**Compound 1 (ACS01): Isoacorone**

**IUPAC Name:** (1S, 8S)-1-Isopropyl-4,8-dimethylspiro [4.5] decan-2,7-dione



**Chemical formula :** C15H24O2

**Exact mass :** 236.18

**Molecular weight :** 236.35 g/m

**Melting point :** 96-97 oC

**Physical state :** Crystals

**Specific rotation : -**00.003 to -00.006

**M/z :** 236.18 (100%), 237.18 (16.6%), 238.18 (1.6%)

**Elemental analysis :** C: 76.23, H: 10.24, O: 13.54



**1H NMR spectrum of Isoacorone**

A graph of a person's body

Description automatically generated with medium confidence

**13C NMR spectrum of Isoacorone**

A graph with numbers and lines

Description automatically generated

**DEPT spectrum of Isoacorone**

**Compound 2 (ACS02): Cis-asarone (β- asarone)**

**IUPAC Name :** 1, 2, 4 trimethoxy -5-(prop -1-en-1-yl) benzene



**Molecular Formula :** C12H16O3

**Molecular weight :** 208.257 g/m

**Colour :** Yellowish oily liquid

**Melting point :** 62.00 to 63.00 °C.

A graph of a red line

Description automatically generated

**1H NMR spectrum of β-Asarone**

A graph of a person with a red line

Description automatically generated

**13C NMR spectrum of Beta asarone**

**Compound 3 (ACS03): Trans-asarone (α - asarone**)

**IUPAC Name :** Trans-1, 2, 4-trimethoxy -5(2-propenyl) benzene



**Molecular Formula :** C12H16O3

**Molecular Weight :** 208.25

**Colour :** Colourless crystalline solid

**Melting point :** 62 oC



**1H NMR Spectrum of α- asarone**

A graph of a person

Description automatically generated with medium confidence

**13C NMR Spectrum of α- asarone**

**Compound 4 (ACS04): Acoric acid**

**IUPAC Name :** (S)-3[(1S, 4R)-1-isobutryryl-4-methyl-3-oxocyclohexyl) butanoic Acid



**Molecular formula :** C15H24O4

**Molecular weight :** 268.353g/m

**Exact Mass :** 268.17g/m

**M/z :** 268.17(100%), 269.17(16.7%), 270.17(2.1%)

**Elemental analysis :** C: 67.14, H: 9.01, O: 23.85

**Melting point :** 166 oC - 168 oC

**Physical state :** crystalline



**1H NMR Spectrum of Acoric acid**

A graph of a number of objects

Description automatically generated with medium confidence

**13 C NMR Spectrum of Acoric acid**

A graph of a graph

Description automatically generated

**DEPT Spectrum of Acoric acid**

**Compound 5 (ACS05): Acorone**

**IUPAC Name:** 1-Isopropyl-4, 8- dimethylspiro [4.5] decan-2, 7-dione



**Chemical formula :** C15H24O2

**Molecular weight :** 236 g/m

**Melting point :** 100-101 oC

**Physical state : C**rystalline

**Specific rotation :** +00.006 to 0.008



**1H NMR Spectrum of Acorone**

A graph of a bar graph

Description automatically generated with medium confidence

**13C NMR spectral data of compound Acorone**

A graph with numbers and lines

Description automatically generated

**DEPT Spectral data of Acorone**

**Compound 6 (ACS6): Beta sitosterol glycoside**

**IUPAC Name :** 2-((17-(5, 6-dimethylheptan-2-yl)-10, 13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a] phenanthren-3- yl) oxy) -6- (hydroxymethyl) tetrahydro-2H-pyran-3, 4, 5-triol



**Chemical formula :** C34H58O6

**Molecular weight :** 562.82g/m

**Exact Mass :** 562.42

**Physical state : S**olid white powder

**M/z** **:** 562.42(100%), 563.43(37.7%), 564.43(8.1%), 565.43(1.2%)

**Elemental analysis :** C: 72.56, H: 10.39, O: 17.06



**1H NMR Spectrum of compound β-Sitosterol glycoside**

A graph of a graph

Description automatically generated

**13 C NMR Spectrum of compound β-Sitosterol glycoside**

A graph of a graph

Description automatically generated

**DEPT Spectrum of β-Sitosterol glycoside**

**Compound 7 (ACS07): 2, 3, 4-Trihydoxybutyl tetradecanoate**

**IUPAC Name :** 2, 3, 4-Trihydoxybutyl tetradecanoate



**Chemical formula :** C18H36O5

**Molecular weight :** 332.47 g/m



**1H NMR Spectrum of compound 2, 3, 4-Trihydoxybutyl tetradecanoate**

A graph of a person with a ruler

Description automatically generated

**13 C NMR Spectrum of compound 2, 3, 4-Trihydoxybutyl tetradecanoate**

A graph of a graph

Description automatically generated

**DEPT Spectrum of compound 2, 3, 4-Trihydoxybutyl tetradecanoate**

**Compound 8 (ACS08): Stearic acid**

**IUPAC Name :** Octadenaoic acid



**Chemical formula :** C18H36O2 , CH3(CH2)16COOH

**Molecular weight :** 284.48 g/mol

**Melting point :** 69.3%

**Boiling point :** 3610C

**Physical state :** Saturated fatty acid

**Density :** 941kg/m

A graph of a person

Description automatically generated

**1H NMR Spectrum of compound Stearic acid**

A graph of a graph

Description automatically generated with medium confidence

**13C NMR Spectrum of compound Stearic acid**

A graph of a person

Description automatically generated

**DEPT Spectrum of compound stearic acid**