

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081823\
 Data File : VY015194.D
 Acq On : 18 Aug 2023 14:37
 Operator : SY/MD
 Sample : 04086-05
 Misc : 5.06g/5.2mL/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 B-PP09A

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_Y\methods\82Y081423S.M
 Title : SW846 8260

Signal : TIC: VY015194.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.071	32	41	55	rBV	60945	90663	3.08%	0.355%
2	2.241	61	69	79	rBV	106919	174055	5.91%	0.682%
3	2.894	166	176	197	rBV	1344148	2942767	100.00%	11.529%
4	3.241	223	233	252	rBV	445150	1036903	35.24%	4.062%
5	3.686	297	306	320	rVB	38358	96753	3.29%	0.379%
6	3.930	334	346	364	rBV3	42927	147736	5.02%	0.579%
7	4.759	457	482	509	rBV	464297	2341152	79.56%	9.172%
8	5.235	543	560	585	rBV	323975	1162477	39.50%	4.554%
9	5.741	630	643	661	rBV	198667	619521	21.05%	2.427%
10	6.094	682	701	714	rBV	32879	110710	3.76%	0.434%
11	6.228	714	723	735	rVV4	16745	51619	1.75%	0.202%
12	6.533	759	773	785	rBV4	42111	135898	4.62%	0.532%
13	6.679	785	797	805	rBV2	63695	199375	6.78%	0.781%
14	6.789	805	815	826	rVV	240168	720244	24.48%	2.822%
15	6.978	836	846	864	rVB	51254	161159	5.48%	0.631%
16	7.521	929	935	946	rVB2	28612	77541	2.63%	0.304%
17	7.716	956	967	969	rBV	102725	225191	7.65%	0.882%
18	7.777	969	977	985	rVV5	305681	978962	33.27%	3.835%
19	7.868	985	992	1003	rVB	144760	369561	12.56%	1.448%
20	7.996	1003	1013	1021	rBV	238787	560253	19.04%	2.195%
21	8.137	1028	1036	1047	rVB2	116980	283834	9.65%	1.112%
22	8.271	1049	1058	1061	rVV2	109909	249270	8.47%	0.977%
23	8.326	1061	1067	1076	rVV2	224966	686853	23.34%	2.691%
24	8.411	1076	1081	1092	rVB2	61176	142213	4.83%	0.557%
25	8.545	1092	1103	1115	rVB	96424	216468	7.36%	0.848%
26	8.685	1117	1126	1138	rBV	327683	721057	24.50%	2.825%
27	8.844	1147	1152	1159	rVV	16001	30940	1.05%	0.121%
28	8.966	1168	1172	1186	rVB2	18088	49263	1.67%	0.193%
29	9.179	1193	1207	1213	rBV3	192448	524246	17.81%	2.054%
30	9.240	1213	1217	1224	rVV2	50951	95222	3.24%	0.373%
31	9.368	1233	1238	1244	rVV2	43562	82347	2.80%	0.323%
32	9.459	1244	1253	1260	rVB5	20992	54804	1.86%	0.215%
33	9.612	1270	1278	1288	rVB	126342	246032	8.36%	0.964%
34	9.746	1288	1300	1307	rBV2	162587	403942	13.73%	1.583%
35	9.819	1307	1312	1315	rBV	37955	67557	2.30%	0.265%
36	9.953	1324	1334	1346	rBV	60769	167878	5.70%	0.658%

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37	10.106	1354	1359	1364	rVB4	17976	36801	1.25%	0.144%
38	10.179	1364	1371	1375	rBV	455888	793283	26.96%	3.108%
39	10.240	1375	1381	1388	rVB	1672542	2832532	96.25%	11.097%
40	10.368	1394	1402	1408	rVB4	34040	86496	2.94%	0.339%
41	10.606	1431	1441	1452	rVB7	25564	85095	2.89%	0.333%
42	11.490	1578	1586	1593	rVV	433601	696751	23.68%	2.730%
43	11.593	1595	1603	1612	rVV	208991	339888	11.55%	1.332%
44	11.697	1612	1620	1632	rVV	672757	1197092	40.68%	4.690%
45	12.026	1663	1674	1682	rBV	289726	445033	15.12%	1.744%
46	12.325	1715	1723	1729	rBV	42146	64536	2.19%	0.253%
47	12.477	1741	1748	1759	rVB	361338	588134	19.99%	2.304%
48	12.672	1773	1780	1785	rBV	104543	162251	5.51%	0.636%
49	12.733	1785	1790	1793	rVV	137512	207755	7.06%	0.814%
50	12.764	1793	1795	1799	rVV	67482	92165	3.13%	0.361%
51	12.813	1799	1803	1814	rVB	71513	106253	3.61%	0.416%
52	12.971	1822	1829	1837	rVB	68750	108284	3.68%	0.424%
53	13.117	1846	1853	1860	rBV	184171	267694	9.10%	1.049%
54	13.422	1897	1903	1916	rVB2	469013	858938	29.19%	3.365%
55	13.623	1933	1936	1940	rVV2	51403	79871	2.71%	0.313%
56	13.666	1940	1943	1953	rVB3	20554	46795	1.59%	0.183%
57	13.971	1987	1993	1999	rVB2	44829	66007	2.24%	0.259%
58	14.081	2006	2011	2017	rVB2	18468	29643	1.01%	0.116%
59	14.684	2103	2110	2116	rBV3	22596	44012	1.50%	0.172%
60	15.233	2191	2200	2206	rBV	19890	33693	1.14%	0.132%
61	16.489	2399	2406	2415	rBV2	15444	31000	1.05%	0.121%

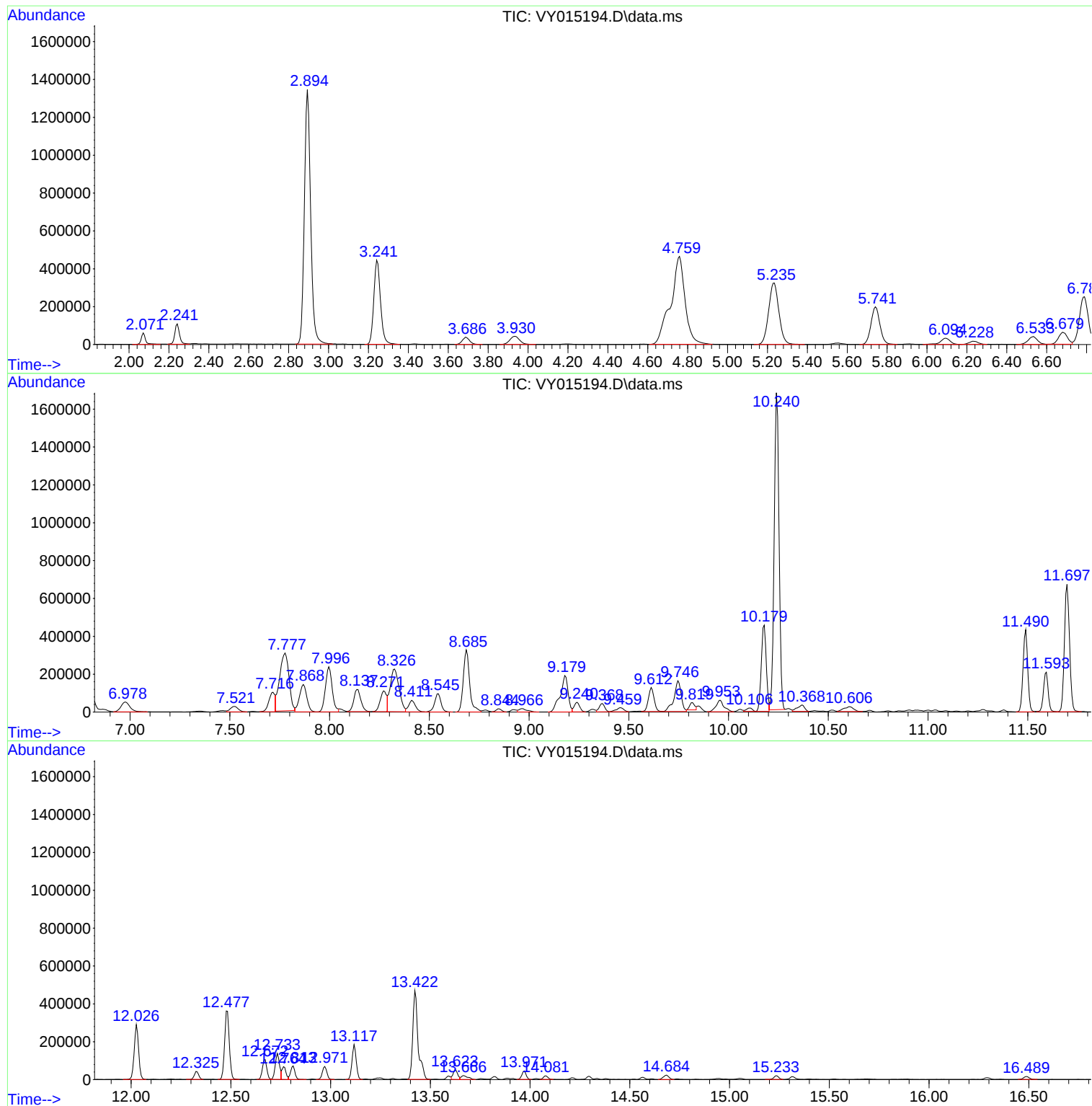
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Quant Title : SW846 8260

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



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
B-PP09A

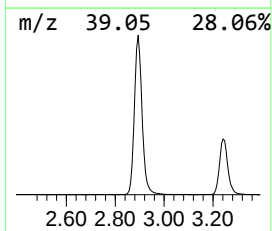
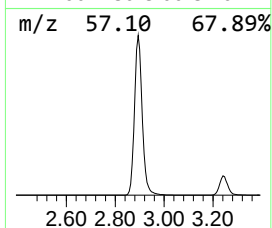
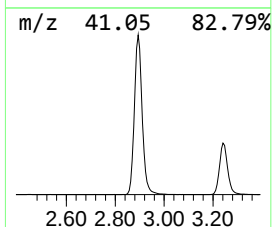
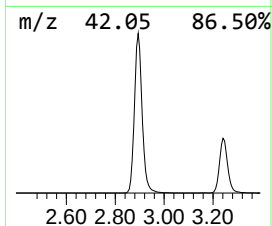
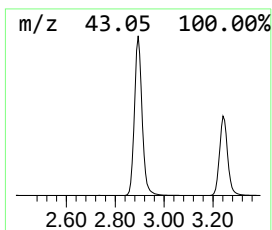
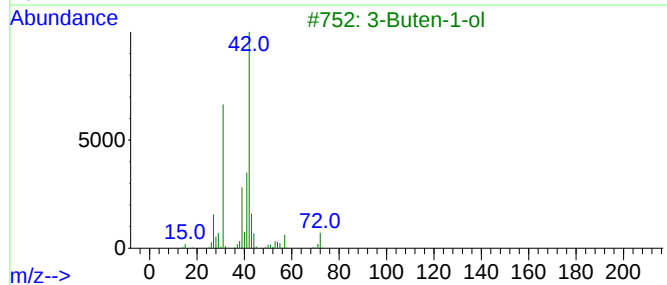
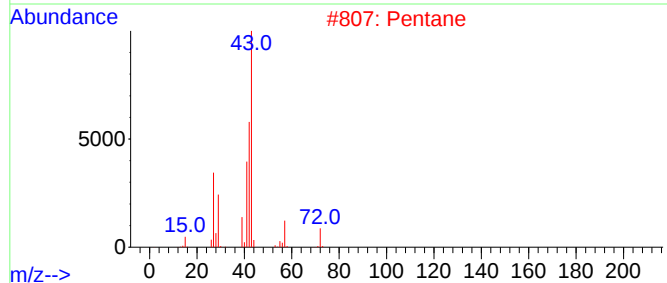
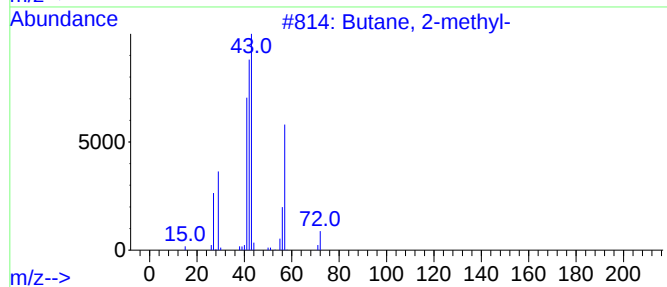
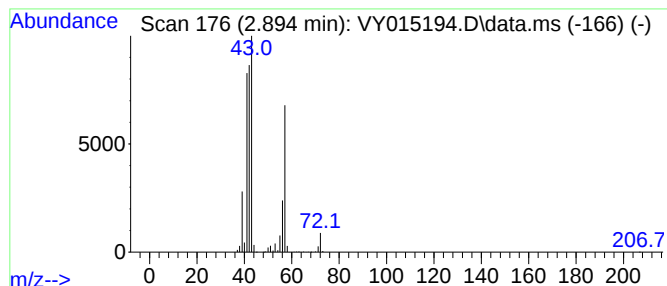
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.894	150.30 ug/l	2942770	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			Pentane	72	C5H12	000109-66-0	45
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5			Methane, isocyanato-	57	C2H3NO	000624-83-9	9



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Misc : 5.06g/5.2mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
B-PP09A

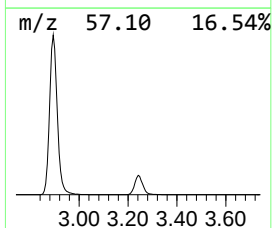
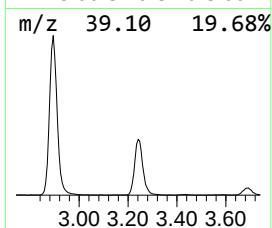
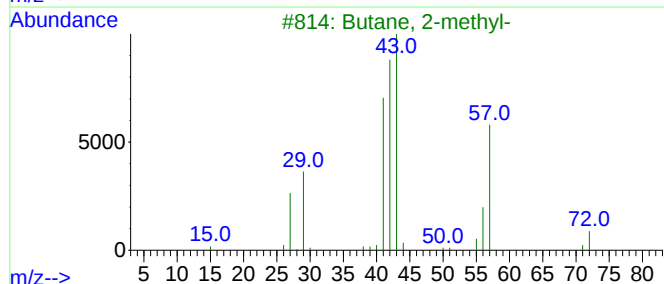
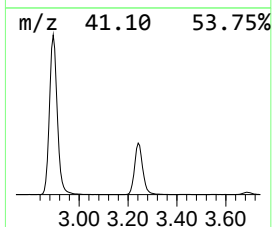
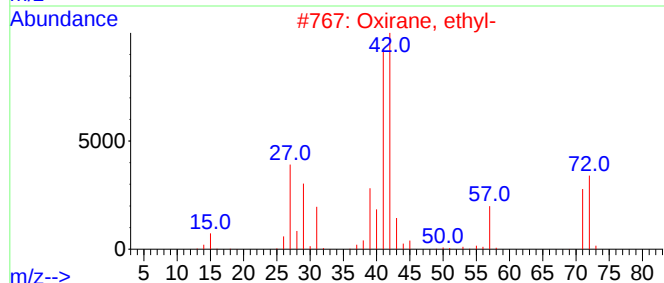
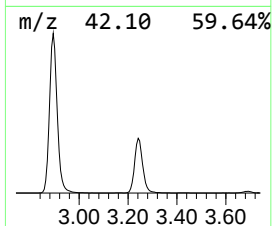
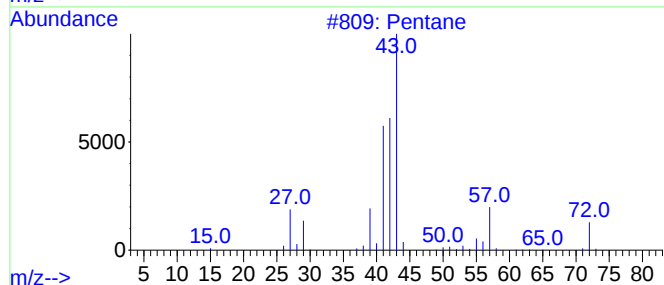
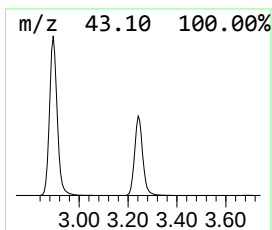
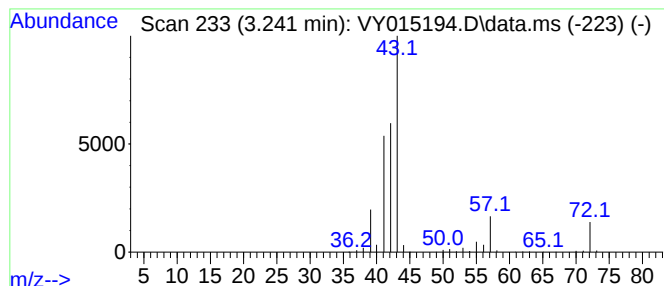
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.241	52.96 ug/l	1036900	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3			Butane, 2-methyl-	72	C5H12	000078-78-4	38
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	25
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081823\
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Sample : 04086-05
Misc : 5.06g/5.2mL/MSVOA_Y/soil
ALS Vial : 13 Sample Multiplier: 1

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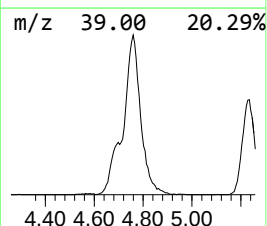
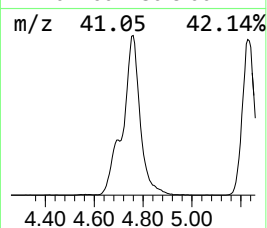
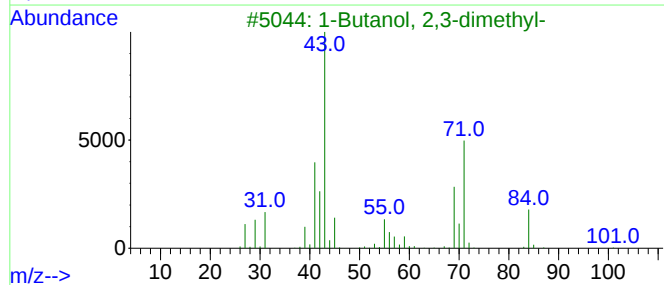
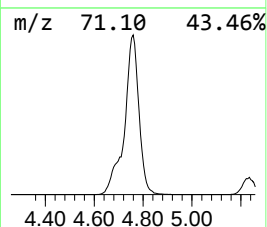
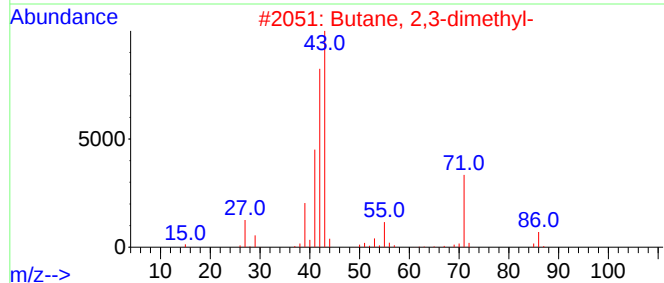
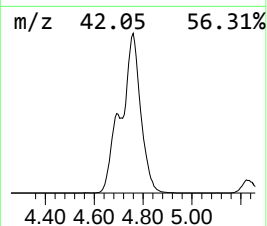
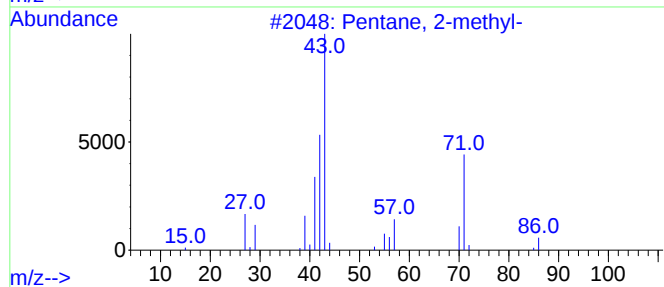
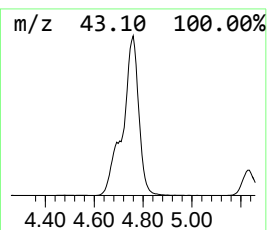
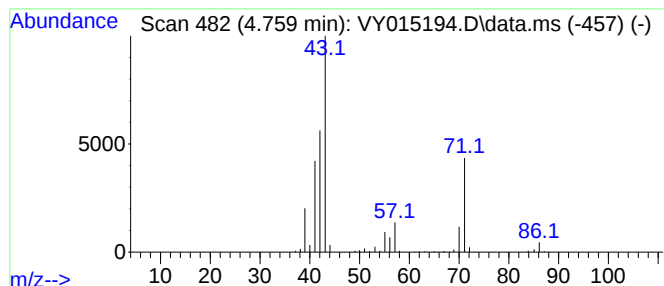
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.759	119.57 ug/l	2341150	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
3			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4			N-Vinylformamide	71	C3H5NO	013162-05-5	38
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38



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Instrument :
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ClientSampleId :
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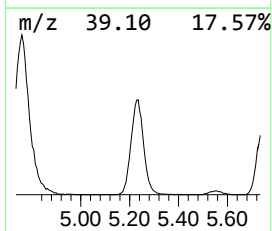
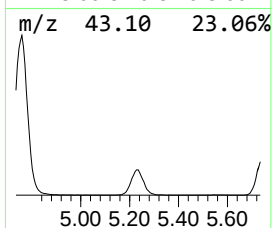
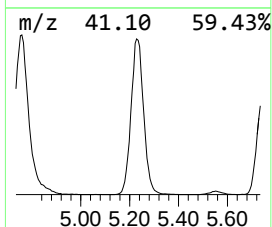
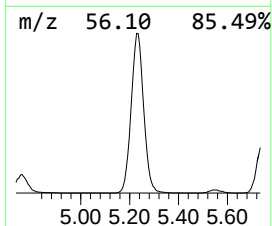
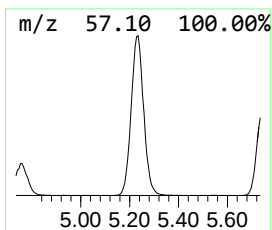
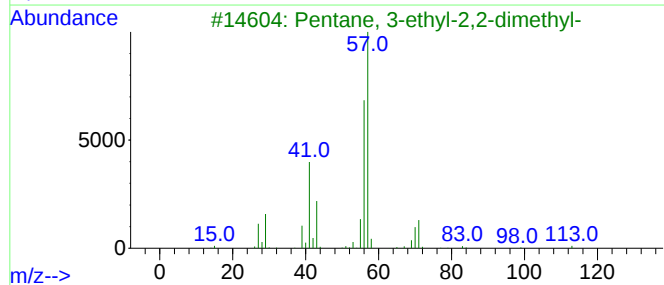
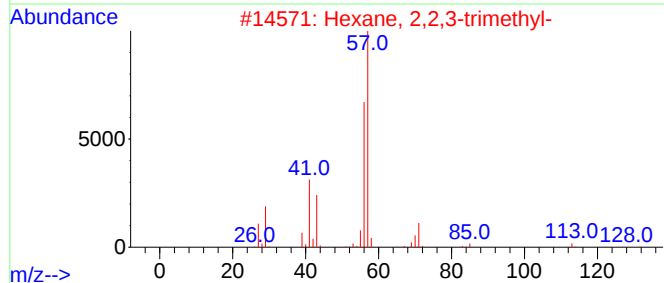
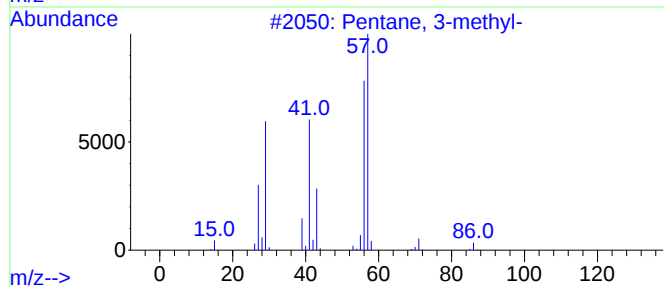
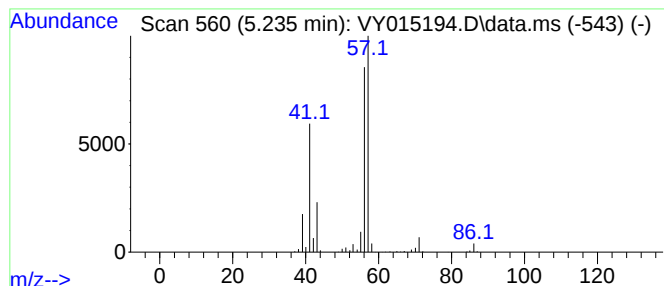
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.235	59.37 ug/l	1162480	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59
5			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40



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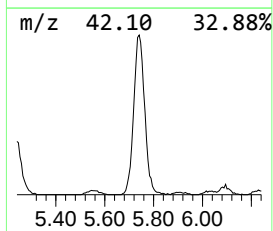
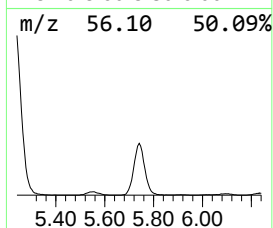
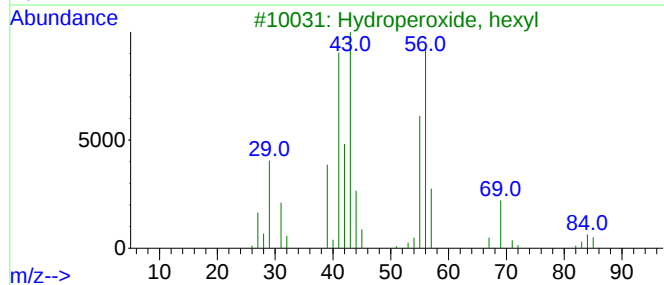
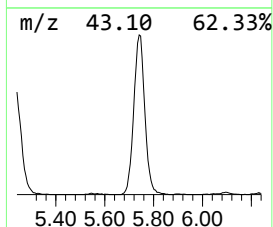
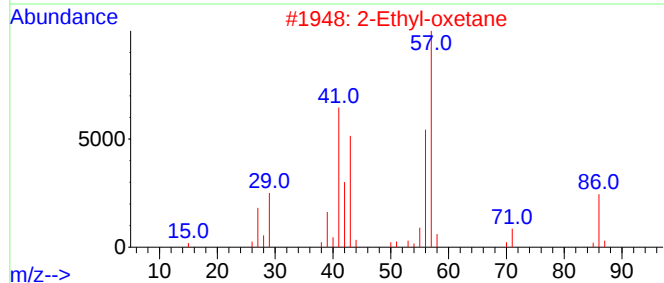
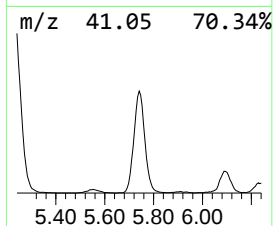
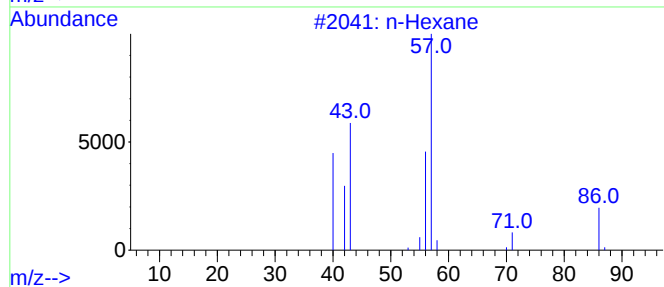
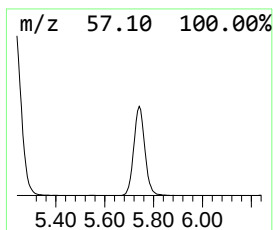
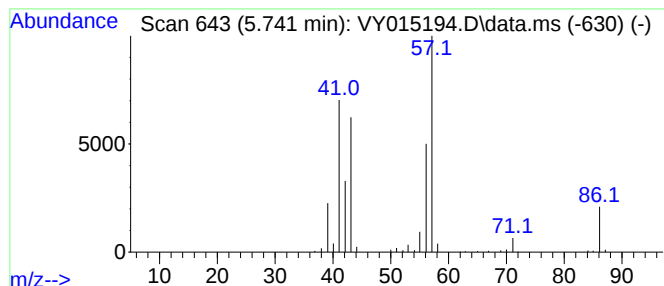
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Quant Title : SW846 8260

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

Peak Number 5 n-Hexane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.741	31.64 ug/l	619521	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	87
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	80
3			Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	38
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	38
5			Methane, isocyanato-	57	C2H3NO	000624-83-9	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081823\
Data File : VY015194.D
Acq On : 18 Aug 2023 14:37
Operator : SY/MD
Sample : 04086-05
Misc : 5.06g/5.2mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
B-PP09A

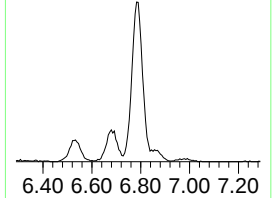
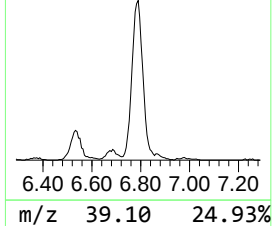
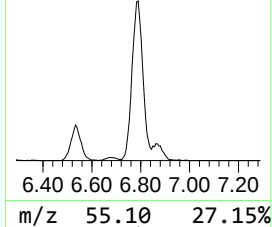
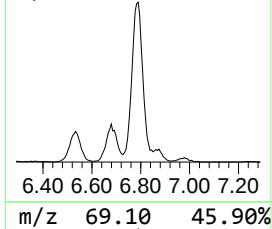
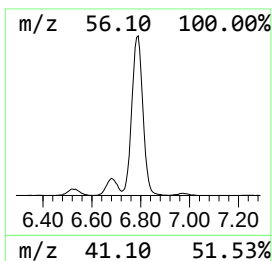
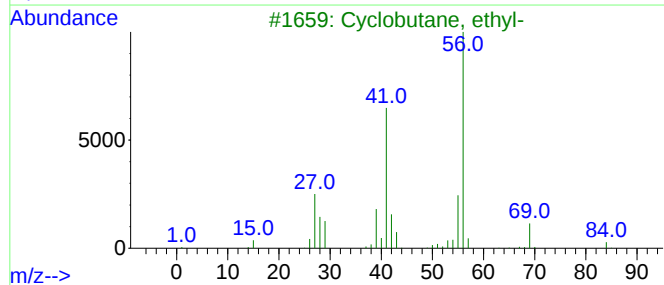
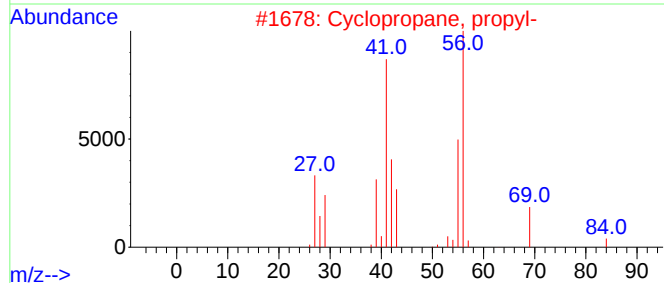
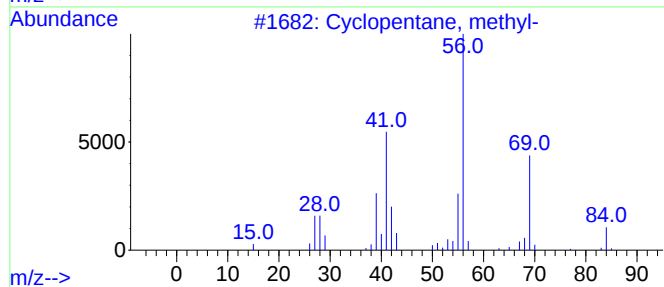
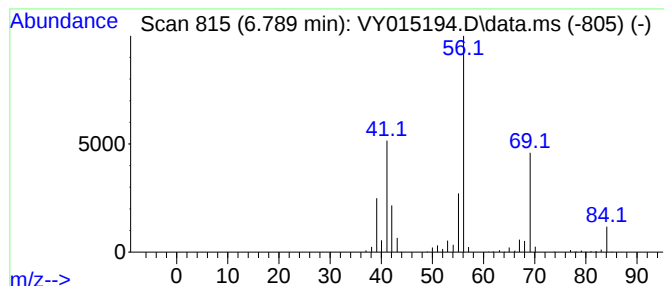
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.789	36.79 ug/l	720244	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopropane, propyl-	84	C6H12	002415-72-7	72
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
5			1-Hexene	84	C6H12	000592-41-6	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081823\
Data File : VY015194.D
Acq On : 18 Aug 2023 14:37
Operator : SY/MD
Sample : 04086-05
Misc : 5.06g/5.2mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
B-PP09A

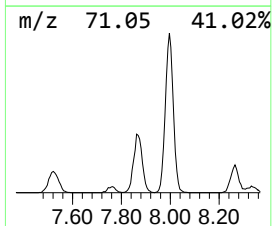
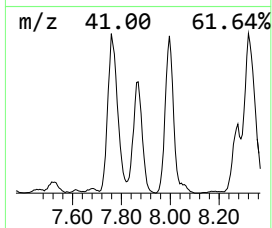
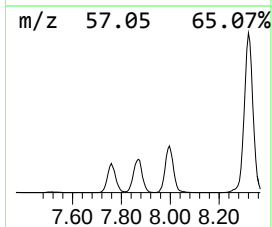
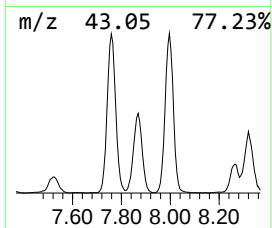
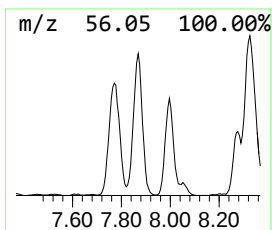
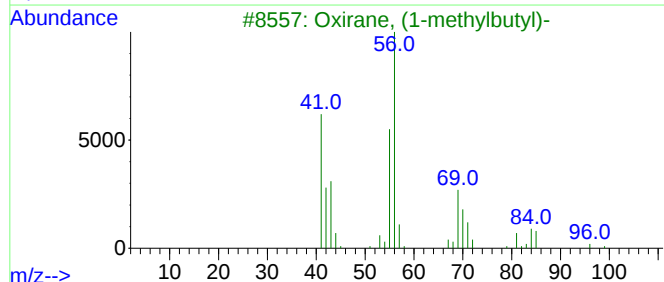
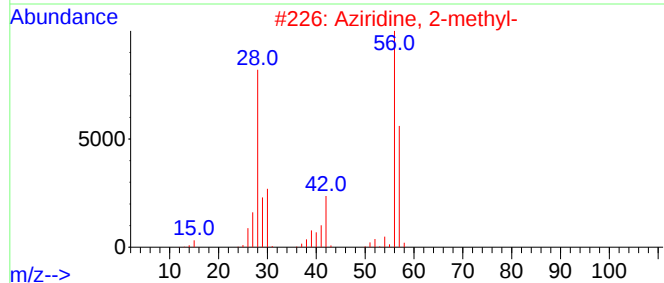
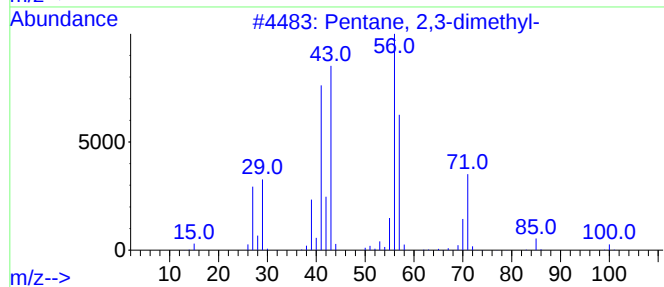
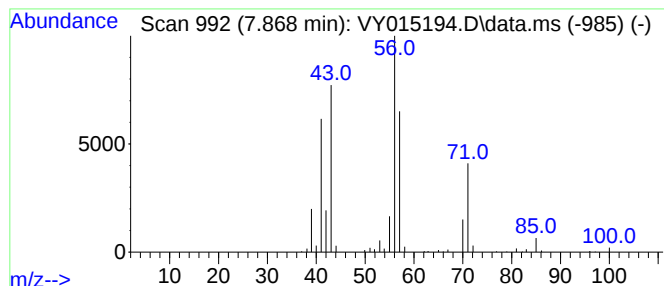
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.868	18.88 ug/l	369561	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	46
3			Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	40
4			Heptane	100	C7H16	000142-82-5	38
5			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081823\
Data File : VY015194.D
Acq On : 18 Aug 2023 14:37
Operator : SY/MD
Sample : 04086-05
Misc : 5.06g/5.2mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
B-PP09A

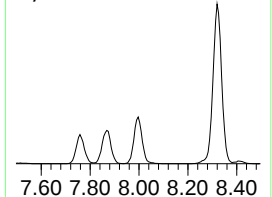
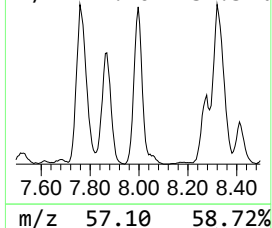
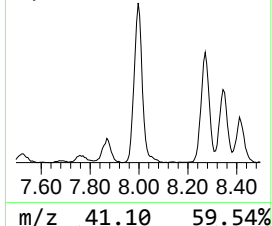
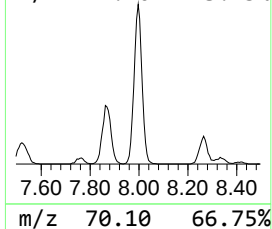
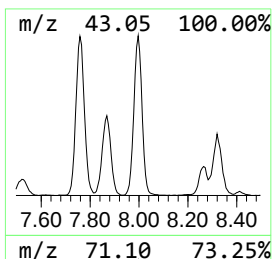
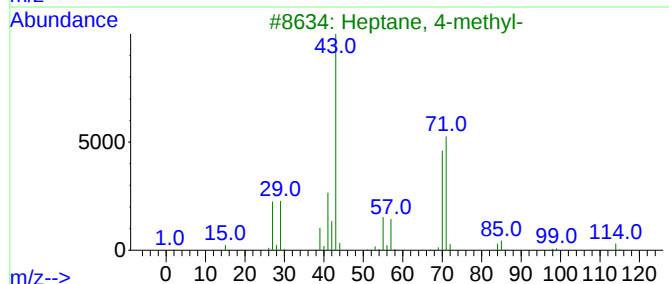
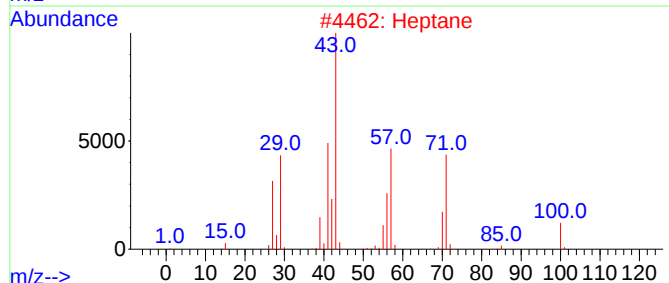
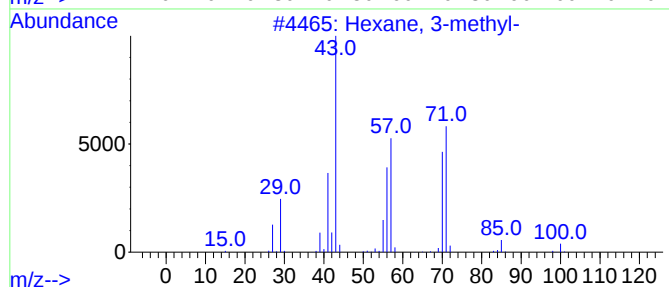
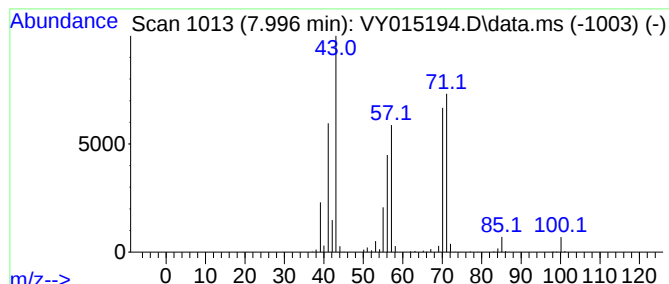
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Quant Title : SW846 8260

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

Peak Number 8 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.996	28.61 ug/l	560253	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane	100	C7H16	000142-82-5	72
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081823\
Data File : VY015194.D
Acq On : 18 Aug 2023 14:37
Operator : SY/MD
Sample : 04086-05
Misc : 5.06g/5.2mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

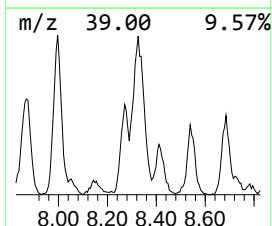
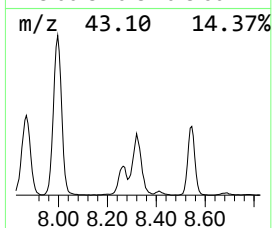
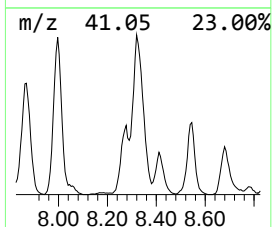
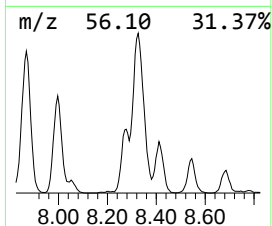
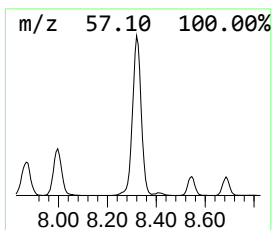
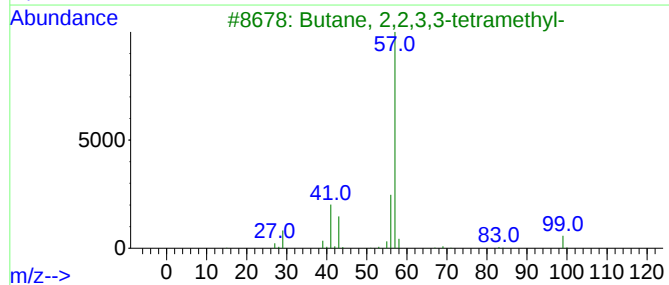
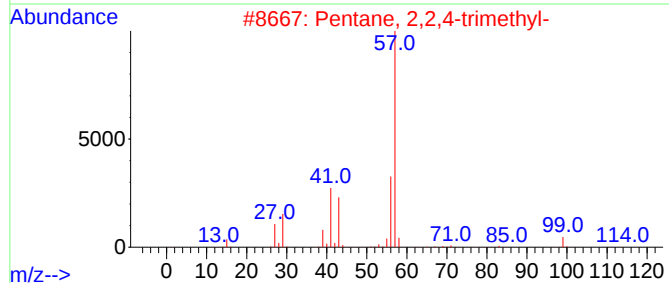
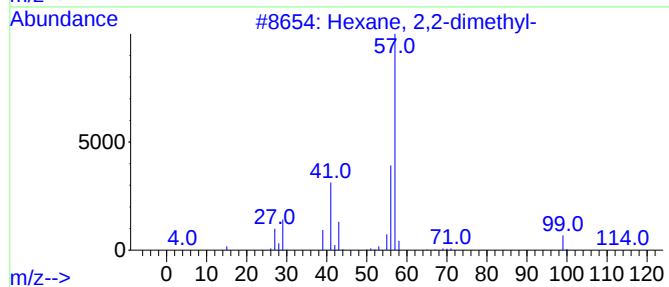
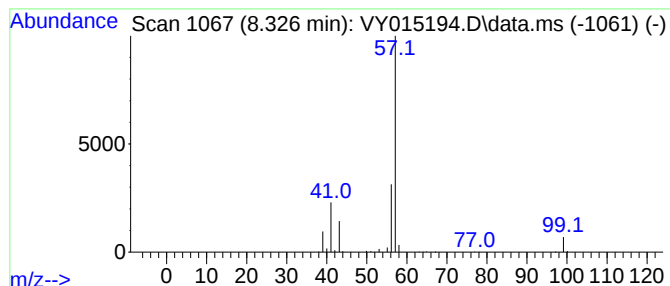
Instrument :
MSVOA_Y
ClientSampleId :
B-PP09A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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

Peak Number 9 Hexane, 2,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.326	47.63 ug/l	686853	1,4-Difluorobenzene	8.685	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	56
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	56
3	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	36
5	Azetidine	57	C3H7N	000503-29-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081823\
Data File : VY015194.D
Acq On : 18 Aug 2023 14:37
Operator : SY/MD
Sample : 04086-05
Misc : 5.06g/5.2mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
B-PP09A

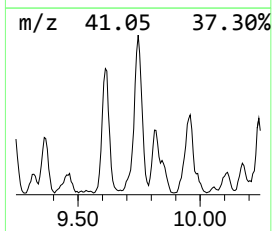
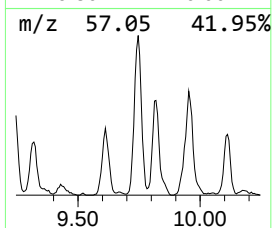
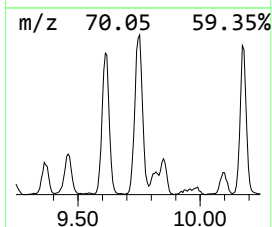
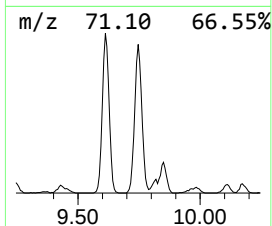
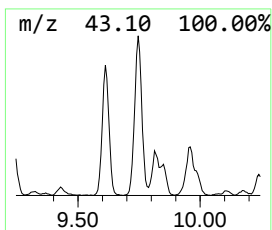
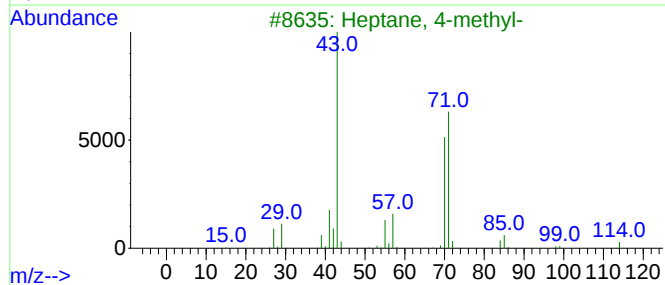
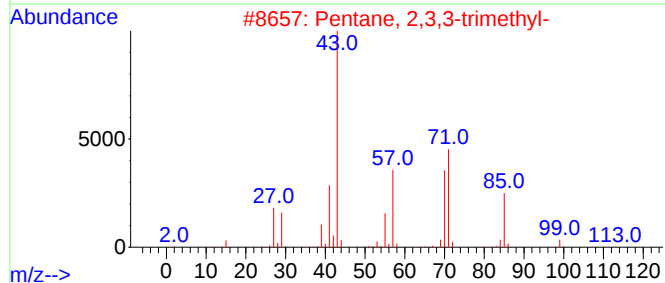
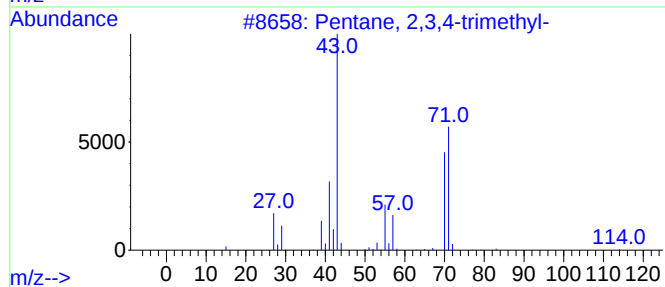
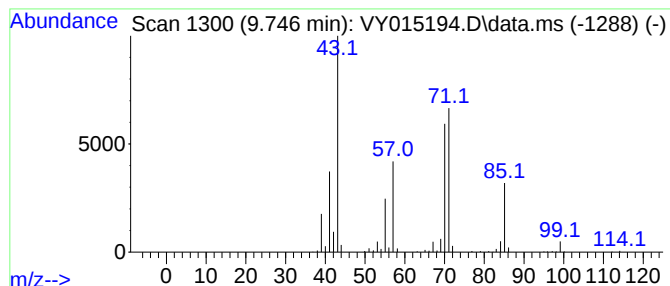
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Quant Title : SW846 8260

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

Peak Number 10 Pentane, 2,3,4-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.746	28.01 ug/l	403942	1,4-Difluorobenzene	8.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	81
2			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	59
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081823\
Data File : VY015194.D
Acq On : 18 Aug 2023 14:37
Operator : SY/MD
Sample : 04086-05
Misc : 5.06g/5.2mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
B-PP09A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.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
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Pentane	3.241	53.0	ug/l	1036900	1	7.783	978962	50.0
Pentane, 2-methyl-	4.759	119.6	ug/l	2341150	1	7.783	978962	50.0
Pentane, 3-methyl-	5.235	59.4	ug/l	1162480	1	7.783	978962	50.0
n-Hexane	5.741	31.6	ug/l	619521	1	7.783	978962	50.0
Cyclopentane, m...	6.789	36.8	ug/l	720244	1	7.783	978962	50.0
Pentane, 2,3-di...	7.868	18.9	ug/l	369561	1	7.783	978962	50.0
Hexane, 3-methyl-	7.996	28.6	ug/l	560253	1	7.783	978962	50.0
Hexane, 2,2-dim...	8.326	47.6	ug/l	686853	2	8.685	721057	50.0
Pentane, 2,3,4-...	9.746	28.0	ug/l	403942	2	8.685	721057	50.0