

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090123\
 Data File : VX037460.D
 Acq On : 01 Sep 2023 13:21
 Operator : JC/MD
 Sample : 04189-01
 Misc : 0.90g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SB-02(22-23)

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\82X081723W.M
 Title : SW846 8260

Signal : TIC: VX037460.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.940	295	304	315	rBV	25429	61765	7.39%	0.946%
2	5.385	694	705	721	rBV	76972	244343	29.24%	3.743%
3	5.544	721	731	748	rVB	183551	522971	62.59%	8.011%
4	5.952	788	798	816	rBV	99752	267450	32.01%	4.097%
5	6.757	919	930	949	rBV	265010	633897	75.87%	9.711%
6	7.123	983	990	1000	rBV2	11171	24999	2.99%	0.383%
7	8.647	1233	1240	1250	rBV	537011	835543	100.00%	12.800%
8	10.055	1465	1471	1479	rBV	493500	690095	82.59%	10.572%
9	10.311	1508	1513	1517	rVB4	6325	11604	1.39%	0.178%
10	10.585	1552	1558	1562	rBV3	7175	11337	1.36%	0.174%
11	10.671	1565	1572	1575	rBV3	5333	10829	1.30%	0.166%
12	10.781	1582	1590	1594	rBV	21489	30480	3.65%	0.467%
13	10.854	1594	1602	1606	rVV3	14634	26621	3.19%	0.408%
14	10.896	1606	1609	1613	rVV	12385	16308	1.95%	0.250%
15	11.030	1627	1631	1634	rVV3	9383	14528	1.74%	0.223%
16	11.085	1634	1640	1650	rVB	358406	520614	62.31%	7.975%
17	11.219	1655	1662	1666	rBV3	9423	15091	1.81%	0.231%
18	11.427	1693	1696	1700	rBV	15487	22299	2.67%	0.342%
19	11.482	1700	1705	1710	rVB8	9777	18746	2.24%	0.287%
20	11.634	1726	1730	1734	rVB3	12353	15203	1.82%	0.233%
21	11.683	1734	1738	1740	rBV	13193	15724	1.88%	0.241%
22	11.713	1740	1743	1746	rBV	43624	45757	5.48%	0.701%
23	11.780	1751	1754	1759	rVB3	13475	20809	2.49%	0.319%
24	11.835	1759	1763	1766	rBV2	12925	19321	2.31%	0.296%
25	11.890	1766	1772	1777	rVB3	25107	36566	4.38%	0.560%
26	11.945	1777	1781	1784	rBV	20560	28936	3.46%	0.443%
27	11.975	1784	1786	1789	rVV2	10238	10925	1.31%	0.167%
28	12.024	1789	1794	1800	rVB	484223	654487	78.33%	10.026%
29	12.152	1810	1815	1819	rBV5	6762	11756	1.41%	0.180%
30	12.244	1825	1830	1836	rBV6	12610	24081	2.88%	0.369%
31	12.311	1836	1841	1843	rBV4	20883	31358	3.75%	0.480%
32	12.420	1848	1859	1864	rBV	26352	68125	8.15%	1.044%
33	12.469	1864	1867	1872	rVB4	23720	43402	5.19%	0.665%
34	12.549	1872	1880	1882	rBV4	23091	44144	5.28%	0.676%
35	12.579	1882	1885	1889	rVB2	17646	28037	3.36%	0.429%
36	12.683	1898	1902	1906	rBV3	35145	47066	5.63%	0.721%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
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37	12.817	1920	1924	1930	rVB4	34972	56434	6.75%	0.865%
38	12.884	1930	1935	1938	rBV3	55393	86539	10.36%	1.326%
39	12.981	1948	1951	1958	rBV4	23483	33952	4.06%	0.520%
40	13.091	1965	1969	1974	rBV5	14639	26003	3.11%	0.398%

41	13.140	1974	1977	1983	rVB7	8934	14686	1.76%	0.225%
42	13.207	1985	1988	1991	rBV3	16051	18700	2.24%	0.286%
43	13.292	1996	2002	2008	rVB3	74813	131629	15.75%	2.016%
44	13.347	2008	2011	2013	rBV2	18110	21199	2.54%	0.325%
45	13.384	2013	2017	2020	rBV2	59407	73162	8.76%	1.121%

46	13.414	2020	2022	2026	rVV4	18242	20352	2.44%	0.312%
47	13.500	2032	2036	2040	rBV5	12711	23345	2.79%	0.358%
48	13.585	2046	2050	2053	rBV4	17411	25800	3.09%	0.395%
49	13.670	2060	2064	2067	rBV3	11894	21529	2.58%	0.330%
50	13.701	2067	2069	2071	rVV2	23374	24187	2.89%	0.371%

51	13.737	2071	2075	2078	rVV2	33437	44641	5.34%	0.684%
52	13.780	2078	2082	2084	rVV	38522	60722	7.27%	0.930%
53	13.841	2088	2092	2099	rBV2	67984	86744	10.38%	1.329%
54	13.908	2099	2103	2110	rVB8	28962	70009	8.38%	1.072%
55	13.987	2110	2116	2119	rBV6	16326	34696	4.15%	0.532%

56	14.073	2126	2130	2132	rBV4	17469	21597	2.58%	0.331%
57	14.103	2132	2135	2137	rVV3	19913	23658	2.83%	0.362%
58	14.134	2138	2140	2143	rVB2	13008	12636	1.51%	0.194%
59	14.213	2151	2153	2161	rVB3	23679	39005	4.67%	0.598%
60	14.420	2184	2187	2188	rBV3	9885	10567	1.26%	0.162%

61	14.481	2193	2197	2200	rVV3	18666	31843	3.81%	0.488%
62	14.518	2200	2203	2206	rVB	20135	22818	2.73%	0.350%
63	14.609	2215	2218	2221	rBV2	49849	65324	7.82%	1.001%
64	14.634	2221	2222	2226	rVV	25175	26176	3.13%	0.401%
65	14.670	2226	2228	2232	rVB3	16957	18680	2.24%	0.286%

66	14.725	2233	2237	2239	rBV5	9393	13463	1.61%	0.206%
67	14.780	2243	2246	2253	rVV3	28497	45349	5.43%	0.695%
68	14.847	2254	2257	2260	rVB2	15989	19123	2.29%	0.293%
69	14.957	2273	2275	2284	rVB7	16294	29066	3.48%	0.445%
70	15.182	2307	2312	2314	rBV5	10028	16319	1.95%	0.250%

71	15.213	2314	2317	2320	rVB	19707	23162	2.77%	0.355%
72	15.377	2340	2344	2347	rBV5	8094	12626	1.51%	0.193%
73	15.414	2347	2350	2354	rVB3	13909	19374	2.32%	0.297%
74	15.475	2357	2360	2367	rVB2	10727	17438	2.09%	0.267%
75	15.609	2378	2382	2386	rBV	11503	20145	2.41%	0.309%

76	15.646	2386	2388	2397	rVV6	11282	21757	2.60%	0.333%
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ClientSampleId :
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Title : SW846 8260

77	15.743	2399	2404	2409	rVB8	9345	18167	2.17%	0.278%
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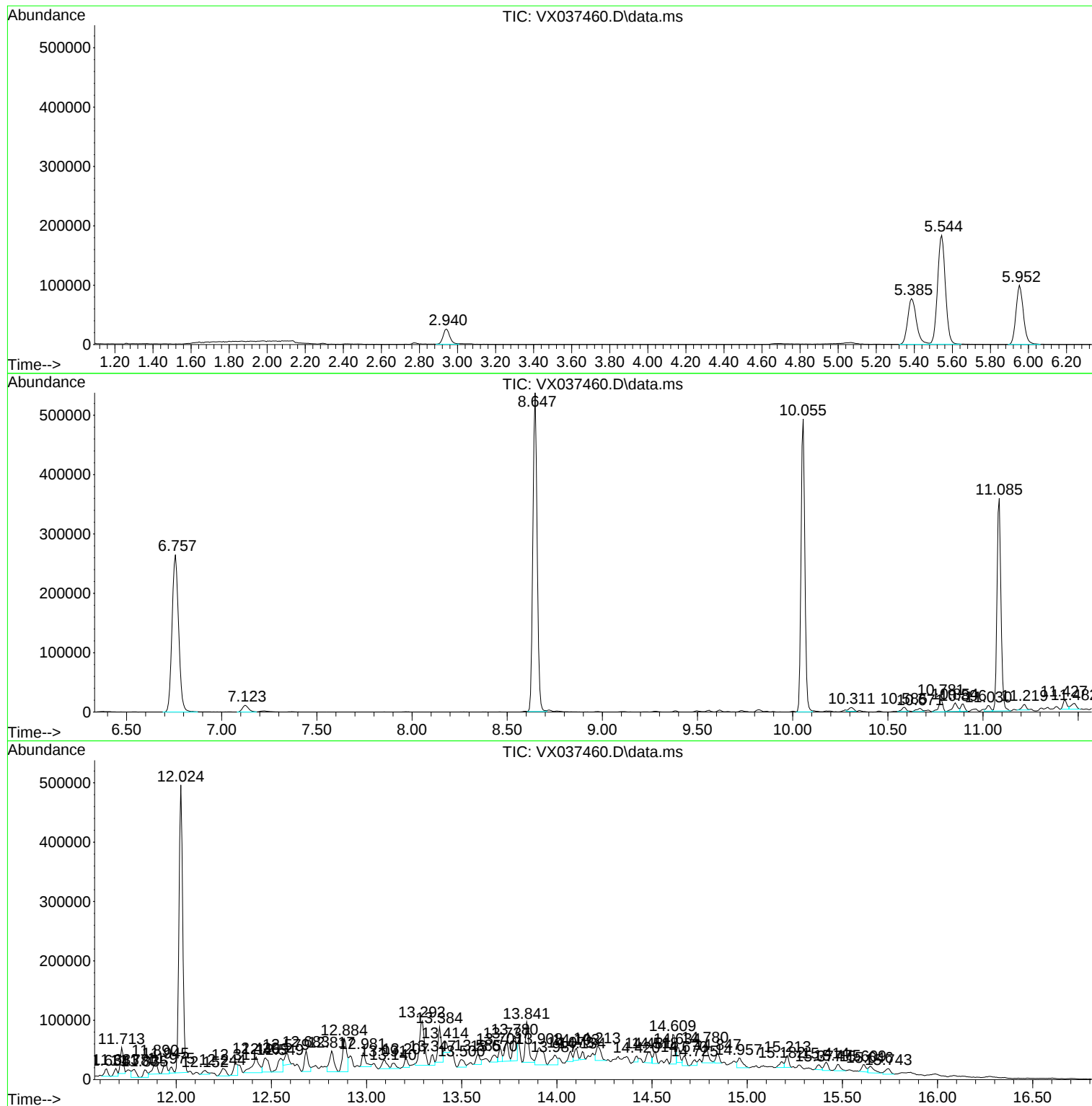
Sum of corrected areas: 6527839

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090123\
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Instrument :
MSVOA_X
ClientSampleId :
SB-02(22-23)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090123\
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB-02(22-23)

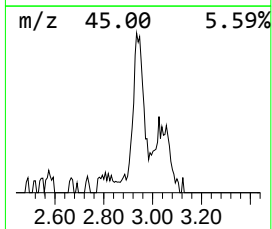
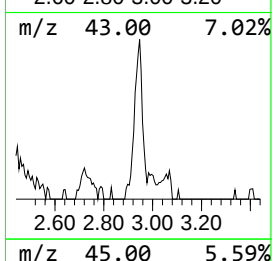
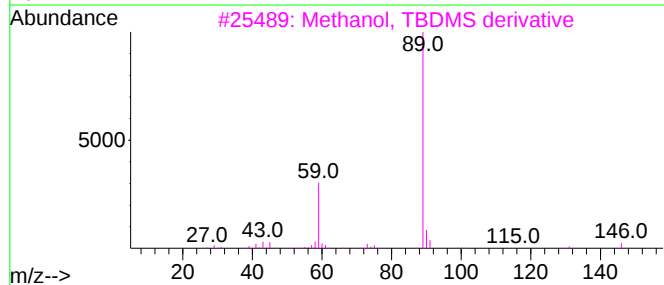
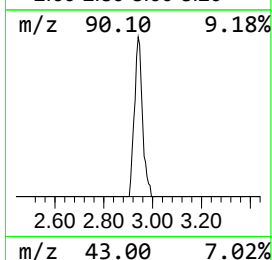
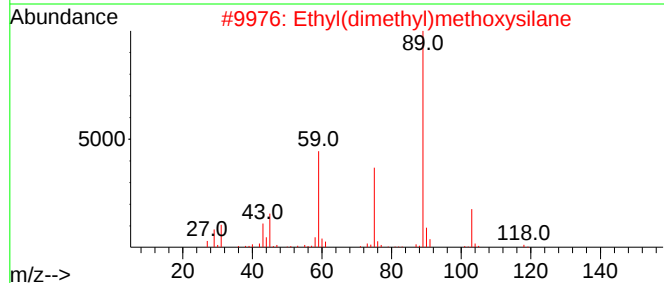
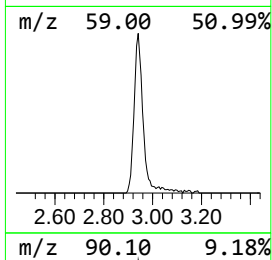
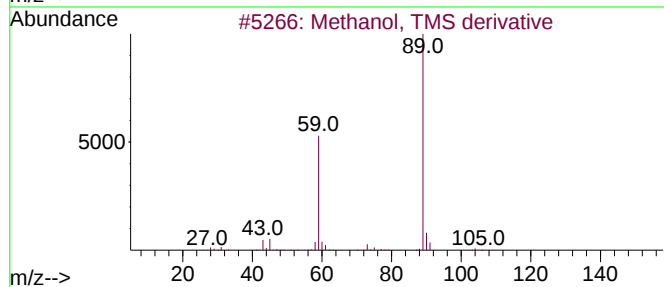
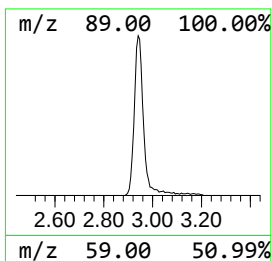
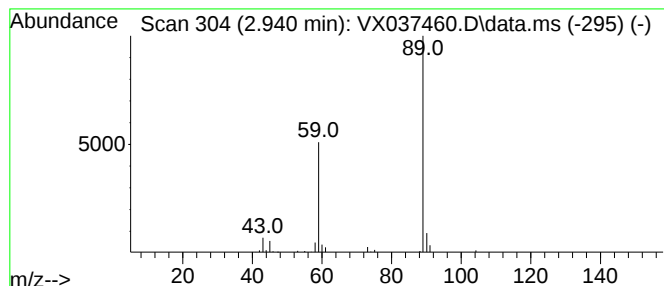
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 1 Methanol, TMS derivative Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.940	5.91 ug/l	61765	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	91
2			Ethyl(dimethyl)methoxysilane	118	C5H14OSi	052686-75-6	83
3			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	83
4			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	74
5			Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB-02(22-23)

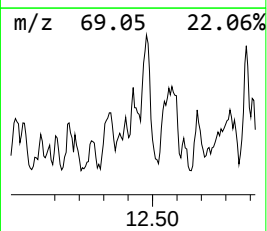
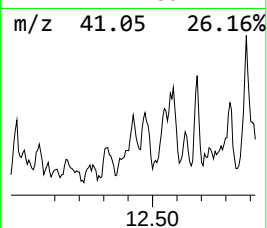
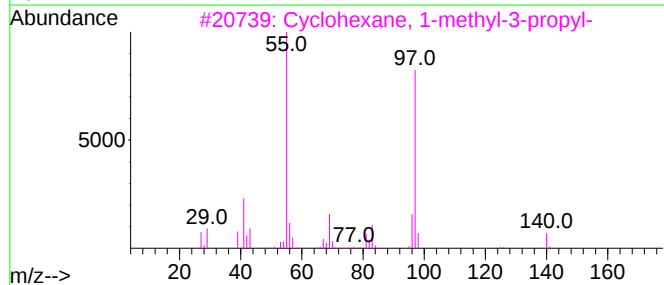
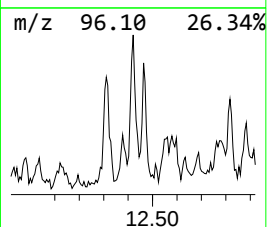
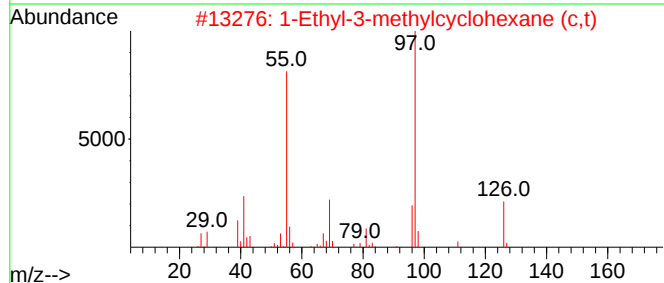
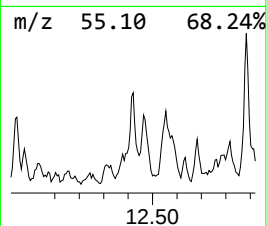
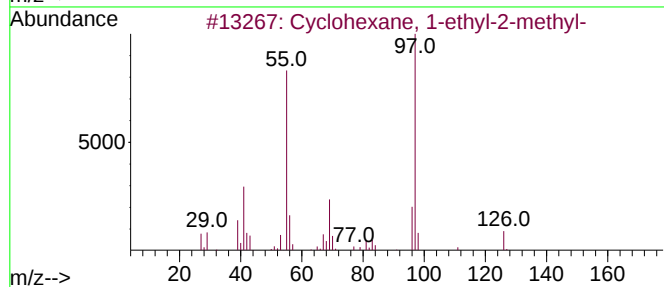
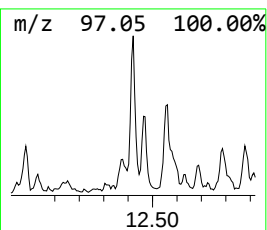
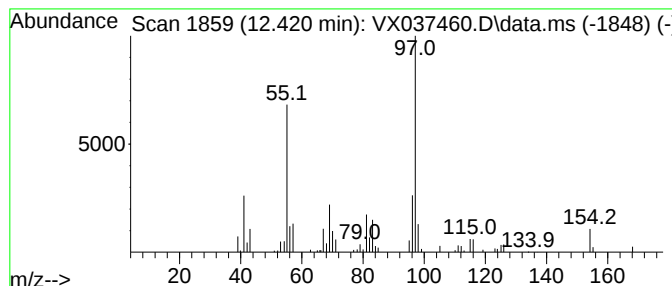
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	5.20 ug/l	68125	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	76
2			1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	72
3			Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	64
4			Succinic acid, di(2-methylcycloh...	310	C18H30O4	1000329-83-0	59
5			Oxalic acid, butyl cyclohexylmet...	242	C13H22O4	1000309-68-2	59



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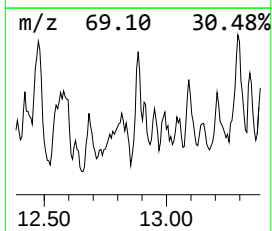
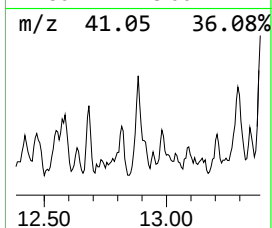
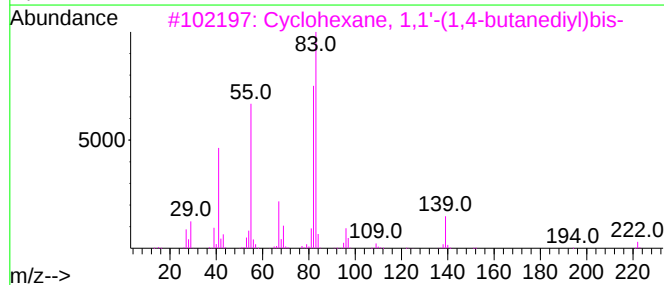
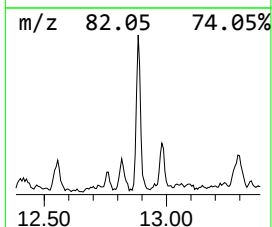
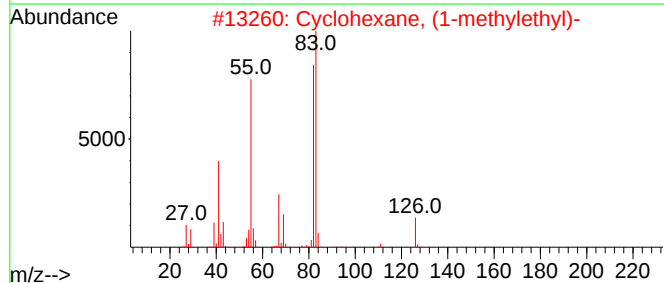
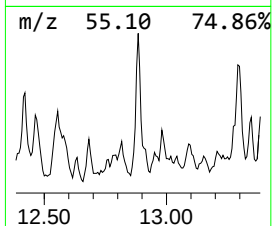
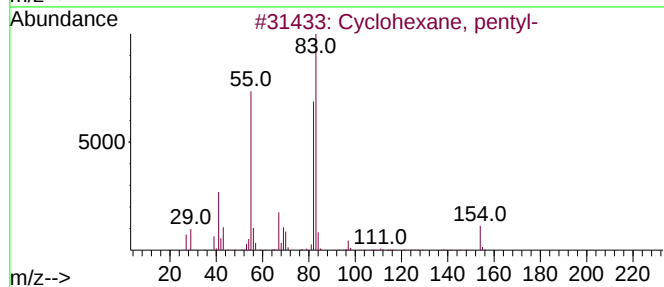
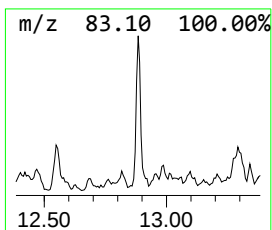
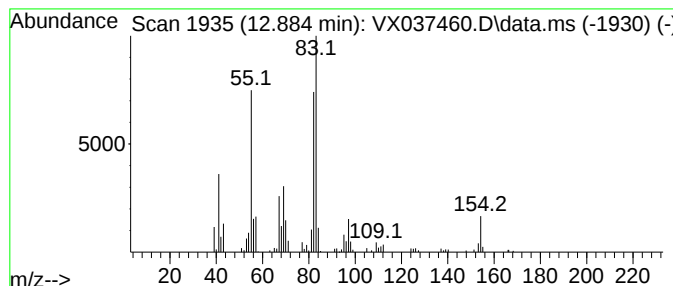
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclohexane, pentyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	6.61 ug/l	86539	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, pentyl-	154	C11H22	004292-92-6	90
2			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	83
3			Cyclohexane, 1,1'-(1,4-butanediyl)-	222	C16H30	006165-44-2	78
4			Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	72
5			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	64



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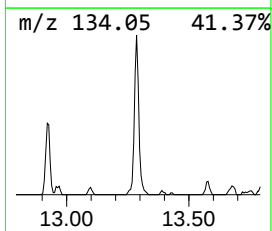
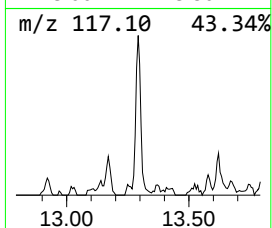
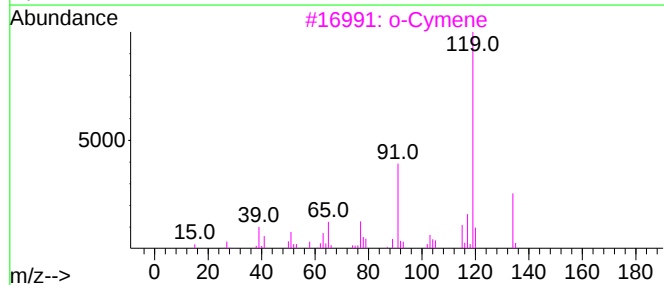
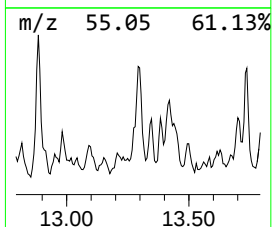
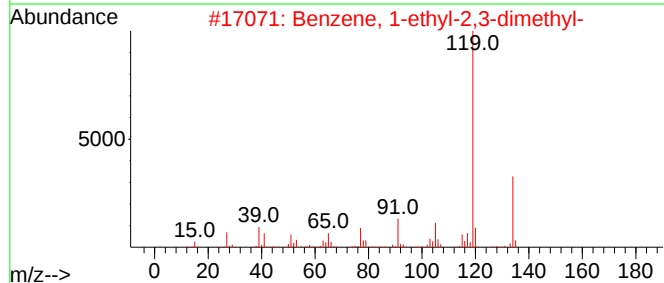
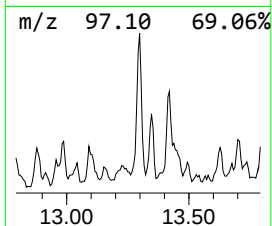
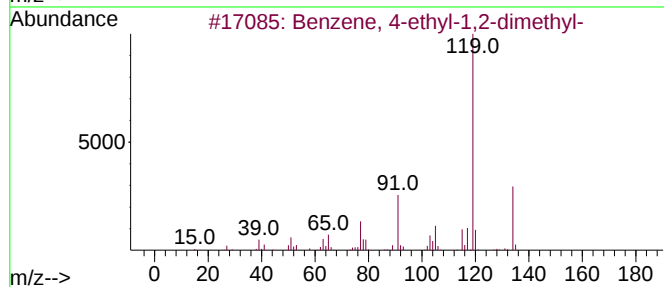
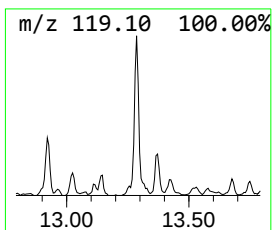
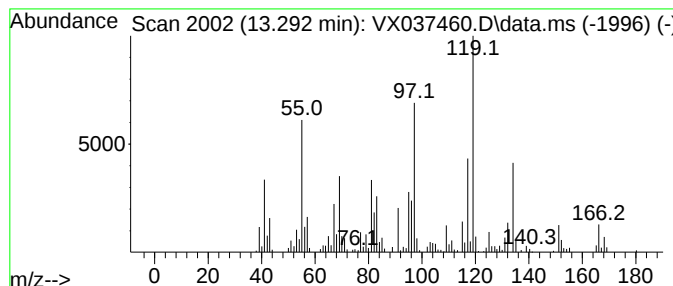
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Quant Title : SW846 8260

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

Peak Number 4 unknown13.292 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	10.06 ug/l	131629	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	41
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	41
3			o-Cymene	134	C10H14	000527-84-4	41
4			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	38
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090123\
Data File : VX037460.D
Acq On : 01 Sep 2023 13:21
Operator : JC/MD
Sample : 04189-01
Misc : 0.90g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB-02(22-23)

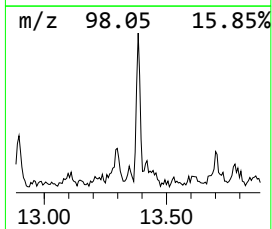
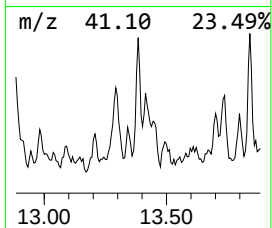
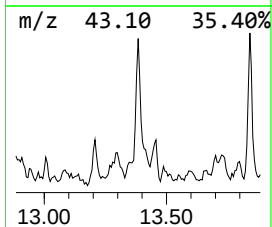
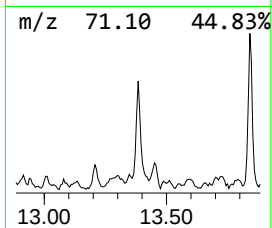
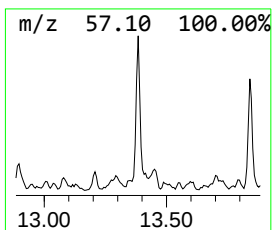
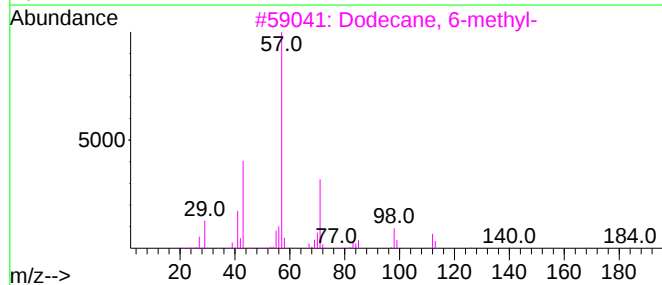
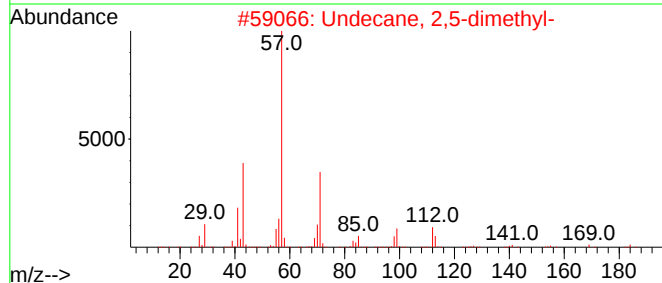
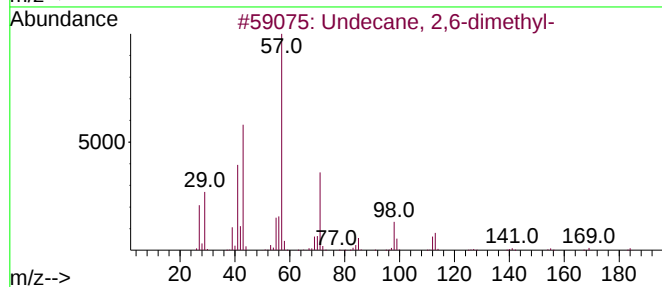
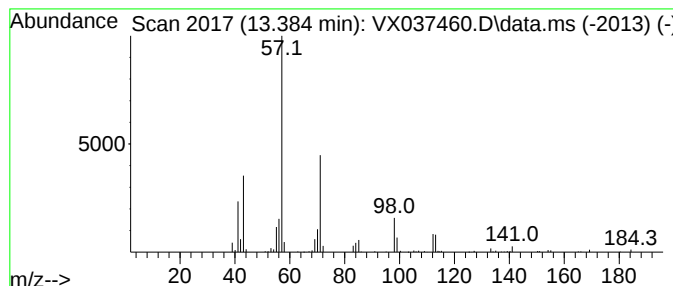
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Quant Title : SW846 8260

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

Peak Number 5 Undecane, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.384	5.59 ug/l	73162	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	94
2			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	87
3			Dodecane, 6-methyl-	184	C13H28	006044-71-9	76
4			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	68
5			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090123\
Data File : VX037460.D
Acq On : 01 Sep 2023 13:21
Operator : JC/MD
Sample : 04189-01
Misc : 0.90g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB-02(22-23)

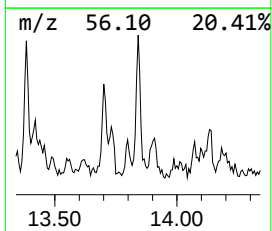
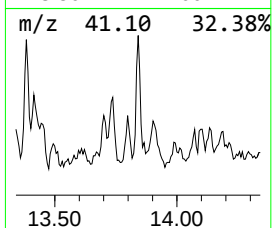
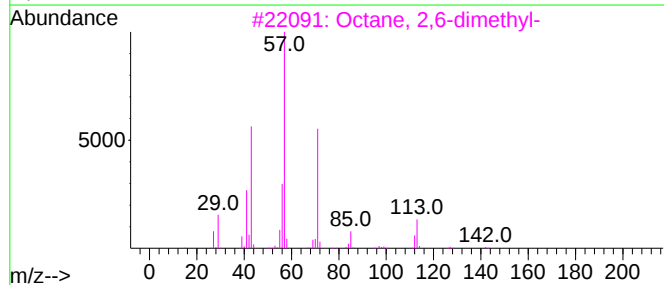
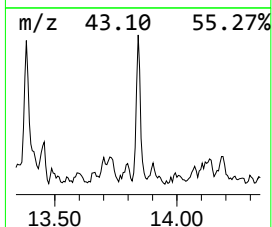
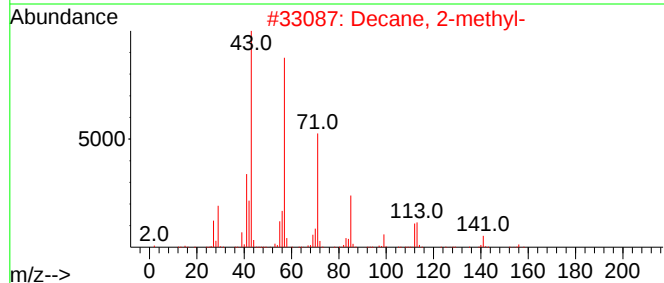
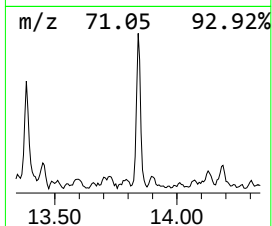
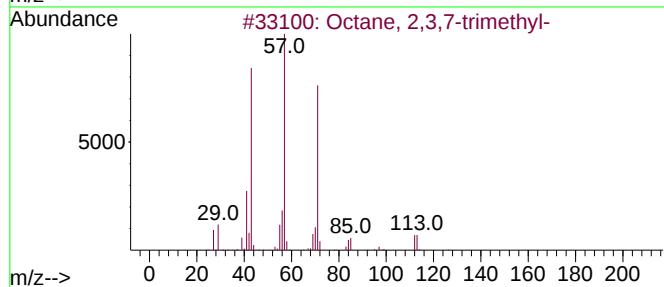
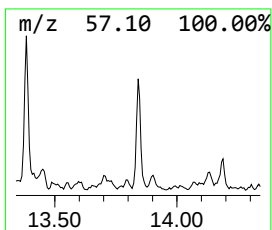
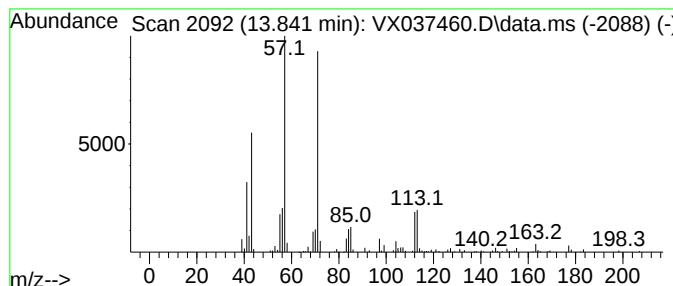
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Quant Title : SW846 8260

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

Peak Number 6 Octane, 2,3,7-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	6.63 ug/l	86744	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	78
2			Decane, 2-methyl-	156	C11H24	006975-98-0	78
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
4			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	64
5			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090123\
Data File : VX037460.D
Acq On : 01 Sep 2023 13:21
Operator : JC/MD
Sample : 04189-01
Misc : 0.90g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB-02(22-23)

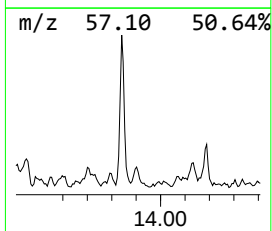
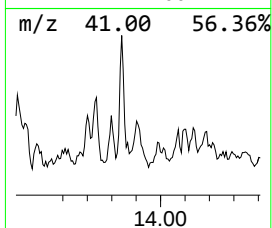
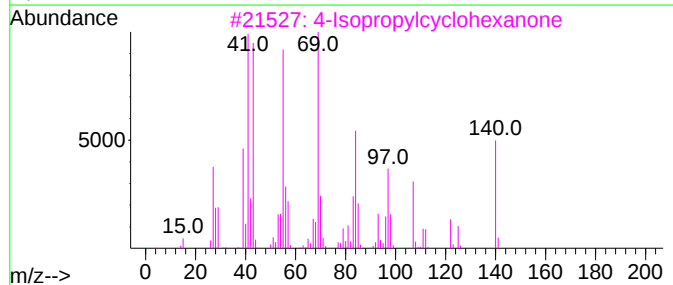
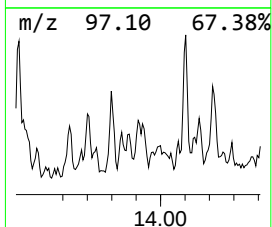
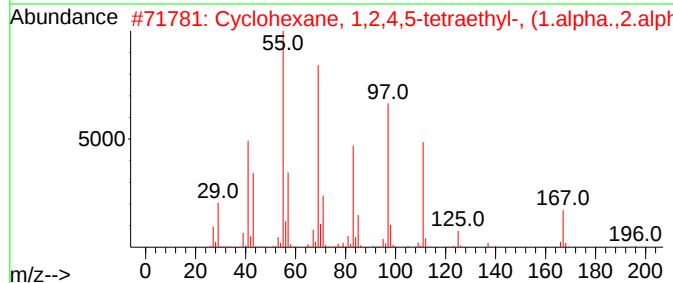
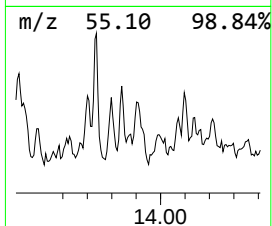
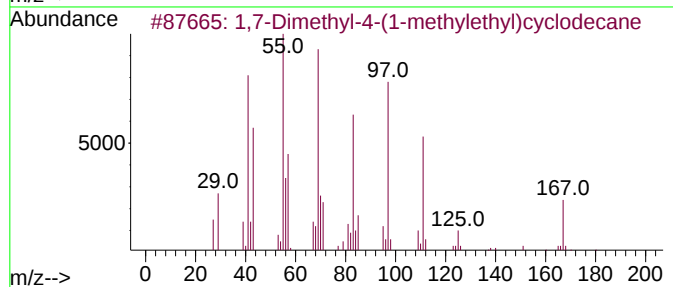
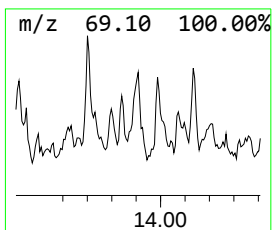
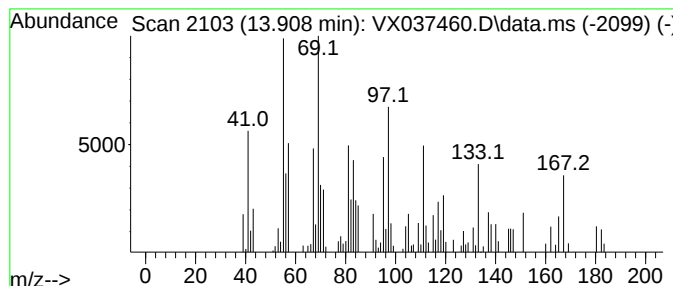
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 7 unknown13.908 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.908	5.35 ug/l	70009	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	47
2			Cyclohexane, 1,2,4,5-tetraethyl-...	196	C14H28	061142-24-3	43
3			4-Isopropylcyclohexanone	140	C9H16O	005432-85-9	30
4			Cyclopentane, pentyl-	140	C10H20	003741-00-2	25
5			6-Tridecene, (Z)-	182	C13H26	006508-77-6	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090123\
Data File : VX037460.D
Acq On : 01 Sep 2023 13:21
Operator : JC/MD
Sample : 04189-01
Misc : 0.90g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB-02(22-23)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.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
Methanol, TMS d...	2.940	5.9	ug/l	61765	1	5.544	522971	50.0
Cyclohexane, 1-...	12.421	5.2	ug/l	68125	4	12.024	654487	50.0
Cyclohexane, pe...	12.884	6.6	ug/l	86539	4	12.024	654487	50.0
unknown13.292	13.292	10.1	ug/l	131629	4	12.024	654487	50.0
Undecane, 2,6-d...	13.384	5.6	ug/l	73162	4	12.024	654487	50.0
Octane, 2,3,7-t...	13.841	6.6	ug/l	86744	4	12.024	654487	50.0
unknown13.908	13.908	5.3	ug/l	70009	4	12.024	654487	50.0