★★★ ＜第37回知的財産翻訳検定試験【第18回英文和訳】＞ ★★★
≪１級課題 -化学-≫

【解答にあたっての注意】

１．問題の指示により和訳してください。

２．解答語数に特に制限はありません。適切な箇所で改行してください。

３．課題文に段落番号がある場合、これを訳文に記載してください。

４．課題は４題あります。それぞれの課題の指示に従い、４題すべて解答してください。

問１．質量分析に使用するキャリブレーション用ポリマー発明に関する従来技術の一部です。下記の***** START *****, ***** END *****の間の英文を日本語に翻訳してください。

[0006] With the growing potential of mass spectrometry for the rapid screening of peptides and proteins, the use of internal calibrants is particularly appealing for maximizing mass accuracy and thereby improving peptide identification. However, most biological and synthetic macromolecular calibrants consist predominately of H, C, N, and O, which all exhibit a mass defect that is either positive or negligibly negative. As a result, these calibrants exhibit a similar positive mass defect to those expected for biological analytes, increasing the likelihood that the analyte signal might be obscured, shifted, or misidentified because of a nearby or overlapping calibrant signal. An ideal internal calibrant set would have a mass defect signature that clearly differentiates it from the majority of peptide analytes. Mass-defect labeling has been explored to tag peptide analytes (Yao et al. 2008; Bajrami et al. 2009); however, the concept of incorporating a mass defect label into a calibrant has only been demonstrated to date by the inclusion of multiple fluorine atoms into calibrants (Fishman et al. 2001). However, while the negative mass defect of multiple fluorine atoms can provide contrast relative to the positive mass defect observed in most synthetic or biological polymers, a significant number of fluorine atoms (greater than 100) would be required to maximize the mass-defect offset relative to common analytes. An attractive alternative

is the incorporation of iodine, which exhibits a much larger negative mass defect (Shi et al. 2009), nearly 60 times greater per atom than F. In order to design calibrants with an optimized mass defect, the mass-defect distributions among natural peptides were first calculated, and this data set used to identify tris-iodinated cores as the ideal initiating groups for the synthesis of dendrimer-based mass-defect calibrants.

[0007] *** START ***For rapid screening of unknown proteomic and peptidomic analytes, internal calibrants can assure optimal mass accuracy; however, they should be designed to minimize the likelihood that a calibrant peak might obscure, or be confused with the analyte. The concept of "averagine" was proposed in order to model the average composition of an amino acid residue: $C_{4.9384}H_{7.7583}N_{1.3577}O_{1.4773}S_{0.0417}$. The averagine concept can also be used as a tool to identify the most populated mass defect associated with any nominal mass. In this case of averagine with a mass of 111.05431, it is comprised of a Nominal Mass of 110.9981 and a mass defect of 0.0562055. To aid in our calibrant design, we propose the concept of "scarcine." If averagine traces the most common mass defect for a given nominal mass (for a given population of compounds, such as peptides), then scarcine is the least common mass defect for a given nominal mass. To better define the targets for a mass-defect calibrant, we have mapped the population of all peptides (MW 0-2400) with respect to their nominal mass and mass defect (see FIGS. 5 and 6.) *** END ***While the nominal mass of each possible peptide is measured on the x-axis and its corresponding mass defect is measured on the y-axis, the z-axis represents the population of peptides with that specific mass (the population values calculated for a 1 u width in the nominal mass, and a 0.01 u width in the mass defect). It should be noted that these initial population calculations were determined assuming an unbiased statistical incorporation of the 20 most common proteinogenic amino acids residues, rather than the actual frequency of occurrence, and without taking into consideration the effect of post-translational modifications.

問２．以下は、"Fluidic channel coated with metal catalysts and devices and methods relating thereto"と題する特許出願の記載の一部です。下記の*** START ***, *** END ***の間の英文を日本語に翻訳してください。

[0040] Currently, there is a problem in coating fluidic channels with catalysts having controlled dimensions and morphology. Controlled dimension of the coating is important to prevent clogging. Controlled morphology of the catalyst is also needed for improved catalyst efficacy, particularly in continuous flow catalysis. The invention described herein solves these two problems.

[0041] The technology described herein differs significantly from what currently exists in the field. Currently, there is no process or method available prior to this disclosure to coat fluidic channels with catalysts having controlled dimensions and morphology (see De Jong, Krijn P. (ed.), Synthesis of Solid Catalysts, May 2009, Wiley-VCH, Weinheim). Currently used approaches have several drawbacks as follows.

[0042] In one approach, a catalyst is typically supported on a catalyst support and tested in a reaction flask. The disadvantages of this approach is that there is a need for preparing the supported catalyst and it needs to be separated and reused after the reaction (see Gaur, Miller, Stellwagen, Sanampudi, Kumar, and Spivey, Synthesis, characterization, and testing of supported Au catalysts prepared from atomically-tailored Au38(SC12H25)24 clusters, Phys. Chem. Chem. Phys, 2012, 14(5), 1627-1634; and Turner et al., Nature, 454, 981-983, 2008). Another disadvantage is the poor reproducibility and process control of the supported catalyst preparation.

[0043] In a second approach, catalysts are supported within large columns and the reagents are flown through such fixed bed reactor columns (see De Jong, Krijn P. (ed.), Synthesis of Solid Catalysts, May 2009, Wiley-VCH, Weinheim). The disadvantage with this approach is that there is no control over the structure of the catalyst (the micro and nano precision) and hence the surface area of the catalysts.

[0044] In a third approach, the catalysts are embedded within microfluidic channels and catalysis is carried out as in the previous case (Ismagilov et al.,

Oxidation of organic compounds in a microstructured catalytic reactor, Chemical Engineering Journal, 2008, 135S, S57-S65). However, fabrication of microfluidic catalyst beds is expensive and impractical for large numbers of experiments.

*** START ***

[0045] Chip-based millifluidics, and related hand-held apparatus, as disclosed herein, offer a technology very different from tubular millifluidics with demonstrated advantages over traditional microfluidics for higher throughput controlled synthesis of ultrasmall nanoclusters and as probes for mapping time-resolved growth of nanomaterials. A central theme of these novel investigations is the utility of millifluidics for mapping the time-resolved chemistry of the growth of metallic structures in general and catalysts in particular.

[0046] Also provided is a demonstration of continuous flow catalytic activity of the as-formed gold nanostructures, for example, the reduction of 4-nitrophenol and ferricyanide. While microfluidics-based continuous flow catalysis of gold nanoparticles impregnated on alumina has been previously utilized for synthesis of polypyridine derivatives, the ability to control the dimension, and morphology of the embedded gold nanostructured catalysts within continuous flow channels can provide superior continuous flow catalysis applications. With the ability to embed atomically precise catalysts, these tools can revolutionize catalysis from the point of view of practical as well as fundamental investigations. Such systems can also lead to advances in the field of bio-sensing, electrophoresis, and enhanced optical detection. Additionally, the flower-like gold morphology obtained through this formation process has applications in surface-enhanced Raman spectroscopy, catalysis, bio-imaging, and super-hydrophobic coatings.

*** END ***

問３．バイポーラ膜電気透析プロセスに関する下記の英文を日本語に翻訳してください。図は参考ですので、図中の英語の翻訳は不要です。

[0102] Figure la demonstrates the configuration of a membrane cell and the flow of the respective ions when subjected to an electric potential between a cathode and anode.

[0103] The product stream from the salt compartment was then directed to an iminodiacetic acid (IDA) crystallizer operating at 20°C. This resulted in a crystallizer stream comprising solid IDA, soluble monosodium iminodiacetic acid (IDA), and soluble MSIDA. The resulting crystallizer stream was then directed to a filtration system whereby the solid IDA was separated and dried, for use in downstream glyphosate production. The soluble IDA and MSIDA exiting the filtration system was recirculated and mixed with the feed stream for contact with the two-compartment bipolar membrane electrodialysis process. Figure 2 shows the 2-compartment BME process in the context of this overall disodium iminodiacetic acid (DSIDA) conversion and recirculation process.

[0104] When the process had been started and the soluble IDA and MSIDA exiting the filtration system was continually recirculated as a source of the feed composition for the two-compartment bipolar membrane electrodialysis process, the following values were observed:

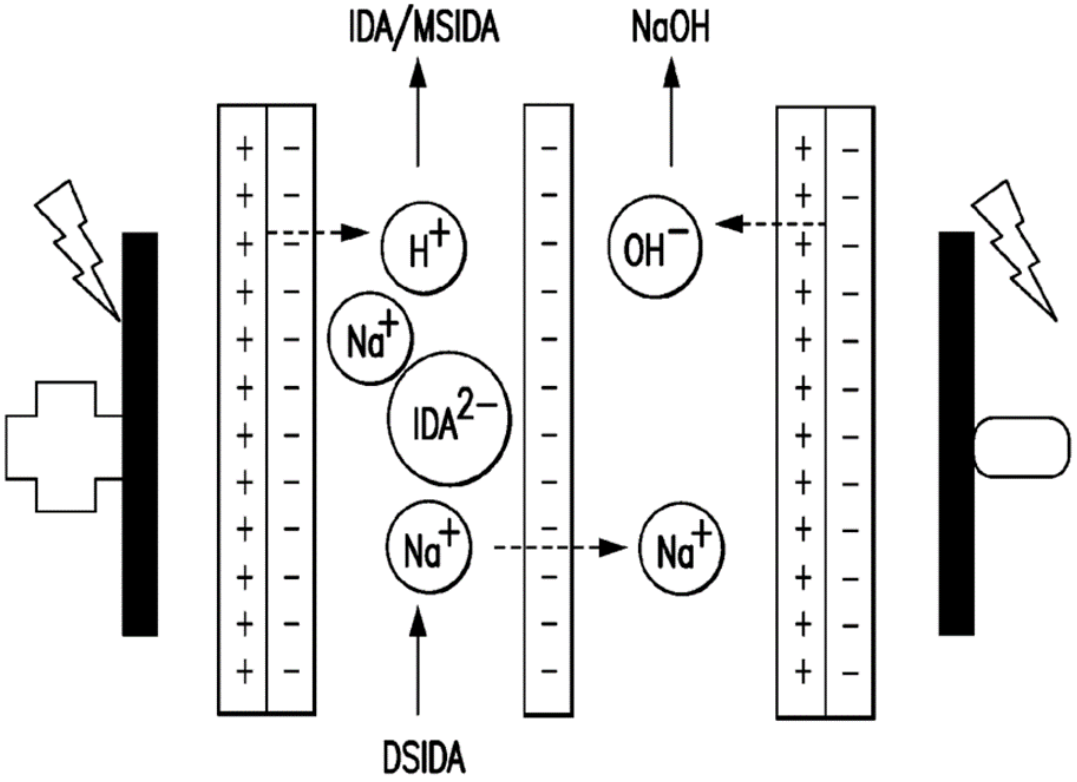
IDA/MSIDA
NaOH
H+
Na+
IDA2−
OH−
Na+
Na+
DSIDA

FIG. 1a

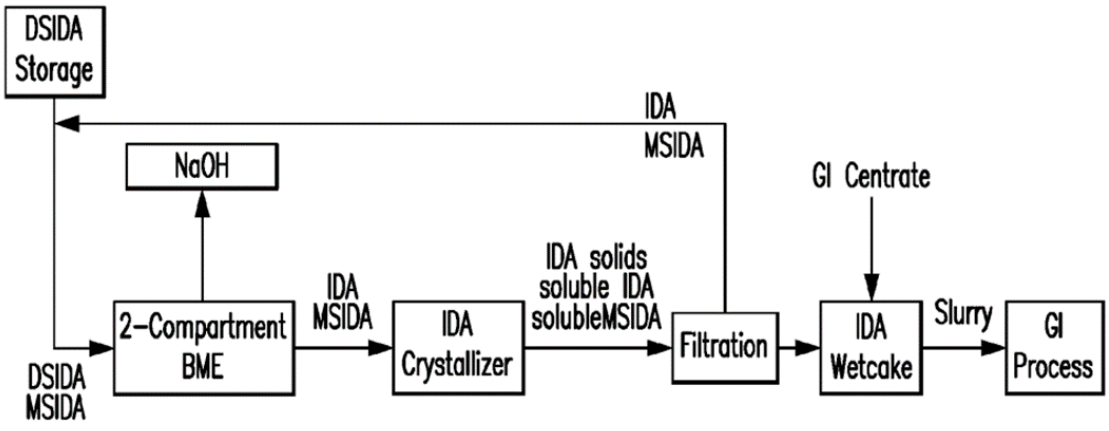
DSIDA Storage
IDA MSIDA
NaOH
GI Centrate
IDA solids soluble IDA solubleMSIDA
IDA MSIDA
2−Compartment BME
IDA Crystallizer
Filtration
IDA Wetcake
Slurry
GI Process
DSIDA MSIDA

FIG. 2

問４．以下は、"Combinatorial Chemistry Computational System and Enhanced Selection Method"と題する特許出願の特許請求の範囲の記載の一部です。Claim 1 にあたる下記英文クレームを日本語に翻訳してください。

1. A method for identifying one or more potentially useful molecular combinations comprising:

applying a selection procedure to a compound of interest to identify a first set of one or more candidate molecules, the selection procedure comprising:

providing a chemical synthesis scheme for a compound of interest, a virtual scaffold molecule of the compound of interest, and a virtual reactant fragment to react with the virtual scaffold molecule according to the chemical synthesis scheme;

preparing the virtual reactant fragment and the virtual scaffold molecule for analyzing combinations of the virtual reactant fragment and the virtual scaffold molecule;

designating a remaining scaffold subset and a remaining fragment subset if a product molecule can be formed from the virtual scaffold molecule and the virtual reactant fragment;

rotating the remaining fragment subset about an axis connecting the remaining scaffold subset and the remaining fragment subset through 360 degrees in increments of less than or equal to 5 degrees; and

identifying potentially useful combinations of the virtual reactant fragment and the virtual scaffold molecule, by:

recording as a potential product increment each increment at which a steric collision is not detected; and

recording a separation distance between the remaining fragment subset and the remaining scaffold subset at each increment and identifying a set of product increments for which the separation distances are less than or equal to a predetermined criterion distance to identify the one or more potentially useful molecular combinations;

identifying a set of combinatorial fragments from the first set of one or more candidates; and

applying the selection procedure to the set of combinatorial fragments to identify a second set of one or more candidate molecules that are the one or more potentially useful molecular combinations.