

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
 Data File : VN068549.D
 Acq On : 18 Sep 2021 4:47
 Operator : JC/MD
 Sample : M3798-02
 Misc : 6.35g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NAPL-06-(30-32)

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_N\methods\82N090721W.M
 Title : SW846 8260

Signal : TIC: VN068549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.711	255	269	271	rBV2	17207	26043	1.02%	0.134%
2	7.319	1968	1987	2008	rBV5	9316	26103	1.02%	0.135%
3	8.019	2226	2248	2259	rBV2	337699	809426	31.77%	4.173%
4	8.083	2260	2272	2306	rVB	689042	1554888	61.04%	8.016%
5	8.434	2378	2403	2430	rBV2	303574	705856	27.71%	3.639%
6	8.965	2580	2601	2634	rBV	826914	1736127	68.15%	8.951%
7	9.215	2678	2694	2709	rBV4	12613	26333	1.03%	0.136%
8	10.443	3130	3152	3187	rBV	1244778	2391802	93.89%	12.331%
9	10.977	3337	3351	3370	rBV3	90475	168855	6.63%	0.871%
10	11.524	3540	3555	3562	rBV5	28973	57705	2.27%	0.297%
11	11.629	3582	3594	3616	rVB2	47982	86545	3.40%	0.446%
12	11.747	3618	3638	3659	rBV	1309984	2391018	93.86%	12.327%
13	11.881	3677	3688	3697	rBV7	20214	33452	1.31%	0.172%
14	11.958	3698	3717	3721	rVV9	55784	127719	5.01%	0.658%
15	11.988	3724	3728	3738	rVV2	83161	129905	5.10%	0.670%
16	12.031	3740	3744	3758	rVB3	44429	68891	2.70%	0.355%
17	12.122	3758	3778	3783	rBV9	17756	42409	1.66%	0.219%
18	12.178	3788	3799	3812	rVB3	68082	120324	4.72%	0.620%
19	12.256	3812	3828	3841	rBV6	190955	430649	16.91%	2.220%
20	12.371	3862	3871	3882	rVB2	205823	321538	12.62%	1.658%
21	12.455	3882	3902	3905	rBV7	129443	286673	11.25%	1.478%
22	12.733	3994	4006	4028	rBV	1123643	2006141	78.75%	10.343%
23	12.900	4060	4068	4084	rVB6	157964	319678	12.55%	1.648%
24	12.983	4084	4099	4108	rBV5	153692	331787	13.02%	1.711%
25	13.055	4115	4126	4139	rVB6	401578	762234	29.92%	3.930%
26	13.200	4172	4180	4188	rBV4	130742	180203	7.07%	0.929%
27	13.248	4189	4198	4204	rVV5	136871	226787	8.90%	1.169%
28	13.286	4204	4212	4225	rVB2	318686	505084	19.83%	2.604%
29	13.568	4310	4317	4325	rVB6	164963	237478	9.32%	1.224%
30	13.608	4326	4332	4340	rVB3	99640	117966	4.63%	0.608%
31	13.678	4346	4358	4378	rVB	1410345	2547407	100.00%	13.133%
32	13.911	4438	4445	4454	rVB3	55046	75818	2.98%	0.391%
33	13.999	4467	4478	4489	rBV5	166147	289272	11.36%	1.491%
34	14.321	4589	4598	4610	rVB8	38275	66686	2.62%	0.344%
35	14.383	4611	4621	4636	rVB8	30525	62142	2.44%	0.320%
36	14.463	4639	4651	4659	rBV8	19459	41576	1.63%	0.214%

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NAPL-06-(30-32)

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

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Title : SW846 8260

37	14.514	4663	4670	4676	rBV7	21982	29127	1.14%	0.150%
38	14.852	4790	4796	4807	rVB9	19705	28184	1.11%	0.145%
39	14.917	4812	4820	4833	rVV4	14626	27115	1.06%	0.140%

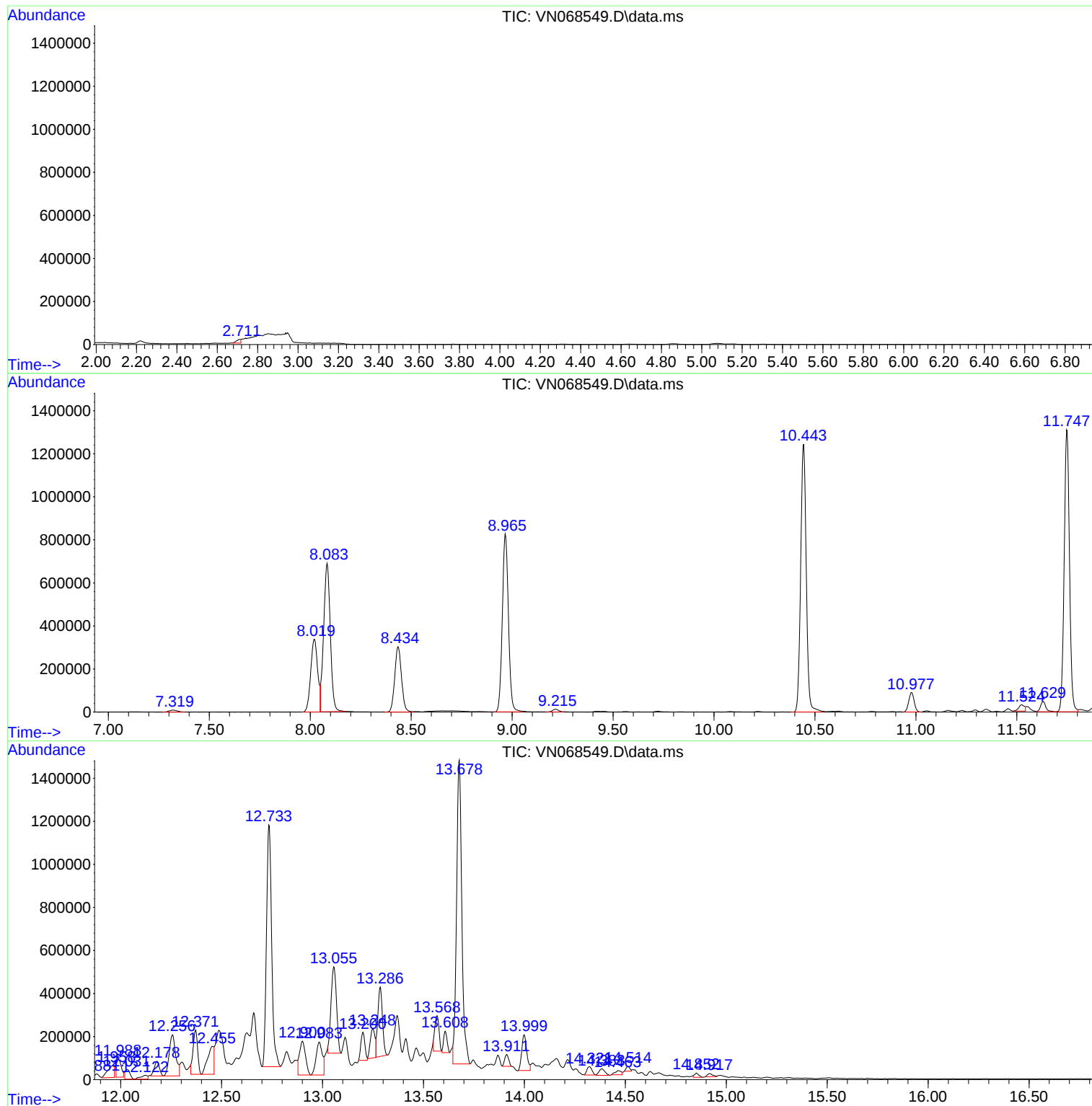
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



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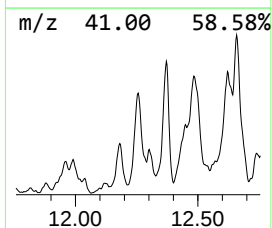
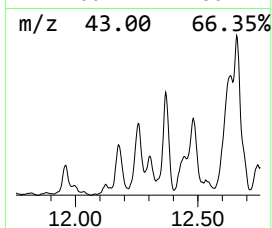
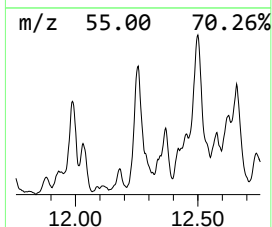
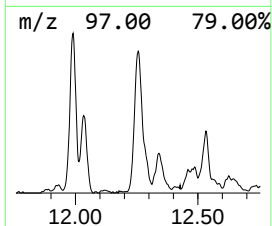
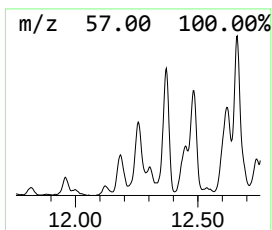
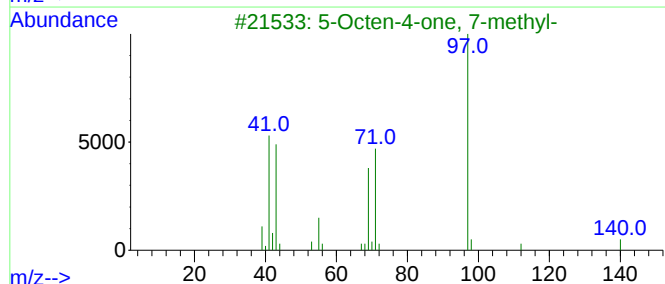
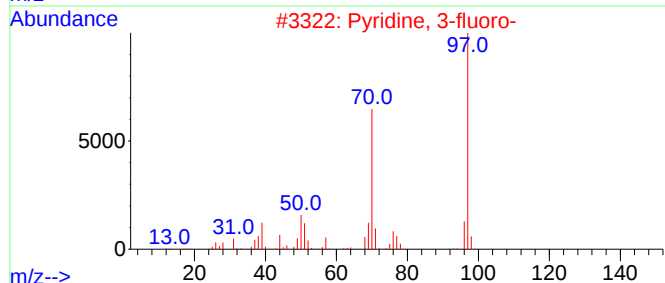
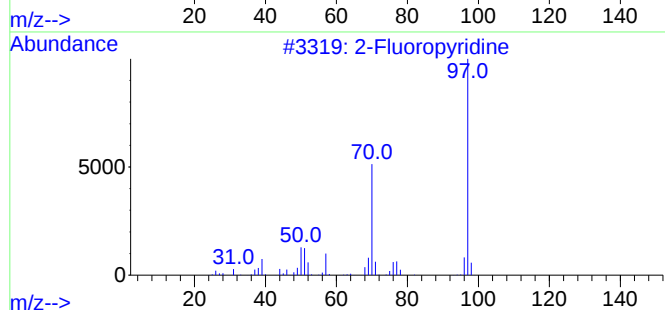
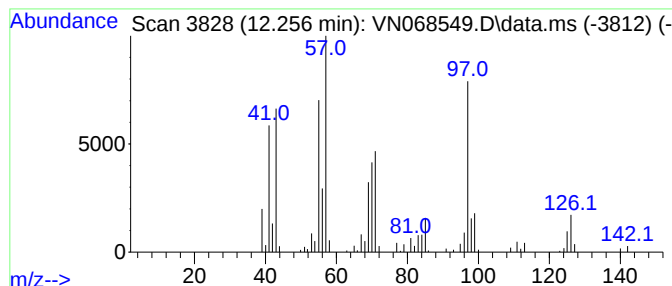
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown12.256 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	9.01 ug/l	430649	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Fluoropyridine	97	C5H4FN	000372-48-5	49
2			Pyridine, 3-fluoro-	97	C5H4FN	000372-47-4	46
3			5-Octen-4-one, 7-methyl-	140	C9H16O	032064-78-1	45
4			6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	43
5			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	35



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ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(30-32)

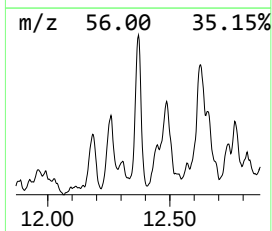
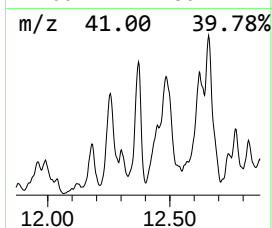
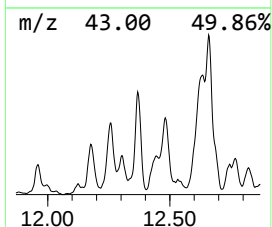
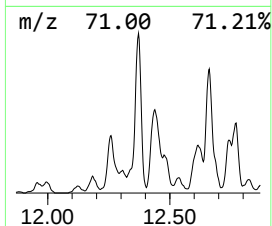
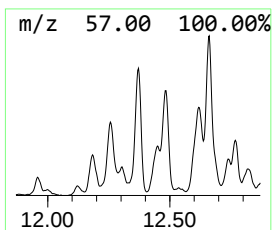
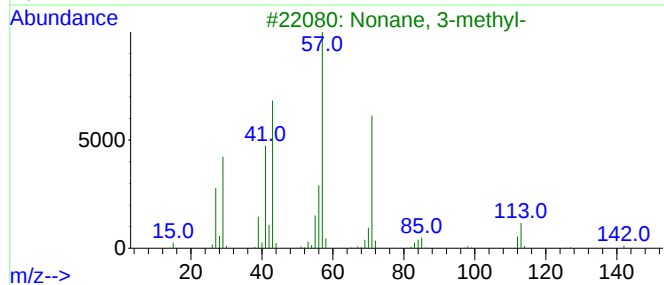
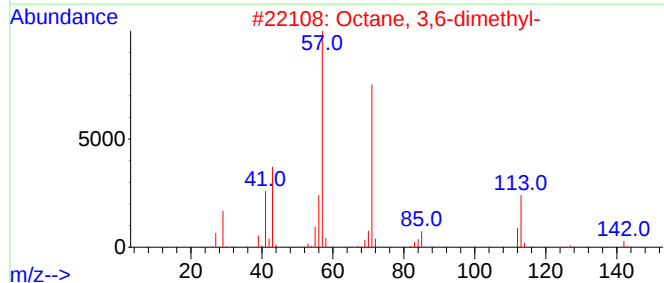
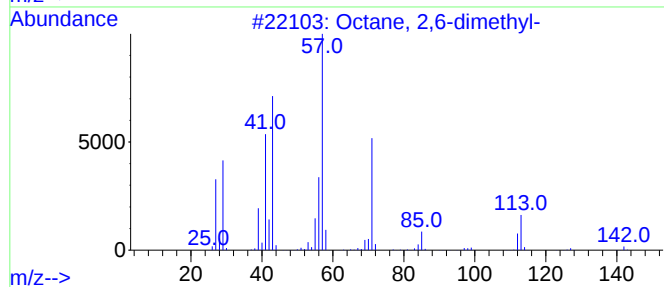
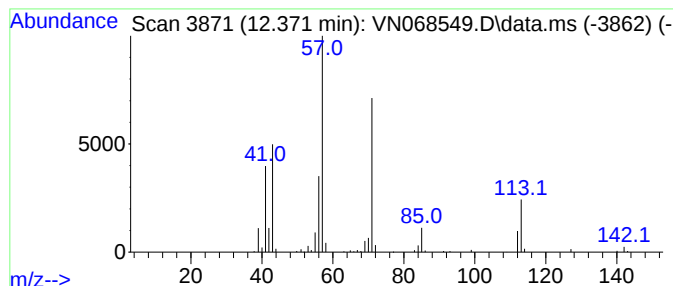
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.371	6.72 ug/l	321538	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
2			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	87
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	83
4			Tridecane, 7-methyl-	198	C14H30	026730-14-3	53
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47



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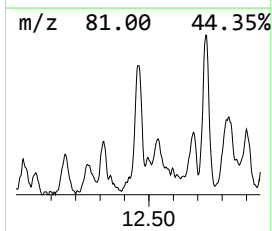
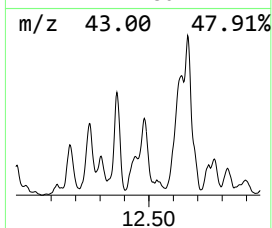
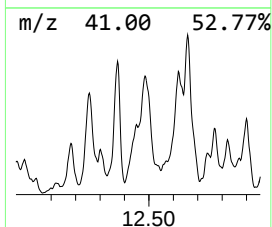
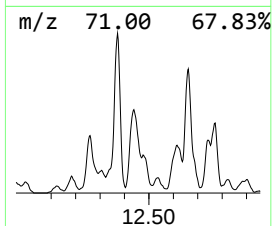
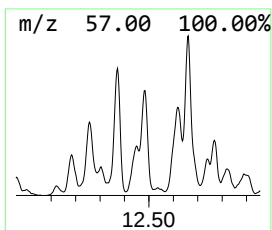
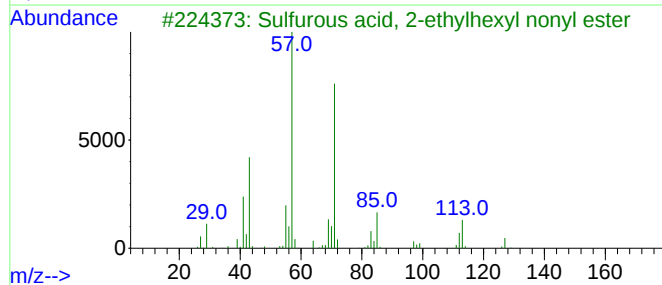
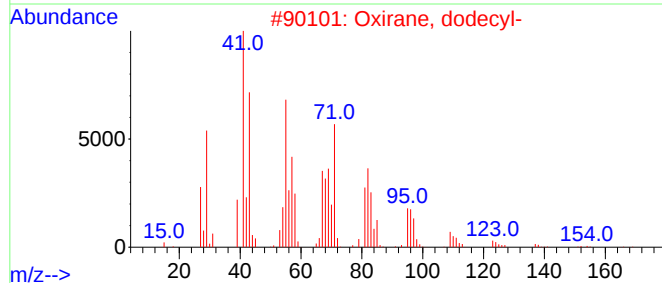
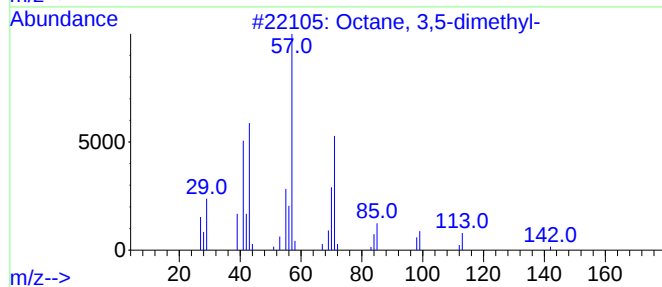
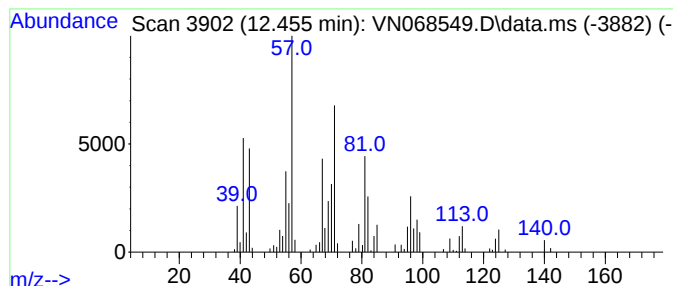
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown12.455 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.455	5.99 ug/l	286673	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	46
2			Oxirane, dodecyl-	212	C14H28O	003234-28-4	43
3			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	27
4			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	25
5			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	22



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ClientSampleId :
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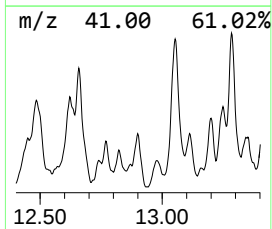
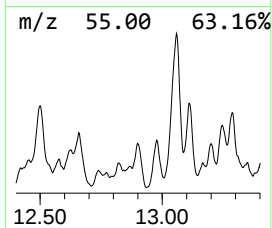
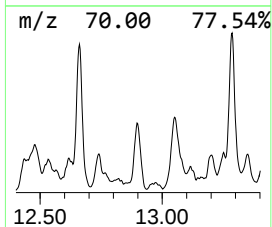
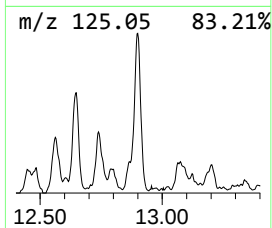
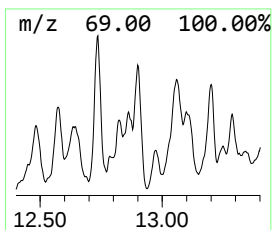
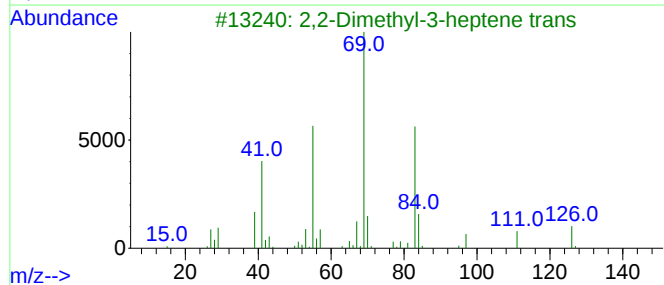
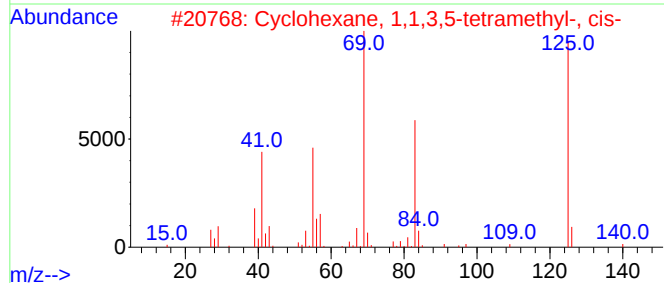
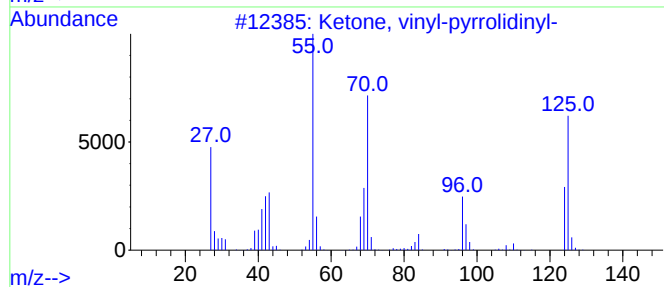
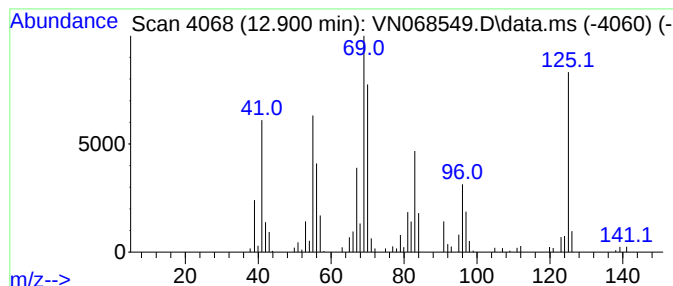
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.900 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.900	6.27 ug/l	319678	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ketone, vinyl-pyrrolidinyl-	125	C7H11NO	042104-70-1	45
2			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	43
3			2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	27
4			1-Octene, 3,3-dimethyl-	140	C10H20	074511-51-6	27
5			Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	001678-81-5	27



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Instrument :
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ClientSampleId :
NAPL-06-(30-32)

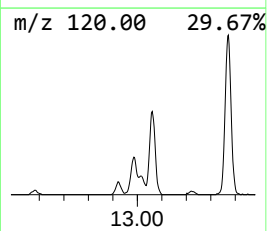
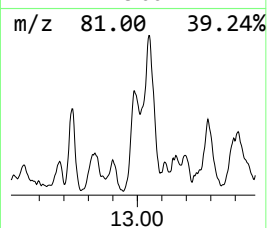
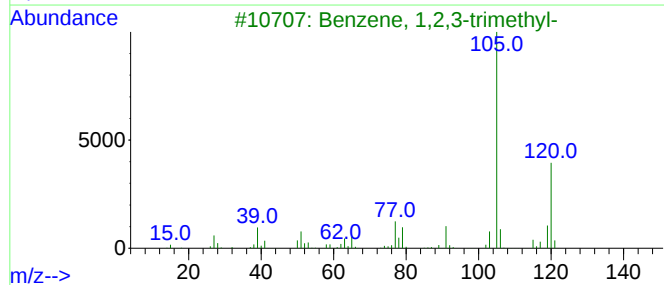
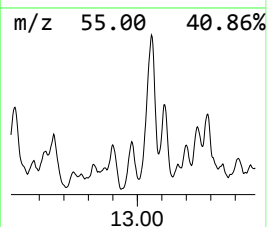
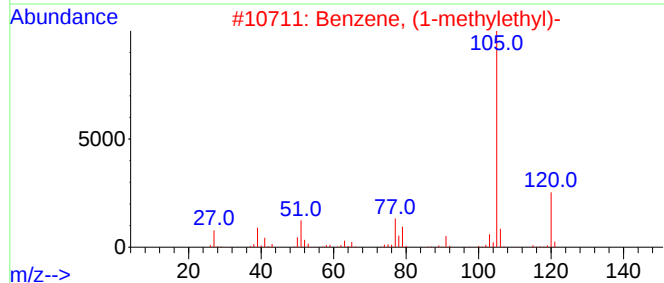
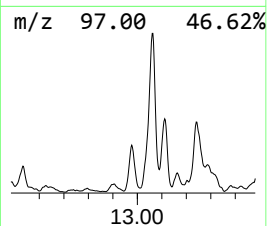
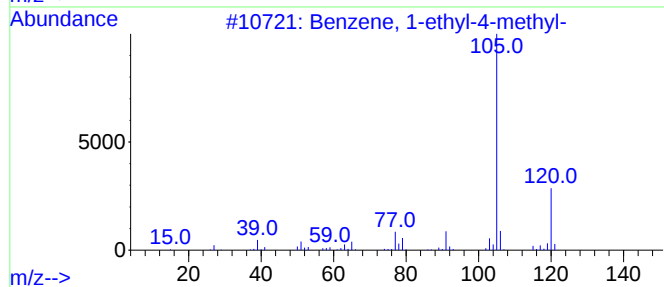
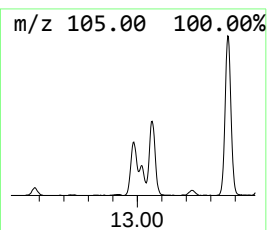
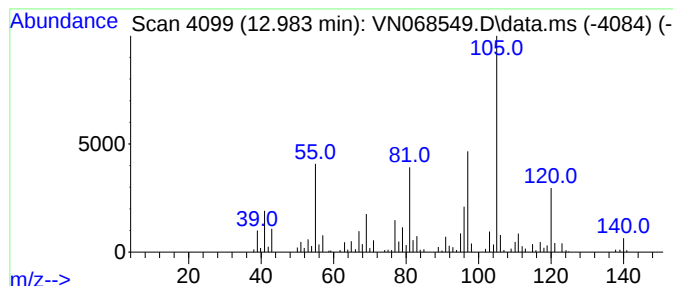
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Quant Title : SW846 8260

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

Peak Number 5 unknown12.983 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	6.51 ug/l	331787	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	46
2			Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	42
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	42
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	42
5			Mesitylene	120	C9H12	000108-67-8	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068549.D
Acq On : 18 Sep 2021 4:47
Operator : JC/MD
Sample : M3798-02
Misc : 6.35g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(30-32)

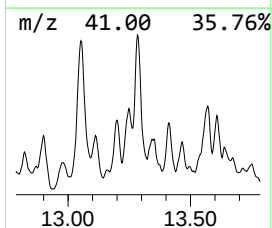
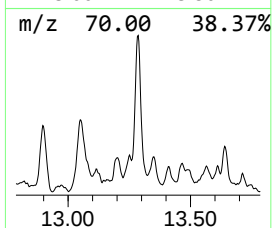
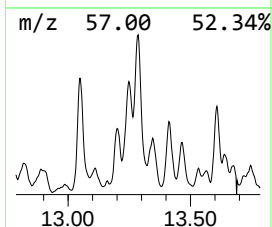
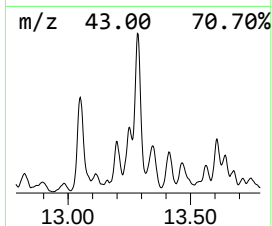
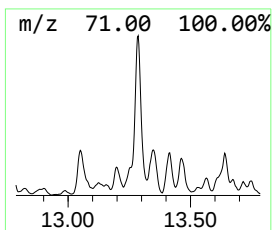
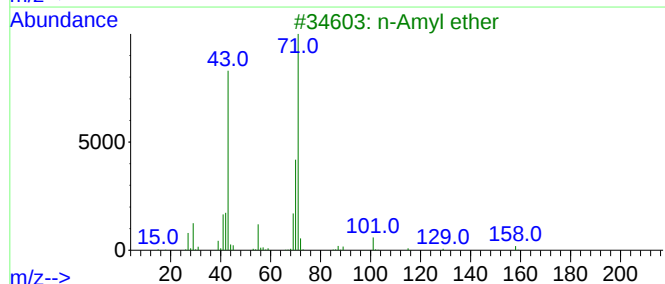
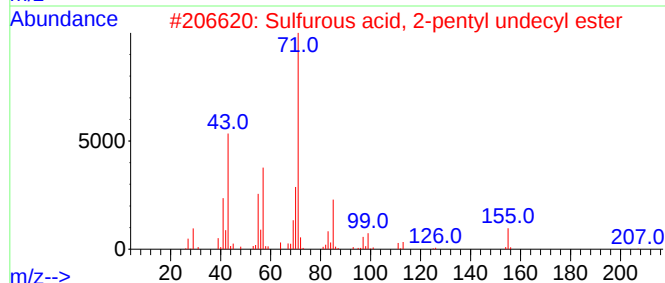
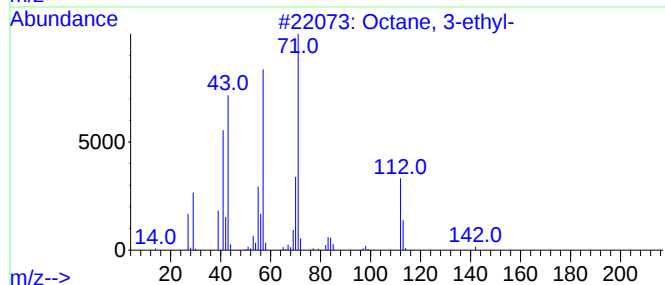
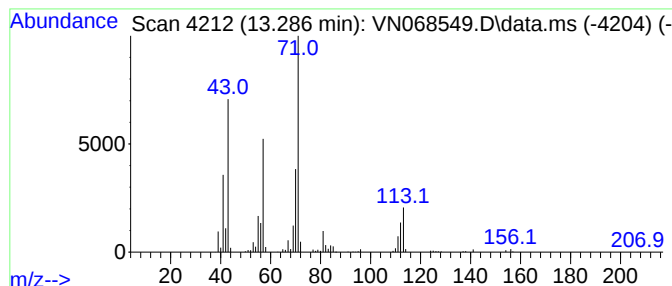
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Quant Title : SW846 8260

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

Peak Number 6 Octane, 3-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	9.91 ug/l	505084	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-ethyl-	142	C10H22	005881-17-4	64
2			Sulfurous acid, 2-pentyl undecyl...	306	C16H34O3S	1000309-16-0	59
3			n-Amyl ether	158	C10H22O	000693-65-2	53
4			Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	53
5			Decane, 3,3,6-trimethyl-	184	C13H28	062338-14-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068549.D
Acq On : 18 Sep 2021 4:47
Operator : JC/MD
Sample : M3798-02
Misc : 6.35g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(30-32)

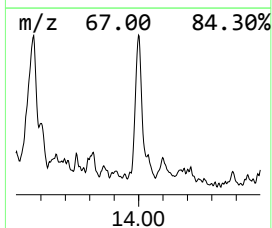
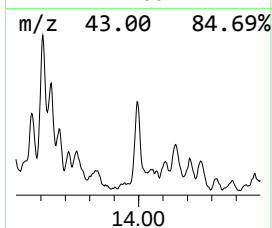
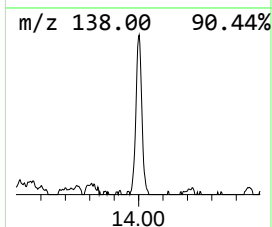
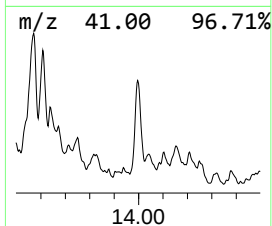
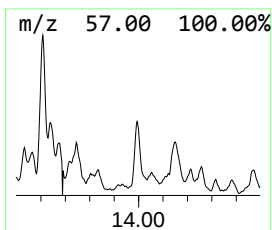
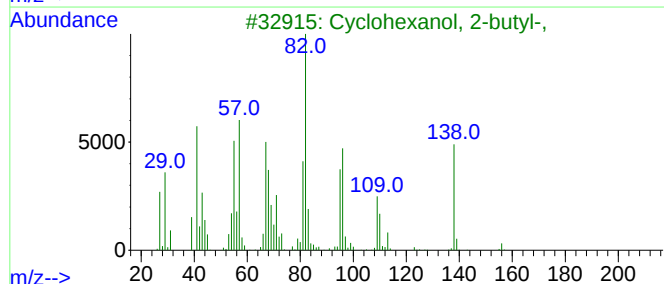
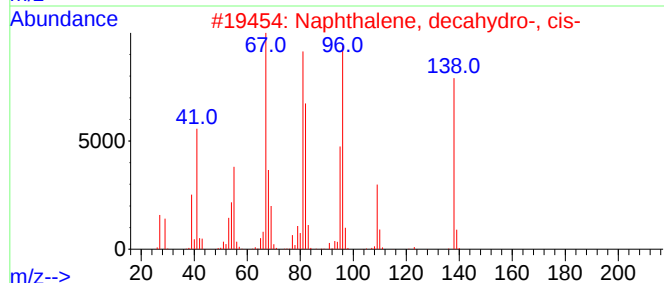
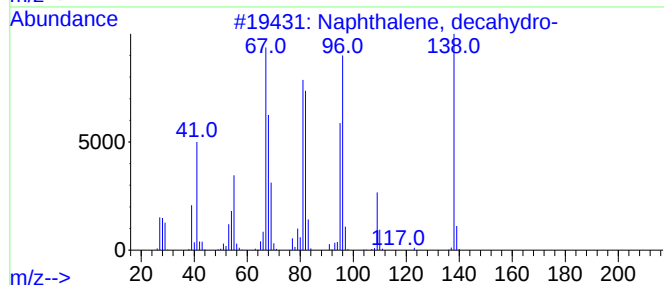
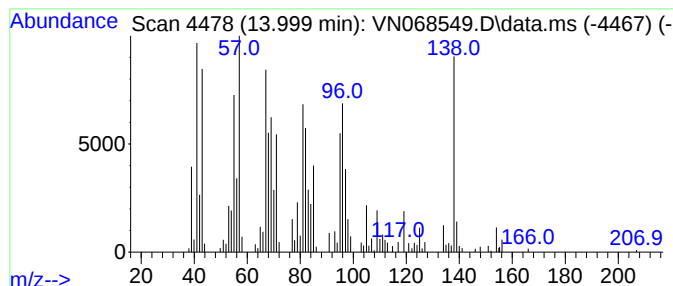
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, decahydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.999	5.68 ug/l	289272	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	97
2			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	64
3			Cyclohexanol, 2-butyl-,	156	C10H20O	036159-49-6	58
4			Spiro[4.5]decane	138	C10H18	000176-63-6	58
5			9-Borabicyclo[3.3.1]nonane, 9-hy...	138	C8H15BO	063366-65-4	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068549.D
Acq On : 18 Sep 2021 4:47
Operator : JC/MD
Sample : M3798-02
Misc : 6.35g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(30-32)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Octane, 2,6-dim...	12.371	6.7	ug/l	321538	3	11.746	2391020	50.0
unknown12.455	12.455	6.0	ug/l	286673	3	11.746	2391020	50.0
unknown12.900	12.900	6.3	ug/l	319678	4	13.678	2547410	50.0
unknown12.983	12.983	6.5	ug/l	331787	4	13.678	2547410	50.0
Octane, 3-ethyl-	13.286	9.9	ug/l	505084	4	13.678	2547410	50.0
Naphthalene, de...	13.999	5.7	ug/l	289272	4	13.678	2547410	50.0