LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052925\
Data File : VX046400.D
Acq On : 29 May 2025 15:33
Operator : JC/MD
Sample : Q2139-01
Misc : 1.18g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

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\82X050525W.M
Title : SW846 8260

Signal : TIC: VX046400.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.075	317	326	347	rBV	1370201	2600954	100.00%	12.914%
2	4.020	471	481	495	rBV2	20356	60110	2.31%	0.298%
3	4.184	498	508	516	rVV	32231	95479	3.67%	0.474%
4	4.276	516	523	538	rVV2	23763	70187	2.70%	0.348%
5	5.105	644	659	676	rBV2	32660	120846	4.65%	0.600%
6	5.379	695	704	710	rBV	45277	133483	5.13%	0.663%
7	5.483	710	721	734	rVV2	394859	1426369	54.84%	7.082%
8	5.599	734	740	754	rVB	135373	428285	16.47%	2.127%
9	5.806	761	774	788	rBV	531447	1538250	59.14%	7.638%
10	5.952	789	798	810	rVB	51017	140328	5.40%	0.697%
11	6.166	819	833	841	rBV4	59162	238119	9.16%	1.182%
12	6.239	841	845	853	rVV2	27818	73495	2.83%	0.365%
13	6.336	853	861	874	rVB2	34530	98580	3.79%	0.489%
14	6.592	893	903	921	rBV	422757	1033324	39.73%	5.131%
15	6.757	921	930	943	rVB	114469	283166	10.89%	1.406%
16	7.367	1018	1030	1042	rVV3	60226	159698	6.14%	0.793%
17	7.550	1055	1060	1069	rVV2	17046	36641	1.41%	0.182%
18	7.647	1069	1076	1085	rVV2	23505	47468	1.83%	0.236%
19	8.269	1173	1178	1182	rBV	16904	28234	1.09%	0.140%
20	8.427	1199	1204	1214	rVB2	15134	29175	1.12%	0.145%
21	8.647	1234	1240	1246	rVV	249500	406861	15.64%	2.020%
22	8.714	1246	1251	1264	rVB	341240	553046	21.26%	2.746%
23	8.909	1277	1283	1288	rBV	36185	52272	2.01%	0.260%
24	9.507	1374	1381	1385	rVV4	18833	41289	1.59%	0.205%
25	9.555	1385	1389	1394	rVV	28702	45422	1.75%	0.226%
26	9.616	1394	1399	1403	rVV	18164	33244	1.28%	0.165%
27	9.824	1427	1433	1437	rBV3	24143	49112	1.89%	0.244%
28	9.903	1441	1446	1451	rVB	59051	88303	3.40%	0.438%
29	10.006	1456	1463	1466	rBV	60414	87464	3.36%	0.434%
30	10.049	1466	1470	1477	rVV	252967	371548	14.29%	1.845%
31	10.189	1486	1493	1498	rVV2	45386	87780	3.37%	0.436%
32	10.299	1498	1511	1516	rVV2	136913	324054	12.46%	1.609%
33	10.354	1516	1520	1532	rVB	239432	344624	13.25%	1.711%
34	10.579	1551	1557	1561	rBV2	62402	105102	4.04%	0.522%
35	10.640	1564	1567	1570	rBV	55443	67407	2.59%	0.335%
36	10.775	1581	1589	1593	rBV2	86239	140872	5.42%	0.699%

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Instrument :
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ClientSampleId :
BELL-25-0010

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Title : SW846 8260

37	10.854	1593	1602	1606	rVV3	105898	190487	7.32%	0.946%
38	10.890	1606	1608	1613	rVB2	27969	37720	1.45%	0.187%
39	10.957	1613	1619	1622	rBV4	24613	48080	1.85%	0.239%
40	11.025	1628	1630	1633	rVV2	26325	29338	1.13%	0.146%
41	11.079	1633	1639	1650	rVB2	310909	537700	20.67%	2.670%
42	11.189	1650	1657	1660	rBV2	91464	142016	5.46%	0.705%
43	11.214	1660	1661	1666	rVB4	46796	45709	1.76%	0.227%
44	11.305	1669	1676	1684	rBV2	73286	148860	5.72%	0.739%
45	11.378	1684	1688	1694	rVV	222485	373642	14.37%	1.855%
46	11.427	1694	1696	1698	rVV	88419	111424	4.28%	0.553%
47	11.451	1698	1700	1701	rVV	102559	104932	4.03%	0.521%
48	11.476	1701	1704	1709	rVB	430801	496151	19.08%	2.464%
49	11.610	1722	1726	1733	rVB2	136327	233078	8.96%	1.157%
50	11.677	1733	1737	1740	rBV2	28580	37208	1.43%	0.185%
51	11.713	1740	1743	1745	rBV2	82555	90500	3.48%	0.449%
52	11.750	1745	1749	1759	rVB	367549	533966	20.53%	2.651%
53	11.835	1759	1763	1765	rBV3	27393	41391	1.59%	0.206%
54	11.890	1765	1772	1776	rVB4	66490	119012	4.58%	0.591%
55	11.939	1776	1780	1783	rBV	99866	131972	5.07%	0.655%
56	11.969	1783	1785	1788	rVB3	55402	54550	2.10%	0.271%
57	12.018	1788	1793	1799	rBV2	280351	428317	16.47%	2.127%
58	12.085	1799	1804	1810	rBV3	108495	239290	9.20%	1.188%
59	12.171	1815	1818	1825	rVB4	65684	107953	4.15%	0.536%
60	12.244	1825	1830	1832	rBV	121480	176781	6.80%	0.878%
61	12.268	1832	1834	1837	rVB	124160	121432	4.67%	0.603%
62	12.311	1837	1841	1848	rVB3	208782	387241	14.89%	1.923%
63	12.421	1848	1859	1863	rBV	393435	511353	19.66%	2.539%
64	12.463	1863	1866	1872	rVB2	103664	145285	5.59%	0.721%
65	12.530	1873	1877	1879	rBV	77119	109064	4.19%	0.542%
66	12.555	1879	1881	1884	rVB	55428	51219	1.97%	0.254%
67	12.610	1887	1890	1893	rVB	66967	74637	2.87%	0.371%
68	12.640	1893	1895	1899	rVB2	36902	41869	1.61%	0.208%
69	12.695	1899	1904	1906	rBV2	67244	111373	4.28%	0.553%
70	12.817	1917	1924	1927	rBV3	94267	136824	5.26%	0.679%
71	12.884	1931	1935	1938	rBV2	63923	102984	3.96%	0.511%
72	12.975	1944	1950	1954	rVB3	85763	190951	7.34%	0.948%
73	13.042	1954	1961	1964	rBV4	70110	122250	4.70%	0.607%
74	13.164	1974	1981	1985	rBV3	94316	163665	6.29%	0.813%
75	13.213	1985	1989	1991	rVV	53315	61517	2.37%	0.305%
76	13.262	1992	1997	1999	rVV2	173813	234243	9.01%	1.163%

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ClientSampleId :
BELL-25-0010

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

77	13.292	1999	2002	2007	rVV2	205556	280444	10.78%	1.392%
78	13.335	2007	2009	2012	rVV3	22747	29199	1.12%	0.145%
79	13.384	2012	2017	2019	rVV2	29695	48103	1.85%	0.239%
80	13.420	2019	2023	2032	rVB	146992	261949	10.07%	1.301%
81	13.500	2032	2036	2039	rBV2	37245	55017	2.12%	0.273%
82	13.542	2039	2043	2046	rBV	32223	38881	1.49%	0.193%
83	13.585	2046	2050	2054	rBV3	47209	75727	2.91%	0.376%
84	13.664	2060	2063	2067	rBV2	32121	50664	1.95%	0.252%
85	13.847	2087	2093	2099	rVB4	72064	138476	5.32%	0.688%
86	13.926	2099	2106	2111	rBV4	58044	113370	4.36%	0.563%
87	14.036	2120	2124	2127	rVB3	66619	71598	2.75%	0.356%
88	14.073	2127	2130	2133	rBV2	31043	36543	1.40%	0.181%
89	14.225	2149	2155	2163	rVB3	101732	176397	6.78%	0.876%
90	14.371	2175	2179	2182	rBV2	24349	27652	1.06%	0.137%
91	14.481	2192	2197	2205	rVB3	50269	90224	3.47%	0.448%
92	14.615	2215	2219	2221	rBV	57375	79051	3.04%	0.393%
93	14.670	2225	2228	2233	rVB2	29323	39021	1.50%	0.194%
94	15.560	2369	2374	2379	rVB	41136	61002	2.35%	0.303%

Sum of corrected areas: 20139893

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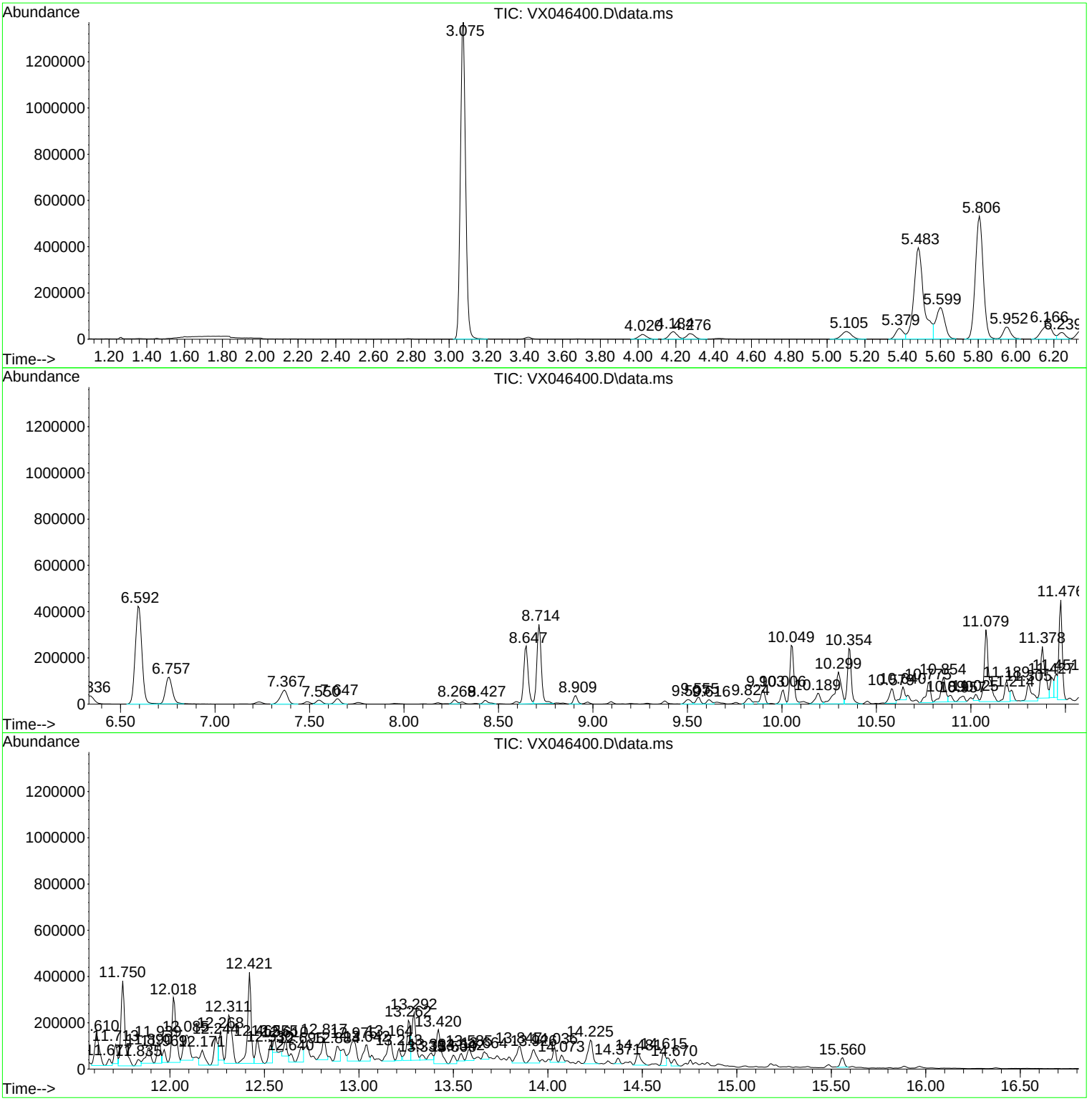
Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052925\
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Instrument :
MSVOA_X
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BELL-25-0010

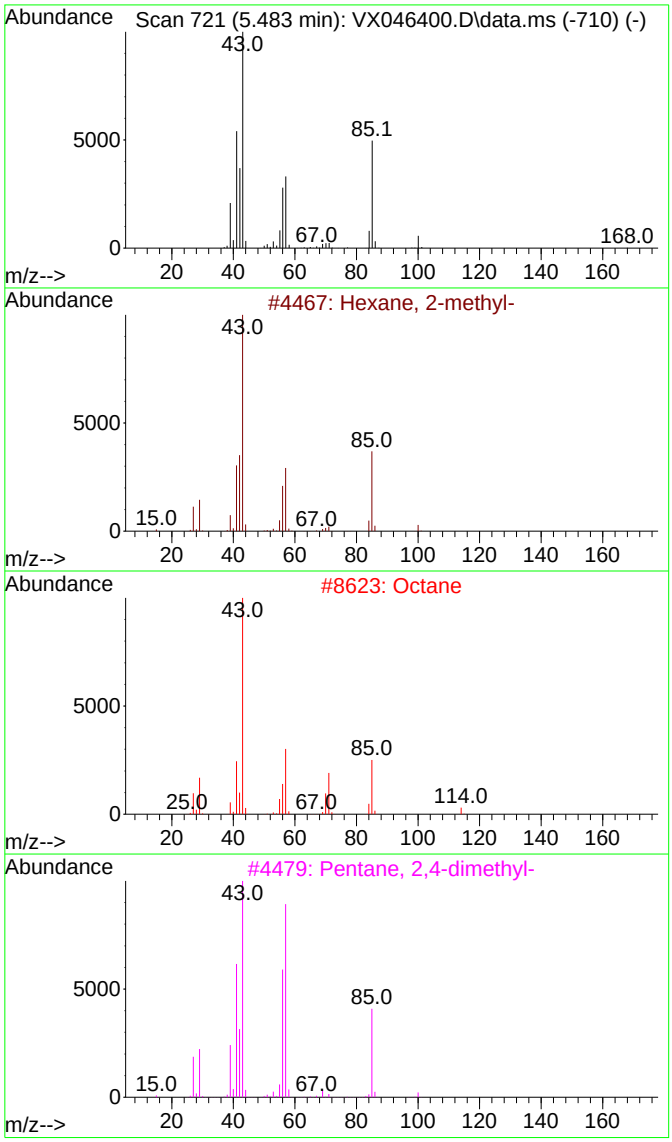
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

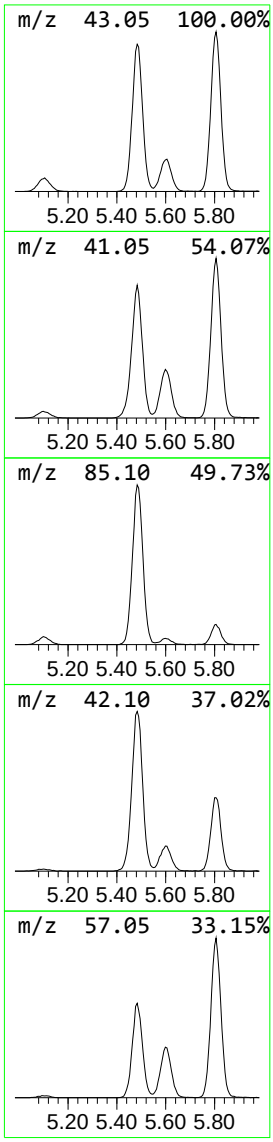
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.483	166.52 ug/l	1426370	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2-methyl-	100	C7H16	000591-76-4	90
2	Octane	114	C8H18	000111-65-9	59
3	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	58
4	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	50
5	2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	50





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

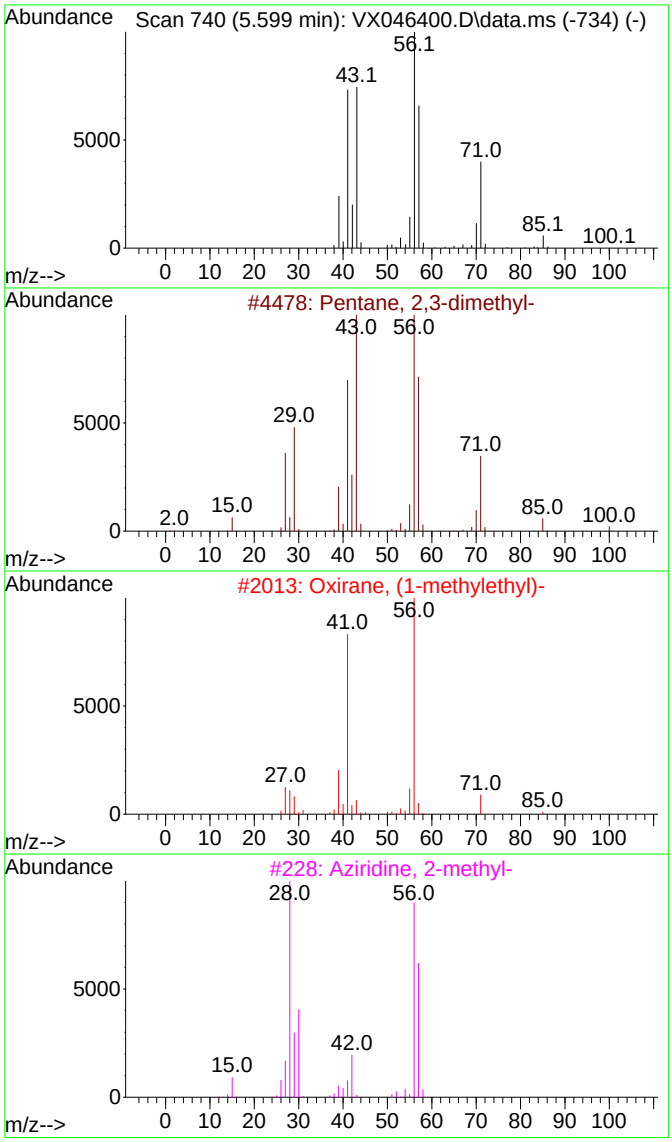
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

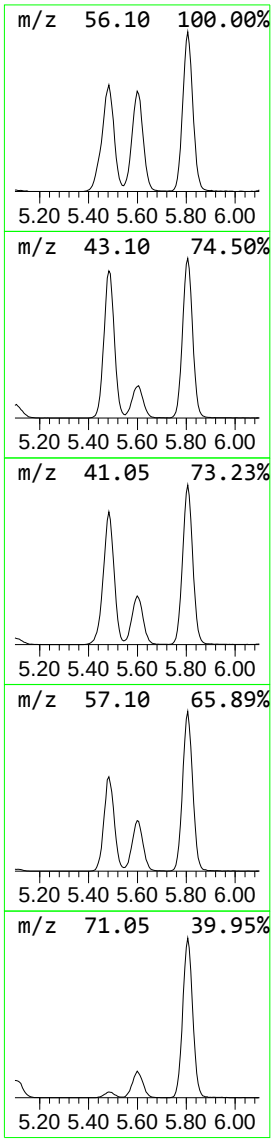
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.599	50.00 ug/l	428285	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	78
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	46
3	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
4	Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	39
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	37





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MSVOA_X
ClientSampleId :
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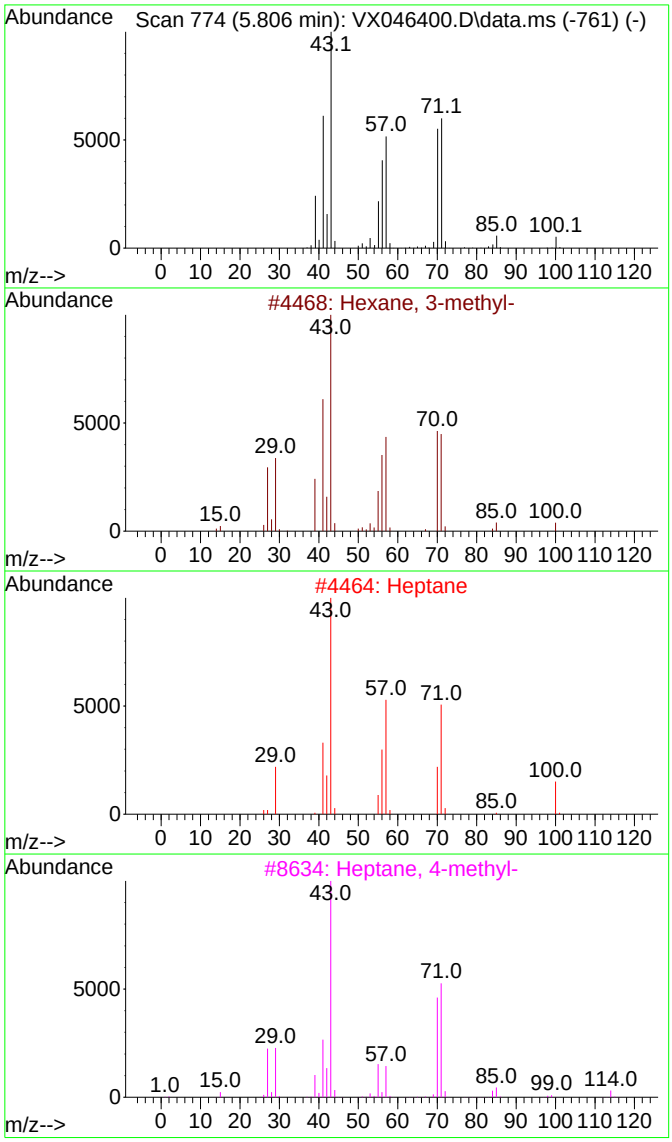
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

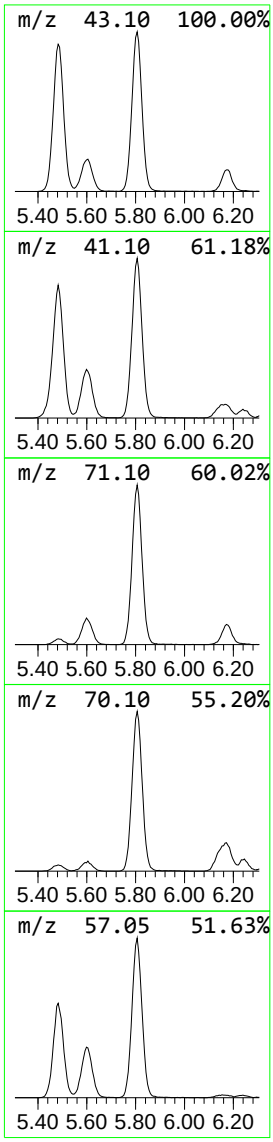
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.806	179.58 ug/l	1538250	Pentafluorobenzene	5.544

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	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	53





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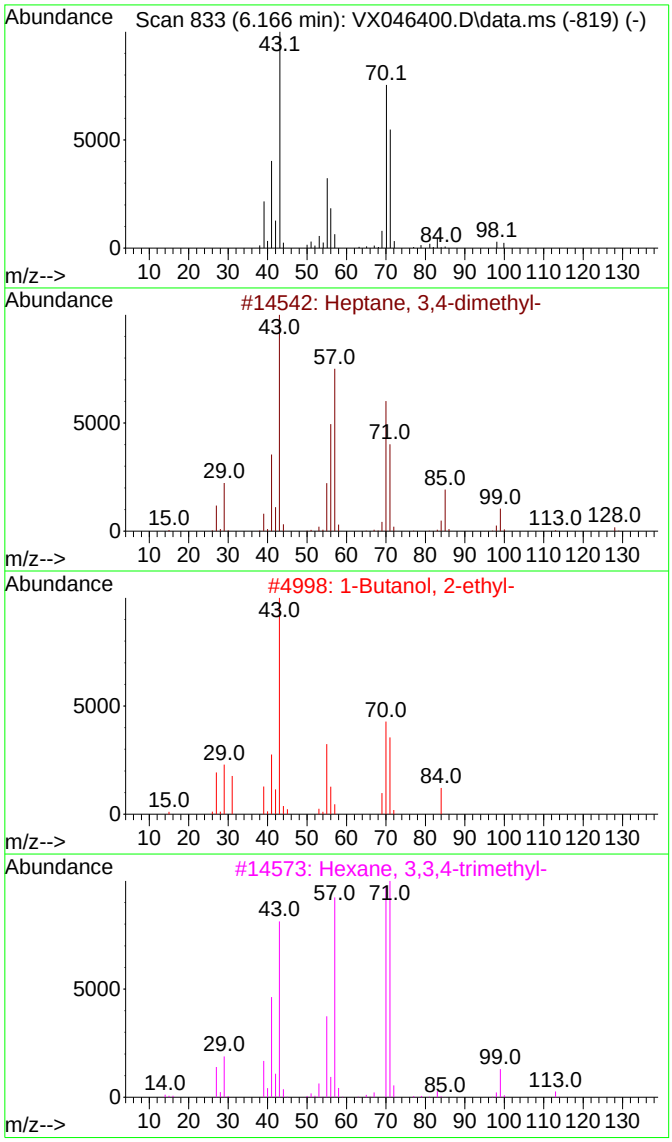
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

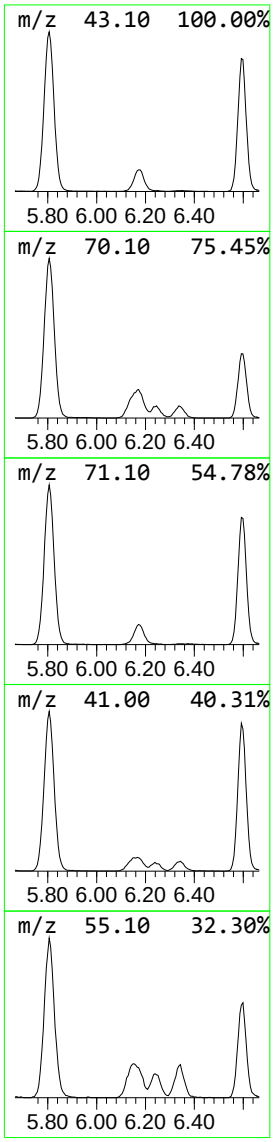
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heptane, 3,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.166	42.05 ug/l	238119	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	64
2	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	64
3	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	56
4	Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	56
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	50





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Data File : VX046400.D
Acq On : 29 May 2025 15:33
Operator : JC/MD
Sample : Q2139-01
Misc : 1.18g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

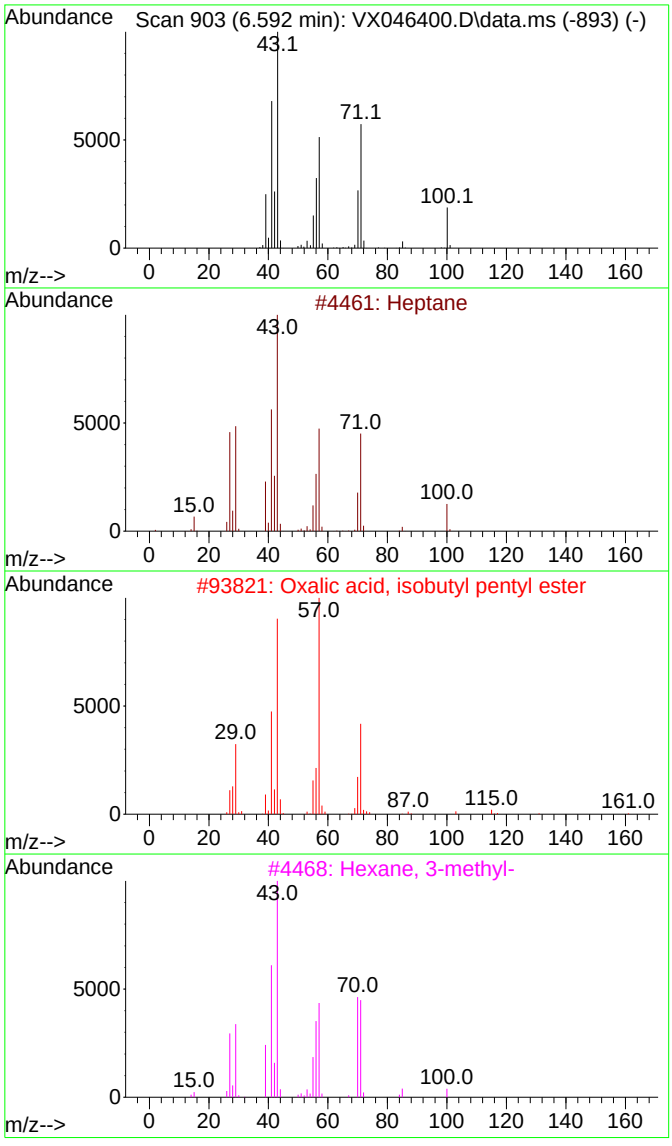
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

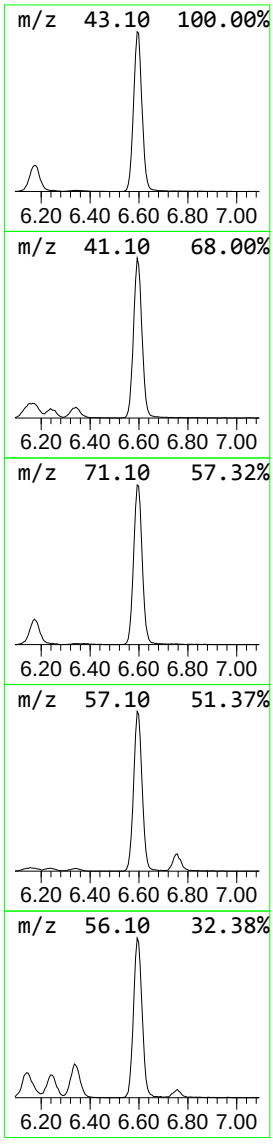
****

Peak Number 5 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.592	182.46 ug/l	1033320	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	42
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	42
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	38





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Data File : VX046400.D
Acq On : 29 May 2025 15:33
Operator : JC/MD
Sample : Q2139-01
Misc : 1.18g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

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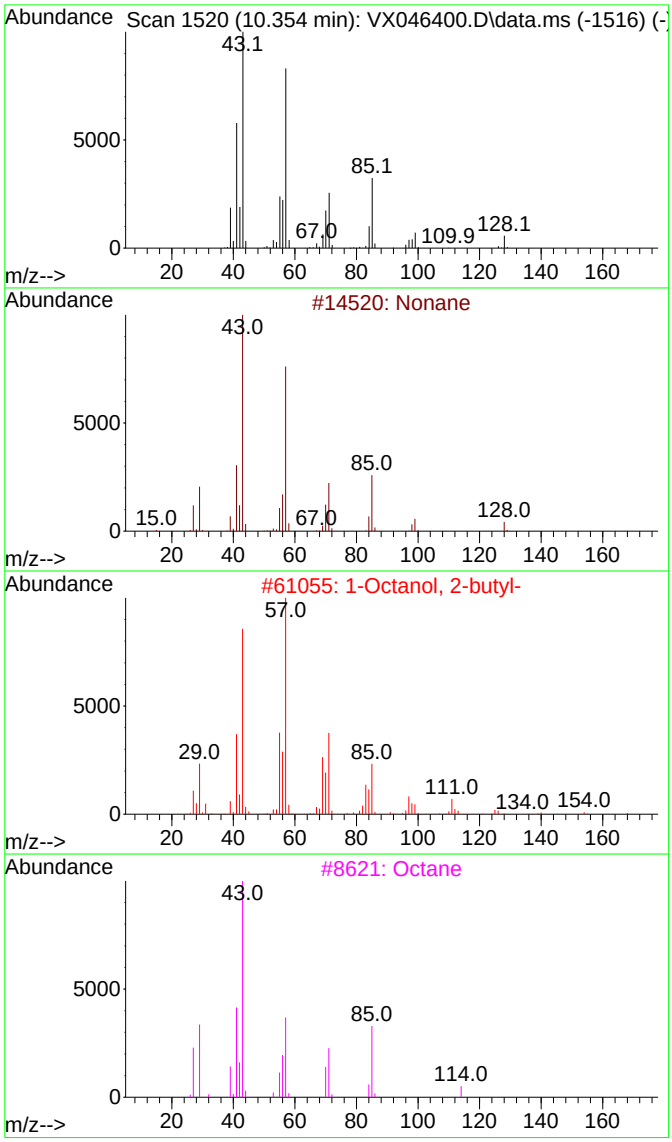
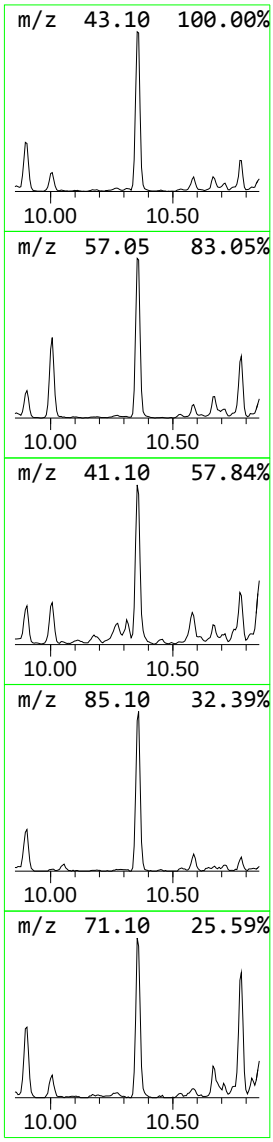
Peak Number 6 Nonane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.354	46.38 ug/l	344624	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	93
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	53
3	Octane	114	C8H18	000111-65-9	53
4	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	50
5	2-Nonanol, trimethylacetate	228	C14H28O2	1000463-21-6	47





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Data File : VX046400.D
Acq On : 29 May 2025 15:33
Operator : JC/MD
Sample : Q2139-01
Misc : 1.18g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

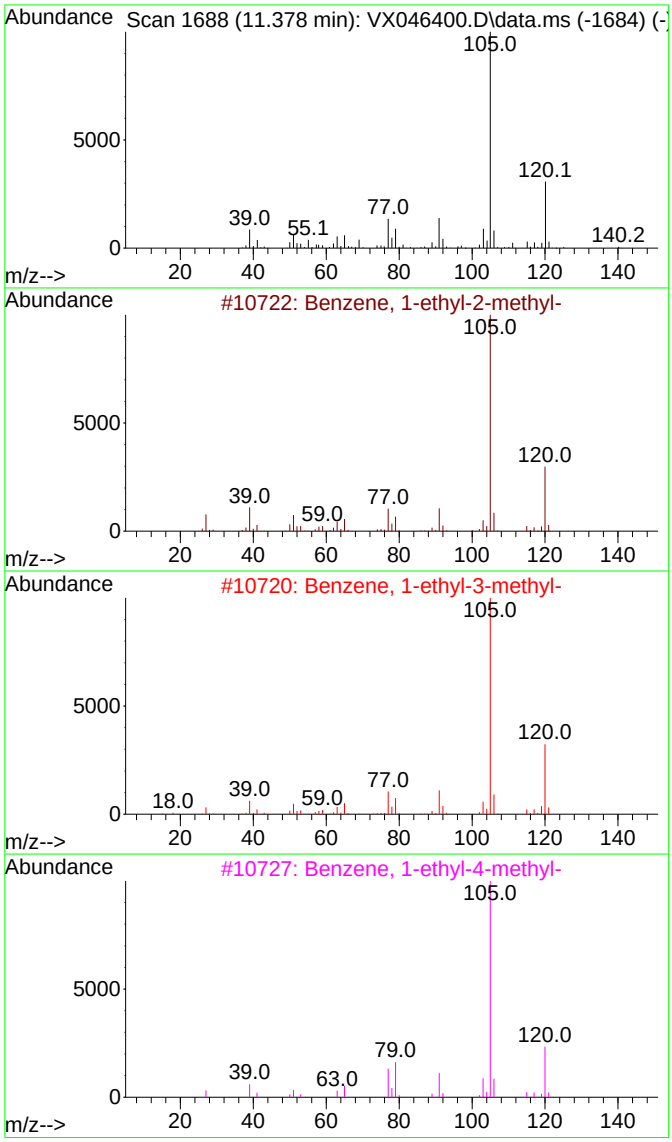
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

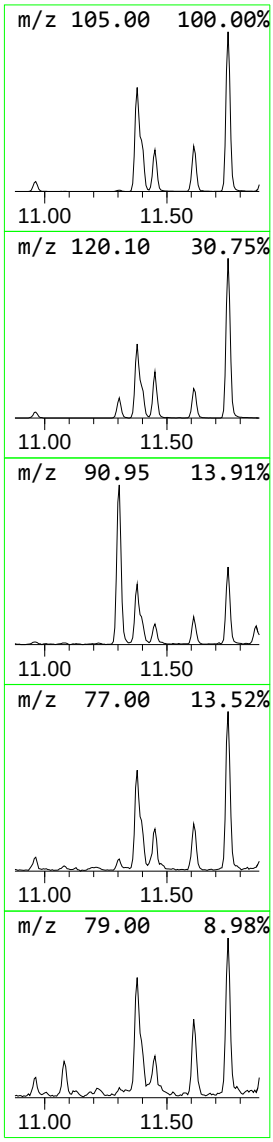
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	43.62 ug/l	373642	1,4-Dichlorobenzene-d4	12.018

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-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	91





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Data File : VX046400.D
Acq On : 29 May 2025 15:33
Operator : JC/MD
Sample : Q2139-01
Misc : 1.18g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

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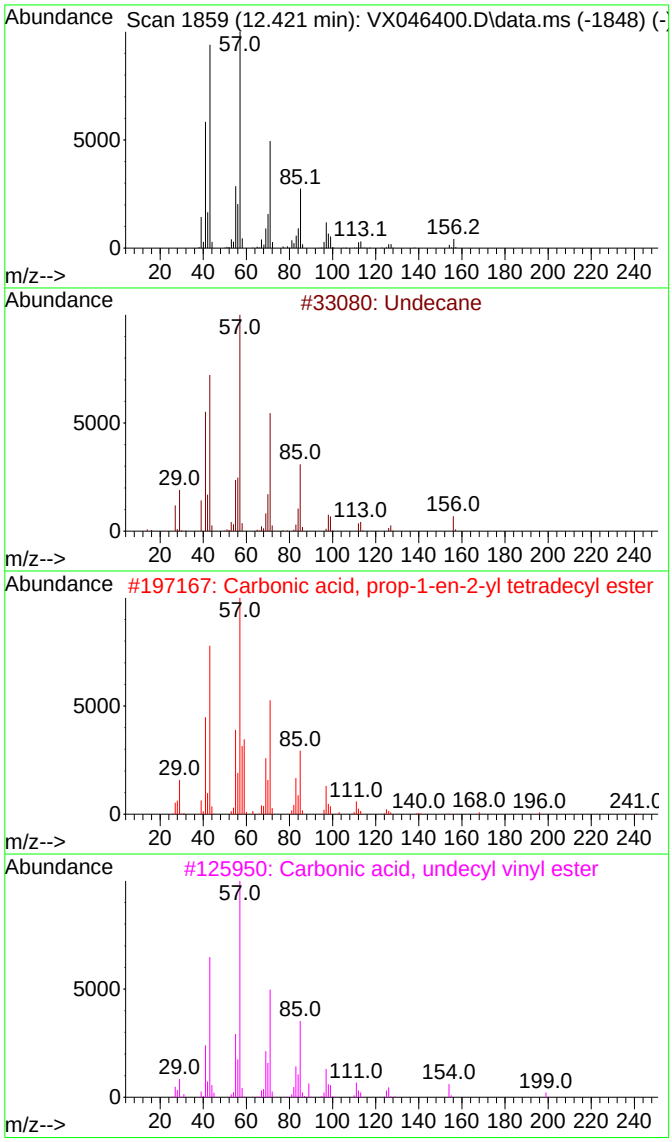
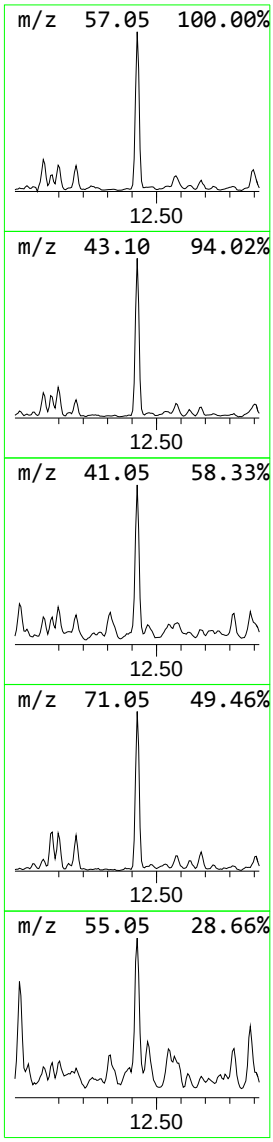
Peak Number 8 Undecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	59.69 ug/l	511353	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	93
2	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	90
3	Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	83
4	Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	78
5	Decane	142	C10H22	000124-18-5	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052925\
Data File : VX046400.D
Acq On : 29 May 2025 15:33
Operator : JC/MD
Sample : Q2139-01
Misc : 1.18g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

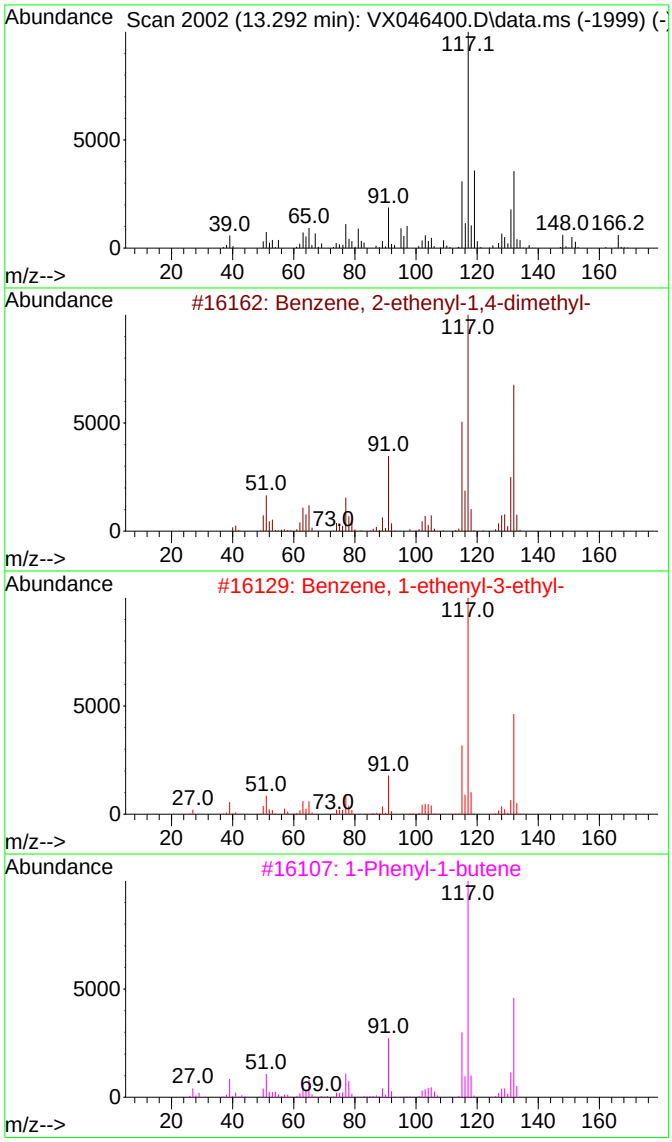
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

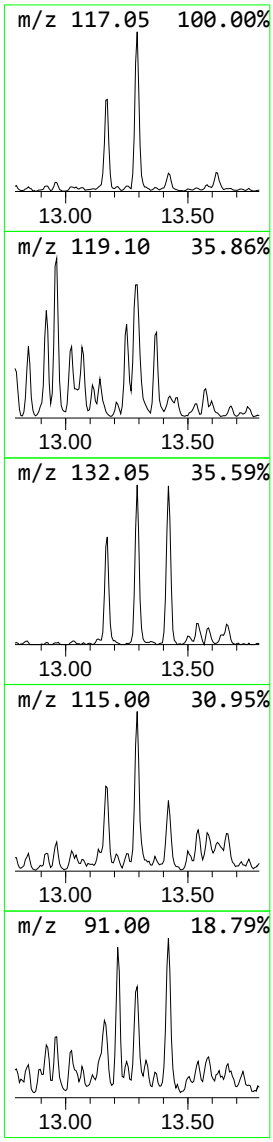
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	32.74 ug/l	280444	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	94
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	89
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052925\
Data File : VX046400.D
Acq On : 29 May 2025 15:33
Operator : JC/MD
Sample : Q2139-01
Misc : 1.18g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

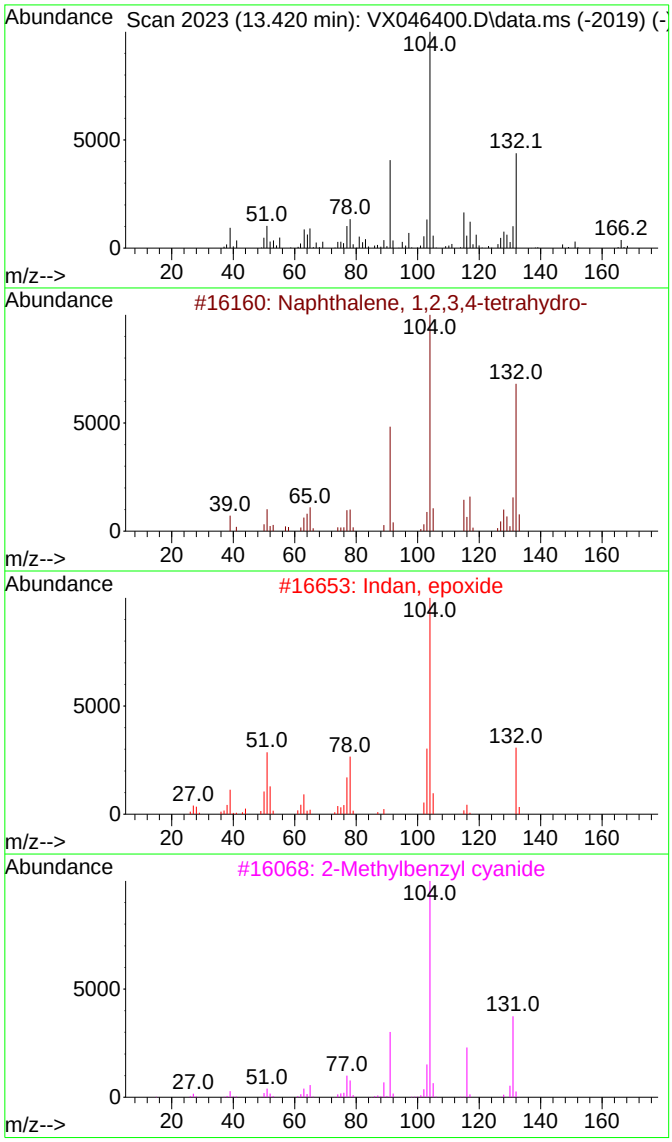
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

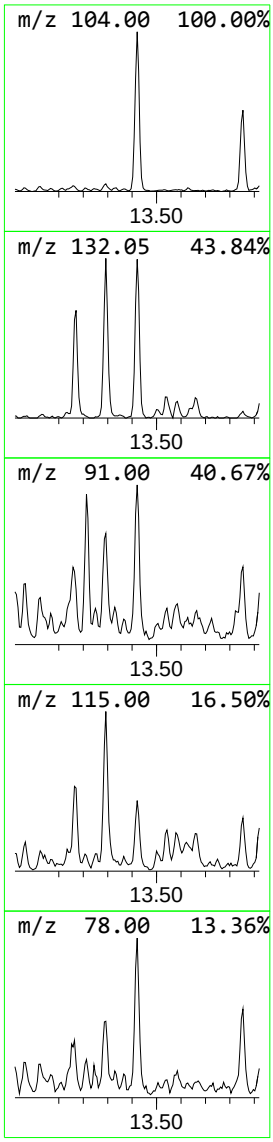
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	30.58 ug/l	261949	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	87
2	Indan, epoxide	132	C9H8O	000768-22-9	50
3	2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	46
4	Benzene, cyclobutyl-	132	C10H12	004392-30-7	45
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-92-1	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052925\
Data File : VX046400.D
Acq On : 29 May 2025 15:33
Operator : JC/MD
Sample : Q2139-01
Misc : 1.18g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BELL-25-0010

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexane, 2-methyl-	5.483	166.5	ug/l	1426370	1	5.544	428285	50.0
Pentane, 2,3-di...	5.599	50.0	ug/l	428285	1	5.544	428285	50.0
Hexane, 3-methyl-	5.806	179.6	ug/l	1538250	1	5.544	428285	50.0
Heptane, 3,4-di...	6.166	42.0	ug/l	238119	2	6.757	283166	50.0
Heptane	6.592	182.5	ug/l	1033320	2	6.757	283166	50.0
Nonane	10.354	46.4	ug/l	344624	3	10.055	371548	50.0
Benzene, 1-ethy...	11.378	43.6	ug/l	373642	4	12.018	428317	50.0
Undecane	12.421	59.7	ug/l	511353	4	12.018	428317	50.0
Benzene, 2-ethe...	13.292	32.7	ug/l	280444	4	12.018	428317	50.0
Naphthalene, 1,...	13.420	30.6	ug/l	261949	4	12.018	428317	50.0