

CLAIMS:

1. A sample preparation method (100) comprising:
 - 5 - providing a sample (10) comprising an organic molecule (20), wherein the organic molecule (20) comprises a target group (21), wherein the target group (21) is a nucleophilic group, and/or an acidic group;
 - a derivatization stage (110) comprising: derivatizing the target group (21) of the organic molecule (20) with a moiety (31) comprising one or more of (i) a hydrocarbon
10 comprising group and (ii) a 3rd period atom comprising group, wherein the 3rd period atom is selected from the group consisting of Si, P, and S, thereby providing a derivatized organic molecule (30);
 - a separation stage (120) comprising: subjecting the sample (10) to a separation process to provide a fraction (35) comprising the derivatized organic molecule (30);
15 - a preparation stage (130) comprising: introducing the derivatized organic molecule (30) into a porous single crystal (40), to provide a derivatized organic molecule doped porous single crystal (50).
2. The sample preparation method (100) according to any one of the preceding
20 claims, wherein the sample (10) comprises a protic solvent, wherein the separation stage (120) further comprises executing a solvent exchange by replacing at least part of the protic solvent by an aprotic solvent, and wherein, the separation stage (120) comprises subjecting the sample to an LC process or GC process.
- 25 3. The sample preparation method (100) according to any one of the preceding claims, wherein the porous single crystal (40) comprises a metal-organic framework material, wherein the metal-organic framework material is tpt-ZnX_2 based where X = Cl or Br or I.
4. The sample preparation method (100) according to any one of the preceding
30 claims, wherein the organic molecule (20) is selected from the group consisting of an organic biomolecule, and wherein the target group (21) is selected from the group consisting of -OH, -COOH, -NH₂, -NRH, and -SH.

5. The sample preparation method (100) according to any one of the preceding claims, wherein the moiety (31) comprises the hydrocarbon comprising group, wherein the moiety comprises an aliphatic group and/or an alkyl group and/or a methyl group, and/or an aromatic group, especially wherein the aromatic group comprises a phenyl group or a benzyl group.
6. The sample preparation method (100) according to any one of the preceding claims, wherein the moiety (31) comprises the 3rd period atom comprising group, wherein the 3rd period atom is selected from the group consisting of Si, P, and S.
7. The sample preparation method (100) according to claim 6, wherein the 3rd period atom comprises Si, and wherein the moiety (31) comprises a group selected from the group consisting of -SiR₃, -SiArR₂, -SiAr₂R, -SiAr₃, wherein R is selected from the group consisting of methyl, ethyl, propyl, isopropyl, and wherein Ar is -C₆H₅.
8. The sample preparation method (100) according to any one of the preceding claims, wherein the separation stage (120) comprises providing N fractions (35), wherein N $\geq$ 2, and wherein the preparation stage (130) comprises contacting the N fractions with N porous single crystals (40), respectively, to provide N organic molecule doped porous single crystals (50).
9. The sample preparation method (100) according to any one of the preceding claims, wherein the sample preparation method (100) further comprise a pre-analysis stage (145) after the separation stage (120), the pre-analysis stage (145) comprising subjecting at least part of the fraction (35) to a mass spectrometry process (124) to attempt to identify the derivatized organic molecule (30), wherein the pre-analysis stage (145) comprises providing the fraction (35) to the preparation stage (130) if the identification of the derivatized organic molecule (30) with the mass spectrometry process (124) is unsuccessful, and wherein the pre-analysis stage (145) comprises terminating the sample preparation method (100) if the identification of the derivatized organic molecule (30) with the mass spectrometry process (124) is successful.
10. An X-ray analysis method (200) of an organic molecule (20), the method comprising a sample providing stage and an analysis stage (240), wherein the sample providing

stage comprises providing the derivatized organic molecule doped porous single crystal (50) *obtainable* according to any one of the preceding claims 1-9, and wherein the analysis stage (240) comprises subjecting the derivatized organic molecule doped porous single crystal (50) to single crystal X-ray analysis.

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11. The X-ray analysis method (200) according to claim 10, comprising subjecting each of the N derivatized organic molecule doped porous single crystals (50) according to claim 8 to a single crystal X-ray analysis, respectively.

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12. A system (300) comprising:

- a derivatization unit (310), configured to derivatize a target group (21) of an organic molecule (20) with a moiety (31) comprising one or more of (i) a hydrocarbon comprising group and (ii) a 3rd period atom comprising group, wherein the 3rd period atom is selected from the group consisting of Si, P, and S, thereby providing a derivatized organic molecule (30), wherein the target group (21) is a nucleophilic group, and/or an acidic group;
- a separation unit (320), functionally coupled to the derivatization unit (310), configured to subject a sample (10) comprising the derivatized organic molecule (30) to a separation process to provide a fraction (35) comprising the derivatized organic molecule (30);
- a preparation unit (330), functionally coupled to the separation unit (320), configured to introduce the derivatized organic molecule (30) into a porous single crystal (40), to provide a derivatized organic molecule doped porous single crystal (50);
- an analysis unit (340), functionally coupled to the preparation unit (330), configured to subject the organic molecule doped porous single crystal (50) to single crystal X-ray analysis;
- a control system (350), configured to control the derivatization unit (310), the separation unit (320), the preparation unit (330) and the analysis unit (340).

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13. The system (300) according to claim 12, wherein the separation unit (320) comprises one or more of a LC system (322a) and a GC system (322b), especially one or more of a LCMS system (325a) and a GCMS system (325b).

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14. The system (300) according to any one of the preceding claims 12-13, further comprising a solvent exchange unit, functionally coupled to the separation unit (320) and to the preparation unit (330), configured to solvent exchange the fraction (35) comprising the

derivatized organic molecule (30) from the separation unit (320) and to provide a solvent-exchange fraction comprising the derivatized organic molecule (30) to the preparation unit (330), and wherein the separation unit (120) is configured to provide N fractions (35), wherein $N \geq 2$, and wherein the preparation unit (330) is configured to introduce the derivatized organic molecule (30) of each of the N fractions (35) into a respective porous single crystal (40), to provide respective derivatized organic molecule doped porous single crystals (50).

15. The system (300) according to any one of the preceding claims 12-15, wherein the system (300) is configured to execute the sample preparation method (100) according to any one of the preceding claims 1-9 and/or the X-ray analysis method (200) according to any one of the preceding claims 10-11.