

Supporting information

Comparison of antidiabetic potential of (+) and (-)-Hopeaphenol, a pair of enantiomers isolated from *Ampelocissus indica* (L.) and *Vateria indica* Linn, with respect to inhibition of digestive enzymes and induction of glucose uptake in L6 myotubes

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Figure S1 ^1H -NMR Spectrum of Compound 1, (+)- hopeaphenol (CD_3COCD_3 , 500 MHz)

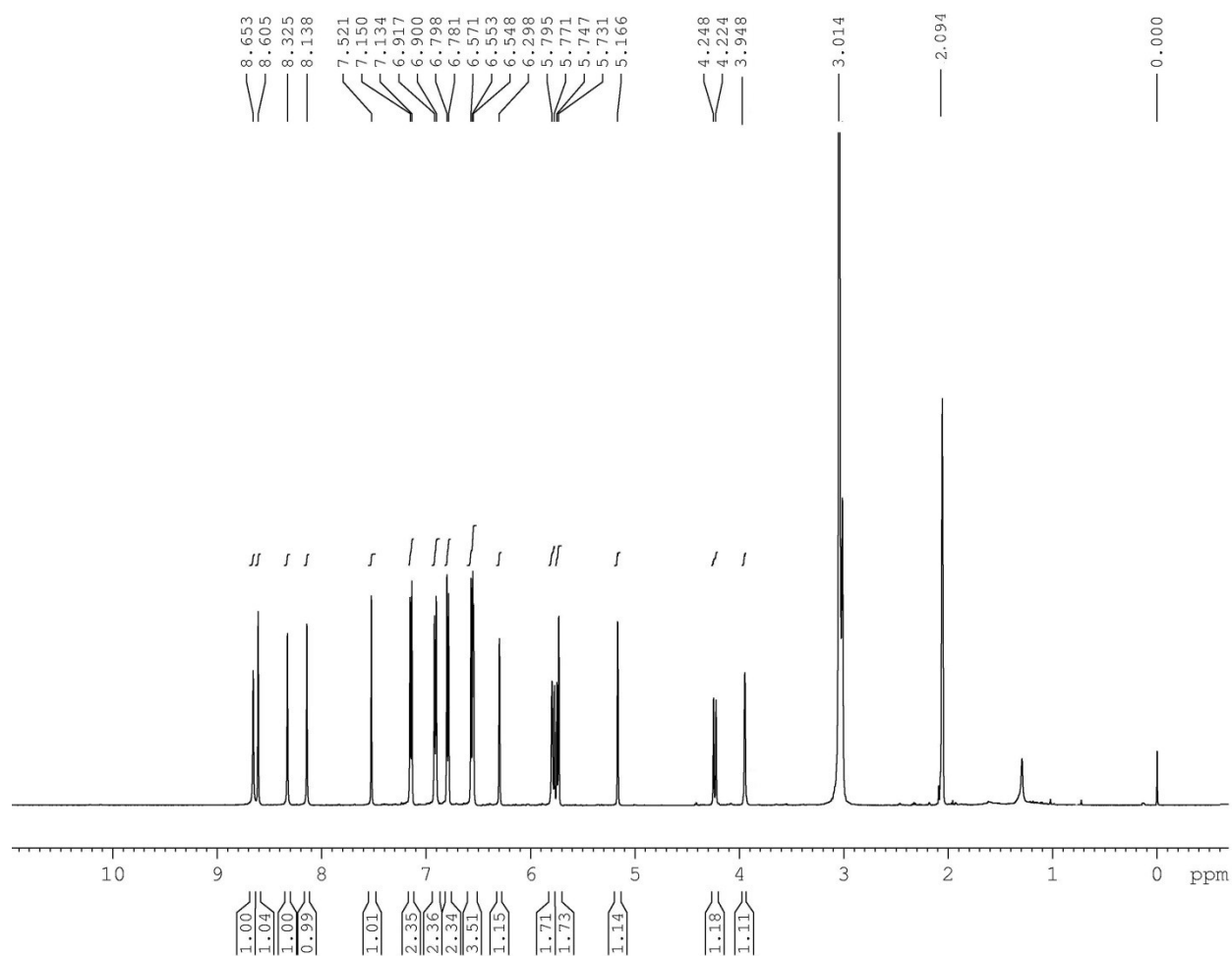


Figure S2 ^{13}C -NMR Spectrum of compound 1,(+)-hopeaphenol (CD_3COCD_3 125MHz)

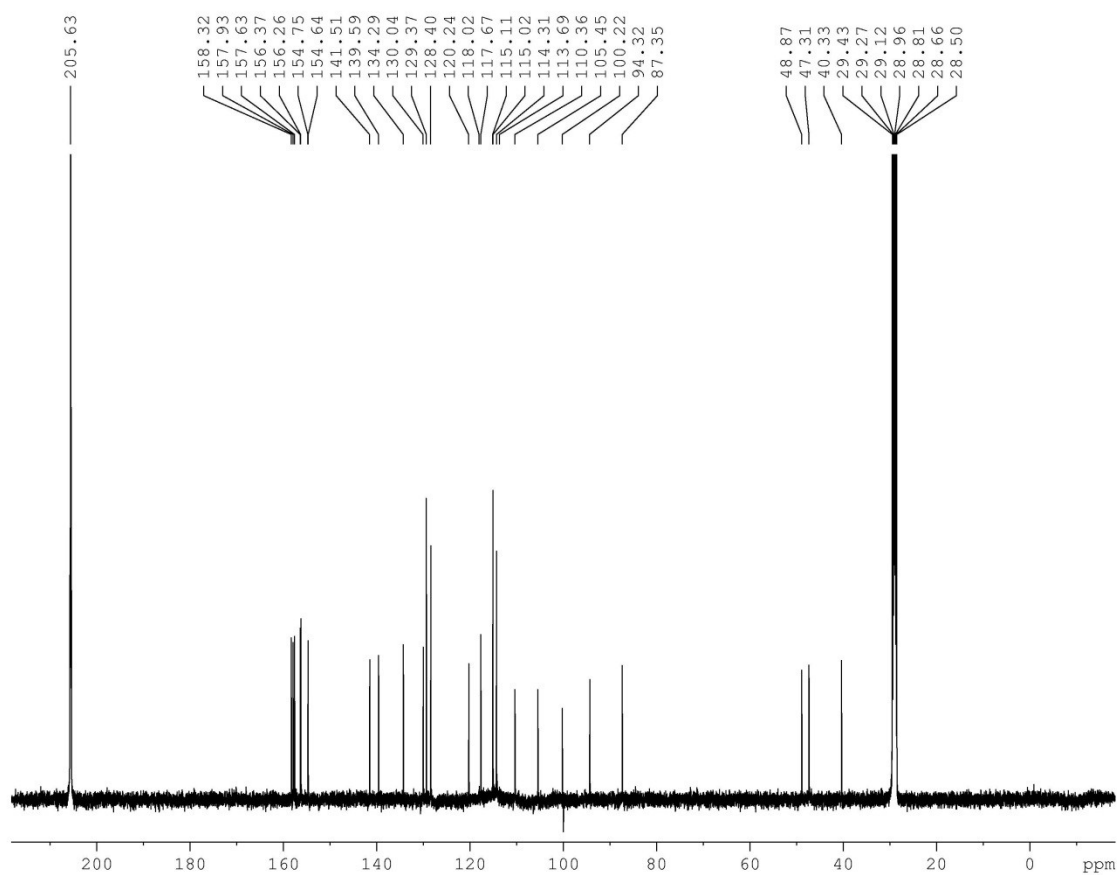


Figure S3 ^1H - ^1H COSY Spectrum of Compound 1, (+)-hopeaphenol (CD_3COCD_3)

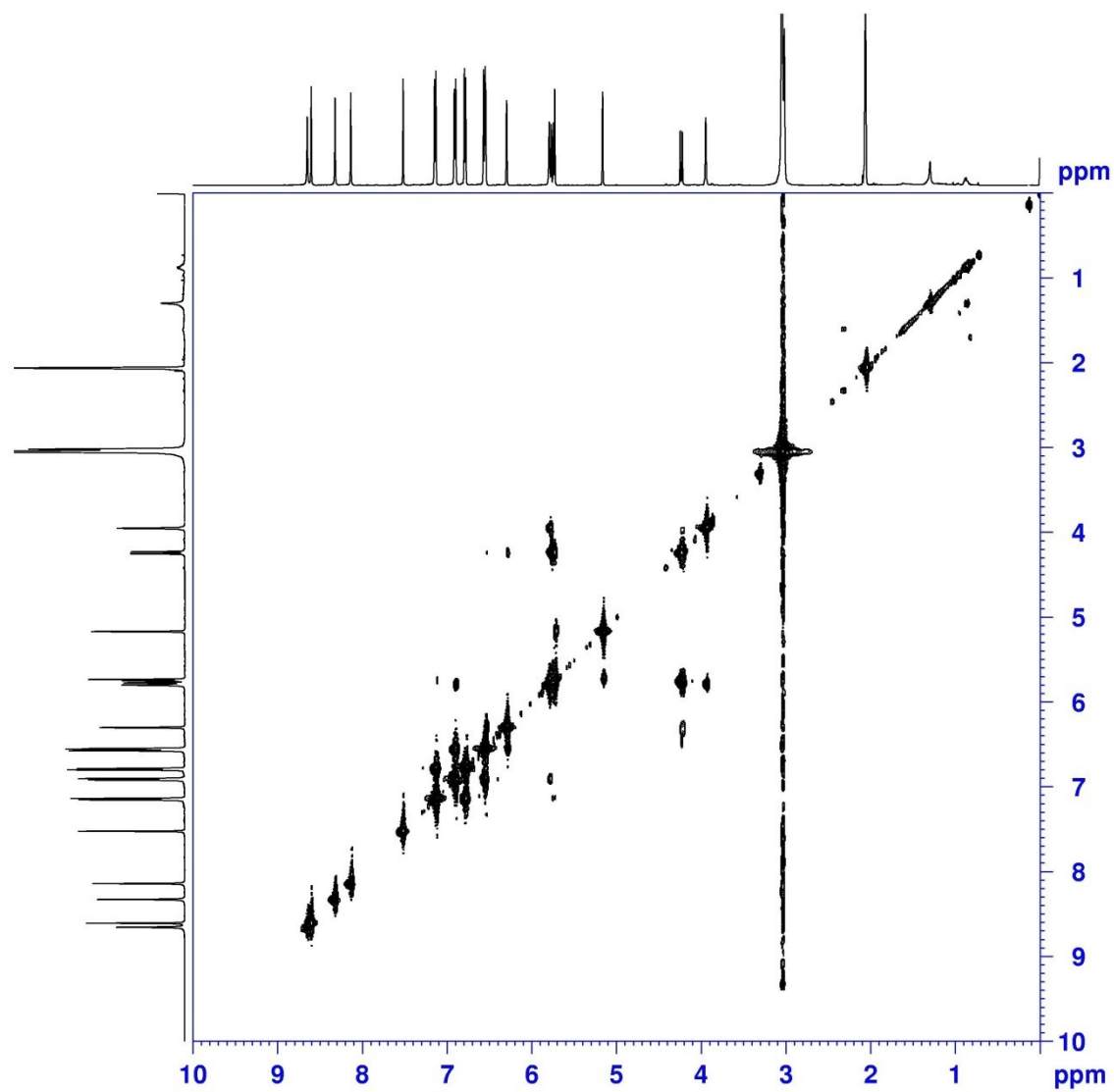


Figure S4 HMQC-Spectrum of Compound 1, (+)-hopeaphenol, (CD_3COCD_3)

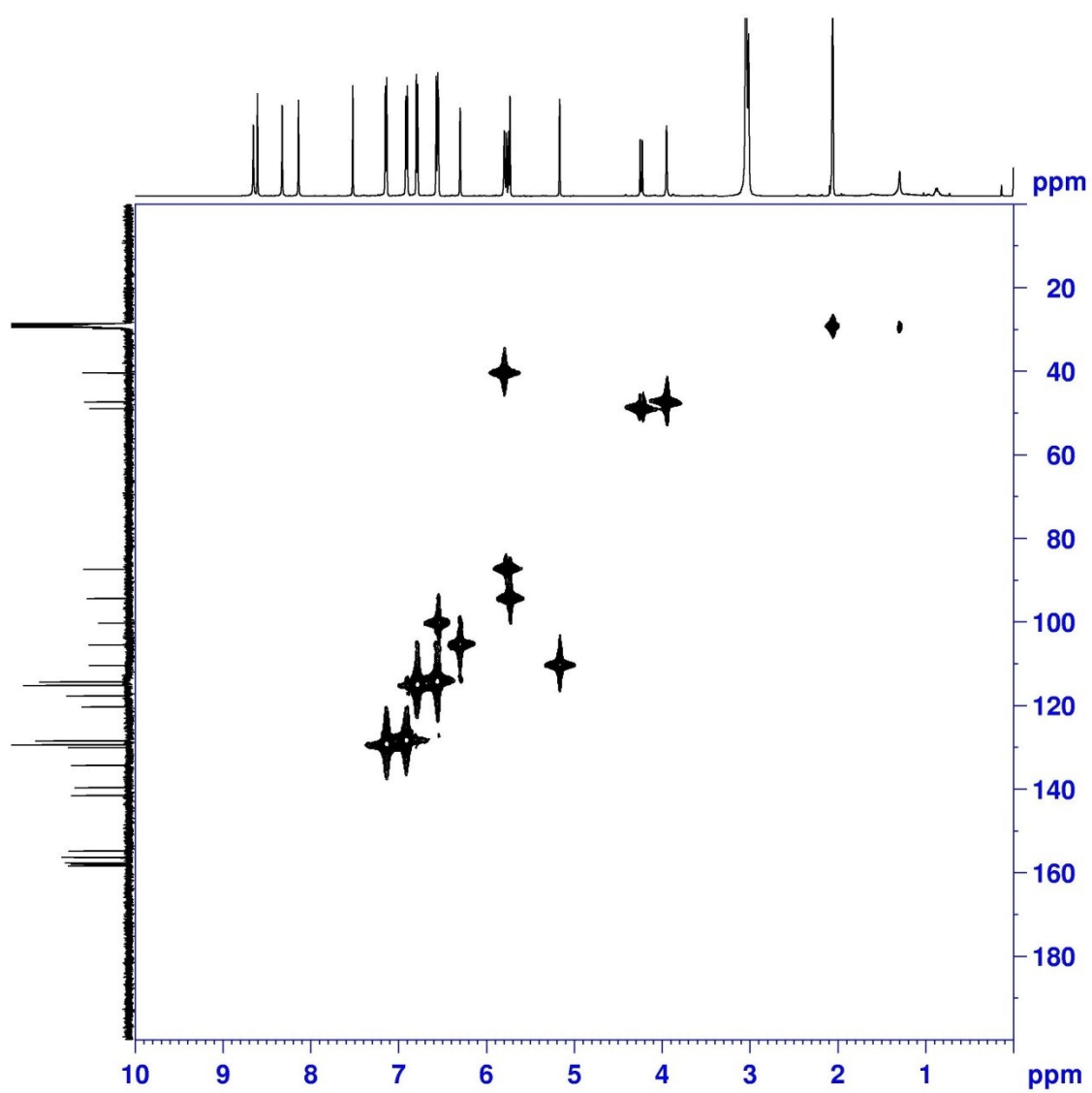


Figure S5 DEPT-135 Specrrum of Compound 1,(+)-hopeaphenol,(CD₃COCD₃)

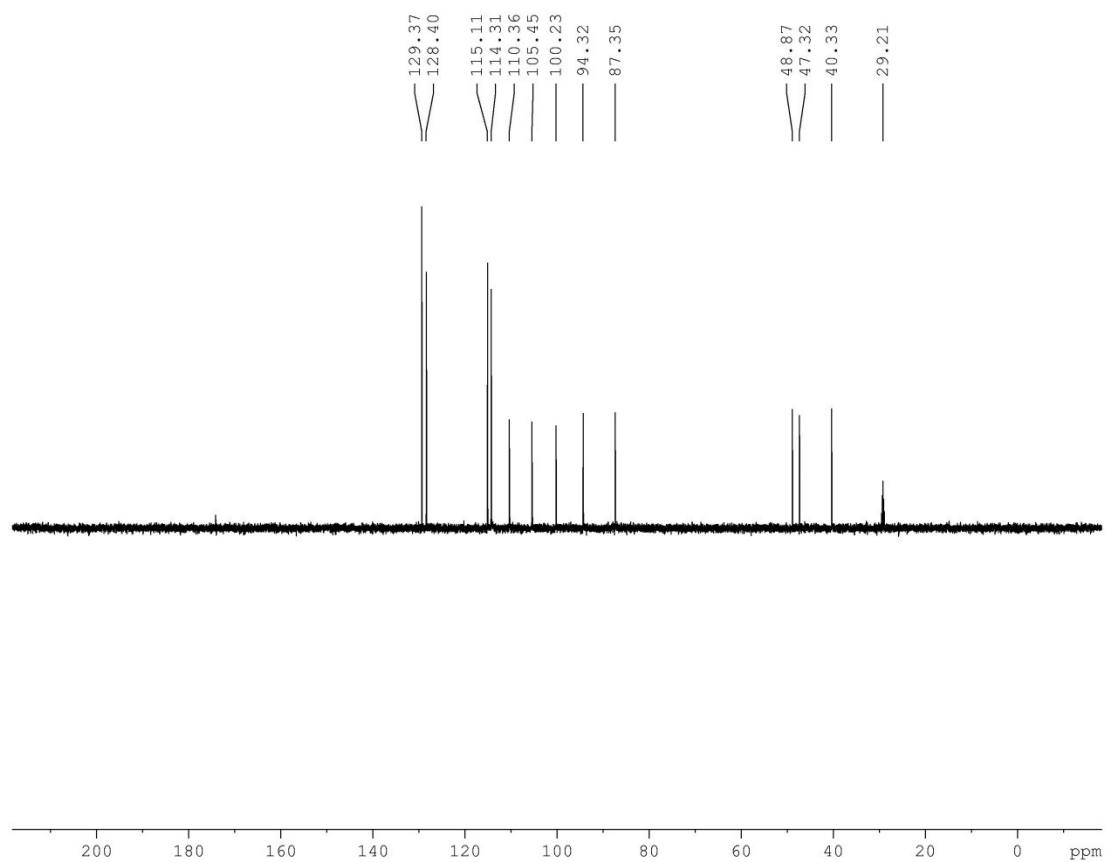


Figure S6 HMBC Spectrum of Compound 1, (+)- hopeaphenol, (CD₃COCD₃)

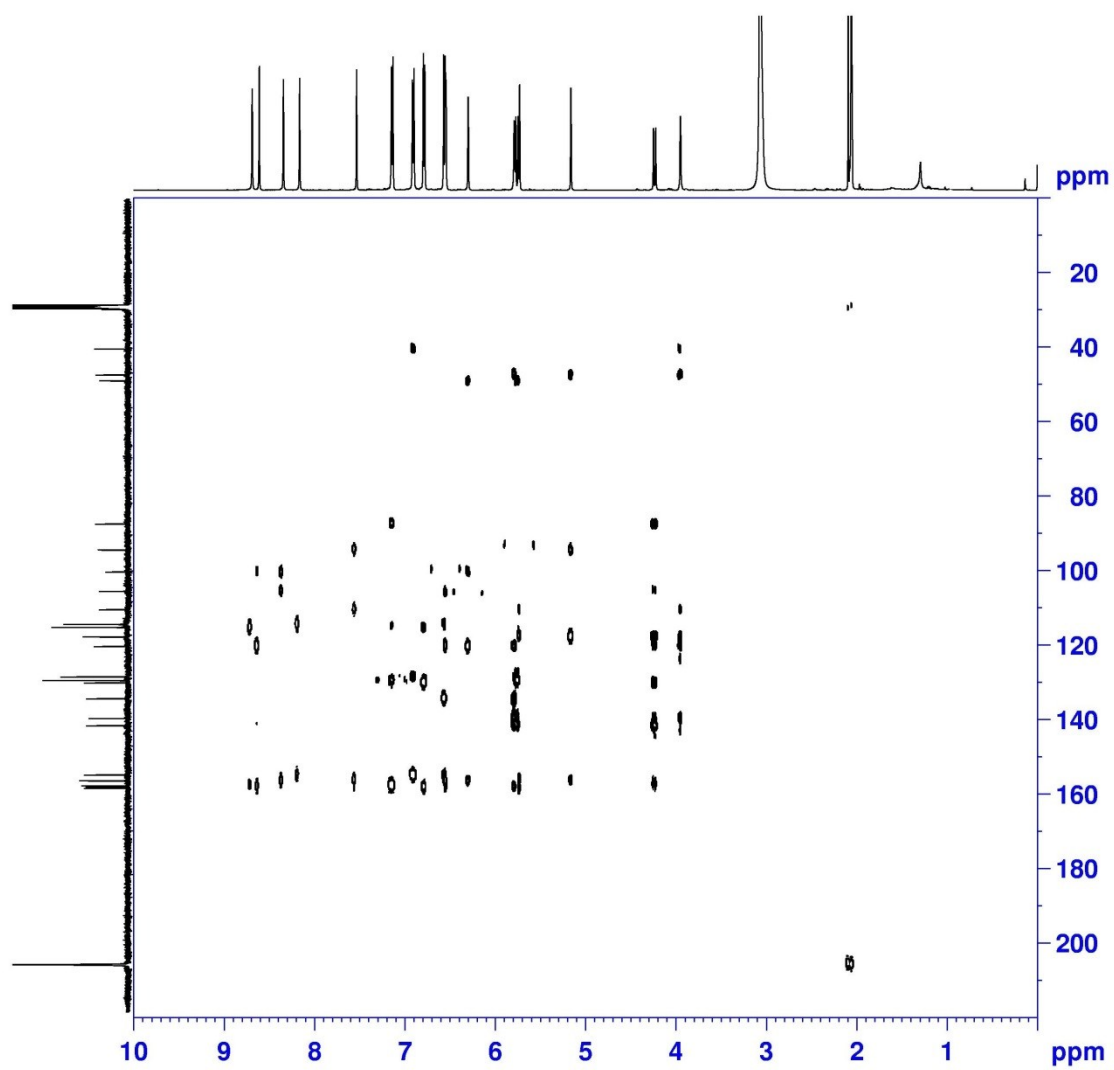


Figure S7 NOESY Spectrum of Compound 1, (+)- hopeaphenol, (CD₃COCD₃)

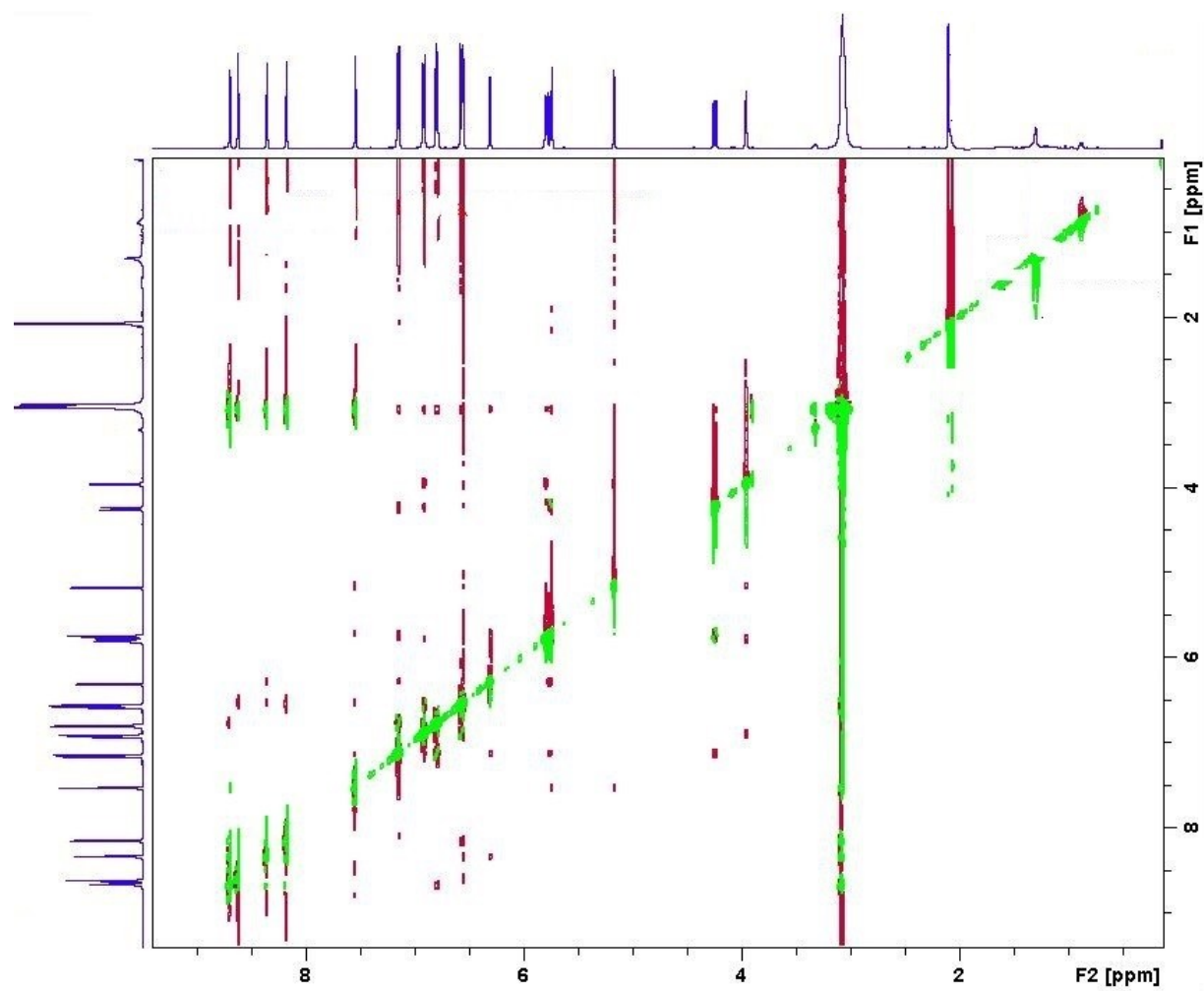


Figure S8 ^1H -NMR Spectrum of Compound 2, (-)- hopeaphenol (CD_3COCD_3 , 500 MHz)

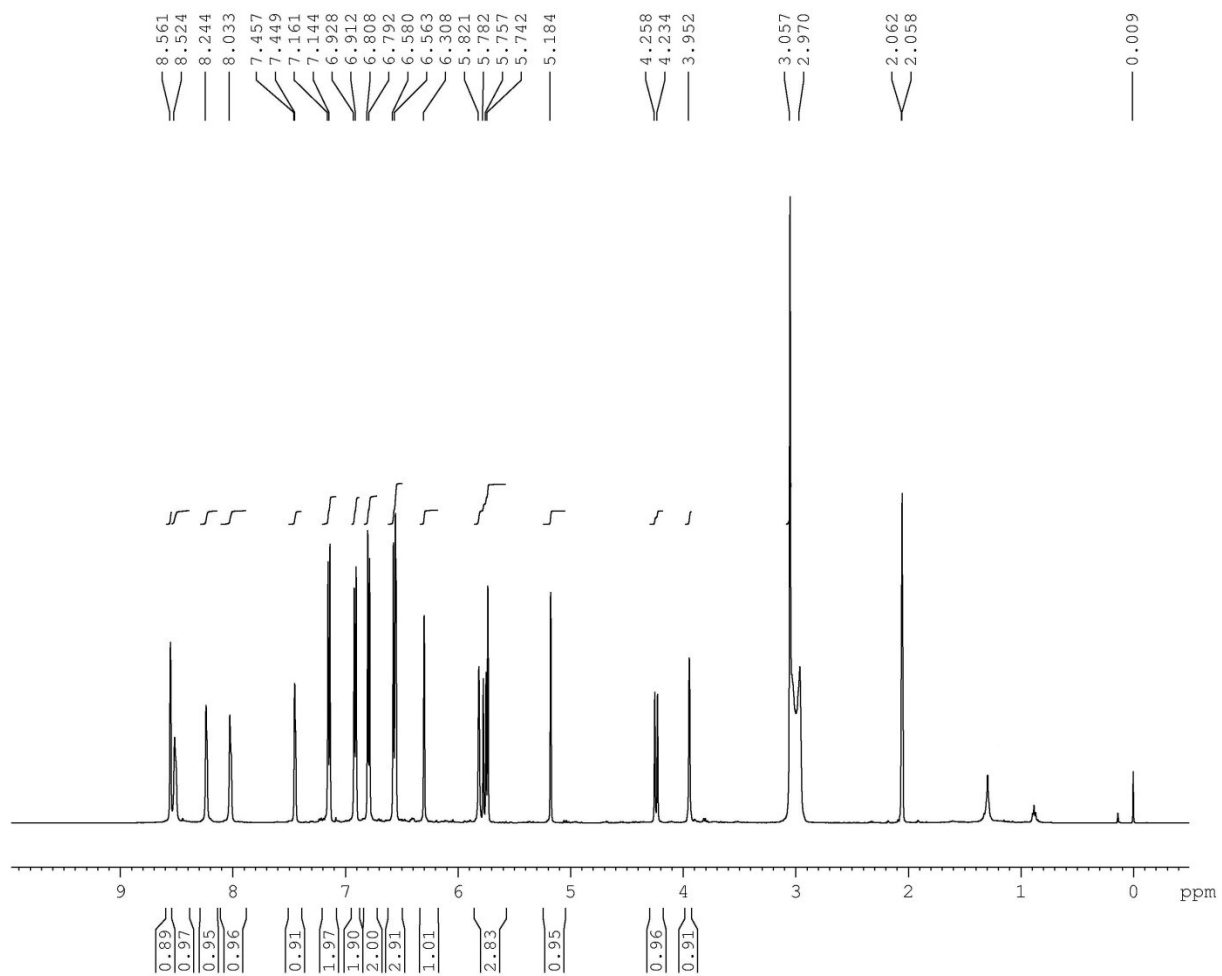


Figure S9 ^{13}C -NMR Spectrum of compound 2,(-)-hopeaphenol, (CD_3COCD_3 , 125 MHz)

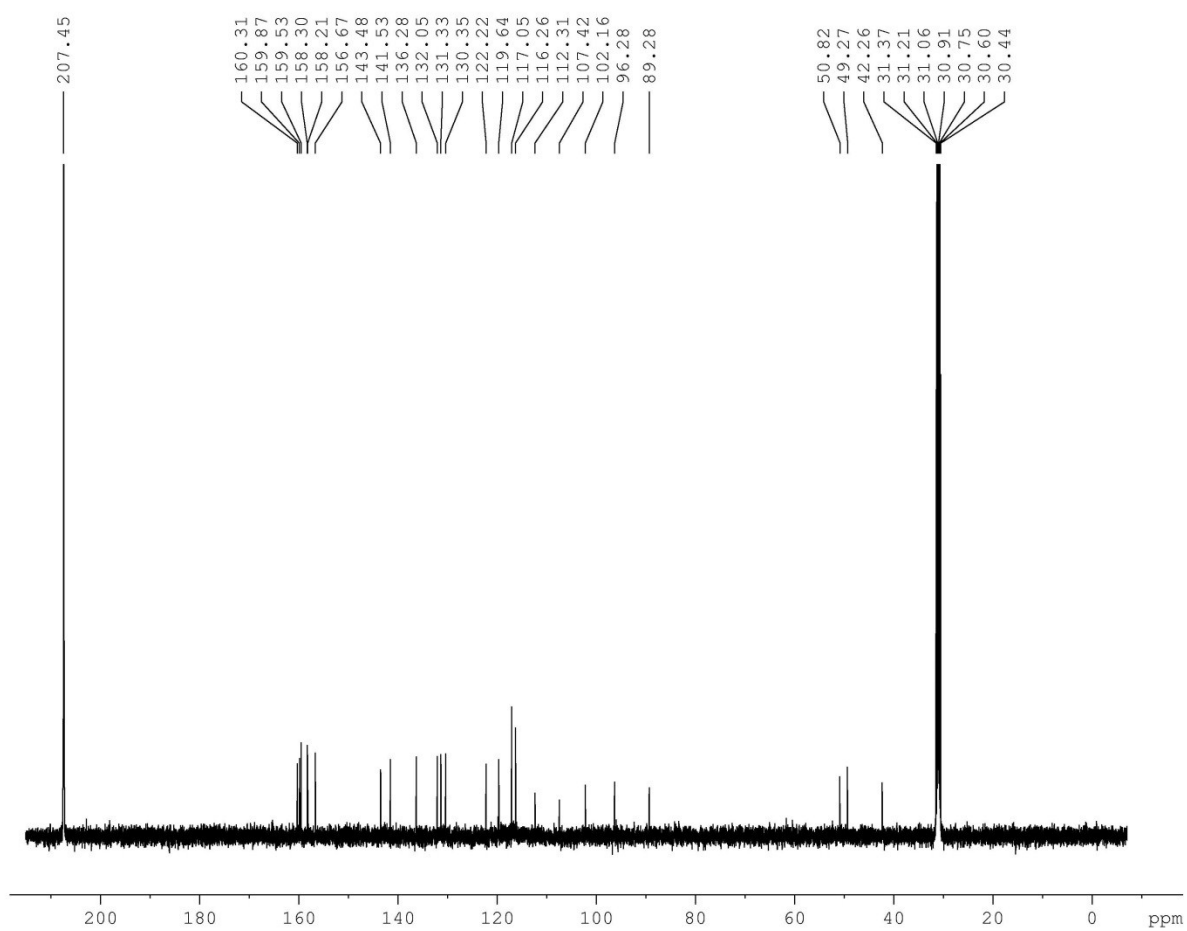


Figure S10 ^1H - ^1H COSY Spectrum of Compound 2, (-)-hopeaphenol, (CD_3COCD_3)

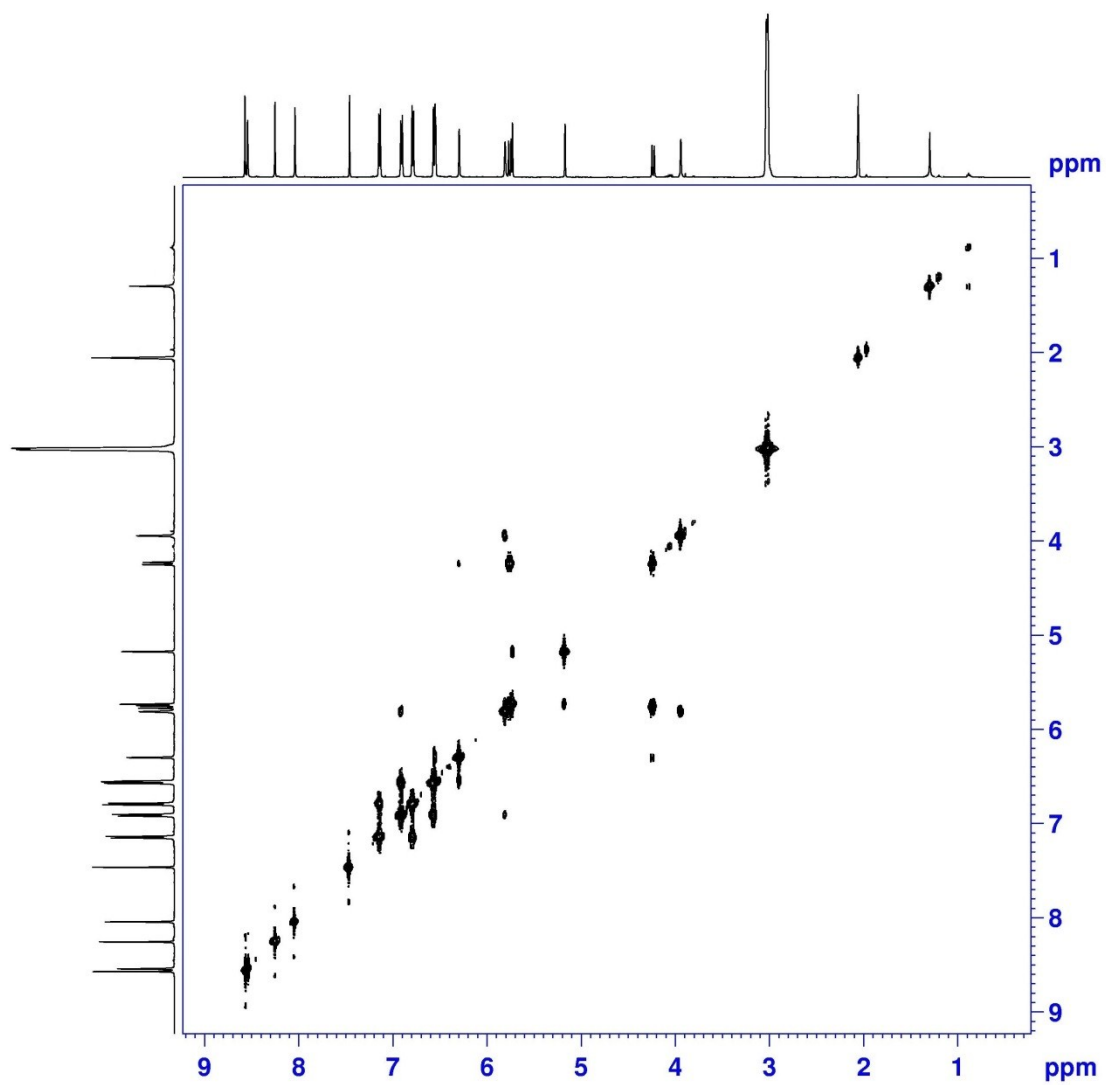


Figure S11 HMQC-Spectrum of Compound 2, (-)-hopeaphenol, (CD_3COCD_3)

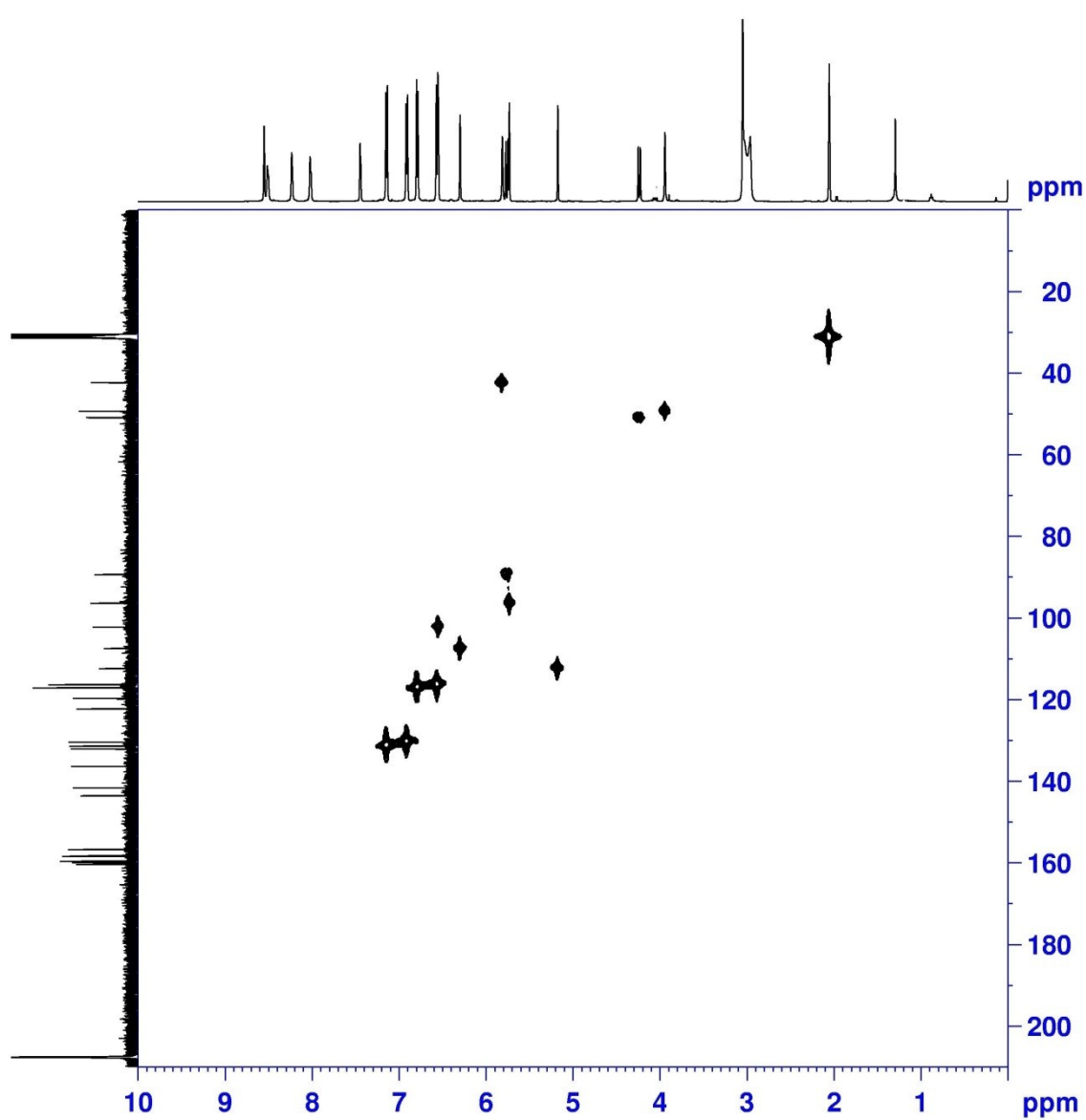


Figure S12 DEPT-135 Spectrum of Compound 2,(-)-hopeaphenol, (CD₃COCD₃)

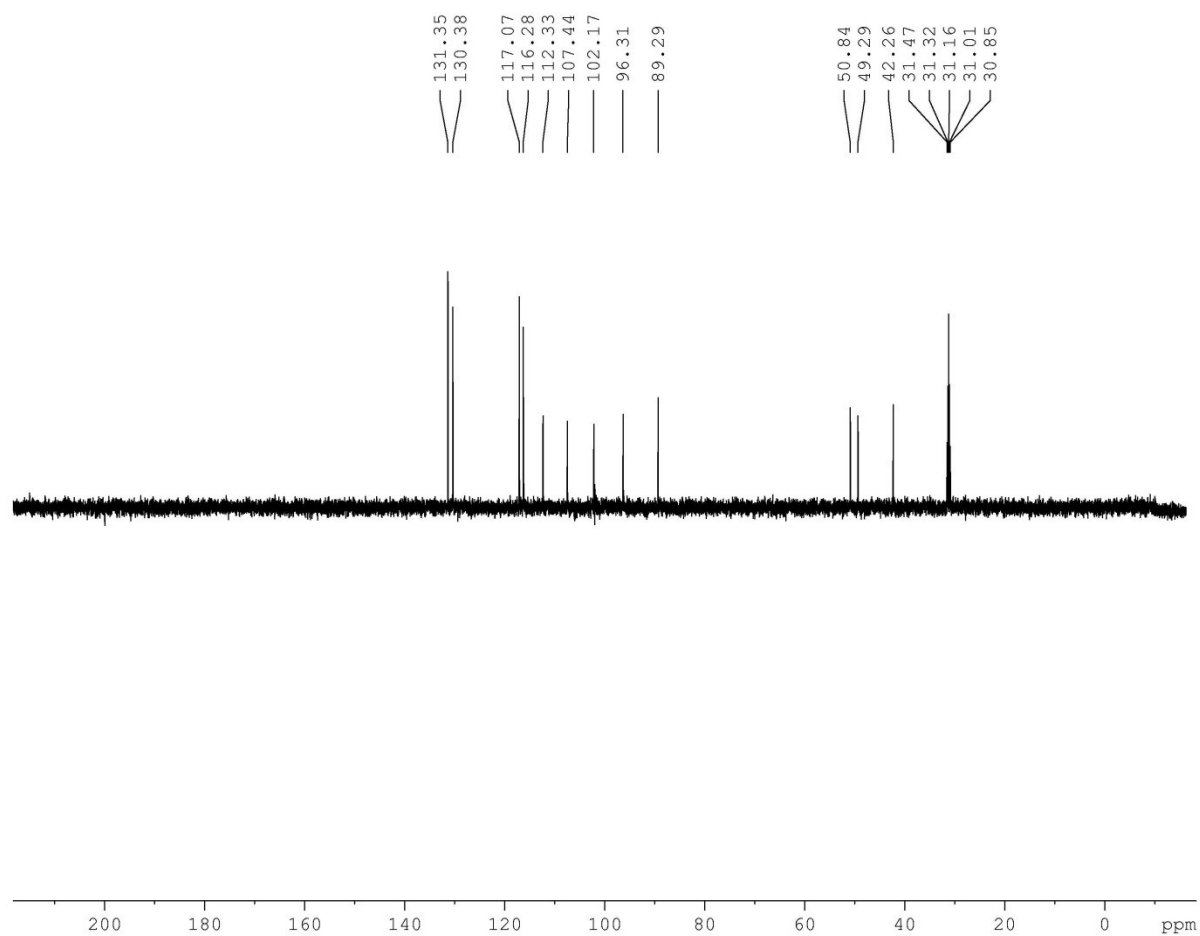


Figure S13 HMBC Spectrum of Compound 2, (-)- hopeaphenol, (CD₃COCD₃)

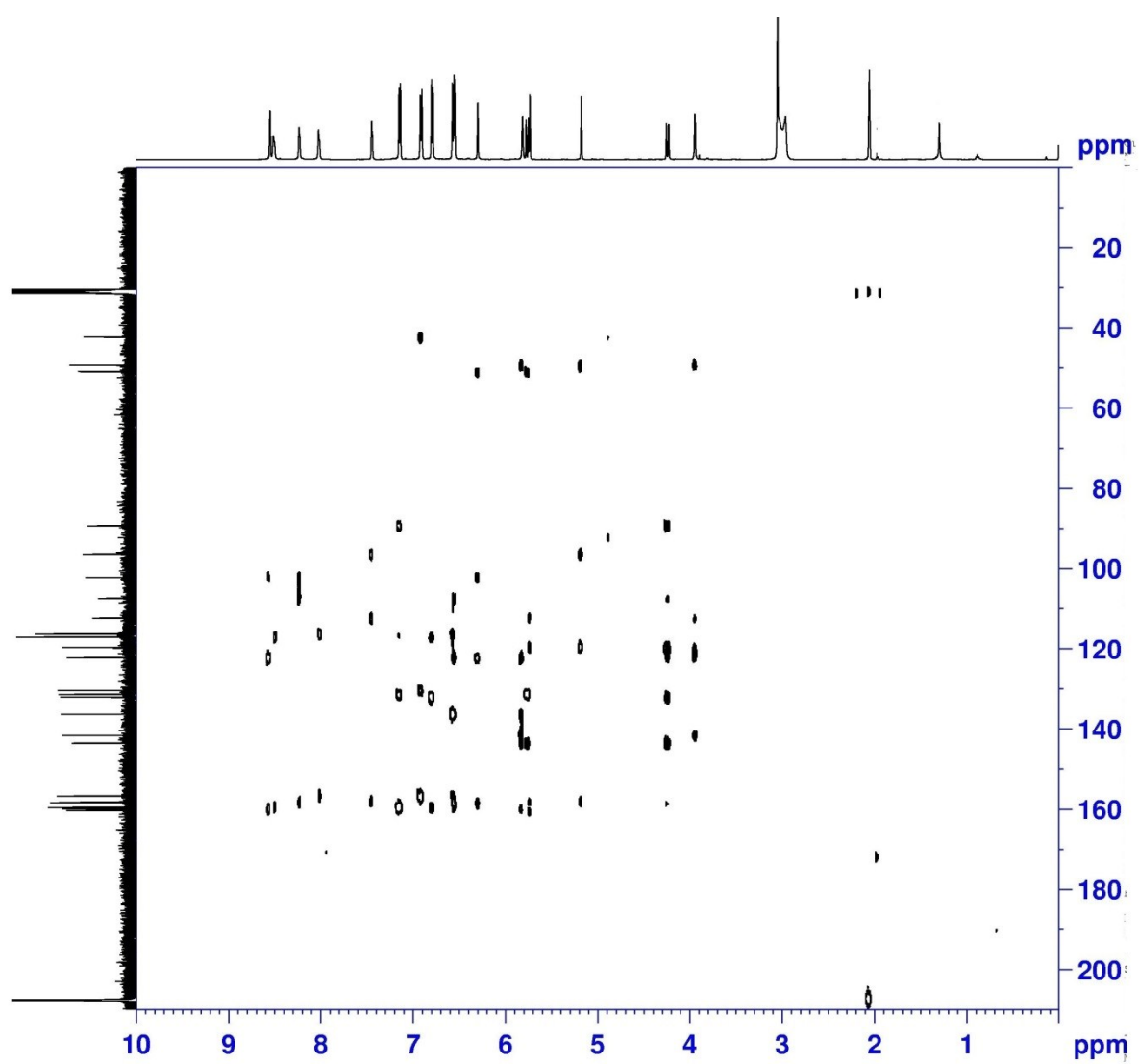


Figure S14 NOESY Spectrum of Compound 2, (-)- hopeaphenol, (CD₃COCD₃)

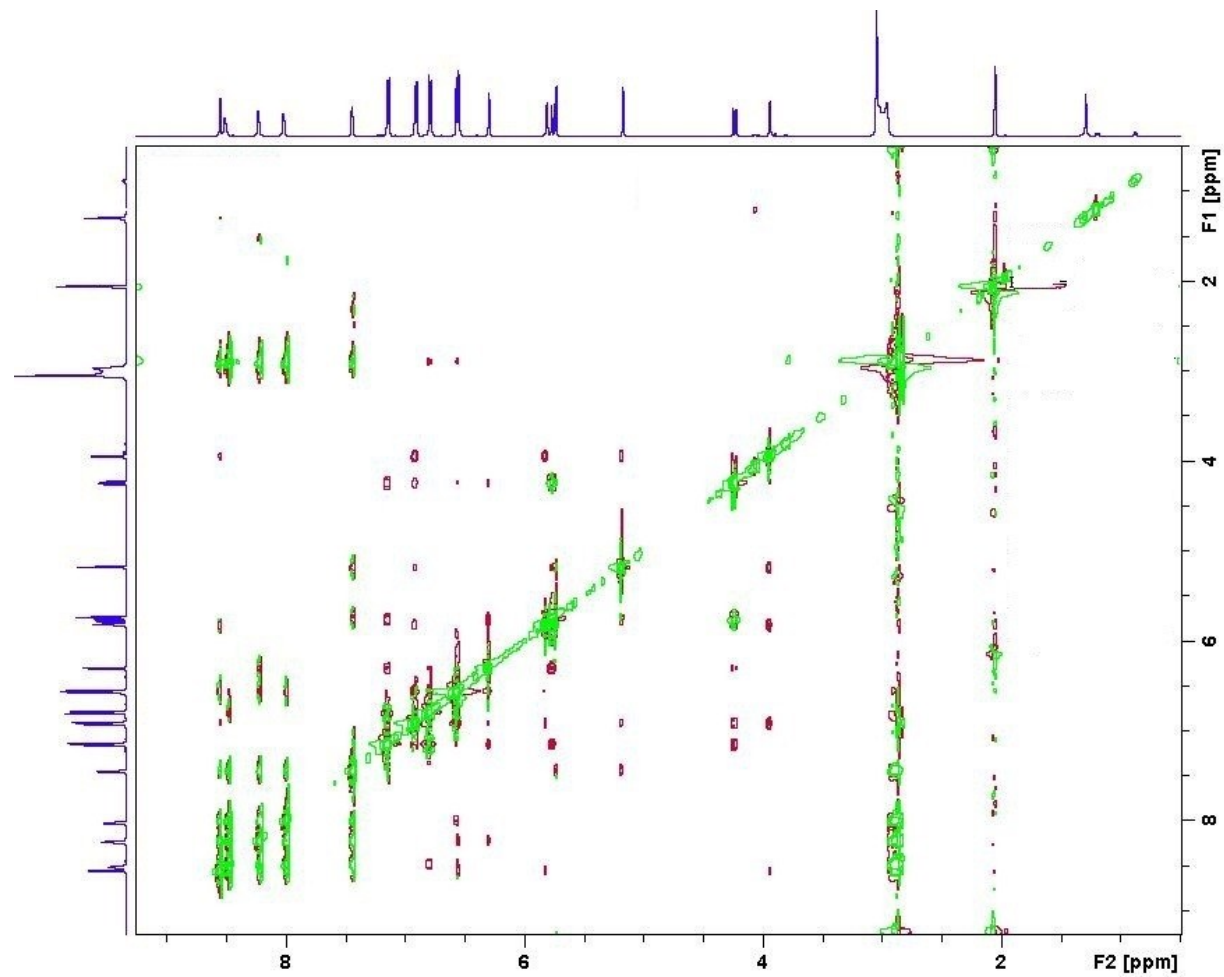
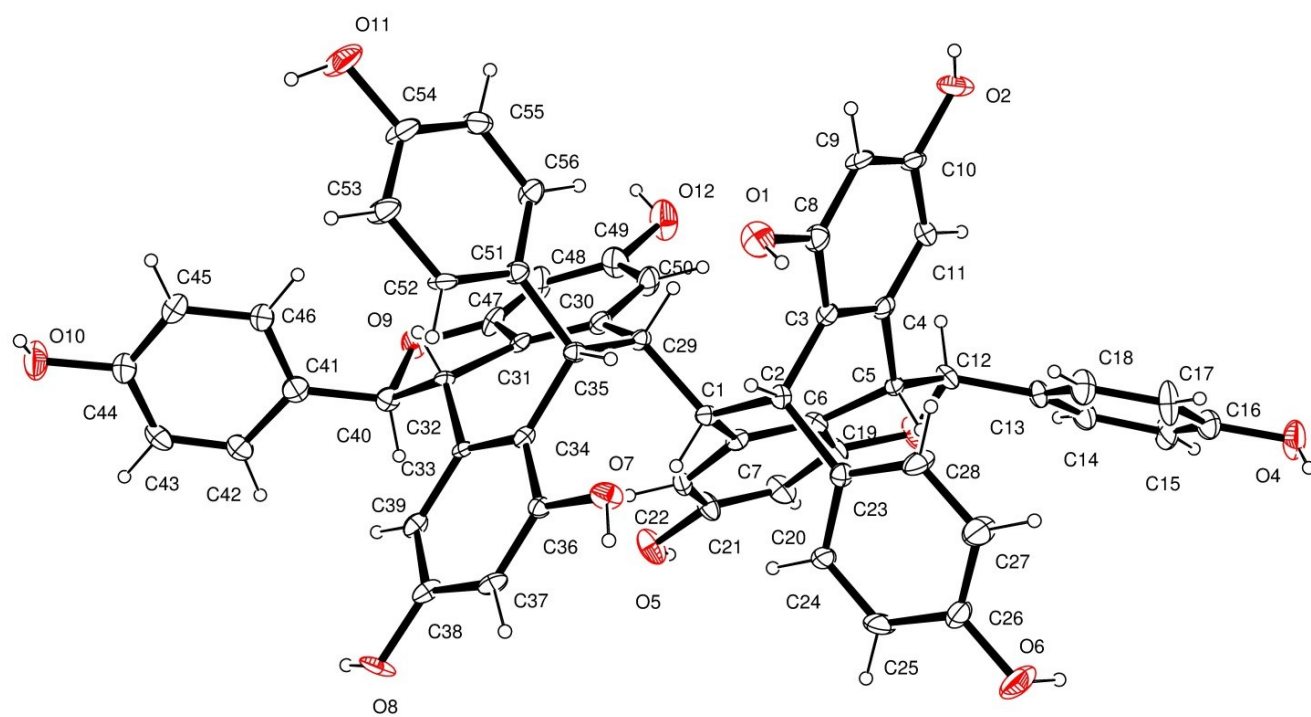


Figure S15 ORTEP Structure of Compound 1, (+)- hopeaphenol



X-ray crystallographic details of (+)-hopeaphenol

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_audit_creation_method SHELXL-2014

_chemical_name_systematic

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety 'C₅₆ H₄₂ O₁₂'

_chemical_formula_sum 'C₅₆ H₄₂ O₁₂'

_chemical_formula_weight 906.89

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_atom_type_description

_atom_type_scatter_dispersion_real

_atom_type_scatter_dispersion_imag

_atom_type_scatter_source

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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'H' 'H' 0.0000 0.0000

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'O' 'O' 0.0106 0.0060

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_space_group_name_Hall      'P 2ac 2ab'

```

```

_shelx_space_group_comment

```

```

;
```

The symmetry employed for this shelxl refinement is uniquely defined by the following loop, which should always be used as a source of symmetry information in preference to the above space-group names.

They are only intended as comments.

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loop_

```

```

_space_group_symop_operation_xyz

```

```

'x, y, z'

```

```

'x+1/2, -y+1/2, -z'

```

```

'-x, y+1/2, -z+1/2'

```

```

'-x+1/2, -y, z+1/2'

```

```

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```

```

_cell_length_b      20.8486(7)

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```

_cell_length_c      24.0242(9)

```

```

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```

```

_cell_angle_beta     90

```

```

_cell_angle_gamma    90

```

```

_cell_volume         5623.9(3)

```

```

_cell_formula_units_Z      4

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```

_cell_measurement_temperature  296(2)

```

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 _exptl_crystal_density_method 'not-measured'
 _exptl_crystal_density_diffn 1.071
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 _exptl_crystal_size_min 0.150
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 _shelx_estimated_absorpt_T_max 0.989
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 _exptl_absorpt_correction_T_max 0.9888
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 _exptl_special_details
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 _diffn_radiation_wavelength 0.71073
 _diffn_radiation_type MoK\alpha

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 _diffrn_detector_area_resol_mean 0
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 _diffrn_reflns_av_unetl/netl 0.1198
 _diffrn_reflns_av_R_equivalents 0.0654
 _diffrn_reflns_limit_h_min -13
 _diffrn_reflns_limit_h_max 11
 _diffrn_reflns_limit_k_min -24
 _diffrn_reflns_limit_k_max 24
 _diffrn_reflns_limit_l_min -28
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 _diffrn_reflns_theta_max 24.999
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 _diffrn_measured_fraction_theta_full 0.972
 _diffrn_reflns_Laue_measured_fraction_max 0.999
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_reflns_Friedel_fraction_max 0.946

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_reflns_special_details

Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

Structure factors included contributions from the .fab file.

_reflns_Friedel_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences

_computing_data_collection 'Bruker APEX2'

_computing_cell_refinement 'Bruker SAINT'

_computing_data_reduction 'Bruker SAINT'

_computing_structure_solution 'SHELXL-2014 (Sheldrick, 2013)'

_computing_structure_refinement 'SHELXL-2014 (Sheldrick, 2014)'

_computing_molecular_graphics 'Bruker SHELXTL'

_computing_publication_material 'Bruker SHELXTL'

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_refine_ls_matrix_type full

_refine_ls_weighting_scheme calc

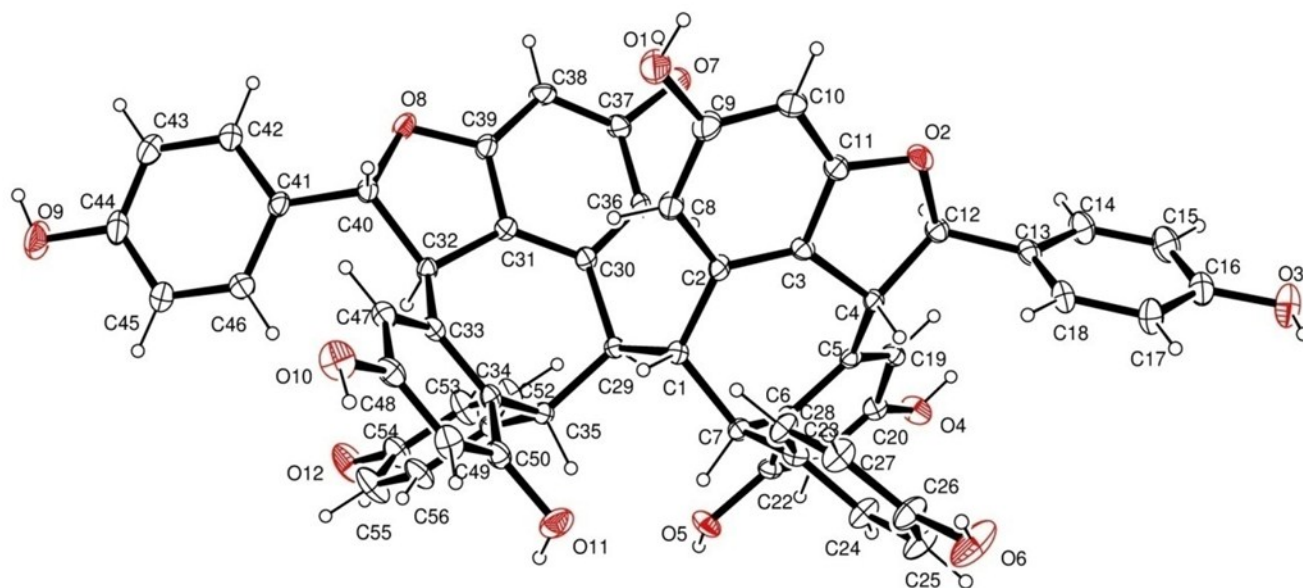
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 _refine_ls_extinction_coef .
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 (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
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 _refine_ls_restrained_S_all 1.011
 _refine_ls_shift/su_max 0.001
 _refine_ls_shift/su_mean 0.000

Figure S16 ORTEP Structure of Compound 2, (-)- hopeaphenol



X-ray crystallographic details of (-)-hopeaphenol

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_audit_creation_method SHELXL-2014

_chemical_name_systematic

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety 'C₅₆ H₄₂ O₁₂'

_chemical_formula_sum 'C₅₆ H₄₂ O₁₂'

_chemical_formula_weight 906.89

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scatter_dispersion_real

_atom_type_scatter_dispersion_imag

_atom_type_scatter_source

'C' 'C' 0.0033 0.0016

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'H' 'H' 0.0000 0.0000

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'O' 'O' 0.0106 0.0060

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_space_group_crystal_system orthorhombic

_space_group_IT_number 19

_space_group_name_H-M_alt 'P 21 21 21'

_space_group_name_Hall 'P 2ac 2ab'

_shelx_space_group_comment

The symmetry employed for this shelxl refinement is uniquely defined by the following loop, which should always be used as a source of symmetry information in preference to the above space-group names.

They are only intended as comments.

loop_

_space_group_symop_operation_xyz

'x, y, z'

'x+1/2, -y+1/2, -z'

'-x, y+1/2, -z+1/2'

'-x+1/2, -y, z+1/2'

_cell_length_a 11.2315(2)

_cell_length_b 20.8456(5)

_cell_length_c 24.0263(6)

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 90

_cell_volume 5625.2(2)

_cell_formula_units_Z 4

_cell_measurement_temperature 296(2)

_cell_measurement_reflns_used 6862

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_cell_measurement_theta_max 24.75

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_reflns_Friedel_fraction_full 0.909

_reflns_special_details

Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

Structure factors included contributions from the .fab file.

_reflns_Friedel_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.

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_computing_cell_refinement 'Bruker SAINT'

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_computing_structure_solution 'SHELXL-2014 (Sheldrick, 2013)'

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_computing_molecular_graphics 'Bruker SHELXTL'

_computing_publication_material 'Bruker SHELXTL'

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_refine_ls_structure_factor_coef Fsqd

_refine_ls_matrix_type full

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_refine_ls_weighting_details

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_atom_sites_solution_hydrogens geom

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 _refine_ls_extinction_coef .
 _refine_ls_abs_structure_details
 Flack x determined using 2604 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$
 (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
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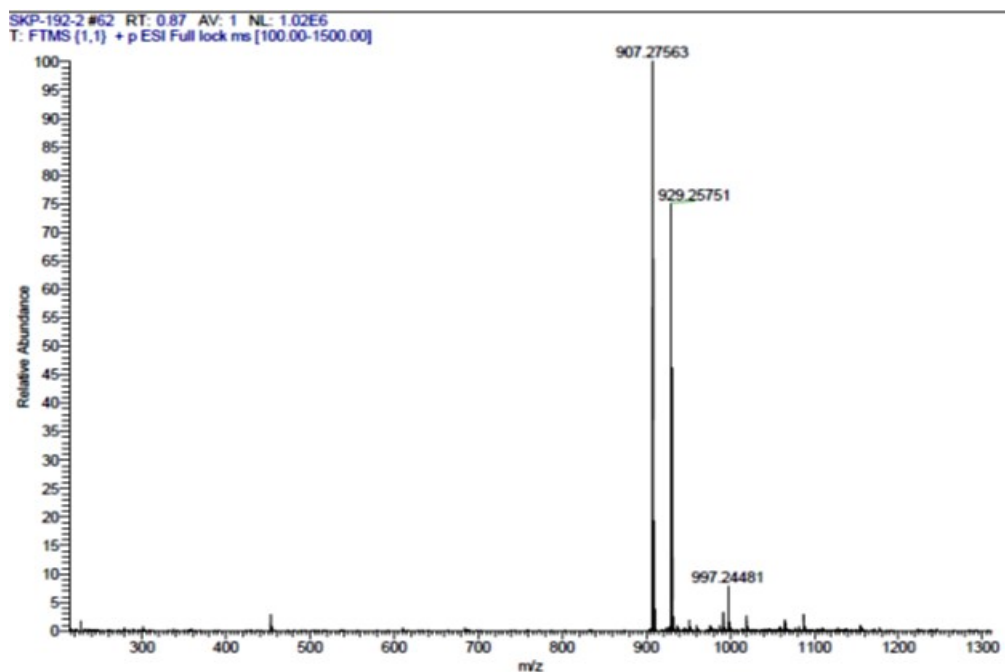


Figure S17 HRMS Spectrum of Compound 1 (+)-hopeaphenol

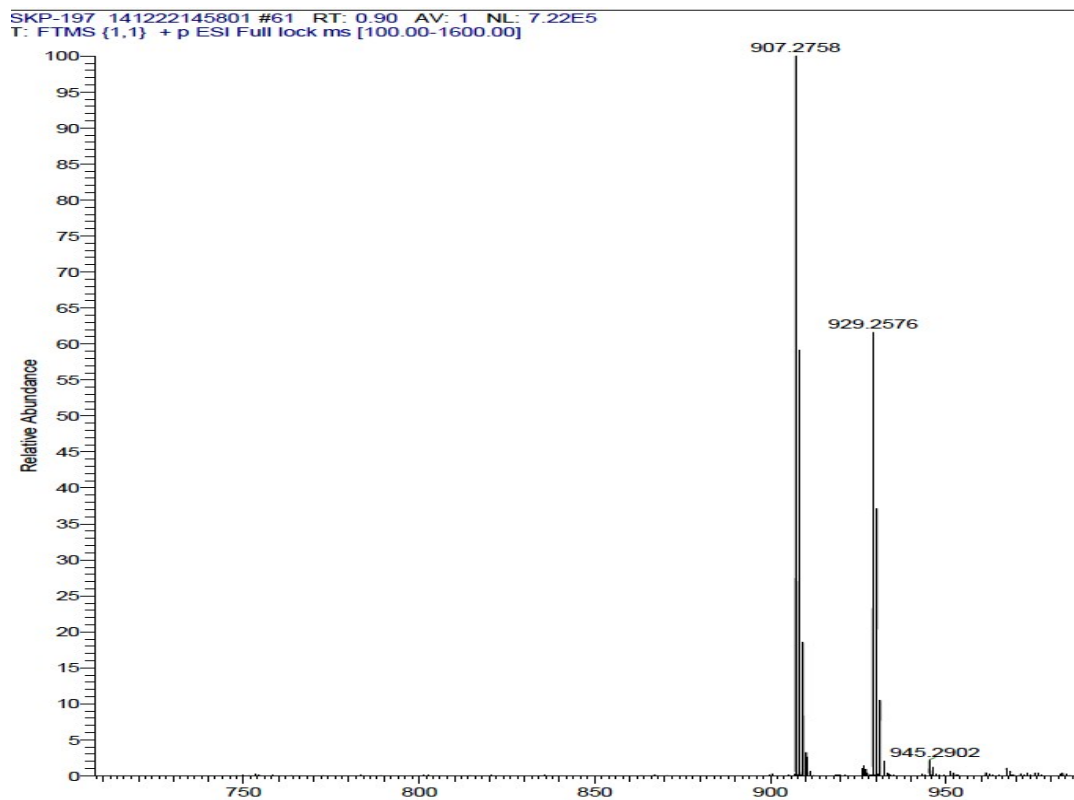
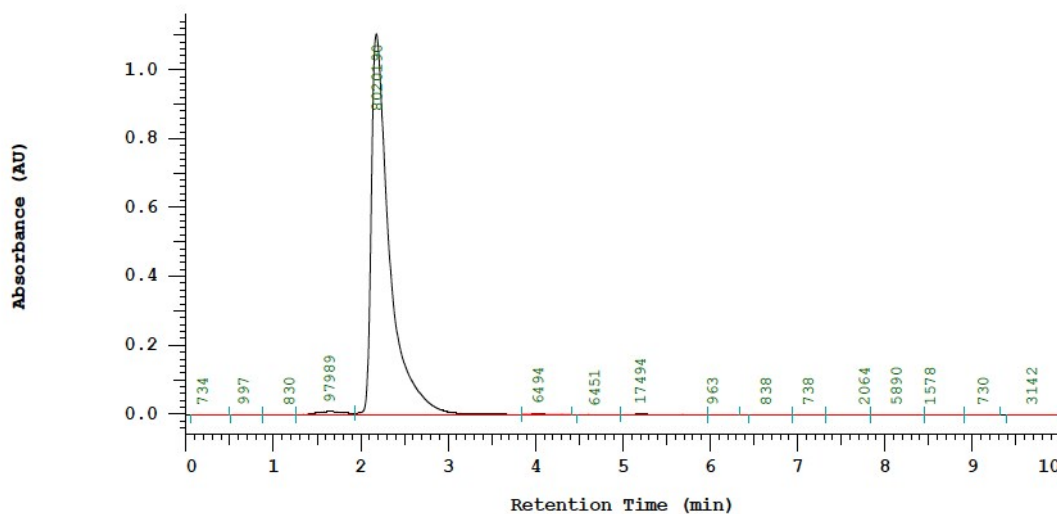


Figure S18 HRMS Spectrum of Compound 2 (-)-hopeaphenol

Sample Name: (+)-hopeaphenol
Sample Description:

Chrom Type: Fixed WL Chromatogram, 254 nm



Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

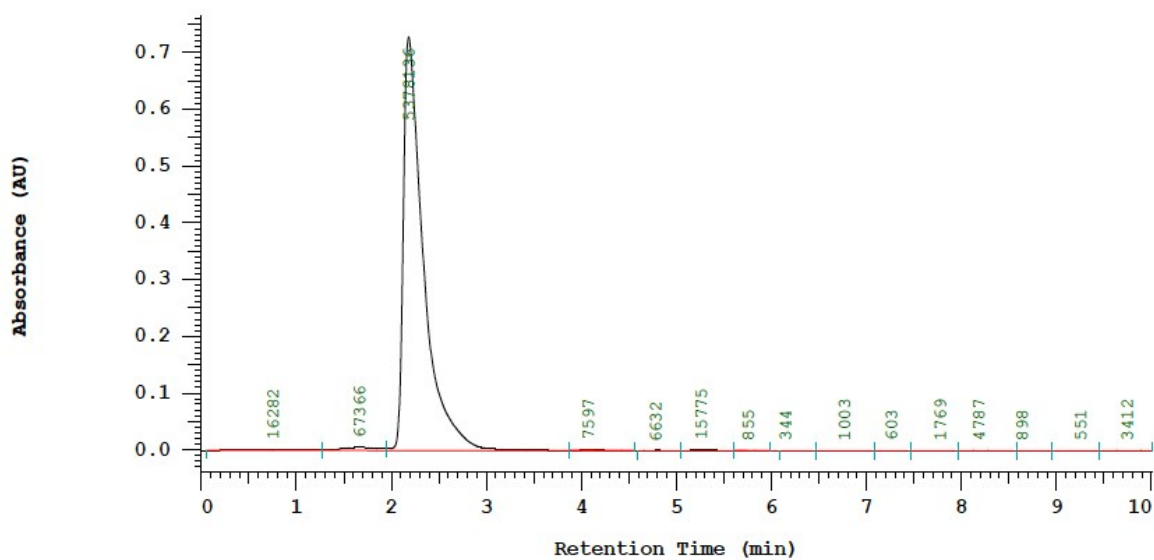
No.	RT	Name	Area	Height	Area %	Purity
1	0.19		734	58	0.009	0.9889
2	0.66		997	108	0.012	0.9899
3	1.18		830	62	0.010	0.9487
4	1.65		97989	4705	1.200	0.9985
5	2.18		8020190	552461	98.201	0.9964
6	4.03		6494	401	0.080	0.0547
7	4.75		6451	362	0.079	-0.0851
8	5.20		17494	641	0.214	0.9111
9	6.03		963	63	0.012	0.9950
10	6.64		838	58	0.010	0.9411
11	7.12		738	48	0.009	0.9464
12	7.76		2064	117	0.025	0.9788
13	8.13		5890	248	0.072	0.9893
14	8.51		1578	102	0.019	0.9879
15	9.12		730	54	0.009	0.9904
16	9.68		3142	175	0.038	0.9820
			8167122	559663	100.000	

Peak rejection level: 0

Figure S19 HPLC Profile of Compound 1 (+)-hopeaphenol

Sample Name: (-)- hopeaphenol
Sample Description:

Chrom Type: Fixed WL Chromatogram, 254 nm



Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

No.	RT	Name	Area	Height	Area %	Purity
1	0.75		16282	377	0.296	-0.9401
2	1.67		67366	2850	1.224	0.9188
3	2.18		5378136	364113	97.677	0.9943
4	4.07		7597	411	0.138	0.9967
5	4.80		6632	385	0.120	0.9994
6	5.26		15775	633	0.287	0.9999
7	5.75		855	70	0.016	0.9997
8	6.15		344	18	0.006	0.9999
9	6.77		1003	67	0.018	0.9996
10	7.26		603	46	0.011	0.9997
11	7.77		1769	110	0.032	0.9999
12	8.18		4787	209	0.087	1.0000
13	8.64		898	63	0.016	0.9999
14	9.25		551	46	0.010	1.0000
15	9.75		3412	213	0.062	0.9999
			5506010	369611	100.000	

Peak rejection level: 0

Figure S20 HPLC Profile of Compound 2 (-)-hopeaphenol

Materials and Methods used for preliminary biological screening of different extracts of VI and AI

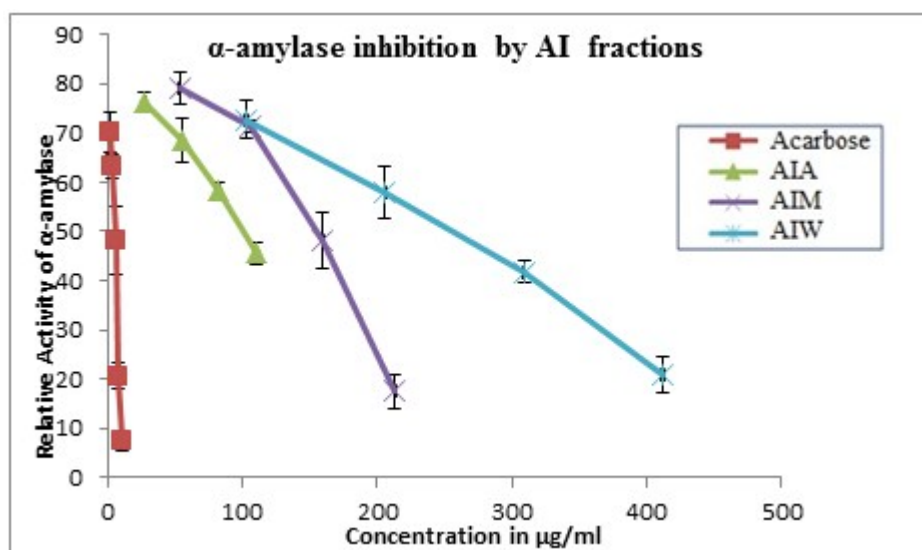


Figure S21 Graph showing the relative decrease in the activity of α -Amylase by the fractions of AI

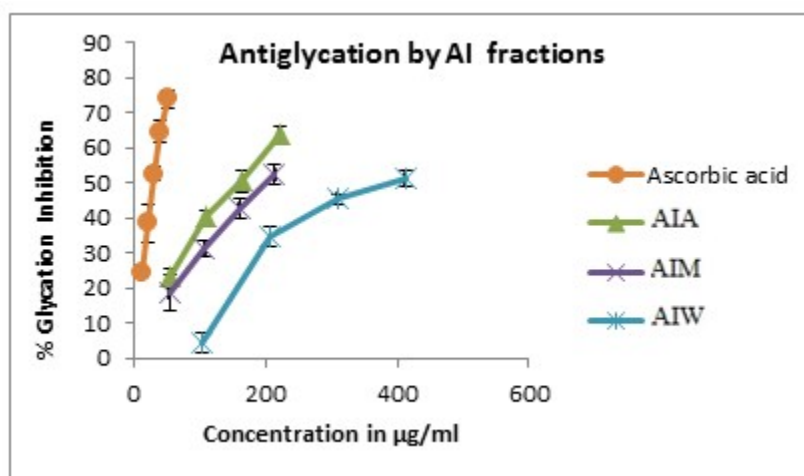


Figure S22 Graph showing the % Inhibition of glycation by fractions of AI

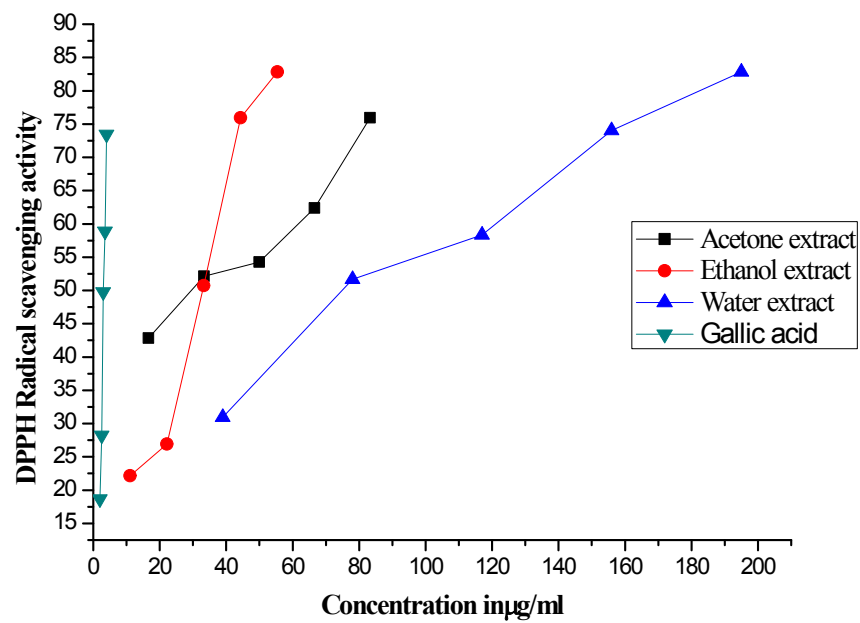


Figure S23 Graph showing the DPPH Radical scavenging activity by fractions of VI

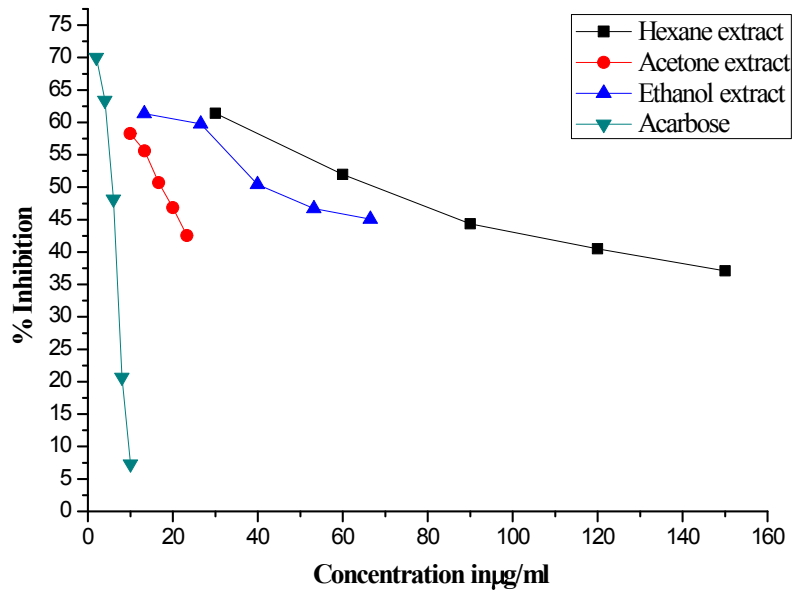


Figure S24 α -Amylase inhibition activity of different extracts of VI