

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY040921\
 Data File : VY004359.D
 Acq On : 09 Apr 2021 15:46
 Operator : SY/MD
 Sample : M1983-02
 Misc : 2.35G/5ML/MSVOA_Y/SOIL
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 16873

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\82Y032921S.M

Title : SW846 8260

Signal : TIC: VY004359.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.960	340	351	386	rBV	2260672	6366211	8.23%	1.385%
2	6.539	760	774	788	rBV	818199	2753009	3.56%	0.599%
3	6.704	788	801	810	rVV	1467148	4680260	6.05%	1.018%
4	6.808	810	818	833	rVV	672983	2105870	2.72%	0.458%
5	7.539	919	938	955	rBV	2707509	7755703	10.03%	1.687%
6	7.777	955	977	987	rVV2	22732390	61151921	79.08%	13.303%
7	7.887	987	995	1006	rVV	10500235	25881817	33.47%	5.630%
8	8.021	1006	1017	1033	rVV	27919919	76605167	99.07%	16.665%
9	8.283	1049	1060	1067	rVV3	5620343	13898320	17.97%	3.023%
10	8.356	1067	1072	1078	rVV2	1936058	4396922	5.69%	0.957%
11	8.429	1078	1084	1095	rVB	2461567	5507397	7.12%	1.198%
12	8.557	1095	1105	1120	rBV	17997193	36060918	46.64%	7.845%
13	8.697	1120	1128	1143	rBV	469437	972768	1.26%	0.212%
14	9.008	1172	1179	1187	rVB	519813	1041006	1.35%	0.226%
15	9.191	1195	1209	1215	rBV	5963674	14306738	18.50%	3.112%
16	9.246	1215	1218	1226	rVB	1074089	1923992	2.49%	0.419%
17	9.374	1232	1239	1245	rBV	1345957	2437921	3.15%	0.530%
18	9.466	1245	1254	1261	rVB2	446387	1252839	1.62%	0.273%
19	9.612	1270	1278	1288	rVB2	403124	804371	1.04%	0.175%
20	9.764	1291	1303	1307	rBV	464254	895562	1.16%	0.195%
21	9.825	1307	1313	1316	rVV	760209	1350845	1.75%	0.294%
22	9.965	1325	1336	1348	rBV	836995	2320986	3.00%	0.505%
23	10.185	1364	1372	1376	rBV2	1927413	3716400	4.81%	0.808%
24	10.252	1376	1383	1390	rVB	32891781	77325476	100.00%	16.822%
25	10.374	1396	1403	1410	rVB4	1104907	2413394	3.12%	0.525%
26	10.526	1423	1428	1436	rVB	632633	1111872	1.44%	0.242%
27	10.624	1436	1444	1450	rBV	783804	1557463	2.01%	0.339%
28	11.038	1508	1512	1516	rVV	1011102	1560765	2.02%	0.340%
29	11.093	1516	1521	1527	rVB	875358	1517333	1.96%	0.330%
30	11.295	1543	1554	1564	rVB4	705320	2145943	2.78%	0.467%
31	11.709	1612	1622	1631	rVV4	1882259	5581351	7.22%	1.214%
32	12.002	1663	1670	1672	rBV3	558040	1058476	1.37%	0.230%
33	12.032	1673	1675	1682	rVV	623203	924398	1.20%	0.201%
34	12.496	1745	1751	1759	rVB2	1021383	1908332	2.47%	0.415%
35	12.806	1798	1802	1808	rVB2	1146273	1786452	2.31%	0.389%
36	12.916	1813	1820	1826	rBV	29395914	54588884	70.60%	11.875%

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37	13.154	1848	1859	1868	rBV	10380623	16837546	21.77%	3.663%
38	13.245	1869	1874	1879	rVV	1599386	2403444	3.11%	0.523%
39	13.489	1907	1914	1922	rVB2	1721004	3158682	4.08%	0.687%
40	13.751	1952	1957	1962	rBV	825950	1161424	1.50%	0.253%
41	14.404	2057	2064	2071	rVB	465257	1045221	1.35%	0.227%
42	14.611	2093	2098	2103	rVB	983369	1326959	1.72%	0.289%
43	15.141	2180	2185	2192	rBV2	594312	1264428	1.64%	0.275%
44	15.434	2229	2233	2241	rVB	515376	813278	1.05%	0.177%

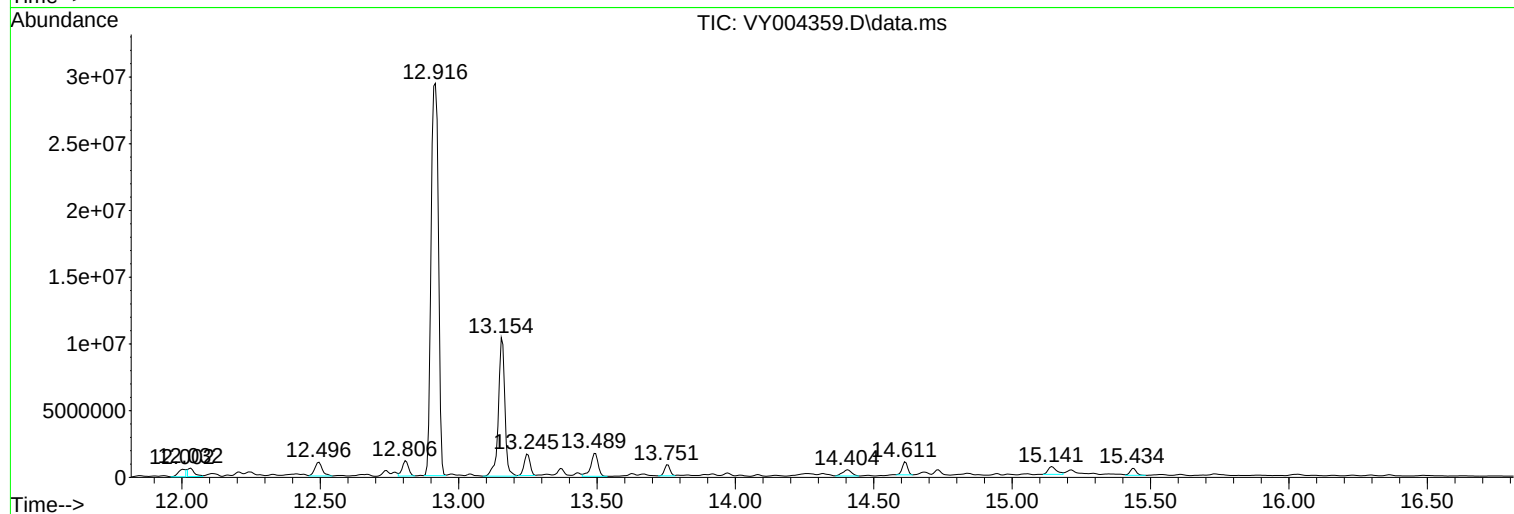
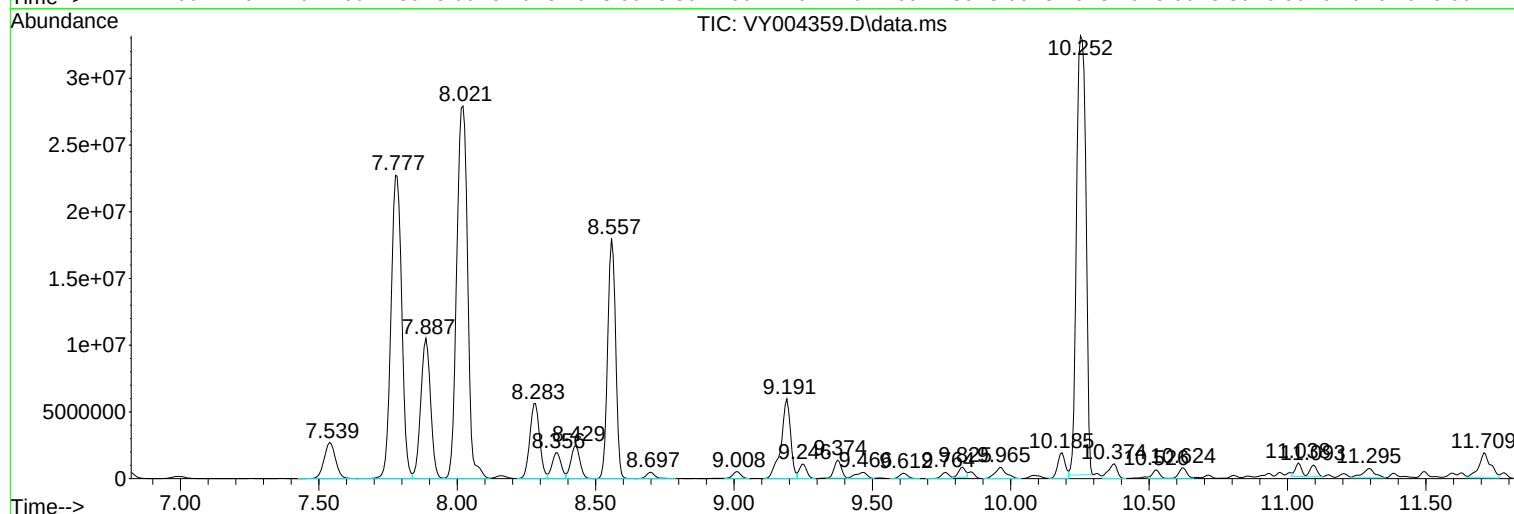
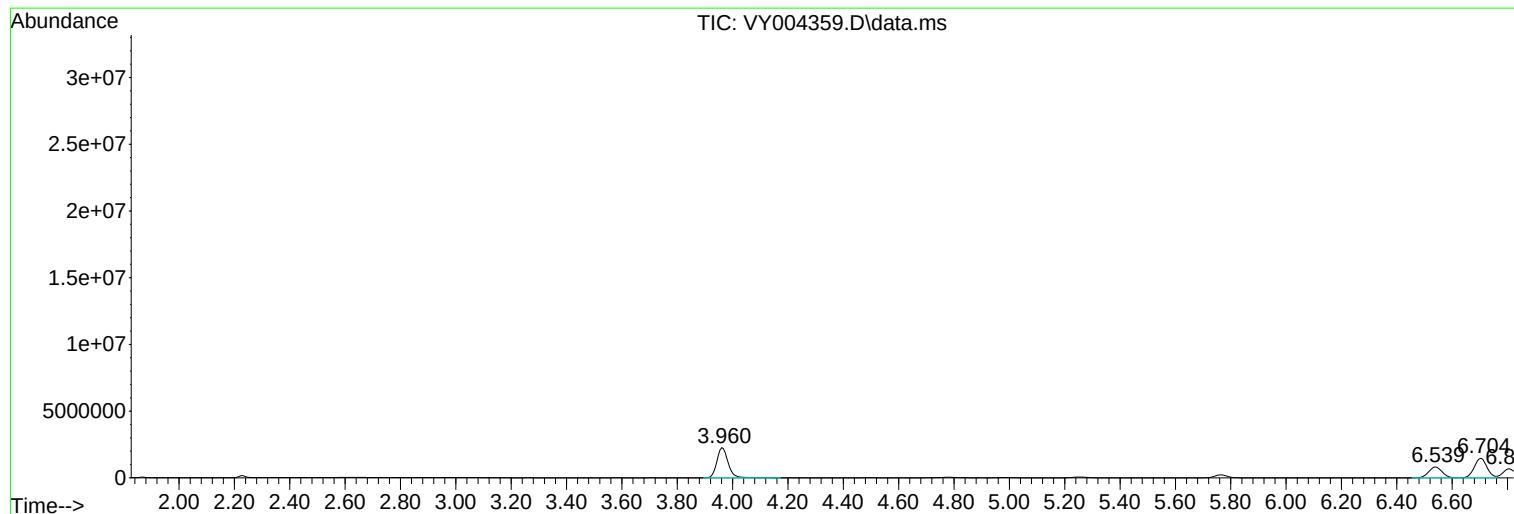
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032921S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Misc : 2.35G/5ML/MSVOA_Y/SOIL
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Instrument :
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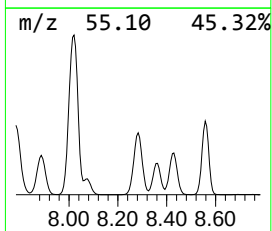
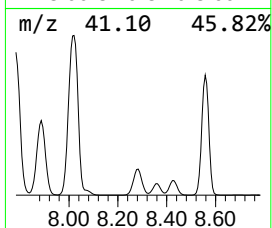
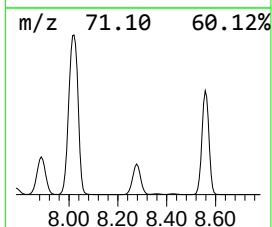
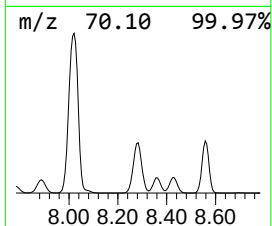
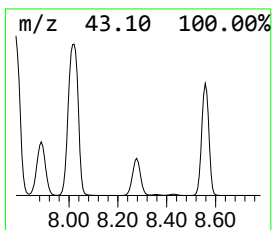
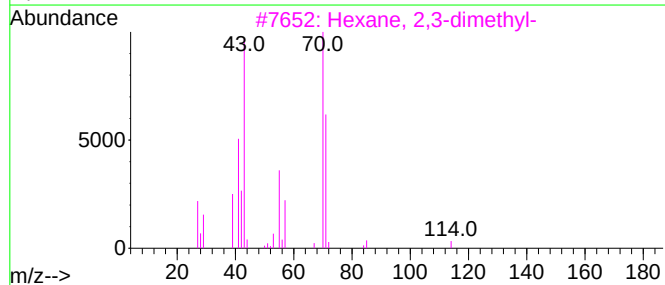
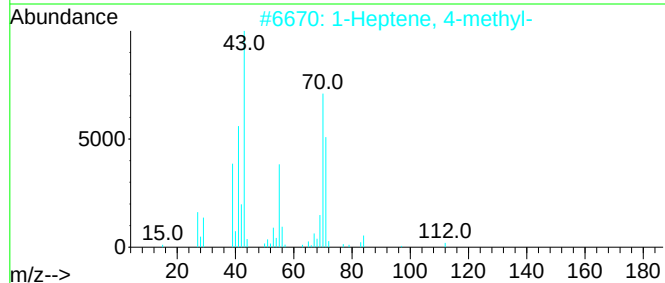
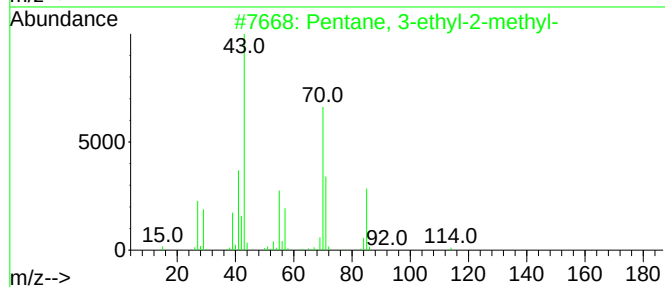
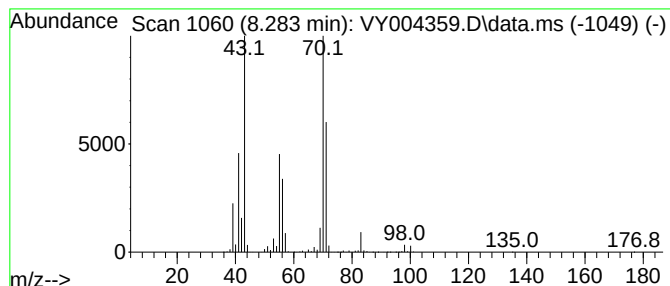
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032921S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Pentane, 3-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.283	714.37 ug/l	13898300	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	72
2			1-Heptene, 4-methyl-	112	C8H16	013151-05-8	64
3			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	45
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	43
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	43



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Instrument :
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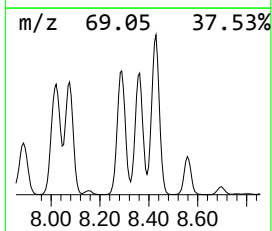
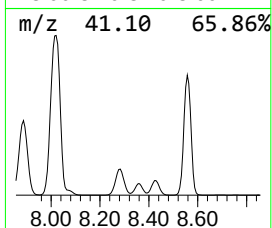
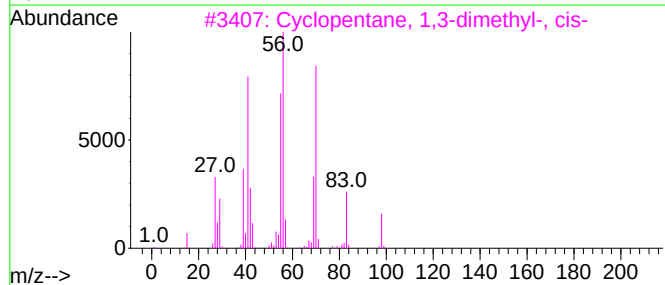
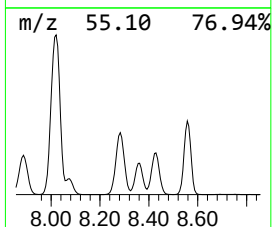
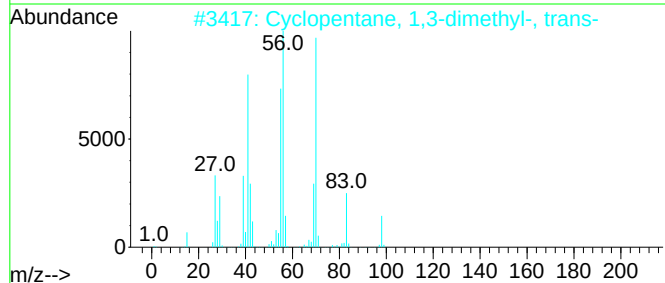
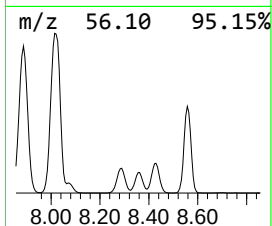
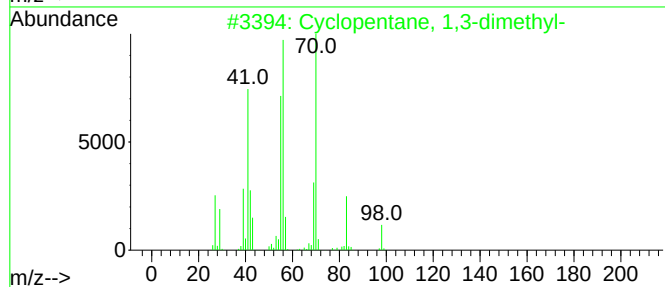
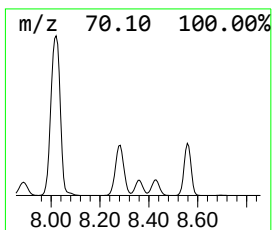
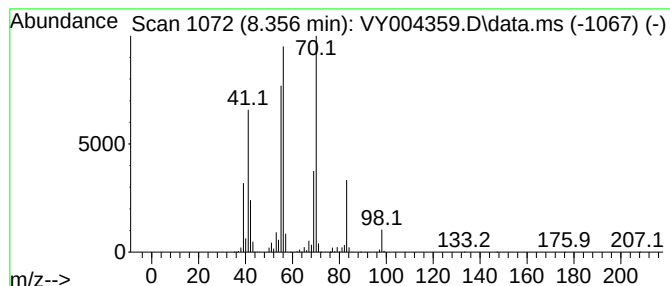
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032921S.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclopentane, 1,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.356	226.00 ug/l	4396920	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	91
2			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	87
3			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	87
4			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	64
5			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	59



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Misc : 2.35G/5ML/MSVOA_Y/SOIL
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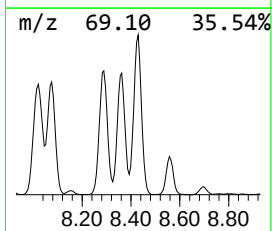
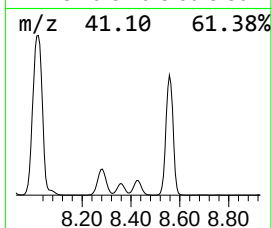
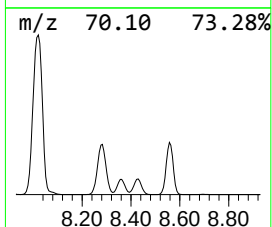
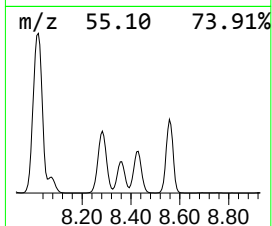
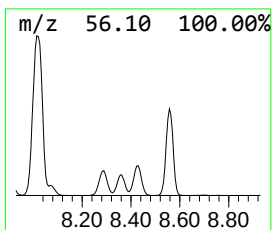
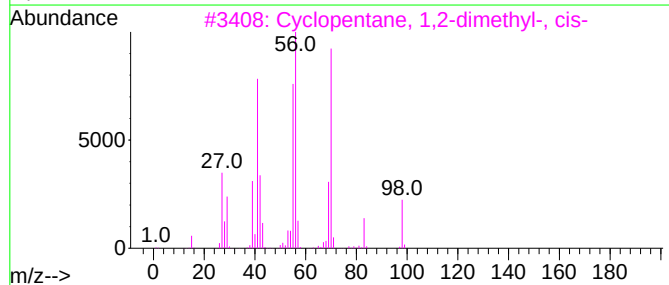
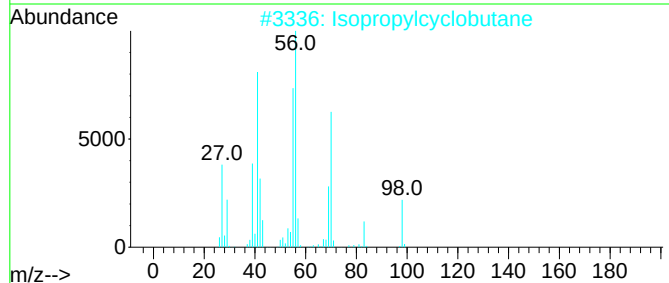
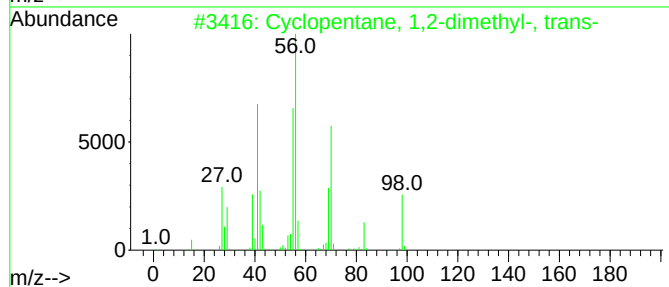
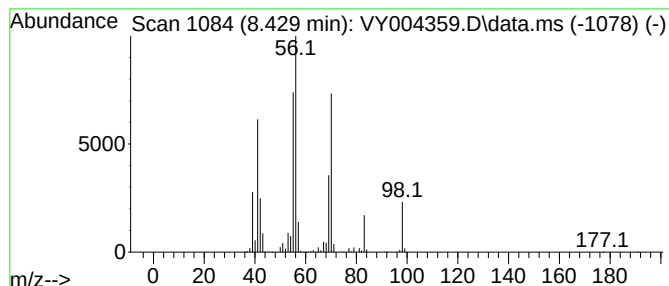
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Peak Number 3 Cyclopentane, 1,2-dimethyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.429	283.08 ug/l	5507400	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	95
2			Isopropylcyclobutane	98	C7H14	000872-56-0	93
3			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	91
4			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	91
5			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	90



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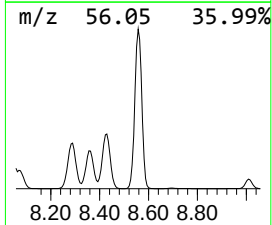
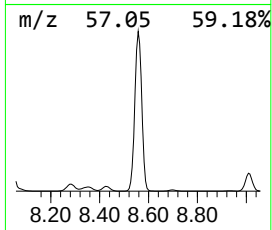
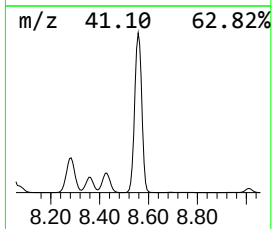
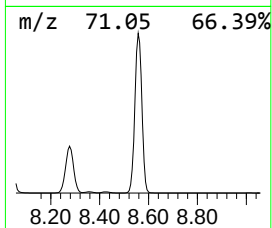
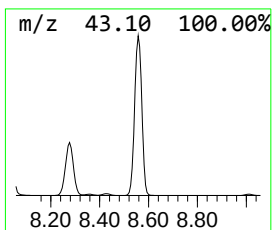
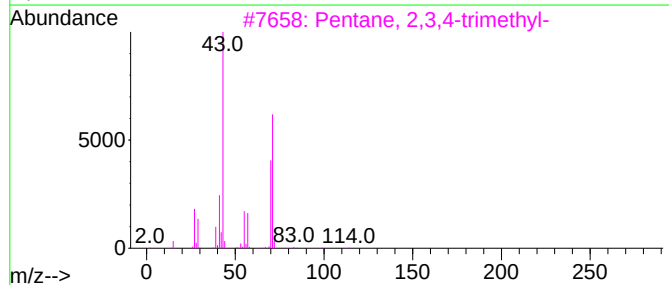
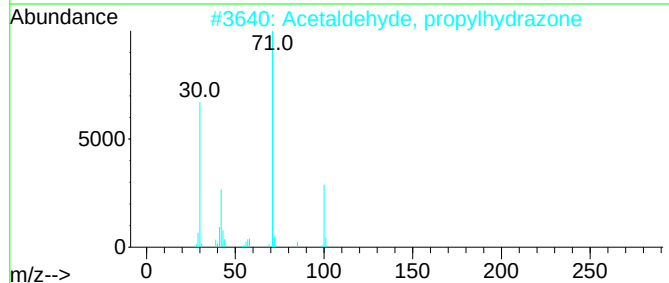
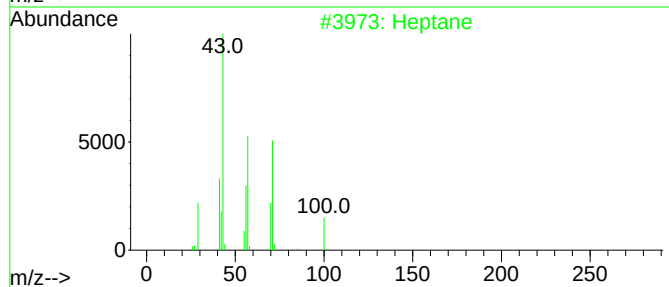
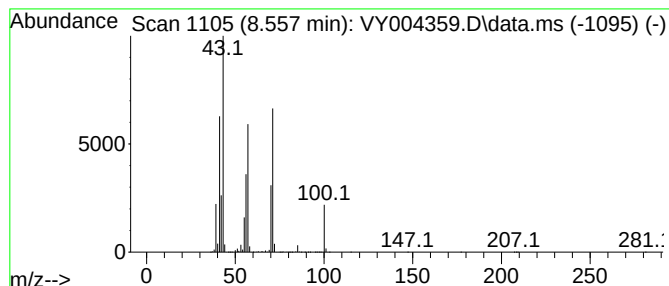
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.557	1853.52 ug/l	36060900	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	49
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	40
4			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	40
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	40



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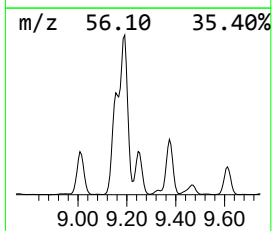
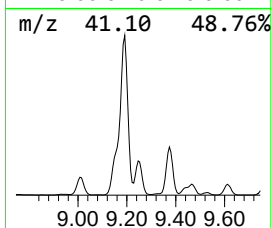
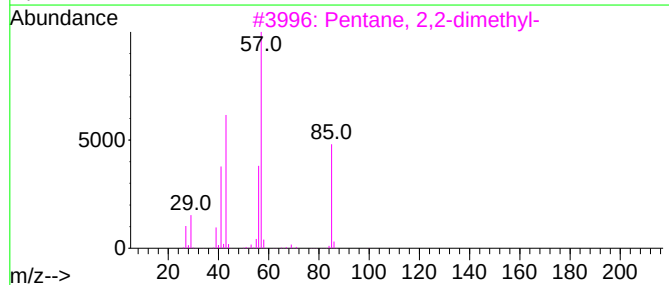
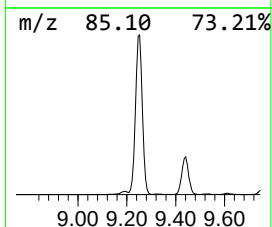
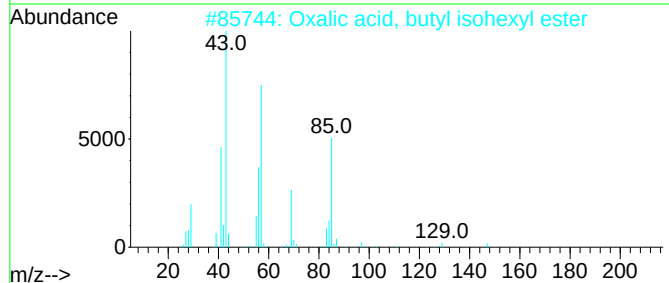
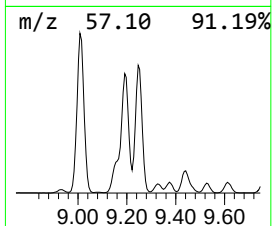
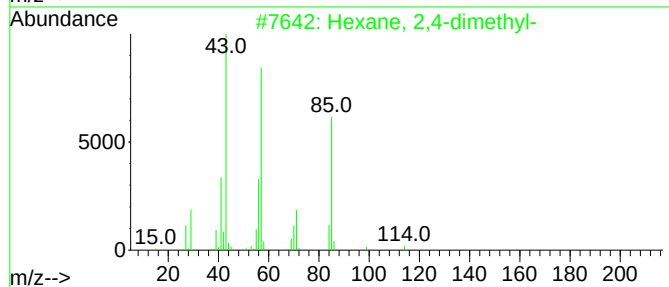
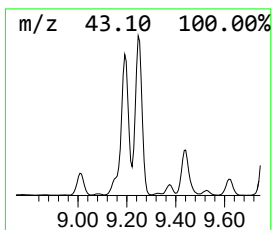
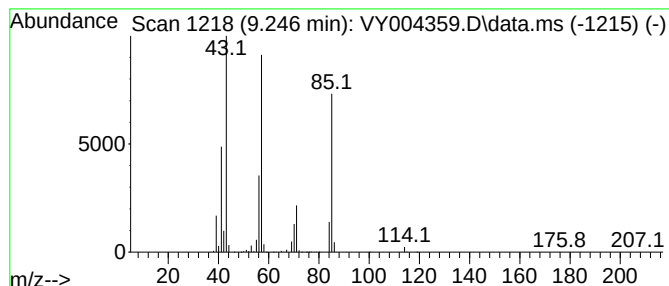
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexane, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.246	98.89 ug/l	1923990	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	95
2			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	72
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64
4			Sulfurous acid, butyl hexyl ester	222	C10H22O3S	1000309-17-3	64
5			Hexane, 2-methyl-	100	C7H16	000591-76-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY040921\
Data File : VY004359.D
Acq On : 09 Apr 2021 15:46
Operator : SY/MD
Sample : M1983-02
Misc : 2.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
16873

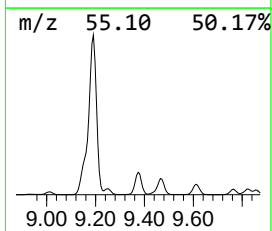
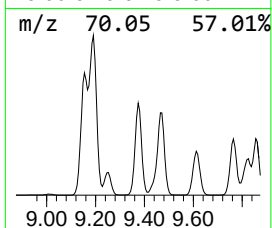
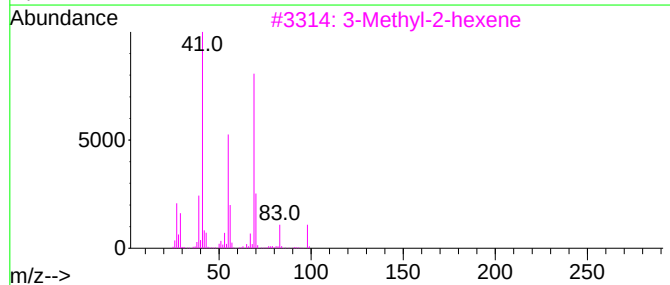
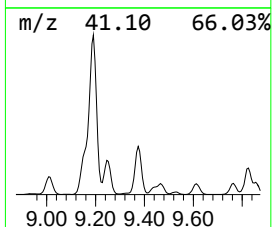
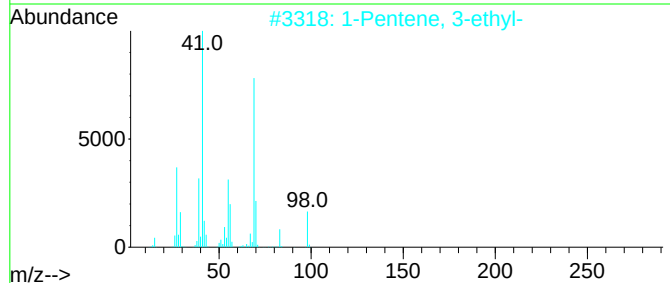
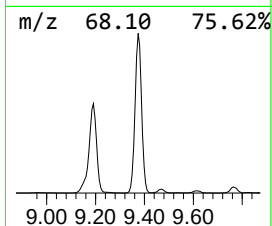
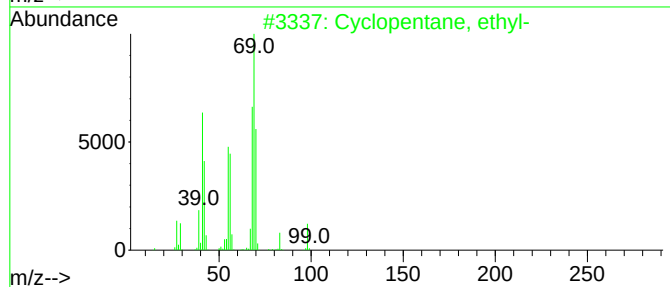
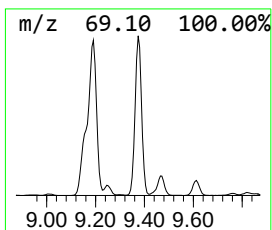
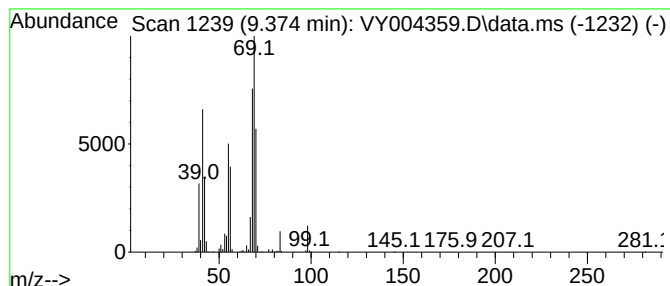
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopentane, ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.374	125.31 ug/l	2437920	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, ethyl-	98	C7H14	001640-89-7	97
2			1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	43
3			3-Methyl-2-hexene	98	C7H14	017618-77-8	38
4			3-Hexene, 3-methyl-, (E)-	98	C7H14	003899-36-3	35
5			Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY040921\
Data File : VY004359.D
Acq On : 09 Apr 2021 15:46
Operator : SY/MD
Sample : M1983-02
Misc : 2.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
16873

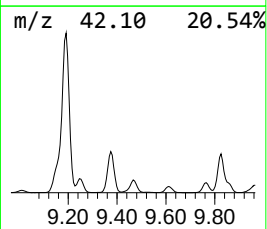
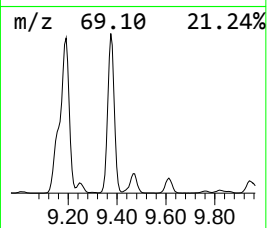
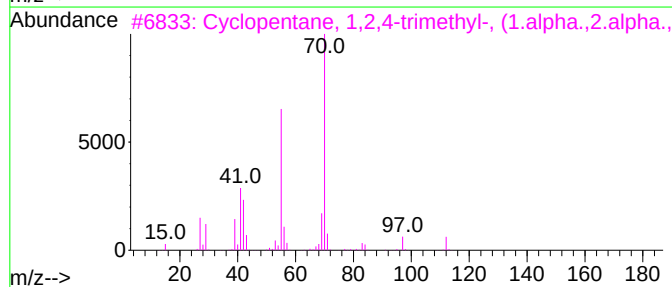
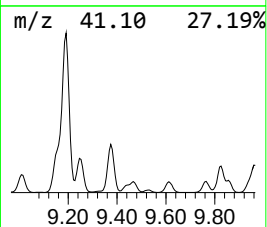
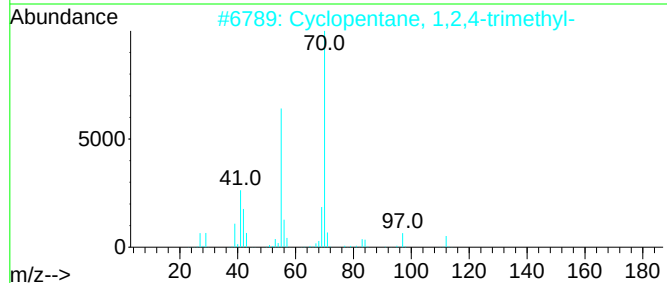
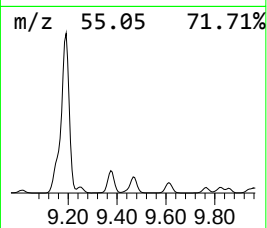
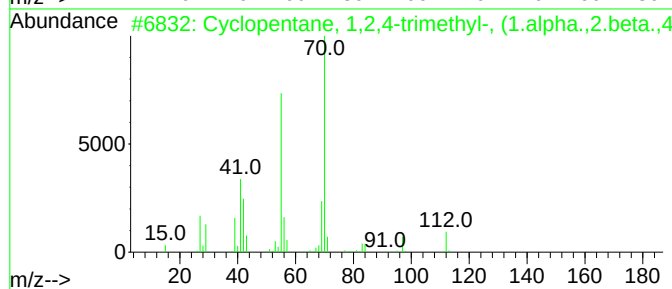
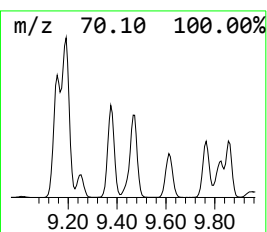
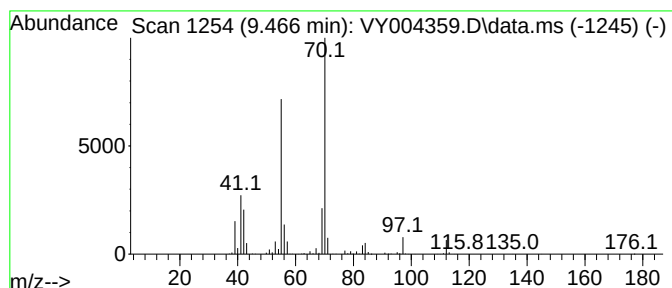
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclopentane, 1,2,4-trimeth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.466	64.40 ug/l	1252840	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	016883-48-0	94
2			Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	91
3			Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	004850-28-6	91
4			Hexane, 2-methyl-4-methylene-	112	C8H16	003404-80-6	78
5			Octane, 3-methyl-6-methylene-	140	C10H20	074630-07-2	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY040921\
Data File : VY004359.D
Acq On : 09 Apr 2021 15:46
Operator : SY/MD
Sample : M1983-02
Misc : 2.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
16873

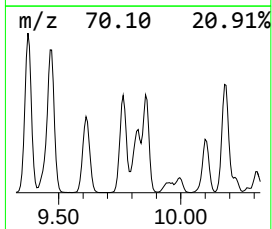
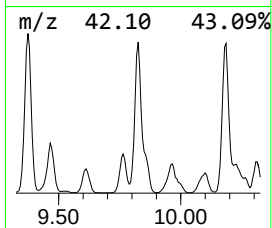
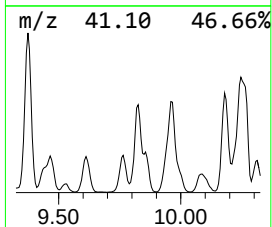
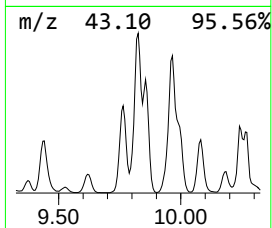
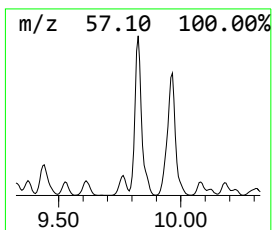
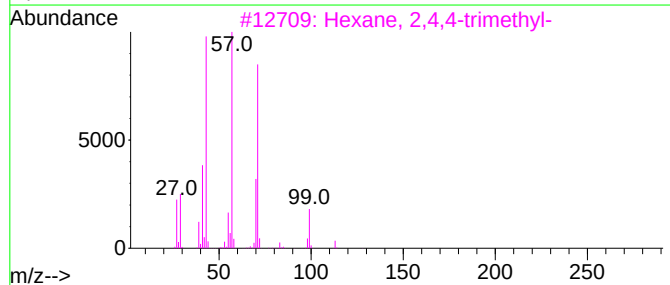
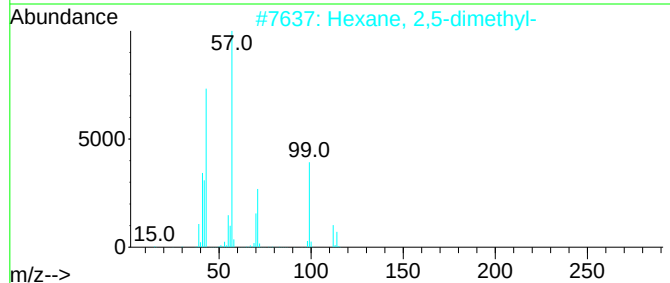
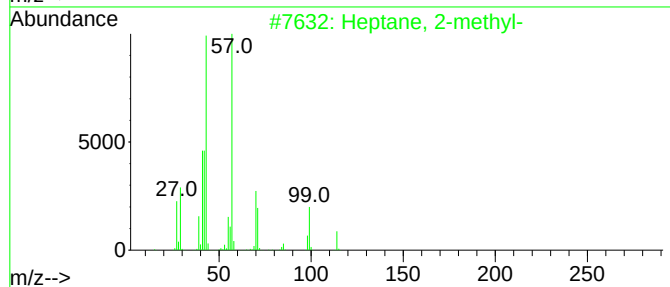
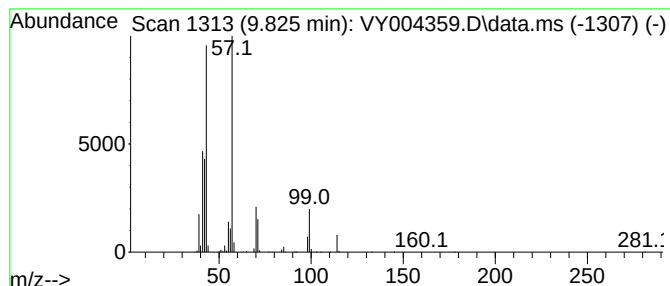
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.825	69.43 ug/l	1350850	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	97
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	72
3			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	37
4			Butane, 1-(ethenyloxy)-3-methyl-	114	C7H14O	039782-38-2	35
5			Heptane, 3-ethyl-	128	C9H20	015869-80-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY040921\
Data File : VY004359.D
Acq On : 09 Apr 2021 15:46
Operator : SY/MD
Sample : M1983-02
Misc : 2.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
16873

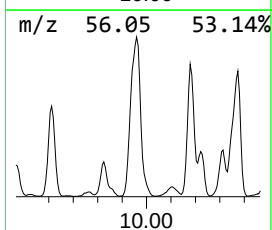
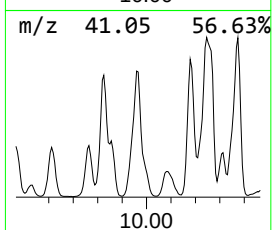
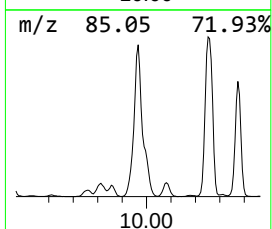
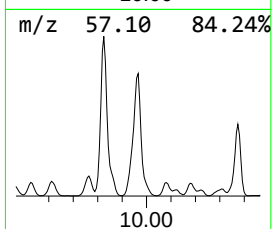
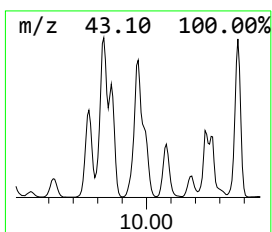
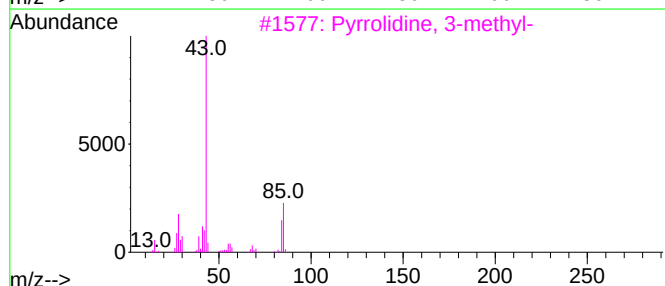
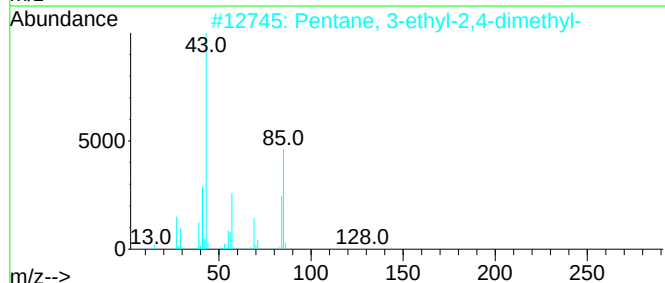
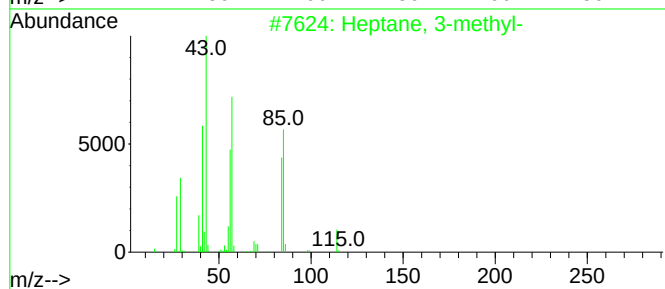
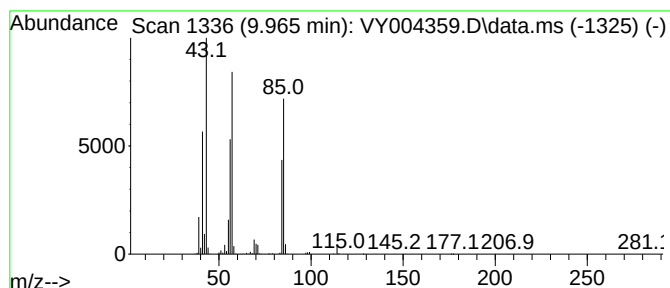
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032921S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.965	119.30 ug/l	2320990	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	94
2			Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53
3			Pyrrolidine, 3-methyl-	85	C5H11N	034375-89-8	50
4			Pentane, 2,3,3,4-tetramethyl-	128	C9H20	016747-38-9	50
5			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY040921\
Data File : VY004359.D
Acq On : 09 Apr 2021 15:46
Operator : SY/MD
Sample : M1983-02
Misc : 2.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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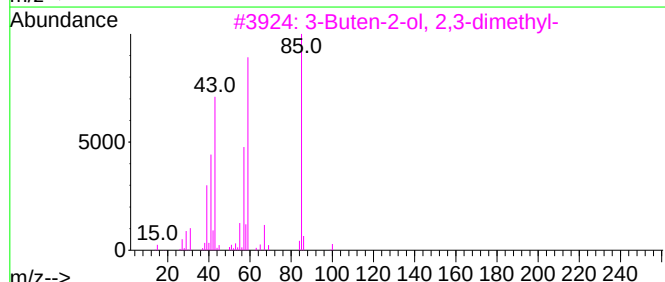
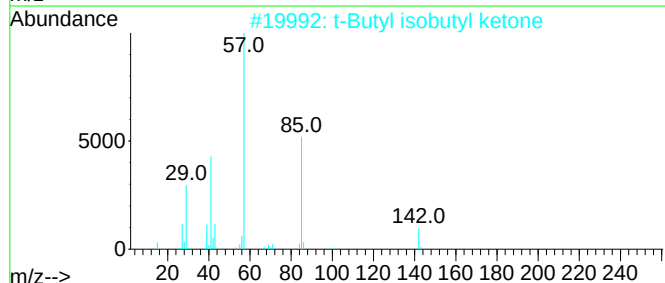
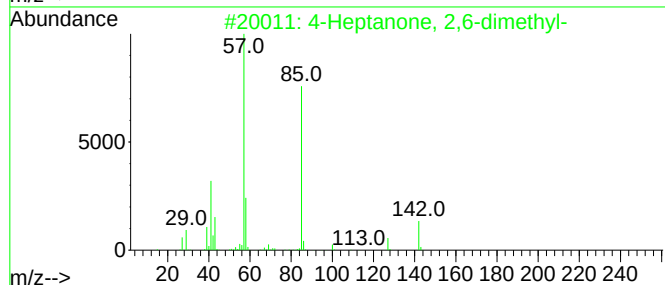
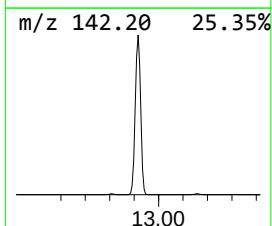
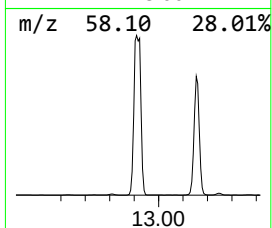
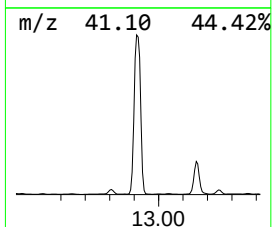
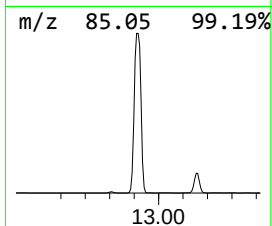
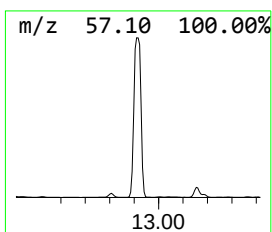
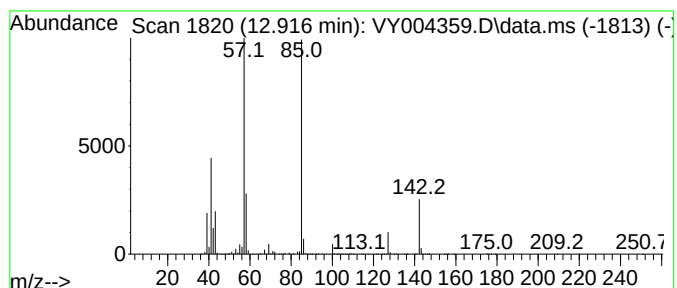
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032921S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 4-Heptanone, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.916	864.11 ug/l	54588900	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
3			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50
4			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	43
5			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY040921\
Data File : VY004359.D
Acq On : 09 Apr 2021 15:46
Operator : SY/MD
Sample : M1983-02
Misc : 2.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
16873

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032921S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Cyclopentane, 1...	8.356	226.0	ug/l	4396920	2	8.697	972768	50.0
Cyclopentane, 1...	8.429	283.1	ug/l	5507400	2	8.697	972768	50.0
Heptane	8.557	1853.5	ug/l	36060900	2	8.697	972768	50.0
Hexane, 2,4-dim...	9.246	98.9	ug/l	1923990	2	8.697	972768	50.0
Cyclopentane, e...	9.374	125.3	ug/l	2437920	2	8.697	972768	50.0
Cyclopentane, 1...	9.466	64.4	ug/l	1252840	2	8.697	972768	50.0
Heptane, 2-methyl-	9.825	69.4	ug/l	1350850	2	8.697	972768	50.0
Heptane, 3-methyl-	9.965	119.3	ug/l	2320990	2	8.697	972768	50.0
4-Heptanone, 2,...	12.916	864.1	ug/l	54588900	4	13.428	3158680	50.0