

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
 Data File : VX039952.D
 Acq On : 25 Jan 2024 14:32
 Operator : JC/MD
 Sample : P1235-05
 Misc : 1.25g/10mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1104

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\82X011024W.M
 Title : SW846 8260

Signal : TIC: VX039952.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	694	705	715	rBV	54938	158363	28.67%	2.886%
2	5.550	715	732	741	rBV2	95355	337700	61.13%	6.155%
3	5.824	767	777	789	rVB2	41188	120363	21.79%	2.194%
4	5.952	789	798	814	rBV2	66815	178101	32.24%	3.246%
5	6.178	824	835	844	rBV7	5221	22436	4.06%	0.409%
6	6.257	844	848	856	rVV7	4331	10374	1.88%	0.189%
7	6.349	856	863	872	rVB5	3675	10613	1.92%	0.193%
8	6.611	896	906	917	rBV2	36575	90092	16.31%	1.642%
9	6.763	922	931	946	rBV	154787	372825	67.49%	6.795%
10	7.379	1022	1032	1043	rBV5	13252	33763	6.11%	0.615%
11	7.659	1072	1078	1084	rVB4	3591	6695	1.21%	0.122%
12	8.275	1174	1179	1182	rBV4	3808	5585	1.01%	0.102%
13	8.598	1227	1232	1234	rBV2	5314	7657	1.39%	0.140%
14	8.647	1234	1240	1246	rVV	331203	509724	92.27%	9.290%
15	8.720	1246	1252	1264	rVB	344029	552447	100.00%	10.069%
16	8.915	1279	1284	1289	rBV	8284	12676	2.29%	0.231%
17	9.098	1309	1314	1320	rVB4	4266	7230	1.31%	0.132%
18	9.385	1354	1361	1369	rBV4	3000	5586	1.01%	0.102%
19	9.513	1375	1382	1385	rBV5	5441	10748	1.95%	0.196%
20	9.561	1385	1390	1395	rVV2	8119	12207	2.21%	0.222%
21	9.616	1395	1399	1403	rVV3	4176	7227	1.31%	0.132%
22	9.830	1428	1434	1440	rBV6	4593	10528	1.91%	0.192%
23	9.903	1441	1446	1451	rVB2	8737	13157	2.38%	0.240%
24	10.006	1456	1463	1466	rBV	7939	13067	2.37%	0.238%
25	10.055	1466	1471	1479	rVB	321524	448852	81.25%	8.181%
26	10.195	1487	1494	1499	rBV	27336	39320	7.12%	0.717%
27	10.299	1502	1511	1517	rVV	83880	136820	24.77%	2.494%
28	10.360	1517	1521	1533	rVB2	25921	39682	7.18%	0.723%
29	10.586	1549	1558	1562	rBV4	9710	18002	3.26%	0.328%
30	10.640	1562	1567	1576	rVB	25187	40154	7.27%	0.732%
31	10.781	1582	1590	1594	rBV4	11901	19614	3.55%	0.357%
32	10.854	1598	1602	1606	rVV4	12162	21349	3.86%	0.389%
33	10.964	1613	1620	1623	rBV4	4623	8389	1.52%	0.153%
34	11.079	1634	1639	1651	rVB	282438	383059	69.34%	6.981%
35	11.189	1654	1657	1660	rVV2	11118	14884	2.69%	0.271%
36	11.220	1660	1662	1666	rVB3	6681	7462	1.35%	0.136%

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37	11.305	1672	1676	1679	rBV	8420	11192	2.03%	0.204%
38	11.378	1684	1688	1694	rVV	25883	49344	8.93%	0.899%
39	11.433	1694	1697	1698	rVV	13240	16455	2.98%	0.300%
40	11.476	1701	1704	1710	rVB	43663	56512	10.23%	1.030%
41	11.616	1722	1727	1734	rVB4	17175	31681	5.73%	0.577%
42	11.683	1734	1738	1740	rBV3	5106	6634	1.20%	0.121%
43	11.713	1740	1743	1746	rBV2	16869	21091	3.82%	0.384%
44	11.750	1746	1749	1759	rVB	40952	64445	11.67%	1.175%
45	11.835	1759	1763	1765	rBV3	6940	9228	1.67%	0.168%
46	11.890	1768	1772	1776	rVB4	12162	15990	2.89%	0.291%
47	11.939	1776	1780	1784	rBV3	16236	24307	4.40%	0.443%
48	12.018	1788	1793	1800	rBV	355474	473266	85.67%	8.625%
49	12.073	1800	1802	1804	rVV2	10168	12283	2.22%	0.224%
50	12.104	1804	1807	1810	rVB	13457	16188	2.93%	0.295%
51	12.171	1816	1818	1825	rVB2	17986	25634	4.64%	0.467%
52	12.244	1825	1830	1832	rBV3	13302	20405	3.69%	0.372%
53	12.268	1832	1834	1837	rVV	15008	18223	3.30%	0.332%
54	12.311	1837	1841	1848	rVB6	27727	58364	10.56%	1.064%
55	12.421	1855	1859	1863	rVB	107496	122232	22.13%	2.228%
56	12.463	1863	1866	1873	rVB5	16489	30295	5.48%	0.552%
57	12.555	1873	1881	1883	rBV6	15590	34028	6.16%	0.620%
58	12.579	1883	1885	1893	rVB5	10309	17817	3.23%	0.325%
59	12.634	1893	1894	1899	rVB4	6634	7433	1.35%	0.135%
60	12.683	1899	1902	1905	rBV3	10620	15968	2.89%	0.291%
61	12.817	1920	1924	1930	rVB2	18516	27951	5.06%	0.509%
62	12.890	1930	1936	1942	rBV5	19979	49741	9.00%	0.907%
63	12.939	1942	1944	1947	rVV2	11657	15931	2.88%	0.290%
64	12.975	1947	1950	1955	rVV4	25759	37218	6.74%	0.678%
65	13.042	1957	1961	1964	rVB	19708	23765	4.30%	0.433%
66	13.164	1977	1981	1985	rVB6	5726	10575	1.91%	0.193%
67	13.268	1993	1998	2001	rVV	82377	110426	19.99%	2.013%
68	13.292	2001	2002	2008	rVV4	24330	22272	4.03%	0.406%
69	13.347	2008	2011	2013	rVV3	6838	7633	1.38%	0.139%
70	13.384	2013	2017	2019	rVV	15529	19082	3.45%	0.348%
71	13.414	2019	2022	2032	rVB7	18287	46416	8.40%	0.846%
72	13.494	2032	2035	2041	rBV7	5862	10781	1.95%	0.196%
73	13.591	2047	2051	2055	rBV6	6115	10623	1.92%	0.194%
74	13.676	2061	2065	2067	rBV4	10733	14983	2.71%	0.273%
75	13.731	2071	2074	2077	rVV3	18273	25708	4.65%	0.469%
76	13.768	2077	2080	2082	rVV	16241	18649	3.38%	0.340%

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77	13.798	2082	2085	2088	rVV4	8994	12417	2.25%	0.226%
78	13.835	2088	2091	2099	rVV4	18683	35919	6.50%	0.655%
79	13.908	2099	2103	2110	rVB9	6829	12884	2.33%	0.235%
80	14.036	2120	2124	2128	rBV	54411	57829	10.47%	1.054%
81	14.219	2151	2154	2160	rVB5	4566	7855	1.42%	0.143%
82	14.402	2180	2184	2187	rBV5	4058	6640	1.20%	0.121%
83	14.432	2187	2189	2193	rVV3	6236	8597	1.56%	0.157%
84	14.499	2197	2200	2206	rVB5	5120	8628	1.56%	0.157%
85	14.609	2215	2218	2224	rBV4	5763	7062	1.28%	0.129%
86	14.756	2238	2242	2245	rBV	15563	18190	3.29%	0.332%
87	15.487	2358	2362	2368	rBV7	6752	13295	2.41%	0.242%

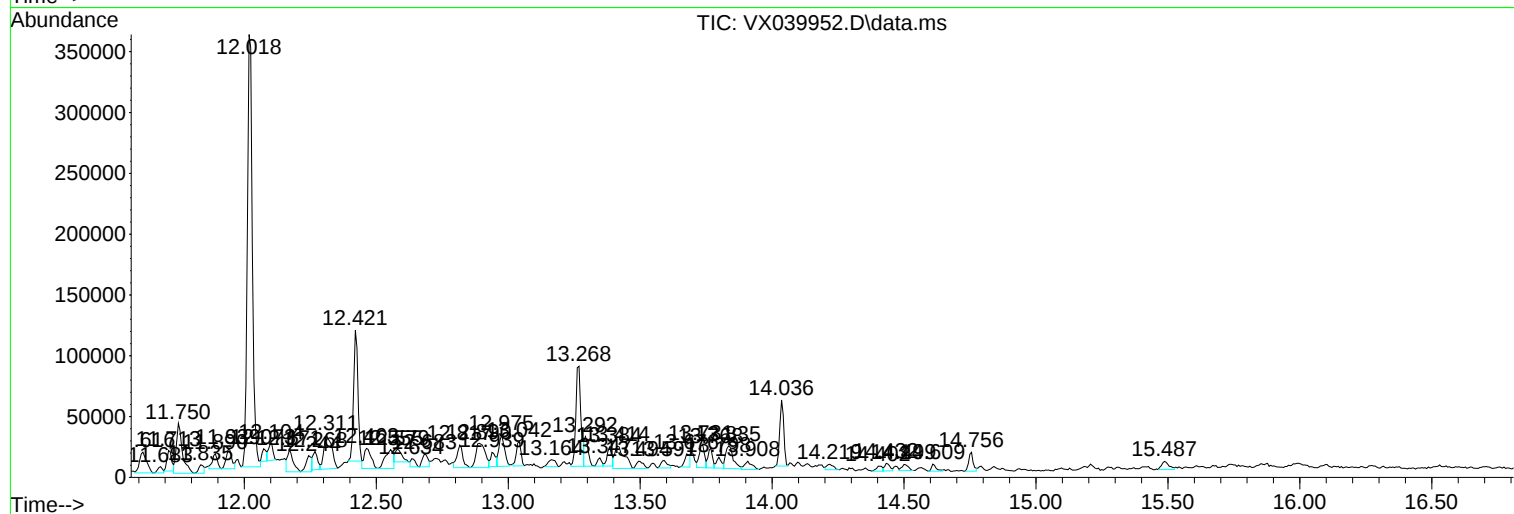
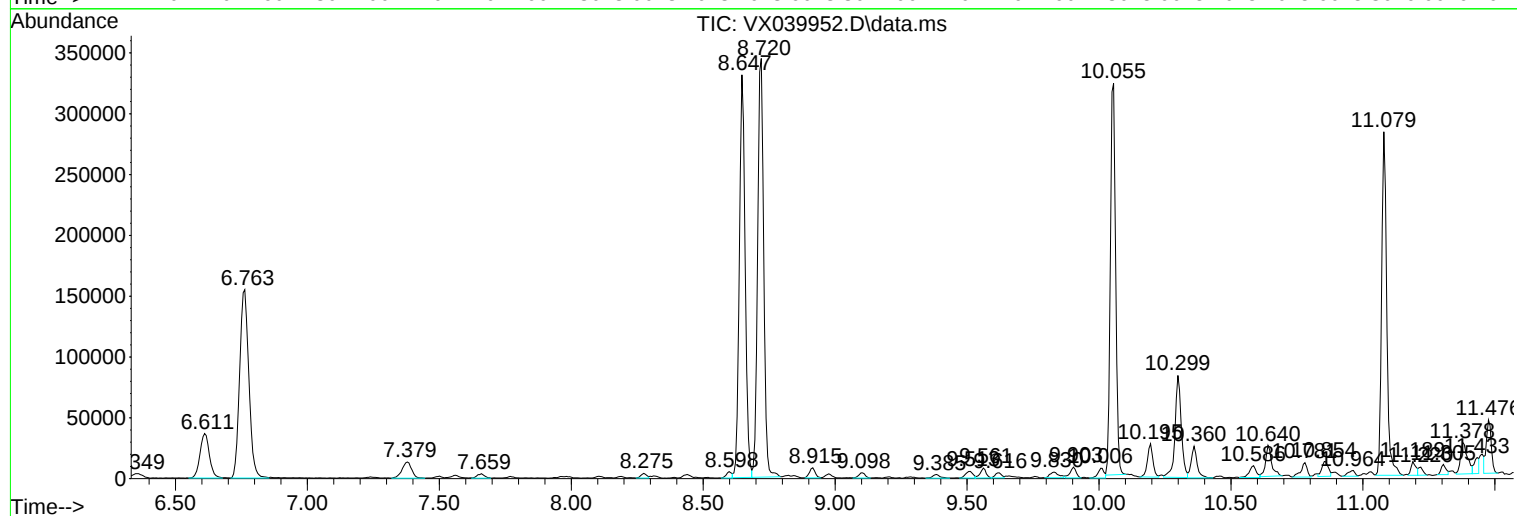
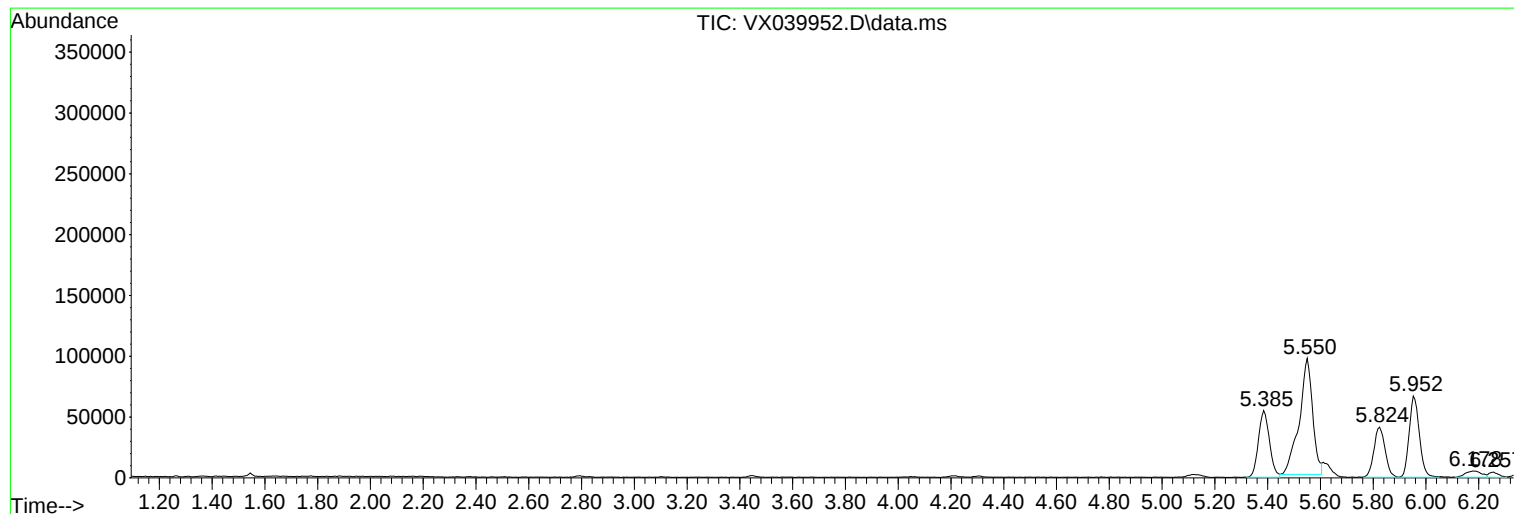
Sum of corrected areas: 5486836

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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



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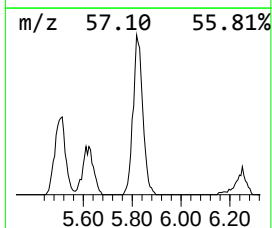
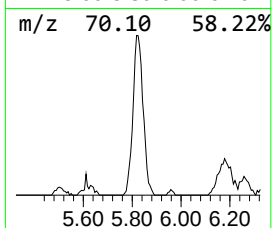
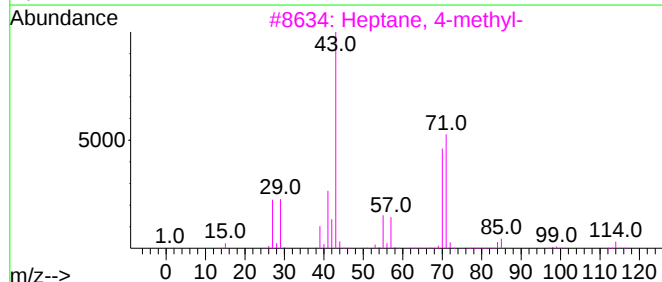
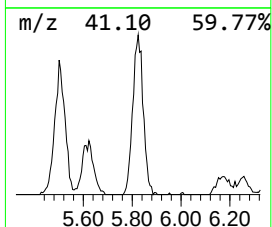
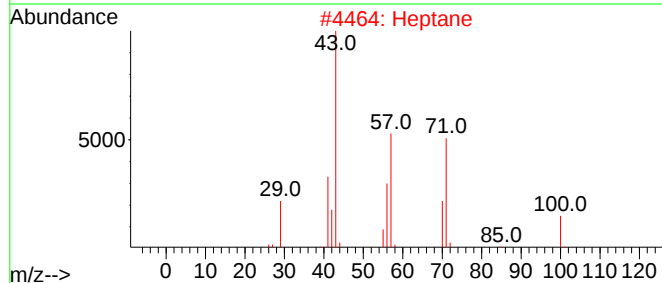
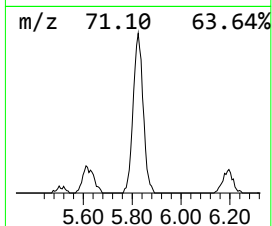
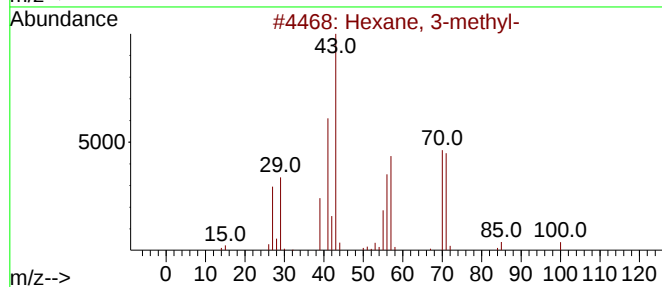
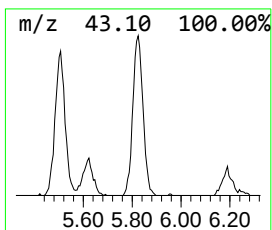
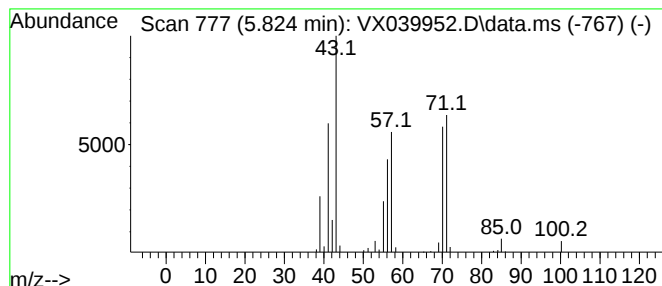
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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.
5.824	17.82 ug/l	120363	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



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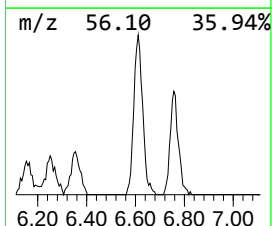
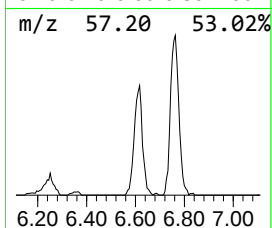
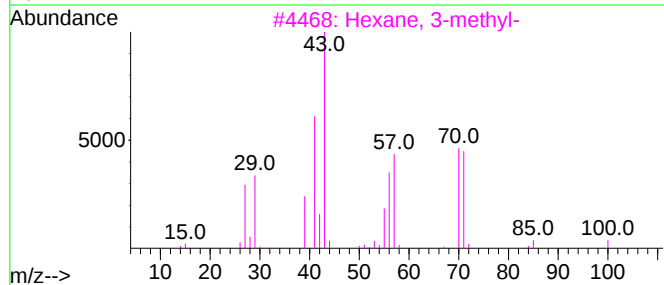
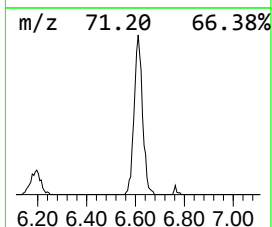
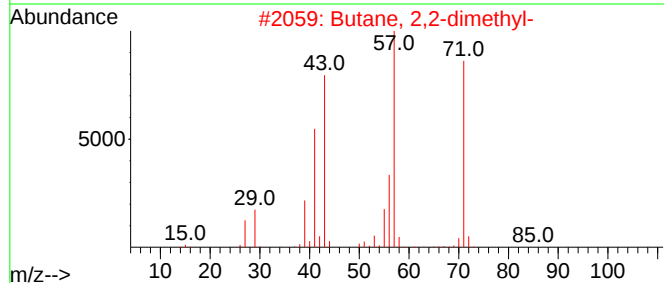
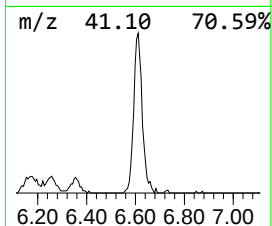
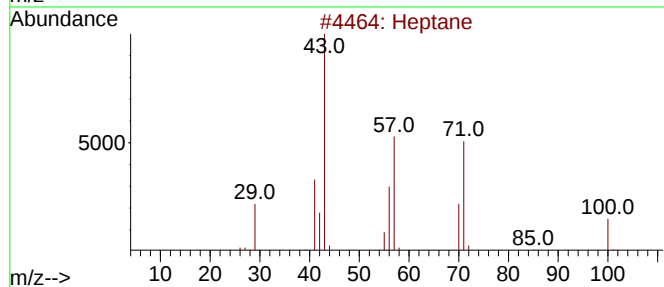
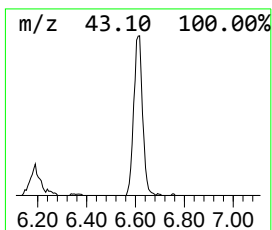
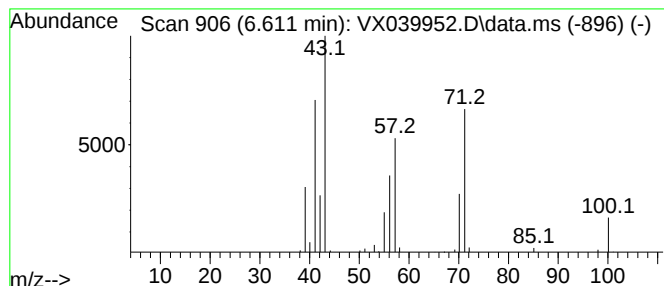
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.611	12.08 ug/l	90092	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	42
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
5			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	38



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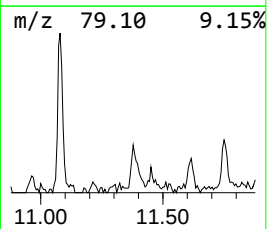
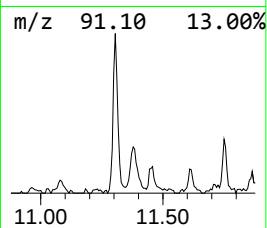
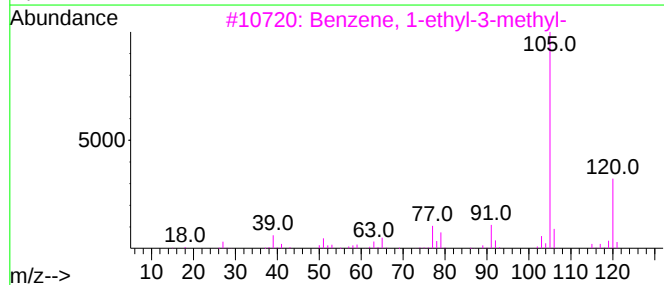
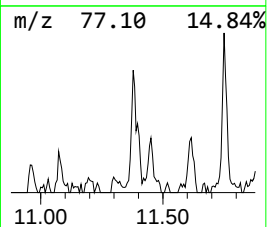
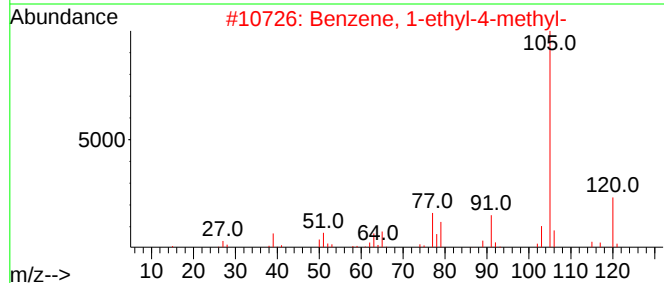
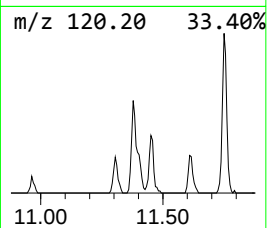
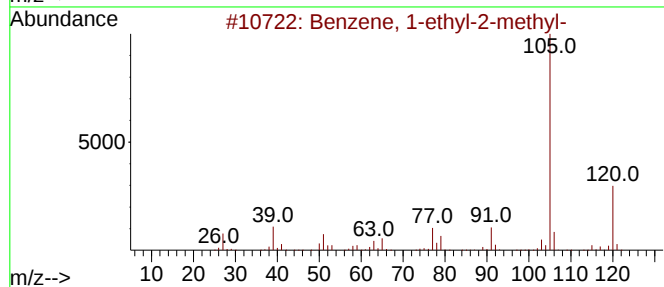
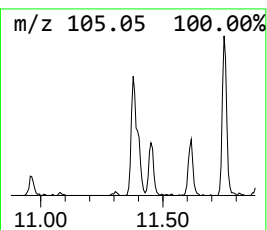
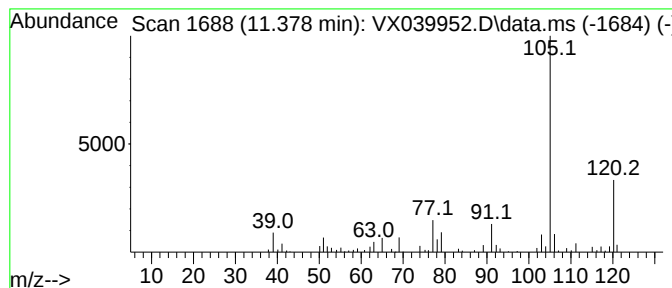
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	5.21 ug/l	49344	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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Sample : P1235-05
Misc : 1.25g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1104

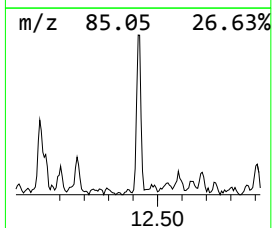
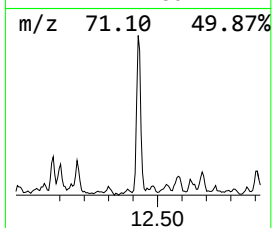
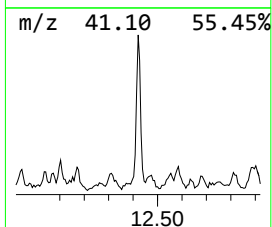
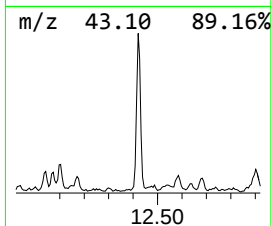
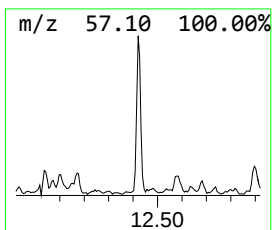
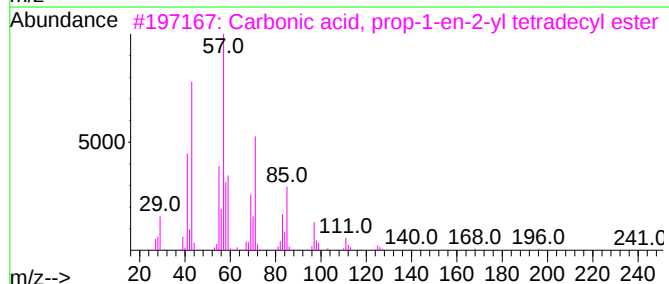
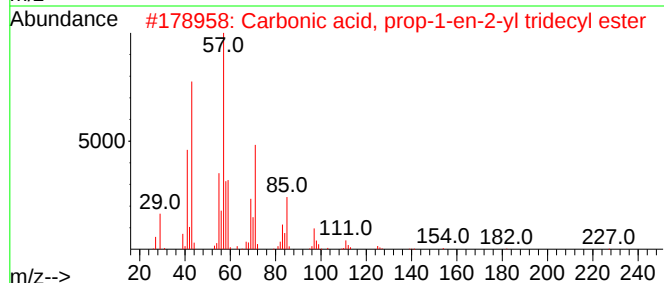
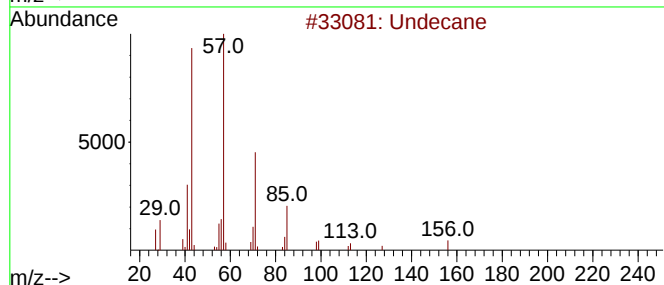
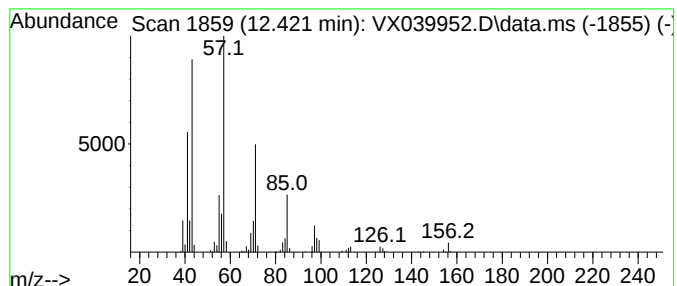
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Quant Title : SW846 8260

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

Peak Number 4 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	12.91 ug/l	122232	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	90
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	90
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	83
4			Tetradecane	198	C14H30	000629-59-4	80
5			Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039952.D
Acq On : 25 Jan 2024 14:32
Operator : JC/MD
Sample : P1235-05
Misc : 1.25g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1104

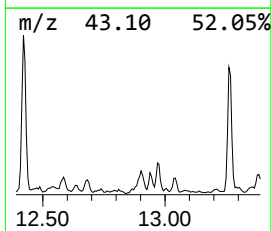
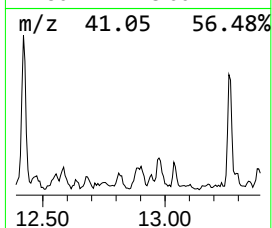
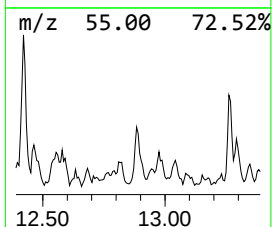
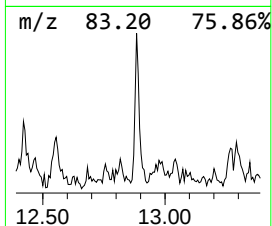
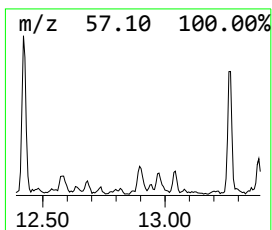
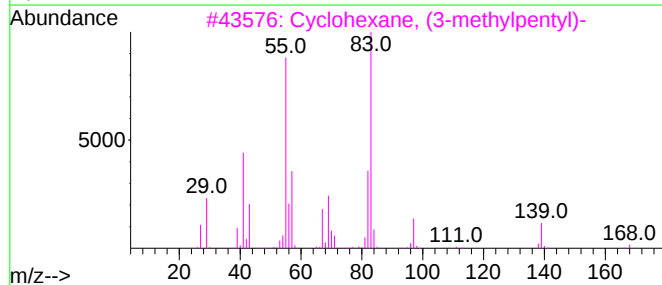
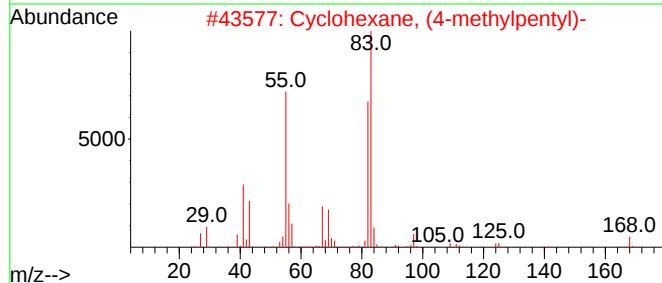
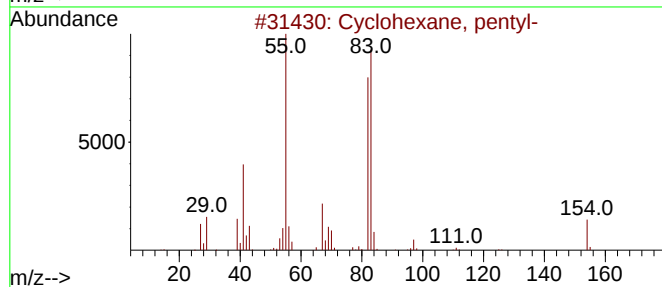
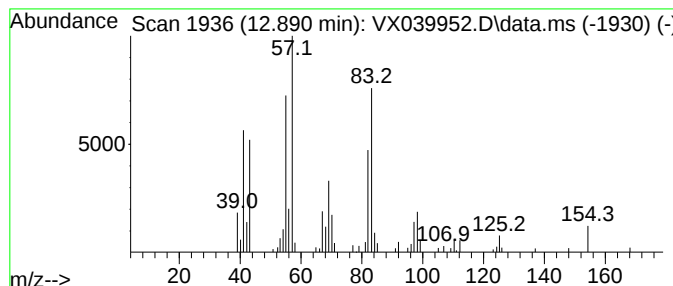
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, pentyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	5.26 ug/l	49741	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, pentyl-	154	C11H22	004292-92-6	64
2			Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	64
3			Cyclohexane, (3-methylpentyl)-	168	C12H24	061142-38-9	58
4			Cyclohexane, propyl-	126	C9H18	001678-92-8	53
5			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039952.D
Acq On : 25 Jan 2024 14:32
Operator : JC/MD
Sample : P1235-05
Misc : 1.25g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1104

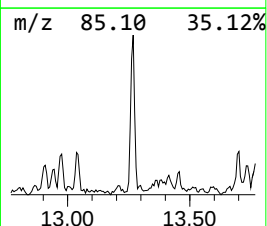
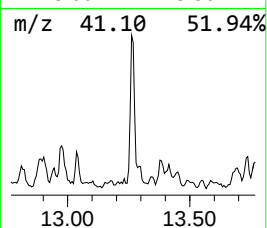
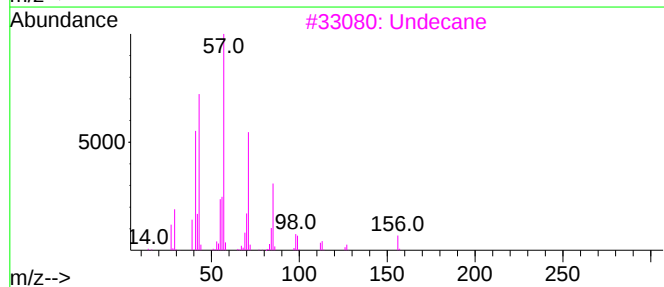
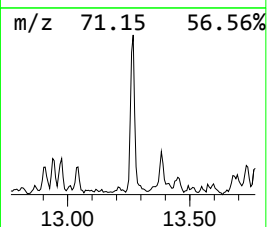
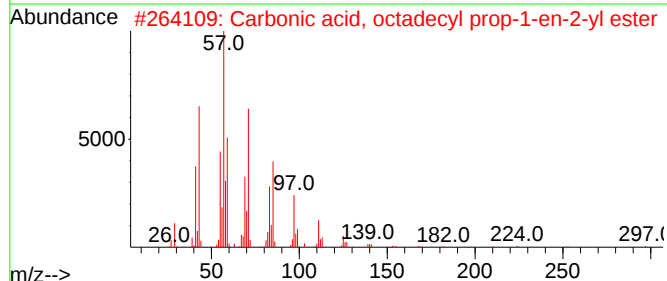
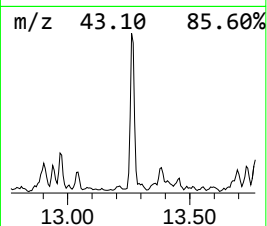
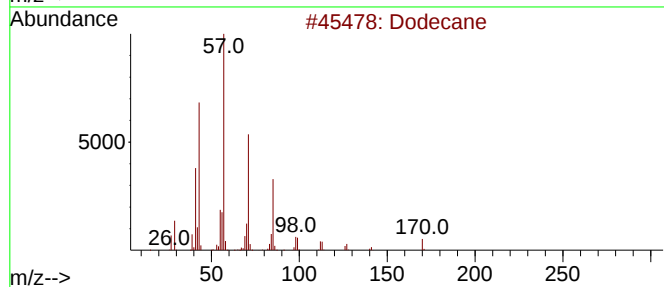
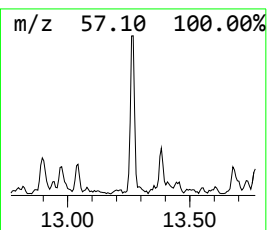
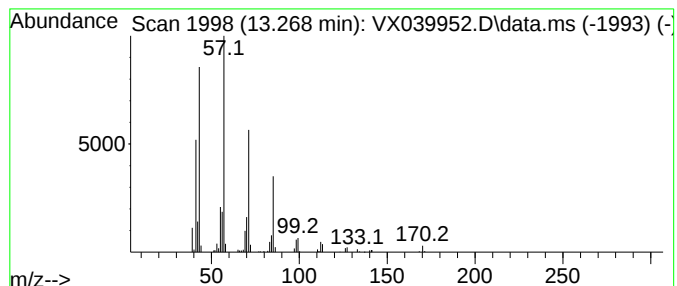
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	11.67 ug/l	110426	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
3			Undecane	156	C11H24	001120-21-4	86
4			Tetradecane	198	C14H30	000629-59-4	86
5			Tridecane	184	C13H28	000629-50-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039952.D
Acq On : 25 Jan 2024 14:32
Operator : JC/MD
Sample : P1235-05
Misc : 1.25g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1104

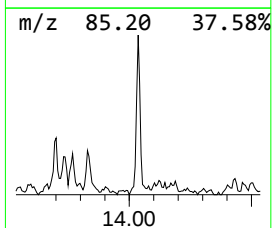
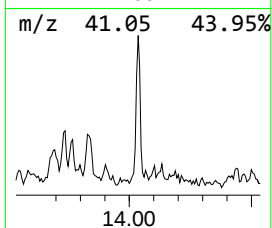
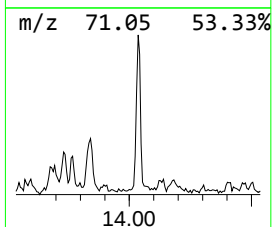
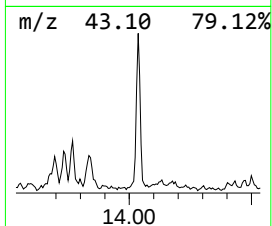
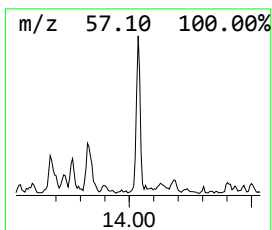
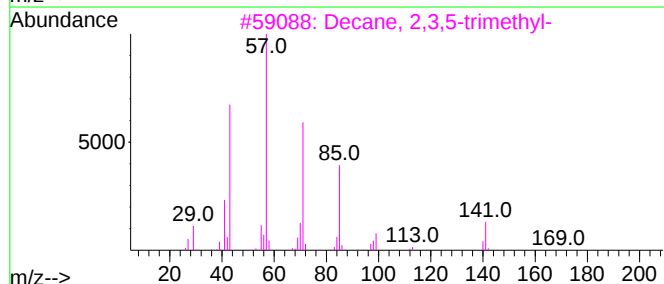
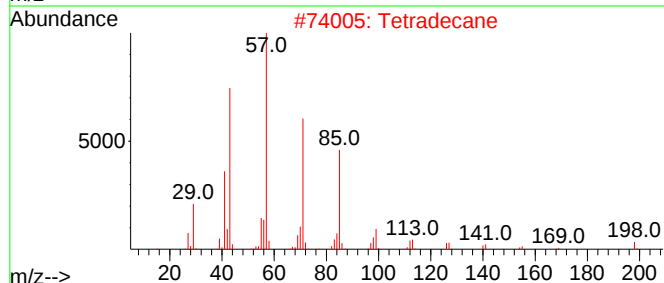
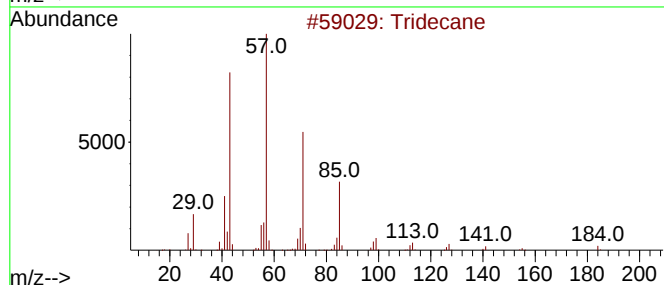
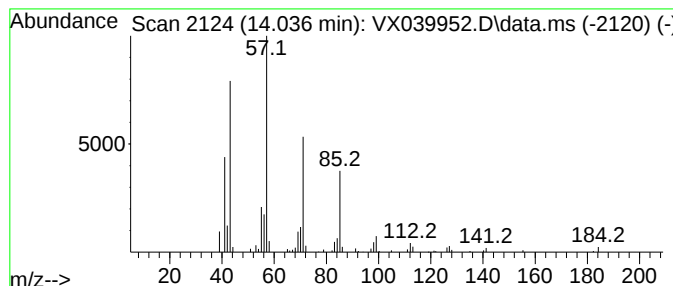
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 7 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.036	6.11 ug/l	57829	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	93
2			Tetradecane	198	C14H30	000629-59-4	86
3			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
4			Hexadecane	226	C16H34	000544-76-3	86
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039952.D
Acq On : 25 Jan 2024 14:32
Operator : JC/MD
Sample : P1235-05
Misc : 1.25g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1104

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.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
Hexane, 3-methyl-	5.824	17.8	ug/l	120363	1	5.550	337700	50.0
Heptane	6.611	12.1	ug/l	90092	2	6.763	372825	50.0
Benzene, 1-ethy...	11.378	5.2	ug/l	49344	4	12.024	473266	50.0
Undecane	12.421	12.9	ug/l	122232	4	12.024	473266	50.0
Cyclohexane, pe...	12.890	5.3	ug/l	49741	4	12.024	473266	50.0
Dodecane	13.268	11.7	ug/l	110426	4	12.024	473266	50.0
Tridecane	14.036	6.1	ug/l	57829	4	12.024	473266	50.0