

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
 Data File : VY014651.D
 Acq On : 14 Jul 2023 16:39
 Operator : SY/MD
 Sample : 03619-01
 Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RT3471

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\82Y071323S.M

Title : SW846 8260

Signal : TIC: VY014651.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.211	60	64	67	rBV	11645	19448	1.61%	0.193%
2	2.894	168	176	189	rBV	52064	117326	9.72%	1.163%
3	3.241	226	233	245	rVB2	44317	109738	9.09%	1.088%
4	3.430	258	264	271	rVB3	5886	12830	1.06%	0.127%
5	3.686	297	306	317	rVB2	14089	37877	3.14%	0.375%
6	3.936	338	347	359	rBV3	10272	32560	2.70%	0.323%
7	4.710	460	474	476	rBV	40125	112931	9.36%	1.119%
8	5.229	546	559	577	rVB2	30048	109451	9.07%	1.085%
9	5.546	602	611	625	rBV7	3633	13464	1.12%	0.133%
10	5.741	631	643	658	rBV2	55986	181324	15.02%	1.797%
11	6.088	695	700	712	rVB3	7901	23360	1.94%	0.232%
12	6.527	761	772	783	rVB5	8813	30387	2.52%	0.301%
13	6.679	787	797	805	rBV3	10673	33933	2.81%	0.336%
14	6.783	805	814	824	rVB3	39726	119218	9.88%	1.182%
15	6.978	836	846	858	rBV	38160	113858	9.43%	1.128%
16	7.460	918	925	930	rBV4	6440	17183	1.42%	0.170%
17	7.521	930	935	944	rVB3	12583	31557	2.61%	0.313%
18	7.716	956	967	972	rBV	168420	415904	34.46%	4.122%
19	7.783	972	978	987	rVV	322811	780506	64.67%	7.735%
20	7.868	987	992	1002	rVB2	22703	57531	4.77%	0.570%
21	7.996	1004	1013	1020	rBV2	45437	109057	9.04%	1.081%
22	8.143	1027	1037	1048	rVB2	174981	427607	35.43%	4.238%
23	8.277	1048	1059	1060	rVV4	19818	43564	3.61%	0.432%
24	8.319	1060	1066	1076	rVV	73276	205325	17.01%	2.035%
25	8.411	1076	1081	1092	rVB2	14087	33974	2.82%	0.337%
26	8.545	1094	1103	1116	rVB	40243	85255	7.06%	0.845%
27	8.685	1116	1126	1137	rBV	450154	909473	75.36%	9.014%
28	8.771	1137	1140	1148	rVB2	10577	21251	1.76%	0.211%
29	9.179	1194	1207	1213	rBV3	74089	179489	14.87%	1.779%
30	9.240	1213	1217	1225	rVB2	16308	30687	2.54%	0.304%
31	9.368	1233	1238	1245	rVB3	9631	18107	1.50%	0.179%
32	9.459	1245	1253	1257	rBV6	7636	17566	1.46%	0.174%
33	9.520	1257	1263	1271	rVB2	15320	30710	2.54%	0.304%
34	9.612	1271	1278	1287	rVB2	32821	67066	5.56%	0.665%
35	9.746	1288	1300	1307	rBV2	35508	91025	7.54%	0.902%
36	9.819	1307	1312	1324	rVB4	23660	58044	4.81%	0.575%

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Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

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Peak Location: TOP

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37	9.959	1326	1335	1346	rBV3	22465	61939	5.13%	0.614%
38	10.112	1354	1360	1364	rVB2	12002	20412	1.69%	0.202%
39	10.179	1364	1371	1377	rBV	704881	1206870	100.00%	11.961%
40	10.240	1377	1381	1388	rVB	99936	167664	13.89%	1.662%
41	10.368	1395	1402	1409	rVB6	14853	36425	3.02%	0.361%
42	10.575	1431	1436	1440	rBV	14899	30501	2.53%	0.302%
43	10.691	1450	1455	1463	rVB3	10175	24579	2.04%	0.244%
44	10.947	1492	1497	1503	rVB	19429	33824	2.80%	0.335%
45	11.209	1534	1540	1545	rBV4	9414	17176	1.42%	0.170%
46	11.276	1545	1551	1556	rBV6	8025	16833	1.39%	0.167%
47	11.490	1578	1586	1596	rBV	647172	1051690	87.14%	10.423%
48	11.697	1612	1620	1626	rBV	98612	198389	16.44%	1.966%
49	11.929	1653	1658	1664	rVB2	9546	15191	1.26%	0.151%
50	12.026	1664	1674	1682	rBV	54936	101328	8.40%	1.004%
51	12.233	1705	1708	1713	rVB5	7153	12370	1.02%	0.123%
52	12.325	1719	1723	1729	rBV5	11355	20630	1.71%	0.204%
53	12.477	1742	1748	1759	rBV	509186	811681	67.26%	8.044%
54	12.733	1785	1790	1793	rBV	23787	36365	3.01%	0.360%
55	12.806	1798	1802	1809	rVB4	23568	42597	3.53%	0.422%
56	12.971	1822	1829	1831	rBV	10791	20536	1.70%	0.204%
57	13.002	1831	1834	1838	rVB2	8439	12335	1.02%	0.122%
58	13.117	1845	1853	1859	rVB4	24644	49761	4.12%	0.493%
59	13.312	1877	1885	1896	rVV2	42124	92998	7.71%	0.922%
60	13.422	1896	1903	1912	rVV	613757	956891	79.29%	9.484%
61	13.508	1914	1917	1923	rVB7	5957	12368	1.02%	0.123%
62	13.629	1933	1937	1940	rBV4	9337	16505	1.37%	0.164%
63	13.703	1945	1949	1953	rVB2	12617	18612	1.54%	0.184%
64	13.873	1972	1977	1981	rBV5	9496	17275	1.43%	0.171%
65	13.965	1988	1992	1997	rVB3	8389	14348	1.19%	0.142%
66	14.020	1997	2001	2007	rBV3	12689	23853	1.98%	0.236%
67	14.300	2042	2047	2051	rBV3	16555	28178	2.33%	0.279%
68	14.416	2063	2066	2069	rBV2	10314	12330	1.02%	0.122%
69	14.459	2069	2073	2079	rVB3	14261	23436	1.94%	0.232%
70	14.556	2086	2089	2095	rBV6	7575	15692	1.30%	0.156%
71	14.654	2102	2105	2114	rVB8	10871	24905	2.06%	0.247%
72	14.745	2115	2120	2122	rBV5	11382	20354	1.69%	0.202%
73	14.776	2122	2125	2132	rVB3	17361	29465	2.44%	0.292%
74	15.056	2167	2171	2175	rVB3	12042	18867	1.56%	0.187%
75	15.208	2189	2196	2204	rBV3	7638	25205	2.09%	0.250%
76	15.312	2210	2213	2219	rVB	13162	18606	1.54%	0.184%

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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

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Title : SW846 8260

77	16.470	2400	2403	2409	rBV8	16952	32462	2.69%	0.322%
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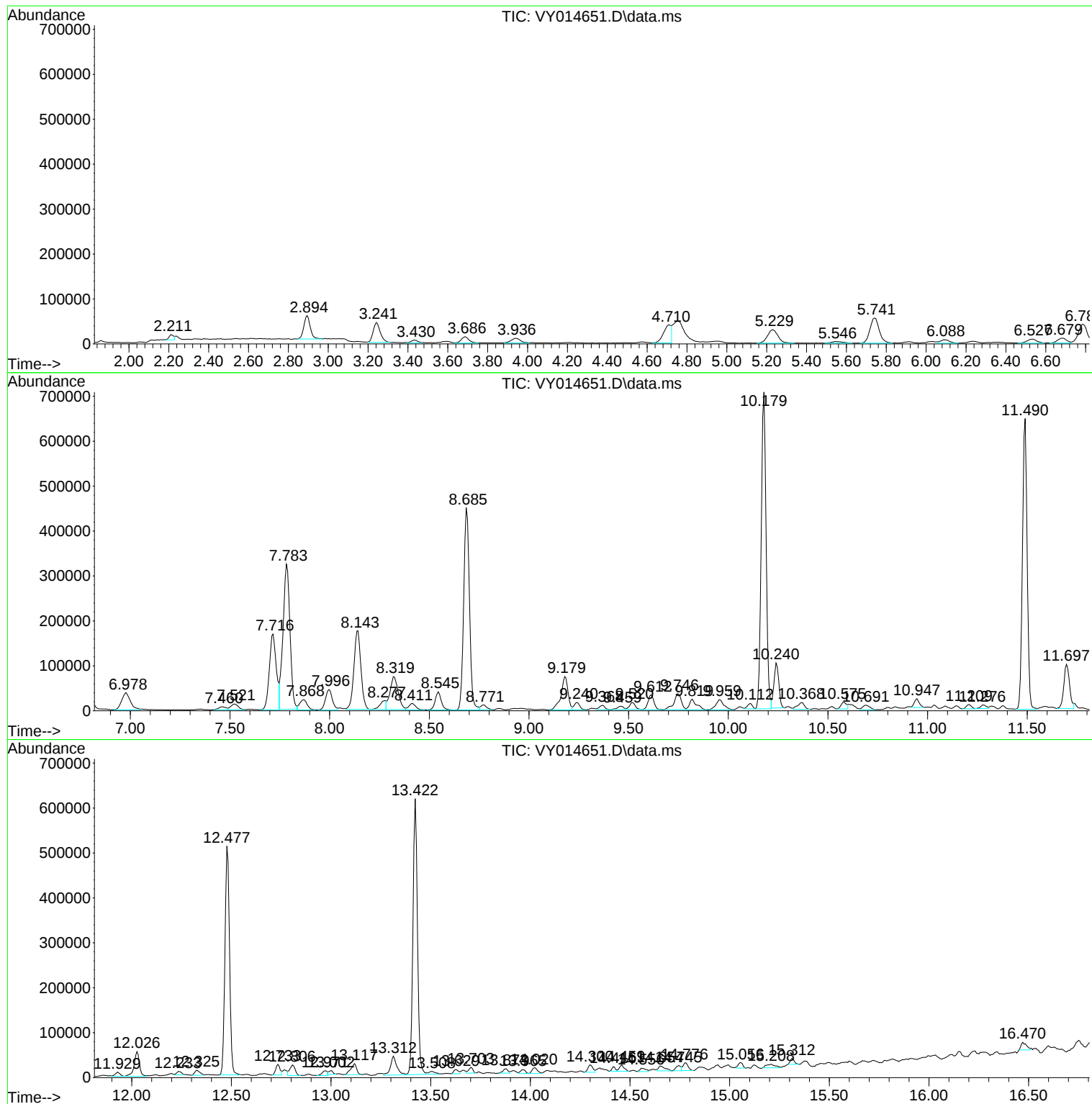
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
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Instrument :
MSVOA_Y
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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



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Operator : SY/MD
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Instrument :
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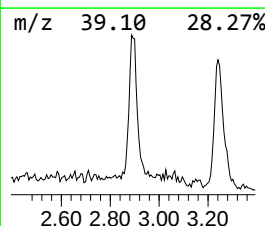
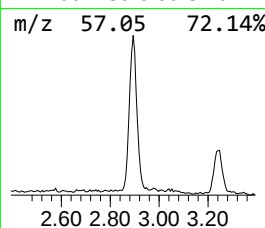
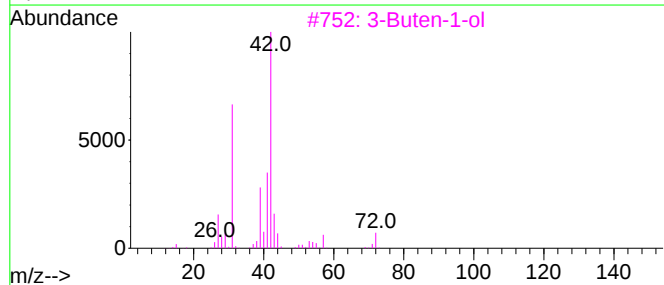
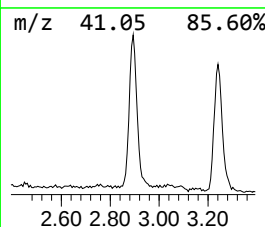
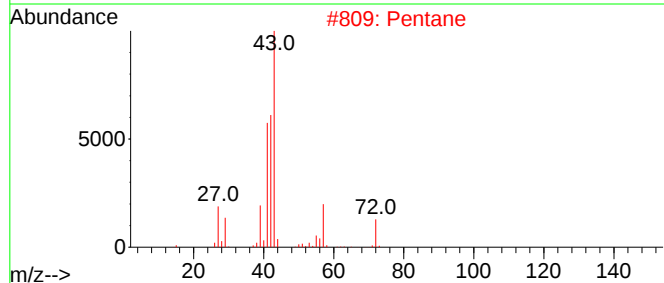
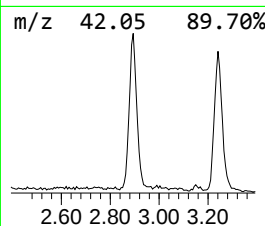
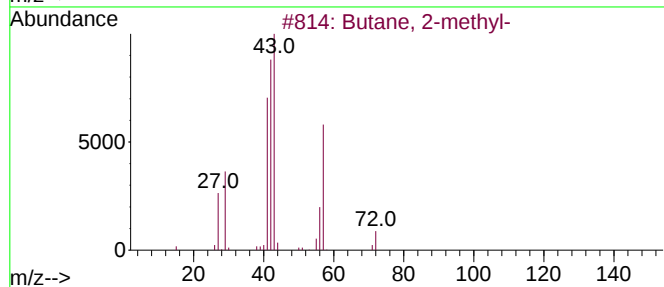
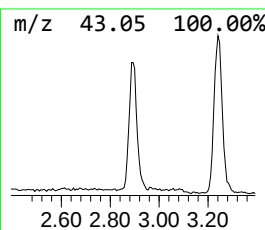
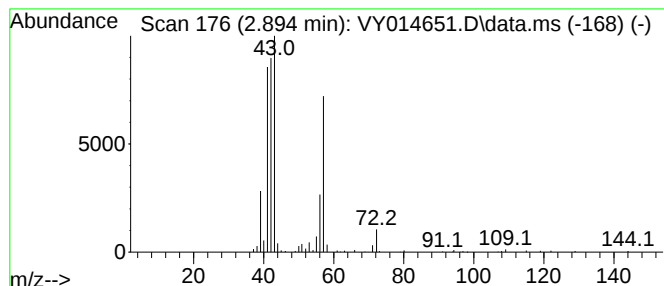
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.894	7.52 ug/l	117326	Pentafluorobenzene	7.789

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	25
4			1,1-Diisobutoxy-butane	202	C12H26O2	013002-16-9	22
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	12



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Instrument :
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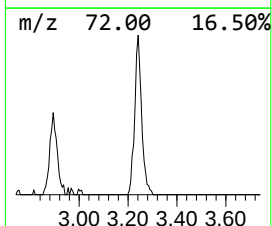
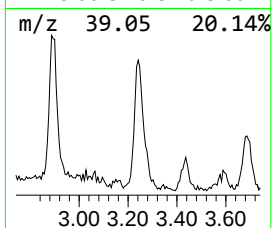
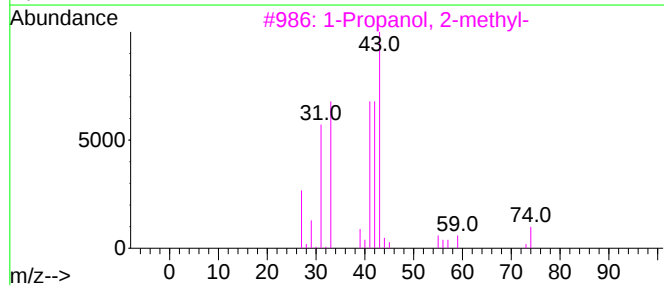
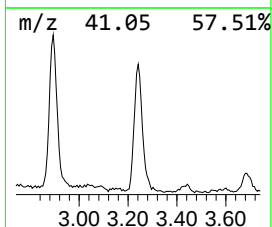
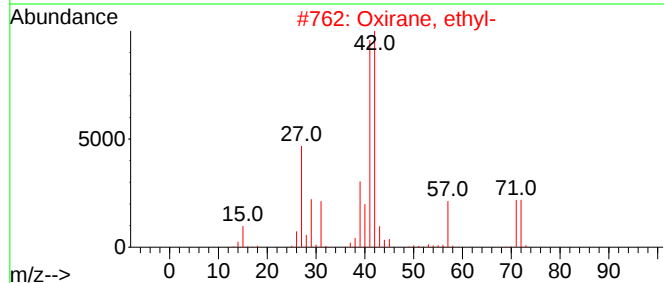
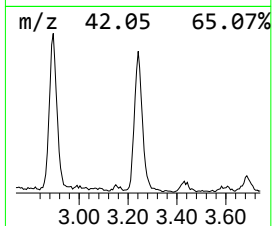
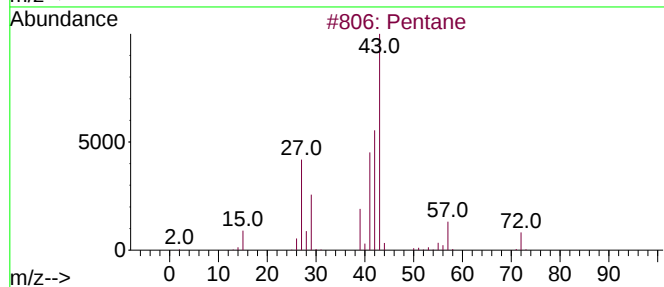
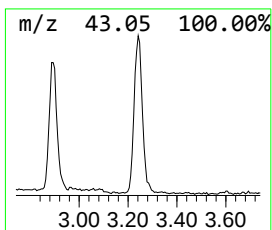
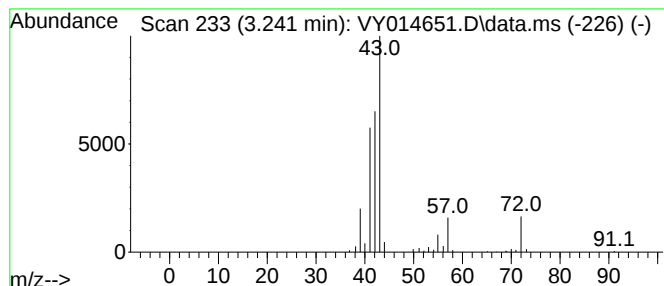
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.241	7.03 ug/l	109738	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	50
4			Butane, 2-methyl-	72	C5H12	000078-78-4	39
5			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38



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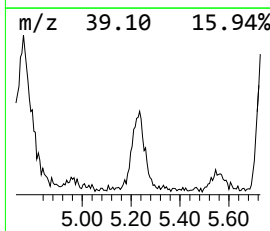
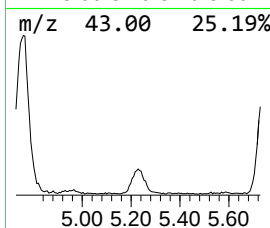
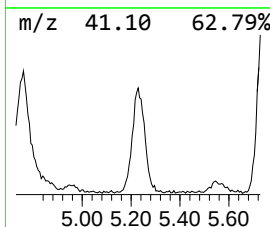
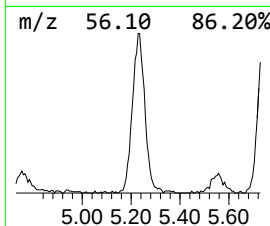
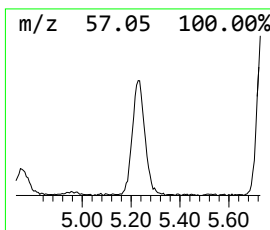
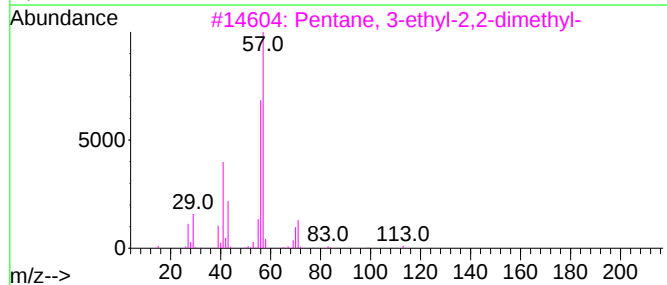
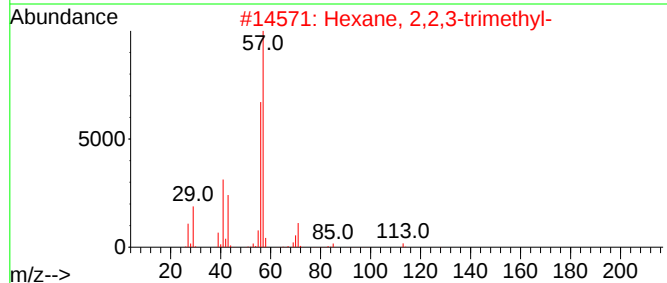
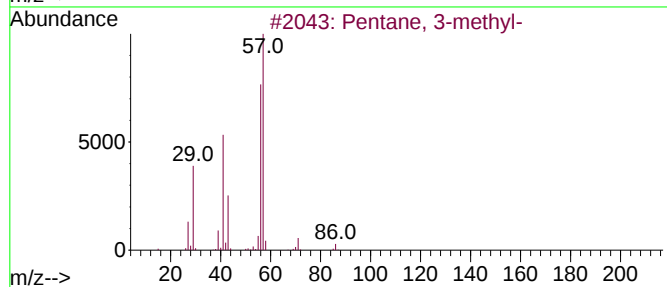
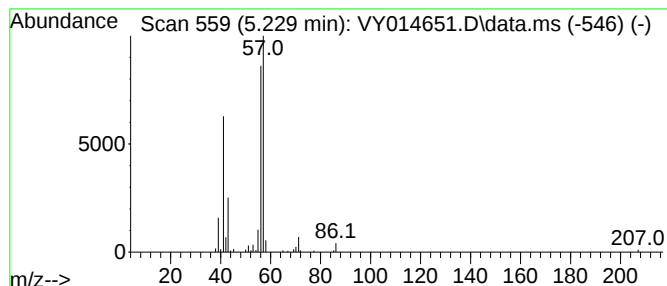
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.229	7.01 ug/l	109451	Pentafluorobenzene	7.789

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			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	56
5			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	56



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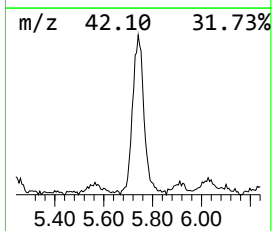
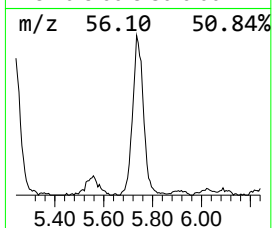
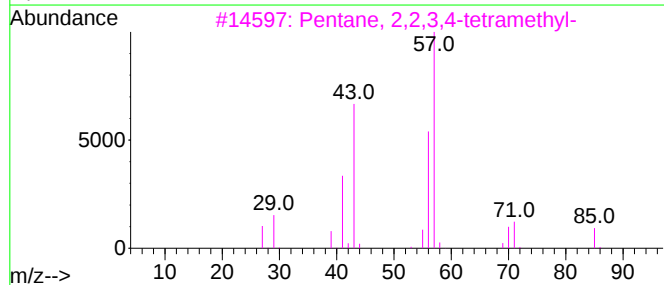
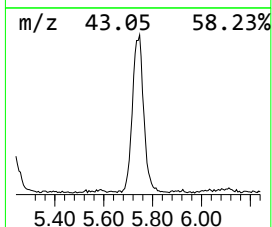
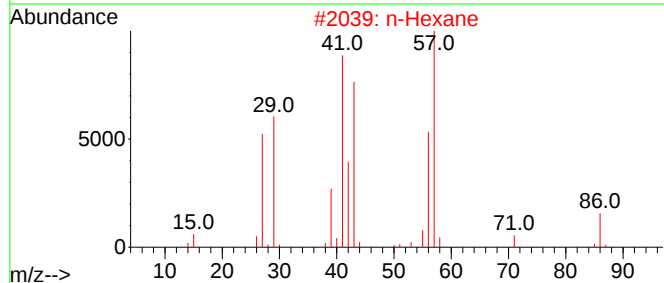
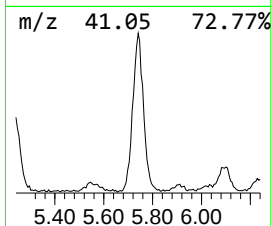
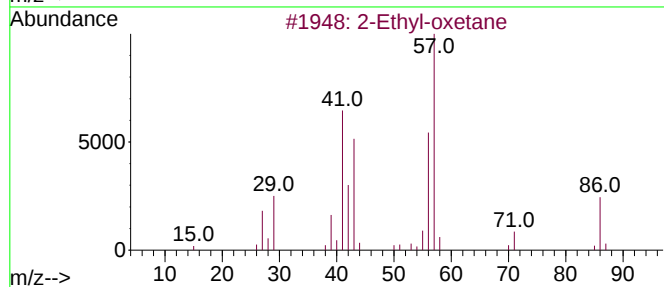
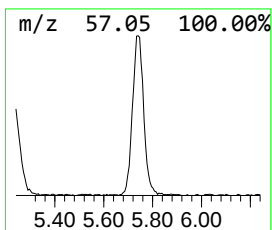
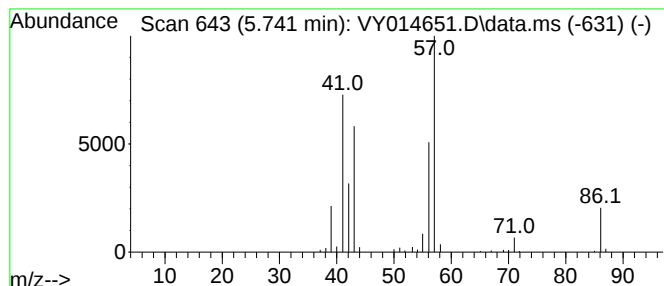
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Quant Title : SW846 8260

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

Peak Number 5 2-Ethyl-oxetane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.741	11.62 ug/l	181324	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	90
2			n-Hexane	86	C6H14	000110-54-3	78
3			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	50
4			Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	50
5			Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
Data File : VY014651.D
Acq On : 14 Jul 2023 16:39
Operator : SY/MD
Sample : 03619-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT3471

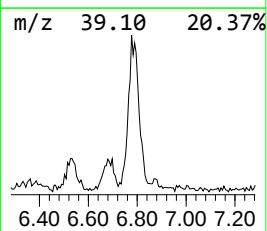
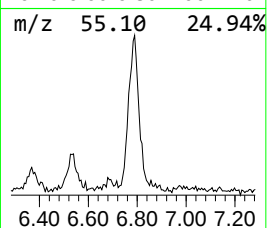
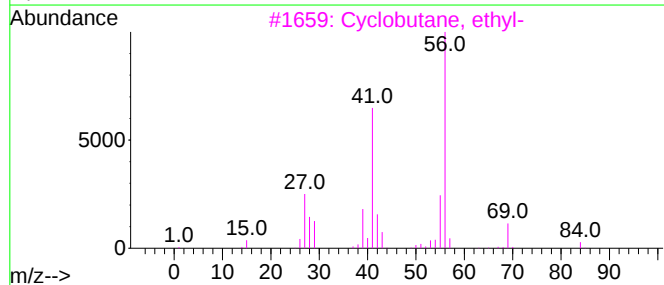
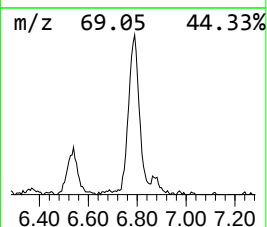
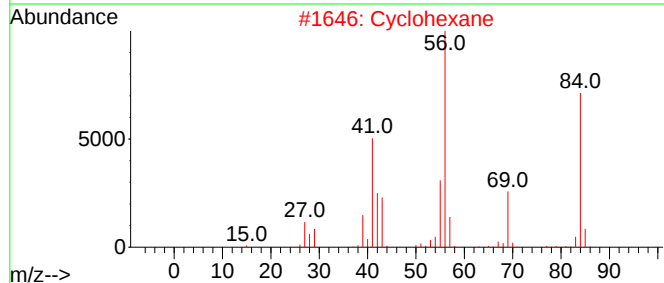
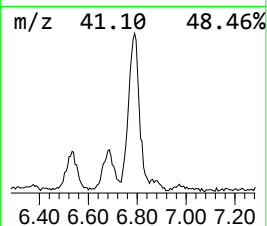
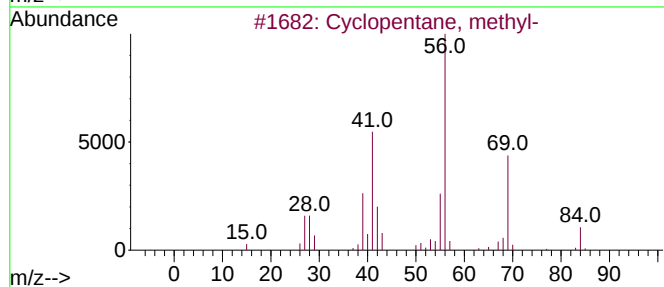
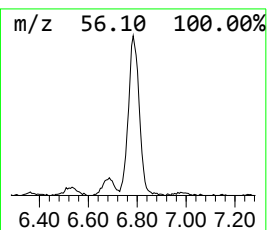
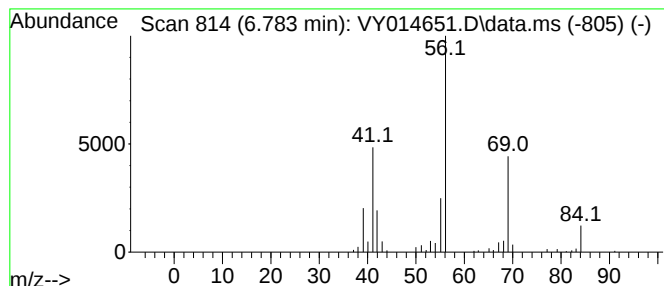
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.783	7.64 ug/l	119218	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclohexane	84	C6H12	000110-82-7	83
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	78
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
Data File : VY014651.D
Acq On : 14 Jul 2023 16:39
Operator : SY/MD
Sample : 03619-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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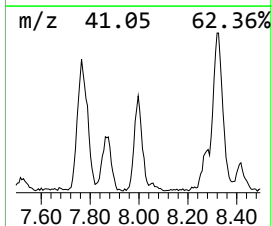
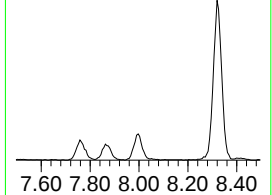
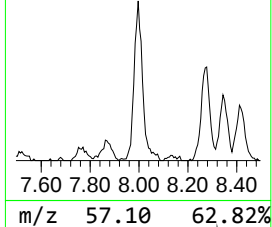
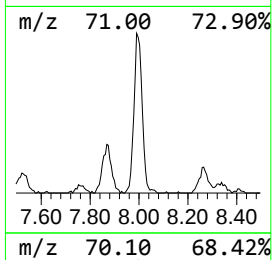
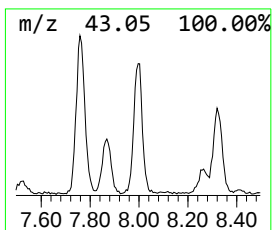
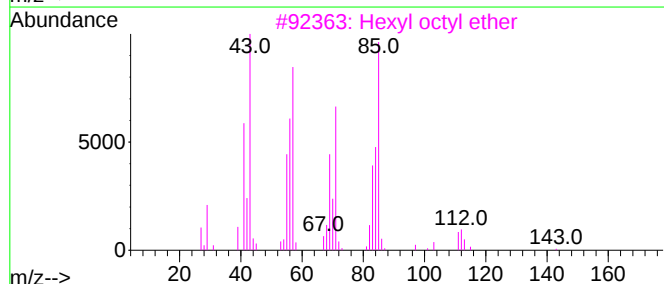
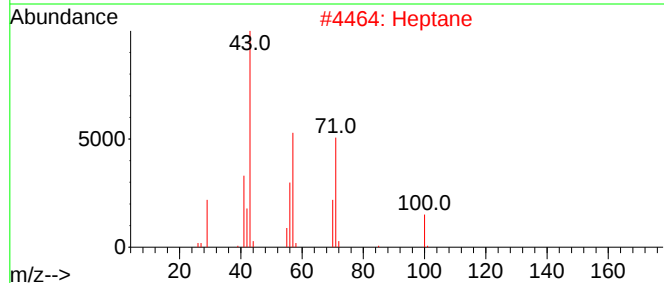
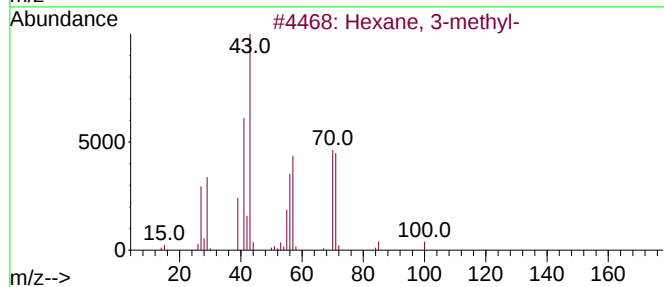
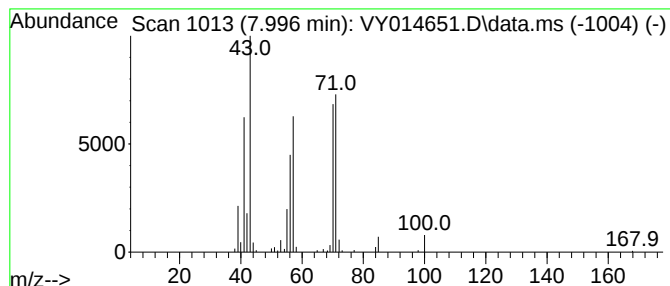
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Quant Title : SW846 8260

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

Peak Number 8 Hexane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.996	6.99 ug/l	109057	Pentafluorobenzene	7.789

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	83
3		Hexyl octyl ether	214	C14H30O	017071-54-4	59
4		Heptane, 4-methyl-	114	C8H18	000589-53-7	59
5		3,4-Diethyl hexane	142	C10H22	019398-77-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
Data File : VY014651.D
Acq On : 14 Jul 2023 16:39
Operator : SY/MD
Sample : 03619-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT3471

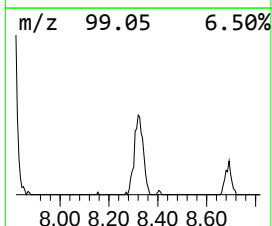
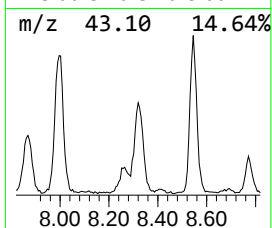
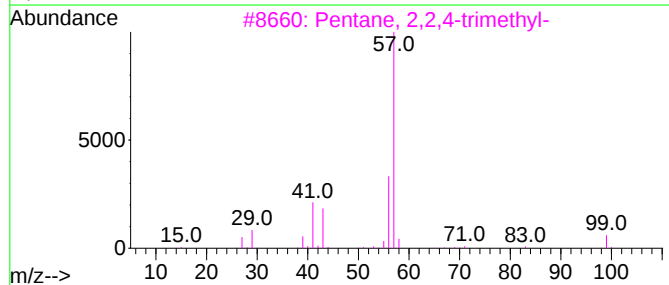
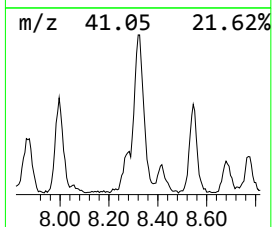
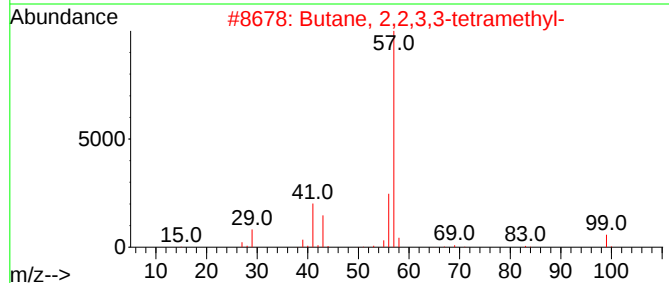
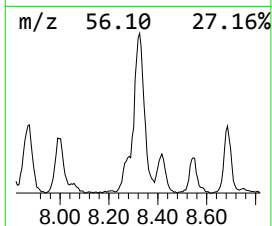
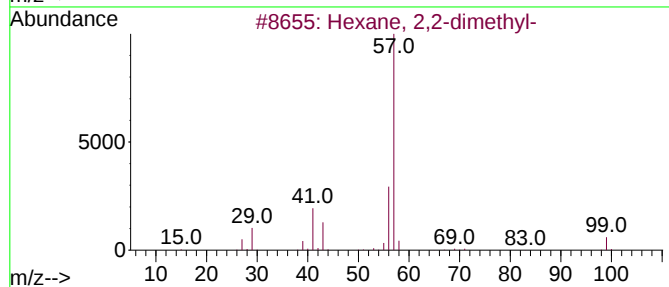
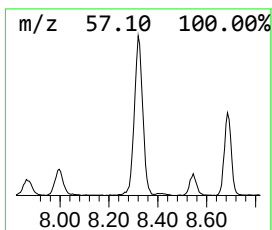
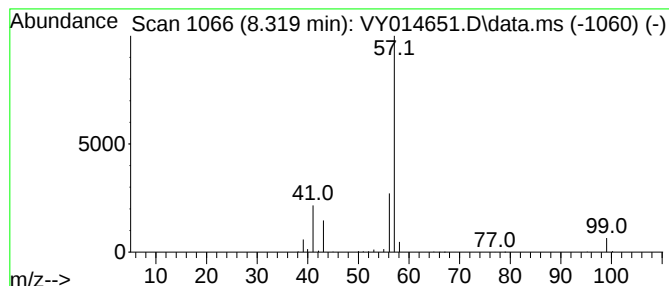
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.319	11.29 ug/l	205325	1,4-Difluorobenzene	8.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	39
5			Acetamide, N-2-propenyl-	99	C5H9NO	000692-33-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
Data File : VY014651.D
Acq On : 14 Jul 2023 16:39
Operator : SY/MD
Sample : 03619-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT3471

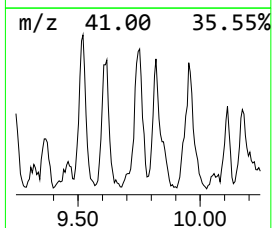
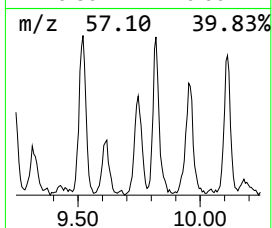
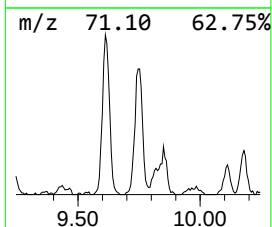
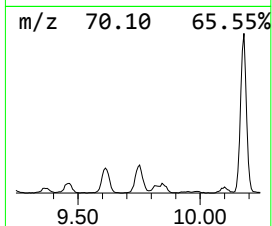
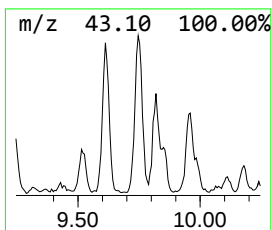
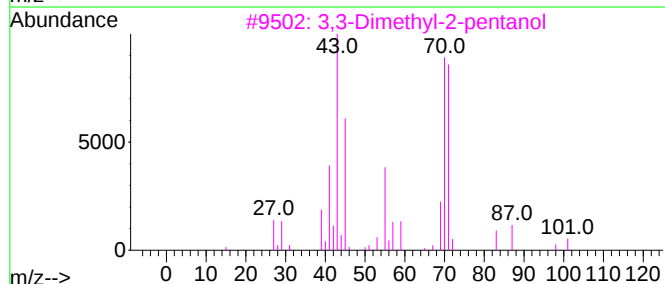
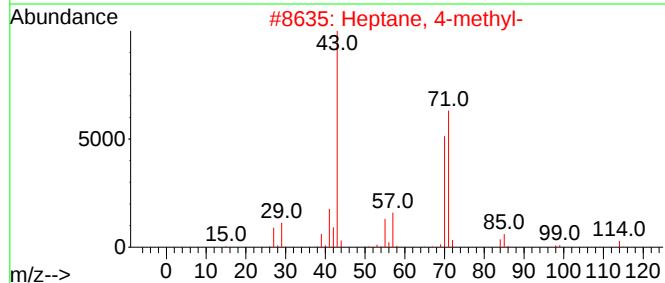
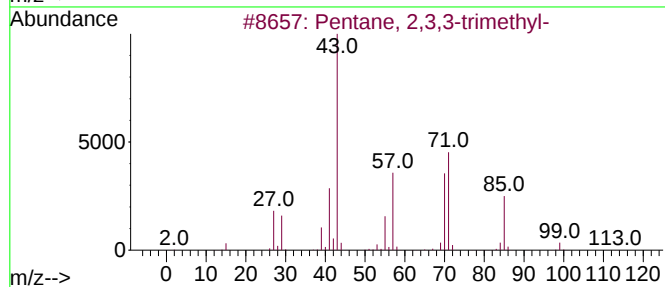
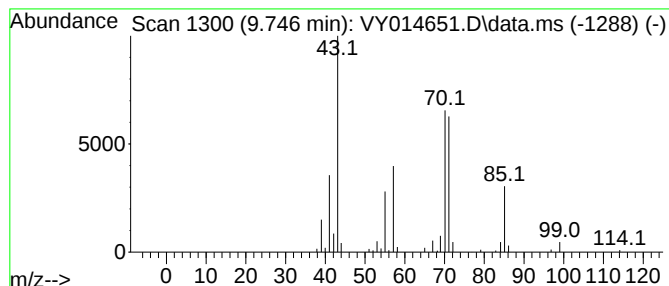
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.746	5.00 ug/l	91025	1,4-Difluorobenzene	8.685

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3		3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	59
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
Data File : VY014651.D
Acq On : 14 Jul 2023 16:39
Operator : SY/MD
Sample : 03619-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT3471

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.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	7.0	ug/l	109738	1	7.789	780506	50.0
Pentane, 3-methyl-	5.229	7.0	ug/l	109451	1	7.789	780506	50.0
2-Ethyl-oxetane	5.741	11.6	ug/l	181324	1	7.789	780506	50.0
Cyclopentane, m...	6.783	7.6	ug/l	119218	1	7.789	780506	50.0
Hexane, 3-methyl-	7.996	7.0	ug/l	109057	1	7.789	780506	50.0
Hexane, 2,2-dim...	8.319	11.3	ug/l	205325	2	8.685	909473	50.0
Pentane, 2,3,3-...	9.746	5.0	ug/l	91025	2	8.685	909473	50.0