CSO BROADBAND MOLECULAR LINE SURVEYS I: BENCHMARKING GOBASIC ANALYSIS SOFTWARE

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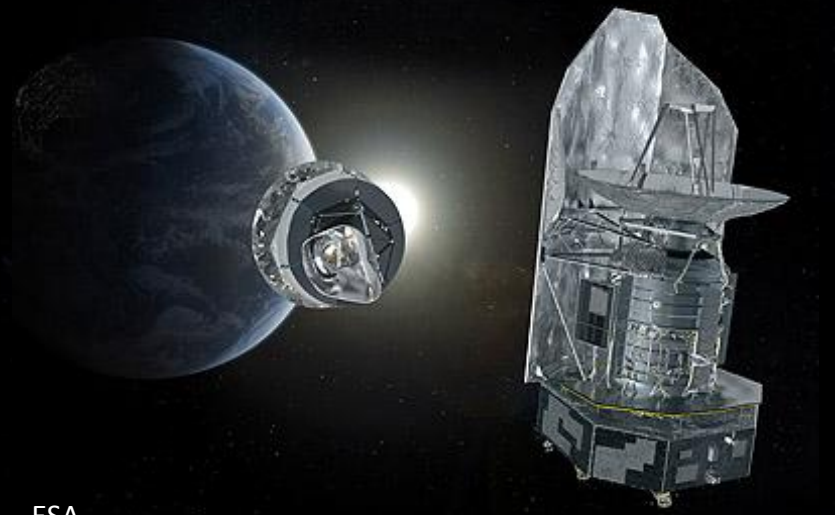
Motivation for GOBASIC

- Vast broadband datasets from the CSO, ALMA, and the Herschel Space Observatory

ESO/B. Tafreshi (twanight.org)

Smallest CSO dataset ~ 30 GHz of data, 32 surveys now on hand



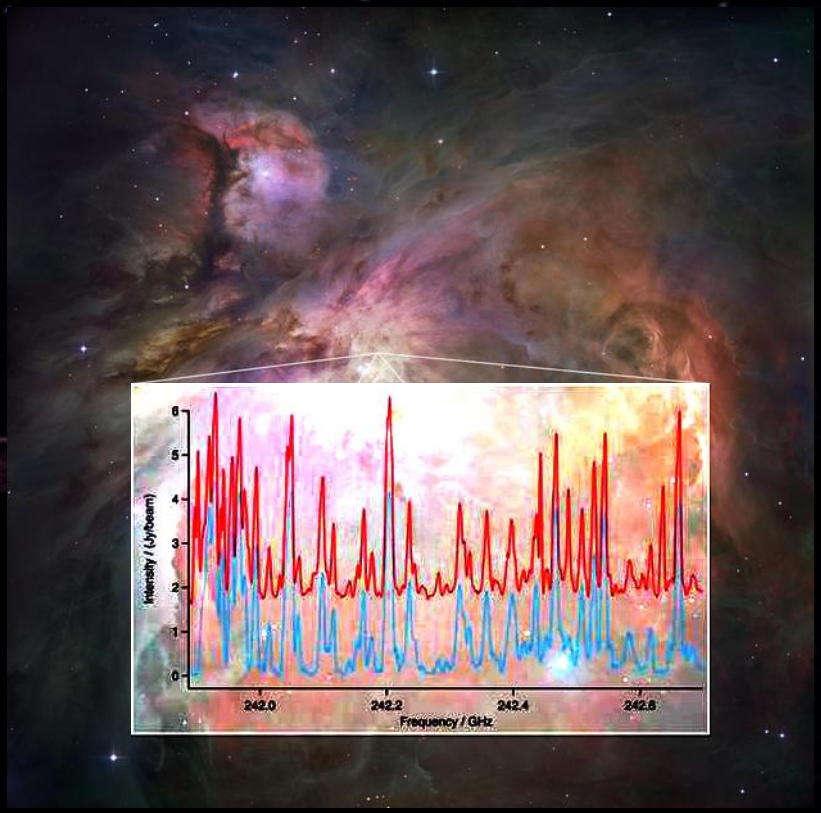
Jacob C. Laas

ESA

Motivation for GOBASIC

- Probed sources with many complex molecules and many components of gas

Increased sensitivity leads to line dense spectra with complex line blending



ALMA ethyl cyanide overlay on Orion spectrum. Fortman, et al., NRAO/AUI/NSF, NASA

Approach of GOBASIC

Time required for analysis

- Import JPL/CDMS catalogs with no special formatting required
- Little user input necessary
- Fast global, derivative-free pattern search optimization
- Parallel processing capabilities
- LTE assumptions

Complexity of Analysis

- Global analysis
- Simultaneous multi-molecule, multi-component fitting up to four components
- Iterative analysis procedure

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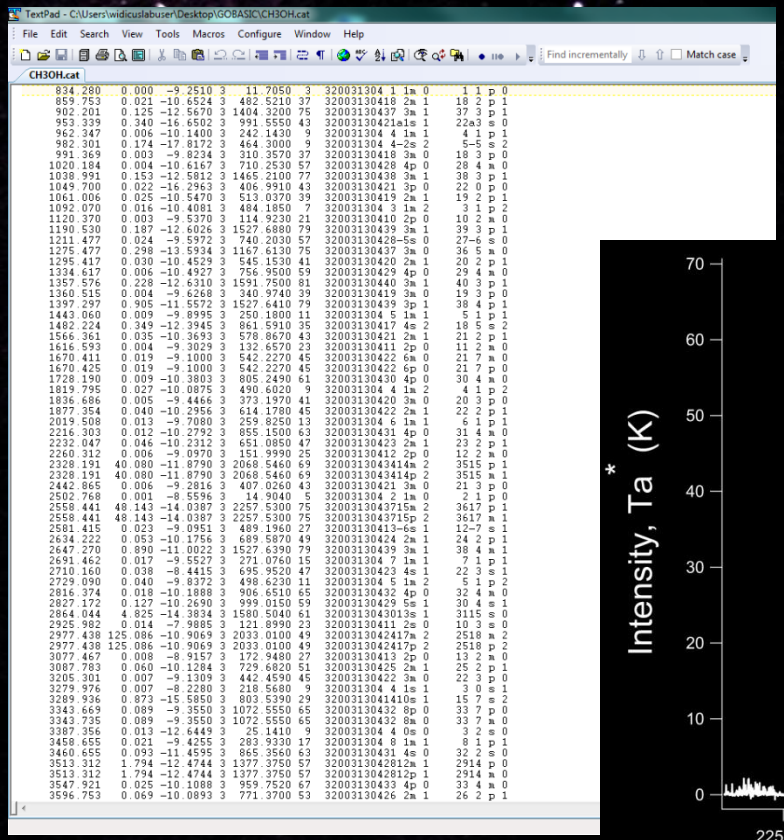
Input deconvolved observational data and JPL/CDMS catalog



834.280	0.000	-9.2510	3	11.7050	3	320031304	1	1m	0	1	1	p	0
859.753	0.021	-10.6524	3	482.5210	37	32003130418	2	m	1	18	2	p	1
902.201	0.125	-12.5670	3	1404.3200	75	32003130437	3	m	1	37	3	p	1
953.339	0.340	-16.6502	3	991.5550	43	320031304	21	a1s	1	22	a3	s	0
962.347	0.006	-10.1400	3	242.1430	9	320031304	4	1m	1	4	1	p	1
982.301	0.174	-17.8172	3	464.3000	9	320031304	4	-2s	2	5	-5	s	2
991.369	0.003	-9.8234	3	310.3570	37	32003130418	3	m	0	18	3	p	0
1020.184	0.004	-10.6167	3	710.2530	57	32003130428	4	p	0	28	4	m	0
1038.991	0.153	-12.5812	3	1465.2100	77	32003130438	3	m	1	38	3	p	1
1049.700	0.022	-16.2963	3	406.9910	43	32003130421	3	p	0	22	0	p	0
1061.006	0.025	-10.5470	3	513.0370	39	32003130419	2	m	1	19	2	p	1
1092.070	0.016	-10.4081	3	484.1850	7	320031304	3	1m	2	3	1	p	2
1120.370	0.003	-9.5370	3	114.9230	21	32003130410	2	p	0	10	2	m	0
1190.530	0.187	-12.6026	3	1527.6880	79	32003130439	3	m	1	39	3	p	1
1211.477	0.024	-9.5972	3	740.2030	57	32003130428	-5	s	0	27	-6	s	0
1275.477	0.298	-13.5934	3	1167.6130	75	32003130437	3	m	0	36	5	m	0
1295.417	0.030	-10.4529	3	545.1530	41	32003130420	2	m	1	20	2	p	1
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1360.515	0.004	-9.6268	3	340.9740	39	32003130419	3	m	1	19	3	p	0
1397.297	0.905	-11.5572	3	1527.6410	79	32003130439	3	p	1	38	4	p	1
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1566.361	0.035	-10.3693	3	578.8670	43	32003130421	2	m	1	21	2	p	1
1616.593	0.004	-9.3029	3	132.6570	23	32003130411	2	p	0	11	2	m	0
1670.411	0.019	-9.1000	3	542.2270	45	32003130422	6	m	0	21	7	m	0
1670.425	0.019	-9.1000	3	542.2270	45	32003130422	6	p	0	21	7	p	0
1728.190	0.009	-10.3803	3	805.2490	61	32003130430	4	p	0	30	4	m	0
1819.795	0.027	-10.0875	3	490.6020	9	320031304	4	1m	2	4	1	p	2
1836.686	0.005	-9.4466	3	373.1970	41	32003130420	3	m	0	20	3	p	0
1877.354	0.040	-10.2956	3	614.1780	45	32003130422	2	m	1	22	2	p	1
2019.508	0.013	-9.7080	3	259.8250	13	320031304	6	1m	1	6	1	p	1
2216.303	0.012	-10.2792	3	855.1500	63	32003130431	4	p	0	31	4	m	0
2232.047	0.046	-10.2312	3	651.0850	47	32003130423	2	m	1	23	2	p	1
2260.312	0.006	-9.0970	3	151.9990	25	32003130412	2	p	0	12	2	m	0
2328.191	40.080	-11.8790	3	2068.5460	69	320031304	314	m	2	3515	p	1	
2328.191	40.080	-11.8790	3	2068.5460	69	320031304	314	p	2	3515	m	1	
2442.865	0.006	-9.2816	3	407.0260	43	32003130421	3	m	0	21	3	p	0
2502.768	0.001	-8.5596	3	14.9040	5	320031304	2	1m	0	2	1	p	0
2558.441	48.143	-14.0387	3	2257.5300	75	320031304	3715	m	2	3617	p	1	
2558.441	48.143	-14.0387	3	2257.5300	75	320031304	3715	p	2	3617	m	1	
2581.415	0.023	-9.0951	3	489.1960	27	320031304	13	-6s	1	12	-7	s	1
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2647.270	0.890	-11.0022	3	1527.6390	79	32003130439	3	m	1	38	4	m	1
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2816.374	0.018	-10.1888	3	906.6510	65	32003130432	4	p	0	32	4	m	0
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2864.044	4.825	-14.3834	3	1580.5040	61	320031304	303	s	1	3115	s	0	
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2977.438	125.086	-10.9069	3	2033.0100	49	320031304	2417	m	2	2518	m	2	
2977.438	125.086	-10.9069	3	2033.0100	49	320031304	2417	p	2	2518	p	2	
3077.467	0.008	-8.9157	3	172.9480	27	32003130413	2	p	0	13	2	m	0
3087.783	0.060	-10.1284	3	729.6820	51	32003130425	2	m	1	25	2	p	1
3205.301	0.007	-9.1309	3	442.4590	45	32003130422	3	m	0	22	3	p	0
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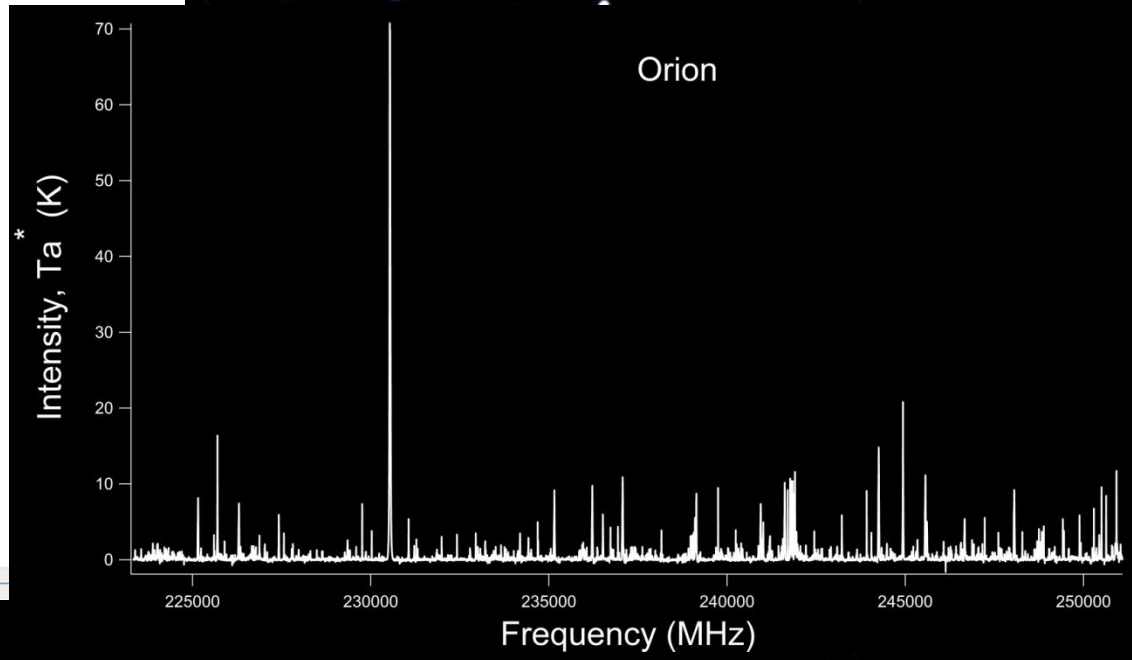
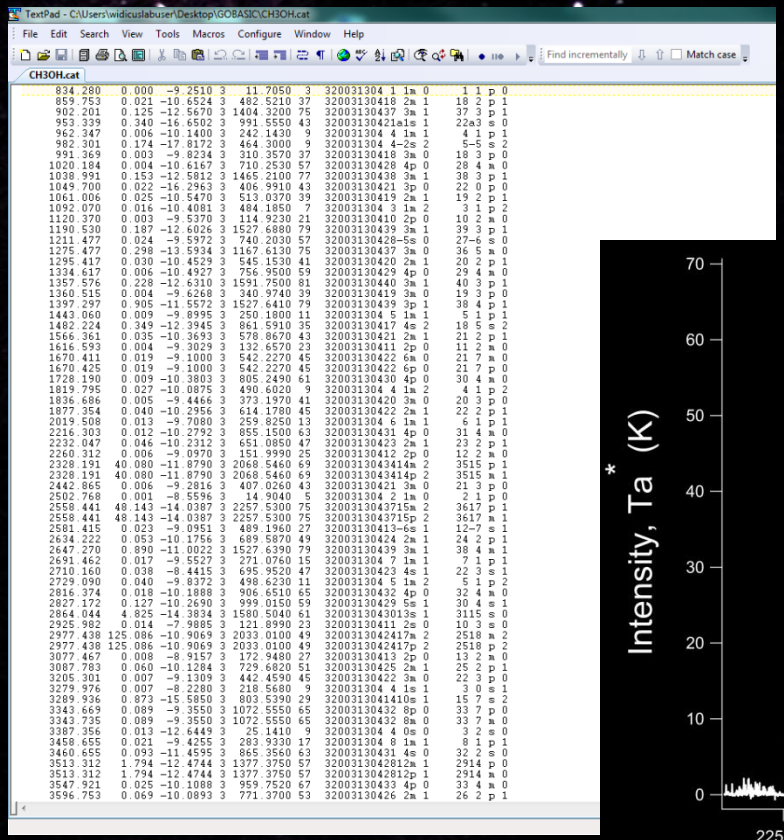
3289.936	0.873	-15.5850	3	803.5390	29	320031304	1410	m	1	15	7	s	2
3343.669	0.089	-9.3550	3	1072.5550	65	32003130432	8	p	0	33	7	p	0
3343.735	0.089	-9.3550	3	1072.5550	65	32003130432	8	m	0	33	7	m	0
3387.356	0.013	-12.6449	3	25.1410	9	320031304	4	0s	0	3	2	s	0
3458.655	0.021	-9.4255	3	283.9330	17	320031304	8	1m	1	8	1	p	1
3460.655	0.093	-11.4595	3	865.3560	63	32003130431	4	s	0	32	2	s	0
3513.312	1.794	-12.4744	3	1377.3750	57	320031304	2812	m	1	2914	p	0	
3513.312	1.794	-12.4744	3	1377.3750	57	320031304	2812	p	1	2914	m	0	
3547.921	0.025	-10.1088	3	959.7520	67	32003130433	4	p	0	33	4	m	0
3596.753	0.069	-10.0893	3	771.3700	53	32003130426	2	m	1	26	2	p	1





Input deconvolved observational data and JPL/CDMS catalog

- Internal selection of catalog data for line intensity and uncertainty limits
- Internal calibration of observational data for telescope efficiency and beam dilution

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LTE population diagram equations from Goldsmith and Langer (1999) *ApJ* **517** used to simulate spectra:

$$T_a = \frac{hc^3 N_T A_{ul} g_u e^{-E_u/kT}}{8\pi k \nu^2 \Delta v Q(T)} \left(\frac{1 - e^{-\tau}}{\tau} \right)$$

$$\tau = \frac{N_T}{Q(T)\Delta v} \frac{c^3}{8\pi\nu^3} A_{ul} g_u e^{-E_u/kT} \left(e^{h\nu/kT} - 1 \right)$$

Pattern search optimization to minimize difference between simulated spectrum and observational spectrum:

$$f(N_T, (m, c, i), \Delta v(m, c, i), T(m, c, i), v(m, c, i)) = ||\mathrm{obs}(\nu) - T_{\mathrm{spec}}(\nu)||$$

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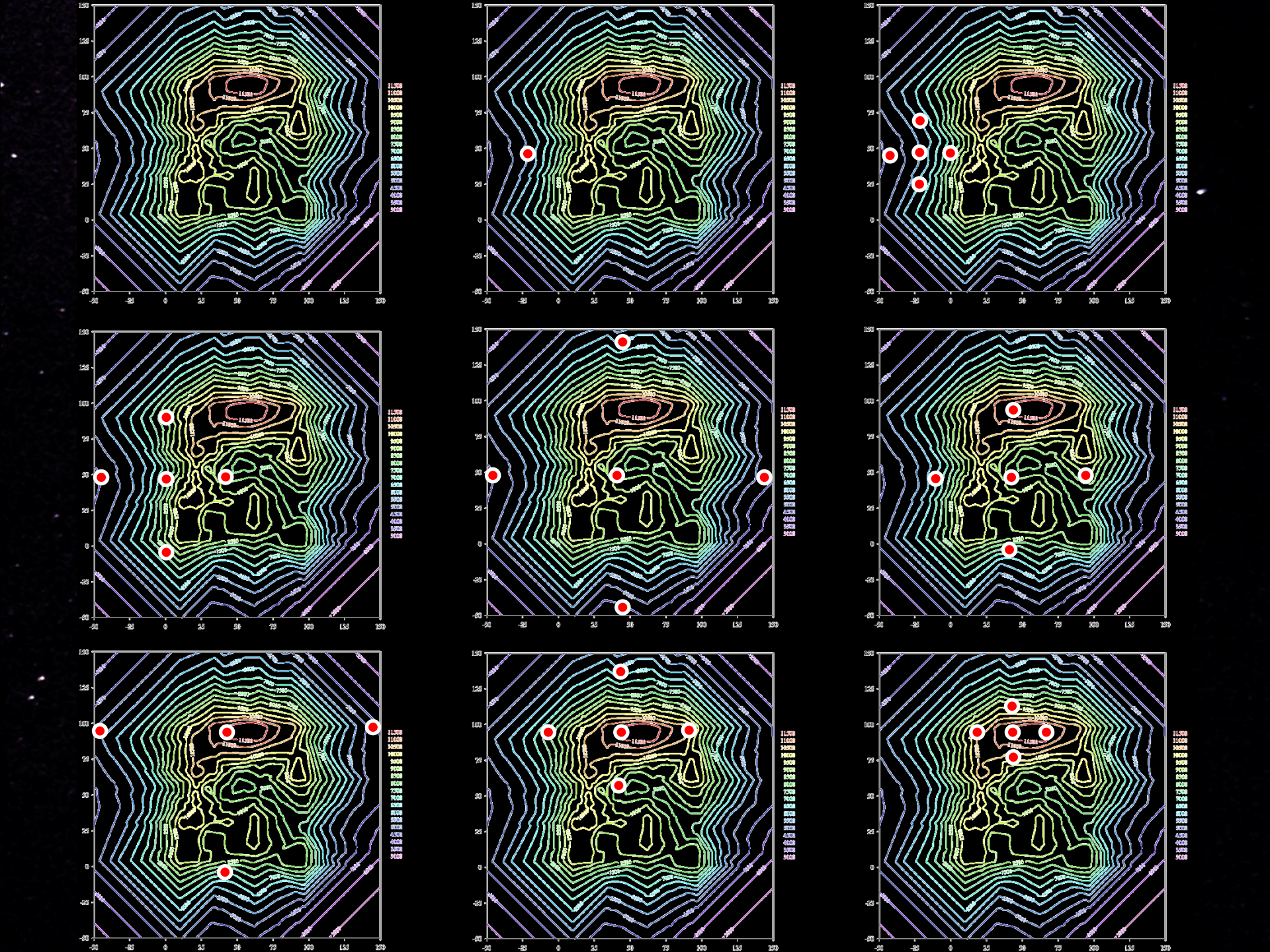
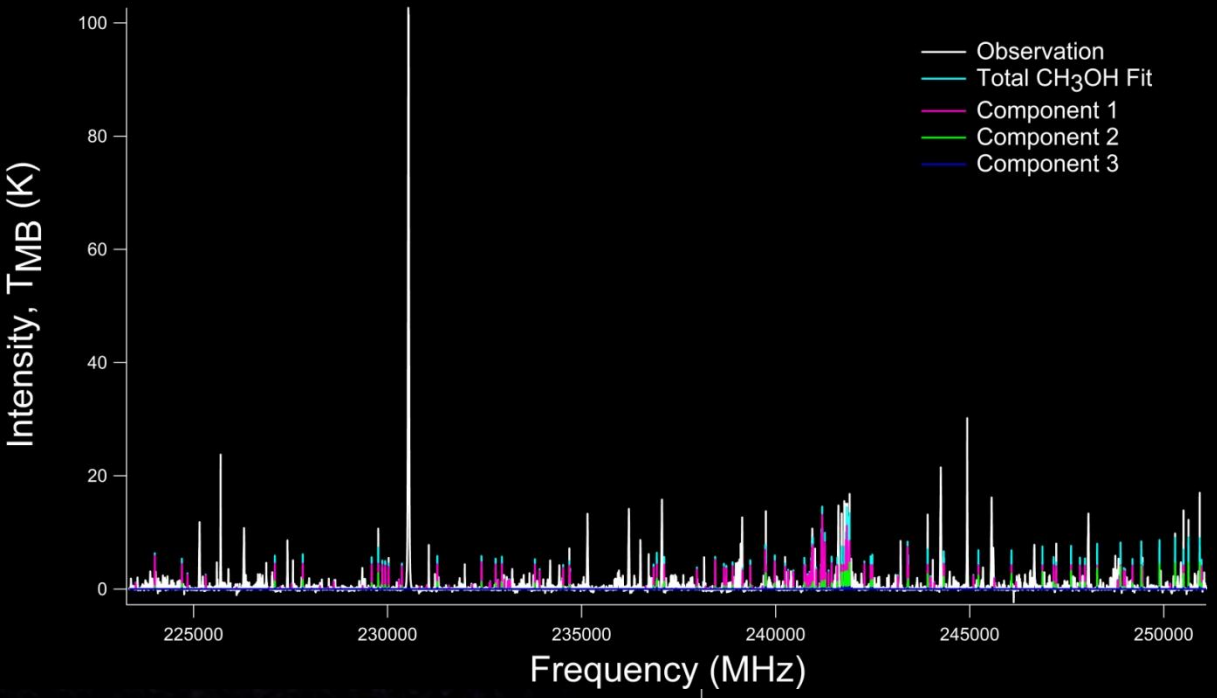
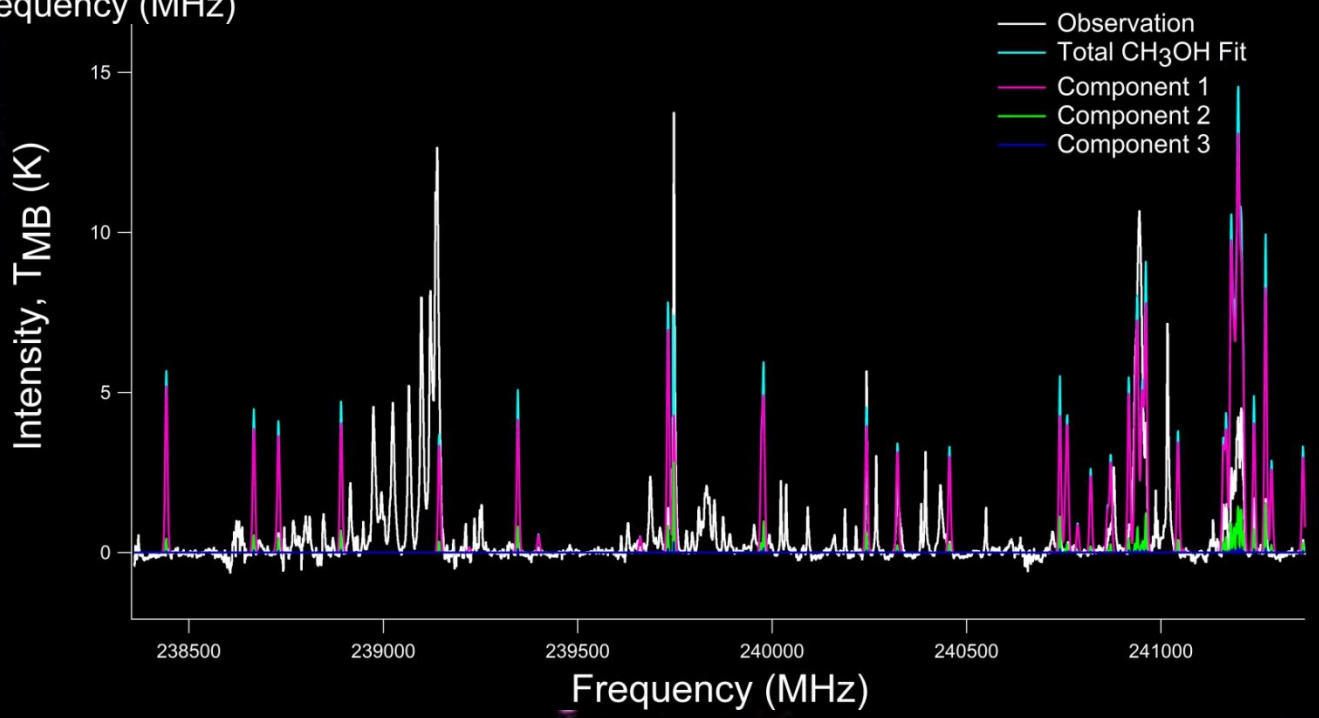
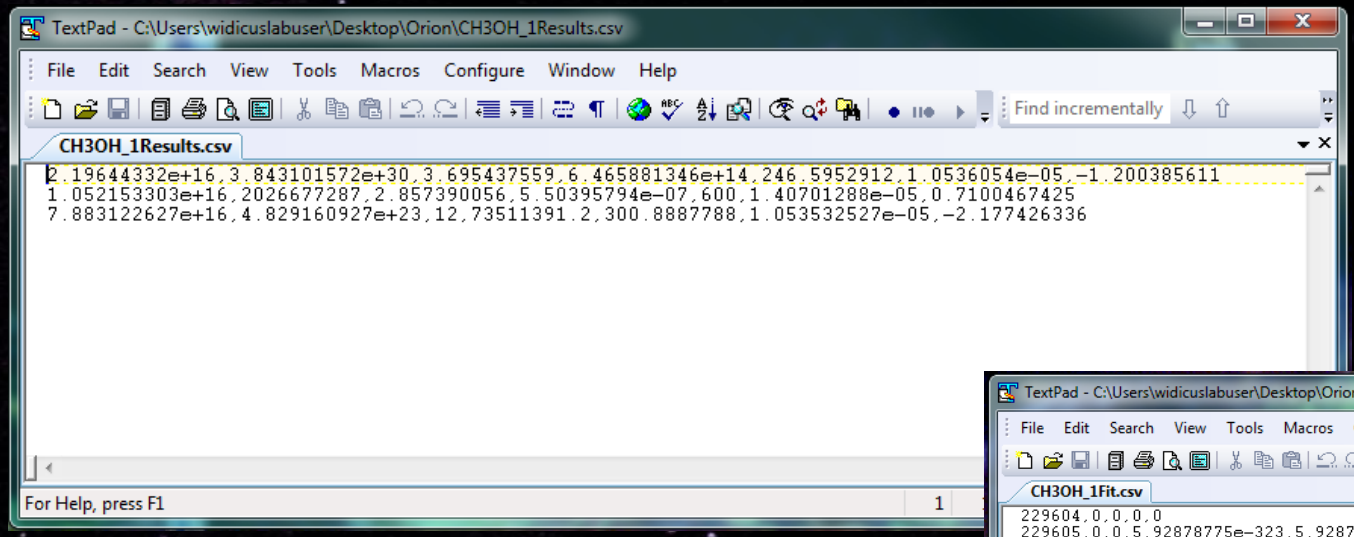
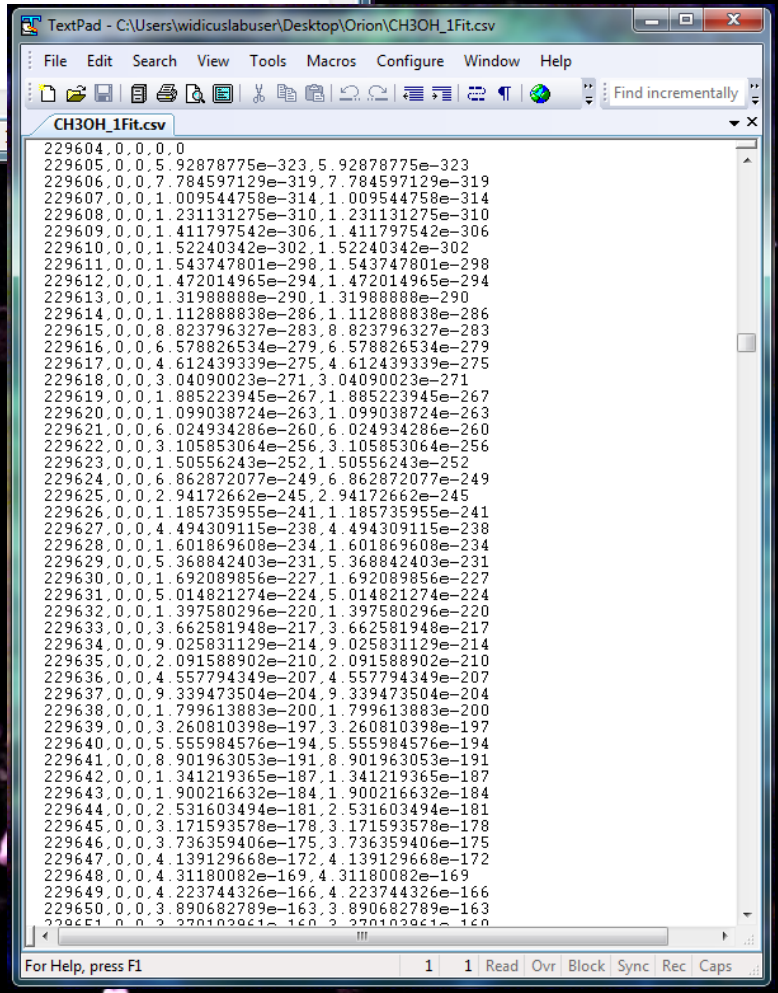




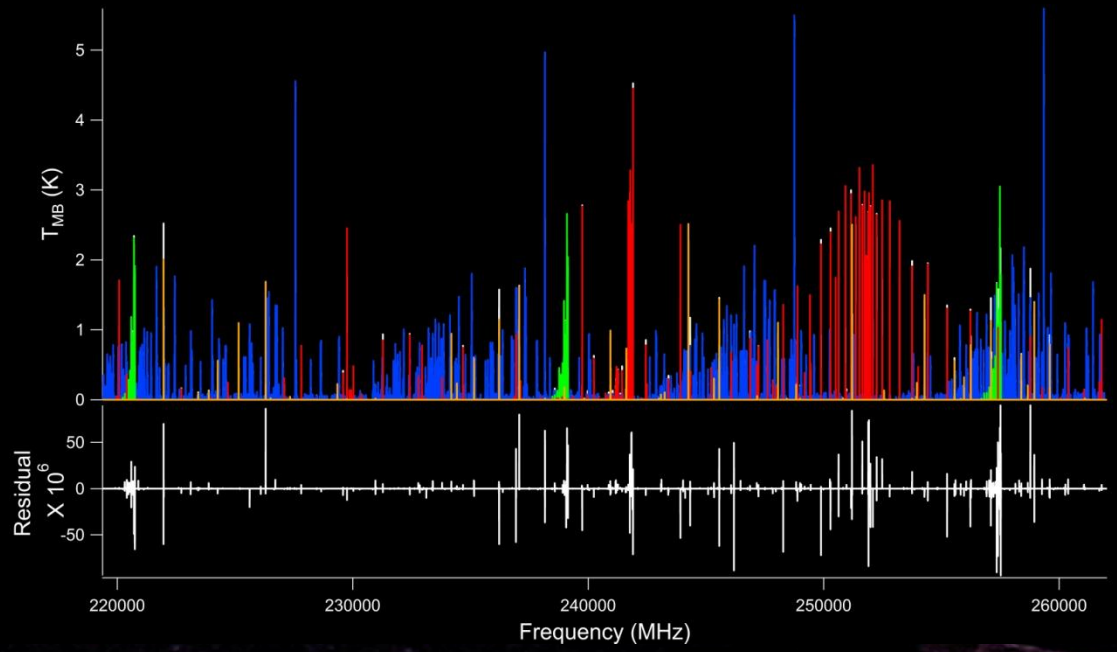
Output figures show best fit simulations for each component and total simulated spectrum



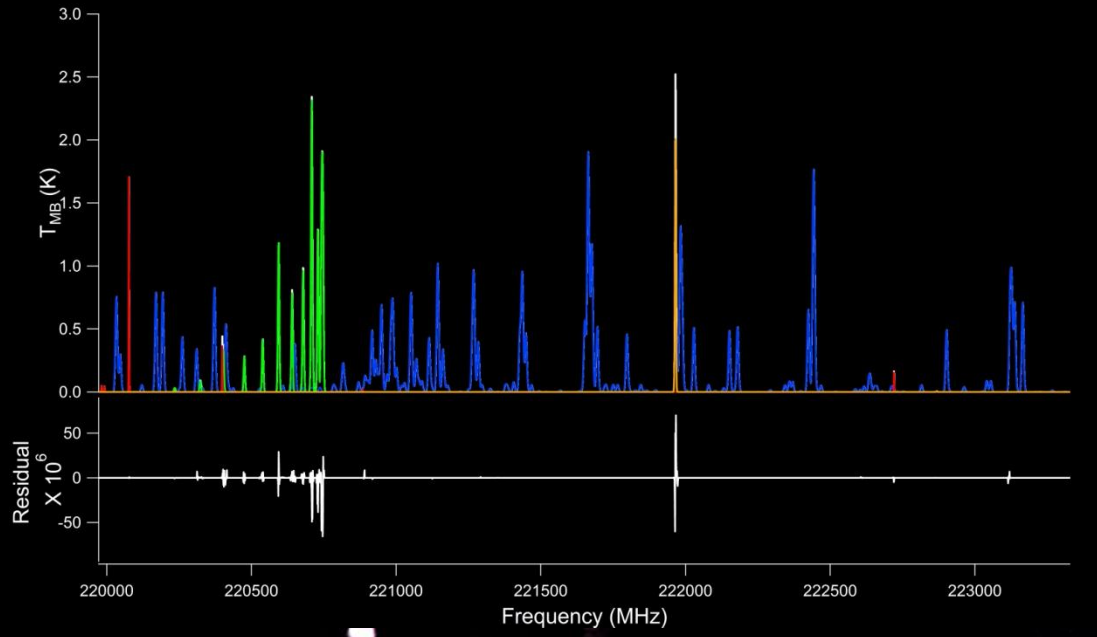


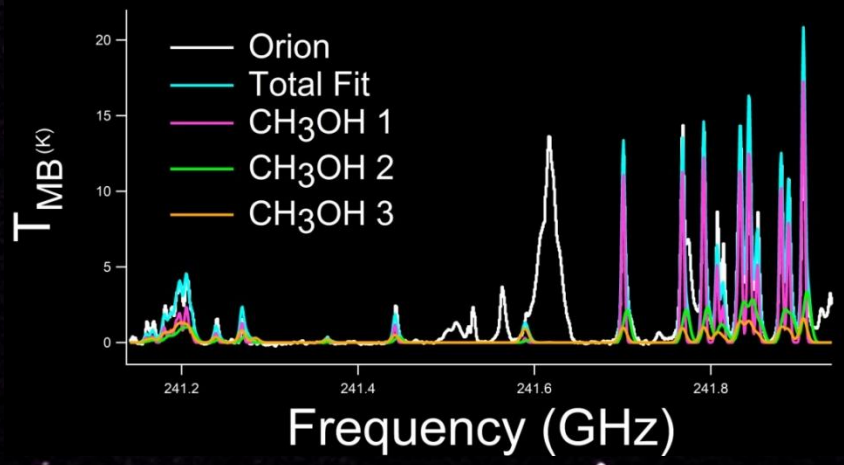


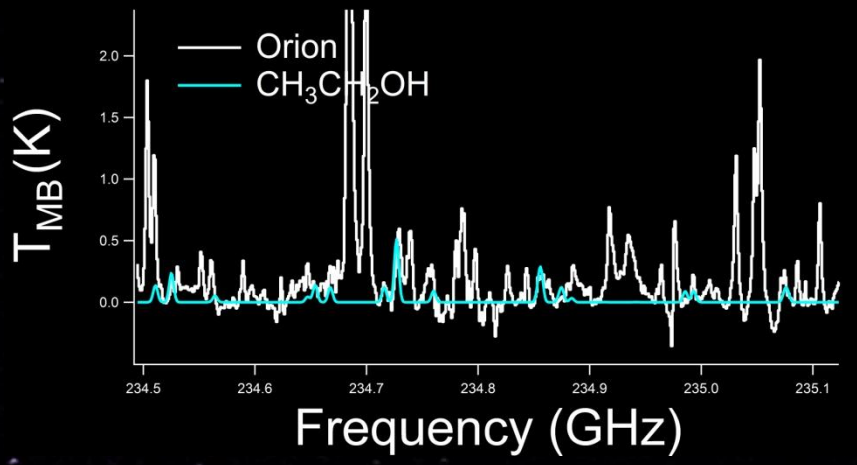
Output files in .csv format include best fit variables with associated errors and simulated spectra for each component

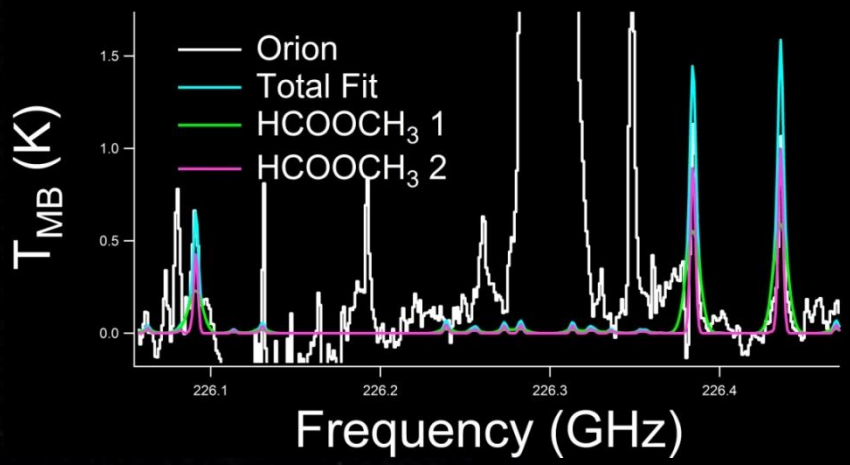


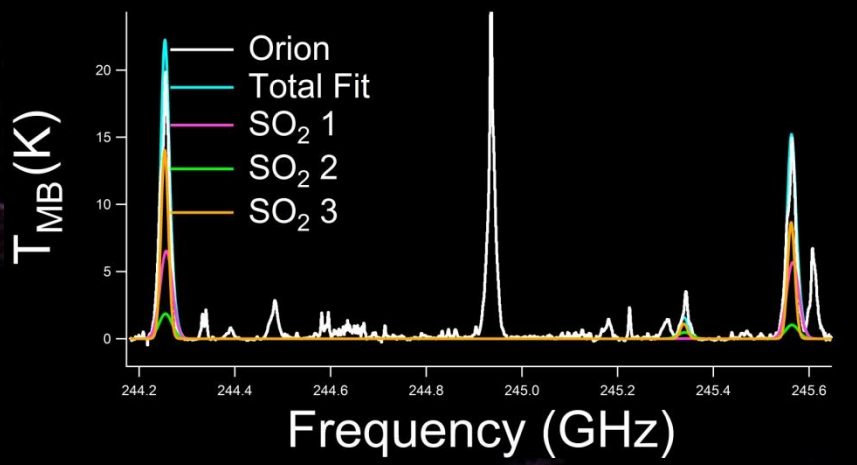
Noiseless simulated spectral fit test. Six molecule spectrum simulated. Residual multiplied by 10^6 as to be visible.

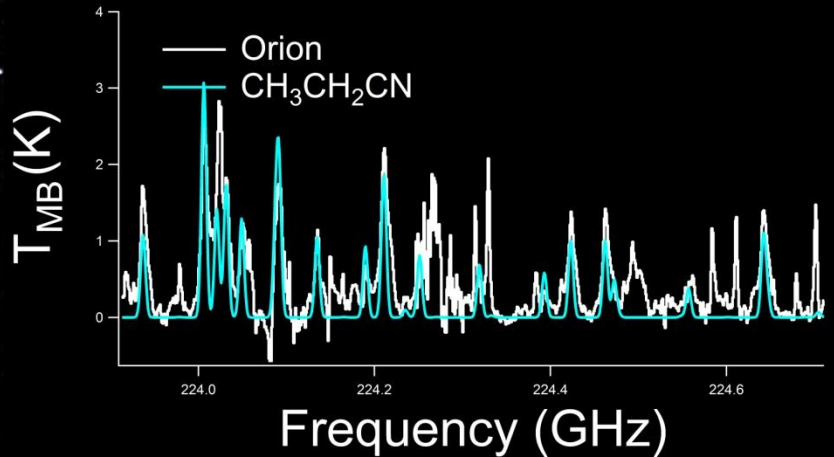




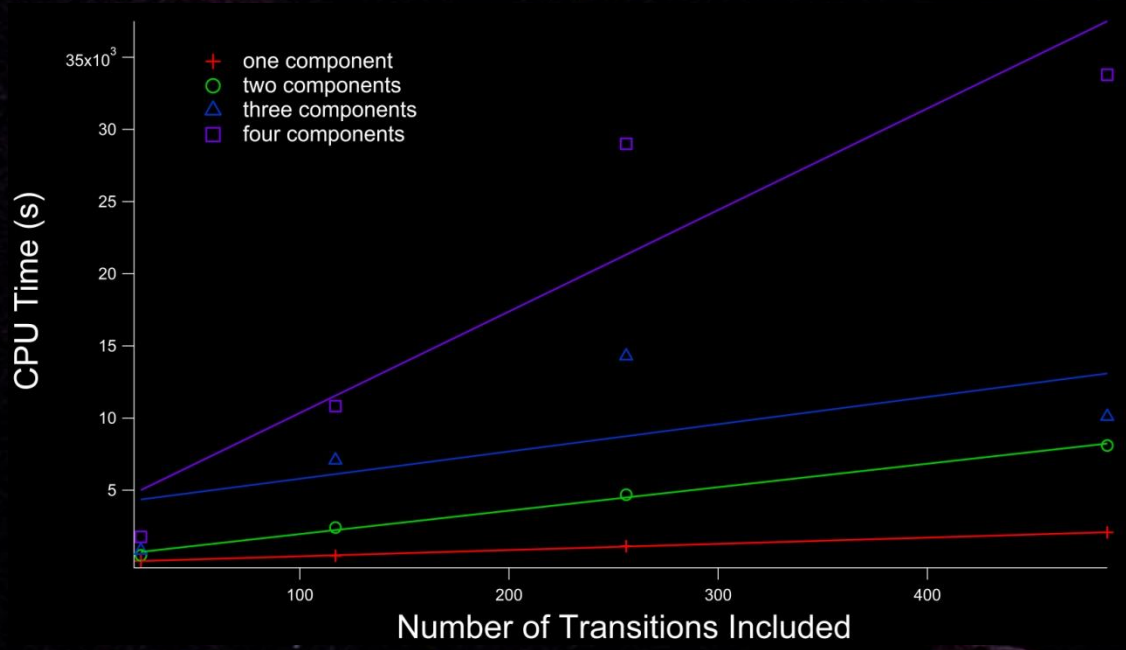






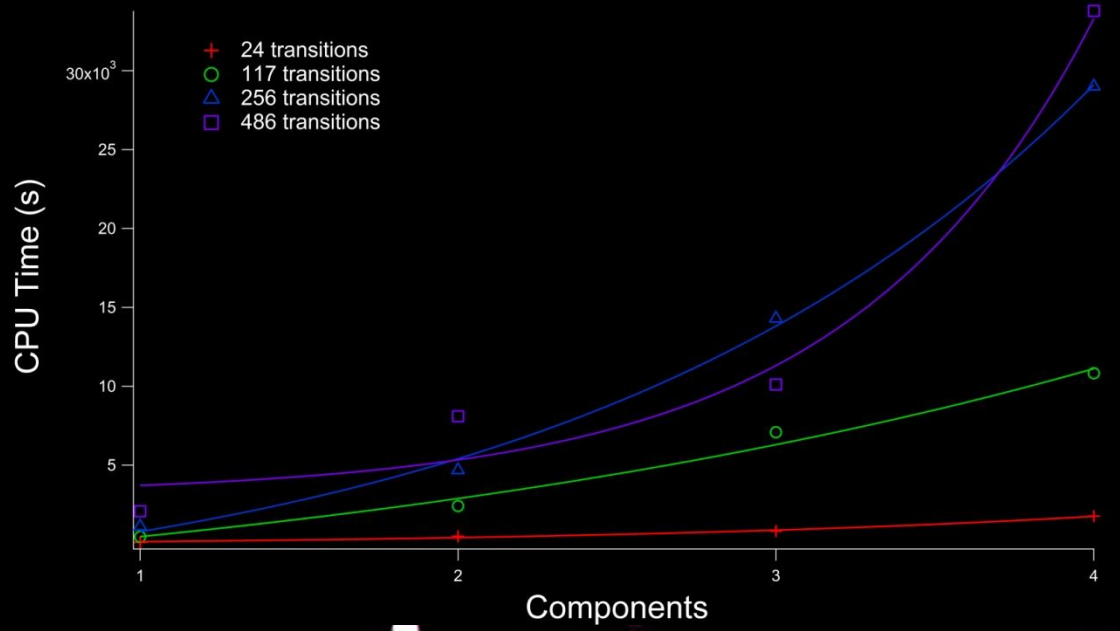


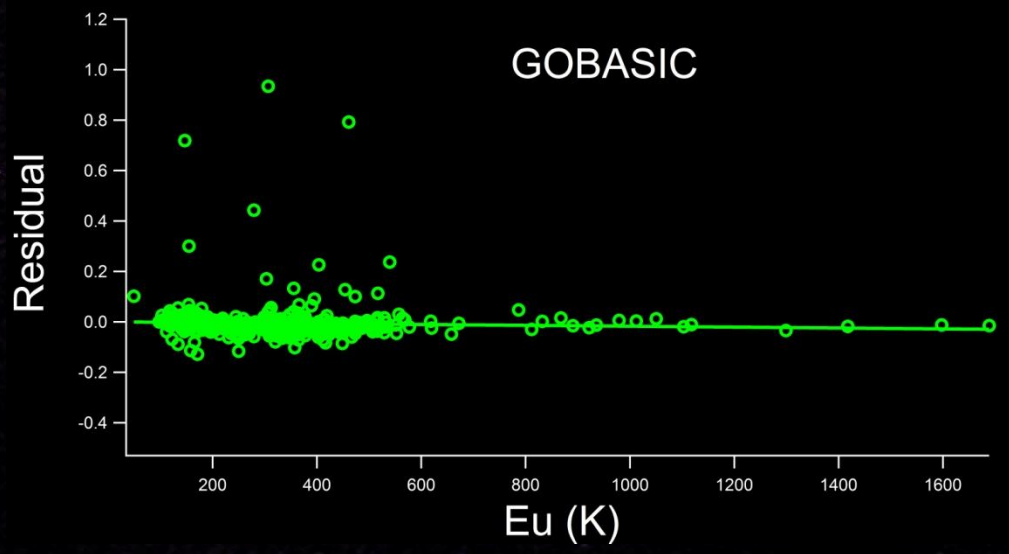
- Fit test on Orion showed good match to observational data and to previous analysis of Orion of Blake et al. 1986 *ApJS* **60**.



Time benchmarking trials used CH_3OH analysis on Orion broadband line survey

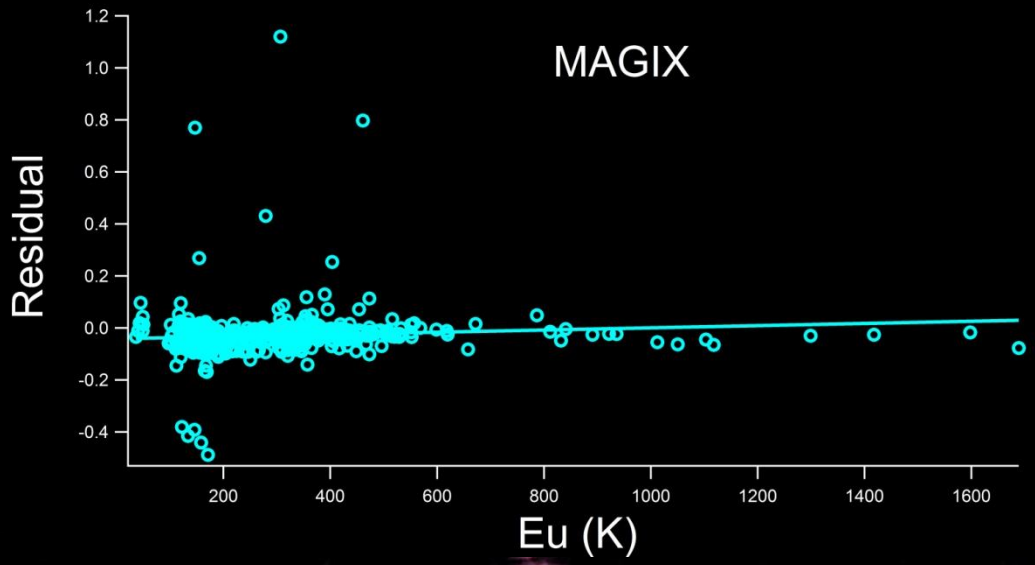
CPU time ~ 7(trans) + $150e^{1.3(components)}$





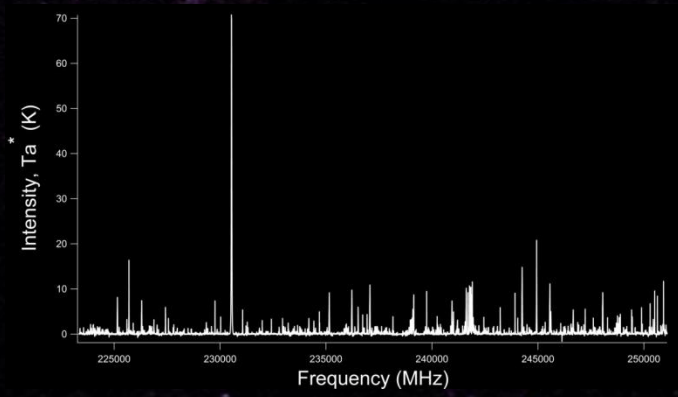
Single component methyl formate fit on CSO survey of W3. Comparison of residual vs upper state energy. Positive residual is under prediction, negative residual is over prediction.

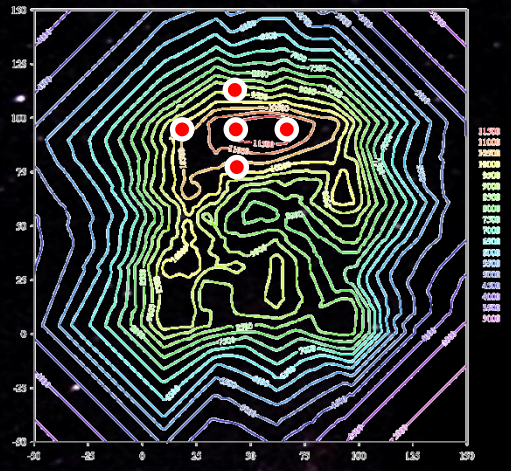
Over prediction of lower E_u(K) lines with MAGIX results in skewing toward lower temperatures.



Möller et al. 2013 *A&A* **549**

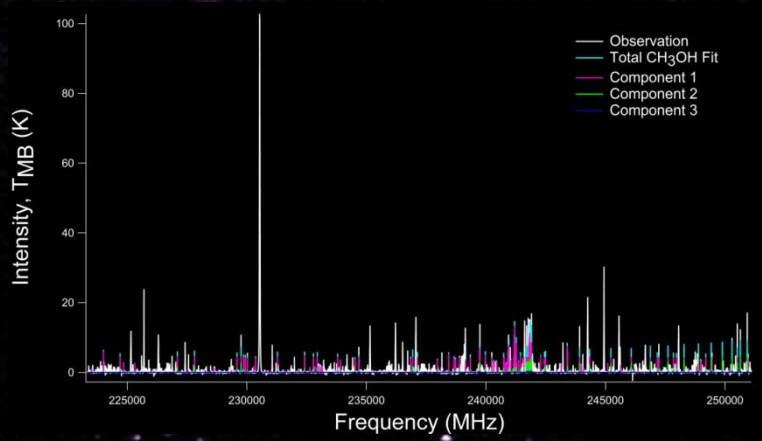
Summary



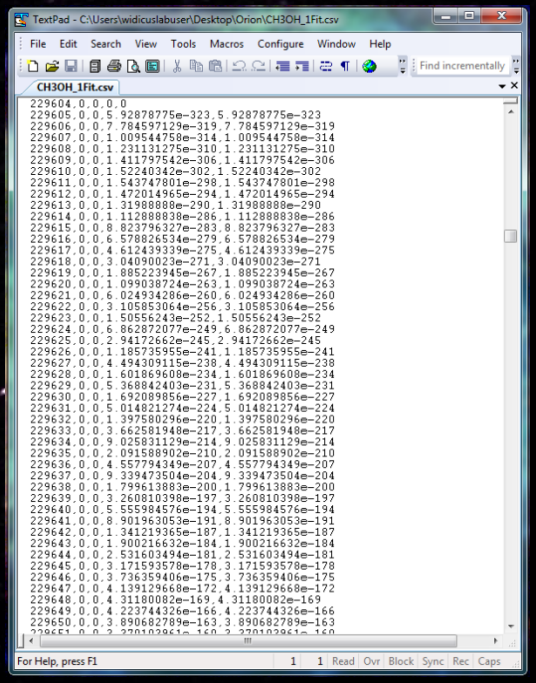


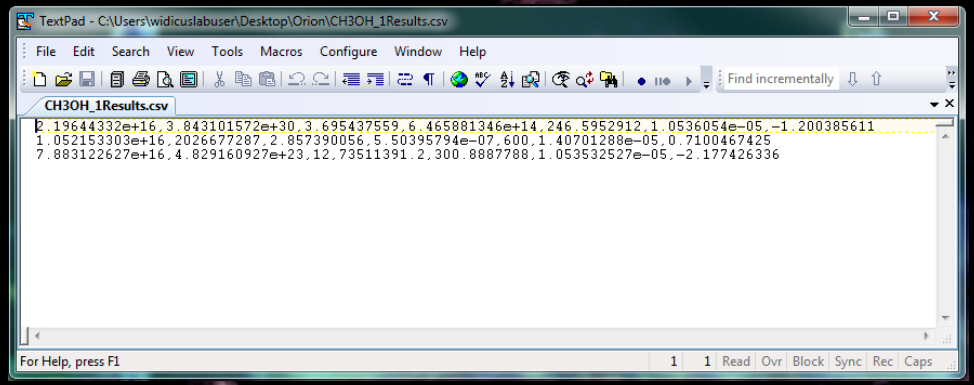
- GOBASIC analysis is fast, robust, and easy with little data calibration and user input required.

Summary

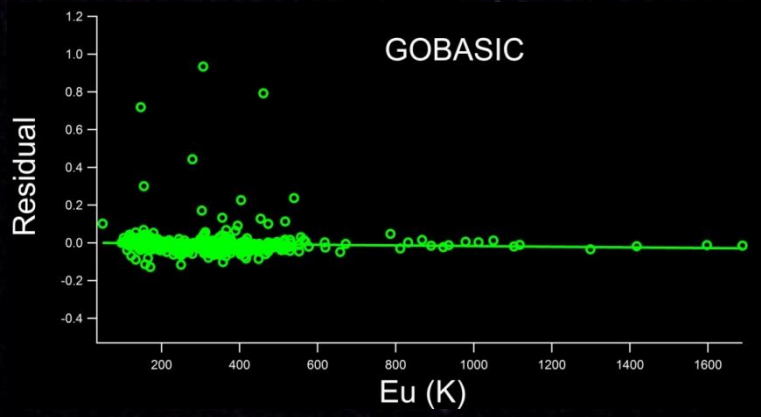


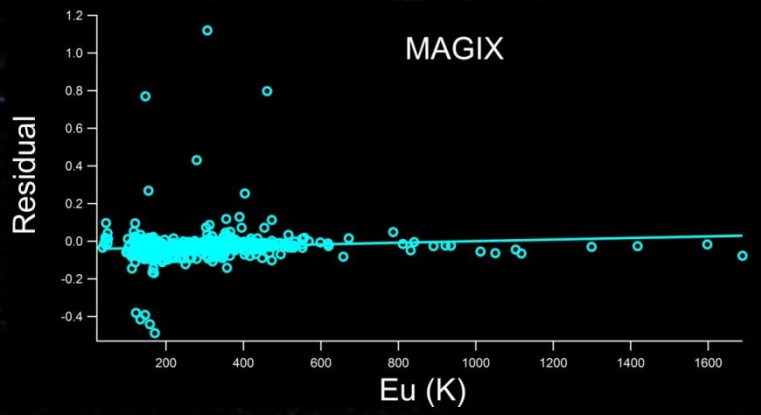
- Final results are provided conveniently as graphs, simulation files, and tables of best fit parameters.





Summary





- Compared to MAGIX and rotation diagram analysis, GOBASIC is less susceptible to skewed results from incorrect line shape analysis.

Future Work

- Complete Analysis of CSO and HIFI surveys (James Sanders TI07)
- Expand use of GOBASIC beyond Widicus Weaver lab (Paper submitted to ApJS)

Acknowledgements

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Emory College Undergraduate Research Matching Grant