

Supplementary Material

A fast and convenient synthesis of new water-soluble, polyanionic dendrimers.

Grzegorz M. Salamończyk

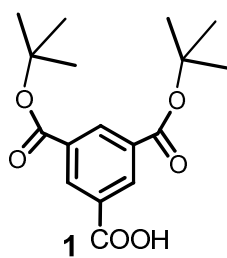
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Sienkiewicza 112, 90-363 Łódź, Poland.*

Tel.: + 48-42-684-7113; fax: +48-42-684-7126; e-mail: gmsalamo@cbmm.lodz.pl

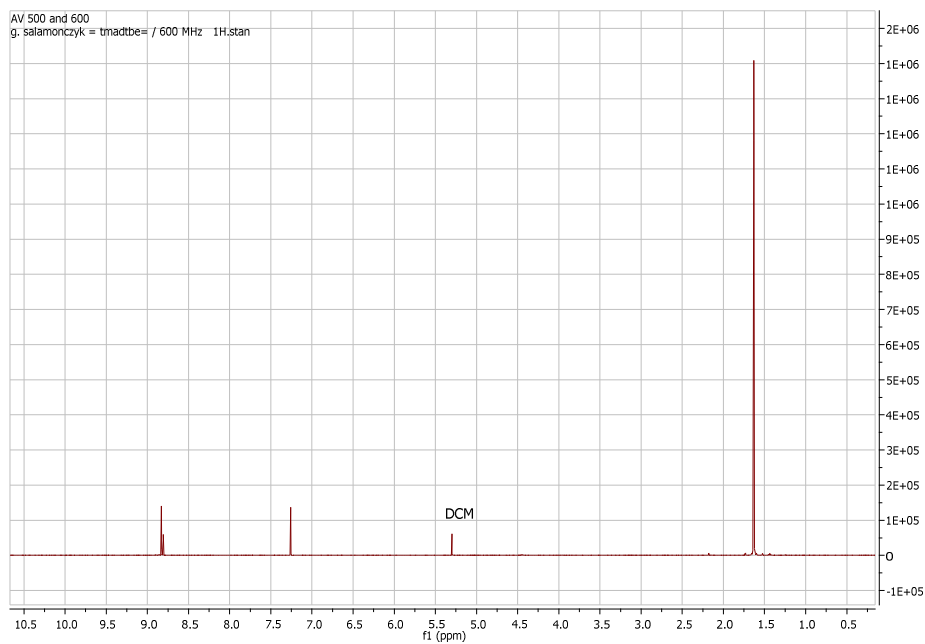
The NMR and Mass spectra.

Spectra of the acid 1	pages S2 – S3
Spectra of the benzyl-type alcohol 2	pages S3 – S4
Spectra of the dendrimer 4	pages S5 - S7
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Spectra of the dendrimer 7	pages S10 - S12
Spectra of the dendrimer 8 (9)	pages S13 - S14
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Spectra of the dendrimer 11 (12)	pages S18 - S21
Spectra of the dendrimer 14	pages S21 – S23
Spectra of the dendrimer 15 (16)	pages S24 - S25
Spectra of the dendrimer 17	pages S26 – S28
Spectra of the dendrimer 18 (19)	pages S28 – S30
Spectra of the dendrimer 21	pages S31 – S32
Spectra of the dendrimer 22 (23)	pages S33 – S35

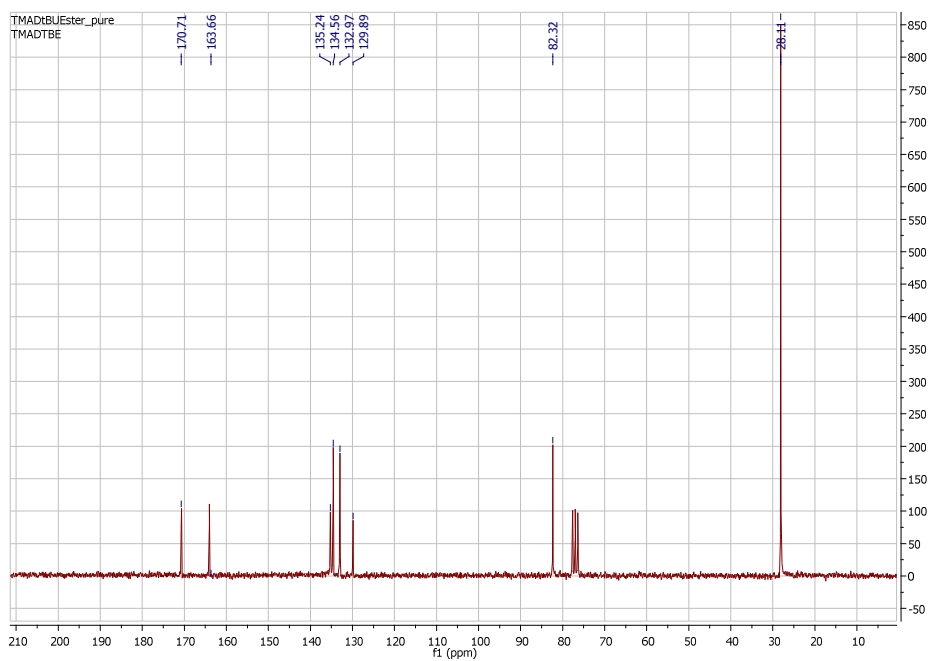
Spectra of the acid **1**.



^1H NMR



^{13}C NMR



Mass Spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 70.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Odd and Even Electron Ions

18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

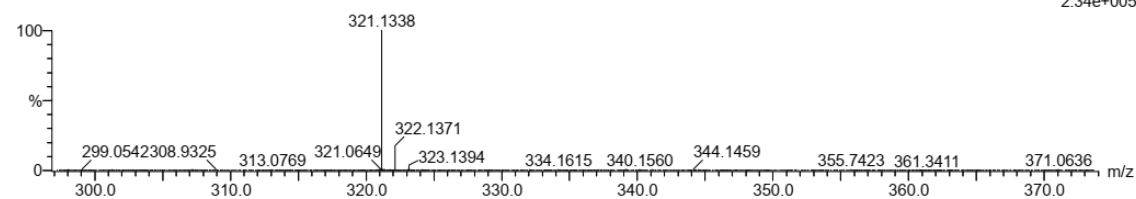
Elements Used:

C: 0-30 H: 0-25 O: 0-7

Salamo

200203_TMADTBE_APCInA 16 (0.177) Cm (14:24-(3:11+41:72))

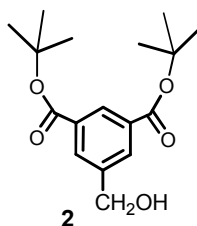
TOF MS AP-
2.34e+005



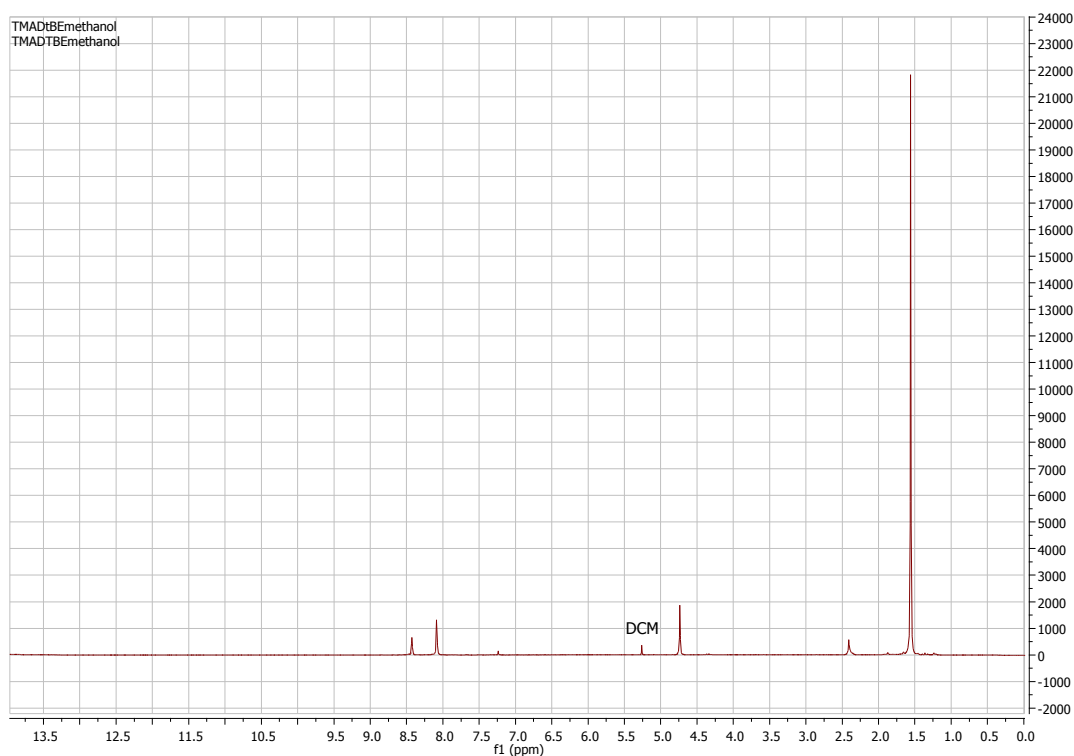
Minimum: -1.5
Maximum: 5.0 5.0 70.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
321.1338	321.1338	0.0	0.0	7.5	1539.8	n/a	n/a	C17 H21 O6

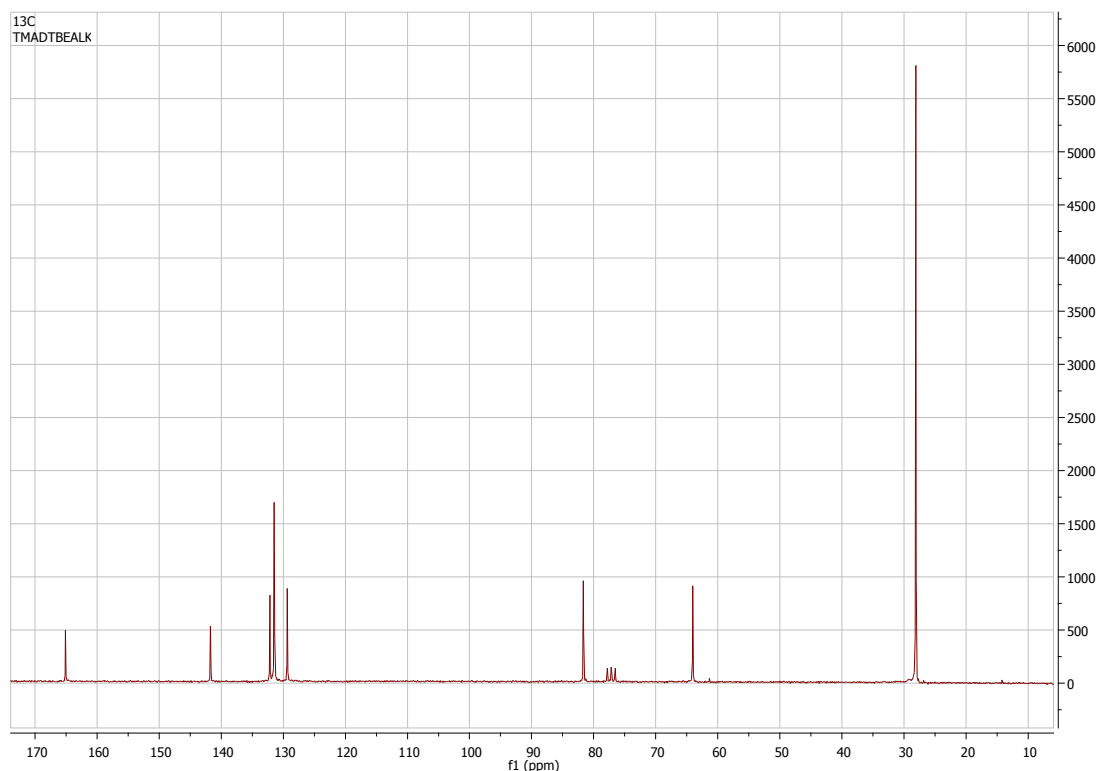
Spectra of the benzyl-type alcohol 2



¹H NMR



¹³C NMR



Mass Spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 70.0

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Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Odd and Even Electron Ions

18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

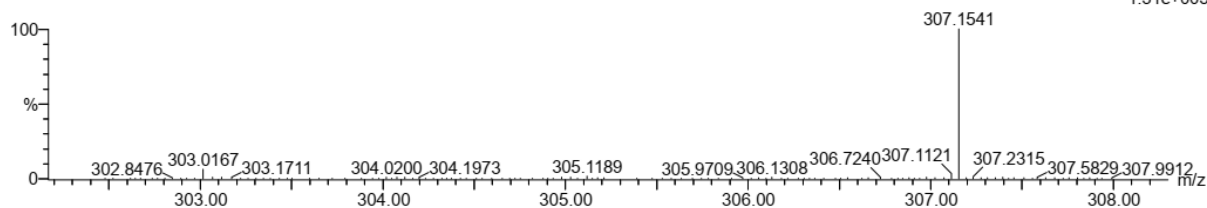
Elements Used:

C: 0-30 H: 0-25 O: 0-7

Salmo

200203_TMADTBEalk_APCInA 16 (0.177) Cm (14:20-(3:11+36:72))

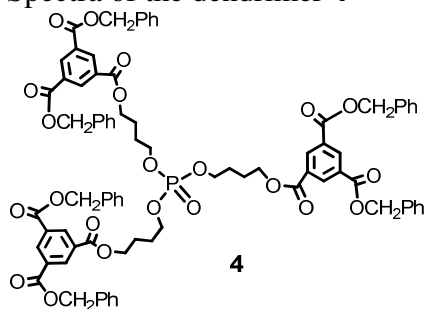
TOF MS AP-
1.31e+005



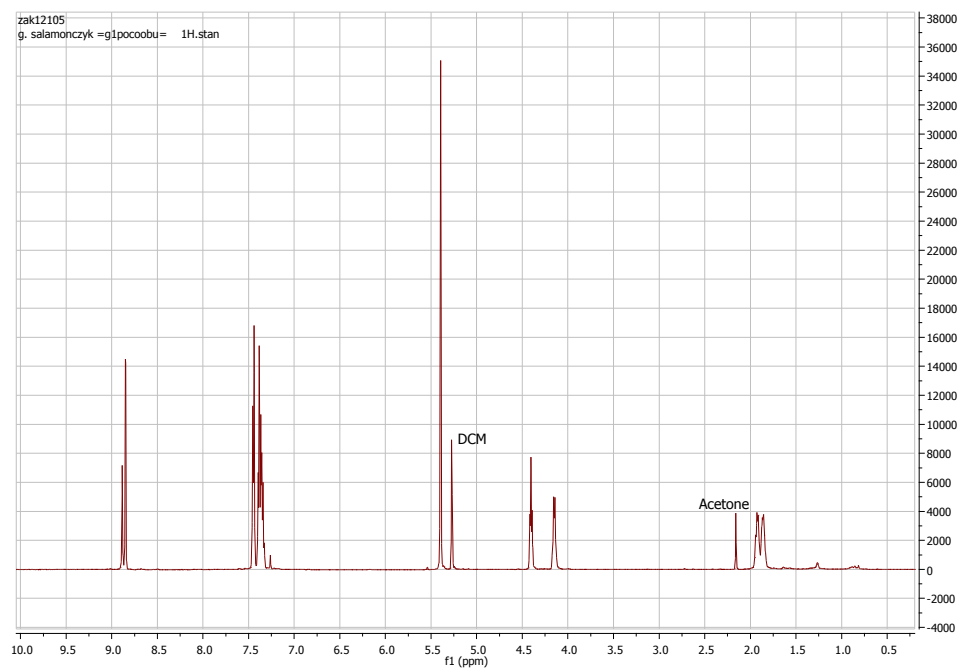
Minimum: -1.5
Maximum: 5.0 5.0 70.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
307.1541	307.1545	-0.4	-1.3	6.5	271.9	n/a	n/a	C17 H23 O5

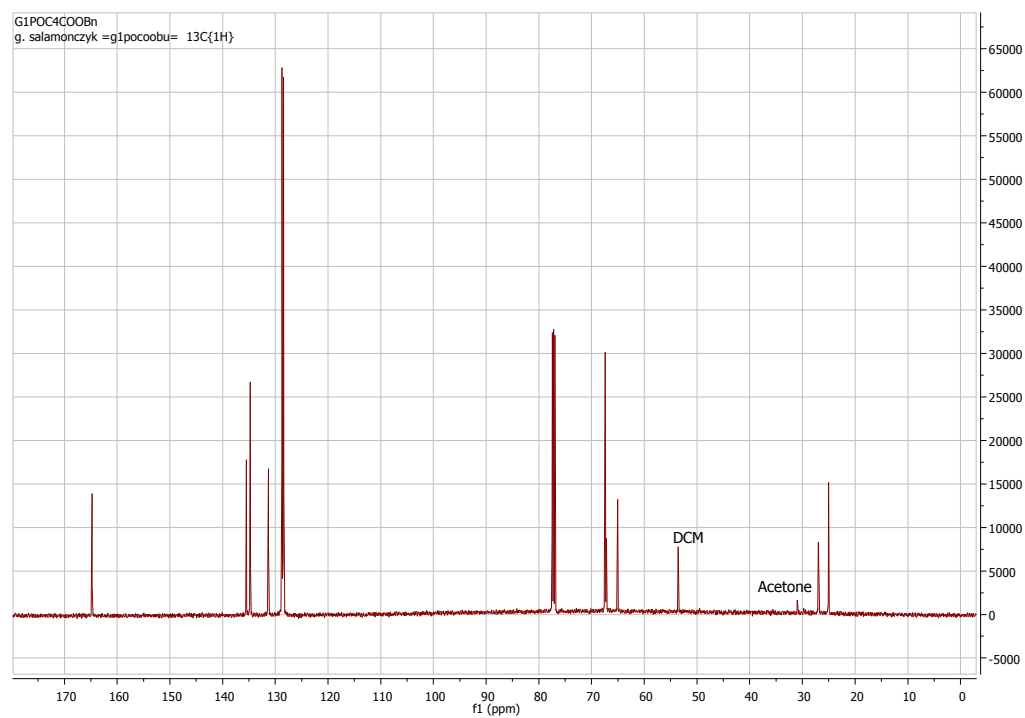
Spectra of the dendrimer **4**



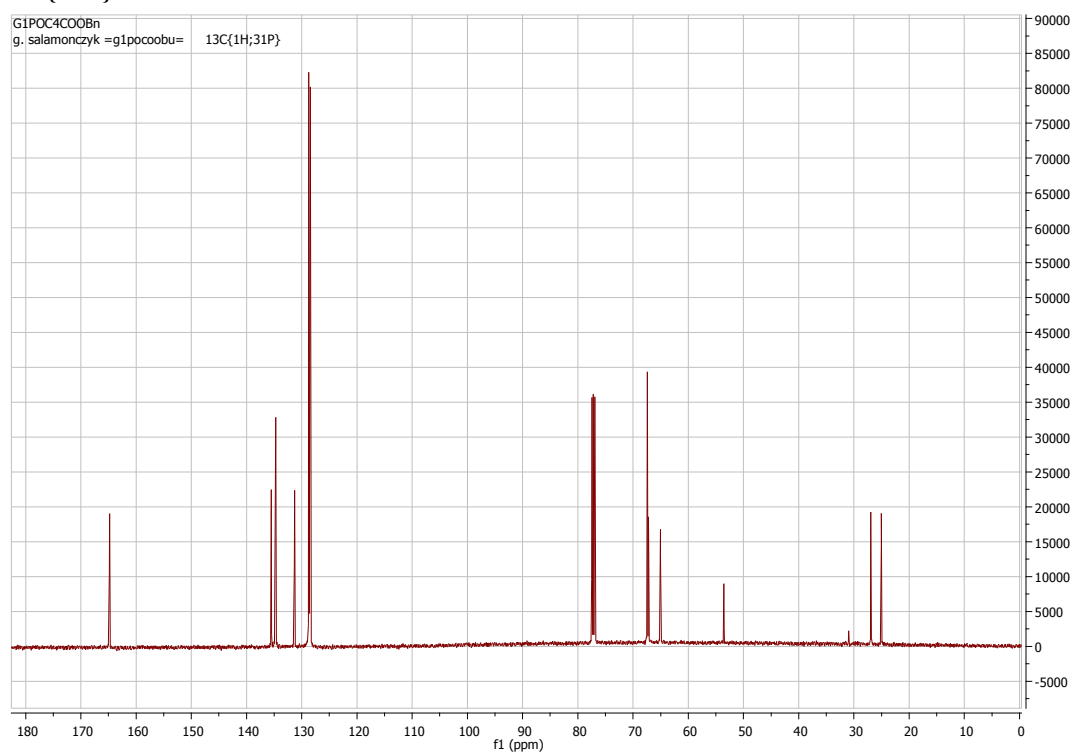
^1H NMR



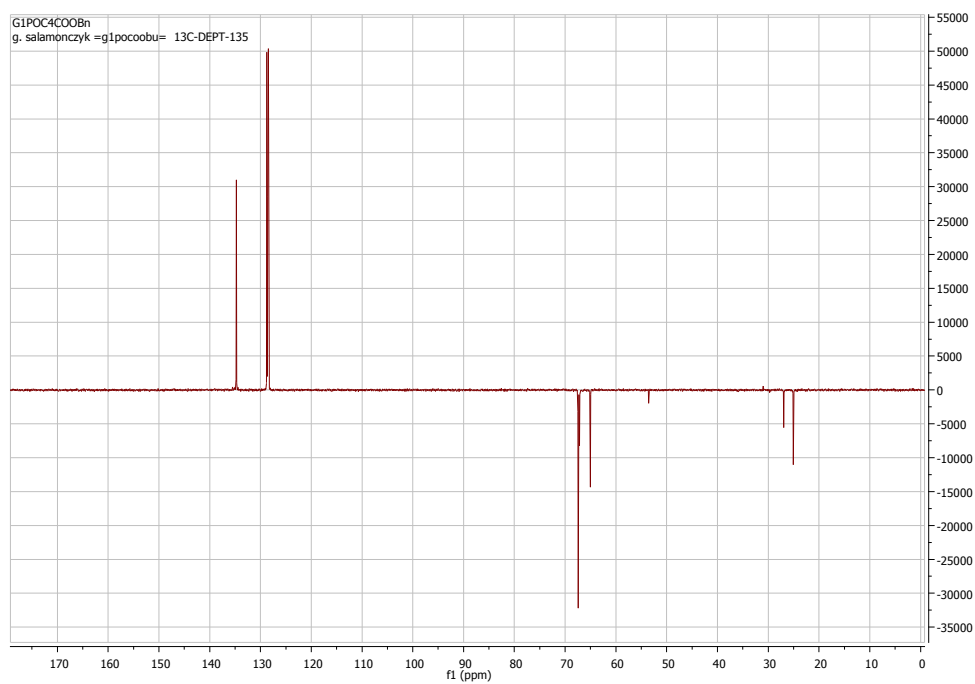
^{13}C NMR



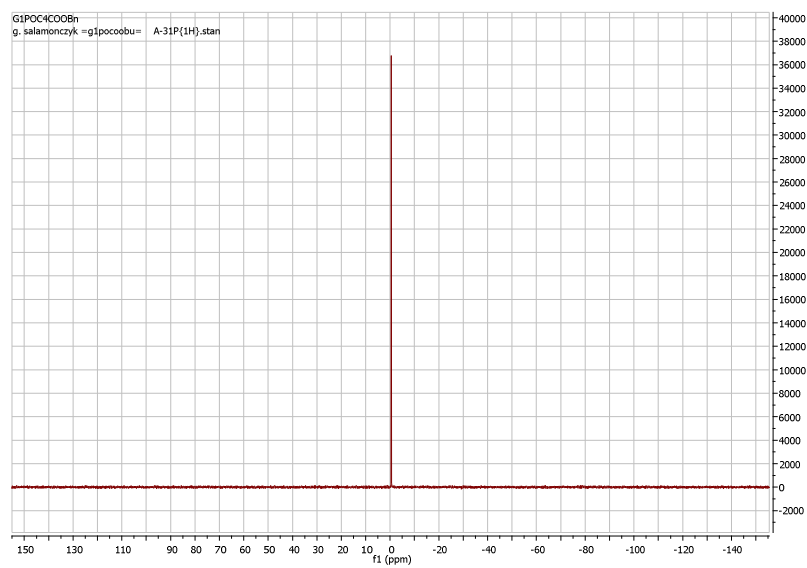
$^{13}\text{C}\{^{31}\text{P}\}$ NMR



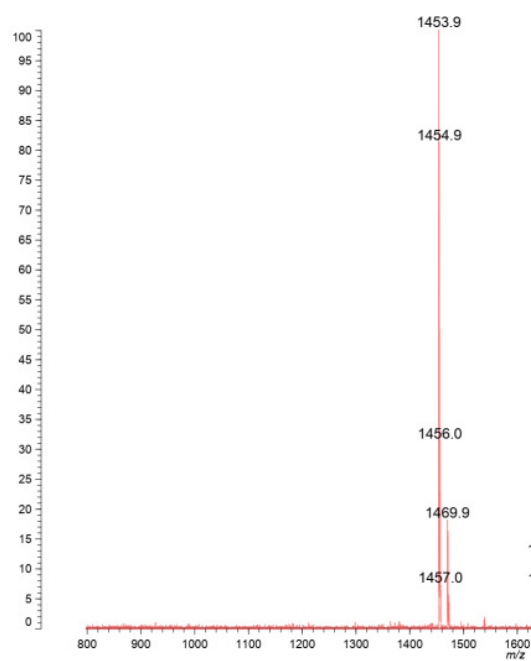
^{13}C DEPT-135 NMR



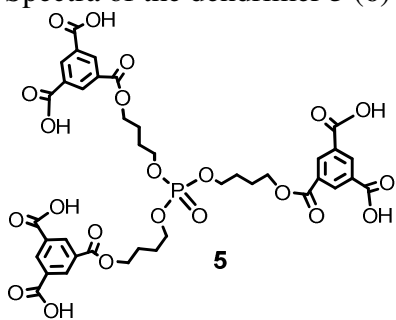
³¹P NMR



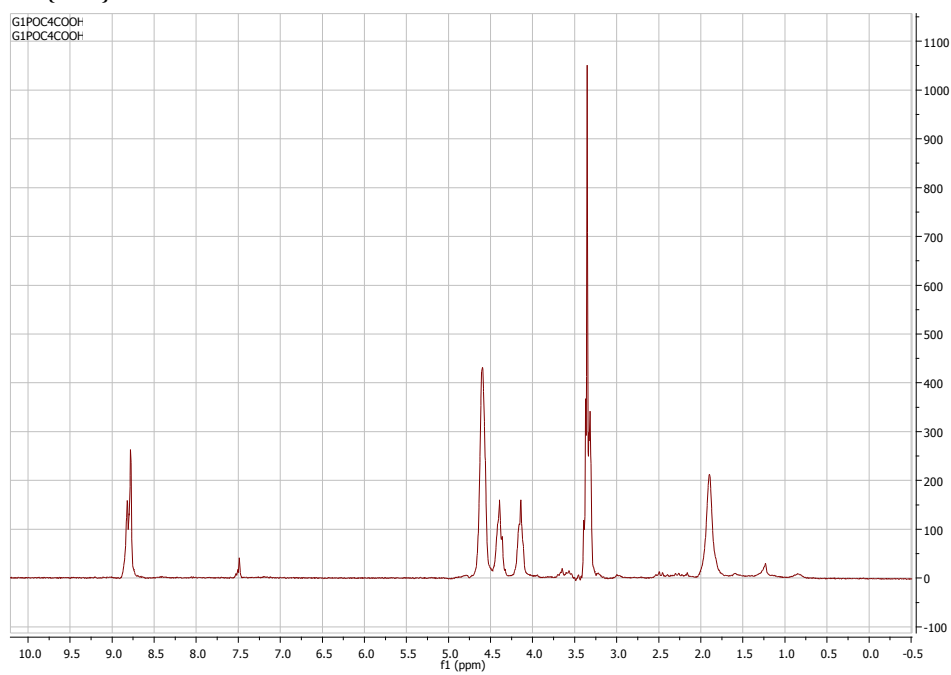
Mass Spectrum



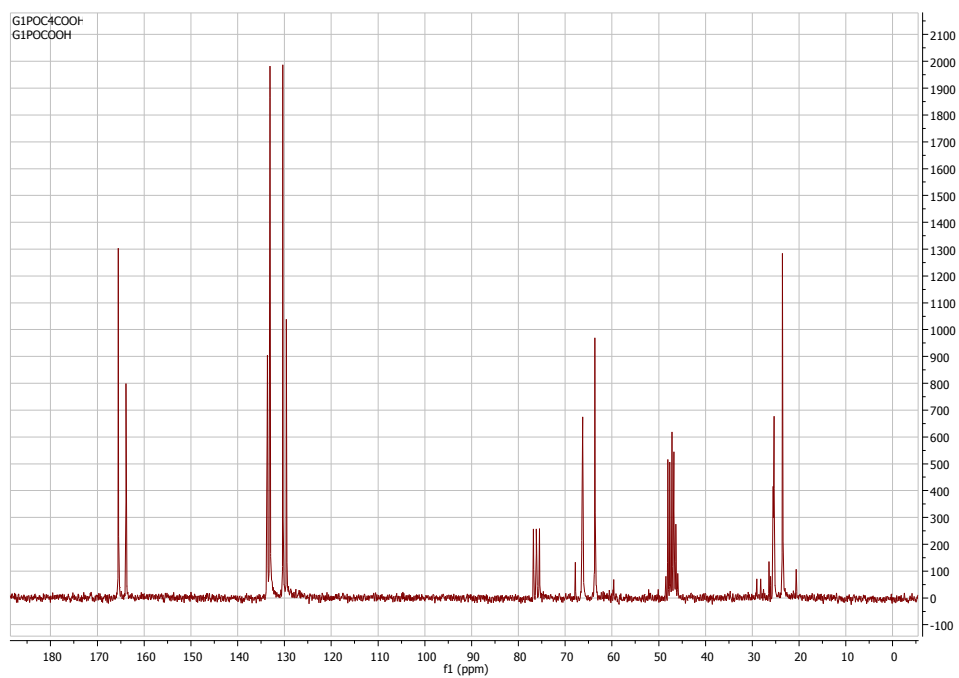
Spectra of the dendrimer **5** (**6**)



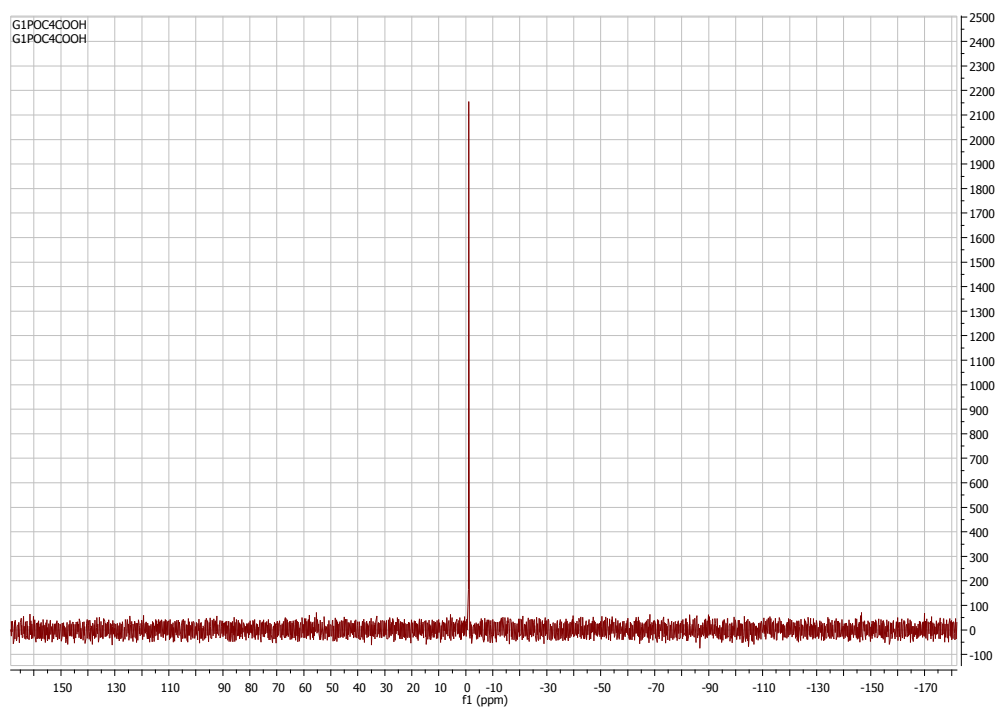
$^1\text{H} \{^3\text{1P}\}$ NMR



^{13}C NMR



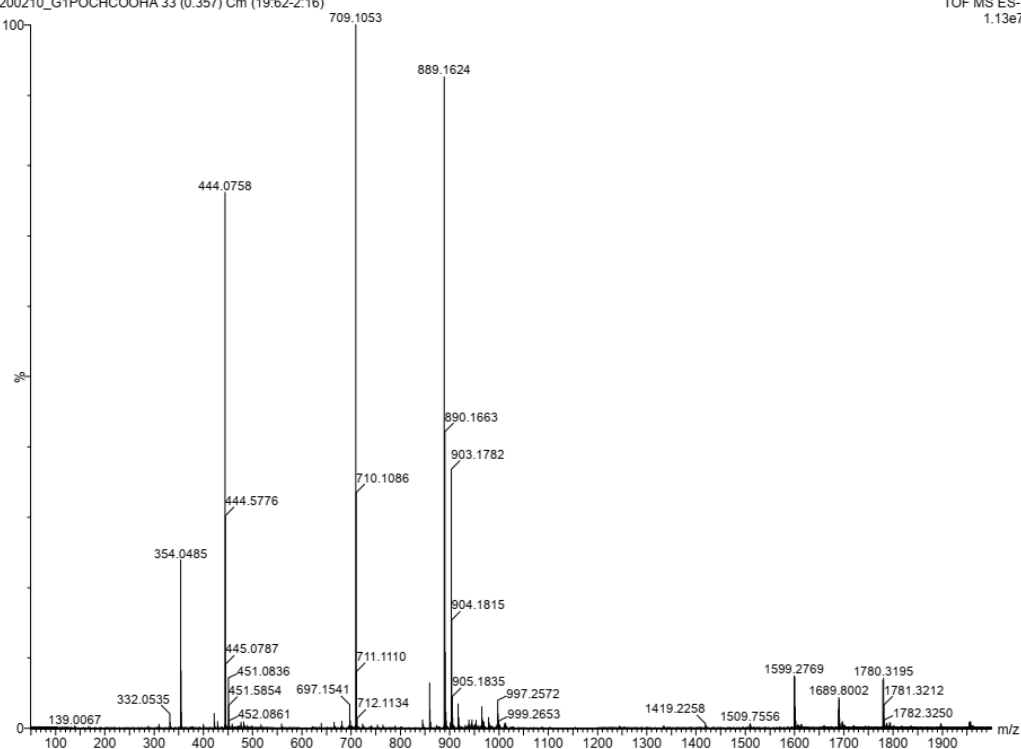
^{31}P NMR



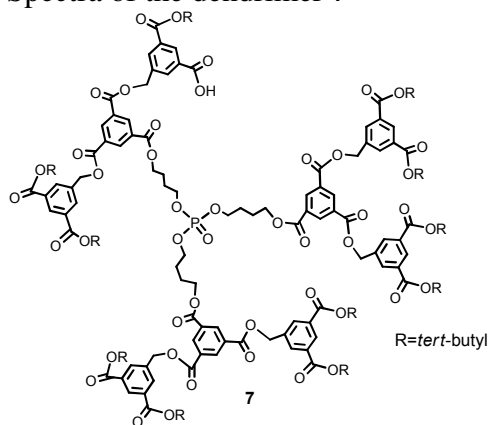
Mass Spectrum

Salamonczyk
200210_G1POCHCOOHA 33 (0.357) Cm (19:62-2:16)

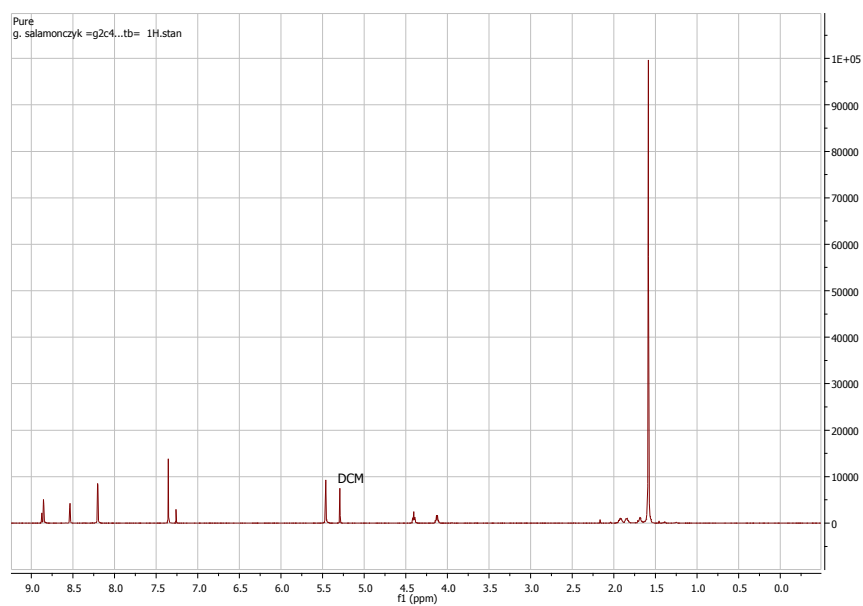
TOF MS ES-
1.13e7



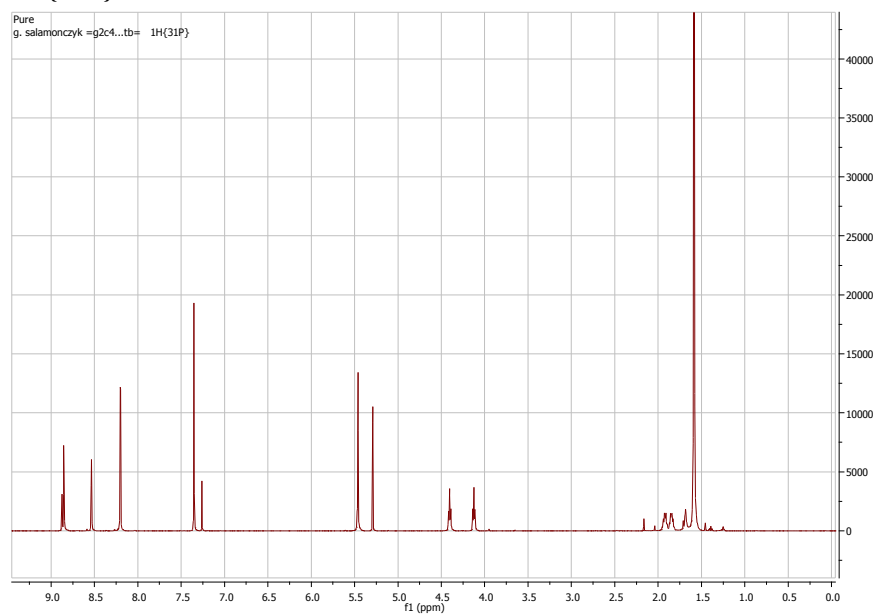
Spectra of the dendrimer **7**



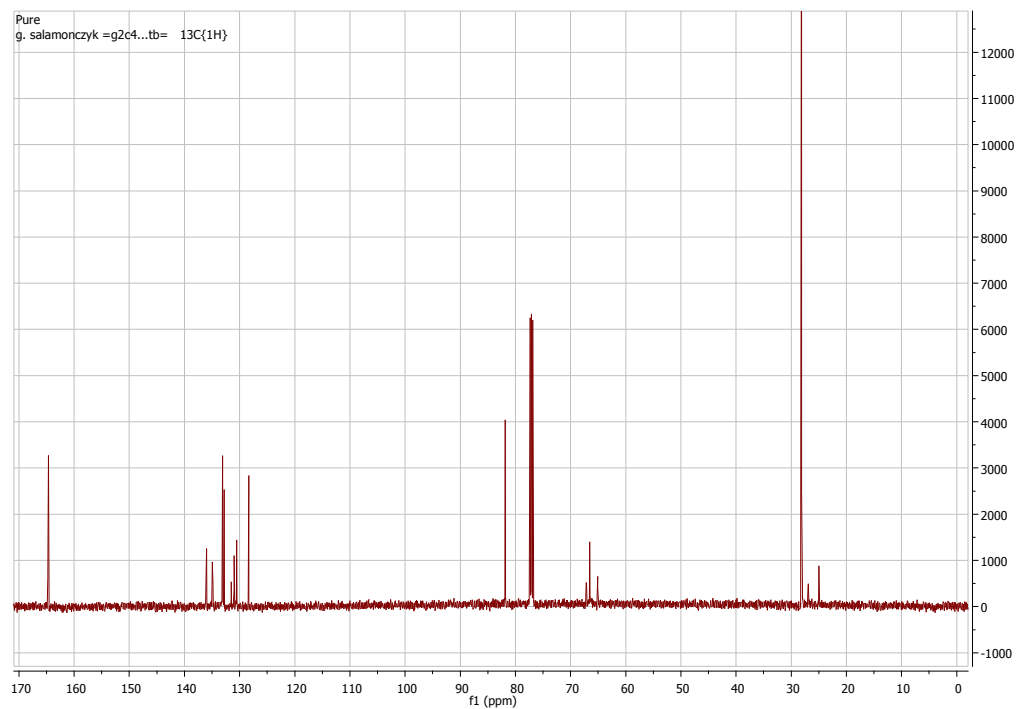
^1H NMR



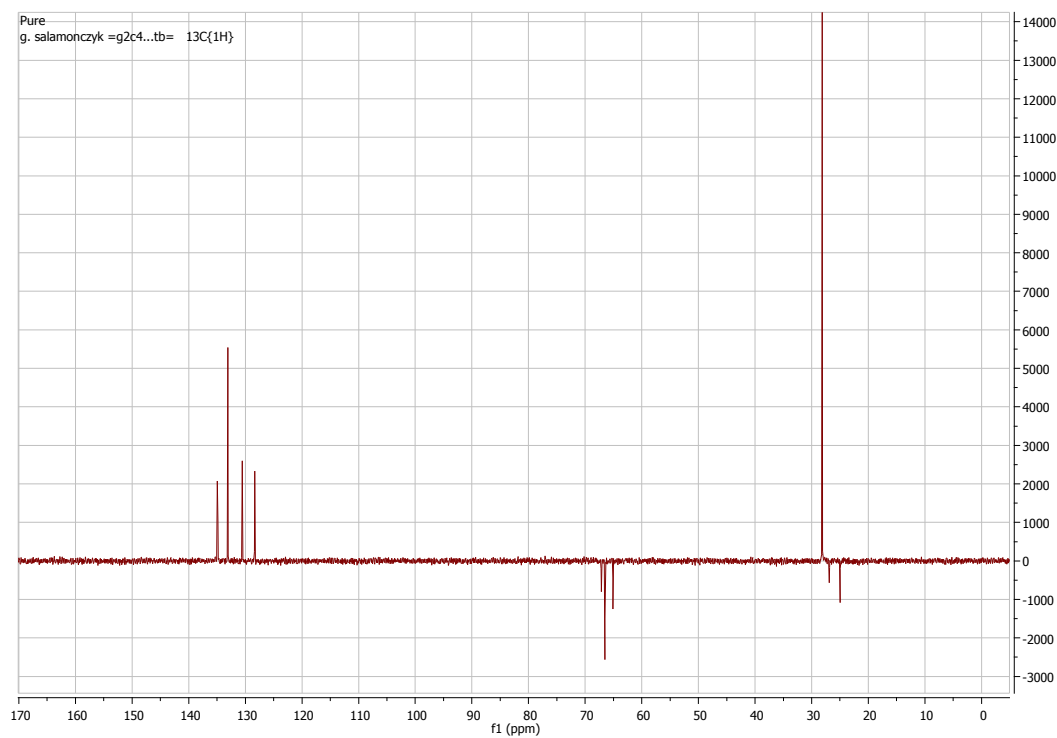
$^1\text{H} \{^3\text{P}\}$ NMR



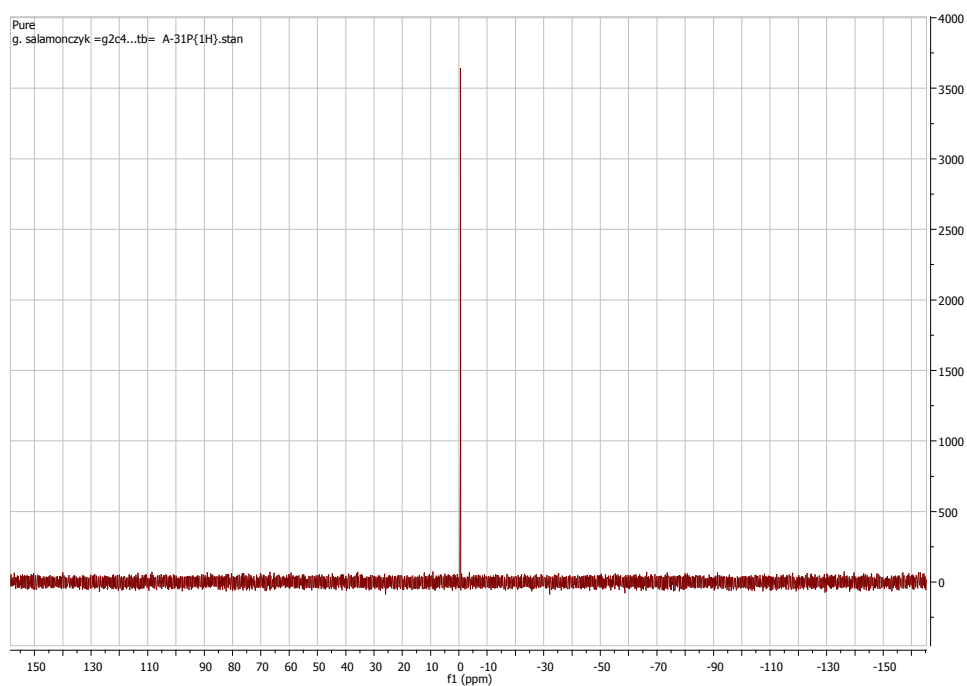
¹³C NMR



¹³C DEPT-135 NMR



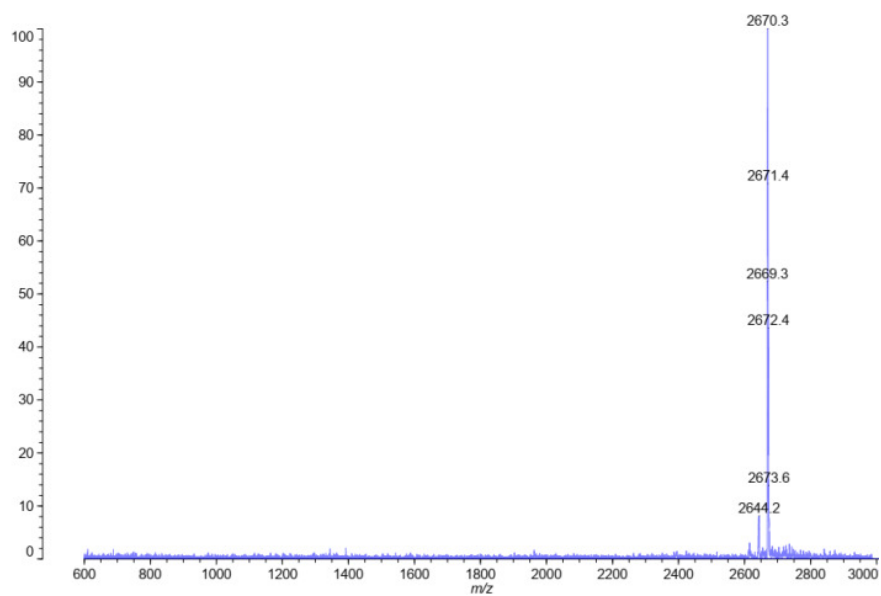
^{31}P NMR



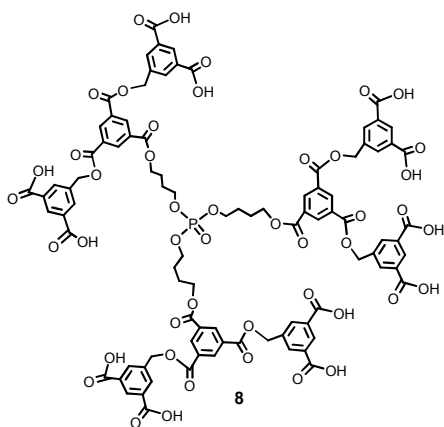
Mass Spectrum

G.Salamonczyk, G2C4POCOCOOTB; linear pos

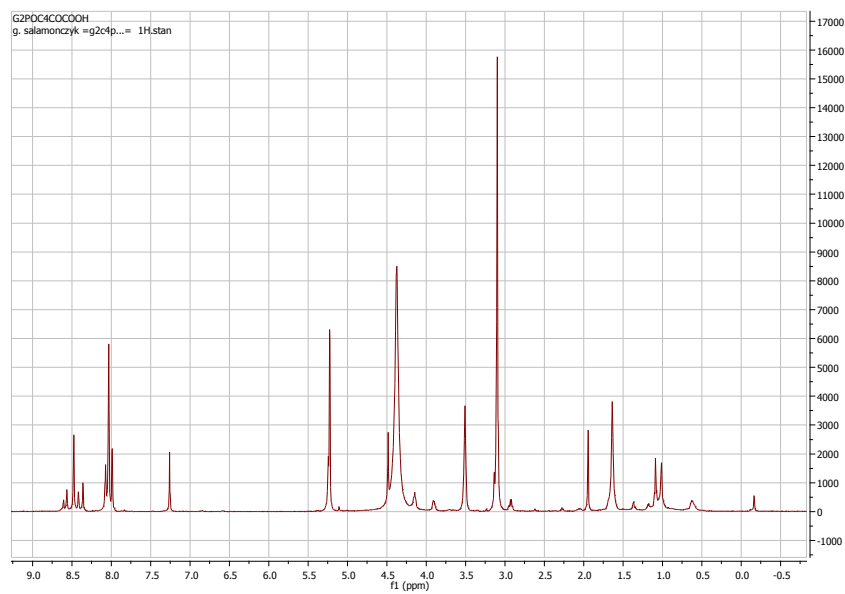
Data: hr870001.F8[c] 10 Jul 2020 13:01 Cal: PEG 2000 (06/2020) 22 Jun 2020 12:42
Shimadzu Biotech Axima Performance 2.9.1.20100121: Mode Linear_2018, Power: 80, Blanked, P.Ext. @ 3000 (bin 78)
%Int. 1.3 mV[sum= 266 mV] Profiles 1-200 Smooth Av 5 -Baseline 20



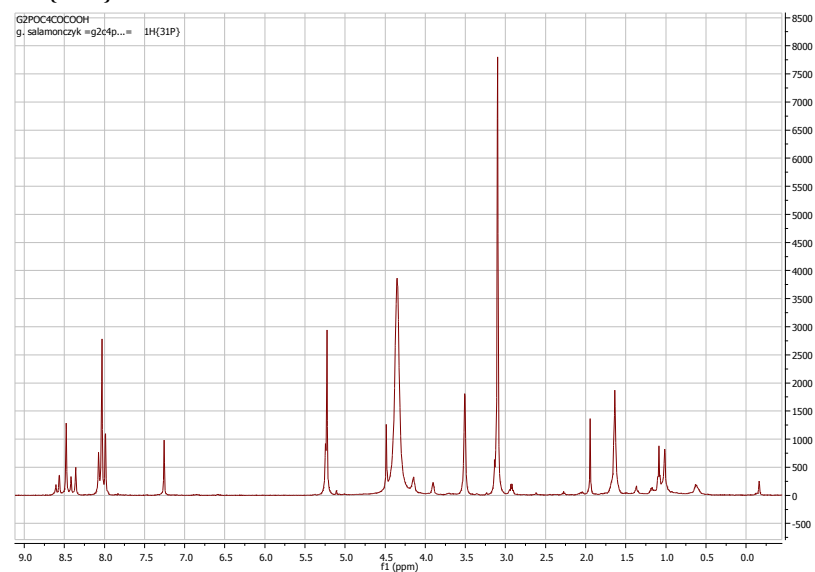
Spectra of the dendrimer **8** (9)



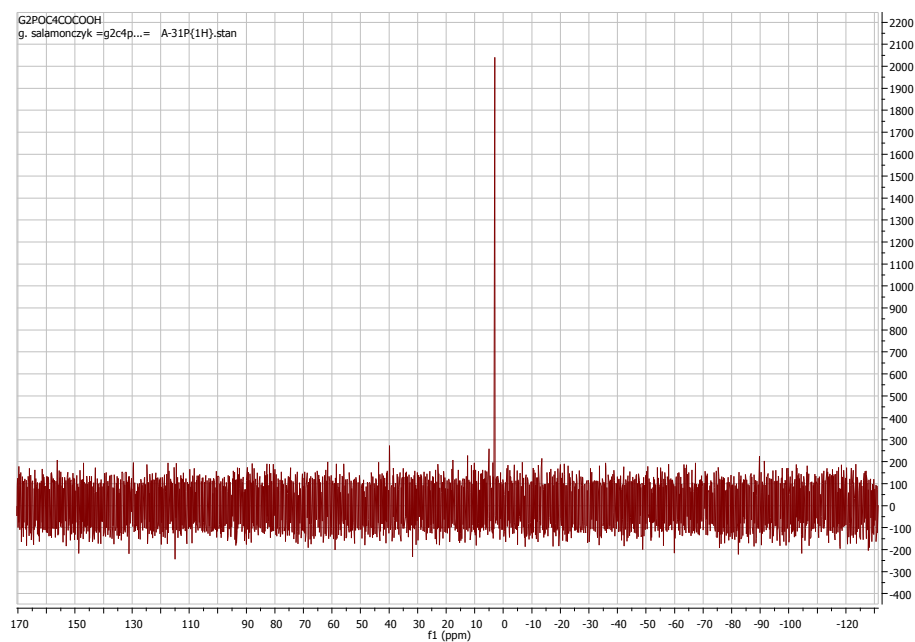
^1H NMR



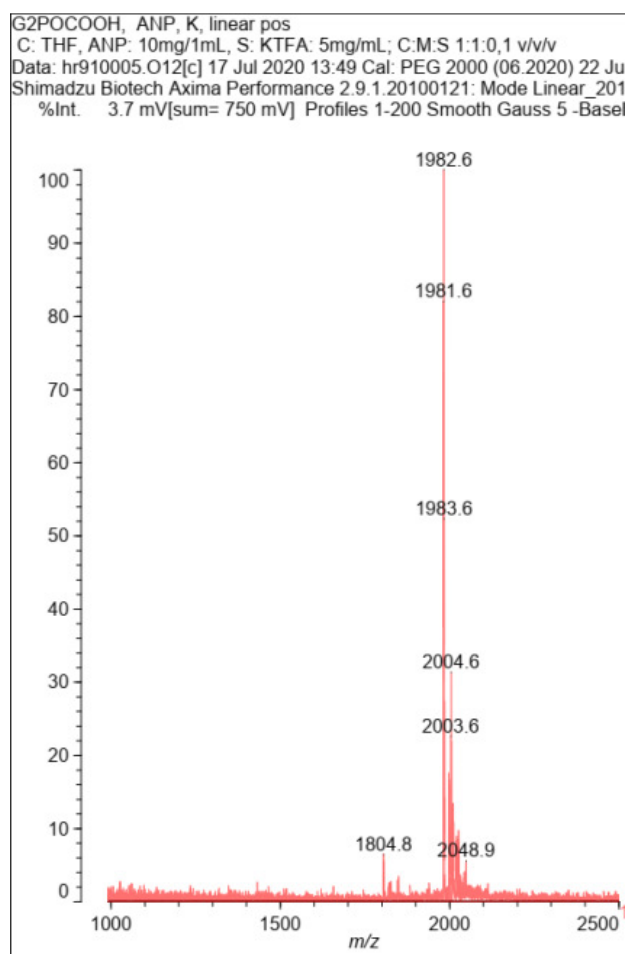
$^1\text{H} \{^3\text{P}\}$ NMR



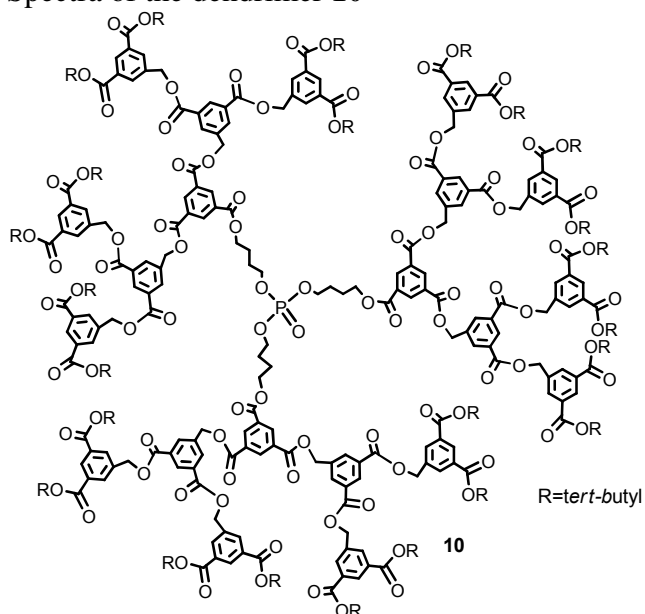
^{31}P NMR



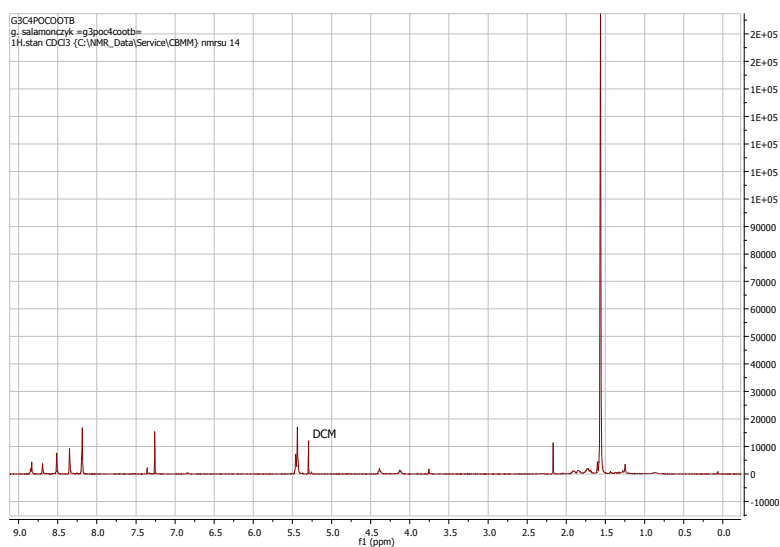
Mass Spectrum



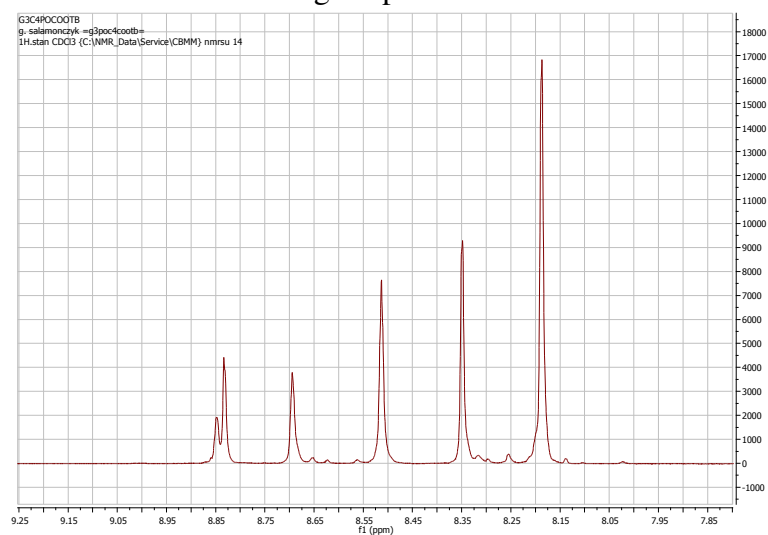
Spectra of the dendrimer **10**



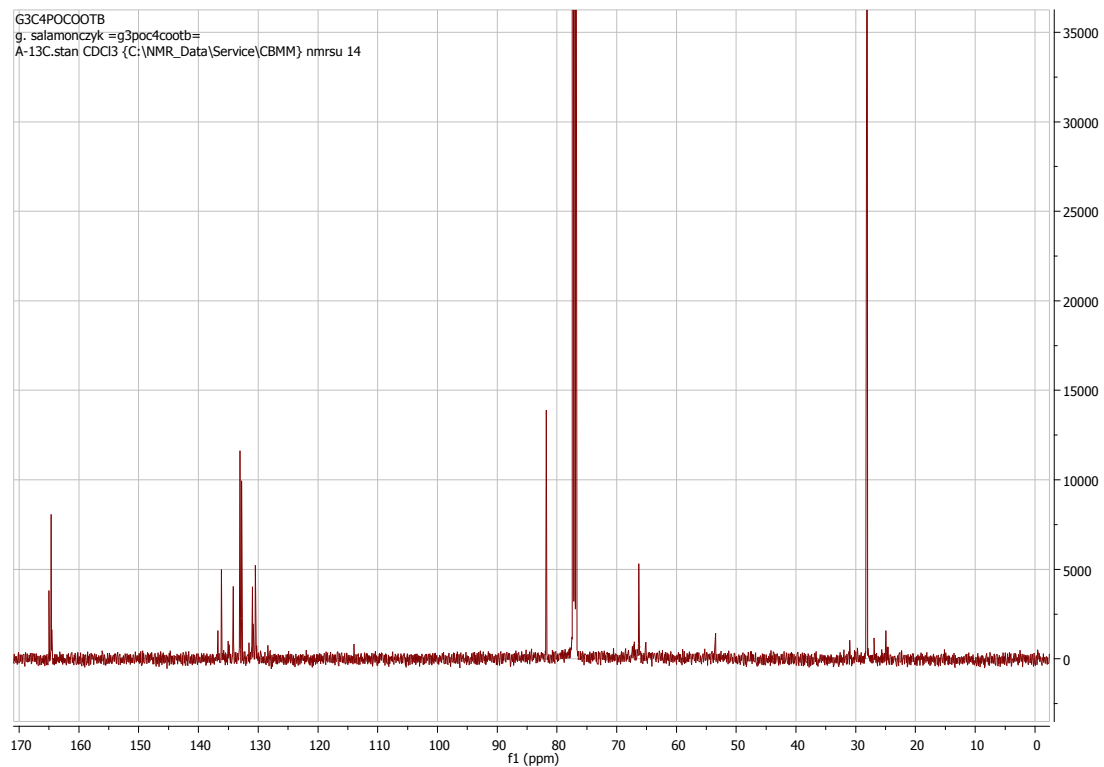
¹H NMR



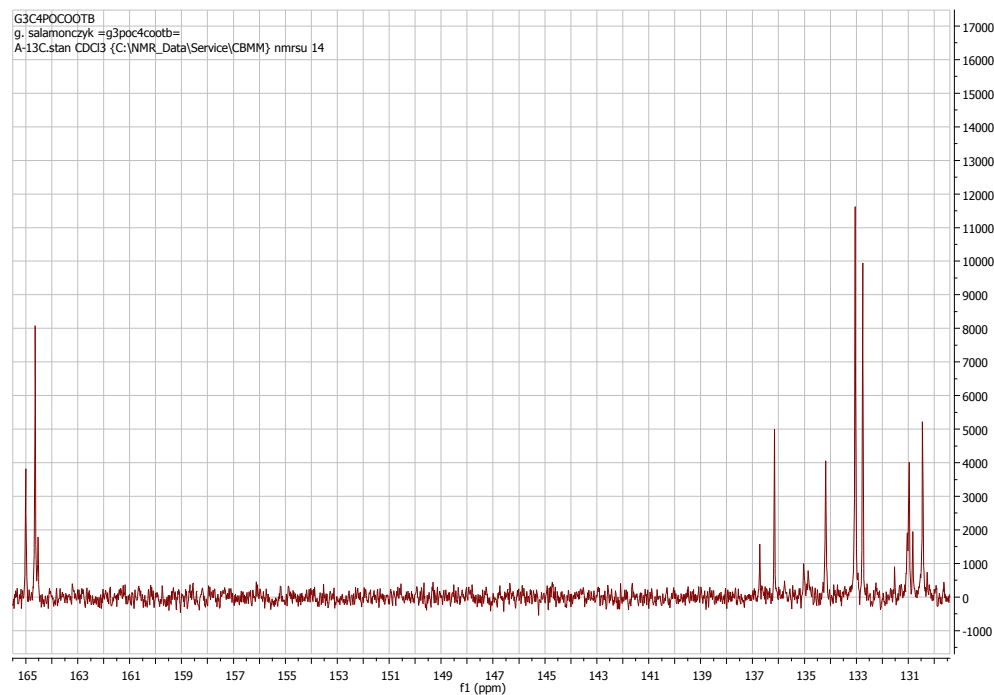
¹H NMR – aromatic range expansion



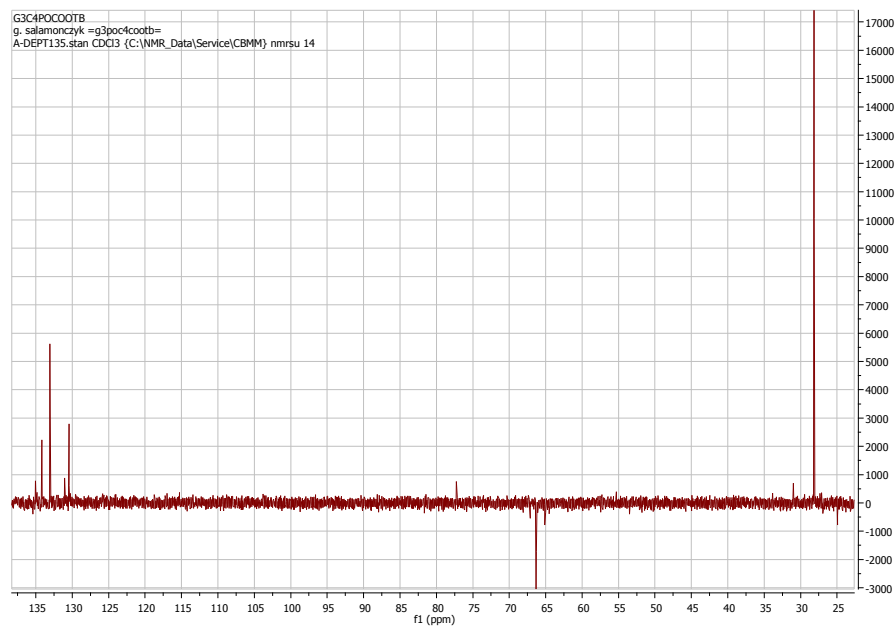
^{13}C NMR



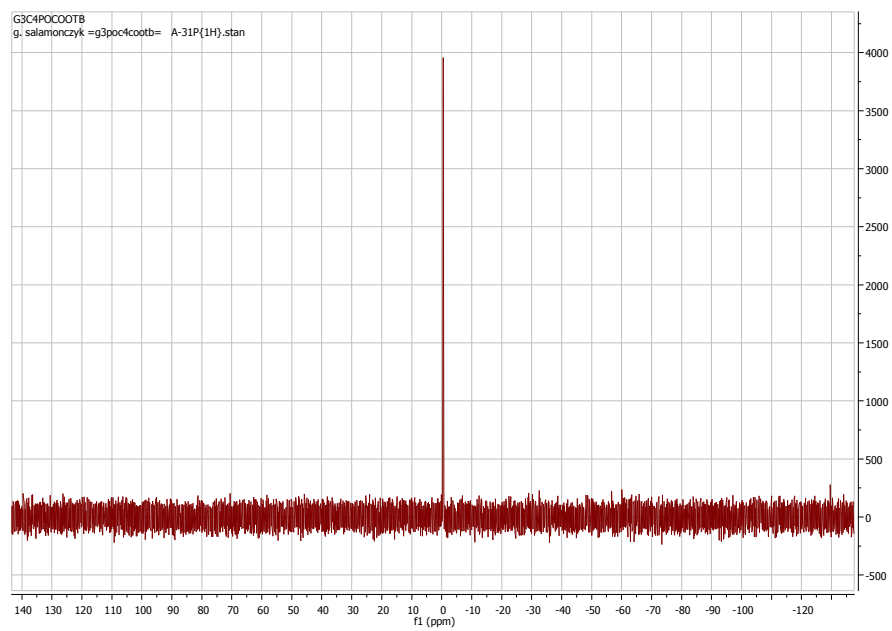
^{13}C NMR – aromatic and carbonyl range expansion



^{13}C NMR – DEPT 135

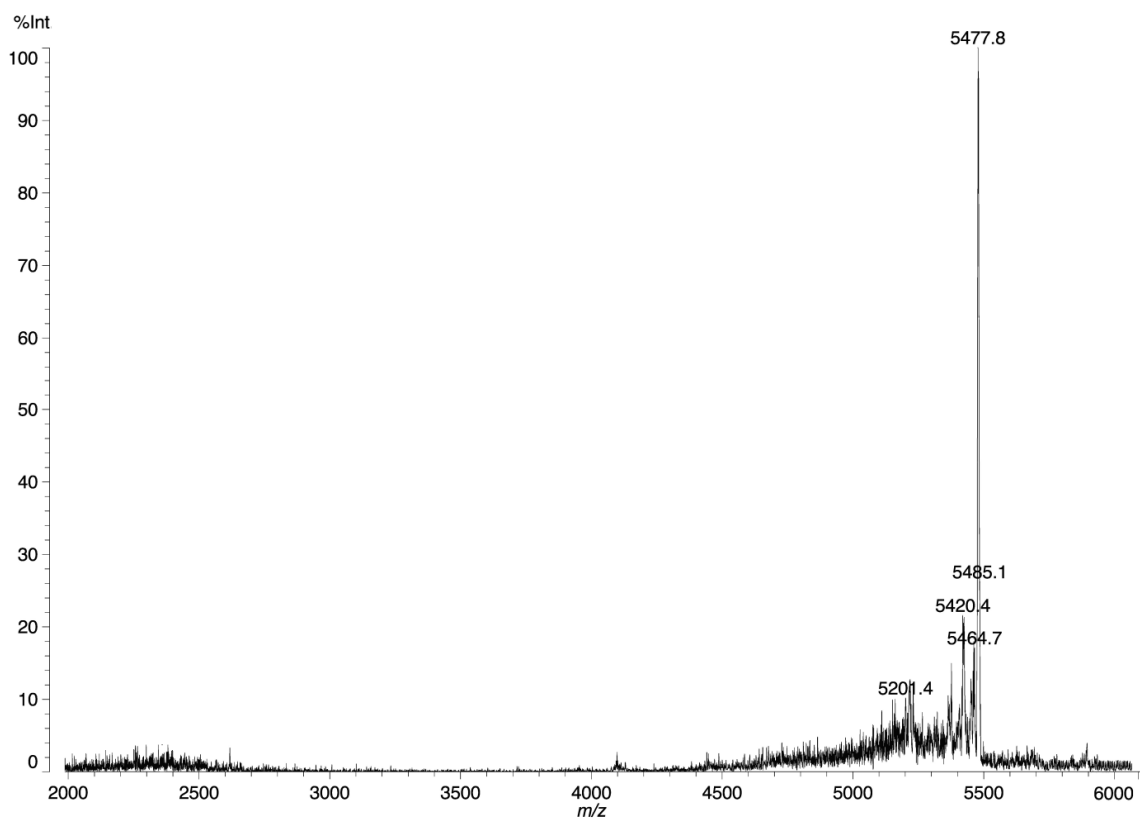


^{31}P NMR

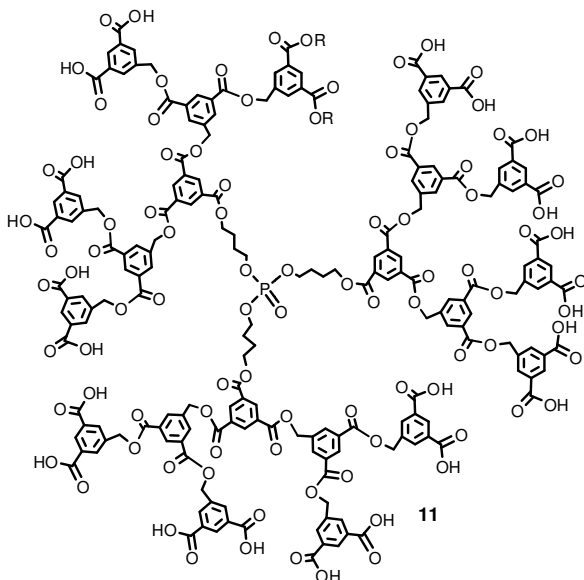


MALDI TOF Mass Spectrum

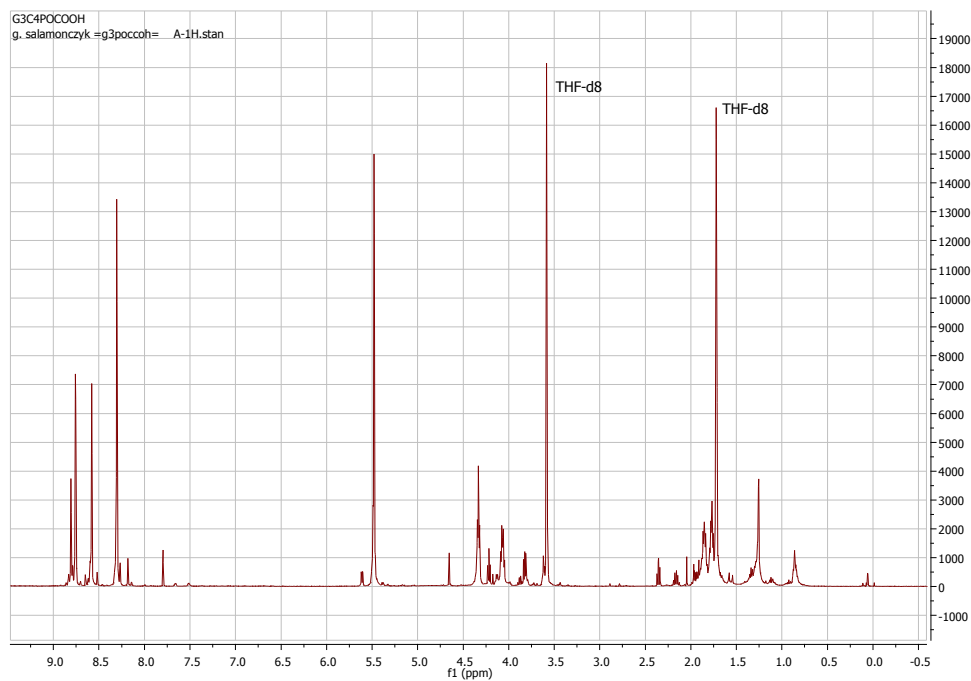
iC4POCOOTB; linear pos
THF; M: DCTB 10mg/1ml CH₂Cl₂; S: KTFA 5mg/1ml H₂O, P/M/S 10/10/1 v/v/v
ta: hw480003.D20[c] 4 Sep 2020 13:07 Cal: PEG 2000 (06.2020) 22 Jun 2020 12:42
1.9 mV[sum= 372 mV] Profiles 1-200 Smooth Av 5 -Baseline 60



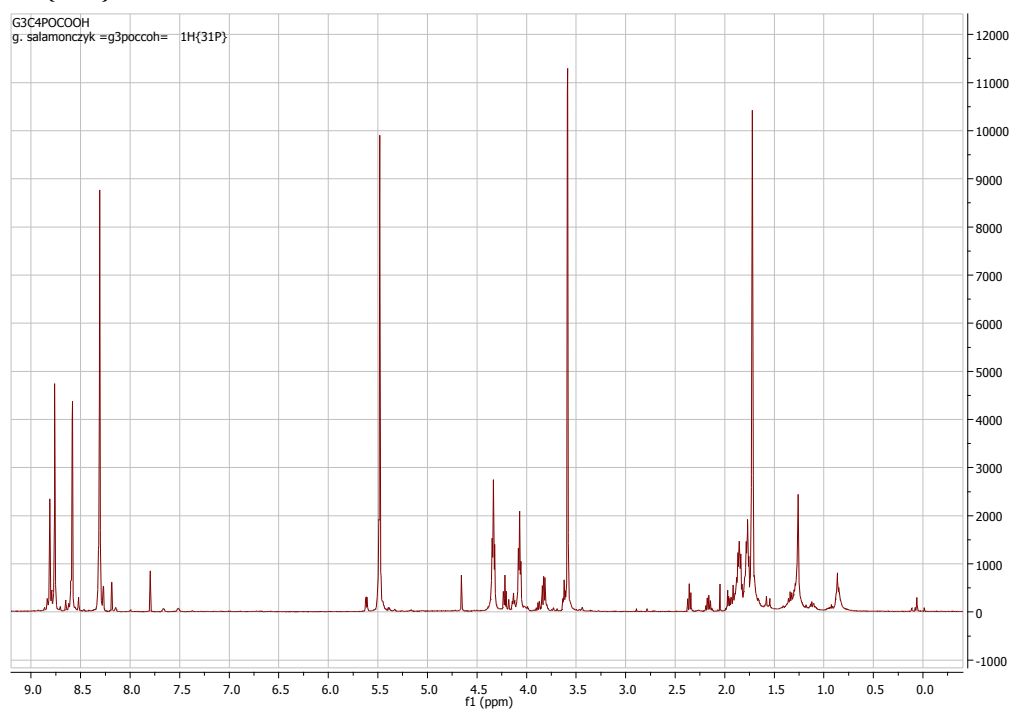
Spectra of the dendrimer **11** (**12**)



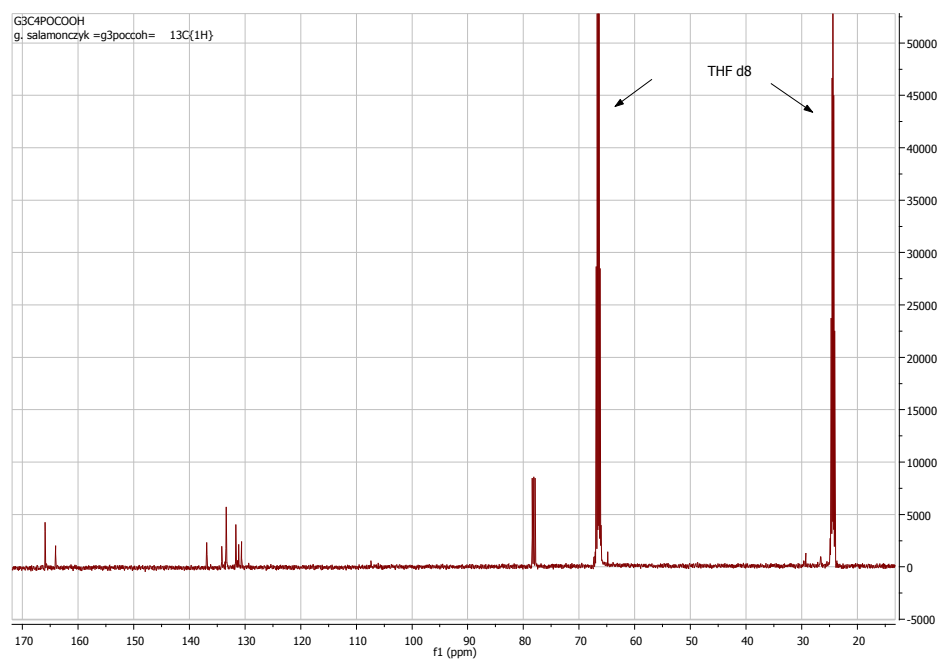
^1H NMR



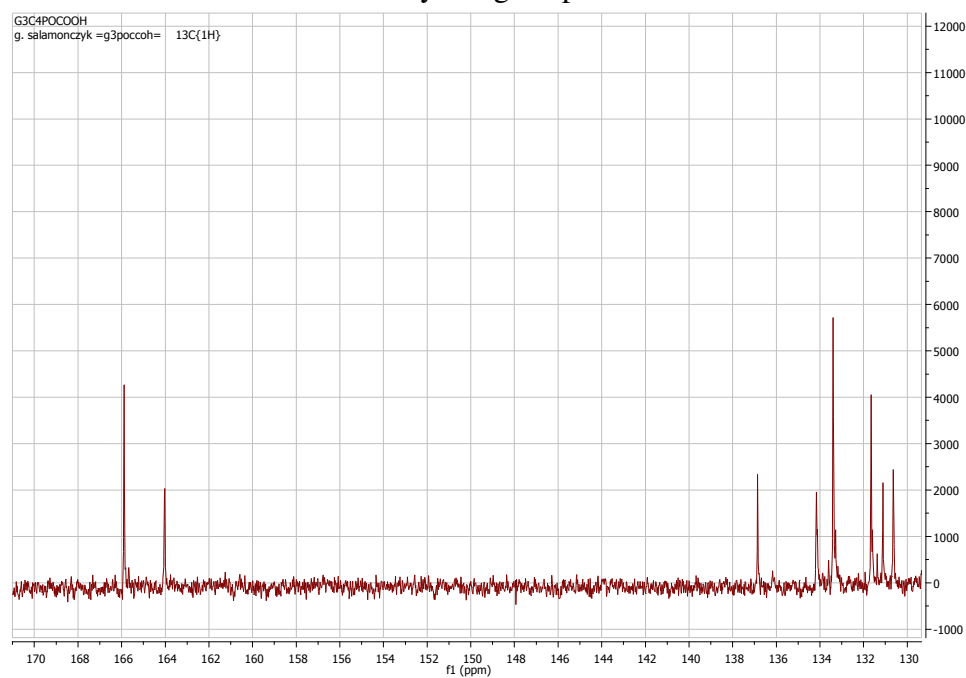
$^1\text{H} \{^3\text{P}\}$ NMR



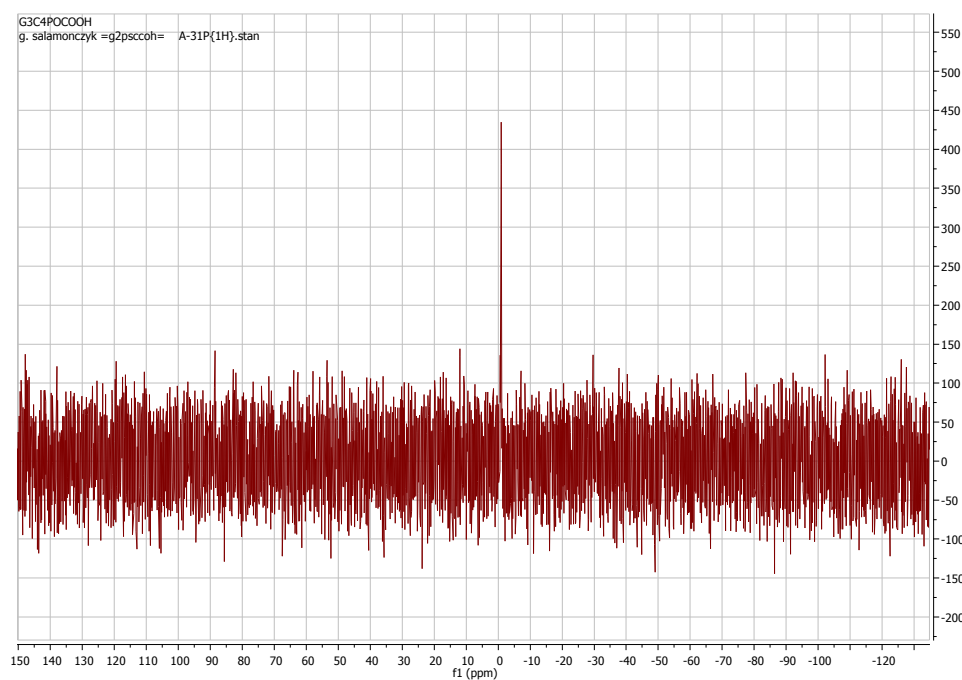
^{13}C NMR



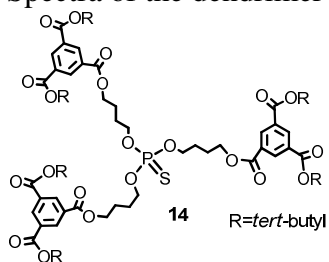
^{13}C NMR – aromatic and carbonyl range expansion



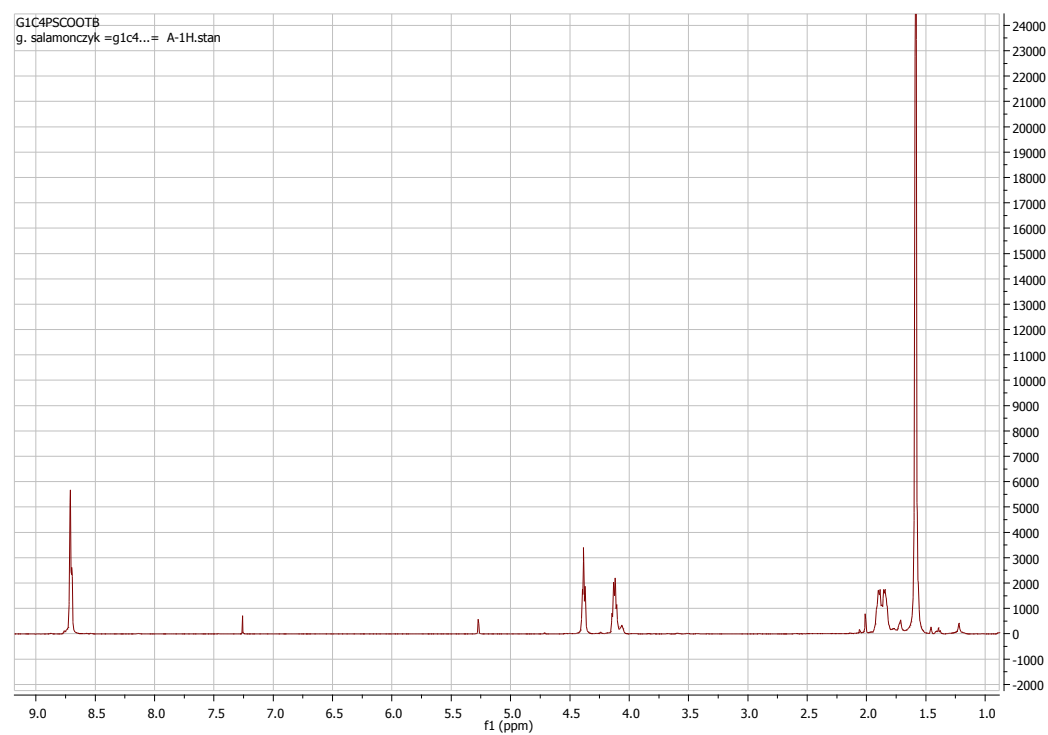
^{31}P NMR



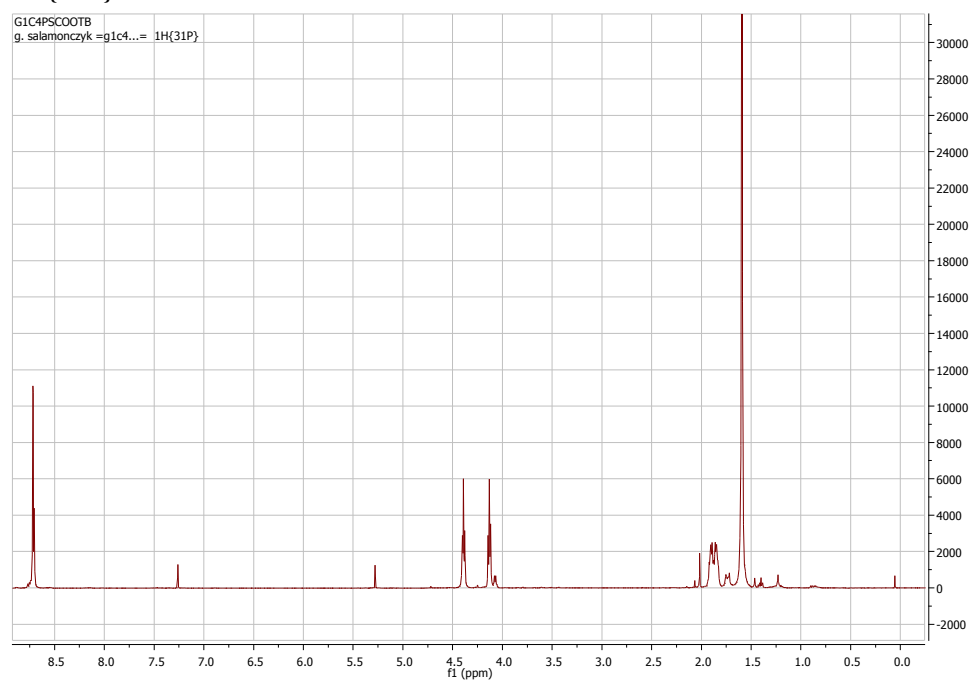
Spectra of the dendrimer **14**



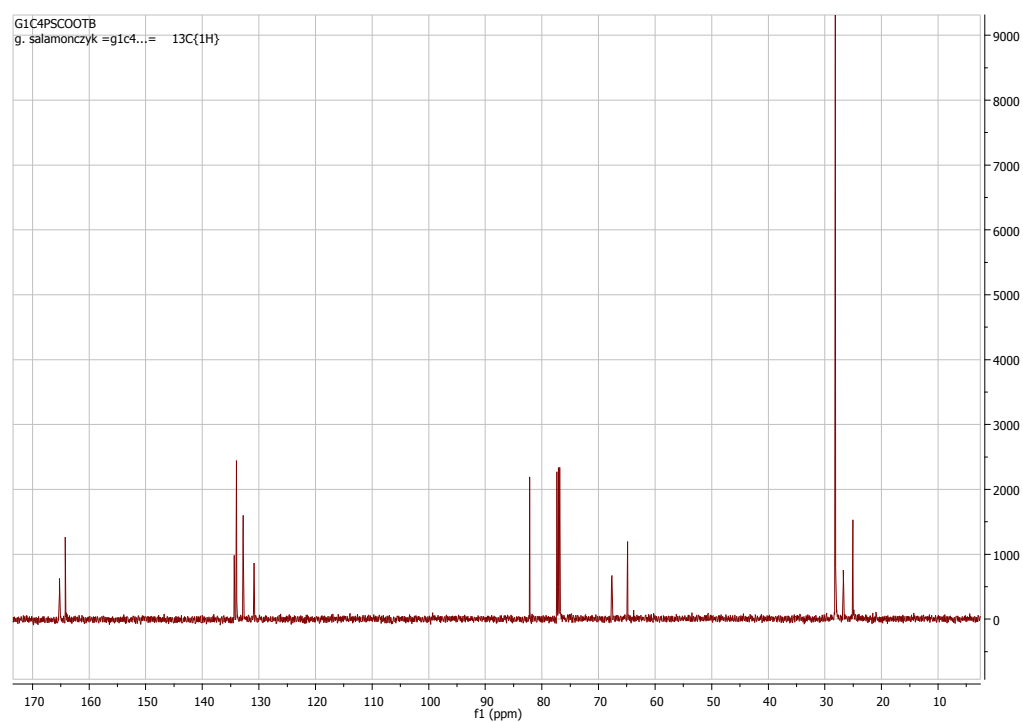
^1H NMR



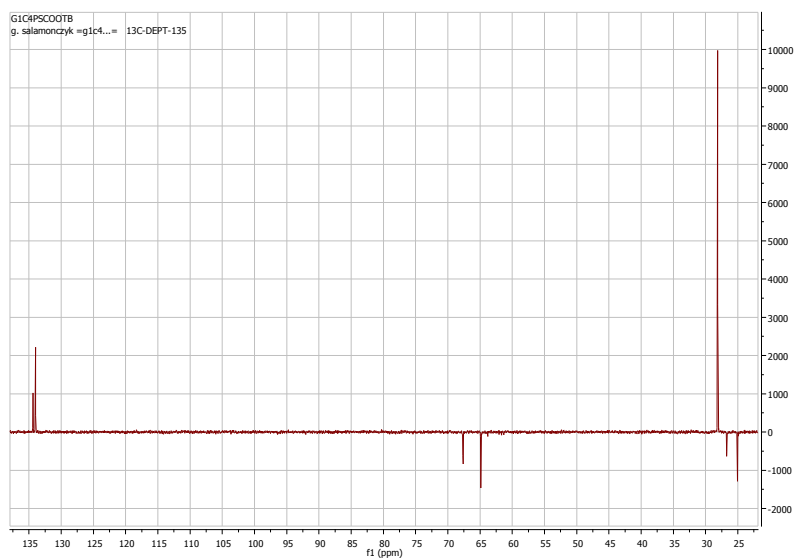
$^1\text{H} \{^3\text{P}\}$ NMR



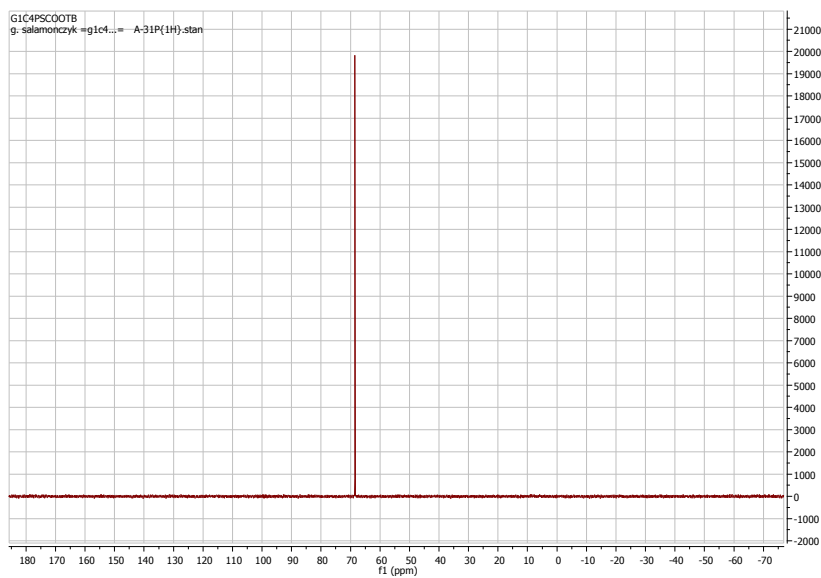
^{13}C NMR



^{13}C NMR – DEPT 135

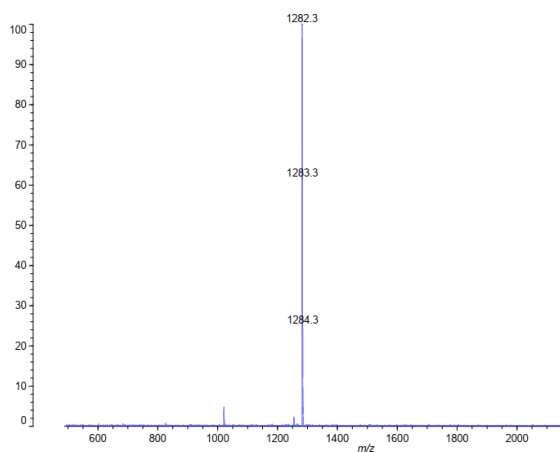


^{31}P NMR

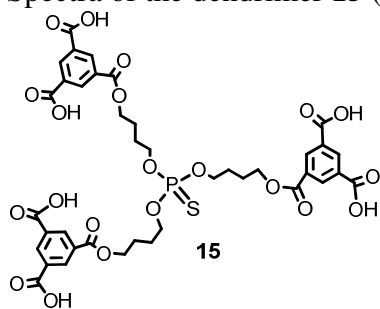


Mass Spectrum

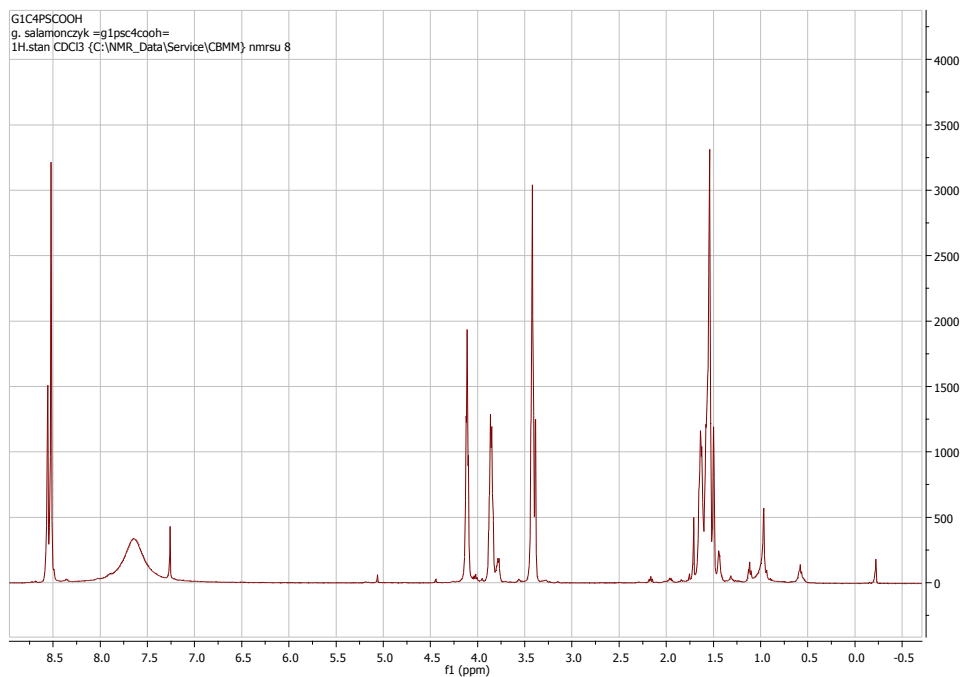
G1PSCOOTB, ANP, K, linear pos
C: THF, ANP: 10mg/mL, S: KTFA: 5mg/mL; C:MS 1:1:0.1 v/v/v
Data: hr910001.K1[c] 17 Jul 2020 12:25 Cal: PEG 2000 (110) 10.19 29 Oct 2019 11:50
Shimadzu Biotech Axima Performance 2.9.1.20100121: Mode Linear, 2018, Power: 67, Blanked, P.Ext. @ 2000 (bin 64)
%Int. 4.8 mV[sum= 960 mV] Profiles 1-200 Smooth Gauss 5-Baseline 60



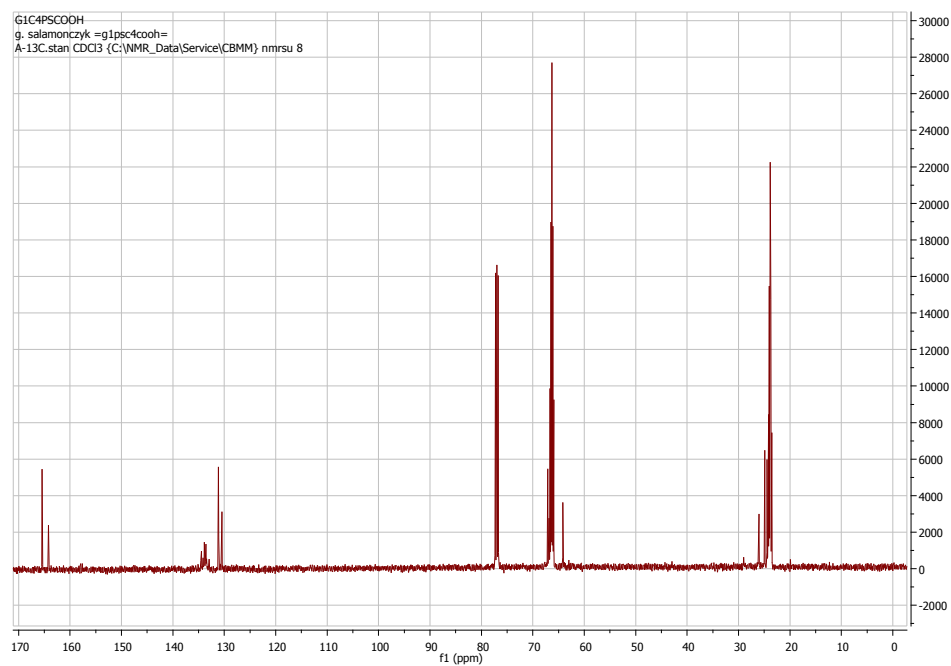
Spectra of the dendrimer **15** (**16**)



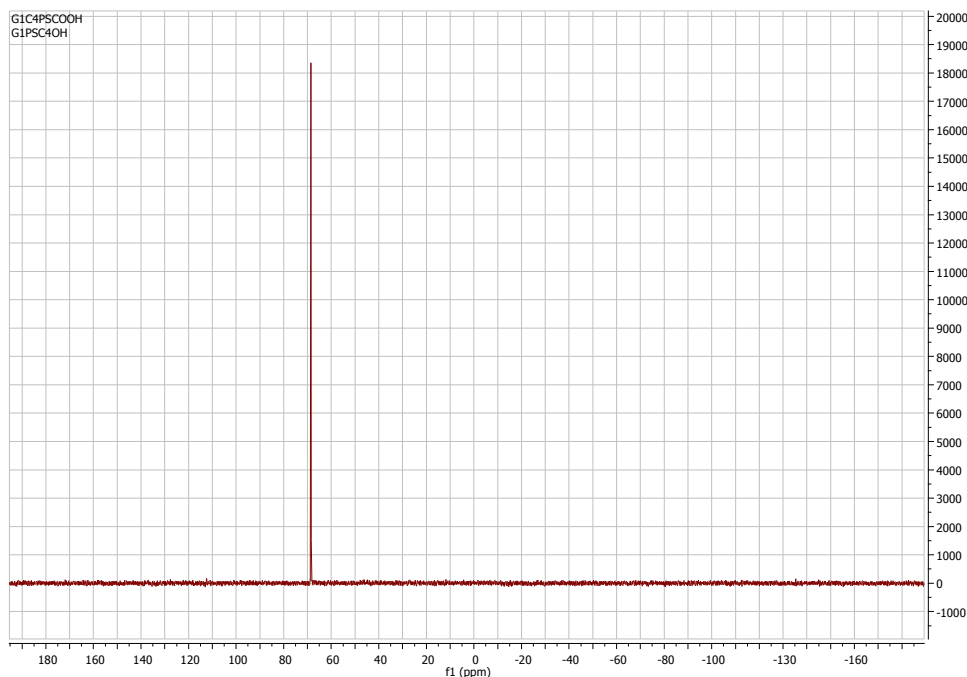
^1H NMR



^{13}C NMR



³¹P NMR



Mass Spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 70.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Odd and Even Electron Ions

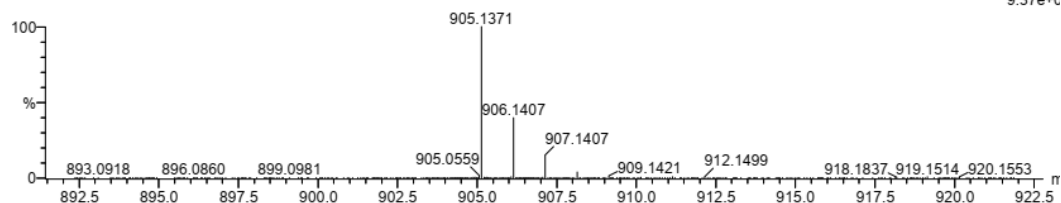
409 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-45 H: 0-45 O: 0-25 P: 0-2 S: 0-2

200831_G1PSC4COOHn1A 46 (0.480) Cm (46:72-2:38)

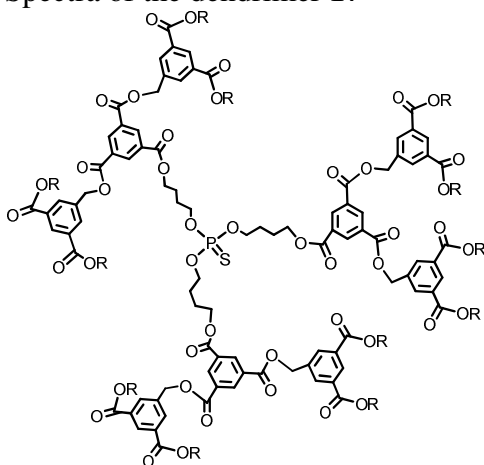
TOF MS E
9.37e+0



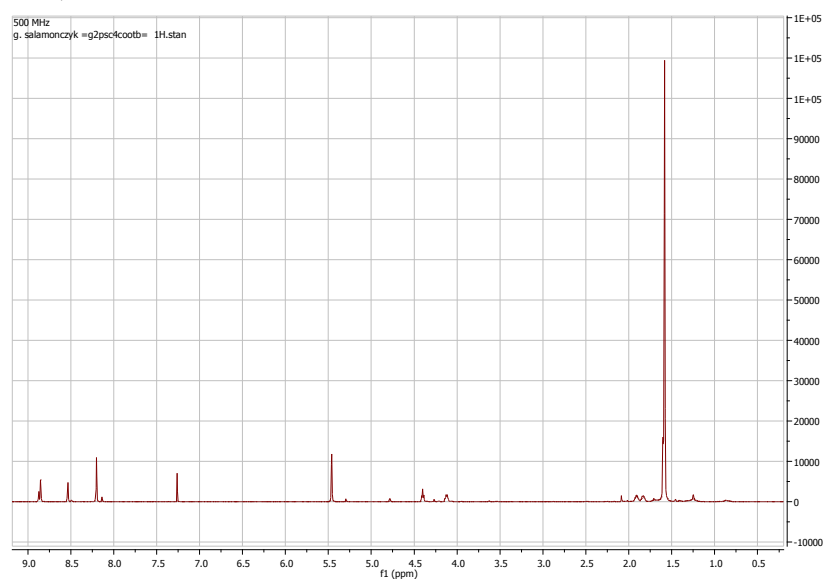
Minimum: -1.5
Maximum: 70.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
905.1371	905.1364	0.7	0.8	21.5	1913.6	2.795	6.11	C39 H38 O21 P S
	905.1398	-2.7	-3.0	16.5	1920.2	9.318	0.01	C36 H42 O21 P S2
	905.1340	3.1	3.4	12.5	1910.9	0.074	92.82	C32 H43 O24 P2 S
	905.1339	3.2	3.5	25.5	1922.3	11.459	0.00	C43 H38 O16 P S2
	905.1330	4.1	4.5	26.5	1915.9	5.071	0.63	C42 H34 O21 P
	905.1413	-4.2	-4.6	26.5	1916.3	5.452	0.43	C42 H33 O23

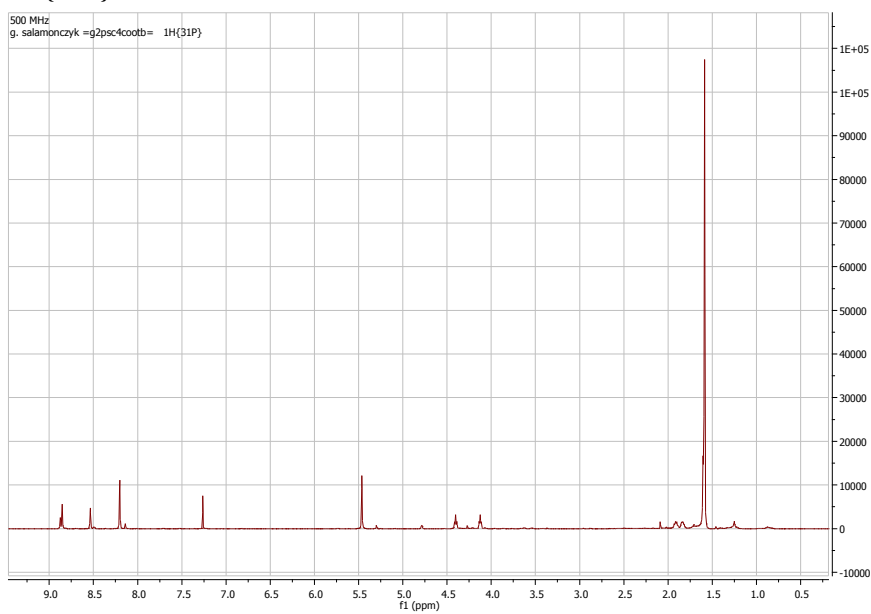
Spectra of the dendrimer **17**



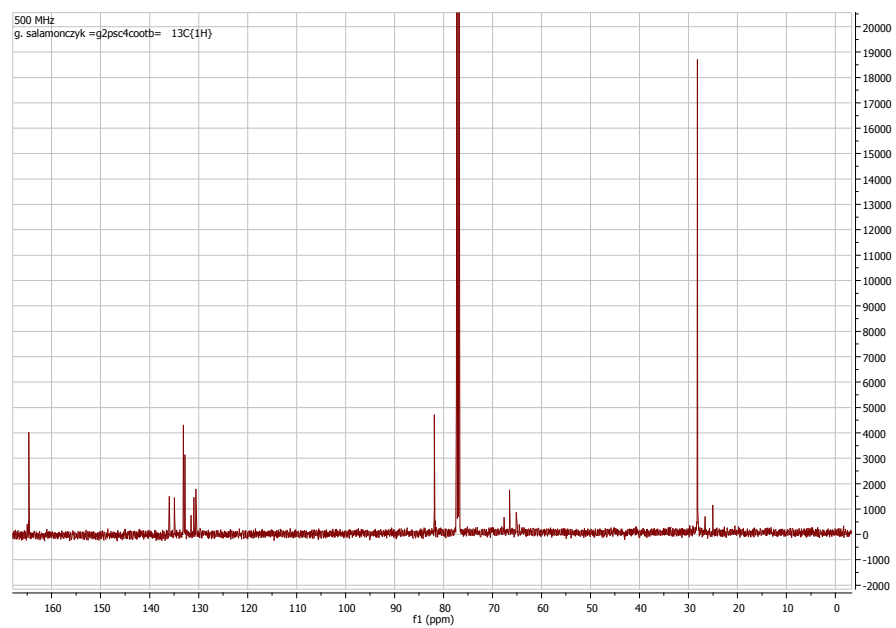
^1H NMR



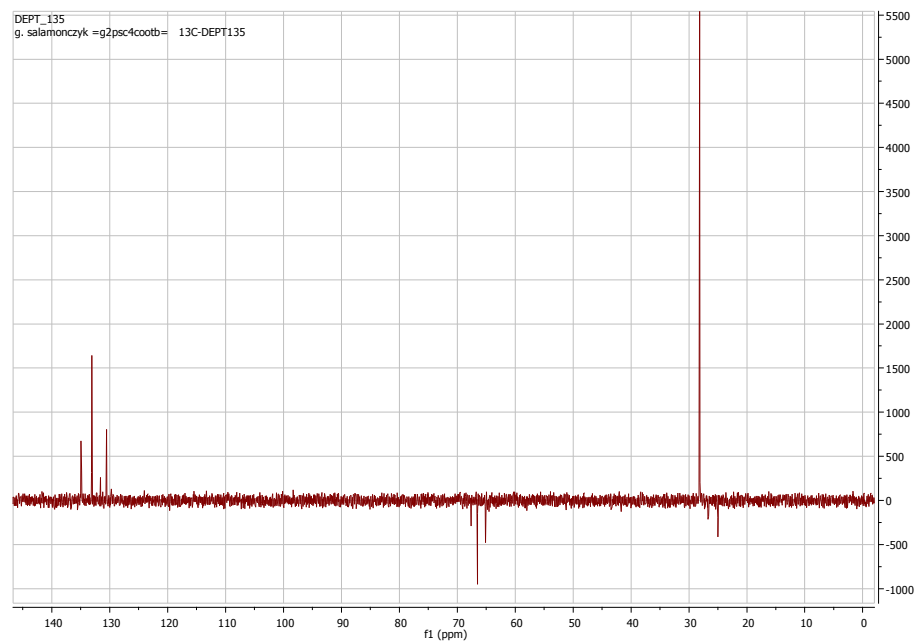
^1H $\{^3\text{P}\}$ NMR



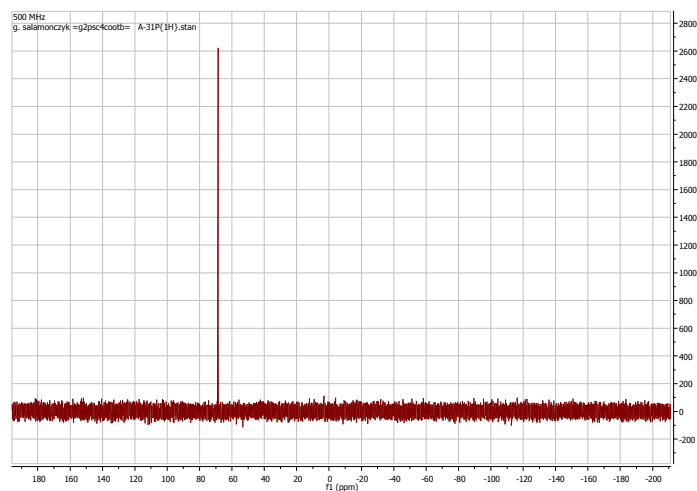
^{13}C NMR



^{13}C NMR – DEPT 135

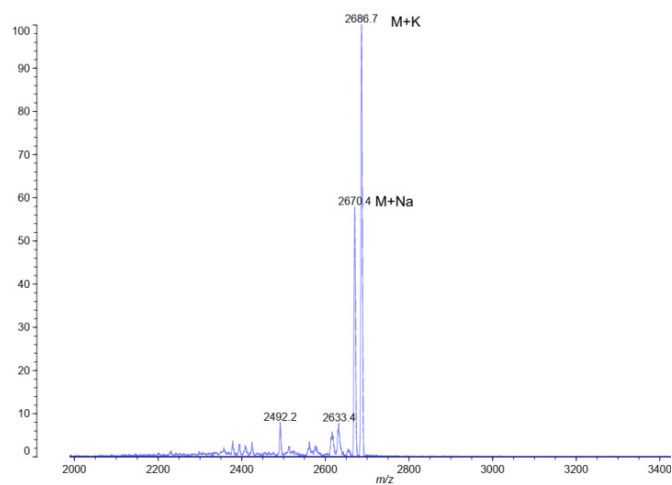


³¹P NMR

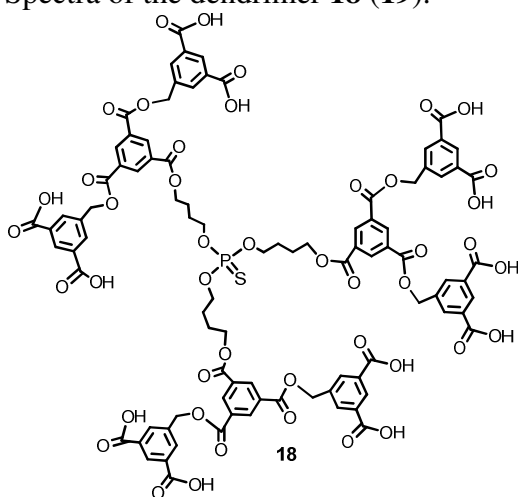


Mass Spectrum

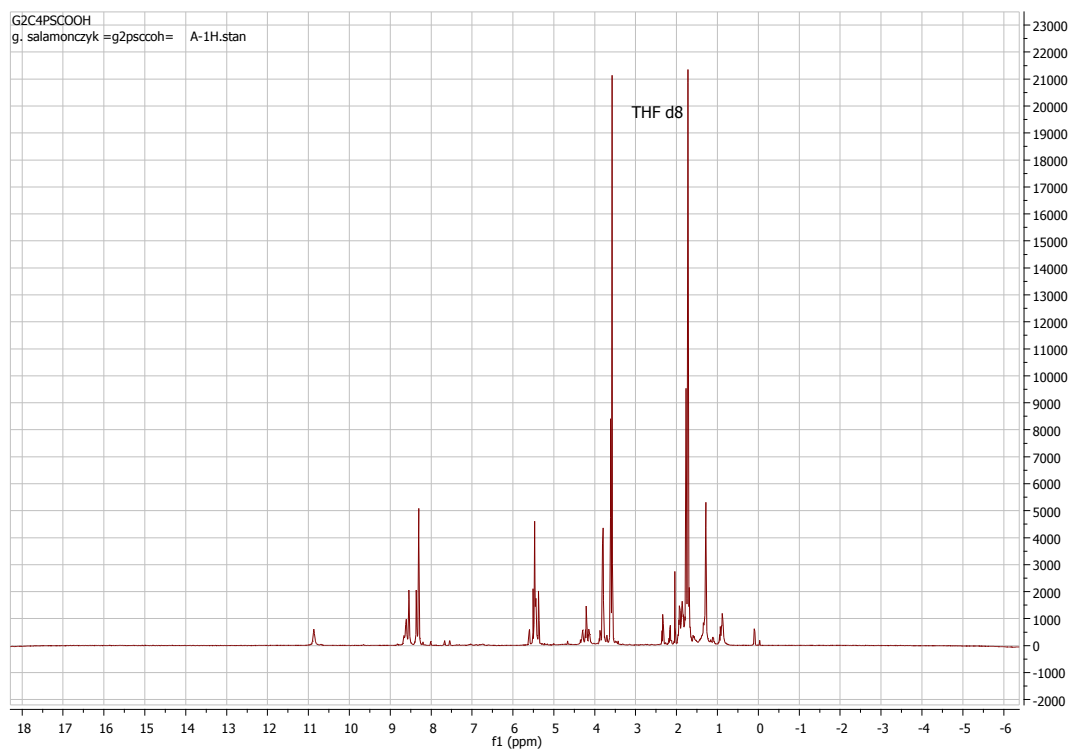
G2C4PSCOOTB, linear pos
C: THF, M: DCTB 10mg/1ml CH₂Cl₂, S: KTFA 5mg/1ml H₂O, P/M/S 10/10/1 v/v/v
Data: hw490003.H19[c] 4 Sep 2020 13:19 Cal: PEG 2000 (06/2020) 22 Jun 2020 12:42
%Int. 6.4 mV[sum= 1270 mV] Profiles 1-200 Smooth Av 10 -Baseline 80



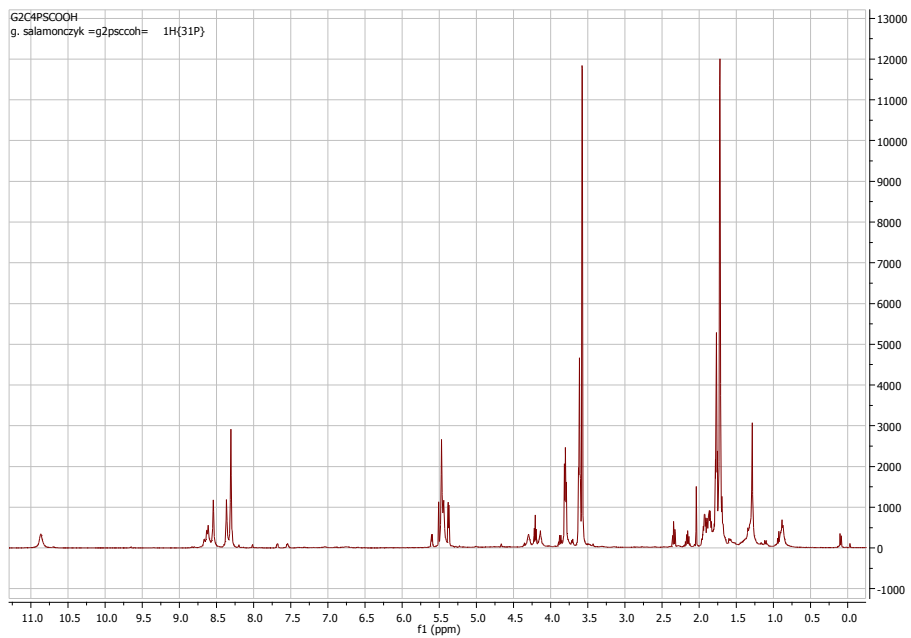
Spectra of the dendrimer **18** (**19**).



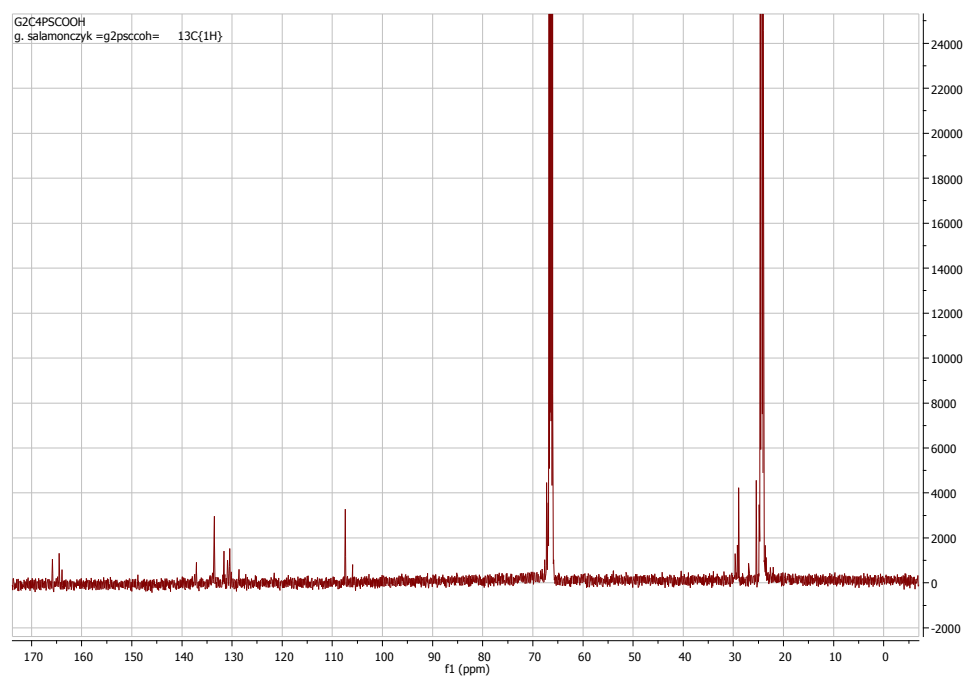
^1H NMR



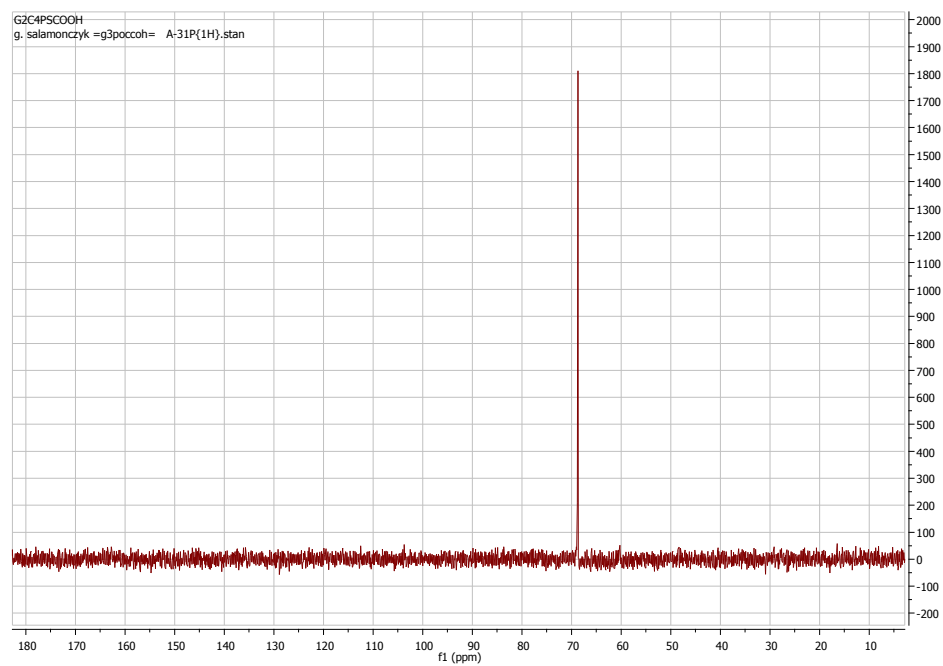
$^1\text{H} \{^3\text{P}\}$ NMR



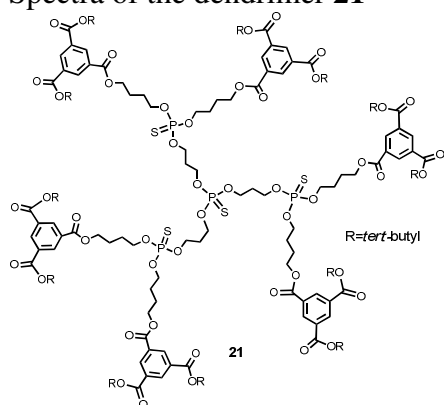
^{13}C NMR



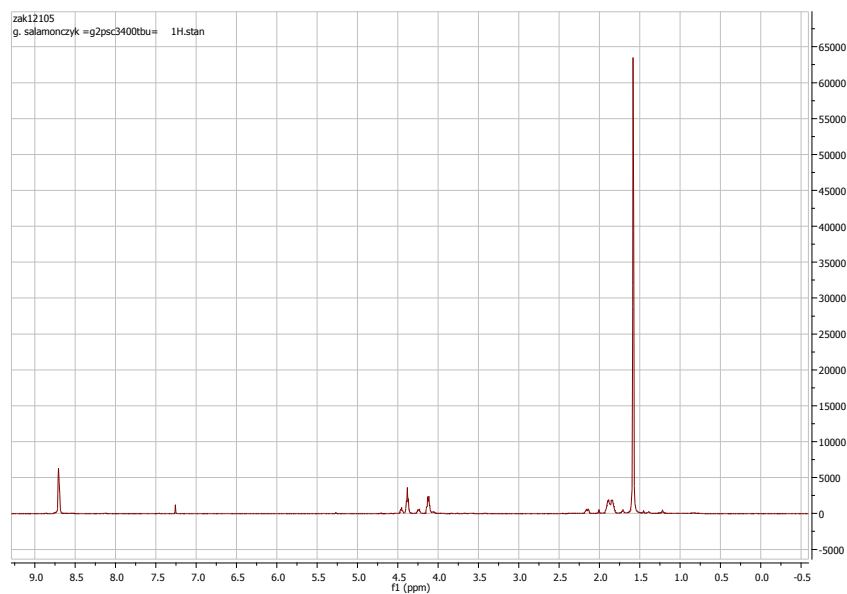
^{31}P NMR



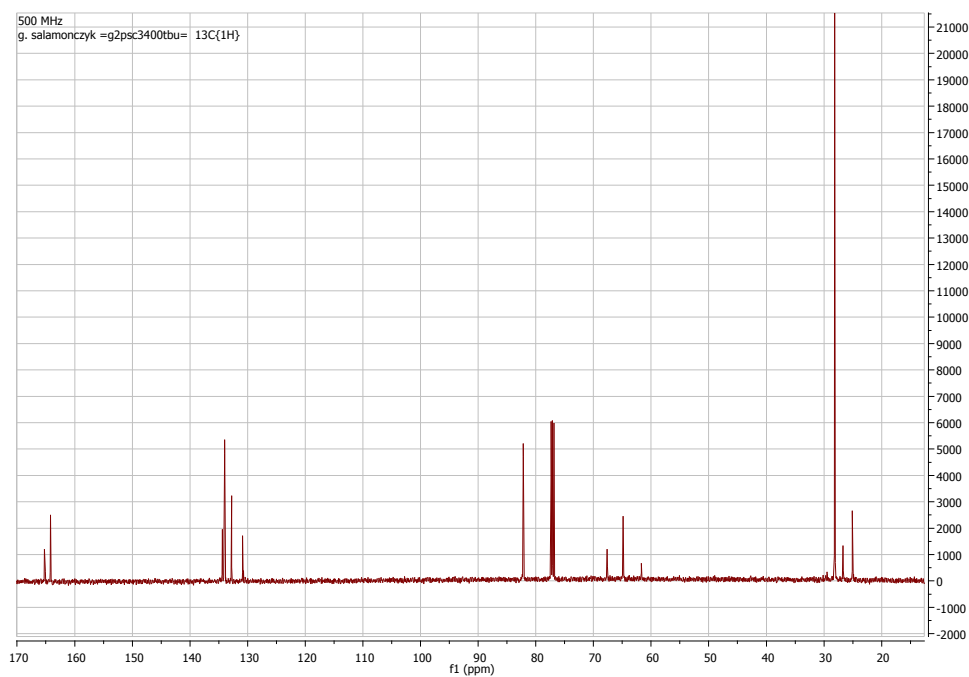
Spectra of the dendrimer **21**



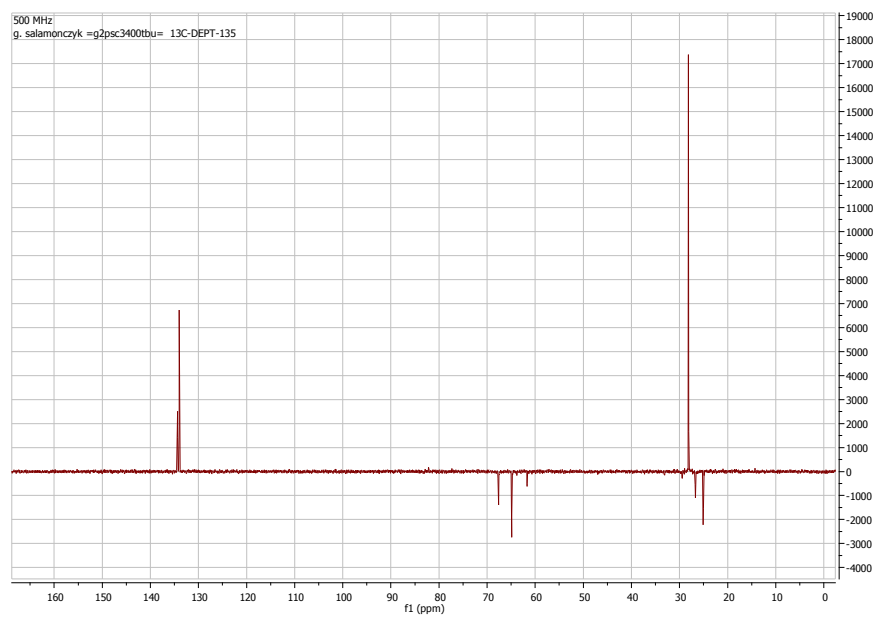
^1H NMR



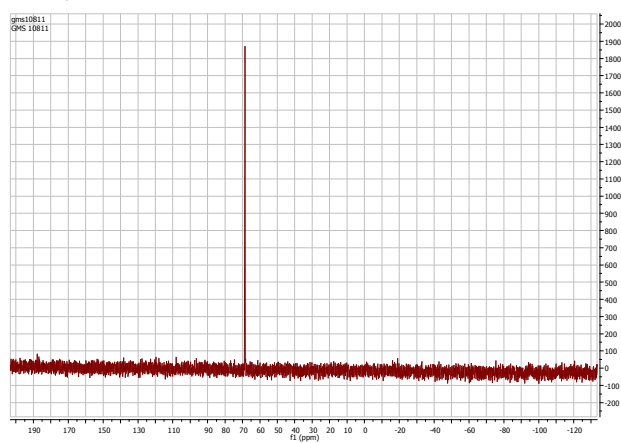
^{13}C NMR



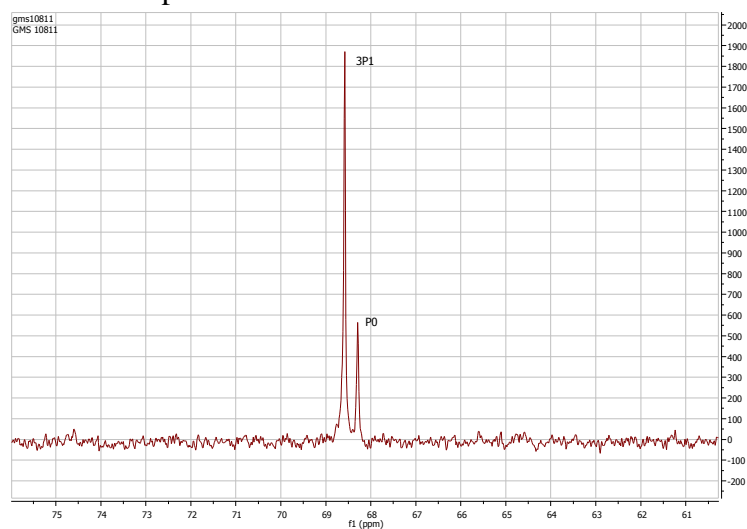
^{13}C NMR – DEPT 135



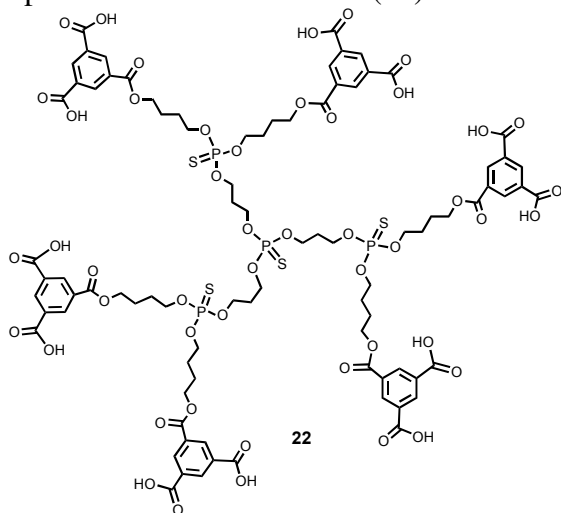
^{31}P NMR



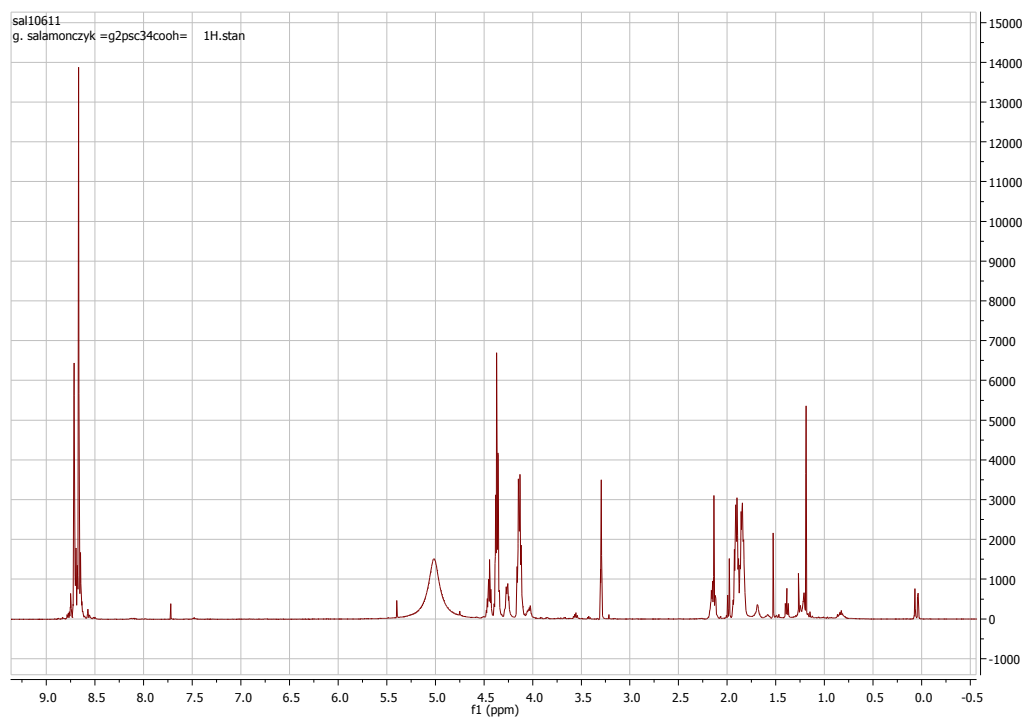
^{31}P NMR-expansion



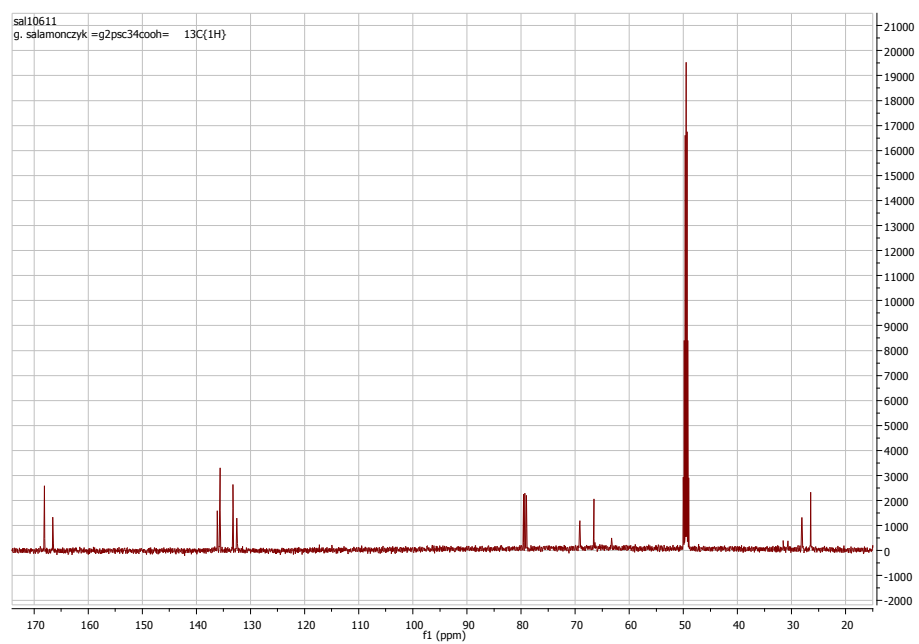
Spectra of the dendrimer **22** (**23**)



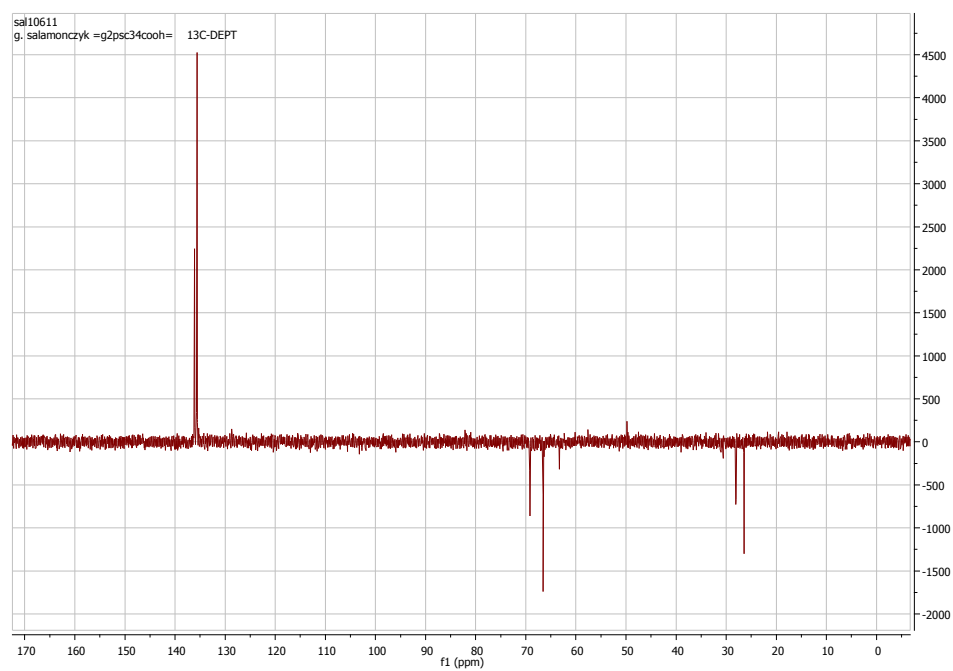
¹H NMR



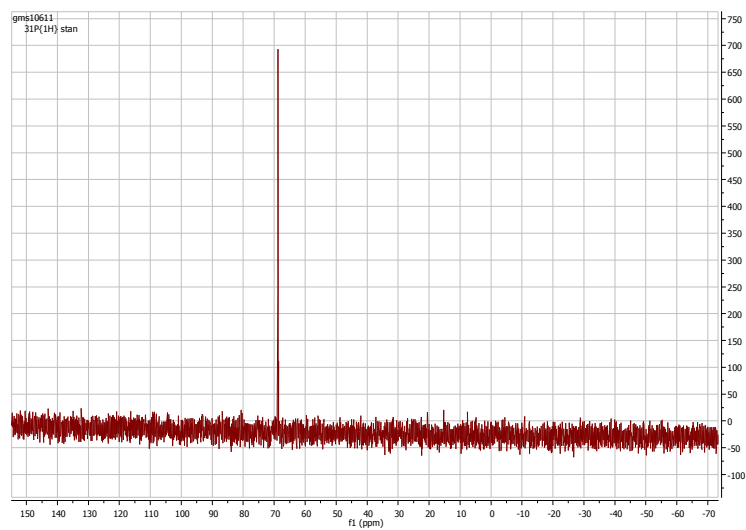
^{13}C NMR



^{13}C NMR – DEPT 135



^{31}P NMR



^{31}P NMR-expansion

