

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021422\
 Data File : VX027018.D
 Acq On : 14 Feb 2022 17:03
 Operator : JC/MD
 Sample : N1486-06
 Misc : 5.00g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 X3946

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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_X\Method\SFAMXML021422WMA.M
 Title : VOC Analysis

Signal : TIC: VX027018.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	58	rVB	62764	71899	7.86%	0.491%
2	1.672	92	96	103	rBV	30733	38583	4.22%	0.264%
3	2.191	175	181	191	rVB	17757	28290	3.09%	0.193%
4	2.294	192	198	205	rBV	122269	193572	21.17%	1.323%
5	2.410	210	217	249	rVB	66630	230823	25.24%	1.578%
6	2.727	260	269	271	rBV3	1404	2941	0.32%	0.020%
7	2.788	271	279	297	rVB	354722	726577	79.44%	4.967%
8	2.995	311	313	316	rBV	134	101	0.01%	0.001%
9	3.081	325	327	333	rVB3	328	443	0.05%	0.003%
10	3.428	382	384	386	rVB	176	144	0.02%	0.001%
11	3.611	404	414	430	rVB	213878	509705	55.73%	3.484%
12	3.922	463	465	467	rBV	143	125	0.01%	0.001%
13	3.983	474	475	478	rBV	125	164	0.02%	0.001%
14	4.135	499	500	503	rBV2	80	105	0.01%	0.001%
15	4.489	547	558	602	rBV	103188	341273	37.31%	2.333%
16	4.904	614	626	642	rBV	162531	536286	58.64%	3.666%
17	5.068	642	653	673	rVB2	78829	331842	36.28%	2.268%
18	5.379	691	704	723	rVB	98732	306928	33.56%	2.098%
19	5.507	723	725	727	rBV2	141	129	0.01%	0.001%
20	5.550	727	732	734	rBV3	375	685	0.07%	0.005%
21	5.678	734	753	766	rVB	109908	350450	38.32%	2.396%
22	5.849	778	781	785	rBV2	152	289	0.03%	0.002%
23	5.970	787	801	812	rBV2	189387	547341	59.85%	3.741%
24	6.092	812	821	836	rVB	133763	372080	40.68%	2.543%
25	6.440	875	878	880	rBV	134	104	0.01%	0.001%
26	6.483	884	885	888	rBV	153	160	0.02%	0.001%
27	6.605	899	905	909	rBV3	375	642	0.07%	0.004%
28	6.653	912	913	916	rBV2	186	206	0.02%	0.001%
29	6.763	921	931	946	rBV	117219	294511	32.20%	2.013%
30	6.922	956	957	959	rBV2	175	158	0.02%	0.001%
31	7.001	969	970	972	rBV	106	103	0.01%	0.001%
32	7.043	975	977	980	rVV2	163	169	0.02%	0.001%
33	7.123	980	990	1004	rBV	179729	400397	43.78%	2.737%
34	7.306	1012	1020	1032	rBV	103281	238829	26.11%	1.633%
35	7.434	1032	1041	1055	rVB	156136	341019	37.29%	2.331%
36	7.653	1075	1077	1079	rBV3	239	292	0.03%	0.002%

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37	7.714	1086	1087	1089	rVB	177	116	0.01%	0.001%
38	7.751	1091	1093	1095	rVB2	171	127	0.01%	0.001%
39	7.818	1102	1104	1106	rBV2	322	354	0.04%	0.002%
40	7.946	1120	1125	1127	rBV3	390	510	0.06%	0.003%
41	8.123	1151	1154	1159	rBV2	142	306	0.03%	0.002%
42	8.183	1159	1164	1168	rVB2	415	836	0.09%	0.006%
43	8.330	1181	1188	1199	rVV	61337	110533	12.09%	0.756%
44	8.592	1222	1231	1233	rBV2	209294	462856	50.61%	3.164%
45	8.909	1277	1283	1288	rBV	248207	362569	39.64%	2.478%
46	8.952	1288	1290	1303	rVB	39517	62228	6.80%	0.425%
47	9.055	1303	1307	1309	rVB	261	391	0.04%	0.003%
48	9.074	1309	1310	1311	rBV	152	101	0.01%	0.001%
49	9.159	1317	1324	1336	rBV	368010	693886	75.87%	4.743%
50	9.275	1336	1343	1352	rVB	542338	820637	89.73%	5.609%
51	9.415	1357	1366	1378	rBV	101982	230397	25.19%	1.575%
52	9.525	1378	1384	1393	rVV	257577	482597	52.77%	3.299%
53	9.610	1393	1398	1415	rVB	150839	245922	26.89%	1.681%
54	9.793	1425	1428	1429	rBV2	142	113	0.01%	0.001%
55	9.897	1443	1445	1448	rBV	219	289	0.03%	0.002%
56	9.945	1452	1453	1457	rVB	222	131	0.01%	0.001%
57	10.061	1465	1472	1481	rBV	216926	346159	37.85%	2.366%
58	10.171	1488	1490	1491	rBV	137	104	0.01%	0.001%
59	10.201	1491	1495	1501	rVB2	744	1166	0.13%	0.008%
60	10.244	1501	1502	1505	rVB	216	177	0.02%	0.001%
61	10.305	1507	1512	1517	rVB	1510	2248	0.25%	0.015%
62	10.360	1518	1521	1525	rVB3	227	249	0.03%	0.002%
63	10.445	1532	1535	1537	rBV	115	153	0.02%	0.001%
64	10.659	1564	1570	1583	rBV	345594	506560	55.39%	3.463%
65	10.799	1591	1593	1594	rBV	175	140	0.02%	0.001%
66	10.963	1615	1620	1629	rVB	352395	474217	51.85%	3.242%
67	11.092	1637	1641	1642	rBV2	267	250	0.03%	0.002%
68	11.122	1642	1646	1650	rVB2	2176	2844	0.31%	0.019%
69	11.201	1653	1659	1670	rBV	545470	745140	81.47%	5.093%
70	11.305	1674	1676	1680	rVB3	434	459	0.05%	0.003%
71	11.378	1685	1688	1694	rBV3	188	361	0.04%	0.002%
72	11.476	1699	1704	1711	rBV	210861	233960	25.58%	1.599%
73	11.543	1714	1715	1718	rBV3	224	214	0.02%	0.001%
74	11.750	1744	1749	1754	rVB2	2137	2792	0.31%	0.019%
75	11.841	1762	1764	1767	rBV	387	425	0.05%	0.003%
76	11.933	1776	1779	1780	rBV	813	844	0.09%	0.006%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.M
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77	11.975	1780	1786	1790	rVV	240579	310558	33.96%	2.123%
78	12.043	1790	1797	1806	rVV2	454326	914581	100.00%	6.252%
79	12.128	1808	1811	1812	rVV2	1096	1245	0.14%	0.009%
80	12.152	1812	1815	1821	rVB	1759	2209	0.24%	0.015%
81	12.268	1832	1834	1835	rBV2	149	103	0.01%	0.001%
82	12.323	1835	1843	1850	rBV	316369	389810	42.62%	2.665%
83	12.427	1857	1860	1863	rBV3	638	840	0.09%	0.006%
84	12.482	1865	1869	1872	rVB4	368	470	0.05%	0.003%
85	12.622	1890	1892	1895	rBV2	204	207	0.02%	0.001%
86	12.652	1895	1897	1898	rBV	167	158	0.02%	0.001%
87	12.664	1898	1899	1903	rVB3	241	215	0.02%	0.001%
88	12.768	1911	1916	1920	rBV	3462	4577	0.50%	0.031%
89	12.945	1940	1945	1953	rVB	117954	148964	16.29%	1.018%
90	13.055	1960	1963	1967	rVV	266	237	0.03%	0.002%
91	13.116	1967	1973	1985	rVB	668120	809609	88.52%	5.534%
92	13.262	1995	1997	2000	rVB2	265	298	0.03%	0.002%
93	13.591	2046	2051	2060	rBV	316541	375085	41.01%	2.564%
94	13.719	2070	2072	2075	rBV2	114	102	0.01%	0.001%
95	13.756	2075	2078	2080	rBV2	598	604	0.07%	0.004%
96	13.963	2108	2112	2120	rVV	6422	7854	0.86%	0.054%
97	14.042	2123	2125	2130	rVB2	181	194	0.02%	0.001%
98	14.634	2220	2222	2226	rBV2	129	158	0.02%	0.001%
99	14.755	2240	2242	2245	rBV2	518	446	0.05%	0.003%
100	15.749	2403	2405	2409	rBV3	202	178	0.02%	0.001%

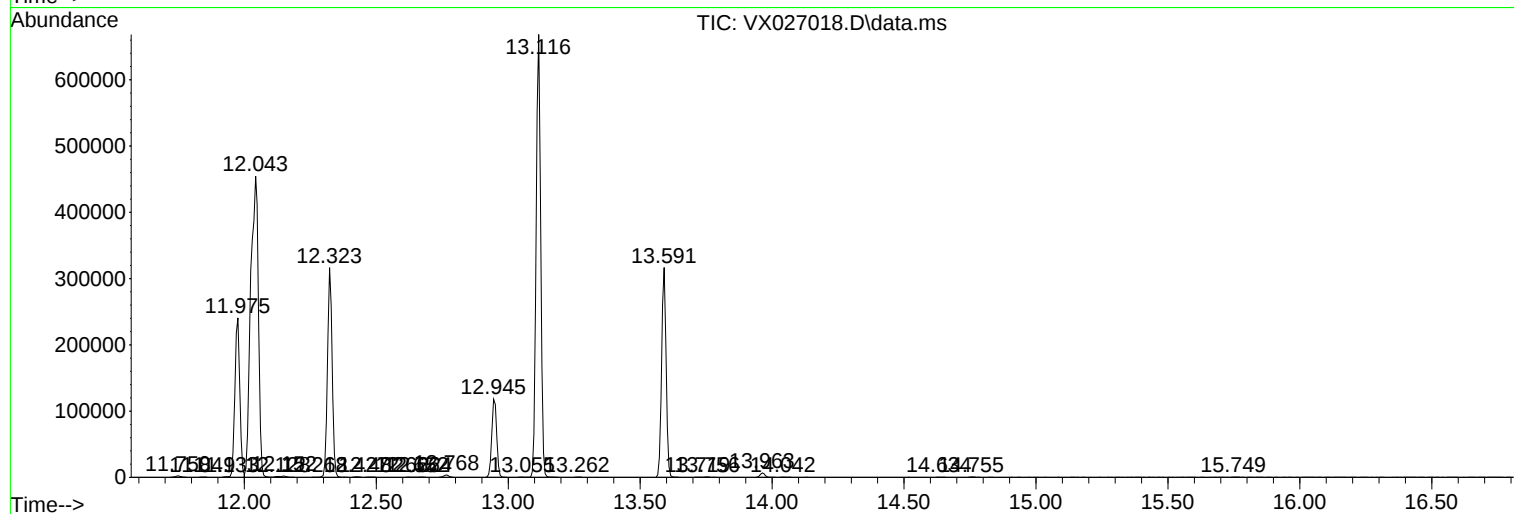
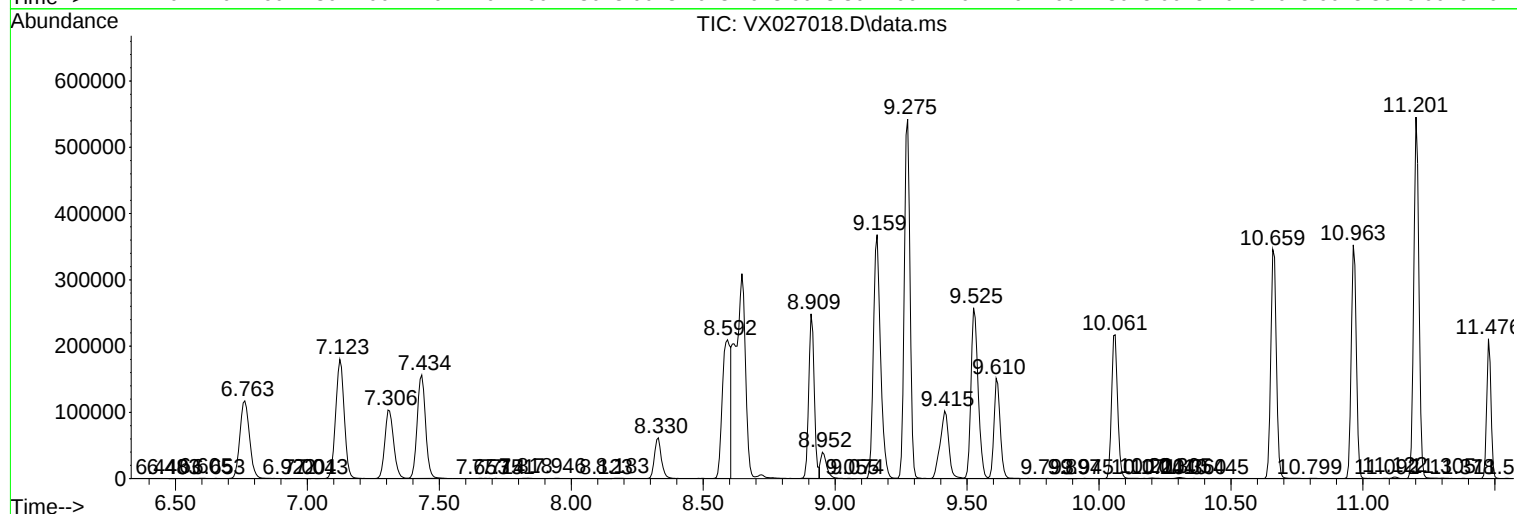
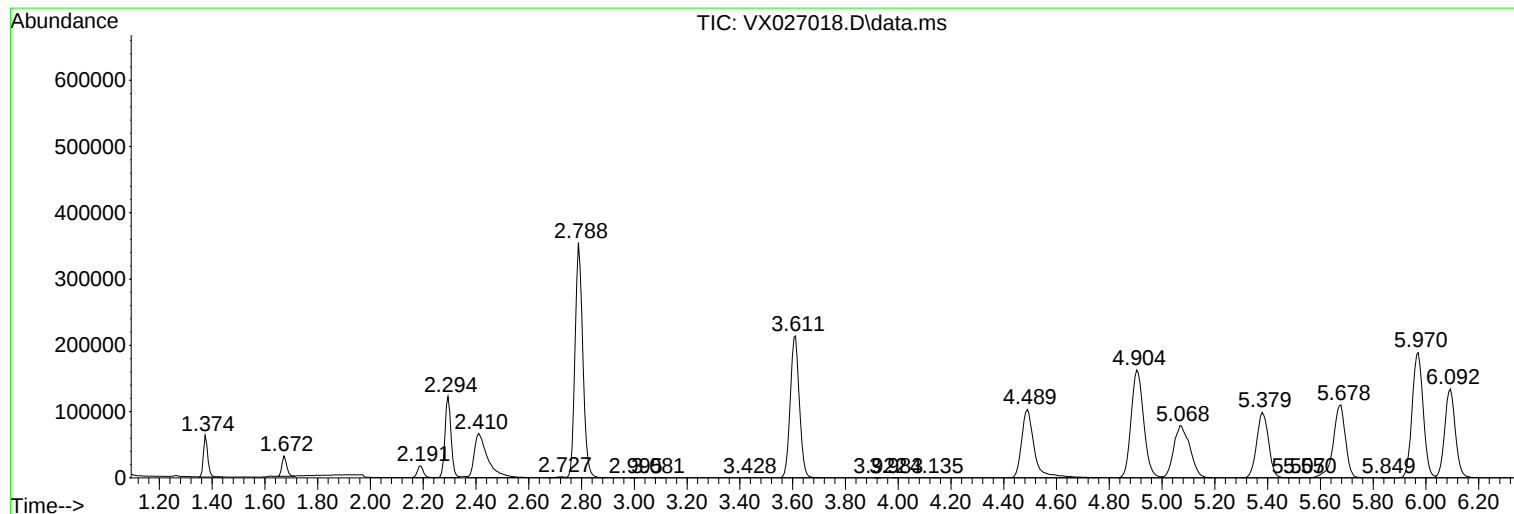
Sum of corrected areas: 14629428

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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
X3946

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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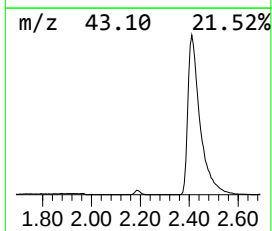
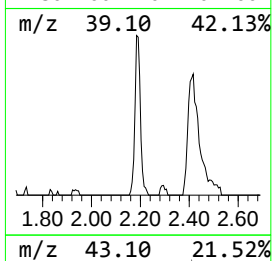
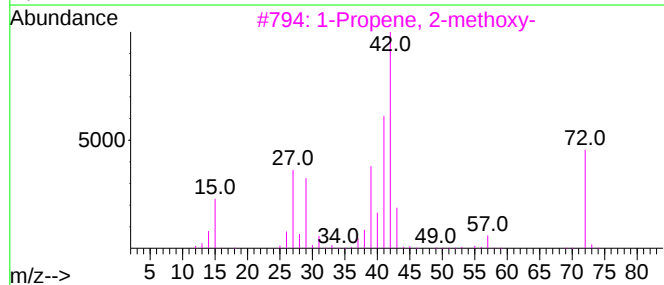
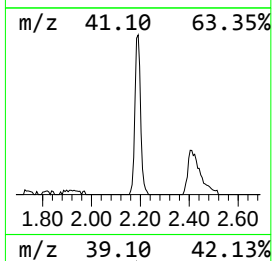
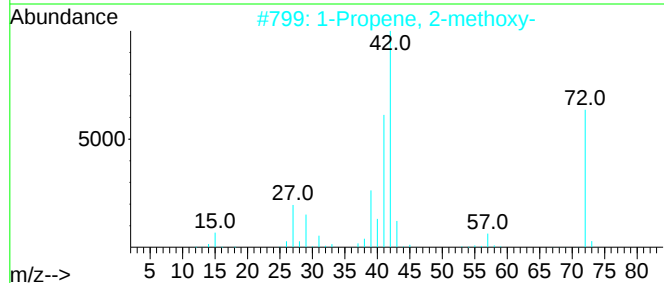
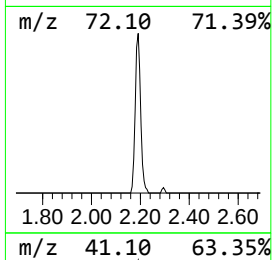
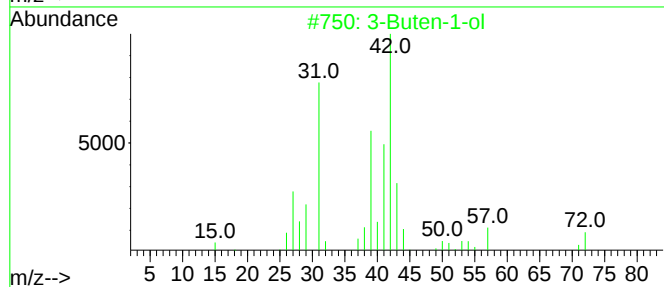
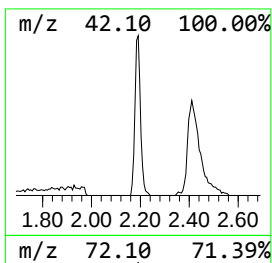
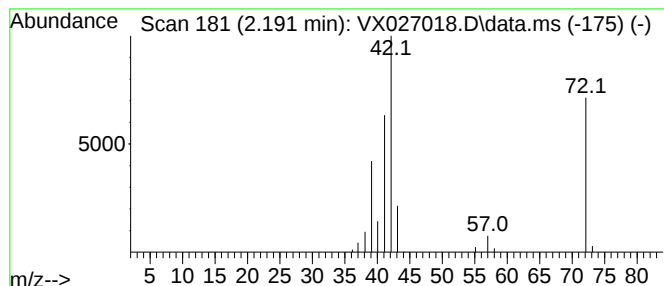
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 3-Buten-1-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.191	4.80 ug/L	28290	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-1-ol			72	C4H8O	000627-27-0	78
2	1-Propene, 2-methoxy-			72	C4H8O	000116-11-0	59
3	1-Propene, 2-methoxy-			72	C4H8O	000116-11-0	59
4	1-Propene, 2-methoxy-			72	C4H8O	000116-11-0	59
5	1-Propene, 3-methoxy-			72	C4H8O	000627-40-7	47



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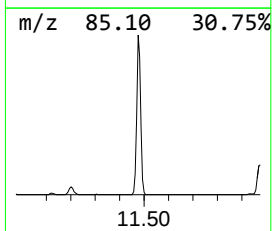
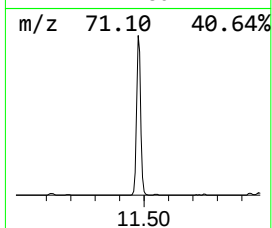
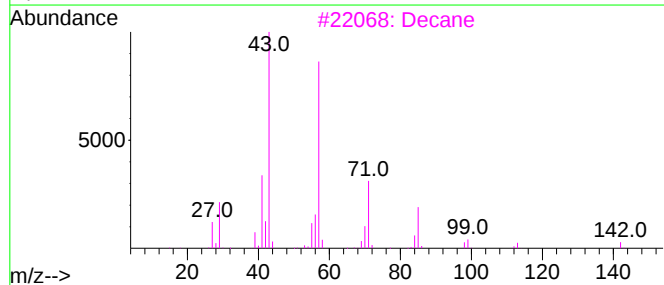
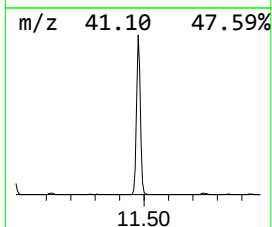
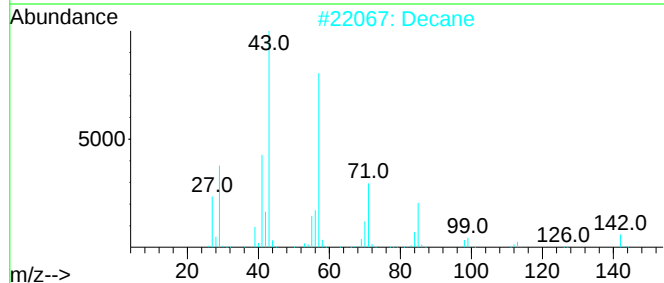
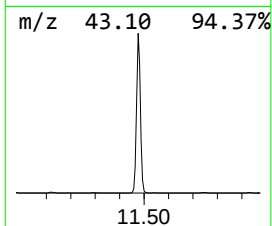
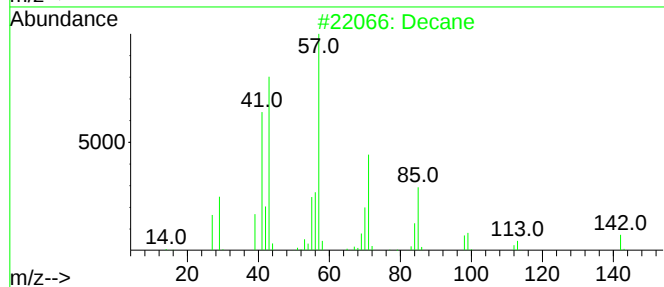
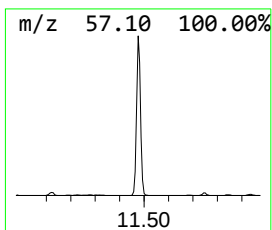
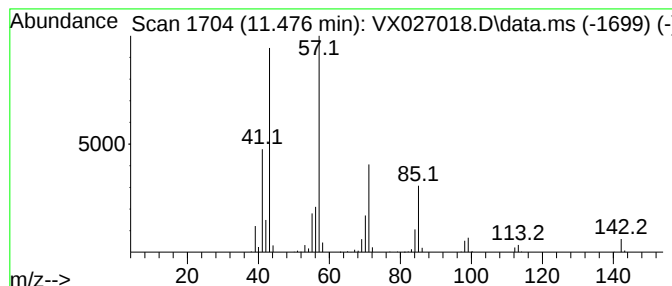
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Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.476	12.79 ug/L	233960	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decane		142	C10H22	000124-18-5	97
2	Decane		142	C10H22	000124-18-5	95
3	Decane		142	C10H22	000124-18-5	94
4	Decane		142	C10H22	000124-18-5	91
5	Nonane		128	C9H20	000111-84-2	86



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Buten-1-ol	2.191	4.8	ug/L	28290	1	6.763	294511	50.0
(DEL) Alkane: S...	11.476	12.8	ug/L	233960	3	12.024	914581	50.0