

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010825\
 Data File : VX044620.D
 Acq On : 08 Jan 2025 12:10
 Operator : JC/MD
 Sample : Q1007-01
 Misc : 1.25g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WD-01

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\82X010725W.M
 Title : SW846 8260

Signal : TIC: VX044620.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	22	29	35	rBV	12781	17293	1.84%	0.218%
2	1.557	67	77	78	rBV4	9366	20060	2.13%	0.253%
3	1.624	81	88	91	rVV7	6474	19830	2.11%	0.250%
4	4.251	509	519	529	rBV5	6564	22975	2.44%	0.290%
5	5.385	694	705	719	rBV2	97812	296737	31.53%	3.747%
6	5.538	719	730	747	rVB	168893	502464	53.39%	6.345%
7	5.952	788	798	815	rBV	118395	338875	36.01%	4.279%
8	6.751	921	929	945	rBV	272358	689602	73.27%	8.708%
9	8.641	1233	1239	1250	rBV	575027	941166	100.00%	11.884%
10	10.049	1465	1470	1486	rBV	564228	831112	88.31%	10.495%
11	10.305	1506	1512	1517	rBV5	5121	10503	1.12%	0.133%
12	10.354	1517	1520	1530	rVB5	5947	9698	1.03%	0.122%
13	11.079	1634	1639	1651	rBV	497932	675138	71.73%	8.525%
14	11.189	1654	1657	1664	rVB7	6725	11149	1.18%	0.141%
15	11.476	1698	1704	1710	rVB2	27313	36933	3.92%	0.466%
16	11.896	1766	1773	1777	rBV6	7467	12348	1.31%	0.156%
17	12.018	1788	1793	1800	rBV	633898	838296	89.07%	10.585%
18	12.097	1804	1806	1811	rVB2	9861	11966	1.27%	0.151%
19	12.171	1815	1818	1822	rVB2	8810	10565	1.12%	0.133%
20	12.219	1822	1826	1838	rBV	28610	50527	5.37%	0.638%
21	12.329	1838	1844	1848	rVB9	4616	10941	1.16%	0.138%
22	12.421	1855	1859	1863	rBV	69301	80706	8.58%	1.019%
23	12.469	1863	1867	1874	rVB9	4628	11183	1.19%	0.141%
24	12.585	1882	1886	1890	rVB3	9224	15930	1.69%	0.201%
25	12.817	1919	1924	1927	rVB3	11443	14876	1.58%	0.188%
26	12.902	1928	1938	1942	rBV5	21642	56916	6.05%	0.719%
27	12.939	1942	1944	1947	rVV2	17790	20143	2.14%	0.254%
28	12.975	1947	1950	1954	rVV4	28747	38235	4.06%	0.483%
29	13.036	1957	1960	1965	rVB	26342	30804	3.27%	0.389%
30	13.268	1993	1998	2001	rBV	207963	251852	26.76%	3.180%
31	13.347	2007	2011	2013	rBV4	10677	15918	1.69%	0.201%
32	13.384	2013	2017	2020	rVV	45566	55857	5.93%	0.705%
33	13.414	2020	2022	2026	rVB5	12372	16631	1.77%	0.210%
34	13.597	2047	2052	2056	rBV7	10743	22402	2.38%	0.283%
35	13.676	2060	2065	2068	rVV3	47916	78722	8.36%	0.994%
36	13.737	2071	2075	2077	rVV2	49222	67652	7.19%	0.854%

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37	13.768	2077	2080	2083	rVV2	48595	62266	6.62%	0.786%
38	13.798	2083	2085	2087	rVV3	20320	23469	2.49%	0.296%
39	13.835	2087	2091	2099	rVV3	68311	128165	13.62%	1.618%
40	13.902	2099	2102	2108	rVB7	15146	26446	2.81%	0.334%
41	14.036	2119	2124	2128	rBV	262211	283426	30.11%	3.579%
42	14.097	2132	2134	2137	rVV3	17019	20836	2.21%	0.263%
43	14.134	2137	2140	2143	rVB3	23759	26703	2.84%	0.337%
44	14.219	2151	2154	2160	rVB3	31488	44314	4.71%	0.560%
45	14.353	2171	2176	2179	rBV4	14816	24458	2.60%	0.309%
46	14.408	2181	2185	2187	rVV	34724	48627	5.17%	0.614%
47	14.432	2187	2189	2192	rVV	49722	53882	5.73%	0.680%
48	14.469	2192	2195	2197	rVV2	27712	31772	3.38%	0.401%
49	14.499	2197	2200	2207	rVB3	43392	78894	8.38%	0.996%
50	14.560	2207	2210	2215	rVB	33733	47418	5.04%	0.599%
51	14.615	2215	2219	2225	rBV3	69681	111476	11.84%	1.408%
52	14.719	2232	2236	2238	rBV5	12402	20099	2.14%	0.254%
53	14.755	2238	2242	2245	rVV	237889	261721	27.81%	3.305%
54	14.792	2245	2248	2251	rVV3	28856	37644	4.00%	0.475%
55	14.841	2252	2256	2259	rVV4	24022	34578	3.67%	0.437%
56	14.932	2269	2271	2274	rBV4	8904	9450	1.00%	0.119%
57	15.097	2295	2298	2302	rBV5	23515	38545	4.10%	0.487%
58	15.176	2308	2311	2313	rBV4	14184	17902	1.90%	0.226%
59	15.213	2313	2317	2324	rVV	78718	111136	11.81%	1.403%
60	15.274	2324	2327	2331	rVB2	32150	41429	4.40%	0.523%
61	15.487	2358	2362	2368	rVB	89117	121613	12.92%	1.536%
62	15.920	2430	2433	2441	rVB5	20734	35934	3.82%	0.454%
63	16.377	2503	2508	2513	rVB2	20916	41264	4.38%	0.521%

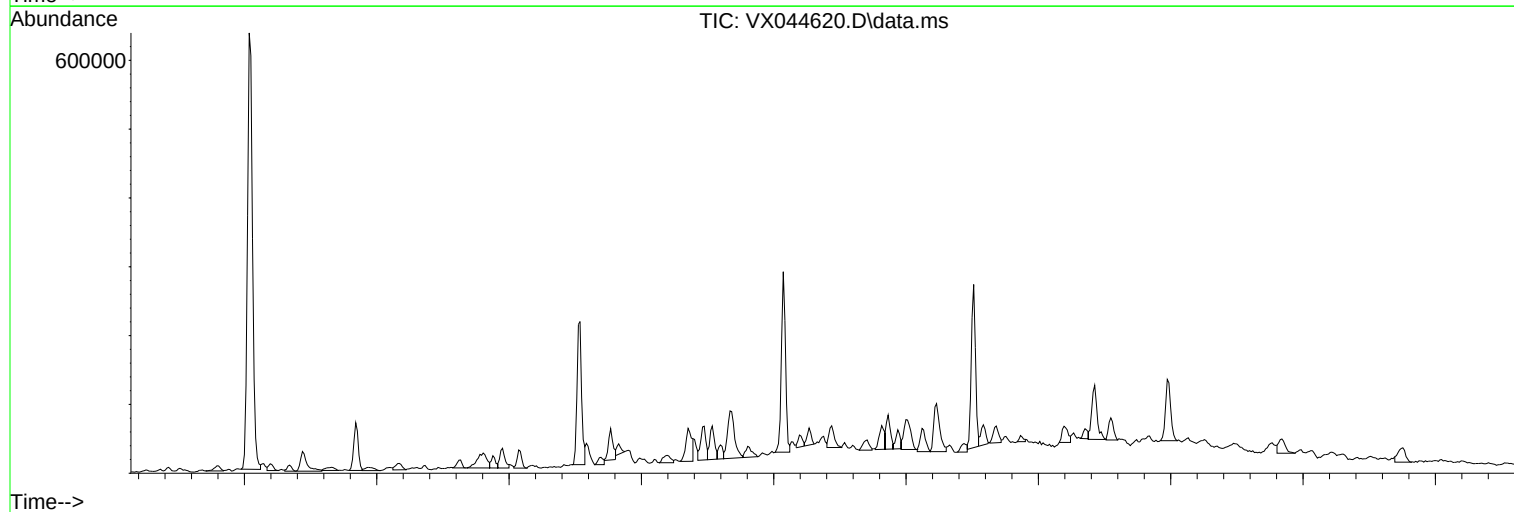
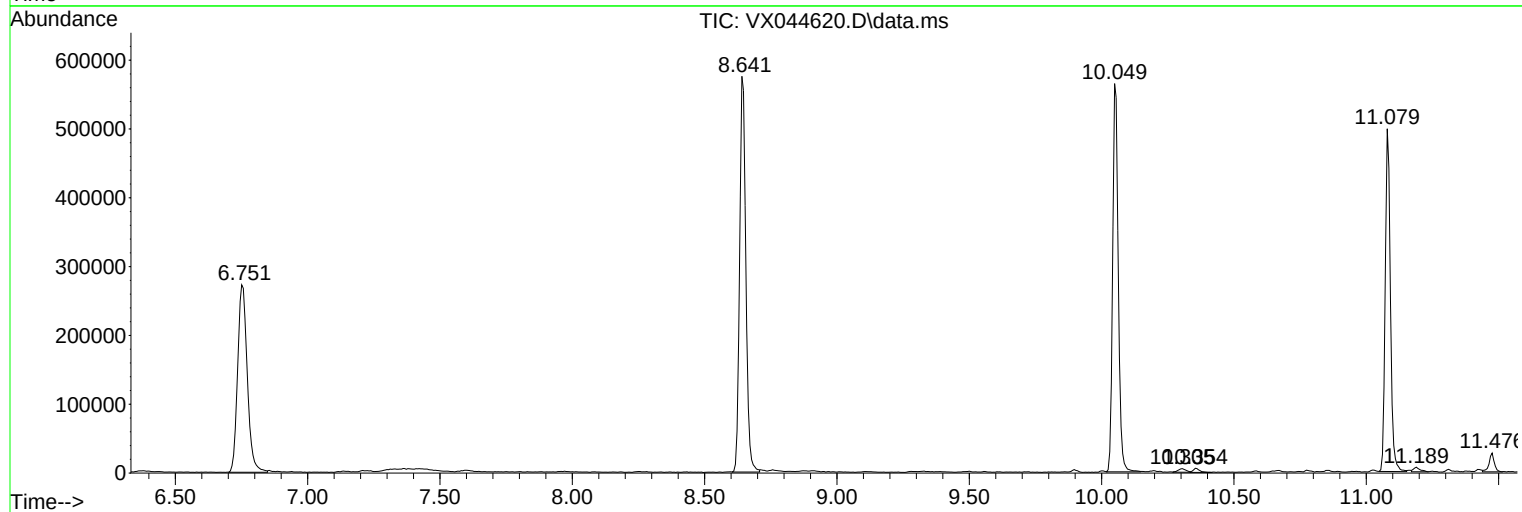
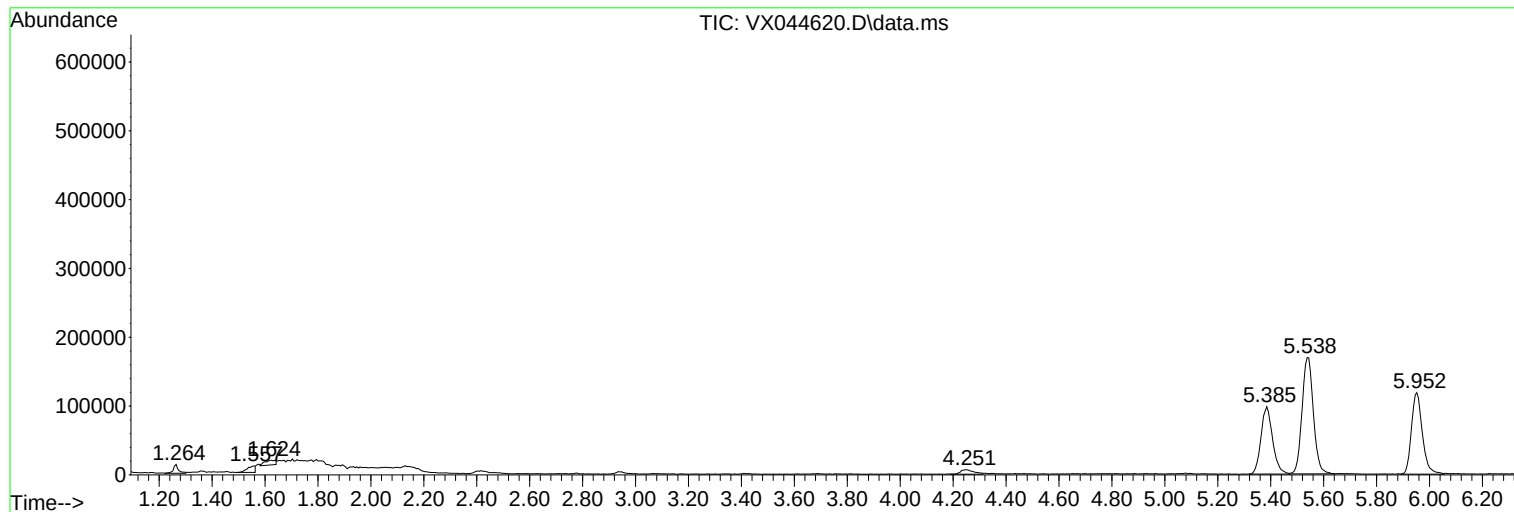
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ClientSampleId :
WD-01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X010725W.M
Quant Title : SW846 8260

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



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MSVOA_X
ClientSampleId :
WD-01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X010725W.M
Quant Title : SW846 8260

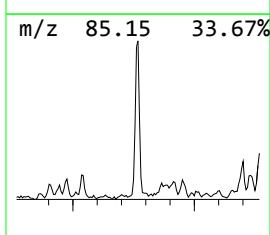
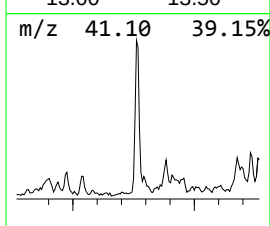
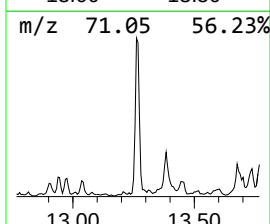
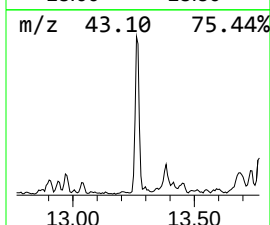
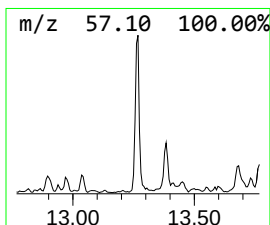
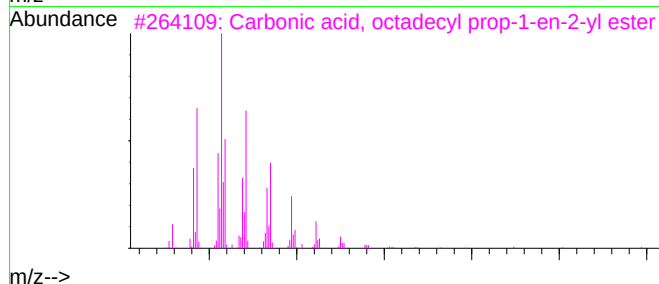
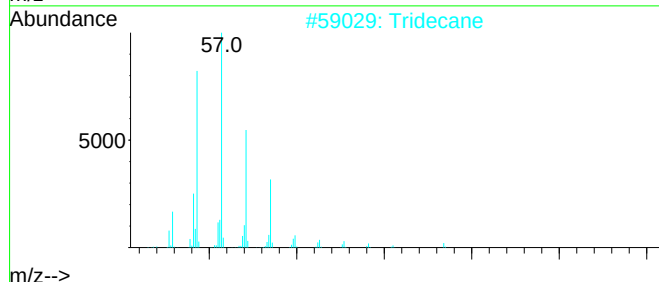
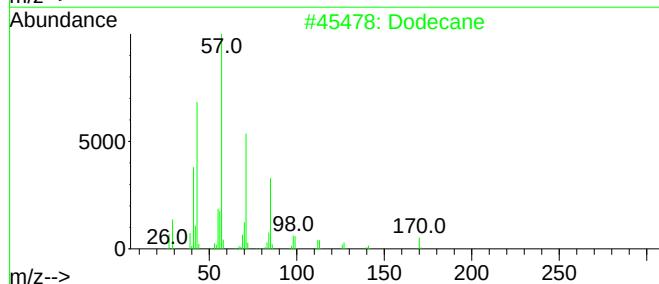
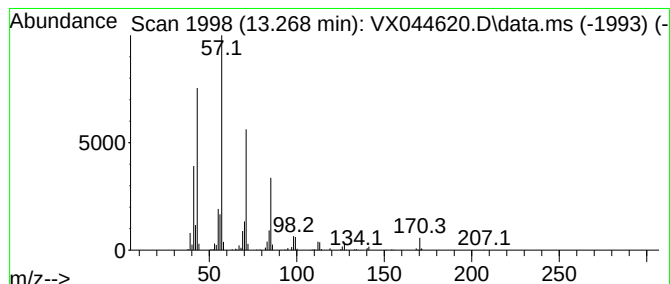
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	15.02 ug/l	251852	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	96
2	Tridecane	184	C13H28	000629-50-5	90
3	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
4	Tetradecane	198	C14H30	000629-59-4	87
5	Undecane	156	C11H24	001120-21-4	86



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X010725W.M
Quant Title : SW846 8260

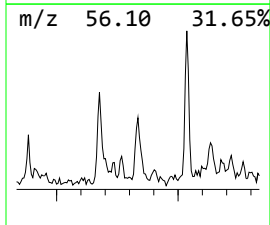
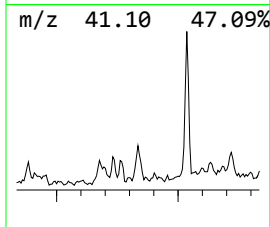
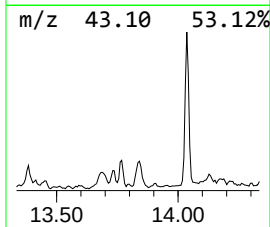
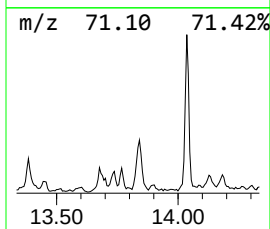
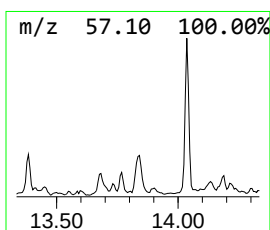
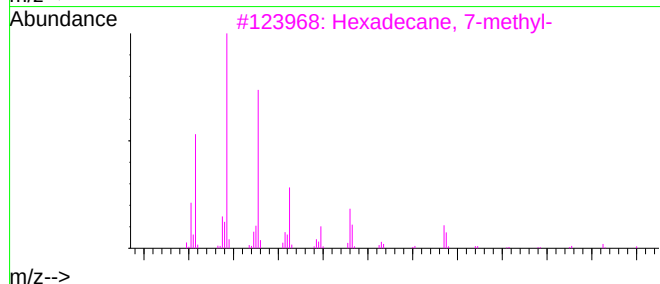
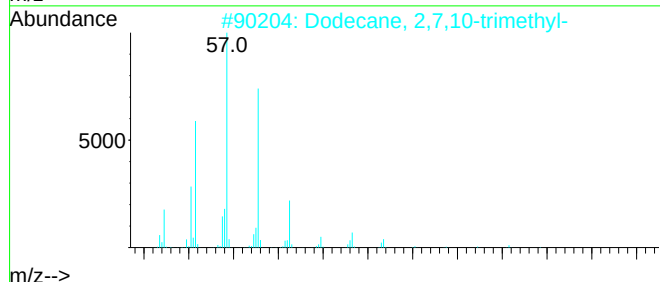
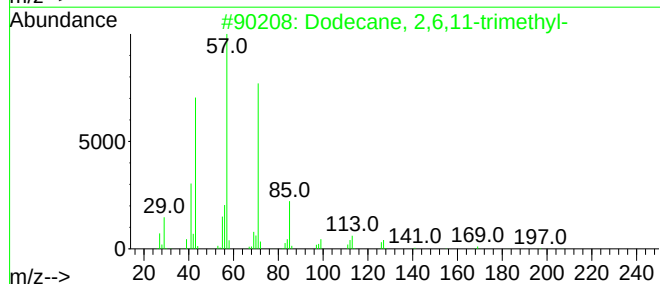
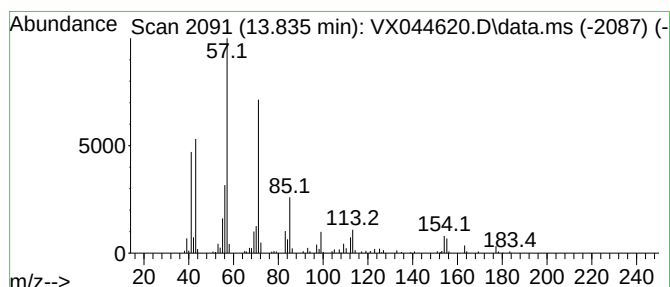
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecane, 2,6,11-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.835	7.64 ug/l	128165	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	80
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
3	Hexadecane, 7-methyl-	240	C17H34	026730-20-1	72
4	Decane, 2-methyl-	156	C11H24	006975-98-0	72
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64



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Misc : 1.25g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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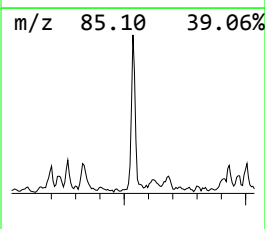
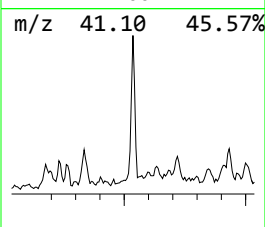
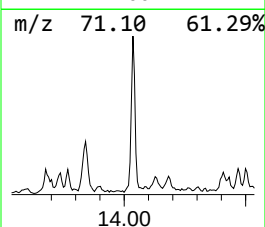
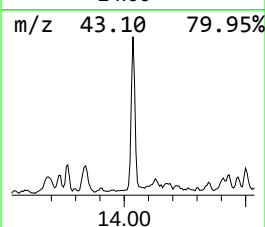
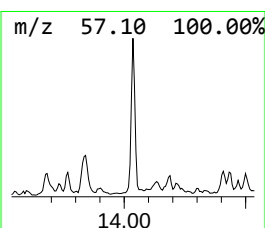
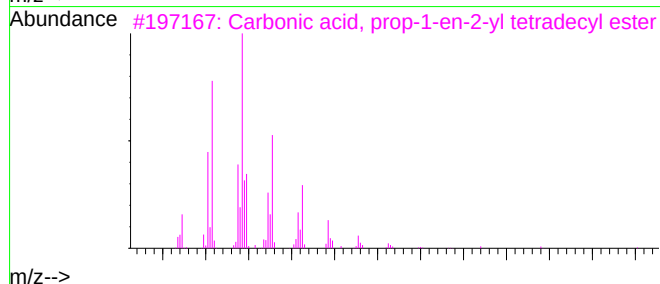
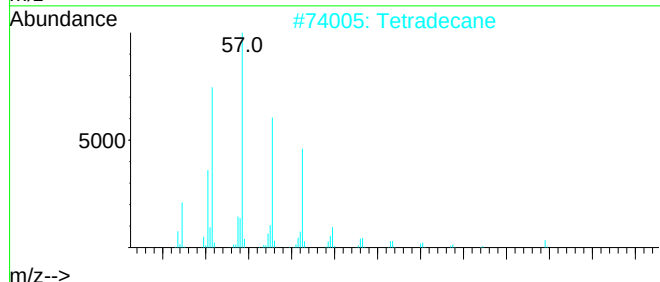
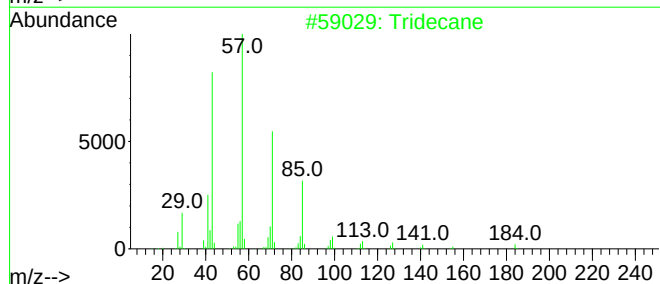
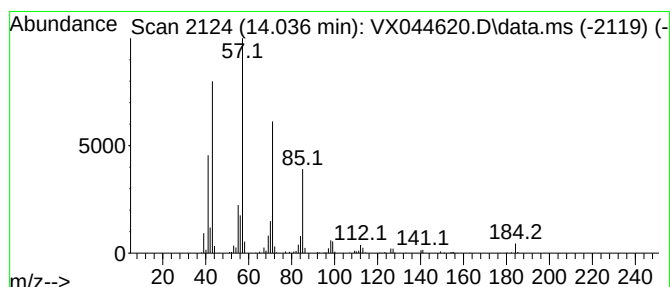
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X010725W.M
Quant Title : SW846 8260

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

Peak Number 3 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.036	16.90 ug/l	283426	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	91
2			Tetradecane	198	C14H30	000629-59-4	90
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	90
4			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	83
5			Nonane	128	C9H20	000111-84-2	81



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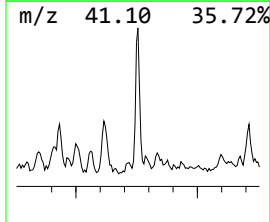
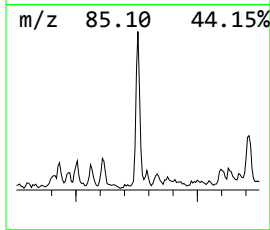
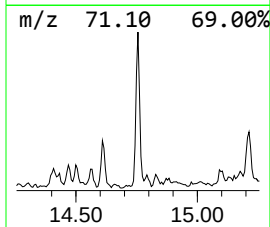
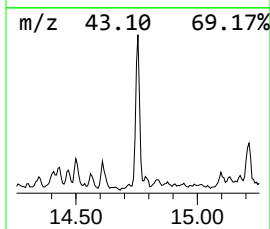
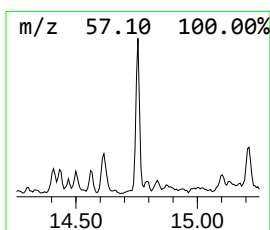
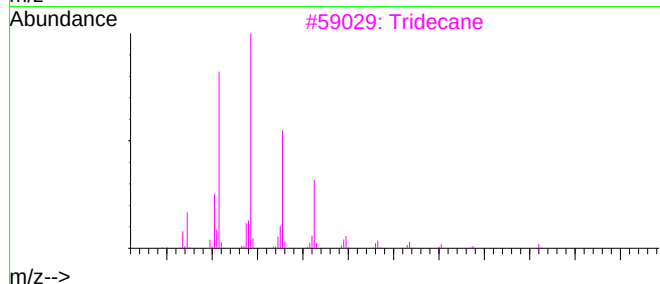
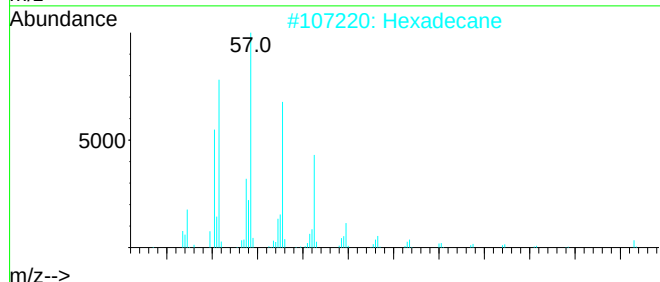
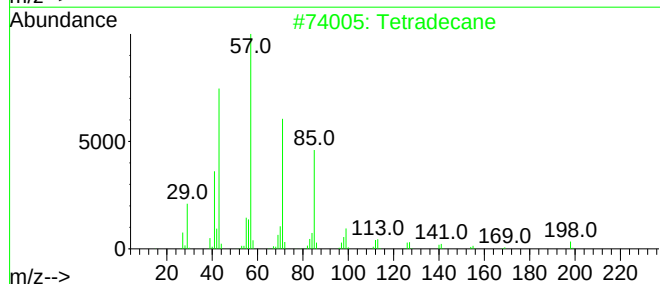
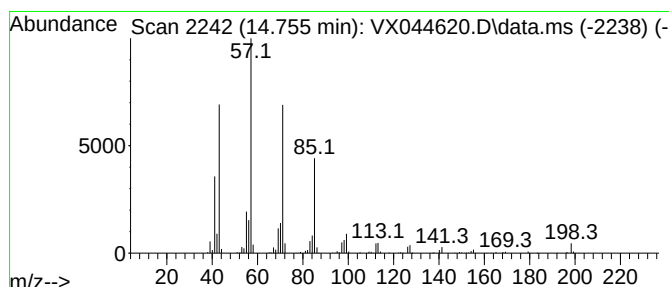
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Quant Title : SW846 8260

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

Peak Number 5 Tetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.756	15.61 ug/l	261721	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	98
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tridecane	184	C13H28	000629-50-5	90
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	86
5	Eicosane	282	C20H42	000112-95-8	80



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Operator : JC/MD
Sample : Q1007-01
Misc : 1.25g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WD-01

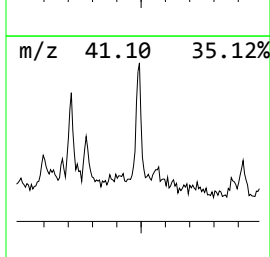
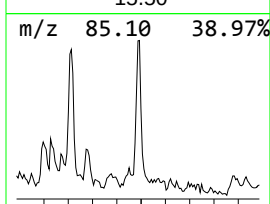
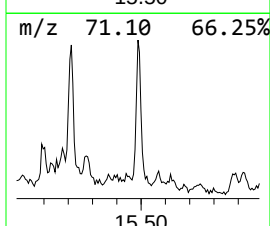
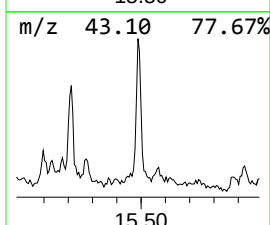
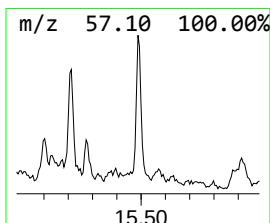
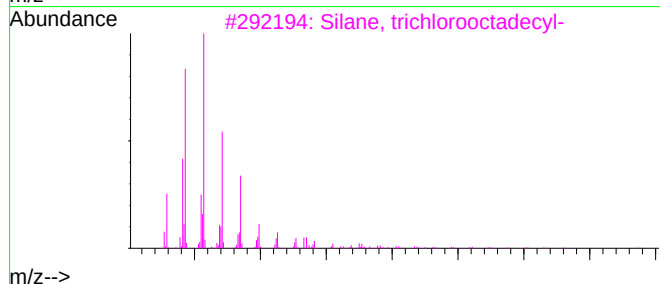
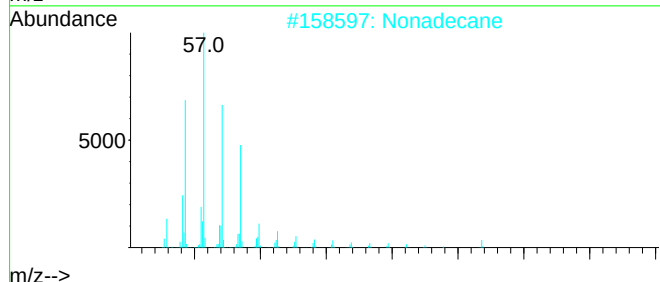
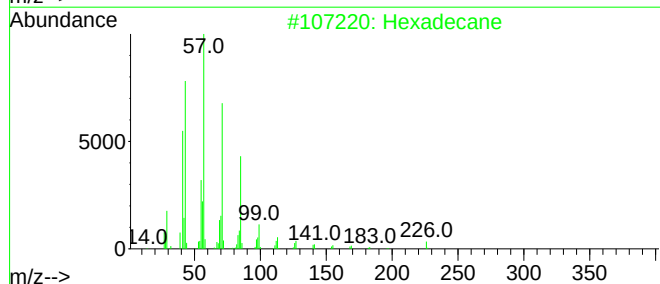
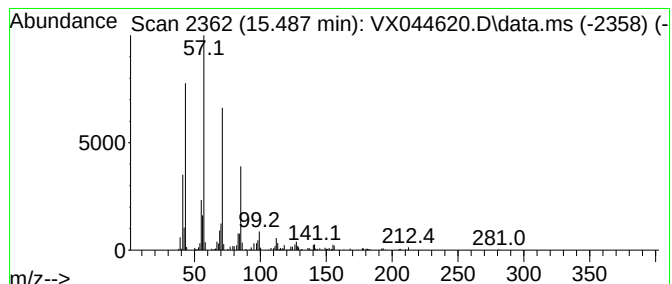
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.487	7.25 ug/l	121613	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	86
2	Nonadecane		268	C19H40	000629-92-5	86
3	Silane, trichlorooctadecyl-		386	C18H37Cl3Si	000112-04-9	86
4	Tridecane		184	C13H28	000629-50-5	86
5	Tetradecane		198	C14H30	000629-59-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010825\
Data File : VX044620.D
Acq On : 08 Jan 2025 12:10
Operator : JC/MD
Sample : Q1007-01
Misc : 1.25g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WD-01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X010725W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dodecane	13.268	15.0	ug/l	251852	4	12.024	838296	50.0
Dodecane, 2,6,1...	13.835	7.6	ug/l	128165	4	12.024	838296	50.0
Tridecane	14.036	16.9	ug/l	283426	4	12.024	838296	50.0
Tetradecane	14.756	15.6	ug/l	261721	4	12.024	838296	50.0
Hexadecane	15.487	7.3	ug/l	121613	4	12.024	838296	50.0