LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044877.D
Acq On : 26 Sep 2021 07:48
Operator : SY/MD
Sample : M3888-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20898

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_U\Method\82U092421W.M
Title : SW846 8260

Signal : TIC: VU044877.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	36	44	53	rBV2	10765	16017	1.23%	0.111%
2	1.684	101	107	116	rVB	34560	40733	3.13%	0.281%
3	2.289	286	295	309	rBV	16096	28137	2.16%	0.194%
4	2.626	387	400	415	rBV	366800	618171	47.53%	4.269%
5	2.761	430	442	464	rBV	66121	135987	10.46%	0.939%
6	2.951	490	501	523	rVB	21113	38706	2.98%	0.267%
7	3.182	557	573	591	rBV	67104	157099	12.08%	1.085%
8	4.256	894	907	925	rVB2	8774	19974	1.54%	0.138%
9	4.449	952	967	990	rBV	45105	111140	8.55%	0.768%
10	4.562	990	1002	1015	rVB7	6261	15787	1.21%	0.109%
11	4.706	1033	1047	1075	rVB	82575	186952	14.37%	1.291%
12	4.986	1121	1134	1148	rBV2	9974	24960	1.92%	0.172%
13	5.295	1214	1230	1243	rBV	189229	400106	30.76%	2.763%
14	5.378	1243	1256	1277	rVB	332957	679585	52.25%	4.693%
15	5.706	1342	1358	1370	rBV	229737	469500	36.10%	3.242%
16	5.777	1370	1380	1394	rVB	106251	213650	16.43%	1.475%
17	6.157	1490	1498	1512	rBV3	8391	21809	1.68%	0.151%
18	6.253	1515	1528	1566	rVB	500248	971961	74.73%	6.712%
19	6.523	1601	1612	1642	rBV2	20557	62638	4.82%	0.433%
20	6.771	1677	1689	1706	rBV	118129	214778	16.51%	1.483%
21	7.475	1895	1908	1924	rBV	42487	74233	5.71%	0.513%
22	7.726	1979	1986	1998	rVB2	11290	18538	1.43%	0.128%
23	7.902	2019	2041	2053	rBV	753794	1300601	100.00%	8.982%
24	7.973	2053	2063	2077	rVB	230918	393965	30.29%	2.721%
25	8.449	2201	2211	2233	rVV5	5497	15229	1.17%	0.105%
26	8.552	2233	2243	2258	rVB	11492	19341	1.49%	0.134%
27	8.687	2275	2285	2289	rBV3	8765	13691	1.05%	0.095%
28	8.729	2289	2298	2310	rVV	80134	134649	10.35%	0.930%
29	8.800	2310	2320	2337	rVB3	35454	69370	5.33%	0.479%
30	8.915	2342	2356	2374	rVB2	9870	18809	1.45%	0.130%
31	9.420	2500	2513	2524	rBV	684679	1116602	85.85%	7.711%
32	9.571	2551	2560	2576	rVB	33923	57845	4.45%	0.399%
33	9.658	2576	2587	2590	rVV3	41867	61308	4.71%	0.423%
34	9.693	2591	2598	2615	rVB	187716	313082	24.07%	2.162%
35	9.828	2630	2640	2647	rBV2	16902	28727	2.21%	0.198%
36	9.918	2659	2668	2684	rVB2	47003	76184	5.86%	0.526%

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Instrument : MSVOA_U
ClientSampleId : 20898

Integration Parameters: RTEINT.P
Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

37	10.111	2715	2728	2745	rBV6	124117	344651	26.50%	2.380%
38	10.234	2746	2766	2778	rVV3	44414	127143	9.78%	0.878%
39	10.365	2794	2807	2816	rBV4	16191	32569	2.50%	0.225%
40	10.635	2878	2891	2902	rBV	537776	856187	65.83%	5.913%
41	10.687	2902	2907	2918	rVV3	18969	35597	2.74%	0.246%
42	10.748	2919	2926	2937	rVB5	11660	20404	1.57%	0.141%
43	10.915	2968	2978	2989	rBV2	24807	39220	3.02%	0.271%
44	11.002	2989	3005	3010	rBV4	25363	45275	3.48%	0.313%
45	11.092	3028	3033	3045	rVB	17115	26194	2.01%	0.181%
46	11.237	3067	3078	3085	rBV2	20670	36702	2.82%	0.253%
47	11.295	3085	3096	3114	rVB5	27651	64127	4.93%	0.443%
48	11.378	3115	3122	3139	rVB6	11506	26252	2.02%	0.181%
49	11.471	3140	3151	3162	rVB	94968	147917	11.37%	1.022%
50	11.539	3163	3172	3179	rBV	24614	39006	3.00%	0.269%
51	11.616	3190	3196	3223	rVB2	23099	50850	3.91%	0.351%
52	11.732	3223	3232	3240	rBV7	10206	20197	1.55%	0.139%
53	11.815	3246	3258	3274	rVB	712141	1122404	86.30%	7.751%
54	11.896	3274	3283	3293	rVV	33095	53560	4.12%	0.370%
55	11.954	3293	3301	3314	rVB8	10318	18755	1.44%	0.130%
56	12.063	3323	3335	3363	rBV	339995	661502	50.86%	4.568%
57	12.314	3401	3413	3428	rBV	261748	412937	31.75%	2.852%
58	12.510	3466	3474	3483	rVB7	15048	24380	1.87%	0.168%
59	12.819	3552	3570	3583	rBV2	55120	109627	8.43%	0.757%
60	13.024	3626	3634	3644	rVB3	10549	19001	1.46%	0.131%
61	13.455	3759	3768	3779	rVB4	11918	19750	1.52%	0.136%
62	13.523	3779	3789	3801	rVB3	26604	42885	3.30%	0.296%
63	13.629	3811	3822	3839	rVB3	30311	50847	3.91%	0.351%
64	13.860	3881	3894	3905	rBV3	7209	15416	1.19%	0.106%
65	14.008	3932	3940	3952	rBV3	15508	25115	1.93%	0.173%
66	14.089	3952	3965	3980	rBV	710416	1137058	87.43%	7.853%
67	14.211	3994	4003	4021	rVB3	44043	95079	7.31%	0.657%
68	14.680	4138	4149	4158	rBV7	7592	14454	1.11%	0.100%
69	15.227	4306	4319	4337	rVB	160658	263809	20.28%	1.822%
70	15.413	4364	4377	4394	rBV	120835	198402	15.25%	1.370%
71	15.957	4536	4546	4553	rBV2	11879	17962	1.38%	0.124%
72	16.265	4632	4642	4658	rBV2	16398	31278	2.40%	0.216%
73	16.410	4676	4687	4694	rBV2	27656	45525	3.50%	0.314%
74	16.452	4694	4700	4711	rVB	15376	23685	1.82%	0.164%
75	16.642	4743	4759	4773	rBV5	10003	24554	1.89%	0.170%

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ClientSampleId : 20898

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Title : SW846 8260

Sum of corrected areas: 14480140

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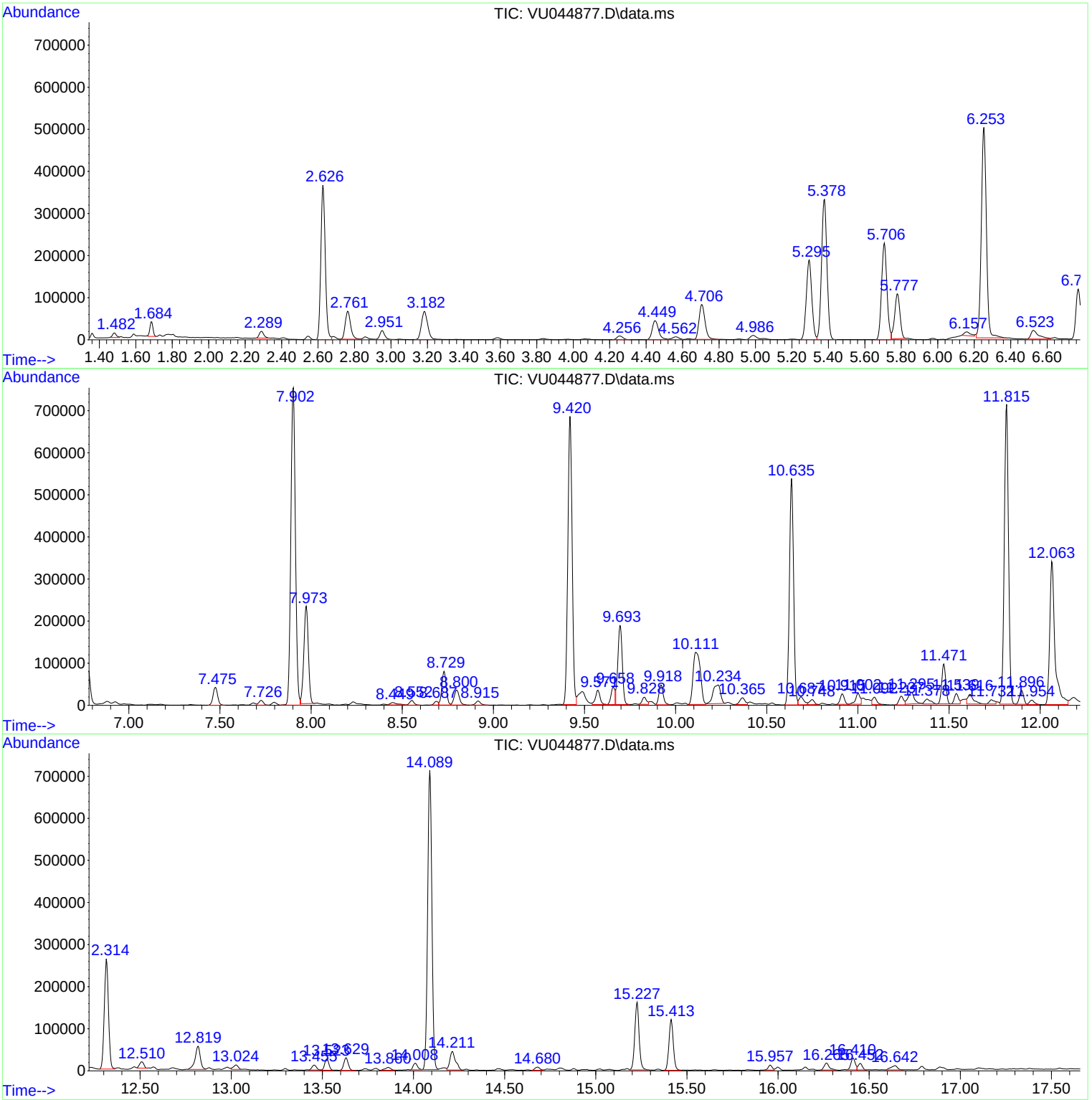
Instrument :
MSVOA_U
ClientSampleId :
20898

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
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ALS Vial : 52 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20898

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

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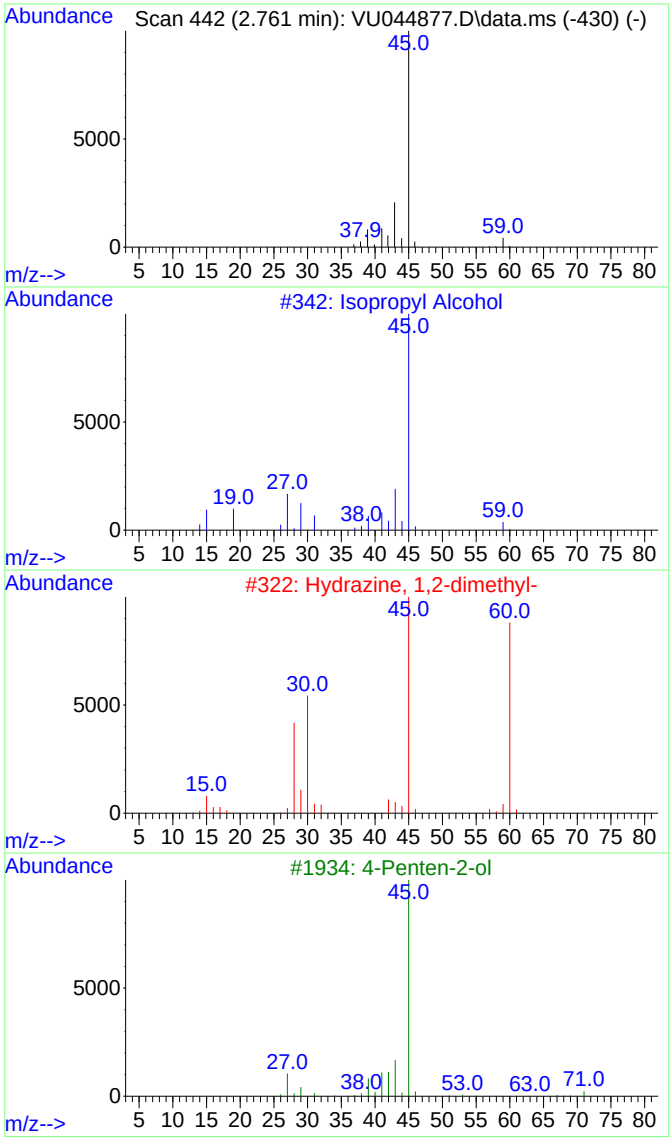
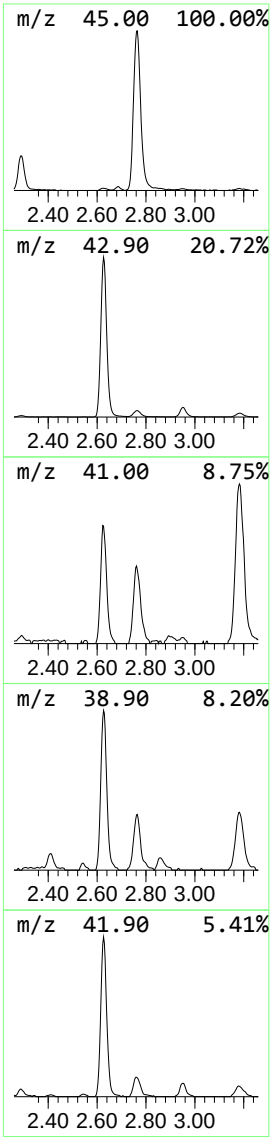
Peak Number 1 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.761	10.01 ug/l	135987	Pentafluorobenzene	5.378

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3	4-Penten-2-ol	86	C5H10O	000625-31-0	9
4	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
5	Formamide	45	CH3NO	000075-12-7	5





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Instrument : MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

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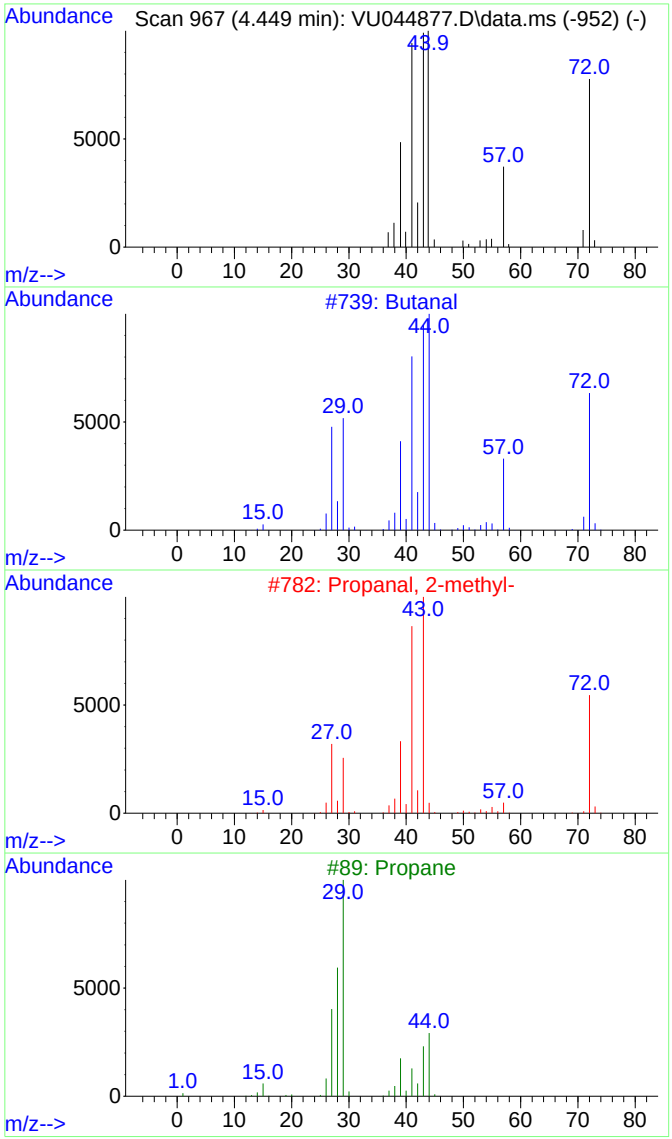
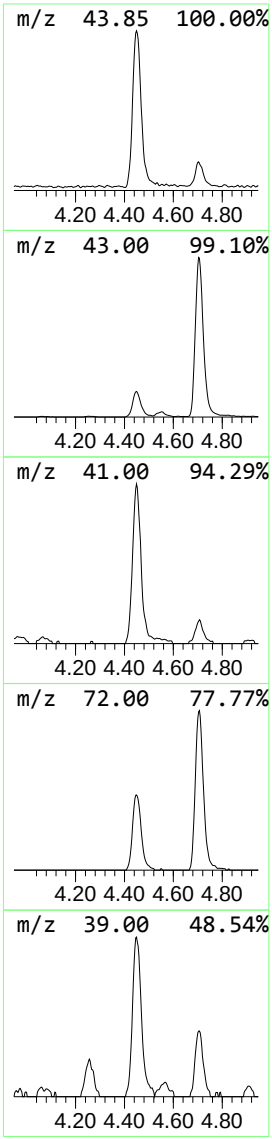
Peak Number 2 Butanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.449	8.18 ug/l	111140	Pentafluorobenzene	5.378

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
3	Propane	44	C3H8	000074-98-6	47
4	Ethene, ethoxy-	72	C4H8O	000109-92-2	40
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38





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Instrument : MSVOA_U
ClientSampleId : 20898

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

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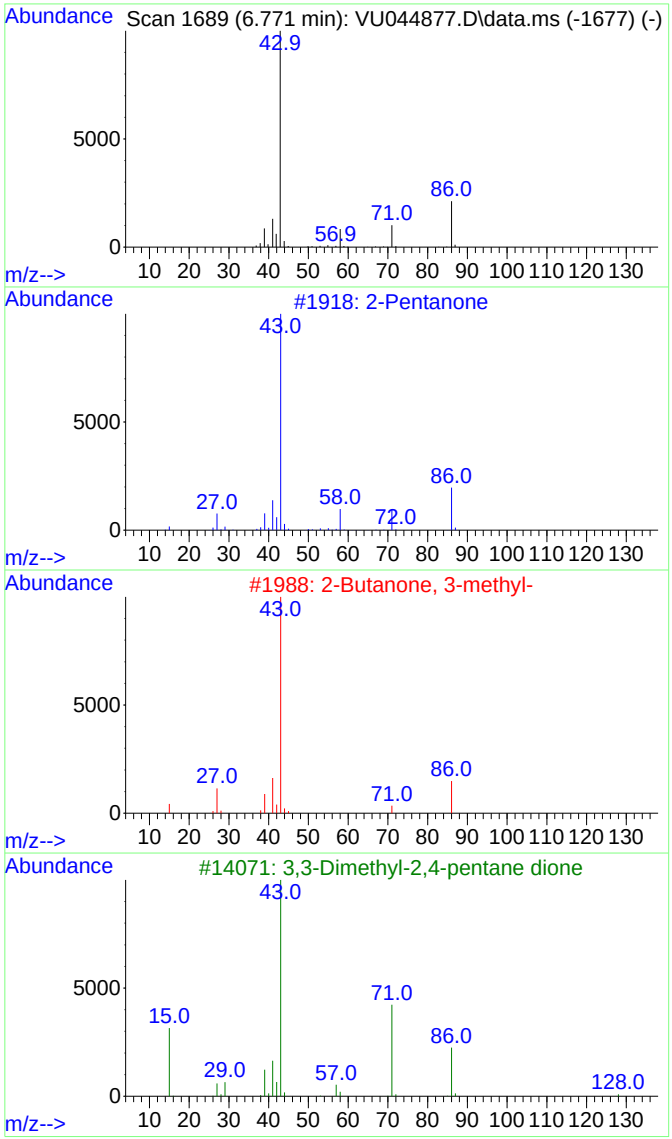
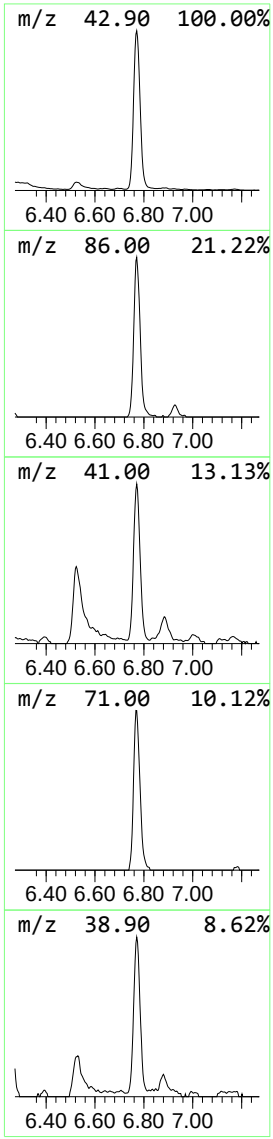
Peak Number 3 2-Pentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.771	11.05 ug/l	214778	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	36
4	Butane	58	C4H10	000106-97-8	9
5	2,3-Butanedione	86	C4H6O2	000431-03-8	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

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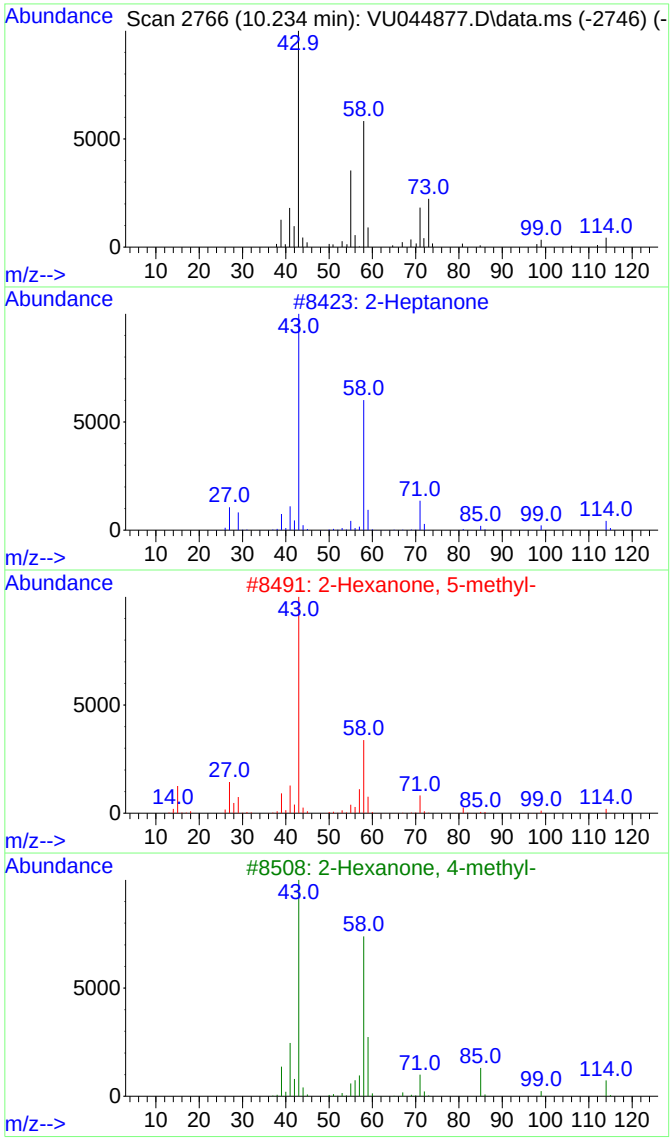
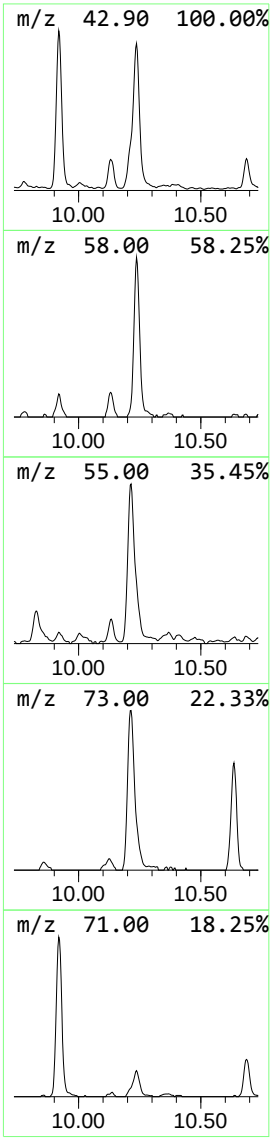
Peak Number 4 2-Heptanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.234	5.69 ug/l	127143	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	64
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	47
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43
4	S-[2-[N,N-Dimethylamino]ethyl]mo...	261	C10H19N3O3S	1000212-14-3	43
5	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	43





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

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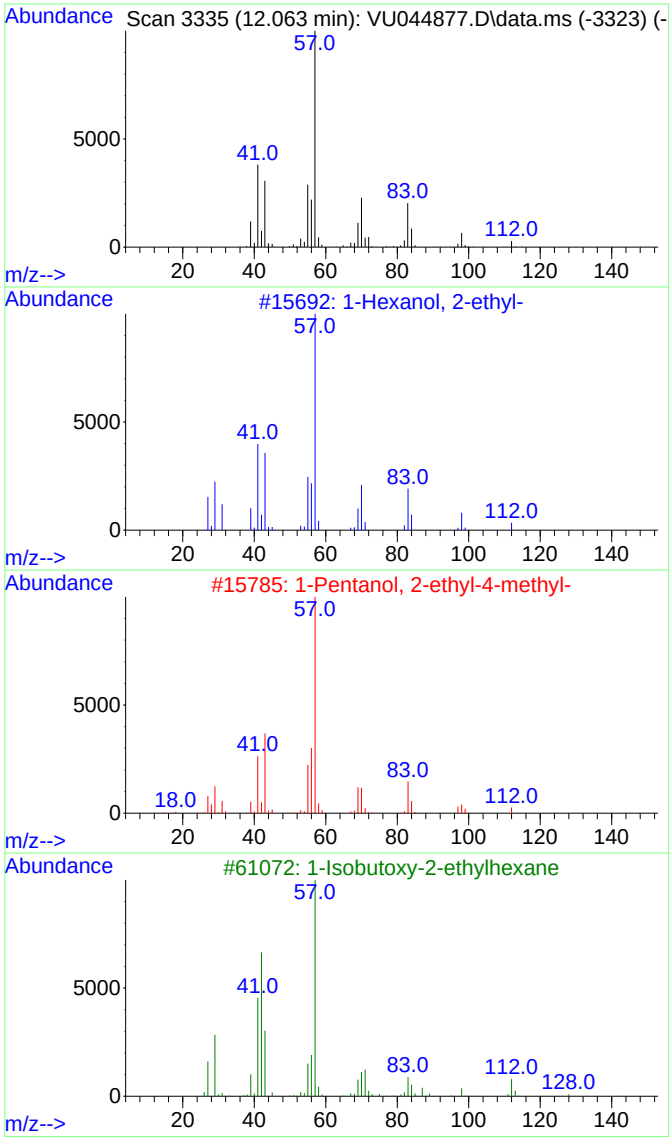
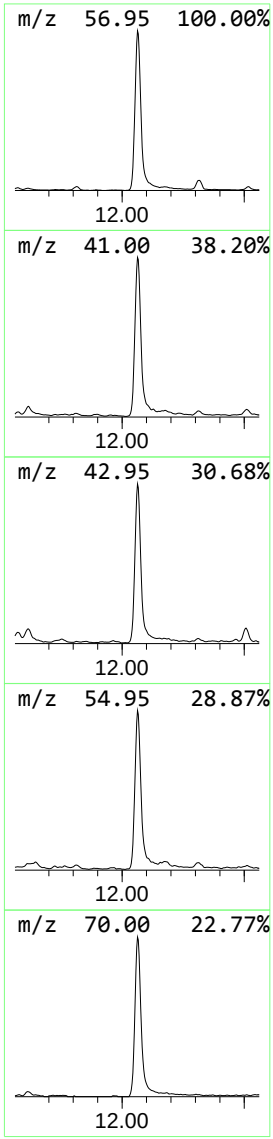
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	29.47 ug/l	661502	1,4-Dichlorobenzene-d4	11.816

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	56
3	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53





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ALS Vial : 52 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20898

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

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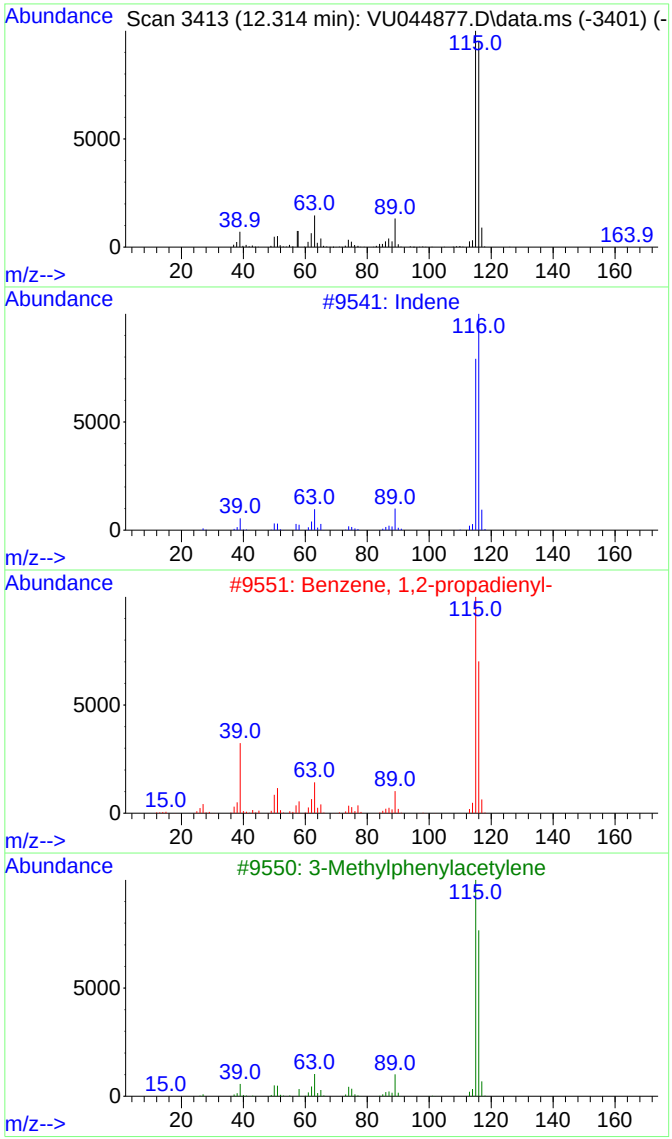
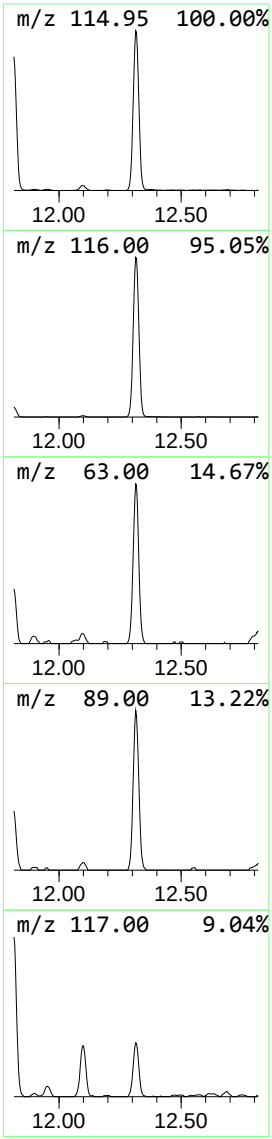
Peak Number 6 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.314	18.40 ug/l	412937	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	95
2	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90





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ClientSampleId : 20898

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Quant Title : SW846 8260

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

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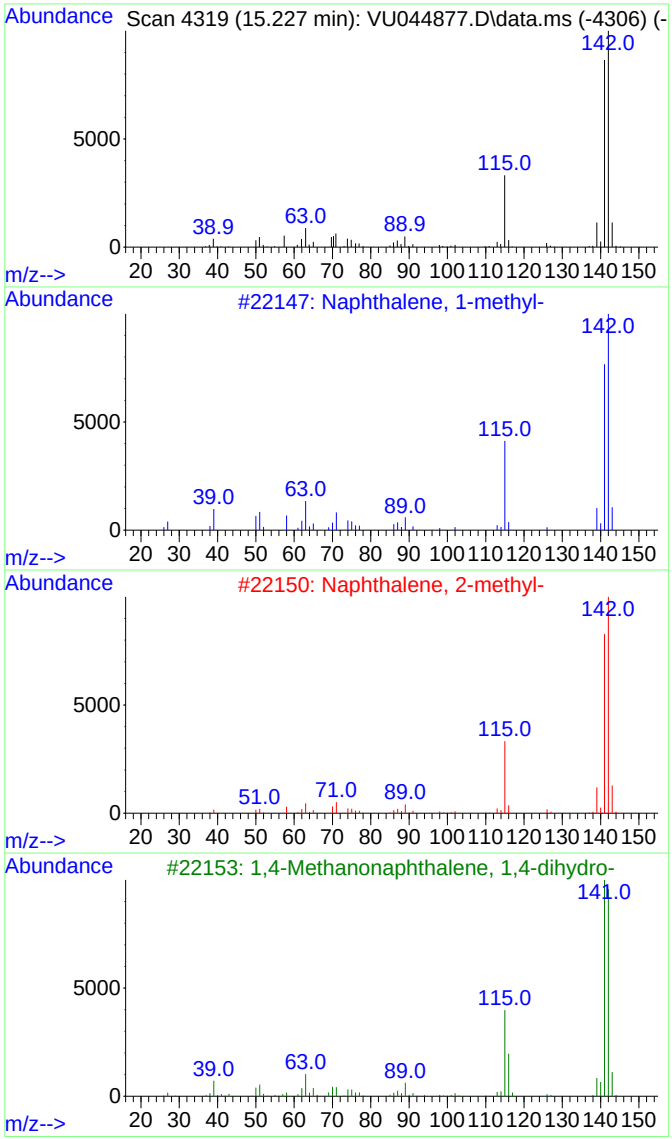
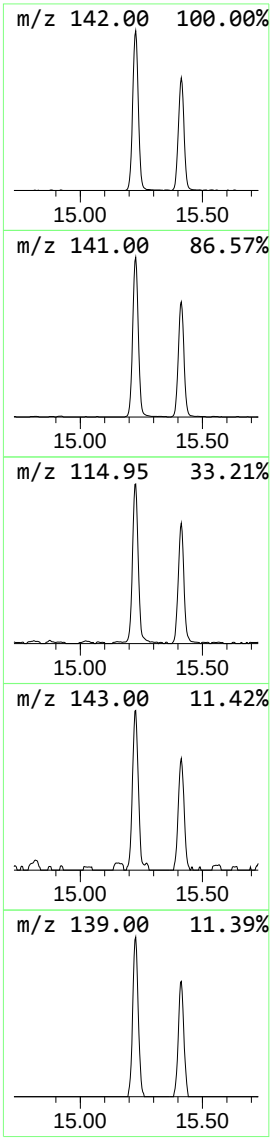
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	11.75 ug/l	263809	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044877.D
Acq On : 26 Sep 2021 07:48
Operator : SY/MD
Sample : M3888-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20898

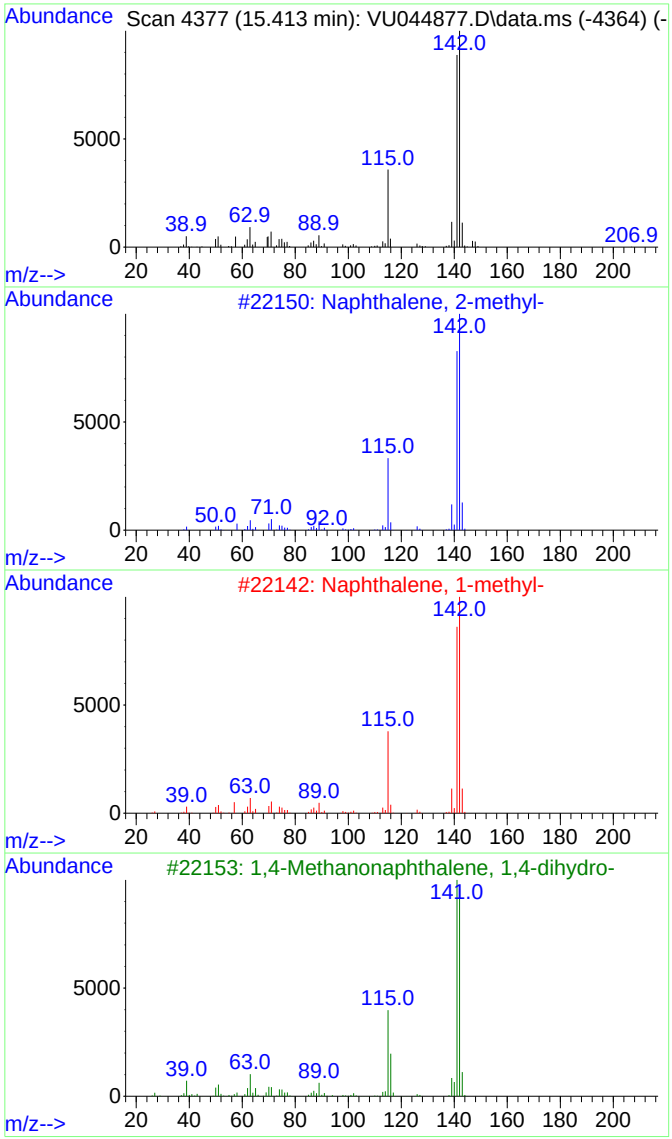
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

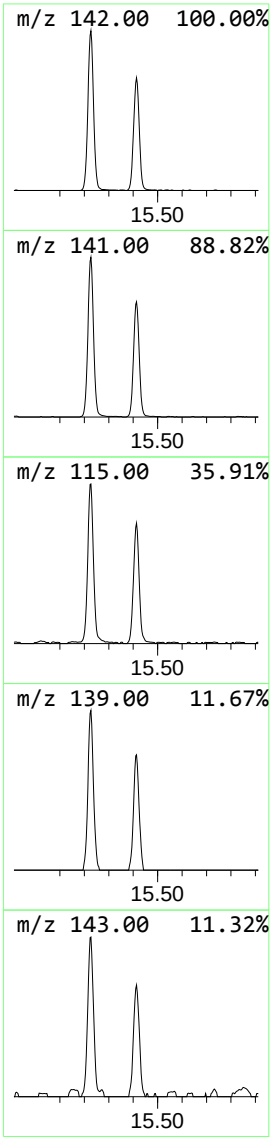
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.413	8.84 ug/l	198402	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044877.D
Acq On : 26 Sep 2021 07:48
Operator : SY/MD
Sample : M3888-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20898

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.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
Isopropyl Alcohol	2.761	10.0	ug/l	135987	1	5.378	679585	50.0
Butanal	4.449	8.2	ug/l	111140	1	5.378	679585	50.0
2-Pentanone	6.771	11.1	ug/l	214778	2	6.253	971961	50.0
2-Heptanone	10.234	5.7	ug/l	127143	3	9.420	1116600	50.0
1-Hexanol, 2-et...	12.063	29.5	ug/l	661502	4	11.816	1122400	50.0
Indene	12.314	18.4	ug/l	412937	4	11.816	1122400	50.0
Naphthalene, 1-...	15.227	11.8	ug/l	263809	4	11.816	1122400	50.0
Naphthalene, 2-...	15.413	8.8	ug/l	198402	4	11.816	1122400	50.0