MESSI: Multi Ensemble Strategy for Structural Identification

https://github.com/Sarotti-Lab/MESSI

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Instructive, general recommendations and case study

Workflow and general recommendations

Step 1: Despite the new MESSI can handle any amount of isomers, keeping the number of candidates to a minimum has several advantages, as it reduces both the overall computational cost and the probability that the calculated data for an incorrect isomer ends up having better fit with the experimental values than the correct candidate.

Step 2: The conformational search should provide a good description of the conformational landscape of the system under study. Improper computational work might lead to potentially negative consequences in the overall results. Systematic sampling is always recommended, but impractical in highly flexible molecules. In those cases, stochastic searches using a reasonably large number of steps should be carried out. To avoid missing potentially relevant conformations, all conformations within a safe energy window from the corresponding global minimum should be kept. For this application, we recommend a 10 kcal/mol cutoff value using the MMFFaq force field.

Step 3: All conformations found in Step 2 must be fully optimized at the PCM/B3LYP/6-31G* level.

Step 4: After removing duplicates, all structures found must be submitted to NMR calculations at the level A (PCM/mPW1PW91/6-31+G**). In parallel, the same PCM/B3LYP/6-31G* optimized structures must be used as inputs for single point energy calculations at level B (SMD/B3LYP/6-31+G**). Important: MESSI requires that all conformations found to be considered, not just the most stable ones. Therefore, keeping only the most stable conformations found in Step 3 could give erroneous results. In the same way, it is important to respect the suggested theory levels, since MESSI was optimized for those levels.

Step 5: The output files must be compiled in a folder. Additionally, an Excel file with the experimental data and labels is needed. The NMR data must be assigned (know which shift corresponds to which nuclei). Using unassigned or misassigned NMR data can lead to erroneous results. The chemical shifts of equivalent nuclei that show fast interconversion should be averaged (such as the case of methyl groups, or some methylene groups). Treating the signal of each individual proton independently is wrong (for example, computing three different chemical shifts for the same methyl group). Another problem arises when dealing with diastereotopic methylene protons, which are ofen arbitrarily correlated. Unless the discrimination of both signals as pro-R and pro-S is made using additional NMR information (such as NOE or J coupling), the most convenient way to tackle this issue is to treat them as interchangeable signals.

Step 6: Run the script `messi.py` to perform the PCM-DP4+, SMD-DP4+ and MESSI probabilities calculations. The script opens a pop-up window that requests to select the folder that contains the Gaussian output files (either as *.log or *.out), and the Excel input file. The script feeds on the corresponding NMR and SCRF/SMD single point Gaussian output files. Both types of calculations could be run separately or together through the "*link*" option. The script automatically extracts the isotropic shielding values and energies from each output and classifies them per isomer. Finally, the chemical shifts are averaged according the filter type and correlated with the experimental data to use it in the DP4+ formalism. The results are printed in an Excel file named '*MESSI_Results.xlsx*'.

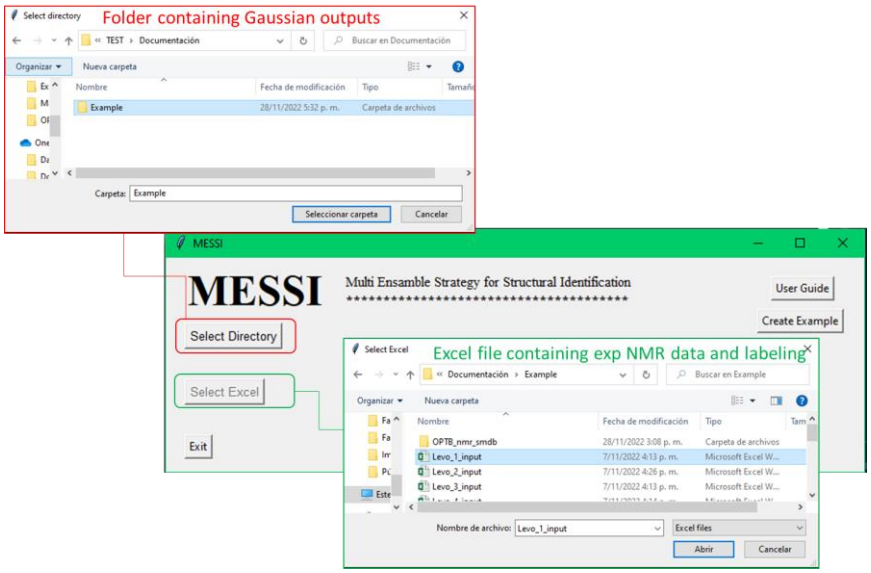


Figure 1.

Installation Requirements

MESSI needs python 3.8 or later to work. The module can be installed by console using:

```
pip3 install messi_nmr
```

MESSI needs `tkinter` module to work. It will be automatically installed by pip in Windows and macOS, but for linux it must be installed separately by `apt-get`.

Once installed the python module, the program can be executed by console using:

```
messi
```

or generate a messi.py shortcut on the desktop, which allows direct execution of the program without the use of a console, using:

```
messi_exe
```

In order to test the correct software operation is recommended to run the provided example, which could be download by clicking the buttom `Create Example`. This will create a folder name `Example_messi_nmr` in the desktop containing all the files needed to run the example.

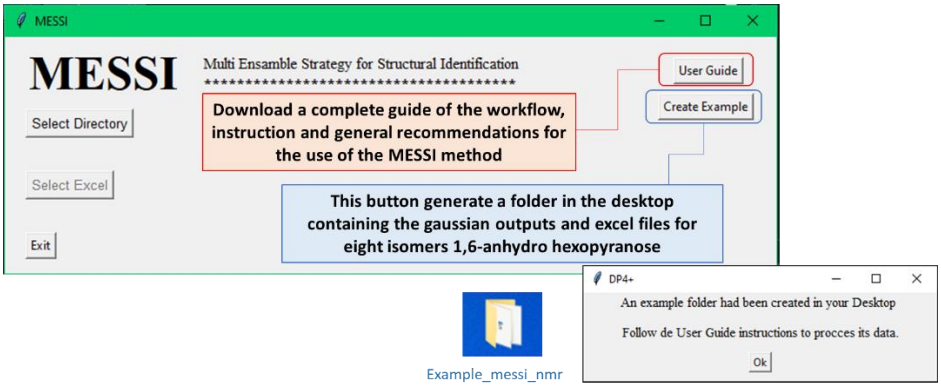


Figure 2.

Terms of use. To run MESSI is required that the information is located in a folder containing the following files:

1) The Gaussian output files of the NMR and SCRF/SMD calculations (all conformers for all isomers).
2) An excel file containing the experimental data and the labels of each nucleus associated with each experimental value.

Technical requirements.

1) The output files: must be named following the next convention: ***n_*_m*.log*** or ***.out***, where ***n*** represent the isomer number and could be from *1* to *N* where *N* is the number of candidate structures under study, and ***m*** indicate the conformer number. For instance,

1_NewNatProd_c01.log (*Conformer 1 for isomer 1 of the compound names* NewNatProd)

1_ NewNatProd _c02.log (*Conformer 2 for isomer 1 of the compound names* NewNatProd)

2_ NewNatProd _c01.log (*Conformer 1 for isomer 2 of the compound names* NewNatProd)

The NMR and SCRF/SMD energies calculation could be in the same or different outputs. If they are separated, both file must begin with the same name (***n_*_m*.log*** or ***.out***) and a suffix must be added in order to differentiate the calculation type. If the number of files for NMR calculations does not match the number of SMD energy calculations the script will not run. The script handles outputs from Gaussian 09 and 16.

Note: *Name files adequately is essential in order to match SMD energy with the NMR data for each conformer.*

2) The input excel file: The experimental data and the labels of the candidate structures must be placed in an excel file following the next rules. The excel file should be constituted by one sheet; containing the data of the NMR chemical shifts (*named* 'shifts').

"shifts" sheet: the first column *"nuclei"* contains the identity of the atom 'c or C' for ^{13}C and 'h or H' for hydrogen atoms. The second column *"sp2"* contains the hybridization of the atoms: *0* for sp^3 C or H attached to; *1* for sp^2/sp C or H attached to). The third column *"exp_data"* contains the experimental chemical shifts. The column *"exchange"* allows to indicate interchangeable signals (for example, two diastereotopic hydrogens). Any character can be used to indicate a pair of interchangeable signals, which will cause that the experimental and calculated values to be ordered upside-down. When dealing with more than one pair of interchangeable signals, different characters should be used to differentiate them. For example, it can be used the letter "a to indicate one pair, and the letter "b" to indicate the other pair. The following columns are intended to place the labels of the nuclei associated to the corresponding chemical shift. If two or more values are added in that region, the isotropic shielding values will be averaged (as in the case of methyl groups or equivalent methylene groups). If the isomers under study have different labeling schemes (as in the case of constitutional isomers), three columns for each isomer should be provided as indicated below.

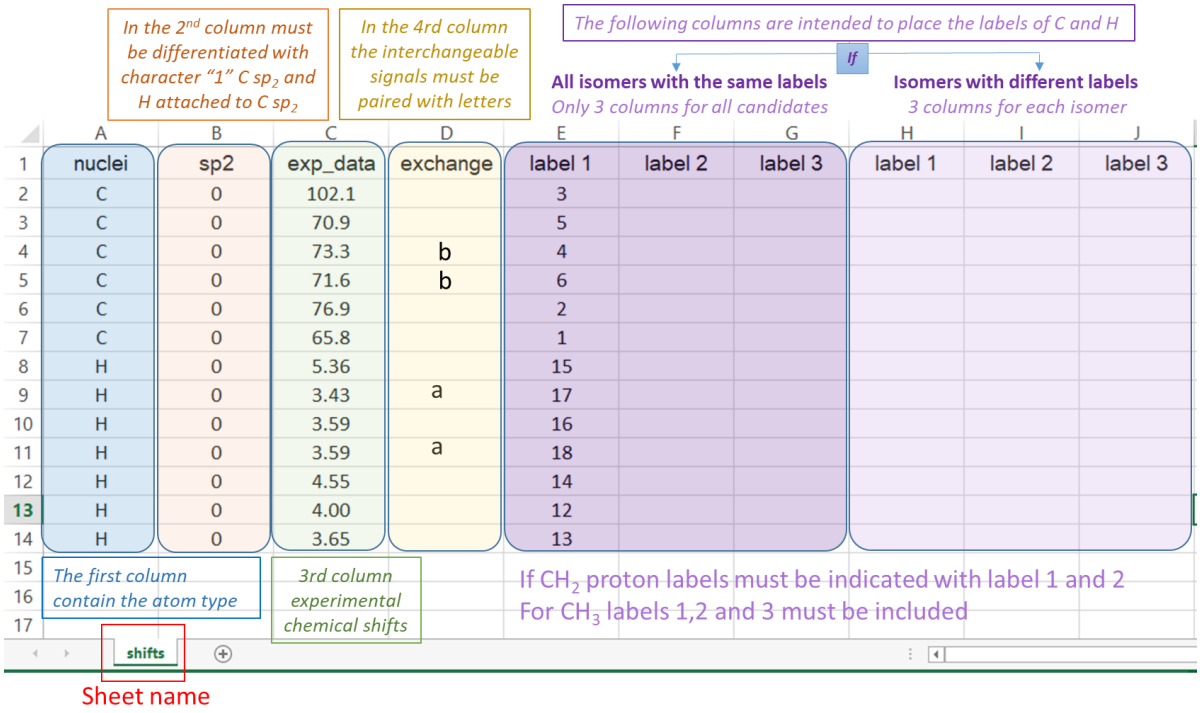


Figure 2. Technical requirements for the excel assembly.

3) The output excel file: once the messi.py is executed, a file named '*MESSI_Results.xlsx*' is created in the folder containing the Gaussian output files. The file contains *n+1* sheets where *n* is the number candidate structures:

Results sheet: contain the PCM-DP4+ (row 19, standard DP4+), SMD-DP4+ (row 20, standard DP4+ using the energies computed at the SMD/B3LYP/6-31+G** level), and the DP4+ results computed for the selected 16 ensembles (rows 3-18). The averaged values of those 16 calculations (MESSI) are shown in row 2. If both ^{1}H and ^{13}C are used, the probabilities shown correspond to the full DP4+ results. In case only ^{1}H, or ^{13}C, data are used (not recommended), the probabilities shown correspond to H-DP4+ or C-DP4+ values, respectively.

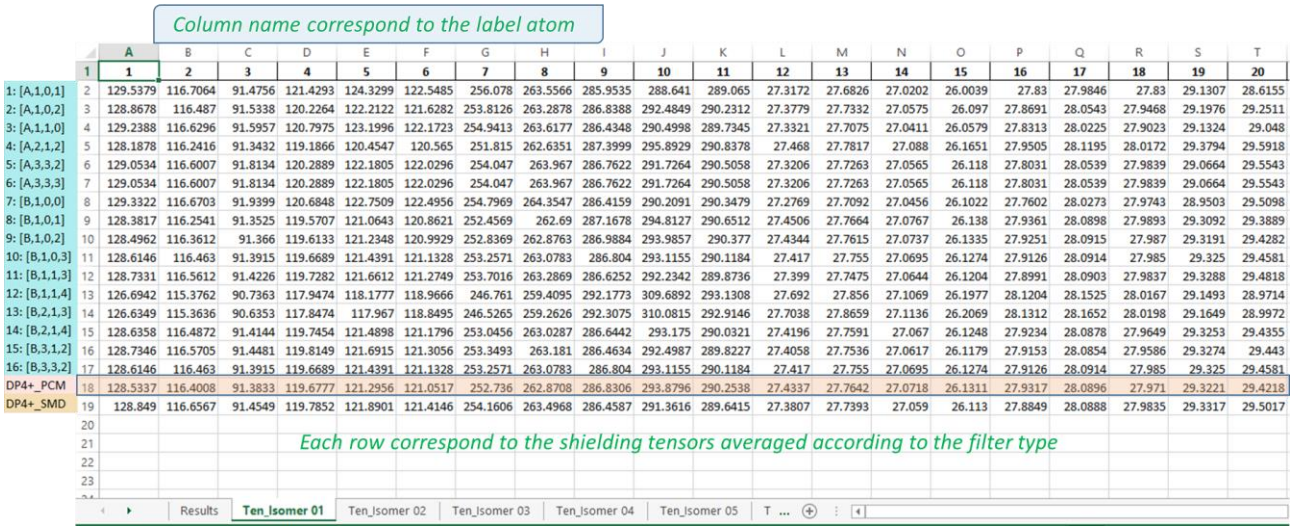
Filter	Isomer 01	Isomer 02	Isomer 03	Isomer 04	Isomer 05	Isomer 06	Isomer 07	Isomer 08
MESSI	99.99	0	0	0	0	0	0	0
1: [A,1,0,1]	100	0	0	0	0	0	0	0
2: [A,1,0,2]	100	0	0	0	0	0	0	0
3: [A,1,1,0]	100	0	0	0	0	0	0	0
4: [A,2,1,2]	100	0	0	0	0	0	0	0
5: [A,3,3,2]	100	0	0	0	0	0	0	0
6: [A,3,3,3]	99.99	0	0	0	0	0	0.01	0
7: [B,1,0,0]	100	0	0	0	0	0	0	0
8: [B,1,0,1]	100	0	0	0	0	0	0	0
9: [B,1,0,2]	100	0	0	0	0	0	0	0
10: [B,1,0,3]	100	0	0	0	0	0	0	0
11: [B,1,1,3]	99.98	0	0	0	0.01	0	0	0
12: [B,1,1,4]	99.91	0	0	0.04	0.04	0	0	0.01
13: [B,2,1,3]	100	0	0	0	0	0	0	0
14: [B,2,1,4]	100	0	0	0	0	0	0	0
15: [B,3,1,2]	100	0	0	0	0	0	0	0
16: [B,3,3,2]	100	0	0	0	0	0	0	0
DP4+_PCM	100	0	0	0	0	0	0	0
DP4+_SMD	100	0	0	0	0	0	0	0

Results | Ten_Isomer 01 | Ten_Isomer 02 | Ten_Isomer 03 | Ten_Isomer 04 | Ten_Isomer 05 | T ...

NOTE: It is important to point out that ensembles 4, 11 y 12 are created by removing all conformations within 1 kcal/mol from the corresponding global minimum. In some systems with flat potential energy

surface, the full conformational space could be confined within that energy window. This will cause all the conformations of that isomer to be eliminated, and therefore its probability will be zero. To indicate that situation, the corresponding cells will be highlighted in gray (in the given example, column H, rows 13 and 14).

Ten_isomers sheets: the Excel file contains as many sheets as candidate structures are considered, labeled as "Tens_Isomer N", **where N is the isomer number.** Each cell contains the isotropic shielding values corresponding to each ensemble (row) and Gaussian label (column). For example, the value shown in cell C2 (91.5338) is the isotropic shielding value of the atom nº 3 (according to Gaussian labeling scheme) computed using ensemble 2 [A-1-0-2].



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
	1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1: [A,1,0,1]	2	129.5379	116.7064	91.4756	121.4293	124.3299	122.5485	256.078	263.5566	285.9535	288.641	289.065	27.3172	27.6826	27.0202	26.0039	27.83	27.9846	27.83	29.1307	28.6155
2: [A,1,0,2]	3	128.8678	116.487	91.5338	120.2264	122.2122	121.6282	253.8126	263.2878	286.8388	292.4849	290.2312	27.3779	27.7332	27.0575	26.097	27.8691	28.0543	27.9468	29.1976	29.2511
3: [A,1,1,0]	4	129.2388	116.6296	91.5957	120.7975	123.1996	122.1723	254.9413	263.6177	286.4348	290.4998	289.7345	27.3321	27.7075	27.0411	26.0579	27.8313	28.0225	27.9023	29.1324	29.048
4: [A,2,1,2]	5	128.1878	116.2416	91.3432	119.1866	120.4547	120.565	251.815	262.6351	287.3999	295.8929	290.8378	27.468	27.7817	27.088	26.1651	27.9505	28.1195	28.0172	29.3794	29.5918
5: [A,3,3,2]	6	129.0534	116.6007	91.8134	120.2889	122.1805	122.0296	254.047	263.967	286.7622	291.7264	290.5058	27.3206	27.7263	27.0565	26.118	27.8031	28.0539	27.9839	29.0664	29.5543
6: [A,3,3,3]	7	129.0534	116.6007	91.8134	120.2889	122.1805	122.0296	254.047	263.967	286.7622	291.7264	290.5058	27.3206	27.7263	27.0565	26.118	27.8031	28.0539	27.9839	29.0664	29.5543
7: [B,1,0,0]	8	129.3322	116.6703	91.9399	120.6848	122.7509	122.4956	254.7969	264.3547	286.4159	290.2091	290.3479	27.2769	27.7092	27.0456	26.1022	27.7602	28.0273	27.9743	28.9503	29.5098
8: [B,1,0,1]	9	128.3817	116.2541	91.3525	119.5707	121.0643	120.8621	252.4569	262.69	287.1678	294.8127	290.6512	27.4506	27.7664	27.0767	26.138	27.9361	28.0898	27.9893	29.3092	29.3889
9: [B,1,0,2]	10	128.4962	116.3612	91.366	119.6133	121.2348	120.9929	252.8369	262.8763	286.9884	293.9857	290.377	27.4344	27.7615	27.0737	26.1335	27.9251	28.0915	27.987	29.3191	29.4282
10: [B,1,0,3]	11	128.6146	116.463	91.3915	119.6689	121.4391	121.1328	253.2571	263.0783	286.804	293.1155	290.1184	27.417	27.755	27.0695	26.1274	27.9126	28.0914	27.985	29.325	29.4581
11: [B,1,1,3]	12	128.7331	116.5612	91.4226	119.7282	121.6612	121.2749	253.7016	263.2869	286.6252	292.2342	289.8736	27.399	27.7475	27.0644	26.1204	27.8991	28.0903	27.9837	29.3288	29.4818
12: [B,1,1,4]	13	126.6942	115.3762	90.7363	117.9474	118.1777	118.9666	246.761	259.4095	292.1773	309.6892	293.1308	27.692	27.856	27.1069	26.1977	28.1204	28.1525	28.0167	29.1493	28.9714
13: [B,2,1,3]	14	126.6349	115.3636	90.6353	117.8474	117.967	118.8495	246.5265	259.2626	292.3075	310.0815	292.9146	27.7038	27.8659	27.1136	26.2069	28.1312	28.1652	28.0198	29.1649	28.9972
14: [B,2,1,4]	15	128.6358	116.4872	91.4144	119.7454	121.4898	121.1796	253.0456	263.0287	286.6442	293.175	290.0321	27.4196	27.7591	27.067	26.1248	27.9234	28.0878	27.9649	29.3253	29.4355
15: [B,3,1,2]	16	128.7346	116.5705	91.4481	119.8149	121.6915	121.3056	253.3493	263.181	286.4634	292.4987	289.8227	27.4058	27.7536	27.0617	26.1179	27.9153	28.0854	27.9586	29.3274	29.443
16: [B,3,3,2]	17	128.6146	116.463	91.3915	119.6689	121.4391	121.1328	253.2571	263.0783	286.804	293.1155	290.1184	27.417	27.755	27.0695	26.1274	27.9126	28.0914	27.985	29.325	29.4581
DP4+_PCM	18	128.5337	116.4008	91.3833	119.6777	121.2956	121.0517	252.736	262.8708	286.8306	293.8796	290.2538	27.4337	27.7642	27.0718	26.1311	27.9317	28.0896	27.971	29.3221	29.4218
DP4+_SMD	19	128.849	116.6567	91.4549	119.7852	121.8901	121.4146	254.1606	263.4968	286.4587	291.3616	289.6415	27.3807	27.7393	27.059	26.113	27.8849	28.0888	27.9835	29.3317	29.5017

Figure 3. Excel output

Case study: 1,6-anhydrohexopyranosides

In order to illustrate the MESSI workflow, we present the analysis of the 1,6-anhydrohexopyranosides family. As indicated in the Figure 4, there are eight possible isomers.

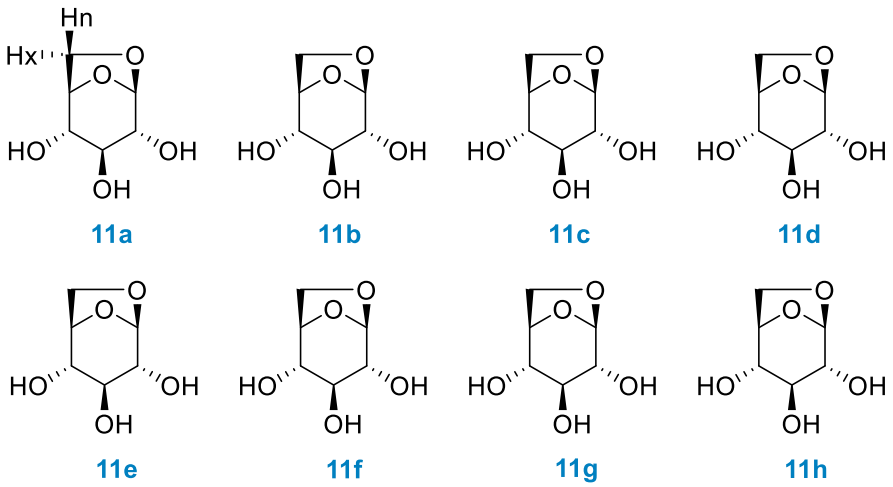


Figure 4

Following the recommended computational procedure, a total number of 130 conformers were found after the optimization at the PCM/B3LYP/6-31G* level (the standard for DP4+ calculations). Each structure was submitted to NMR and SCRF calculations at the PCM/mPW1PW91/6-31+G** and SMD/B3LYP/6-31+G**

levels respectively. The corresponding output files are provided in the Folder “Example”. According to Gaussian numbering scheme, the labels corresponding to each nuclei are given in Figure 5.

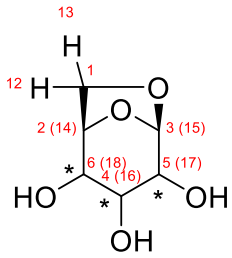


Figure 5. Carbon label followed by its corresponding proton(s) label(s) between parenthesis

MESSI

MESSI calculations were run using the experimental NMR data of all the diastereoisomers (which are provided in the same folder). Once the script is run, the Excel report file ““**MESSI_Results”** is generated.

MESSI input and output excel files

INPUTS	**OUTPUTS**
Experimenta Data of Isomer 1	*Results*

	A	B	C	D	E	F	G
1	nuclei	sp2	exp_data	exchange	label 1	label 2	label 3
2	C	0	102.1		3		
3	C	0	70.9		5		
4	C	0	73.3		4		
5	C	0	71.6		6		
6	C	0	76.9		2		
7	C	0	65.8		1		
8	H	0	5.36		15		
9	H	0	3.43		17		
10	H	0	3.59		16		
11	H	0	3.59		18		
12	H	0	4.55		14		
13	H	0	4		12		
14	H	0	3.65		13		
15							
16							
17							

shifts

	A	B	C	D	E	F	G	H	I
1	Filter	Isomer 01	Isomer 02	Isomer 03	Isomer 04	Isomer 05	Isomer 06	Isomer 07	Isomer 08
2	MESSI	99.99	0	0	0	0	0	0	0
3	1: [A,1,0,1]	100	0	0	0	0	0	0	0
4	2: [A,1,0,2]	100	0	0	0	0	0	0	0
5	3: [A,1,1,0]	100	0	0	0	0	0	0	0
6	4: [A,2,1,2]	100	0	0	0	0	0	0	0
7	5: [A,3,3,2]	100	0	0	0	0	0	0	0
8	6: [A,3,3,3]	99.99	0	0	0	0	0	0.01	0
9	7: [B,1,0,0]	100	0	0	0	0	0	0	0
10	8: [B,1,0,1]	100	0	0	0	0	0	0	0
11	9: [B,1,0,2]	100	0	0	0	0	0	0	0
12	10: [B,1,0,3]	100	0	0	0	0	0	0	0
13	11: [B,1,1,3]	99.98	0	0	0	0.01	0	0	0
14	12: [B,1,1,4]	99.91	0	0	0.04	0.04	0	0	0.01
15	13: [B,2,1,3]	100	0	0	0	0	0	0	0
16	14: [B,2,1,4]	100	0	0	0	0	0	0	0
17	15: [B,3,1,2]	100	0	0	0	0	0	0	0
18	16: [B,3,3,2]	100	0	0	0	0	0	0	0
19	DP4+_PCM	100	0	0	0	0	0	0	0
20	DP4+_SMD	100	0	0	0	0	0	0	0

Results | Ten_Isomer 01 | Ten_Isomer 02 | Ten_Isomer 03 | Ten_Isomer 04 | Ten_Isomer 05

Experimenta Data of Isomer 2	*Results*

	A	B	C	D	E	F	G
1	nuclei	sp2	exp_data	exchange	label 1	label 2	label 3
2	C	0	101.3		3		
3	C	0	71.9		5		
4	C	0	70.8		4		
5	C	0	64.9		6		
6	C	0	74.9		2		
7	C	0	64.1		1		
8	H	0	5.3		15		
9	H	0	3.69		17		
10	H	0	3.82		16		
11	H	0	3.94		21		
12	H	0	4.41		14		
13	H	0	4.21		12		
14	H	0	3.55		13		
15							
16							
17							

shifts

	A	B	C	D	E	F	G	H	I
1	Filter	Isomer 01	Isomer 02	Isomer 03	Isomer 04	Isomer 05	Isomer 06	Isomer 07	Isomer 08
2	MESSI	0	100	0	0	0	0	0	0
3	1: [A,1,0,1]	0	100	0	0	0	0	0	0
4	2: [A,1,0,2]	0	100	0	0	0	0	0	0
5	3: [A,1,1,0]	0	100	0	0	0	0	0	0
6	4: [A,2,1,2]	0	100	0	0	0	0	0	0
7	5: [A,3,3,2]	0	100	0	0	0	0	0	0
8	6: [A,3,3,3]	0	100	0	0	0	0	0	0
9	7: [B,1,0,0]	0	100	0	0	0	0	0	0
10	8: [B,1,0,1]	0	100	0	0	0	0	0	0
11	9: [B,1,0,2]	0	100	0	0	0	0	0	0
12	10: [B,1,0,3]	0	100	0	0	0	0	0	0
13	11: [B,1,1,3]	0	100	0	0	0	0	0	0
14	12: [B,1,1,4]	0	100	0	0	0	0	0	0
15	13: [B,2,1,3]	0	100	0	0	0	0	0	0
16	14: [B,2,1,4]	0	100	0	0	0	0	0	0
17	15: [B,3,1,2]	0	100	0	0	0	0	0	0
18	16: [B,3,3,2]	0	100	0	0	0	0	0	0
19	DP4+_PCM	0	100	0	0	0	0	0	0
20	DP4+_SMD	0	100	0	0	0	0	0	0

Results | Ten_Isomer 01 | Ten_Isomer 02 | Ten_Isomer 03 | Ten_Isomer 04 | Ten_Isomer 05

Experimenta Data of Isomer 3	*Results*

	A	B	C	D	E	F	G
1	nuclei	sp2	exp_data	exchange	label 1	label 2	label 3
2	C	0	101.7		3		
3	C	0	70.5		5		
4	C	0	70.5		4		
5	C	0	69.9		6		
6	C	0	74.9		2		
7	C	0	63.8		1		
8	H	0	5.38		15		
9	H	0	3.79		17		
10	H	0	3.65		16		
11	H	0	3.81		18		
12	H	0	4.46		14		
13	H	0	3.98		12		
14	H	0	3.6		13		
15							
16							

shifts

Experimenta Data of Isomer 4

	A	B	C	D	E	F	G	H	I
1	Filter	Isomer 01	Isomer 02	Isomer 03	Isomer 04	Isomer 05	Isomer 06	Isomer 07	Isomer 08
2	MESSI	0	0	99.99	0	0	0	0	0.01
3	1: [A,1,0,1]	0	0	100	0	0	0	0	0
4	2: [A,1,0,2]	0	0	100	0	0	0	0	0
5	3: [A,1,1,0]	0	0	99.96	0	0	0	0	0.04
6	4: [A,2,1,2]	0	0	100	0	0	0	0	0
7	5: [A,3,3,2]	0	0	100	0	0	0	0	0
8	6: [A,3,3,3]	0	0	100	0	0	0	0	0
9	7: [B,1,0,0]	0	0	99.99	0	0	0	0	0.01
10	8: [B,1,0,1]	0	0	100	0	0	0	0	0
11	9: [B,1,0,2]	0	0	100	0	0	0	0	0
12	10: [B,1,0,3]	0	0	100	0	0	0	0	0
13	11: [B,1,1,3]	0	0	99.97	0	0.01	0	0	0.02
14	12: [B,1,1,4]	0	0	99.97	0	0.01	0	0	0.02
15	13: [B,2,1,3]	0	0	100	0	0	0	0	0
16	14: [B,2,1,4]	0	0	100	0	0	0	0	0
17	15: [B,3,1,2]	0	0	100	0	0	0	0	0
18	16: [B,3,3,2]	0	0	100	0	0	0	0	0
19	DP4+_PCM	0	0	100	0	0	0	0	0
20	DP4+_SMD	0	0	100	0	0	0	0	0

Results | Ten_Isomer 01 | Ten_Isomer 02 | Ten_Isomer 03 | Ten_Isomer 04 | Ten_Isomer 05

Results

	A	B	C	D	E	F	G
1	nuclei	sp2	exp_data	exchange	label 1	label 2	label 3
2	C	0	101.5		3		
3	C	0	70.2		5		
4	C	0	63.5		4		
5	C	0	70.1		6		
6	C	0	76.8		2		
7	C	0	65.4		1		
8	H	0	5.42		15		
9	H	0	3.7		17		
10	H	0	3.73		16		
11	H	0	3.78		18		
12	H	0	4.62		14		
13	H	0	3.78		12		
14	H	0	3.78		13		
15							
16							

shifts

Experimenta Data of Isomer 5

	A	B	C	D	E	F	G	H	I
1	Filter	Isomer 01	Isomer 02	Isomer 03	Isomer 04	Isomer 05	Isomer 06	Isomer 07	Isomer 08
2	MESSI	0	0	0	87.5	0	0	0	12.5
3	1: [A,1,0,1]	0	0	0	100	0	0	0	0
4	2: [A,1,0,2]	0	0	0	100	0	0	0	0
5	3: [A,1,1,0]	0	0	0	99.89	0	0	0	0.11
6	4: [A,2,1,2]	0	0	0	100	0	0	0	0
7	5: [A,3,3,2]	0	0	0	100	0	0	0	0
8	6: [A,3,3,3]	0	0	0	100	0	0	0	0
9	7: [B,1,0,0]	0	0	0	100	0	0	0	0
10	8: [B,1,0,1]	0	0	0	100	0	0	0	0
11	9: [B,1,0,2]	0	0	0	100	0	0	0	0
12	10: [B,1,0,3]	0	0	0	100	0	0	0	0
13	11: [B,1,1,3]	0	0	0	0.04	0	0	0	99.96
14	12: [B,1,1,4]	0	0	0	0.02	0	0	0	99.98
15	13: [B,2,1,3]	0	0	0	100	0	0	0	0
16	14: [B,2,1,4]	0	0	0	100	0	0	0	0
17	15: [B,3,1,2]	0	0	0	100	0	0	0	0
18	16: [B,3,3,2]	0	0	0	100	0	0	0	0
19	DP4+_PCM	0	0	0	100	0	0	0	0
20	DP4+_SMD	0	0	0	100	0	0	0	0

Results | Ten_Isomer 01 | Ten_Isomer 02 | Ten_Isomer 03 | Ten_Isomer 04 | Ten_Isomer 05

Results

	A	B	C	D	E	F	G
1	nuclei	sp2	exp_data	exchange	label 1	label 2	label 3
2	C	0	101.9		3		
3	C	0	66.6		5		
4	C	0	70.9		4		
5	C	0	72.2		6		
6	C	0	76.4		2		
7	C	0	65.3		1		
8	H	0	5.31		15		
9	H	0	3.68		17		
10	H	0	3.86		16		
11	H	0	3.85		18		
12	H	0	4.51		14		
13	H	0	4.14		12		
14	H	0	3.65		13		
15							
16							
17							

shifts

Experimenta Data of Isomer 6

	A	B	C	D	E	F	G	H	I
1	Filter	Isomer 01	Isomer 02	Isomer 03	Isomer 04	Isomer 05	Isomer 06	Isomer 07	Isomer 08
2	MESSI	0	0	0.32	0	99.68	0	0	0
3	1: [A,1,0,1]	0	0	0	0	100	0	0	0
4	2: [A,1,0,2]	0	0	0	0	100	0	0	0
5	3: [A,1,1,0]	0.01	0	5.06	0	94.93	0	0	0
6	4: [A,2,1,2]	0	0	0	0	100	0	0	0
7	5: [A,3,3,2]	0	0	0	0	100	0	0	0
8	6: [A,3,3,3]	0	0	0	0	100	0	0	0
9	7: [B,1,0,0]	0	0	0.11	0	99.89	0	0	0
10	8: [B,1,0,1]	0	0	0	0	100	0	0	0
11	9: [B,1,0,2]	0	0	0	0	100	0	0	0
12	10: [B,1,0,3]	0	0	0	0	100	0	0	0
13	11: [B,1,1,3]	0	0	0	0	100	0	0	0
14	12: [B,1,1,4]	0	0	0	0	100	0	0	0
15	13: [B,2,1,3]	0	0	0	0	100	0	0	0
16	14: [B,2,1,4]	0	0	0	0	100	0	0	0
17	15: [B,3,1,2]	0	0	0	0	100	0	0	0
18	16: [B,3,3,2]	0	0	0	0	100	0	0	0
19	DP4+_PCM	0.11	0	0	0	99.89	0	0	0
20	DP4+_SMD	0	0	0	0	100	0	0	0

Results | Ten_Isomer 01 | Ten_Isomer 02 | Ten_Isomer 03 | Ten_Isomer 04 | Ten_Isomer 05

Results

	A	B	C	D	E	F	G
1	nuclei	sp2	exp_data	exchange	label 1	label 2	label 3
2	C	0	101.2		3		
3	C	0	69.1		5		
4	C	0	69.2		4		
5	C	0	67.1		6		
6	C	0	74.8		2		
7	C	0	65.1		1		
8	H	0	5.24		15		
9	H	0	3.61		17		
10	H	0	4.09		16		
11	H	0	3.87		18		
12	H	0	4.36		14		
13	H	0	4.28		12		
14	H	0	3.58		13		
15							
16							

shifts

Experimenta Data of Isomer 7

	A	B	C	D	E	F	G	H	I
1	Filter	Isomer 01	Isomer 02	Isomer 03	Isomer 04	Isomer 05	Isomer 06	Isomer 07	Isomer 08
2	MESSI	0	0	1.31	0.04	0	98.66	0	0
3	1: [A,1,0,1]	0	0	0	0	0	100	0	0
4	2: [A,1,0,2]	0	0	0	0	0	100	0	0
5	3: [A,1,1,0]	0	0	20.91	0.57	0	78.52	0	0
6	4: [A,2,1,2]	0	0	0	0	0	100	0	0
7	5: [A,3,3,2]	0	0	0	0	0	100	0	0
8	6: [A,3,3,3]	0	0	0	0	0	100	0	0
9	7: [B,1,0,0]	0	0	0	0	0	100	0	0
10	8: [B,1,0,1]	0	0	0	0	0	100	0	0
11	9: [B,1,0,2]	0	0	0	0	0	100	0	0
12	10: [B,1,0,3]	0	0	0	0	0	100	0	0
13	11: [B,1,1,3]	0	0	0	0	0	100	0	0
14	12: [B,1,1,4]	0	0	0	0	0	100	0	0
15	13: [B,2,1,3]	0	0	0	0	0	100	0	0
16	14: [B,2,1,4]	0	0	0	0	0	100	0	0
17	15: [B,3,1,2]	0	0	0	0	0	100	0	0
18	16: [B,3,3,2]	0	0	0	0	0	100	0	0
19	DP4+_PCM	0	0	0	0	0	100	0	0
20	DP4+_SMD	0	0	0	0	0	100	0	0

Results | Ten_Isomer 01 | Ten_Isomer 02 | Ten_Isomer 03 | Ten_Isomer 04 | Ten_Isomer 05

Results

	A	B	C	D	E	F	G
1	nuclei	sp2	exp_data	exchange	label 1	label 2	label 3
2	C	0	101.9		3		
3	C	0	74.7		5		
4	C	0	74.7		4		
5	C	0	71.4		6		
6	C	0	75.8		2		
7	C	0	65.4		1		
8	H	0	5.26		15		
9	H	0	3.42		17		
10	H	0	3.4		16		
11	H	0	3.69		18		
12	H	0	4.46		14		
13	H	0	3.98		12		
14	H	0	3.66		13		
15							
16							

shifts

	A	B	C	D	E	F	G	H	I
1	Filter	Isomer 01	Isomer 02	Isomer 03	Isomer 04	Isomer 05	Isomer 06	Isomer 07	Isomer 08
2	MESSI	12.66	0	0	0	0	0	87.33	0
3	1: [A,1,0,1]	0	0	0	0	0	0	99.99	0
4	2: [A,1,0,2]	0	0	0	0	0	0	100	0
5	3: [A,1,1,0]	1.39	0	0	0	0	0	98.61	0
6	4: [A,2,1,2]	0	0	0	0	0	0	100	0
7	5: [A,3,3,2]	0	0	0	0	0	0	100	0
8	6: [A,3,3,3]	0	0	0	0	0	0	99.99	0.01
9	7: [B,1,0,0]	0.27	0	0	0	0	0	99.73	0
10	8: [B,1,0,1]	0.17	0	0	0	0	0	99.83	0
11	9: [B,1,0,2]	0.08	0	0	0	0	0	99.92	0
12	10: [B,1,0,3]	0.03	0	0	0	0	0	99.96	0
13	11: [B,1,1,3]	100	0	0	0	0	0	0	0
14	12: [B,1,1,4]	100	0	0	0	0	0	0	0
15	13: [B,2,1,3]	0.21	0	0	0	0	0	99.79	0
16	14: [B,2,1,4]	0.12	0	0	0	0	0	99.88	0
17	15: [B,3,1,2]	0.08	0	0	0	0	0	99.92	0
18	16: [B,3,3,2]	0.26	0	0	0	0	0	99.74	0
19	DP4+_PCM	0	0	0	0	0	0	99.99	0.01
20	DP4+_SMD	0.01	0	0	0	0	0	99.98	0

Results | Ten_Isomer 01 | Ten_Isomer 02 | Ten_Isomer 03 | Ten_Isomer 04 | Ten_Isomer 05

Experimenta Data of Isomer 8

	A	B	C	D	E	F	G
1	nuclei	sp2	exp_data	exchange	label 1	label 2	label 3
2	C	0	101.9		3		
3	C	0	72.9		5		
4	C	0	70.3		4		
5	C	0	69.9		6		
6	C	0	77.6		2		
7	C	0	66		1		
8	H	0	5.3		15		
9	H	0	3.54		17		
10	H	0	3.58		16		
11	H	0	3.88		18		
12	H	0	4.59		14		
13	H	0	3.74		12		
14	H	0	3.74		13		
15							
16							

shifts

Results

	A	B	C	D	E	F	G	H	I
1	Filter	Isomer 01	Isomer 02	Isomer 03	Isomer 04	Isomer 05	Isomer 06	Isomer 07	Isomer 08
2	MESSI	0	0	0	0	0	0	0	100
3	1: [A,1,0,1]	0	0	0	0	0	0	0	100
4	2: [A,1,0,2]	0	0	0	0	0	0	0	100
5	3: [A,1,1,0]	0	0	0	0	0	0	0	100
6	4: [A,2,1,2]	0	0	0	0	0	0	0	100
7	5: [A,3,3,2]	0	0	0	0	0	0	0	100
8	6: [A,3,3,3]	0	0	0	0	0	0	0	100
9	7: [B,1,0,0]	0	0	0	0	0	0	0	100
10	8: [B,1,0,1]	0	0	0	0	0	0	0	100
11	9: [B,1,0,2]	0	0	0	0	0	0	0	100
12	10: [B,1,0,3]	0	0	0	0	0	0	0	100
13	11: [B,1,1,3]	0	0	0	0	0	0	0	100
14	12: [B,1,1,4]	0	0	0	0	0	0	0	100
15	13: [B,2,1,3]	0	0	0	0	0	0	0	100
16	14: [B,2,1,4]	0	0	0	0	0	0	0	100
17	15: [B,3,1,2]	0	0	0	0	0	0	0	100
18	16: [B,3,3,2]	0	0	0	0	0	0	0	100
19	DP4+_PCM	0	0	0	0	0	0	0	100
20	DP4+_SMD	0	0	0	0	0	0	0	100

Results | Ten_Isomer 01 | Ten_Isomer 02 | Ten_Isomer 03 | Ten_Isomer 04 | Ten_Isomer 05