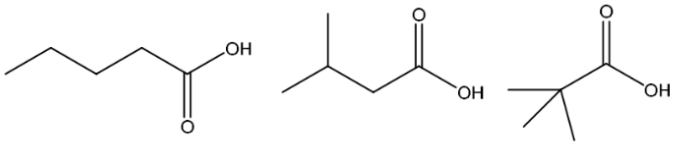
1. 9701/42/O/N/16 Q8b

8(b)(i)



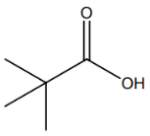
2 correct = 1 mark
3 correct = 2 marks

2

8(b)(ii) 2-methyl butanoic acid

1 **1**

8(c)(i)



1 **1**

8(c)(ii)

δ/ppm	environment of the carbon atom	hybridisation of the carbon atom
27	alkyl / CH_3	sp^3
41	next to carboxyl / $(CH_3)_3\underline{\mathbf{C}}$	sp^3
179	carboxyl / CO_2H	sp^2

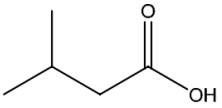
2

8(d)(i)

δ/ppm	type of proton	number of protons	splitting
0.9	alkane / CH / CH_3	6	doublet
1.6	alkane / CH	1	***[multiplet]***
2.4	alkyl next to C = O / $CH_{(2)}CO$ / CH	2	doublet
11.5	OH / CO_2H / carboxylic acid	1	singlet

4

8(d)(ii)

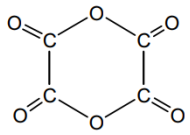


1 **1**

8(e) $CDCl_3$ **OR** D_2O, DMSO, CD_2Cl_2, CCl_4

1 **1**

2. 9701/41/M/J/16 Q2c

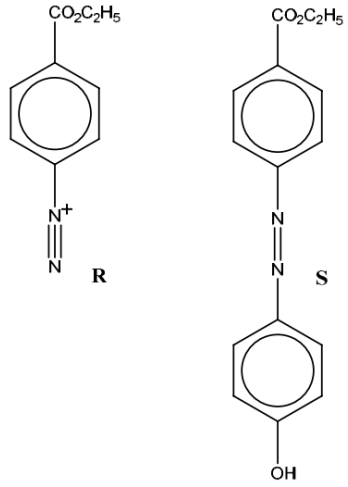
(c) (i)	CH_3 at δ 15 CH_2O at δ 65	[1] [1]
(ii)	Only one peak, so only one type / environment of C atom	[1]
(d) (i)	**M** is $HO_2C–CO_2H$ **N** is $CH_3OCO–CO_2H$ **O** is $CH_3OCO–COOCH_3$	[3]
(ii)	**L** is 	[1]

3. 9701/42/M/J/16 Q6b

(b) (i)	δ 26 is **C**H3-CO δ 52 is **C**H3-O δ 169 is CH3**CO** δ 167 is phenyl-**C**O Phenyl ethanoate is **B** methyl benzoate is **A** M1 = any two correct δ linked to phenylethanoate / methyl benzoate M2 = the rest correct	2
(ii)	heat with H_3O^+ (to hydrolyse the ester) then add Br_2(aq) / bromine water decolourises/gives white ppt. (with phenol from **B**)	3

4. 9701/41/O/N/17 Q6d

6(d)(i)	7 peaks	**1**
6(d)(ii)	$CDCl_3$ will produce no signal in the spectrum **or** $CHCl_3$ would produce a signal / would be detected	**1**
6(d)(iii)	<table><tr><th>*δ/ppm*</th><th>group responsible for the peak</th><th>number of H atoms responsible for the peak</th><th>splitting pattern</th></tr><tr><td>*1.2*</td><td>$CH_{(3)}$</td><td>3</td><td>triplet</td></tr><tr><td>*3.5*</td><td>$CH_{(2)}O$</td><td>2</td><td>quartet</td></tr><tr><td>*5.5*</td><td>NH_2</td><td>2</td><td>singlet (broad)</td></tr><tr><td>*7.1–7.4*</td><td>H attached to aromatic / benzene ring</td><td>4</td><td>*multiplet*</td></tr></table>	**4**
6(d)(iv)	neighbouring / adjacent carbon **atom** has two protons / H (attached to it) **or** there is an adjacent CH_2(O) group	**1**
6(d)(v)	peak at 5.5 / NH_2 peak will disappear **and** NH_2 / protons exchange / swap with deuterium	**1**

6(e)(i)	$NaNO_2 + HCl$ ***or*** HNO_2	**1**
6(e)(ii)		
	structure of diazonium salt **R**	**1**
	structure of azo dye **S**	**1**

5. 9701/42/O/N/17 Q3c

3(c)(ii)	5 or 6 peaks	**1**
	OH/NH protons exchange with deuterium ***or*** –OH / –NH + D_2O → –OD / –ND + DHO	**1**

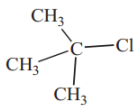
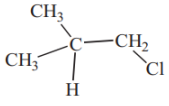
6. 9701/41/M/J/17 Q6d

6(d)(i)

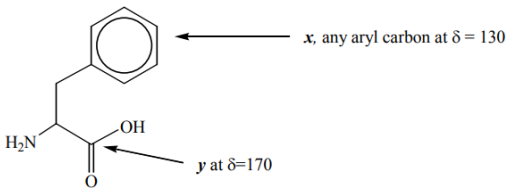
δ value	number of H atoms	group	splitting	result with D_2O
1.4	**3**	**CH_3 / methyl**	**doublet**	**peak remains**
2.7	**1**	**OH / hydroxyl / alcohol**	**singlet**	**peak disappears**
4.0	**1**	**CH**	**quartet**	**peak remains**

the three groups are in their correct places wrt the δ values	**1**
no. of H atoms for each peak agrees with group column	**1**
splitting patterns doublet, singlet and quartet are assigned to correct groups	**1**
peak identified as OH disappears with D_2O, no other peak disappears	**1**

7. 9701/42/M/J/17 Q2e

2(e)(i)	**4** peaks	**1**
2(e)(ii)	 	**1 + 1**
	number of peaks = 2 number of peaks = 3	**1**

8. 9701/42/F/M/17 Q7e

7(e)(i)	seven	**1**
7(e)(ii)		**1**

9. 9701/41/O/N/18 Q5a(i)

5(a)(i)	[1] for each correct answer number of peaks **F** 3 **G** 6	**2**

10. 9701/41/M/J/18 Q7e

7(e)(i)	propanoic acid	**1**
7(e)(ii)	propan-1-ol would have peak at 0.5–6.0 because of OH group	**1**
	propanal would have peak at 9.3–10.5 because of CHO / aldehyde	**1**

11. 9701/42/M/J/18 Q8d

8(d)(i)	4	**1**
8(d)(ii)	range δ 25–5	**1**
	range δ 190–220	**1**
	one peak in first range and three peaks in second range	**1**
8(d)(iii)	1	**1**
8(d)(iv)	singlet	**1**
	neighbouring / adjacent (carbon) atom has no protons / H	**1**

12. 9701/41/O/N/19 Q4d

4(d)(iv)	6	**1**
4(d)(v)	• 25–50 • 110–160 • 190–220 Award 1 mark for two points, award 2 marks for three points	**2**

13. 9701/41/O/N/19 Q9c

9(c)(i)	2 [1]	**1**
9(c)(ii)	CH_2 next to ester **and** terminal CH_3 are circled [1]	**1**
9(c)(iii)	• one less peak • the lost peak is NH_2 / aryl amine • protons exchange with D **OR** protons are labile **OR** valid equation •✓✓ for two marks [2]	**2**

14. 9701/42/O/N/19 Q8g

8(g)(i)	**M1:** δ12.7 is COOH **M2:** δ3.3 is CH **and** δ1.1 is CH_3	**2**
8(g)(ii)	quadruplet / quartet 3 H / protons on neighbouring / adjacent carbon / carbons / C	**1**
8(g)(iii)	2 (butanedioic acid) and 3 (methylpropanedioic acid)	**1**

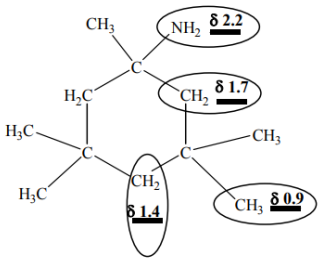
15. 9701/41/M/J/19 Q8b

8(b)	TMS: Reference $CDCl_3$: Solvent	**1**
8(c)(i)	**M1**: CH_3CO **M2**: CH_3CH_2O **M3**: $(CO)CH_2O$	**3**
8(c)(ii)	$CH_3COCH_2OCH_2CH_3$	**1**
8(d)	$HCO_2C(CH_3)_3$	**1**
8(e)(i)	this is a (carbon) atom which has four different atoms or groups attached to it	**1**
8(e)(ii)	$CH_3CH_2CH(CH_3)COOH$	**1**

16. 9701/42/M/J/19 Q8

8(a)	4-chloro-3,5-dimethylphenol **OR** 3,5-dimethyl-4-chlorophenol [1] **ALLOW** 2,6-dimethyl-4-hydroxychlorobenzene and 2-chloro-5-hydroxy-1,3-dimethylbenzene	**1**
8(b)(i)	carbon-13 NMR = 5 peaks [1] proton NMR = 3 peaks [1]	**2**
8(b)(ii)	**OH** proton had disappeared due to proton exchange with D / D_2O [1] **ALLOW** $OH + D_2O \rightarrow OD + HOD$	**1**

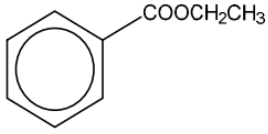
17. 9701/42/F/M/19 Q6c

6(c)(i)	six	1
6(c)(ii)	**M1** peak at δ 0.9 is due to **12 H** **M2** peak at 2.2 is due to **2 H** **M3/M4** peaks at 1.2, 1.4 and 1.7 are **all singlets**	4
6(c)(iii)		2
6(c)(iv)	NH / NH_2 protons **AND** exchange with D_2O / D OR $–NH_2 + D_2O \rightarrow –ND_2 + H_2O$	1

18. 9701/41/O/N/20 Q8b(iv)

8(b)(iv)	5 / five [1]	1

19. 9701/41/O/N/20 Q9

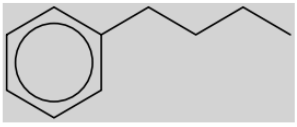
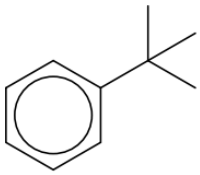
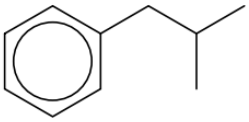
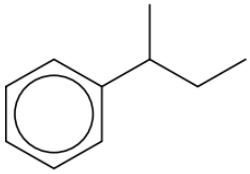
9(a)	(because $CDCl_3$ / it) does not give a peak [1] **OR** because $CHCl_3$ does give a peak	1
9(b)	as a **standard / reference** for (chemical shift measurements) [1]	1
9(c)	ester [1]	1
9(d)(i)	• (δ = 1.4) triplet • (δ = 1.4) two H on neighbouring C atom • (δ = 4.3) quartet / quadruplet • (δ = 4.3) three H on neighbouring C atom mark as • ✓ • ✓ [2]	2
9(d)(ii)	aryl group / arene / phenyl [1]	1
9(d)(iii)	 **OR** $C_6H_5CO_2C_2H_5$ [1]	1

20. 9701/42/O/N/20 Q6d

6(d)(ii)	Clockwise from left: absorption at σ = 1.9 to 2.1 absorption at σ = 6.5 to 7 [1] absorption at σ = 3 to 3.5 absorption at σ = 1 to 1.5 [1]	2
6(d)(iii)	the peak at 6.6 to 6.8 / due to NH would disappear [1] H exchanges with D [1]	2

6(f)(i)	$LiAlH_4$ [1]	1
6(f)(ii)	2 [1]	1

21. 9701/41/M/J/20 Q6c

5(c)(i)	$CH_3CH_2CH^+CH_3$ $(CH_3)_2CHCH_2^+$ $(CH_3)_3C^+$ Each correct structure = 1 mark	3
5(c)(ii)	 number of peaks in carbon-13 NMR = 8  number of peaks in carbon-13 NMR = 6  number of peaks in carbon-13 NMR = 7  number of peaks in carbon-13 NMR = 8 Two correct organic products = 1 mark three correct organic products = 2 marks all products linked correctly to NMR = 2 marks	4

22. 9701/41/M/J/20 Q6d

6(d)	<table><tr><th>chemical shift (δ)</th><th>environment of the carbon atom</th><th>hybridisation of the carbon atom</th></tr><tr><td>27</td><td>**C**H_3 circled</td><td>sp^3</td></tr><tr><td>163</td><td>**C**OOH circled</td><td>sp^2</td></tr><tr><td>192</td><td>**C**=O(COOH) circled</td><td>sp^2</td></tr></table> Award one mark for each correct column	2
6(e)	<table><tr><th>chemical shift (δ)</th><th>group responsible for the peak</th><th>splitting pattern</th><th>number of ^1H atoms responsible for the peak</th></tr><tr><td>1.3</td><td>alkane / CH / CH_3</td><td>triplet</td><td>3</td></tr><tr><td>2.2</td><td>CH_3CO **or** alkyl / CH next to C=O</td><td>singlet</td><td>3</td></tr><tr><td>4.0</td><td>CH_2O **or** alkyl / CH next to electronegative atom / C=O</td><td>quartet / quadruplet</td><td>2</td></tr></table> Award one mark for every three correct responses.	3
6(f)	CH **AND** CH_3 **circled** these protons do not exchange with D_2O **OR** OH and NH protons exchange with D_2O	2

23. 9701/42/M/J/20 Q5e

<table>
<tr><td>5(e)(i)</td><td>5 peaks</td><td>1</td></tr>
<tr><td>5(e)(ii)</td><td>
<table>
<tr><th>environment of carbon atom</th><th>chemical shift range (δ)</th></tr>
<tr><td>carbonyl / RCOR</td><td>190–220</td></tr>
<tr><td>arene / benzene</td><td>110–160</td></tr>
</table>
Award one mark for each correct for each row
</td><td>2</td></tr>
</table>

24. 9701/42/F/M/20 Q5d

<table>
<tr><td>5(d)(i)</td><td>5</td><td>1</td></tr>
<tr><td>5(d)(ii)</td><td>M1 only one peak
M2 singlet at δ 6.0–9.0 ppm

OR

M1 singlet(s) only
M2 only one peak at δ 6.0–9.0 ppm</td><td>2</td></tr>
</table>

25. 9701/41/O/N/21 Q7a

<table>
<tr><td>7(a)</td><td>6 [1]</td><td>1</td></tr>
</table>

26. 9701/41/O/N/21 Q9e

<table>
<tr><td>9(e)(i)</td><td>a [1]</td><td>1</td></tr>
<tr><td>9(e)(iii)</td><td>d [1]</td><td>1</td></tr>
<tr><td>9(e)(iii)</td><td>b, c, f [1]</td><td>1</td></tr>
<tr><td>9(e)(iv)</td><td>f [1]</td><td>1</td></tr>
</table>

27. 9701/42/O/N/21 Q8b

<table>
<tr><td>8(b)</td><td>alanine because glutamic acid would have more than two / three peaks / absorb^{ns} / proton environments [1]

reason why alanine has a doublet given as one neighbouring proton [1]
glutamic acid would have (two) triplet(s) OR a multiplet [1]

reason why alanine has a quartet / quadruplet given as three neighbouring protons [1]</td><td>3</td></tr>
</table>

28. 9701/41/M/J/21 Q6b

6(b)(ii)

compound	number of peaks in proton NMR	number of peaks in carbon-13 NMR
HCO_2H	2	1
HO_2CCO_2H	1	1
$HO_2CCH_2CH_2CO_2H$	2	2

one mark for three, four or five correct
two marks for six correct

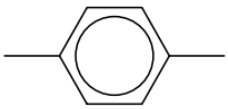
2

6(b)(iii) OH peak disappears **AND** proton / H exchanges with deuterium **1**

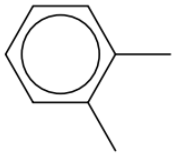
29. 9701/42/M/J/21 Q6

6(a)

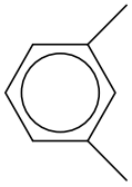
three peaks



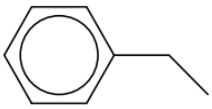
four peaks



five peaks



six peaks

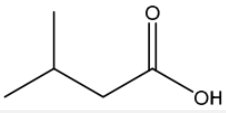


correct isomers and correct assignment to peaks: mark as • ✓ • ✓ • ✓ • ✓

4

30. 9701/42/M/J/21 Q8c

8(c)(i)



1

8(c)(ii)

chemical shift (δ)	environment of proton	splitting pattern (words required)	number of ^1H atoms responsible for the peak
0.95	alkane / CH_3	doublet	6
1.90	alkane / CH **ALLOW** alkyne	multiplet	1
2.20	R / alkyl / CH_2 next to C=O / COOH	doublet	2

mark as • • ✓ • • ✓ • • ✓

3

31. 9701/41/O/N/22 Q9b

9(b)	5 5 5 4 4	**2**
9(c)	4 [1] singlet, (two) triplet(s), multiplet (any order) [1]	**2**
9(d)(i)	**D** = $CH_3CH_2CO_2CH_2CH_3$ [1] **E** = $(CH_3)_2CHCO_2CH_3$	**2**
9(d)(ii)	O-CH_2 **labelled F** **AND** three protons on neighbouring **carbon** / adjacent CH_3	**1**
9(d)(iii)	**both CH_3 in** isopropyl group **labelled G** **AND** alkane / alkyl (protons)	**1**

32. 9701/42/O/N/22 Q8

8(a)	C* marked on CH of T and nowhere else	**1**
8(b)(i)	R – $C_6H_5CH_2COCH_2CH_3$ [1] 3.7 is C_6H_5**CH_2**$COCH_2CH_3$ 2.5 is $C_6H_5CH_2CO$**CH_2**CH_3 1.0 is $C_6H_5CH_2COCH_2$**CH_3** [1]	**2**
8(b)(ii)	singlet **and** no H on neighbouring C	**1**
8(c)(i)	P and T	**1**
8(c)(ii)	P	**1**
8(d)	$CDCl_3$ or CCl_4	**1**
8(e)	no difference **and** no protons that exchange with D	**1**
8(f)	6 5 [1] 4 3 [1]	**2**

33. 9701/41/M/J/22 Q6b

6(b)		carbon-13 NMR	proton NMR
	number of peaks in $CDCl_3$	4	5

1

34. 9701/42/M/J/22 Q7

7(a)	TMS reference **OR** standard **OR** to define d = 0 D_2O solvent **OR** identification of **O-H / N-H** protons / group	**1**

7(b)(i)	<table><tr><th>ketone</th><th>number of peaks observed in proton NMR spectrum</th><th>number of peaks observed in carbon-13 NMR spectrum</th></tr><tr><td>pentan-2-one</td><td>4</td><td>5</td></tr><tr><td>pentan-3-one</td><td>2</td><td>3</td></tr><tr><td>3-methylbutanone</td><td>3</td><td>4</td></tr></table> three for one mark, six for two marks	**2**
7(b)(ii)	**M1** 3-methylbutanone **M2** 3-methylbutanone **AND** pentan-2-one	**2**