LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044870.D
Acq On : 26 Sep 2021 05:04
Operator : SY/MD
Sample : M3888-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20897

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: VU044870.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.687	101	108	131	rVB	341574	439912	4.25%	0.769%
2	1.790	134	140	153	rVB2	81796	107534	1.04%	0.188%
3	2.690	411	420	435	rVB	93836	161061	1.56%	0.282%
4	2.793	435	452	466	rBV3	52537	192583	1.86%	0.337%
5	5.295	1214	1230	1243	rBV3	205552	439977	4.25%	0.769%
6	5.378	1243	1256	1274	rVB	335277	684150	6.62%	1.196%
7	5.706	1343	1358	1367	rBV	231251	467716	4.52%	0.818%
8	5.780	1367	1381	1431	rVB	4687060	9423328	91.12%	16.474%
9	6.253	1515	1528	1580	rVB	510315	1035148	10.01%	1.810%
10	7.475	1895	1908	1923	rBV	98538	168432	1.63%	0.294%
11	7.902	2023	2041	2051	rBV	760513	1296298	12.54%	2.266%
12	7.973	2051	2063	2093	rVV	6109423	10341255	100.00%	18.079%
13	8.275	2145	2157	2176	rVB	67258	116876	1.13%	0.204%
14	8.732	2287	2299	2309	rBV2	324881	556950	5.39%	0.974%
15	8.799	2309	2320	2340	rVB	728855	1270522	12.29%	2.221%
16	9.420	2496	2513	2521	rBV	687782	1118391	10.81%	1.955%
17	9.468	2521	2528	2545	rVV	382813	627771	6.07%	1.097%
18	9.574	2545	2561	2577	rVV	581998	945959	9.15%	1.654%
19	9.697	2578	2599	2621	rBV	3060941	5081016	49.13%	8.883%
20	9.832	2626	2641	2650	rBV3	158295	294936	2.85%	0.516%
21	10.105	2714	2726	2745	rVB4	2734264	4799319	46.41%	8.390%
22	10.369	2790	2808	2821	rBV6	166821	402426	3.89%	0.704%
23	10.635	2879	2891	2903	rBV	539961	890247	8.61%	1.556%
24	10.700	2903	2911	2929	rVB2	69073	155358	1.50%	0.272%
25	10.912	2966	2977	2986	rBV2	74796	147289	1.42%	0.257%
26	10.976	2988	2997	2999	rVV	135278	198735	1.92%	0.347%
27	10.999	3000	3004	3020	rVV	211636	437820	4.23%	0.765%
28	11.092	3021	3033	3049	rVB	165191	298083	2.88%	0.521%
29	11.295	3087	3096	3106	rBV	108946	209385	2.02%	0.366%
30	11.404	3121	3130	3140	rVB	115962	191848	1.86%	0.335%
31	11.471	3140	3151	3162	rVB	661856	1011862	9.78%	1.769%
32	11.539	3162	3172	3180	rBV	138064	210775	2.04%	0.368%
33	11.732	3223	3232	3244	rVB	79317	125621	1.21%	0.220%
34	11.815	3246	3258	3270	rVB	706487	1102559	10.66%	1.928%
35	11.896	3272	3283	3292	rBV	242855	392654	3.80%	0.686%
36	11.947	3292	3299	3313	rVB5	95157	169672	1.64%	0.297%

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ALS Vial : 45 Sample Multiplier: 1

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

37	12.095	3339	3345	3359	rVB	130243	204032	1.97%	0.357%
38	12.314	3401	3413	3426	rBV	1128412	1798432	17.39%	3.144%
39	12.815	3555	3569	3584	rBV	274618	483928	4.68%	0.846%
40	14.089	3951	3965	3982	rBV	4223846	6936210	67.07%	12.126%
41	14.208	3993	4002	4019	rVB	152518	262087	2.53%	0.458%
42	15.018	4241	4254	4277	rVB4	70197	163901	1.58%	0.287%
43	15.224	4307	4318	4334	rBV	567921	897540	8.68%	1.569%
44	15.413	4364	4377	4395	rBV	428346	718904	6.95%	1.257%
45	16.410	4677	4687	4694	rBV	69188	113803	1.10%	0.199%
46	16.606	4737	4748	4771	rVB7	37492	108323	1.05%	0.189%

Sum of corrected areas: 57200628

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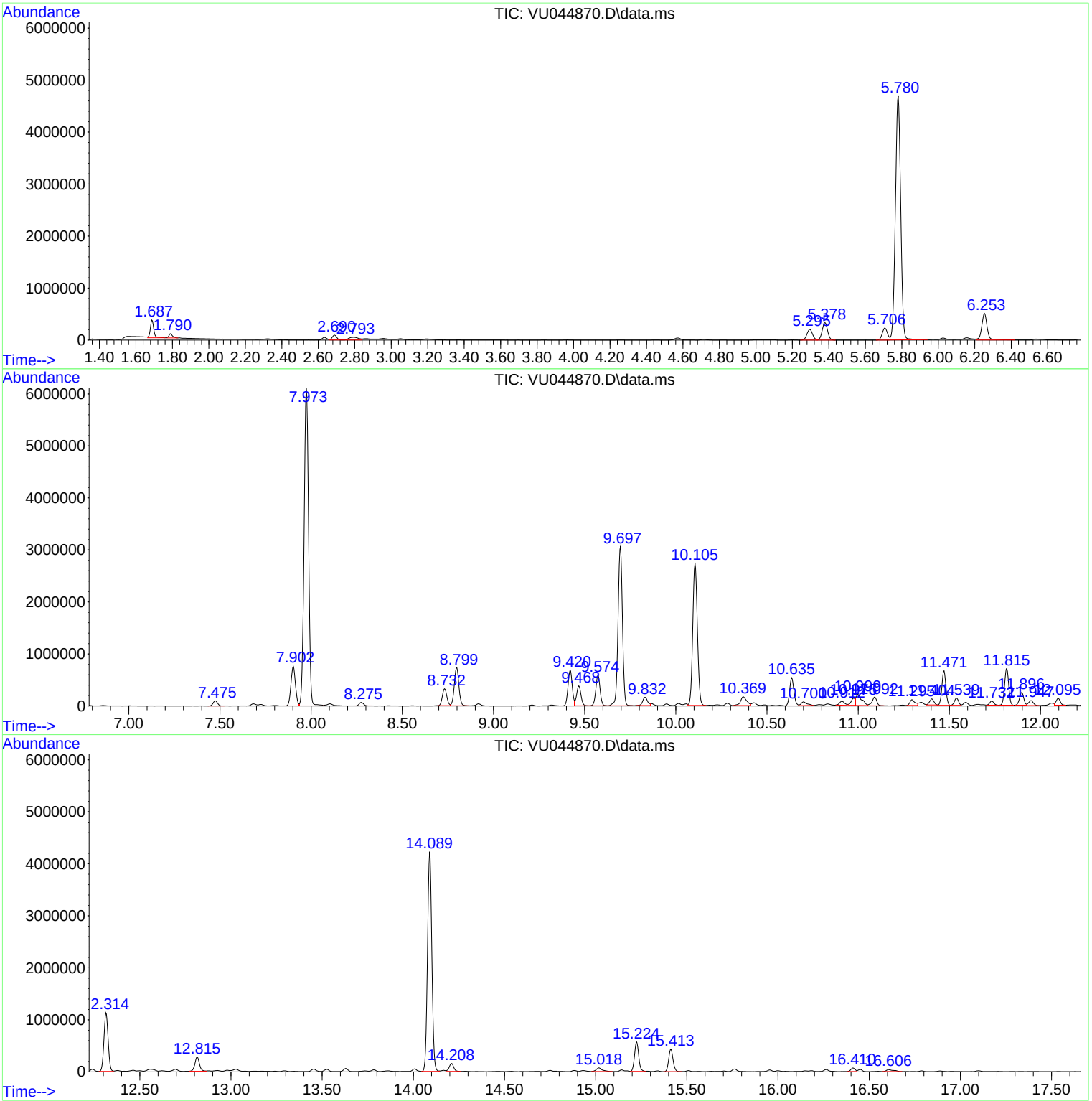
MSVOA_U
ClientSampleId :
20897

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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Data File : VU044870.D
Acq On : 26 Sep 2021 05:04
Operator : SY/MD
Sample : M3888-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20897

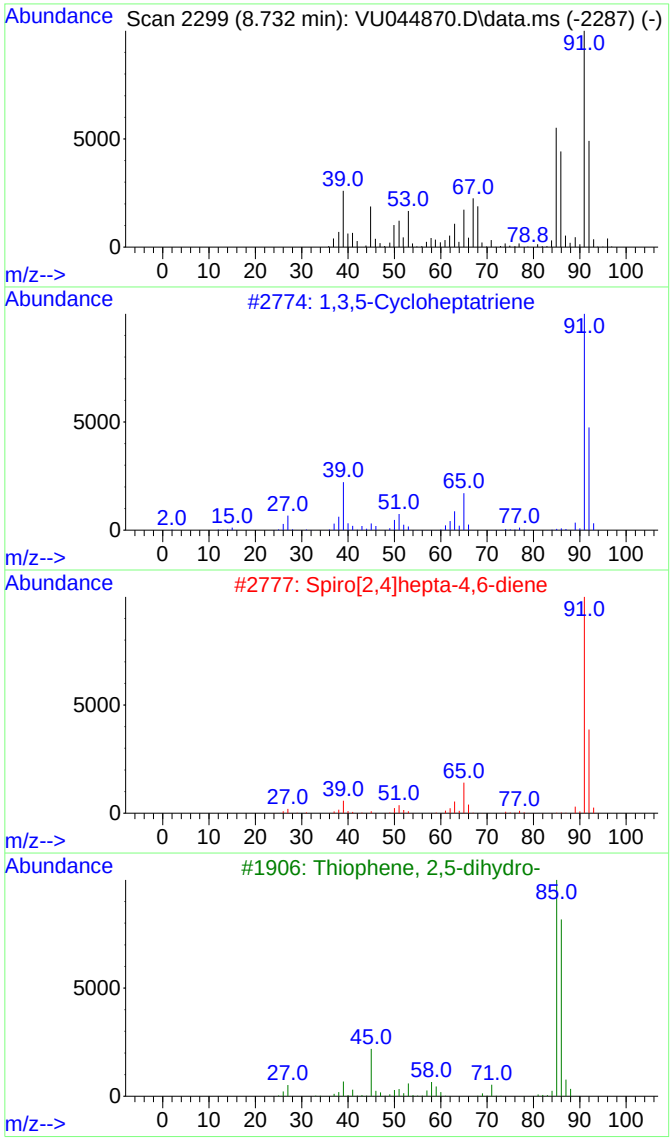
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

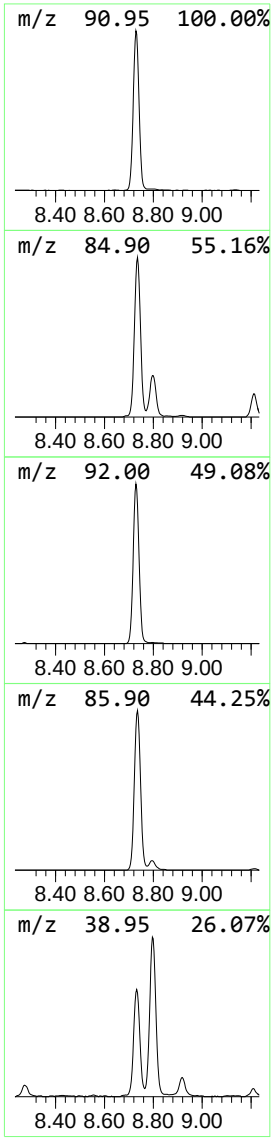
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.732	24.90 ug/l	556950	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	70
2	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	70
3	Thiophene, 2,5-dihydro-	86	C4H6S	001708-32-3	38
4	Toluene	92	C7H8	000108-88-3	38
5	2,5-Norbornadiene	92	C7H8	000121-46-0	38





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Acq On : 26 Sep 2021 05:04
Operator : SY/MD
Sample : M3888-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20897

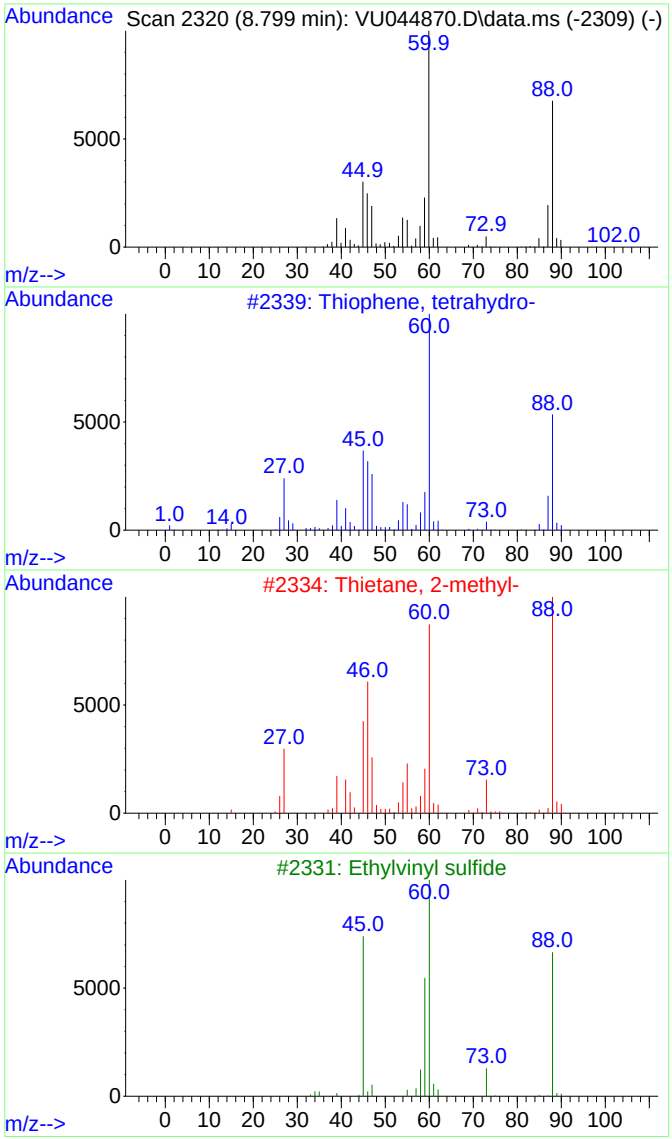
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

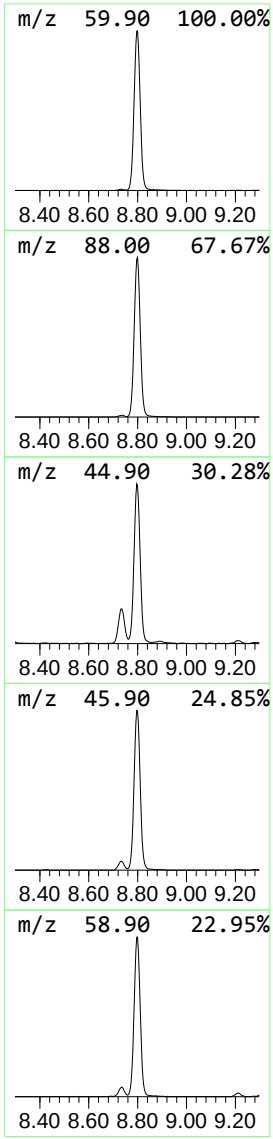
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Thiophene, tetrahydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.799	56.80 ug/l	1270520	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2	Thietane, 2-methyl-	88	C4H8S	017837-41-1	43
3	Ethylvinyl sulfide	88	C4H8S	000627-50-9	40
4	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33
5	Acetic acid, nitro-, ethyl ester	133	C4H7NO4	000626-35-7	25





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Acq On : 26 Sep 2021 05:04
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Sample : M3888-06
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ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20897

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

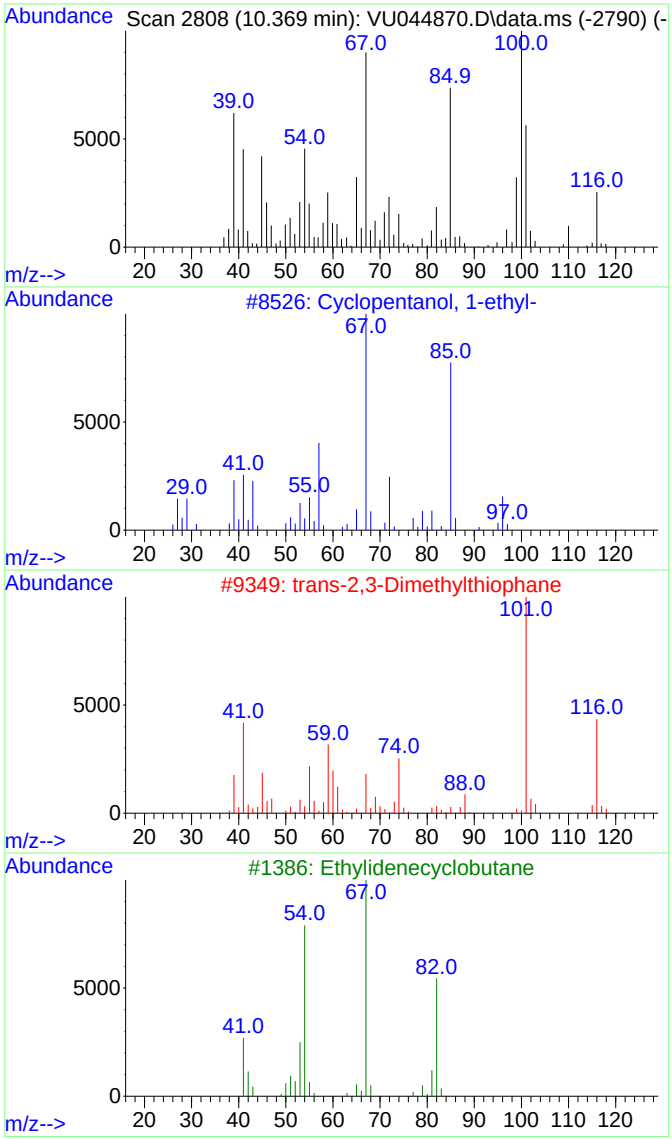
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

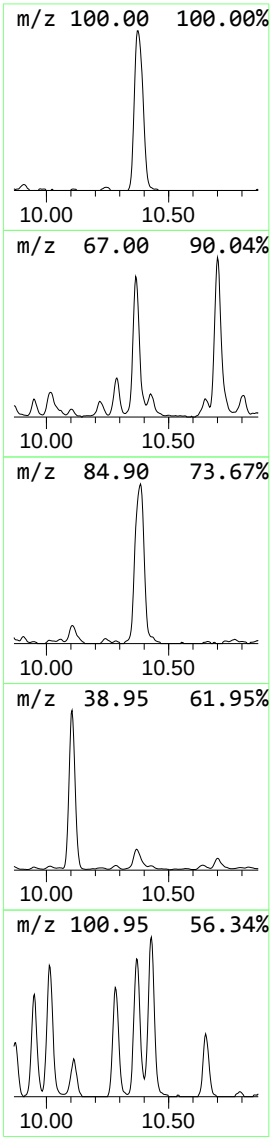
****

Peak Number 4 unknown10.368 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.368	17.99 ug/l	402426	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanol, 1-ethyl-	114	C7H14O	001462-96-0	27
2	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	15
3	Ethylidenecyclobutane	82	C6H10	001528-21-8	11
4	Bicyclo[3.1.0]hexane	82	C6H10	000285-58-5	11
5	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	11





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Sample : M3888-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20897

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

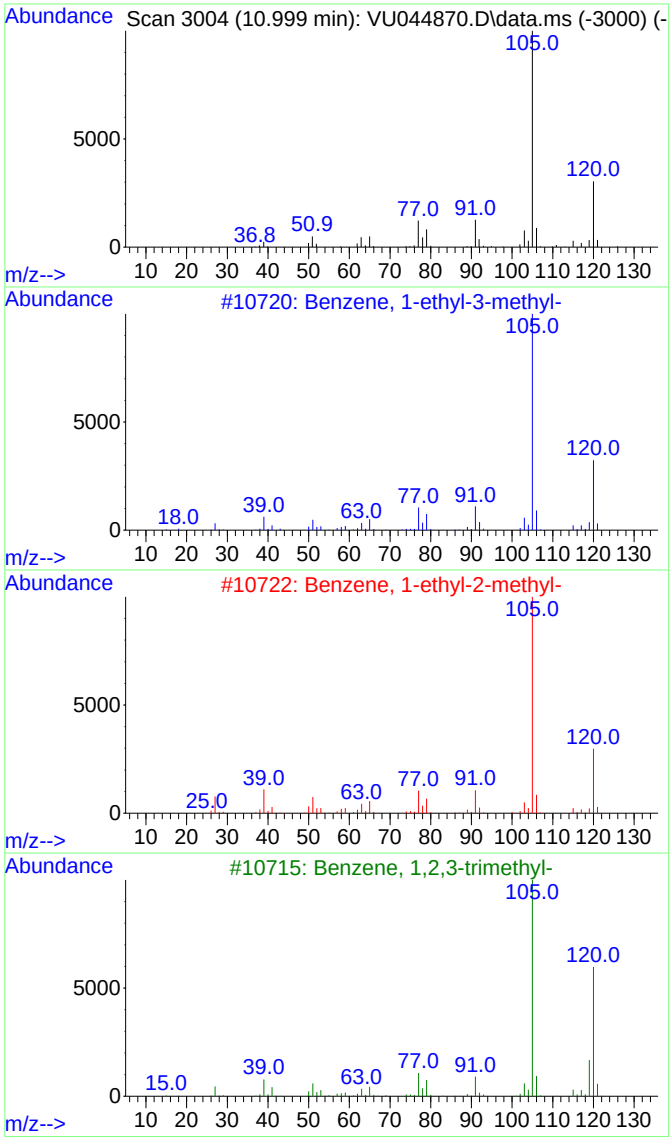
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

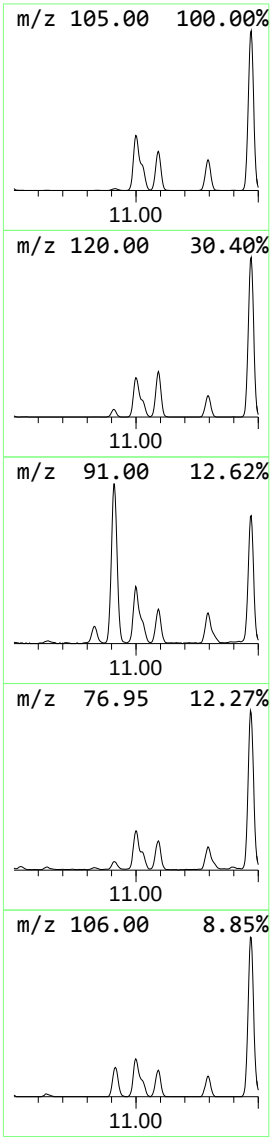
****

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.999	19.85 ug/l	437820	1,4-Dichlorobenzene-d4	11.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





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ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20897

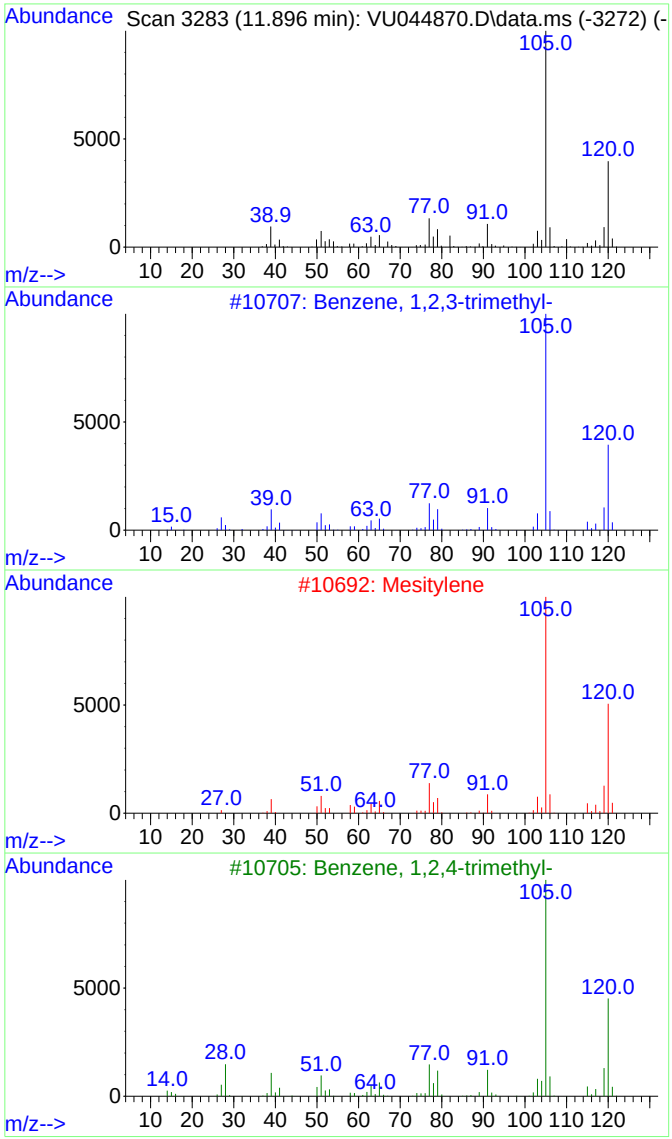
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

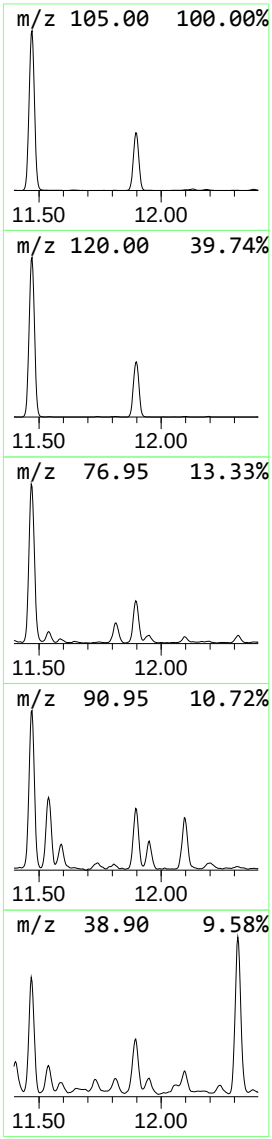
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.896	17.81 ug/l	392654	1,4-Dichlorobenzene-d4	11.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Mesitylene	120	C9H12	000108-67-8	97
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90





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Instrument : MSVOA_U
ClientSampleId : 20897

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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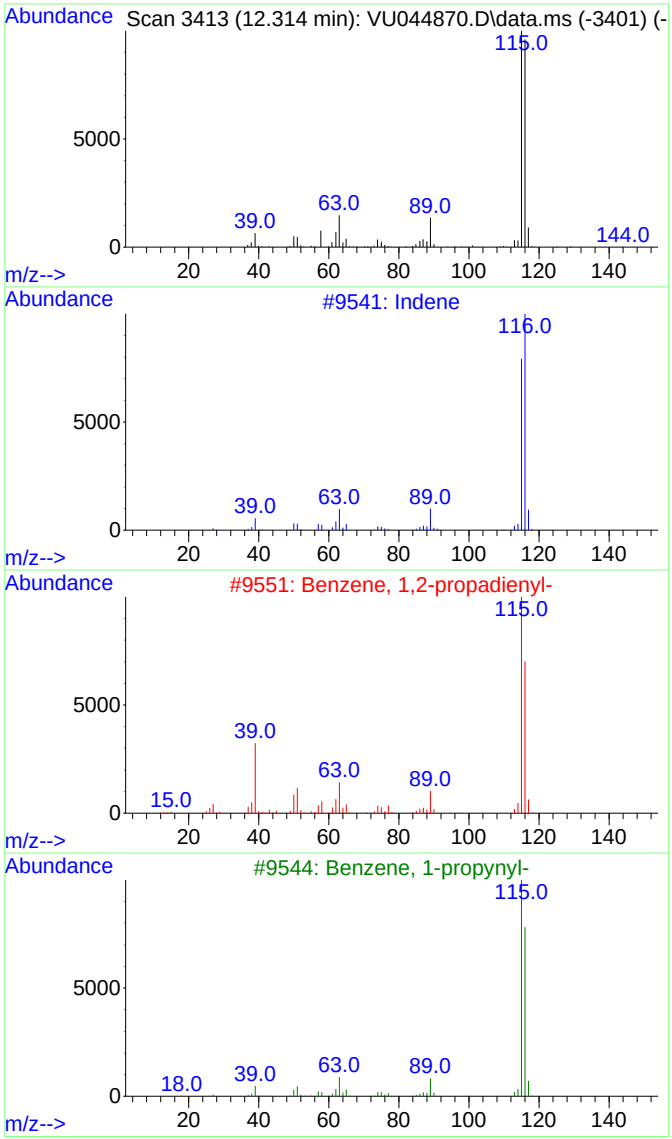
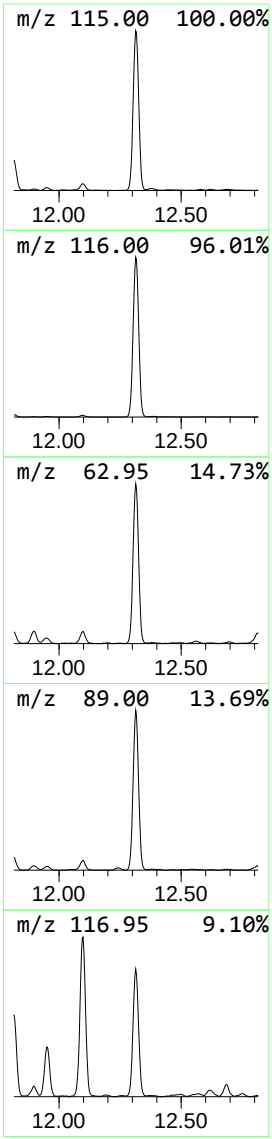
Peak Number 7 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.314	81.56 ug/l	1798430	1,4-Dichlorobenzene-d4	11.815

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	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90





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Quant Title : SW846 8260

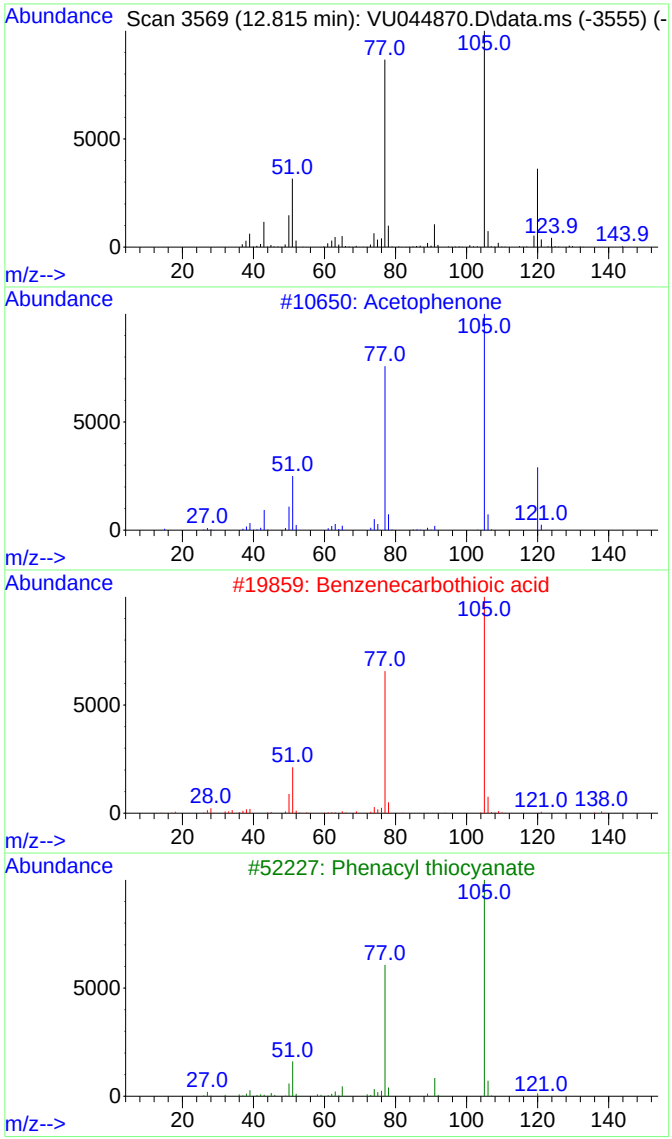
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

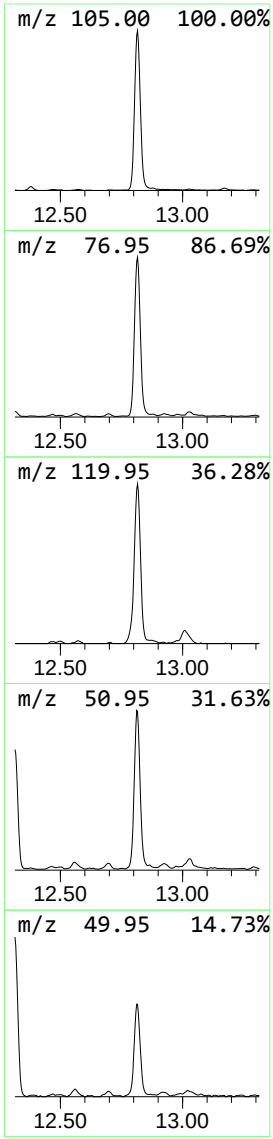
****

Peak Number 8 Acetophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.815	21.95 ug/l	483928	1,4-Dichlorobenzene-d4	11.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone	120	C8H8O	000098-86-2	94
2	Benzenecarbothioic acid	138	C7H6OS	000098-91-9	64
3	Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	64
4	Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	59
5	Propan-1-one, 3-nitro-1-phenyl-	179	C9H9NO3	062847-52-3	59





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ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20897

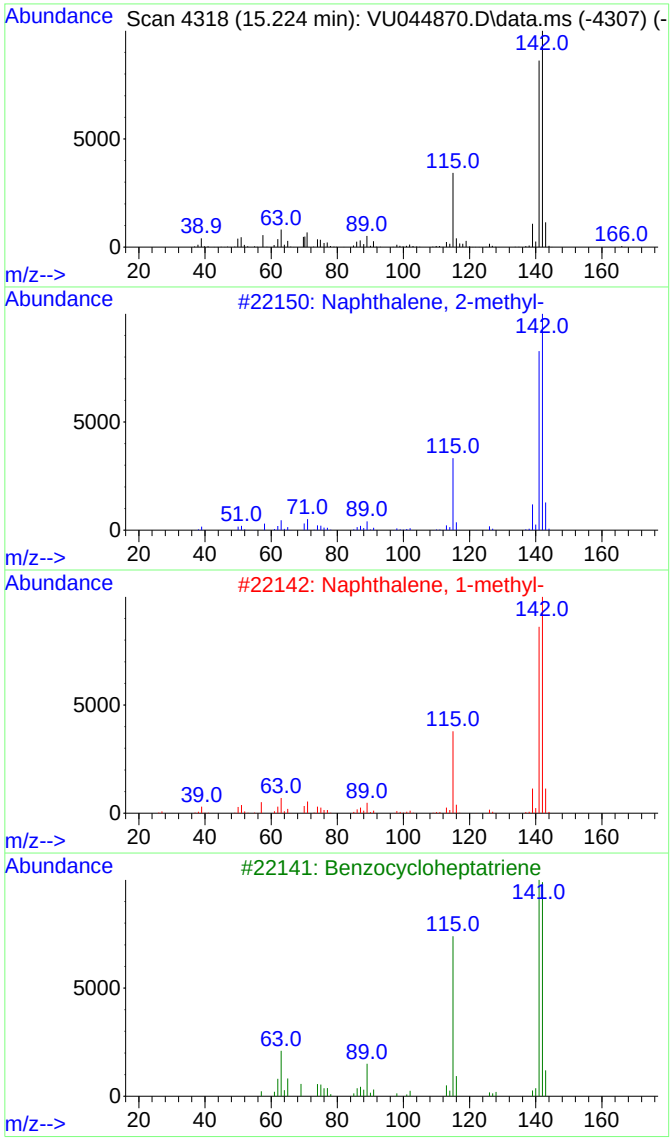
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

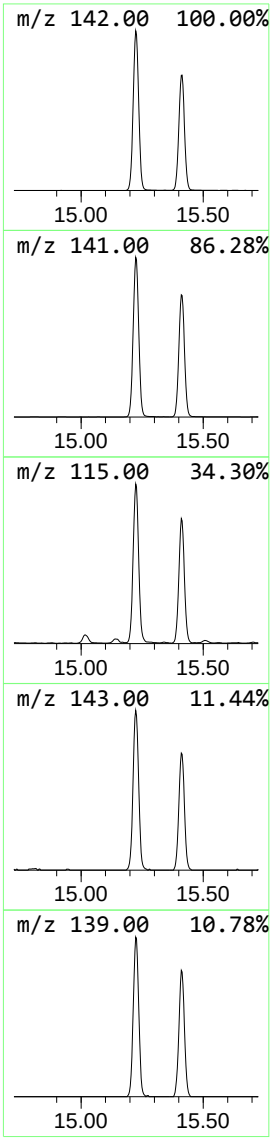
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.224	40.70 ug/l	897540	1,4-Dichlorobenzene-d4	11.815

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	Benzocycloheptatriene	142	C11H10	000264-09-5	90
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044870.D
Acq On : 26 Sep 2021 05:04
Operator : SY/MD
Sample : M3888-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20897

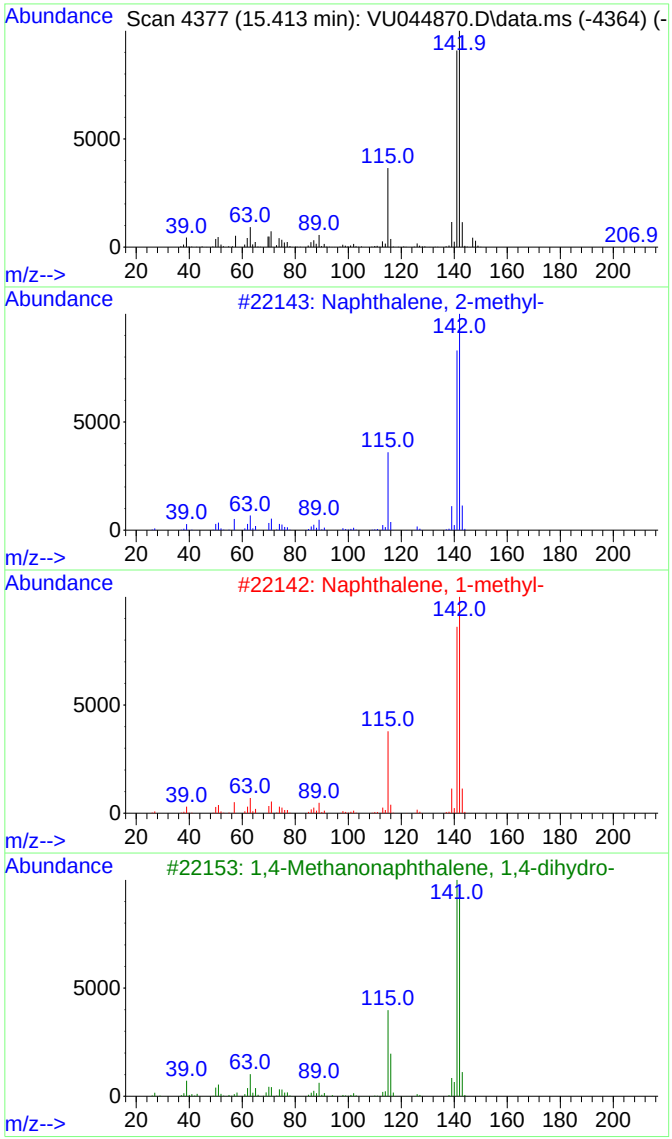
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

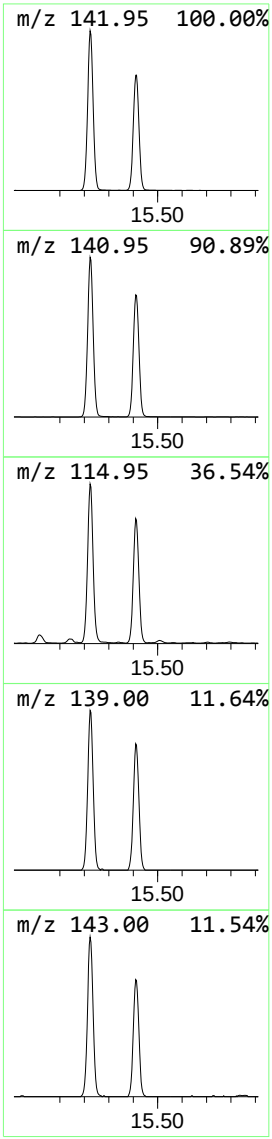
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.413	32.60 ug/l	718904	1,4-Dichlorobenzene-d4	11.815

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	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044870.D
Acq On : 26 Sep 2021 05:04
Operator : SY/MD
Sample : M3888-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 20897

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
1,3,5-Cyclohept...	8.732	24.9	ug/l	556950	3	9.420	1118390	50.0
Thiophene, tetr...	8.799	56.8	ug/l	1270520	3	9.420	1118390	50.0
unknown10.368	10.368	18.0	ug/l	402426	3	9.420	1118390	50.0
Benzene, 1-ethy...	10.999	19.9	ug/l	437820	4	11.815	1102560	50.0
Benzene, 1,2,3-...	11.896	17.8	ug/l	392654	4	11.815	1102560	50.0
Indene	12.314	81.6	ug/l	1798430	4	11.815	1102560	50.0
Acetophenone	12.815	21.9	ug/l	483928	4	11.815	1102560	50.0
Naphthalene, 2-...	15.224	40.7	ug/l	897540	4	11.815	1102560	50.0
Naphthalene, 1-...	15.413	32.6	ug/l	718904	4	11.815	1102560	50.0