

Supporting Information

Water Soluble Pentacene

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General Experimental Methods

Reactions were performed in standard glassware except where noted. The following reagents were used as purchased without further purification: zinc iodide (Aldrich), 3-thiopropionic acid (Alfa Aesar), chloranil (Aldrich), potassium carbonate (J. T. Baker), ethanol (Pharmco-AAPER), methanol (MeOH, Pharmco-AAPER), chloroform (CHCl_3 , Pharmco-AAPER), dichloromethane (DCM, Pharmco-AAPER), benzene (Sigma-Aldrich), hexanes (Pharmco-AAPER), acetone (Pharmco-AAPER), buffer solution (K_2CO_3 - K_3BO_3 -KOH, pH=10, Fisher Scientific), dimethylsulfoxide (DMSO, Alfa Aesar). All NMR solvents including acetone- d_6 , methanol- d_4 , D_2O and acetic acid- d_4 were purchased from Cambridge Isotope Laboratories.

^1H NMR Spectra

^1H NMR spectra were obtained on a Varian Mercury Plus 400 FT-NMR operating at 399.768 MHz or a Varian INOVA 500 FT-NMR operating at 499.763 MHz. All chemical shift (δ_{H}) values are reported in parts per million (ppm) relative to residual solvent protons unless otherwise noted.

^{13}C NMR Spectra

^{13}C NMR spectra were obtained on a Varian Mercury Plus 400 FT-NMR operating at 100.522 MHz or a Varian INOVA 500 FT-NMR operating at 125.666 MHz. All chemical shift (δ_{C}) values are reported in parts per million (ppm) relative to residual solvent signal or K_2CO_3 (160.64 ppm in D_2O)¹ unless otherwise noted.

¹ Y. Kim, J. Choi, S. Nam, S. Jeong and Y. Yoon, *Energy Fuels*, 2012, **26**, 1449.

Mass Spectrometry

Matrix assisted laser desorption ionization (MALDI-TOF-MS, S₈ as matrix) and laser desorption ionization (LDI-TOF-MS) mass spectra was acquired on a Shimadzu Kratos Axima-CFR mass spectrometer in reflectron mode. Electrospray ionization high resolution mass spectra were acquired at the Notre Dame Mass Spectrometry & Proteomics Facility in Notre Dame, Indiana.

Solid State FTIR Spectroscopy

Infrared spectra of solid samples were acquired using a Thermo Scientific spectrometer (NICOLET iS10) with diamond ATR accessory (Smart iTR).

Thermogravimetric Analysis

Thermogravimetric analysis was completed using a TA Instruments TGA Q5000 instrument. Samples weighing between 5 - 15 mg were heated from 35 °C - 550 °C with the ramp rate set to 5 °C/min.

UV-Vis Spectroscopy

UV-visible spectra were obtained on a Nicolet Evolution 300 spectrometer using 1 cm quartz cells. In order to obtain the decay profile of WSP **4** in solution with exposure to light and air, dilute solutions (2.0×10^{-4} M) of WSP **4** were prepared in aqueous buffer (pH = 10). The cells were protected from light until each experiment began, at which point an initial spectrum was recorded. The cells were placed in a tank containing water to maintain a constant temperature (25 °C) and irradiated with an overhead 15 watt, 120 volt incandescent light bulb. The solutions were repeatedly scanned at prescribed intervals until less than 5% of WSP **4** remained. Because WSP **4**

is slow to decay, water was added periodically to offset evaporation and maintain a constant concentration.

Computational Modeling

Gaussian archive entries

NOTE: All species had zero imaginary frequencies, as determined from frequency calculations at the B3LYP/6-31G(d) level

Conformer A of Table 1

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1\1\GINC-MILLER4\FOpt\RB3LYP\6-31G(d)\C28H20K2O4S2\JHODGSON\04-Aug-
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6678\S,-0.188725594,-3.22748793,-1.3008103753\S,0.188725594,3.22748793
,-1.3008103753\C,0.510638732,-3.907097033,0.2828746749\C,-0.510638732,
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60798369\C,0.9103714609,2.647310035,2.0060798369\O,-0.0183492998,1.787
7973565,2.1773640895\O,0.0183492998,-1.7877973565,2.1773640895\H,0.871
1032472,-4.898265894,-0.0135415215\H,-0.8711032472,4.898265894,-0.0135
415215\H,0.0026979592,-4.5743605436,2.2461171371\H,-0.0026979592,4.574
3605436,2.2461171371\C,1.2647696252,0.6684781519,-1.1318132963\C,-1.26
47696252,-0.6684781519,-1.1318132963\C,1.1907294355,-0.7926078741,-1.2
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.1439072887,2.1284363722\K,-1.9380542274,0.1439072887,2.1284363722\H,1
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3.7236278891,-0.5275294439,-1.0407610578\C,3.6530509903,-0.9103688726,
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-1.6547118708,-1.2779424662\C,-4.87894496,1.6547118708,-1.2779424662\H
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Conformer B of Table 1

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783\S,-0.6168778588,-2.5647968423,1.8769185276\S,0.6168778588,2.564796
8423,-1.8769185276\C,-0.7107120154,-4.0047497829,0.6930787775\C,0.7107
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36168\H,0.017925939,3.811407655,0.1277336168\H,-0.3421338689,-4.849288
4232,1.2853136008\H,0.3421338689,4.8492884232,-1.2853136008\C,-1.28213
28128,-0.1680301686,0.6141240482\C,1.2821328128,0.1680301686,-0.614124
0482\C,-1.0003548451,0.9961709528,-0.2273493462\C,1.0003548451,-0.9961
709528,0.2273493462\H,1.8489425211,-2.7780616429,1.0939437175\H,-1.848
9425211,2.7780616429,-1.0939437175\O,-1.6958780594,-2.7315339552,-1.64
27801521\O,1.6958780594,2.7315339552,1.6427801521\C,-2.5787562821,-0.2
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3,3.2887305967,0.2613639868\H,-6.8645987497,1.3020382794,1.6928724876\H,
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pole=0.,0.,0.\PG=CI [X(C28H20K2O4S2)]\@

Conformer C of Table 1

1\1\GINC-MILLER4\FOpt\RB3LYP\6-31G(d)\C28H20K2O4S2\JHODGSON\16-Aug-
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Conformer D of Table 1

1\1\GINC-MILLER4\FOpt\RB3LYP\6-31G(d)\C28H20K2O4S2\JHODGSON\17-Aug-2012\0\# rb3lyp/6-31G* opt freq=noraman\wsp_cs6s_6drb3\0,1\C,-0.4036993946,5.0831488207,-0.7268292573\C,0.4036993946,-5.0831488207,0.7268292573\C,-0.4069882527,1.3135161784,-0.4025965966\C,0.4069882527,-1.3135161784,0.4025965966\C,-0.0395383289,3.7467504556,-0.3494600825\C,0.0395383289,-3.7467504556,0.3494600825\C,0.3208758547,6.1565698431,-0.292276481\C,-0.3208758547,-6.1565698431,0.292276481\C,-0.7596868586,2.6366879623,-0.7675360372\C,0.7596868586,-2.6366879623,0.7675360372\C,0.7668973755,1.1223141463,0.4489453547\C,-0.7668973755,-1.1223141463,-0.4489453547\C,1.1170081979,3.5580357714,0.5017276101\C,-1.1170081979,-3.5580357714,-0.5017276101\C,1.8460944135,4.7158345631,0.9360478516\C,-1.8460944135,-4.7158345631,-0.9360478516\C,1.4630641592,5.969960238,0.5531472094\C,-1.4630641592,-5.969960238,-0.5531472094\C,1.4807695309,2.2708870401,0.8714019088\C,-1.4807695309,-2.2708870401,-0.8714019088\C,-1.1553200786,0.1872387219,-0.8287794639\C,1.1553200786,-0.1872387219,0.8287794639\S,2.5986447929,-0.4221352796,1.8815897325\S,-2.5986447929,0.4221352796,-1.8815897325\C,3.959924906,-0.3444693025,0.6234710466\C,-3.959924906,0.3444693025,-0.6234710466\C,5.3074669588,-0.506032542,1.3190064354\C,-5.3074669588,0.506032542,-1.3190064354\C,6.5048836394,-0.4217528544,0.3521168351\C,-6.5048836394,0.4217528544,-0.3521168351\O,7.6502647898,-0.6309242914,0.8516437191\O,-7.6502647898,0.6309242914,-0.8516437191\O,-6.2711546307,0.1455220275,0.8630409112\O,6.2711546307,-0.1455220275,-0.8630409112\K,-8.7351971567,0.2715031382,1.4014016225\K,8.7351971567,-0.2715031382,-1.4014016225\H,-3.8020459846,1.1380847357,0.1105865108\H,3.8020459846,-1.1380847357,-0.1105865108\H,2.3360959648,2.1306075537,1.5230481015\H,-2.3360959648,-2.1306075537,-1.5230481015\H,1.6263458399,-2.7767563168,1.4037077191\H,-1.6263458399,2.7767563168,-1.4037077191\H,2.7121230653,4.5703891176,1.577506159\H,-2.7121230653,-4.5703891176,-1.577506159\H,1.2713751216,-5.2202954276,1.3678358298\H,-1.2713751216,5.2202954276,-1.3678358298\H,2.0234441613,6.8389514752,0.8880254933\H,-2.0234441613,-6.8389514752,-0.8880254933\H,-0.0355588382,-7.1636729697,0.5848666351\H,0.0355588382,7.1636729697,-0.5848666351\H,3.9066585454,0.6129700058,0.1010909693\H,-3.9066585454,-0.6129700058,-0.1010909693\H,5.4464538765,0.2672601678,2.0859586181\H,-5.4464538765,-0.2672601678,-2.0859586181\H,5.3694359644,-1.4654260933,1.8468699453\H,-5.3694359644,1.4654260933,-1.8468699453\\Version=AM64L-G03Rev E.01\State=1-AG\HF=-3376.2833812\RMSD=9.369e-09\RMSF=3.381e-06\Thermal=0.\Dipole=0.,0.,0.\PG=CI [X(C28H20K2O4S2)]\@

Conformer E of Table 1

1\1\GINC-MILLER4\FOpt\RB3LYP\6-31G(d)\C28H20K2O4S2\JHODGSON\16-Aug-2012\0\# rb3lyp/6-31G* opt freq=noraman\wsp_cs5s_6drb3\0,1\C,0.7339142084,-3.6473191261,-0.5680508722\C,-0.7339142084,3.6473191261,0.5680508

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72471,-0.0523125163\C,-5.580695612,-0.5545972471,0.0523125163\O,-6.101
9915388,-1.4578916632,-0.6669259154\O,6.1019915388,1.4578916632,0.6669
259154\O,-6.0680248915,0.6013058097,0.2476071554\O,6.0680248915,-0.601
3058097,-0.2476071554\K,7.9529257955,-0.1054417326,1.3602933558\K,-7.9
529257955,0.1054417326,-1.3602933558\H,3.6355892435,-1.1510093113,-1.0
929765556\H,-3.6355892435,1.1510093113,1.0929765556\H,4.4073102355,-0.
3784125767,-2.4711701339\H,-4.4073102355,0.3784125767,2.4711701339\H,4.
.3651642133,1.8371231257,-1.2783700461\H,-4.3651642133,-1.8371231257,1.
.2783700461\H,1.7455426769,-2.3536813529,-1.9324861468\H,-1.7455426769
,2.3536813529,1.9324861468\H,1.4179440134,2.6006356267,-1.8875079202\H
, -1.4179440134,-2.6006356267,1.8875079202\H,3.515653182,1.1150604552,0.
.0703448425\H,-3.515653182,-1.1150604552,-0.0703448425\H,1.9453782379,
-4.8123610181,-1.9469197598\H,-1.9453782379,4.8123610181,1.9469197598\H
H,1.2245132927,5.0603442201,-1.9074848914\H,-1.2245132927,-5.060344220
1,1.9074848914\H,1.3035855308,-6.9978986611,-0.9941028876\H,-1.3035855
308,6.9978986611,0.9941028876\H,0.2776664482,7.1220761884,-0.932139189
9\H,-0.2776664482,-7.1220761884,0.9321391899\\Version=AM64L-G03RevE.01
\State=1-AG\HF=-3376.2829138\RMSE=6.758e-09\RMSE=4.974e-06\Thermal=0.
Dipole=0.,0.,0.\PG=CI [X(C28H20K2O4S2)]\@

Conformer F of Table 1

1\1\GINC-MILLER1\FOpt\RB3LYP\6-31G(d)\C28H20K2O4S2\JHODGSON\16-Aug-
2012\0\#\rb3lyp/6-31G* opt freq=norman\wsp_cs4s_6drb3\0,1\C,0.4487984
334,2.8184083697,-0.0193093148\C,-0.4487984334,-2.8184083697,0.0193093
148\C,0.1919738501,1.4238476634,-0.0141144114\C,-0.1919738501,-1.42384
76634,0.0141144114\C,1.9878219237,4.7587194646,-0.0557315938\C,-1.9878
219237,-4.7587194646,0.0557315938\C,1.732721176,3.3460664837,-0.043751
7544\C,-1.732721176,-3.3460664837,0.0437517544\C,1.1225277841,-0.88924
48132,0.0118580829\C,-1.1225277841,0.8892448132,-0.0118580829\C,-1.338

2012076,-0.5122787204,0.0052283674\C,1.3382012076,0.5122787204,-0.0052
283674\C,2.8625628254,2.4427480131,-0.064989553\C,-2.8625628254,-2.442
7480131,0.064989553\C,2.6377023163,1.073429229,-0.0280128554\C,-2.6377
023163,-1.073429229,0.0280128554\C,3.2675331413,5.2356082673,-0.102019
2819\C,-3.2675331413,-5.2356082673,0.1020192819\C,-3.1319475766,2.2504
45355,1.6103366841\C,3.1319475766,-2.250445355,-1.6103366841\C,4.19118
55243,2.9844439713,-0.1327721645\C,-4.1911855243,-2.9844439713,0.13277
21645\C,4.3840018233,4.3371379796,-0.1494922041\C,-4.3840018233,-4.337
1379796,0.1494922041\C,-4.285418208,1.3275580261,2.0199219412\C,4.2854
18208,-1.3275580261,-2.0199219412\C,-5.3691003606,1.3401391739,0.92560
33253\C,5.3691003606,-1.3401391739,-0.9256033253\S,-2.5169007778,2.026
5216171,-0.1396378728\S,2.5169007778,-2.0265216171,0.1396378728\O,5.75
78291457,-2.4786992085,-0.5345643575\O,-5.7578291457,2.4786992085,0.53
45643575\O,5.7027966158,-0.2332835111,-0.4020121435\O,-5.7027966158,0.
2332835111,0.4020121435\K,-5.6952607026,1.5072600803,-1.8247798944\K,5.
.6952607026,-1.5072600803,1.8247798944\H,-0.3973182263,3.4955723336,-0.
.014022946\H,0.3973182263,-3.4955723336,0.014022946\H,1.1403494804,5.4
398862785,-0.0318529921\H,-1.1403494804,-5.4398862785,0.0318529921\H,-
2.264887182,2.160467638,2.2700456789\H,2.264887182,-2.160467638,-2.270
0456789\H,-3.4795643709,3.2857922984,1.6186514113\H,3.4795643709,-3.28
57922984,-1.6186514113\H,-4.7066959116,1.718310483,2.9564502189\H,4.70
66959116,-1.718310483,-2.9564502189\H,-3.5020033416,-0.4216820846,0.03
63864575\H,3.5020033416,0.4216820846,-0.0363864575\H,-3.9437717299,0.3
059911357,2.201232021\H,3.9437717299,-0.3059911357,-2.201232021\H,-5.0
209973441,-2.2845338421,0.1974342078\H,5.0209973441,2.2845338421,-0.19
74342078\H,3.4489399808,6.3073092776,-0.1128825991\H,-3.4489399808,-6.
3073092776,0.1128825991\H,-5.389664268,-4.7453307365,0.2082119543\H,5.
389664268,4.7453307365,-0.2082119543\\Version=AM64L-G03RevE.01\State=1
-AG\HF=-3376.290142\RMSE=5.119e-09\RMSE=7.834e-06\Thermal=0.\Dipole=0.
,0,0.\PG=CI [X(C28H20K2O4S2)]\@

Two molecule stack of conformer B (c.f. Fig. 6 (a))

1\1\GINC-MILLER6\FOpt\RB3LYP\6-31G(d)\C56H40K4O8S4\JHODGSON\14-Aug-
2012\0\# rb3lyp/6-31G* opt\dimolwsp_cs1c5_6drb3\0,1\C,2.7265560086,5.6
051514537,1.9901683638\C,2.8907821569,4.3642147282,1.2884009911\C,2.84
74198509,4.3736256073,-0.1594066394\C,2.6452469239,5.6252769076,-0.833
0096383\C,2.4974030936,6.7835117929,-0.1236568372\C,2.5369022345,6.773
6070795,1.3091344323\C,3.0666734215,3.1588483015,1.9520510664\C,3.2208
967601,1.9238636238,1.2746965721\C,3.1998166911,1.9336220789,-0.189374
9924\C,2.9989392093,3.1751199294,-0.8464667143\C,3.3478298601,0.720352
3239,-0.908948197\C,3.4560928998,-0.5123988311,-0.2113232116\C,3.48752
4985,-0.5215400072,1.2526498669\C,3.3573772199,0.6961969492,1.96957638
38\C,3.5511959859,-1.7528453459,-0.8915068505\C,3.6717518803,-2.970071
0682,-0.2270072012\C,3.7372557752,-2.9801145157,1.2219194971\C,3.65009
62385,-1.7700437224,1.9092273336\C,3.7513020693,-4.2183208677,-0.93235

05677\C,3.8937266928,-5.3960890699,-0.2537379373\C,3.9669787025,-5.406
4035856,1.1779252986\C,3.892393814,-4.2423564536,1.8919163944\S,3.3951
710562,0.6857802988,3.7684958859\C,1.7520664105,-0.0423805694,4.248584
6806\C,0.5421947781,0.8707884631,4.0673438979\C,0.112936231,1.08683781
79,2.6022867802\O,-0.2789336278,2.2312915153,2.2737431714\S,3.32446723
53,0.7299836508,-2.7063818725\C,4.9634741564,1.5020980788,-3.146329613
9\O,0.1747540611,0.0749227829,1.8270484652\K,0.2420643989,-1.983528199
1,0.3288649277\O,0.3561848642,-2.4334616284,-2.2709235468\C,-0.0538914
604,-1.2932017685,-2.592359438\O,-0.0928274189,-0.2753463393,-1.824698
3081\C,-0.5509823965,-1.0933072481,-4.0377729101\C,-1.7684181281,-0.18
22613507,-4.1607726159\S,-3.3576130591,-0.8999961032,-3.5048313959\C,-
3.2831080145,-0.6871061533,-1.7196871332\C,-3.4375397029,0.6047008276,
-1.1507834631\C,-3.5123739898,0.7508978132,0.3040689046\C,-3.480800959
3,-0.4014354423,1.1302324664\C,-3.2268740292,-1.6775776262,0.566253790
2\C,-3.1373833004,-1.8276191299,-0.8857841439\C,-3.5421307873,1.780425
4656,-1.9413382078\C,-3.6566940755,3.0546002812,-1.3887745785\C,-3.686
9211133,3.1963998331,0.0525493984\C,-3.635590102,2.0556069706,0.843572
4746\C,-3.736290848,4.2402929466,-2.1941957091\C,-3.8325721801,5.47382
62278,-1.6121167387\C,-3.8555033422,5.6140253767,-0.1863839867\C,-3.78
47103911,4.5117562772,0.6178002054\C,-3.0309140667,-2.8236186667,1.375
1805971\C,-2.7606201479,-4.0797667512,0.8440055527\C,-2.6855003125,-4.
2310633745,-0.5950047855\C,-2.8758264759,-3.1187379034,-1.4061182858\C
, -2.5403874267,-5.2333400662,1.6703865696\C,-2.2656585299,-6.450045059
5,1.1121656716\C,-2.1865736331,-6.5985714197,-0.3111051024\C,-2.388319
6172,-5.5273791848,-1.1348399809\S,-3.7398118183,-0.2338744968,2.90066
37618\C,-5.4476237872,-0.9415120092,3.1213074711\C,-6.5921560982,-0.04
51106088,2.6545174237\C,-6.7726095947,-0.0119553255,1.1213625268\O,-7.
1719276888,1.0690059204,0.6042314109\O,-6.5115644026,-1.0829257264,0.4
933737377\K,-6.5240176768,0.1976179543,-1.7321285659\K,-0.211587317,1.
7902528609,-0.3232415021\H,-2.0084850365,0.0168544444,-5.2111915195\H,
0.2704704324,-0.6226309336,-4.5993359879\H,-1.5827382498,0.7685857307,
-3.6588748551\H,-0.7382351024,-2.0698094052,-4.4927922481\H,-3.5186416
543,1.6847553463,-3.0212789061\H,-3.0752737455,-2.7019530867,2.4519231
526\H,-2.7846272152,-3.2331030765,-2.4791115509\H,-3.6770175319,2.1606
095275,1.9205179648\H,-3.7164885661,4.136953569,-3.2768964033\H,-2.605
0929296,-5.1173379233,2.7497932982\H,-2.3243669301,-5.6347115012,-2.21
44631075\H,-3.8009320395,4.6071247589,1.7000356646\H,-3.8931115427,6.3
638660175,-2.2328058982\H,-2.1081583992,-7.3184947871,1.746067011\H,-1.
.9645436683,-7.5758006068,-0.7308959884\H,-3.9321307166,6.6061350726,0
.2489485863\H,-5.4947681988,-1.9023125233,2.6045342431\H,-5.4907492425
, -1.1140169124,4.2025323051\H,-7.5237233274,-0.4544038,3.0752287374\H,
6.4900427101,0.9752144802,3.0349718905\H,2.9578948535,3.1827384968,-1
.9300868572\H,3.7086098182,-1.7766008572,2.9924156572\H,3.5239590478,-
1.7481513199,-1.9735110905\H,3.065950217,3.1511773634,3.0351105733\H,2
.6215762699,5.6314312049,-1.9203408289\H,3.9410294871,-4.2516038104,2.
9786354076\H,3.6927710651,-4.1998582262,-2.0167106016\H,2.7543548755,5

.5914642152,3.0766279494\H,2.3516697845,7.7266008918,-0.6435039064\H,4
.0806131655,-6.3549996532,1.6959485613\H,3.9524170323,-6.3356203352,-0
.7954505225\H,2.4143917327,7.708082475,1.8495746762\H,-0.3083010155,0.
3953842481,4.5797407062\H,0.7042129856,1.8425477368,4.5415475622\H,1.6
092864329,-0.9739438925,3.6967670504\H,1.9044750551,-0.2854905363,5.30
62918\H,4.7599098944,2.0202355898,-4.089868163\H,5.2090008368,2.238597
0109,-2.3793100199\C,6.108124597,0.5034764444,-3.2942440126\H,6.967908
2104,1.0449699504,-3.7179839059\C,6.5576311519,-0.0960407635,-1.946713
2148\H,5.8539455925,-0.3021305814,-3.9889117239\O,6.8574289523,-1.3231
648536,-1.9217334196\O,6.579111085,0.6945950662,-0.954774681\K,6.66425
61007,-1.3095237758,0.6369493155\Version=AM64L-G03RevE.01\State=1-A\H
F=-6752.6639511\RMSD=4.455e-09\RMSF=2.482e-05\Thermal=0.\Dipole=0.0869
97,-0.5000852,-0.0967594\PG=C01 [X(C56H40K4O8S4)]\@

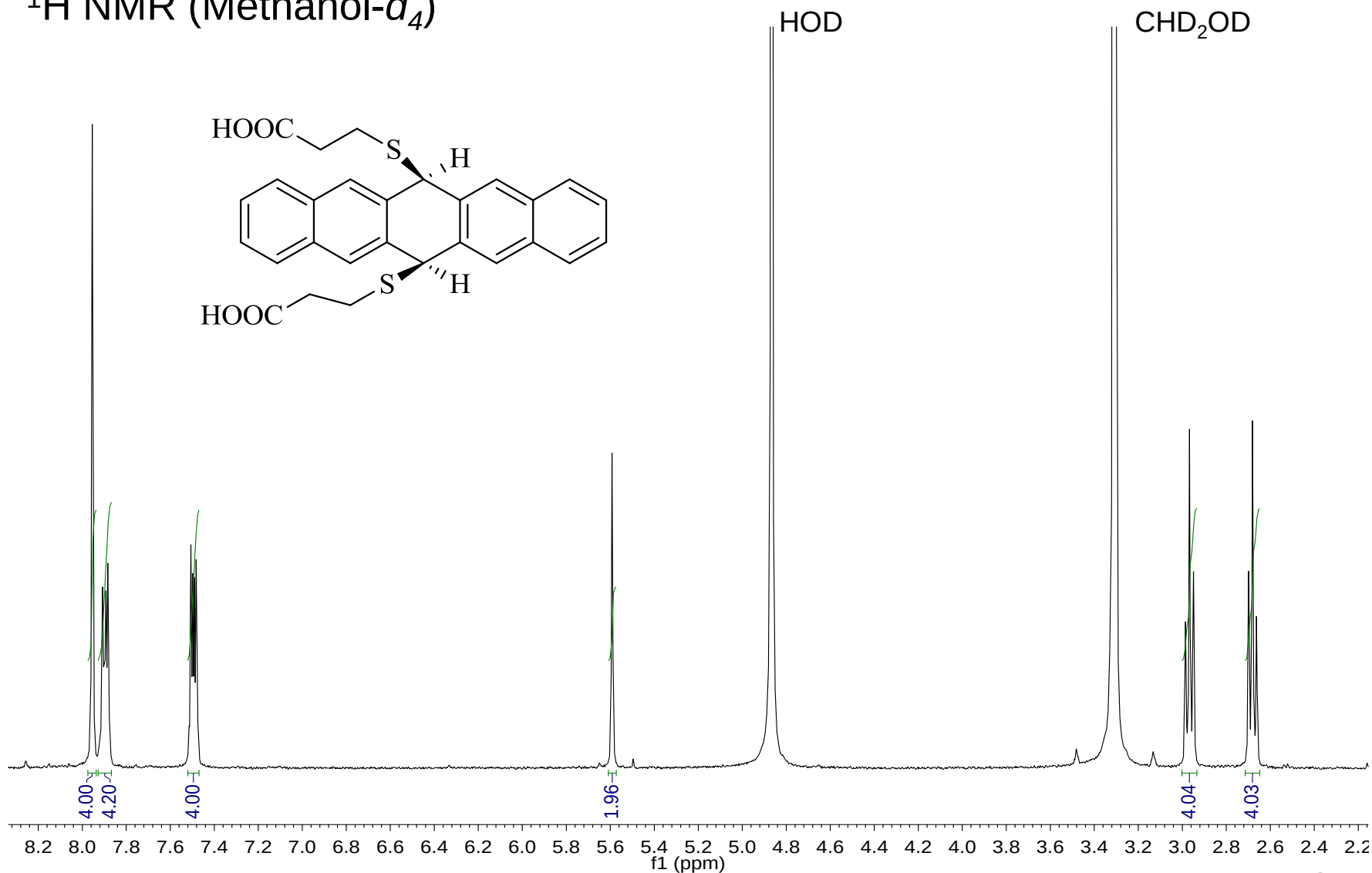
Two molecule stack of conformer E (c.f. Fig. 6 (b))

1\1\GINC-MILLER4\FOpt\RB3LYP\6-31G(d)\C56H40K4O8S4\JHODGSON\11-Aug-
2012\0\# rb3lyp/6-31G* opt\dimolwsp_cs2cc_6drb3\0,1\C,-0.1032428717,1.
4679680396,4.3907837252\C,-0.6413361936,0.6771061322,3.3207169043\C,-1
.3511014107,1.3462413076,2.2492306437\C,-1.4963250657,2.7755159685,2.3
04188968\C,-0.9694874264,3.4846249372,3.3476866328\C,-0.2612102378,2.8
246227774,4.4036220908\C,-0.5119789452,-0.7040769544,3.2886742004\C,-1
.0687869268,-1.5022043437,2.2599018881\C,-1.7846929133,-0.8297281634,1
.1739271548\C,-1.878822973,0.5850978985,1.2130296388\C,-2.363797601,-1
.60473703,0.1364786238\C,-2.3277016155,-3.0222060992,0.1867570047\C,-1
.6315723809,-3.6919336937,1.2852940595\C,-0.9605342957,-2.9164270723,2
.2644377566\C,-2.9403031552,-3.829293369,-0.8033859558\C,-2.9396814058
, -5.2160695747,-0.7485838197\C,-2.2769406016,-5.8779432117,0.355736602
6\C,-1.6422084268,-5.108723426,1.3204403801\C,-2.2909317493,-7.3124697
378,0.4051193866\C,-2.9105803143,-8.0421403508,-0.569555359\C,-3.56183
19966,-7.3871853936,-1.6654272976\C,-3.5745408492,-6.0237050397,-1.751
0719438\S,0.037520723,-3.7291488638,3.5282977543\C,1.7373915681,-3.554
0899702,2.7899781902\C,1.9694556684,-4.4424175545,1.573544037\C,3.3473
746564,-4.2604739567,0.9057164118\O,4.269266466,-3.6820764148,1.553032
748\S,-3.0590204525,-0.7929317422,-1.3134779644\C,-4.8783694714,-0.797
8602613,-0.9722253136\C,-5.3420226303,0.4192257608,-0.1765724707\C,-6.
8592440854,0.4890693081,0.0378348833\O,-7.3171244572,1.5481958264,0.60
70429743\O,3.4517142208,-4.7188960681,-0.2737580792\O,-7.5768837711,-0
.475455623,-0.3337800218\K,5.8015291841,-3.7234016971,-0.568542834\K,-
9.6980548291,0.5499705862,0.5377022618\H,1.8955940374,-2.4989053594,2.
5521356207\H,-5.1467391537,-1.7330370718,-0.4762593374\H,2.4206984909,
-3.8120637757,3.6040947771\H,-5.352016275,-0.8051285601,-1.9586138251\
H,1.8721918674,-5.4998970178,1.8537927059\H,-5.0102926948,1.3327343121
, -0.6880091501\H,0.0101058446,-1.2039611091,4.0966685066\H,-3.41915861
24,-3.337602833,-1.6423076128\H,-1.1324820939,-5.6018430059,2.14009447
98\H,-2.3890250192,1.0887794399,0.3998798201\H,1.2062994309,-4.2625174

759,0.8107322966\H,-4.8652743994,0.4260833847,0.8132333193\H,0.4335214
245,0.9599788461,5.1885002035\H,-4.066649947,-5.5231010833,-2.5817801
264\H,-1.7921950372,-7.8051272243,1.2364533854\H,-2.0399253246,3.29370
4971,1.5163819811\H,0.153103407,3.415053146,5.2170884527\H,-4.04605497
13,-7.9877411093,-2.4312604337\H,-2.9120515433,-9.1280532587,-0.522698
0822\H,-1.0828248589,4.5652250485,3.3753172547\C,3.6711206991,6.073516
2291,1.6099593447\C,3.0037737147,5.2500493778,0.6420527222\C,2.3175543
678,5.8939036648,-0.4585804488\C,2.3412064261,7.3268550873,-0.53898560
35\C,2.9921134853,8.0719379962,0.4031040325\C,3.6669389203,7.434936045
5,1.4952576461\C,2.9945656277,3.8647171024,0.7264965767\C,2.3509122746
,3.0420221195,-0.2305041766\C,1.6334502594,3.694160486,-1.3259123933\C
,1.6527977094,5.109742442,-1.3905153046\C,0.9340097447,2.9035079809,-2
.2726207212\C,1.0350617031,1.4891189775,-2.2429146135\C,1.7730744403,0
.833817741,-1.1611910655\C,2.3766319862,1.6256395818,-0.1507161091\C,0
.4489860296,0.6741112396,-3.2417254064\C,0.5735876687,-0.7078149557,-3
.2517472081\C,1.3109061234,-1.3594467227,-2.1880419553\C,1.8640285825,
-0.581609452,-1.1778122318\C,1.4541855684,-2.7894399659,-2.2231895982\
C,0.8957434031,-3.516082718,-3.2376874659\C,0.1571664373,-2.8735933091
, -4.2836250733\C,0.0032455703,-1.5164669407,-4.2913454188\S,3.08421169
7,0.8377600987,1.3060183094\C,4.9010322432,0.8300641652,0.9520894689\C
,5.3571108538,-0.4072024601,0.1834347609\C,6.8732755983,-0.48505236,-0
.0369426998\O,7.5931861099,0.4899539258,0.3014090489\S,-0.0889176307,3
.6977250532,-3.5281278342\C,-1.7745344154,3.5310849821,-2.7569070302\C
, -1.983459756,4.4281408788,-1.5426254624\C,-3.353850268,4.2578275575,-
0.8563913179\O,-3.4392081513,4.7130171559,0.3257387097\O,7.3277587821,
-1.5608816258,-0.5764956508\O,-4.2896421187,3.6902613347,-1.4935547849
\K,9.709119411,-0.5587056499,-0.5542779283\K,-5.7815439859,3.706074107
6,0.657938038\H,5.1682698064,1.7518221601,0.4311639432\H,-1.9304860871
,2.4778563659,-2.5088232894\H,5.3817530669,0.8607552467,1.9346092524\H
, -2.4722763736,3.7850474736,-3.5599171113\H,5.0250181093,-1.3075909998
,0.7173573805\H,-1.8839784228,5.4832745225,-1.8309224177\H,3.491645547
3,3.3872033912,1.5630206202\H,-0.0926859006,1.1606073671,-4.0449589331
\H,2.3921375731,-1.0723091975,-0.3681062278\H,1.1259299178,5.589991566
1,-2.2069562109\H,4.8754074057,-0.4363432968,-0.8035941068\H,-1.210831
1146,4.248048615,-0.7894196815\H,4.1809140445,5.5867733671,2.438258481
8\H,-0.5552218811,-1.0215306756,-5.0822963041\H,2.0227869412,-3.294498
8373,-1.4448158132\H,1.8246146846,7.8058202879,-1.3674071067\H,4.17587
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524731,0.3329050618\\Version=AM64L-G03RevE.01\State=1-A\HF=-6752.62218
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8,0.0032546\PG=C01 [X(C56H40K4O8S4)]\@

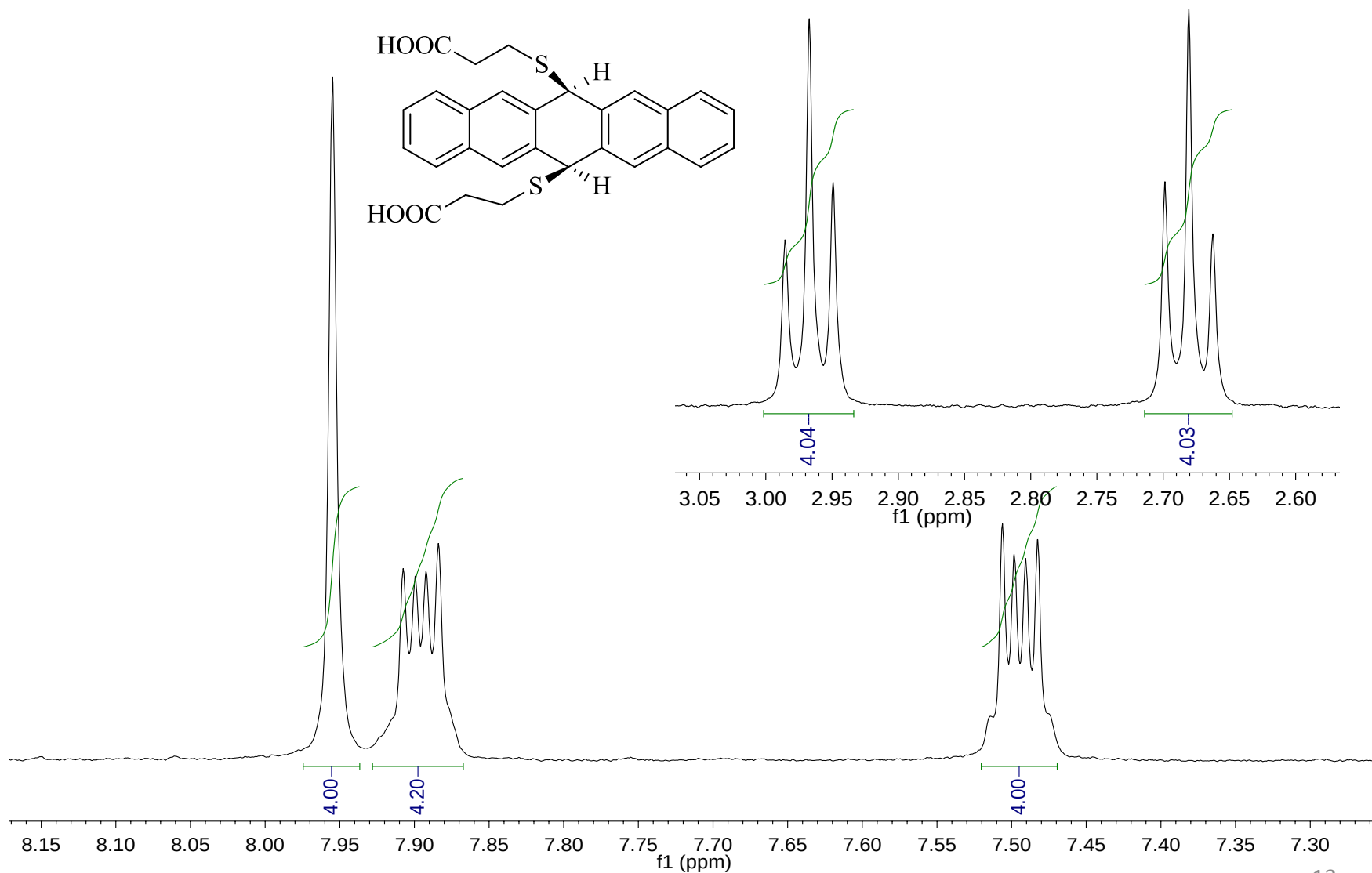
syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfaneydiyl))dipropionic acid (**2**)

^1H NMR (Methanol- d_4)



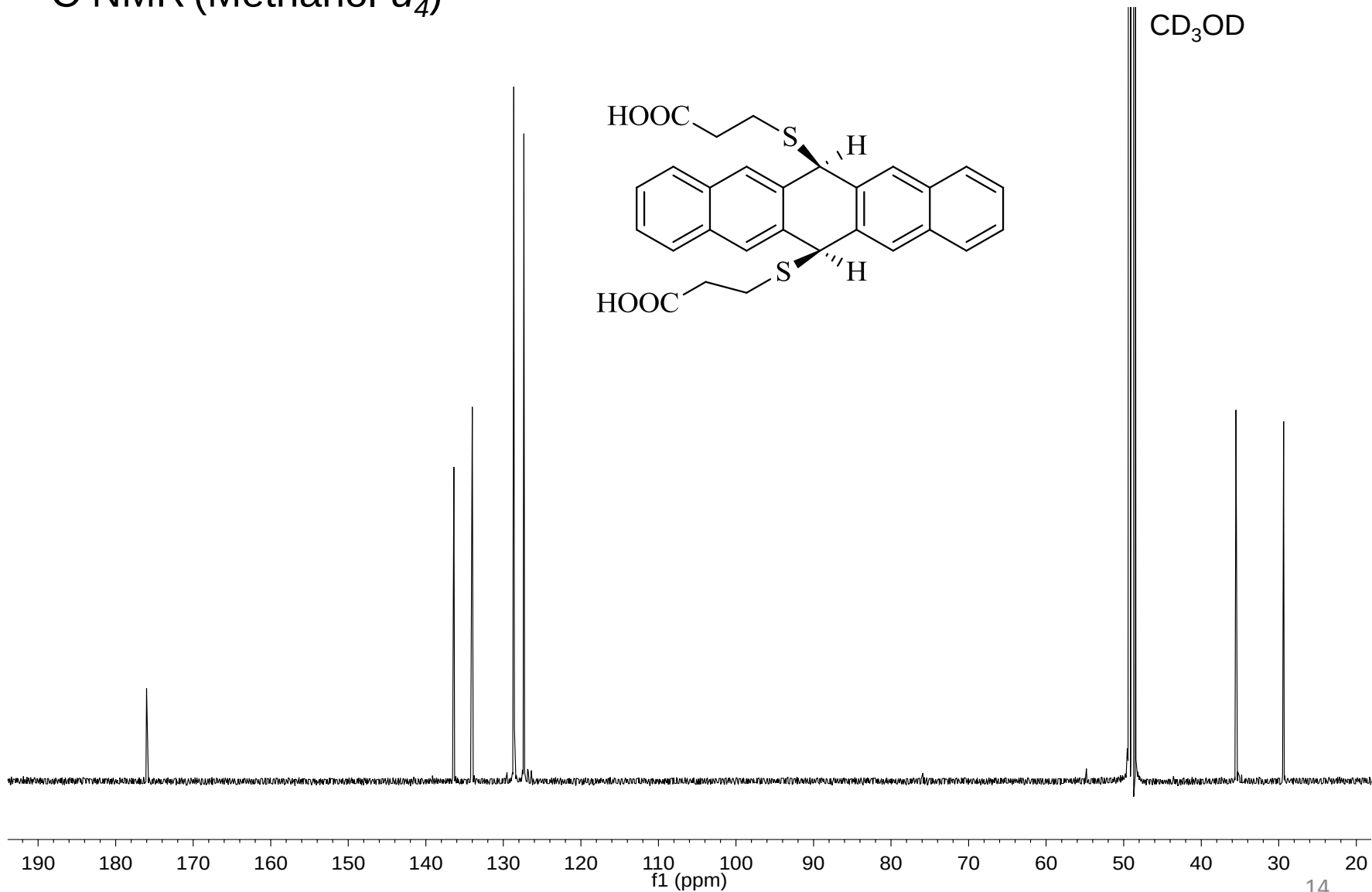
syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfanediyl))dipropionic acid (**2**)

^1H NMR (Methanol- d_4)



syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfaneydiyl))dipropionic acid **(2)**

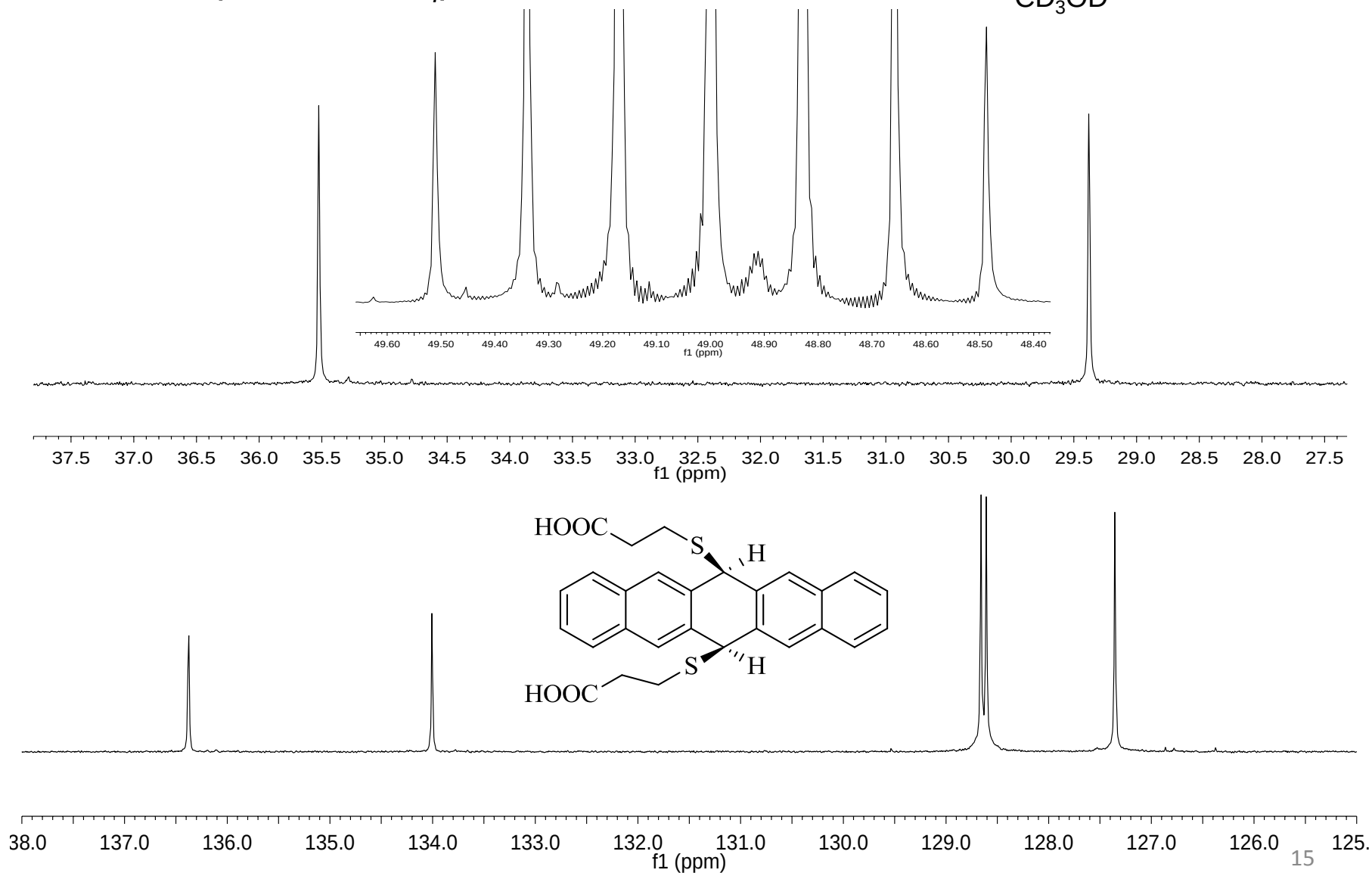
¹³C NMR (Methanol-*d*₄)



syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfaneydiyl))dipropionic acid (**2**)

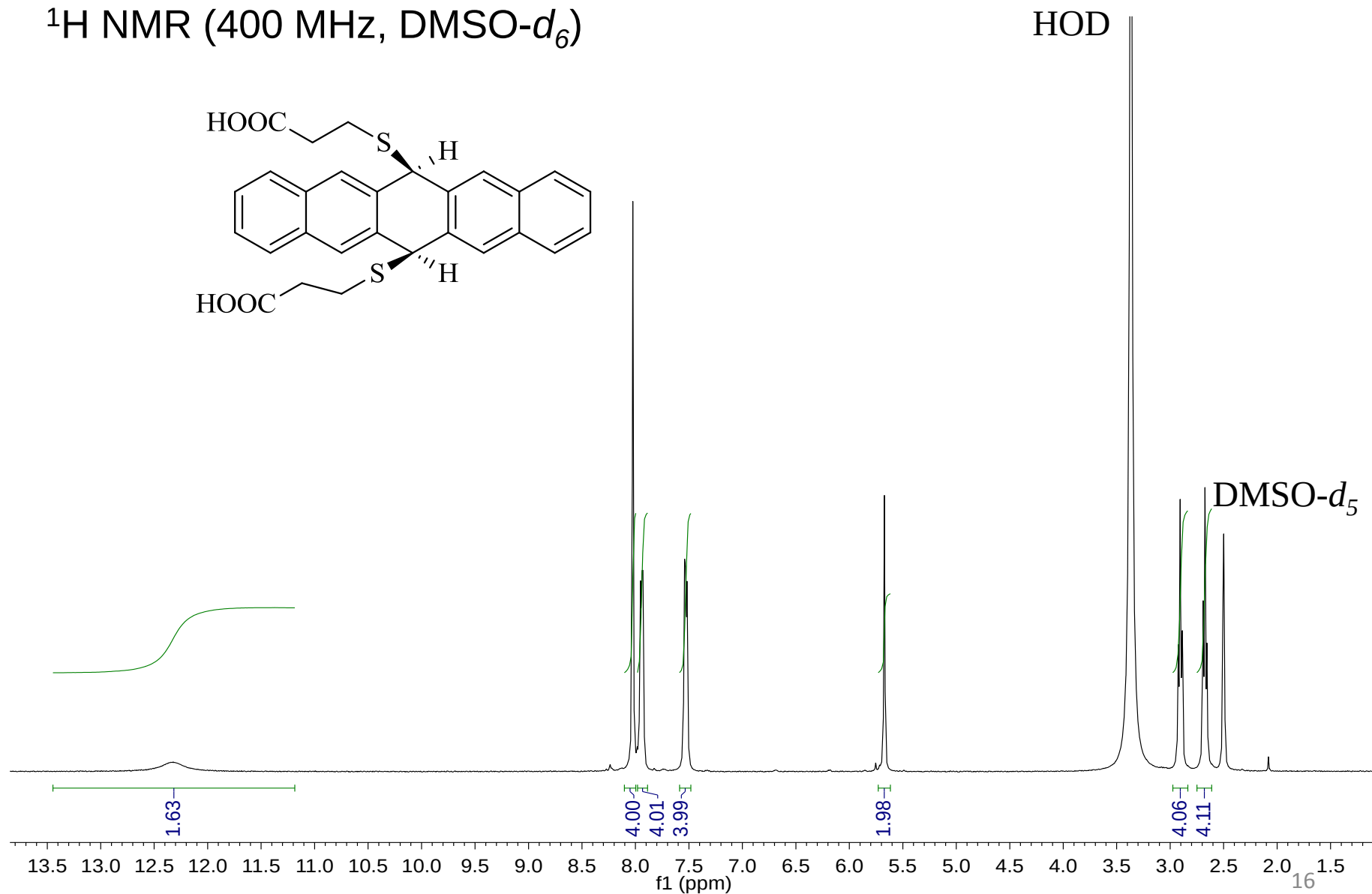
^{13}C NMR (Methanol- d_4)

CD_3OD



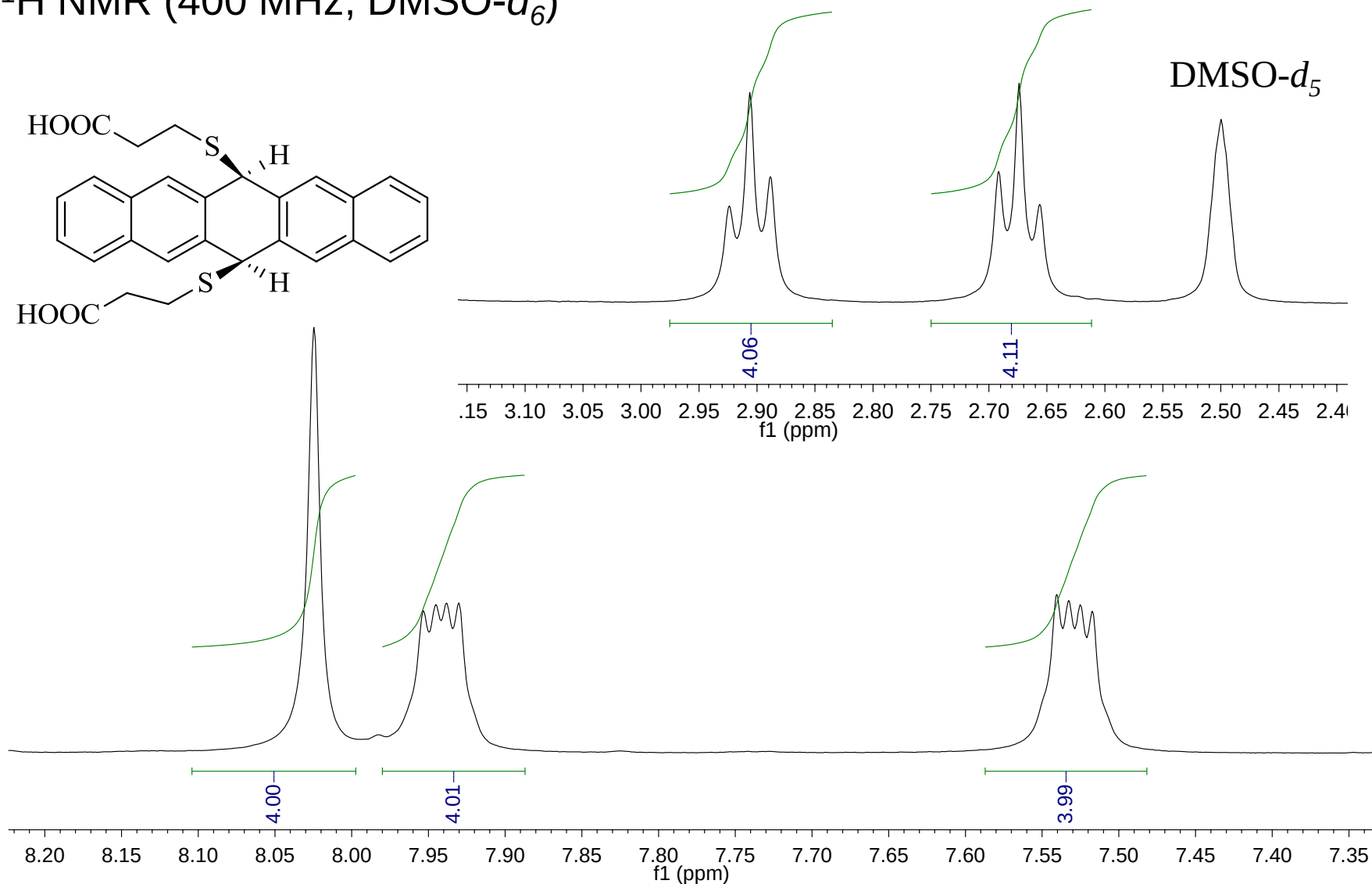
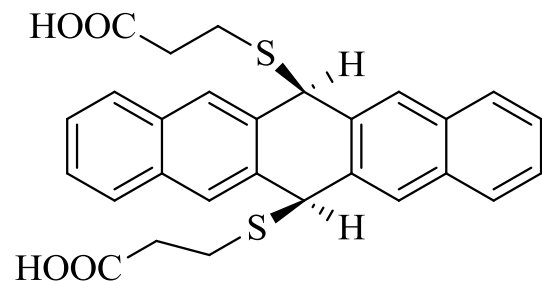
syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfaneydiyl))dipropionic acid (**2**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$)



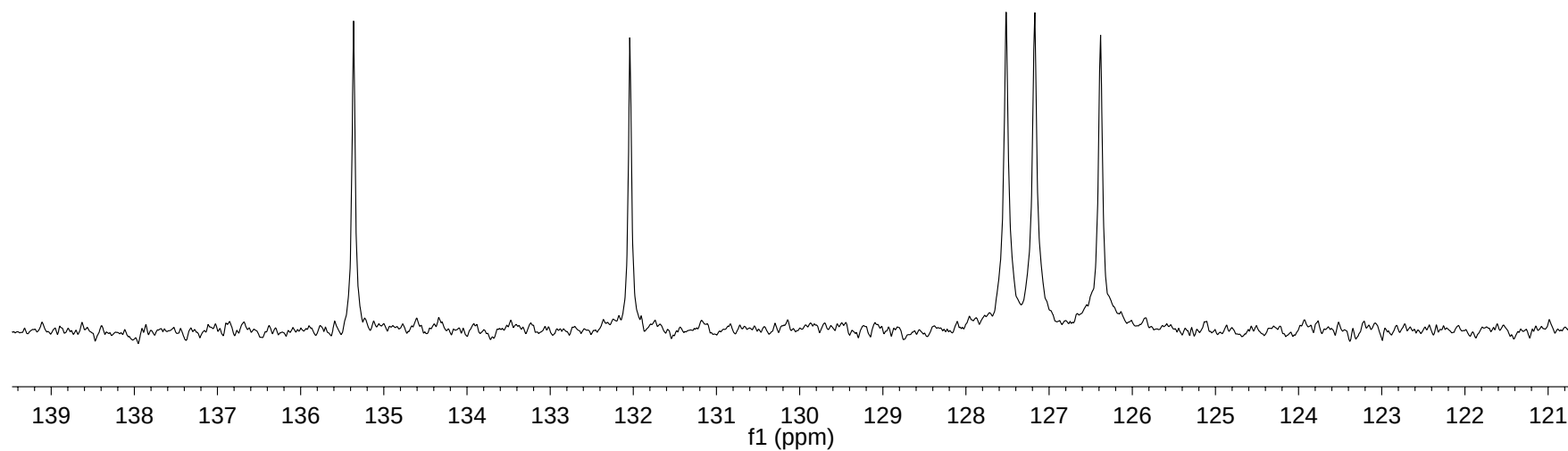
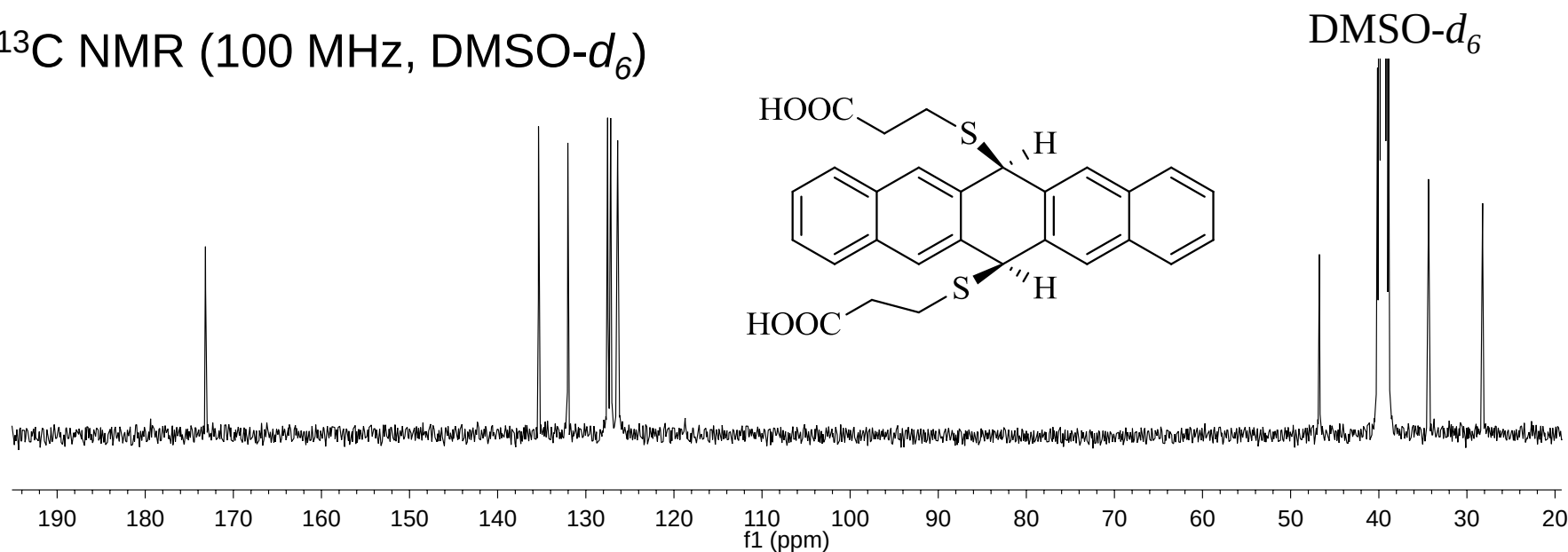
syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfaneydiyl))dipropionic acid (**2**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$)

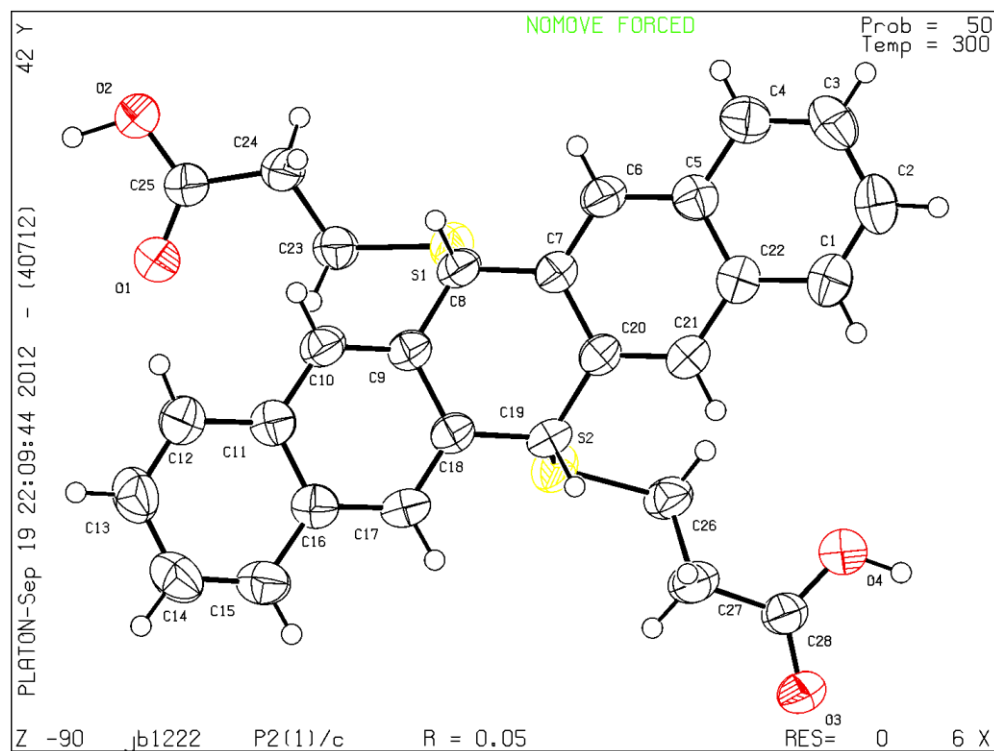
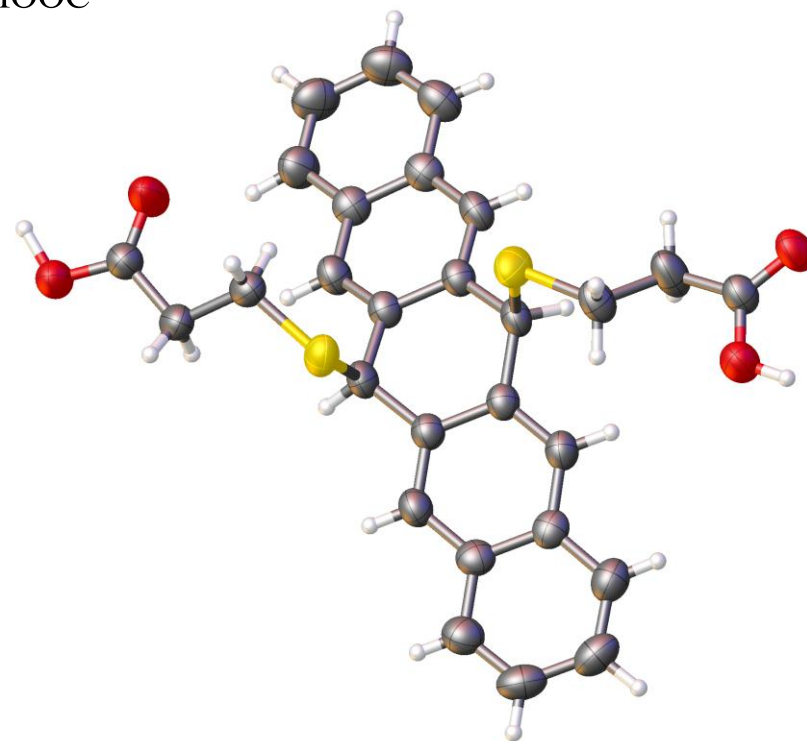
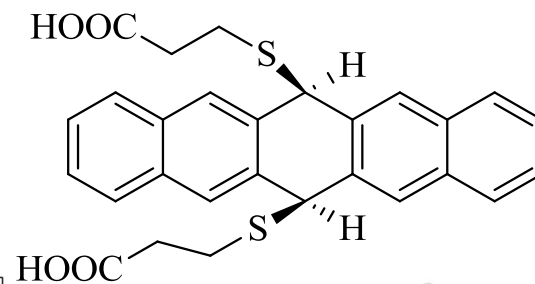


syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfaneydiyl))dipropionic acid (**2**)

^{13}C NMR (100 MHz, $\text{DMSO-}d_6$)

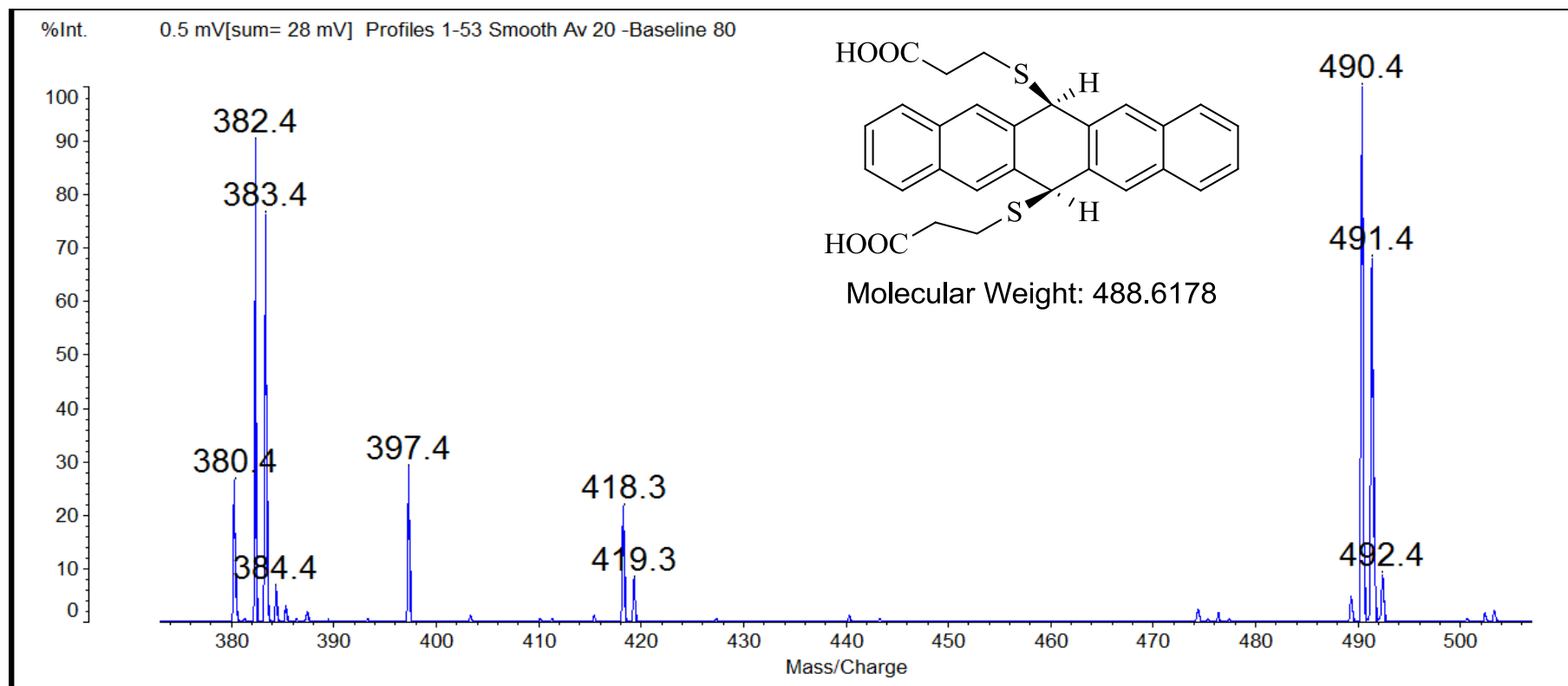


Single crystal X-ray structure of major isomer of **2**:
syn-3,3'-((6,13-dihdropentacene-6,13-diyl)-
bis(sulfanediyl))dipropanoic acid

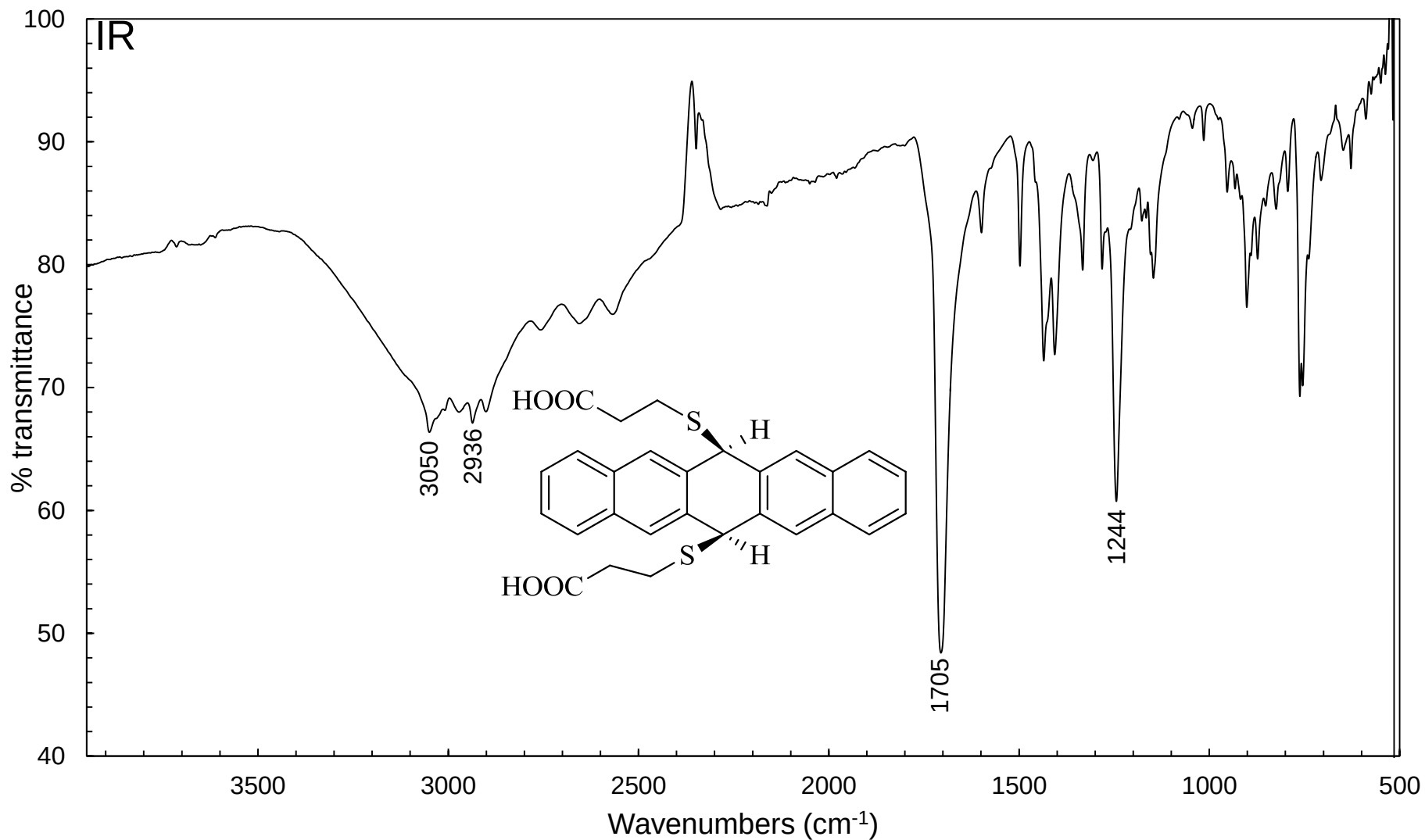


syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfaneydiyl))dipropionic acid (**2**)

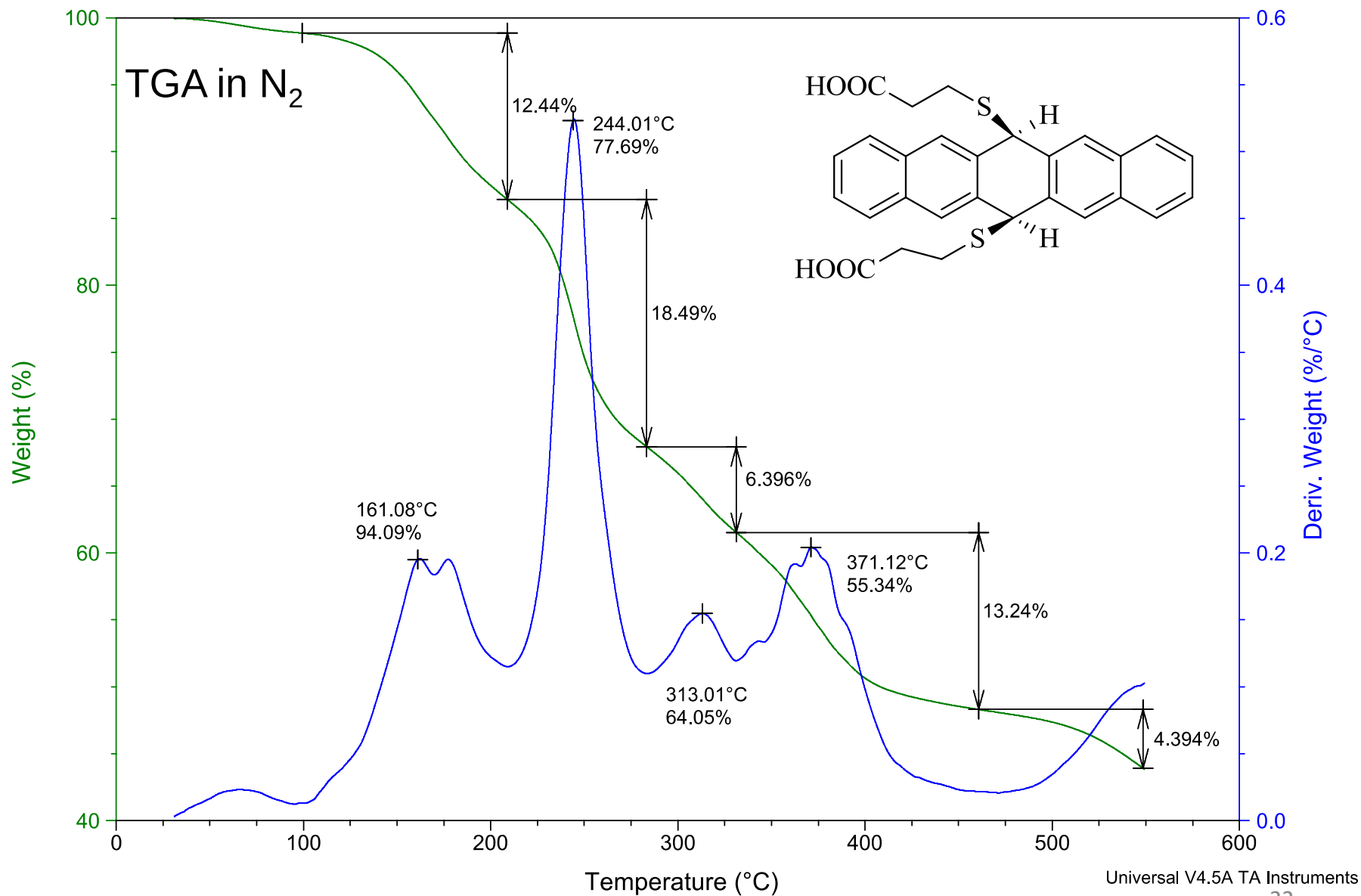
LDI MS



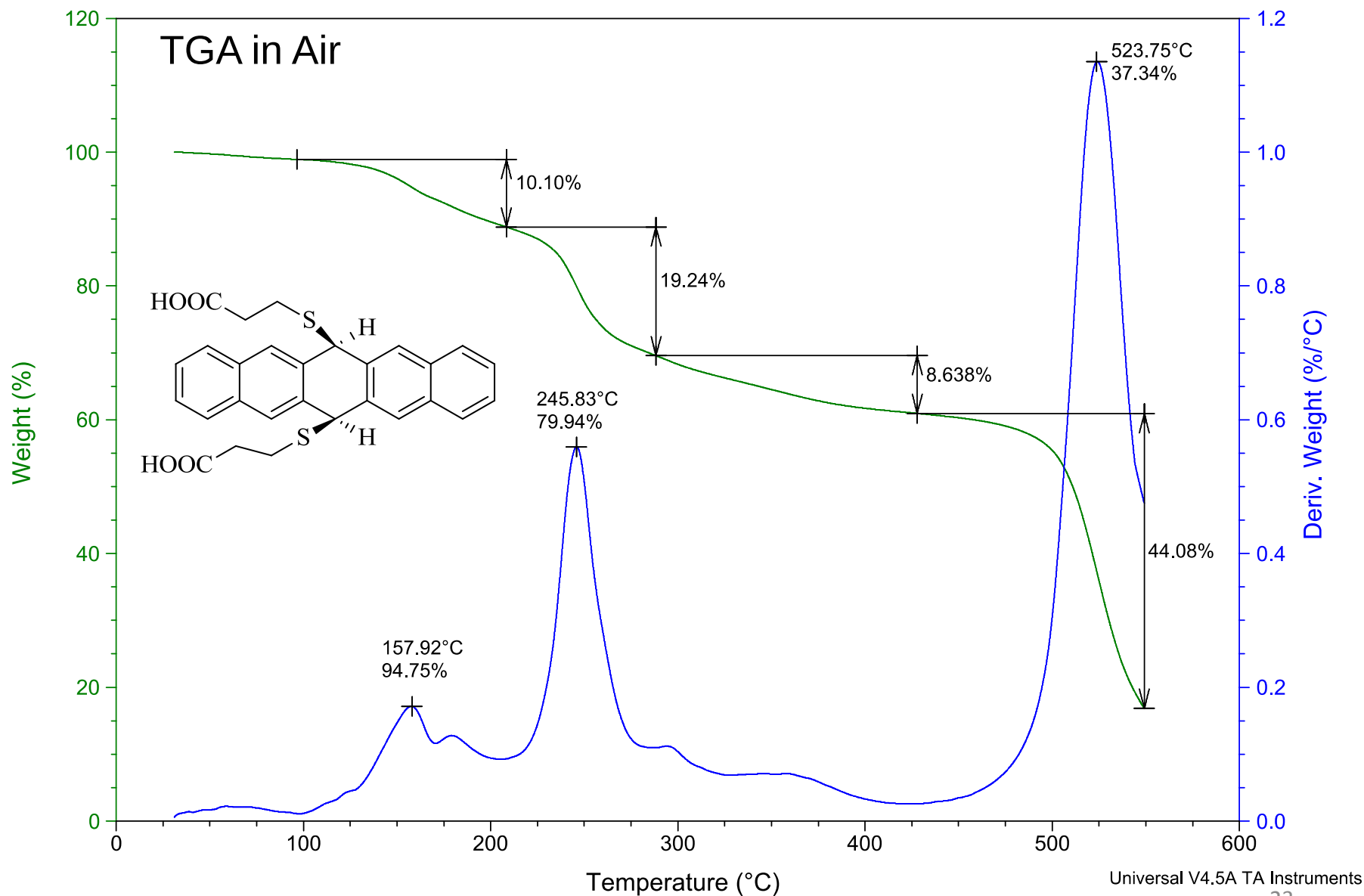
syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfanediyl))dipropionic acid (**2**)



syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfanediyl))dipropionic acid (**2**)

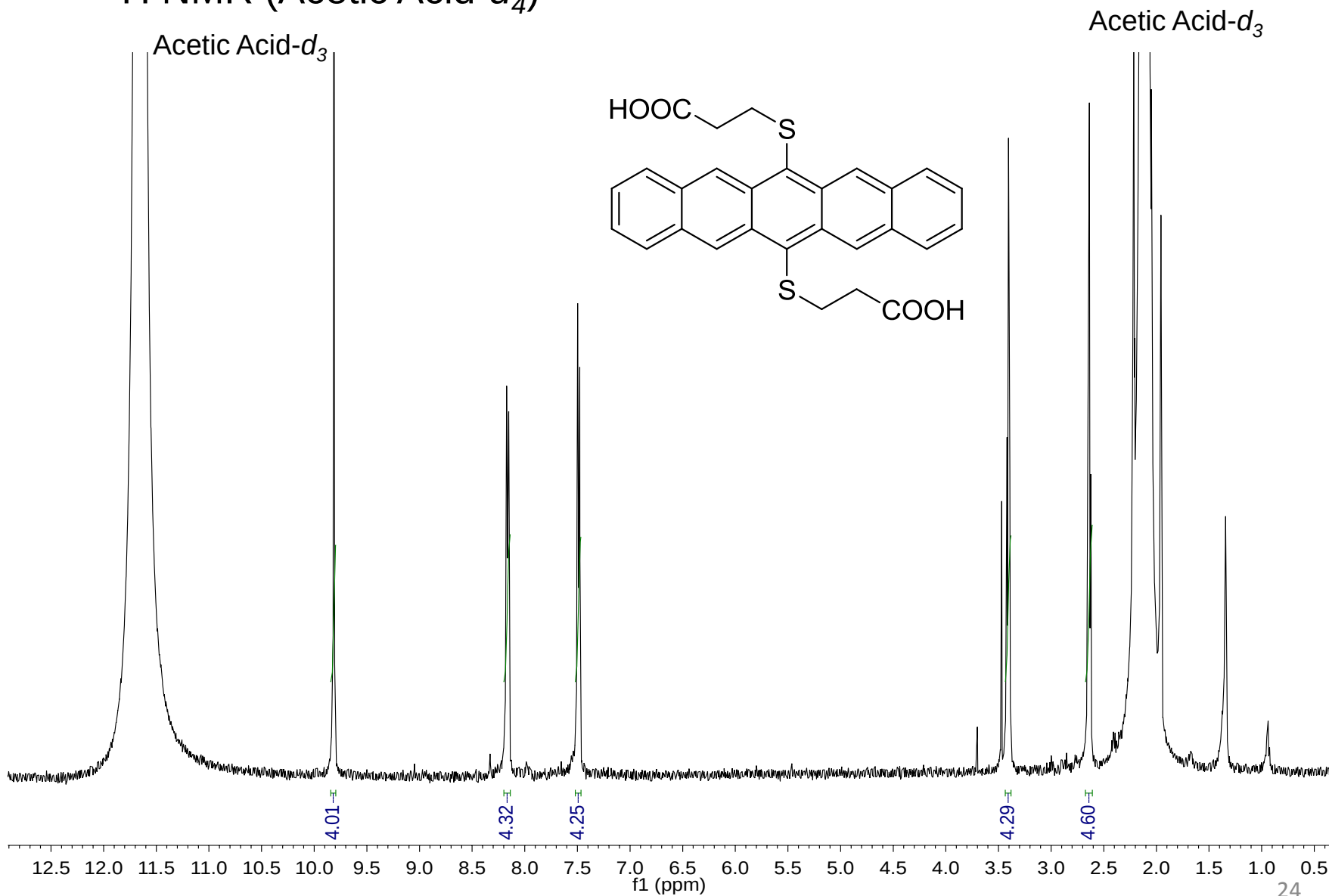


syn-3,3'-((6,13-dihydropentacene-6,13-diyl)bis(sulfanediyl))dipropionic acid (**2**)



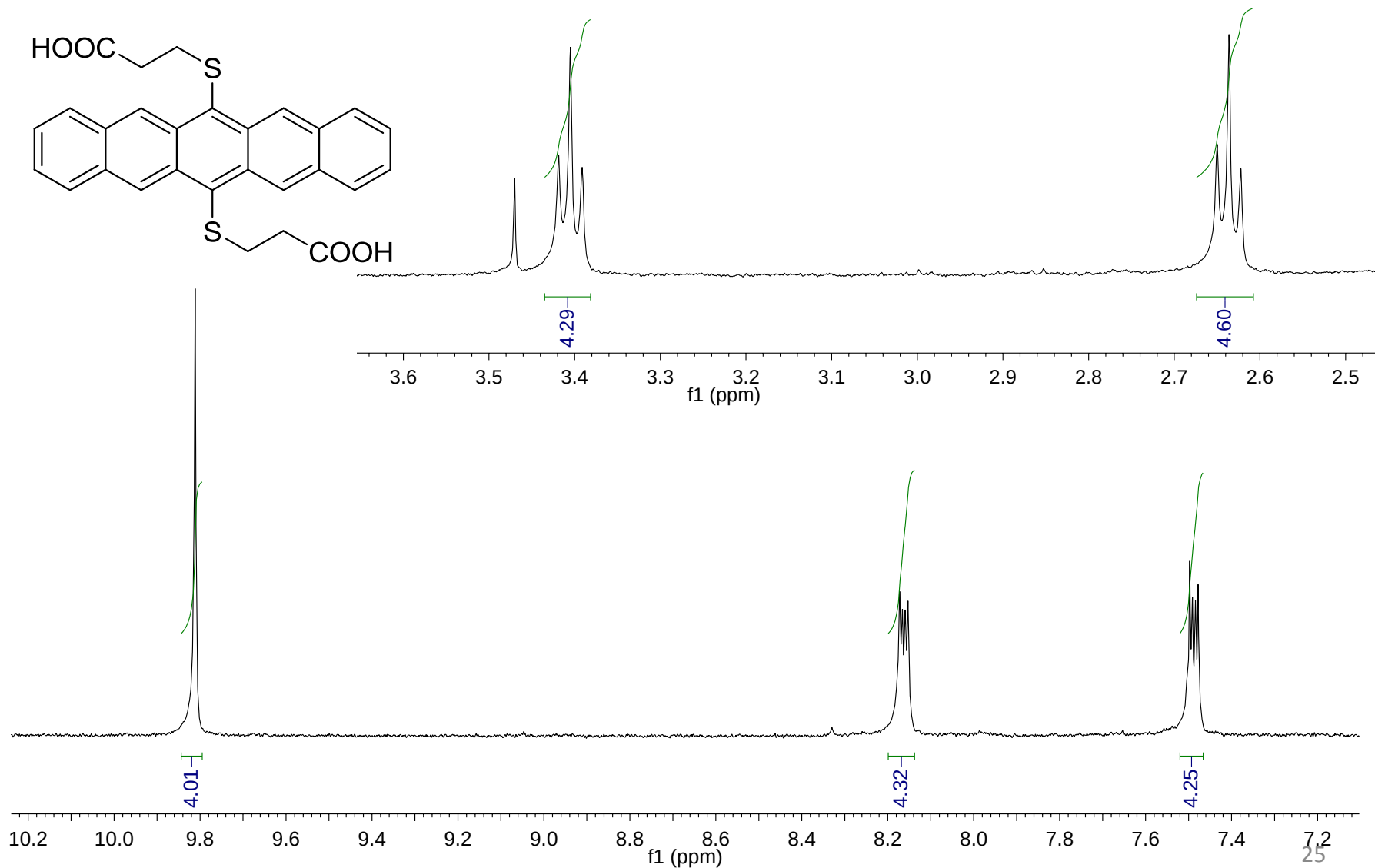
3,3'-(Pentacene-6,13-diylbis(sulfaneydiyl))dipropionic acid (**3**)

^1H NMR (Acetic Acid- d_4)



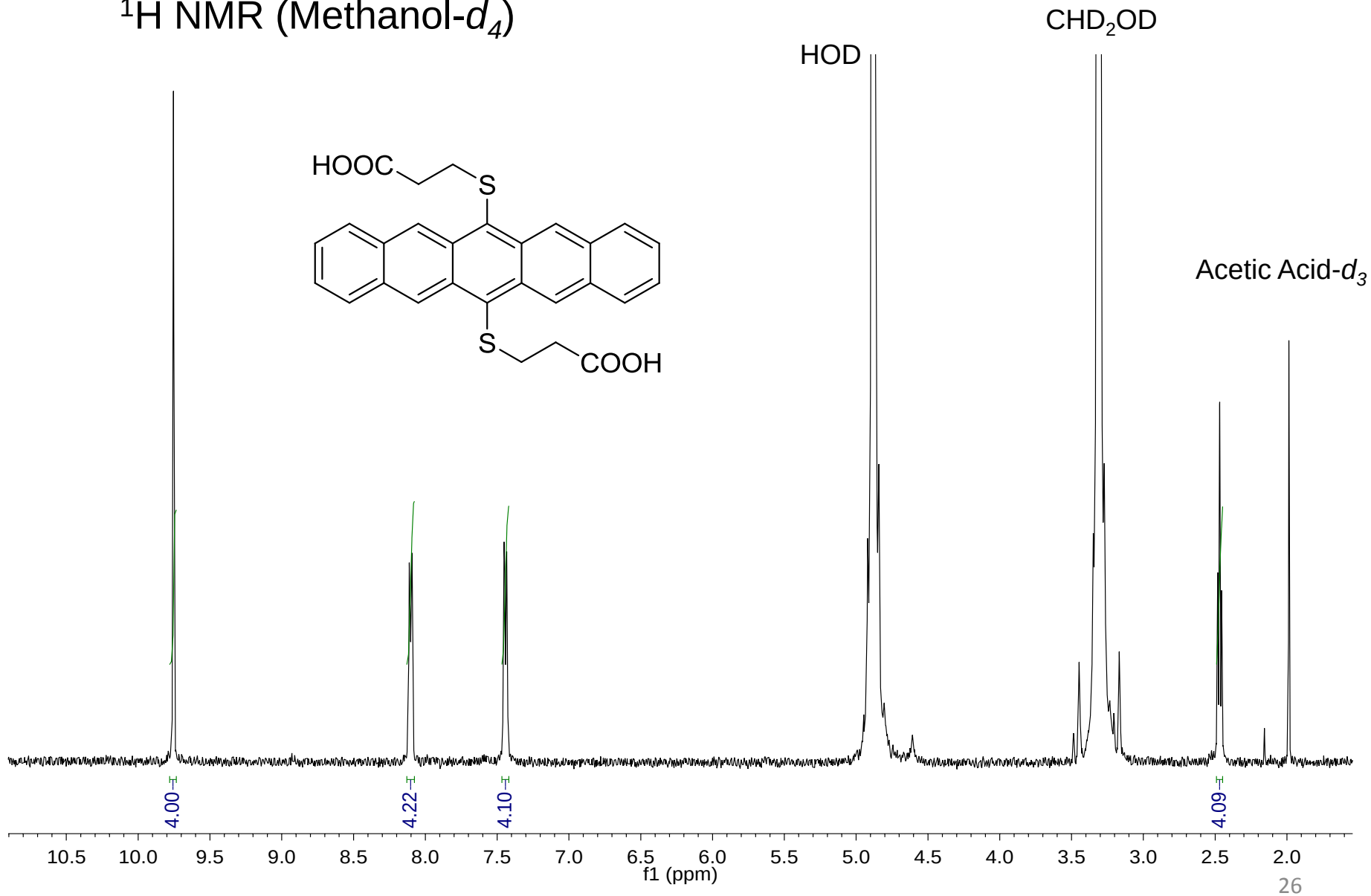
3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)

^1H NMR (Acetic Acid- d_4)



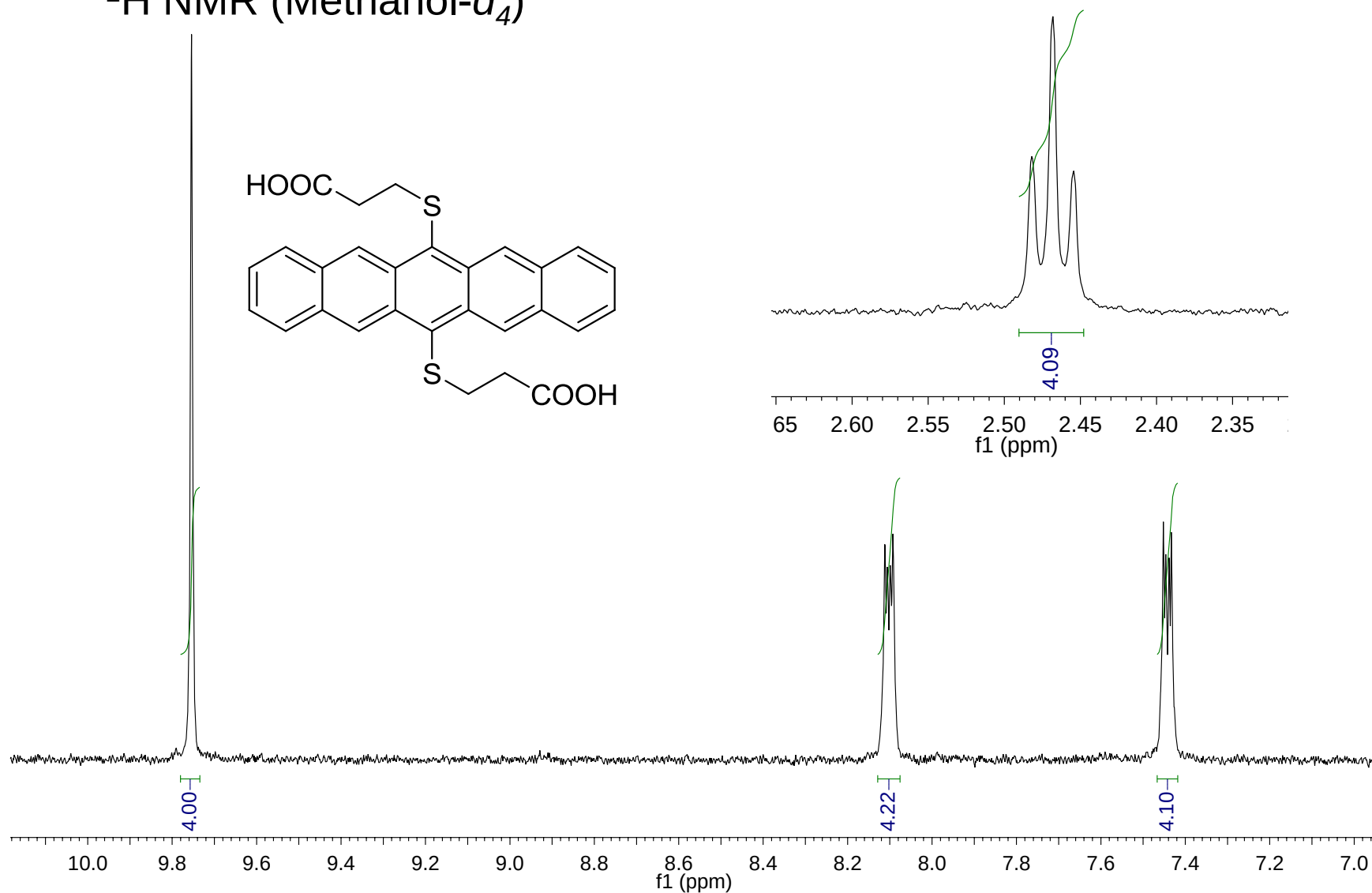
3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)

¹H NMR (Methanol-*d*₄)



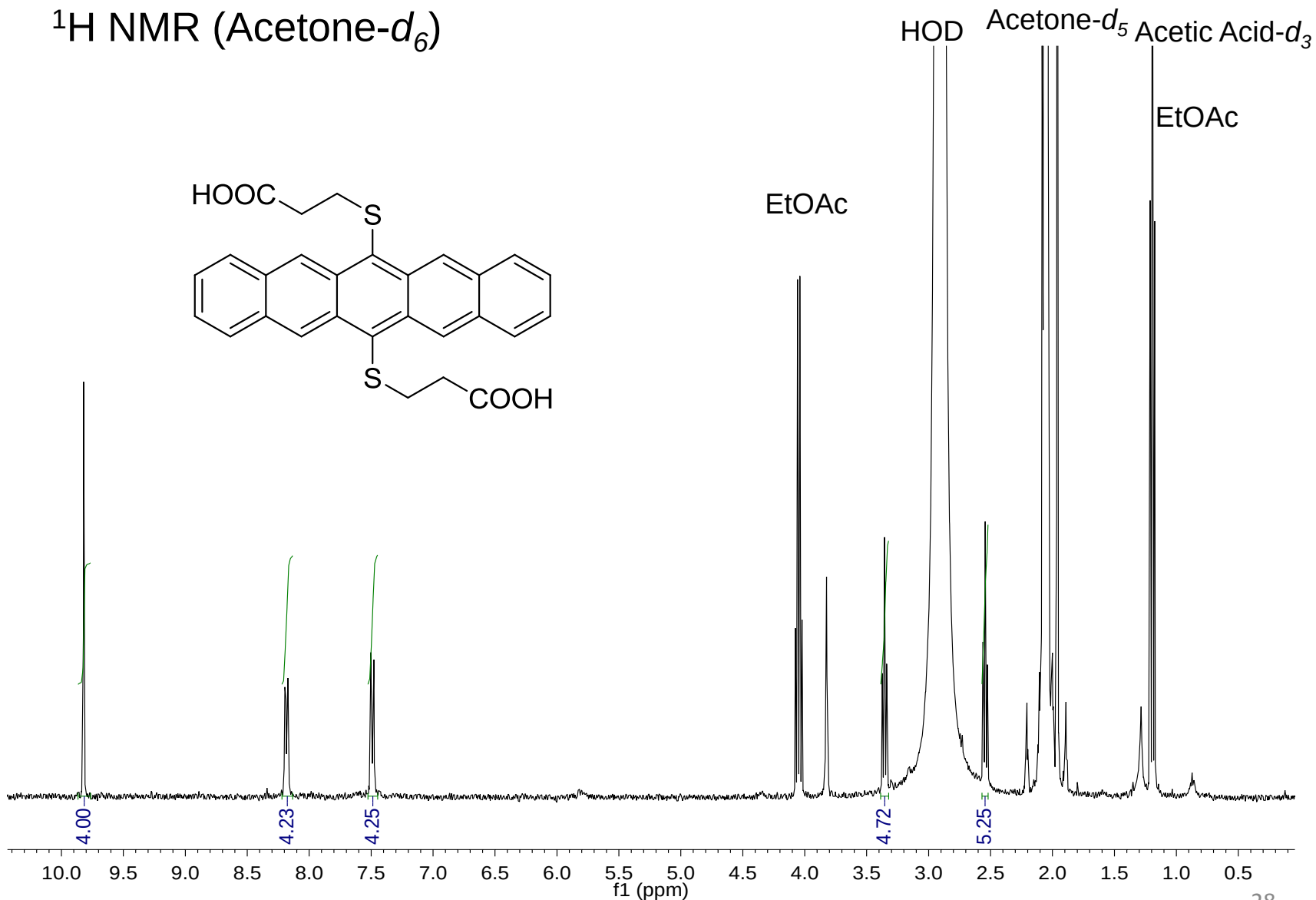
3,3'-(Pentacene-6,13-diylbis(sulfaneydiyl))dipropionic acid (**3**)

^1H NMR (Methanol- d_4)



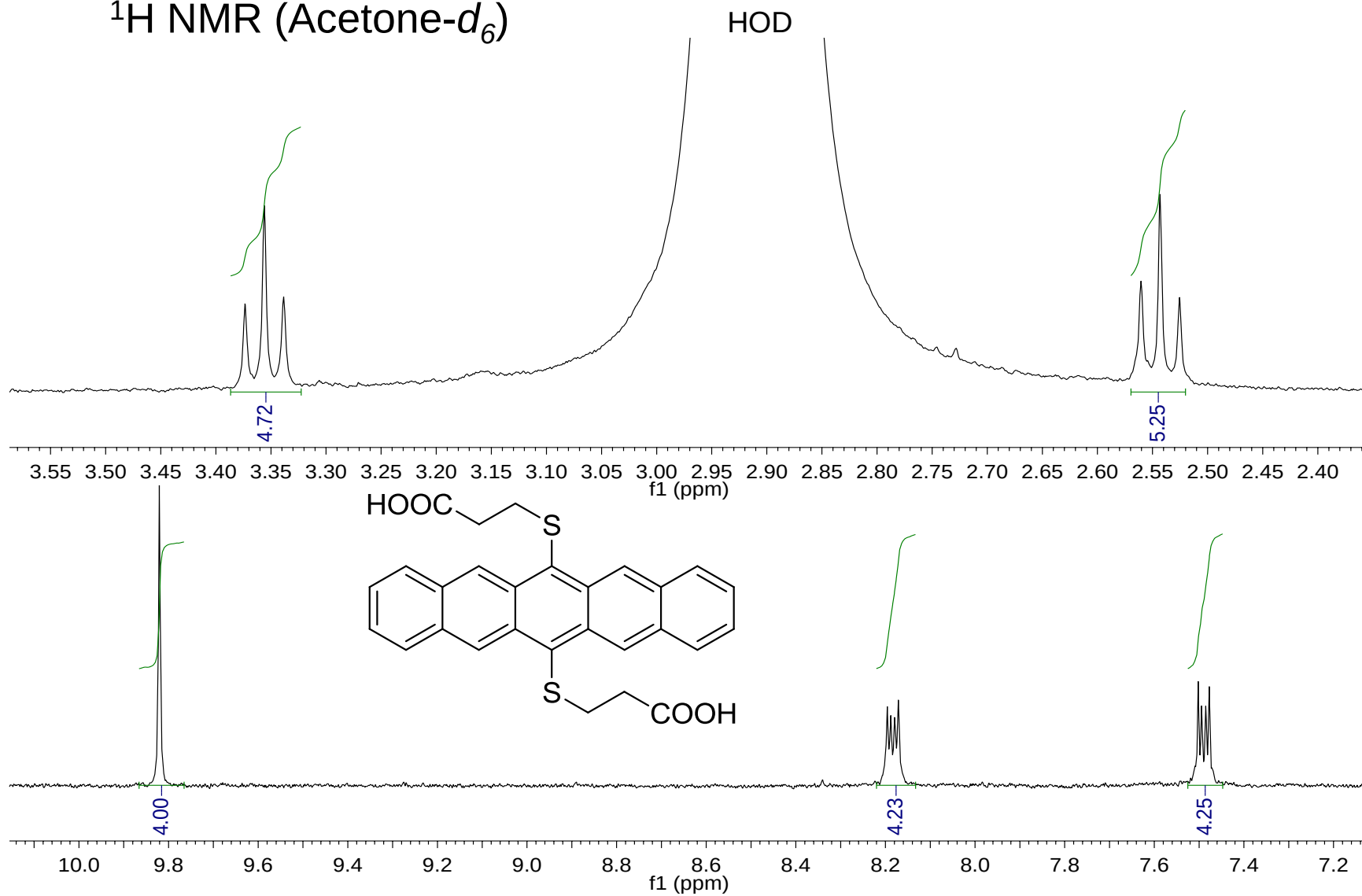
3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)

^1H NMR (Acetone- d_6)



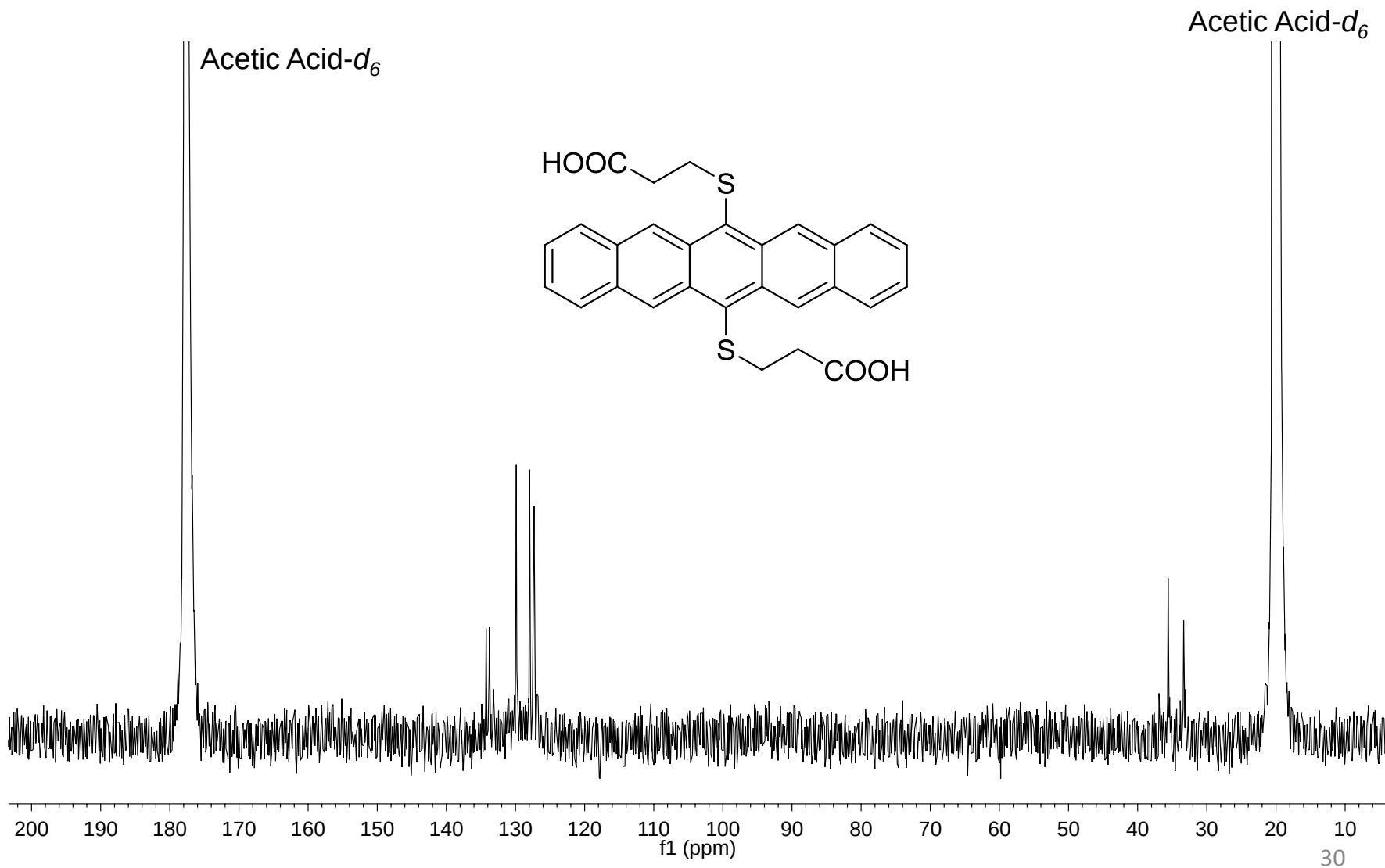
3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)

^1H NMR (Acetone- d_6)



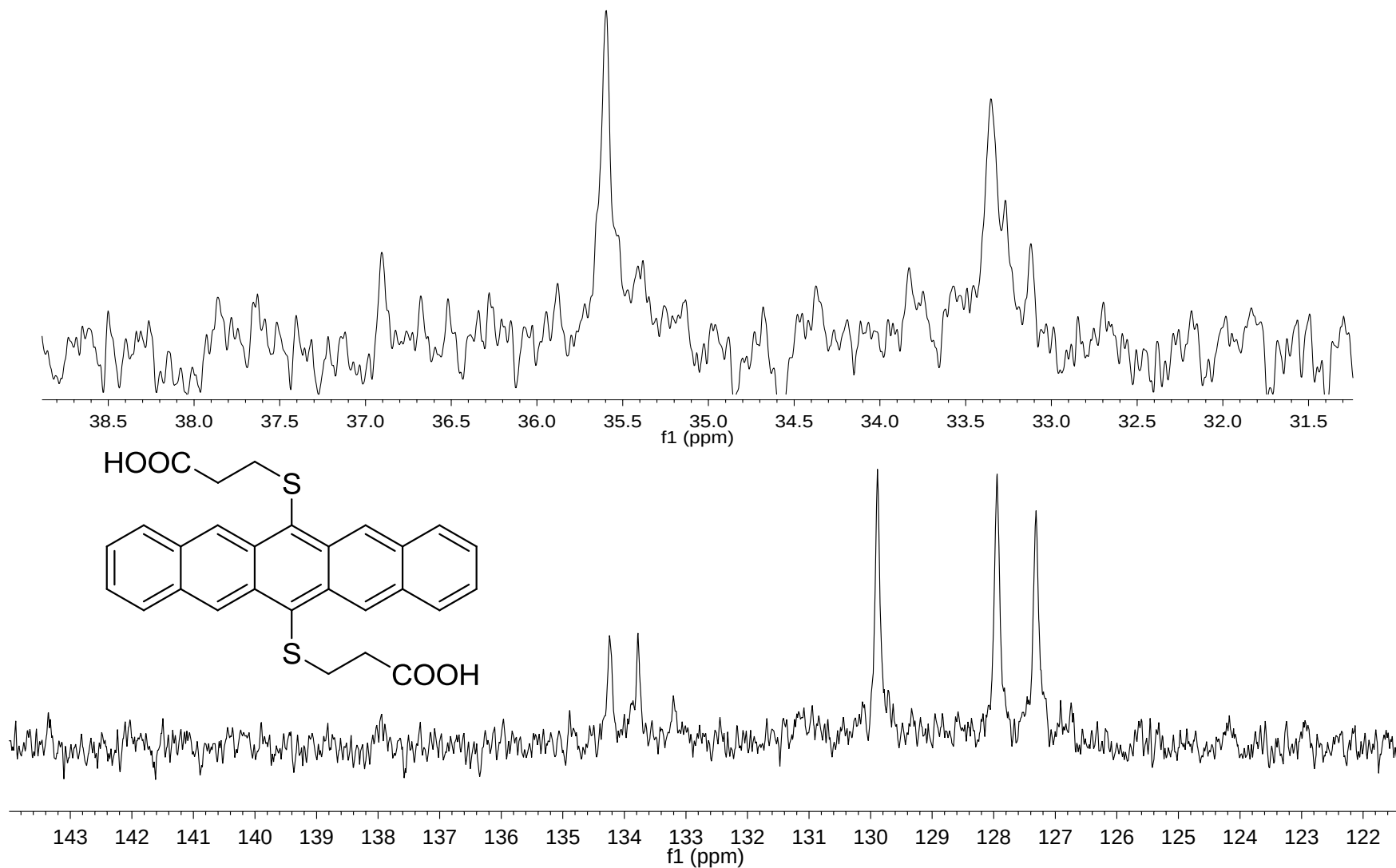
3,3'-(Pentacene-6,13-diylbis(sulfaneyl))dipropionic acid (**3**)

^{13}C NMR (Acetic Acid- d_4) at 80 °C



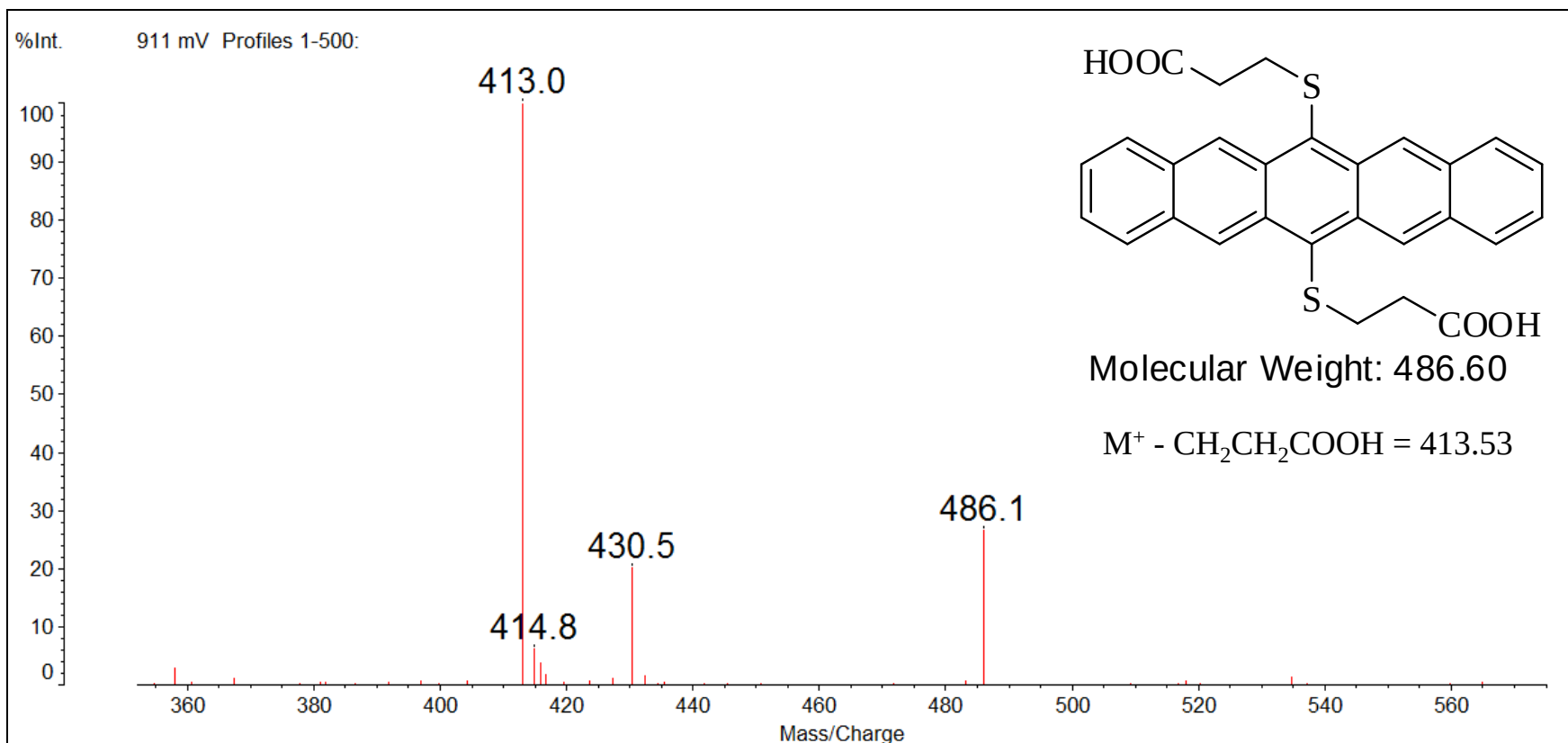
3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)

^{13}C NMR (Acetic Acid- d_4) at 80 °C



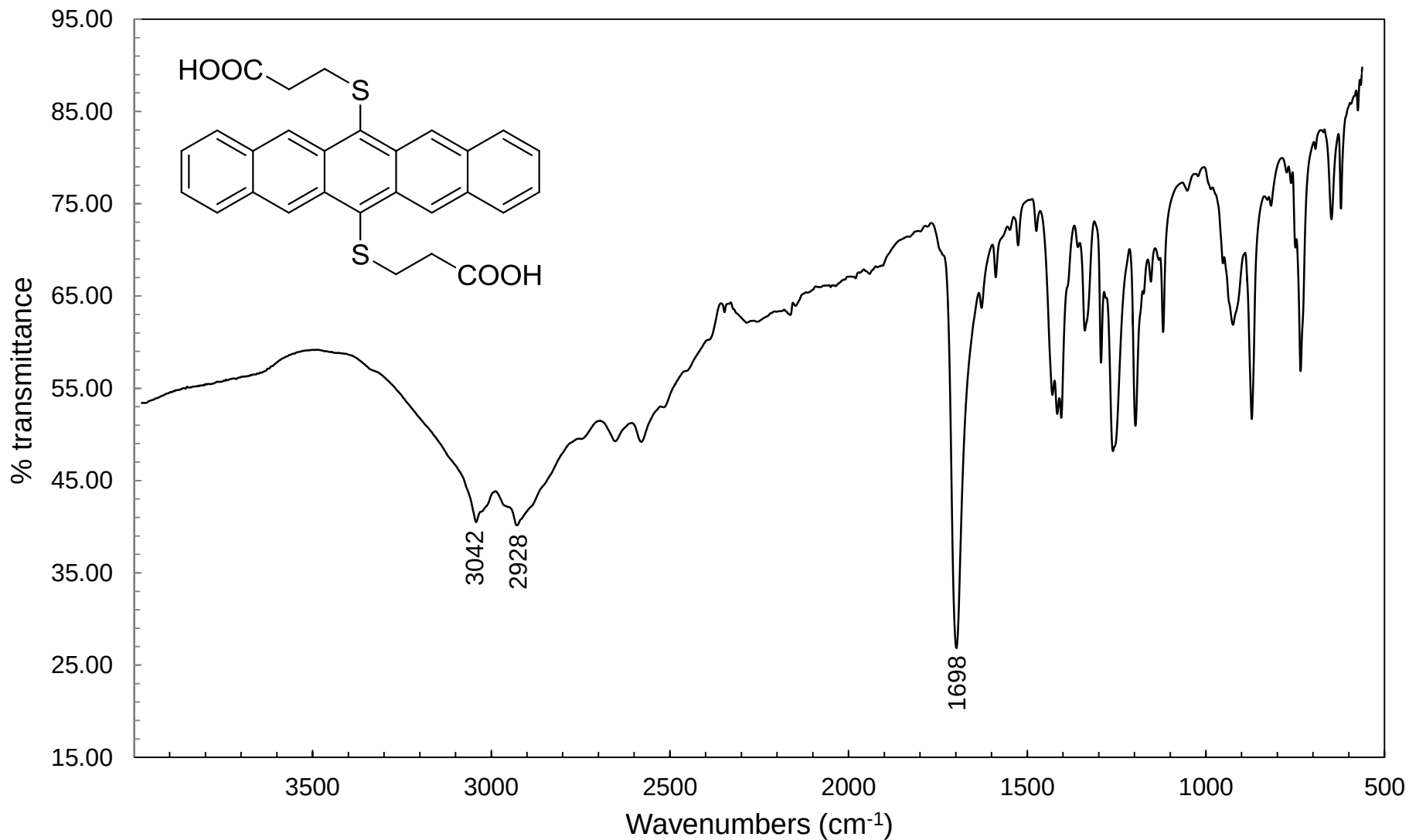
3,3'-(Pentacene-6,13-diylbis(sulfaneydiyl))dipropionic acid (**3**)

LDI MS

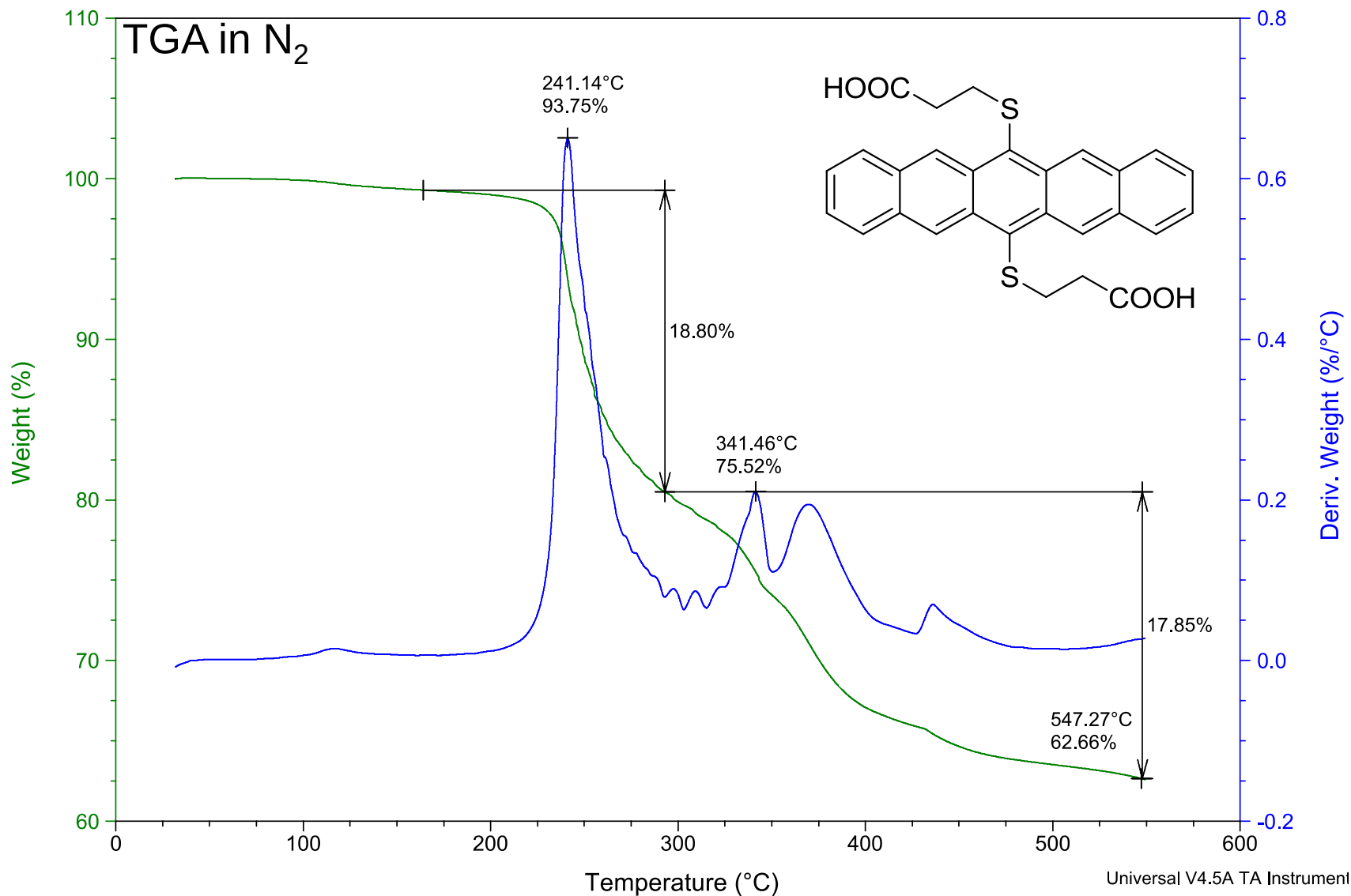


3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)

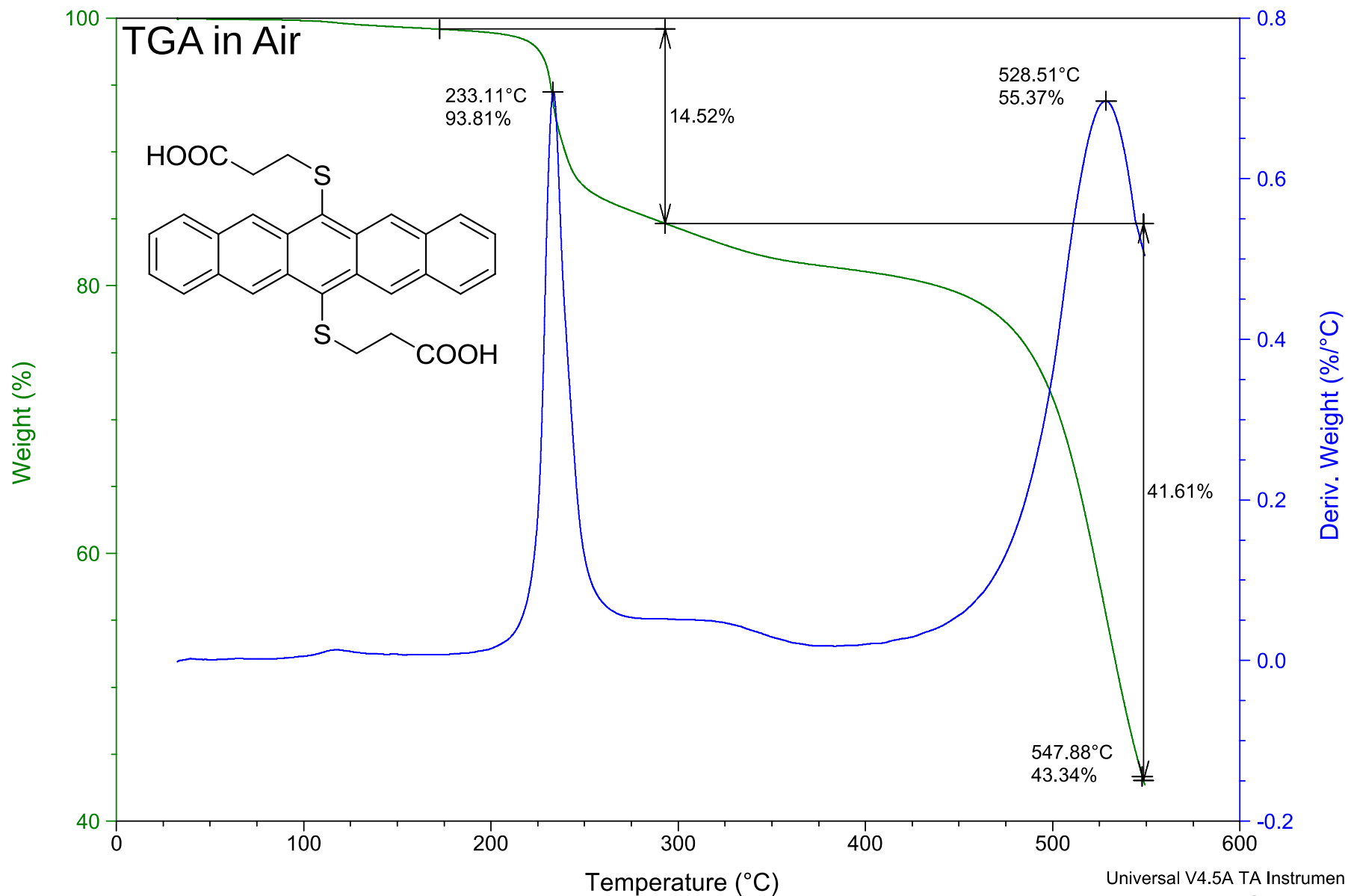
IR



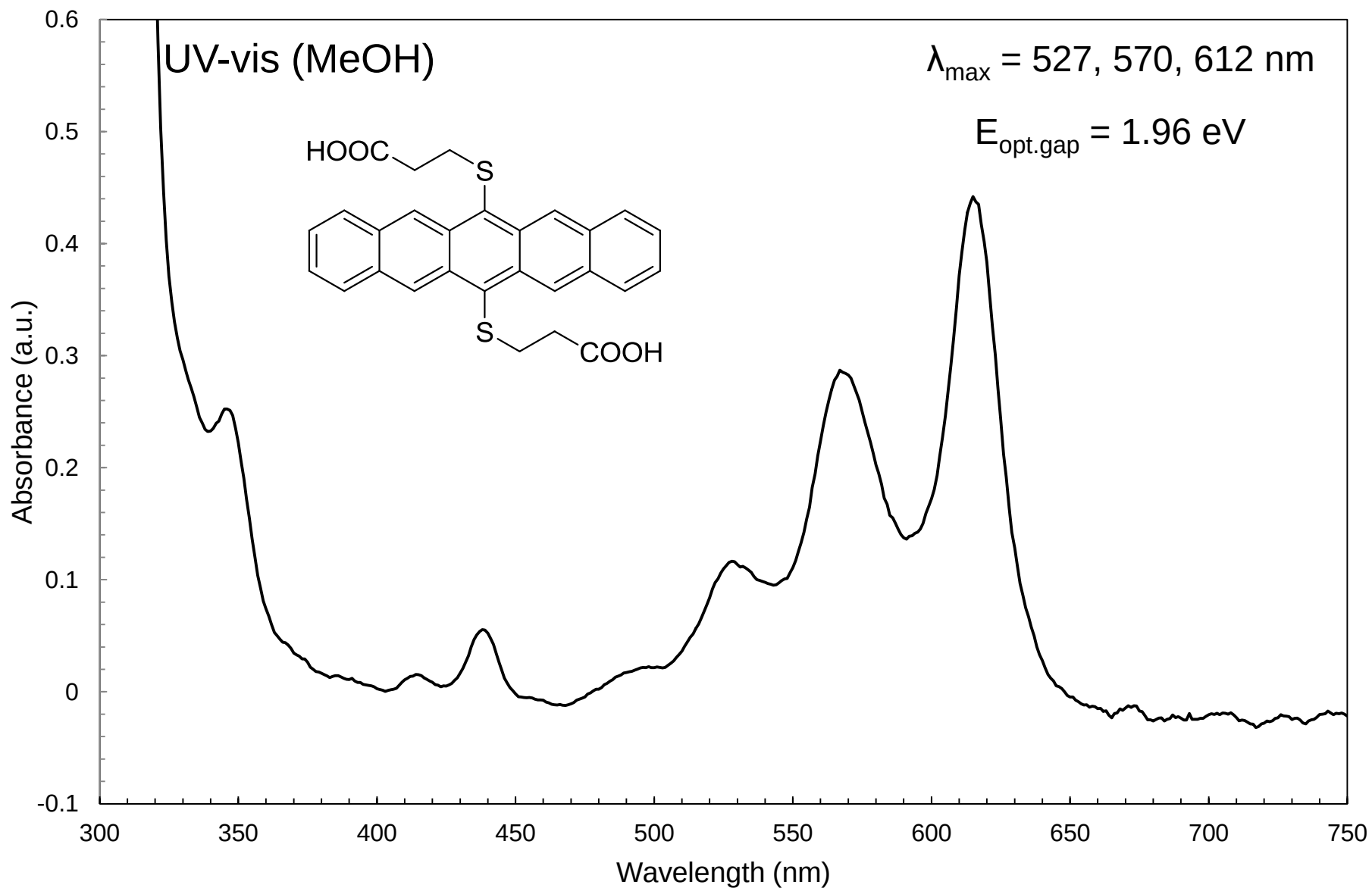
3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)



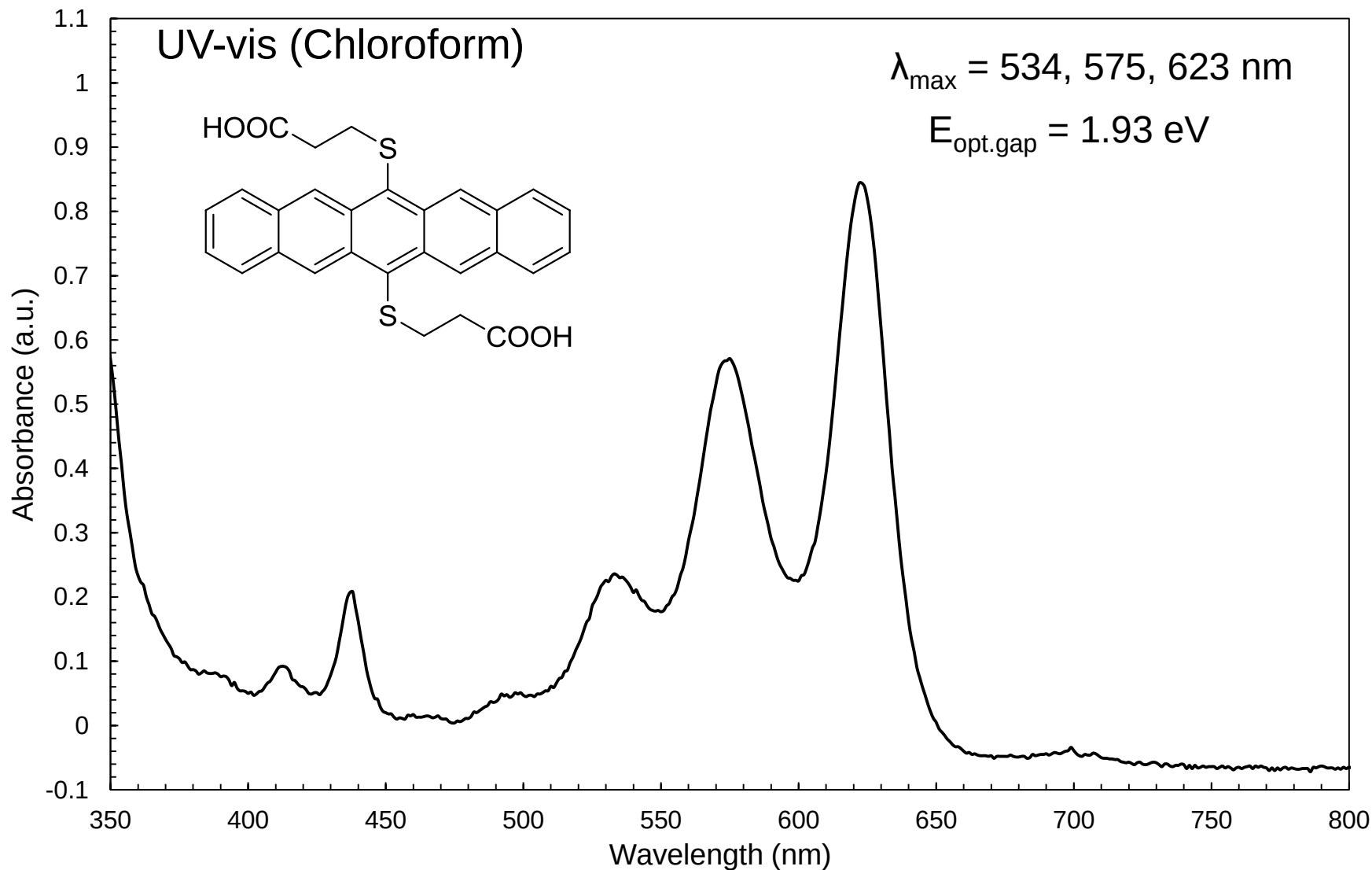
3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)



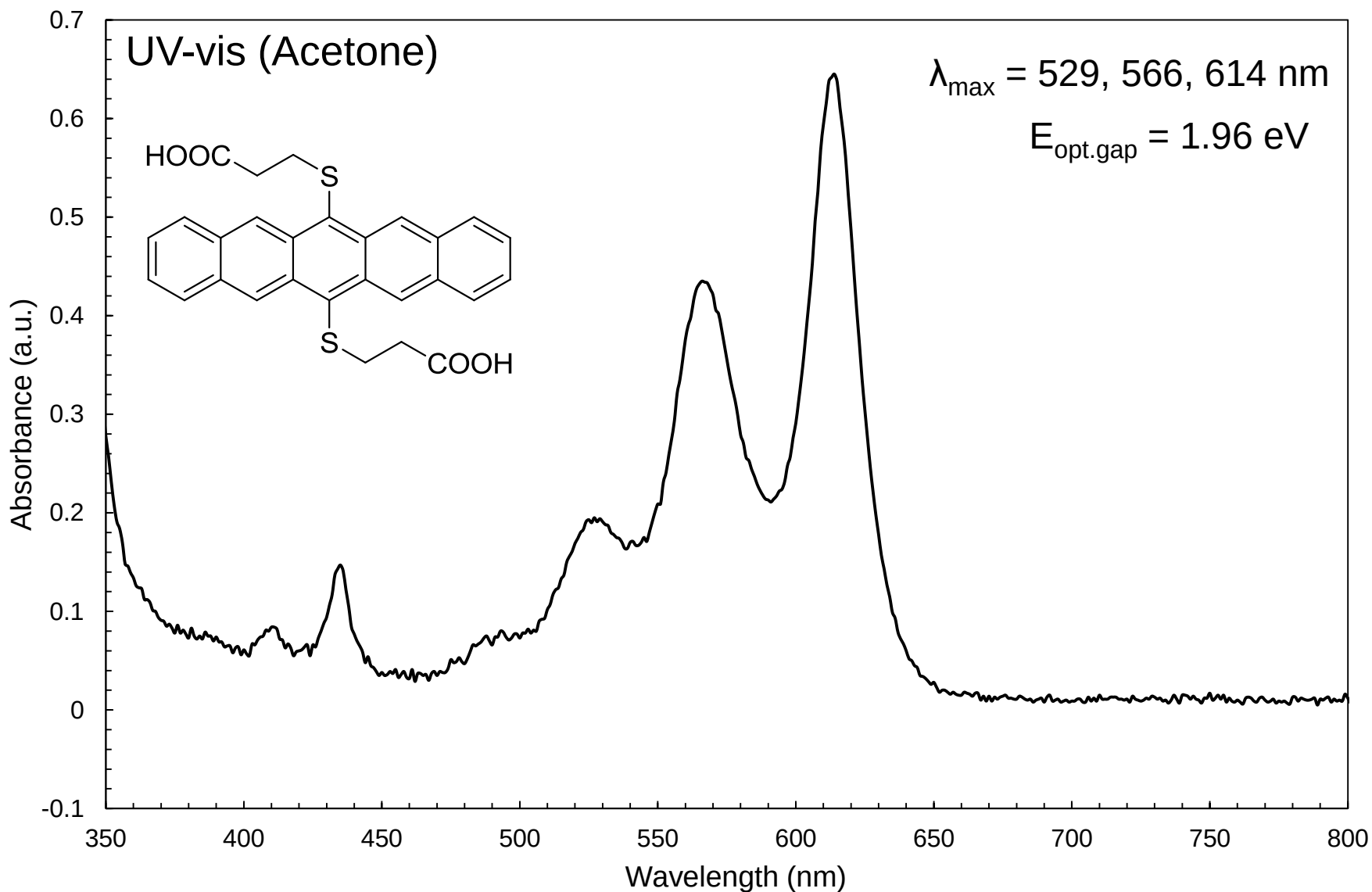
3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)



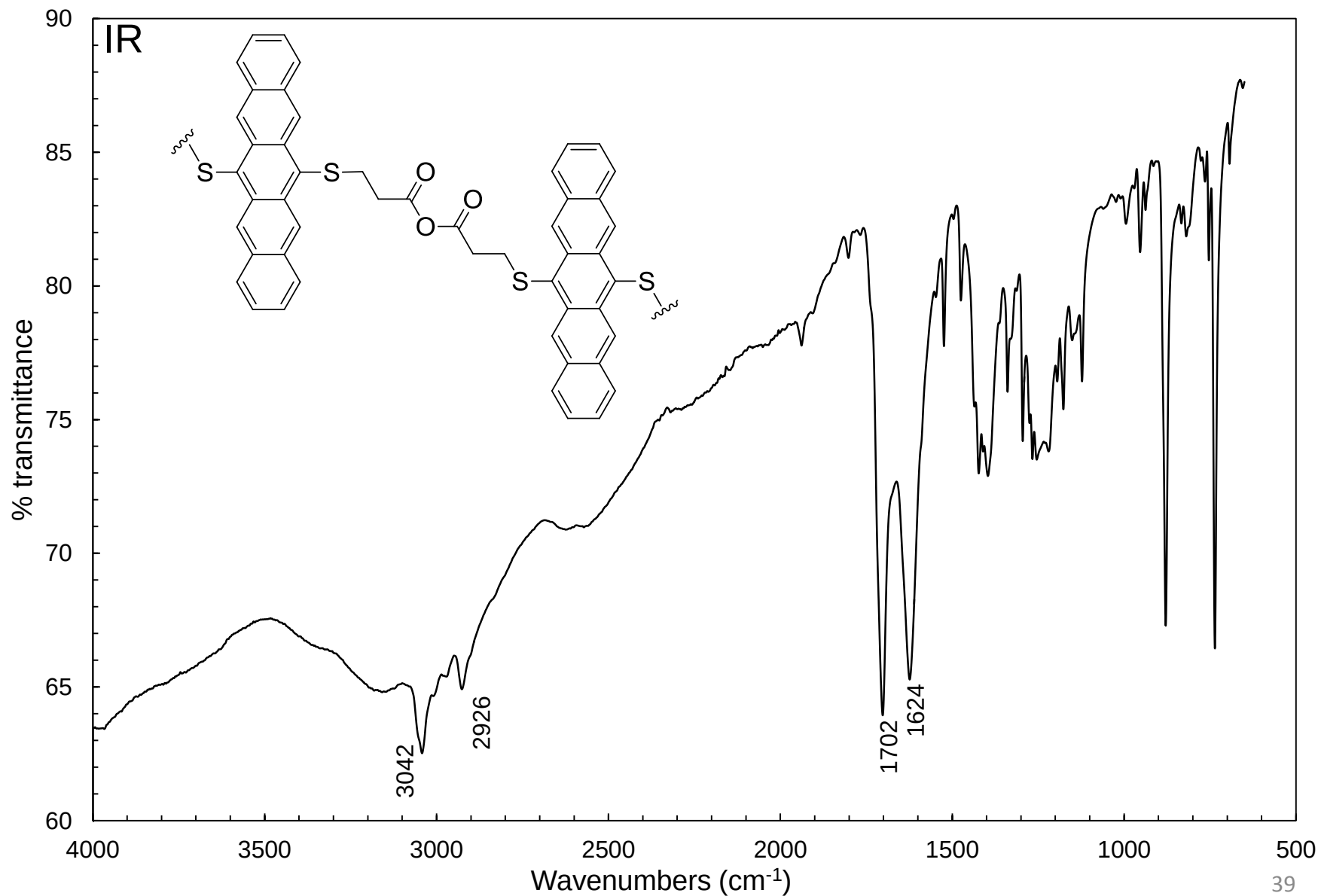
3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)



3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropionic acid (**3**)

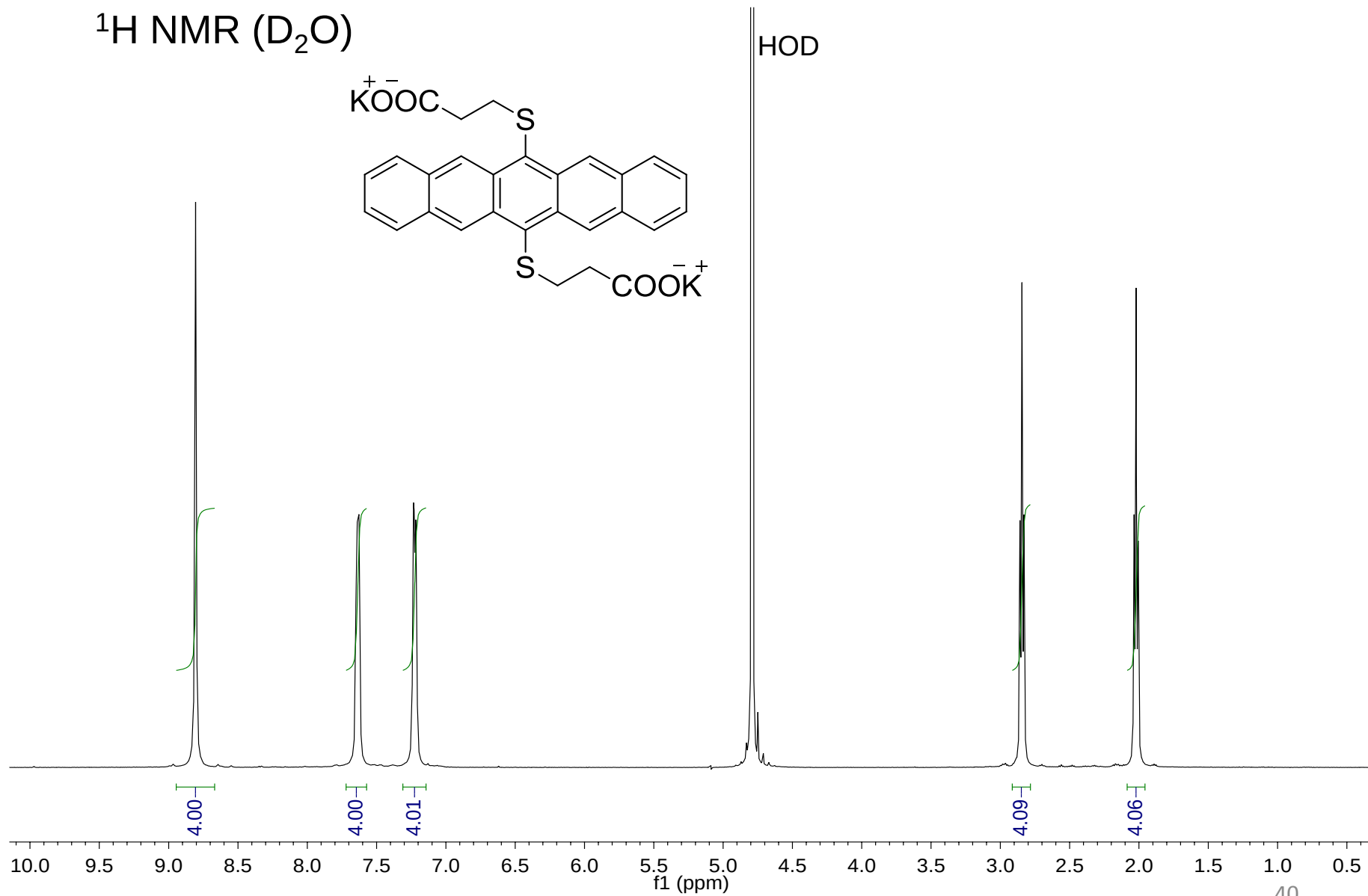
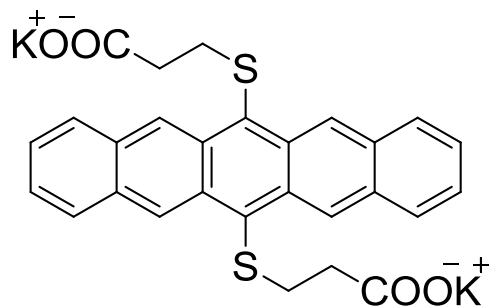


Anhydride of 3,3'-(Pentacene-6,13-diylbis(sulfanediyl))dipropanoic acid (3)



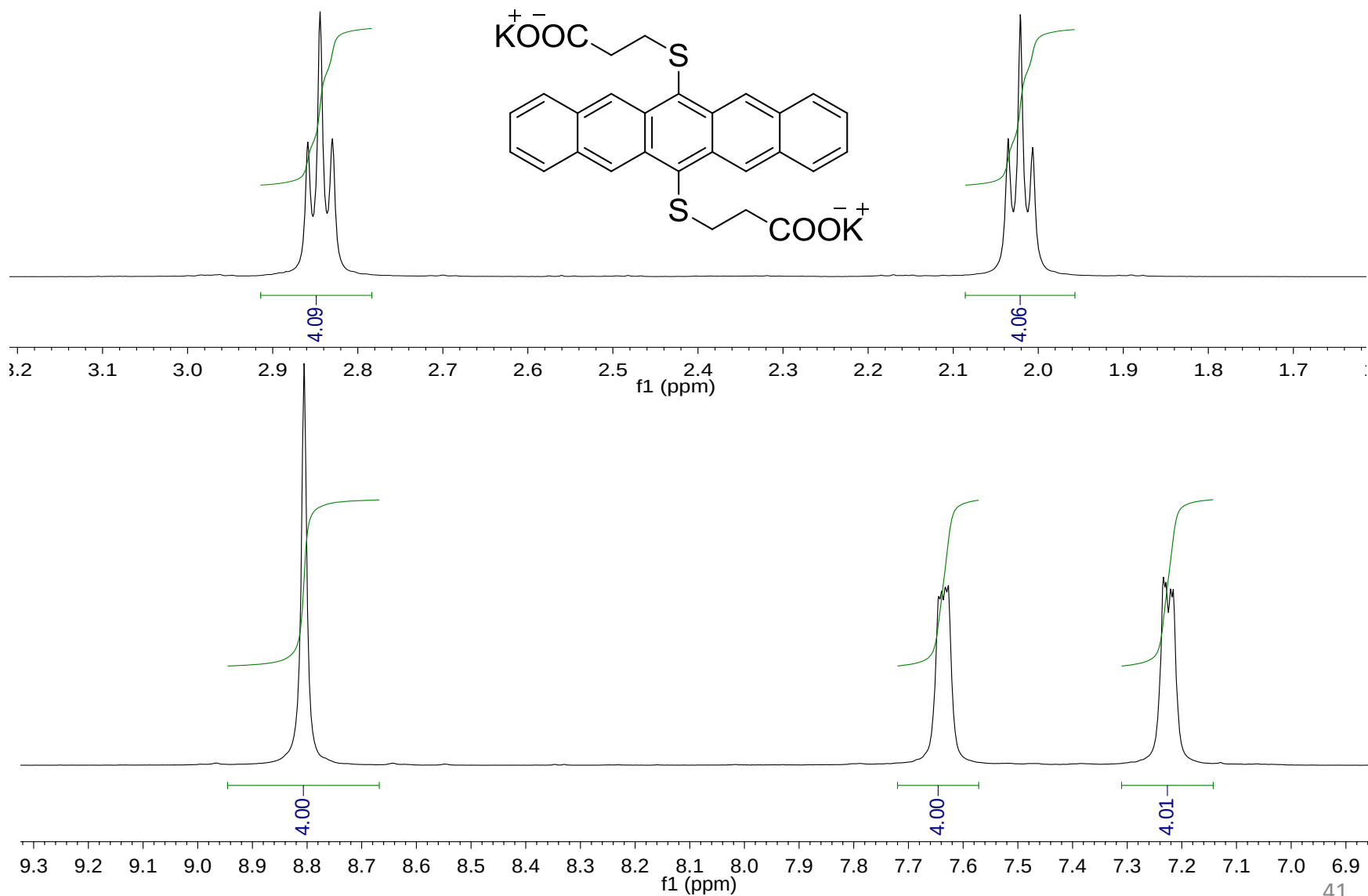
Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropanoate (**4**)

^1H NMR (D_2O)



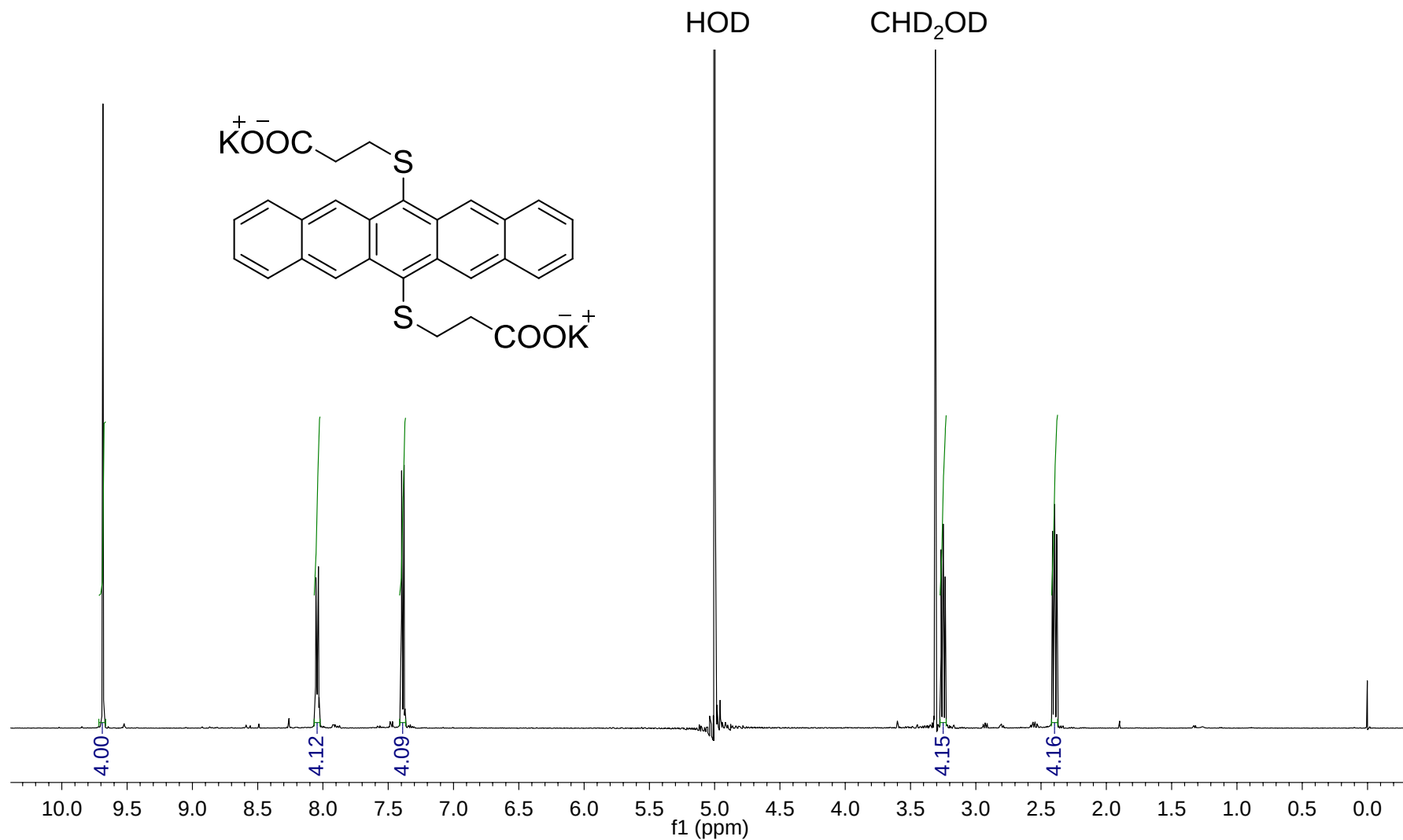
Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (**4**)

^1H NMR (D_2O)

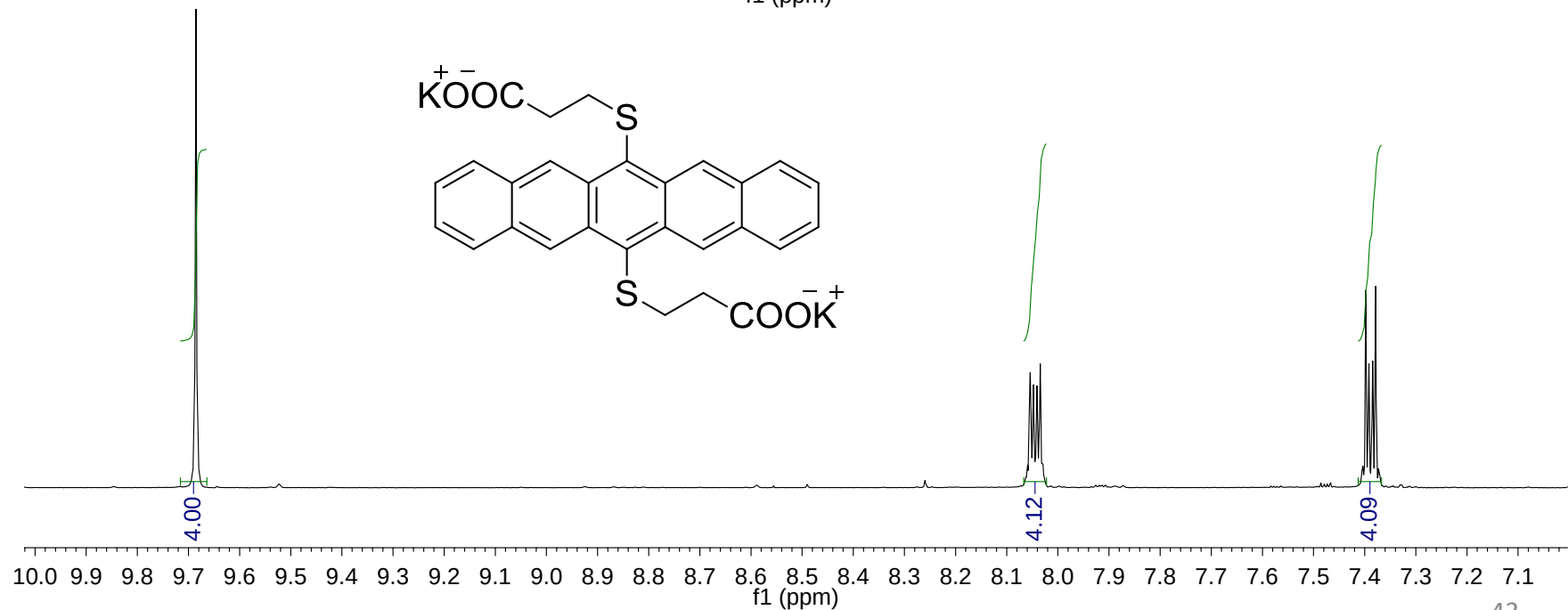
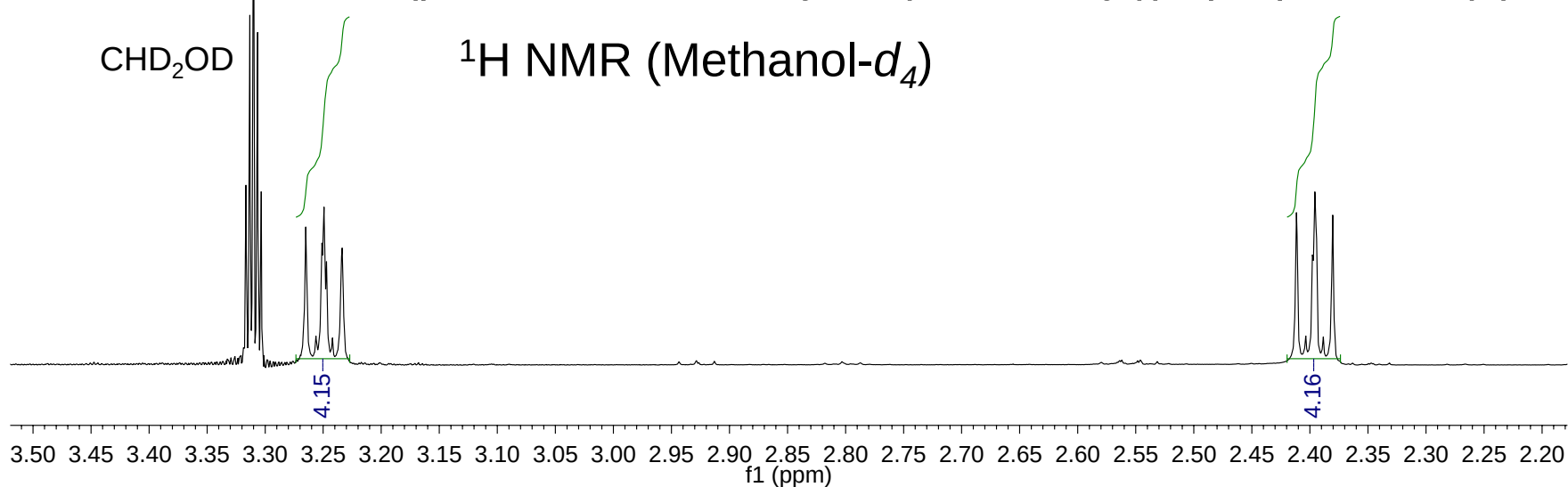


Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (**4**)

^1H NMR (Methanol- d_4)

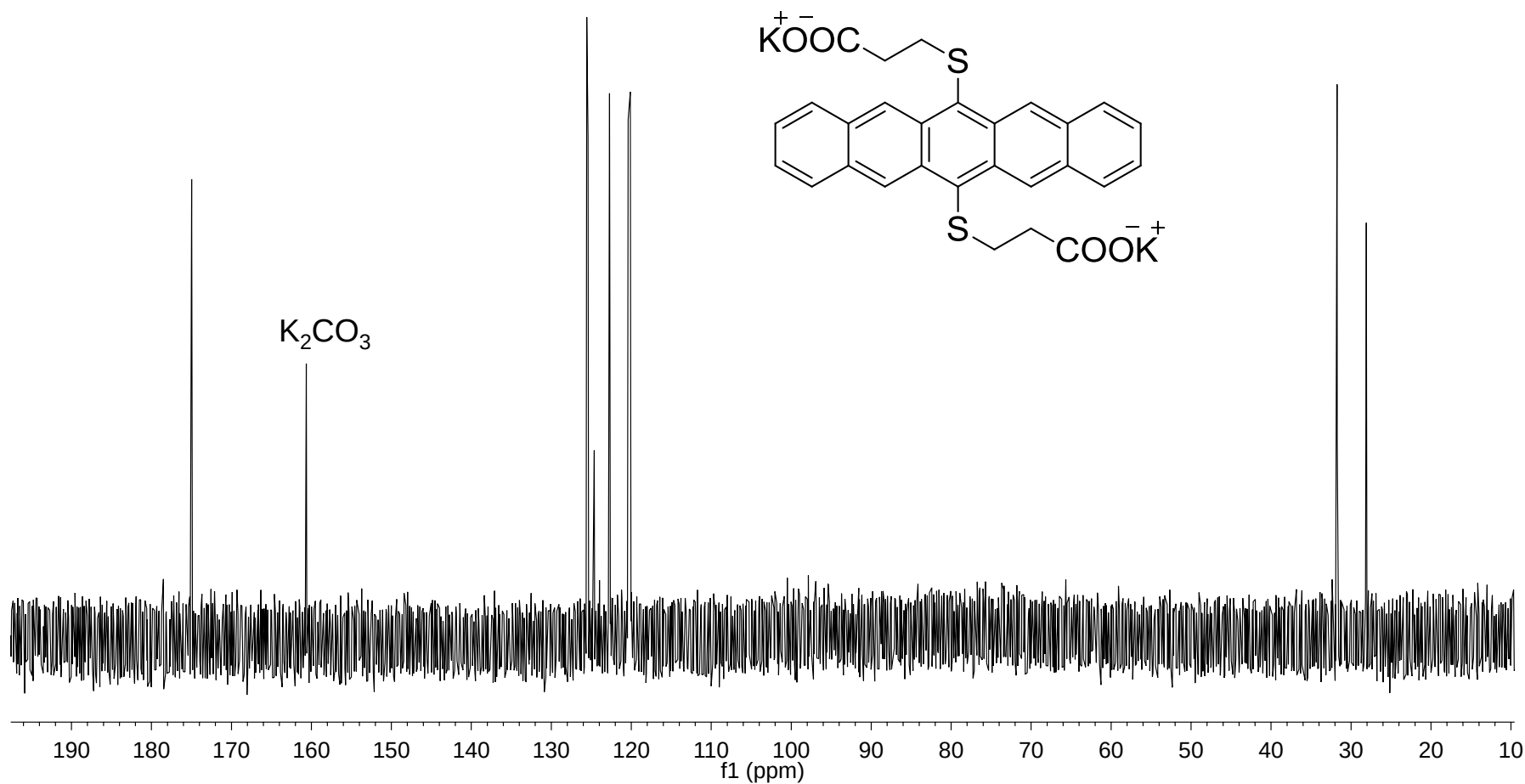


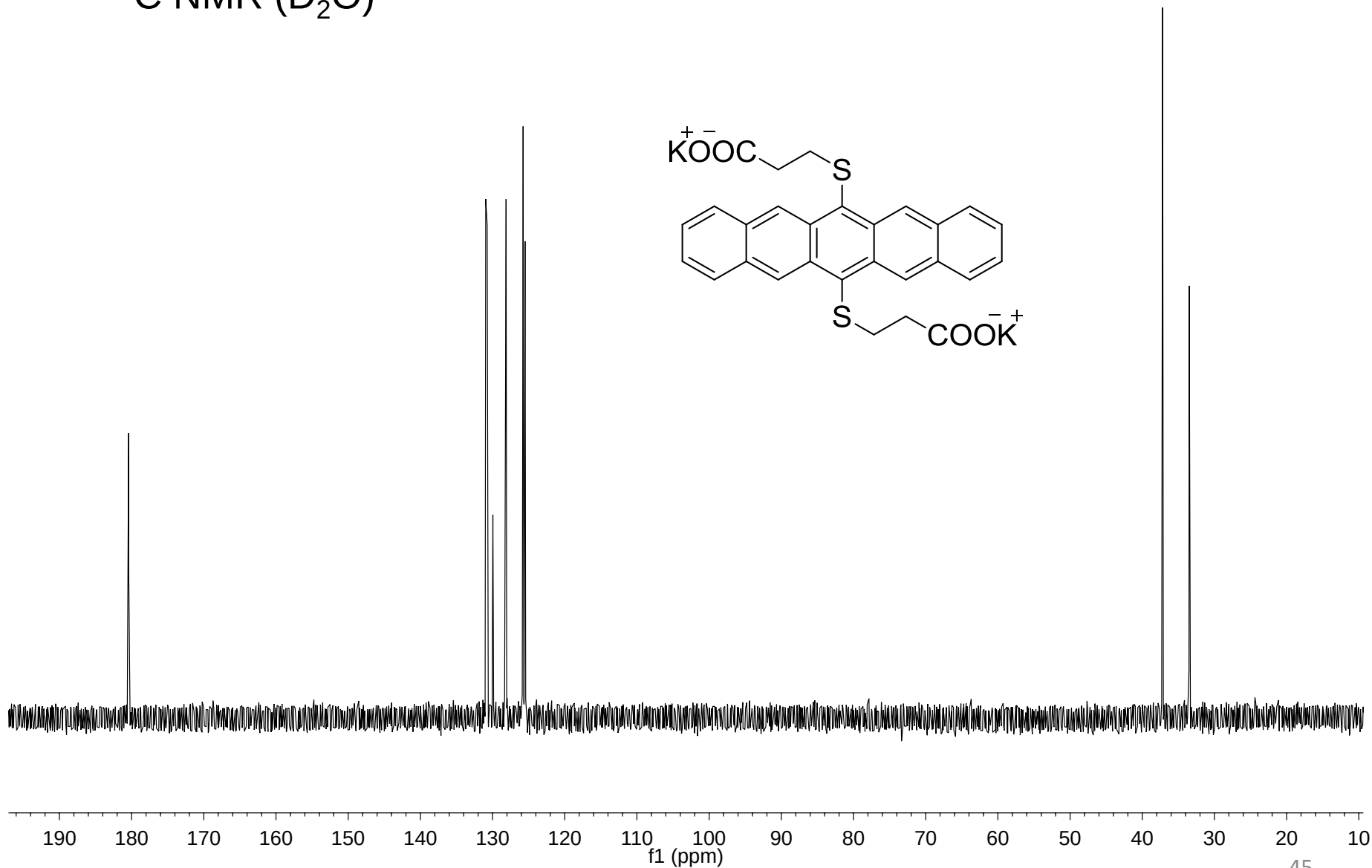
Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (4)



Potassium 3,3'-(pentacene-6,13-diylbis(sulfaneydiyl))dipropionate (**4**)

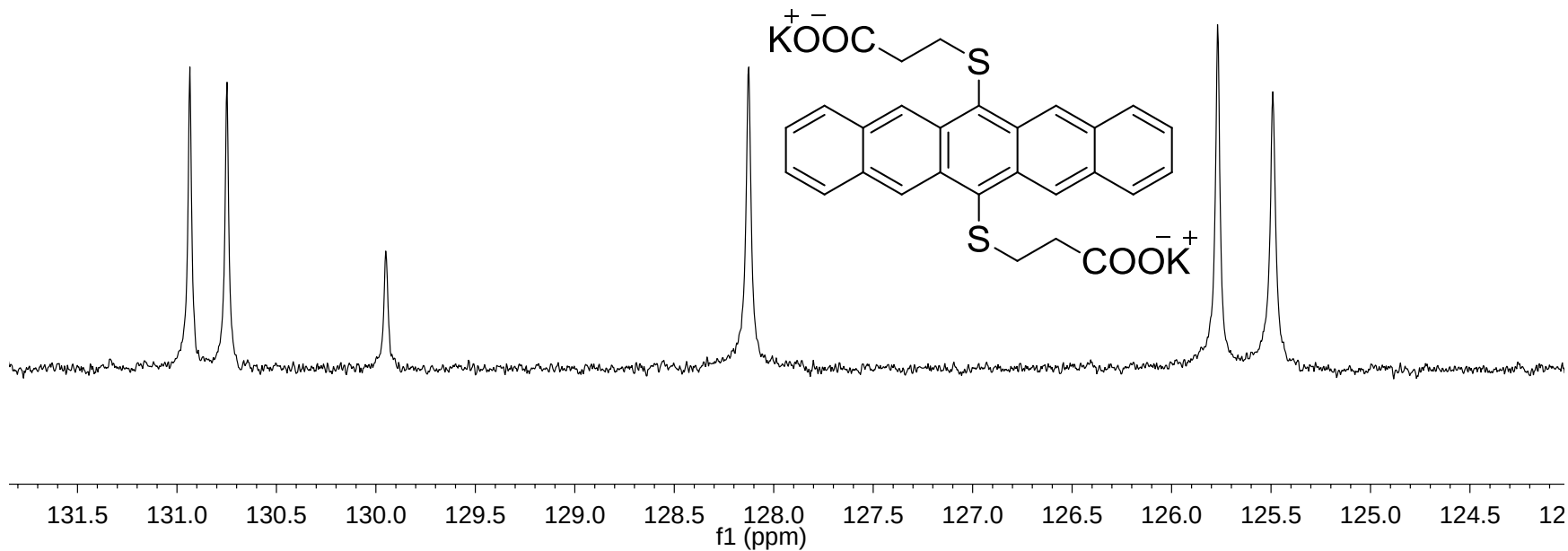
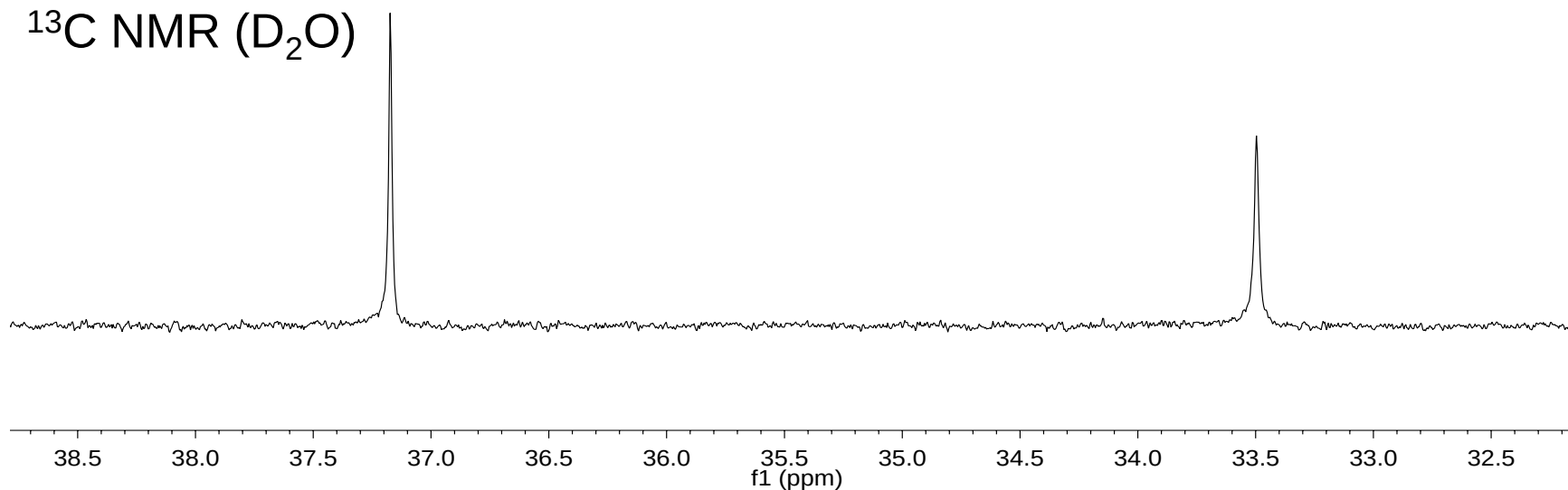
^{13}C NMR (D_2O with K_2CO_3)



Potassium 3,3'-(pentacene-6,13-diylbis(sulfaneydiyl))dipropanoate (**4**) ^{13}C NMR (D_2O)

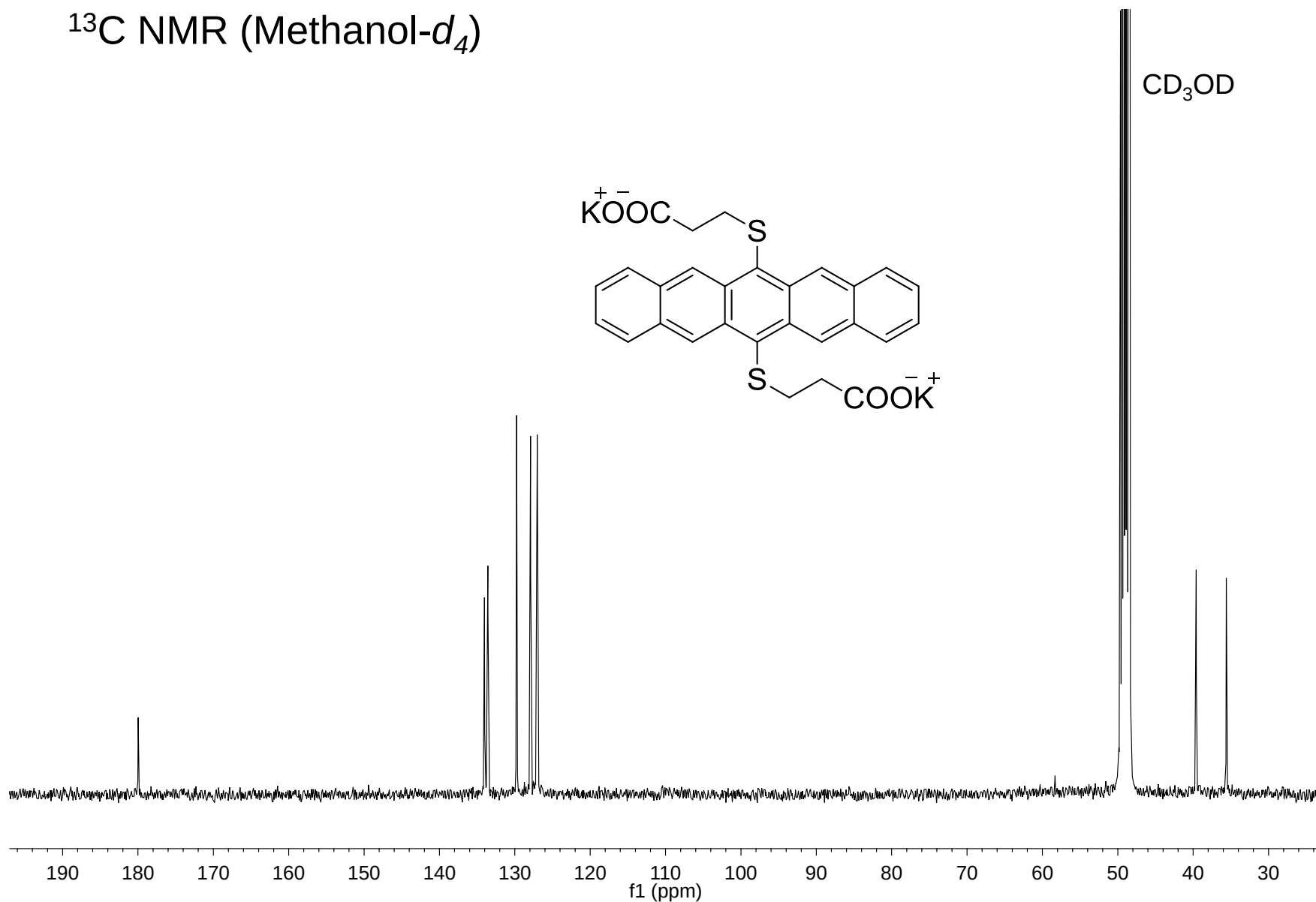
Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropanoate (**4**)

^{13}C NMR (D_2O)

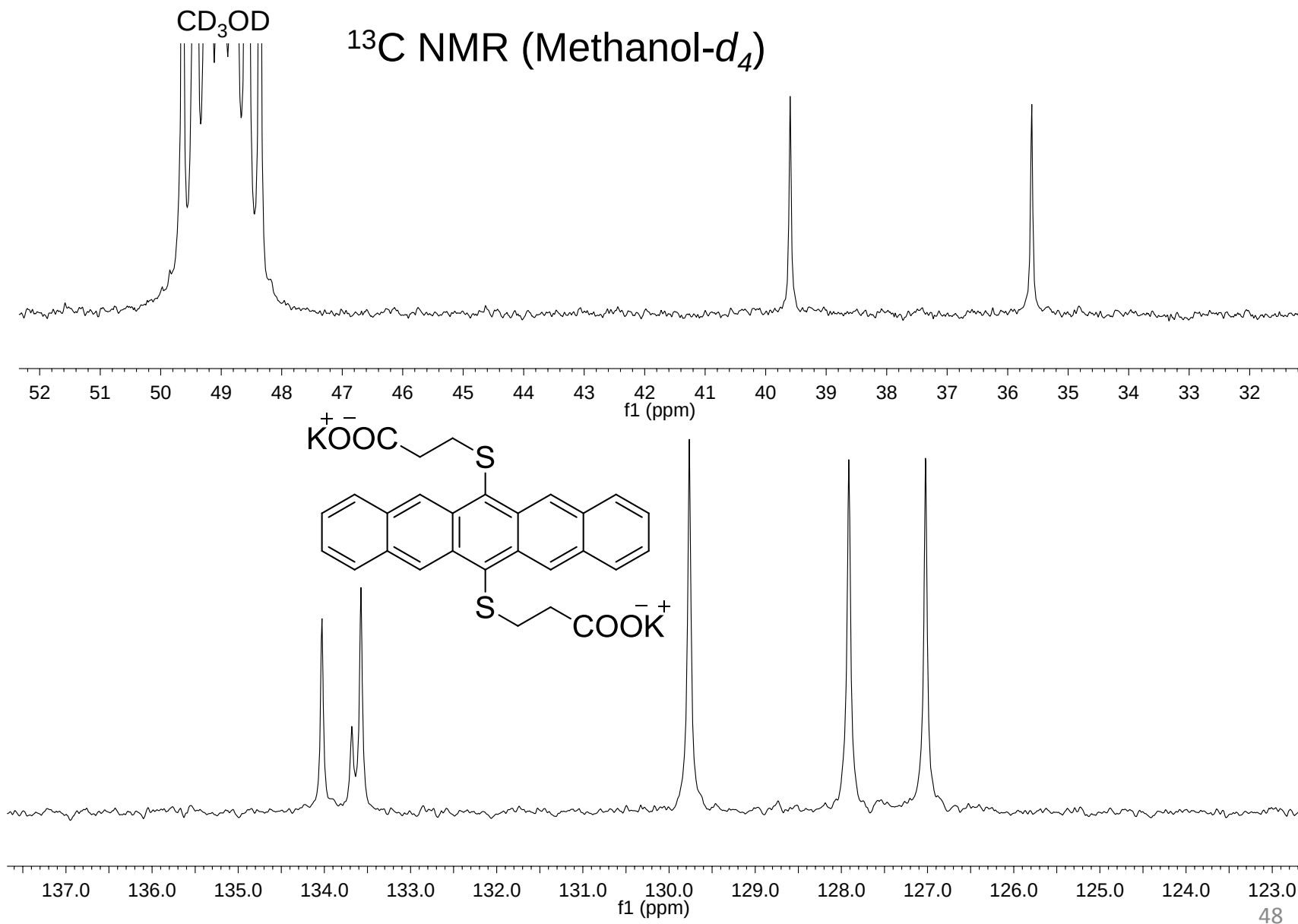


Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (**4**)

^{13}C NMR (Methanol- d_4)

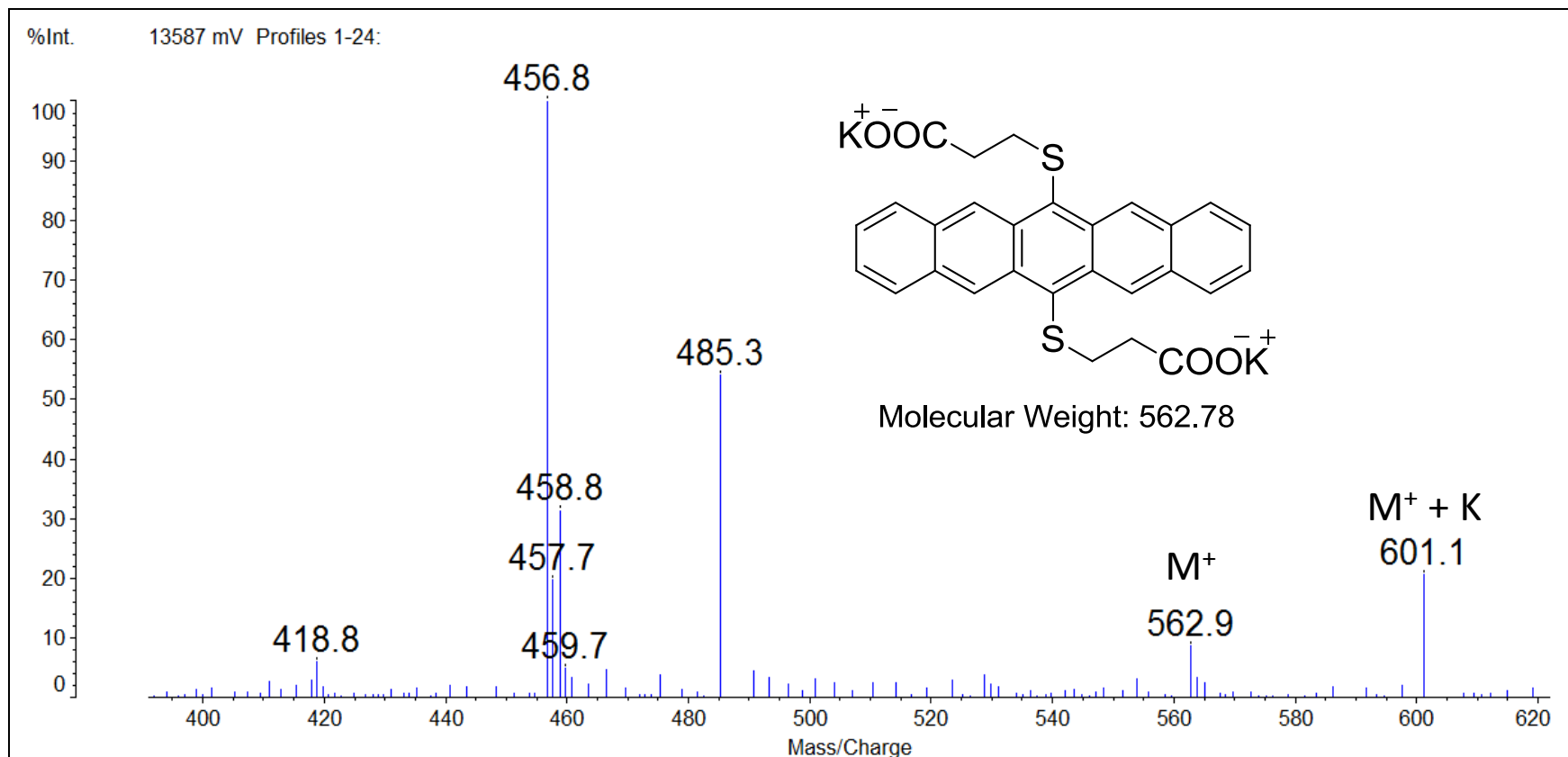


Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (**4**)

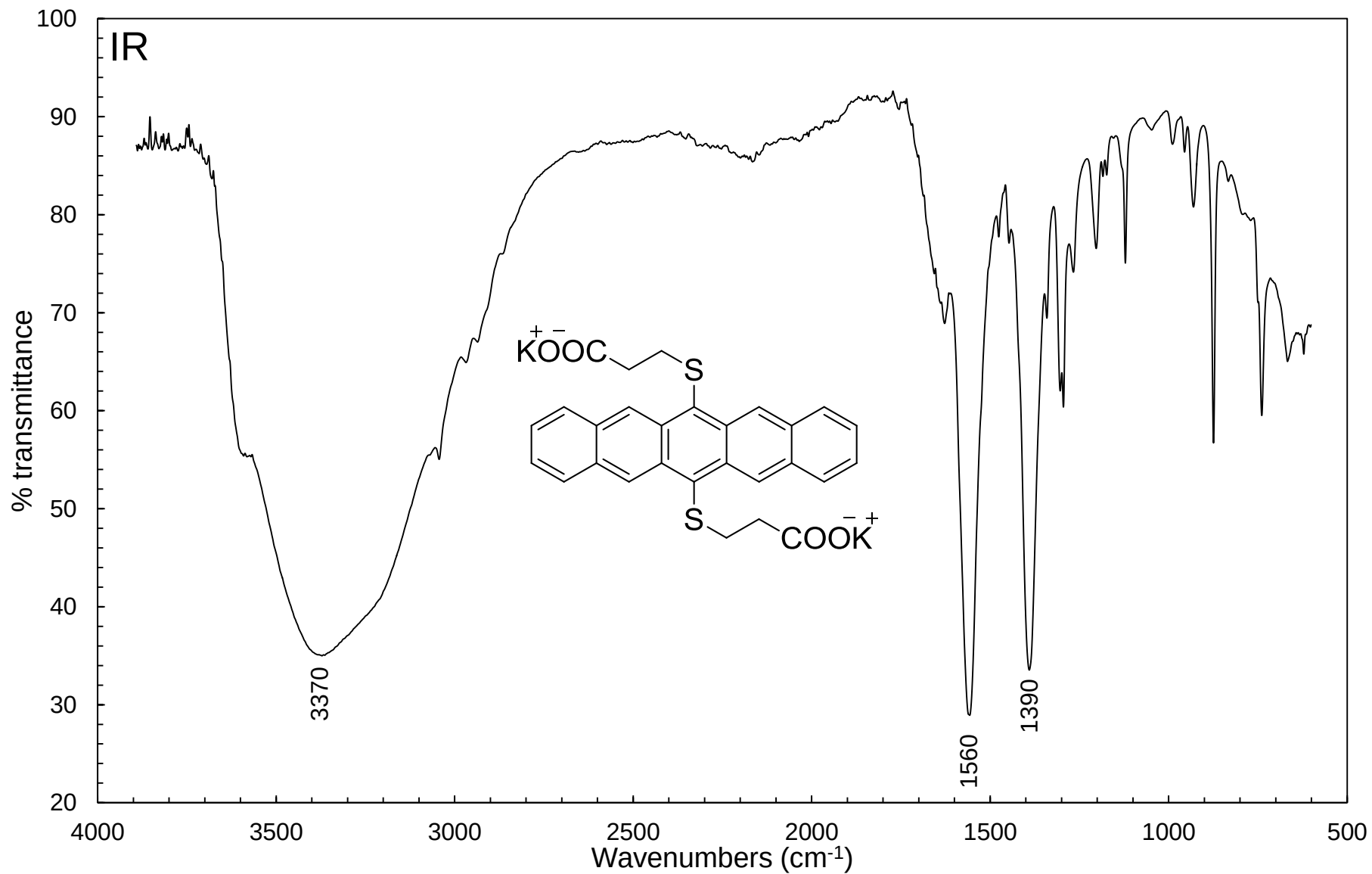


Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (**4**)

MALDI MS (matrix: sulfur)

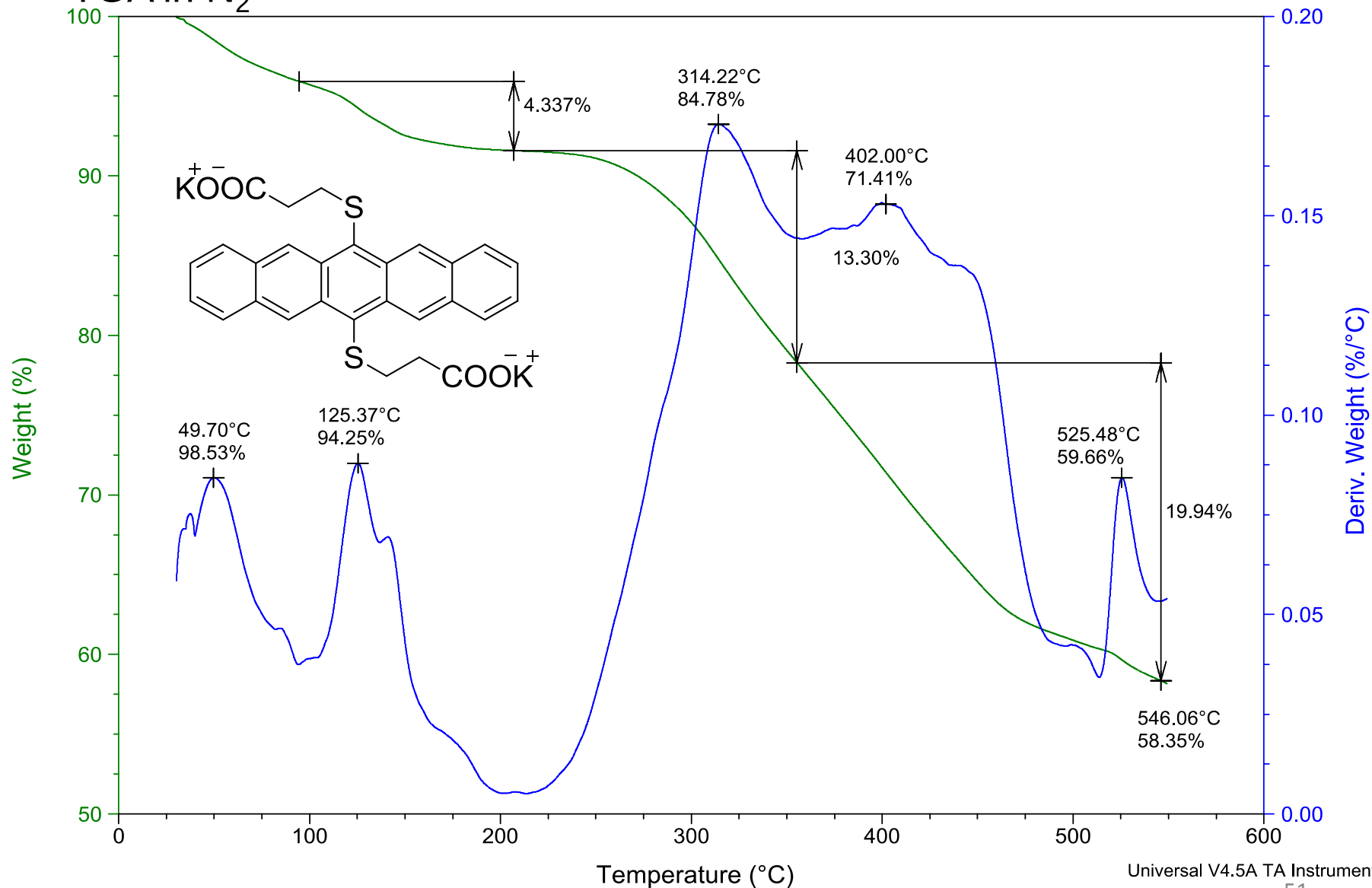


Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (**4**)

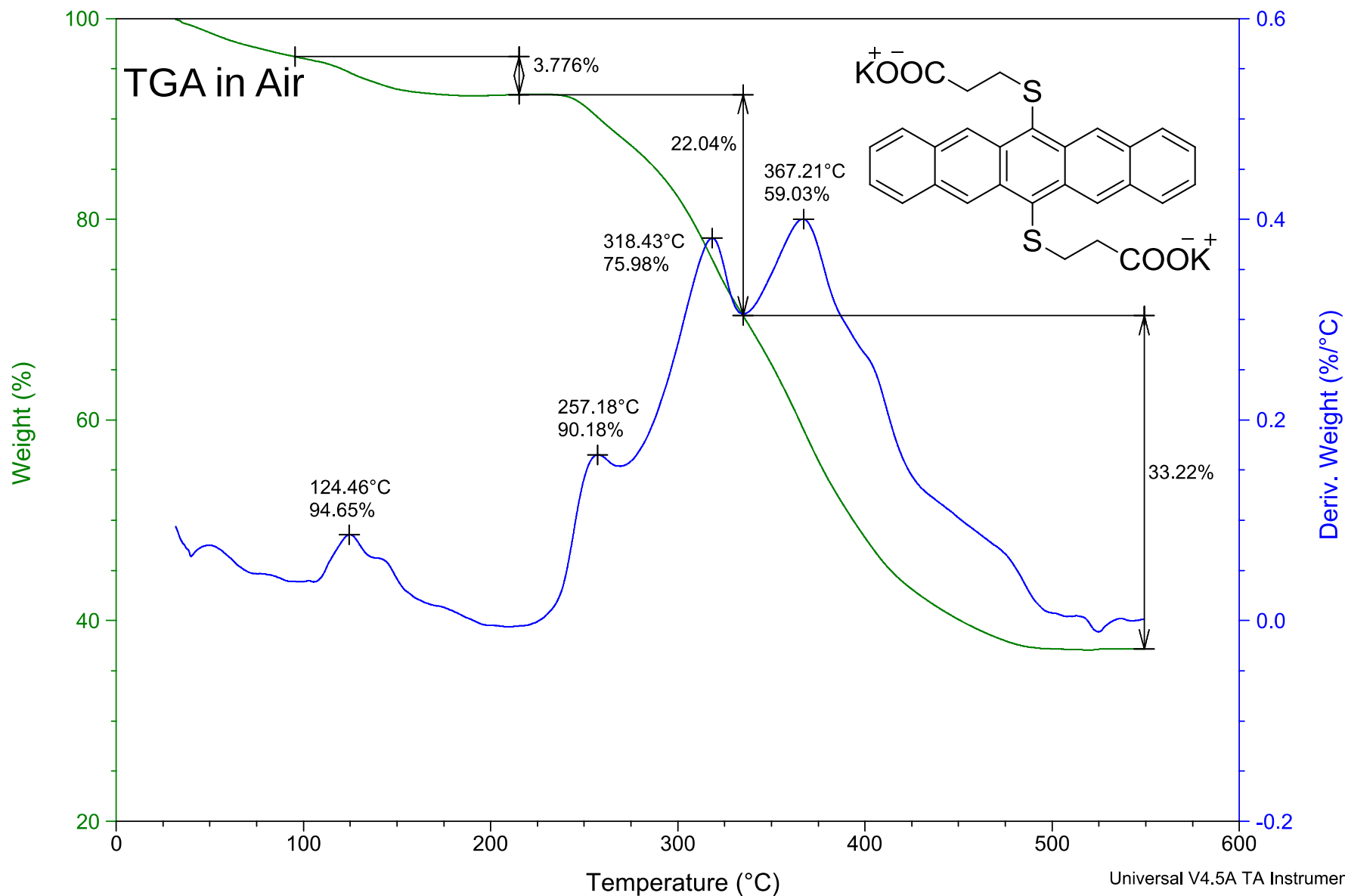


Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (**4**)

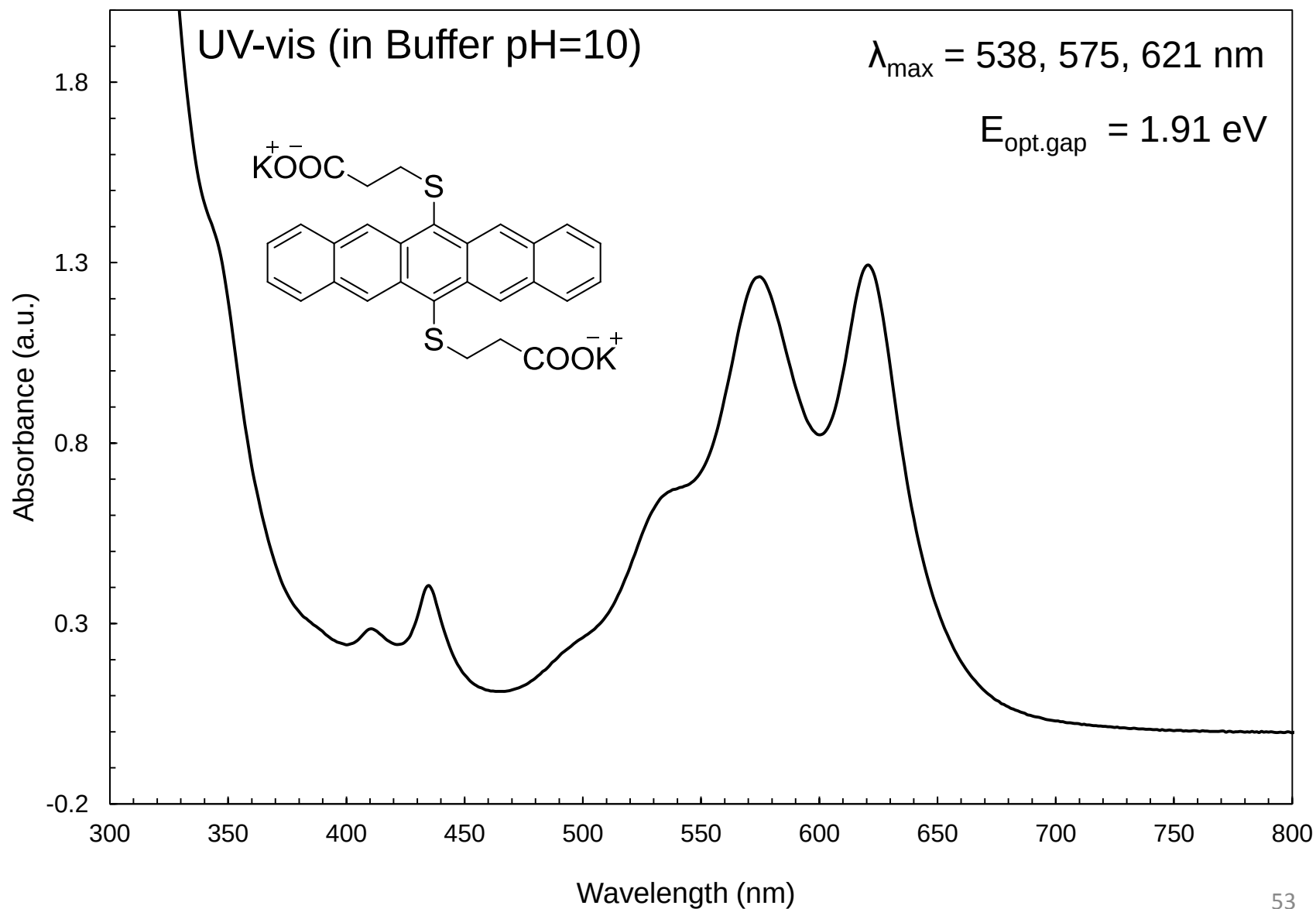
TGA in N₂



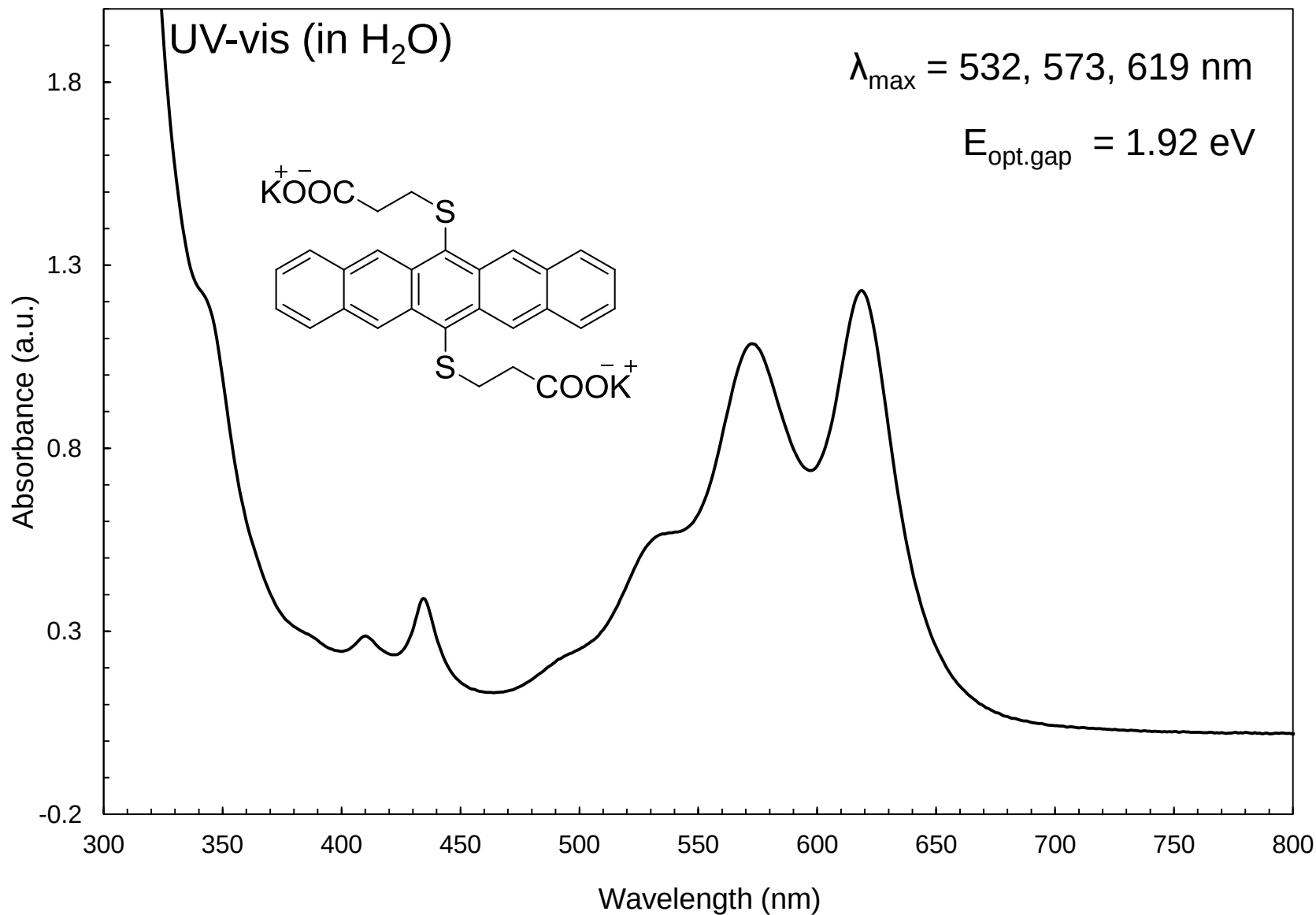
Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (4)



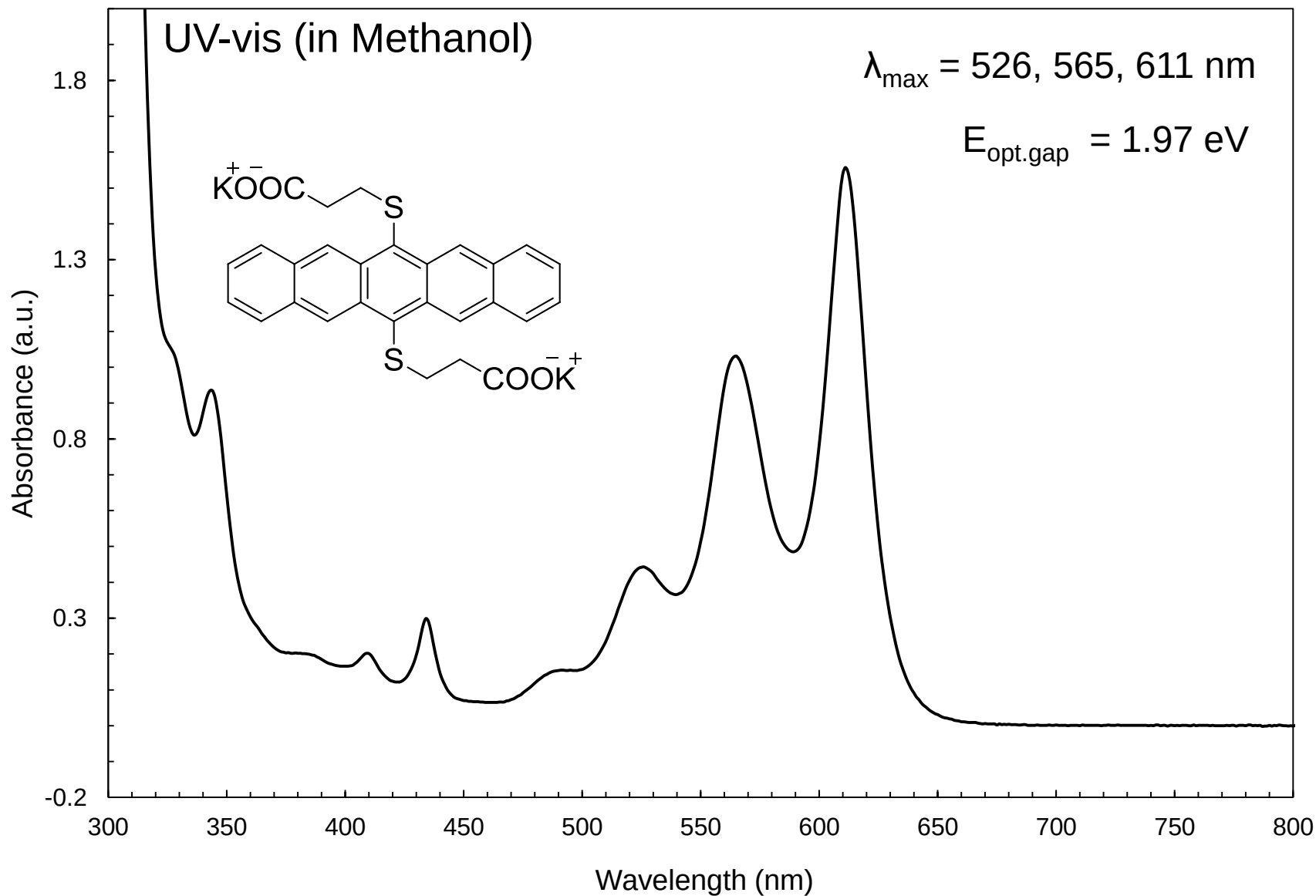
Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (**4**)



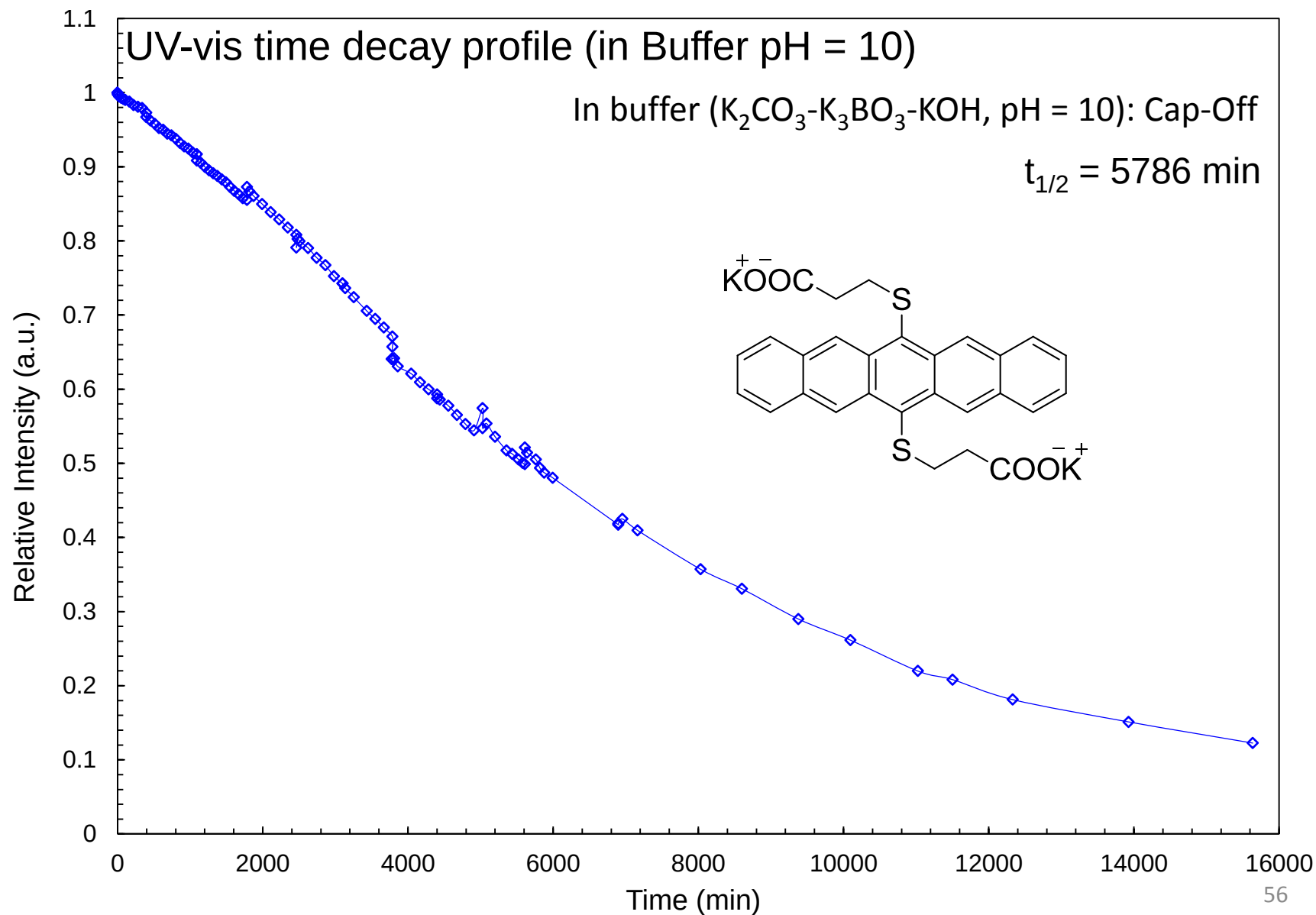
Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropionate (**4**)



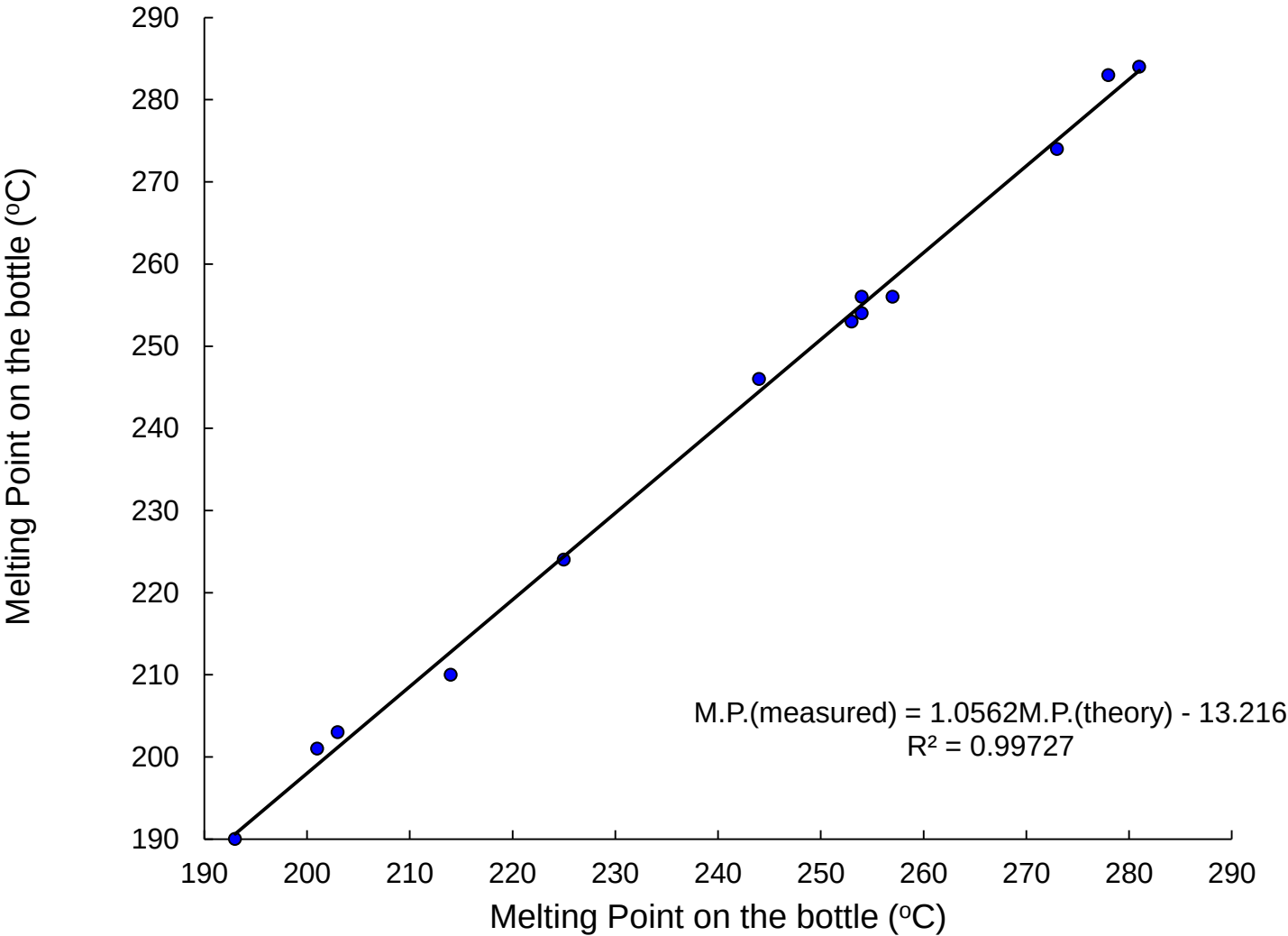
Potassium 3,3'-(pentacene-6,13-diylbis(sulfanediyl))dipropanoate (**4**)



Potassium 3,3'-(pentacene-6,13-diylbis(sulfaneydiyl))dipropionate (4)



Melting point apparatus calibration



Melting point apparatus calibration

NO.	Chemical		M.P. on bottle /°C	M.P. measured/°C
1	2,2'-Biquinoline	crystal	193	190
2	4-hydroxyquinoline	powder	201	201
3	m-hydroxybenzoic acid	crystal	203	203
4	p-hydroxybenzoic acid	powder	214	210
5	4,4'-sulfonyl diphenol	crystal	225	224
6	dicyanobenzene	powder	244	246
7	tetra bromo hydroquinone	crystal	253	253
8	tritycene	powder	254	254
9	4-quinolin carboxylic acid	powder	254	256
10	pentaerythritol	crystal	257	256
11	4-iodobenzoic acid	powder	273	274
12	3-quinolin carboxylic acid	powder	278	283
13	tetraphenylmethane	crystal	281	284

NO.	Name	M.P. measured /°C	M.P. calibrated /°C
3	3,3'-[(6,13-pentacenediyl) bis(sulfanediyl)]dipropanoic acid	235	235
4	Potassium 3,3'-[(pentacene-6,13-diyl)bis(sulfanediyl)]dipropanoate	278	276