

Identification of unknown compound

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April 26, 2017

Task 0: Classification of an unknown substance

Assign the general name to displayed substances:

CARBOHYDRATE

PEPTIDE

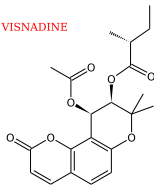
STEROID

TERPENE

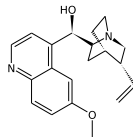
ALKALOID

COUMARINE

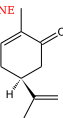
VISNADINE



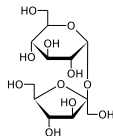
QUININE



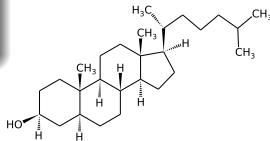
CARVONE



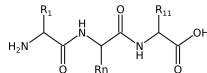
SACHAROSA



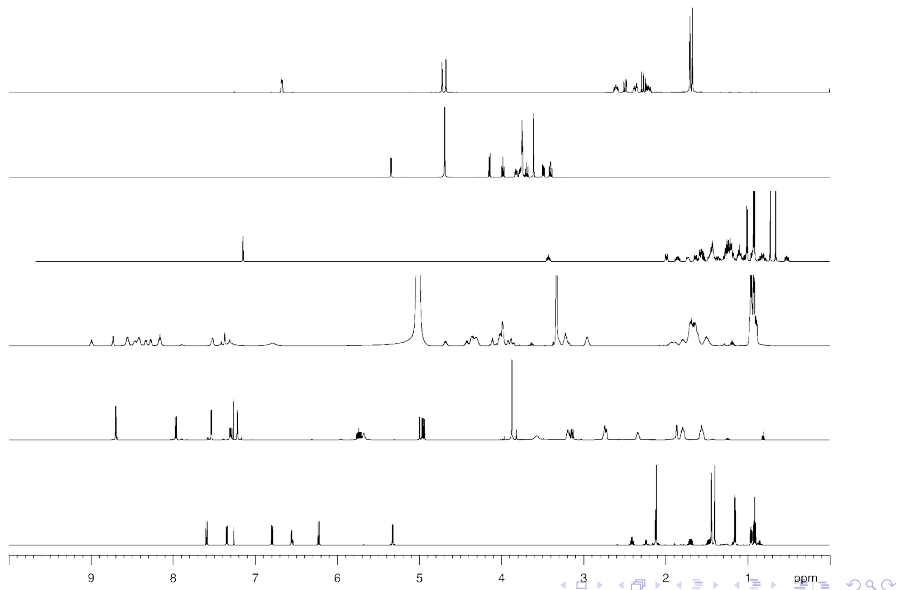
DIHYDROCHOLESTEROL



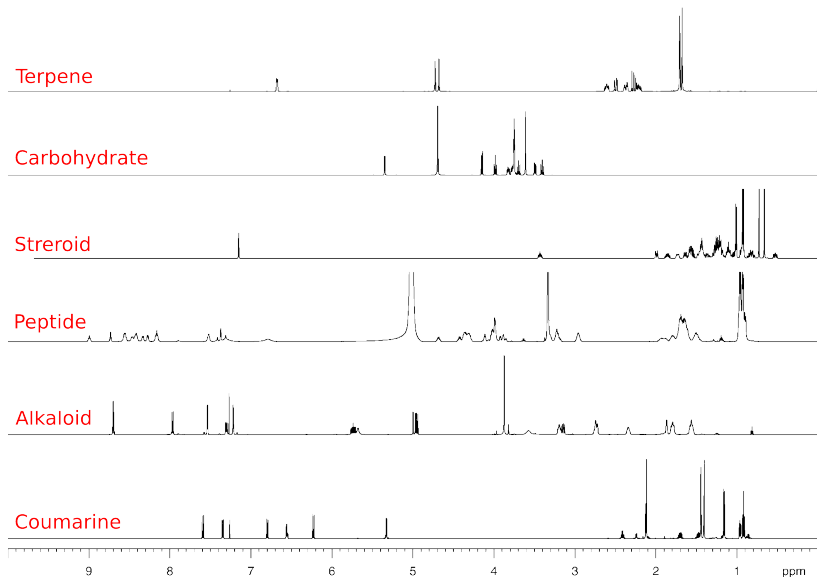
SGGLRLHLGLS



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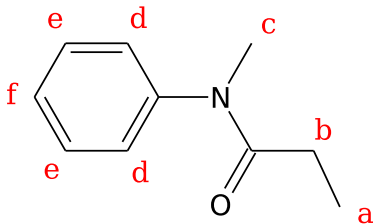


Task 1: C₁₀H₁₃NO

δ [ppm]	Multiplicity	Integral
1.05	triplet	3
1.75	singlet	3
3.70	quartet	2
7-7.60	complex multiplet	5

Task 1: C₁₀H₁₃NO

δ [ppm]	Multiplicity	Integral
1.05 a	triplet	3
1.75 c	singlet	3
3.70 b	quartet	2
7-7.60 d-f	complex multiplet	5

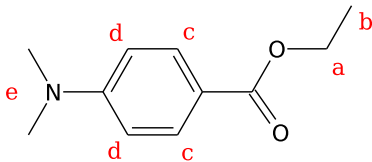


Task 2: $C_{11}H_{15}NO_2$

δ [ppm]	Multiplicity	J (Hz)	Integral
1.30	triplet	7	3
3.00	singlet	-	6
4.25	quartet	7	2
6.65	dublet	8	2
7.80	dublet	8	2

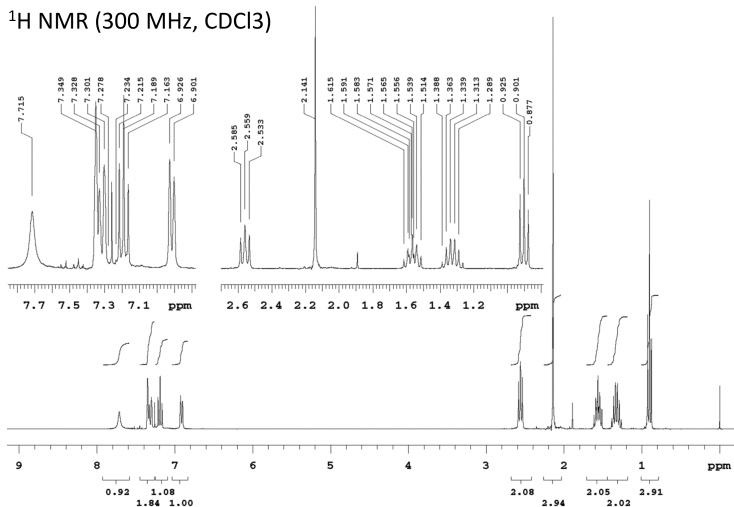
Task 2: $C_{11}H_{15}NO_2$

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1.30 b	triplet	7	3
3.00 e	singlet	-	6
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6.65 d	dublet	8	2
7.80 c	dublet	8	2



Task 3: C₁₂H₁₇NO - ¹H/COSY

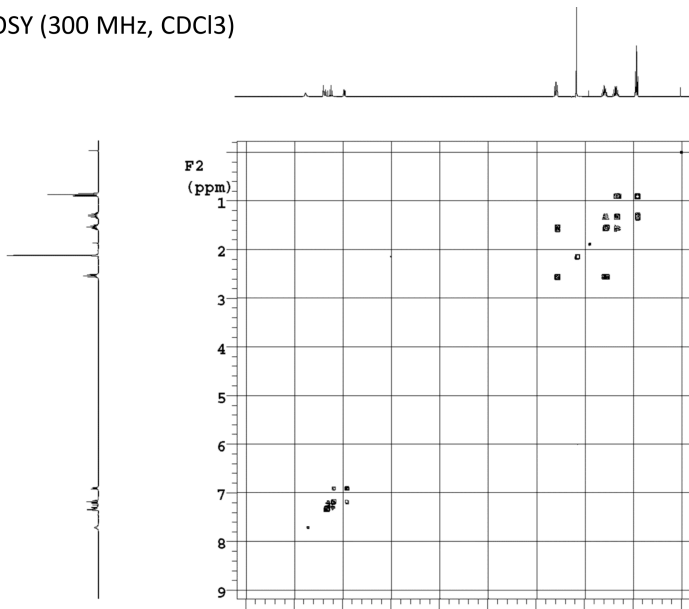
¹H NMR (300 MHz, CDCl₃)



SOLUTION

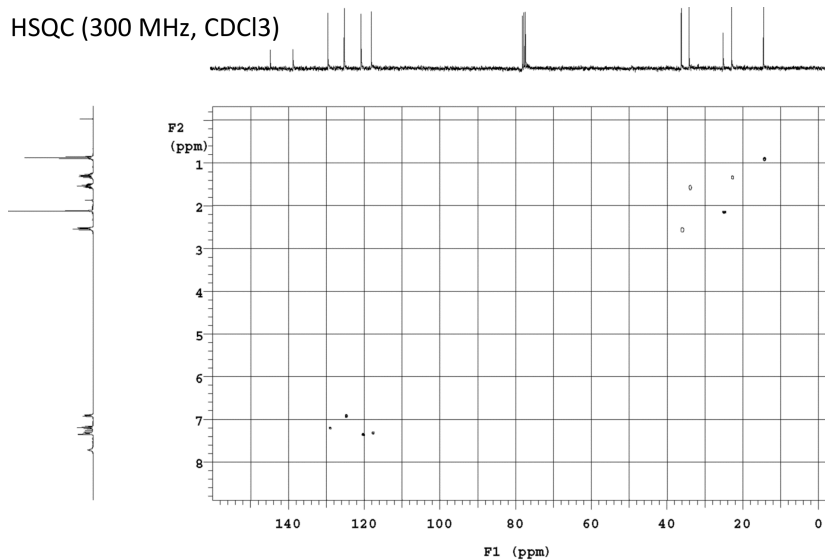
Task 3: $C_{12}H_{17}NO$ - $^1H/COSY$

COSY (300 MHz, $CDCl_3$)



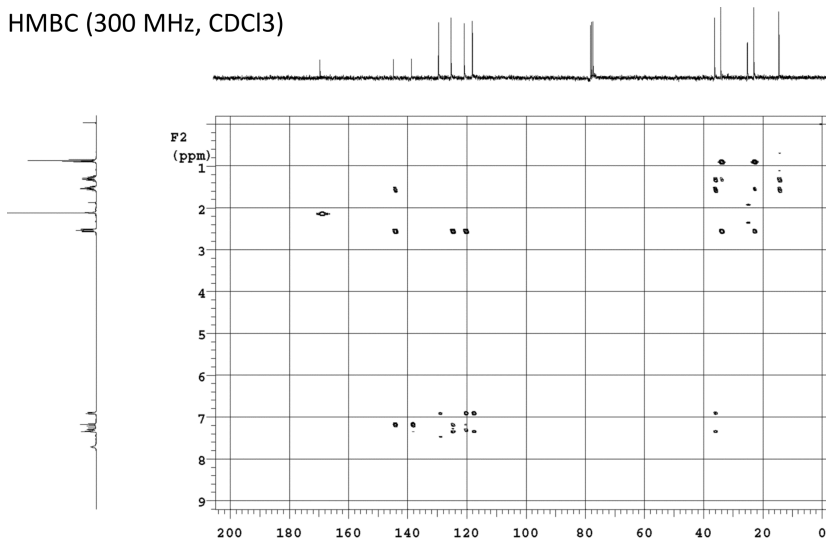
Task 3: $C_{12}H_{17}NO$ - 1H - ^{13}C /HSQC, HMBC

HSQC (300 MHz, $CDCl_3$)

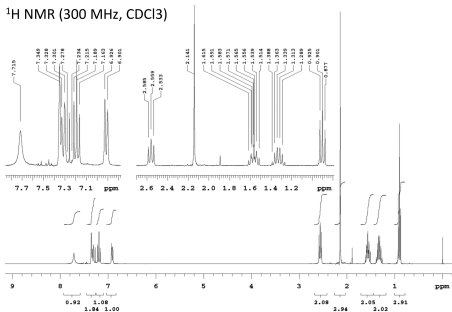


Task 3: $C_{12}H_{17}NO$ - 1H - ^{13}C /HSQC, HMBC

HMBC (300 MHz, $CDCl_3$)



^1H NMR (300 MHz, CDCl_3)



COSY (300 MHz, CDCl_3)

