

Electronic Supplementary Data

One-step synthesis of 3-formyl-2-furylcarbinols and elaboration to unprecedented furotropones

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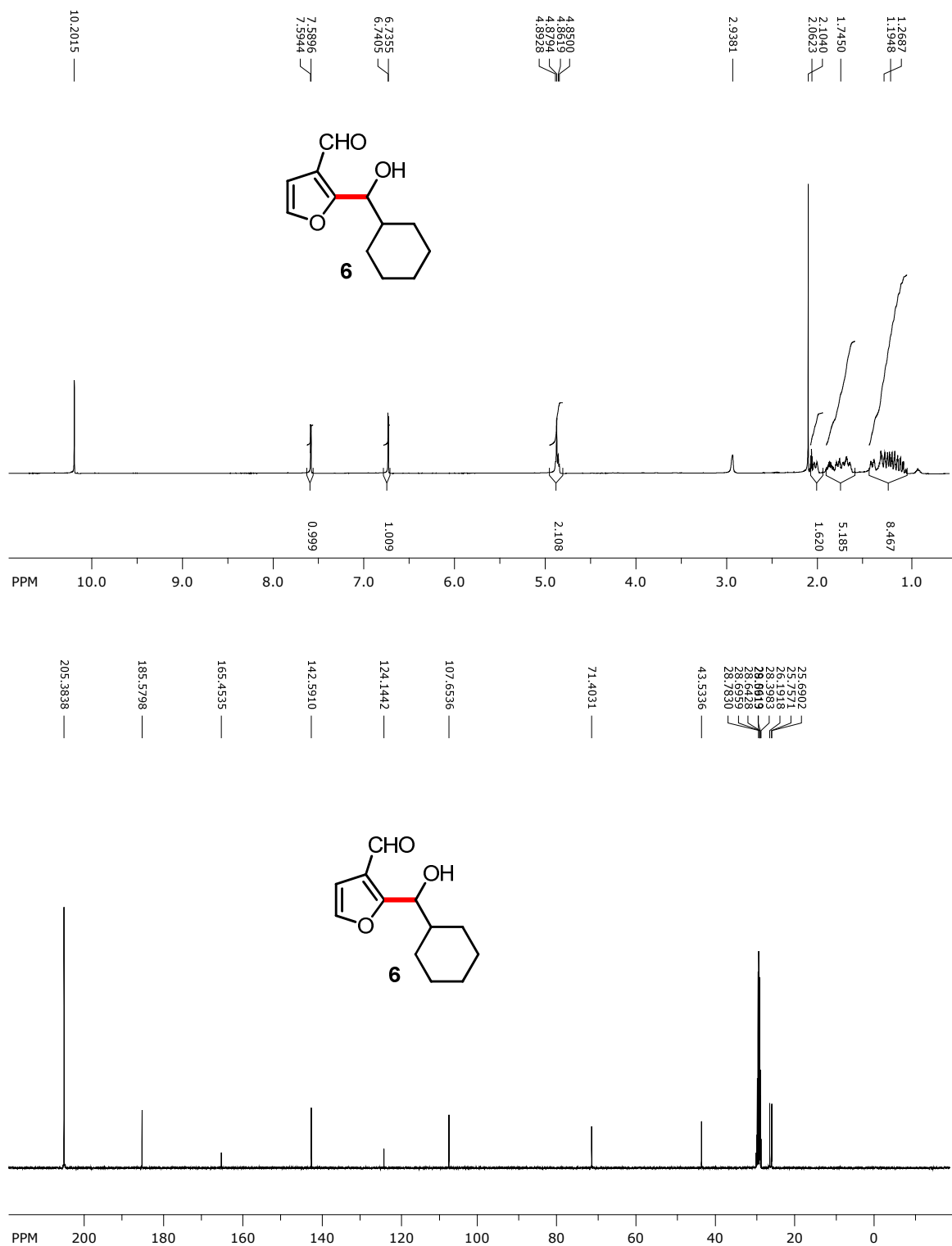


Fig. S1- ¹H and ¹³C-NMR spectra of 2-(cyclohexyl(hydroxy)methyl)furan-3-carbaldehyde (**6**)

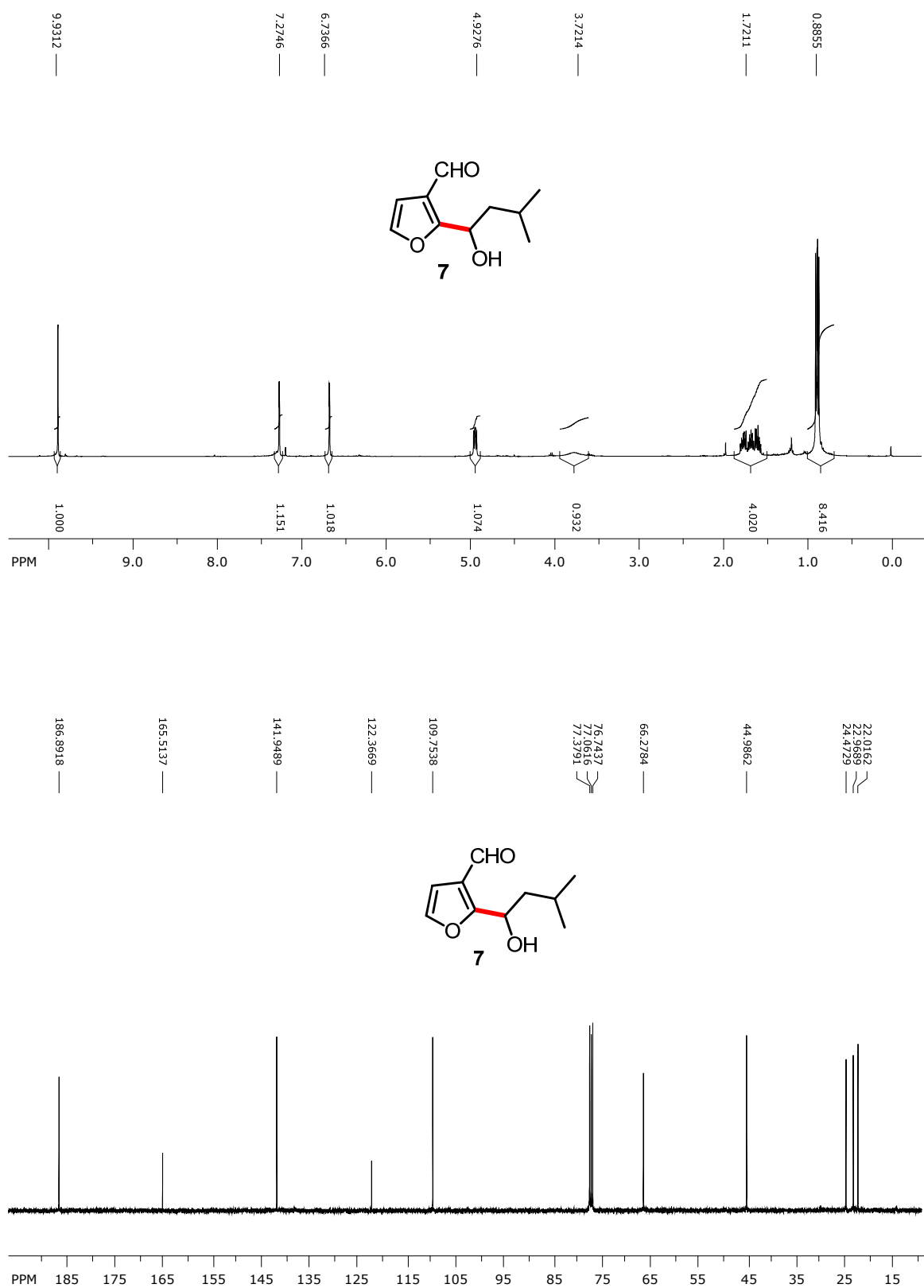


Fig. S2- ¹H and ¹³C-NMR spectra of 2-(1-hydroxy-3-methylbutyl)furan-3-carbaldehyde (**7**).

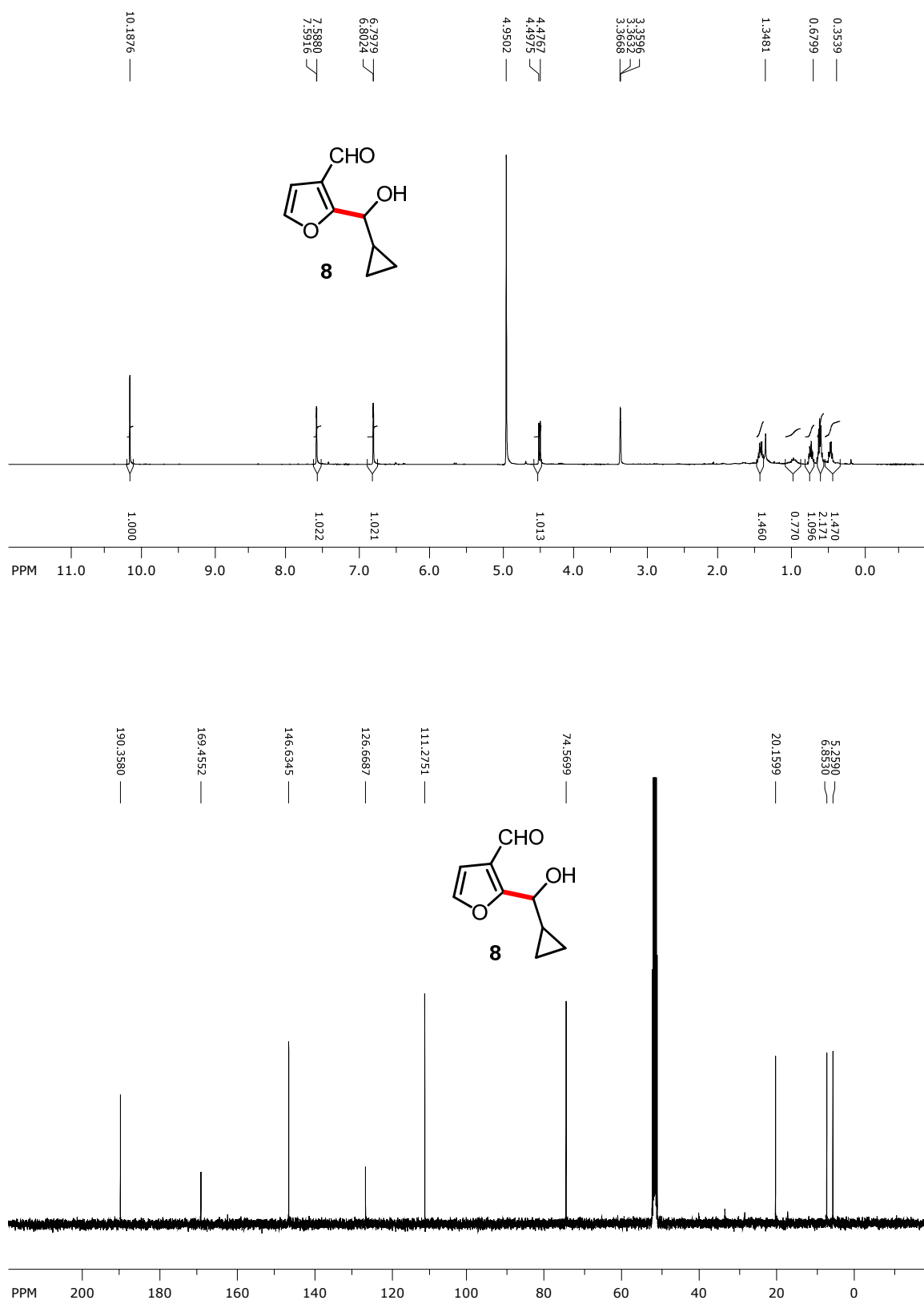


Fig. S3- ¹H and ¹³C-NMR spectra of 2-(cyclopropyl(hydroxy)methyl)furan-3-carbaldehyde (**8**).

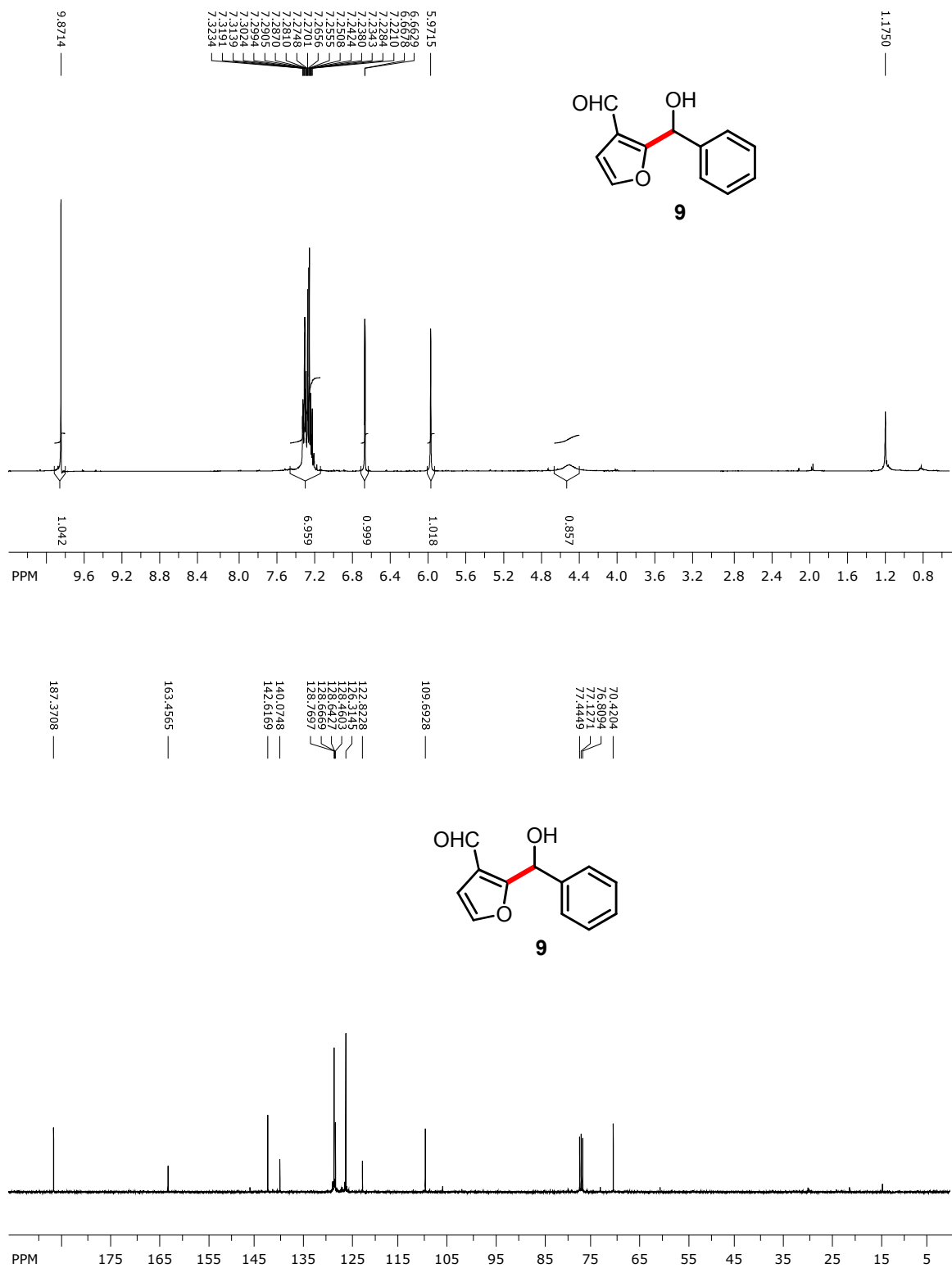


Fig. S4- ¹H and ¹³C-NMR spectra of 2-(hydroxy(phenyl)methyl)furan-3-carbaldehyde (**9**).

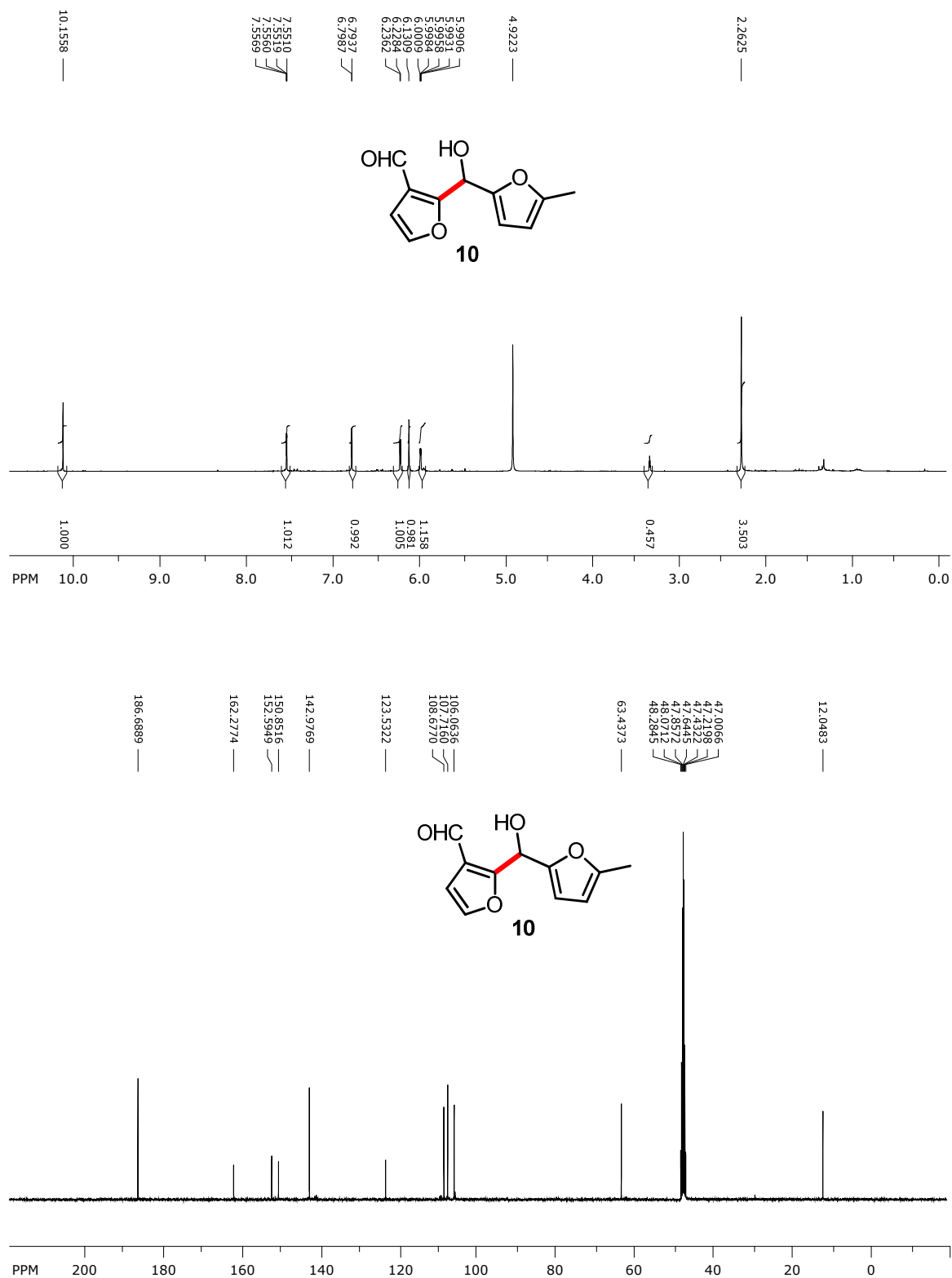


Fig. S5- ¹H and ¹³C-NMR spectra of 2-(hydroxy(5-methylfuran-2-yl)methyl)furan-3-carbaldehyde (**10**).

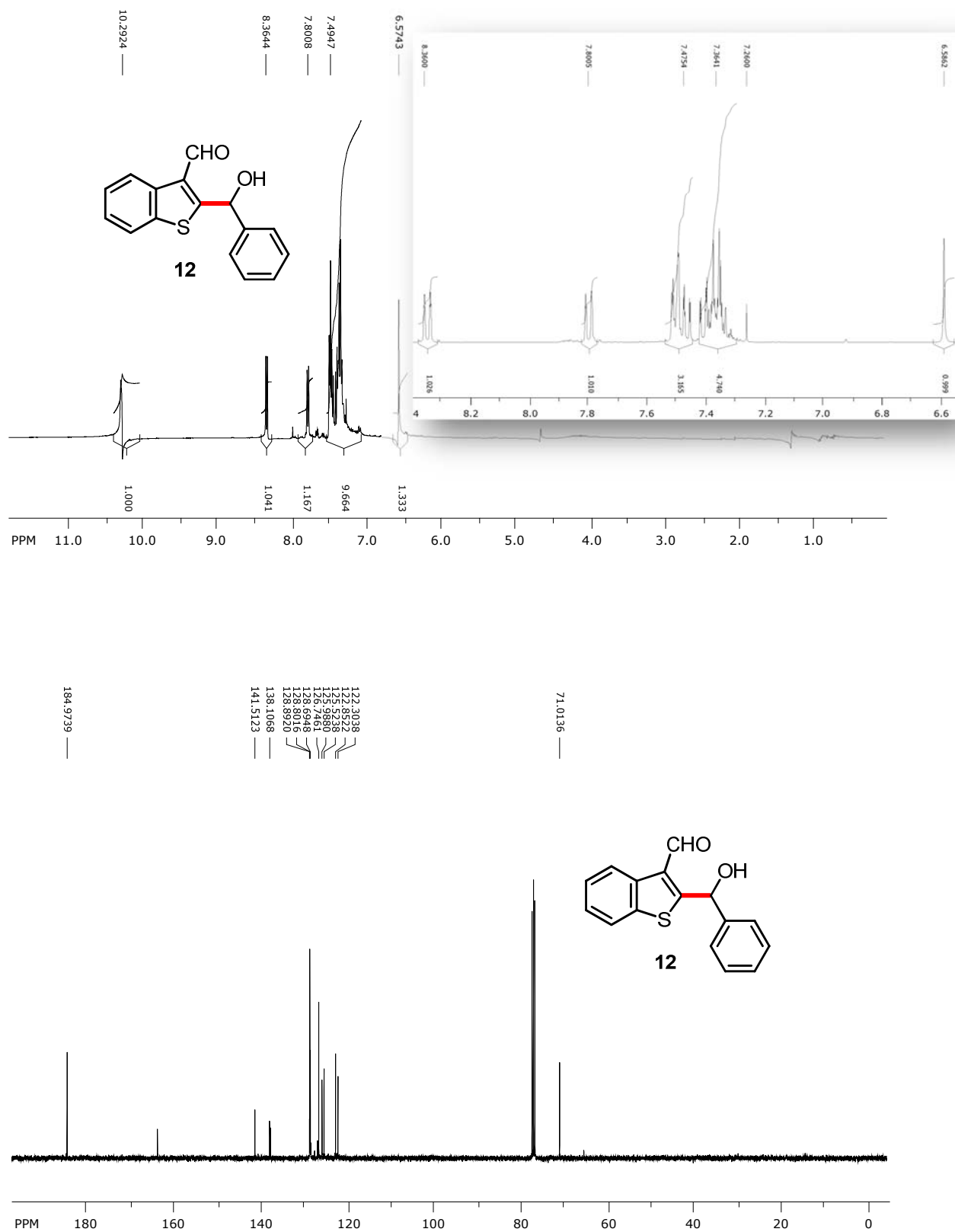


Fig. S7- ¹H and ¹³C-NMR spectra of 2-(hydroxyphenylmethyl)benzo[*b*]thiophene-3-carbaldehyde (**12**).

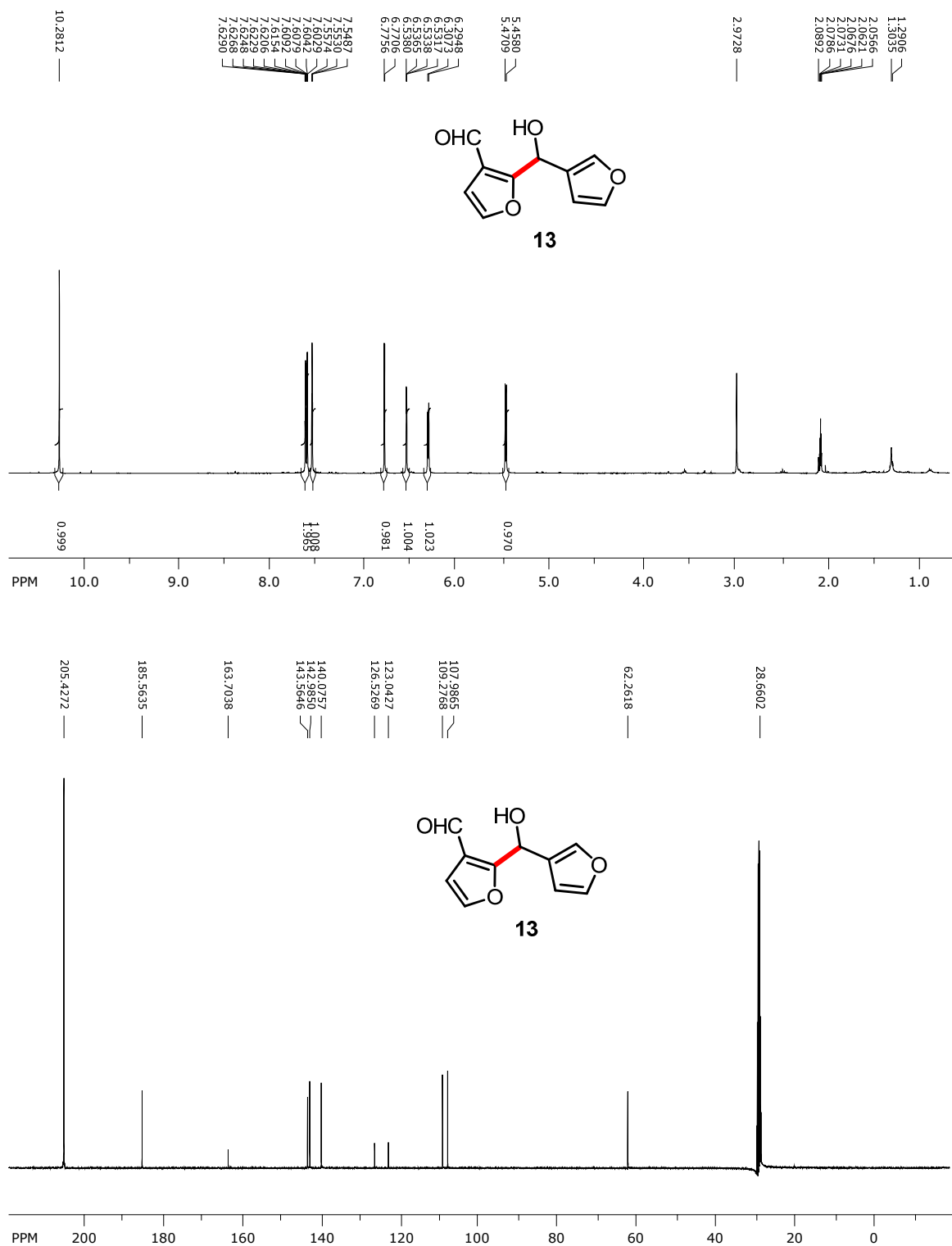


Fig. S8- ¹H and ¹³C-NMR spectra of 2-((furan-3-yl)(hydroxy)methyl)furan-3-carbaldehyde (**13**).

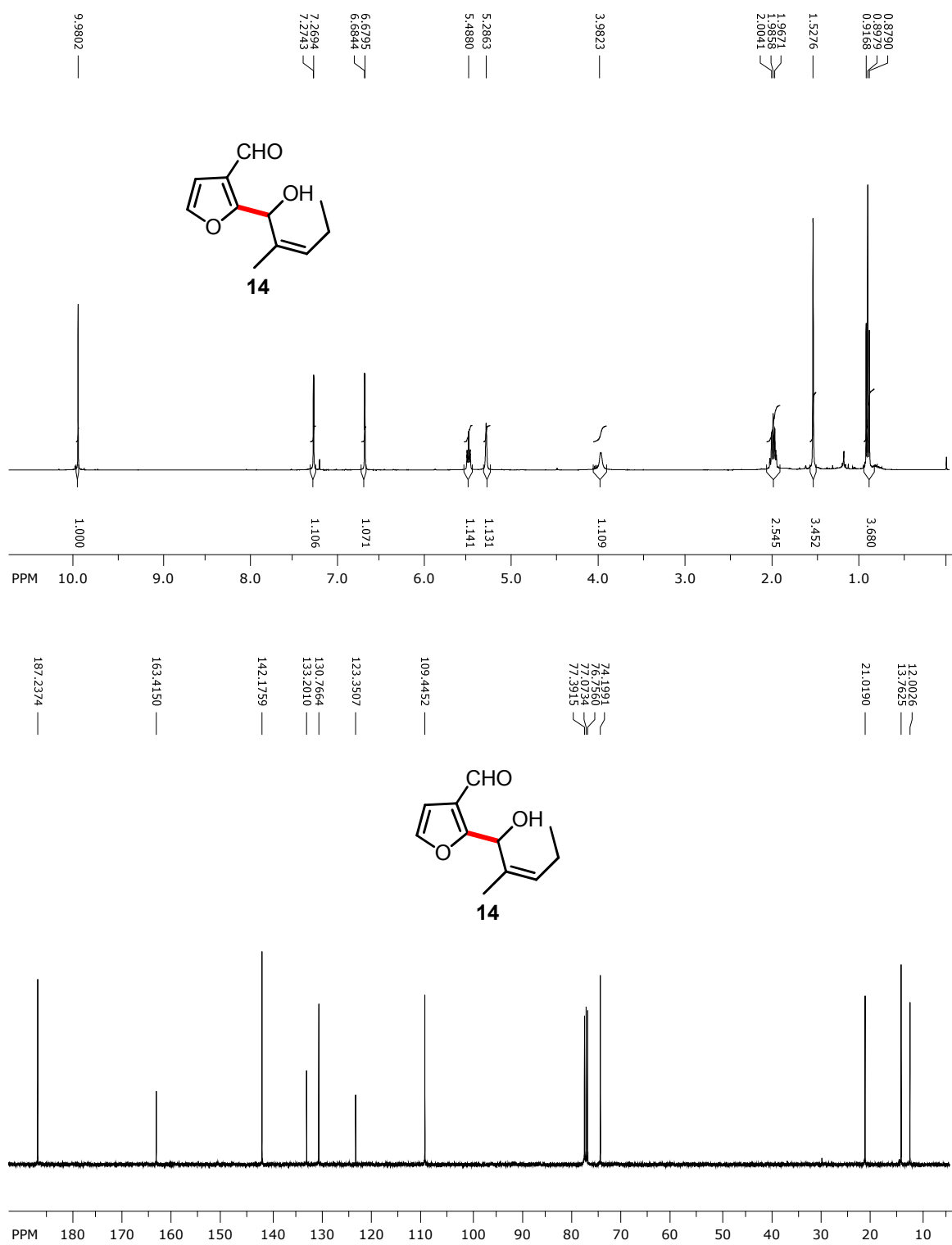


Fig. S9- ¹H and ¹³C-NMR spectra of 2-(1-hydroxy-2-methylpent-2-enyl)furan-3-carbaldehyde (**14**).

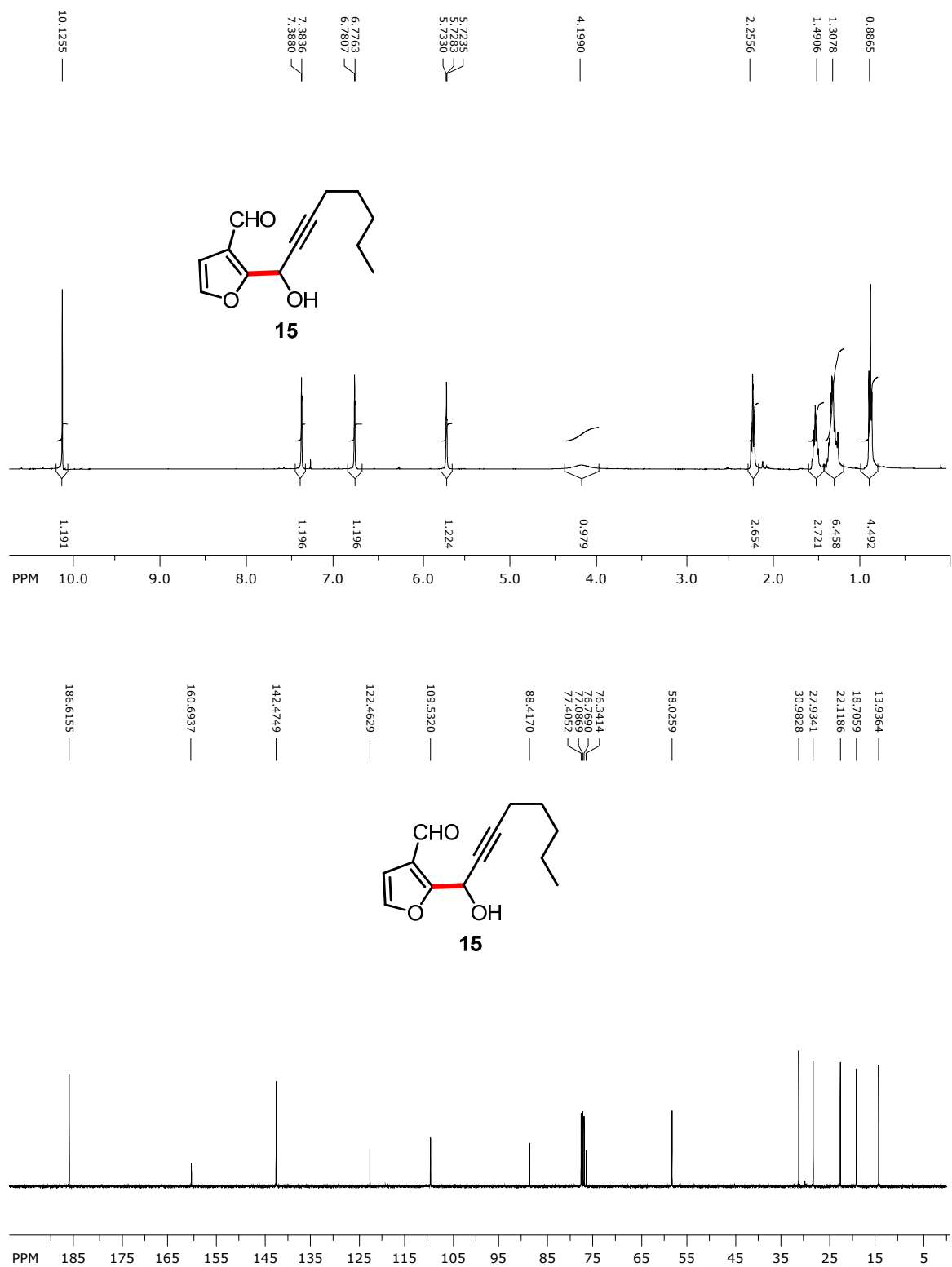


Fig. S10- ¹H and ¹³C-NMR spectra of 2-(1-hydroxyoct-2-ynyl)furan-3-carbaldehyde (**15**).

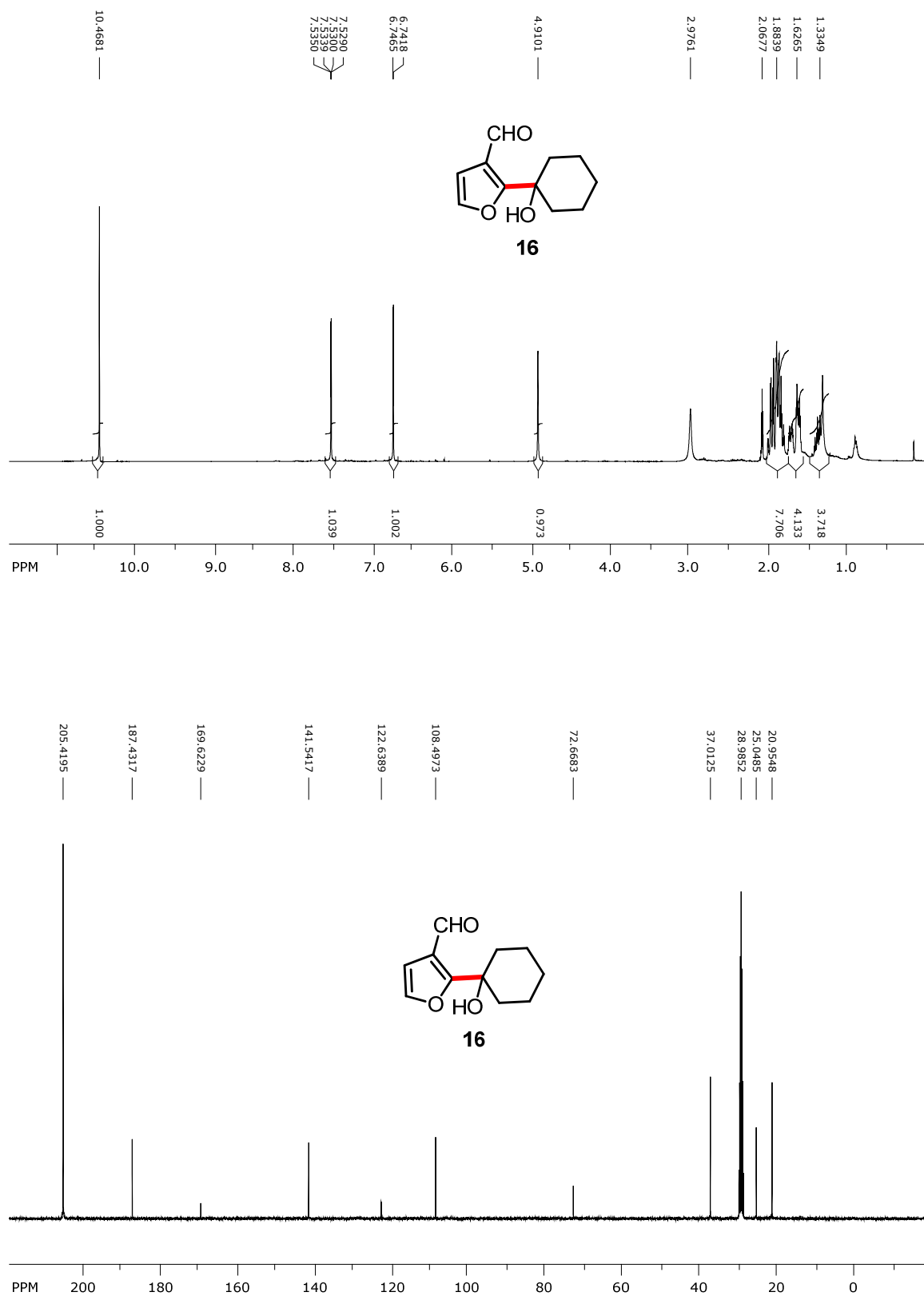


Fig. S11- ¹H and ¹³C-NMR spectra of 2-(1-hydroxycyclohexyl)furan-3-carbaldehyde (**16**).

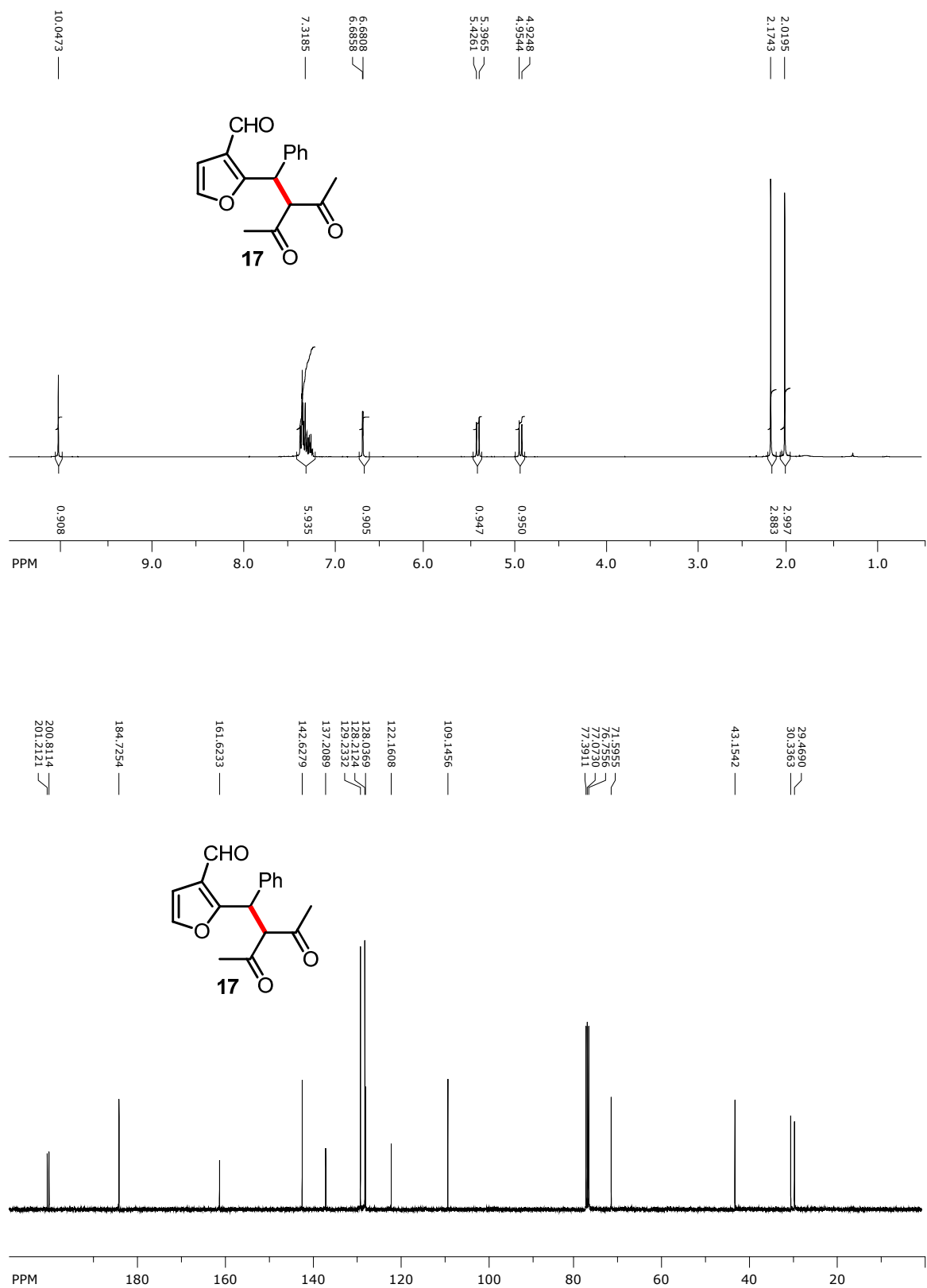


Fig. S12- ¹H and ¹³C-NMR spectra of 2-(2-acetyl-3-oxo-1-phenylbutyl)furan-3-carbaldehyde (**17**).

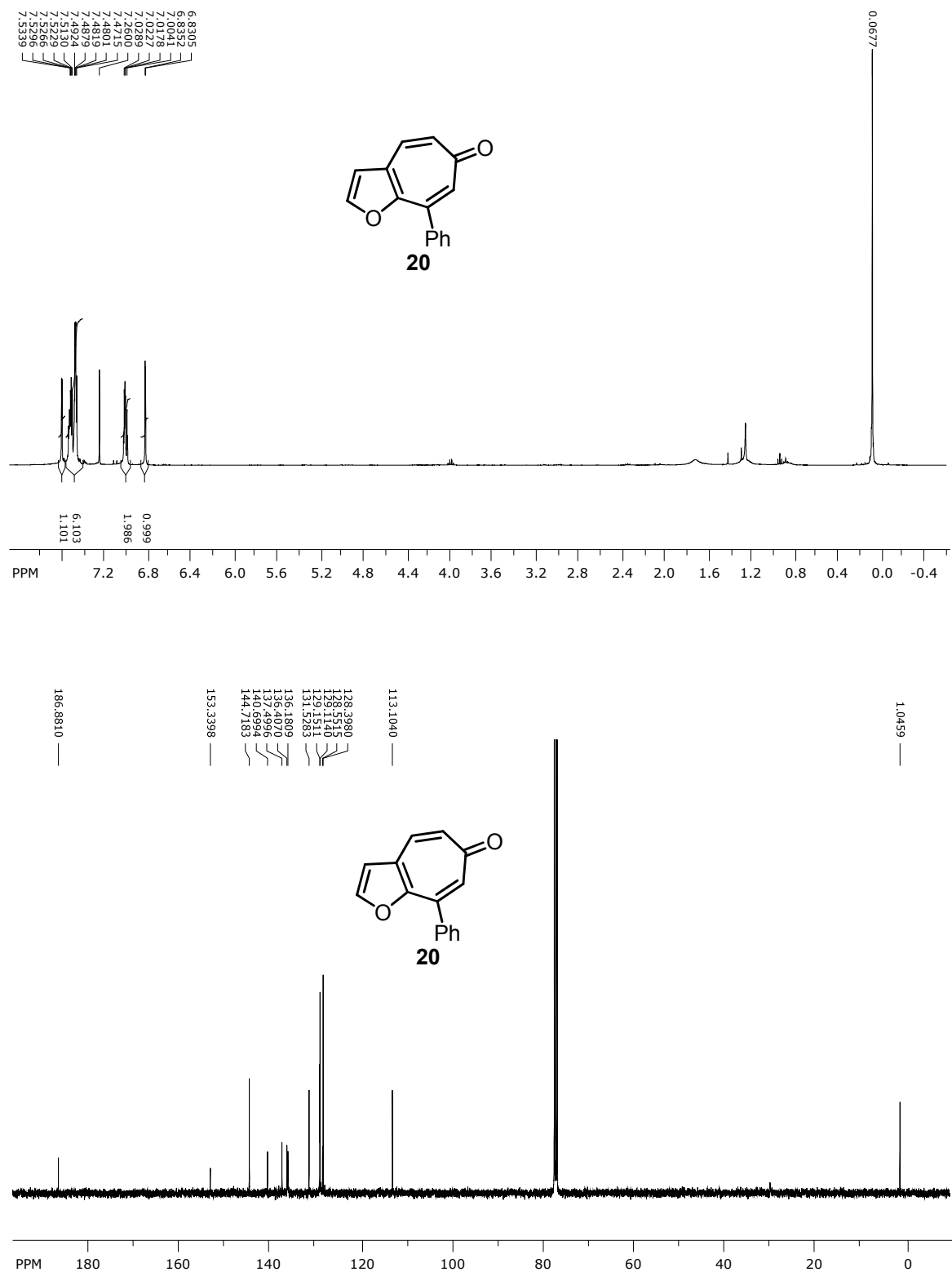
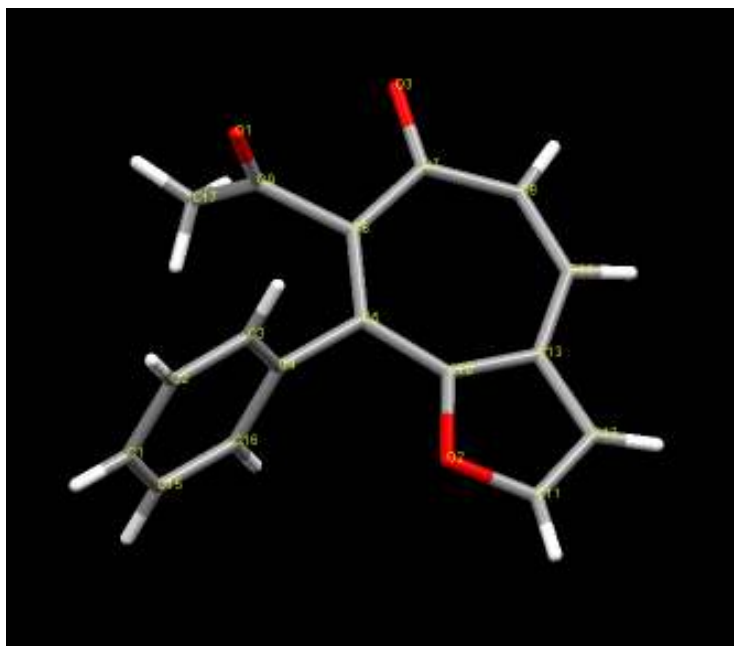


Fig. S15- ¹H and ¹³C-NMR spectra of 8-phenyl-6*H*-cyclohepta[*b*]furan-6-one (**20**).

Crystal structure information of the furotropone 19



A colorless specimen of $C_{17}H_{12}O_3$, approximate dimensions 0.30 mm x 0.30 mm x 0.40 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The total exposure time was 5.06 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 7545 reflections to a maximum θ angle of 25.05° (0.84 Å resolution), of which 2339 were independent (average redundancy 3.226, completeness = 99.9%, $R_{\text{int}} = 5.49\%$, $R_{\text{sig}} = 5.93\%$) and 1343 (57.42%) were greater than $2\sigma(F^2)$. The final cell constants of $a = 9.1041(15)$ Å, $b = 16.164(3)$ Å, $c = 9.2635(16)$ Å, $\beta = 103.874(5)^\circ$, volume = $1323.4(4)$ Å³, are based upon the refinement of the XYZ-centroids of 825 reflections above $20\sigma(I)$ with $5.183^\circ < 2\theta < 42.88^\circ$. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.937.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P 1 21/c 1$, with $Z = 4$ for the formula unit, $C_{17}H_{12}O_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 182 variables converged at $R1 = 4.97\%$, for the observed data and $wR2 = 13.79\%$ for all data. The goodness-of-fit was 0.961. The largest peak in the final difference electron density synthesis was $0.145 \text{ e}^-/\text{\AA}^3$ and the

largest hole was $-0.197 \text{ e}^-/\text{\AA}^3$ with an RMS deviation of $0.040 \text{ e}^-/\text{\AA}^3$. On the basis of the final model, the calculated density was 1.326 g/cm^3 and $F(000)$, 552 e^- .

Table 1. Sample and crystal data for SCI80

Identification code	SCI80	
Chemical formula	$\text{C}_{17}\text{H}_{12}\text{O}_3$	
Formula weight	264.28	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.30 x 0.30 x 0.40 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 9.1041(15) Å	$\alpha = 90^\circ$
	b = 16.164(3) Å	$\beta = 103.874(5)^\circ$
	c = 9.2635(16) Å	$\gamma = 90^\circ$
Volume	1323.4(4) Å ³	
Z	4	
Density (calculated)	1.326 Mg/cm ³	
Absorption coefficient	0.091 mm ⁻¹	
F(000)	552	

Table 2. Data collection and structure refinement for SCI80.

Theta range for data collection	2.30 to 25.05°	
Index ranges	-10 ≤ h ≤ 10, -19 ≤ k ≤ 18, -11 ≤ l ≤ 10	
Reflections collected	7545	
Independent reflections	2339 [R(int) = 0.0549]	
Coverage of independent reflections	99.9%	
Absorption correction	multi-scan	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F ²	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\sum w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	2339 / 0 / 182	
Goodness-of-fit on F ²	0.961	
$\Delta/\sigma_{\text{max}}$	0.001	
Final R indices	1343 data;	R1 = 0.0497, wR2 =

	I>2σ(I)	0.1117
	all data	R1 = 0.1028, wR2 = 0.1379
Weighting scheme	w=1/[σ ² (F _o ²)+(0.0678P) ² +0.0000P] where P=(F _o ² +2F _c ²)/3	
Largest diff. peak and hole	0.145 and -0.197 eÅ ⁻³	
R.M.S. deviation from mean	0.040 eÅ ⁻³	

Table 3. Bond lengths (Å) for SCI80.

O1-C9	1.202(3)	O2-C11	1.371(3)
O2-C10	1.372(3)	O3-C7	1.238(3)
C1-C2	1.373(4)	C1-C15	1.374(4)
C1-H1	0.93	C2-C3	1.381(3)
C2-H2	0.93	C3-C4	1.387(3)
C3-H3A	0.93	C4-C16	1.384(3)
C4-C5	1.498(3)	C5-C6	1.366(3)
C5-C10	1.427(3)	C6-C7	1.475(3)
C6-C9	1.507(4)	C7-C8	1.445(4)
C8-C14	1.340(4)	C8-H8	0.93
C9-C17	1.493(4)	C10-C13	1.379(3)
C11-C12	1.333(4)	C11-H11	0.93
C12-C13	1.418(3)	C12-H12	0.93
C13-C14	1.422(4)	C14-H14	0.93
C15-C16	1.384(4)	C15-H15	0.93
C16-H16	0.93	C17-H17A	0.96
C17-H17B	0.96	C17-H17C	0.96

Table 4. Bond angles (°) for SCI80.

C11-O2-C10	106.49(19)	C2-C1-C15	120.0(3)
C2-C1-H1	120.0	C15-C1-H1	120.0
C1-C2-C3	120.4(3)	C1-C2-H2	119.8
C3-C2-H2	119.8	C2-C3-C4	120.1(3)
C2-C3-H3A	119.9	C4-C3-H3A	119.9
C16-C4-C3	118.9(2)	C16-C4-C5	121.2(2)
C3-C4-C5	119.9(2)	C6-C5-C10	123.9(2)
C6-C5-C4	119.9(2)	C10-C5-C4	116.2(2)
C5-C6-C7	130.8(2)	C5-C6-C9	119.1(2)
C7-C6-C9	110.2(2)	O3-C7-C8	118.4(2)

O3-C7-C6	116.3(2)	C8-C7-C6	125.2(2)
C14-C8-C7	130.4(3)	C14-C8-H8	114.8
C7-C8-H8	114.8	O1-C9-C17	122.4(3)
O1-C9-C6	121.2(3)	C17-C9-C6	116.3(3)
O2-C10-C13	109.4(2)	O2-C10-C5	116.7(2)
C13-C10-C5	133.9(2)	C12-C11-O2	110.8(2)
C12-C11-H11	124.6	O2-C11-H11	124.6
C11-C12-C13	107.4(2)	C11-C12-H12	126.3
C13-C12-H12	126.3	C10-C13-C12	106.0(2)
C10-C13-C14	126.5(2)	C12-C13-C14	127.5(2)
C8-C14-C13	129.0(2)	C8-C14-H14	115.5
C13-C14-H14	115.5	C1-C15-C16	119.9(3)
C1-C15-H15	120.1	C16-C15-H15	120.1
C15-C16-C4	120.6(3)	C15-C16-H16	119.7
C4-C16-H16	119.7	C9-C17-H17A	109.5
C9-C17-H17B	109.5	H17A-C17-H17B	109.5
C9-C17-H17C	109.5	H17A-C17-H17C	109.5
H17B-C17-H17C	109.5		

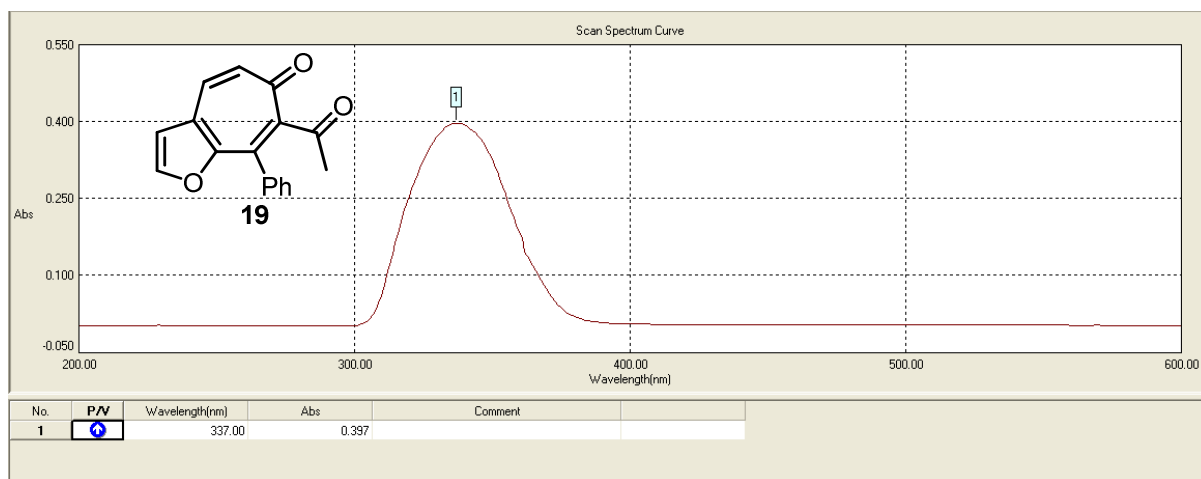


Fig. S16- Absorption spectrum of 7-acetyl-8-phenyl-6H-cyclohepta[*b*]furan-6-one (**19**) recorded with 0.0000348 M solution in ethanol (*l* = 1 cm).

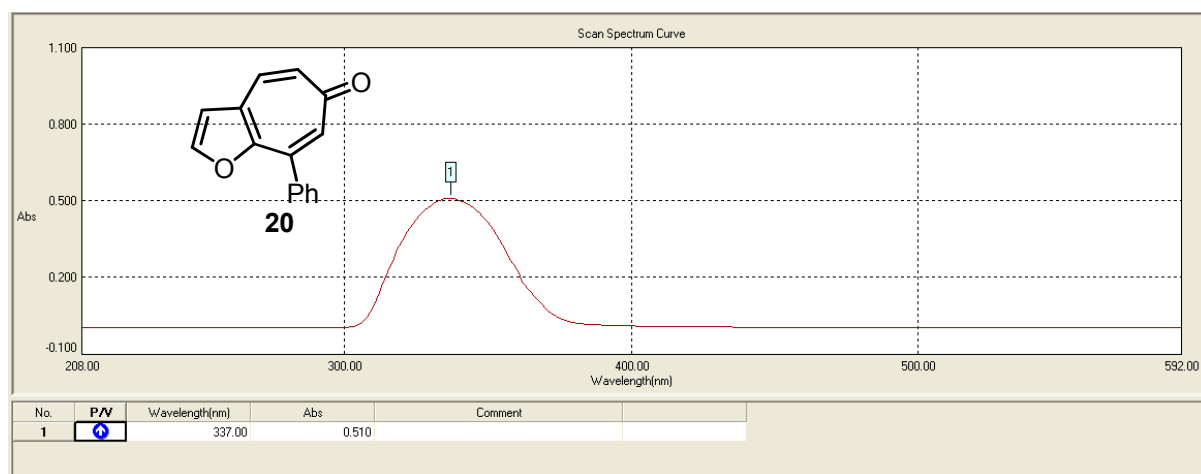


Fig. S17- Absorption spectrum of 8-phenyl-6H-cyclohepta[*b*]furan-6-one (**20**) recorded with 0.0000594 M solution in ethanol (*l* = 1 cm).

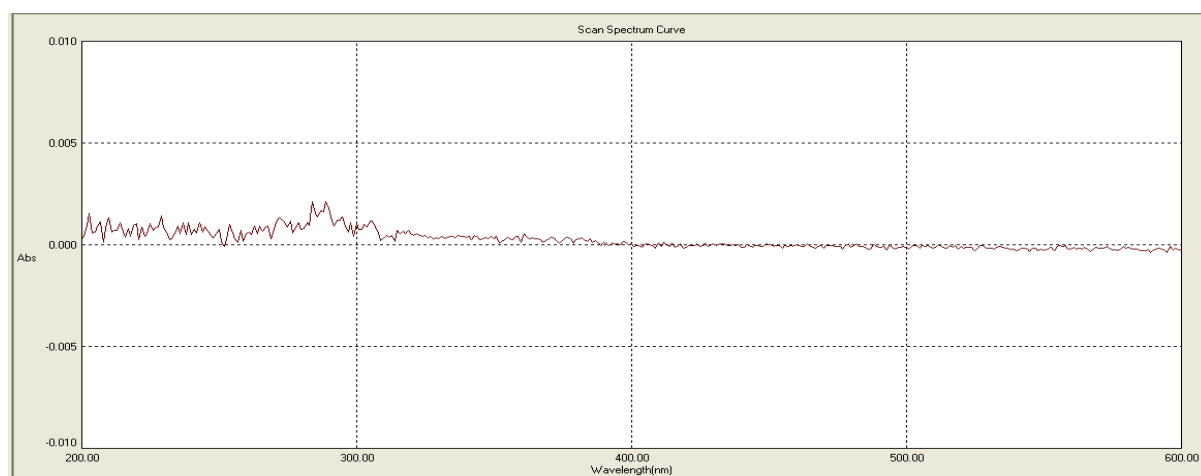


Fig. S18- Absorption spectrum of blank run in ethanol.

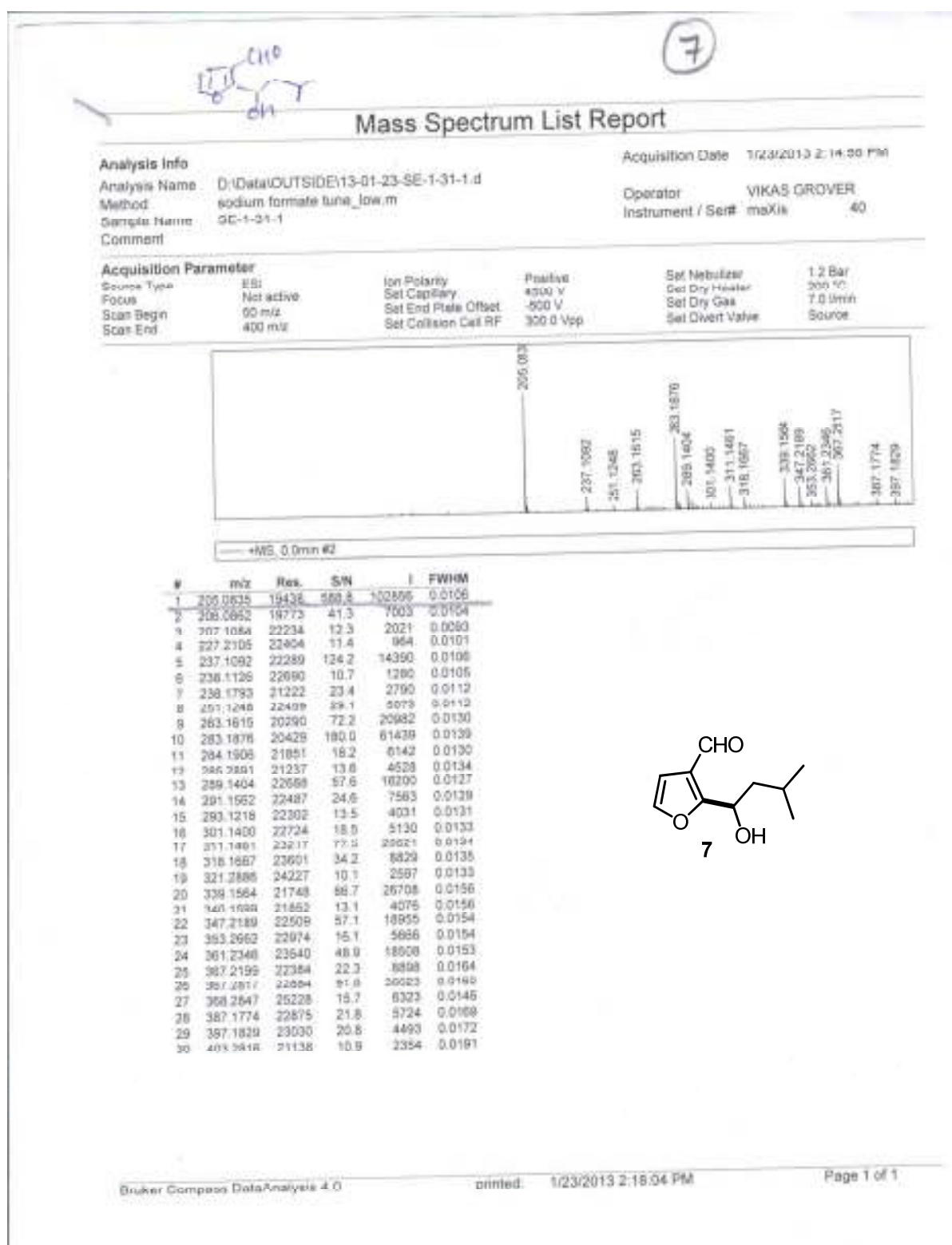


Fig. S19- HRMS spectrum of 2-(1-hydroxy-3-methylbutyl)furan-3-carbaldehyde (7).

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Mass Spectrum List Report

Analysis Info

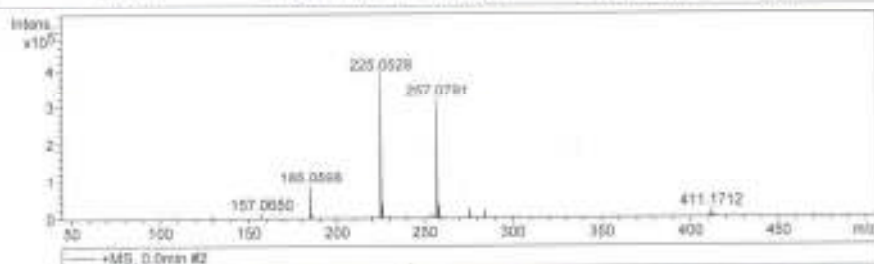
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Operator: VIKAS GROVER
Instrument / Ser#: mXis 40

Acquisition Parameter

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Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Oven Valve	Source



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1	122.0302	16422	15.4	563	0.0074
2	129.0710	20170	151.8	8959	0.0264
3	157.0650	17761	158.2	12190	0.0268
4	185.0598	16326	911.7	84736	0.0113
5	186.0627	19554	54.0	5419	0.0095
6	191.1175	17240	16.4	2255	0.0111
7	220.1438	21351	13.4	4492	0.0103
8	225.0528	19889	1066.1	267583	0.0143
9	225.0554	19354	111.5	40331	0.0117
10	230.1643	19836	13.5	5127	0.0117
11	239.0673	18537	12.5	5292	0.0126
12	254.0794	20547	35.2	12591	0.0126
13	257.0791	15658	883.7	317700	0.0164
14	258.0816	19254	100.8	35542	0.0134
15	275.1389	19417	111.9	26491	0.0142
16	283.1301	18418	18.6	3751	0.0154
17	284.0891	19671	112.0	22134	0.0144
18	300.1200	19678	25.2	3212	0.0153
19	327.1318	21188	11.8	1051	0.0154
20	338.1918	17705	13.4	1118	0.0190
21	358.1740	19812	18.6	1940	0.0181
22	367.1842	17134	10.0	1217	0.0214
23	377.2181	19859	18.4	2021	0.0180
24	411.1712	20189	120.8	19508	0.0204
25	412.1740	20895	21.5	3208	0.0199
26	413.2888	20000	59.0	8375	0.0207
27	414.2700	22477	10.2	1492	0.0184
28	431.1964	21172	15.5	2535	0.0204
29	468.1419	22114	10.0	551	0.0212

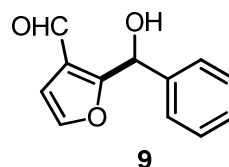


Fig. S20- HRMS spectrum of 2-(hydroxy(phenyl)methyl)furan-3-carbaldehyde (9).

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Mass Spectrum List Report

Analysis Info

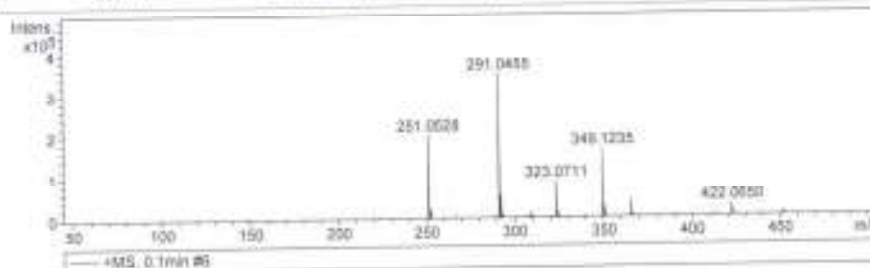
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Operator: VIKAS GROVER
 Instrument / Ser#: maXis 40

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 L/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	PWHR
1	237.0723	18977	12.1	1193	0.0125
2	251.0628	18207	1861.7	186424	0.0165
3	252.0550	19340	222.3	23417	0.0130
4	253.0611	12251	33.3	3450	0.0207
5	267.0486	18832	45.1	3548	0.0142
6	288.0391	19531	18.4	2840	0.0147
7	288.0297	17596	21.3	3428	0.0160
8	291.0455	16102	1081.6	247283	0.0161
9	291.1174	16745	127.2	22352	0.0174
10	292.0478	18922	289.8	52798	0.0150
11	292.1208	17226	14.1	2573	0.0170
12	293.0431	14380	43.4	8025	0.0204
13	309.1298	21009	38.7	10102	0.0147
14	321.0547	18984	11.3	3042	0.0188
15	323.0711	18239	327.8	87985	0.0177
16	324.0736	20012	21.1	8344	0.0162
17	325.1242	19880	11.5	3067	0.0164
18	339.0648	17910	14.8	3827	0.0189
19	349.1235	18780	830.0	163891	0.0208
20	350.1290	20809	138.1	26363	0.0168
21	351.1228	14513	18.8	3490	0.0242
22	385.1174	20042	398.6	40343	0.0182
23	386.1186	21077	42.7	4806	0.0174
24	413.2084	21800	55.0	6391	0.0150
25	414.0796	18748	11.6	1383	0.0221
26	422.0650	20013	179.3	27930	0.0211
27	422.5665	20434	78.4	12385	0.0207
28	423.0688	18820	23.3	6343	0.0227
29	423.5003	18106	10.4	1888	0.0233

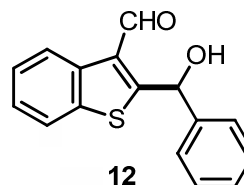


Fig. S21- HRMS spectrum of 2-(hydroxy(phenyl)methyl)benzo[b]thiophene-3-carbaldehyde (12).

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Mass Spectrum List Report

Analysis Info:

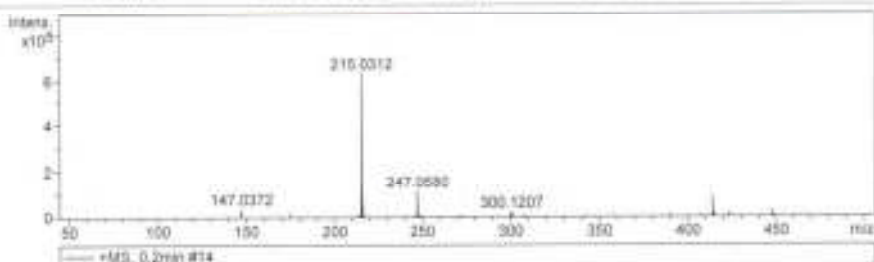
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 Method: sodium formate tune_low.m
 Sample Name: SN-01-008
 Comment:

Acquisition Date: 5/15/2013 1:32:02 PM

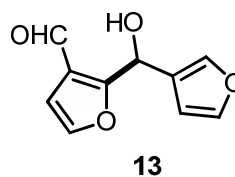
Operator: VIKAS GROVER
 Instrument / Ser#: maXis 40

Acquisition Parameter:

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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Diverter Valve	Source



#	m/z	Rel.	SN	I	FWHM
1	119.0368	10636	88.3	1230	0.0061
2	122.0460	15957	93.8	1815	0.0078
3	139.0646	20064	114.9	4911	0.0069
4	147.0372	15109	702.5	37719	0.0097
5	148.0402	19306	40.9	2254	0.0077
6	152.0600	18923	31.6	1918	0.0080
7	158.9583	22019	20.4	1241	0.0072
8	175.0302	17902	298.2	17972	0.0098
9	176.0364	18542	17.1	1002	0.0095
10	198.0948	18861	12.2	1699	0.0100
11	213.0143	18571	38.4	8006	0.0114
12	215.0312	14190	3863.6	621308	0.0140
13	216.0330	18365	269.4	60625	0.0118
14	217.0352	17949	14.0	3254	0.0121
15	217.1205	18138	11.1	2583	0.0120
16	245.0416	20271	26.7	9781	0.0121
17	247.0580	18811	317.4	115295	0.0147
18	248.0607	18178	18.6	8613	0.0138
19	249.0637	20497	26.2	6065	0.0121
20	263.0521	19454	11.5	2801	0.0135
21	271.0930	20382	41.2	8539	0.0134
22	273.1096	20126	66.4	9402	0.0136
23	300.1207	20602	100.3	22767	0.0146
24	301.1366	19835	84.9	18864	0.0152
25	307.0940	20058	33.7	7792	0.0153
26	308.0448	18374	26.4	5775	0.0159
27	318.1672	18858	10.2	1824	0.0160
28	320.2217	21526	12.2	2210	0.0149
29	328.1153	19782	13.9	2107	0.0166
30	329.0630	20816	11.2	1655	0.0160

Fig. S22- HRMS spectrum of 2-((furan-3-yl)(hydroxy)methyl)furan-3-carbaldehyde (**13**).

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Mass Spectrum List Report

Analysis Info

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Method sodium formate tune_low.m
Sample Name SE-01-015
Comment

Acquisition Date 4/10/2013 4:19:40 PM

Operator VIKAS GROVER

Instrument / Set# maXis 40

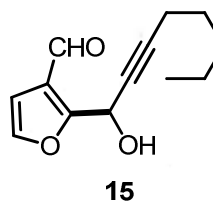
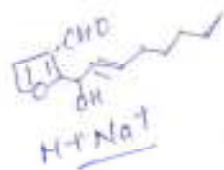
Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-520 V	Set Dry Gas	7.0 l/min
Scan End	400 m/z	Set Collision Cell RF	350.0 Vpp	Set Glycerol Valve	Source



HRMS: 0.5mm #01

#	m/z	Res.	S/N	I	FWHM
1	243.0992	1761.3	8183.3	389352	0.0133
2	275.1254	18122	2547.2	134768	0.0153
3	301.1416	18295	4101.3	232960	0.0165
4	329.2066	20866	813.5	42068	0.0158
5	332.2590	21116	1131.4	67813	0.0157
6	359.2196	18520	9039.6	871340	0.0194
7	363.2501	20749	722.1	89855	0.0175



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Fig. S23- HRMS spectrum of 2-(1-hydroxyoct-2-ynyl)furan-3-carbaldehyde (15).

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Mass Spectrum List Report

Analysis Info

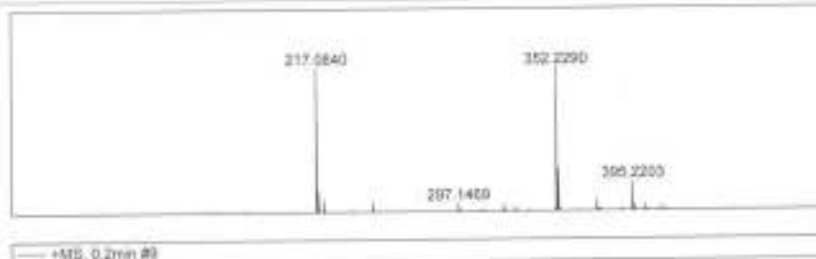
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Method sodium formate tune_low.m
Sample Name SN-040-1
Comment

Acquisition Date 4/26/2013 2:21:11 PM

Operator VIKAS GROVER
Instrument / Sent maxis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	160 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Desolv Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	217.0840	15776	5123.4	1255345	0.0158
2	218.0868	15444	4244.0	178131	0.0133
3	219.0891	16882	325.4	12539	0.0131
4	221.1511	17798	2785.6	102561	0.0124
5	249.1103	18216	4323.5	78864	0.0137
6	267.1469	19133	2522.0	63500	0.0155
7	311.1818	19938	696.2	20911	0.0156
8	323.1625	19680	1514.7	47691	0.0164
9	329.1305	20165	1243.7	39942	0.0163
10	352.2290	14739	18569.5	1206710	0.0239
11	375.1573	15041	1083.2	89705	0.0167
12	395.2203	17363	4044.7	242251	0.0228

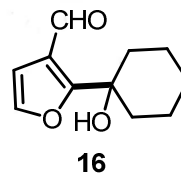


Fig. S24- HRMS spectrum of 2-(1-hydroxycyclohexyl)furan-3-carbaldehyde (16).

17

Mass Spectrum List Report

Analysis Info

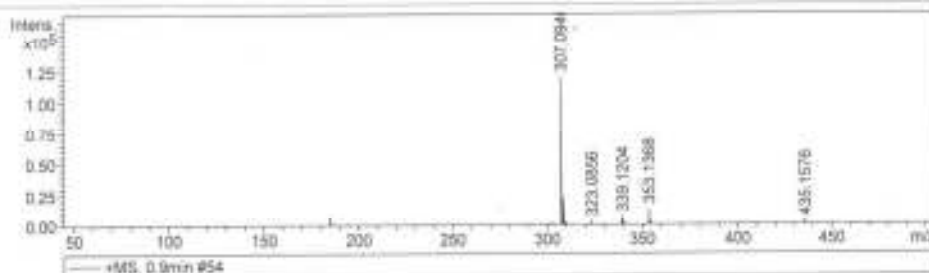
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Method: tune_low.m
Sample Name: SE-06
Comment:

Acquisition Date: 8/24/2012 12:41:14 PM

Operator: VIKAS GROVER
Instrument / Ser#: mxiXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End-Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	129.0705	17427	77.9	864	0.0074
2	178.0152	21301	1.9	43	0.0084
3	231.1016	18985	33.6	478	0.0122
4	265.0831	19410	25.4	383	0.0137
5	267.1008	24043	20.9	318	0.0111
6	299.1288	18948	10.0	820	0.0159
7	302.1309	20580	34.5	2143	0.0147
8	304.0859	20493	18.2	1189	0.0148
9	307.0948	20881	1785.2	119057	0.0147
10	308.0978	21708	337.2	22351	0.0142
11	309.1006	21543	42.0	2758	0.0143
12	323.0858	20385	99.9	3354	0.0158
13	324.0900	19647	10.4	577	0.0183
14	339.1204	21659	147.8	6978	0.0157
15	340.1243	23607	31.0	1487	0.0144
16	353.1368	21861	278.3	13387	0.0162
17	354.1400	20952	52.7	2539	0.0170
18	389.1345	21952	10.7	298	0.0177
19	400.8989	22957	16.7	347	0.0174
20	402.8970	24888	32.2	688	0.0162
21	404.8950	23383	14.7	323	0.0173
22	423.1148	18381	14.5	394	0.0218
23	435.1575	21128	117.2	3188	0.0206
24	436.1618	21959	35.4	976	0.0199
25	437.1661	20091	10.3	273	0.0218
26	448.1387	23580	20.7	504	0.0189
27	453.1645	26632	11.3	257	0.0170
28	459.1781	19983	17.5	372	0.0230
29	503.1839	21896	48.8	919	0.0230
30	504.1871	22184	16.1	317	0.0227

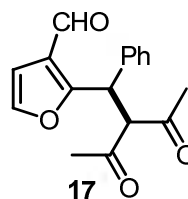


Fig. S25- HRMS spectrum of 2-(2-acetyl-3-oxo-1-phenylbutyl)furan-3-carbaldehyde (17).

Mass Spectrum List Report

Analysis Info

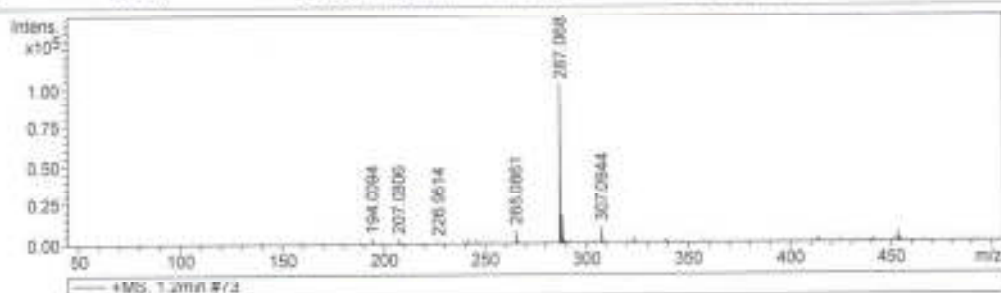
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 Method sodium formate tune_low.m
 Sample Name SEO-284
 Comment

Acquisition Date 8/28/2012 4:12:47 PM

Operator VIKAS GROVER
 Instrument / Ser# maXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	194.0594	19877	100.3	3359	0.0099
2	207.0606	18934	81.6	2549	0.0108
3	226.0614	20124	39.5	1674	0.0113
4	265.0651	21092	89.5	8333	0.0128
5	287.0663	21436	1003.3	101851	0.0134
6	288.0714	20887	177.0	17480	0.0138
7	289.0736	20902	23.8	2366	0.0138
8	307.0644	21370	122.1	9990	0.0144

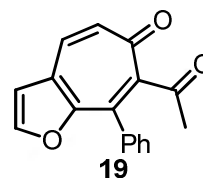


Fig. S26- HRMS spectrum of 7-acetyl-8-phenyl-6H-cyclohepta[b]furan-6-one (19).

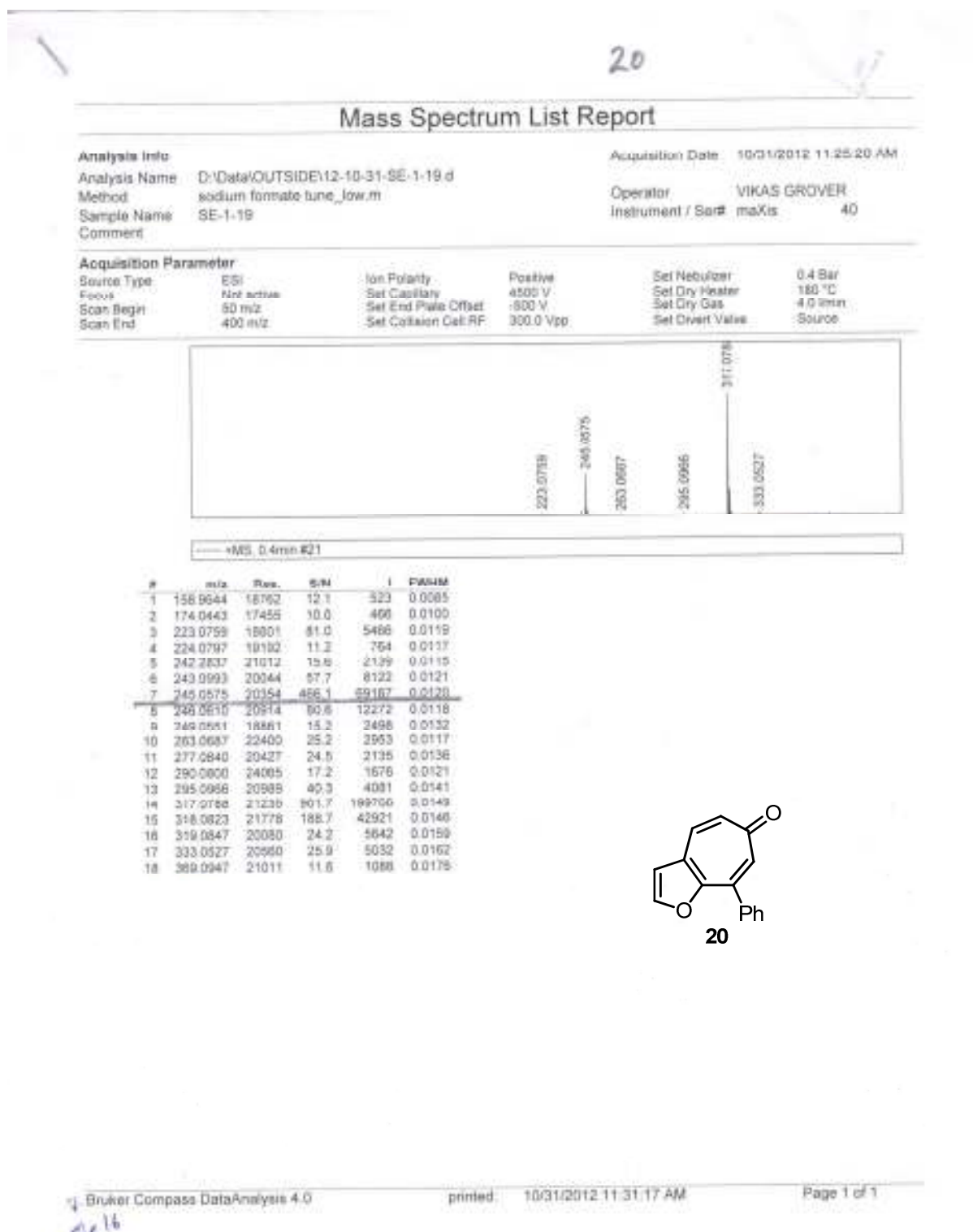


Fig. S27- HRMS spectrum of 8-phenyl-6H-cyclohepta[b]furan-6-one (**20**).

Mass Spectrum List Report

Analyte Info

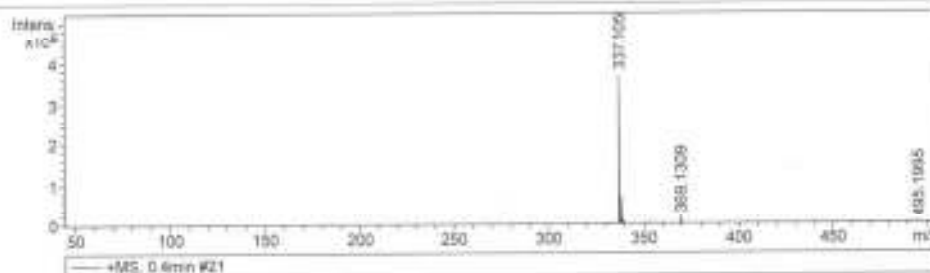
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 Comment:

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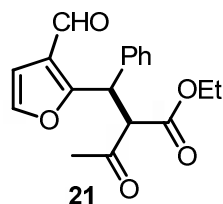
Operator: VIKAS GROVER
 Instrument / Ser#: maXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3000 V	Set Dry Heater	160 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	157.0651	19978	34.5	455	0.0079
2	186.0598	19070	127.1	2603	0.0087
3	332.1492	21324	13.0	1863	0.0158
4	334.0987	21369	16.3	3454	0.0158
5	337.1050	21211	2795.5	367081	0.0159
6	358.1083	20845	450.3	70765	0.0162
7	339.1107	21607	70.0	10614	0.0157
8	363.0931	9843	39.3	4580	0.0359
9	369.1309	22100	248.2	18734	0.0167
10	370.1342	21309	48.0	3541	0.0174
11	371.1278	8031	10.9	756	0.0416
12	405.0918	23305	46.0	1165	0.0174
13	405.1052	21493	62.3	1371	0.0190
14	435.1031	22195	30.3	558	0.0196
15	467.1670	24288	33.8	1102	0.0192
16	483.1713	15582	12.7	713	0.0310
17	491.1543	24457	51.1	3361	0.0201
18	491.5567	22539	27.0	1777	0.0218
19	492.1574	24953	12.5	824	0.0197
20	495.1985	33627	82.0	5389	0.0210
21	496.2025	23032	22.6	1486	0.0215

Fig. S28- HRMS spectrum of ethyl 2-((3-formylfuran-2-yl)(phenyl)methyl)-3-oxobutanoate (**21**).