

The synthesis of new amphiphilic *p*-tert-butylthiacalix[4]arenes containing peptide fragments and their interaction with DNA

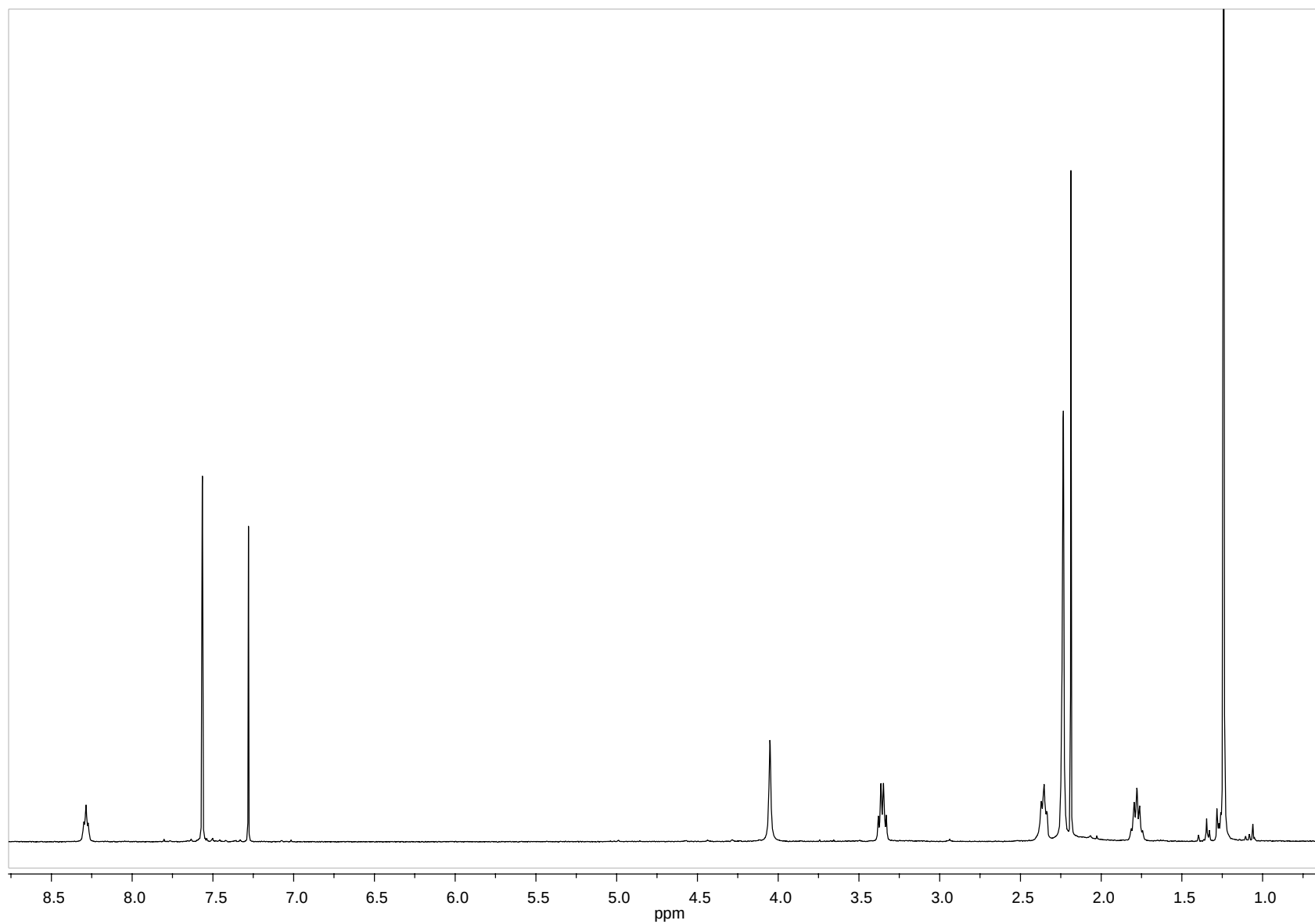
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^aKazan (Volga Region) Federal University, A.M. Butlerov Chemical Institute, 420008
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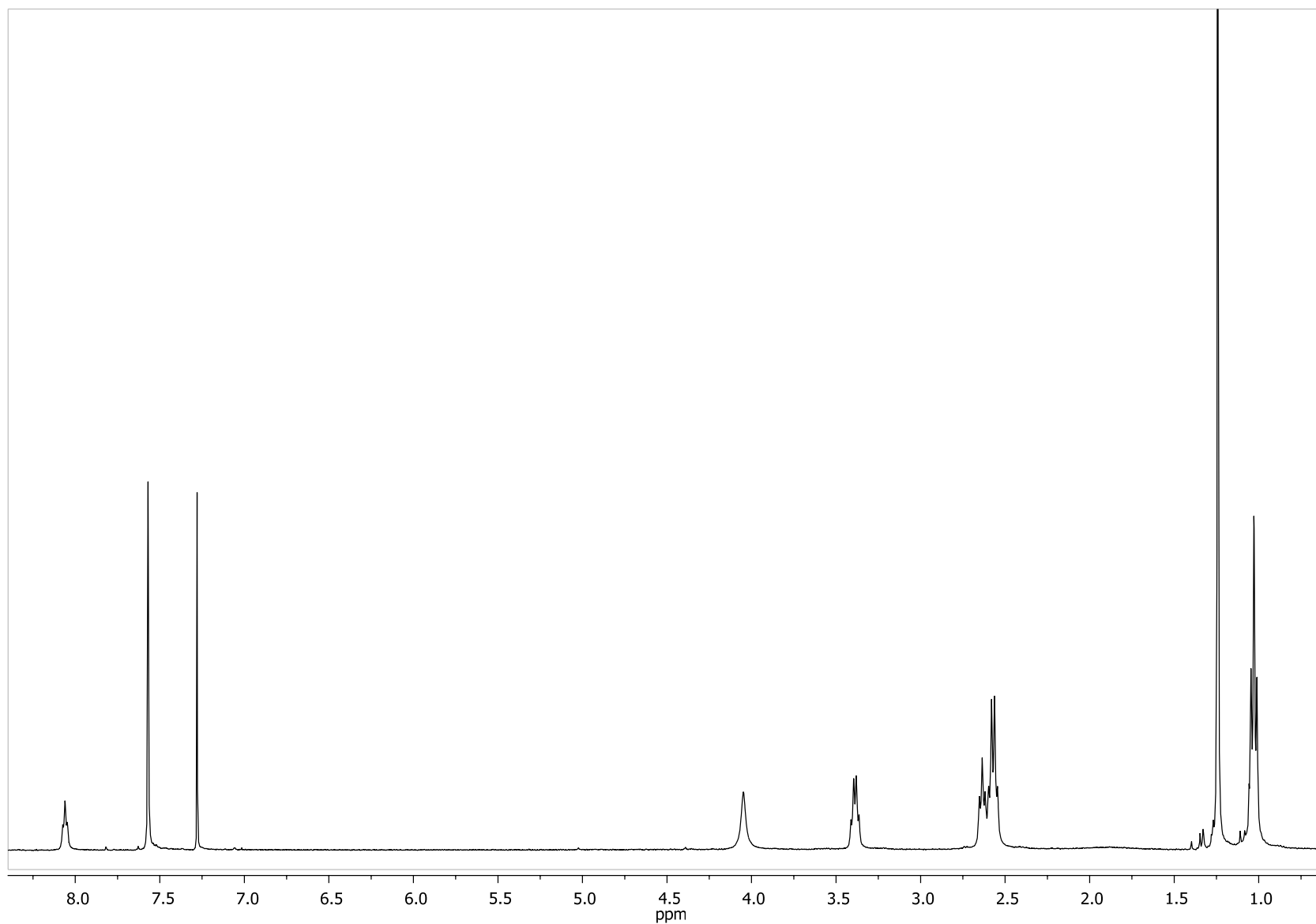
^bA. E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Centre of the
Russian Academy of Sciences, 420088 Kazan, Russian Federation

Electronic Supplementary Information

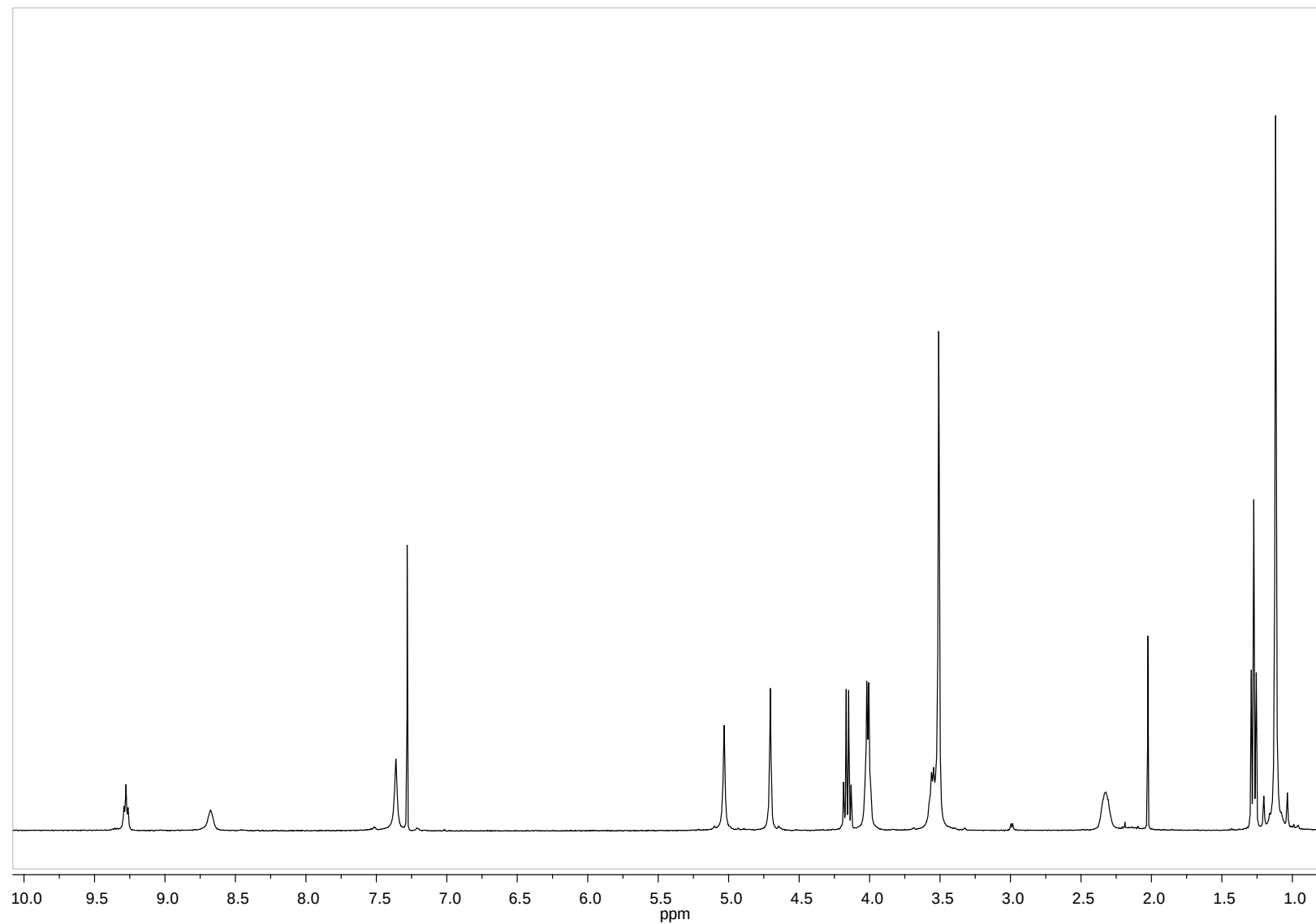
^1H NMR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethylaminopropyl)carbamoylmethoxy)-2,8,14,20-tetratetrathiacalix[4]arene (1,3-*alternate*-5), CDCl_3 , 298 K, 400 MHz



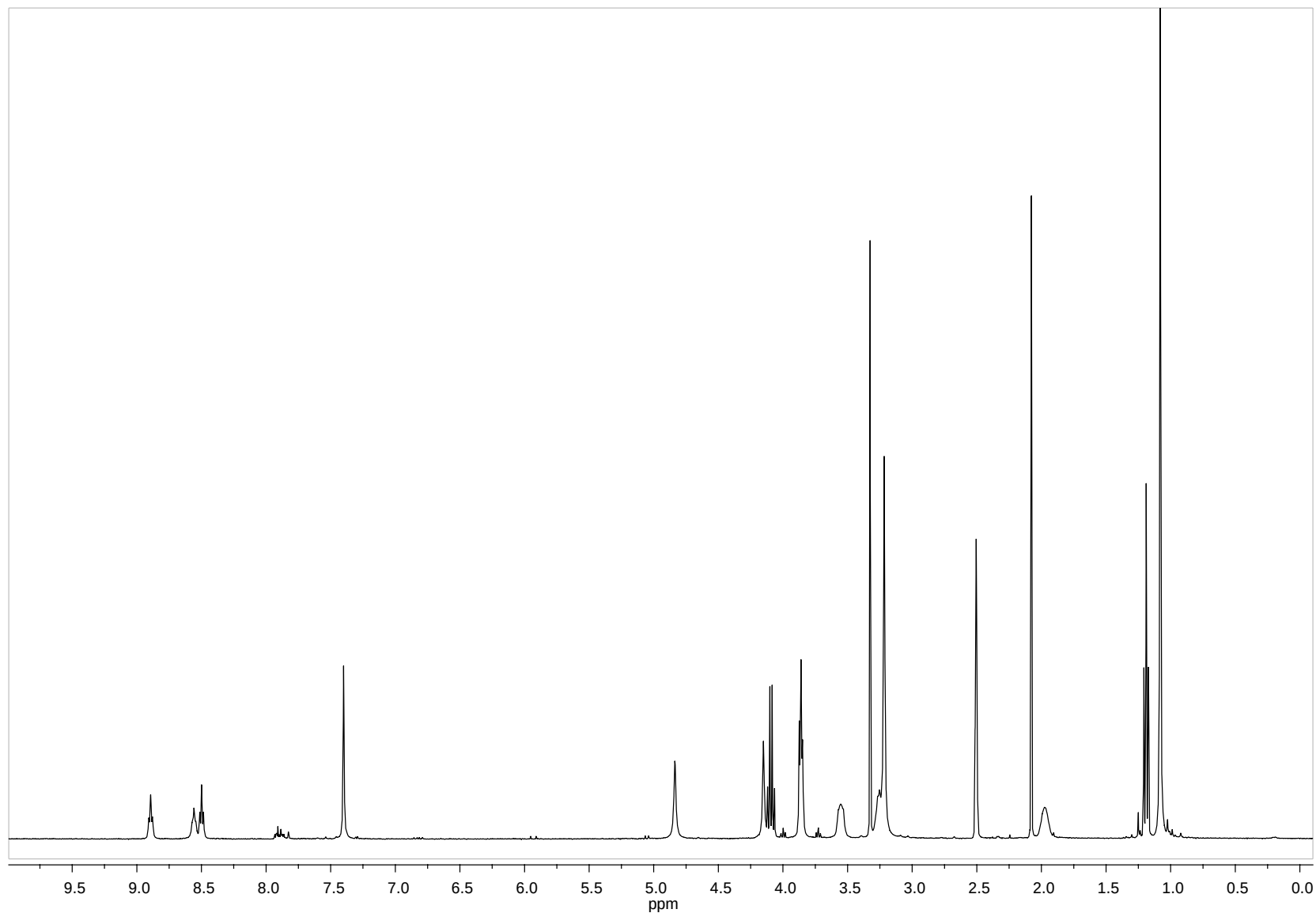
^1H NMR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(*N*-(2',2'-diethylaminoethyl)carbamoylmethoxy)-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*-6), CDCl_3 , 298 K, 400 MHz



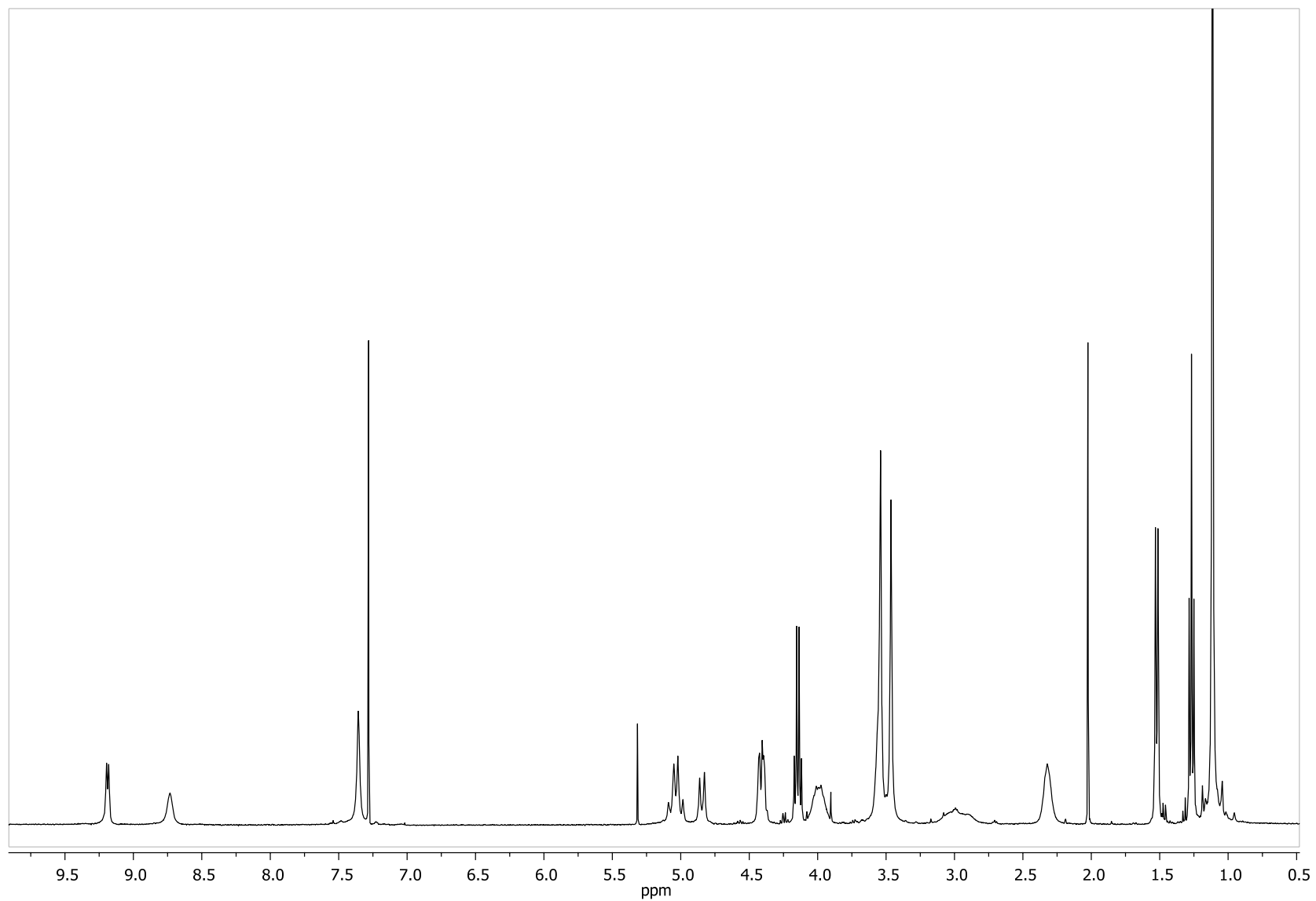
¹H NMR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{ethoxycarbonylmethyl}amidocarbonylmethyl)ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-14), CDCl₃, 298 K, 400 MHz



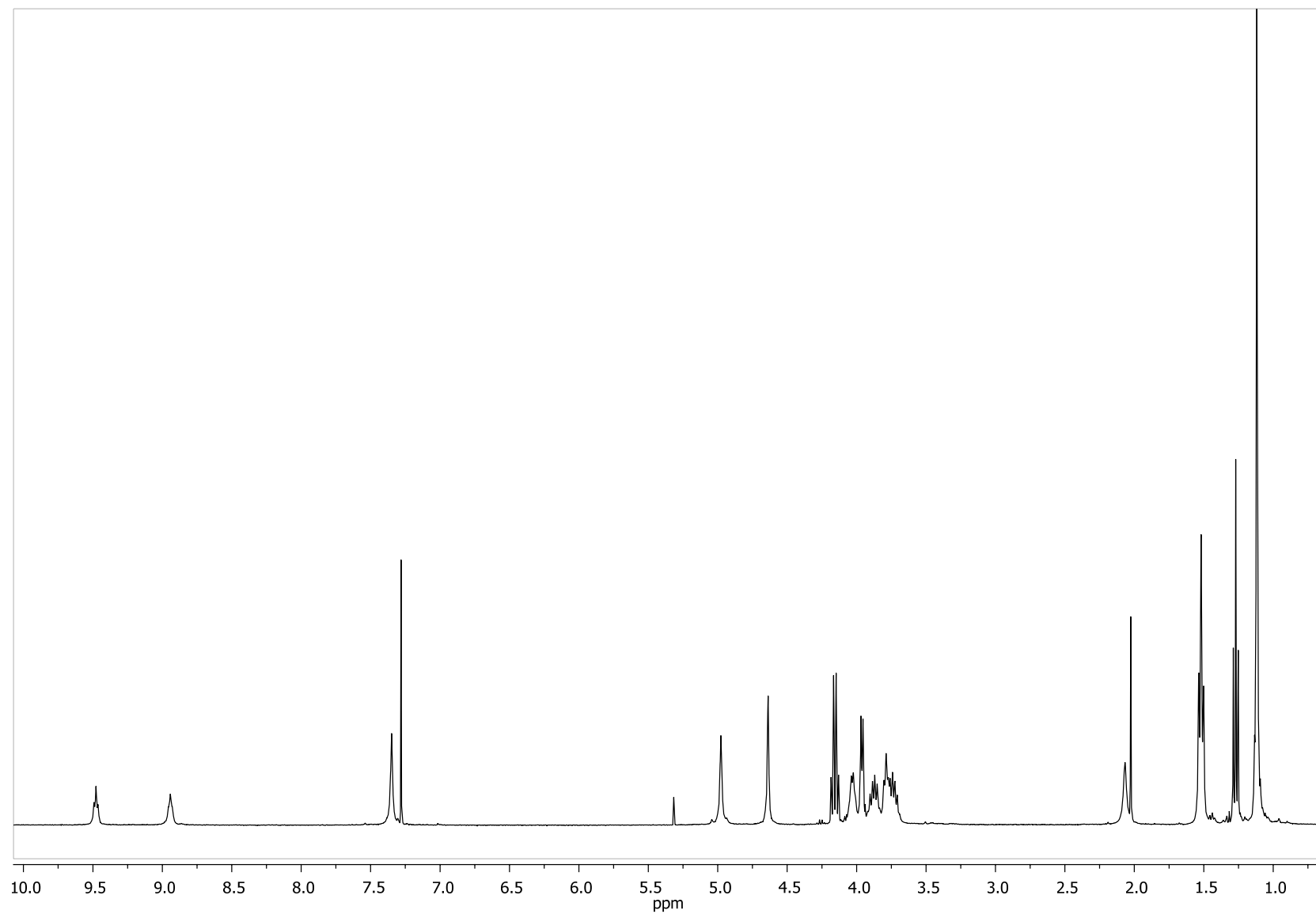
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tetrathiacalix[4]arene tetrabromide (*cone*-15), DMSO-d₆, 298 K, 400 MHz**



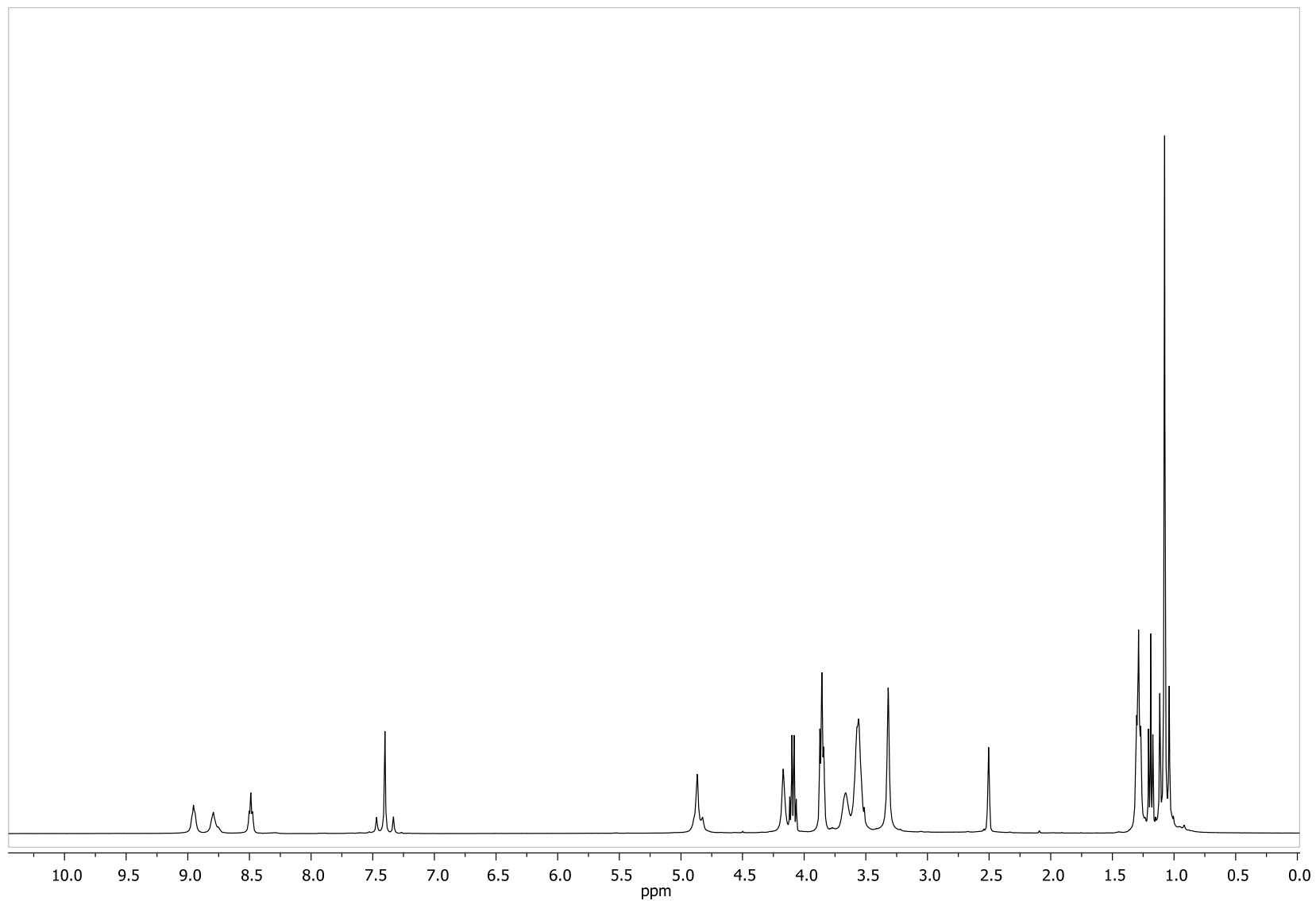
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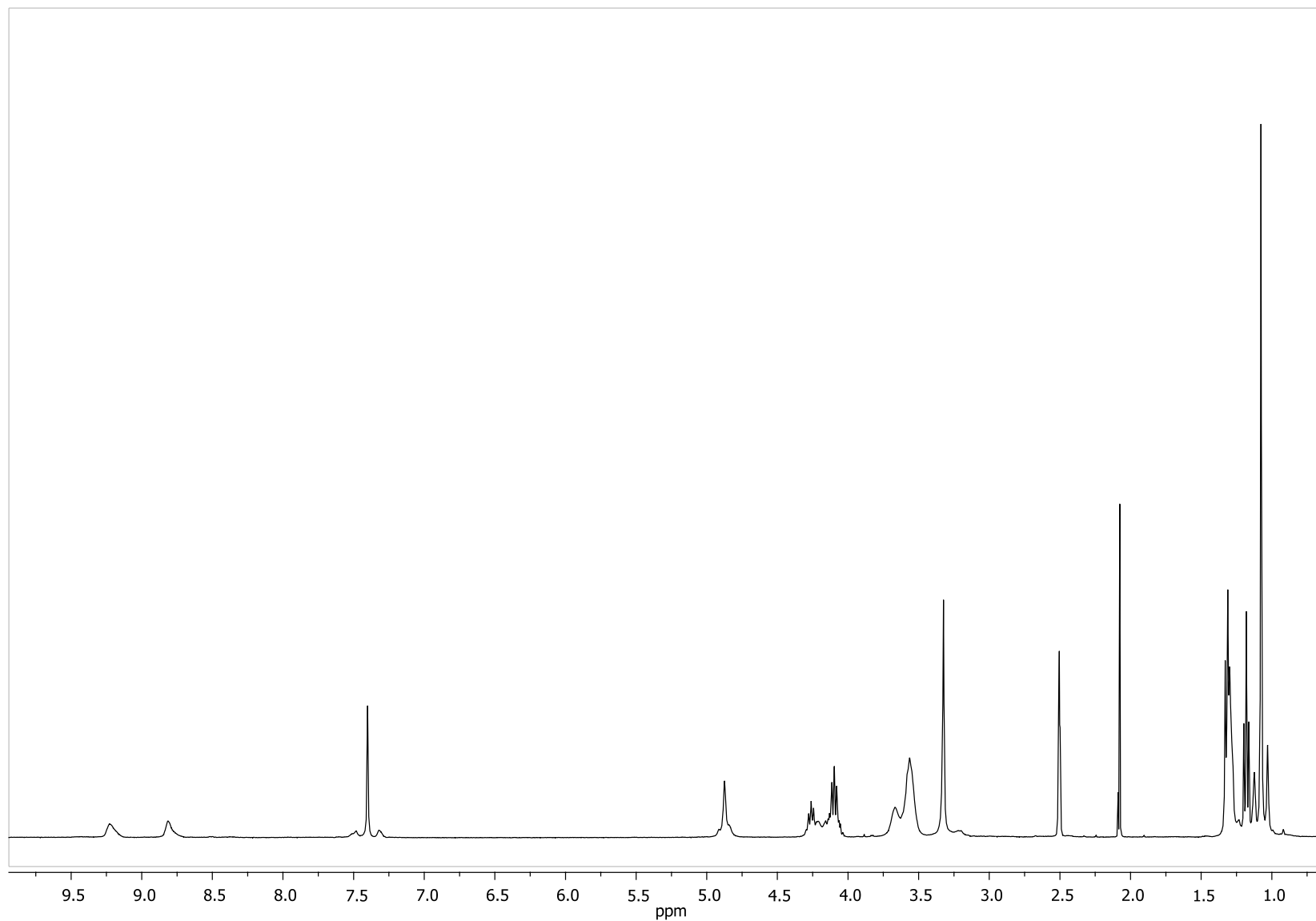
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CDCl₃, 298 K, 400 MHz**



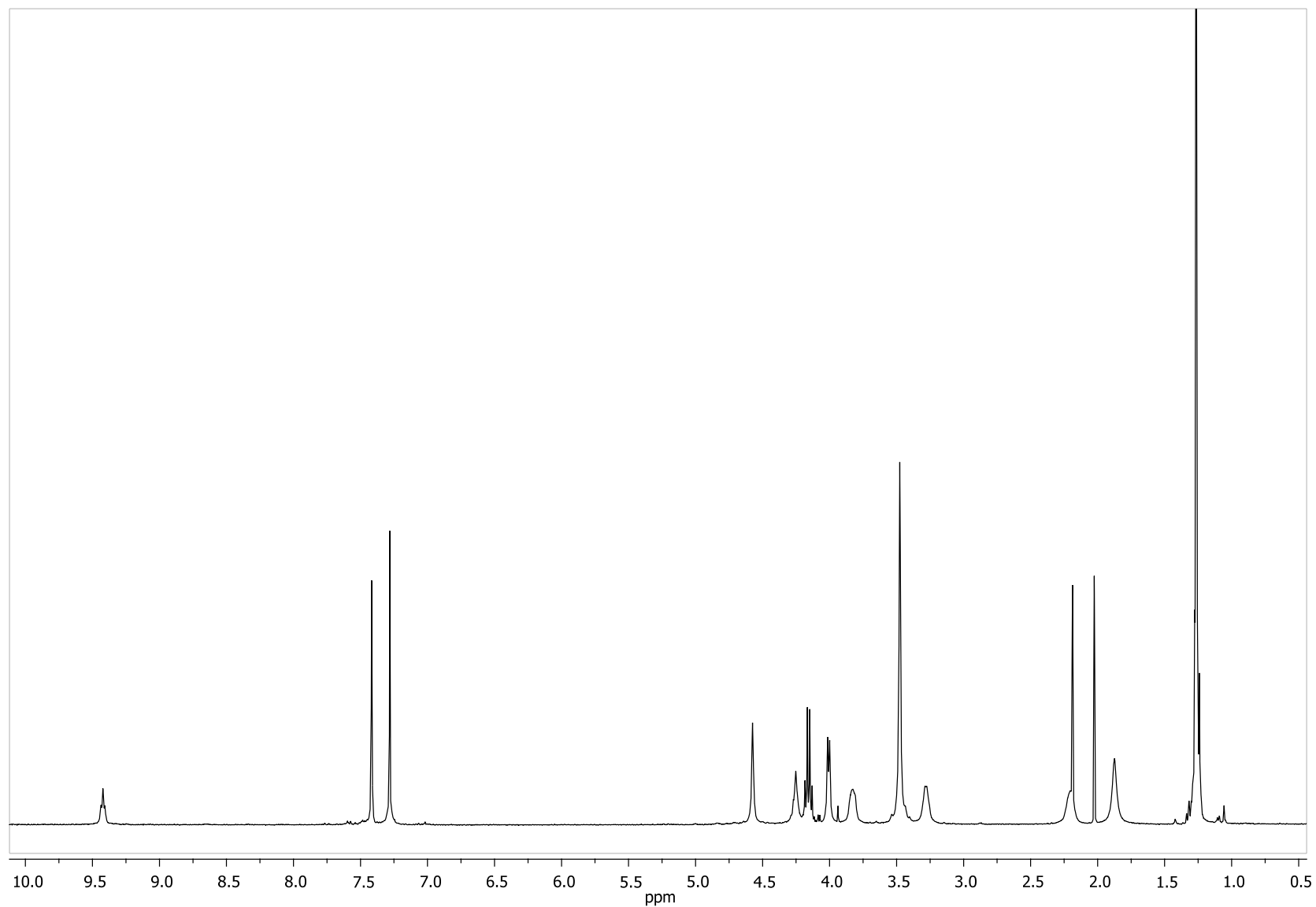
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tetrabromide (*cone*-18), DMSO-d₆, 298 K, 400 MHz**



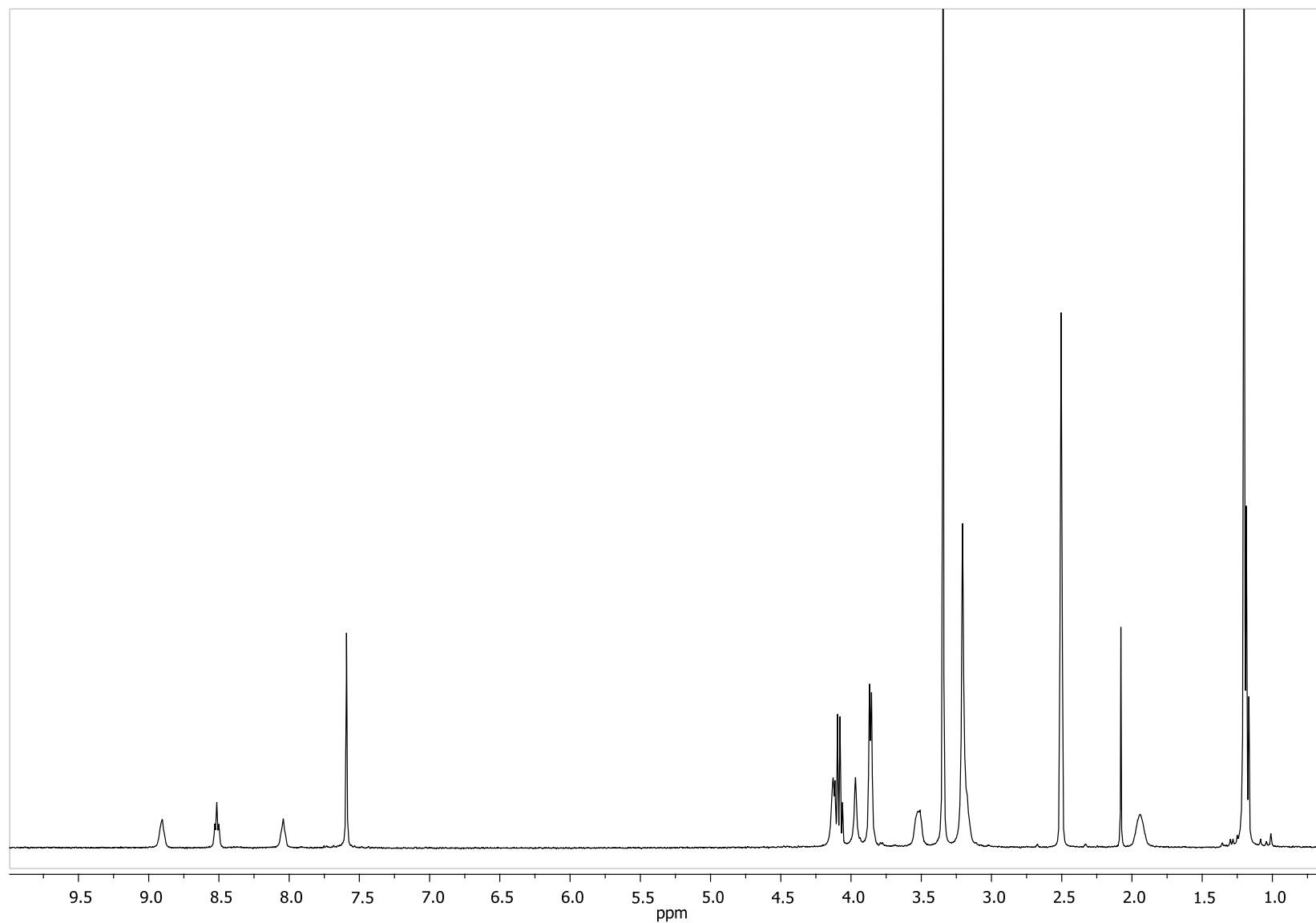
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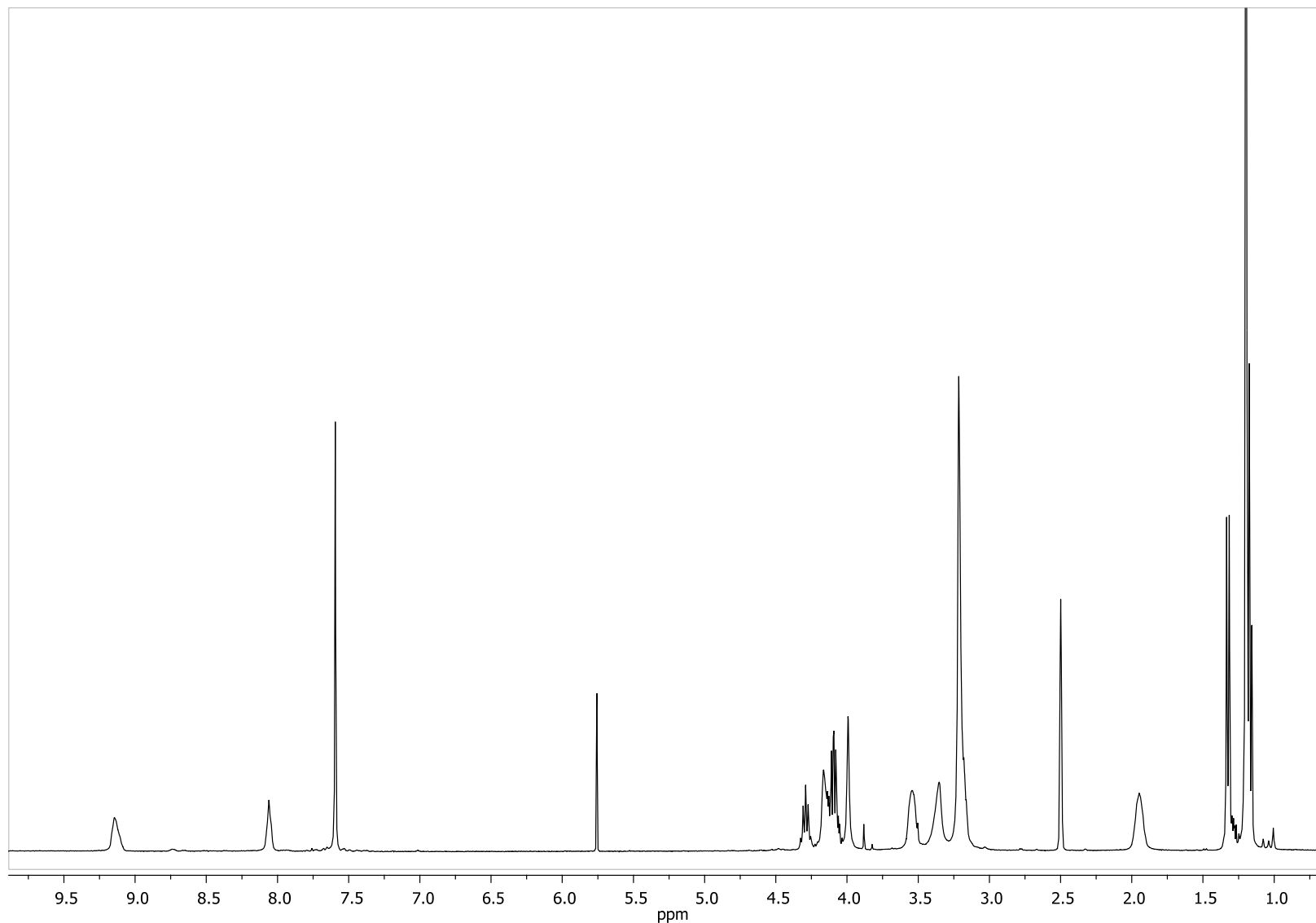
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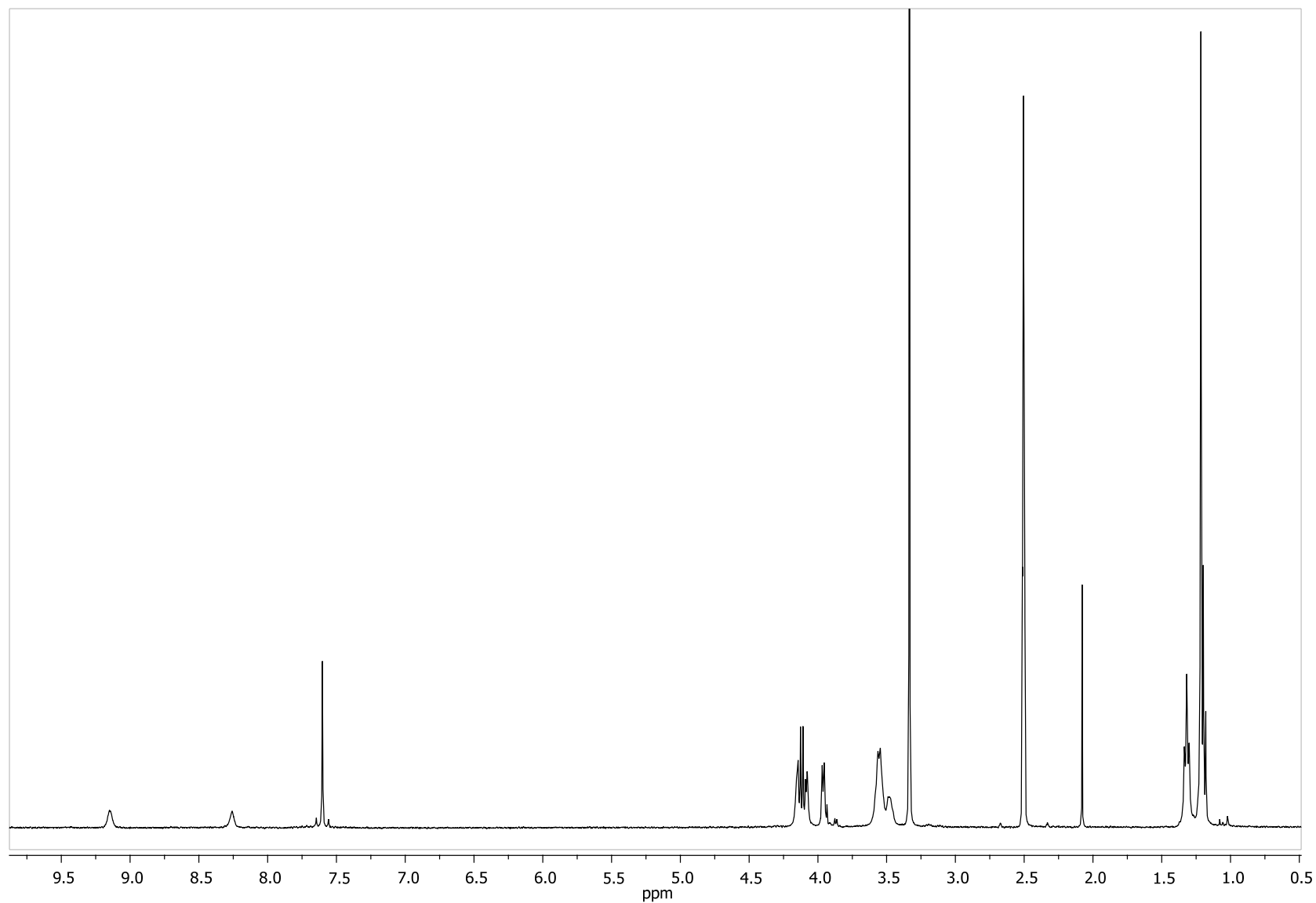
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tetrathiacalix[4]arene tetrabromide (1,3-*alternate*-21), DMSO-d₆, 298 K, 400 MHz**



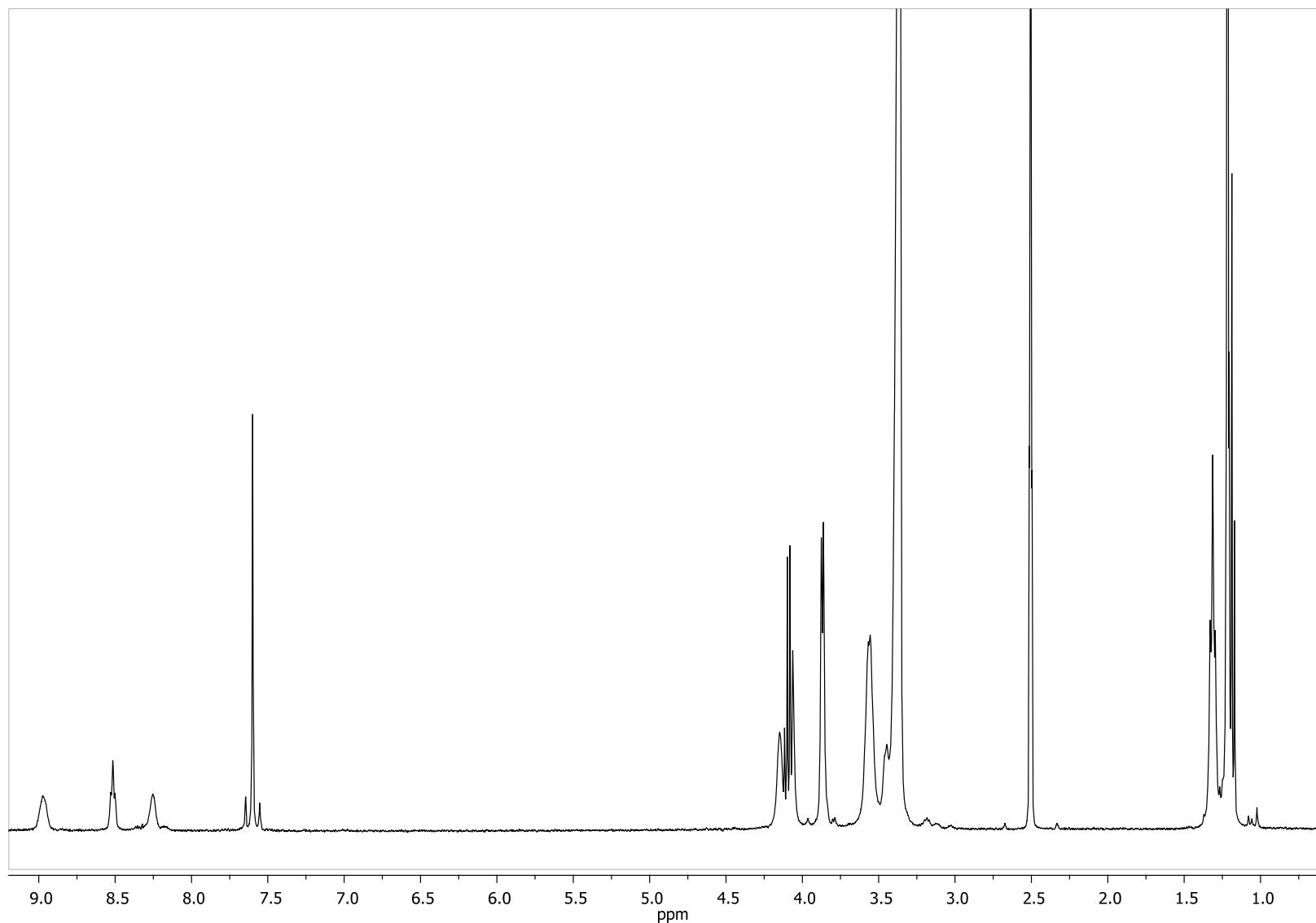
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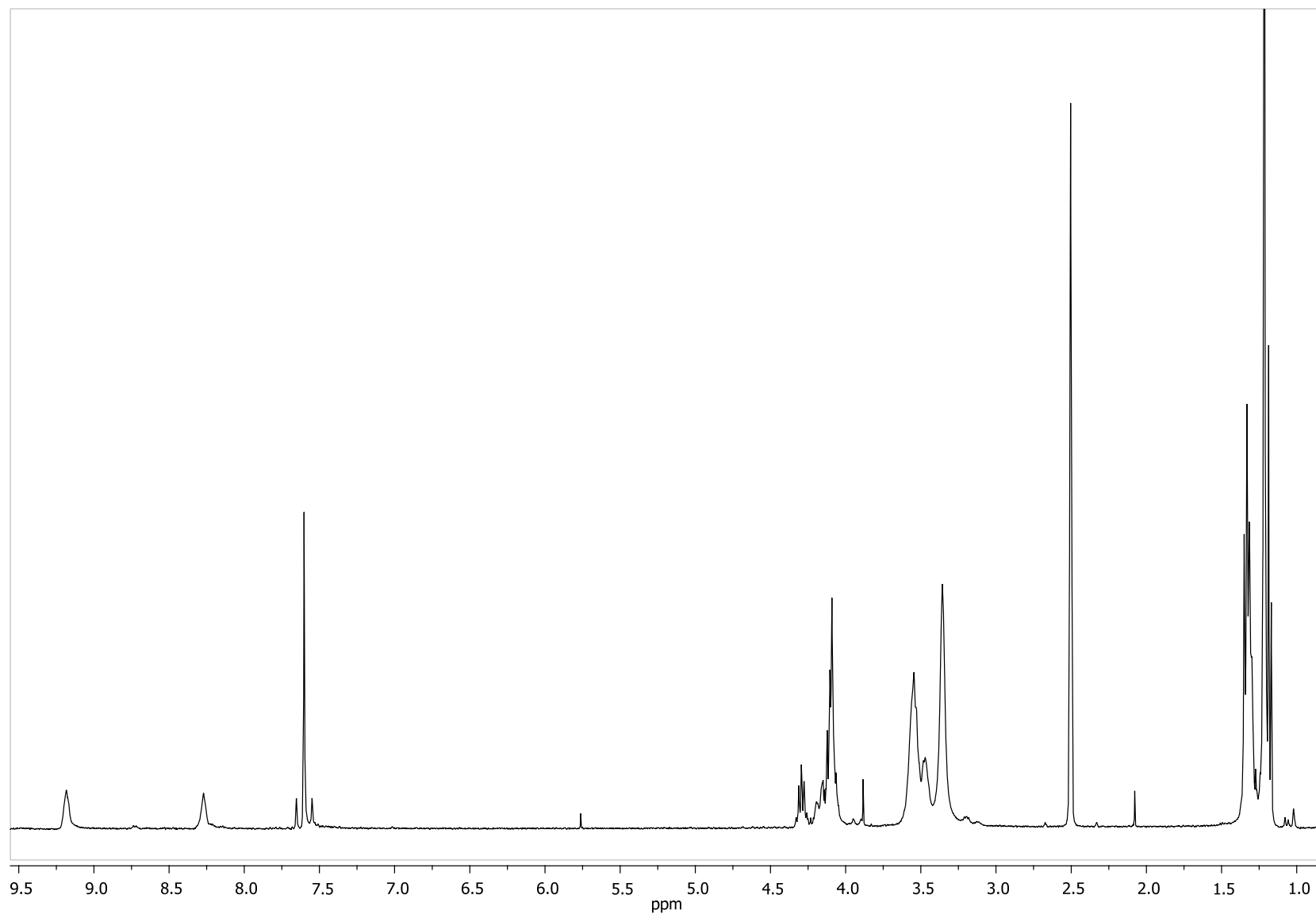
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alternate-23), DMSO-d₆, 298 K, 400 MHz**



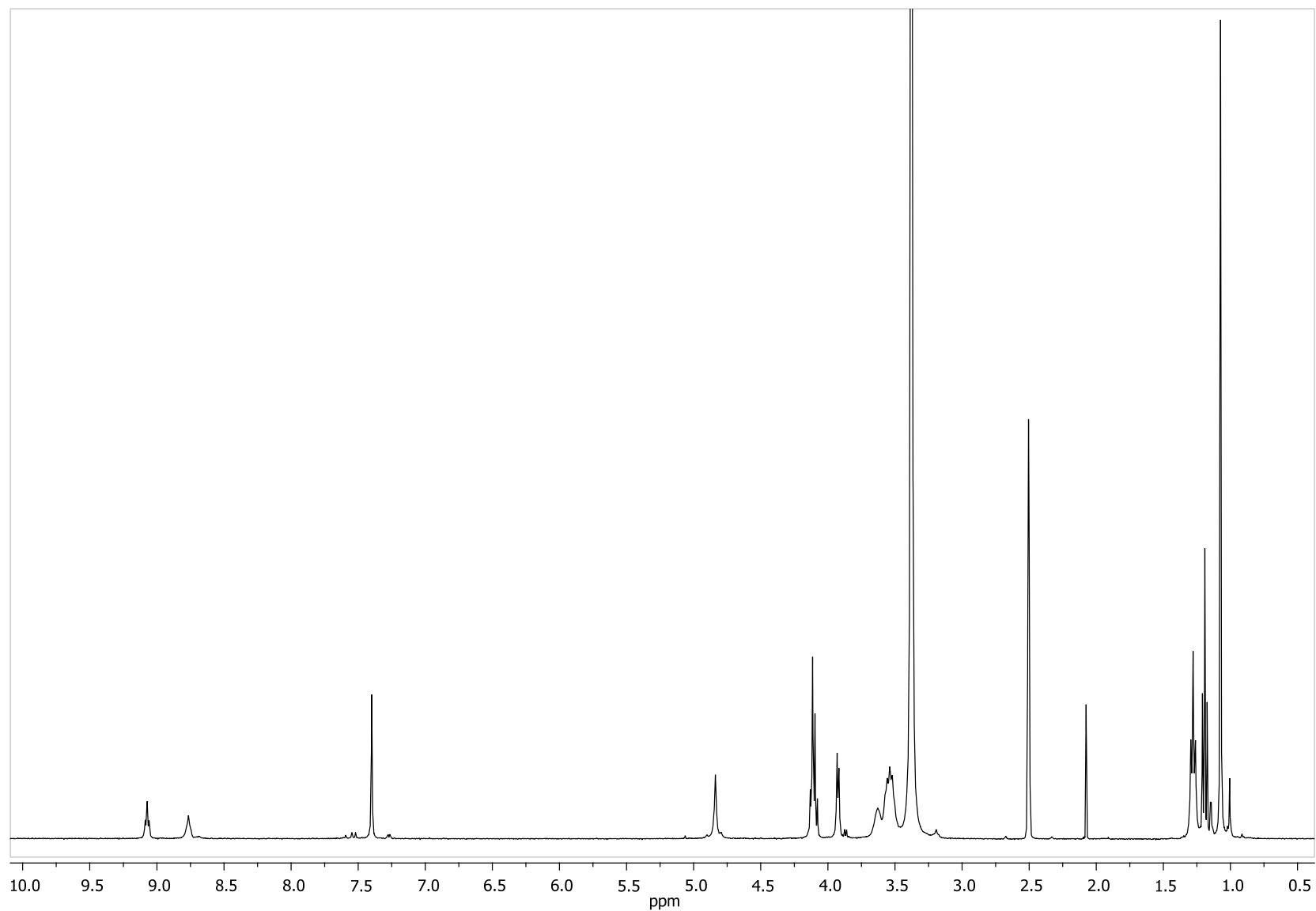
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tetrabromide (1,3-alternate-24), DMSO-d₆, 298 K, 400 MHz**



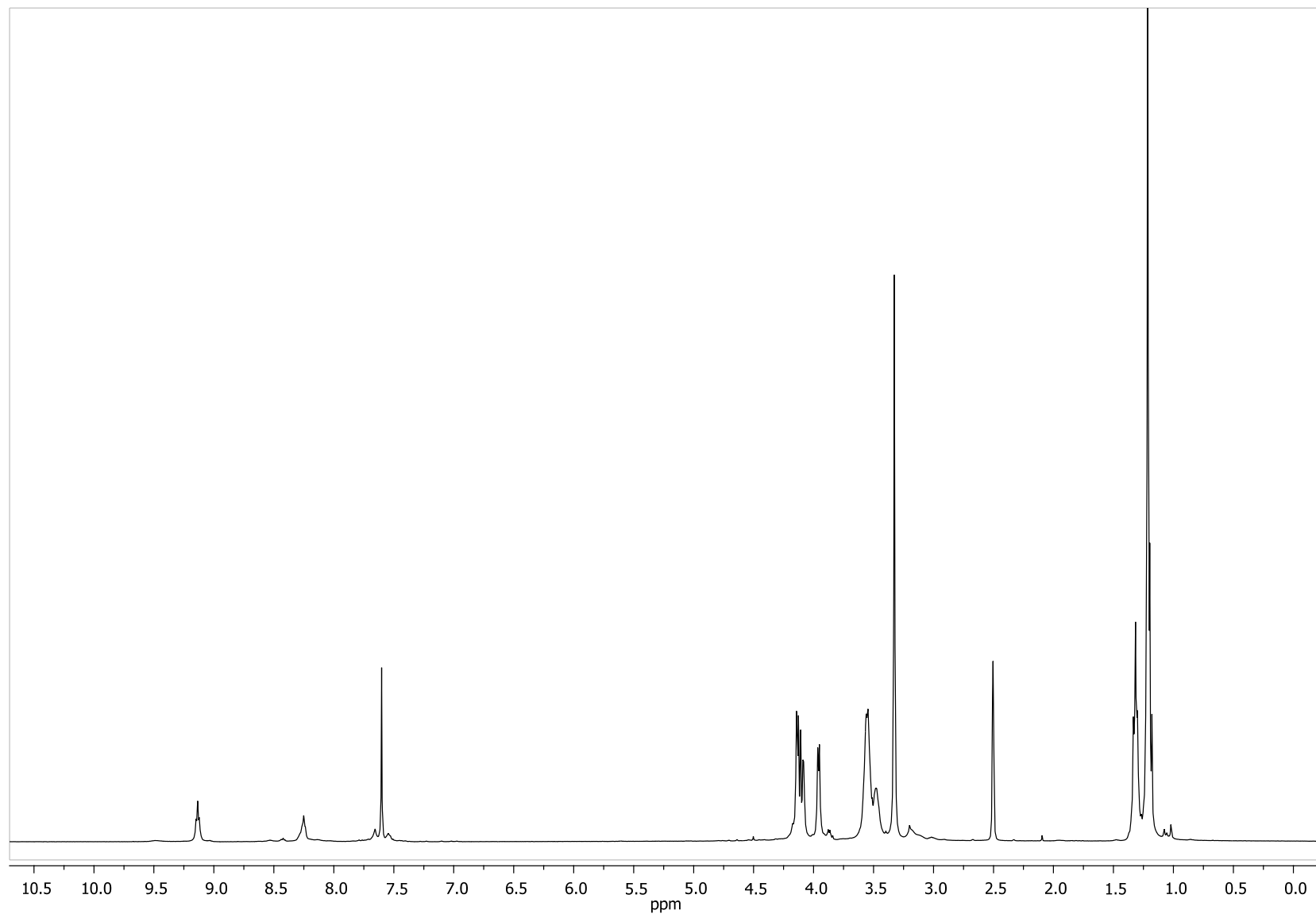
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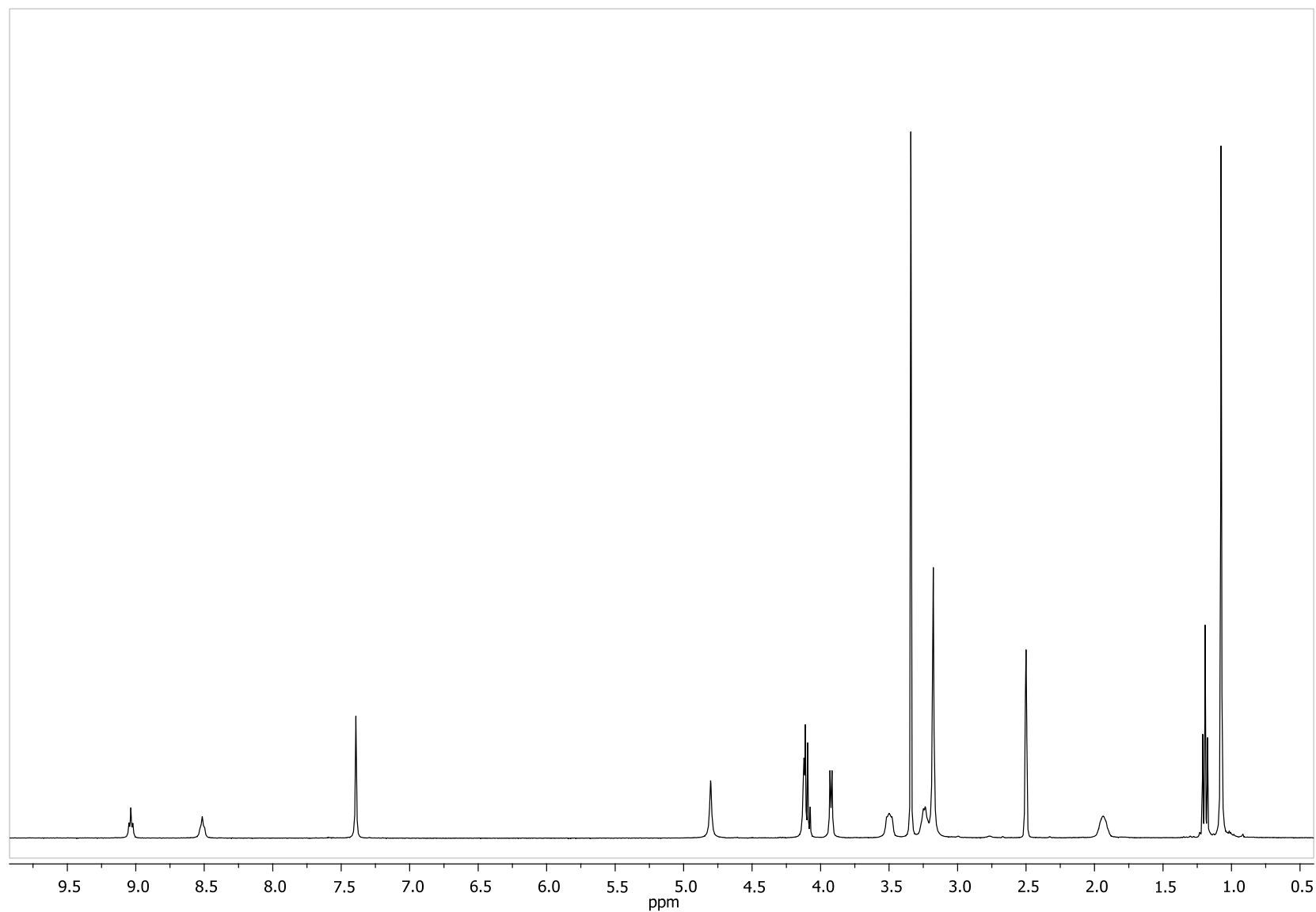
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DMSO-d₆, 298 K, 400 MHz**



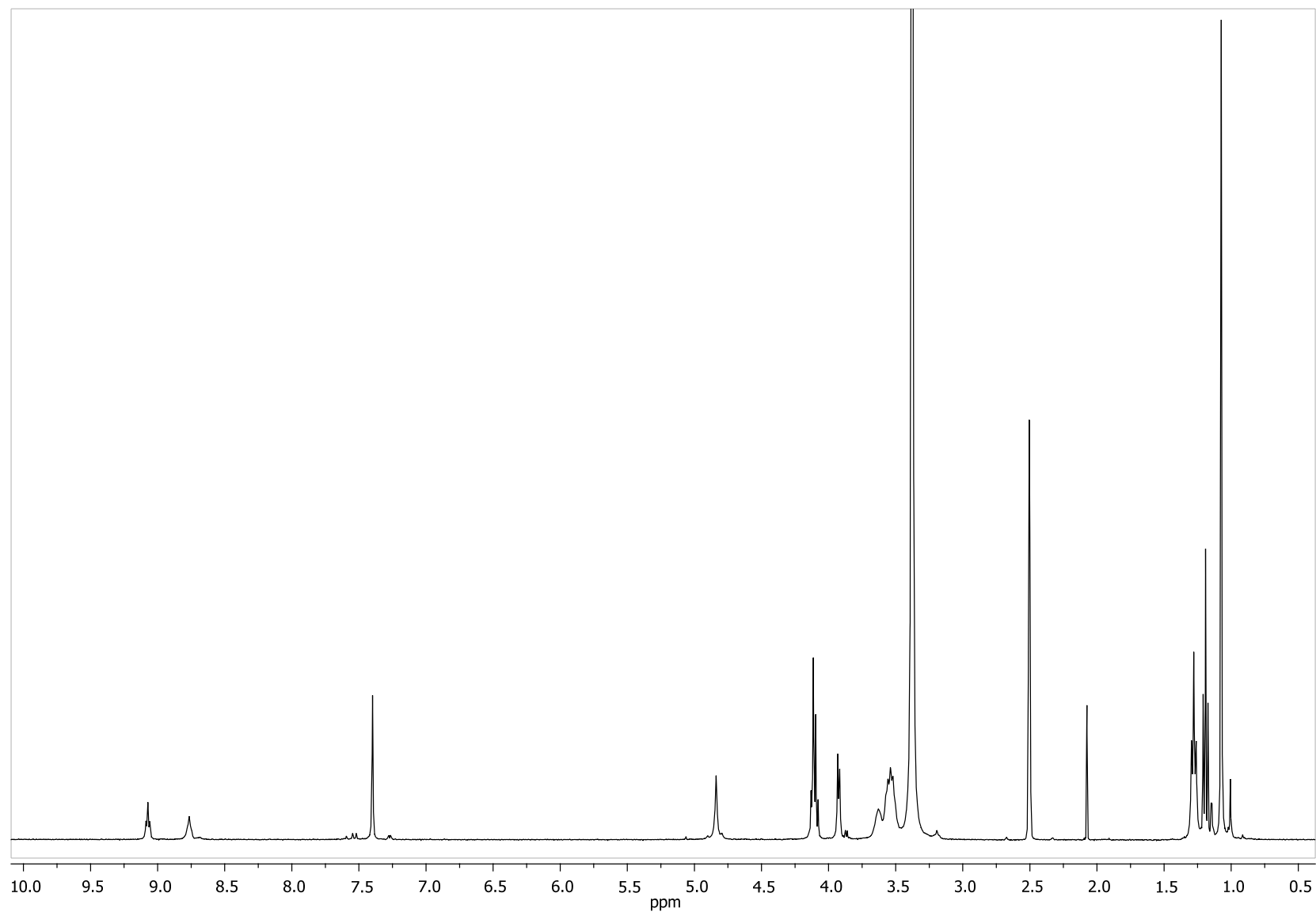
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alternate-27), DMSO-d₆, 298 K, 400 MHz**



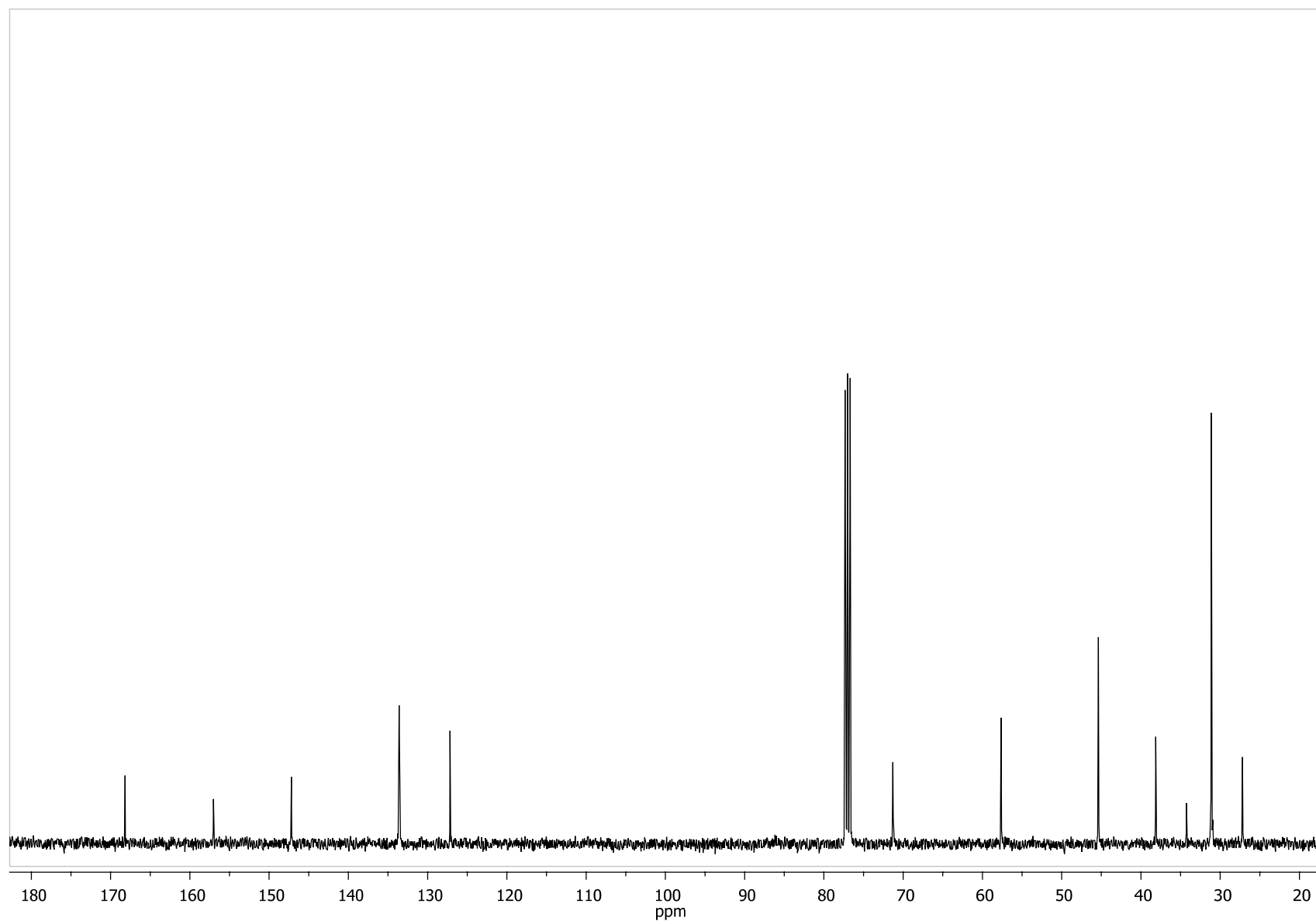
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DMSO-d₆, 298 K, 400 MHz**



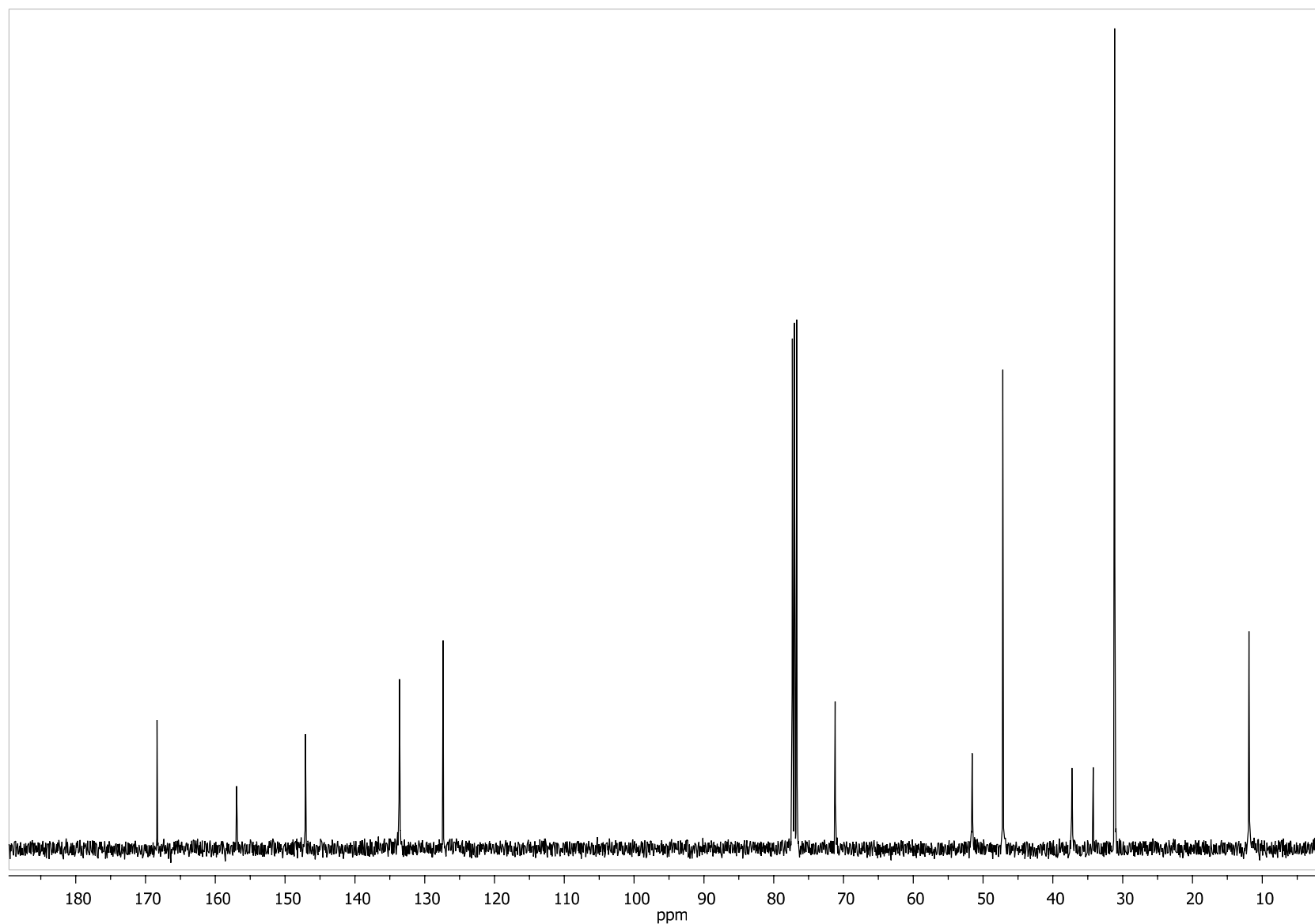
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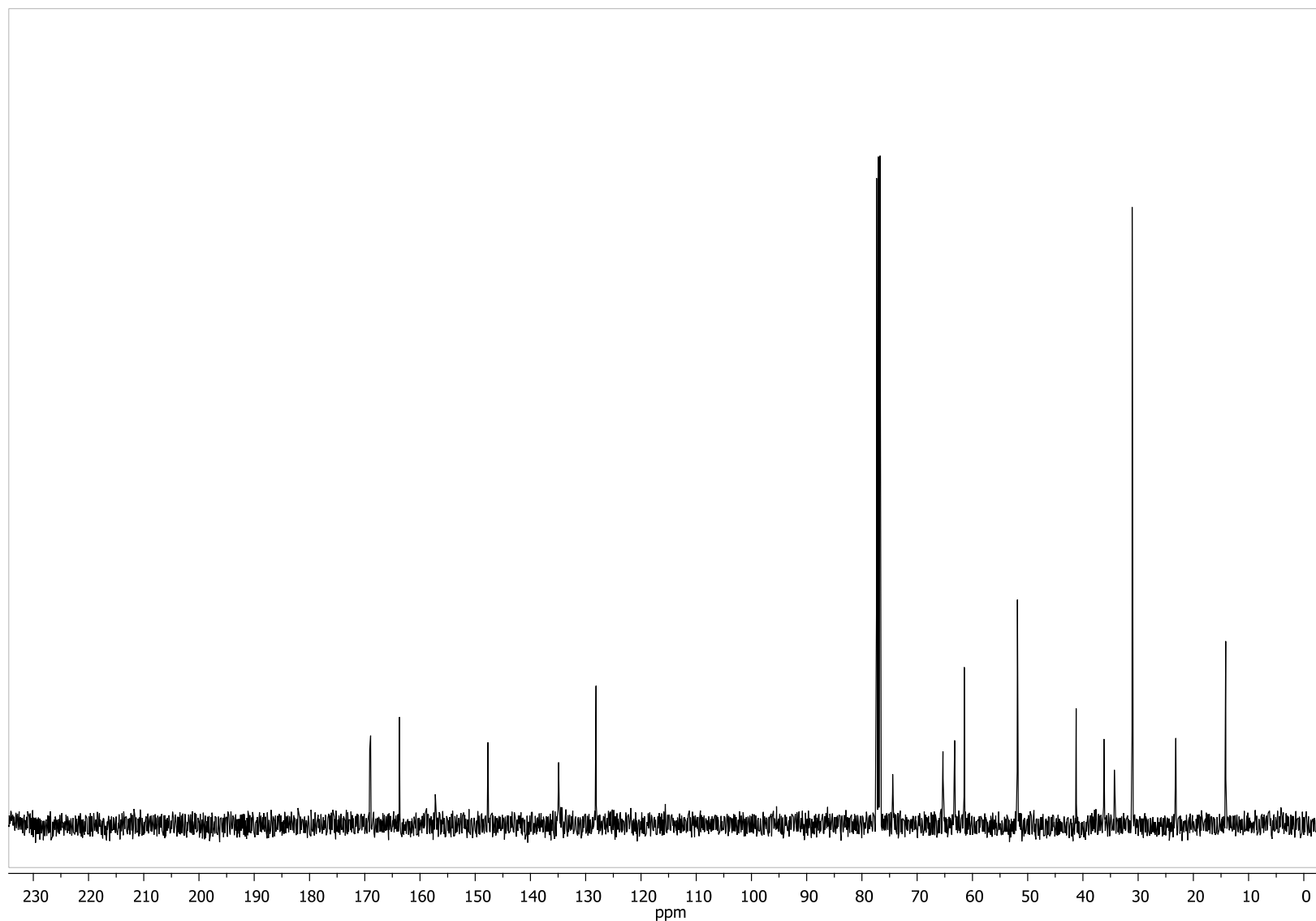
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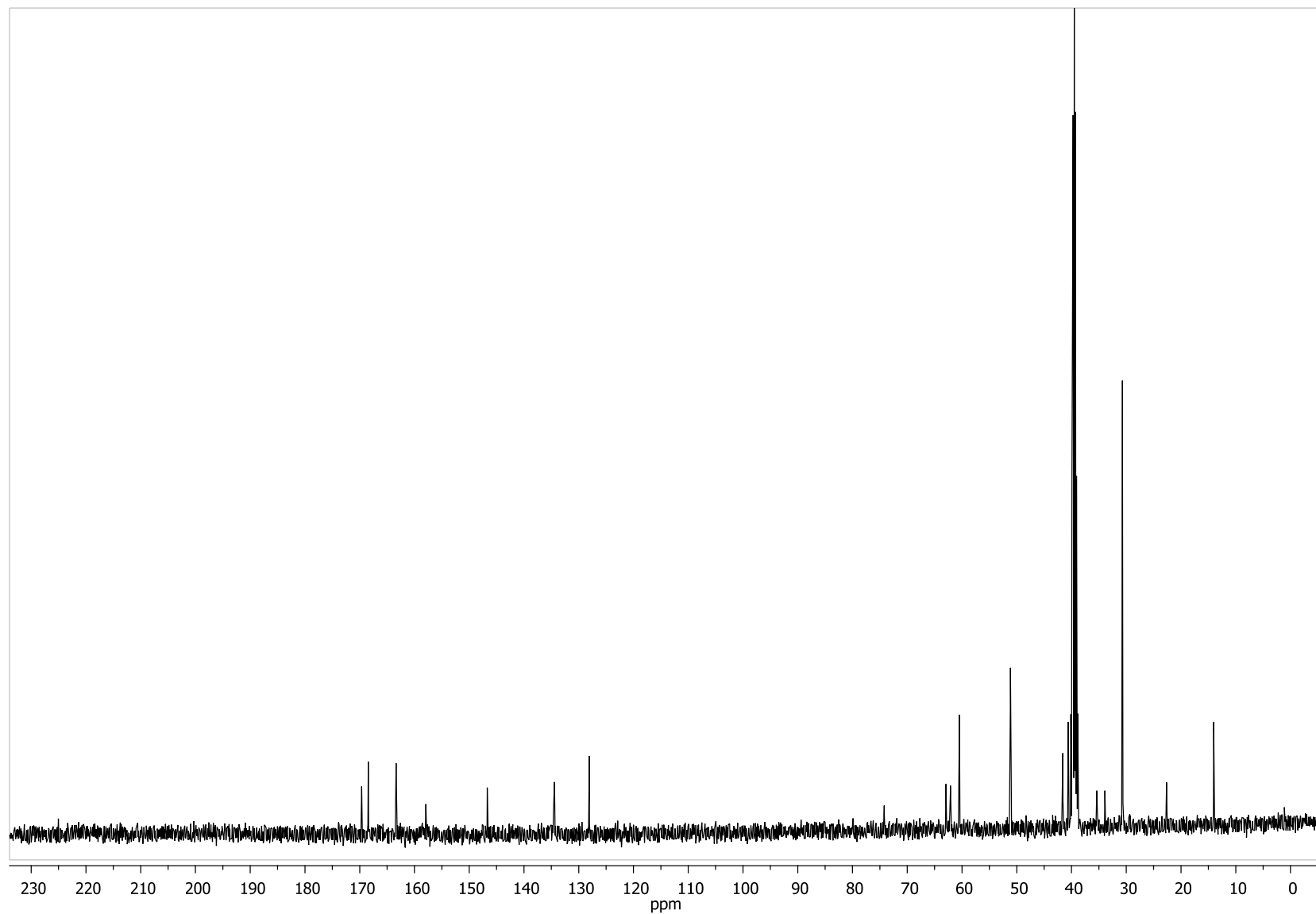
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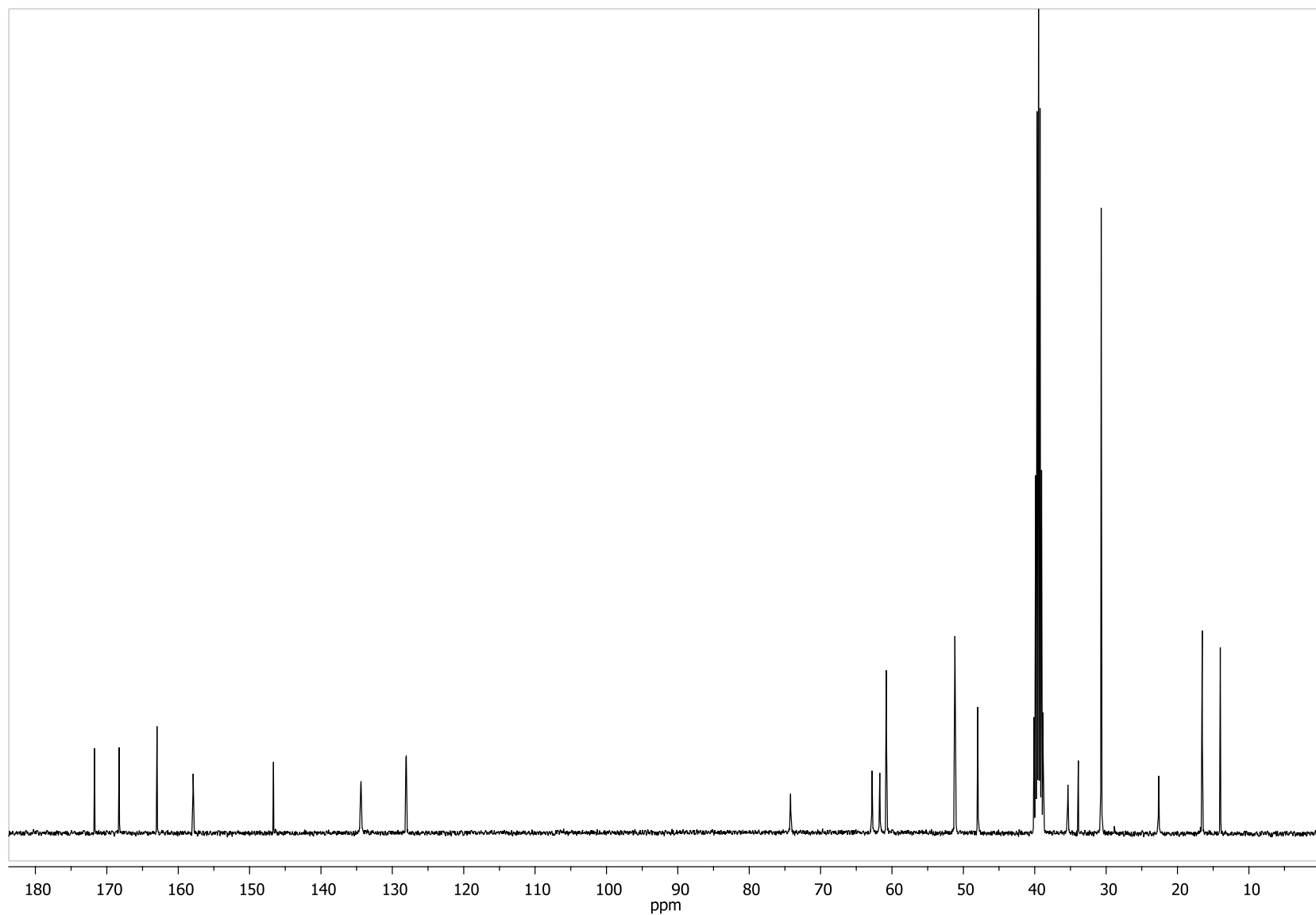
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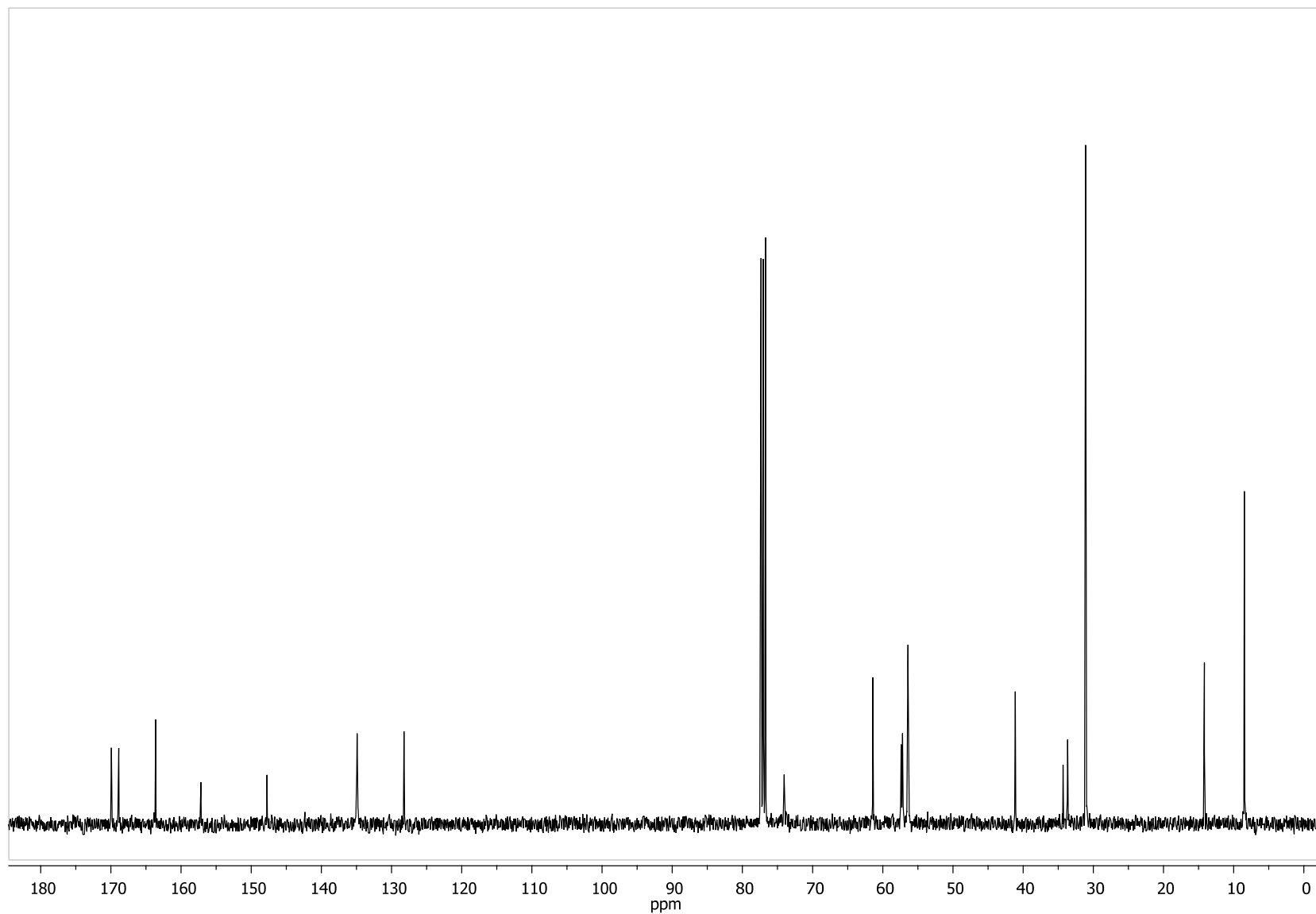
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tetrathiacalix[4]arene tetrabromide (*cone*-15), DMSO- d_6 , 298 K, 100 MHz**



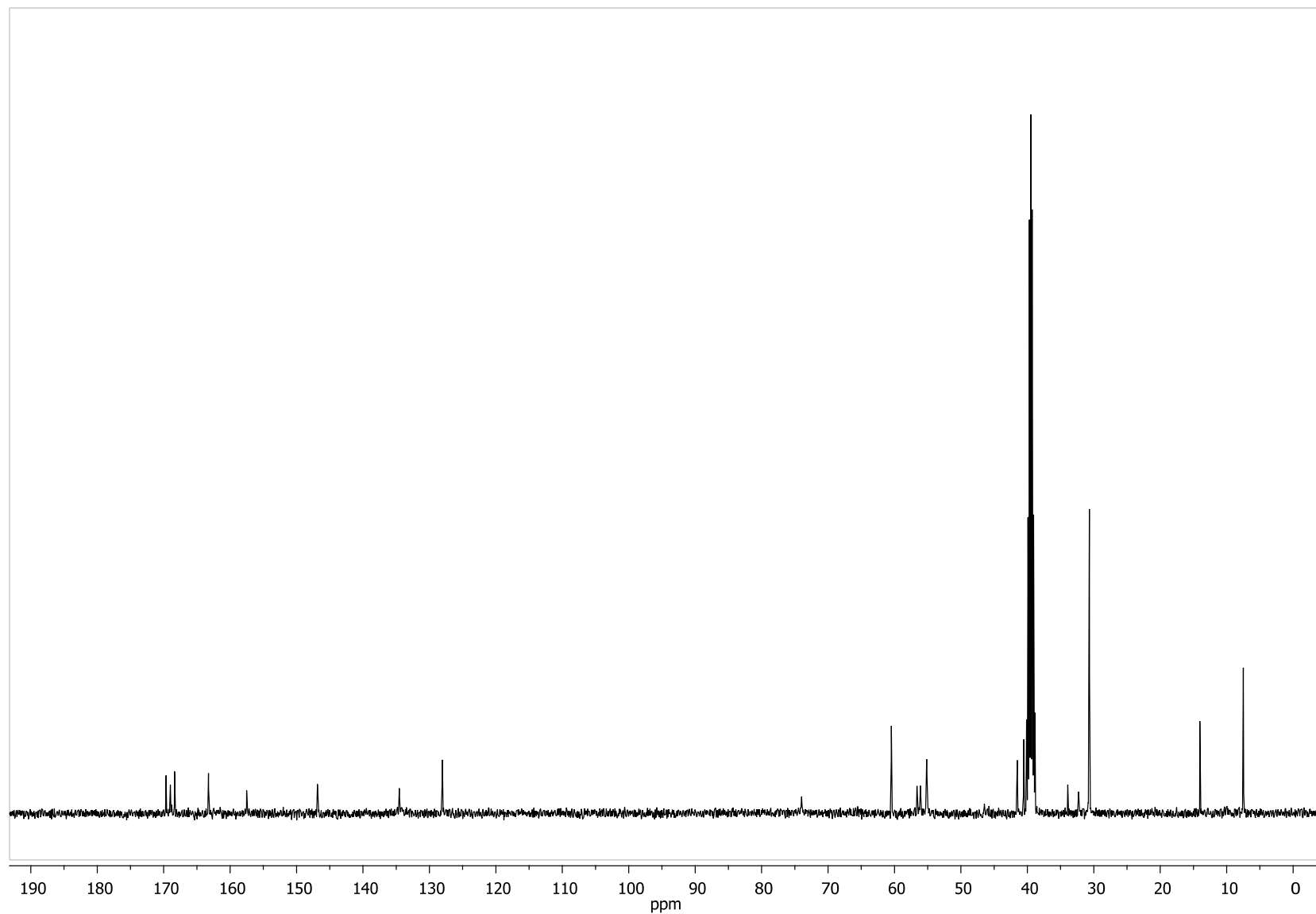
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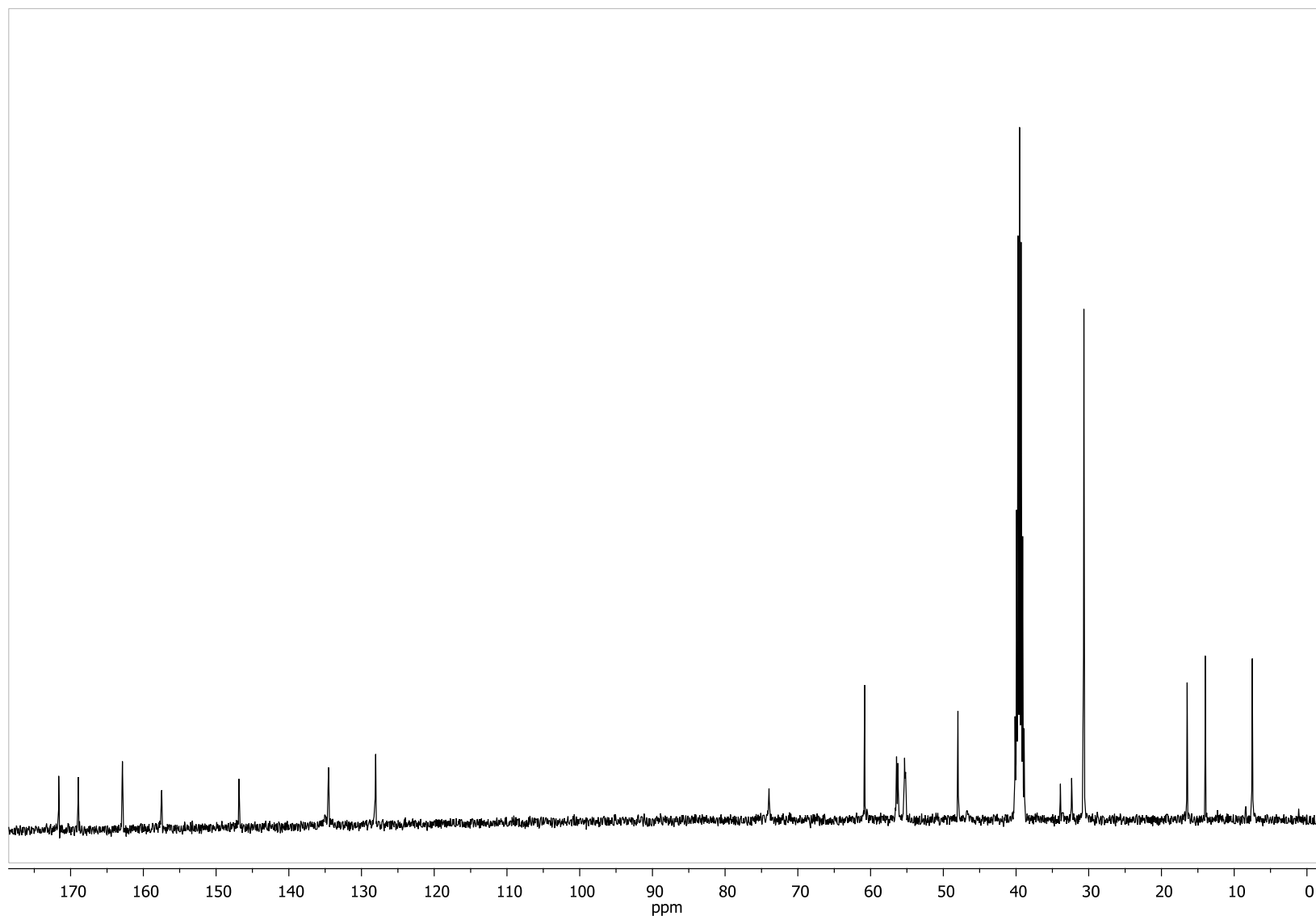
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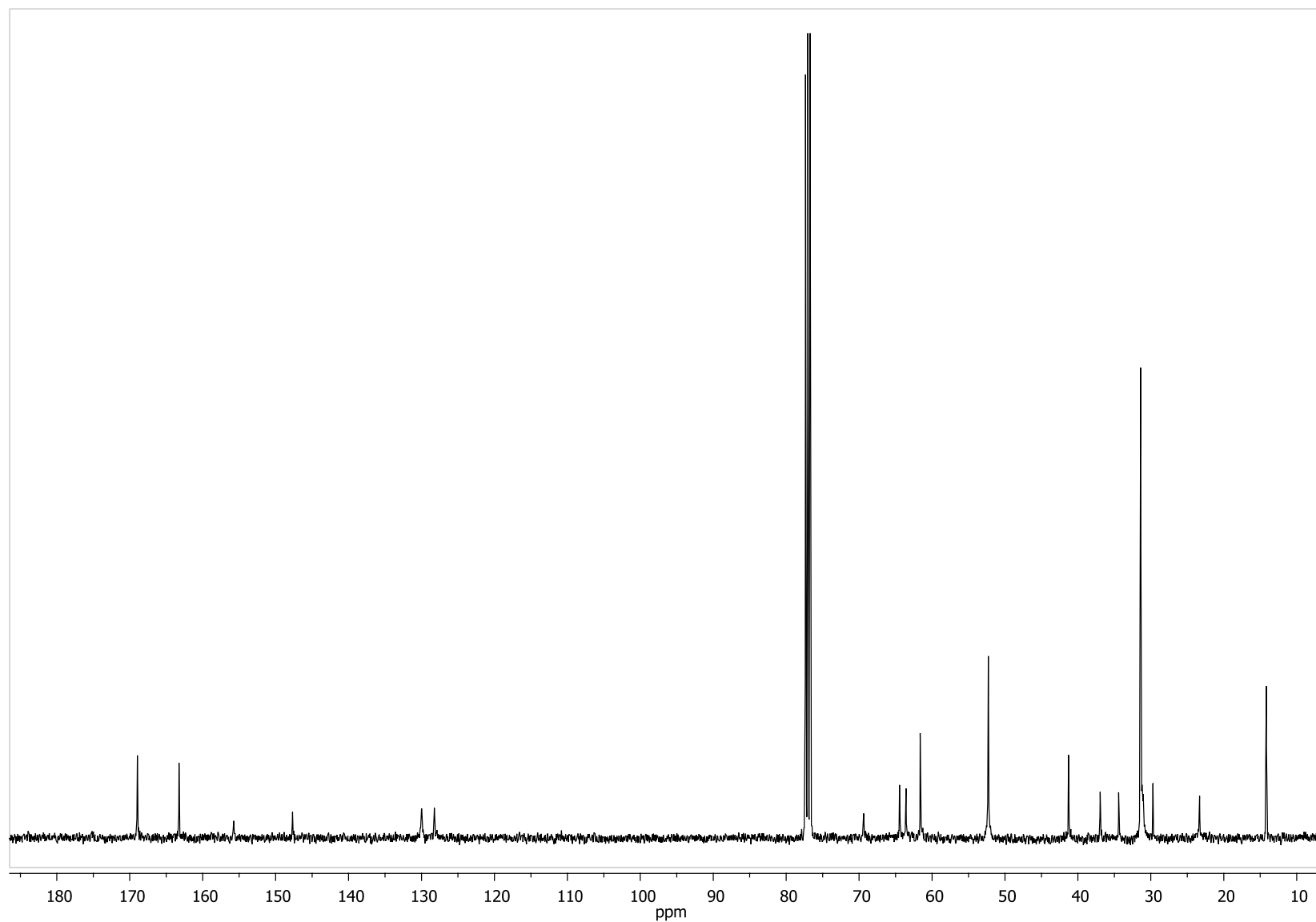
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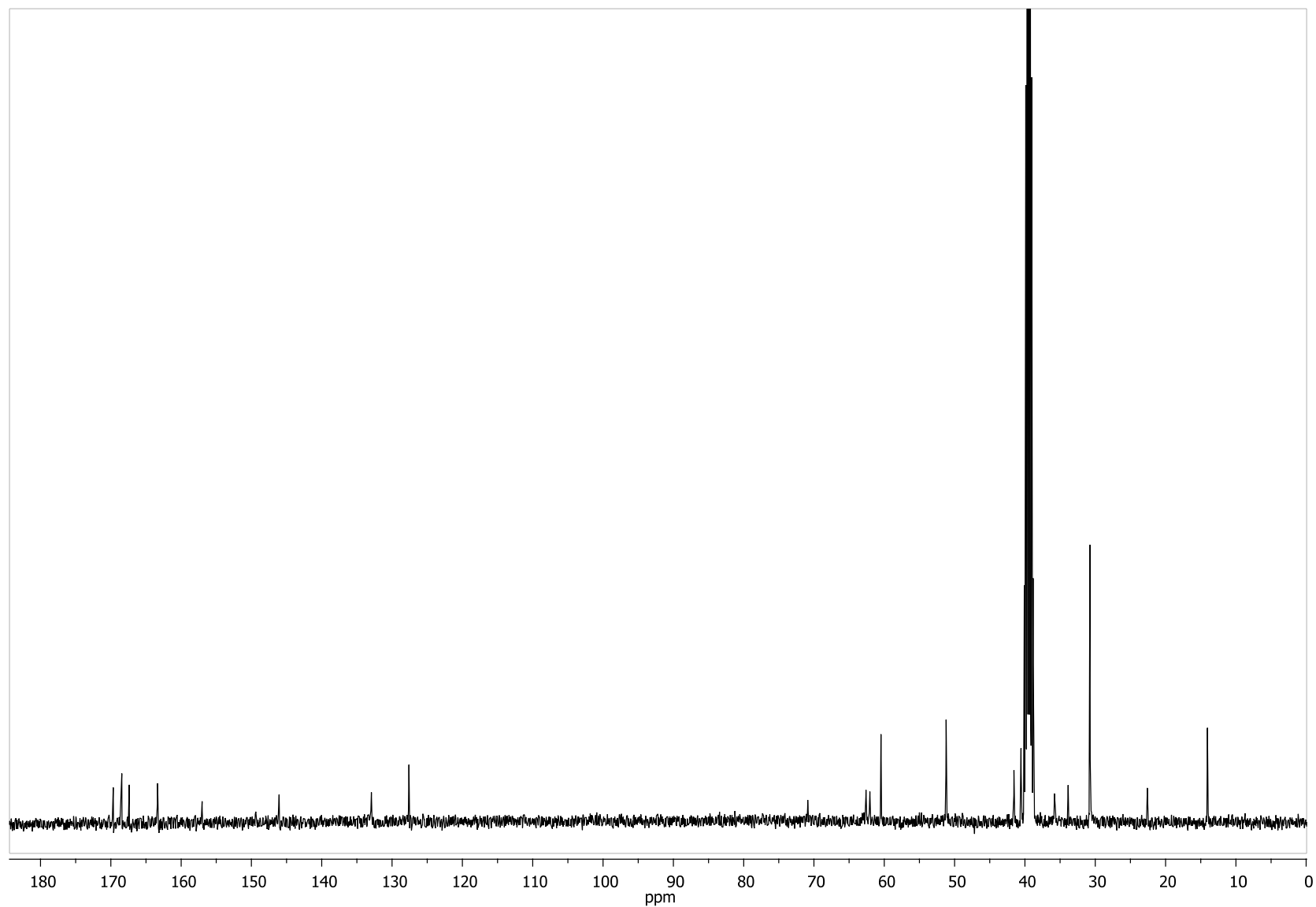
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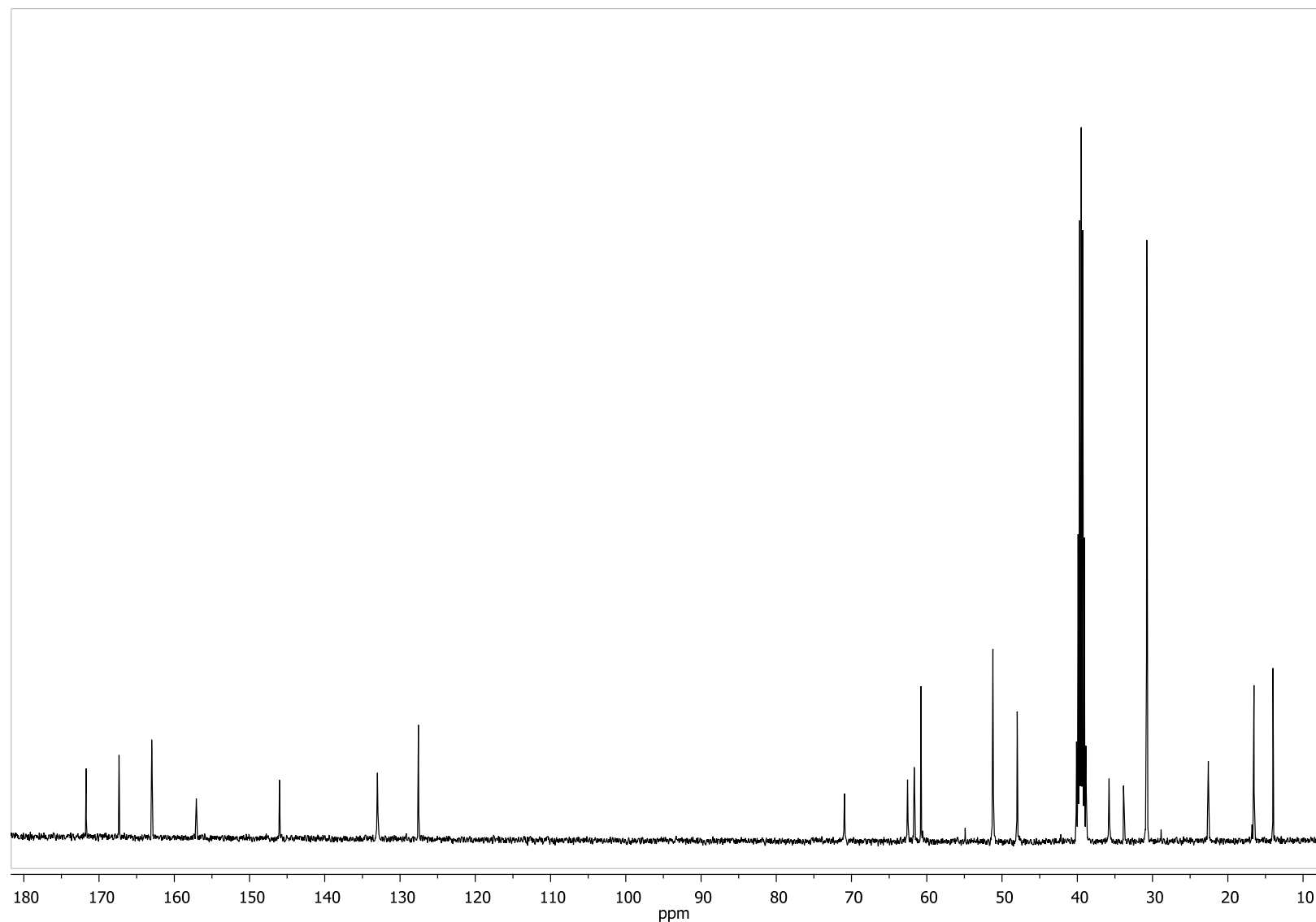
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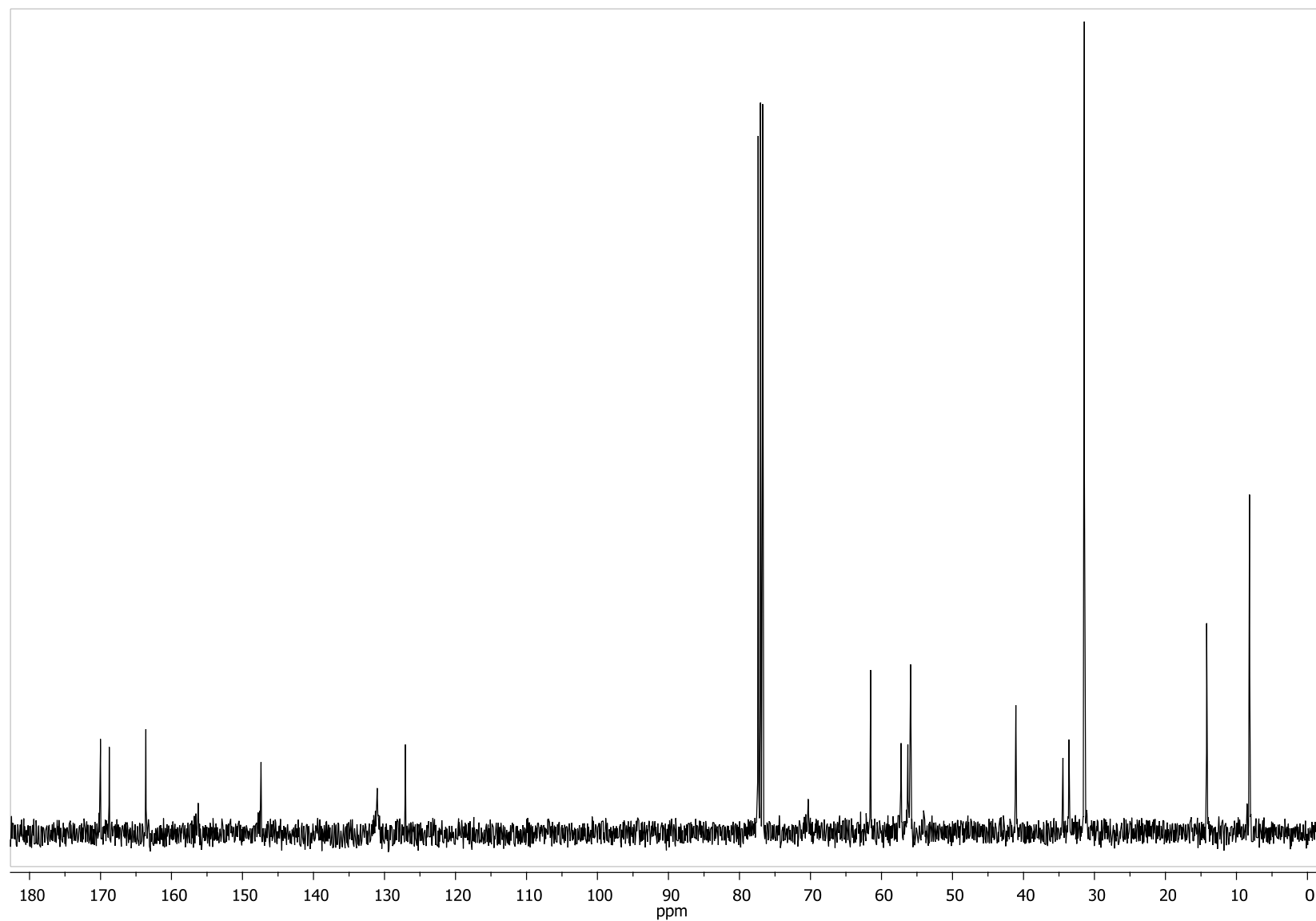
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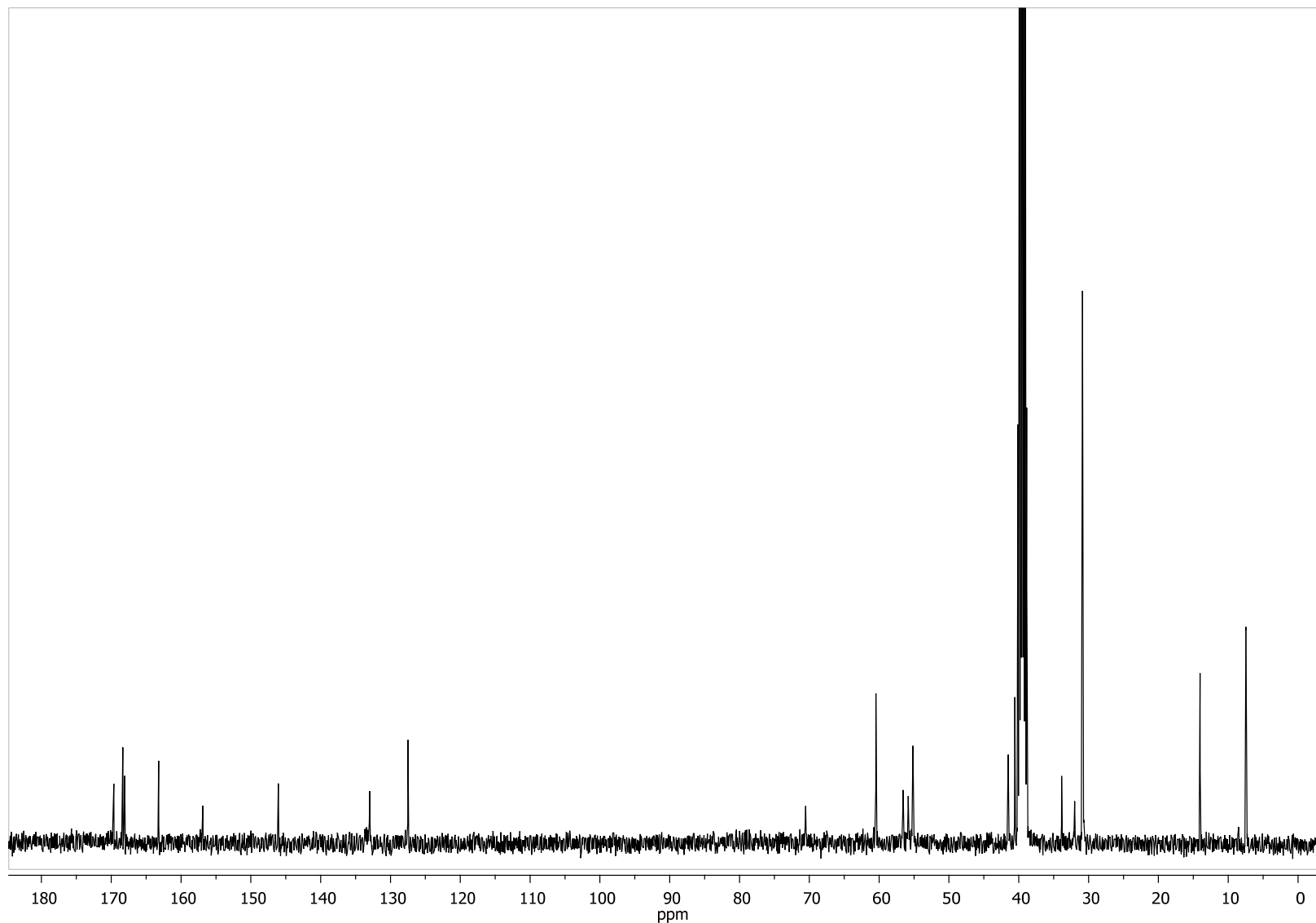
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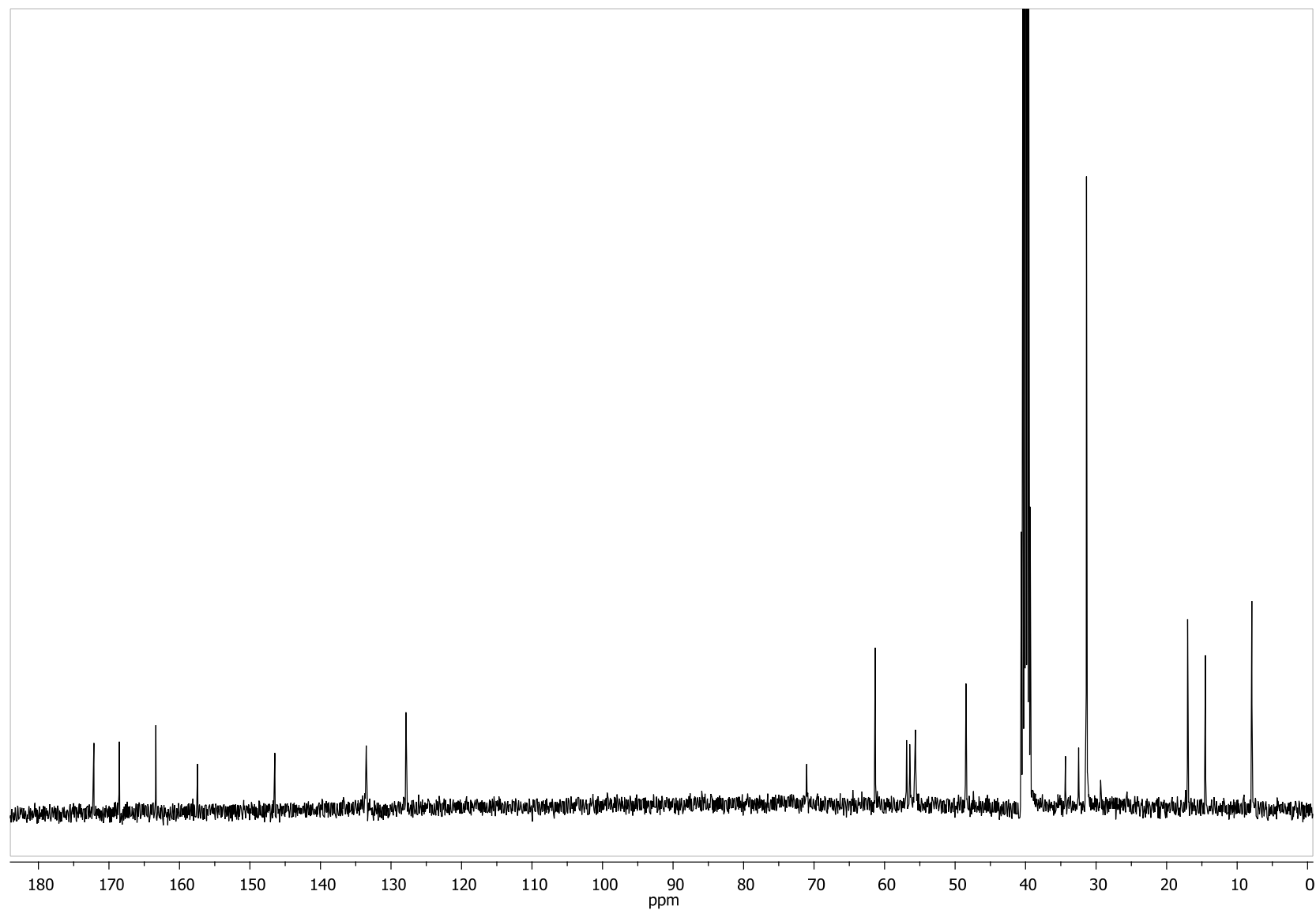
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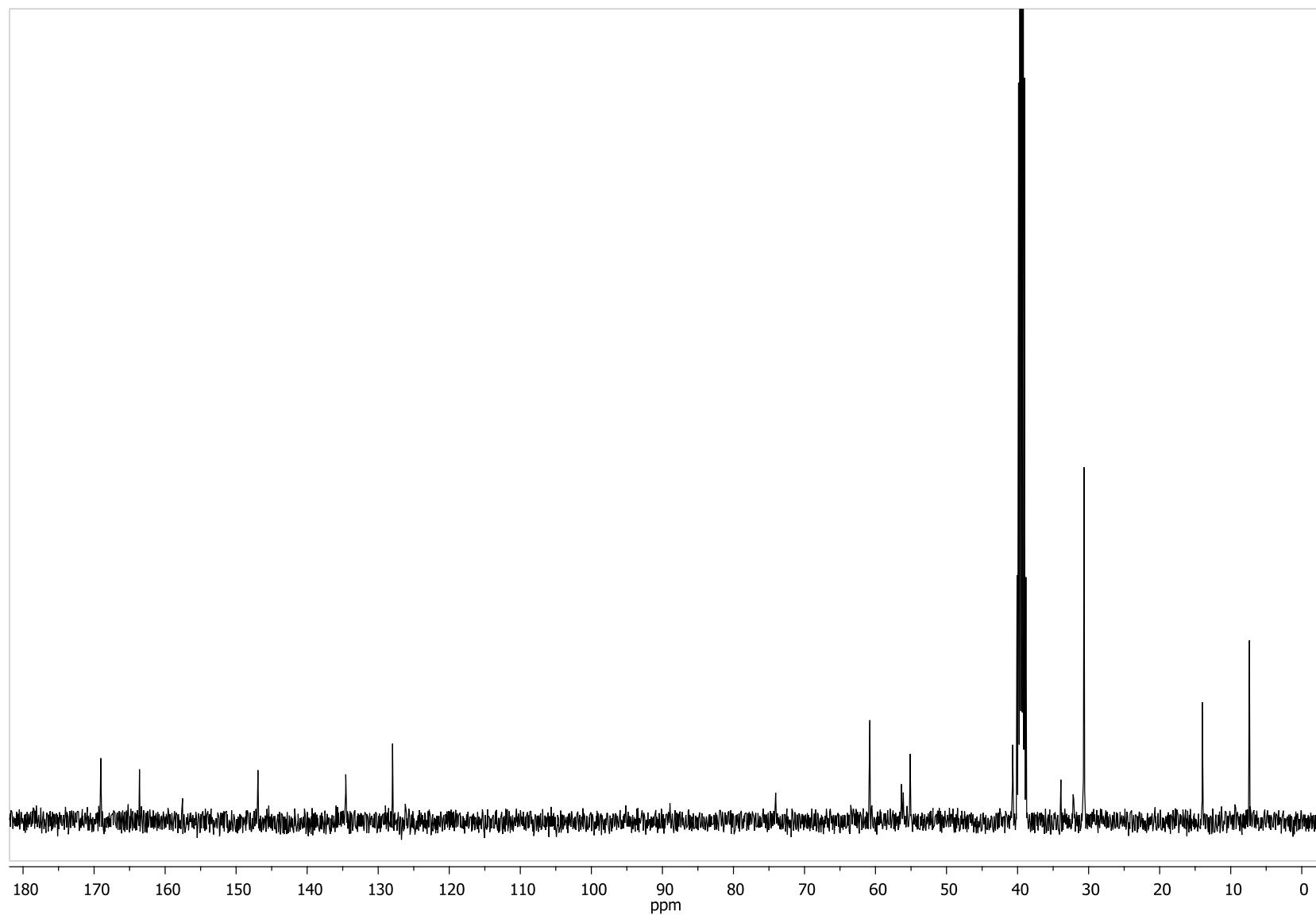
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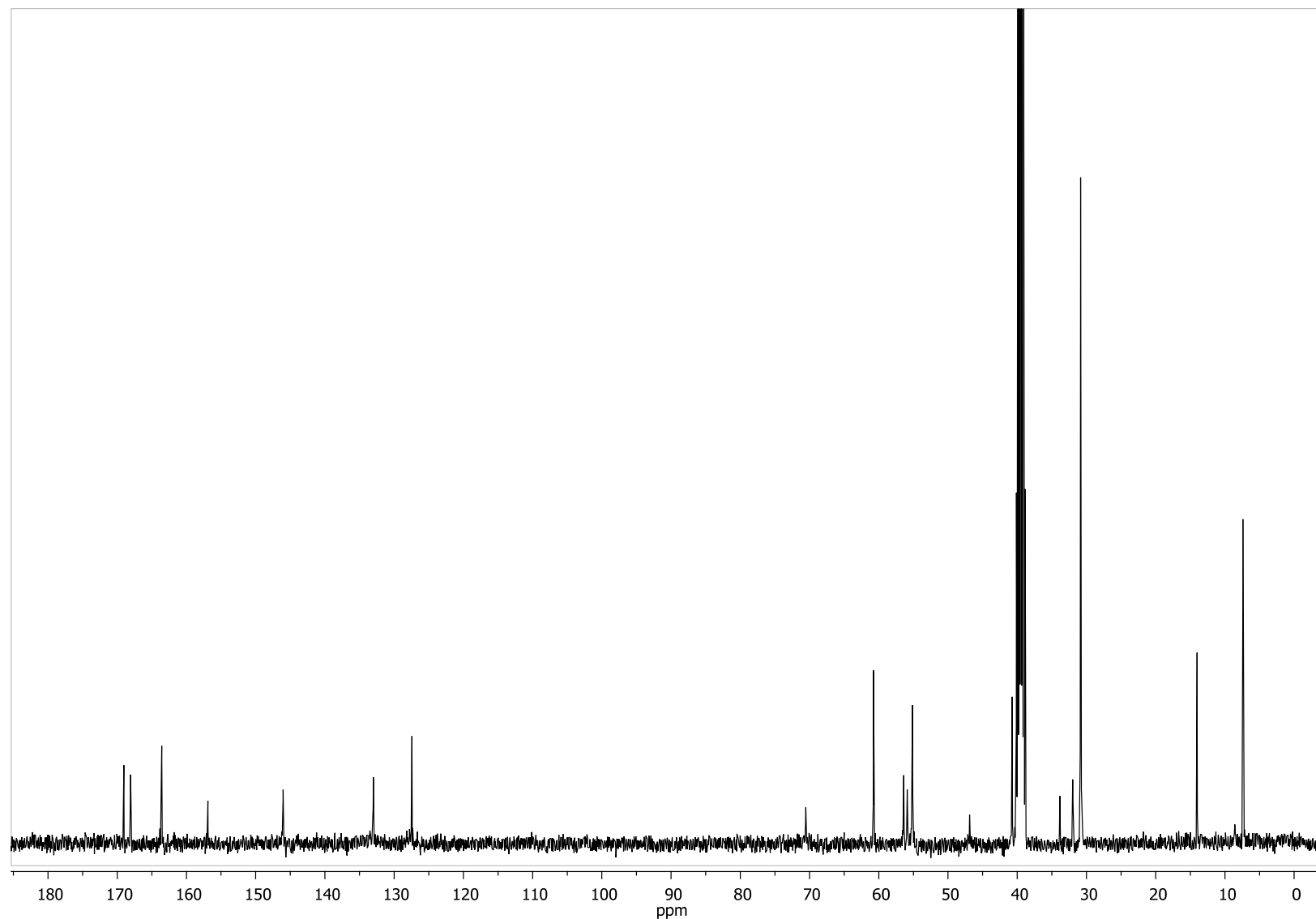
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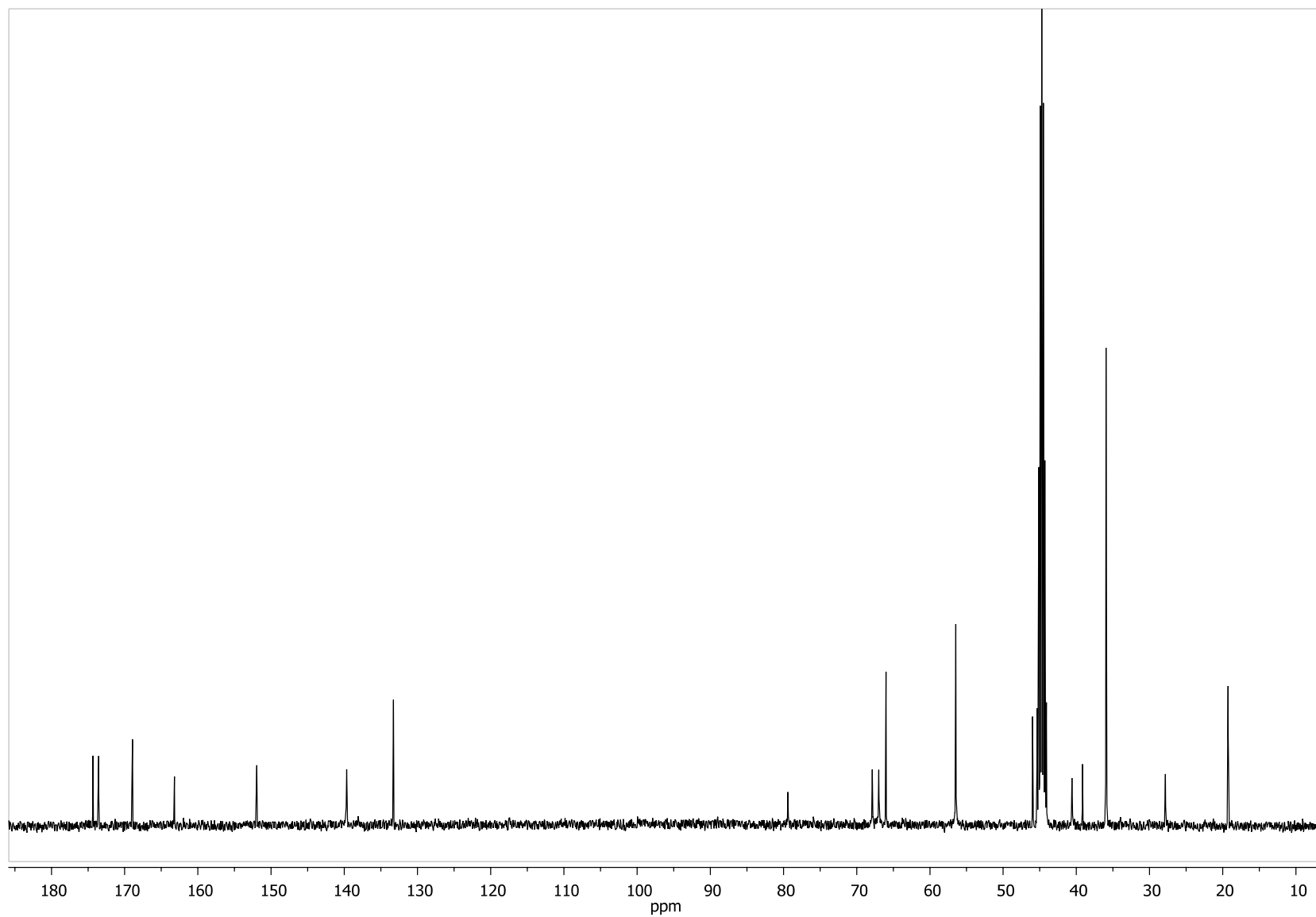
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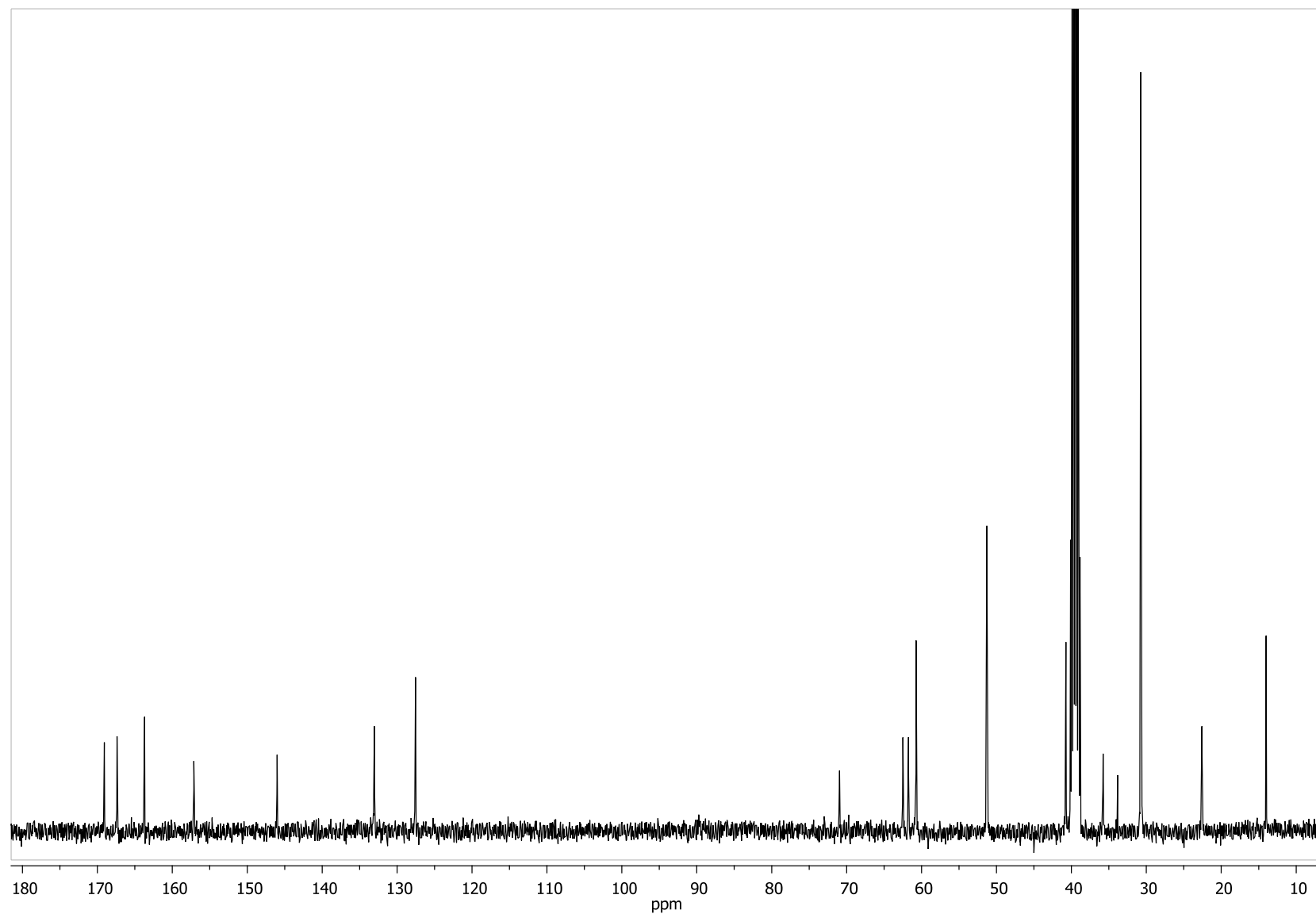
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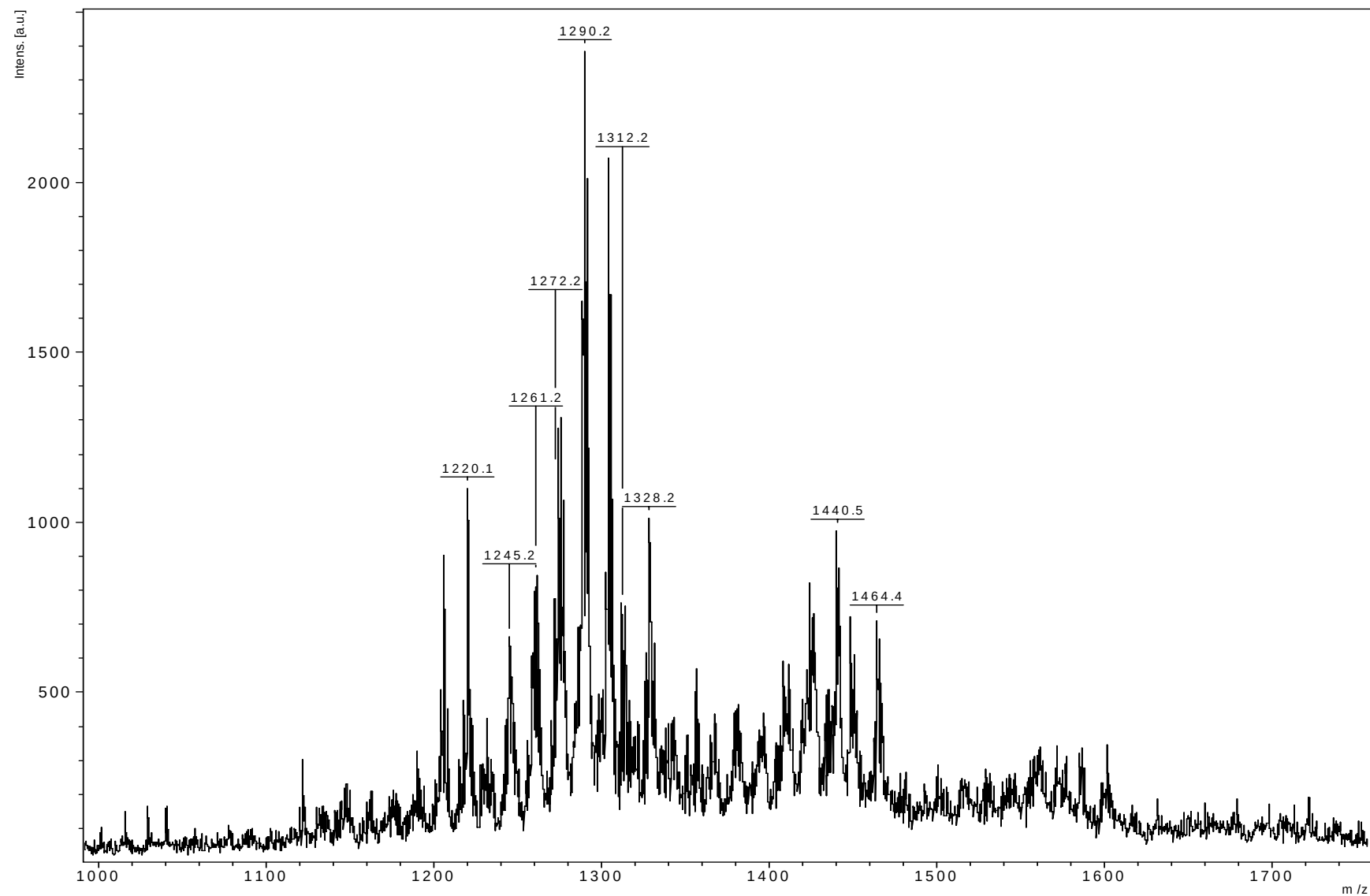
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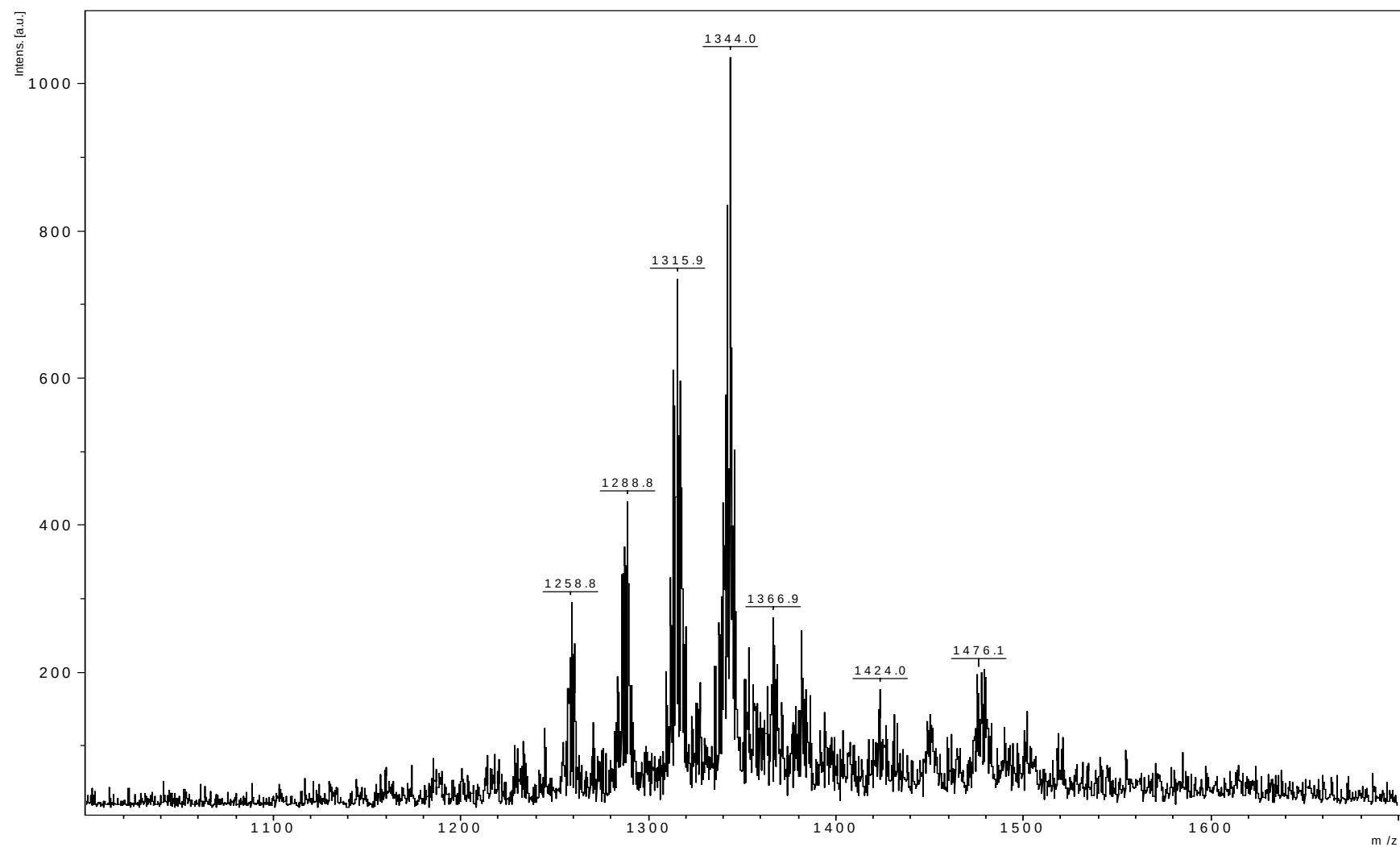
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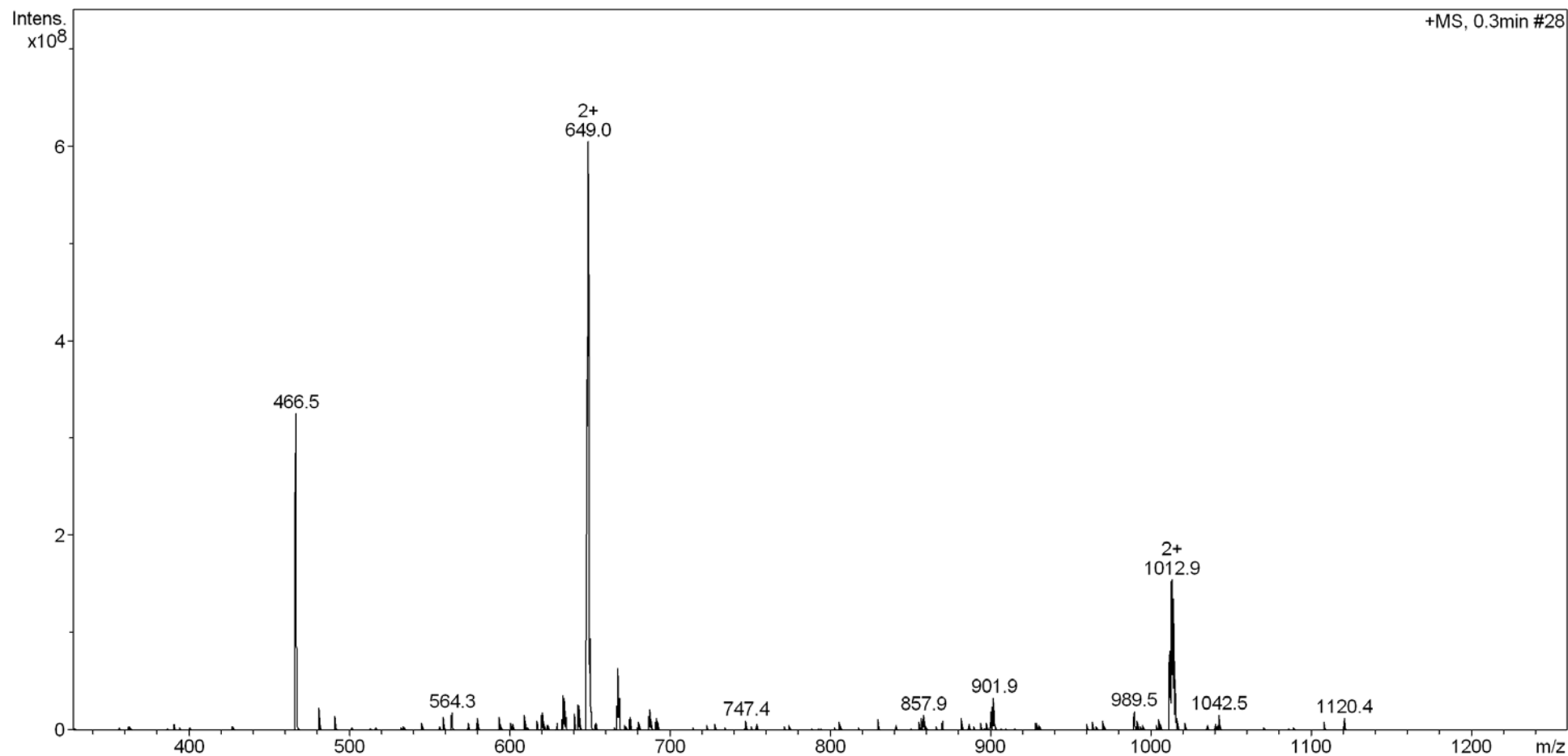
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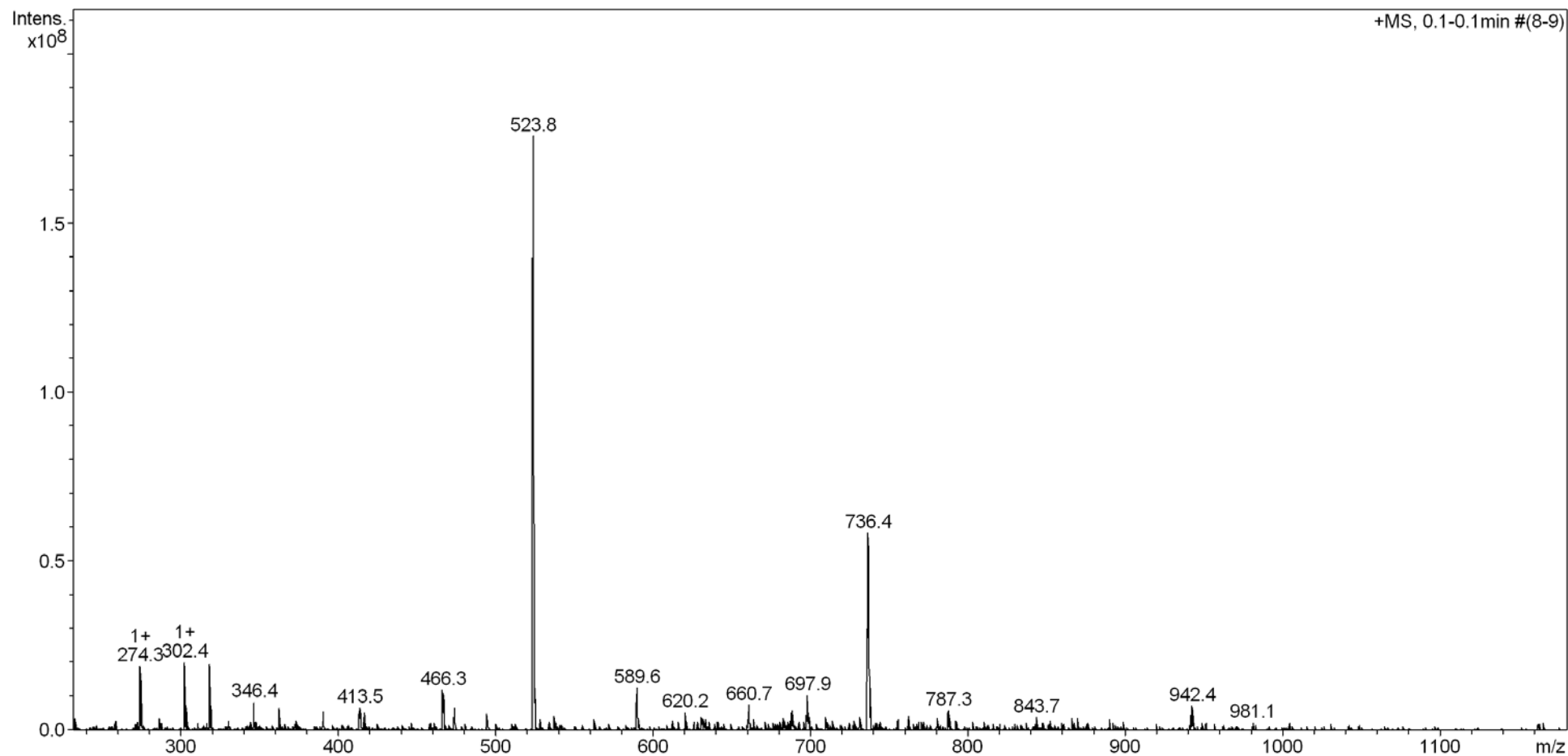
Mass spectrum (MALDI-TOF, 4-nitroaniline matrix) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethylaminoethyl)carbamoylmethoxy)-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*-6).



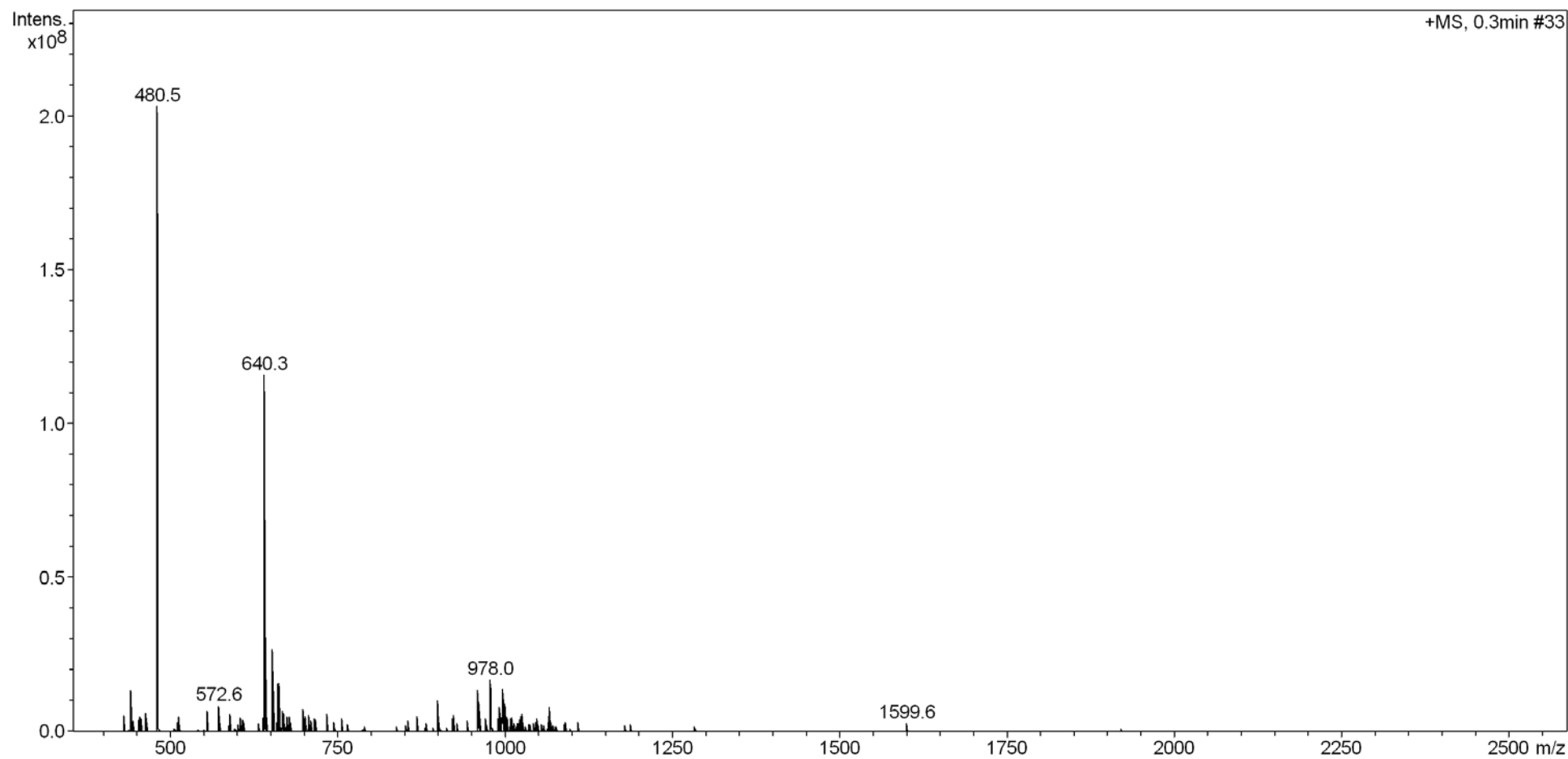
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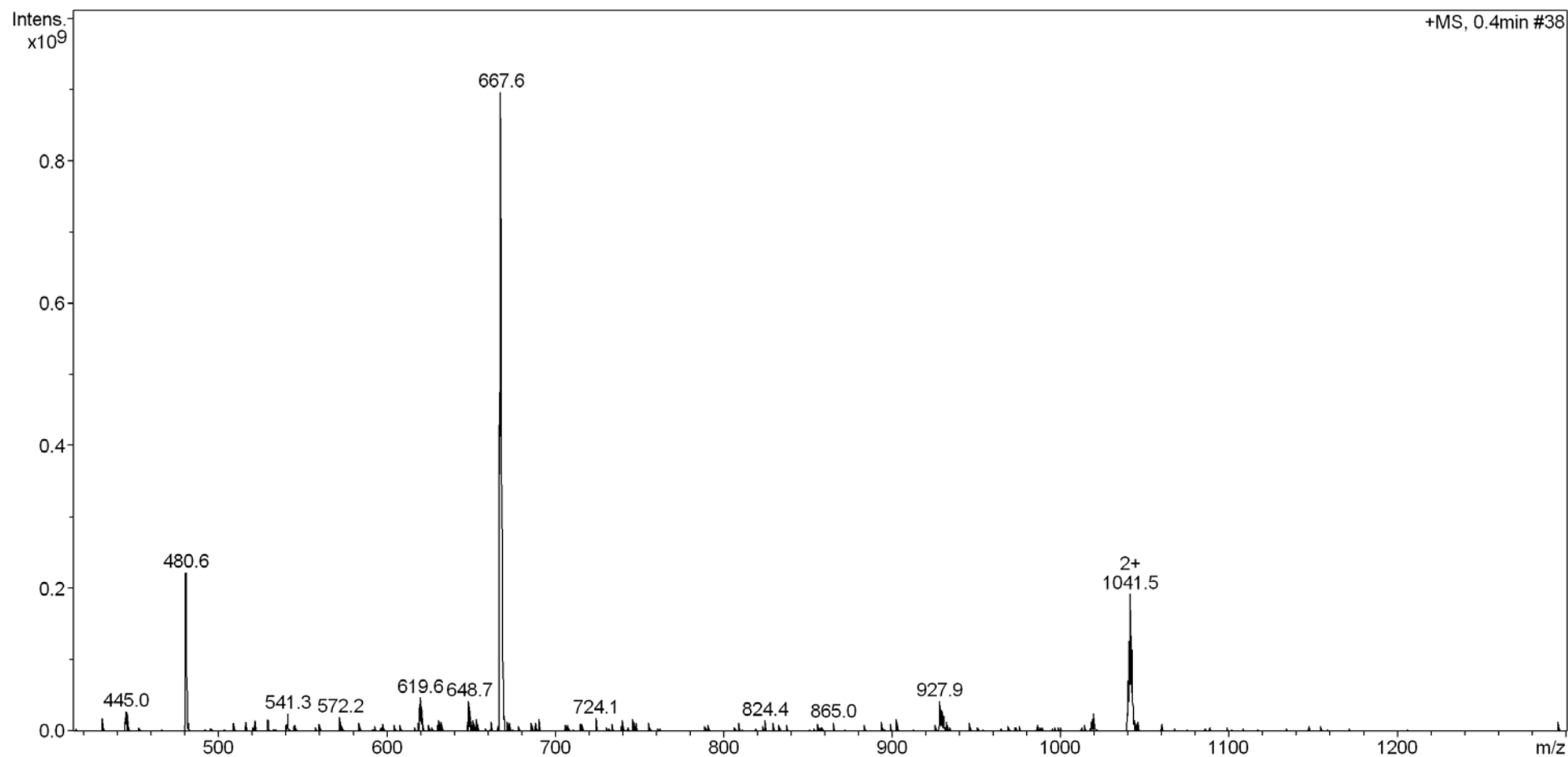
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{([ethoxycarbonylmethyl]amidocarbonylmethyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-15).



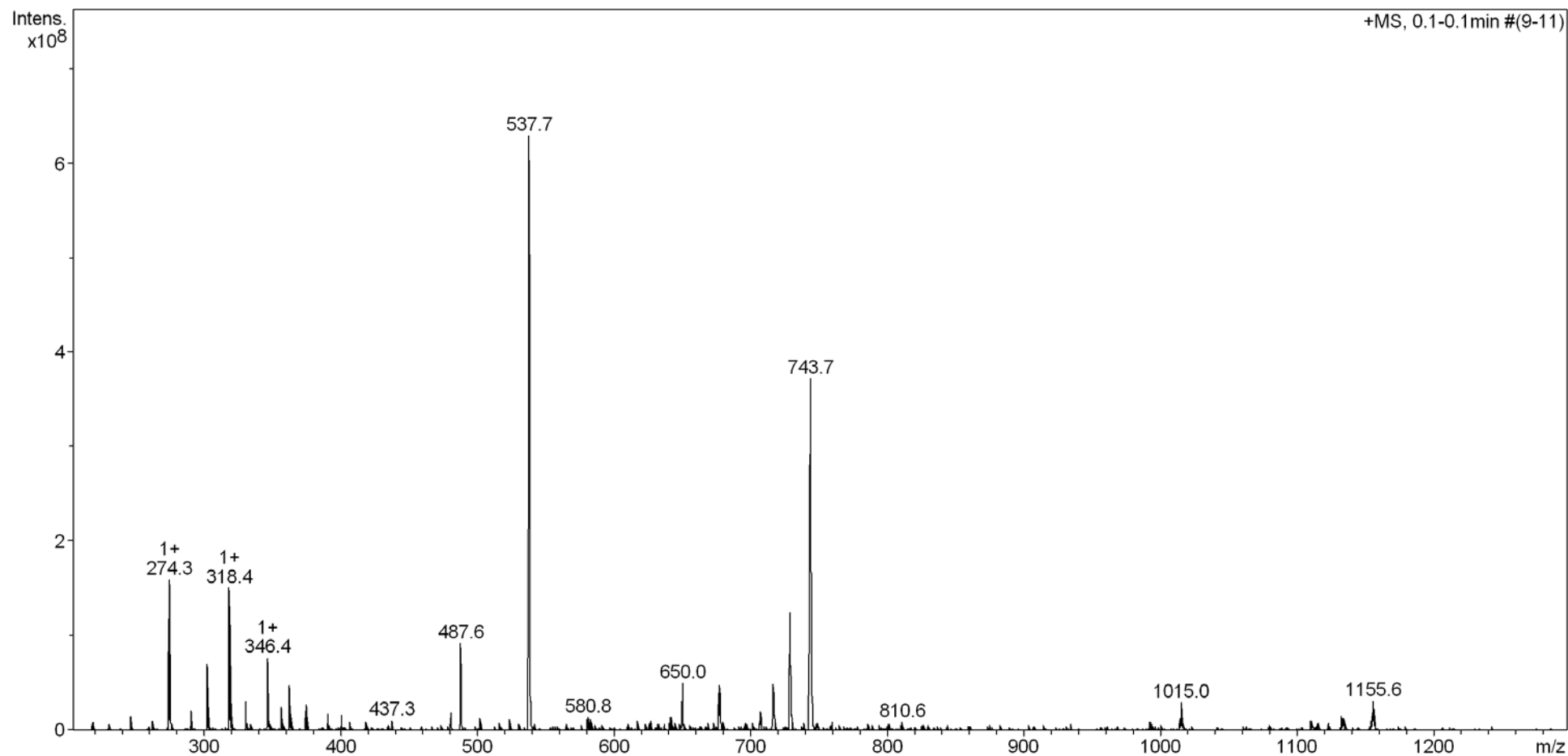
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{(ethoxycarbonyl[S-methyl]methyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-16).



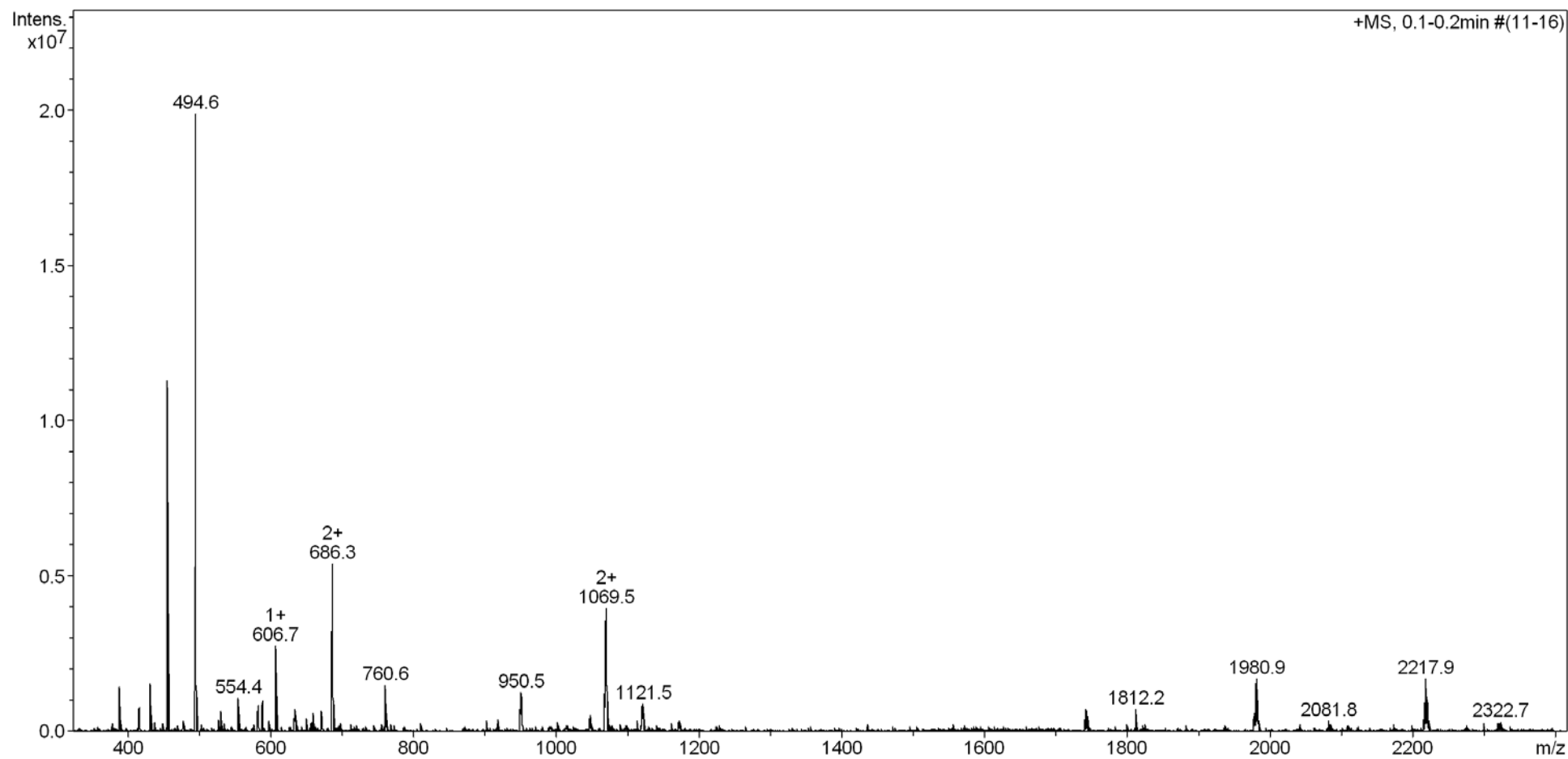
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{ethoxycarbonylmethyl)amidocarbonylmethyl})ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-17).



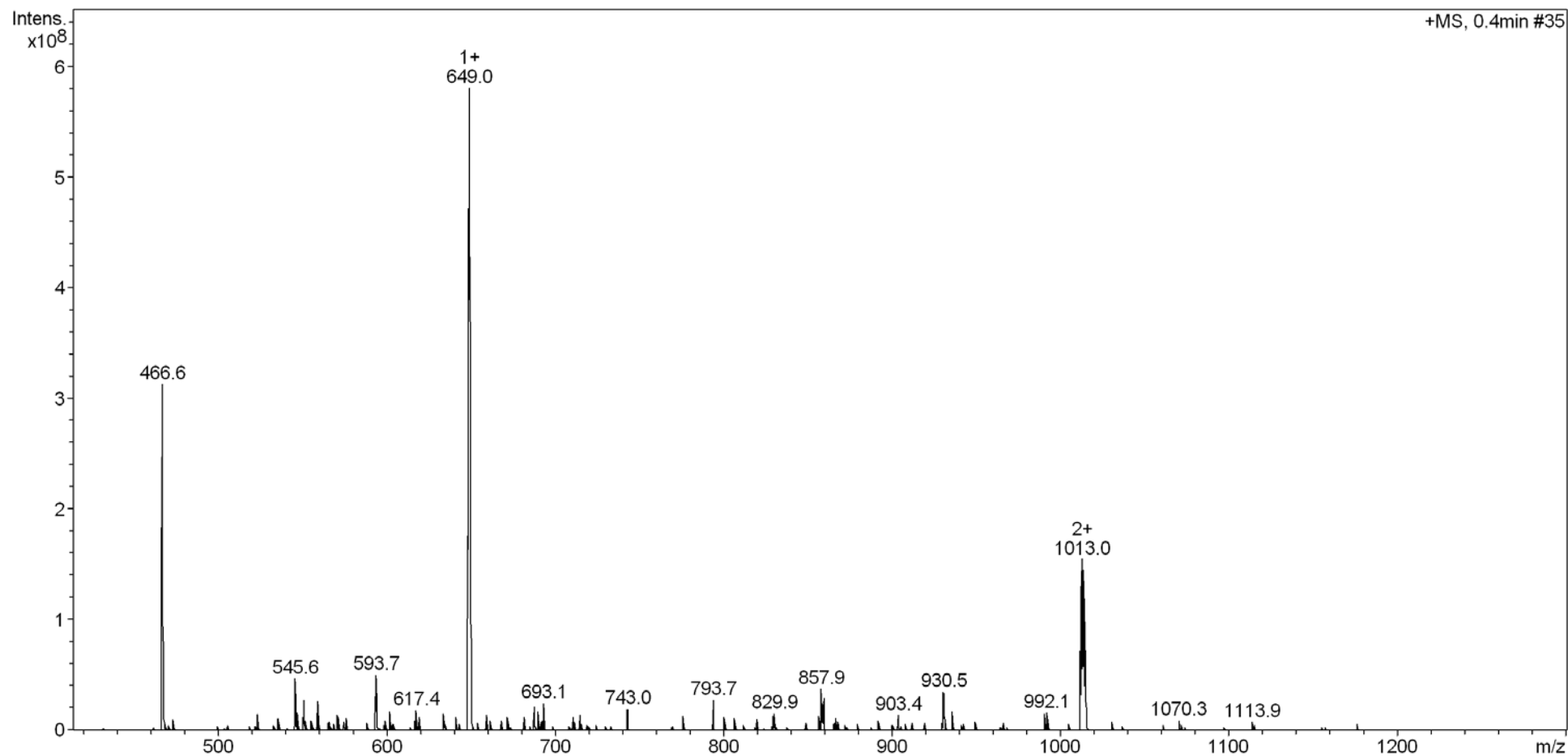
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{(ethoxycarbonylmethyl)amidocarbonylmethyl}ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-18).



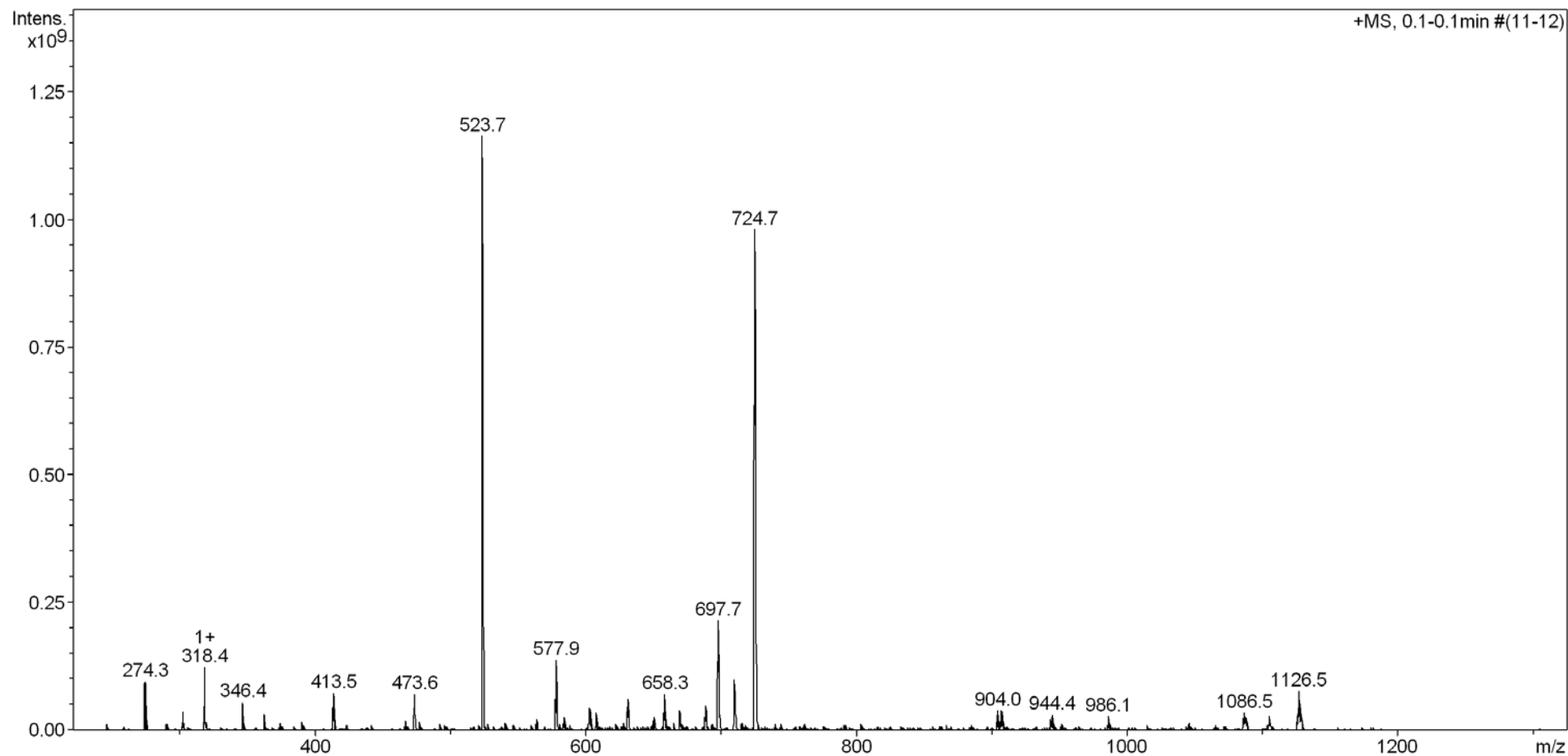
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{(ethoxycarbonyl[S-methyl]methyl)amidocarbonylmethyl}ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-19).



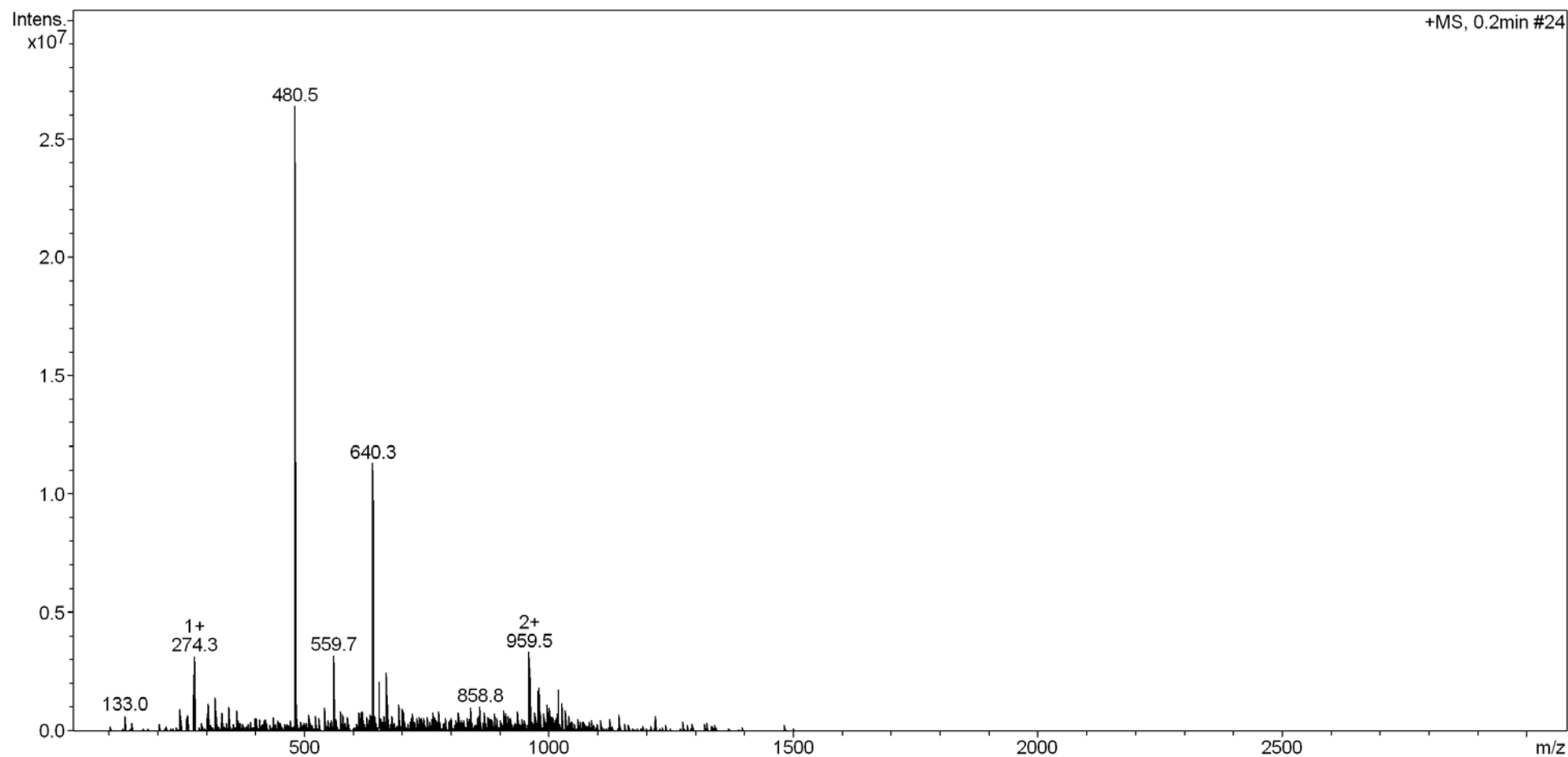
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{(ethoxycarbonylmethyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (1,3-*alternate*-20).



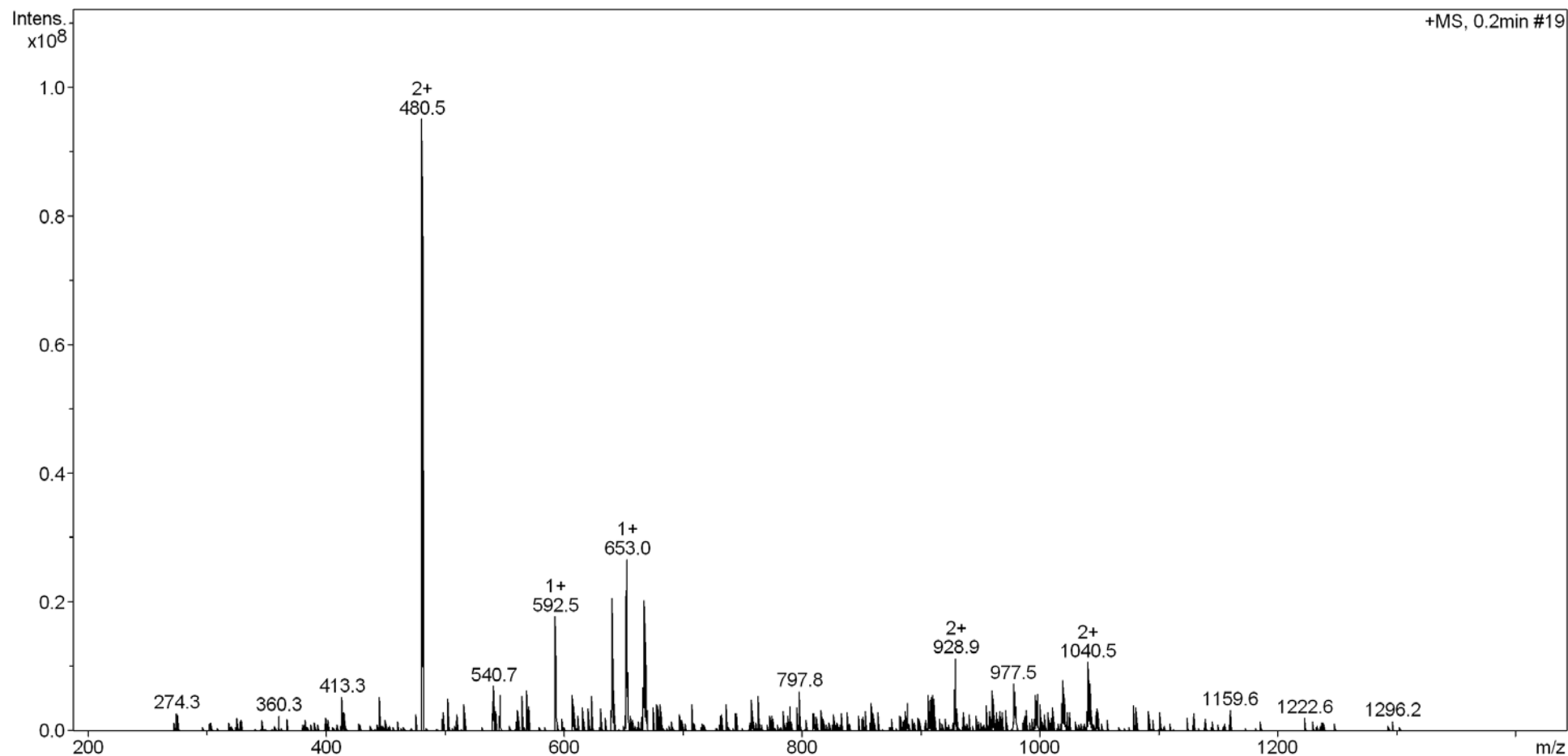
**Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-
{([ethoxycarbonylmethyl]amidocarbonylmethyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-
tetrathiacalix[4]arene tetrabromide (1,3-*alternate*-21).**



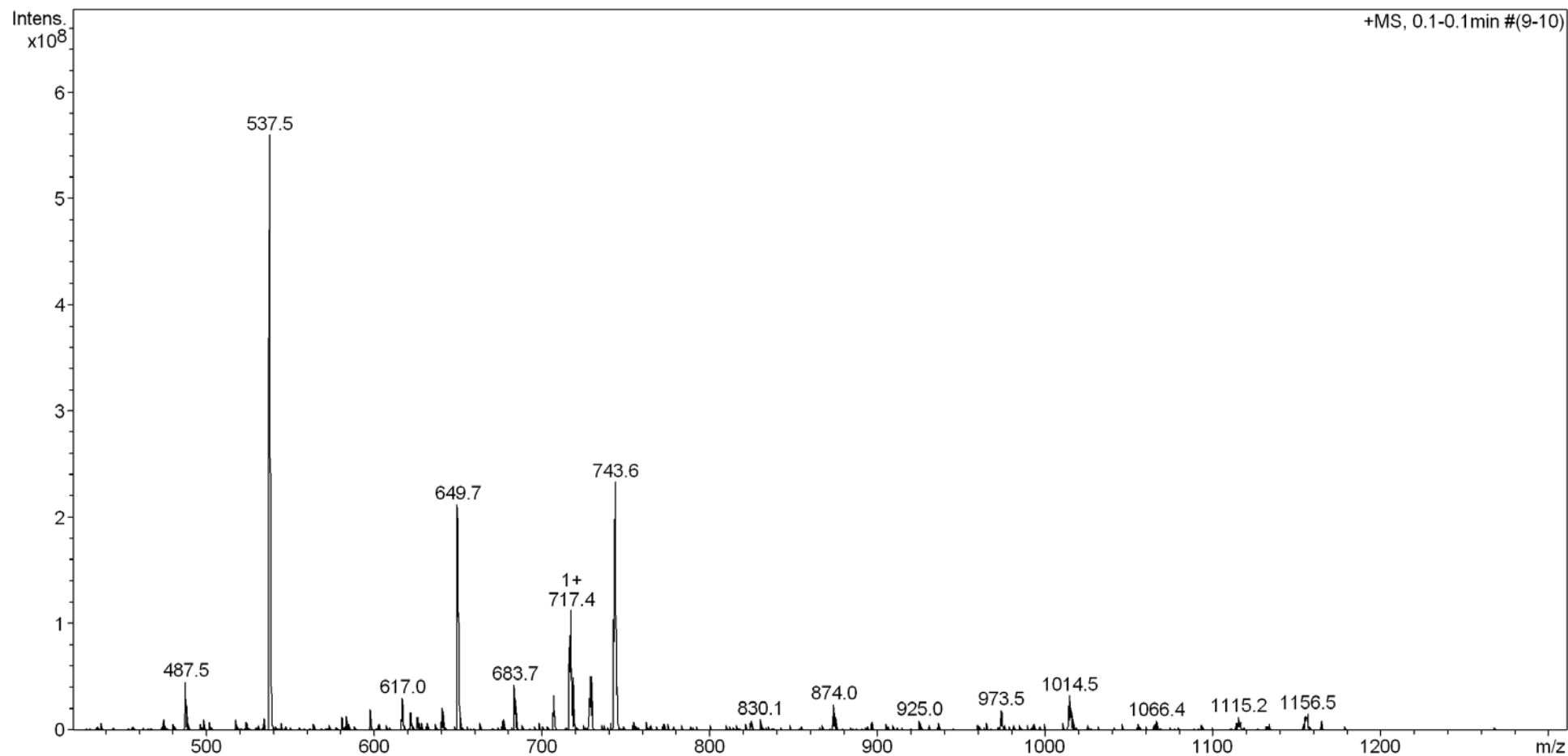
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{(ethoxycarbonyl[S-methyl]methyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (1,3-*alternate*-22).



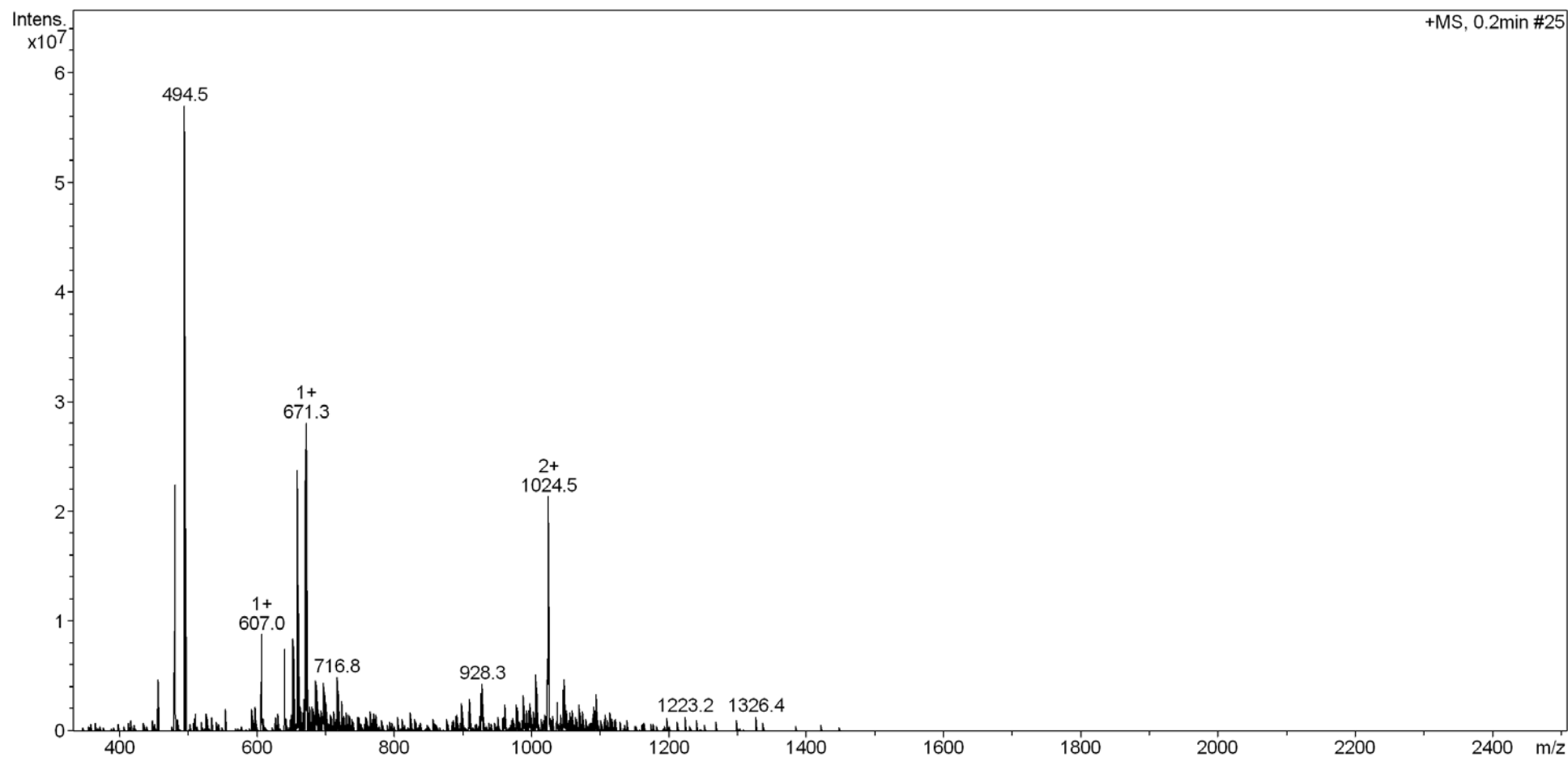
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{(ethoxycarbonylmethyl)amidocarbonylmethyl})ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (1,3-*alternate*-23).



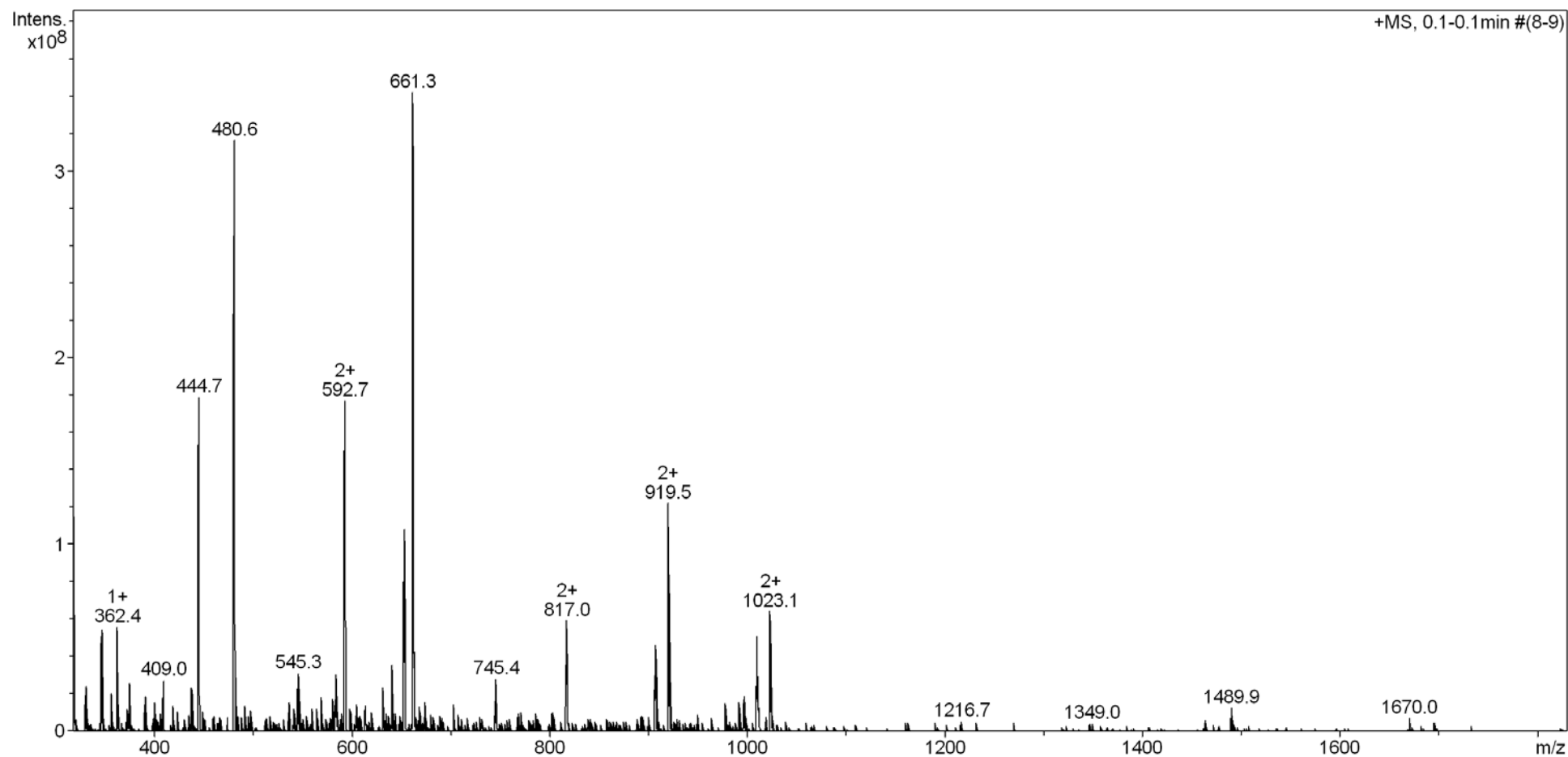
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{ethoxycarbonylmethyl)amidocarbonylmethyl}ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (1,3-alternate-24).



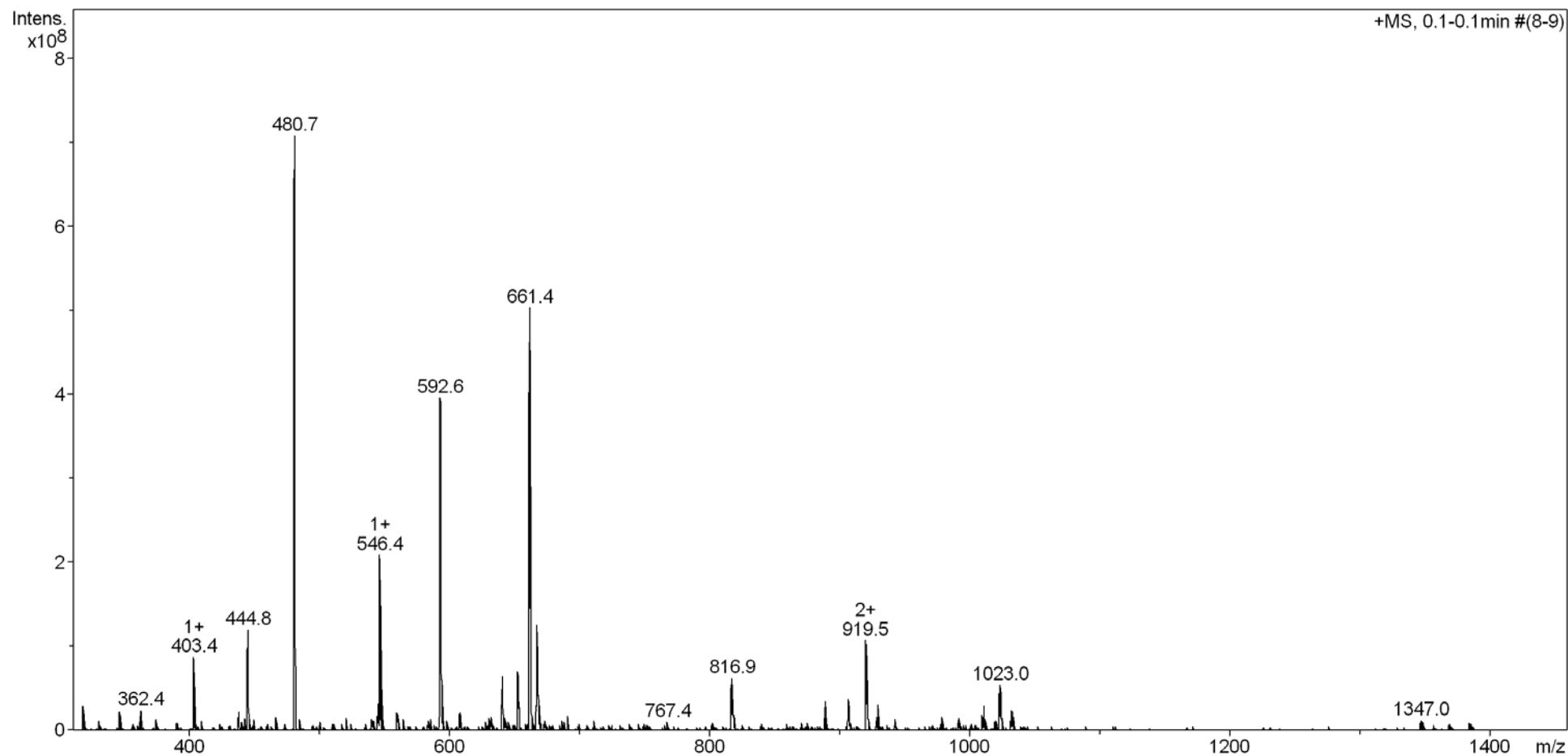
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{(ethoxycarbonyl[S-methyl]methyl)amidocarbonylmethyl}ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (1,3-*alternate*-25).



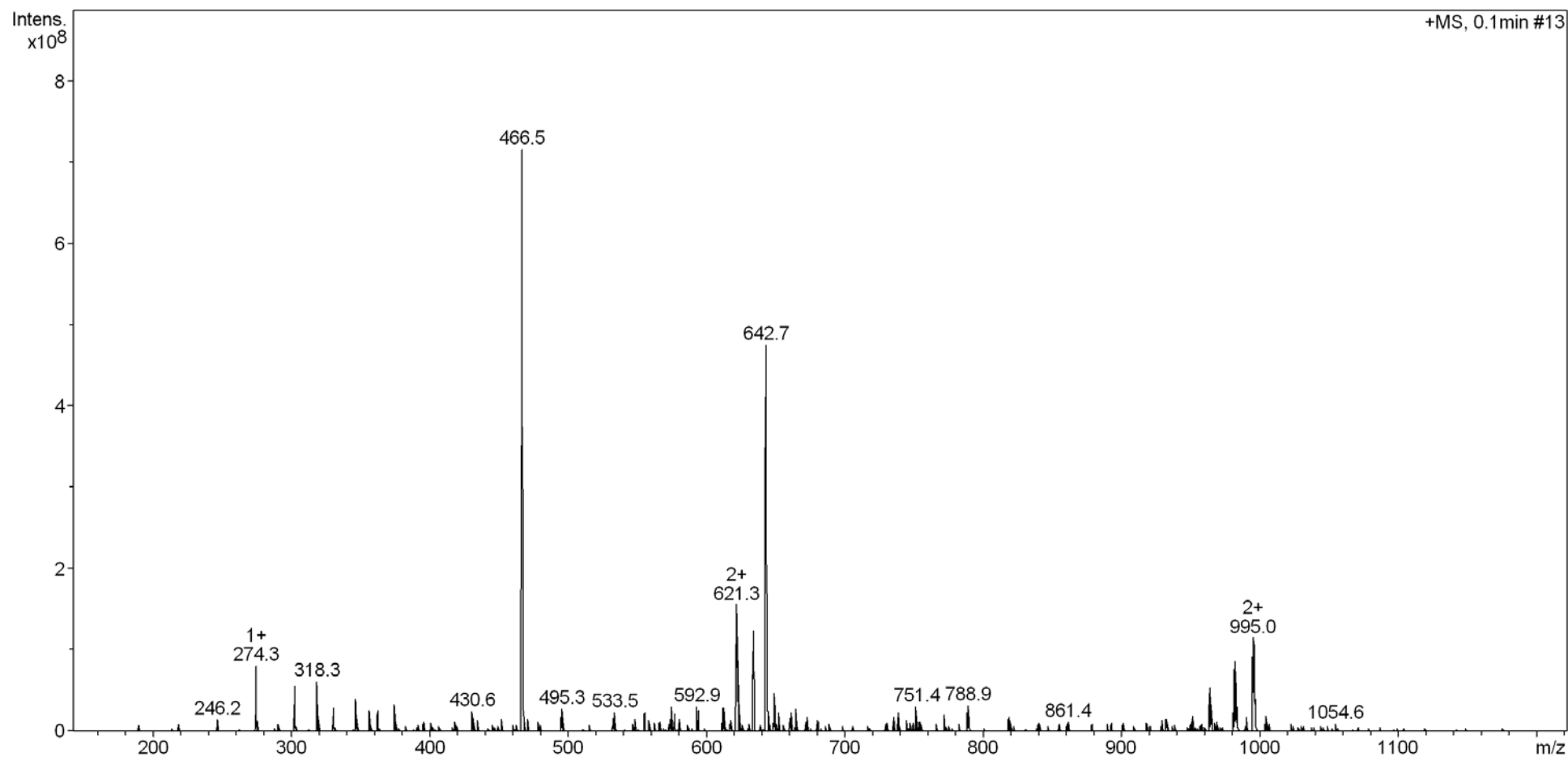
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{ethoxycarbonylmethyl)amidocarbonylmethyl})ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetranitrate (*cone*-26).



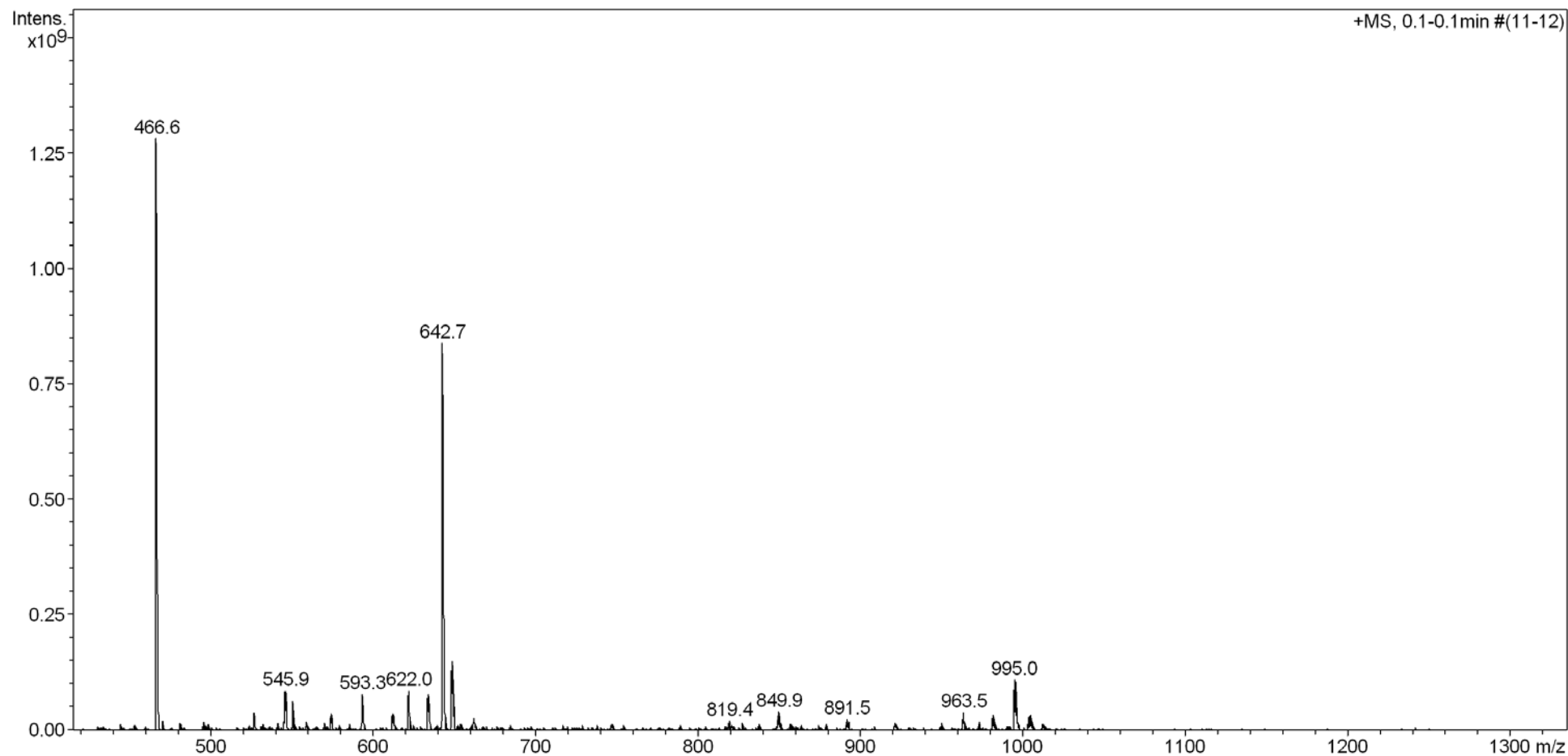
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{ethoxycarbonylmethyl)amidocarbonylmethyl})ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetranitrate (1,3-*alternate*-27).



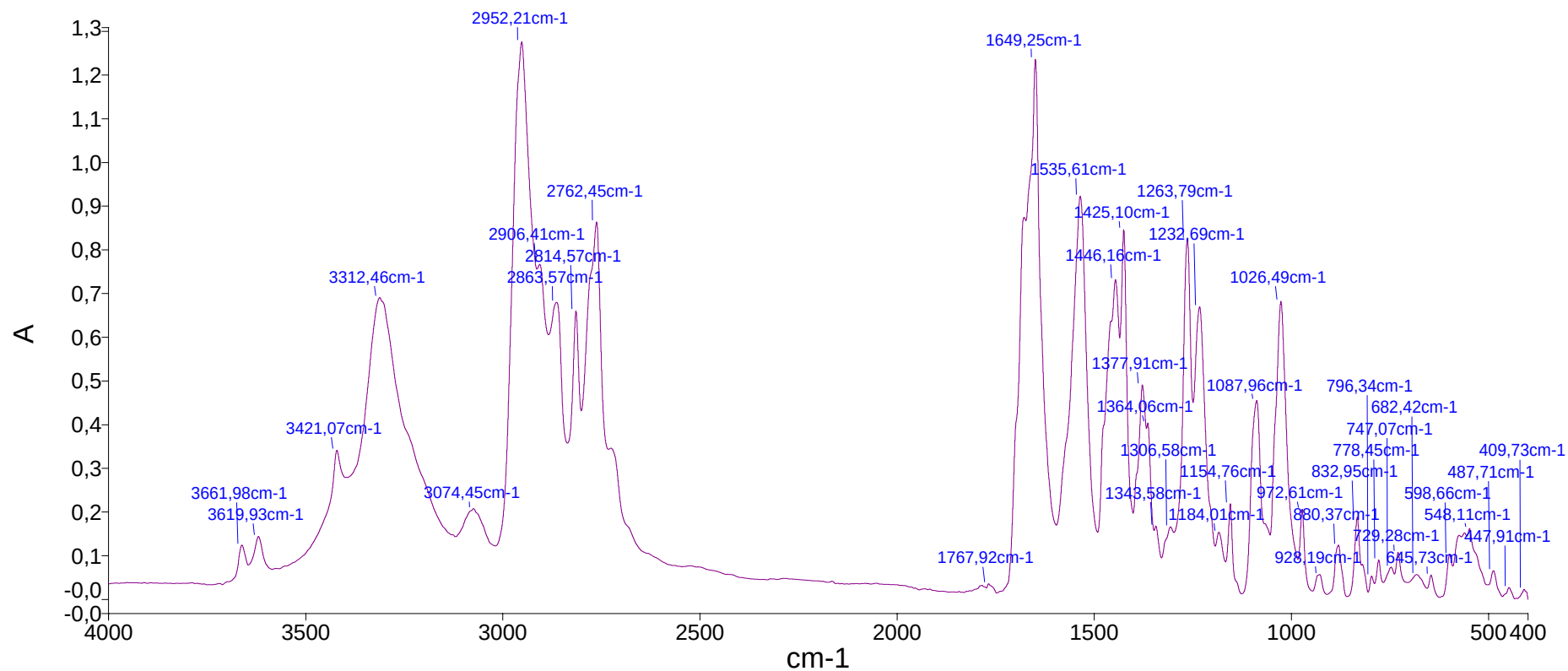
Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{(ethoxycarbonylmethyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetranitrate (*cone*-28).



Mass spectrum (ESI) of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{ethoxycarbonylmethyl}amidocarbonylmethyl)ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetranitrate (1,3-*alternate*-29).



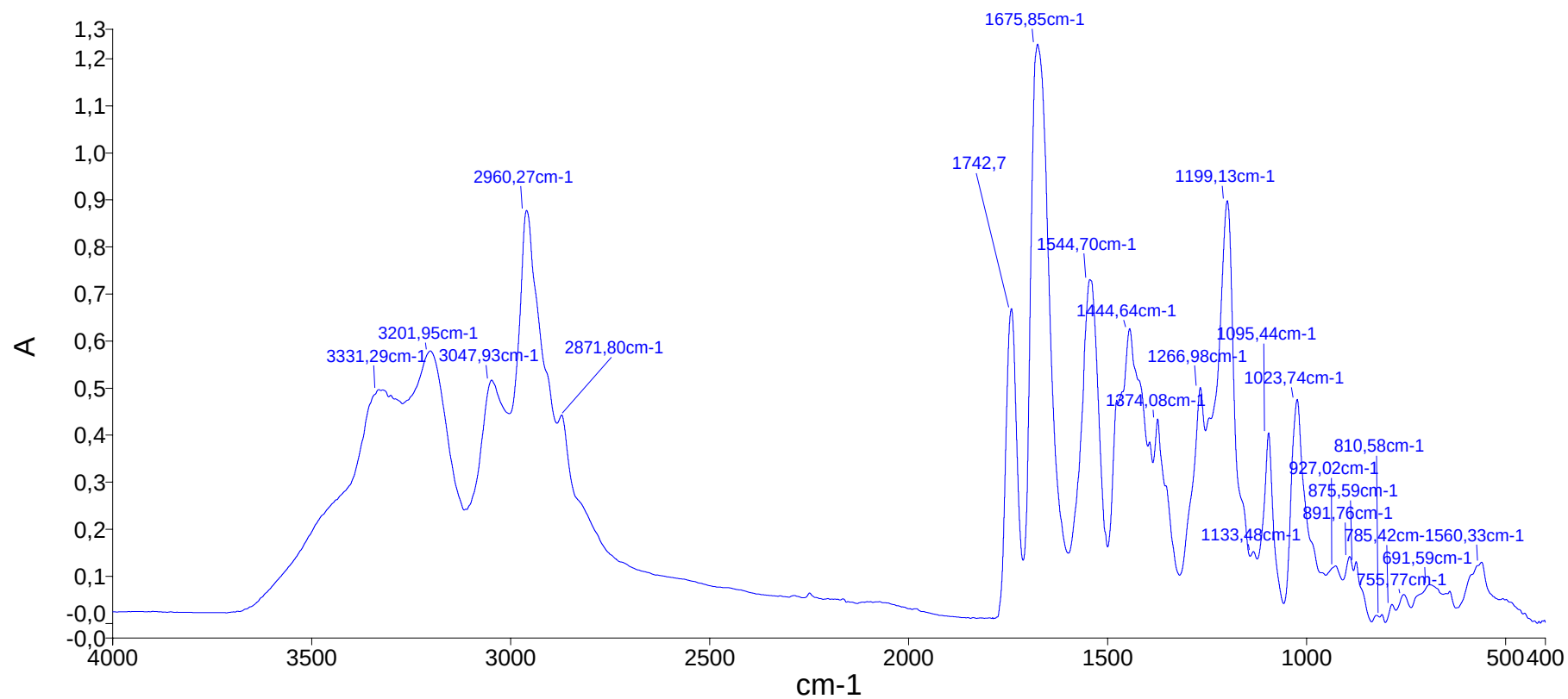
IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethylaminopropyl)carbamoylmethoxy]-2,8,14,20-tetratetrathiacalix[4]arene (1,3-*alternate*-5).



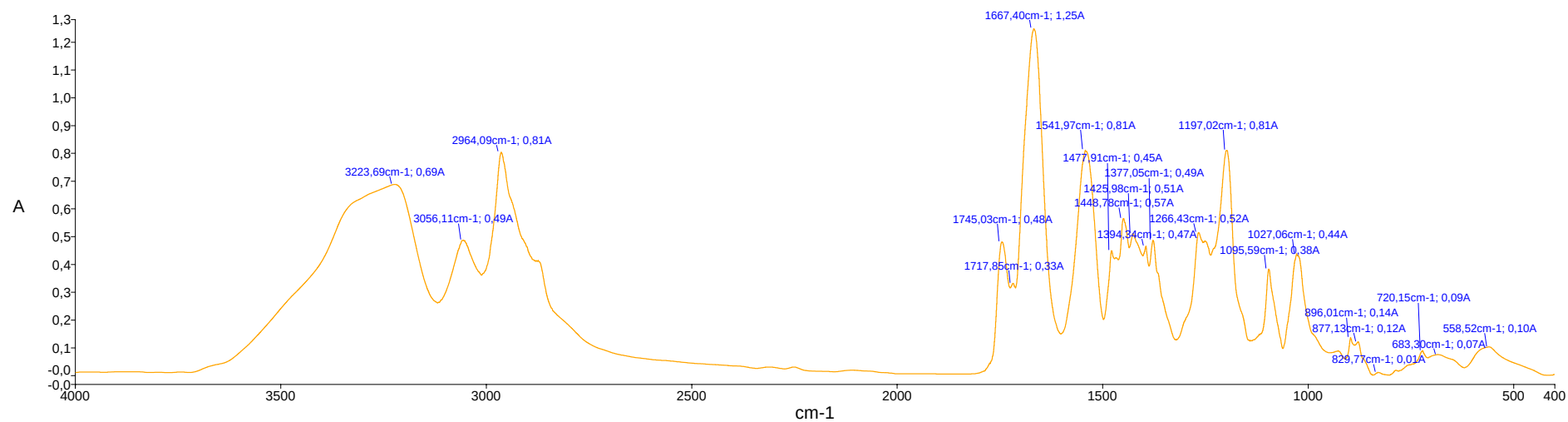
IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethylaminoethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*-6).



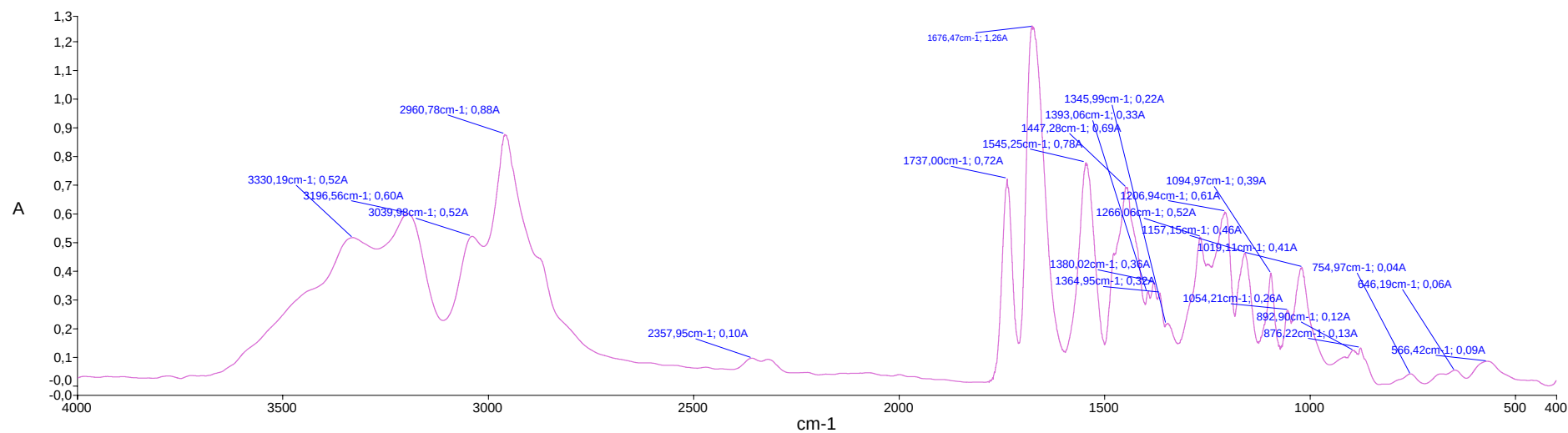
IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{(ethoxycarbonylmethyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-14).



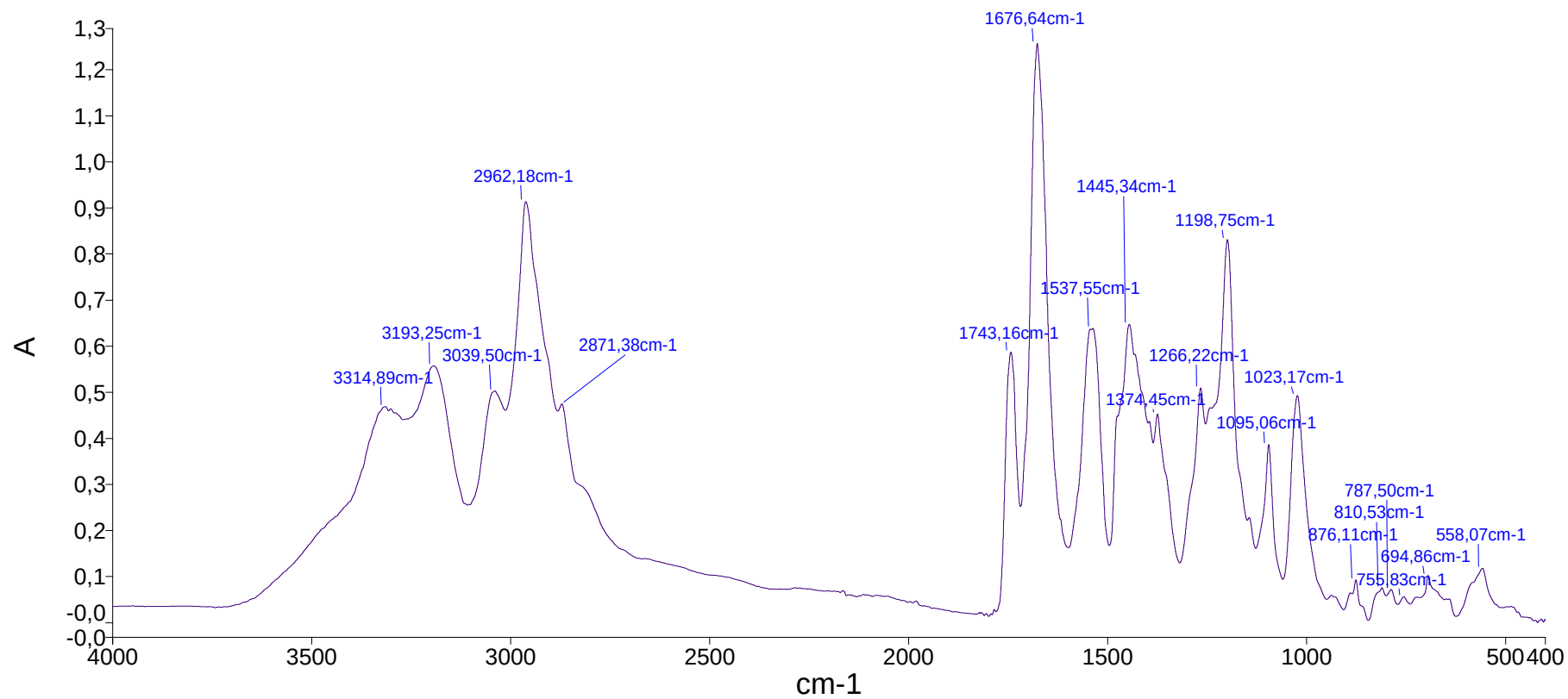
**IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-
{([ethoxycarbonylmethyl]amidocarbonylmethyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-
tetrathiacalix[4]arene tetrabromide (*cone*-15).**



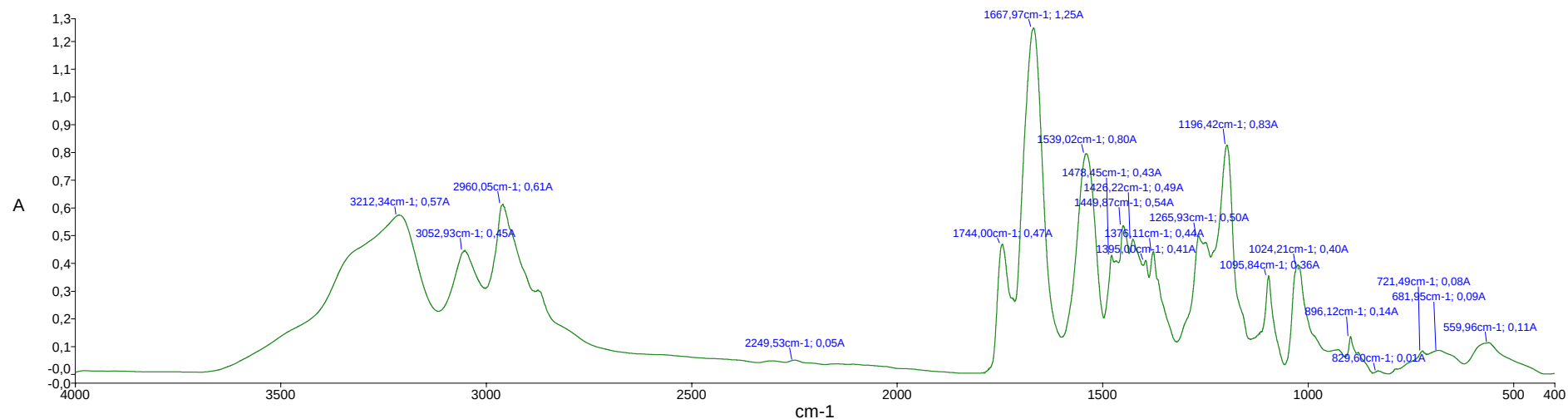
IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{(ethoxycarbonyl[S-methyl]methyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy)-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-16).



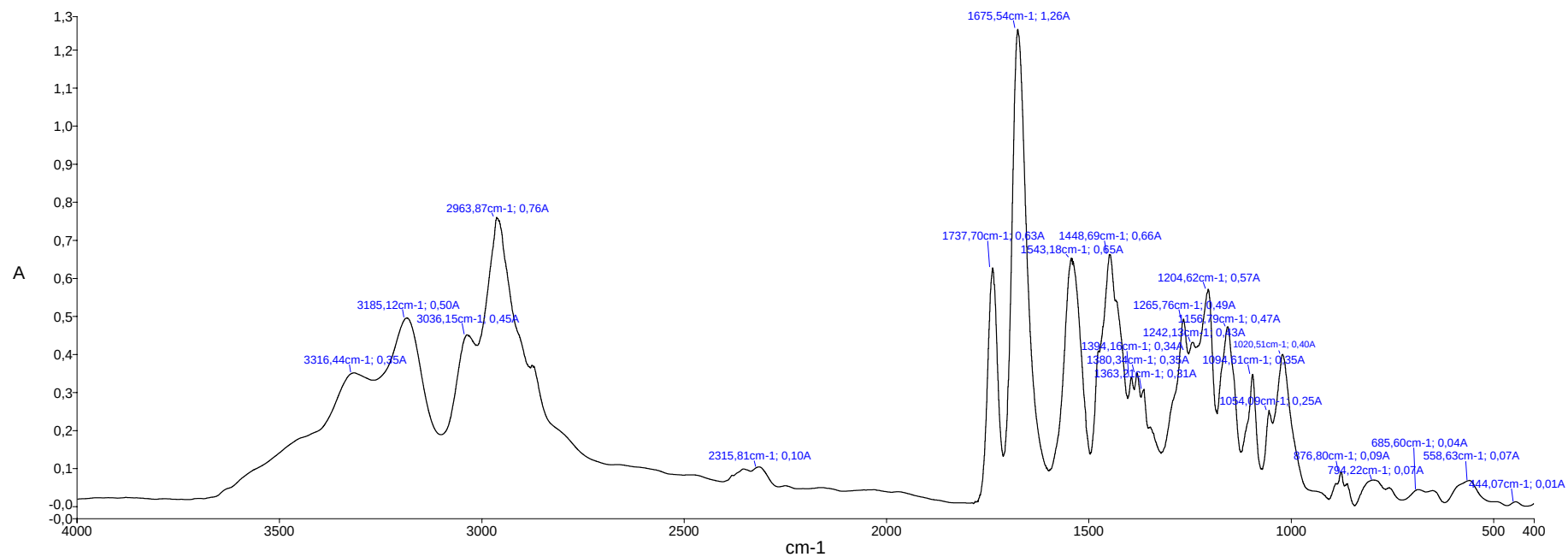
**IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-
{(ethoxycarbonylmethyl)amidocarbonylmethyl})ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-17).**



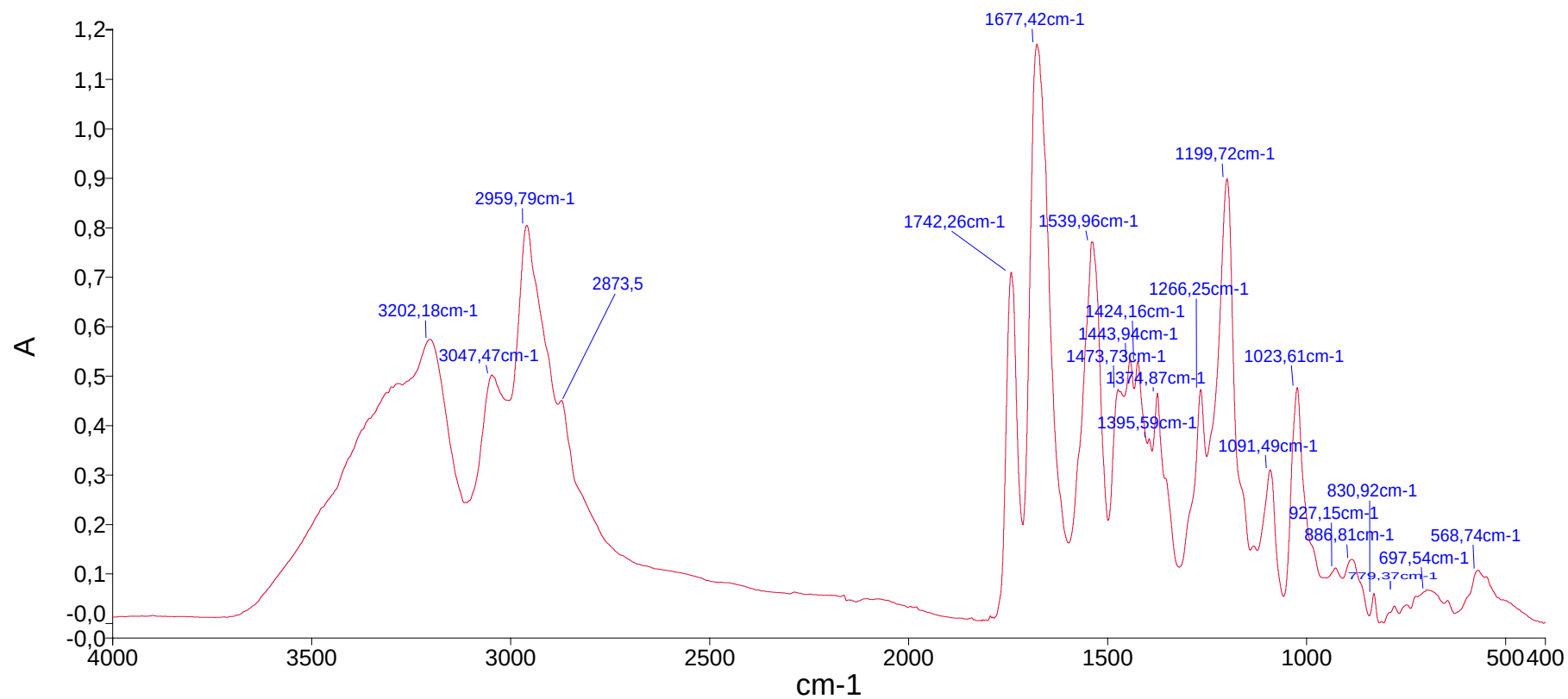
IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{ethoxycarbonylmethyl)amidocarbonylmethyl}ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-18).



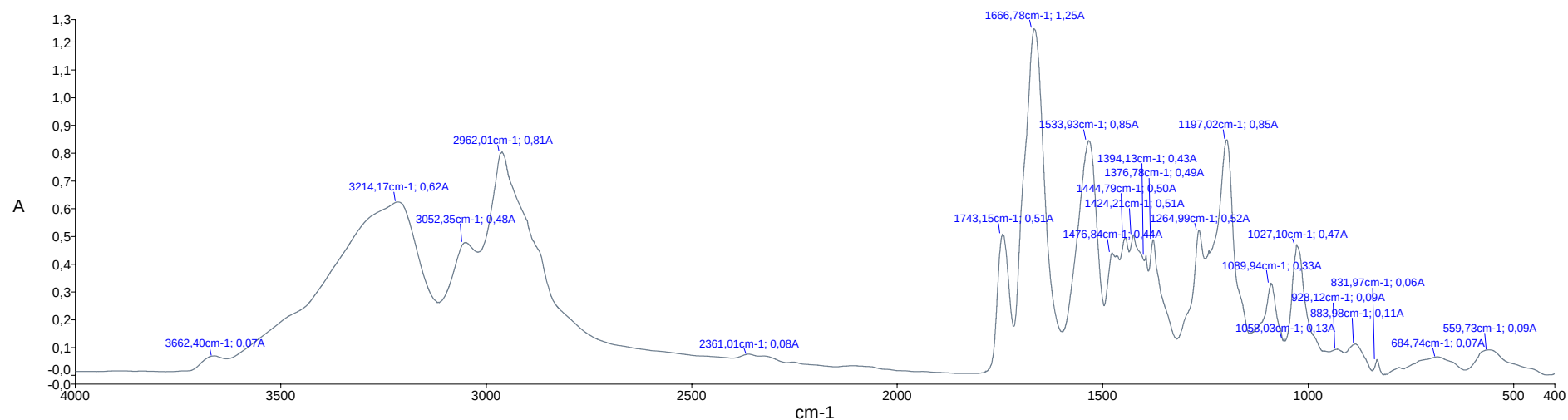
IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{(ethoxycarbonyl[S-methyl]methyl)amidocarbonylmethyl}ammoniummethyl)carbamoylmethoxy)]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (*cone*-19).



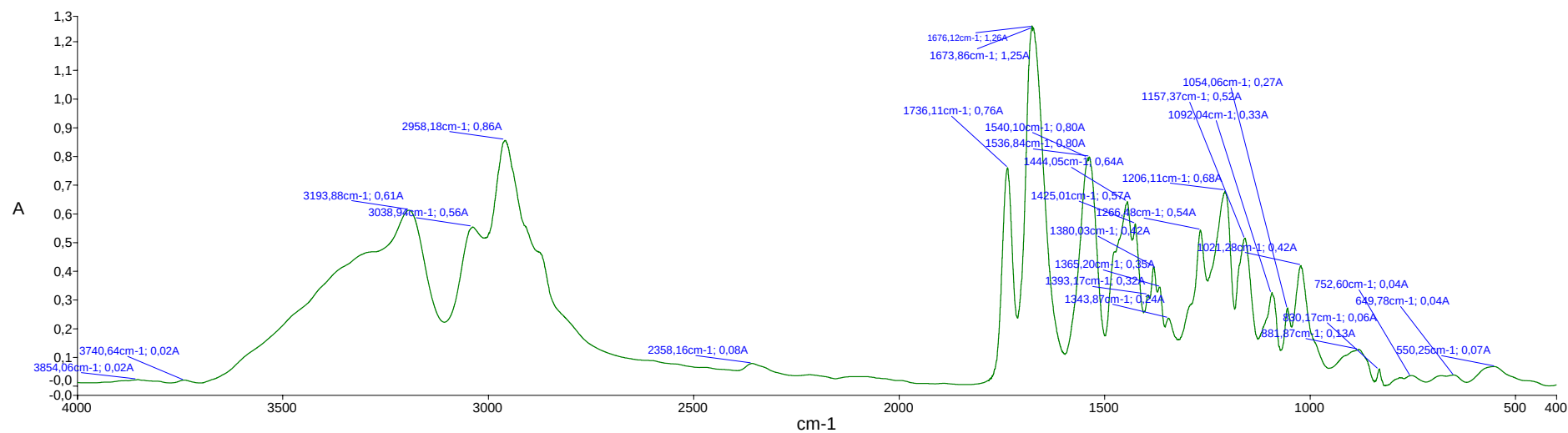
IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{ethoxycarbonylmethyl}amidocarbonylmethyl)ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (1,3-alternate-20).



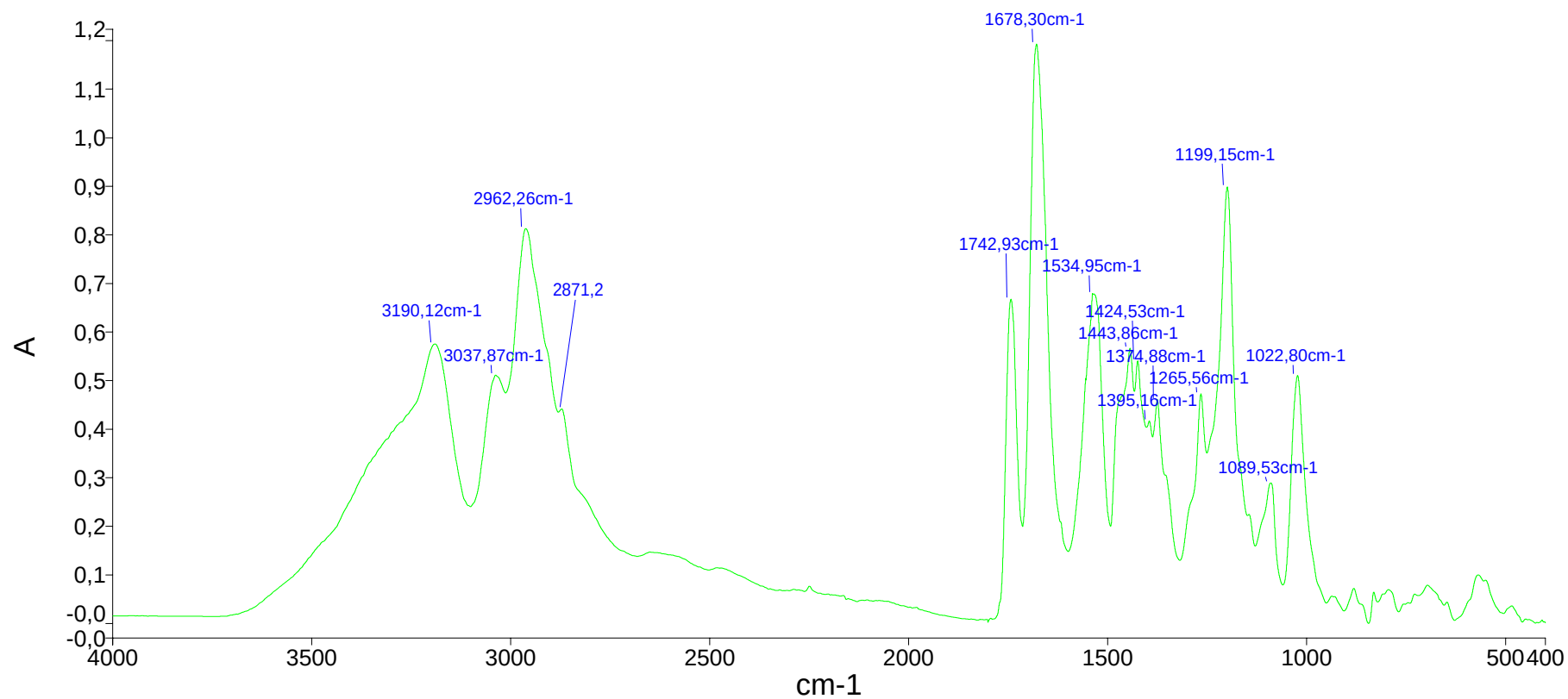
**IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-
 {[ethoxycarbonylmethyl]amidocarbonylmethyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-
 tetrathiacalix[4]arene tetrabromide (1,3-*alternate*-21).**



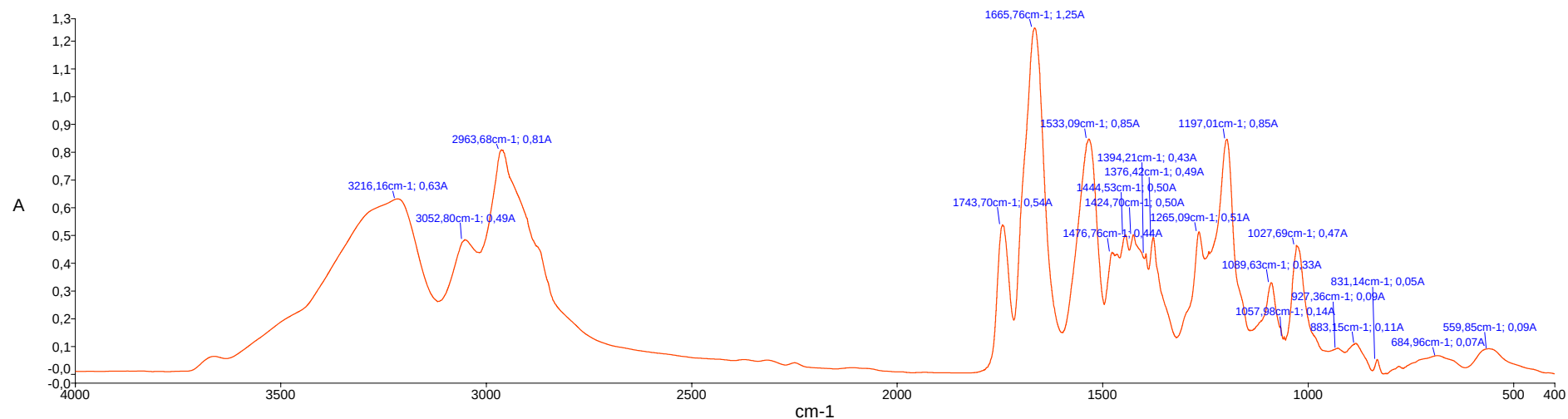
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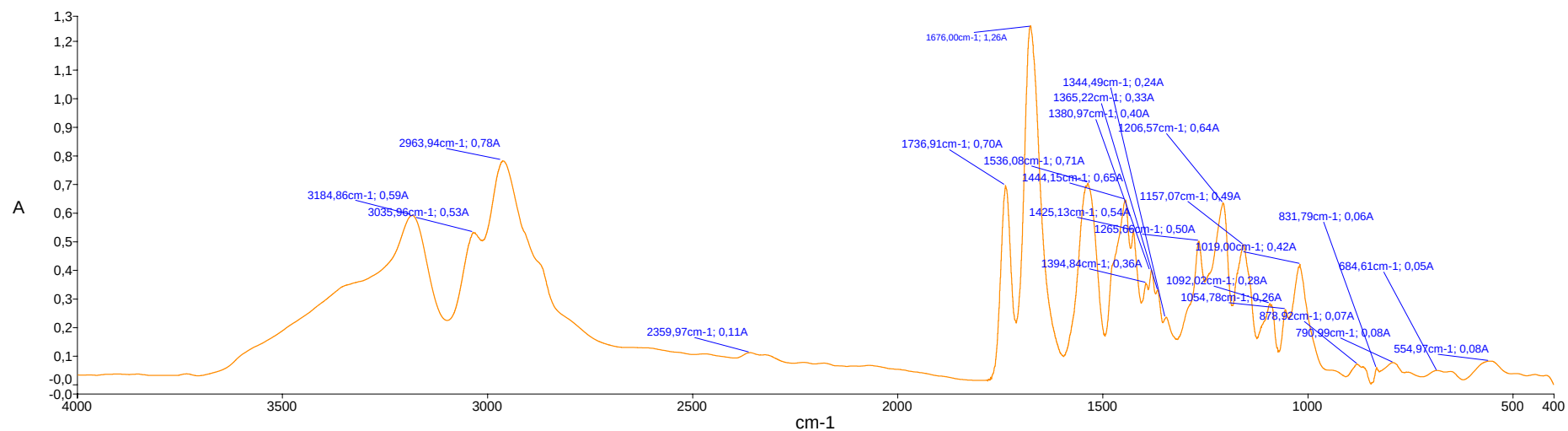
**IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-
{(ethoxycarbonylmethyl)amidocarbonylmethyl})ammoniummethyl)carbamoylethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (1,3-
alternate-23).**



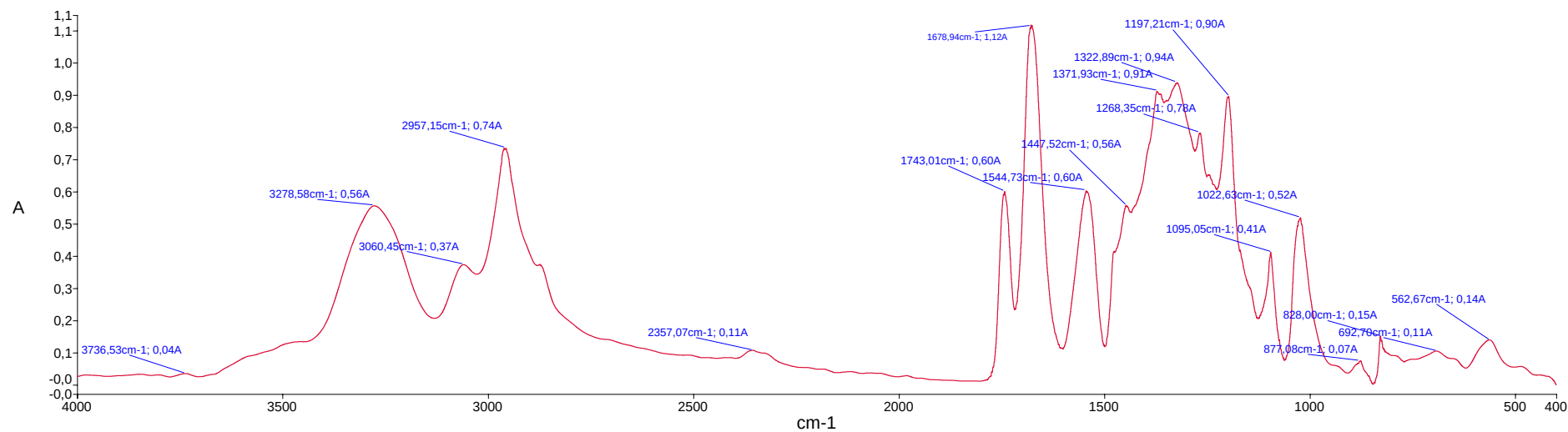
IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{ethoxycarbonylmethyl)amidocarbonylmethyl}ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (1,3-alternate-24).



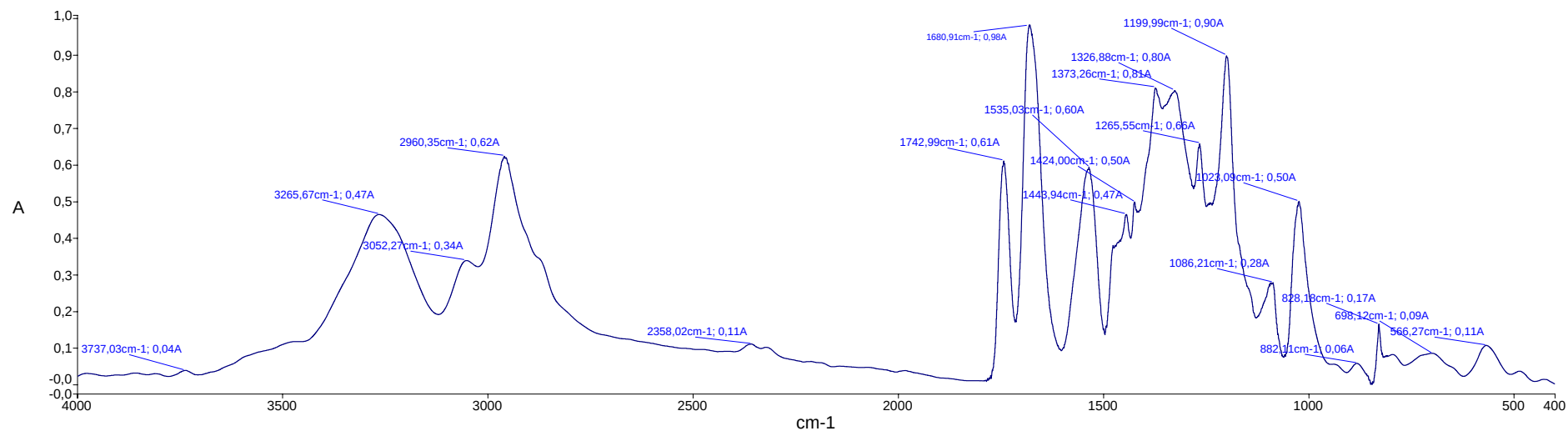
IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{(ethoxycarbonyl[S-methyl]methyl)amidocarbonylmethyl}ammoniummethyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide (1,3-*alternate*-25).



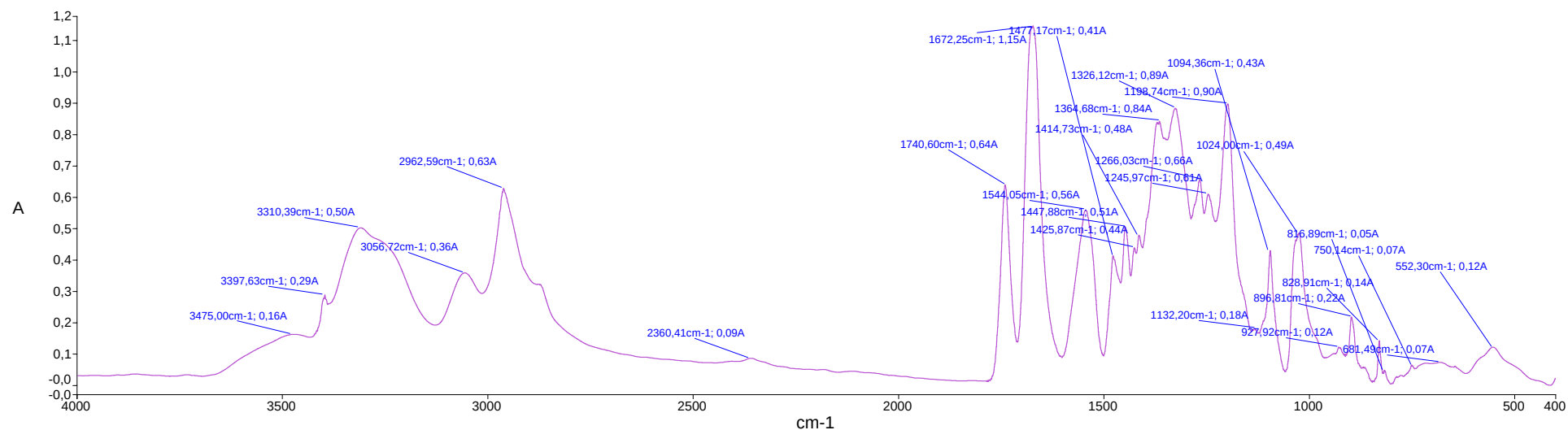
**IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-
{(ethoxycarbonylmethyl)amidocarbonylmethyl})ammoniummethyl)carbamoylemethoxy]-2,8,14,20-tetrathiocalix[4]arene tetranitrate (*cone*-26).**



IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(2',2'-diethyl-2'-{(ethoxycarbonylmethyl)amidocarbonylmethyl})ammoniummethyl)carbamoylethoxy]-2,8,14,20-tetrathiacalix[4]arene tetranitrate (1,3-*alternate*-27).



IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{ethoxycarbonylmethyl}amidocarbonylmethyl)ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetranitrate (*cone*-28).



IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(N-(3',3'-dimethyl-3'-{(ethoxycarbonylmethyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetranitrate (1,3-*alternate*-29).

