

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070324\
 Data File : VX042160.D
 Acq On : 03 Jul 2024 13:38
 Operator : JC/MD
 Sample : P3106-04
 Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FILTER-1

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\82X061824W.M
 Title : SW846 8260

Signal : TIC: VX042160.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	22	28	40	rBV2	21986	31328	1.41%	0.126%
2	2.941	296	304	318	rBV2	9579	26525	1.20%	0.107%
3	4.245	499	518	534	rBV	110623	408331	18.44%	1.642%
4	5.391	696	706	721	rBV2	52320	216516	9.78%	0.871%
5	5.538	722	730	748	rVB	123622	368147	16.63%	1.481%
6	5.952	789	798	805	rBV2	67035	183592	8.29%	0.738%
7	6.025	805	810	822	rVB2	16813	50346	2.27%	0.202%
8	6.214	830	841	853	rBV4	16608	97304	4.39%	0.391%
9	6.592	896	903	915	rVB3	16075	42116	1.90%	0.169%
10	6.757	920	930	946	rBV	182643	446461	20.16%	1.796%
11	7.275	1000	1015	1022	rBV2	175605	688079	31.08%	2.767%
12	7.586	1061	1066	1072	rVB2	17747	34619	1.56%	0.139%
13	8.269	1172	1178	1182	rBV	19543	31818	1.44%	0.128%
14	8.427	1199	1204	1214	rBV	17679	33212	1.50%	0.134%
15	8.592	1225	1231	1234	rBV	18029	30874	1.39%	0.124%
16	8.647	1234	1240	1247	rVV	381277	605085	27.33%	2.434%
17	8.714	1247	1251	1257	rVV	96813	147741	6.67%	0.594%
18	8.873	1272	1277	1279	rBV2	14852	25770	1.16%	0.104%
19	8.909	1279	1283	1290	rVV	73172	124563	5.63%	0.501%
20	8.970	1290	1293	1305	rVB2	16579	31893	1.44%	0.128%
21	9.287	1338	1345	1357	rBV3	20532	71342	3.22%	0.287%
22	9.494	1370	1379	1385	rBV3	16571	34278	1.55%	0.138%
23	9.561	1385	1390	1394	rVB	18019	27286	1.23%	0.110%
24	9.903	1442	1446	1451	rVB	52548	73428	3.32%	0.295%
25	10.006	1457	1463	1466	rBV	41993	55557	2.51%	0.223%
26	10.055	1466	1471	1487	rVV	387803	584913	26.42%	2.352%
27	10.195	1487	1494	1499	rVV	52507	82265	3.72%	0.331%
28	10.299	1502	1511	1517	rVV2	298137	510417	23.05%	2.053%
29	10.360	1517	1521	1527	rVB	119147	156882	7.09%	0.631%
30	10.586	1552	1558	1563	rBV3	25364	38820	1.75%	0.156%
31	10.640	1563	1567	1577	rVV	167173	250751	11.33%	1.008%
32	10.738	1577	1583	1586	rBV	22947	36138	1.63%	0.145%
33	10.781	1586	1590	1594	rVB2	33772	48184	2.18%	0.194%
34	10.854	1598	1602	1606	rBV3	24654	31632	1.43%	0.127%
35	11.025	1623	1630	1634	rBV2	27459	47467	2.14%	0.191%
36	11.086	1634	1640	1649	rVB	372830	589488	26.62%	2.371%

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37	11.189	1654	1657	1661	rVV	45740	47655	2.15%	0.192%
38	11.305	1670	1676	1679	rBV	20864	31160	1.41%	0.125%
39	11.378	1684	1688	1694	rVV	89530	154954	7.00%	0.623%
40	11.451	1694	1700	1701	rVV2	128549	181238	8.19%	0.729%
41	11.476	1701	1704	1714	rVB	253010	312983	14.14%	1.259%
42	11.616	1722	1727	1734	rBV2	42952	86776	3.92%	0.349%
43	11.683	1734	1738	1742	rBV	228519	292793	13.22%	1.178%
44	11.750	1745	1749	1756	rVB	225287	298765	13.49%	1.202%
45	11.902	1769	1774	1778	rVB	320941	383194	17.31%	1.541%
46	11.994	1782	1789	1790	rVV2	77987	135790	6.13%	0.546%
47	12.024	1790	1794	1800	rVV	469038	736476	33.26%	2.962%
48	12.085	1800	1804	1810	rVB3	120210	259428	11.72%	1.043%
49	12.171	1815	1818	1822	rVB2	71234	77498	3.50%	0.312%
50	12.219	1822	1826	1832	rBV2	167389	299415	13.52%	1.204%
51	12.317	1837	1842	1848	rVB3	99653	163463	7.38%	0.657%
52	12.421	1854	1859	1863	rBV2	448216	570295	25.76%	2.294%
53	12.555	1878	1881	1883	rVB2	27662	26210	1.18%	0.105%
54	12.591	1883	1887	1889	rVV4	36608	58625	2.65%	0.236%
55	12.738	1905	1911	1915	rBV6	37757	73358	3.31%	0.295%
56	12.811	1917	1923	1927	rVB3	122647	185048	8.36%	0.744%
57	12.921	1932	1941	1946	rBV5	149248	397360	17.95%	1.598%
58	12.969	1946	1949	1957	rVV4	124858	236497	10.68%	0.951%
59	13.042	1957	1961	1964	rVB3	102479	113865	5.14%	0.458%
60	13.164	1977	1981	1986	rVB3	32636	50397	2.28%	0.203%
61	13.213	1986	1989	1991	rBV2	29563	39722	1.79%	0.160%
62	13.268	1993	1998	2000	rBV	530516	640444	28.93%	2.576%
63	13.292	2000	2002	2007	rVB4	166669	209489	9.46%	0.843%
64	13.341	2007	2010	2013	rBV4	61820	74214	3.35%	0.298%
65	13.420	2014	2023	2028	rBV8	165186	461480	20.84%	1.856%
66	13.518	2033	2039	2042	rBV2	60947	98106	4.43%	0.395%
67	13.548	2042	2044	2047	rVV2	44007	46900	2.12%	0.189%
68	13.609	2047	2054	2060	rVB6	154348	278640	12.58%	1.121%
69	13.677	2060	2065	2071	rBV3	150603	286711	12.95%	1.153%
70	13.737	2071	2075	2077	rVV	136212	182058	8.22%	0.732%
71	13.774	2077	2081	2088	rVV	1659601	2214095	100.00%	8.905%
72	13.841	2088	2092	2100	rVB7	248734	466255	21.06%	1.875%
73	13.920	2100	2105	2108	rBV5	65472	145877	6.59%	0.587%
74	14.036	2118	2124	2127	rBV2	556046	716744	32.37%	2.883%
75	14.067	2127	2129	2132	rVB3	105137	119676	5.41%	0.481%
76	14.140	2138	2141	2143	rBV3	85310	115542	5.22%	0.465%

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Title : SW846 8260

77	14.219	2150	2154	2159	rVB3	206754	322670	14.57%	1.298%
78	14.268	2160	2162	2165	rVB3	35516	31806	1.44%	0.128%
79	14.347	2172	2175	2181	rVB5	93923	147937	6.68%	0.595%
80	14.426	2181	2188	2193	rVB5	228770	434459	19.62%	1.747%
81	14.475	2193	2196	2198	rBV2	101381	150262	6.79%	0.604%
82	14.634	2215	2222	2226	rBV	1087548	1550747	70.04%	6.237%
83	14.670	2226	2228	2232	rVB4	69691	77723	3.51%	0.313%
84	14.719	2233	2236	2239	rBV4	69134	104172	4.70%	0.419%
85	14.756	2239	2242	2243	rVV	459103	474170	21.42%	1.907%
86	14.780	2243	2246	2251	rVV	779097	1026679	46.37%	4.129%
87	14.847	2254	2257	2260	rVB4	62873	76080	3.44%	0.306%
88	15.182	2308	2312	2313	rBV2	83862	101651	4.59%	0.409%
89	15.207	2313	2316	2320	rVB2	172266	222089	10.03%	0.893%
90	15.371	2339	2343	2346	rBV2	120829	171901	7.76%	0.691%
91	15.408	2347	2349	2354	rVV4	72063	109379	4.94%	0.440%
92	15.481	2356	2361	2368	rVV2	287538	563954	25.47%	2.268%
93	15.560	2369	2374	2378	rVV	232511	375231	16.95%	1.509%
94	15.609	2378	2382	2386	rVV	351102	559618	25.28%	2.251%
95	15.646	2386	2388	2397	rVB	173818	258060	11.66%	1.038%
96	15.835	2412	2419	2423	rBV	64657	147720	6.67%	0.594%
97	15.920	2429	2433	2439	rVB	84913	140941	6.37%	0.567%
98	15.987	2440	2444	2449	rVV	50256	78803	3.56%	0.317%
99	16.091	2456	2461	2467	rBV3	80928	154876	7.00%	0.623%
100	16.597	2540	2544	2549	rVB3	29313	51496	2.33%	0.207%

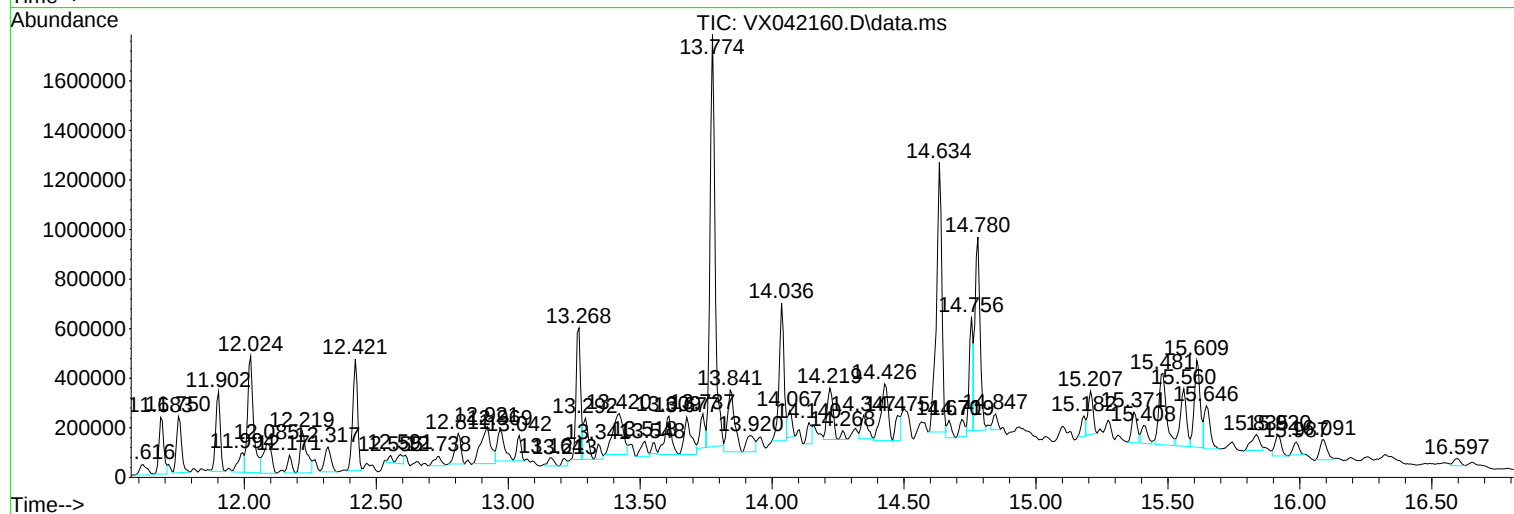
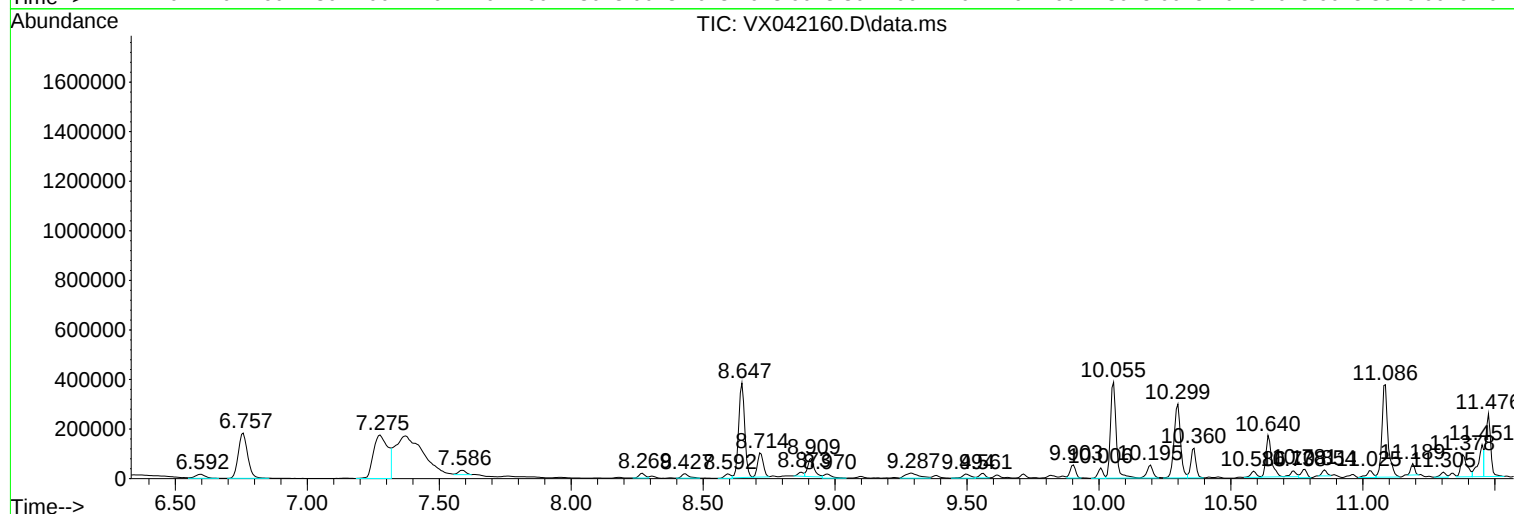
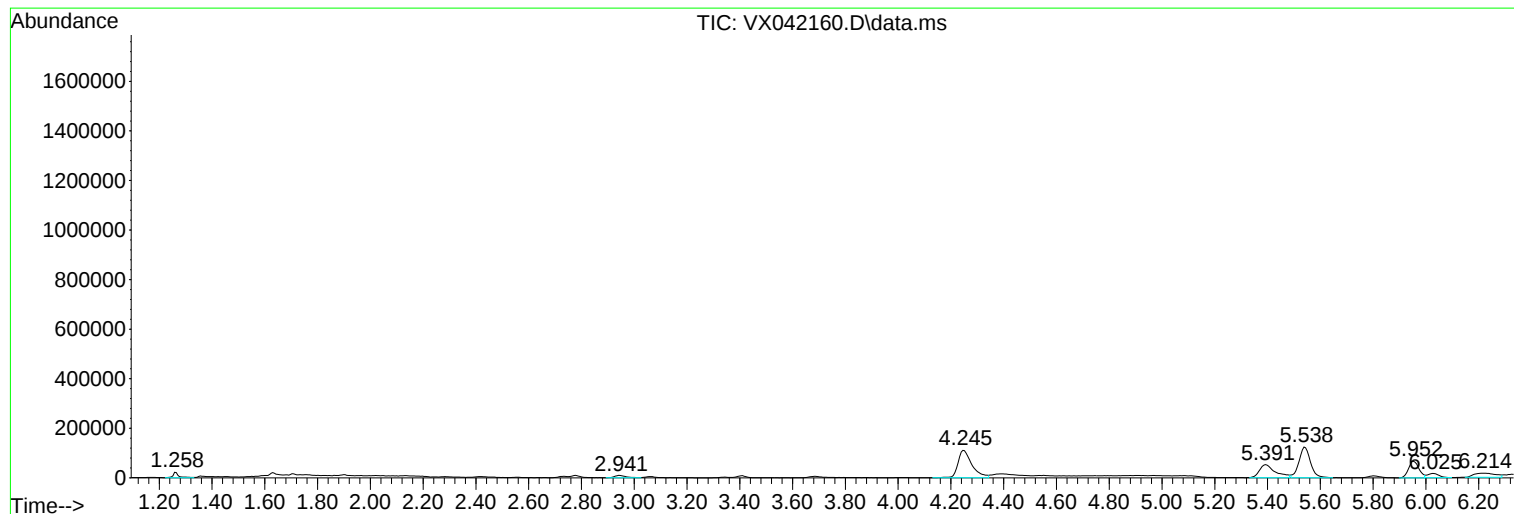
Sum of corrected areas: 24864788

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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



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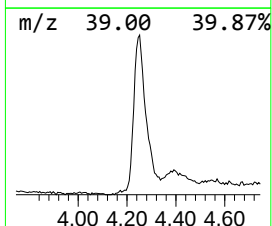
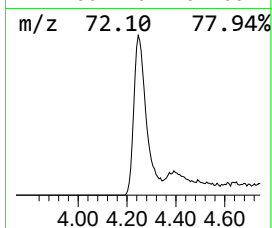
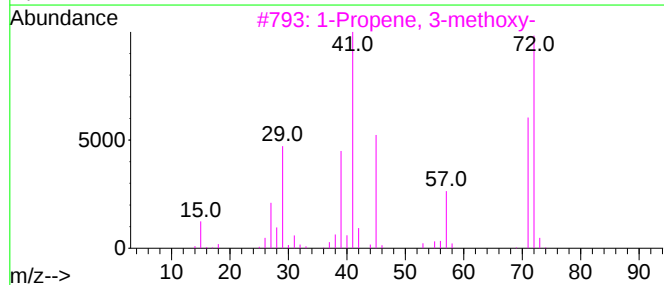
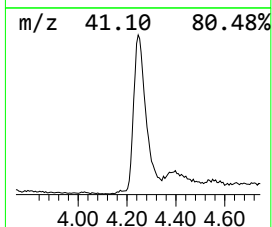
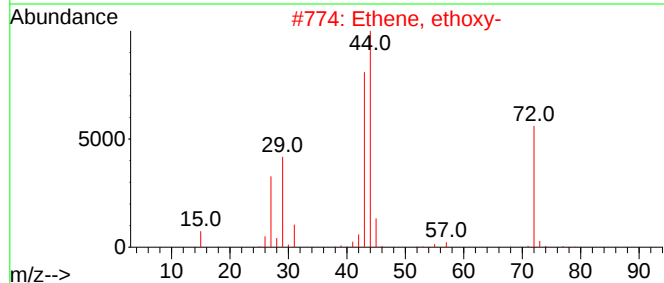
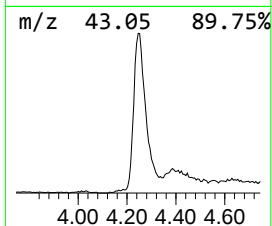
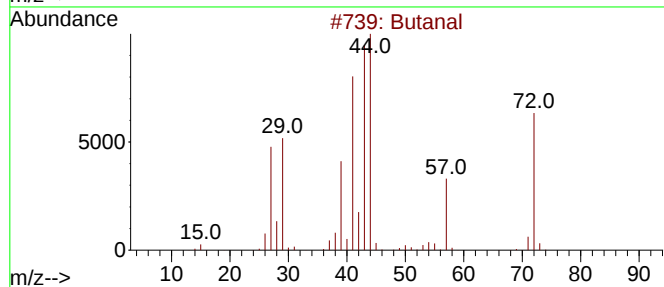
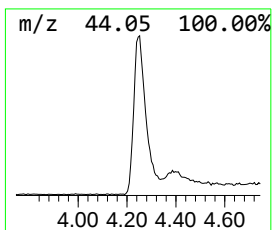
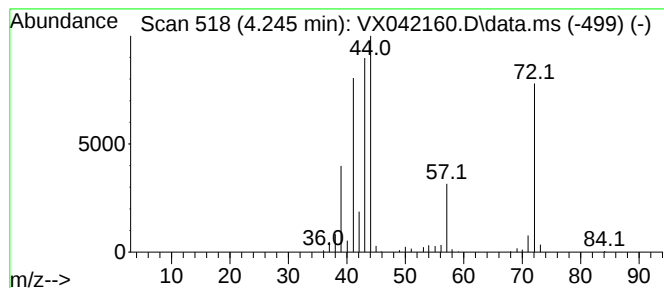
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.245	55.46 ug/l	408331	Pentafluorobenzene	5.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	58
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5			Isobutylene epoxide	72	C4H8O	000558-30-5	35



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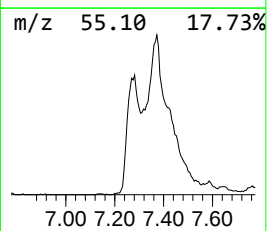
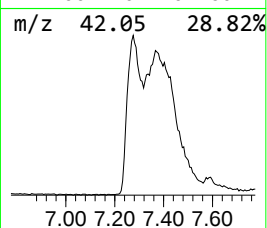
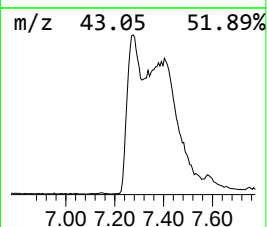
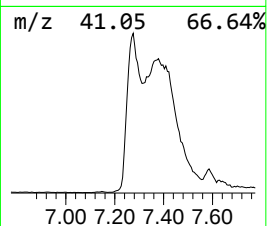
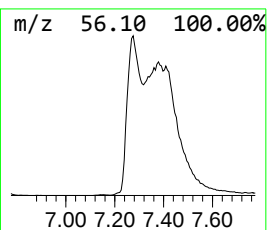
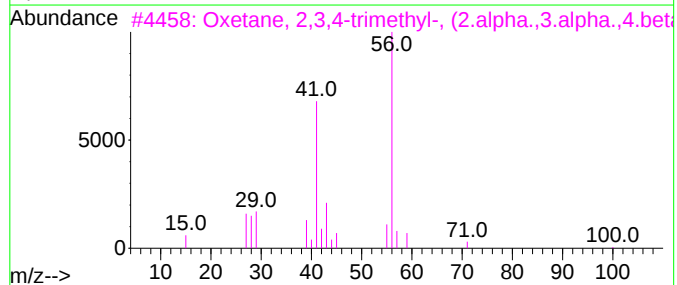
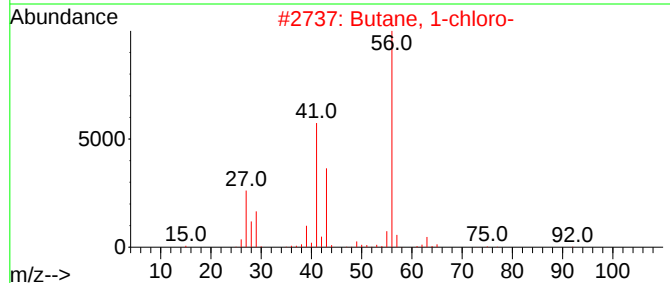
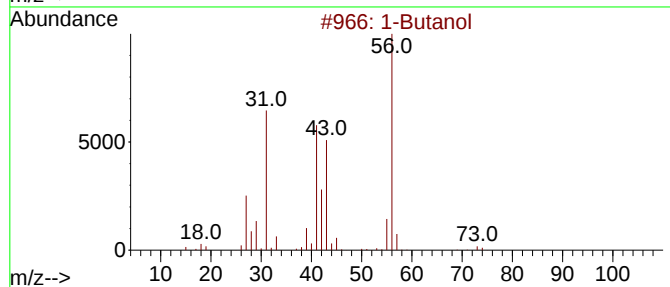
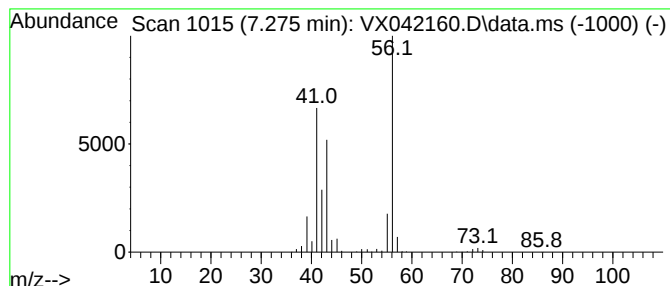
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.275	77.06 ug/l	688079	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	45
3			Oxetane, 2,3,4-trimethyl-, (2.alpha...	100	C6H12O	032347-12-9	38
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
5			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9



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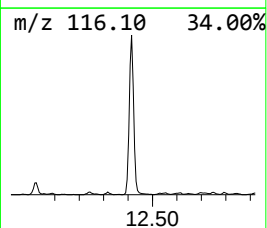
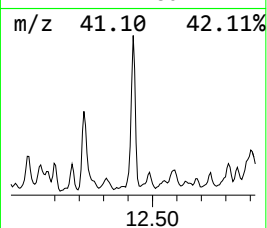
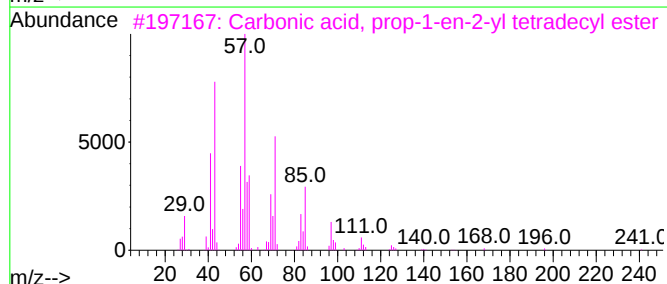
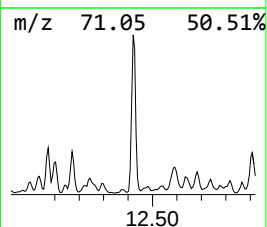
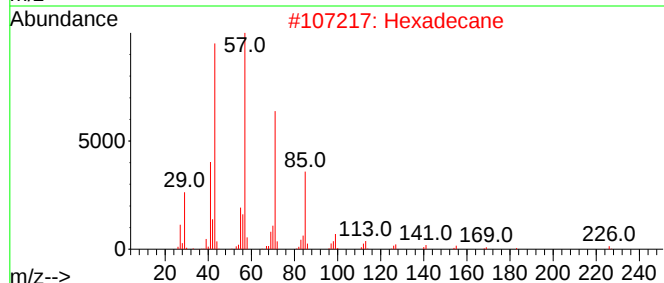
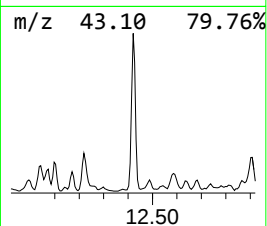
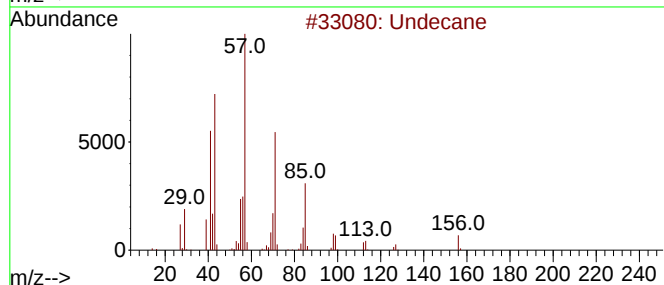
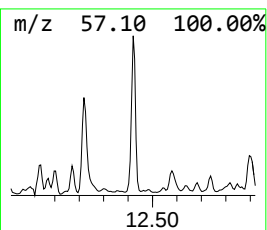
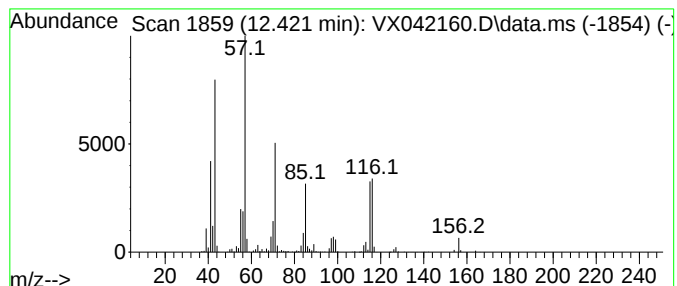
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Quant Title : SW846 8260

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

Peak Number 3 Undecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	38.72 ug/l	570295	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	96
2			Hexadecane	226	C16H34	000544-76-3	52
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	52
4			Decane	142	C10H22	000124-18-5	50
5			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070324\
Data File : VX042160.D
Acq On : 03 Jul 2024 13:38
Operator : JC/MD
Sample : P3106-04
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FILTER-1

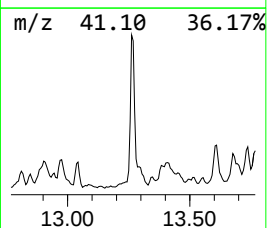
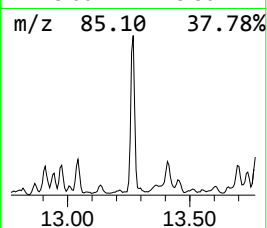
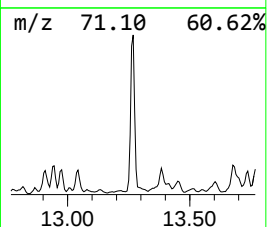
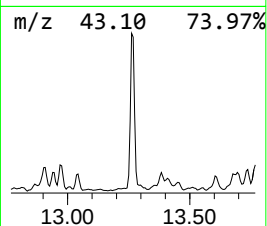
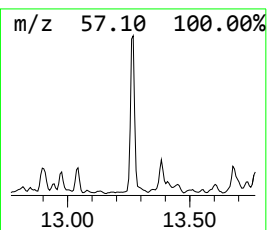
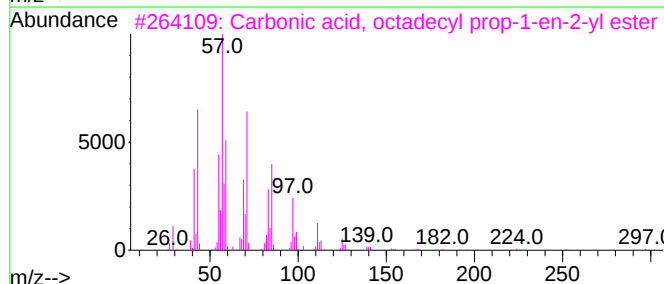
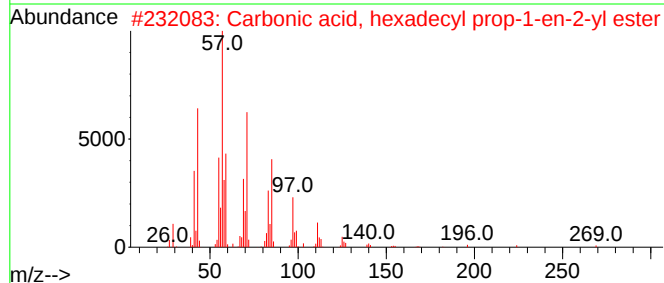
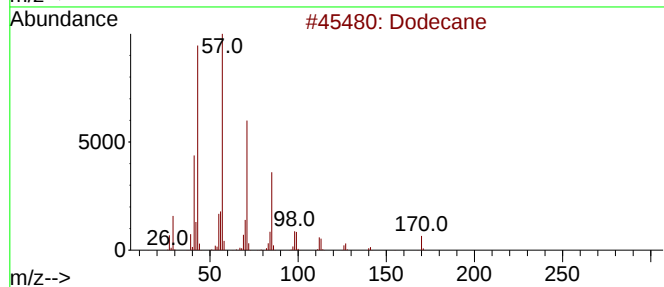
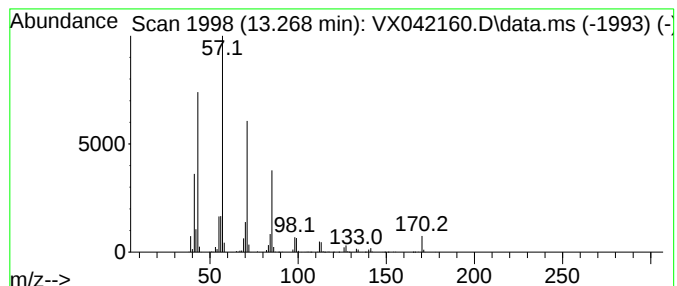
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Quant Title : SW846 8260

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

Peak Number 4 Dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	43.48 ug/l	640444	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	96
2			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	90
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	90
5			Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070324\
Data File : VX042160.D
Acq On : 03 Jul 2024 13:38
Operator : JC/MD
Sample : P3106-04
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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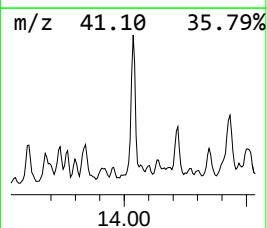
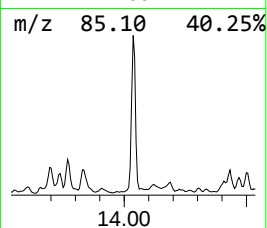
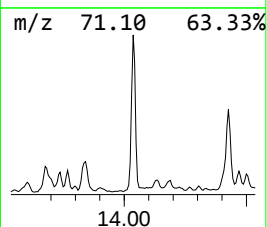
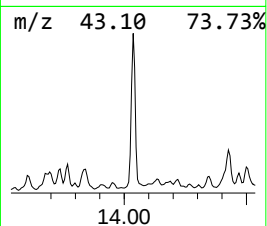
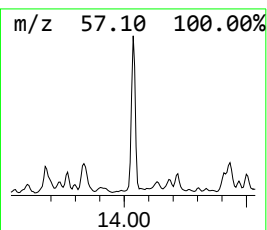
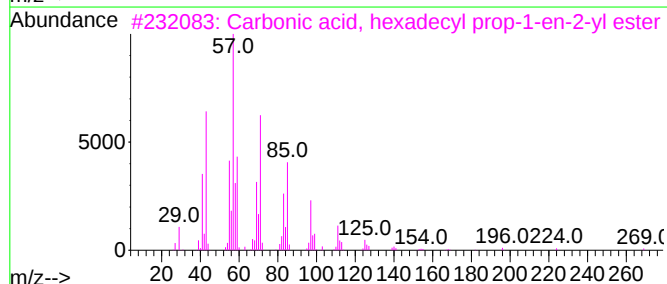
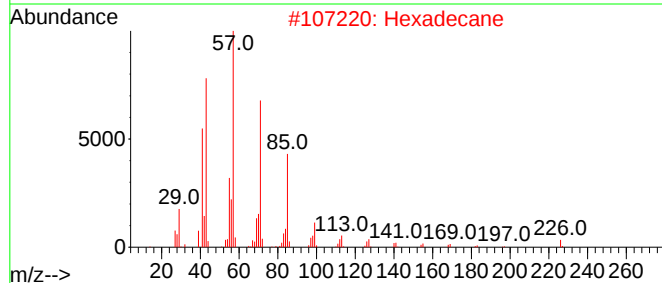
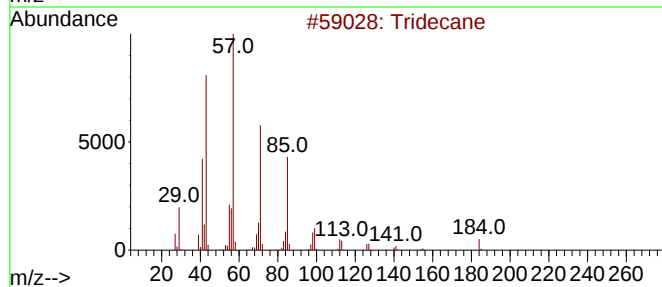
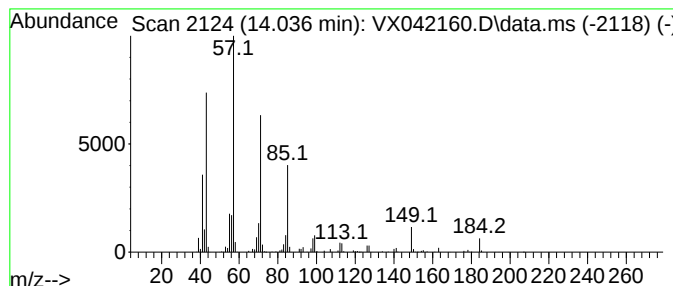
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Quant Title : SW846 8260

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

Peak Number 5 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.036	48.66 ug/l	716744	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	98
2			Hexadecane	226	C16H34	000544-76-3	86
3			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	86
4			Dodecane	170	C12H26	000112-40-3	86
5			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070324\
Data File : VX042160.D
Acq On : 03 Jul 2024 13:38
Operator : JC/MD
Sample : P3106-04
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FILTER-1

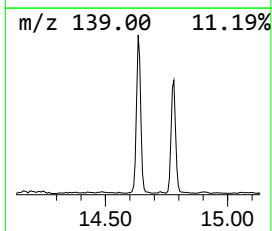
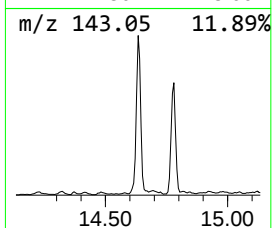
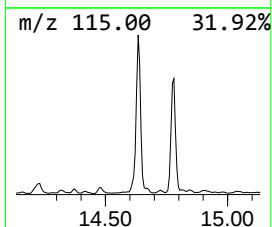
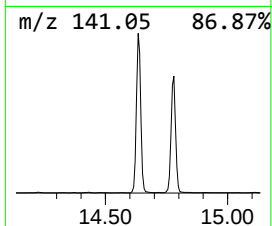
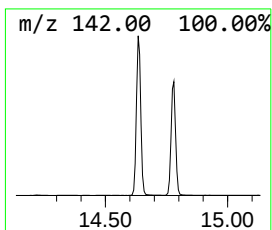
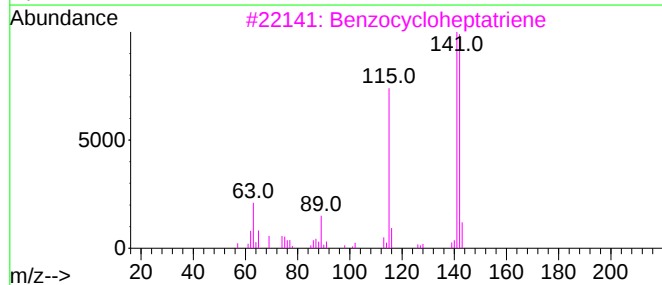
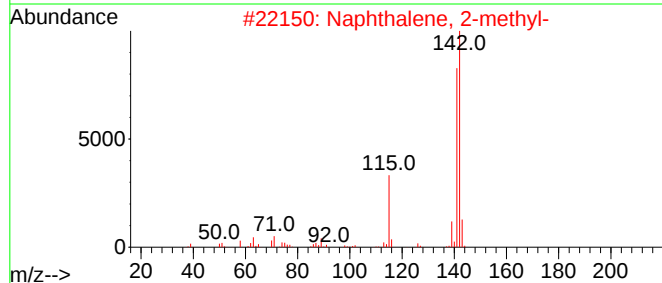
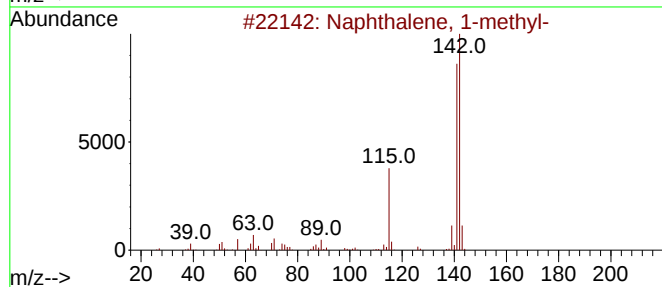
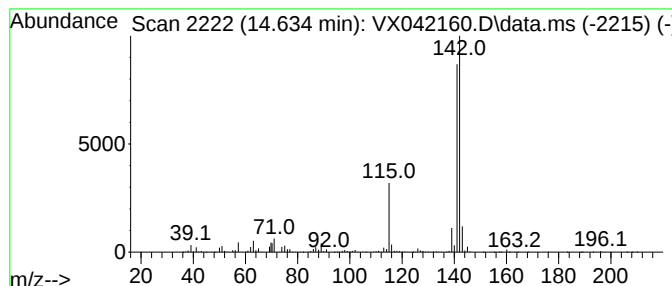
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	105.28 ug/l	1550750	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070324\
Data File : VX042160.D
Acq On : 03 Jul 2024 13:38
Operator : JC/MD
Sample : P3106-04
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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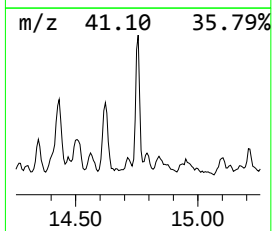
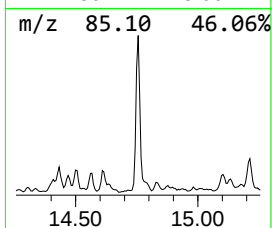
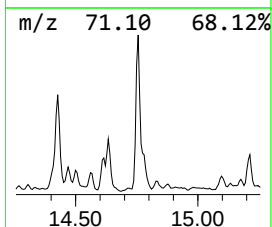
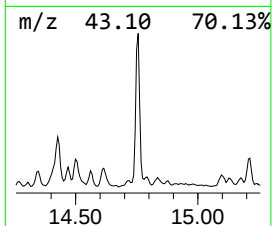
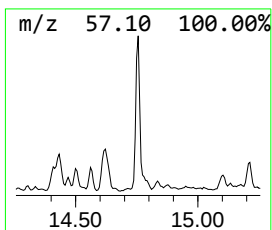
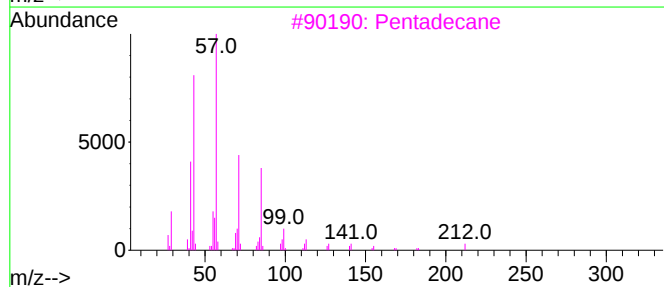
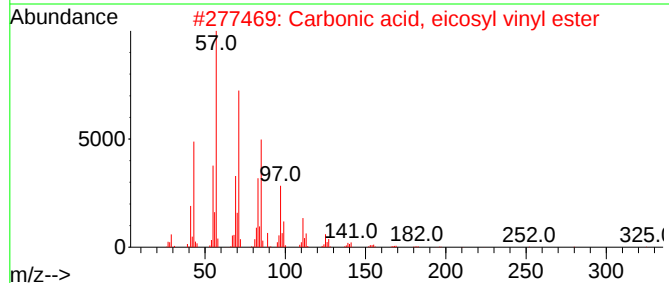
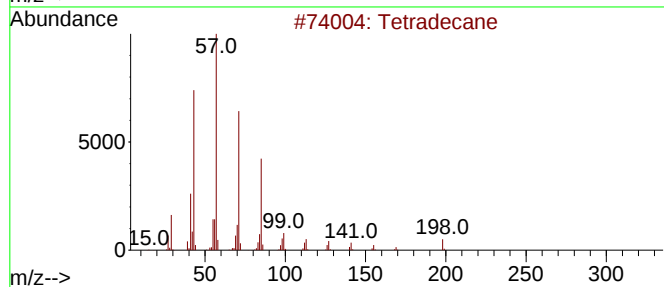
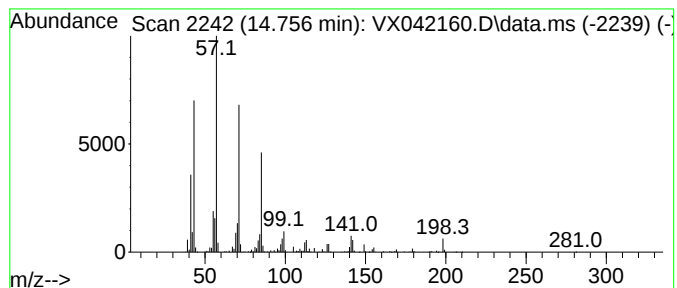
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Quant Title : SW846 8260

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

Peak Number 7 Carbonic acid, eicosyl vinyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.756	32.19 ug/l	474170	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	97
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	83
3			Pentadecane	212	C15H32	000629-62-9	80
4			Eicosane	282	C20H42	000112-95-8	80
5			Tridecane	184	C13H28	000629-50-5	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070324\
Data File : VX042160.D
Acq On : 03 Jul 2024 13:38
Operator : JC/MD
Sample : P3106-04
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FILTER-1

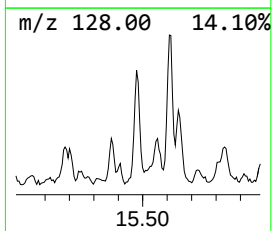
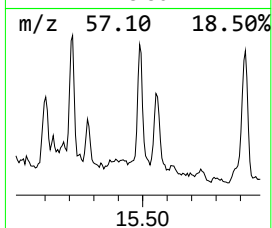
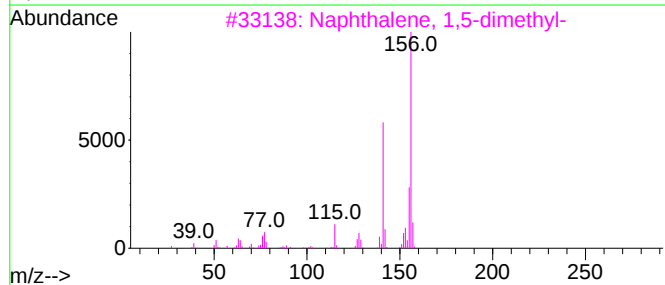
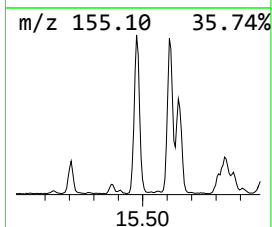
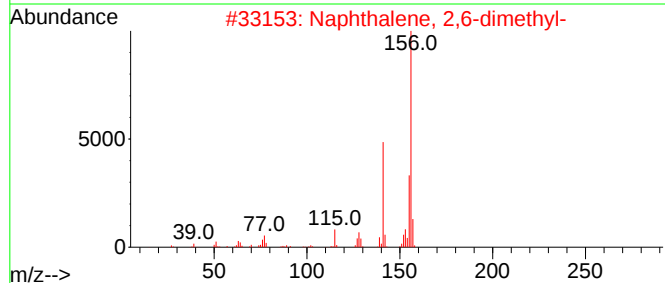
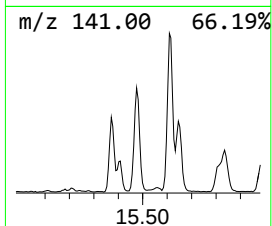
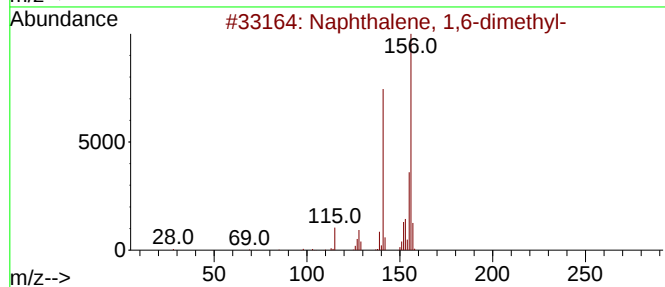
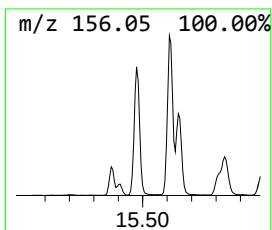
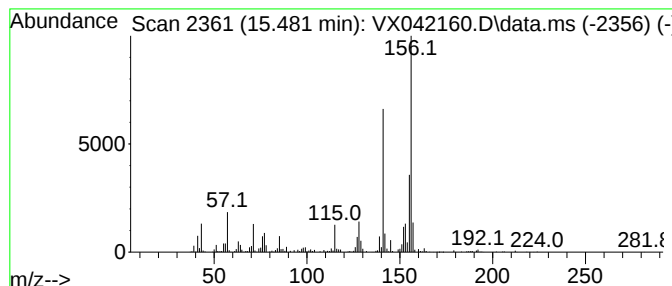
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	38.29 ug/l	563954	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070324\
Data File : VX042160.D
Acq On : 03 Jul 2024 13:38
Operator : JC/MD
Sample : P3106-04
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FILTER-1

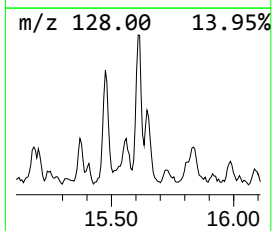
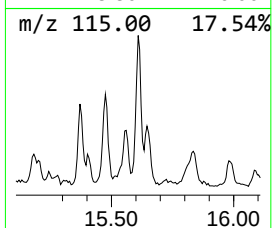
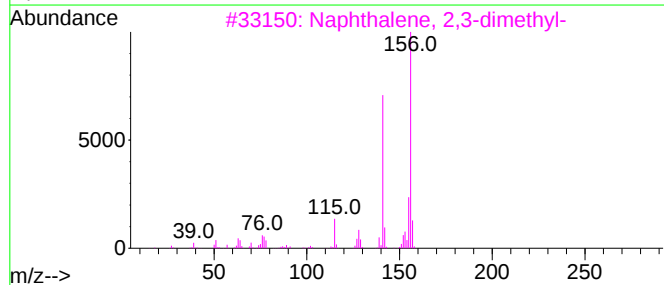
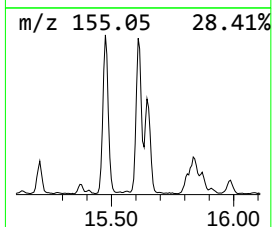
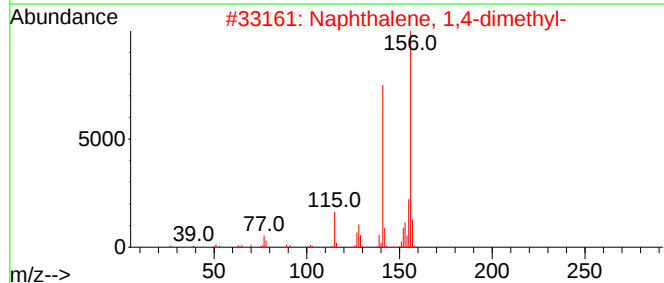
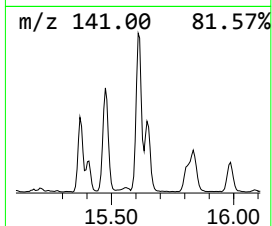
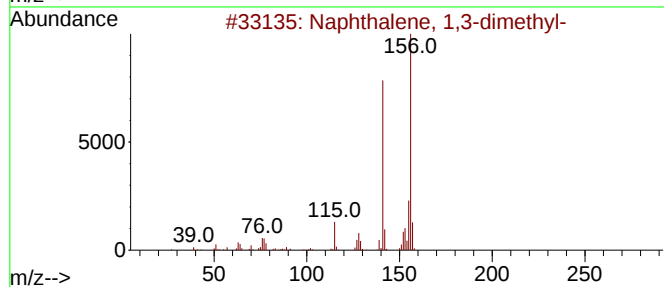
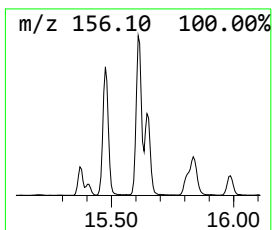
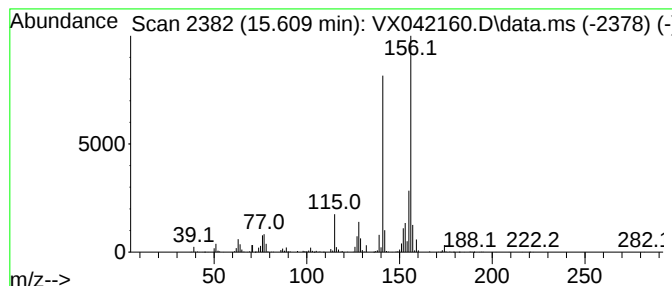
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	37.99 ug/l	559618	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
2			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070324\
Data File : VX042160.D
Acq On : 03 Jul 2024 13:38
Operator : JC/MD
Sample : P3106-04
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FILTER-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.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
Butanal	4.245	55.5	ug/l	408331	1	5.538	368147	50.0
1-Butanol	7.275	77.1	ug/l	688079	2	6.757	446461	50.0
Undecane	12.421	38.7	ug/l	570295	4	12.024	736476	50.0
Dodecane	13.268	43.5	ug/l	640444	4	12.024	736476	50.0
Tridecane	14.036	48.7	ug/l	716744	4	12.024	736476	50.0
Naphthalene, 1-...	14.634	105.3	ug/l	1550750	4	12.024	736476	50.0
Carbonic acid, ...	14.756	32.2	ug/l	474170	4	12.024	736476	50.0
Naphthalene, 1,...	15.481	38.3	ug/l	563954	4	12.024	736476	50.0
Naphthalene, 1,...	15.609	38.0	ug/l	559618	4	12.024	736476	50.0