

## ANALYSIS OF ALTERNATIVES

### PUBLIC VERSION

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**Substance:** Diglyme (Bis(2-methoxyethyl)ether)  
CAS No 111-96-6

**Use title:** Use of Diglyme as solvent in the manufacturing  
process of [REDACTED] products by process used in  
the electronic industry in several applications.

**Use number:** 2

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## LIST OF ABBREVIATIONS

<b>AoA:</b>	Analysis of alternatives
<b>MSDS:</b>	Materials safety data sheet
<b>GESTIS:</b>	Information system on hazardous substances of the German Social Accident Insurance
<b>GHS:</b>	Globally harmonized system for the labelling of chemicals
<b>PubChem:</b>	Open chemistry database of the National Institutes of Health (NIH) in the USA
<b>UV:</b>	ultraviolet light
<b>ml:</b>	milli-liter
<b>µl:</b>	micro-liter

[REDACTED]

[REDACTED]

[REDACTED]

<b>CAS No.:</b>	Chemical abstracts service number
<b>REACH:</b>	Registration, evaluation, authorization and restriction of chemicals in the European Union
<b>EC No.:</b>	Chemical substance number in the European Union
<b>NMR:</b>	Nuclear magnetic resonance spectroscopy
<b>CSR:</b>	Chemical safety report
<b>THF:</b>	Tetrahydrofuran
<b>DMF:</b>	N,N-Dimethylformamide
<b>CDCl<sub>3</sub>:</b>	deuterated Chloroform
<b>SOCl<sub>2</sub>:</b>	Thionyl chloride

[REDACTED]

<b>n.a.:</b>	not available or not assessed
<b>hPa:</b>	hecto-Pascal
<b>ca.:</b>	circa



## DECLARATION

We, BASF Switzerland AG, request that the information given within this document, must be erased or blanked out, especially for the following information:

- regarding the synthesis schemes,
- the description of the production process [REDACTED] and its inherent analytical data, [REDACTED] and the trade name and application of [REDACTED]

and it is not to be made available to personal not involved in the verification of our appraisal for authorization of Diglyme as process solvent for our [REDACTED] production at our facility in Schweizerhalle/Switzerland.

We hereby declare that, to the best of our knowledge of today the information is not publicly available, and in accordance with due measures of protection that we have implemented, a member of the public should not be able to obtain access to this information without our consent or that of the third party whose commercial interests are at stake.

Date, Place:

25.7.2019, Basel

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## 1 SUMMARY

Use of Diglyme in the [REDACTED] production at BASF Schweiz AG, Schweizerhalle production site

BASF Schweiz AG (before its predecessor Ciba Specialty Chemicals Ltd. and even before Ciba-Geigy Ltd.) produces and sells since [REDACTED] products by process under the trade names [REDACTED].

These commercial products are used in the electronic industry as UV-light-patternable encapsulation materials / dielectrics for electronic parts like computer chips and integrated circuits. They were qualified over many years for specific applications by our customer. These products are used e.g. in safety relevant electronic systems, where a continued quality and reliability is of utmost importance. In order to fulfill the stringent quality measures [REDACTED], the production processes and the outcoming product compositions must be kept constant, fulfilling the product specifications.

The production processes for the manufacturing of [REDACTED] result in product by process polymeric materials. [REDACTED], Diglyme is the main solvent over the whole production processes, which is present in all [REDACTED] reaction steps. The final product compositions are precipitated at the end [REDACTED] in water to give the raw products in the form of filterable powders. Extensive washing [REDACTED] is then needed to get rid of the large part of [REDACTED] residues to fulfill the very demanding quality measures for electronic applications. The products are dried in a closed oven to remove residual traces of Diglyme in the wet cakes. The products are then finally purified [REDACTED].

Diglyme has the right polarity and viscosity to enable the dissolution of the starting materials, the intermediates and the final [REDACTED] resins, which are formed as products by process. In addition, Diglyme is chemically inert, compatible and safe in combination with all starting materials, intermediates [REDACTED] and the resulting [REDACTED] resins during the whole process under the chosen reaction conditions. One reaction step must be conducted at -[REDACTED]°C. With a melting point of -64°C, Diglyme fulfills as well this criterium. Moreover, Diglyme is completely miscible with water in any ratio, so that the final products can be simply precipitated at the end of the [REDACTED] syntheses in water, where the solvent residues, [REDACTED] side products [REDACTED] are dissolved in water, and the products by process are obtained as filterable powders. Diglyme is readily available in large quantities and is as well an ideal solvent from an economical point of view.

Diglyme is labelled with the H-phrase H360 (May damage fertility or the unborn child.).

Diglyme has been taken up recently in Annex 1.17 of ChemOOR. Since Diglyme is the main solvent for all processes, a potential ban of the use of Diglyme represents a serious problem for our production [REDACTED] and is an enormous threat for our business [REDACTED].



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Therefore, we apply for an authorization of Diglyme as process solvent for [REDACTED] production processes at our production plant in CH-4133 Schweizerhalle, Switzerland.

In order to support our application, we have conducted an Analysis of Alternatives (AoA), to explore the possibility of a replacement of Diglyme by another solvent.

Any solvent replacing Diglyme must fulfill at least the same criteria as described above for Diglyme and must lead to the same final product by process compositions.

To add a benefit compared to Diglyme, a potentially alternative solvent must have additionally a significantly better (eco)toxicity profile than Diglyme. Therefore, it must at least not be labelled with the H-phrases H361 (Suspected of damaging fertility or the unborn child.), H360 (May damage fertility or the unborn child.), H351 (Suspected of causing cancer.) and H350 (May cause cancer.).

A total of 106 solvents commonly used in the chemical industry (including the solvents which were tested in other AoAs for Diglyme in the European Union) have been assessed by these selection criteria mentioned above. After this assessment, none of the tested solvents fulfilled all the criteria to be considered as potential alternative for Diglyme.

Pyridine was one solvent out of the 106 tested candidates. Even that it failed in the assessment test, [REDACTED] we have checked Pyridine experimentally as replacement solvent [REDACTED]

[REDACTED] In the experiment, we have substituted all Diglyme parts with Pyridine. Unfortunately, this resulted in a product by process which contained new additional compounds, which was not acceptable.

Even in the case that a solvent candidate would have been identified in this assessment as a potential replacement for Diglyme, extensive studies would have been necessary to be executed with the target to get exactly the same product by process compositions and qualities for [REDACTED], as in the current processes made in Diglyme. Since these [REDACTED] resins are complex mixtures, a solvent replacement would be much more difficult compared to the production of a single molecule in a given purity.

In addition, the new products by process would have to be requalified in lengthy test series [REDACTED]. Finally, we would have to develop [REDACTED] new processes, which must ensure for [REDACTED] products by process consistent qualities and safe production conditions. All these developments would take years, and it is still not sure if such a replacement would be successful at all.

So far, we have shown [REDACTED], that we can use Diglyme safely as process solvent for the production of [REDACTED] under appropriate safety measures exceeding local EHS requirements (see as well the CSR, which is added to this application). Since we could identify no solvent with replacement potential, we are applying for a long-term authorization for Diglyme for our [REDACTED] production processes at our production site in CH-4133 Schweizerhalle [REDACTED]

## 2 THE [REDACTED] PRODUCTION PROCESSES

The [REDACTED] products are produced in multistep processes, where the first [REDACTED] process steps involve the solvent Diglyme and are made subsequently in [REDACTED] reactor [REDACTED]

[REDACTED]  
[REDACTED]  
[REDACTED]  
[REDACTED]

[REDACTED] The raw products are then isolated [REDACTED] as filterable powders after precipitation in water.

### [REDACTED] Synthesis [REDACTED]

#### Process step 1 [REDACTED]

[REDACTED]

#### Process step 2 [REDACTED]

[REDACTED]

#### Process step 3 [REDACTED]

[REDACTED]

[REDACTED]

#### Process step 4 [REDACTED]

[REDACTED]

#### Process step 5 [REDACTED]

[REDACTED]

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### **Synthesis**

The process is similar to the process of

#### **Process step 1**

#### **Process step 2**

#### **Process step 3**

#### **Process step 4**

#### **Process step 5**



## ANALYSIS OF ALTERNATIVES

### ANNUAL TONNAGE

[REDACTED]

[REDACTED]

[REDACTED]

[REDACTED]

## 4 THE SOLVENT DIGLYME

### 4.1 General purpose and benefits of Diglyme

Diglyme is a versatile solvent with dipolar aprotic properties which is used in a variety of applications. The most important applications are:


- Solvent for the synthesis of electronic materials
- Solvent for the synthesis of pharmaceuticals and other chemicals
- Solvent for purification processes
- Solvent for the production of plastic and rubber products
- Solvent for the production of binding agents
- Solvent for electrolytes in sealed batteries
- Solvent for polytetrafluoroethylene etchant solutions
- Solvent for scientific research and development

The first mentioned use is subject to this application: **solvent for the synthesis of [REDACTED] for the electronic industry as products by process at one industrial site.**

The key functionalities of diglyme are based on the following desirable physicochemical properties:

- Highly solubilizing substance in which the starting materials, intermediates and the final product by process are able to go into solution (eventually with a further co-solvent), even if they show mostly a poor or limited solubility in classical organic solvents.
- The solvent is 100% miscible in every ratio with water, which is needed to precipitate the product by process from water at the end of the [REDACTED] synthesis route.
- Chemical inertness towards all starting materials, intermediates and the final product by process
- Excellent chemical stability under the reaction conditions
- High boiling point of 162°C
- Low vapor pressure at 20°C: 3mm Hg

The following substance is subject of this analysis of alternatives (AoA).

Parameter	Value
Chemical name	<b>Diglyme</b>
CAS number	111-96-6
EC number	203-924-4
Molecular formula	C <sub>6</sub> H <sub>14</sub> O <sub>3</sub>
Molecular weight	134.17 g/mol
Molecular structure	

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Physical state (20°C and 1013 hPa)	Colorless liquid
Melting point	- 64°C
Boiling point (at 1013 hPa)	162°C
Relative density	0.943 g/cm <sup>3</sup> at 25°C
Vapor pressure	0.99hPa at 25°C
Vapor density	4.63 (air = 1.0)
Water solubility	100% miscible
Flash point	57°C
Signal word / Pictogram	 Danger
H hazard statement	H226 Flammable liquid and vapor. H360 May damage fertility or the unborn child
P precautionary statements	P201, P210, P280, P308+P313, P370+P378

Diglyme is categorized as a Substance of Very High Concern (SVHC) and is listed on Annex XIV of Regulation (EC) No 1907/2006. Adverse effects are evaluated in detail in the CSR.

### 4.2 Purpose and benefits of Diglyme

Diglyme (Bis(2-methoxyethyl)ether; CAS No 111-96-6) is used as a well-established organic solvent for the synthesis of , which are used in the electronic industry e.g. as insulation materials and as dielectrics.


The polar aprotic solvent Diglyme has the advantage to dissolve the intermediates and the final product during all reaction steps of processes. Its rather high boiling point of 162°C limits the emissions during the use of this solvent. Very importantly, Diglyme is chemically inert towards the different reactive functional groups of the all starting materials, intermediates, final products and side products, which occur during these processes. Some starting materials and intermediates are very aggressive and acidic. The chemical inertness of Diglyme is important for the product quality and for the overall process safety. Another advantage is its low melting point of -64°C, to allow the performance at -°C. The processes, which yield polymeric products by process are well adapted to the viscosity and polarity of Diglyme to give constant and reproducible product qualities. The complete water miscibility of Diglyme is another important factor during the work up of the final product, since the final products are precipitated in water. The products precipitate as filterable solids. The side products are water soluble and are washed out of the product filter cakes during the filtration steps. The residual Diglyme is washed out as well and the waste water is then burned under controlled conditions.



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The AoA below has been done specifically for [REDACTED] but is valid as well for [REDACTED].

Diglyme fulfills the following specific selection criteria for the [REDACTED] production process, and is therefore an ideal solvent:

Diglyme [111-96-6]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible with current production process	
b) compatibility with [REDACTED]	compatible with current production process	
c) compatibility with thionyl chloride (4)	no changes in <sup>1</sup> H-NMR detected (own experiment) and compatible with current production process	
d) compatibility with acid chloride (5)	compatible with current production process	
e) compatibility with [REDACTED]	compatible with current production process	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS), compatible with current production process	
g) 100% miscible with water	100% miscible (GESTIS), compatible with current production process	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360 (MSDS)	
i) melting point below -20°C	-64°C (MSDS), compatible with current production process	
j) other selection criteria	suitable solvent to dissolve intermediates and final product in the current production process	

Diglyme was added to REACH Annex XIV in August 2014 in the European Union, and more recently in Switzerland in November 2018. Therefore, an alternative solvent must be searched for.

In this AoA a study on a total of 106 different solvents was performed by BASF trying to identify solvent alternatives for Diglyme in the production process of our [REDACTED] products [REDACTED]. The detailed study is described in chapter 5. One of the evaluated solvents with rather promising physicochemical properties has been thoroughly evaluated as alternative processing solvent [REDACTED], but finally failed.

## 5 IDENTIFICATION OF POSSIBLE ALTERNATIVES

### 5.1 Considered solvents

To find a potential alternative to the solvent Diglyme, we have assessed a total of 106 typical solvents which are commonly used in the chemical industry and / or which were assessed by other companies in the European Union during their Analysis of Alternatives for the substitution of Diglyme (Novartis, Roche Diagnostics, Merck, Bracco Imaging, Maflon, Ajinomoto, Acton, Life Technologies, PMC Isochem).

The assessed solvents are belonging to a variety of 14 different chemical classes:

- Glymes
- Acetals
- Ethers
- Alcohols
- Esters
- Ketones
- Nitriles
- Amines
- Amides
- Carbonates
- Aliphatic hydrocarbons
- Aromatic hydrocarbons
- Chlorinated solvents
- Miscellaneous solvents

### 5.2 The solvent selection criteria

We have assessed these solvents against nine general **selection criteria a) to i)**, which are relevant for the [REDACTED] production process, plus one optional selection criterium **j)**. These selection criteria must be fulfilled at least, that these solvents might be considered as potential alternatives for Diglyme in our production process [REDACTED].

Many of the data to the selection criteria have been retrieved either from the MSDS from Sigma-Aldrich (or from other companies, if specifically named), or from the GESTIS database ([www.dguv.de/ifa/gestis-database](http://www.dguv.de/ifa/gestis-database)). GESTIS is the information system on hazardous substances of the German Social Accident Insurance. Another source of information was the open chemistry database PubChem of the National Institutes of Health (NIH) in the USA (<https://pubchem.ncbi.nlm.nih.gov>). Other data we have obtained from own experiments, from common expert knowhow or were derived from common theory in Organic Chemistry, e.g. from the text book "March's Advanced Organic Chemistry", 6<sup>th</sup> edition, 2007, John Wiley & Sons Inc., Hoboken, New Jersey, USA.



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### a) Chemical compatibility of the assessed solvent with the starting material

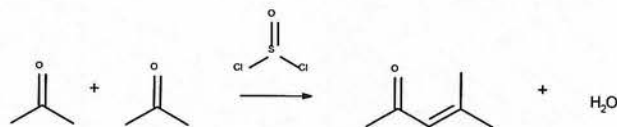
is e.g. incompatible with solvents R-OH bearing a hydroxy functional group (alcohols), since they would react with through , in competition to the wanted reaction with :

### b) Chemical compatibility of the assessed solvent with the starting material

is e.g. incompatible with solvents bearing an ester or a carbonate functional group, since they can react with the hydroxy group of , in competition to the wanted reaction of and :

### c) Chemical compatibility of the assessed solvent with the reagent thionyl chloride

Thionyl chloride (4) is very reactive and aggressive. It can react with different functional groups, especially with the hydroxyl group of alcohols or with carboxylic acid groups to give chlorides or acid chlorides. It can react as well dangerously with amides (e.g. DMF), or also with ethers, e.g. in the combination with THF an explosion can occur. In the case of ketones, thionyl chloride can trigger condensation reactions leading to different side products, e.g. dimers or trimers:



Journal of the Korean Chemical Society, 49(5), 470-472; 2005

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Journal of Chemical Research, (4), 252-253; 2005

The water which is formed in such reactions will consume the reagent thionyl chloride (4) in competition to the wanted reaction [REDACTED]

The compatibility of some of the assessed solvents with thionyl chloride has been tested in own experiments (chapter 7.1.), or information has been obtained from the MSDS (Sigma-Aldrich, if no other information is given) or from the GESTIS database or from general theory in Organic Chemistry.

- d) Chemical compatibility of the assessed solvent with the intermediate carboxylic acid chloride [REDACTED]:

Carboxylic acid chlorides (5) can react e.g. with solvents bearing a hydroxy, a primary or secondary amine functional group through the formation of esters or amides, in competition to the wanted reaction with [REDACTED]

[REDACTED]

[REDACTED]

[REDACTED]

- e) Chemical compatibility of the assessed solvent with [REDACTED]

[REDACTED] can react e.g. with solvents bearing a ketone function to form [REDACTED], or with solvents bearing ester or carbonate functions to form [REDACTED], in competition to the wanted reaction [REDACTED]

[REDACTED]

[REDACTED]

**f) Chemical compatibility of the assessed solvent with acidic conditions:**

During the [REDACTED] production processes, different acidic intermediates are formed [REDACTED]

[REDACTED] Therefore, the solvents must be chemically inert against acidic conditions.

The acid compatibility/incompatibility for each solvent was checked in its MSDS (MSDS from Sigma-Aldrich, if no other information is given) and in the GESTIS database.

**g) 100% miscibility of the assessed solvent with water**

At the end of the [REDACTED] reaction steps, the reaction mixture is precipitated in water [REDACTED] The resulting solid raw product is then filtered and washed with water to get rid of the [REDACTED] water-soluble side products. For this isolation process, the alternative solvent must be 100% miscible with water.

The water miscibility data for each solvent was checked in the MSDS (Sigma-Aldrich, if no other information is given) or in the GESTIS database or in PubChem.

Where no literature data was available, or to confirm the literature data, we have checked the water miscibility in own experiments (chapter 7.2.).

**h) Toxicology: the assessed solvents must not contain the H350, H351, H360 and H361 phrases:**

With this Analysis of Alternatives for Diglyme we are looking for solvents, which are toxicologically more benign than Diglyme, which is labelled itself with the GHS phrase H360 (May damage fertility or the unborn child.).

Therefore, alternative solvents must at least not be labelled with the GHS-phrases H360 (may damage fertility or the unborn child) or H361 (suspected of damaging fertility or the unborn child), and additionally must not be labelled with the GHS-phrases H350 (may cause cancer) or H351 (suspected of causing cancer).

The GHS phrases of the assessed solvents were retrieved from the MSDS (Sigma-Aldrich, if no other information is given) or from the GESTIS database.

**i) Melting point of the assessed solvent must be below -20°C:**

Process step [REDACTED] has to be performed at -[REDACTED]°C. Therefore, the melting point of an alternative solvent must be below this temperature to ensure the same reaction temperature window like in Diglyme. The melting points have been retrieved from the MSDS (Sigma-Aldrich, if no other information is given) or from GESTIS database.



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### j) Other selection criteria

In some cases, additional selection criteria and tests have been added for further evaluation, e.g. a full experimental study in the case of the solvent Pyridine.

The selection criteria described above were assessed in tables for each solvent, and the results for each criterium was rated accordingly with a color code (green, yellow, red or white):

If a specific selection criterium is met, then the color code is **green**.

If a specific selection criterium is borderline, then the color code is **yellow**.

If a specific selection criterium is not met, then the color code is **red**.

If a specific selection criterium is not, or could not be assessed, or if the needed data were not available, then the comment "n. a." was added and the neutral color code white was attributed, which will not influence the overall rating.

For each solvent, an **overall rating** was given, based on the results of the specific selection criteria described above:

If *none* of the selection criteria mentioned above are *borderline* or *not met* (none of the color codes are yellow or red), then the **overall rating** for this solvent is "**potentially an alternative solvent**" for Diglyme. The color code for the **overall rating** is in this case **green**.

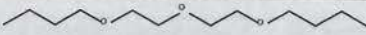
If at *least one* or more selection criteria mentioned above are *borderline* or *not met* (at least one of the color codes is yellow or red), then the **overall rating** for this solvent is "**not an alternative solvent**" for Diglyme. The color code for the **overall rating** is in this case **red**.

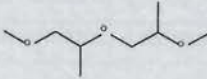
In the following section, for each assessed solvent, the specific **selection criteria** have been checked and compiled in tables, and the **overall rating** has been assigned.

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### 5.3 The solvent assessment


#### 5.3.1 Glymes:


<b>Butyl-diglyme [112-73-2]</b>		
selection criteria	comment	result
a) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
b) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 3g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-60°C (MSDS)	
j) other selection criteria	n. a.	
Butyl-diglyme is not 100% miscible with water and not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

<b>Di-propylene-glycol-di-methyl-ether [111109-77-4]</b>		
selection criteria	comment	result
a) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
b) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	very small changes in <sup>1</sup> H-NMR detected (own experiment)	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 526g/l (GESTIS) & own experiment	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
Di-propylene-glycol-di-methyl-ether is not 100% miscible with water and is not 100% inert with thionyl chloride, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	




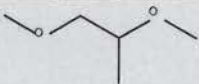
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Di-ethylene-glycol-di-ethyl-ether [112-36-7]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	very small changes in <sup>1</sup> H-NMR detected (own experiment)	yellow
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not compatible with strong acids (MSDS)	red
g) 100% miscible with water	miscible: > 100g/l (GESTIS) & own experiment	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	n. a.	white
j) other selection criteria	n. a.	white
Diethylene-glycol-di-ethyl-ether not compatible with acidic conditions and is not 100% inert with thionyl chloride, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Ethylene-glycol-diethyl-ether [629-14-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	white
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 34g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360Df (MSDS)	red
i) melting point below -20°C	-74°C (MSDS)	green
j) other selection criteria	n. a.	white
Ethylene-glycol-diethyl-ether is a toxic CMR compound, not compatible with acidic conditions and not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red
















## ANALYSIS OF ALTERNATIVES


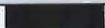
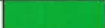

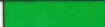

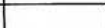








Ethylene-glycol-di-methyl-ether [110-71-4]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	yellow
g) 100% miscible with water	100% miscible (GESTIS)	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360 (MSDS)	red
i) melting point below -20°C	-58°C (MSDS)	green
j) other selection criteria	n. a.	
Ethylene-glycol-di-methyl-ether is a toxic CMR compound and not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Propylene-glycol-di-methyl-ether [7778-85-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	very small changes in <sup>1</sup> H-NMR detected (own experiment)	yellow
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, almost insoluble in water (GESTIS) & own experiment	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
Propylene-glycol-di-methyl-ether is not 100% miscible with water, not 100% inert with thionyl chloride and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

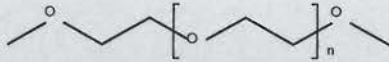



# ANALYSIS OF ALTERNATIVES

<b>Tetra-ethylene-glycol-di-methyl-ether [143-24-8]</b> 		
selection criteria	comment	result
a) compatibility with 	compatible (common theory in Organic Chemistry)	
b) compatibility with 	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with 	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360FD (MSDS)	
i) melting point below -20°C	-30°C (MSDS)	
j) other selection criteria	n. a.	
Tetra-ethylene-glycol-di-methyl-ether is a toxic CMR compound and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

<b>Triethylene glycol dimethyl ether [112-49-2]</b> 		
selection criteria	comment	result
a) compatibility with 	compatible (common theory in Organic Chemistry)	
b) compatibility with 	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with 	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	
g) 100% miscible with water	well soluble in water (GESTIS: 990g/l)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360D (MSDS)	
i) melting point below -20°C	-45°C (MSDS)	
j) other selection criteria	n. a.	
Triethylene glycol dimethyl ether is a toxic CMR compound and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	


# ANALYSIS OF ALTERNATIVES


Polyglyme 250 [24991-55-7]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	very small changes in <sup>1</sup> H-NMR detected (own experiment)	yellow
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	n. a. (GESTIS) / not negatively rated (MSDS)	
g) 100% miscible with water	100% miscible (own experiment)	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360 (see AoA for Diglyme, Merck p28)	red
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
Polyglyme 250 is a toxic CMR compound and is not 100% inert with thionyl chloride, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Methoxyethoxyethane [5137-45-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	n. a.	
g) 100% miscible with water	not 100% miscible (own experiment)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	n. a.	
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
Methoxyethoxyethane is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red



# ANALYSIS OF ALTERNATIVES


Dibutoxyethane [112-48-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	n. a.	
g) 100% miscible with water	not 100% miscible, poor solubility in water (PubChem)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
Dibutoxyethane is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red


Methoxypropoxyethane [17081-22-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	n. a.	
g) 100% miscible with water	not 100% miscible with water in analogy to the tested solvent Methoxyethoxyethane which contains one CH <sub>2</sub> -unit less.	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	n. a.	
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
Methoxypropoxyethane is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red




## ANALYSIS OF ALTERNATIVES

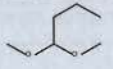
## 5.3.2 Acetals:

Dimethoxymethane [109-87-5]		
		
selection criteria	comment	result
	compatible (common theory in Organic Chemistry)	
	compatible (common theory in Organic Chemistry)	
	n. a.	
	n. a.	
	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with acids (MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 285g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	n. a.	
i) melting point below -20°C	-105°C (MSDS)	
j) other selection criteria	n. a.	
Dimethoxymethane is not 100% miscible with water and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

1,1-Dimethoxyethane [534-15-6]		
		
selection criteria	comment	result
	compatible (common theory in Organic Chemistry)	
	compatible (common theory in Organic Chemistry)	
	n. a.	
	n. a.	
	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not compatible with strong acids (MSDS)	
g) 100% miscible with water	not 100% miscible (own experiment)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	n. a.	
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
1,1-Dimethoxyethane is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

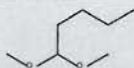
## ANALYSIS OF ALTERNATIVES

1,1-Dimethoxypropane [4744-10-9]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not compatible (common theory in Organic Chemistry)	red
g) 100% miscible with water	not 100% miscible (own experiment)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	n. a.	
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
1,1-dimethoxypropane is not 100% miscible with water and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

1,1-Dimethoxybutane [4461-87-4]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not compatible (common theory in Organic Chemistry)	red
g) 100% miscible with water	In analogy to dimethoxymethane, 1,1-dimethoxyethane and 1,1-dimethoxypropane this solvent is not 100% miscible in water.	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	n. a.	
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
1,1-dimethoxybutane is not 100% miscible with water and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red




## ANALYSIS OF ALTERNATIVES


1,1-Dimethoxypentane [26450-58-8]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not compatible (common theory in Organic Chemistry)	red
g) 100% miscible with water	In analogy to dimethoxymethane, 1,1-dimethoxyethane and 1,1-dimethoxypropane this solvent is not 100% miscible in water.	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	n. a.	
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
1,1-dimethoxypentane is not 100% miscible with water and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red



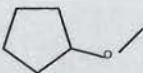
## ANALYSIS OF ALTERNATIVES

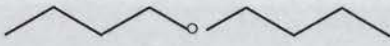
### 5.3.3 Ethers:

1,4-Dioxane [123-91-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	100% miscible (GESTIS)	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H351 (MSDS)	red
i) melting point below -20°C	10°C (MSDS)	red
j) other selection criteria	n. a.	
1,4-dioxane is a toxic CMR compound, is not compatible with acidic conditions and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

2-Methyltetrahydrofuran [96-47-9]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with strong acids (GESTIS) / not compatible with strong acids (MSDS)	red
g) 100% miscible with water	not 100% miscible, solubility in water: 150g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-20°C (MSDS)	yellow
j) other selection criteria	n. a.	
2-Methyltetrahydrofuran is not 100% miscible with water, is not compatible with acidic conditions and has a melting point just at -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red


## ANALYSIS OF ALTERNATIVES


Cyclopentyl methyl ether [5614-37-9]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	no changes in <sup>1</sup> H-NMR detected (own experiment)	green
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	n. a. (GESTIS) / not compatible with acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible (own experiment)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-140°C (MSDS)	green
j) other selection criteria	n. a.	white
Cyclopentyl methyl ether is not 100% miscible with water and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Dibutyl ether [142-96-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	white
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with strong acids (GESTIS) / not compatible with strong acids (MSDS)	red
g) 100% miscible with water	not 100% miscible, solubility in water: 0.3g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-98°C (MSDS)	green
j) other selection criteria	n. a.	white
Dibutyl ether is not 100% miscible with water and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red




# ANALYSIS OF ALTERNATIVES

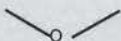
<b>Diisopropyl ether [108-20-3]</b> <div>  </div>		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 12g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-85°C (MSDS)	
j) other selection criteria	n. a.	
Diisopropyl ether is not 100% miscible with water and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

<b>Methyl-tert-butylether [1634-04-4]</b> <div>  </div>		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 26g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-109°C (MSDS)	
j) other selection criteria	n. a.	
Methyl-tertbutyl ether is not 100% miscible with water and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

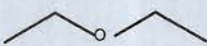


## ANALYSIS OF ALTERNATIVES

Tetrahydrofuran [109-99-9]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	risk of explosion (GESTIS)	red
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not compatible with acids (MSDS)	red
g) 100% miscible with water	100% miscible (GESTIS)	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H351 (MSDS)	red
i) melting point below -20°C	-108°C (MSDS)	green
j) other selection criteria	n. a.	white
Tetrahydrofuran is a toxic CMR compound, is not compatible with thionyl chloride and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Dimethylether [115-10-6]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	white
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with hydrochloric acid (GESTIS) / not compatible with strong acids (MSDS)	red
g) 100% miscible with water	not 100% miscible, solubility in water: 70g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-141°C (MSDS)	green
j) other selection criteria	highly flammable gas (GESTIS)	red
Dimethyl ether is not 100% miscible with water, is not compatible with acidic conditions and is a highly flammable gas, therefore this compound is not an alternative for diglyme.		
overall rating	not an alternative solvent	red


## ANALYSIS OF ALTERNATIVES

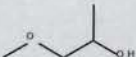
Diethylether [60-29-7]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with sulfuric and nitric acid (GESTIS [REDACTED]) / not compatible with strong acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 69g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-116°C (MSDS)	green
j) other selection criteria	highly flammable	red
Dimethyl ether is not 100% miscible with water and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red



## ANALYSIS OF ALTERNATIVES


### 5.3.4 Alcohols:


1-Butanol [71-36-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	Red
b) compatibility with [REDACTED]	possible transesterification	Red
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	Red
d) compatibility with acid chloride (5)	possible formation of ester	Red
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	Green
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	Yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 77g/l (GESTIS)	Red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	Green
i) melting point below -20°C	-90°C (MSDS)	Green
j) other selection criteria	n. a.	
1-butanol is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	Red

1-methoxy-2-propanol [107-98-2]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	Red
b) compatibility with [REDACTED]	possible transesterification	Red
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	Red
d) compatibility with acid chloride (5)	possible formation of ester	Red
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	Green
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	Green
g) 100% miscible with water	100% miscible (GESTIS)	Green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	Green
i) melting point below -20°C	-97°C (GESTIS)	Green
j) other selection criteria	n. a.	
1-methoxy-2-propanol is not compatible with [REDACTED], therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	Red




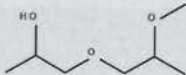
# ANALYSIS OF ALTERNATIVES

<b>2-Butanol [78-92-2]</b>		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with acids (MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 85g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-108°C (MSDS)	
j) other selection criteria	n. a.	
2-Butanol is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

<b>rac-Butan-1,3-diol [107-88-0]</b>		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-57°C (MSDS)	
j) other selection criteria	n. a.	
rac-Butan-1,3-diol is not compatible with [REDACTED], therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	


## ANALYSIS OF ALTERNATIVES


Cyclohexanol [108-93-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 40g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	20°C (MSDS)	
j) other selection criteria	n. a.	
Cyclohexanol is not compatible with [REDACTED], is not 100% miscible with water and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

Di(propyleneglycol) monomethyl ether [34590-94-8]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-83°C (MSDS)	
j) other selection criteria	n. a.	
Di(propyleneglycol) monomethyl ether is not compatible with [REDACTED] and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	




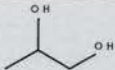
# ANALYSIS OF ALTERNATIVES

Ethylene glycol [107-21-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	can react dangerously with sulfuric or nitric acid (GESTIS [REDACTED]) / not compatible with strong acids (MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-13°C (MSDS)	
j) other selection criteria	n. a.	
Ethylene glycol is not compatible with [REDACTED], is not compatible with acidic conditions and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

Isopropanol [67-63-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not compatible with strong acids (GESTIS) / not compatible with acids (MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-89°C (MSDS)	
j) other selection criteria	n. a.	
Isopropanol is not compatible with [REDACTED] and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	


## ANALYSIS OF ALTERNATIVES


1,5-Pentanediol [111-29-5]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-16°C (MSDS)	
j) other selection criteria	n. a.	
1,5-Pentanediol is not compatible with [REDACTED] and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

1,2-Propanediol [57-55-6]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-60°C (MSDS)	
j) other selection criteria	n. a.	
1,2-Propanediol is not compatible with [REDACTED], therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	





# ANALYSIS OF ALTERNATIVES

<b>1,3-Propanediol [504-63-2]</b>		
<b>selection criteria</b>	<b>comment</b>	<b>result</b>
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-27°C (MSDS)	
j) other selection criteria	n. a.	
1,3-Propanediol is not compatible with [REDACTED], therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

<b>tert-Butanol [75-65-0]</b>		
<b>selection criteria</b>	<b>comment</b>	<b>result</b>
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	23°C (MSDS)	
j) other selection criteria	n. a.	
tert-Butanol is not compatible with [REDACTED] and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

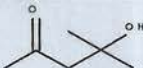
## ANALYSIS OF ALTERNATIVES

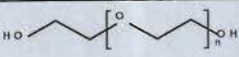
Methanol [67-56-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	Red
b) compatibility with [REDACTED]	possible transesterification	Red
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	Red
d) compatibility with acid chloride (5)	possible formation of ester	Red
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	Green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not compatible with acids (MSDS)	Red
g) 100% miscible with water	100% miscible (GESTIS)	Green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	Green
i) melting point below -20°C	-98°C (MSDS)	Green
j) other selection criteria	n. a.	
Methanol is not compatible with [REDACTED] and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	Red

Ethanol [64-17-5]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	Red
b) compatibility with [REDACTED]	possible transesterification	Red
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	Red
d) compatibility with acid chloride (5)	possible formation of ester	Red
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	Green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	Yellow
g) 100% miscible with water	100% miscible (GESTIS)	Green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	Green
i) melting point below -20°C	-114°C (MSDS)	Green
j) other selection criteria	n. a.	
Ethanol is not compatible with [REDACTED] and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	Red



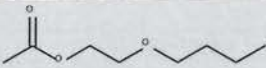
# ANALYSIS OF ALTERNATIVES

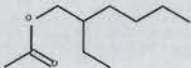
4-Hydroxy-4-methyl-2-pentanone [123-42-2]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]		
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-47°C (GESTIS)	
j) other selection criteria	n. a.	
4-Hydroxy-4-methyl-2-pentanone is not compatible with [REDACTED] and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

Polyethyleneglycole MW400 [25322-68-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	
b) compatibility with [REDACTED]	possible transesterification	
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	
d) compatibility with acid chloride (5)	possible formation of ester	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	4-8°C (MSDS)	
j) other selection criteria	n. a.	
Polyethyleneglycole MW400 is not compatible with [REDACTED] and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

## ANALYSIS OF ALTERNATIVES

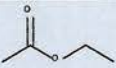
## 5.3.5 Esters:

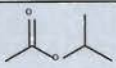
2-Butoxyethyl acetate [112-07-2]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	significant changes in <sup>1</sup> H-NMR detected (own experiment)	red
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 15g/l (GESTIS) & own experiment	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-64°C (GESTIS)	green
j) other selection criteria	n. a.	white
2-Butoxyethyl acetate is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

2-Ethylhexyl acetate [103-09-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	n. a.	white
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 0.088g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-92°C (MSDS)	green
j) other selection criteria	n. a.	white
2-Ethylhexyl acetate is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

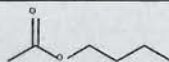



# ANALYSIS OF ALTERNATIVES

Ethyl acetate [141-78-6]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	can react dangerously with strong acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 85.3g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-84°C (MSDS)	green
j) other selection criteria	n. a.	
Ethyl acetate is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Isopropyl acetate [108-21-4]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not compatible with acids (MSDS)	red
g) 100% miscible with water	not 100% miscible, solubility in water: 31g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-73°C (MSDS)	green
j) other selection criteria	n. a.	
Isopropyl acetate is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

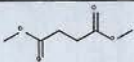
# ANALYSIS OF ALTERNATIVES


n-Butyl acetate [123-86-4]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 4.3g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-78°C (MSDS)	green
j) other selection criteria	n. a.	
n-Butyl acetate is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

gamma-Butyrolacton [96-48-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	significant changes in <sup>1</sup> H-NMR detected (own experiment)	red
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	yellow
g) 100% miscible with water	100% miscible (GESTIS) and own experiment	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-45°C (MSDS)	green
j) other selection criteria	n. a.	
gamma-Butyrolacton is not compatible with [REDACTED] and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

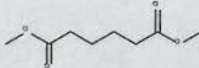


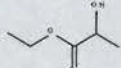
# ANALYSIS OF ALTERNATIVES

Dimethylsuccinate [106-65-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 75g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	16°C (MSDS)	red
j) other selection criteria	n. a.	
Dimethylsuccinate is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Dimethylglutarate [1119-40-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 4.3g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-38°C (MSDS)	green
j) other selection criteria	n. a.	
Dimethylglutarate is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red


# ANALYSIS OF ALTERNATIVES

Dimethyladipate [627-93-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: < 1g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	8°C (MSDS)	red
j) other selection criteria	n. a.	
Dimethyladipate is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Ethyllactate [97-64-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	possible alcoholysis of [REDACTED]	red
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	possible formation of alkyl chloride	red
d) compatibility with acid chloride (5)	possible formation of ester	red
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	hydrolysis in water (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-26°C (MSDS)	green
j) other selection criteria	n. a.	
Ethyllactate is not compatible with [REDACTED], therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

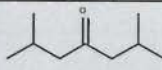



# ANALYSIS OF ALTERNATIVES

Methylacetate [79-20-9]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible transesterification	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	can react with strong acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 240-250g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-98°C (MSDS)	green
j) other selection criteria	n. a.	
Methylacetate is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

## ANALYSIS OF ALTERNATIVES

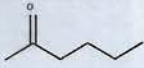
## 5.3.6 Ketones:

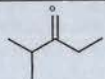
2,6-Dimethyl-4-heptanone [108-83-8]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 0.5g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-46°C (MSDS)	green
j) other selection criteria	n. a.	
2,6-Dimethyl-4-heptanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

2-Butanone [78-93-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	significant changes in <sup>1</sup> H-NMR detected (own experiment)	red
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 292g/l (GESTIS) & own experiment	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-87°C (MSDS)	green
j) other selection criteria	n. a.	
2-butanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

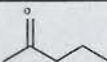



## ANALYSIS OF ALTERNATIVES

2-Hexanone [591-78-6]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 17g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H361f (MSDS)	red
i) melting point below -20°C	-57°C (MSDS)	green
j) other selection criteria	n. a.	
2-hexanone is not compatible with [REDACTED], is not 100% miscible with water and is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

2-Methyl-3-pentanone [565-69-5]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	significant changes in <sup>1</sup> H-NMR detected (own experiment)	red
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not assessed (GESTIS) / not negatively rated (MSDS)	
g) 100% miscible with water	not 100% miscible (own experiment)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
2-Methyl-3-pentanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red


## ANALYSIS OF ALTERNATIVES


<b>2-Pentanone [107-87-9]</b>		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 43g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-78°C (MSDS)	green
j) other selection criteria	n. a.	
2-Pentanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	red

<b>3,3-Dimethyl-2-butanone [75-97-8]</b>		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	significant changes in <sup>1</sup> H-NMR detected (own experiment)	red
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 19g/l (GESTIS) & own experiment	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-50°C (GESTIS)	green
j) other selection criteria	n. a.	
3,3-Dimethyl-2-butanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	red

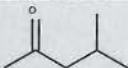


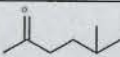
# ANALYSIS OF ALTERNATIVES

3-Methyl-2-butanone [563-80-4]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 6g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-92°C (MSDS)	green
j) other selection criteria	n. a.	
3-Methyl-2-butanone is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

3-Pentanone [96-22-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 35g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-42°C (MSDS)	green
j) other selection criteria	n. a.	
3-Pentanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red


## ANALYSIS OF ALTERNATIVES


<b>4-Methyl-2-pentanone [108-10-1]</b>		
<b>selection criteria</b>	<b>comment</b>	<b>result</b>
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 19g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-80°C (MSDS)	green
j) other selection criteria	n. a.	
4-Methyl-2-pentanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	red

<b>5-Methyl-2-hexanone [110-12-3]</b>		
<b>selection criteria</b>	<b>comment</b>	<b>result</b>
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 3.1g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-74°C (MSDS)	green
j) other selection criteria	n. a.	
5-Methyl-2-hexanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	red

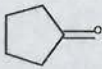


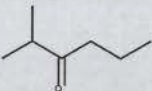
## ANALYSIS OF ALTERNATIVES

Acetone [67-64-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	significant changes in <sup>1</sup> H-NMR detected (own experiment)	red
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	100% miscible (GESTIS)	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-94°C (MSDS)	green
j) other selection criteria	n. a.	white
Acetone is not compatible with [REDACTED], therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Cyclohexanone [108-94-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	white
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	Can react dangerously with mineral acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 103g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-47°C (MSDS)	green
j) other selection criteria	n. a.	white
Cyclohexanone is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

## ANALYSIS OF ALTERNATIVES


Cyclopentanone [120-92-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	significant changes in <sup>1</sup> H-NMR detected (own experiment)	red
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 9.81g/l (GESTIS) and own experiment	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-51°C (MSDS)	green
j) other selection criteria	n. a.	
Cyclopentanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red


2-Methylhexanone [7379-12-6]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (MSDS) / GESTIS n. a.	
g) 100% miscible with water	not 100% miscible	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
2-Methylhexanone is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red



## ANALYSIS OF ALTERNATIVES

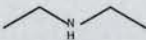
### 5.3.7 Nitriles:

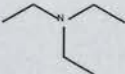
Acetonitrile [75-05-8]		
selection criteria	comment	result
a) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
b) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	significant changes in <sup>1</sup> H-NMR detected (own experiment)	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	n. a.	
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not compatible with acids (MSDS)	
g) 100% miscible with water	100% miscible (GESTIS) & own experiment	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-48°C (MSDS)	
j) other selection criteria	Can decompose to very toxic HCN (GESTIS)	
Acetonitrile is not compatible with thionyl chloride, is not compatible with acidic conditions and can form very toxic HCN on decomposition, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

Butyronitrile [109-74-0]		
selection criteria	comment	result
a) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
b) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	n. a.	
f) compatibility with acidic conditions	can react dangerously with strong acids (GESTIS) / not compatible with strong acids (MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 33g/l (GESTIS) and own experiment	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-112°C (MSDS)	
j) other selection criteria	n. a.	
Butyronitrile is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

## ANALYSIS OF ALTERNATIVES


## 5.3.8 Amines:


Diethylamine [109-89-7]		
selection criteria	comment	result
a) compatibility with [REDACTED]	[REDACTED]	Red
b) compatibility with [REDACTED]	[REDACTED]	Red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	possible formation of [REDACTED]	Red
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	Green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	Yellow
g) 100% miscible with water	100% miscible (GESTIS) & own experiment	Green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	Green
i) melting point below -20°C	-50°C (MSDS)	Green
j) other selection criteria	n. a.	
Diethylamine is not compatible with [REDACTED] and is not compatible with acidic conditions, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	Red

Triethylamine [121-44-8]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	Green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	Green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	Green
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	Green
g) 100% miscible with water	not 100% miscible, solubility in water: 80g/l (GESTIS)	Red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	Green
i) melting point below -20°C	-115°C (MSDS)	Green
j) other selection criteria	n. a.	
Triethylamine is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	Red



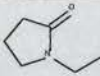
# ANALYSIS OF ALTERNATIVES

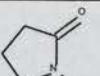
N-Methylmorpholine [109-02-4]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	reacts strongly with SOCl <sub>2</sub> (own experiment)	red
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	100% miscible (GESTIS) & own experiment	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-66°C (MSDS)	green
j) other selection criteria	n. a.	white
N-Methylmorpholine is not compatible with thionyl chloride, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Pyridine [110-86-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	very small changes in <sup>1</sup> H-NMR detected (own experiment)	yellow
d) compatibility with acid chloride (5)	n. a.	white
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with sulfuric and nitric acid (GESTIS [REDACTED]) / not compatible with strong acids (MSDS)	yellow
g) 100% miscible with water	100% miscible (GESTIS) and own experiment	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-42°C (MSDS)	green
j) other selection criteria	Pyridine was tested experimentally as alternative solvent in the [REDACTED] process but failed due to formation of [REDACTED] side products (chapter 7.3.)	red
Pyridine is not 100% inert with thionyl chloride, not compatible with acidic conditions and experimentally failed as solvent in the [REDACTED] process, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

## ANALYSIS OF ALTERNATIVES


## 5.3.9 Amides:

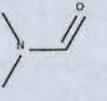
1-Ethyl-2-pyrrolidone [2687-91-4]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	not compatible (MSDS)	red
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	100% miscible (GESTIS)	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360D (MSDS)	red
i) melting point below -20°C	-120°C (MSDS)	green
j) other selection criteria	n. a.	
1-Ethyl-2-pyrrolidone is not compatible with acid chlorides and is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

1-Methyl-2-pyrrolidone [872-50-4]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with nitric acid (GESTIS [REDACTED]) / not compatible with strong acids (MSDS)	yellow
g) 100% miscible with water	100% miscible (GESTIS)	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360D (MSDS)	red
i) melting point below -20°C	-24°C (MSDS)	green
j) other selection criteria	n. a.	
1-Methyl-2-pyrrolidone is not compatible with acidic conditions and is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red




## ANALYSIS OF ALTERNATIVES

N,N-Dimethylacetamide [127-19-5]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360D (MSDS)	
i) melting point below -20°C	-20°C (MSDS)	
j) other selection criteria	n. a.	
N,N-Dimethylacetamide is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

N,N-Dimethylformamide [68-12-2]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	can react dangerously with SOCl <sub>2</sub> (GESTIS)	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	100% miscible (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360D (MSDS)	
i) melting point below -20°C	-61°C (MSDS)	
j) other selection criteria	n. a.	
N,N-Dimethylformamide is not compatible with thionyl chloride and is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

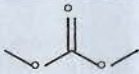
## ANALYSIS OF ALTERNATIVES

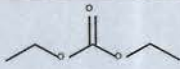
Acetamide [60-35-5]		
<b>selection criteria</b>	<b>comment</b>	<b>result</b>
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not compatible with strong acids (GESTIS) / not compatible with strong acids (MSDS)	red
g) 100% miscible with water	100% miscible (GESTIS)	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H351 (MSDS)	red
i) melting point below -20°C	80°C (MSDS)	red
j) other selection criteria	n. a.	
Acetamide is not compatible with acidic conditions, is a toxic CMR compound and its melting point is above -20°C, therefore this compound is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	red



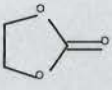
## ANALYSIS OF ALTERNATIVES

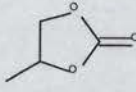
## 5.3.10 Carbonates:

Dimethyl carbonate [616-38-6]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible [REDACTED]	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 139g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-2°C (MSDS)	red
j) other selection criteria	n. a.	
Dimethyl carbonate is not compatible with [REDACTED], is not compatible with acidic conditions, is not 100% miscible with water and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Diethyl carbonate [105-58-8]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible [REDACTED]	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 19.2g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-43°C (MSDS)	green
j) other selection criteria	n. a.	
Diethyl carbonate is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

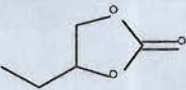
## ANALYSIS OF ALTERNATIVES

Ethylene carbonate [96-49-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible [REDACTED]	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 778g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	35°C (MSDS)	red
j) other selection criteria	n. a.	
Ethylene carbonate is not compatible with [REDACTED], is not compatible with acidic conditions, is not 100% miscible with water and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Propylene carbonate [108-32-7]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	possible [REDACTED]	red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	red
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 240g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-55°C (MSDS)	green
j) other selection criteria	n. a.	
Propylene carbonate is not compatible with [REDACTED], is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red





# ANALYSIS OF ALTERNATIVES

1,2-Butylenecarbonate [4437-85-8]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	Green
b) compatibility with [REDACTED]	possible [REDACTED]	Red
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	possible formation of [REDACTED]	Red
f) compatibility with acidic conditions	n. a.	
g) 100% miscible with water	not 100% miscible (own experiment)	Red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS from ABCR)	Green
i) melting point below -20°C	n. a.	
j) other selection criteria	n. a.	
1,2-Butylenecarbonate is not compatible with [REDACTED] and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	Red

## ANALYSIS OF ALTERNATIVES

### 5.3.11 Aliphatic hydrocarbons:

<b>n-Heptane [142-82-5]</b>		
<b>selection criteria</b>	<b>comment</b>	<b>result</b>
a) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
b) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
e) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	<span style="background-color: green; color: green;">          </span>
g) 100% miscible with water	not 100% miscible, solubility in water: 2.2mg/l (GESTIS)	<span style="background-color: red; color: red;">          </span>
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	<span style="background-color: green; color: green;">          </span>
i) melting point below -20°C	-91°C (MSDS)	<span style="background-color: green; color: green;">          </span>
j) other selection criteria	n. a.	<span style="background-color: green; color: green;">          </span>
n-Heptane is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	<span style="background-color: red; color: red;">          </span>

<b>n-Pentane [109-66-0]</b>		
<b>selection criteria</b>	<b>comment</b>	<b>result</b>
a) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
b) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
e) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<span style="background-color: green; color: green;">          </span>
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	<span style="background-color: green; color: green;">          </span>
g) 100% miscible with water	not 100% miscible, solubility in water: 39mg/l (GESTIS)	<span style="background-color: red; color: red;">          </span>
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	<span style="background-color: green; color: green;">          </span>
i) melting point below -20°C	-130°C (MSDS)	<span style="background-color: green; color: green;">          </span>
j) other selection criteria	Not suitable for production due to very high flammability.	<span style="background-color: red; color: red;">          </span>
n-Pentane is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	<span style="background-color: red; color: red;">          </span>

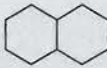


# ANALYSIS OF ALTERNATIVES

Cis- / trans-decaline [91-17-8]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 6mg/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-125°C (MSDS)	
j) other selection criteria	n. a.	
Cis- / trans-decaline is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	

Cis-decaline [493-01-6]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	not 100% miscible, highly insoluble (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-43°C (MSDS)	
j) other selection criteria	n. a.	
Cis-decaline is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	


## ANALYSIS OF ALTERNATIVES

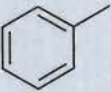
Trans-decaline [493-02-7]		
selection criteria	comment	result
a) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<div></div>
b) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<div></div>
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	<div></div>
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	<div></div>
e) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<div></div>
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	<div></div>
g) 100% miscible with water	not 100% miscible, highly insoluble (GESTIS)	<div></div>
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	<div></div>
i) melting point below -20°C	-32°C (MSDS)	<div></div>
j) other selection criteria	n. a.	<div></div>
Trans-decaline is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	<div></div>



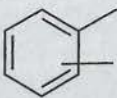
# ANALYSIS OF ALTERNATIVES

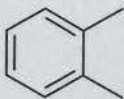
## 5.3.12 Aromatic hydrocarbons:

1,2,3,4-tetrahydronaphthalene [119-64-2]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	green
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	green
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 0.05g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H351 (MSDS)	red
i) melting point below -20°C	-35°C (MSDS)	green
j) other selection criteria	n. a.	
1,2,3,4-tetrahydronaphthalene is not 100% miscible with water and is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Toluene [108-88-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	green
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	green
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with strong acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 520mg/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H361d (MSDS)	red
i) melting point below -20°C	-93°C (MSDS)	green
j) other selection criteria	n. a.	
Toluene is not compatible with acidic conditions, is not 100% miscible with water and is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

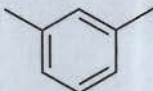
## ANALYSIS OF ALTERNATIVES

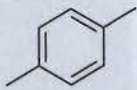
Xylenes, mixture of isomers [1330-20-7]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	green
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	green
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 0.2g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	0°C	red
j) other selection criteria	n. a.	
Xylenes, mixture of isomers is not compatible with acidic conditions, is not 100% miscible with water and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

ortho-Xylene [95-47-6]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	green
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	green
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 0.18g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-26°C (MSDS)	green
j) other selection criteria	n. a.	
ortho-xylene is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red




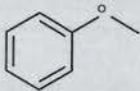
## ANALYSIS OF ALTERNATIVES

meta-Xylene [108-38-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	green
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	green
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 0.174g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-48°C (MSDS)	green
j) other selection criteria	n. a.	
meta-xylene is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

para-Xylene [106-42-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	green
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	green
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 0.2g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	13°C (MSDS)	red
j) other selection criteria	n. a.	
para-xylene is not compatible with acidic conditions, is not 100% miscible with water and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

## ANALYSIS OF ALTERNATIVES

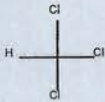
Benzene [71-43-2]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	green
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	green
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with acids (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 1.77g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H350 (MSDS)	red
i) melting point below -20°C	6°C (MSDS)	red
j) other selection criteria	n. a.	
Benzene is not compatible with acidic conditions, is not 100% miscible with water, is a toxic CMR compound and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

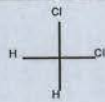
Anisole [100-66-3]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	not 100% miscible, solubility in water: 0.14g/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	-37°C (MSDS)	green
j) other selection criteria	n. a.	
Anisole is not compatible with acidic conditions and it is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red



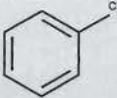
## ANALYSIS OF ALTERNATIVES

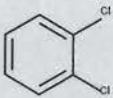
### 5.3.13 Chlorinated solvents:

<b>Chloroform [67-66-3]</b>		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	
e) compatibility with [REDACTED]	risk of [REDACTED] formation	
f) compatibility with acidic conditions	can react dangerously with mineral acids (GESTIS) / not negatively rated (MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 8g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H351 & H361d (MSDS)	
i) melting point below -20°C	-63°C (MSDS)	
j) other selection criteria	n. a.	
Chloroform is not compatible with [REDACTED], is not compatible with acidic conditions, is not 100% miscible with water and is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

<b>Methylenechloride [75-09-2]</b>		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 20g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H351 (MSDS)	
i) melting point below -20°C	-97°C (MSDS)	
j) other selection criteria	n. a.	
Methylene chloride is not 100% miscible with water and is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

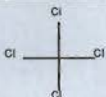
## ANALYSIS OF ALTERNATIVES

Chlorobenzene [108-90-7]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 0.4g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-45°C (MSDS)	
j) other selection criteria	n. a.	
Chlorobenzene is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

1,2-Dichlorobenzene [95-50-1]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	not 100% miscible, solubility in water: 0.08g/l (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	-18°C (MSDS)	
j) other selection criteria	n. a.	
1,2-Dichlorobenzene is not 100% miscible with water and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	




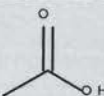
# ANALYSIS OF ALTERNATIVES

Carbontetrachloride [56-23-5]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	compatible (common theory in Organic Chemistry)	green
d) compatibility with acid chloride (5)	compatible (common theory in Organic Chemistry)	green
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	not 100% miscible, solubility in water: 800mg/l (GESTIS)	red
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H351 (MSDS)	red
i) melting point below -20°C	-23°C (MSDS)	green
j) other selection criteria	n. a.	
Carbontetrachloride is not 100% miscible with water and is a toxic CMR compound, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

## ANALYSIS OF ALTERNATIVES


### 5.3.14 Miscellaneous solvents:


Sulfolane [126-33-0]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	green
g) 100% miscible with water	n. a.	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	H360 (GESTIS)	red
i) melting point below -20°C	20°C (MSDS)	red
j) other selection criteria	n. a.	
Sulfolane is a toxic CMR compound and has a melting point above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red

Acetic acid [64-19-7]		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
b) compatibility with [REDACTED]	n. a.	
c) compatibility with thionyl chloride (4)	possible formation of acid chloride	red
d) compatibility with acid chloride (5)	possible formation of mixed acid anhydride	red
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	green
f) compatibility with acidic conditions	can react dangerously with strong acids (GESTIS) / not negatively rated (MSDS)	yellow
g) 100% miscible with water	100% miscible (GESTIS)	green
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	green
i) melting point below -20°C	16°C (MSDS)	red
j) other selection criteria	n. a.	
Acetic acid is not compatible with thionyl chloride, acid chlorides, is not compatible with acidic conditions and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	red




## ANALYSIS OF ALTERNATIVES

<b>Water [7732-18-5]</b>		
selection criteria	comment	result
a) compatibility with [REDACTED]	hydrolysis of [REDACTED]	
b) compatibility with [REDACTED]	n. a.	
c) compatibility with thionyl chloride (4)	hydrolysis of thionyl chloride	
d) compatibility with acid chloride (5)	hydrolysis of acid chloride	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water		
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (MSDS)	
i) melting point below -20°C	0°C	
j) other selection criteria	n. a.	
Water is not compatible with [REDACTED], thionyl chloride, acid chlorides, and its melting point is above -20°C, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

<b>Octamethyltrisiloxane [107-51-7]</b>		
selection criteria	comment	result
a) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
b) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
c) compatibility with thionyl chloride (4)	n. a.	
d) compatibility with acid chloride (5)	n. a.	
e) compatibility with [REDACTED]	compatible (common theory in Organic Chemistry)	
f) compatibility with acidic conditions	not negatively rated (in GESTIS and in MSDS)	
g) 100% miscible with water	not 100% miscible, highly insoluble (GESTIS)	
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (GESTIS)	
i) melting point below -20°C	-82°C (MSDS)	
j) other selection criteria	n. a.	
Octamethyltrisiloxane is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
<b>overall rating</b>	<b>not an alternative solvent</b>	

## ANALYSIS OF ALTERNATIVES

Decamethyltetrasiloxane [141-62-8]		
selection criteria	comment	result
a) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<div></div>
b) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<div></div>
c) compatibility with thionyl chloride (4)	n. a.	<div></div>
d) compatibility with acid chloride (5)	n. a.	<div></div>
e) compatibility with <span style="background-color: black; color: black;">XXXXXXXXXX</span>	compatible (common theory in Organic Chemistry)	<div></div>
f) compatibility with acidic conditions	not negatively rated (GESTIS) / not compatible with strong acids (MSDS)	<div></div>
g) 100% miscible with water	not 100% miscible, solubility in water: 0.006mg/l (GESTIS)	<div></div>
h) toxicology (H-phrases): must <b>not</b> contain H350, H351, H360, H361	free (GESTIS)	<div></div>
i) melting point below -20°C	-68°C (MSDS)	<div></div>
j) other selection criteria	n. a.	<div></div>
Decamethyltetrasiloxane is not compatible with acidic conditions and is not 100% miscible with water, therefore this solvent is not an alternative for diglyme.		
overall rating	not an alternative solvent	<div></div>



## 6 CONCLUSIONS

After the assessment of 106 different solvents, none of them could be identified as potential alternative to Diglyme for the production of [REDACTED]  
[REDACTED]

Even if a solvent would have been found to be a potential alternative, extensive experimental test studies would have been necessary, to confirm or disconfirm it as a valid alternative to Diglyme in [REDACTED] production processes. Such tests would have taken several years, since [REDACTED] are products by process. Their compositions made with an alternative solvent would have to match exactly the compositions resulting from the current production processes. The outcome of such experiments is in addition uncertain.

Since [REDACTED] are used in different electronic applications, where some of them can be critical like e.g. in security systems, where a malfunction could be fatal, the requalification of [REDACTED] would take additionally some years, again with uncertain outcome.

To avoid a rupture [REDACTED] on the market and since we have shown [REDACTED] to be able to work with the solvent Diglyme under safe and controlled conditions, BASF is applying for an authorization for the use of Diglyme [REDACTED], to be able to further produce [REDACTED] at the production site in CH-4133 Schweizerhalle.

## 7 ANNEX

### 7.1 Own experiments for thionyl chloride compatibility

To decide in some cases, if a particular solvent was inert against thionyl chloride or not, we made the following experiment:

To 1ml of a solvent in a test tube was added 100µl of thionyl chloride at room temperature and the substances were well mixed. The test tube was then closed with a bubble counter.

After 2 hours, 50µl of the reaction mixture was taken for an  $^1\text{H-NMR}$  in  $\text{CDCl}_3$ .

After 3 days, 50µl of the reaction mixture was taken for an  $^1\text{H-NMR}$  in  $\text{CDCl}_3$ .

These NMR spectra were then compared to an  $^1\text{H-NMR}$  spectrum of 50µl of the pure solvent in  $\text{CDCl}_3$ .

Then the compared NMR spectra were rated with the comments "no changes", "very small changes" and "significant changes".

### 7.2 Own experiments for water miscibility

Some data about water miscibility were not available in the MSDS or in the GESTIS database. To decide in these cases, if a particular solvent is 100% water miscible or not, we made the following experiment:

To a 10ml measurement cylinder we added 5ml of the solvent and 5ml of deionized water. Then a magnetic stirrer was added, and the cylinder was closed with a stopper. After stirring of the mixture for 15 minutes, the phases were allowed to separate during 1 hour. Then it was checked if no phase separation occurred (100% miscible) or if a phase separation occurred (not 100% miscible).

### 7.3 Experimental feasibility study with Pyridine as potential alternative for Diglyme



Since the selection criteria a) to i) in the assessment of Pyridine gave two borderline results (chapter 5.3.8), [REDACTED] we have checked this solvent experimentally as substitute for Diglyme in the [REDACTED] process.

In the following table, some additional key data are given for the solvent Pyridine (MSDS):

Parameter	Value
Chemical name	Pyridine



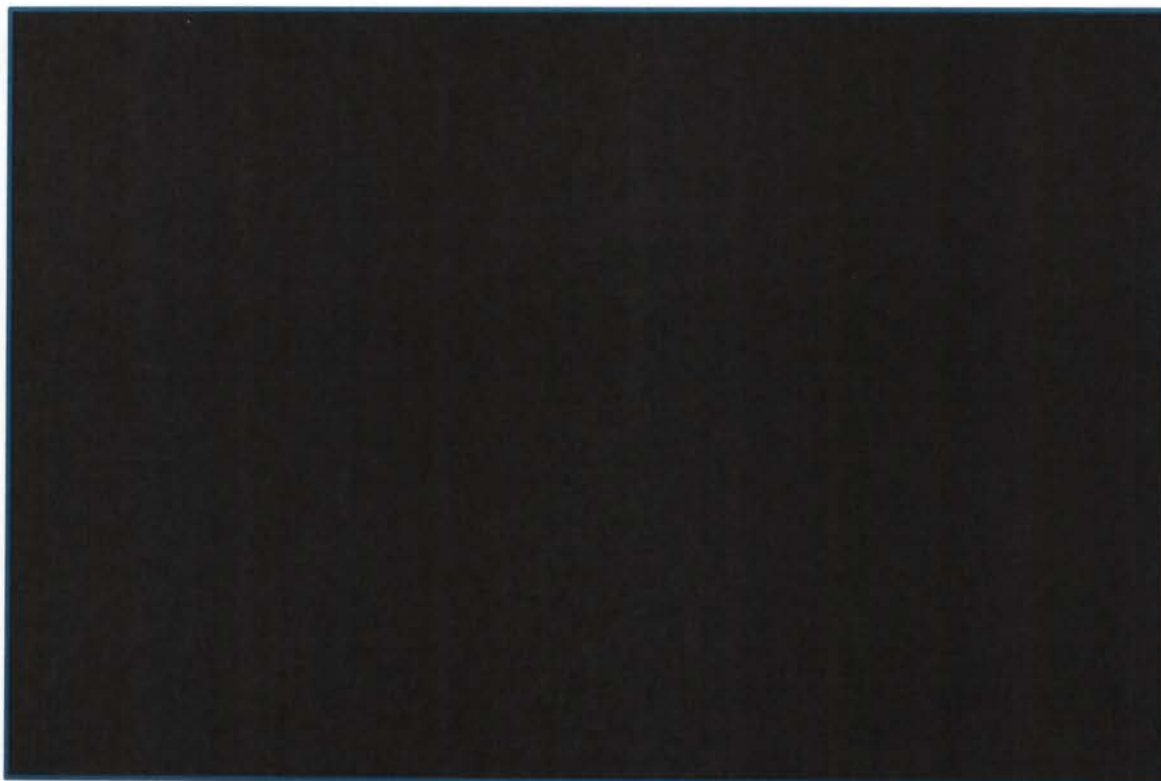
# ANALYSIS OF ALTERNATIVES

CAS number	110-86-1
EC number	203-809-9
Molecular formula	C <sub>5</sub> H <sub>5</sub> N
Molecular weight	79.10 g/mol
Molecular structure	
Physical state (20°C and 1013 hPa)	Colorless liquid
Melting point	- 42°C
Boiling point (at 1013 hPa)	115°C
Relative density	0.978 g/cm <sup>3</sup> at 25°C
Vapor pressure	20 mmHg at 25°C
Vapor density	Not available
Water solubility	Miscible
Surface tension	Not available
Flash point	17°C
Autoignition temperature	482°C
Signal word / Pictogram	 Danger
H hazard statement	H225 Highly flammable liquid and vapor.  H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled.  H315 Causes skin irritation.  H319 Causes serious eye irritation.
P precautionary statements	P210, P261, P280, P305+P351+P338, P370+P378, P403+P235

Pyridine has been checked as substitute for Diglyme under the analogous conditions of the production process in the solvent Diglyme, but in a down-scaled version compared to the production process. All the parts of Diglyme have been replaced by Pyridine during the synthesis.

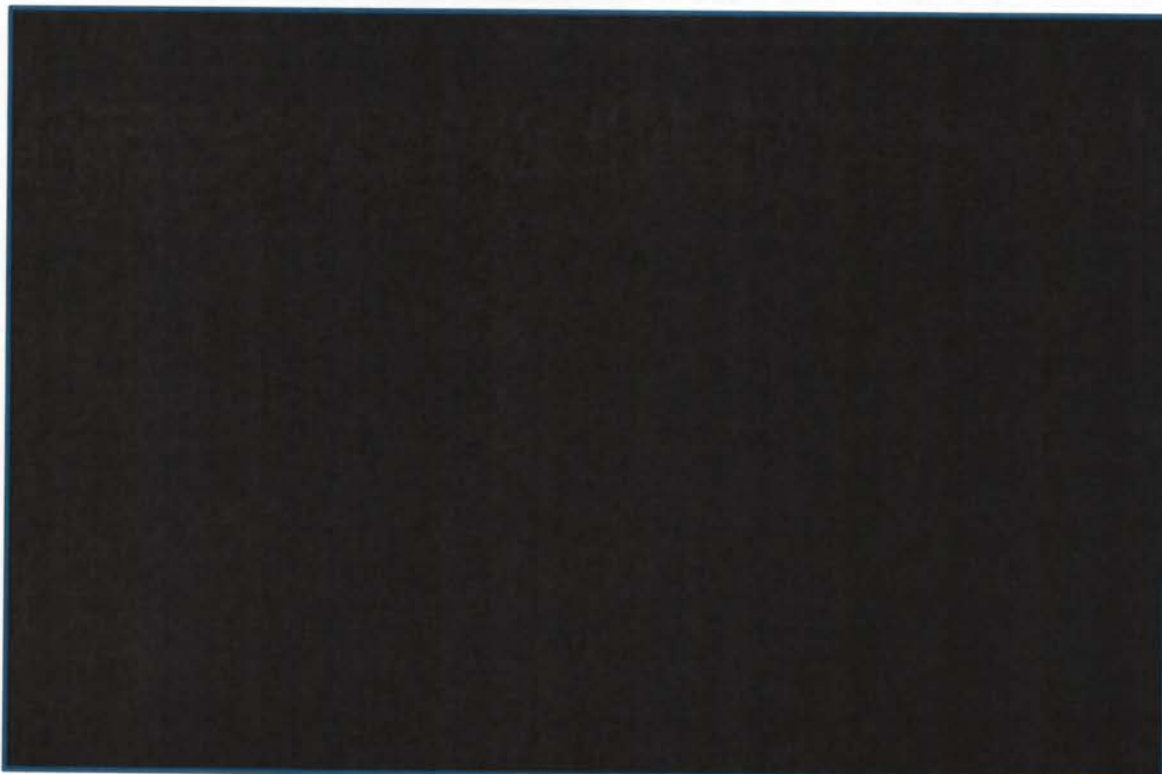
After completion of the process with Pyridine instead of Diglyme, a final product named "P" was obtained. The following <sup>1</sup>H-NMR spectrum of the raw product "P" was obtained:

## ANALYSIS OF ALTERNATIVES



Picture 1: full  $^1\text{H}$ -NMR of the raw product [REDACTED] P" (small-scale experiment with Pyridine as solvent)

A representative sample of [REDACTED] raw product from a current large-scale production in Diglyme was then taken as first comparative sample, named [REDACTED] D1". The  $^1\text{H}$ -NMR spectrum is shown below [REDACTED]:

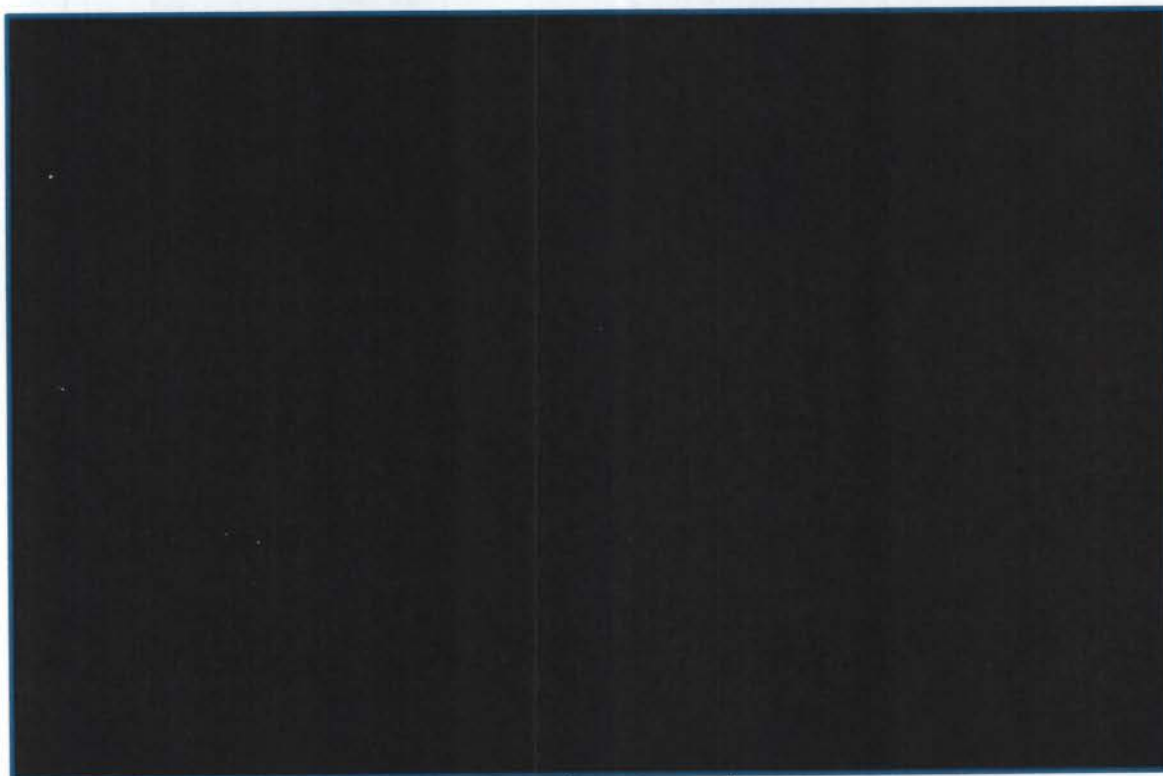




## ANALYSIS OF ALTERNATIVES

Picture 2: full  $^1\text{H}$ -NMR of the raw product [REDACTED] D1" (from current large-scale production in Diglyme)

A second comparative example, named [REDACTED] D2", was then synthesized with Diglyme as solvent in the same reactor and on the same scale like [REDACTED] P" in Pyridine. The  $^1\text{H}$ -NMR spectrum is shown below [REDACTED]:



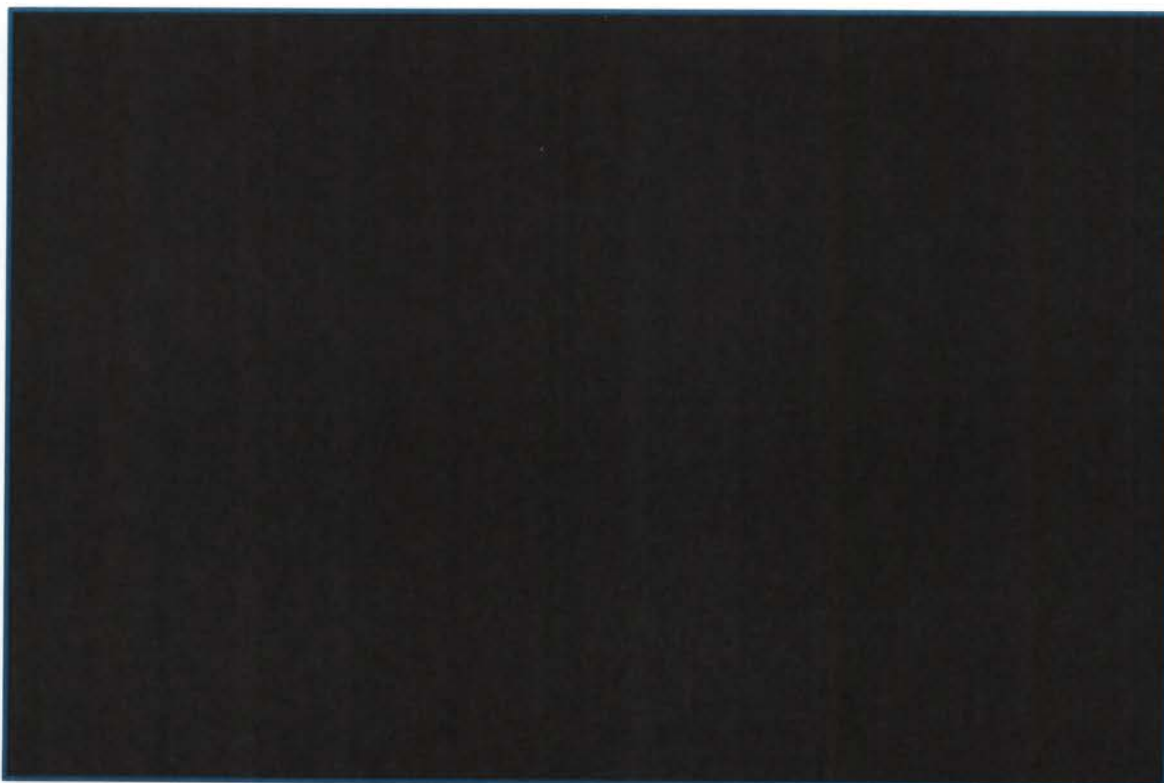
Picture 3: full  $^1\text{H}$ -NMR of the raw product [REDACTED] D2" (small-scale with Diglyme as solvent)

This second experiment in Diglyme on the small scale was made for better comparison of the [REDACTED] products made with Diglyme as solvent, since there are inevitable scale-up differences between [REDACTED] D1" and [REDACTED] D2", which can lead to slightly different  $^1\text{H}$ -NMR spectra.

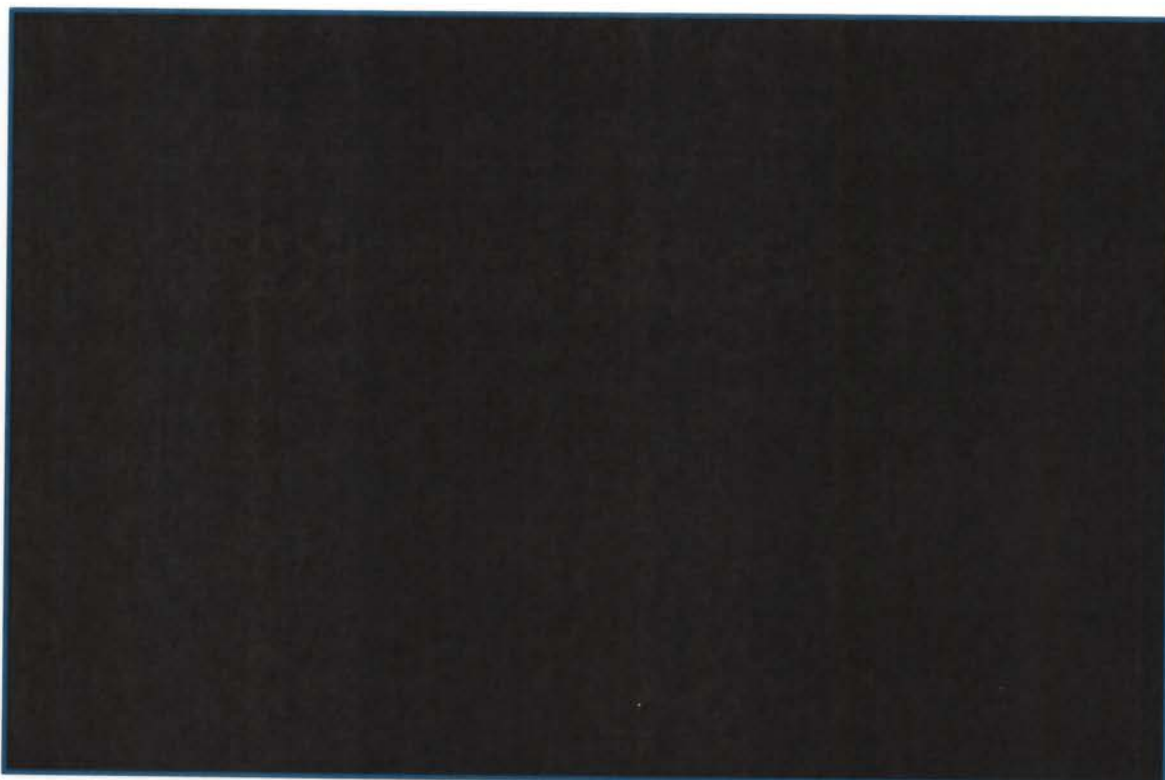
The comparison of the three  $^1\text{H}$ -NMR spectra of [REDACTED] P", [REDACTED] D1" and [REDACTED] D2" revealed, that [REDACTED] D1" and [REDACTED] D2" (both made by using Diglyme as solvent) showed a very similar peak pattern with slight differences which can be attributed to scale up effects.

On the other hand, the  $^1\text{H}$ -NMR spectrum of [REDACTED] P" (made with Pyridine as solvent) showed **significantly different** peaks especially in the [REDACTED] region when compared to the spectra of [REDACTED] D1" and [REDACTED] D2", which were made with Diglyme as solvent. Below, the magnified [REDACTED] regions [REDACTED] of all three  $^1\text{H}$ -NMR spectra are shown:

## ANALYSIS OF ALTERNATIVES

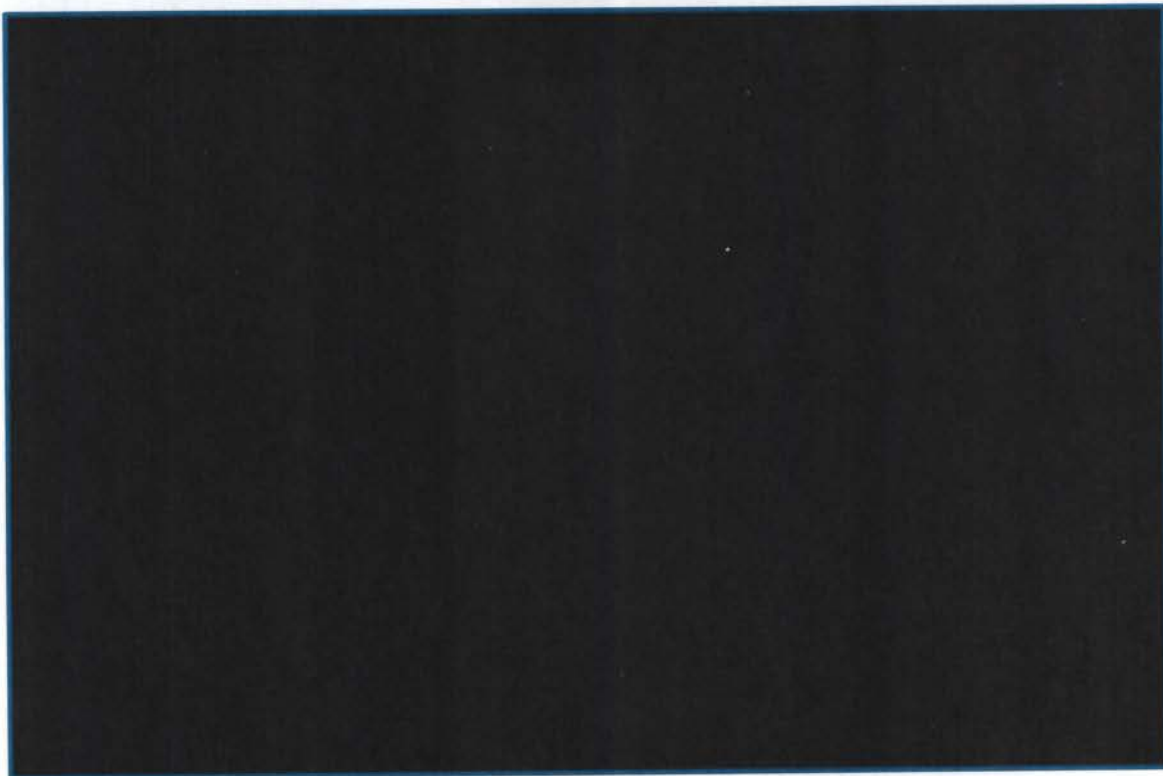


Picture 4: [REDACTED] region of the  $^1\text{H}$ -NMR [REDACTED] of the raw product [REDACTED]  
P" (small-scale made with Pyridine as solvent)



Picture 5: [REDACTED] region of the  $^1\text{H}$ -NMR [REDACTED] of the raw product [REDACTED]  
D1" (from current large-scale production in Diglyme)





Picture 6: [REDACTED] region of the  $^1\text{H}$ -NMR [REDACTED] of the raw product [REDACTED] D2" (small-scale with Diglyme as solvent)

The spectra of the comparative samples [REDACTED] D1" and [REDACTED] D2" made with Diglyme as solvent are very similar and are both cleaner and both significantly different to the spectrum of the [REDACTED] P" made with Pyridine as solvent.

Especially [REDACTED] NEW peaks are occurring, which are not present in the samples made with Diglyme as solvent.

Therefore, the use of Pyridine instead of Diglyme changes significantly the composition of the product by process [REDACTED], which is not acceptable.

With this, Pyridine has been excluded as well as potential alternative solvent to Diglyme in an experiment involving all [REDACTED] reaction steps of the [REDACTED] synthesis process.