

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042470.D
 Acq On : 23 Jul 2024 14:34
 Operator : JC/MD
 Sample : P3263-19ME
 Misc : 5.15g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CK9ME

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042470.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	27	rBV	35316	42612	6.87%	0.785%
2	1.368	43	46	47	rBV	11094	10765	1.74%	0.198%
3	1.642	86	91	95	rBV2	12693	33113	5.34%	0.610%
4	2.270	189	194	211	rBV	71786	137104	22.12%	2.527%
5	2.721	262	268	284	rBV	33777	84785	13.68%	1.563%
6	3.123	333	334	339	rBV2	260	358	0.06%	0.007%
7	3.178	341	343	347	rBV	161	186	0.03%	0.003%
8	3.343	361	370	372	rBV3	729	1573	0.25%	0.029%
9	3.599	407	412	413	rBV3	782	1138	0.18%	0.021%
10	3.849	446	453	462	rVV3	2340	6836	1.10%	0.126%
11	4.068	487	489	492	rBV2	198	215	0.03%	0.004%
12	4.294	524	526	530	rBV2	114	147	0.02%	0.003%
13	4.379	538	540	542	rBV2	140	138	0.02%	0.003%
14	4.501	551	560	577	rBV	39114	137321	22.15%	2.531%
15	5.056	638	651	667	rBV	76491	242609	39.14%	4.472%
16	5.318	688	694	695	rBV2	253	406	0.07%	0.007%
17	5.385	703	705	715	rVB4	783	1671	0.27%	0.031%
18	5.550	724	732	733	rBV3	1147	2040	0.33%	0.038%
19	5.739	761	763	766	rBV	197	185	0.03%	0.003%
20	5.836	777	779	784	rBV	154	217	0.04%	0.004%
21	5.879	784	786	788	rBV	130	157	0.03%	0.003%
22	5.964	788	800	813	rBV2	214739	619890	100.00%	11.427%
23	6.379	860	868	873	rBV5	2159	5144	0.83%	0.095%
24	6.617	903	907	908	rBV2	377	484	0.08%	0.009%
25	6.757	921	930	956	rVB	214345	523788	84.50%	9.655%
26	7.019	971	973	976	rBV3	317	385	0.06%	0.007%
27	7.104	983	987	989	rBV3	1041	1689	0.27%	0.031%
28	7.226	1001	1007	1012	rBV4	1962	4075	0.66%	0.075%
29	7.312	1012	1021	1041	rVB	122612	283634	45.76%	5.228%
30	7.610	1067	1070	1075	rBV2	174	290	0.05%	0.005%
31	7.678	1080	1081	1084	rBV2	164	144	0.02%	0.003%
32	7.812	1100	1103	1106	rBV2	184	200	0.03%	0.004%
33	7.976	1123	1130	1140	rBV5	1874	5205	0.84%	0.096%
34	8.165	1157	1161	1165	rVB3	490	580	0.09%	0.011%
35	8.257	1172	1176	1179	rVB3	357	460	0.07%	0.008%
36	8.330	1182	1188	1206	rBV	64570	119391	19.26%	2.201%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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 Title : VOC Analysis

37	8.647	1234	1240	1252	rBV	312836	502539	81.07%	9.264%
38	8.952	1285	1290	1303	rBV	48662	78816	12.71%	1.453%
39	9.110	1315	1316	1320	rVB2	928	874	0.14%	0.016%
40	9.196	1328	1330	1332	rVB2	151	158	0.03%	0.003%
41	9.238	1332	1337	1338	rBV	251	260	0.04%	0.005%
42	9.275	1338	1343	1351	rVB	8622	13392	2.16%	0.247%
43	9.330	1351	1352	1355	rBV2	161	138	0.02%	0.003%
44	9.397	1357	1363	1381	rBV	163973	346715	55.93%	6.391%
45	9.726	1411	1417	1422	rBV4	2324	5200	0.84%	0.096%
46	9.982	1456	1459	1461	rVB	165	147	0.02%	0.003%
47	10.006	1461	1463	1465	rBV2	120	146	0.02%	0.003%
48	10.055	1465	1471	1483	rBV	438574	606603	97.86%	11.182%
49	10.311	1510	1513	1515	rBV2	500	572	0.09%	0.011%
50	10.354	1518	1520	1524	rVB3	367	396	0.06%	0.007%
51	10.500	1543	1544	1547	rVB2	164	159	0.03%	0.003%
52	10.537	1547	1550	1552	rBV2	129	142	0.02%	0.003%
53	10.646	1566	1568	1571	rVB	245	206	0.03%	0.004%
54	10.811	1593	1595	1598	rBV	130	144	0.02%	0.003%
55	10.878	1602	1606	1611	rBV3	540	898	0.14%	0.017%
56	10.963	1613	1620	1629	rBV3	7006	12170	1.96%	0.224%
57	11.098	1639	1642	1647	rVB3	346	467	0.08%	0.009%
58	11.134	1647	1648	1652	rBV2	140	193	0.03%	0.004%
59	11.195	1652	1658	1670	rVV	267530	346883	55.96%	6.394%
60	11.305	1674	1676	1678	rVV3	279	306	0.05%	0.006%
61	11.439	1692	1698	1702	rBV4	1495	2492	0.40%	0.046%
62	11.488	1702	1706	1711	rVB3	2925	4192	0.68%	0.077%
63	11.634	1728	1730	1734	rBV3	574	811	0.13%	0.015%
64	11.701	1737	1741	1743	rBV	5019	6307	1.02%	0.116%
65	11.732	1743	1746	1748	rVV	9371	12417	2.00%	0.229%
66	11.762	1748	1751	1763	rVB2	28110	43227	6.97%	0.797%
67	11.860	1763	1767	1772	rVB4	1066	1756	0.28%	0.032%
68	11.939	1775	1780	1783	rBV3	3015	4238	0.68%	0.078%
69	11.982	1783	1787	1789	rBV2	5469	6610	1.07%	0.122%
70	12.024	1789	1794	1803	rVB	461688	587980	94.85%	10.838%
71	12.232	1823	1828	1837	rBV5	1163	2447	0.39%	0.045%
72	12.323	1837	1843	1851	rBV	358929	477319	77.00%	8.799%
73	12.524	1873	1876	1877	rBV2	196	182	0.03%	0.003%
74	12.597	1883	1888	1896	rBV3	2956	6448	1.04%	0.119%
75	12.713	1904	1907	1909	rVB2	378	385	0.06%	0.007%
76	12.768	1912	1916	1920	rBV2	565	987	0.16%	0.018%

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Instrument :
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 ClientSampleId :
 A4CK9ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

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 Title : VOC Analysis

77	12.872	1927	1933	1937	rBV2	15859	21807	3.52%	0.402%
78	13.030	1955	1959	1964	rBV2	1606	1976	0.32%	0.036%
79	13.116	1971	1973	1976	rBV2	409	380	0.06%	0.007%
80	13.164	1977	1981	1986	rBV3	704	909	0.15%	0.017%
81	13.219	1989	1990	1993	rBV2	349	354	0.06%	0.007%
82	13.280	1998	2000	2001	rBV2	251	137	0.02%	0.003%
83	13.402	2015	2020	2027	rVV3	1198	2035	0.33%	0.038%
84	13.554	2044	2045	2047	rBV	165	142	0.02%	0.003%
85	13.683	2062	2066	2072	rBV2	2824	3888	0.63%	0.072%
86	13.731	2072	2074	2077	rVB3	682	648	0.10%	0.012%
87	13.786	2079	2083	2088	rVB2	656	1188	0.19%	0.022%
88	13.884	2096	2099	2103	rVB2	1305	1469	0.24%	0.027%
89	14.134	2136	2140	2145	rVB	1819	2181	0.35%	0.040%
90	14.195	2148	2150	2153	rBV	234	274	0.04%	0.005%
91	14.365	2176	2178	2181	rVB2	494	502	0.08%	0.009%
92	14.426	2182	2188	2196	rVB	8659	12712	2.05%	0.234%
93	14.969	2275	2277	2281	rBV2	354	217	0.04%	0.004%
94	15.176	2308	2311	2316	rVB3	2133	2560	0.41%	0.047%
95	15.347	2335	2339	2343	rBV4	2241	3465	0.56%	0.064%
96	15.487	2359	2362	2370	rBV4	1412	2273	0.37%	0.042%
97	15.908	2430	2431	2434	rBV3	541	601	0.10%	0.011%
98	15.957	2434	2439	2449	rVB	10435	16904	2.73%	0.312%
99	16.572	2536	2540	2546	rBV4	2115	3729	0.60%	0.069%
100	16.664	2553	2555	2556	rBV2	563	318	0.05%	0.006%

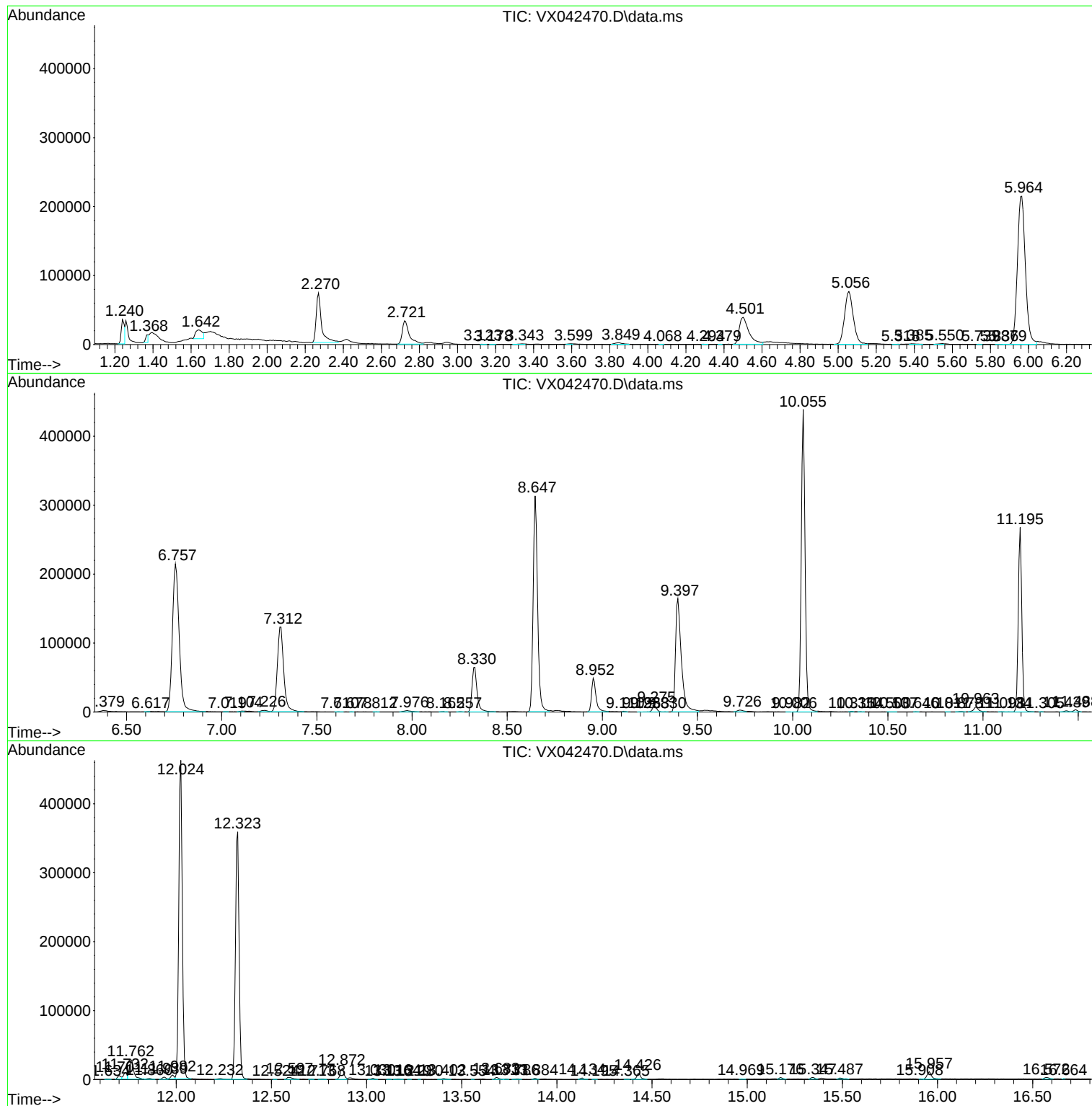
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CK9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CK9ME

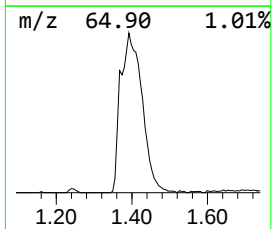
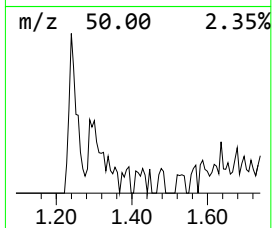
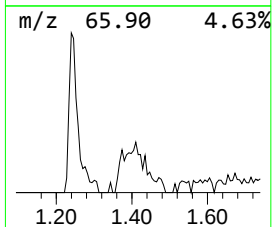
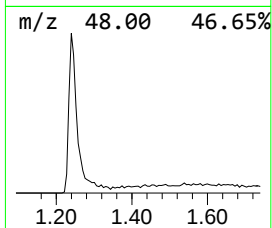
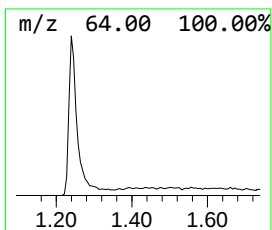
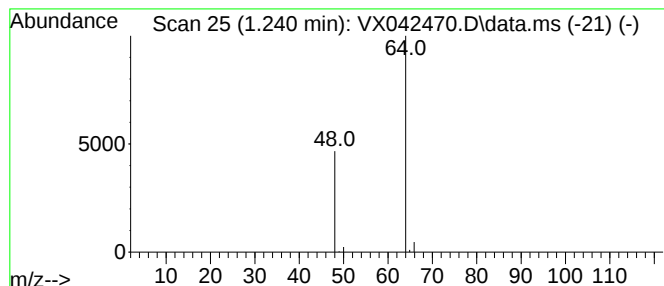
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	4.07 ug/L	42612	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CK9ME

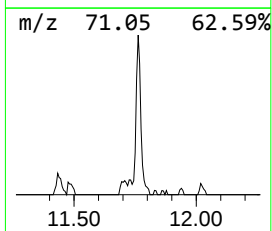
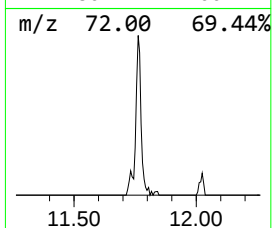
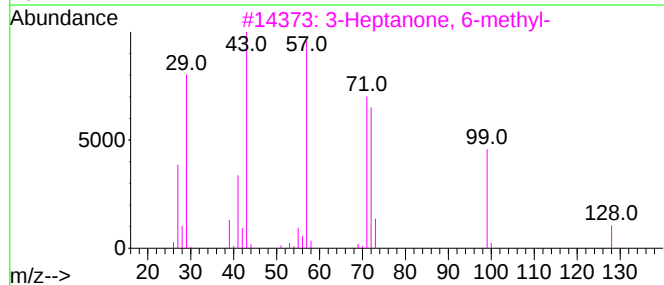
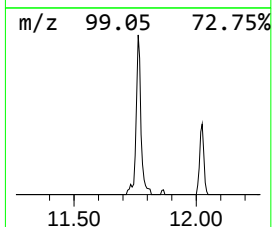
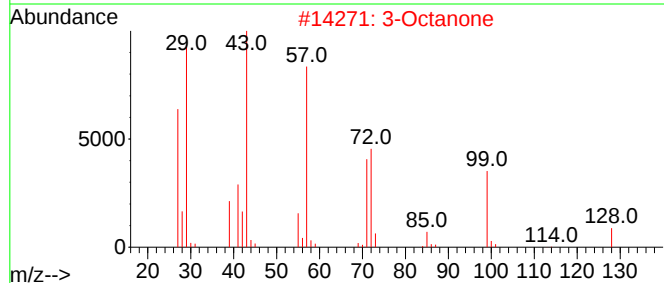
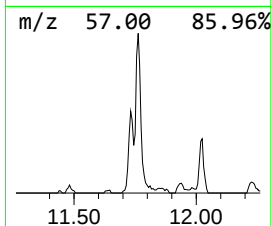
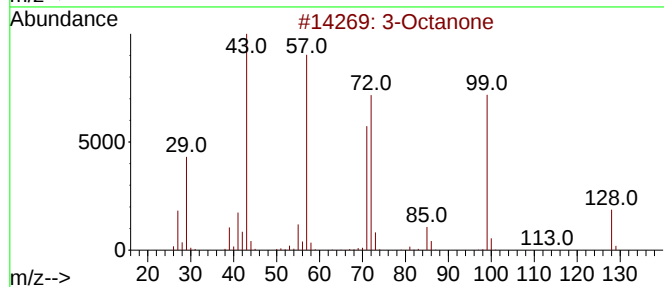
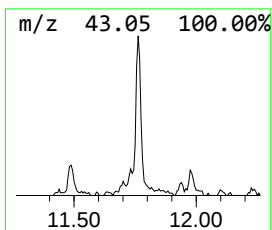
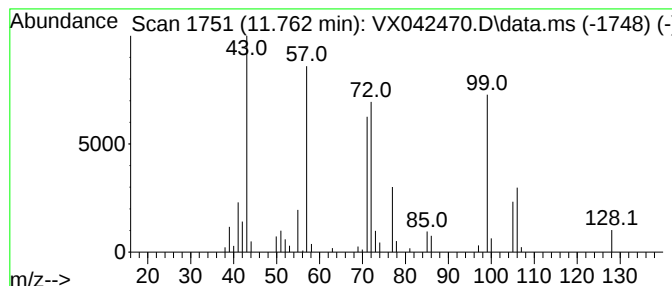
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 3-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.762	3.68 ug/L	43227	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Octanone	128	C8H16O	000106-68-3	70
2		3-Octanone	128	C8H16O	000106-68-3	62
3		3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	53
4		3-Octanone	128	C8H16O	000106-68-3	50
5		3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	49



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	4.1	ug/L	42612	1	6.757	523788	50.0
3-Octanone	11.762	3.7	ug/L	43227	3	12.024	587980	50.0