

Small Molecule Identification with MOLGEN and Mass Spectrometry

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Supporting Information

This file contains supporting information for the abovementioned article and includes:

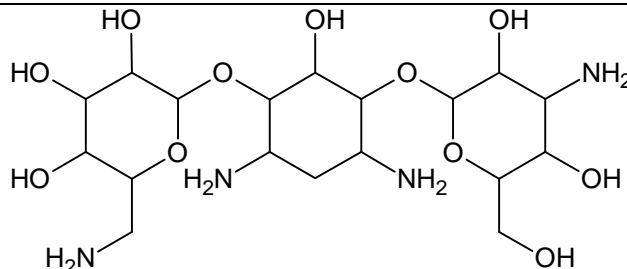
Table SI-1: The LC Challenges for CASMI 2012. Pages 1-3.

Table SI-2: The GC Challenges for CASMI 2012. Page 4.

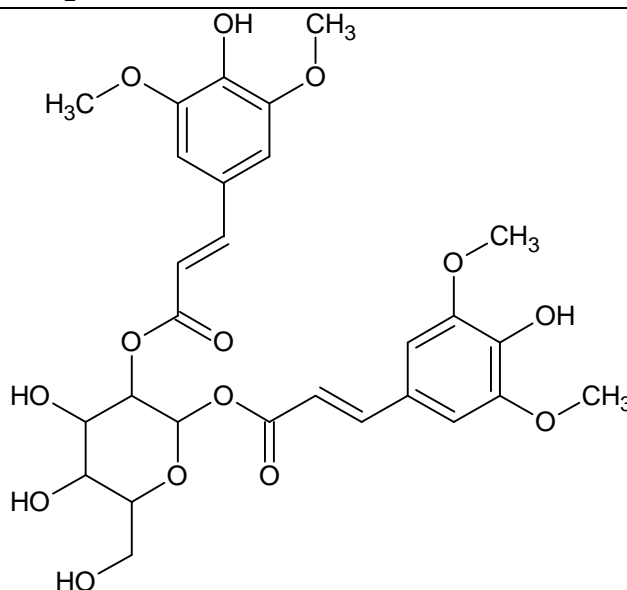
[1]: E. L. Schymanski and S. Neumann. CASMI: Challenges and Solutions, Metabolites, in review.

Table SI-1: The LC Challenges for CASMI 2012. Source: [1].

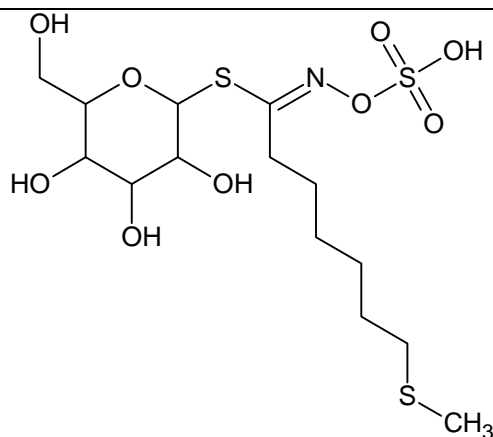
Challenge 1
Kanamycin A
 $C_{18}H_{36}N_4O_{11}$
PubChem: 6032
ChemSpider: 5810



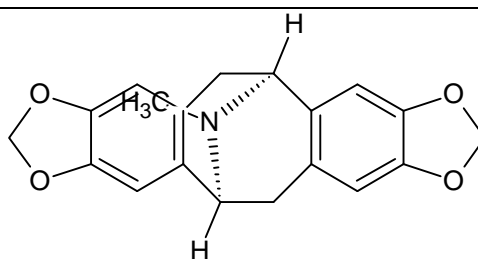
Challenge 2
1,2-Bis-O-sinapoyl-beta-D-glucoside
 $C_{28}H_{32}O_{14}$
PubChem: 5280665
ChemSpider: 4444262



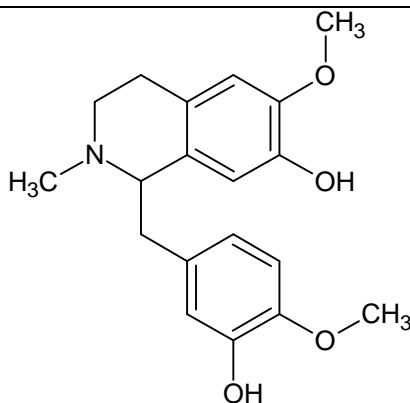
Challenge 3
Glucosquerellin
 $C_{14}H_{27}NO_9S_3$
PubChem: 46173875
ChemSpider: NA



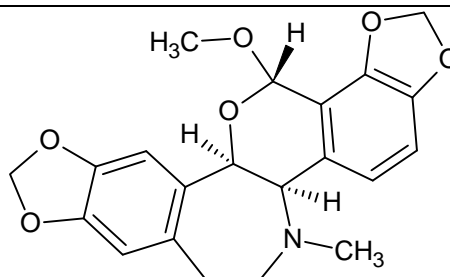
Challenge 4
Escholtzine
 $C_{19}H_{17}NO_4$
PubChem: 12304178
ChemSpider: 16740500



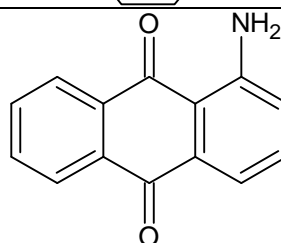
Challenge 5
Reticuline
 $C_{19}H_{23}NO_4$
PubChem: 10233
ChemSpider: 9816



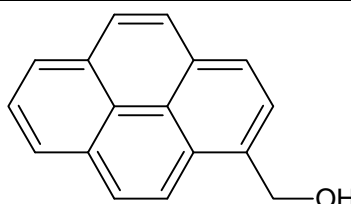
Challenge 6
Rheadine
 $C_{21}H_{21}NO_6$
PubChem: 197775
ChemSpider: 171184



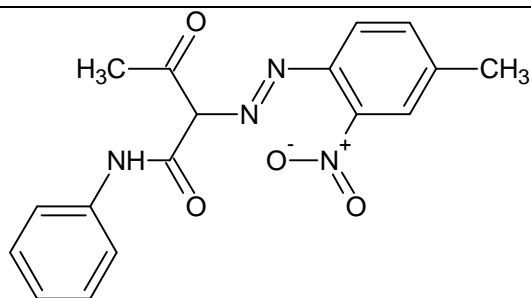
Challenge 10
1-Aminoanthraquinone
 $C_{14}H_9NO_2$
PubChem: 6710
ChemSpider: 6454



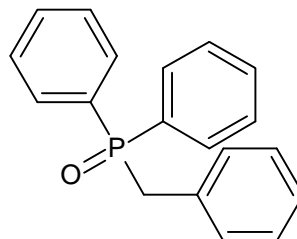
Challenge 11
1-Pyrenemethanol
 $C_{17}H_{12}O$
PubChem: 104977
ChemSpider: 94729



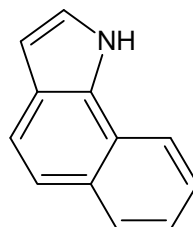
Challenge 12
alpha-(o-Nitro-p-tolyl
azo)acetoacetanilide
 $C_{17}H_{16}N_4O_4$
PubChem: 221491
ChemSpider: 192174



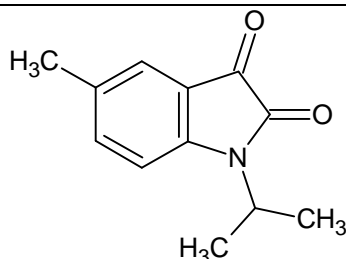
Challenge 13
Benzyl-diphenyl phosphine
oxide
 $C_{19}H_{17}OP$
PubChem: 76293
ChemSpider: 68772



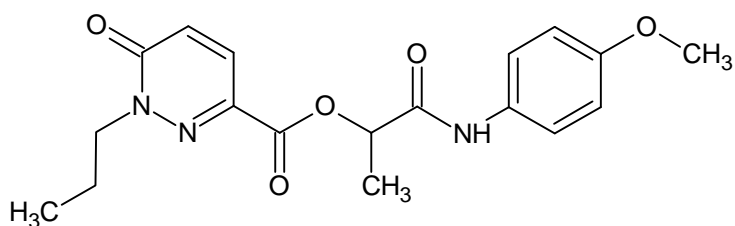
Challenge 14
1H-Benz[g]indole
 $C_{12}H_9N$
PubChem: 98617
ChemSpider: 89061



Challenge 15
1-Isopropyl-5-methyl-1H-
indole-2,3-dione
 $C_{12}H_{13}NO_2$
PubChem: 2145522
ChemSpider: 1606080



Challenge 16
1-[(4-Methoxyphenyl) amino]-
1-oxo-2-propanyl 6-oxo-1-
propyl-1,6-dihydro-3-
pyridinecarboxylate
 $C_{18}H_{21}N_3O_5$
PubChem: 18091616
ChemSpider: 16896706



Challenge 17
Nitrin
 $C_{13}H_{13}N_3$
PubChem: 68380
ChemSpider: 61666

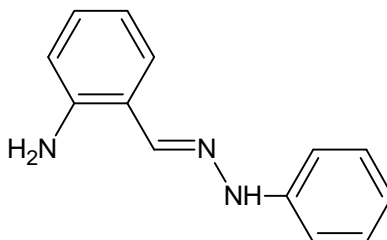


Table SI-2: The GC Challenges for CASMI 2012. Source: [23].

Challenge 1 Phthalic anhydride $C_8H_4O_3$ PubChem: 6811 ChemSpider: 6552		Challenge 2 Phthalimide $C_8H_5NO_2$ PubChem: 6809 ChemSpider: 6550	
Challenge 3 2-Chlorobenzyl alcohol C_7H_7ClO PubChem: 28810 ChemSpider: 26799		Challenge 4 4-Chlorobenzyl alcohol C_7H_7ClO PubChem: 13397 ChemSpider: 12823	
Challenge 5 1,4-Dichlorobenzene $C_6H_4Cl_2$ PubChem: 4685 ChemSpider: 13866817		Challenge 6 Acenaphthene $C_{12}H_{10}$ PubChem: 6734 ChemSpider: 6478	
Challenge 7 4-Chlorobenzoic acid $C_7H_5ClO_2$ PubChem: 6318 ChemSpider: 6079		Challenge 8 Fluorene $C_{13}H_{10}$ PubChem: 6853 ChemSpider: 6592	
Challenge 9 Methyl 2-chlorobenzoate $C_8H_7ClO_2$ PubChem: 11895 ChemSpider: 11402		Challenge 10 2,4,6-Trichlorophenol $C_6H_3Cl_3O$ PubChem: 6914 ChemSpider: 21106172	
Challenge 11 Formothion $C_6H_{12}NO_4PS_2$ PubChem: 17345 ChemSpider: 16412		Challenge 12 alpha-Hexachloro- cyclohexane $C_6H_6Cl_6$ PubChem: 727 ChemSpider: 10468511	
Challenge 13 Dimethyl carbonotrithioate $C_3H_6S_3$ PubChem: 16840 ChemSpider: 15959		Challenge 14 O,O,O-Trimethyl thiophosphate $C_3H_9O_3PS$ PubChem: 9038 ChemSpider: 8686	
Challenge 15 Dibenzofuran $C_{12}H_8O$ PubChem: 568 ChemSpider: 551		Challenge 16 O,S,S-Trimethyl phosphorodithioate $C_3H_9PS_2O_2$ PubChem: 31435 ChemSpider: 29165	