

First Principles Prediction of pK_a s of Anti-inflammatory Oxicams

Junming Ho and Michelle L. Coote¹

ARC Centre of Excellence for Free Radical Chemistry and Biotechnology, Research

School of Chemistry, Australian National University, Canberra ACT 0200, Australia

Marco Franco-Pérez and Rodolfo Gómez-Balderas

Laboratorio de Fisicoquímica Analítica, Unidad de Investigación Multidisciplinaria, FES

Cuautitlán, Universidad Nacional Autónoma de México, Cuautitlán Izcalli, Estado de

México, 54700, México.

SUPPORTING INFORMATION

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¹ Correspondence author. Email: mcoote@rsc.anu.edu.au

Table S1. M05-2X/6-311+G(3df,2p) electronic energies and solvation free energies obtained from the various solvent models.

	M05-2X	ΔG_{solv} (kJ mol ⁻¹)		
		CPCM	SMD	COSMO-RS
H+piroxicam (gas)	-1443.407455	-233.3	-261.0	-232.2
H+piroxicam (CPCM)	-1443.395182	-266.8		-266.6
Zwit-piroxicam-(O)	-1443.009925	-100.2	-133.4	-116.9
Piroxicam	-1443.029827	-50.3	-69.8	-51.3
Zwit-piroxicam-(N)	-1443.015395	-68.3	-98.7	-79.9
O-piroxicam	-1442.5041	-226.9	-248.7	-259.2
H+tenoxicam (gas)	-1764.161517	-243.0	-260.3	-229.4
H+tenoxicam (CPCM)	-1764.149128	-274.9		-262.8
Zwit-tenoxicam-(O)	-1763.767051	-105.2	-131.7	-110.4
Tenoxicam	-1763.78479	-56.4	-67.4	-45.7
Zwit-tenoxicam-(N)	-1763.771047	-73.2	-96.1	-74.0
O-tenoxicam	-1763.262888	-229.1	-244.2	-250.0
H+lornoxicam (gas)	-2223.762899	-235.3	-257.9	-229.3
H+lornoxicam (CPCM)	-2223.750453	-268.3		-264.1
Zwit-lornoxicam-(O)	-2223.371591	-92.9	-125.1	-104.7
Lornoxicam	-2223.387961	-44.9	-61.0	-42.5
Zwit-lornoxicam-(N)	-2223.375016	-61.8	-88.8	-69.4
O-lornoxicam	-2222.870784	-207.9	-229.3	-234.5
H+meloxicam (gas)	-1803.489659	-237.5	-244.2	-225.2
H+meloxicam (CPCM)	-1803.485018	-265.3	-266.5	-254.7
Zwit-meloxicam-(O) (gas)	-1803.094038	-100.7	-118.4	-107.9
Zwit-meloxicam-(O) (CPCM)	-1803.088937	-130.5	-140.7	-136.9
Meloxicam	-1803.115166	-57.0	-74.1	-52.9
Zwit-meloxicam-(N) (gas)	-1803.105182	-77.9	-92.6	-79.2
Zwit-meloxicam-(N) (CPCM)	-1803.102058	-90.3	-104.9	-92.4
O-meloxicam	-1802.595358	-225.2	-243.9	-249.7
H+isoxicam	-1480.470469	-247.7	-255.8	-241.2
Zwit-isoxicam-(O)	-1480.073278	-112.2	-128.3	-124.7
Isoxicam	-1480.10593	-58.2	-73.6	-57.4
Zwit-isoxicam-(N)	-1480.081858	-75.1	-92.9	-84.4
O-isoxicam	-1479.583488	-222.9	-248.0	-259.6
H+sudoxicam	-1764.16063	-248.1		-232.5
Zwit-sudoxicam-(O)	-1763.768301	-105.6		-107.5
Sudoxicam	-1763.791442	-59.6		-51.5
O-sudoxicam	-1763.273146	-225.0		-244.7
H+propoxicam	-1448.225811	-227.6		-222.9
Zwit-propoxicam-(O)	-1447.815994	-134.6		-148.5
Propoxicam	-1447.829285	-41.4		-47.4
O-propoxicam	-1447.289794	-244.3		-278.7
H+propoxicam-Q1	-1408.888304	-262.2		-241.9
Zwit-propoxicam-Q1	-1408.470183	-165.5		-170.4
H+propoxicam-Q2	-1448.208377	-253.5		-243.2

Zwit-propoxicam-Q2	-1447.782866	-165.0	-181.7
H+hybrid	-1444.378442	-283.9	-279.8
Zwit-hybrid-(O)	-1443.976133	-130.4	-139.5
Hybrid	-1444.004393	-81.9	-80.6
O-hybrid	-1443.483809	-231.2	-248.6

Table S2. CPCM-UAKS Solution free energies^a (kJ mol⁻¹) of selected species calculated on gas and solution phase conformers.

	Gas phase conformer	Solution phase conformer	$\Delta G(\text{Soln} - \text{Gas})$
H+piroxicam	-3789285.9	-3789289.7	-3.8
H+tenoxicam	-4631521.8	-4631523.7	-1.9
H+lornoxicam	-5838228.0	-5838230.8	-2.8
H+meloxicam	-4734707.8	-4734724.6	-16.7
Zwit-meloxicam (O)	-4733570.9	-4733589.3	-18.3
Zwit-mleoxicam (N)	-4733573.4	-4733578.0	-4.6

^a G_{soln} calculated as $G_{\text{gas}}^* + \Delta G_{\text{solv}}^*$ where G_{gas}^* is calculated at the M05-2X/6-311+G(3df,2p) level in conjunction with thermal corrections at B3LYP/6-31+G* (scaled).

Table S3. Gas phase optimised geometries of all the studied species in their gas phase conformation.

NOTE: All species had zero imaginary frequencies, as determined from frequency calculations at the B3LYP/6-31+G(d) level.

h+piroxicam

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trafine)\opt calc\1,1\C,0.0903667176,-0.2356495633,-0.0614910431\C,0
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879493219\C,2.4424870647,0.0486092981,1.4465952828\C,2.4801904681,-0.0
181759174,0.0362391786\C,1.3227672667,-0.1544557387,-0.7203305749\H,-0
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6677643,3.4908610663\C,4.8660079935,0.6242834552,1.6408303635\C,6.1080
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zwit-piroxicam

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piroxicam

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zwit-piroxicam-N.a3

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o-piroxicam

```
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9706142228,-0.0594284694,-0.5342253488\H,-0.9620297889,0.0816469427,1.9542407315\H,1.213893584,0.1433721749,3.1922622244\H,1.2057775458,-0.126196183,-1.7715760451\S,3.9560453968,-0.0175069758,-0.816885105\O,3.8264032659,-0.7991268752,-2.0616589696\O,4.4233660983,1.371933187,-0.8890266779\N,4.8894185665,-0.8751273973,0.2606411088\C,4.9626793505,-2.3347191474,0.0862249083\H,5.8542749714,-2.6647141195,0.6236447708\H,4.0736480336,-2.8407561046,0.4943874429\H,5.0701746396,-2.5749890643,-0.9727055305\C,3.6919263154,0.0437934722,2.2388834084\O,3.5912267945,0.4571761902,3.4366703581\C,4.8894653188,-0.3792798826,1.6180025145\C,6.1979552206,-0.429242959,2.2629016555\O,7.2157532877,-0.8668159532,1.6974377558\N,6.2203661619,0.0214736078,3.5868909721\H,5.304587158,0.331459875,3.9462216541\H,8.816231177,-0.6614478987,3.1240852043\C,8.6121413127,-0.3000172929,4.1225201271\C,7.2880927458,0.0794835035,4.4588922064\C,9.5962500108,-0.187975109,5.0954990678\N,6.9717994614,0.5409648657,5.6899097963\C,9.2739325576,0.2892414519,6.3727539886\H,10.6191026379,-0.4730194236,4.855346885\C,7.9422361075,0.6364205706,6.6019966262\H,10.0205265821,0.389852601,7.1561881806\H,7.63111045,1.01507141,7.576488317\\Version=EM64L-G03RevE.01\State=1-A\HF=-1442.2333455\RMSD=8.648e-09\RMSF=2.090e-05\Thermal=0.\Dipole=-1.0487457,-0.9939247,0.6145425\PG=C01 [X(C15H12N3O4S1)]\@

h+tenoxicam

1\1\GINC-X147\FOpt\RB3LYP\6-31+G(d)\C13H12N3O4S2(1+)\JMH502\08-Jan-2010\0\0\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\opt calc\1,1\C,-0.0317916646,-0.0322906801,-0.017084414\S,0.0417924553,-0.1184780325,2.7159647054\O,1.4706136838,-0.2668330912,2.977413986\O,-0.8737024174,0.4384876907,3.7060229453\N,-0.53356055,-1.6847314846,2.284853798\C,-2.0143234321,-1.8385324516,2.313786778\H,-2.4981837892,-1.3155583295,1.4799579297\H,-2.2388701547,-2.9061122094,2.2416444495\H,-2.3924400089,-1.4536344531,3.2610657659\C,0.2695179425,-1.4413383836,-0.0436512188\O,0.7709541374,-1.9173366861,-1.1763317876\C,0.1031506019,-2.2101738082,1.1083765893\C,0.6564390769,-3.5313385563,1.173184996\O,1.112986413,-4.1558701712,0.1830440511\N,0.6859588992,-4.1036749645,2.4494060538\H,0.8560875727,-5.1477426381,4.9150469174\C,1.2497025629,-5.776122964,4.1230107883\C,1.2121313181,-5.318942351,2.7938332993\C,1.7934680007,-7.0207841791,4.3929689908\N,1.7160171163,-6.1192167898,1.8194106913\C,2.3039685191,-7.8255716622,3.3542972098\H,1.8257909739,-7.3768624512,5.418310565\C,2.2522945335,-7.3424523144,2.0677606308\H,2.7320450323,-8.8012524447,3.5519213966\H,2.6212349747,-7.879254437,1.2015449803\H,0.9722315239,-2.8805643719,-1.0578982128\H,0.368033656,-3.4824964661,3.192545673\C,-0.1848848376,0.7083359627,1.1476894102\C,-0.4202891502,2.0843708755,0.9336232506\H,-0.5682265835,2.8140475158,1.7207779552\C,-0.4431041696,2.3718168705,-0.413803803\H,-0.6154724938,3.3366783226,-0.8747551265\S,-0.1684083551,0.9925494615,-1.4143894378\H,1.6783077208,-5.7174147422,0.8683657071\\Version=EM64L-G03RevE.01\State=1-A\HF=-1763.8835698\RMSD=8.313e-09\RMSF=2.428e-05\Thermal=0.\Dipole=0.3506784,-4.3945124,0.4109844\PG=C01 [X(C13H12N3O4S2)]\@

zwit-tenoxicam

1\1\GINC-X139\FOpt\RB3LYP\6-31+G(d)\C13H11N3O4S2\JMH502\10-Jan-2010\0\0\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\opt calc\0,1\C,0.008811321,0.0079783422,-0.0237228828\C,0.0146755917,0.0025696508,1.3552126685\S,1.6015783532,0.0080891705,2.1658440331\O,2.0869185561,1.3884199018,2.1974589626\O,1.5169318098,-0.7821326161,3.3992691007\N,2.5019857345,-0.8590320066,1.0405898177\C,2.5958462291,-2.3193097725,1.2243316842\H,3.4848475773,-2.6538782379,0.6843438882\H,2.7188922027,-2.5442046179,2.2839210431\H,1.7083089523,-2.8388582822\O,0.8349567247\C,1.1836768273,-0.0134695524,-0.9116876137\O,1.0266797818,0.3318542648,-2.124671416\C,2.4315948259,-0.3884765046,-0.3142691449\C,3.6658207235,-0.3761309566,-1.0225669912\O,4.7861492215,-0.7166021353,-0.5703171606\N,3.5625282254,0.0480981669,-2.3804658717\H,2.5722296327,0.2710208346,-2.6553248268\H,3.424600801,0.8932575991,-4.9185338425\C,4.422531627,0.6505424797,-4.5697322732\C,4.5861875888,0.1937253084,-3.2347854751\C,5.5283578123,0.7769636996,-5.3803404096\N,5.8510860878,-0.1037866864,-2.8164341065\C,6.824112773,0.4587446273,-4.90241803

65\H,5.4037593657,1.1277222636,-6.4008880966\C,6.9458114784,0.01987869
86,-3.6076395891\H,7.7002671034,0.556773416,-5.5323088056\H,7.88985206
46,-0.2476428317,-3.1465672414\H,5.8630106853,-0.4327750797,-1.8199335
337\S,-1.6187129551,0.1228173277,-0.6243053248\C,-2.2532075673,0.13595
41052,0.9903376376\C,-1.2735876762,0.0745328168,1.9501259385\H,-3.3235
693411,0.186520661,1.1461886081\H,-1.4527569507,0.0738201204,3.0189123
775\\Version=EM64L-G03RevE.01\State=1-A\HF=-1763.4916214\RMSD=3.455e-0
9\RMSF=1.144e-05\Thermal=0.\Dipole=1.8955602,-0.4102892,-4.0225342\PG=
C01 [X(C13H11N3O4S2)]\@

tenoxicam

1\1\GINC-X143\FOpt\RB3LYP\6-31+G(d)\C13H11N3O4S2\JMH502\17-Dec-2009\0\
\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultraf
ine)\\opt calc\\0,1\C,0.0299440644,-0.2334488435,-0.0892649327\C,0.124
9256627,-0.4394483103,1.2878132117\N,1.2695060762,-0.3382327563,1.9712
114771\C,2.3806249064,-0.0184450436,1.293154824\C,2.403856056,0.212768
7485,-0.0918643648\C,1.1980023247,0.0977119903,-0.7801018673\N,3.51402
29912,0.0529148821,2.1217899413\C,4.8053316449,0.3610075391,1.80900650
63\C,5.7568561363,0.3245710916,2.9268099652\N,5.3207055837,-0.21192690
83,4.1875621155\S,5.8148834698,0.6938831438,5.5498616107\C,7.557161176
9,0.8321206312,5.2015687624\C,7.943865672,0.9040084992,3.8769274895\C,
7.0384546338,0.8028256872,2.7490605223\O,7.5096641524,1.2436784814,1.5
793964815\H,6.7733361693,1.1054954944,0.911573915\O,5.6207008869,-0.13
59380298,6.7404795323\O,5.2055012113,2.0168871089,5.4422556972\C,5.462
3234301,-1.6839127175,4.3197748196\H,6.5125798579,-1.9997586679,4.2680
524011\H,4.9111833923,-2.1417215777,3.4943088678\H,5.0238613807,-2.003
3401841,5.2652261796\H,3.311085116,-0.0878667803,3.1082277092\O,5.1827
189729,0.6615843851,0.6526810785\H,3.3284227167,0.4735405219,-0.587829
6406\H,1.1752997622,0.2701179524,-1.8529983619\H,-0.9248294472,-0.3281
28411,-0.5972727588\H,-0.75328868,-0.6979952464,1.8759626931\S,9.65957
35243,1.152649739,3.75514766\C,9.8194801646,1.1384763546,5.4819972066\
C,8.6222423424,0.9615754245,6.1302921439\H,10.7980538583,1.2631039424,
5.9279905901\H,8.5021238111,0.9244606771,7.2064509518\\Version=EM64L-G
03RevE.01\State=1-A\HF=-1763.5047053\RMSD=4.516e-09\RMSF=5.444e-06\The
rmal=0.\Dipole=0.7592258,-0.9512807,-0.6851932\PG=C01 [X(C13H11N3O4S2)
]\@

zwit-tenoxicam-N.a3

1\1\GINC-V1299\FOpt\RB3LYP\6-31+G(d)\C13H11N3O4S2\JMH502\21-Jun-2010\0\
\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultraf
ine)\\opt calc\\0,1\S,-0.0168489756,-0.0433016689,0.0496933493\C,0.012
2016747,-0.039714019,1.7859021015\C,1.2844311562,-0.0235026074,2.29964
36026\C,2.2525686255,-0.009327984,1.2608641851\C,1.7226085133,-0.00443
48142,-0.014074513\C,2.4972430896,0.0343844264,-1.2369553487\C,3.83774
20361,0.3863662991,-1.209435929\N,4.4642707342,0.7613300877,0.01880694
65\S,4.0212903541,-0.1111717773,1.3931692359\C,4.6887289426,0.43135284
48,-2.4117627433\N,4.0389890056,0.0988596475,-3.5876511589\C,4.6869966
484,0.0559713998,-4.75400501\C,4.0217619198,-0.2999887972,-5.966187567
2\C,4.7116439759,-0.3456064801,-7.1543651187\C,6.0970236037,-0.0409578
13,-7.2046111178\C,6.7229721236,0.3006042246,-6.0335554976\N,6.0297225
479,0.3447143834,-4.8670043876\H,-0.9205255321,-0.054394702,2.33542342
16\H,1.5246641598,-0.0243914224,3.3561999539\O,4.4708221968,0.63236597
18,2.5740124039\O,4.4056653196,-1.5087890622,1.1999748203\H,5.36283613
2,2.3142423452,1.1164184407\C,4.8068549252,2.1876540667,0.1879151238\H
,3.9080393461,2.8197157202,0.2047513256\H,5.4451690977,2.4668077744,-0
.6519776989\O,1.8269441543,-0.3137880747,-2.342175117\H,2.4908670438,-
0.2289566286,-3.1029765308\O,5.8951051751,0.7621244864,-2.3344061581\H
,2.964446077,-0.53308228,-5.909114151\H,4.1899741237,-0.6201754516,-8.
0672181234\H,6.6530052718,-0.0749918629,-8.134184717\H,7.7762990311,0.
5497763812,-5.9646098582\H,6.4540847396,0.598163136,-3.954743013\\Vers
ion=EM64L-G03RevE.01\State=1-A\HF=-1763.4922433\RMSD=5.069e-09\RMSF=1.
613e-05\Thermal=0.\Dipole=-0.3366505,0.8163997,-3.3237278\PG=C01 [X(C1
3H11N3O4S2)]\@

o-tenoxicam


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1\1\GINC-X137\FOpt\RB3LYP\6-31+G(d)\C13H10N3O4S2(1-)\JMH502\09-Jan-201
0\0\#\ B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ul
trafine)\opt calc\ -1,1\C,-0.0156052172,0.0341969295,0.005943795\C,-0
.0142430394,-0.0125626679,1.3812937021\S,1.5767519572,-0.0209150391,2.
173590794\O,1.5039544634,-0.8650082769,3.3807873419\O,2.0319368852,1.3
679814493,2.3004395813\N,2.4807045685,-0.8160087498,1.0152986736\C,2.6
246957796,-2.2746754324,1.1640439271\H,1.7393114165,-2.8112634442,0.78
91469763\H,3.5038302499,-2.5583896933,0.5817272585\H,2.7909859995,-2.5
255863882,2.2125637063\C,1.1527965161,0.0446664263,-0.9105209968\O,0.9
440462196,0.4109666908,-2.1098766659\C,2.3975693219,-0.3222141275,-0.3
411573547\C,3.6668490302,-0.3397924059,-1.061189354\O,4.733312044,-0.7
211985998,-0.5485981897\N,3.5914724621,0.0792326786,-2.3938416131\H,2.
6451878887,0.335976864,-2.7122078844\H,6.2420994474,-0.4605258379,-2.0
639132498\C,5.9642017511,-0.1333033361,-3.0562471449\C,4.6059948433,0.
1698829221,-3.3258109384\C,6.8858594935,0.0055133453,-4.0854825055\N,4
.1982874448,0.5848025352,-4.5460104753\C,6.4688638835,0.4345962333,-5.
352203624\H,7.9338802109,-0.2210891906,-3.8974439033\C,5.1102323752,0.
7077165014,-5.5134691862\H,7.1647030433,0.554032729,-6.178493335\H,4.7
261693215,1.0462265897,-6.4765622017\S,-1.646527186,0.1479077821,-0.59
20259292\C,-2.288400293,0.1002031574,1.0262519131\C,-1.306283948,0.020
9478721,1.9802389563\H,-3.3592007143,0.1362198836,1.1850953603\H,-1.48
08861157,-0.0166494668,3.0497556049\Version=EM64L-G03RevE.01\State=1-
A\HF=-1762.9871777\RMSD=5.727e-09\RMSF=1.585e-05\Thermal=0.\Dipole=-0.
908044,-0.8789459,-0.51608\PG=C01 [X(C13H10N3O4S2)]\@

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h+lornoxicam

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1\1\GINC-X142\FOpt\RB3LYP\6-31+G(d)\C13H11Cl1N3O4S2(1+)\JMH502\08-Jan-
2010\0\#\ B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid
=ultrafine)\opt calc\ 1,1\C,-0.0384805005,-0.0352867516,-0.0231762798
\S,0.0241368045,-0.1074055234,2.7111811672\O,1.4534254226,-0.238496640
9,2.9762739554\O,-0.9005934217,0.450208663,3.6916538778\N,-0.536222942
2,-1.6776258954,2.2846049387\C,-2.0157741575,-1.8458341353,2.311996376
8\H,-2.5028715667,-1.3343773971,1.4729925481\H,-2.2290600993,-2.916134
9746,2.2475590939\H,-2.3997952719,-1.4576456038,3.255520981\C,0.271854
1973,-1.4403043775,-0.0420928459\O,0.7758876118,-1.9181334141,-1.17339
26963\C,0.1090468578,-2.2053707753,1.1135828537\C,0.6695097168,-3.5225
880196,1.1847072112\O,1.1320962504,-4.1472445368,0.1972373124\N,0.6981
990559,-4.0922386659,2.4623387818\H,0.8649057092,-5.1315954588,4.93030
48786\C,1.2641256556,-5.759394065,4.1406013122\C,1.2288642686,-5.30474
78266,2.8105511422\C,1.8127799891,-7.0010649389,4.4146542727\N,1.73963
64296,-6.1044193875,1.8392501941\C,2.3304092652,-7.8053251981,3.379158
1609\H,1.8432842308,-7.3551551137,5.4407424606\C,2.2807284954,-7.32472
28601,2.0915807237\H,2.7623353613,-8.77866307,3.5799489456\H,2.6549713
554,-7.8613509962,1.2275276491\H,0.9839091908,-2.879479814,-1.05042054
96\H,0.3757771419,-3.4723470256,3.204295233\C,-0.201933059,0.711437195
,1.1352135498\C,-0.4408799553,2.0844332007,0.9251974594\H,-0.597892427
8,2.8190941282,1.7054598626\C,-0.4533948025,2.3676132103,-0.4256959525
\S,-0.1655518521,0.9778367271,-1.4345636733\H,1.703095035,-5.704817601
8,0.8872821532\C1,-0.7274170614,3.9041780956,-1.1328019676\Version=EM
64L-G03RevE.01\State=1-A\HF=-2223.4697226\RMSD=6.093e-09\RMSF=1.851e-0
5\Thermal=0.\Dipole=0.6038574,-5.6158535,1.0161994\PG=C01 [X(C13H11Cl1
N3O4S2)]\@

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zwit-lornoxicam

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1\1\GINC-X139\FOpt\RB3LYP\6-31+G(d)\C13H10Cl1N3O4S2\JMH502\09-Jan-2010
\0\#\ B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ult
rafine)\opt calc\ 0,1\C,0.0067071845,0.0066350037,-0.022061544\C,0.01
51046517,0.0023991566,1.355049125\S,1.6080101542,0.0061005399,2.160283
0427\O,2.0901188356,1.3869799294,2.1876980812\O,1.5242082603,-0.783506
0609,C,3.393357751\N,2.4992866046,-0.8616820011,1.03105962\C,2.598616024
1,-2.3217427022,1.2167289773\H,3.4877398044,-2.6536207171,0.6754313974
\H,2.724388761,-2.5448404505,2.2763330417\H,1.7120328849,-2.8441239516
,0.8294628185\C,1.1758405373,-0.0179944402,-0.9161237509\O,1.008817878
1,0.3241924663,-2.128773013\C,2.4251611571,-0.3919356598,-0.3241203724
\C,3.6571902256,-0.3794332637,-1.0375514788\O,4.7785403436,-0.71772304

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33,-0.5879427303\N,3.5482734564,0.0423849113,-2.3952221838\H,2.5584813
778,0.2640810482,-2.6687981783\H,3.3993575962,0.8859426941,-4.93299097
2\C,4.3991179632,0.6456736384,-4.5877655327\C,4.5691810611,0.189931606
5,-3.2536733251\C,5.5016539803,0.7745797266,-5.4027998043\N,5.83598354
29,-0.104485017,-2.8398925243\C,6.799761009,0.4597152477,-4.9296893396
\H,5.3722214871,1.1246841256,-6.4229364793\C,6.9276138102,0.0215096837
, -3.6352422401\H,7.6732865767,0.5595711097,-5.5629184417\H,7.873952533
1,-0.2436994677,-3.1776522485\H,5.8541035679,-0.4331623327,-1.84411445
02\S,-1.6203534652,0.1329880227,-0.6311476222\C,-2.2416335191,0.149240
7153,0.9995922799\C,-1.2664138613,0.0817389585,1.9618899161\H,-1.44955
844,0.0823521513,3.0292954603\Cl,-3.9465726648,0.2391737152,1.28154642
1\\Version=EM64L-G03RevE.01\State=1-A\HF=-2223.0809356\RMSD=6.471e-09\
RMSF=2.187e-05\Thermal=0.\Dipole=2.5695069,-0.4429331,-4.1685961\PG=C0
1 [X(C13H10Cl1N3O4S2)]\\@

lornoxicam

1\1\GINC-X140\FOpt\RB3LYP\6-31+G(d)\C13H10Cl1N3O4S2\JMH502\17-Dec-2009
\0\#\ B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ult
rafine)\opt calc\0,1\C,0.0261126309,-0.2456450887,-0.0893889837\C,0.
1220046485,-0.4498382261,1.2879482206\N,1.2666450535,-0.3446505425,1.9
70646557\C,2.3762814571,-0.0226481837,1.2915400697\C,2.3987735854,0.20
7015418,-0.0935230313\C,1.1928633399,0.0878445616,-0.7811696786\N,3.50
99250766,0.0528209767,2.1203735197\C,4.799903119,0.3638024512,1.807184
1006\C,5.7526080748,0.3307892602,2.9245121299\N,5.3218970386,-0.207354
0284,4.1863618661\S,5.8148401165,0.696866954,5.5477521766\C,7.55842689
89,0.839765353,5.194703271\C,7.9387373062,0.915101888,3.8701216049\C,7
.0323269868,0.812600724,2.7445129639\O,7.5029734587,1.2540872193,1.574
7741556\H,6.7669535893,1.1134689035,0.906617913\O,5.6293371274,-0.1343
682008,6.7380060932\O,5.2066857862,2.0199540447,5.443098996\C,5.460661
9472,-1.6801824582,4.3165984099\H,6.5099930787,-1.9979536661,4.2603341
587\H,4.9054346187,-2.1355062908,3.4926058825\H,5.0249655424,-1.999719
1765,5.263219281\H,3.3061304384,-0.0872713634,3.1066876365\O,5.1773593
697,0.6645448655,0.6510449736\H,3.3223320579,0.4696158401,-0.590400292
9\H,1.169221997,0.2589071618,-1.8542324688\H,-0.9285828022,-0.34349808
95,-0.5968976576\H,-0.7552524772,-0.71008407,1.8767029054\S,9.65591531
4,1.1709457096,3.7324001259\C,9.8102901218,1.1513498158,5.4714369442\C
,8.6185844087,0.9689665508,6.1274904166\Cl,11.3594986043,1.3509218399,
6.2046076418\H,8.5075648725,0.9295540285,7.2039528461\\Version=EM64L-G
03RevE.01\State=1-A\HF=-2223.0926074\RMSD=7.552e-09\RMSF=1.283e-05\The
rmal=0.\Dipole=0.2183341,-1.0289967,-0.9304321\PG=C01 [X(C13H10Cl1N3O4
S2)]\\@

zwit-lornoxicam-N.a3

1\1\GINC-V1295\FOpt\RB3LYP\6-31+G(d)\C13H10Cl1N3O4S2\JMH502\21-Jun-201
0\0\#\ B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ult
rafine)\opt calc\0,1\S,-0.0157440179,-0.0544714825,0.0472635221\C,0.
0110040327,-0.0426958772,1.7943655417\C,1.2750350583,-0.0198355218,2.3
252041316\C,2.2444482561,-0.0075528031,1.2885873\S,4.0145683882,-0.105
694419,1.4359601242\N,4.4639662981,0.7634626268,0.0633863777\C,3.84927
73941,0.3841365106,-1.1693056823\C,2.5105701813,0.0279961226,-1.206449
5442\C,1.7277803885,-0.0098085934,0.0098830673\C,4.7086000764,0.429445
2328,-2.3664770146\N,4.0660716596,0.0953661148,-3.5449536993\C,4.72093
87215,0.0526423872,-4.708311832\N,6.0635949384,0.3430149388,-4.8135373
23\C,6.7635403398,0.2996127358,-5.9761711306\C,6.1443909309,-0.0432288
063,-7.1505415517\C,4.7594172334,-0.3496983025,-7.1079749078\C,4.06281
90814,-0.3045977287,-5.923461687\C,4.8115542151,2.1893335718,0.2304861
555\H,3.9151188387,2.8246093065,0.2366096575\H,5.4587095902,2.46206475
26,-0.6045954155\H,5.3594385669,2.316823154,1.163597042\O,4.3985747426
, -1.5037040438,1.2499087233\O,4.4495080043,0.6419177748,2.6188802613\H
,1.4998547811,-0.0157339199,3.3844840799\Cl,-1.4715084758,-0.067083452
6,2.682737507\O,1.8474881536,-0.3230489775,-2.3152438634\H,2.516756116
7,-0.2366253602,-3.0722455702\O,5.913773696,0.7614722846,-2.2805309269
\H,6.4833118514,0.5975925391,-3.8997654954\H,7.8160839659,0.5502679022
, -5.9013906143\H,6.7055613082,-0.0767318188,-8.0770027516\H,4.24315620
95,-0.625248111,-8.0235696606\H,3.005514578,-0.5390693726,-5.872368129

9\\Version=EM64L-G03RevE.01\\State=1-A\\HF=-2223.0809713\\RMSD=8.300e-09\\
RMSF=9.258e-06\\Thermal=0.\\Dipole=0.2413641,0.8300639,-3.6879234\\PG=C01
[X(C13H10Cl1N3O4S2)]\\@

o-lornoxicam

1\\1\\GINC-X137\\FOpt\\RB3LYP\\6-31+G(d)\\C13H9Cl1N3O4S2(1-)\\JMH502\\09-Jan-2
010\\0\\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=
ultrafine)\\opt calc\\-1,1\\C,-0.0162598267,0.0339275189,0.003736712\\C,
-0.019689113,-0.0141127892,1.3770746331\\S,1.5731498324,-0.012704175,2.
1714795491\\O,1.5020698026,-0.8574058385,3.3772255792\\O,2.0145335406,1.
3799546783,2.2963417056\\N,2.4791465468,-0.8011357602,1.0123713664\\C,2.
6402317244,-2.2583158205,1.1632794965\\H,1.7616730522,-2.8048595339,0.7
874284213\\H,3.5236239253,-2.531987089,0.5828218298\\H,2.8076420692,-2.5
05867775,2.2123013772\\C,1.1494041386,0.0492337168,-0.9138969042\\O,0.93
16727558,0.4111217437,-2.1132793994\\C,2.3951104392,-0.3087349538,-0.34
45404128\\C,3.6655560426,-0.3187074328,-1.0648924978\\O,4.733226559,-0.6
908619319,-0.5492626879\\N,3.586949104,0.0958031758,-2.3973748864\\H,2.6
399738824,0.3443313389,-2.7187405834\\H,6.2440047156,-0.4161205483,-2.0
643762033\\C,5.9623729238,-0.0963406531,-3.0580681734\\C,4.6019956311,0.
1921138972,-3.3298690387\\C,6.8828253664,0.0466474773,-4.0881073371\\N,4.
1898756297,0.5973709419,-4.5512101418\\C,6.4615189186,0.4654826965,-5.
3565720582\\H,7.9329599281,-0.1686674965,-3.8990511838\\C,5.1003753629,0.
.7247674748,-5.5195174748\\H,7.1561972441,0.5876401972,-6.1833693554\\H,
4.7130196423,1.0550734181,-6.4840039257\\S,-1.6432078174,0.1490574382,-
0.6144198483\\C,-2.2772653817,0.0963755655,1.0145068278\\C,-1.3103167937
,0.0164661438,1.9797262572\\H,-1.4976826757,-0.0224008643,3.045984652\\C
1,-3.9963857307,0.1491494992,1.292906708\\Version=EM64L-G03RevE.01\\Sta
te=1-A\\HF=-2222.5798899\\RMSD=5.858e-09\\RMSF=1.161e-05\\Thermal=0.\\Dipol
e=-0.9987269,-0.8789471,-0.3999886\\PG=C01 [X(C13H9Cl1N3O4S2)]\\@

h+meloxicam.alc2

1\\1\\GINC-V173\\FOpt\\RB3LYP\\6-31+G(d)\\C14H14N3O4S2(1+)\\JMH502\\13-Jan-201
0\\0\\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ul
trafine)\\opt calc\\1,1\\C,-0.0038993411,0.0508654982,-0.0353754353\\C,-
0.0205269273,0.0426054793,1.3625483486\\C,1.1730257727,0.0155218818,2.0
843938446\\C,2.4038955304,-0.0006046378,1.4087902493\\C,2.3968678031,-0.
0079983043,-0.0037368794\\C,1.2119525076,0.0215742136,-0.7286215752\\C,3
.6697562261,-0.0354402429,2.1478031969\\C,4.8813406244,0.2886036991,1.5
487450151\\N,4.9547916027,0.7925287075,0.205453479\\S,3.970293006,-0.132
2238677,-0.8629023388\\C,6.1166522288,-0.0026256062,2.2205321844\\N,7.26
18766608,0.0806658712,1.4052835855\\C,8.5188908938,-0.217808109,1.80875
39562\\N,8.844987762,-0.56778387,3.0551464821\\C,10.1965821398,-0.829501
0691,3.2542749331\\C,10.9488195168,-0.6799141601,2.1388628492\\S,9.91366
43556,-0.1909498657,0.7854799937\\H,1.1623612779,0.0128259926,3.1690566
279\\H,-0.9673636236,0.0602640423,1.8936073912\\H,-0.9363556538,0.078684
6921,-0.5912753858\\H,1.238178224,0.0257933328,-1.8138613181\\O,4.470187
5592,-1.5031384406,-0.7781276232\\O,3.8938515174,0.5835917313,-2.132910
7891\\C,4.8195692781,2.2680730412,0.0717918475\\H,3.8534155709,2.6295828
596,0.4445730666\\H,4.9353940487,2.5386860953,-0.9780728069\\H,5.6200884
929,2.7308431011,0.6553618284\\O,3.5818541559,-0.4535384742,3.403572638
3\\H,4.486557034,-0.4664806237,3.8068036832\\O,6.2229355266,-0.334876161
6,3.4203366876\\H,7.0654101298,0.2721777494,0.4217580002\\H,8.0977401505
, -0.6407189667,3.7532054625\\H,10.5344271028,-1.1218696312,4.2395995768
\\C,12.4213972446,-0.8713771048,1.9533852217\\H,12.9084697183,0.05258954
54,1.622400372\\H,12.6344981399,-1.6521427938,1.2147784598\\H,12.8723848
416,-1.1711527717,2.9037199809\\Version=EM64L-G03RevE.01\\State=1-A\\HF=
-1803.2054848\\RMSD=7.581e-09\\RMSF=1.380e-05\\Thermal=0.\\Dipole=3.156156
6,0.6376576,2.130439\\PG=C01 [X(C14H14N3O4S2)]\\@

zwit-meloxicam-enolate

1\\1\\GINC-V183\\FOpt\\RB3LYP\\6-31+G(d)\\C14H13N3O4S2\\JMH502\\14-Jan-2010\\0\\
\\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultraf
ine)\\opt calc\\0,1\\C,0.0026845687,0.0311449352,-0.0556980631\\C,-0.005
6430755,0.1060757746,1.3359672041\\C,1.2111329038,0.1079666876,2.020907
982\\C,2.4150497463,0.0430712132,1.3093886532\\C,2.4092448291,-0.0352081

343,-0.082815871\C,1.1982327655,-0.0544298221,-0.7909026924\H,-0.95175
 94145,0.1557642425,1.8662489227\H,1.2193545957,0.1631352919,3.10623195
 34\H,3.3612686021,0.05144823,1.8441058793\H,3.3344661035,-0.0826659896
 ,-0.647599758\C,1.2248907328,-0.1514247949,-2.2854409102\S,-1.52880952
 41,0.0932753746,-0.9853196163\N,-1.1470989864,-0.9292142154,-2.2598990
 363\C,0.0431185794,-0.563168068,-2.9717596174\C,-0.0456971966,-0.65725
 71877,-4.3914796104\O,-1.0267561524,-1.0319182661,-5.0636801517\N,1.16
 9428237,-0.2908751354,-5.0689942771\H,1.9354606693,-0.0177119734,-4.37
 73003602\C,1.2867545497,-0.2577247886,-6.3875287045\O,-2.5946765841,-0
 .531935681,-0.1930939039\O,-1.687399335,1.4513266812,-1.5100505937\C,-
 1.4171789823,-2.3682728564,-2.0952350914\H,-0.6336826368,-2.8700391665
 ,-1.5086706008\H,-2.3837079234,-2.4998976188,-1.6079745013\H,-1.461240
 0421,-2.8038175281,-3.096437972\O,2.3161263853,0.1550742533,-2.8666999
 981\N,0.3067648122,-0.5856994237,-7.2479571825\S,2.7261491452,0.222044
 33,-7.2584214779\C,0.6397726881,-0.4711742479,-8.5908795496\C,1.904584
 5818,-0.0499941127,-8.8112083993\C,2.6097418049,0.1886281134,-10.10956
 91442\H,1.933677488,-0.0343501181,-10.9410313863\H,2.9342694043,1.2313
 67073,-10.2081411907\H,3.4952291024,-0.4497897755,-10.2131633419\H,-0.
 1040945759,-0.7161411177,-9.3376067228\H,-0.5834553863,-0.8777204826,-
 6.8110698918\\Version=EM64L-G03RevE.01\State=1-A\HF=-1802.8131922\RMSE
 =8.881e-09\RMSE=2.038e-05\Thermal=0.\Dipole=2.4405764,-0.8930804,-3.64
 42334\PG=C01 [X(C14H13N3O4S2)]\@

meloxicam

1\1\GINC-X135\FOpt\RB3LYP\6-31+G(d)\C14H13N3O4S2\JMH502\17-Dec-2009\0\
 \# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultraf
 ine)\opt calc\0,1\C,-0.013397038,-0.0529187509,0.0525224273\C,0.1328
 265879,-0.3083544237,1.4129808323\C,1.4195588439,-0.3941018417,1.95105
 35854\C,2.5367873981,-0.2198197397,1.1273093473\C,2.3812575625,0.02519
 83664,-0.2370551693\C,1.0975199008,0.1018580524,-0.7998939163\H,-0.747
 3497179,-0.4381034684,2.035076789\H,1.5476724582,-0.5927289587,3.01133
 50446\H,3.5358501598,-0.2796655817,1.5498572294\H,3.2450240607,0.15547
 67718,-0.8799472499\C,0.9159323888,0.3382707107,-2.2413484652\S,-1.648
 1322264,0.1598843657,-0.6565948606\N,-1.3943114753,-0.503296886,-2.206
 9124019\C,-0.2729960235,0.0867840164,-2.8861591196\C,-0.4341663636,0.4
 476511621,-4.2961019215\O,0.528867056,0.827385378,-5.0000124195\N,-1.6
 961194277,0.3490203121,-4.8060851662\H,-2.4501817919,0.1254826421,-4.1
 616686556\C,-2.0869878823,0.6297899778,-6.1092979338\O,-2.5964876414,-
 0.7015595962,0.0534128671\O,-1.908604227,1.5873170639,-0.8316942202\C,
 -1.4792126451,-1.9823189913,-2.2903796637\H,-0.6219925111,-2.471390712
 1,-1.8089958468\H,-2.4067589101,-2.3138388646,-1.8230800056\H,-1.49244
 96863,-2.251525043,-3.34977946\O,1.9838574707,0.8433843474,-2.86673244
 18\H,1.7363177593,0.9408616846,-3.8318641603\N,-3.3338024669,0.5024927
 17,-6.4675485351\S,-0.9863331217,1.1621850724,-7.3684607789\C,-3.48097
 42738,0.8303782827,-7.7972651933\C,-2.3535516764,1.2081904534,-8.47069
 73107\C,-2.2077512089,1.6148580075,-9.9060801973\H,-3.1841405718,1.571
 24289,-10.400433316\H,-1.8267785368,2.6389156378,-10.005956926\H,-1.52
 479632,0.9529650289,-10.4532258161\H,-4.4703318669,0.7732237208,-8.238
 8148247\\Version=EM64L-G03RevE.01\State=1-A\HF=-1802.830045\RMSE=7.155
 e-09\RMSE=1.034e-05\Thermal=0.\Dipole=1.3069063,-1.1030742,-0.0278919\
 PG=C01 [X(C14H13N3O4S2)]\@

zwit-meloxicam.alb2

1\1\GINC-V1281\FOpt\RB3LYP\6-31+G(d)\C14H13N3O4S2\JMH502\29-May-2010\0\
 \#B3LYP/6-31+G(d) Opt=gdiis freq=noraman maxdisk=458752000 INT(grid=u
 ltrafine)\zwit-meloxicam-enolate.UAKS confsearch\0,1\C,0.0268440158,
 -0.0096370406,-0.014711263\C,0.0672527366,-0.0220617516,1.3783410006\C
 ,1.3068452966,0.0125620602,2.0200105703\C,2.4844790569,0.0663062055,1.
 2647637059\C,2.4305886281,0.0729253038,-0.1285416508\C,1.1966153012,0.
 0221236139,-0.7947608675\H,-0.8594733131,-0.062465452,1.9425776973\H,1
 .3531366168,0.0015521528,3.1057169596\H,3.448192066,0.1003122147,1.766
 2546028\H,3.3352521258,0.1152845956,-0.7259388477\C,1.1670144769,0.006
 1720052,-2.2888630534\S,-1.5395111699,0.0243676052,-0.8851572981\N,-1.
 1556543783,-0.8979127258,-2.2331288244\C,-0.0059598314,-0.4377489008,-
 2.9546566701\C,-0.119340707,-0.4739148089,-4.3825057042\O,-1.069003291

7,-0.8681886592,-5.0705462053\N,1.057835603,-0.0053349984,-5.052120520
6\H,1.8206922371,0.2838658008,-4.3297841852\C,1.1327363525,0.067832467
9,-6.3656781586\O,-2.5414128834,-0.7027878802,-0.0965376714\O,-1.78619
70983,1.4015744541,-1.3173951456\C,-1.3685974021,-2.3543655582,-2.1613
934001\H,-0.5484152856,-2.8642020676,-1.6351259476\H,-2.3130630864,-2.
555558469,-1.6551938845\H,-1.4301377978,-2.7211174389,-3.1888355131\O,
2.2236860819,0.4105533817,-2.8944059743\N,2.217514851,0.5376294954,-7.
0222930161\S,-0.1114245812,-0.4065538737,-7.4987419535\C,2.1132100621,
0.545689727,-8.4159667091\C,0.932185195,0.0735176467,-8.8619476857\C,0.
4595124028,-0.0675644382,-10.2758452539\H,1.2335947029,0.278215765,-1
0.9684215975\H,0.2280743789,-1.1113802417,-10.5194690916\H,-0.44593266
11,0.5240137463,-10.4564459264\H,2.9484555501,0.9135652839,-8.99710110
07\H,3.0338663636,0.8699528143,-6.5221427745\\Version=EM64L-G03RevE.01
\State=1-A\HF=-1802.8064214\RMSD=8.018e-09\RMSF=3.947e-05\Thermal=0.\D
ipole=3.2587665,-0.2940708,-3.5696265\PG=C01 [X(C14H13N3O4S2)]\@

o-meloxicam

1\1\GINC-X139\FOpt\RB3LYP\6-31+G(d)\C14H12N3O4S2(1-)\JMH502\09-Jan-201
0\0\#\B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ul
trafine)\opt calc\1,1\C,-0.0375881281,-0.0896495712,0.0316323876\C,
-0.0190726931,0.0069737182,1.4298244215\C,1.1913189463,0.067155738,2.1
188896922\C,2.4147139973,0.0284205725,1.4307385343\C,2.3680403762,-0.0
432351571,0.0287100053\C,1.16505624,-0.1116734198,-0.6757821173\H,-0.9
831317617,-0.1427798378,-0.5033353705\H,-0.9558930887,0.0329396761,1.9
826841205\H,1.2283874011,0.1496459645,3.2006345007\H,1.1826729921,-0.1
860342492,-1.7592525769\S,3.9373469611,-0.0061854589,-0.8344638791\O,3
.8119567746,-0.8019897718,-2.0699775091\O,4.3749174595,1.3916682907,-0
.9218122454\N,4.9026012722,-0.8346408106,0.2401982768\C,5.0119918897,-
2.293507911,0.0750616432\H,5.9172123071,-2.5976605002,0.6050227527\H,4
.1407000209,-2.8193276678,0.4958083008\H,5.1146106139,-2.5374357162,-0
.9833694853\C,3.6993412355,0.0786223588,2.2224308519\O,3.6088681685,0.
5001995491,3.4196233291\C,4.8967061796,-0.3306093161,1.5930270131\C,6.
1966710603,-0.3519695391,2.2433028212\O,7.242914375,-0.7680400431,1.71
28156263\N,6.2166857248,0.1009588933,3.5627925406\H,5.3047340071,0.408
4544281,3.9403135988\C,7.3211868149,0.132298233,4.3657199662\C,9.54976
84185,-0.0000751404,5.4124486274\N,7.2816559474,0.559989384,5.60586706
68\C,8.5308249322,0.4818738228,6.181047469\H,8.6427540648,0.8068692605
,7.212456152\S,8.920420135,-0.402032507,3.8152813501\C,10.9911123139,-
0.1872336368,5.7795516372\H,11.3090354333,-1.2362604607,5.697967989\H,
11.6630115255,0.4050530794,5.14254487\H,11.1531203683,0.1290685446,6.8
175419375\\Version=EM64L-G03RevE.01\State=1-A\HF=-1802.3151743\RMSD=2.
678e-09\RMSF=9.241e-06\Thermal=0.\Dipole=-0.806869,-1.1165707,0.601228
2\PG=C01 [X(C14H12N3O4S2)]\@

h+isoxicam.a2

1\1\GINC-V1282\FOpt\RB3LYP\6-31+G(d)\C14H14N3O5S1(1+)\JMH502\30-May-20
10\0\#\B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ul
trafine)\opt calc\1,1\C,-0.0089379566,0.0139460756,0.0150551538\C,0.
0018240915,-0.0033643617,1.4129640855\C,1.209512463,-0.0160259656,2.11
12776138\C,2.4270213088,-0.0084069528,1.4117233649\C,2.3926350746,-0.0
069168204,-0.0004812102\C,1.1934240305,0.0083388475,-0.7019085504\H,3.
8195406655,2.653222695,0.4380153168\S,3.9511406509,-0.0994998045,-0.89
03911828\N,4.9410484965,0.8333069252,0.1637377612\C,4.9020088876,0.320
2397979,1.5050491841\C,3.7075490989,-0.027040156,2.1254983198\C,6.1534
176964,0.0440983914,2.1502145085\N,7.287131803,0.1470190481,1.32356999
92\C,8.543414023,-0.148801432,1.7251068694\C,9.7457056142,-0.183827498
4,0.970255811\C,10.7276552839,-0.5486890986,1.8507516947\O,10.20239082
, -0.7342615461,3.0908443184\N,8.8601553528,-0.4624593911,2.985258286\H
,1.2200189483,-0.0256297869,3.1959131157\H,-0.9346230308,-0.0040739759
,1.9624137767\H,-0.9524269143,0.0304116306,-0.5223818089\H,1.198349097
,0.019873158,-1.7873985253\O,4.4741281355,-1.4630201991,-0.8250618276\O
,3.8383360929,0.6226381783,-2.154231196\C,4.7823520865,2.3072937117,0
.0423128966\H,4.8716859317,2.5860531589,-1.0080068602\H,5.588762739,2.
7777358766,0.6114755484\O,3.6514863338,-0.4542888319,3.379897027\H,4.5
639542581,-0.4553458508,3.7653080524\O,6.2928521378,-0.2961369013,3.34

38210778\H,7.0997364219,0.3304807635,0.3382535988\H,9.8556644763,0.027
5276822,-0.0832093164\C,12.1887574922,-0.7677636772,1.721676464\H,12.4
989903389,-0.6108718146,0.6865999396\H,12.7394577405,-0.0739868098,2.3
671306085\H,12.4516562062,-1.7884927102,2.0213438344\H,8.2589403315,-0
.636344351,3.78806627\Version=EM64L-G03RevE.01\State=1-A\HF=-1480.187
6012\RMSD=7.136e-09\RMSF=1.342e-05\Thermal=0.\Dipole=3.555474,0.725889
1,1.5451094\PG=C01 [X(C14H14N3O5S1)]\@

zwit-isoxicam.a2

1\1\GINC-V1287\FOpt\RB3LYP\6-31+G(d)\C14H13N3O5S1\JMH502\30-May-2010\0
\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultraf
ine)\opt calc\0,1\C,-0.0721263089,0.1236225877,-0.1097756933\C,-0.11
70121699,0.0633409807,1.2882016623\C,1.0600911299,-0.03801278,2.028909
8977\C,2.306487876,-0.0768072173,1.3861392\C,2.32482536,-0.0341436203,
-0.0190695094\C,1.1562383951,0.0708735734,-0.7714619891\H,4.1577005933
,2.6790518984,0.4807021008\S,3.921921956,-0.1707901895,-0.8214595904\N
,4.8777343712,0.6714817284,0.2695303657\C,4.8013754966,0.1868227784,1.
6176320888\C,3.5543133561,-0.1738918392,2.2117787512\C,6.0476622714,0.
1007831233,2.3041625432\N,5.9393046828,-0.377811375,3.6507031646\C,6.9
970686346,-0.5874631467,4.4224141759\C,7.0810076444,-1.200931619,5.714
6214828\C,8.4047369052,-1.2452398809,6.0250294278\O,9.158042236,-0.694
1042517,5.0334174721\N,8.2525484566,-0.2310835627,4.0855282413\H,1.040
5323749,-0.0893369277,3.1125677371\H,-1.0746295234,0.0980596166,1.8012
175099\H,-0.9911421544,0.2083782655,-0.6836272681\H,1.2162775104,0.116
0492269,-1.8546004661\O,4.3220607147,-1.5796884273,-0.8005351587\O,3.8
884586293,0.5778997317,-2.0838181931\C,5.0215212076,2.1258226848,0.083
8496376\H,5.1427225799,2.3435673867,-0.9776899362\H,5.9267832372,2.429
9867026,0.6150505835\O,3.4256541741,-0.5906425202,3.4075558605\O,7.177
3795605,0.4010226773,1.8705849264\H,4.9423351812,-0.6094123262,3.92397
33485\H,6.2530892495,-1.5730698928,6.2990009031\C,9.1606945534,-1.7536
651204,7.1991861793\H,8.4736663074,-2.2093737366,7.9157602745\H,9.8976
458037,-2.502966482,6.8893341183\H,9.6981157983,-0.9373156137,7.695201
8704\H,8.5684677631,-0.0052924993,3.1388761793\Version=EM64L-G03RevE.
01\State=1-A\HF=-1479.7941517\RMSD=6.504e-09\RMSF=8.690e-06\Thermal=0.
\Dipole=1.522221,-0.0397942,4.4648979\PG=C01 [X(C14H13N3O5S1)]\@

isoxicam

1\1\GINC-X138\FOpt\RB3LYP\6-31+G(d)\C14H13N3O5S1\JMH502\09-Jan-2010\0\
\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultraf
ine)\opt calc\0,1\C,0.0004226818,-0.0305157577,-0.0171885064\C,-0.01
38679261,-0.0269816283,1.3816838881\C,1.1796094662,-0.0060739651,2.103
499671\C,2.4120441908,0.0097031066,1.4317435719\C,2.4029115665,-0.0182
44258,0.0234399259\C,1.2168040376,-0.028480795,-0.7049133349\H,-0.9326
139081,-0.0385572618,-0.5734653424\H,-0.9610649232,-0.0359884936,1.913
6555951\H,1.1726378103,0.0020604361,3.1880551435\H,1.2501343886,-0.033
2727628,-1.7899977352\S,3.9837206046,-0.1109806847,-0.8208385217\O,4.4
869443526,-1.4807552003,-0.7389084036\O,3.8840284373,0.583904907,-2.10
63906979\N,4.9385957183,0.8433906835,0.2205748247\C,4.839703754,2.3092
944902,0.0136094245\H,3.8717306693,2.707115184,0.346031567\H,5.6357455
072,2.7780943182,0.5980221349\H,4.9901094708,2.531983777,-1.043002284\
C,3.6804534234,0.0532139436,2.1783814305\O,3.5891732686,-0.3090035227,
3.4614042725\C,4.8716770659,0.4099799815,1.5900062977\C,6.1238636203,0
.323810511,2.3507931011\O,6.1286665044,0.0953588536,3.5801380202\N,7.2
693601889,0.507184802,1.6292655368\H,8.4602756302,0.1037484646,4.33587
94712\C,9.0450348587,0.2852687758,3.4498171424\C,8.5719265811,0.483896
2359,2.1191091631\N,9.551301671,0.6768343874,1.2564741186\C,10.4000997
165,0.3720848382,3.3163774509\H,4.5092539546,-0.2213041561,3.849452913
2\H,7.1644361055,0.5901365495,0.621578009\O,10.7193166721,0.6036692108
,2.0221796406\C,11.5329648436,0.2618094475,4.2769782141\H,12.126295300
2,1.1835833683,4.2898081336\H,11.1530405003,0.0773701188,5.2851966607\
H,12.2017924571,-0.5612998045,3.9994906992\Version=EM64L-G03RevE.01\St
ate=1-A\HF=-1479.8229097\RMSD=5.794e-09\RMSF=5.449e-06\Thermal=0.\Dip
ole=-1.2264904,1.0065979,1.4456692\PG=C01 [X(C14H13N3O5S1)]\@

zwit-isoxicam-N.a2

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1\1\GINC-V1289\FOpt\RB3LYP\6-31+G(d)\C14H13N3O5S1\JMH502\31-May-2010\0
\0\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultraf
ine)\opt calc\0,1\C,-0.0974174031,0.2221916876,-0.1105538266\C,-0.14
31956699,0.0624884183,1.2796958117\C,1.0294055415,-0.1090475625,2.0137
569415\C,2.2768723855,-0.1244205597,1.366017882\C,2.2944992181,0.00696
80024,-0.0352345745\C,1.1295902321,0.1914245003,-0.7759632474\H,4.3287
394128,2.6727935424,0.5104768766\S,3.8847787714,-0.1471569042,-0.83768
83933\N,4.8695331865,0.6126132873,0.2933906743\C,4.7560693704,0.113286
0104,1.6273464261\C,3.5250553019,-0.251929728,2.1375517332\C,6.0205989
054,0.0312976419,2.3832113599\N,5.8929887047,-0.4598794189,3.678495324
4\C,6.9862705624,-0.5903488016,4.4096302406\C,7.1105474127,-1.18856980
82,5.7129585551\C,8.4305132832,-1.1800172922,6.0281925064\O,9.16720212
13,-0.6044991592,5.0350885419\N,8.2415340148,-0.1713727561,4.084765314
2\H,0.9971496299,-0.2237468363,3.0916009936\H,-1.0998334983,0.07789474
91,1.7949655111\H,-1.0148767112,0.3628257842,-0.6753962897\H,1.1910578
16,0.3055847248,-1.853854412\O,4.2338823958,-1.5679359547,-0.872345383
3\O,3.8903132254,0.6560011071,-2.0649263846\C,5.148934487,2.0511039336
,0.1243954351\H,5.3039792948,2.2615227321,-0.9336320578\H,6.0689102184
,2.2668173084,0.6706137133\O,3.3490829116,-0.7515286429,3.3691115953\O
,7.1054979494,0.3834912421,1.8843687299\H,6.2964522551,-1.5896815819,6
.2973461592\C,9.2051593907,-1.6480989406,7.208021336\H,8.536783508,-2.
1301107231,7.9253397505\H,9.9762464109,-2.3659349885,6.90061997446\H,9.
7045527173,-0.8067349958,7.7023776482\H,8.5788622032,0.0005044973,3.13
95120653\H,4.2574116674,-0.7672433363,3.805459566\Version=EM64L-G03Re
vE.01\State=1-A\HF=-1479.7991896\RMSD=7.324e-09\RMSF=2.074e-06\Thermal
=0.\Dipole=0.5745965,0.1851138,3.6382296\PG=C01 [X(C14H13N3O5S1)]\@

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o-isoxicam

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1\1\GINC-X137\FOpt\RB3LYP\6-31+G(d)\C14H12N3O5S1(1-)\JMH502\09-Jan-201
0\0\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ul
trafine)\opt calc\1,1\C,-0.0243439631,0.0280564713,0.0037008476\C,-
0.0208864096,-0.0428747136,1.4036370235\C,1.1819658946,-0.0673999997,2
.1079428396\C,2.4130710875,-0.0169689453,1.434171705\C,2.3816395426,0.
0286325961,0.0307404035\C,1.1863169735,0.0607063209,-0.6894259837\H,-0
.9641959377,0.0531291486,-0.5433291316\H,-0.9637747648,-0.0771001579,1
.9457485785\H,1.2076640516,-0.1307467337,3.1913182629\H,1.216002884,0.
1160559805,-1.7737879797\S,3.9625793771,0.0108783707,-0.8110806944\O,4
.429369663,-1.3791360495,-0.8741615825\O,3.8368421427,0.7856856751,-2.
0603976124\N,4.894831714,0.8740362201,0.2636087594\C,4.9726328514,2.33
22400521,0.0795798491\H,4.0838496408,2.8434772411,0.4816424614\H,5.863
3831256,2.6634981325,0.6177037196\H,5.0839689171,2.5649372057,-0.98062
13213\C,3.6888397752,-0.0317650684,2.2437164699\O,3.5862931238,-0.4376
348114,3.4455960872\C,4.8867725065,0.3882406451,1.6241009493\C,6.18904
85146,0.4416581362,2.2803493379\O,7.2177522932,0.8704292699,1.73087604
54\N,6.1970744208,0.0019570719,3.6073927472\H,9.026222904,0.7033444439
,3.199536424\C,8.6519340564,0.3432459619,4.143054515\C,7.2923823957,-0
.0207915064,4.435276231\N,7.1535069286,-0.4291579383,5.6905529199\C,9.
3096810023,0.1202158111,5.3114446161\H,5.2786150471,-0.3050134388,3.96
50953149\O,8.4527919613,-0.3379449021,6.2517381565\C,10.7342121868,0.2
782016903,5.7255903011\H,11.1599981515,-0.6793646617,6.0515242407\H,11
.3279391915,0.6535225547,4.8869068882\H,10.8281844834,0.9833945248,6.5
613088784\Version=EM64L-G03RevE.01\State=1-A\HF=-1479.3055578\RMSD=6.
602e-09\RMSF=1.557e-05\Thermal=0.\Dipole=-0.5391044,1.247044,0.1313968
\PG=C01 [X(C14H12N3O5S1)]\@

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h+sudoxicam.a2

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1\1\GINC-X119\FOpt\RB3LYP\6-31+G(d)\C13H12N3O4S2(1+)\JMH502\06-Jul-201
0\0\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ult
rafine)\opt calc\1,1\C,-0.006771716,0.0469027247,-0.0234586337\C,-0.
0190655471,0.0434839516,1.3745137688\C,1.1767844142,0.0200573758,2.092
6305482\C,2.4055426744,0.0030365098,1.4129835325\C,2.394141585,-0.0089
338435,0.000288757\C,1.2069309235,0.0165837309,-0.7207087191\C,3.67338
50527,-0.0288367253,2.1478159828\C,4.8835365671,0.294084337,1.54298294
04\N,4.9518147211,0.7956245336,0.198631162\S,3.964775075,-0.1343112674
,-0.8640870966\C,6.1200653338,0.0010893861,2.2087169725\N,7.2623498237

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,0.0815146286,1.3849750027\C,8.5192749984,-0.2181060912,1.7807113574\S
,9.909644696,-0.1961007507,0.7489543804\C,10.9229481836,-0.6784868338,
2.0946523256\C,10.1992239876,-0.8301070326,3.2243826532\N,8.8494794748
, -0.566632788,3.0302961994\O,3.5905638755,-0.4435859215,3.404425035\H,
4.4959586338,-0.4564869694,3.8054058559\H,1.1694591135,0.0211297273,3.
1773307024\H,-0.9642350813,0.0620271221,1.9084657537\H,-0.9410129095,0
.0718002937,-0.576480699\H,1.2293897411,0.0170018368,-1.8060445198\O,4
.4677148333,-1.5037984784,-0.7750546448\O,3.883595658,0.5770497798,-2.
1360230564\C,4.812291261,2.2707188342,0.0621721218\H,3.846800869,2.630
6428688,0.4380431358\H,4.9230022256,2.5389198568,-0.988859184\H,5.6140
475482,2.7370504485,0.641175702\O,6.2345502207,-0.3307444224,3.4077486
685\H,7.0580017597,0.2745104442,0.4028880068\H,8.1015453059,-0.6356973
47,3.729223364\H,10.5473843845,-1.1211767919,4.2062019033\H,11.9857841
888,-0.8178390491,1.9538375419\\Version=EM64L-G03RevE.01\State=1-A\HF=
-1763.8802564\RMSD=3.925e-09\RMSF=1.975e-05\Thermal=0.\Dipole=3.144926
8,0.6493679,2.1849509\PG=C01 [X(C13H12N3O4S2)]\@

zwit-sudoxicam

1\1\GINC-V1347\FOpt\RB3LYP\6-31+G(d)\C13H11N3O4S2\JMH502\15-Jun-2010\0
\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultraf
ine)\opt calc\0,1\C,0.0000050372,-0.0006507833,-0.0016491311\C,0.000
5954625,-0.0011611079,1.3919613035\C,1.2222978521,-0.0007963369,2.0681
818867\C,2.4219545907,0.0080625231,1.3467069732\C,2.4074731907,0.00521
59937,-0.047618017\C,1.1918456385,-0.0112557368,-0.7478445229\H,-0.942
262202,-0.0076663437,1.9302528658\H,1.2374858798,-0.0041827948,3.15480
35551\H,3.3716960442,0.0151441776,1.8750932535\H,3.3293099136,0.015315
5046,-0.6197666992\C,1.2091271699,-0.0266229612,-2.2450970212\S,-1.539
9869684,0.0677875965,-0.9167695394\N,-1.139365555,-0.8733301454,-2.247
5077639\C,0.0339992495,-0.4348665785,-2.9456809331\C,-0.0622794122,-0.
4542448519,-4.3670388513\O,-1.0362335792,-0.820020074,-5.0545771024\N,
1.1388665475,-0.0163851592,-5.0297630984\H,1.9009382476,0.2405214948,-
4.3244855082\C,1.2467489739,0.0899188675,-6.3438851977\O,-2.5815927593
, -0.6295316994,-0.1533149649\O,-1.740187166,1.4467886309,-1.3670977629
\C,-1.3671774591,-2.3264566621,-2.1598814957\H,-0.564143117,-2.8368396
43,-1.6083055715\H,-2.3246983979,-2.5118288756,-1.6723676706\H,-1.4092
264183,-2.7081098636,-3.1829476384\O,2.2863543028,0.3418859592,-2.8165
525024\N,0.2653493188,-0.2216059674,-7.2142045668\S,2.6665437394,0.654
8894314,-7.1980282517\C,0.5814863452,-0.0298688288,-8.5492859431\C,1.8
340008659,0.4369028398,-8.7342498194\H,2.3294474895,0.6713584345,-9.66
49289558\H,-0.158700689,-0.2555768316,-9.3048923901\H,-0.6112587219,-0
.5616667671,-6.7806501174\\Version=EM64L-G03RevE.01\State=1-A\HF=-1763
.491265\RMSD=5.129e-09\RMSF=2.273e-05\Thermal=0.\Dipole=2.2926898,-0.7
00968,-3.2984296\PG=C01 [X(C13H11N3O4S2)]\@

sudoxicam

1\1\GINC-V1363\FOpt\RB3LYP\6-31+G(d)\C13H11N3O4S2\JMH502\15-Jun-2010\0
\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultraf
ine)\opt calc\0,1\C,-0.074420677,0.2098113473,0.0873164831\C,-0.0151
970568,0.1280013814,1.4825993594\C,1.2113154305,-0.0001886581,2.134508
3955\C,2.4032661493,-0.0506077775,1.3947315443\C,2.3181324457,0.009535
0251,-0.0102430589\C,1.0994731546,0.1481053353,-0.6682416487\H,-1.0321
483526,0.3177113124,-0.4138340272\H,-0.9301595736,0.168825761,2.066881
2506\H,1.2617416708,-0.0584658697,3.2163731863\H,1.075187651,0.2073580
964,-1.7519542946\S,3.8369281735,-0.1701789042,-0.9493147995\O,4.21668
59376,-1.5812804549,-0.9743239177\O,3.7336939344,0.6089281393,-2.18528
05662\N,4.9296915904,0.6302145624,0.0869278429\C,4.954213728,2.1092410
603,-0.0304460938\H,4.0439814254,2.5693709612,0.3762870059\H,5.8173014
905,2.4697353947,0.5353455527\H,5.0718325955,2.3822941221,-1.079363189
9\C,3.7074352831,-0.1643174652,2.0675837408\O,3.651659497,-0.594725785
9,3.3315656091\C,4.8932859846,0.1211792341,1.4308651837\C,6.1672297908
, -0.1210778561,2.1093637592\O,6.2303421205,-0.422228709,3.3223693638\N
, 7.2932101405,-0.0023957423,1.3458184153\C,8.6015164406,-0.1792527587,
1.7746537103\C,10.7097429967,-0.5571772388,2.9114509932\N,9.595165633,
-0.0443024582,0.9378486091\C,10.7920342318,-0.260461628,1.5819054079\H
, 11.7107539194,-0.1842699063,1.0119399336\H,7.1742897698,0.1517184918,

0.3478891851\H,4.5911759487,-0.6137649726,3.675297662\S,9.0441499251,-
0.5830816108,3.4236662199\H,11.5108724759,-0.7612993863,3.6091778486\\
Version=EM64L-G03RevE.01\State=1-A\HF=-1763.5100696\RMSD=6.313e-09\RMS
F=4.141e-06\Thermal=0.\Dipole=-1.0689732,1.1705817,0.8817224\PG=C01 [X
(C13H11N3O4S2)]\\@

o-sudoxicam

1\1\GINC-V1310\FOpt\RB3LYP\6-31+G(d)\C13H10N3O4S2(1-)\JMH502\15-Jun-20
10\0\#\B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ul
trafine)\opt calc\\-1,1\C,0.0018792637,0.0003223939,0.0018973029\C,0.
0021173362,0.0005257544,1.4035175235\C,1.203487338,0.0004547469,2.1107
743068\C,2.4356982098,-0.003934947,1.4374691639\C,2.4076277104,0.02126
76144,0.0333434735\C,1.213804059,0.0141603382,-0.6897393249\H,-0.93671
46675,-0.0059572104,-0.5476981458\H,-0.9418915275,-0.0015765162,1.9446
052658\H,1.2264502404,0.0079977788,3.1960206213\H,1.2454709074,0.01418
37199,-1.7754283674\S,3.9888452424,0.101155765,-0.8048869351\O,3.87280
23315,-0.6062972886,-2.0938157095\O,4.4411436209,1.4968938043,-0.78939
56256\N,4.9313573129,-0.8096348202,0.2225218344\C,5.0288613783,-2.2547
808807,-0.0413037493\H,5.9240227946,-2.6043529677,0.477633997\H,4.1470
72239,-2.7990859826,0.3312363039\H,5.1430944584,-2.4262801324,-1.11266
66662\C,3.7098087273,-0.0218670675,2.24721386\O,3.6074594268,0.3174188
005,3.4692438774\C,4.9116802765,-0.3996903529,1.6065128352\C,6.2017739
113,-0.4789850756,2.2706340385\O,7.2521392223,-0.867658373,1.728000816
2\N,6.2076741389,-0.1186809861,3.6191628323\H,5.2934189091,0.171330857
8,4.0050415087\C,7.3020264489,-0.1550330111,4.4341478551\C,9.498423361
4,-0.3794902087,5.4914151885\N,7.2473851242,0.1870034074,5.7031331375\
C,8.4842142965,0.0586630375,6.2913415611\H,8.5817627816,0.3104854671,7
.3430702849\S,8.9020612392,-0.6650698079,3.8688617821\H,10.5363791045,
-0.5460977593,5.7496695074\\Version=EM64L-G03RevE.01\State=1-A\HF=-176
2.9968335\RMSD=3.051e-09\RMSF=9.264e-06\Thermal=0.\Dipole=-1.4687619,-
1.1027965,0.1154971\PG=C01 [X(C13H10N3O4S2)]\\@

h+propoxicam-q1.a2

1\1\GINC-V1381\FOpt\RB3LYP\6-31+G(d)\C14H20N3O4S1(1+)\JMH502\19-Jun-20
10\0\#\B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ul
trafine)\opt calc\\1,1\C,0.4045888951,-0.5768326361,-0.0421177928\C,0.
.2419206101,-0.3198317117,1.3221655036\C,1.3403765204,0.0119695302,2.1
174770582\C,2.619879057,0.0955945268,1.5497079998\C,2.7633365336,-0.18
30597294,0.1730543727\C,1.6748494054,-0.5121953369,-0.6261823671\H,-0.
4552523216,-0.8271621916,-0.6563482274\H,-0.7458301547,-0.3752749189,1
.7697821471\H,1.2162631155,0.2113231912,3.176647297\H,1.8155773749,-0.
705840855,-1.6850380366\S,4.4165653236,-0.1290488164,-0.5303253728\O,5
.1696288666,-1.3312811113,-0.1479861802\O,4.3463463237,0.2986769016,-1
.9253532385\N,5.0861518486,1.1403962561,0.3991779076\C,4.6957798003,2.
5145788273,-0.0079834248\H,3.6486120444,2.7354040369,0.2327080355\H,5.
3390951352,3.2135177844,0.5327563807\H,4.8605342379,2.6271878995,-1.08
01942539\C,3.8004531314,0.4134789099,2.3681478849\O,3.6714114726,0.163
6318219,3.6676919365\C,4.9846722066,0.849816272,1.8052530647\C,6.21701
13175,0.7654832733,2.5659637637\O,6.2626834714,0.572014458,3.795639618
8\N,7.3807763753,0.8303657669,1.8105256473\C,8.6513632215,0.57805101,2
.3561019419\H,4.5448139467,0.3447161625,4.1073969912\H,7.248040801,0.9
828783882,0.8153052014\H,8.6406011167,0.7693333338,3.4302823444\N,9.11
89987241,-0.9106255091,2.1975660129\H,9.4271701416,1.1664338499,1.8616
433644\C,10.4790188873,-1.0238321896,2.8289175051\C,8.1599376455,-1.84
87862852,2.8872056988\H,10.8366334602,-2.0488246463,2.7188039668\H,11.
166420418,-0.3383669151,2.3292338273\H,10.40222689,-0.7710816801,3.888
0944159\H,8.565435225,-2.8600505092,2.8200448662\H,8.0510609868,-1.545
2278704,3.9284019626\H,7.1958783934,-1.804376326,2.381653498\C,9.19908
7435,-1.2718293181,0.7380739062\H,9.8834018552,-0.5841310352,0.2364358
565\H,9.5741248023,-2.2932328969,0.6517486479\H,8.2013910275,-1.213717
8088,0.2996548513\\Version=EM64L-G03RevE.01\State=1-A\HF=-1408.6201338
\RMSD=6.868e-09\RMSF=3.508e-06\Thermal=0.\Dipole=4.063573,-0.3924617,1
.3299434\PG=C01 [X(C14H20N3O4S1)]\\@

zwit-propoxicam-q1

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1\1\GINC-V1305\FOpt\RB3LYP\6-31+G(d)\C14H19N3O4S1\JMH502\16-Jun-2010\0
\\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultraf
ine)\opt calc\0,1\C,0.3332150651,-0.5782401271,0.0421760285\C,0.2037
017224,-0.3615685108,1.4194027767\C,1.3289517125,-0.1123354505,2.20568
45983\C,2.606488725,-0.0661110845,1.6295002899\C,2.7115123987,-0.30454
64578,0.2482492255\C,1.5971312049,-0.5537848396,-0.5510967124\H,-0.546
5440573,-0.7663584207,-0.5677126583\H,-0.7807128174,-0.3848004345,1.88
01881626\H,1.2445407616,0.05005952,3.2754459227\H,1.7244951882,-0.7156
275322,-1.6172600726\S,4.36634392,-0.29029314,-0.4398920012\O,5.018616
8216,-1.5613902028,-0.0897353145\O,4.3017775606,0.1410237244,-1.842377
4519\N,5.0542893071,0.9215491273,0.4781571526\C,4.9336958194,2.3113200
153,0.0129547782\H,3.9591950454,2.7501918451,0.2734297584\H,5.73048530
32,2.8806917836,0.4983263662\H,5.0784967583,2.3475554141,-1.0677726211
\C,3.8051437379,0.1958304273,2.5028173444\O,3.676079355,-0.0747411721,
3.7422670948\C,4.9958074118,0.6738176727,1.8937206578\C,6.260823968,0.
7883538919,2.5760503401\O,7.3471912525,1.0843969716,2.0606077617\N,6.2
185405966,0.4629829568,3.96245573\C,7.3522518554,-0.0244821088,4.57722
86496\H,5.2658664032,0.2409943843,4.3009359446\H,7.3192128519,0.054244
8917,5.6665835085\N,7.5731845501,-1.6280863767,4.3519986029\H,8.256430
7535,0.4174318074,4.1547367027\C,8.8448856457,-2.0094818101,5.03096732
46\C,6.4164007787,-2.3628776537,4.9530790971\H,9.0014418715,-3.0869792
926,4.9378726658\H,9.6731420194,-1.4766495361,4.5590593866\H,8.7862819
385,-1.7380387968,6.0877034423\H,6.5396941454,-3.4335047289,4.77187351
43\H,6.390059174,-2.1691690947,6.0282257127\H,5.4918888586,-2.01125551
08,4.4899909038\C,7.6611478402,-1.9458752668,2.8834837837\H,8.43240191
32,-1.3238597774,2.4293579479\H,7.900330729,-3.0072026955,2.7761621339
\H,6.7055794617,-1.7338922594,2.4036417578\\Version=EM64L-G03RevE.01\S
tate=1-A\HF=-1408.2060795\RMSD=4.055e-09\RMSF=1.457e-06\Thermal=0.\Dip
ole=1.8037451,-1.8841228,3.8122635\PG=C01 [X(C14H19N3O4S1)]\@

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h+propoxicam-q2.a3b2

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1\1\GINC-V1349\FOpt\RB3LYP\6-31+G(d)\C15H22N3O4S1(1+)\JMH502\19-Jun-20
10\0\\#B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ult
rafine)\h+propoxicam-q2 confsearch\1,1\C,5.0090075457,0.2326372468,-
1.1654123081\C,4.7488569446,1.57398984,-0.8695763552\C,3.5094204686,1.
960521655,-0.3560869928\C,2.5125582823,1.00107322,-0.127748904\C,2.791
0941552,-0.3440778788,-0.4501743375\C,4.0234641485,-0.738792598,-0.958
4285975\H,5.9782215487,-0.0616933869,-1.5569825834\H,5.5165849205,2.32
37581095,-1.0360171068\H,3.3064838375,3.0007268231,-0.1243147977\H,4.2
104892935,-1.7848109329,-1.1806536053\S,1.4782600282,-1.5464484076,-0.
2134831548\O,0.4818939557,-1.4112523831,-1.284734159\O,2.0521731819,-2
.8494463343,0.1144729991\N,0.7435341337,-0.9032552089,1.1874898547\C,1
.4445138036,-1.1806285807,2.4670048502\H,2.3822904026,-0.6180903501,2.
5549919568\H,0.7758660834,-0.883763792,3.27920308\H,1.6460779402,-2.25
01528541,2.5377073553\C,1.1901012684,1.3808159175,0.3962905123\O,0.850
907479,2.6542815837,0.2018385254\C,0.33913811,0.4615937113,0.974198892
9\C,-1.0667464291,0.7876281641,1.1775976944\O,-1.5168117658,1.95137225
32,1.0299554933\N,-1.8945617411,-0.2638976008,1.4512242426\C,-3.326226
8879,-0.1258295587,1.5894261687\H,-0.0789740796,2.7721749353,0.5410673
753\H,-1.4513905862,-1.1758585639,1.5064877039\H,-3.545190005,0.928871
7144,1.7682761607\C,-4.1744151726,-0.6914065627,0.4372007316\H,-3.6617
81554,-0.6759390748,2.4780404051\N,-4.0802450582,-0.0215827936,-0.9383
471814\H,-3.9457476369,-1.7472429089,0.2661059031\H,-5.225627698,-0.61
48446958,0.7307751978\C,-5.2325819306,-0.5360066435,-1.7674543352\C,-4
.1915523144,1.4806941977,-0.826907388\H,-5.1526708848,-0.1217261015,-2
.7736816404\H,-5.1819516824,-1.6254210074,-1.8105431376\H,-6.171837646
5,-0.2214661253,-1.309713773\H,-4.23443982,1.8933097353,-1.8363360063\
H,-5.1108169368,1.7240677809,-0.2898019924\H,-3.3214760582,1.870144932
2,-0.295163261\C,-2.79419387,-0.3865309694,-1.6503304275\H,-2.81239936
79,0.0726644005,-2.640067787\H,-1.9388122678,-0.0248807552,-1.08876157
11\H,-2.7372621382,-1.4718411515,-1.7444137002\\Version=EM64L-G03RevE.
01\State=1-A\HF=-1447.9337618\RMSD=9.962e-09\RMSF=2.739e-06\Thermal=0.
\Dipole=-4.7229027,0.3085768,-0.4755073\PG=C01 [X(C15H22N3O4S1)]\@

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zwit-propoxicam-q2

1\1\GINC-V1422\FOpt\RB3LYP\6-31+G(d)\C15H21N3O4S1\JMH502\16-Jun-2010\0
\\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultraf
ine)\opt calc\0,1\C,4.9169171347,0.3022213315,-1.0014019144\C,4.5160
690169,1.6218873512,-0.75866179\C,3.2280569541,1.8978784649,-0.2987992
545\C,2.3154091353,0.8599493645,-0.0629852487\C,2.7365559674,-0.453586
5903,-0.332224388\C,4.0202045665,-0.7471537215,-0.7907134139\H,5.92334
24247,0.0910614895,-1.3535219942\H,5.2141167959,2.4383026026,-0.927196
462\H,2.8992828821,2.9159405006,-0.1154515261\H,4.3066283218,-1.779670
2901,-0.9671527235\S,1.5274215745,-1.7485123353,-0.0630740527\O,0.5925
994143,-1.7517283971,-1.2032469963\O,2.2217780813,-2.9901293027,0.3057
698544\N,0.7281147402,-1.1406498017,1.2662960141\C,1.251116784,-1.4613
445947,2.6028869799\H,2.0947428454,-0.8125894777,2.8813193325\H,0.4297
771002,-1.3117277047,3.3081675502\H,1.5622682144,-2.5068015054,2.63402
95906\C,0.9235058732,1.1892350786,0.4186970852\O,0.4975029575,2.361972
4762,0.1721779819\C,0.1702748237,0.1703108902,1.053682871\C,-1.2399073
413,0.2857222324,1.366913056\O,-1.9385826341,-0.6580351217,1.805505103
\N,-1.8311361504,1.5047079969,1.068030071\C,-3.2534572461,1.6150297254
,0.9414531257\H,-1.1882158076,2.2023773685,0.6661909461\H,-3.578663842
6,2.6207453631,1.2443575489\C,-3.8228570281,1.4563683727,-0.4854387114
\H,-3.7232844971,0.9045798531,1.6271828214\N,-3.7037073938,0.092244969
9,-1.1840315953\H,-4.8973988947,1.6683130381,-0.4546991355\H,-3.347832
4595,-2.1693057236,-1.1657401338\C,-4.593184655,0.1389272836,-2.3950918
903\C,-2.2910415659,-0.1908393161,-1.6595472227\H,-4.4994824211,-0.803
6552628,-2.9372416613\H,-5.6276762861,0.2826753699,-2.0778225648\H,-4.
2803778315,0.9656661772,-3.036036366\H,-2.3129958754,-1.1042390389,-2.
2559556082\H,-1.9533316823,0.6508668146,-2.2661700862\H,-1.6228738577,
-0.3372507159,-0.8172999776\C,-4.1604673257,-1.0280818065,-0.279953436
5\H,-4.1534152954,-1.9522567603,-0.8614101863\H,-3.4669435316,-1.10122
7676,0.5657389902\H,-5.1759199852,-0.8064024194,0.057552418\\Version=E
M64L-G03RevE.01\State=1-A\HF=-1447.5106949\RMSD=5.412e-09\RMSF=9.302e-
07\Thermal=0.\Dipole=-4.257167,1.2743537,-2.1260563\PG=C01 [X(C15H21N3
O4S1)]\@

h+propoxicam.a2

1\1\GINC-V1464\FOpt\RB3LYP\6-31+G(d)\C15H22N3O4S1(1+)\JMH502\08-Jul-20
10\0\\#B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ult
rafine)\h+propoxicam confsearch\1,1\C,-4.945706633,1.1239455656,0.57
27707777\C,-4.4357909648,2.1837111296,-0.1833145529\C,-3.120119889,2.1
54698366,-0.6487739821\C,-2.2970084026,1.0551962232,-0.3625494687\C,-2
.8273100495,0.0049168524,0.4167951022\C,-4.1374542218,0.0238264311,0.8
805640782\H,-5.972816534,1.1497089416,0.9245178378\H,-5.0674900394,3.0
356991955,-0.4162612082\H,-2.7249762285,2.9741344039,-1.2397508978\H,-
4.5192341078,-0.8076264897,1.4649328631\S,-1.7321787085,-1.3565780493,
0.8332508841\O,-0.7911192199,-0.9267990933,1.8726435571\O,-2.505503688
1,-2.5876627742,0.9702808632\N,-0.8242750032,-1.4440569855,-0.61343151
13\C,-1.4966645434,-2.1118923556,-1.7567270028\H,-2.3155284028,-1.5069
912465,-2.165800999\H,-0.7466171894,-2.2672826878,-2.5367138329\H,-1.8
790284622,-3.0786099463,-1.4271881827\C,-0.9036838168,1.0015509519,-0.
8291605949\O,-0.359545962,2.186410458,-1.1156094991\C,-0.1968048809,-0
.182266145,-0.9001020948\C,1.2453135572,-0.1863462184,-1.0772317244\O,
1.8926004063,0.8838346208,-1.3315889962\N,1.8896816465,-1.3568312696,-
0.8924258401\C,3.3170059211,-1.5743793808,-1.1083733245\H,0.5818656597
,2.0239215827,-1.3877658704\H,1.3017218437,-2.1356461693,-0.6090272126
\H,3.6441993935,-0.9255075002,-1.927487949\C,4.2108255423,-1.379997259
,0.1397698982\H,3.4250888091,-2.6073420453,-1.4503966765\C,4.747392879
7,0.0316863817,0.3973452704\H,3.7095436424,-1.7865480504,1.0254123408\H,
5.1096157038,-1.9942247668,0.0011947195\H,5.4355652308,0.0261736973,
1.2486267114\H,5.2958246345,0.3877563749,-0.480004466\N,3.7100523281,1.
0940487259,0.6904648147\C,2.9265865476,0.8312327379,1.9430802573\C,4.
3377195002,2.4551831713,0.7236741011\H,3.5555168585,3.1993121377,0.882
3740442\H,5.0634758816,2.497398684,1.538972831\H,4.8335083042,2.640880
9495,-0.2305921008\H,2.2153944285,1.6462541836,2.0856717641\H,2.378315
2636,-0.1054792709,1.8481845127\H,3.6152070953,0.7850440313,2.79006229
15\H,3.0321818695,1.0865809064,-0.1174155326\\Version=EM64L-G03RevE.01
\State=1-A\HF=-1447.956302\RMSD=6.455e-09\RMSF=2.102e-06\Thermal=0.\Di

pole=4.1532875,1.3168389,-0.2365801\PG=C01 [X(C15H22N3O4S1)]\@

zwit-propoxicam

1\1\GINC-V1292\FOpt\RB3LYP\6-31+G(d)\C15H21N3O4S1\JMH502\08-May-2010\0
\\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafi
ne)\opt calc\0,1\C,4.9454804813,0.2743042137,-0.9811021283\C,4.6207
369735,1.6232363343,-0.7937689099\C,3.3409538875,1.9922716078,-0.37839
02968\C,2.3612271634,1.0205025022,-0.1327985384\C,2.7080161587,-0.3255
680173,-0.3430824816\C,3.9819824942,-0.7114221711,-0.7578769857\H,5.94
51266353,-0.0096673454,-1.2993787183\H,5.3708888791,2.3896046641,-0.97
22062049\H,3.0695036726,3.034279972,-0.2415541762\H,4.2109615634,-1.76
46265167,-0.8899053702\S,1.4281148031,-1.5469988229,-0.0495606554\O,0.
5303683366,-1.5832655015,-1.2200073954\O,2.0489687744,-2.7944961051,0.
417419139\N,0.6029913596,-0.8290312354,1.2100680294\C,1.0924934762,-1.
0694254991,2.57731914\H,1.9582755191,-0.4373396996,2.8233345227\H,0.26
90156937,-0.8319699649,3.2555661843\H,1.3588622714,-2.1214290175,2.692
4129119\C,0.974872639,1.4525458458,0.2817474659\O,0.6300737678,2.63580
04589,-0.0040383428\C,0.1239738987,0.4930169099,0.8943665779\C,-1.2883
108375,0.6872078911,1.052443888\O,-2.0675863239,-0.2463886775,1.457852
7145\N,-1.8218442543,1.8961279223,0.6978894847\C,-3.2465128211,2.07618
41048,0.534435033\H,-1.1382538105,2.5728270447,0.3360188465\H,-3.48940
14557,3.1301874581,0.7083698443\C,-3.7862350301,1.685610993,-0.868689
2761\H,-3.7525871553,1.4956115175,1.3122842795\H,-4.8840125625,1.72435
85082,-0.8505229031\H,-3.4701573263,2.4450841237,-1.5955999734\C,-3.29
06921664,0.3546256239,-1.4484451964\H,-3.7762697609,0.1564952061,-2.41
1281321\H,-2.2116499134,0.3990679976,-1.6165040241\N,-3.5112646728,-0.
8575711483,-0.5784202237\H,-2.9777758006,-0.6416047098,0.3610623081\C,
-4.9421728384,-1.1191160436,-0.2786366358\H,-5.0084808546,-1.991518657
9,0.3745423411\H,-5.374038743,-0.2584528727,0.2329649574\H,-5.48643332
71,-1.311395395,-1.2087531452\C,-2.8392363035,-2.0585304823,-1.1643006
594\H,-2.9841087818,-2.9007650016,-0.4846029525\H,-3.2810588203,-2.283
8339293,-2.1399381618\H,-1.7688988885,-1.8596281914,-1.2605059917\\Ver
sion=EM64L-G03RevE.01\State=1-A\HF=-1447.5466246\RMSD=5.777e-09\RMSF=7
.362e-06\Thermal=0.\Dipole=-3.2704601,0.0544033,-0.9749873\PG=C01 [X(C
15H21N3O4S1)]\@

propoxicam.alb2

1\1\GINC-V1289\FOpt\RB3LYP\6-31+G(d)\C15H21N3O4S1\JMH502\11-Jul-2010\0
\\#B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafi
ne)\propoxicam confsearch\0,1\C,5.0888677888,-0.949736489,0.04415031
75\C,5.2079891766,0.444381055,0.0547666935\C,4.0736048064,1.2546658697
,0.0063083283\C,2.7942889854,0.6799810218,-0.0565235983\C,2.7002165996
, -0.7250922805,-0.0924323733\C,3.8260850711,-1.5421799958,-0.032144869
3\H,5.9760070485,-1.575119867,0.0906042831\H,6.1915987337,0.9031833517
,0.1060381534\H,4.1611825083,2.3356570358,0.0200957137\H,3.7101246292,
-2.621560037,-0.0445583936\S,1.0674626939,-1.4402722092,-0.2849118957\O,
0.6643422714,-1.3316454247,-1.6873294834\O,1.0190988156,-2.733357637
6,0.4066957642\N,0.1383496121,-0.3348599762,0.6029847696\C,0.085508647
3,-0.5578536736,2.0657410982\H,1.0343159311,-0.3003440661,2.555953914\H,
-0.705749528,0.0830528678,2.4625709344\H,-0.1607796908,-1.6015127828
,2.2628886974\C,1.5858199763,1.522899716,-0.0810733235\O,1.7976887062,
2.8005089729,-0.4192569633\C,0.3349954203,1.0294198784,0.1961904443\C,
-0.8546530055,1.8894272925,0.047621829\O,-0.7278412766,3.1233374982,-0.
1625972657\N,-2.0620157867,1.2976104671,0.1481402472\C,-3.2988702356,
2.0315464562,-0.1070486863\H,0.8970209328,3.2508234812,-0.374724718\H,
-2.1294759249,0.2762556982,0.1139131124\H,-3.3540764878,2.3087000331,-
1.1709208192\C,-4.5285292512,1.2034649316,0.2827251201\H,-3.2704431859
,2.9684954413,0.458298619\C,-4.6754045122,-0.1151745563,-0.4940291572\H,
-4.5202830566,1.0150460504,1.3639783061\H,-5.417629948,1.81604063,0.
0844681867\H,-5.6958422289,-0.5221608522,-0.3536982392\H,-4.5683528988
,0.0994131591,-1.5646661494\N,-3.6605499557,-1.1228894579,-0.138143698
2\C,-3.9709683371,-1.793418293,1.1239094711\C,-3.4710106852,-2.1037981
372,-1.2085896286\H,-2.682557439,-2.8073363282,-0.9246880603\H,-4.3926
046437,-2.6788901588,-1.4219455076\H,-3.1549736558,-1.5969733091,-2.12
54555066\H,-3.1617933368,-2.4852701189,1.3786912254\H,-4.0616620975,-1

.0648420598,1.9351264093\H,-4.9162011862,-2.3682141972,1.0703516984\\V
ersion=EM64L-G03RevE.01\State=1-A\HF=-1447.5608646\RMSD=5.304e-09\RMSF
=2.608e-06\Thermal=0.\Dipole=-0.3100389,-0.2302846,1.111342\PG=C01 [X(
C15H21N3O4S1)]\\@

o-propoxycam.alb3c2d2

1\1\GINC-V1378\FOpt\RB3LYP\6-31+G(d)\C15H20N3O4S1(1-)\JMH502\09-Jul-20
10\0\#\B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ult
rafine)\o-propoxycam confsearch\\-1,1\C,5.1981313511,0.9089592589,-1.
1226845956\C,4.5733879355,2.1577629376,-0.9962615918\C,3.2375660983,2.
2451595481,-0.6073231229\C,2.4885014381,1.089728953,-0.3286093303\C,3.
1313292622,-0.149042015,-0.4898362881\C,4.4702597716,-0.2545866296,-0.
870415746\H,6.2423502289,0.8433269732,-1.4205813805\H,5.1358738163,3.0
667456086,-1.2012665841\H,2.7316908069,3.2009274475,-0.5117605473\H,4.
9250182186,-1.2370402116,-0.9598096489\S,2.1352841373,-1.6104978476,-0
.2098739452\O,1.3506509832,-1.867099742,-1.4245326584\O,3.007866991,-2
.678415643,0.3172343818\N,1.1385611313,-1.0782060908,1.0092610553\C,1.
5804297854,-1.2991825053,2.3956938063\H,2.3262228041,-0.5520197751,2.7
107864813\H,0.6861292223,-1.2150158955,3.016576085\H,1.9985980016,-2.3
022417002,2.495515305\C,1.048994577,1.2380131534,0.1062356246\O,0.5014
714546,2.3645595998,-0.146144747\C,0.4215476591,0.1477079666,0.7385760
654\C,-0.964542195,0.154714211,1.2305548167\O,-1.4603188492,-0.7939441
041,1.8739266752\N,-1.6874858915,1.2915145805,0.9536181726\C,-3.024152
2284,1.5124002712,1.4586920893\H,-1.1618140103,2.0300539115,0.47383640
98\H,-3.0821181232,2.5275042896,1.8794217167\C,-4.1330248873,1.3599983
504,0.3968218393\H,-3.1913127918,0.8002160048,2.274359903\C,-4.2317611
933,-0.0660791046,-0.151728092\H,-5.0827454531,1.6701771197,0.85842300
98\H,-3.9398426581,2.0462889647,-0.4391331026\H,-3.2384560958,-0.36913
51467,-0.4953403919\H,-4.5065261628,-0.7640039747,0.6652087513\N,-5.15
49623754,-0.2022291676,-1.2890707333\C,-4.9580212892,-1.4738643987,-1.
9729774431\C,-6.5486939881,-0.0366168177,-0.9067394976\H,-7.187515252,
-0.1200407566,-1.794643955\H,-6.8847056012,-0.7989359192,-0.1695765632
\H,-6.7119619184,0.9524480644,-0.4682746161\H,-5.6019114319,-1.5210371
736,-2.8602889195\H,-3.9164628804,-1.5625512656,-2.297545851\H,-5.1920
973982,-2.3496113297,-1.3314108371\\Version=EM64L-G03RevE.01\State=1-A
\HF=-1447.0278528\RMSD=5.078e-09\RMSF=6.812e-06\Thermal=0.\Dipole=-0.2
532378,1.0449816,0.04363\PG=C01 [X(C15H20N3O4S1)]\\@

h+hybrid

1\1\GINC-V1374\FOpt\RB3LYP\6-31+G(d)\C17H14N3O3S1(1+)\JMH502\15-Jun-20
10\0\#\B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ul
trafine)\opt calc\\1,1\C,0.0508454582,0.0776917001,-0.0940510864\C,0.
0793685997,0.0370918138,1.2964893157\C,1.3110739479,-0.0739925405,1.94
61499158\C,2.4926017135,-0.1470184163,1.2001055464\C,2.4547430315,-0.1
220581166,-0.1929049767\C,1.2269473307,-0.0069390945,-0.874041806\H,-0
.8479877091,0.0912792064,1.8584153657\H,1.3470392447,-0.1064511328,3.0
307437844\H,3.4481209427,-0.2434841998,1.7069774274\H,3.3799355224,-0.
2397193495,-0.7509854191\C,1.139853975,-0.0184620213,-2.3269560209\S,-
1.5022630634,0.354617145,-0.9329758588\N,-1.1840969585,-0.6476031896,-
2.2752969076\C,-0.0137494991,-0.3289604904,-2.9976231939\C,-0.18885764
67,-0.3215581833,-4.4263163567\N,0.8230898603,-0.0944020571,-5.3721288
071\C,-1.3977515416,-0.5206707631,-5.0674784539\C,-2.6547522162,-0.803
6505731,-4.2951224122\C,-1.1444517257,-0.3949553481,-6.4688445426\O,-2
.612510082,-0.2509694694,-0.1996677833\O,-1.564142463,1.7566453739,-1.
351978203\O,2.2603214808,0.272368123,-3.076628967\H,2.8429546585,0.876
368402,-2.5859226058\C,-2.2675313397,-1.4046997754,-2.9310523167\H,-3.
1145323542,-1.4262379659,-2.2437351156\H,-1.9145188322,-2.4341769027,-
3.063848763\H,-3.2969677206,-1.5177171486,-4.8254174584\H,-3.239918181
6,0.1157037982,-4.1580467262\H,1.7800311509,0.1121869352,-5.1049865097
\C,-1.9002222445,-0.4644425528,-7.6419346707\C,-1.2657711301,-0.273661
2136,-8.8805756291\C,0.0926619261,-0.0189969417,-8.9476211654\N,0.8345
326158,0.0494709338,-7.8021245929\C,0.2579925281,-0.1271804441,-6.5952
930609\H,-2.9677976128,-0.6596797021,-7.6047450397\H,-1.8312667271,-0.
3211702107,-9.8042189017\H,0.6332214528,0.1366048743,-9.8725646026\H,1
.8311309649,0.2369845345,-7.8728310464\\Version=EM64L-G03RevE.01\State

=1-A\HF=-1444.1003121\RMSD=7.117e-09\RMSF=1.036e-05\Thermal=0.\Dipole=2.5409901,-0.5552478,-4.9918138\PG=C01 [X(C17H14N3O3S1)]\@

zwit-hybrid

1\1\GINC-V1398\FOpt\RB3LYP\6-31+G(d)\C17H13N3O3S1\JMH502\15-Jun-2010\0
\\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\\opt calc\\0,1\C,0.0334195459,0.0676464786,-0.0950309278\C,-0.0074637852,0.4158454958,1.2545173074\C,1.1834356585,0.4501379127,1.9825994761\C,2.3976684808,0.1496286132,1.3537993831\C,2.4247732583,-0.1991220823,0.0045757287\C,1.2407398946,-0.2553775617,-0.7454381852\H,-0.9587074953,0.6465541481,1.7244625989\H,1.162325058,0.7130948709,3.0367392611\H,3.3243181325,0.1843622602,1.9208991581\H,3.356133041,-0.4348731656,-0.5008172262\C,1.292639129,-0.650039566,-2.1834554817\S,-1.4951821455,0.1461365661,-1.0363963592\N,-1.1533785196,-1.1469097505,-2.0714731441\C,0.0682956049,-1.0165308978,-2.8057254877\C,-0.0356629729,-1.2417101065,-4.179012296\N,1.0655089305,-1.2430699669,-5.0452793333\C,-1.2096373323,-1.4838673106,-4.9071667502\C,-2.5214969456,-1.5140987892,-4.1759389971\C,-0.83196656,-1.6228403858,-6.2599192043\O,-2.6344526657,-0.2512916599,-0.1955533907\O,-1.5527030625,1.4390301655,-1.7367808114\O,2.3912521743,-0.6174337838,-2.8159053099\C,-2.2575102639,-1.8987801149,-2.6984121974\H,-3.1467551758,-1.7555919742,-2.0815327889\H,-1.9785148176,-2.9586055434,-2.6481074444\H,-3.2133119656,-2.2515772845,-4.6062684079\H,-3.0261271658,-0.5384434965,-4.2209574525\H,1.9884253677,-1.0324429735,-4.6438585926\C,-1.4658278929,-1.8517890263,-7.4953332672\C,-0.6931898589,-1.9159409186,-8.6681604423\C,0.6795856241,-1.7562537423,-8.6434923097\N,1.3064073332,-1.5288968991,-7.433691473\C,0.6079263038,-1.458835452,-6.2892246791\H,-2.5432599702,-1.9726511716,-7.5497775661\H,-1.1720911963,-2.0906606534,-9.6259921831\H,1.3219841555,-1.7912369858,-9.5123774022\H,2.3134875739,-1.4077044194,-7.4124959219\\Version=EM64L-G03RevE.01\State=1-A\HF=-1443.7062282\RMSD=9.211e-09\RMSF=9.939e-06\Thermal=0.\Dipole=1.1919375,-1.5010077,-3.1679497\PG=C01 [X(C17H13N3O3S1)]\@

hybrid

1\1\GINC-V1395\FOpt\RB3LYP\6-31+G(d)\C17H13N3O3S1\JMH502\15-Jun-2010\0
\\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\\opt calc\\0,1\C,-0.0080704983,0.0825057005,-0.0474335406\C,-0.0479088807,0.2581093016,1.3341593221\C,1.1491103314,0.2774144649,2.0507701323\C,2.3656540523,0.119133794,1.3742901857\C,2.3955870431,-0.0759470726,-0.004362518\C,1.2009818555,-0.1052200341,-0.7545800166\H,-1.0044777693,0.3803406372,1.8330729547\H,1.1336730696,0.4165623464,3.1277103558\H,3.2988160747,0.1299886797,1.9311266654\H,3.34309171,-0.2472545331,-0.5063275689\C,1.1912043305,-0.3624215984,-2.1839877909\S,-1.5106664254,0.2104259272,-0.9926968228\N,-1.1405410316,-0.9544091338,-2.1669751232\C,0.0805101115,-0.7894603914,-2.8614812771\C,0.0057116623,-1.1072151445,-4.2705861289\N,1.0648021874,-1.1342104895,-5.163524798\C,-1.1747146989,-1.416064154,-4.9317986752\C,-2.4837937543,-1.4922900791,-4.201468268\C,-0.8328249076,-1.6267690547,-6.3031596584\O,-2.6560585198,-0.2929666442,-0.2262438524\O,-1.5778718248,1.5483586823,-1.590476293\O,2.3851309494,-0.248430147,-2.8837556828\H,2.7976228843,0.609248403,-2.6863497963\C,-2.2018998561,-1.8177404686,-2.7282199916\H,-3.0856782251,-1.6959252171,-2.1003315115\H,-1.8592642048,-2.8558019135,-2.6366643238\H,-3.1253759395,-2.2808632948,-4.6158782648\H,-3.0431447371,-0.5491794453,-4.284962904\H,2.0241870126,-0.9254359946,-4.925445415\C,-1.516126545,-1.9550101049,-7.4849025421\C,-0.7661234185,-2.0696740816,-8.6518410358\C,0.6283644299,-1.8585272917,-8.6186896681\N,1.3182405045,-1.5461021288,-7.5161816467\C,0.582078585,-1.441573283,-6.4100135413\H,-2.5920954261,-2.1115984013,-7.493808544\H,-1.2426718185,-2.3195173184,-9.5952069195\H,1.2115612004,-1.9477557604,-9.5328888287\\Version=EM64L-G03RevE.01\State=1-A\HF=-1443.7246824\RMSD=8.743e-09\RMSF=2.709e-05\Thermal=0.\Dipole=0.8588912,-0.5573263,0.3764433\PG=C01 [X(C17H13N3O3S1)]\@

o-hybrid

1\1\GINC-V1387\FOpt\RB3LYP\6-31+G(d)\C17H12N3O3S1(1-)\JMH502\15-Jun-20

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10\0\#\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ul
trafine)\opt calc\ -1,1\C,0.0196325688,0.0669645761,-0.0746428052\C,-
0.0302933293,0.3649721309,1.2885401587\C,1.1537697562,0.3829818298,2.0
26635561\C,2.373517518,0.1161108013,1.3874513682\C,2.4074918689,-0.184
8844939,0.0281833981\C,1.2279638533,-0.232212238,-0.7357849891\H,-0.98
78428357,0.5727987957,1.7575539411\H,1.1263416485,0.6091309459,3.09010
57019\H,3.2998093204,0.1409253991,1.9582794253\H,3.3393083258,-0.39061
89483,-0.4902929939\C,1.3081949053,-0.5840856138,-2.1882994637\S,-1.49
83695542,0.1675711918,-1.0239299762\N,-1.1359324735,-1.0521633151,-2.1
081475906\C,0.1055815618,-0.9218663157,-2.8313999065\C,-0.0047258966,-
1.1653759909,-4.2277292949\N,1.0631721502,-1.1774577473,-5.1076309017\
C,-1.1889845637,-1.4337806347,-4.9192489505\C,-2.4940929206,-1.5011976
839,-4.1810014122\C,-0.8338147359,-1.607758216,-6.2864930887\O,-2.6399
322491,-0.2839669924,-0.199662645\O,-1.5883765868,1.512447561,-1.62387
38334\O,2.4387573259,-0.533739644,-2.7783133571\C,-2.2114366856,-1.861
477871,-2.7058658322\H,-3.0988501937,-1.7498305134,-2.0789733476\H,-1.
8830457269,-2.9081708583,-2.6506640257\H,-3.1591957102,-2.2720375313,-
4.6010265917\H,-3.0471739101,-0.5497088965,-4.2277959687\H,2.007001183
5,-0.9784969117,-4.7846200486\C,-1.4970566561,-1.8863988188,-7.4909947
145\C,-0.7288106381,-1.9797825046,-8.657971816\C,0.6610487373,-1.79435
38394,-8.603655679\N,1.3412204786,-1.5244367609,-7.4719862968\C,0.5998
396857,-1.4391820171,-6.3731610315\H,-2.5765227398,-2.0231806879,-7.52
27326393\H,-1.201386626,-2.1928113166,-9.6144897999\H,1.2598860847,-1.
8645177471,-9.5106974531\\Version=EM64L-G03RevE.01\State=1-A\HF=-1443.
2114743\RMSD=7.288e-09\RMSF=5.496e-06\Thermal=0.\Dipole=-0.8781558,-0.
8516952,1.0421491\PG=C01 [X(C17H12N3O3S1)]\\@

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Table S4. Gas phase optimised geometries of all the studied species in their *solution phase* conformation (if different from gas phase).

NOTE: All species had zero imaginary frequencies, as determined from frequency calculations at the B3LYP/6-31+G(d) level.

h+piroxicam.alc2

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1\1\GINC-V1298\FOpt\RB3LYP\6-31+G(d)\C15H14N3O4S1(1+)\JMH502\01-May-20
10\0\#\ B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ul
trafine)\opt calc\1,1\C,0.1338004972,-0.2597682601,-0.0987937791\C,0
.041960864,-0.168853755,1.2930854072\C,1.1901830946,-0.0096554743,2.07
0019641\C,2.4507462472,0.0631937778,1.4571678581\C,2.521196566,-0.0466
305107,0.0510813796\C,1.3819143492,-0.2021264267,-0.7295567215\S,4.141
8249982,-0.0461516028,-0.7229536573\N,4.9647781825,1.0459355751,0.3224
753091\C,4.8723288966,0.6280278804,1.6959533048\C,3.6720118125,0.22011
82977,2.2572739392\C,6.099016473,0.500930024,2.4491195188\N,7.25844636
09,0.6016778117,1.6483371792\C,8.5521941959,0.4259601282,2.0348682543\
N,9.4787042371,0.3345803488,1.034344101\C,10.8171264218,0.1790706054,1
.2488371085\C,11.2972452702,0.0993208388,2.5312396807\C,10.3737866922,
0.180685802,3.5942578221\C,9.0180850894,0.341822345,3.3625741834\H,1.1
206871904,0.0635128153,3.1500311144\H,-0.9288604786,-0.2193302394,1.77
67073925\H,-0.7641473713,-0.3765920734,-0.6981875295\H,1.467399764,-0.
271829608,-1.8094852636\O,4.7908766509,-1.3427547015,-0.5283590214\O,4
.0582437771,0.5746292065,-2.042755389\C,4.6818102705,2.4864445535,0.08
05881158\H,3.6639215643,2.762194265,0.3817445507\H,4.824525323,2.70261
60261,-0.9786314733\H,5.3949567618,3.068619476,0.6704135438\O,3.558038
8063,-0.1171742914,3.5356367266\H,4.4399961864,-0.0037806748,3.9767205
89\O,6.1593000425,0.2809932958,3.6667234703\H,7.0215458219,0.687497105
3,0.657086517\H,9.1573249384,0.3659272917,0.0697955918\H,11.4336842891
,0.1227930867,0.3595241785\H,12.3593024215,-0.0252434209,2.7065356056\
H,10.7274875299,0.118131654,4.6191515707\H,8.2974187365,0.3997267393,4
.1660288939\Version=EM64L-G03RevE.01\State=1-A\HF=-1443.1212521\RMSD=
7.134e-09\RMSF=7.296e-06\Thermal=0.\Dipole=4.1003059,1.068628,1.045369
5\PG=C01 [X(C15H14N3O4S1)]\@
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h+tenoxicam.a2

```
1\1\GINC-V1401\FOpt\RB3LYP\6-31+G(d)\C13H12N3O4S2(1+)\JMH502\28-May-20
10\0\#\ B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ul
trafine)\opt calc\1,1\S,0.0115130337,0.0898879769,0.1118562133\C,0.0
764903736,0.0642824058,1.8371220514\C,1.3596777424,0.0135176395,2.3349
303939\C,2.3031948315,-0.015520742,1.283162006\C,1.7441302966,0.013357
0349,0.013017763\C,2.5123616628,0.0467636488,-1.2086326963\C,3.8659539
44,-0.2758881751,-1.1869672816\N,4.4976082644,-0.8234119731,-0.0157089
827\S,4.082713846,0.0220271183,1.4288255816\O,4.5600956766,1.390865223
,1.2445180979\O,4.506593901,-0.792932179,2.5632412081\H,1.6103885161,-
0.007294104,3.3887797386\H,-0.8461177499,0.0822461258,2.4041085794\C,4
.4309757859,-2.307714629,0.0873951222\H,3.3966890273,-2.6691396566,0.1
337818168\H,4.9743776113,-2.6278005283,0.9767121284\H,4.912013004,-2.7
231713156,-0.8021020221\O,1.8787614847,0.4718848661,-2.2942458136\H,2.
522372763,0.4900524983,-3.0502035413\C,4.6908268375,0.0432514195,-2.3
253918855\O,4.2570280233,0.3772827905,-3.4375895432\N,6.0759864681,-0.
0132215258,-2.048532241\H,6.2552887308,-0.2111890909,-1.0619258545\C,7
.1028794882,0.3159257531,-2.8803302963\N,8.3433729541,0.3975673386,-2.
312235285\C,9.4798461111,0.6952024915,-3.006289277\C,9.411232139,0.939
1194873,-4.354272426\C,8.1485678602,0.8732601963,-4.9794185223\C,7.003
26548,0.5670880903,-4.263811471\H,8.4310666015,0.2447200932,-1.3105547
755\H,10.3936397813,0.723911509,-2.4246148798\H,10.3109913198,1.176934
9868,-4.9093362051\H,8.0661715886,1.0642132582,-6.0453300597\H,6.02775
31286,0.5189143798,-4.7266958007\Version=EM64L-G03RevE.01\State=1-A\H
F=-1763.8706244\RMSD=6.469e-09\RMSF=4.135e-05\Thermal=0.\Dipole=3.7329
562,-0.4464975,-2.546306\PG=C01 [X(C13H12N3O4S2)]\@
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h+lornoxicam.a2

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1\1\GINC-V1286\FOpt\RB3LYP\6-31+G(d)\C13H11Cl1N3O4S2(1+)\JMH502\28-May-2010\0\0\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\opt calc\1,1\,S,0.0082342774,0.0845076164,0.1076392512\C,0.072087709,0.0588286616,1.8481141388\C,1.3544517868,0.0103979857,2.3542447658\C,2.2944670695,-0.0144869968,1.3029728208\C,1.7459163207,0.0122941206,0.0293557305\C,2.5201255307,0.0530085599,-1.1859352103\C,3.8770364827,-0.2568530294,-1.156739861\N,4.504684569,-0.8010894405,0.0184074346\S,4.0755986453,0.0366482402,1.4605087125\H,1.5949999706,-0.0103890813,3.4100905085\Cl,-1.3763158282,0.0828369652,2.7647731327\O,4.5378944145,1.4110807026,1.2841347624\O,4.4945675189,-0.7774365049,2.5968467861\C,4.453757587,-2.2866022719,0.1177341869\H,3.423210522,-2.6595133035,0.1540600018\H,4.9931520153,-2.602926474,1.0108002534\H,4.9469891721,-2.694076772,-0.7686930718\O,1.887119831,0.470043085,-2.2755090743\H,2.5345669714,0.4946169354,-3.0281149675\O,4.2719207874,0.3977723638,-3.4052511863\C,4.7044215882,0.0674751829,-2.2912529317\N,6.0892606421,0.019403962,-2.01068879\H,6.2689030171,-0.175526561,-1.0238604661\C,7.1164260655,0.3518664114,-2.8414091212\N,8.3557149115,0.4387423523,-2.2714723127\C,9.4920968237,0.740521662,-2.9639682107\C,9.4246175099,0.9832738248,-4.3122293111\C,8.1632433142,0.9118567594,-4.9392339283\C,7.018005055,0.6016411269,-4.2251488605\H,6.0435434781,0.5492491889,-4.6897427315\H,8.4428302376,0.2864660835,-1.2696495771\H,10.4048466301,0.773233647,-2.3808600163\H,10.3242639519,1.2243511124,-4.8660735986\H,8.0816605984,1.1017241872,-6.0054038064\Version=EM64L-G03RevE.01\State=1-A\HF=-2223.4567063\RMSD=8.589e-09\RMSF=3.369e-05\Thermal=0.\Dipole=4.9556804,-0.4308136,-3.2565773\PG=C01 [X(C13H11Cl1N3O4S2)]\@
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h+meloxicam

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1\1\GINC-X149\FOpt\RB3LYP\6-31+G(d)\C14H14N3O4S2(1+)\JMH502\08-Jan-2010\0\0\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\opt calc\1,1\C,0.0936605277,-0.216337144,-0.0788544102\C,0.019503302,-0.1485168843,1.3154717918\C,1.1789062922,-0.0173884467,2.0806820564\C,2.4326592377,0.0501734583,1.4528674256\C,2.4855252974,-0.0362531956,0.043985416\C,1.3346824278,-0.1637955162,-0.7243177711\H,-0.8129223132,-0.3115918688,-0.6689939017\H,-0.9460001076,-0.1950514691,1.8099400579\H,1.1233267887,0.0386520153,3.1625380111\H,1.4058432539,-0.2167878173,-1.8062355505\S,4.0972282565,-0.049547836,-0.7507132909\O,4.7263933262,-1.3578682934,-0.5756720181\O,4.0048774491,0.5883832941,-2.0611597572\N,4.9472016509,1.0205874459,0.297623888\C,4.6762139086,2.4668686163,0.0766553761\H,3.6636650777,2.7494203392,0.389495835\H,5.4000657351,3.0351962273,0.6670764575\H,4.81257698,2.6943184298,-0.9810058995\C,3.6649246726,0.1808657061,2.2380009728\O,3.5662658154,-0.1744119611,3.5128522875\C,4.8621138246,0.5851510086,1.6648880485\C,6.0908893819,0.4409693119,2.3972260006\O,6.1924265433,0.1943280786,3.6093470536\N,7.2582814982,0.5607082804,1.6151984918\C,8.5022099792,0.3668207187,2.101165358\C,10.6345509288,-0.010571742,3.3335510528\N,9.5989577305,0.3919538968,1.3298540031\C,10.80221267,0.1803293655,2.0063584195\H,11.7252643143,0.1847039915,1.4423561185\H,7.0853116183,0.6710952732,0.6137907967\H,4.4506267968,-0.0786084711,3.9493438\S,8.9137856724,0.0662303415,3.7542942454\C,11.6698374584,-0.2671073339,4.3845935954\H,11.5071414754,-1.2318117962,4.8781252322\H,12.6643683757,-0.2821552871,3.9296407324\H,11.6595751166,0.5125793867,5.1544337424\H,9.5611278705,0.5402914597,0.325681133\Version=EM64L-G03RevE.01\State=1-A\HF=-1803.1995681\RMSD=4.609e-09\RMSF=2.427e-05\Thermal=0.\Dipole=3.3928713,1.117574,1.1433738\PG=C01 [X(C14H14N3O4S2)]\@
```

zwit-meloxicam-enolate.alb2

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1\1\GINC-V1281\FOpt\RB3LYP\6-31+G(d)\C14H13N3O4S2\JMH502\29-May-2010\0\0\#B3LYP/6-31+G(d) Opt=gdiis freq=noraman maxdisk=458752000 INT(grid=ultrafine)\zwit-meloxicam-enolate.UAKS confsearch\0,1\C,0.0268440158,-0.0096370406,-0.014711263\C,0.0672527366,-0.0220617516,1.3783410006\C,1.3068452966,0.0125620602,2.0200105703\C,2.4844790569,0.0663062055,1.2647637059\C,2.4305886281,0.0729253038,-0.1285416508\C,1.1966153012,0.0221236139,-0.7947608675\H,-0.8594733131,-0.062465452,1.9425776973\H,1.3531366168,0.0015521528,3.1057169596\H,3.448192066,0.1003122147,1.766
```

2546028\H,3.3352521258,0.1152845956,-0.7259388477\C,1.1670144769,0.006
1720052,-2.2888630534\S,-1.5395111699,0.0243676052,-0.8851572981\N,-1.
1556543783,-0.8979127258,-2.2331288244\C,-0.0059598314,-0.4377489008,-
2.9546566701\C,-0.119340707,-0.4739148089,-4.3825057042\O,-1.069003291
7,-0.8681886592,-5.0705462053\N,1.057835603,-0.0053349984,-5.052120520
6\H,1.8206922371,0.2838658008,-4.3297841852\C,1.1327363525,0.067832467
9,-6.3656781586\O,-2.5414128834,-0.7027878802,-0.0965376714\O,-1.78619
70983,1.4015744541,-1.3173951456\C,-1.3685974021,-2.3543655582,-2.1613
934001\H,-0.5484152856,-2.8642020676,-1.6351259476\H,-2.3130630864,-2.
555558469,-1.6551938845\H,-1.4301377978,-2.7211174389,-3.1888355131\O,
2.2236860819,0.4105533817,-2.8944059743\N,2.217514851,0.5376294954,-7.
0222930161\S,-0.1114245812,-0.4065538737,-7.4987419535\C,2.1132100621,
0.545689727,-8.4159667091\C,0.932185195,0.0735176467,-8.8619476857\C,0
.4595124028,-0.0675644382,-10.2758452539\H,1.2335947029,0.278215765,-1
0.9684215975\H,0.2280743789,-1.1113802417,-10.5194690916\H,-0.44593266
11,0.5240137463,-10.4564459264\H,2.9484555501,0.9135652839,-8.99710110
07\H,3.0338663636,0.8699528143,-6.5221427745\\Version=EM64L-G03RevE.01
\State=1-A\HF=-1802.8064214\RMSD=8.018e-09\RMSF=3.947e-05\Thermal=0.\D
ipole=3.2587665,-0.2940708,-3.5696265\PG=C01 [X(C14H13N3O4S2)]\@

zwit-meloxicam

1\1\GINC-X138\FOpt\RB3LYP\6-31+G(d)\C14H13N3O4S2\JMH502\10-Jan-2010\0\
\# B3LYP/6-31+G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultraf
ine)\opt calc\0,1\C,-0.0125371863,0.0228708364,-0.0307915771\C,-0.03
35515143,-0.0075741822,1.3689040506\C,1.1550886932,-0.0203876195,2.097
0525451\C,2.3944992497,-0.0035087306,1.4337122375\C,2.3894080895,-0.00
52433342,0.0261811917\C,1.2073398906,0.0210550972,-0.7098133972\H,-0.9
430115912,0.0402065248,-0.5915290399\H,-0.9839734833,-0.0152107212,1.8
957145127\H,1.1403144873,-0.0338555345,3.1812515502\H,1.2506001986,0.0
363869557,-1.7944993131\S,3.9793026482,-0.1198548251,-0.7824566213\O,4
.4329949799,-1.5074644319,-0.6827734443\O,3.9142940173,0.5565417766,-2
.0820218321\N,4.9142992084,0.818699719,0.2536702964\C,5.0900007779,2.2
492431534,-0.0625394002\H,5.9975378446,2.5821522956,0.4439521779\H,5.2
197032543,2.361555221,-1.1387090912\H,4.230863005,2.8474545058,0.27254
27605\C,3.6556507057,0.0402211935,2.1911933254\O,3.5280151997,-0.34918
48258,3.4719904062\C,4.8493180397,0.4472319805,1.631428463\C,6.1249310
559,0.54625205,2.3698791356\O,7.1689795562,0.9458342639,1.8389467531\N
,6.0644975163,0.1733669516,3.7130670827\C,7.1749105225,0.2211583429,4.
4096843255\C,9.4396802763,0.3968234034,5.5166869145\N,7.2221650865,-0.
1421999095,5.7184798817\C,8.4665522114,-0.0510300136,6.3370193632\H,8.
5538675513,-0.3333811723,7.3782704606\H,6.3850208639,-0.4714646531,6.1
829821025\S,8.7882238657,0.7226610117,3.8934568064\C,10.8873217027,0.6
186046353,5.8300556076\H,11.0920308886,0.3613923203,6.8747027704\H,11.
5347011075,0.0005081946,5.196103123\H,11.1765294005,1.6654076611,5.676
187095\H,4.4306645126,-0.2508510288,3.8937543076\\Version=EM64L-G03Rev
E.01\State=1-A\HF=-1802.8169836\RMSD=4.585e-09\RMSF=1.482e-05\Thermal=
0.\Dipole=0.2842263,0.6762933,3.8456869\PG=C01 [X(C14H13N3O4S2)]\@