

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020524\
 Data File : VY017224.D
 Acq On : 05 Feb 2024 13:19
 Operator : SY/MD
 Sample : P1366-05
 Misc : 4.58g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EB-1-4-6

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\82Y020124S.M
 Title : SW846 8260

Signal : TIC: VY017224.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.729	463	477	493	rBV6	10451	39301	2.55%	0.345%
2	6.704	789	801	815	rBV3	32952	106171	6.90%	0.931%
3	7.734	960	970	975	rBV	60393	146662	9.53%	1.286%
4	7.801	975	981	988	rVV	117740	277225	18.02%	2.430%
5	7.887	988	995	1008	rVV	127812	318947	20.73%	2.796%
6	8.155	1030	1039	1052	rBV	53647	123425	8.02%	1.082%
7	8.338	1054	1069	1084	rBV	656857	1538684	100.00%	13.488%
8	8.704	1120	1129	1139	rBV	226689	444056	28.86%	3.893%
9	9.021	1172	1181	1189	rVB2	7744	17055	1.11%	0.150%
10	9.203	1202	1211	1215	rBV	92864	187221	12.17%	1.641%
11	9.252	1215	1219	1226	rVV	115027	220343	14.32%	1.931%
12	9.331	1226	1232	1246	rVB	72353	148718	9.67%	1.304%
13	9.630	1272	1281	1292	rBV	517604	981986	63.82%	8.608%
14	9.764	1292	1303	1310	rBV	402547	868336	56.43%	7.612%
15	9.947	1326	1333	1348	rVB3	24431	60659	3.94%	0.532%
16	10.124	1351	1362	1368	rBV	261468	456868	29.69%	4.005%
17	10.191	1368	1373	1378	rVV	282464	483589	31.43%	4.239%
18	10.252	1378	1383	1397	rVV	843675	1468775	95.46%	12.875%
19	10.380	1397	1404	1412	rVB2	17141	30578	1.99%	0.268%
20	10.575	1431	1436	1442	rVB4	10563	21040	1.37%	0.184%
21	10.648	1442	1448	1455	rVB	54895	94964	6.17%	0.832%
22	10.910	1485	1491	1500	rBV2	13998	29480	1.92%	0.258%
23	11.045	1506	1513	1518	rVB4	9330	17818	1.16%	0.156%
24	11.221	1538	1542	1546	rVV	10506	17663	1.15%	0.155%
25	11.295	1546	1554	1565	rVB7	7607	24262	1.58%	0.213%
26	11.502	1579	1588	1594	rVV	381969	676543	43.97%	5.930%
27	11.575	1594	1600	1613	rVV2	64235	151980	9.88%	1.332%
28	11.715	1613	1623	1626	rVV2	24253	54799	3.56%	0.480%
29	11.752	1626	1629	1640	rVB	46934	75696	4.92%	0.664%
30	11.947	1657	1661	1665	rBV	20596	31887	2.07%	0.280%
31	12.038	1670	1676	1683	rVV2	12771	28378	1.84%	0.249%
32	12.124	1683	1690	1696	rVB	21739	37141	2.41%	0.326%
33	12.337	1720	1725	1729	rBV	11958	18366	1.19%	0.161%
34	12.477	1740	1748	1758	rBV2	278207	668254	43.43%	5.858%
35	12.569	1758	1763	1769	rBV2	14387	34080	2.21%	0.299%
36	12.636	1769	1774	1779	rBV	55495	98194	6.38%	0.861%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

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Stop Thrs : 0

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Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

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37	12.745	1785	1792	1796	rBV3	17195	29164	1.90%	0.256%
38	12.843	1800	1808	1814	rVV2	66200	142257	9.25%	1.247%
39	12.892	1814	1816	1825	rVB	12118	18442	1.20%	0.162%
40	12.983	1825	1831	1834	rBV	10726	19712	1.28%	0.173%
41	13.081	1839	1847	1851	rVV	67503	113548	7.38%	0.995%
42	13.130	1851	1855	1860	rVB	22722	33288	2.16%	0.292%
43	13.184	1860	1864	1870	rVB	25038	38278	2.49%	0.336%
44	13.294	1870	1882	1886	rBV	64450	140019	9.10%	1.227%
45	13.434	1897	1905	1910	rBV	319718	525158	34.13%	4.603%
46	13.489	1910	1914	1925	rVB	90754	196361	12.76%	1.721%
47	13.654	1934	1941	1949	rBV4	38012	80062	5.20%	0.702%
48	13.837	1967	1971	1976	rVB3	11922	21936	1.43%	0.192%
49	14.392	2058	2062	2072	rVB3	22551	50538	3.28%	0.443%

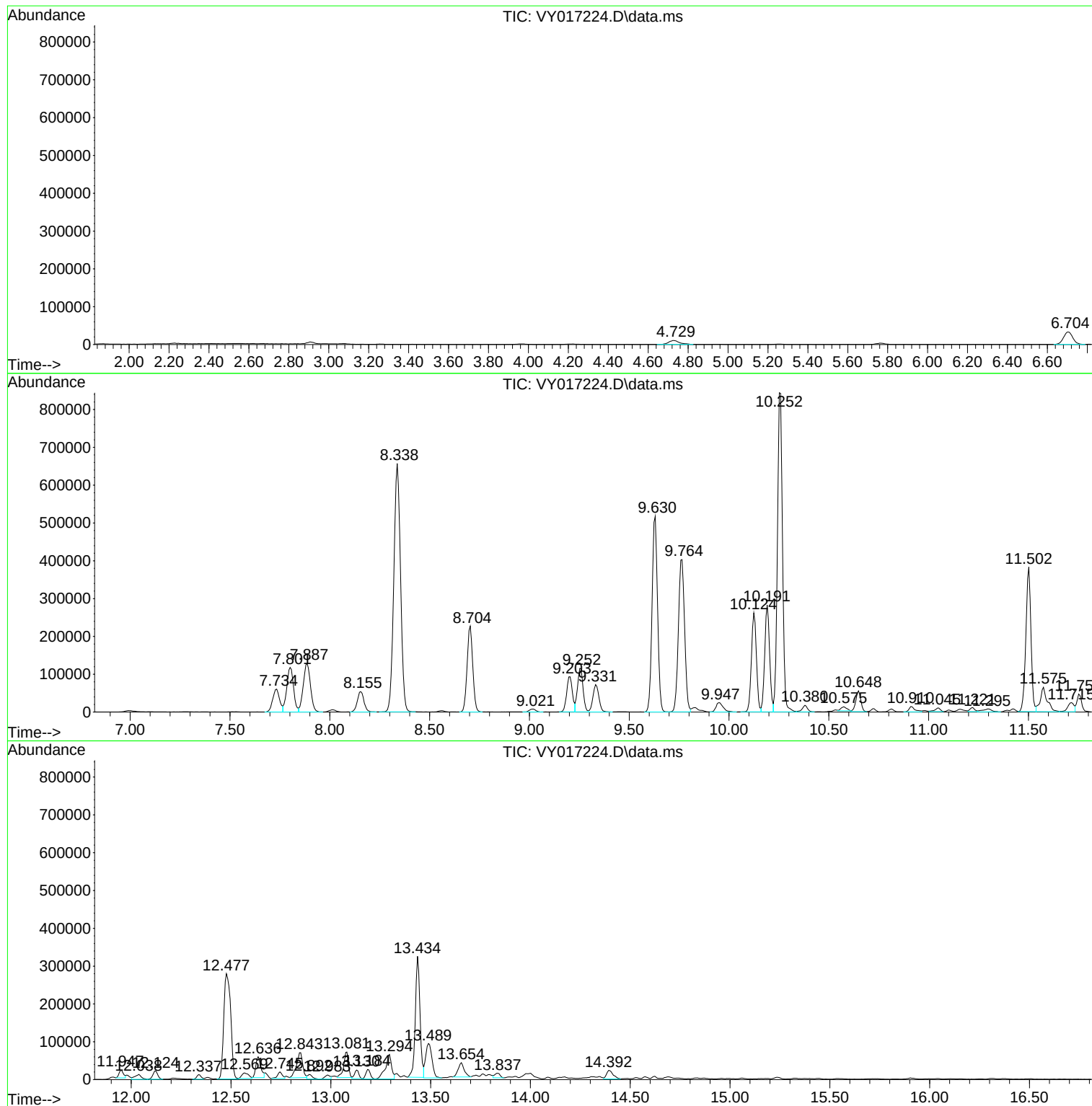
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_Y
ClientSampleId :
EB-1-4-6

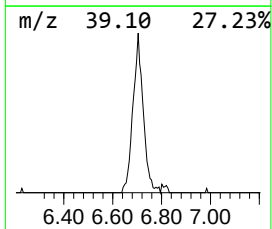
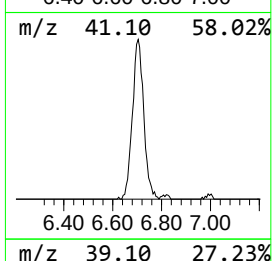
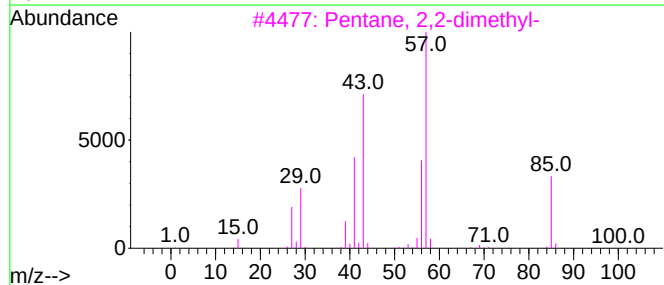
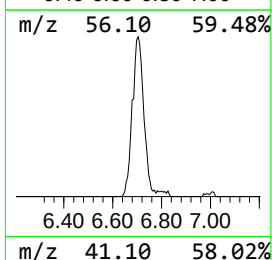
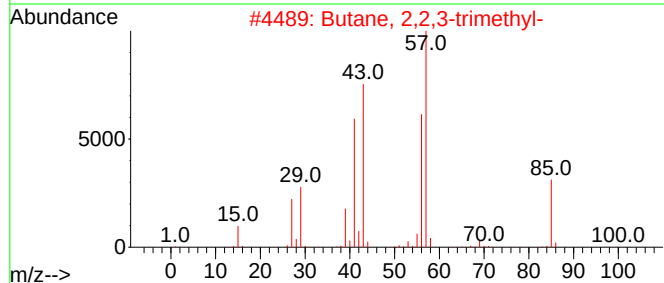
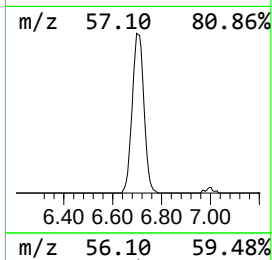
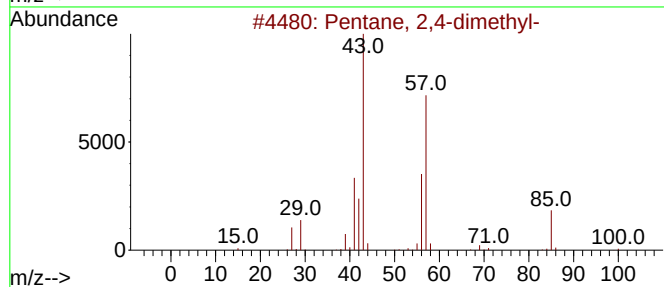
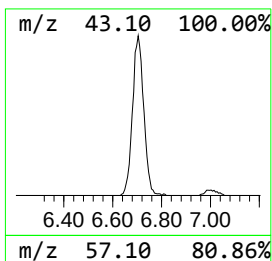
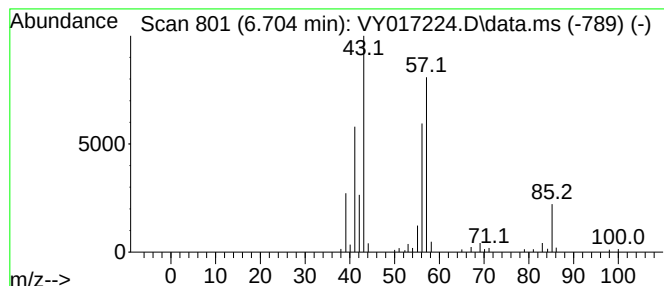
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	19.15 ug/l	106171	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	64
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50
4			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	50
5			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	43



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EB-1-4-6

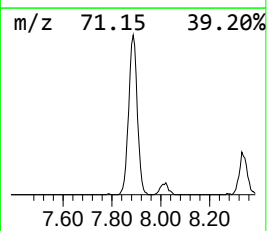
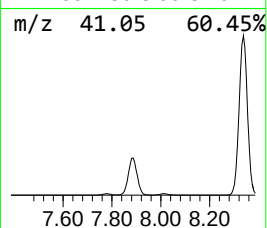
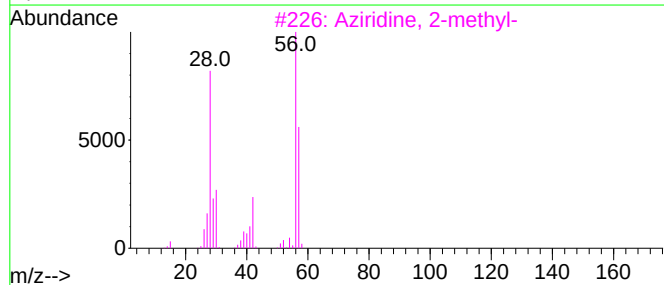
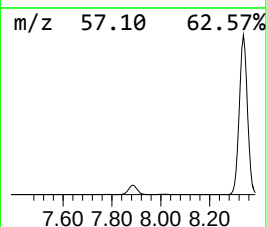
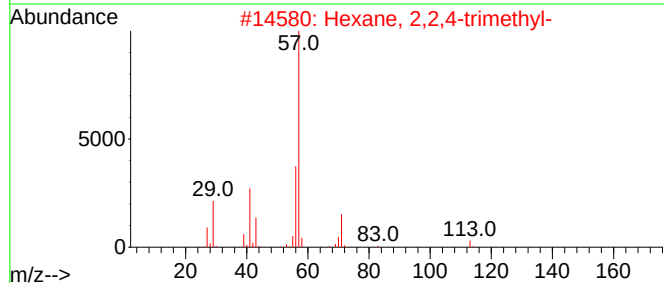
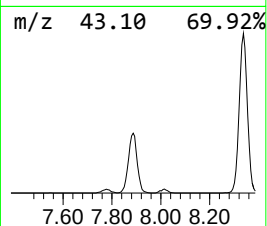
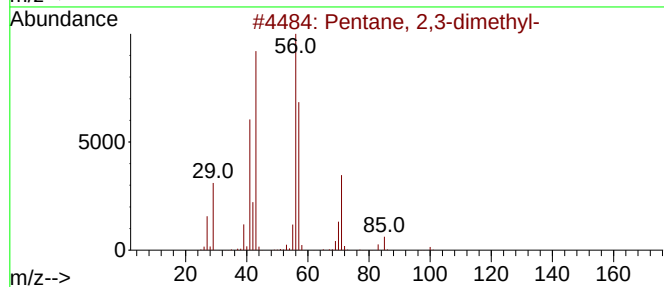
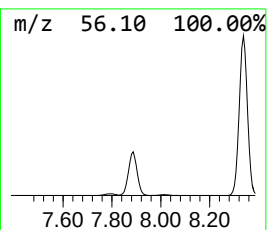
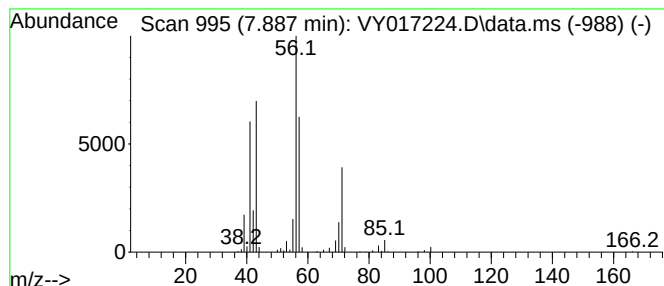
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.887	57.52 ug/l	318947	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50
3			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	38
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020524\
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Operator : SY/MD
Sample : P1366-05
Misc : 4.58g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EB-1-4-6

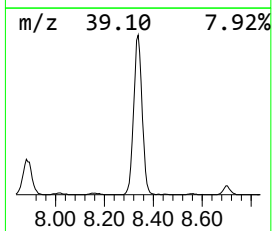
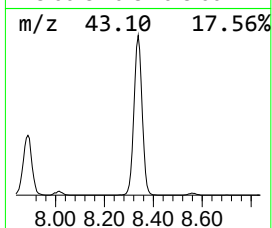
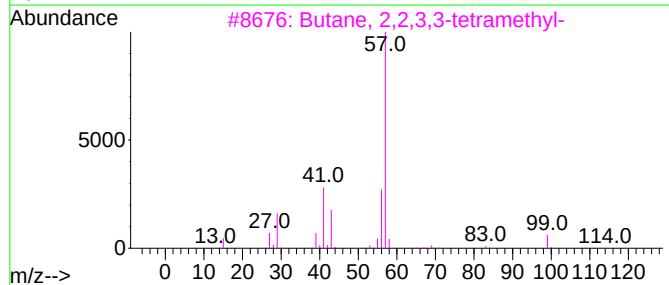
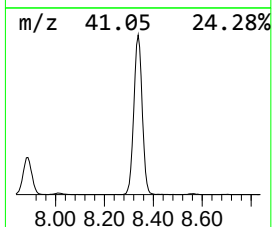
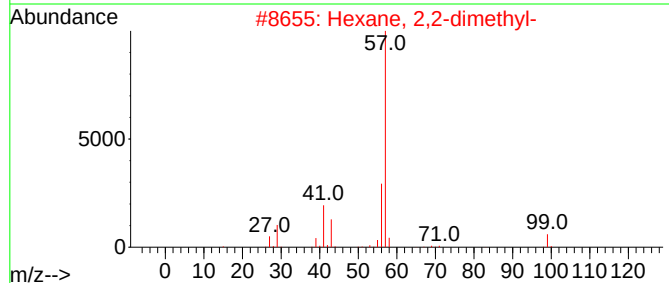
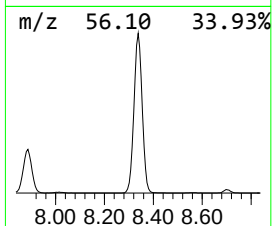
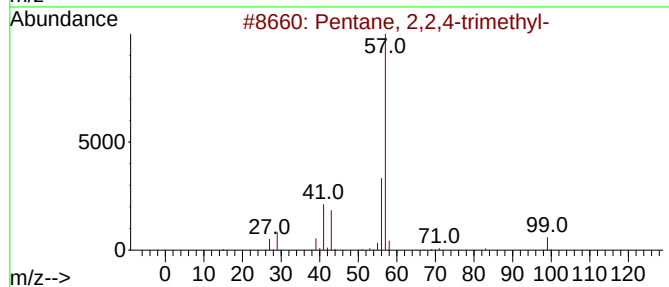
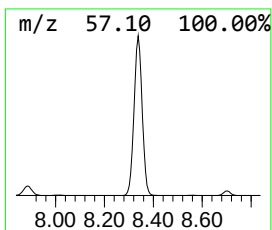
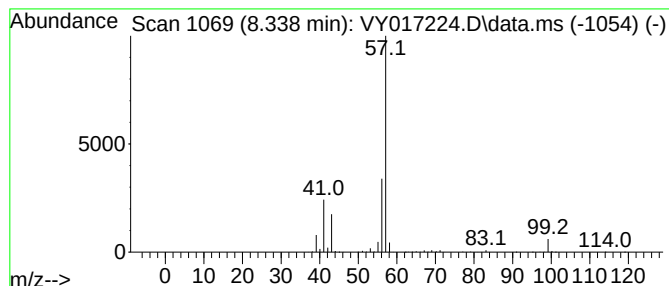
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.338	173.25 ug/l	1538680	1,4-Difluorobenzene	8.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	78
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64



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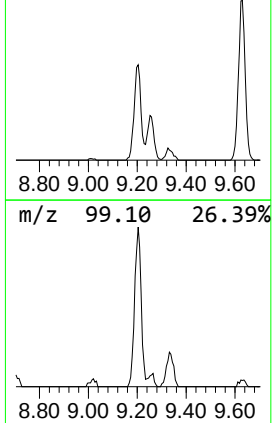
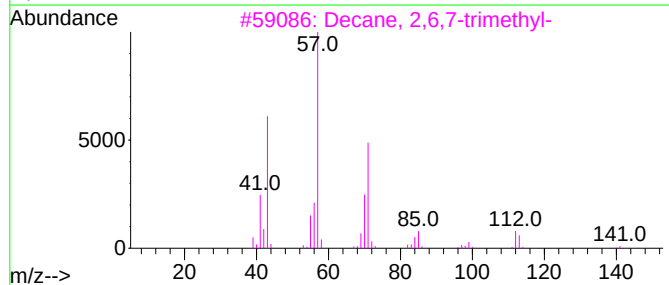
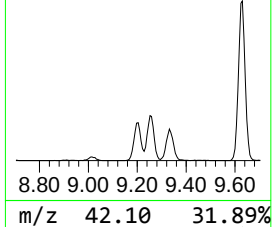
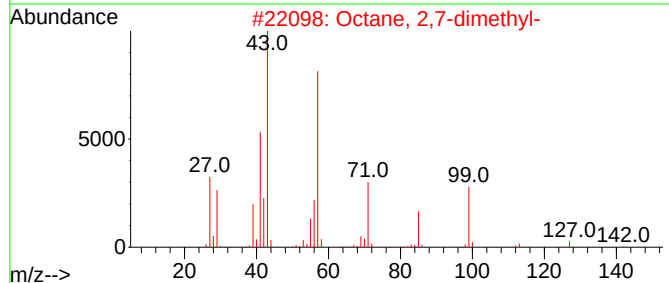
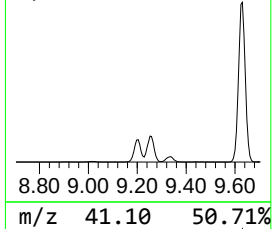
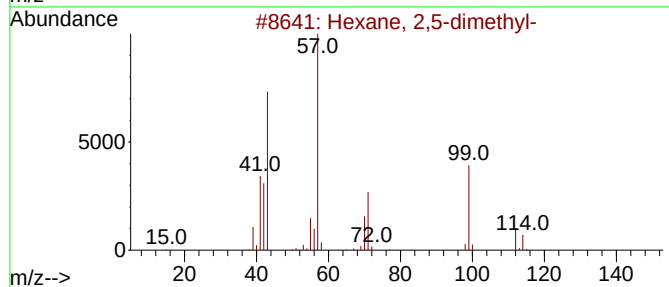
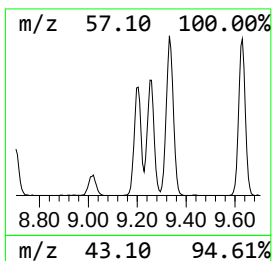
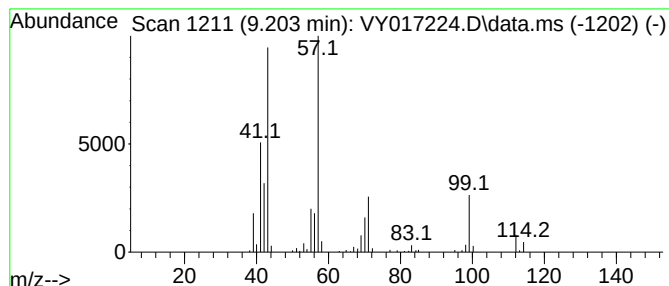
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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

Peak Number 4 Hexane, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.203	21.08 ug/l	187221	1,4-Difluorobenzene	8.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	91
2			Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	59
3			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	53
4			Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	53
5			Pentane, 1-(2-propenyloxy)-	128	C8H16O	023186-70-1	50



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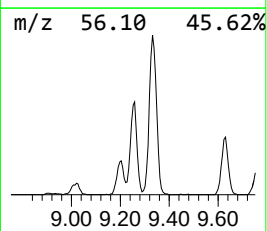
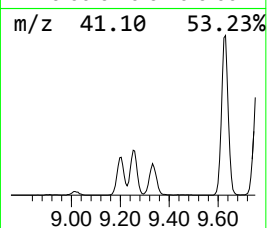
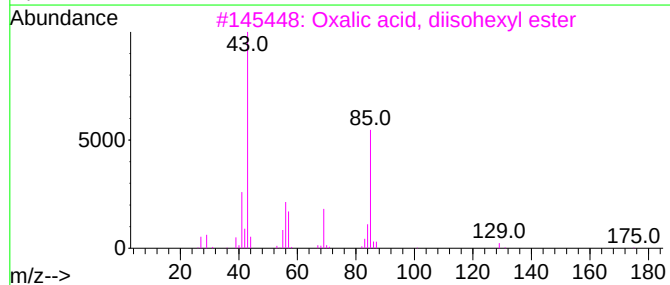
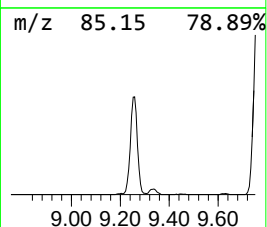
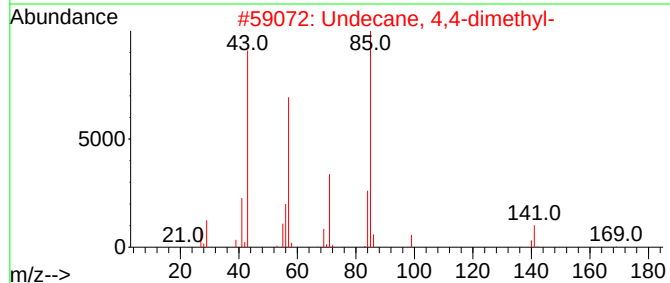
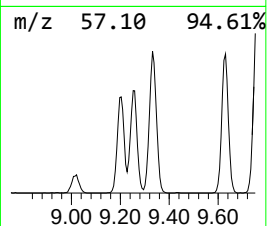
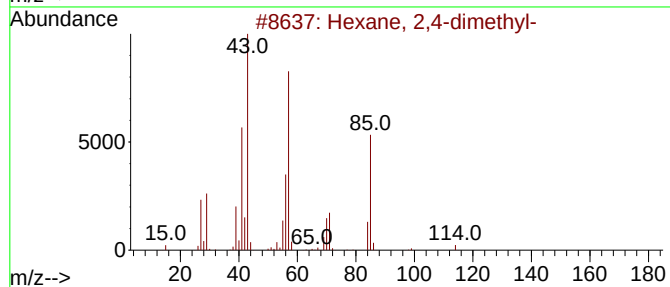
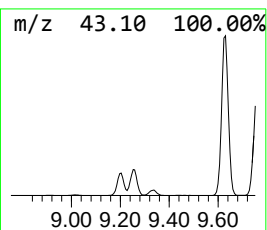
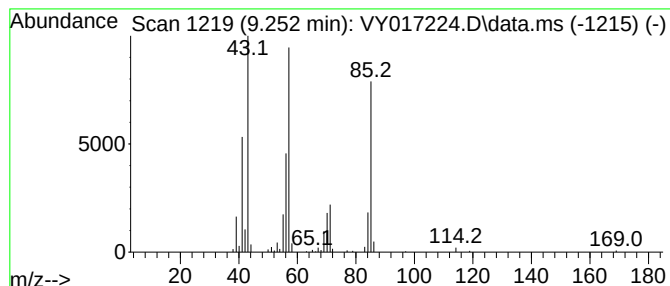
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Quant Title : SW846 8260

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

Peak Number 5 Hexane, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.252	24.81 ug/l	220343	1,4-Difluorobenzene	8.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	96
2			Undecane, 4,4-dimethyl-	184	C13H28	017312-68-4	59
3			Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	59
4			4,4-Dimethyl octane	142	C10H22	015869-95-1	59
5			Sulfurous acid, butyl isohexyl e...	222	C10H22O3S	1000309-17-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020524\
Data File : VY017224.D
Acq On : 05 Feb 2024 13:19
Operator : SY/MD
Sample : P1366-05
Misc : 4.58g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EB-1-4-6

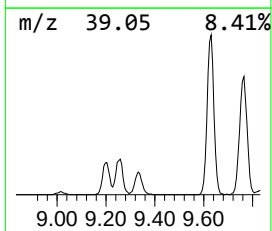
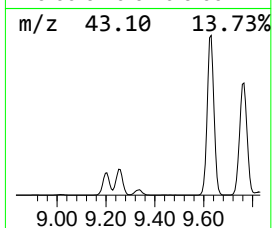
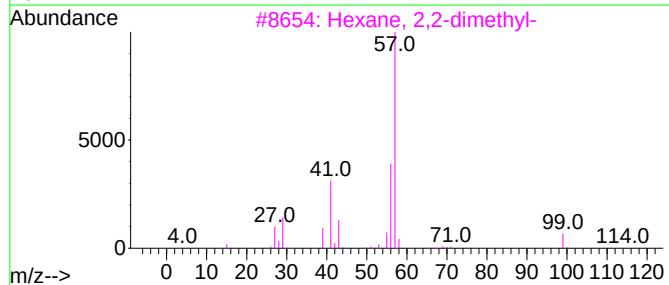
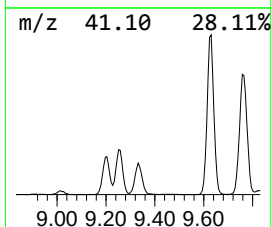
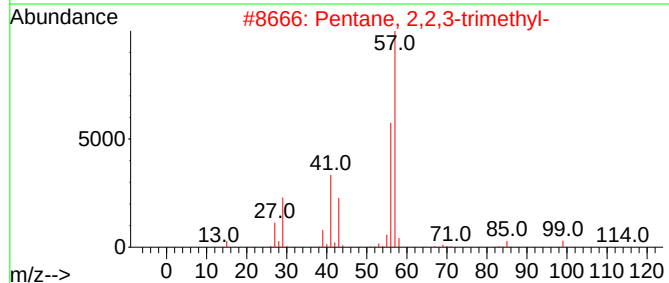
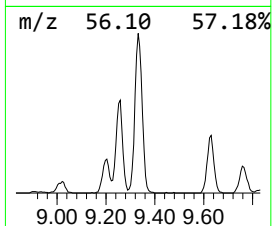
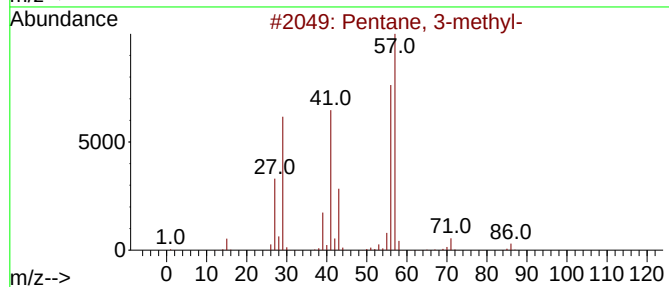
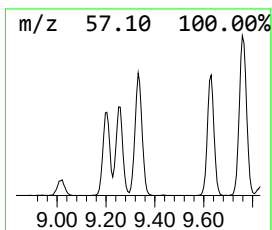
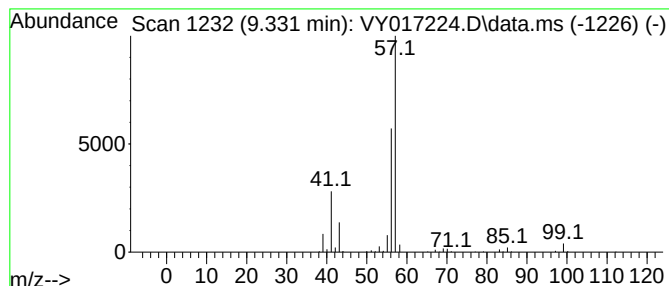
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.331	16.75 ug/l	148718	1,4-Difluorobenzene	8.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	64
2			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	64
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4			Decane, 2,2,8-trimethyl-	184	C13H28	062238-01-1	56
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020524\
Data File : VY017224.D
Acq On : 05 Feb 2024 13:19
Operator : SY/MD
Sample : P1366-05
Misc : 4.58g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EB-1-4-6

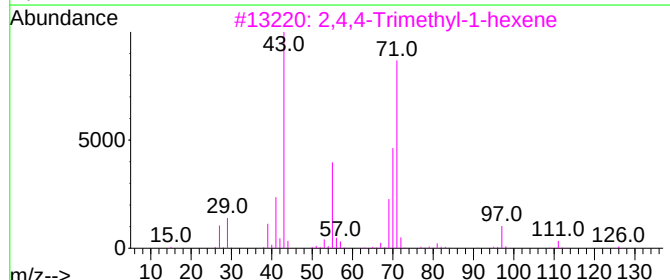
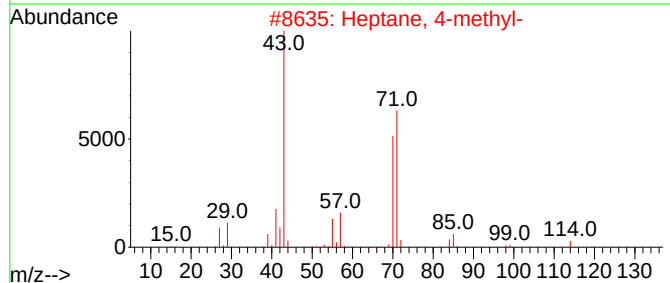
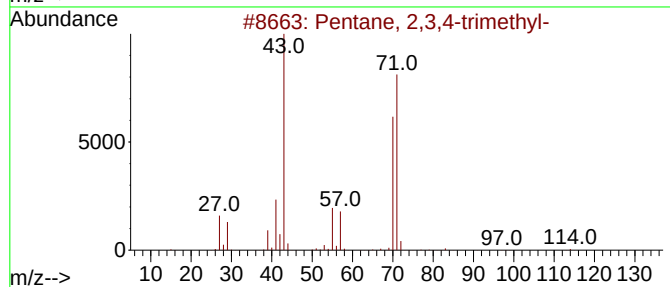
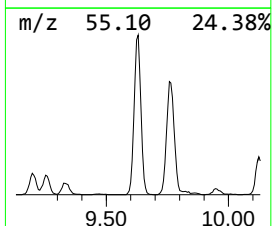
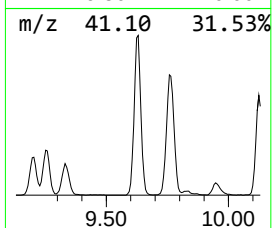
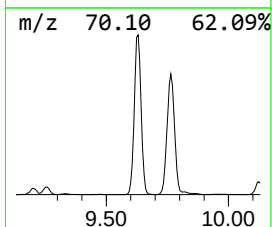
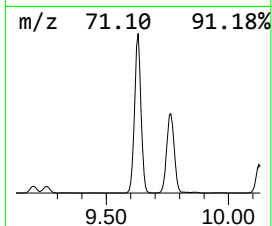
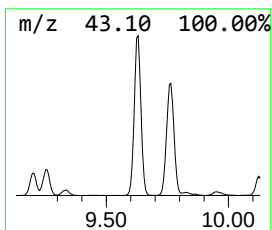
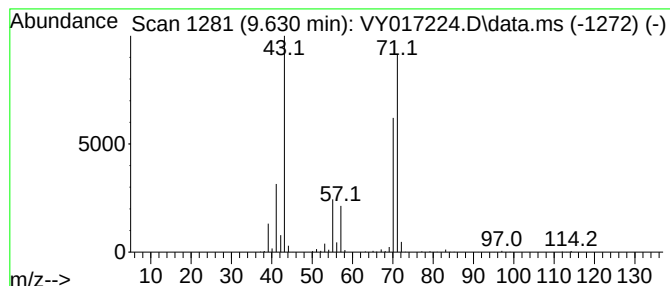
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.630	110.57 ug/l	981986	1,4-Difluorobenzene	8.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020524\
Data File : VY017224.D
Acq On : 05 Feb 2024 13:19
Operator : SY/MD
Sample : P1366-05
Misc : 4.58g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EB-1-4-6

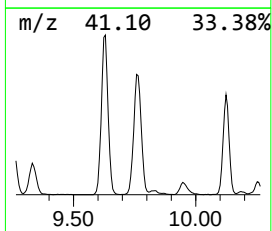
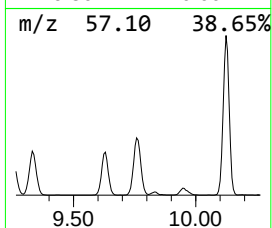
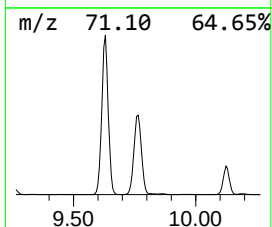
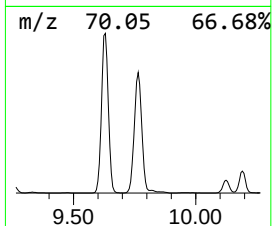
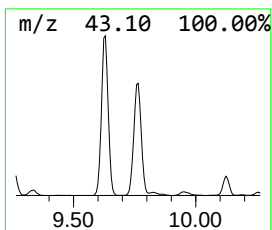
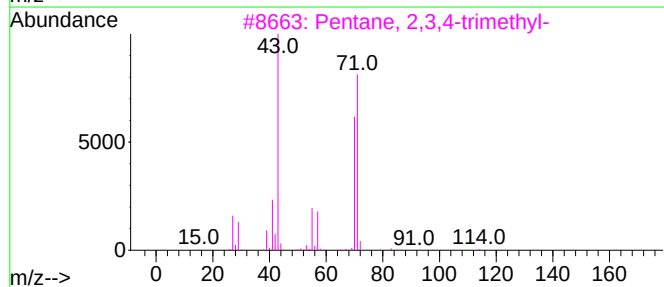
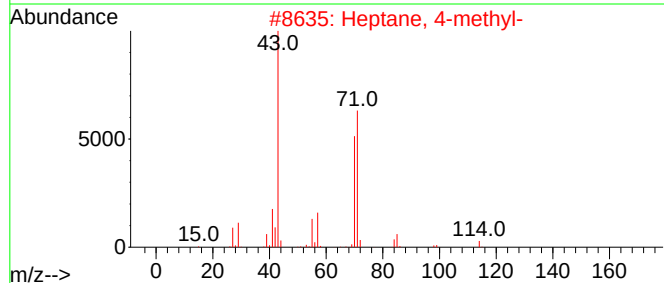
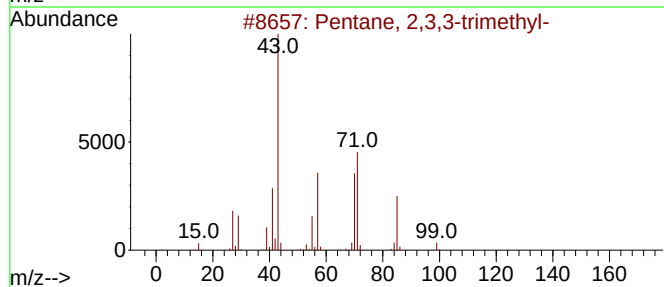
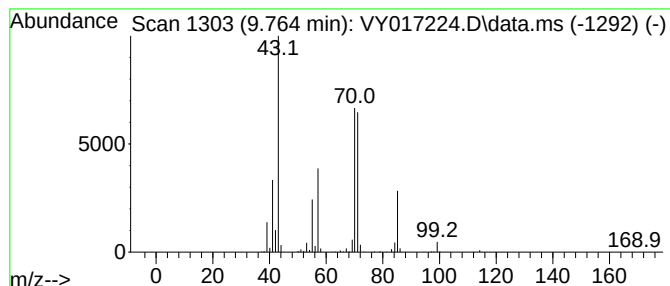
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Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.764	97.77 ug/l	868336	1,4-Difluorobenzene	8.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020524\
Data File : VY017224.D
Acq On : 05 Feb 2024 13:19
Operator : SY/MD
Sample : P1366-05
Misc : 4.58g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

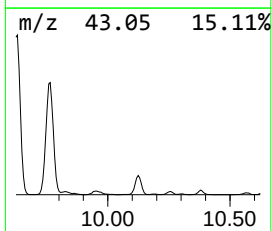
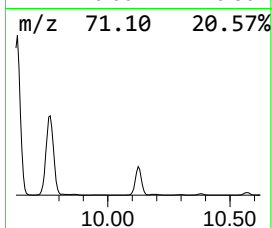
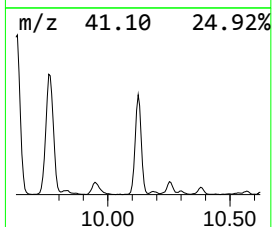
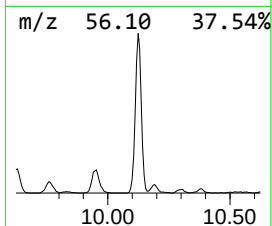
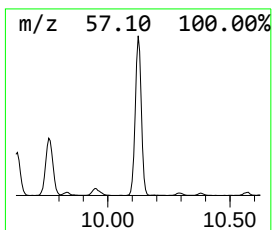
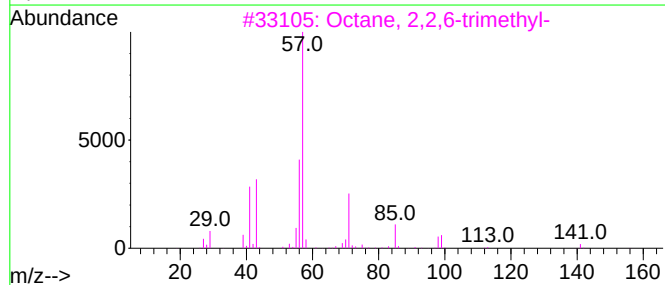
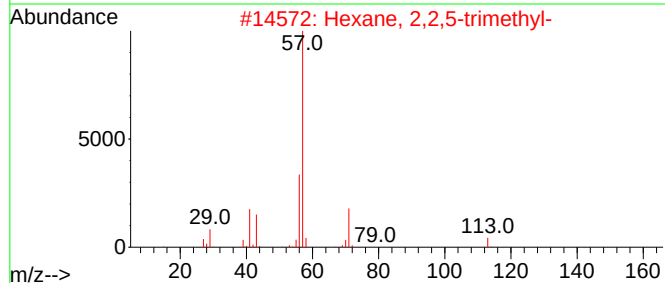
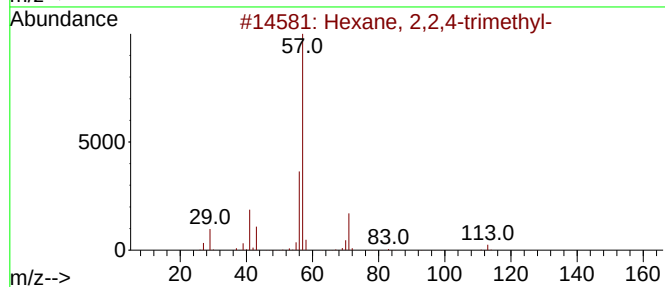
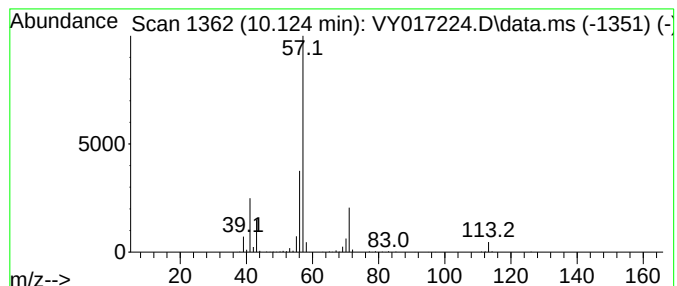
Instrument :
MSVOA_Y
ClientSampleId :
EB-1-4-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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

Peak Number 9 Hexane, 2,2,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.124	33.76 ug/l	456868	Chlorobenzene-d5	11.502	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	83
2	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	83
3	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	72
4	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	64
5	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020524\
Data File : VY017224.D
Acq On : 05 Feb 2024 13:19
Operator : SY/MD
Sample : P1366-05
Misc : 4.58g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EB-1-4-6

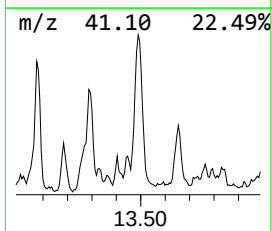
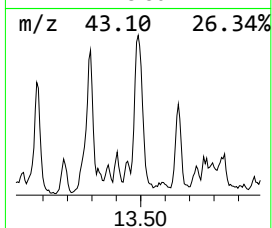
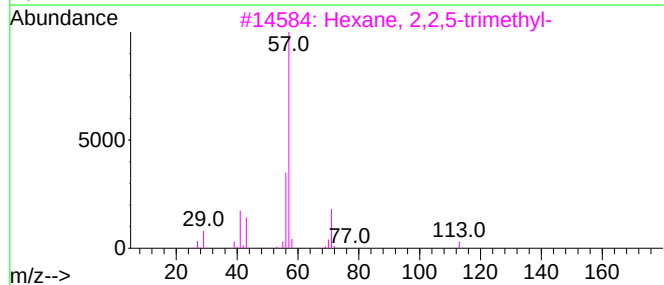
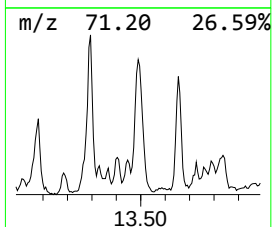
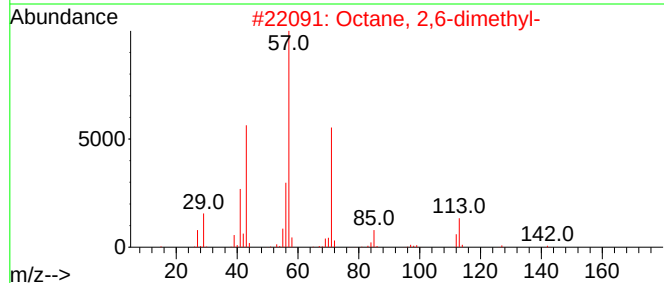
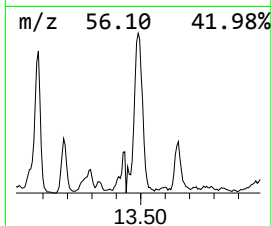
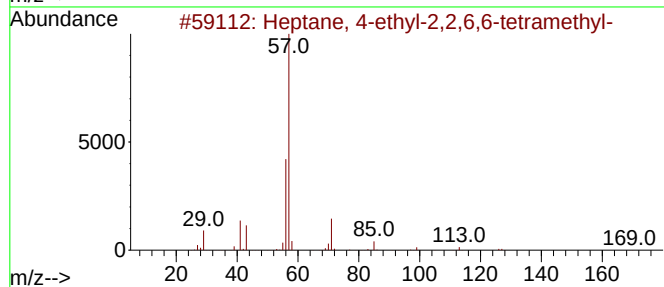
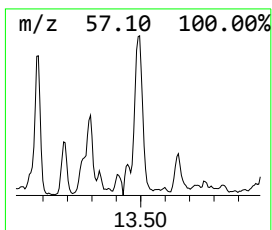
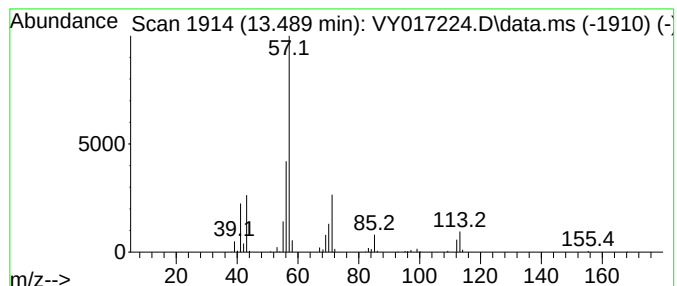
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Quant Title : SW846 8260

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

Peak Number 10 Heptane, 4-ethyl-2,2,6,6-te... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.489	18.70 ug/l	196361	1,4-Dichlorobenzene-d4	13.434

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 4-ethyl-2,2,6,6-tetrame...	184	C13H28	062108-31-0	72
2		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
3		Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64
4		Heptane, 5-ethyl-2,2,3-trimethyl-	170	C12H26	062199-06-8	64
5		Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020524\
Data File : VY017224.D
Acq On : 05 Feb 2024 13:19
Operator : SY/MD
Sample : P1366-05
Misc : 4.58g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EB-1-4-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.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, 2,3-di...	7.887	57.5	ug/l	318947	1	7.801	277225	50.0
Pentane, 2,2,4-...	8.338	173.3	ug/l	1538680	2	8.704	444056	50.0
Hexane, 2,5-dim...	9.203	21.1	ug/l	187221	2	8.704	444056	50.0
Hexane, 2,4-dim...	9.252	24.8	ug/l	220343	2	8.704	444056	50.0
Pentane, 3-methyl-	9.331	16.8	ug/l	148718	2	8.704	444056	50.0
Pentane, 2,3,4-...	9.630	110.6	ug/l	981986	2	8.704	444056	50.0
Pentane, 2,3,3-...	9.764	97.8	ug/l	868336	2	8.704	444056	50.0
Hexane, 2,2,4-t...	10.124	33.8	ug/l	456868	3	11.502	676543	50.0
Heptane, 4-ethy...	13.489	18.7	ug/l	196361	4	13.434	525158	50.0