LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042854.D
Acq On : 31 Mar 2021 13:59
Operator : SY/MD
Sample : M1836-14 10X
Misc : 11.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : B6-10-12

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\82U032421W.M
Title : SW846 8260

Signal : TIC: VU042854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.298	1216	1231	1244	rBV2	94018	197336	32.48%	2.825%
2	5.382	1244	1257	1275	rVB	148805	303489	49.96%	4.344%
3	5.710	1345	1359	1376	rBV	105512	214105	35.24%	3.065%
4	6.256	1514	1529	1546	rBV	213925	403841	66.48%	5.781%
5	7.906	2021	2042	2059	rBV	335270	577578	95.08%	8.268%
6	9.423	2498	2514	2538	rBV	319054	521420	85.83%	7.464%
7	9.578	2553	2562	2571	rBV	4354	6461	1.06%	0.092%
8	9.703	2593	2601	2610	rBV5	4754	8203	1.35%	0.117%
9	9.754	2610	2617	2628	rVB5	3676	6448	1.06%	0.092%
10	10.259	2763	2774	2789	rBV9	3617	10006	1.65%	0.143%
11	10.365	2798	2807	2815	rBV7	5574	10153	1.67%	0.145%
12	10.639	2878	2892	2908	rBV	280068	445260	73.29%	6.374%
13	10.815	2939	2947	2959	rVB8	4846	7914	1.30%	0.113%
14	10.909	2965	2976	2987	rBV3	13049	24608	4.05%	0.352%
15	11.031	2999	3014	3020	rBV2	12470	22303	3.67%	0.319%
16	11.317	3088	3103	3114	rBV9	4891	11604	1.91%	0.166%
17	11.423	3128	3136	3142	rBV5	5355	8071	1.33%	0.116%
18	11.475	3143	3152	3164	rVB2	50057	77472	12.75%	1.109%
19	11.648	3200	3206	3218	rVB	11885	17997	2.96%	0.258%
20	11.719	3220	3228	3235	rBV5	5653	8838	1.45%	0.127%
21	11.819	3246	3259	3274	rBV	386941	607493	100.00%	8.696%
22	11.902	3274	3285	3298	rVB	17845	33828	5.57%	0.484%
23	12.008	3311	3318	3326	rVB10	5158	8164	1.34%	0.117%
24	12.105	3337	3348	3362	rBV2	30766	57687	9.50%	0.826%
25	12.192	3366	3375	3392	rVB4	33428	73886	12.16%	1.058%
26	12.307	3398	3411	3427	rBV10	6704	17670	2.91%	0.253%
27	12.385	3428	3435	3452	rVB2	15104	25260	4.16%	0.362%
28	12.471	3452	3462	3467	rBV2	22746	35365	5.82%	0.506%
29	12.503	3467	3472	3481	rVB	19605	25534	4.20%	0.365%
30	12.577	3485	3495	3503	rBV	35768	51350	8.45%	0.735%
31	12.616	3503	3507	3517	rVB2	9740	13739	2.26%	0.197%
32	12.690	3517	3530	3538	rBV	27276	56647	9.32%	0.811%
33	12.822	3562	3571	3575	rBV4	8280	12954	2.13%	0.185%
34	12.880	3585	3589	3598	rVB4	11079	15306	2.52%	0.219%
35	12.944	3598	3609	3611	rBV8	9426	15267	2.51%	0.219%
36	12.979	3613	3620	3628	rVB	24064	36012	5.93%	0.515%

LSC Area Percent Report

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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : B6-10-12

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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Title : SW846 8260

37	13.034	3628	3637	3652	rVB2	36537	66412	10.93%	0.951%
38	13.118	3652	3663	3668	rBV3	16858	29122	4.79%	0.417%
39	13.262	3702	3708	3712	rBV4	9305	11528	1.90%	0.165%
40	13.298	3713	3719	3729	rVB2	29265	44800	7.37%	0.641%
41	13.359	3730	3738	3746	rVB4	16306	24088	3.97%	0.345%
42	13.413	3746	3755	3761	rBV2	19502	30643	5.04%	0.439%
43	13.462	3761	3770	3783	rVV3	78244	141262	23.25%	2.022%
44	13.568	3797	3803	3809	rBV	10559	12792	2.11%	0.183%
45	13.632	3815	3823	3846	rVB3	48141	101893	16.77%	1.459%
46	13.741	3848	3857	3864	rBV3	17690	29660	4.88%	0.425%
47	13.793	3864	3873	3880	rBV2	26265	40435	6.66%	0.579%
48	13.844	3880	3889	3902	rBV6	38982	79276	13.05%	1.135%
49	13.950	3916	3922	3937	rVB5	31105	61094	10.06%	0.875%
50	14.092	3959	3966	3974	rVB	42388	59506	9.80%	0.852%
51	14.198	3986	3999	4012	rVB3	41054	84447	13.90%	1.209%
52	14.294	4014	4029	4041	rBV5	46572	102420	16.86%	1.466%
53	14.355	4042	4048	4055	rVB3	14233	19974	3.29%	0.286%
54	14.400	4058	4062	4069	rVV4	5010	6764	1.11%	0.097%
55	14.494	4080	4091	4100	rBV2	38854	68623	11.30%	0.982%
56	14.613	4122	4128	4135	rVB3	9055	13395	2.20%	0.192%
57	14.690	4136	4152	4172	rBV4	81462	201927	33.24%	2.890%
58	14.818	4184	4192	4200	rBV3	23695	37285	6.14%	0.534%
59	14.886	4205	4213	4222	rVB3	44682	72272	11.90%	1.035%
60	14.947	4222	4232	4246	rVB7	13498	26376	4.34%	0.378%
61	15.024	4246	4256	4271	rBV4	54333	105594	17.38%	1.511%
62	15.230	4304	4320	4329	rBV2	191745	374317	61.62%	5.358%
63	15.278	4330	4335	4349	rVB3	33658	57513	9.47%	0.823%
64	15.355	4350	4359	4367	rBV5	17987	30152	4.96%	0.432%
65	15.420	4367	4379	4389	rVV	114872	196866	32.41%	2.818%
66	15.474	4390	4396	4402	rVV5	20215	31620	5.20%	0.453%
67	15.513	4402	4408	4419	rVB8	16421	28490	4.69%	0.408%
68	15.587	4420	4431	4445	rBV4	15120	37358	6.15%	0.535%
69	15.770	4472	4488	4498	rBV8	12290	27601	4.54%	0.395%
70	15.934	4525	4539	4556	rBV5	38009	91391	15.04%	1.308%
71	16.018	4556	4565	4582	rVB5	9067	23384	3.85%	0.335%
72	16.156	4598	4608	4615	rBV2	42904	70194	11.55%	1.005%
73	16.191	4615	4619	4629	rVB2	16019	22691	3.74%	0.325%
74	16.269	4629	4643	4654	rBV2	79839	145202	23.90%	2.078%
75	16.416	4679	4689	4696	rBV	110358	179469	29.54%	2.569%
76	16.455	4696	4701	4717	rVB	65637	102599	16.89%	1.469%

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Instrument : MSVOA_U
ClientSampleId : B6-10-12

Integration Parameters: RTEINT.P
Integrator: RTE
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Title : SW846 8260

77	16.651	4745	4762	4775	rBV2	21986	52907	8.71%	0.757%
78	16.793	4799	4806	4816	rBV4	12990	21554	3.55%	0.309%
79	16.892	4830	4837	4844	rBV9	4245	6804	1.12%	0.097%
80	17.127	4903	4910	4923	rVB2	6977	11923	1.96%	0.171%
81	17.336	4970	4975	4984	rVB5	7398	9583	1.58%	0.137%
82	17.387	4984	4991	5003	rVB5	7138	12297	2.02%	0.176%
83	17.548	5033	5041	5051	rVB3	7311	11287	1.86%	0.162%

Sum of corrected areas: 6986059

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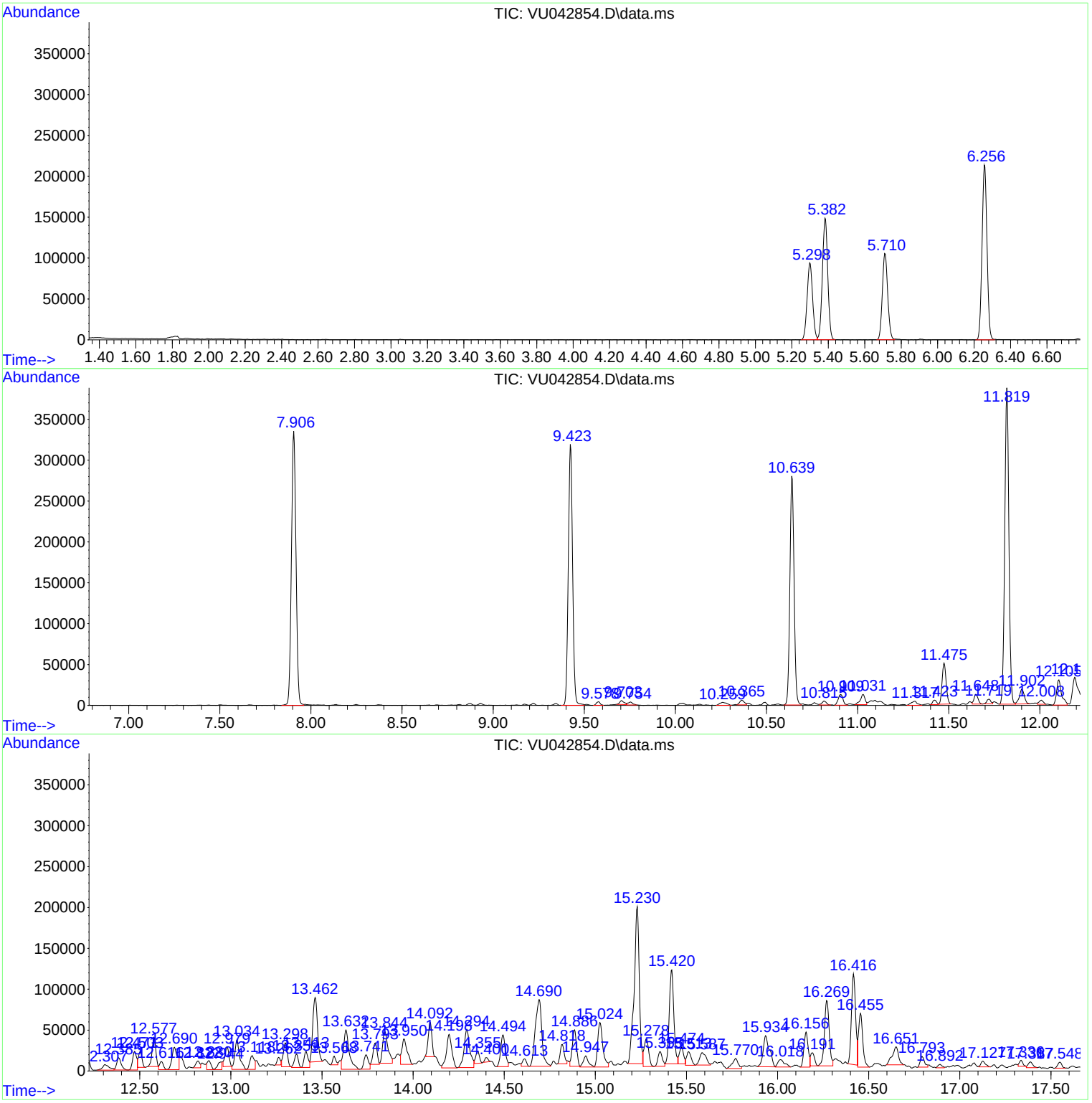
Instrument :
MSVOA_U
ClientSampleId :
B6-10-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042854.D
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Operator : SY/MD
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Instrument : MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

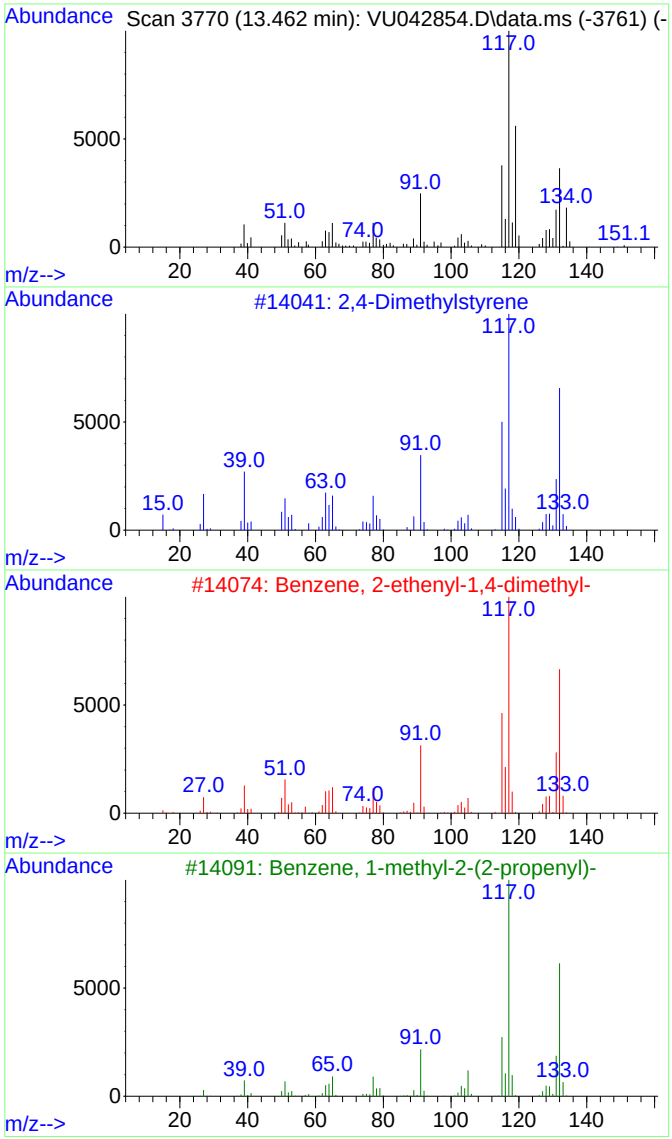
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

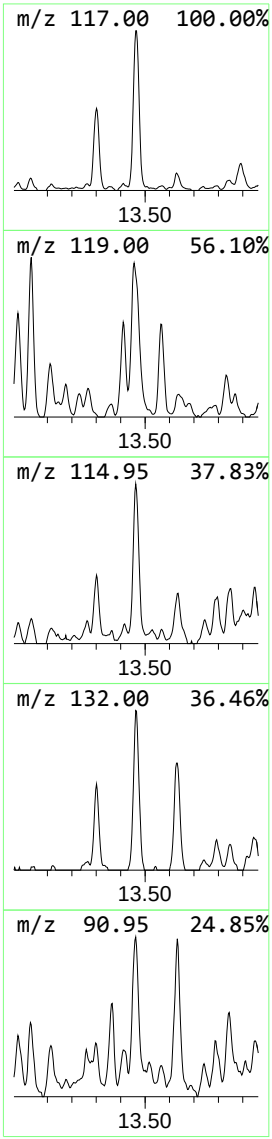
****

Peak Number 1 2,4-Dimethylstyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.462	11.63 ug/l	141262	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethylstyrene	132	C10H12	002234-20-0	91
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70





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Operator : SY/MD
Sample : M1836-14 10X
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
B6-10-12

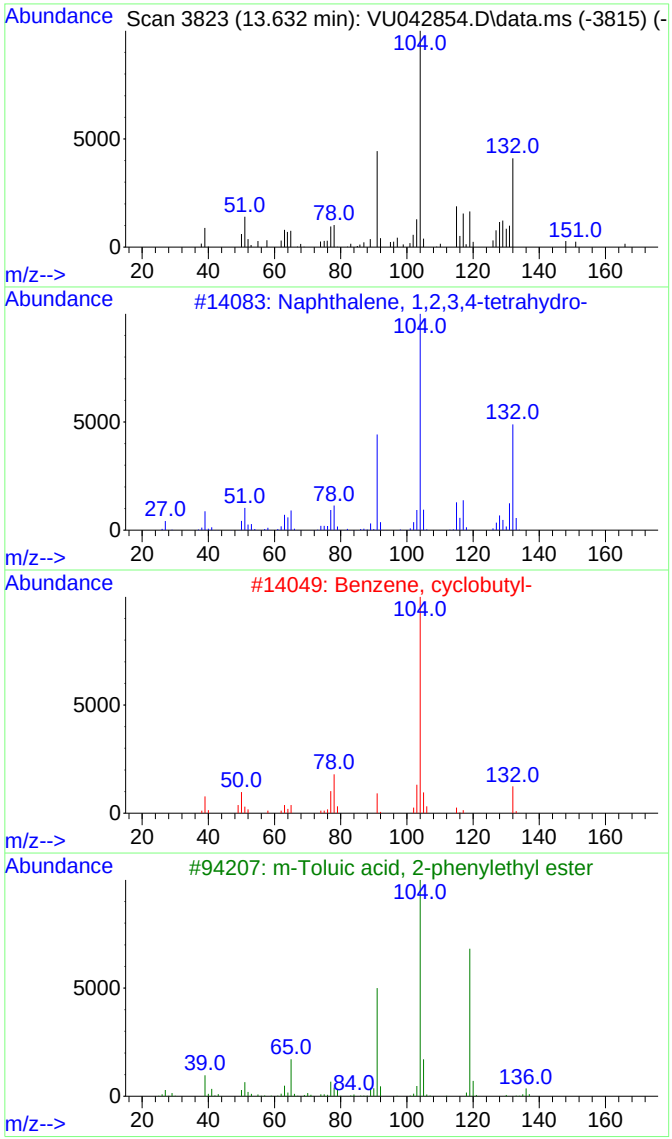
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

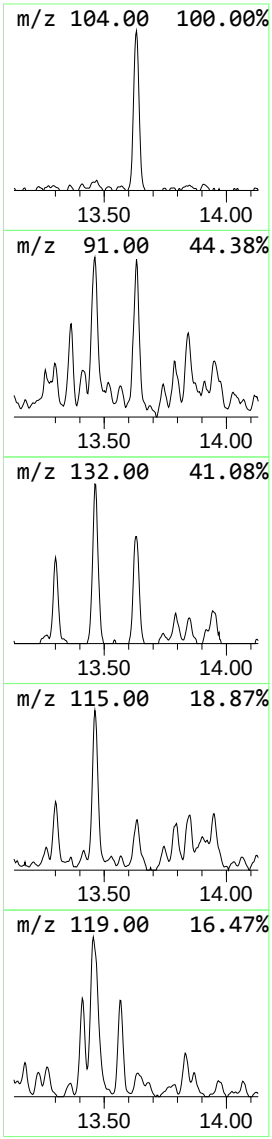
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.632	8.39 ug/l	101893	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	90
2	Benzene, cyclobutyl-	132	C10H12	004392-30-7	42
3	m-Toluic acid, 2-phenylethyl ester	240	C16H16O2	006641-74-3	38
4	Pentafluoropropionic acid, 2-phe...	268	C11H9F5O2	081089-48-7	38
5	Acetic acid, trichloro-, 2-pheny...	266	C10H9Cl3O2	071965-07-6	38





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MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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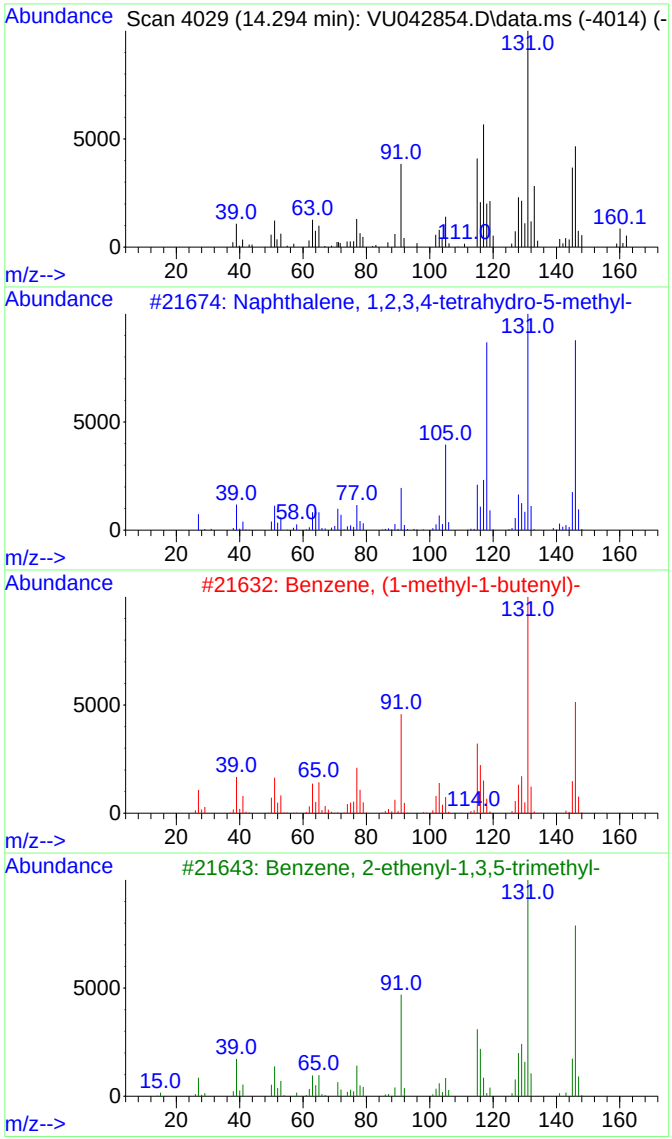
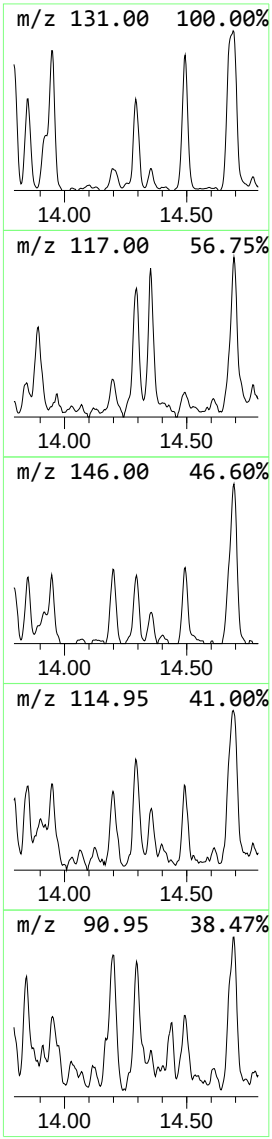
****
Peak Number 3 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.294	8.43 ug/l	102420	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	74
2	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	64
3	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	60
4	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	53
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	49





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Instrument : MSVOA_U
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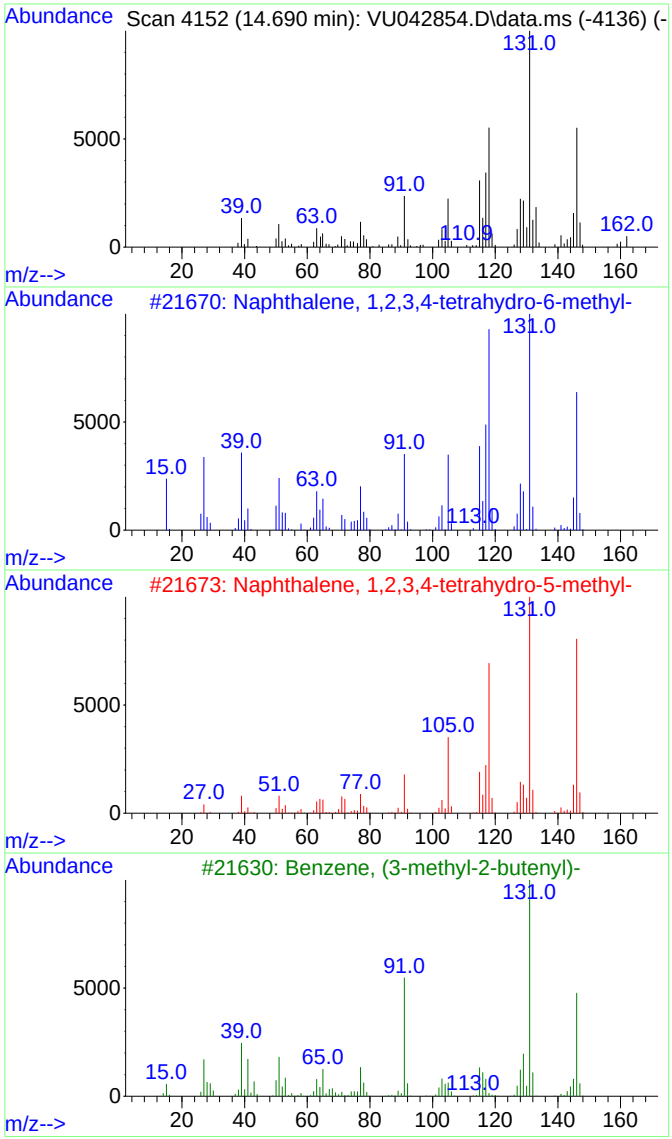
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

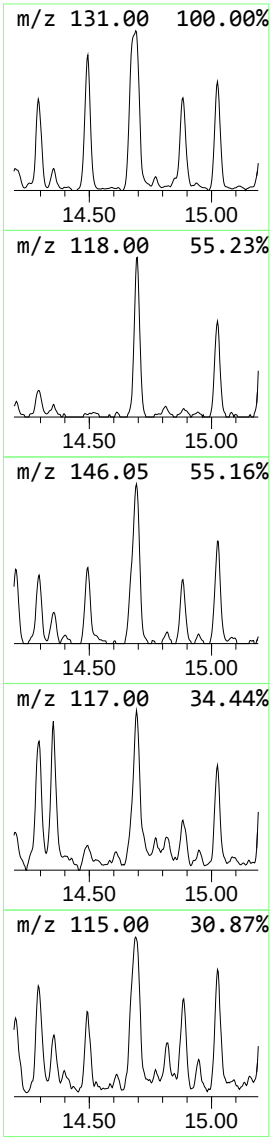
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.690	16.62 ug/l	201927	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
3	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	86
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	68
5	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	64





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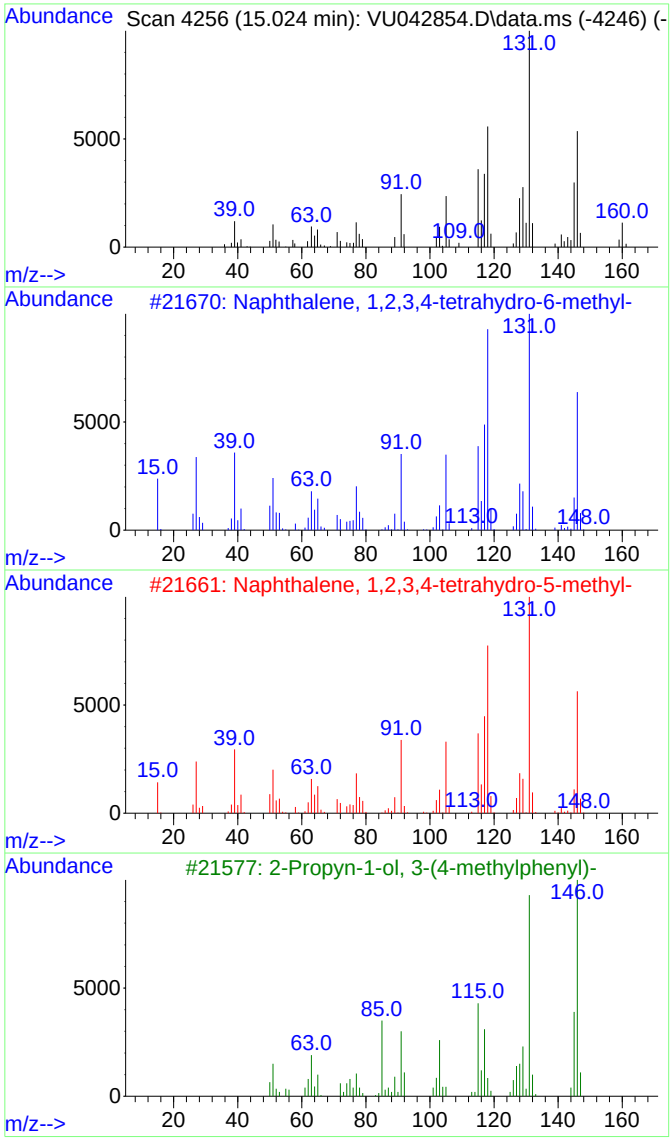
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

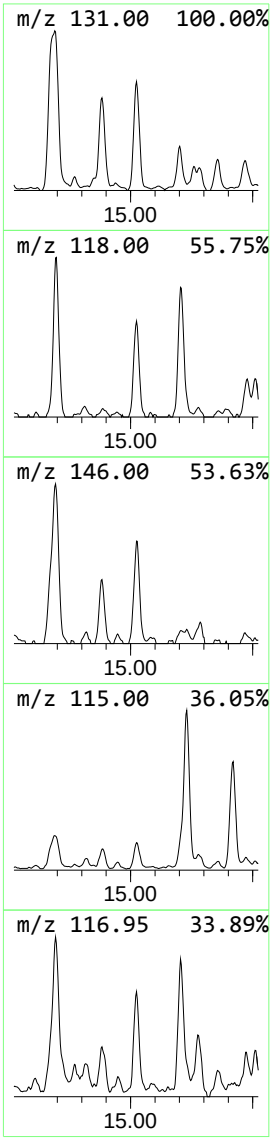
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propyn-1-ol, 3-(4-methylp... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.024	8.69 ug/l	105594	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	89
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	81
3	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	68
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	58
5	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	58





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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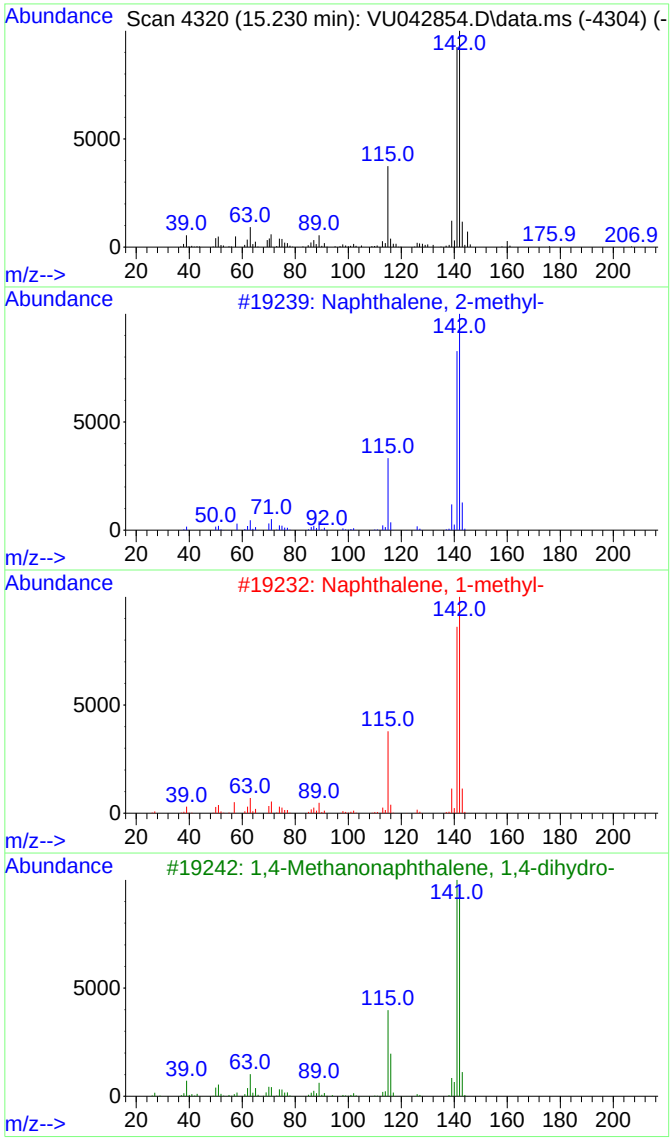
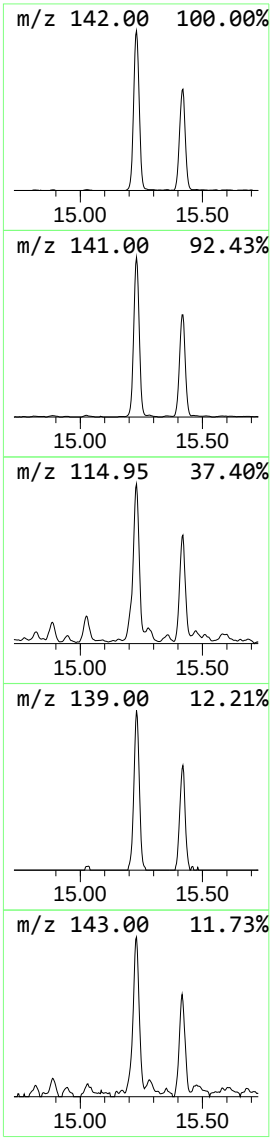
Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.230	30.81 ug/l	374317	1,4-Dichlorobenzene-d4	11.819

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	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	94
5	Benzocycloheptatriene	142	C11H10	000264-09-5	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042854.D
Acq On : 31 Mar 2021 13:59
Operator : SY/MD
Sample : M1836-14 10X
Misc : 11.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : B6-10-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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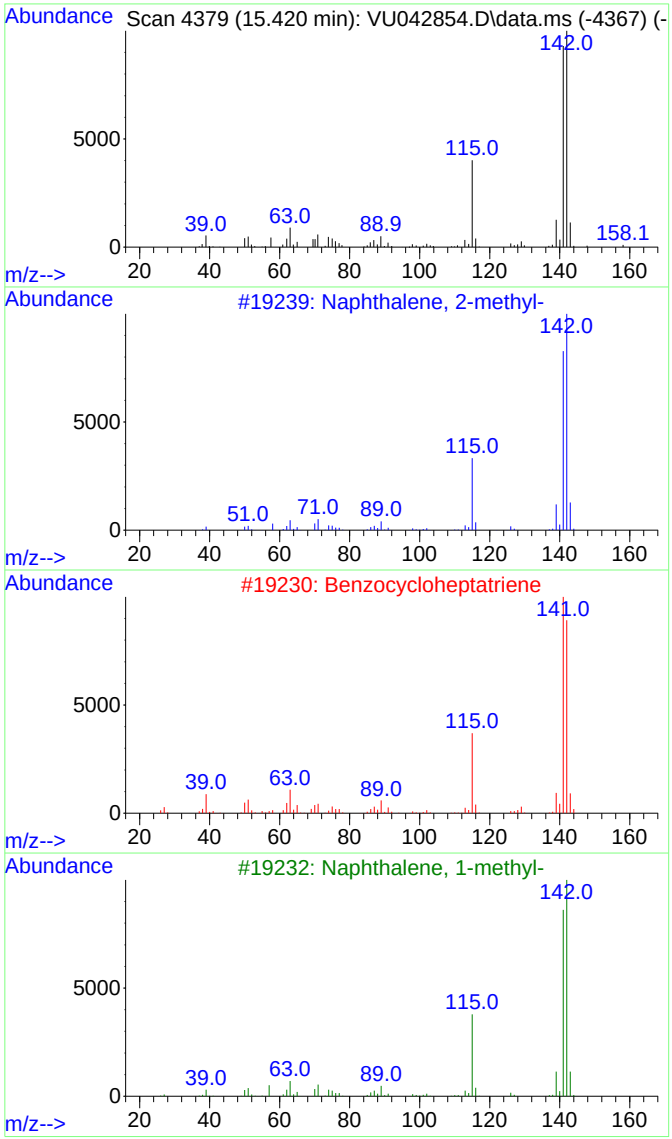
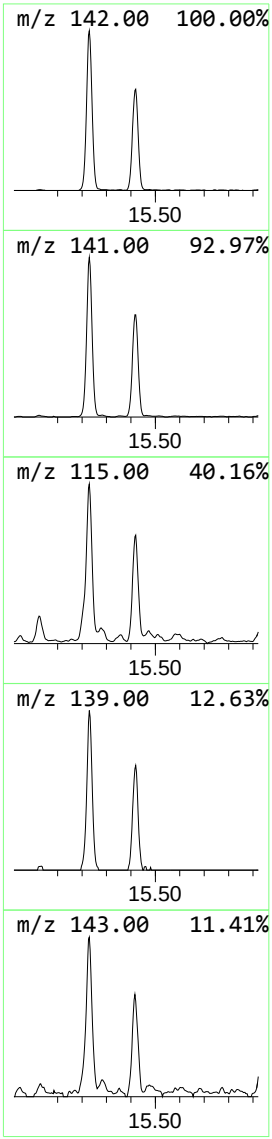
Peak Number 7 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.420	16.20 ug/l	196866	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Benzocycloheptatriene	142	C11H10	000264-09-5	97
3	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042854.D
Acq On : 31 Mar 2021 13:59
Operator : SY/MD
Sample : M1836-14 10X
Misc : 11.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
B6-10-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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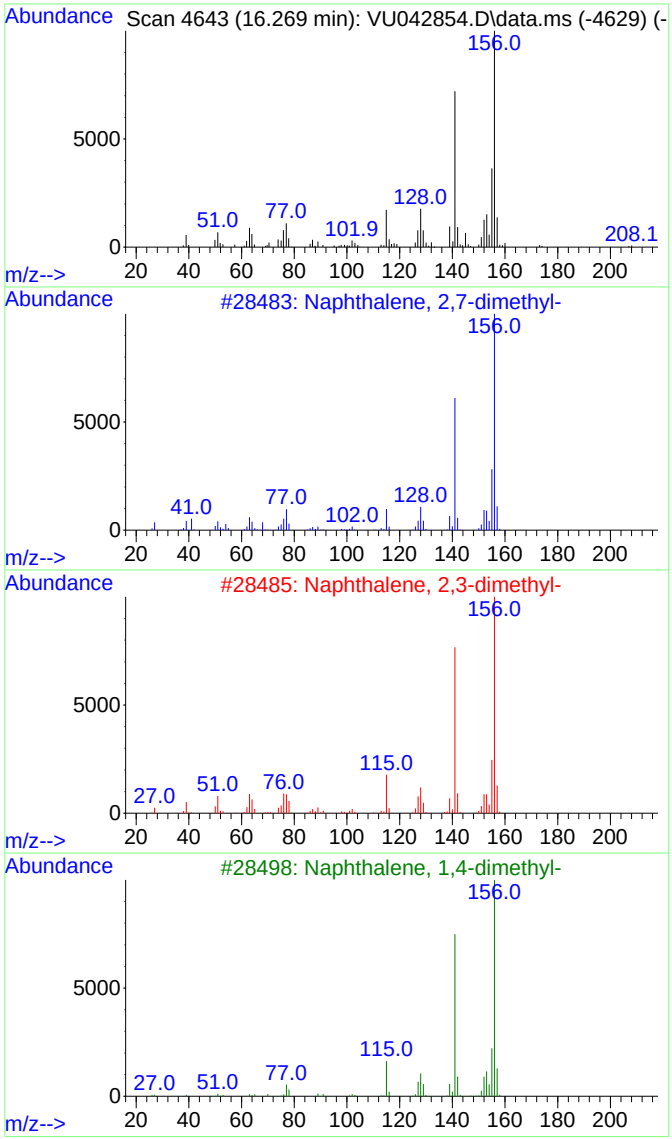
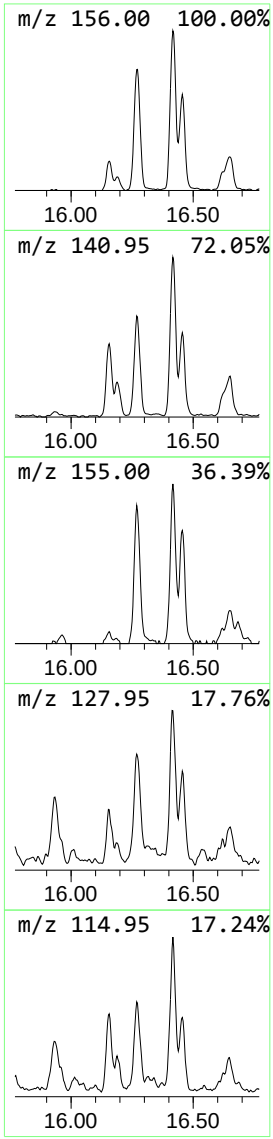
Peak Number 8 Naphthalene, 2,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.269	11.95 ug/l	145202	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042854.D
Acq On : 31 Mar 2021 13:59
Operator : SY/MD
Sample : M1836-14 10X
Misc : 11.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
B6-10-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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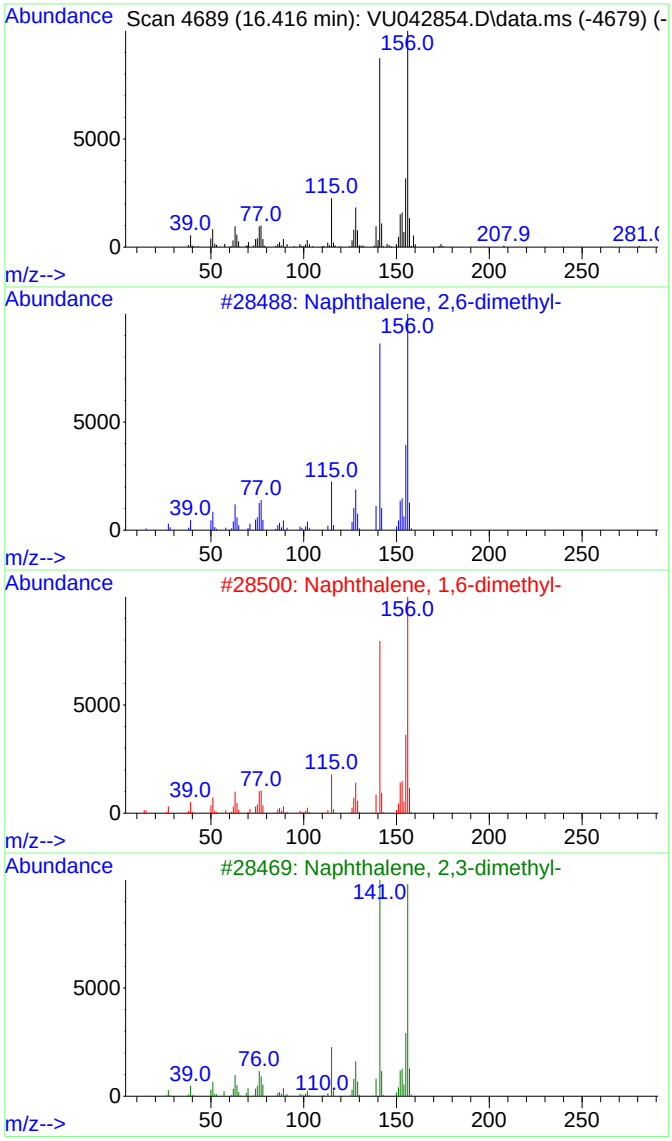
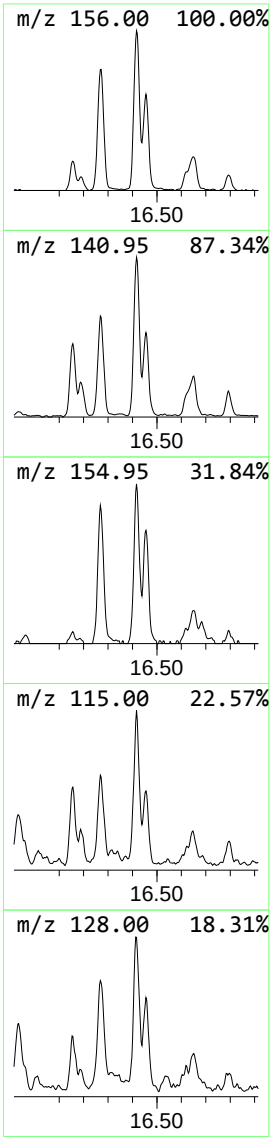
Peak Number 9 Naphthalene, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.416	14.77 ug/l	179469	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	98
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042854.D
Acq On : 31 Mar 2021 13:59
Operator : SY/MD
Sample : M1836-14 10X
Misc : 11.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
B6-10-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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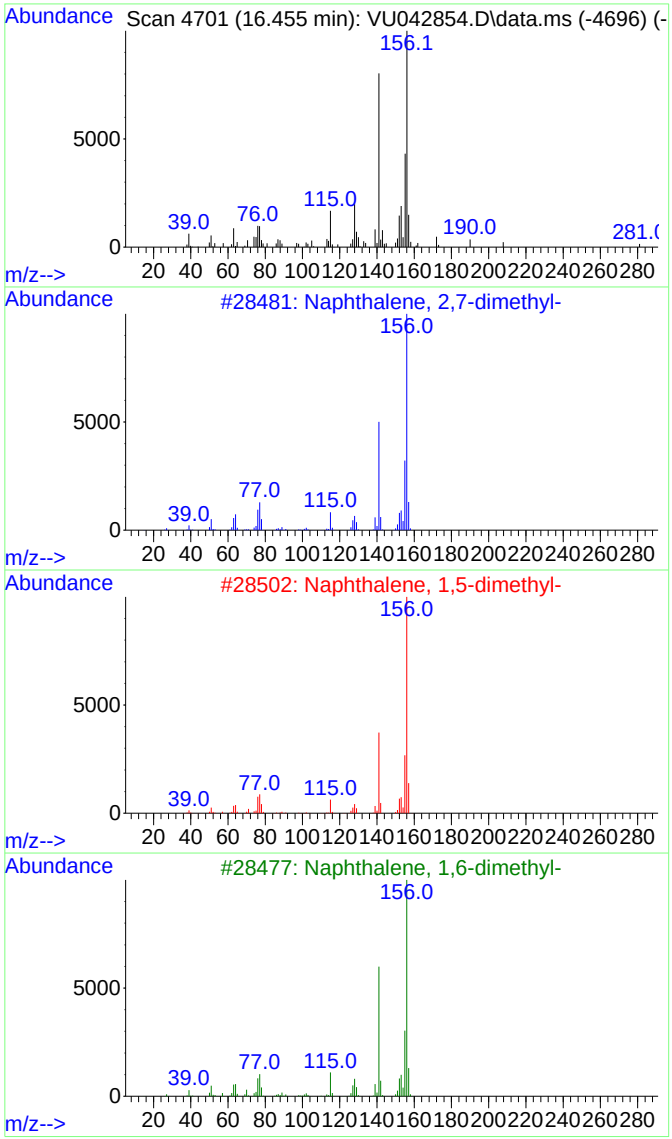
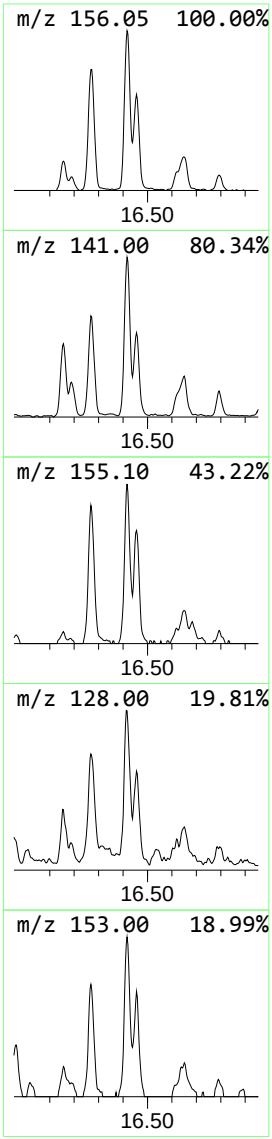
Peak Number 10 Naphthalene, 1,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.455	8.44 ug/l	102599	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	93
2	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	90
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	90
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	90
5	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042854.D
Acq On : 31 Mar 2021 13:59
Operator : SY/MD
Sample : M1836-14 10X
Misc : 11.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : B6-10-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2,4-Dimethylsty...	13.462	11.6	ug/l	141262	4	11.819	607493	50.0
Naphthalene, 1,...	13.632	8.4	ug/l	101893	4	11.819	607493	50.0
Naphthalene, 1,...	14.294	8.4	ug/l	102420	4	11.819	607493	50.0
Naphthalene, 1,...	14.690	16.6	ug/l	201927	4	11.819	607493	50.0
2-Propyn-1-ol, ...	15.024	8.7	ug/l	105594	4	11.819	607493	50.0
Naphthalene, 1-...	15.230	30.8	ug/l	374317	4	11.819	607493	50.0
Benzocyclohepta...	15.420	16.2	ug/l	196866	4	11.819	607493	50.0
Naphthalene, 2,...	16.269	11.9	ug/l	145202	4	11.819	607493	50.0
Naphthalene, 2,...	16.416	14.8	ug/l	179469	4	11.819	607493	50.0
Naphthalene, 1,...	16.455	8.4	ug/l	102599	4	11.819	607493	50.0