

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020822\
 Data File : VX026847.D
 Acq On : 09 Feb 2022 01:38
 Operator : JC/MD
 Sample : N1425-03 200X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31377

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\82X020822W.M
 Title : SW846 8260

Signal : TIC: VX026847.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	56	61	70	rBV	180899	214012	31.62%	3.351%
2	2.111	157	168	181	rBV2	2620	11312	1.67%	0.177%
3	5.391	695	706	717	rBV	76507	220434	32.57%	3.452%
4	5.556	722	733	747	rVB	136641	385565	56.97%	6.038%
5	5.958	790	799	810	rBV	84738	224987	33.24%	3.523%
6	6.763	920	931	947	rBV	210230	499797	73.85%	7.826%
7	7.378	1025	1032	1043	rVB3	8686	19994	2.95%	0.313%
8	8.604	1227	1233	1235	rBV3	5071	8622	1.27%	0.135%
9	8.653	1235	1241	1247	rVV	427841	676759	100.00%	10.597%
10	8.720	1247	1252	1258	rVB	30386	46012	6.80%	0.720%
11	9.104	1307	1315	1320	rVB	4891	7876	1.16%	0.123%
12	9.512	1375	1382	1386	rBV4	4824	8246	1.22%	0.129%
13	9.567	1386	1391	1395	rVB	8849	12378	1.83%	0.194%
14	10.055	1466	1471	1478	rVB	449615	595540	88.00%	9.326%
15	10.195	1488	1494	1499	rBV	27154	36690	5.42%	0.575%
16	10.299	1503	1511	1518	rVV	79211	121274	17.92%	1.899%
17	10.360	1518	1521	1528	rVB	8991	12234	1.81%	0.192%
18	10.585	1553	1558	1562	rBV2	6042	10221	1.51%	0.160%
19	10.640	1562	1567	1576	rVB	44132	60517	8.94%	0.948%
20	10.780	1582	1590	1594	rVB4	6140	10636	1.57%	0.167%
21	10.860	1597	1603	1608	rBV3	7512	12548	1.85%	0.196%
22	10.963	1614	1620	1624	rBV	8391	10827	1.60%	0.170%
23	11.079	1634	1639	1646	rBV	349987	460055	67.98%	7.204%
24	11.305	1671	1676	1683	rBV	22899	29141	4.31%	0.456%
25	11.378	1683	1688	1696	rBV	67234	124141	18.34%	1.944%
26	11.451	1696	1700	1704	rBV	32336	40348	5.96%	0.632%
27	11.615	1722	1727	1733	rVB	43218	57356	8.48%	0.898%
28	11.756	1745	1750	1759	rVB	122550	157869	23.33%	2.472%
29	11.890	1769	1772	1777	rVB	11160	14831	2.19%	0.232%
30	11.969	1782	1785	1789	rVV	12827	15057	2.22%	0.236%
31	12.024	1789	1794	1800	rVV	457703	550122	81.29%	8.614%
32	12.091	1800	1805	1810	rBV	42621	54568	8.06%	0.854%
33	12.243	1824	1830	1832	rBV2	43187	54973	8.12%	0.861%
34	12.268	1832	1834	1838	rVB	37661	41664	6.16%	0.652%
35	12.317	1838	1842	1852	rVB3	55527	93835	13.87%	1.469%
36	12.420	1852	1859	1862	rBV3	9111	18533	2.74%	0.290%

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37	12.463	1862	1866	1871	rVB	25157	29470	4.35%	0.461%
38	12.530	1873	1877	1879	rBV	25434	32003	4.73%	0.501%
39	12.554	1879	1881	1885	rVB	27037	29349	4.34%	0.460%
40	12.615	1885	1891	1894	rBV	35368	43454	6.42%	0.680%
41	12.646	1894	1896	1900	rVB	11522	11933	1.76%	0.187%
42	12.701	1900	1905	1908	rBV	27136	41739	6.17%	0.654%
43	12.798	1917	1921	1923	rBV2	6278	7849	1.16%	0.123%
44	12.847	1926	1929	1933	rVB2	12683	16143	2.39%	0.253%
45	12.920	1933	1941	1945	rBV	19656	32070	4.74%	0.502%
46	12.963	1945	1948	1955	rVB	31397	41356	6.11%	0.648%
47	13.024	1955	1958	1960	rBV	10154	13754	2.03%	0.215%
48	13.042	1960	1961	1964	rVV2	7814	8055	1.19%	0.126%
49	13.170	1974	1982	1986	rBV3	39760	67518	9.98%	1.057%
50	13.213	1986	1989	1992	rVV2	14709	16510	2.44%	0.259%
51	13.255	1992	1996	1998	rVV2	12491	18829	2.78%	0.295%
52	13.292	1998	2002	2007	rVV2	88259	120766	17.84%	1.891%
53	13.335	2007	2009	2012	rVV	7012	7286	1.08%	0.114%
54	13.371	2012	2015	2018	rVV	7278	7627	1.13%	0.119%
55	13.420	2019	2023	2032	rVB	65054	90334	13.35%	1.415%
56	13.505	2032	2037	2040	rBV2	11511	15484	2.29%	0.242%
57	13.542	2040	2043	2046	rVV	17174	22069	3.26%	0.346%
58	13.585	2046	2050	2054	rVV2	24210	40450	5.98%	0.633%
59	13.640	2054	2059	2060	rVV4	10138	18516	2.74%	0.290%
60	13.664	2060	2063	2069	rVB2	22661	33815	5.00%	0.530%
61	13.780	2079	2082	2088	rVB2	6434	10590	1.56%	0.166%
62	13.853	2088	2094	2099	rVB	35557	50690	7.49%	0.794%
63	13.926	2099	2106	2111	rBV3	33406	53726	7.94%	0.841%
64	13.975	2111	2114	2117	rVV	9565	11064	1.63%	0.173%
65	14.036	2121	2124	2127	rVB3	6777	8117	1.20%	0.127%
66	14.078	2127	2131	2135	rBV2	24699	30778	4.55%	0.482%
67	14.231	2148	2156	2162	rBV	81589	127409	18.83%	1.995%
68	14.322	2168	2171	2176	rBV2	9646	12659	1.87%	0.198%
69	14.377	2176	2180	2184	rVB	22522	28870	4.27%	0.452%
70	14.420	2184	2187	2192	rVB3	6349	8781	1.30%	0.138%
71	14.481	2192	2197	2203	rBV2	49336	67409	9.96%	1.056%
72	14.615	2215	2219	2221	rBV	34807	44020	6.50%	0.689%
73	14.639	2221	2223	2226	rVV	25752	30678	4.53%	0.480%
74	14.670	2226	2228	2233	rVB2	18838	24390	3.60%	0.382%
75	14.731	2233	2238	2240	rBV2	7616	10444	1.54%	0.164%
76	14.780	2244	2246	2249	rVV2	9202	11527	1.70%	0.181%

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77	14.822	2249	2253	2255	rVV	11202	16529	2.44%	0.259%
78	14.847	2255	2257	2263	rVB5	10138	11493	1.70%	0.180%
79	14.908	2263	2267	2273	rBV2	11256	19026	2.81%	0.298%
80	15.054	2284	2291	2294	rBV4	5059	8829	1.30%	0.138%
81	15.188	2307	2313	2320	rBV3	22239	44356	6.55%	0.695%
82	15.249	2320	2323	2332	rVB8	3040	7989	1.18%	0.125%
83	15.377	2339	2344	2349	rBV3	6272	10783	1.59%	0.169%
84	15.481	2351	2361	2366	rBV4	12007	23002	3.40%	0.360%
85	15.615	2378	2383	2387	rVV4	10158	19672	2.91%	0.308%
86	15.651	2387	2389	2397	rVB2	4996	7946	1.17%	0.124%

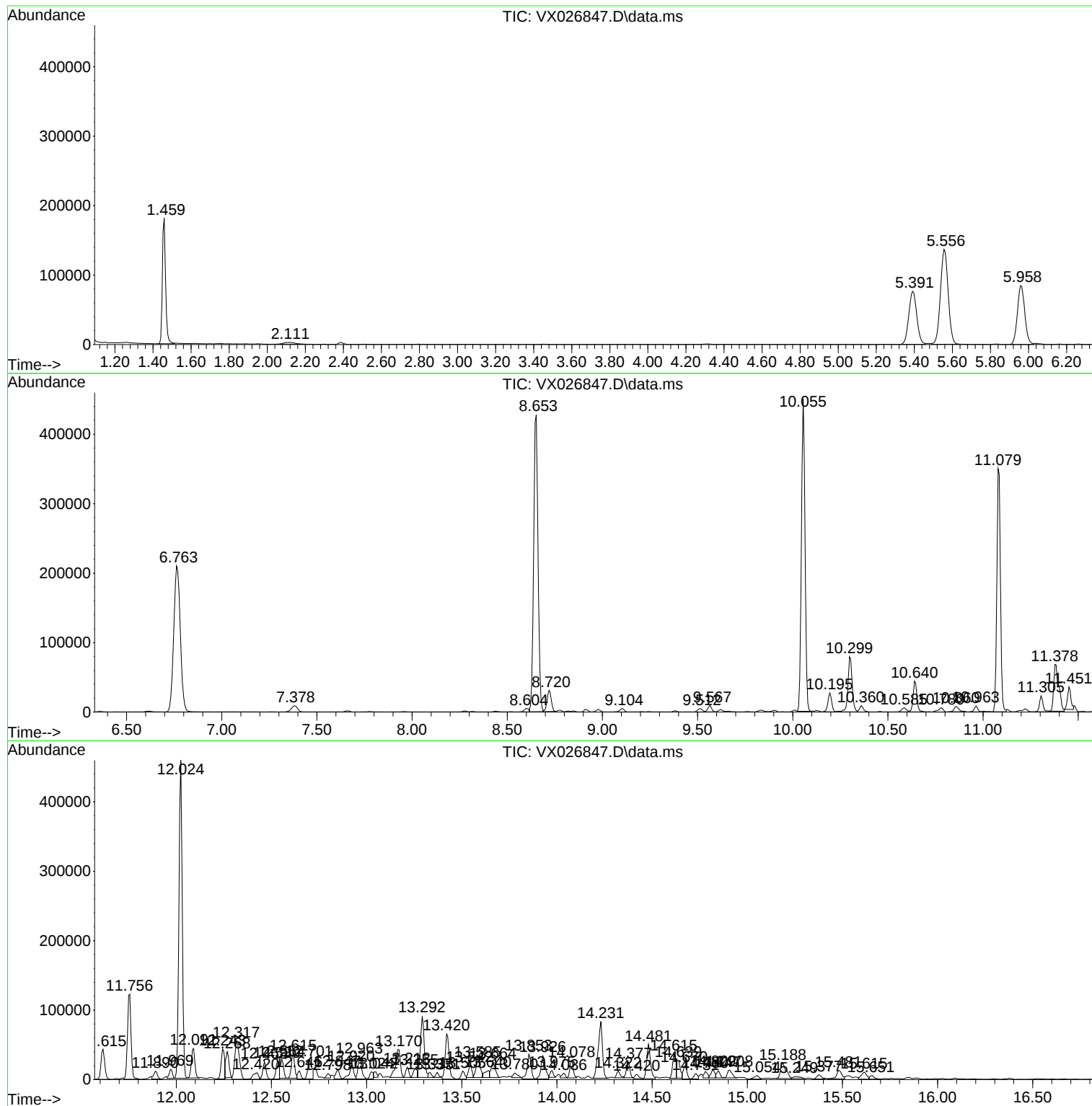
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.M
Quant Title : SW846 8260

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



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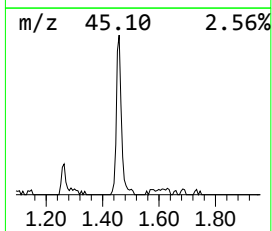
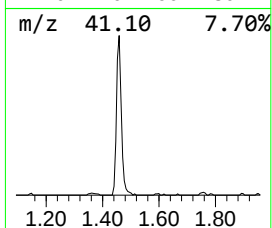
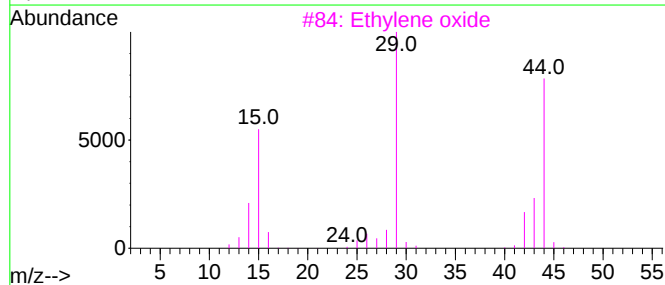
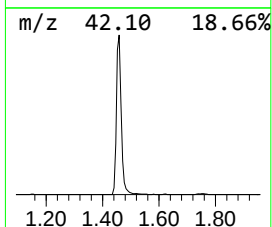
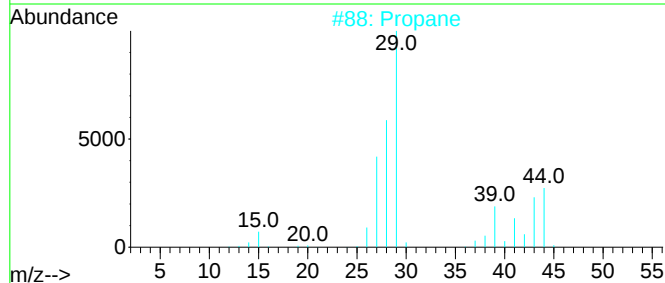
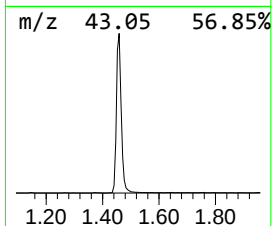
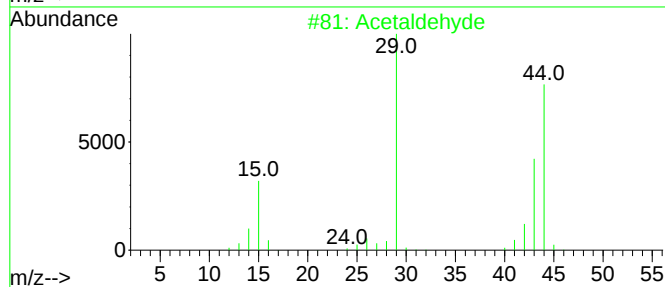
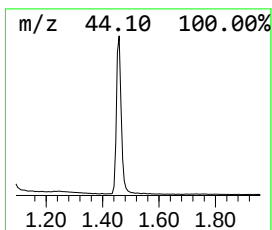
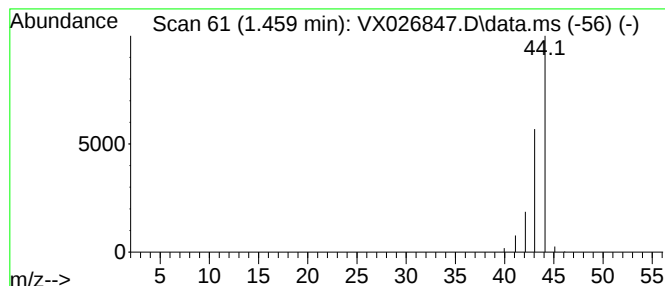
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.459 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.459	27.75 ug/l	214012	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Carbon dioxide	44	CO2	000124-38-9	3



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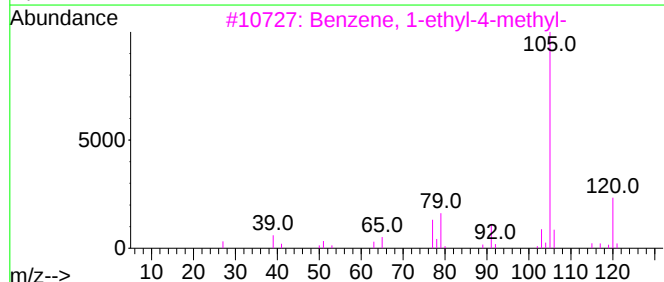
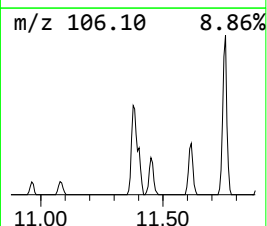
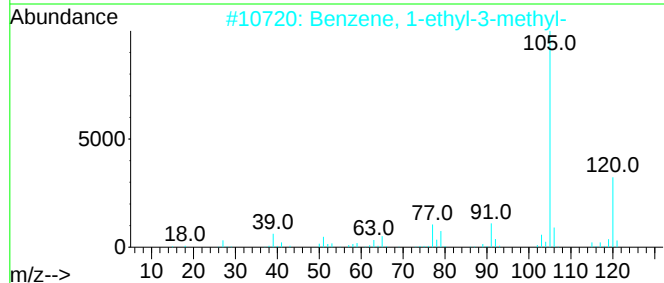
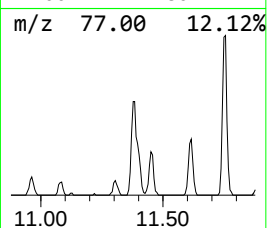
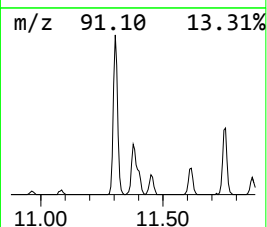
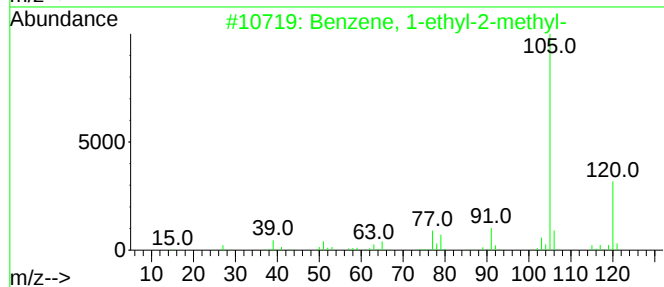
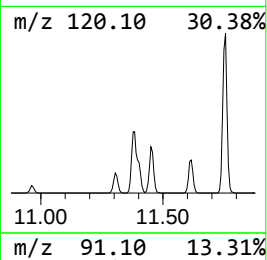
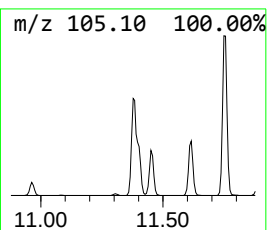
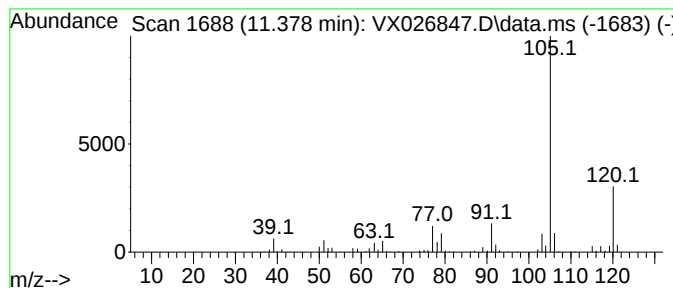
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	11.28 ug/l	124141	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-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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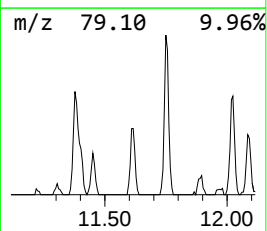
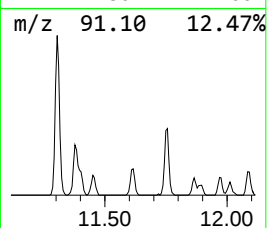
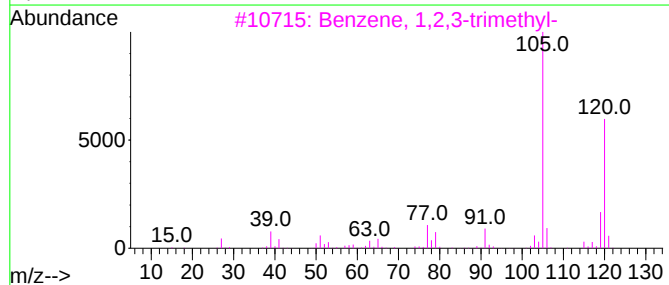
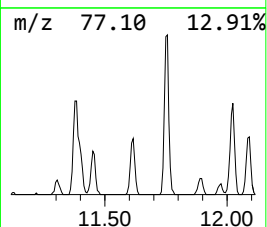
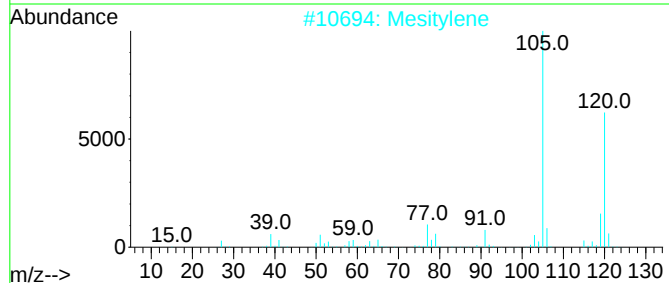
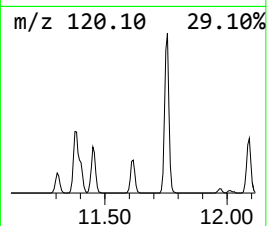
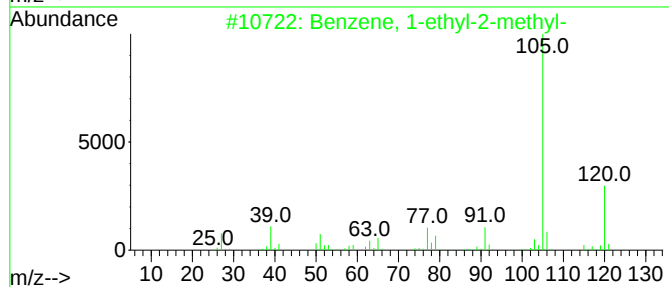
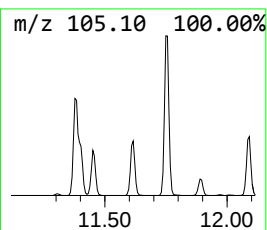
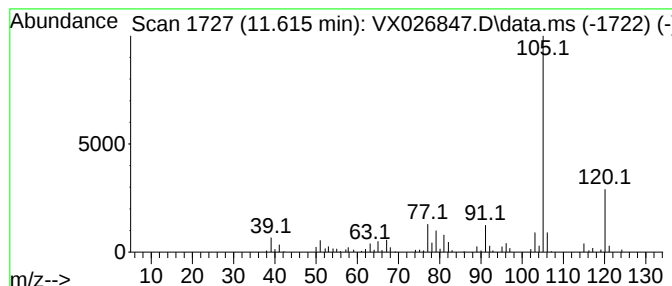
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	5.21 ug/l	57356	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	93
2			Mesitylene	120	C9H12	000108-67-8	90
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



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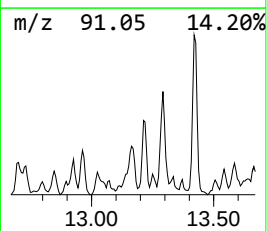
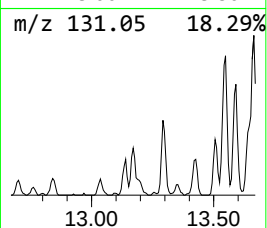
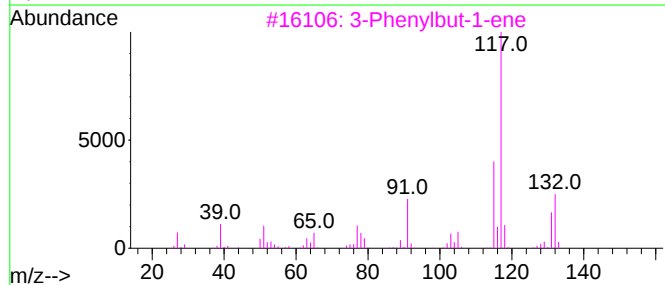
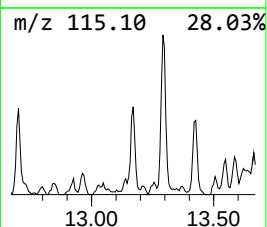
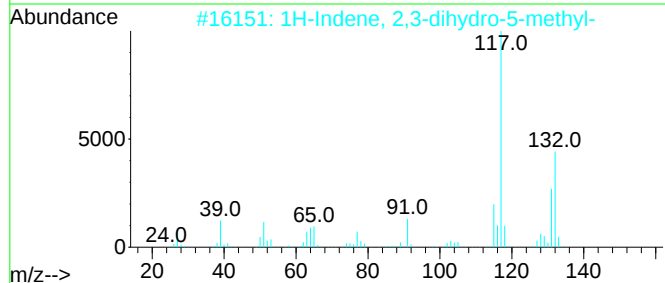
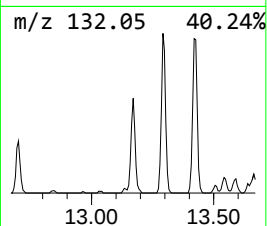
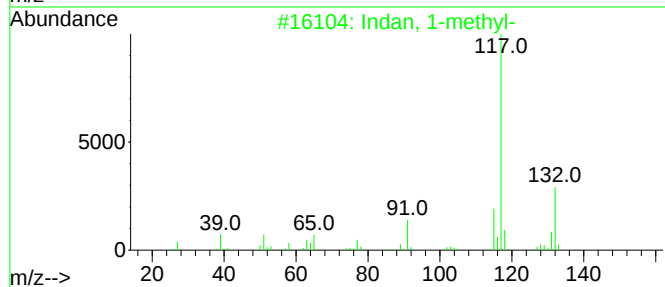
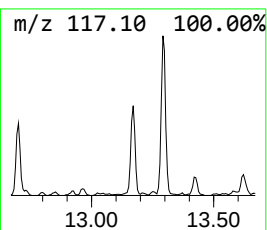
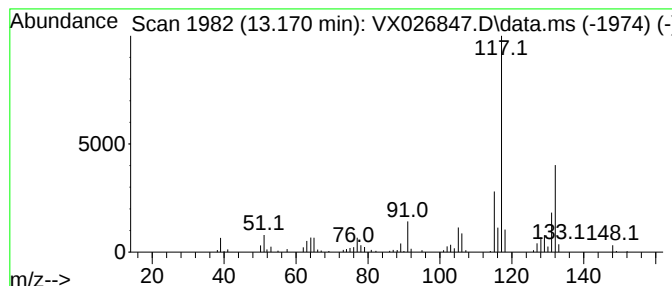
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Quant Title : SW846 8260

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

Peak Number 4 Indan, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	6.14 ug/l	67518	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	94
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020822\
Data File : VX026847.D
Acq On : 09 Feb 2022 01:38
Operator : JC/MD
Sample : N1425-03 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31377

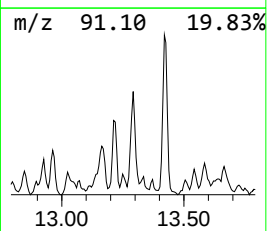
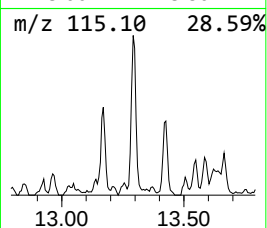
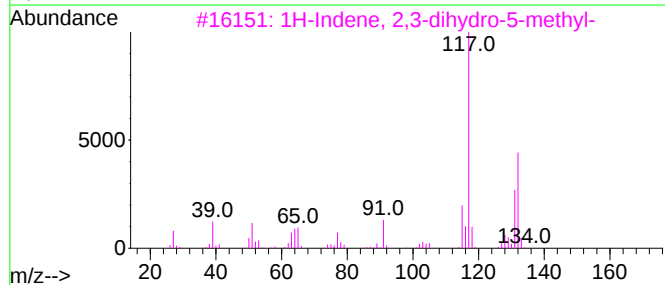
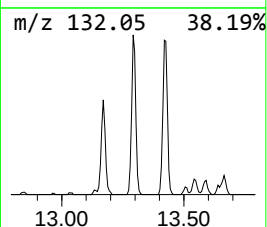
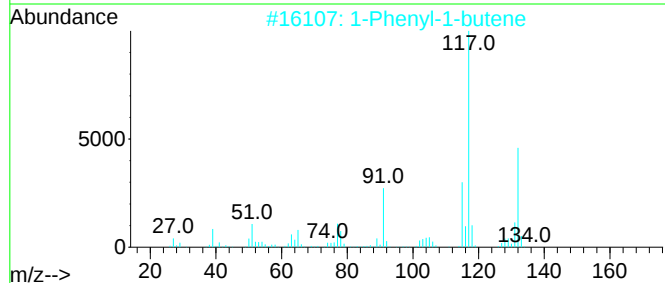
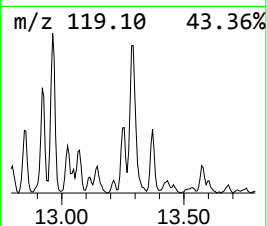
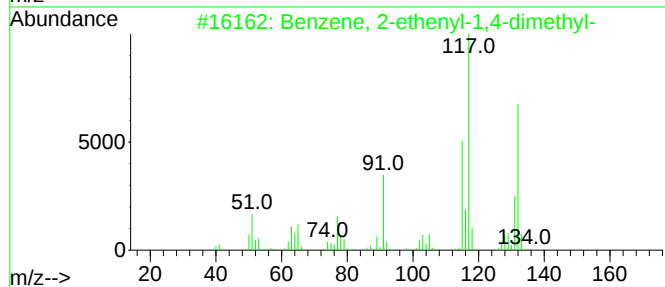
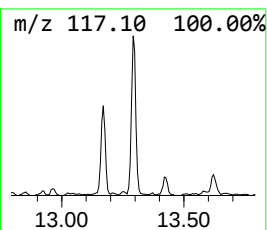
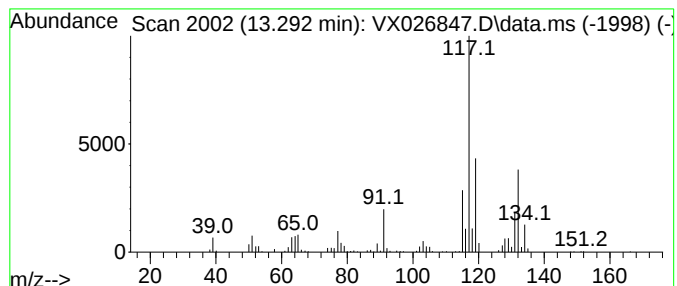
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	10.98 ug/l	120766	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	70
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	70
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
4			Indan, 1-methyl-	132	C10H12	000767-58-8	70
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020822\
Data File : VX026847.D
Acq On : 09 Feb 2022 01:38
Operator : JC/MD
Sample : N1425-03 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31377

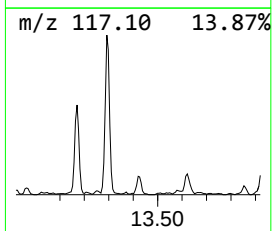
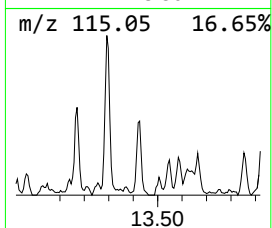
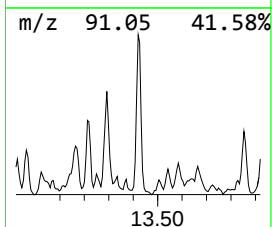
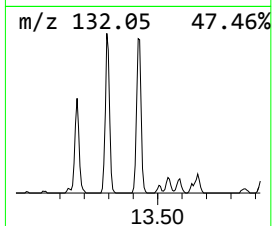
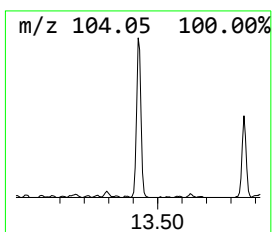
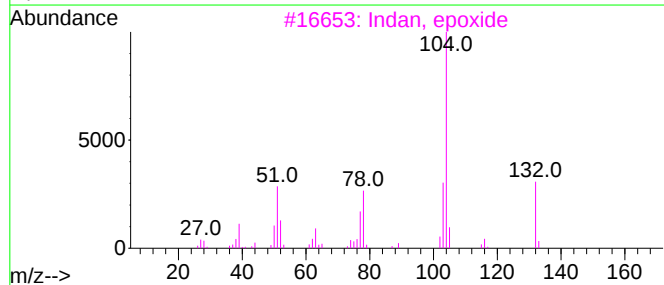
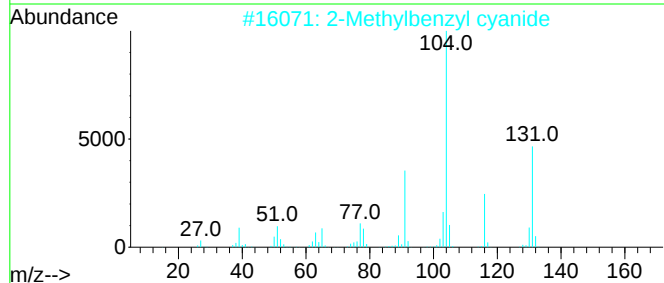
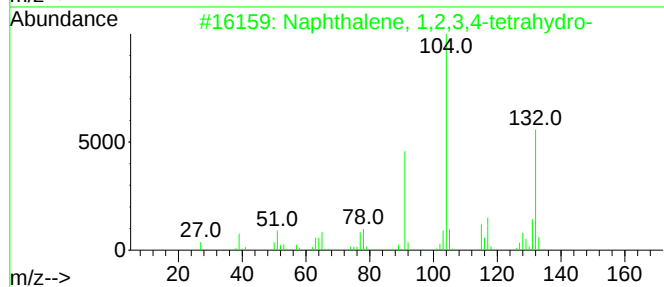
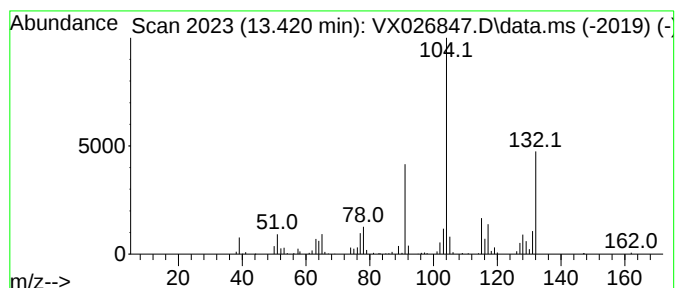
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	8.21 ug/l	90334	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	46
3			Indan, epoxide	132	C9H8O	000768-22-9	38
4			3-Pyridinecarbonitrile	104	C6H4N2	000100-54-9	38
5			4-Cyanobenzoic acid, 2-phenyleth...	251	C16H13NO2	131786-46-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020822\
Data File : VX026847.D
Acq On : 09 Feb 2022 01:38
Operator : JC/MD
Sample : N1425-03 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

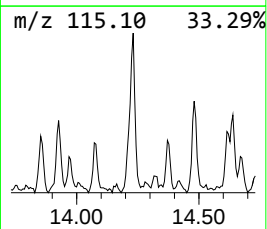
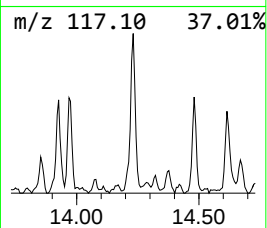
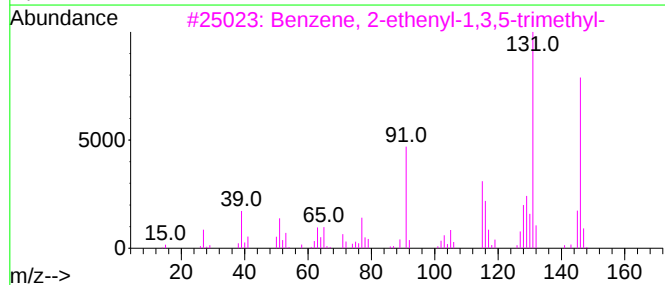
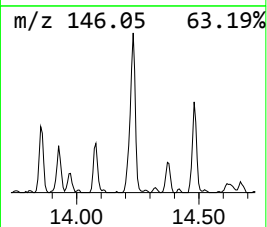
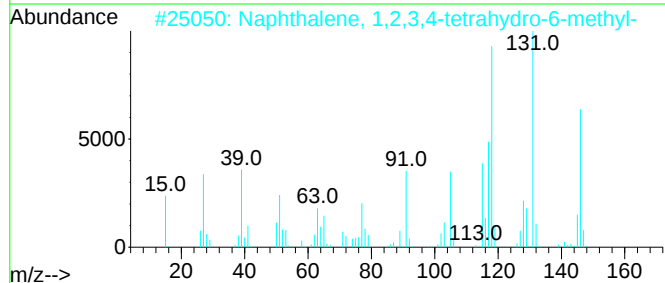
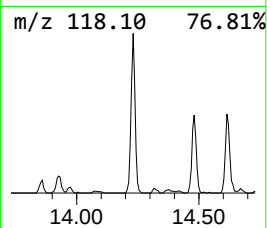
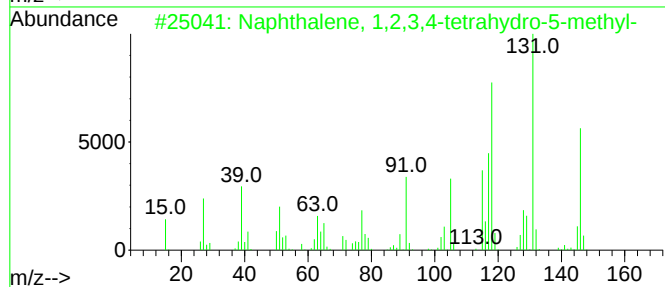
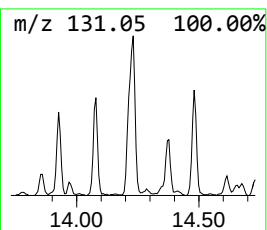
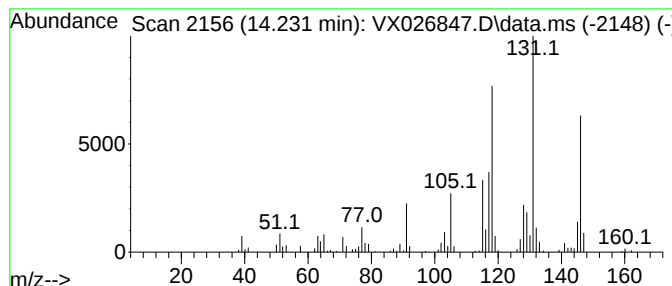
Instrument :
MSVOA_X
ClientSampleId :
31377

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.231	11.58 ug/l	127409	1,4-Dichlorobenzene-d4			12.024
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	002809-64-5	96
2	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	001680-51-9	96
3	Benzene, 2-ethenyl-1,3,5-trimethyl-		146	C11H14	000769-25-5	83
4	Benzene, (1,2-dimethyl-1-propenyl)-		146	C11H14	000769-57-3	60
5	Benzene, (3-methyl-2-butenyl)-		146	C11H14	004489-84-3	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020822\
Data File : VX026847.D
Acq On : 09 Feb 2022 01:38
Operator : JC/MD
Sample : N1425-03 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31377

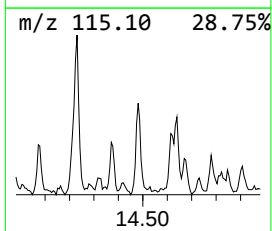
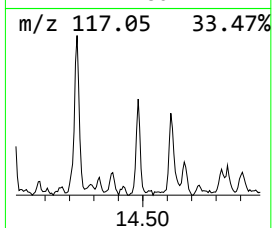
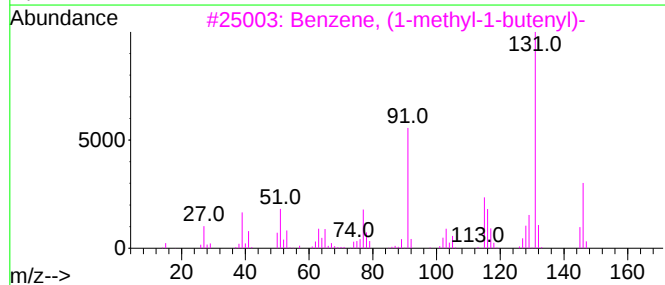
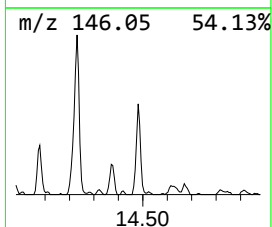
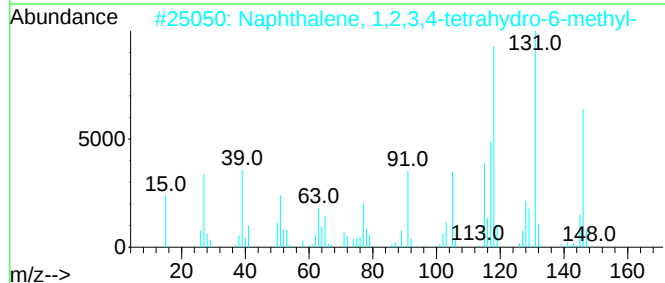
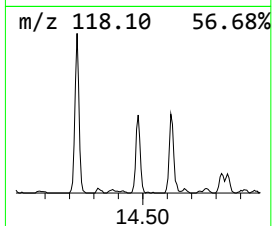
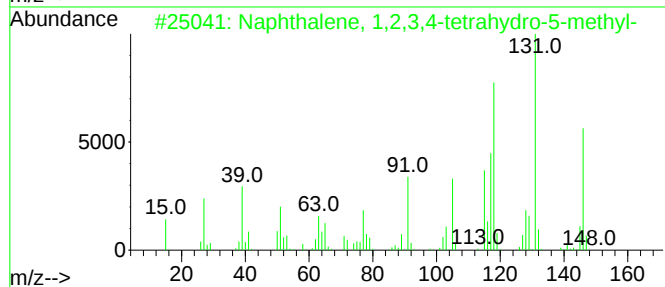
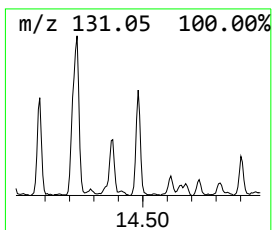
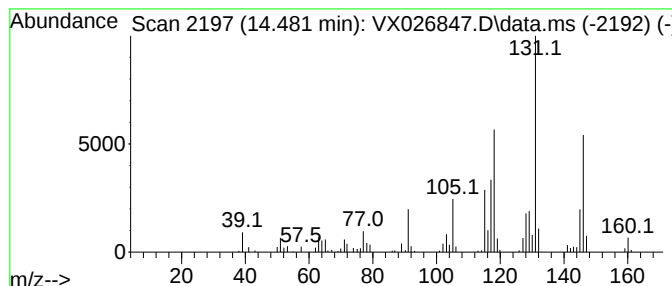
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	6.13 ug/l	67409	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
3			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	76
4			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	76
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020822\
Data File : VX026847.D
Acq On : 09 Feb 2022 01:38
Operator : JC/MD
Sample : N1425-03 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31377

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.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
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Benzene, 1,2,3-...	11.616	5.2	ug/l	57356	4	12.024	550122	50.0
Indan, 1-methyl-	13.170	6.1	ug/l	67518	4	12.024	550122	50.0
Benzene, 2-ethe...	13.292	11.0	ug/l	120766	4	12.024	550122	50.0
Naphthalene, 1,...	13.420	8.2	ug/l	90334	4	12.024	550122	50.0
Naphthalene, 1,...	14.231	11.6	ug/l	127409	4	12.024	550122	50.0
Naphthalene, 1,...	14.481	6.1	ug/l	67409	4	12.024	550122	50.0