Total synthesis of high loading capacity PEG-based supports. Evaluation and improvement of the process by use of ultrafiltration and PEG as solvent.

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Supporting information

Examples of calculations

The determination of the green metrics can be done in a very easy way considering the mass of all the reagents and auxiliaries used in the reaction. Alternatively, we also show here how they can be calculated using the general formalism we developed.[1]
The results are presented here in tables, we generally used a spreadsheet application (Excel) to perform the calculations.

- One step transformation without recycling: Preparation of 1

$$PEG_{6000} + 2\ NaOH + 2\ BrPr \longrightarrow \mathbf{1}$$

AE = $M_1/[M_{PEG}+2M_{NaOH}+2M_{BrPr}]$= **0.962798251**

-Reaction

compound	M	volume mL	density	mass g	mol
PEG_{6000}	6185			40	0.006467259
THF		30	0.8892	26.676	
NaOH	40			5.34	0.1335
H_2O		11		11	
BrPr 80%w in toluene	118.96	4.3	1.335	4.5924	0.038604573

stoichiometric ratio between NaOH and PEG	φ_1=mol $_{NaOH}$/2/mol $_{PEG}$	10.32121875
ratio between the mass of the excess of NaOH and the mass of the reactants in a stoichiometric amount	$b_1=(\varphi_1-1)*2M_{NaOH}/[M_{PEG}+2M_{NaOH}+2M_{BrPr}]$	0.114671178
stoichiometric ratio between BrPr and PEG	φ_2= mol $_{BrPr}$/2/mol $_{PEG}$	2.984616047
ratio between the mass of the excess of BrPr and the mass of the reactants in a stoichiometric amount	$b_2=(\varphi_2-1)*2M_{BrPr}/[M_{PEG}+2M_{NaOH}+2M_{BrPr}]$	0.072610435

- Workup

by extraction/precipitation

	M	volume mL	density	mass g	Yield
CH_2Cl_2		200	1,3	260	
aq. KH_2PO_4		80	1.1527	92.216	
H_2O		40	1	40	
Na_2SO_4				10	
Et_2O (precipitation)		450	0.7134	321.03	
Et_2O (washing)		200	0.7134	142.68	
product 1 ($C_{286}H_{566}O_{141}$)	**6261**			**39**	**0.96316483**

Mass of reactants	$= m_{PEG} + m_{NaOH} + m_{BrPr}$	49.9324
Mass of auxiliaries	$= m_{THF} + m_{H2O} + m_{CH2Cl2} + m_{aq.\ KH2PO4} + m_{H2O} + m_{aq.\ Na2SO4} + m_{Et2O} + m_{toluene}$	904.750

[1] J. Augé, *Green Chem.*, 2008, **10**, 225-231; J. Augé and M.-C. Scherrmann *New J. Chem.*, 2012, **36**, 1091–1098.

Reaction mass efficiency	$RME = \frac{mass\ of\ product}{mass\ of\ reactants}$ $RME = \frac{\varepsilon AE}{1 + b_1 + b_2}$	**0.781055988**
Global mass efficiency	$GME = \frac{mass\ of\ product}{mass\ of\ react. + mass\ of\ auxiliaries}$	**0.040851278**
E	$E = \frac{mass\ of\ waste}{mass\ of\ product}$	**23.47903**

by ultrafiltration

	M	volume mL	density	mass g	Yield
H_2O Ultrafiltration 1		160	1,3	160	
H_2O Ultrafiltration 2		120	1	120	
H_2O Ultrafiltration 3		120	1	120	
product 1 ($C_{286}H_{566}O_{141}$)	**6261**			**38.5**	**0.950816563**

Mass of reactants	= $m_{PEG} + m_{NaOH} + m_{BrPr}$	49.9324
Mass of auxiliaries	= $m_{THF} + m_{H2O} + m_{H2O\ (UF)} + m_{toluene}$	438.8241
Mass of auxiliaries (without H_2O used in the workup)	= $m_{THF} + m_{H2O} + m_{toluene}$	38.8241

Reaction mass efficiency	$RME = \frac{mass\ of\ product}{mass\ of\ reactants}$ $RME = \frac{\varepsilon AE}{1 + b_1 + b_2}$	**0.771042449**
Global mass efficiency	$GME = \frac{mass\ of\ product}{mass\ of\ react. + mass\ of\ auxiliaries}$	**0.0787713**
E	$E = \frac{mass\ of\ waste}{mass\ of\ product}$	**11.6949**
E* *(without H_2O used in the workup)*	$E^* = \frac{mass\ of\ waste\ (without\ water)}{mass\ of\ product}$	**1.305363**

- One step transformation with solvent recycling: Preparation of 19

18 + NaN_3 ⟶ **19**

AE = $M_{19}/[M_{18}+M_{NaN3}]$= **0.931891148**

Reaction

compound	M	volume mL	density	mass g	mol
18	1445.66			20	0.013834512
PEG_{400}		16	1.128	18.048	
NaN_3	65.01			0.99	0.015228426

stoichiometric ratio between NaN_3 and **18**	$\varphi = mol_{NaN3}/mol_{18}$	1.100756345
ratio between the mass of the excess of NaN_3 and the mass of the reactants in a stoichiometric amount	**b**= $(\varphi-1)^* M_{NaN3}/[M_{18} + M_{NaN3}]$	0.004335937

Workup

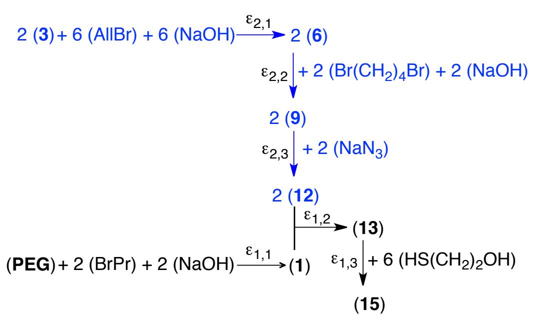
	M	**volume mL**	**density**	**mass g**	**yield**
Et_2O		40	0.7134	28.536	
H_2O		20	1	20	
Na_2SO_4				5	
product 19 ($C_{72}H_{118}N_{12}O_{16}$)	**1407.78**			**19.1**	**0.980696771**

Mass of reactants	$= m_{18} + m_{NaN3}$	20.99
Mass of auxiliaries	$= m_{PEG400} + m_{Et2O} + m_{H2O} + m_{Na2SO4}$	71.584
Mass of auxiliaries (1 recycling of PEG)	$= m_{PEG400}/2 + m_{Et2O} + m_{H2O} + m_{Na2SO4}$	62.56
Mass of auxiliaries (2 recycling of PEG)	$= m_{PEG400}/3 + m_{Et2O} + m_{H2O} + m_{Na2SO4}$	59.552
Mass of auxiliaries (3 recycling of PEG)	$= m_{PEG400}/4 + m_{Et2O} + m_{H2O} + m_{Na2SO4}$	58.048

Reaction mass efficiency	$RME = \frac{mass\ of\ product}{mass\ of\ reactants}$ $RME = \frac{\varepsilon AE}{1+b}$	**0.909957122**
Global mass efficiency	$GME = \frac{mass\ of\ product}{mass\ of\ react. + mass\ of\ auxiliaries}$	**0.206321429** (1st use of PEG_{400}) **0.228605625** (2nd use of PEG_{400}) **0.237143354**(3rd use of PEG_{400}) **0.241655912**(4th use of PEG_{400})
E	$E = \frac{mass\ of\ waste}{mass\ of\ product}$	**3.846806283** (1st use of PEG_{400}) **3.37434555** (2nd use of PEG_{400}) **3.216858639** (3rd use of PEG_{400}) **3.138115183** (4th use of PEG_{400})

- Multi-step transformation: Preparation of 15

For a linear multi-step synthesis, the calculation of GME can be easy but for a multi-sequence convergent synthesis, the problem is more difficult and a general formalism allows for the calculation.[1] The calculation of GRME (global reaction mass efficiency) of **15** is detailed below.



Compound	M	coef.	coef*M
3	136.16	2	272.32
AllBr	120.98	6	725.88
NaOH	40	6	240
dibromobutane	215.91	2	431.82
NaOH	40	2	80
NaN_3	65.01	2	130.02
PEG_{6000}	6185	1	6185
BrPr	118.96	2	237.92
NaOH	40	2	80
mercaptoethanol	78.133	6	468.798

The global atom economy is:

$$GAE = \frac{\nu_P M_P}{\sum M}$$

were P refers to the product **15** and

$$\sum M = \nu_{a1} M_{A1} + \nu_{a2} M_{A2} + \sum_{i=1}^{z} \nu_{b1,i} M_{B1,i} + \sum_{j=1}^{m} \nu_{b2,j} M_{B2,j}$$

$\Sigma M = M_{PEG} + 2\ M_3 + 2\ M_{BrPr} + 2\ M_{NaOH} + 6\ M_{SH(CH2)2OH} + 6M_{AllBr} + 6M_{NaOH} + 2\ M_{Br(CH2)4Br} + 2\ M_{NaOH} + 2M_{NaN3}$
$GAE = M_{15} / \Sigma M = 7437/8851.758 = 0.840172088$

There are 2 branches in the synthesis of **15**, and therefore two possibilities to carry out the calculation: Either considering the main branch starting from PEG (black branch) or by considering that the reference compound is pentaerythritol **3** (blue branch). As we have demonstrated,[1] the final result is exactly the same. We chose here to consider that the black branch is the main branch.

Total yield from PEG (black branch): $\Pi\varepsilon_{(PEG)} = \varepsilon_{1,1}\varepsilon_{1,2}\varepsilon_{1,3} = 0.845246869$
Total yield from pentaeryhritol **3** (blue branch):
For this calculation, we have to considerate the stoichiometric ratio between **12** and **1**:
$\varphi_{1,2} = mol_{12}/mol_{1}/2 = 1.139607295$
$\Pi\varepsilon_{(3)} = \varepsilon_{2,1}\varepsilon_{2,2}\varepsilon_{2,3}(\varepsilon_{1,2}/\varphi)\varepsilon_{1,3} = 0.418203894$

number of moles of the reference molecule = mol of PEG	$x_1=$	0.006467259
number of moles of **3** necessary to give **15** from x_1 mol of PEG	$x_2=2x_1\Pi\ \varepsilon_{(PEG)}/\Pi\ \varepsilon_{(3)}$	0.02614242
3/PEG (scale ratio)	$\sigma_2=x_2/2x_1=\Pi\ \varepsilon_{(PEG)}/\Pi\ \varepsilon_{(3)}$	2.021135818
ratio between the mass of the excess of **3** and the mass of all the reactants in the ideal case*, for the total synthesis with respect to PEG	$a_2=(\sigma_2-1)2M_3/\Sigma M$	0.031414743

* Ideal case: All the yields (not necessary the last one) are 100% and all the reactions are carried out in the stoichiometric amount.

For the main branch (branch 1 in black): there are 3 steps, involving 2 reagents (step 1), no reagents (step 2) and 1 reagent (step 3). Hence, we have to calculate the ratios between the mass of the excess of every reactant and the mass of all the reactants used in the total synthesis, with respect to PEG. These ratios are $b_{1,1}$ (branch 1, step 1, reactant 1), $b_{1,1*}$ (branch 1, step 1, reactant 2), $b_{1,3}$ (branch 1, step 3, reactant 1). They are calculated using the formula given below.[1]

$$b_{1,i} = \left[\varphi_{1,i}\,(\varepsilon_{1,1}\,\varepsilon_{1,2}...\varepsilon_{1,i-1}) - 1\right] \frac{\nu_{b1,i} M_{B1,i}}{\sum M}$$

$$\varphi_{1,i} = \frac{mol\,number\ \ of\ B_{1,i} / \nu_{1,i}}{mol\,number\ \ of\ P_{1,i-1} / \nu_{p1,i-1}}$$

Branch 1 step 1	PEG+ 2 NaOH + 2 BrPr→1	yield = $\varepsilon_{1,1}$= 0.950816563 (purification by UF)
stoichiometric ratio between NaOH and PEG	$\varphi_{1,1} = mol_{NaOH}/2/mol_{PEG}$	10.32121875
ratio between the mass of the excess of NaOH and the mass of the reactants in the ideal case, for the total synthesis with respect to PEG	$b_{11}=(\varphi_{1,1}-1)2M_{NaOH}/\Sigma M$	0.08424287
stoichiometric ratio between BrPr and PEG	$\varphi_{1,1*} = mol_{BrPr}/2/mol_{PEG}$	2.984616047
ratio between the mass of the excess of BrPr and the mass of the reactants in the ideal case, for the total synthesis with respect to PEG	$b_{1,1*}=(\varphi_{1,1*}-1)2M_{BrPr}/\Sigma M$	0.053343059

Branch 1 step 2	2 **(12)** + **(1)** → **(13)** **no reagent is added :** $b_{1,2} = 0$	yield = $\varepsilon_{1,2}$= 0.948803923
Branch 1 step 3	**(13)** + 6 ($HS(CH_2)_2OH$)→ **(15)**	yield = $\varepsilon_{1,3}$= 0.936936937
stoichiometric ratio between $HS(CH_2)_2OH$ and **13**	$\varphi_{1,3}$ = mol $_{HS(CH2)2OH}$ /6/mol$_{\mathbf{10}}$	4.6164421
ratio between the mass of the excess of $HS(CH_2)_2OH$ and the mass of the reactants in the ideal case, for the total synthesis with respect to PEG	$b_{1,3} = (\varphi_{1,3}\varepsilon_{1,2}\varepsilon_{1,1}-1)6M_{HS(CH2)2OH}/\Sigma M$	0.167604108

For the second branch (branch 2 in blue): there are 3 steps, involving 2 reagents (step 1 and step 2) and 1 reagent (step 3). Hence, we have to calculate the ratios between the mass of the excess of every reactant and the mass of all the reactants used in the total synthesis, with respect to PEG, in the ideal case; *ie*, all the yields (not necessary the last one) are 100% and all the reactions are carried out in the stoichiometric amount. These ratios are $b_{2,1}$ (branch 2, step 1, reactant 1), $b_{2,1*}$ (branch 2, step 1, reactant 2), $b_{2,2}$ (branch 2, step 2, reactant 1), $b_{2,2*}$ (branch 2, step 2, reactant 2) and $b_{2,3}$ (branch 2, step 3, reactant 1). They are calculated using the formula given below.

$$b_{2,j} = \left[\sigma_2 \varphi_{2,j}\left(\varepsilon_{2,1} \ldots \varepsilon_{2,j-1}\right) - 1\right] \frac{\nu_{b2,j} M_{B2,j}}{\sum M} \qquad \varphi_{2,j} = \frac{mol\ number\ of\ \ B_{2,j} / \nu_{b2,j}}{mol\ number\ of\ \ P_{2,j-1} / \nu_{P2,j-1}}$$

Branch 2 step 1	**3** + 3 NaOH + 3 AllBr →**6** + **7** **7** + NaOH + AllBr →**6**	yield = $\varepsilon_{2,1}$= 0.747438763 (2 steps)
stoichiometric ratio between NaOH and **3**	$\varphi_{2,1}$ = mol$_{NaOH}$/3/mol$_3$	1.505573179
ratio between the mass of the excess of NaOH and the mass of the reactants, and the mass of the reactants in the ideal case, for the total synthesis with respect to PEG	$b_{2,1}=(\sigma_2\varphi_{2,1}-1)6M_{NaOH}/\Sigma M$	0.055391516
stoichiometric ratio between AllBr and **3**	$\varphi_{2,1*}$ = mol$_{AllBr}$/3/mol$_3$	1.503536293
ratio between the mass of the excess of AllBr and the mass of the reactants, and the mass of the reactants in the ideal case, for the total synthesis with respect to PEG	$b_{2,1*} =(\sigma_2\varphi_{2,1*} -1)6M_{AllBr}/\Sigma M$	0.167194043
Branch 2 step 2	**6** + $Br(CH_2)_4Br$ + NaOH→**7**	yield = $\varepsilon_{2,2}$= 0.728932412 (method in water with recovery of dibromobutane)
stoichiometric ratio between NaOH and **6**	$\varphi_{2,2}$ = mol $_{NaOH}$/mol$_4$	9.859230769
ratio between the mass of the excess of NaOH and the mass of the reactants, and the mass of the reactants in the ideal case, for the total synthesis with respect to PEG	$b_{2,2}=(\sigma_2\varphi_{2,2}\varepsilon_{2,1} -1)2M_{NaOH}/\Sigma M$	0.125571404
stoichiometric ratio between $Br(CH_2)_4Br$ and **4**	$\varphi_{2,2*}$ = mol$_{Br(CH2)4Br}$ /mol$_6$	1.250574159
ratio between the mass of the excess of $Br(CH_2)_4Br$ and the mass of the reactants in the ideal case, for the total synthesis with respect to PEG	$b_{2,2*} =(\sigma_2\varphi_{2,2*}\varepsilon_{2,1} -1)2M_{Br(CH2)4Br}/\Sigma M$	0.043378873
Branch 2 step 3	**9** + NaN_3 → **12**	yield = $\varepsilon_{2,3}$= 0.983996563 (method in PEG_{400})
stoichiometric ratio between **NaN_3** and **9**	$\varphi_{2,3}$ = mol $_{NaN3}$/mol$_6$	1.098593293
ratio between the mass of the excess of NaN_3 and the mass of the reactants in the ideal case, for the total synthesis with respect to PEG	$b_{2,3}=(\sigma_2\varphi_{2,3}\varepsilon_{2,1}\varepsilon_{2,2} -1)2M_{NaN3}/\Sigma M$	0.003080923

The general expression of GRME is:

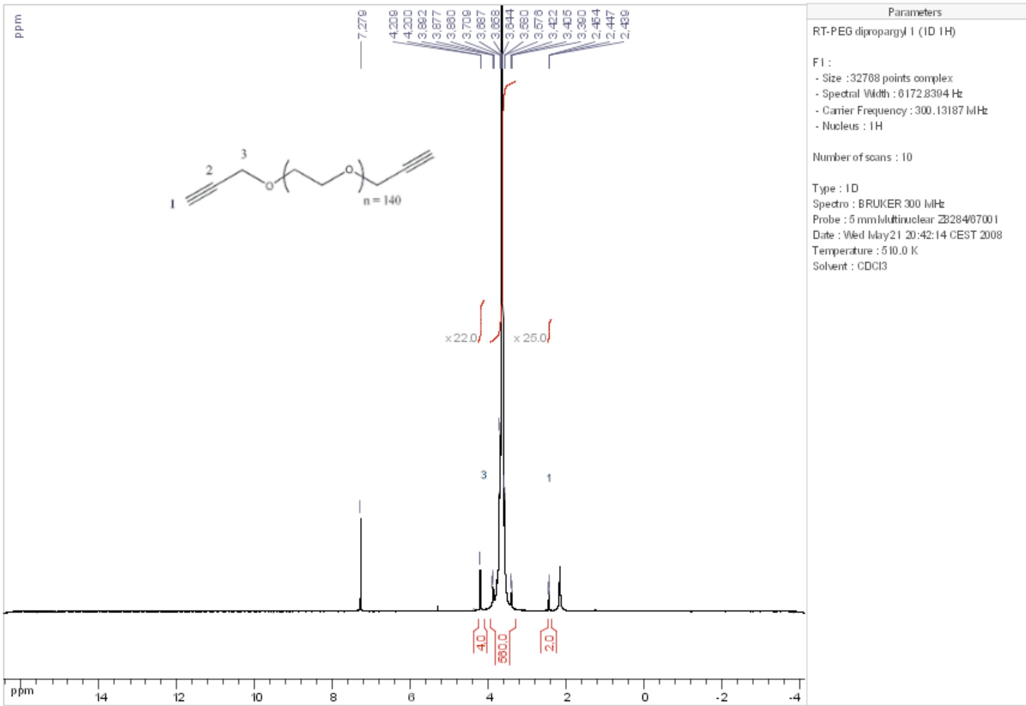
$$GRME = \frac{GAE \prod_{i=1}^{z} \varepsilon_{1,i}}{1 + a_2 + \sum_{i=1}^{z} b_{1,i} + \sum_{j=1}^{m} b_{2,j}}$$

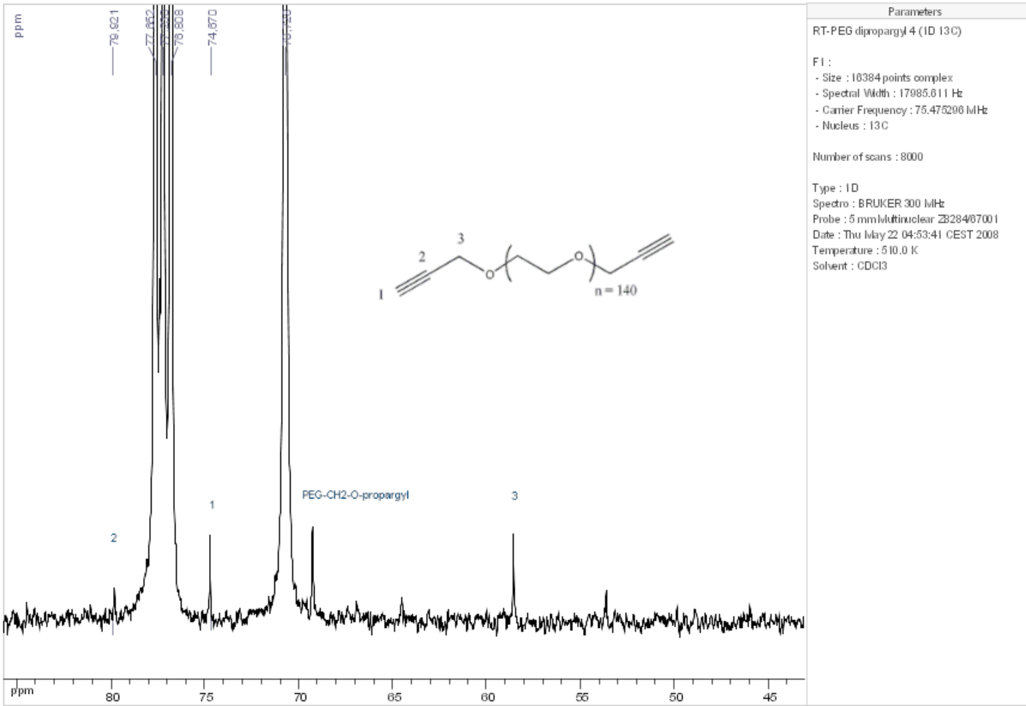
Applied to the synthesis of **15** it becomes:

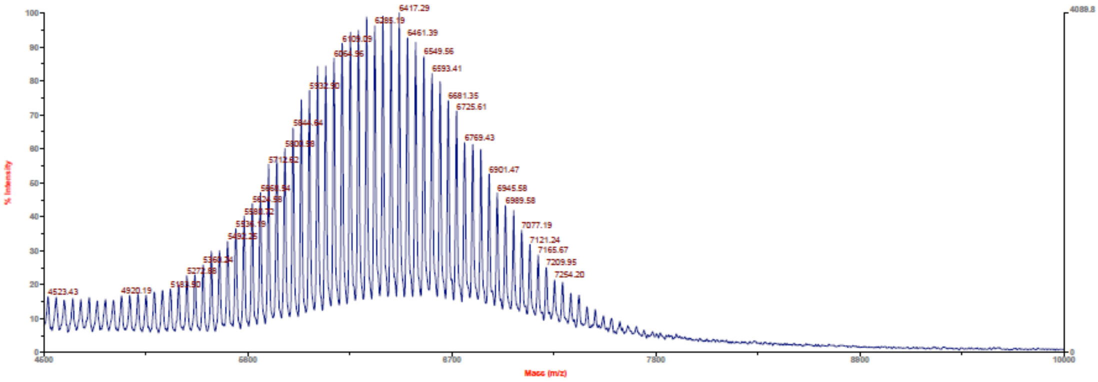
$$GRME = \frac{GAE \prod_{i=1}^{3} \varepsilon_{1,i}}{1 + a_2 + \sum_{i=1}^{3} b_{1,i} + \sum_{j=1}^{3} b_{2,j}} = \frac{GAE\varepsilon_{1,1}\varepsilon_{1,2}\varepsilon_{1,3}}{1 + a_2 + (b_{1,1} + b_{1,1*} + b_{1,2} + b_{1,3}) + (b_{2,1} + b_{2,1*} + b_{2,2} + b_{2,2*} + b_{2,3})}$$

GRME = 0.41020332

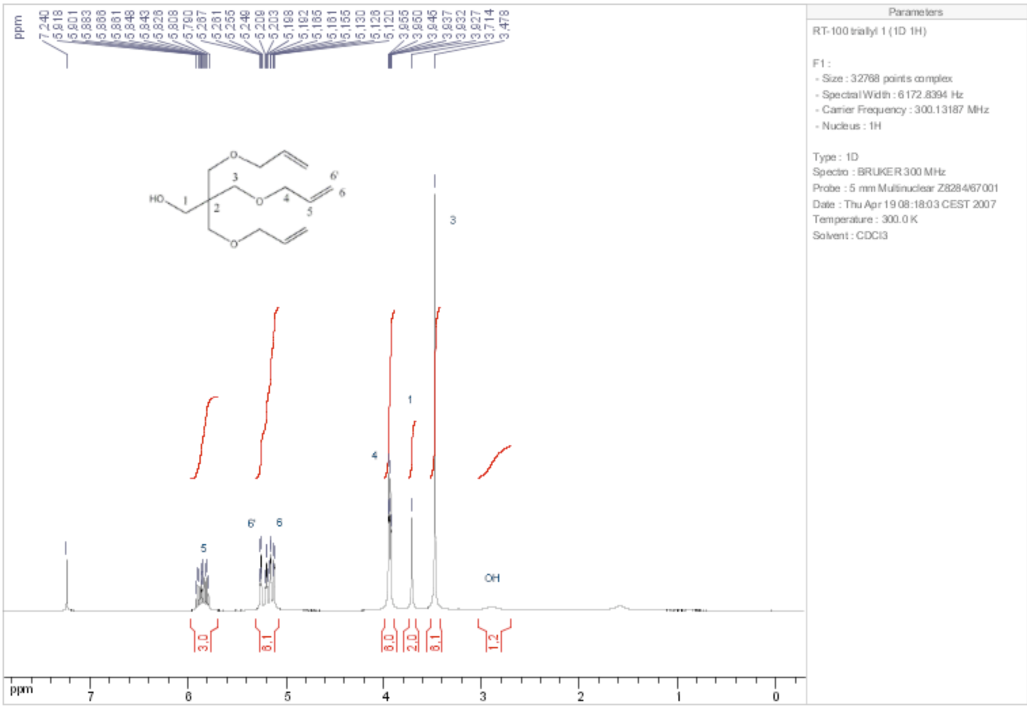
Bis propargylated PEG$_{6000}$ (1)

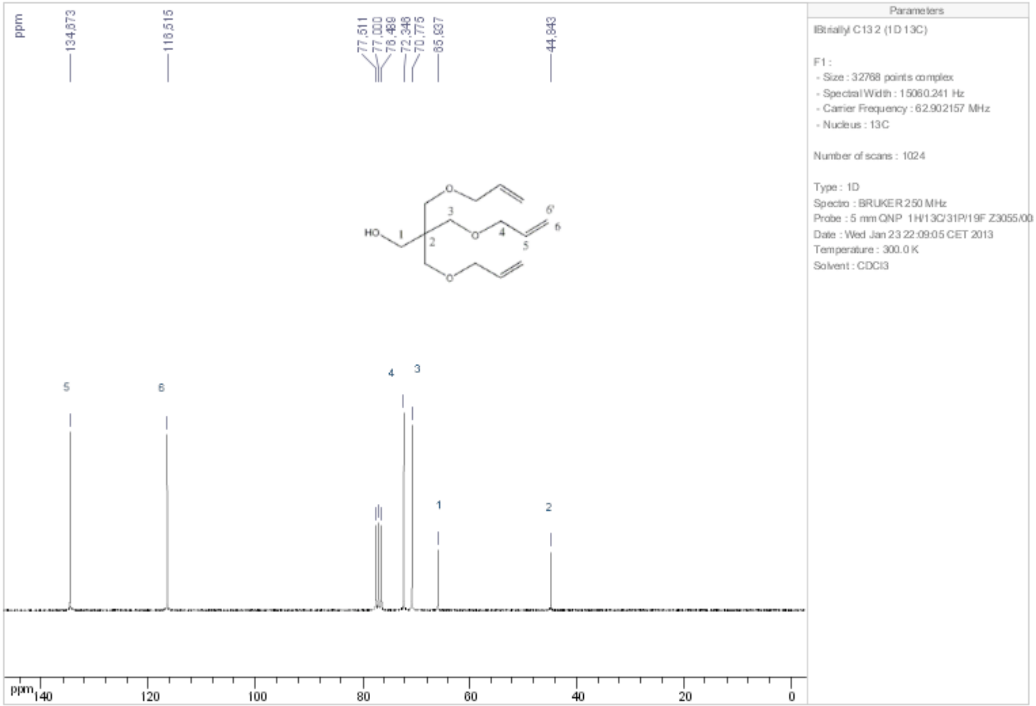




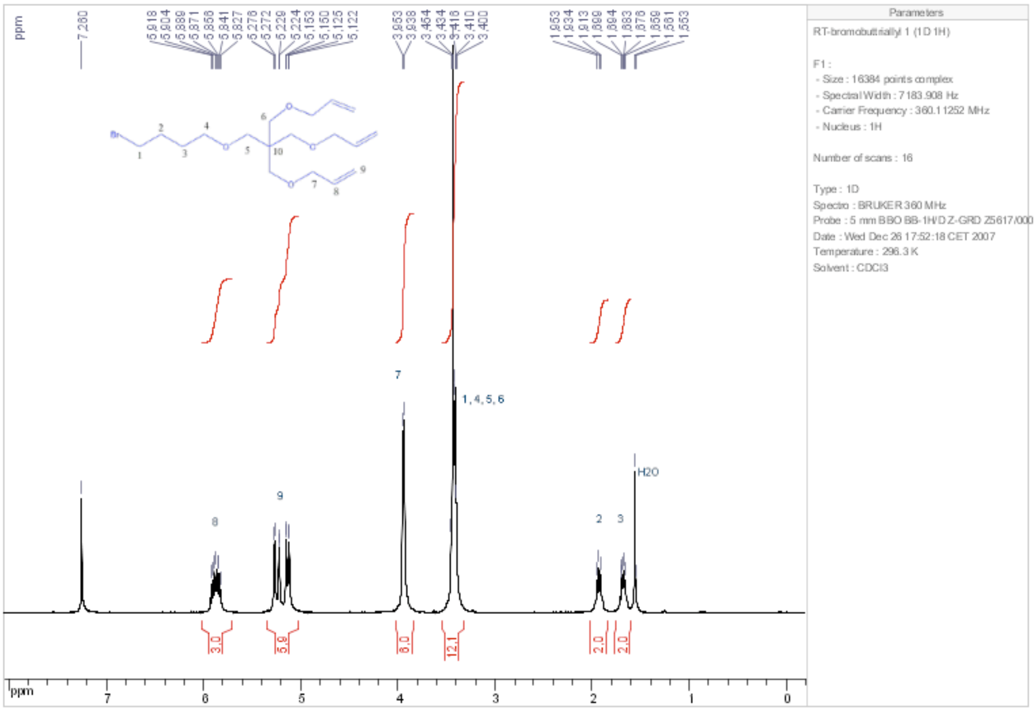


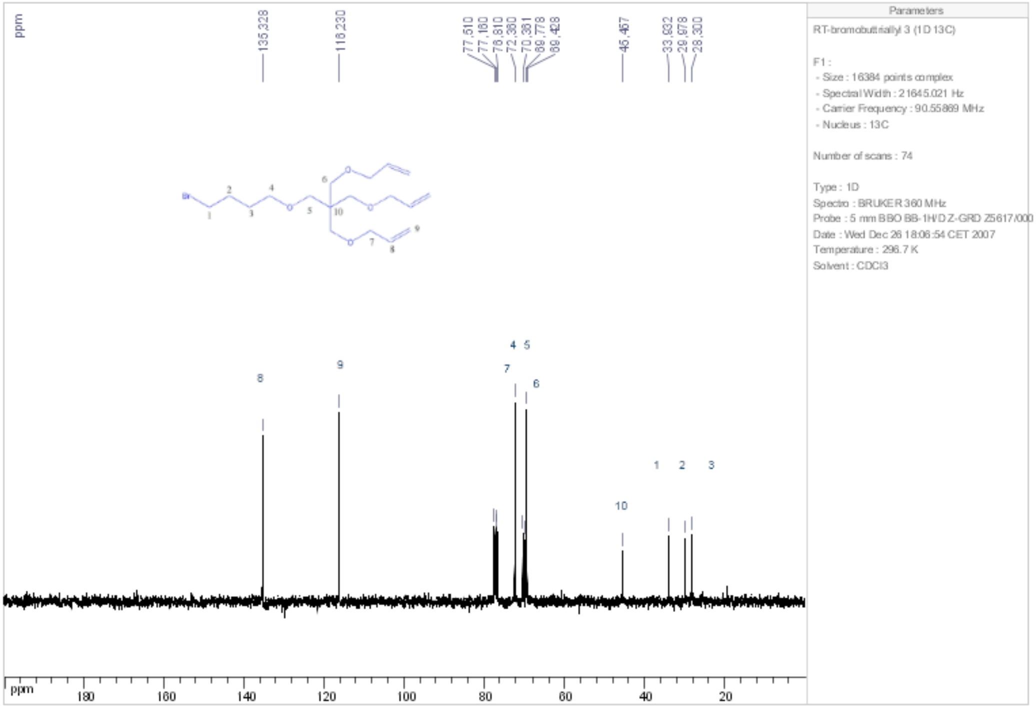
Pentaerythritol triallyl ether 6



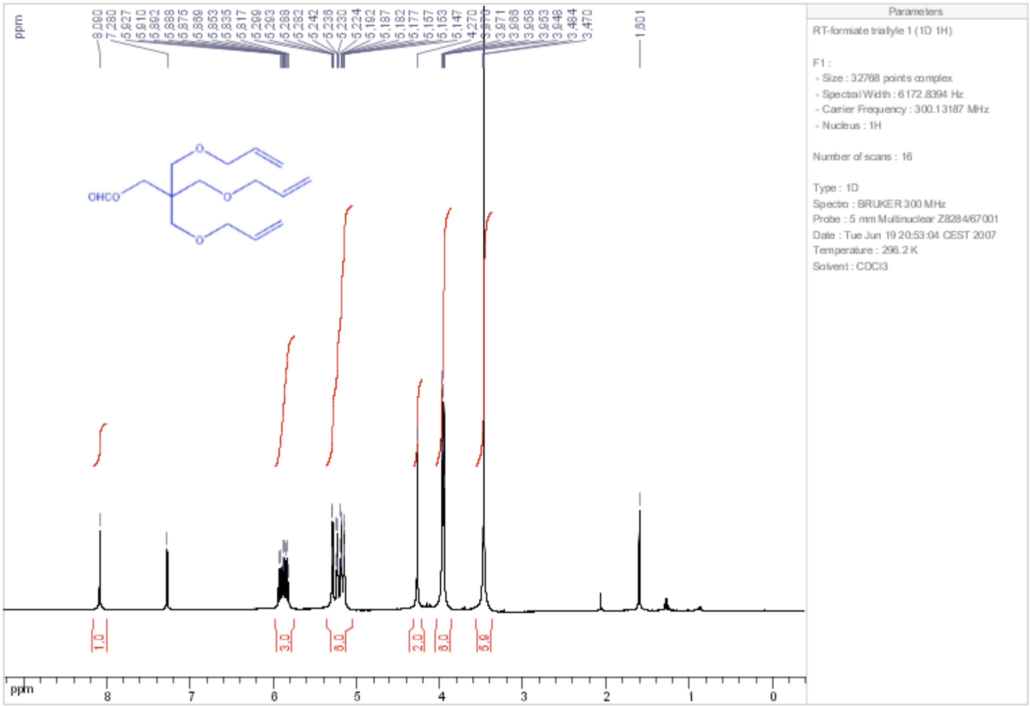


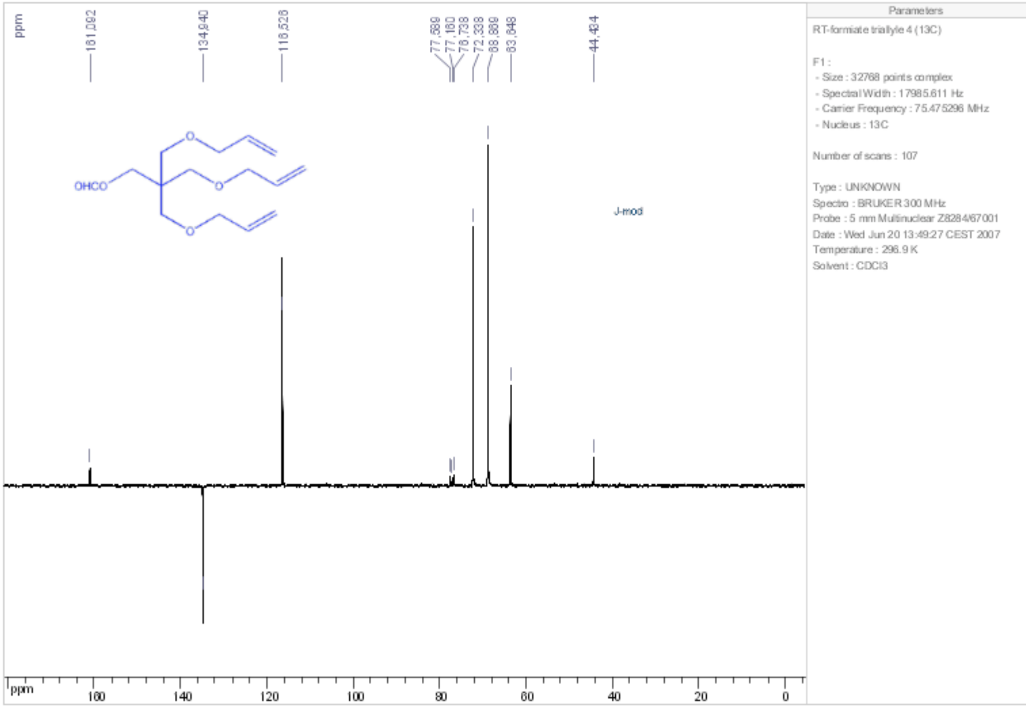
Compound 9



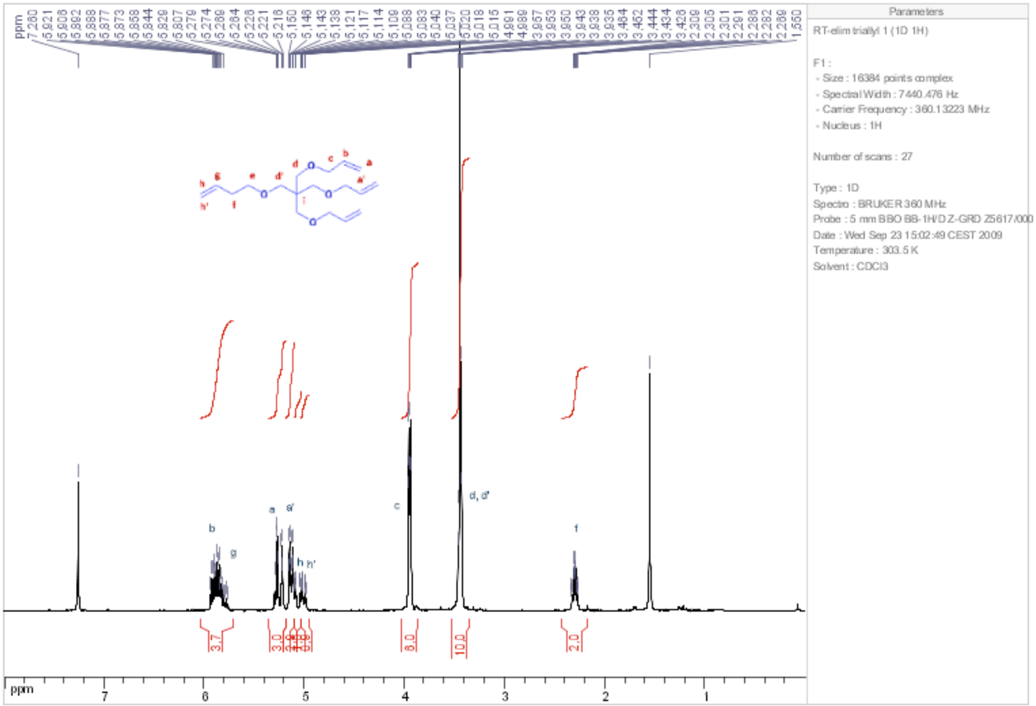


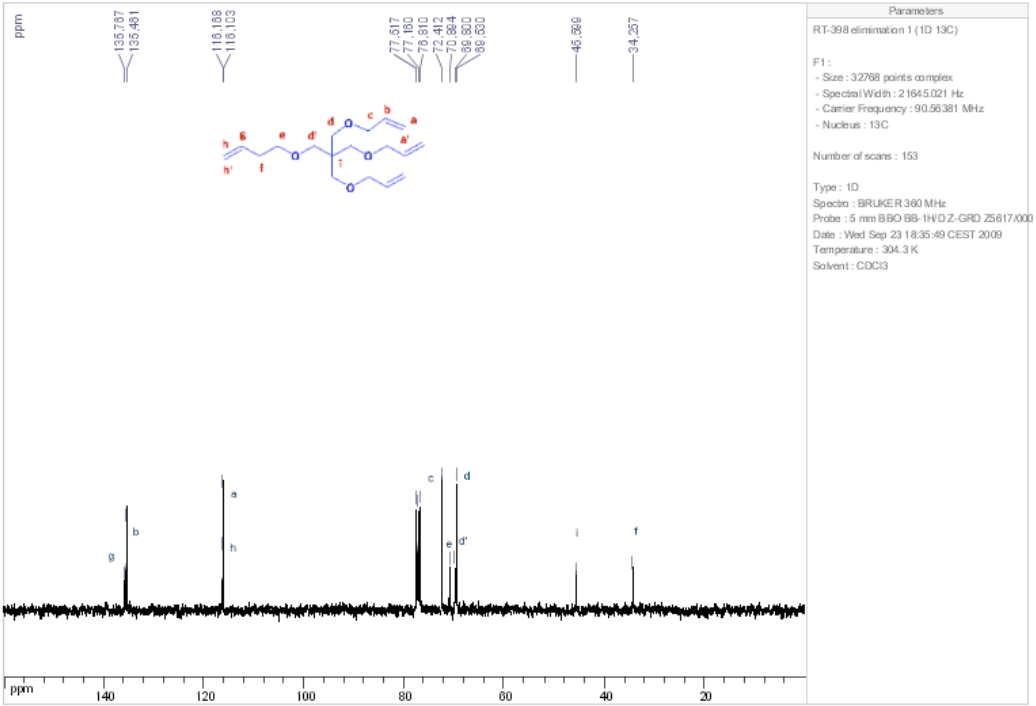
Compound 10





Compound 11

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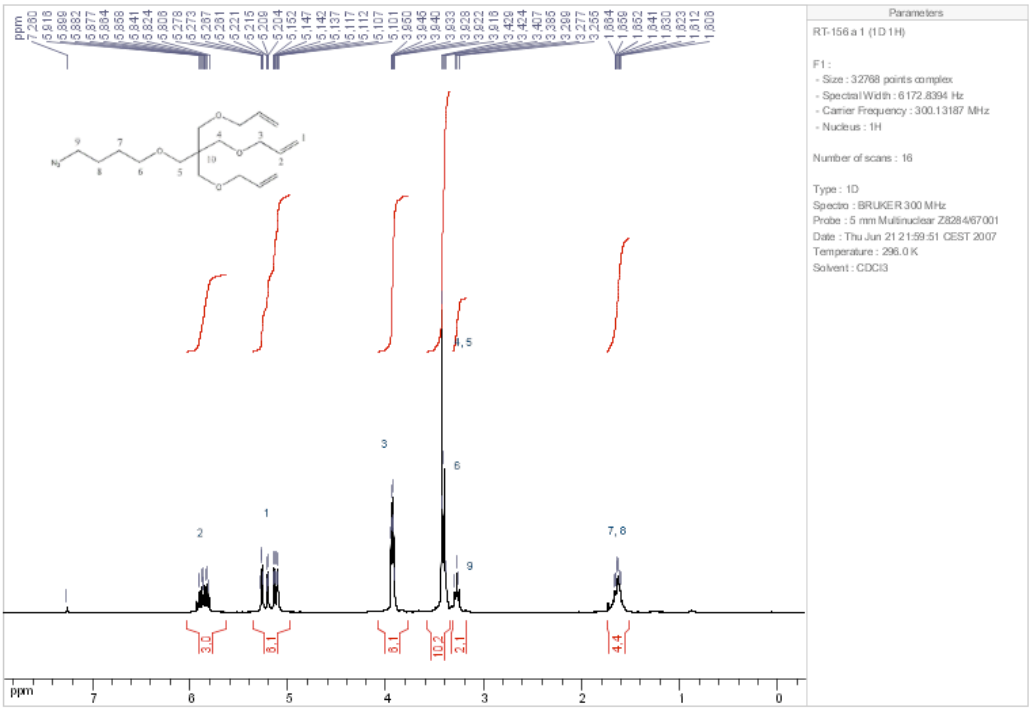
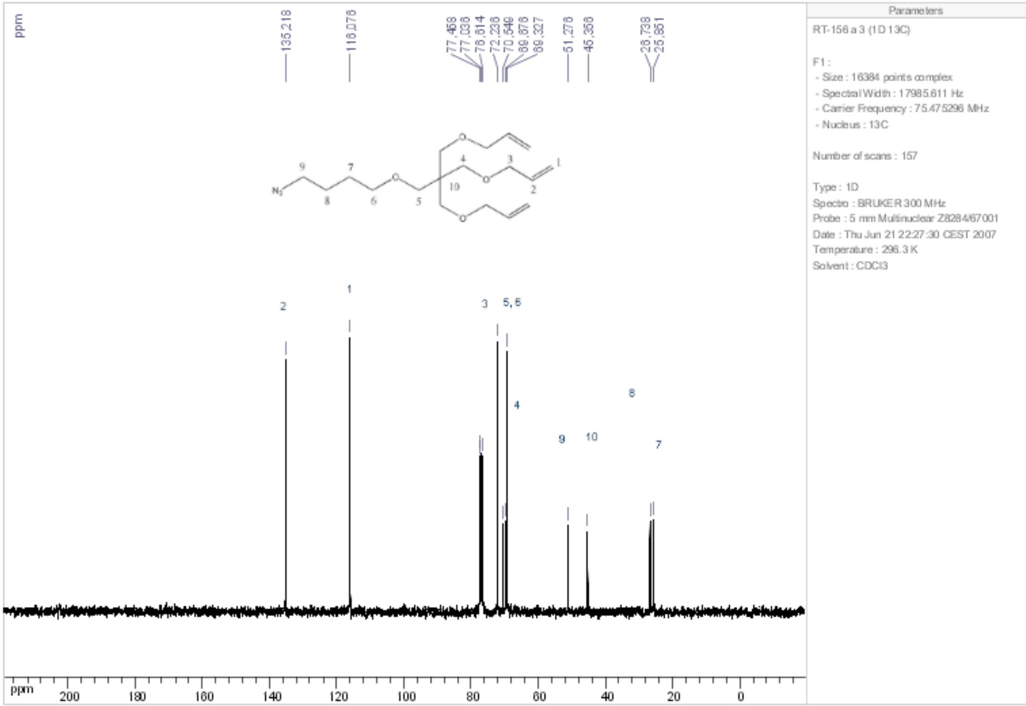
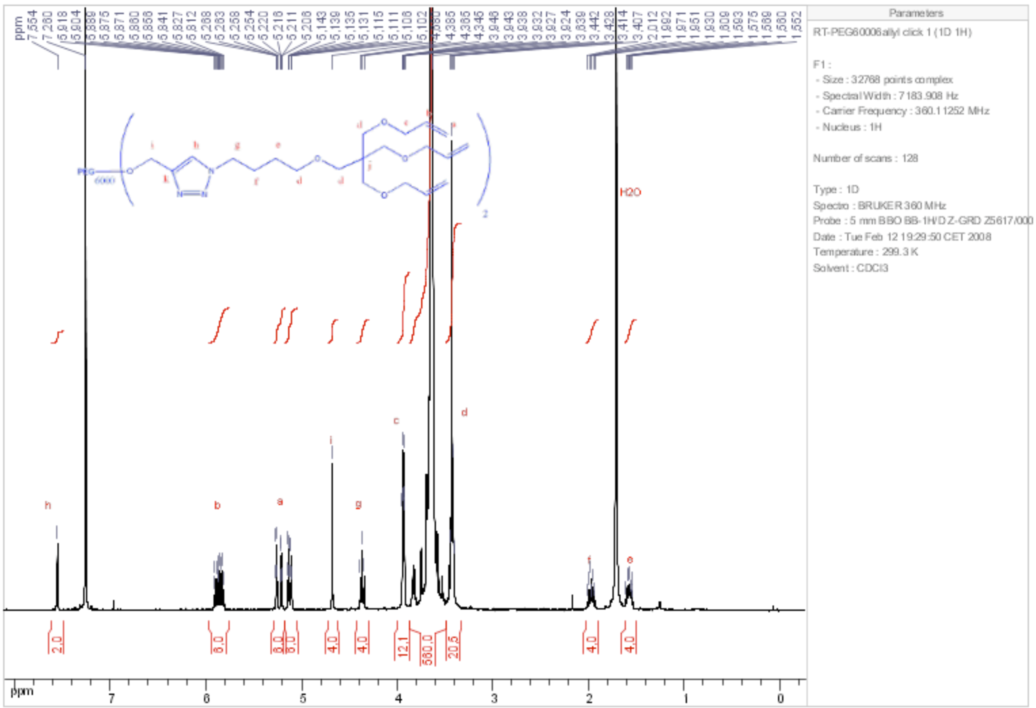
135.481
116.188
116.103
77.517
77.180
76.810
72.412
70.884
69.800
69.530
45.569
34.257
Parameters
RT-398 elimination 1 (1D 13C)
F1 :
- Size : 32768 points complex
- Spectral Width : 21645.021 Hz
- Carrier Frequency : 90.56381 MHz
- Nucleus : 13C
Number of scans : 153
Type : 1D
Spectro : BRUKER 360 MHz
Probe : 5 mm BBO BB-1H/D Z-GRD Z5617/000
Date : Wed Sep 23 18:35:49 CEST 2009
Temperature : 304.3 K
Solvent : CDCl3
ppm
140
120
100
80
60
40
20

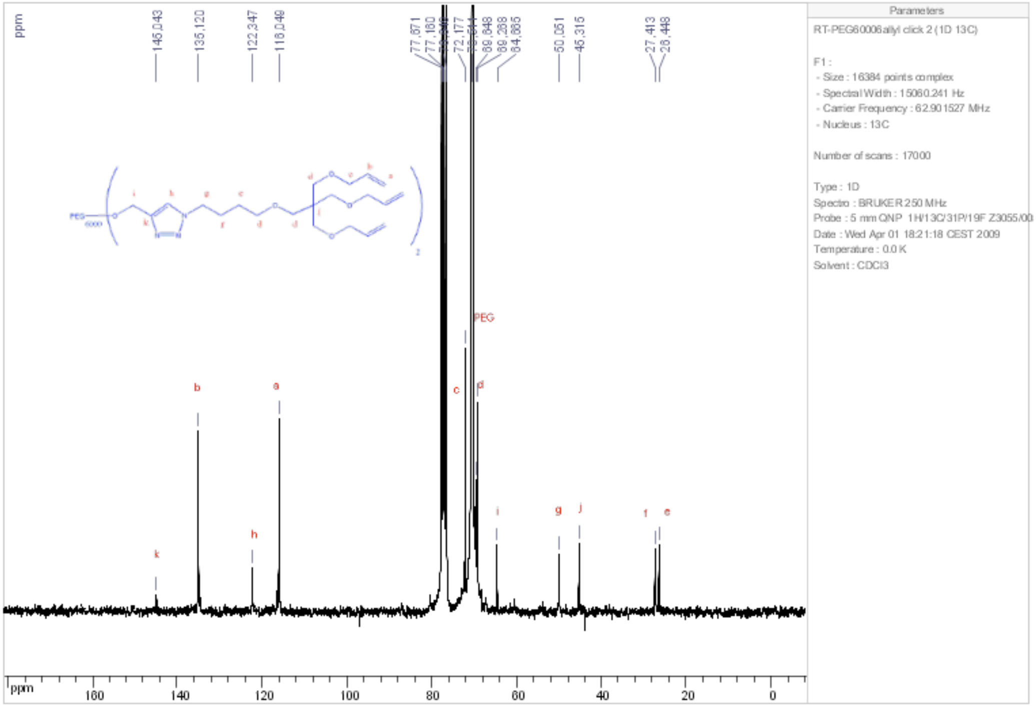
Compound 12


ppm
Parameters
RT-156 a 1 (1D 1H)
F1 :
- Size : 32768 points complex
- Spectral Width : 6172.8394 Hz
- Carrier Frequency : 300.13187 MHz
- Nucleus : 1H
Number of scans : 16
Type : 1D
Spectro : BRUKER 300 MHz
Probe : 5 mm Multinuclear Z8284/67001
Date : Thu Jun 21 21:59:51 CEST 2007
Temperature : 296.0 K
Solvent : CDCl3
3.0
6.1
6.1
10.2
2.1
4.4
ppm
7
6
5
4
3
2
1
0



PEG$_{6000}$ with 6 allyl functions (13)

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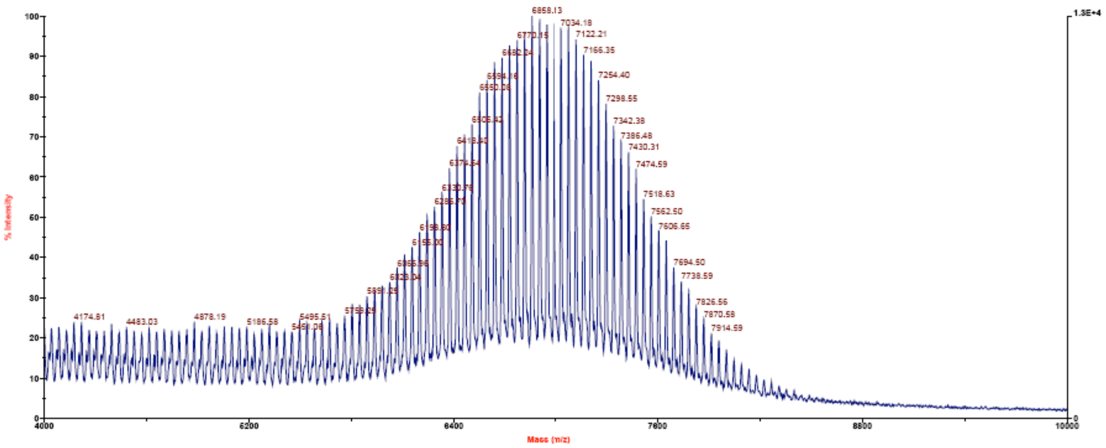
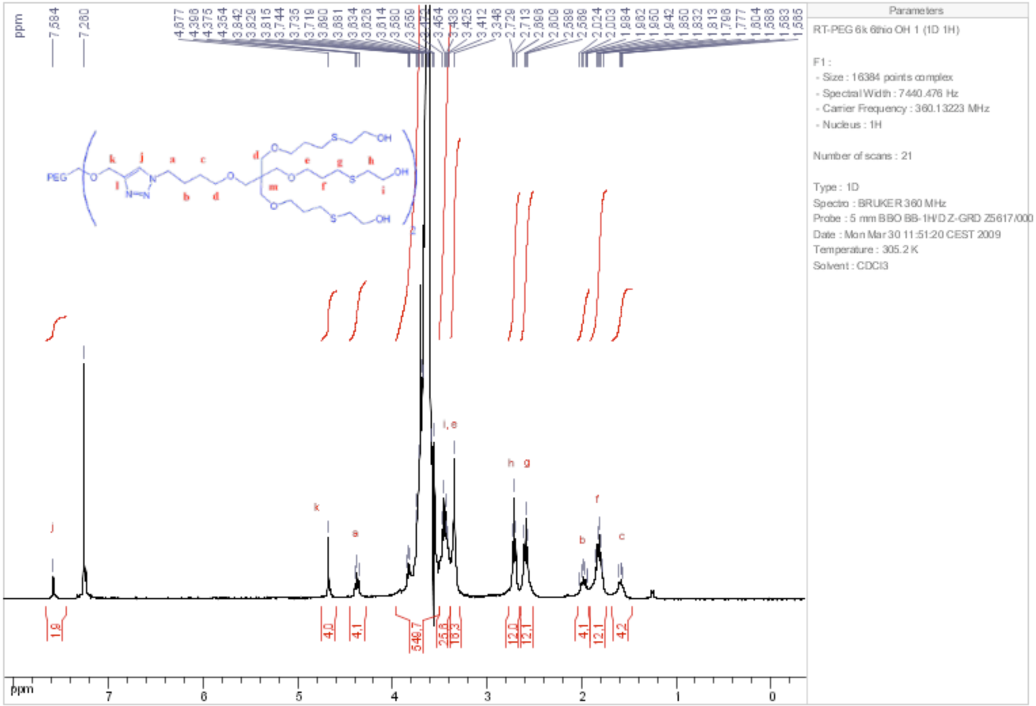
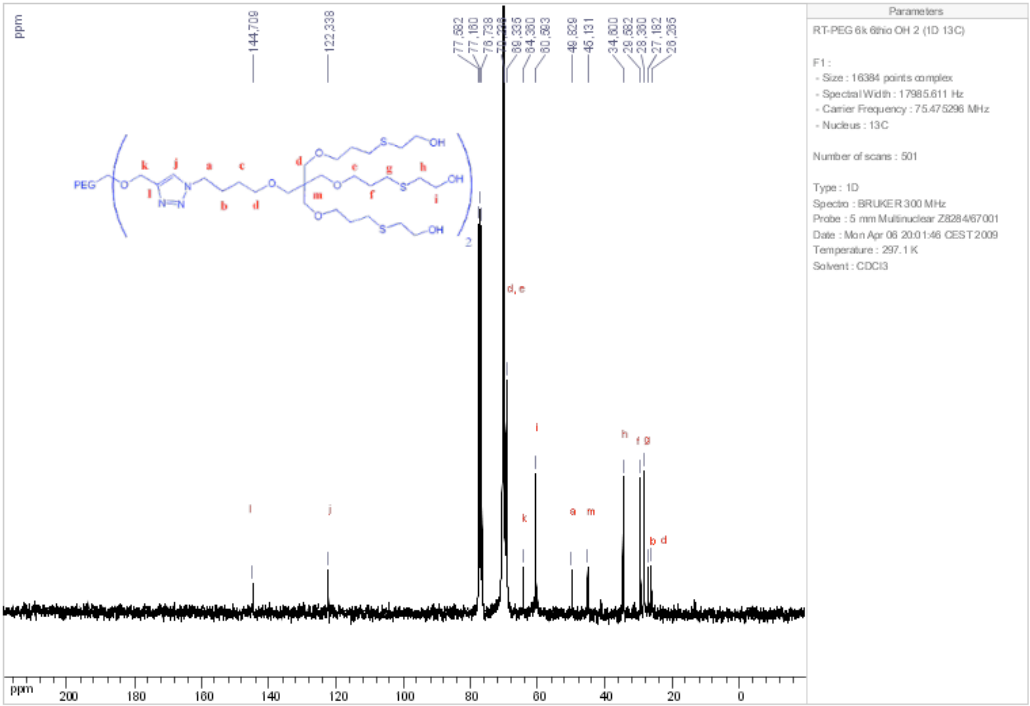
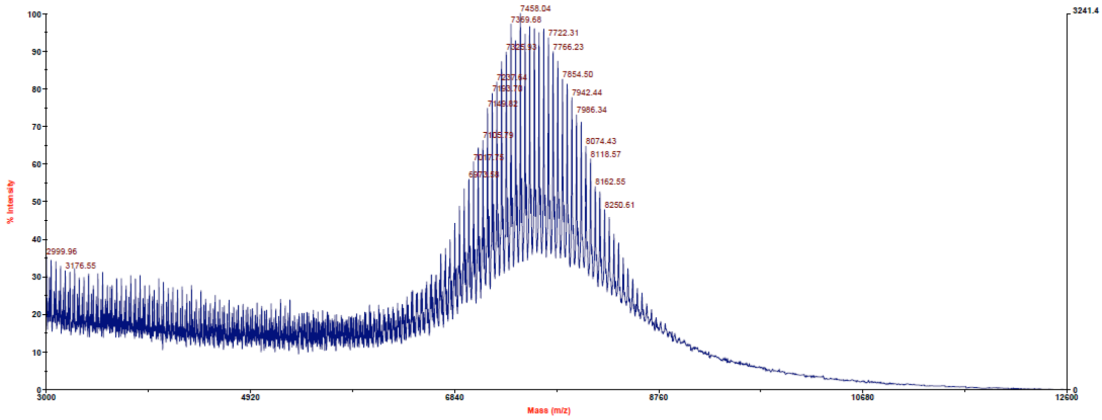
116,049
77,671
77,160
72,177
69,648
69,288
64,885
50,051
45,315
27,413
26,448
PEG
6000
k
b
h
a
c
d
i
g
j
f
e
2
Parameters
RT-PEG60006allyl click 2 (1D 13C)
F1 :
- Size : 16384 points complex
- Spectral Width : 15060.241 Hz
- Carrier Frequency : 62.901527 MHz
- Nucleus : 13C
Number of scans : 17000
Type : 1D
Spectro : BRUKER 250 MHz
Probe : 5 mm QNP 1H/13C/31P/19F Z3055/00
Date : Wed Apr 01 18:21:18 CEST 2009
Temperature : 0.0 K
Solvent : CDCl3
ppm
160
140
120
100
80
60
40
20
0


% Intensity
Mass (m/z)
1.3E+4
6858.13
7034.18
6770.15
7122.21
6682.24
7166.35
6594.16
6550.08
7254.40
7298.55
6506.42
7342.38
6418.40
7386.48
7430.31
6374.64
7474.59
6330.79
6286.70
7518.63
7562.50
6198.60
7606.65
6155.00
6066.96
7694.50
6023.04
7738.59
5891.29
7826.56
5759.29
7870.58
4174.81
4483.03
4878.19
5186.58
5495.51
7914.59
4000
10000

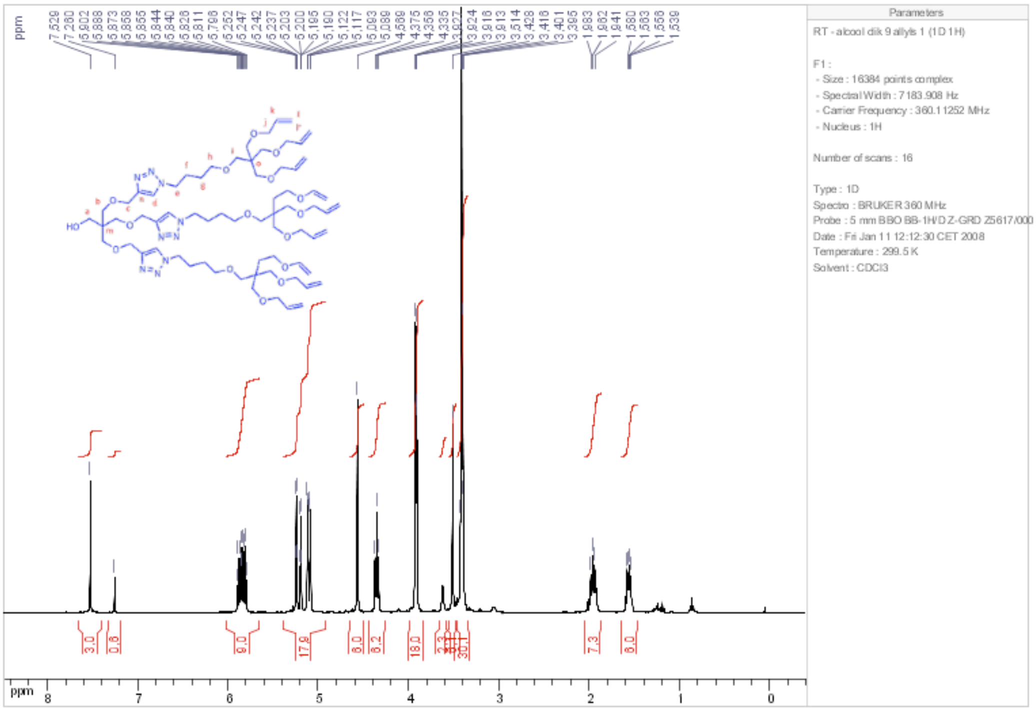
PEG$_{6000}$ with 6 alcohol functions (15)

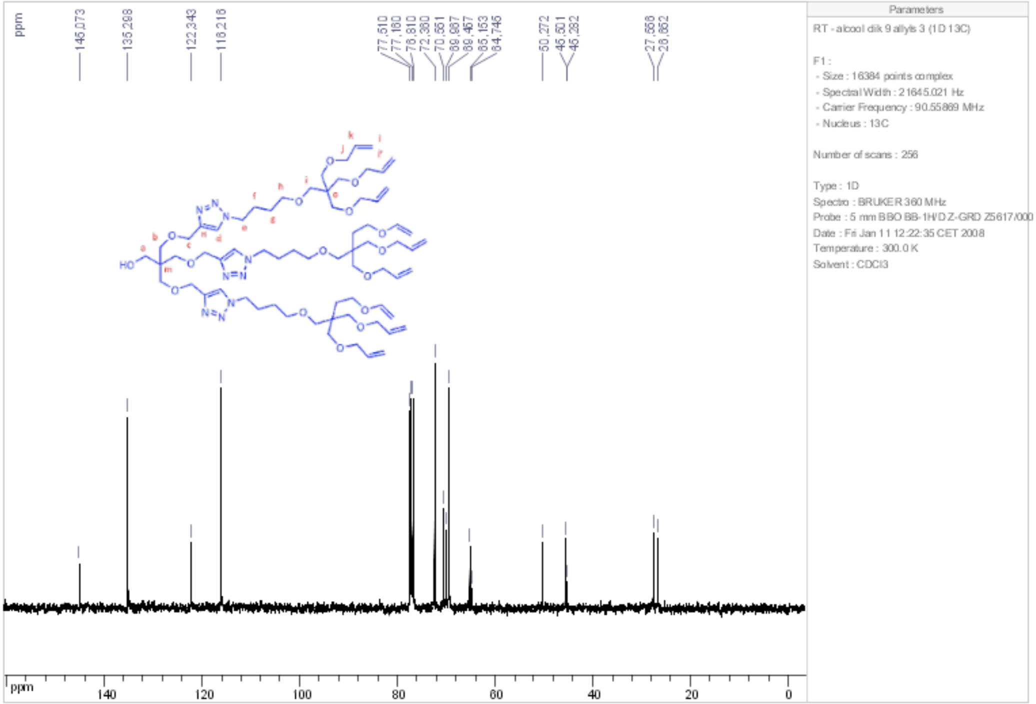




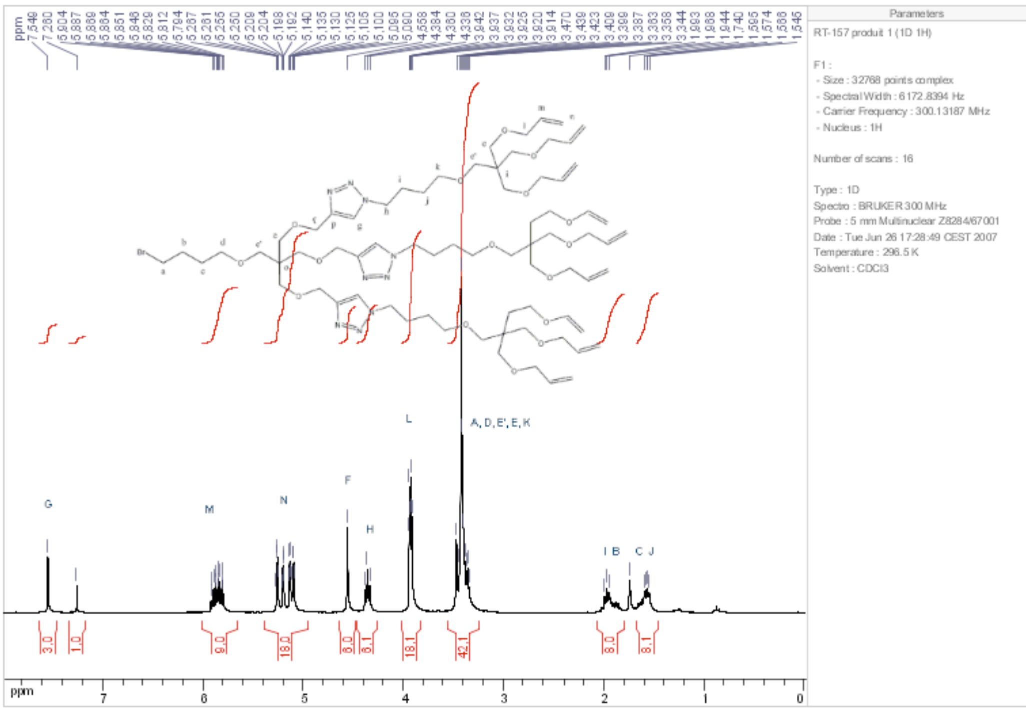

% Intensity
Mass (m/z)
7458.04
7722.31
7766.23
7854.50
7942.44
7986.34
8074.43
8118.57
8162.55
8250.61
2999.96
3176.55
3241.4

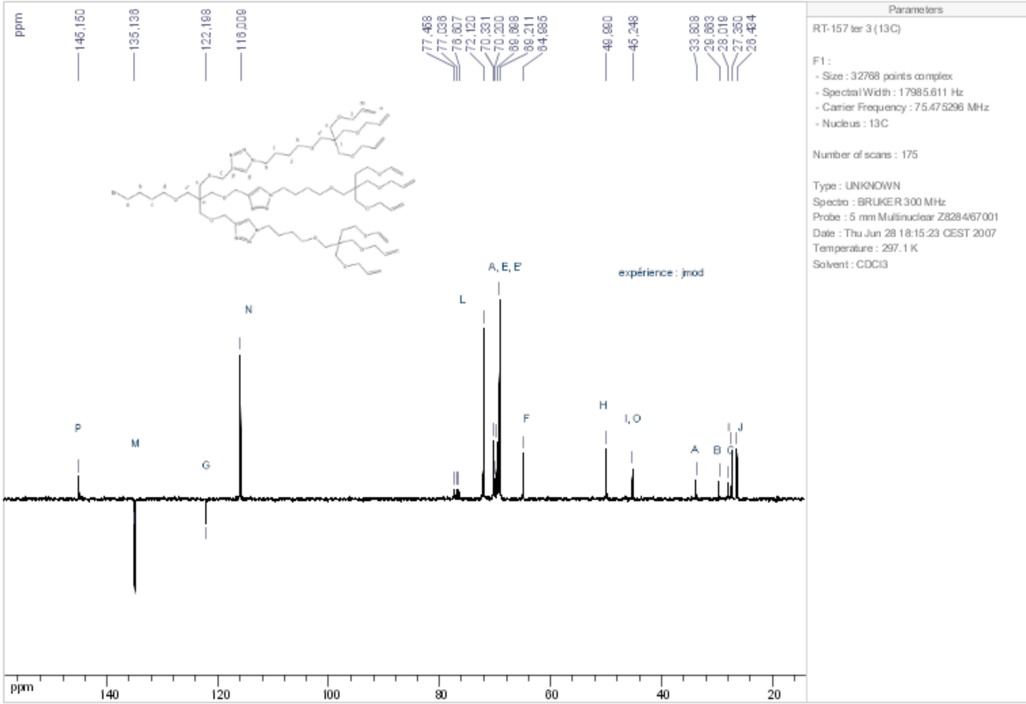
Compound 17


Parameters
RT - alcool dik 9 allyls 1 (1D 1H)
F1 :
- Size : 16384 points complex
- Spectral Width : 7 183.908 Hz
- Carrier Frequency : 360.11252 MHz
- Nucleus : 1H
Number of scans : 16
Type : 1D
Spectro : BRUKER 360 MHz
Probe : 5 mm BBO BB-1H/D Z-GRD Z5617/000
Date : Fri Jan 11 12:12:30 CET 2008
Temperature : 299.5 K
Solvent : CDCl3
ppm

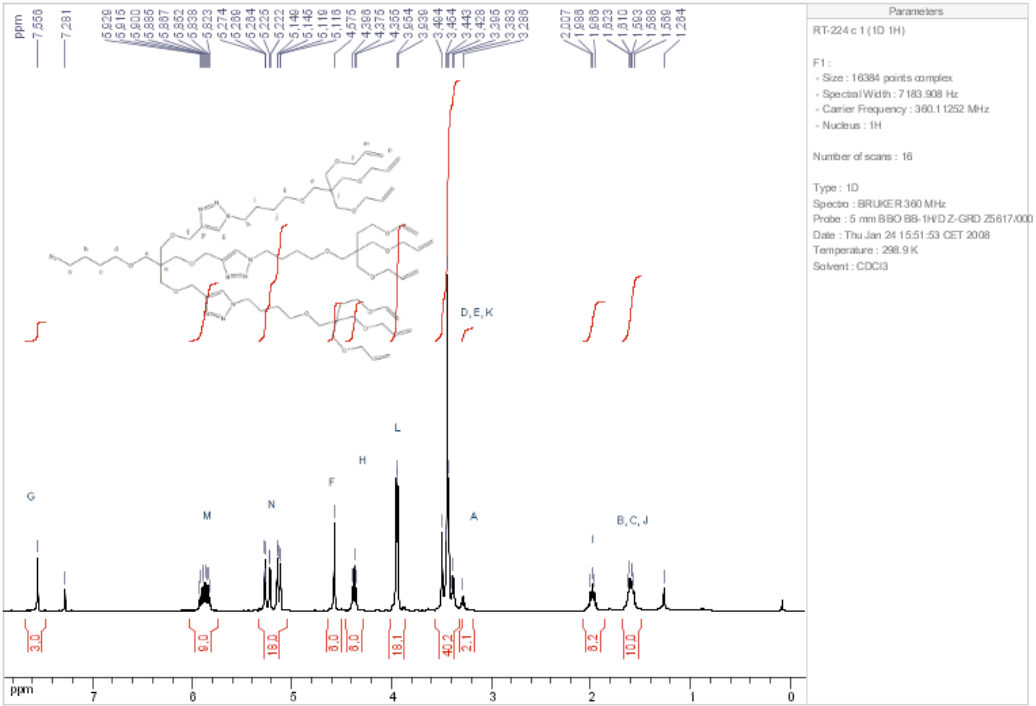

Parameters
RT - alcool dik 9 allyls 3 (1D 13C)
F1 :
- Size : 16384 points complex
- Spectral Width : 21645.021 Hz
- Carrier Frequency : 90.55869 MHz
- Nucleus : 13C
Number of scans : 256
Type : 1D
Spectro : BRUKER 360 MHz
Probe : 5 mm BBO BB-1H/D Z-GRD Z5617/000
Date : Fri Jan 11 12:22:35 CET 2008
Temperature : 300.0 K
Solvent : CDCl3
ppm

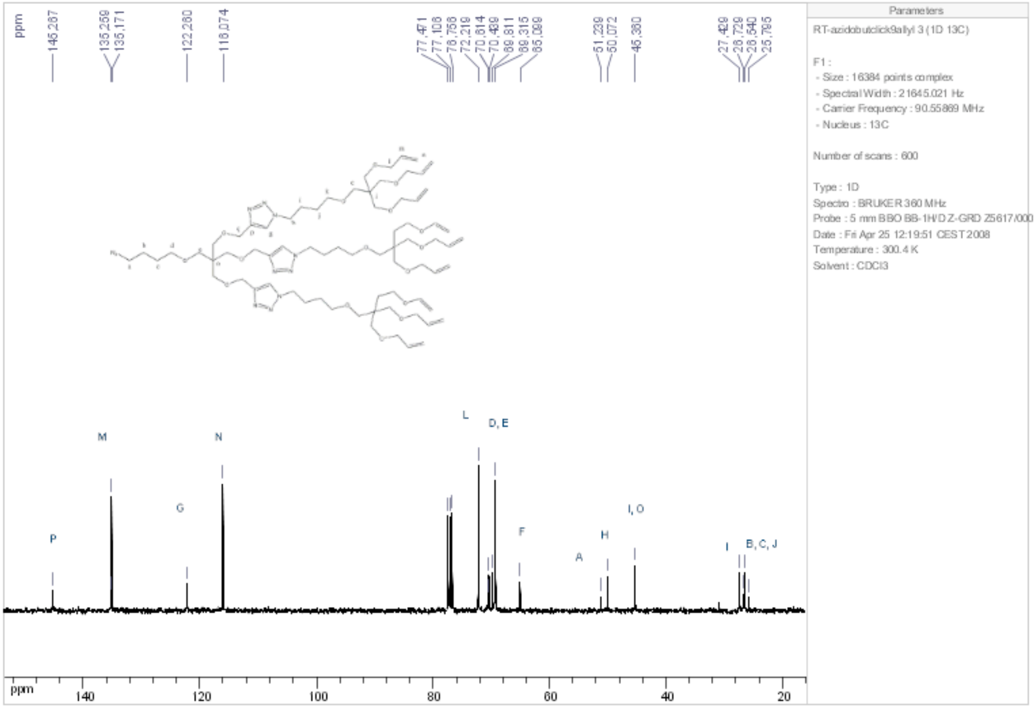
Compound 18


Parameters
RT-157 produit 1 (1D 1H)
F1 :
- Size : 32768 points complex
- Spectral Width : 6172.8394 Hz
- Carrier Frequency : 300.13187 MHz
- Nucleus : 1H
Number of scans : 16
Type : 1D
Spectro : BRUKER 300 MHz
Probe : 5 mm Multinuclear Z8284/67001
Date : Tue Jun 26 17:28:49 CEST 2007
Temperature : 296.5 K
Solvent : CDCl3
A, D, E', E, K
ppm

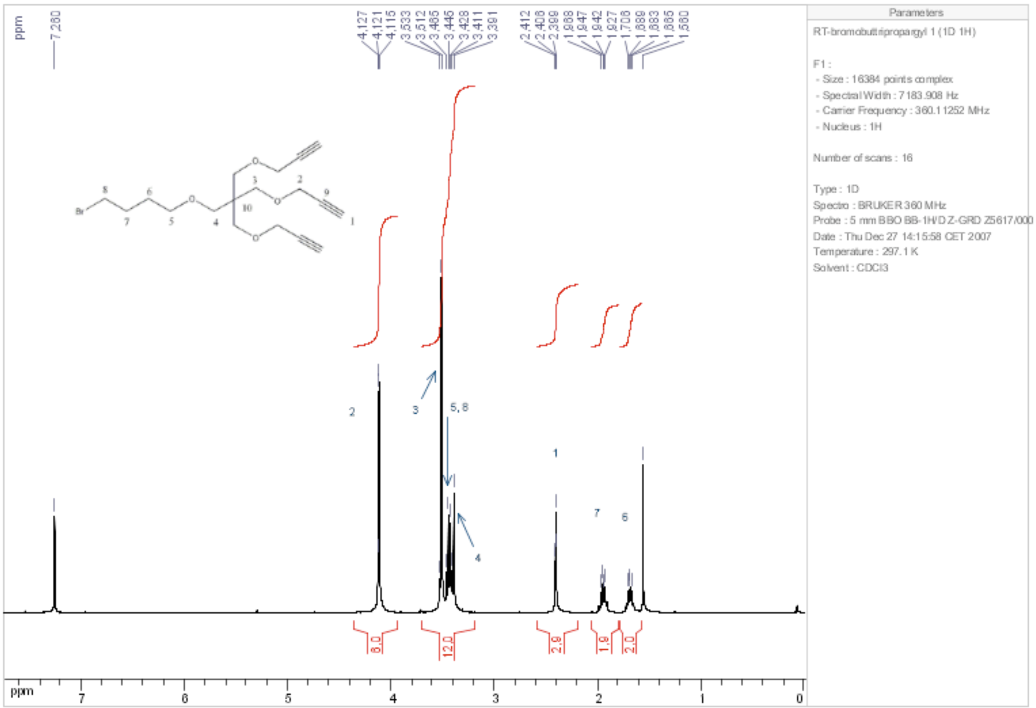

Parameters
RT-157 ter 3 (13C)
F1 :
- Size : 32768 points complex
- Spectral Width : 17985.611 Hz
- Carrier Frequency : 75.475296 MHz
- Nucleus : 13C
Number of scans : 175
Type : UNKNOWN
Spectro : BRUKER 300 MHz
Probe : 5 mm Multinuclear Z8284/67001
Date : Thu Jun 28 18:15:23 CEST 2007
Temperature : 297.1 K
Solvent : CDCl3
expérience : jmod
ppm

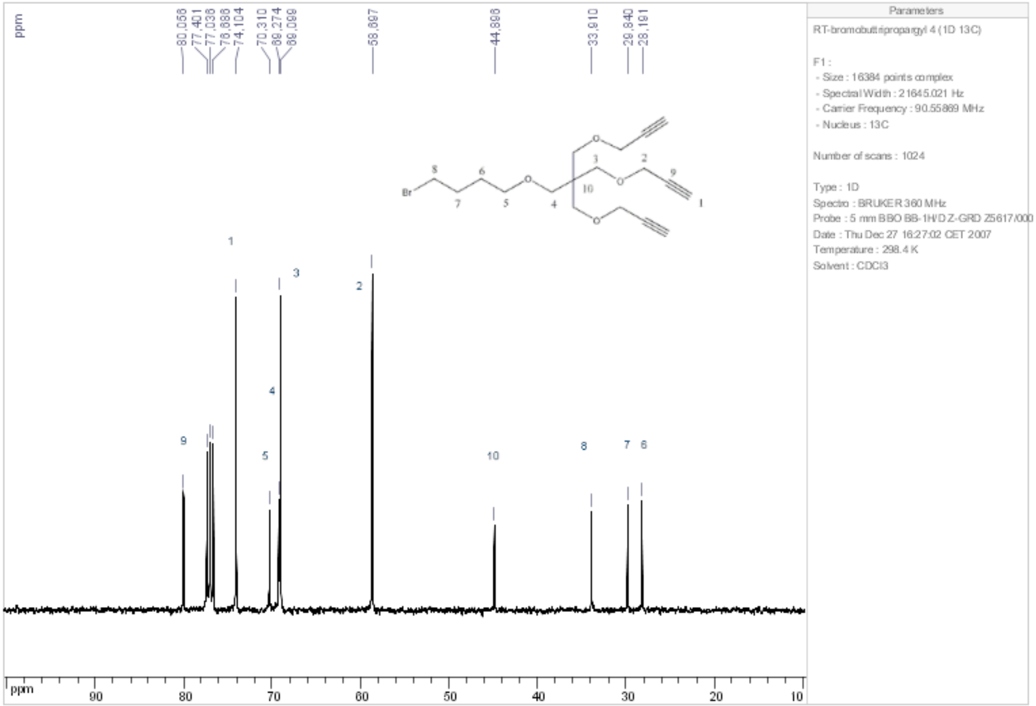
Compound 19


Parameters
RT-224 c 1 (1D 1H)
F1 :
- Size : 16384 points complex
- Spectral Width : 7183.908 Hz
- Carrier Frequency : 360.11252 MHz
- Nucleus : 1H
Number of scans : 16
Type : 1D
Spectro : BRUKER 360 MHz
Probe : 5 mm BBO BB-1H/D Z-GRD Z5617/000
Date : Thu Jan 24 15:51:53 CET 2008
Temperature : 298.9 K
Solvent : CDCl3
ppm

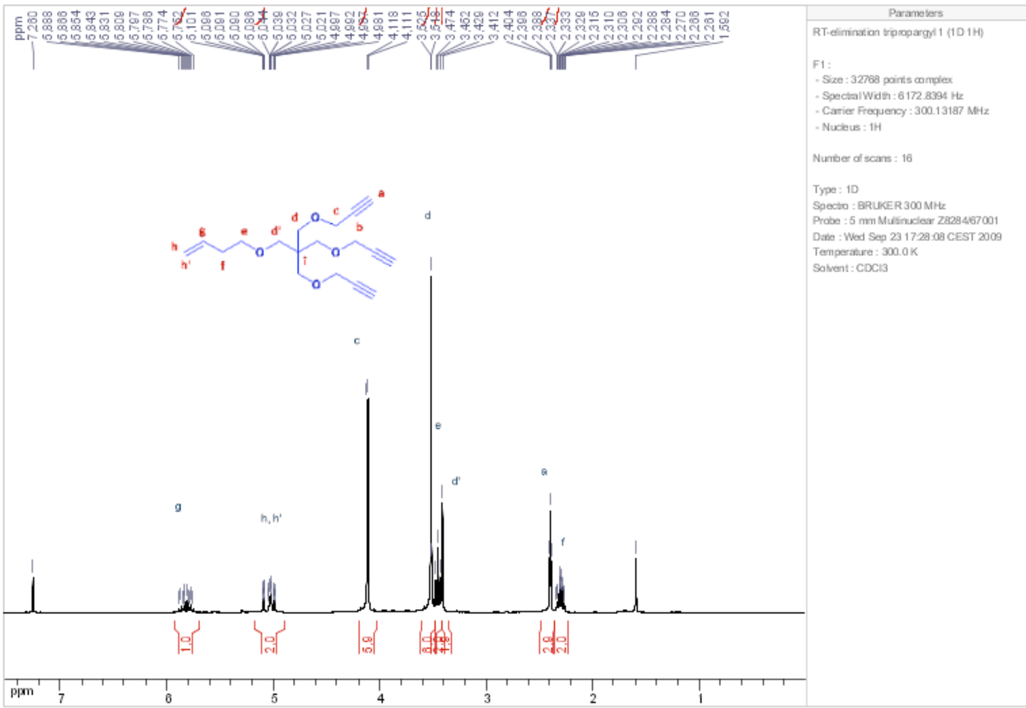


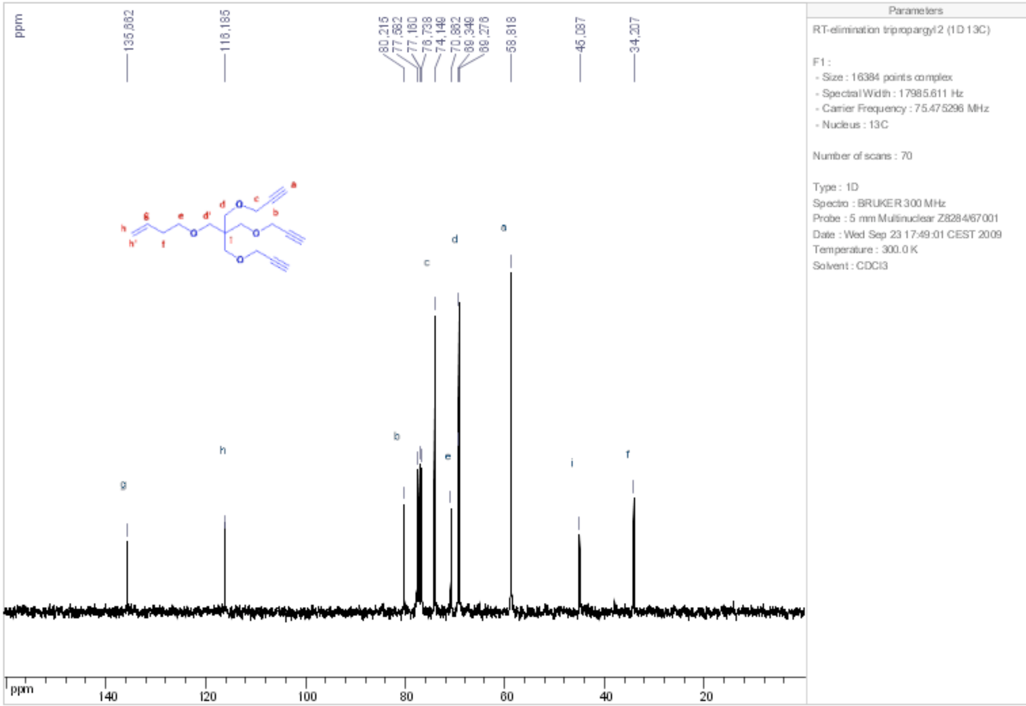
Compound 20



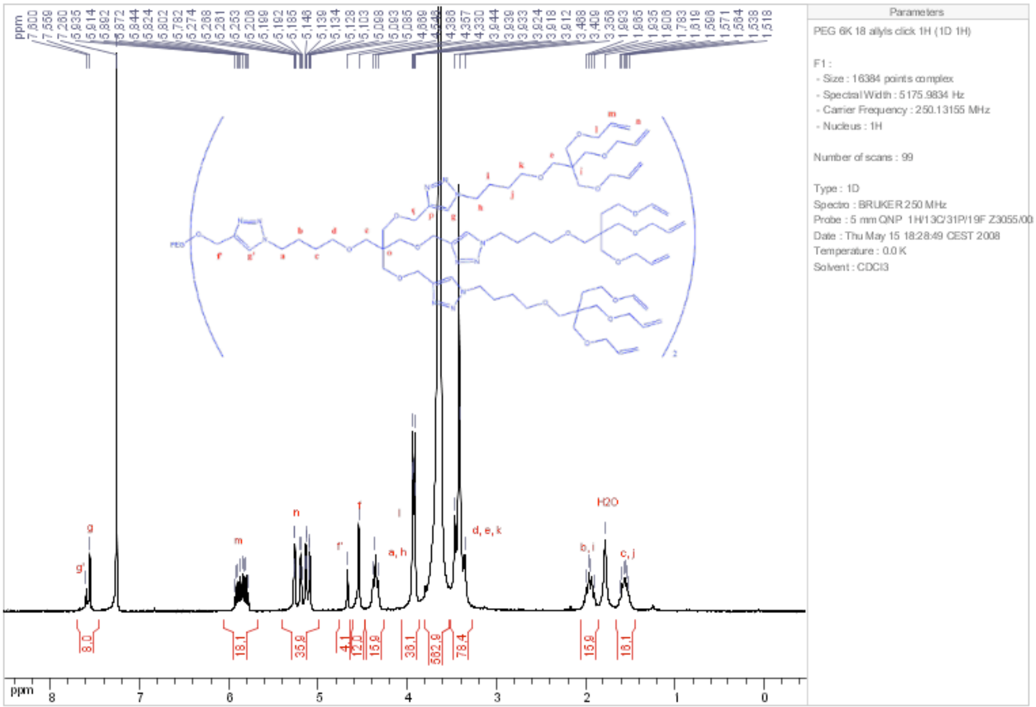


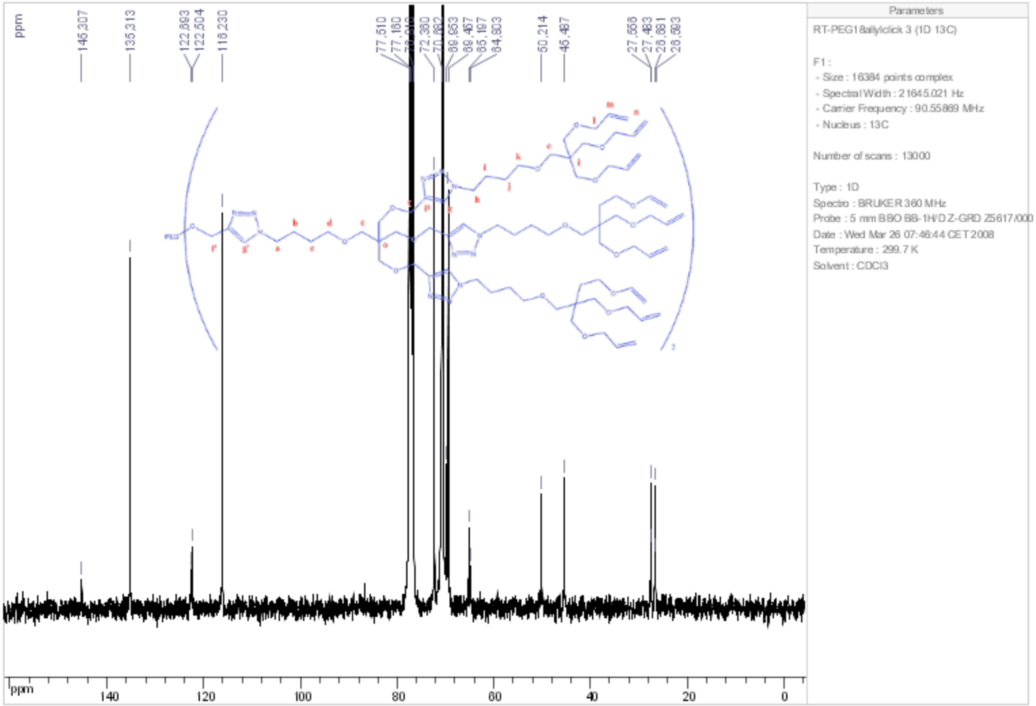
Compound 21

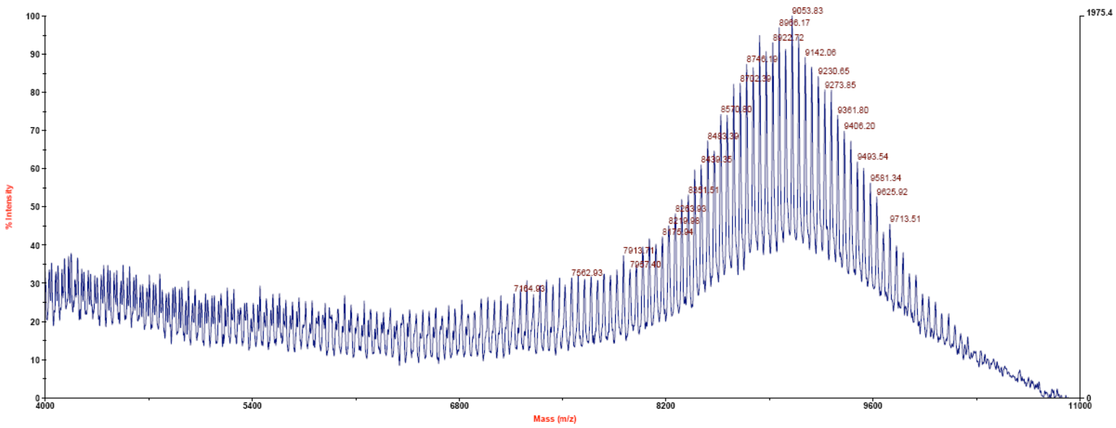




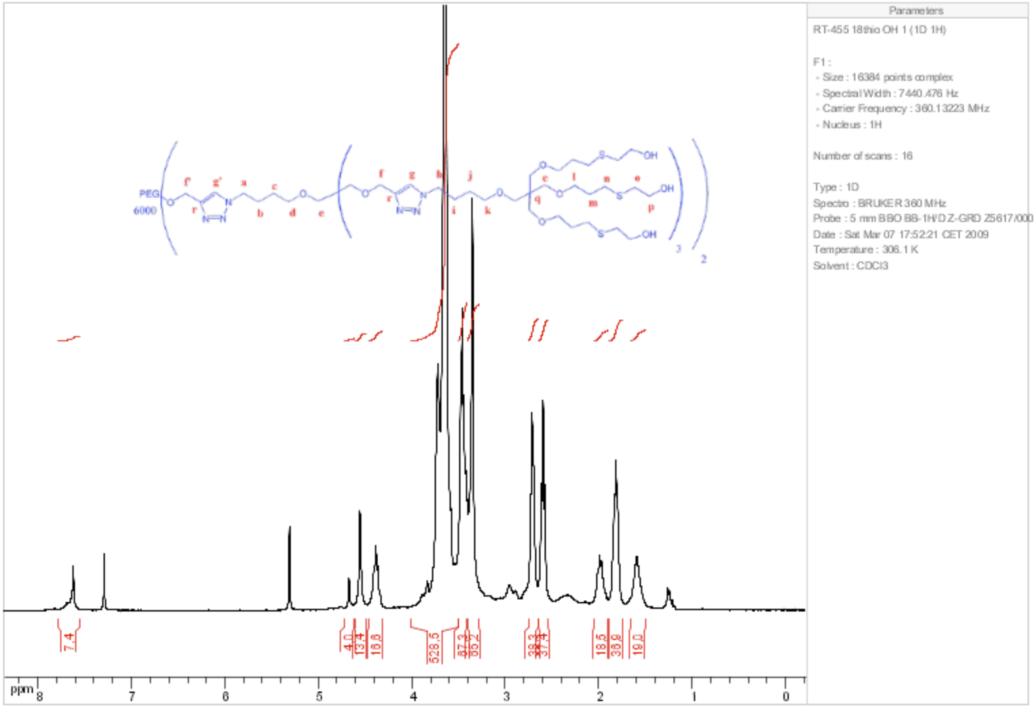
PEG$_{6000}$ with 18 allyl functions (22)

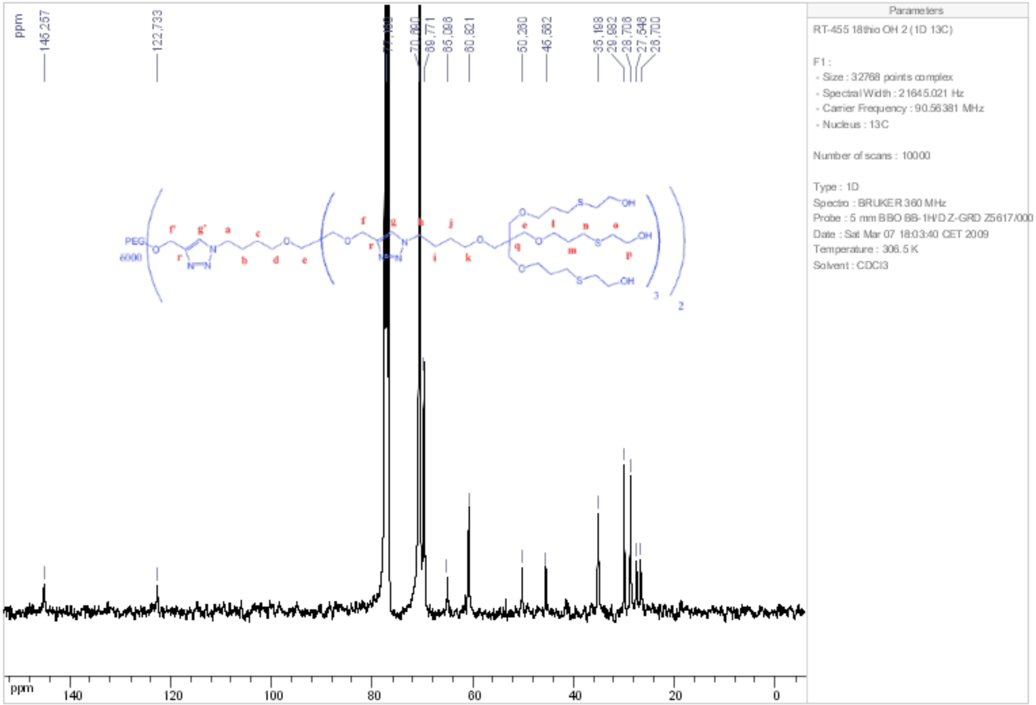


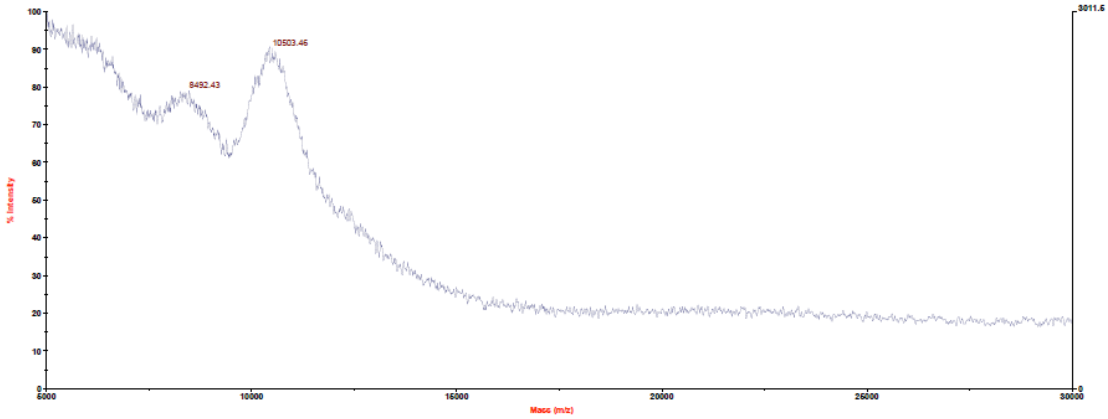

ppm
145.307
135.313
122.893
122.504
116.230
77.510
77.180
72.380
69.853
69.457
65.197
64.803
50.214
45.487
27.558
27.483
26.581
26.593
Parameters
RT-PEG18allylclick 3 (1D 13C)
F1 :
- Size : 16384 points complex
- Spectral Width : 21645.021 Hz
- Carrier Frequency : 90.55869 MHz
- Nucleus : 13C
Number of scans : 13000
Type : 1D
Spectro : BRUKER 360 MHz
Probe : 5 mm BBO BB-1H/D Z-GRD Z5617/000
Date : Wed Mar 26 07:46:44 CET 2008
Temperature : 299.7 K
Solvent : CDCl3
ppm
140
120
100
80
60
40
20
0


9053.83
8966.17
8922.72
9142.06
8746.19
9230.65
8702.39
9273.85
8570.60
9361.80
9406.20
9493.54
9581.34
9625.92
9713.51
7562.93
1975.4
% Intensity
Mass (m/z)
4000
5400
6800
8200
9600
11000

PEG_{6000} with 18 alcohol functions (23)






10503.46
8492.43
3011.5
% Intensity
Mass (m/z)
0
10
20
30
40
50
60
70
80
90
100
5000
10000
15000
20000
25000
30000