

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
 Data File : VX044792.D
 Acq On : 31 Jan 2025 13:30
 Operator : JC/MD
 Sample : Q1189-11ME
 Misc : 14.77g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44R2ME

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: VX044792.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	35	rBV2	14655	32086	1.67%	0.290%
2	1.368	43	46	49	rBV	68820	73832	3.84%	0.668%
3	1.557	72	77	78	rBV4	3967	5570	0.29%	0.050%
4	1.642	86	91	97	rBV2	15715	34560	1.80%	0.313%
5	2.282	190	196	211	rBV	204433	346535	18.04%	3.134%
6	2.721	263	268	273	rBV2	3454	6083	0.32%	0.055%
7	2.940	297	304	313	rVV	4978	12272	0.64%	0.111%
8	3.422	376	383	390	rBV4	1283	3424	0.18%	0.031%
9	3.599	402	412	429	rVB	241743	566281	29.48%	5.122%
10	4.483	549	557	580	rBV2	42383	169838	8.84%	1.536%
11	5.056	639	651	675	rBV2	128292	448247	23.34%	4.054%
12	5.373	689	703	726	rBV	613596	1920616	100.00%	17.371%
13	5.666	745	751	760	rVB4	2535	7490	0.39%	0.068%
14	5.958	789	799	820	rBV2	350743	1011370	52.66%	9.147%
15	6.757	921	930	953	rBV	235586	600006	31.24%	5.427%
16	7.226	1001	1007	1011	rBV3	1272	2437	0.13%	0.022%
17	7.306	1011	1020	1028	rBV	202526	458362	23.87%	4.146%
18	7.757	1087	1094	1104	rBV7	2694	6976	0.36%	0.063%
19	8.269	1174	1178	1181	rBV5	2214	3479	0.18%	0.031%
20	8.324	1181	1187	1202	rVV	147575	250805	13.06%	2.268%
21	8.427	1202	1204	1208	rVV4	1512	2503	0.13%	0.023%
22	8.592	1226	1231	1234	rBV3	9181	16585	0.86%	0.150%
23	8.647	1234	1240	1255	rVV	485185	820993	42.75%	7.425%
24	8.769	1257	1260	1266	rVB2	8982	15543	0.81%	0.141%
25	8.909	1279	1283	1285	rBV2	5018	6439	0.34%	0.058%
26	8.952	1285	1290	1303	rVB	98093	169375	8.82%	1.532%
27	9.098	1309	1314	1319	rVB4	4328	7159	0.37%	0.065%
28	9.275	1338	1343	1351	rVB3	9664	17946	0.93%	0.162%
29	9.391	1357	1362	1376	rBV	190964	350542	18.25%	3.170%
30	9.500	1376	1380	1386	rVV5	6893	14665	0.76%	0.133%
31	9.555	1386	1389	1394	rVV2	6373	9197	0.48%	0.083%
32	9.616	1394	1399	1403	rVV	15377	23615	1.23%	0.214%
33	9.653	1403	1405	1409	rVB3	3506	3685	0.19%	0.033%
34	9.823	1428	1433	1437	rVV5	3930	7478	0.39%	0.068%
35	9.866	1437	1440	1442	rVV2	2300	3081	0.16%	0.028%
36	9.903	1442	1446	1451	rVB4	4469	6892	0.36%	0.062%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

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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	10.000	1457	1462	1465	rBV3	4325	6152	0.32%	0.056%
38	10.055	1465	1471	1487	rVB	470899	705630	36.74%	6.382%
39	10.275	1498	1507	1509	rBV6	8084	14348	0.75%	0.130%
40	10.360	1517	1521	1529	rVB2	16509	24883	1.30%	0.225%
41	10.451	1532	1536	1542	rVB3	3678	5679	0.30%	0.051%
42	10.592	1550	1559	1565	rBV5	10490	27055	1.41%	0.245%
43	10.646	1565	1568	1570	rBV2	6354	7702	0.40%	0.070%
44	10.750	1581	1585	1586	rBV3	3085	3897	0.20%	0.035%
45	10.774	1586	1589	1594	rVB	11222	15351	0.80%	0.139%
46	10.854	1594	1602	1605	rBV5	11776	21724	1.13%	0.196%
47	10.890	1605	1608	1613	rVB4	8028	12304	0.64%	0.111%
48	10.945	1613	1617	1621	rVB5	1989	2661	0.14%	0.024%
49	11.006	1621	1627	1628	rBV5	5445	9059	0.47%	0.082%
50	11.030	1628	1631	1634	rVB3	5513	6526	0.34%	0.059%
51	11.079	1637	1639	1641	rBV3	3878	3560	0.19%	0.032%
52	11.189	1649	1657	1665	rBV	342839	482903	25.14%	4.368%
53	11.335	1677	1681	1686	rVB5	6036	8338	0.43%	0.075%
54	11.384	1686	1689	1693	rBV4	6919	9276	0.48%	0.084%
55	11.433	1693	1697	1700	rBV3	7658	12003	0.62%	0.109%
56	11.476	1700	1704	1709	rVB	43219	50872	2.65%	0.460%
57	11.591	1721	1723	1726	rBV4	2078	2784	0.14%	0.025%
58	11.628	1726	1729	1733	rVV4	6706	8941	0.47%	0.081%
59	11.683	1734	1738	1740	rVV3	10291	15548	0.81%	0.141%
60	11.713	1740	1743	1746	rVV	30991	34982	1.82%	0.316%
61	11.756	1746	1750	1760	rVB	97836	156444	8.15%	1.415%
62	11.847	1760	1765	1768	rBV6	5198	11427	0.59%	0.103%
63	11.884	1769	1771	1776	rVB4	9249	12054	0.63%	0.109%
64	12.018	1788	1793	1800	rBV	495501	649419	33.81%	5.874%
65	12.103	1804	1807	1812	rVB3	9465	12505	0.65%	0.113%
66	12.171	1815	1818	1821	rBV2	5838	5942	0.31%	0.054%
67	12.238	1826	1829	1830	rBV3	2493	2968	0.15%	0.027%
68	12.317	1837	1842	1849	rBV	533819	685265	35.68%	6.198%
69	12.420	1855	1859	1864	rBV	61321	68705	3.58%	0.621%
70	12.573	1881	1884	1891	rVB2	21415	36746	1.91%	0.332%
71	12.640	1891	1895	1898	rBV5	4334	7316	0.38%	0.066%
72	12.683	1899	1902	1905	rVB	13230	14423	0.75%	0.130%
73	12.762	1912	1915	1919	rBV5	3208	4818	0.25%	0.044%
74	12.817	1921	1924	1929	rVB5	10626	15279	0.80%	0.138%
75	12.890	1929	1936	1942	rBV7	14225	39916	2.08%	0.361%
76	12.975	1947	1950	1957	rVV4	13562	18433	0.96%	0.167%

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Instrument :
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 ClientSampleId :
 A44R2ME

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

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Peak separation: 5

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

77	13.036	1957	1960	1964	rVB3	9289	10564	0.55%	0.096%
78	13.079	1964	1967	1970	rBV	7549	9050	0.47%	0.082%
79	13.268	1994	1998	2001	rBV	48955	57837	3.01%	0.523%
80	13.347	2008	2011	2013	rBV3	5454	7105	0.37%	0.064%
81	13.384	2013	2017	2021	rBV	28519	38485	2.00%	0.348%
82	13.621	2053	2056	2061	rVB6	7691	10681	0.56%	0.097%
83	13.682	2063	2066	2067	rBV2	4698	5232	0.27%	0.047%
84	13.737	2071	2075	2077	rBV2	10707	11483	0.60%	0.104%
85	13.768	2077	2080	2083	rBV2	6653	6674	0.35%	0.060%
86	13.841	2088	2092	2096	rBV	35220	41953	2.18%	0.379%
87	13.993	2114	2117	2119	rBV4	4799	5321	0.28%	0.048%
88	14.036	2120	2124	2128	rBV	39120	43269	2.25%	0.391%
89	14.438	2187	2190	2194	rVB2	7192	8684	0.45%	0.079%
90	14.518	2198	2203	2206	rVB4	9447	15342	0.80%	0.139%
91	14.609	2215	2218	2221	rBV	10344	12018	0.63%	0.109%
92	14.719	2234	2236	2238	rBV3	2441	2482	0.13%	0.022%
93	14.755	2238	2242	2245	rBV	22275	28839	1.50%	0.261%
94	14.841	2253	2256	2260	rBV4	6081	8684	0.45%	0.079%
95	15.213	2313	2317	2321	rVB3	7547	10389	0.54%	0.094%
96	15.414	2346	2350	2356	rVB6	13055	19724	1.03%	0.178%
97	15.487	2359	2362	2370	rVB2	10708	17856	0.93%	0.161%
98	16.084	2456	2460	2464	rBV6	2009	3997	0.21%	0.036%
99	16.371	2502	2507	2514	rVB6	2474	4970	0.26%	0.045%
100	16.597	2541	2544	2552	rVB10	2854	6023	0.31%	0.054%

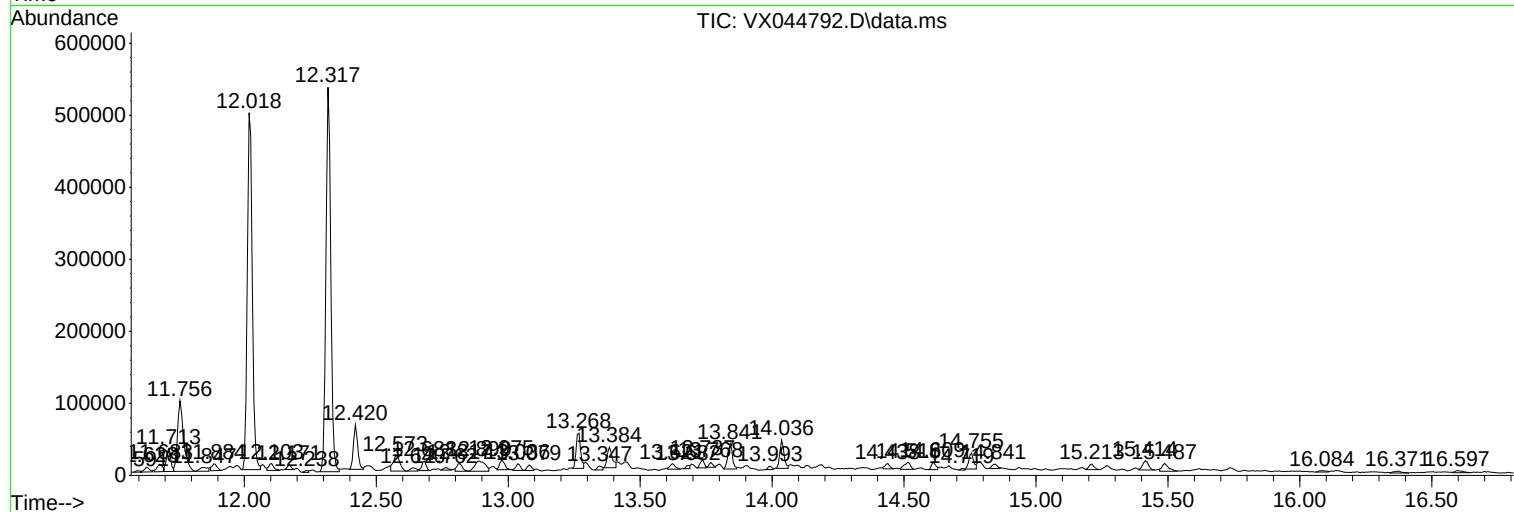
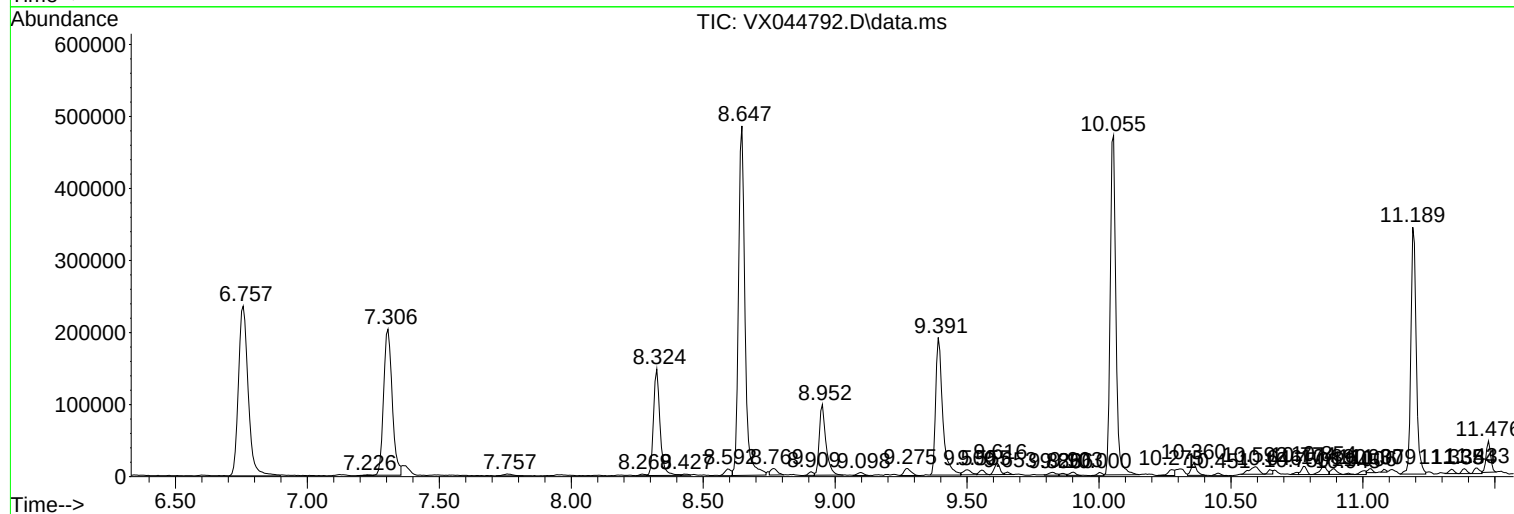
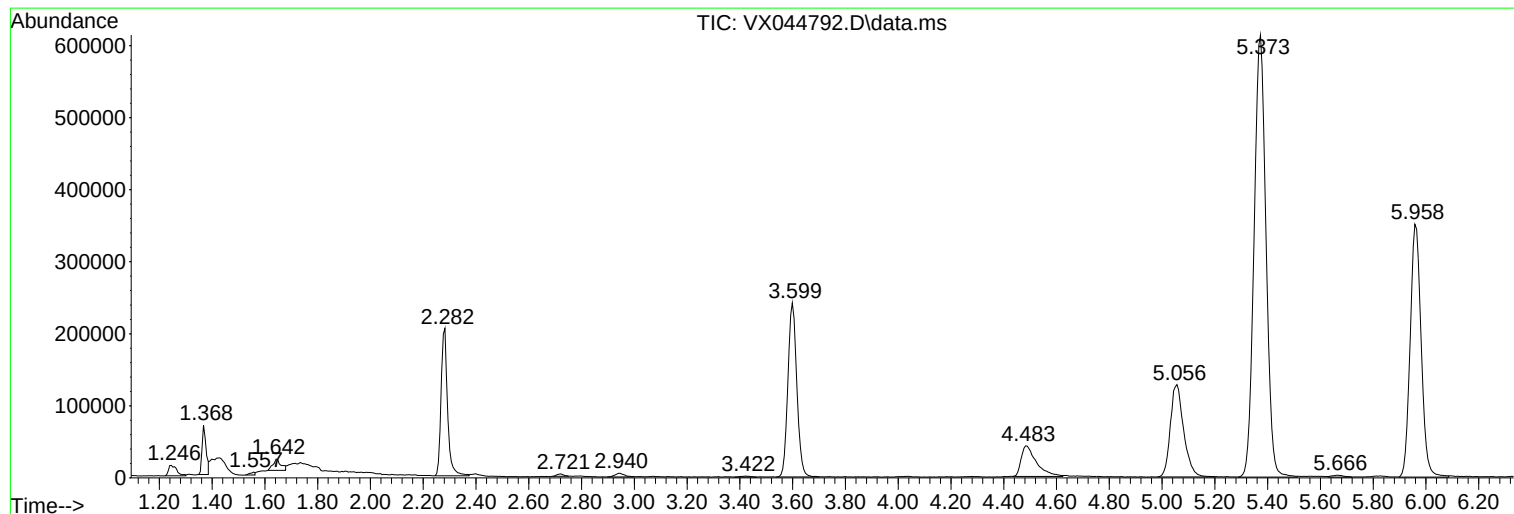
Sum of corrected areas: 11056467

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R2ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044792.D
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Operator : JC/MD
Sample : Q1189-11ME
Misc : 14.77g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

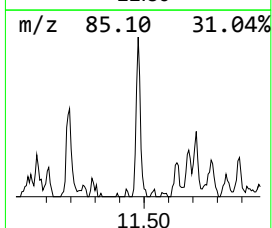
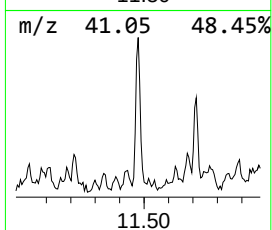
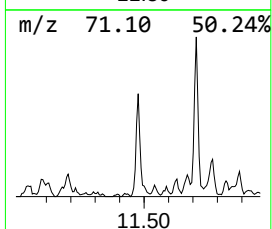
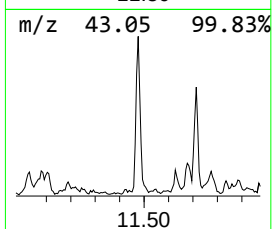
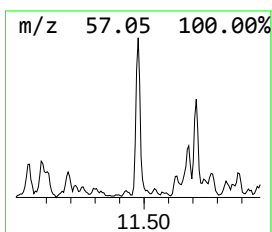
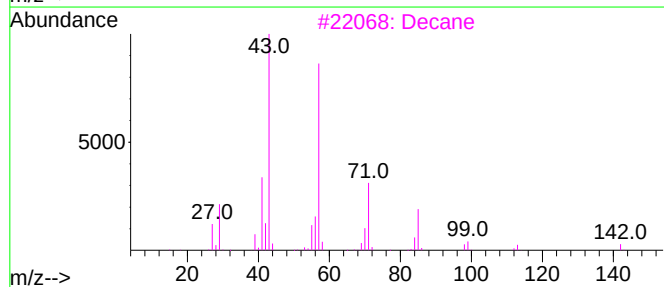
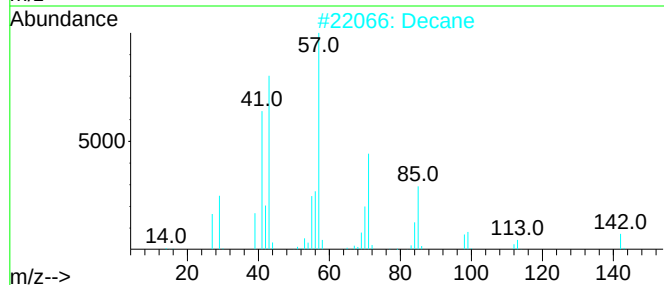
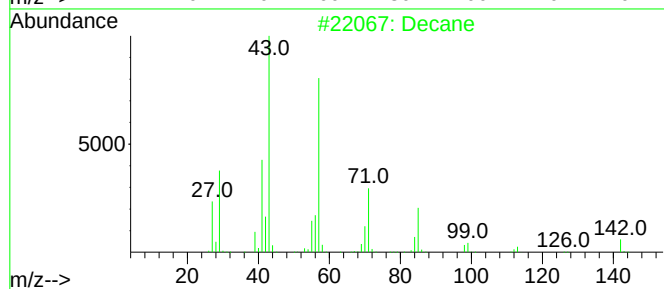
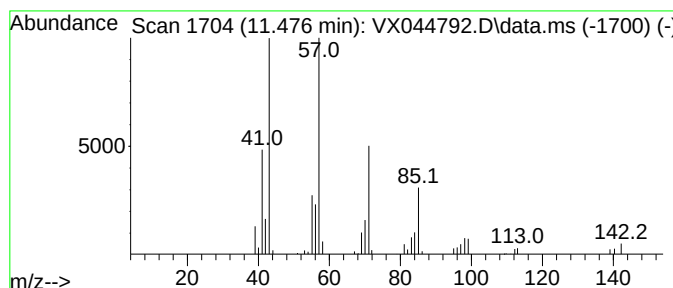
Instrument :
MSVOA_X
ClientSampleId :
A44R2ME

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 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.476	3.92 ug/L	50872	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decane		142	C10H22	000124-18-5	94
2	Decane		142	C10H22	000124-18-5	93
3	Decane		142	C10H22	000124-18-5	90
4	Tetradecane		198	C14H30	000629-59-4	80
5	Decane		142	C10H22	000124-18-5	70



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Instrument :
MSVOA_X
ClientSampleId :
A44R2ME

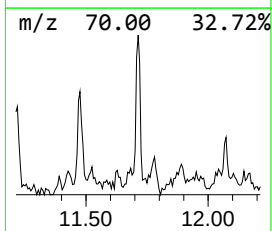
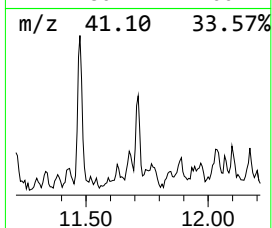
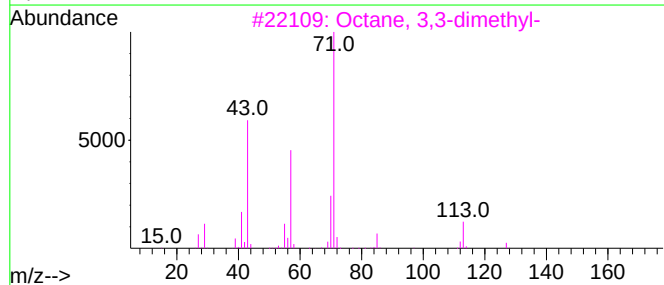
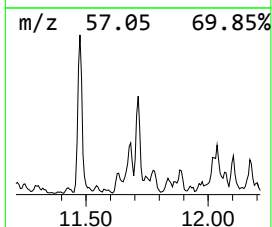
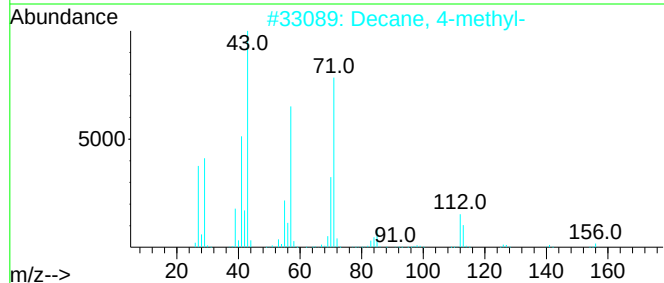
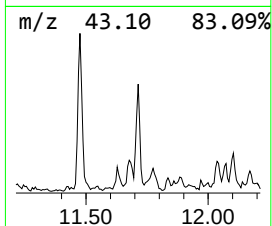
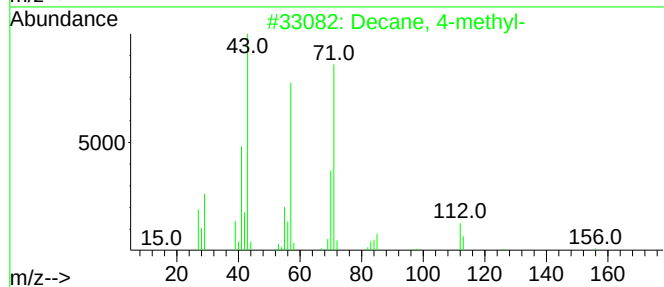
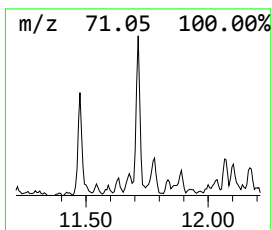
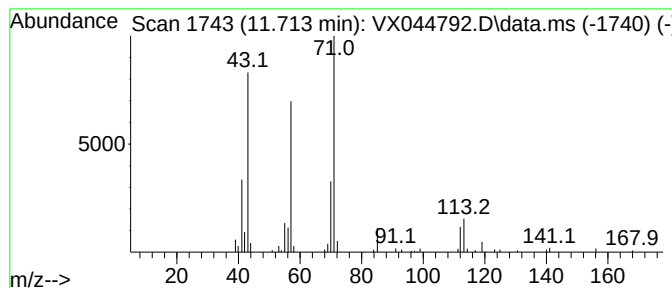
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.713	2.69 ug/L	34982	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decane, 4-methyl-	156	C11H24	002847-72-5	90
2		Decane, 4-methyl-	156	C11H24	002847-72-5	80
3		Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	78
4		Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	78
5		Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72



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Instrument :
MSVOA_X
ClientSampleId :
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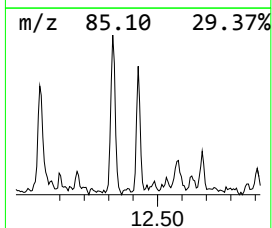
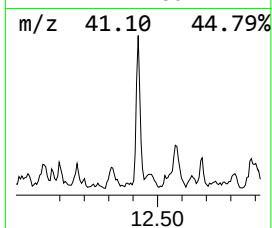
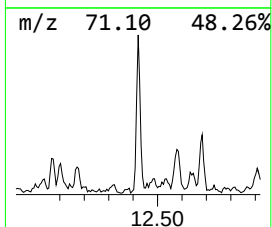
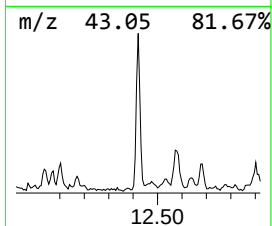
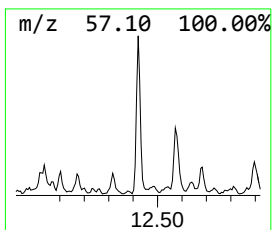
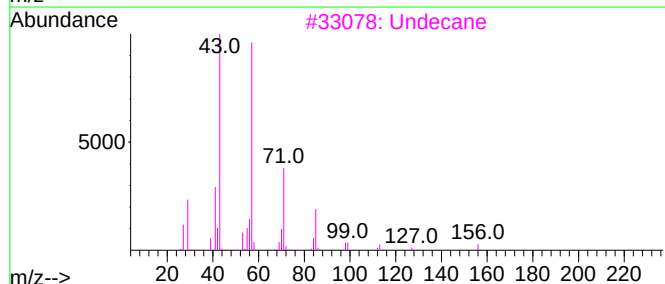
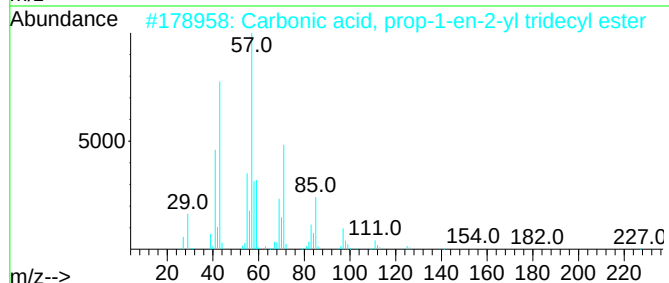
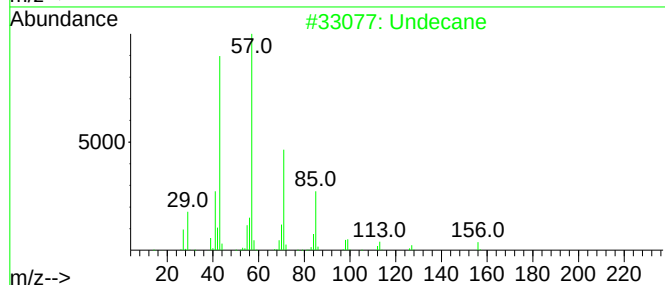
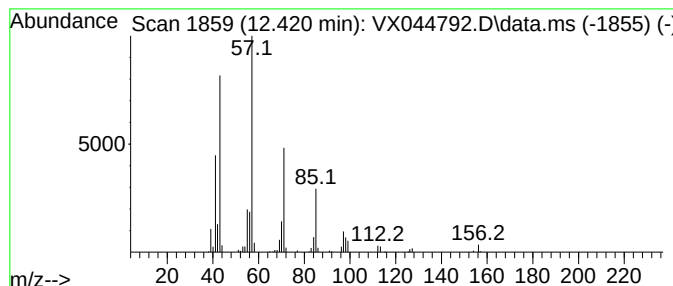
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	5.29 ug/L	68705	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	90
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	90
3			Undecane	156	C11H24	001120-21-4	87
4			Undecane	156	C11H24	001120-21-4	81
5			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044792.D
Acq On : 31 Jan 2025 13:30
Operator : JC/MD
Sample : Q1189-11ME
Misc : 14.77g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R2ME

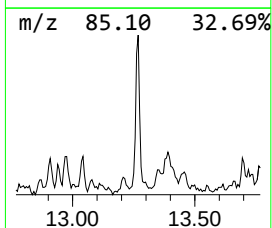
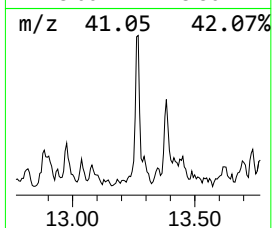
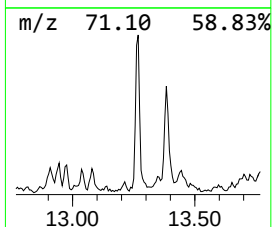
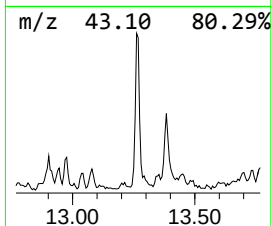
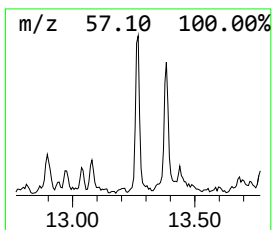
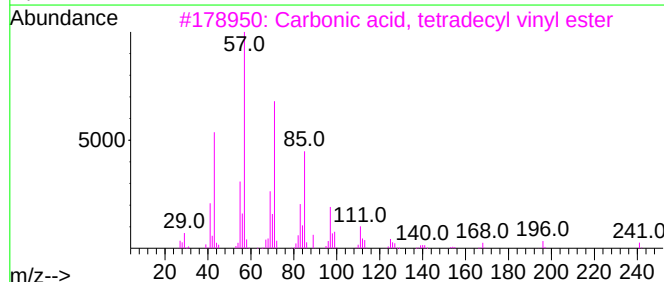
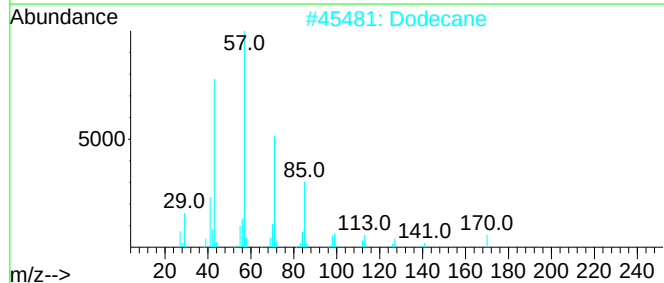
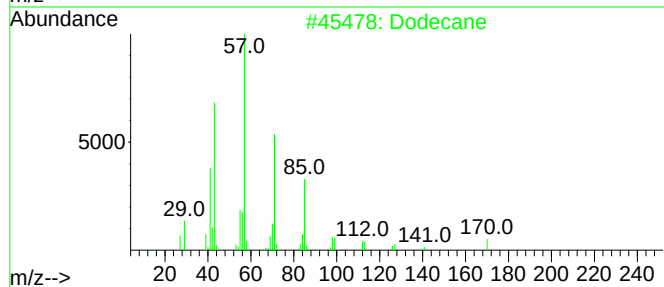
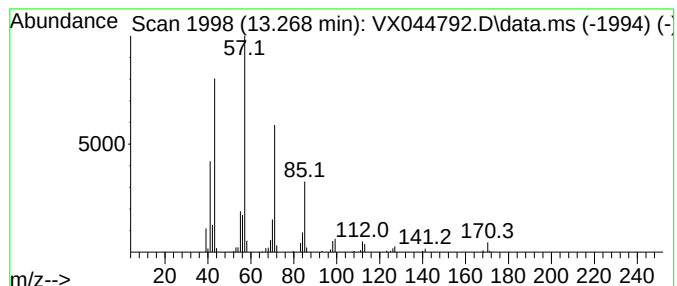
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Quant Title : VOC Analysis

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	4.45 ug/L	57837	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	96
2			Dodecane	170	C12H26	000112-40-3	91
3			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	90
4			Undecane	156	C11H24	001120-21-4	86
5			Tetradecane	198	C14H30	000629-59-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044792.D
Acq On : 31 Jan 2025 13:30
Operator : JC/MD
Sample : Q1189-11ME
Misc : 14.77g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R2ME

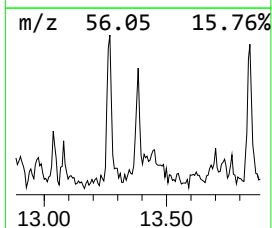
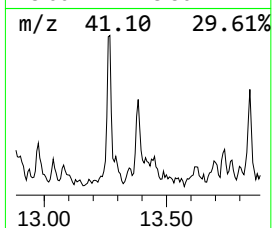
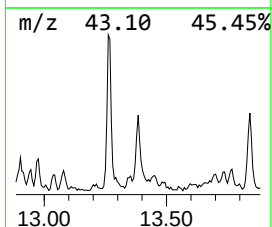
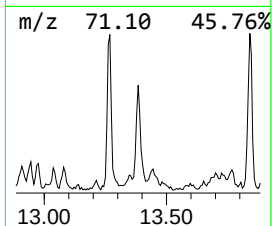
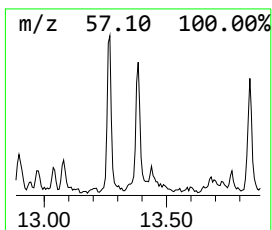
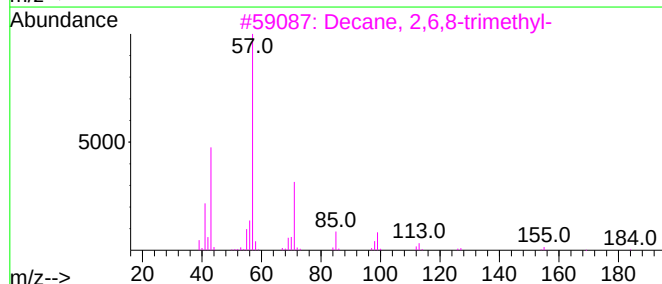
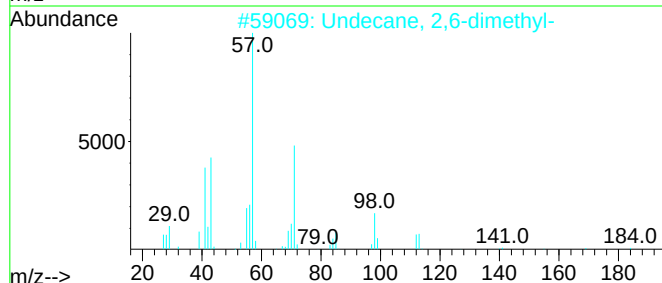
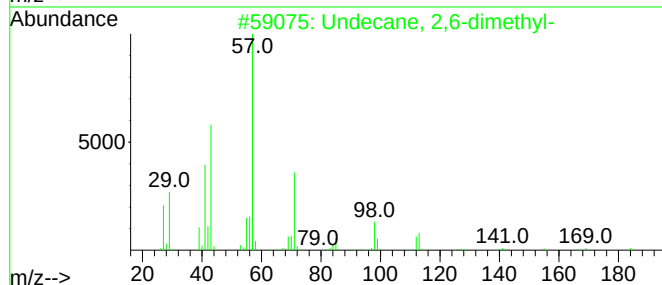
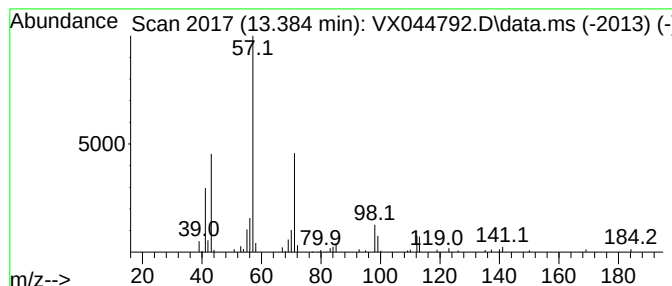
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Quant Title : VOC Analysis

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.384	2.96 ug/L	38485	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	91
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	90
3			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	80
4			5-Ethyldecane	170	C12H26	017302-36-2	78
5			Dodecane, 6-methyl-	184	C13H28	006044-71-9	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VOX013125\
Data File : VX044792.D
Acq On : 31 Jan 2025 13:30
Operator : JC/MD
Sample : Q1189-11ME
Misc : 14.77g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R2ME

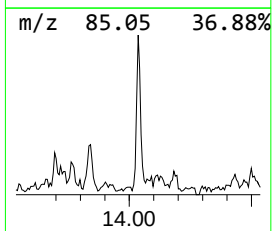
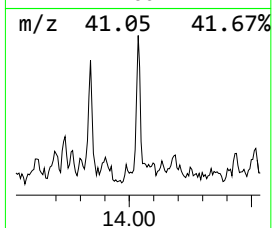
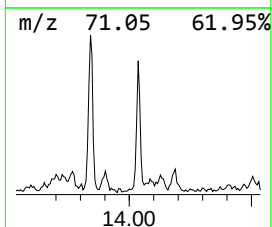
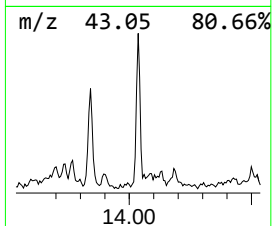
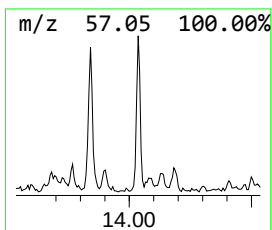
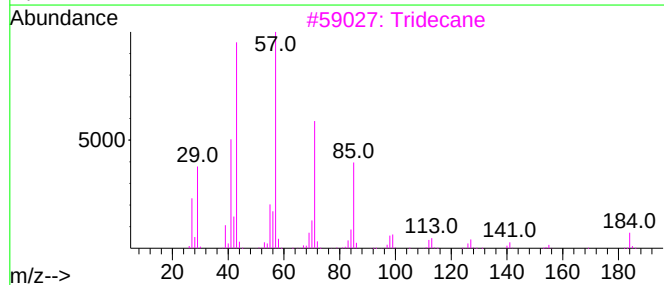
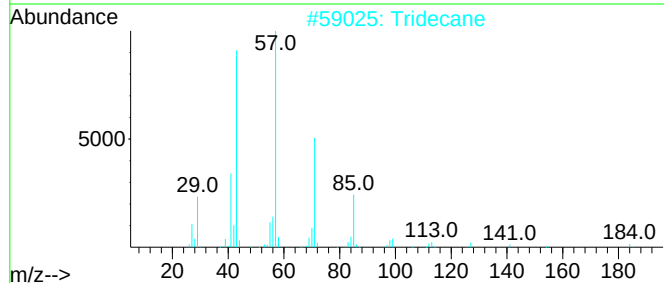
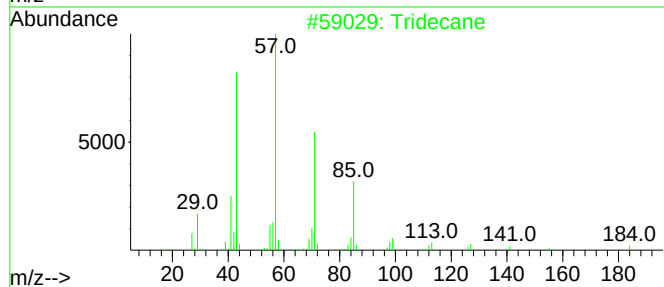
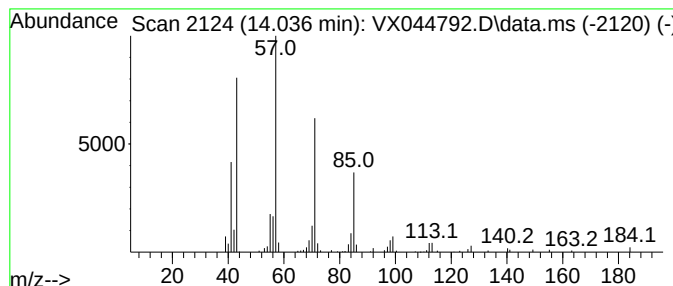
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Quant Title : VOC Analysis

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

Peak Number 12 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.036	3.33 ug/L	43269	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	96
2		Tridecane	184	C13H28	000629-50-5	91
3		Tridecane	184	C13H28	000629-50-5	87
4		Hexadecane	226	C16H34	000544-76-3	86
5		Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044792.D
Acq On : 31 Jan 2025 13:30
Operator : JC/MD
Sample : Q1189-11ME
Misc : 14.77g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44R2ME

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

						--Internal Standard--			
TIC Top	Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL)	Alkane: S...	11.476	3.9	ug/L	50872	3	12.024	649419	50.0
(DEL)	Alkane: S...	11.713	2.7	ug/L	34982	3	12.024	649419	50.0
(DEL)	Alkane: S...	12.421	5.3	ug/L	68705	3	12.024	649419	50.0
(DEL)	Alkane: S...	13.268	4.5	ug/L	57837	3	12.024	649419	50.0
(DEL)	Alkane: S...	13.384	3.0	ug/L	38485	3	12.024	649419	50.0
(DEL)	Alkane: S...	14.036	3.3	ug/L	43269	3	12.024	649419	50.0