LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

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\82U052622W.M
Title : SW846 8260

Signal : TIC: VU048721.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.752	428	439	462	rBV	22399	44999	1.01%	0.171%
2	3.044	515	530	549	rBV2	34166	81839	1.83%	0.312%
3	3.170	549	569	597	rVV	188335	440717	9.86%	1.679%
4	3.362	612	629	650	rVB2	106910	244613	5.47%	0.932%
5	5.292	1212	1229	1242	rBV	224532	478059	10.70%	1.821%
6	5.375	1242	1255	1271	rVV	338459	699357	15.65%	2.664%
7	5.462	1272	1282	1301	rVB4	22071	53828	1.20%	0.205%
8	5.703	1343	1357	1368	rBV	220856	442166	9.89%	1.684%
9	5.777	1368	1380	1382	rBV	273286	400842	8.97%	1.527%
10	5.822	1383	1394	1412	rVB	2109947	4469360	100.00%	17.023%
11	6.250	1512	1527	1564	rVB	473991	940055	21.03%	3.581%
12	7.256	1824	1840	1854	rVB3	29656	65056	1.46%	0.248%
13	7.388	1856	1881	1893	rBV6	54750	132808	2.97%	0.506%
14	7.623	1941	1954	1964	rBV	317674	588849	13.18%	2.243%
15	7.684	1964	1973	2014	rVB	566645	1115602	24.96%	4.249%
16	7.899	2014	2040	2054	rBV	663809	1168114	26.14%	4.449%
17	8.037	2070	2083	2111	rBV	704062	1302149	29.14%	4.960%
18	8.176	2112	2126	2139	rVV	1051631	1798486	40.24%	6.850%
19	8.266	2140	2154	2173	rVB	1251031	2117123	47.37%	8.064%
20	8.684	2273	2284	2287	rBV	40315	60524	1.35%	0.231%
21	8.716	2288	2294	2309	rVV	89572	157350	3.52%	0.599%
22	8.822	2313	2327	2341	rVB3	41882	92373	2.07%	0.352%
23	9.102	2389	2414	2425	rBV2	23471	61673	1.38%	0.235%
24	9.336	2475	2487	2501	rBV2	110178	225395	5.04%	0.858%
25	9.417	2501	2512	2524	rBV	699652	1220716	27.31%	4.650%
26	9.484	2525	2533	2550	rVB	214824	408991	9.15%	1.558%
27	9.571	2551	2560	2568	rBV	98833	174694	3.91%	0.665%
28	9.693	2587	2598	2606	rBV	184017	305678	6.84%	1.164%
29	10.098	2712	2724	2738	rVB	67275	121425	2.72%	0.462%
30	10.269	2754	2777	2790	rBV4	42783	127111	2.84%	0.484%
31	10.404	2811	2819	2828	rVB2	30916	52253	1.17%	0.199%
32	10.484	2836	2844	2853	rVB2	36330	61663	1.38%	0.235%
33	10.632	2877	2890	2908	rBV	661472	1105129	24.73%	4.209%
34	10.732	2909	2921	2935	rVB6	41935	121975	2.73%	0.465%
35	10.861	2951	2961	2968	rBV2	44001	75187	1.68%	0.286%
36	10.906	2968	2975	2995	rVB4	61124	120428	2.69%	0.459%

LSC Area Percent Report

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ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

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\82U052622W.M
Title : SW846 8260

37	11.015	2995	3009	3018	rBV3	46762	125486	2.81%	0.478%
38	11.291	3085	3095	3112	rBV	43279	79948	1.79%	0.305%
39	11.417	3113	3134	3142	rVV3	57022	136131	3.05%	0.519%
40	11.468	3142	3150	3163	rVB	156999	252226	5.64%	0.961%
41	11.642	3188	3204	3214	rBV7	30448	75962	1.70%	0.289%
42	11.812	3245	3257	3272	rBV	858513	1358664	30.40%	5.175%
43	11.896	3274	3283	3289	rBV2	40409	67389	1.51%	0.257%
44	12.095	3333	3345	3355	rBV2	143302	248517	5.56%	0.947%
45	12.188	3368	3374	3392	rVB6	19384	46212	1.03%	0.176%
46	12.680	3518	3527	3542	rBV	120782	191097	4.28%	0.728%
47	12.973	3603	3618	3627	rBV	120567	193906	4.34%	0.739%
48	13.024	3627	3634	3648	rVB2	28742	46411	1.04%	0.177%
49	13.455	3759	3768	3779	rVB3	50485	83248	1.86%	0.317%
50	13.831	3877	3885	3897	rBV3	31452	52129	1.17%	0.199%
51	14.085	3951	3964	3983	rBV	407352	673451	15.07%	2.565%
52	14.208	3990	4002	4014	rVB	28599	56903	1.27%	0.217%
53	15.224	4307	4318	4343	rVB	473547	796318	17.82%	3.033%
54	15.410	4364	4376	4389	rBV	333011	558065	12.49%	2.126%
55	16.262	4630	4641	4650	rBV	31077	53620	1.20%	0.204%
56	16.410	4677	4687	4694	rBV	48767	82363	1.84%	0.314%

Sum of corrected areas: 26254633

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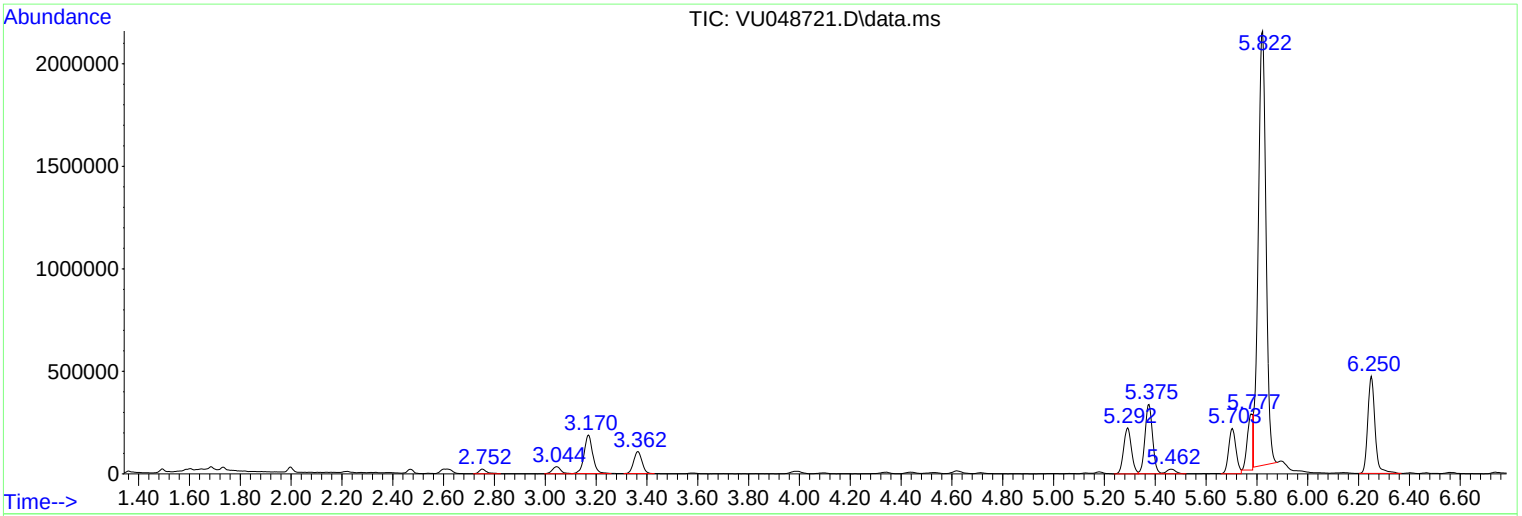
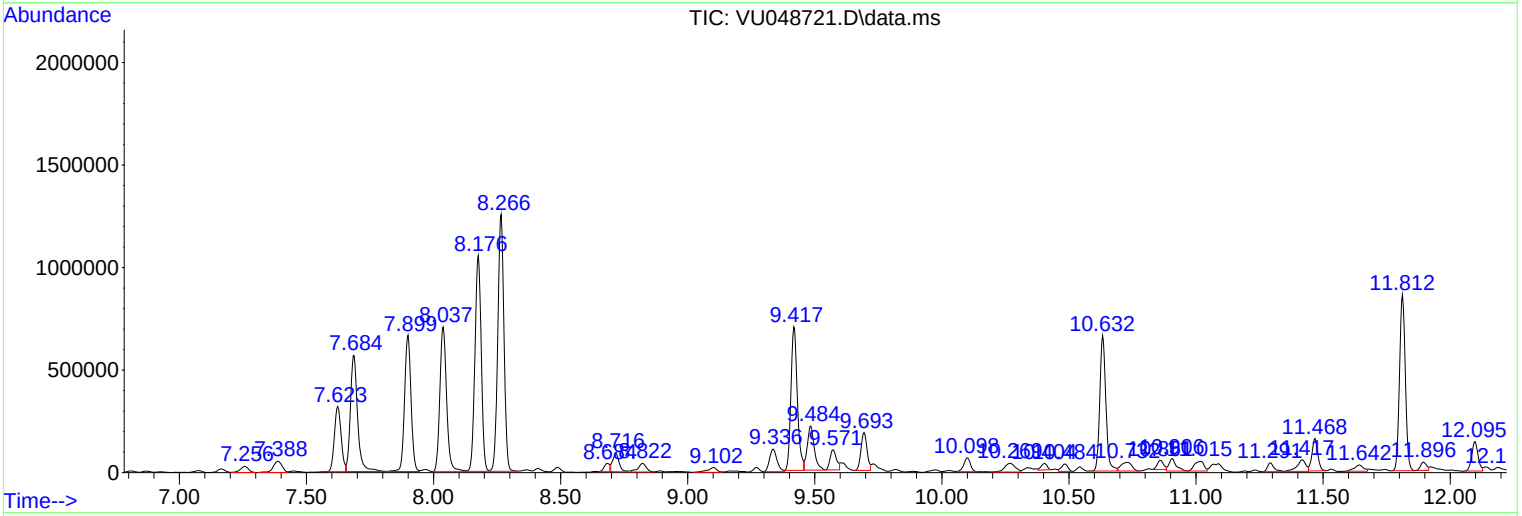
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

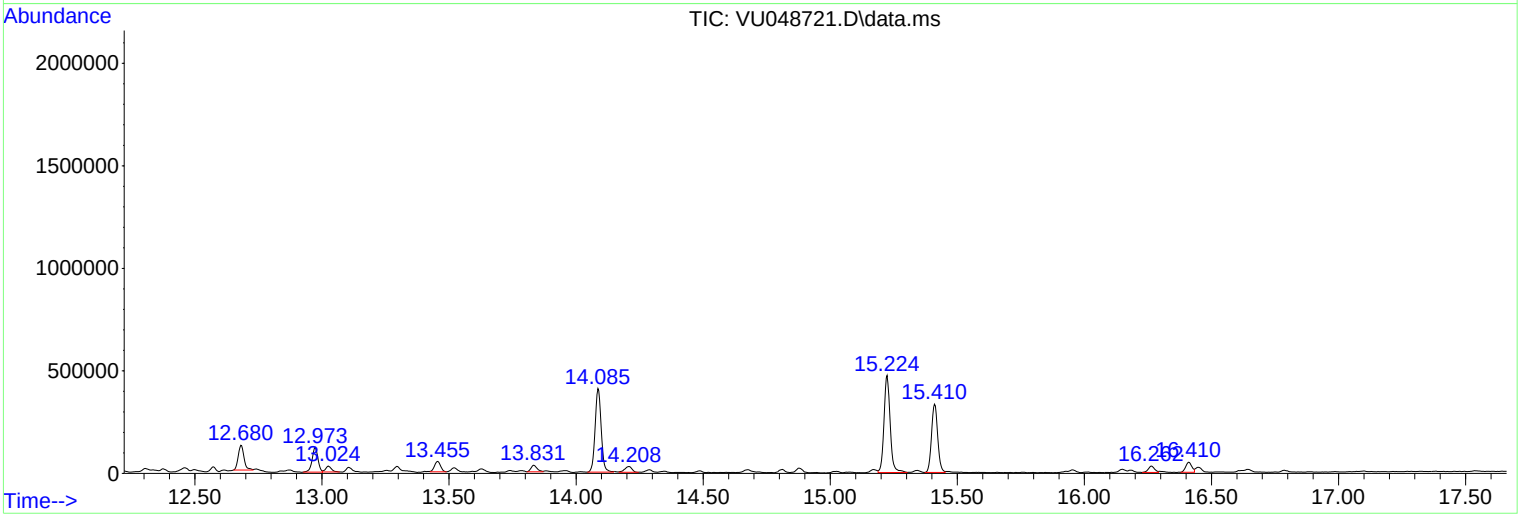
Instrument :
MSVOA_U
ClientSampleId :
TW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
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ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

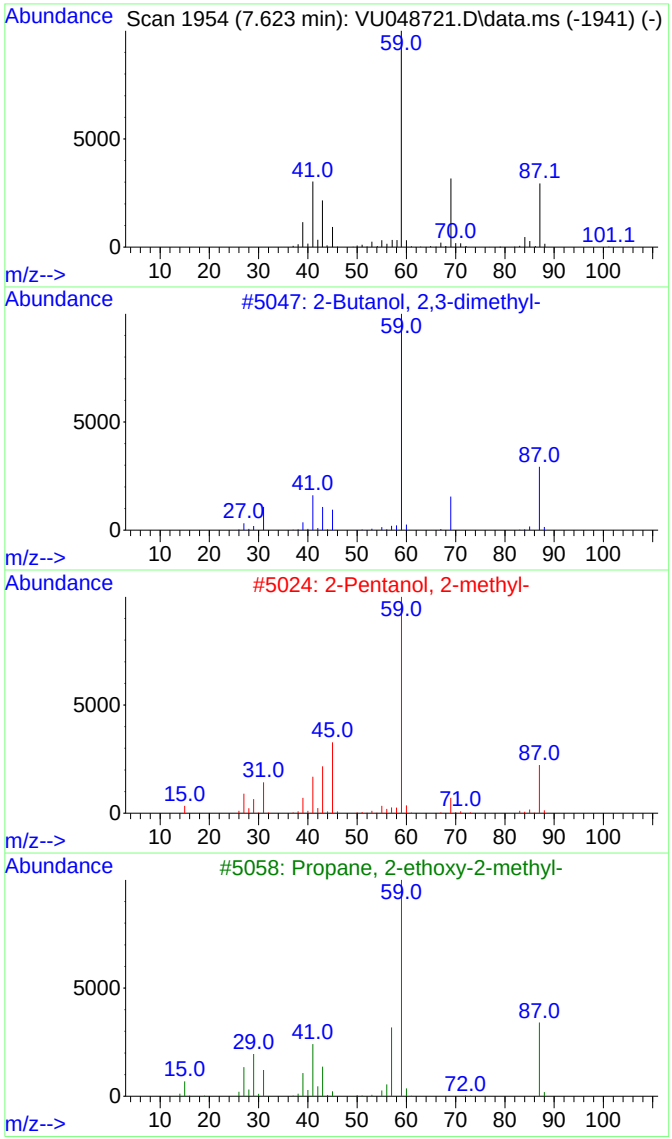
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

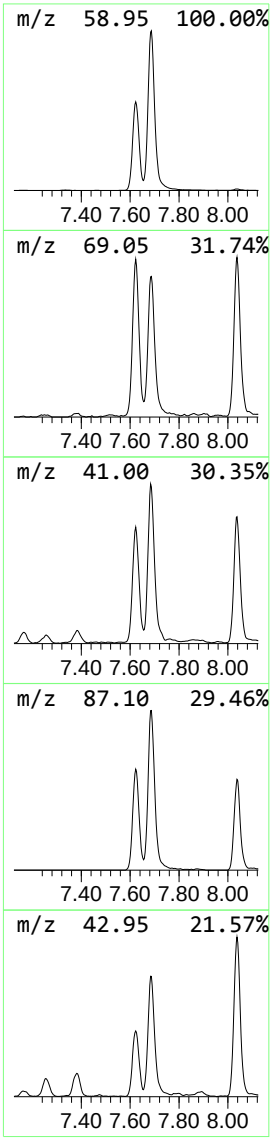
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.623	31.32 ug/l	588849	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
4	Amylene hydrate	88	C5H12O	000075-85-4	42
5	3-Heptanol	116	C7H16O	000589-82-2	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

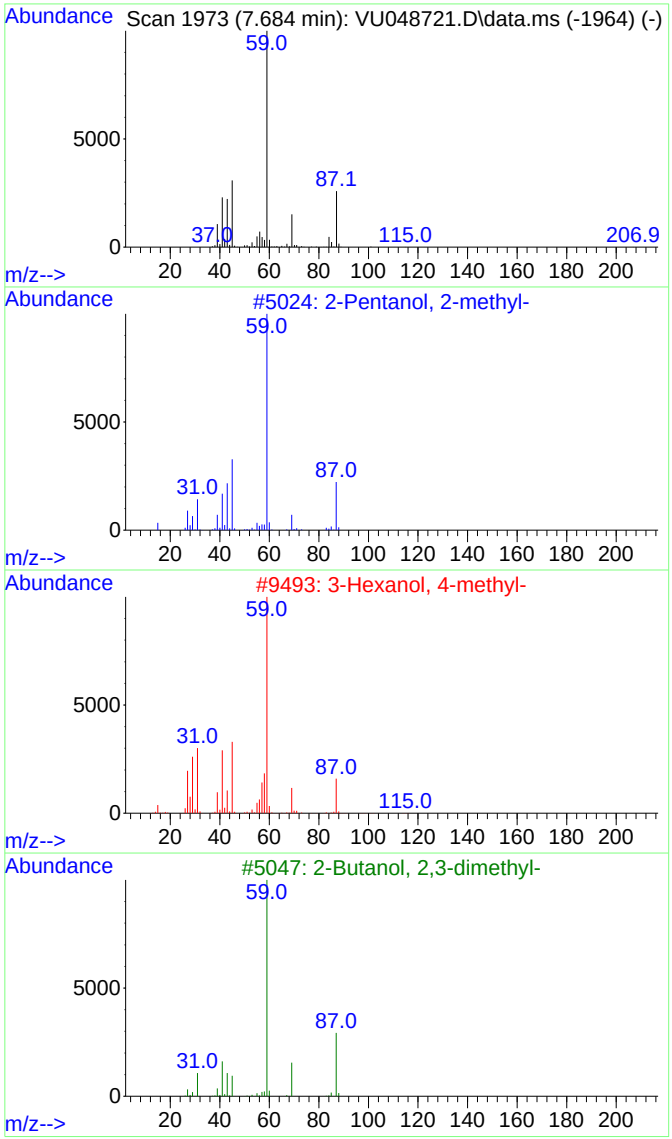
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

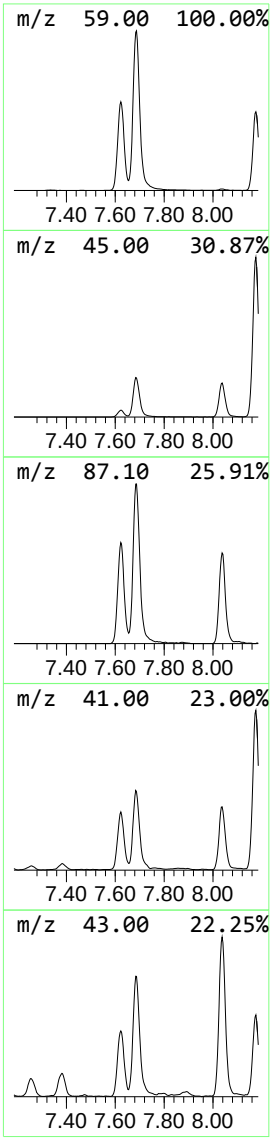
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.684	59.34 ug/l	1115600	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	78
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	64
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	53
5	3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

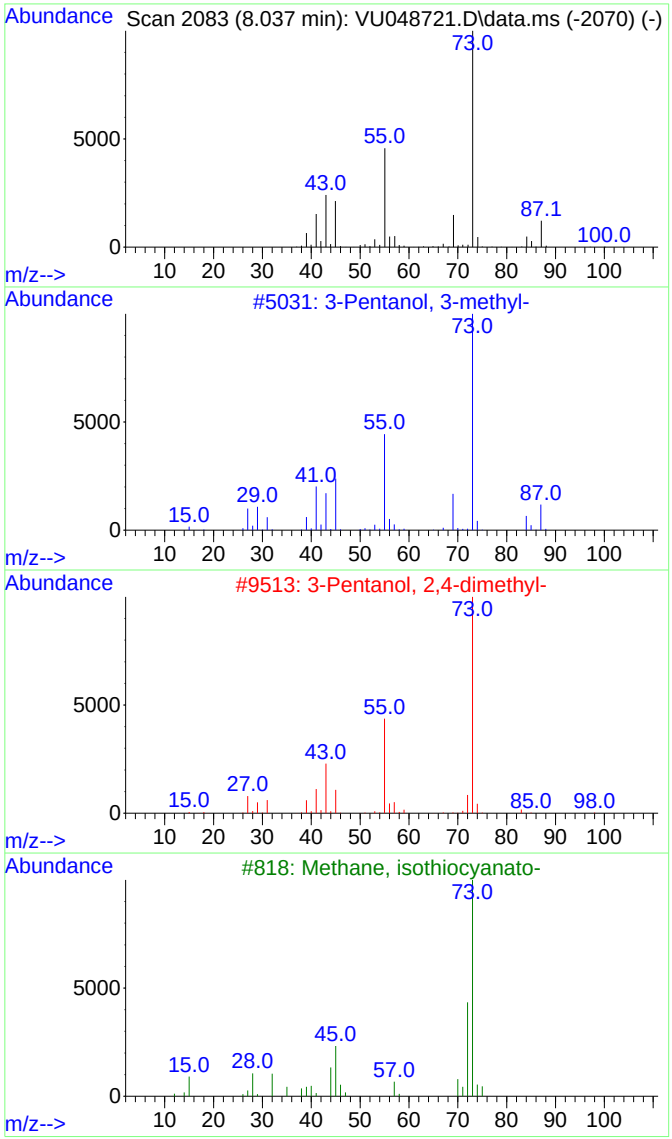
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

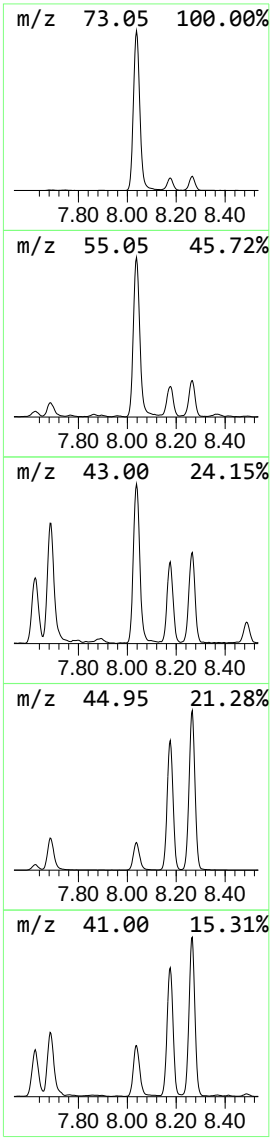
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Pentanol, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.037	53.34 ug/l	1302150	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5	3-Methylpentan-3-yl propyl carbo...	188	C10H20O3	1000372-82-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

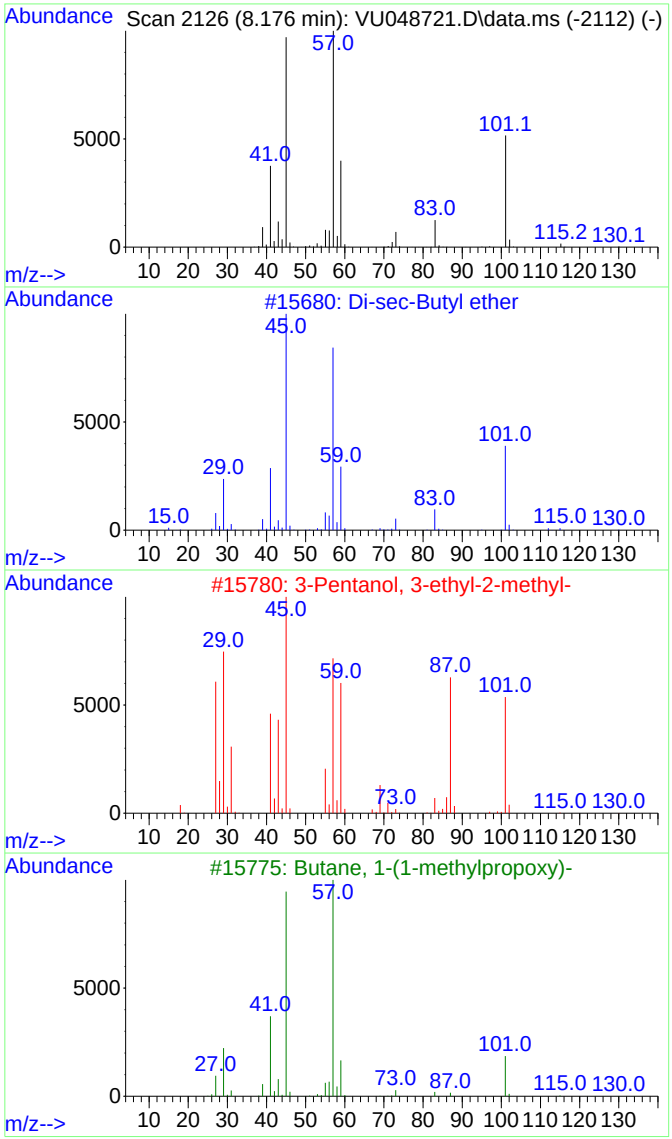
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

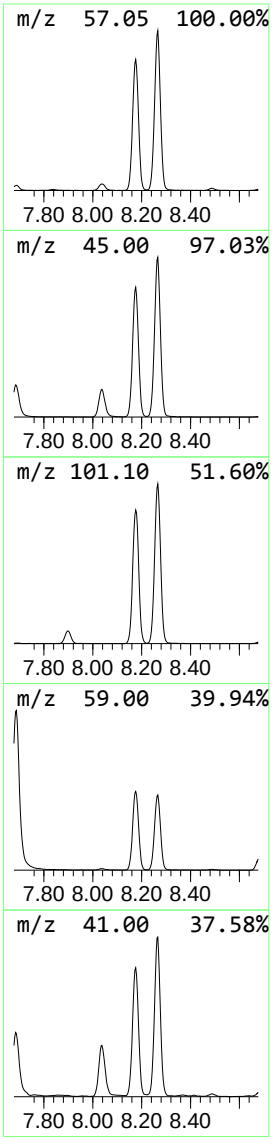
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Di-sec-Butyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.176	73.67 ug/l	1798490	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	72
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	47
4	2-Hydroxy-3-pentanone	102	C5H10O2	005704-20-1	36
5	Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

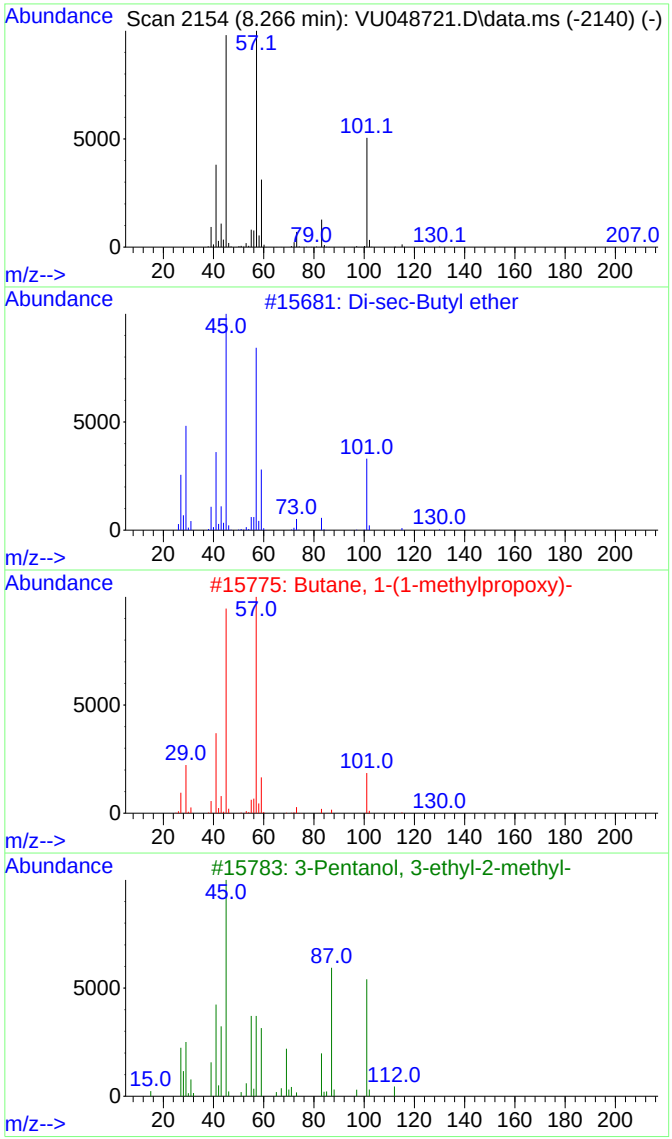
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

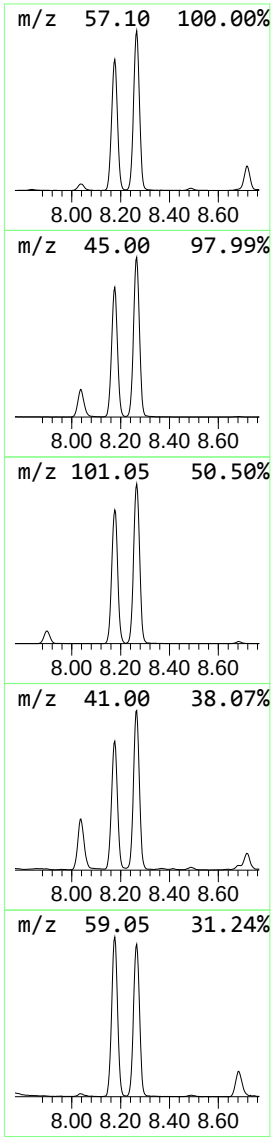
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 1-(1-methylpropoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.266	86.72 ug/l	2117120	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	39
4	Diethyl carbitol	162	C8H18O3	000112-36-7	38
5	Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	36





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Data File : VU048721.D
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ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

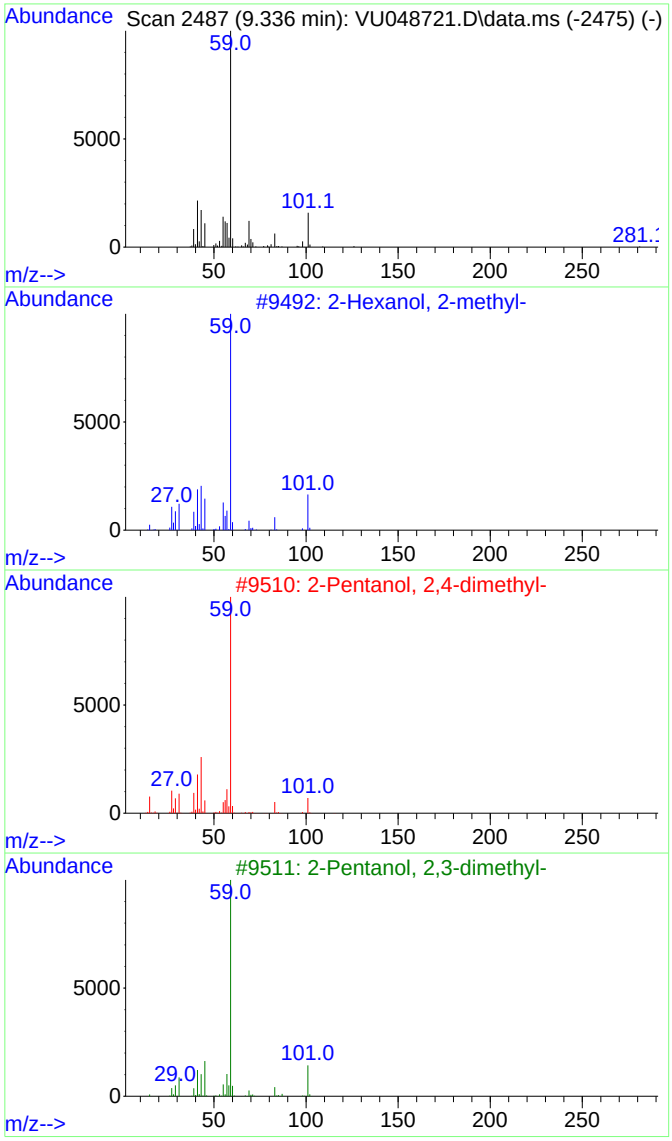
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

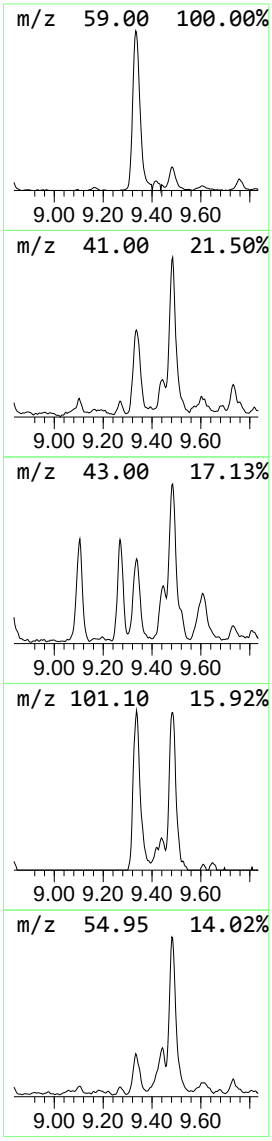
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Hexanol, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.336	9.23 ug/l	225395	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	72
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	72
3	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	64
4	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	64
5	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

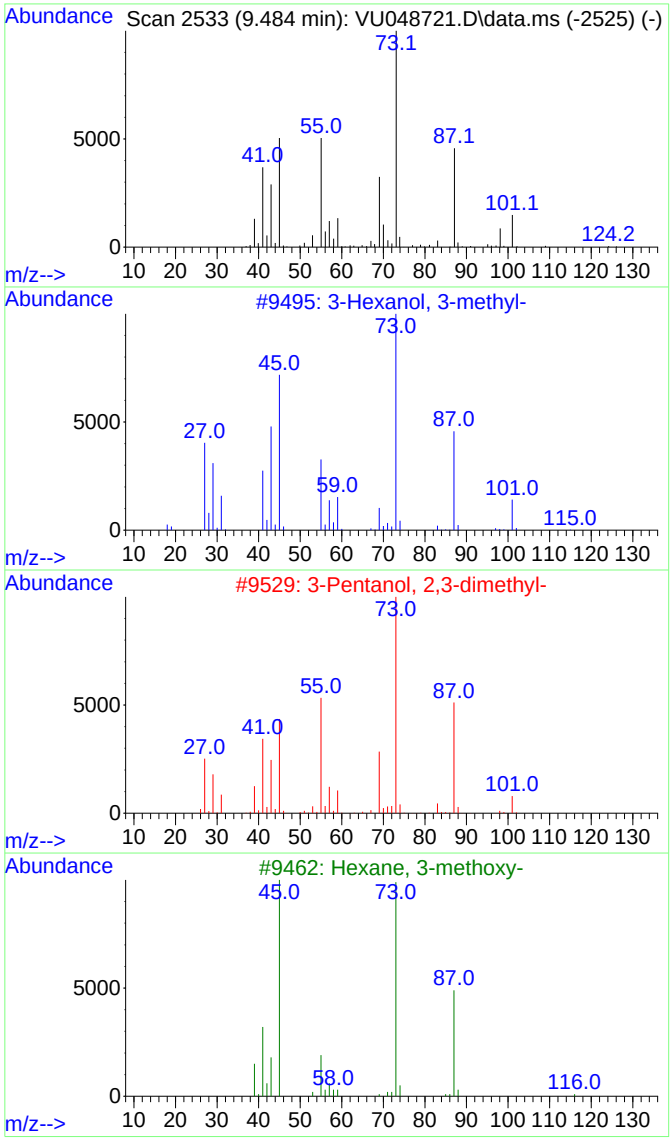
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

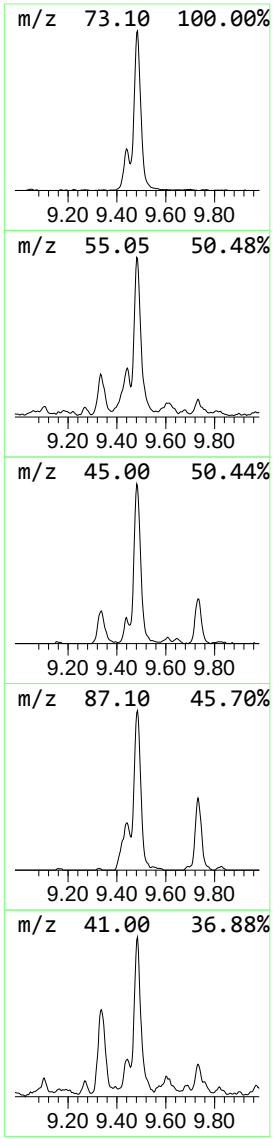
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3-Hexanol, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.484	16.75 ug/l	408991	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	72
2	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	72
3	Hexane, 3-methoxy-	116	C7H16O	054658-01-4	42
4	1,3-Dioxolane, 2-ethyl-	102	C5H10O2	002568-96-9	38
5	3-Heptanol, 3-methyl-	130	C8H18O	005582-82-1	35





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Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

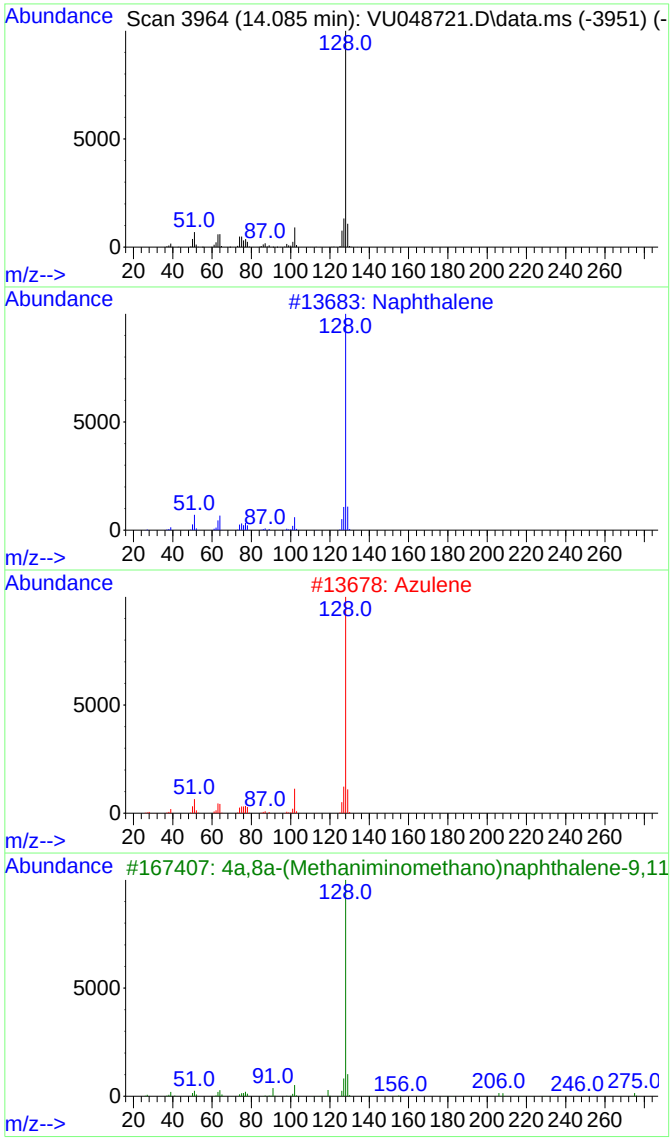
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

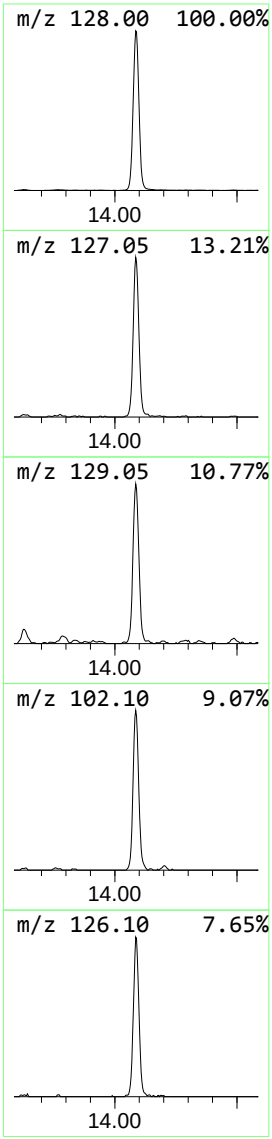
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Azulene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	24.78 ug/l	673451	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	94
3	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
4	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	58
5	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

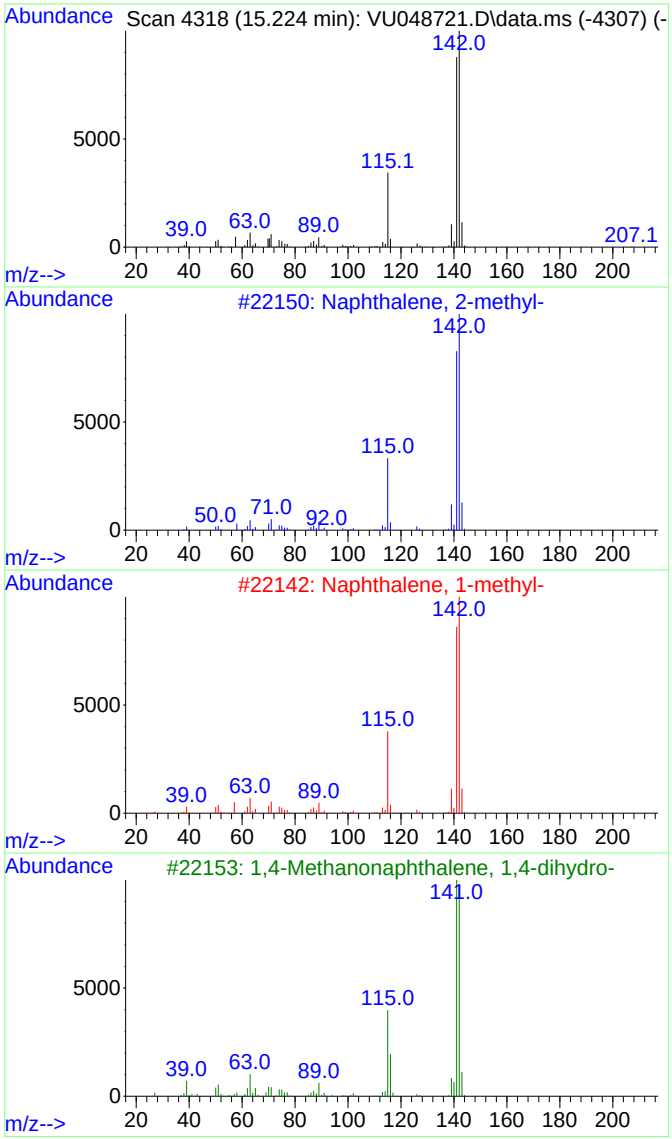
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

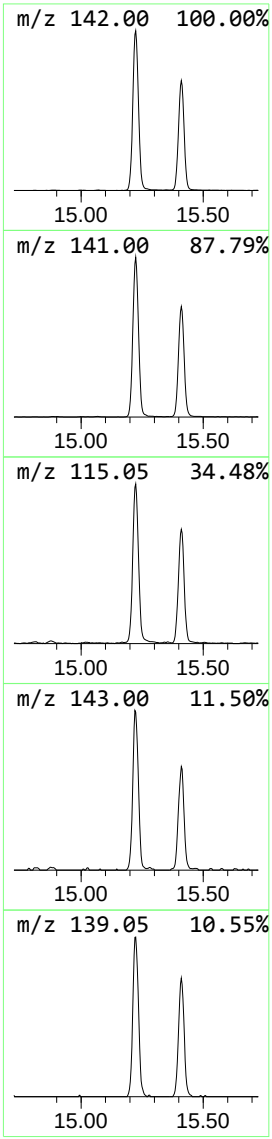
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,4-Methanonaphthalene, 1,4... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.224	29.31 ug/l	796318	1,4-Dichlorobenzene-d4	11.812

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	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

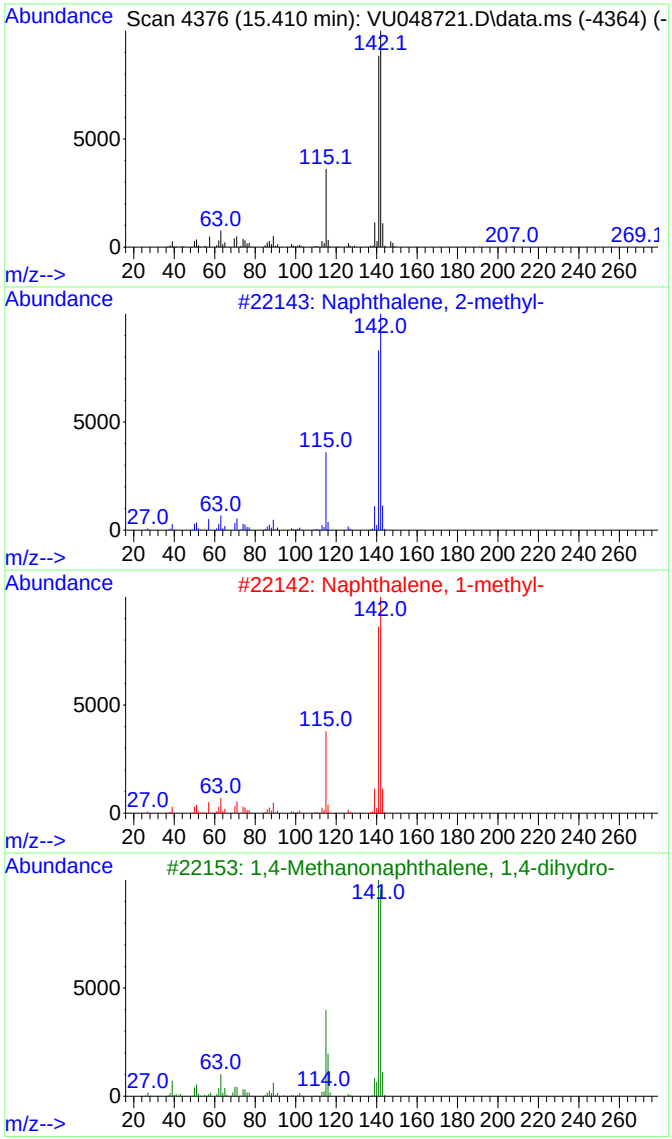
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

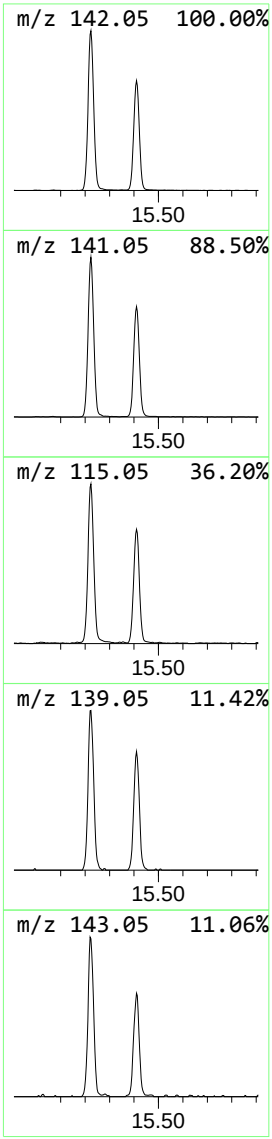
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzocycloheptatriene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	20.54 ug/l	558065	1,4-Dichlorobenzene-d4	11.812

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	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048721.D
Acq On : 28 May 2022 03:11
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.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-Butanol, 2,3-...	7.623	31.3	ug/l	588849	2	6.250	940055	50.0
2-Pentanol, 2-m...	7.684	59.3	ug/l	1115600	2	6.250	940055	50.0
3-Pentanol, 3-m...	8.037	53.3	ug/l	1302150	3	9.417	1220720	50.0
Di-sec-Butyl ether	8.176	73.7	ug/l	1798490	3	9.417	1220720	50.0
Butane, 1-(1-me...	8.266	86.7	ug/l	2117120	3	9.417	1220720	50.0
2-Hexanol, 2-me...	9.336	9.2	ug/l	225395	3	9.417	1220720	50.0
3-Hexanol, 3-me...	9.484	16.8	ug/l	408991	3	9.417	1220720	50.0
Azulene	14.086	24.8	ug/l	673451	4	11.812	1358660	50.0
1,4-Methanonaph...	15.224	29.3	ug/l	796318	4	11.812	1358660	50.0
Benzocyclohepta...	15.410	20.5	ug/l	558065	4	11.812	1358660	50.0