

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102825\
 Data File : VX048399.D
 Acq On : 28 Oct 2025 15:11
 Operator : JC/MD
 Sample : Q3472-12 20X
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-5

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_X\Method\82X102025W.M
 Title : SW846 8260

Signal : TIC: VX048399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.373	692	703	714	rBV3	68350	221509	27.70%	4.246%
2	5.537	715	730	761	rVB3	121234	543152	67.93%	10.412%
3	5.818	764	776	788	rBV3	49109	163748	20.48%	3.139%
4	5.940	788	796	820	rVB	83059	246841	30.87%	4.732%
5	6.147	820	830	831	rBV4	6970	13465	1.68%	0.258%
6	6.245	840	846	854	rVB6	6061	15803	1.98%	0.303%
7	6.342	854	862	873	rVB8	6945	20864	2.61%	0.400%
8	6.598	894	904	917	rBV2	13575	35885	4.49%	0.688%
9	6.745	918	928	947	rBV	207818	552197	69.06%	10.586%
10	8.634	1228	1238	1257	rBV	461826	790536	98.87%	15.155%
11	10.037	1463	1468	1487	rVB	515127	759318	94.97%	14.556%
12	10.341	1514	1518	1526	rVB2	6936	9676	1.21%	0.185%
13	11.061	1631	1636	1649	rBV	432290	618841	77.40%	11.863%
14	11.366	1681	1686	1691	rBV	4819	9770	1.22%	0.187%
15	11.457	1698	1701	1708	rVB	23695	31137	3.89%	0.597%
16	11.738	1743	1747	1757	rVB2	10754	18294	2.29%	0.351%
17	12.006	1785	1791	1797	rBV	598496	799538	100.00%	15.327%
18	12.085	1802	1804	1808	rVB2	8458	8843	1.11%	0.170%
19	12.158	1813	1816	1822	rVB3	6105	8718	1.09%	0.167%
20	12.298	1834	1839	1845	rVB6	10400	20175	2.52%	0.387%
21	12.408	1847	1857	1860	rBV	44232	61328	7.67%	1.176%
22	12.445	1860	1863	1870	rVB4	6611	11801	1.48%	0.226%
23	12.536	1870	1878	1880	rBV5	6998	15441	1.93%	0.296%
24	12.670	1896	1900	1903	rBV4	5272	9672	1.21%	0.185%
25	12.798	1917	1921	1926	rVB5	7761	10385	1.30%	0.199%
26	12.872	1928	1933	1940	rVV6	7926	18004	2.25%	0.345%
27	12.957	1940	1947	1951	rVB7	9232	19997	2.50%	0.383%
28	13.024	1951	1958	1961	rBV6	8088	11532	1.44%	0.221%
29	13.146	1972	1978	1982	rVB6	7537	12160	1.52%	0.233%
30	13.250	1989	1995	1997	rVV2	23533	31362	3.92%	0.601%
31	13.274	1997	1999	2004	rVB2	19612	22850	2.86%	0.438%
32	13.402	2017	2020	2030	rVB3	15305	26516	3.32%	0.508%
33	13.829	2084	2090	2096	rVB6	7031	12458	1.56%	0.239%
34	13.902	2097	2102	2109	rVV4	5498	8905	1.11%	0.171%
35	14.207	2146	2152	2159	rBV3	11606	20885	2.61%	0.400%
36	14.457	2189	2193	2202	rVB9	5790	11528	1.44%	0.221%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102825\
Data File : VX048399.D
Acq On : 28 Oct 2025 15:11
Operator : JC/MD
Sample : Q3472-12 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5

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_X\Method\82X102025W.M

Title : SW846 8260

37	14.591	2212	2215	2221	rBV6	6738	12524	1.57%	0.240%
38	16.060	2450	2456	2461	rBV5	5265	10804	1.35%	0.207%

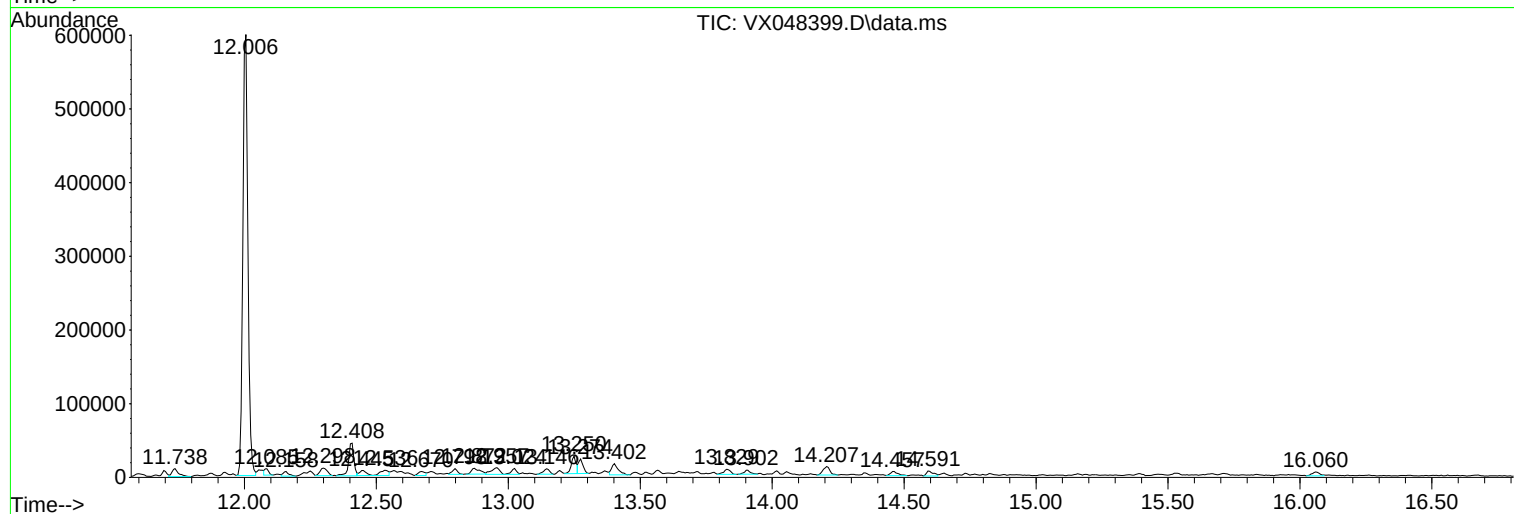
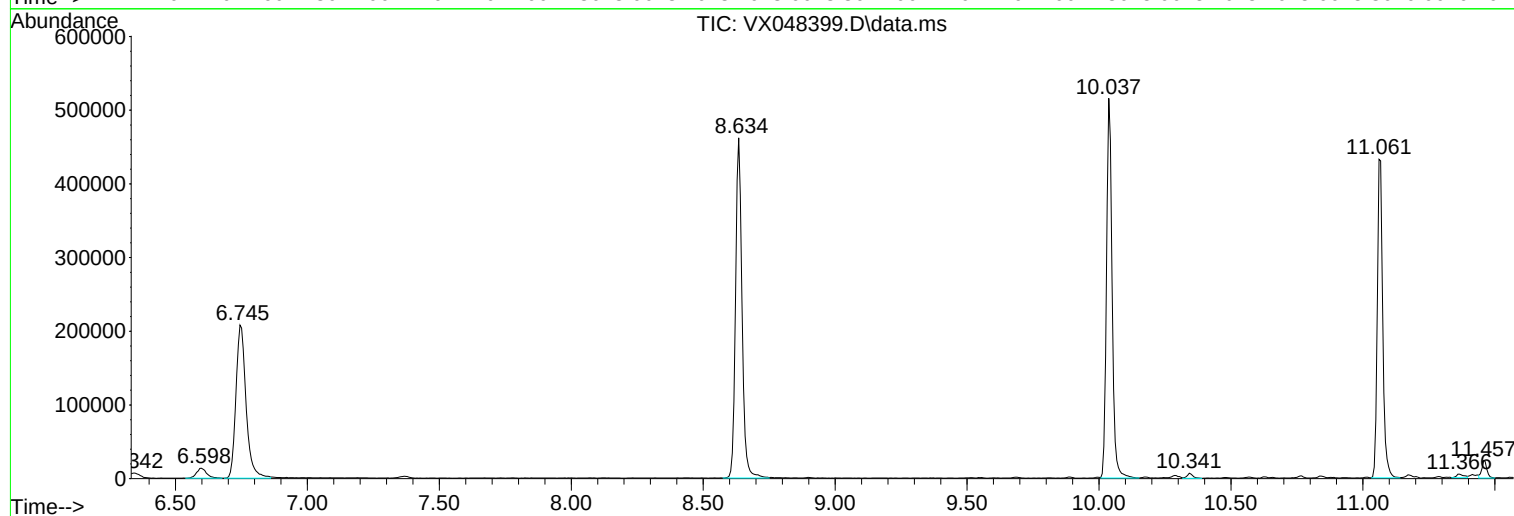
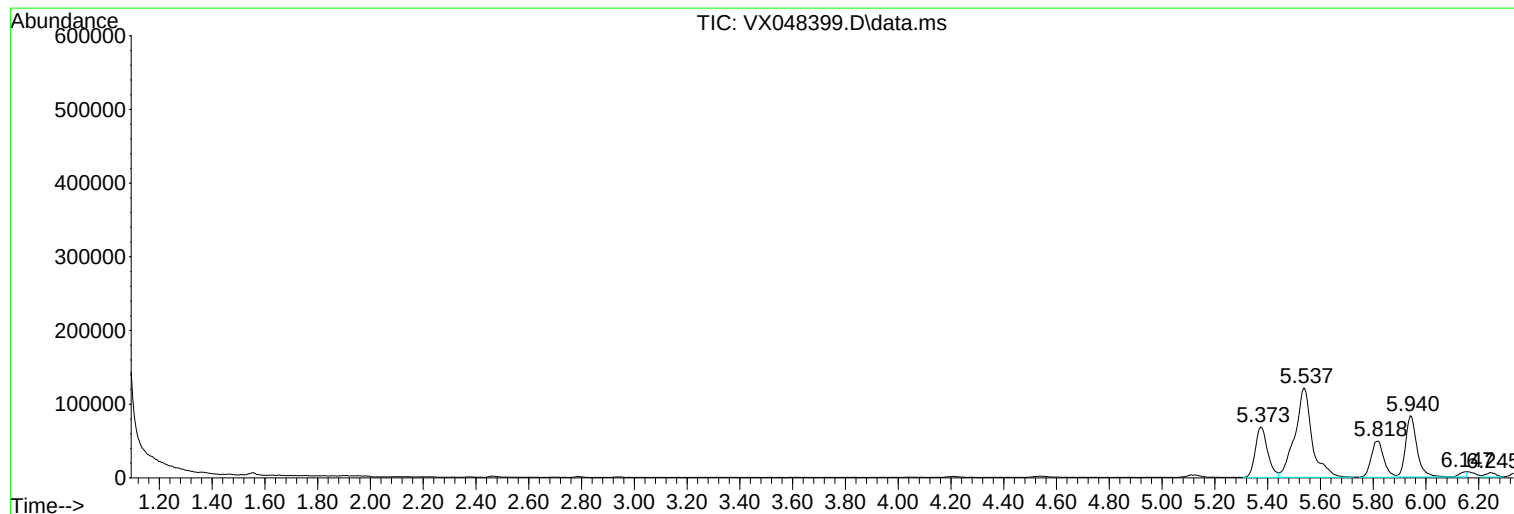
Sum of corrected areas: 5216462

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102825\
Data File : VX048399.D
Acq On : 28 Oct 2025 15:11
Operator : JC/MD
Sample : Q3472-12 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102025W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102825\
Data File : VX048399.D
Acq On : 28 Oct 2025 15:11
Operator : JC/MD
Sample : Q3472-12 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5

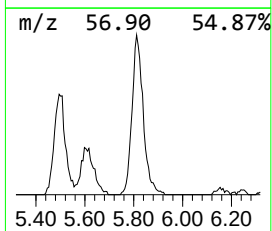
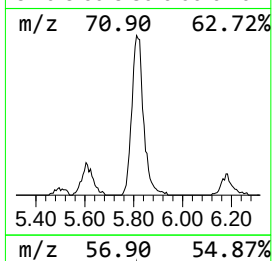
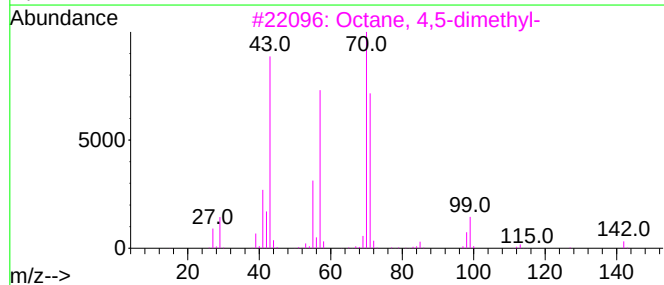
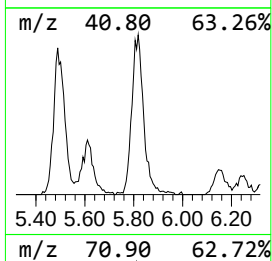
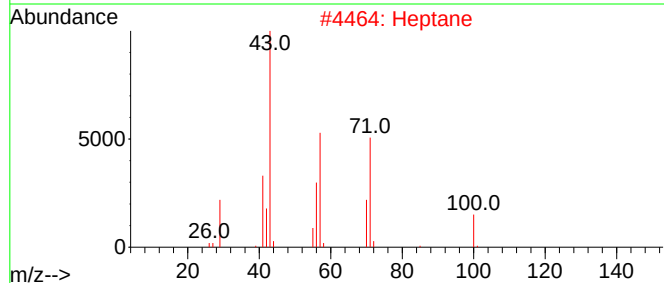
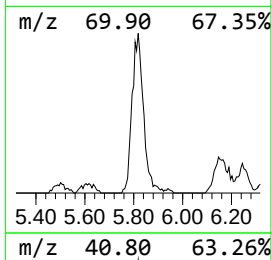
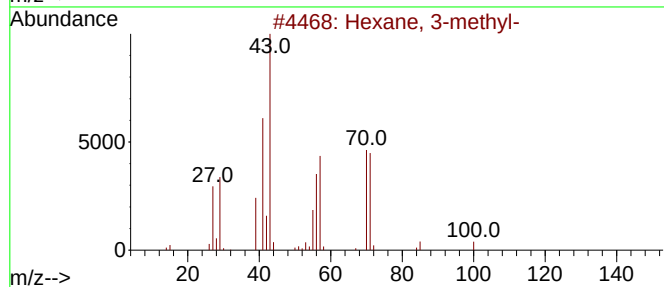
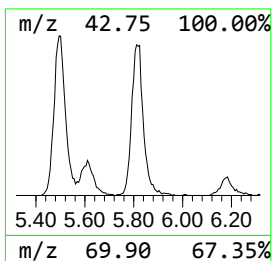
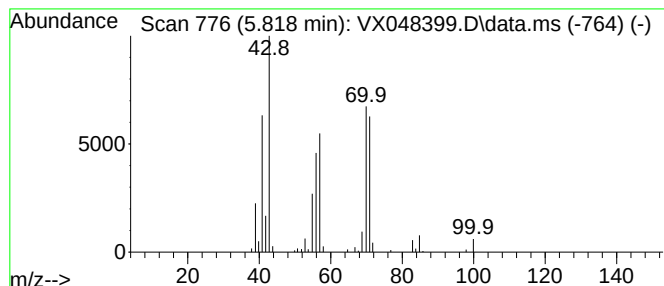
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102025W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.818	15.07 ug/l	163748	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Heptane	100	C7H16	000142-82-5	72
3			Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	59
4			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	53
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102825\
Data File : VX048399.D
Acq On : 28 Oct 2025 15:11
Operator : JC/MD
Sample : Q3472-12 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102025W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	5.818	15.1	ug/l	163748	1	5.544	543152	50.0