Supporting Information

Absorption-mode: The Next Generation of Fourier Transform Mass Spectra

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Supplementary I: Load the Modified Spectrum into Bruker DataAnalysis Software

The raw transient ('fid' file) was processed and phase corrected using MatLab. The pre-processed file was then written in old Xmass format (Bruker), with appropriate parameters based on the data and a rescaled m/z range which is then readable by DataAnalysis for further analysis. The procedure and syntax for phase correction in MatLab are available in the previous paper.[26]

After phase correction, the real part of the spectrum (consisting of just the intensity values only) is written out as a 32 bit binary file (eg. floats) with a file name of '1r'. In this case, the spectrum data is written in 32 bit using syntax '[phid] = newfid(sf);' (see Supplementary II)

Then all need to do is to create the corresponding 'proc' and 'procs' parameter files in the same directory as the '1r' file. Users just have to make sure their parameters are set correctly and consistently with the original method file, so that DataAnalysis can calculate the right *m/z* array for the spectrum. Details of parameter settings are available from Bruker on request.

Supplementary II: MatLab Functions 'newfid' with Full Comments (Start with %)

```
%#############################################################################
%#
%#                  function newfid
%#
%#     usage: [phid] = newfid(sf);
%#     generate the transient ('phid') and absorption-mode ('1r') file for the phase corrected
%#     spectrum
%#     sf is spectrum after phase correction (complex number)
%#
%#############################################################################

function [phid]=newfid(sf);

% the MatLab syntax 'fft' (fast Fourier transform) and 'ifft' (inverse fast Fourier transform) generate
even symmetry data around the zero frequency point which adds redundant information, thus this
part of data is discarded during the data processing
sf2=rot90(sf);
sf2=rot90(sf2); % the negative half of data
```

```
sff=[sf;sf2]; % generate a symmetric spectrum for ifft (inverse fast Fourier transform)
newfid=ifft(sff);
newfid =real(newfid);
newfid = newfid (1:(length(phid)/2)); % discard the half of data

% generate the phase corrected transient file named 'phid'
fid=fopen('phid','w');
fwrite(fid, newfid,'int32');
fclose(fid);

% read the new transient (phid)
[fidspec,s,f,m]=readfid;

s=fft(fidspec,length(fidspec)*2); % zero fill
s=s((length(s)/2+1):length(s)); % discard the half of data
s=real(s);

%generate the '1r' file
fid = fopen('1r', 'w');
fwrite(fid, s, 'int32');
fclose(fid);
end
```

Table S1. Noise level (in RMS) of oil and ubiquitin charge states spectra in both magnitude and absorption-mode display.

Noise level (RMS) of crude oil spectrum			
***m/z* range**	**Magnitude-mode**	**Absorption-mode**	**Ratio**
300.30-301.05	699892.09	495412.99	1.41
500.56-501.1	836396.19	553054.63	1.51
699.71-700.30	938281.32	711066.96	1.32
899.98-900.56	965850.73	676193.80	1.43
Noise level (RMS) of ubiquitin charge states spectrum			
***m/z* range**	**Magnitude-mode**	**Absorption-mode**	**Ratio**
555-560	1099373.2806	777392.4059	1.41
990-995	1628990.0643	1152204.5984	1.41
1665-1670	1886997.2299	1335085.2547	1.41
2700-2705	2452423.2363	1735824.9276	1.41

Table S2. Peak assignment for both of the magnitude and absorption-mode in Fig. 4 and 5B, (H) indicates the $[M+H]^+$ ion as APPI generate both radical and protonated species.

No.	Formula	Magnitude *m/z*	Magnitude Error(ppm)	Absorption *m/z*	Absorption Error(ppm)
1	$C_{52}H_{62}S_2$	750.42891	0.23	750.42881	0.09
2	$C_{49}H_{66}S_3$	N/A	N/A	750.43208	-0.05
3	$C_{53}H_{66}OS$	750.48332	0.57	750.48294	0.07
4	$C_{52}H_{67}NS^{13}C$	750.50210	-0.17	750.50267	0.59
5	$C_{52}H_{67}S^{13}C_2(H)$	N/A	N/A	750.51028	-0.07
6	$C_{54}H_{70}S$	750.51951	0.32	750.51922	-0.07
7	$C_{51}H_{74}S_2$	750.52251	-0.19	750.52262	-0.04
8	$C_{53}H_{72}O^{13}C_2$	750.56433	-0.20	750.56458	0.13
9	$C_{55}H_{74}O$	750.57369	0.36	750.57339	-0.04
10	$C_{52}H_{78}OS$	750.57608	0.39	750.57574	-0.07
11	$C_{54}H_{75}N^{13}C$	750.59281	0.07	750.59282	0.08
12	$C_{54}H_{76}{}^{13}C_2$	750.60078	-0.11	750.60066	-0.27
13	$C_{51}H_{80}S^{13}C_2$	750.60442	0.25	750.60431	0.11
14	$C_{56}H_{78}$	750.60989	0.12	750.60978	-0.03
15	$C_{53}H_{82}S$	750.61319	0.03	750.61316	-0.01
16	$C_{50}H_{86}S_2$	N/A	N/A	750.61647	-0.11
17	$C_{53}H_{83}NO(H)$	750.65490	0.21	750.65497	0.31
18	$C_{52}H_{84}O^{13}C_2$	750.65801	-0.49	750.65825	-0.17
19	$C_{54}H_{86}O$	750.66738	0.08	750.66729	-0.04
20	$C_{53}H_{87}N^{13}C$	750.68672	0.08	750.68671	0.07
21	$C_{54}H_{87}N(H)$	750.69125	0.16	750.69108	-0.07
22	$C_{53}H_{88}{}^{13}C_2$	750.69484	0.11	750.69468	-0.11
23	$C_{54}H_{88}{}^{13}C(H)$	750.70024	1.35	750.69895	-0.37
24	$C_{55}H_{90}$	750.70385	0.20	750.70364	-0.08
25	$C_{52}H_{94}S$	N/A	N/A	750.70707	-0.01
26	$C_{51}H_{96}O^{13}C_2$	750.75272	0.59	750.75232	0.05
27	$C_{52}H_{100}{}^{13}C_2$	750.78883	0.23	750.78870	0.05
28	$C_{53}H_{100}{}^{13}C(H)$	750.79325	0.16	750.79313	0.00
29	$C_{54}H_{102}$	750.79761	0.01	750.79762	0.03
30	$C_{51}H_{62}S_2{}^{13}C$	751.43211	0.01	751.43220	0.13
31	$C_{48}H_{66}S_3{}^{13}C$	N/A	N/A	751.43583	0.48
32	$C_{52}H_{66}OS^{13}C$	N/A	N/A	751.48632	0.11
33	$C_{53}H_{69}NS$	751.51440	-0.16	751.51454	0.03
34	$C_{53}H_{70}S^{13}C$	751.52292	0.39	751.52263	0.00
35	$C_{50}H_{74}S_2{}^{13}C$	N/A	N/A	751.52631	0.41
36	$C_{54}H_{74}O^{13}C$	751.57726	0.65	751.57657	-0.27
37	$C_{51}H_{78}OS^{13}C$	N/A	N/A	751.58055	0.55
38	$C_{53}H_{75}N^{13}C_2$	751.59635	0.32	751.59631	0.27
39	$C_{55}H_{77}N$	751.60509	0.05	751.60499	-0.08
40	$C_{55}H_{78}{}^{13}C$	751.61332	0.21	751.61312	-0.05
41	$C_{52}H_{82}S^{13}C$	751.61642	-0.15	751.61666	0.17
42	$C_{53}H_{82}S(H)$	751.62124	0.32	751.62085	-0.20
43	$C_{50}H_{86}S_2(H)$	N/A	N/A	751.62442	0.07
44	$C_{53}H_{86}O^{13}C$	751.67074	0.09	751.67061	-0.08
45	$C_{54}H_{86}O(H)$	751.67512	-0.03	751.67511	-0.04
46	$C_{52}H_{87}N^{13}C_2$	751.69017	0.21	751.69024	0.31

47	$C_{53}H_{87}N^{13}C(H)$	751.69467	0.25	751.69454	0.08
48	$C_{54}H_{89}N$	751.69898	0.04	751.69890	-0.07
49	$C_{54}H_{90}{}^{13}C$	751.70721	0.20	751.70703	-0.04
50	$C_{55}H_{90}(H)$	N/A	N/A	751.71107	-0.61
51	$C_{52}H_{94}S(H)$	751.71478	-0.16	751.71491	0.01
52	$C_{52}H_{99}{}^{13}C_2(H)$	751.79686	0.49	751.79635	-0.19
53	$C_{53}H_{102}{}^{13}C$	751.80094	-0.03	751.80099	0.04
54	$C_{54}H_{102}(H)$	751.80545	0.03	751.80541	-0.03
55	$C_{51}H_{68}$	680.53179	0.35	680.53149	-0.10
56	$C_{48}H_{72}S$	680.53496	0.04	680.53490	-0.04
57	$C_{45}H_{76}S_2$	680.53805	-0.36	680.53824	-0.08
58	$C_{53}H_{64}$	700.50054	0.41	700.50020	-0.07
59	$C_{50}H_{68}S$	700.50368	0.08	700.50360	-0.03
60	$C_{47}H_{72}S_2$	700.50689	-0.15	700.50699	-0.01
61	$C_{54}H_{72}$	720.56309	0.33	720.56272	-0.18
62	$C_{51}H_{76}S$	720.56624	0.02	720.56616	-0.09
63	$C_{48}H_{80}S_2$	N/A	N/A	720.56953	-0.09
64	$C_{56}H_{68}$	N/A	N/A	740.53146	-0.13
65	$C_{53}H_{72}S$	740.53495	0.03	740.53486	-0.09
66	$C_{50}H_{76}S_2$	N/A	N/A	740.53823	-0.09
67	$C_{57}H_{76}$	N/A	N/A	760.59404	-0.15
68	$C_{54}H_{80}S$	760.59752	0.00	760.59748	-0.05
69	$C_{51}H_{84}S_2$	N/A	N/A	760.60087	-0.03
70	$C_{58}H_{84}$	N/A	N/A	780.65657	-0.23
71	$C_{55}H_{88}S$	780.65992	-0.27	780.66006	-0.09
72	$C_{52}H_{92}S_2$	N/A	N/A	780.66350	0.01
73	$C_{60}H_{80}$	N/A	N/A	800.62534	-0.15
74	$C_{57}H_{84}S$	800.62882	-0.01	800.62875	-0.10
75	$C_{54}H_{88}S_2$	N/A	N/A	800.63205	-0.18
76	$C_{61}H_{88}$	N/A	N/A	820.68784	-0.26
77	$C_{58}H_{92}S$	820.69115	-0.34	820.69136	-0.08
78	$C_{55}H_{96}S_2$	N/A	N/A	820.69485	0.06

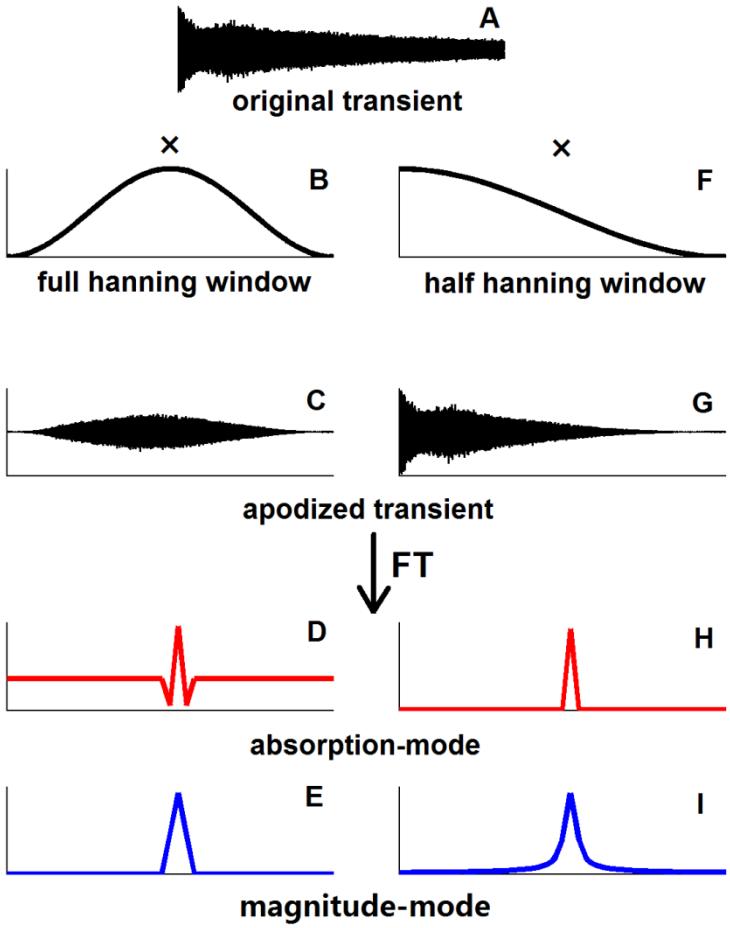

Figure S1. Transient, window function and its corresponding peak shape by simulation.

A: original transient; B to E: full hanning window, apodized transient, and its corresponding peak shape in the absorption and magnitude-mode; F to I: half hanning window, apodized transient, and its peak shape in the absorption and magnitude-mode.

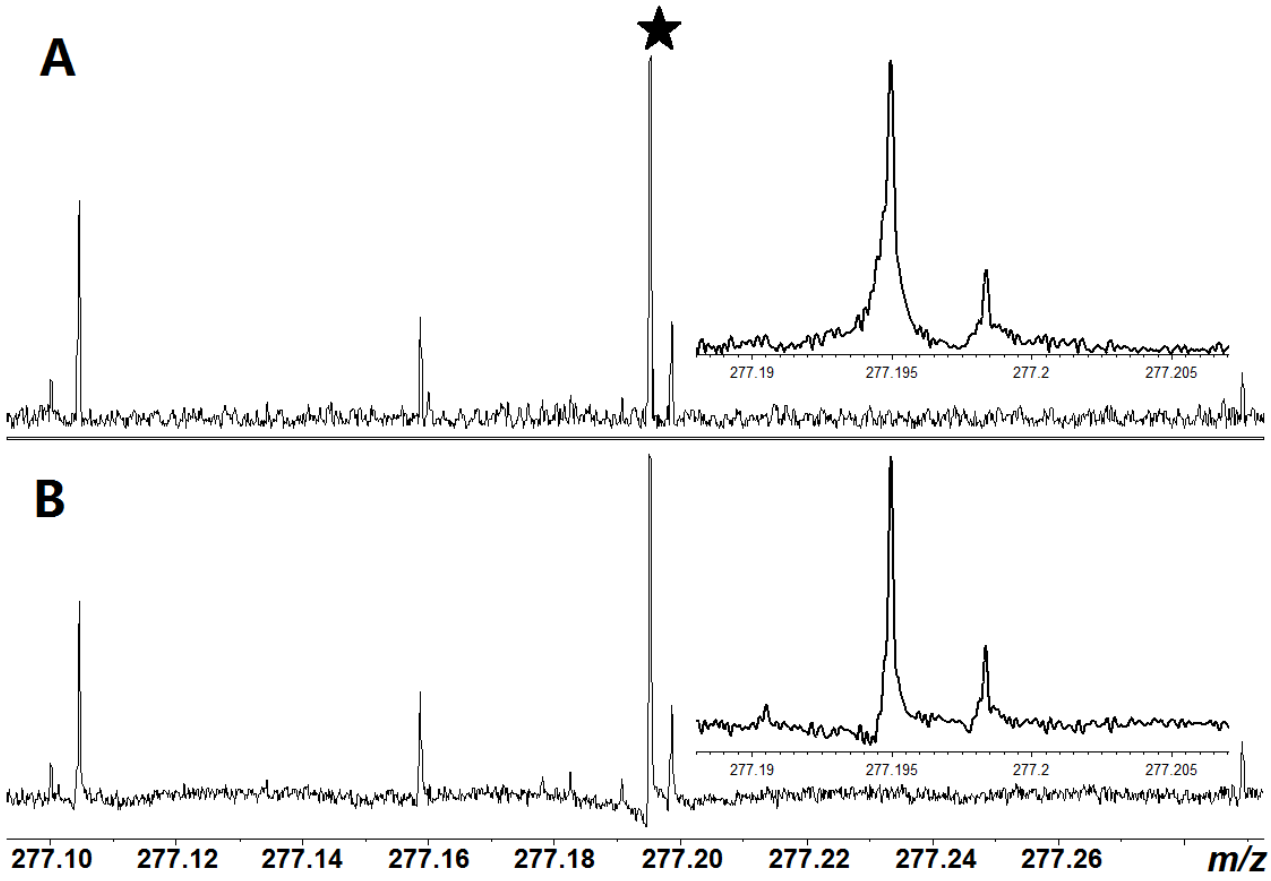

Figure S2. A: zoom in of oil spectrum in the low *m/z* region with magnitude-mode and, B: absorption-mode, inset: further zoom in of labelled peaks from the **unapodized** spectrum to show the wiggles and broad "tails". Note the asymmetric peak shape of the absorption-mode spectrum causes a slightly negative shift in *m/z* (mentioned in the text).

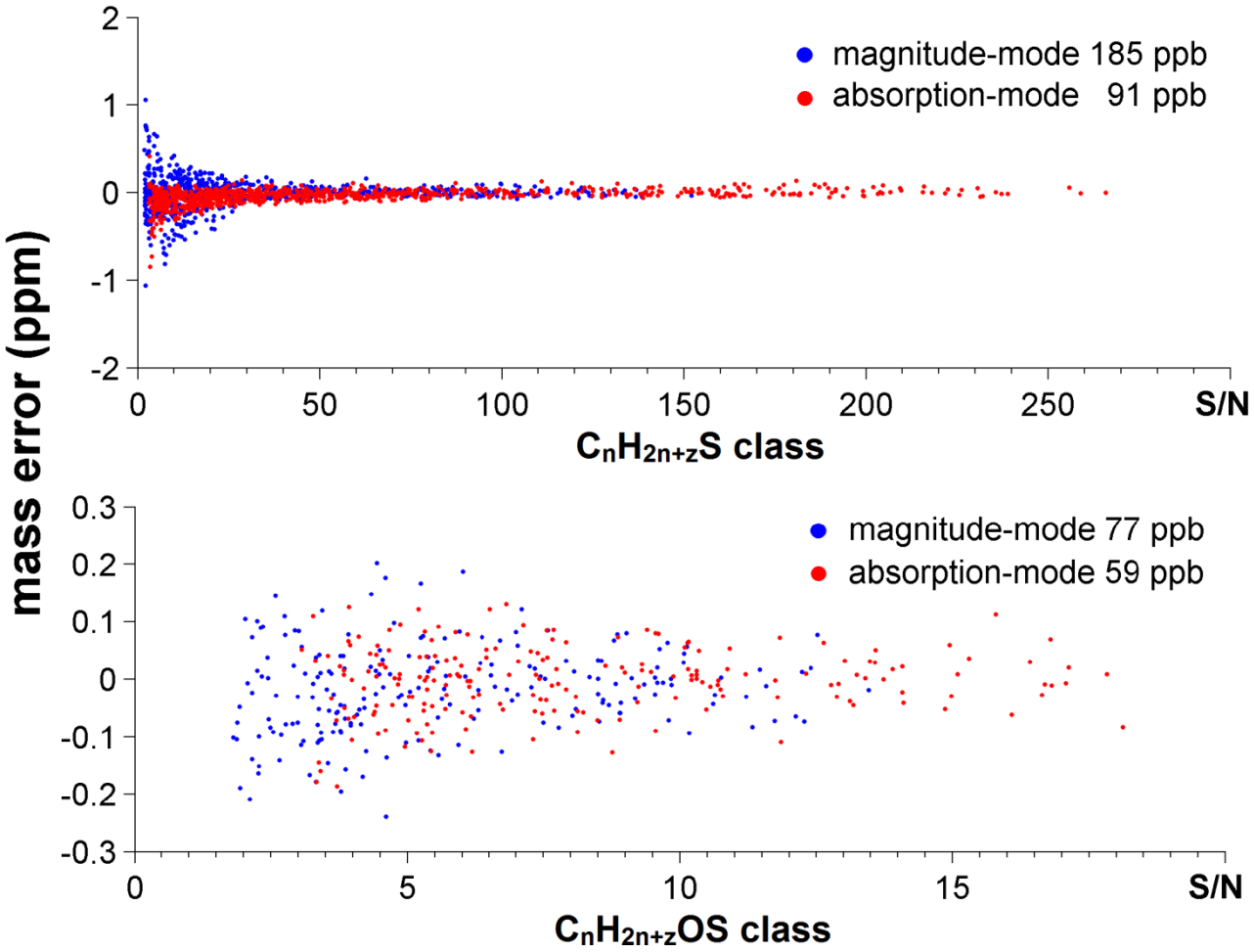

Figure S3. RMS mass error distribution to show the mass accuracy improvement for different compounds in the crude oil, huge for $C_nH_{2n+z}S$ (top), while intermediate for $C_nH_{2n+z}OS$ (bottom).