Supplementary Material

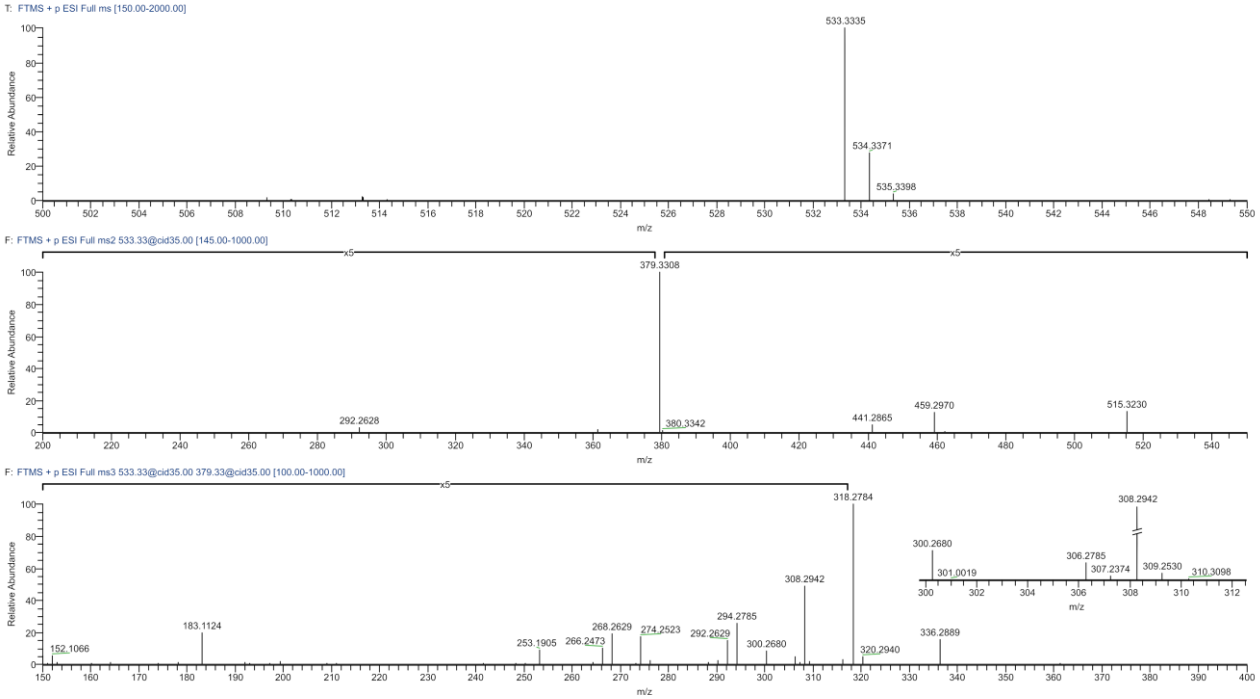


Figure S1. High resolution ESI MS data of favilipid A (**1**): MS spectrum (top panel), 533.33→MS^2 spectrum (middle panel), and 533.33→379.33→MS^3 spectrum (bottom panel).

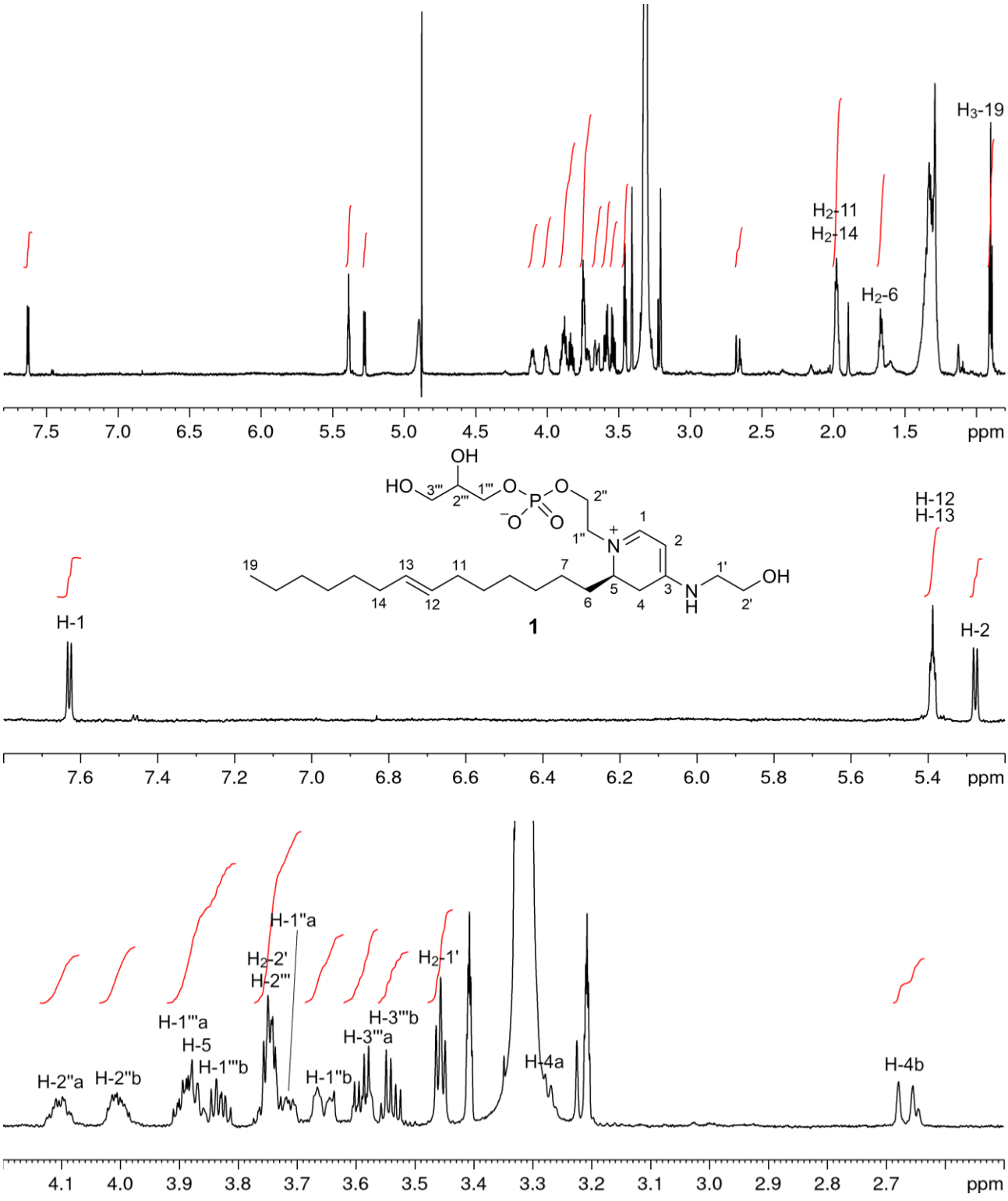


Figure S2. ^{1}H-NMR spectrum of favilipid A (**1**) (700 MHz, CD_3OD): full spectrum (top panel), low-field expansion (middle panel), middle-field expansion (bottom panel)

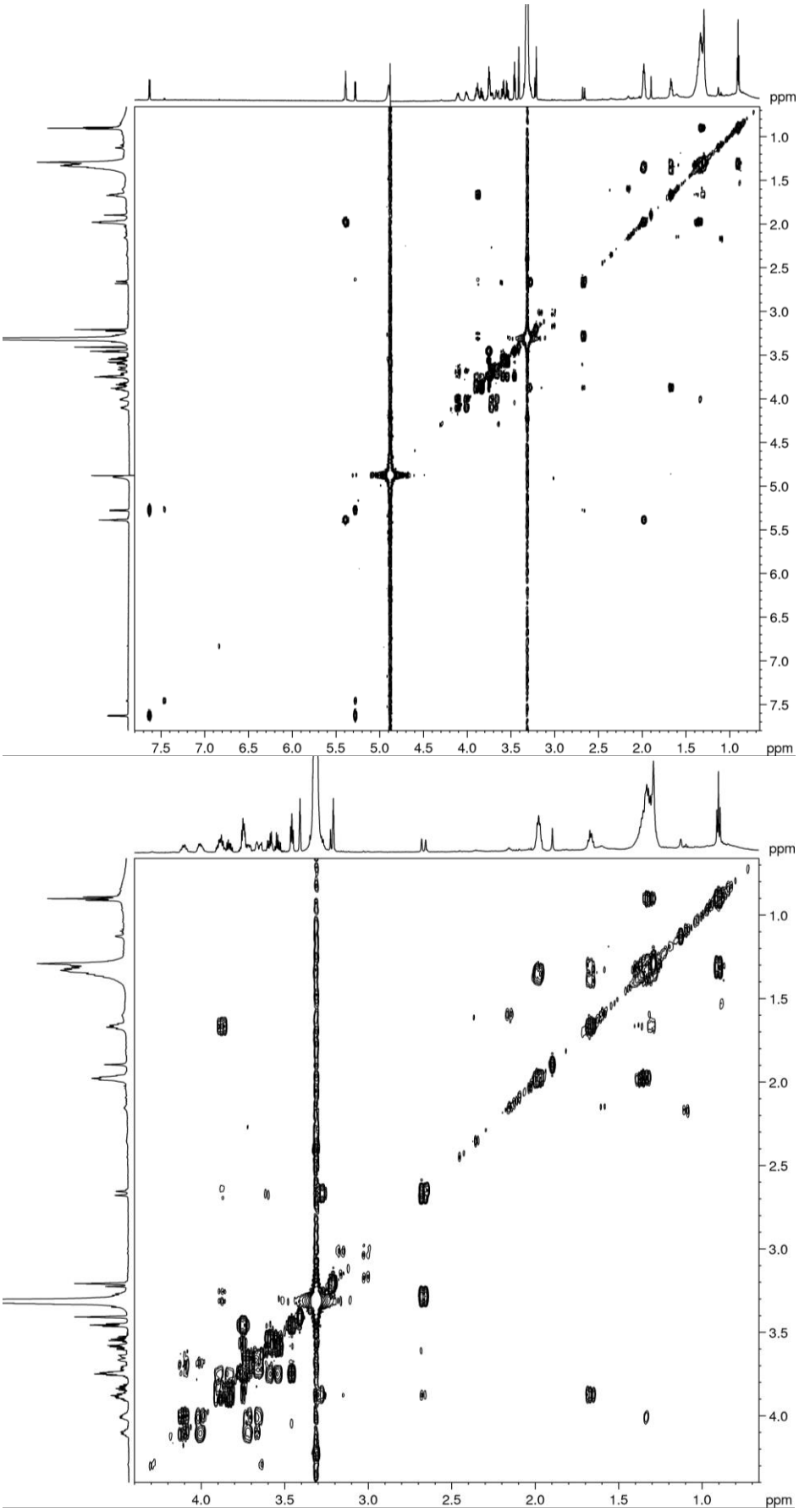


Figure S3. COSY spectrum of favilipid A (**1**) (700 MHz, CD_3OD): full spectrum (top panel), high-field expansion (bottom panel)

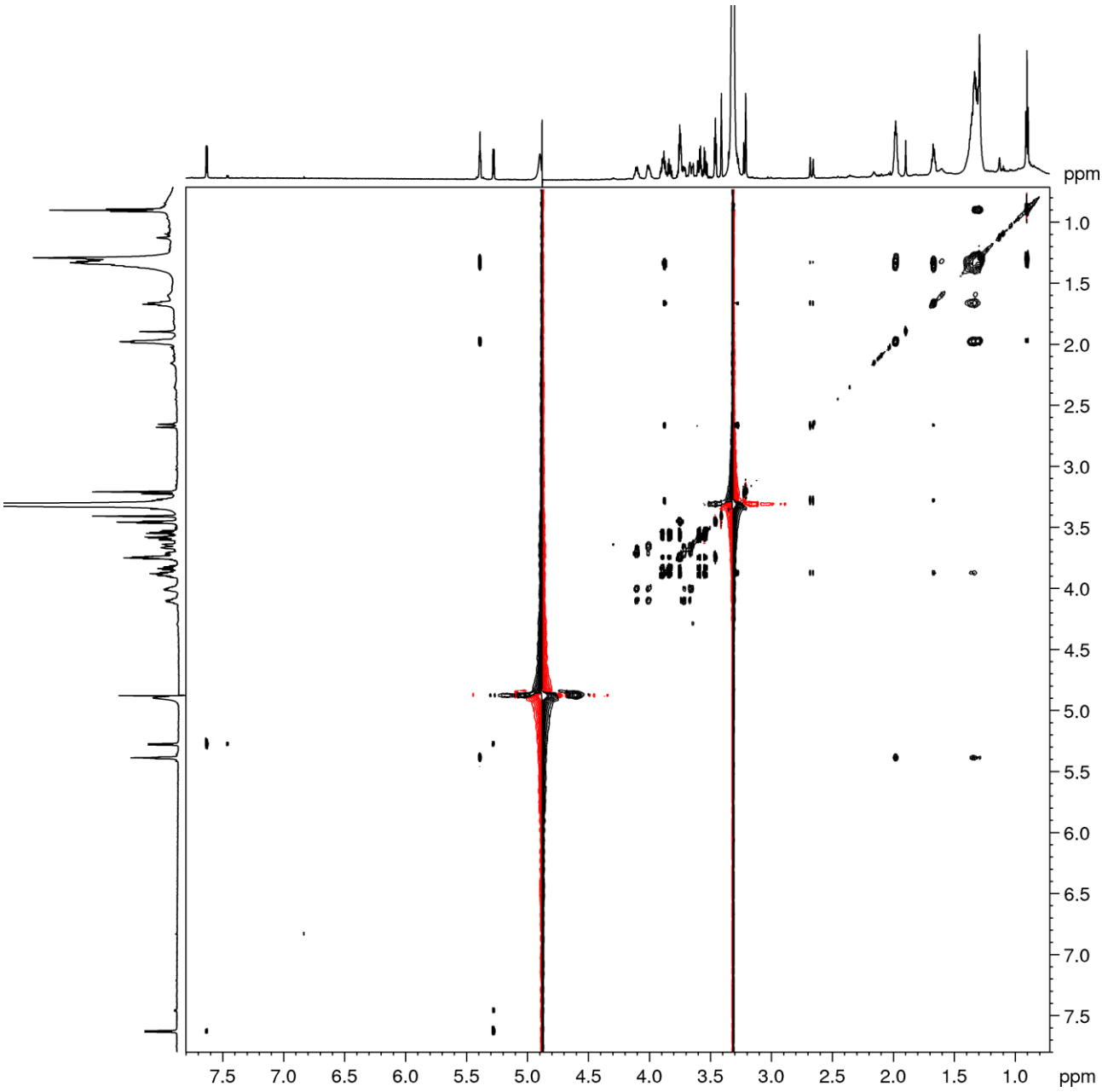


Figure S4. TOCSY spectrum of favilipid A (**1**) (700 MHz, CD_3OD).

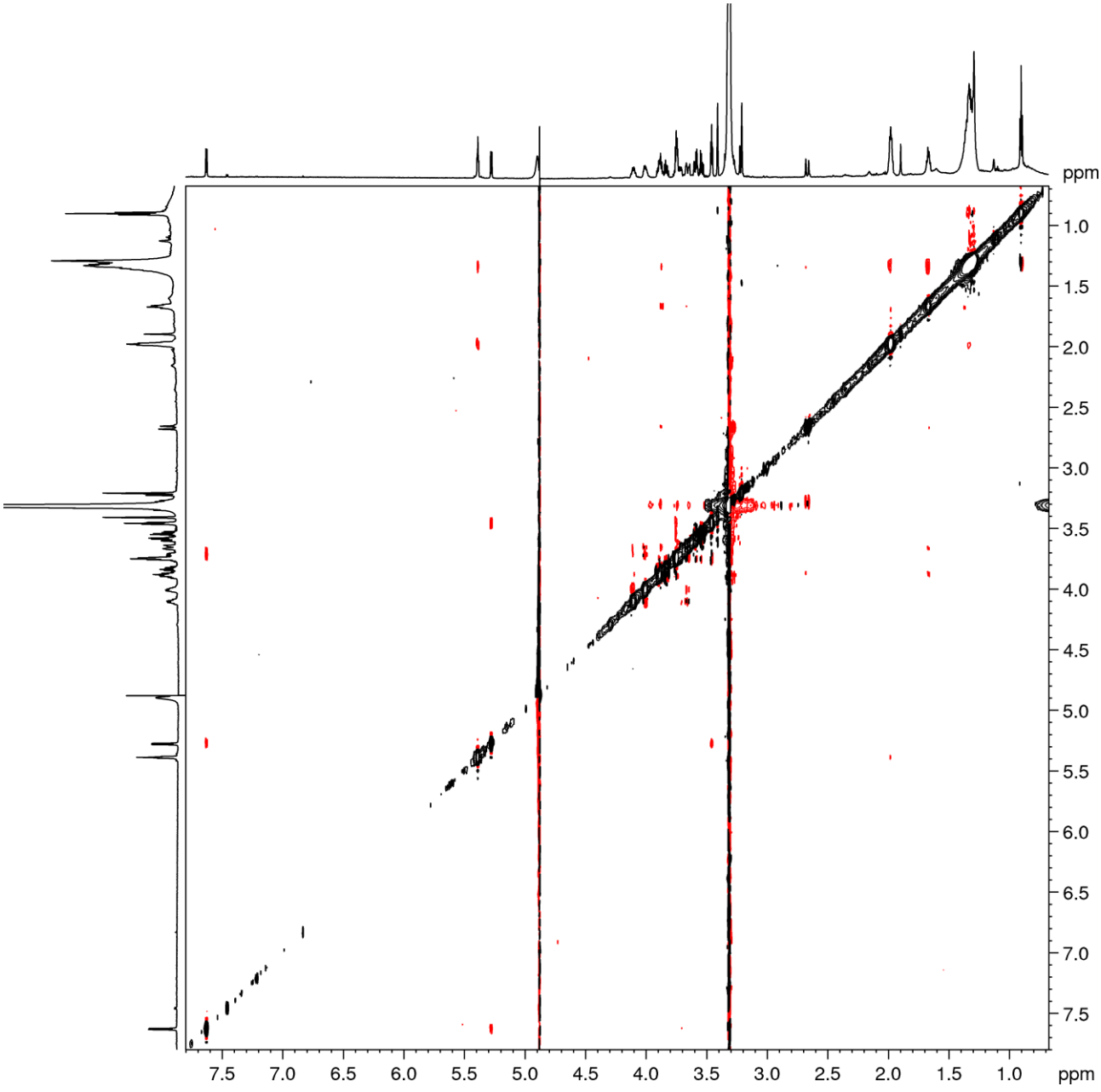


Figure S5. ROESY spectrum of favilipid A (**1**) (700 MHz, CD_3OD).

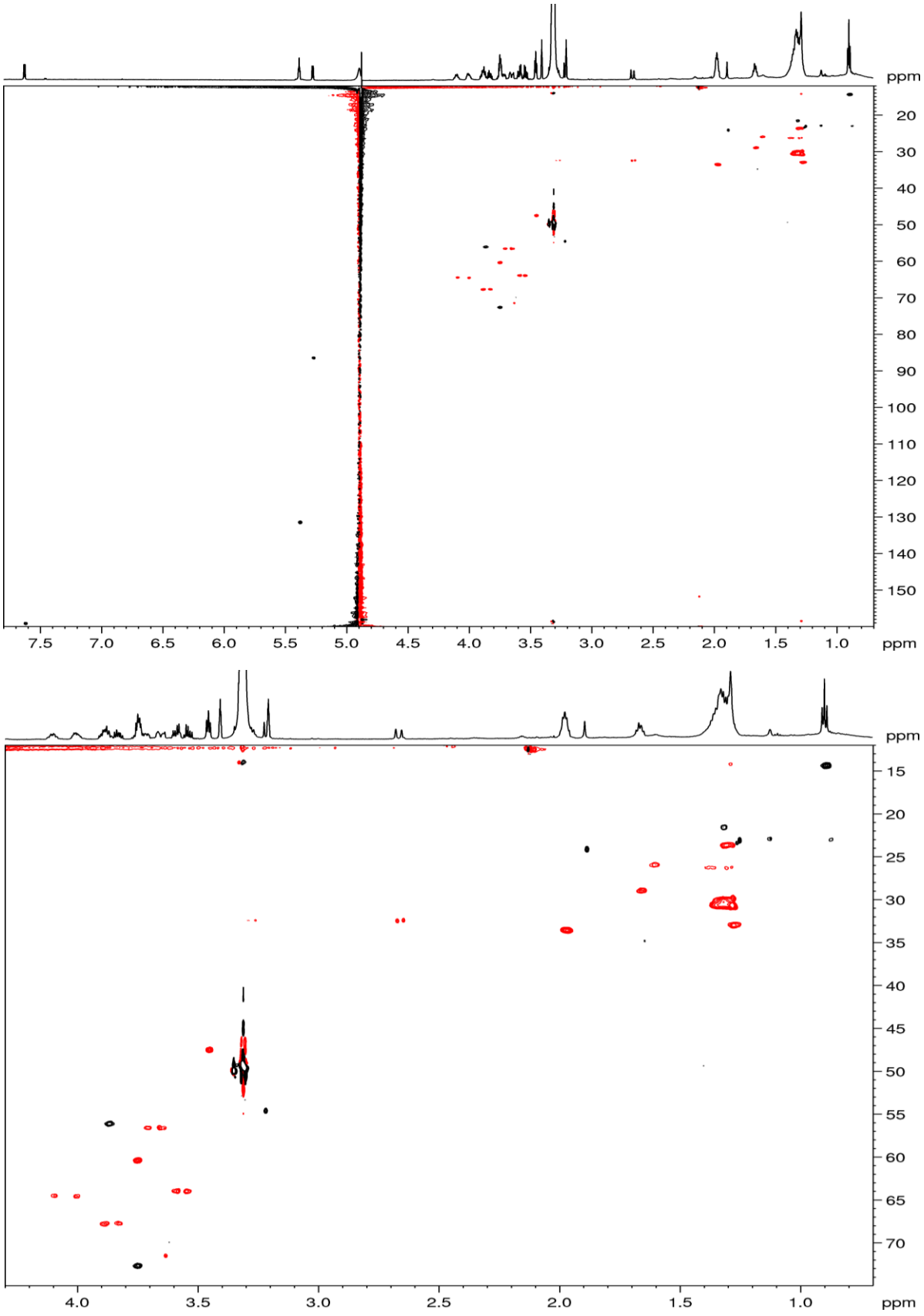


Figure S6. ^{13}C-HSQC spectrum of favilipid A (**1**) (700 MHz, CD_3OD): full spectrum (top panel), high-field expansion (bottom panel)

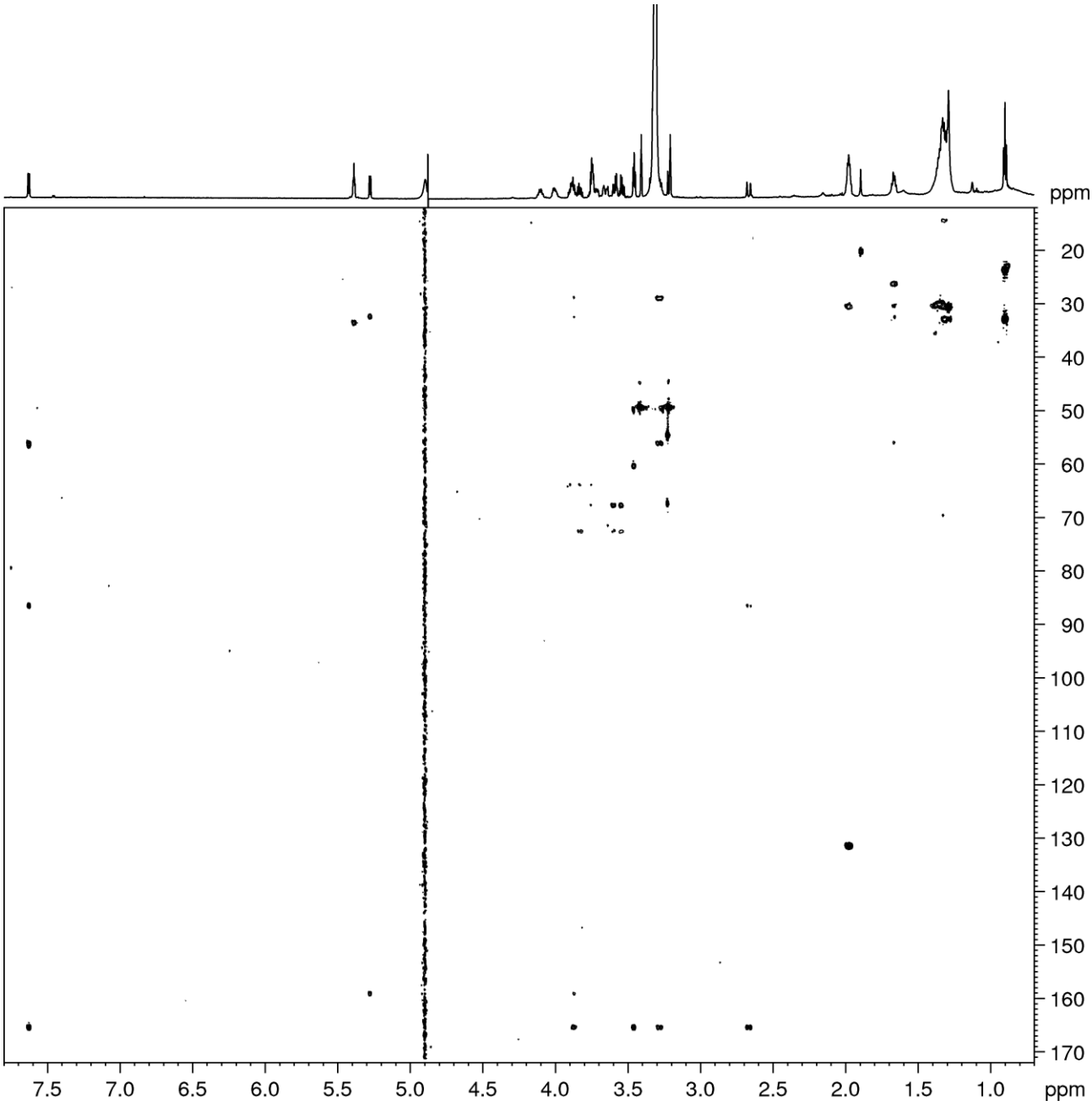


Figure S7. ^{13}C-HMBC spectrum of favilipid A (**1**) (700 MHz, CD_3OD).

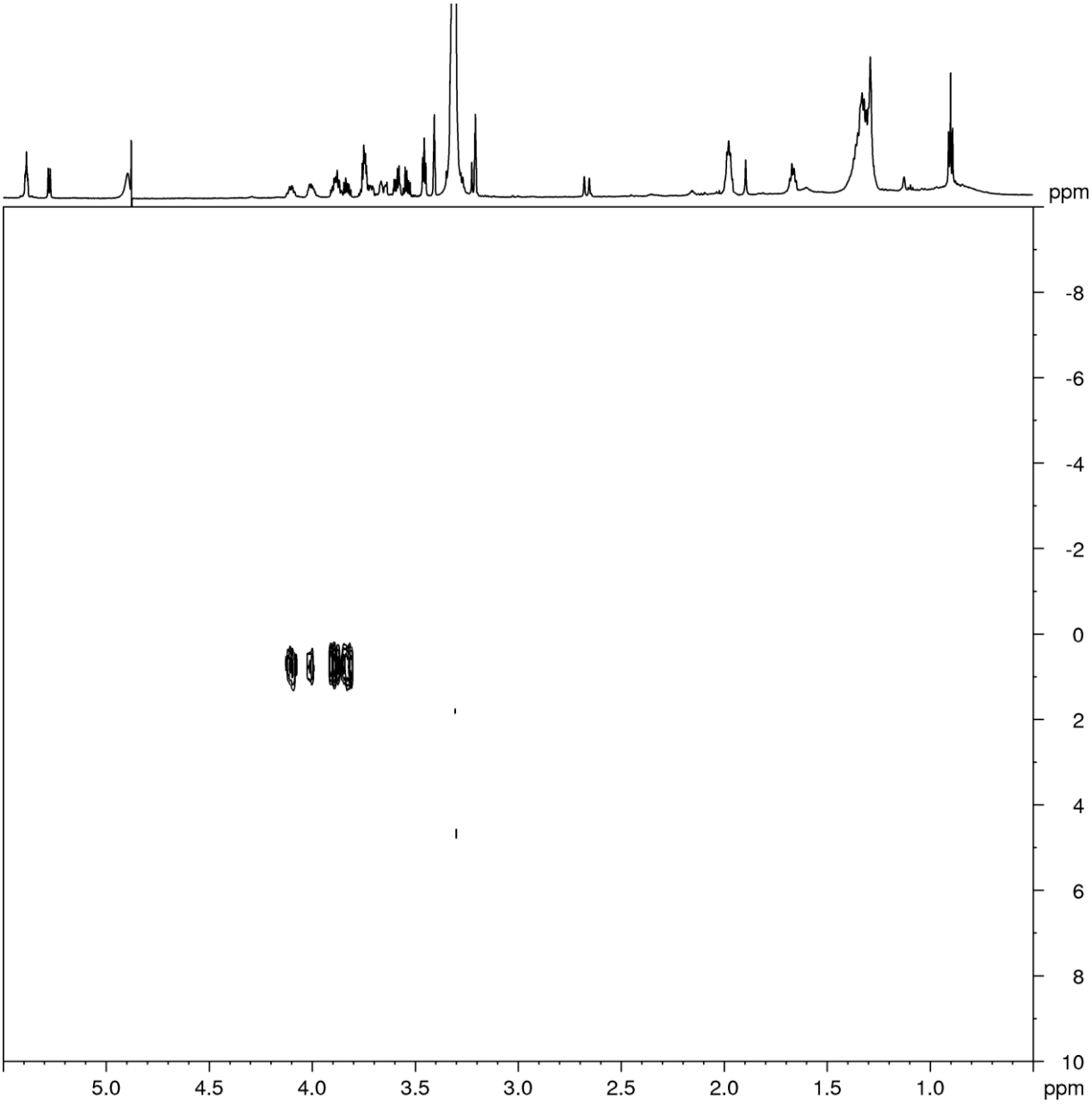


Figure S8. ^{31}P-HMBC spectrum of favilipid A (**1**) (700 MHz, CD_3OD).

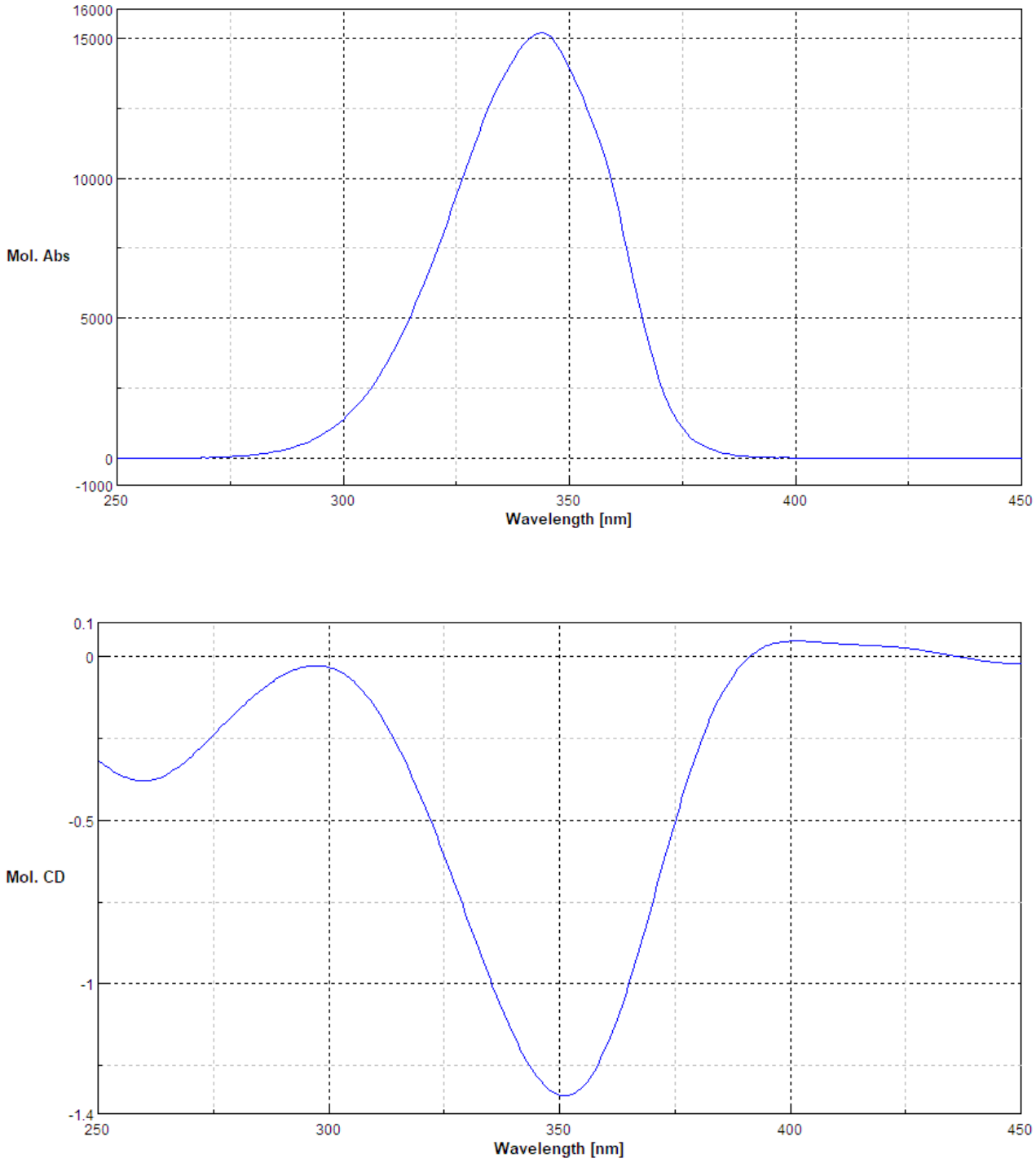
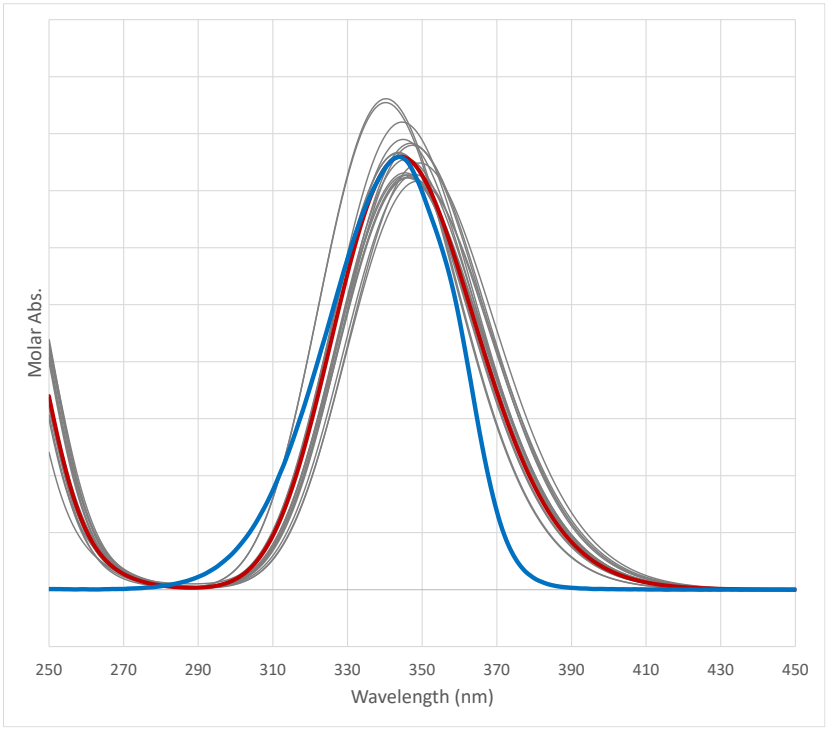


Figure S9. UV and ECD spectra of favilipid A (**1**) in MeOH.



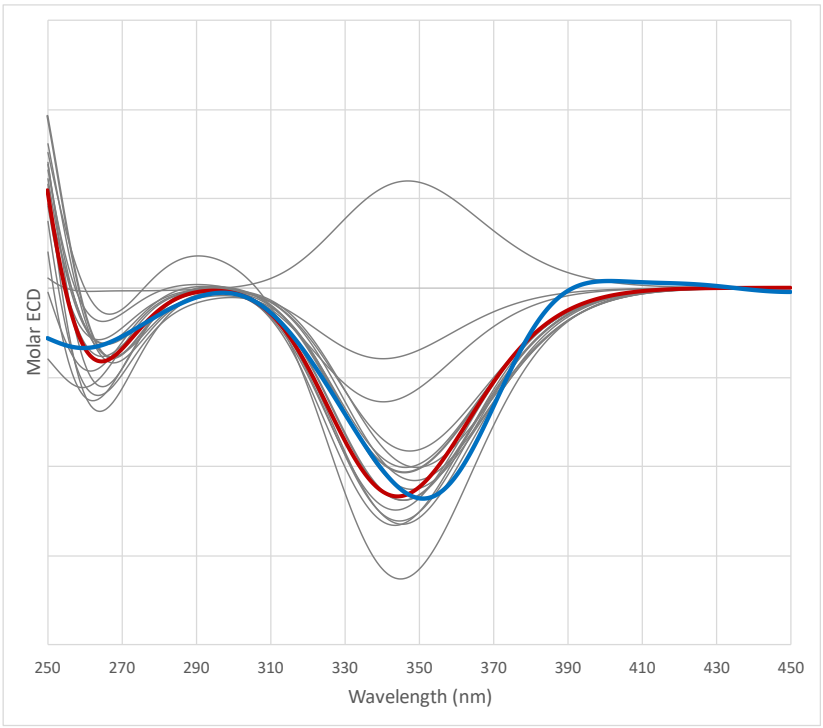


Figure S10. UV (top panel) and ECD (bottom panel) spectra of individual conformers and predicted average spectra of favilipid A (**1**) in MeOH.
Grey lines: spectra of individual conformers calculated at the B3LYP/6-311+G(2d,p)/SMD(MeOH)//B3LYP/6-31G(d,p)/SMD(MeOH) level of theory. The half-band width σ = 0.35 eV was used to generate the spectra. All the predicted spectra are shifted by +37 nm to match experimental and predicted UV maxima (see text for details). The only conformer showing positive ECD at 350 nm is conformer #11, whose population is 1.3%.
Red line: average UV and ECD spectra according to the Boltzmann statistics and B3LYP/6-31G+(d,p)/SMD(MeOH) energies.
Blue line: experimental UV and ECD spectra.

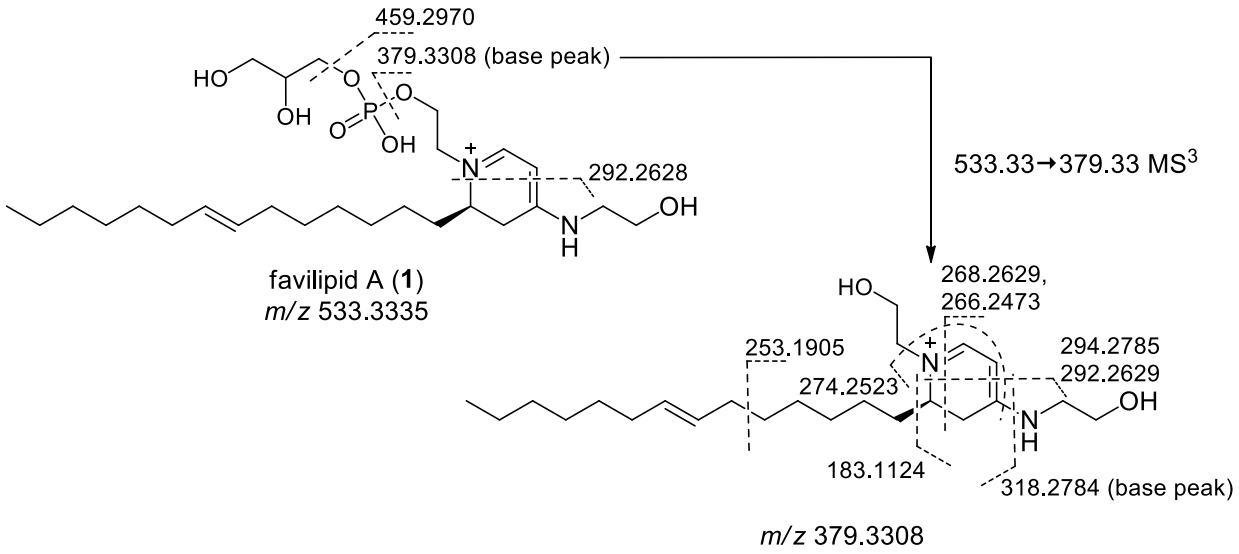


Figure S11. Interpretation of MS^2 and MS^3 spectra of favilipid A (**1**).

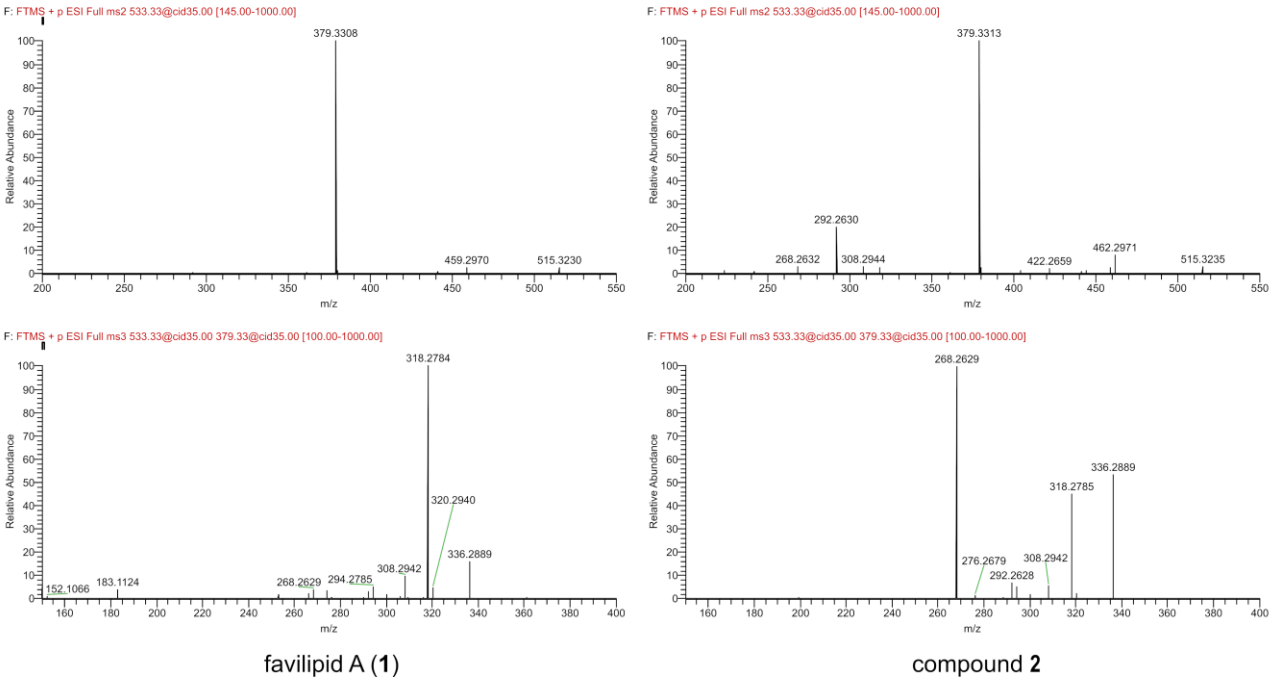


Figure S12. 533.33→MS^2 and 533.33→379.33→MS^3 spectra of favilipid A (**1**) and of its isomer **2**.

Table S1. Cartesian coordinates of the 16 low-energy conformers of the model compound **1m** of favilipid A used for prediction of the ECD spectrum.

```
favilipd model compound conf #01
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7668160 Hartree
C          -1.30690         0.27700        -1.52780
C          -2.29580         1.16970        -1.10170
C          -2.79880         1.04880         0.19640
C          -2.16920         0.01790         1.09990
C          -1.72000        -1.23230         0.33240
C          -2.86800        -2.17390        -0.09050
C          -3.55430        -2.86550         1.09200
C          -4.37220         2.94700         0.00270
C           0.15250        -1.66790        -1.33080
C           1.44410        -1.43710        -0.55910
C           5.44960        -0.12950         0.72050
H          -0.78660         0.46130        -2.46380
H          -2.58670         1.97420        -1.76430
H          -1.29700         0.49250         1.56950
H          -2.85090        -0.26400         1.90600
H          -1.03020        -1.78770         0.97320
H          -5.11370         3.39190         0.66640
H          -2.44770        -2.93800        -0.75450
H          -3.60290        -1.61180        -0.67970
H          -4.31150        -3.56890         0.72900
H          -2.83240        -3.43240         1.69240
H          -3.63750         3.71020        -0.27490
H          -4.87260         2.58850        -0.90240
H          -4.05900        -2.15460         1.75490
H          -0.13870        -2.71660        -1.21250
H           0.31350        -1.47720        -2.39500
H           1.29040        -1.57330         0.51570
H           2.19330        -2.15800        -0.90510
H           6.20210        -0.82180         0.33750
H           5.22250        -0.37580         1.76250
H           5.83350         0.89430         0.65650
H          -3.99690         1.69180         1.67600
N          -0.95000        -0.81740        -0.86990
N          -3.73300         1.84170         0.70870
O           4.28100        -0.29400        -0.11010
O           1.90710        -0.09800        -0.82710
O           3.16490         2.03790        -0.38260
O           2.53650         0.49000         1.63180
P           2.96050         0.64630         0.18260

favilipd model compound conf #02
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7654640 Hartree
C           1.35780        -0.06340         1.41000
C           2.20670         1.00740         1.11290
C           2.58020         1.22010        -0.21770
C           1.98860         0.31120        -1.26760
C           1.78290        -1.11360        -0.73720
C           3.11190        -1.88740        -0.61180
C           2.98400        -3.35100        -0.18110
C           3.91950         3.24520         0.25200
C          -0.00180        -2.00700         0.86080
C          -1.33150        -1.61420         0.23000
C          -5.26700         0.12130        -0.77190
H           0.89330        -0.12610         2.39010
H           2.47110         1.69540         1.90500
H           1.02340         0.74460        -1.56320
H           2.61920         0.28130        -2.16060
H           1.12520        -1.64480        -1.42990
H           4.52820         3.91340        -0.35710
H           3.77820        -1.35730         0.07960
H           3.58560        -1.84200        -1.60020
H           3.96800        -3.83250        -0.19960
H           2.59410        -3.44810         0.83780
H           3.12860         3.82580         0.73850
H           4.55070         2.78860         1.02090
H           2.32640        -3.91330        -0.85470
H           0.28420        -2.98920         0.47790
H          -0.10850        -2.07880         1.94670
H          -1.22670        -1.48530        -0.85160
H          -2.06260        -2.40660         0.42520
H          -6.04200        -0.63500        -0.63240
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H          -5.01390         0.19350        -1.83450
H          -5.63500         1.08810        -0.41170
H           3.53060         2.30710        -1.61510
N           1.06830        -1.04670         0.56680
N           3.35170         2.22270        -0.62060
O          -4.12630        -0.31380        -0.00250
O          -1.78640        -0.38750         0.83510
O          -2.98810         1.82210         0.94950
O          -2.29220         0.87240        -1.38840
P          -2.78020         0.63540         0.02970

favilipd model compound conf #03
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7646274 Hartree
C           1.12930         0.26360         1.45560
C           2.00890         1.28860         1.09300
C           2.62880         1.23460        -0.15820
C           2.23600         0.11400        -1.08910
C           1.90700        -1.18220        -0.33700
C           3.13520        -1.94820         0.20000
C           4.02960        -2.51930        -0.90500
C           3.87810         3.34970         0.12650
C          -0.01360        -1.87310         1.17920
C          -1.27640        -1.80810         0.33240
C          -4.57150         2.11960         0.02220
H           0.51450         0.37330         2.34450
H           2.12550         2.13130         1.76160
H           1.34850         0.45240        -1.64080
H           3.01820        -0.07370        -1.82830
H           1.36060        -1.83590        -1.02220
H           4.59890         3.89590        -0.48210
H           2.76760        -2.77190         0.82300
H           3.71800        -1.29030         0.85650
H           4.83310        -3.12030        -0.46540
H           3.45940        -3.16790        -1.58120
H           3.01680         3.99570         0.32700
H           4.34770         3.07710         1.07680
H           4.50020        -1.73460        -1.50680
H           0.42560        -2.86950         1.07210
H          -0.26300        -1.72080         2.23260
H          -1.03750        -1.90300        -0.73280
H          -1.93660        -2.63320         0.62290
H          -4.59290         2.97250         0.70310
H          -5.52870         1.59030         0.07090
H          -4.39280         2.47240        -0.99870
H           3.83670         2.04170        -1.54740
N           0.98800        -0.87450         0.79030
N           3.47310         2.15570        -0.60820
O          -3.49270         1.26990         0.46770
O          -1.92690        -0.54720         0.58360
O          -2.72710         0.19990        -1.77540
O          -4.34340        -1.09770        -0.20150
P          -3.19830        -0.11230        -0.36490

favilipd model compound conf #04
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7645088 Hartree
C          -1.87210         1.17080        -1.32900
C          -3.08380         1.31040        -0.64460
C          -3.29660         0.55170         0.51010
C          -2.15440        -0.29600         1.01280
C          -1.30690        -0.86690        -0.13090
C          -1.96170        -2.03190        -0.90430
C          -2.12440        -3.30540        -0.06810
C          -5.56750         1.43250         0.94080
C           0.30170         0.17880        -1.81130
C           1.38390         1.05640        -1.19300
C           5.54780         0.80150         0.32960
H          -1.62660         1.86200        -2.13150
H          -3.79520         2.04690        -0.99440
H          -1.52760         0.34950         1.64320
H          -2.51820        -1.10590         1.64960
H          -0.36200        -1.21330         0.29270
H          -6.33200         1.23060         1.69100
H          -1.32770        -2.25360        -1.77060
H          -2.93370        -1.70980        -1.29770
H          -2.51270        -4.11770        -0.69220
H          -1.16300        -3.63280         0.34560
H          -5.30250         2.49450         0.97750
H          -5.96920         1.19950        -0.05040
```

H	-2.82260	-3.17120	0.76490
H	0.63230	-0.86140	-1.84560
H	0.13430	0.51720	-2.83900
H	2.27390	1.01540	-1.82850
H	1.04570	2.09550	-1.13430
H	6.05720	1.76160	0.22440
H	5.82570	0.14740	-0.50290
H	5.84000	0.33880	1.27850
H	-4.44330	0.02860	2.07380
N	-0.97370	0.22750	-1.08160
N	-4.40810	0.59680	1.23490
O	4.13290	1.08390	0.30790
O	1.69180	0.65030	0.15830
O	2.97410	-0.54560	1.96770
O	3.35490	-1.23630	-0.53010
P	3.07150	-0.16160	0.50460

favilipd model compound conf #05
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7643324 Hartree

C	1.30210	-0.05690	1.30160
C	2.26150	0.92510	1.03740
C	2.79340	1.02230	-0.24950
C	2.22070	0.13200	-1.32350
C	1.70950	-1.22260	-0.80450
C	2.78570	-2.32270	-0.67680
C	3.93710	-2.07550	0.30290
C	4.29330	2.91630	0.27810
C	-0.13620	-1.94920	0.78380
C	-1.44620	-1.53520	0.12740
C	-5.55710	0.04690	-0.39530
H	0.77880	-0.04900	2.25350
H	2.52140	1.61830	1.82640
H	1.38650	0.68610	-1.77430
H	2.95350	-0.04170	-2.11690
H	0.97640	-1.58290	-1.53050
H	5.03690	3.47880	-0.28650
H	3.18690	-2.47290	-1.68730
H	2.27930	-3.25810	-0.40920
H	4.60090	-2.94740	0.31580
H	4.54320	-1.20790	0.02110
H	3.52650	3.60670	0.64540
H	4.78180	2.43870	1.13330
H	3.57780	-1.92290	1.32630
H	0.12390	-2.95340	0.43760
H	-0.25760	-1.98420	1.86960
H	-1.33140	-1.44110	-0.95690
H	-2.20300	-2.29860	0.34030
H	-6.28760	-0.68810	-0.05140
H	-5.47440	-0.00240	-1.48580
H	-5.88100	1.04850	-0.09270
H	4.00120	1.92520	-1.57870
N	0.97140	-1.03740	0.47270
N	3.71050	1.91410	-0.60770
O	-4.30280	-0.29890	0.22870
O	-1.85940	-0.27410	0.69020
O	-3.07600	1.92750	0.77040
O	-2.73300	0.74690	-1.54200
P	-2.98840	0.65470	-0.04810

favilipd model compound conf #06
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7636565 Hartree

C	1.29970	0.67030	1.41450
C	2.28220	1.47570	0.83880
C	3.21570	0.89200	-0.02070
C	3.17260	-0.60380	-0.18740
C	1.75290	-1.17890	-0.09380
C	1.77340	-2.71570	-0.07250
C	2.44270	-3.33160	-1.30770
C	4.42700	2.99530	-0.49060
C	-0.13870	-1.24690	1.65780
C	-1.35330	-1.17920	0.74060
C	-5.50740	0.20420	-0.08530
H	0.65860	1.09290	2.18220
H	2.33140	2.51670	1.13000
H	3.61010	-0.88700	-1.14690
H	3.80250	-1.04070	0.60180
H	1.18010	-0.84350	-0.97190
H	2.28380	-3.05450	0.83830

H	0.74760	-3.09120	-0.02680
H	2.29980	-4.41740	-1.30160
H	2.00170	-2.94390	-2.23400
H	3.52040	-3.14340	-1.33940
H	3.54570	3.56040	-0.80940
H	4.66430	3.25880	0.54550
H	5.27050	3.26170	-1.12750
H	0.07660	-2.29300	1.88290
H	-0.36470	-0.74770	2.60260
H	-1.15940	-1.65560	-0.22440
H	-2.18370	-1.69930	1.23160
H	-6.18420	-0.11350	0.71050
H	-5.59700	-0.47930	-0.93570
H	-5.76770	1.22130	-0.39780
H	4.83300	1.03410	-1.20410
N	1.06050	-0.60080	1.09900
N	4.19220	1.56060	-0.62070
O	-4.17540	0.16080	0.46760
O	-1.69190	0.20770	0.53580
O	-2.86300	2.14070	-0.58130
O	-2.88270	-0.20720	-1.74290
P	-2.90900	0.62940	-0.47670

favilipd model compound conf #07
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7635054 Hartree

C	1.92800	0.01090	1.61320
C	3.06340	0.68210	1.14990
C	3.21010	0.88480	-0.22660
C	2.08760	0.42970	-1.12740
C	1.41370	-0.84320	-0.60000
C	2.28790	-2.09710	-0.81130
C	1.64430	-3.42440	-0.40050
C	5.35400	2.10500	-0.04280
C	-0.18690	-1.17120	1.38090
C	-1.28180	-0.11410	1.46240
C	-5.35100	1.25810	0.36260
H	1.69930	0.01250	2.67640
H	3.75280	1.09730	1.87320
H	1.35640	1.24830	-1.17390
H	2.44760	0.25780	-2.14580
H	0.46710	-0.97410	-1.12730
H	6.05650	2.52020	-0.76560
H	3.24130	-1.97080	-0.28380
H	2.52360	-2.12680	-1.88250
H	2.30650	-4.25710	-0.66250
H	1.46450	-3.47930	0.67850
H	5.01160	2.90450	0.62280
H	5.86320	1.33980	0.55110
H	0.68920	-3.58470	-0.91450
H	-0.51520	-1.99990	0.75250
H	-0.00420	-1.55460	2.39030
H	-2.16560	-0.56310	1.92560
H	-0.95540	0.73320	2.07410
H	-5.69230	2.05290	1.02900
H	-5.75790	0.29910	0.69830
H	-5.69210	1.46920	-0.65670
H	4.22260	1.65130	-1.78300
N	1.07850	-0.65170	0.83830
N	4.23470	1.52410	-0.77720
O	-3.90950	1.25440	0.43380
O	-1.59080	0.40370	0.15030
O	-2.96480	0.73450	-1.93200
O	-3.59200	-1.20730	-0.29070
P	-3.07130	0.20070	-0.51710

favilipd model compound conf #08
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7634115 Hartree

C	1.78020	-0.14540	1.75500
C	2.80790	0.68650	1.30050
C	2.92000	0.93050	-0.07170
C	1.85450	0.36210	-0.97510
C	1.33160	-0.99190	-0.47950
C	2.28980	-2.18080	-0.70650
C	2.50560	-2.51660	-2.18560
C	4.89680	2.40230	0.12810
C	-0.08710	-1.69360	1.52130
C	-1.39510	-0.92730	1.64790
C	-4.14180	1.19720	-2.13610

H	1.57940	-0.21630	2.82120
H	3.44430	1.17060	2.02950
H	1.02870	1.08640	-0.99280
H	2.21870	0.26920	-2.00090
H	0.39130	-1.19660	-0.99530
H	5.53280	2.92390	-0.58720
H	1.86030	-3.05360	-0.20120
H	3.25140	-1.97490	-0.22040
H	3.12250	-3.41690	-2.28080
H	1.55210	-2.71020	-2.69170
H	4.45990	3.13290	0.81710
H	5.50690	1.69490	0.69850
H	3.01660	-1.71170	-2.72460
H	-0.22160	-2.56800	0.87980
H	0.19810	-2.04380	2.51780
H	-2.13390	-1.57550	2.13410
H	-1.25210	-0.02840	2.25810
H	-3.86560	1.18530	-3.19210
H	-4.23120	2.23390	-1.79510
H	-5.09620	0.67800	-2.00260
H	3.82160	1.84330	-1.61780
N	1.01120	-0.88780	0.96950
N	3.85560	1.70000	-0.61480
O	-3.08370	0.51360	-1.43070
O	-1.85480	-0.55800	0.33310
O	-4.44060	-0.40880	0.58650
O	-2.97470	1.72460	0.86990
P	-3.19980	0.37880	0.20030

favilipd model compound conf #09
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7632852 Hartree

C	1.19600	0.04410	1.34260
C	1.93380	1.20080	1.07290
C	2.43980	1.39170	-0.21650
C	2.10330	0.35960	-1.26550
C	2.00610	-1.05030	-0.66780
C	3.39430	-1.63800	-0.33790
C	3.39630	-3.08280	0.16860
C	3.44820	3.59530	0.27310
C	0.16810	-2.08800	0.77600
C	-1.13160	-1.89470	0.00600
C	-4.37890	2.05940	0.46550
H	0.62900	-0.02780	2.26660
H	2.01180	1.95770	1.84230
H	1.14000	0.64910	-1.70690
H	2.84420	0.36350	-2.07040
H	1.50780	-1.69780	-1.39370
H	4.03940	4.30710	-0.30300
H	3.89850	-0.99150	0.39070
H	3.97800	-1.58020	-1.26510
H	4.42710	-3.43190	0.29540
H	2.89850	-3.18060	1.13930
H	2.53790	4.09080	0.62700
H	4.03210	3.26330	1.13730
H	2.90180	-3.75840	-0.53950
H	0.61130	-3.03790	0.46980
H	-0.03760	-2.13380	1.84890
H	-0.93540	-1.79580	-1.06740
H	-1.77130	-2.76930	0.17180
H	-4.34480	2.80570	1.26150
H	-5.33770	1.53200	0.50110
H	-4.26240	2.55520	-0.50380
H	3.41400	2.52290	-1.56170
N	1.13470	-1.00960	0.53820
N	3.12320	2.46620	-0.59210
O	-3.28460	1.15100	0.71220
O	-1.78270	-0.71000	0.50290
O	-2.62340	0.40250	-1.69080
O	-4.24260	-1.05870	-0.27130
P	-3.06490	-0.09990	-0.32600

favilipd model compound conf #10
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7632841 Hartree

C	-0.93440	0.42410	-1.05210
C	-1.92610	1.38520	-0.82770
C	-2.82760	1.19160	0.22190
C	-2.61510	-0.00310	1.11910
C	-2.05350	-1.21000	0.35640

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C          -3.07650        -1.94520        -0.53600
C          -4.18730        -2.64500         0.25370
C          -4.08370         3.28350        -0.17920
C           0.20740        -1.70140        -0.69530
C           1.22110        -1.69080         0.44480
C           4.60390         2.17580         0.19060
H          -0.12830         0.63600        -1.74880
H          -1.91980         2.28560        -1.42780
H          -1.90160         0.30270         1.89640
H          -3.54080        -0.28090         1.62880
H          -1.65910        -1.91680         1.09150
H          -4.96240         3.74340         0.27300
H          -2.52990        -2.69350        -1.12140
H          -3.51020        -1.23770        -1.25310
H          -4.82680        -3.21910        -0.42560
H          -3.77150        -3.34330         0.99030
H          -3.23850         3.97560        -0.10190
H          -4.28760         3.08800        -1.23670
H          -4.83010        -1.93560         0.78580
H          -0.19990        -2.71340        -0.78870
H           0.69660        -1.44110        -1.63650
H           0.73660        -1.90810         1.40100
H           1.97040        -2.46740         0.25830
H           4.41620         3.19140         0.54410
H           4.82680         2.19850        -0.88120
H           5.45100         1.75000         0.73800
H          -4.37750         1.82200         1.33550
N          -0.90370        -0.76960        -0.47640
N          -3.80400         2.03870         0.52840
O           3.39770         1.42550         0.44810
O           1.83630        -0.39300         0.58310
O           4.35940        -0.95850         0.85090
O           3.41750        -0.31410        -1.48640
P           3.36550        -0.15910         0.02480

favilipd model compound conf #11
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7632499 Hartree
C          -1.51970        -1.51660        -0.28250
C          -2.68140        -1.33980         0.47560
C          -3.51870        -0.26070         0.17750
C          -3.14350         0.61480        -0.99370
C          -1.62140         0.75330        -1.13000
C          -0.98810         1.64960        -0.04100
C          -1.38150         3.12520        -0.17120
C          -5.21680        -0.82260         1.88430
C           0.10910        -0.93600        -1.99780
C           1.45600        -0.36400        -1.58020
C           4.13510         1.78930         1.23210
H          -0.97410        -2.45340        -0.21580
H          -2.94720        -2.09700         1.20150
H          -3.55800         0.14400        -1.89570
H          -3.60410         1.60170        -0.90860
H          -1.39970         1.17920        -2.11230
H          -6.14350        -0.35590         2.21850
H           0.09920         1.56590        -0.11200
H          -1.26510         1.27350         0.95100
H          -0.84190         3.72300         0.57130
H          -1.12710         3.51750        -1.16350
H          -5.43200        -1.84100         1.54370
H          -4.51690        -0.86830         2.72450
H          -2.45170         3.29020        -0.00720
H           0.17950        -2.02500        -2.05110
H          -0.12440        -0.56380        -3.00090
H           2.19870        -0.68300        -2.31930
H           1.44380         0.72950        -1.54860
H           3.75500         2.79520         1.42150
H           4.92900         1.83440         0.47980
H           4.53030         1.37000         2.16360
H          -5.21520         0.77290         0.48050
N          -1.02010        -0.60930        -1.11280
N          -4.66550        -0.01650         0.80000
O           3.01780         1.01290         0.75160
O           1.79260        -0.89060        -0.28180
O           3.28900        -1.39950         1.67680
O           4.37120        -0.72070        -0.60980
P           3.24840        -0.58010         0.40240

favilipd model compound conf #12
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Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7631985 Hartree

C	1.32020	0.34420	1.36870
C	2.23400	1.31270	0.95310
C	3.13180	1.00460	-0.07350
C	3.15000	-0.41410	-0.57260
C	1.76210	-1.06680	-0.55270
C	1.83320	-2.55140	-0.94960
C	2.69230	-3.45790	-0.06020
C	4.19850	3.23420	-0.11680
C	-0.05840	-1.62620	1.17230
C	-1.30770	-1.33670	0.34940
C	-5.49260	0.08920	-0.09610
H	0.70620	0.54530	2.24140
H	2.25830	2.25710	1.48120
H	3.54410	-0.46360	-1.59140
H	3.84360	-0.96750	0.07440
H	1.13110	-0.55360	-1.29350
H	0.81710	-2.95240	-1.01860
H	2.22510	-2.56850	-1.97360
H	2.60930	-4.49500	-0.40350
H	3.75260	-3.18760	-0.09660
H	2.37650	-3.43090	0.98880
H	3.27260	3.80050	-0.25770
H	4.48350	3.27280	0.93980
H	4.98820	3.68850	-0.71510
H	0.17490	-2.68890	1.08700
H	-0.25390	-1.41550	2.22630
H	-1.13890	-1.51470	-0.71640
H	-2.10880	-1.99910	0.69660
H	-6.15760	-0.49380	0.54430
H	-5.54880	-0.28940	-1.12170
H	-5.79680	1.14120	-0.07190
H	4.65000	1.51570	-1.28470
N	1.11230	-0.82860	0.77110
N	4.02860	1.85330	-0.55830
O	-4.16220	-0.07390	0.43780
O	-1.68330	0.03970	0.55890
O	-2.92300	2.18160	0.08400
O	-2.84690	0.32030	-1.75540
P	-2.91130	0.71300	-0.29060

favilipd model compound conf #13

Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7631374 Hartree

C	1.55640	0.08520	-1.52040
C	2.54430	-0.83300	-1.15410
C	2.82400	-1.02040	0.20130
C	1.95170	-0.31640	1.20990
C	1.39940	1.03460	0.72480
C	2.34560	2.23730	0.92890
C	3.69060	2.21230	0.19610
C	4.62740	-2.67080	-0.17520
C	-0.13080	1.80070	-1.16280
C	-1.48740	1.11320	-1.19820
C	-4.08180	-2.36440	-0.45670
H	1.24190	0.14140	-2.55960
H	3.03380	-1.40440	-1.93170
H	1.11420	-0.99360	1.42450
H	2.48950	-0.16580	2.15070
H	0.49870	1.23760	1.30710
H	5.31810	-3.20460	0.47770
H	2.51660	2.30640	2.01100
H	1.79960	3.14670	0.64960
H	4.24150	3.13550	0.40910
H	4.32090	1.37500	0.51420
H	4.04510	-3.39840	-0.75050
H	5.20120	-2.04640	-0.86720
H	3.56390	2.15080	-0.89020
H	-0.16960	2.67580	-0.51080
H	0.10400	2.14220	-2.17560
H	-2.22330	1.81120	-1.61190
H	-1.44880	0.21880	-1.83000
H	-3.64780	-3.26450	-0.89680
H	-4.83220	-1.94990	-1.13720
H	-4.54980	-2.61890	0.50040
H	3.85590	-1.93610	1.66330
N	0.95620	0.92790	-0.69130
N	3.75660	-1.84810	0.65810
O	-2.99410	-1.43530	-0.26840

O -1.86130 0.74130 0.14440
O -3.38720 -0.13430 1.94500
O -4.42740 0.71810 -0.30360
P -3.30260 0.01960 0.43910

favilipd model compound conf #14
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7624681 Hartree
C -1.86310 -0.95700 1.15080
C -3.16150 -1.32330 0.78730
C -3.75630 -0.69760 -0.31290
C -2.91620 0.26800 -1.11160
C -1.92580 1.04290 -0.23250
C -2.56170 2.16080 0.62170
C -3.11010 3.32520 -0.20960
C -5.88700 -1.94010 -0.14290
C 0.17400 0.37740 1.03560
C 1.15730 -0.20090 0.01770
C 6.25350 0.38610 0.17860
H -1.32760 -1.54120 1.89460
H -3.64290 -2.12910 1.32550
H -2.36300 -0.32500 -1.85280
H -3.54570 0.96630 -1.66790
H -1.17160 1.48820 -0.88670
H -6.83000 -1.91210 -0.68870
H -1.79130 2.54160 1.30210
H -3.35530 1.73590 1.24830
H -3.47280 4.12030 0.45090
H -2.33190 3.75440 -0.85230
H -5.46910 -2.95050 -0.20320
H -6.07400 -1.69390 0.90700
H -3.94750 3.02410 -0.84820
H 0.29950 1.46210 1.09580
H 0.36610 -0.04700 2.02450
H 1.09660 -1.29530 0.01580
H 0.94200 0.17140 -0.98980
H 6.76850 1.20520 0.68390
H 6.50960 0.39780 -0.88610
H 6.55660 -0.56670 0.62390
H -5.30600 -0.47860 -1.57280
N -1.21130 0.08760 0.65560
N -4.98190 -0.96650 -0.74520
O 4.84100 0.61420 0.37020
O 2.46940 0.22890 0.42580
O 4.02260 -1.84630 0.20220
O 3.70340 -0.23120 -1.81440
P 3.78210 -0.43670 -0.31060

favilipd model compound conf #15
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7623296 Hartree
C -1.84030 0.43870 1.51330
C -2.77620 -0.55930 1.22870
C -2.80180 -1.11150 -0.05640
C -1.76440 -0.63930 -1.04580
C -1.40960 0.83920 -0.84180
C -2.52100 1.78240 -1.34790
C -2.19610 3.27710 -1.27730
C -4.61850 -2.71550 0.43540
C -0.02480 1.97470 1.00000
C 1.26290 1.24380 1.35100
C 4.11930 -1.68010 -1.75860
H -1.67360 0.73920 2.54490
H -3.39320 -0.93730 2.03330
H -0.87100 -1.26170 -0.89980
H -2.10410 -0.79410 -2.07380
H -0.48780 1.04850 -1.38800
H -5.15940 -3.45620 -0.15360
H -3.44970 1.58030 -0.80020
H -2.70560 1.50250 -2.39260
H -3.00610 3.85700 -1.73370
H -2.08710 3.62790 -0.24550
H -4.13680 -3.21520 1.28250
H -5.32830 -1.97410 0.81530
H -1.27230 3.51400 -1.81820
H 0.15520 2.67710 0.18530
H -0.34450 2.54290 1.87940
H 1.99710 1.97960 1.70030
H 1.08500 0.51210 2.14710
H 3.83240 -1.98350 -2.76720

H	4.29390	-2.57140	-1.14670
H	5.03080	-1.07560	-1.80410
H	-3.54030	-2.43660	-1.37400
N	-1.11490	1.07110	0.59930
N	-3.62620	-2.08300	-0.42780
O	3.01760	-0.90610	-1.23750
O	1.75540	0.57360	0.17410
O	4.34600	0.59970	0.41220
O	2.97120	-1.41970	1.31360
P	3.13700	-0.31160	0.28710

favilipd model compound conf #16
Energy at B3LYP/6-31+G(d,p)/SMD(MeOH): -1183.7621729 Hartree

C	1.15900	-0.00440	1.25970
C	2.00970	1.07020	0.98500
C	2.61180	1.15290	-0.27150
C	2.22270	0.13620	-1.31490
C	1.83590	-1.23650	-0.73780
C	3.02010	-2.19300	-0.47910
C	4.07260	-1.75540	0.54420
C	3.84230	3.24080	0.21710
C	-0.00520	-2.08900	0.79140
C	-1.31590	-1.87540	0.04690
C	-4.42420	2.19340	0.45710
H	0.57820	-0.00270	2.17770
H	2.13320	1.83710	1.73830
H	1.36430	0.55810	-1.85460
H	3.02510	0.00280	-2.04660
H	1.19580	-1.72150	-1.47900
H	4.54500	3.85980	-0.34080
H	3.49800	-2.35370	-1.45410
H	2.60880	-3.16450	-0.17940
H	4.82700	-2.54270	0.65320
H	4.59560	-0.84280	0.23890
H	2.97640	3.84920	0.49900
H	4.33210	2.87600	1.12540
H	3.63460	-1.58340	1.53330
H	0.39240	-3.07060	0.51990
H	-0.18380	-2.08100	1.86980
H	-1.14690	-1.82960	-1.03480
H	-1.98550	-2.71480	0.26620
H	-4.41490	2.90460	1.28520
H	-5.41070	1.72230	0.39350
H	-4.20160	2.71820	-0.47750
H	3.79550	2.11220	-1.58320
N	1.00180	-1.06640	0.48150
N	3.43990	2.12620	-0.63400
O	-3.40480	1.21430	0.75000
O	-1.90460	-0.64480	0.51000
O	-2.76400	0.49300	-1.66530
O	-4.36790	-0.98790	-0.24870
P	-3.19280	-0.02580	-0.30260