

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV01122\
 Data File : VV028517.D
 Acq On : 11 Oct 2022 12:42
 Operator : SY/MD
 Sample : N5079-05DL 20X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFZ02DL

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_V\Method\SFAMVLM100722WMA.M
 Title : VOC Analysis

Signal : TIC: VV028517.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	104	rVB	157191	163968	12.79%	1.585%
2	1.561	156	162	175	rVB	119964	140215	10.94%	1.356%
3	2.101	321	330	348	rVB	267461	386855	30.17%	3.740%
4	2.577	475	478	482	rBV3	620	495	0.04%	0.005%
5	2.896	573	577	582	rVB2	528	511	0.04%	0.005%
6	2.928	584	587	591	rBV4	918	830	0.06%	0.008%
7	2.976	600	602	607	rBV4	372	287	0.02%	0.003%
8	3.108	638	643	647	rBV4	554	543	0.04%	0.005%
9	3.185	653	667	684	rBV	45137	96431	7.52%	0.932%
10	3.391	729	731	734	rVB	536	247	0.02%	0.002%
11	3.423	735	741	742	rBV	324	226	0.02%	0.002%
12	3.436	742	745	747	rVV3	457	260	0.02%	0.003%
13	3.484	757	760	761	rBV	539	268	0.02%	0.003%
14	3.571	781	787	790	rBV3	346	336	0.03%	0.003%
15	3.590	790	793	797	rVV2	444	284	0.02%	0.003%
16	3.625	800	804	806	rBV2	324	260	0.02%	0.003%
17	3.654	810	813	816	rBV2	298	201	0.02%	0.002%
18	3.709	829	830	833	rVB2	406	192	0.01%	0.002%
19	3.760	844	846	850	rBV2	308	205	0.02%	0.002%
20	3.809	857	861	865	rBV3	265	224	0.02%	0.002%
21	3.892	877	887	917	rBV	61476	235457	18.37%	2.277%
22	4.339	1012	1026	1051	rBV2	194150	487854	38.05%	4.717%
23	4.600	1091	1107	1128	rBV	223085	557509	43.49%	5.391%
24	4.757	1154	1156	1159	rBV3	421	185	0.01%	0.002%
25	4.780	1159	1163	1167	rBV4	573	431	0.03%	0.004%
26	4.831	1175	1179	1188	rVB4	726	930	0.07%	0.009%
27	4.876	1189	1193	1194	rBV2	302	198	0.02%	0.002%
28	5.040	1224	1244	1280	rBV2	493653	1282048	100.00%	12.396%
29	5.275	1314	1317	1320	rBV2	546	372	0.03%	0.004%
30	5.448	1367	1371	1374	rBV3	498	442	0.03%	0.004%
31	5.487	1379	1383	1385	rBV3	429	332	0.03%	0.003%
32	5.564	1405	1407	1410	rBV	273	191	0.01%	0.002%
33	5.612	1410	1422	1451	rBV	335038	678973	52.96%	6.565%
34	5.821	1484	1487	1489	rBV3	560	353	0.03%	0.003%
35	5.908	1506	1514	1524	rBV6	2872	5227	0.41%	0.051%
36	6.063	1549	1562	1590	rBV	271852	566812	44.21%	5.481%

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 Title : VOC Analysis

37	6.313	1629	1640	1654	rVB	11658	22856	1.78%	0.221%
38	6.403	1664	1668	1670	rBV3	355	233	0.02%	0.002%
39	6.477	1688	1691	1693	rVB2	417	206	0.02%	0.002%
40	6.513	1697	1702	1707	rBV3	530	572	0.04%	0.006%
41	6.535	1707	1709	1712	rVB3	534	242	0.02%	0.002%
42	6.603	1727	1730	1732	rBV	444	286	0.02%	0.003%
43	6.699	1755	1760	1761	rBV2	357	297	0.02%	0.003%
44	6.751	1771	1776	1786	rVB5	2035	2622	0.20%	0.025%
45	6.799	1789	1791	1792	rBV2	551	240	0.02%	0.002%
46	6.834	1797	1802	1804	rBV3	380	257	0.02%	0.002%
47	6.928	1822	1831	1838	rBV7	4432	8176	0.64%	0.079%
48	6.982	1838	1848	1881	rVB	169874	320485	25.00%	3.099%
49	7.133	1887	1895	1906	rBV3	8583	15274	1.19%	0.148%
50	7.201	1915	1916	1919	rVB	633	189	0.01%	0.002%
51	7.310	1937	1950	1981	rBV	588342	1038284	80.99%	10.039%
52	7.616	2035	2045	2069	rBV	119325	214882	16.76%	2.078%
53	7.902	2130	2134	2138	rBV2	390	404	0.03%	0.004%
54	7.985	2154	2160	2161	rBV2	569	389	0.03%	0.004%
55	8.085	2179	2191	2228	rBV	314325	645883	50.38%	6.245%
56	8.757	2397	2400	2401	rBV	401	201	0.02%	0.002%
57	8.847	2416	2428	2459	rBV	479351	798850	62.31%	7.724%
58	9.062	2492	2495	2500	rVB2	792	555	0.04%	0.005%
59	9.124	2512	2514	2517	rBV2	404	194	0.02%	0.002%
60	9.230	2543	2547	2550	rBV2	495	333	0.03%	0.003%
61	9.252	2550	2554	2556	rBV	323	191	0.01%	0.002%
62	9.281	2561	2563	2567	rVB2	465	224	0.02%	0.002%
63	9.349	2580	2584	2586	rBV2	398	227	0.02%	0.002%
64	9.542	2642	2644	2647	rBV3	262	193	0.02%	0.002%
65	9.583	2654	2657	2660	rBV3	437	277	0.02%	0.003%
66	9.731	2691	2703	2726	rBV2	75465	140938	10.99%	1.363%
67	9.924	2761	2763	2765	rBV3	846	449	0.04%	0.004%
68	10.098	2815	2817	2819	rBV3	685	395	0.03%	0.004%
69	10.210	2840	2852	2867	rVV	360604	569925	44.45%	5.511%
70	10.323	2885	2887	2890	rVB	602	289	0.02%	0.003%
71	10.368	2900	2901	2905	rBV2	413	210	0.02%	0.002%
72	10.416	2912	2916	2917	rBV	435	237	0.02%	0.002%
73	10.474	2922	2934	2957	rVB	144455	241632	18.85%	2.336%
74	10.603	2972	2974	2978	rBV	233	213	0.02%	0.002%
75	10.641	2983	2986	2990	rBV2	289	261	0.02%	0.003%
76	10.879	3058	3060	3064	rVV2	480	205	0.02%	0.002%

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Title : VOC Analysis

77	10.924	3069	3074	3082	rVV5	736	823	0.06%	0.008%
78	11.008	3097	3100	3103	rBV2	245	178	0.01%	0.002%
79	11.078	3119	3122	3123	rBV	632	261	0.02%	0.003%
80	11.239	3161	3172	3193	rBV	502691	793534	61.90%	7.673%
81	11.525	3253	3261	3270	rBV5	4419	6755	0.53%	0.065%
82	11.561	3270	3272	3275	rVB2	332	191	0.01%	0.002%
83	11.615	3275	3289	3308	rBV	561169	891580	69.54%	8.621%
84	12.066	3427	3429	3432	rBV2	285	188	0.01%	0.002%
85	12.098	3435	3439	3441	rBV2	353	272	0.02%	0.003%
86	12.149	3452	3455	3460	rBV2	581	549	0.04%	0.005%
87	12.316	3499	3507	3512	rBV2	2038	2691	0.21%	0.026%
88	12.358	3517	3520	3525	rBV4	532	615	0.05%	0.006%
89	12.413	3534	3537	3542	rBV4	775	605	0.05%	0.006%
90	12.464	3552	3553	3558	rBV2	219	181	0.01%	0.002%
91	12.548	3577	3579	3582	rBV	419	252	0.02%	0.002%
92	12.593	3590	3593	3596	rBV3	633	396	0.03%	0.004%
93	12.927	3695	3697	3700	rBV	399	212	0.02%	0.002%
94	13.268	3800	3803	3804	rBV	508	273	0.02%	0.003%
95	13.390	3836	3841	3844	rBV	505	429	0.03%	0.004%
96	13.516	3870	3880	3893	rBV7	1160	2720	0.21%	0.026%
97	13.577	3895	3899	3900	rBV3	591	423	0.03%	0.004%
98	13.619	3910	3912	3915	rBV	339	204	0.02%	0.002%
99	13.821	3971	3975	3980	rBV4	582	639	0.05%	0.006%
100	14.146	4073	4076	4080	rBV3	503	435	0.03%	0.004%

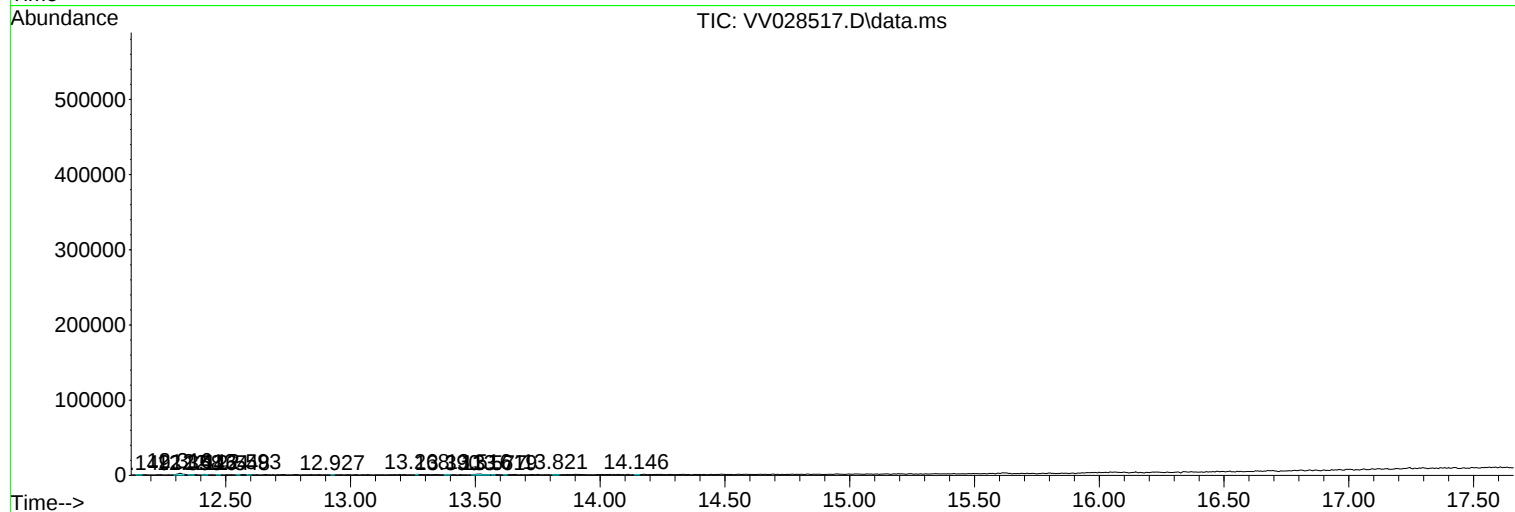
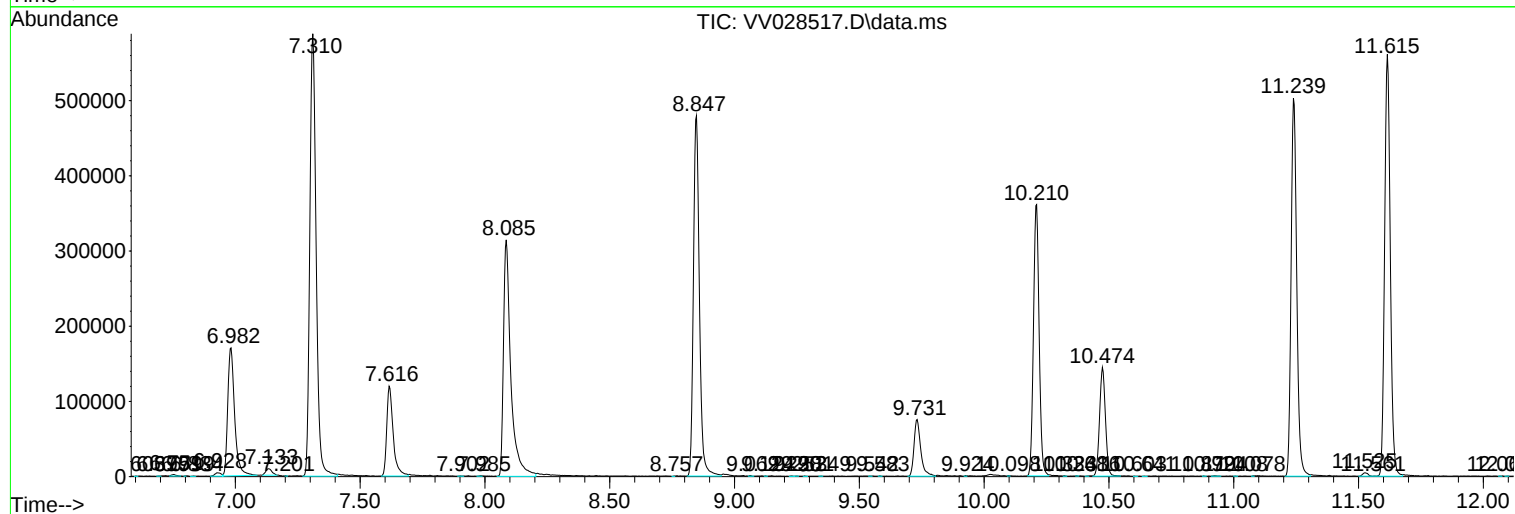
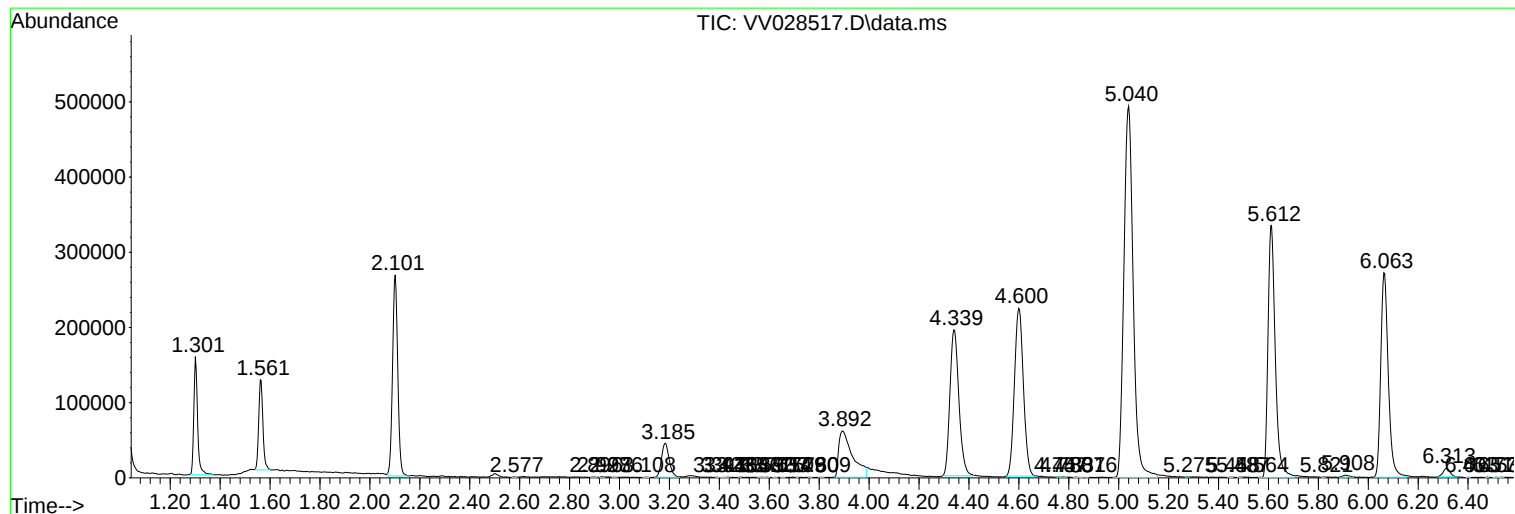
Sum of corrected areas: 10342334

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

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



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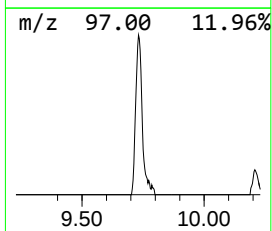
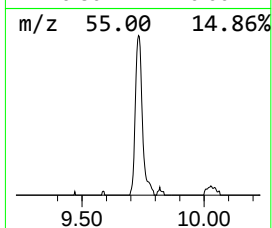
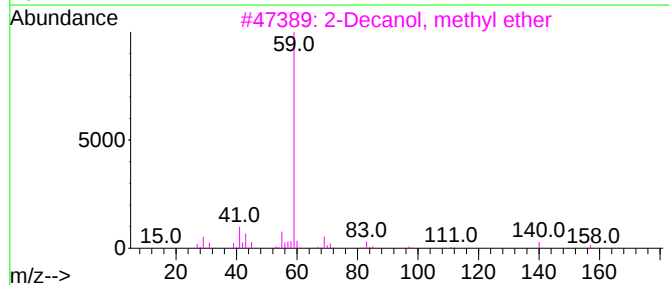
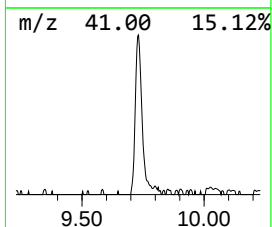
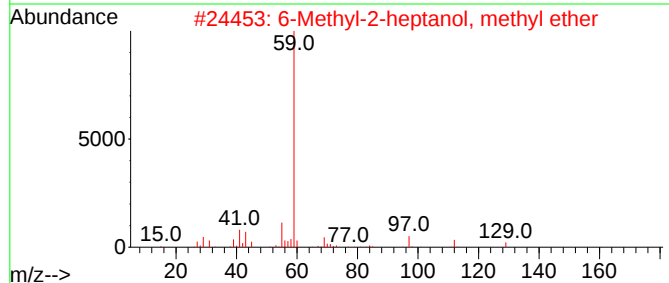
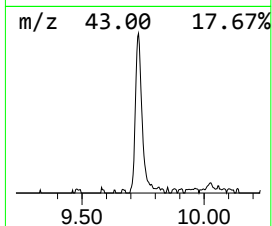
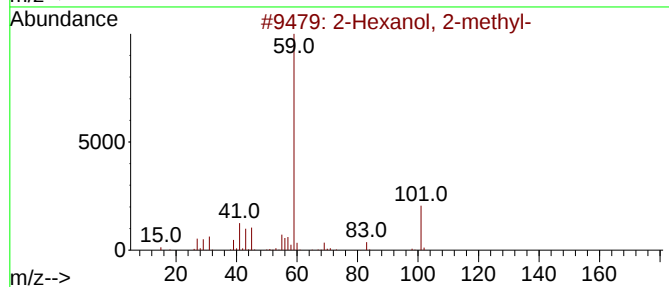
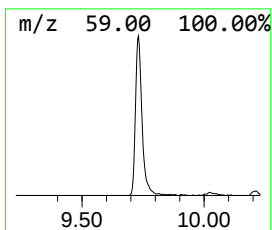
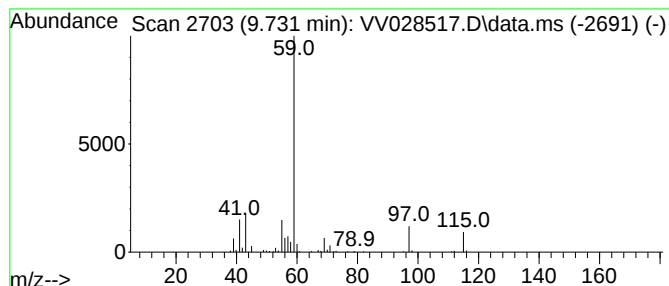
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2-Hexanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.731	8.82 ug/L	140938	Chlorobenzene-d5	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-			116	C7H16O	000625-23-0	64
2	6-Methyl-2-heptanol, methyl ether			144	C9H20O	1000365-52-0	64
3	2-Decanol, methyl ether			172	C11H24O	1000333-83-9	59
4	2-Heptanol, 2-methyl-			130	C8H18O	000625-25-2	56
5	2-Heptanol, 2-methyl-			130	C8H18O	000625-25-2	56



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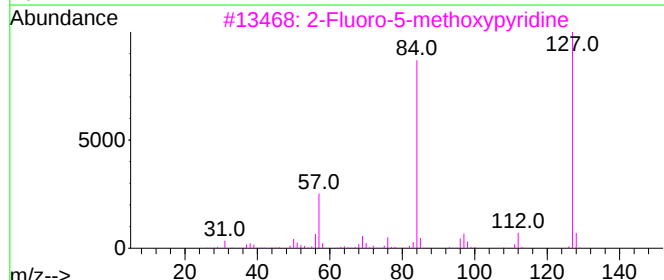
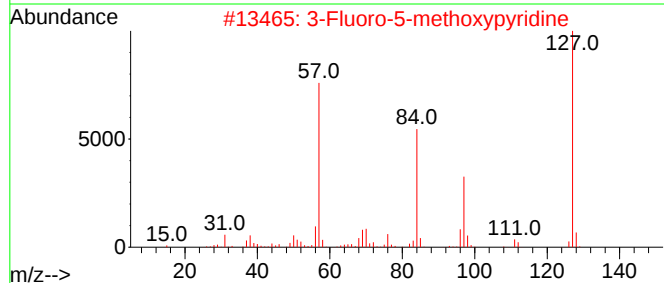
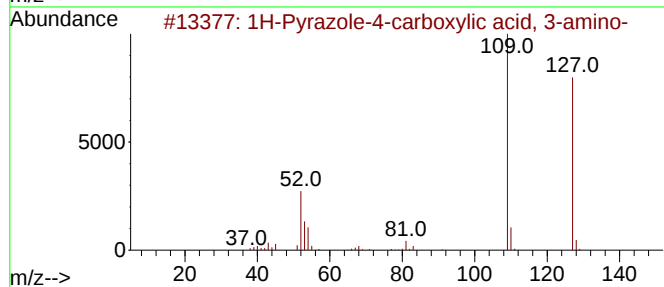
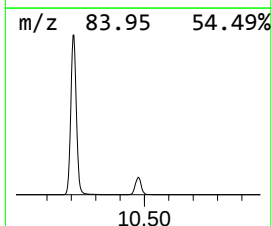
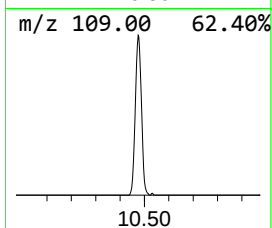
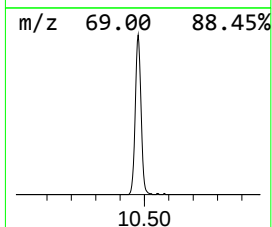
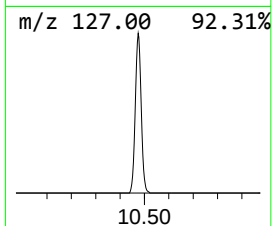
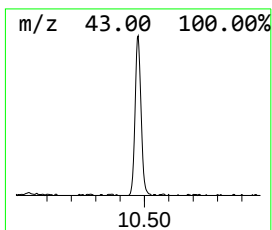
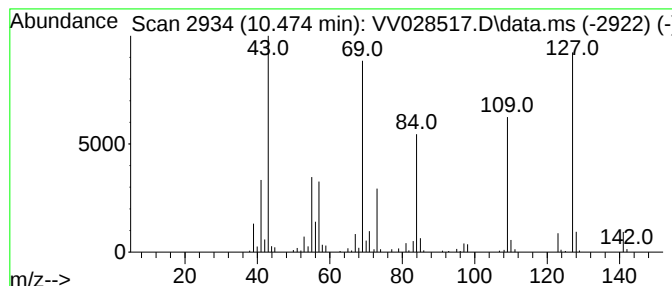
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Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.474	15.23 ug/L	241632	1,4-Dichlorobenzene-d4	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	38
2			3-Fluoro-5-methoxypyridine	127	C6H6FNO	1060801-62-8	35
3			2-Fluoro-5-methoxypyridine	127	C6H6FNO	136888-79-4	35
4			2-Fluoro-5-methoxypyridine	127	C6H6FNO	136888-79-4	35
5			2-Nonen-4-one	140	C9H16O	032064-72-5	27



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Hexanol, 2-me...	9.731	8.8	ug/L	140938	2	8.847	798850	50.0
unknown-01	10.474	15.2	ug/L	241632	3	11.239	793534	50.0