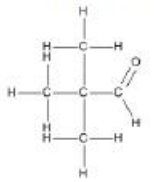
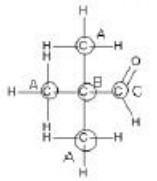
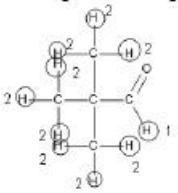
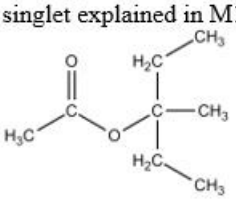
Mark Scheme

Q1.

Question Number	Answer	Additional Guidance	Mark
	An answer that makes reference to the following points: • displayed formula of aldehyde (1) • three different carbon environments indicated (1) • two different proton environments indicated (1) • no splitting as there are no hydrogens on the adjacent carbon atom(s)	Example of displayed formula:  Allow CH_3 groups but aldehyde group must be displayed Example of three carbon environments:  Example of two proton environments:  Stand alone mark	(4)

Q2.

Question Number	Answer	Additional Guidance	Mark
	An answer that makes reference to the following points: **Peak at 2.50 ppm** • identified as C**H**$_3$CO (as relative peak area = 3 / singlet so no protons on adjacent C) **(1)** **Peak at 1.56 ppm** • 2 C**H**$_2$ groups as relative peak area = 4 **(1)** • (the 2 C**H**$_2$ groups / hydrogen environment) next to CH_3 groups as peak is a quartet **(1)** **Peak at 0.92 ppm** • 2 C**H**$_3$ groups as relative peak area = 6 **(1)** • (the 2 C**H**$_3$ groups / hydrogen environment) next to CH_2 groups as peak is a triplet **(1)** **Peak at 1.43 ppm** • C**H**$_3$ group with no protons on adjacent carbon atoms as (relative peak area = 3 and) singlet **(1)** • structure of **Q** **(1)**	Allow credit for annotations on table in p14 and on labelled structures Allow adjacent protons / hydrogens for protons on adjacent C Penalise H^+ for protons once only Allow ester group / H-C-C=O / CH_3 on left of structure given is indicated Do not award if aldehyde / ketone mentioned Allow 4 protons / hydrogens Allow 6 protons / hydrogens Allow just CH_3 identified in M6 if singlet explained in M1 	(7)

Q3.

Acceptable Answers	Additional Guidance	Mark
This question assesses a student's ability to show a coherent and logically structured answer with linkages and fully-sustained reasoning. Marks are awarded for indicative content and for how the answer is structured and shows lines of reasoning. The following table shows how the marks should be awarded for indicative content. Guidance on how the mark scheme should be applied: The mark for indicative content should be added to the mark for lines of reasoning. For example, an answer with five indicative marking points that is partially structured with some linkages and lines of reasoning scores 4 marks (3 marks for indicative content and 1 mark for partial structure and some linkages and lines of reasoning). If there are no linkages between points, the same five indicative marking points would yield an overall score of 3 marks (3 marks for indicative content and no marks for linkages). The following table shows how the marks should be awarded for structure and lines of reasoning.		(6)

Number of indicative marking points seen in answer	Number of marks awarded for indicative marking points
6	4
5-4	3
3-2	2
1	1
0	0

		Number of marks awarded for structure of answer and sustained line of reasoning		
	Answer shows a coherent and logical structure with linkages and fully sustained lines of reasoning demonstrated throughout.	2		
	Answer is partially structured with some linkages and lines of reasoning.	1		
	Answer has no linkages between points and is unstructured.	0		
	Comment: Look for the indicative marking points first, then consider the mark for structure of answer and sustained line of reasoning		In general it would be expected that 5 or 6 indicative points would get 2 reasoning marks, and 3 or 4 indicative points would get 1 mark for reasoning, and 0, 1 or 2 indicative points would score zero marks for reasoning.	

	Indicative content • **IP1 -** Similarity **both** ^{1}H NMR spectra have a peak (which is a singlet with relative peak area 1) for OH • **IP2 -** ^{13}C spectra 3 peaks for propan-1-ol **and** 2 peaks for propan-2-ol	**General points to note** If there is any incorrect chemistry, deduct mark(s) from the reasoning. If no reasoning mark(s) awarded do not deduct mark(s). e.g. Mention of splitting on the ^{13}C spectra Deduct 1 reasoning mark if the similarity in IP1 has not been explicitly mentioned All IP can be shown on clearly labelled diagrams of structures and/or spectra Allow carbon environments for peaks Ignore any reference to peak areas	

	• **IP3 -** ^{1}H spectra number of peaks 4 peaks for propan-1-ol **and** 3 peaks for propan-2-ol		
	• **IP4 -** ^{1}H spectra relative peak areas (relative) peak areas 3 : 2 : 2 : 1 for propan-1-ol, 6 : 1 : 1 for propan-2-ol	Allow ratios in any order e.g. 1 : 2 : 2 :3	
	• **IP5 -** ^{1}H splitting pattern for propan-1-ol 2 triplets, 1 sextet / split into 6 and 1 singlet	Allow hextet for sextet Ignore missing singlet if this has been given in similarity	
	• **IP6 -** ^{1}H splitting pattern for propan-2-ol 1 doublet, 1 septet / split into 7 and 1 singlet	Allow heptet for septet Ignore missing singlet if this has been given in similarity	

Q4.

Question Number	Answer	Mark
(i)	**The only correct answer is B** (alkaline iodine solution) ***A*** *is not correct because this oxidising agent would react with phenylethanal and not with phenylethanone which is the wrong way round* ***C*** *is not correct because test is for aldehydes and so would react with phenylethanal and not with phenylethanone which is the wrong way round* ***D*** *is not correct because test is for aldehydes and so would react with phenylethanal and not with phenylethanone which is the wrong way round*	**(1)**

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Question Number	Answer	Additional Guidance	Mark
(ii)	An answer that makes reference to the following points: • formation of yellow/orange/red (crystalline) precipitate **(1)** • (Filter then) recrystallisation of products **(1)** • determination of melting temperature **(1)** • comparison (and hence identification) from use of database/known values **(1)**	Colour and state are both required Allow solid for ppt Ignore any conditions given with the use of 2,4-DNPH Penalise M3 if any reference to boiling temperature Award only in the context of melting temperature of the hydrazones or as a TE of boiling temperature Max 3 out of 4 if test is only carried out with one of the carbonyls	**(4)**

<table>
<tr><th>Question Number</th><th>Answer</th><th>Additional Guidance</th><th>Mark</th></tr>
<tr>
<td>* (iii)</td>
<td>
This question assesses the student's ability to show a coherent and logically structured answer with linkages and fully sustained reasoning.

Marks are awarded for indicative content and for how the answer is structured and shows lines of reasoning.

The following table shows how the marks should be awarded for indicative content.
<table>
<tr><th>Number of indicative marking points seen in answer</th><th>Number of marks awarded for indicative marking points</th></tr>
<tr><td>6</td><td>4</td></tr>
<tr><td>5-4</td><td>3</td></tr>
<tr><td>3-2</td><td>2</td></tr>
<tr><td>1</td><td>1</td></tr>
<tr><td>0</td><td>0</td></tr>
</table>

The following table shows how the marks should be awarded for structure and lines of reasoning
<table>
<tr><th></th><th>Number of marks awarded for structure of answer and sustained lines of reasoning</th></tr>
<tr><td>Answer shows a coherent logical structure with linkages and fully sustained lines of reasoning demonstrated throughout</td><td>2</td></tr>
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</table>
</td>
<td>
Guidance on how the mark scheme should be applied: The mark for indicative content should be added to the mark for lines of reasoning. For example, a response with four indicative marking points that is partially structured with some linkages and lines of reasoning scores 4 marks (3 marks for indicative content and 1 mark for partial structure and some linkages and lines of reasoning).
If there were no linkages between the points, then the same indicative marking points would yield and overall score of 3 marks (3 marks for indicative content and zero marks for linkages).

In general it would be expected that 5 or 6 indicative points would get 2 reasoning marks, and 3 or 4 indicative points would get 1 mark for reasoning, and 0, 1 or 2 indicative points would score zero marks for reasoning. If there is any incorrect chemistry, deduct mark(s) from the reasoning. If no reasoning mark(s) awarded do not deduct mark(s).

If there is no mention of protons/hydrogens in the response then deduct one structure and reasoning mark
</td>
<td>(6)</td>
</tr>
</table>

	Indicative content **Similarities** • **IP1**: aromatic hydrogens will give similar/same peaks • **IP2**: both have a peak in the range 1.7-3.0 (ppm) (due to the hydrogen of the H–C–C=O type) **Differences** • **IP3** (Hydrogen environments): Phenylethanone has one less peak/hydrogen environment than phenylethanal • **IP4** (Splitting patterns): a singlet for phenylethanone but a doublet and a triplet in phenylethanal • **IP5** (Peak area ratios): relative peak (area) ratio in phenylethanone is 3 but in phenylethanal the peak (area) ratio is 2 to 1 • **IP6** (Chemical shifts): (Only) phenylethanal has an aldehyde (hydrogen) peak in the range 9 – 10.1 (ppm)	Ignore references to C^{13} nmr Accept annotations on a structure towards crediting the following IPs Allow either a single chemical shift value or a range within the stated values Penalise incorrect chemical shifts Both have peaks in the range 6.5-8.4 (ppm) Ignore any splitting description Ignore any splitting pattern given for this peak to award this mark Allow any difference of one in the number of peaks stated All these splitting patterns required for this IP Ignore the splitting pattern for this IP and ignore any peak areas given for the aryl hydrogens Ignore the splitting pattern for this IP	

Q5.

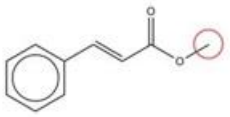
Question Number	Answer	Mark
	The only correct answer is C (6 ..... 7) ***A*** *is not correct because there are six non-equivalent carbons in isoamyl acetate and seven in amyl acetate* ***B*** *is not correct because all carbons of amyl acetate generate their own peak in the spectrum* ***D*** *is not correct because the two methyl groups on the branched chain are equivalent*	**(1)**

Q6.

Question Number	Answer	Mark
	The only correct answer is B (6) ***A*** *is not correct because four carbon atoms in the aromatic ring are non-equivalent and not just three, so the correct total of non-equivalent carbon atoms and therefore peaks is six* ***C*** *is not correct because there are two sets of equivalent carbon atoms in the aromatic ring and not just one which means that the correct total of non-equivalent carbon atoms and therefore peaks is six* ***D*** *is not correct because this is the total number of carbon atoms in antifebrin but carbon atoms 2 and 6 in the aromatic ring are equivalent, as are 3 and 5, which gives a correct total of six non-equivalent carbon atoms and therefore six peaks*	**(1)**

Q7.

Question Number	Answer	Additional Guidance	Mark
(i)	An answer that makes reference to the following points: • peak due to tetramethylsilane (1) • so (chemical) shifts (due to other hydrogen atoms) can be compared (1)	 Allow TMS / $Si(CH_3)_4$ Name must be correct if given Allow "a reference" / "a standard" "calibration" Ignore "to allow other molecules to be compared"	(2)

Question Number	Answer	Additional Guidance	Mark
(ii)	An answer that makes reference to the following points: • **M1** circle around $–CH_3$ group in $-OCH_3$ (1) • **M2** singlet as no neighbouring hydrogen atoms (1) • **M3** peak area of 3 means there are 3 hydrogen atoms in this environment (1)	Allow 'protons' for hydrogen atoms  Award whole $-OCH_3$ circled Do not award if C=O included in circle M1 is a stand alone mark Award "has no adjacent hydrogen atoms" Award "no hydrogens on adjacent carbon" Ignore "there is no adjacent C atom" Award "(relative) peak area of three for a $–CH_3$ group" For M3 must relate to (relative) peak area / integral Ignore references to chemical shift value for ester δ = 3.0 to 4.0 (ppm) Ignore references to relative heights of peaks **Comment** M2 and / or M3 dependent on $-CH_3$ group being included in the circled group	(3)

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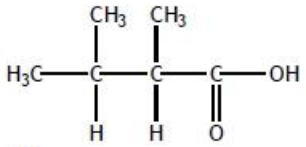
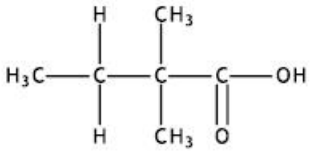
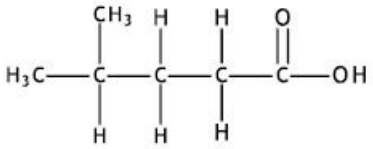
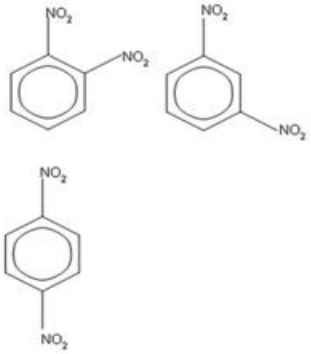
Q8.

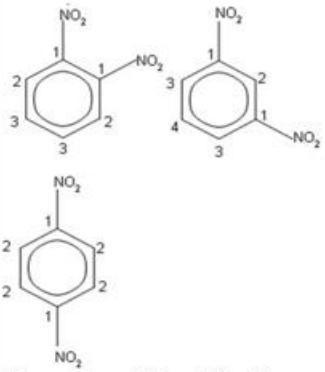
Question Number	Acceptable Answers	Additional Guidance	Mark
(i)	Any two of the following $(CH_3)_2CHCH(CH_3)COOH$ /  **(1)** $CH_3CH_2C(CH_3)_2COOH$ /  **(1)** $(CH_3)_2CHCH_2CH_2COOH$ /  **(1)**	Allow displayed or skeletal formulae	**(2)**

Question Number	Acceptable Answers	Additional Guidance	Mark
(ii)		Do not award other types of structure	**(1)**

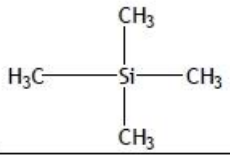
Q9.

Question Number	Acceptable Answers	Additional Guidance	Mark
(i)	$C_6H_4^+$	Allow $H_4C_6^+$ Do not award just C_6H_4	**(1)**

Question Number	Acceptable Answers	Additional Guidance	Mark
(ii)	• 3 correct formulae **(2)**	Examples of formulae  Allow (1) for any 2 correct formulae Allow (2) for three disubstituted benzenes with incorrect substituents / (1) for any two disubstituted benzenes with incorrect substituents Allow incorrectly displayed formulae of NO_2 groups **In (c)(ii) and (iii):** Allow Kekule structures Allow hydrogen atoms shown on benzene Ignore connectivity of NO_2 groups Penalise missing circle in benzene once only	**(2)**

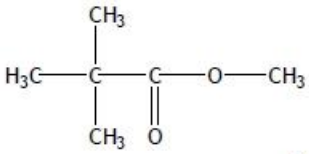
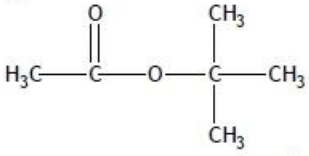
Question Number	Acceptable Answers	Additional Guidance	Mark
(iii)	• **D** identified as 1,3-dinitrobenzene **and** 4 different carbon environments labelled **(1)** • 3 different carbon environments labelled on 1,2-dinitrobenzene **(1)** • 2 different carbon environments labelled on 1,4-dinitrobenzene **(1)**	 Examples of identification These labels may be shown on the structures in (c)(ii) The identification of **D** can be assumed if it is the only structure with 4 carbon environments labelled Allow any form of identification of the carbon environments e.g. numbers, letters, equivalent carbon environments circled TE on disubstituted benzene substituents in (ii) Penalise only half the carbon environments labelled once only	**(3)**

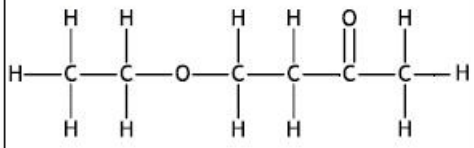
Q10.

Question Number	Acceptable Answers	Additional Guidance	Mark
(i)	$(CH_3)_4Si$	Allow partially or fully displayed formula Ignore connectivity 	**(1)**

Question Number	Acceptable Answers	Additional Guidance	Mark
(ii)	An answer that makes reference to any **two** of the following: • single peak / all H or all C in same environment / no splitting pattern **(1)** • (TMS) peak to the right / upfield / out of the way of other peaks / peak doesn't overlap with other peaks **(1)** • (TMS) low boiling temperature / volatile / can be easily removed **(1)** • gives a strong signal so only a small amount needed **(1)**	Allow 12 H or 4 C in the same environment Ignore references to inertness / non-toxicity / cost / non-polar(ity) Ignore chemical shift = 0 12 H / 4 C are equivalent so gives a strong signal scores 2 marks	**(2)**

Q11.

Question Number	Acceptable Answers	Additional Guidance	Mark
(i)	$C(CH_3)_3COOCH_3$ **or**  **(1)** $CH_3COOC(CH_3)_3$ **or**  **(1)**	Allow displayed or skeletal formulae	**(2)**

Question Number	Acceptable Answers	Additional Guidance	Mark
(ii)	An answer that makes reference to the following points: • the chemical shift δ 2.2 identified **(1)** • four remaining chemical shifts identified **(2)** • two splitting patterns given **and** explained **(2)**	$CH_3C{=}O$ / methyl attached to C=O Identifies 2 or 3 chemical shifts correctly scores 1 δ 1.2 3.5 3.8 2.6 (2.2)  1 specific splitting patterns explained scores 1	(5)

Q12.

Question Number	Answer	Additional Guidance	Mark
	• number of peaks in first product (1) • number of peaks in second product (1)	Number of peaks in the ^{13}C NMR spectrum: 4 | 6	(2)

Q13.

Question Number	Answer	Additional Guidance	Mark
(i)	An answer that makes reference to • **(M1)** (similarity) all have arene C–H absorptions Either 3030 (cm^{-1}) **or** 750 and/or 700 (cm^{-1}) **(1)** • **(M2)** only phenol and phenylmethanol have O–H 3750 - 3200 (cm^{-1}) **(1)** • **(M3)** only benzoic acid has O–H 3300 - 2500 (cm^{-1}) **(1)** • **(M4)** only benzoic acid has C=O 1700 - 1680 (cm^{-1}) **(1)** • **(M5)** only phenylmethanol has alkane C–H absorptions either 2962 - 2853 (cm^{-1}) or 1485 - 1365 (cm^{-1}) **(1)**	Bond and wavenumber ranges necessary for each mark Do not award 880/830/780 (cm^{-1}) Do not award –OH / C–OH by penalising once only in M2 and M3 All 5 correct bonds with no wavenumber ranges scores (3) 4 correct etc scores (2) and 3 correct etc scores (1) All 5 correct wavenumber ranges with no bonds or incorrect bonds scores (3) 4 correct etc scores (2) and 3 correct etc scores (1) Penalise any additional peaks once only Ignore references to different fingerprint regions	**(5)**

Question Number	Answer	Additional Guidance	Mark
(ii)	An answer that makes reference to • five peaks (in the ^{13}C NMR spectrum) **(1)** • (four) aromatic peaks within the chemical shift range of 165 - 105 (ppm) **(1)** • (one) peak (for the C-OH) within the chemical shift range of 75 - 55 (ppm) **(1)**	Allow any range within the stated ranges Penalise single values as opposed to ranges once only Accept annotations on diagram Penalise additional peaks once only when three or more types of peak are stated	**(3)**

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Question Number	Answer	Additional Guidance	Mark
(iii)	An answer that makes reference to • suitable formula of fragment ion **(1)** • matching *m*/*z* value **(1)**	Example of a suitable formula $C_6H_5COO^+$ or $C_6H_5CO^+$ Do not award $C_7H_5O_2^+$ or $C_7H_5O^+$ *m*/*z* = 121 or 105 Allow $COOH^+$ (1) Do not award bond to the fragment, e.g. $-COOH^+$ *m*/*z* = 45 (1) No TE on incorrect fragment ions such as CH_3^+	**(2)**