

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
 Data File : VX029841.D
 Acq On : 28 Jun 2022 20:12
 Operator : JC/MD
 Sample : N3494-14
 Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SP-EXC-1-5-GR

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\82X062822W.M
 Title : SW846 8260

Signal : TIC: VX029841.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.636	77	90	94	rBV	22379	51616	1.09%	0.307%
2	1.910	131	135	139	rBV	58892	70657	1.50%	0.420%
3	3.075	317	326	336	rVB2	29366	66656	1.41%	0.396%
4	3.416	374	382	393	rBV	63376	139552	2.96%	0.829%
5	5.391	694	706	713	rBV2	130883	406617	8.63%	2.415%
6	5.458	714	717	724	rVV3	62204	159594	3.39%	0.948%
7	5.550	724	732	747	rVB2	249310	737627	15.65%	4.380%
8	5.812	765	775	786	rBV2	21805	65862	1.40%	0.391%
9	5.958	788	799	807	rBV2	147164	406880	8.63%	2.416%
10	6.031	807	811	822	rVB2	31653	81174	1.72%	0.482%
11	6.598	894	904	913	rBV	54444	133990	2.84%	0.796%
12	6.763	922	931	950	rBV	393476	964985	20.47%	5.730%
13	7.373	1023	1031	1041	rVB2	29960	70324	1.49%	0.418%
14	8.433	1200	1205	1210	rBV	28419	49340	1.05%	0.293%
15	8.647	1234	1240	1248	rVB	788625	1277167	27.09%	7.584%
16	8.909	1278	1283	1291	rBV	77571	121567	2.58%	0.722%
17	9.500	1376	1380	1387	rBV5	18958	50673	1.07%	0.301%
18	9.903	1442	1446	1451	rVB	55563	77279	1.64%	0.459%
19	10.006	1459	1463	1467	rBV	52141	74378	1.58%	0.442%
20	10.061	1467	1472	1473	rVV	731378	1028161	21.81%	6.106%
21	10.080	1473	1475	1482	rVB	784190	1046470	22.20%	6.214%
22	10.195	1489	1494	1499	rVB	80644	109349	2.32%	0.649%
23	10.305	1507	1512	1517	rVV	101697	141708	3.01%	0.842%
24	10.360	1517	1521	1532	rVB	104727	154267	3.27%	0.916%
25	10.659	1564	1570	1582	rVB	426864	644454	13.67%	3.827%
26	10.781	1582	1590	1594	rBV3	43270	73758	1.56%	0.438%
27	10.964	1613	1620	1624	rBV	64353	96802	2.05%	0.575%
28	11.085	1634	1640	1651	rVB	599059	856750	18.17%	5.088%
29	11.189	1651	1657	1660	rBV	51650	81894	1.74%	0.486%
30	11.311	1672	1677	1684	rBV2	69644	107898	2.29%	0.641%
31	11.384	1685	1689	1695	rBV2	53915	111285	2.36%	0.661%
32	11.482	1701	1705	1711	rVB2	130222	173030	3.67%	1.028%
33	11.634	1723	1730	1734	rBV5	24930	49067	1.04%	0.291%
34	11.719	1741	1744	1746	rBV	43645	48258	1.02%	0.287%
35	11.756	1746	1750	1759	rVB	63170	114483	2.43%	0.680%
36	12.024	1789	1794	1800	rBV	724581	1072742	22.75%	6.370%

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37	12.171	1810	1818	1822	rVB4	36539	68892	1.46%	0.409%
38	12.250	1826	1831	1834	rBV4	61065	102459	2.17%	0.608%
39	12.341	1838	1846	1851	rBV	3588010	4714348	100.00%	27.995%
40	12.427	1855	1860	1863	rVV	107241	126610	2.69%	0.752%
41	12.469	1864	1867	1873	rVB5	31189	64515	1.37%	0.383%
42	12.616	1888	1891	1895	rVV	41123	52366	1.11%	0.311%
43	12.920	1934	1941	1944	rVB7	30222	64851	1.38%	0.385%
44	13.042	1956	1961	1964	rVB4	27422	52417	1.11%	0.311%
45	13.292	2000	2002	2008	rVB4	53270	74812	1.59%	0.444%
46	13.390	2013	2018	2020	rBV2	32419	52576	1.12%	0.312%
47	13.420	2020	2023	2033	rVB9	34922	86755	1.84%	0.515%
48	13.774	2078	2081	2085	rBV	115375	154267	3.27%	0.916%
49	13.847	2089	2093	2096	rBV5	34348	49176	1.04%	0.292%
50	14.640	2220	2223	2227	rVB	71547	83621	1.77%	0.497%
51	14.786	2244	2247	2253	rVB2	41522	57470	1.22%	0.341%
52	15.414	2348	2350	2355	rVB6	33378	50028	1.06%	0.297%
53	15.481	2357	2361	2365	rVB2	41464	68230	1.45%	0.405%

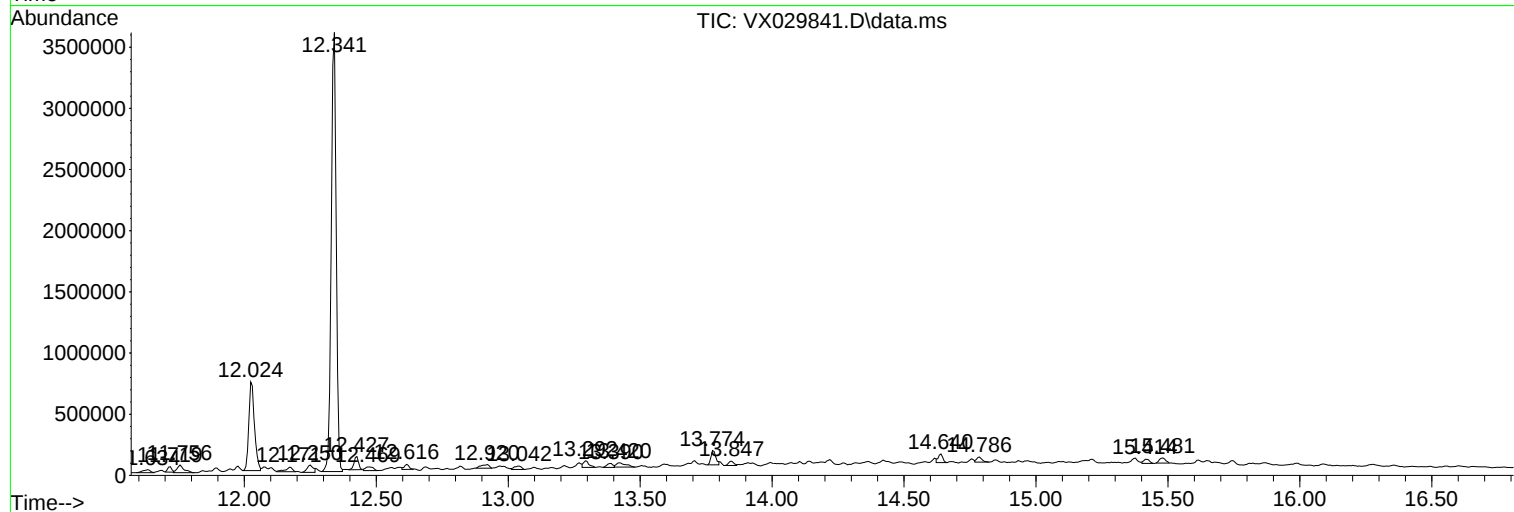
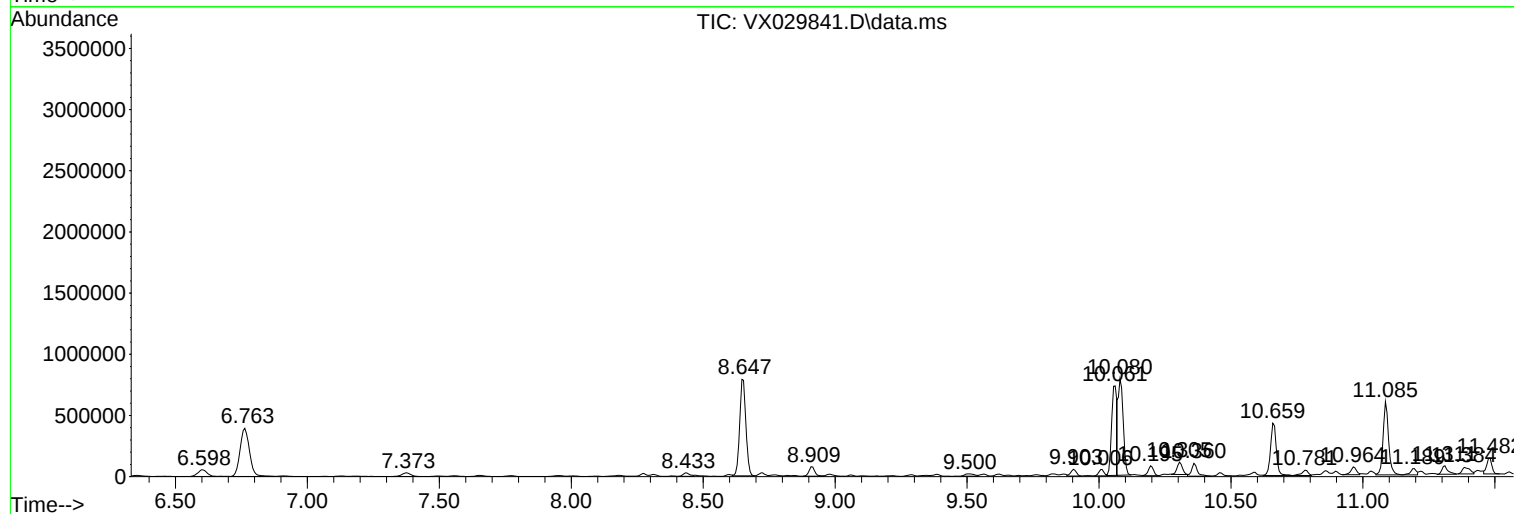
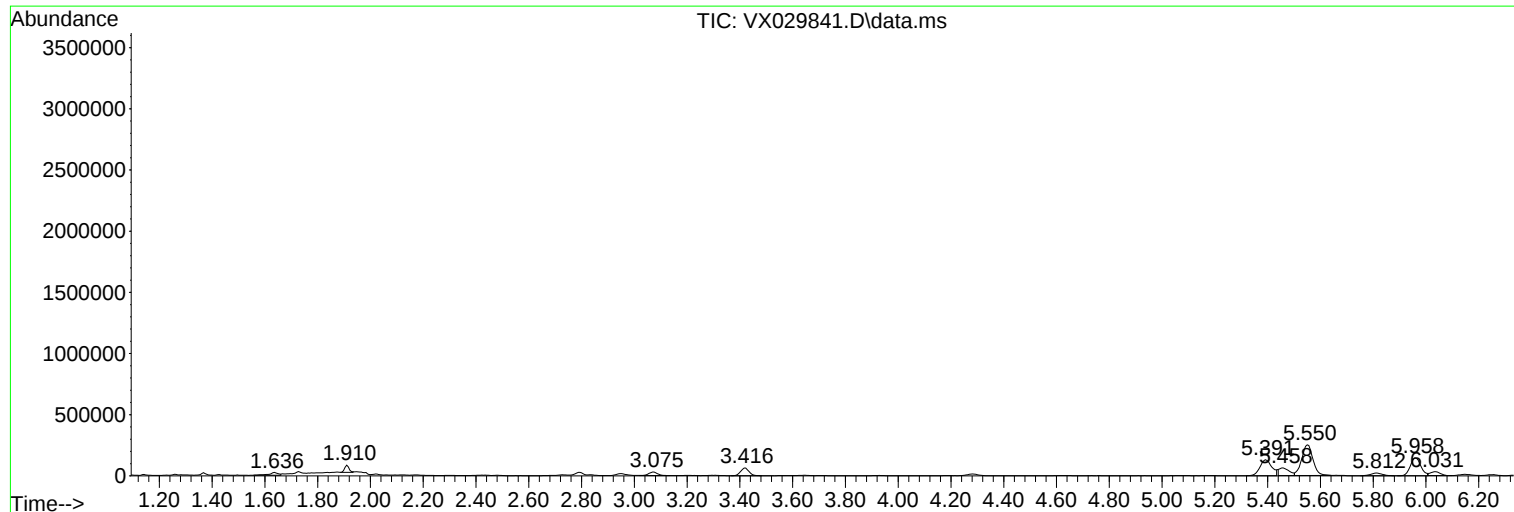
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Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
SP-EXC-1-5-GR

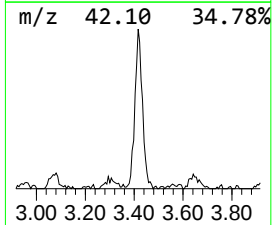
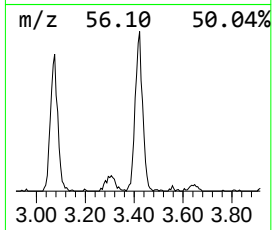
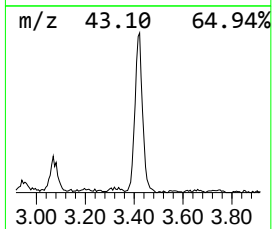
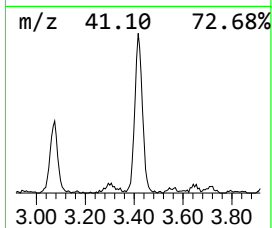
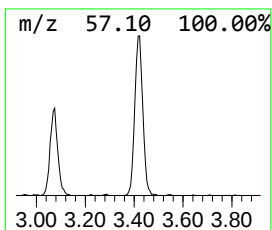
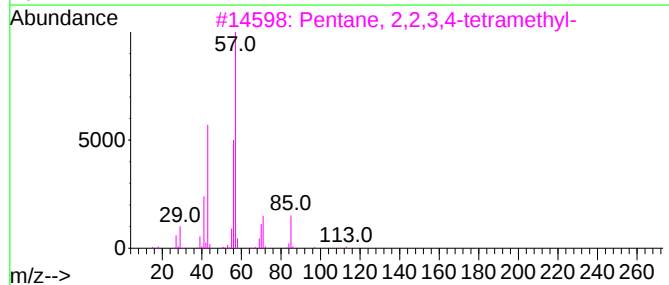
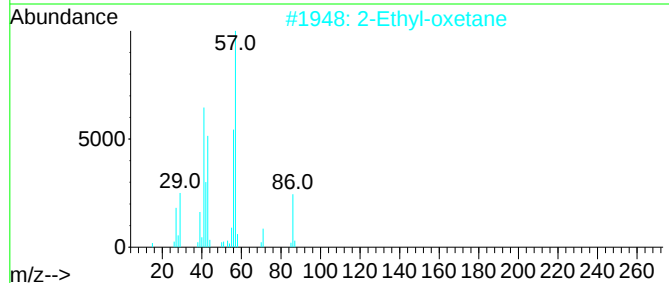
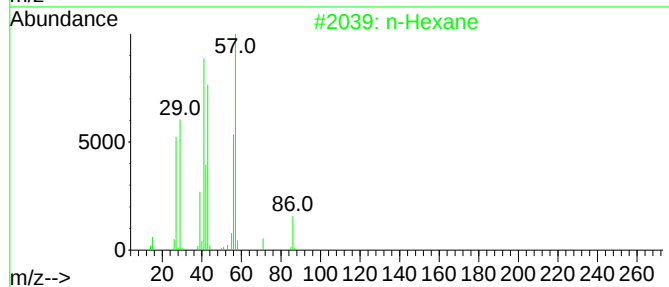
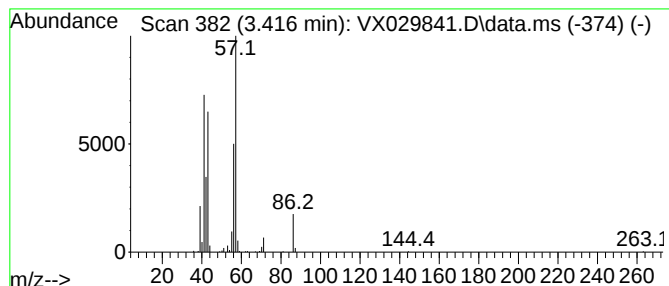
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Quant Title : SW846 8260

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

Peak Number 1 n-Hexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.416	9.46 ug/l	139552	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	91
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	43
3			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	42
4			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	38
5			2(3H)-Furanone, dihydro-3-methyl-	100	C5H8O2	001679-47-6	37



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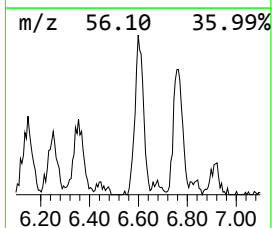
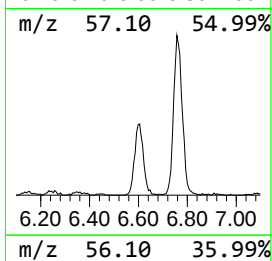
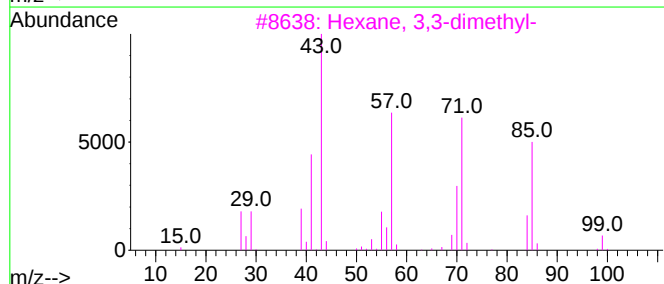
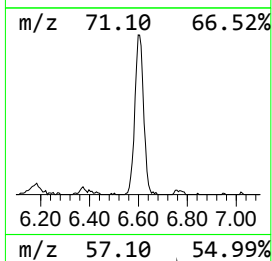
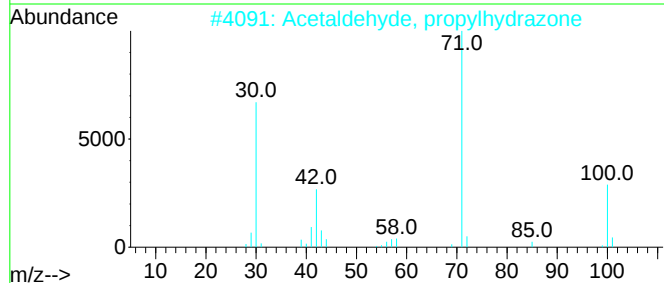
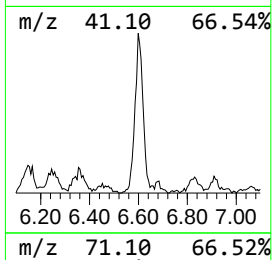
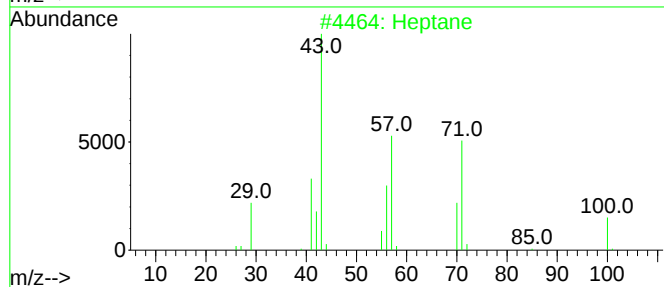
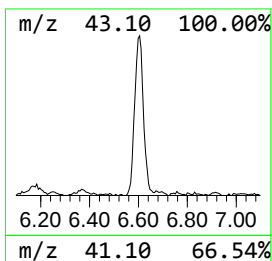
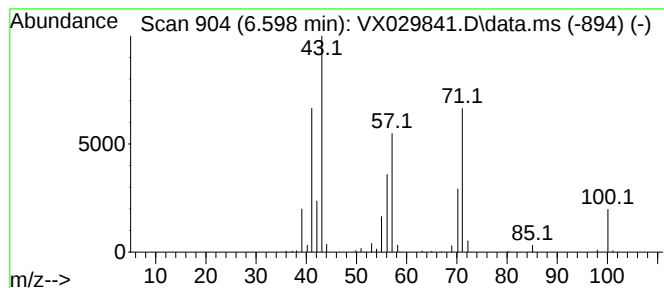
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	6.94 ug/l	133990	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	47
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
5			Isobutyl 3-methylbutan-2-yl carb...	188	C10H20O3	1000372-77-0	38



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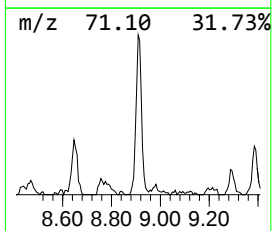
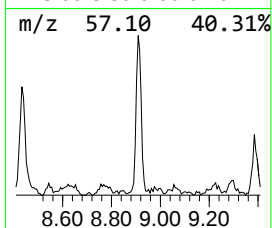
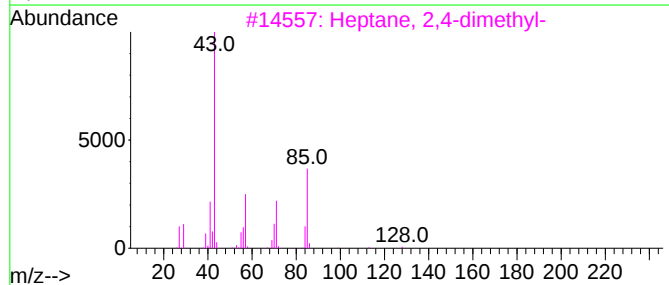
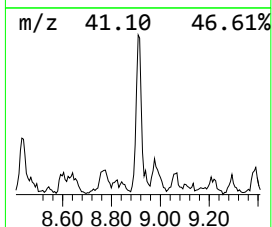
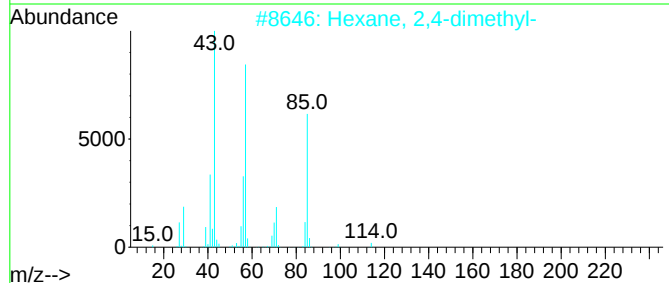
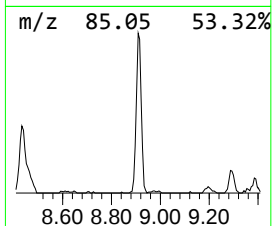
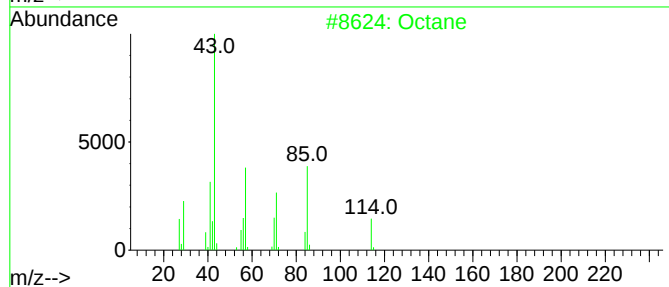
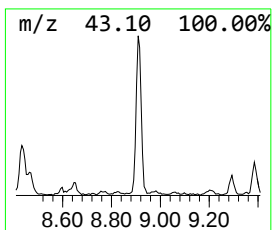
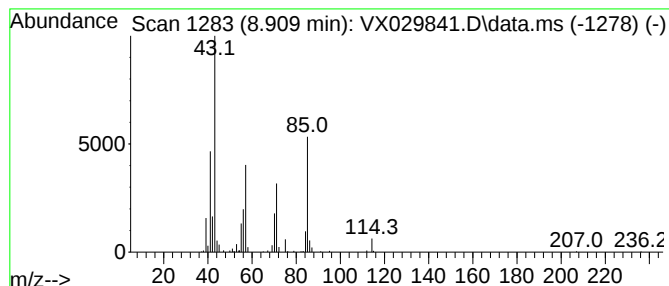
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Peak Number 3 Octane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.909	5.91 ug/l	121567	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane	114	C8H18	000111-65-9	91
2		Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
3		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
4		Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	53
5		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50



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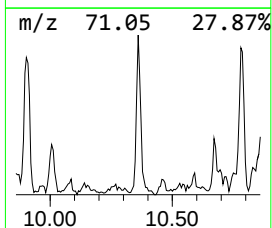
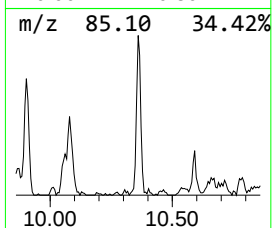
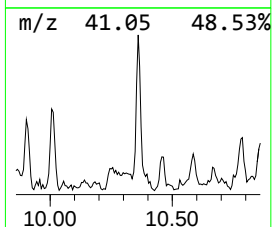
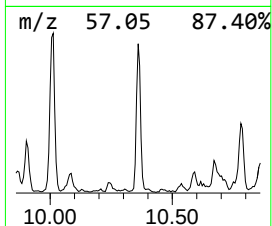
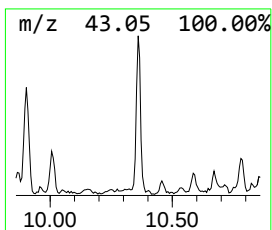
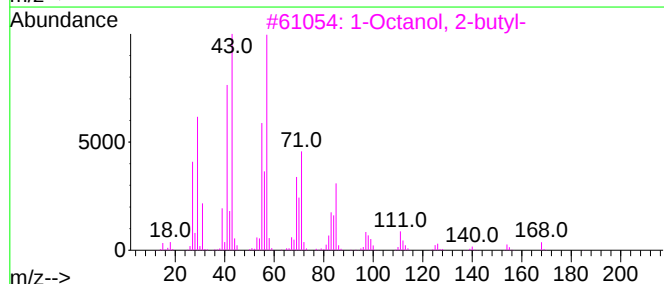
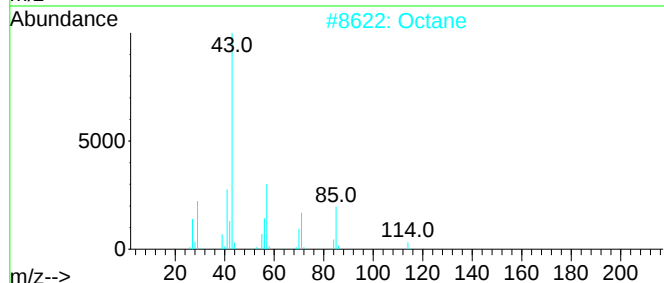
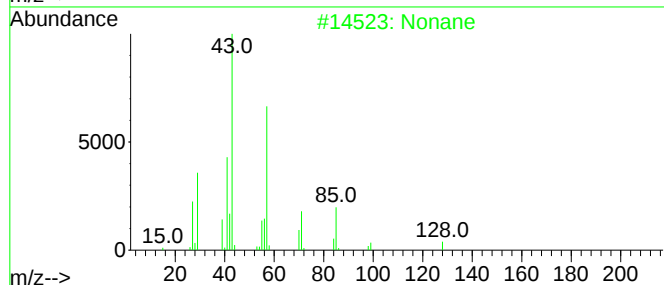
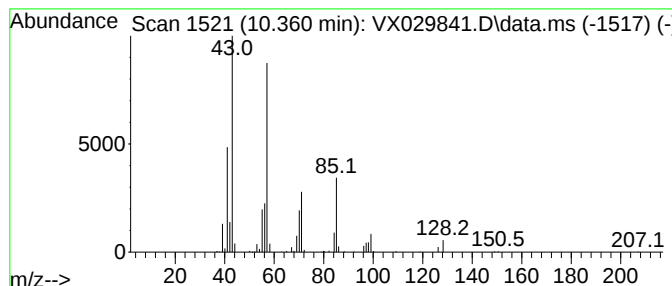
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Quant Title : SW846 8260

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

Peak Number 4 Nonane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	7.50 ug/l	154267	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane	128	C9H20	000111-84-2	95
2			Octane	114	C8H18	000111-65-9	64
3			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	64
4			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	58
5			Decane	142	C10H22	000124-18-5	50



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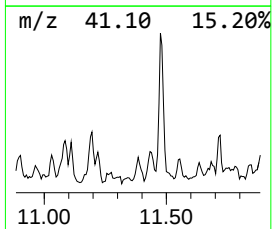
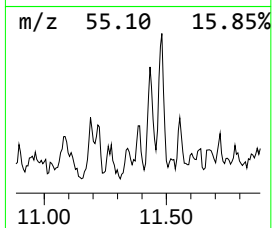
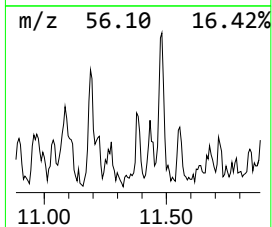
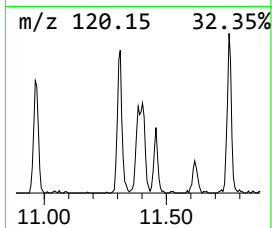
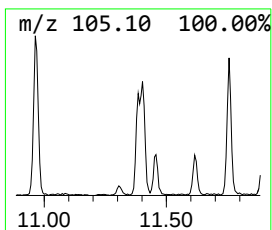
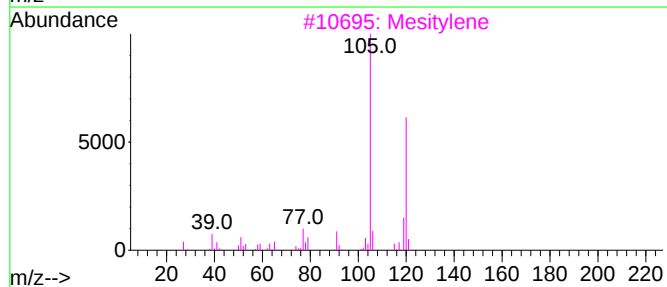
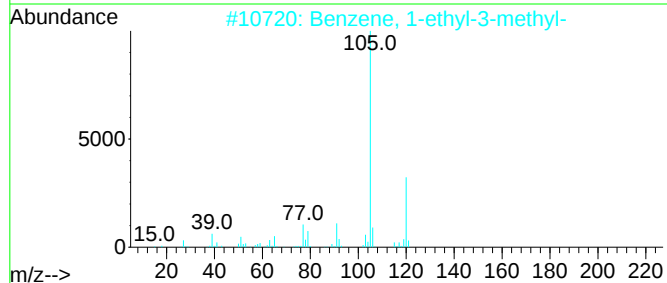
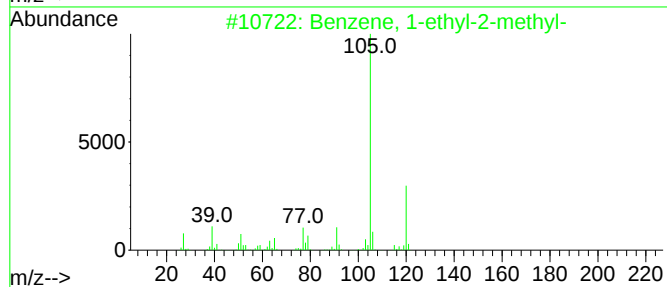
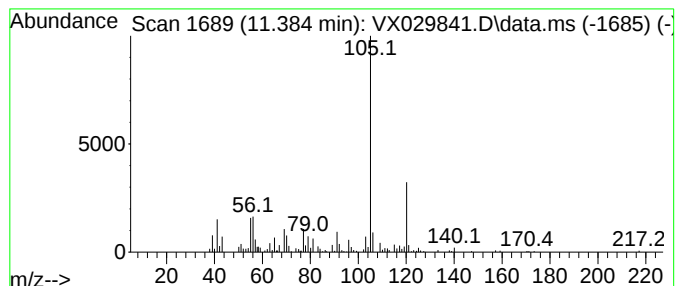
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	5.19 ug/l	111285	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93
3			Mesitylene	120	C9H12	000108-67-8	81
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	76
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029841.D
Acq On : 28 Jun 2022 20:12
Operator : JC/MD
Sample : N3494-14
Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-1-5-GR

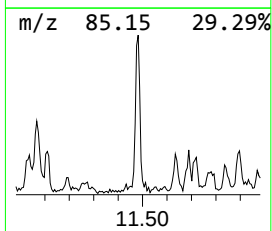
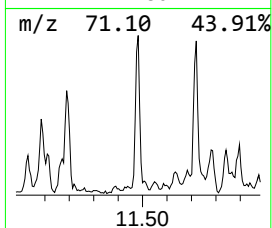
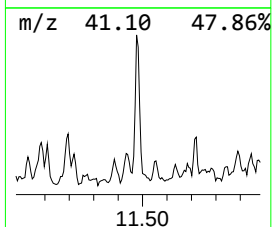
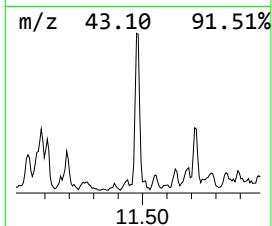
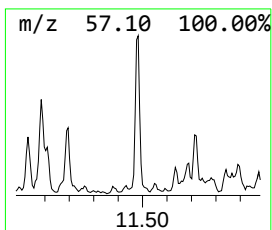
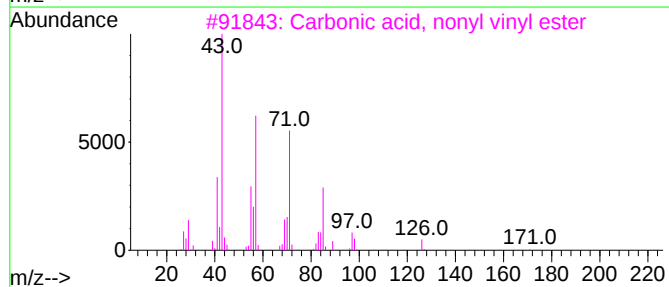
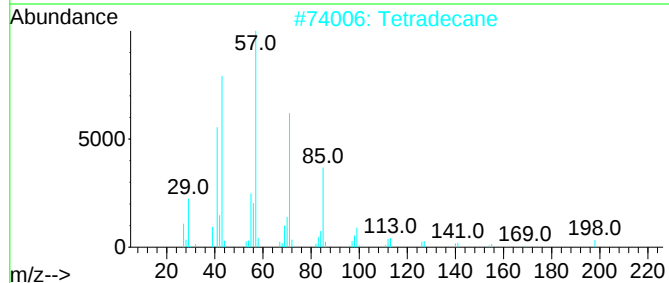
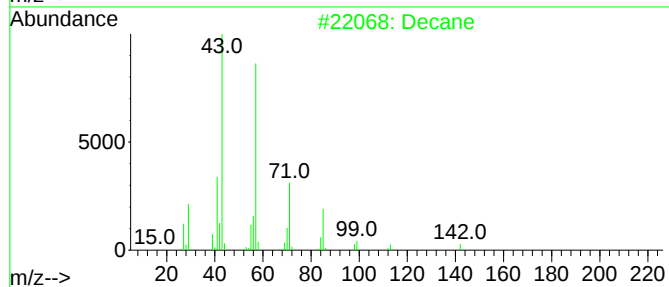
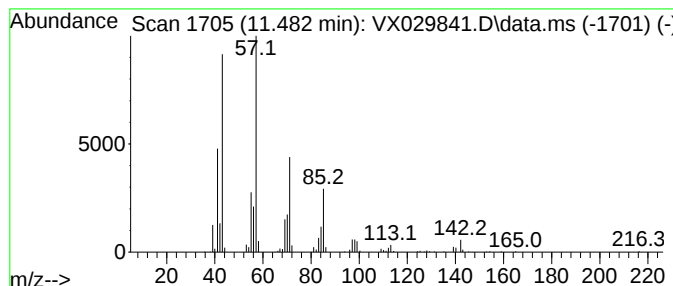
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Quant Title : SW846 8260

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

Peak Number 6 Decane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.482	8.06 ug/l	173030	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	91
2			Tetradecane	198	C14H30	000629-59-4	86
3			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	80
4			Undecane	156	C11H24	001120-21-4	78
5			Methyl tetratriacontyl ether	509	C35H72O	1000406-30-1	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029841.D
Acq On : 28 Jun 2022 20:12
Operator : JC/MD
Sample : N3494-14
Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-1-5-GR

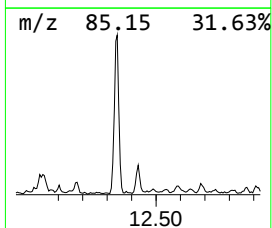
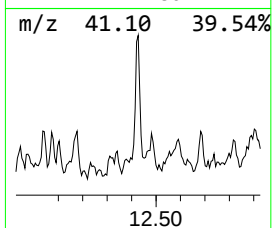
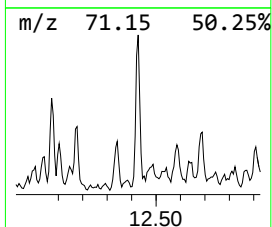
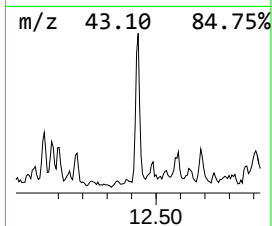
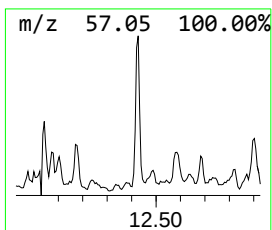
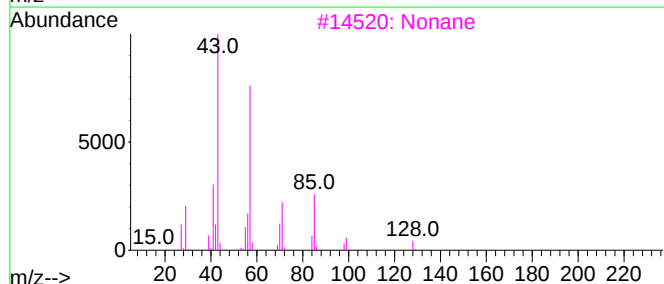
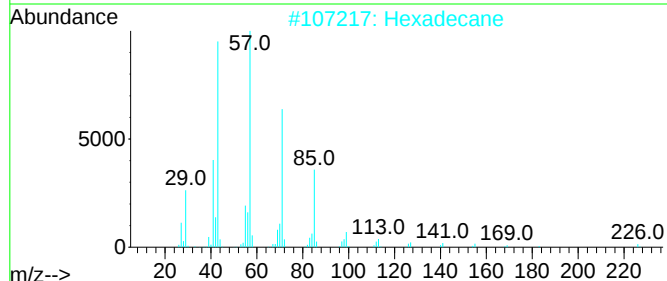
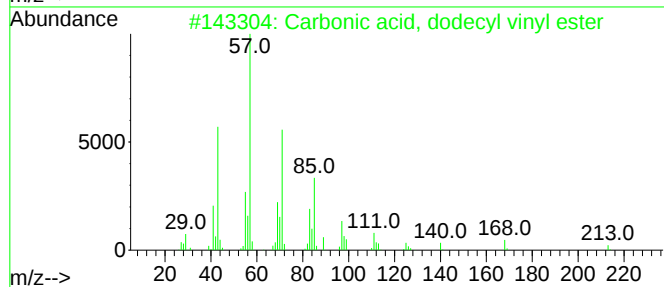
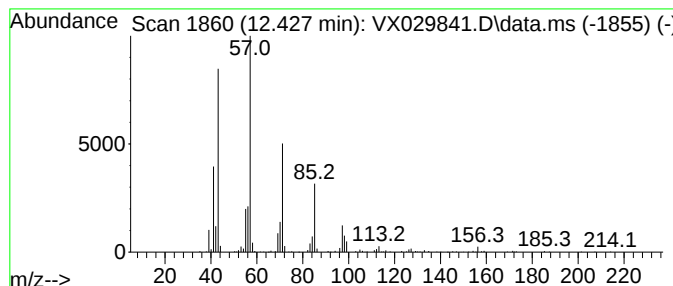
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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

Peak Number 7 Carbonic acid, dodecyl vinyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	5.90 ug/l	126610	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	83
2			Hexadecane	226	C16H34	000544-76-3	72
3			Nonane	128	C9H20	000111-84-2	59
4			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	53
5			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029841.D
Acq On : 28 Jun 2022 20:12
Operator : JC/MD
Sample : N3494-14
Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-1-5-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.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
n-Hexane	3.416	9.5	ug/l	139552	1	5.556	737627	50.0
Heptane	6.598	6.9	ug/l	133990	2	6.763	964985	50.0
Octane	8.909	5.9	ug/l	121567	3	10.055	1028160	50.0
Nonane	10.360	7.5	ug/l	154267	3	10.055	1028160	50.0
Benzene, 1-ethy...	11.384	5.2	ug/l	111285	4	12.024	1072740	50.0
Decane	11.482	8.1	ug/l	173030	4	12.024	1072740	50.0
Carbonic acid, ...	12.427	5.9	ug/l	126610	4	12.024	1072740	50.0