130.38 , 130.24 , 129.00 , 39.85 , 32.84.

CFTV05_41_D2O.3.fid

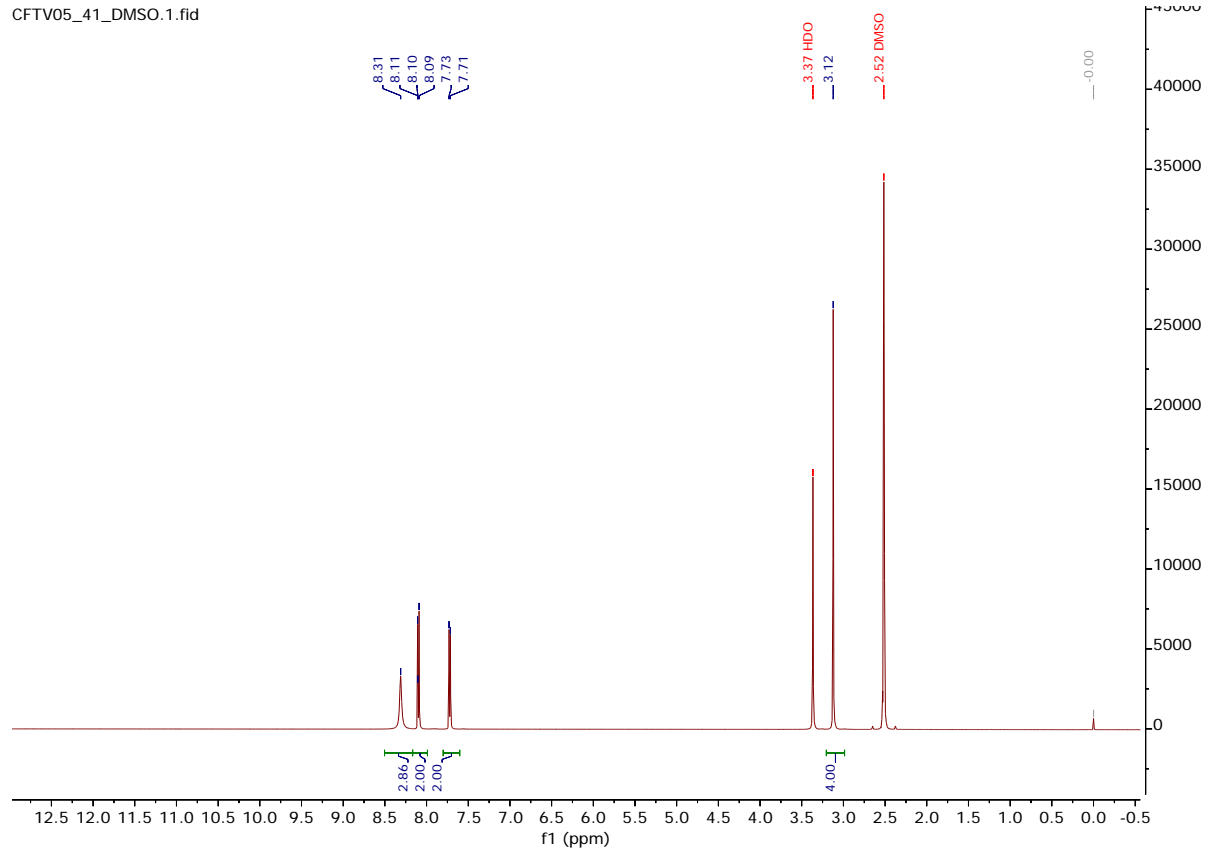


Impurities found in ^{13}C -NMR spectrum: None, or below 1 %.

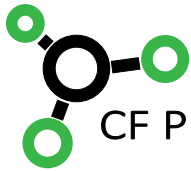


^1H NMR (500 MHz, DMSO- d_6) δ 8.31 (s, 3H), 8.10 (d, $J = 8.5$ Hz, 2H), 7.72 (d, $J = 8.1$ Hz, 2H), 3.12 (s, 4H)

CFTV05_41_DMSO.1.fid



Impurities found in ^1H -NMR spectrum: None, or below 1 %.



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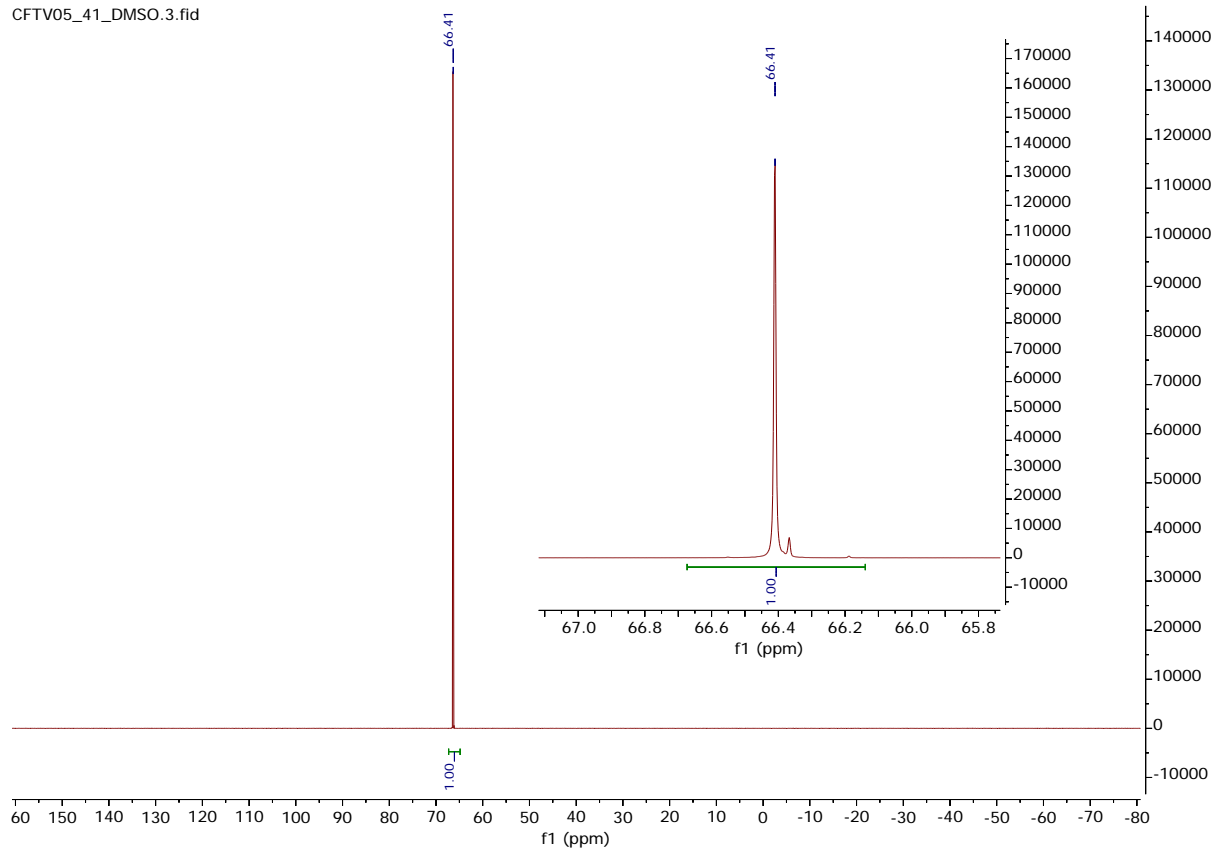
Czech Republic

Phone: +420770645920

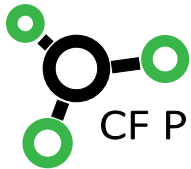
Email: sales@cfplus.cz

^{19}F NMR (471 MHz, $\text{DMSO-}d_6$) δ 66.41.

CFTV05_41_DMSO.3.fid

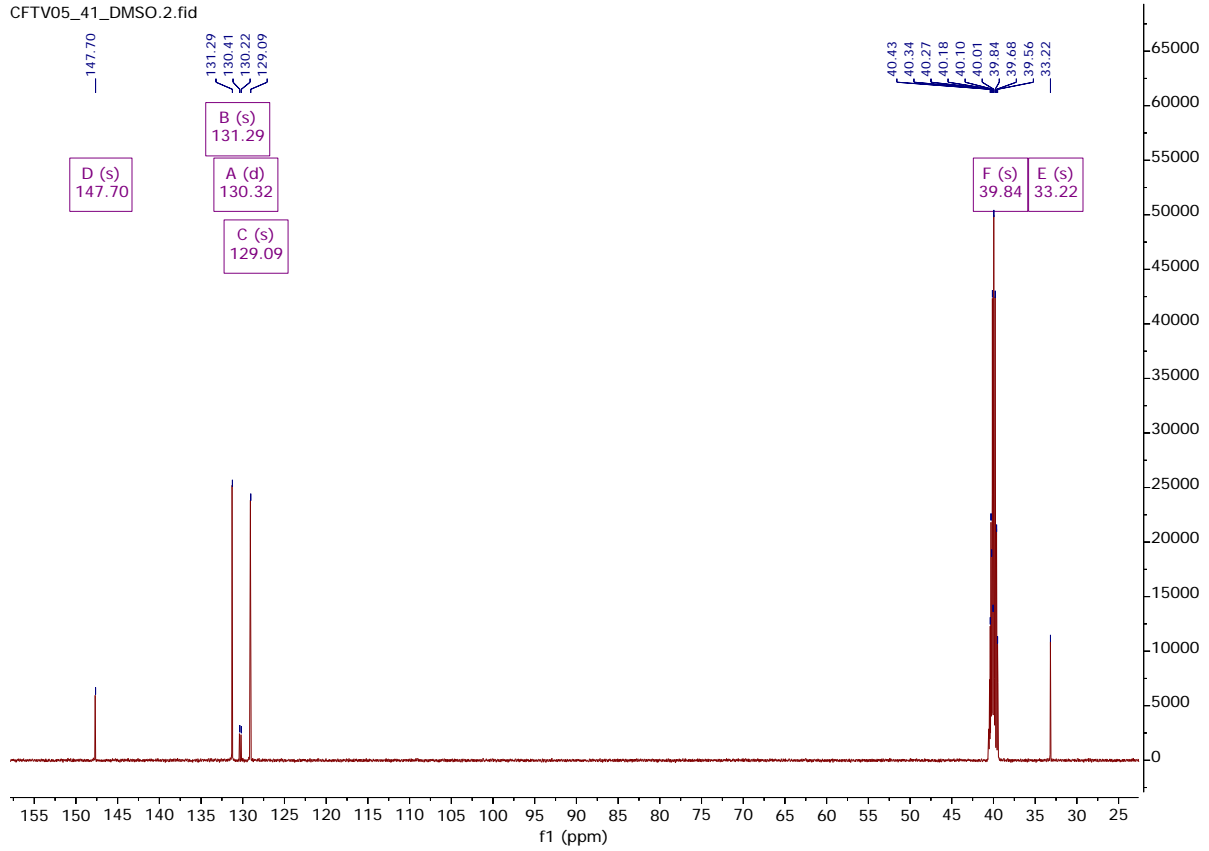


Impurities found in ^{19}F -NMR spectrum: None, or below 1 %.

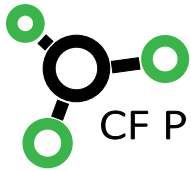


^{13}C NMR (126 MHz, DMSO- d_6) δ 147.70 , 131.29 , 130.32 (d, $J = 23.3$ Hz), 129.09 , 39.84 , 33.22.

CFTV05_41_DMSO.2.fid



Impurities found in ^{13}C -NMR spectrum: None, or below 1 %.



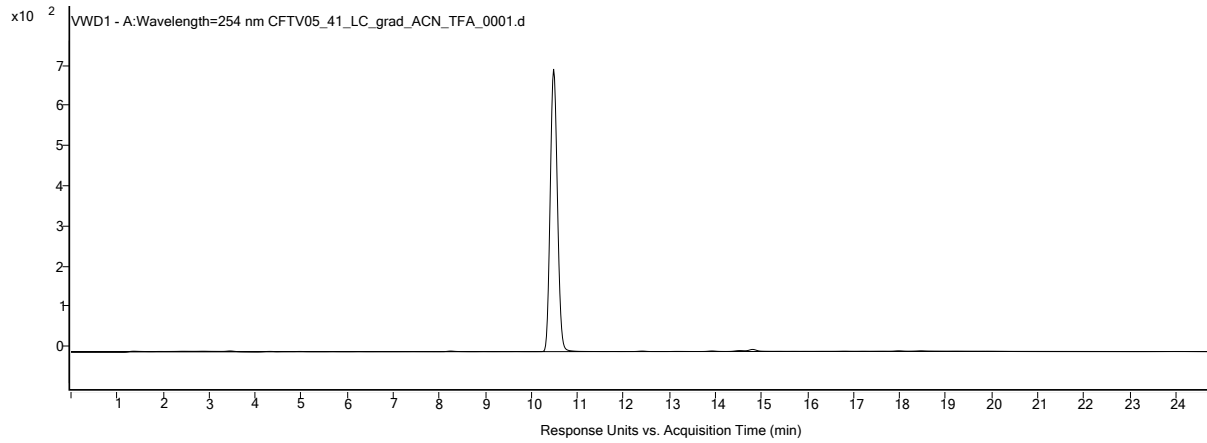
HPLC Spectrum

Method: Gradient elution:

0 – 15 min 95% - 20% 0.1% TFA, 5% - 80% acetonitrile

15 – 18 min 20% - 95% 0.1% TFA, 80% - 5% acetonitrile

18 – 25 min 95% 0.1% TFA, 5% acetonitrile



Peak	Area	Percentage
10.483 min	7635.51	98,93 %
14.812 min	81.9	1,06 %