

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
 Data File : VX044797.D
 Acq On : 31 Jan 2025 15:26
 Operator : JC/MD
 Sample : Q1189-13ME
 Misc : 19.85g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44R4ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMXML012825WMA.M
 Title : VOC Analysis

Signal : TIC: VX044797.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	27	rBV	12411	15546	1.42%	0.125%
2	1.368	42	46	49	rBV	67396	72436	6.62%	0.585%
3	1.575	73	80	82	rBV3	5039	10405	0.95%	0.084%
4	1.648	89	92	96	rBV	13931	15922	1.46%	0.129%
5	2.130	169	171	172	rBV2	661	570	0.05%	0.005%
6	2.276	188	195	210	rBV	204129	333834	30.52%	2.694%
7	2.563	240	242	247	rVV3	924	1274	0.12%	0.010%
8	2.660	254	258	259	rVV2	724	843	0.08%	0.007%
9	2.678	259	261	264	rVV2	806	1094	0.10%	0.009%
10	2.721	264	268	274	rVV2	1855	4211	0.38%	0.034%
11	2.770	274	276	282	rVV3	978	1338	0.12%	0.011%
12	2.947	297	305	315	rBV3	3966	10418	0.95%	0.084%
13	3.422	379	383	387	rBV3	748	1171	0.11%	0.009%
14	3.605	407	413	418	rVV3	2136	4116	0.38%	0.033%
15	3.873	453	457	459	rBV2	407	495	0.05%	0.004%
16	4.215	510	513	518	rVB2	374	559	0.05%	0.005%
17	4.263	518	521	524	rBV2	505	674	0.06%	0.005%
18	4.495	549	559	579	rBV2	43850	177506	16.23%	1.433%
19	4.867	619	620	626	rVB3	449	637	0.06%	0.005%
20	5.056	639	651	667	rVB	125025	374610	34.25%	3.023%
21	5.221	676	678	681	rVB3	523	523	0.05%	0.004%
22	5.288	687	689	692	rVB2	462	522	0.05%	0.004%
23	5.373	696	703	713	rVV6	4499	12731	1.16%	0.103%
24	5.550	731	732	736	rVV2	552	671	0.06%	0.005%
25	5.958	788	799	823	rBV2	345980	990523	90.55%	7.994%
26	6.117	823	825	827	rVB3	821	671	0.06%	0.005%
27	6.330	858	860	863	rBV2	428	468	0.04%	0.004%
28	6.452	878	880	884	rVB2	359	487	0.04%	0.004%
29	6.629	907	909	911	rBV2	525	595	0.05%	0.005%
30	6.757	919	930	954	rBV	251990	623996	57.05%	5.036%
31	6.958	961	963	967	rVB3	539	569	0.05%	0.005%
32	7.117	984	989	997	rVB4	920	2119	0.19%	0.017%
33	7.220	1001	1006	1009	rBV4	504	1084	0.10%	0.009%
34	7.306	1012	1020	1038	rVV	199840	445766	40.75%	3.598%
35	7.476	1045	1048	1049	rBV2	505	546	0.05%	0.004%
36	7.610	1068	1070	1074	rVV2	390	608	0.06%	0.005%

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 Misc : 19.85g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44R4ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMXML012825WMA.M
 Title : VOC Analysis

37	7.799	1098	1101	1104	rVB	508	596	0.05%	0.005%
38	7.976	1128	1130	1133	rVB2	640	649	0.06%	0.005%
39	8.062	1141	1144	1146	rVV2	474	542	0.05%	0.004%
40	8.092	1146	1149	1154	rVB3	535	858	0.08%	0.007%
41	8.147	1156	1158	1162	rBV3	411	513	0.05%	0.004%
42	8.214	1166	1169	1172	rBV2	362	496	0.05%	0.004%
43	8.324	1180	1187	1206	rBV	135086	240315	21.97%	1.939%
44	8.537	1219	1222	1225	rVB3	504	565	0.05%	0.005%
45	8.647	1233	1240	1249	rBV	468629	787125	71.96%	6.353%
46	8.903	1278	1282	1285	rBV4	1388	2262	0.21%	0.018%
47	8.952	1285	1290	1304	rVV	90295	151426	13.84%	1.222%
48	9.226	1334	1335	1340	rBV2	430	627	0.06%	0.005%
49	9.269	1340	1342	1348	rVB4	1071	1517	0.14%	0.012%
50	9.391	1357	1362	1377	rBV	158233	348938	31.90%	2.816%
51	9.610	1396	1398	1405	rVB4	675	819	0.07%	0.007%
52	9.708	1410	1414	1420	rVB4	1443	2160	0.20%	0.017%
53	10.055	1465	1471	1491	rBV	479322	752900	68.83%	6.076%
54	10.195	1491	1494	1495	rBV2	831	730	0.07%	0.006%
55	10.238	1500	1501	1506	rVB5	580	631	0.06%	0.005%
56	10.305	1506	1512	1517	rBV3	2398	4199	0.38%	0.034%
57	10.348	1517	1519	1521	rVV2	616	751	0.07%	0.006%
58	10.555	1546	1553	1559	rBV3	3641	5519	0.50%	0.045%
59	10.665	1564	1571	1583	rVV3	7186	15470	1.41%	0.125%
60	10.781	1588	1590	1593	rVB2	664	708	0.06%	0.006%
61	10.811	1593	1595	1597	rBV2	404	504	0.05%	0.004%
62	10.878	1603	1606	1610	rVB3	490	621	0.06%	0.005%
63	10.945	1612	1617	1621	rBV3	4318	6089	0.56%	0.049%
64	11.134	1644	1648	1652	rVV6	3916	6236	0.57%	0.050%
65	11.195	1652	1658	1670	rVV	319156	456217	41.71%	3.682%
66	11.293	1672	1674	1675	rVV2	849	621	0.06%	0.005%
67	11.317	1675	1678	1684	rVB4	1364	2010	0.18%	0.016%
68	11.433	1693	1697	1703	rVV3	3101	5206	0.48%	0.042%
69	11.488	1703	1706	1710	rVB4	3482	4601	0.42%	0.037%
70	11.567	1717	1719	1723	rVB4	551	589	0.05%	0.005%
71	11.707	1740	1742	1744	rBV3	567	522	0.05%	0.004%
72	11.750	1746	1749	1752	rBV3	1763	2491	0.23%	0.020%
73	11.811	1755	1759	1763	rBV	10669	12829	1.17%	0.104%
74	11.854	1763	1766	1772	rVB	2892	3913	0.36%	0.032%
75	11.933	1775	1779	1783	rVB3	1275	1684	0.15%	0.014%
76	11.969	1783	1785	1788	rBV3	1034	1117	0.10%	0.009%

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Instrument :
 MSVOA_X
 ClientSampleId :
 A44R4ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

77	12.018	1788	1793	1803	rBV	571478	767170	70.13%	6.192%
78	12.244	1824	1830	1832	rBV4	2219	3576	0.33%	0.029%
79	12.317	1837	1842	1849	rBV	526431	706172	64.56%	5.699%
80	12.414	1855	1858	1863	rVB2	8456	10721	0.98%	0.087%
81	12.463	1864	1866	1872	rVB7	3315	4576	0.42%	0.037%
82	12.555	1875	1881	1885	rBV6	4984	10674	0.98%	0.086%
83	12.756	1910	1914	1919	rBV4	10605	14689	1.34%	0.119%
84	12.817	1919	1924	1927	rBV4	13649	20757	1.90%	0.168%
85	12.981	1945	1951	1957	rBV4	23138	62078	5.68%	0.501%
86	13.042	1958	1961	1963	rBV2	12686	15899	1.45%	0.128%
87	13.292	1998	2002	2007	rVB3	63568	95749	8.75%	0.773%
88	13.414	2018	2022	2030	rBV9	47740	121608	11.12%	0.981%
89	13.798	2078	2085	2089	rBV3	104122	209061	19.11%	1.687%
90	13.841	2090	2092	2095	rBV3	63191	75320	6.89%	0.608%
91	14.213	2150	2153	2157	rVB2	133700	166436	15.22%	1.343%
92	14.323	2168	2171	2175	rBV2	96429	143261	13.10%	1.156%
93	14.615	2216	2219	2220	rBV	184655	206576	18.89%	1.667%
94	14.780	2243	2246	2250	rVB	329273	404399	36.97%	3.264%
95	15.414	2346	2350	2354	rVB2	308537	442801	40.48%	3.574%
96	15.475	2357	2360	2364	rVB	288683	383820	35.09%	3.098%
97	15.609	2378	2382	2386	rBV	490220	763477	69.80%	6.162%
98	15.652	2386	2389	2398	rVB2	281872	503987	46.07%	4.067%
99	15.810	2410	2415	2428	rVB	519726	1093861	100.00%	8.828%
100	16.651	2549	2553	2558	rBV	137896	228839	20.92%	1.847%

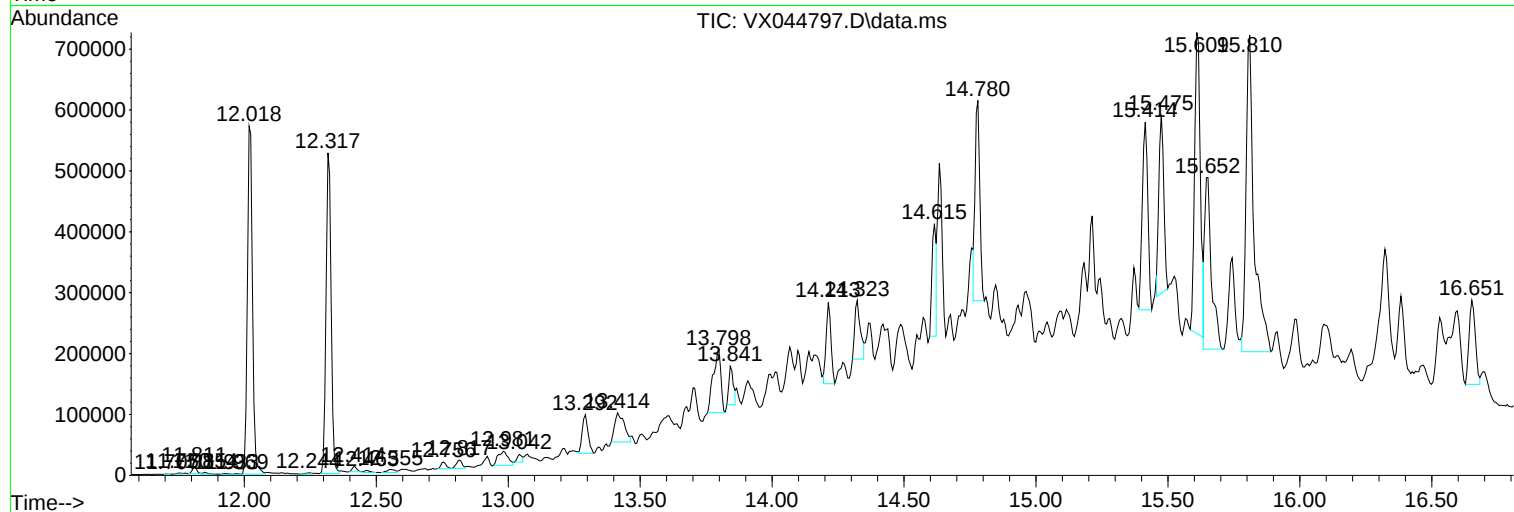
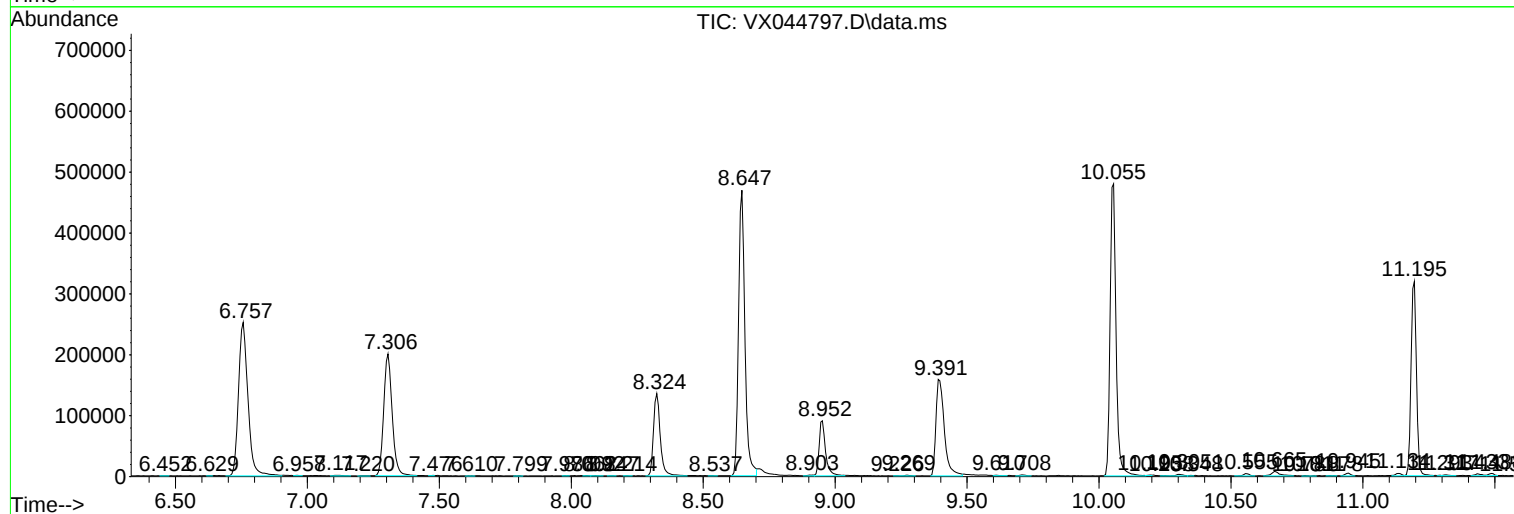
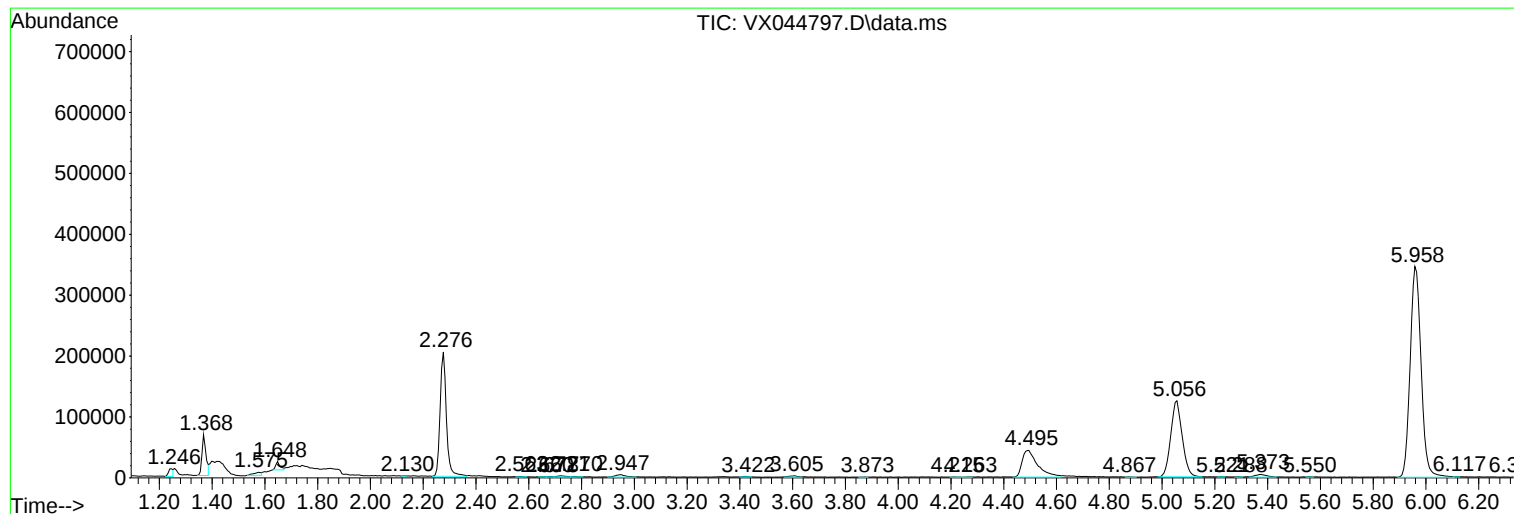
Sum of corrected areas: 12390611

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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



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Data File : VX044797.D
Acq On : 31 Jan 2025 15:26
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R4ME

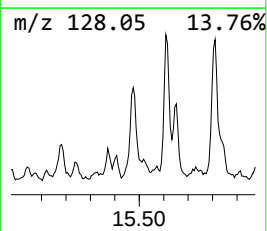
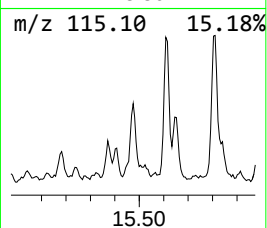
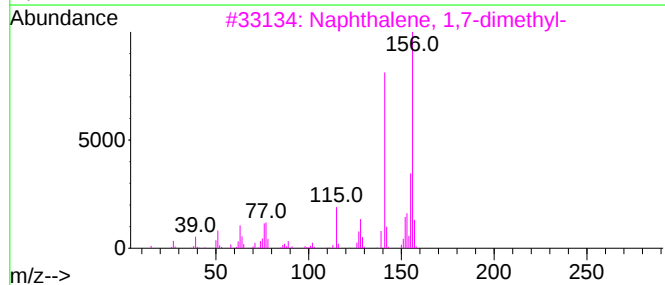
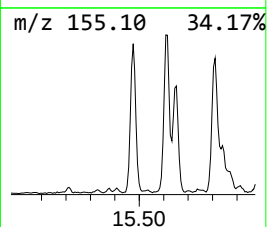
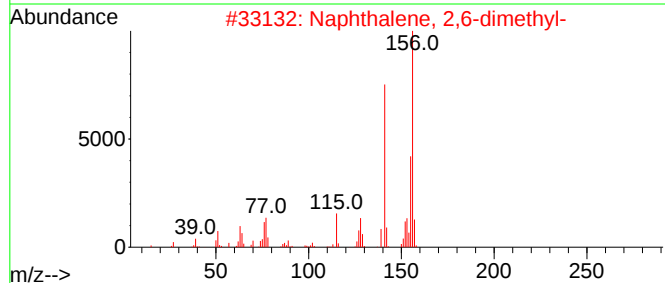
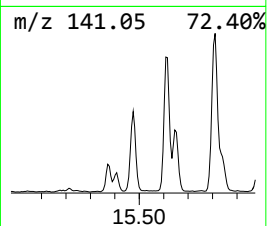
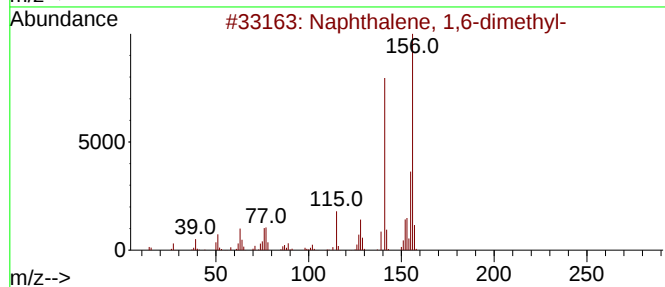
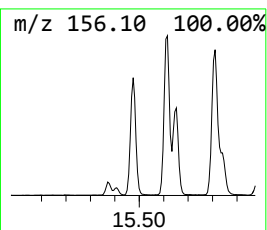
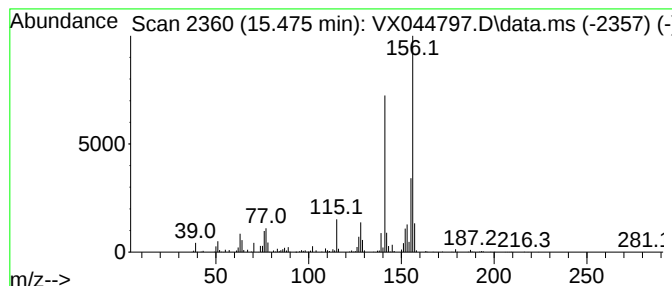
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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

Peak Number 12 Naphthalene, 1,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	25.02 ug/L	383820	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	98
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	98
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	98
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R4ME

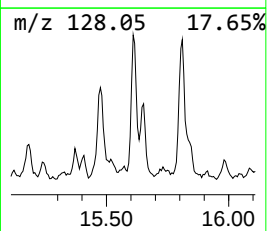
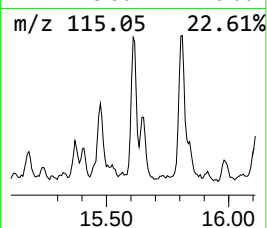
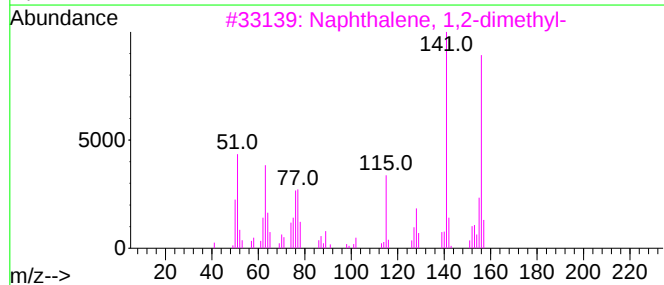
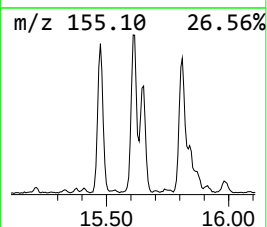
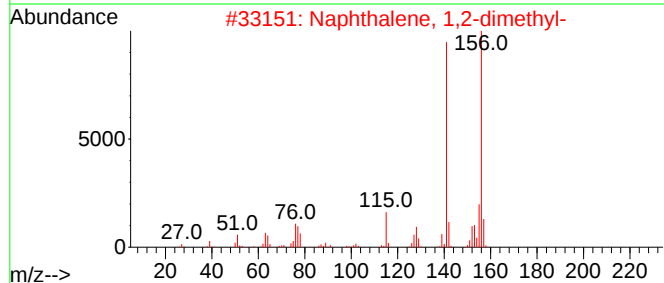
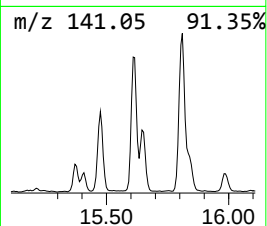
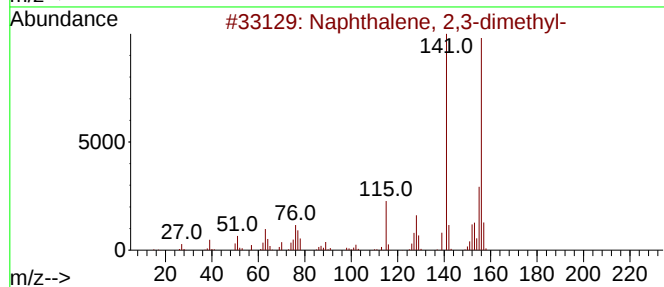
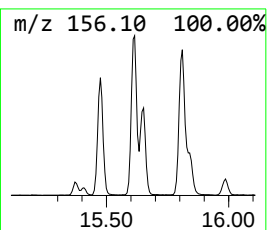
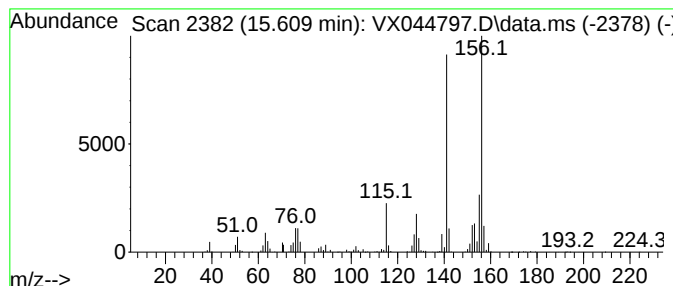
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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

Peak Number 13 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	49.76 ug/L	763477	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	98
3			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97



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Instrument :
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ClientSampleId :
A44R4ME

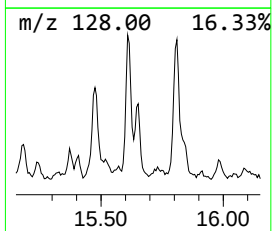
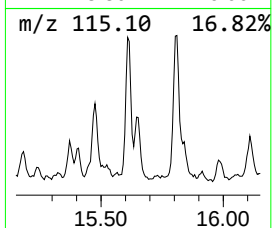
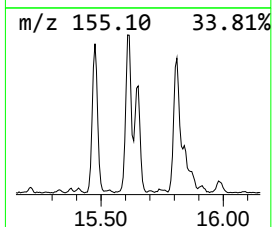
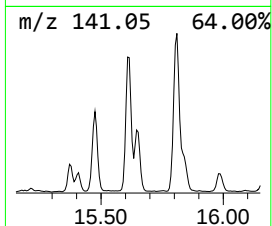
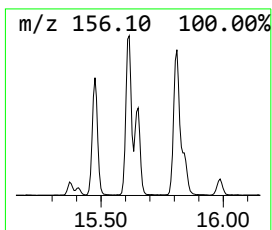
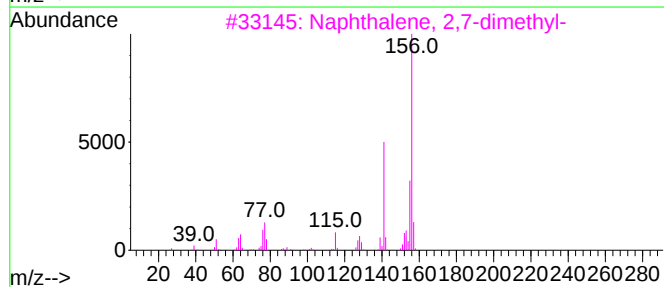
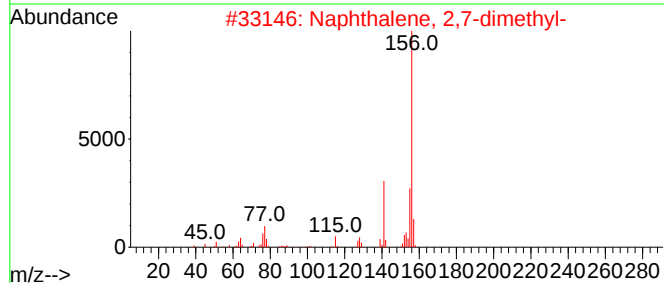
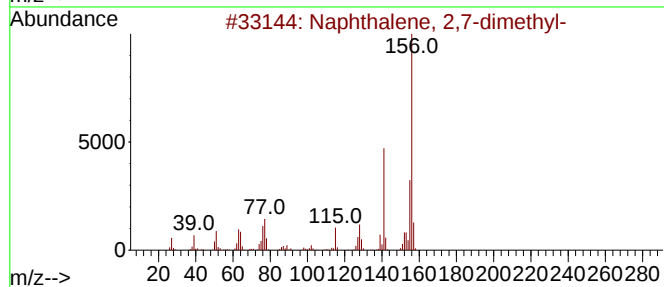
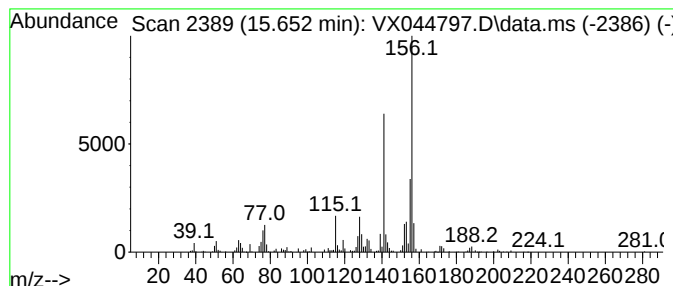
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Quant Title : VOC Analysis

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

Peak Number 14 Naphthalene, 2,7-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	32.85 ug/L	503987	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VOX013125\
Data File : VX044797.D
Acq On : 31 Jan 2025 15:26
Operator : JC/MD
Sample : Q1189-13ME
Misc : 19.85g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R4ME

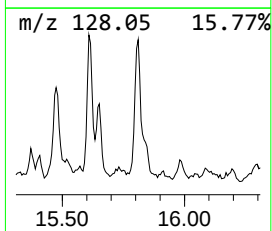
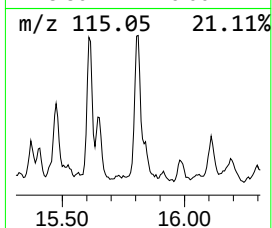
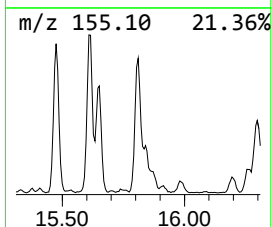
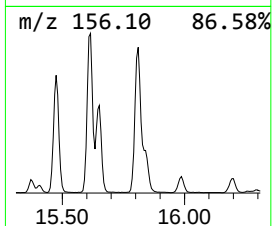
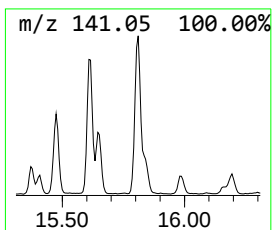
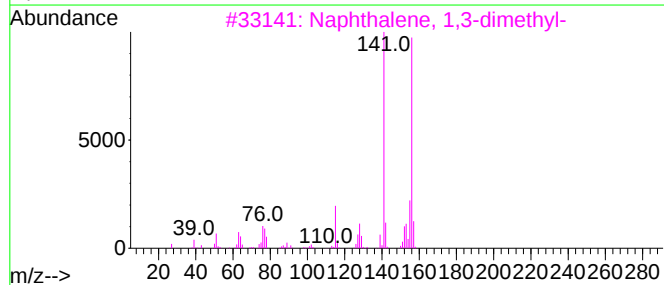
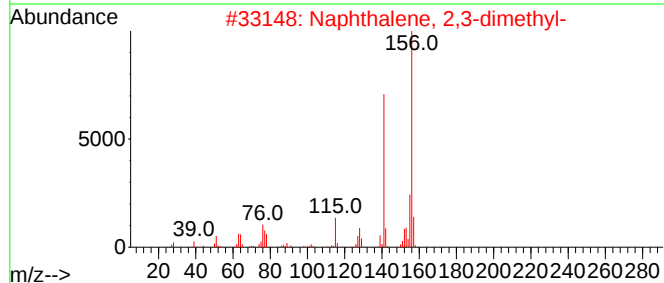
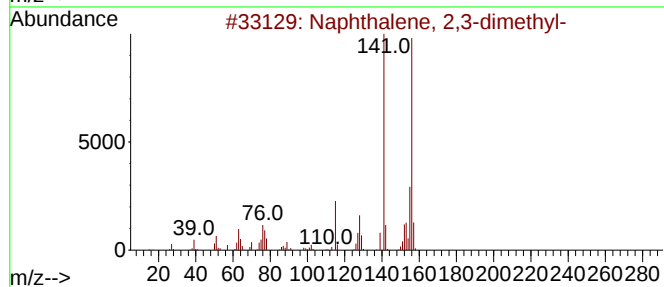
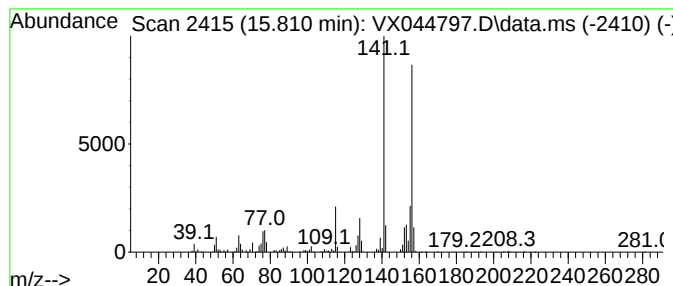
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Quant Title : VOC Analysis

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

Peak Number 15 Naphthalene, 1,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.810	71.29 ug/L	1093860	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	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\VOX013125\
Data File : VX044797.D
Acq On : 31 Jan 2025 15:26
Operator : JC/MD
Sample : Q1189-13ME
Misc : 19.85g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R4ME

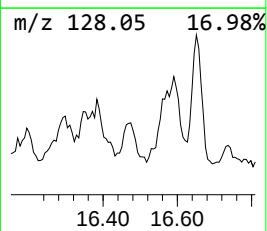
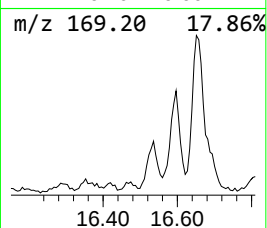
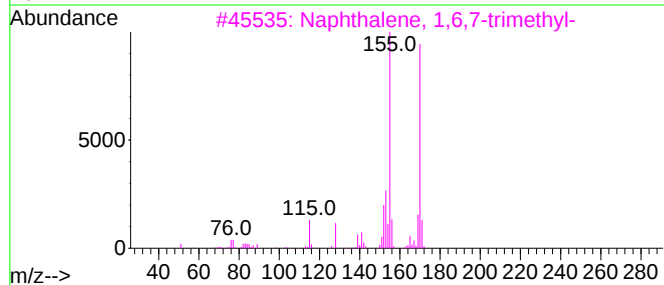
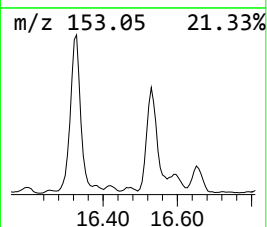
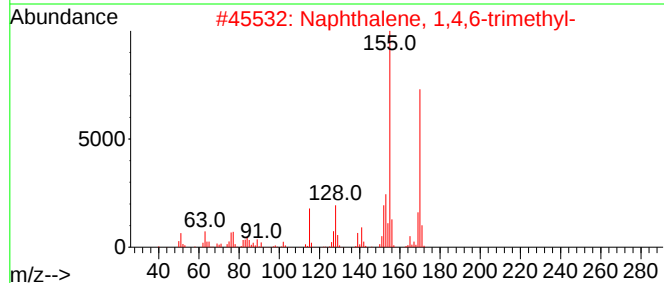
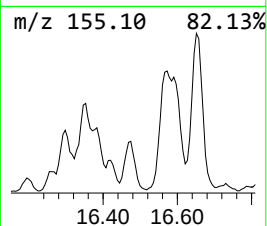
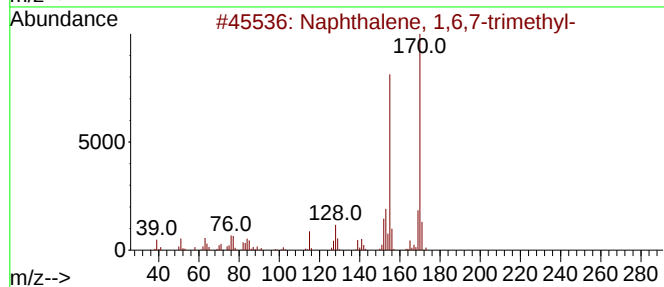
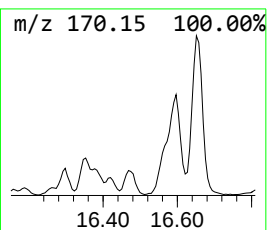
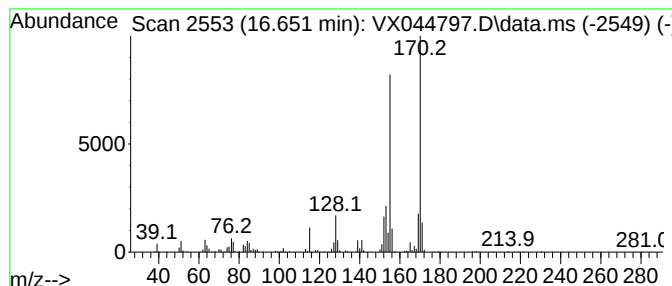
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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

Peak Number 16 Naphthalene, 1,6,7-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.651	14.91 ug/L	228839	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	97
2			Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	96
3			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	96
4			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	94
5			Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044797.D
Acq On : 31 Jan 2025 15:26
Operator : JC/MD
Sample : Q1189-13ME
Misc : 19.85g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Naphthalene, 1,...	15.475	25.0	ug/L	383820	3	12.024	767170	50.0
Naphthalene, 2,...	15.609	49.8	ug/L	763477	3	12.024	767170	50.0
Naphthalene, 2,...	15.652	32.9	ug/L	503987	3	12.024	767170	50.0
Naphthalene, 1,...	15.810	71.3	ug/L	1093860	3	12.024	767170	50.0
Naphthalene, 1,...	16.651	14.9	ug/L	228839	3	12.024	767170	50.0