

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092525\
 Data File : VV039177.D
 Acq On : 25 Sep 2025 13:40
 Operator : SY/MD
 Sample : Q3168-05
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 TOTES COMP#1

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_V\Method\82V092225W.M
 Title : SW846 8260

Signal : TIC: VV039177.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.101	14	19	32	rVB2	29945	44600	1.85%	0.180%
2	1.233	47	60	63	rBV2	52518	122411	5.07%	0.493%
3	1.362	94	100	114	rVB	89951	123160	5.10%	0.496%
4	2.056	309	316	325	rBV2	27623	42601	1.76%	0.172%
5	2.121	327	336	360	rVV	364220	685467	28.38%	2.762%
6	2.230	362	370	392	rVB3	42161	121073	5.01%	0.488%
7	2.571	469	476	488	rBV2	21550	43805	1.81%	0.177%
8	3.635	797	807	817	rBV5	18732	47145	1.95%	0.190%
9	3.818	853	864	875	rBV3	11782	32426	1.34%	0.131%
10	3.883	876	884	921	rVB2	80005	240714	9.97%	0.970%
11	4.503	1060	1077	1096	rBV3	428690	1136728	47.06%	4.581%
12	4.600	1096	1107	1155	rVB	499987	1414492	58.56%	5.701%
13	4.944	1202	1214	1249	rBV	449159	1123662	46.52%	4.528%
14	5.256	1300	1311	1316	rBV8	13334	24950	1.03%	0.101%
15	5.464	1362	1376	1386	rBV3	21200	54952	2.27%	0.221%
16	5.535	1387	1398	1432	rVV	815494	1849081	76.55%	7.452%
17	6.111	1570	1577	1606	rBV	83376	217523	9.01%	0.877%
18	6.227	1607	1613	1627	rVV5	16204	34249	1.42%	0.138%
19	6.506	1685	1700	1714	rVB4	17789	43716	1.81%	0.176%
20	7.165	1896	1905	1916	rBV3	43520	83890	3.47%	0.338%
21	7.239	1917	1928	1963	rVV	1171969	2267065	93.86%	9.136%
22	7.410	1975	1981	1995	rVB2	12803	25624	1.06%	0.103%
23	7.644	2047	2054	2068	rVB5	25126	48641	2.01%	0.196%
24	7.863	2111	2122	2134	rBV2	17148	31963	1.32%	0.129%
25	7.950	2139	2149	2167	rBV4	22864	59076	2.45%	0.238%
26	8.079	2180	2189	2213	rBV2	123249	276135	11.43%	1.113%
27	8.178	2213	2220	2238	rVV3	48656	93120	3.86%	0.375%
28	8.776	2389	2406	2436	rBV	1384991	2415491	100.00%	9.735%
29	8.995	2453	2474	2491	rBV3	102566	267707	11.08%	1.079%
30	9.069	2493	2497	2514	rVB2	23974	47786	1.98%	0.193%
31	9.175	2516	2530	2536	rBV	89832	158558	6.56%	0.639%
32	9.532	2634	2641	2655	rVB2	46614	83442	3.45%	0.336%
33	9.632	2663	2672	2692	rBV	393206	689863	28.56%	2.780%
34	9.744	2699	2707	2718	rBV5	91562	168466	6.97%	0.679%
35	9.850	2736	2740	2753	rVB5	15931	28393	1.18%	0.114%
36	9.940	2761	2768	2777	rBV3	20624	34015	1.41%	0.137%

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Peak Location: TOP

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37	10.001	2777	2787	2811	rBV	1079594	1798232	74.45%	7.247%
38	10.123	2818	2825	2842	rVB9	23745	71892	2.98%	0.290%
39	10.291	2869	2877	2893	rVB4	48330	90988	3.77%	0.367%
40	10.368	2894	2901	2903	rBV2	23446	27962	1.16%	0.113%
41	10.451	2920	2927	2935	rBV5	34026	51901	2.15%	0.209%
42	10.506	2935	2944	2968	rVV	1016665	1598684	66.18%	6.443%
43	10.628	2975	2982	2987	rBV3	42575	61336	2.54%	0.247%
44	10.667	2988	2994	3008	rVV3	107102	202305	8.38%	0.815%
45	10.728	3009	3013	3023	rVB3	46214	67859	2.81%	0.273%
46	10.789	3025	3032	3038	rBV5	25512	47090	1.95%	0.190%
47	10.869	3052	3057	3067	rVB3	53020	74412	3.08%	0.300%
48	10.966	3079	3087	3099	rBV	340554	526646	21.80%	2.122%
49	11.082	3117	3123	3136	rVB3	49905	80463	3.33%	0.324%
50	11.172	3142	3151	3172	rVB	1540371	2405442	99.58%	9.694%
51	11.464	3233	3242	3250	rBV2	166871	323109	13.38%	1.302%
52	11.593	3276	3282	3291	rVB3	54483	84587	3.50%	0.341%
53	11.709	3304	3318	3325	rBV	197668	332213	13.75%	1.339%
54	11.754	3325	3332	3347	rVB6	181655	367978	15.23%	1.483%
55	11.834	3348	3357	3370	rBV4	347307	634284	26.26%	2.556%
56	11.956	3390	3395	3405	rVB6	29879	46579	1.93%	0.188%
57	12.069	3424	3430	3447	rVB10	47816	107120	4.43%	0.432%
58	12.162	3451	3459	3474	rBV	324947	553376	22.91%	2.230%
59	12.602	3588	3596	3603	rBV4	75121	124836	5.17%	0.503%
60	12.664	3608	3615	3638	rVB	209851	424749	17.58%	1.712%
61	12.828	3659	3666	3677	rVB3	126843	211317	8.75%	0.852%
62	12.963	3701	3708	3714	rBV8	33899	55252	2.29%	0.223%
63	13.156	3761	3768	3771	rBV5	34500	51310	2.12%	0.207%
64	13.252	3791	3798	3807	rBV2	138969	209481	8.67%	0.844%

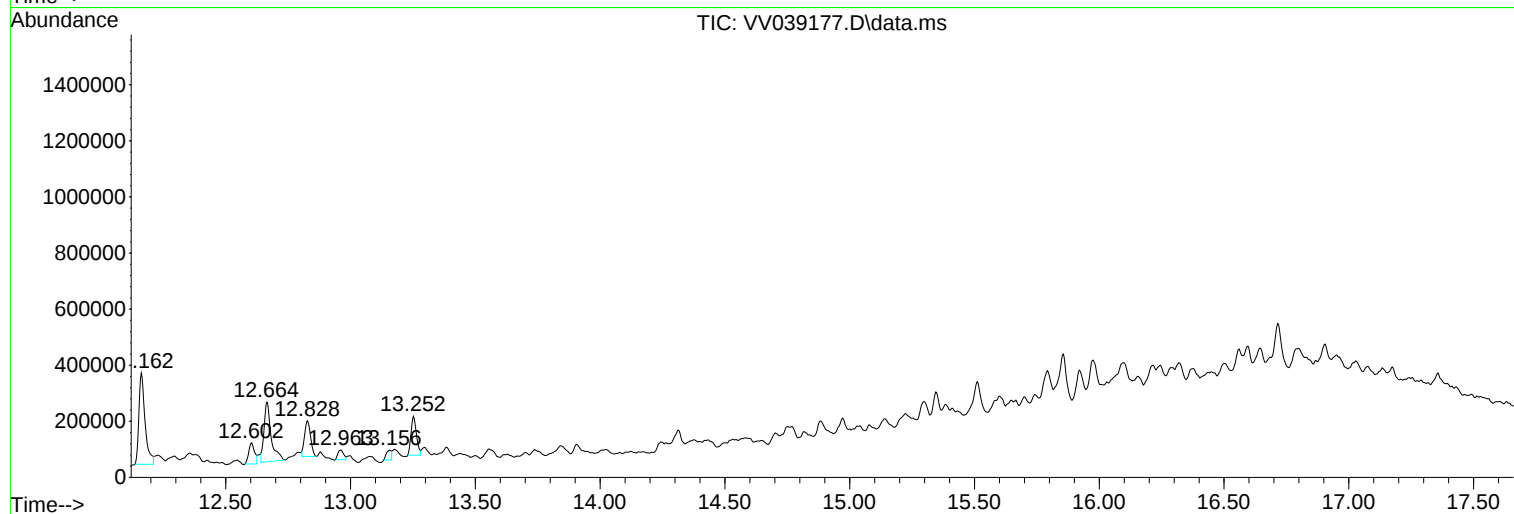
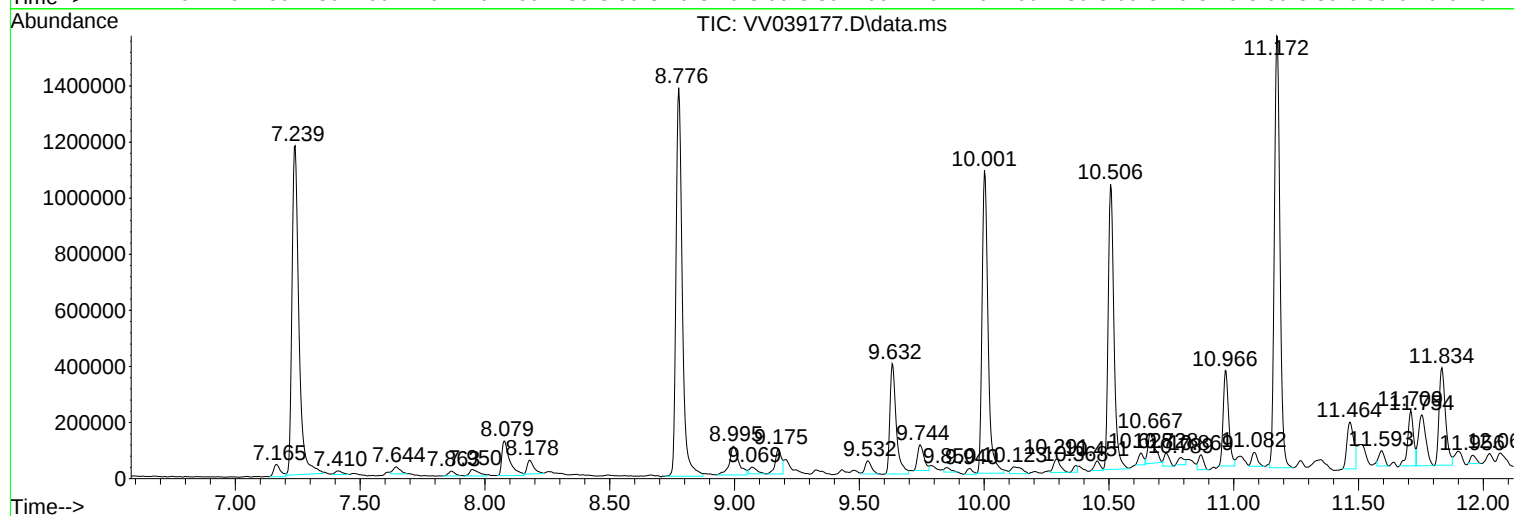
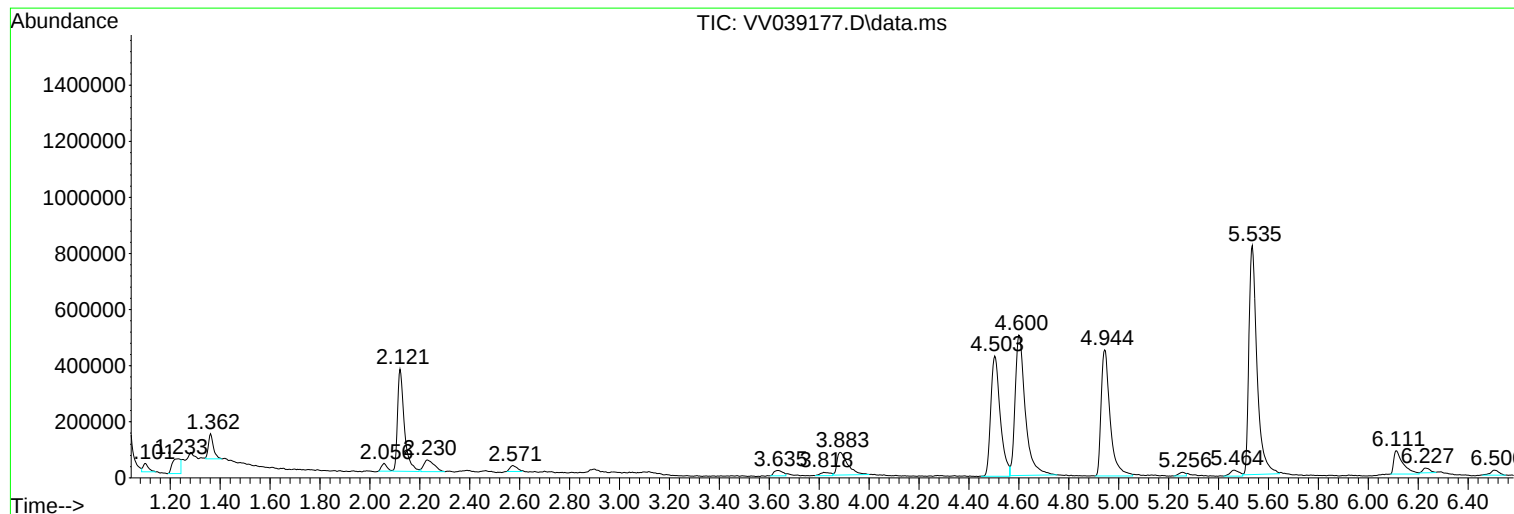
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Instrument :
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ClientSampleId :
TOTES COMP#1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V092225W.M
Quant Title : SW846 8260

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



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MSVOA_V
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TOTES COMP#1

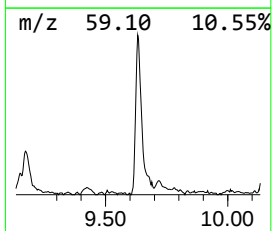
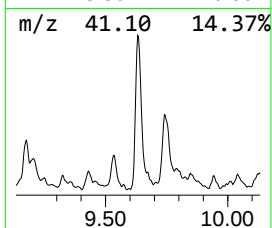
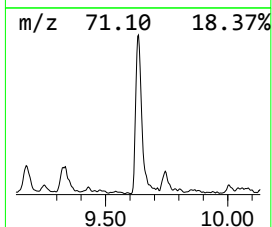
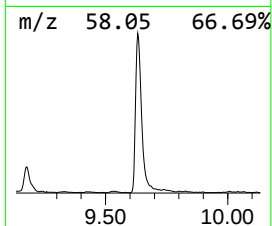
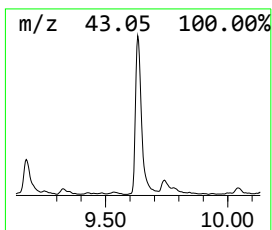
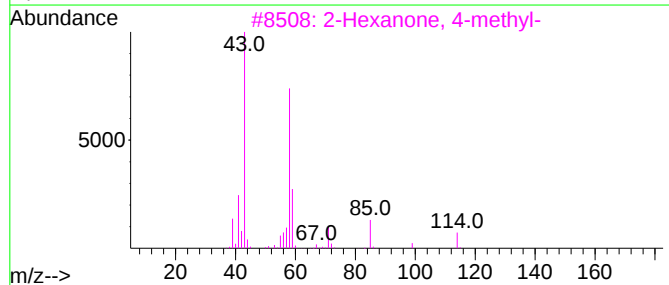
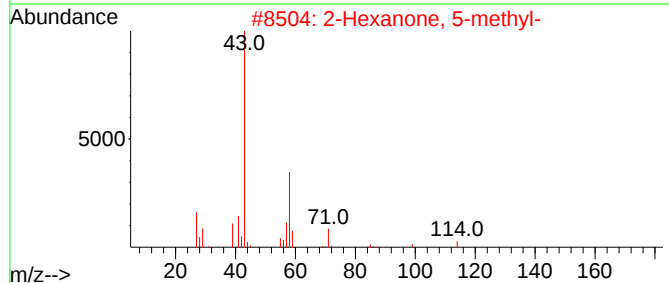
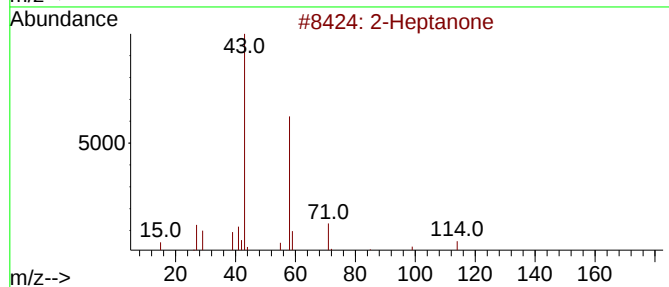
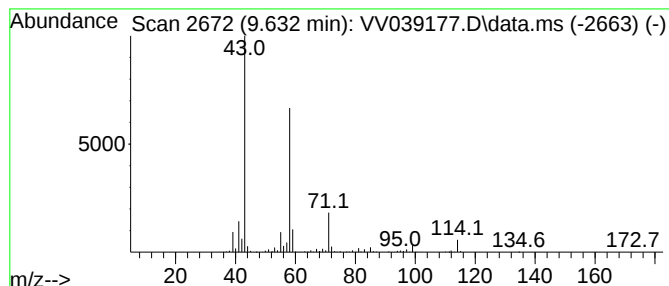
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V092225W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Heptanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.632	14.28 ug/l	689863	Chlorobenzene-d5	8.776

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptanone	114	C7H14O	000110-43-0	91
2		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
3		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64
4		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	56
5		2-Propenoic acid, 2-(dimethylami...	143	C7H13NO2	002439-35-2	47



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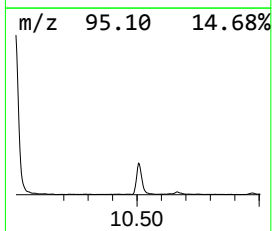
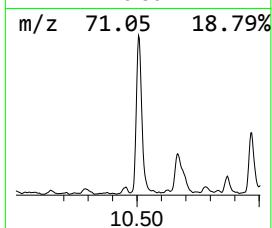
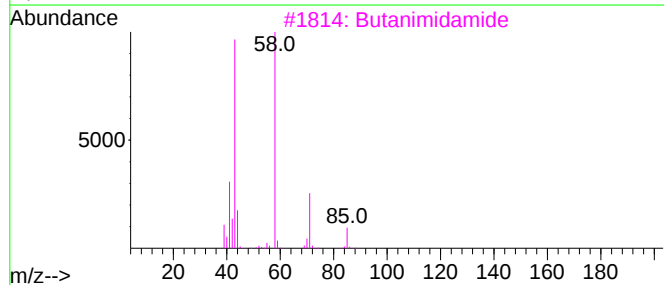
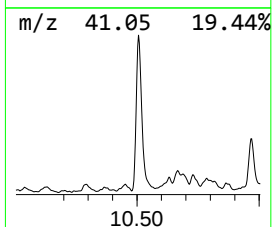
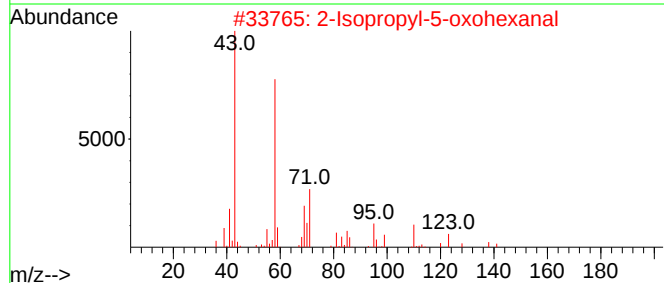
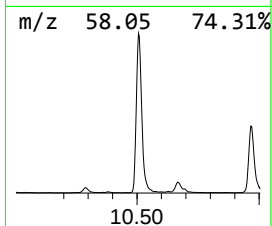
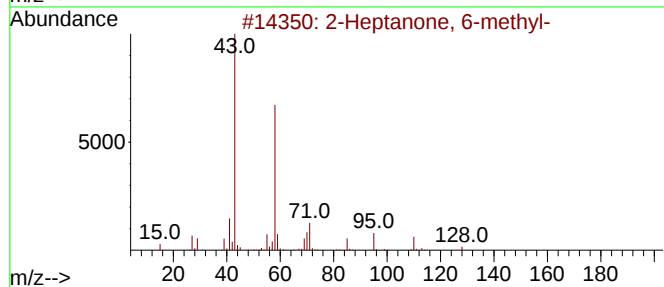
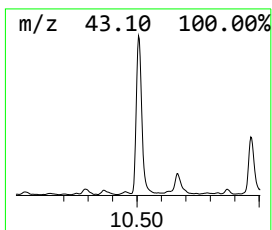
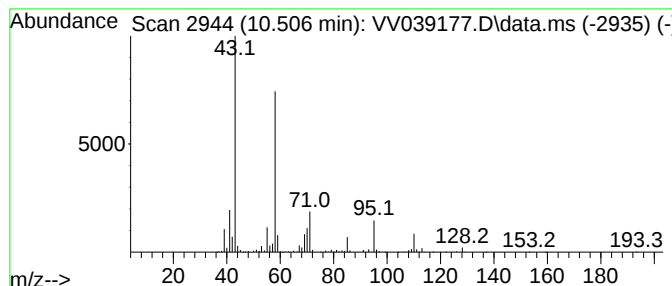
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V092225W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Heptanone, 6-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.506	33.23 ug/l	1598680	1,4-Dichlorobenzene-d4	11.175

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	91
2		2-Isopropyl-5-oxohexanal	156	C9H16O2	015303-46-5	83
3		Butanimidamide	86	C4H10N2	000107-90-4	64
4		2-Octanone	128	C8H16O	000111-13-7	50
5		2-(Dimethylamino)-N-(5-ethyl-1,3...	214	C8H14N4OS	111750-46-0	38



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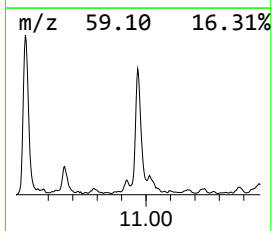
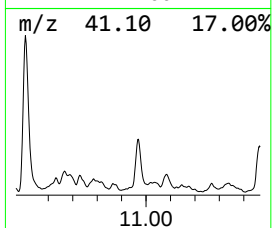
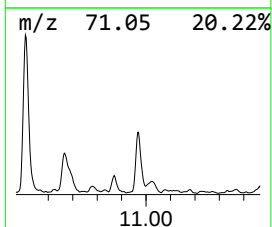
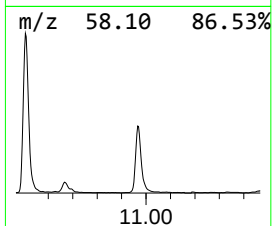
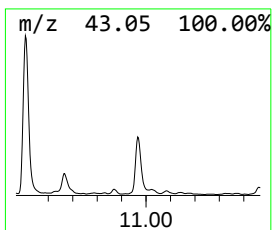
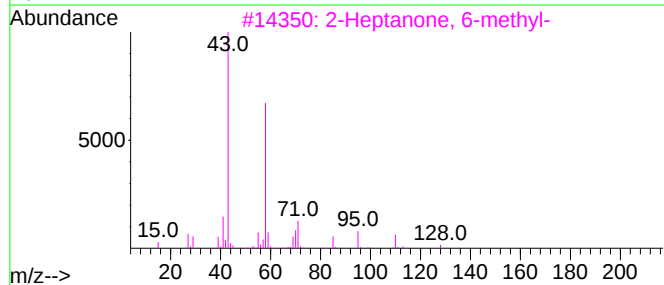
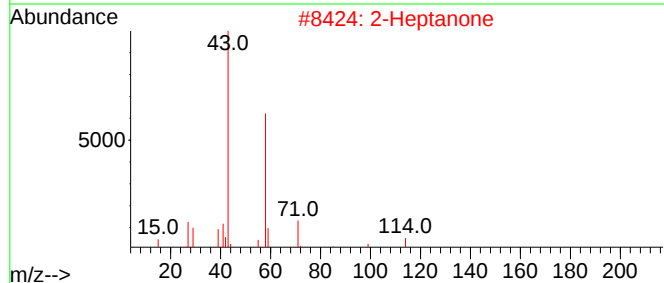
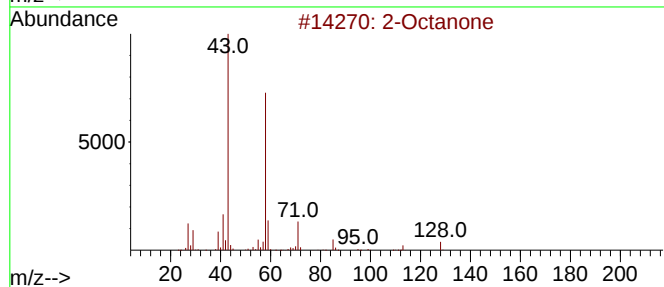
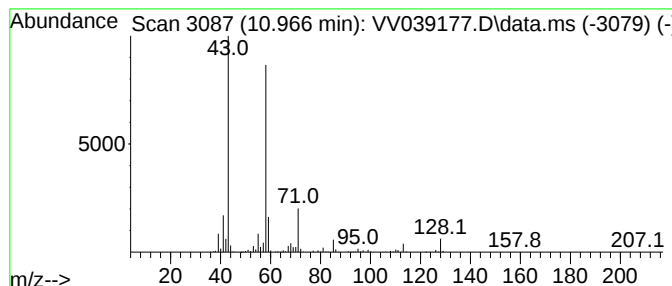
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Peak Number 4 2-Octanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.966	10.95 ug/l	526646	1,4-Dichlorobenzene-d4	11.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octanone	128	C8H16O	000111-13-7	87
2			2-Heptanone	114	C7H14O	000110-43-0	72
3			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	64
4			2-Butoxy-N-(2-(dimethylamino)eth...	315	C18H25N3O2	1000425-82-7	53
5			Pentanal, 2,4-dimethyl-	114	C7H14O	027944-79-2	53



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TOTES COMP#1

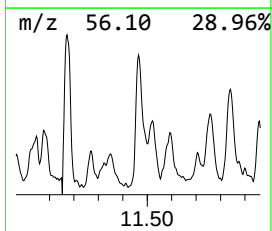
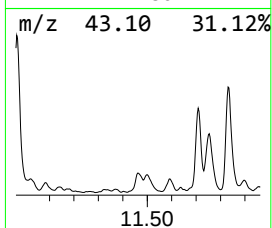
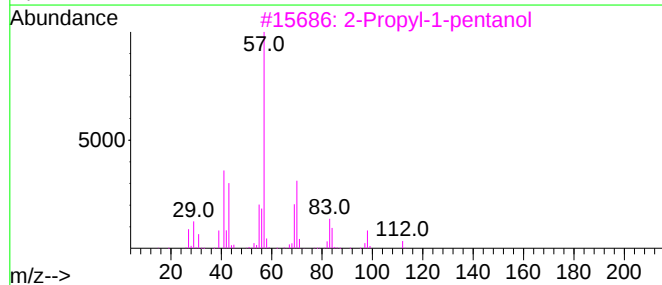
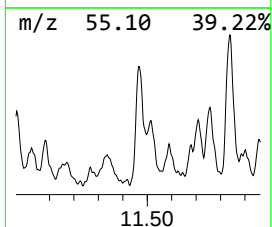
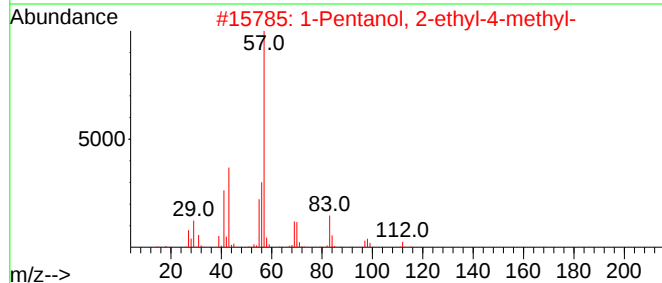
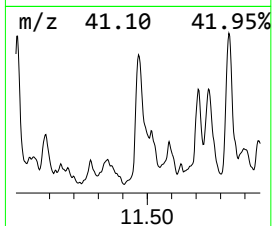
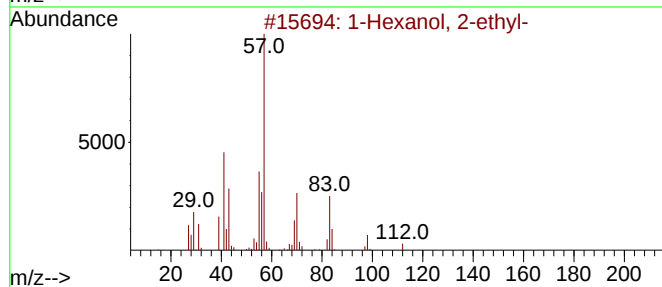
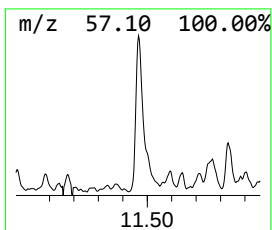
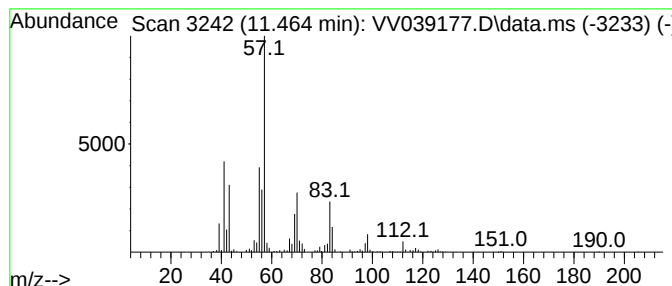
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.464	6.72 ug/l	323109	1,4-Dichlorobenzene-d4	11.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
4			Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	59
5			1,2-Cyclopentanediol, 3-methyl-	116	C6H12O2	027583-37-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092525\
Data File : VV039177.D
Acq On : 25 Sep 2025 13:40
Operator : SY/MD
Sample : Q3168-05
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

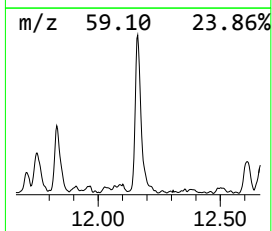
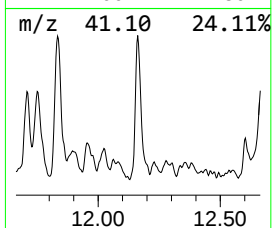
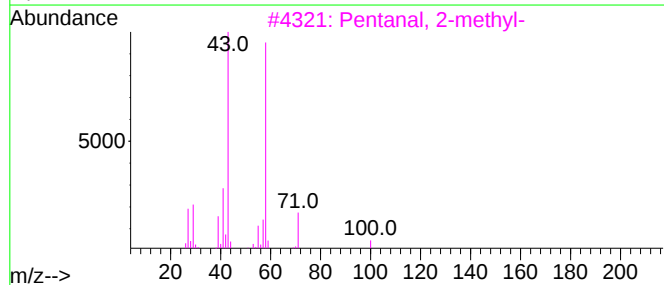
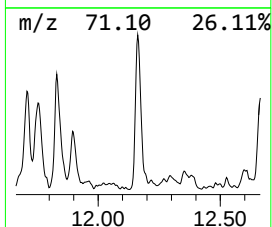
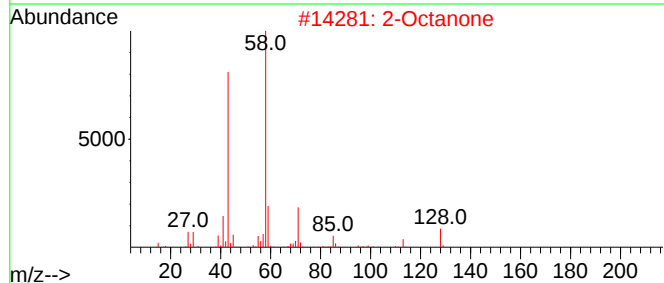
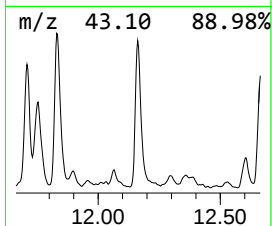
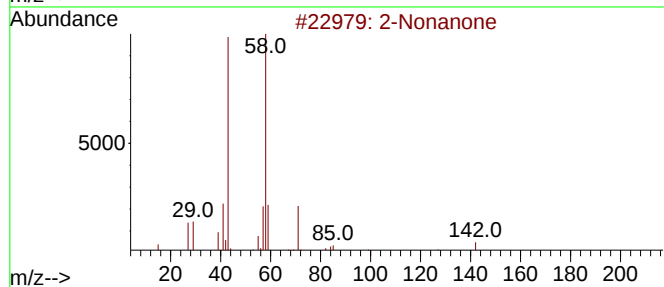
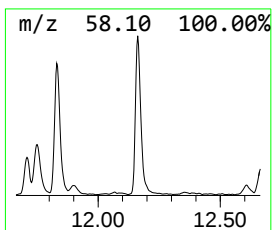
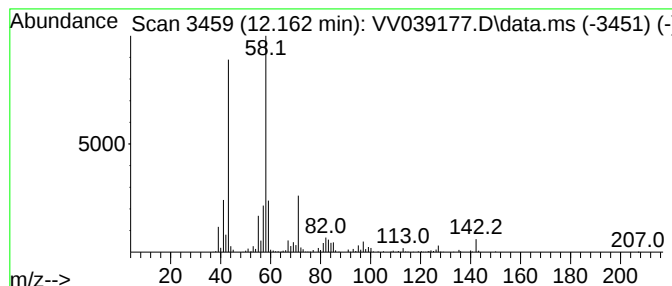
Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V092225W.M
Quant Title : SW846 8260

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

Peak Number 9 2-Nonanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.162	11.50 ug/l	553376	1,4-Dichlorobenzene-d4	11.175	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	91
2	2-Octanone	128	C8H16O	000111-13-7	64
3	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	58
4	2-Undecanone	170	C11H22O	000112-12-9	56
5	2-Dodecanone	184	C12H24O	006175-49-1	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092525\
Data File : VV039177.D
Acq On : 25 Sep 2025 13:40
Operator : SY/MD
Sample : Q3168-05
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V092225W.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
2-Heptanone	9.632	14.3	ug/l	689863	3	8.776	2415490	50.0
2-Heptanone, 6-...	10.506	33.2	ug/l	1598680	4	11.175	2405440	50.0
2-Octanone	10.966	10.9	ug/l	526646	4	11.175	2405440	50.0
1-Hexanol, 2-et...	11.464	6.7	ug/l	323109	4	11.175	2405440	50.0
2-Nonanone	12.162	11.5	ug/l	553376	4	11.175	2405440	50.0