Results of experiment series I: C4-compounds

GC-MS-Results (total ion chromtogram and identification).
PK: Number of peak identified
RT: Retention time of the chromatogram
Area Pct: % of the total measured area in the total ion chromatogram
Ref: Reference Number
CAS: CAS Number
Qual: Quality of identification, above 80 % the compounds is regarded as identified.

Table 1: Experiment with 1-Butanol, Headspace analysis (100 µL at 200 °C),

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	8.97	3.76	Oxygen(DOT)	113642	007782-44-7	1
2	9.58	16.36	Carbon dioxide	113671	000124-38-9	3
3	9.65	5.37	Acetaldehyde	430	000075-07-0	91
4	9.73	0.29	Ethanol	108331	000064-17-5	86
5	9.78	9.86	Acetone	109708	000067-64-1	87
6	9.88	0.29	Propanoic acid, 2-hydroxy-2-methyl-	2492	000594-61-6	78
7	10.16	6.65	Butanal	110540	000123-72-8	95
8	10.64	0.22	Pentanal	114638	000110-62-3	78
9	10.70	11.15	Benzene	115810	000071-43-2	95
10	11.03	1.03	2-Pentanone	7171	000107-87-9	86
11	11.17	0.30	2-Penten-1-ol, (E)-	114699	001576-96-1	40
12	12.56	15.30	Toluene	117282	000108-88-3	94
13	14.88	3.39	Ethylbenzene	117388	000100-41-4	94
14	15.08	4.62	Benzene, 1,3-dimethyl-	117394	000108-38-3	97
15	15.62	5.05	Benzene, 1,3-dimethyl-	117397	000108-38-3	97
16	17.00	0.30	Benzene, propyl-	117470	000103-65-1	91
17	17.21	6.03	Benzene, 1-ethyl-4-methyl-	46776	000622-96-8	95
18	17.54	2.19	Benzene, 1-ethyl-2-methyl-	46774	000611-14-3	95
19	17.82	2.19	Benzene, 1,2,3-trimethyl-	119303	000526-73-8	97
20	18.06	1.05	2-Hexenal, 2-ethyl-	12970	000645-62-5	90
21	18.40	0.48	Benzene, 1-ethyl-3-methyl-	119287	000620-14-4	93
22	18.64	1.14	Indane	120527	000496-11-7	91
23	18.82	0.31	Benzene, 1-propynyl-	51770	000673-32-5	90
24	18.93	0.36	Benzene, 1,2-diethyl-	119273	000135-01-3	96
25	19.45	0.58	Benzene, 2-ethyl-1,4-dimethyl-	53593	001758-88-9	97
26	19.59	1.50	Benzene, 1-ethyl-2,4-dimethyl-	120822	000874-41-9	94
27	20.73	0.23	Benzene, 2-ethenyl-1,4-dimethyl-	52571	002039-89-6	93

Table 2: Experiment with 1-Butanol, SPE-analysis

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	8.71	24.56	Phenol	40630	000108-95-2	95
2	9.87	3.87	Benzaldehyde, 2-hydroxy-	121296	000090-02-8	94
3	10.04	8.98	Phenol, 2-methyl-	119787	000095-48-7	97
4	10.28	6.91	Benzaldehyde, 2-methyl-	117472	000529-20-4	96
5	10.40	26.87	Phenol, 4-methyl-	48443	000106-44-5	95
6	10.54	3.11	Benzaldehyde, 2-methyl-	38042	000529-20-4	96
7	11.58	2.55	Benzenemethanol, 2-methyl-	118905	000089-95-2	94
8	11.67	5.64	Phenol, 2,3-dimethyl-	48509	000526-75-0	97
9	11.94	9.93	Phenol, 2-ethyl-	119665	000090-00-6	90
10	12.38	5.27	Phenol, 3,4-dimethyl-	121291	000095-65-8	97
11	13.68	2.31	Benzene, diethylmethyl-	119917	025550-13-4	76

Table 3: Experiment with 1-Butanal, Headspace analysis (100 µL at 200 °C),

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	9.40	11.82	TRIDEUTEROACETONITRILE	113662	002206-26-0	3
2	9.48	1.04	Acetaldehyde	108064	000075-07-0	91
3	9.62	2.76	2-Propanone	113790	000067-64-1	59
4	9.81	0.40	Propanal, 2-methyl-	109227	000078-84-2	94
5	9.98	45.97	Butanal	107914	000123-72-8	94
6	10.50	8.68	Benzene	115810	000071-43-2	95
7	10.81	0.39	2-Pentanone	7171	000107-87-9	86
8	10.95	0.44	3-Heptene, (E)-	2212	014686-14-7	86
9	12.22	0.43	Butanal, 2-ethyl-	6527	000097-96-1	91
10	12.32	4.96	Toluene	117292	000108-88-3	94
11	13.22	0.69	Hexanal	10785	000066-25-1	91
12	13.71	0.59	2-Ethyl-trans-2-butenal	2904	063883-69-2	93
13	14.76	0.77	Ethylbenzene	117388	000100-41-4	94
14	14.96	1.07	Benzene, 1,3-dimethyl-	117394	000108-38-3	97
15	15.10	0.76	4-Heptanone	6294	000123-19-3	91
16	15.45	0.70	3-Heptanone	112009	000106-35-4	91
17	15.53	1.36	Benzene, 1,3-dimethyl-	117394	000108-38-3	97
18	16.46	0.19	2-Pentenal, 2-ethyl-	13048	003491-57-4	81
19	16.99	2.48	Hexanal, 2-ethyl-	24918	000123-05-7	87
20	17.15	0.92	Benzene, 1-ethyl-2-methyl-	119293	000611-14-3	95
21	17.50	0.32	Benzene, 1-ethyl-2-methyl-	119282	000611-14-3	95
22	17.78	0.34	Benzene, 1,2,3-trimethyl-	119303	000526-73-8	97
23	18.00	11.80	2-Hexenal, 2-ethyl-	12970	000645-62-5	96
24	18.12	0.71	2-Hexenal, 2-ethyl-	12970	000645-62-5	95
25	18.61	0.30	Indane	120527	000496-11-7	95
26	42.78	0.12	Gibberellin A3	128639	000077-06-5	59

Table 4: Experiment with 1-Butanal, SPE analysis

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	3.65	14.47	1-Butanol	111809	000071-36-3	90
2	3.85	0.77	2-Pentanone	114657	000107-87-9	62
3	3.99	1.05	2-Butanol	114259	000078-92-2	80
4	4.90	0.26	Butanal, 2-ethyl-	2054	000097-96-1	76
5	4.98	3.17	1,3,5-Cycloheptatriene	117298	000544-25-2	91
6	5.27	0.37	3-Hexanone	112056	000589-38-8	81
7	5.34	0.66	Cyclopentanone	114490	000120-92-3	49
8	5.53	0.86	Formamide	113691	000075-12-7	46
9	5.85	1.53	2-Ethyl-trans-2-butenal	2904	063883-69-2	95
10	6.45	0.14	2-Hexenal	1524	000505-57-7	97
11	6.64	0.23	Ethylbenzene	117388	000100-41-4	93
12	6.83	1.44	4-Heptanone	109874	000123-19-3	91
13	7.08	2.99	3-Heptanone	112010	000106-35-4	91
14	7.26	2.20	3-Heptanol	19637	000589-82-2	83
15	7.39	0.33	2-Pentenal, 2-ethyl-	3487	003491-57-4	47
16	7.46	0.26	2-Cyclopenten-1-one, 3,4,5-trimethyl-	119929	055683-21-1	90
17	7.89	0.58	2-Pentenal, 2-ethyl-	13048	003491-57-4	93
18	7.99	0.38	Cyclohexane, 1,2-dimethyl-, cis-	111704	002207-01-4	89
19	8.33	1.30	Hexanal, 2-ethyl-	24918	000123-05-7	91
20	8.42	0.22	Benzaldehyde	119466	000100-52-7	97
21	8.50	0.27	Benzene, 1-ethyl-2-methyl-	119282	000611-14-3	94
22	8.73	0.50	Bicyclo[2.2.1]heptan-2-ol, exo-	115871	000497-37-0	98
23	8.91	13.41	Phenol	40630	000108-95-2	94
24	9.07	1.04	Benzene, 1,2,3-trimethyl-	119277	000526-73-8	83
25	9.27	18.27	2-Hexenal, 2-ethyl-	12970	000645-62-5	96
26	9.34	0.90	2-Hexenal, 2-ethyl-	12970	000645-62-5	93
27	9.61	0.42	2-Piperidinone	115328	000675-20-7	27
28	9.68	0.58	1-Hexanol, 2-ethyl-	118096	000104-76-7	80
29	9.77	0.30	Benzenemethanol	116085	000100-51-6	96
30	9.84	0.84	Benzene, 1,1'-(1-ethenyl-1,3-propanediyl)bis-	44791	061141-97-7	78
31	10.11	3.69	Phenol, 2-methyl-	119787	000095-48-7	97
32	10.35	2.61	Ethanone, 1-phenyl-	117111	000098-86-2	76
33	10.47	6.74	Phenol, 4-methyl-	48443	000106-44-5	94
34	10.61	1.18	Benzaldehyde, 4-methyl-	117450	000104-87-0	89
35	11.10	0.38	Butane, 1-[(2-methyl-2-propenyl)oxy]-	6885	053907-74-7	50
36	11.20	0.63	Heptane, 1-(2-butenyloxy)-, (E)-	22166	056052-77-8	59
37	11.53	1.16	Phenol, 2-ethyl-	117292	000090-00-6	60
38	11.63	0.47	Benzenemethanol, 2-methyl-	44887	000089-95-2	93
39	11.70	2.25	Phenol, 2,5-dimethyl-	48522	000095-87-4	94
40	12.02	2.05	Phenol, 3-ethyl-	48507	000620-17-7	90
41	12.14	1.87	Ethanone, 1-(3-methylphenyl)-	53339	000585-74-0	93
42	12.37	1.68	Naphthalene	121778	000091-20-3	95
43	12.47	0.88	Phenol, 2,4-dimethyl-	117285	000105-67-9	83
44	13.20	0.90	Phenol, 2-(1-methylethyl)-	118666	000088-69-7	42
45	13.58	0.46	Ethanone, 1-(4-ethylphenyl)-	122176	000937-30-4	95
46	13.68	0.42	Benzene, 2,4-diethyl-1-methyl-	60096	001758-85-6	90
47	13.85	0.58	1H-Inden-1-one, 2,3-dihydro-	45083	000083-33-0	90
48	14.11	0.43	Naphthalene, 1-methyl-	123000	000090-12-0	95
49	14.40	0.68	Ethanone, 1-(2,4-dimethylphenyl)-	122151	000089-74-7	86
50	14.60	0.23	Benzene, 1-ethenyl-3-ethyl-, mixt. with 1-ethenyl-4-ethylbenzene	118264	055319-72-7	60
51	15.27	1.00	Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro-	120301	006674-22-2	64

Table 5: Experiment with Butendiol, Headspace analysis (100 µL at 200 °C)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	9.60	19.05	Carbon dioxide	113670	000124-38-9	4
2	9.66	3.40	Acetaldehyde	108064	000075-07-0	91
3	9.74	0.24	Ethanol	108332	000064-17-5	86
4	9.81	10.49	Furan	108396	000110-00-9	91
5	9.94	0.36	1,3-Cyclopentadiene	113626	000542-92-7	91
6	10.01	1.22	Propanal, 2-methyl-	398	000078-84-2	70
7	10.18	12.53	2-Butanone	109957	000078-93-3	91
8	10.28	0.40	Furan, 2-methyl-	32366	000534-22-5	95
9	10.39	2.06	Furan, tetrahydro-	109005	000109-99-9	91
10	10.70	15.02	Benzene	30179	000071-43-2	95
11	11.03	0.35	2-Pentanone	979	000107-87-9	72
12	11.16	0.44	Cyclopentanol	112441	000096-41-3	80
13	12.56	15.34	Toluene	117282	000108-88-3	94
14	14.87	3.18	Ethylbenzene	117388	000100-41-4	94
15	15.07	4.39	p-Xylene	117401	000106-42-3	97
16	15.62	3.30	Benzene, 1,3-dimethyl-	117397	000108-38-3	97
17	17.19	2.46	Benzene, 1-ethyl-4-methyl-	46776	000622-96-8	95
18	17.32	0.28	cis-Bicyclo[4.3.0]nona-3,7-diene	5105	000000-00-0	91
19	17.55	0.69	Benzene, 1-ethyl-2-methyl-	46774	000611-14-3	95
20	17.83	0.72	Benzene, 1,2,3-trimethyl-	119303	000526-73-8	97
21	18.65	2.20	Tetracyclo[3.3.1.0(2,8).0(4,6)]-non-2-ene	52502	1000191-13-7	81
22	18.83	0.99	Benzene, 1-propynyl-	120369	000673-32-5	94
23	19.62	0.88	1-Phenyl-1-butene	120545	000824-90-8	86

Table 6: Experiment with Butendiol, SPE-analysis

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	3.19	5.71	2-Butanone	109955	000078-93-3	86
2	3.31	1.18	Chloroform	116499	000067-66-3	96
3	3.39	2.08	Furan, tetrahydro-	109006	000109-99-9	91
4	3.48	1.69	3-Buten-1-ol	108983	000627-27-0	91
5	3.73	4.94	1-Butanol	111808	000071-36-3	87
6	3.99	1.32	2-Pentanone	114657	000107-87-9	83
7	4.09	0.79	Cyclopentanol	114683	000096-41-3	72
8	4.73	0.40	Crotonaldehyde, 2-methyl-	14362	1000150-33-4	87
9	4.86	0.15	2-Pentanone, 3-methyl-	115482	000565-61-7	58
10	4.93	0.39	1H-Pyrrole	113943	000109-97-7	64
11	5.02	0.13	Toluene	117292	000108-88-3	90
12	5.10	3.52	Toluene	117292	000108-88-3	95
13	5.39	0.87	2-Furanol, tetrahydro-	1128	005371-52-8	49
14	5.44	1.67	Cyclopentanone	114490	000120-92-3	62
15	5.63	0.42	2-Undecanol	22928	001653-30-1	45
16	6.16	0.20	2-Furanmethanol	115200	000098-00-0	53
17	6.30	0.76	Cyclopentanone, 2-methyl-	109040	001120-72-5	95
18	6.40	0.20	Cyclopentanone, 3-methyl-	114216	001757-42-2	94
19	6.71	0.56	Ethylbenzene	117388	000100-41-4	90
20	6.86	0.90	Benzene, 1,3-dimethyl-	117395	000108-38-3	92
21	7.14	0.36	3-Heptanone	4018	000106-35-4	76
22	7.27	1.25	p-Xylene	117401	000106-42-3	97
23	7.46	0.35	2-Cyclopenten-1-one, 2-methyl-	113922	001120-73-6	95
24	7.67	0.70	2-Furanmethanol, tetrahydro-	115681	000097-99-4	53
25	8.06	0.41	Cyclopentanone, 2-ethyl-	33691	004971-18-0	95
26	8.23	1.06	3-Cyclohexene-1-carboxaldehyde	115964	000100-50-5	98

27	8.37	0.38	Hexanal, 2-ethyl-	117792	000123-05-7	58
28	8.54	1.25	Benzene, 1-ethyl-2-methyl-	119281	000611-14-3	90
29	8.76	0.48	3-Cyclohexene-1-carboxaldehyde, 1-methyl-	41190	000931-96-4	96
30	8.90	10.85	Phenol	117987	000108-95-2	94
31	9.10	0.38	Benzene, 1,2,3-trimethyl-	119277	000526-73-8	87
32	9.15	0.32	Cyclopropane, tetramethylmethylene-	3174	054376-39-5	70
33	9.22	0.41	3-Octyne	116214	015232-76-5	49
34	9.29	1.70	IMIDAZOLE-1,4,5-D3	288	053716-57-7	42
35	9.46	2.02	2-Furanmethanol, tetrahydro-	115681	000097-99-4	59
36	9.61	0.54	Benzene, 1,2,3-trimethyl-	5078	000526-73-8	53
37	9.85	1.03	Benzene, 1-ethenyl-2-methyl-	120522	000611-15-4	81
38	9.94	1.00	Furan, 2-butyltetrahydro-	117848	001004-29-1	50
39	10.01	2.19	Benzene, 1-propynyl-	120369	000673-32-5	91
40	10.16	6.91	Phenol, 2-methyl-	48963	000095-48-7	95
41	10.40	2.38	Acetophenone	119121	000098-86-2	93
42	10.50	7.91	Phenol, 4-methyl-	48443	000106-44-5	94
43	10.74	0.50	Indan, 1-methyl-	120549	000767-58-8	93
44	11.03	1.61	Phenol, 2,3-dimethyl-	48509	000526-75-0	96
45	11.53	0.98	Phenol, 2-ethyl-	48508	000090-00-6	95
46	11.61	0.30	1H-Indene, 2,3-dihydro-5-methyl-	52578	000874-35-1	91
47	11.72	3.03	Phenol, 2,4-dimethyl-	48524	000105-67-9	97
48	11.78	1.18	2-Methylindene	58801	002177-47-1	96
49	11.89	0.56	Benzene, (1-methyl-2-cyclopropen-1-yl)-	121918	065051-83-4	96
50	12.02	2.64	Phenol, 4-ethyl-	119667	000123-07-9	86
51	12.18	1.76	Phenol, 2,3-dimethyl-	119666	000526-75-0	90
52	12.38	3.38	Naphthalene	121777	000091-20-3	94
53	12.64	0.47	Phenol, 2,3,5-trimethyl-	118678	000697-82-5	70
54	13.08	0.27	Phenol, 2,3,6-trimethyl-	54900	002416-94-6	95
55	13.22	0.91	Phenol, 2-ethyl-5-methyl-	121148	001687-61-2	81
56	13.48	0.60	Phenol, 3-ethyl-5-methyl-	118690	000698-71-5	76
57	13.58	1.04	Phenol, 2,3,5-trimethyl-	118679	000697-82-5	86
58	13.87	1.63	1H-Inden-1-one, 2,3-dihydro-	122070	000083-33-0	96
59	14.11	1.08	Naphthalene, 2-methyl-	123002	000091-57-6	94
60	14.38	1.09	Naphthalene, 2-methyl-	123001	000091-57-6	89
61	14.57	0.74	Pentane, 1,1'-oxybis-	120979	000693-65-2	38
62	14.71	0.68	1H-Inden-1-ol, 2,3-dihydro-	122168	006351-10-6	91
63	15.29	0.63	3-ETHYLADAMANTAN-1-OL	26202	015598-87-5	38
64	15.56	0.65	Naphthalene, 2-ethyl-	122921	000939-27-5	97
65	15.73	0.42	Butanoic acid, 3-methylphenyl ester	25108	007476-80-4	53
66	16.86	0.25	Acenaphthene	123839	000083-32-9	93
67	17.10	0.31	1-Naphthalenol	123100	000090-15-3	95
68	17.22	1.03	2-Naphthalenol	123093	000135-19-3	93
69	18.16	0.34	Fluorene	124603	000086-73-7	96
70	20.59	0.16	Phenanthrene	76766	000085-01-8	93

Results of experiment series II: Deuterated Glucose

Fig. 1: Total ion chromatogram of the not-deuterated Glucose:

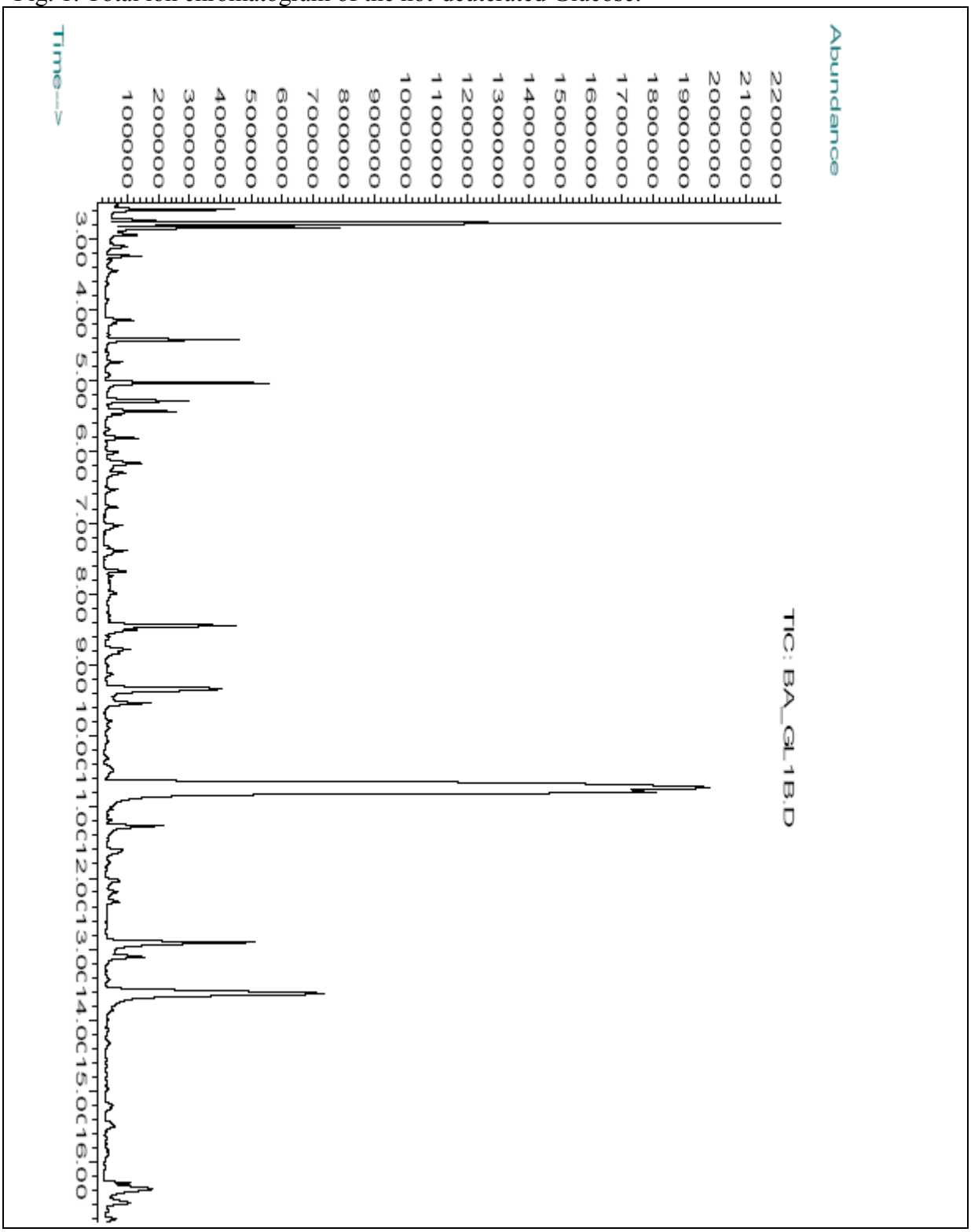


Table 7: As table the main peaks (not-deuterated glucose):

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	2.59	1.44	Amylene Hydrate	19551	000075-85-4	86
2	2.78	11.77	2-Butanone, 3-methyl-	109139	000563-80-4	86
3	4.42	1.82	Toluene	117281	000108-88-3	91
4	5.03	2.53	Cyclopentanone	111214	000120-92-3	97
5	5.28	1.17	Tetrachloroethylene	124590	000127-18-4	99
6	5.43	1.31	1-Propen-1-one, 2-methyl-	114016	000598-26-5	50
7	6.17	0.85	Cyclohexane, nitro-	7041	001122-60-7	59
8	8.46	3.54	1-CYCLOPENTEN-4-OL	808	014320-38-8	59
9	9.35	4.31	Acetic acid, propyl ester	120944	000109-60-4	45
10	9.56	1.11	Pentane, 2,3,4-trimethyl-	4129	000565-75-3	64
11	10.74	51.11	Phenol	40630	000108-95-2	94
12	11.28	1.44	Ethanol, 2-(2-ethoxyethoxy)-	110886	000111-90-0	86
13	12.93	4.23	Phenol, 2-methyl-	48963	000095-48-7	98
14	13.11	1.09	Acetophenone	119045	000098-86-2	97
15	13.64	10.00	Phenol, 3-methyl-	119786	000108-39-4	97
16	16.38	2.29	Phenol, 2-ethyl-	119665	000090-00-6	93

The GC-MS of the experiment with normal glucose was used to get the product and the retension time of these products. In the product solution of the experiment with deuterated glucose e.g. deuterated phenol has the same retention time like phenol, but a different MS-spektrum. Here the MS-spectrum of a compound is first compared with the literature data and than with the MS-spectrum of the deuterated compound. An increase of the molecular weight of a key fragment give the information, how many deuterium atoms are in this key fragment. Not for all compounds a clear quantification of the key compounds is possilbe, but for 3-methyl-2-butanon (1), hydroxyaceton (2), toluene (3), three different cyclopentanones (4-6) and three different phenols (7-9).

Fig. 2*:* Total ion chromatogram of the deuterated Glucose:

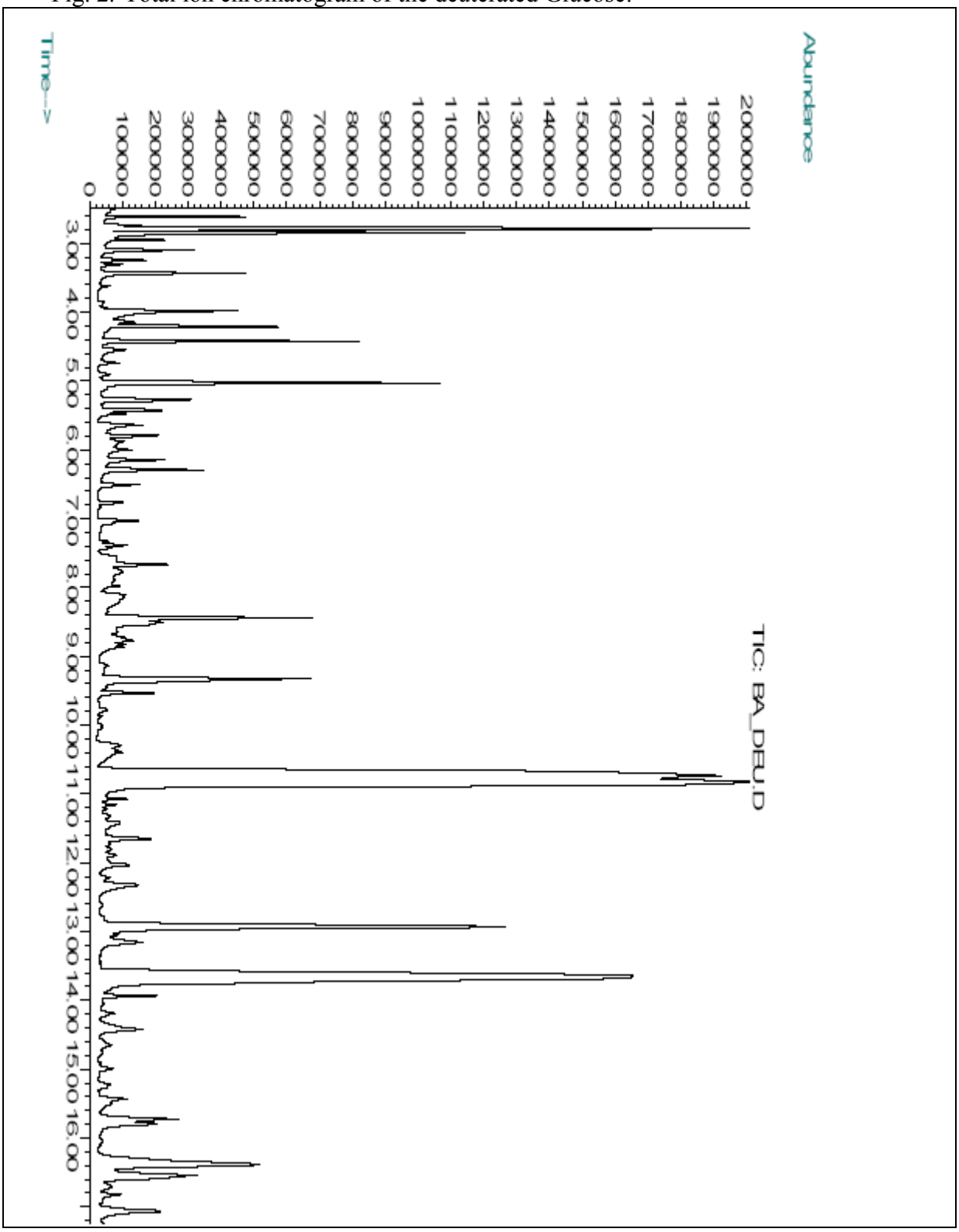


Fig. 3: Area % of identified products in the total ion chromatogram (Glucose conversion, most important deuterated compounds in black).

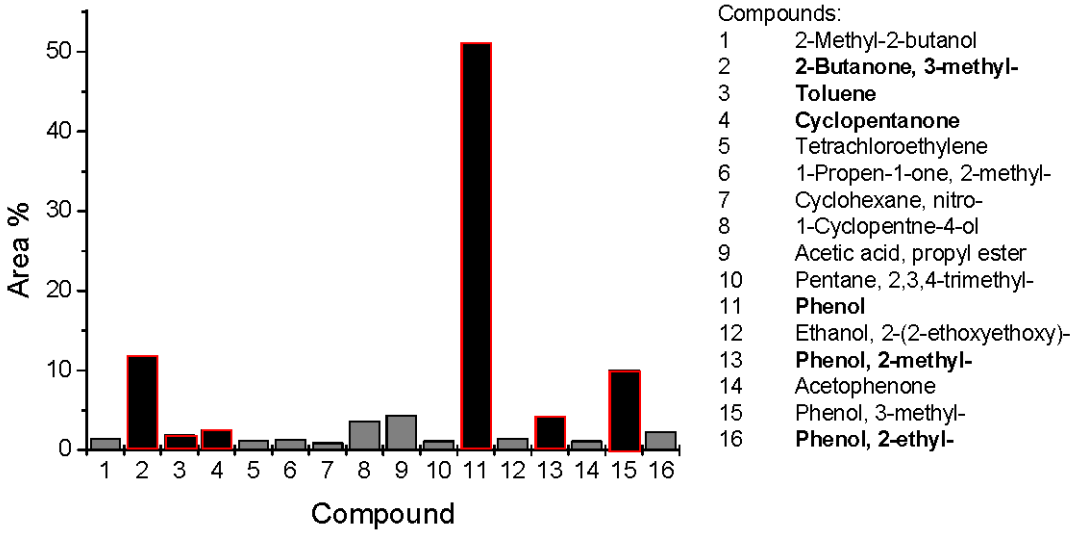


Figure 3 shows the strong dominance of phenol in the total ion chromatogram. In addition, 3-methylbutanone, cyclopentanone and toluene show strong peaks. The methyl-cyclopentanones and hydroxyacetone are minor compounds. Trichloroethylene and the nitro-compound (Nr. 5 and 7 in Fig. 3) are artefacts from sample preparation.

Compound 1: 3-methyl-2-butanon

Fig. 4: Non-deuterated product MS spectrum in comparison with literature:

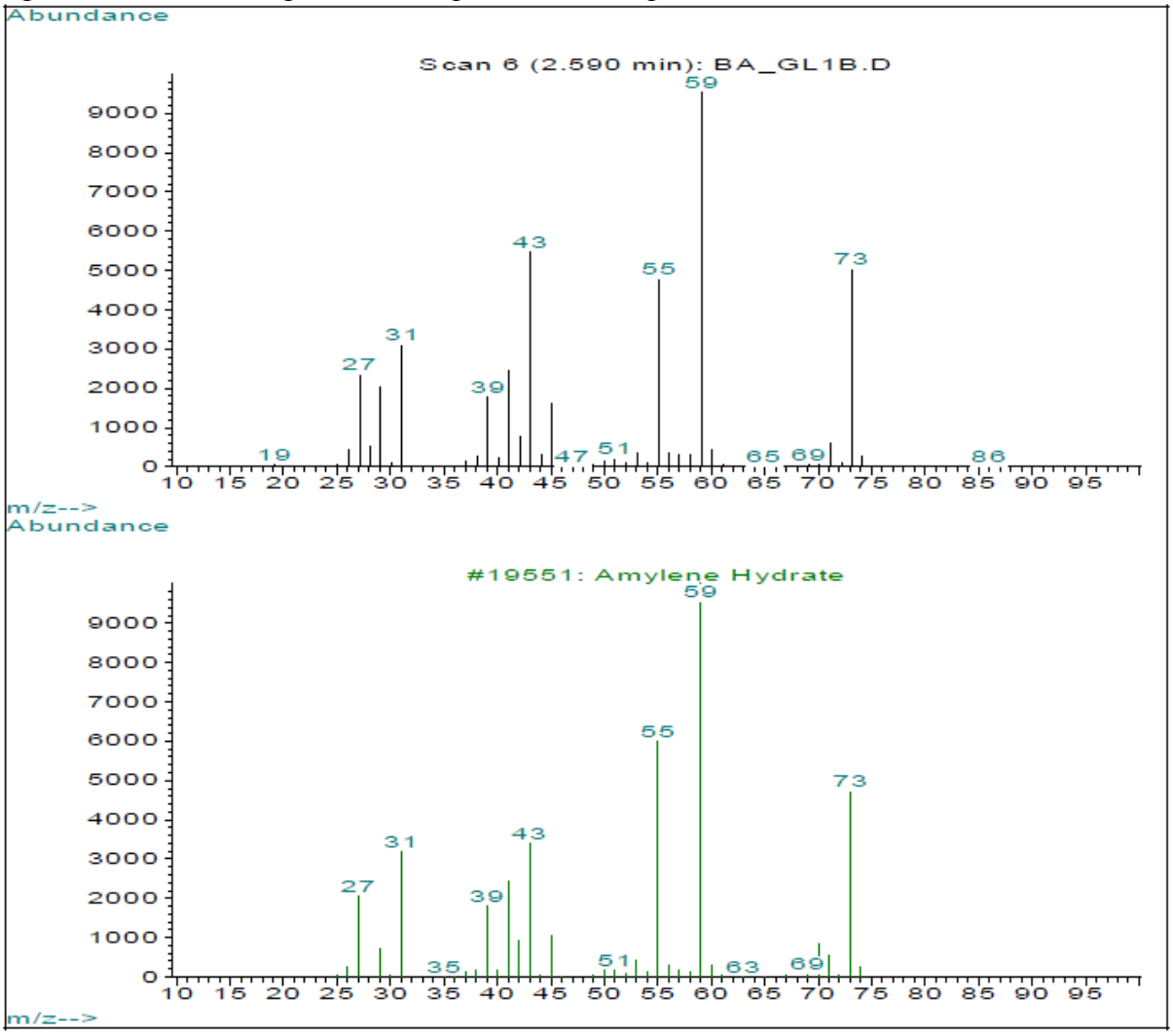
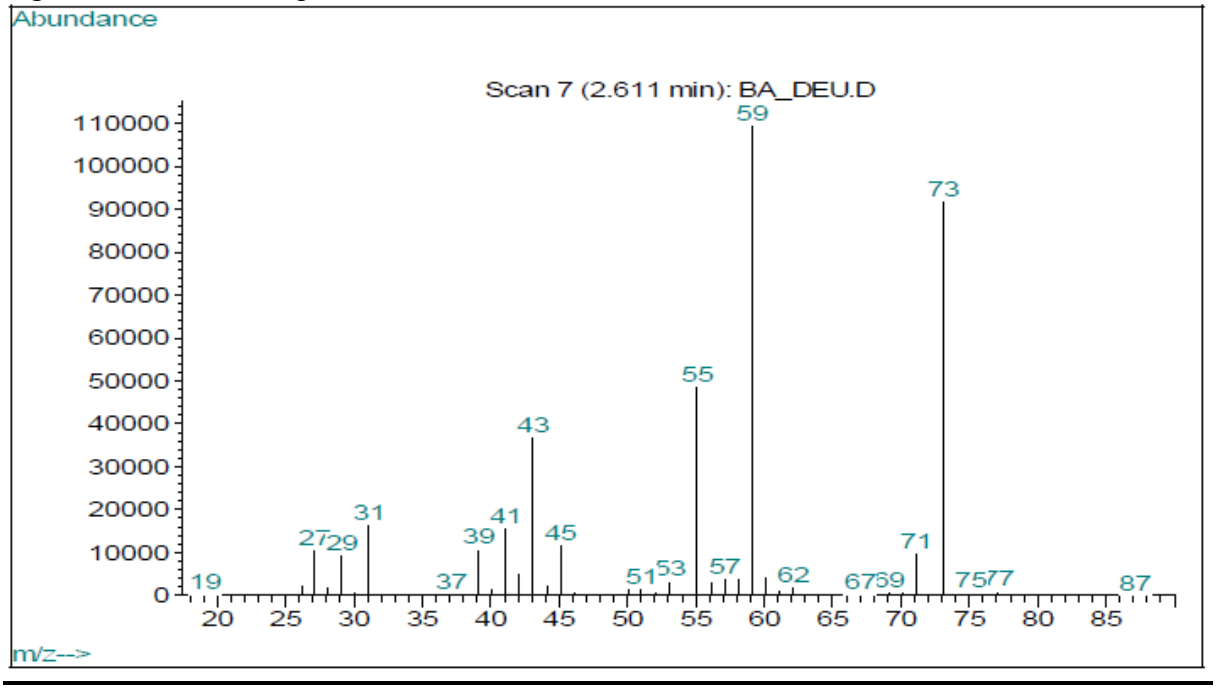


Fig. 5: Deuterated compound:



Compound 2: Hydroxyacetone

Fig. 6: Non-deuterated product MS spectrum in comparison with literature:

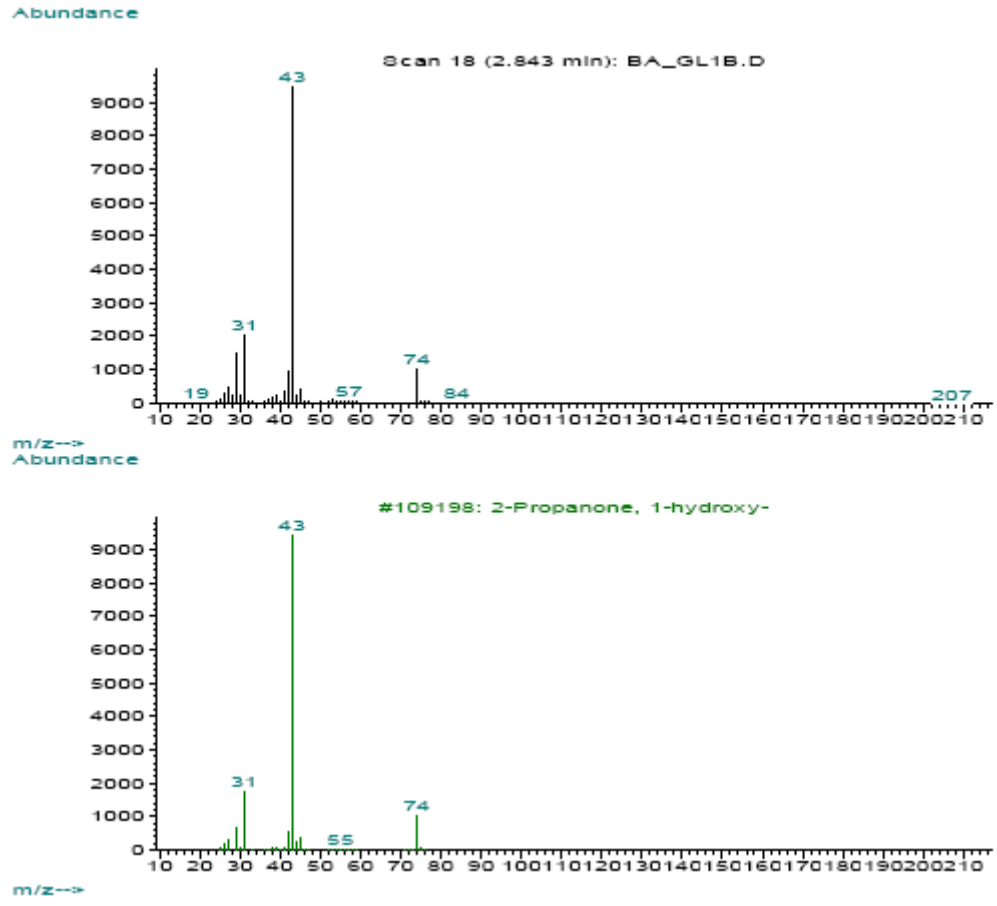
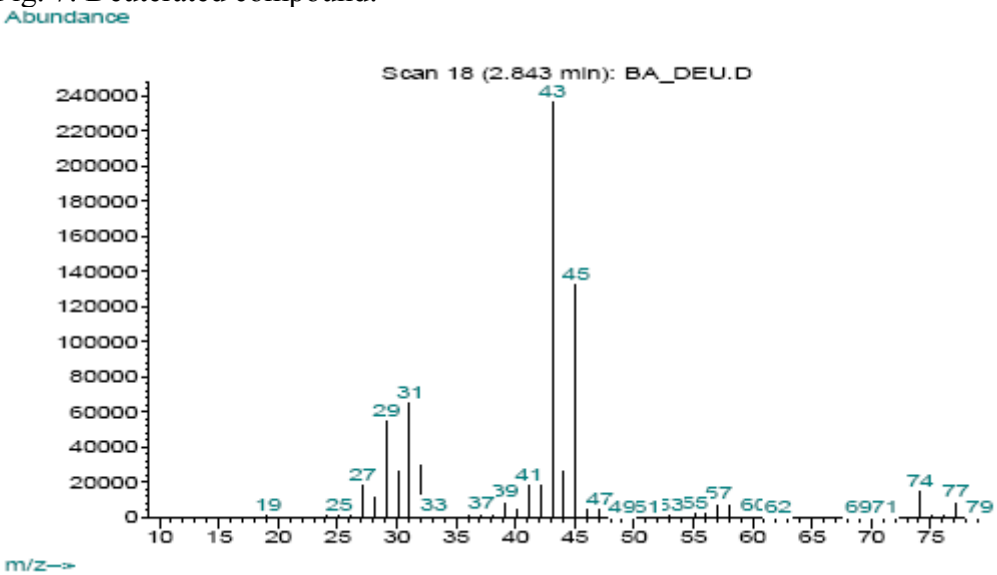


Fig. 7: Deuterated compound:



In the deuterated sample the mass increase was Δm = 3 u. The main peaks are the same but a shift of the peaks m/z 32 and m/z 43 to m/z 44 and m/z 45 is obvious. The splitted CH_2OH fragment is not able to have a OD- group therefore the increase of m/z31 to m/z 32 should be a consequence of the a CHD-OH-fragment formed.

This together with the mass increase of m/z 43 to m/z 44 and m/z 45 hints to a deuteration ration of 3 from 6 possible positions.

Compound 3: Toluene

Fig. 8: Non-deuterated product MS spectrum in comparison with literature:

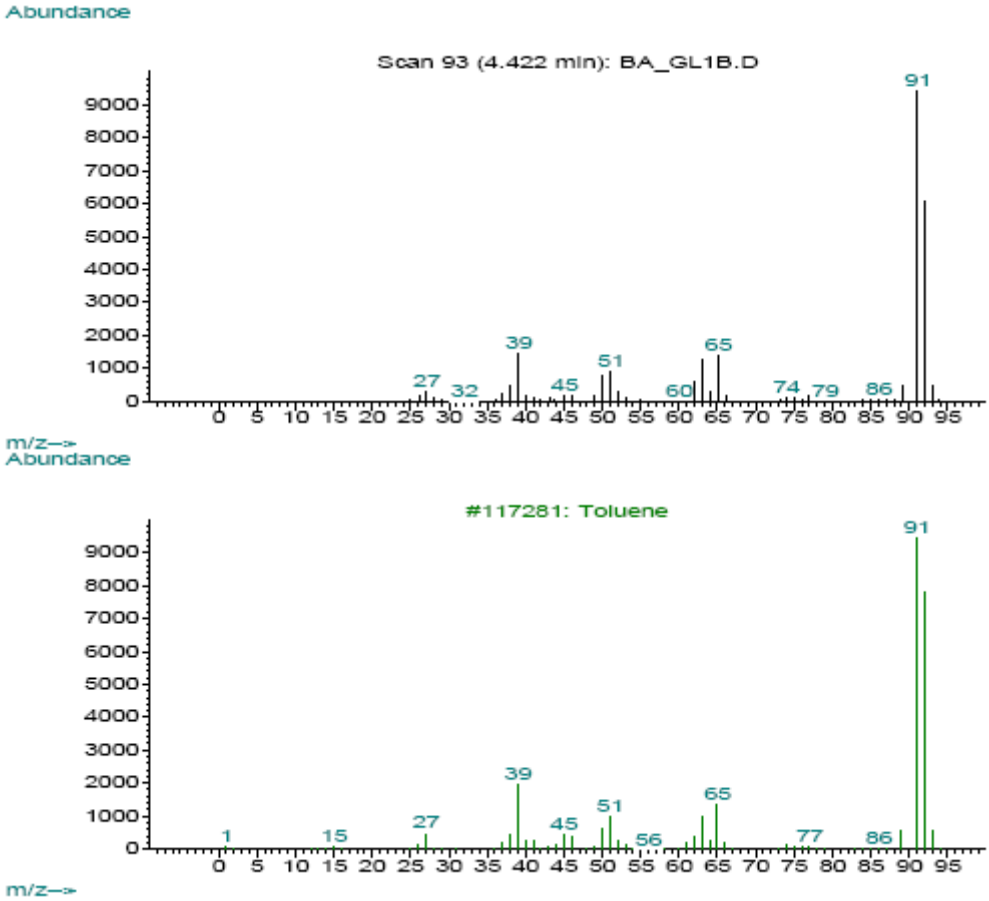
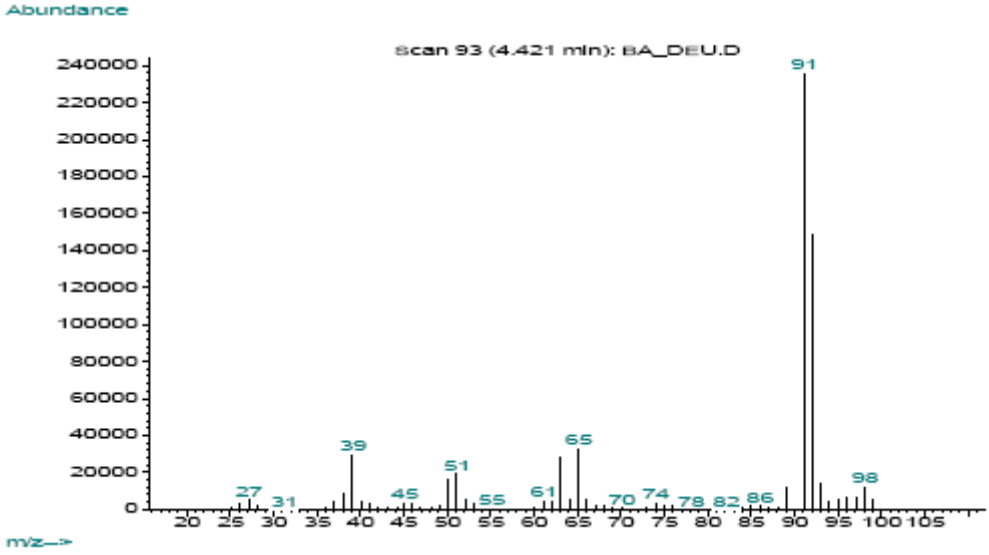


Fig. 9: Deuterated toluene:



In the spectrum of the deuterated glucose experiment, there is a significant increase of mass of $\Delta m = 5$ u for m/z 93 to m/z 99 found. The five D-atoms are uniformly distributed at all C-atoms of the toluene. Four of them 4, but at lower intensity are found in the C5H5

-fragment at m/z 67, 68, 69 and 70 also. The last D-atom is separated by the formation of the C2H2-fragmente from the C7H7-Fragment.

Compound 4: Cyclopentanone

Fig. 10: Non-deuterated product MS spectrum in comparison with literature:

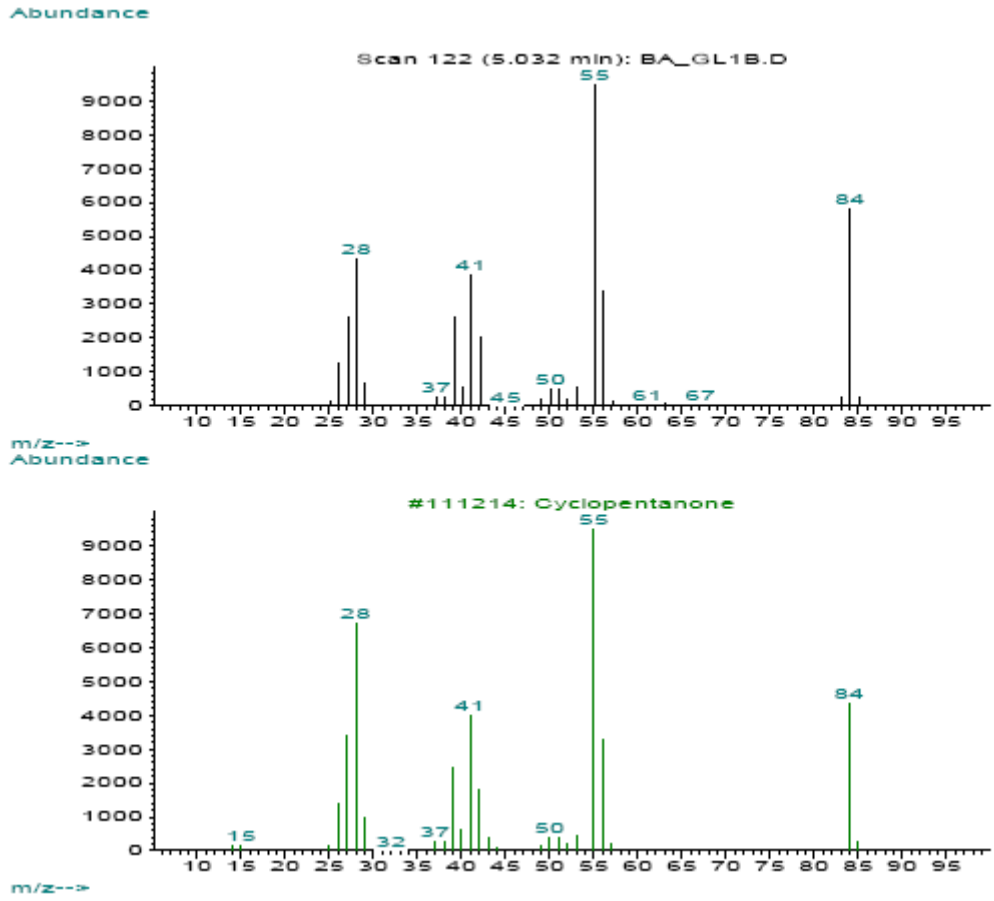
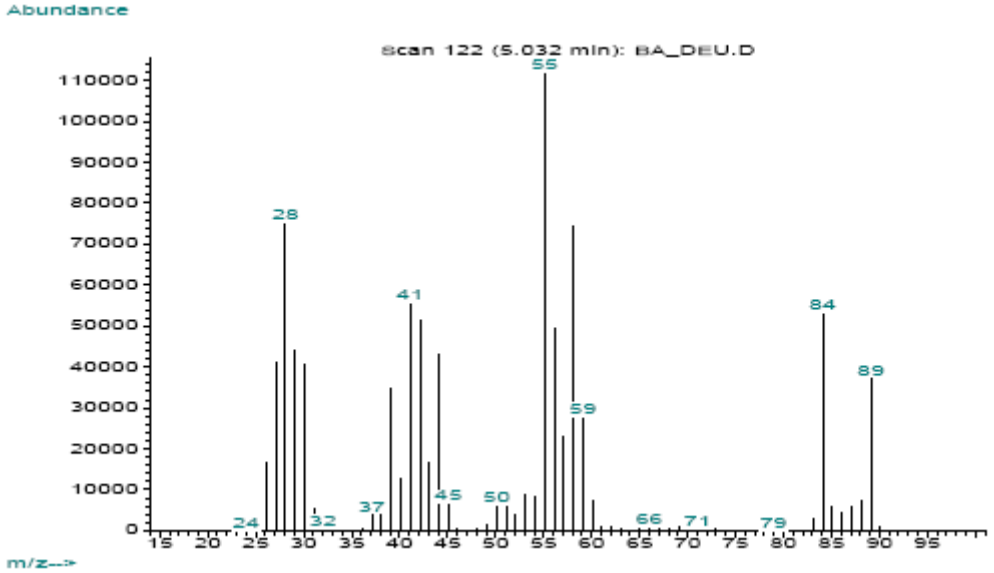


Fig. 10: Deuterated product:



In the samples of deuterated glucose conversion, the molecular mass is increased by $\Delta m = 4$, corresponding to C5D4H3O. Now the fragments are investigated for an mass increase. At three C-atoms, not bonded to oxygen, the mass of the fragment is increased. There is one C-atom left, which has to be bonded to deuterium. The mass increase of m/z 55 and m/z 56 of $\Delta m = 3$ u to m/z 57, 58, 59, relative to the non-deuterated glucose experiments hints to 3 deuterium in the main fragment. This is formed by splitting of a C2H4D1 fragment. Only this way the strong peak at m/z 58 can be explained. The peak at m/z 30 prove the splitting off a C2D3 fragment with m/z 58, forming a carbonyl group. The three deuterium atoms can be found here again. Also the mass difference in respect of the molecule ion C5D4H3O, hints to this assumption