Combined Prioritization and Dereplication Based Rapid Identification of New 8-Alkylated Coumarine: Podurins A and B from Leaves of *Murraya paniculata* and Cytotoxic Evaluation†

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†This paper is offered in memory of Professor Ramarao Poduri (June 30, 1955 - December 7, 2024); our teacher and a researcher of pharmacology and toxicology, former director of NIPER Mohali.

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Figure S.1: Schematic representation of isolation scheme

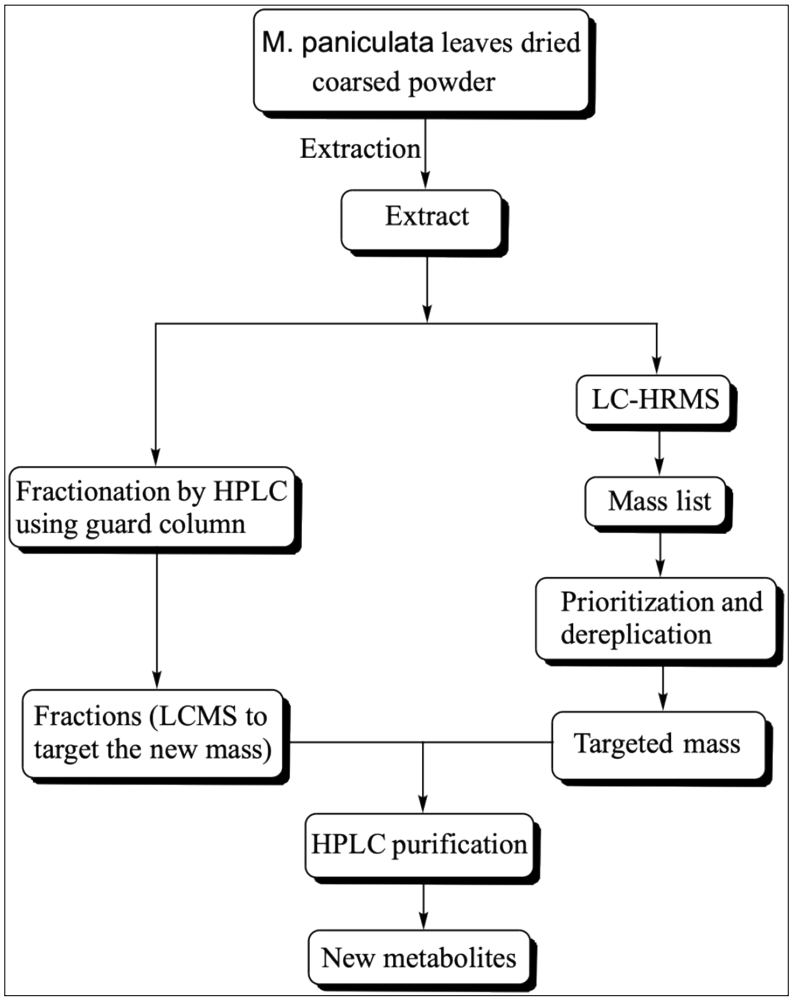

Figure S.2. NMR Data of Mexoticin and Acacetin

Mexoticin 500 mg, white solid, HRESIMS *m/z* 291.1217 [M+H-H_2O] +1 (calcd for $C_{16}H_{20}O_6$ + H^+ , 308.1260) ^{1}H NMR (500 MHz, $CDCl_3$)δ: 1.32 (6H, d, J= 5), 2.33 (1H, d, J= 20), 2.89 (1H,d, J=5), 3.59 (1H, brs s), 3.94 (6H, d, J=5), 6.14 (1H, d, J=10), 6.35 (1H, S), 7.99 (1H, d, J=5). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 161.2, 155.8, 154.2, 138.8, 111, 107.5, 104, 90.4, 78.5, 73, 56.2, 56, 26.2, 25.1, 23.9.

Acacetin 10mg, powder, HRESIMS *m/z* 285.0757 [M+H]$^+$ (calcd for $C_{16}H_{12}O_5$ + H^+, 284.0685), ^{1}H NMR (600 MHz, dmso-d6)δ: 3.86 (3H, S), 6.21 (1H, d, J= <5), 6.51 (1H, d, J= 6), 6.87 (1H, S), 7.11 (2H, d, J= 12), 8.03 (2H, d, J= 12), 12.92 (1H, S). ^{13}C NMR (151 MHz, dmso-d6) δ: 182.2, 164.9, 163.7, 162.8, 161.9, 157.8, 128.8, 123.3, 115.1, 104.2, 104, 99.4, 94.5, 56.

Spectral information of compound Podurin A

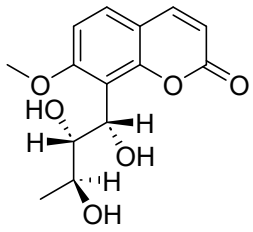

Figure S.3. X-ray data of Podurin A

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sk5c_auto

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

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Datablock: sk5c_auto

Bond precision: C-C = 0.0035 A Wavelength=1.54184

Cell:	a=9.78624(14)	b=14.74804(17) beta=114.7462(18)	c=10.33498(15)
	alpha=90		gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	1354.65(4)	1354.65(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C14 H14 O6	C14 H14 O6
Sum formula	C14 H14 O6	C14 H14 O6
Mr	278.25	278.25
Dx,g cm-3	1.364	1.364
Z	4	4
Mu (mm-1)	0.913	0.913
F000	584.0	584.0
F000’	586.13	
h,k,lmax	11,17,12	11,17,12
Nref	2477	2459

Tmin,Tmax	0.858,0.896	0.467,1.000
Tmin’	0.856	

Correction method= # Reported T Limits: Tmin=0.467 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 68.110

R(reflections)= 0.0599(2137) wR2(reflections)=

0.1851(2459)

S = 1.082 Npar= 186

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

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_refine_diff_density_min given = -0.697 Test value = -0.600

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75 The relevant atom site should be identified.

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -0.70 eA-3
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range
3.4 Ratio PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of
C00H Check PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) .....
O00J Check PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be
LIST 4 Please Check PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.512
Check PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600
6 Report

-5 16 2, -10 9 3, 6 11 4, -5 10 9, -8 8 10, -5 8 11,

Alert level G

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report

H002 H004

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records
1 Report PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0010 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 34
Note

O001	O002	H002	O003	O004	H004	O005	C006

C007	C008	H008	C009	C00A	C00B	H00B	C00C		
C00D	H00D	C00E	H00E	C00F	H00F	C00G	H00G		
C00H H00J	C00I H00K	H00A	H00C	H00H	O00J	C00K	H00I		
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		Chirality	at C008		(Centro	SpGr)		S	Verify
PLAT793_ALERT_4_GModel has		Chirality	at C00B		(Centro	SpGr)		R	Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints 1									Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta (Max) Still 74%									Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 12									Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 5.162									Note
Predicted wR2: Based on SigI**2 3.59 or SHELX Weight 17.11									
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3									Info

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0 ALERT level A = Most likely a serious problem - resolve or explain

0 ALERT level B = A potentially serious problem, consider carefully

9 ALERT level C = Check. Ensure it is not caused by an omission or oversight

16 ALERT level G = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

8	ALERTtype	2	Indicator that the structure model may be wrong or deficient
6	ALERTtype	3	Indicator that the structure quality may be low
6	ALERTtype	4	Improvement, methodology, query or suggestion
2	ALERTtype	5	Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

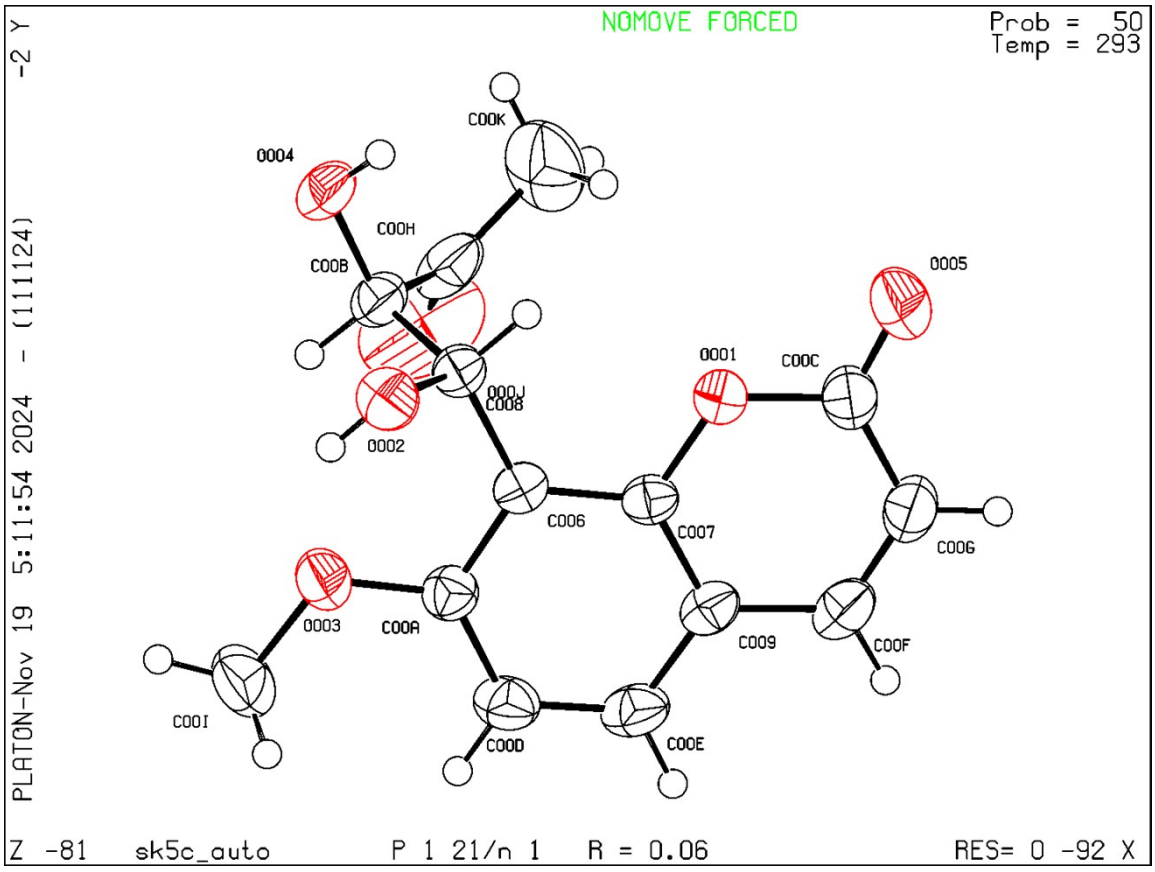
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation); however, if you intend to submit to Acta Crystallographica Section C or E or IUCrData, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the Notes for Authors of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 11/11/2024; check.def file version of 11/11/2024

Datablock sk5c_auto - ellipsoid plot



Spectral information of Podurin B

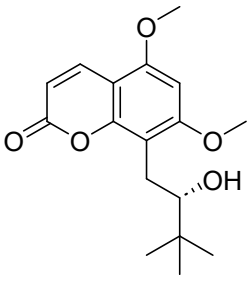


Figure S.4. X-ray data of Podurin B

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sk10a_autored

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sk10a_autored

Bond precision: C-C = 0.0060 A Wavelength=1.54184

Cell:	a=6.7946(1)	b=9.8825(1)	c=22.9394(3)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	1540.33(3)	1540.33(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C17 H22 O5	C17 H22 O5
Sum formula	C17 H22 O5	C17 H22 O5
Mr	306.35	306.34
Dx,g cm-3	1.321	1.321
Z	4	4
Mu (mm-1)	0.795	0.795
F000	656.0	656.0
F000’	658.15	
h,k,lmax	8,11,27	8,11,27
Nref	2812[1650]	2435
Tmin,Tmax	0.895,0.931	0.895,1.000
Tmin’	0.895	

Correction method= # Reported T Limits: Tmin=0.895 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 1.48/0.87 Theta(max)= 68.114

R(reflections)= 0.0566(2173) wR2(reflections)=

0.1984(2435)

S = 1.084 Npar= 206

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT420_ALERT_2_B D-H Bond Without Acceptor O4 --H4 . Please Check

---

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.48 Report
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5
Check PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.006 Ang.

PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report

5 9 6, 7 5 8, 7 3 12, 2 5 24,

PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 69 %

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note PLAT003_ALERT_2_G
Number of Uiso or U(i,j) Restrained non-H-Atoms 2 Report PLAT007_ALERT_5_G Number of Unrefined
Donor-H Atoms ..... 1 Report

H4

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.14 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 2
Report PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records
2 Report PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0010 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at ..... 0.5 Check

H1A	H1B	H1C	H1D	H1E	H1F		
PLAT412_ALERT_2_G	Short Intra	XH3 ..	XHn	H1D	..H2C	.	2.12 Ang.
					x,y,z =	1_555	Check
PLAT415_ALERT_2_G	Short Inter	D-H..H-X		H1C	..H4	.	1.52 Ang.

			1-x,-1/2+y,3/2-z			=	3_646	Check	
PLAT415_ALERT_2_G	Short	Inter	D-H..H-X	H1D	..H4	.	1.96	Ang.	
			1-x,-1/2+y,3/2-z			=	3_646	Check	
PLAT432_ALERT_2_G	Short	Inter	X...Y Contact O4		..C1	.	2.95	Ang.	
1-x,1/2+y,3/2-z						=	3_656	Check	

PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder	!	Report
PLAT791_ALERT_4_G Model has Chirality at C4 (Sohncke SpGr)	S	Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints	3	Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still	72%	Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	7	Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value	8.123	Note
Predicted wR2: Based on SigI**2 2.44 or SHELX Weight	18.30	
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	2	Info

---

0 ALERT level A = Most likely a serious problem - resolve or explain

1 ALERT level B = A potentially serious problem, consider carefully

6 ALERT level C = Check. Ensure it is not caused by an omission or oversight

24 ALERT level G = General information/check it is not something unexpected

2	ALERTtype	1	CIF construction/syntax error, inconsistent or missing data
11	ALERTtype	2	Indicator that the structure model may be wrong or deficient
9	ALERTtype	3	Indicator that the structure quality may be low
7	ALERTtype	4	Improvement, methodology, query or suggestion
2	ALERTtype	5	Informative message, check

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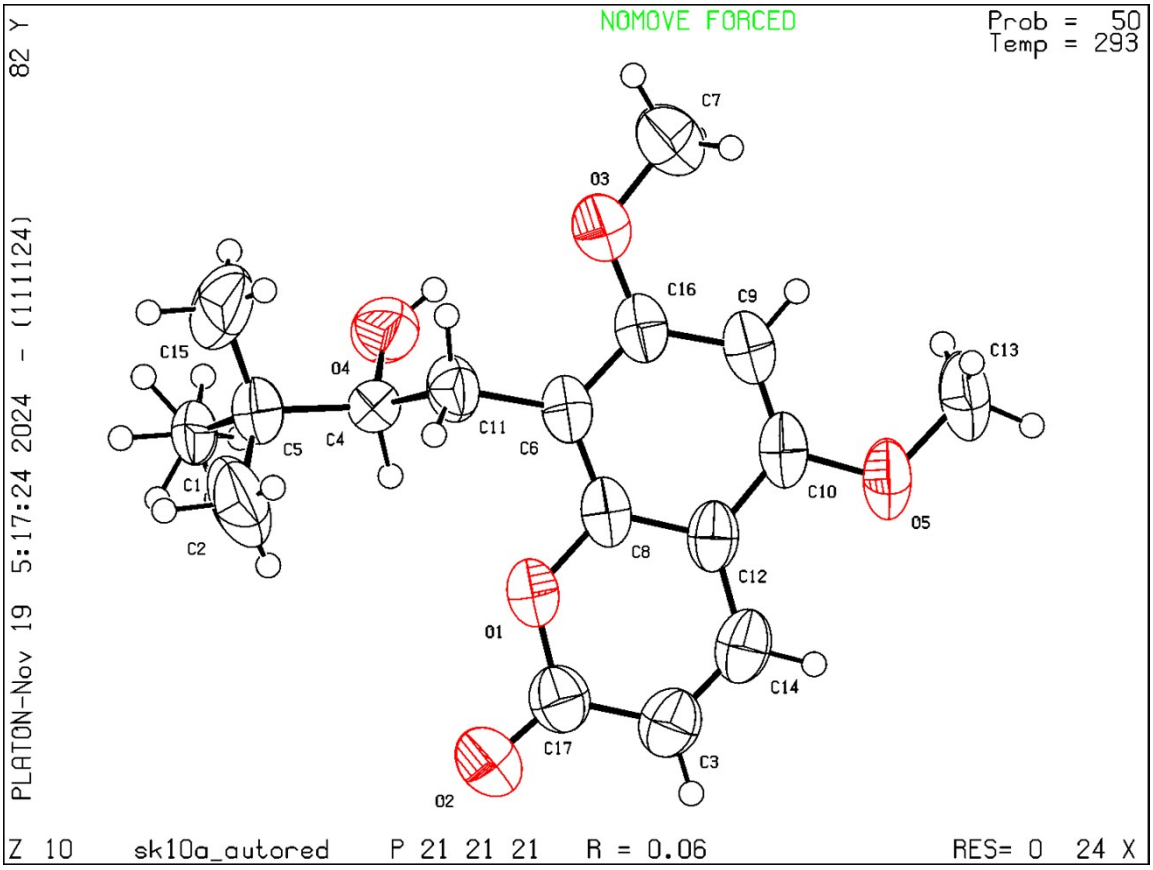
PLATON version of 11/11/2024; check.def file version of 11/11/2024

Datablock sk10a_autored - ellipsoid plot



Spectral information of Mexoticin

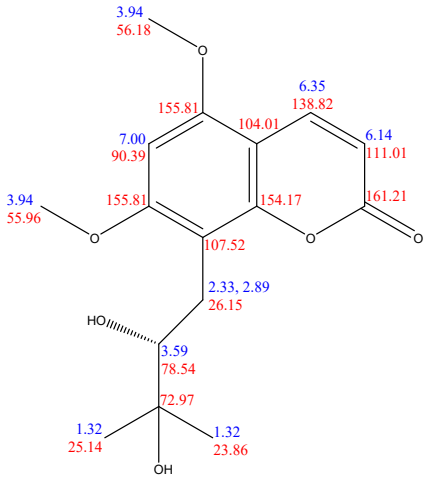


Figure S.5. ^{1}H NMR spectrum of Mexoticin in $CDCl_3$

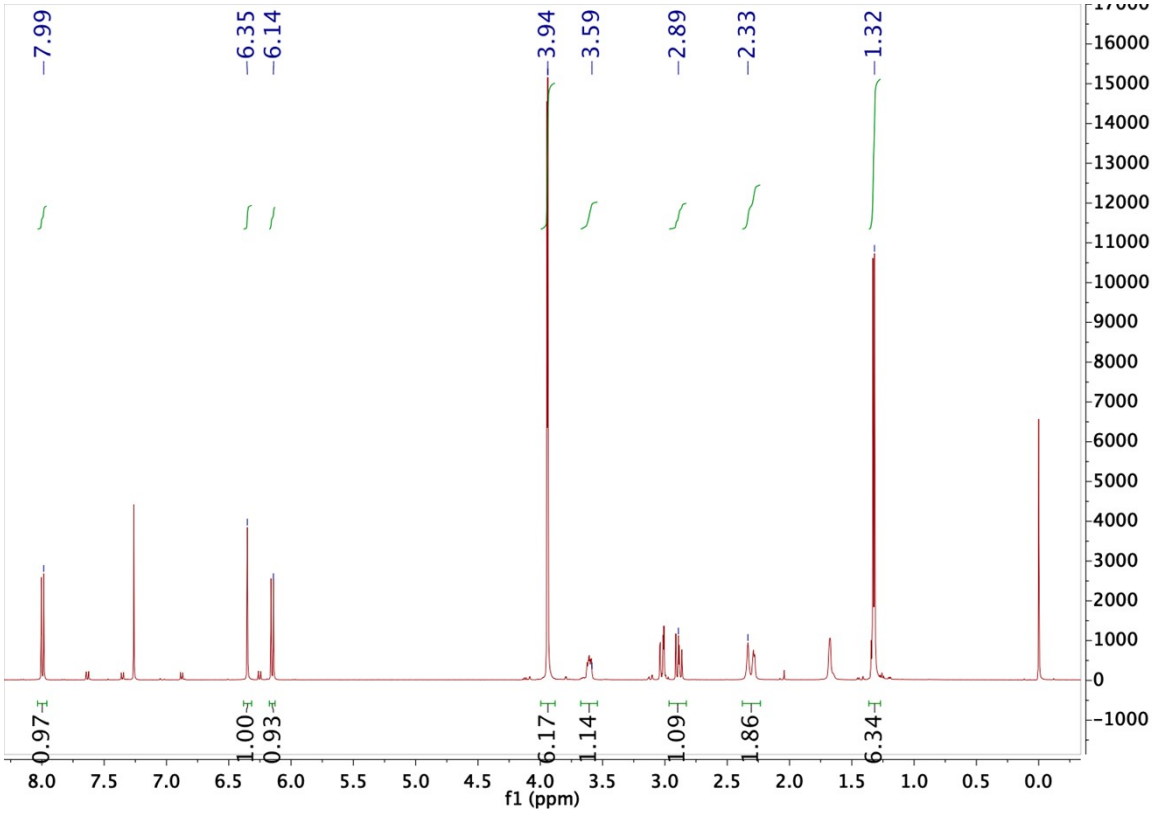


Figure S.6. ^{13}C NMR spectrum of Mexoticin in $CDCl_3$

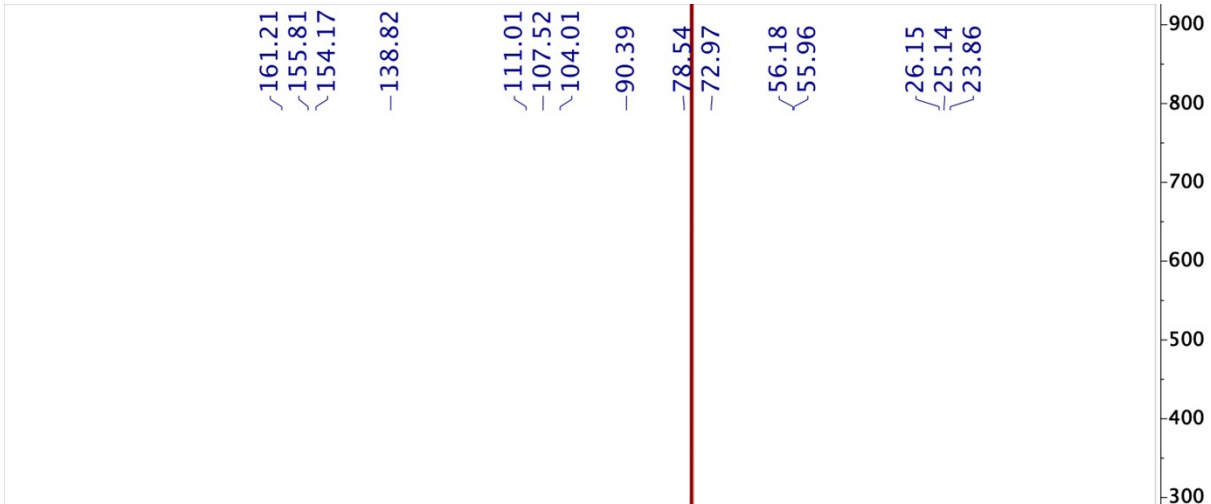
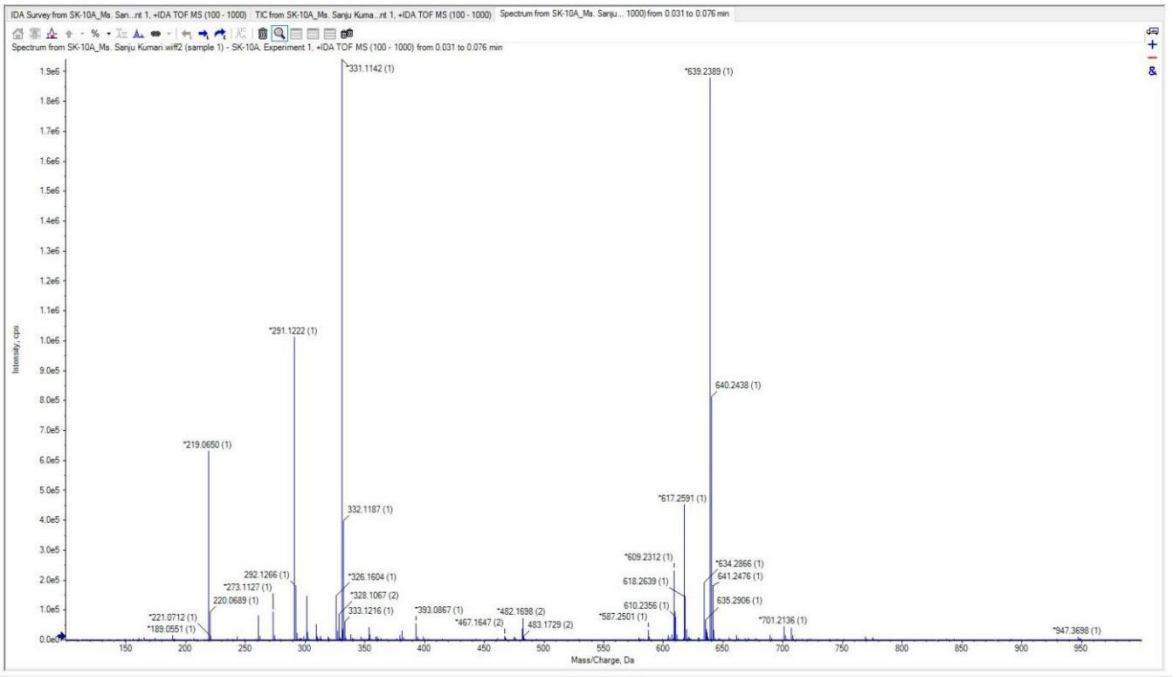


Figure S.7. HRMS spectrum of Mexoticin



Spectral information of Vanillin

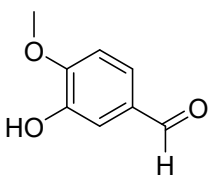


Figure S.8. X-ray data of Vanillin

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sk8c2_auto

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

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Datablock: sk8c2_auto

Bond precision: C-C = 0.0019 A Wavelength=1.54184

Cell:	a=5.9418(1)	b=25.5269(5) beta=94.027(2)	c=4.9770(1)
	alpha=90		gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	753.03(2)	753.03(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C8 H8 O4	C8 H8 O4
Sum formula	C8 H8 O4	C8 H8 O4
Mr	168.14	168.14
Dx,g cm-3	1.483	1.483
Z	4	4
Mu (mm-1)	1.031	1.031
F000	352.0	352.0
F000’	353.33	
h,k,lmax	7,30,5	7,30,5
Nref	1355	1347
Tmin,Tmax	0.857,0.893	0.550,1.000
Tmin’	0.857	

Correction method= # Reported T Limits: Tmin=0.550 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 68.108

R(reflections)= 0.0392(1157) wR2(reflections)=

0.0996(1347)

S = 1.056 Npar= 1

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O003 - H003 . 1.03 Ang.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.427 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report

7 5 0, -3 26 2, 0 22 4, 1 22 4, -4 6 5,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note PLAT007_ALERT_5_G
Number of Unrefined Donor-H Atoms ..... 1 Report

H001

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 20 Note

O001 H001 O002 O003 O004 C005 C006 H006

C007 C008 C009 H009 C00A C00B H00B C00C

H00A H00C H00D H003

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note

PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 76% Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.651 Note

Predicted wR2: Based on SigI**2 2.73 or SHELX Weight 9.43

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

---

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2 ALERTtype 2 Indicator that the structure model may be wrong or deficient

5 ALERTtype 3 Indicator that the structure quality may be low

3 ALERTtype 4 Improvement, methodology, query or suggestion

2 ALERTtype 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

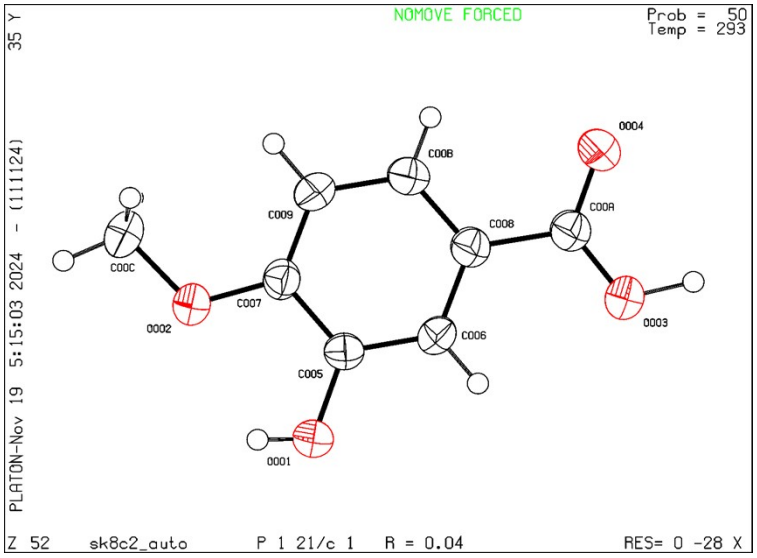
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation); however, if you intend to submit to Acta Crystallographica Section C or E or IUCrData, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the Notes for Authors of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 11/11/2024; check.def file version of 11/11/2024

Datablock sk8c2_auto - ellipsoid plot



Spectral information of Acacetin

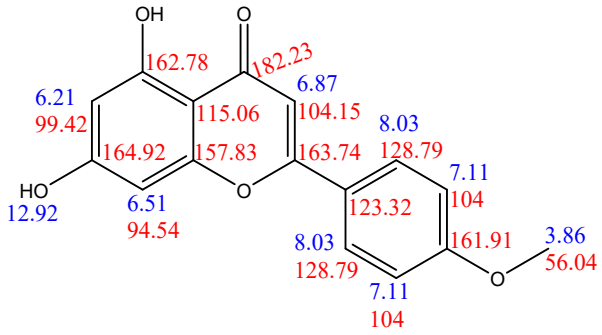


Figure S.9. ^{1}H NMR spectrum of Acacetin in DMSO

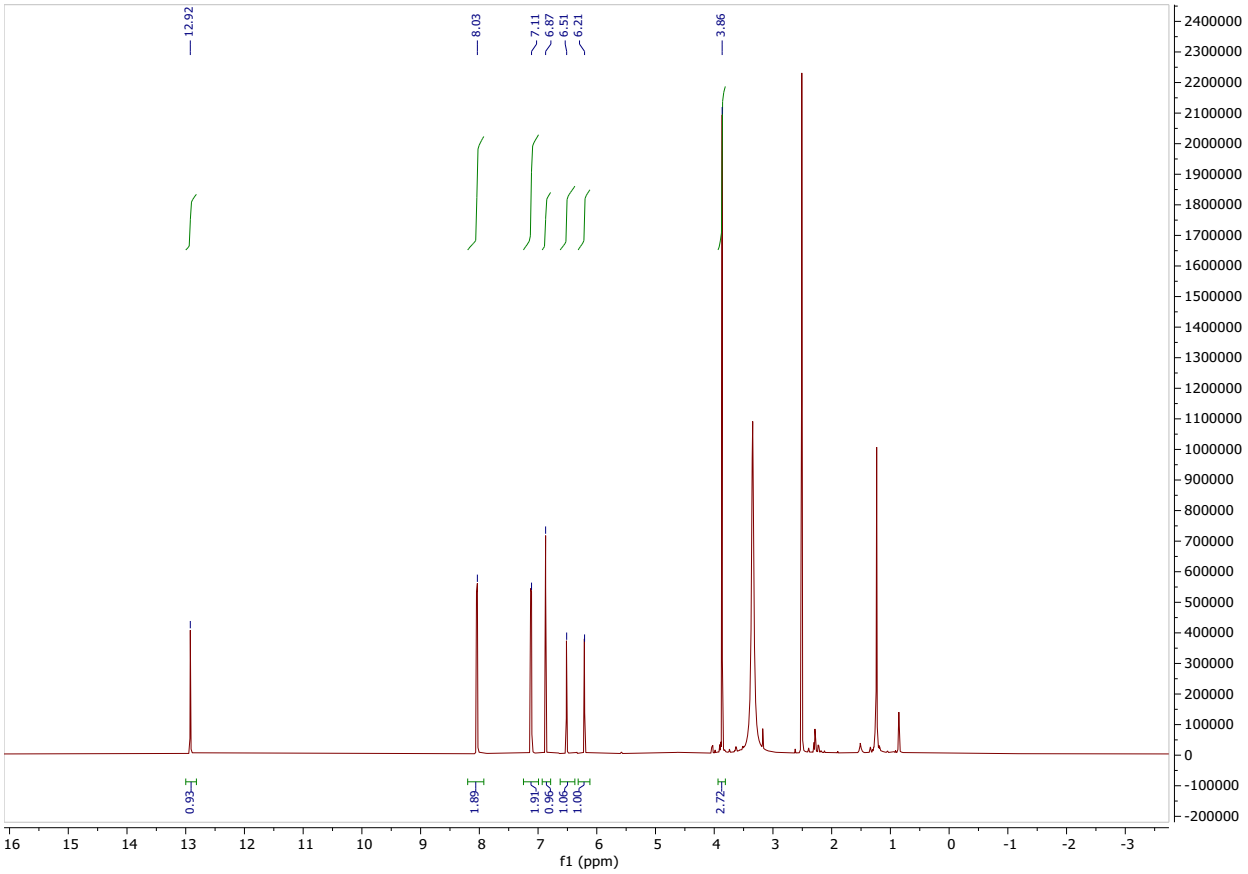


Figure S.10. ^{13}C NMR spectrum of Acacetin in DMSO

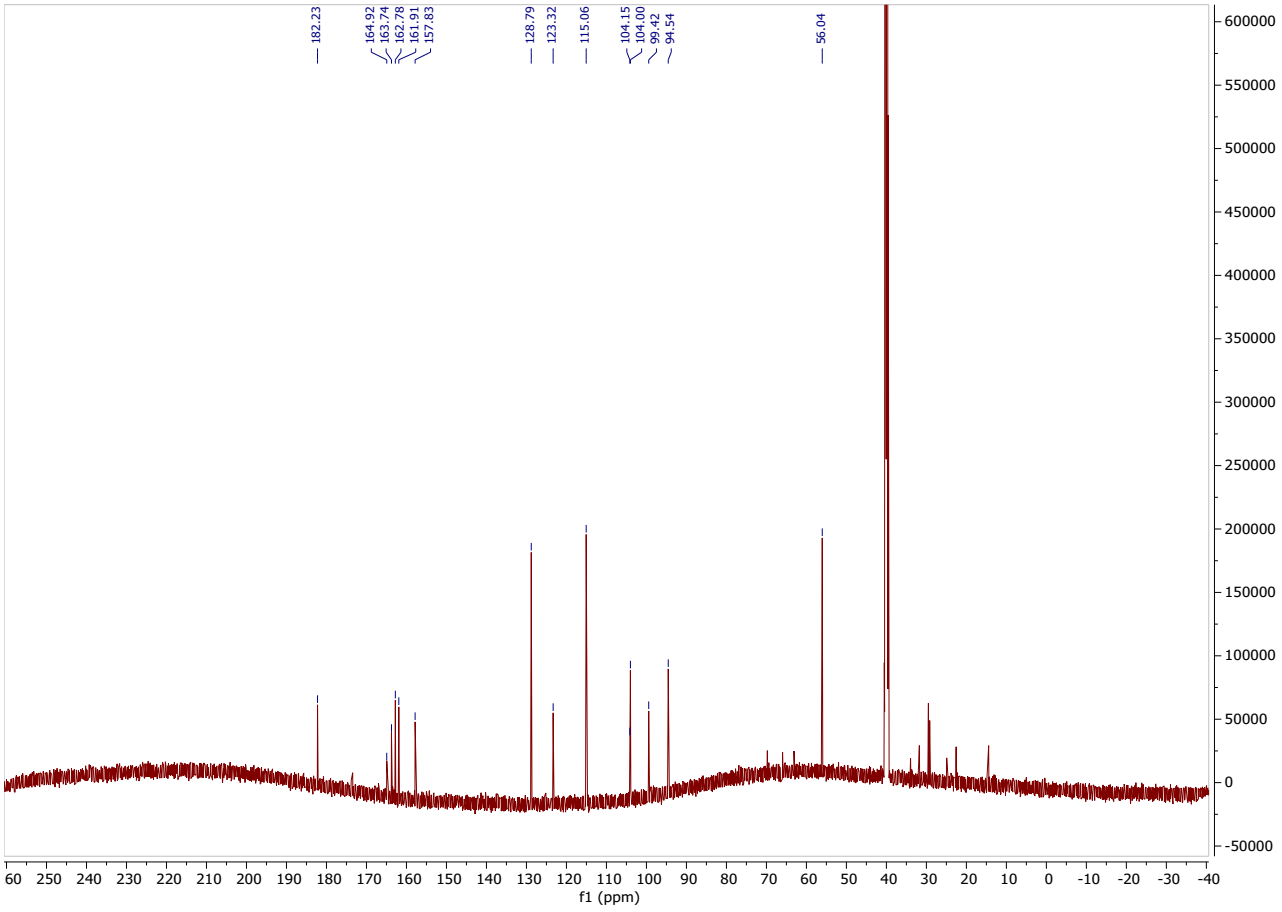


Figure S.11. DEPT-135 NMR spectrum of Acacetin in DMSO

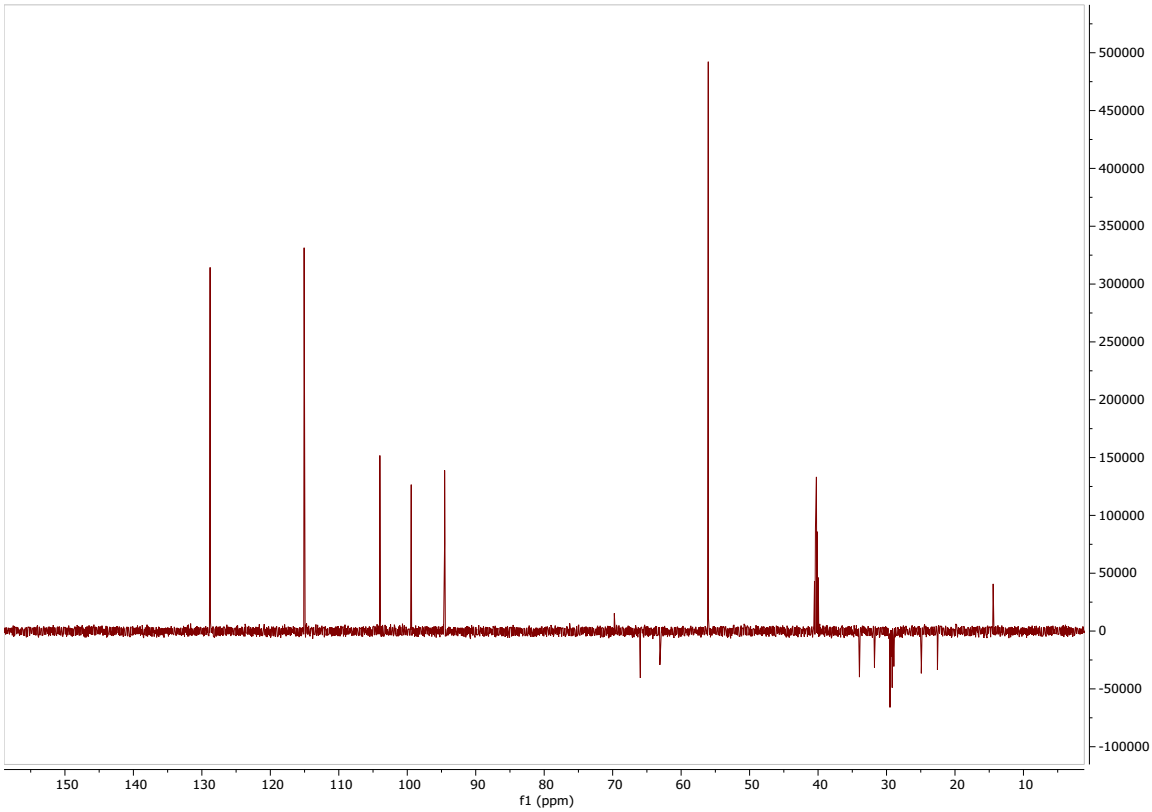


Figure S.12. ^{1}H-^{1}H COSY NMR spectrum of Acacetin in DMSO

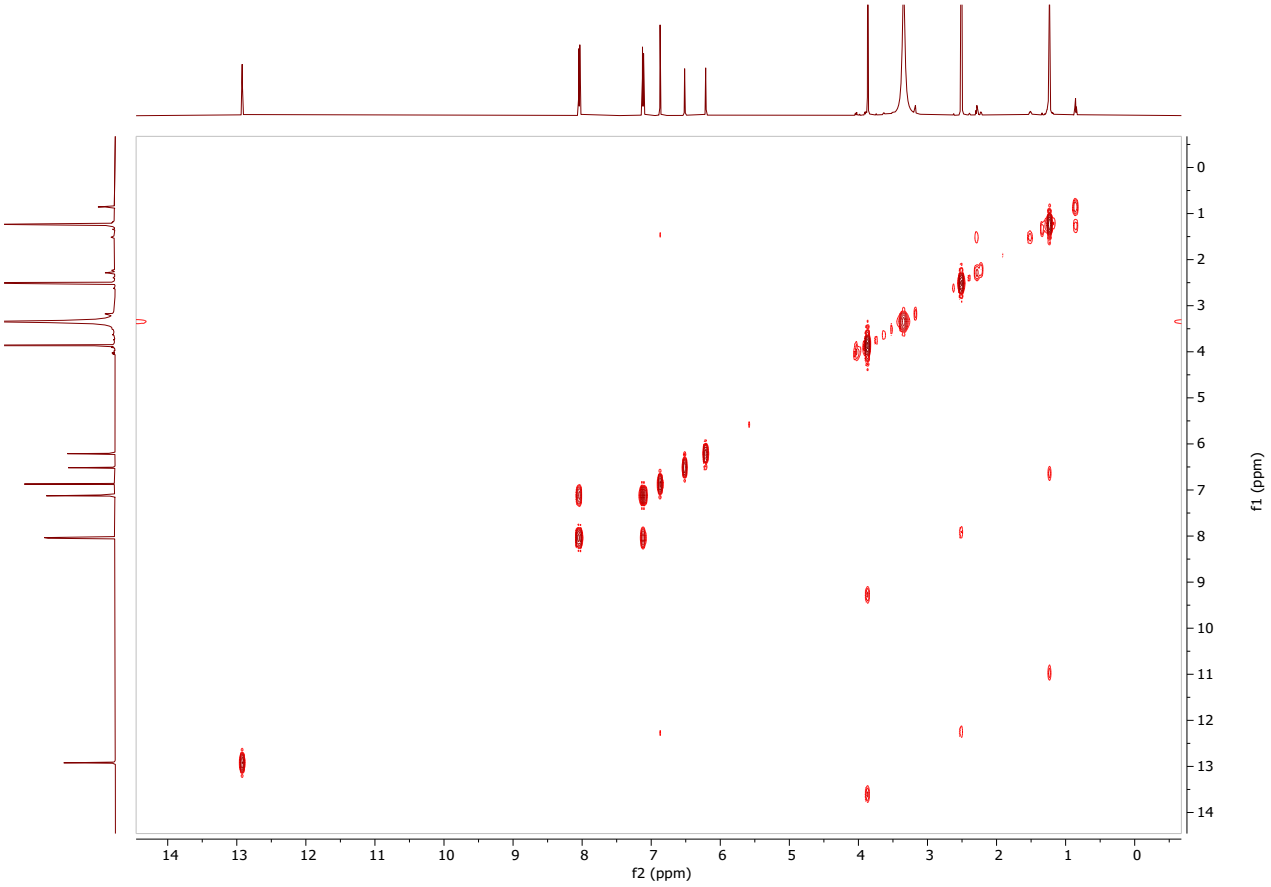


Figure S.13. HSQC NMR spectrum of Acacetin in DMSO

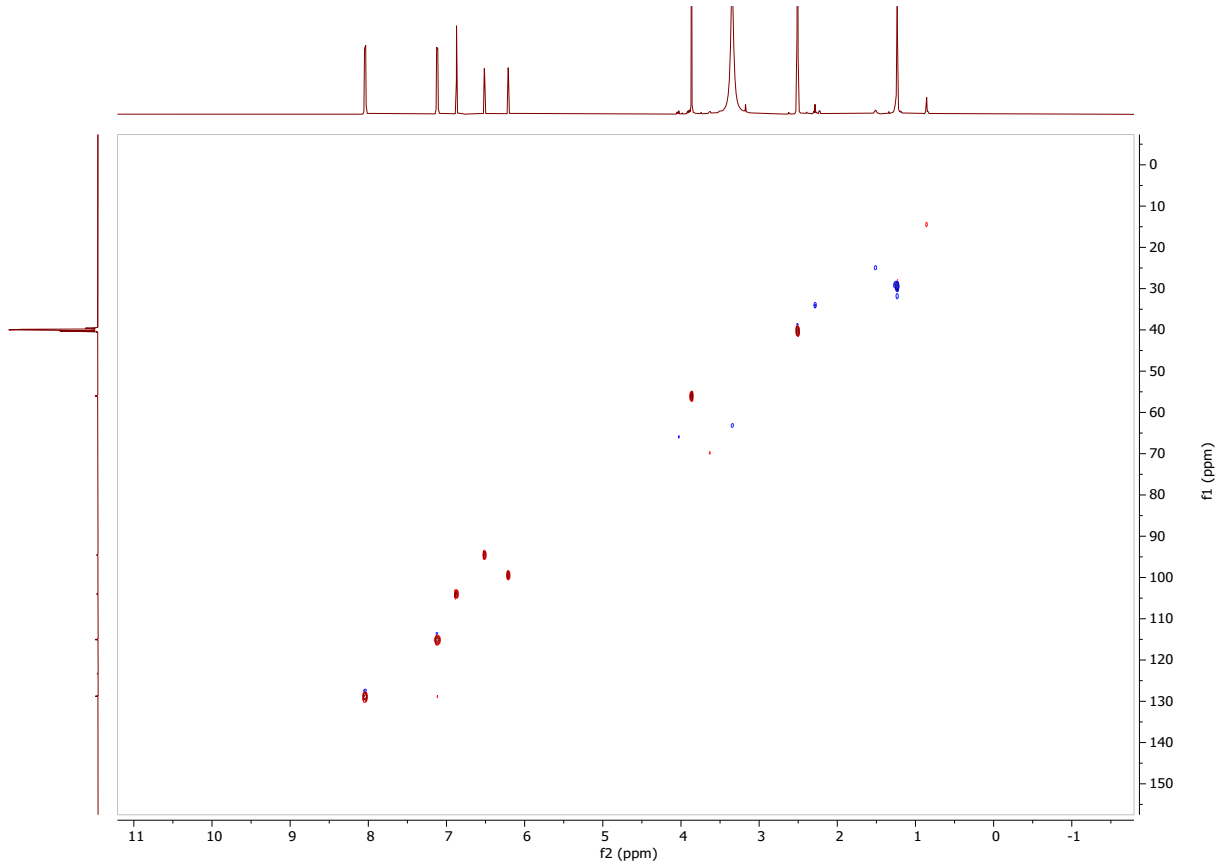


Figure S.14. HMBC NMR spectrum of Acacetin in DMSO

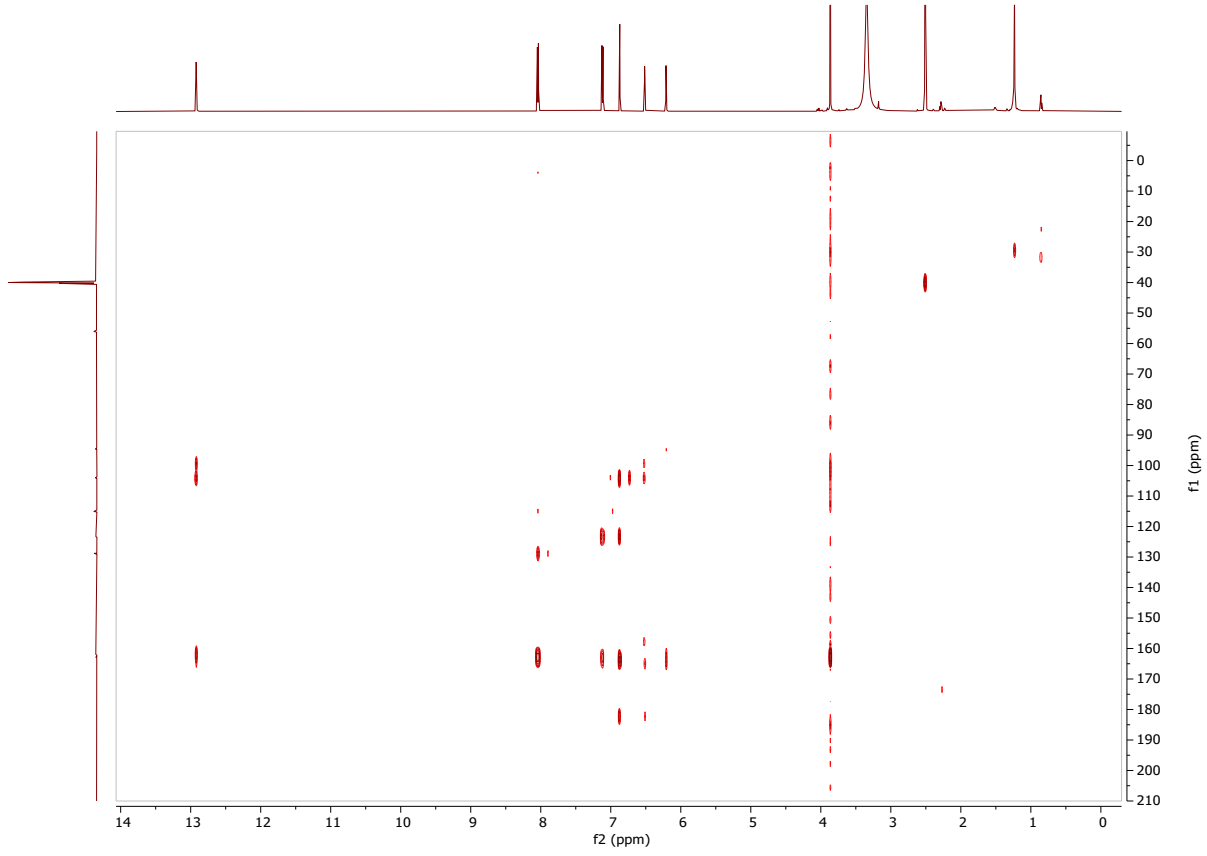


Figure S.15. HRMS spectrum of Acacetin

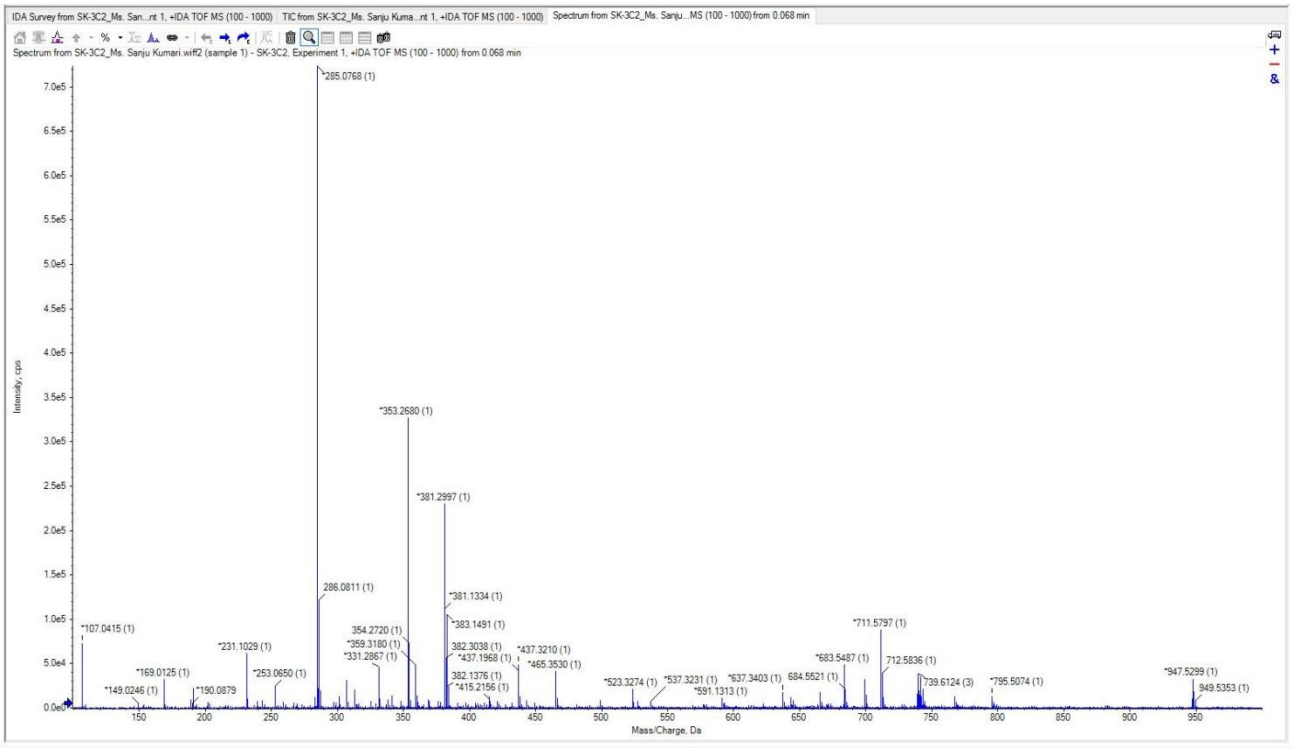


Figure S.16. Flow chart of isolation scheme of compounds

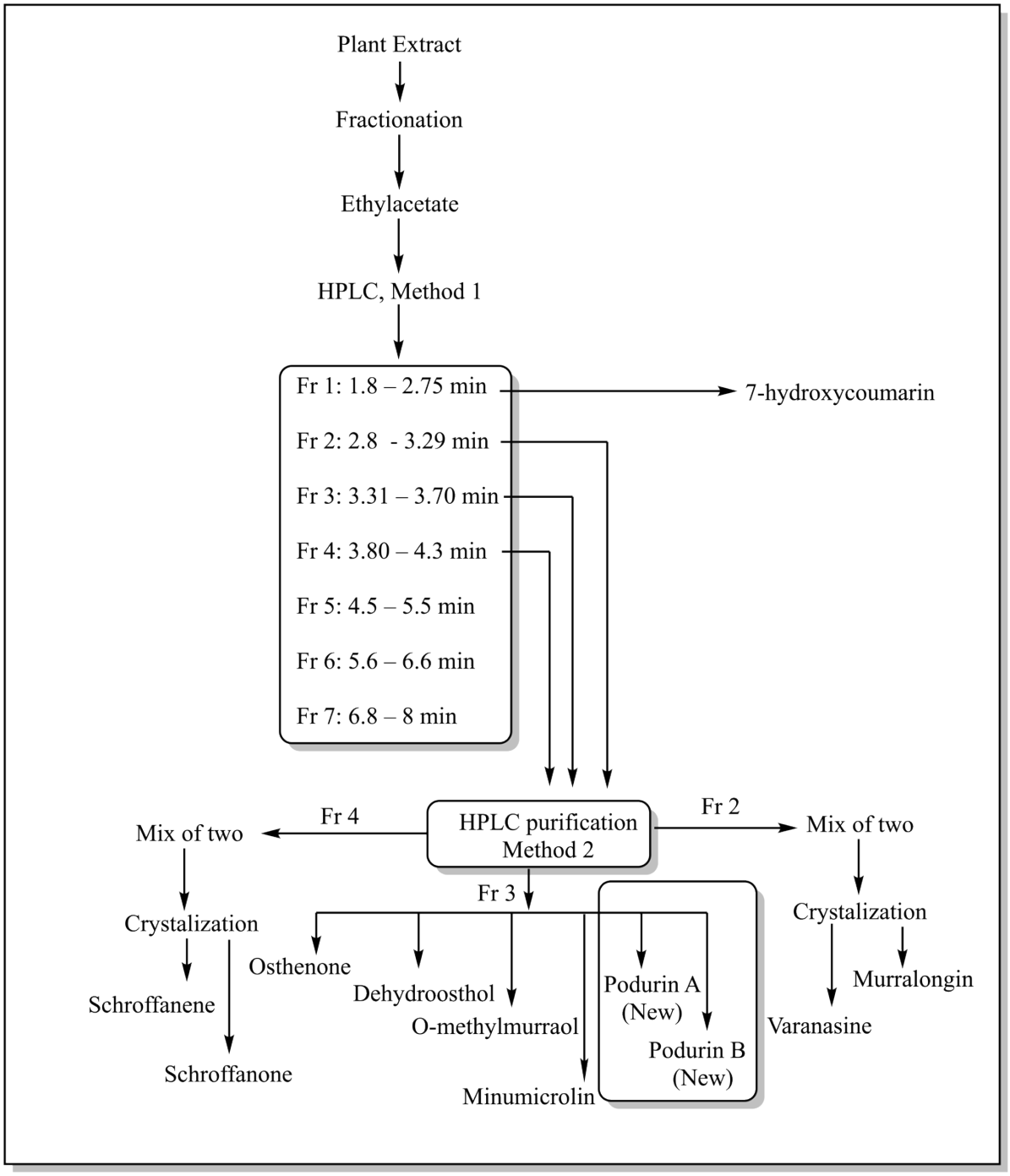


Figure S.17. ^{1}H NMR spectrum of Podurin A in $CDCl_3$

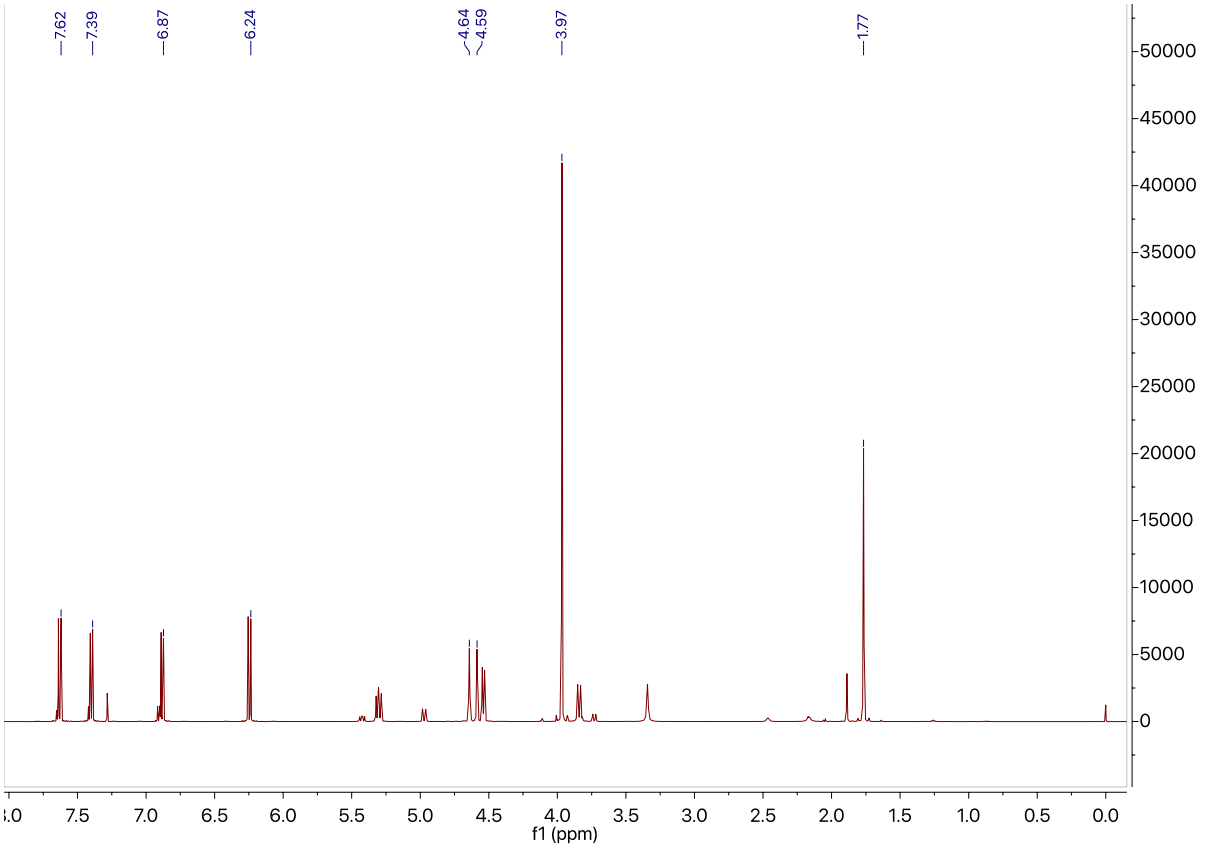


Figure S.18. ^{13}C NMR spectrum of Podurin A in $CDCl_3$

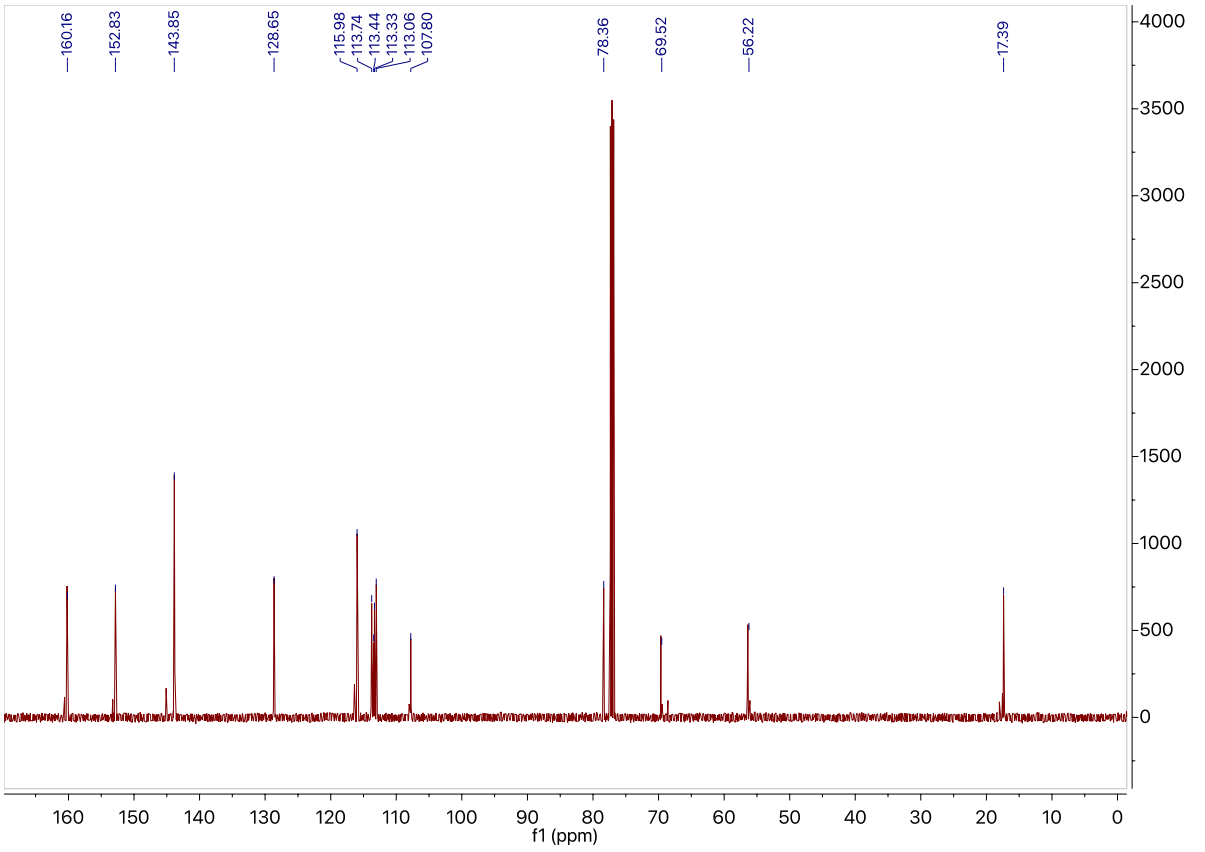


Figure S.19. COSY NMR spectrum of Podurin A in $CDCl_3$

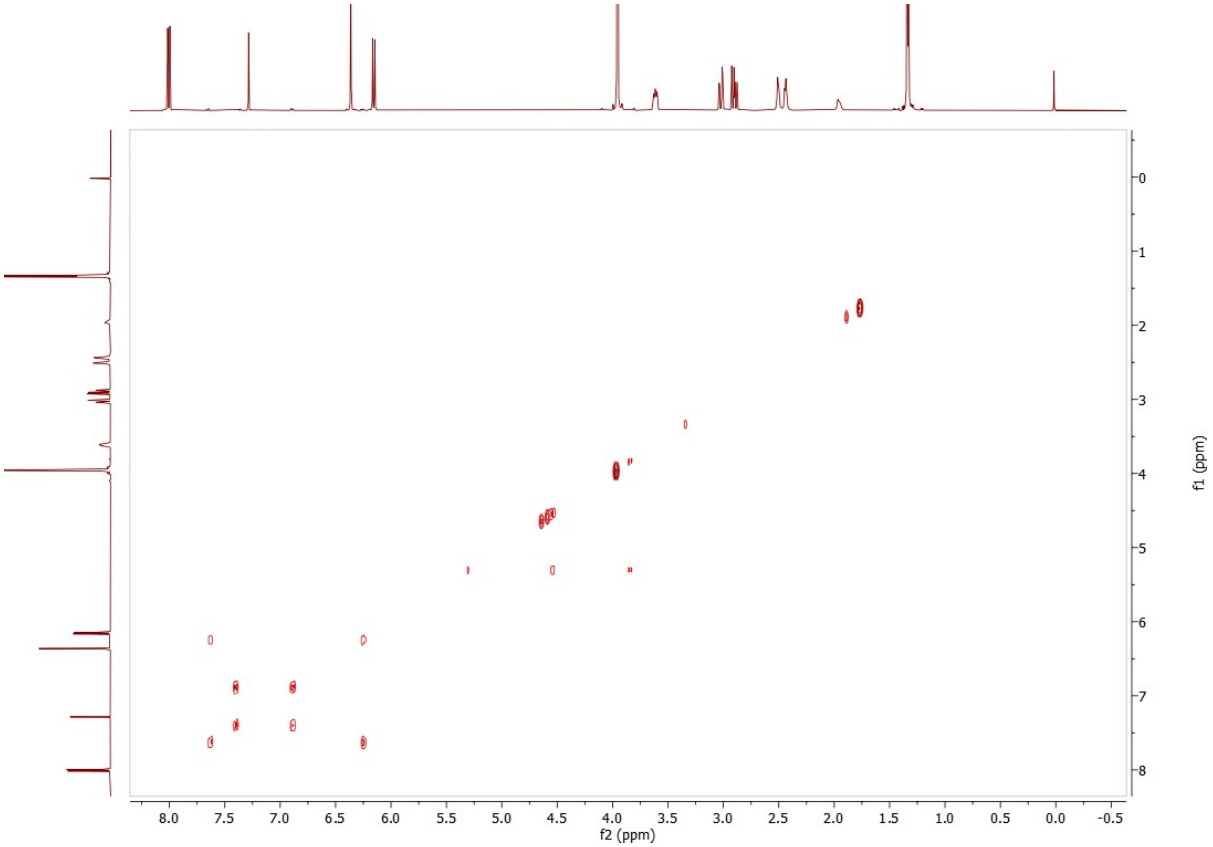


Figure S.20. HSQC NMR spectrum of Podurin A in $CDCl_3$

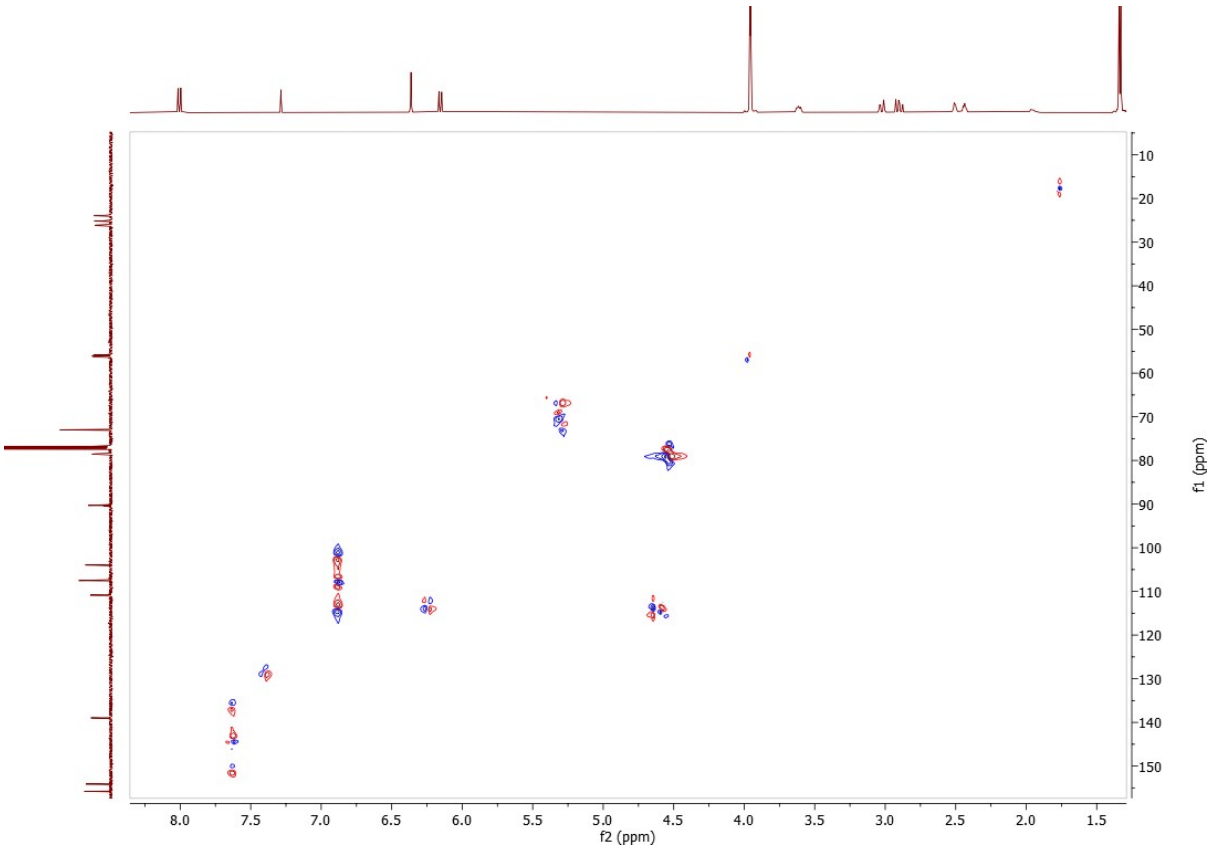


Figure S.21. HMBC NMR spectrum of Podurin A in $CDCl_3$

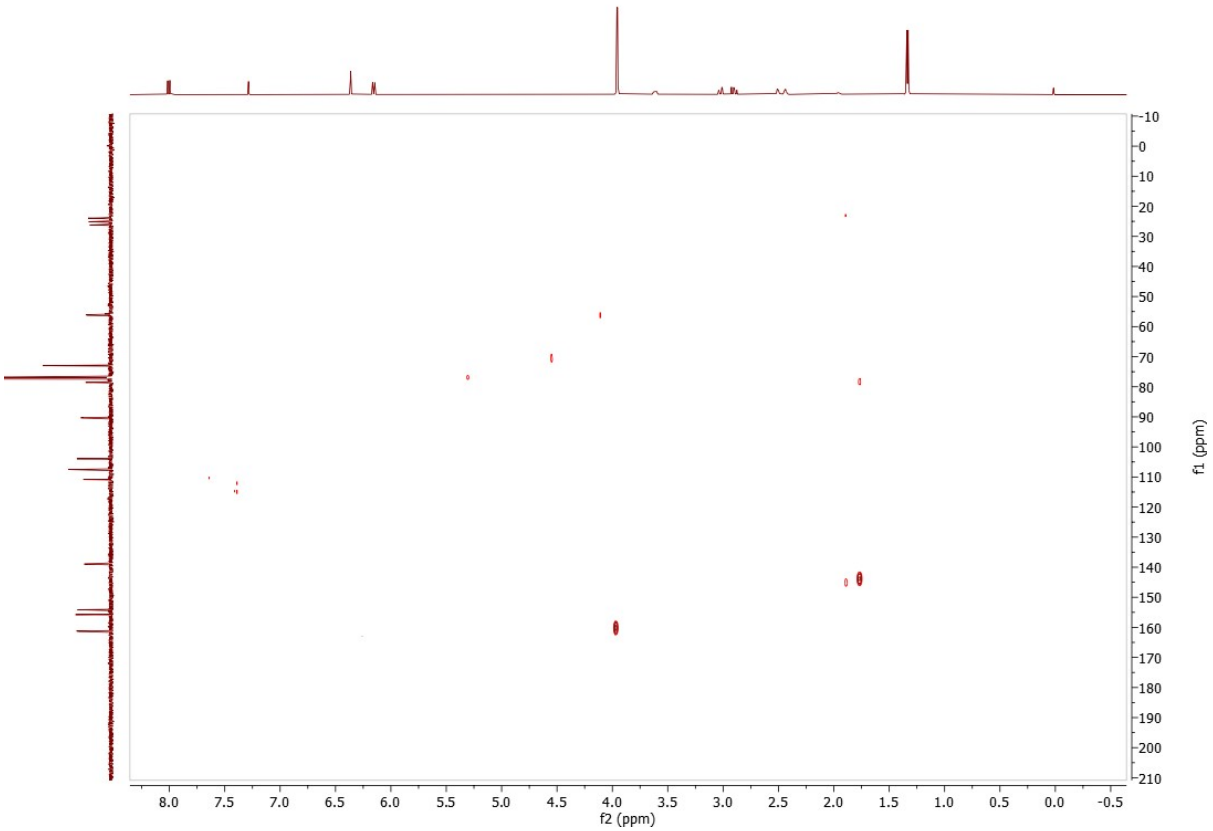
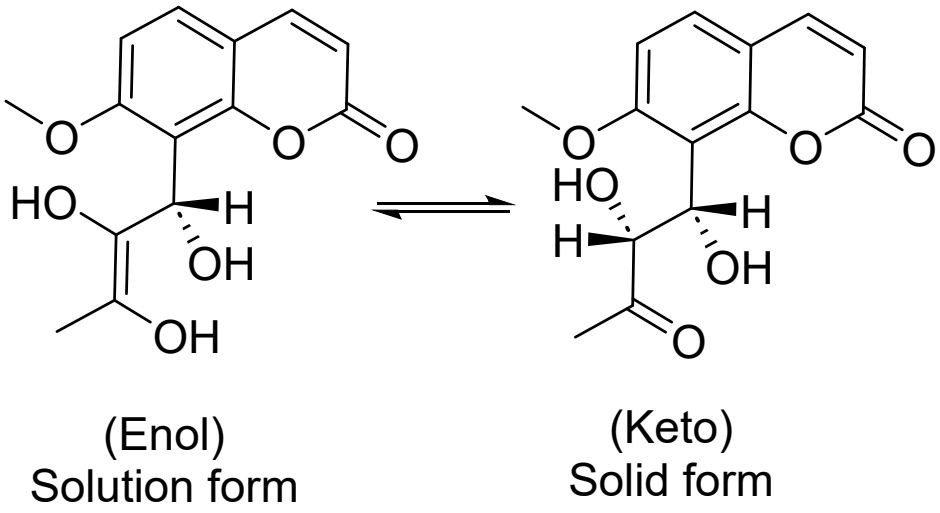


Figure S.22. Keto-enol conversion of Podurin A



(Enol)
Solution form

(Keto)
Solid form