

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071823\
 Data File : VD076777.D
 Acq On : 18 Jul 2023 14:49
 Operator : KP/SY
 Sample : 03645-07
 Misc : 5.92G/5.0ml/MSVOA_D/SOIL
 ALS Vial : 14 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: VD076777.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	386299	743527	62.69%	8.918%
2	1.893	45	52	58	rBV	57462	73194	6.17%	0.878%
3	2.105	82	88	93	rBV	46596	62147	5.24%	0.745%
4	2.275	109	117	125	rBV	106785	154034	12.99%	1.848%
5	2.934	221	229	238	rBV2	71883	156062	13.16%	1.872%
6	3.299	282	291	300	rVB2	35283	78545	6.62%	0.942%
7	4.799	535	546	569	rVB8	38282	175054	14.76%	2.100%
8	5.322	625	635	646	rBV6	8088	27894	2.35%	0.335%
9	5.834	710	722	734	rBV4	42487	134833	11.37%	1.617%
10	6.887	891	901	910	rVB4	11866	34539	2.91%	0.414%
11	7.804	1046	1057	1062	rBV2	153118	377796	31.85%	4.532%
12	7.875	1062	1069	1078	rVB	205697	487514	41.11%	5.848%
13	8.087	1098	1105	1112	rBV4	12796	27554	2.32%	0.330%
14	8.234	1120	1130	1140	rBV3	125753	300746	25.36%	3.607%
15	8.357	1144	1151	1159	rVV6	5959	13496	1.14%	0.162%
16	8.504	1171	1176	1182	rVB4	6603	14027	1.18%	0.168%
17	8.634	1190	1198	1205	rBV3	33761	69290	5.84%	0.831%
18	8.775	1212	1222	1235	rBV	376226	781911	65.93%	9.379%
19	9.269	1296	1306	1314	rBV2	53297	118037	9.95%	1.416%
20	9.904	1408	1414	1421	rBV3	13433	26671	2.25%	0.320%
21	10.046	1428	1438	1447	rVB5	10245	28212	2.38%	0.338%
22	10.269	1468	1476	1482	rBV	644408	1186021	100.00%	14.226%
23	10.334	1482	1487	1493	rVB	66208	123962	10.45%	1.487%
24	10.457	1500	1508	1514	rVB3	41265	76085	6.42%	0.913%
25	10.610	1530	1534	1539	rBV5	10491	15315	1.29%	0.184%
26	11.128	1617	1622	1626	rBV3	13364	21730	1.83%	0.261%
27	11.375	1655	1664	1674	rVB6	13872	35618	3.00%	0.427%
28	11.469	1674	1680	1684	rBV5	7328	13589	1.15%	0.163%
29	11.581	1691	1699	1711	rBV	555391	945390	79.71%	11.340%
30	11.687	1711	1717	1725	rVV3	12889	26003	2.19%	0.312%
31	11.792	1725	1735	1745	rVV3	81056	182369	15.38%	2.187%
32	12.122	1780	1791	1798	rBV3	22771	53423	4.50%	0.641%
33	12.328	1822	1826	1831	rVB5	9748	18254	1.54%	0.219%
34	12.575	1860	1868	1877	rVB	399779	660544	55.69%	7.923%
35	12.828	1905	1911	1914	rBV2	13907	23112	1.95%	0.277%
36	12.898	1918	1923	1929	rVV4	40286	75422	6.36%	0.905%

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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

37	13.210	1970	1976	1983	rVB2	42639	70551	5.95%	0.846%
38	13.398	2003	2008	2016	rBV8	6040	14636	1.23%	0.176%
39	13.516	2020	2028	2038	rVB	540215	883491	74.49%	10.597%
40	13.839	2077	2083	2087	rBV5	16872	26469	2.23%	0.317%

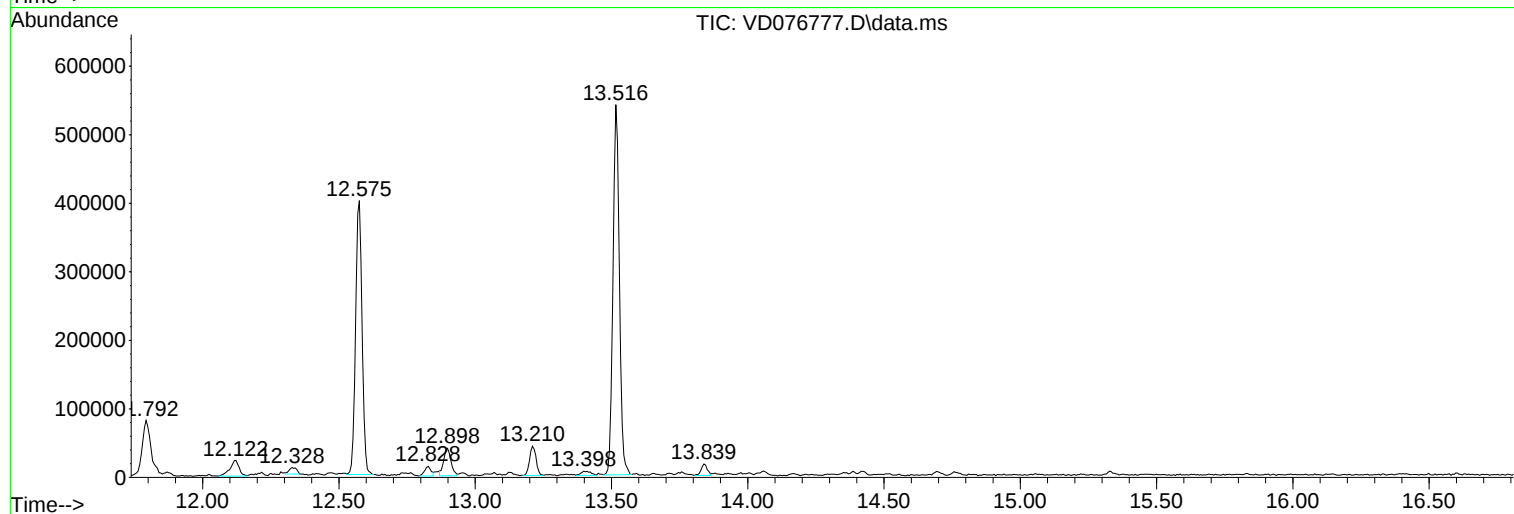
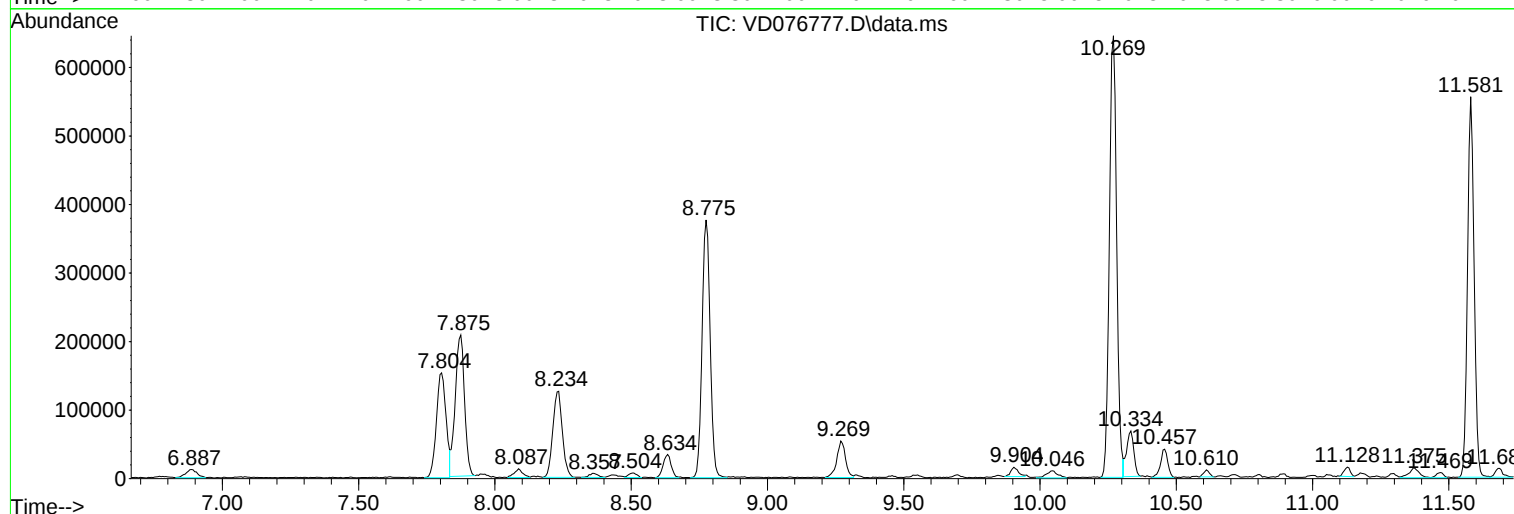
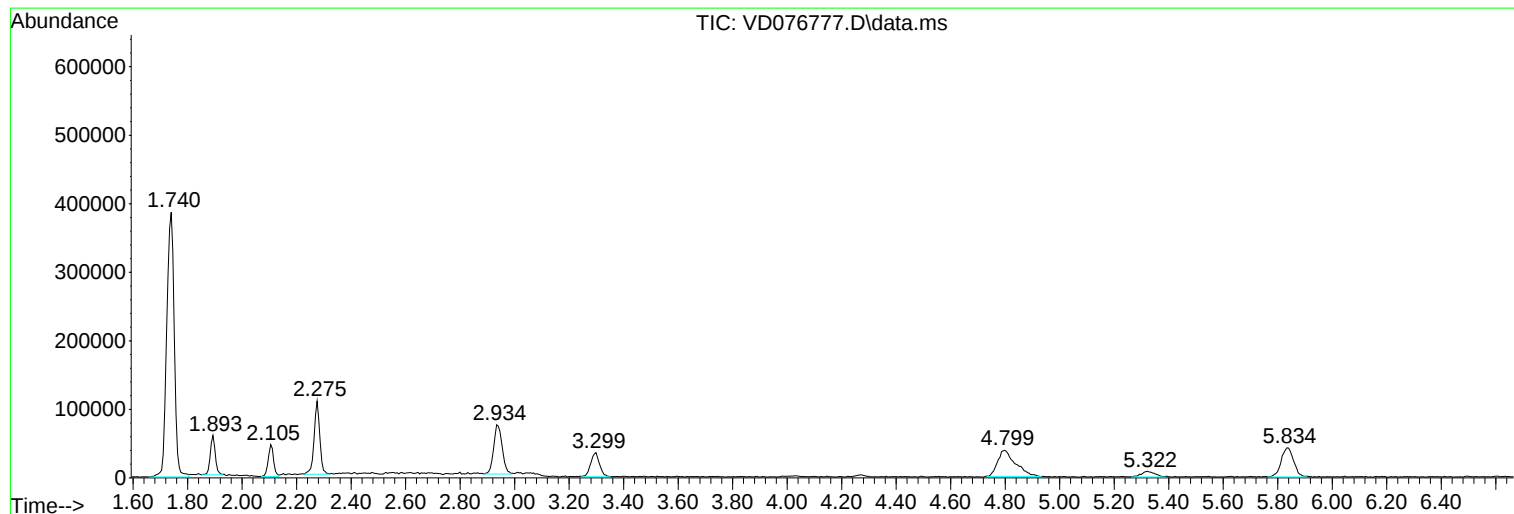
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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



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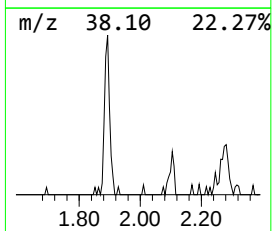
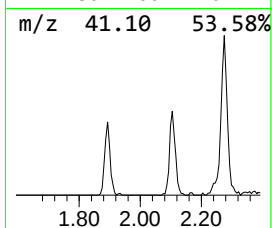
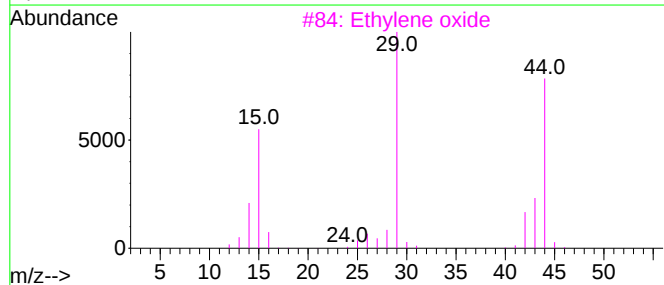
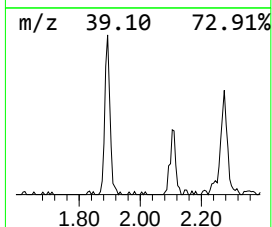
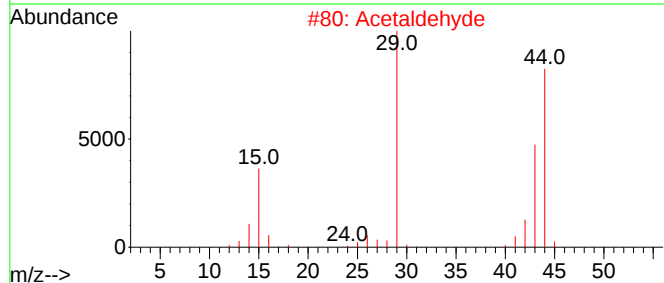
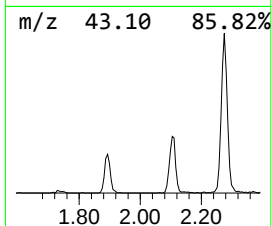
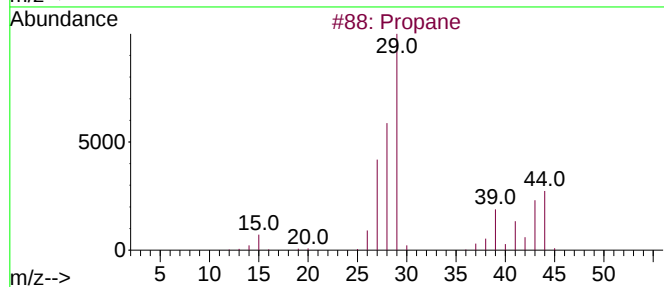
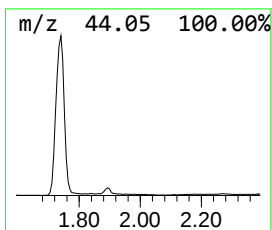
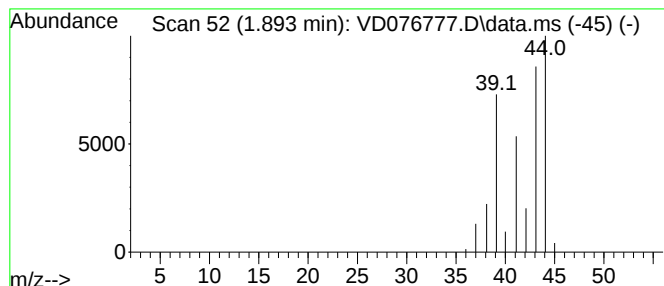
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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

Peak Number 2 Propane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.893	7.51 ug/l	73194	Pentafluorobenzene	7.875

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



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
DUP

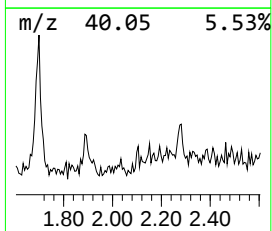
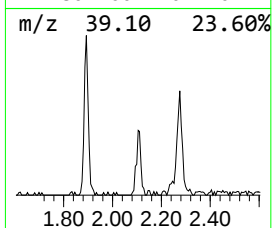
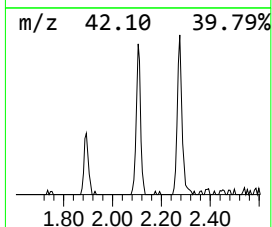
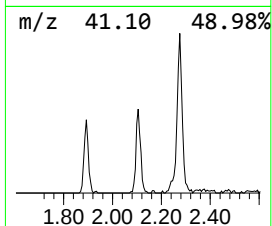
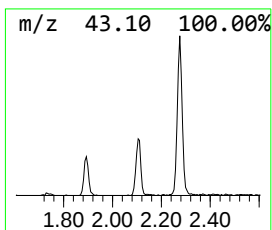
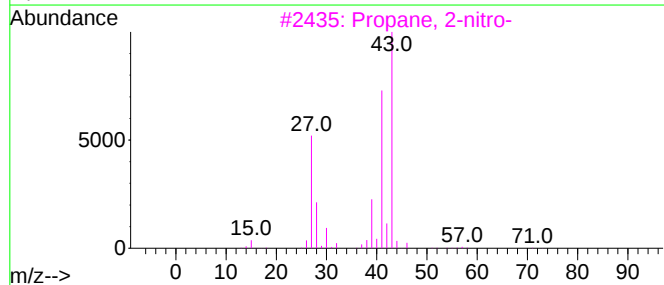
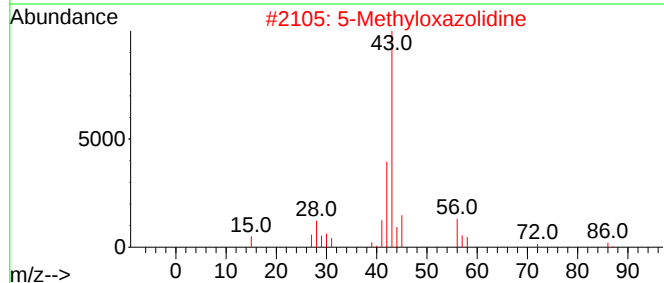
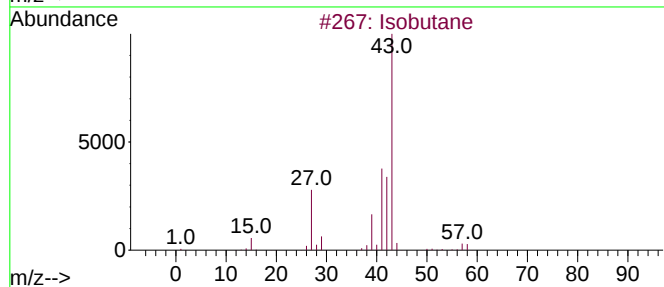
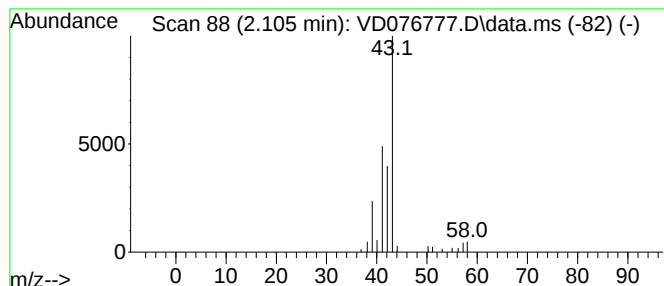
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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

Peak Number 3 Isobutane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.105	6.37 ug/l	62147	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	72
2			5-Methyloxazolidine	87	C4H9NO	058328-22-6	4
3			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
4			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4
5			Hydrogen azide	43	HN3	007782-79-8	2



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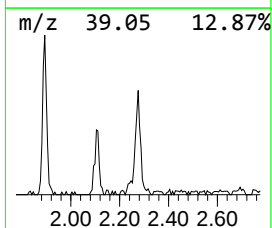
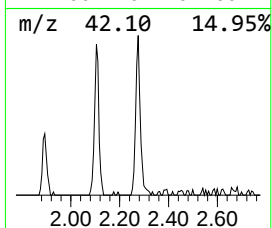
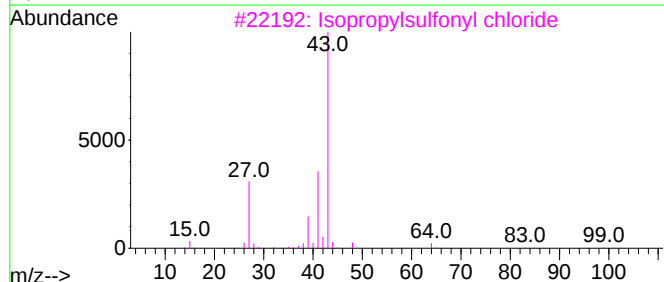
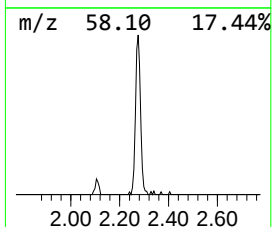
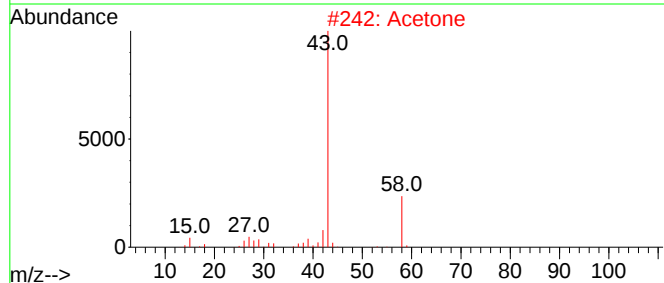
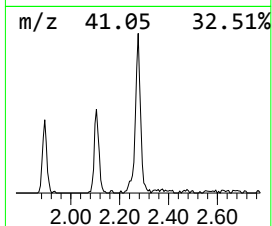
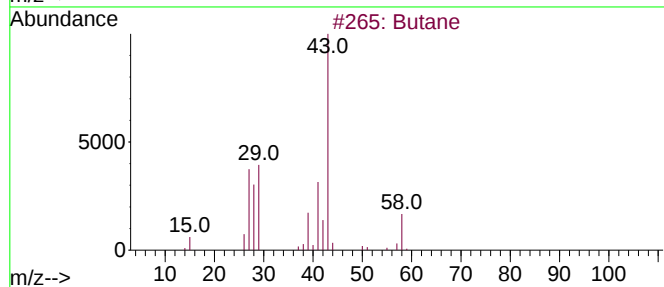
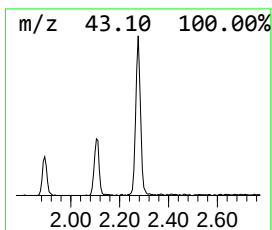
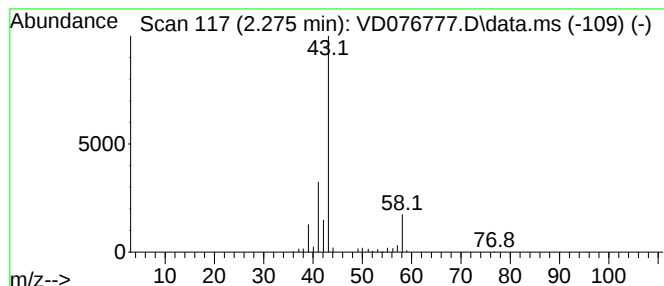
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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	15.80 ug/l	154034	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	64
2			Acetone	58	C3H6O	000067-64-1	9
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Methyl glyoxal	72	C3H4O2	000078-98-8	9
5			Isobutane	58	C4H10	000075-28-5	5



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Misc : 5.92G/5.0ml/MSVOA_D/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
DUP

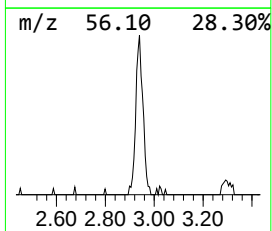
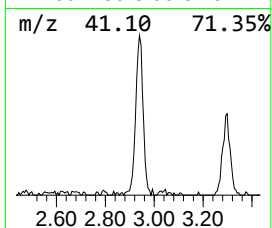
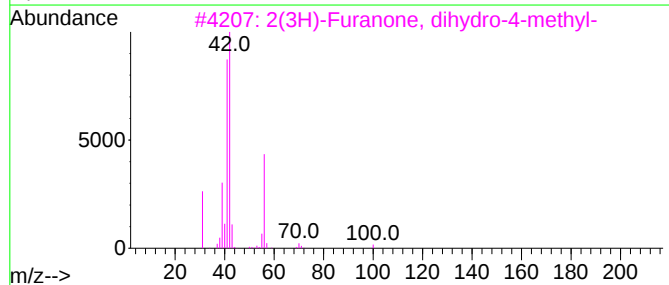
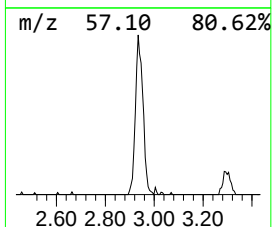
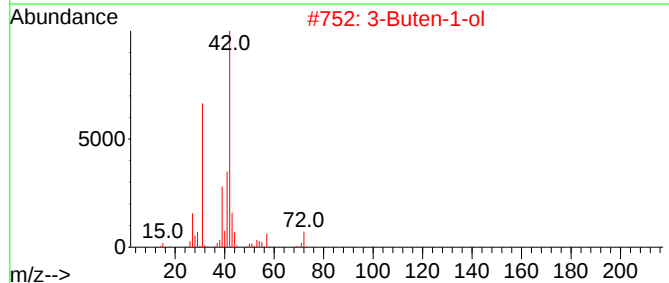
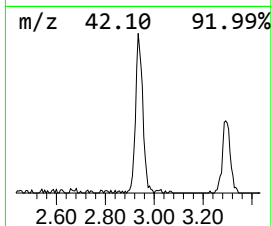
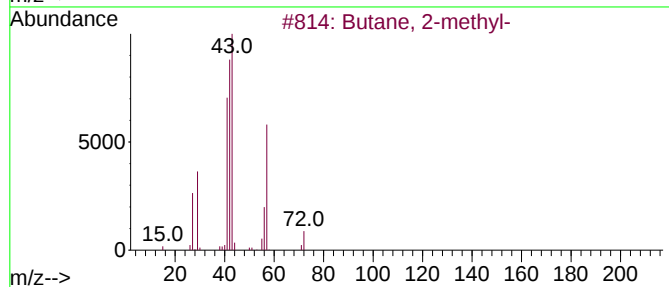
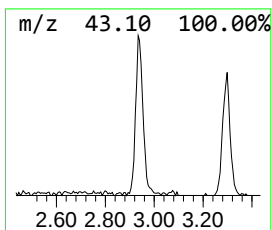
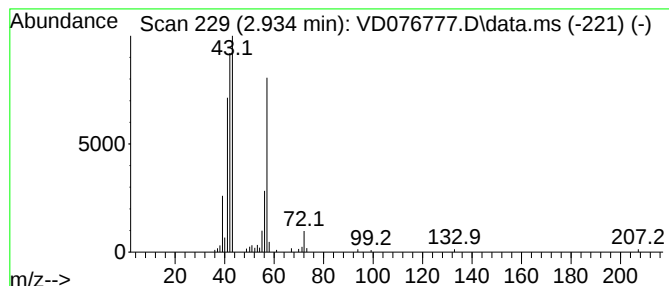
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

TIC Library : C:\Database\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.
2.934	16.01 ug/l	156062	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
4			Pentane	72	C5H12	000109-66-0	28
5			Butane, 1-isocyano-	83	C5H9N	002769-64-4	10



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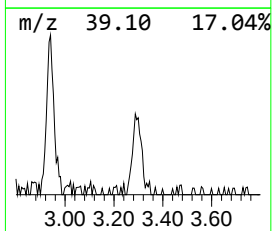
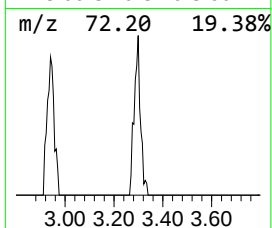
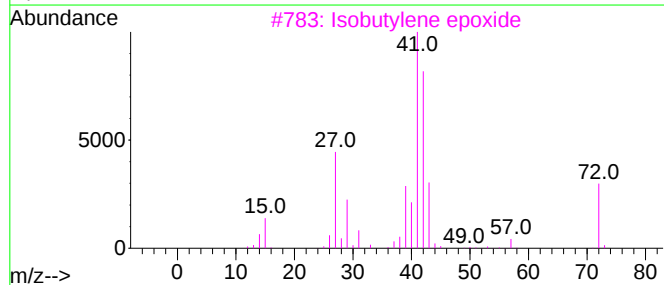
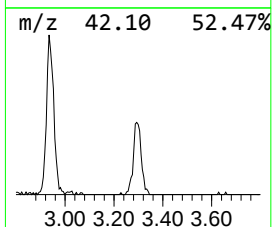
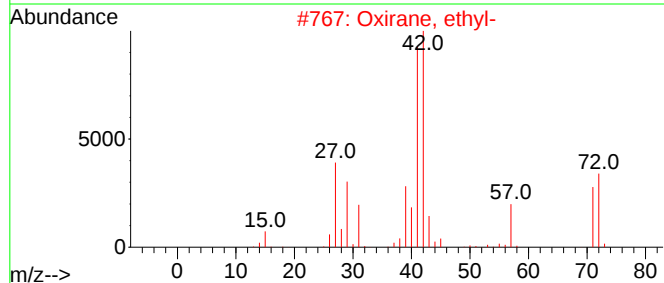
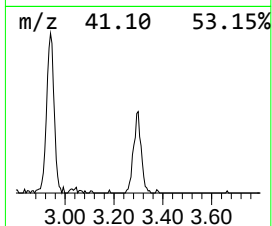
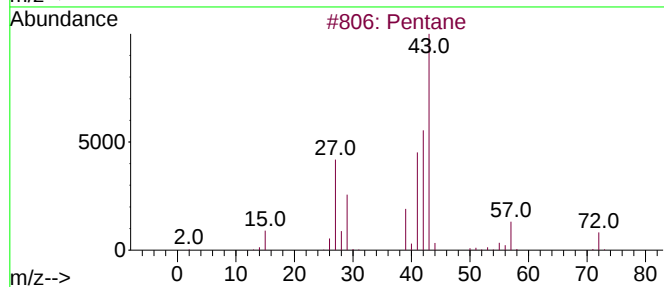
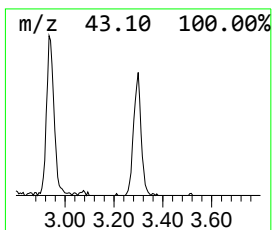
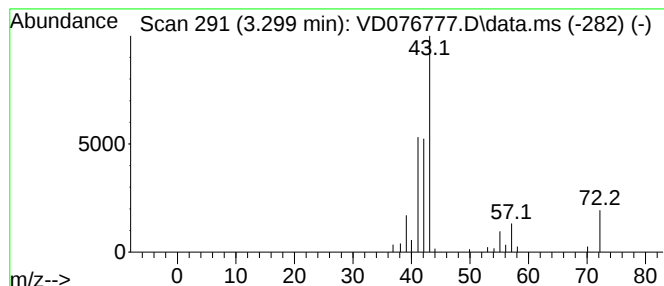
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071423S.M
Quant Title : SW846 8260

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

Peak Number 6 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.299	8.06 ug/l	78545	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	64
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3			Isobutylene epoxide	72	C4H8O	000558-30-5	50
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5			Butanal	72	C4H8O	000123-72-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071823\
Data File : VD076777.D
Acq On : 18 Jul 2023 14:49
Operator : KP/SY
Sample : 03645-07
Misc : 5.92G/5.0ml/MSVOA_D/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
DUP

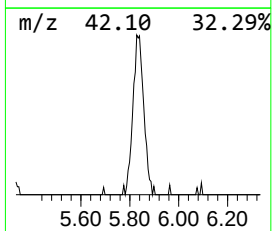
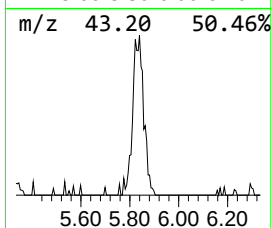
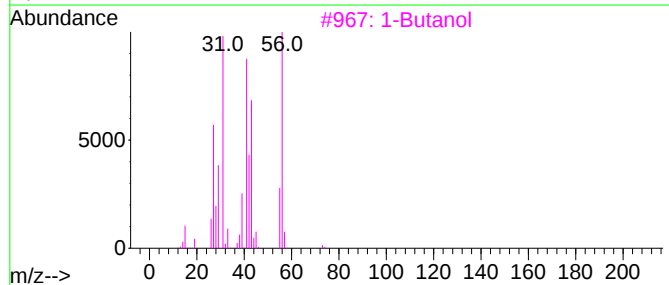
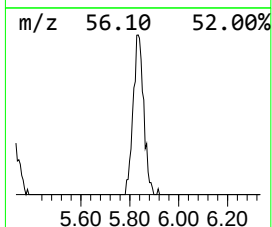
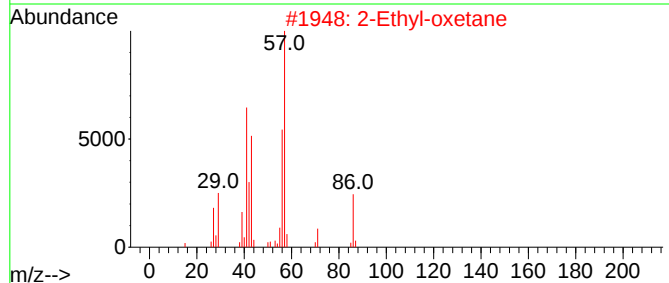
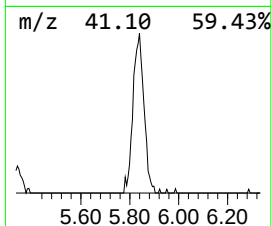
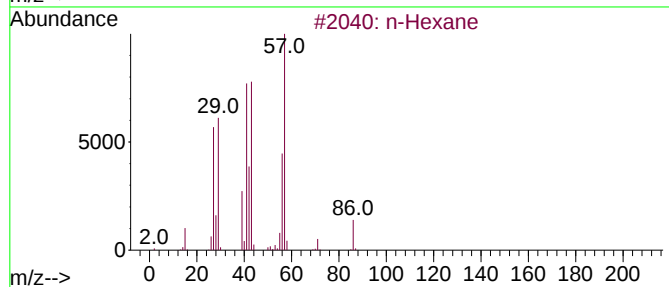
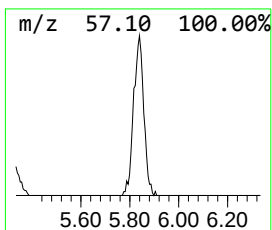
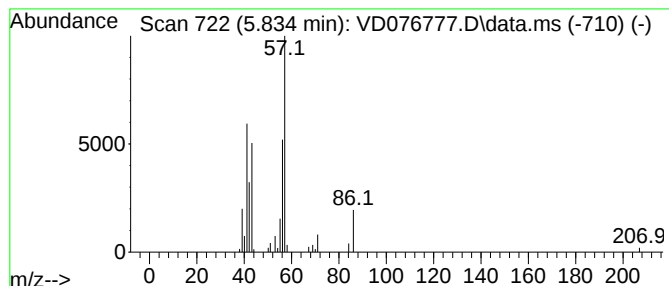
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Quant Title : SW846 8260

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

Peak Number 8 n-Hexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	13.83 ug/l	134833	Pentafluorobenzene	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	72
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	56
3			1-Butanol	74	C4H10O	000071-36-3	37
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	37
5			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071823\
Data File : VD076777.D
Acq On : 18 Jul 2023 14:49
Operator : KP/SY
Sample : 03645-07
Misc : 5.92G/5.0ml/MSVOA_D/SOIL
ALS Vial : 14 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	7.5	ug/l	73194	1	7.875	487514	50.0
Isobutane	2.105	6.4	ug/l	62147	1	7.875	487514	50.0
Butane	2.275	15.8	ug/l	154034	1	7.875	487514	50.0
Butane, 2-methyl-	2.934	16.0	ug/l	156062	1	7.875	487514	50.0
Pentane	3.299	8.1	ug/l	78545	1	7.875	487514	50.0
n-Hexane	5.834	13.8	ug/l	134833	1	7.875	487514	50.0