

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051625\
 Data File : VY022295.D
 Acq On : 16 May 2025 16:48
 Operator : SY/MD
 Sample : Q2032-04
 Misc : 6.39g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TP-24

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\82Y051525S.M
 Title : SW846 8260

Signal : TIC: VY022295.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.824	13	17	27	rVB3	24313	39501	2.49%	0.395%
2	2.086	53	60	63	rBV4	11894	30952	1.95%	0.310%
3	2.196	70	78	85	rBV	59720	118282	7.46%	1.183%
4	2.489	120	126	137	rBV8	16462	58980	3.72%	0.590%
5	2.842	178	184	193	rVB	46192	97136	6.12%	0.972%
6	3.177	231	239	249	rVB2	40090	96175	6.06%	0.962%
7	3.872	345	353	362	rBV	10714	29665	1.87%	0.297%
8	4.616	465	475	476	rBV2	16666	36824	2.32%	0.368%
9	5.128	545	559	571	rBV3	23930	87146	5.49%	0.872%
10	5.640	629	643	656	rBV3	62686	199425	12.57%	1.995%
11	7.634	956	970	975	rBV	209105	528531	33.32%	5.286%
12	7.707	975	982	991	rVV	364808	883854	55.73%	8.840%
13	7.786	991	995	1007	rVB4	17794	43317	2.73%	0.433%
14	7.921	1007	1017	1026	rBV	80876	188454	11.88%	1.885%
15	8.061	1031	1040	1053	rBV	200707	455117	28.70%	4.552%
16	8.183	1053	1060	1070	rVB2	11851	27862	1.76%	0.279%
17	8.469	1096	1107	1119	rVB	108249	214731	13.54%	2.148%
18	8.609	1122	1130	1143	rBV	586839	1185961	74.78%	11.862%
19	9.164	1216	1221	1228	rVV2	9369	18097	1.14%	0.181%
20	9.292	1232	1242	1248	rBV4	7637	18085	1.14%	0.181%
21	9.536	1277	1282	1287	rVB2	11957	19582	1.23%	0.196%
22	9.689	1301	1307	1310	rVV2	10917	22960	1.45%	0.230%
23	9.749	1310	1317	1320	rVV	35383	78028	4.92%	0.780%
24	9.780	1320	1322	1328	rVB	27853	36809	2.32%	0.368%
25	9.890	1329	1340	1351	rBV	53739	143756	9.06%	1.438%
26	10.103	1363	1375	1387	rBV	926998	1586038	100.00%	15.864%
27	10.298	1399	1407	1412	rVB	47992	84270	5.31%	0.843%
28	10.359	1412	1417	1421	rBV2	28732	45736	2.88%	0.457%
29	10.481	1433	1437	1441	rBV2	10860	18558	1.17%	0.186%
30	11.085	1529	1536	1541	rVB8	10281	23257	1.47%	0.233%
31	11.200	1547	1555	1559	rBV3	15752	35283	2.22%	0.353%
32	11.304	1566	1572	1578	rBV3	23545	45970	2.90%	0.460%
33	11.414	1583	1590	1602	rVB	836745	1313362	82.81%	13.136%
34	11.524	1602	1608	1612	rBV4	8347	15998	1.01%	0.160%
35	11.652	1624	1629	1636	rVB5	13525	31668	2.00%	0.317%
36	12.401	1743	1752	1763	rVB	582837	947151	59.72%	9.473%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
Title : SW846 8260

37	13.346	1897	1907	1916	rVB	657566	1026270	64.71%	10.265%
38	13.883	1989	1995	2001	rVB2	63469	102584	6.47%	1.026%
39	14.151	2032	2039	2044	rBV4	9660	16989	1.07%	0.170%
40	15.139	2193	2201	2208	rBV	26696	45557	2.87%	0.456%

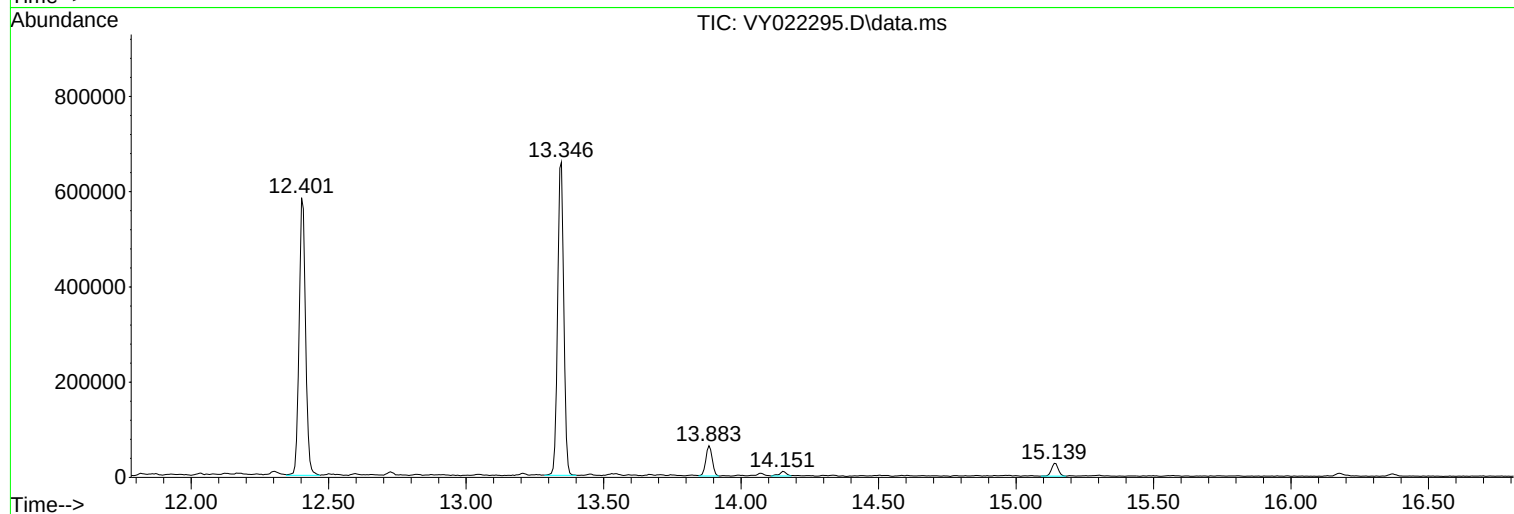
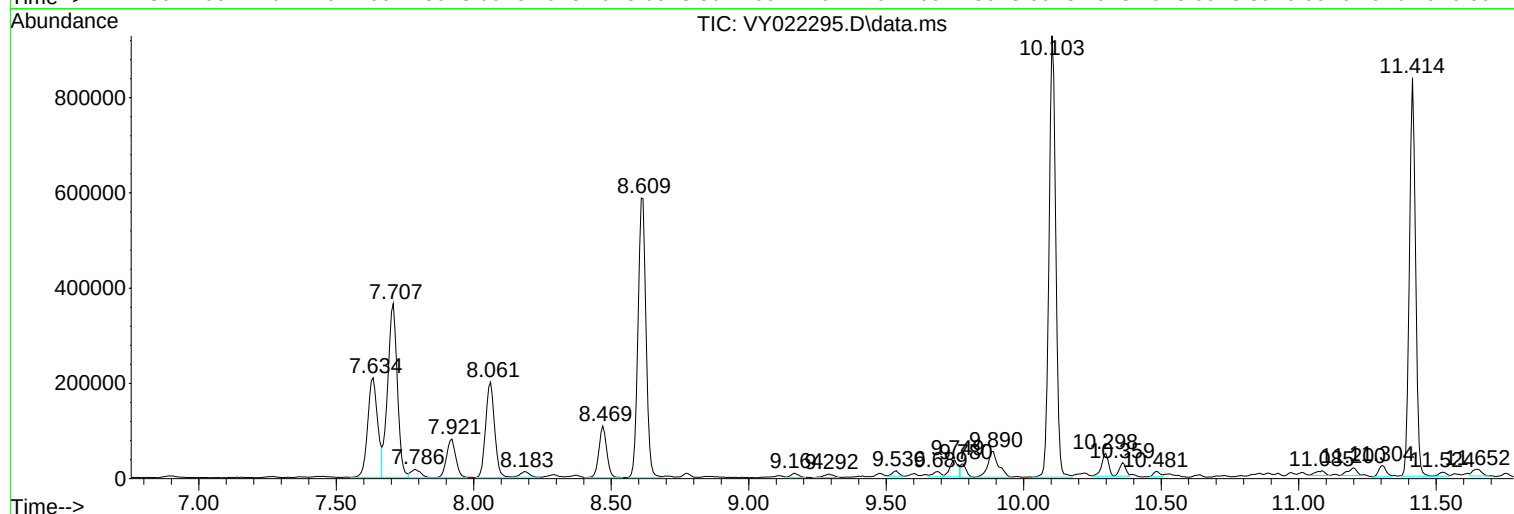
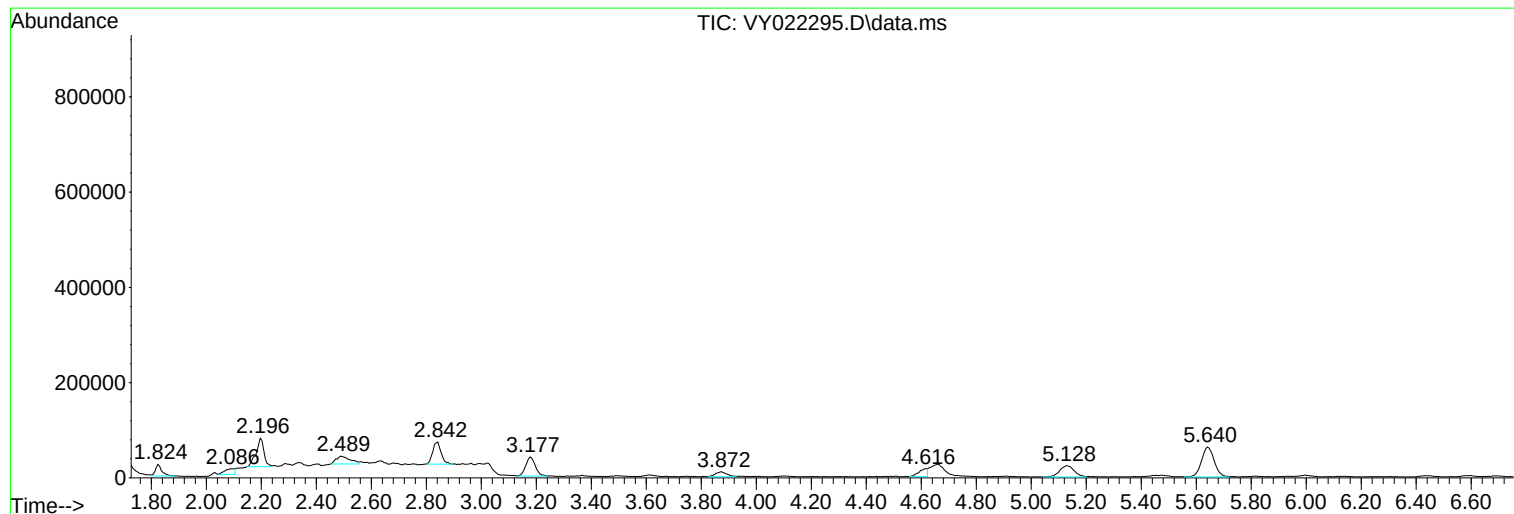
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051625\
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MSVOA_Y
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
Quant Title : SW846 8260

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



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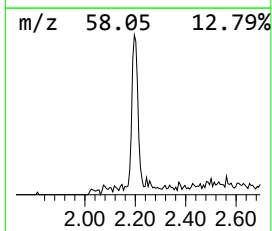
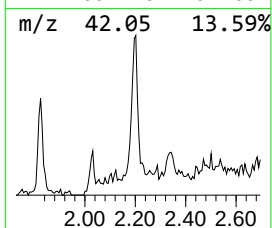
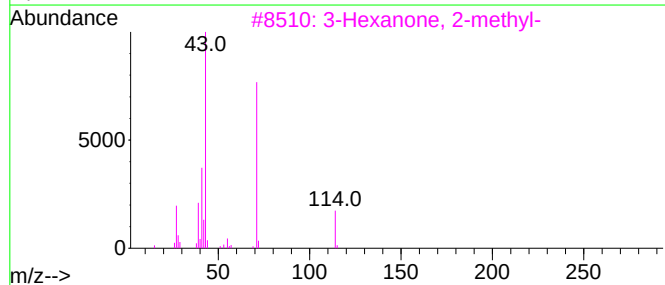
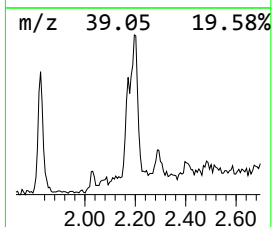
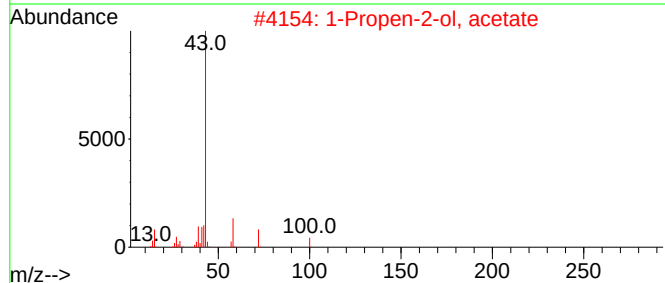
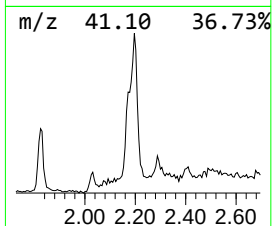
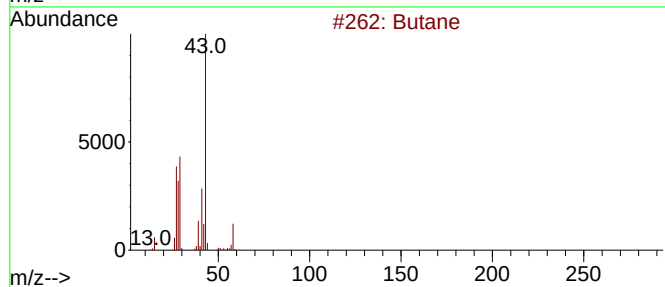
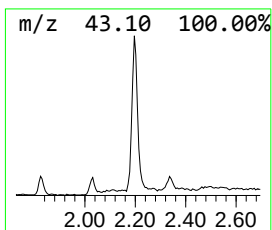
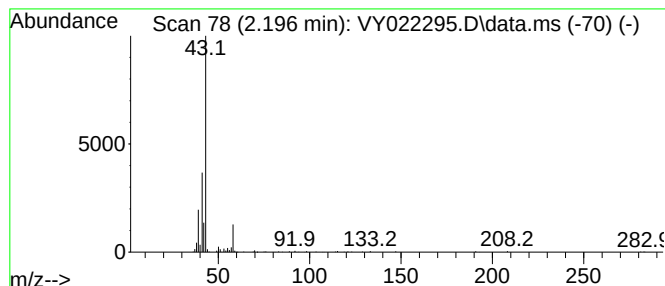
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.196	6.69 ug/l	118282	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	50
2	1-Propen-2-ol, acetate			100	C5H8O2	000108-22-5	39
3	3-Hexanone, 2-methyl-			114	C7H14O	007379-12-6	25
4	Propane, 2-nitro-			89	C3H7NO2	000079-46-9	9
5	Formic acid, chloro-, (3,4,4-tri...			194	C7H11ClO4	107323-92-2	9



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-24

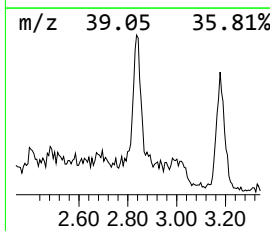
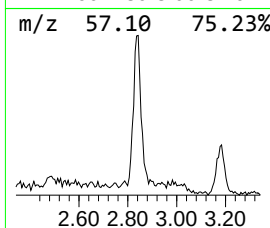
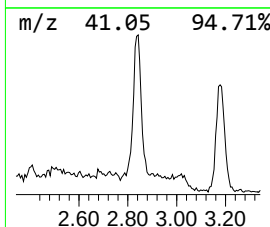
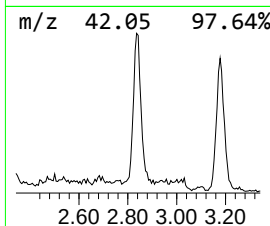
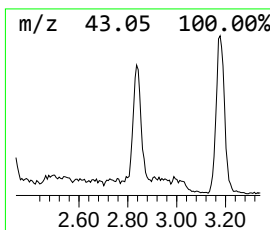
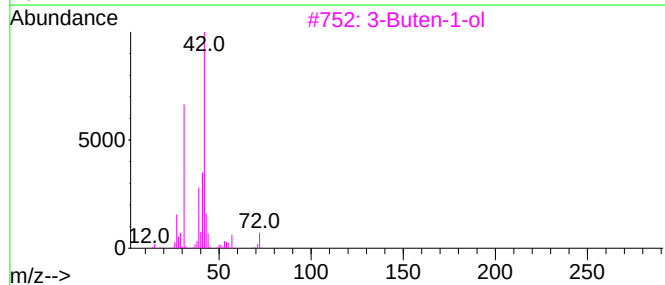
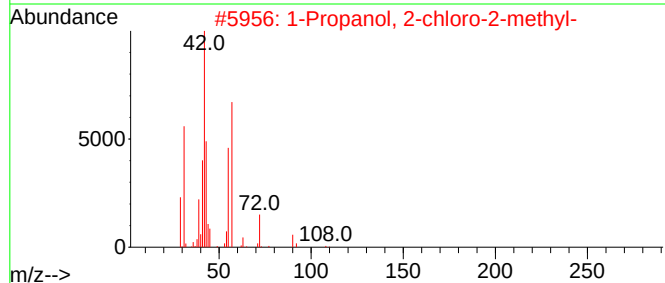
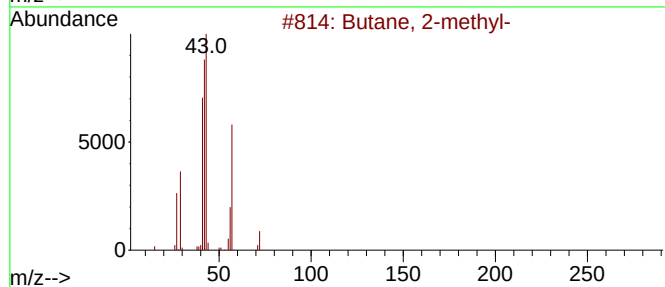
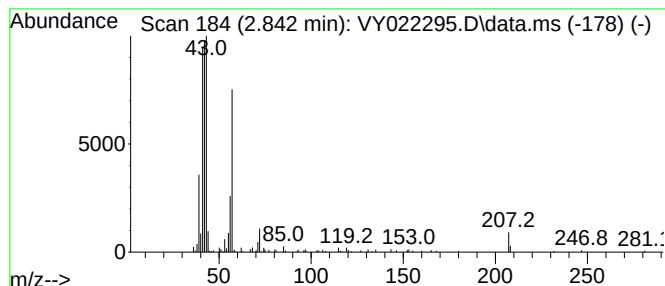
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.842	5.50 ug/l	97136	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			1-Propanol, 2-chloro-2-methyl-	108	C4H9ClO	000558-38-3	38
3			3-Buten-1-ol	72	C4H8O	000627-27-0	37
4			Pentane	72	C5H12	000109-66-0	28
5			Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	10



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Misc : 6.39g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-24

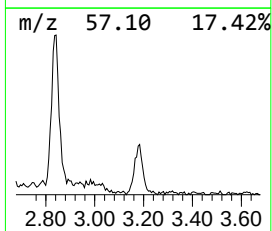
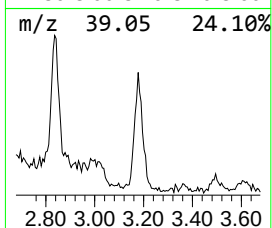
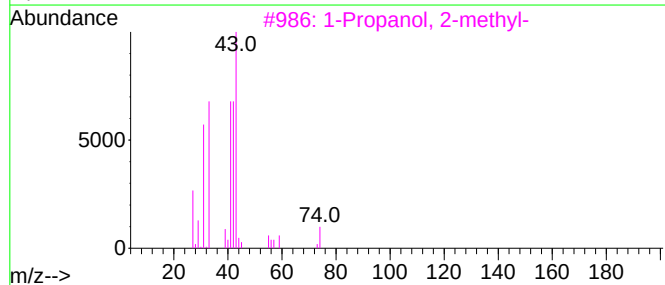
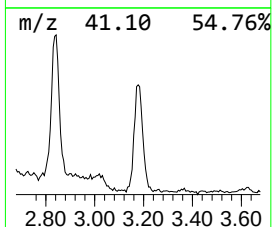
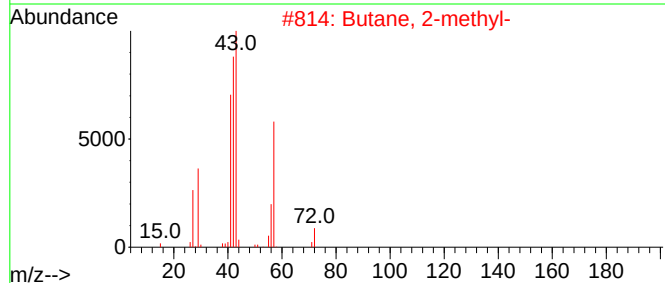
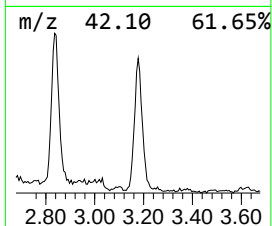
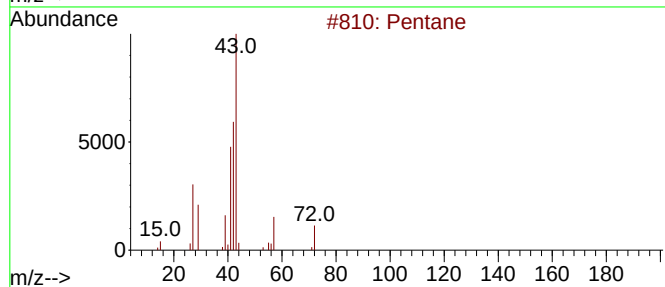
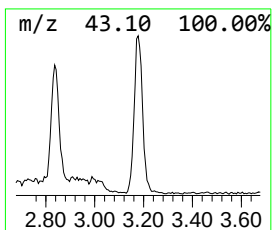
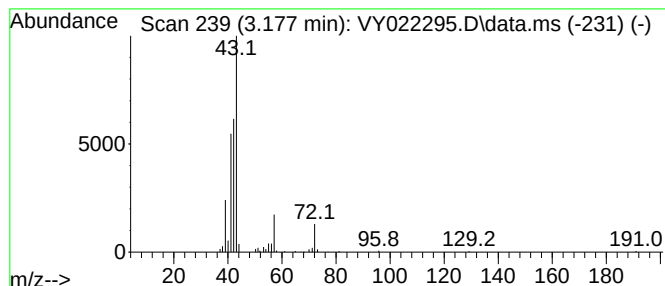
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.177	5.44 ug/l	96175	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Butane, 2-methyl-	72	C5H12	000078-78-4	50
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	50
4			Oxirane, ethyl-	72	C4H8O	000106-88-7	40
5			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38



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Misc : 6.39g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 20 Sample Multiplier: 1

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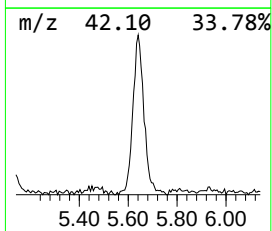
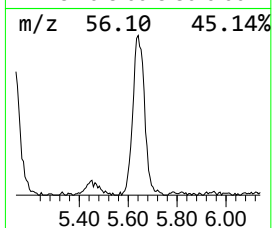
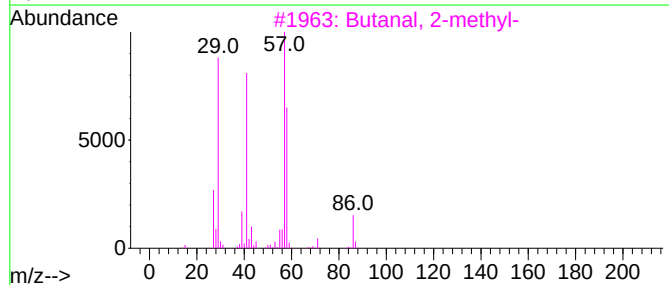
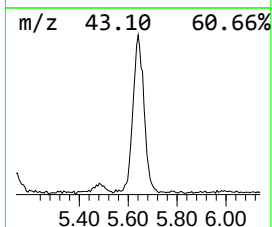
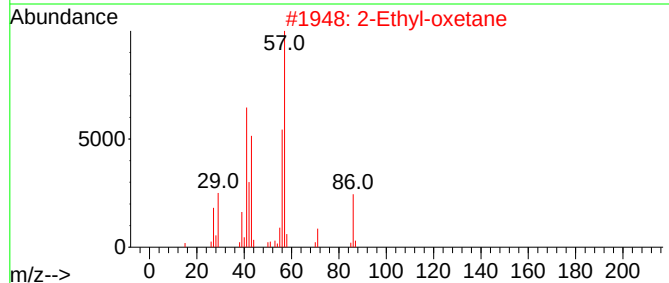
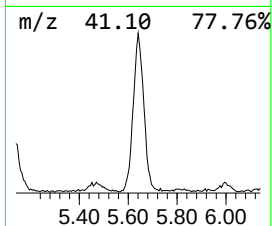
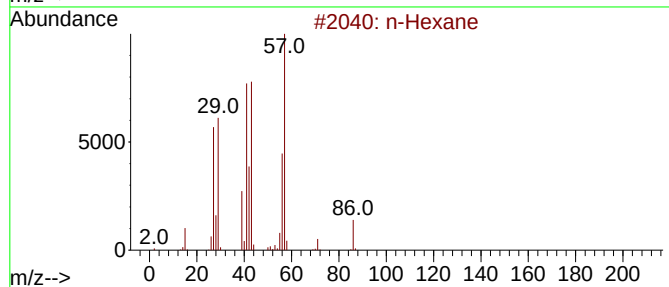
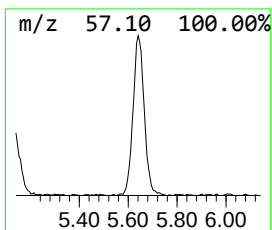
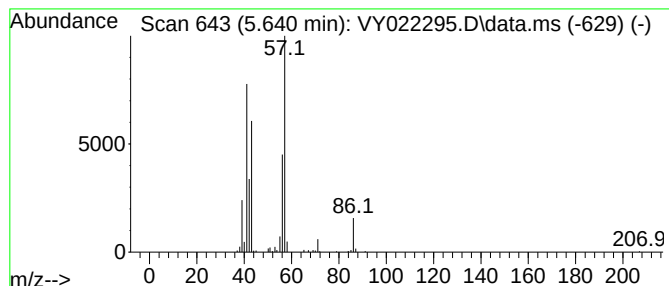
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.640	11.28 ug/l	199425	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	91
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	91
3			Butanal, 2-methyl-	86	C5H10O	000096-17-3	38
4			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
5			Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	38



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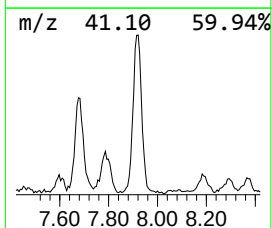
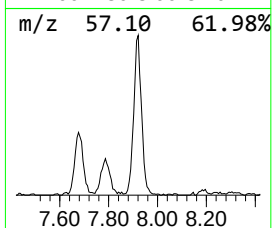
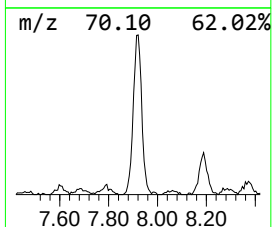
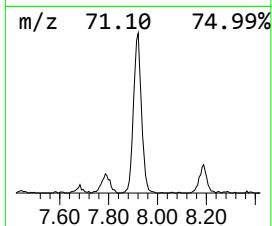
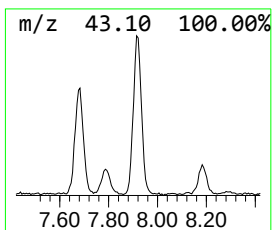
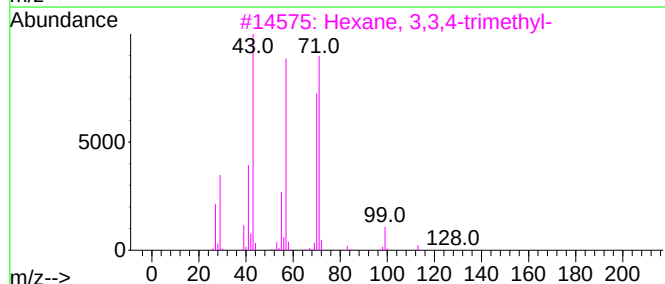
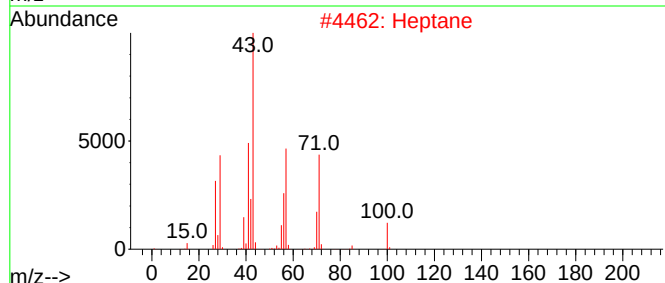
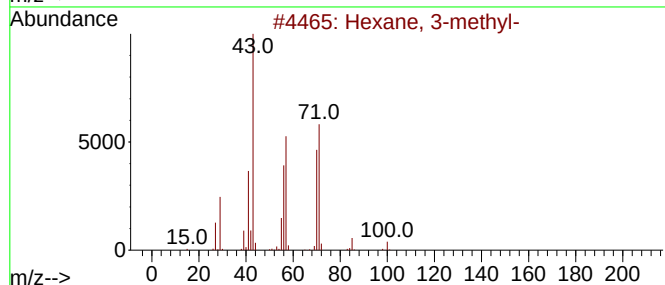
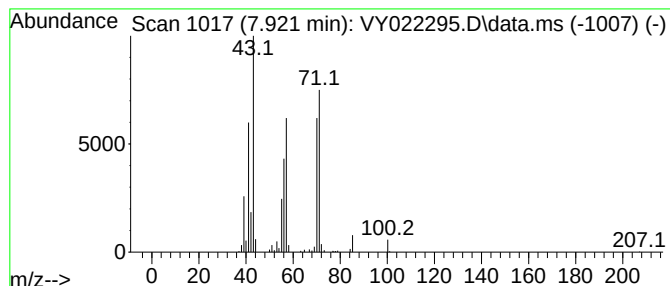
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
Quant Title : SW846 8260

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

Peak Number 5 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.921	10.66 ug/l	188454	Pentafluorobenzene	7.707

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	80
3			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	59
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051625\
Data File : VY022295.D
Acq On : 16 May 2025 16:48
Operator : SY/MD
Sample : Q2032-04
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-24

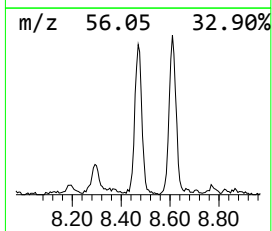
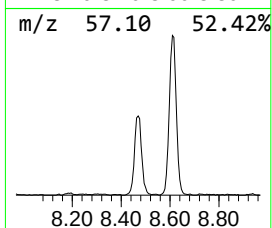
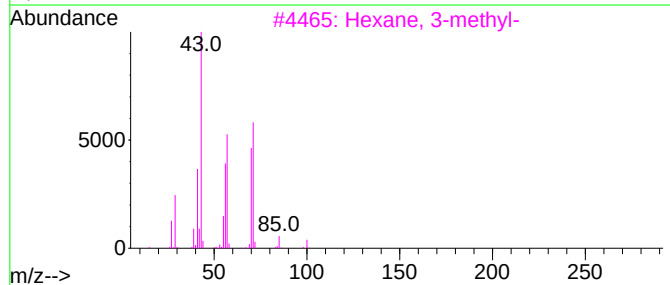
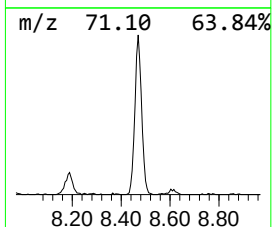
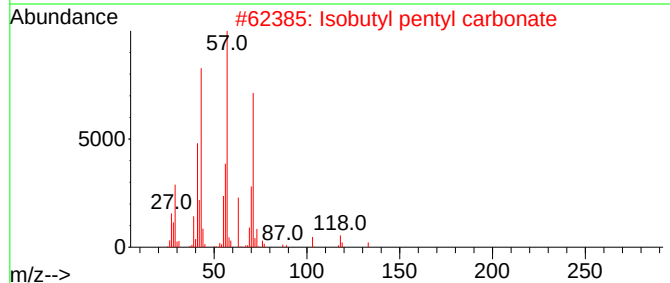
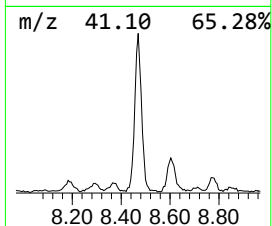
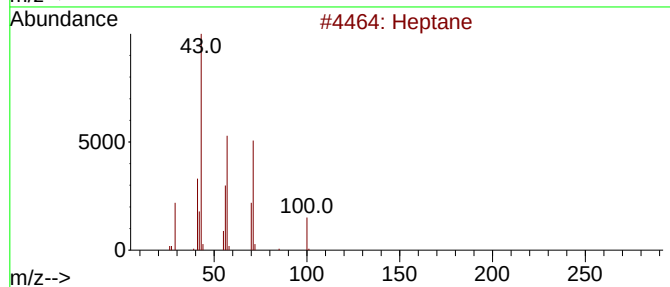
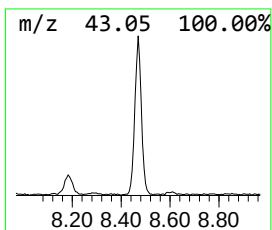
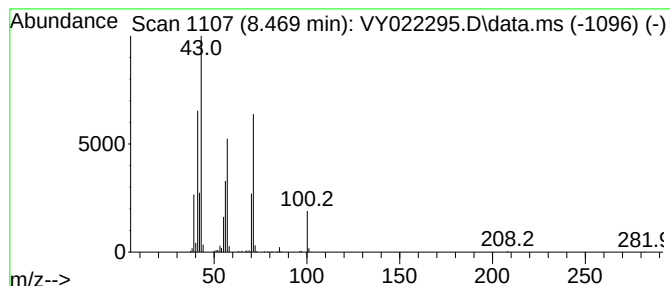
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Quant Title : SW846 8260

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

Peak Number 6 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	9.05 ug/l	214731	1,4-Difluorobenzene	8.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	83
2			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	50
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
5			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051625\
Data File : VY022295.D
Acq On : 16 May 2025 16:48
Operator : SY/MD
Sample : Q2032-04
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-24

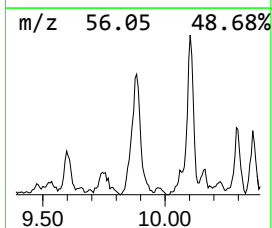
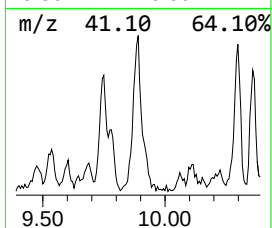
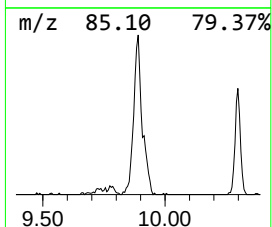
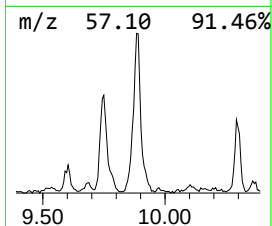
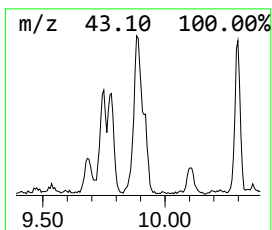
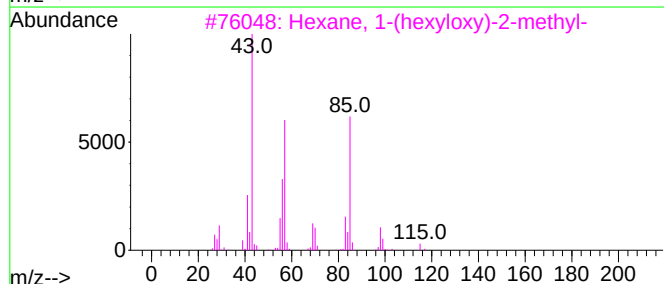
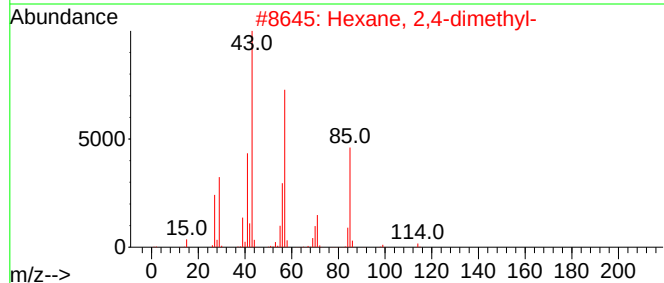
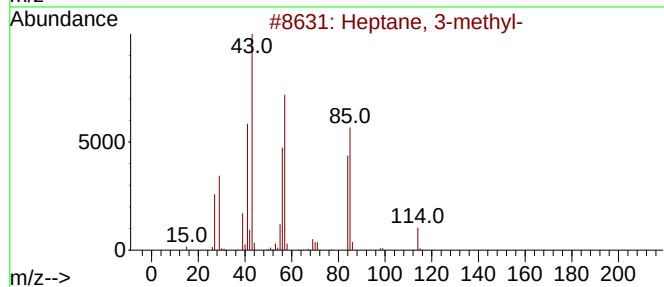
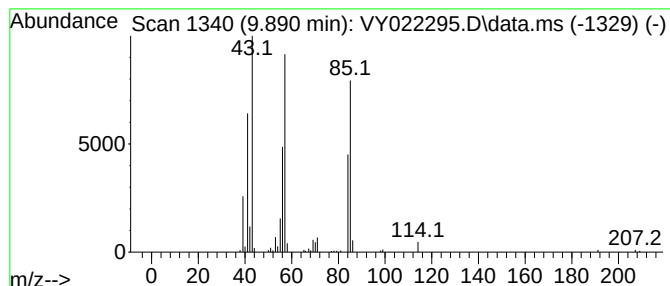
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Quant Title : SW846 8260

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

Peak Number 7 Heptane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.890	6.06 ug/l	143756	1,4-Difluorobenzene	8.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	94
2			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
3			Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	64
4			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
5			Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051625\
Data File : VY022295.D
Acq On : 16 May 2025 16:48
Operator : SY/MD
Sample : Q2032-04
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.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
Butane	2.196	6.7	ug/l	118282	1	7.707	883854	50.0
Butane, 2-methyl-	2.842	5.5	ug/l	97136	1	7.707	883854	50.0
Pentane	3.177	5.4	ug/l	96175	1	7.707	883854	50.0
n-Hexane	5.640	11.3	ug/l	199425	1	7.707	883854	50.0
Hexane, 3-methyl-	7.921	10.7	ug/l	188454	1	7.707	883854	50.0
Heptane	8.469	9.1	ug/l	214731	2	8.616	1185960	50.0
Heptane, 3-methyl-	9.890	6.1	ug/l	143756	2	8.616	1185960	50.0