

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071723\
 Data File : VD076757.D
 Acq On : 17 Jul 2023 16:26
 Operator : KP/SY
 Sample : 03645-07
 Misc : 5.93G/5.0ml/MSVOA_D/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 DUP

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_D\Method\82D071423S.M
 Title : SW846 8260

Signal : TIC: VD076757.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.740	12	26	37	rBV	341827	684734	55.96%	7.369%
2	1.893	47	52	60	rVB	66048	84151	6.88%	0.906%
3	2.105	83	88	93	rBV	59534	77371	6.32%	0.833%
4	2.275	108	117	125	rVB	124351	192449	15.73%	2.071%
5	2.940	222	230	239	rBV	91372	193794	15.84%	2.086%
6	3.081	252	254	267	rVB3	6944	13010	1.06%	0.140%
7	3.293	277	290	300	rBV2	47284	103203	8.43%	1.111%
8	4.787	532	544	545	rBV2	31566	53705	4.39%	0.578%
9	5.322	628	635	636	rBV3	9195	14975	1.22%	0.161%
10	5.834	710	722	736	rBV2	79247	245074	20.03%	2.638%
11	6.881	890	900	910	rVB3	15470	47358	3.87%	0.510%
12	7.805	1048	1057	1062	rBV	159503	393060	32.12%	4.230%
13	7.875	1062	1069	1078	rVV	222534	537347	43.91%	5.783%
14	7.963	1078	1084	1089	rVB4	7339	16663	1.36%	0.179%
15	8.087	1098	1105	1111	rBV3	17323	38813	3.17%	0.418%
16	8.228	1121	1129	1141	rVB2	130186	319769	26.13%	3.442%
17	8.363	1146	1152	1160	rVV8	7631	18743	1.53%	0.202%
18	8.434	1160	1164	1169	rVV5	5994	12362	1.01%	0.133%
19	8.499	1169	1175	1184	rVB6	9144	22909	1.87%	0.247%
20	8.628	1190	1197	1210	rBV3	46059	97711	7.99%	1.052%
21	8.775	1214	1222	1236	rVV	394131	788957	64.48%	8.491%
22	9.269	1295	1306	1314	rBV2	68423	153844	12.57%	1.656%
23	9.546	1345	1353	1360	rVB3	5919	12750	1.04%	0.137%
24	9.904	1408	1414	1425	rVB5	22909	52529	4.29%	0.565%
25	10.046	1430	1438	1448	rVB6	15632	38310	3.13%	0.412%
26	10.269	1468	1476	1483	rBV	663938	1223607	100.00%	13.169%
27	10.334	1483	1487	1494	rVB	67451	124622	10.18%	1.341%
28	10.457	1499	1508	1515	rVB2	60432	107659	8.80%	1.159%
29	10.610	1529	1534	1540	rVB5	11775	21115	1.73%	0.227%
30	10.893	1577	1582	1588	rVB3	10244	16309	1.33%	0.176%
31	11.122	1614	1621	1627	rBV3	18980	36072	2.95%	0.388%
32	11.187	1627	1632	1636	rVB3	9175	14515	1.19%	0.156%
33	11.298	1645	1651	1656	rBV7	8149	15281	1.25%	0.164%
34	11.381	1656	1665	1671	rVV8	17793	43441	3.55%	0.468%
35	11.469	1675	1680	1689	rVB4	10867	21111	1.73%	0.227%
36	11.581	1689	1699	1710	rBV	599669	1028604	84.06%	11.070%

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Filtering: 5

Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	11.681	1710	1716	1725	rVV	14877	32942	2.69%	0.355%
38	11.793	1725	1735	1745	rVV3	93516	227577	18.60%	2.449%
39	11.863	1745	1747	1756	rVB4	9547	16169	1.32%	0.174%
40	12.122	1779	1791	1798	rBV5	25996	64454	5.27%	0.694%
41	12.334	1823	1827	1832	rVB4	12174	24325	1.99%	0.262%
42	12.575	1861	1868	1879	rVB	457046	751722	61.43%	8.090%
43	12.828	1904	1911	1913	rBV3	17094	27279	2.23%	0.294%
44	12.898	1917	1923	1929	rVV4	53811	101605	8.30%	1.094%
45	13.134	1958	1963	1969	rVB6	7384	12699	1.04%	0.137%
46	13.210	1971	1976	1982	rVV	51217	80357	6.57%	0.865%
47	13.404	2003	2009	2014	rBV7	7964	16229	1.33%	0.175%
48	13.516	2021	2028	2038	rBV	626050	999990	81.72%	10.762%
49	13.840	2078	2083	2089	rBV4	24556	41992	3.43%	0.452%
50	14.051	2114	2119	2126	rVB8	7611	15898	1.30%	0.171%
51	14.692	2223	2228	2234	rBV6	7627	12315	1.01%	0.133%

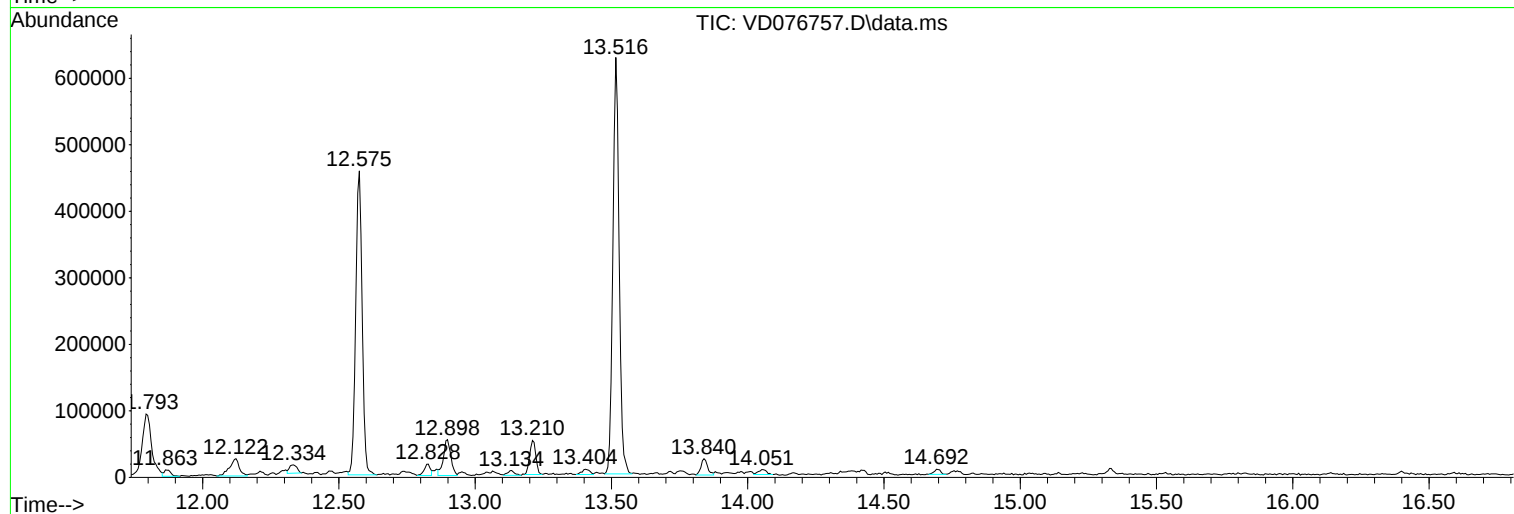
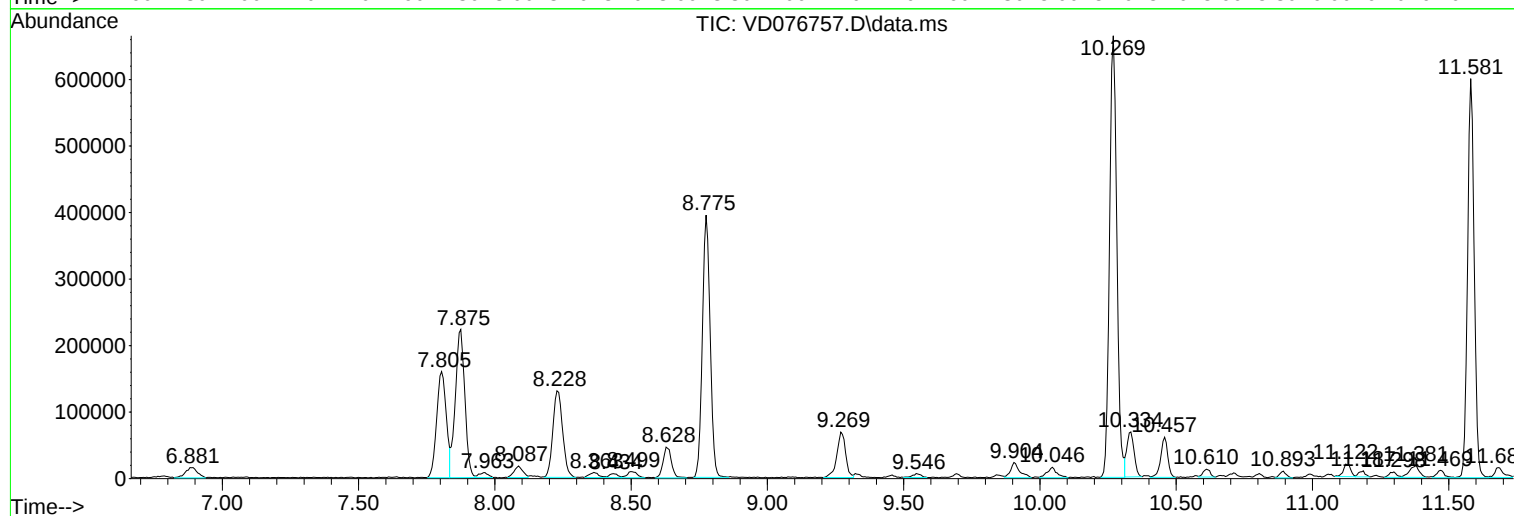
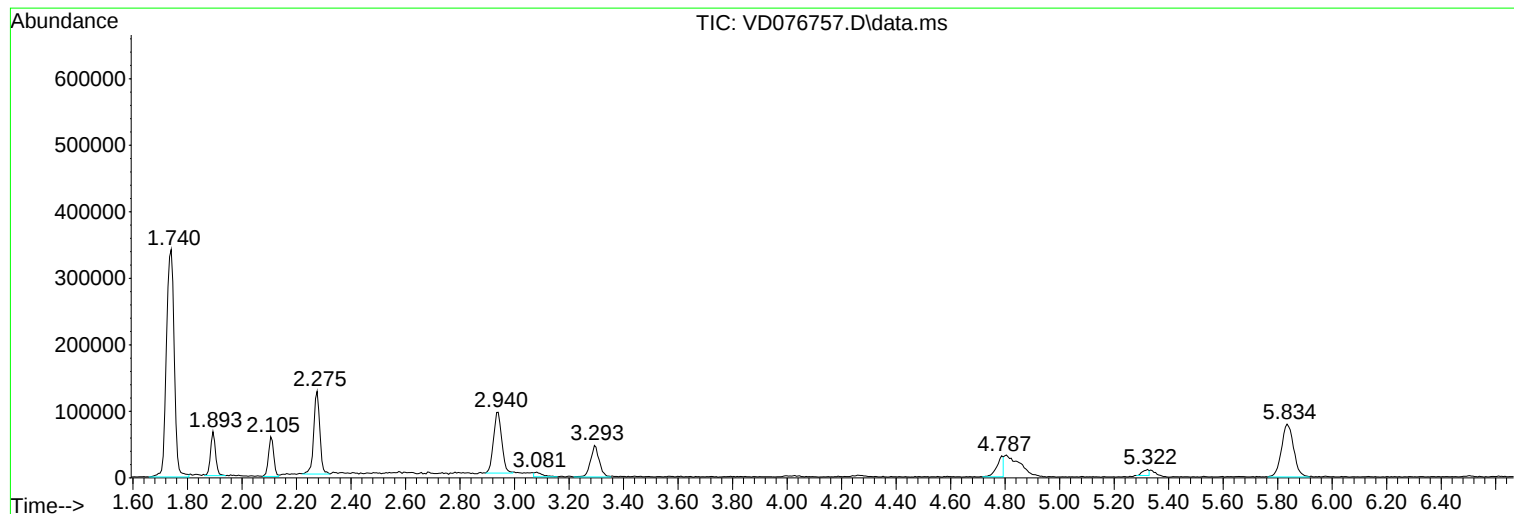
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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



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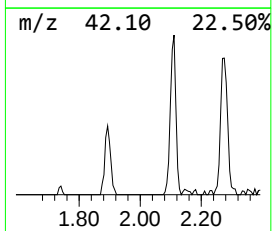
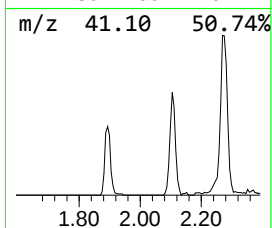
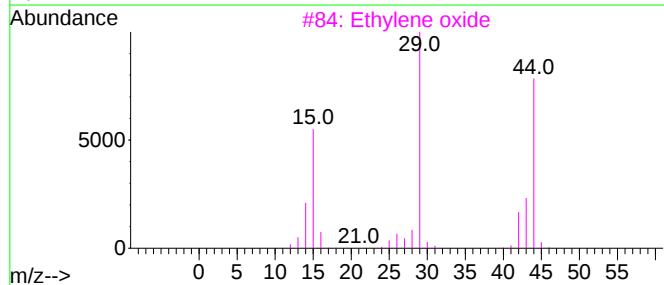
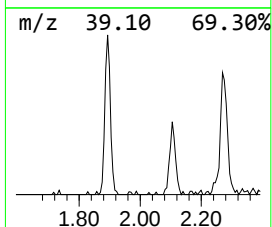
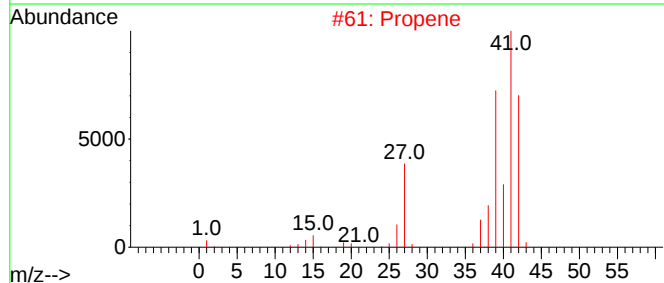
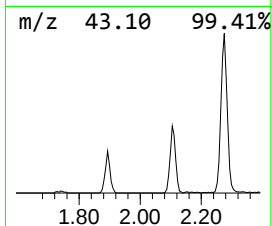
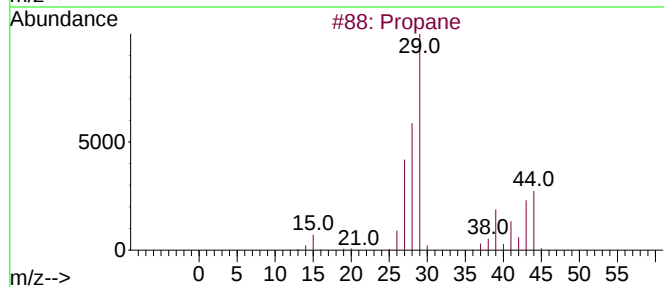
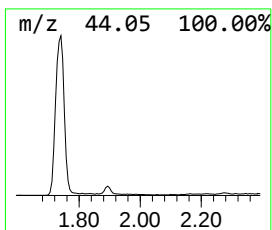
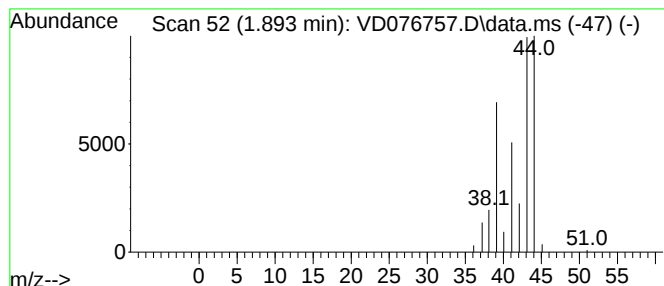
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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

Peak Number 2 Propane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.893	7.83 ug/l	84151	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			Propene	42	C3H6	000115-07-1	9
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Acetaldehyde	44	C2H4O	000075-07-0	5
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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Misc : 5.93G/5.0ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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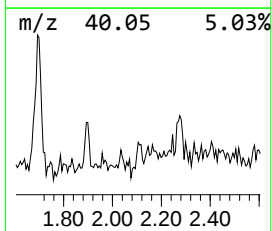
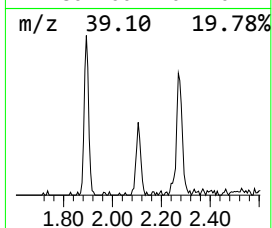
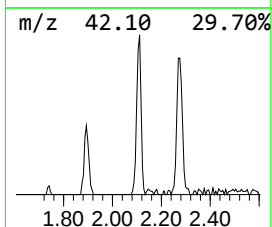
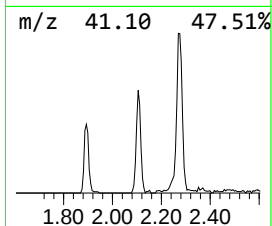
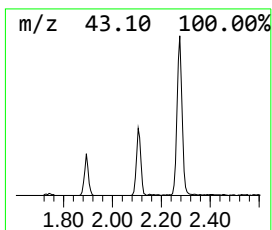
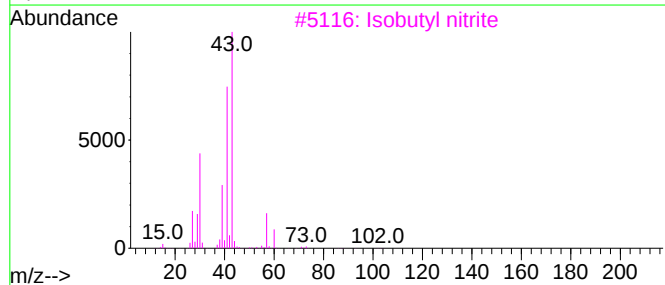
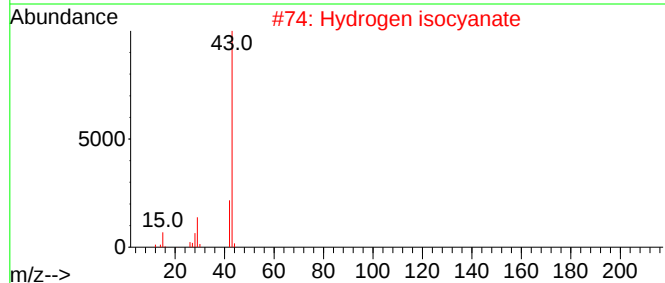
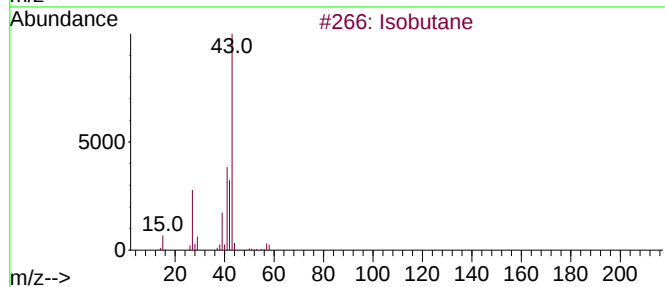
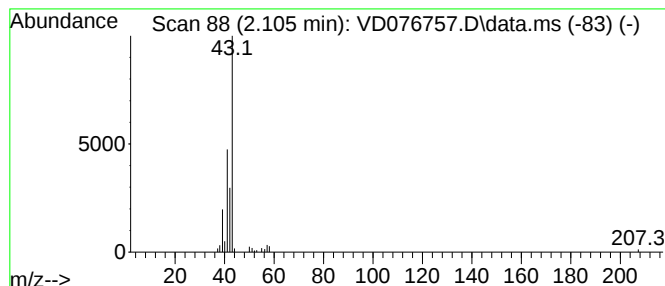
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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

Peak Number 3 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.105	7.20 ug/l	77371	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	64
2			Hydrogen isocyanate	43	CHNO	000075-13-8	4
3			Isobutyl nitrite	103	C4H9NO2	000542-56-3	4
4			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	4
5			Oxirane, trimethyl-	86	C5H10O	005076-19-7	4



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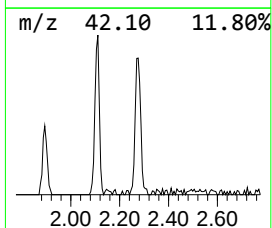
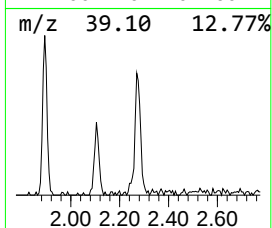
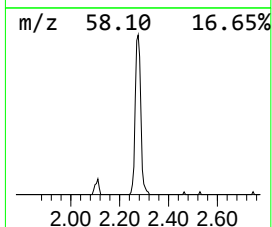
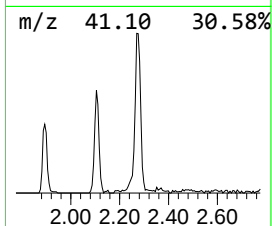
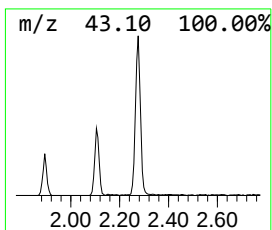
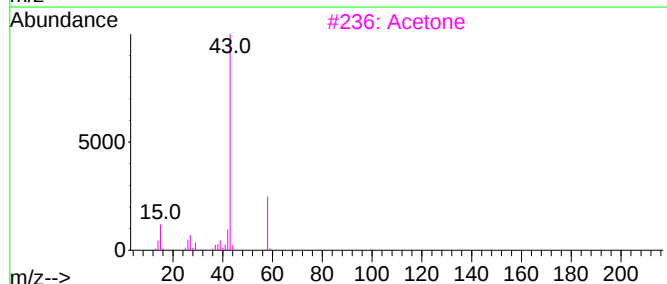
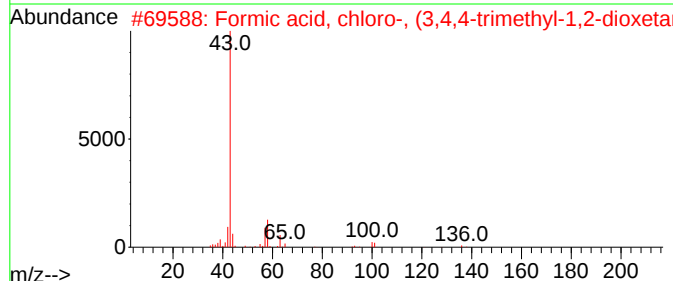
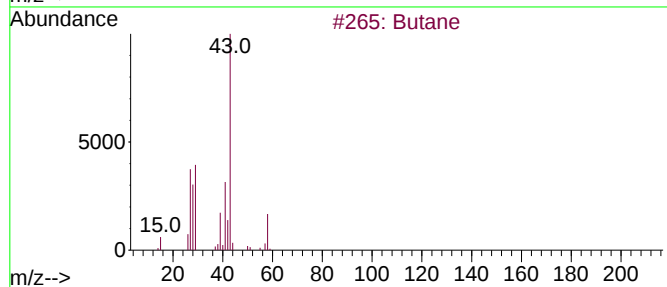
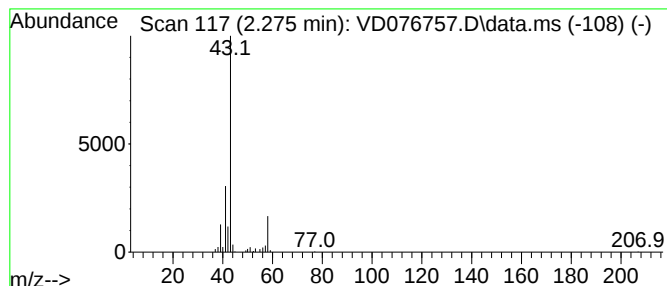
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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

Peak Number 4 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	17.91 ug/l	192449	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	39
3			Acetone	58	C3H6O	000067-64-1	9
4			Methyl glyoxal	72	C3H4O2	000078-98-8	9
5			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9



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Instrument :
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ClientSampleId :
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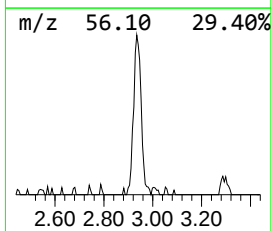
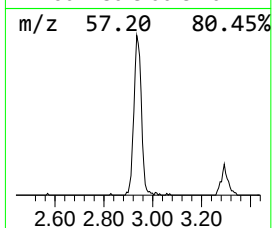
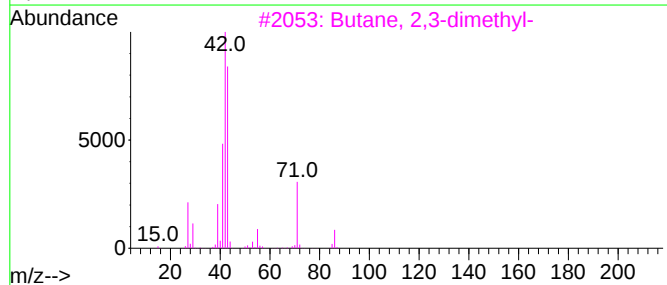
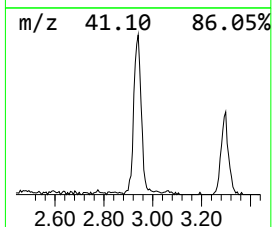
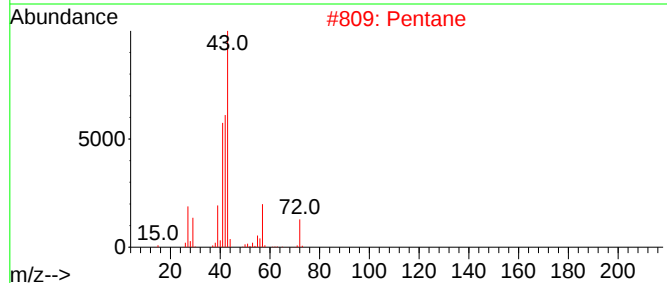
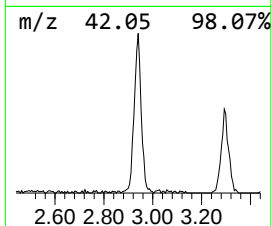
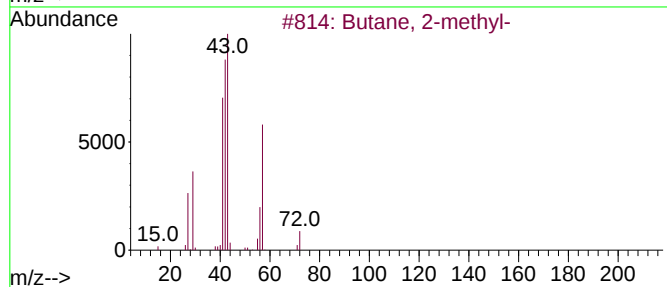
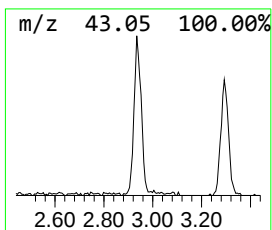
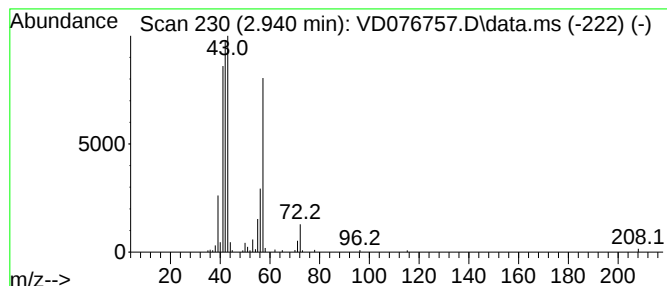
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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

Peak Number 5 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.940	18.03 ug/l	193794	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	38
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	28
4			Butane, 2-chloro-3-methyl-	106	C5H11Cl	000631-65-2	28
5			Butane, 1-isocyano-	83	C5H9N	002769-64-4	22



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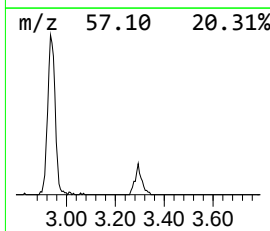
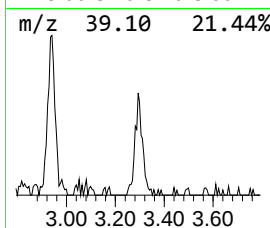
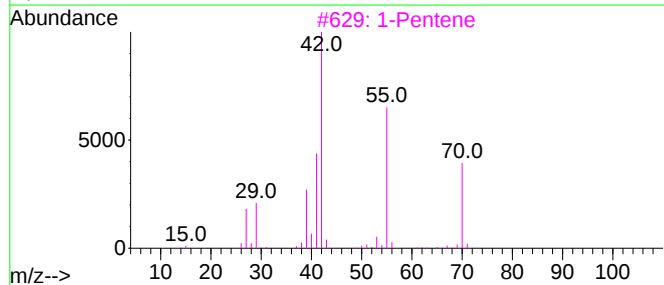
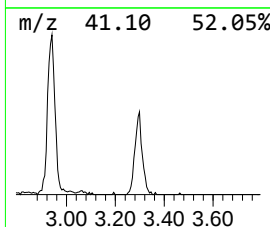
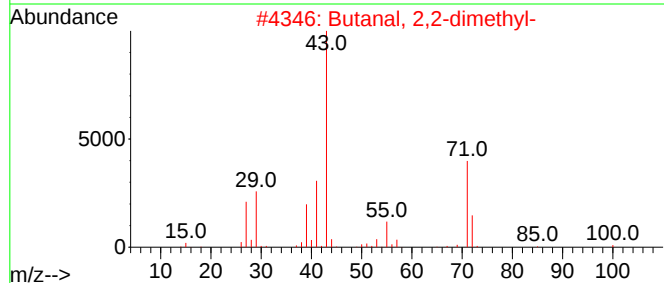
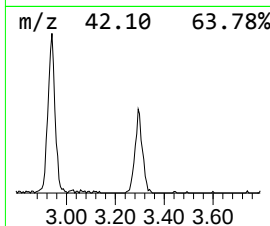
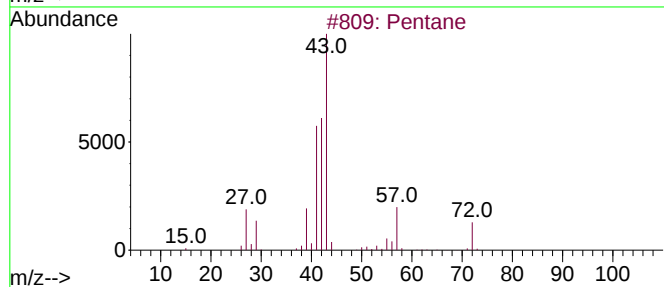
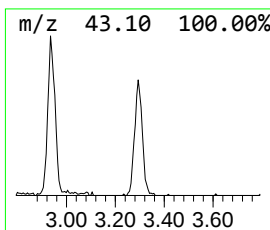
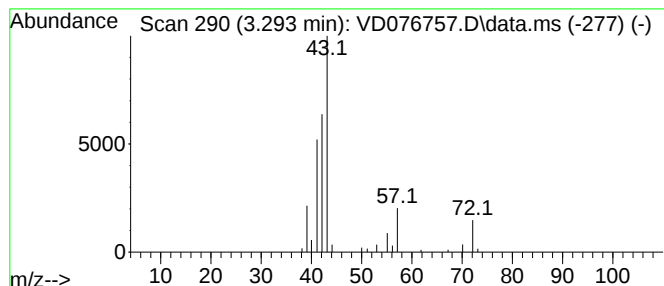
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Quant Title : SW846 8260

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

Peak Number 6 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.293	9.60 ug/l	103203	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	25
3			1-Pentene	70	C5H10	000109-67-1	17
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5			Butane, 2-methyl-	72	C5H12	000078-78-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071723\
Data File : VD076757.D
Acq On : 17 Jul 2023 16:26
Operator : KP/SY
Sample : 03645-07
Misc : 5.93G/5.0ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
DUP

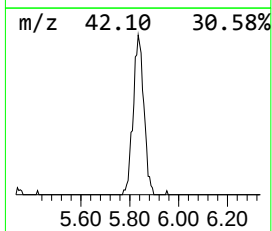
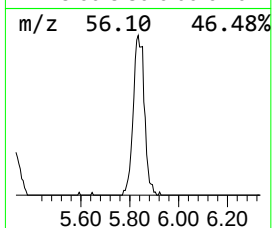
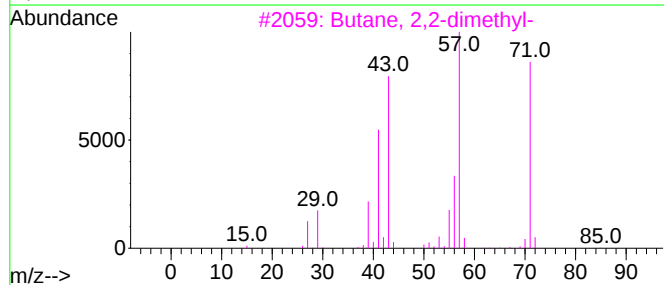
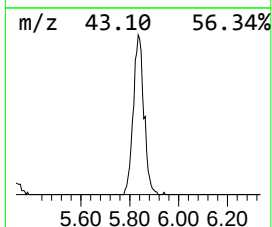
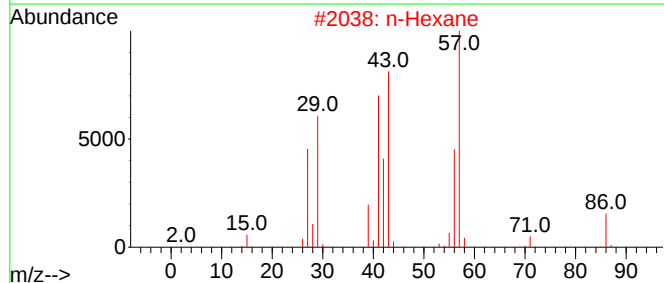
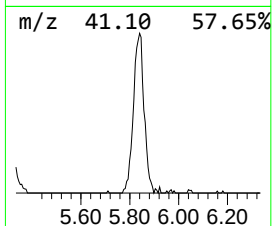
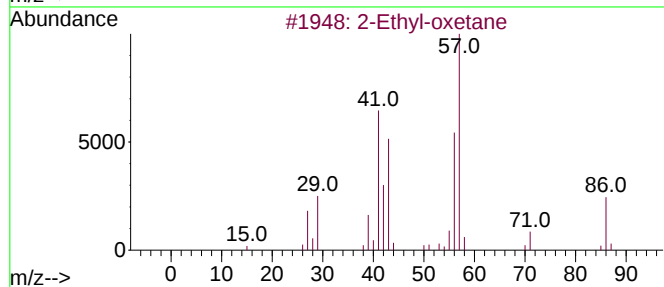
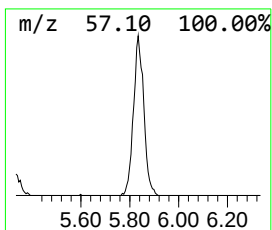
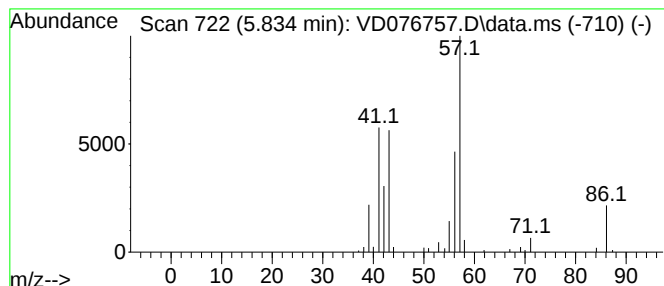
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Quant Title : SW846 8260

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

Peak Number 7 2-Ethyl-oxetane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	22.80 ug/l	245074	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	91
2			n-Hexane	86	C6H14	000110-54-3	83
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	32
4			Methane, isocyanato-	57	C2H3NO	000624-83-9	32
5			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071723\
Data File : VD076757.D
Acq On : 17 Jul 2023 16:26
Operator : KP/SY
Sample : 03645-07
Misc : 5.93G/5.0ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
DUP

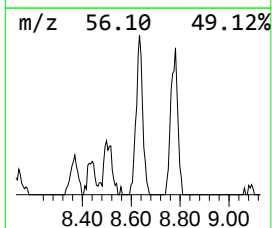
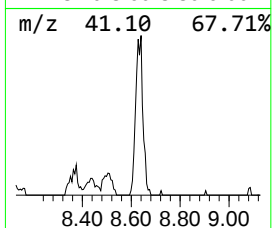
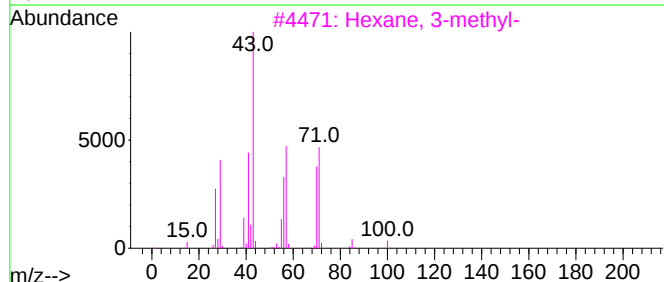
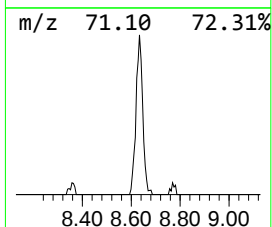
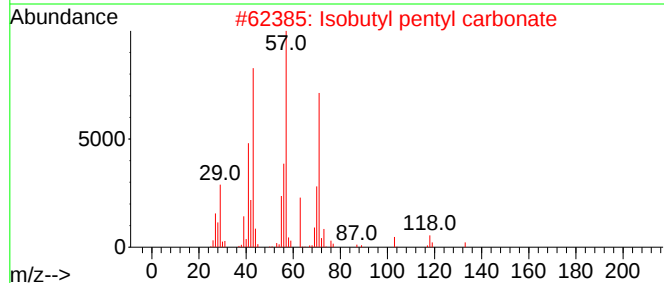
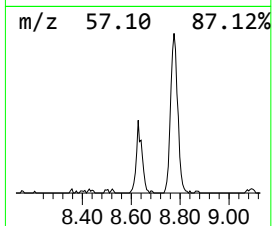
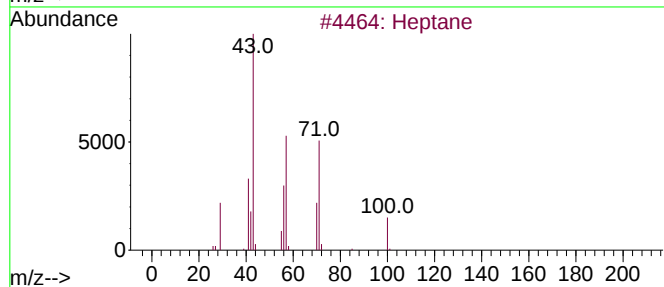
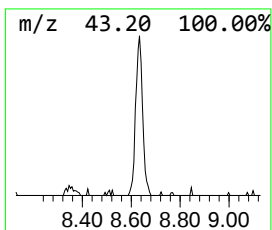
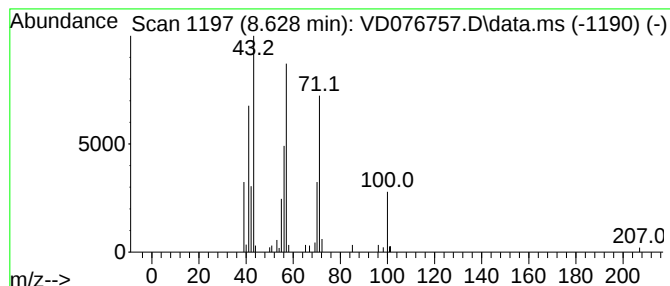
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Quant Title : SW846 8260

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

Peak Number 8 Heptane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.628	6.19 ug/l	97711	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	83
2			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	72
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
4			3-Hexanone	100	C6H12O	000589-38-8	49
5			Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071723\
Data File : VD076757.D
Acq On : 17 Jul 2023 16:26
Operator : KP/SY
Sample : 03645-07
Misc : 5.93G/5.0ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
DUP

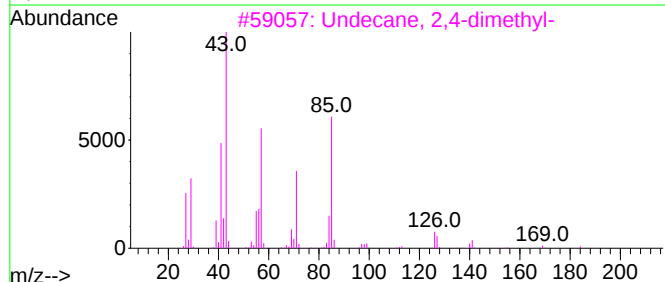
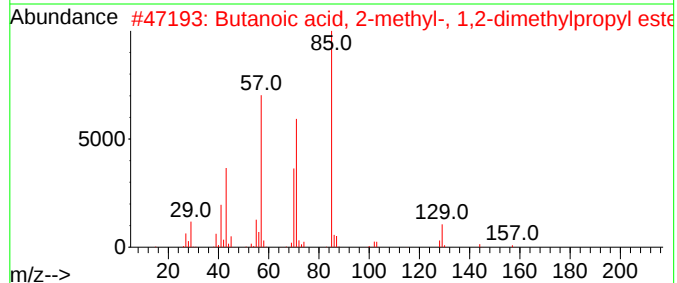
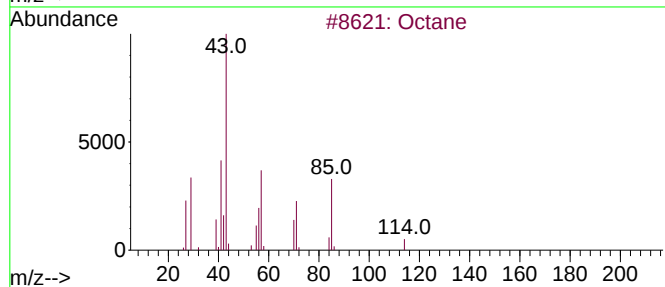
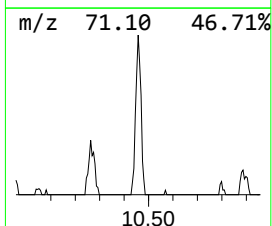
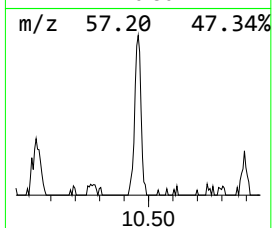
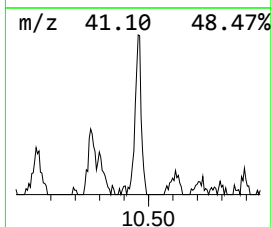
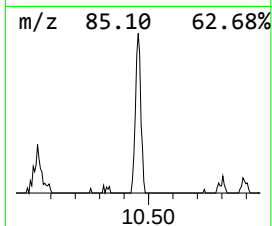
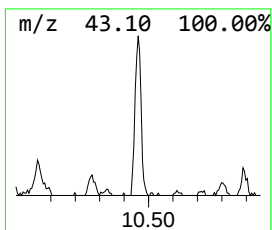
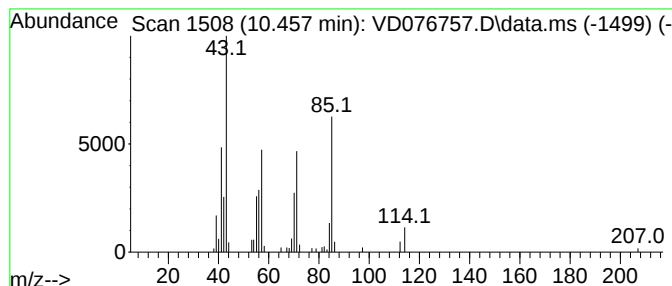
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Quant Title : SW846 8260

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

Peak Number 9 Octane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.457	5.23 ug/l	107659	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	90
2			Butanoic acid, 2-methyl-, 1,2-di...	172	C10H20O2	084696-83-3	50
3			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	50
4			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	47
5			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071723\
Data File : VD076757.D
Acq On : 17 Jul 2023 16:26
Operator : KP/SY
Sample : 03645-07
Misc : 5.93G/5.0ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
DUP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane	1.893	7.8	ug/l	84151	1	7.875	537347	50.0
Isobutane	2.105	7.2	ug/l	77371	1	7.875	537347	50.0
Butane	2.275	17.9	ug/l	192449	1	7.875	537347	50.0
Butane, 2-methyl-	2.940	18.0	ug/l	193794	1	7.875	537347	50.0
Pentane	3.293	9.6	ug/l	103203	1	7.875	537347	50.0
2-Ethyl-oxetane	5.834	22.8	ug/l	245074	1	7.875	537347	50.0
Heptane	8.628	6.2	ug/l	97711	2	8.775	788957	50.0
Octane	10.457	5.2	ug/l	107659	3	11.581	1028600	50.0