

Supporting Information

Antibacterial and Antiproliferative Polyketides, Diketopiperazine and Isochromanone from a Marine-derived Fungal Strain *Fusarium graminearum* FM1010 in Hawaii

KH Ahammad Uz Zaman^a, Ariel M. Sarotti^b, Xiaohua Wu^a, Lela DeVine^c, Shugeng Cao,^{a,*}

^aDepartment of Pharmaceutical Sciences, Daniel K. Inouye College of Pharmacy, University of Hawai'i at Hilo, Hilo, Hawaii 96720, United States

^bInstituto de Química Rosario (CONICET), Facultad de Ciencias Bioquímicas y Farmacéuticas, Universidad Nacional de Rosario, Suipacha 531, Rosario 2000, Argentina

^cDepartment of Cellular and Molecular Biology, Barnard College of Columbia University, USA

*Corresponding author

Table of Contents

Figures	Content	Page
Fig. S1	HRESIMS of compound 1	4
Fig. S2	¹ H NMR spectrum of compound 1 in DMSO-d ₆ (400MHz)	5
Fig. S3	¹³ C NMR spectrum of compound 1 in DMSO-d ₆ (100MHz)	6
Fig. S4	HSQC spectrum of compound 1 in DMSO-d ₆ (400MHz)	7
Fig. S5	COSY spectrum of compound 1 in DMSO-d ₆ (400MHz)	8
Fig. S6	HMBC spectrum of compound 1 in DMSO-d ₆ (400MHz)	9
Fig. S7	ROESY spectrum of compound 1 in DMSO-d ₆ (400MHz)	10
Fig. S8	DP4+ probability of compound 1	11
Fig. S9	Marfey analysis of <i>D</i> -valine hydrolyzed from 1	12
Fig. S10	Experimental and calculated ECD spectrum of 1	13
Fig. S11	IR spectrum of compound 1	14
Fig. S12	HRESIMS of compound 2	15
Fig. S13	¹ H NMR spectrum of compound 2 in DMSO-d ₆ (400MHz)	16
Fig. S14	DEPTQ spectrum of compound 2 in DMSO-d ₆ (100MHz)	17
Fig. S15	HSQC spectrum of compound 2 in DMSO-d ₆ (400MHz)	18
Fig. S16	COSY spectrum of compound 2 in DMSO-d ₆ (400MHz)	19
Fig. S17	HMBC spectrum of compound 2 in DMSO-d ₆ (400MHz)	20
Fig. S18	ROESY spectrum of compound 2 in DMSO-d ₆ (400MHz)	21
Fig. S19	DP4+ probability of compound 2	22
Fig. S20	Marfey analysis of allo- <i>D</i> -isoleucine hydrolyzed from 2	23
Fig. S21	Experimental and calculated ECD spectrum of 2	24
Fig. S22	IR spectrum of compound 2	25
Fig. S23	HRESIMS of compound 3	26
Fig. S24	¹ H NMR spectrum of compound 3 in CD ₃ OD (400MHz)	27
Fig. S25	DEPTQ spectrum of compound 3 in CD ₃ OD (100MHz)	28
Fig. S26	HSQC spectrum of compound 3 in CD ₃ OD (400MHz)	29

Fig. S27	COSY spectrum of compound 3 in CD ₃ OD (400MHz)	30
Fig. S28	HMBC spectrum of compound 3 in CD ₃ OD (400MHz)	31
Figures	Content	Page
Fig. S29	ROESY spectrum of compound 3 in CD ₃ OD (400MHz)	32
Fig. S30	IR spectrum of compound 3	33
Fig. S31	HRESIMS of compound 4	34
Fig. S32	¹ H NMR spectrum of compound 4 in CD ₃ OD (400MHz)	35
Fig. S33	HSQC spectrum of compound 4 in CD ₃ OD (400MHz)	36
Fig. S34	COSY spectrum of compound 4 in CD ₃ OD (400MHz)	37
Fig. S35	HMBC spectrum of compound 4 in CD ₃ OD (400MHz)	38
Fig. S36	ROESY spectrum of compound 4 in CD ₃ OD (400MHz)	39
Fig. S37	IR spectrum of compound 4	40
Fig. S38	HRESIMS of compound 5	41
Fig. S39	¹ H NMR spectrum of compound 5 in CD ₃ OD (400MHz)	42
Fig. S40	HSQC spectrum of compound 5 in CD ₃ OD (400MHz)	43
Fig. S41	COSY spectrum of compound 5 in CD ₃ OD (400MHz)	44
Fig. S42	HMBC spectrum of compound 5 in CD ₃ OD (400MHz)	45
Fig. S43	ROESY spectrum of compound 5 in CD ₃ OD (400MHz)	46
Fig. S44	IR spectrum of compound 5	47
Fig. S45	HRESIMS of compound 6	48
Fig. S46	¹ H NMR spectrum of compound 6 in CD ₃ OD (400MHz)	49
Fig. S47	DEPTQ spectrum of compound 6 in CD ₃ OD (100MHz)	50
Fig. S48	HSQC spectrum of compound 6 in CD ₃ OD (400MHz)	51
Fig. S49	COSY spectrum of compound 6 in CD ₃ OD (400MHz)	52
Fig. S50	HMBC spectrum of compound 6 in CD ₃ OD (400MHz)	53
Fig. S51	IR spectrum of compound 6	54
Table S1	¹ H and ¹³ C NMR Spectroscopic Data, and COSY & HMBC correlations for Compounds 6 in CD ₃ OD	55
Fig. S52	Structures of the known compounds 7–11	56
	Cartesian coordinates	57-104

Fig. S1: HRESIMS of compound 1

KH Ahammad Zaman S-2021-7
Synapt2_1580n 23 (0.465) Cm (23:24-5:9)

1: TOF MS ES-
1.12e6

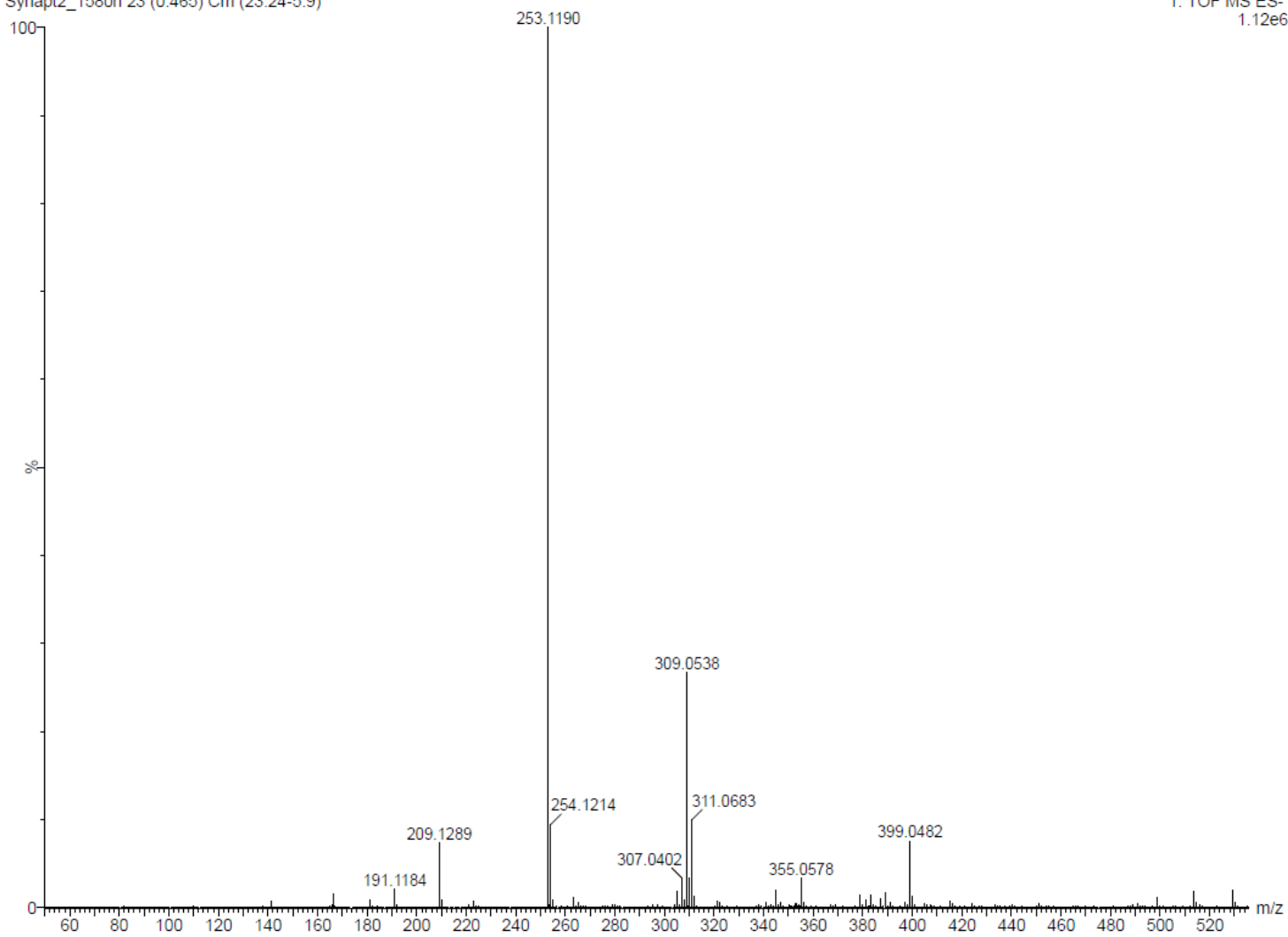


Fig. S2: ^1H NMR spectrum of compound 1 in DMSO-d_6 (400MHz)

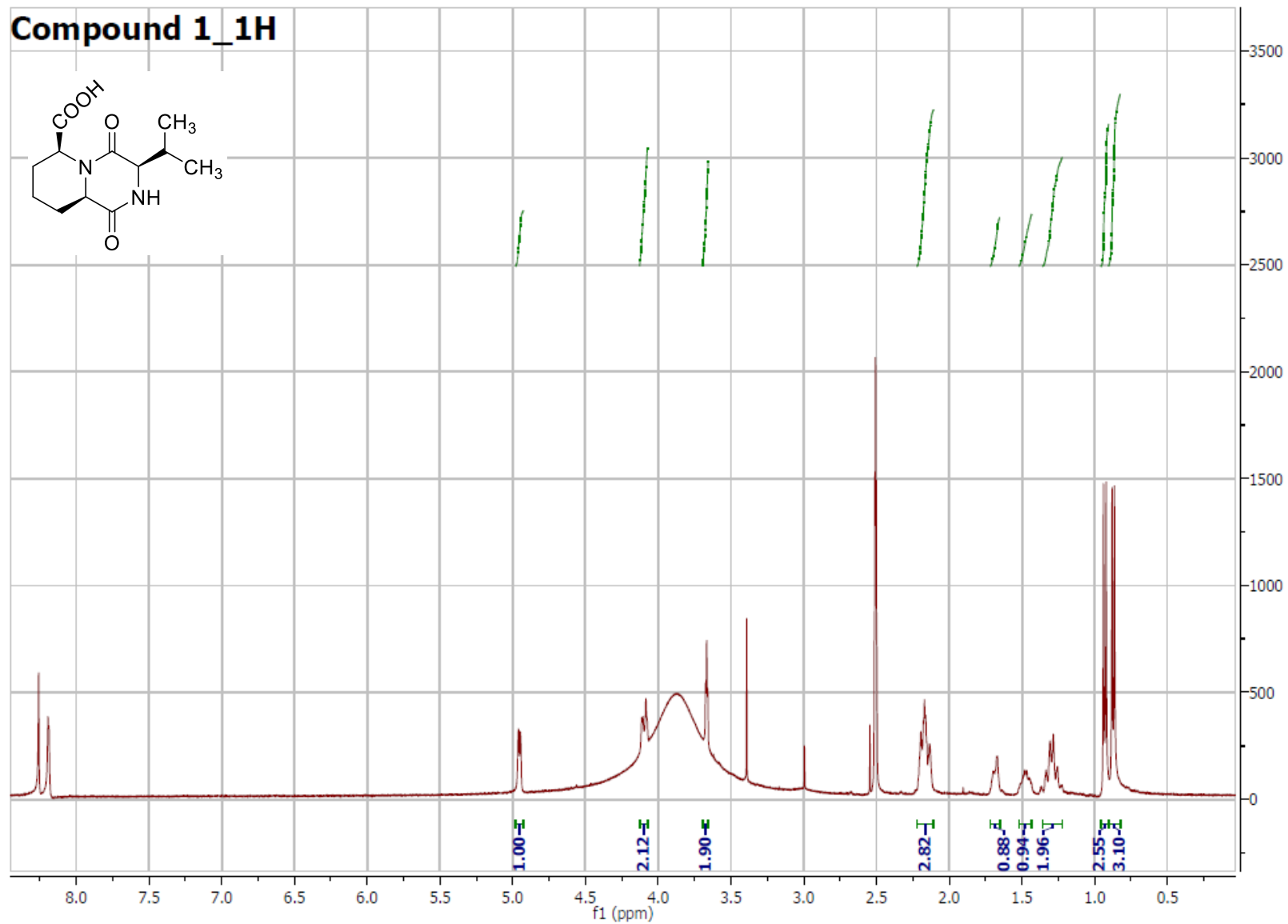


Fig. S3: ¹³C NMR spectrum of compound 1 in DMSO-d₆ (100MHz)

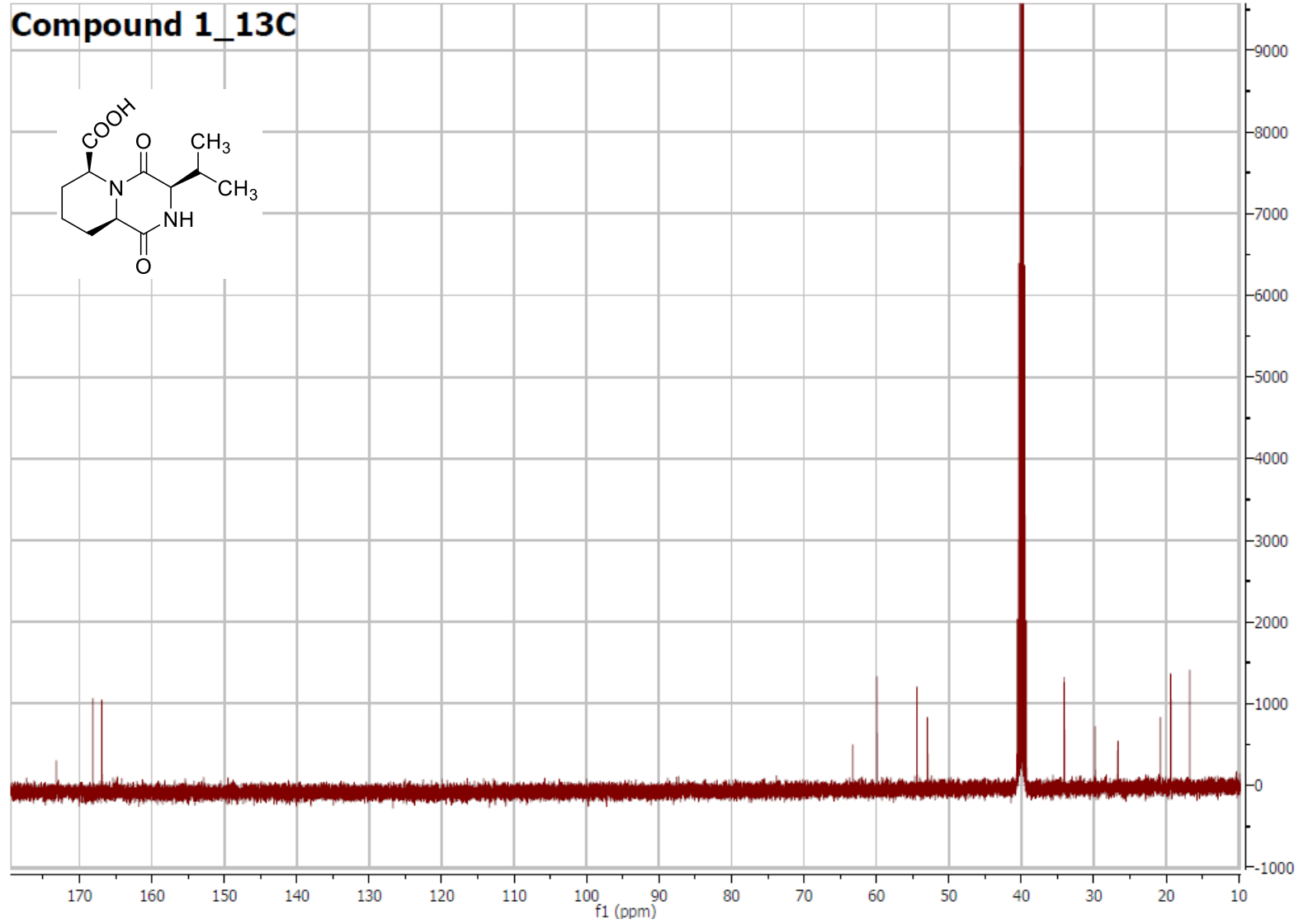


Fig. S4: HSQC spectrum of compound 1 in DMSO-d₆ (400MHz)

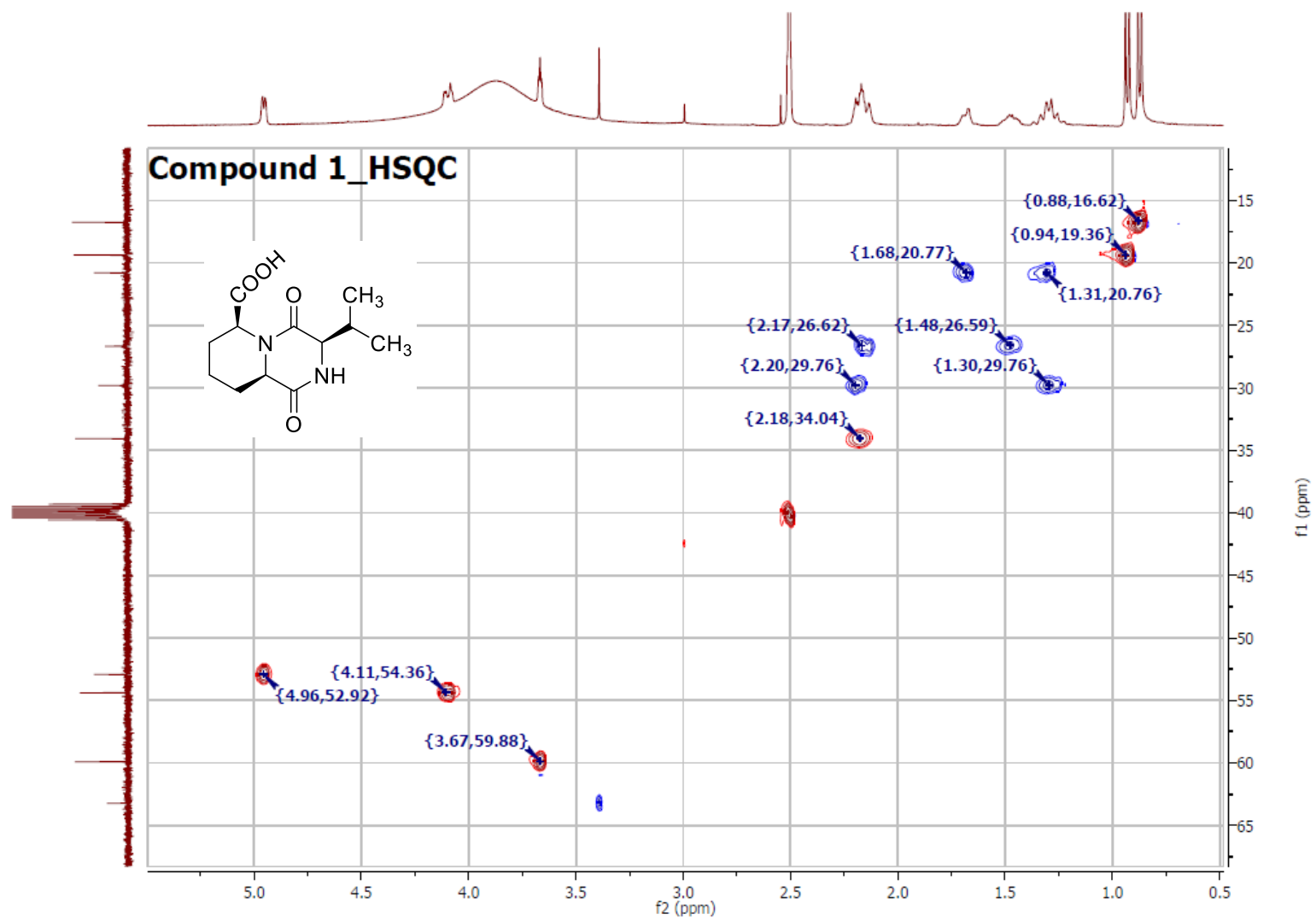


Fig. S5: COSY spectrum of compound 1 in DMSO-d₆ (400MHz)

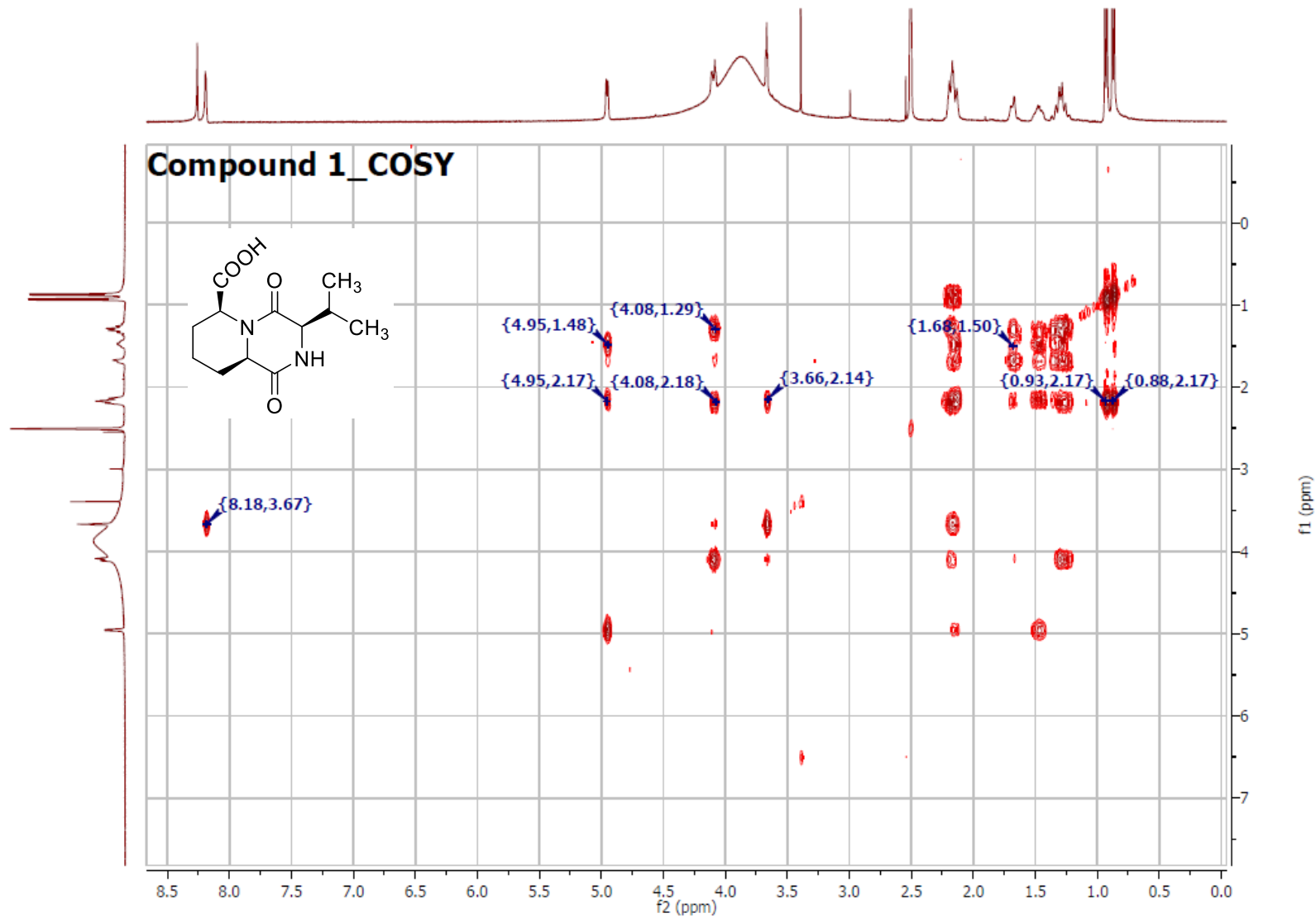


Fig. S6: HMBC spectrum of compound 1 in DMSO-d₆ (400MHz)

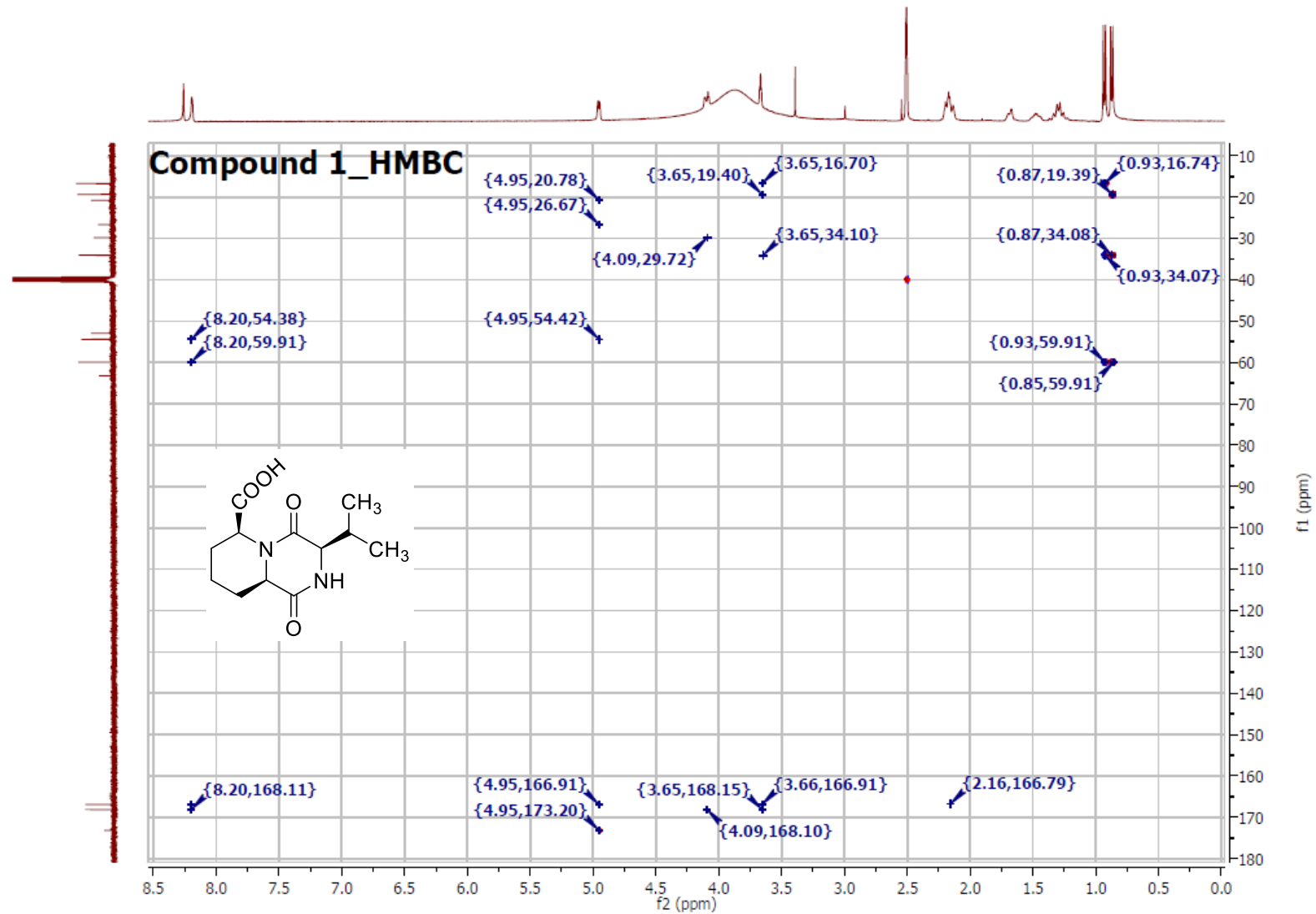
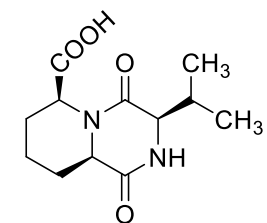


Fig. S7: ROESY spectrum of compound 1 in DMSO-d₆ (400MHz)



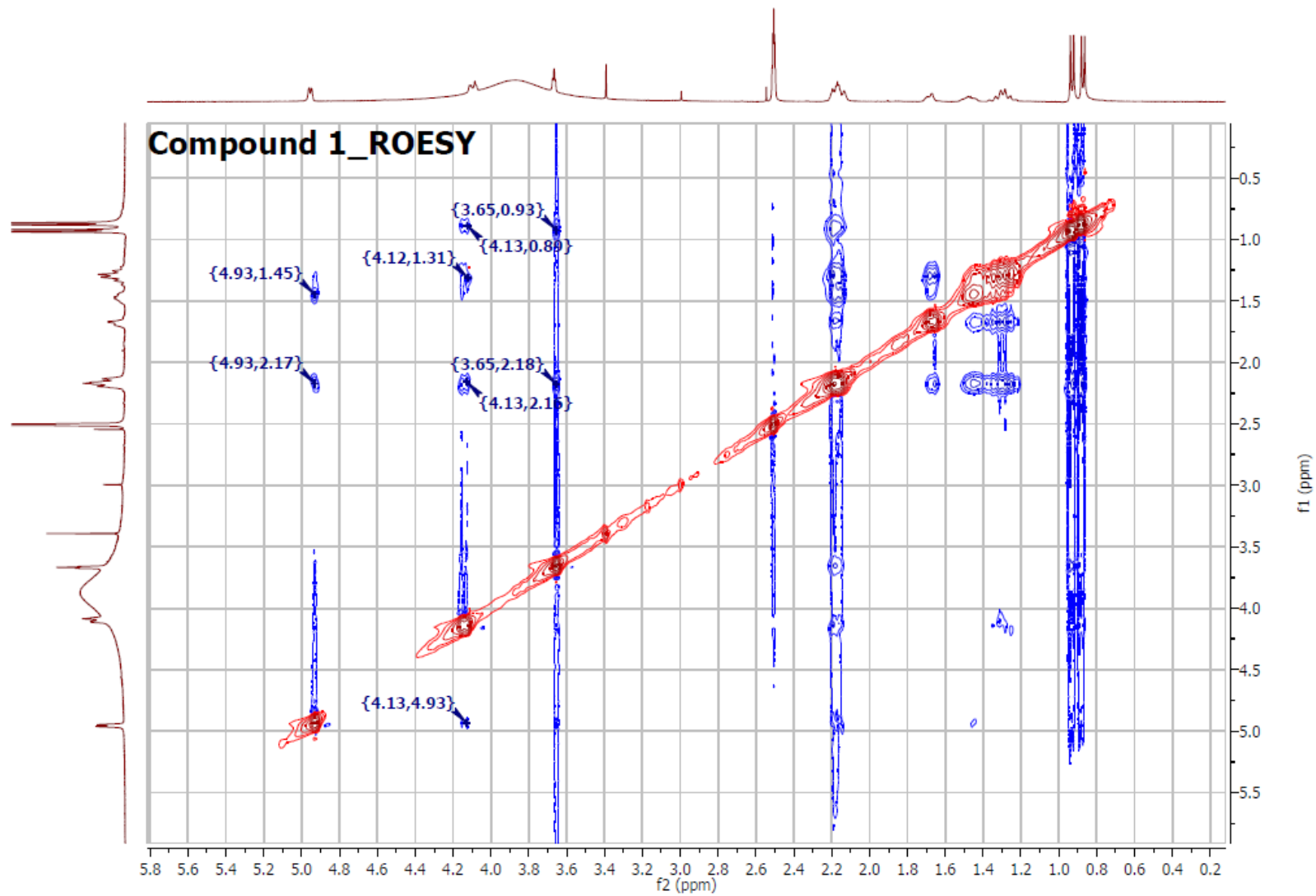
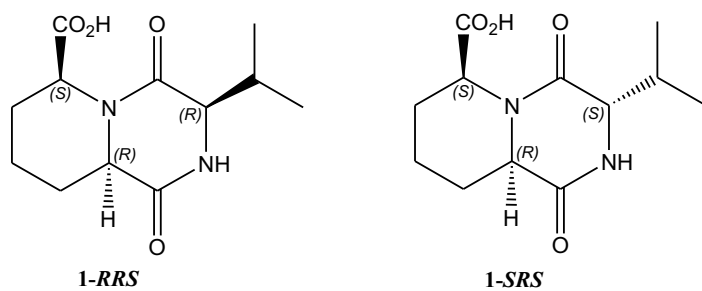


Fig. S8: DP4+ probability of compound 1





















	1-RRS	1-SRS
sDP4+ (H data)	 99.91%	 0.09%
sDP4+ (C data)	 99.63%	 0.37%
sDP4+ (all data)	 100.00%	 0.00%
uDP4+ (H data)	 84.56%	 15.44%
uDP4+ (C data)	 99.62%	 0.38%
uDP4+ (all data)	 99.93%	 0.07%
DP4+ (H data)	 99.98%	 0.02%
DP4+ (C data)	 100.00%	 0.00%
DP4+ (all data)	 100.00%	 0.00%

Fig. S9: Marfey analysis of *D*-valine hydrolyzed from 1

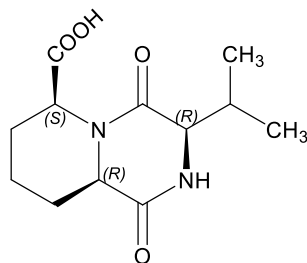
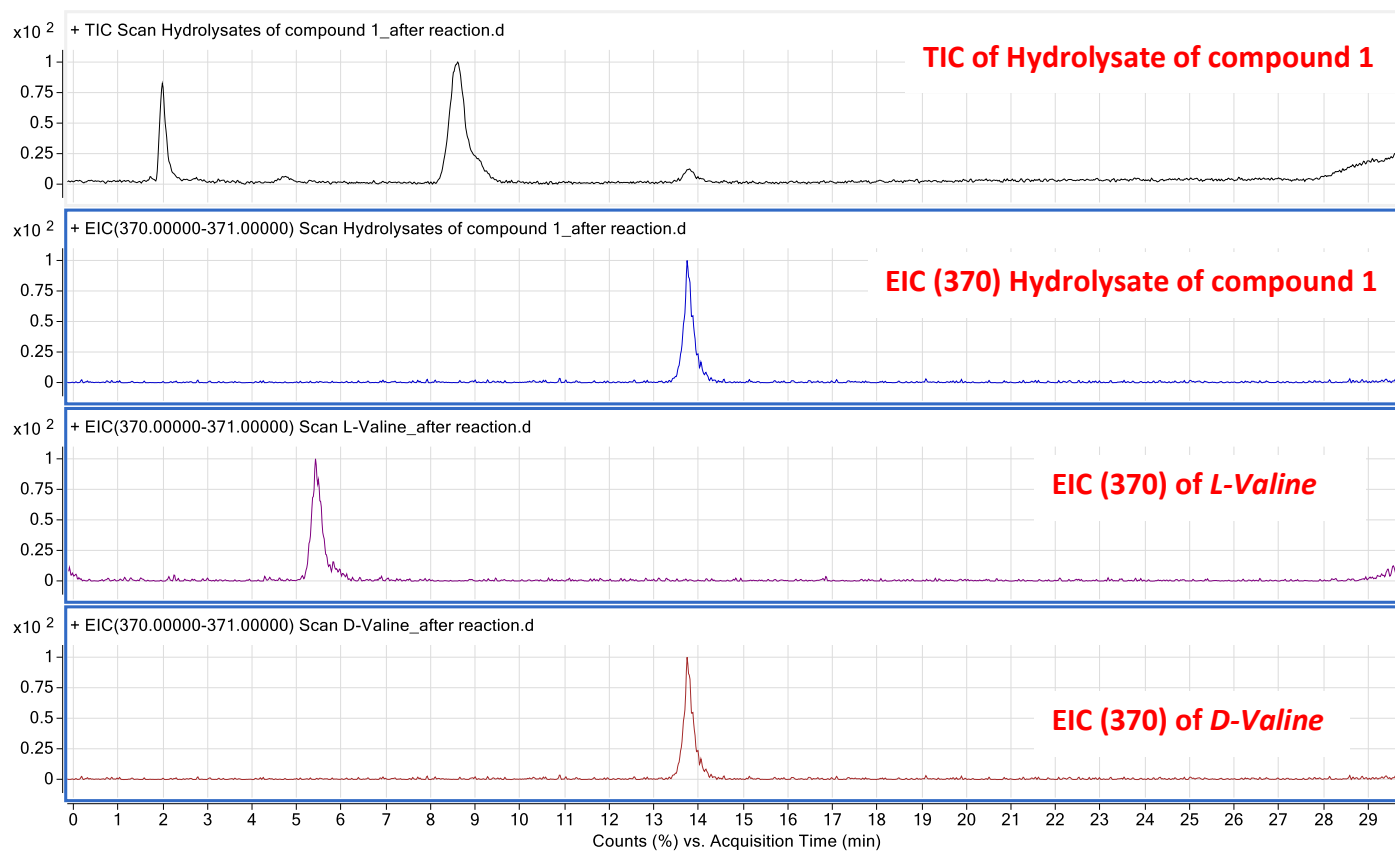


Fig. S10: Experimental and calculated ECD spectrum of 1

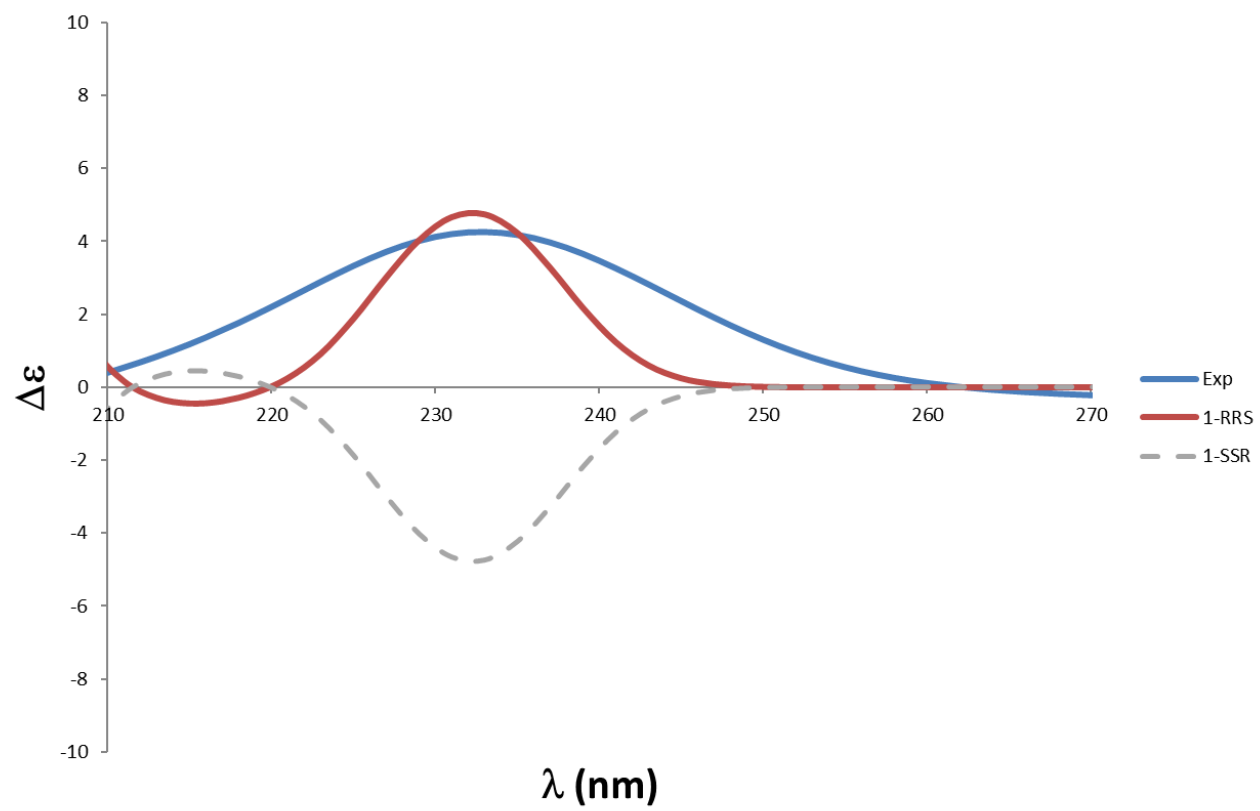


Fig. S11: IR spectrum of compound 1

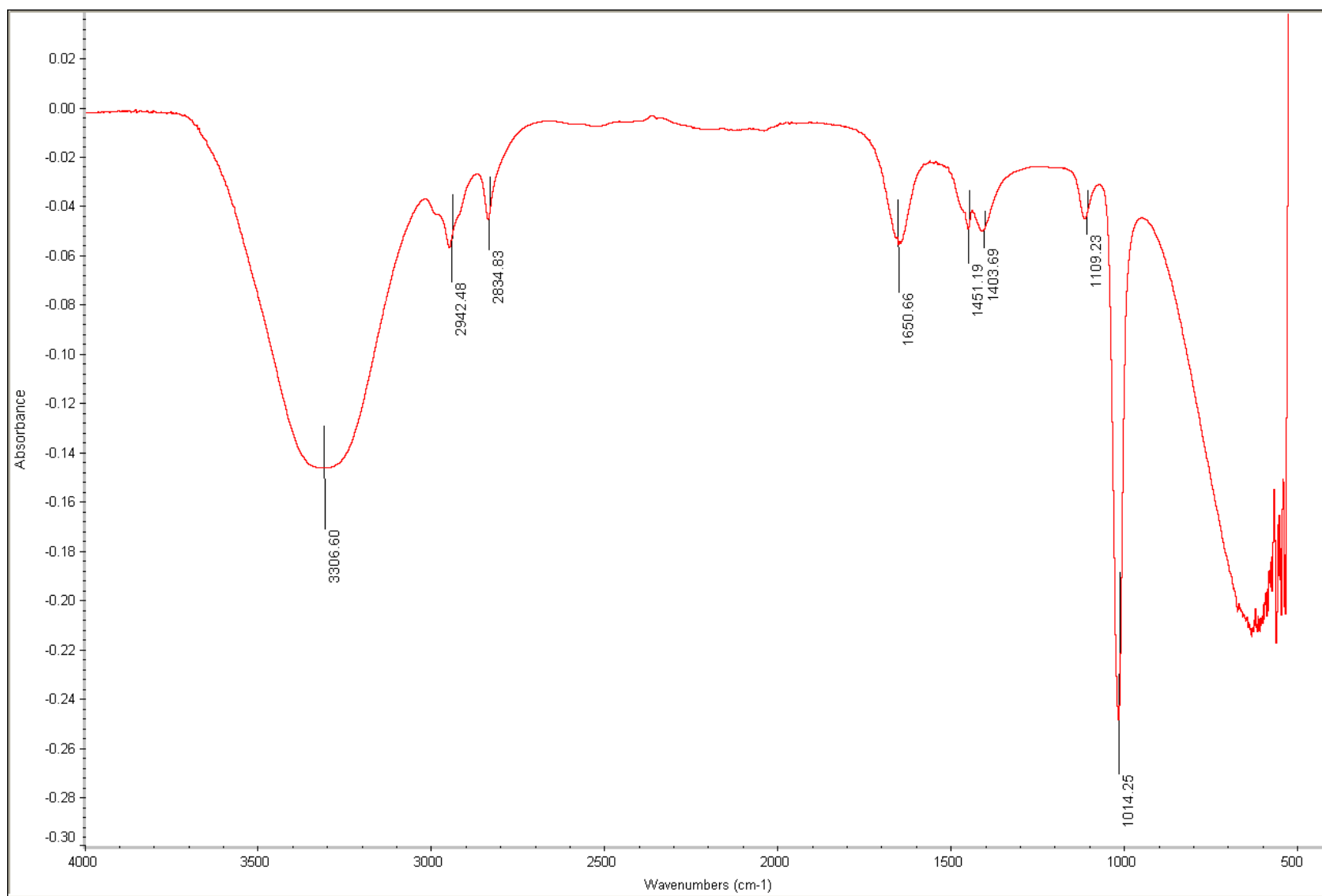


Fig. S12: HRESIMS of compound 2

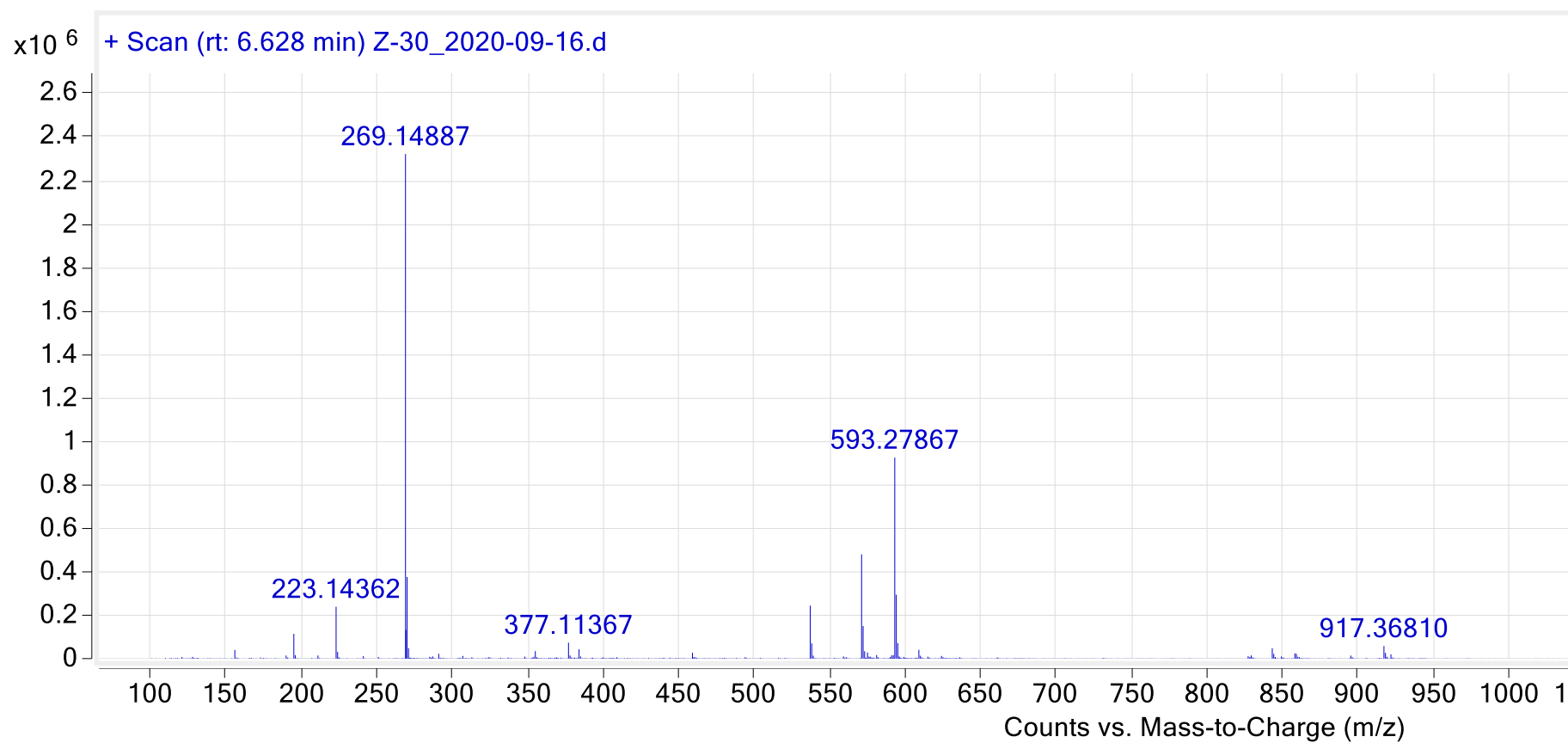


Fig. S13: ¹H NMR spectrum of compound 2 in DMSO-d₆ (400MHz)

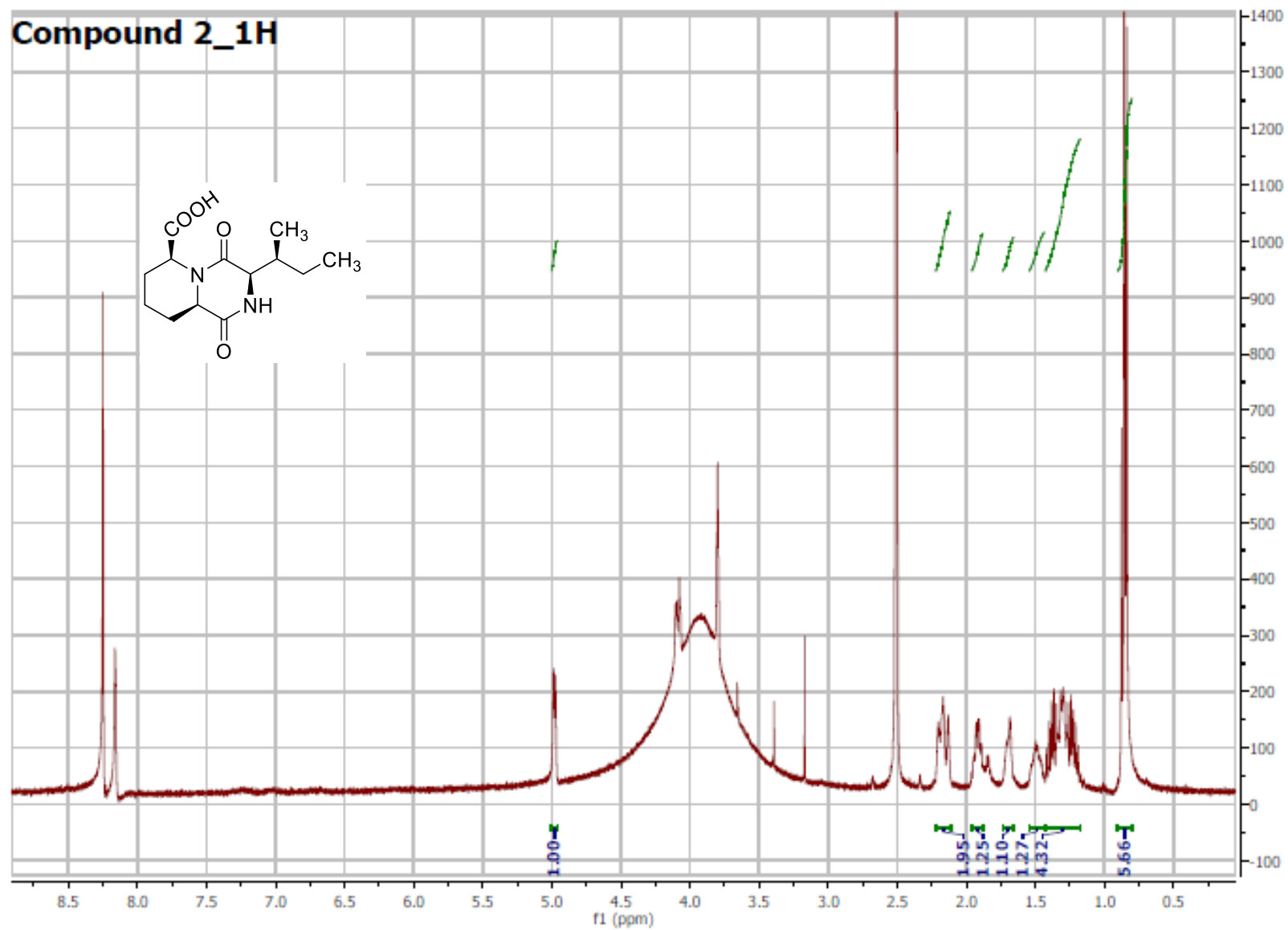


Fig. S14: DEPTQ spectrum of compound 2 in DMSO-d₆ (100MHz)

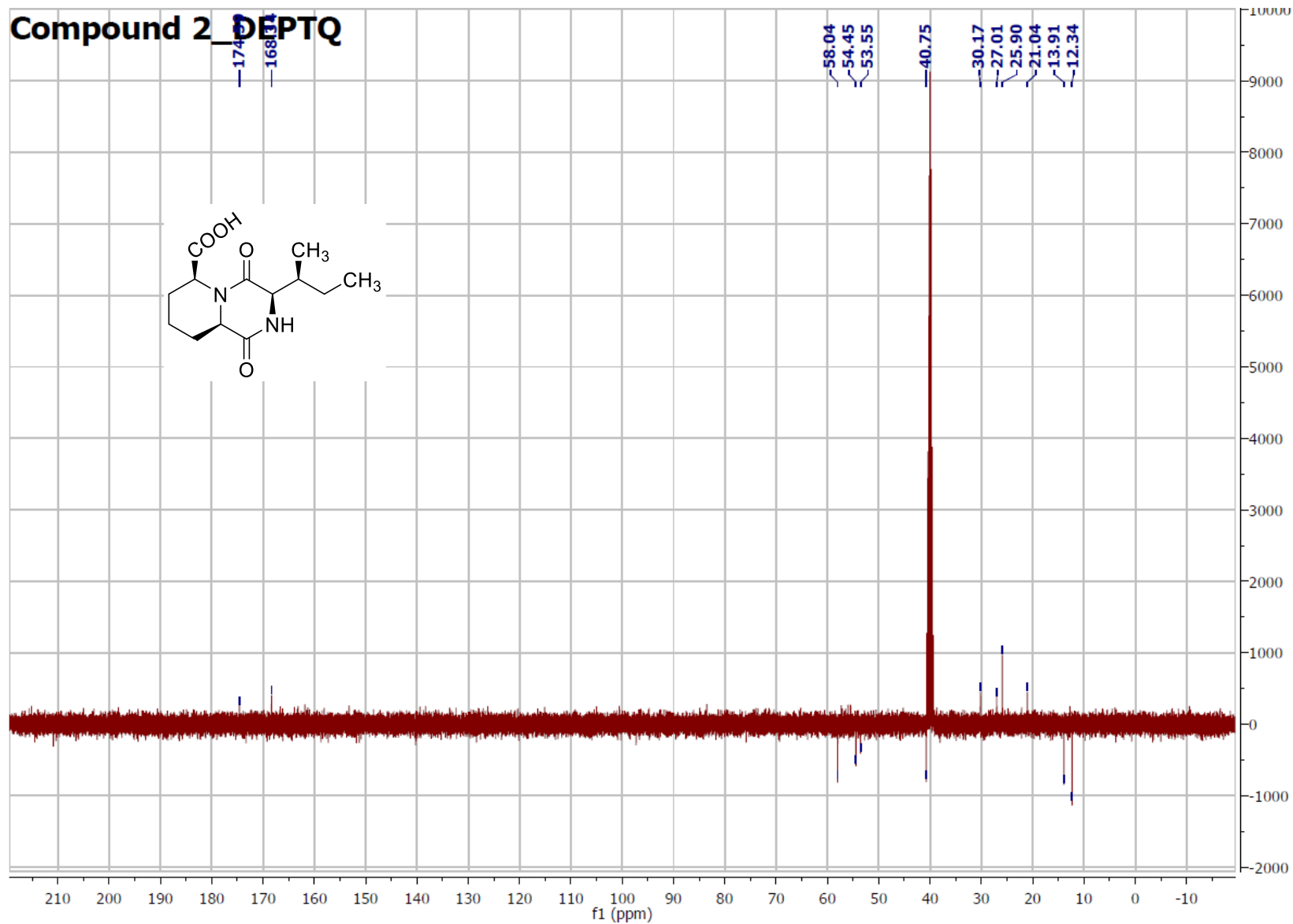


Fig. S15: HSQC spectrum of compound 2 in DMSO-d₆ (400MHz)

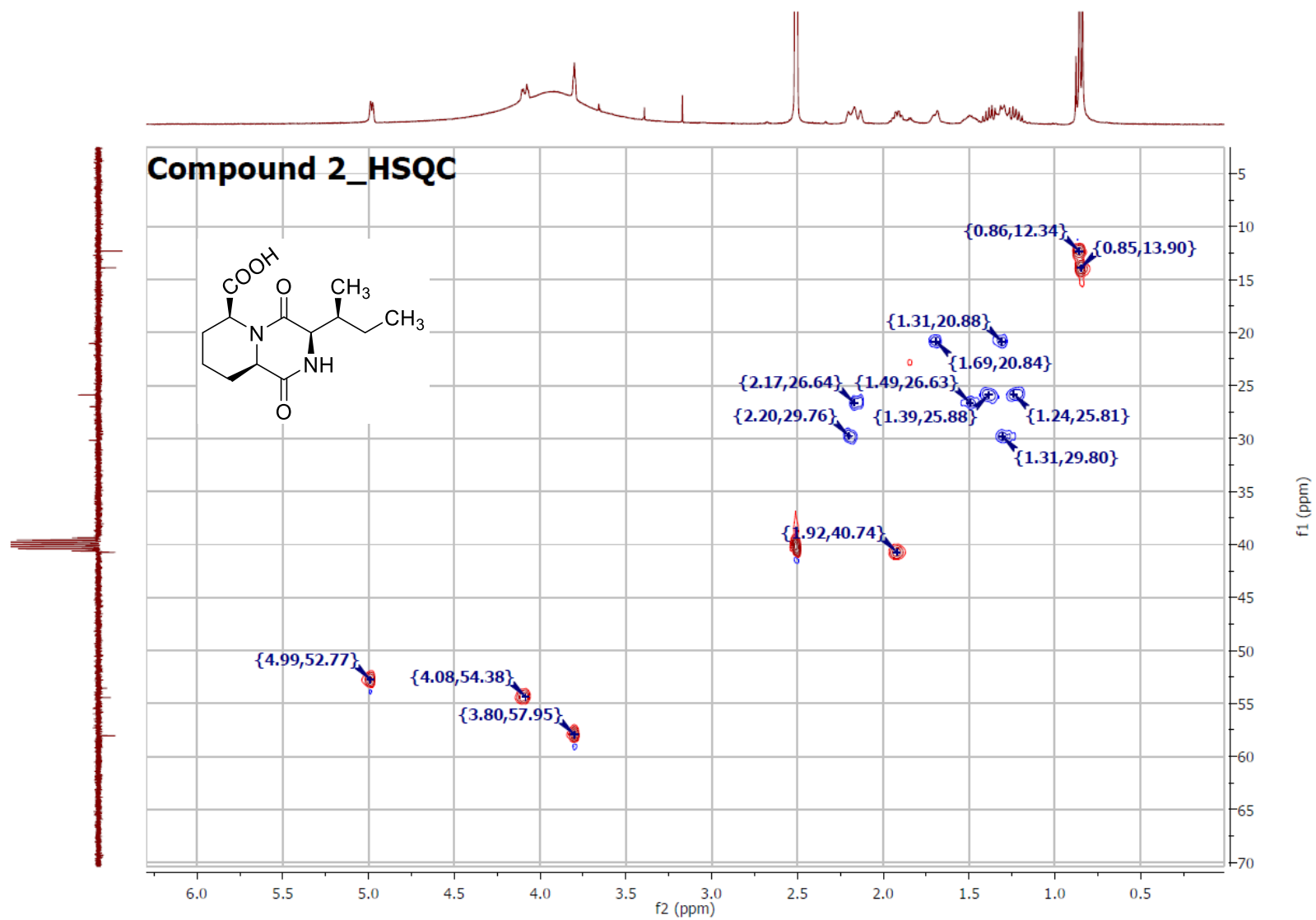


Fig. S16: COSY spectrum of compound 2 in DMSO-d₆ (400MHz)

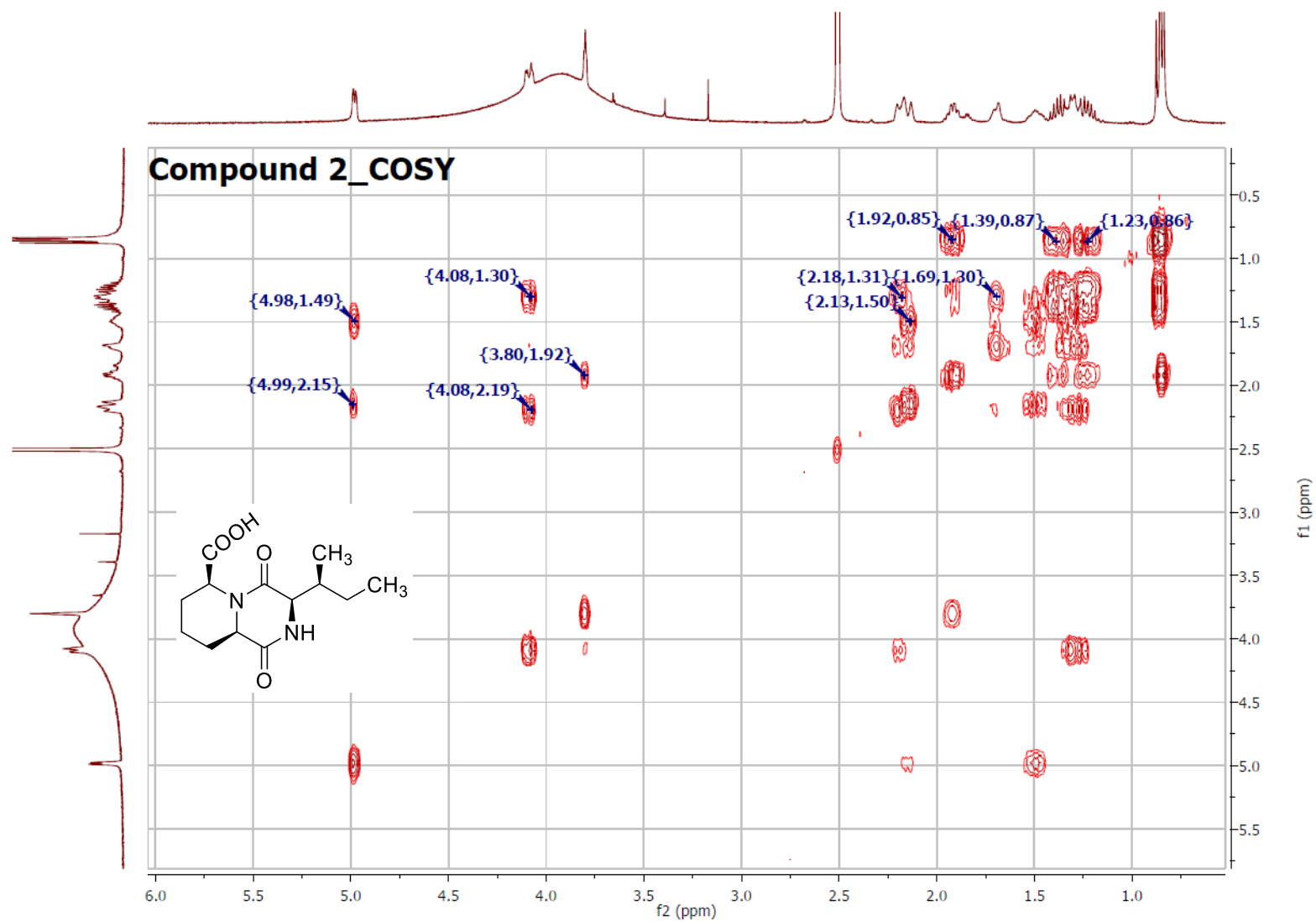


Fig. S17: HMBC spectrum of compound 2 in DMSO-d₆ (400MHz)

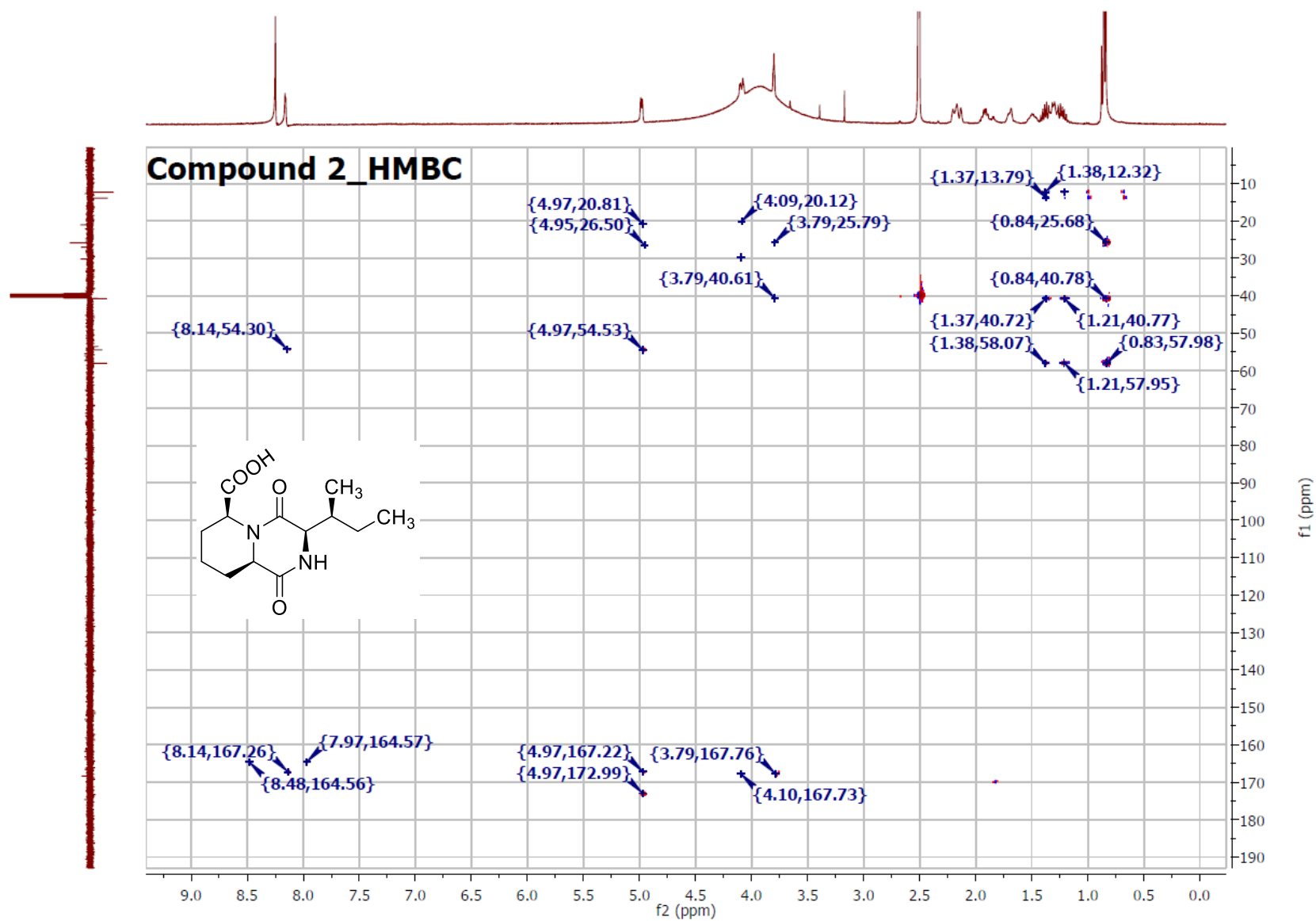


Fig. S18: ROESY spectrum of compound 2 in DMSO-d₆ (400MHz)

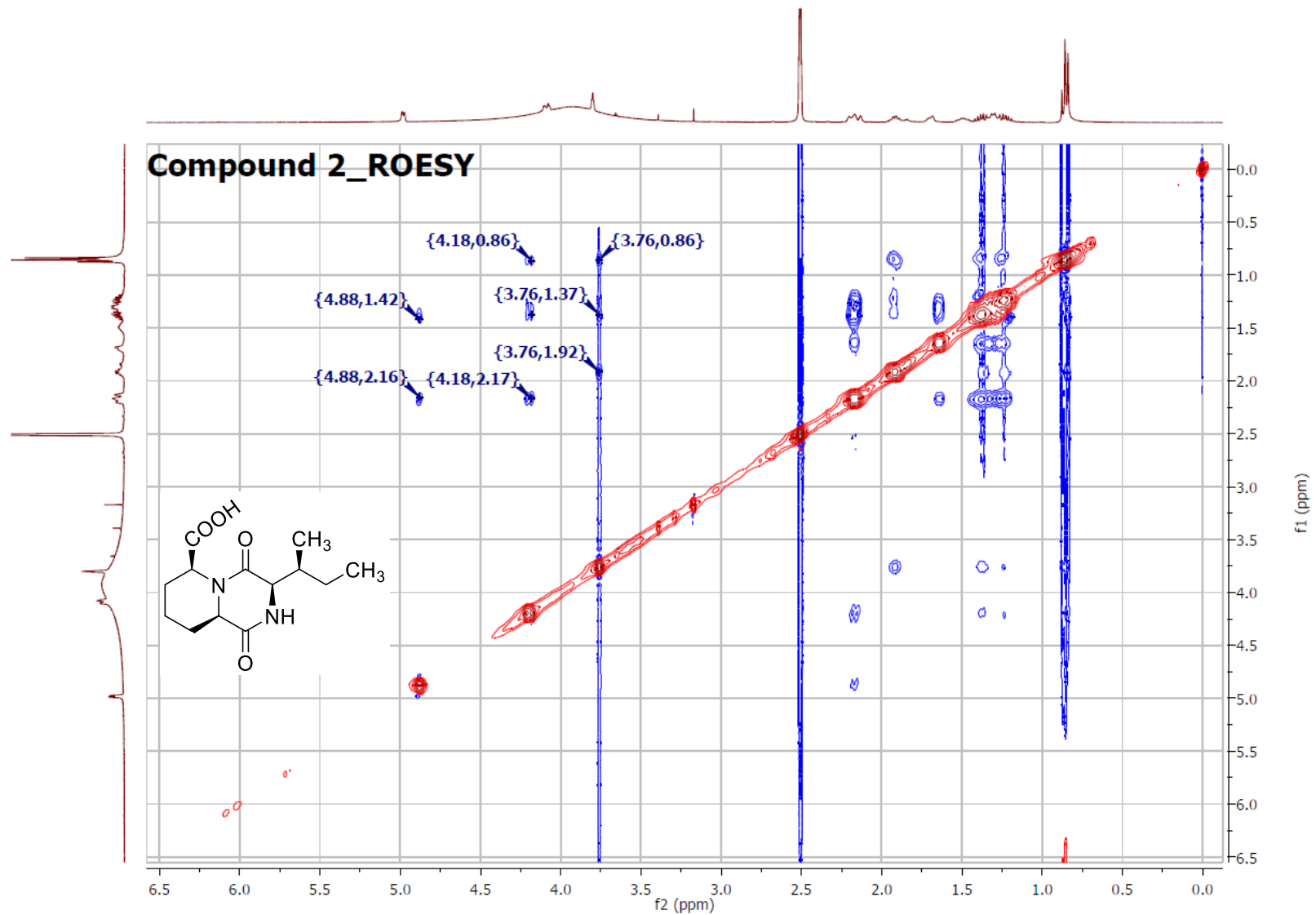
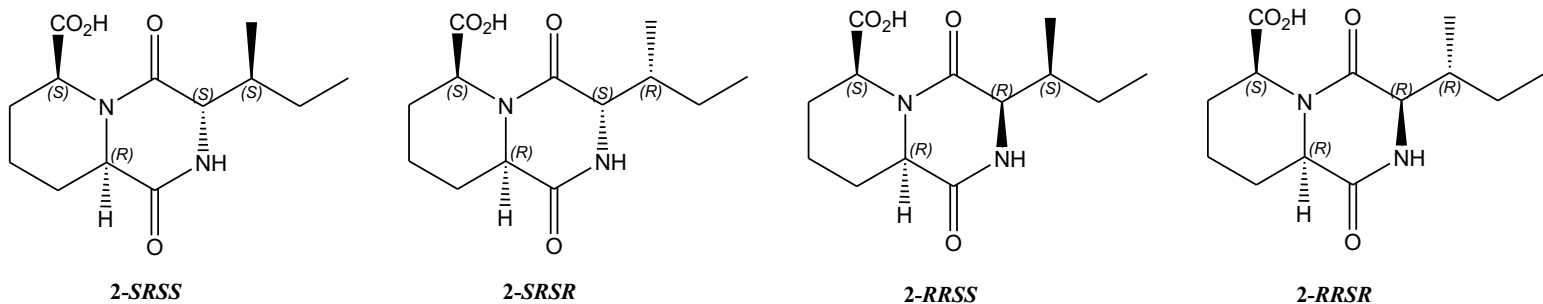


Fig. S19: DP4+ probability of compound 2



	2-SRSS	2-SRSR	2-RRSS	2-RRSR
sDP4+ (H data)	1.96%	0.09%	77.91%	20.03%
sDP4+ (C data)	0.00%	0.00%	98.99%	1.01%
sDP4+ (all data)	0.00%	0.00%	99.74%	0.26%
uDP4+ (H data)	2.77%	86.55%	8.12%	2.56%
uDP4+ (C data)	0.02%	0.04%	96.13%	3.82%
uDP4+ (all data)	0.01%	0.40%	98.37%	1.23%
DP4+ (H data)	0.78%	1.16%	90.71%	7.35%
DP4+ (C data)	0.00%	0.00%	99.96%	0.04%
DP4+ (all data)	0.00%	0.00%	100.00%	0.00%

Fig. S20: Marfey analysis of allo-*D*- isoleucine hydrolyzed from 2

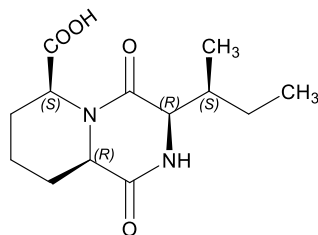
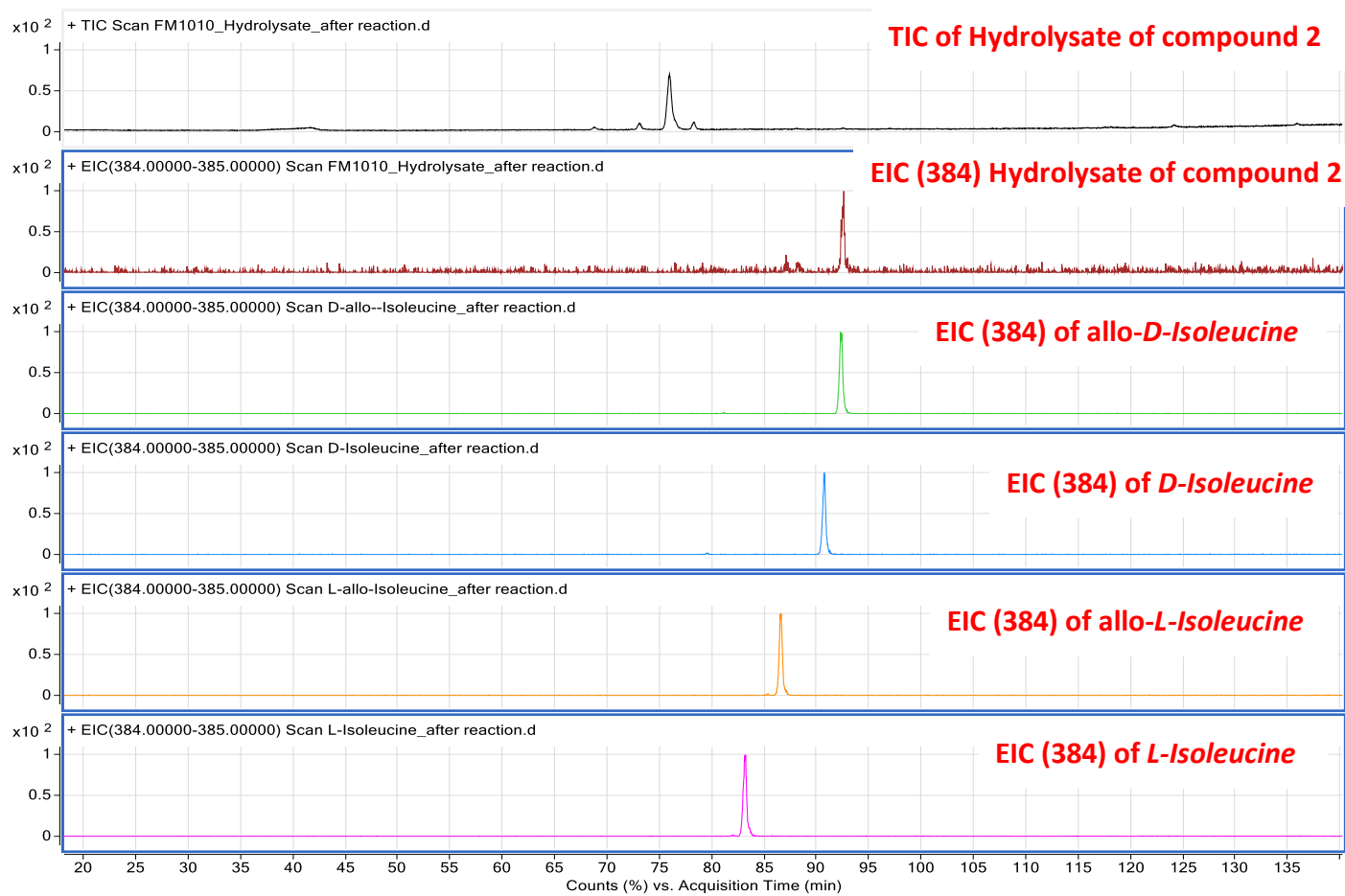


Fig. S21: Experimental and calculated ECD spectrum of 2

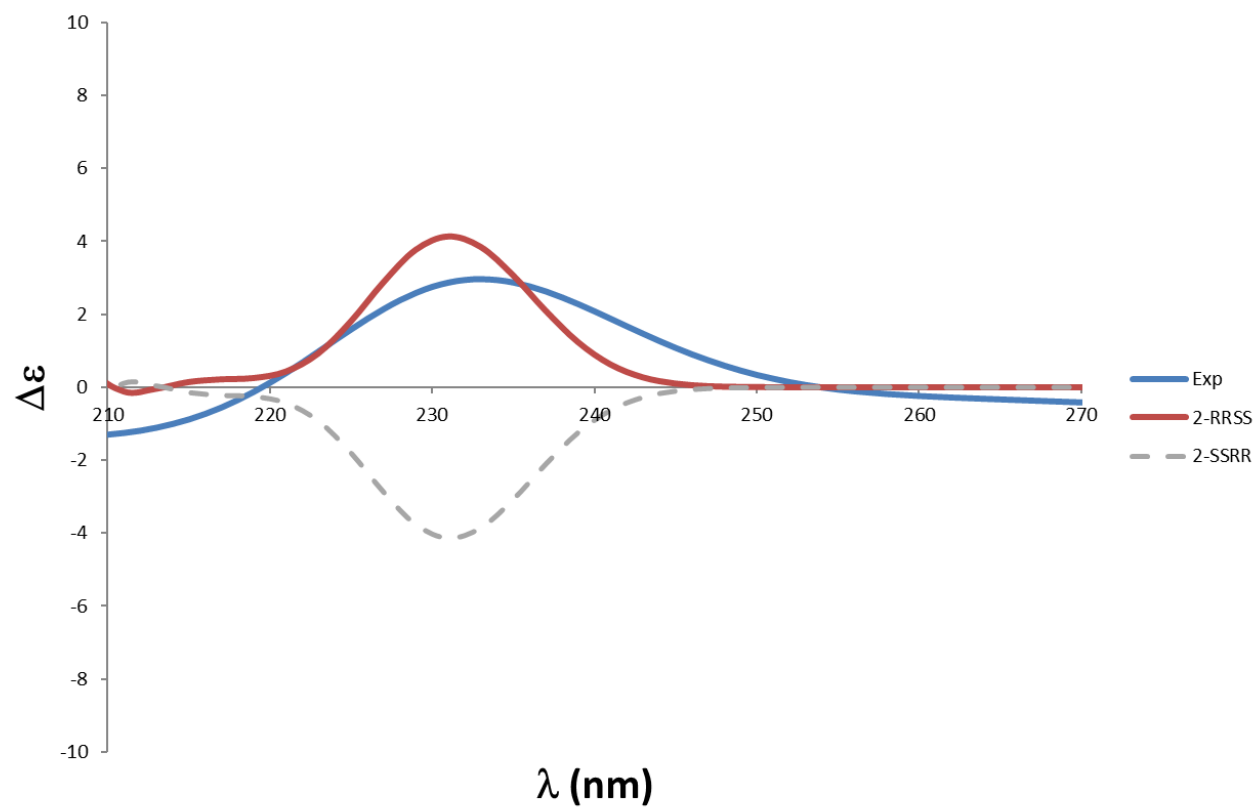


Fig. S22: IR spectrum of compound 2

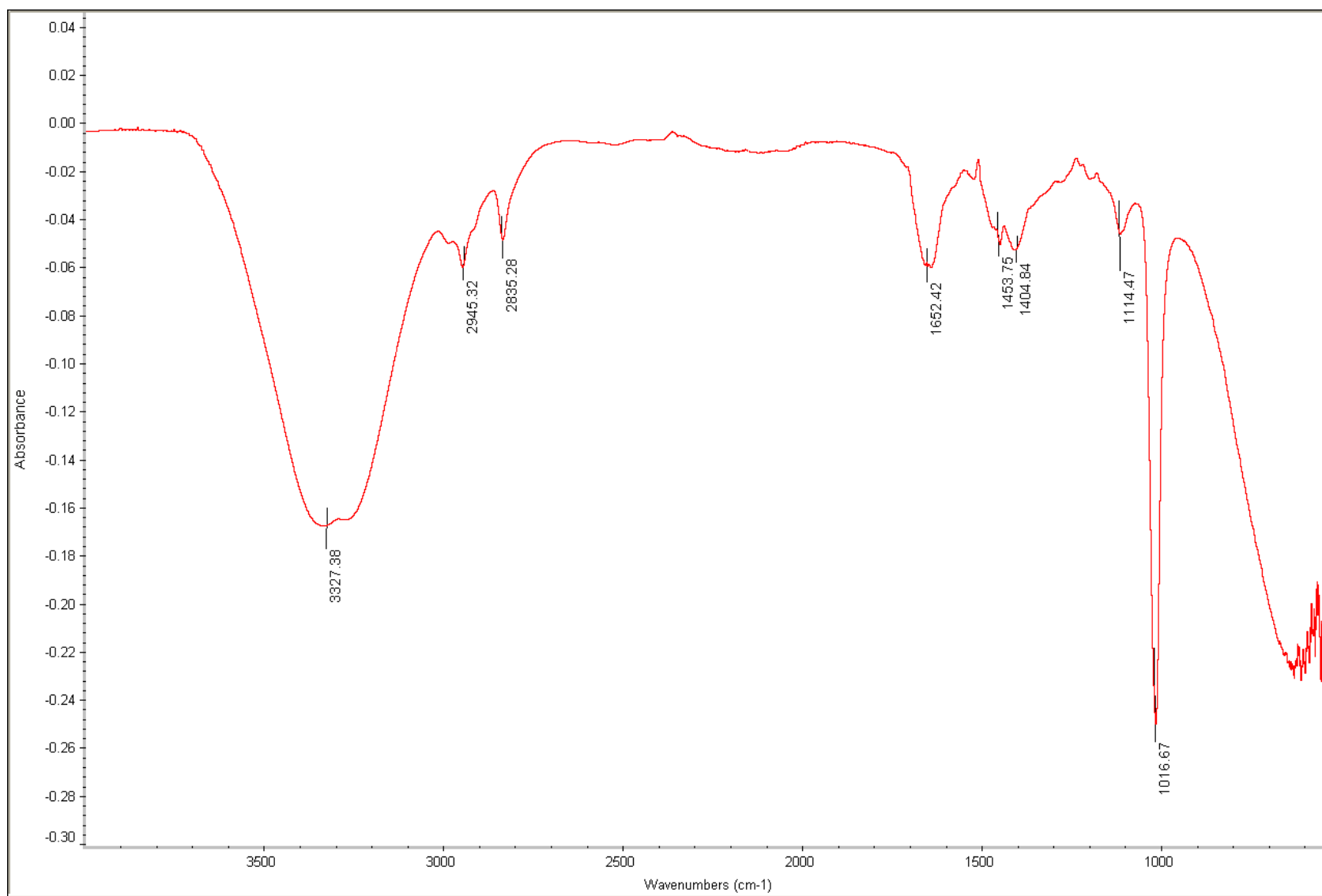


Fig. S23: HRESIMS of compound 3

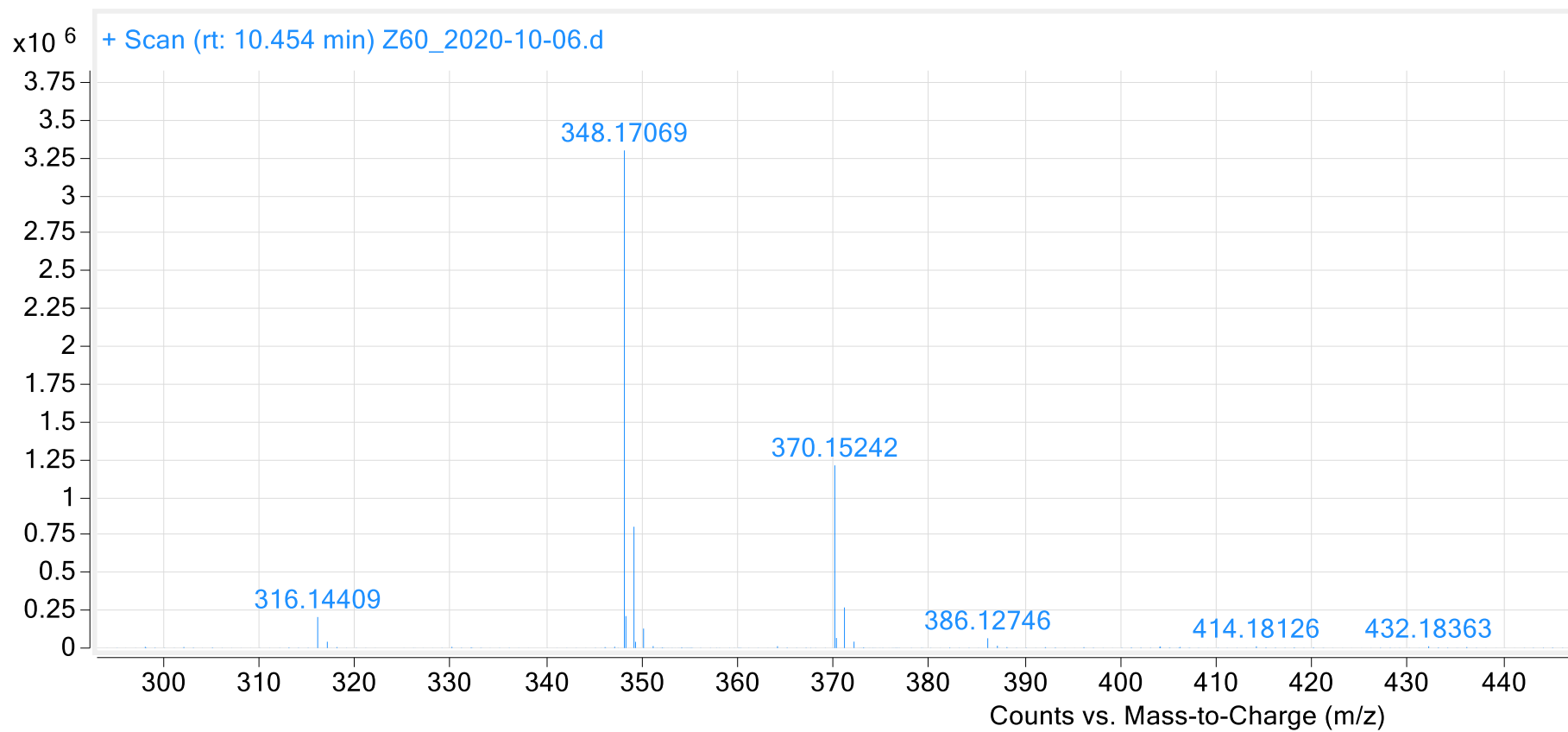


Fig. S24: ¹H NMR spectrum of compound 3 in CD₃OD (400MHz)

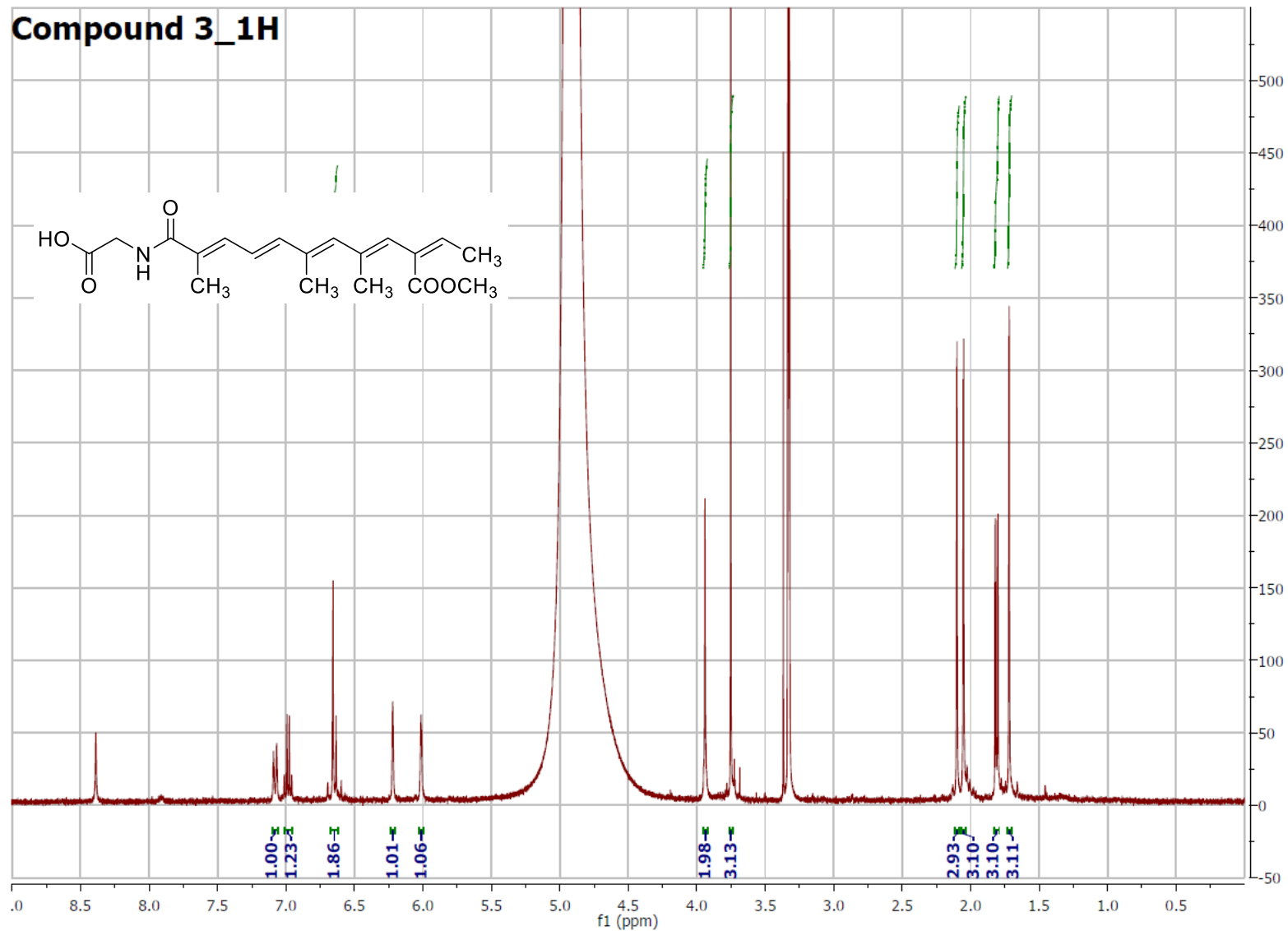


Fig. S25: DEPTQ NMR spectrum of compound 3 in CD₃OD (100MHz)

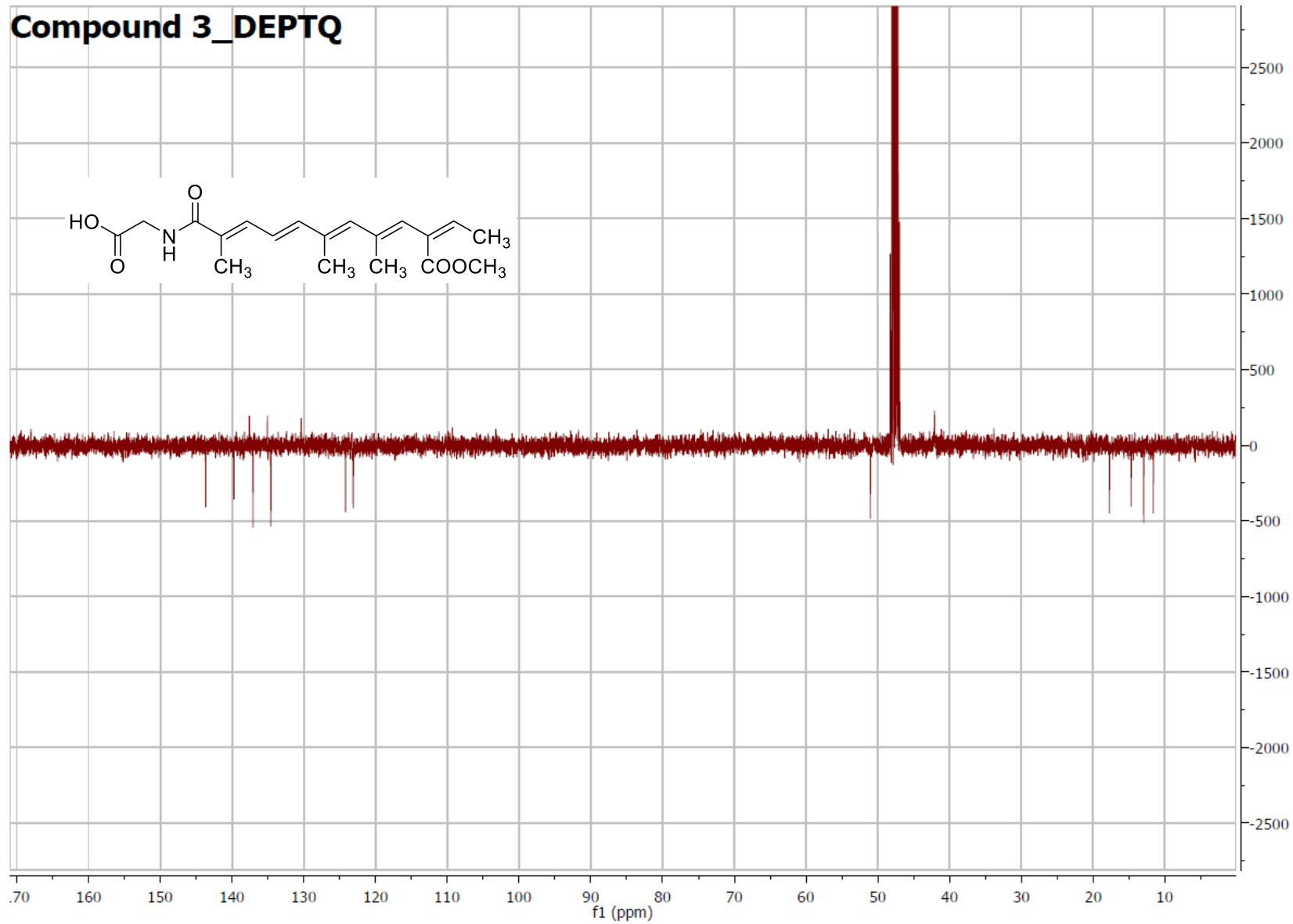
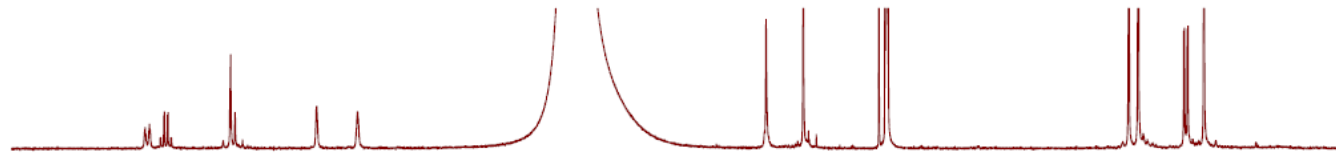


Fig. S26: HSQC spectrum of compound 3 in CD₃OD (400MHz)



Compound 3_HSQC

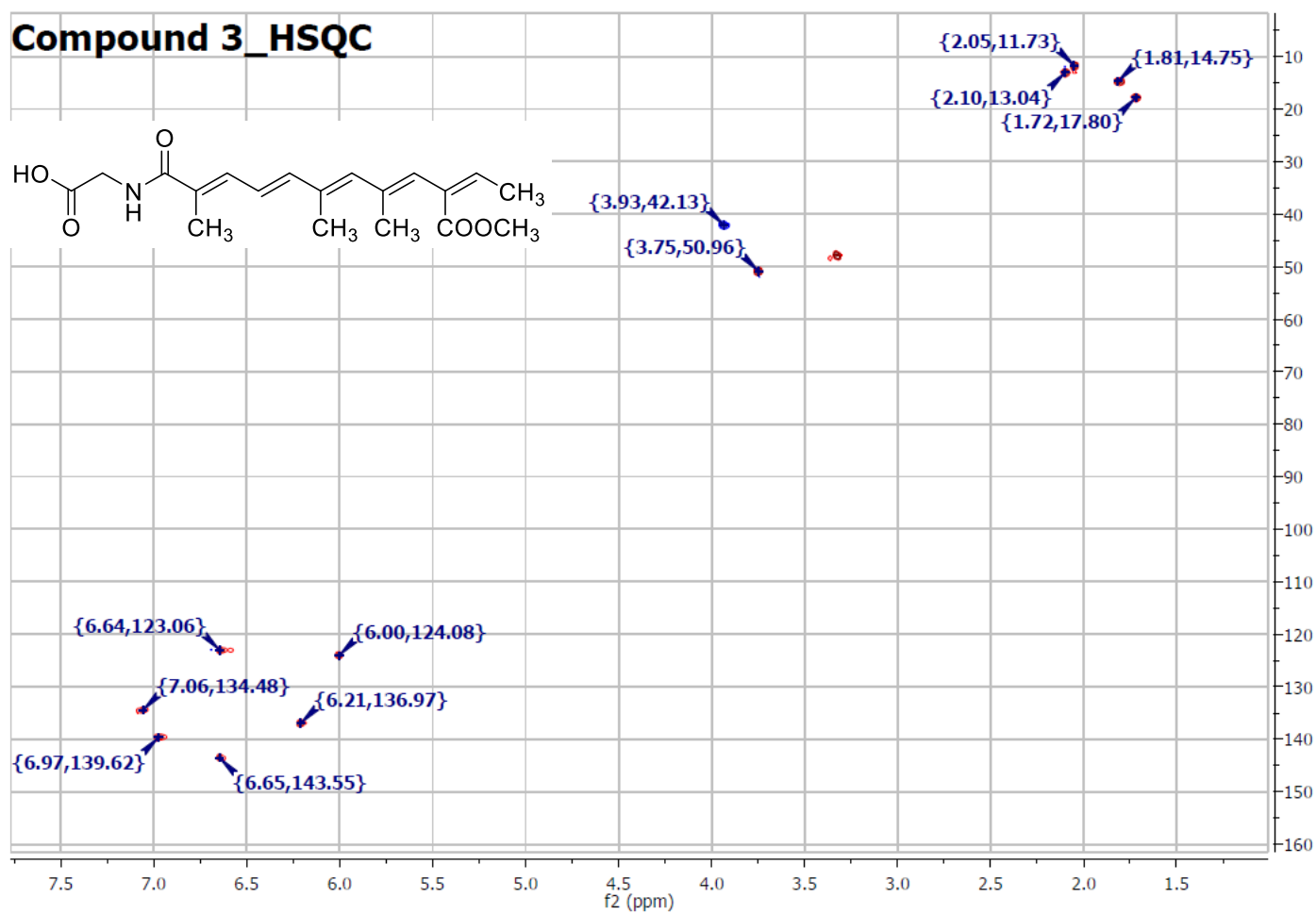


Fig. S27: COSY spectrum of compound 3 in CD₃OD (400MHz)

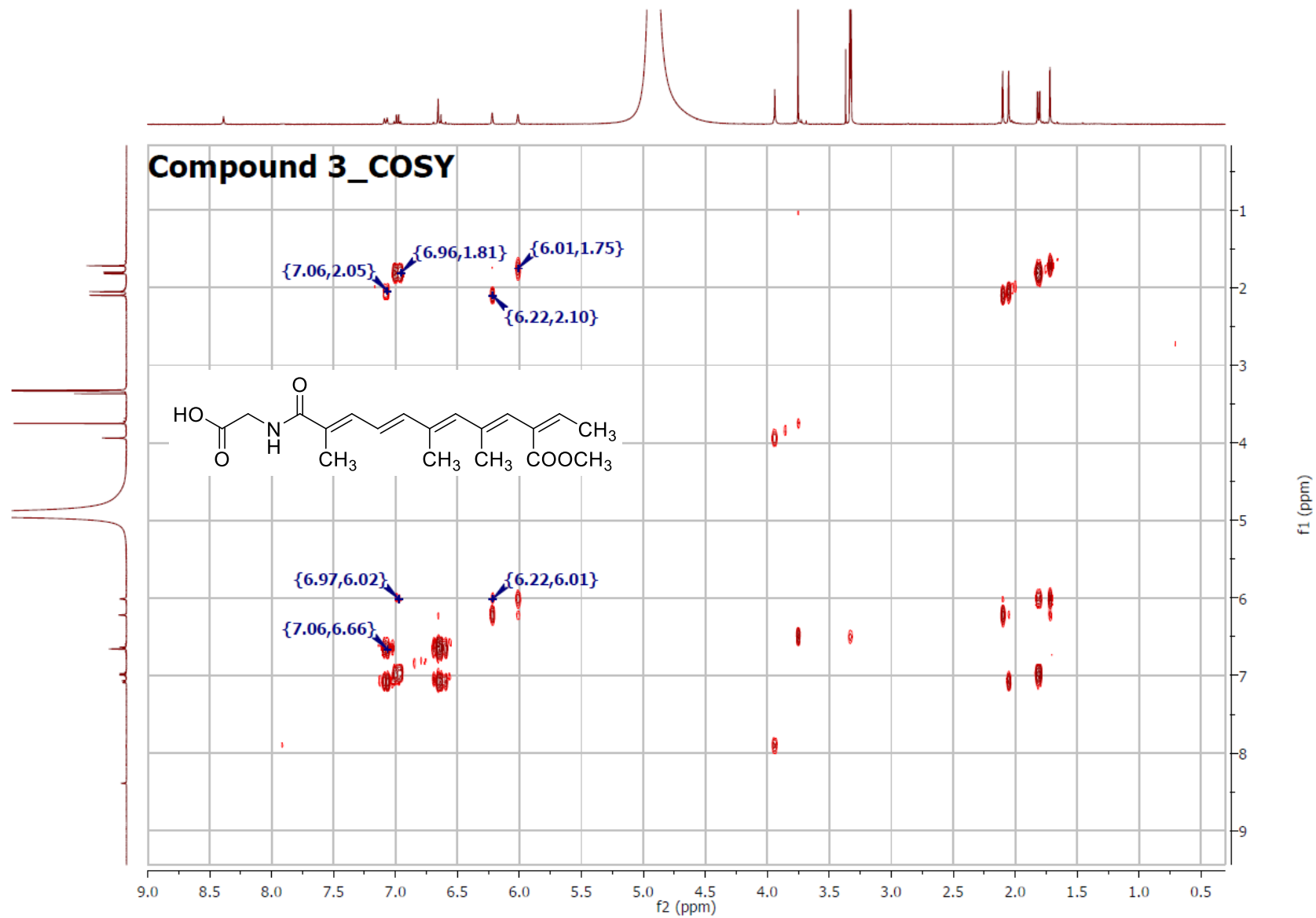


Fig. S28: HMBC spectrum of compound 3 in CD₃OD (400MHz)

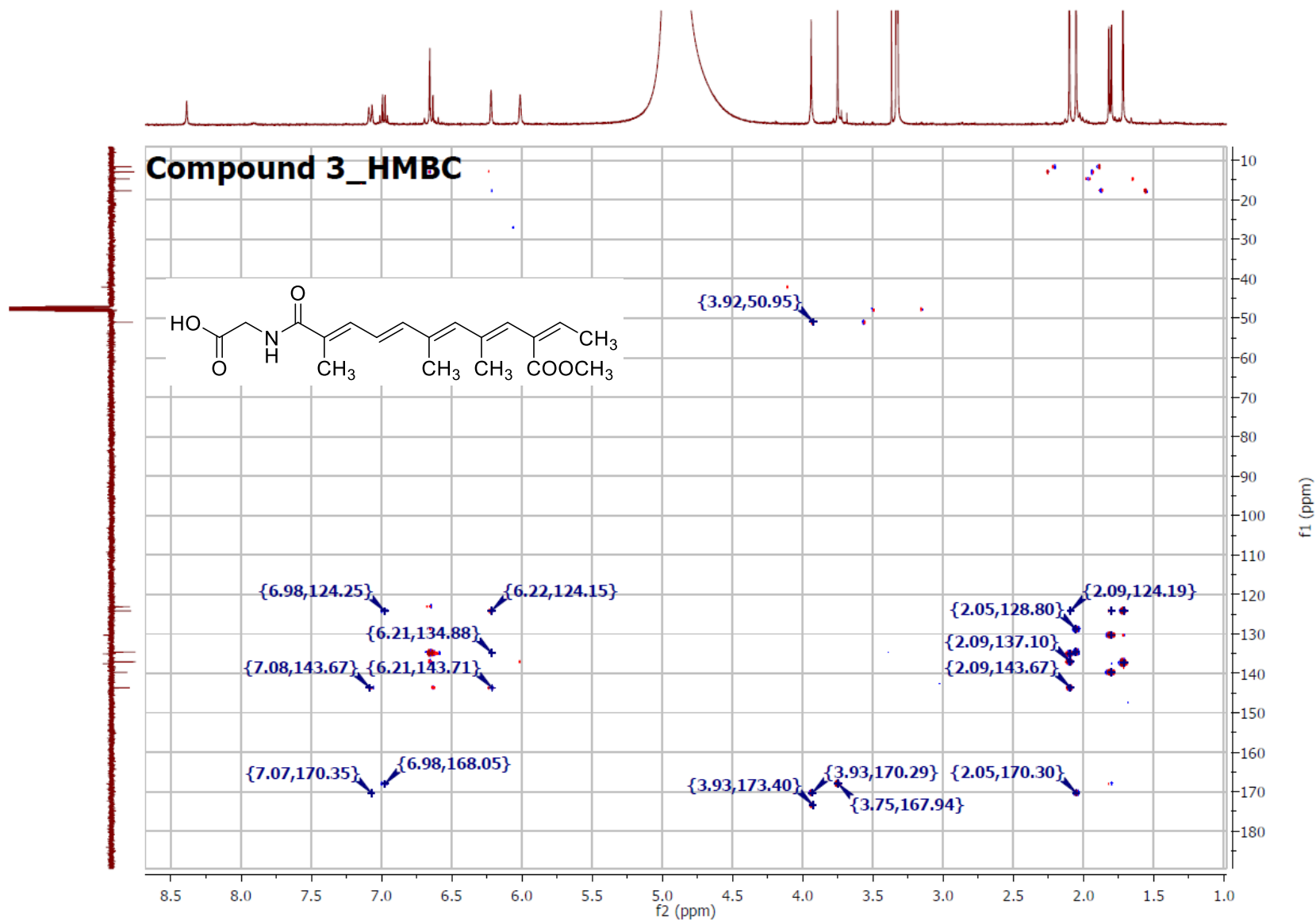


Fig. S29: ROESY spectrum of compound 3 in CD₃OD (400MHz)

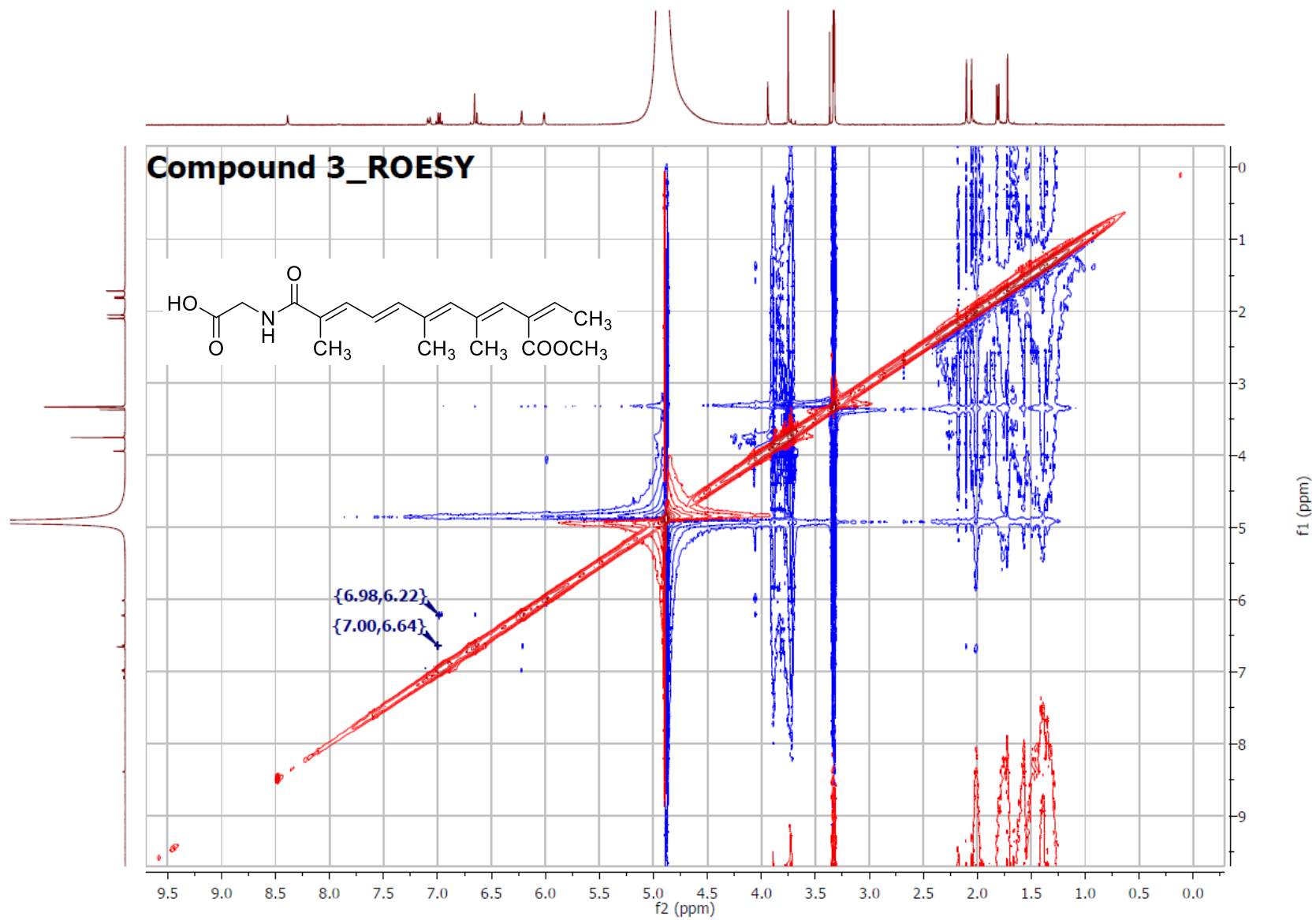


Fig. S30: IR spectrum of compound 3

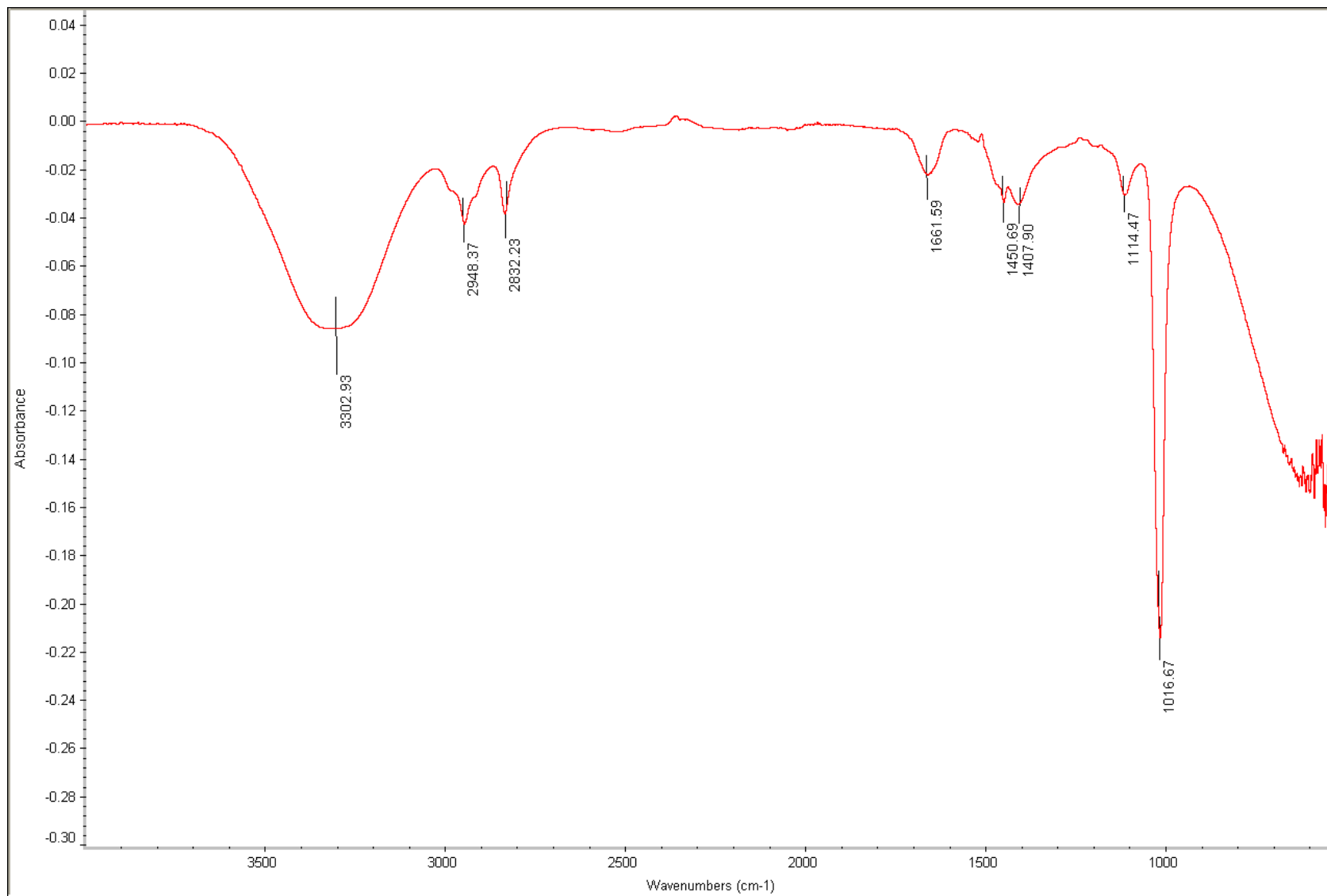


Fig. S31: HRESIMS of compound 4

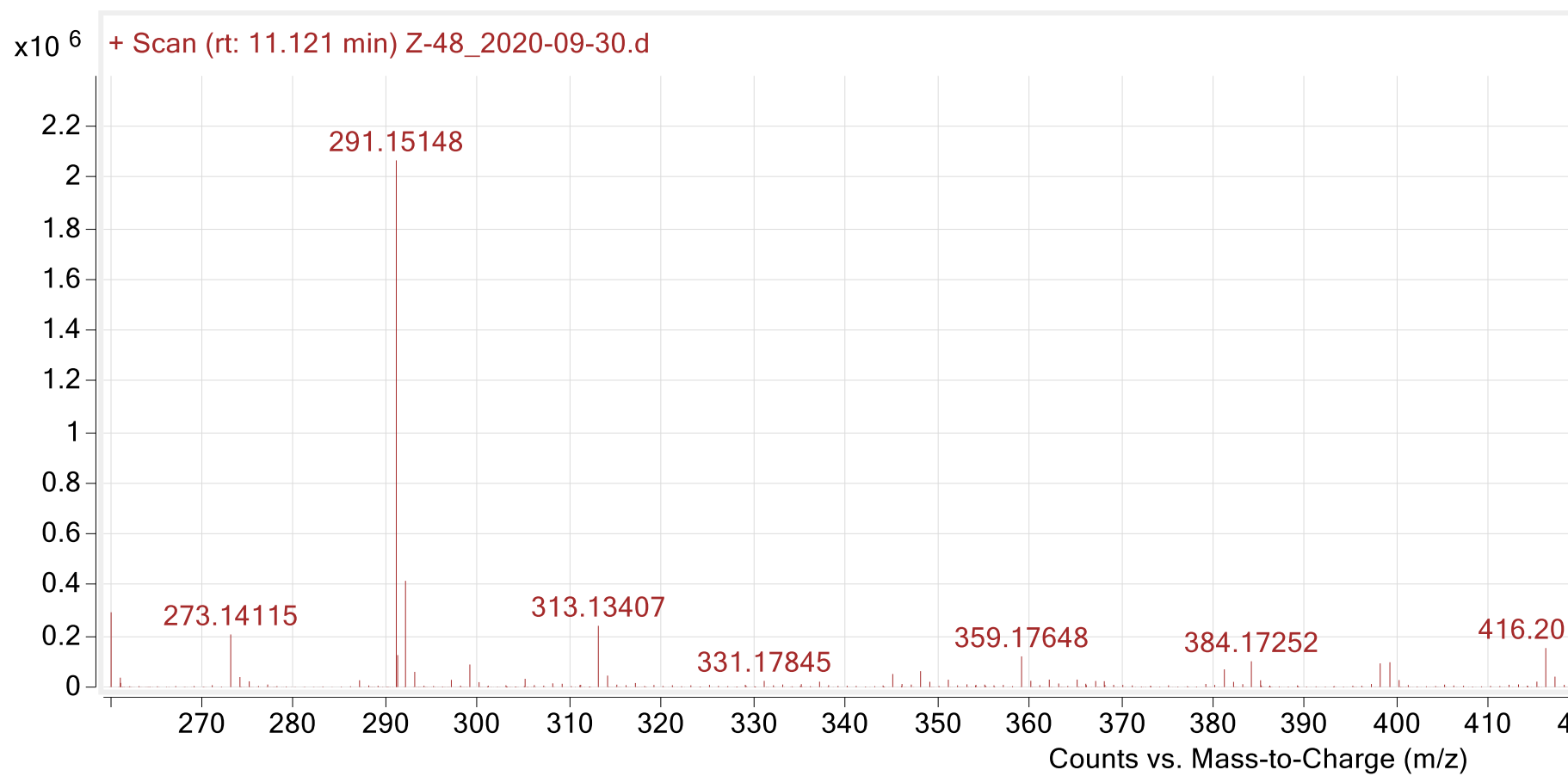


Fig. S32: ¹H NMR spectrum of compound 4 in CD₃OD (400MHz)

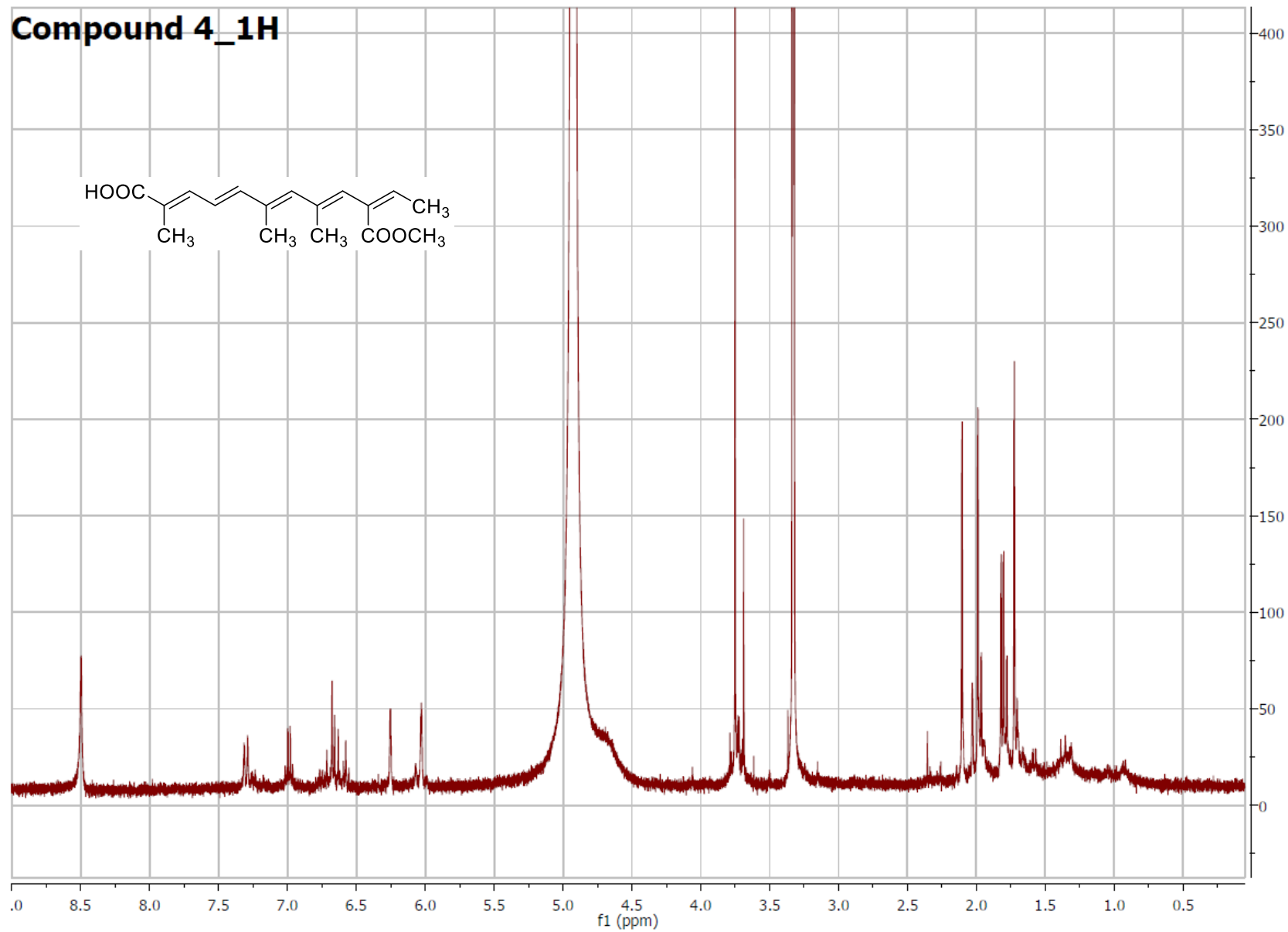


Fig. S33: HSQC spectrum of compound 4 in CD₃OD (400MHz)

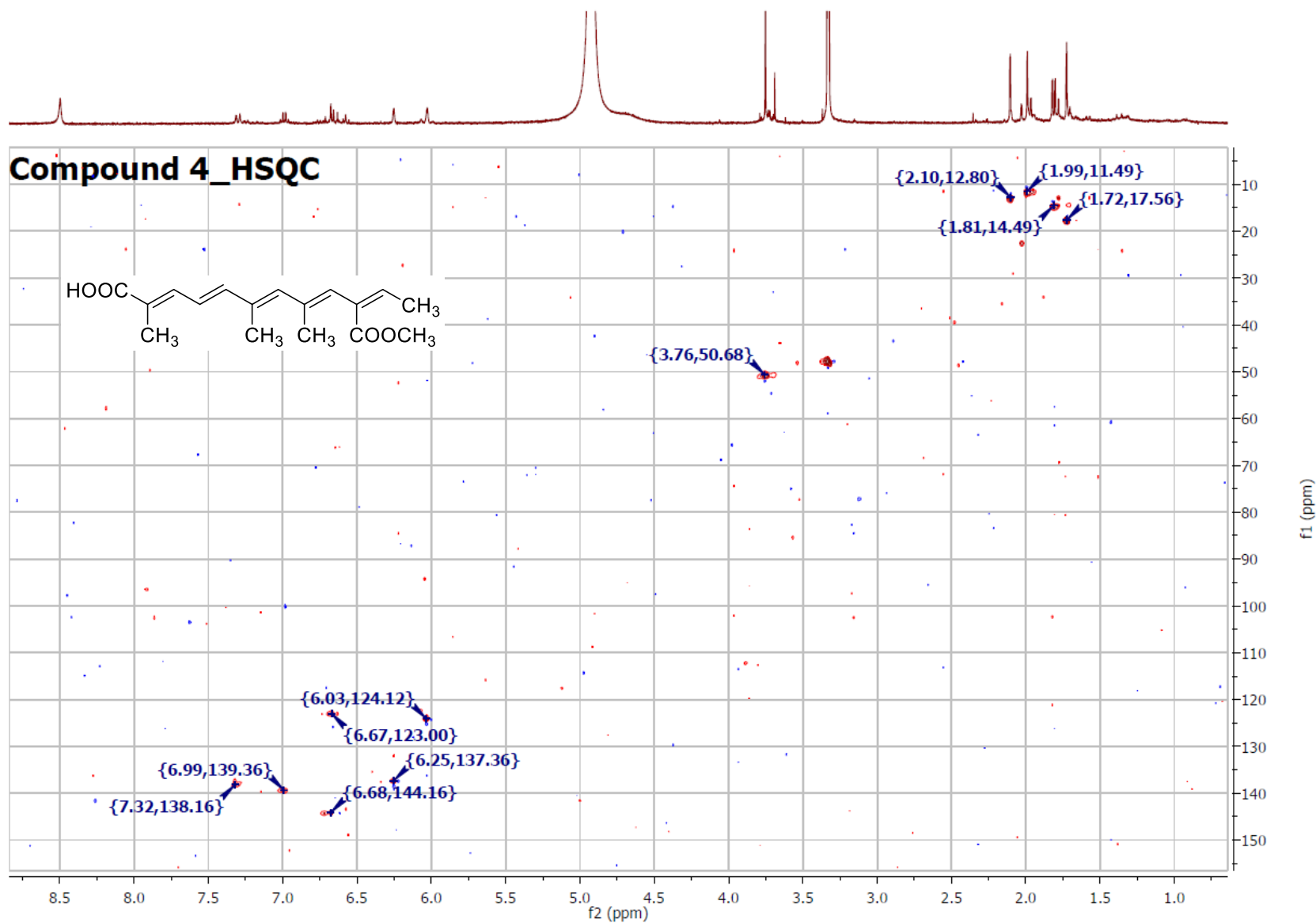


Fig. S34: COSY spectrum of compound 4 in CD₃OD (400MHz)

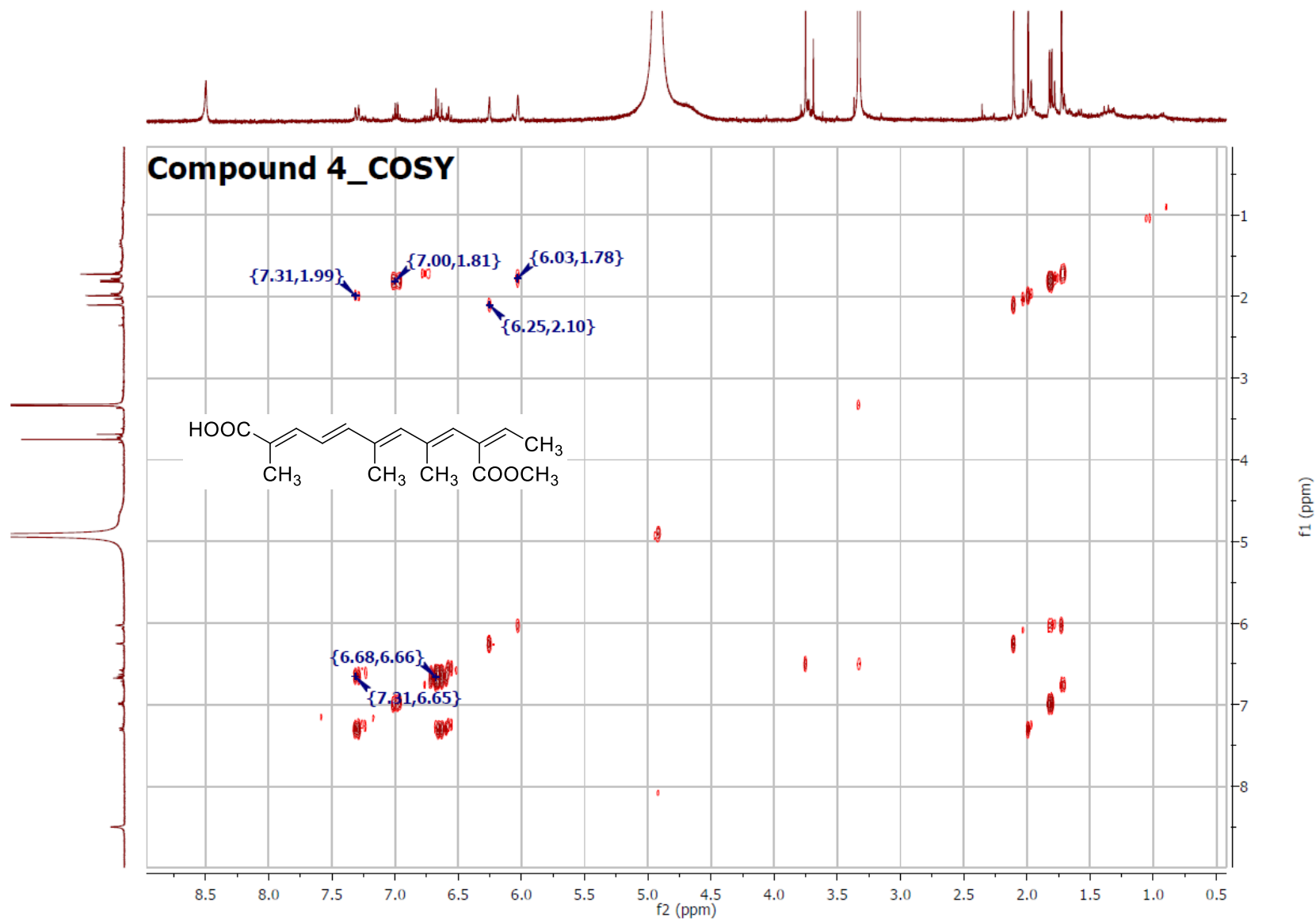


Fig. S35: HMBC spectrum of compound 4 in CD₃OD (400MHz)

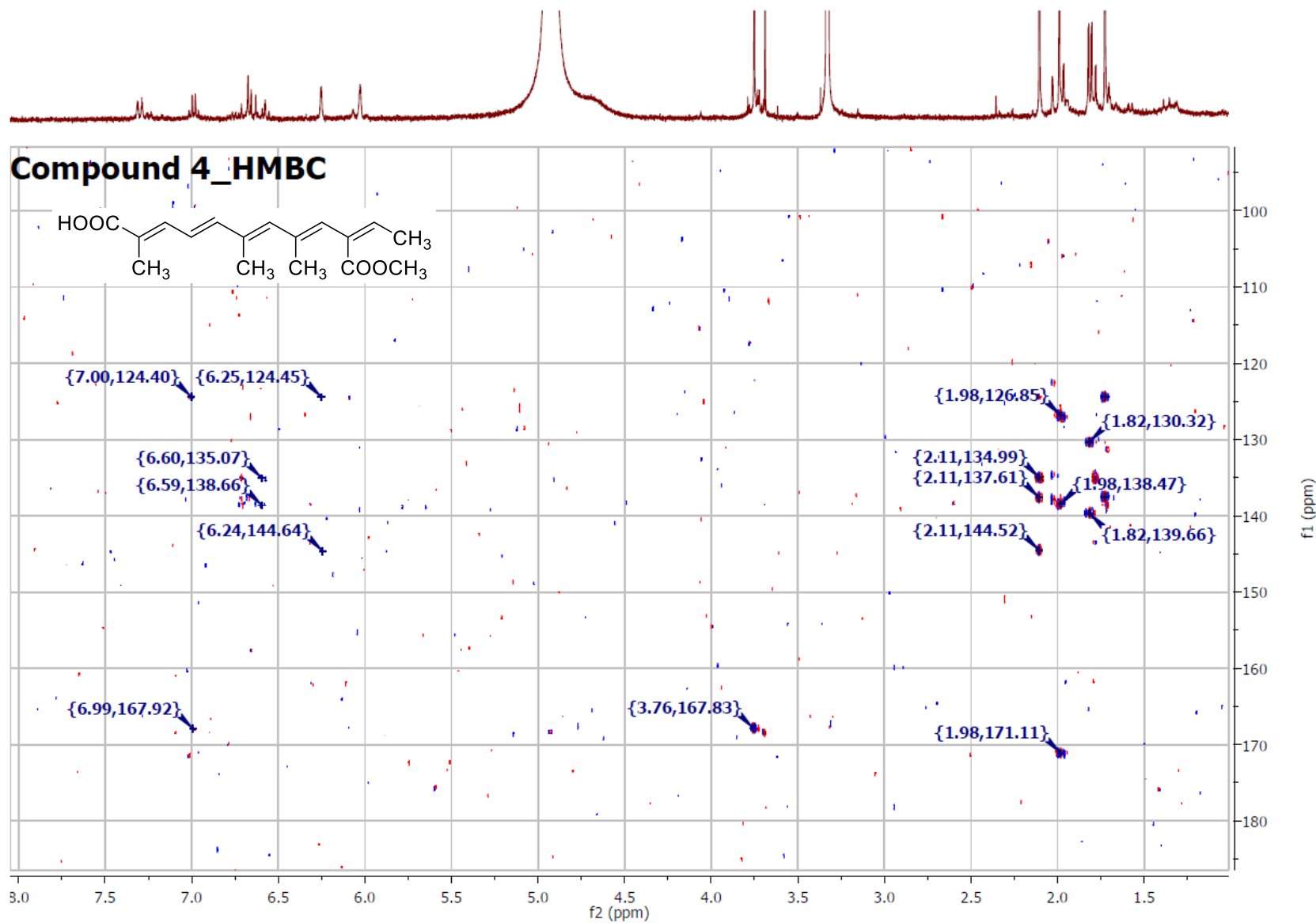


Fig. S37: IR spectrum of compound 4

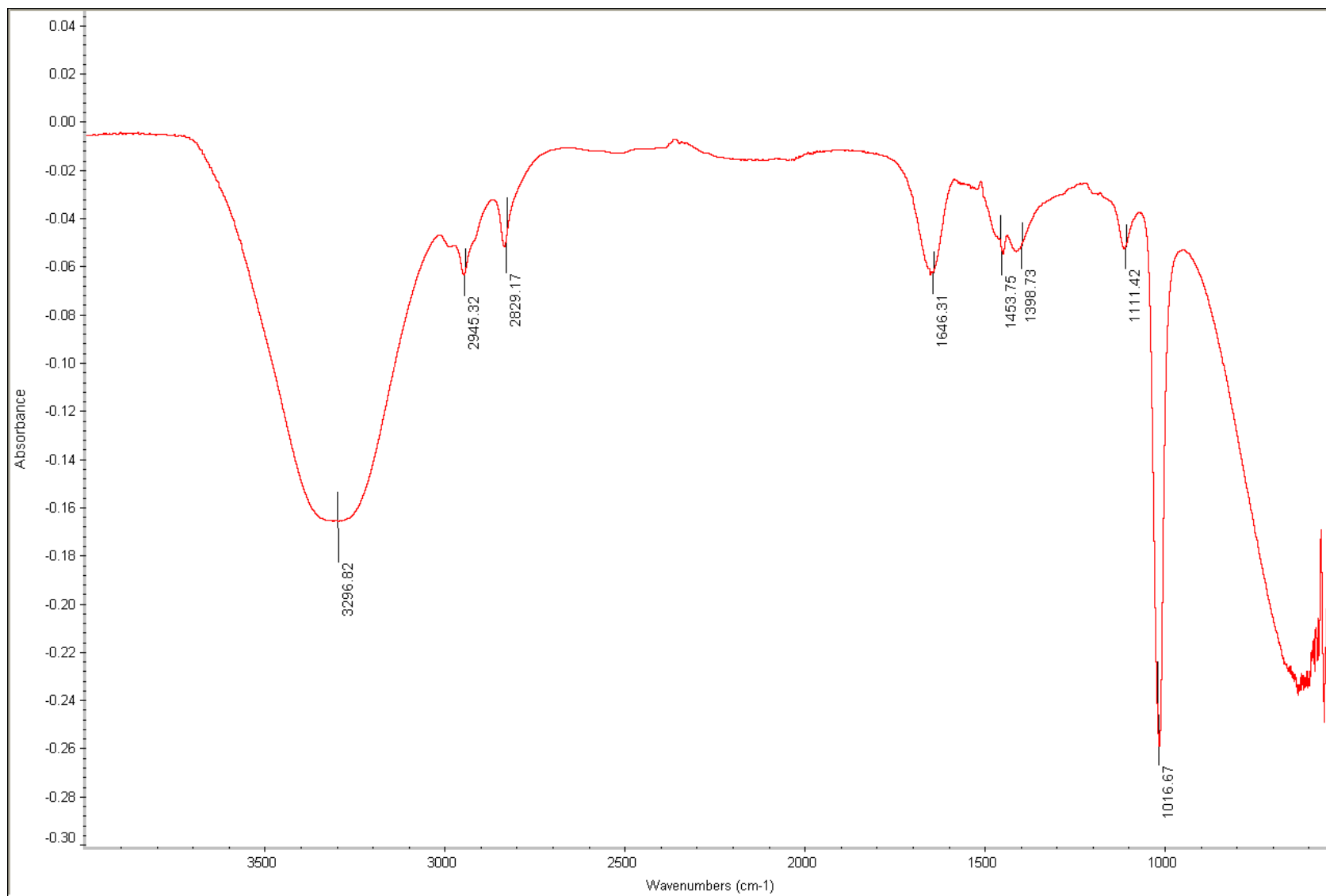


Fig. S38: HRESIMS of compound 5

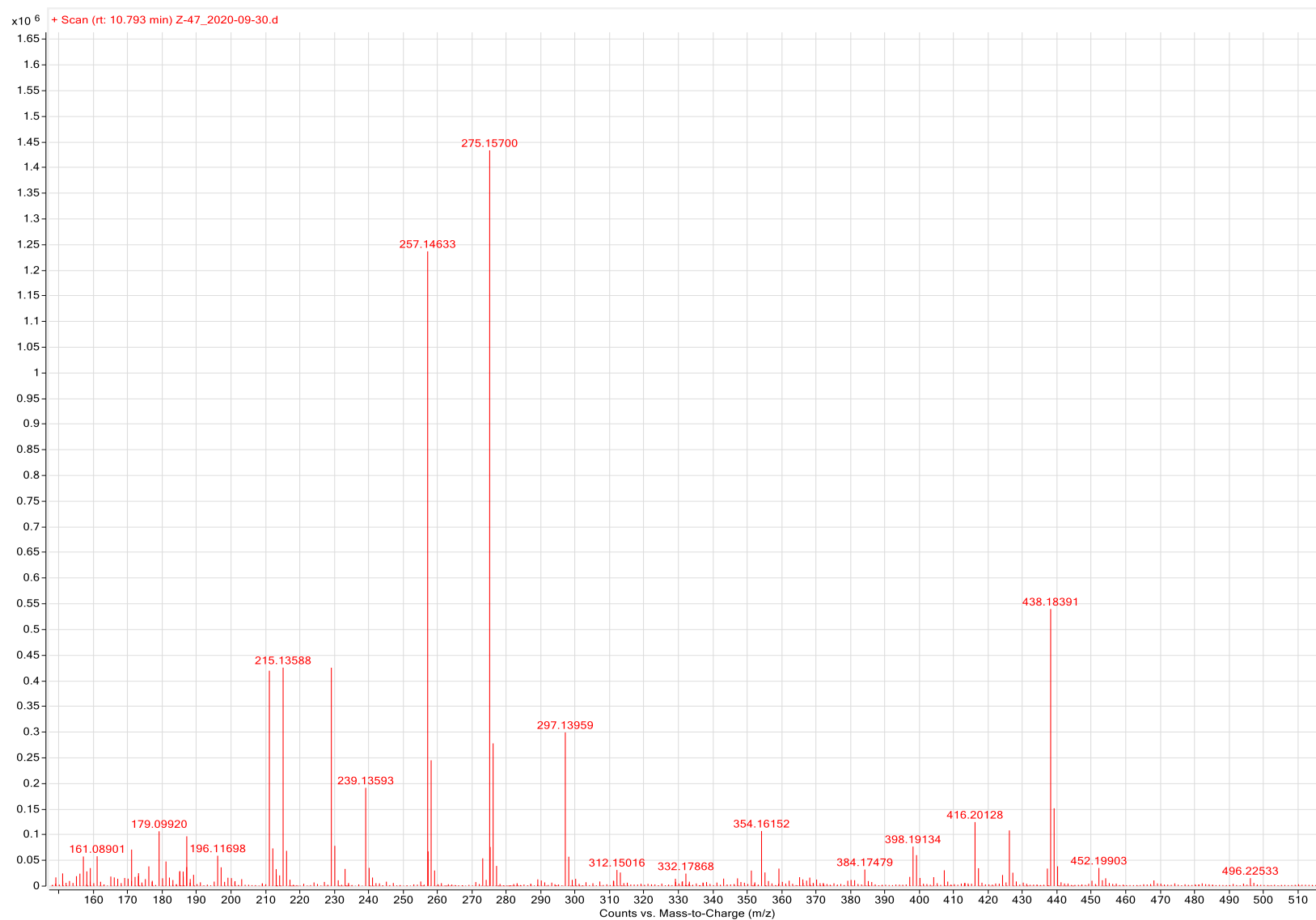


Fig. S39: ¹H NMR spectrum of compound 5 in CD₃OD (400MHz)

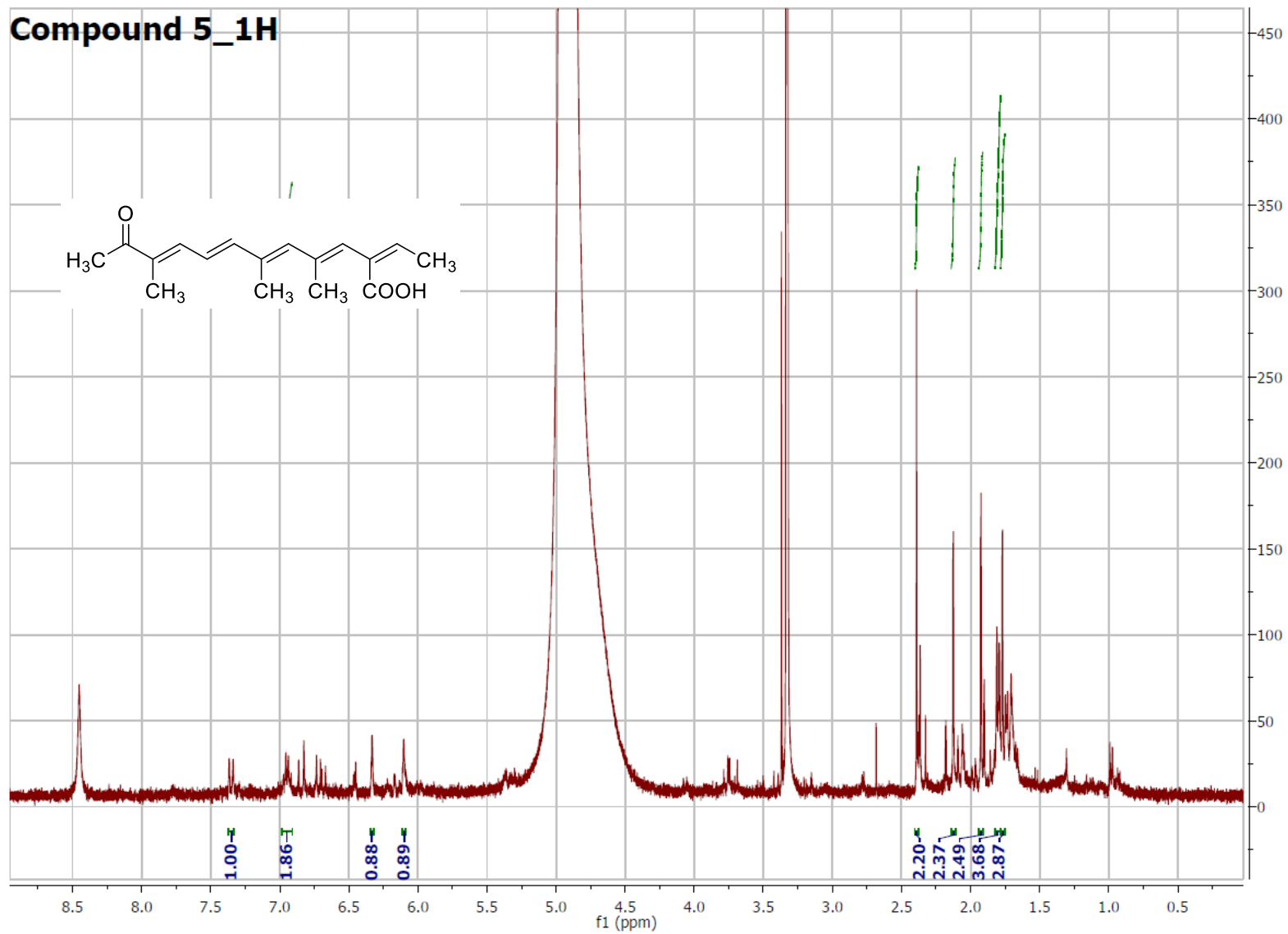


Fig. S40: HSQC spectrum of compound 5 in CD₃OD (400MHz)

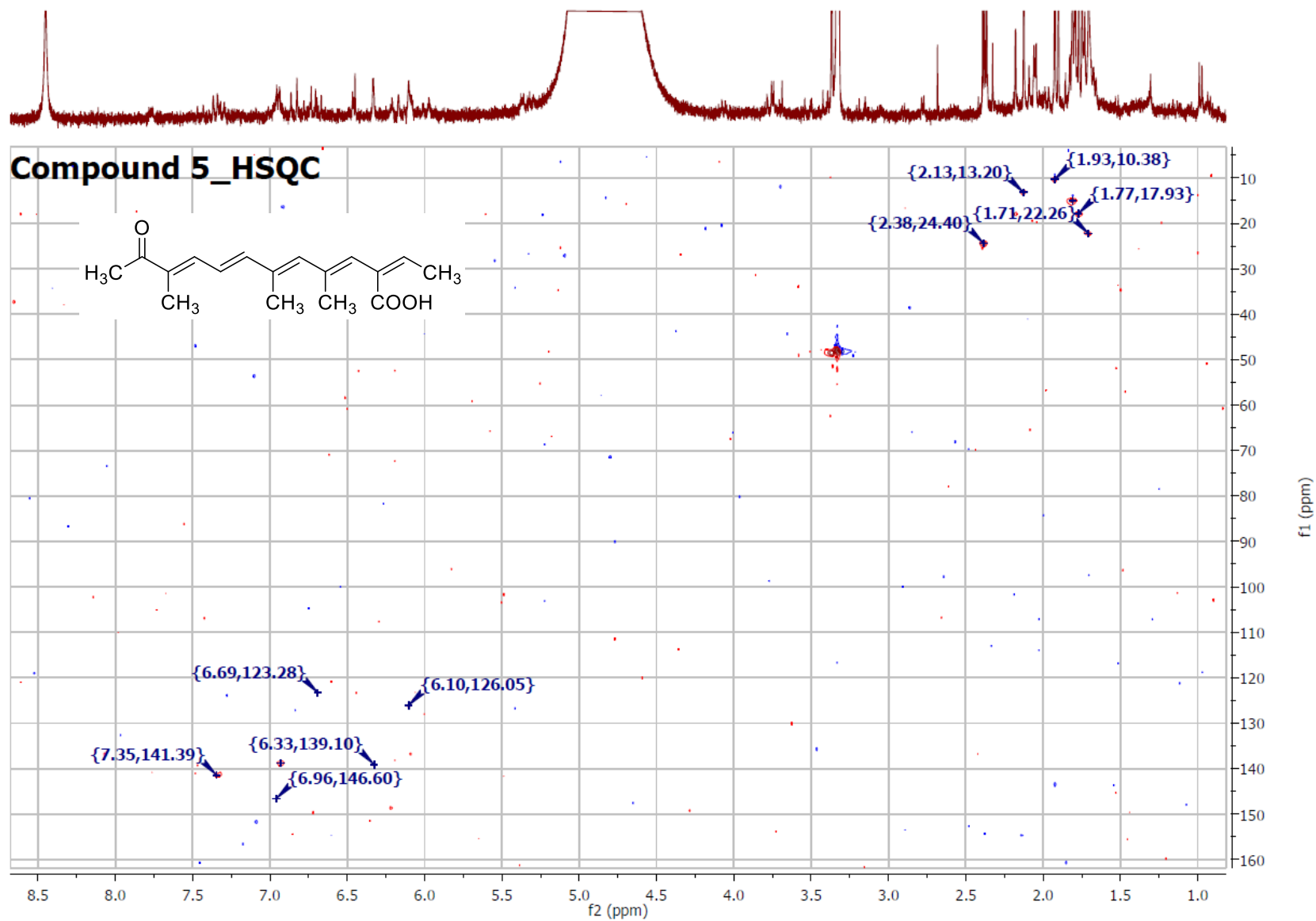


Fig. S41: COSY spectrum of compound 5 in CD₃OD (400MHz)

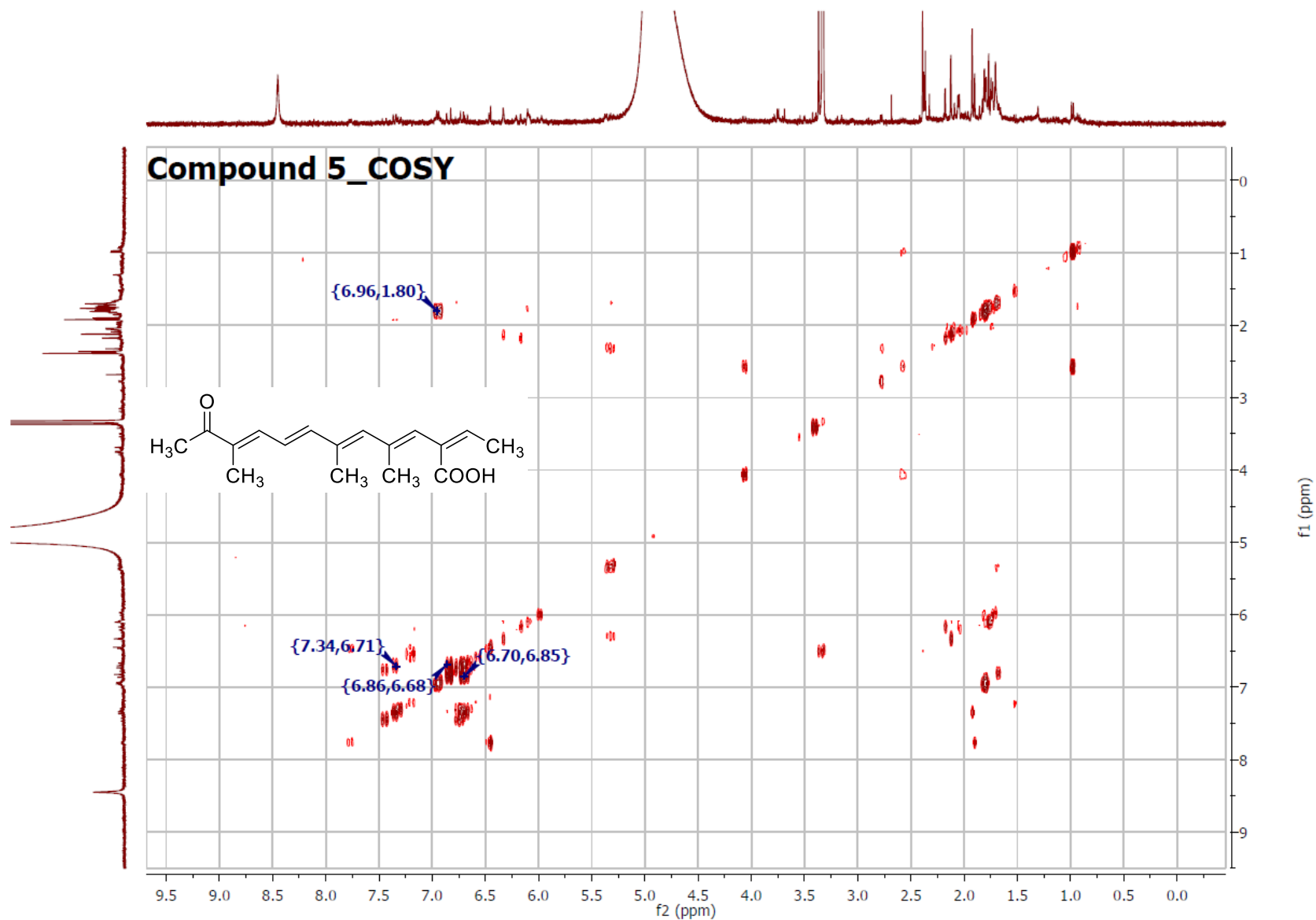


Fig. S42: HMBC spectrum of compound 5 in CD₃OD (400MHz)

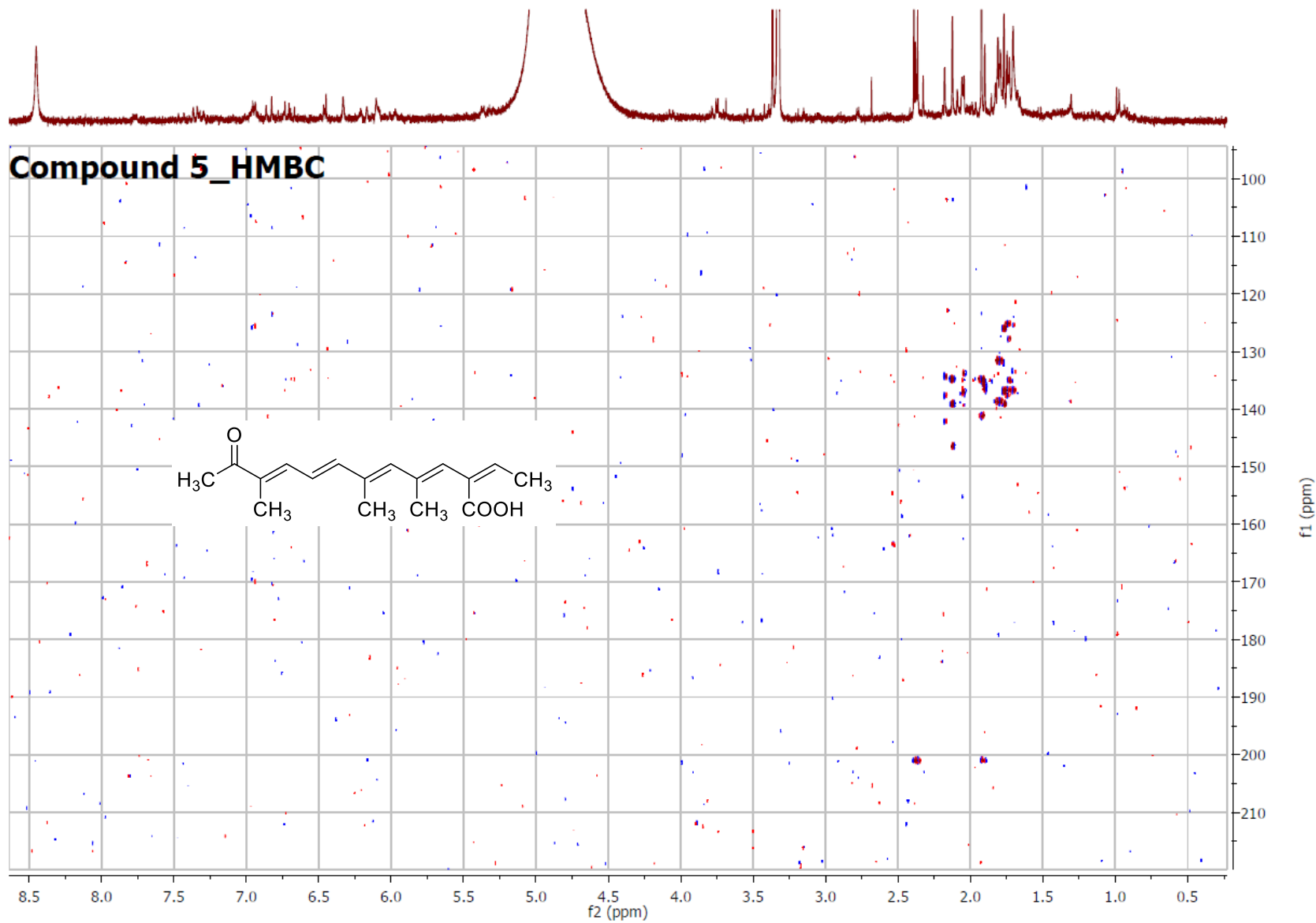


Fig. S43: ROESY spectrum of compound 5 in CD₃OD (400MHz)

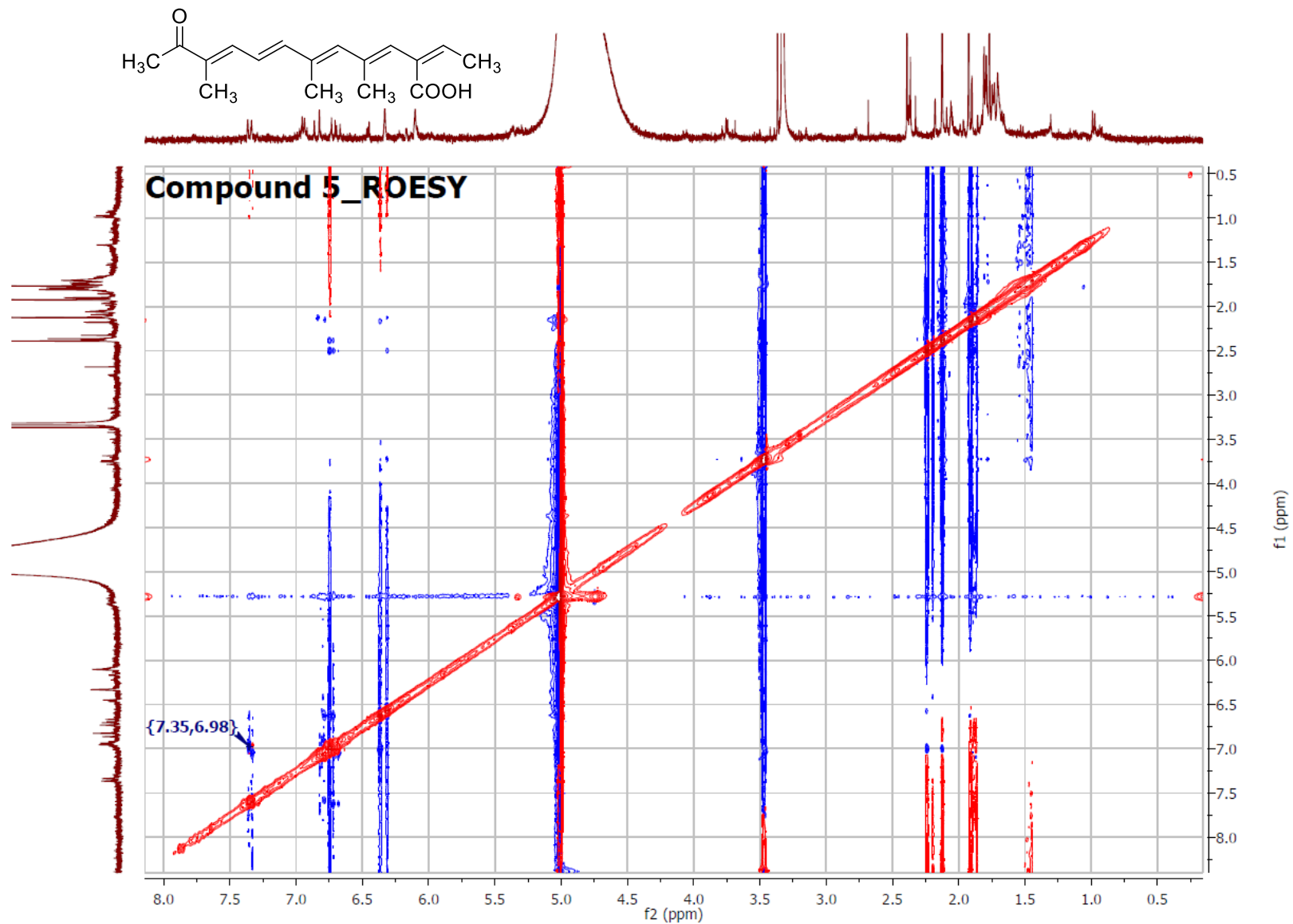


Fig. S44: IR spectrum of compound 5

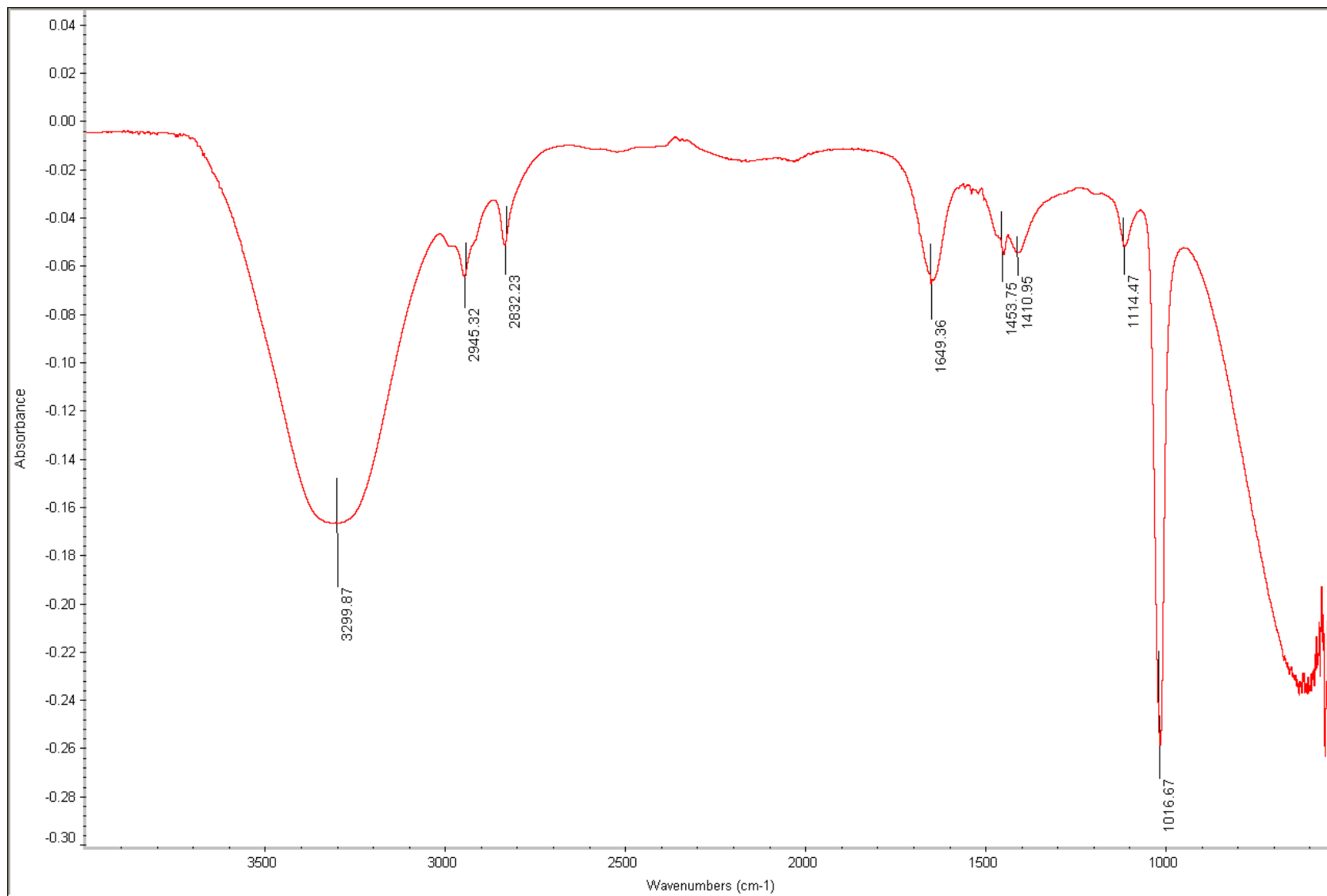


Fig. S45: HRESIMS of compound 6

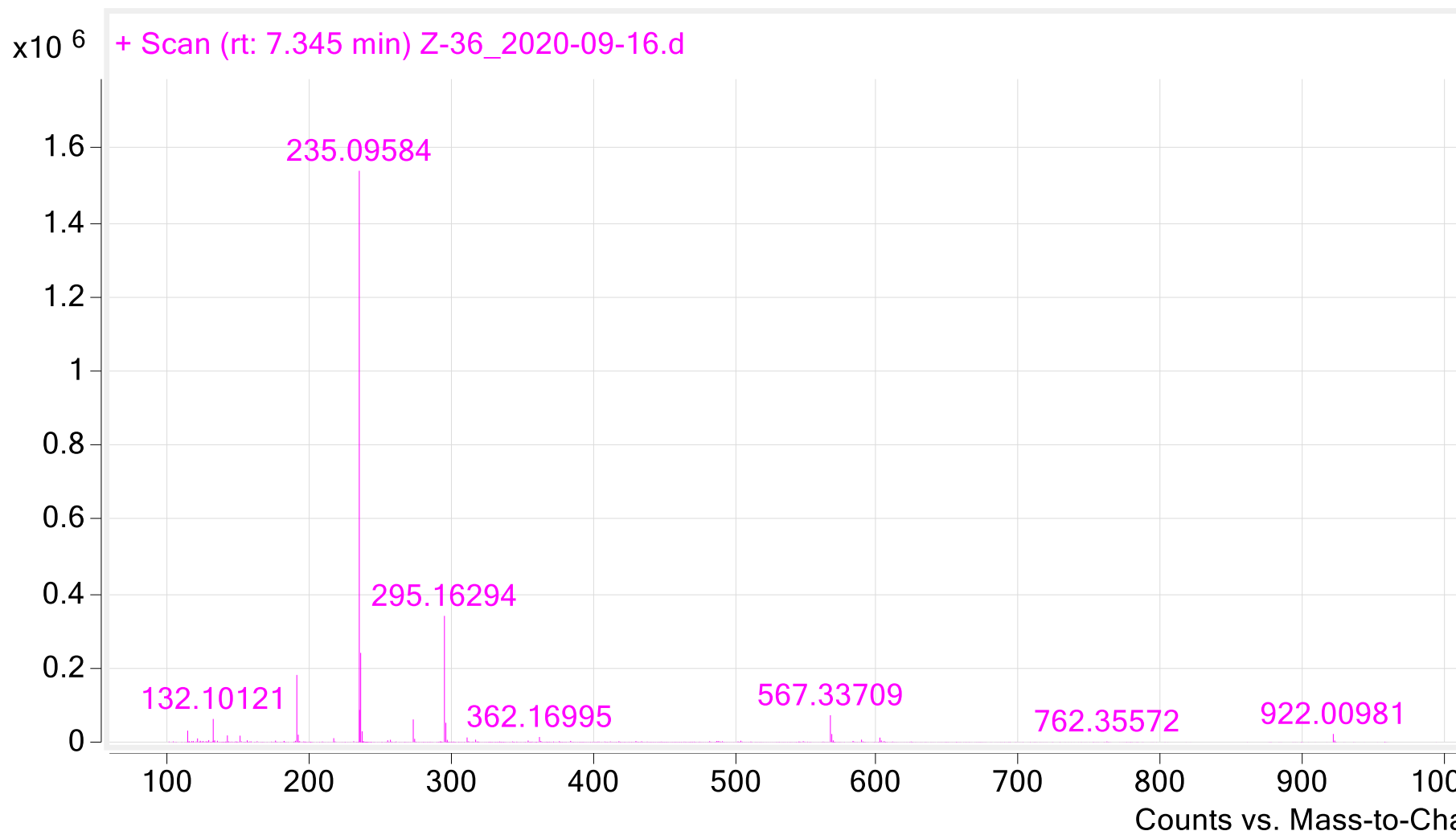


Fig. S46: ¹H spectrum of compound 6 in CD₃OD (400MHz)

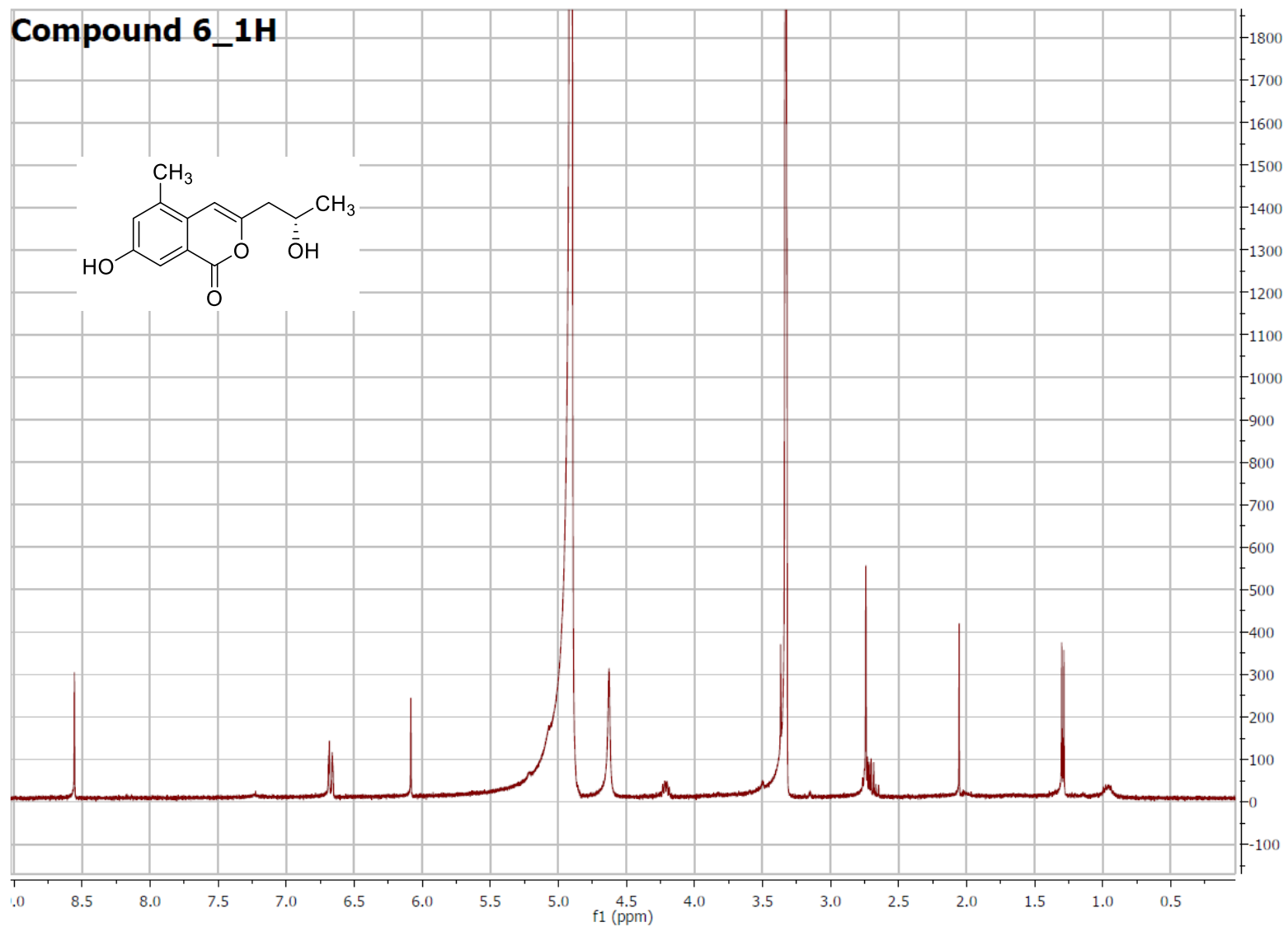


Fig. S47: DEPTQ spectrum of compound 6 in CD₃OD (400MHz)

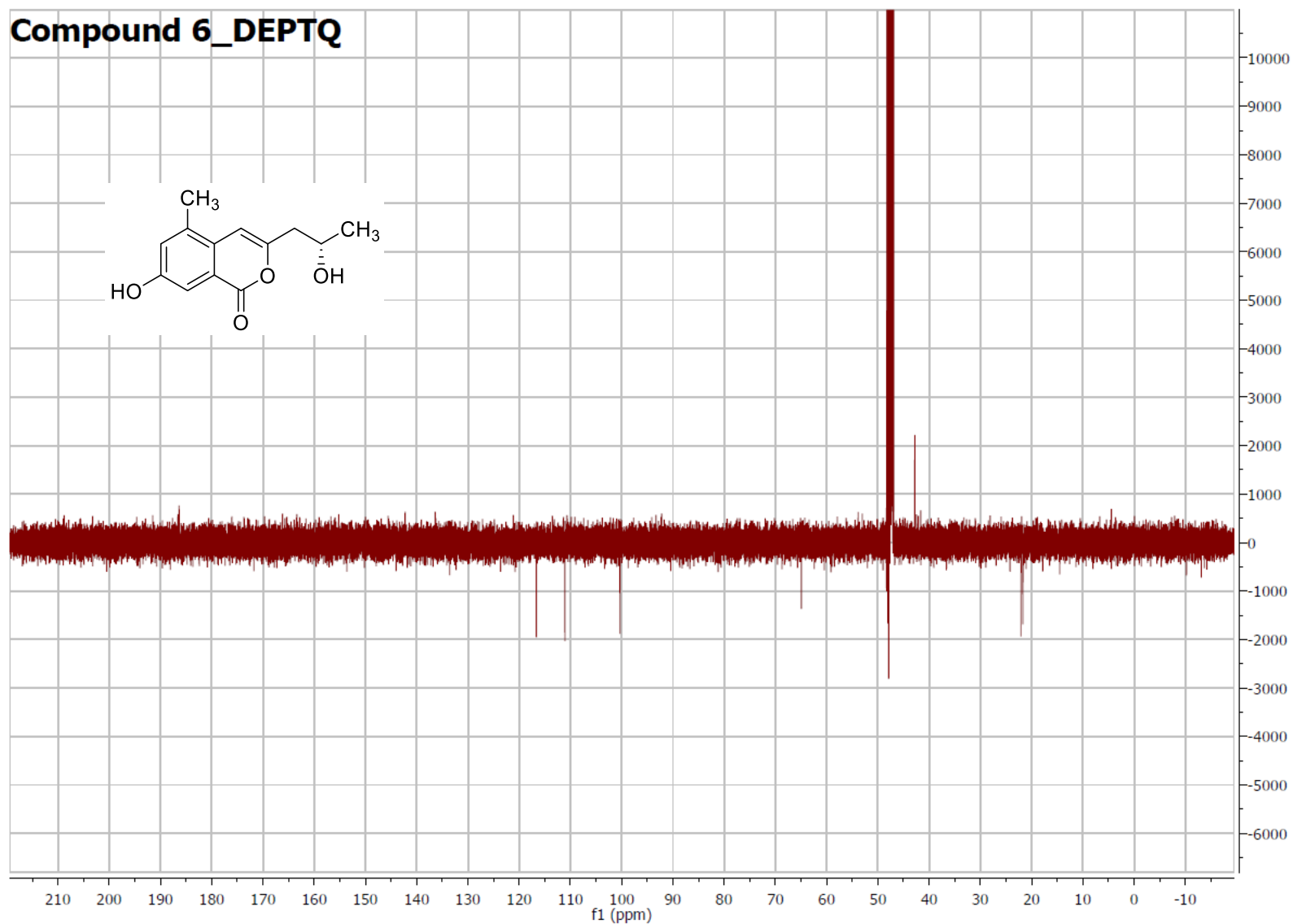


Fig. S48: HSQC spectrum of compound 6 in CD₃OD (400MHz)

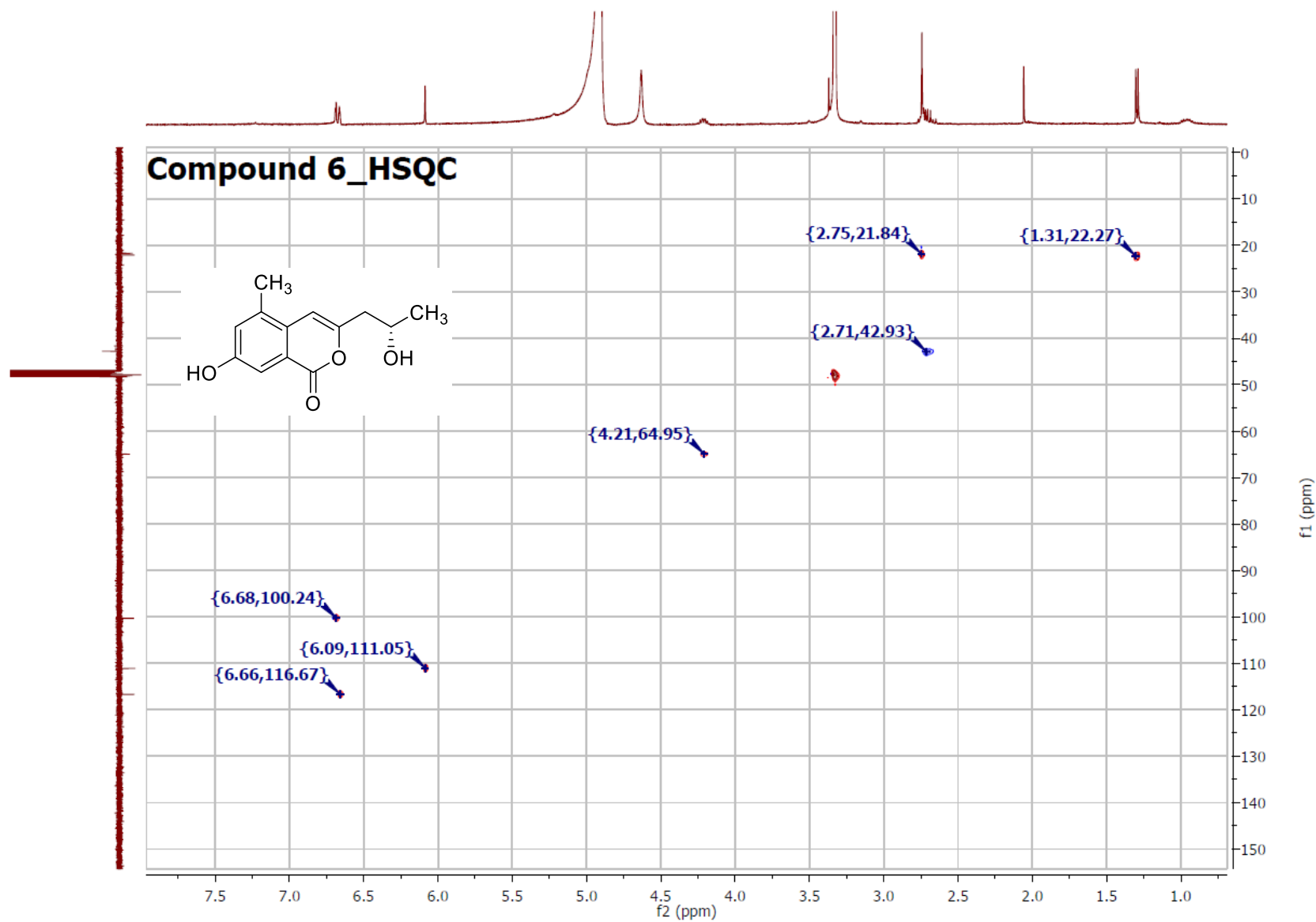


Fig. S49: COSY spectrum of compound 6 in CD₃OD (400MHz)

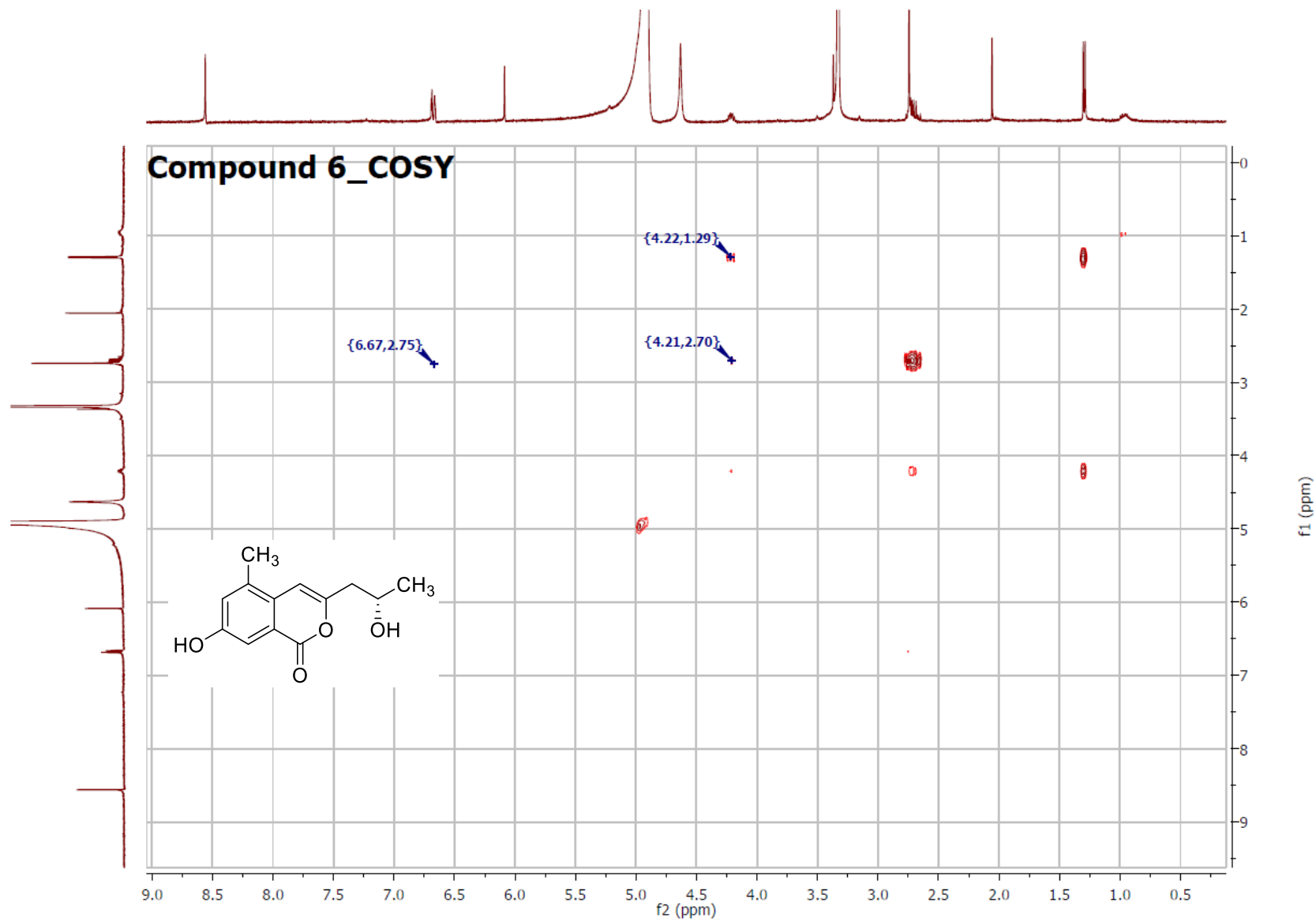


Fig. S50: HMBC spectrum of compound 6 in CD₃OD (400MHz)

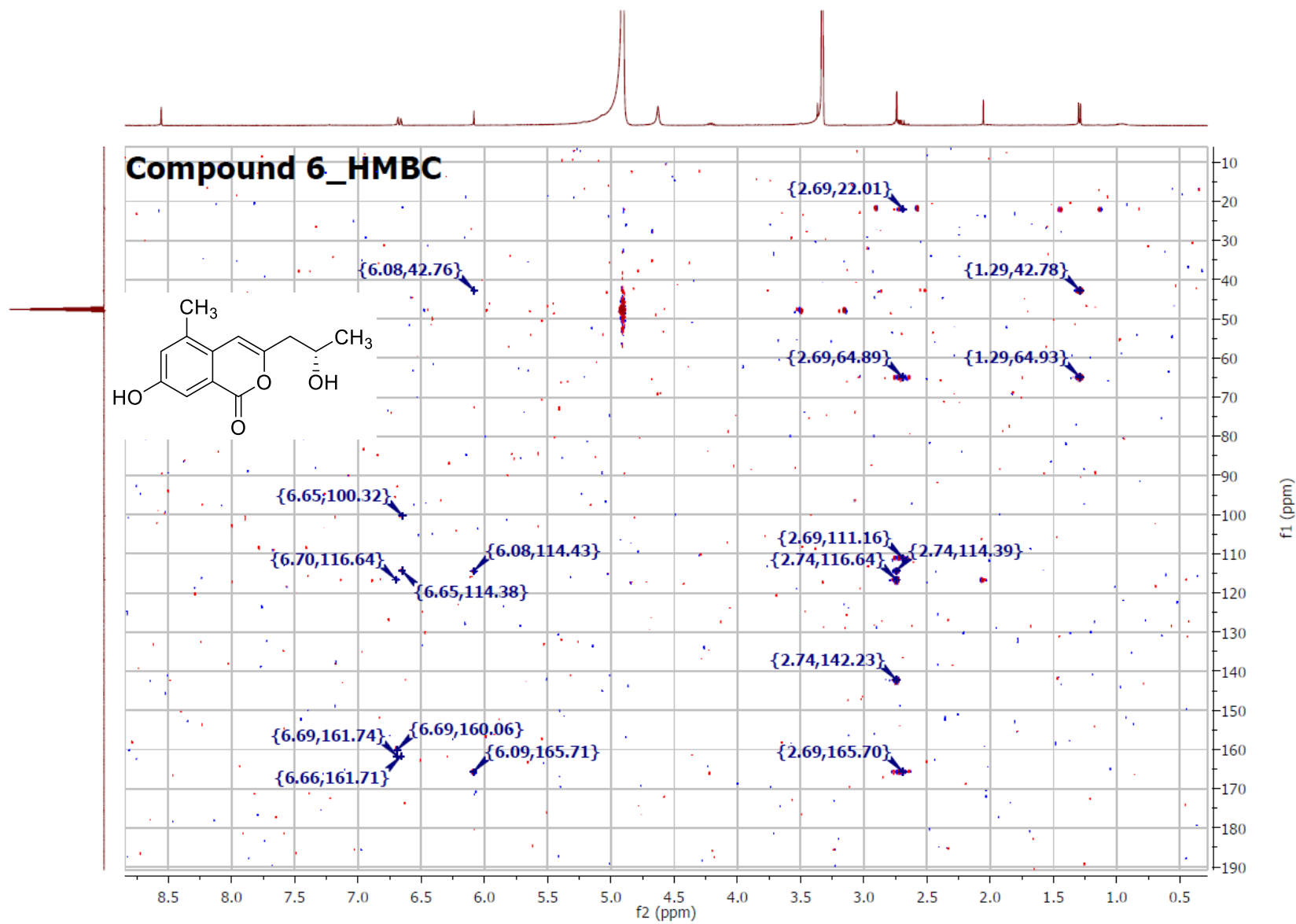


Fig. S51: IR spectrum of compound 6

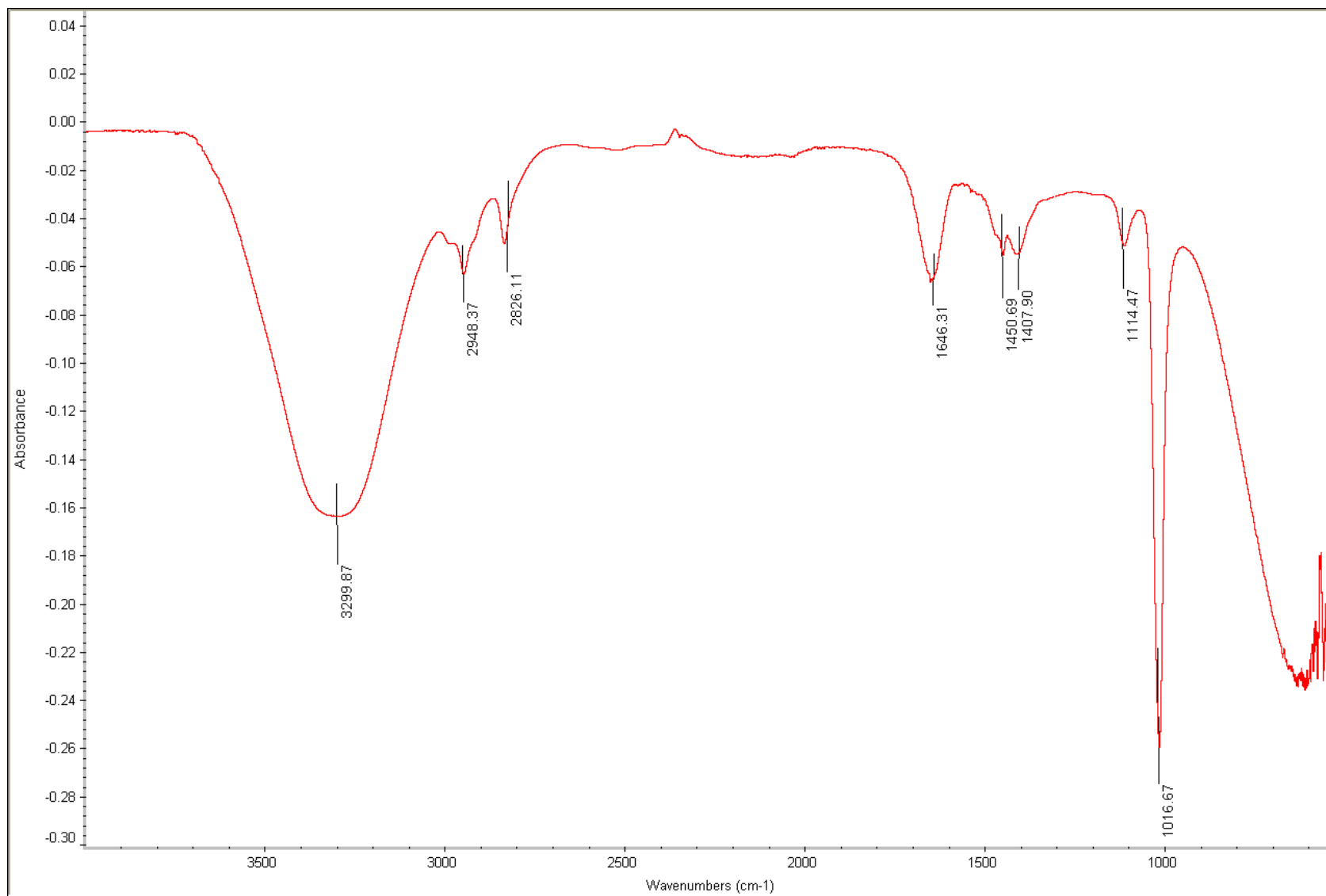
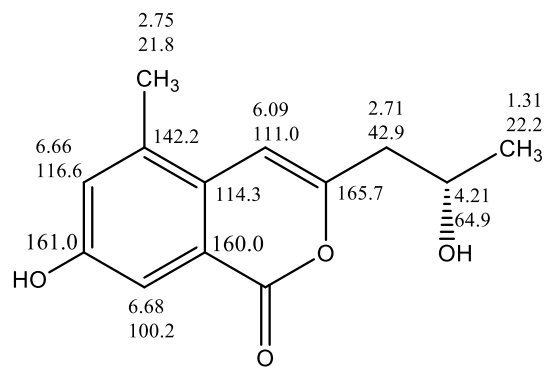
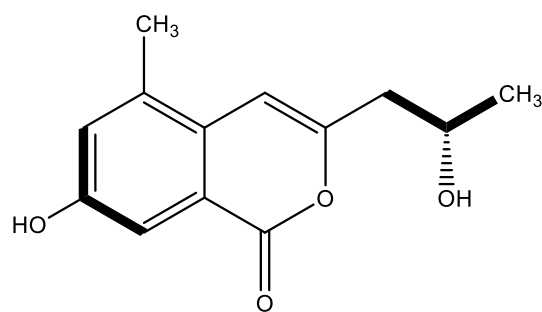


Table S1. ^1H and ^{13}C NMR Spectroscopic Data, and COSY & HMBC correlations for Compounds **6** in CD_3OD

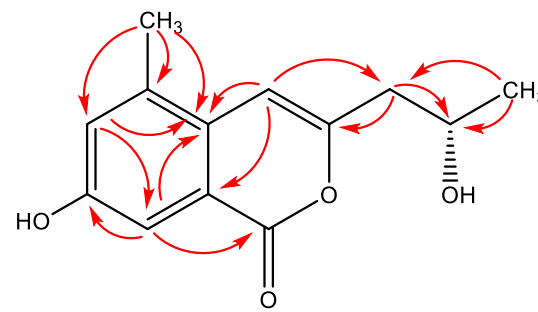
No.	δ_{C}	δ_{H} J (Hz)
1		
3	165.7, C	
4	6.09, s	111.0, CH
4a	114.3, C	
5	142.2, C	
6	6.66, d (2)	116.6, CH
7	161.0, C	
8	6.68, d (2)	100.2, CH
8a	160.0, C	
9	2.71, dd (5,10)	42.9, CH_2
10	4.21, m	64.9, CH
11	1.31, d (6)	22.2, CH_3
12	2.75, s	21.8, CH_3



Chemical Formula: $\text{C}_{13}\text{H}_{14}\text{O}_4$
Exact Mass: 234.08921

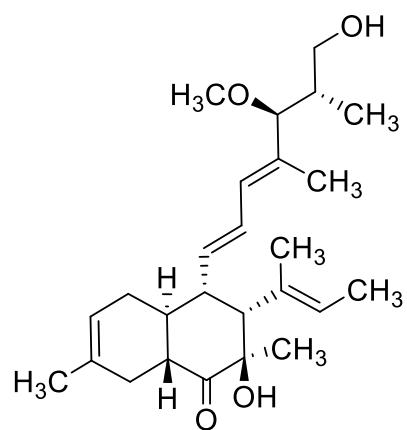


— COSY

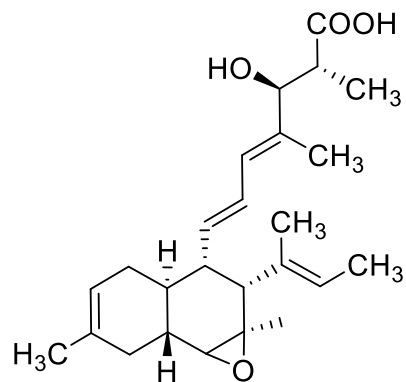


↷ HMBC

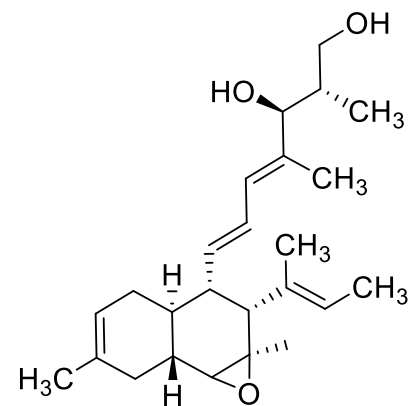
Fig. S52: Structures of the known compounds **7–11**



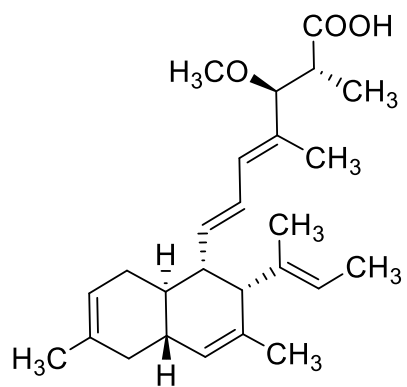
7: Fusarielin F



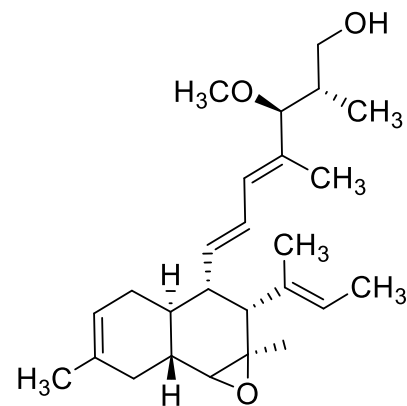
8: Fusarielin G



9: Fusarielin H



10: Fusarielin M



11: 3-O-methyl-fusarielin

Cartesian Coordinates of the most stable conformations found for each isomer.

1-RRS_c001

C 1.778910 -0.752246 -0.708964
C 0.579418 1.437201 -0.346881
C 3.123494 1.375539 -0.253680
C 1.825322 1.781023 0.478476
C 2.900080 0.175404 -1.200413
N 0.516355 -0.018162 -0.574839
C -0.636130 -0.700814 -0.840816
C -1.955483 0.072235 -0.709735
N -1.812222 1.252216 0.134747
C -0.685615 1.988422 0.317040
O -0.640547 -1.878088 -1.188709
C -3.080450 -0.860471 -0.195880
C -2.828789 -1.351274 1.237047
C -4.462882 -0.205744 -0.337976
O -0.671265 3.042140 0.940227
C 2.205775 -1.497204 0.560878
O 3.275157 -2.055680 0.667992
O 1.276609 -1.496085 1.541906
H 0.653066 1.953420 -1.320517
H 1.604812 -1.544503 -1.444659
H 3.891340 1.128995 0.487559
H 3.512398 2.220062 -0.834135
H 1.743239 1.259867 1.439021
H 1.799672 2.849704 0.700060
H 3.812450 -0.415419 -1.312411
H 2.617512 0.526490 -2.199646
H -2.227582 0.377443 -1.735473
H -2.651980 1.672058 0.515877
H -3.040682 -1.727268 -0.863594
H -2.846958 -0.525423 1.957760
H -3.604685 -2.066936 1.531023
H -1.859714 -1.852720 1.318524
H -4.591709 0.652505 0.335595
H -5.249343 -0.924197 -0.082684
H -4.645492 0.140079 -1.362556

H 1.653193 -2.033261 2.264981

1-RRS_c002

C 1.950775 -0.377281 -0.433822
C 0.437205 1.643032 -0.415778
C 2.868463 1.930458 0.160447
C 1.444351 2.386701 0.468081
C 2.976811 0.424221 0.395948
N 0.583778 0.173522 -0.307840
C -0.418470 -0.647841 -0.764678
C -1.860018 -0.141827 -0.722555
N -1.971402 1.205784 -0.186474
C -0.981284 2.130891 -0.101441
O -0.205115 -1.789570 -1.158640
C -2.742785 -1.152982 0.062749
C -2.328512 -1.268197 1.536007
C -4.235045 -0.821202 -0.083619
O -1.190674 3.299535 0.196625
C 2.059632 -1.830906 0.020291
O 2.782119 -2.641758 -0.509130
O 1.417278 -2.065669 1.192711
H 0.636083 1.936809 -1.462643
H 2.249452 -0.377162 -1.490192
H 3.587151 2.460360 0.796022
H 3.125646 2.172625 -0.880912
H 1.206236 2.193683 1.521879
H 1.304319 3.456382 0.297349
H 2.807898 0.212334 1.458621
H 3.972698 0.046444 0.140453
H -2.204785 -0.154759 -1.768865
H -2.900546 1.580103 -0.032024
H -2.556273 -2.114499 -0.427942
H -2.452746 -0.314283 2.061488
H -2.950207 -2.013268 2.045039
H -1.283054 -1.577566 1.635394
H -4.505538 0.111394 0.429464
H -4.843462 -1.613647 0.365495
H -4.530774 -0.729998 -1.135909
H 1.595657 -3.000777 1.405172

1-RRS_c003

C 1.767852 -0.850502 -0.621360
C 0.553053 1.355301 -0.359636
C 3.085216 1.338329 -0.599301
C 1.882224 1.805535 0.250368
C 2.780169 0.031300 -1.364933
N 0.495687 -0.127135 -0.403398
C -0.678271 -0.775291 -0.736195
C -1.956780 0.071050 -0.636647
N -1.778203 1.174247 0.303193
C -0.646962 1.928272 0.402807
O -0.715289 -1.947351 -1.083199
C -3.179467 -0.803089 -0.269697
C -3.074336 -1.411777 1.136136
C -4.494479 -0.030713 -0.457999
O -0.585641 2.972828 1.033425
C 2.373851 -1.398971 0.688431
O 3.483551 -1.870936 0.724867
O 1.588244 -1.341294 1.783167
H 0.485303 1.747938 -1.389435
H 1.520201 -1.731080 -1.222166
H 3.948605 1.191498 0.057355
H 3.366166 2.116850 -1.317668
H 1.945966 1.400550 1.267218
H 1.855370 2.891891 0.357528
H 3.689380 -0.554366 -1.519165
H 2.365287 0.253974 -2.355118
H -2.131217 0.466146 -1.653891
H -2.604906 1.591299 0.714960
H -3.157601 -1.623630 -0.994598
H -3.054691 -0.640867 1.915335
H -3.937814 -2.056835 1.331120
H -2.174846 -2.027346 1.235537
H -4.607904 0.788784 0.264494
H -5.348943 -0.699541 -0.310340
H -4.573457 0.396331 -1.464832
H 0.753376 -0.904008 1.527178

1-RRS_c004

C 1.557110 -0.978931 -0.641769

C 0.726243 1.394864 -0.439063
C 3.227532 0.958035 -0.624948
C 2.101480 1.617478 0.198987
C 2.736844 -0.309282 -1.362268
N 0.431550 -0.048532 -0.511612
C -0.830493 -0.559056 -0.642278
C -1.985257 0.449695 -0.537696
N -1.594563 1.601548 0.273235
C -0.359824 2.166464 0.316877
O -1.035575 -1.750393 -0.858365
C -3.296184 -0.154054 0.034118
C -4.011664 -1.061840 -0.976407
C -3.089033 -0.847839 1.388617
O -0.123965 3.221663 0.890052
C 2.008950 -1.602383 0.683508
O 3.018646 -2.263022 0.791369
O 1.166471 -1.373277 1.713782
H 0.743352 1.814385 -1.460938
H 1.191617 -1.824630 -1.233908
H 4.056671 0.703869 0.043845
H 3.626074 1.667723 -1.359159
H 2.069714 1.204493 1.213477
H 2.253600 2.693185 0.307973
H 3.540529 -1.042338 -1.465230
H 2.398894 -0.055683 -2.373679
H -2.197536 0.776190 -1.571160
H -2.330100 2.148721 0.706058
H -3.950053 0.718152 0.198583
H -3.419929 -1.955414 -1.183766
H -4.985668 -1.368860 -0.578613
H -4.190273 -0.538888 -1.924431
H -2.489434 -1.754473 1.269316
H -4.055989 -1.130112 1.819648
H -2.580021 -0.191623 2.103510
H 1.540799 -1.854498 2.476350

1-RRS_c005

C 1.941355 -0.304317 -0.379322
C 0.359610 1.664043 -0.430522
C 2.754184 2.039873 0.234224

C 1.304698 2.447401 0.486944
C 2.905557 0.538654 0.481388
N 0.557106 0.202810 -0.311985
C -0.397818 -0.655484 -0.801914
C -1.862408 -0.231634 -0.736434
N -2.037215 1.133512 -0.264587
C -1.087070 2.098436 -0.173032
O -0.121982 -1.774416 -1.222088
C -2.650855 -1.255550 0.132111
C -2.164537 -1.286993 1.587633
C -4.163769 -1.007912 0.041906
O -1.351144 3.265494 0.086526
C 2.010783 -1.732373 0.165478
O 1.518347 -2.108790 1.205029
O 2.845448 -2.490736 -0.578489
H 0.586524 1.963714 -1.469975
H 2.280185 -0.316677 -1.423449
H 3.429936 2.595592 0.894468
H 3.041955 2.288560 -0.797615
H 1.034862 2.250582 1.532324
H 1.133746 3.510602 0.304163
H 2.696180 0.322272 1.535803
H 3.925836 0.197786 0.272041
H -2.242020 -0.316731 -1.766154
H -2.983260 1.472545 -0.133414
H -2.434845 -2.225808 -0.329051
H -2.313694 -0.317873 2.078222
H -2.727933 -2.036772 2.154389
H -1.102722 -1.545061 1.655786
H -4.459343 -0.070346 0.531285
H -4.708413 -1.811686 0.548912
H -4.510541 -0.975039 -0.998364
H 2.890581 -3.357196 -0.131956

1-RRS_c006

C 1.827505 -0.720296 -0.749901
C 0.613476 1.467450 -0.325251
C 3.126555 1.374392 -0.000378
C 1.774361 1.756157 0.634886
C 2.968708 0.254864 -1.052266

N 0.537583 0.012416 -0.579523
C -0.608231 -0.665715 -0.806730
C -1.943862 0.071162 -0.716651
N -1.821758 1.343490 -0.021239
C -0.694802 2.073869 0.182815
O -0.610222 -1.875967 -1.091953
C -3.017224 -0.836696 -0.056413
C -2.677696 -1.183223 1.400330
C -4.419048 -0.220254 -0.179950
O -0.707897 3.179143 0.706445
C 2.127066 -1.610571 0.484555
O 3.085350 -1.440556 1.202180
O 1.254920 -2.608019 0.690897
H 0.815253 1.977050 -1.281267
H 1.680984 -1.394651 -1.601715
H 3.812673 1.048634 0.783292
H 3.573710 2.249691 -0.486067
H 1.606701 1.181352 1.553132
H 1.732374 2.813188 0.904933
H 3.892174 -0.324345 -1.138596
H 2.775864 0.689612 -2.040894
H -2.258348 0.242498 -1.760529
H -2.674735 1.808949 0.266025
H -2.997526 -1.760015 -0.644311
H -2.645400 -0.287780 2.031372
H -3.437500 -1.854925 1.814200
H -1.710791 -1.690887 1.479672
H -5.174464 -0.932386 0.168499
H -4.659870 0.040567 -1.217648
H -4.534252 0.683195 0.433809
H 0.554322 -2.584735 -0.009402

1-RRS_c007

C 1.747395 -0.675085 -0.427520
C 0.716988 1.607768 -0.433947
C 3.118890 1.367234 0.262663
C 1.813746 2.122557 0.505354
C 2.886478 -0.130666 0.462361
N 0.523116 0.146064 -0.301202
C -0.635018 -0.440907 -0.756404

C -1.941736 0.343543 -0.659587
N -1.736048 1.742261 -0.310348
C -0.563714 2.419877 -0.228650
O -0.662530 -1.595346 -1.170438
C -2.940366 -0.310434 0.348968
C -3.539532 -1.620425 -0.178595
C -2.330811 -0.476470 1.747458
O -0.509977 3.625329 -0.020424
C 1.550458 -2.139009 -0.042800
O 2.083081 -3.057053 -0.620094
O 0.885188 -2.290790 1.130963
H 1.043805 1.819023 -1.468375
H 2.071364 -0.689331 -1.476515
H 3.899626 1.718310 0.947156
H 3.479505 1.562112 -0.757603
H 1.918149 3.196125 0.333040
H 1.486150 1.989031 1.544330
H 2.626612 -0.321683 1.510367
H 3.788576 -0.709778 0.236359
H -2.394366 0.280639 -1.659582
H -2.559744 2.322298 -0.191838
H -3.763677 0.418060 0.423416
H -2.776981 -2.396811 -0.271787
H -4.319426 -1.973945 0.505568
H -3.996525 -1.481844 -1.165794
H -1.520816 -1.213781 1.740868
H -3.095062 -0.819528 2.453634
H -1.926681 0.469439 2.123848
H 0.867246 -3.251628 1.297891

1-RRS_c008

C 1.876663 -0.443609 -0.765953
C 0.411239 1.563988 -0.353624
C 2.807867 1.576711 0.510359
C 1.325410 1.884650 0.840558
C 2.949631 0.660978 -0.721860
N 0.532808 0.140726 -0.701917
C -0.496005 -0.723832 -0.923545
C -1.933516 -0.222069 -0.799960
N -2.022966 1.165690 -0.365891

C -1.016914 2.032722 -0.087764
O -0.293304 -1.900000 -1.218513
C -2.745478 -1.179482 0.118152
C -2.243970 -1.163521 1.568589
C -4.250359 -0.885830 0.036260
O -1.218621 3.171872 0.315903
C 2.083076 -1.435909 0.383477
O 1.515826 -1.425562 1.452645
O 3.061241 -2.317209 0.076815
H 0.737989 2.166453 -1.215403
H 1.968375 -1.014899 -1.693622
H 3.280459 1.105956 1.379102
H 3.361217 2.503299 0.320444
H 0.993047 1.273086 1.685142
H 1.177602 2.933150 1.107656
H 3.936785 0.189406 -0.752284
H 2.858484 1.248036 -1.643294
H -2.356941 -0.305428 -1.812699
H -2.946951 1.548121 -0.199767
H -2.565891 -2.175088 -0.302152
H -1.179558 -1.411780 1.633936
H -2.392978 -0.180985 2.032296
H -2.796327 -1.897873 2.165647
H -4.506617 0.087108 0.476969
H -4.814716 -1.641038 0.593994
H -4.611881 -0.896862 -0.999397
H 3.162015 -2.897175 0.855162

1-RRS_c009

C 1.911933 -0.575615 -0.460736
C 0.544008 1.593439 -0.395002
C 3.051504 1.705620 -0.254368
C 1.737242 2.296297 0.251790
C 3.100224 0.223671 0.113107
N 0.608940 0.111069 -0.264593
C -0.474189 -0.604533 -0.762720
C -1.852617 0.060537 -0.702011
N -1.829735 1.284762 0.086130
C -0.772152 2.135970 0.178688
O -0.358514 -1.737973 -1.202584

C -2.905583 -0.948737 -0.170382
C -2.613438 -1.403611 1.266713
C -4.331404 -0.395084 -0.312930
O -0.850667 3.250747 0.673826
C 1.930135 -1.944476 0.240822
O 2.629086 -2.850153 -0.130594
O 1.228372 -2.011426 1.400093
H 0.551751 1.846181 -1.470268
H 2.067185 -0.771937 -1.527172
H 3.903738 2.229508 0.192703
H 3.133179 1.833663 -1.343229
H 1.672178 2.192927 1.342212
H 1.647496 3.363120 0.033396
H 3.099193 0.131899 1.207625
H 4.013959 -0.260503 -0.244810
H -2.119923 0.287055 -1.748458
H -2.714277 1.677741 0.386304
H -2.807807 -1.817236 -0.830118
H -2.622642 -0.560704 1.967590
H -3.374119 -2.118899 1.597303
H -1.643009 -1.906311 1.337819
H -4.524715 0.444557 0.368081
H -5.062282 -1.172289 -0.065878
H -4.536350 -0.056746 -1.335685
H 0.721813 -1.183270 1.498066

1-RRS_c010

C 1.781191 -0.834337 -0.727334
C 0.599543 1.498572 -0.594139
C 3.054549 1.180339 0.101183
C 1.986744 2.140223 -0.423807
C 3.099980 -0.047960 -0.808005
N 0.596802 0.028631 -0.798727
C -0.604037 -0.626068 -0.877170
C -1.843393 0.260038 -0.639943
N -1.552323 1.210785 0.433642
C -0.357468 1.845853 0.567385
O -0.684947 -1.830755 -1.093884
C -3.102302 -0.582455 -0.342552
C -3.026031 -1.330652 0.997711

C -4.377119 0.269879 -0.442923
O -0.094609 2.632999 1.464997
C 1.803434 -1.705828 0.537232
O 2.498892 -2.688982 0.646413
O 1.026515 -1.235800 1.540826
H 0.136522 1.945063 -1.487942
H 1.726277 -1.551495 -1.550318
H 2.833036 0.887040 1.135095
H 4.026634 1.685844 0.112559
H 1.857966 2.993343 0.247727
H 2.317791 2.525848 -1.395503
H 3.911467 -0.733387 -0.545646
H 3.265110 0.268507 -1.846028
H -2.030109 0.813000 -1.577979
H -2.242491 1.382517 1.152902
H -3.124903 -1.334946 -1.138226
H -3.045755 -0.646572 1.855351
H -3.886964 -2.000587 1.098652
H -2.116733 -1.933170 1.059333
H -4.415306 1.050833 0.327908
H -5.265405 -0.357025 -0.309096
H -4.457881 0.763036 -1.418899
H 1.142042 -1.859077 2.283065

1-RRS_c011

C 1.565803 -1.024036 -0.556634
C 0.680061 1.344046 -0.448367
C 3.163648 0.952693 -0.822873
C 2.095060 1.652373 0.044813
C 2.638339 -0.365565 -1.435002
N 0.417928 -0.113088 -0.349725
C -0.852165 -0.620834 -0.554158
C -1.989690 0.411474 -0.493357
N -1.601366 1.540971 0.352797
C -0.377137 2.140121 0.323665
O -1.056564 -1.808625 -0.765416
C -3.344311 -0.161849 -0.000591
C -4.016502 -1.056253 -1.052248
C -3.236953 -0.857531 1.364492
O -0.136037 3.212914 0.855617

C 2.175438 -1.529491 0.768875
O 3.219581 -2.133374 0.796583
O 1.468333 -1.280158 1.889636
H 0.597199 1.653710 -1.505066
H 1.164393 -1.913272 -1.052387
H 4.045984 0.751757 -0.207020
H 3.490131 1.617482 -1.630801
H 2.170329 1.326618 1.088929
H 2.222428 2.736864 0.054661
H 3.449118 -1.084554 -1.573012
H 2.195763 -0.182115 -2.421187
H -2.137193 0.755447 -1.532856
H -2.341190 2.096197 0.768506
H -3.986583 0.725067 0.122787
H -3.438901 -1.967722 -1.217970
H -5.021402 -1.334922 -0.716101
H -4.120365 -0.534425 -2.011700
H -2.657509 -1.782172 1.285385
H -4.234855 -1.116066 1.734632
H -2.762063 -0.212127 2.112431
H 0.676714 -0.767889 1.636226

1-RRS_c012

C 1.768918 -0.535694 -0.380174
C 0.564976 1.664452 -0.443434
C 2.952484 1.618179 0.329310
C 1.584490 2.268442 0.528405
C 2.833823 0.107175 0.534475
N 0.487881 0.193675 -0.310305
C -0.603490 -0.484992 -0.802277
C -1.975883 0.166267 -0.675992
N -1.895834 1.595392 -0.405154
C -0.786184 2.367121 -0.289023
O -0.516134 -1.624157 -1.249476
C -2.846862 -0.541891 0.413571
C -3.294607 -1.944862 -0.016511
C -2.169466 -0.553782 1.790939
O -0.838093 3.576053 -0.100145
C 1.598249 -1.976872 0.103210
O 1.056177 -2.309615 1.133389

O 2.288163 -2.832900 -0.681536
H 0.907218 1.900976 -1.467405
H 2.125600 -0.559008 -1.418348
H 3.682048 2.032698 1.034522
H 3.327183 1.837109 -0.681011
H 1.236174 2.110198 1.556969
H 1.608940 3.346536 0.354298
H 2.552121 -0.098427 1.574099
H 3.788181 -0.397880 0.346188
H -2.467886 0.011036 -1.645725
H -2.767635 2.103671 -0.302803
H -3.750506 0.084998 0.483442
H -2.443993 -2.626007 -0.093993
H -3.999899 -2.349764 0.718079
H -3.797543 -1.924897 -0.990833
H -1.271257 -1.180930 1.790954
H -2.859311 -0.952504 2.543071
H -1.881439 0.455255 2.105573
H 2.188071 -3.712836 -0.271731

1-RRS_c013

C 1.594549 -0.979075 -0.698911
C 0.794399 1.413712 -0.380970
C 3.288185 0.946537 -0.448150
C 2.133334 1.584267 0.346039
C 2.806165 -0.254662 -1.291146
N 0.467825 -0.026492 -0.481438
C -0.794033 -0.515113 -0.524652
C -1.937971 0.504021 -0.526060
N -1.552836 1.677035 0.254351
C -0.310194 2.227412 0.301241
O -1.017352 -1.734801 -0.603672
C -3.294740 -0.038025 -0.005592
C -3.962926 -0.995912 -1.002527
C -3.204829 -0.638569 1.405118
O -0.076376 3.307169 0.823768
C 1.938349 -1.752656 0.598743
O 3.009645 -1.667878 1.153477
O 0.963306 -2.551982 1.053185
H 0.887241 1.827561 -1.399221

H 1.222390 -1.719576 -1.416649
H 4.063829 0.623002 0.248639
H 3.738510 1.688348 -1.118375
H 2.045531 1.115644 1.332811
H 2.290880 2.651541 0.514141
H 3.609208 -0.986578 -1.414332
H 2.526087 0.079119 -2.297948
H -2.083910 0.787524 -1.583958
H -2.292466 2.260611 0.628939
H -3.934982 0.857354 0.052227
H -3.390190 -1.919928 -1.103767
H -4.971966 -1.247218 -0.657540
H -4.056534 -0.537411 -1.994938
H -2.635738 -1.572355 1.398128
H -4.209170 -0.857829 1.783355
H -2.725607 0.050641 2.109249
H 0.176443 -2.485948 0.455986

1-RRS_c014

C 1.858632 -0.786329 -0.573509
C 0.607930 1.507631 -0.314824
C 3.015423 1.525046 -0.891383
C 1.965769 2.070500 0.073540
C 3.173942 0.022843 -0.652155
N 0.606396 0.024136 -0.424724
C -0.567142 -0.583627 -0.737018
C -1.842067 0.266675 -0.609339
N -1.670613 1.276488 0.428131
C -0.517317 1.971796 0.619313
O -0.641710 -1.761752 -1.118595
C -3.084829 -0.616977 -0.346682
C -3.033894 -1.329690 1.013417
C -4.382463 0.188560 -0.517740
O -0.390011 2.889194 1.414536
C 1.952846 -1.809145 0.610770
O 2.763998 -1.708895 1.500780
O 1.083517 -2.824941 0.566813
H 0.363890 1.910526 -1.313716
H 1.716730 -1.366348 -1.492274
H 3.982667 2.014320 -0.733013

H 2.717361 1.741426 -1.927374
H 2.206855 1.796817 1.107468
H 1.890975 3.160657 0.042169
H 3.688642 -0.119860 0.301584
H 3.803039 -0.432688 -1.424416
H -1.986387 0.753461 -1.591572
H -2.473767 1.578600 0.964739
H -3.052149 -1.381838 -1.129352
H -2.130260 -1.937749 1.113375
H -3.061800 -0.621442 1.849732
H -3.897532 -1.995278 1.117592
H -4.498769 0.965250 0.249745
H -5.250448 -0.473564 -0.431222
H -4.430052 0.677868 -1.497812
H 0.453191 -2.687061 -0.184102

1-RRS_c015

C 1.708535 -0.616276 -0.778372
C 0.570914 1.590637 -0.370912
C 2.938574 1.240636 0.495651
C 1.524064 1.787034 0.819182
C 2.934828 0.316309 -0.738011
N 0.466287 0.160563 -0.689977
C -0.684075 -0.546821 -0.875767
C -2.029399 0.160206 -0.722199
N -1.891928 1.577234 -0.400663
C -0.765495 2.283511 -0.127804
O -0.651260 -1.742999 -1.161586
C -2.954017 -0.536509 0.325875
C -3.505376 -1.880161 -0.169717
C -2.287345 -0.658777 1.702833
O -0.789684 3.450863 0.243263
C 1.783342 -1.635001 0.363601
O 1.274464 -1.524393 1.456230
O 2.578010 -2.673350 0.020997
H 0.988774 2.115280 -1.244015
H 1.703763 -1.187010 -1.711002
H 3.323386 0.697225 1.365041
H 3.636842 2.064577 0.310211
H 1.101330 1.250390 1.674284

H 1.544820 2.850685 1.066146
H 3.839764 -0.298470 -0.773281
H 2.930565 0.911735 -1.658553
H -2.517896 0.068977 -1.703195
H -2.747080 2.095724 -0.229028
H -3.811625 0.148296 0.426040
H -2.708865 -2.619515 -0.272444
H -4.251154 -2.259083 0.538659
H -3.993730 -1.775080 -1.146399
H -1.425229 -1.333005 1.671389
H -3.000996 -1.056473 2.433018
H -1.942946 0.313834 2.071780
H 2.610204 -3.262353 0.798434

1-RRS_c016

C 1.706455 -1.009786 -0.467887
C 0.591162 1.258144 -0.579395
C 3.075081 1.057489 -1.113914
C 2.004847 1.732150 -0.232694
C 2.710187 -0.406624 -1.462506
N 0.486088 -0.204610 -0.421337
C -0.716025 -0.848511 -0.324414
C -1.946346 0.083674 -0.346938
N -1.621418 1.285403 0.422761
C -0.460603 1.980009 0.274245
O -0.807560 -2.068559 -0.238755
C -3.222369 -0.630358 0.166282
C -4.339214 0.352712 0.558903
C -3.743423 -1.606717 -0.901296
O -0.267995 3.087648 0.756096
C 2.357856 -1.249860 0.898581
O 3.461600 -1.731743 1.029935
O 1.575511 -0.905448 1.943607
H 0.377660 1.526232 -1.630362
H 1.400399 -2.005882 -0.805527
H 4.035702 1.091772 -0.589250
H 3.208537 1.624628 -2.042550
H 2.182070 1.518689 0.826970
H 2.030365 2.819674 -0.330014
H 3.599472 -1.040997 -1.485790

H 2.248753 -0.457333 -2.455150
H -2.122709 0.361517 -1.402775
H -2.367818 1.791974 0.879939
H -2.937485 -1.209709 1.052533
H -4.583494 1.039808 -0.261834
H -5.250410 -0.205607 0.798353
H -4.097885 0.947449 1.447915
H -4.075686 -1.063938 -1.796620
H -4.604096 -2.163748 -0.514768
H -2.972041 -2.323163 -1.187298
H 2.077888 -1.146029 2.745386

1-RRS_c017

C 1.648743 -0.913814 -0.454197
C 0.872850 1.518550 -0.433568
C 3.329400 1.010931 -0.290923
C 2.205311 1.920545 0.199153
C 3.006205 -0.430826 0.097872
N 0.559856 0.075207 -0.239410
C -0.680160 -0.363671 -0.696536
C -1.862786 0.602713 -0.595563
N -1.494401 1.844730 0.073554
C -0.257077 2.408483 0.096573
O -0.842444 -1.496670 -1.124212
C -3.084823 -0.032756 0.136107
C -3.831006 -1.053320 -0.733575
C -2.708612 -0.610081 1.508194
O -0.047041 3.541700 0.504528
C 1.347262 -2.245977 0.252607
O 1.791483 -3.294996 -0.133501
O 0.685291 -2.141974 1.432244
H 0.948005 1.711928 -1.518425
H 1.733225 -1.142291 -1.522322
H 4.285915 1.311294 0.151279
H 3.440442 1.098428 -1.381213
H 2.119920 1.862245 1.291629
H 2.380979 2.970632 -0.046043
H 2.993396 -0.506668 1.193515
H 3.765161 -1.133447 -0.259779
H -2.170099 0.808985 -1.633720

H -2.244460 2.461804 0.365663
H -3.770163 0.813420 0.303255
H -3.212055 -1.930262 -0.933406
H -4.744435 -1.377766 -0.222658
H -4.123685 -0.617062 -1.696434
H -2.073640 -1.496884 1.402398
H -3.609473 -0.914837 2.051187
H -2.183242 0.128692 2.124653
H 0.395864 -1.216915 1.542071

1-RRS_c018

C 1.521398 -1.072023 -0.707732
C 0.776502 1.433061 -0.668544
C 3.195665 0.734980 -0.155780
C 2.261482 1.827546 -0.675780
C 2.945044 -0.545510 -0.952799
N 0.501280 -0.020023 -0.791209
C -0.797996 -0.455792 -0.713604
C -1.828044 0.662377 -0.450772
N -1.273828 1.564646 0.563454
C 0.020184 1.983699 0.559798
O -1.093335 -1.642707 -0.812148
C -3.229238 0.170417 -0.019139
C -3.966232 -0.518324 -1.177477
C -3.212677 -0.706126 1.243994
O 0.504484 2.738058 1.390501
C 1.495549 -1.819340 0.633900
O 2.008580 -2.902341 0.795343
O 0.906536 -1.123794 1.634052
H 0.303360 1.918200 -1.536257
H 1.276625 -1.835747 -1.449819
H 3.025622 0.563141 0.914373
H 4.236401 1.059037 -0.267601
H 2.347131 2.738203 -0.076613
H 2.555066 2.073393 -1.703440
H 3.643879 -1.345226 -0.689367
H 3.071650 -0.343250 -2.024236
H -1.955998 1.217417 -1.396690
H -1.858777 1.872492 1.329713
H -3.783199 1.093130 0.216740

H -3.466503 -1.449226 -1.454720
H -4.995640 -0.750372 -0.882453
H -4.012648 0.128498 -2.062521
H -2.713859 -1.657483 1.046240
H -4.239309 -0.912032 1.566837
H -2.694896 -0.217782 2.077874
H 0.968978 -1.688266 2.427856

1-RRS_c019

C 1.764552 -0.806969 -0.713805
C 0.583137 1.520094 -0.603499
C 3.022628 1.217649 0.120675
C 1.968920 2.163557 -0.453906
C 3.091837 -0.030190 -0.760891
N 0.589069 0.056616 -0.847339
C -0.612449 -0.603545 -0.906416
C -1.849903 0.274589 -0.630882
N -1.546211 1.206522 0.456402
C -0.343565 1.827554 0.591930
O -0.691651 -1.805658 -1.135644
C -3.101338 -0.578203 -0.330798
C -3.007356 -1.343837 0.998882
C -4.380995 0.269496 -0.405774
O -0.053910 2.576566 1.513136
C 1.674635 -1.590784 0.604313
O 1.015754 -1.284970 1.571118
O 2.482998 -2.675320 0.571585
H 0.095821 1.982745 -1.475556
H 1.735280 -1.546287 -1.518278
H 2.769522 0.948111 1.153585
H 3.995387 1.721447 0.146901
H 1.840379 3.042318 0.183537
H 2.308699 2.508005 -1.438333
H 3.894327 -0.709179 -0.456294
H 3.295234 0.263002 -1.798926
H -2.053485 0.847000 -1.553347
H -2.198274 1.308747 1.222807
H -3.129052 -1.320126 -1.136230
H -3.042604 -0.673514 1.866812
H -3.854731 -2.032425 1.089925

H -2.085223 -1.926680 1.056694
H -4.409605 1.043549 0.372106
H -5.264802 -0.362250 -0.264599
H -4.477768 0.770772 -1.376226
H 2.394746 -3.108622 1.441442

1-RRS_c021

C 1.972370 -0.087581 -0.344642
C 0.253200 1.700729 -0.358728
C 2.465661 2.200873 0.699092
C 0.959283 2.456203 0.772250
C 2.748332 0.696788 0.739885
N 0.535856 0.250485 -0.295024
C -0.345356 -0.659063 -0.835715
C -1.834594 -0.371083 -0.654234
N -2.105866 1.061355 -0.688187
C -1.230218 2.065641 -0.422701
O 0.017812 -1.719985 -1.328346
C -2.375139 -1.039539 0.652908
C -3.871442 -0.736112 0.834884
C -2.135528 -2.556289 0.676877
O -1.577701 3.234850 -0.315469
C 2.272085 -1.568032 -0.123915
O 3.106982 -2.180778 -0.745853
O 1.650960 -2.069901 0.974515
H 0.667864 2.079486 -1.310700
H 2.374251 0.150563 -1.338426
H 2.982507 2.697447 1.528361
H 2.866512 2.633747 -0.228680
H 0.559057 2.116100 1.736371
H 0.717615 3.516861 0.669044
H 2.458900 0.297452 1.718899
H 3.816089 0.491774 0.603468
H -2.333332 -0.838860 -1.510994
H -3.071406 1.363639 -0.741476
H -1.824568 -0.582692 1.487173
H -4.457608 -1.121696 -0.009945
H -4.245112 -1.223350 1.741776
H -4.076059 0.334835 0.938427
H -2.623075 -3.046674 -0.174680

H -2.558237 -2.981237 1.594395
H -1.073542 -2.804569 0.639729
H 1.953868 -2.994397 1.045201

1-RRS_c022

C 1.724263 -1.011307 -0.428908
C 0.569640 1.241038 -0.548144
C 3.044818 1.069125 -1.110296
C 1.974988 1.759331 -0.236484
C 2.647441 -0.378907 -1.479393
N 0.491877 -0.212359 -0.269637
C -0.721248 -0.871740 -0.281412
C -1.953814 0.054097 -0.321900
N -1.644647 1.264364 0.444629
C -0.505455 1.991264 0.246784
O -0.803799 -2.091398 -0.241524
C -3.235441 -0.663338 0.177287
C -4.355278 0.319162 0.562661
C -3.747048 -1.637016 -0.897532
O -0.348775 3.129748 0.659975
C 2.475477 -1.238969 0.900847
O 3.591892 -1.695669 0.928371
O 1.809310 -0.922960 2.029852
H 0.354199 1.417354 -1.617067
H 1.402561 -2.005301 -0.755324
H 3.996280 1.068209 -0.569236
H 3.207707 1.641696 -2.030563
H 2.174204 1.586316 0.827467
H 1.975245 2.843003 -0.371888
H 3.530320 -1.014079 -1.580913
H 2.119537 -0.398752 -2.440192
H -2.114700 0.321318 -1.382926
H -2.412847 1.788432 0.844042
H -2.960690 -1.244450 1.065942
H -4.594341 1.006814 -0.259110
H -5.267512 -0.240596 0.793612
H -4.120777 0.911542 1.454890
H -4.070331 -1.091377 -1.794220
H -4.612094 -2.192736 -0.519691
H -2.976168 -2.355447 -1.179797

H 0.939720 -0.560181 1.775572

1-RRS_c023

C -1.737883 -0.939338 0.615376
C -0.653537 1.360369 0.443818
C -3.171846 1.195663 0.753829
C -2.027397 1.759816 -0.107117
C -2.789301 -0.153538 1.402786
N -0.516168 -0.112828 0.416506
C 0.675566 -0.744337 0.302013
C 1.923074 0.153064 0.341138
N 1.626392 1.349320 -0.446439
C 0.470458 2.061644 -0.330546
O 0.753805 -1.977378 0.185108
C 3.195741 -0.584792 -0.145857
C 4.333595 0.382625 -0.516253
C 3.680586 -1.566378 0.934198
O 0.327942 3.184887 -0.789552
C -2.280205 -1.493108 -0.725446
O -3.378585 -1.224099 -1.154569
O -1.448233 -2.323378 -1.368916
H -0.570290 1.708187 1.487680
H -1.414204 -1.807124 1.202131
H -4.056228 1.068579 0.126224
H -3.432402 1.907429 1.546162
H -2.103752 1.382891 -1.133159
H -2.059464 2.849481 -0.168814
H -3.670829 -0.789656 1.520132
H -2.381854 0.014149 2.407408
H 2.085016 0.434093 1.398236
H 2.398971 1.868475 -0.843436
H 2.920640 -1.159034 -1.038407
H 4.571678 1.066323 0.309163
H 5.241031 -0.188933 -0.736813
H 4.117271 0.978801 -1.410373
H 4.004666 -1.026335 1.833948
H 4.539463 -2.137351 0.565259
H 2.896443 -2.273096 1.210815
H -0.610256 -2.422715 -0.850826

1-RRS_c024
 C 1.512135 -1.033477 -0.704326
 C 0.756293 1.460897 -0.664467
 C 3.173091 0.784558 -0.143012
 C 2.237184 1.862843 -0.687712
 C 2.940562 -0.507442 -0.927493
 N 0.491171 0.010231 -0.827581
 C -0.805915 -0.435206 -0.733004
 C -1.836551 0.672211 -0.429932
 N -1.275670 1.555804 0.597208
 C 0.021393 1.966857 0.594826
 O -1.095515 -1.621468 -0.850831
 C -3.230855 0.164468 0.006005
 C -3.978932 -0.498080 -1.160594
 C -3.197087 -0.743499 1.246581
 O 0.522551 2.685833 1.446052
 C 1.415469 -1.683074 0.684067
 O 0.917893 -1.186272 1.667787
 O 2.015972 -2.895594 0.688582
 H 0.265014 1.966063 -1.510119
 H 1.284340 -1.815594 -1.432632
 H 2.988258 0.625921 0.926492
 H 4.213527 1.112593 -0.246415
 H 2.321109 2.785649 -0.107379
 H 2.526952 2.087181 -1.721631
 H 3.642088 -1.297314 -0.641356
 H 3.086103 -0.320125 -1.999227
 H -1.978162 1.249521 -1.360234
 H -1.833524 1.790749 1.408088
 H -3.784461 1.079426 0.270441
 H -3.479010 -1.419752 -1.467024
 H -5.003728 -0.742228 -0.859189
 H -4.038854 0.170352 -2.028719
 H -2.700040 -1.689022 1.019384
 H -4.219756 -0.957441 1.577099
 H -2.667058 -0.279526 2.086297
 H 1.940772 -3.235014 1.600385

1-RRS_c026
 C 1.954232 -0.041420 -0.300033

C 0.192254 1.713984 -0.368269
 C 2.383344 2.280707 0.699617
 C 0.870779 2.501876 0.757075
 C 2.698183 0.784572 0.773662
 N 0.514256 0.274425 -0.286884
 C -0.331675 -0.660690 -0.841293
 C -1.827454 -0.426698 -0.651593
 N -2.146331 0.996399 -0.694801
 C -1.303007 2.030702 -0.438730
 O 0.073805 -1.699757 -1.347467
 C -2.330504 -1.100887 0.667379
 C -3.844022 -0.886584 0.833377
 C -1.991282 -2.597586 0.729056
 O -1.687322 3.189396 -0.342712
 C 2.195876 -1.512561 0.042828
 O 1.755541 -2.078616 1.018155
 O 3.107784 -2.061629 -0.788082
 H 0.597920 2.096145 -1.322912
 H 2.371789 0.160004 -1.295572
 H 2.881400 2.804433 1.523725
 H 2.782038 2.705768 -0.232793
 H 0.471805 2.165385 1.722840
 H 0.604603 3.554898 0.637171
 H 2.399744 0.394337 1.753703
 H 3.773043 0.601394 0.660021
 H -2.317340 -0.918621 -1.499762
 H -3.121598 1.266314 -0.744662
 H -1.814536 -0.590457 1.492382
 H -4.400072 -1.336007 -0.000209
 H -4.191696 -1.365141 1.755111
 H -4.116539 0.172416 0.899241
 H -2.413830 -3.134848 -0.129013
 H -2.418706 -3.032514 1.639653
 H -0.914348 -2.775730 0.740412
 H 3.252046 -2.971196 -0.465154

1-RRS_c027
 C 1.744418 -0.838737 -0.605946
 C 0.597151 1.413665 -0.503790
 C 3.150261 1.304517 -0.497561

C 1.889153 1.866758 0.194191
 C 2.853862 0.000402 -1.265933
 N 0.510778 -0.057214 -0.496397
 C -0.649343 -0.770767 -0.390446
 C -1.953154 0.046454 -0.389598
 N -1.721440 1.315041 0.299829
 C -0.610299 2.086511 0.155613
 O -0.644559 -1.997531 -0.340996
 C -3.134819 -0.753438 0.223315
 C -4.304000 0.149059 0.654444
 C -3.637251 -1.807035 -0.777611
 O -0.560798 3.254354 0.518759
 C 2.176753 -1.385876 0.758342
 O 1.820751 -0.987511 1.842485
 O 3.067916 -2.393433 0.597483
 H 0.608815 1.774082 -1.546759
 H 1.530195 -1.712620 -1.226790
 H 3.922832 1.128455 0.259505
 H 3.566380 2.038412 -1.197495
 H 1.838010 1.517147 1.229508
 H 1.891595 2.958104 0.218680
 H 3.751393 -0.617014 -1.366594
 H 2.515950 0.231620 -2.283247
 H -2.202063 0.244197 -1.448667
 H -2.528314 1.826676 0.634162
 H -2.751883 -1.272638 1.109871
 H -4.659602 0.777821 -0.172986
 H -5.147274 -0.472452 0.973578
 H -4.054670 0.796612 1.502852
 H -4.065231 -1.325198 -1.667390
 H -4.425950 -2.415078 -0.320504
 H -2.828846 -2.469771 -1.088957
 H 3.310425 -2.689269 1.495225

1-RRS_c028
 C 1.707128 -1.011001 -0.614259
 C 0.582534 1.338003 -0.769926
 C 3.110562 1.074825 -0.379777
 C 1.982726 1.950092 -0.927673
 C 3.014940 -0.311713 -1.018437

N 0.531742 -0.145656 -0.768524
C -0.676364 -0.753451 -0.530636
C -1.850750 0.235005 -0.346743
N -1.383187 1.256767 0.597470
C -0.167212 1.858111 0.476050
O -0.785121 -1.968353 -0.408647
C -3.146477 -0.461663 0.117402
C -4.215196 0.543668 0.580585
C -3.713092 -1.332926 -1.016327
O 0.253591 2.724318 1.228309
C 1.863171 -1.568483 0.808151
O 2.540189 -2.536218 1.067382
O 1.232385 -0.832389 1.751940
H -0.017882 1.672671 -1.629438
H 1.552623 -1.894604 -1.238033
H 3.040978 1.002457 0.712513
H 4.077125 1.536803 -0.610037
H 1.960286 2.921306 -0.425743
H 2.169125 2.128034 -1.993735
H 3.844179 -0.962959 -0.725709
H 3.044362 -0.217341 -2.111662
H -2.059932 0.714359 -1.319231
H -1.948194 1.513354 1.394704
H -2.882848 -1.118794 0.955289
H -3.936458 1.095497 1.485932
H -4.439779 1.277174 -0.203942
H -5.144296 0.012181 0.812706
H -3.999740 -0.715196 -1.878112
H -4.611913 -1.857177 -0.673621
H -2.986035 -2.078501 -1.341775
H 1.418351 -1.268706 2.604945

1-SRS_c001

C -1.658682 -0.901492 0.509288
C -0.218886 1.175609 0.450046
C -2.532076 1.287678 1.508216
C -1.580528 1.878599 0.447011
C -2.282190 -0.221561 1.737747
N -0.390710 -0.259951 0.156547
C 0.612907 -1.051004 -0.329703

C 1.942413 -0.350227 -0.625175
N 1.698867 1.025860 -1.052608
C 0.746571 1.848539 -0.536316
O 0.484714 -2.258794 -0.504341
C 2.942283 -0.457920 0.568550
C 3.251945 -1.920278 0.922028
C 4.238611 0.306361 0.259472
O 0.664103 3.037317 -0.813233
C -2.668099 -0.985709 -0.641372
O -3.808536 -1.365164 -0.489668
O -2.165985 -0.624288 -1.841265
H 0.231175 1.292878 1.451551
H -1.422192 -1.945402 0.741418
H -3.566670 1.452803 1.188840
H -2.413071 1.818295 2.460045
H -2.007942 1.777855 -0.556590
H -1.411744 2.945920 0.603828
H -3.209409 -0.742449 1.988415
H -1.590696 -0.369555 2.575202
H 2.368631 -0.890611 -1.476606
H 2.363710 1.474684 -1.670460
H 2.466019 0.019290 1.438420
H 3.744312 -2.426772 0.082545
H 3.930778 -1.961986 1.781291
H 2.351474 -2.489865 1.162331
H 4.737601 -0.111131 -0.625310
H 4.937099 0.223636 1.099266
H 4.059757 1.371902 0.083087
H -2.885920 -0.764984 -2.485543

1-SRS_c004

C -1.660844 -0.808642 0.653660
C -0.259076 1.289666 0.308944
C -2.624419 1.515825 1.201467
C -1.627652 1.953337 0.112270
C -2.334959 0.081885 1.700426
N -0.401078 -0.177322 0.170553
C 0.579700 -0.980910 -0.300678
C 1.932748 -0.341698 -0.596941
N 1.728568 1.012052 -1.102120

C 0.779633 1.880406 -0.655011
O 0.416538 -2.200681 -0.469206
C 2.895019 -0.410866 0.629997
C 3.139082 -1.858856 1.080963
C 4.225803 0.285649 0.308477
O 0.749521 3.059086 -0.975769
C -2.608639 -1.171810 -0.517928
O -3.713287 -0.694581 -0.642594
O -2.126723 -2.082889 -1.372717
H 0.102189 1.519823 1.324606
H -1.358467 -1.756194 1.115244
H -3.637542 1.570662 0.798650
H -2.573109 2.202510 2.054805
H -2.001453 1.675014 -0.879509
H -1.478966 3.034954 0.103448
H -3.258250 -0.409317 2.019147
H -1.673809 0.113605 2.575295
H 2.365586 -0.938529 -1.406197
H 2.436160 1.423600 -1.698413
H 2.413141 0.137509 1.453266
H 3.805047 -1.872145 1.950690
H 2.214093 -2.375362 1.348976
H 3.618784 -2.440016 0.283876
H 4.732864 -0.204939 -0.532985
H 4.897839 0.233387 1.171657
H 4.091144 1.343483 0.060764
H -1.214457 -2.352553 -1.093941

1-SRS_c005

C -1.902931 -0.291856 0.500075
C -0.084619 1.453163 0.279651
C -2.444078 2.190466 0.748579
C -1.151061 2.519659 0.006811
C -2.949888 0.822844 0.291453
N -0.572569 0.088060 -0.024516
C 0.321774 -0.946696 -0.147920
C 1.742955 -0.641269 -0.619824
N 1.948089 0.766735 -0.920764
C 1.200427 1.810437 -0.478468
O 0.011800 -2.115709 0.056700

C 2.785706 -1.229218 0.373871
C 4.204285 -1.154462 -0.206907
C 2.712085 -0.573257 1.759193
O 1.521574 2.977875 -0.657221
C -2.470168 -1.552806 -0.148385
O -3.124085 -2.372657 0.452594
O -2.330156 -1.555796 -1.496031
H 0.166298 1.503131 1.354054
H -1.820012 -0.523800 1.569863
H -3.204357 2.955136 0.552219
H -2.267381 2.188552 1.833949
H -1.339087 2.570943 -1.073015
H -0.734445 3.484165 0.305317
H -3.201318 0.869747 -0.775001
H -3.856661 0.526673 0.829798
H 1.839677 -1.202508 -1.559198
H 2.798769 1.036091 -1.401111
H 2.506844 -2.284517 0.474131
H 4.552044 -0.117489 -0.299960
H 4.913117 -1.671796 0.448630
H 4.262510 -1.625346 -1.196013
H 2.932587 0.499761 1.707457
H 3.444256 -1.027282 2.435812
H 1.723443 -0.703255 2.214864
H -2.764902 -2.373497 -1.801944

1-SRS_c008

C -1.910384 -0.269541 0.446850
C -0.067597 1.461969 0.292686
C -2.424230 2.213634 0.750224
C -1.119303 2.545263 0.030295
C -2.938635 0.863100 0.253477
N -0.567074 0.108816 -0.038800
C 0.316287 -0.935092 -0.160390
C 1.740702 -0.642335 -0.629195
N 1.965188 0.768404 -0.903703
C 1.227545 1.814598 -0.450504
O -0.009024 -2.100384 0.043551
C 2.777457 -1.262460 0.350611
C 4.194922 -1.202349 -0.234557

C 2.719840 -0.626492 1.745977
O 1.564820 2.980615 -0.607664
C -2.441308 -1.473929 -0.334325
O -2.455147 -1.569800 -1.539265
O -3.056627 -2.349766 0.492424
H 0.176187 1.491495 1.369603
H -1.849836 -0.545850 1.507599
H -3.173920 2.990726 0.561856
H -2.260665 2.185956 1.837372
H -1.294808 2.621090 -1.050046
H -0.696171 3.498767 0.354025
H -3.168007 0.934194 -0.816424
H -3.860120 0.568976 0.768673
H 1.826091 -1.187203 -1.579350
H 2.819614 1.034735 -1.378985
H 2.481560 -2.314422 0.435879
H 4.558951 -0.169841 -0.314480
H 4.897892 -1.740166 0.410795
H 4.241598 -1.659942 -1.230440
H 2.960359 0.442817 1.709688
H 3.444899 -1.104500 2.413755
H 1.729750 -0.744271 2.201933
H -3.424117 -3.046611 -0.083181

1-SRS_c009

C -1.663671 -0.757515 0.611998
C -0.210881 1.306274 0.421370
C -2.665448 1.558467 1.079266
C -1.536719 2.030193 0.136193
C -2.411700 0.135453 1.618387
N -0.387102 -0.145630 0.236536
C 0.547969 -0.984570 -0.299199
C 1.918198 -0.385716 -0.613557
N 1.780727 1.017064 -0.992989
C 0.899275 1.901074 -0.453337
O 0.325119 -2.178907 -0.478864
C 2.928573 -0.607440 0.556890
C 3.140201 -2.099381 0.853986
C 4.272408 0.073062 0.253439
O 0.968481 3.108332 -0.642465

C -2.518534 -1.055579 -0.624510
O -2.416074 -0.541650 -1.713783
O -3.466775 -1.975793 -0.327812
H 0.087802 1.508579 1.463565
H -1.447850 -1.725563 1.071622
H -3.618265 1.592589 0.539071
H -2.768464 2.242543 1.929606
H -1.802206 1.821347 -0.904314
H -1.358916 3.103917 0.221017
H -3.347131 -0.357626 1.899362
H -1.796841 0.180574 2.525219
H 2.281530 -0.934520 -1.488770
H 2.524579 1.447127 -1.529637
H 2.498248 -0.128196 1.449377
H 3.583394 -2.608682 -0.010929
H 3.827465 -2.218482 1.699234
H 2.205472 -2.612487 1.089694
H 4.721649 -0.335974 -0.661512
H 4.978639 -0.103307 1.071965
H 4.173411 1.156832 0.134018
H -3.981922 -2.110485 -1.145573

1-SRS_c010

C -1.718577 -0.722365 0.664351
C -0.206429 1.262350 0.278131
C -2.649144 1.651283 0.893107
C -1.504150 1.996720 -0.087556
C -2.432380 0.286255 1.579265
N -0.424542 -0.193995 0.218445
C 0.525923 -1.110975 -0.125384
C 1.882218 -0.604731 -0.612543
N 1.862233 0.807233 -0.971948
C 0.951239 1.744004 -0.601407
O 0.331175 -2.321349 -0.056472
C 3.001812 -0.980768 0.401525
C 4.392271 -0.721542 -0.194452
C 2.834181 -0.276817 1.754266
O 1.050852 2.923705 -0.914340
C -2.644933 -1.159054 -0.476523
O -3.723229 -1.673358 -0.279457

O -2.161349 -0.914360 -1.713744
H 0.075560 1.542998 1.306666
H -1.520706 -1.644777 1.218686
H -3.600413 1.647432 0.349173
H -2.738557 2.424582 1.664636
H -1.772681 1.707549 -1.109178
H -1.292361 3.067498 -0.104256
H -3.381436 -0.153192 1.897290
H -1.817488 0.406856 2.478785
H 2.070987 -1.178643 -1.528143
H 2.622755 1.169601 -1.535164
H 2.885038 -2.060987 0.551907
H 4.572499 0.349999 -0.349225
H 5.173679 -1.084419 0.482115
H 4.521695 -1.233013 -1.156211
H 2.908837 0.812139 1.648730
H 3.618433 -0.594486 2.450062
H 1.869364 -0.513049 2.217630
H -2.830821 -1.262020 -2.333563

1-SRS_c011

C -1.521531 -0.812515 0.687123
C -0.294881 1.362043 0.304093
C -2.773489 1.414513 0.909532
C -1.676345 1.937187 -0.047655
C -2.360417 0.098749 1.598951
N -0.326556 -0.107111 0.207587
C 0.684641 -0.891922 -0.265421
C 1.961804 -0.215329 -0.757729
N 1.756533 1.199856 -1.046662
C 0.785035 2.015207 -0.561021
O 0.592895 -2.117277 -0.295289
C 3.173986 -0.443402 0.199900
C 2.900986 0.049681 1.627253
C 3.653371 -1.901495 0.185442
O 0.764849 3.221064 -0.774233
C -2.391709 -1.402929 -0.427943
O -3.290517 -2.182767 -0.207188
O -2.094810 -0.952610 -1.666956
H -0.049313 1.649923 1.339138

H -1.188949 -1.685903 1.255041
H -3.702603 1.266193 0.347603
H -2.997009 2.160382 1.680703
H -1.900964 1.649061 -1.079628
H -1.601404 3.026093 -0.024968
H -3.234522 -0.466995 1.933250
H -1.760227 0.312050 2.491394
H 2.193276 -0.718324 -1.704036
H 2.475348 1.683230 -1.574268
H 3.979528 0.178518 -0.220264
H 2.128344 -0.556301 2.115877
H 3.809153 -0.025135 2.235135
H 2.581348 1.097679 1.641667
H 2.885480 -2.575338 0.574066
H 4.555653 -2.005999 0.798790
H 3.897320 -2.230807 -0.831422
H -2.708341 -1.413562 -2.270374

1-SRS_c015

C -1.749538 -0.468679 0.517772
C -0.213364 1.528503 0.284643
C -2.632298 1.903564 0.862909
C -1.433881 2.432377 0.079436
C -2.954102 0.487879 0.386186
N -0.506907 0.113306 -0.036315
C 0.518612 -0.779996 -0.230124
C 1.865607 -0.258266 -0.730243
N 1.830891 1.167414 -1.027016
C 0.973273 2.085050 -0.511354
O 0.371618 -1.987429 -0.064665
C 3.050614 -0.620639 0.220595
C 2.805239 -0.164771 1.665415
C 3.426141 -2.107426 0.150655
O 1.123260 3.290815 -0.658451
C -2.157622 -1.776691 -0.157425
O -2.664355 -2.700636 0.434706
O -2.074726 -1.714909 -1.508504
H 0.070340 1.594434 1.350019
H -1.592982 -0.720303 1.574673
H -3.502904 2.553546 0.718635

H -2.410018 1.902794 1.939838
H -1.673042 2.475283 -0.990655
H -1.148563 3.441560 0.384746
H -3.257591 0.523920 -0.666990
H -3.783222 0.048936 0.951572
H 2.028653 -0.791463 -1.676056
H 2.628274 1.568189 -1.509023
H 3.902765 -0.044987 -0.172213
H 2.564956 0.903210 1.721670
H 1.986418 -0.733128 2.122652
H 3.700227 -0.331238 2.274666
H 2.618264 -2.738346 0.528105
H 4.326733 -2.294371 0.746735
H 3.636998 -2.415539 -0.880553
H -2.401663 -2.575689 -1.829991

1-SRS_c016

C -1.719552 -0.692716 0.712050
C -0.227783 1.290200 0.165706
C -2.632957 1.711952 0.841856
C -1.543946 1.977513 -0.217103
C -2.405747 0.370380 1.574001
N -0.427540 -0.176000 0.173398
C 0.526398 -1.072764 -0.158224
C 1.895890 -0.578862 -0.605413
N 1.866502 0.812278 -1.032745
C 0.925936 1.747261 -0.732325
O 0.332799 -2.299702 -0.109327
C 2.975002 -0.893148 0.474472
C 4.383488 -0.635627 -0.078673
C 2.742986 -0.132039 1.786026
O 1.001886 2.907308 -1.111078
C -2.640231 -1.212500 -0.422736
O -3.718248 -0.722312 -0.669574
O -2.170229 -2.269280 -1.097528
H 0.052359 1.609876 1.181825
H -1.460217 -1.560479 1.330237
H -3.610745 1.705671 0.356862
H -2.638963 2.518982 1.583938
H -1.858501 1.592896 -1.194229

H -1.344779 3.043812 -0.341011
H -3.355932 -0.041655 1.924491
H -1.781879 0.526403 2.462928
H 2.132055 -1.193505 -1.482264
H 2.625503 1.153484 -1.610709
H 2.871462 -1.968060 0.668385
H 4.551004 0.431141 -0.273304
H 5.142214 -0.954772 0.643832
H 4.559643 -1.186665 -1.010531
H 1.763887 -0.359806 2.222957
H 2.809532 0.951788 1.634258
H 3.502783 -0.407791 2.525104
H -1.278727 -2.521261 -0.745109

1-SRS_c017

C -1.763304 -0.436219 0.464694
C -0.186426 1.540192 0.294897
C -2.603283 1.944358 0.860531
C -1.388935 2.469628 0.099450
C -2.945177 0.547224 0.344541
N -0.502391 0.136889 -0.051300
C 0.508623 -0.772867 -0.242506
C 1.865186 -0.270960 -0.735951
N 1.858427 1.159851 -1.010020
C 1.014235 2.086001 -0.487732
O 0.338894 -1.977745 -0.077836
C 3.044104 -0.669680 0.207464
C 2.807957 -0.231483 1.659339
C 3.392858 -2.161654 0.113520
O 1.186414 3.290768 -0.617670
C -2.155523 -1.679215 -0.338431
O -2.211996 -1.737940 -1.544551
O -2.605247 -2.658261 0.479345
H 0.094212 1.583617 1.362295
H -1.625346 -0.732075 1.512725
H -3.460861 2.613019 0.723467
H -2.391431 1.914634 1.939219
H -1.618251 2.539965 -0.971158
H -1.088935 3.466719 0.429490
H -3.226704 0.611469 -0.713203

H -3.794385 0.113923 0.885151
H 2.015644 -0.792652 -1.690291
H 2.662491 1.552103 -1.487800
H 3.906391 -0.103633 -0.176981
H 1.977981 -0.790545 2.107834
H 3.699549 -0.424238 2.265904
H 2.588223 0.840022 1.732041
H 2.573735 -2.783750 0.481177
H 4.290385 -2.374517 0.705628
H 3.597267 -2.456737 -0.922725
H -2.898627 -3.381027 -0.106748

1-SRS_c021

C -1.997323 -0.145681 0.302084
C -0.278752 1.567357 0.470145
C -2.456540 2.095226 -0.750717
C -0.960529 2.422746 -0.623320
C -2.722835 0.582709 -0.850016
N -0.530241 0.131672 0.196913
C 0.330758 -0.575839 -0.571005
C 1.794103 -0.134764 -0.657826
N 2.087716 1.056164 0.123202
C 1.187657 1.948968 0.609470
O 0.030284 -1.606128 -1.195649
C 2.721176 -1.323117 -0.266419
C 4.192161 -0.995784 -0.564170
C 2.524742 -1.765587 1.189677
O 1.500366 3.014424 1.121498
C -2.565712 -1.574396 0.529633
O -3.545125 -1.653508 1.239619
O -2.054687 -2.624032 -0.096589
H -0.731289 1.795766 1.440361
H -2.287744 0.344978 1.234462
H -2.875089 2.612257 -1.621905
H -2.985034 2.486282 0.129686
H -0.450575 2.231849 -1.578086
H -0.807677 3.478687 -0.378827
H -2.372377 0.179160 -1.808474
H -3.796032 0.379382 -0.777076
H 1.967064 0.068819 -1.726409

H 3.052907 1.360304 0.177903
H 2.414420 -2.141955 -0.925516
H 4.589405 -0.220734 0.104511
H 4.811958 -1.886136 -0.414641
H 4.334327 -0.661512 -1.599084
H 2.752217 -0.953343 1.889200
H 3.189884 -2.604083 1.422091
H 1.498408 -2.099324 1.376635
H -1.267239 -2.342324 -0.641878

1-SRS_c023

C -1.723660 -0.643549 0.692209
C -0.225080 1.352134 0.313225
C -2.732451 1.712811 0.605158
C -1.478918 2.053047 -0.236518
C -2.540881 0.428250 1.436353
N -0.421406 -0.106289 0.284166
C 0.488037 -1.025721 -0.144809
C 1.852554 -0.547448 -0.631044
N 1.914481 0.894224 -0.828522
C 1.020446 1.835288 -0.430457
O 0.244981 -2.230417 -0.140208
C 2.977697 -1.092786 0.295635
C 4.363229 -0.854843 -0.321086
C 2.894560 -0.525328 1.718456
O 1.193077 3.032526 -0.623295
C -2.492622 -1.168443 -0.525483
O -2.351111 -0.810009 -1.671655
O -3.423240 -2.072715 -0.142118
H -0.072014 1.670980 1.356325
H -1.553620 -1.501986 1.347263
H -3.593685 1.600794 -0.062574
H -2.974133 2.536205 1.286908
H -1.616452 1.716927 -1.268648
H -1.283226 3.126986 -0.257852
H -3.503500 -0.004283 1.726050
H -2.009571 0.656484 2.367987
H 1.976805 -1.030715 -1.608952
H 2.720247 1.274217 -1.311853
H 2.799293 -2.173891 0.337884

H 4.609830 0.213751 -0.367616
H 5.139321 -1.335818 0.284215
H 4.430184 -1.266051 -1.335770
H 3.024733 0.563466 1.720765
H 3.682874 -0.954078 2.346888
H 1.933950 -0.757551 2.192200
H -3.889674 -2.346526 -0.954374

1-SRS_c024

C -1.976963 -0.215510 0.380989
C -0.342177 1.600231 0.530469
C -2.648261 2.056742 -0.445056
C -1.166392 2.465150 -0.451410
C -2.837299 0.541590 -0.636664
N -0.562073 0.172786 0.248502
C 0.237286 -0.529814 -0.610138
C 1.691674 -0.081363 -0.767006
N 1.999119 1.145709 -0.042553
C 1.121714 2.019216 0.518288
O -0.142249 -1.537402 -1.199076
C 2.635801 -1.250649 -0.364011
C 4.094760 -0.937059 -0.726578
C 2.489330 -1.637599 1.113885
O 1.457040 3.100169 0.984708
C -2.204917 -1.725441 0.364790
O -3.090699 -2.277377 -0.243411
O -1.403206 -2.361327 1.253231
H -0.694268 1.791911 1.551412
H -2.267542 0.099377 1.395143
H -3.186899 2.605639 -1.226038
H -3.098526 2.356791 0.512581
H -0.748300 2.337428 -1.459750
H -1.042077 3.517421 -0.176952
H -2.540462 0.228531 -1.644476
H -3.886699 0.258407 -0.510963
H 1.828856 0.088540 -1.845694
H 2.954414 1.483351 -0.072816
H 2.302891 -2.093333 -0.980281
H 4.509186 -0.128292 -0.110149
H 4.724306 -1.816939 -0.555313

H 4.200452 -0.652450 -1.780715
H 2.756876 -0.803050 1.772246
H 3.153051 -2.476322 1.351902
H 1.464775 -1.943402 1.350017
H -1.623778 -3.308536 1.179265

1-SRS_c030

C -1.529947 -0.760111 0.679618
C -0.271460 1.397576 0.309809
C -2.770941 1.481745 0.808756
C -1.631939 1.977368 -0.112913
C -2.395365 0.177415 1.540570
N -0.314041 -0.072206 0.233497
C 0.664540 -0.873038 -0.277654
C 1.958275 -0.226059 -0.763888
N 1.798434 1.201940 -1.013493
C 0.848899 2.034206 -0.513813
O 0.533294 -2.094295 -0.334496
C 3.167548 -0.514308 0.181444
C 2.918238 -0.042354 1.620176
C 3.599859 -1.986260 0.133391
O 0.873568 3.246341 -0.687490
C -2.320949 -1.294926 -0.519213
O -2.279826 -0.875143 -1.652286
O -3.143508 -2.297137 -0.130828
H -0.068089 1.697250 1.350056
H -1.233240 -1.632277 1.267986
H -3.676030 1.329489 0.210409
H -3.019510 2.242913 1.557151
H -1.816094 1.661080 -1.144035
H -1.550333 3.066113 -0.107750
H -3.287187 -0.368150 1.863830
H -1.823609 0.404850 2.448244
H 2.167377 -0.713123 -1.723659
H 2.538038 1.677760 -1.518834
H 3.990618 0.089922 -0.230569
H 2.131081 -0.634762 2.102097
H 3.827937 -0.156044 2.219799
H 2.629085 1.013891 1.657645
H 2.813667 -2.643040 0.514503

H 4.502867 -2.132350 0.737120
H 3.825161 -2.302002 -0.891975
H -3.631268 -2.575297 -0.928948

1-SRS_c032

C -1.867169 -0.320190 0.309692
C -0.432150 1.640276 0.420829
C -2.658268 1.773146 -0.830915
C -1.234589 2.338507 -0.703328
C -2.680776 0.235143 -0.878130
N -0.458758 0.173515 0.203318
C 0.498135 -0.419696 -0.551042
C 1.898547 0.191430 -0.595005
N 1.982319 1.483961 0.070757
C 0.958036 2.246969 0.530285
O 0.332751 -1.481074 -1.174673
C 2.966282 -0.779682 0.011381
C 2.578639 -1.273362 1.411683
C 3.326435 -1.937068 -0.929098
O 1.105893 3.370334 0.990399
C -2.199678 -1.808583 0.606691
O -3.132186 -2.016225 1.352398
O -1.546529 -2.788037 -0.003929
H -0.913749 1.834634 1.384502
H -2.242571 0.160743 1.216385
H -3.140247 2.188198 -1.723620
H -3.254810 2.104774 0.030195
H -0.689454 2.202155 -1.648000
H -1.254772 3.412532 -0.493219
H -2.254628 -0.141794 -1.816053
H -3.709793 -0.132486 -0.808954
H 2.130101 0.312222 -1.663281
H 2.895081 1.922094 0.130291
H 3.866167 -0.153377 0.113390
H 1.728648 -1.964021 1.366330
H 3.415699 -1.812939 1.867124
H 2.314458 -0.442820 2.075145
H 3.626389 -1.569298 -1.917785
H 2.483336 -2.617432 -1.066135
H 4.167188 -2.503400 -0.513152

H -0.832078 -2.403447 -0.583511

1-SRS_c035

C 1.855794 -0.362982 -0.529981
C 0.059077 1.450155 -0.365446
C 2.375888 2.054054 -1.154529
C 1.167804 2.506490 -0.338214
C 2.915257 0.757430 -0.553907
N 0.547518 0.096058 -0.015921
C -0.356545 -0.906001 0.239691
C -1.794958 -0.502393 0.570404
N -1.837567 0.868845 1.063782
C -1.087900 1.886097 0.561715
O -0.044362 -2.092389 0.208449
C -2.767018 -0.753809 -0.629912
C -2.825647 -2.235789 -1.028354
C -4.175772 -0.235464 -0.299061
O -1.293565 3.063158 0.821799
C 2.449412 -1.511726 0.283813
O 3.090464 -2.410753 -0.208395
O 2.345887 -1.315603 1.619614
H -0.349987 1.426131 -1.391672
H 1.724533 -0.763091 -1.543496
H 3.154841 2.824854 -1.142596
H 2.093732 1.901582 -2.206439
H 1.465958 2.688394 0.701291
H 0.739856 3.440462 -0.710083
H 3.247719 0.951138 0.473190
H 3.777892 0.377756 -1.111571
H -2.096135 -1.162122 1.391636
H -2.624334 1.159625 1.631297
H -2.387194 -0.174824 -1.485670
H -3.215426 -2.843956 -0.202350
H -3.499448 -2.363867 -1.883099
H -1.844533 -2.633864 -1.292688
H -4.584196 -0.744636 0.584347
H -4.855531 -0.434843 -1.134351
H -4.191052 0.843071 -0.113175
H 2.793912 -2.077799 2.031350

1-SRS_c036

C -1.939999 -0.172552 0.427922
C -0.269826 1.617043 0.529211
C -2.589718 2.101699 -0.402528
C -1.102720 2.490079 -0.438363
C -2.808542 0.586962 -0.584084
N -0.525199 0.194573 0.259472
C 0.225253 -0.511057 -0.642007
C 1.698016 -0.132513 -0.789533
N 2.045455 1.105371 -0.101443
C 1.202352 2.003565 0.472697
O -0.211646 -1.476711 -1.260393
C 2.577675 -1.332354 -0.327943
C 4.058680 -1.088313 -0.652596
C 2.369325 -1.677404 1.153034
O 1.572493 3.083059 0.915951
C -2.098883 -1.694024 0.506505
O -1.463543 -2.400289 1.255291
O -3.123537 -2.144582 -0.247682
H -0.589652 1.821778 1.558083
H -2.207309 0.168858 1.439186
H -3.135248 2.655302 -1.175455
H -3.017921 2.411240 0.562165
H -0.706772 2.353305 -1.454348
H -0.960347 3.541938 -0.171239
H -2.535198 0.265955 -1.595667
H -3.863090 0.332929 -0.437759
H 1.862850 -0.004032 -1.869286
H 3.008941 1.416358 -0.149728
H 2.227958 -2.175183 -0.935206
H 4.487465 -0.284681 -0.039502
H 4.644829 -1.989951 -0.444653
H 4.208322 -0.830941 -1.708630
H 2.650230 -0.837579 1.799446
H 2.994160 -2.533813 1.430233
H 1.328256 -1.941310 1.365897
H -3.159072 -3.108393 -0.098950

1-SRS_c038

C -1.803641 -0.508373 0.415167

C -0.597502 1.622457 0.472181
C -2.963053 1.530055 -0.470664
C -1.606657 2.249992 -0.518757
C -2.815588 0.006028 -0.614118
N -0.505158 0.170096 0.249960
C 0.422441 -0.383477 -0.590855
C 1.763553 0.333270 -0.751405
N 1.767125 1.673882 -0.174379
C 0.736257 2.351459 0.394199
O 0.242391 -1.461886 -1.149936
C 2.941406 -0.504219 -0.156945
C 2.713861 -0.867627 1.316663
C 3.276272 -1.735600 -1.008761
O 0.835339 3.500575 0.804865
C -1.706626 -2.031997 0.454850
O -2.461802 -2.780257 -0.118733
O -0.782475 -2.453981 1.352265
H -0.961479 1.778183 1.495027
H -2.148267 -0.225517 1.421820
H -3.618466 1.922211 -1.256810
H -3.456219 1.755179 0.486490
H -1.183627 2.181679 -1.530793
H -1.709887 3.312974 -0.279371
H -2.462768 -0.266616 -1.615508
H -3.775475 -0.497568 -0.465702
H 1.926885 0.408865 -1.835675
H 2.633082 2.200021 -0.223303
H 3.808477 0.173722 -0.207206
H 1.873577 -1.561511 1.429604
H 3.607255 -1.350754 1.727598
H 2.505866 0.020800 1.922737
H 2.456122 -2.456844 -1.001386
H 4.177636 -2.222490 -0.619368
H 3.468228 -1.459100 -2.052489
H -0.806684 -3.428506 1.318242

1-SRS_c042

C 1.719841 -0.776400 -0.684463
C 0.079153 1.255561 -0.624695
C 2.625655 1.576462 -0.762402

C 1.245150 2.149118 -1.080149
C 2.721299 0.173653 -1.362779
N 0.382170 -0.194127 -0.542791
C -0.556265 -1.042977 -0.010484
C -1.840468 -0.394044 0.525889
N -1.509284 0.886440 1.156730
C -0.532177 1.726355 0.713819
O -0.371657 -2.252242 0.080771
C -2.988776 -0.306214 -0.522771
C -3.321673 -1.691625 -1.096552
C -4.233252 0.342111 0.100090
O -0.219543 2.762645 1.280201
C 2.254313 -1.166714 0.701359
O 1.915358 -0.680108 1.755143
O 3.222938 -2.105085 0.594542
H -0.724369 1.372778 -1.364886
H 1.629975 -1.700994 -1.259787
H 2.786045 1.542104 0.322005
H 3.399269 2.227985 -1.184119
H 1.100695 3.121145 -0.601155
H 1.172399 2.296076 -2.164669
H 3.722324 -0.256367 -1.256487
H 2.501675 0.215624 -2.437444
H -2.170767 -1.071078 1.319570
H -1.906565 1.110787 2.059912
H -2.650085 0.336904 -1.347719
H -2.455592 -2.165837 -1.565918
H -3.675523 -2.366619 -0.307574
H -4.116616 -1.607670 -1.846036
H -4.613129 -0.263580 0.933630
H -5.035582 0.421934 -0.641684
H -4.022173 1.348265 0.475912
H 3.534236 -2.281055 1.502455

1-SRS_c044

C 1.865816 -0.329866 -0.480534
C 0.038217 1.461429 -0.373738
C 2.354582 2.083224 -1.148254
C 1.132025 2.533131 -0.352164
C 2.905379 0.806922 -0.515031

N 0.541511 0.119004 -0.005620
C -0.349328 -0.894518 0.247059
C -1.793318 -0.510216 0.575301
N -1.858871 0.867038 1.049183
C -1.120790 1.889950 0.541847
O -0.019018 -2.076411 0.213747
C -2.764969 -0.793620 -0.618277
C -2.802800 -2.281602 -0.996387
C -4.180662 -0.292675 -0.290376
O -1.345208 3.066599 0.787866
C 2.427297 -1.406269 0.453002
O 2.479337 -1.325185 1.657631
O 3.019807 -2.394175 -0.256515
H -0.364146 1.420388 -1.402117
H 1.759269 -0.768164 -1.481048
H 3.122430 2.865209 -1.141956
H 2.086108 1.907766 -2.200202
H 1.417060 2.735758 0.687037
H 0.695532 3.454944 -0.743990
H 3.213937 1.022414 0.514908
H 3.785505 0.434883 -1.051313
H -2.080800 -1.163264 1.406825
H -2.648355 1.151521 1.615986
H -2.396717 -0.220739 -1.483199
H -3.478261 -2.431470 -1.846346
H -1.816669 -2.667917 -1.259277
H -3.179728 -2.884285 -0.160462
H -4.578652 -0.795928 0.601137
H -4.859581 -0.513951 -1.120873
H -4.212028 0.787898 -0.119229
H 3.408584 -2.999319 0.402666

1-SRS_c045

C -1.514326 -0.839951 0.696987
C -0.323037 1.345503 0.189520
C -2.716650 1.415000 1.015188
C -1.738764 1.865337 -0.087723
C -2.279813 0.077531 1.654550
N -0.325833 -0.132913 0.136164
C 0.714869 -0.880438 -0.293629

C 1.989153 -0.183845 -0.756331
N 1.726279 1.192262 -1.157973
C 0.702485 1.988224 -0.748723
O 0.667777 -2.122843 -0.324895
C 3.157608 -0.294083 0.275298
C 2.809353 0.312686 1.640805
C 3.672652 -1.734079 0.408745
O 0.607923 3.164434 -1.069068
C -2.425735 -1.407829 -0.422723
O -3.569506 -1.047818 -0.582833
O -1.867102 -2.355241 -1.185949
H -0.028306 1.658917 1.203307
H -1.117006 -1.701275 1.246750
H -3.715322 1.310208 0.587595
H -2.772963 2.177600 1.800955
H -2.059505 1.482271 -1.063377
H -1.687695 2.952764 -0.171216
H -3.148504 -0.472591 2.026220
H -1.630763 0.265299 2.518925
H 2.293584 -0.738734 -1.650939
H 2.414901 1.658700 -1.737805
H 3.964675 0.311531 -0.164077
H 2.477305 1.352966 1.553338
H 2.023358 -0.262527 2.145769
H 3.688882 0.304678 2.293520
H 2.913688 -2.392805 0.839761
H 4.557892 -1.756466 1.054040
H 3.955198 -2.150053 -0.565049
H -0.932035 -2.508519 -0.894891

2-RRSR_c001

C 1.924063 -0.838949 -0.760143
C 1.059473 1.464714 -0.200251
C 3.557373 0.996363 -0.048558
C 2.304942 1.512426 0.692238
C 3.201267 -0.063788 -1.115703
N 0.786590 0.072857 -0.603618
C -0.439841 -0.375845 -1.003703
C -1.620445 0.592770 -0.841859
N -1.351640 1.603660 0.174690

C -0.137494 2.120944 0.495139
O -0.610240 -1.489339 -1.491440
C -2.927373 -0.182463 -0.542870
C -4.156131 0.725625 -0.712719
C -2.887499 -0.885665 0.830175
O 0.005935 3.064686 1.261622
C 2.159302 -1.753939 0.447360
O 3.134070 -2.464541 0.556535
O 1.170691 -1.717604 1.367867
H 1.253632 2.072457 -1.101972
H 1.665300 -1.522305 -1.575923
H 4.255446 0.572776 0.681441
H 4.081394 1.828489 -0.532794
H 2.101590 0.904085 1.580885
H 2.432418 2.539196 1.040725
H 4.015126 -0.780763 -1.247908
H 3.031612 0.415555 -2.086681
H -1.746434 1.077305 -1.826377
H -2.138558 2.094186 0.582864
H -2.964103 -0.958396 -1.315615
H -4.212097 1.502905 0.061981
H -4.152162 1.225270 -1.688870
H -5.081777 0.146422 -0.644999
H -2.924304 -0.135043 1.631488
H -1.925318 -1.400366 0.934106
H 1.419795 -2.368192 2.051859
C -4.013652 -1.906576 1.033065
H -5.005245 -1.440216 1.020831
H -3.904795 -2.414454 1.997889
H -3.993729 -2.673844 0.249853

2-RRSR_c003

C 1.869938 -0.716922 -0.802807
C 0.790895 1.483905 -0.201170
C 3.326129 1.333732 -0.333909
C 2.110760 1.707664 0.541181
C 2.999405 0.187803 -1.320148
N 0.650175 0.059632 -0.564487
C -0.545745 -0.493783 -0.933225
C -1.781668 0.401454 -0.742466

N -1.578441 1.363689 0.334961
C -0.403196 1.983649 0.620449
O -0.638590 -1.609275 -1.435061
C -3.087072 -0.412179 -0.552587
C -4.305655 0.435155 -0.959778
C -3.293522 -0.996912 0.861640
O -0.298478 2.886046 1.439968
C 2.341775 -1.535681 0.403416
O 3.404987 -2.115177 0.431956
O 1.456606 -1.577620 1.423526
H 0.801355 2.092638 -1.123702
H 1.614720 -1.463483 -1.562699
H 4.158146 1.043140 0.316389
H 3.666468 2.207557 -0.901562
H 2.088304 1.103790 1.455126
H 2.147325 2.750603 0.862470
H 3.878948 -0.431315 -1.512216
H 2.673178 0.595316 -2.283864
H -1.884847 0.938452 -1.703021
H -2.389262 1.737299 0.813261
H -2.995962 -1.246283 -1.256888
H -4.440620 1.307130 -0.305353
H -4.214864 0.803035 -1.988425
H -5.224419 -0.157775 -0.896362
H -4.255313 -1.527117 0.843746
H -3.427184 -0.178390 1.583536
H 1.853352 -2.160332 2.099012
C -2.211551 -1.952488 1.376188
H -2.040257 -2.775012 0.674877
H -2.517048 -2.379616 2.338643
H -1.253309 -1.447053 1.529905

2-RRSR_c004

C 2.045084 -0.484594 -0.523800
C 0.733000 1.677046 -0.357298
C 3.225511 1.714032 0.003804
C 1.884747 2.299986 0.437072
C 3.202984 0.203092 0.228747
N 0.747523 0.194501 -0.305219
C -0.352295 -0.507166 -0.743856

C -1.698473 0.224870 -0.791719
N -1.680242 1.456869 -0.018886
C -0.599471 2.266304 0.126701
O -0.277928 -1.668121 -1.130678
C -2.891320 -0.687596 -0.396865
C -4.198769 -0.137820 -0.994223
C -3.052040 -0.919661 1.120193
O -0.666422 3.392862 0.598753
C 2.046830 -1.947847 -0.087354
O 2.638983 -2.818573 -0.680499
O 1.483224 -2.130405 1.131167
H 0.846621 1.990389 -1.411844
H 2.265914 -0.502052 -1.599074
H 4.043983 2.165649 0.575953
H 3.415001 1.939556 -1.055696
H 1.721512 2.115673 1.506157
H 1.836620 3.381494 0.291304
H 3.094100 -0.000390 1.300814
H 4.134214 -0.269388 -0.102034
H -1.831454 0.458848 -1.863319
H -2.565369 1.886538 0.223886
H -2.674149 -1.649065 -0.875241
H -4.475646 0.833933 -0.562824
H -4.124758 -0.011860 -2.080603
H -5.029120 -0.822911 -0.792632
H -3.950877 -1.536934 1.252429
H -3.275147 0.035594 1.615545
H 1.582068 -3.080486 1.327933
C -1.875927 -1.597042 1.830399
H -1.614568 -2.545898 1.350612
H -2.134433 -1.802705 2.875631
H -0.977494 -0.973305 1.830983

2-RRSR_c005

C 2.052105 -0.619763 -0.369255
C 0.988121 1.670975 -0.299307
C 3.335154 1.386070 0.555531
C 2.005225 2.108378 0.760049
C 3.104759 -0.122547 0.643080
N 0.825667 0.200888 -0.337993

C -0.251708 -0.347681 -0.991520
C -1.571097 0.420050 -0.997823
N -1.469970 1.724735 -0.361519
C -0.334661 2.414859 -0.084173
O -0.206952 -1.456217 -1.514921
C -2.685906 -0.458325 -0.356632
C -4.068623 0.172909 -0.585120
C -2.401163 -0.763870 1.127952
O -0.342712 3.575538 0.305516
C 1.732766 -2.066264 0.012982
O 1.072507 -2.407094 0.968269
O 2.429343 -2.931919 -0.755797
H 1.370103 2.005718 -1.280922
H 2.472932 -0.615841 -1.383160
H 4.061418 1.696752 1.315381
H 3.763287 1.652046 -0.421803
H 1.604516 1.883141 1.756376
H 2.106089 3.193755 0.690602
H 2.753731 -0.377174 1.650322
H 4.030173 -0.682111 0.465654
H -1.830743 0.547550 -2.060318
H -2.319950 2.265808 -0.252197
H -2.643489 -1.400596 -0.915921
H -4.209615 1.085122 0.010396
H -4.224474 0.427260 -1.640756
H -4.864921 -0.518958 -0.295519
H -2.435812 0.171137 1.703417
H -1.379563 -1.150396 1.224884
H 2.227479 -3.821285 -0.408814
C -3.365317 -1.783131 1.747028
H -4.395901 -1.412522 1.785228
H -3.064378 -2.019679 2.773437
H -3.366187 -2.721523 1.178998

2-RRSR_c006

C 1.715952 -1.030373 -0.669445
C 0.960904 1.369429 -0.469178
C 3.406777 0.865634 -0.965837
C 2.412630 1.586596 -0.031151
C 2.801166 -0.421803 -1.570513

N 0.633562 -0.068834 -0.438718
C -0.646251 -0.549741 -0.398242
C -1.754122 0.498593 -0.214284
N -1.246868 1.663255 0.511964
C -0.002189 2.193243 0.392311
O -0.903400 -1.742730 -0.536944
C -3.017802 -0.038829 0.510653
C -2.680421 -0.673902 1.868861
C -3.880917 -0.982667 -0.352866
O 0.330274 3.254060 0.904051
C 2.328903 -1.602306 0.613488
O 3.335251 -2.276781 0.620246
O 1.631051 -1.311532 1.732335
H 0.846365 1.745641 -1.501790
H 1.259836 -1.893574 -1.165999
H 4.314566 0.624085 -0.402749
H 3.714190 1.532750 -1.779540
H 2.510104 1.220170 0.996949
H 2.597436 2.662033 0.006868
H 3.571186 -1.177450 -1.743643
H 2.335420 -0.205885 -2.538974
H -2.049977 0.804093 -1.231203
H -1.912162 2.237048 1.017533
H -3.629072 0.860271 0.699544
H -2.133650 -1.610932 1.731130
H -2.065862 -0.008004 2.484623
H -3.600206 -0.891614 2.422994
H -4.716120 -1.315886 0.277938
H -3.295068 -1.872622 -0.597901
H 2.095513 -1.764781 2.461779
C -4.454858 -0.360104 -1.631382
H -5.014146 0.560130 -1.418121
H -5.143246 -1.057823 -2.121060
H -3.675994 -0.115355 -2.363101

2-RRSR_c008

C 1.753635 -1.079700 -0.663360
C 1.185828 1.368377 -0.454342
C 3.627200 0.660980 -0.605457
C 2.569368 1.443850 0.201664

C 3.003995 -0.530265 -1.367197
N 0.735879 -0.034285 -0.515909
C -0.573790 -0.414974 -0.615585
C -1.624943 0.697889 -0.491467
N -1.099244 1.832853 0.265193
C 0.186767 2.269623 0.276111
O -0.899933 -1.581199 -0.820437
C -2.958135 0.228393 0.154247
C -2.734590 -0.442508 1.518350
C -3.803856 -0.621518 -0.815805
O 0.533599 3.317374 0.805419
C 2.129358 -1.776383 0.649484
O 3.037972 -2.572963 0.734951
O 1.343717 -1.442559 1.696001
H 1.262640 1.770613 -1.480166
H 1.303203 -1.869936 -1.273050
H 4.405837 0.303236 0.076845
H 4.123872 1.323835 -1.323359
H 2.478642 1.039877 1.216219
H 2.835982 2.497159 0.308588
H 3.721551 -1.346383 -1.481401
H 2.701671 -0.221878 -2.374712
H -1.853211 1.014325 -1.524314
H -1.766780 2.470038 0.685166
H -3.522449 1.161401 0.325266
H -2.253034 -1.416847 1.394569
H -2.096750 0.173642 2.161817
H -3.685087 -0.591217 2.039799
H -3.301531 -1.578593 -0.980567
H -3.831255 -0.113553 -1.790952
H 1.658192 -1.981094 2.447219
C -5.243905 -0.847831 -0.341256
H -5.284548 -1.438649 0.580247
H -5.818544 -1.389489 -1.100799
H -5.759276 0.102722 -0.151208

2-RRSR_c009

C -1.992323 -0.808853 0.786406
C -1.086227 1.482962 0.181866
C -3.526211 0.968917 -0.275479

C -2.200255 1.481402 -0.872590
C -3.284418 0.003898 0.906339
N -0.815776 0.093186 0.609339
C 0.396415 -0.369053 0.986060
C 1.606113 0.561838 0.906912
N 1.355872 1.707827 0.044762
C 0.153671 2.225477 -0.317589
O 0.555702 -1.528210 1.406780
C 2.872555 -0.219323 0.462650
C 4.134474 0.635178 0.664211
C 2.742388 -0.770508 -0.972232
O 0.044796 3.251626 -0.974318
C -2.063240 -1.860384 -0.351295
O -2.982305 -1.921513 -1.134782
O -1.036991 -2.722203 -0.393860
H -1.433382 2.055110 1.057491
H -1.813161 -1.358641 1.717807
H -4.098947 0.461796 -1.053949
H -4.129194 1.812706 0.080005
H -1.880796 0.840000 -1.702199
H -2.292838 2.495299 -1.266830
H -4.116203 -0.699050 1.004459
H -3.233209 0.564910 1.847551
H 1.780936 0.902745 1.942205
H 2.151587 2.263614 -0.246231
H 2.925128 -1.071375 1.149489
H 4.191532 1.472213 -0.045213
H 4.180054 1.049024 1.678793
H 5.036863 0.035444 0.515298
H 2.696499 0.063757 -1.684894
H 1.788421 -1.304896 -1.061733
H -0.401613 -2.517380 0.338325
C 3.870838 -1.726985 -1.375876
H 4.845058 -1.227164 -1.410765
H 3.681828 -2.143799 -2.370948
H 3.948470 -2.566400 -0.674225

2-RRSR_c010

C 2.034589 -0.451077 -0.471403
C 0.695762 1.700958 -0.374625

C 3.177690 1.770868 0.045372
C 1.820603 2.348030 0.438718
C 3.165374 0.263427 0.294696
N 0.728778 0.221054 -0.304342
C -0.348688 -0.501813 -0.761783
C -1.714792 0.188750 -0.802247
N -1.720056 1.444697 -0.068592
C -0.655893 2.276601 0.070266
O -0.239406 -1.655490 -1.163350
C -2.868548 -0.749146 -0.350613
C -4.209458 -0.245203 -0.913454
C -2.971563 -0.958400 1.174694
O -0.749975 3.414956 0.508694
C 1.978273 -1.879899 0.073063
O 1.559525 -2.194360 1.163309
O 2.621978 -2.735305 -0.752609
H 0.829877 2.004312 -1.429623
H 2.280634 -0.502223 -1.540080
H 3.977240 2.239800 0.630281
H 3.390250 1.983233 -1.012513
H 1.634103 2.175018 1.505799
H 1.763968 3.426842 0.277007
H 3.025078 0.074166 1.365561
H 4.112782 -0.201927 -0.000202
H -1.880280 0.384617 -1.876531
H -2.614451 1.864172 0.157563
H -2.641147 -1.712520 -0.820649
H -4.505385 0.719726 -0.479270
H -4.172058 -0.124564 -2.002451
H -5.011041 -0.954914 -0.682822
H -3.860441 -1.580282 1.347946
H -3.185477 0.003699 1.660966
H 2.603511 -3.602564 -0.305953
C -1.766117 -1.616946 1.853454
H -1.508650 -2.569923 1.380505
H -1.989130 -1.812222 2.908727
H -0.870811 -0.990022 1.821100

2-RRSR_c011

C 1.748402 -1.047495 -0.465352

C 1.294107 1.410649 -0.493328
C 3.596572 0.621177 0.120732
C 2.518347 1.668694 0.392487
C 3.026016 -0.777650 0.361155
N 0.762924 0.042485 -0.301989
C -0.529080 -0.256384 -0.665728
C -1.601857 0.813118 -0.498086
N -1.047458 2.146526 -0.302062
C 0.256839 2.517429 -0.289476
O -0.861621 -1.375853 -1.043771
C -2.587541 0.468275 0.667395
C -1.862942 0.353902 2.016310
C -3.470114 -0.768906 0.405777
O 0.612344 3.681810 -0.155530
C 1.228350 -2.416975 -0.035934
O 1.491587 -3.442981 -0.616924
O 0.612264 -2.389373 1.173724
H 1.623151 1.505417 -1.544133
H 2.007882 -1.151073 -1.527215
H 4.465192 0.785138 0.768714
H 3.951692 0.712031 -0.915893
H 2.211262 1.633057 1.445738
H 2.866419 2.683686 0.187901
H 2.779068 -0.891218 1.423395
H 3.754948 -1.555429 0.108144
H -2.170470 0.803311 -1.435487
H -1.699483 2.914066 -0.181100
H -3.261624 1.339742 0.714689
H -1.197473 -0.516121 2.036007
H -1.264043 1.245194 2.230503
H -2.591565 0.239236 2.826532
H -4.143865 -0.861486 1.268524
H -2.842025 -1.665332 0.399346
H 0.371656 -3.314883 1.365722
C -4.305109 -0.726362 -0.878659
H -4.881818 0.204571 -0.958747
H -5.018970 -1.557261 -0.897983
H -3.676730 -0.821372 -1.770038

2-RRSR_c012

C 2.043862 -0.532369 -0.788818
C 0.899048 1.623371 -0.165044
C 3.178547 1.090773 0.840781
C 1.742527 1.601227 1.120519
C 3.276969 0.346791 -0.506007
N 0.815544 0.266848 -0.726022
C -0.317270 -0.359448 -1.150929
C -1.655181 0.373304 -1.056734
N -1.557649 1.660999 -0.382101
C -0.450886 2.291056 0.085125
O -0.285537 -1.497807 -1.614027
C -2.723222 -0.550970 -0.405769
C -4.132195 0.035071 -0.587895
C -2.392795 -0.867902 1.066590
O -0.497756 3.375644 0.653432
C 1.976134 -1.695817 0.206228
O 1.319322 -1.735393 1.222066
O 2.821380 -2.683997 -0.163507
H 1.394896 2.278606 -0.898074
H 2.123847 -0.976257 -1.784774
H 3.490204 0.427619 1.654925
H 3.889416 1.924712 0.830737
H 1.240257 0.939854 1.833335
H 1.743602 2.608784 1.541530
H 4.170796 -0.283525 -0.545348
H 3.367635 1.064260 -1.330022
H -1.964131 0.540600 -2.100476
H -2.417790 2.170672 -0.214912
H -2.660931 -1.482791 -0.980015
H -4.282886 0.942582 0.012853
H -4.330205 0.285674 -1.637325
H -4.897142 -0.681215 -0.273774
H -2.482039 0.048827 1.665391
H -1.344857 -1.183560 1.139123
H 2.751113 -3.375662 0.521357
C -3.273593 -1.964461 1.677984
H -4.327186 -1.668352 1.734786
H -2.944444 -2.197748 2.696554
H -3.216354 -2.889333 1.091097

2-RRSR_c013

C 1.807146 -1.087378 -0.409179
C 1.444818 1.391875 -0.403262
C 3.673576 0.493848 0.329478
C 2.620998 1.575163 0.562711
C 3.035643 -0.884195 0.505687
N 0.853905 0.038415 -0.297083
C -0.406813 -0.204108 -0.791985
C -1.447618 0.912363 -0.732697
N -0.878562 2.193346 -0.336865
C 0.431225 2.521415 -0.207062
O -0.738363 -1.305048 -1.219840
C -2.640714 0.550120 0.209502
C -2.160949 0.198853 1.624875
C -3.566959 -0.517775 -0.405468
O 0.806723 3.661637 0.034434
C 1.206628 -2.441869 -0.042573
O 1.481729 -3.469494 -0.615448
O 0.495146 -2.407526 1.113025
H 1.837998 1.516405 -1.428755
H 2.135099 -1.185482 -1.452422
H 4.507717 0.611218 1.030736
H 4.092802 0.591120 -0.682332
H 2.247782 1.524009 1.593613
H 3.018551 2.581170 0.410960
H 2.714398 -1.005026 1.547188
H 3.747821 -1.687063 0.285790
H -1.846407 0.992282 -1.754459
H -1.515339 2.975251 -0.226959
H -3.227157 1.482210 0.272319
H -1.614929 -0.750901 1.632531
H -1.496162 0.974336 2.020093
H -3.008028 0.110411 2.311864
H -3.041195 -1.476509 -0.444246
H -3.771198 -0.244624 -1.450252
H 0.211562 -3.327250 1.271438
C -4.901451 -0.673252 0.333656
H -4.765575 -1.040950 1.356597
H -5.546825 -1.389428 -0.186924
H -5.443370 0.279606 0.391394

2-RRSR_c016

C 2.017320 -0.842262 -0.466361
C 1.136404 1.563381 -0.290699
C 3.596349 1.121100 -0.020118
C 2.406618 1.944016 0.469209
C 3.307955 -0.358570 0.227175
N 0.879844 0.096171 -0.285881
C -0.292336 -0.332048 -0.899327
C -1.494242 0.616974 -0.868894
N -1.275064 1.736679 0.036840
C -0.071842 2.329092 0.266250
O -0.387844 -1.431366 -1.422887
C -2.792654 -0.161106 -0.523265
C -4.030838 0.720621 -0.753011
C -2.744592 -0.779404 0.889203
O 0.051939 3.388488 0.863262
C 1.696460 -2.224332 0.128346
O 2.214722 -3.233688 -0.271150
O 0.914044 -2.211839 1.236378
H 1.264875 1.888354 -1.338616
H 2.197837 -0.999346 -1.535267
H 4.509233 1.416728 0.508933
H 3.773406 1.304422 -1.089586
H 2.250343 1.780361 1.542783
H 2.559336 3.017811 0.336643
H 3.217563 -0.523366 1.309363
H 4.120189 -1.002038 -0.124427
H -1.604804 0.983708 -1.904250
H -2.078092 2.282480 0.326755
H -2.818891 -0.982561 -1.248444
H -4.121022 1.519849 -0.004485
H -4.009584 1.188039 -1.744674
H -4.947126 0.126846 -0.690997
H -2.670807 0.019736 1.639416
H -1.830893 -1.380561 0.976880
H 0.585851 -1.302137 1.366742
C -3.940752 -1.681097 1.216843
H -4.881276 -1.121385 1.261791
H -3.800607 -2.163900 2.189899

H -4.054980 -2.473926 0.467890

2-RRSR_c018

C 2.128087 -0.427878 -0.399015
C 0.708037 1.655729 -0.459773
C 3.100180 1.824345 0.303602
C 1.678460 2.342429 0.507874
C 3.120799 0.312026 0.522663
N 0.779430 0.179141 -0.361974
C -0.218528 -0.588247 -0.913694
C -1.630145 -0.007022 -0.995389
N -1.726052 1.323652 -0.414560
C -0.706729 2.203570 -0.241639
O -0.024764 -1.732419 -1.310512
C -2.654781 -1.011511 -0.394206
C -4.097886 -0.558839 -0.664161
C -2.408923 -1.402164 1.083325
O -0.886319 3.374128 0.068669
C 2.144390 -1.894202 0.025421
O 2.868570 -2.723322 -0.472637
O 1.412258 -2.126445 1.144153
H 0.998028 1.951310 -1.484692
H 2.504873 -0.417824 -1.430115
H 3.790444 2.312759 1.000914
H 3.448066 2.066416 -0.711021
H 1.352276 2.149632 1.537817
H 1.600216 3.419272 0.342632
H 2.858170 0.094165 1.564913
H 4.115447 -0.108640 0.339528
H -1.851849 0.049666 -2.074278
H -2.647827 1.732847 -0.315671
H -2.482347 -1.921560 -0.979822
H -4.365773 0.362549 -0.132658
H -4.269231 -0.390433 -1.734264
H -4.802777 -1.329303 -0.332413
H -1.369654 -1.735341 1.188999
H -3.027057 -2.290031 1.276154
H 1.536138 -3.072873 1.344941
C -2.717461 -0.355791 2.164037
H -2.069226 0.521285 2.085949

H -2.565304 -0.792739 3.157669
H -3.757201 -0.010899 2.119496

2-RRSR_c022

C 1.708135 -1.067789 -0.418877
C 1.306529 1.406338 -0.503978
C 3.583838 0.578172 0.148594
C 2.525565 1.653000 0.391603
C 2.980949 -0.802503 0.414212
N 0.751764 0.049692 -0.308387
C -0.535872 -0.230941 -0.702058
C -1.598471 0.841549 -0.509563
N -1.028740 2.172624 -0.339306
C 0.280171 2.527227 -0.316831
O -0.868484 -1.340147 -1.109746
C -2.543122 0.498273 0.691100
C -1.773975 0.387689 2.015850
C -3.425726 -0.745423 0.460793
O 0.649747 3.688120 -0.189942
C 1.096091 -2.358133 0.129467
O 0.541285 -2.468335 1.200001
O 1.406430 -3.411260 -0.657095
H 1.646953 1.490660 -1.552114
H 1.971062 -1.229096 -1.472642
H 4.450114 0.736467 0.801157
H 3.949701 0.641168 -0.886426
H 2.207106 1.640240 1.441858
H 2.897294 2.657056 0.174863
H 2.710849 -0.884233 1.473758
H 3.699511 -1.600604 0.195096
H -2.197656 0.832883 -1.427142
H -1.671811 2.947621 -0.218279
H -3.219051 1.367271 0.756907
H -1.101883 -0.477478 2.015549
H -1.177354 1.284718 2.212900
H -2.477152 0.267501 2.847514
H -4.072394 -0.837962 1.343824
H -2.792668 -1.638344 0.442392
H 1.043765 -4.198141 -0.208173
C -4.299113 -0.713842 -0.798225

H -4.882002 0.214305 -0.866581
H -5.010036 -1.547590 -0.791321
H -3.697324 -0.811378 -1.707546

2-RRSR_c023

C 1.754304 -1.111228 -0.351917
C 1.460547 1.381005 -0.399996
C 3.626321 0.435687 0.447606
C 2.594079 1.548636 0.617841
C 2.943694 -0.922386 0.614181
N 0.836237 0.043388 -0.308505
C -0.405361 -0.173697 -0.860960
C -1.439895 0.943473 -0.778405
N -0.849133 2.230650 -0.437650
C 0.461929 2.533505 -0.265655
O -0.727282 -1.258824 -1.334475
C -2.584468 0.590371 0.228659
C -2.037949 0.285159 1.630976
C -3.513281 -0.512128 -0.316848
O 0.854218 3.671467 -0.039754
C 1.038729 -2.389195 0.088974
O 0.367818 -2.505891 1.089925
O 1.394263 -3.433152 -0.691256
H 1.904090 1.487145 -1.406821
H 2.119095 -1.255733 -1.377402
H 4.430142 0.540881 1.185355
H 4.094488 0.507767 -0.544736
H 2.172603 1.522031 1.630821
H 3.026136 2.541089 0.470830
H 2.562522 -1.015883 1.638087
H 3.646869 -1.746519 0.447809
H -1.887122 1.007148 -1.779915
H -1.473799 3.025077 -0.350799
H -3.183594 1.514606 0.289386
H -1.475326 -0.654899 1.645552
H -1.372612 1.083659 1.976841
H -2.854753 0.204073 2.354728
H -2.971307 -1.462410 -0.345384
H -3.764328 -0.276244 -1.360508
H 0.956997 -4.216450 -0.307244

C -4.813371 -0.670404 0.480877
H -4.627148 -1.004022 1.507311
H -5.464747 -1.414530 0.009127
H -5.371745 0.273357 0.532515

2-RRSR_c024

C 1.918096 -0.562330 -0.831740
C 0.723785 1.589596 -0.267674
C 3.230701 1.403899 0.162511
C 1.856223 1.803087 0.748317
C 3.091870 0.417295 -1.014779
N 0.660358 0.167437 -0.648084
C -0.483390 -0.527481 -0.919196
C -1.810274 0.233866 -0.826431
N -1.709199 1.408369 0.030481
C -0.594119 2.141124 0.281652
O -0.457504 -1.697089 -1.292917
C -2.993336 -0.681095 -0.412508
C -4.325619 -0.074288 -0.886561
C -3.061056 -1.010838 1.093662
O -0.620156 3.202125 0.892402
C 2.173806 -1.516807 0.338503
O 1.698212 -1.442904 1.448349
O 3.068163 -2.468204 -0.017221
H 0.936551 2.194037 -1.165806
H 1.818458 -1.188272 -1.722307
H 3.842288 0.958522 0.955159
H 3.773931 2.289990 -0.185524
H 1.627567 1.191101 1.626000
H 1.835732 2.848700 1.061205
H 4.010432 -0.158594 -1.162377
H 2.913985 0.965242 -1.947743
H -2.011582 0.552846 -1.864589
H -2.568864 1.839311 0.350592
H -2.825708 -1.613140 -0.963608
H -4.556974 0.871951 -0.377714
H -4.319485 0.120923 -1.965366
H -5.154556 -0.758320 -0.675315
H -3.967340 -1.613297 1.243607
H -3.225778 -0.085377 1.663498

H 3.202439 -3.027053 0.771459
C -1.864173 -1.763567 1.684571
H -1.657923 -2.684349 1.129071
H -2.068910 -2.033827 2.727055
H -0.947185 -1.167230 1.679051

2-RRSR_c029

C 1.738864 -0.919883 -0.796140
C 1.093904 1.487890 -0.449181
C 3.384742 0.693981 0.328762
C 2.137525 1.547871 0.677792
C 3.127428 -0.254182 -0.859041
N 0.685847 0.094475 -0.673028
C -0.592557 -0.368111 -0.764811
C -1.753910 0.597511 -0.555237
N -1.318697 1.981885 -0.386753
C -0.059921 2.452952 -0.194838
O -0.823202 -1.553686 -1.002825
C -2.673618 0.175052 0.635925
C -1.908652 0.140807 1.966861
C -3.450694 -1.138211 0.409851
O 0.174582 3.618890 0.099694
C 1.679032 -1.895793 0.383486
O 1.263085 -1.653422 1.493971
O 2.239072 -3.079321 0.047934
H 1.557204 1.867881 -1.372813
H 1.563863 -1.507050 -1.701892
H 3.681241 0.111932 1.207654
H 4.235797 1.338033 0.080775
H 1.665890 1.169431 1.590108
H 2.395269 2.596004 0.844792
H 3.887310 -1.040603 -0.906514
H 3.193071 0.295201 -1.805444
H -2.347047 0.537735 -1.475875
H -2.040920 2.672458 -0.209757
H -3.423357 0.982123 0.694324
H -1.140174 -0.639795 1.967142
H -1.419739 1.097857 2.178887
H -2.598758 -0.066364 2.792354
H -4.111717 -1.263736 1.278468

H -2.749841 -1.977898 0.420630
H 2.201795 -3.637177 0.847821
C -4.290879 -1.197096 -0.870499
H -4.939890 -0.317337 -0.974993
H -4.937457 -2.081777 -0.863528
H -3.658470 -1.267857 -1.761458

2-RRSR_c030

C 1.822039 -0.943063 -0.761767
C 1.259739 1.472078 -0.332624
C 3.456031 0.535835 0.551247
C 2.213482 1.405357 0.871498
C 3.240617 -0.345639 -0.695004
N 0.810987 0.117792 -0.683496
C -0.472418 -0.275663 -0.920912
C -1.602192 0.744636 -0.794150
N -1.128777 2.068234 -0.400722
C 0.130153 2.466810 -0.087623
O -0.729909 -1.436667 -1.235855
C -2.728414 0.270513 0.178366
C -2.174074 -0.069741 1.569240
C -3.591783 -0.854740 -0.427821
O 0.384940 3.592842 0.322626
C 1.617783 -1.958772 0.366992
O 1.100075 -1.745006 1.439625
O 2.168781 -3.148689 0.037221
H 1.808705 1.893512 -1.189081
H 1.690925 -1.487023 -1.701109
H 3.688454 -0.094557 1.416211
H 4.335445 1.167468 0.382534
H 1.658614 0.974086 1.710515
H 2.489756 2.426798 1.141824
H 3.965050 -1.165313 -0.729338
H 3.396141 0.242764 -1.606912
H -2.043398 0.814236 -1.799399
H -1.833493 2.777817 -0.229576
H -3.384305 1.151553 0.282227
H -1.531963 -0.956128 1.536485
H -1.583289 0.759106 1.974611
H -2.987210 -0.264433 2.275256

H -2.997948 -1.770842 -0.491784
H -3.842489 -0.584272 -1.463590
H 2.033183 -3.735819 0.804808
C -4.892214 -1.113763 0.341921
H -4.703740 -1.480958 1.356623
H -5.497584 -1.869848 -0.170543
H -5.499916 -0.203243 0.424657

2-RRSR_c031

C 2.105427 -0.372723 -0.347630
C 0.640460 1.679652 -0.482482
C 3.001919 1.912459 0.352214
C 1.563248 2.401446 0.505804
C 3.047700 0.403951 0.594499
N 0.748350 0.207873 -0.369142
C -0.209085 -0.587636 -0.952533
C -1.645398 -0.074069 -1.013324
N -1.784955 1.275511 -0.486829
C -0.795443 2.187915 -0.311455
O 0.039462 -1.712879 -1.372745
C -2.594075 -1.103435 -0.329681
C -4.067030 -0.728745 -0.553283
C -2.266556 -1.425311 1.148661
O -1.015407 3.360205 -0.034484
C 2.062133 -1.811370 0.170585
O 1.477381 -2.179828 1.163959
O 2.908511 -2.599100 -0.528744
H 0.951981 1.975350 -1.500939
H 2.517177 -0.385908 -1.365241
H 3.659064 2.424889 1.064204
H 3.376186 2.149472 -0.654222
H 1.210321 2.214987 1.527970
H 1.466389 3.473912 0.322664
H 2.744675 0.192879 1.627016
H 4.059609 0.005433 0.459706
H -1.908047 -0.074413 -2.083569
H -2.719726 1.657858 -0.404071
H -2.402277 -2.025769 -0.890108
H -4.354753 0.198713 -0.043343
H -4.291051 -0.609254 -1.620400

H -4.719712 -1.517619 -0.163126
H -1.209067 -1.704278 1.226254
H -2.830985 -2.334361 1.398882
H 2.877006 -3.474562 -0.098976
C -2.585320 -0.355102 2.202647
H -1.985234 0.549070 2.068115
H -2.370964 -0.747420 3.203246
H -3.641822 -0.062055 2.189714

2-RRSR_c054

C 2.068791 -0.671227 -0.422561
C 1.047838 1.634430 -0.291805
C 3.422479 1.300075 0.469326
C 2.115094 2.044937 0.728490
C 3.168491 -0.204545 0.555032
N 0.853187 0.166501 -0.331738
C -0.260372 -0.356998 -0.943730
C -1.545496 0.470938 -0.962843
N -1.406905 1.743855 -0.272422
C -0.248791 2.404192 -0.016285
O -0.271780 -1.478685 -1.439610
C -2.726038 -0.368624 -0.397193
C -4.067089 0.335030 -0.661160
C -2.519781 -0.730177 1.087551
O -0.219643 3.553972 0.402791
C 1.809307 -2.145017 -0.120084
O 2.377760 -3.050680 -0.682719
O 1.026933 -2.327514 0.973561
H 1.396191 1.966377 -1.286846
H 2.454256 -0.646468 -1.450141
H 4.183066 1.593289 1.201974
H 3.817130 1.563757 -0.522552
H 1.748721 1.822030 1.738540
H 2.233449 3.128717 0.661758
H 2.859276 -0.460471 1.575635
H 4.072940 -0.780578 0.331526
H -1.758828 0.648172 -2.029525
H -2.241153 2.303097 -0.136376
H -2.704995 -1.295581 -0.982112
H -4.190053 1.236115 -0.044968

H -4.166030 0.626747 -1.713794
H -4.906832 -0.325259 -0.425494
H -2.540333 0.186318 1.692366
H -1.517900 -1.158605 1.211685
H 0.970639 -3.293487 1.096170
C -3.548865 -1.728220 1.632408
H -4.564518 -1.317318 1.637409
H -3.305578 -2.006658 2.663853
H -3.562994 -2.648189 1.034943

2-RRSS_c001

C 2.034840 -0.848735 -0.715799
C 1.017971 1.430373 -0.352042
C 3.548271 1.162019 -0.255478
C 2.286655 1.672450 0.474801
C 3.228437 -0.014114 -1.204829
N 0.836123 -0.015378 -0.576657
C -0.369071 -0.605977 -0.829890
C -1.623275 0.267991 -0.691276
N -1.379494 1.442296 0.138122
C -0.196970 2.087213 0.308671
O -0.468291 -1.780679 -1.172330
C -2.812830 -0.568038 -0.155190
C -2.575365 -1.046881 1.285216
C -4.143829 0.193636 -0.326644
O -0.095618 3.143143 0.920246
C 2.401966 -1.630896 0.550433
O 3.416647 -2.284948 0.648010
O 1.486434 -1.544535 1.540624
H 1.135065 1.936421 -1.326644
H 1.797022 -1.621721 -1.454073
H 4.291760 0.851725 0.486707
H 4.006838 1.972229 -0.833996
H 2.160840 1.159679 1.435136
H 2.347557 2.739854 0.695644
H 4.089534 -0.677397 -1.317030
H 2.977327 0.360612 -2.203832
H -1.881408 0.582958 -1.717659
H -2.180865 1.931933 0.518576
H -2.840106 -1.448814 -0.806783

H -2.561679 -0.209834 1.993260
H -3.364171 -1.737496 1.598950
H -1.621507 -1.576478 1.368620
H -4.187023 0.606550 -1.344572
H -4.180564 1.056990 0.356021
H 1.819113 -2.114422 2.260178
C -5.391419 -0.666474 -0.092052
H -5.395386 -1.541500 -0.753155
H -6.302120 -0.091715 -0.293519
H -5.452287 -1.027231 0.939991

2-RRSS_c002

C 2.009600 -0.715857 -0.797122
C 0.816908 1.451263 -0.305684
C 3.362272 1.412871 -0.363434
C 2.106345 1.791829 0.452264
C 3.089021 0.238877 -1.329306
N 0.752496 -0.000617 -0.552720
C -0.406709 -0.700854 -0.730657
C -1.725200 0.041342 -0.479474
N -1.536786 1.236991 0.333455
C -0.409351 1.985545 0.439012
O -0.417799 -1.873561 -1.093859
C -2.767413 -0.913802 0.156635
C -2.335268 -1.389310 1.552130
C -4.188723 -0.312935 0.193167
O -0.366190 3.040934 1.058586
C 2.527680 -1.499453 0.414503
O 3.593092 -2.075314 0.417565
O 1.686500 -1.507193 1.472271
H 0.831349 1.982740 -1.273508
H 1.795787 -1.484773 -1.546714
H 4.172344 1.149611 0.325382
H 3.715053 2.274681 -0.941539
H 2.085599 1.249921 1.404462
H 2.084435 2.855792 0.695784
H 3.996977 -0.339774 -1.516220
H 2.742164 0.616399 -2.298149
H -2.093836 0.324863 -1.478724
H -2.350017 1.641454 0.782769

H -2.783766 -1.783327 -0.509975
H -2.300491 -0.560858 2.269248
H -3.045949 -2.130763 1.934068
H -1.345890 -1.855474 1.524263
H -4.219679 0.556075 0.869201
H -4.841667 -1.059206 0.664147
H 2.115166 -2.066525 2.148001
C -4.780552 0.073440 -1.167558
H -4.244081 0.907193 -1.635440
H -5.825970 0.383082 -1.060443
H -4.753984 -0.772389 -1.865114

2-RRSS_c003

C 2.156615 -0.505003 -0.513236
C 0.799704 1.622737 -0.418012
C 3.290448 1.740185 -0.079360
C 1.938488 2.310047 0.343013
C 3.309639 0.236869 0.195620
N 0.850199 0.148530 -0.282194
C -0.245085 -0.605290 -0.629865
C -1.635308 0.014913 -0.494903
N -1.600938 1.368829 0.036396
C -0.542917 2.218841 0.020475
O -0.149195 -1.768247 -1.007716
C -2.540817 -0.915854 0.360238
C -2.021335 -1.056048 1.798459
C -4.021913 -0.481816 0.344823
O -0.636818 3.400906 0.324588
C 2.200905 -1.951730 -0.027230
O 2.813134 -2.826132 -0.593357
O 1.649981 -2.110898 1.202879
H 0.914400 1.878261 -1.487370
H 2.356512 -0.552235 -1.591631
H 4.102323 2.230986 0.469487
H 3.465535 1.934037 -1.147527
H 1.787933 2.163101 1.420034
H 1.860859 3.382611 0.151806
H 3.222844 0.066567 1.275534
H 4.247704 -0.222153 -0.134699
H -2.040643 0.026968 -1.517701

H -2.481606 1.807947 0.279136
H -2.470389 -1.892582 -0.132388
H -2.040975 -0.095515 2.325960
H -2.648636 -1.757921 2.359417
H -0.994058 -1.433513 1.819537
H -4.139501 0.485282 0.857575
H -4.573330 -1.199483 0.966060
H 1.779021 -3.051472 1.426574
C -4.678714 -0.418639 -1.039363
H -4.255950 0.373736 -1.668314
H -5.752150 -0.219365 -0.949208
H -4.559791 -1.367085 -1.576813

2-RRSS_c005

C 1.809891 -1.015215 -0.633954
C 1.125436 1.397314 -0.343198
C 3.599270 0.802972 -0.425210
C 2.472549 1.482442 0.380033
C 3.080614 -0.403873 -1.242734
N 0.744195 -0.014099 -0.540635
C -0.535228 -0.414423 -0.813143
C -1.603938 0.690072 -0.754946
N -1.220182 1.717128 0.213002
C 0.042997 2.176595 0.412765
O -0.811390 -1.571124 -1.118113
C -3.031385 0.177045 -0.428277
C -3.662514 -0.541295 -1.630744
C -3.078222 -0.655214 0.870668
O 0.306015 3.144751 1.113054
C 2.120959 -1.721914 0.690044
O 3.090826 -2.430125 0.850088
O 1.197805 -1.510566 1.652634
H 1.224816 1.887336 -1.328703
H 1.428881 -1.807462 -1.287596
H 4.384444 0.479030 0.266083
H 4.063793 1.524703 -1.107130
H 2.356916 1.009665 1.361887
H 2.688483 2.535671 0.571054
H 3.839419 -1.186506 -1.316282
H 2.834222 -0.094154 -2.264794

H -1.638625 1.130742 -1.767293
H -1.954373 2.272313 0.637456
H -3.620143 1.094379 -0.256012
H -3.127444 -1.467209 -1.851992
H -4.712096 -0.779444 -1.431235
H -3.636815 0.093173 -2.525604
H -2.452834 -0.164821 1.628548
H -2.622378 -1.632166 0.678402
H 1.482830 -2.045877 2.417734
C -4.490888 -0.837298 1.437640
H -4.968480 0.129400 1.643354
H -4.460178 -1.396796 2.379248
H -5.141825 -1.389910 0.751330

2-RRSS_c006

C 2.149945 -0.467695 -0.445088
C 0.768967 1.643872 -0.442233
C 3.227677 1.792281 0.062175
C 1.843733 2.346150 0.394596
C 3.246661 0.287934 0.333730
N 0.828845 0.173017 -0.295368
C -0.236769 -0.596725 -0.696740
C -1.644150 -0.029676 -0.544474
N -1.654010 1.362352 -0.120056
C -0.608693 2.227642 -0.110594
O -0.100394 -1.745393 -1.105138
C -2.456379 -0.939829 0.424524
C -1.842087 -0.974398 1.831506
C -3.950007 -0.556006 0.479932
O -0.738528 3.420945 0.131429
C 2.119059 -1.889362 0.119689
O 1.673160 -2.202280 1.200595
O 2.815164 -2.736293 -0.669896
H 0.958098 1.896578 -1.501527
H 2.414382 -0.524977 -1.509065
H 3.995207 2.289389 0.666466
H 3.472020 1.993663 -0.990914
H 1.623505 2.194550 1.458913
H 1.766308 3.417746 0.197788
H 3.086074 0.110654 1.403847

H 4.212705 -0.155987 0.067796
H -2.098117 -0.112745 -1.541757
H -2.550743 1.795387 0.068361
H -2.381045 -1.941821 -0.014895
H -1.849256 0.020432 2.292264
H -2.421142 -1.644109 2.477217
H -0.809262 -1.336702 1.816605
H -4.067708 0.431700 0.951318
H -4.436370 -1.258466 1.169081
H 2.806873 -3.597837 -0.211856
C -4.694194 -0.584163 -0.860835
H -4.342905 0.190443 -1.553113
H -5.766758 -0.418483 -0.711184
H -4.573512 -1.552979 -1.360428

2-RRSS_c008

C 2.149939 -0.643066 -0.350367
C 1.027848 1.616757 -0.408097
C 3.417316 1.460793 0.355243
C 2.078147 2.164564 0.564276
C 3.234790 -0.042101 0.567686
N 0.902997 0.145880 -0.315368
C -0.195731 -0.481726 -0.851448
C -1.538528 0.241887 -0.817775
N -1.432563 1.613228 -0.342638
C -0.301702 2.349936 -0.200080
O -0.150163 -1.627807 -1.286475
C -2.549807 -0.594169 0.022253
C -2.110995 -0.720621 1.488355
C -3.979359 -0.034136 -0.133651
O -0.318872 3.544975 0.066344
C 1.894841 -2.064529 0.154592
O 1.303681 -2.348726 1.171860
O 2.568075 -2.968531 -0.590227
H 1.359641 1.874777 -1.430263
H 2.519737 -0.703916 -1.382221
H 4.167497 1.847245 1.054726
H 3.794137 1.661010 -0.658225
H 1.728665 2.011231 1.593055
H 2.145443 3.242699 0.402687

H 2.939525 -0.228131 1.607330
H 4.166942 -0.589573 0.387569
H -1.900244 0.241159 -1.857241
H -2.288597 2.145761 -0.238506
H -2.525755 -1.589563 -0.437889
H -2.093408 0.258353 1.981851
H -2.801252 -1.362666 2.044267
H -1.113543 -1.163926 1.572035
H -4.163828 0.183027 -1.195881
H -4.067964 0.923714 0.400632
H 2.411776 -3.833957 -0.167396
C -5.077136 -0.980162 0.368305
H -5.024535 -1.948751 -0.143151
H -6.069980 -0.556548 0.180556
H -4.996810 -1.165559 1.444329

2-RRSS_c010

C -2.083445 -0.834592 0.746179
C -1.064779 1.450296 0.320987
C -3.558947 1.137190 -0.010260
C -2.243263 1.632915 -0.643776
C -3.306489 0.036764 1.043353
N -0.862194 0.008038 0.578511
C 0.337886 -0.566800 0.810641
C 1.603580 0.285177 0.728535
N 1.373302 1.542364 0.031766
C 0.187296 2.168121 -0.183646
O 0.444698 -1.772087 1.097358
C 2.761063 -0.521579 0.078334
C 2.456885 -0.883755 -1.383145
C 4.104425 0.219155 0.248667
O 0.105084 3.267636 -0.713291
C -2.299474 -1.751557 -0.486461
O -3.266779 -1.669205 -1.207496
O -1.342468 -2.668990 -0.686476
H -1.314053 1.942269 1.275112
H -1.880905 -1.491917 1.599927
H -4.213473 0.753196 -0.794659
H -4.080387 1.971493 0.473530
H -2.022770 1.071026 -1.558933

H -2.292849 2.688499 -0.918253
H -4.175859 -0.621096 1.127838
H -3.155852 0.487894 2.031853
H 1.892556 0.484423 1.774857
H 2.183706 2.078407 -0.255715
H 2.811830 -1.448459 0.660730
H 2.375433 0.010626 -2.011491
H 3.247868 -1.514327 -1.799656
H 1.520010 -1.444131 -1.467793
H 4.184015 0.577158 1.285183
H 4.128787 1.115082 -0.390414
H -0.649067 -2.581956 0.016275
C 5.334239 -0.639871 -0.069276
H 5.351819 -1.545432 0.548824
H 6.256430 -0.082685 0.128191
H 5.356867 -0.950494 -1.118891

2-RRSS_c011

C -1.925914 -0.833381 0.331574
C -1.167410 1.550783 0.378589
C -3.396970 1.013812 -0.646737
C -2.160989 1.906474 -0.733591
C -2.975695 -0.453315 -0.736454
N -0.793835 0.118791 0.340546
C 0.341679 -0.316283 0.984762
C 1.551607 0.613812 1.047123
N 1.245270 1.968620 0.610057
C 0.029921 2.502098 0.329325
O 0.434684 -1.447474 1.450298
C 2.763788 0.052882 0.232406
C 3.423686 -1.143006 0.932558
C 2.387454 -0.231009 -1.234709
O -0.126934 3.687640 0.066150
C -1.516937 -2.276759 0.050366
O -2.026259 -3.230479 0.589760
O -0.673967 -2.388834 -1.007605
H -1.668177 1.750184 1.343526
H -2.396330 -0.850466 1.323572
H -4.099760 1.250257 -1.453889
H -3.926016 1.198605 0.299325

H -1.668602 1.778886 -1.706289
H -2.406744 2.965739 -0.629971
H -2.547004 -0.648759 -1.726572
H -3.832728 -1.124118 -0.611125
H 1.848286 0.632713 2.105618
H 2.006796 2.638474 0.591293
H 3.495225 0.878303 0.235092
H 2.758371 -2.009340 0.947292
H 4.352595 -1.419451 0.423655
H 3.676441 -0.900953 1.971767
H 1.800498 0.614000 -1.616683
H 1.727719 -1.106854 -1.273605
H -0.528419 -3.346213 -1.124419
C 3.592362 -0.448370 -2.157306
H 4.271606 0.413483 -2.136410
H 3.264495 -0.584392 -3.193904
H 4.172013 -1.335240 -1.878757

2-RRSS_c014

C 2.112253 -0.662925 -0.747446
C 0.985713 1.551158 -0.326456
C 3.332799 1.157679 0.584949
C 1.912802 1.696312 0.891866
C 3.351568 0.247799 -0.659207
N 0.881680 0.134290 -0.704738
C -0.269048 -0.545470 -0.968664
C -1.607314 0.186668 -0.874043
N -1.480151 1.552162 -0.382408
C -0.352798 2.239404 -0.071036
O -0.253736 -1.733686 -1.283841
C -2.609064 -0.651386 -0.029548
C -2.169743 -0.758824 1.437893
C -4.045386 -0.111664 -0.189371
O -0.375614 3.386421 0.359447
C 2.121842 -1.690288 0.389942
O 1.540119 -1.596017 1.447187
O 2.943882 -2.720601 0.090060
H 1.422744 2.110010 -1.168635
H 2.131988 -1.229411 -1.682316
H 3.704933 0.606019 1.454979

H 4.031823 1.985533 0.420759
H 1.466022 1.130739 1.715359
H 1.930844 2.749565 1.179590
H 4.247476 -0.380618 -0.676127
H 3.381657 0.854198 -1.572123
H -1.993868 0.213913 -1.904794
H -2.333486 2.075019 -0.221049
H -2.571067 -1.650654 -0.479411
H -2.212827 0.215404 1.939674
H -2.820685 -1.445230 1.988260
H -1.146567 -1.139021 1.523406
H -4.242000 0.065211 -1.256788
H -4.139608 0.865019 0.309464
H 2.927306 -3.318650 0.861088
C -5.129439 -1.047617 0.358851
H -5.069874 -2.035877 -0.112791
H -6.128202 -0.642715 0.161270
H -5.039628 -1.187624 1.441021

2-RRSS_c015

C 2.053095 -0.594928 -0.820641
C 0.801124 1.547083 -0.379947
C 3.264489 1.392844 0.254902
C 1.849978 1.833713 0.707750
C 3.213108 0.411748 -0.933294
N 0.773606 0.106724 -0.674793
C -0.339938 -0.670723 -0.785347
C -1.714534 -0.035819 -0.582320
N -1.646968 1.355809 -0.155389
C -0.552108 2.140940 0.003653
O -0.262306 -1.868596 -1.050683
C -2.553502 -0.905963 0.395883
C -1.951296 -0.921111 1.808283
C -4.040058 -0.494068 0.432168
O -0.621034 3.300179 0.394671
C 2.278017 -1.546470 0.359540
O 1.796798 -1.446783 1.465509
O 3.163092 -2.512551 0.025486
H 1.088387 2.089400 -1.294485
H 2.011789 -1.216408 -1.719186

H 3.784619 0.927429 1.099228
H 3.864212 2.262398 -0.036979
H 1.553337 1.283249 1.605931
H 1.811855 2.899691 0.941442
H 4.150520 -0.145032 -1.027716
H 3.082754 0.961184 -1.873158
H -2.194759 -0.083310 -1.570204
H -2.516525 1.816460 0.088392
H -2.492088 -1.918527 -0.019656
H -1.990563 0.072315 2.270718
H -2.514434 -1.607651 2.450391
H -0.907275 -1.250552 1.802094
H -4.141959 0.521433 0.845396
H -4.538411 -1.146817 1.160635
H 3.281273 -3.063560 0.822199
C -4.786675 -0.586853 -0.904340
H -4.417295 0.134112 -1.643339
H -5.854837 -0.386248 -0.765817
H -4.689652 -1.587643 -1.342207

2-RRSS_c017

C 1.855246 -0.829765 -0.451752
C 1.008080 1.550712 -0.513874
C 3.427120 1.121666 0.033100
C 2.209292 1.993193 0.328123
C 3.085621 -0.335993 0.338810
N 0.714043 0.106682 -0.352781
C -0.483080 -0.396435 -0.809782
C -1.698653 0.530172 -0.838523
N -1.412724 1.836487 -0.258822
C -0.198447 2.438050 -0.187826
O -0.601646 -1.562330 -1.173450
C -2.961271 -0.104483 -0.171505
C -3.677335 -1.053577 -1.146294
C -2.715941 -0.800596 1.184101
O -0.054573 3.614655 0.117424
C 1.534047 -2.228587 0.068503
O 1.992668 -3.238089 -0.411959
O 0.841546 -2.210823 1.234699
H 1.257799 1.739594 -1.573993

H 2.125542 -0.964876 -1.507073
H 4.282923 1.440213 0.639218
H 3.724431 1.230620 -1.019916
H 1.945639 1.924592 1.391130
H 2.390256 3.048483 0.111955
H 2.877738 -0.440591 1.410656
H 3.918677 -1.005587 0.099487
H -1.936085 0.653342 -1.908001
H -2.197478 2.452573 -0.078202
H -3.636748 0.747466 0.010354
H -3.049054 -1.916179 -1.381122
H -4.614141 -1.412591 -0.705773
H -3.924390 -0.546525 -2.087164
H -2.052300 -1.658433 1.025708
H -3.681318 -1.216356 1.502645
H 0.746548 -3.145929 1.495472
C -2.160237 0.075072 2.313864
H -1.136491 0.401915 2.112688
H -2.146592 -0.487614 3.254435
H -2.774801 0.969822 2.473347

2-RRSS_c020

C -1.913896 -0.770213 0.275613
C -1.088413 1.593758 0.392257
C -3.288862 1.139507 -0.726863
C -2.023504 1.994798 -0.754017
C -2.908827 -0.338897 -0.823437
N -0.764060 0.151529 0.352328
C 0.328831 -0.326720 1.038593
C 1.585305 0.535609 1.087733
N 1.328383 1.922777 0.725409
C 0.143710 2.501727 0.406393
O 0.349784 -1.450583 1.530242
C 2.724923 -0.058722 0.193484
C 3.316366 -1.339349 0.798738
C 2.280499 -0.230049 -1.272687
O 0.035246 3.697720 0.166203
C -1.455017 -2.183111 -0.088921
O -0.719048 -2.464660 -1.007899
O -2.119671 -3.107101 0.638922

H -1.620238 1.802110 1.338614
H -2.419924 -0.811943 1.249219
H -3.952391 1.407764 -1.557030
H -3.848006 1.328732 0.200850
H -1.497477 1.862382 -1.708123
H -2.241020 3.059876 -0.646372
H -2.439765 -0.532882 -1.795375
H -3.792075 -0.983737 -0.749745
H 1.929710 0.495189 2.129938
H 2.115056 2.563092 0.731801
H 3.513700 0.712041 0.216913
H 2.593084 -2.158096 0.776739
H 4.209356 -1.645620 0.244902
H 3.611955 -1.183986 1.843248
H 1.756592 0.680965 -1.589634
H 1.549955 -1.045877 -1.340261
H -1.827488 -3.975119 0.302168
C 3.437775 -0.490360 -2.244292
H 3.070328 -0.538404 -3.275281
H 3.946917 -1.437403 -2.035384
H 4.187639 0.309904 -2.196662

2-RRSS_c024

C 1.839156 -0.797850 -0.405500
C 0.968780 1.573645 -0.532921
C 3.377708 1.181053 0.078860
C 2.143958 2.044480 0.329866
C 3.043648 -0.274630 0.403715
N 0.691427 0.129520 -0.357854
C -0.485995 -0.395855 -0.840139
C -1.727492 0.492831 -0.849475
N -1.461723 1.824551 -0.320160
C -0.258424 2.447001 -0.249304
O -0.567974 -1.557823 -1.226717
C -2.936791 -0.167692 -0.109302
C -3.655468 -1.170494 -1.026494
C -2.607339 -0.816075 1.252681
O -0.137235 3.634269 0.023828
C 1.455533 -2.145915 0.207368
O 0.868859 -2.296314 1.254671

O 2.005492 -3.164064 -0.491086
H 1.240605 1.752185 -1.589364
H 2.132572 -0.966447 -1.449821
H 4.215129 1.519175 0.699937
H 3.699572 1.275170 -0.968426
H 1.856239 1.990784 1.387432
H 2.318903 3.097765 0.099336
H 2.801957 -0.361384 1.469910
H 3.893154 -0.937350 0.203880
H -2.013281 0.577287 -1.910120
H -2.257322 2.430943 -0.154823
H -3.635023 0.664623 0.077694
H -3.005137 -2.016536 -1.261832
H -4.559166 -1.550063 -0.536832
H -3.959023 -0.702111 -1.970988
H -1.916288 -1.652333 1.095235
H -3.542525 -1.259339 1.620867
H 1.777015 -3.977864 -0.003582
C -2.042974 0.110360 2.336855
H -1.034240 0.454653 2.094466
H -1.983271 -0.424500 3.291365
H -2.676740 0.993147 2.488926

2-RRSS_c026

C 1.917683 -0.750249 -0.727982
C 1.048324 1.569893 -0.283242
C 3.239190 0.839376 0.790677
C 1.881671 1.554822 1.008935
C 3.247336 -0.006893 -0.497624
N 0.791717 0.191006 -0.722656
C -0.410496 -0.329407 -1.100026
C -1.653511 0.558533 -1.060049
N -1.379992 1.893123 -0.536784
C -0.204623 2.421976 -0.113185
O -0.503814 -1.497397 -1.475360
C -2.829466 -0.093934 -0.265050
C -3.497924 -1.229249 -1.053620
C -2.403363 -0.504094 1.158316
O -0.116651 3.552323 0.351361
C 1.717621 -1.826216 0.344243

O 1.092482 -1.704034 1.373165
O 2.407467 -2.944888 0.026879
H 1.625101 2.087271 -1.065509
H 1.941192 -1.266246 -1.691595
H 3.454364 0.202097 1.654955
H 4.054622 1.569145 0.732442
H 1.298856 1.029680 1.772147
H 2.013982 2.587375 1.338963
H 4.058141 -0.741956 -0.482171
H 3.426229 0.632241 -1.370276
H -1.977237 0.650376 -2.107695
H -2.173653 2.512860 -0.413235
H -3.573327 0.714986 -0.167529
H -2.821580 -2.078837 -1.167075
H -4.409091 -1.563878 -0.547445
H -3.785002 -0.892665 -2.057588
H -1.834548 0.320845 1.606802
H -1.715008 -1.355554 1.099905
H 2.265126 -3.572400 0.760544
C -3.575310 -0.848534 2.085010
H -4.285842 -0.015046 2.156934
H -3.214780 -1.064469 3.096759
H -4.128283 -1.728912 1.739981

2-RRSS_c028

C 2.122049 -0.860283 -0.601100
C 0.994964 1.494744 -0.322079
C 3.377348 1.387058 -0.989087
C 2.392523 1.995492 0.006500
C 3.471426 -0.118012 -0.733808
N 0.917778 0.012294 -0.417871
C -0.294958 -0.538651 -0.683339
C -1.519031 0.378097 -0.521215
N -1.261585 1.380530 0.506377
C -0.069097 2.018414 0.651499
O -0.441251 -1.714656 -1.050329
C -2.802138 -0.433182 -0.220647
C -2.738208 -1.144332 1.140704
C -4.055609 0.455468 -0.377717
O 0.133838 2.930467 1.437162

C 2.206930 -1.876053 0.589622
O 3.051385 -1.807676 1.451225
O 1.288764 -2.849010 0.584777
H 0.730139 1.901200 -1.314227
H 1.919639 -1.440638 -1.508272
H 4.372423 1.830384 -0.873561
H 3.051430 1.604445 -2.016443
H 2.659761 1.723593 1.034482
H 2.369636 3.087539 -0.037853
H 4.010238 -0.273176 0.204618
H 4.051852 -0.613359 -1.519571
H -1.663673 0.870244 -1.500762
H -2.028966 1.720460 1.071733
H -2.834153 -1.201284 -1.001751
H -2.730749 -0.432621 1.974785
H -3.604734 -1.798736 1.273269
H -1.843273 -1.767957 1.219587
H -3.969793 1.027581 -1.312248
H -4.098643 1.199709 0.431826
H 0.640075 -2.686607 -0.145327
C -5.374858 -0.325656 -0.398782
H -5.372190 -1.079949 -1.194803
H -6.219411 0.347918 -0.580150
H -5.562891 -0.840135 0.549138

2-RRSS_c032

C 2.221059 -0.388860 -0.373949
C 0.716391 1.651741 -0.451984
C 3.153583 1.938356 0.104256
C 1.734707 2.421792 0.394837
C 3.245718 0.445967 0.421124
N 0.864150 0.186511 -0.311489
C -0.125323 -0.639389 -0.788991
C -1.574720 -0.150363 -0.739046
N -1.684126 1.196391 -0.195022
C -0.700365 2.127887 -0.113546
O 0.111349 -1.771499 -1.198106
C -2.424403 -1.192832 0.048562
C -2.110928 -1.171217 1.551916
C -3.937679 -1.133652 -0.268450

O -0.914361 3.291058 0.203896
C 2.222503 -1.788037 0.245135
O 1.687341 -2.093904 1.286324
O 3.043801 -2.614366 -0.439681
H 0.892366 1.923109 -1.508914
H 2.539157 -0.476130 -1.420836
H 3.879013 2.493725 0.709787
H 3.410143 2.122937 -0.949037
H 1.499888 2.278248 1.456947
H 1.604225 3.484639 0.179405
H 3.057277 0.292780 1.490631
H 4.242578 0.047434 0.202137
H -1.925165 -0.161504 -1.783399
H -2.608348 1.553481 0.011065
H -2.079488 -2.153933 -0.348262
H -2.369184 -0.214502 2.017961
H -2.677120 -1.957309 2.064342
H -1.046411 -1.354973 1.733574
H -4.390928 -2.009039 0.215478
H -4.074687 -1.285059 -1.348294
H 3.044767 -3.458346 0.050003
C -4.726725 0.112603 0.161687
H -4.558950 0.365858 1.214623
H -5.801576 -0.059226 0.036984
H -4.485678 0.993209 -0.447396

2-RRSS_c035

C 1.767118 -0.833694 -0.759620
C 0.902672 1.516894 -0.451255
C 3.363554 1.019681 0.010071
C 2.066689 1.673361 0.540502
C 3.071328 -0.067376 -1.043734
N 0.630718 0.087453 -0.680401
C -0.602572 -0.468223 -0.870255
C -1.817955 0.460187 -0.810371
N -1.520483 1.696864 -0.093095
C -0.313913 2.301865 0.041827
O -0.734768 -1.663966 -1.123950
C -3.094244 -0.216343 -0.224880
C -3.805657 -1.055420 -1.298909

C -2.888517 -1.046602 1.060707
O -0.181149 3.421595 0.520348
C 1.870666 -1.670932 0.519949
O 1.351706 -1.428803 1.585257
O 2.671587 -2.743037 0.317075
H 1.187852 1.987183 -1.407237
H 1.573414 -1.540743 -1.570615
H 3.917679 0.588060 0.851319
H 4.020756 1.774413 -0.436956
H 1.762410 1.202308 1.480160
H 2.199377 2.739080 0.736246
H 3.893084 -0.786187 -1.112946
H 2.969104 0.387159 -2.036281
H -2.045548 0.702820 -1.862781
H -2.305377 2.263369 0.208170
H -3.762838 0.623629 0.027495
H -3.175586 -1.891448 -1.612610
H -4.746631 -1.456622 -0.906181
H -4.044695 -0.453191 -2.184408
H -2.300552 -1.936338 0.811618
H -3.882272 -1.407832 1.359015
H 2.705067 -3.225059 1.164951
C -2.244894 -0.328275 2.253170
H -1.191643 -0.094308 2.073473
H -2.284769 -0.969904 3.140936
H -2.765123 0.606345 2.498057

2-RRSS_c037

C 2.037403 -0.865348 -0.733392
C 0.958465 1.508408 -0.607044
C 3.402036 1.107970 0.054932
C 2.373281 2.093747 -0.497933
C 3.395268 -0.147121 -0.818758
N 0.897428 0.046499 -0.852891
C -0.332646 -0.562592 -0.878646
C -1.523477 0.369584 -0.574488
N -1.152579 1.283368 0.508112
C 0.079304 1.850443 0.614447
O -0.468282 -1.760801 -1.100874
C -2.807361 -0.424291 -0.249171

C -2.711812 -1.181644 1.086644
C -4.048986 0.488941 -0.333826
O 0.426661 2.580779 1.530726
C 1.942108 -1.630150 0.595561
O 1.311498 -1.289121 1.569568
O 2.708236 -2.744765 0.562290
H 0.466113 1.991978 -1.464728
H 1.958558 -1.611502 -1.528152
H 3.166119 0.855979 1.096282
H 4.395286 1.570786 0.051205
H 2.298548 2.980670 0.136810
H 2.700818 2.418277 -1.493242
H 4.175173 -0.858073 -0.528777
H 3.584991 0.130280 -1.863699
H -1.718582 0.954278 -1.490947
H -1.777009 1.403533 1.294560
H -2.878429 -1.172393 -1.047678
H -2.766850 -0.506300 1.950191
H -3.537372 -1.893473 1.181630
H -1.777156 -1.743071 1.153734
H -4.017581 1.038574 -1.285095
H -4.007961 1.252517 0.457111
H 2.618461 -3.164894 1.438457
C -5.384384 -0.257881 -0.238837
H -5.454112 -1.039434 -1.005466
H -6.224435 0.429785 -0.386591
H -5.518609 -0.735730 0.737243

2-RRSS_c038

C 2.012256 -0.691607 -0.836087
C 0.708183 1.545327 -0.496799
C 3.219105 1.369006 -0.015189
C 2.060417 2.270496 -0.440274
C 3.279744 0.170797 -0.963411
N 0.779583 0.098925 -0.819311
C -0.380277 -0.635473 -0.804502
C -1.636152 0.146654 -0.369061
N -1.289407 1.045724 0.733931
C -0.116427 1.731915 0.794579
O -0.407087 -1.826612 -1.094511

C -2.797388 -0.800524 0.003727
C -2.509850 -1.614543 1.276960
C -4.150191 -0.064175 0.112998
O 0.218016 2.445972 1.728379
C 2.091572 -1.539847 0.442293
O 1.498500 -1.329025 1.474896
O 2.966670 -2.559831 0.285796
H 0.112763 2.016646 -1.293861
H 1.953374 -1.393992 -1.671461
H 3.080666 1.035655 1.020883
H 4.157912 1.933021 -0.050964
H 1.939371 3.107861 0.252039
H 2.284120 2.682449 -1.431970
H 4.146891 -0.467919 -0.769071
H 3.365938 0.524390 -1.998944
H -1.950841 0.747682 -1.238270
H -1.861114 1.052315 1.568319
H -2.858497 -1.507560 -0.831807
H -2.525099 -0.991482 2.180148
H -3.278530 -2.384575 1.405835
H -1.537473 -2.109219 1.222638
H -4.101189 0.697894 0.904965
H -4.892287 -0.796234 0.457618
H 2.983737 -3.038709 1.135844
C -4.658547 0.578556 -1.182726
H -4.019102 1.402689 -1.519560
H -5.664185 0.989781 -1.041303
H -4.711148 -0.156747 -1.994954

2-RRSS_c054

C -2.166919 -0.667910 0.412318
C -1.053711 1.594307 0.402553
C -3.474336 1.421032 -0.256986
C -2.149117 2.129943 -0.526150
C -3.293554 -0.082240 -0.466013
N -0.920607 0.122306 0.310174
C 0.204679 -0.494472 0.801655
C 1.530226 0.265790 0.776358
N 1.400514 1.613952 0.245449
C 0.258301 2.338463 0.131412

O 0.195882 -1.651039 1.209568
C 2.592722 -0.564977 0.000788
C 2.216033 -0.735854 -1.478045
C 4.003039 0.029653 0.197463
O 0.254327 3.527173 -0.161373
C -1.995200 -2.125386 -0.008188
O -2.566893 -3.045390 0.527075
O -1.295180 -2.260297 -1.163257
H -1.342974 1.853070 1.437407
H -2.494401 -0.701299 1.459586
H -4.255448 1.799833 -0.926078
H -3.808885 1.625035 0.770421
H -1.842494 1.973544 -1.568155
H -2.215172 3.208661 -0.368159
H -3.049410 -0.273605 -1.517925
H -4.211060 -0.634707 -0.236082
H 1.858847 0.311960 1.826701
H 2.247570 2.154608 0.112862
H 2.571877 -1.549274 0.483597
H 2.206145 0.228293 -1.999631
H 2.933521 -1.385527 -1.988801
H 1.225736 -1.189991 -1.585743
H 4.143317 0.268922 1.261455
H 4.091452 0.980284 -0.349839
H -1.290071 -3.216551 -1.355253
C 5.138330 -0.900342 -0.248031
H 5.086350 -1.861941 0.276523
H 6.114311 -0.453094 -0.029729
H 5.103402 -1.103638 -1.323415

2-SRSR_c003

C -2.135793 -0.540373 0.517040
C -0.646412 1.488314 0.293329
C -3.089703 1.811960 0.795878
C -1.881320 2.360432 0.041147
C -3.361565 0.380223 0.335270
N -0.899645 0.064235 -0.025635
C 0.155564 -0.801345 -0.177522
C 1.489634 -0.255790 -0.686999
N 1.453071 1.174747 -0.948261

C 0.553540 2.069403 -0.465001
O 0.053959 -2.007338 0.021807
C 2.654015 -0.692718 0.247461
C 2.526465 -0.076896 1.647816
C 4.017893 -0.401375 -0.410632
O 0.678992 3.278511 -0.609100
C -2.491186 -1.875023 -0.134840
O -2.986637 -2.798395 0.467528
O -2.374185 -1.844707 -1.484470
H -0.400037 1.568256 1.367199
H -1.995934 -0.761682 1.583164
H -3.971806 2.436707 0.614554
H -2.900544 1.834582 1.878895
H -2.089186 2.384753 -1.036079
H -1.630100 3.379757 0.342604
H -3.635824 0.389750 -0.726497
H -4.194681 -0.070186 0.885587
H 1.636265 -0.768519 -1.647825
H 2.242805 1.594219 -1.425260
H 2.542788 -1.780663 0.334402
H 2.598465 1.016877 1.612511
H 1.571537 -0.346152 2.113975
H 3.317527 -0.439382 2.311071
H 4.189015 0.684664 -0.446807
H 3.986765 -0.745883 -1.454612
H -2.668310 -2.722294 -1.791964
C 5.207972 -1.070101 0.287838
H 5.345158 -0.700132 1.309390
H 6.137367 -0.875300 -0.258535
H 5.073078 -2.157092 0.340655

2-SRSR_c007

C -1.952263 -0.829983 0.678624
C -0.643323 1.294333 0.297406
C -3.104131 1.441902 0.946033
C -2.008850 1.910956 -0.040044
C -2.743856 0.098829 1.614036
N -0.725751 -0.174238 0.210853
C 0.292513 -0.992885 -0.182941
C 1.581441 -0.357115 -0.699939

N 1.428440 1.059168 -1.008912
C 0.451804 1.901443 -0.583005
O 0.207762 -2.217131 -0.138495
C 2.769070 -0.667417 0.258249
C 2.586516 -0.010072 1.632988
C 4.110494 -0.295681 -0.405890
O 0.445972 3.096410 -0.851286
C -2.853482 -1.350247 -0.447207
O -3.856872 -1.993134 -0.233269
O -2.442093 -1.020067 -1.690789
H -0.376879 1.580379 1.328465
H -1.655495 -1.731236 1.223389
H -4.055693 1.348222 0.410694
H -3.263488 2.193636 1.727503
H -2.262145 1.615796 -1.063833
H -1.897732 2.996958 -0.037995
H -3.639693 -0.433495 1.944463
H -2.127657 0.271248 2.504260
H 1.781038 -0.883910 -1.641427
H 2.145714 1.506610 -1.567798
H 2.742708 -1.757779 0.383949
H 2.584752 1.083632 1.552906
H 1.646609 -0.321727 2.102761
H 3.394395 -0.291293 2.315121
H 4.187400 0.797776 -0.496263
H 4.116997 -0.693836 -1.430932
H -3.085187 -1.430282 -2.300179
C 5.346987 -0.824894 0.330537
H 5.447721 -0.388972 1.330113
H 6.260590 -0.585070 -0.224570
H 5.301555 -1.914792 0.443407

2-SRSR_c009

C -2.145645 -0.529391 0.461133
C -0.643743 1.500998 0.306236
C -3.091513 1.821296 0.785781
C -1.872543 2.382327 0.057629
C -3.362189 0.402288 0.286247
N -0.898432 0.084565 -0.038974
C 0.154928 -0.783825 -0.184619

C 1.491747 -0.240327 -0.687805
N 1.465800 1.195617 -0.920681
C 0.566044 2.087271 -0.432418
O 0.046331 -1.989453 0.015060
C 2.656343 -0.703342 0.232890
C 2.542754 -0.107309 1.643052
C 4.019697 -0.416438 -0.428216
O 0.698952 3.297900 -0.555863
C -2.463572 -1.806174 -0.320892
O -2.477577 -1.897834 -1.526204
O -2.899638 -2.782082 0.507843
H -0.406111 1.562758 1.383380
H -2.023100 -0.793978 1.519533
H -3.969205 2.453248 0.607870
H -2.915633 1.818473 1.871315
H -2.067728 2.429818 -1.021037
H -1.622046 3.394208 0.383814
H -3.613092 0.435678 -0.780616
H -4.210111 -0.054148 0.809553
H 1.629124 -0.735911 -1.659105
H 2.258706 1.618256 -1.389467
H 2.534254 -1.791250 0.303925
H 2.628572 0.985853 1.623640
H 1.586040 -0.370719 2.108996
H 3.331637 -0.490051 2.297509
H 4.201133 0.668317 -0.451143
H 3.979864 -0.746935 -1.476342
H -3.144447 -3.530814 -0.067906
C 5.206965 -1.105398 0.255201
H 5.353446 -0.749604 1.280510
H 6.135217 -0.912942 -0.293955
H 5.061712 -2.191633 0.295106

2-SRSR_c010

C -1.712181 -0.984017 0.632472
C -0.705032 1.336999 0.330899
C -3.056858 1.118961 1.264354
C -2.172293 1.755418 0.175965
C -2.513092 -0.255756 1.714498
N -0.590288 -0.129025 0.155247

C 0.511020 -0.734449 -0.343869
C 1.723460 0.142248 -0.637304
N 1.269185 1.443107 -1.121577
C 0.193934 2.122625 -0.635782
O 0.562916 -1.959808 -0.544132
C 2.691706 0.249513 0.584426
C 3.903242 1.124673 0.224466
C 3.117549 -1.124098 1.154098
O -0.050385 3.283840 -0.927331
C -2.598981 -1.471824 -0.540982
O -3.770511 -1.188503 -0.643118
O -1.978070 -2.261051 -1.427383
H -0.367054 1.601923 1.345991
H -1.241814 -1.877153 1.060614
H -4.070963 1.006759 0.875903
H -3.111414 1.779361 2.137986
H -2.511598 1.445883 -0.818983
H -2.215077 2.846181 0.199923
H -3.330747 -0.909773 2.029615
H -1.851878 -0.134309 2.581532
H 2.246680 -0.350243 -1.461116
H 1.883605 1.985554 -1.716543
H 2.135278 0.767530 1.379870
H 4.462261 0.713582 -0.624370
H 3.603788 2.146642 -0.029047
H 4.591207 1.186767 1.074681
H 2.229459 -1.661332 1.505992
H 3.726583 -0.924039 2.045963
H -1.029661 -2.377666 -1.164691
C 3.898933 -2.041881 0.204470
H 3.282976 -2.357755 -0.643098
H 4.209510 -2.948978 0.734383
H 4.806527 -1.563808 -0.180848

2-SRSR_c012

C -1.973336 -0.751698 0.676877
C -0.627724 1.335886 0.222213
C -3.146457 1.522448 0.570459
C -1.945155 1.904558 -0.325978
C -2.862332 0.263224 1.414728

N -0.703999 -0.134492 0.275007
C 0.344065 -0.981911 0.061435
C 1.682957 -0.392220 -0.375169
N 1.574648 0.991288 -0.820668
C 0.559840 1.862884 -0.587411
O 0.246902 -2.197418 0.207502
C 2.758246 -0.610528 0.729674
C 2.409265 0.128053 2.029364
C 4.175380 -0.234117 0.251691
O 0.587349 3.026701 -0.967961
C -2.747365 -1.400595 -0.476228
O -3.753831 -2.049980 -0.300199
O -2.223905 -1.171530 -1.700448
H -0.476898 1.726302 1.242352
H -1.738141 -1.585412 1.344994
H -4.028476 1.357532 -0.058696
H -3.399648 2.348874 1.244284
H -2.081250 1.509656 -1.338207
H -1.833118 2.986722 -0.415952
H -3.789288 -0.240696 1.701299
H -2.347436 0.536781 2.343140
H 1.967922 -1.000359 -1.240767
H 2.347164 1.388321 -1.342811
H 2.738405 -1.690388 0.925744
H 2.382828 1.213720 1.876897
H 1.437907 -0.187268 2.426845
H 3.160181 -0.077923 2.799955
H 4.859587 -0.393276 1.095341
H 4.218527 0.844818 0.041919
H -2.796327 -1.653493 -2.327493
C 4.693666 -1.022369 -0.957630
H 4.646416 -2.102718 -0.775969
H 5.737497 -0.765169 -1.168276
H 4.121178 -0.817461 -1.870271

2-SRSR_c015

C -1.707561 -1.027026 0.565304
C -0.605839 1.266673 0.438970
C -2.846818 1.031087 1.611880
C -2.053924 1.765629 0.515009

C -2.337131 -0.413435 1.818142
N -0.596942 -0.167455 0.071008
C 0.404040 -0.749781 -0.628752
C 1.629353 0.105355 -0.939563
N 1.192889 1.471448 -1.214671
C 0.218618 2.129725 -0.527299
O 0.357054 -1.937020 -0.991336
C 2.720746 0.006806 0.177138
C 3.866658 0.986922 -0.116950
C 3.230684 -1.442104 0.333958
O 0.007960 3.327187 -0.648371
C -2.748455 -1.314232 -0.546329
O -3.905014 -0.967765 -0.470752
O -2.280048 -2.005515 -1.593399
H -0.137012 1.384471 1.429732
H -1.246497 -1.989347 0.817428
H -3.902720 1.014665 1.335030
H -2.764580 1.572472 2.561831
H -2.520869 1.605146 -0.463247
H -2.028979 2.844576 0.680388
H -3.151212 -1.066696 2.143809
H -1.576452 -0.435689 2.608407
H 2.045173 -0.303124 -1.865763
H 1.766277 2.058050 -1.808604
H 2.246348 0.310354 1.123536
H 4.352451 0.746932 -1.072290
H 3.517495 2.023183 -0.159232
H 4.631261 0.935647 0.663301
H 3.788645 -1.718912 -0.572251
H 2.379106 -2.128239 0.378550
H -1.316466 -2.197651 -1.463245
C 4.111903 -1.665755 1.569058
H 5.041165 -1.087214 1.532457
H 4.389061 -2.722123 1.653693
H 3.582909 -1.388723 2.489579

2-SRSR_c024

C -1.714021 -0.985801 0.524737
C -0.595721 1.285556 0.541349
C -2.967883 1.048472 1.460151

C -2.035123 1.823551 0.503917
C -2.461182 -0.383810 1.728657
N -0.582350 -0.135960 0.150194
C 0.402874 -0.732596 -0.584175
C 1.633231 0.114681 -0.907051
N 1.242577 1.511563 -1.074876
C 0.303928 2.163269 -0.337687
O 0.333035 -1.908957 -0.931689
C 2.773835 -0.087230 0.146337
C 3.916440 0.910243 -0.102684
C 3.283963 -1.544760 0.146990
O 0.167158 3.379381 -0.359325
C -2.648626 -1.219529 -0.667077
O -2.719372 -0.550369 -1.671097
O -3.443098 -2.291865 -0.435934
H -0.204669 1.386327 1.567708
H -1.317645 -1.968186 0.794659
H -3.974170 1.017107 1.027353
H -3.060769 1.573639 2.417865
H -2.389546 1.731595 -0.526848
H -2.001562 2.887911 0.744049
H -3.281891 -1.052145 2.005695
H -1.759671 -0.382703 2.571533
H 1.992059 -0.247943 -1.875793
H 1.846816 2.121671 -1.612187
H 2.341958 0.129252 1.136332
H 4.724961 0.763336 0.619408
H 4.342939 0.774135 -1.105906
H 3.584940 1.948976 -0.008305
H 3.839333 -1.721383 -0.785847
H 2.431305 -2.229342 0.120502
H -4.017622 -2.380036 -1.219766
C 4.171930 -1.895562 1.347278
H 5.091437 -1.300853 1.378367
H 4.466680 -2.950147 1.310424
H 3.639881 -1.734844 2.293429

2-SRSR_c032

C -1.977427 -0.752405 0.701010
C -0.643871 1.333044 0.129384

C -3.119799 1.554989 0.614035
C -1.987494 1.862772 -0.385992
C -2.821710 0.286436 1.444312
N -0.704286 -0.142573 0.216171
C 0.350094 -0.959609 0.003204
C 1.692612 -0.363682 -0.396518
N 1.565950 0.997802 -0.896875
C 0.524055 1.851863 -0.714111
O 0.269291 -2.194702 0.120983
C 2.729907 -0.521057 0.756857
C 2.318372 0.250447 2.018397
C 4.151487 -0.121420 0.311527
O 0.519724 2.993427 -1.152448
C -2.760078 -1.425930 -0.456457
O -3.856924 -1.057305 -0.809295
O -2.146865 -2.472264 -1.023757
H -0.472487 1.736092 1.140064
H -1.682671 -1.552429 1.390469
H -4.056068 1.426658 0.067991
H -3.253363 2.399206 1.300840
H -2.192363 1.389097 -1.353066
H -1.881872 2.934040 -0.568167
H -3.751978 -0.195961 1.756311
H -2.281247 0.553168 2.361080
H 2.024940 -0.996046 -1.226506
H 2.329579 1.381574 -1.441148
H 2.733387 -1.594524 0.987305
H 1.348221 -0.083084 2.404258
H 3.054689 0.098306 2.814874
H 2.260569 1.328230 1.825435
H 4.810394 -0.234962 1.182014
H 4.171156 0.950818 0.068235
H -1.263599 -2.612800 -0.595943
C 4.730824 -0.933797 -0.853360
H 5.774792 -0.656414 -1.034593
H 4.188425 -0.771830 -1.792745
H 4.704209 -2.008908 -0.639370

2-SRSR_c034

C -1.971765 -0.707235 0.671011

C -0.626732 1.387647 0.246937
C -3.165921 1.548446 0.422257
C -1.910755 1.940732 -0.392827
C -2.911611 0.323046 1.323318
N -0.696980 -0.081884 0.306371
C 0.326416 -0.937908 0.026445
C 1.675477 -0.361435 -0.391891
N 1.603461 1.048857 -0.750395
C 0.602855 1.927609 -0.485988
O 0.198642 -2.156808 0.114752
C 2.751152 -0.671524 0.691043
C 2.437334 0.016223 2.026991
C 4.177689 -0.324184 0.219245
O 0.668413 3.113040 -0.787326
C -2.626226 -1.351721 -0.555627
O -2.422999 -1.065287 -1.712510
O -3.530596 -2.282958 -0.171901
H -0.542695 1.784260 1.271561
H -1.766725 -1.518523 1.374373
H -3.990881 1.339812 -0.267864
H -3.493417 2.383532 1.052053
H -1.975341 1.530119 -1.405038
H -1.805225 3.023882 -0.479562
H -3.848547 -0.175839 1.589139
H -2.447477 0.636275 2.266084
H 1.936104 -0.926687 -1.293627
H 2.396535 1.462193 -1.227275
H 2.693896 -1.758203 0.834808
H 2.457084 1.108121 1.927752
H 1.453477 -0.274881 2.411733
H 3.180165 -0.259976 2.783317
H 4.860438 -0.541543 1.051080
H 4.258210 0.760517 0.054283
H -3.922662 -2.637725 -0.992080
C 4.662104 -1.079201 -1.024851
H 4.581578 -2.163890 -0.885715
H 5.712203 -0.846986 -1.233545
H 4.090123 -0.820124 -1.923805

2-SRSR_c040

C -1.952894 -0.778774 0.696532
C -0.690459 1.375010 0.323349
C -3.216869 1.450959 0.659588
C -2.023323 1.939727 -0.196422
C -2.868891 0.186786 1.470357
N -0.724930 -0.095762 0.275615
C 0.274546 -0.902764 -0.178757
C 1.568026 -0.269166 -0.682275
N 1.465230 1.173055 -0.860249
C 0.480845 2.003625 -0.431400
O 0.167817 -2.127046 -0.185787
C 2.766906 -0.698139 0.213358
C 2.640656 -0.152694 1.642502
C 4.104433 -0.317917 -0.453736
O 0.517521 3.215615 -0.605684
C -2.681921 -1.368217 -0.515854
O -2.595992 -0.986237 -1.659883
O -3.508226 -2.367711 -0.129286
H -0.555786 1.695487 1.368440
H -1.677413 -1.622104 1.335271
H -4.070589 1.249754 0.003216
H -3.538880 2.234265 1.355204
H -2.139987 1.604648 -1.231571
H -1.948443 3.028937 -0.204442
H -3.772198 -0.352950 1.770883
H -2.348257 0.460991 2.395620
H 1.723725 -0.723031 -1.669715
H 2.218020 1.646661 -1.346375
H 2.704471 -1.793427 0.248699
H 2.679611 0.943233 1.655036
H 1.699254 -0.466532 2.107576
H 3.451427 -0.521507 2.278027
H 4.223054 0.775691 -0.449918
H 4.070438 -0.623558 -1.509492
H -3.956463 -2.680121 -0.937838
C 5.337288 -0.954306 0.199244
H 5.479984 -0.610226 1.229096
H 6.245456 -0.701600 -0.359092
H 5.251457 -2.047406 0.220023

2-SRSR_c041

C -1.947499 -0.805250 0.728558
C -0.649030 1.308432 0.179959
C -3.050520 1.511167 0.962368
C -2.032855 1.890607 -0.132136
C -2.684107 0.174817 1.645815
N -0.725746 -0.168799 0.155403
C 0.284608 -0.974500 -0.237497
C 1.588241 -0.357787 -0.726404
N 1.424752 1.036302 -1.114073
C 0.424713 1.882296 -0.748936
O 0.194562 -2.214205 -0.214350
C 2.737707 -0.607131 0.297230
C 2.496201 0.116079 1.629018
C 4.098361 -0.250449 -0.336245
O 0.390501 3.054524 -1.095171
C -2.867478 -1.372941 -0.383586
O -3.991370 -0.968761 -0.575767
O -2.339606 -2.371059 -1.103306
H -0.354637 1.626236 1.192703
H -1.592256 -1.662836 1.312145
H -4.044366 1.437134 0.517312
H -3.089596 2.296390 1.726515
H -2.355329 1.502072 -1.105124
H -1.928646 2.972354 -0.237029
H -3.582197 -0.324175 2.019880
H -2.040284 0.359093 2.514928
H 1.834238 -0.929298 -1.629441
H 2.132237 1.455316 -1.706063
H 2.721706 -1.690470 0.476663
H 2.495073 1.204396 1.495440
H 1.539895 -0.176098 2.078091
H 3.277720 -0.127667 2.354350
H 4.155842 0.836126 -0.495045
H 4.154193 -0.714465 -1.331440
H -1.416397 -2.554531 -0.792304
C 5.313623 -0.702715 0.482192
H 5.369509 -0.194303 1.450351
H 6.242832 -0.484992 -0.055442
H 5.282934 -1.782546 0.670937

2-SRSR_c045

C 2.255479 -0.302201 -0.255181
C 0.756982 1.613047 -0.539932
C 2.953297 1.904000 0.712600
C 1.507646 2.403765 0.556963
C 3.028375 0.376370 0.880800
N 0.859356 0.168560 -0.278677
C -0.074380 -0.504635 0.459802
C -1.506696 0.031202 0.467527
N -1.657828 1.286905 -0.258190
C -0.672169 2.118432 -0.687577
O 0.175615 -1.547333 1.056952
C -2.466898 -1.070317 -0.068334
C -2.153995 -1.444396 -1.524240
C -3.953879 -0.694501 0.100021
O -0.887835 3.226376 -1.161458
C 2.393126 -1.823012 -0.260556
O 3.165993 -2.442991 0.430421
O 1.670436 -2.386273 -1.259205
H 1.237961 1.807244 -1.506333
H 2.683851 0.019596 -1.216945
H 3.427036 2.401255 1.566816
H 3.530594 2.196188 -0.176941
H 0.965825 2.281022 1.505306
H 1.479296 3.467390 0.300101
H 2.592293 0.060421 1.835599
H 4.066838 0.031828 0.874399
H -1.743334 0.192624 1.528548
H -2.590083 1.676881 -0.338146
H -2.264427 -1.940951 0.567044
H -2.298230 -0.589703 -2.195280
H -1.123410 -1.796130 -1.637631
H -2.820053 -2.247414 -1.859413
H -4.544300 -1.530183 -0.297567
H -4.202145 0.161270 -0.546057
H 1.827036 -3.346569 -1.191104
C -4.406385 -0.410259 1.537494
H -4.155928 -1.244676 2.203502
H -5.491434 -0.265239 1.579604

H -3.944769 0.493684 1.952554

2-SRSR_c047

C 2.208651 -0.555089 -0.344124
C 0.997043 1.566652 -0.504341
C 3.309137 1.509056 0.560323
C 1.947644 2.222099 0.524568
C 3.165958 -0.014121 0.723191
N 0.902095 0.119833 -0.252071
C -0.060533 -0.415352 0.558539
C -1.394374 0.324346 0.675438
N -1.408015 1.604769 -0.021904
C -0.345778 2.284835 -0.528084
O 0.076759 -1.490612 1.134053
C -2.546612 -0.611412 0.206831
C -2.414966 -0.984211 -1.276683
C -3.920684 -0.000748 0.553294
O -0.428109 3.421702 -0.974631
C 2.114975 -2.079248 -0.358988
O 2.839329 -2.815677 0.267215
O 1.236299 -2.516600 -1.293430
H 1.418304 1.698724 -1.508476
H 2.599838 -0.289917 -1.338339
H 3.920902 1.919787 1.371722
H 3.849093 1.721071 -0.374251
H 1.473681 2.171917 1.514834
H 2.058812 3.280640 0.269337
H 2.766977 -0.272469 1.711048
H 4.136147 -0.511499 0.630865
H -1.536612 0.496249 1.753169
H -2.272367 2.134355 -0.015441
H -2.419044 -1.519375 0.808823
H -2.494904 -0.097973 -1.917114
H -1.453923 -1.466956 -1.482098
H -3.202922 -1.683560 -1.573101
H -4.127803 0.855340 -0.106110
H -3.886064 0.396182 1.578335
H 1.250160 -3.490154 -1.235925
C -5.087124 -0.991515 0.454265
H -5.226967 -1.359224 -0.567562

H -6.025256 -0.517900 0.763944
H -4.920854 -1.859706 1.103130

2-SRSR_c051

C -1.686874 -0.778025 0.816374
C -0.519848 1.345131 0.056049
C -2.786530 1.522678 1.170794
C -1.946770 1.892922 -0.067428
C -2.301183 0.205193 1.816639
N -0.562508 -0.133434 0.076246
C 0.396734 -0.930307 -0.444863
C 1.615307 -0.297124 -1.107134
N 1.348539 1.075593 -1.516855
C 0.395427 1.914794 -1.031050
O 0.315553 -2.170904 -0.407707
C 2.919056 -0.426523 -0.252367
C 3.406562 -1.881540 -0.186098
C 2.778180 0.225922 1.136120
O 0.286431 3.076523 -1.396648
C -2.746292 -1.366787 -0.152312
O -3.892654 -0.981588 -0.182942
O -2.311037 -2.360600 -0.936561
H -0.093471 1.696214 1.008717
H -1.244413 -1.625827 1.352579
H -3.833768 1.426688 0.878796
H -2.725429 2.322674 1.918167
H -2.397451 1.475566 -0.975256
H -1.881137 2.973455 -0.209739
H -3.126419 -0.300896 2.324919
H -1.540847 0.415471 2.578930
H 1.767918 -0.890542 -2.015957
H 1.965949 1.494961 -2.203092
H 3.668250 0.152920 -0.814924
H 2.712172 -2.510391 0.378138
H 3.498339 -2.312861 -1.189543
H 4.391071 -1.936561 0.288460
H 2.082965 -0.367778 1.746732
H 2.327173 1.219429 1.017386
H -1.350774 -2.529696 -0.757602
C 4.102789 0.388002 1.891650

H 4.558746 -0.577118 2.134765
H 3.946108 0.923407 2.834377
H 4.827089 0.962291 1.301032

2-SRSR_c056

C -1.681394 -0.770722 0.761934
C -0.528389 1.413460 0.240500
C -2.961562 1.439860 1.003002
C -1.939353 1.959254 -0.035326
C -2.472060 0.156030 1.703381
N -0.543783 -0.056850 0.172822
C 0.381345 -0.838654 -0.453408
C 1.591574 -0.170967 -1.100206
N 1.400849 1.262403 -1.285970
C 0.484814 2.072433 -0.696278
O 0.267290 -2.062615 -0.492339
C 2.924700 -0.482479 -0.345467
C 3.363130 -1.938627 -0.558095
C 2.854987 -0.085928 1.142023
O 0.464071 3.284539 -0.871040
C -2.587846 -1.341445 -0.334303
O -2.698494 -0.923733 -1.463622
O -3.320031 -2.371933 0.148657
H -0.221231 1.721695 1.252556
H -1.296822 -1.626166 1.323181
H -3.917766 1.252382 0.502326
H -3.156440 2.201399 1.766811
H -2.225447 1.633607 -1.039971
H -1.883830 3.049640 -0.040802
H -3.308152 -0.408185 2.127920
H -1.811841 0.411163 2.540871
H 1.662073 -0.631764 -2.093020
H 2.067697 1.753560 -1.871481
H 3.673283 0.167419 -0.826939
H 2.648749 -2.634030 -0.109893
H 3.428045 -2.176514 -1.626392
H 4.351031 -2.115374 -0.120958
H 2.192970 -0.786973 1.668980
H 2.393026 0.906953 1.224635
H -3.888615 -2.671095 -0.585838

C 4.217328 -0.046144 1.844917
H 4.695665 -1.030953 1.868267
H 4.109450 0.291155 2.881790
H 4.902366 0.646721 1.340706

2-SRSR_c073

C 2.218821 -0.289934 -0.312921
C 0.716754 1.634185 -0.531712
C 2.953389 1.899326 0.658420
C 1.508147 2.412035 0.546161
C 3.025907 0.368201 0.813981
N 0.827642 0.189193 -0.285818
C -0.071940 -0.478632 0.500642
C -1.516593 0.015526 0.503853
N -1.687417 1.299450 -0.167387
C -0.717951 2.140078 -0.615536
O 0.217064 -1.494724 1.125296
C -2.428746 -1.092956 -0.102754
C -2.060766 -1.408971 -1.559639
C -3.928971 -0.758804 0.030604
O -0.950487 3.259052 -1.054635
C 2.264991 -1.816505 -0.428068
O 1.668617 -2.447159 -1.270666
O 3.155981 -2.370711 0.420851
H 1.159792 1.838015 -1.514078
H 2.623640 0.054801 -1.276254
H 3.454024 2.387148 1.502766
H 3.508900 2.193174 -0.244345
H 0.992802 2.288594 1.509082
H 1.482631 3.477563 0.297198
H 2.613140 0.048847 1.777509
H 4.066044 0.029335 0.778388
H -1.781174 0.124714 1.563952
H -2.622927 1.687009 -0.213684
H -2.223886 -1.979952 0.509456
H -2.197093 -0.531502 -2.202772
H -1.023413 -1.745470 -1.654344
H -2.705706 -2.206650 -1.944986
H -4.485765 -1.596408 -0.409106
H -4.176855 0.109667 -0.598237

H 3.132412 -3.329641 0.241510
C -4.432568 -0.528288 1.460851
H -4.179555 -1.374742 2.110592
H -5.521991 -0.413346 1.473586
H -4.008838 0.375110 1.916149

2-SRSR_c075

C 1.873970 -0.839376 -0.486358
C 1.123918 1.490000 -0.535946
C 3.492512 0.939317 0.223084
C 2.318324 1.923247 0.346593
C 3.053696 -0.519129 0.437623
N 0.758817 0.094227 -0.244102
C -0.172378 -0.231720 0.705263
C -1.307406 0.760075 0.968476
N -1.121149 2.034606 0.282463
C -0.027163 2.475387 -0.392212
O -0.159681 -1.309034 1.294373
C -2.703117 0.157736 0.601535
C -3.161325 -0.892154 1.623251
C -2.744022 -0.346562 -0.854245
O 0.066089 3.605668 -0.853061
C 1.468099 -2.311242 -0.458696
O 2.106904 -3.186539 0.075338
O 0.397887 -2.552734 -1.254341
H 1.425404 1.538976 -1.589297
H 2.180162 -0.655273 -1.527673
H 4.277205 1.207447 0.939806
H 3.938404 1.037020 -0.777666
H 1.978026 1.969136 1.390561
H 2.614594 2.935932 0.055466
H 2.741135 -0.692274 1.473927
H 3.876326 -1.210713 0.232666
H -1.298978 0.930801 2.054737
H -1.856355 2.726919 0.378874
H -3.396255 1.012360 0.676950
H -2.524362 -1.778898 1.590444
H -3.121354 -0.491460 2.643372
H -4.196125 -1.191508 1.428651
H -2.122833 -1.247211 -0.940363

H -2.282082 0.410547 -1.500913
H 0.229706 -3.511175 -1.186863
C -4.156587 -0.640197 -1.372971
H -4.637276 -1.455624 -0.821710
H -4.127132 -0.931287 -2.428828
H -4.802597 0.243274 -1.291518

2-SRSR_c079

C -2.165934 -0.540657 0.399281
C -0.956969 1.588775 0.507302
C -3.299345 1.508471 -0.491216
C -1.943309 2.233018 -0.495159
C -3.153433 -0.016946 -0.652019
N -0.869675 0.141973 0.261229
C 0.052968 -0.387507 -0.600121
C 1.403728 0.315974 -0.713845
N 1.432841 1.615296 -0.051279
C 0.386978 2.305471 0.474868
O -0.130272 -1.438239 -1.207135
C 2.521582 -0.638323 -0.196442
C 2.337487 -0.989096 1.287032
C 3.916525 -0.057788 -0.510189
O 0.482937 3.450980 0.896335
C -1.971152 -2.056187 0.505706
O -1.217759 -2.585084 1.290579
O -2.835078 -2.742929 -0.271165
H -1.341652 1.729371 1.524778
H -2.537022 -0.256230 1.395218
H -3.935986 1.911380 -1.287370
H -3.816076 1.719503 0.456638
H -1.497485 2.183715 -1.498496
H -2.057236 3.291527 -0.241064
H -2.778871 -0.275474 -1.648897
H -4.124054 -0.508649 -0.533122
H 1.571532 0.457654 -1.791502
H 2.299552 2.139977 -0.083366
H 2.394018 -1.551778 -0.790679
H 2.406006 -0.093567 1.916088
H 1.367770 -1.463115 1.470296
H 3.110393 -1.689724 1.617918

H 4.120761 0.799604 0.148185
H 3.918498 0.330907 -1.539228
H -2.651252 -3.686410 -0.102846
C 5.060182 -1.069928 -0.370841
H 5.162343 -1.432961 0.657020
H 6.016068 -0.616588 -0.655874
H 4.896053 -1.939505 -1.018398

2-SRSR_c083

C 2.140117 -0.478115 -0.456731
C 0.595953 1.513251 -0.239375
C 3.067826 1.900646 -0.499267
C 1.787214 2.382296 0.177967
C 3.325946 0.446158 -0.107415
N 0.847060 0.073807 0.003458
C -0.200619 -0.814334 -0.006401
C -1.589365 -0.319961 0.395728
N -1.601380 1.084197 0.776226
C -0.675912 2.022889 0.450847
O -0.055696 -2.003079 -0.271927
C -2.632741 -0.678373 -0.702413
C -2.344830 0.044899 -2.025306
C -4.082322 -0.424796 -0.241883
O -0.832207 3.215057 0.680073
C 2.459555 -1.845407 0.144017
O 3.029882 -2.721471 -0.462806
O 2.212531 -1.902199 1.475103
H 0.440364 1.663619 -1.322513
H 2.103376 -0.635812 -1.542470
H 3.918055 2.524481 -0.200486
H 2.974898 1.991227 -1.591301
H 1.898458 2.338451 1.268745
H 1.545064 3.416148 -0.078084
H 3.504782 0.391211 0.973247
H 4.213522 0.043798 -0.607464
H -1.827409 -0.911565 1.288325
H -2.437529 1.457223 1.210814
H -2.507984 -1.756471 -0.862196
H -3.064946 -0.260065 -2.792382
H -2.422671 1.133035 -1.913985

H -1.344813 -0.193822 -2.405474
H -4.741229 -0.669154 -1.085232
H -4.232072 0.649982 -0.060326
H 2.493717 -2.793138 1.755074
C -4.533594 -1.229258 0.983589
H -3.992125 -0.948439 1.895009
H -4.381548 -2.304054 0.828512
H -5.599127 -1.068522 1.180708

2-SRSR_c105

C 2.145606 -0.462507 -0.401082
C 0.584365 1.526449 -0.255760
C 3.055819 1.922802 -0.497074
C 1.765154 2.412251 0.155099
C 3.318138 0.480688 -0.063805
N 0.842764 0.094922 0.017088
C -0.197086 -0.801821 0.005605
C -1.590363 -0.316270 0.400914
N -1.618694 1.096623 0.747502
C -0.698057 2.037177 0.414036
O -0.038272 -1.990087 -0.255618
C -2.633849 -0.712132 -0.683601
C -2.357152 -0.019126 -2.024942
C -4.084315 -0.461561 -0.224324
O -0.866700 3.232062 0.619182
C 2.423131 -1.776965 0.332491
O 2.325918 -1.940869 1.526242
O 2.961690 -2.691410 -0.505943
H 0.436977 1.656129 -1.342865
H 2.125026 -0.666742 -1.479511
H 3.898814 2.559206 -0.204242
H 2.974476 1.986141 -1.591994
H 1.865032 2.393302 1.247540
H 1.519738 3.438537 -0.127043
H 3.475741 0.452209 1.020952
H 4.219306 0.075038 -0.537580
H -1.816483 -0.889695 1.308554
H -2.459000 1.469629 1.173889
H -2.498679 -1.792509 -0.817139
H -2.441881 1.070827 -1.939433

H -1.356937 -0.260433 -2.402881
H -3.078356 -0.347360 -2.781391
H -4.743847 -0.734934 -1.058279
H -4.244360 0.616106 -0.070835
H 3.171328 -3.468200 0.046011
C -4.522574 -1.237555 1.024029
H -4.361120 -2.314640 0.896741
H -5.588693 -1.081503 1.221823
H -3.979564 -0.928073 1.925141

2-SRSS_c005

C -2.023567 -0.462353 0.556324
C -0.415091 1.471970 0.298823
C -2.756917 1.922140 1.100538
C -1.600404 2.442261 0.250502
C -3.186736 0.552356 0.577289
N -0.808462 0.094708 -0.077873
C 0.156792 -0.828530 -0.398162
C 1.472526 -0.339177 -1.003019
N 1.505119 1.103181 -1.190973
C 0.729800 2.022645 -0.560961
O -0.015722 -2.036099 -0.269804
C 2.688663 -0.897527 -0.207475
C 3.995125 -0.633669 -0.970561
C 2.726874 -0.369143 1.239608
O 0.921499 3.227816 -0.655983
C -2.547366 -1.715707 -0.141346
O -3.046423 -2.645369 0.448300
O -2.570509 -1.591892 -1.490378
H -0.041001 1.457683 1.338024
H -1.788692 -0.773938 1.582405
H -3.602908 2.618089 1.064728
H -2.449280 1.849035 2.153812
H -1.923404 2.561525 -0.791378
H -1.240881 3.416773 0.588166
H -3.573215 0.661660 -0.443238
H -3.987745 0.120075 1.186637
H 1.497717 -0.806385 -1.997027
H 2.264173 1.498852 -1.733535
H 2.520009 -1.980990 -0.171966

H 4.248354 0.434592 -0.984940
H 4.835914 -1.157353 -0.506592
H 3.927625 -0.982315 -2.008523
H 1.747628 -0.548066 1.704957
H 2.875331 0.719451 1.227177
H -2.962093 -2.421260 -1.822103
C 3.800457 -1.019631 2.120766
H 3.691464 -2.110749 2.135828
H 3.719256 -0.663488 3.153648
H 4.813458 -0.787871 1.774809

2-SRSS_c011

C 1.821005 -0.846511 -0.648255
C 0.490347 1.279552 -0.360284
C 2.890878 1.411661 -1.210670
C 1.857112 1.962953 -0.199760
C 2.506601 0.009643 -1.725908
N 0.627772 -0.168530 -0.128208
C -0.312305 -0.962260 0.461187
C -1.568783 -0.308777 1.032362
N -1.453005 1.139732 1.144802
C -0.552886 1.952991 0.534723
O -0.181266 -2.180215 0.549158
C -2.835640 -0.780370 0.258538
C -4.108168 -0.351652 1.004046
C -2.824923 -0.322517 -1.212742
O -0.575170 3.171635 0.655190
C 2.830643 -1.254515 0.430508
O 3.799798 -1.938462 0.188798
O 2.560786 -0.769245 1.662078
H 0.136358 1.447439 -1.390735
H 1.498303 -1.795552 -1.086288
H 3.877908 1.376313 -0.735716
H 2.986741 2.087602 -2.068007
H 2.195600 1.790719 0.827284
H 1.710443 3.038696 -0.313892
H 3.382974 -0.535294 -2.087030
H 1.812880 0.093567 -2.570726
H -1.645006 -0.717028 2.048122
H -2.135536 1.631012 1.710399

H -2.775904 -1.876361 0.278747
H -4.248824 0.736675 0.972574
H -4.998831 -0.805367 0.559706
H -4.075123 -0.660873 2.056004
H -1.866398 -0.609954 -1.665837
H -2.872117 0.774541 -1.251813
H 3.263524 -1.117467 2.243484
C -3.955442 -0.912158 -2.065156
H -3.949601 -2.008255 -2.026726
H -3.842339 -0.616291 -3.114024
H -4.942255 -0.570482 -1.735010

2-SRSS_c012

C -1.920932 -0.762547 0.733454
C -0.477330 1.277110 0.235436
C -2.741685 1.600570 1.341947
C -1.832106 1.992100 0.162717
C -2.462286 0.160304 1.827795
N -0.685939 -0.185237 0.134947
C 0.220826 -1.030195 -0.407781
C 1.567882 -0.442067 -0.817911
N 1.355891 0.901295 -1.349260
C 0.479251 1.811361 -0.840866
O -0.004024 -2.243097 -0.551764
C 2.614874 -0.503928 0.342372
C 2.816369 -1.946968 0.830419
C 3.943152 0.142316 -0.104713
O 0.449788 2.980290 -1.195264
C -2.981999 -1.094924 -0.346274
O -4.075100 -0.577481 -0.376281
O -2.611706 -2.026575 -1.234228
H -0.006057 1.505772 1.205466
H -1.616022 -1.718752 1.175118
H -3.784076 1.689709 1.029931
H -2.589605 2.290869 2.180182
H -2.306867 1.724148 -0.787798
H -1.643540 3.067025 0.129801
H -3.370388 -0.292218 2.235368
H -1.722525 0.172691 2.637898
H 1.924028 -1.072968 -1.638174

H 2.008413 1.270659 -2.029673
H 2.212582 0.096436 1.173352
H 3.249003 -2.568782 0.036697
H 3.497996 -1.973091 1.685424
H 1.877772 -2.416379 1.134667
H 3.738962 1.144927 -0.499137
H 4.361391 -0.444438 -0.936445
H -1.689317 -2.330505 -1.035574
C 4.991023 0.270677 1.007585
H 4.592713 0.829943 1.863114
H 5.872449 0.808832 0.642516
H 5.329530 -0.704243 1.372688

2-SRSS_c016

C -2.037478 -0.447581 0.500152
C -0.410731 1.483635 0.317603
C -2.759873 1.927820 1.099489
C -1.589275 2.462295 0.277994
C -3.190589 0.575913 0.532172
N -0.807399 0.117802 -0.091782
C 0.156559 -0.806413 -0.411861
C 1.475316 -0.315965 -1.008139
N 1.521737 1.130425 -1.160218
C 0.746161 2.042817 -0.520463
O -0.022242 -2.013983 -0.289371
C 2.688475 -0.903802 -0.230286
C 3.995977 -0.627661 -0.987273
C 2.730683 -0.416200 1.230862
O 0.947055 3.248294 -0.589332
C -2.534387 -1.633449 -0.330232
O -2.685017 -1.627604 -1.529647
O -2.951831 -2.640162 0.470648
H -0.046830 1.446529 1.359997
H -1.822341 -0.803586 1.516118
H -3.601147 2.629815 1.070069
H -2.467251 1.825600 2.154658
H -1.898204 2.609427 -0.764438
H -1.228427 3.425768 0.644772
H -3.551942 0.712122 -0.494053
H -4.009524 0.137468 1.113784

H 1.492155 -0.759041 -2.013472
H 2.284284 1.531756 -1.693551
H 2.512797 -1.986706 -0.224432
H 4.257154 0.438633 -0.971452
H 4.833545 -1.170668 -0.539893
H 3.924428 -0.945818 -2.034695
H 1.752036 -0.607638 1.692348
H 2.880148 0.672208 1.248853
H -3.313664 -3.322638 -0.125416
C 3.805500 -1.091999 2.091188
H 3.697349 -2.183225 2.073624
H 3.725348 -0.766984 3.134412
H 4.817971 -0.849435 1.751155

2-SRSS_c018

C -1.638895 -0.997675 0.706230
C -0.850597 1.375038 0.347067
C -3.302841 0.938602 0.916092
C -2.313487 1.699773 -0.000176
C -2.638178 -0.261963 1.616153
N -0.612428 -0.071235 0.210778
C 0.497747 -0.648781 -0.331706
C 1.615873 0.252130 -0.850144
N 1.176772 1.631372 -1.028763
C 0.092111 2.242941 -0.487615
O 0.616957 -1.870312 -0.404114
C 2.911264 0.166126 0.018999
C 2.639313 0.506079 1.490981
C 3.632676 -1.183713 -0.166910
O -0.132659 3.438599 -0.629800
C -2.385747 -1.752078 -0.398681
O -3.060614 -2.731474 -0.176543
O -2.269146 -1.200862 -1.627544
H -0.664056 1.673327 1.390988
H -1.139147 -1.785696 1.276294
H -4.155618 0.594406 0.320058
H -3.712870 1.608198 1.680525
H -2.473845 1.422534 -1.046803
H -2.441126 2.781616 0.072256
H -3.384045 -0.985670 1.957252

H -2.092628 0.072743 2.506348
H 1.858886 -0.151893 -1.840514
H 1.790090 2.257910 -1.538828
H 3.571199 0.948609 -0.389741
H 2.045327 -0.278999 1.974678
H 3.574417 0.604677 2.050387
H 2.102448 1.456374 1.589105
H 3.710625 -1.390973 -1.243147
H 3.012923 -1.986400 0.245872
H -2.782949 -1.776554 -2.225445
C 5.037186 -1.226796 0.446922
H 5.670879 -0.419489 0.057520
H 5.529868 -2.176634 0.211467
H 5.014360 -1.134756 1.538375

2-SRSS_c024

C -1.915483 -0.762339 0.660863
C -0.463391 1.292701 0.376028
C -2.844822 1.551385 1.266750
C -1.804275 2.030051 0.230660
C -2.562491 0.113274 1.748936
N -0.667523 -0.155998 0.193964
C 0.216898 -0.995241 -0.422190
C 1.565664 -0.399741 -0.826042
N 1.394289 0.999231 -1.207153
C 0.556699 1.885576 -0.604696
O -0.031354 -2.184289 -0.603156
C 2.650826 -0.614541 0.281526
C 2.852946 -2.108592 0.578588
C 3.974038 0.071499 -0.119539
O 0.597795 3.089969 -0.818087
C -2.875181 -1.023494 -0.505031
O -2.851909 -0.494873 -1.591775
O -3.813549 -1.931271 -0.144689
H -0.059233 1.482125 1.384670
H -1.672954 -1.743361 1.077755
H -3.843807 1.609736 0.820098
H -2.857440 2.217617 2.137217
H -2.167909 1.843209 -0.783951
H -1.609834 3.100821 0.315778

H -3.475573 -0.376604 2.100126
H -1.869389 0.130778 2.598560
H 1.871795 -0.953679 -1.719327
H 2.076055 1.423425 -1.824375
H 2.280821 -0.120400 1.193969
H 3.278872 -2.622348 -0.292832
H 3.541168 -2.246652 1.417944
H 1.913619 -2.608972 0.822265
H 3.777960 1.124163 -0.355983
H 4.349914 -0.393963 -1.043485
H -4.395946 -2.044380 -0.919458
C 5.066843 0.023274 0.955467
H 4.711237 0.453869 1.899802
H 5.942015 0.600910 0.638053
H 5.403797 -0.998064 1.159231

2-SRSS_c025

C -1.857472 -0.845259 0.534929
C -0.906278 1.486271 0.313294
C -3.322621 1.205624 0.952869
C -2.325431 2.044164 0.157684
C -3.273837 -0.237348 0.451979
N -0.829601 0.050793 -0.040230
C 0.387044 -0.538648 -0.285105
C 1.529379 0.322797 -0.823714
N 1.123826 1.702817 -1.052120
C 0.072635 2.351400 -0.489052
O 0.567222 -1.744327 -0.141798
C 2.823297 0.238957 0.047509
C 2.544699 0.573549 1.519861
C 3.562201 -1.101768 -0.138874
O -0.098174 3.558531 -0.598342
C -1.927159 -2.207050 -0.153347
O -2.150182 -3.239015 0.435168
O -1.910750 -2.110283 -1.504924
H -0.621278 1.600287 1.374193
H -1.608743 -1.057955 1.582663
H -4.336794 1.605779 0.840587
H -3.081091 1.247005 2.024976
H -2.596436 2.043836 -0.905682

H -2.304920 3.086571 0.483185
H -3.604607 -0.266215 -0.593194
H -3.943181 -0.887451 1.025741
H 1.763274 -0.121187 -1.800661
H 1.772781 2.309553 -1.541444
H 3.477899 1.027578 -0.357716
H 1.945038 -0.212982 1.993623
H 3.476544 0.665152 2.085792
H 2.012644 1.526684 1.620097
H 3.628096 -1.315280 -1.215158
H 2.962317 -1.909736 0.290874
H -2.008321 -3.023421 -1.833268
C 4.976891 -1.115612 0.452546
H 5.592120 -0.303918 0.043137
H 5.480171 -2.060934 0.221358
H 4.969901 -1.010335 1.543037

2-SRSS_c030

C -1.872057 -0.839170 0.480468
C -0.914641 1.498011 0.322399
C -3.339242 1.206447 0.922740
C -2.331104 2.059741 0.157423
C -3.283802 -0.225317 0.391135
N -0.834101 0.068978 -0.051052
C 0.385245 -0.519477 -0.282200
C 1.529053 0.342583 -0.815633
N 1.131125 1.729190 -1.017445
C 0.075719 2.371937 -0.455907
O 0.563046 -1.725006 -0.131886
C 2.829833 0.238643 0.042568
C 2.565087 0.551548 1.522262
C 3.561121 -1.101886 -0.172069
O -0.090020 3.581352 -0.546941
C -1.916886 -2.137084 -0.330147
O -1.985574 -2.201093 -1.535443
O -2.051039 -3.209015 0.483828
H -0.642427 1.597289 1.388270
H -1.635783 -1.090499 1.522569
H -4.351639 1.609279 0.803813
H -3.112993 1.226576 1.998814

H -2.587588 2.078680 -0.909233
H -2.314758 3.095893 0.502583
H -3.589594 -0.232215 -0.661765
H -3.968666 -0.884534 0.936671
H 1.750511 -0.087573 -1.801887
H 1.783244 2.340845 -1.496235
H 3.484883 1.030544 -0.355474
H 1.967777 -0.240948 1.988863
H 3.501963 0.633433 2.081466
H 2.035119 1.503816 1.640617
H 3.615987 -1.298221 -1.252138
H 2.961463 -1.913874 0.250163
H -2.142783 -3.980973 -0.105772
C 4.981031 -1.131182 0.406026
H 5.595435 -0.314475 0.005458
H 5.478973 -2.073916 0.153590
H 4.984260 -1.044968 1.498246

2-SRSS_c034

C -1.823889 -0.797403 0.721052
C -0.503888 1.304457 0.184859
C -2.827593 1.534125 1.164887
C -1.887254 1.944302 0.014024
C -2.451032 0.152391 1.745493
N -0.632675 -0.165320 0.081533
C 0.312710 -0.975966 -0.440943
C 1.585753 -0.372421 -1.019460
N 1.450191 1.052202 -1.288177
C 0.515326 1.903235 -0.787803
O 0.184076 -2.212099 -0.475136
C 2.825250 -0.743635 -0.149603
C 4.118096 -0.366349 -0.888357
C 2.750751 -0.139515 1.266337
O 0.499432 3.097162 -1.051814
C -2.849704 -1.276410 -0.339620
O -3.970508 -0.827976 -0.418004
O -2.416963 -2.250032 -1.150496
H -0.125664 1.552807 1.189097
H -1.450663 -1.695385 1.227693
H -3.855751 1.513179 0.799288

H -2.780203 2.276611 1.970243
H -2.297255 1.618979 -0.949083
H -1.754863 3.026625 -0.041195
H -3.331481 -0.340027 2.167227
H -1.732398 0.270849 2.565985
H 1.709171 -0.883599 -1.982151
H 2.120179 1.487666 -1.911189
H 2.785470 -1.837374 -0.061138
H 4.237884 0.722101 -0.961481
H 4.997838 -0.755315 -0.367738
H 4.130914 -0.780848 -1.903756
H 1.781644 -0.399277 1.713890
H 2.778416 0.956400 1.194927
H -1.478011 -2.476981 -0.927655
C 3.859644 -0.616997 2.212264
H 3.874726 -1.711266 2.284449
H 3.703065 -0.219705 3.221062
H 4.851050 -0.288915 1.882847

2-SRSS_c035

C 1.818155 -0.801837 -0.656796
C 0.509276 1.339598 -0.385004
C 2.972916 1.456892 -1.031740
C 1.866741 2.002099 -0.096593
C 2.594636 0.091947 -1.641207
N 0.615584 -0.113785 -0.176325
C -0.298073 -0.895211 0.465422
C -1.561213 -0.247922 1.025961
N -1.490322 1.206973 1.054098
C -0.593669 2.014198 0.431699
O -0.140087 -2.106947 0.595084
C -2.824606 -0.794172 0.296499
C -4.099129 -0.372165 1.042568
C -2.849834 -0.403225 -1.193823
O -0.657581 3.236310 0.484724
C 2.705716 -1.219760 0.520414
O 2.727751 -0.713362 1.618092
O 3.531993 -2.226760 0.153219
H 0.238897 1.530868 -1.435592
H 1.510399 -1.723936 -1.156864

H 3.907882 1.367473 -0.467882
H 3.169486 2.161404 -1.847917
H 2.118457 1.791742 0.947374
H 1.744226 3.082131 -0.199289
H 3.482095 -0.450824 -1.980775
H 1.960233 0.234430 -2.524129
H -1.609683 -0.604201 2.063037
H -2.203213 1.708423 1.571387
H -2.729739 -1.885583 0.365375
H -4.275748 0.708722 0.965661
H -4.981356 -0.872351 0.632330
H -4.041657 -0.633467 2.106344
H -1.886465 -0.673615 -1.646816
H -2.939132 0.688291 -1.281697
H 4.081462 -2.428243 0.934094
C -3.967407 -1.074182 -2.001895
H -3.919254 -2.166296 -1.912259
H -3.879032 -0.823984 -3.064961
H -4.962361 -0.754792 -1.673817

2-SRSS_c040

C 2.049471 -0.677219 -0.395050
C 0.984358 1.515885 -0.616676
C 3.373558 1.355881 0.244195
C 2.068719 2.168752 0.271724
C 3.139330 -0.136544 0.536740
N 0.809446 0.103890 -0.241314
C -0.102827 -0.288597 0.698892
C -1.352818 0.573441 0.890805
N -1.359266 1.771653 0.059950
C -0.302872 2.329803 -0.588711
O 0.011764 -1.325941 1.344556
C -2.624082 -0.297590 0.673471
C -3.884080 0.461162 1.119193
C -2.721466 -0.829292 -0.770407
O -0.349020 3.428869 -1.125627
C 1.844805 -2.186089 -0.280279
O 2.572063 -2.930911 0.332530
O 0.848857 -2.617695 -1.091436
H 1.322380 1.539174 -1.659837

H 2.362894 -0.517270 -1.438184
H 4.085493 1.774039 0.965054
H 3.838342 1.459064 -0.747359
H 1.686616 2.227272 1.300551
H 2.231280 3.194301 -0.074624
H 2.818959 -0.292751 1.573401
H 4.059227 -0.712230 0.396949
H -1.341071 0.865487 1.952409
H -2.180709 2.364547 0.096688
H -2.483831 -1.152885 1.345262
H -4.133295 1.285036 0.436869
H -4.752446 -0.203744 1.142306
H -3.765063 0.877243 2.127111
H -1.772448 -1.312000 -1.034437
H -2.842055 0.015715 -1.461432
H 0.798324 -3.582772 -0.959600
C -3.857044 -1.836919 -0.987767
H -3.774333 -2.682642 -0.293930
H -3.823671 -2.239570 -2.006228
H -4.845486 -1.385428 -0.848397

2-SRSS_c041

C -1.622824 -0.956828 0.708441
C -0.787531 1.379511 0.229590
C -3.242751 1.023287 0.827663
C -2.244778 1.670650 -0.160777
C -2.622126 -0.173903 1.576550
N -0.551210 -0.075188 0.231458
C 0.614670 -0.681027 -0.137182
C 1.762925 0.194975 -0.629822
N 1.300157 1.509370 -1.064552
C 0.169933 2.155817 -0.679638
O 0.761646 -1.900599 -0.079591
C 2.935303 0.300161 0.397396
C 2.498639 0.958943 1.713420
C 3.647432 -1.041997 0.664612
O -0.081027 3.307936 -1.010818
C -2.357686 -1.714282 -0.403282
O -3.173350 -2.578308 -0.171819
O -2.035098 -1.322457 -1.655245

H -0.610159 1.774771 1.243031
H -1.159345 -1.745798 1.307618
H -4.133500 0.697679 0.278556
H -3.586656 1.759696 1.562864
H -2.400917 1.281304 -1.172069
H -2.368137 2.754097 -0.211787
H -3.391993 -0.868970 1.922481
H -2.082749 0.173564 2.465507
H 2.140994 -0.323909 -1.515792
H 1.929199 2.071583 -1.627317
H 3.665636 0.968659 -0.086408
H 1.788086 0.325929 2.259257
H 3.364841 1.114645 2.365682
H 2.033626 1.936312 1.546191
H 2.957352 -1.721982 1.175757
H 4.464638 -0.833633 1.368740
H -2.554000 -1.893065 -2.253821
C 4.217991 -1.743085 -0.573173
H 3.420987 -2.138844 -1.210244
H 4.845723 -2.590694 -0.276718
H 4.841202 -1.066530 -1.172878

2-SRSS_c045

C -1.613234 -0.985047 0.723497
C -0.825881 1.359978 0.137559
C -3.218735 1.019533 0.898296
C -2.303201 1.594230 -0.200591
C -2.567552 -0.185163 1.613935
N -0.554330 -0.094804 0.164292
C 0.622950 -0.652550 -0.193788
C 1.763033 0.247167 -0.652497
N 1.264011 1.526285 -1.144133
C 0.094266 2.134042 -0.812166
O 0.807817 -1.882917 -0.164412
C 2.886225 0.417847 0.421122
C 2.379660 1.102270 1.698263
C 3.627334 -0.893623 0.755423
O -0.209526 3.250644 -1.207409
C -2.361108 -1.757130 -0.394782
O -3.545037 -1.624631 -0.604581

O -1.607284 -2.611595 -1.097960
H -0.625738 1.772077 1.138879
H -1.085619 -1.734789 1.324868
H -4.166784 0.714807 0.451497
H -3.440068 1.792363 1.643933
H -2.514610 1.115687 -1.163783
H -2.451214 2.667301 -0.337199
H -3.333328 -0.869271 1.989547
H -1.994187 0.156927 2.484336
H 2.198924 -0.280497 -1.505879
H 1.872460 2.079189 -1.737376
H 3.613744 1.093707 -0.055518
H 1.667796 0.465857 2.238736
H 3.215716 1.303195 2.376602
H 1.895095 2.060720 1.484624
H 2.938818 -1.584418 1.255294
H 4.402617 -0.640257 1.490855
H -0.672247 -2.578001 -0.770873
C 4.280032 -1.604783 -0.435307
H 3.530810 -2.039895 -1.103841
H 4.916771 -2.425261 -0.086979
H 4.912791 -0.922433 -1.017721

2-SRSS_c051

C -1.635473 -1.022182 0.694731
C -0.814460 1.336859 0.237374
C -3.135291 1.010799 1.196749
C -2.306124 1.647628 0.064273
C -2.468083 -0.273295 1.738846
N -0.600158 -0.121420 0.108585
C 0.511305 -0.684744 -0.414594
C 1.636446 0.213610 -0.915422
N 1.151027 1.553195 -1.221765
C 0.046850 2.166977 -0.718688
O 0.646285 -1.917819 -0.505142
C 2.879991 0.229435 0.031223
C 2.528477 0.706710 1.446802
C 3.624396 -1.121588 0.017014
O -0.239028 3.328790 -0.970818
C -2.518892 -1.670256 -0.403972

O -3.711029 -1.480554 -0.483543
O -1.872864 -2.485777 -1.246482
H -0.509275 1.647832 1.248831
H -1.083350 -1.837908 1.176168
H -4.134219 0.778973 0.822974
H -3.250200 1.722176 2.023166
H -2.626770 1.259646 -0.909376
H -2.422297 2.732807 0.031847
H -3.221791 -0.963458 2.127533
H -1.802225 -0.028547 2.575589
H 1.952718 -0.247547 -1.858116
H 1.726580 2.143534 -1.811893
H 3.551670 0.978310 -0.417877
H 1.999887 1.665861 1.427488
H 1.901012 -0.025274 1.970690
H 3.432112 0.851969 2.045782
H 3.746977 -1.442541 -1.026308
H 3.001861 -1.888181 0.491508
H -0.909728 -2.510352 -1.013220
C 5.002946 -1.074992 0.686535
H 5.642742 -0.307257 0.233189
H 5.514055 -2.037784 0.578163
H 4.934711 -0.861558 1.758773

2-SRSS_c058

C -1.627398 -0.908844 0.705938
C -0.790373 1.428998 0.236811
C -3.277487 1.054461 0.668426
C -2.221020 1.706798 -0.253800
C -2.689193 -0.113217 1.486337
N -0.547236 -0.023656 0.260516
C 0.594214 -0.643568 -0.154264
C 1.761234 0.216477 -0.625729
N 1.333359 1.558351 -1.006965
C 0.215142 2.216318 -0.607202
O 0.707783 -1.868542 -0.136358
C 2.937862 0.254388 0.401814
C 2.517557 0.870985 1.743265
C 3.618636 -1.113516 0.615181
O 0.003121 3.390877 -0.882245

C -2.251201 -1.647077 -0.483476
O -2.234775 -1.292358 -1.639145
O -2.891307 -2.762395 -0.060884
H -0.681369 1.827670 1.257858
H -1.194286 -1.677019 1.351781
H -4.115236 0.699594 0.057927
H -3.692824 1.793766 1.362922
H -2.303592 1.301551 -1.266797
H -2.350608 2.788949 -0.317436
H -3.472771 -0.802613 1.815293
H -2.207555 0.267431 2.395000
H 2.122043 -0.280743 -1.531016
H 1.985619 2.131778 -1.530799
H 3.682922 0.923940 -0.057514
H 1.794478 0.232517 2.265492
H 3.388191 0.982991 2.398663
H 2.072375 1.863459 1.615533
H 2.912595 -1.796229 1.100123
H 4.440869 -0.952431 1.325860
H -3.281348 -3.171801 -0.856203
C 4.172244 -1.778831 -0.649910
H 3.366713 -2.127890 -1.303563
H 4.777506 -2.653706 -0.387703
H 4.813529 -1.094979 -1.221565

2-SRSS_c062

C -1.647248 -0.967254 0.692178
C -0.857323 1.404777 0.345831
C -3.321866 0.968930 0.837593
C -2.307628 1.710111 -0.066054
C -2.680778 -0.230290 1.563972
N -0.604589 -0.041299 0.237279
C 0.493489 -0.622364 -0.324463
C 1.618827 0.271173 -0.838403
N 1.200920 1.660158 -0.986648
C 0.111647 2.272863 -0.456717
O 0.599337 -1.844693 -0.409818
C 2.920525 0.152738 0.017777
C 2.666222 0.475321 1.496822
C 3.621367 -1.203756 -0.194815

O -0.098845 3.472906 -0.583121
C -2.327288 -1.644649 -0.502551
O -2.410234 -1.203859 -1.625492
O -2.897757 -2.810911 -0.121160
H -0.714687 1.714896 1.392869
H -1.173002 -1.762808 1.272705
H -4.164451 0.627930 0.226202
H -3.739438 1.649425 1.588448
H -2.427169 1.390577 -1.105621
H -2.447011 2.792457 -0.030988
H -3.439498 -0.948806 1.889169
H -2.164222 0.107937 2.470113
H 1.846276 -0.119864 -1.837799
H 1.824166 2.287807 -1.483071
H 3.588076 0.931732 -0.385348
H 2.065456 -0.308227 1.974551
H 3.607495 0.553536 2.049161
H 2.142620 1.430969 1.612241
H 3.684539 -1.396865 -1.274562
H 2.995445 -2.003741 0.213722
H -3.331712 -3.175571 -0.915488
C 5.031713 -1.273927 0.402805
H 5.671152 -0.468332 0.019304
H 5.510090 -2.225861 0.147129
H 5.021583 -1.198773 1.495739

2-SRSS_c075

C -1.964789 -0.815800 0.625798
C -0.572138 1.294394 0.319517
C -2.971991 1.502314 1.119373
C -1.938390 1.943182 0.066393
C -2.686839 0.075301 1.639626
N -0.694356 -0.174894 0.185203
C 0.313185 -0.971896 -0.239135
C 1.670163 -0.320217 -0.485234
N 1.472263 1.027204 -1.009177
C 0.498016 1.889158 -0.607049
O 0.169079 -2.194602 -0.403674
C 2.573243 -0.367341 0.788436
C 2.820394 -1.810885 1.254985

C 3.896231 0.408283 0.581266
O 0.468935 3.065269 -0.937542
C -2.863147 -1.197364 -0.578084
O -3.966888 -0.732512 -0.748945
O -2.339250 -2.109566 -1.406810
H -0.252181 1.533754 1.346941
H -1.670548 -1.756687 1.105869
H -3.969357 1.543418 0.677396
H -2.961311 2.195281 1.969127
H -2.271236 1.655054 -0.937164
H -1.800091 3.026167 0.056132
H -3.616419 -0.423192 1.927304
H -2.059359 0.120181 2.538369
H 2.136618 -0.919275 -1.272075
H 2.200585 1.442471 -1.577602
H 2.025679 0.158697 1.584908
H 3.312941 -2.406925 0.478968
H 3.465653 -1.812421 2.140718
H 1.890247 -2.324736 1.509868
H 4.435719 0.391918 1.537029
H 3.667470 1.463726 0.387869
H -1.435514 -2.367589 -1.091550
C 4.823156 -0.121577 -0.521223
H 5.129643 -1.156621 -0.337834
H 5.733045 0.485681 -0.575332
H 4.355492 -0.089089 -1.513369

2-SRSS_c077

C 2.008454 -0.642145 -0.440088
C 0.924212 1.547552 -0.621456
C 3.334150 1.390482 0.186386
C 2.028355 2.200780 0.242526
C 3.113958 -0.106229 0.479312
N 0.772375 0.133418 -0.249816
C -0.091457 -0.259818 0.736626
C -1.372423 0.551743 0.924408
N -1.402997 1.770301 0.123098
C -0.370026 2.347944 -0.545717
O 0.085304 -1.269116 1.411891
C -2.604920 -0.363350 0.657944

C -3.902510 0.346101 1.075891
C -2.640858 -0.881487 -0.793905
O -0.440298 3.455136 -1.063337
C 1.715409 -2.145033 -0.406229
O 0.858893 -2.679911 -1.072086
O 2.609834 -2.827511 0.339612
H 1.229950 1.582206 -1.674119
H 2.306058 -0.459298 -1.483448
H 4.059371 1.808913 0.893828
H 3.778926 1.496945 -0.813954
H 1.669209 2.257039 1.279729
H 2.182661 3.227289 -0.104728
H 2.814693 -0.265660 1.521372
H 4.040026 -0.667103 0.318854
H -1.394522 0.819669 1.991398
H -2.232496 2.349944 0.181370
H -2.453752 -1.220929 1.325024
H -4.159453 1.169335 0.395720
H -4.747462 -0.348579 1.065272
H -3.827444 0.753259 2.091861
H -1.673999 -1.340396 -1.033551
H -2.761258 -0.030933 -1.478575
H 2.356777 -3.766913 0.263797
C -3.743861 -1.913487 -1.059079
H -3.661612 -2.765377 -0.372939
H -3.664219 -2.303966 -2.079500
H -4.747858 -1.488584 -0.948743

2-SRSS_c080

C 1.895426 -0.867126 -0.346821
C 1.242383 1.495038 -0.377626
C 3.389888 0.782768 0.799524
C 2.248605 1.810261 0.755642
C 2.867004 -0.663045 0.819739
N 0.784564 0.099415 -0.273970
C -0.342429 -0.247555 0.420800
C -1.490613 0.757483 0.473416
N -1.101837 2.093524 0.030571
C 0.119399 2.523686 -0.379140
O -0.489286 -1.357178 0.927515

C -2.727865 0.263870 -0.346764
C -2.381474 0.041711 -1.825936
C -3.431088 -0.971915 0.249767
O 0.347329 3.681792 -0.705101
C 1.442903 -2.316219 -0.511207
O 1.926365 -3.254655 0.075877
O 0.552823 -2.452842 -1.524529
H 1.749473 1.606344 -1.343790
H 2.418569 -0.630966 -1.286444
H 4.021528 0.969455 1.675580
H 4.032127 0.920716 -0.082711
H 1.704568 1.804146 1.710473
H 2.630440 2.824750 0.604686
H 2.339782 -0.882046 1.755477
H 3.689310 -1.380262 0.740025
H -1.784116 0.810288 1.528570
H -1.818194 2.811780 0.028740
H -3.442815 1.101261 -0.285301
H -1.690070 -0.799502 -1.948725
H -3.289482 -0.183590 -2.396240
H -1.919712 0.929128 -2.271254
H -2.771247 -1.840250 0.159009
H -4.306461 -1.171483 -0.383400
H 0.340043 -3.403964 -1.563391
C -3.889335 -0.833922 1.705823
H -3.039423 -0.821459 2.395884
H -4.521559 -1.682523 1.989690
H -4.476538 0.080461 1.863501

2-SRSS_c084

C 1.891555 -0.982861 -0.375818
C 1.396017 1.413215 -0.432280
C 3.543175 0.590086 0.666007
C 2.469164 1.689521 0.646977
C 2.931262 -0.819351 0.737961
N 0.850840 0.055940 -0.267794
C -0.249655 -0.198874 0.505254
C -1.305630 0.900616 0.638507
N -0.880699 2.172428 0.062175
C 0.342165 2.511223 -0.422797

O -0.443390 -1.291041 1.031933
C -2.674194 0.469431 0.019457
C -2.522649 0.035991 -1.445638
C -3.407790 -0.567624 0.892640
O 0.620014 3.637485 -0.814085
C 1.340611 -2.403060 -0.483687
O 1.792983 -3.358030 0.101766
O 0.395021 -2.503595 -1.449477
H 1.866813 1.462393 -1.421453
H 2.379399 -0.799562 -1.345555
H 4.222504 0.750838 1.510995
H 4.154881 0.670164 -0.244637
H 1.970269 1.741150 1.624887
H 2.909452 2.672796 0.453714
H 2.437880 -0.989852 1.701815
H 3.702466 -1.588345 0.633590
H -1.458281 1.028302 1.719968
H -1.549174 2.935346 0.074477
H -3.282707 1.389270 0.038240
H -1.967282 -0.905266 -1.524078
H -3.501523 -0.107442 -1.913030
H -1.987985 0.794042 -2.027976
H -3.369492 -0.233742 1.939139
H -2.865299 -1.517143 0.861099
H 0.122517 -3.440159 -1.455608
C -4.874074 -0.777600 0.495982
H -5.434505 0.166066 0.514836
H -5.365000 -1.467563 1.191228
H -4.972679 -1.202711 -0.508819

6-c01

C 1.874748 1.570511 -0.157148
C 2.554405 -1.154675 0.185586
C 3.180721 1.180260 0.106947
C 0.866836 0.573711 -0.254961
C 1.230713 -0.778729 -0.079570
C 3.529289 -0.171951 0.278495
C 0.219603 -1.843301 -0.170341
O -1.082004 -1.436750 -0.438645
C -1.433131 -0.123380 -0.620141

C -0.521253 0.869841 -0.527450
C 1.542256 3.033077 -0.335736
O 4.842804 -0.440480 0.533486
O 0.421691 -3.028036 -0.032826
C -2.904465 0.036805 -0.848244
C -3.717032 -0.018070 0.469339
O -3.364071 1.065757 1.323887
C -5.214051 0.091853 0.213927
H 2.783368 -2.209079 0.312244
H 3.969608 1.922657 0.186758
H -0.849517 1.890083 -0.684029
H 2.435243 3.653243 -0.218803
H 0.802279 3.373052 0.399478
H 1.124966 3.234712 -1.330182
H 4.956257 -1.399193 0.630641
H -3.249077 -0.756440 -1.522465
H -3.093834 1.003000 -1.328597
H -3.502548 -0.978768 0.964773
H -2.405598 1.018134 1.474905
H -5.446804 1.033262 -0.296377
H -5.756513 0.076485 1.164017
H -5.567023 -0.740795 -0.403797

6-c02

C 2.170002 1.525461 -0.019332
C 2.441214 -1.290596 -0.058524
C 3.412089 0.921703 -0.159020
C 1.016392 0.704729 0.107293
C 1.178966 -0.697496 0.084895
C 3.558324 -0.477684 -0.179434
C 0.015660 -1.584341 0.203929
O -1.217372 -0.958153 0.371546
C -1.379178 0.409448 0.390970
C -0.319738 1.233169 0.257648
C 2.057784 3.031662 -0.003202
O 4.826532 -0.960991 -0.322187
O 0.025143 -2.793306 0.170635
C -2.815052 0.803161 0.555994
C -3.770903 0.169376 -0.488207
O -3.984550 -1.210524 -0.231070

C -5.141450 0.836621 -0.457698
H 2.512037 -2.374589 -0.072001
H 4.308347 1.527494 -0.256911
H -0.489745 2.302505 0.272625
H 3.041009 3.497575 -0.112393
H 1.619559 3.394400 0.934890
H 1.423230 3.398669 -0.819528
H 4.797350 -1.930828 -0.321178
H -2.873826 1.895872 0.502539
H -3.173785 0.499507 1.549607
H -3.327328 0.310380 -1.489423
H -3.114182 -1.636546 -0.159069
H -5.579326 0.764105 0.544258
H -5.812303 0.330550 -1.158377
H -5.073714 1.893432 -0.738315

6-c03

C 1.998474 1.551244 -0.097572
C 2.513166 -1.220037 0.137804
C 3.280676 1.072904 0.134994
C 0.928883 0.622789 -0.218852
C 1.211634 -0.754748 -0.097206
C 3.547139 -0.303492 0.253511
C 0.136622 -1.750488 -0.213365
O -1.136115 -1.255048 -0.457268
C -1.409861 0.084818 -0.567359
C -0.439838 1.014355 -0.459652
C 1.753885 3.036970 -0.216472
O 4.845620 -0.661834 0.482106
O 0.266033 -2.950947 -0.120139
C -2.867118 0.331082 -0.811346
C -3.764222 -0.086138 0.364691
O -3.398376 0.756633 1.459149
C -5.248499 0.057168 0.025137
H 2.677841 -2.290511 0.223965
H 4.114379 1.762612 0.231682
H -0.710219 2.059140 -0.544505
H 2.686334 3.596541 -0.100516
H 1.053115 3.393274 0.548752
H 1.326670 3.299576 -1.192331

H 4.897735 -1.628614 0.544467
H -3.181176 -0.227237 -1.703039
H -3.021714 1.397194 -1.009531
H -3.545356 -1.137166 0.606857
H -3.876705 0.445374 2.243059
H -5.482493 1.094131 -0.241084
H -5.869575 -0.219970 0.886036
H -5.531779 -0.593344 -0.810480

6-c04

C 2.109572 1.471973 -0.034318
C 2.267257 -1.350483 0.084553
C 3.320254 0.824571 0.170419
C 0.930460 0.693286 -0.188325
C 1.036173 -0.713037 -0.124214
C 3.410090 -0.578444 0.230449
C -0.156131 -1.557219 -0.267099
O -1.356389 -0.889512 -0.498717
C -1.461749 0.482868 -0.562311
C -0.376591 1.268361 -0.407289
C 2.058184 2.980526 -0.090930
O 4.651544 -1.106417 0.436004
O -0.194673 -2.764395 -0.201790
C -2.871383 0.924569 -0.812860
C -3.920776 0.365911 0.186161
O -4.189838 -1.008926 -0.050222
C -3.564437 0.633756 1.651478
H 2.294113 -2.435667 0.127617
H 4.235118 1.397744 0.290217
H -0.503151 2.342608 -0.458154
H 3.053435 3.410352 0.052089
H 1.403109 3.392212 0.686926
H 1.677194 3.336490 -1.056237
H 4.584356 -2.074158 0.456217
H -3.181355 0.602492 -1.816114
H -2.892666 2.020069 -0.797156
H -4.865105 0.874467 -0.042358
H -3.341827 -1.482596 -0.013711
H -2.636243 0.123522 1.934384
H -4.365110 0.260810 2.297096

H -3.432557 1.705839 1.842685

6-c05

C -2.009285 1.549330 -0.090624
C -2.503384 -1.227142 0.131392
C -3.288697 1.060067 0.135126
C -0.932577 0.629362 -0.210914
C -1.205021 -0.750747 -0.096963
C -3.545007 -0.318783 0.247255
C -0.121684 -1.737910 -0.214256
O 1.149271 -1.231852 -0.451664
C 1.414076 0.110449 -0.560086
C 0.434729 1.031665 -0.445371
C -1.776690 3.037383 -0.205602
O -4.840818 -0.687479 0.469850
O -0.241971 -2.938808 -0.123515
C 2.864711 0.374151 -0.817455
C 3.805816 -0.114986 0.298034
O 5.121935 0.105328 -0.214324
C 3.596895 0.616406 1.623857
H -2.660265 -2.299191 0.211844
H -4.128232 1.742785 0.230407
H 0.693662 2.079007 -0.537955
H -2.714366 3.588727 -0.093214
H -1.347302 3.305399 -1.178963
H -1.083223 3.399346 0.563759
H -4.887688 -1.654993 0.525361
H 3.016268 1.448887 -0.965424
H 3.168666 -0.130963 -1.743180
H 3.631876 -1.191535 0.444671
H 5.751874 -0.225410 0.444589
H 3.768204 1.691593 1.496793
H 4.297519 0.247206 2.383417
H 2.582375 0.466161 2.008758

6-c06

C -1.773526 1.575499 -0.105005
C -2.447912 -1.158679 0.164218
C -3.070448 1.178021 0.188922
C -0.770212 0.581868 -0.271974

C -1.132113 -0.775406 -0.131986
C -3.416198 -0.179316 0.324412
C -0.126755 -1.835586 -0.292109
O 1.163430 -1.420494 -0.589155
C 1.513212 -0.098620 -0.725617
C 0.606171 0.888405 -0.579367
C -1.442313 3.042597 -0.242441
O -4.722354 -0.455704 0.614537
O -0.326371 -3.025890 -0.189073
C 2.975417 0.069089 -1.020541
C 3.863022 0.302021 0.218365
O 3.518399 1.597826 0.712622
C 3.722370 -0.769854 1.298563
H -2.674615 -2.216781 0.261494
H -3.854492 1.918139 0.321652
H 0.940755 1.912738 -0.678038
H -2.329476 3.660424 -0.077096
H -1.053801 3.276962 -1.241362
H -0.678135 3.353429 0.480585
H -4.832136 -1.417399 0.680703
H 3.112753 0.930390 -1.682728
H 3.331704 -0.821396 -1.549491
H 4.905933 0.309109 -0.140816
H 3.989597 1.730328 1.549719
H 2.705409 -0.784537 1.702248
H 4.416658 -0.572069 2.125702
H 3.950726 -1.765478 0.903352

6-c07

C -1.814689 1.553124 -0.105697
C -2.404415 -1.201171 0.163735
C -3.098076 1.115833 0.192551
C -0.783170 0.590250 -0.275224
C -1.102607 -0.777526 -0.136684
C -3.401703 -0.251280 0.329233
C -0.067167 -1.807655 -0.307165
O 1.212238 -1.353613 -0.607117
C 1.521788 -0.024567 -0.746081
C 0.584838 0.936792 -0.584856
C -1.530059 3.029782 -0.246281

O -4.696412 -0.566652 0.624400
O -0.230564 -3.002461 -0.209214
C 2.976820 0.202988 -1.027921
C 3.836774 0.396608 0.251700
O 3.422154 1.559711 0.962647
C 3.882553 -0.833389 1.158730
H -2.599114 -2.265698 0.259393
H -3.904022 1.831518 0.327366
H 0.879530 1.970863 -0.714972
H -2.436584 3.619211 -0.083610
H -1.148372 3.274209 -1.245359
H -0.778190 3.368592 0.477367
H -4.779265 -1.531094 0.690892
H 3.081608 1.109428 -1.632685
H 3.365058 -0.640904 -1.609344
H 4.853462 0.630152 -0.084206
H 2.517479 1.391904 1.276637
H 2.885397 -1.089520 1.535444
H 4.531817 -0.633761 2.016850
H 4.266539 -1.709502 0.624274

6-c08

C 1.876240 1.556980 -0.160680
C 2.547991 -1.172654 0.188116
C 3.182954 1.158999 0.104864
C 0.868150 0.565273 -0.255953
C 1.229403 -0.790428 -0.077320
C 3.528061 -0.192392 0.279298
C 0.210683 -1.851311 -0.166777
O -1.089907 -1.437463 -0.436574
C -1.434676 -0.123061 -0.620060
C -0.519117 0.866517 -0.528895
C 1.551740 3.021077 -0.341699
O 4.807780 -0.589412 0.539547
O 0.403537 -3.035989 -0.027671
C -2.905342 0.043729 -0.848350
C -3.717668 -0.005882 0.469518
O -3.358277 1.076865 1.323027
C -5.214194 0.111834 0.214805
H 2.794043 -2.219735 0.319872

H 3.961548 1.917466 0.179310
H -0.843663 1.887711 -0.687118
H 2.447141 3.638640 -0.226293
H 0.813747 3.366418 0.392902
H 1.135300 3.223458 -1.336271
H 5.383967 0.189927 0.574904
H -3.253586 -0.748864 -1.521463
H -3.090500 1.010200 -1.329837
H -3.507999 -0.967202 0.965673
H -2.400040 1.023250 1.473622
H -5.442252 1.054127 -0.296022
H -5.756325 0.099855 1.165141
H -5.571794 -0.719335 -0.402245

6-c09

C -1.992772 1.550157 -0.119310
C -2.513400 -1.216859 0.155915
C -3.275891 1.077863 0.120736
C -0.925689 0.617378 -0.226914
C -1.211331 -0.757721 -0.086235
C -3.545437 -0.296114 0.259437
C -0.138967 -1.758013 -0.191368
O 1.136831 -1.268855 -0.439444
C 1.414078 0.068981 -0.574095
C 0.444154 1.002011 -0.475556
C -1.745980 3.033493 -0.262112
O -4.843707 -0.647429 0.494044
O -0.271239 -2.956240 -0.083940
C 2.870460 0.306718 -0.823840
C 3.796670 -0.090084 0.353790
O 5.161400 0.046157 -0.041245
C 3.610067 0.797586 1.576642
H -2.680583 -2.285618 0.256647
H -4.108175 1.770532 0.207260
H 0.712767 2.044738 -0.590266
H -2.677217 3.596201 -0.152676
H -1.321243 3.280272 -1.243138
H -1.043363 3.401684 0.495845
H -4.900103 -1.613062 0.569898
H 3.034880 1.363155 -1.061296

H 3.171252 -0.278753 -1.704999
H 3.581075 -1.133997 0.626175
H 5.339000 -0.613657 -0.729859
H 3.841036 1.839518 1.326184
H 4.287225 0.481155 2.375496
H 2.581382 0.746398 1.946865

6-c10

C 2.000072 1.537835 -0.100774
C 2.506058 -1.238003 0.139466
C 3.282281 1.051117 0.132845
C 0.930470 0.614653 -0.219993
C 1.210153 -0.766158 -0.095649
C 3.545213 -0.324489 0.253707
C 0.127446 -1.757451 -0.210620
O -1.143568 -1.254355 -0.455734
C -1.410696 0.086436 -0.567341
C -0.436969 1.011790 -0.461190
C 1.763915 3.024798 -0.221355
O 4.802769 -0.807544 0.483185
O 0.247308 -2.957380 -0.115955
C -2.866934 0.339259 -0.811120
C -3.765339 -0.074844 0.364964
O -3.397431 0.767522 1.459260
C -5.249239 0.072424 0.025431
H 2.687585 -2.302490 0.230361
H 4.106996 1.757303 0.225373
H -0.703202 2.057570 -0.547237
H 2.698766 3.581352 -0.106973
H 1.065710 3.386178 0.543746
H 1.337478 3.288768 -1.197101
H 5.423279 -0.064485 0.539974
H -3.183361 -0.217672 -1.702850
H -3.017326 1.406055 -1.009025
H -3.549273 -1.126249 0.607626
H -3.872114 0.453856 2.244412
H -5.480404 1.109924 -0.241237
H -5.870997 -0.202568 0.886512
H -5.534346 -0.577688 -0.809879

6-c11

C -2.169809 1.513613 0.017163
 C -2.434263 -1.306041 0.058287
 C -3.411875 0.902419 0.156726
 C -1.017348 0.697344 -0.107873
 C -1.177786 -0.707979 -0.084279
 C -3.555712 -0.495845 0.178150
 C -0.008117 -1.590782 -0.202041
 O 1.223030 -0.958000 -0.370730
 C 1.379355 0.409986 -0.390750
 C 0.317486 1.230143 -0.258030
 C -2.064907 3.020364 0.000426
 O -4.771244 -1.101284 0.315280
 O -0.009219 -2.798359 -0.167087
 C 2.813815 0.809054 -0.555654
 C 3.771748 0.177961 0.488321
 O 3.990444 -1.200808 0.230311
 C 5.139914 0.850186 0.458535
 H -2.523724 -2.385866 0.074765
 H -4.299767 1.526476 0.252447
 H 0.484364 2.300001 -0.273507
 H -3.049713 3.483837 0.109124
 H -1.628176 3.384973 -0.937557
 H -1.432308 3.390877 0.816590
 H -5.460485 -0.423102 0.390015
 H 2.868986 1.901971 -0.501902
 H 3.173577 0.506712 -1.549298
 H 3.327474 0.316816 1.489555
 H 3.121599 -1.630069 0.158296
 H 5.578250 0.779791 -0.543376
 H 5.812423 0.346050 1.159026
 H 5.068409 1.906612 0.739754

6-c12

C 2.109809 1.459776 -0.037255
 C 2.259205 -1.365961 0.084520
 C 3.319921 0.804469 0.167689
 C 0.931566 0.686046 -0.189168
 C 1.034329 -0.723308 -0.123405
 C 3.406666 -0.597294 0.229297

C -0.164595 -1.562693 -0.264947
 O -1.362449 -0.887999 -0.497475
 C -1.461706 0.484560 -0.561808
 C -0.373832 1.265942 -0.407810
 C 2.066458 2.968581 -0.094852
 O 4.590560 -1.245977 0.430353
 O -0.212036 -2.768085 -0.198159
 C -2.869624 0.932111 -0.811954
 C -3.921001 0.376615 0.186786
 O -4.195620 -0.996751 -0.050858
 C -3.563219 0.641665 1.652302
 H 2.304359 -2.447635 0.131623
 H 4.227541 1.395770 0.284122
 H -0.496732 2.340611 -0.459352
 H 3.063492 3.395489 0.047063
 H 1.414099 3.384355 0.683012
 H 1.686668 3.326092 -1.059982
 H 5.302992 -0.593633 0.516736
 H -3.180916 0.611583 -1.815302
 H -2.886873 2.027704 -0.795669
 H -4.863337 0.889281 -0.040943
 H -3.349447 -1.473878 -0.015259
 H -2.637102 0.127322 1.934489
 H -4.365248 0.271322 2.297736
 H -3.427005 1.713068 1.844471

6-c13

C 2.088761 1.549354 0.034716
 C 2.490075 -1.250922 0.060373
 C 3.352803 1.003274 0.210409
 C 0.979874 0.676210 -0.134463
 C 1.206466 -0.716703 -0.118233
 C 3.563207 -0.387899 0.224411
 C 0.088561 -1.655628 -0.287581
 O -1.166183 -1.091544 -0.475965
 C -1.388086 0.262945 -0.488344
 C -0.374380 1.139296 -0.326060
 C 1.905788 3.048719 0.025121
 O 4.847997 -0.813882 0.404194
 O 0.166068 -2.863653 -0.277257

C -2.829708 0.612483 -0.696409
 C -3.756271 0.331750 0.505108
 O -4.949249 1.065072 0.212604
 C -4.062217 -1.148589 0.725639
 H 2.610999 -2.330598 0.065622
 H 4.216110 1.649372 0.341699
 H -0.596091 2.199050 -0.346891
 H 2.862893 3.559598 0.162153
 H 1.233703 3.379518 0.826806
 H 1.474517 3.397209 -0.921534
 H 4.862519 -1.783945 0.392545
 H -3.219035 0.076715 -1.571708
 H -2.898189 1.683402 -0.910906
 H -3.277015 0.744348 1.409066
 H -5.604601 0.839975 0.891314
 H -4.550237 -1.568197 -0.161207
 H -4.738653 -1.274693 1.581569
 H -3.155234 -1.725430 0.924750

6-c14

C 1.568050 -1.633177 -0.023813
 C 2.788477 0.918852 -0.023317
 C 2.948727 -1.493929 -0.061017
 C 0.759220 -0.464599 0.014291
 C 1.392458 0.796376 0.014222
 C 3.565334 -0.229219 -0.061207
 C 0.593626 2.029473 0.055846
 O -0.783591 1.869111 0.078343
 C -1.397653 0.639135 0.079104
 C -0.684357 -0.505006 0.056187
 C 0.944485 -3.008797 -0.024756
 O 4.930859 -0.209671 -0.099005
 O 1.030244 3.159057 0.067193
 C -2.892545 0.805689 0.118778
 C -3.725090 -0.405636 -0.328975
 O -3.523256 -1.547504 0.510405
 C -5.212556 -0.059812 -0.423693
 H 3.226576 1.913092 -0.021179
 H 3.588151 -2.371601 -0.091066
 H -1.218996 -1.444396 0.090525

H 1.713253 -3.786054 -0.056596
H 0.286120 -3.153390 -0.890142
H 0.335220 -3.177114 0.871734
H 5.231276 0.712829 -0.094580
H -3.144014 1.665034 -0.515915
H -3.199049 1.099408 1.136533
H -3.367528 -0.732766 -1.311819
H -3.801269 -1.303573 1.408707
H -5.596761 0.285140 0.545783
H -5.781944 -0.945403 -0.721151
H -5.394147 0.734747 -1.156217

6-c17

C -1.818504 1.538234 -0.110018
C -2.396059 -1.221237 0.165678
C -3.101782 1.091354 0.189190
C -0.785456 0.581819 -0.276373
C -1.100119 -0.789661 -0.134530
C -3.399950 -0.275307 0.329031
C -0.055645 -1.814485 -0.303609
O 1.221849 -1.351360 -0.604764
C 1.523083 -0.020942 -0.745659
C 0.581110 0.935363 -0.586131
C -1.544079 3.016634 -0.252914
O -4.656662 -0.719749 0.623346
O -0.208065 -3.009216 -0.204227
C 2.976829 0.215302 -1.027595
C 3.835440 0.413398 0.252208
O 3.412033 1.572587 0.964742
C 3.890062 -0.817426 1.157582
H -2.606230 -2.279408 0.267736
H -3.899208 1.822471 0.318349
H 0.870508 1.970739 -0.717874
H -2.453998 3.602108 -0.092690
H -1.162834 3.262063 -1.251828
H -0.795463 3.362093 0.470861
H -5.253165 0.040231 0.708100
H 3.076305 1.122542 -1.632090
H 3.369926 -0.626180 -1.609230
H 4.850425 0.654947 -0.083213

H 2.507849 1.397786 1.276393
H 2.894698 -1.081918 1.533125
H 4.537307 -0.614092 2.016368
H 4.281064 -1.689764 0.622055

6-c18

C 2.040632 1.563716 0.032052
C 2.501004 -1.227567 0.060079
C 3.312937 1.044278 0.227709
C 0.953584 0.667355 -0.156418
C 1.209306 -0.720585 -0.138253
C 3.552680 -0.342153 0.243015
C 0.115080 -1.683442 -0.328007
O -1.150397 -1.146713 -0.527573
C -1.399080 0.203095 -0.545376
C -0.406723 1.101502 -0.370621
C 1.825836 3.058843 0.022487
O 4.843080 -0.740924 0.443003
O 0.220257 -2.889292 -0.325642
C -2.848924 0.519368 -0.753113
C -3.743839 0.402736 0.509279
O -5.015835 0.992071 0.239512
C -3.895754 -1.022332 1.037210
H 2.644877 -2.304409 0.065505
H 4.159936 1.708366 0.374540
H -0.650600 2.156413 -0.398105
H 2.769670 3.589556 0.175070
H 1.134862 3.373369 0.814583
H 1.401775 3.400317 -0.929973
H 4.878440 -1.710463 0.431924
H -3.249783 -0.140888 -1.534969
H -2.936529 1.549358 -1.112466
H -3.309288 1.037559 1.290172
H -5.495386 0.388011 -0.350774
H -4.331495 -1.675105 0.268451
H -4.559414 -1.024625 1.907752
H -2.934333 -1.457474 1.323636

6-c19

C 1.994613 1.552455 -0.101375

C 2.509721 -1.217719 0.142034
C 3.276160 1.075531 0.138209
C 0.926289 0.623299 -0.224610
C 1.209298 -0.753763 -0.099629
C 3.542771 -0.300277 0.261562
C 0.136317 -1.751386 -0.223228
O -1.137445 -1.256825 -0.468084
C -1.411576 0.081392 -0.579379
C -0.442557 1.012510 -0.470429
C 1.750477 3.037935 -0.225254
O 4.839875 -0.657264 0.497434
O 0.268063 -2.951424 -0.137216
C -2.869821 0.324066 -0.815429
C -3.762656 -0.095426 0.375552
O -3.398417 0.599301 1.565656
C -5.247866 0.078228 0.056470
H 2.674606 -2.287961 0.230332
H 4.108987 1.765956 0.237058
H -0.709910 2.057472 -0.566546
H 2.682955 3.597630 -0.110541
H 1.050191 3.397438 0.539124
H 1.324116 3.297972 -1.202222
H 4.892264 -1.623664 0.565650
H -3.187846 -0.234600 -1.706413
H -3.024064 1.389734 -1.029746
H -3.558497 -1.146850 0.601570
H -3.617704 1.536766 1.437115
H -5.477017 1.125674 -0.184999
H -5.852424 -0.212364 0.921027
H -5.549291 -0.534585 -0.800687

6-c20

C -1.579848 -1.632397 -0.001873
C -2.784631 0.925824 0.051623
C -2.958587 -1.485986 0.064748
C -0.764375 -0.468491 -0.042310
C -1.390278 0.795967 -0.015870
C -3.567508 -0.217836 0.092196
C -0.585480 2.024801 -0.060832
O 0.789725 1.856989 -0.116711

C 1.396977 0.624333 -0.143167
C 0.677397 -0.515836 -0.113028
C -0.964659 -3.011437 -0.032158
O -4.932190 -0.190879 0.157828
O -1.015748 3.156973 -0.047669
C 2.892052 0.778746 -0.223674
C 3.717929 -0.372209 0.355894
O 3.539844 -1.500003 -0.510533
C 5.198303 -0.002286 0.463314
H -3.216609 1.922609 0.069121
H -3.602522 -2.360333 0.096370
H 1.208474 -1.456247 -0.166375
H -1.737356 -3.784801 0.000677
H -0.293538 -3.172971 0.820641
H -0.371580 -3.168681 -0.941455
H -5.226811 0.733445 0.166574
H 3.152935 1.702571 0.305233
H 3.193016 0.925815 -1.271164
H 3.329610 -0.609819 1.359598
H 4.058616 -2.234352 -0.146178
H 5.598995 0.265623 -0.520526
H 5.780999 -0.848353 0.849203
H 5.348979 0.841689 1.145791

6-c22

C -2.004810 1.551274 -0.094972
C -2.503900 -1.223535 0.134792
C -3.284461 1.065243 0.136059
C -0.930302 0.628860 -0.216614
C -1.205384 -0.750425 -0.098816
C -3.543328 -0.312803 0.252219
C -0.124786 -1.740597 -0.218334
O 1.147176 -1.237676 -0.458837
C 1.413926 0.103512 -0.571913
C 0.436940 1.027497 -0.456713
C -1.769651 3.038584 -0.213974
O -4.838916 -0.678136 0.479897
O -0.248193 -2.940831 -0.127284
C 2.867783 0.358060 -0.821920
C 3.809876 -0.121563 0.310085

O 5.166674 -0.018378 -0.117504
C 3.583334 0.610969 1.631596
H -2.662570 -2.295116 0.217941
H -4.122294 1.749875 0.232690
H 0.697133 2.074261 -0.553453
H -2.705570 3.592218 -0.098430
H -1.344285 3.303822 -1.189927
H -1.072069 3.400696 0.551636
H -4.887909 -1.645381 0.538658
H 3.012568 1.433959 -0.985046
H 3.176618 -0.160036 -1.738459
H 3.647668 -1.193950 0.455580
H 5.385091 0.926458 -0.170871
H 3.743923 1.691833 1.510711
H 4.283648 0.243950 2.388039
H 2.562701 0.467121 2.001793

6c27

C 2.046426 1.562646 0.034765
C 2.500402 -1.229437 0.059935
C 3.318090 1.040326 0.227147
C 0.956916 0.668979 -0.151358
C 1.209558 -0.719399 -0.135101
C 3.554647 -0.346612 0.241245
C 0.112606 -1.679729 -0.323894
O -1.152078 -1.139884 -0.521291
C -1.398186 0.209397 -0.535513
C -0.403350 1.105536 -0.361026
C 1.835377 3.058360 0.026001
O 4.844423 -0.748477 0.438227
O 0.215649 -2.885436 -0.322777
C -2.848049 0.528772 -0.741402
C -3.748682 0.375473 0.513630
O -5.055637 0.871601 0.223580
C -3.933041 -1.066007 0.967630
H 2.641681 -2.306625 0.064070
H 4.166982 1.702408 0.372092
H -0.643639 2.161380 -0.386538
H 2.781084 3.586743 0.175009
H 1.148406 3.374807 0.820925

H 1.408826 3.400979 -0.924991
H 4.877670 -1.718098 0.426470
H -3.258140 -0.103903 -1.537815
H -2.915420 1.569744 -1.082485
H -3.294552 0.959378 1.331639
H -4.981814 1.819476 0.030770
H -4.382053 -1.659662 0.163954
H -4.604416 -1.094531 1.831350
H -2.979754 -1.524346 1.241288