

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
 Data File : VX041283.D
 Acq On : 29 Apr 2024 18:14
 Operator : JC/MD
 Sample : P2183-04 20X
 Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1241

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\82X042224W.M
 Title : SW846 8260

Signal : TIC: VX041283.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.575	69	80	82	rBV8	6438	18495	3.17%	0.302%
2	2.392	207	214	225	rBV	62807	111731	19.15%	1.827%
3	5.391	695	706	718	rBV	70723	208694	35.76%	3.413%
4	5.550	718	732	749	rVB	123283	362077	62.05%	5.921%
5	5.824	768	777	785	rVB5	3612	10511	1.80%	0.172%
6	5.958	788	799	818	rBV	71318	194778	33.38%	3.185%
7	6.610	899	906	914	rBV3	3812	9419	1.61%	0.154%
8	6.763	922	931	951	rBV	178342	435741	74.67%	7.125%
9	8.647	1234	1240	1247	rBV	369475	583559	100.00%	9.542%
10	8.720	1247	1252	1269	rVB	111347	182177	31.22%	2.979%
11	10.055	1465	1471	1482	rBV	389417	538760	92.32%	8.810%
12	10.195	1490	1494	1501	rVB	9063	13478	2.31%	0.220%
13	10.299	1506	1511	1518	rBV	28503	42549	7.29%	0.696%
14	10.640	1563	1567	1574	rBV	7395	10732	1.84%	0.175%
15	11.079	1634	1639	1658	rBV	348100	453966	77.79%	7.423%
16	12.024	1788	1794	1802	rBV	431723	557309	95.50%	9.113%
17	12.420	1855	1859	1864	rBV	19343	24011	4.11%	0.393%
18	12.585	1882	1886	1890	rVB4	3840	6833	1.17%	0.112%
19	12.682	1898	1902	1906	rBV3	4830	5922	1.01%	0.097%
20	12.817	1920	1924	1929	rVB4	12350	17087	2.93%	0.279%
21	12.908	1929	1939	1942	rBV3	20403	52249	8.95%	0.854%
22	12.945	1942	1945	1947	rVV2	17954	22141	3.79%	0.362%
23	12.975	1947	1950	1957	rVV2	35662	52672	9.03%	0.861%
24	13.042	1957	1961	1964	rVV	32802	35356	6.06%	0.578%
25	13.091	1964	1969	1975	rVV6	5995	13197	2.26%	0.216%
26	13.176	1980	1983	1986	rBV4	6514	7337	1.26%	0.120%
27	13.268	1994	1998	2001	rBV	277213	321753	55.14%	5.261%
28	13.347	2008	2011	2014	rBV2	22398	31694	5.43%	0.518%
29	13.384	2014	2017	2020	rBV	54372	68191	11.69%	1.115%
30	13.414	2020	2022	2025	rVB3	23005	25806	4.42%	0.422%
31	13.493	2032	2035	2042	rVB5	16830	29709	5.09%	0.486%
32	13.554	2042	2045	2047	rBV3	13608	14360	2.46%	0.235%
33	13.597	2047	2052	2056	rVB6	17385	35437	6.07%	0.579%
34	13.682	2060	2066	2067	rVV	49511	67302	11.53%	1.101%
35	13.701	2067	2069	2071	rVV	60493	65900	11.29%	1.078%
36	13.737	2071	2075	2077	rVV2	96865	129035	22.11%	2.110%

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Integrator: RTE

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Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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 Title : SW846 8260

37	13.768	2077	2080	2083	rVV	84288	101060	17.32%	1.653%
38	13.798	2083	2085	2088	rVV3	39625	54811	9.39%	0.896%
39	13.835	2088	2091	2096	rVV2	92935	158845	27.22%	2.597%
40	13.908	2099	2103	2109	rVB6	32296	64526	11.06%	1.055%
41	14.036	2120	2124	2128	rBV	345906	381617	65.39%	6.240%
42	14.072	2128	2130	2132	rVV2	18461	20172	3.46%	0.330%
43	14.103	2132	2135	2137	rVV	29245	37391	6.41%	0.611%
44	14.133	2138	2140	2143	rVV2	25687	31263	5.36%	0.511%
45	14.164	2143	2145	2147	rVV2	13716	17490	3.00%	0.286%
46	14.213	2151	2153	2159	rVB4	20459	26909	4.61%	0.440%
47	14.408	2181	2185	2187	rBV2	22469	30653	5.25%	0.501%
48	14.438	2187	2190	2193	rVV3	44102	57899	9.92%	0.947%
49	14.469	2193	2195	2197	rVV	20021	21457	3.68%	0.351%
50	14.499	2197	2200	2207	rVV3	32712	66152	11.34%	1.082%
51	14.560	2207	2210	2215	rVB3	16627	29343	5.03%	0.480%
52	14.609	2215	2218	2226	rVB3	22611	32024	5.49%	0.524%
53	14.755	2238	2242	2245	rBV	65703	72597	12.44%	1.187%
54	14.792	2245	2248	2252	rVB4	18529	21825	3.74%	0.357%
55	14.841	2253	2256	2261	rVB6	7446	11126	1.91%	0.182%
56	14.938	2268	2272	2284	rVB6	9497	27395	4.69%	0.448%
57	15.182	2308	2312	2314	rBV5	5082	8105	1.39%	0.133%
58	15.213	2314	2317	2324	rVB6	8508	13530	2.32%	0.221%
59	15.273	2324	2327	2331	rBV5	4628	6805	1.17%	0.111%
60	15.487	2358	2362	2369	rBV4	10777	20252	3.47%	0.331%
61	15.560	2369	2374	2380	rBV2	27466	42338	7.26%	0.692%

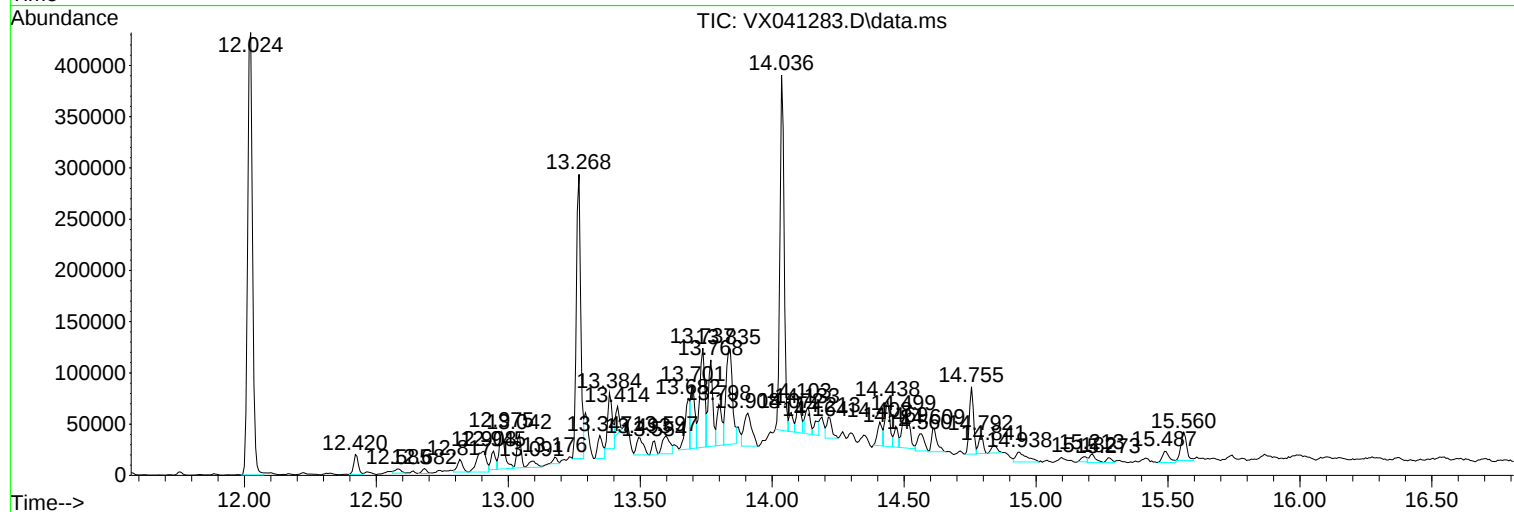
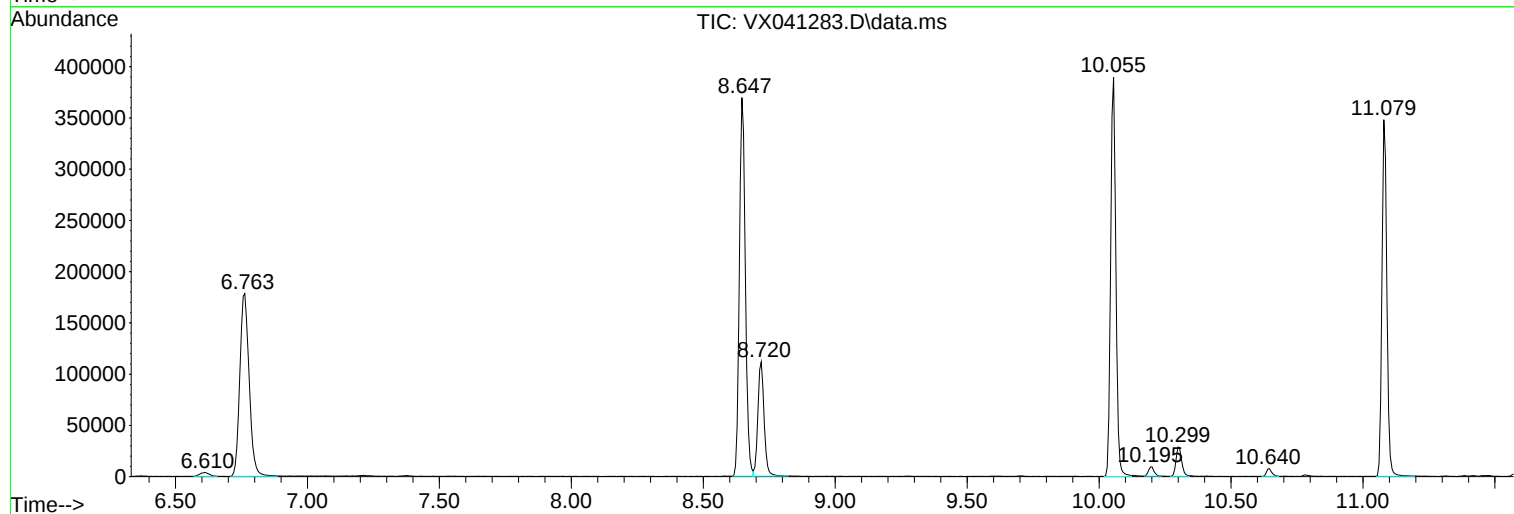
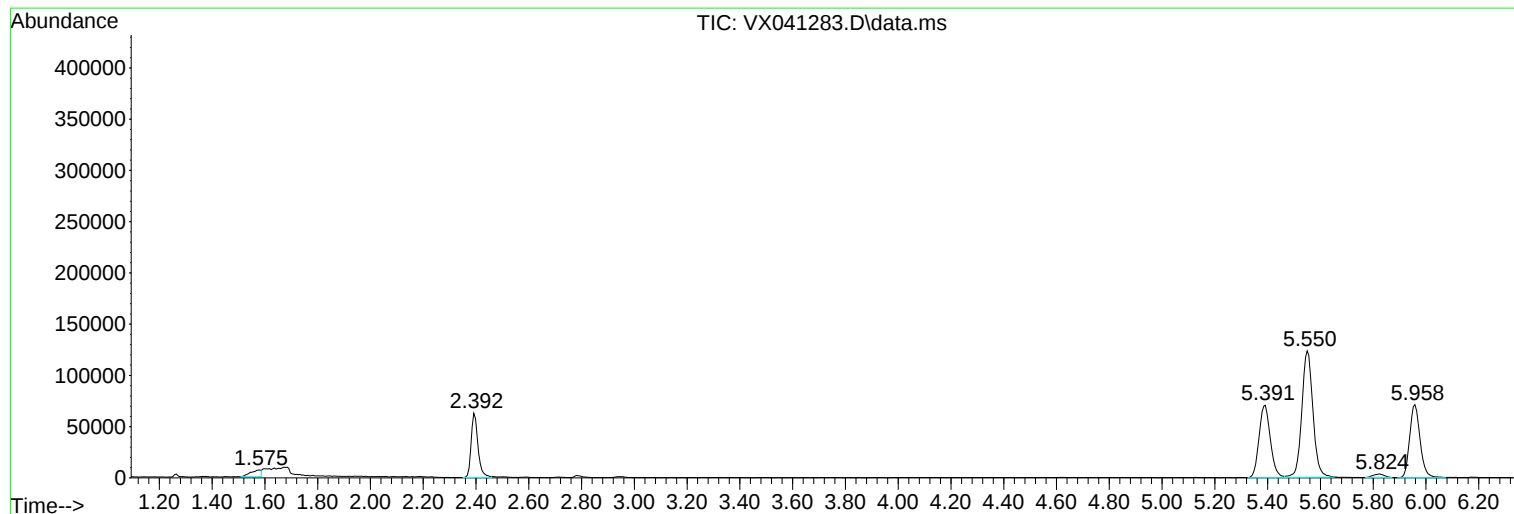
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Instrument :
MSVOA_X
ClientSampleId :
1241

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

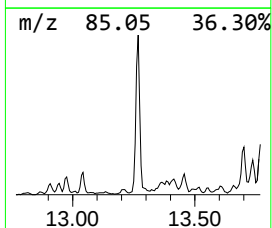
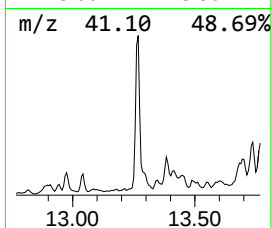
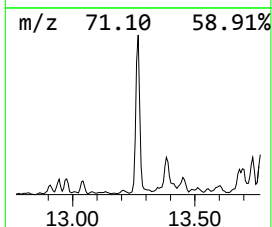
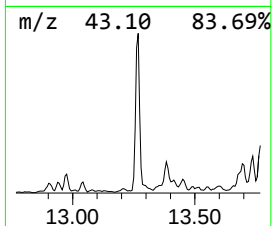
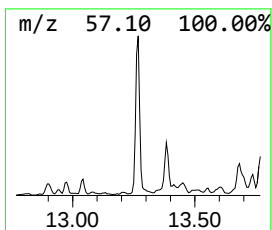
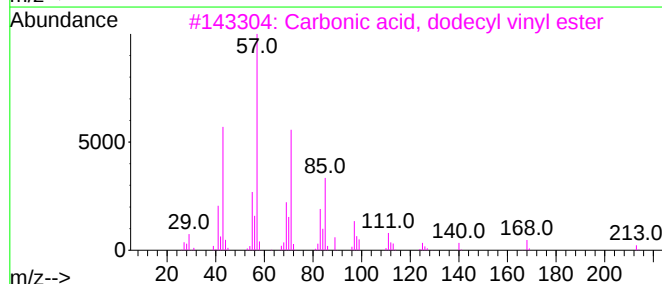
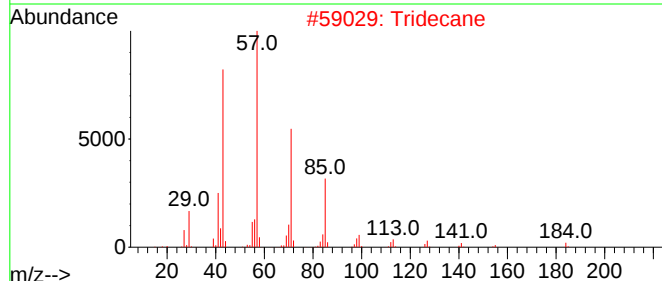
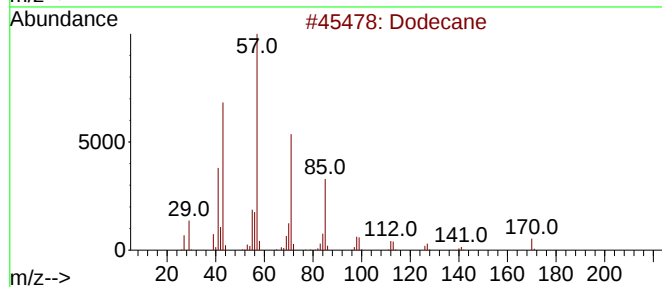
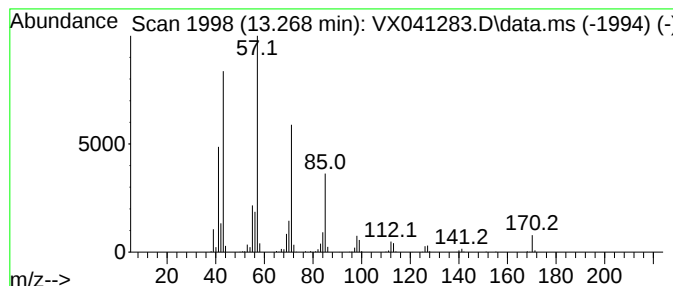
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 1 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	28.87 ug/l	321753	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, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	90
4			Undecane	156	C11H24	001120-21-4	86
5			Hexadecane	226	C16H34	000544-76-3	86



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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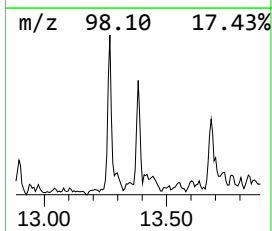
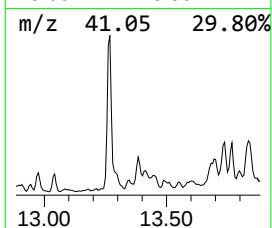
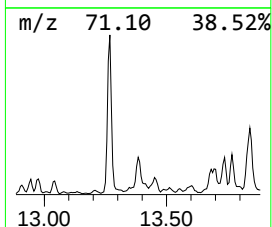
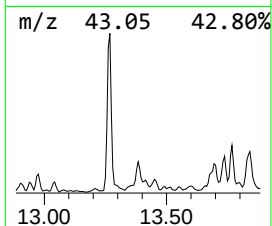
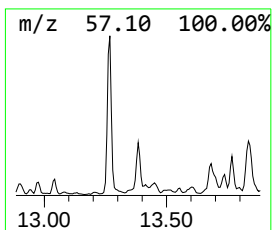
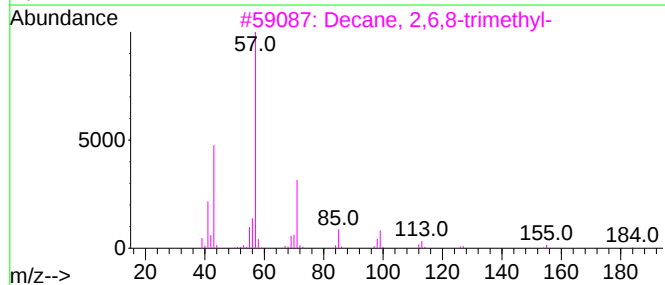
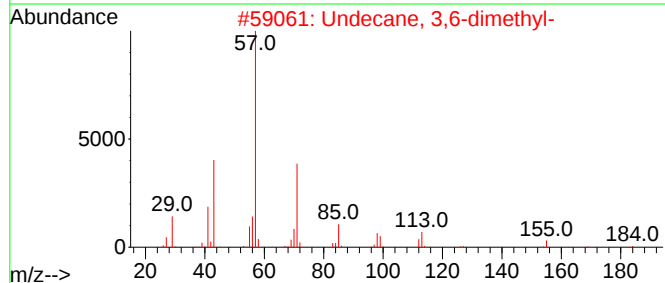
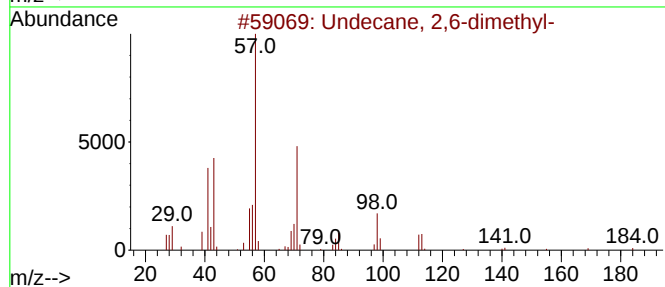
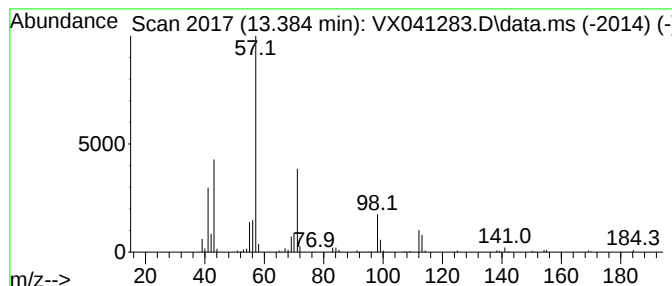
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 2 Undecane, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.384	6.12 ug/l	68191	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, 3,6-dimethyl-	184	C13H28	017301-28-9	87		
3	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	72		
4	Dodecane, 6-methyl-	184	C13H28	006044-71-9	64		
5	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	59		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041283.D
Acq On : 29 Apr 2024 18:14
Operator : JC/MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

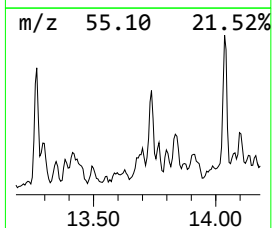
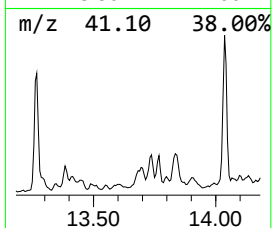
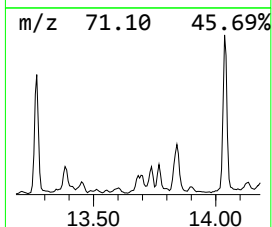
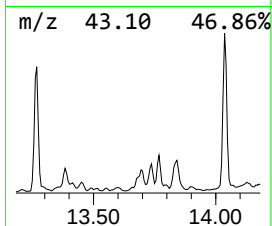
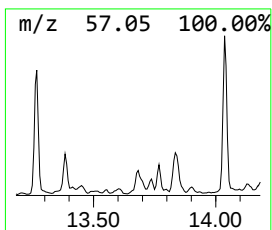
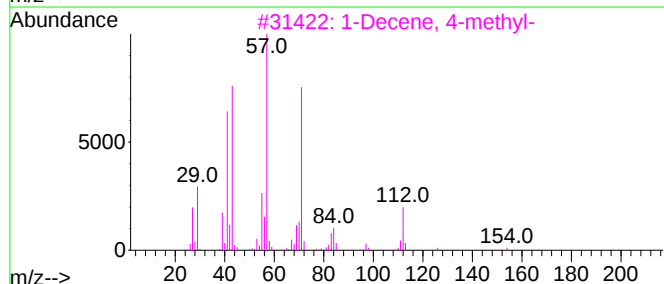
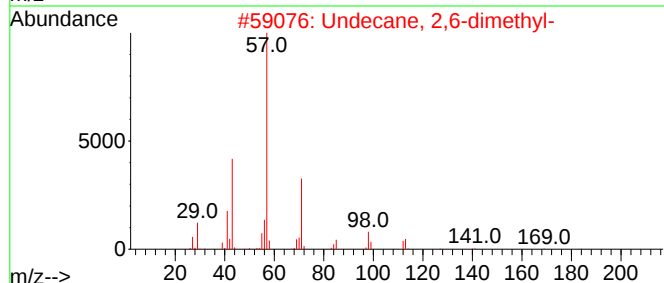
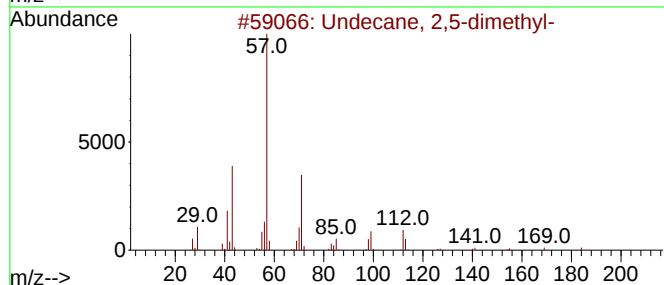
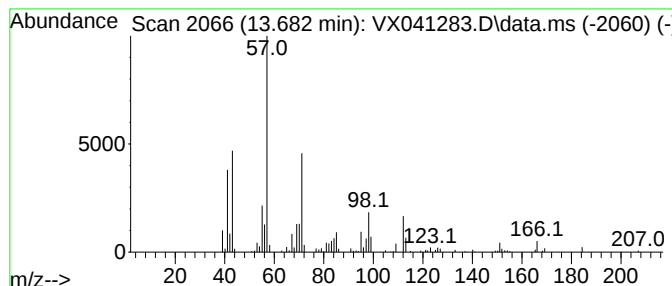
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 3 Undecane, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.682	6.04 ug/l	67302	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	64
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	64
3			1-Decene, 4-methyl-	154	C11H22	013151-29-6	50
4			Tridecane	184	C13H28	000629-50-5	49
5			Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	49



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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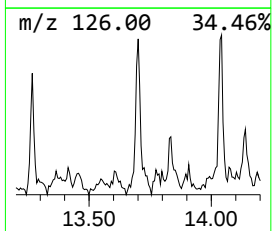
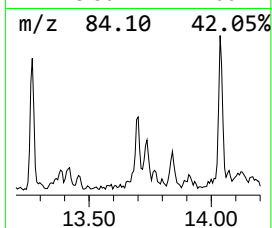
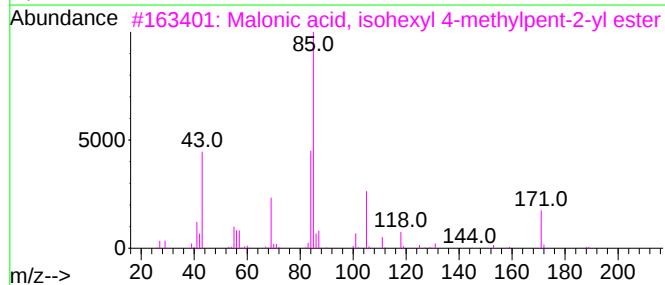
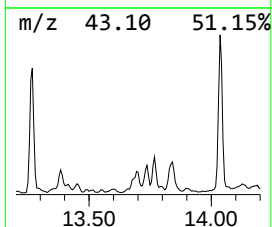
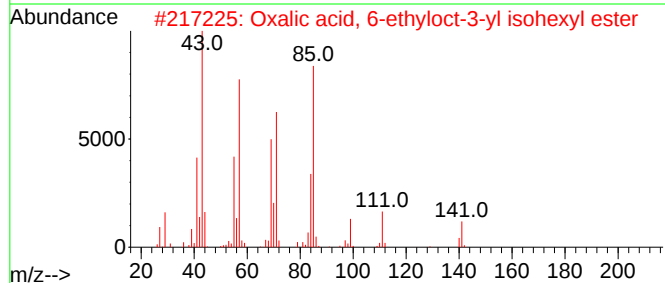
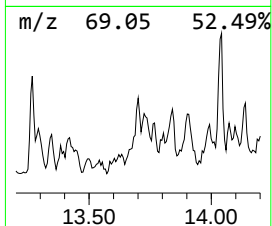
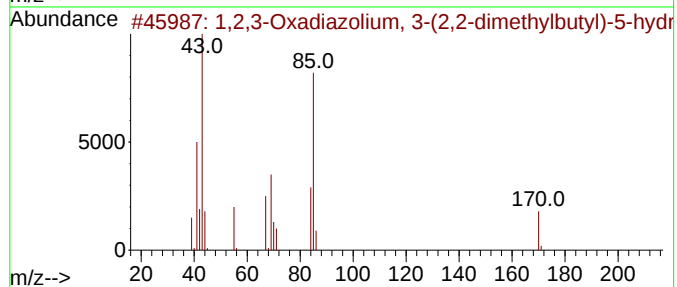
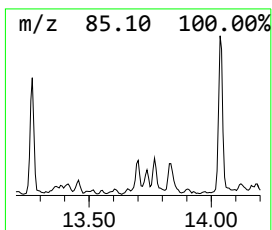
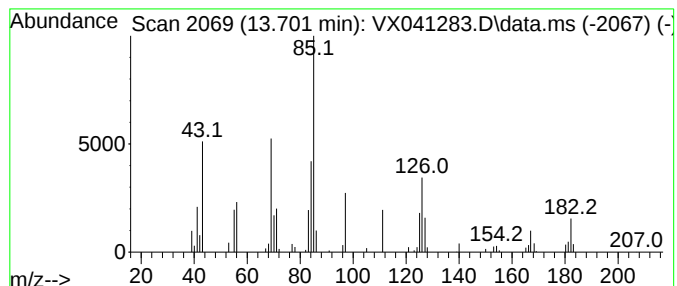
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown13.701 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.701	5.91 ug/l	65900	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,3-Oxadiazolium, 3-(2,2-dimet...	170	C8H14N2O2	054460-94-5	43
2			Oxalic acid, 6-ethyloct-3-yl iso...	314	C18H34O4	1000309-34-3	40
3			Malonic acid, isohexyl 4-methylp...	272	C15H28O4	1000349-33-4	38
4			2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	37
5			O-Hexylhydroxylamine	117	C6H15NO	1000426-05-8	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041283.D
Acq On : 29 Apr 2024 18:14
Operator : JC/MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

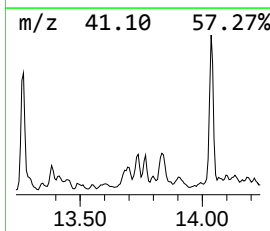
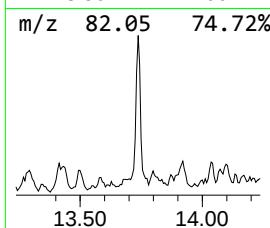
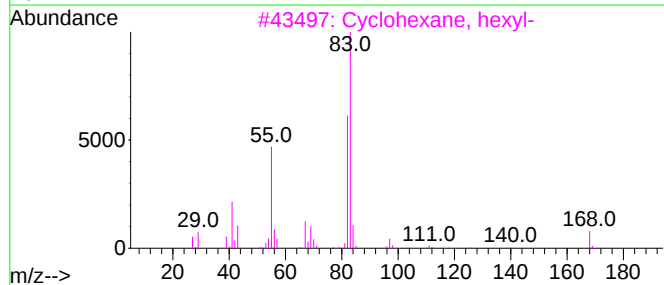
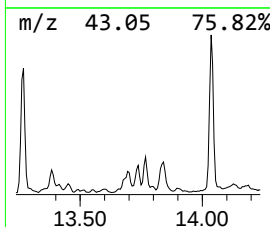
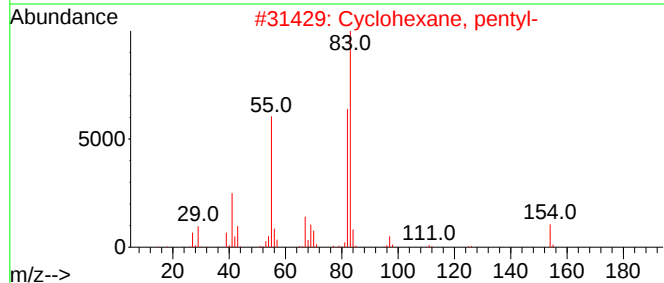
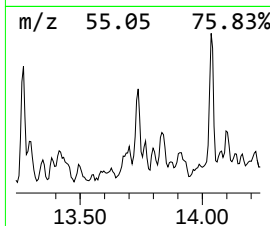
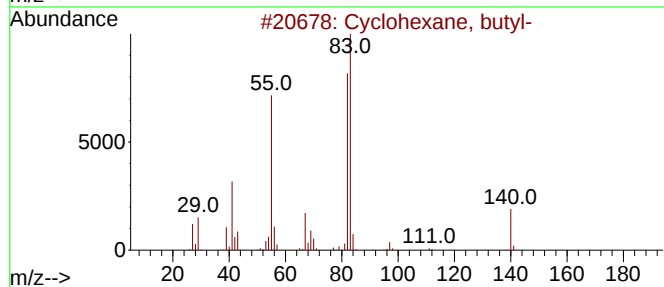
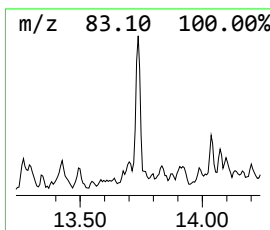
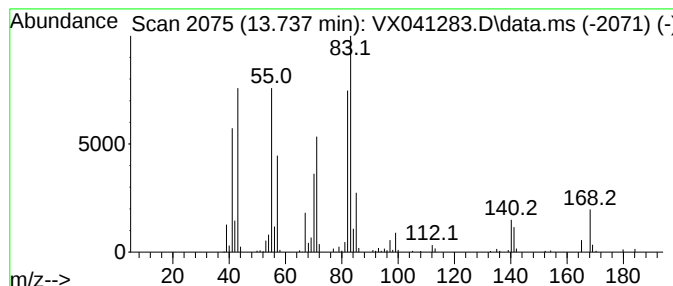
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.737	11.58 ug/l	129035	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, butyl-	140	C10H20	001678-93-9	91
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	60
3			Cyclohexane, hexyl-	168	C12H24	004292-75-5	58
4			Succinic acid, 2-methylpent-3-yl...	284	C16H28O4	1000391-11-2	50
5			Dodecane, 4-methyl-	184	C13H28	006117-97-1	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041283.D
Acq On : 29 Apr 2024 18:14
Operator : JC/MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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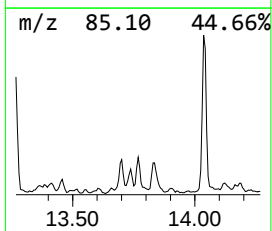
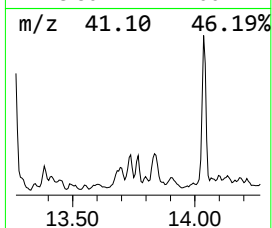
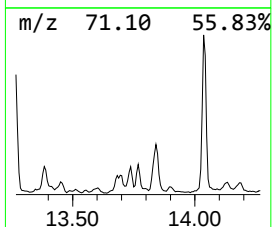
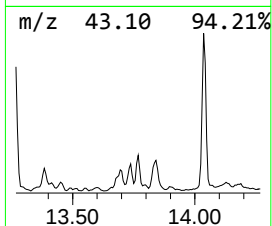
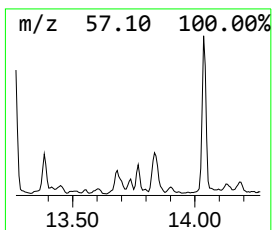
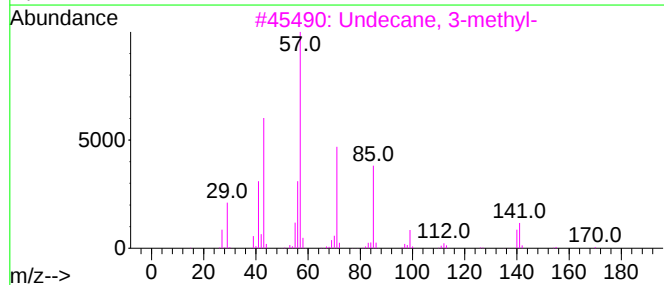
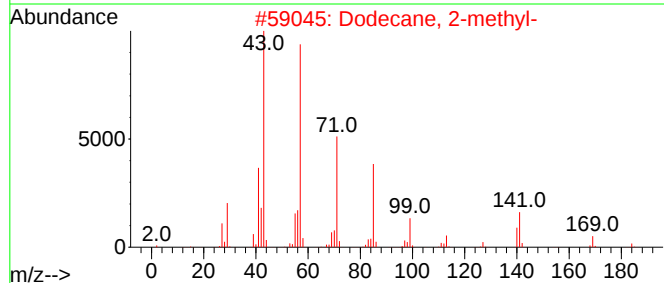
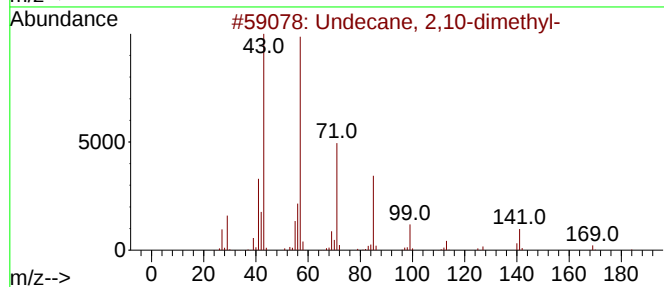
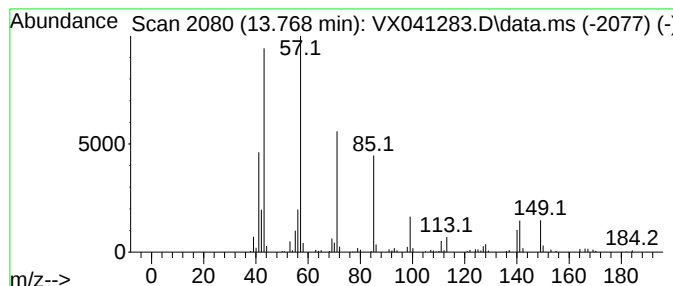
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Quant Title : SW846 8260

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

Peak Number 6 Undecane, 2,10-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.768	9.07 ug/l	101060	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	90
2			Dodecane, 2-methyl-	184	C13H28	001560-97-0	86
3			Undecane, 3-methyl-	170	C12H26	001002-43-3	70
4			Undecane, 2-methyl-	170	C12H26	007045-71-8	64
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041283.D
Acq On : 29 Apr 2024 18:14
Operator : JC/MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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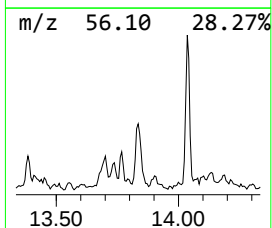
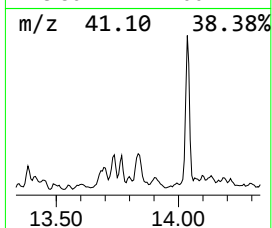
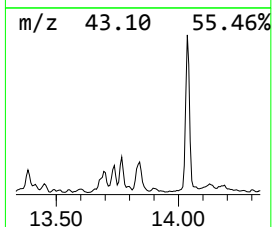
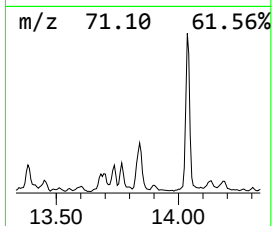
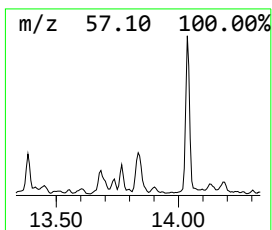
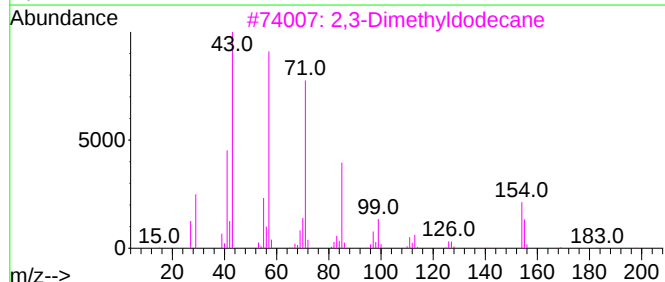
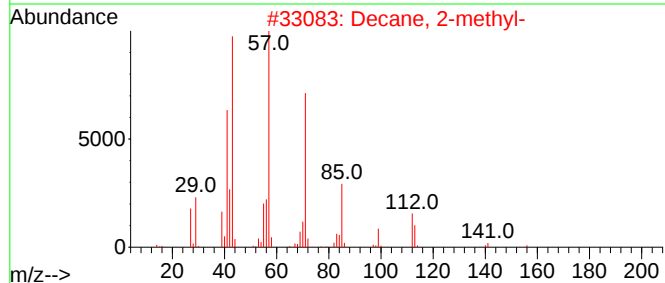
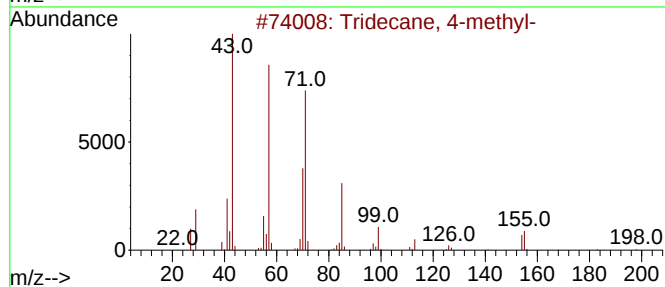
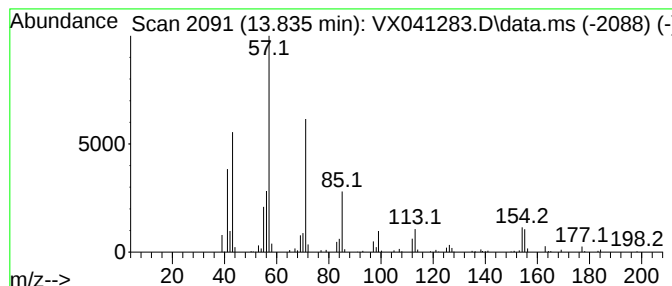
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Quant Title : SW846 8260

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

Peak Number 7 Tridecane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.835	14.25 ug/l	158845	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 4-methyl-	198	C14H30	026730-12-1	90
2			Decane, 2-methyl-	156	C11H24	006975-98-0	83
3			2,3-Dimethyldodecane	198	C14H30	006117-98-2	64
4			Decane, 3-methyl-	156	C11H24	013151-34-3	64
5			Dodecane, 3-methyl-	184	C13H28	017312-57-1	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041283.D
Acq On : 29 Apr 2024 18:14
Operator : JC/MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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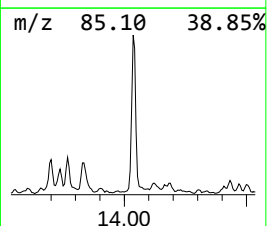
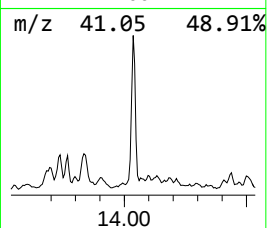
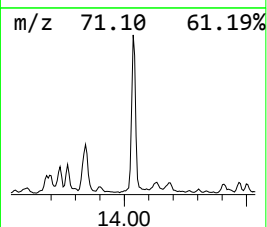
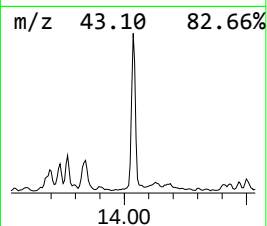
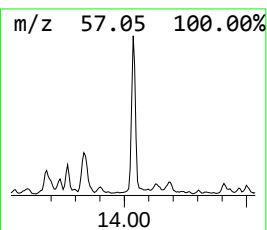
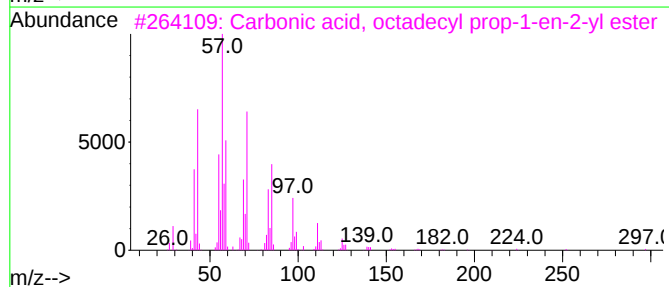
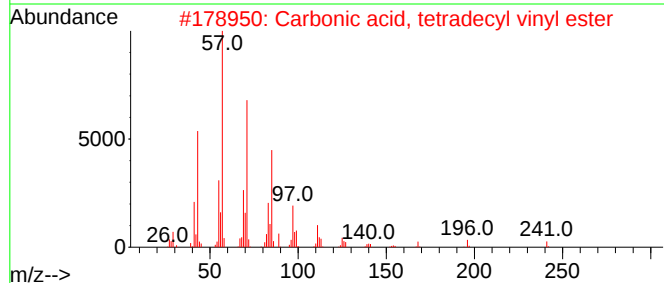
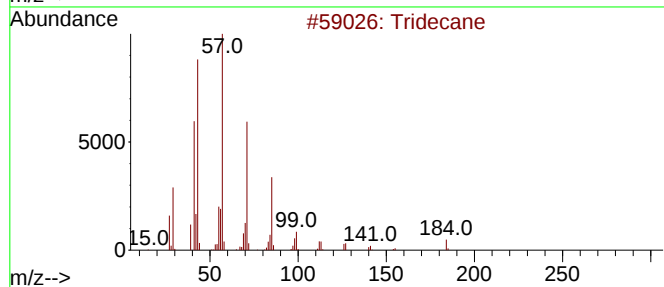
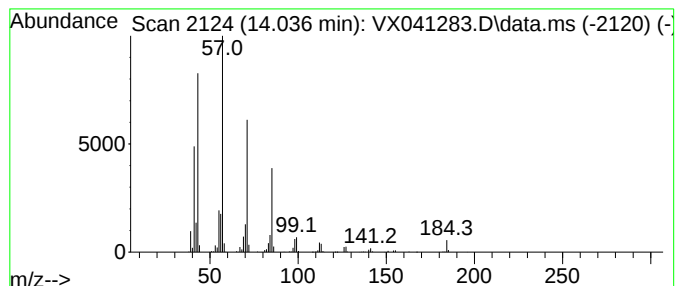
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.036	34.24 ug/l	381617	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	97
2			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	90
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
4			Hexadecane	226	C16H34	000544-76-3	87
5			Pentadecane	212	C15H32	000629-62-9	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041283.D
Acq On : 29 Apr 2024 18:14
Operator : JC/MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

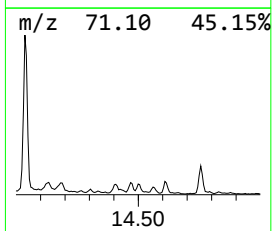
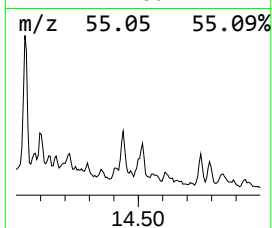
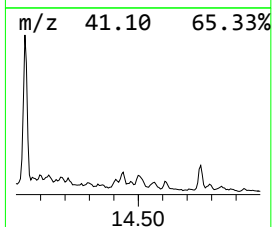
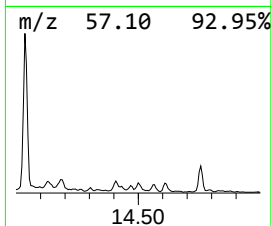
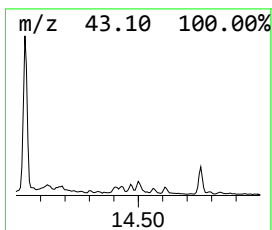
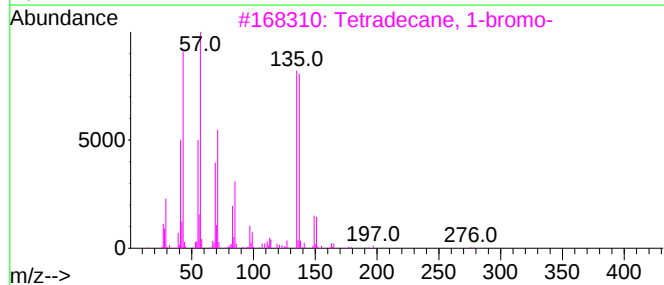
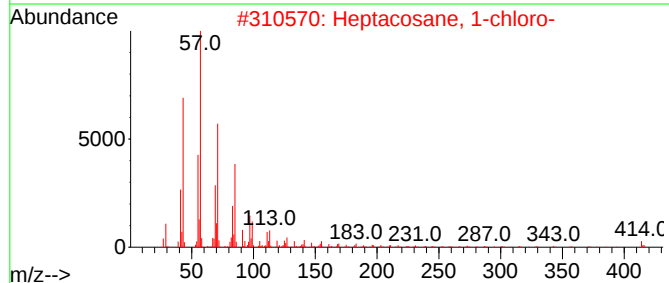
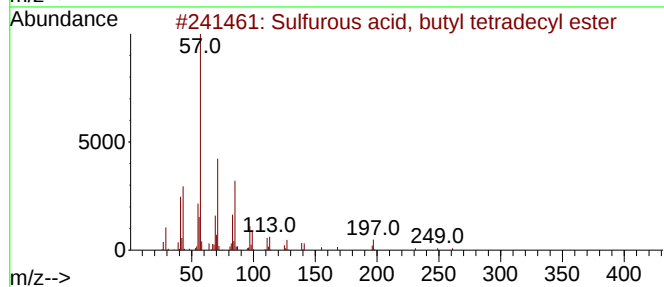
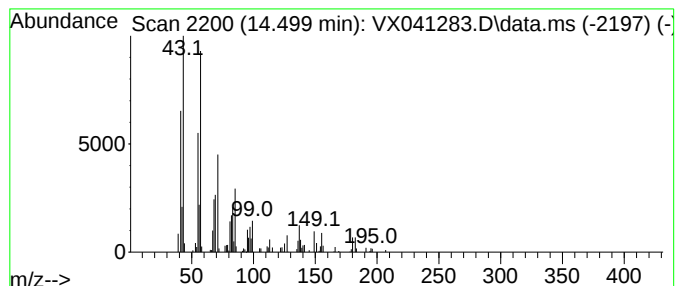
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Quant Title : SW846 8260

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

Peak Number 9 Sulfurous acid, butyl tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.499	5.93 ug/l	66152	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	58
2			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	53
3			Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	53
4			Oxalic acid, allyl decyl ester	270	C15H26O4	1010309-23-8	52
5			Dodecane, 1-bromo-	248	C12H25Br	000143-15-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041283.D
Acq On : 29 Apr 2024 18:14
Operator : JC/MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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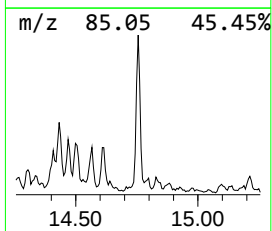
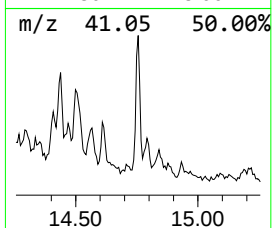
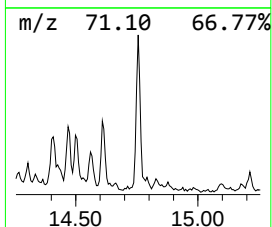
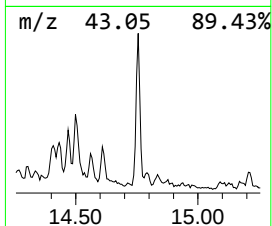
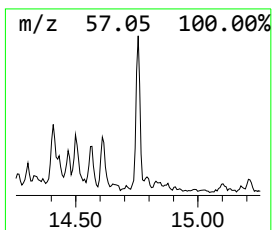
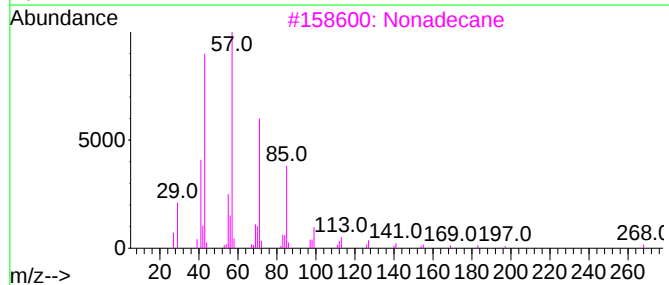
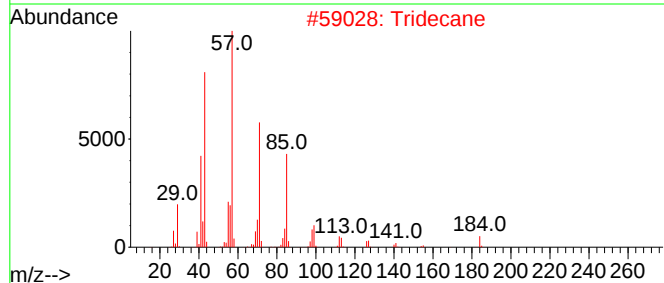
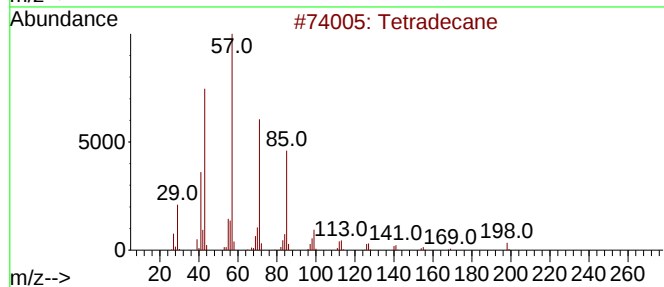
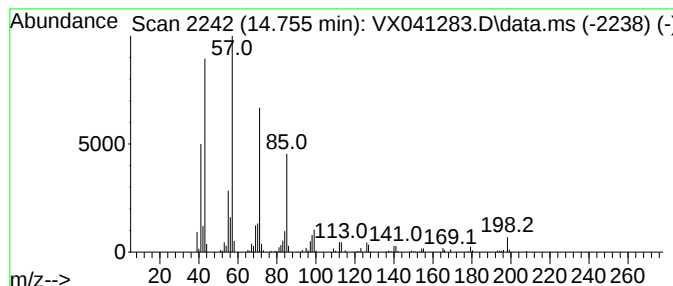
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Quant Title : SW846 8260

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

Peak Number 10 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.755	6.51 ug/l	72597	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	98
2		Tridecane	184	C13H28	000629-50-5	91
3		Nonadecane	268	C19H40	000629-92-5	87
4		Hexadecane	226	C16H34	000544-76-3	87
5		Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041283.D
Acq On : 29 Apr 2024 18:14
Operator : JC/MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.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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Undecane, 2,6-d...	13.384	6.1	ug/l	68191	4	12.024	557309	50.0
Undecane, 2,5-d...	13.682	6.0	ug/l	67302	4	12.024	557309	50.0
unknown13.701	13.701	5.9	ug/l	65900	4	12.024	557309	50.0
Cyclohexane, bu...	13.737	11.6	ug/l	129035	4	12.024	557309	50.0
Undecane, 2,10-...	13.768	9.1	ug/l	101060	4	12.024	557309	50.0
Tridecane, 4-me...	13.835	14.3	ug/l	158845	4	12.024	557309	50.0
Tridecane	14.036	34.2	ug/l	381617	4	12.024	557309	50.0
Sulfurous acid,...	14.499	5.9	ug/l	66152	4	12.024	557309	50.0
Tetradecane	14.755	6.5	ug/l	72597	4	12.024	557309	50.0