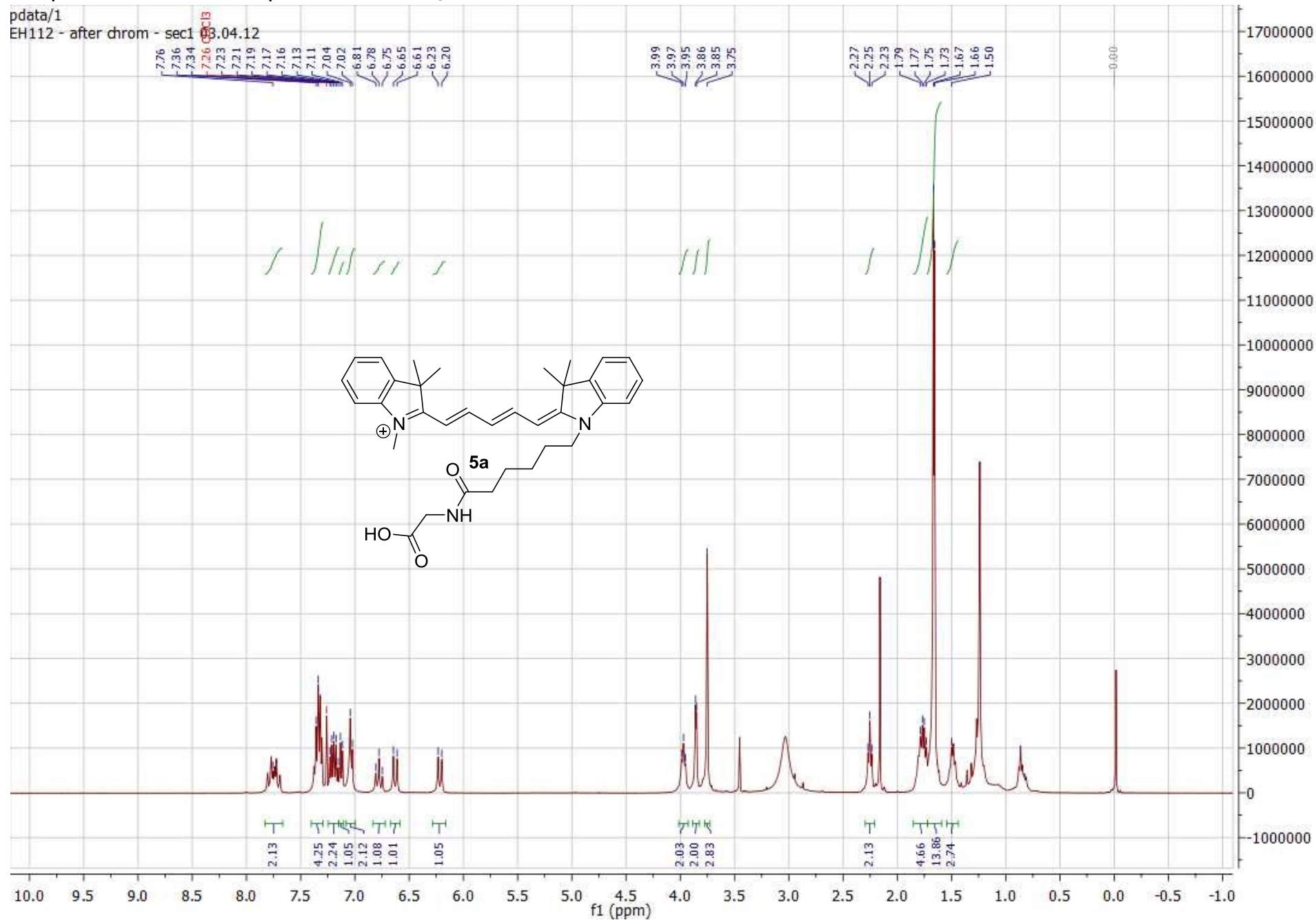
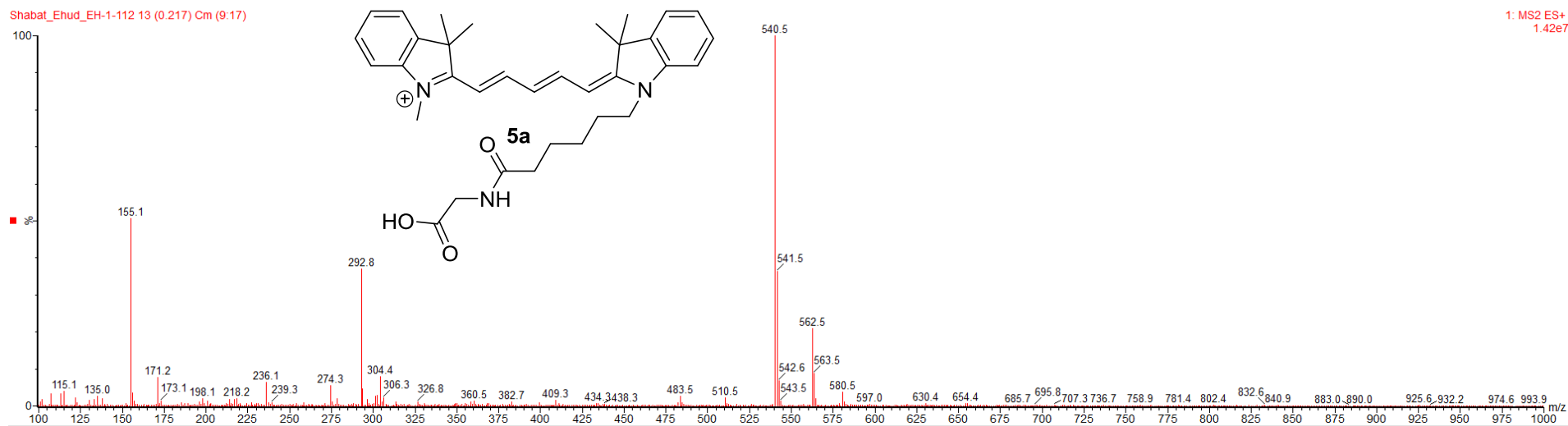


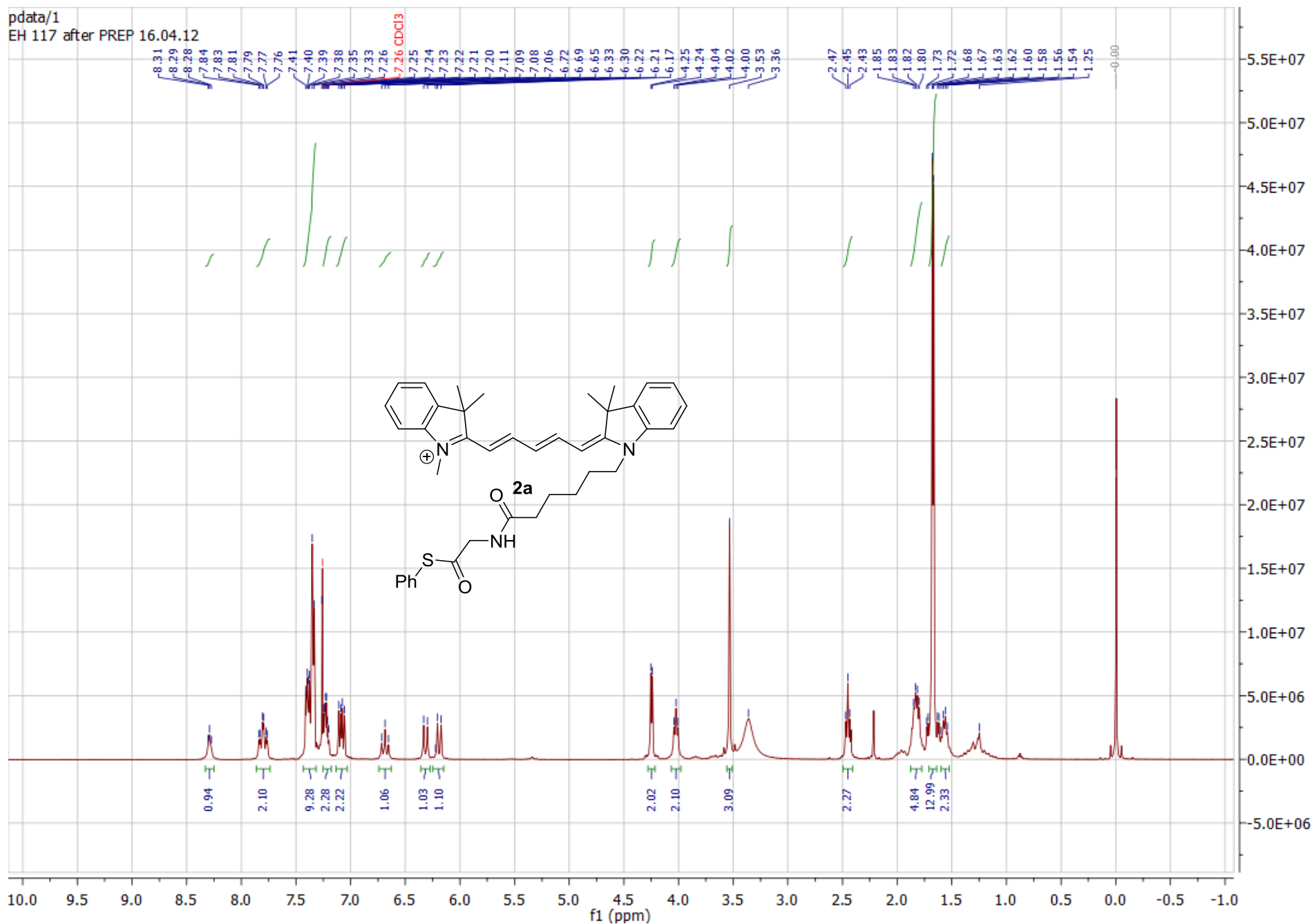
Compound **5a** - ^1H NMR spectrum in CDCl_3



Compound **5a** - MS (ESI+): m/z calc. for $C_{34}H_{42}N_3O_3^+$: 540.32 ; found: 540.5 $[M]^+$



Compound **2a** - ^1H NMR spectrum in CDCl_3



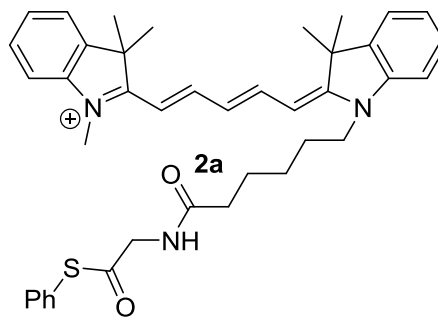
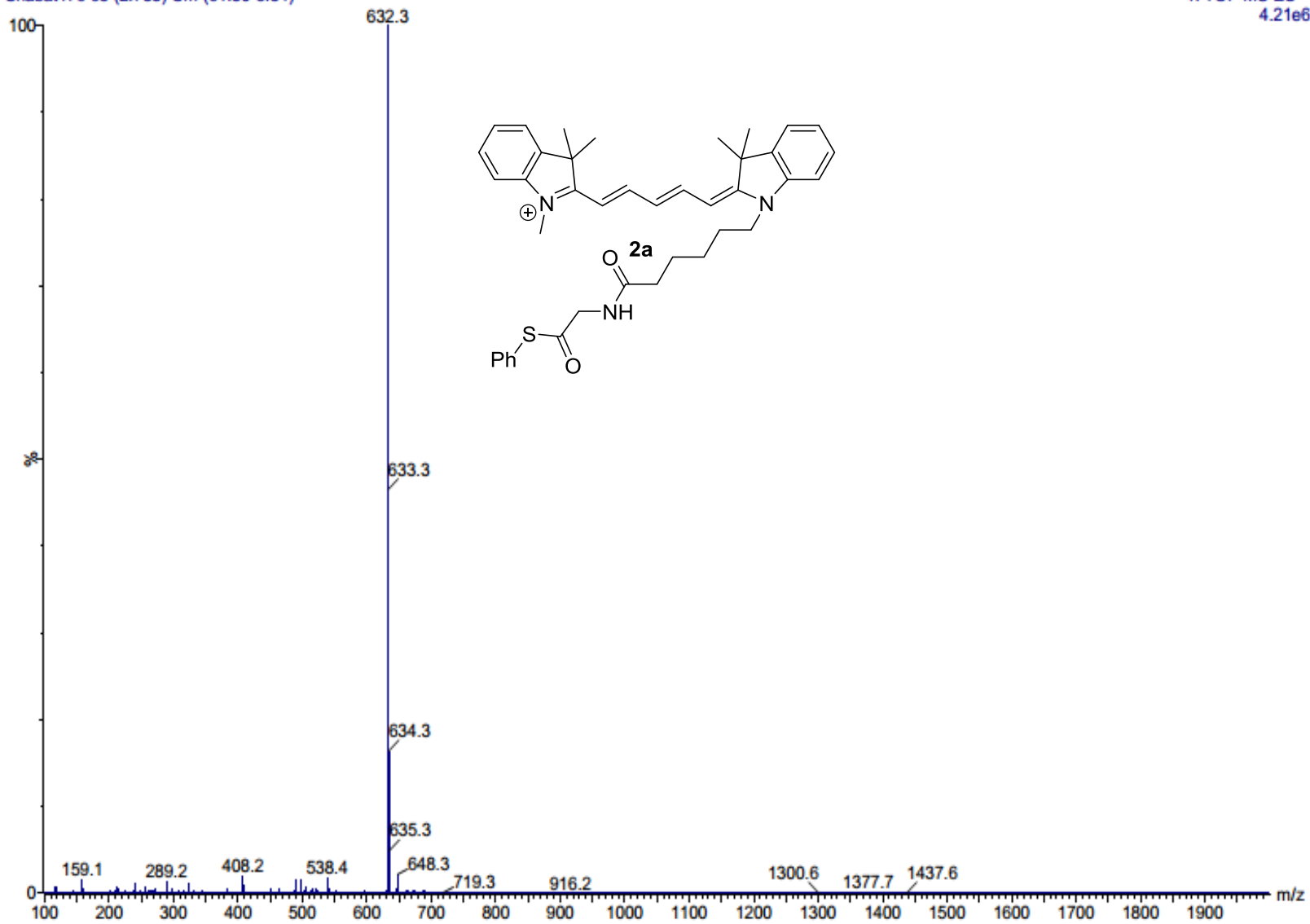
Compound **2a** - MS (ESI+): m/z calc. for $C_{40}H_{46}N_3O_2S^+$: 632.33 ; found: 632.3 $[M]^+$

EH - 117

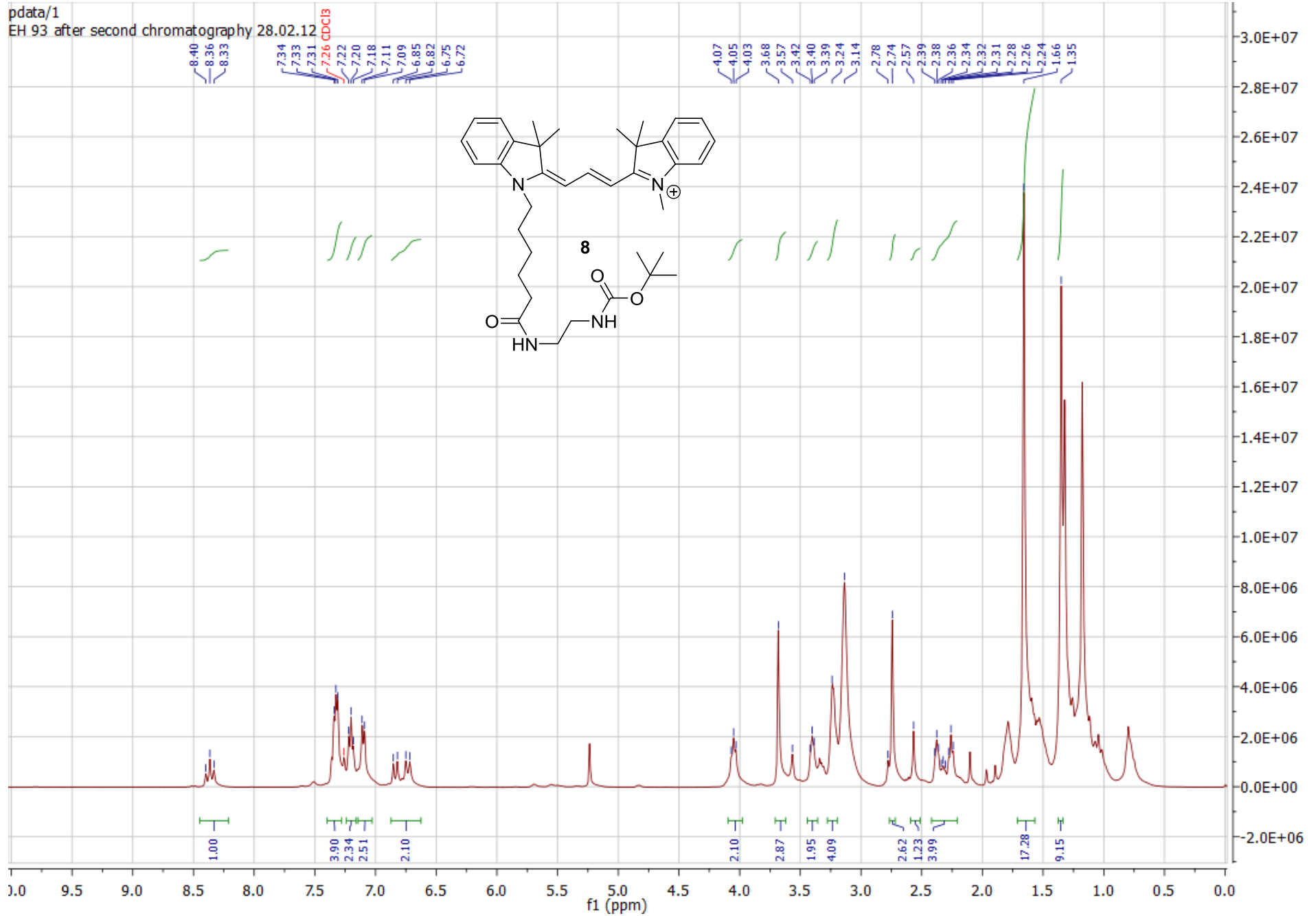
Shabat176 63 (2.788) Cm (61:80-5:34)

Ehud Herbust

1: TOF MS ES+
4.21e6



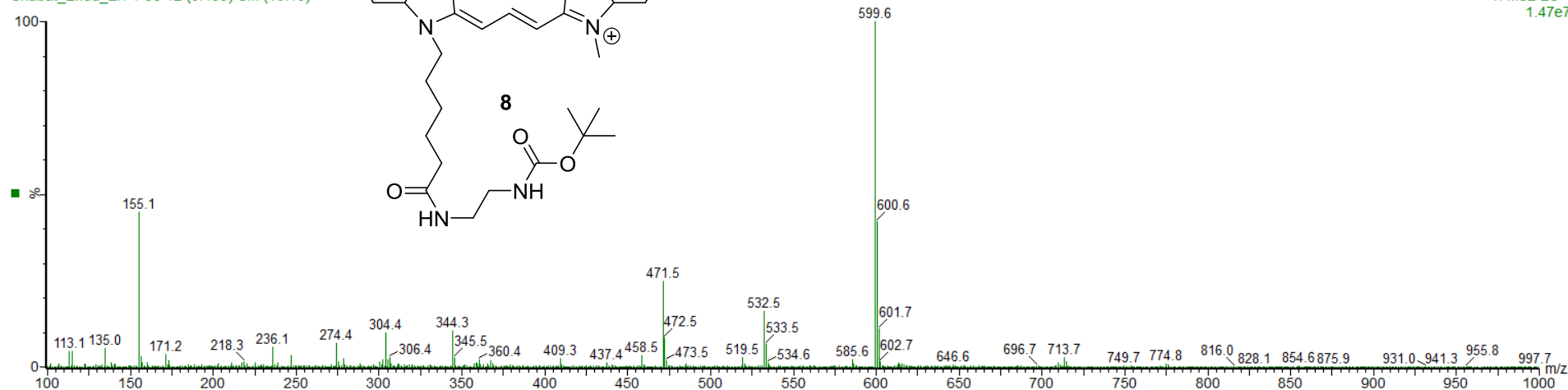
Compound **8** - ^1H NMR spectrum in CDCl_3



Compound **8** - MS (ESI+): m/z calc. for $C_{37}H_{51}N_4O_3^+$: 599.40; found: 599.6 $[M]^+$

13 in MeOH

Shabat_Ehud_EH-1-98 12 (0.199) Cm (10:16)



Ehud

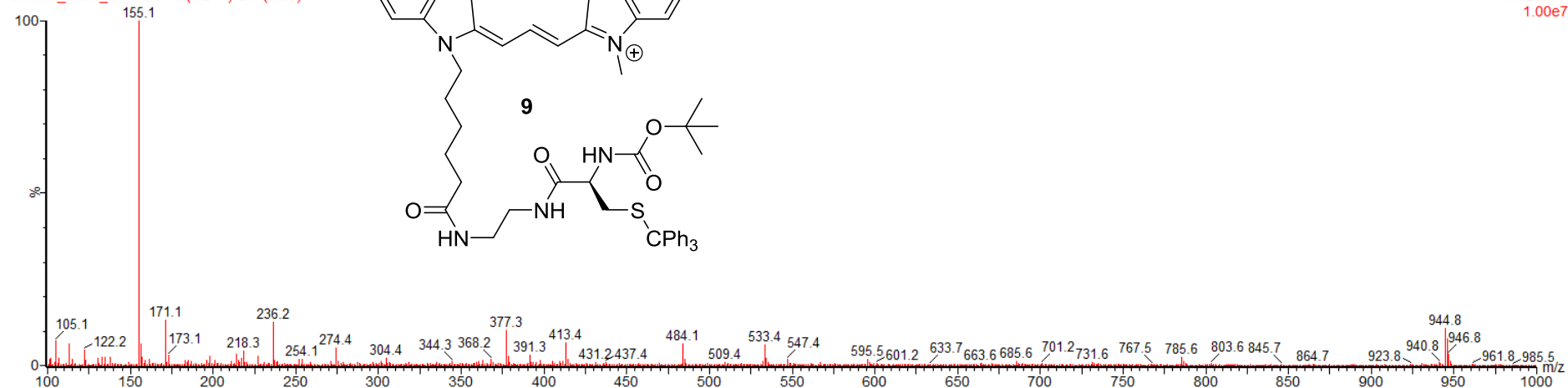
17-Jul-2013

Coll energy 3

1: MS2 ES+
1.47e7

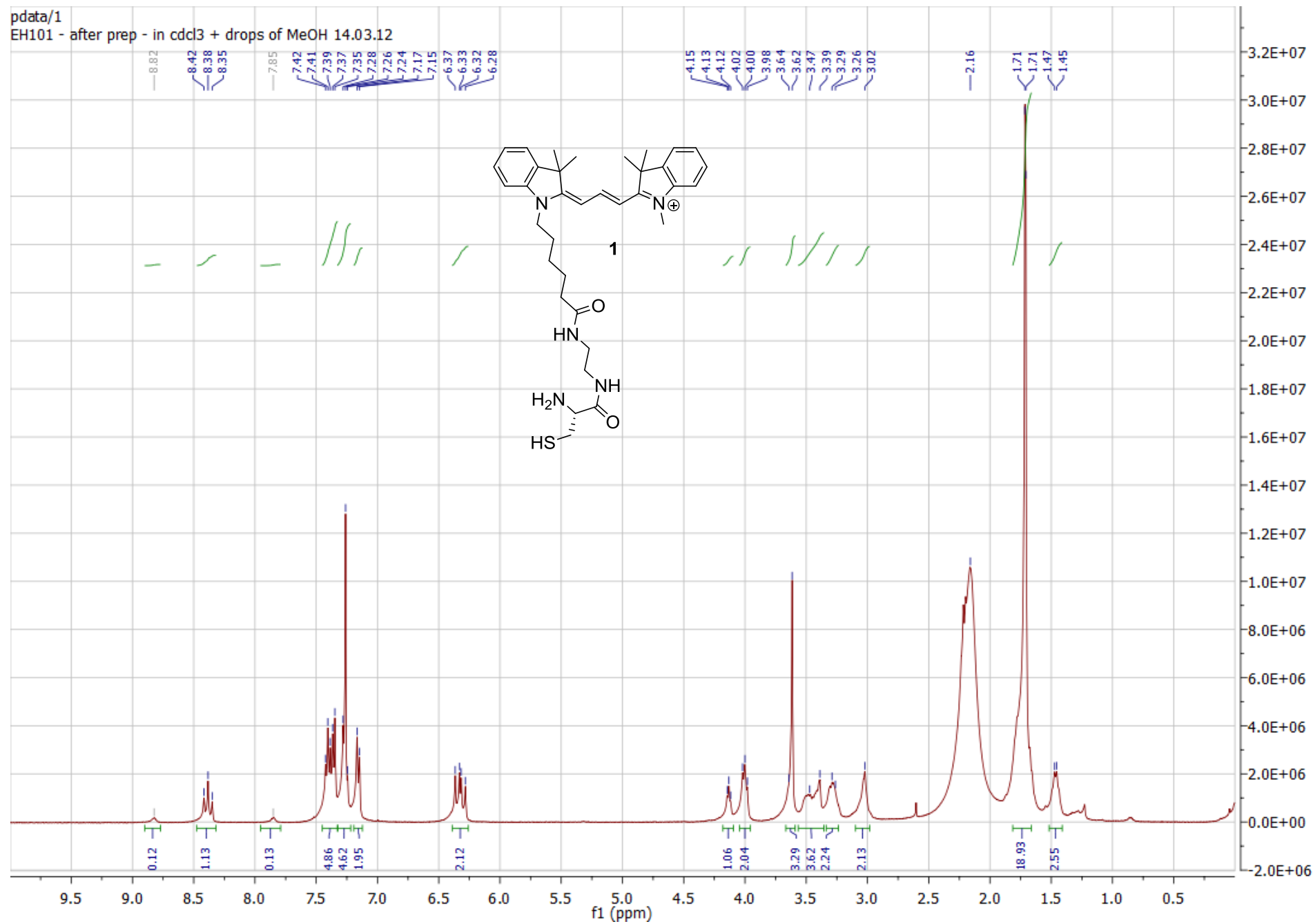
Compound **9** - MS (ESI+): m/z calc. for $C_{59}H_{70}N_5O_4^+$: 944.51; found: 944.8 $[M]^+$

Shabat_Ehud_EH-1-95 13 (0.217) Cm (8:26)



1: MS2 ES+
1.00e7

Compound **1** - ^1H NMR spectrum in CDCl_3



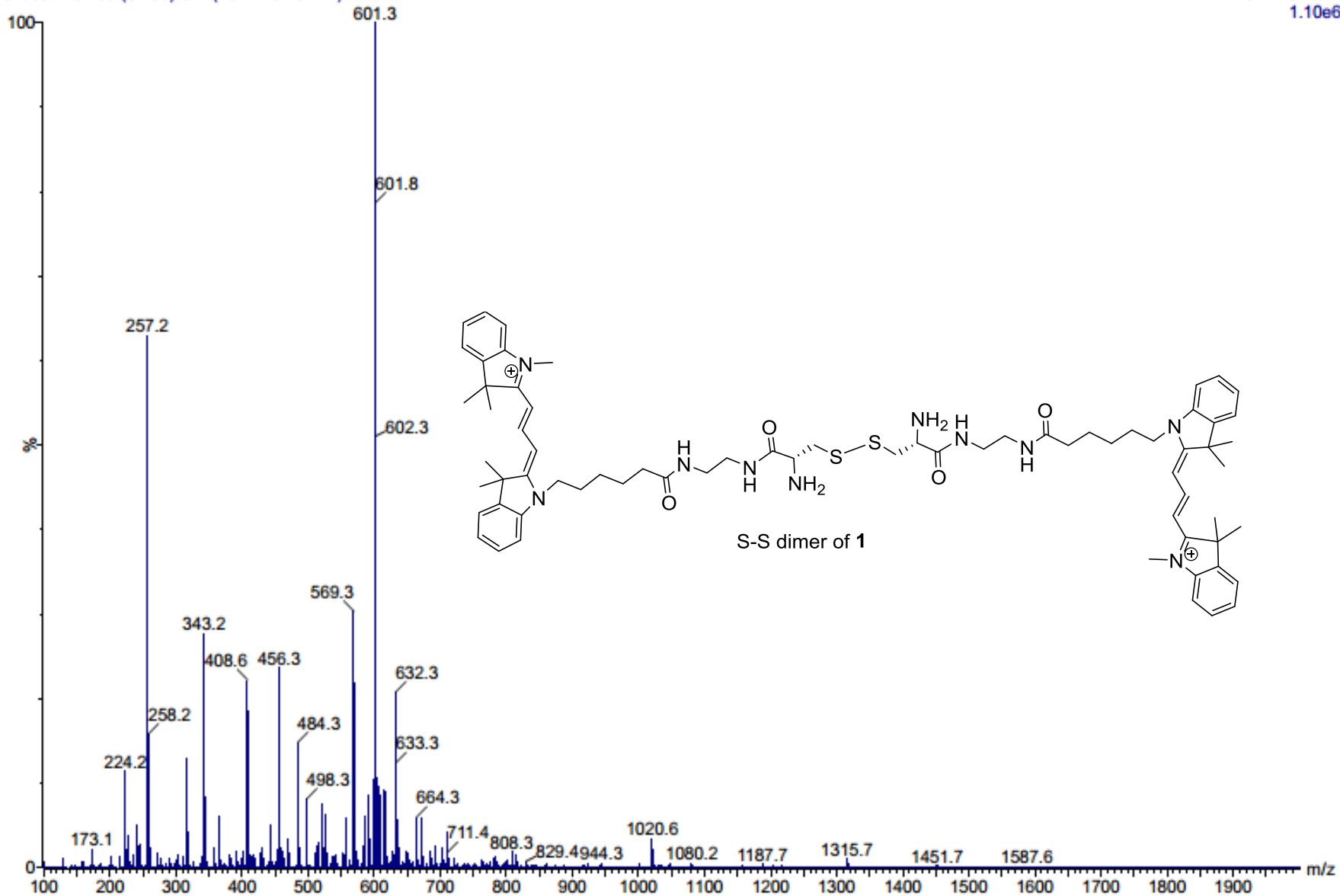
Compound **1** - MS (ESI+): m/z calc. for $C_{70}H_{94}N_{10}O_4S_2^{2+}$: 601.35; found: 601.3 $[M]^+$.

EH - 101

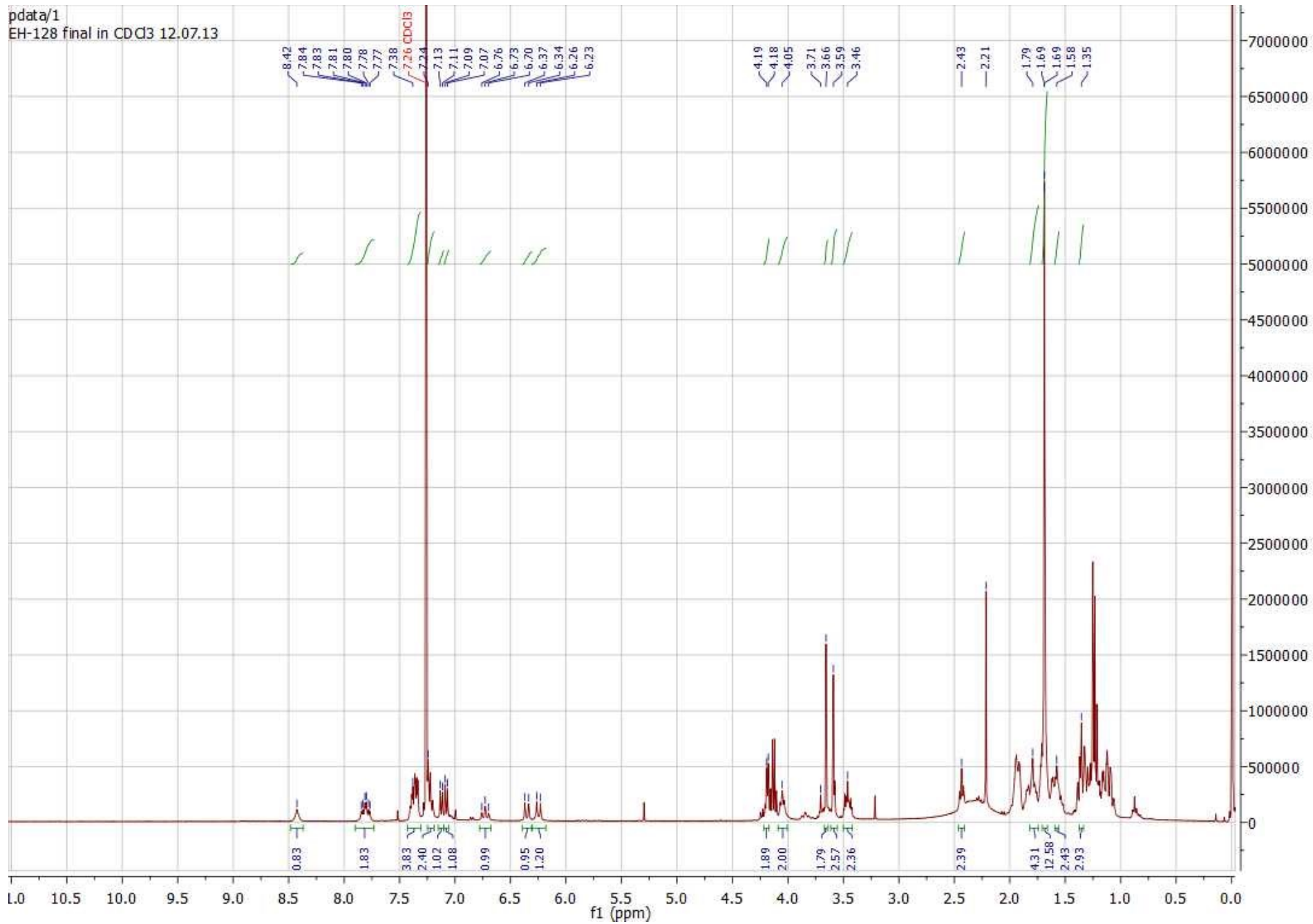
shabat175 199 (8.750) Cm (161:216-28:112)

Ehud Herbust

1: TOF MS ES+
1.10e6



Compound **2b** - ^1H NMR spectrum in CDCl_3



Compound **2b** - MS (ESI+): m/z calc. for $C_{38}H_{48}N_3O_4S^+$: 642.34; found: 642.5 $[M]^+$.

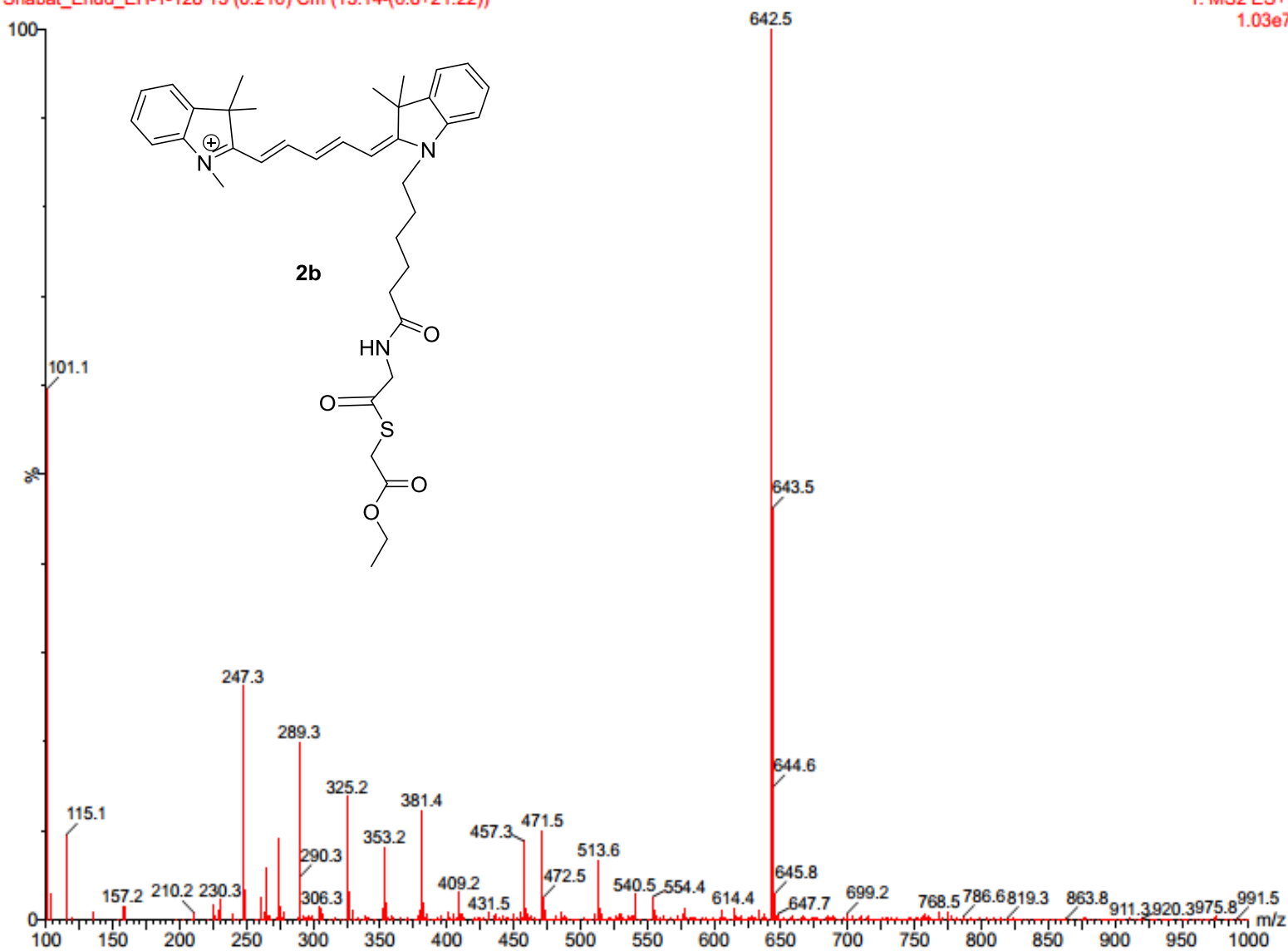
EH-1-128 MeOH ACN

Ehud

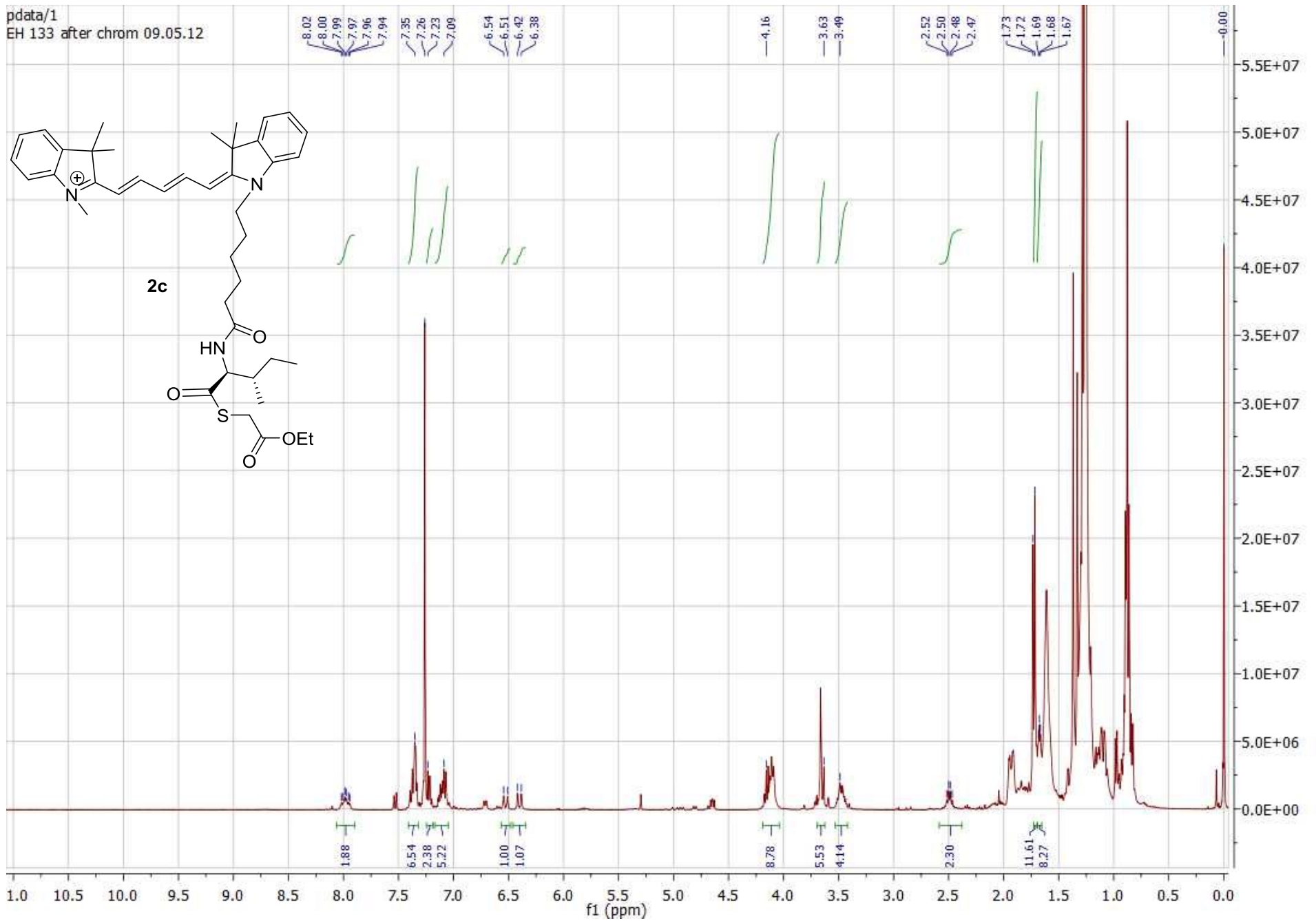
17-Jul-2013
Coll energy 3

Shabat_Ehud_EH-1-128 13 (0.216) Cm (13:14-(6:8+21:22))

1: MS2 ES+
1.03e7



Compound **2c** - ^1H NMR spectrum in CDCl_3



Compound **2c** - MS (ESI+): m/z calc. for $C_{42}H_{56}N_3O_4^+$: 698.40; found: 698.6 [M]⁺.

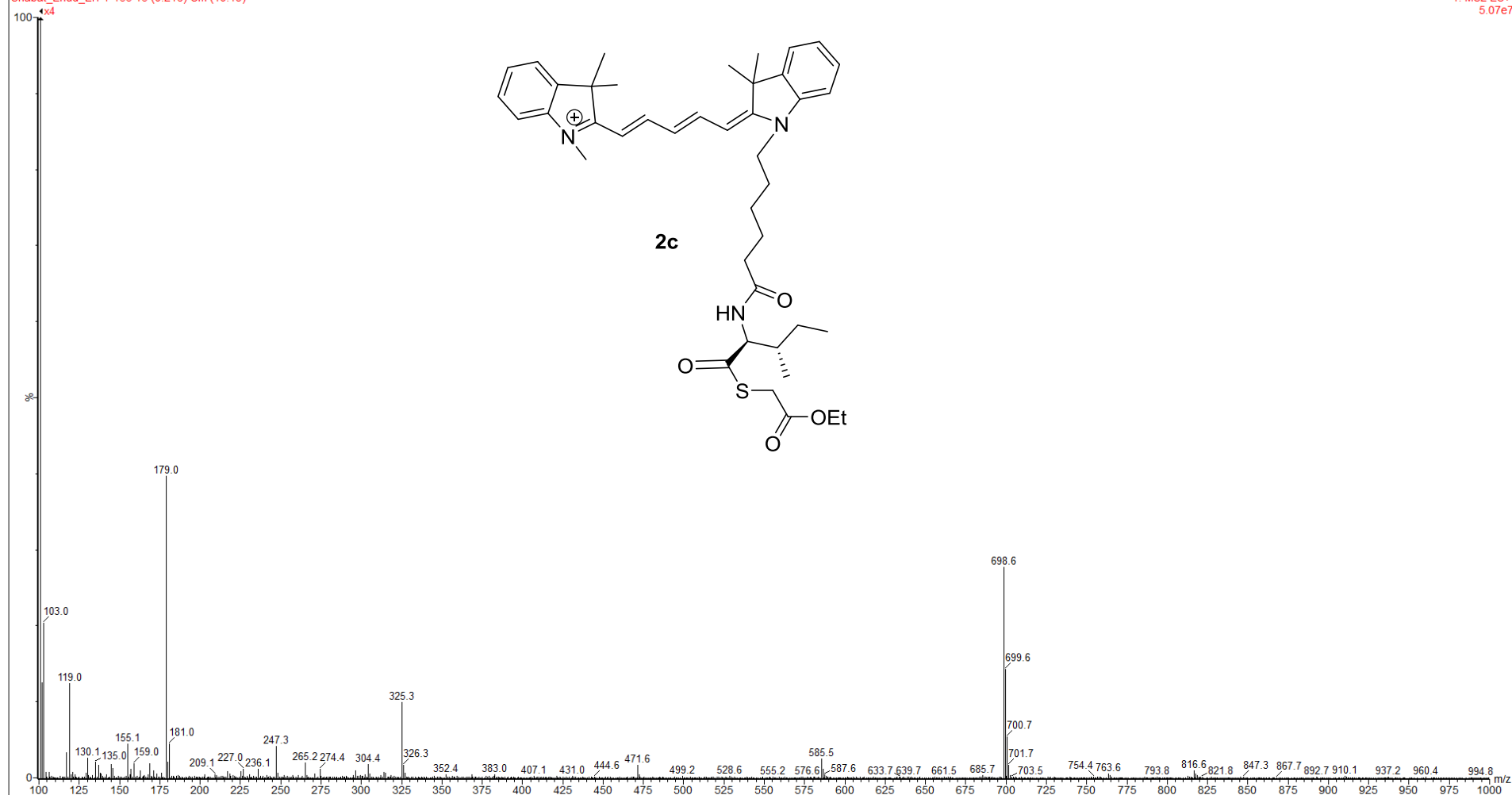
EH-1-133 from DMSO stock dil MeOH

Ehud

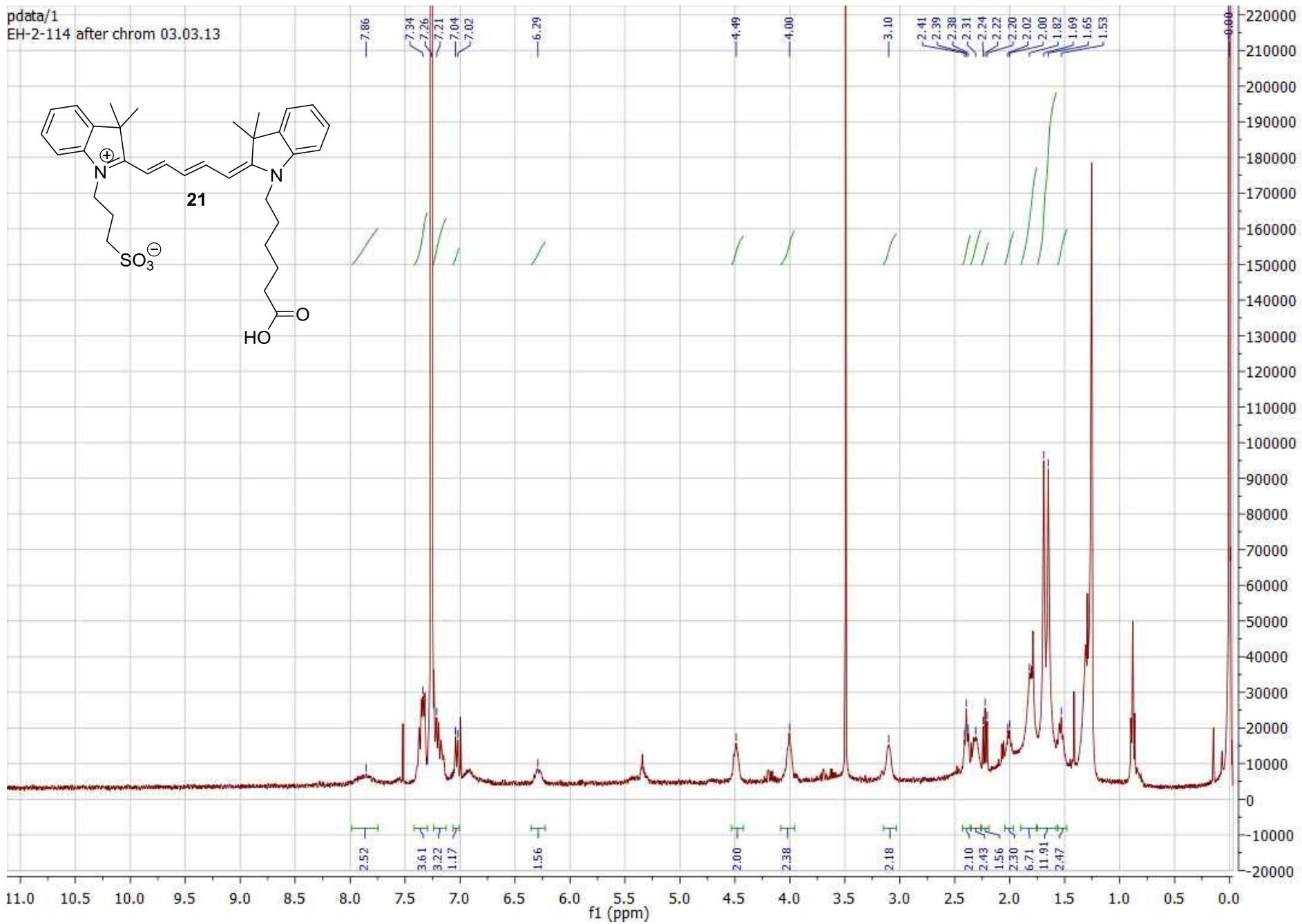
17-Jul-2013
Coll energy 3

1: MS2 ES+
5.07e7

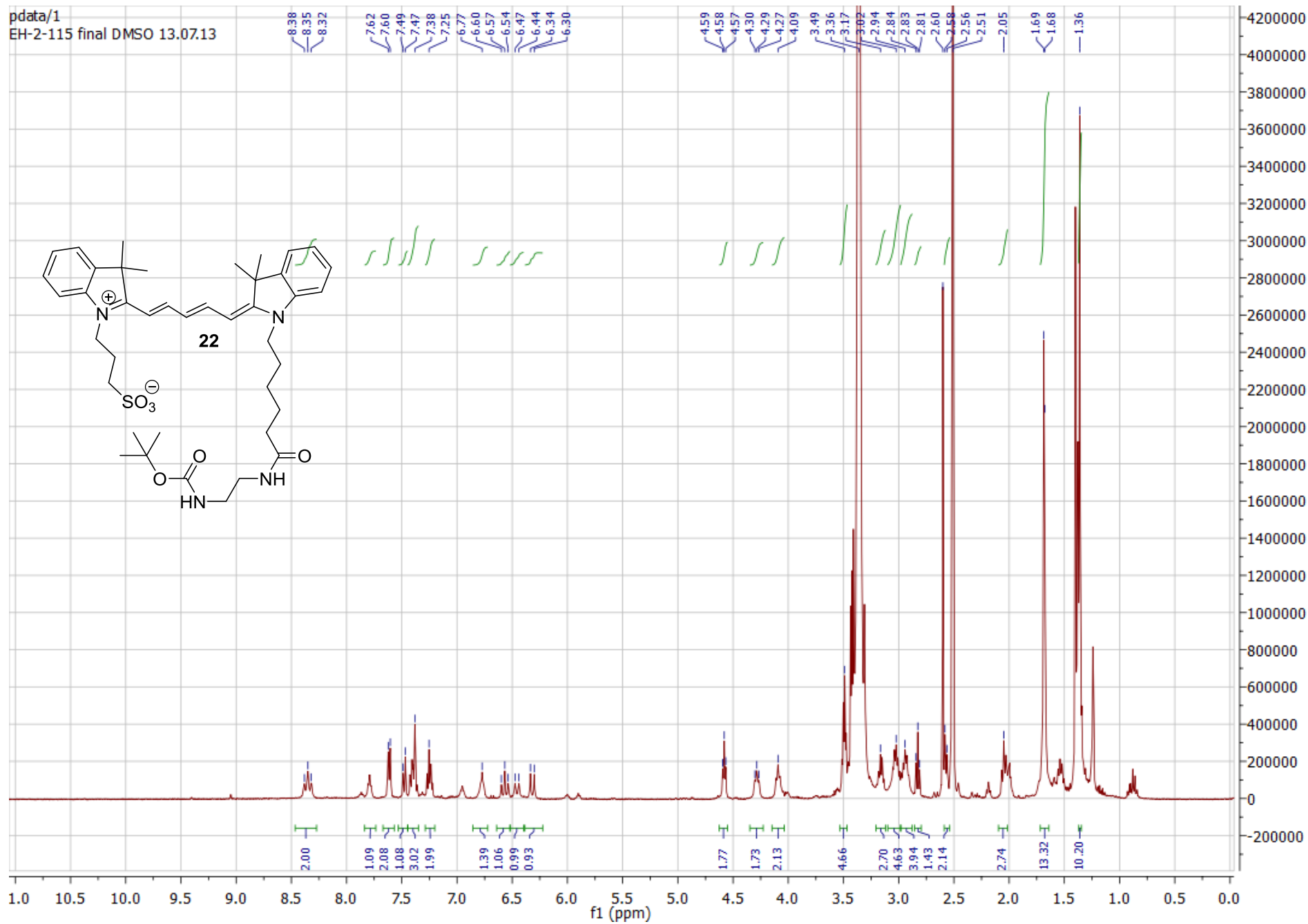
Shabat_Ehud_EH-1-133 13 (0.216) Cm (10:19)



Compound **21** - ^1H NMR spectrum in CDCl_3

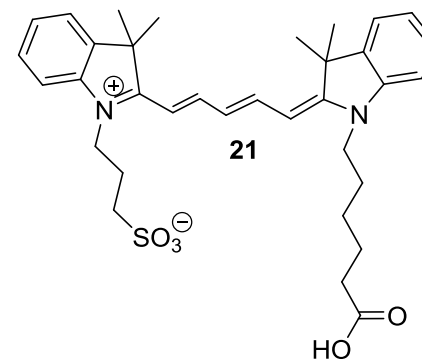
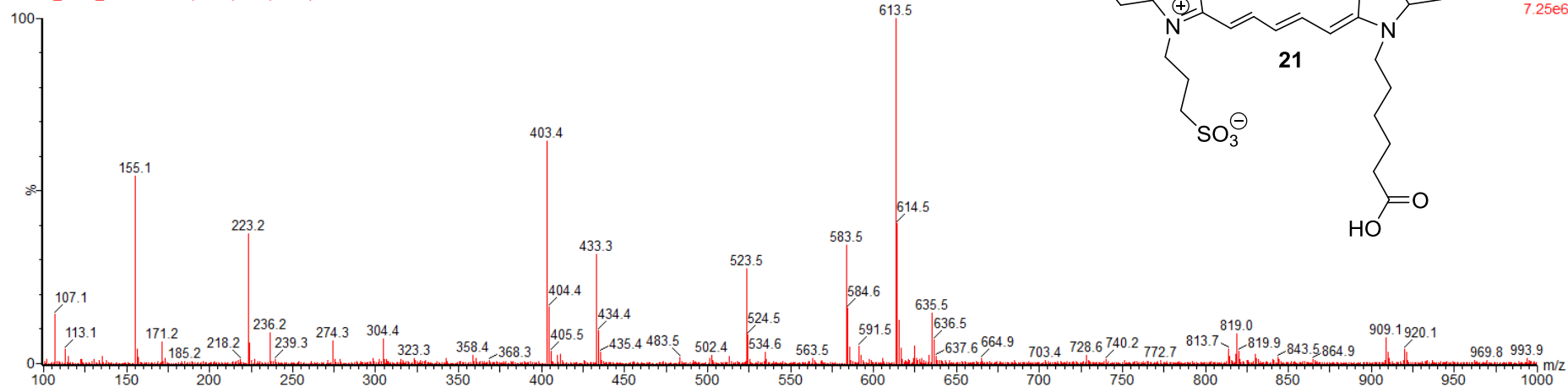


Compound **22** - ^1H NMR spectrum in DMSO-d_6



Compound **21** - MS (ESI+): m/z calc. for $C_{34}H_{42}N_2Na.O_5S^+$: 613.27; found: 613.5 $[M + Na]^+$.

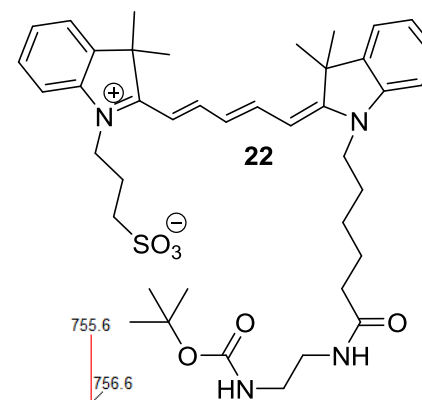
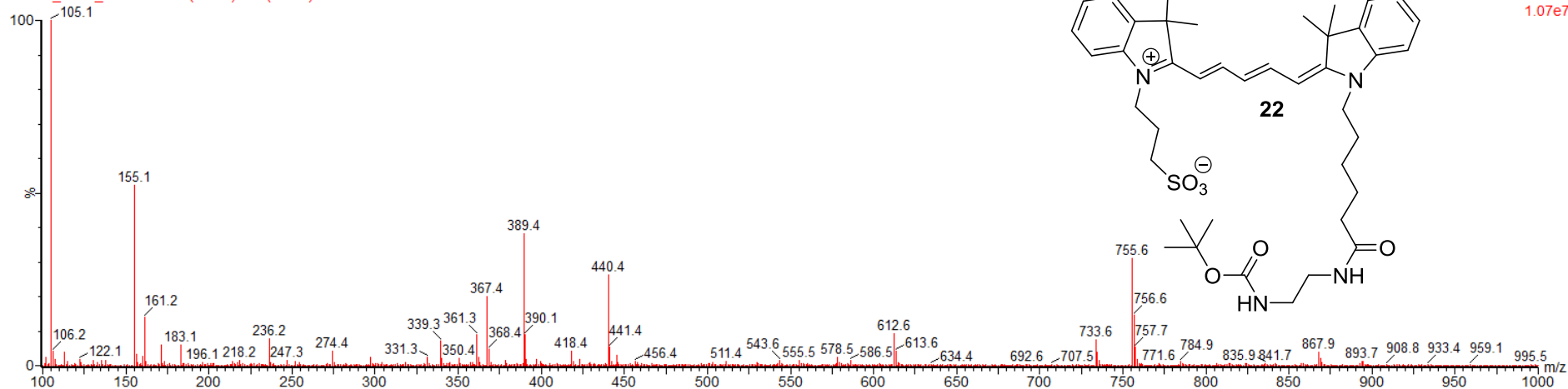
Shabat_Ehud_EH-2-114 14 (0.234) Cm (10:17)



1: MS2 ES+
7.25e6

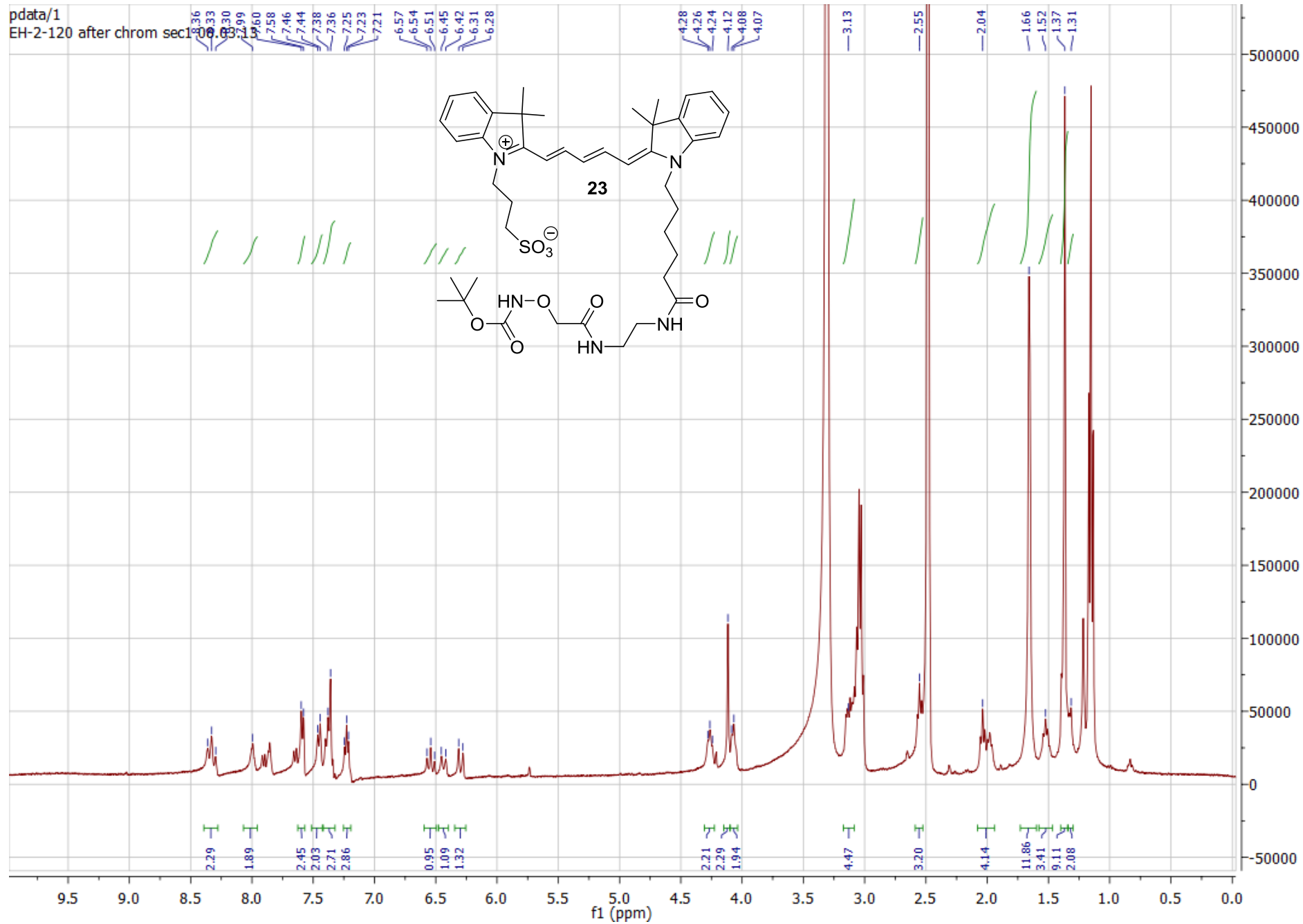
Compound **22** - MS (ESI+): m/z calc. for $C_{41}H_{56}N_4Na.O_6S^+$: 755.38; found: 755.6 $[M + Na]^+$.

Shabat_Ehud_EH-2-115 15 (0.251) Cm (10:21)



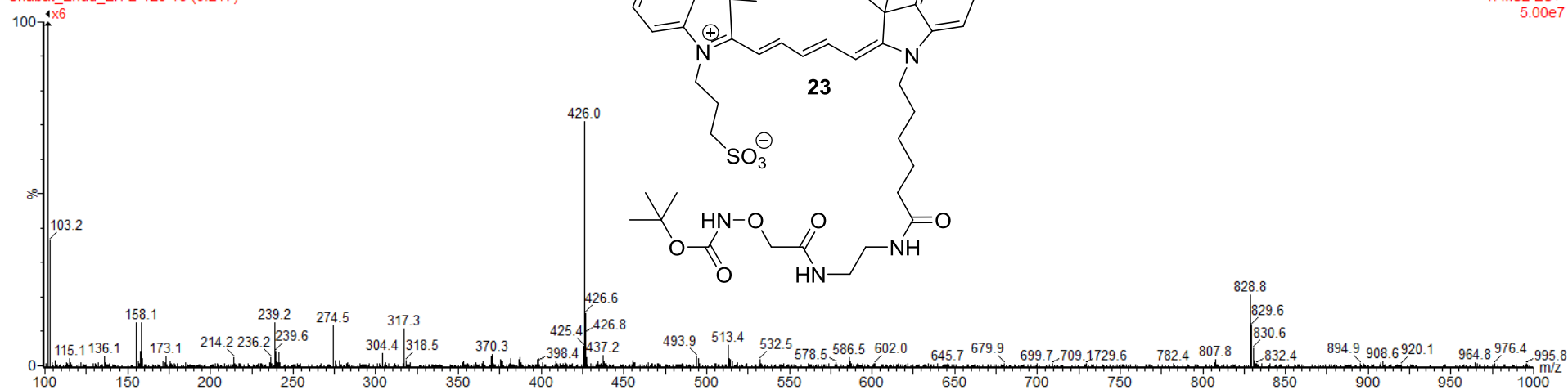
1: MS2 ES+
1.07e7

Compound **23** - ^1H NMR spectrum in DMSO-d_6



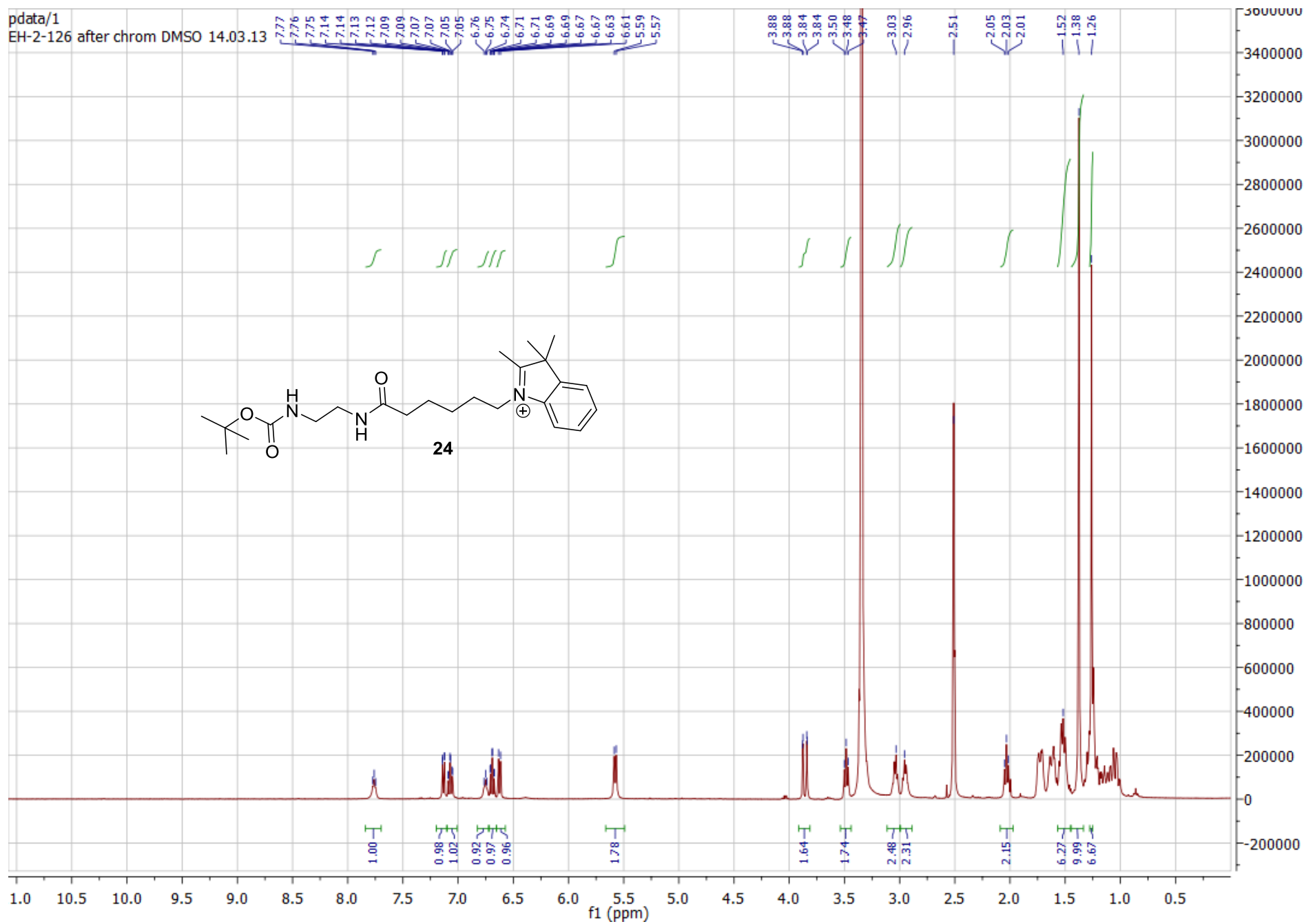
Compound **23** - MS (ESI+): m/z calc. for $C_{43}H_{59}N_5NaO_8S^+$: 828.40; found: 828.7 [M + Na]⁺.

Shabat_Ehud_EH-2-120 13 (0.217)

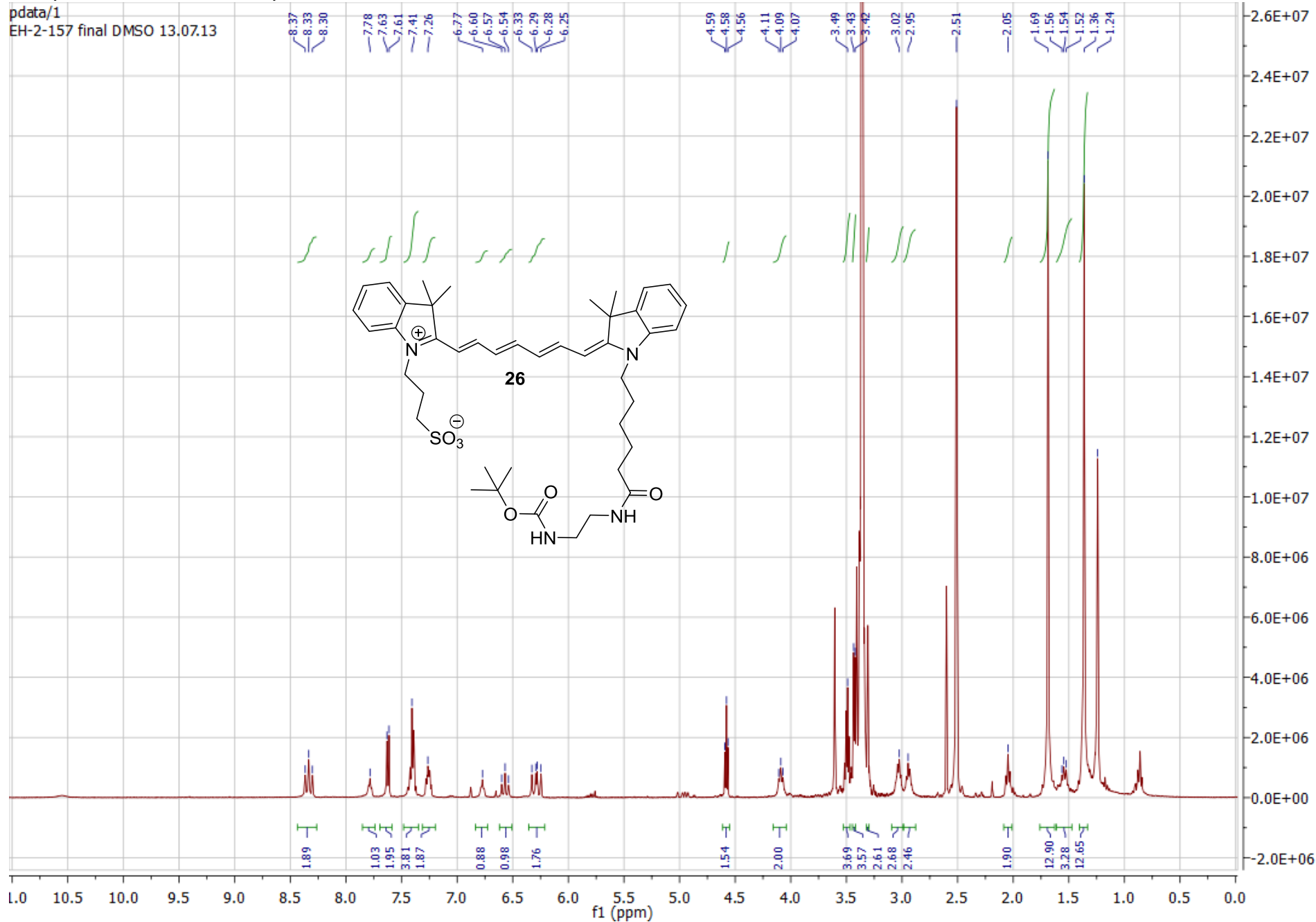


1: MS2 ES+
5.00e7

Compound **24** - ^1H NMR spectrum in DMSO-d_6

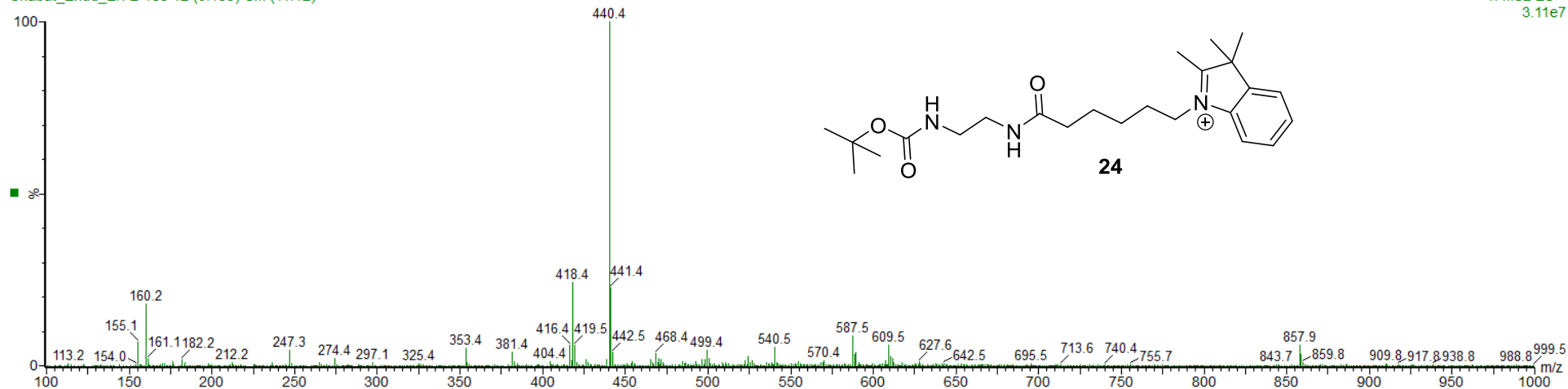


Compound **26** - ^1H NMR spectrum in DMSO-d_6



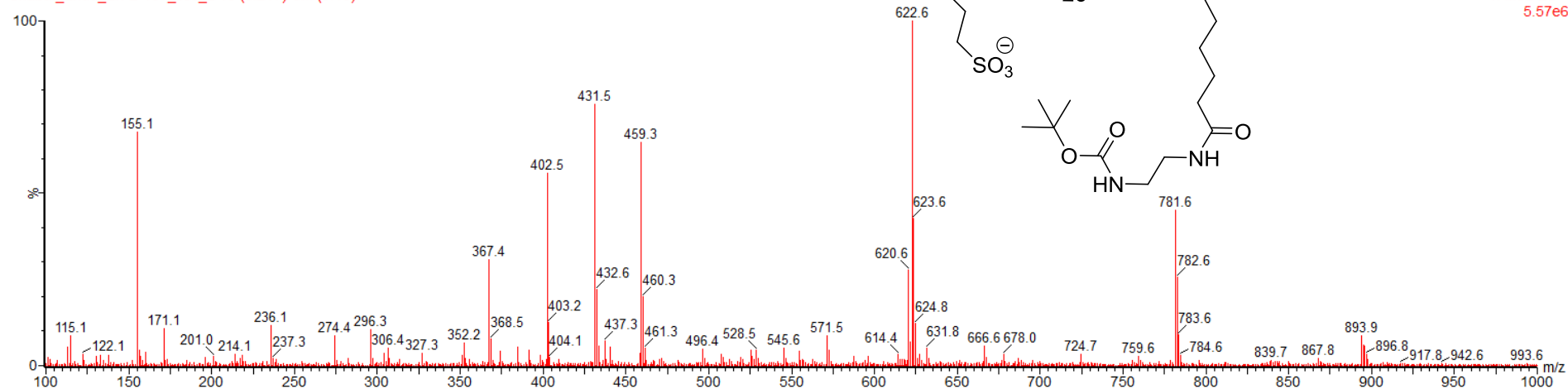
Compound **24** - MS (ESI+): m/z calc. for $C_{24}H_{36}N_3O_3^+$: 416.29; found: 416.4 $[M]^+$.

Shabat_Ehud_EH-2-155 12 (0.199) Cm (11:12)

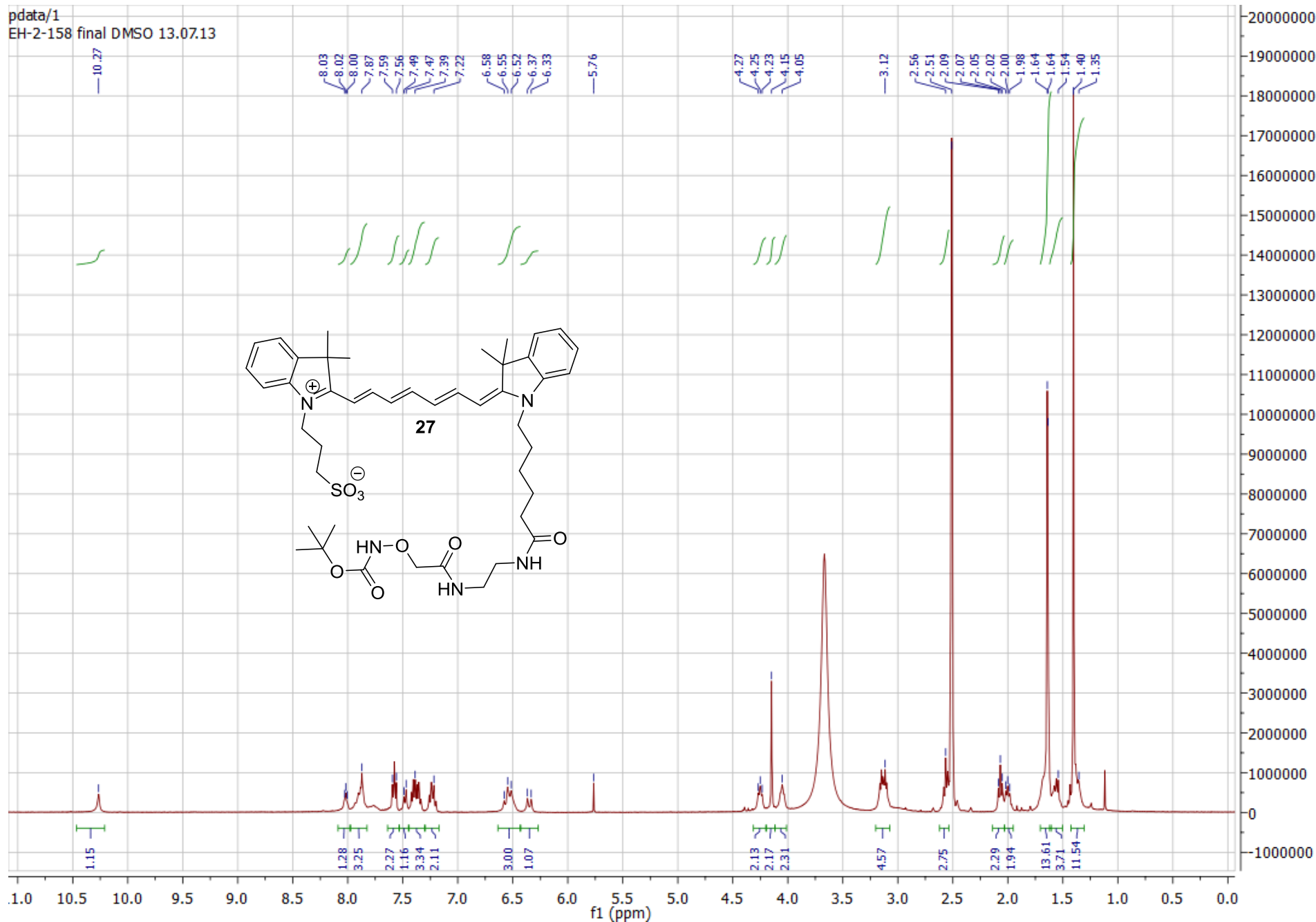


Compound **26** - MS (ESI+): m/z calc. for $C_{43}H_{58}N_4NaO_6S^+$: 781.39; found: 781.6 $[M + Na]^+$.

Shabat_Ehud_EH-2-157_sec_2 13 (0.217) Cm (9:16)



Compound **27** - ^1H NMR spectrum in DMSO- d_6



Compound **27** - MS (ESI+): m/z calc. for $C_{45}H_{61}N_5NaO_8S^+$: 854.41; found: 854.7 $[M + Na]^+$.

EH-2-100 MeOH from DMSO D conc

Ehud

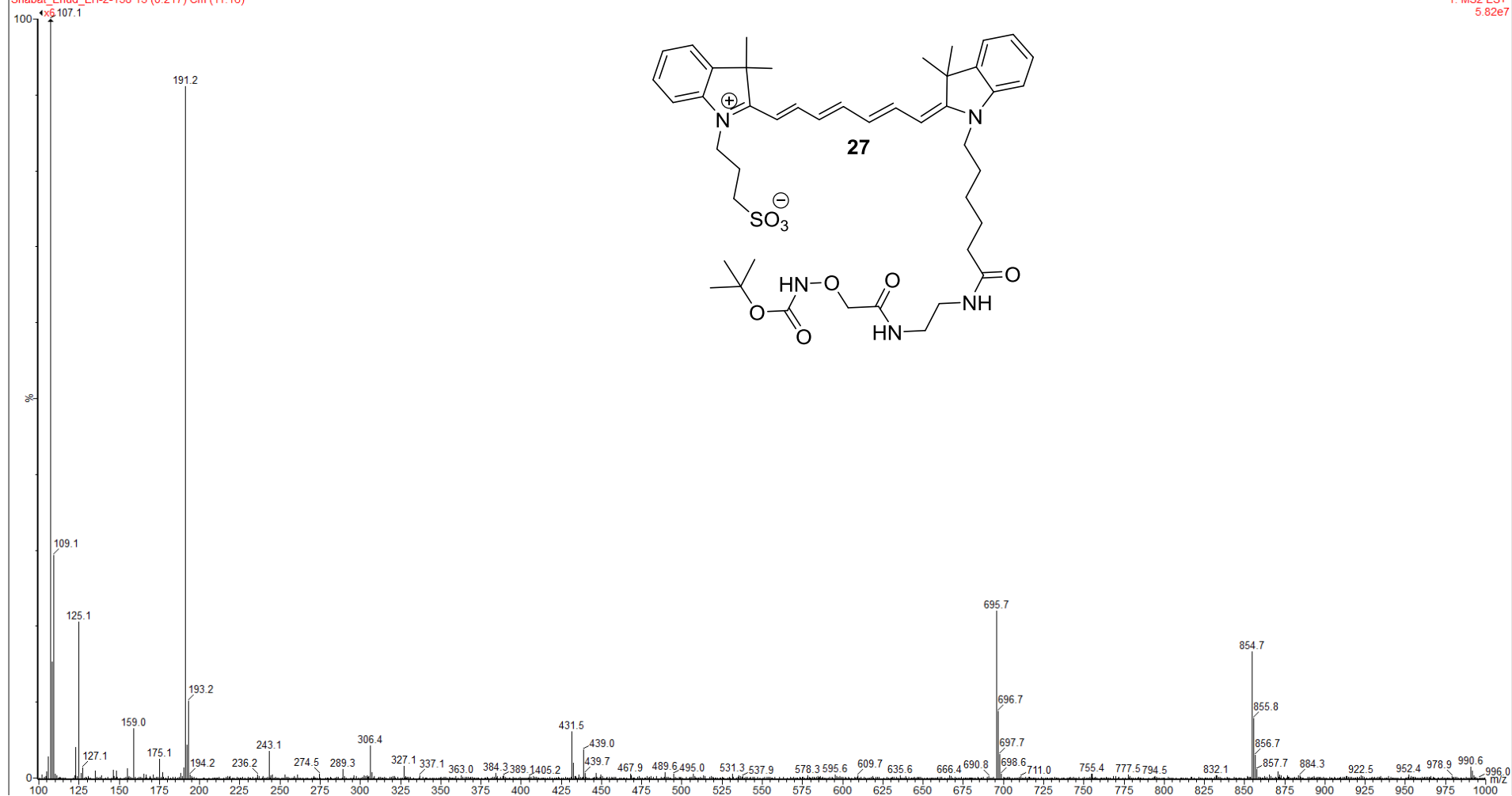
17-Jul-2013

Coll energy 3

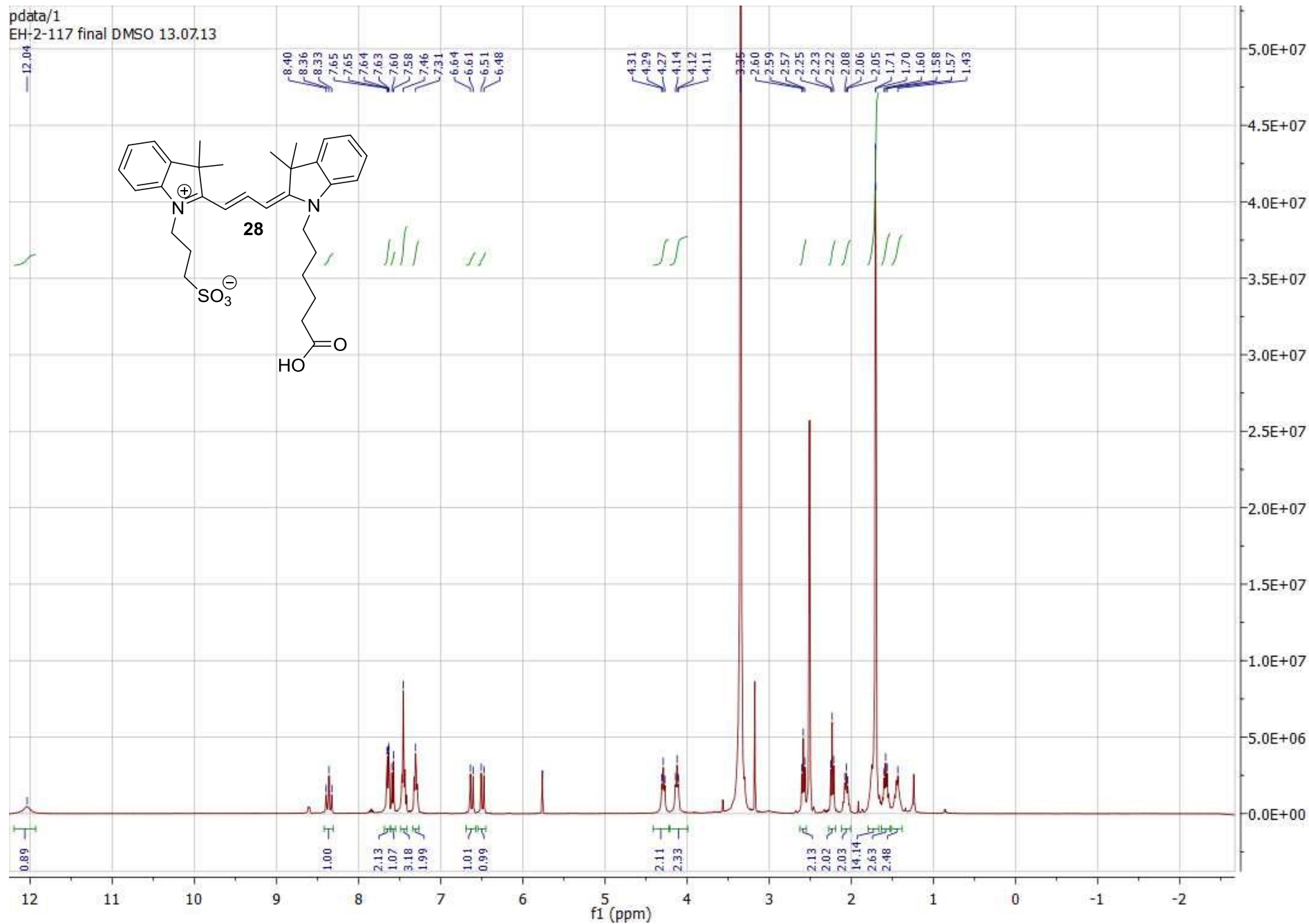
Shabat_Ehud_EH-2-158 13 (0.217) Cm (11:16)

1: MS2 ES+

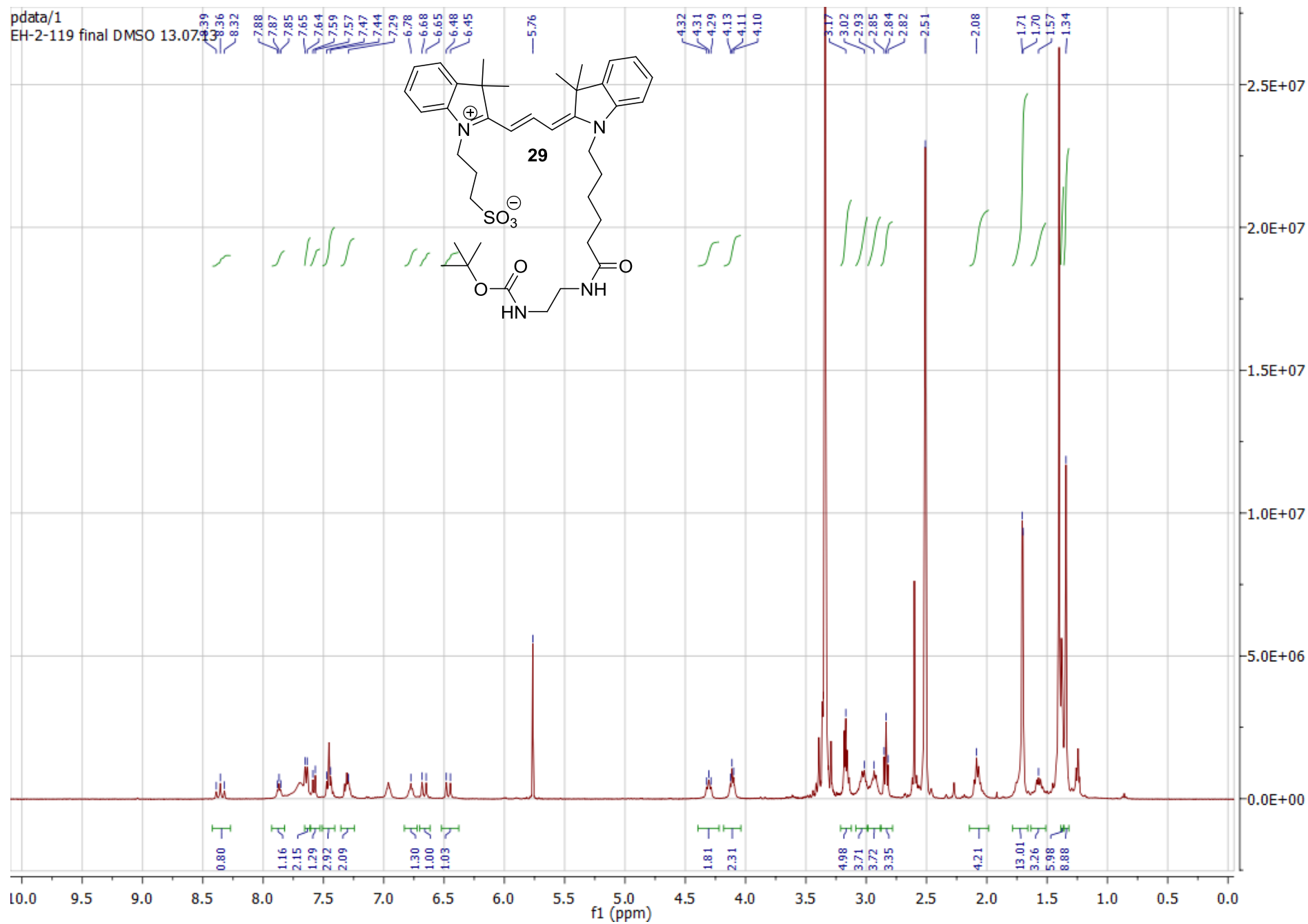
5.82e7



Compound **28** - ^1H NMR spectrum in DMSO-d_6

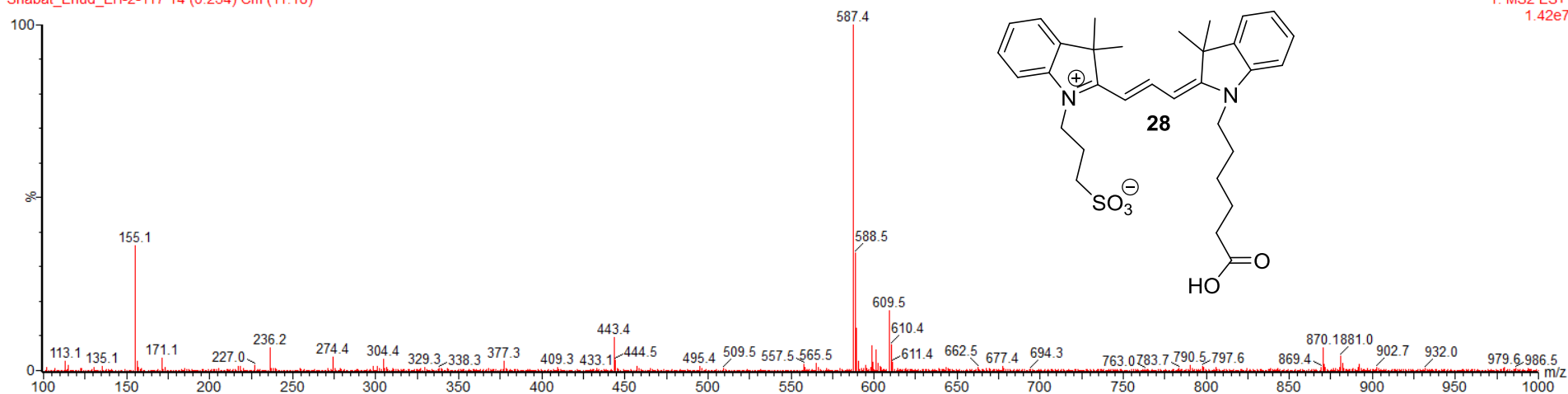


Compound **29** - ^1H NMR spectrum in DMSO- d_6



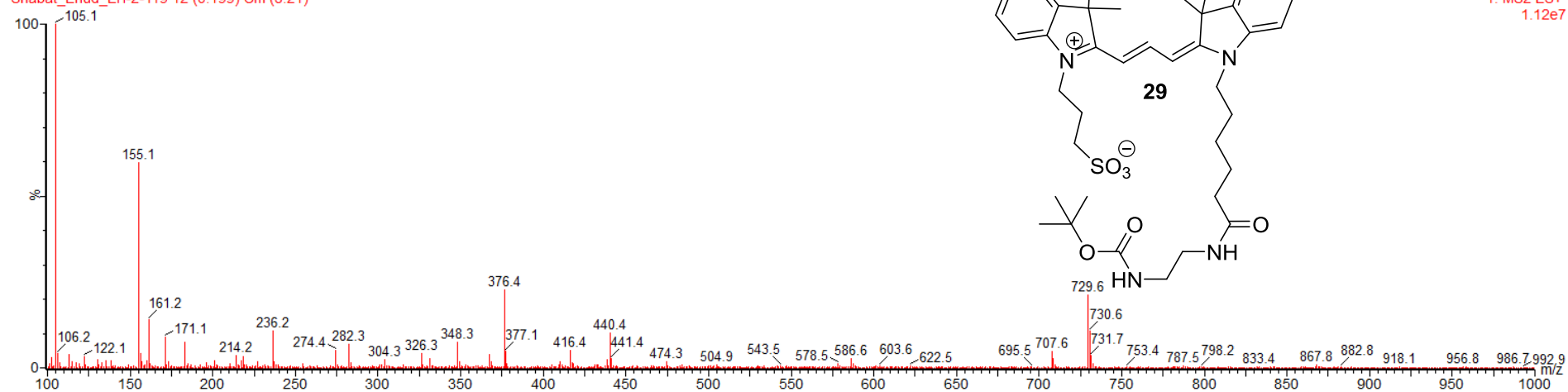
Compound **28** - MS (ESI+): m/z calc. for $C_{32}H_{41}N_2NaO_5S^+$: 587.25; found: 587.4 $[M + Na]^+$.

Shabat_Ehud_EH-2-117 14 (0.234) Cm (11:18)

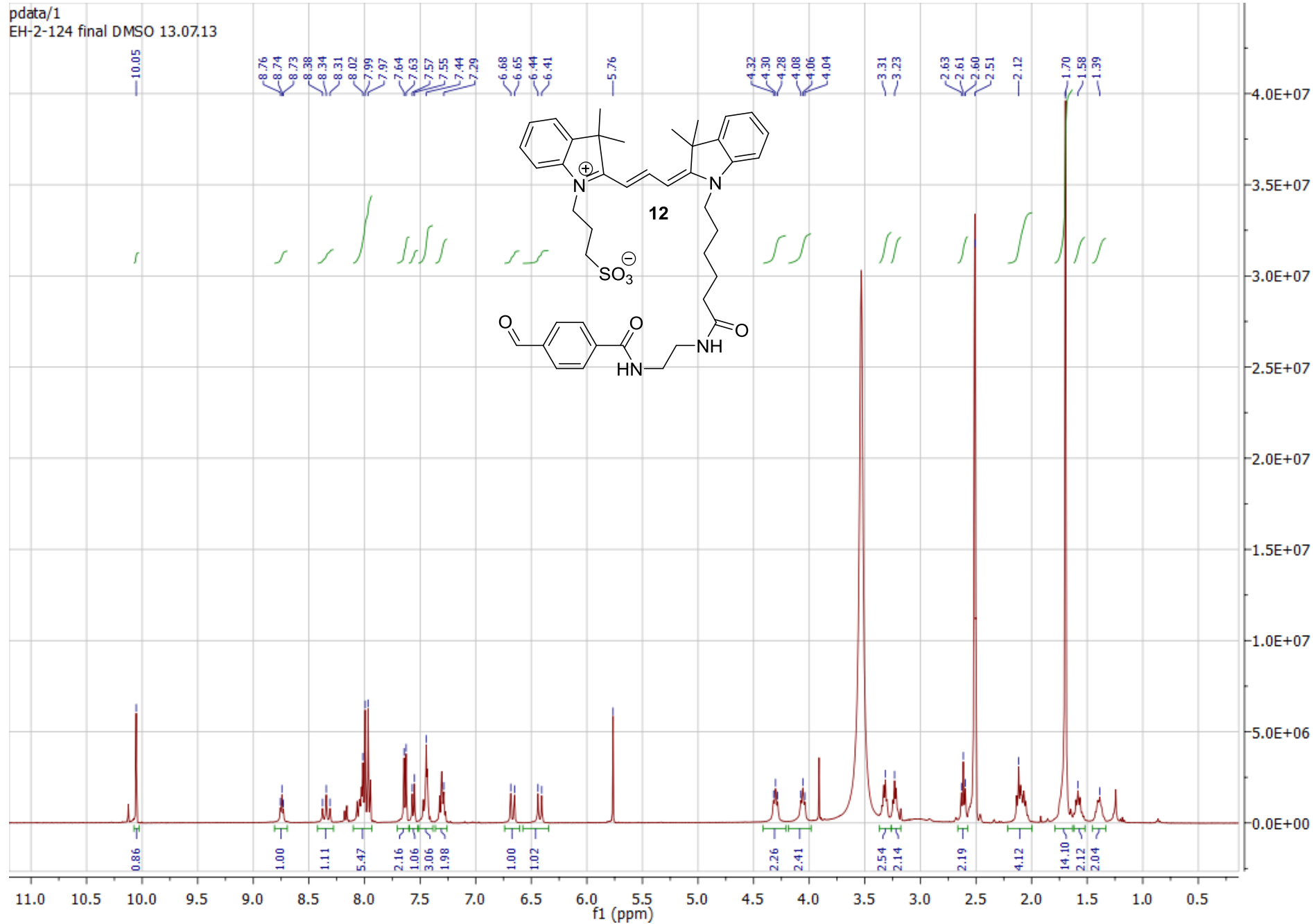


Compound **29** - MS (ESI+): m/z calc. for $C_{39}H_{54}N_4NaO_6S^+$: 729.36; found: 729.6 $[M + Na]^+$.

Shabat_Ehud_EH-2-119 12 (0.199) Cm (8:21)

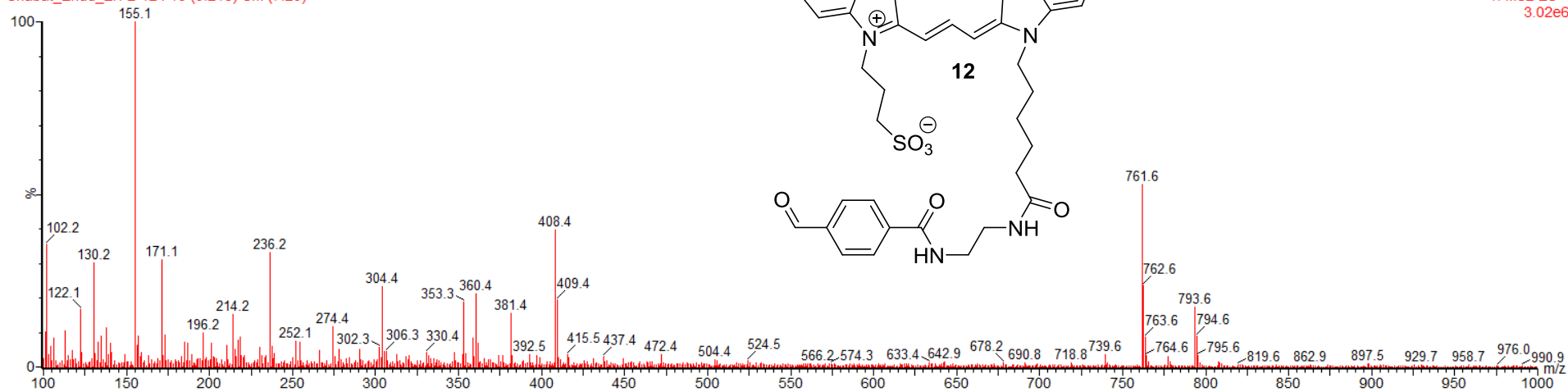


Compound **12** - ^1H NMR spectrum in DMSO-d_6

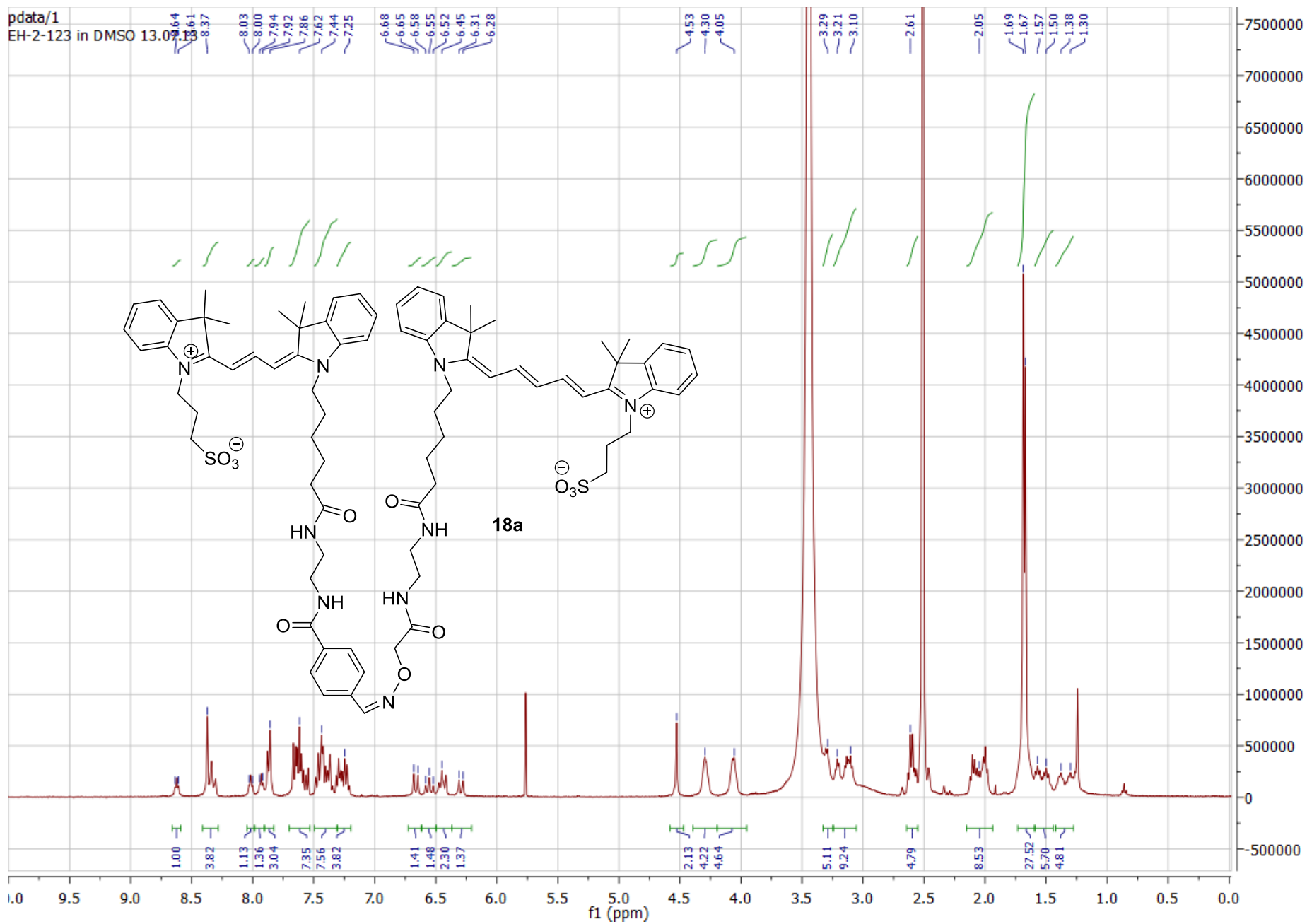


Compound **12** - MS (ESI+): m/z calc. for $C_{42}H_{50}N_4NaO_6S^+$: 761.34; found: 761.6 $[M + Na]^+$.

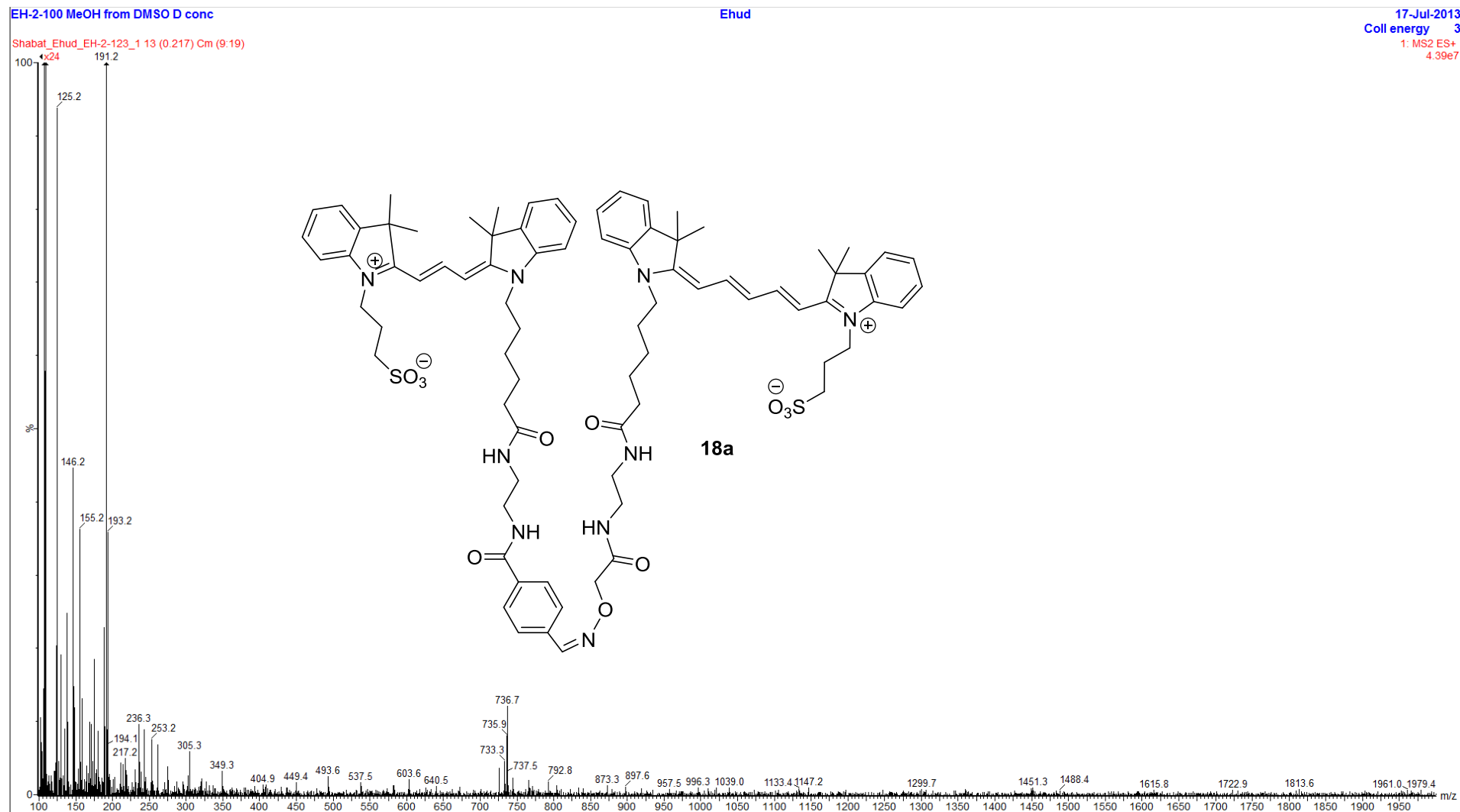
Shabat_Ehud_EH-2-124 13 (0.216) Cm (7:20)



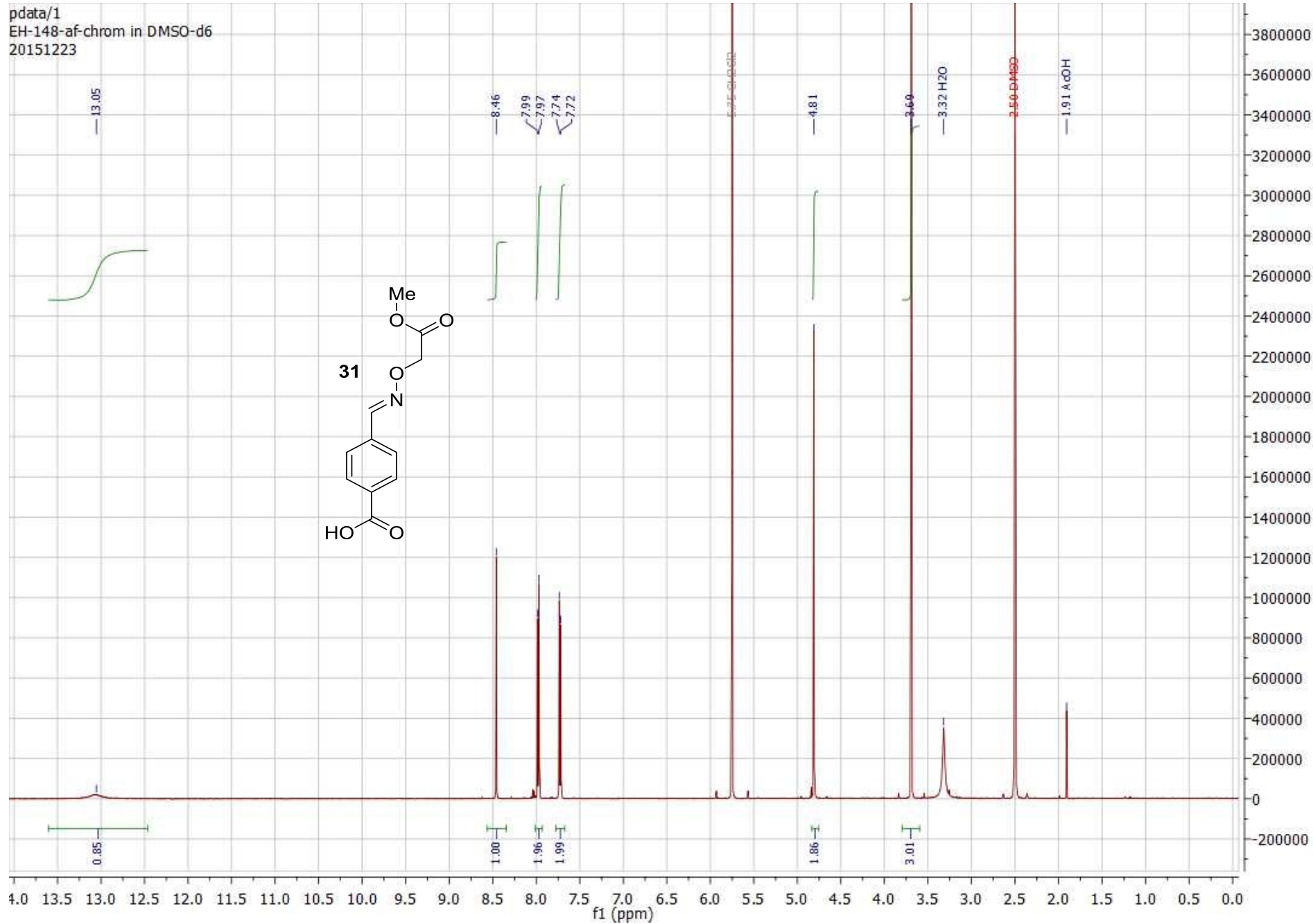
Compound **18a** - ^1H NMR spectrum in DMSO- d_6



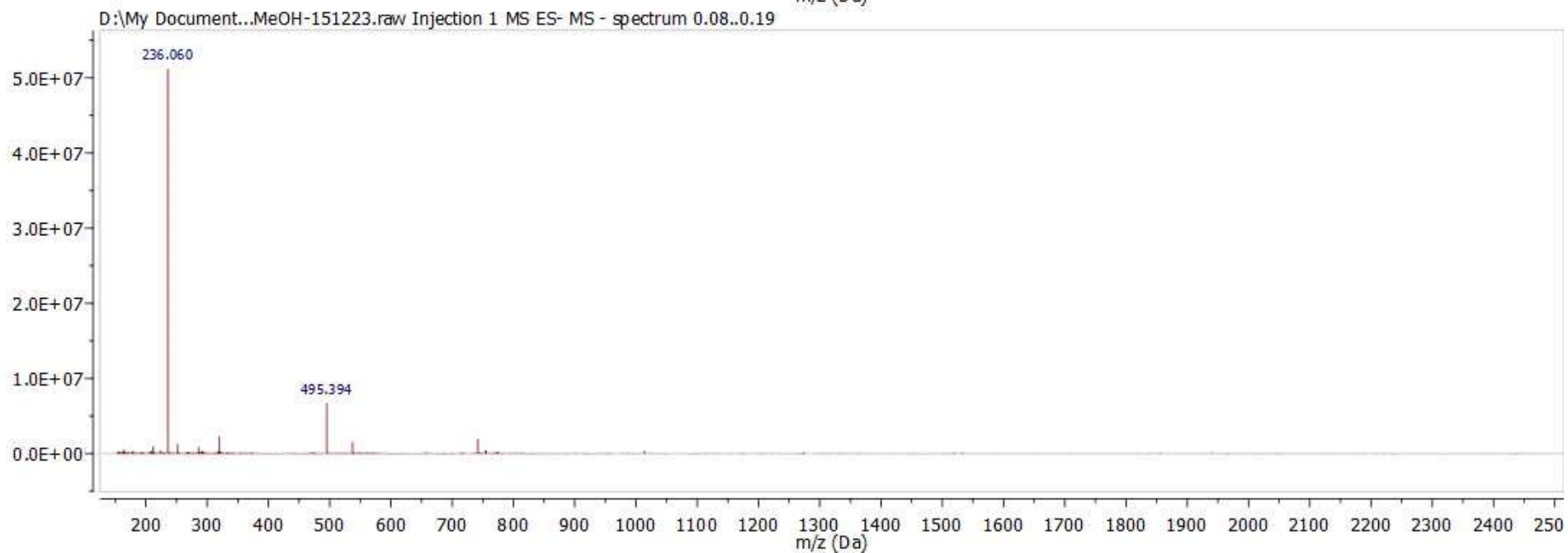
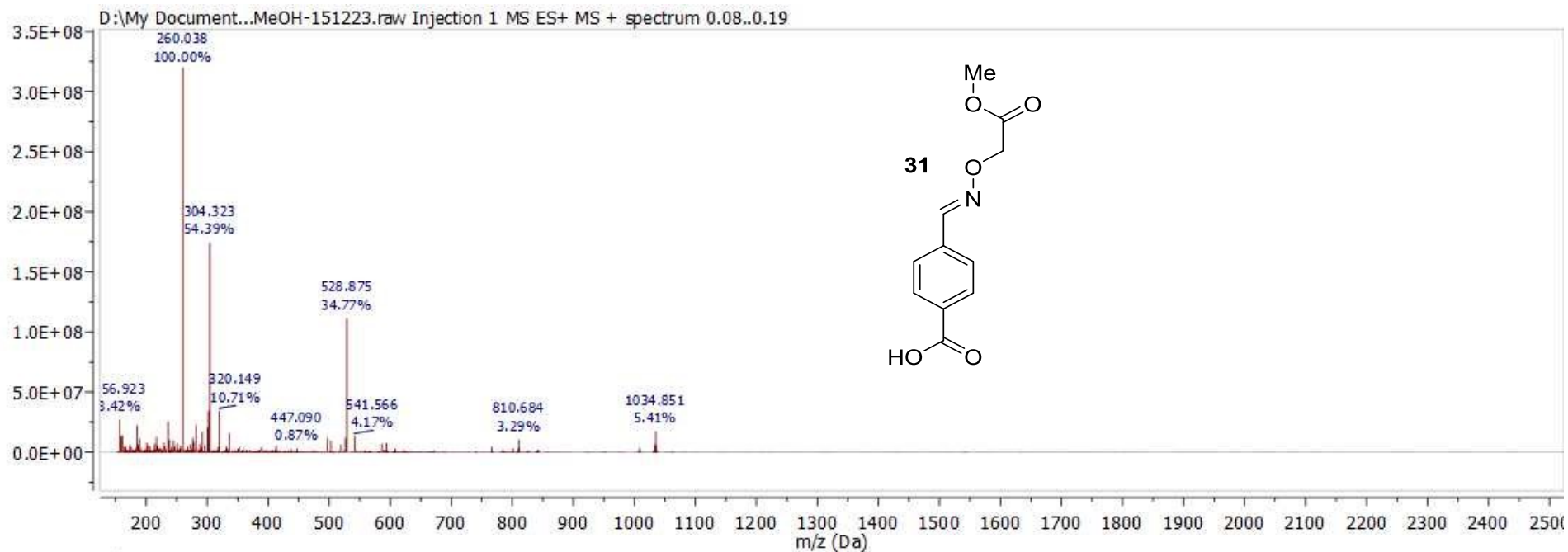
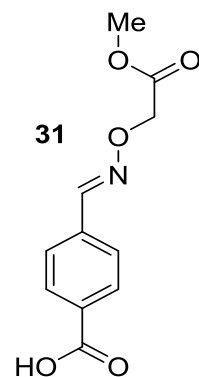
Compound **18a** - MS (ESI+): m/z calc. for $C_{80}H_{99}N_9Na_2O_{11}S_2^{2+}$: 735.83; found: 735.9 $[M + 2Na]^{2+}$.



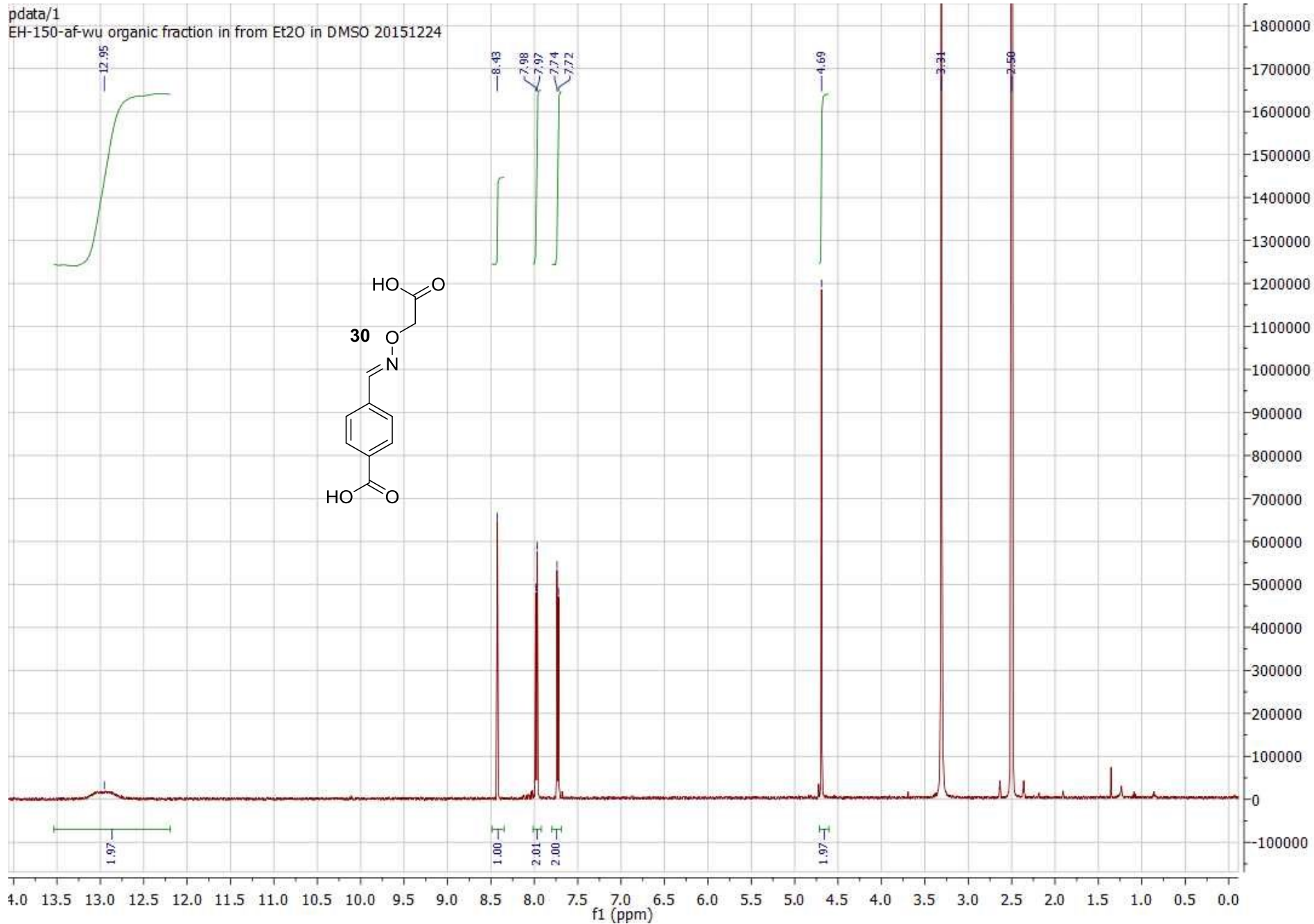
Compound **31**- ^1H NMR spectrum in DMSO- d_6



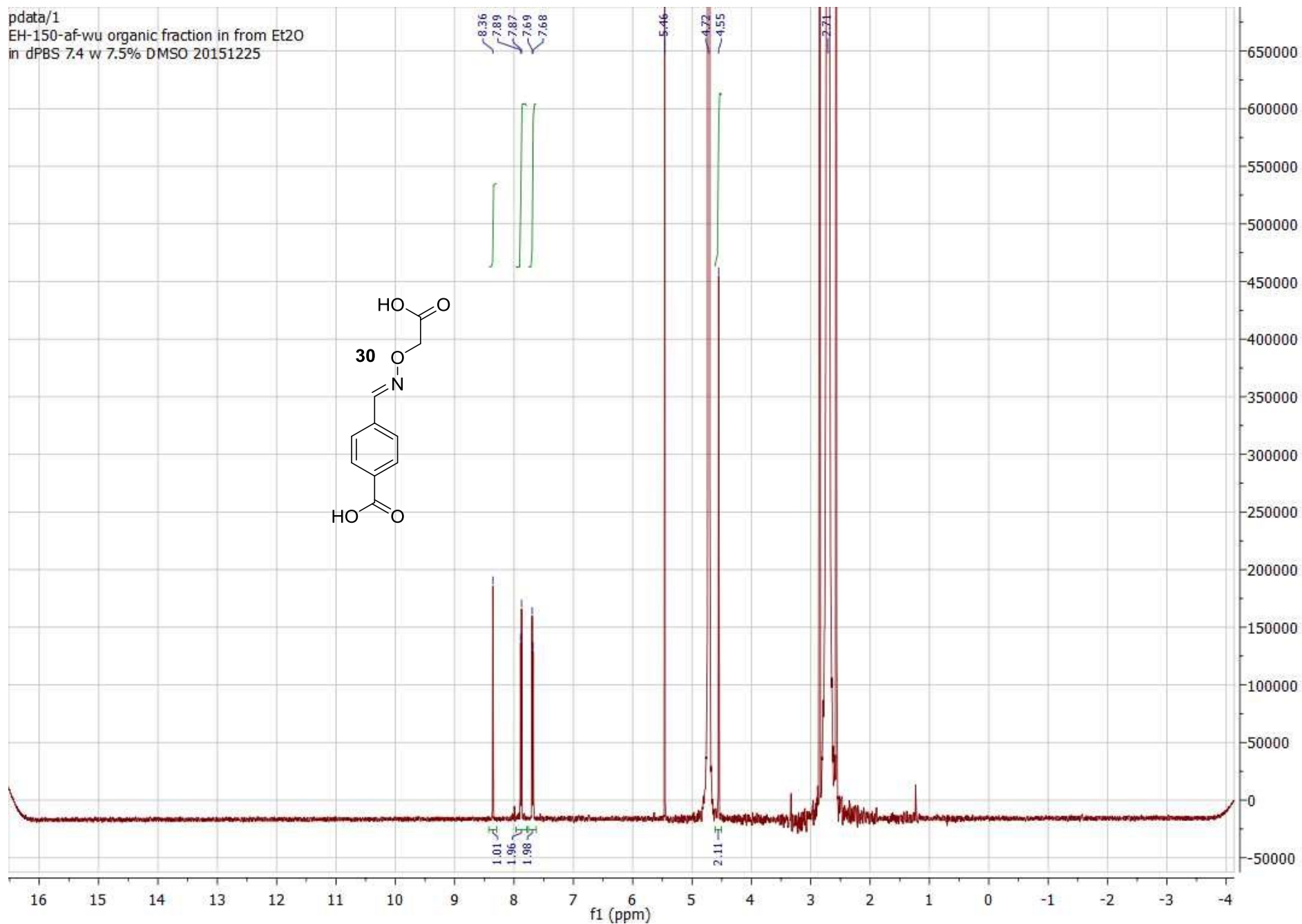
Compound **31** - MS (ESI+): m/z calc. for $C_{11}H_{11}NNaO_5^+$: 260.05; found: 260.038 $[M + Na]^+$; MS (ESI-): m/z calc. for $C_{11}H_{10}NO_5^-$: 236.06; found: 236.06 $[M - H]^-$.



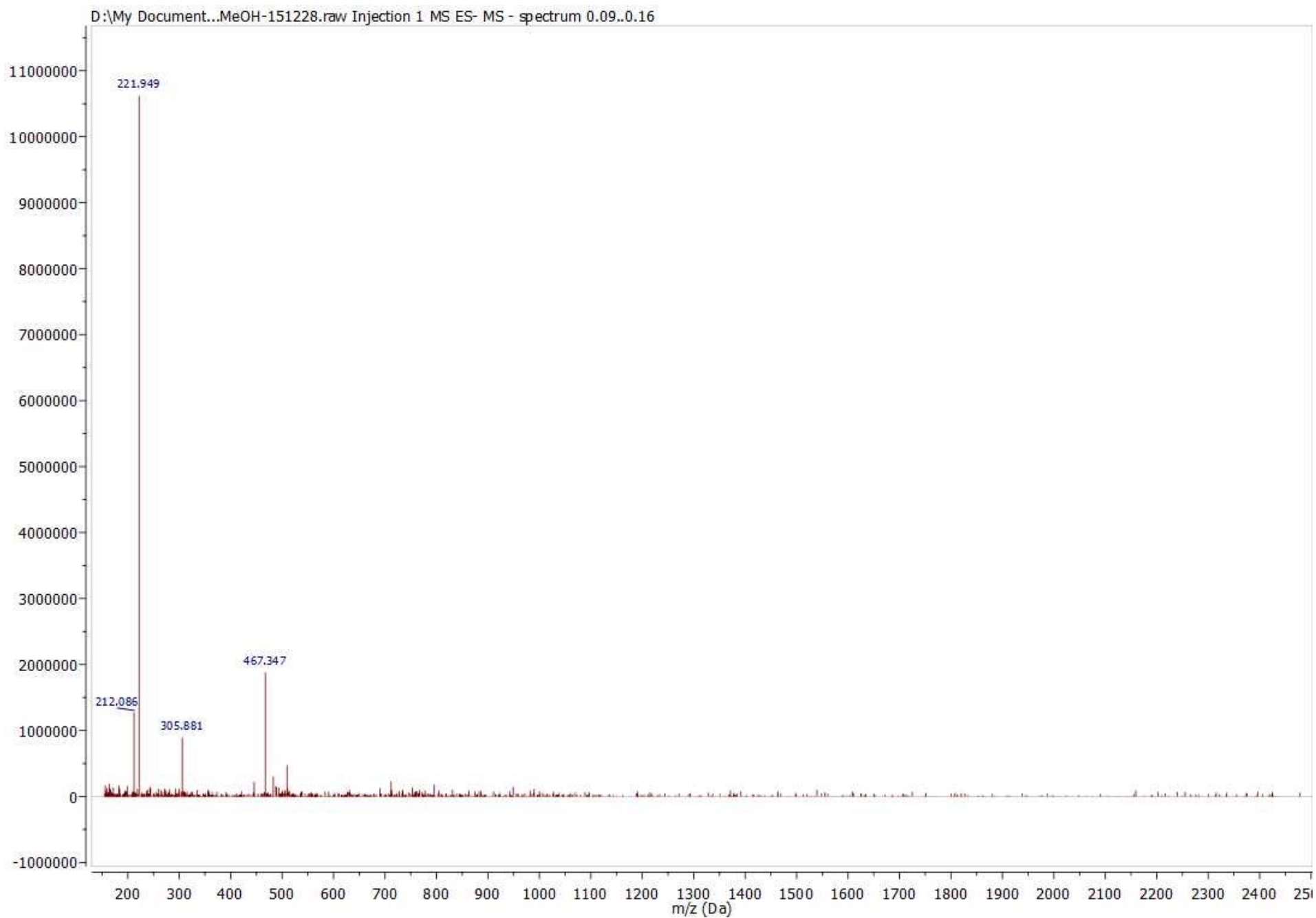
Compound **30** - ^1H NMR spectrum in DMSO-d_6



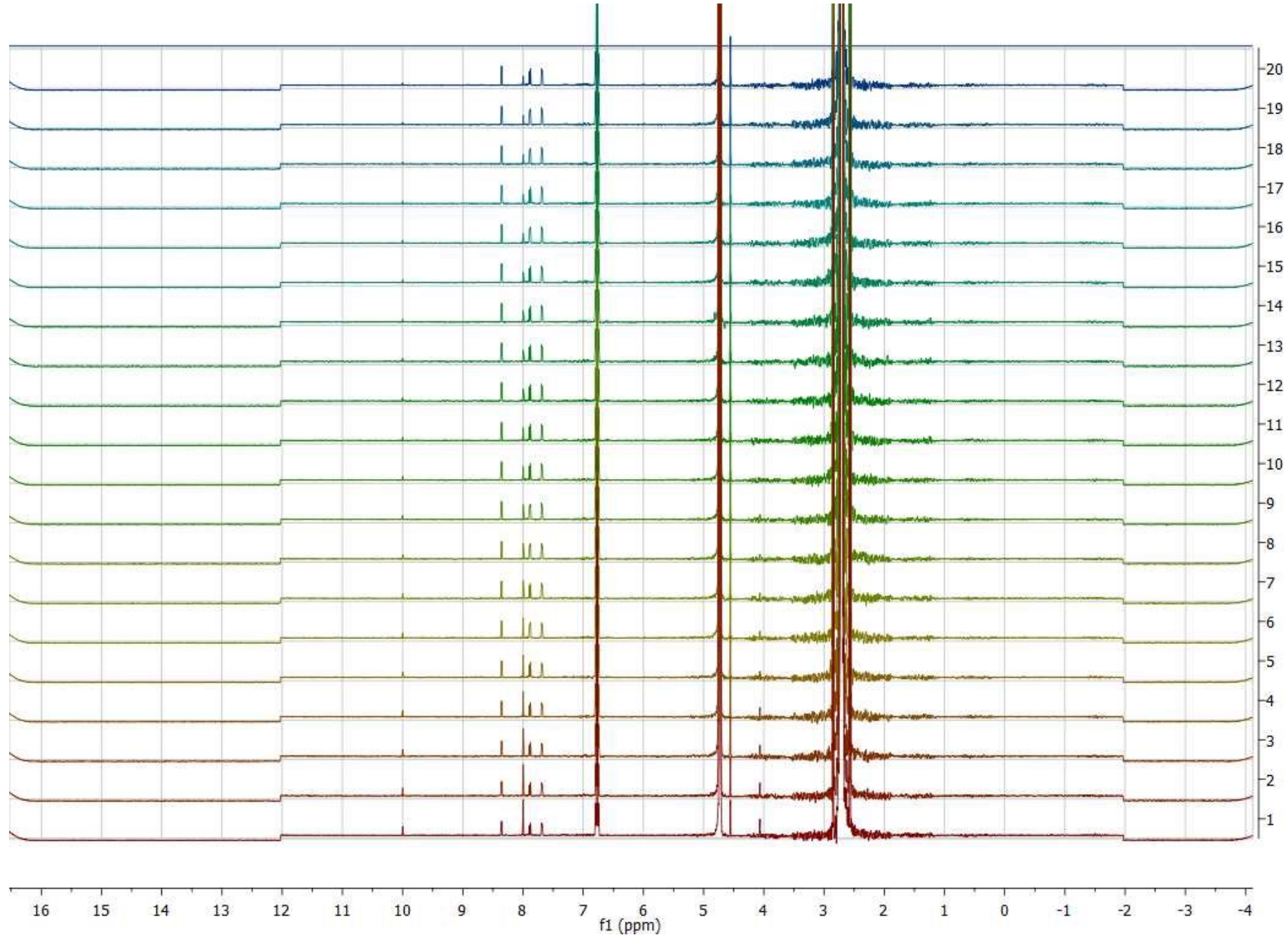
Compound **30**- ^1H NMR spectrum in dPBS (pH 7.4) with 7.5% DMSO (v/v)



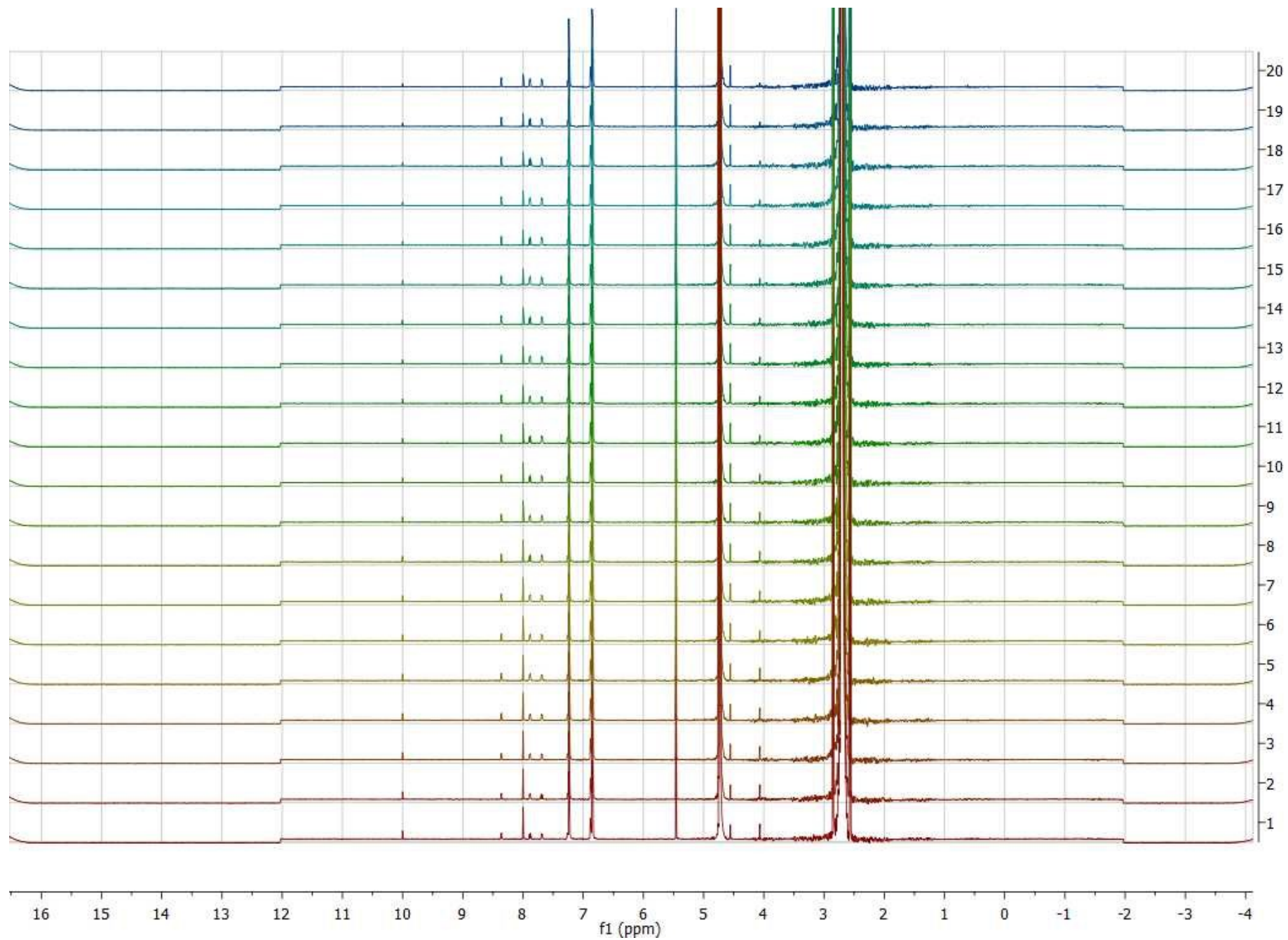
Compound **30** - MS (ESI-): m/z calc. for $C_{10}H_8NO_5^-$: 222.04; found: 221.949 $[M - H]^-$.



^1H NMR spectra of the oxime bond formation reaction between 4-formylbenzoic acid and (aminoxy)acetic acid hemihydrochloride with 10 mM 4-aminophenol in dPBS (pH 7.4) with 7.5% DMSO (v/v)



^1H NMR spectra of the oxime bond formation reaction between 4-formylbenzoic acid and (aminoxy)acetic acid hemihydrochloride with 10 mM aniline in dPBS (pH 7.4) with 7.5% DMSO (v/v)



^1H NMR spectra of the oxime bond formation reaction between 4-formylbenzoic acid and (aminoxy)acetic acid hemihydrochloride with no catalyst in dPBS (pH 7.4) with 7.5% DMSO (v/v)

