Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

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_X\Method\82X112222W.M
Title : SW846 8260

Signal : TIC: VX033246.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	21	rVB	206150	204477	37.98%	3.281%
2	1.264	25	29	33	rBV	39983	39692	7.37%	0.637%
3	1.374	41	47	52	rVB	44371	53770	9.99%	0.863%
4	1.752	105	109	118	rVB	12792	17356	3.22%	0.279%
5	1.953	138	142	151	rVB	5518	9075	1.69%	0.146%
6	2.136	161	172	179	rBV6	7472	26321	4.89%	0.422%
7	2.392	208	214	225	rVB	22652	50394	9.36%	0.809%
8	2.599	238	248	250	rBV3	5722	15905	2.95%	0.255%
9	2.703	261	265	274	rVB2	5086	9993	1.86%	0.160%
10	2.965	298	308	325	rBV4	15180	51073	9.49%	0.820%
11	3.331	361	368	378	rVB2	4163	9439	1.75%	0.151%
12	3.697	417	428	444	rBV2	84568	236057	43.85%	3.788%
13	3.928	455	466	467	rBV4	3418	8470	1.57%	0.136%
14	4.227	501	515	531	rBV	145031	400610	74.42%	6.429%
15	4.562	562	570	589	rVB	47518	142040	26.39%	2.279%
16	5.385	693	705	715	rBV	59246	175069	32.52%	2.809%
17	5.550	722	732	749	rVB	127069	364444	67.70%	5.848%
18	5.958	789	799	805	rBV	61862	161748	30.05%	2.596%
19	6.038	805	812	825	rVV	116683	316084	58.72%	5.072%
20	6.147	825	830	842	rVB5	2875	9494	1.76%	0.152%
21	6.763	922	931	947	rBV	188986	454595	84.45%	7.295%
22	7.245	1004	1010	1024	rBV4	6351	25113	4.66%	0.403%
23	7.379	1027	1032	1041	rVB5	3138	6988	1.30%	0.112%
24	7.580	1060	1065	1072	rVB2	10950	20812	3.87%	0.334%
25	8.647	1234	1240	1246	rBV	275307	431355	80.13%	6.922%
26	8.720	1246	1252	1258	rVV	179292	273146	50.74%	4.383%
27	8.781	1258	1262	1270	rVB	5122	10260	1.91%	0.165%
28	9.250	1333	1339	1345	rBV4	5340	11723	2.18%	0.188%
29	9.488	1373	1378	1383	rBV2	9904	15063	2.80%	0.242%
30	10.055	1463	1471	1484	rBV	399310	535126	99.40%	8.587%
31	10.159	1484	1488	1490	rVV2	5215	6994	1.30%	0.112%
32	10.195	1490	1494	1500	rVB	16290	22492	4.18%	0.361%
33	10.299	1506	1511	1518	rVB	74798	101731	18.90%	1.633%
34	10.445	1530	1535	1541	rVB	46730	60978	11.33%	0.979%
35	10.506	1541	1545	1553	rBV	7202	9422	1.75%	0.151%
36	10.640	1561	1567	1572	rBV	28865	45462	8.44%	0.730%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

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_X\Method\82X112222W.M
Title : SW846 8260

37	10.683	1572	1574	1579	rVB3	4232	5596	1.04%	0.090%
38	10.756	1579	1586	1595	rBV3	9619	19496	3.62%	0.313%
39	11.079	1634	1639	1645	rBV	250704	327923	60.91%	5.262%
40	11.128	1645	1647	1652	rVB2	4721	6129	1.14%	0.098%
41	11.305	1673	1676	1683	rVB3	3907	5881	1.09%	0.094%
42	11.378	1683	1688	1694	rBV	11822	23465	4.36%	0.377%
43	11.451	1698	1700	1708	rVB	9352	11873	2.21%	0.191%
44	11.573	1715	1720	1723	rBV4	5908	8439	1.57%	0.135%
45	11.610	1723	1726	1734	rVB5	10501	20333	3.78%	0.326%
46	11.683	1734	1738	1745	rVB	17067	20264	3.76%	0.325%
47	11.756	1745	1750	1754	rBV	26842	34648	6.44%	0.556%
48	11.988	1779	1788	1789	rBV5	6073	10363	1.93%	0.166%
49	12.024	1789	1794	1801	rVV	419215	538331	100.00%	8.639%
50	12.085	1801	1804	1809	rVB	9520	12566	2.33%	0.202%
51	12.219	1821	1826	1837	rBV	318394	457697	85.02%	7.345%
52	12.305	1837	1840	1853	rVV6	20467	46597	8.66%	0.748%
53	12.414	1853	1858	1863	rVV2	16355	22707	4.22%	0.364%
54	12.561	1879	1882	1885	rBV4	6971	9830	1.83%	0.158%
55	12.695	1900	1904	1911	rVB6	3851	7001	1.30%	0.112%
56	12.762	1911	1915	1918	rBV4	3842	6674	1.24%	0.107%
57	12.799	1918	1921	1925	rVV4	7277	11077	2.06%	0.178%
58	12.847	1925	1929	1936	rVB2	5432	8348	1.55%	0.134%
59	12.920	1936	1941	1945	rBV4	4009	6995	1.30%	0.112%
60	12.963	1945	1948	1956	rVB4	4566	7302	1.36%	0.117%
61	13.286	1998	2001	2007	rVB2	6504	9520	1.77%	0.153%
62	13.420	2017	2023	2030	rVB6	4087	7740	1.44%	0.124%
63	13.774	2078	2081	2086	rVB	44596	55918	10.39%	0.897%
64	13.847	2089	2093	2100	rVB2	17864	27564	5.12%	0.442%
65	13.914	2100	2104	2111	rVB	21509	28064	5.21%	0.450%
66	14.134	2135	2140	2145	rVB	6305	8848	1.64%	0.142%
67	14.225	2150	2155	2159	rBV7	3215	5703	1.06%	0.092%
68	14.634	2217	2222	2230	rVB	24273	36030	6.69%	0.578%
69	14.780	2241	2246	2251	rBV	15612	20405	3.79%	0.327%
70	15.207	2313	2316	2321	rVB2	4322	5908	1.10%	0.095%
71	15.377	2340	2344	2354	rBV6	2159	5868	1.09%	0.094%
72	15.475	2354	2360	2366	rVB5	4124	7557	1.40%	0.121%
73	15.615	2377	2383	2386	rBV3	4369	6881	1.28%	0.110%
74	15.969	2434	2441	2453	rBV4	18691	37461	6.96%	0.601%
75	16.091	2457	2461	2466	rVB5	3785	5729	1.06%	0.092%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

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_X\Method\82X112222W.M
Title : SW846 8260

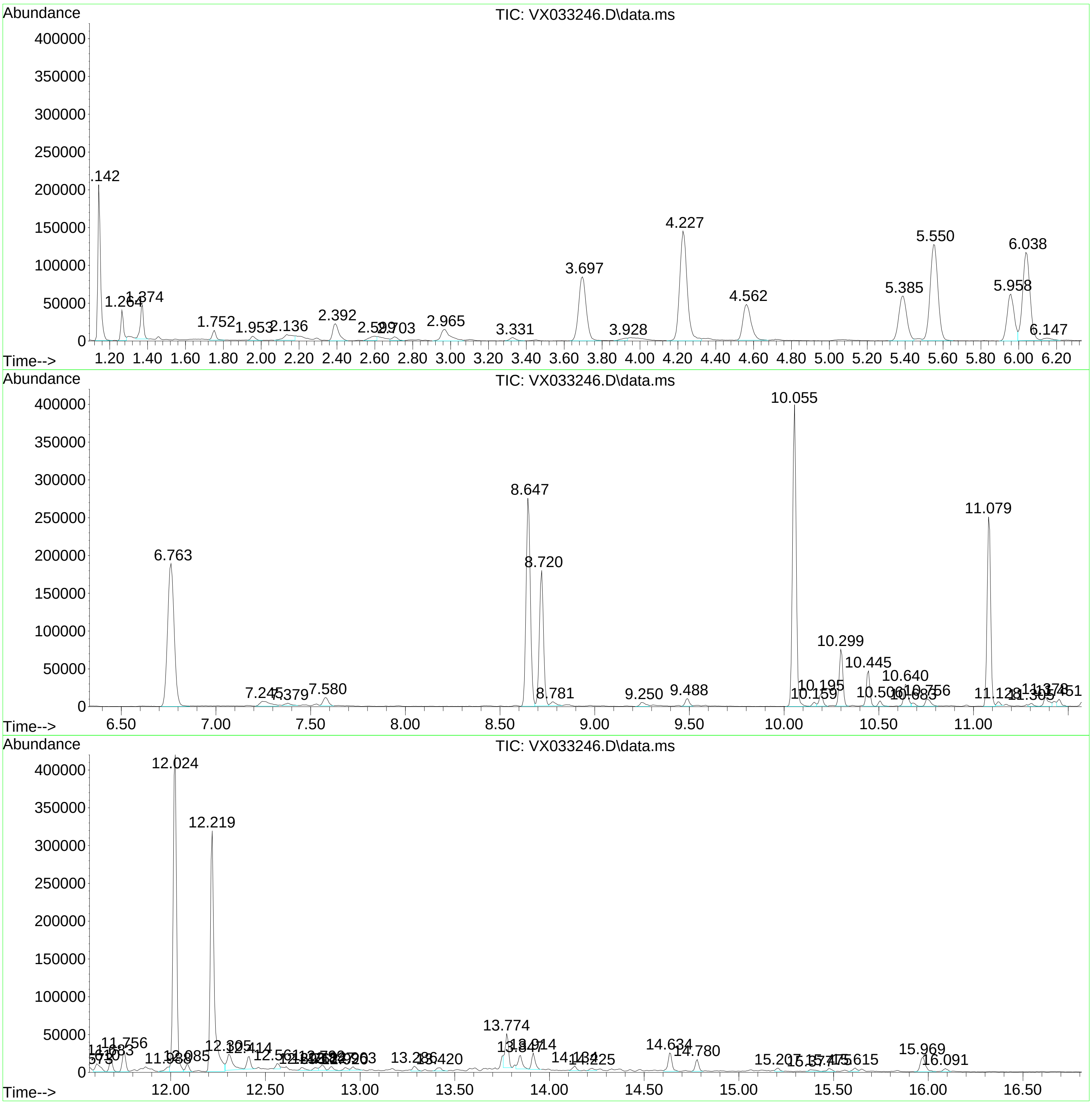
Sum of corrected areas: 6231502

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

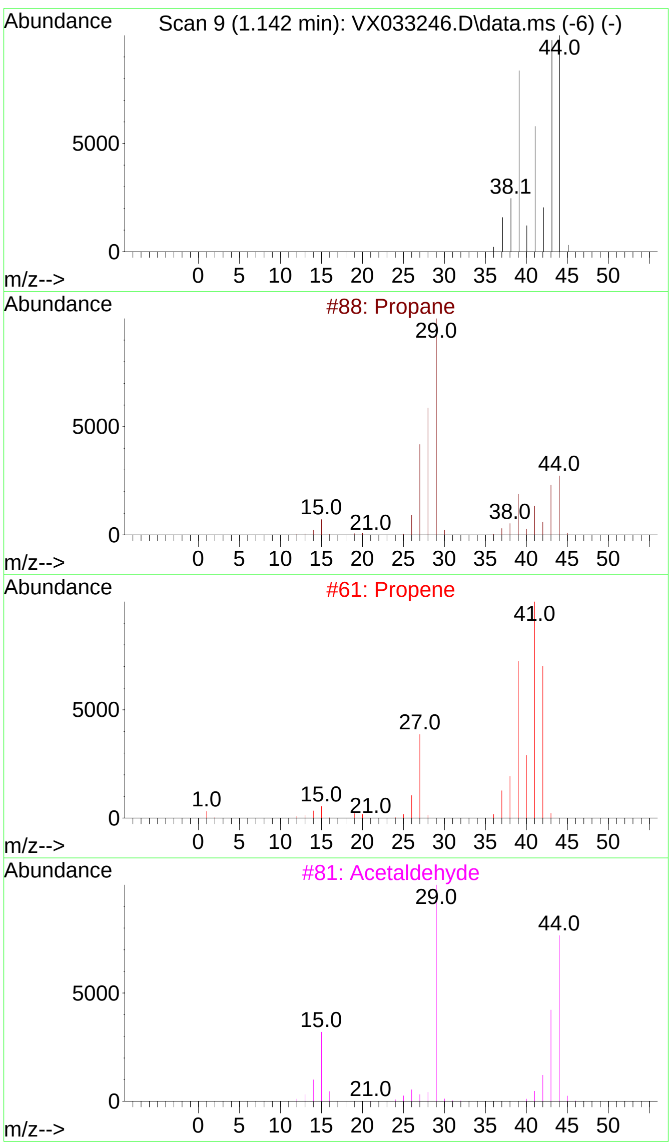
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

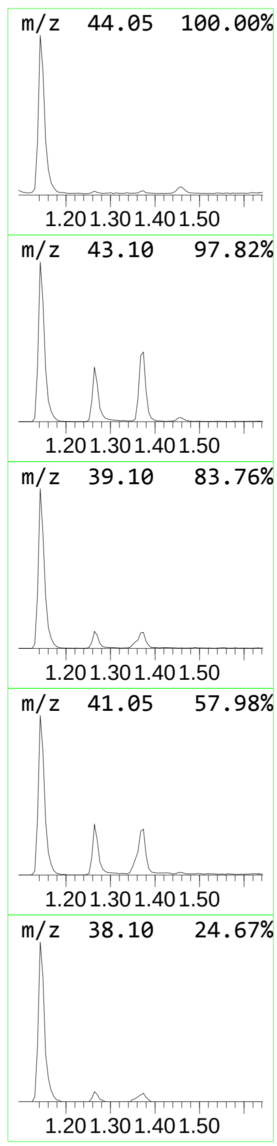
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	28.05 ug/l	204477	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	83
2	Propene	42	C3H6	000115-07-1	9
3	Acetaldehyde	44	C2H4O	000075-07-0	5
4	Cyclopropene	40	C3H4	002781-85-3	2
5	Alanine	89	C3H7NO2	000056-41-7	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ORA-0583

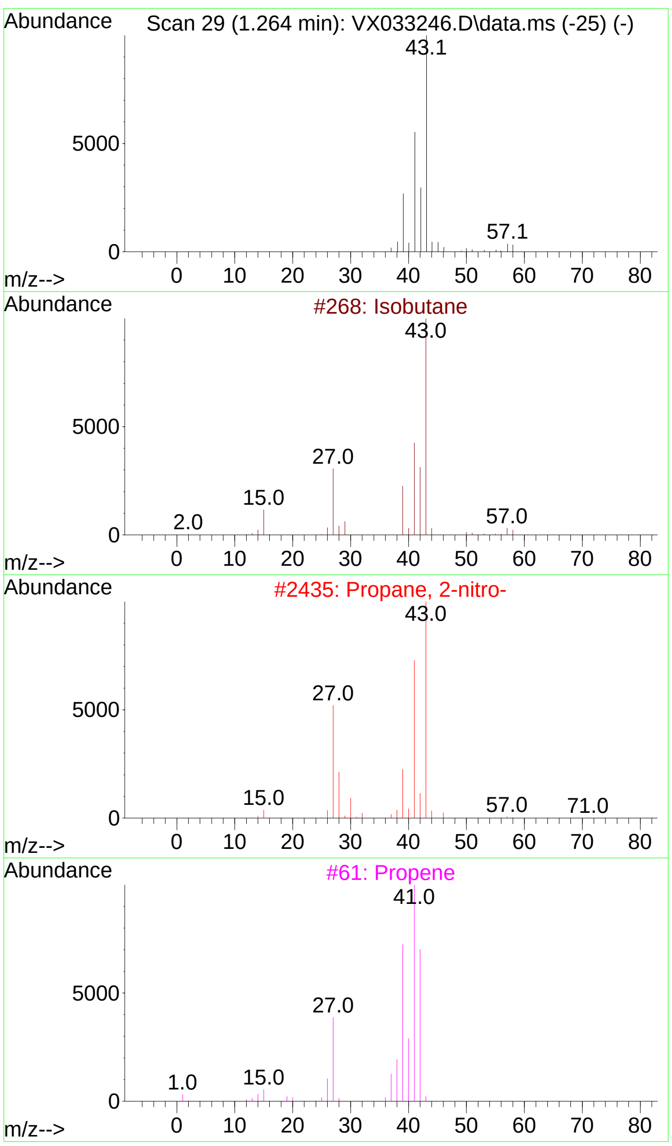
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

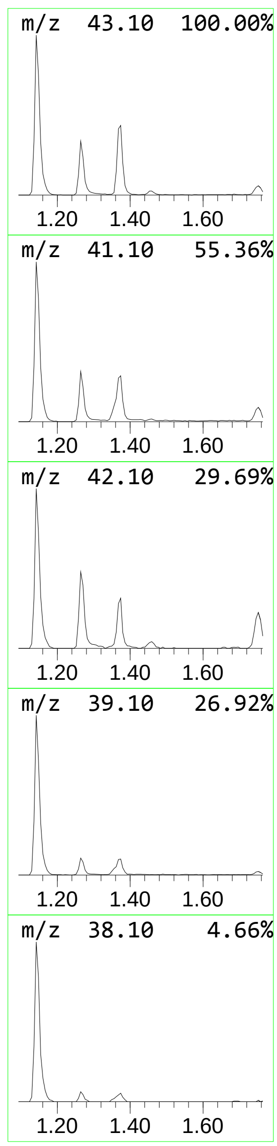
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	5.45 ug/l	39692	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	59
2	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	36
3	Propene	42	C3H6	000115-07-1	5
4	1-Butanol	74	C4H10O	000071-36-3	4
5	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

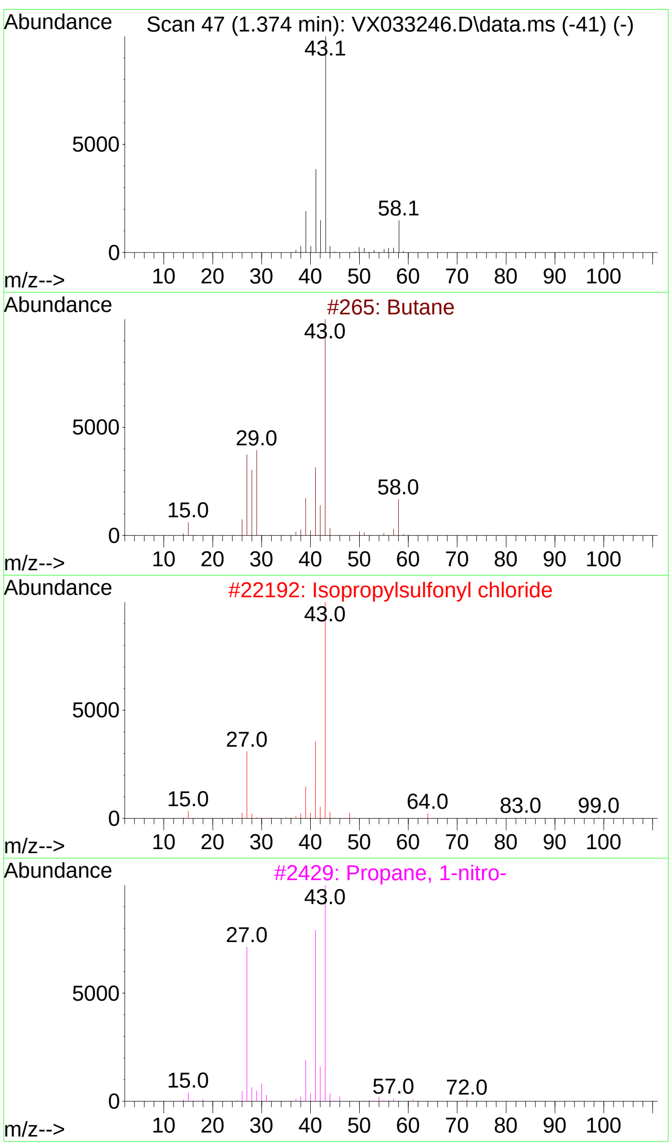
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

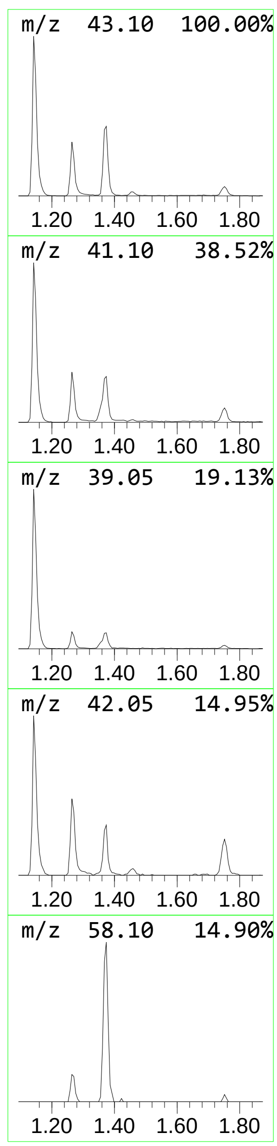
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	7.38 ug/l	53770	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
4	Diazene, dimethyl-	58	C2H6N2	000503-28-6	5
5	Isobutane	58	C4H10	000075-28-5	4





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

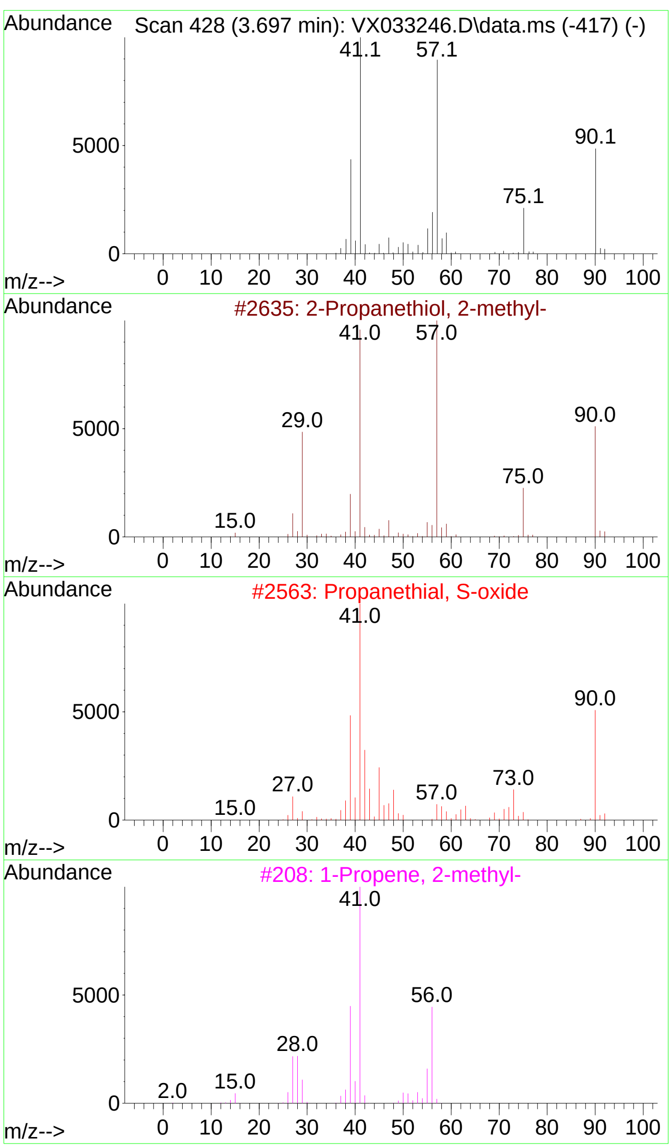
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

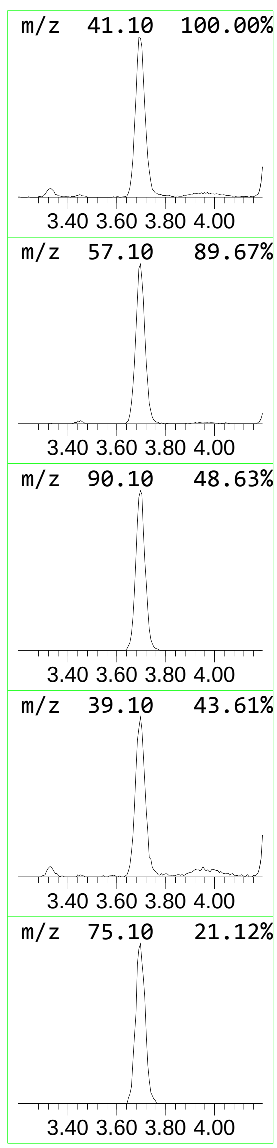
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Propanethiol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.697	32.39 ug/l	236057	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	64
2	Propanethial, S-oxide	90	C3H6OS	032157-29-2	47
3	1-Propene, 2-methyl-	56	C4H8	000115-11-7	38
4	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	32
5	Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	25





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Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On    : 05 Dec 2022  23:08
Operator  : JC/MD
Sample    : N5859-04
Misc      : 5.0mL/MSVOA_X/WATER
ALS Vial  : 31   Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title  : SW846 8260

TIC Library    : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P
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Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

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**********************************************************************
Peak Number  5  Butanal                          Concentration Rank  1

  R.T.     EstConc          Area       Relative to ISTD         R.T.
----------------------------------------------------------------------
  4.227   54.96 ug/l       400610   Pentafluorobenzene           5.556

 Hit# of  5    Tentative ID              MW  MolForm       CAS#       Qual
----------------------------------------------------------------------
 1 Butanal                               72 C4H8O         000123-72-8 94
 2 Ethene, ethoxy-                       72 C4H8O         000109-92-2 52
 3 Propanal, 2-methyl-                   72 C4H8O         000078-84-2 46
 4 1-Propene, 3-methoxy-                 72 C4H8O         000627-40-7 37
 5 Isobutylene epoxide                   72 C4H8O         000558-30-5 27
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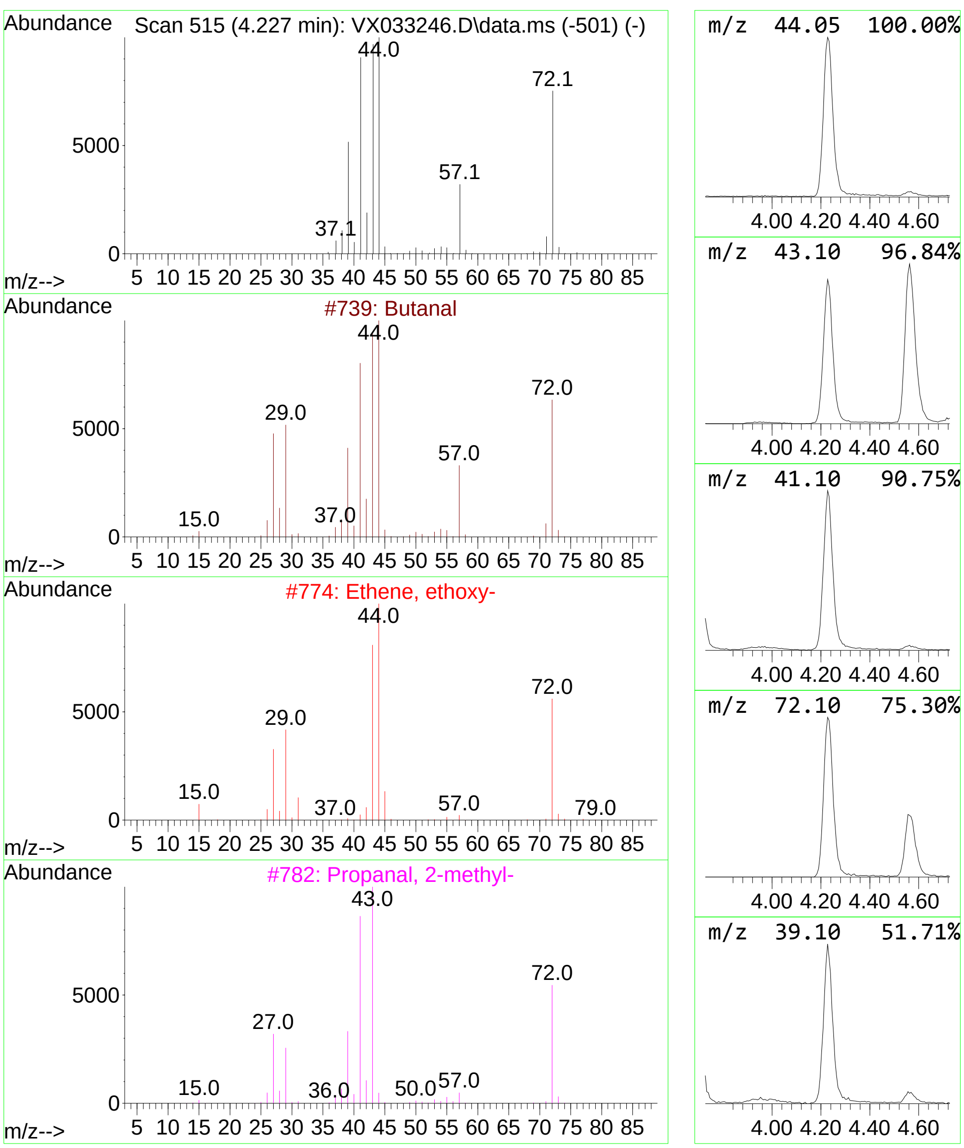


Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

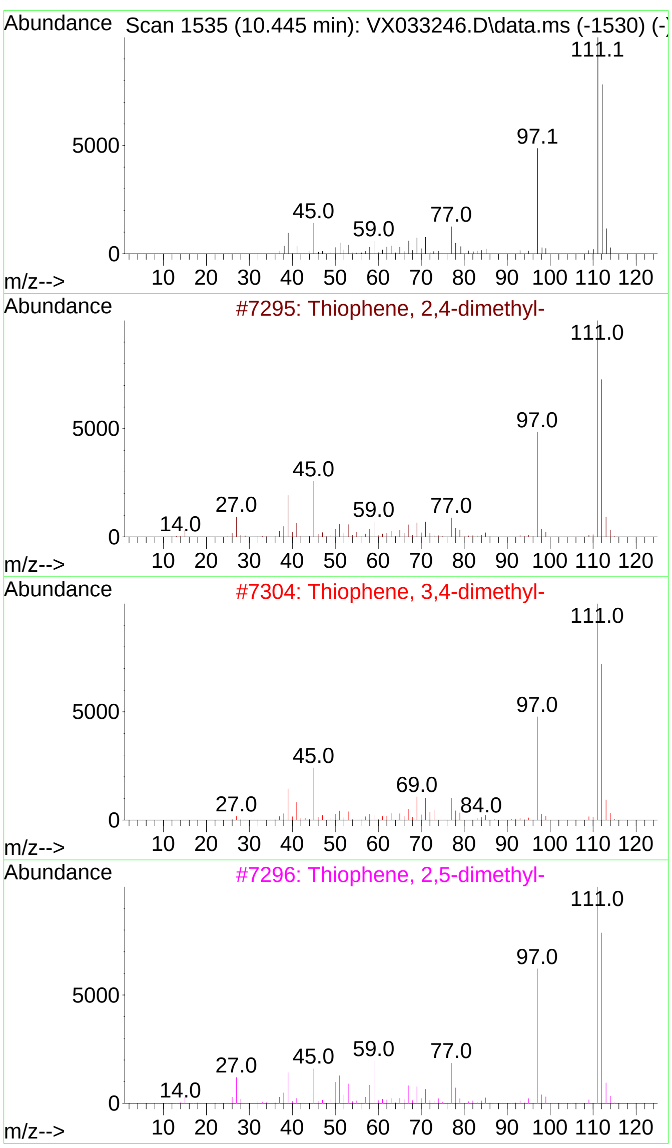
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

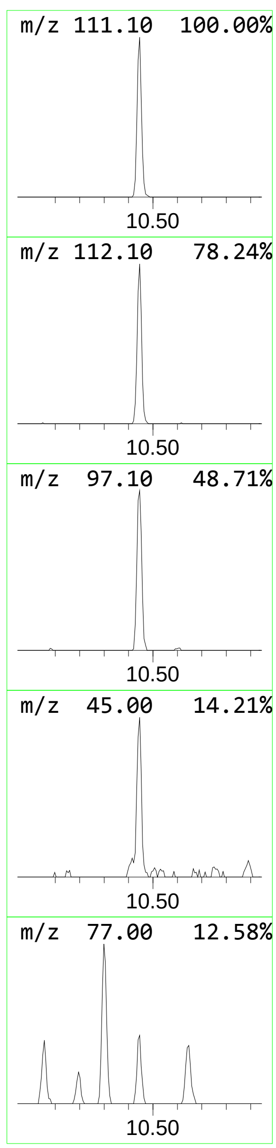
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Thiophene, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.445	5.70 ug/l	60978	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2,4-dimethyl-	112	C6H8S	000638-00-6	91
2	Thiophene, 3,4-dimethyl-	112	C6H8S	000632-15-5	90
3	Thiophene, 2,5-dimethyl-	112	C6H8S	000638-02-8	90
4	2-Thiophenecarboxaldehyde	112	C5H4OS	000098-03-3	45
5	3-Thiophenecarboxaldehyde	112	C5H4OS	000498-62-4	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033246.D
Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

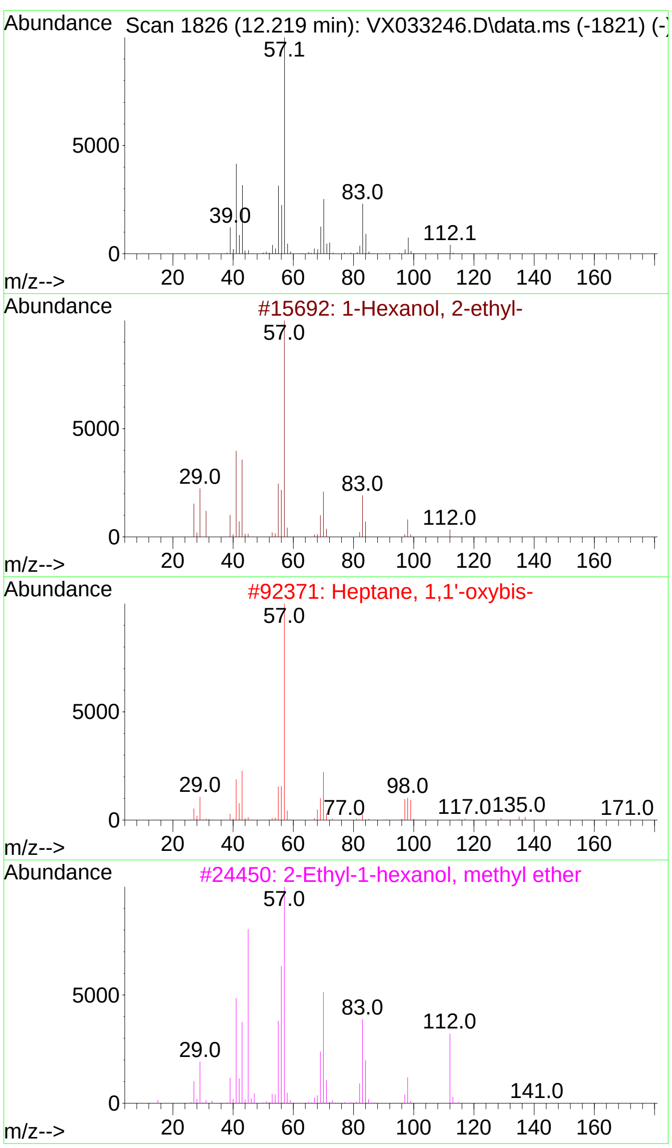
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

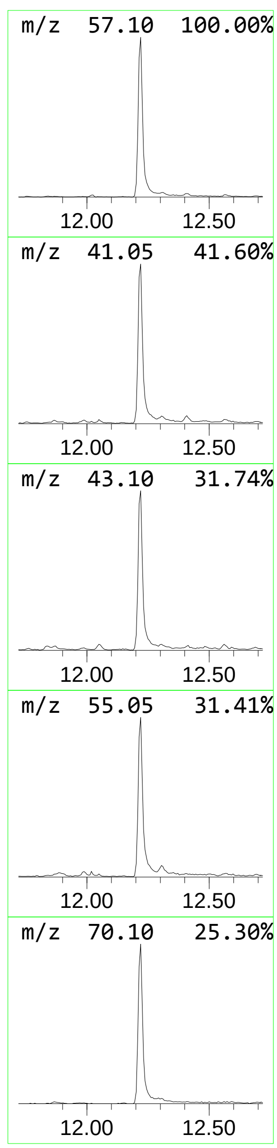
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	42.51 ug/l	457697	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45





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Acq On : 05 Dec 2022 23:08
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane	1.142	28.1	ug/l	204477	1	5.556	364444	50.0
Isobutane	1.264	5.5	ug/l	39692	1	5.556	364444	50.0
Butane	1.374	7.4	ug/l	53770	1	5.556	364444	50.0
2-Propanethiol,...	3.697	32.4	ug/l	236057	1	5.556	364444	50.0
Butanal	4.227	55.0	ug/l	400610	1	5.556	364444	50.0
Thiophene, 2,4-...	10.445	5.7	ug/l	60978	3	10.055	535126	50.0
1-Hexanol, 2-et...	12.219	42.5	ug/l	457697	4	12.024	538331	50.0