

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
 Data File : VN078021.D
 Acq On : 02 Jun 2023 10:47
 Operator : JC\MD
 Sample : VN0602WBS01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VN0602WBS01

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
 Title : SW846 8260

Signal : TIC: VN078021.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.136	26	31	38	rVB	78711	117179	4.90%	0.209%
2	2.371	66	71	76	rBV	84899	116579	4.87%	0.208%
3	2.524	90	97	103	rBV	92142	152847	6.39%	0.273%
4	2.671	117	122	128	rVB2	31495	55148	2.31%	0.098%
5	2.830	141	149	156	rVB2	41039	91652	3.83%	0.163%
6	2.965	164	172	181	rBV2	88905	209958	8.78%	0.374%
7	3.136	191	201	207	rBV2	63775	145177	6.07%	0.259%
8	3.507	254	264	274	rBV	124491	309760	12.95%	0.552%
9	3.971	332	343	358	rBV2	80295	205989	8.61%	0.367%
10	4.195	374	381	390	rBV2	23551	65347	2.73%	0.117%
11	4.359	394	409	410	rBV2	161025	358969	15.01%	0.640%
12	4.442	419	423	437	rVB	94678	247428	10.35%	0.441%
13	4.601	440	450	461	rVV2	49490	155275	6.49%	0.277%
14	4.724	461	471	484	rVB2	67778	203504	8.51%	0.363%
15	5.036	513	524	540	rVB3	149262	495968	20.74%	0.884%
16	5.283	554	566	582	rBV2	104091	341969	14.30%	0.610%
17	5.530	597	608	626	rBV3	39666	139820	5.85%	0.249%
18	5.736	630	643	647	rBV2	139699	420771	17.59%	0.750%
19	5.800	647	654	671	rVB3	263152	906338	37.90%	1.616%
20	6.612	772	792	799	rBV2	341846	1257544	52.58%	2.242%
21	6.683	799	804	824	rVB4	203962	672783	28.13%	1.200%
22	7.494	927	942	950	rBV2	458721	1262309	52.78%	2.251%
23	7.571	950	955	962	rVV2	124095	279398	11.68%	0.498%
24	7.842	982	1001	1015	rBV5	240074	1037139	43.36%	1.849%
25	7.977	1015	1024	1035	rVB	163643	412695	17.26%	0.736%
26	8.171	1046	1057	1063	rBV	481015	1222107	51.10%	2.179%
27	8.236	1063	1068	1079	rVV2	532917	1581136	66.11%	2.819%
28	8.377	1079	1092	1104	rVB3	344713	1233363	51.57%	2.199%
29	8.600	1113	1130	1139	rBV2	431487	1515458	63.36%	2.702%
30	8.689	1139	1145	1158	rVB3	232289	598839	25.04%	1.068%
31	9.106	1208	1216	1229	rBV	712709	1443974	60.37%	2.575%
32	9.359	1251	1259	1268	rBV2	258451	518399	21.67%	0.924%
33	9.618	1292	1303	1310	rBV4	358806	989763	41.38%	1.765%
34	9.694	1310	1316	1323	rVV4	220218	725986	30.35%	1.294%
35	9.747	1323	1325	1333	rVV	151344	243222	10.17%	0.434%
36	9.806	1333	1335	1343	rVV4	15804	34015	1.42%	0.061%

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37	9.894	1343	1350	1361	rVB	188916	379154	15.85%	0.676%
38	10.106	1379	1386	1390	rBV	34987	68912	2.88%	0.123%
39	10.165	1390	1396	1405	rVB	554880	990214	41.40%	1.766%
40	10.318	1415	1422	1432	rBV2	224858	435768	18.22%	0.777%
41	10.453	1437	1445	1456	rBV	766590	1399571	58.52%	2.496%
42	10.571	1458	1465	1471	rVV	1101283	2072869	86.67%	3.696%
43	10.635	1471	1476	1486	rVB	514355	936865	39.17%	1.670%
44	10.841	1504	1511	1514	rBV	221621	391464	16.37%	0.698%
45	10.877	1514	1517	1531	rVV	231345	417082	17.44%	0.744%
46	11.024	1534	1542	1549	rVV2	270988	504563	21.10%	0.900%
47	11.112	1549	1557	1562	rVV	388216	701494	29.33%	1.251%
48	11.171	1562	1567	1568	rVV	250001	367081	15.35%	0.655%
49	11.200	1568	1572	1582	rVV	542304	1034627	43.26%	1.845%
50	11.294	1582	1588	1594	rVV	203848	346913	14.50%	0.619%
51	11.365	1594	1600	1609	rVV	170910	324709	13.58%	0.579%
52	11.477	1612	1619	1627	rVB	126452	236938	9.91%	0.422%
53	11.871	1676	1686	1696	rBV2	937982	2391704	100.00%	4.265%
54	11.971	1696	1703	1712	rVV2	877357	1564665	65.42%	2.790%
55	12.077	1713	1721	1734	rVB	936999	1855830	77.59%	3.309%
56	12.412	1767	1778	1787	rBV3	868029	1737915	72.66%	3.099%
57	12.500	1787	1793	1801	rVV	239378	388696	16.25%	0.693%
58	12.582	1801	1807	1815	rVV2	126942	234518	9.81%	0.418%
59	12.700	1819	1827	1832	rVV	595602	1020308	42.66%	1.819%
60	12.741	1832	1834	1842	rVV2	143671	211316	8.84%	0.377%
61	12.853	1846	1853	1861	rVV	760389	1312519	54.88%	2.340%
62	12.941	1861	1868	1871	rVV	243430	441824	18.47%	0.788%
63	12.988	1871	1876	1881	rVV3	483591	1151619	48.15%	2.053%
64	13.041	1881	1885	1892	rVV	550202	892650	37.32%	1.592%
65	13.129	1894	1900	1904	rVV	476724	804269	33.63%	1.434%
66	13.176	1904	1908	1913	rVV	570770	957996	40.05%	1.708%
67	13.229	1913	1917	1924	rVB	425942	697607	29.17%	1.244%
68	13.441	1945	1953	1957	rBV	516455	923592	38.62%	1.647%
69	13.488	1957	1961	1968	rVB	779358	1290894	53.97%	2.302%
70	13.623	1977	1984	1992	rBV	514867	820033	34.29%	1.462%
71	13.735	1996	2003	2008	rBV2	844821	1402502	58.64%	2.501%
72	13.800	2008	2014	2024	rVB2	878030	1938582	81.05%	3.457%
73	14.065	2051	2059	2063	rBV	368343	617571	25.82%	1.101%
74	14.112	2063	2067	2075	rVB2	357617	612411	25.61%	1.092%
75	14.341	2090	2106	2116	rVB	256903	462681	19.35%	0.825%
76	14.723	2162	2171	2179	rVB2	77217	145859	6.10%	0.260%

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77	15.041	2218	2225	2232	rBV	378756	644784	26.96%	1.150%
78	15.400	2278	2286	2294	rVV3	152190	284080	11.88%	0.507%
79	15.506	2297	2304	2314	rVB2	143943	264658	11.07%	0.472%
80	15.647	2321	2328	2335	rBV	162860	317209	13.26%	0.566%
81	15.847	2354	2362	2370	rVB3	157996	318932	13.33%	0.569%

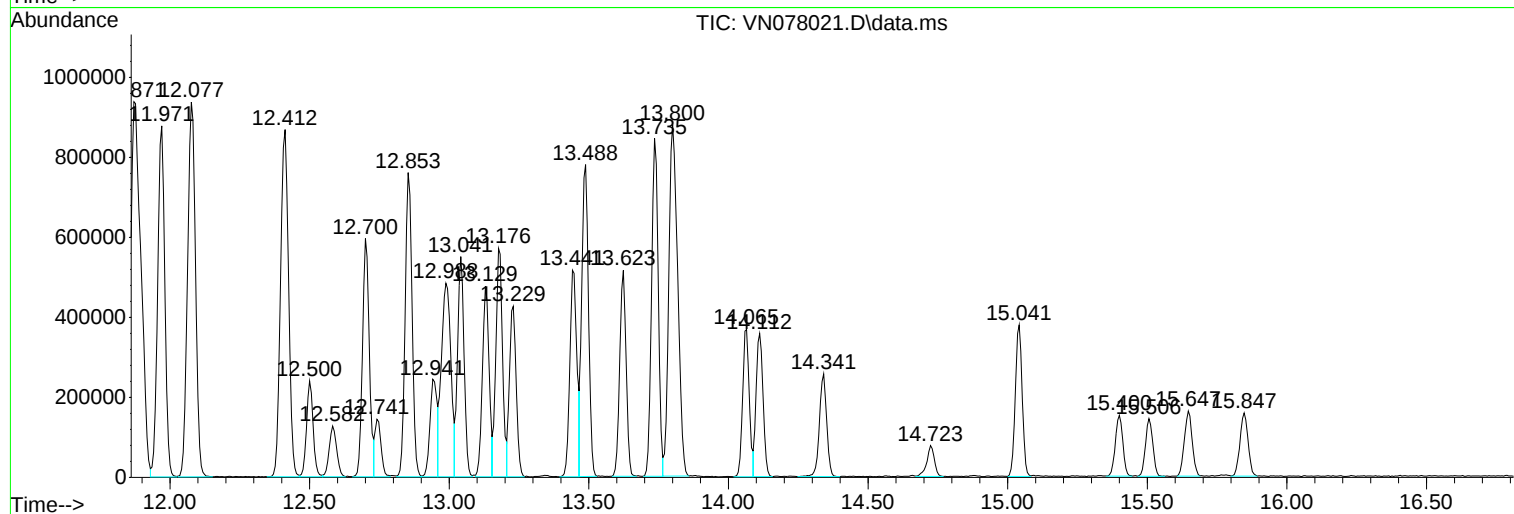
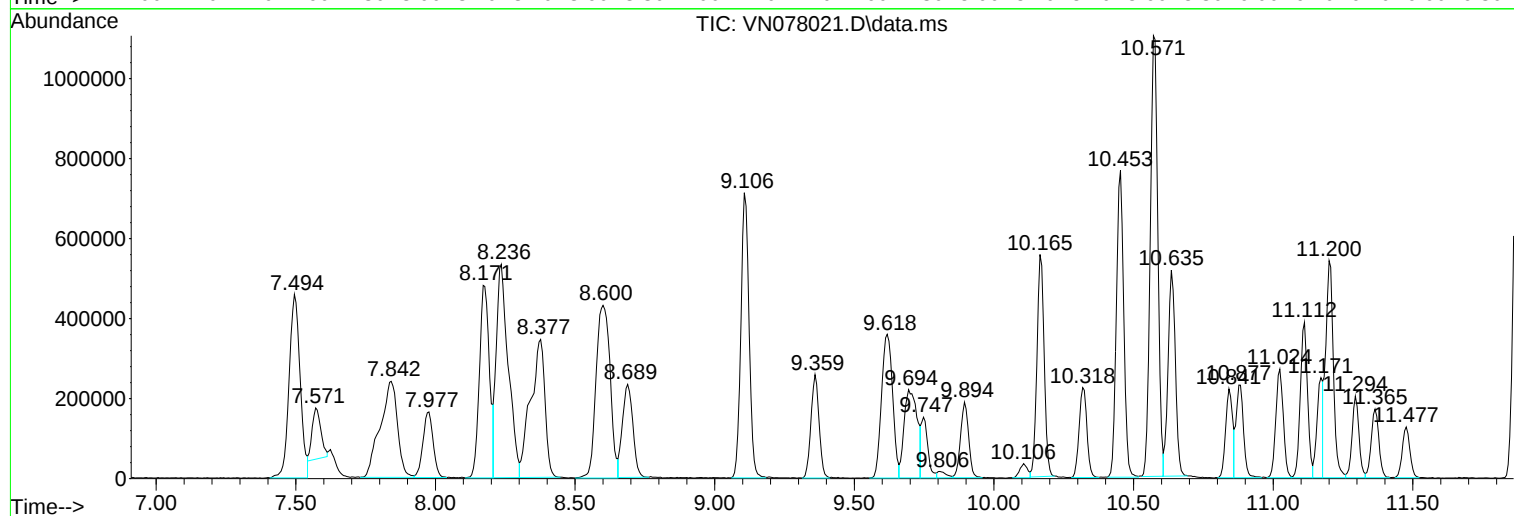
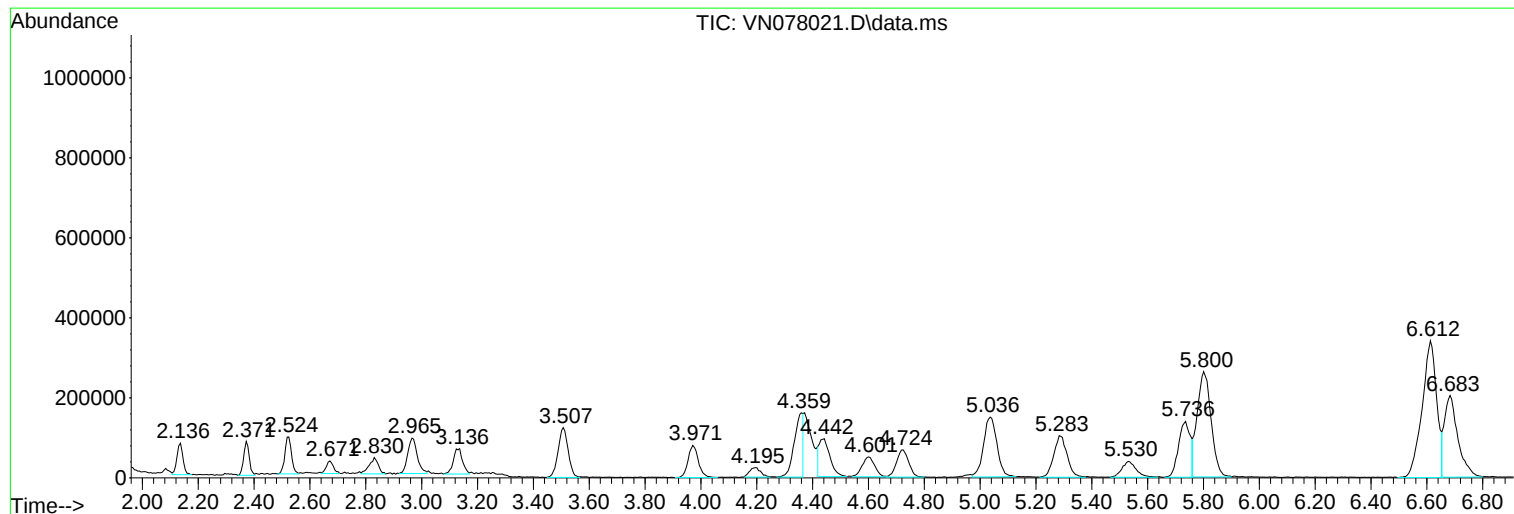
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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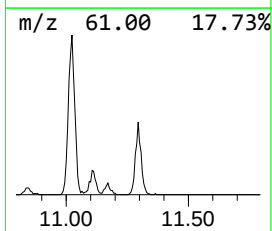
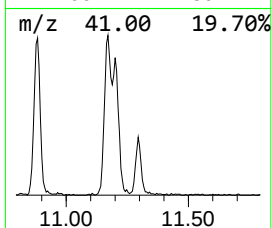
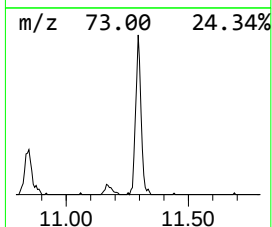
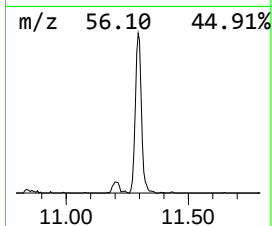
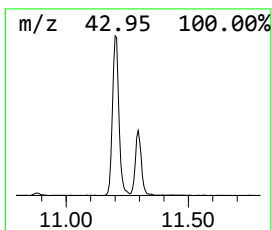
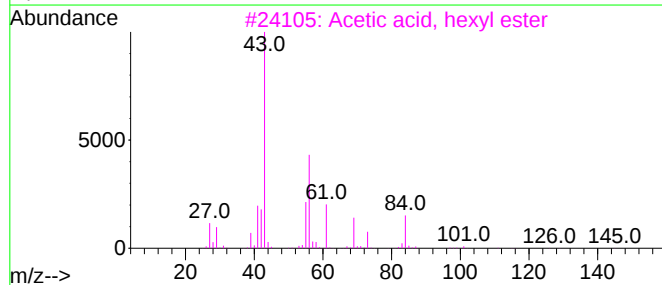
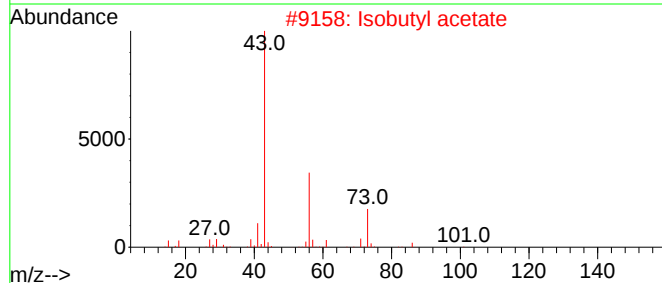
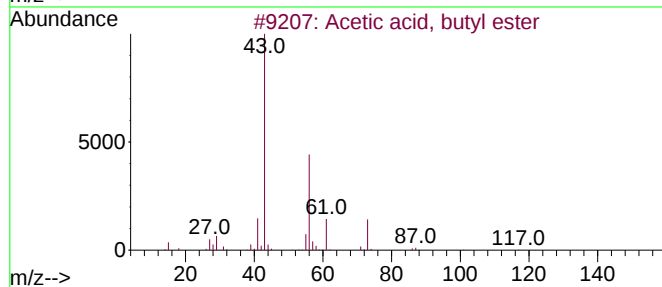
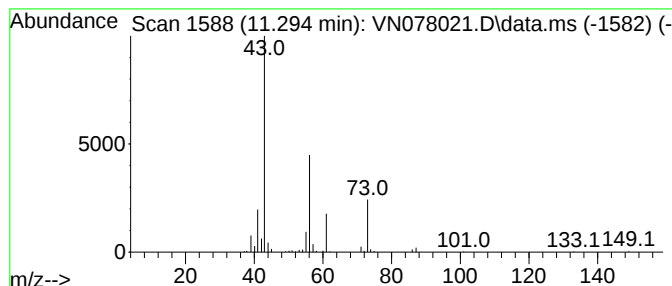
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	7.25 ug/l	346913	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
2			Isobutyl acetate	116	C6H12O2	000110-19-0	40
3			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
4			Butane, 1-propoxy-	116	C7H16O	003073-92-5	23
5			Di-n-propyl ether	102	C6H14O	000111-43-3	17



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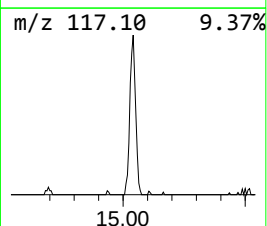
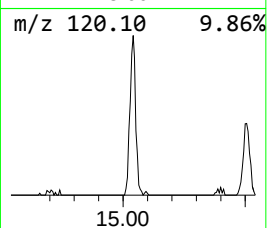
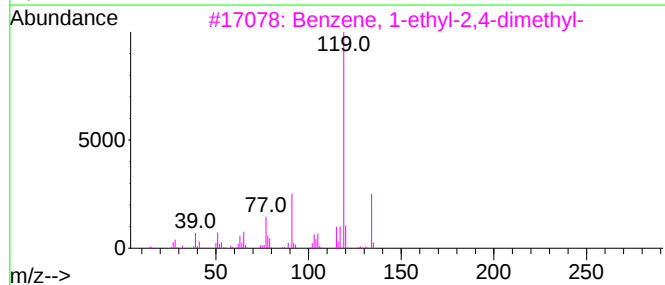
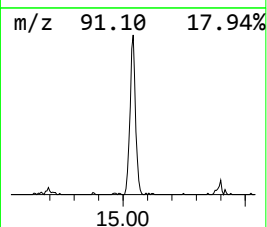
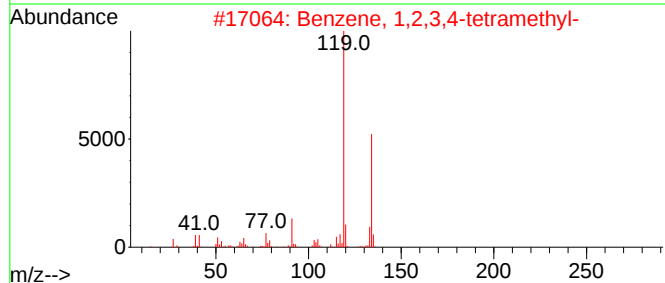
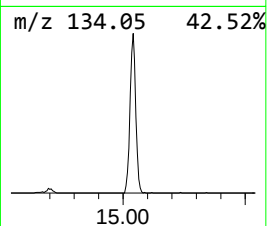
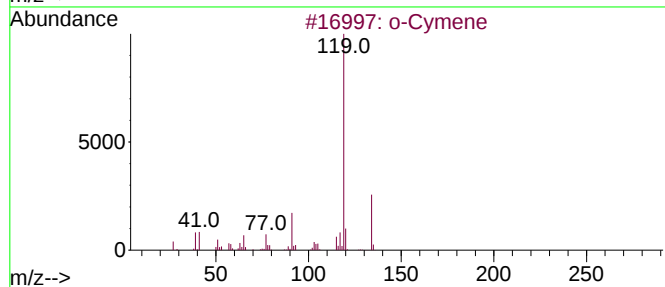
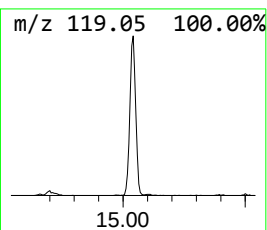
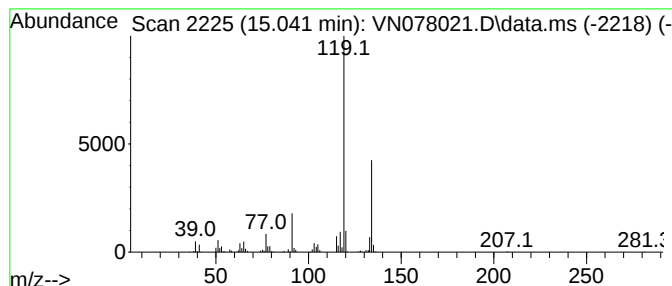
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Peak Number 2 o-Cymene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	16.63 ug/l	644784	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	95
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid, bu...	11.294	7.3	ug/l	346913	3	11.871	2391700	50.0
o-Cymene	15.041	16.6	ug/l	644784	4	13.800	1938580	50.0