

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
 Data File : VX032212.D
 Acq On : 19 Oct 2022 17:00
 Operator : JC/MD
 Sample : N5114-02
 Misc : 1.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FMC-0083

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\82X101922W.M
 Title : SW846 8260

Signal : TIC: VX032212.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.947	296	305	314	rBV	9448	25052	1.59%	0.157%
2	5.391	693	706	720	rBV	127895	377732	24.01%	2.375%
3	5.544	720	731	747	rVB	201042	569268	36.19%	3.579%
4	5.958	785	799	815	rBV	150314	401239	25.51%	2.523%
5	6.757	919	930	948	rBV	292145	694927	44.18%	4.369%
6	8.647	1232	1240	1248	rBV	740109	1156359	73.51%	7.270%
7	8.720	1248	1252	1258	rVB	27716	41925	2.67%	0.264%
8	10.055	1465	1471	1482	rVB	578576	788012	50.10%	4.954%
9	11.085	1634	1640	1651	rBV	553533	809576	51.47%	5.090%
10	11.476	1698	1704	1710	rVB2	16387	25370	1.61%	0.159%
11	12.024	1788	1794	1800	rBV	607914	805347	51.20%	5.063%
12	12.421	1855	1859	1864	rBV	41375	51963	3.30%	0.327%
13	12.902	1929	1938	1942	rBV3	19520	46894	2.98%	0.295%
14	12.975	1947	1950	1956	rVB2	30415	38337	2.44%	0.241%
15	13.042	1957	1961	1965	rBV	28568	31858	2.03%	0.200%
16	13.268	1994	1998	2001	rBV	356824	379278	24.11%	2.384%
17	13.298	2001	2003	2008	rVB3	35388	40196	2.56%	0.253%
18	13.347	2008	2011	2013	rBV3	13208	17655	1.12%	0.111%
19	13.384	2013	2017	2020	rBV	74510	87479	5.56%	0.550%
20	13.500	2032	2036	2037	rBV3	14849	20949	1.33%	0.132%
21	13.585	2047	2050	2052	rBV4	17007	23114	1.47%	0.145%
22	13.683	2060	2066	2067	rBV2	86374	111780	7.11%	0.703%
23	13.701	2067	2069	2071	rVV	81957	85531	5.44%	0.538%
24	13.737	2071	2075	2078	rVV3	128101	166778	10.60%	1.049%
25	13.768	2078	2080	2083	rVB	131708	125302	7.97%	0.788%
26	13.798	2083	2085	2087	rBV2	19769	18078	1.15%	0.114%
27	13.841	2087	2092	2099	rVB2	194382	353833	22.49%	2.225%
28	13.908	2099	2103	2105	rBV2	39516	60121	3.82%	0.378%
29	14.042	2116	2125	2128	rBV	1407414	1572968	100.00%	9.889%
30	14.073	2128	2130	2133	rVV3	68465	100948	6.42%	0.635%
31	14.103	2133	2135	2137	rVV2	71001	92184	5.86%	0.580%
32	14.134	2138	2140	2143	rVV2	77163	102480	6.52%	0.644%
33	14.170	2143	2146	2147	rVV2	48866	64857	4.12%	0.408%
34	14.189	2147	2149	2151	rVV	88744	95606	6.08%	0.601%
35	14.225	2151	2155	2161	rVB3	102962	201253	12.79%	1.265%
36	14.304	2166	2168	2171	rBV2	24445	32672	2.08%	0.205%

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Integrator: RTE

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Peak Location: TOP

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37	14.371	2177	2179	2181	rBV2	27883	31029	1.97%	0.195%
38	14.408	2181	2185	2187	rVV2	119943	162249	10.31%	1.020%
39	14.439	2187	2190	2193	rVV2	171506	219377	13.95%	1.379%
40	14.475	2193	2196	2198	rVV2	174082	234245	14.89%	1.473%
41	14.506	2198	2201	2206	rVV2	228249	348742	22.17%	2.192%
42	14.567	2206	2211	2215	rVB3	155331	227130	14.44%	1.428%
43	14.615	2215	2219	2225	rBV2	345720	506249	32.18%	3.183%
44	14.670	2225	2228	2233	rVB5	93062	147331	9.37%	0.926%
45	14.756	2233	2242	2246	rBV	1240966	1479504	94.06%	9.301%
46	14.792	2246	2248	2251	rVV3	108740	144920	9.21%	0.911%
47	14.847	2254	2257	2260	rVV3	143458	214105	13.61%	1.346%
48	14.908	2264	2267	2277	rVB5	55990	128674	8.18%	0.809%
49	15.048	2286	2290	2293	rVB5	38319	63975	4.07%	0.402%
50	15.103	2294	2299	2302	rBV3	75742	141497	9.00%	0.890%
51	15.182	2308	2312	2315	rBV2	220613	343563	21.84%	2.160%
52	15.213	2315	2317	2320	rVV	232780	254449	16.18%	1.600%
53	15.280	2324	2328	2331	rVB2	130208	174390	11.09%	1.096%
54	15.377	2340	2344	2350	rBV4	96789	147434	9.37%	0.927%
55	15.493	2357	2363	2367	rBV2	446298	677610	43.08%	4.260%
56	15.566	2373	2375	2378	rBV3	32025	30720	1.95%	0.193%
57	15.615	2379	2383	2386	rBV2	101334	138797	8.82%	0.873%
58	15.847	2418	2421	2424	rBV5	22835	35108	2.23%	0.221%
59	15.993	2441	2445	2448	rBV6	33030	61271	3.90%	0.385%
60	16.091	2456	2461	2468	rBV3	57748	136107	8.65%	0.856%
61	16.377	2501	2508	2513	rVB2	62659	150002	9.54%	0.943%
62	16.597	2541	2544	2549	rVB3	30448	49752	3.16%	0.313%
63	16.658	2550	2554	2559	rVB2	24992	41000	2.61%	0.258%

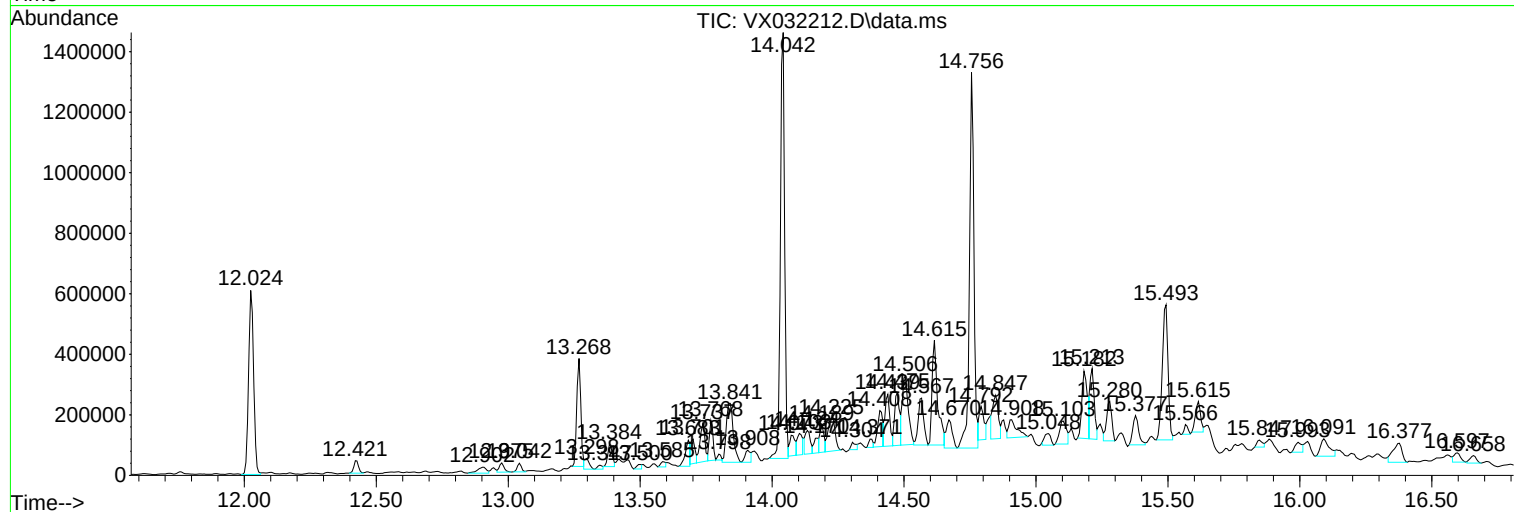
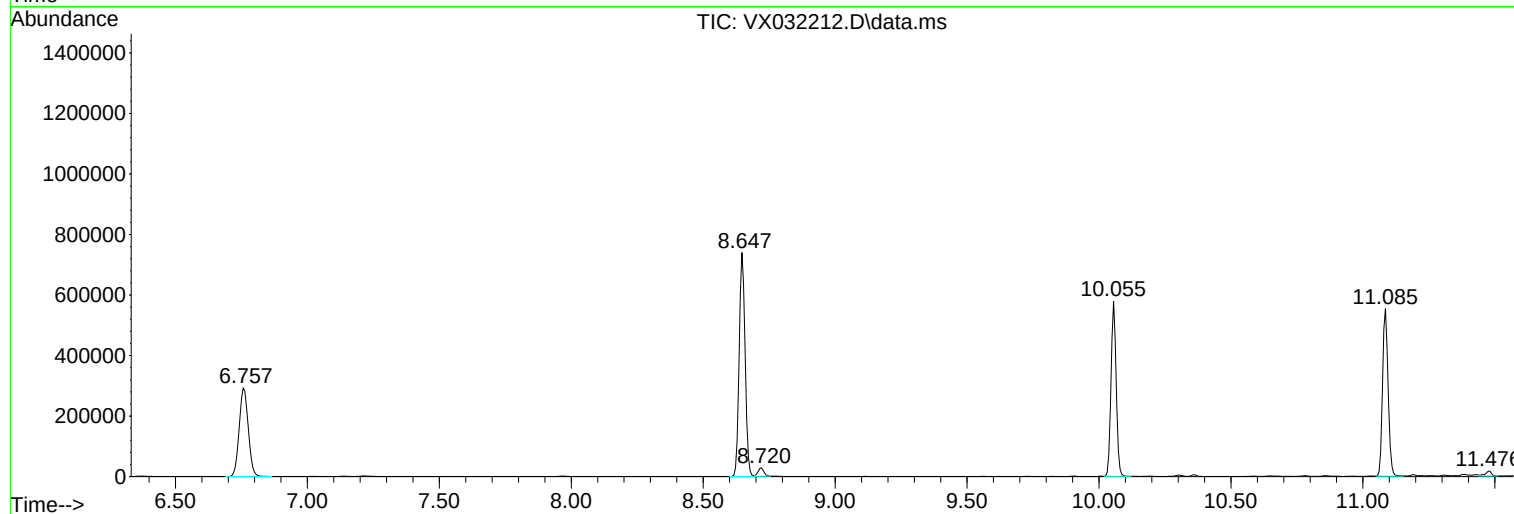
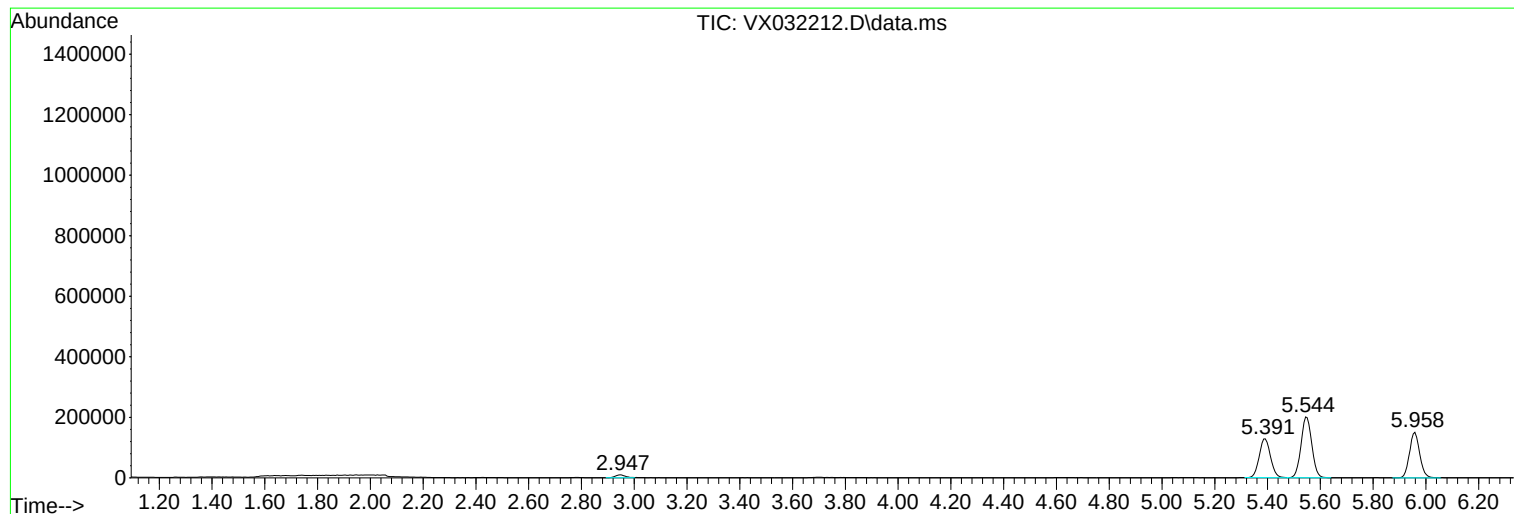
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Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.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 :
FMC-0083

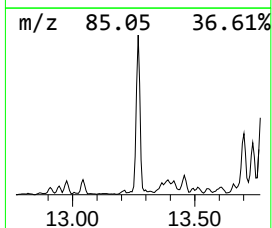
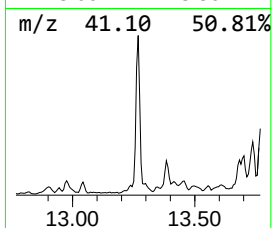
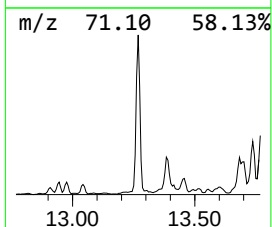
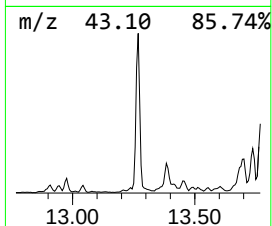
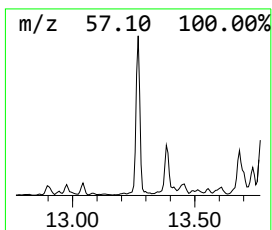
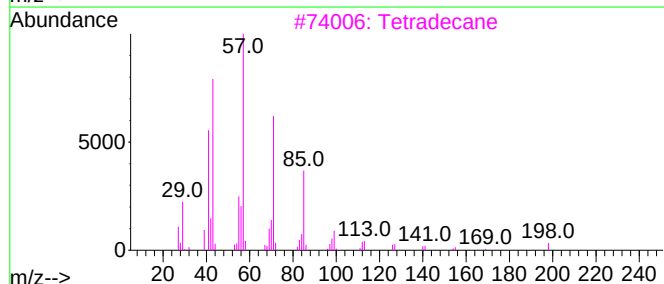
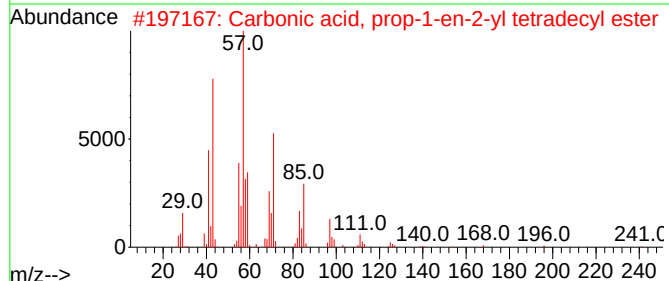
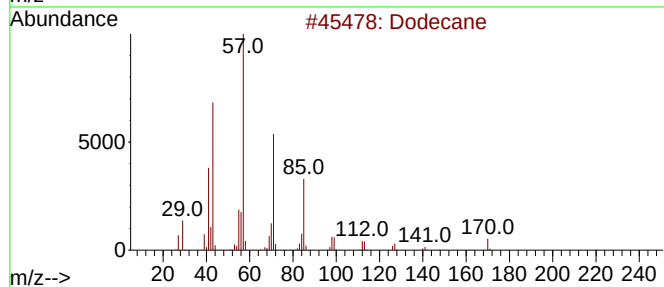
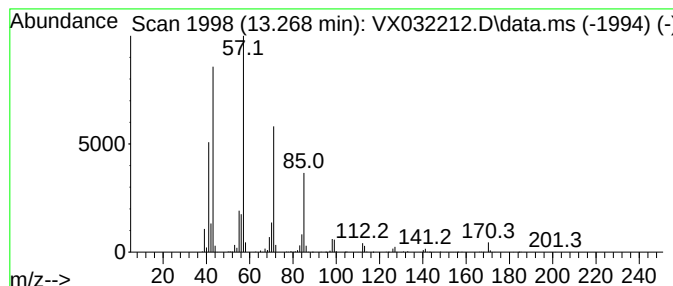
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 1 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	23.55 ug/l	379278	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	90
3			Tetradecane	198	C14H30	000629-59-4	90
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	90
5			Tridecane	184	C13H28	000629-50-5	90



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

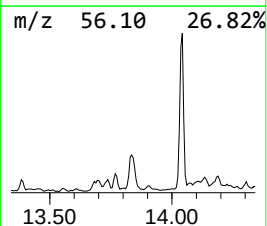
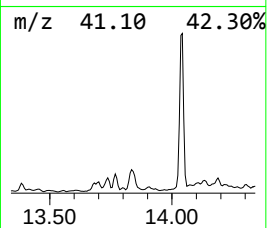
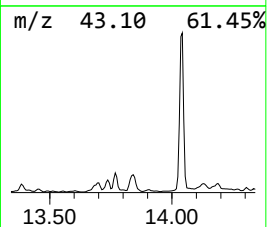
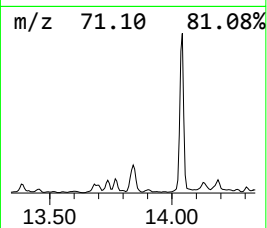
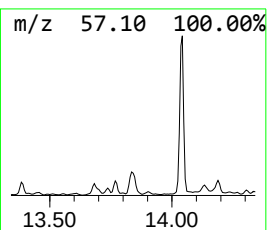
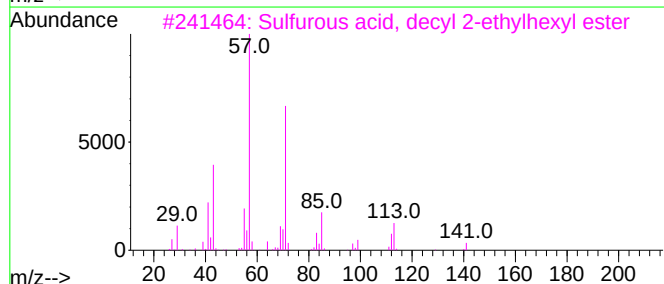
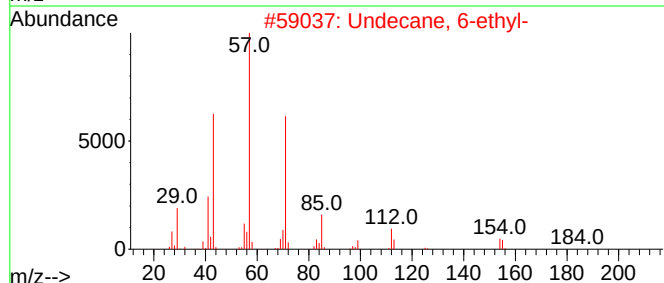
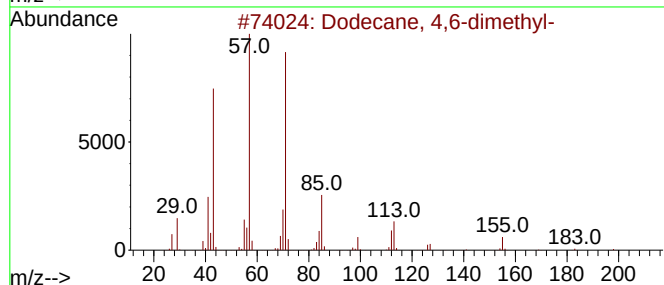
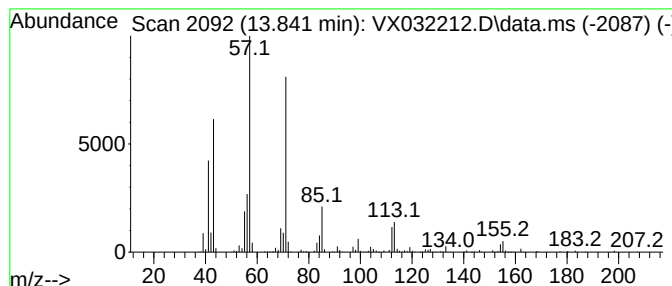
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 2 Dodecane, 4,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	21.97 ug/l	353833	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	91
2			Undecane, 6-ethyl-	184	C13H28	017312-60-6	72
3			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	72
4			Decane, 2-methyl-	156	C11H24	006975-98-0	58
5			Oxalic acid, hexyl neopentyl ester	244	C13H24O4	1000309-73-1	50



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

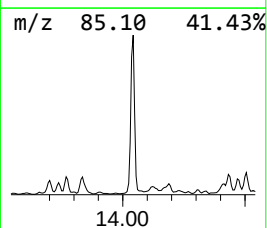
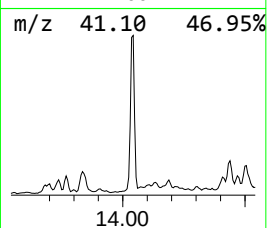
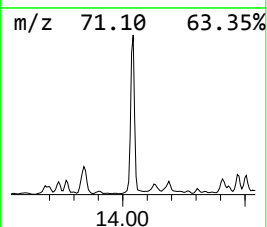
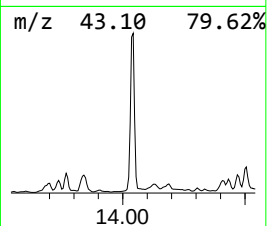
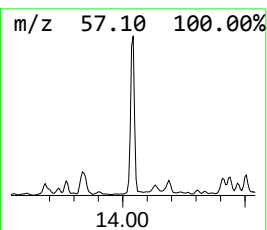
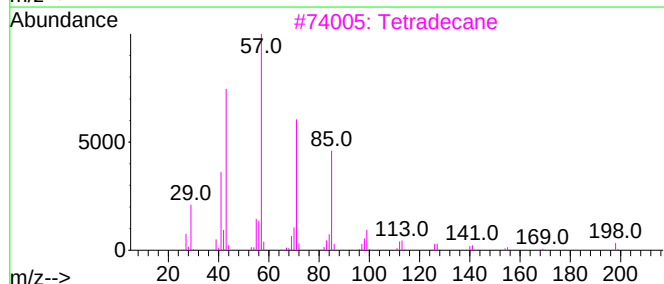
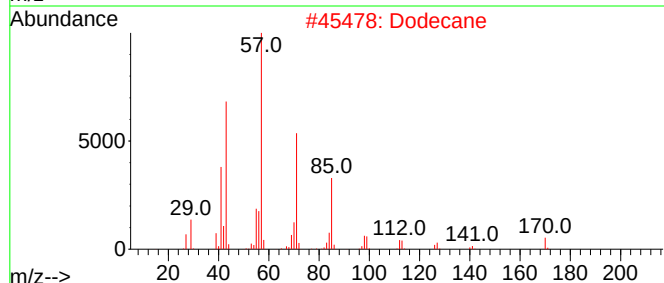
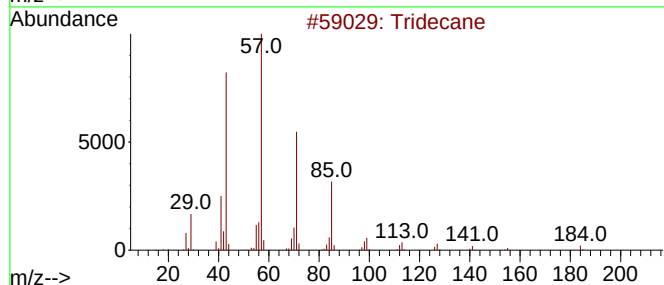
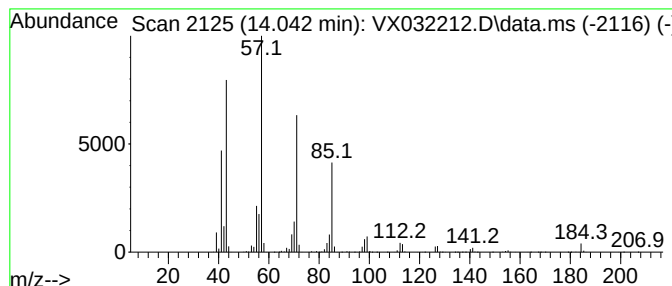
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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.
14.042	97.66 ug/l	1572970	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	97
2			Dodecane	170	C12H26	000112-40-3	90
3			Tetradecane	198	C14H30	000629-59-4	90
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	90
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90



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Instrument :
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ClientSampleId :
FMC-0083

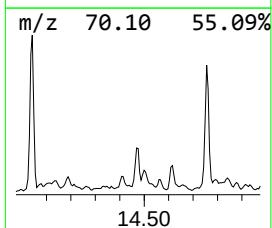
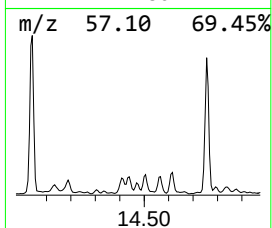
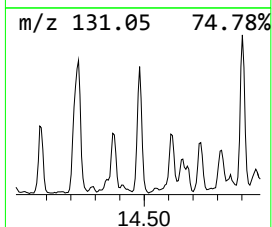
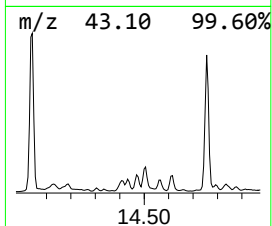
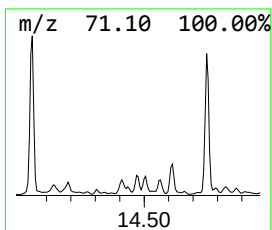
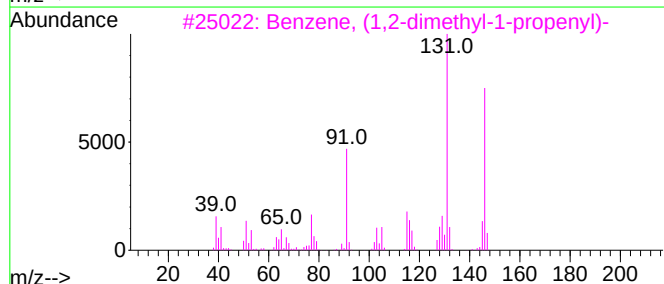
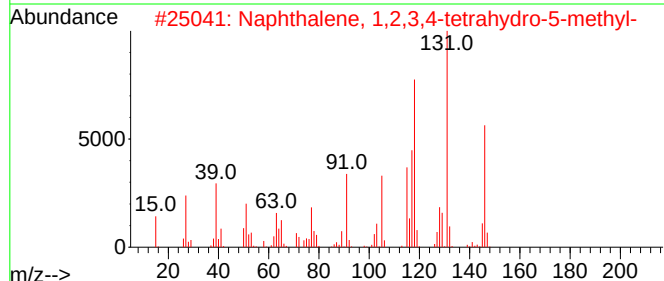
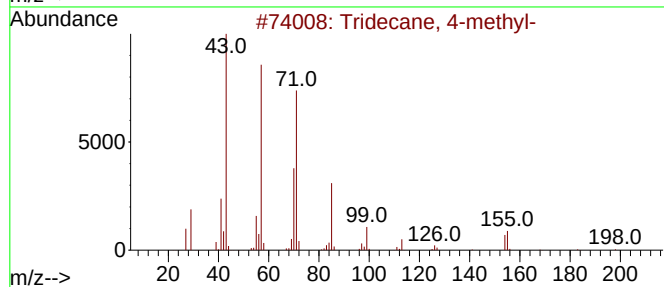
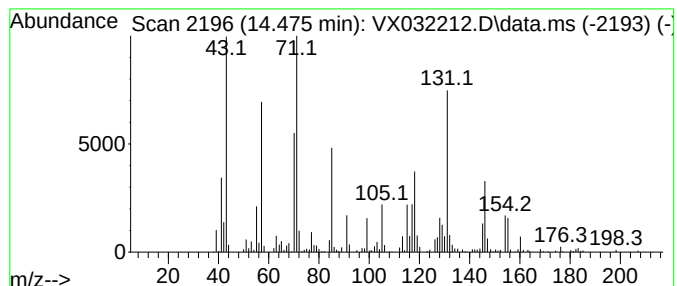
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 4 Tridecane, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.475	14.54 ug/l	234245	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 4-methyl-	198	C14H30	026730-12-1	55
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	46
3			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	38
4			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	38
5			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032212.D
Acq On : 19 Oct 2022 17:00
Operator : JC/MD
Sample : N5114-02
Misc : 1.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

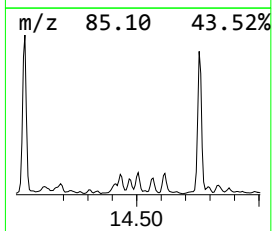
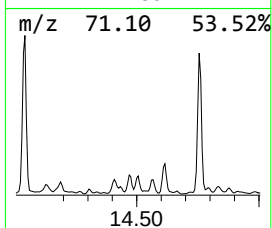
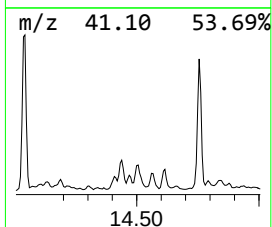
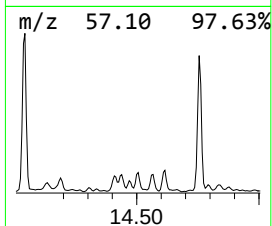
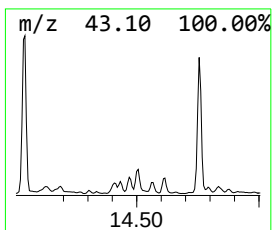
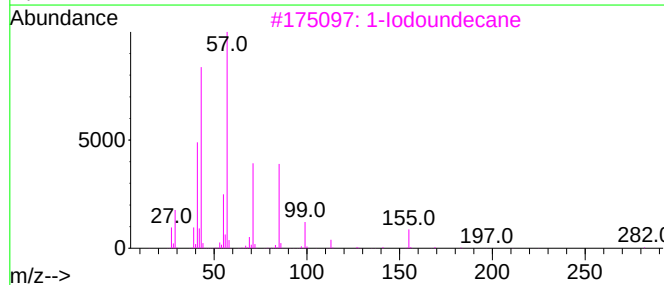
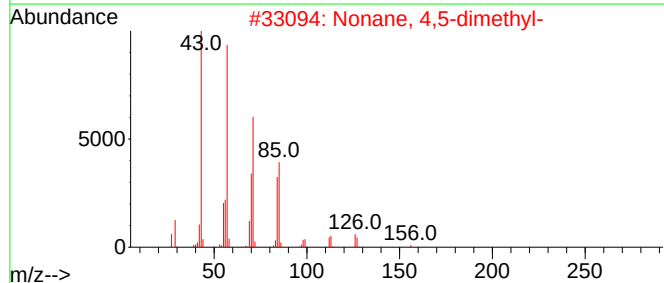
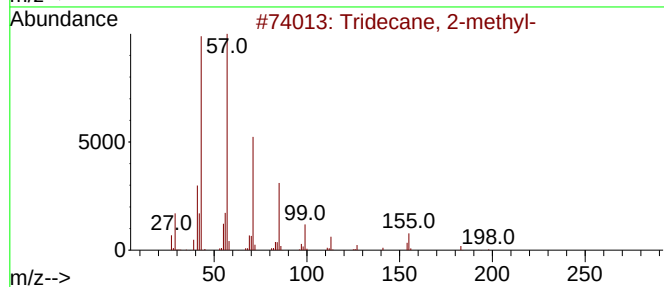
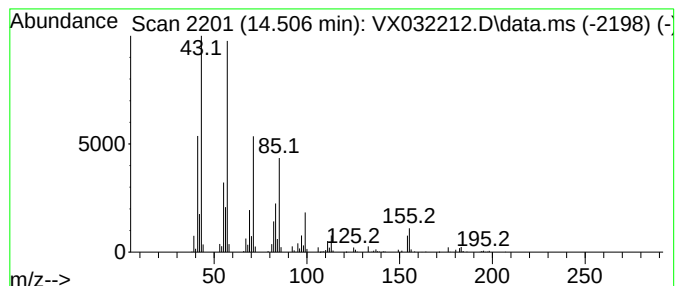
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Quant Title : SW846 8260

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

Peak Number 5 Tridecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.506	21.65 ug/l	348742	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 2-methyl-	198	C14H30	001560-96-9	93
2			Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	64
3			1-Iodoundecane	282	C11H23I	004282-44-4	64
4			Eicosane	282	C20H42	000112-95-8	59
5			Eicosane, 10-methyl-	296	C21H44	054833-23-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032212.D
Acq On : 19 Oct 2022 17:00
Operator : JC/MD
Sample : N5114-02
Misc : 1.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

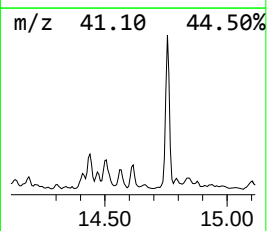
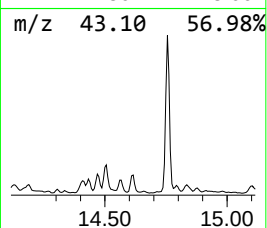
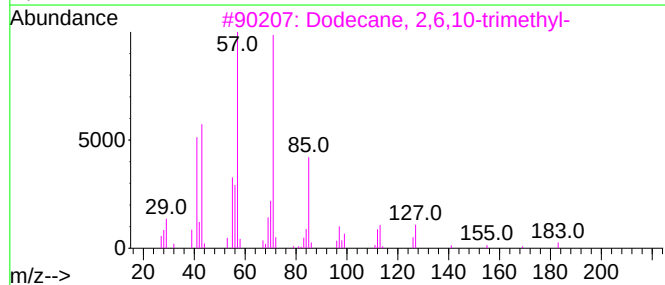
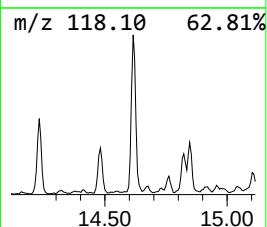
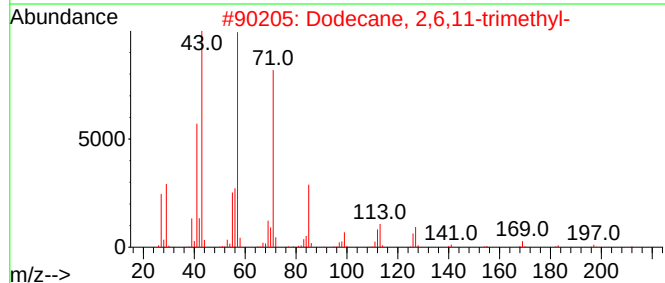
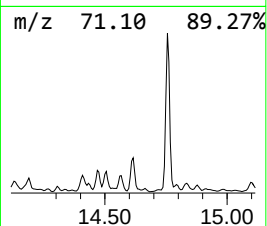
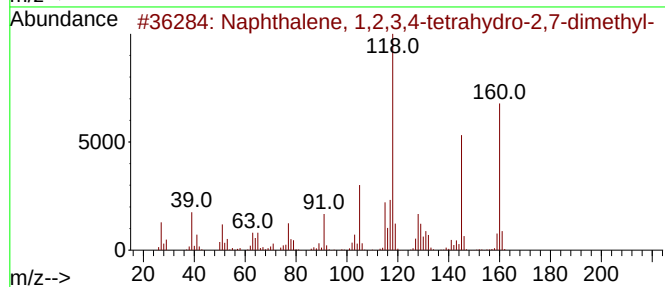
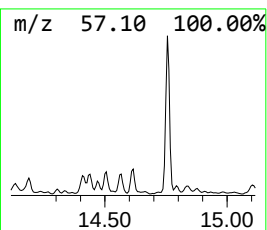
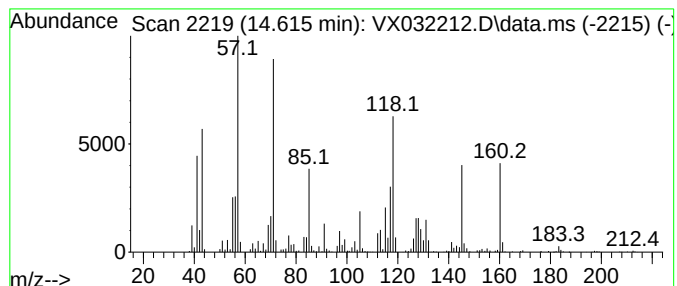
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	31.43 ug/l	506249	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	64
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	52
3			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	42
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	38
5			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032212.D
Acq On : 19 Oct 2022 17:00
Operator : JC/MD
Sample : N5114-02
Misc : 1.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

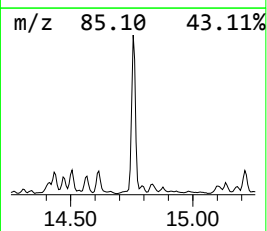
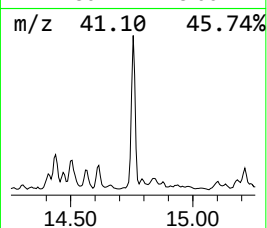
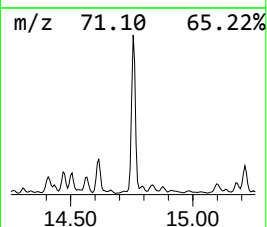
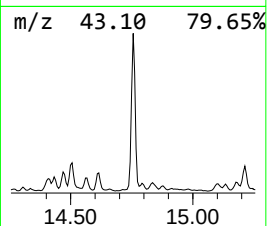
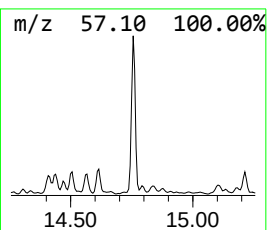
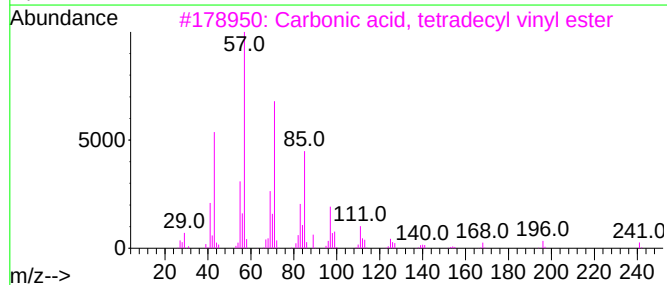
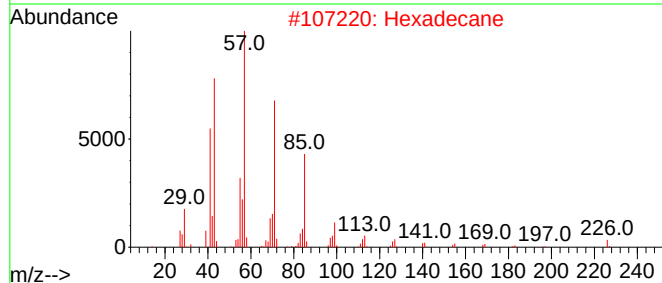
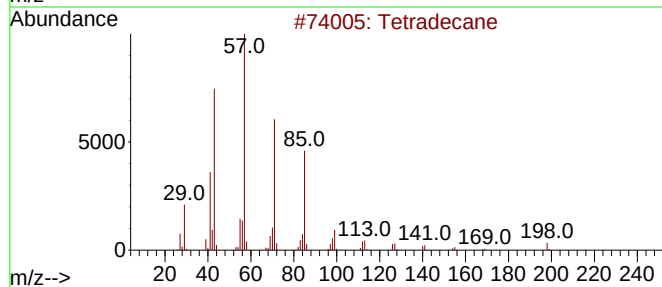
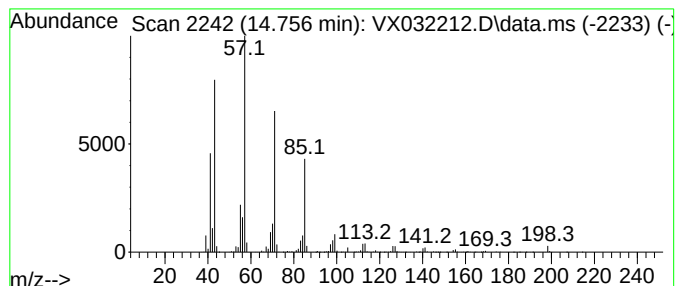
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Quant Title : SW846 8260

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

Peak Number 7 Tetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.756	91.86 ug/l	1479500	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			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	90
4			Tridecane	184	C13H28	000629-50-5	90
5			Dodecane	170	C12H26	000112-40-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032212.D
Acq On : 19 Oct 2022 17:00
Operator : JC/MD
Sample : N5114-02
Misc : 1.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

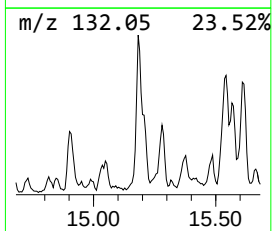
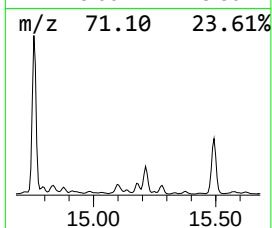
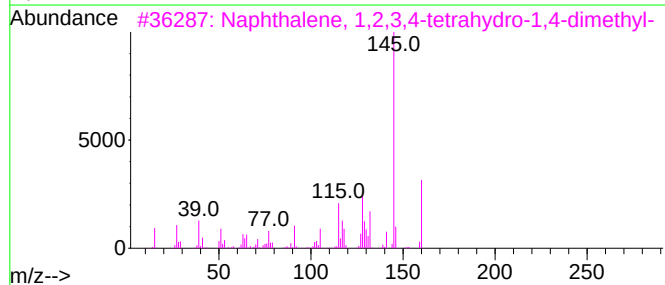
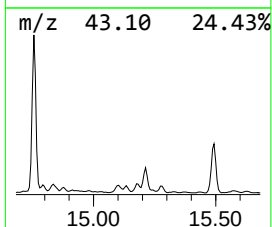
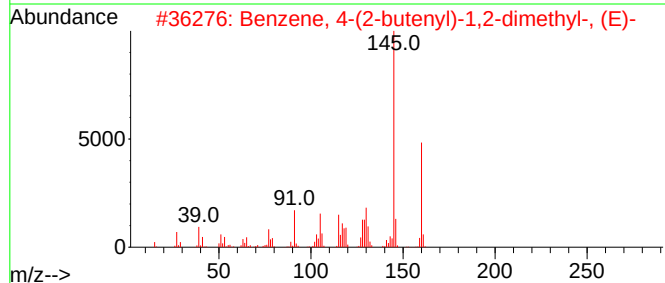
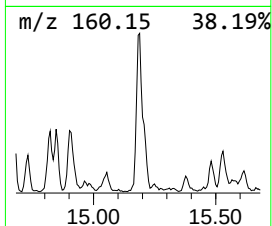
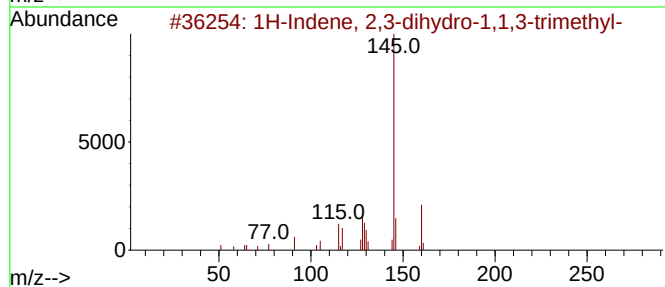
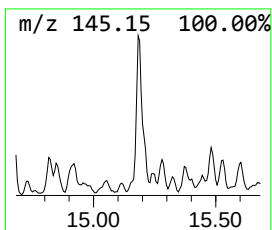
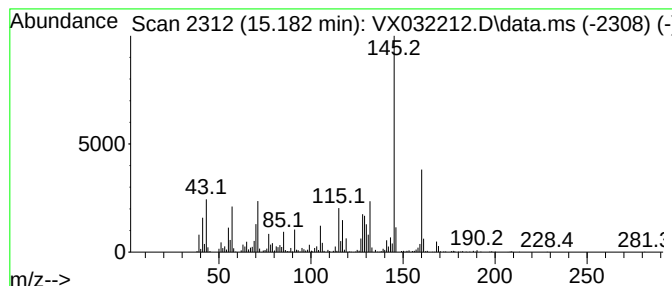
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	21.33 ug/l	343563	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	93
2			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	93
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	93
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	91
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032212.D
Acq On : 19 Oct 2022 17:00
Operator : JC/MD
Sample : N5114-02
Misc : 1.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

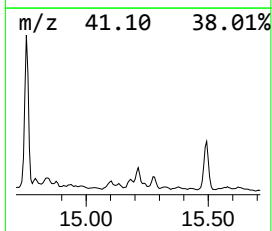
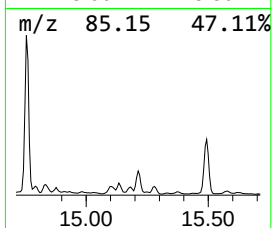
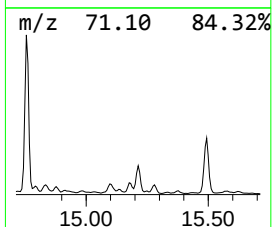
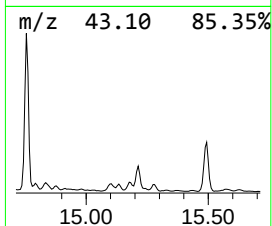
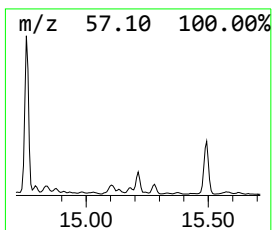
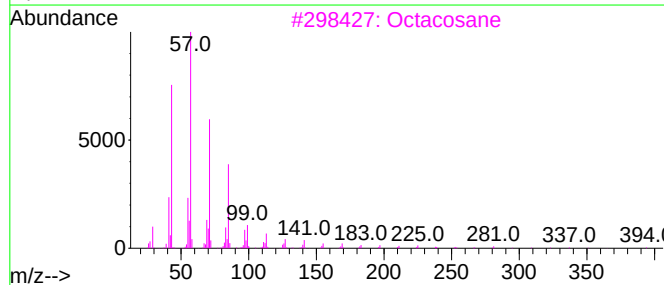
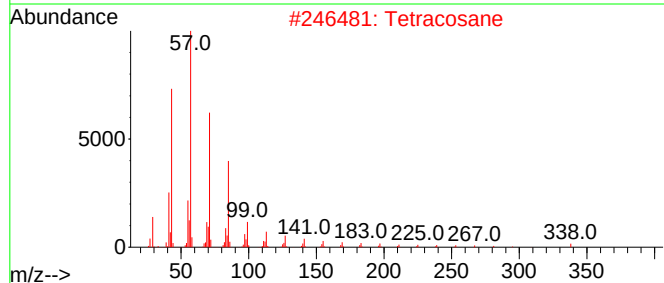
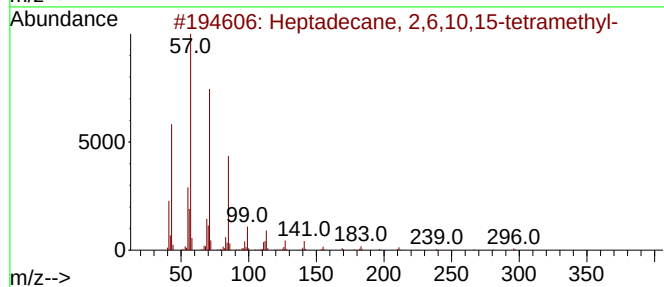
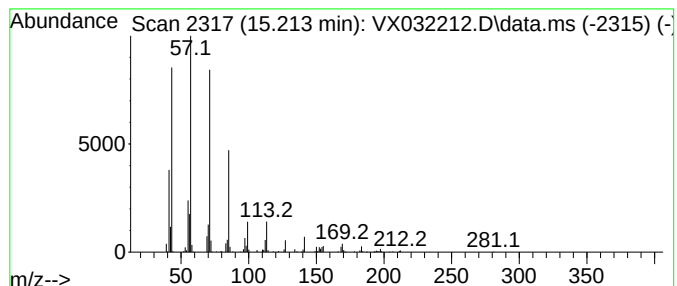
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Quant Title : SW846 8260

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

Peak Number 9 Heptadecane, 2,6,10,15-tetr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.213	15.80 ug/l	254449	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Tetratetracontane	619	C44H90	007098-22-8	90
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032212.D
Acq On : 19 Oct 2022 17:00
Operator : JC/MD
Sample : N5114-02
Misc : 1.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

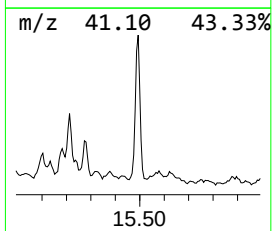
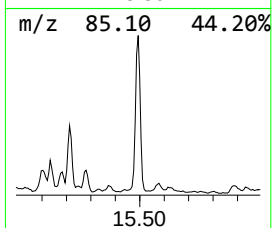
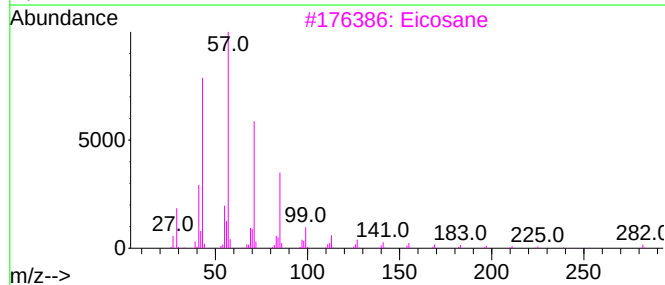
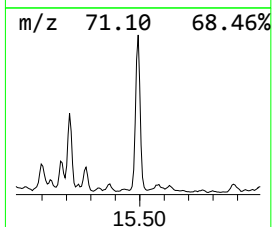
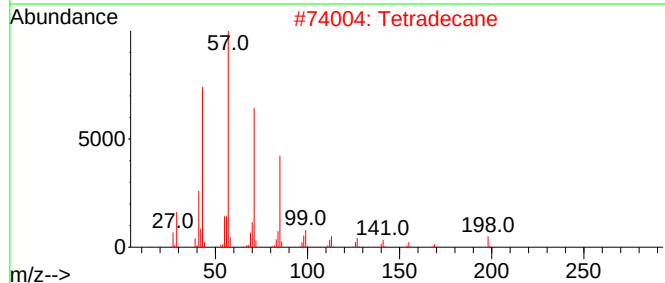
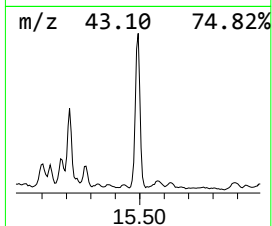
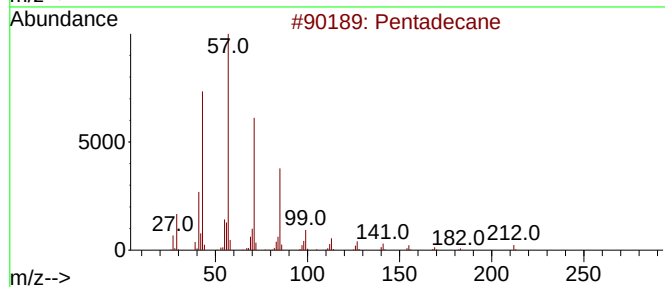
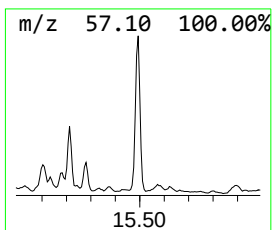
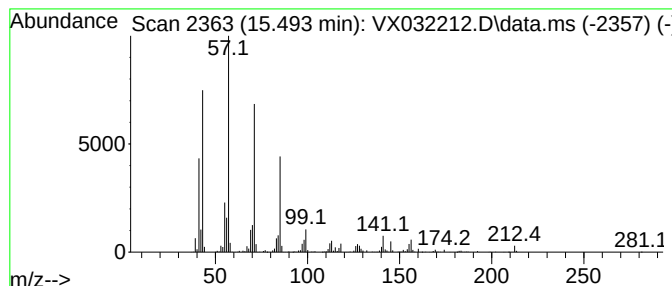
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Quant Title : SW846 8260

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

Peak Number 10 Pentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.493	42.07 ug/l	677610	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	96
2			Tetradecane	198	C14H30	000629-59-4	87
3			Eicosane	282	C20H42	000112-95-8	87
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5			Nonadecane	268	C19H40	000629-92-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032212.D
Acq On : 19 Oct 2022 17:00
Operator : JC/MD
Sample : N5114-02
Misc : 1.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0083

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.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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Dodecane, 4,6-d...	13.841	22.0	ug/l	353833	4	12.024	805347	50.0
Tridecane	14.042	97.7	ug/l	1572970	4	12.024	805347	50.0
Tridecane, 4-me...	14.475	14.5	ug/l	234245	4	12.024	805347	50.0
Tridecane, 2-me...	14.506	21.6	ug/l	348742	4	12.024	805347	50.0
Naphthalene, 1,...	14.615	31.4	ug/l	506249	4	12.024	805347	50.0
Tetradecane	14.756	91.9	ug/l	1479500	4	12.024	805347	50.0
1H-Indene, 2,3-...	15.182	21.3	ug/l	343563	4	12.024	805347	50.0
Heptadecane, 2,...	15.213	15.8	ug/l	254449	4	12.024	805347	50.0
Pentadecane	15.493	42.1	ug/l	677610	4	12.024	805347	50.0