LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092525\
Data File : VV039178.D
Acq On : 25 Sep 2025 14:03
Operator : SY/MD
Sample : Q3168-06
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#2

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: VV039178.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.098	15	18	36	rVB2	30099	49652	1.65%	0.180%
2	1.233	49	60	63	rBV2	37589	70809	2.35%	0.257%
3	1.362	94	100	111	rBV	88924	111756	3.72%	0.405%
4	2.056	310	316	327	rBV2	29635	43354	1.44%	0.157%
5	2.121	328	336	357	rVV	233813	427597	14.22%	1.549%
6	2.227	361	369	389	rVB	106715	221898	7.38%	0.804%
7	3.629	796	805	825	rBV4	33021	90096	3.00%	0.326%
8	3.892	880	887	908	rVB2	27295	68659	2.28%	0.249%
9	4.503	1056	1077	1096	rBV2	412895	1107204	36.82%	4.011%
10	4.603	1096	1108	1147	rVB	436907	1201889	39.97%	4.354%
11	4.944	1202	1214	1252	rBV	453742	1152163	38.32%	4.174%
12	5.252	1295	1310	1330	rBV5	20518	59512	1.98%	0.216%
13	5.535	1387	1398	1431	rBV	727435	1662397	55.29%	6.023%
14	6.130	1574	1583	1603	rBV3	29399	93373	3.11%	0.338%
15	6.227	1604	1613	1633	rVV3	35466	87065	2.90%	0.315%
16	7.169	1896	1906	1913	rBV4	22171	40443	1.35%	0.147%
17	7.239	1917	1928	1947	rBV	925713	1746010	58.07%	6.326%
18	7.609	2033	2043	2045	rBV4	31385	43952	1.46%	0.159%
19	7.635	2045	2051	2073	rVB3	59005	130145	4.33%	0.472%
20	8.082	2181	2190	2210	rBV2	69532	160663	5.34%	0.582%
21	8.172	2210	2218	2240	rVV	120926	233816	7.78%	0.847%
22	8.776	2391	2406	2437	rBV	1109209	1943037	64.62%	7.040%
23	8.976	2451	2468	2469	rBV2	28654	62597	2.08%	0.227%
24	9.069	2491	2497	2512	rVB2	41952	79178	2.63%	0.287%
25	9.172	2514	2529	2546	rVV3	95133	289799	9.64%	1.050%
26	9.246	2547	2552	2567	rVB3	55035	92863	3.09%	0.336%
27	9.323	2568	2576	2591	rVB5	27974	59612	1.98%	0.216%
28	9.429	2600	2609	2617	rBV4	43206	81188	2.70%	0.294%
29	9.532	2634	2641	2655	rVB	65302	111335	3.70%	0.403%
30	9.632	2664	2672	2693	rBV	424138	707476	23.53%	2.563%
31	9.741	2697	2706	2718	rBV2	197902	353778	11.77%	1.282%
32	10.001	2777	2787	2816	rVV	839249	1442552	47.98%	5.226%
33	10.146	2818	2832	2842	rVB7	33462	94110	3.13%	0.341%
34	10.284	2869	2875	2892	rVB	99320	170697	5.68%	0.618%
35	10.368	2892	2901	2916	rBV3	53312	142084	4.73%	0.515%
36	10.451	2919	2927	2935	rVV5	83512	137326	4.57%	0.498%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#2

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

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Peak separation: 5

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

37	10.506	2935	2944	2970	rVB	1837466	2869213	95.42%	10.395%
38	10.628	2976	2982	2986	rBV3	50549	68653	2.28%	0.249%
39	10.667	2987	2994	3011	rVB2	201147	495799	16.49%	1.796%
40	10.866	3051	3056	3068	rVB2	104159	156404	5.20%	0.567%
41	10.966	3076	3087	3099	rBV	549590	899665	29.92%	3.260%
42	11.082	3118	3123	3134	rVB5	79566	122075	4.06%	0.442%
43	11.175	3142	3152	3170	rVB	1144136	1828231	60.80%	6.624%
44	11.265	3175	3180	3188	rVB6	56110	81039	2.70%	0.294%
45	11.709	3310	3318	3325	rBV	364351	549082	18.26%	1.989%
46	11.754	3326	3332	3347	rVB5	241417	485776	16.16%	1.760%
47	11.834	3348	3357	3372	rBV4	472040	985370	32.77%	3.570%
48	12.162	3451	3459	3474	rBV2	484066	886165	29.47%	3.211%
49	12.667	3609	3616	3625	rVB2	291100	415593	13.82%	1.506%
50	12.924	3691	3696	3702	rBV2	139693	181133	6.02%	0.656%
51	15.512	4495	4501	4513	rVB	1933460	3006828	100.00%	10.894%

Sum of corrected areas: 27601111

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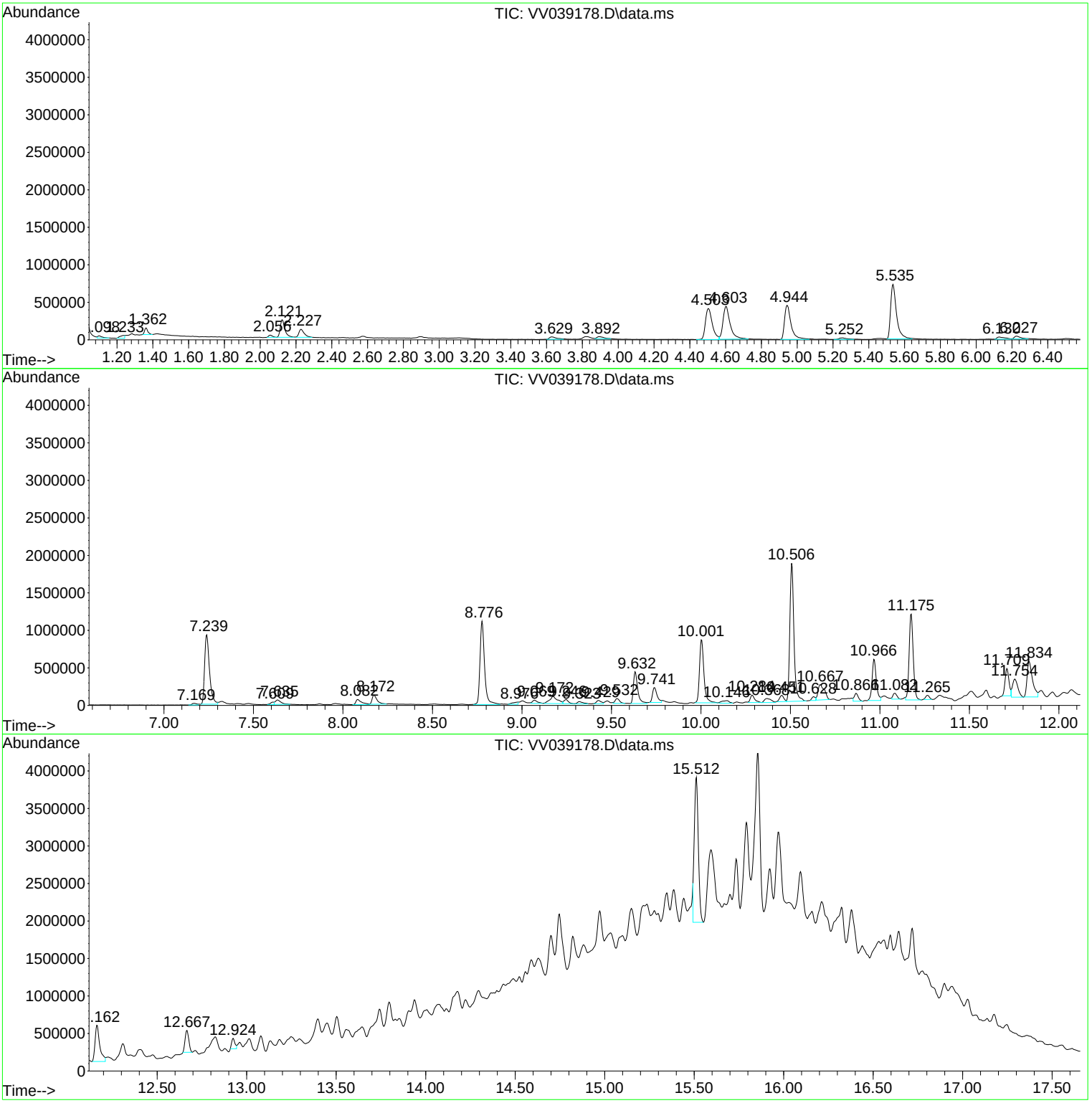
Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#2

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092525\
Data File : VV039178.D
Acq On : 25 Sep 2025 14:03
Operator : SY/MD
Sample : Q3168-06
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#2

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

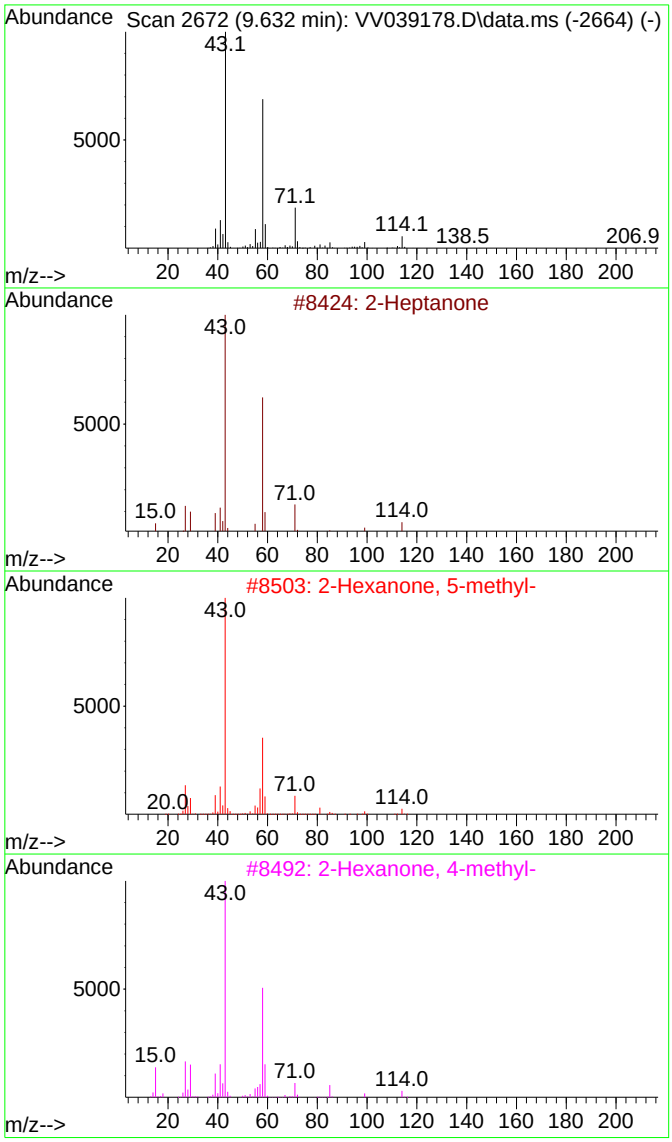
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

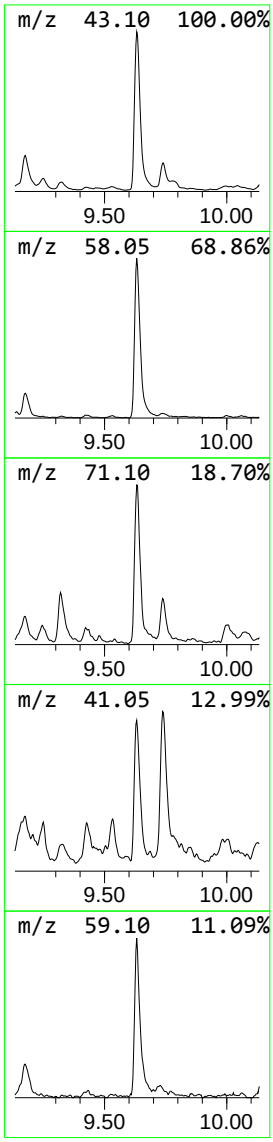
****

Peak Number 1 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.632	18.21 ug/l	707476	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	83
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	72
4	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	42
5	Hexanal, 2-methyl-	114	C7H14O	000925-54-2	42





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Data File : VV039178.D
Acq On : 25 Sep 2025 14:03
Operator : SY/MD
Sample : Q3168-06
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#2

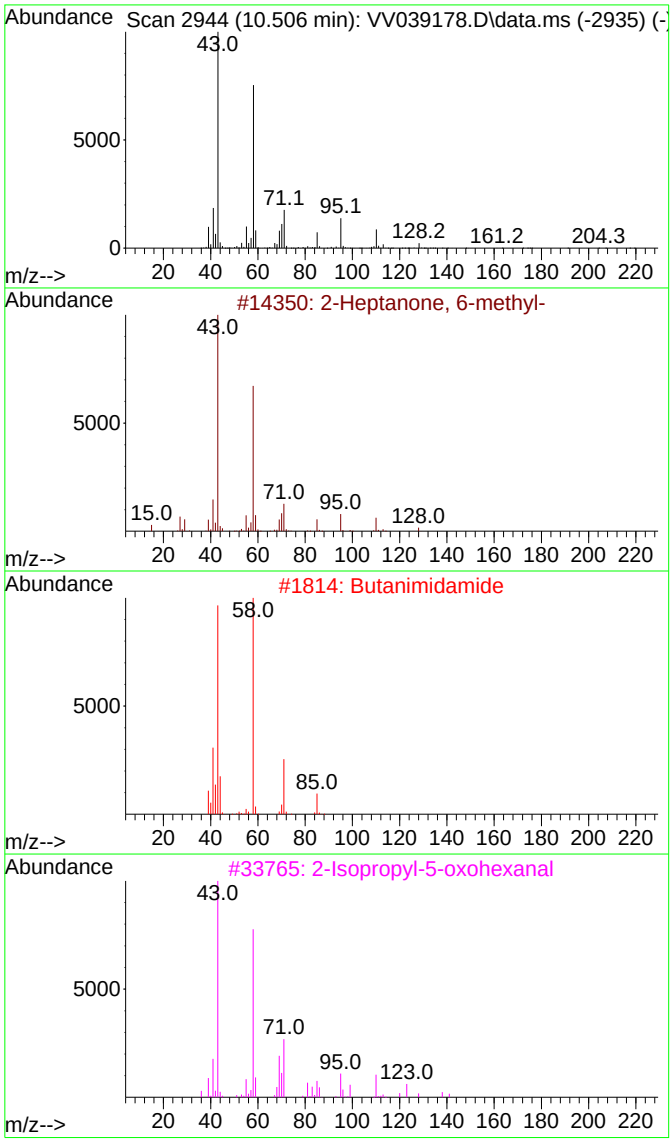
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V092225W.M
Quant Title : SW846 8260

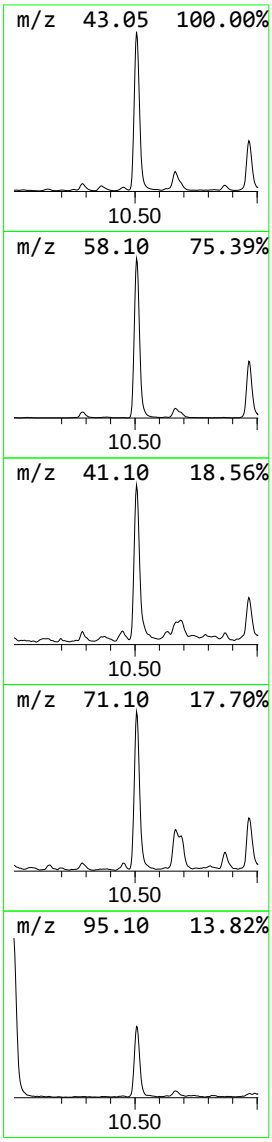
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Heptanone, 6-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.506	78.47 ug/l	2869210	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	94
2	Butanimidamide	86	C4H10N2	000107-90-4	72
3	2-Isopropyl-5-oxohexanal	156	C9H16O2	015303-46-5	64
4	2-Heptanone	114	C7H14O	000110-43-0	59
5	2-Octanone	128	C8H16O	000111-13-7	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092525\
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Acq On : 25 Sep 2025 14:03
Operator : SY/MD
Sample : Q3168-06
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#2

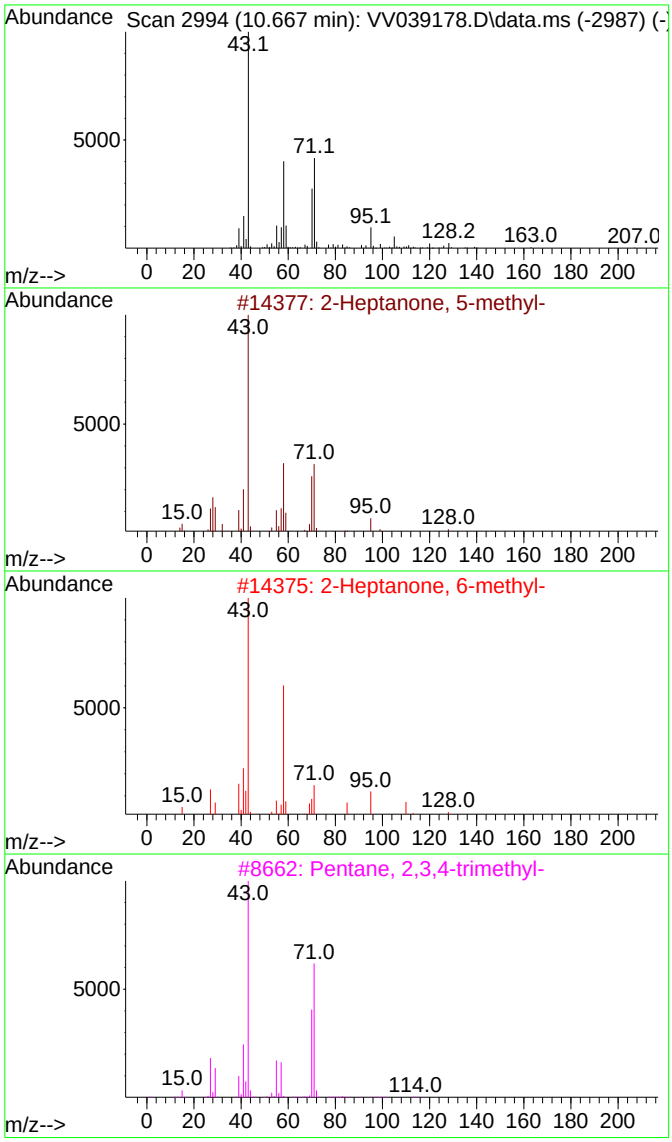
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V092225W.M
Quant Title : SW846 8260

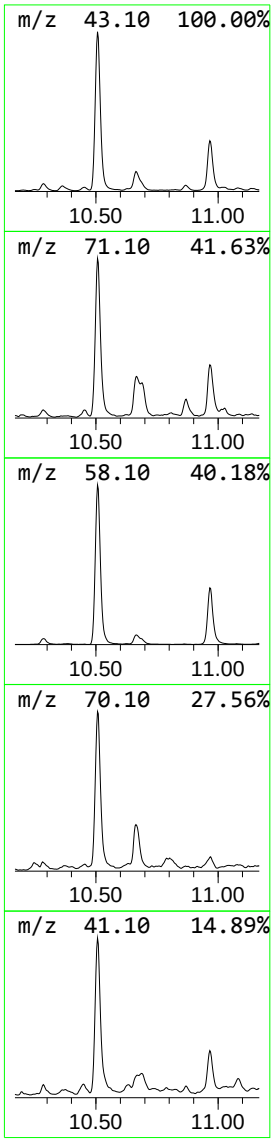
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Heptanone, 5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.667	13.56 ug/l	495799	1,4-Dichlorobenzene-d4	11.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 5-methyl-	128	C8H16O	018217-12-4	87
2	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	50
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	43
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	38
5	2-Heptanone	114	C7H14O	000110-43-0	32





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092525\
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Sample : Q3168-06
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#2

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

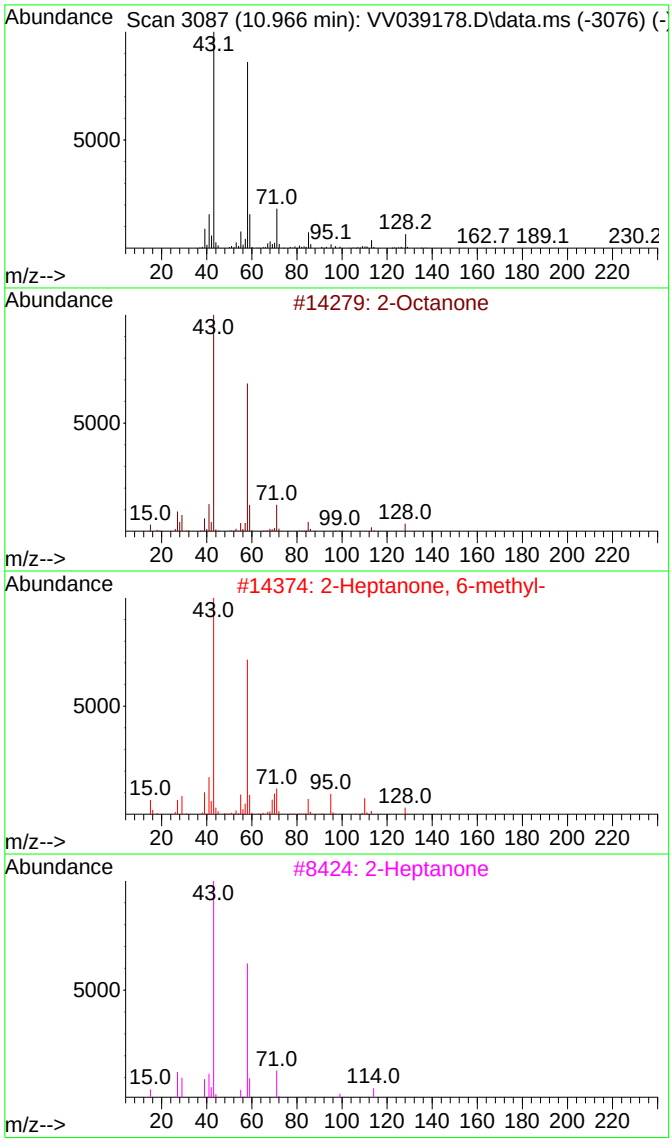
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

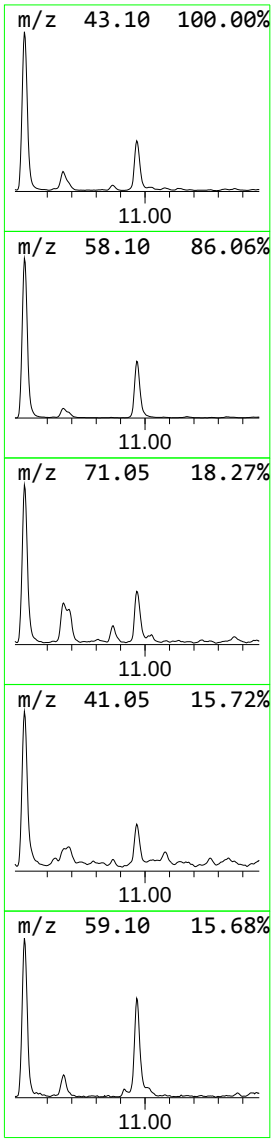
****

Peak Number 4 2-Octanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.966	24.60 ug/l	899665	1,4-Dichlorobenzene-d4	11.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	91
2	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	78
3	2-Heptanone	114	C7H14O	000110-43-0	72
4	2-Hexanone	100	C6H12O	000591-78-6	64
5	Pentanal, 2,3-dimethyl-	114	C7H14O	032749-94-3	53





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Acq On : 25 Sep 2025 14:03
Operator : SY/MD
Sample : Q3168-06
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TOTES COMP#2

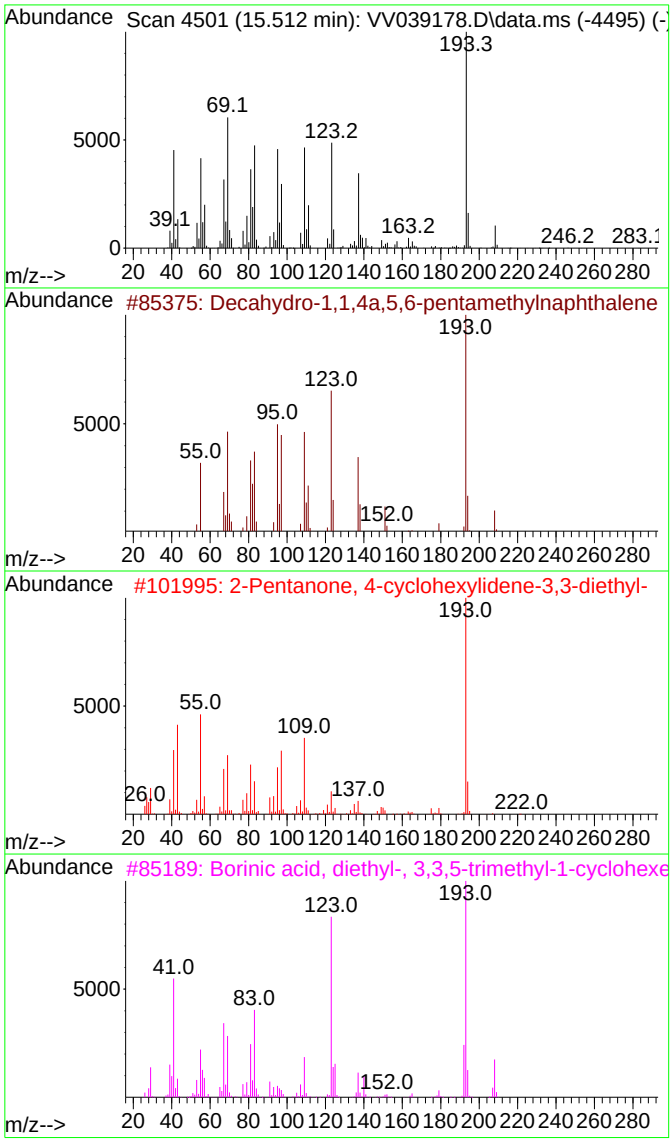
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V092225W.M
Quant Title : SW846 8260

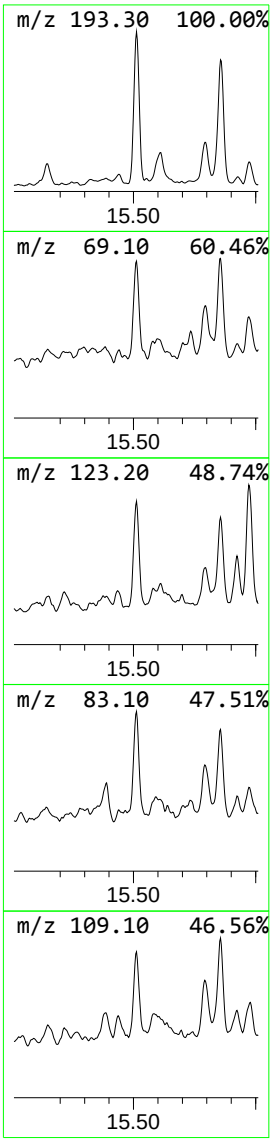
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.512	82.23 ug/l	3006830	1,4-Dichlorobenzene-d4	11.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	87
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	47
3	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	27
4	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22
5	Iminostilbene	193	C14H11N	000256-96-2	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092525\
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TOTES COMP#2

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Heptanone	9.632	18.2	ug/l	707476	3	8.776	1943040	50.0
2-Heptanone, 6-...	10.506	78.5	ug/l	2869210	4	11.175	1828230	50.0
2-Heptanone, 5-...	10.667	13.6	ug/l	495799	4	11.175	1828230	50.0
2-Octanone	10.966	24.6	ug/l	899665	4	11.175	1828230	50.0
Decahydro-1,1,4...	15.512	82.2	ug/l	3006830	4	11.175	1828230	50.0