

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
 Data File : VN068556.D
 Acq On : 18 Sep 2021 7:44
 Operator : JC/MD
 Sample : M3798-09
 Misc : 6.83g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NAPL-07-(8-10)-END-POINT

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: VN068556.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.019	2225	2248	2259	rBV2	373972	907767	1.05%	0.158%
2	8.083	2260	2272	2293	rVB	760618	1751859	2.02%	0.305%
3	8.968	2581	2602	2636	rBV2	919161	1973213	2.28%	0.344%
4	10.443	3135	3152	3186	rBV2	1926974	4069063	4.70%	0.709%
5	11.055	3361	3380	3396	rVB	766184	1367978	1.58%	0.238%
6	11.157	3402	3418	3434	rBV	793120	1722561	1.99%	0.300%
7	11.229	3434	3445	3456	rVV	718639	1262250	1.46%	0.220%
8	11.293	3459	3469	3479	rVV	1125656	1963925	2.27%	0.342%
9	11.347	3479	3489	3502	rVB	1593754	2789861	3.22%	0.486%
10	11.457	3518	3530	3539	rBV	1817948	3054826	3.53%	0.532%
11	11.524	3541	3555	3561	rBV2	2510915	4751243	5.49%	0.828%
12	11.629	3582	3594	3618	rVB	2592383	4726699	5.46%	0.824%
13	11.749	3619	3639	3655	rBV2	1525999	3834512	4.43%	0.668%
14	11.881	3679	3688	3696	rBV	1784209	2760169	3.19%	0.481%
15	11.961	3697	3718	3721	rVV4	5658637	12285424	14.19%	2.141%
16	11.991	3723	3729	3739	rVV	9406859	16272696	18.80%	2.836%
17	12.034	3740	3745	3758	rVB3	5270631	8153587	9.42%	1.421%
18	12.098	3758	3769	3770	rBV4	724182	887447	1.03%	0.155%
19	12.181	3789	3800	3811	rVB4	6000460	10800329	12.48%	1.882%
20	12.256	3812	3828	3842	rBV4	19025324	41607611	48.07%	7.250%
21	12.374	3863	3872	3882	rVB	18569184	27317797	31.56%	4.760%
22	12.457	3882	3903	3907	rBV6	13981622	32002950	36.97%	5.577%
23	12.742	3998	4009	4017	rBV6	6807390	11747988	13.57%	2.047%
24	12.905	4061	4070	4086	rVB4	16949431	37453898	43.27%	6.527%
25	12.983	4086	4099	4107	rBV4	9058738	18512436	21.39%	3.226%
26	13.058	4114	4127	4140	rVV6	42394742	86563929	100.00%	15.084%
27	13.114	4141	4148	4160	rVB2	16245011	24457479	28.25%	4.262%
28	13.203	4172	4181	4189	rBV3	10494422	14831323	17.13%	2.584%
29	13.248	4190	4198	4205	rVV3	8927683	15077533	17.42%	2.627%
30	13.289	4206</							

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37	13.999	4467	4478	4489	rBV4	15215382	25290455	29.22%	4.407%
38	14.099	4510	4515	4522	rBV5	1655646	1944792	2.25%	0.339%
39	14.217	4550	4559	4578	rVB	11011266	16541932	19.11%	2.883%
40	14.324	4590	4599	4611	rVB5	4432831	8356042	9.65%	1.456%
41	14.391	4612	4624	4636	rBV10	1980310	3848620	4.45%	0.671%
42	14.512	4660	4669	4673	rBV4	2859657	3982959	4.60%	0.694%
43	14.539	4675	4679	4691	rVB3	4242931	5724217	6.61%	0.997%
44	14.622	4702	4710	4719	rBV2	1698050	2384600	2.75%	0.416%
45	14.917	4809	4820	4836	rBV2	2173958	4295030	4.96%	0.748%

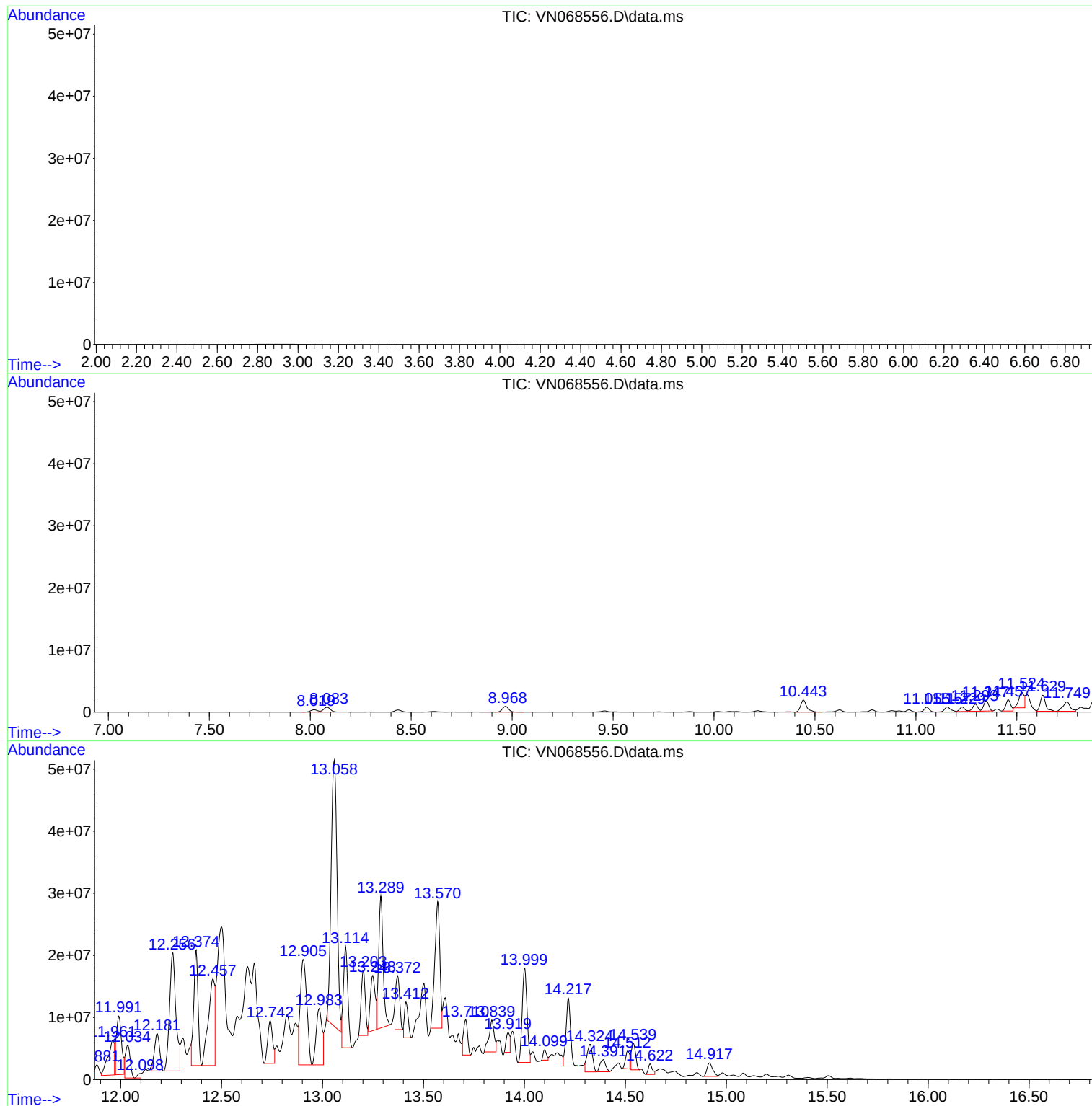
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



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NAPL-07-(8-10)-END-POINT

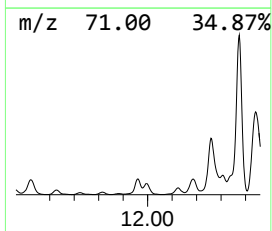
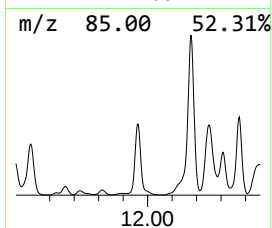
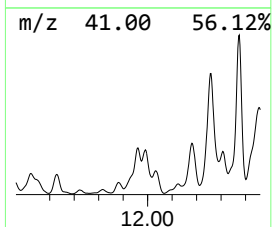
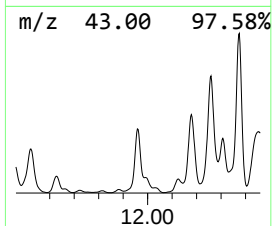
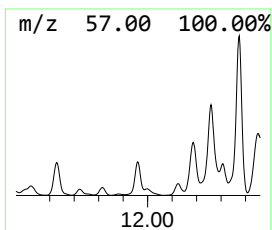
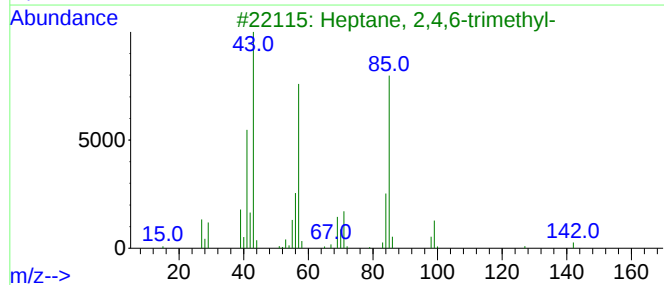
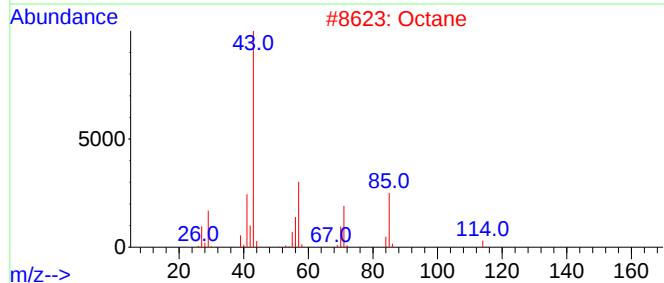
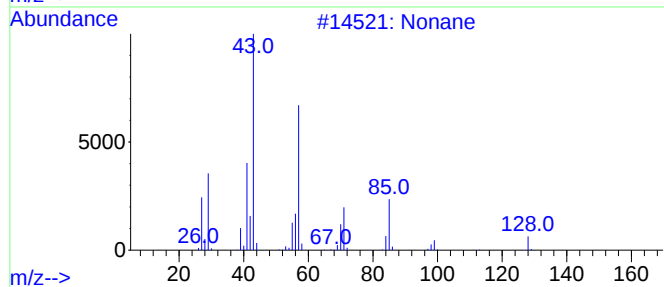
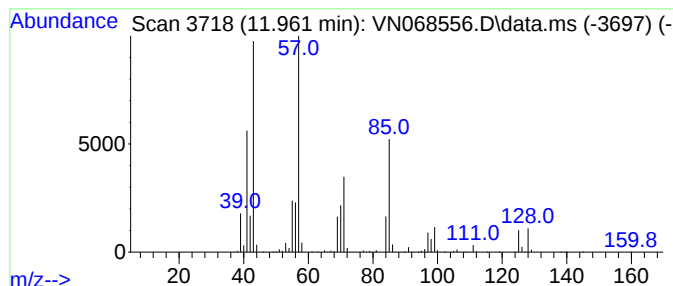
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 1 Nonane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.961	160.19 ug/l	12285400	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane	128	C9H20	000111-84-2	93
2			Octane	114	C8H18	000111-65-9	50
3			Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	49
4			Ether, heptyl hexyl	200	C13H28O	007289-40-9	47
5			Hexanoic acid, 9-decen-1-yl ester	254	C16H30O2	180252-09-9	43



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ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(8-10)-END-POINT

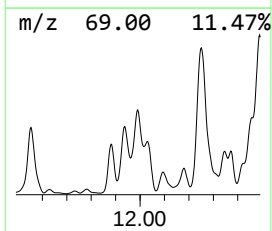
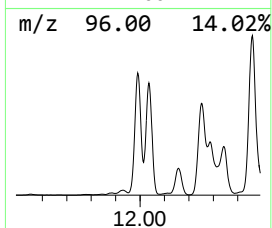
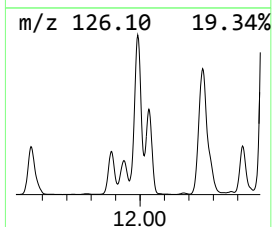
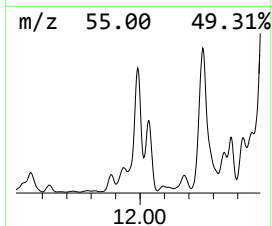
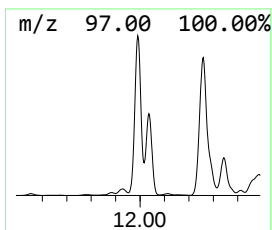
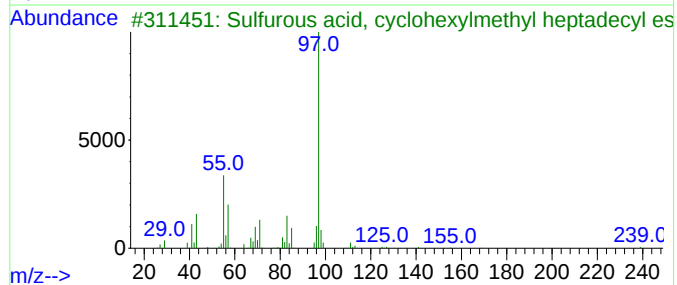
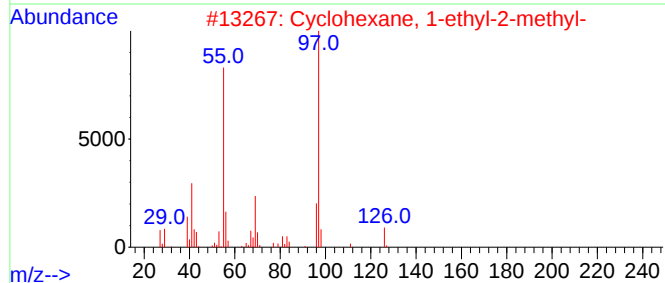
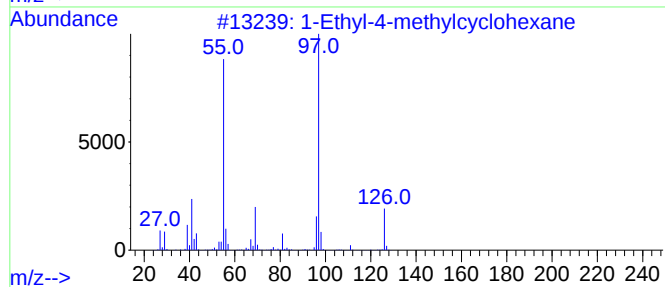
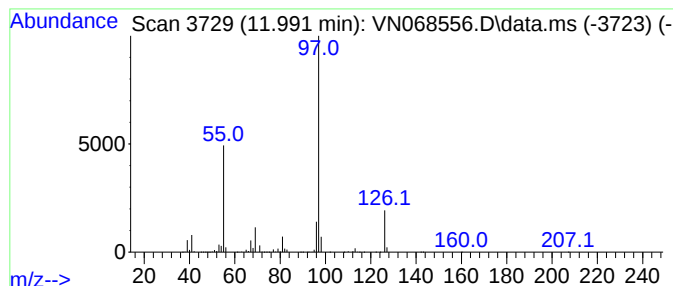
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Ethyl-4-methylcyclohexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.991	212.19 ug/l	16272700	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	91
2			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	78
3			Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	64
4			Thiophene, 2-propyl-	126	C7H10S	001551-27-5	64
5			Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	64



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Misc : 6.83g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 50 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NAPL-07-(8-10)-END-POINT

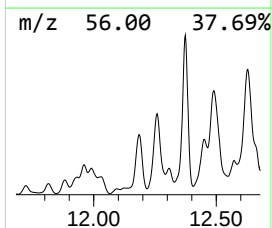
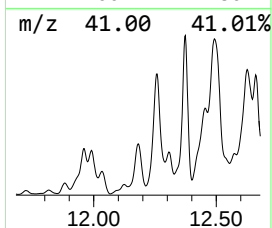
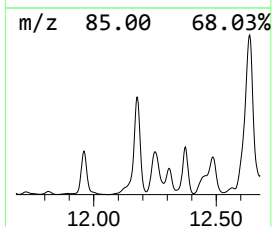
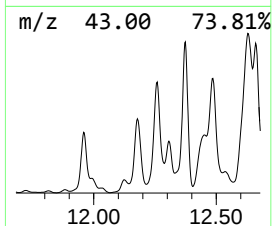
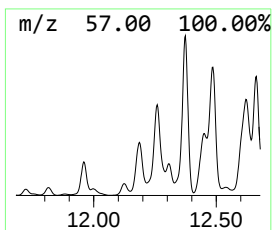
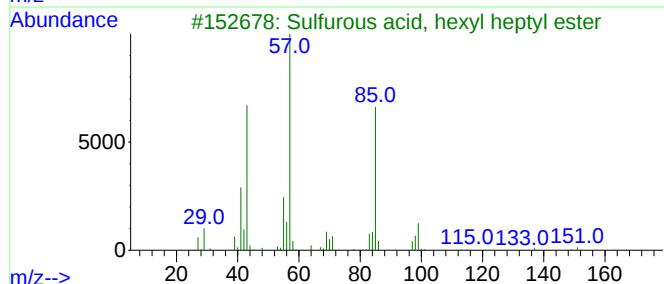
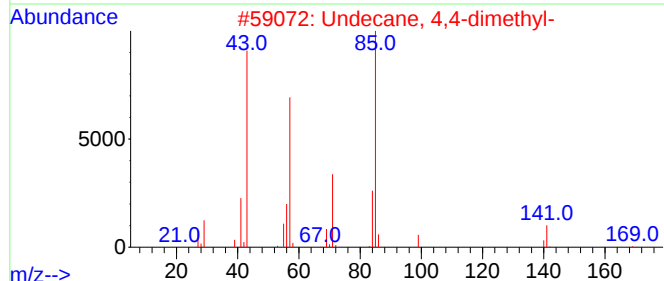
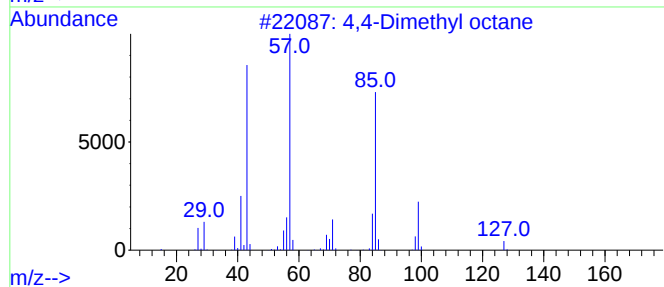
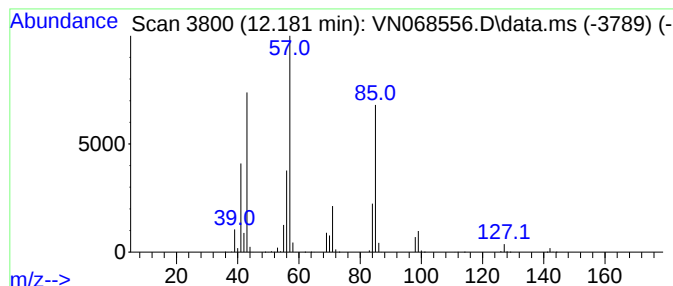
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 3 4,4-Dimethyl octane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.181	140.83 ug/l	10800300	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4-Dimethyl octane	142	C10H22	015869-95-1	59
2			Undecane, 4,4-dimethyl-	184	C13H28	017312-68-4	59
3			Sulfurous acid, hexyl heptyl ester	264	C13H28O3S	1000309-12-9	53
4			Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	52
5			Heptane, 4,4-dimethyl-	128	C9H20	001068-19-5	50



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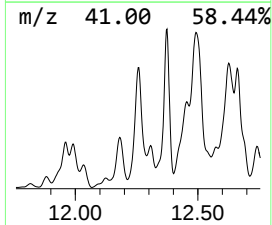
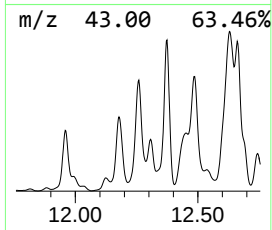
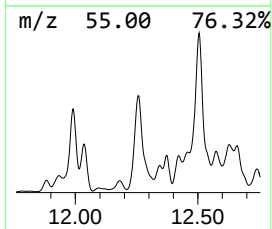
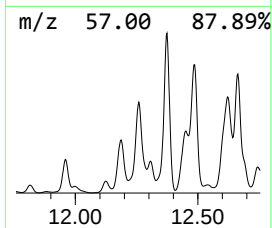
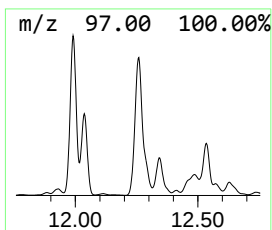
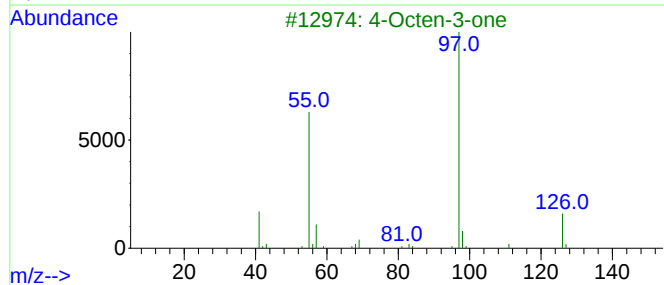
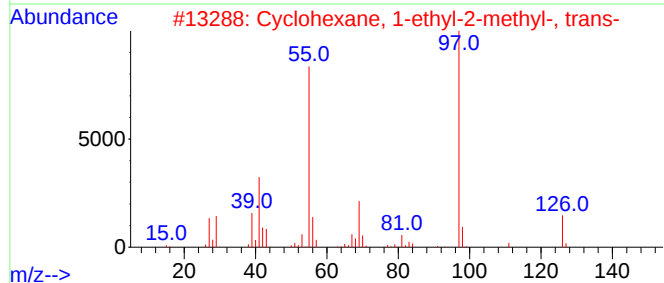
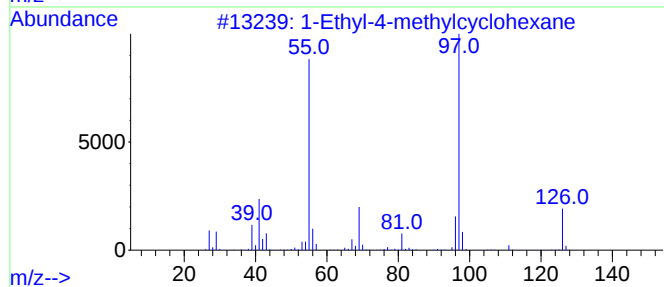
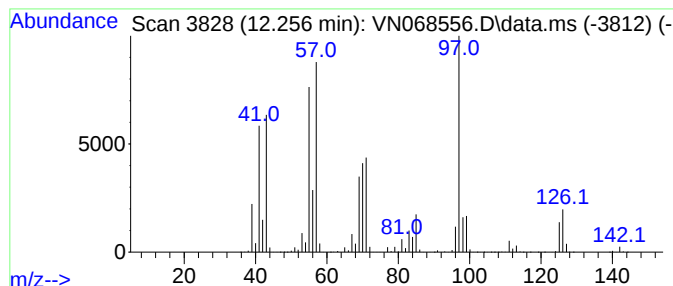
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown12.256 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	542.54 ug/l	41607600	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	38
2			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	38
3			4-Octen-3-one	126	C8H14O	014129-48-7	38
4			Thiophene, 2-propyl-	126	C7H10S	001551-27-5	35
5			Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	30



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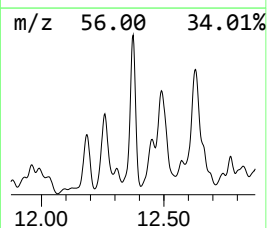
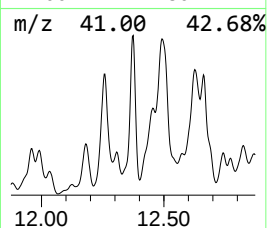
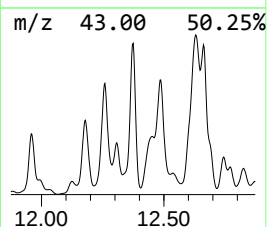
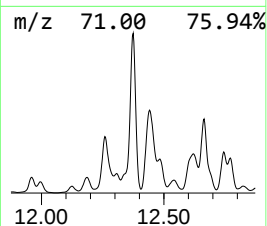
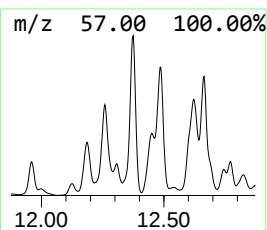
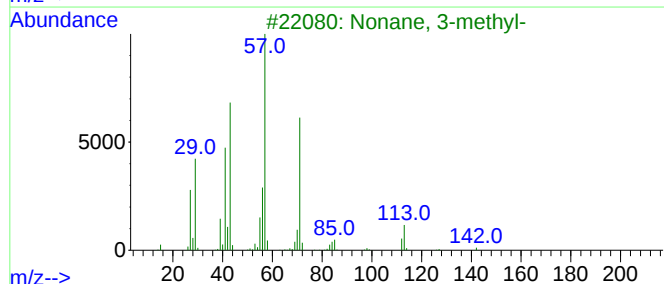
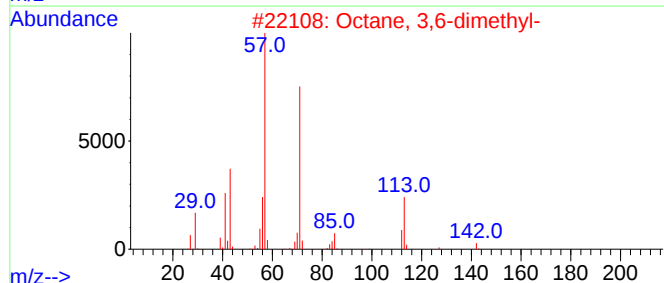
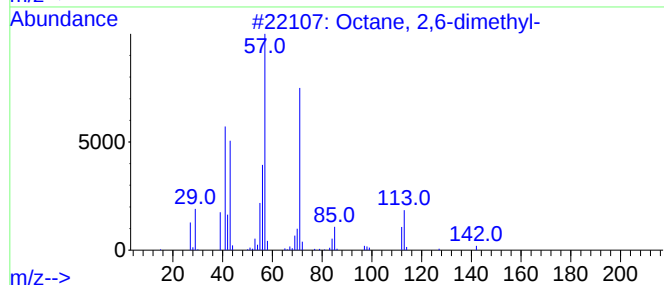
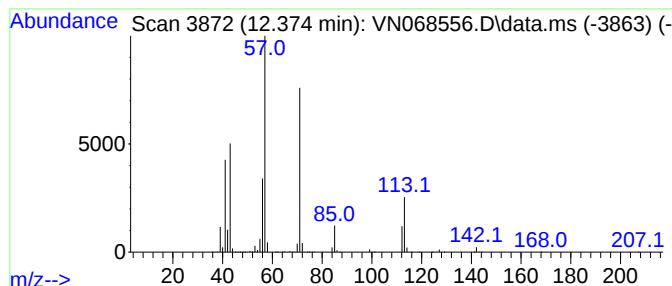
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Quant Title : SW846 8260

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

Peak Number 5 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	356.21 ug/l	27317800	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	91
4			Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	80
5			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068556.D
Acq On : 18 Sep 2021 7:44
Operator : JC/MD
Sample : M3798-09
Misc : 6.83g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(8-10)-END-POINT

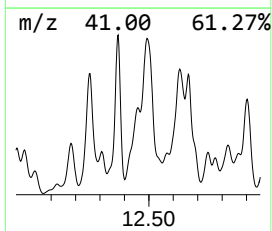
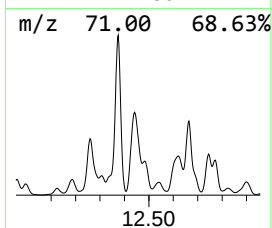
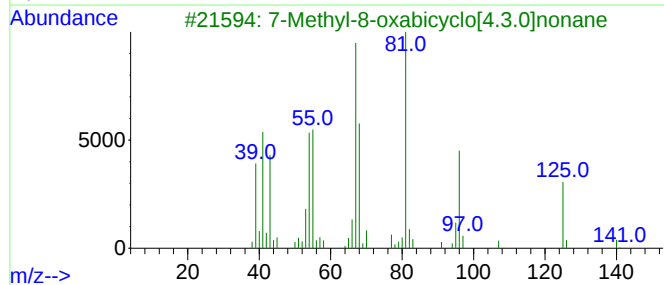
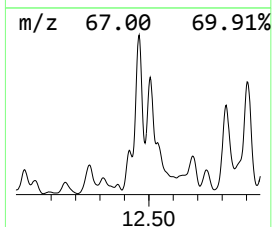
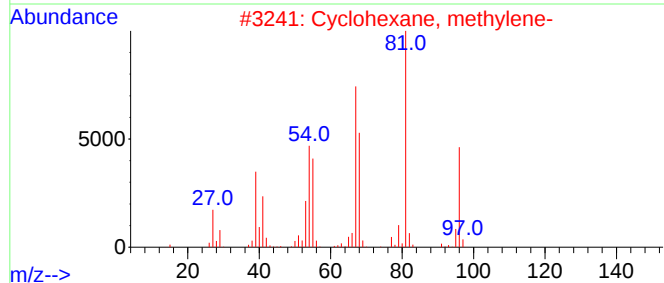
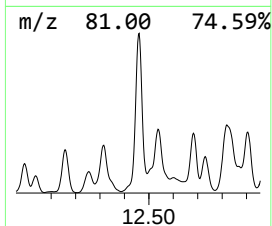
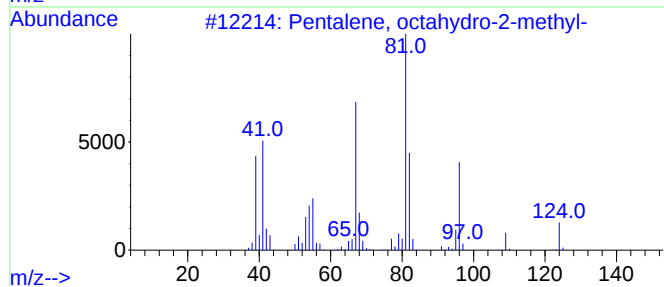
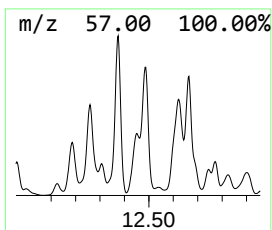
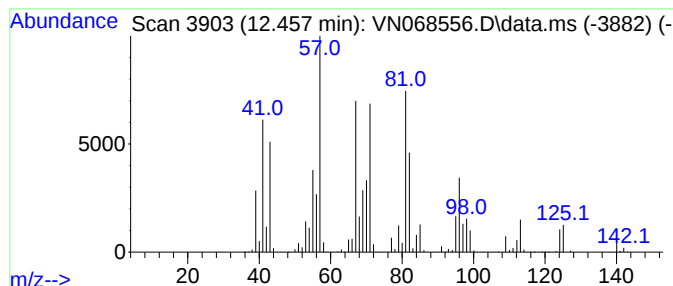
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Quant Title : SW846 8260

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

Peak Number 6 unknown12.457 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	417.30 ug/l	32003000	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	46
2			Cyclohexane, methylene-	96	C7H12	001192-37-6	43
3			7-Methyl-8-oxabicyclo[4.3.0]nonane	140	C9H16O	1000216-87-6	43
4			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	38
5			1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068556.D
Acq On : 18 Sep 2021 7:44
Operator : JC/MD
Sample : M3798-09
Misc : 6.83g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(8-10)-END-POINT

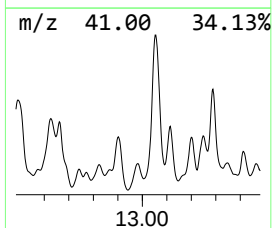
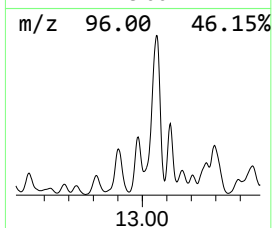
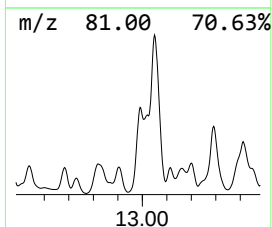
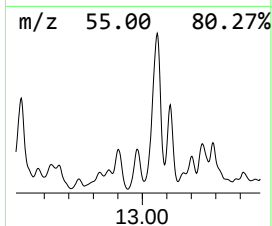
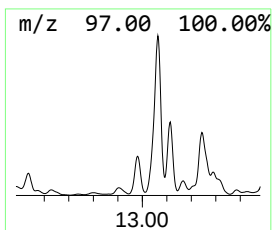
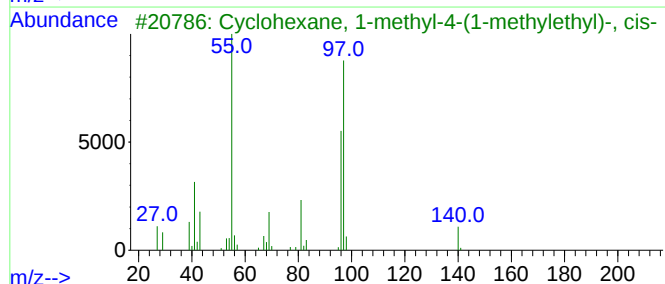
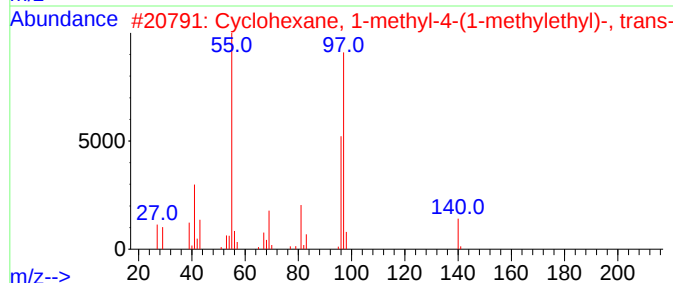
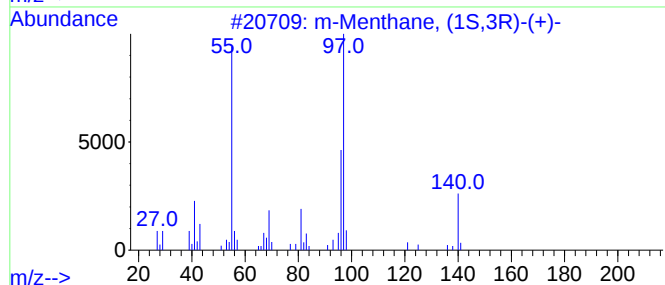
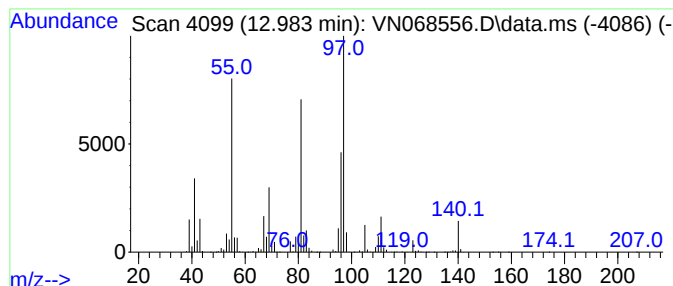
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Quant Title : SW846 8260

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

Peak Number 7 m-Menthane, (1S,3R)-(+)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	121.44 ug/l	18512400	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	83
2			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	81
3			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	72
4			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	64
5			Oxalic acid, di(cyclohexylmethyl...	282	C16H26O4	1000309-68-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068556.D
Acq On : 18 Sep 2021 7:44
Operator : JC/MD
Sample : M3798-09
Misc : 6.83g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(8-10)-END-POINT

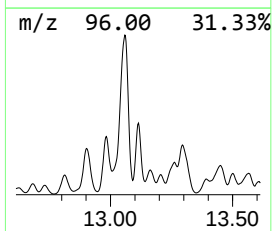
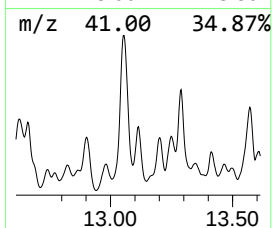
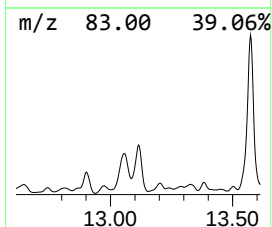
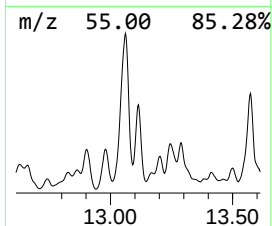
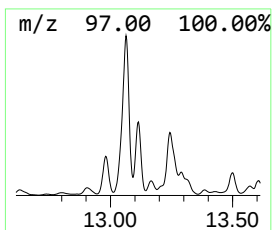
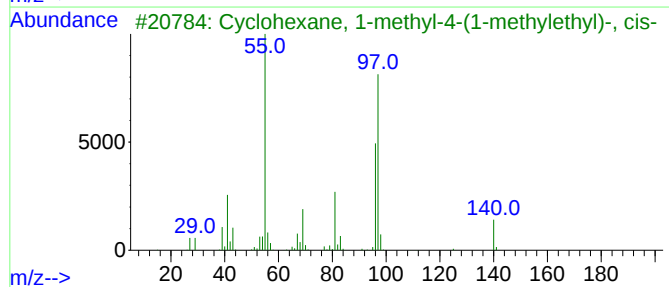
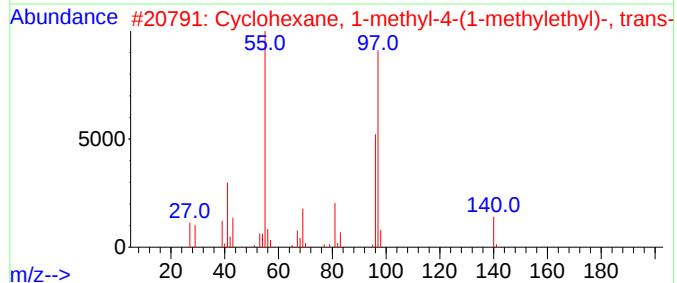
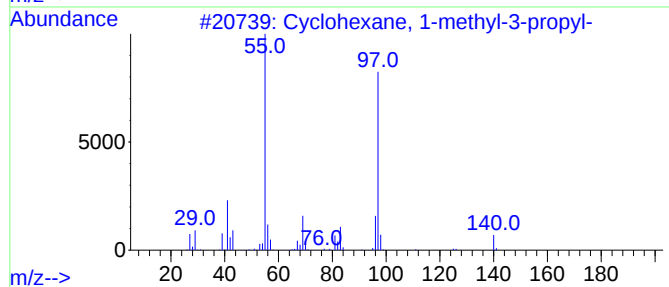
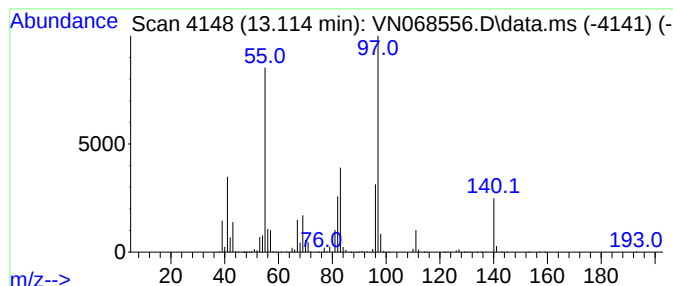
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, 1-methyl-3-pro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.114	160.44 ug/l	24457500	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	58
2			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	53
3			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	53
4			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	53
5			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068556.D
Acq On : 18 Sep 2021 7:44
Operator : JC/MD
Sample : M3798-09
Misc : 6.83g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(8-10)-END-POINT

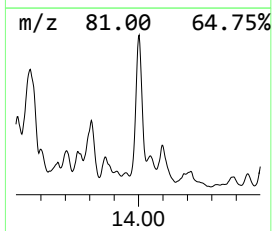
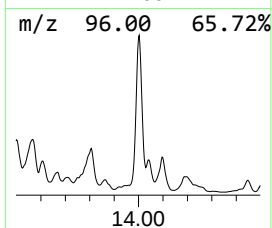
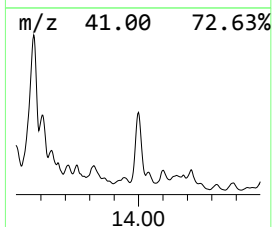
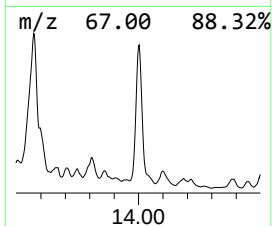
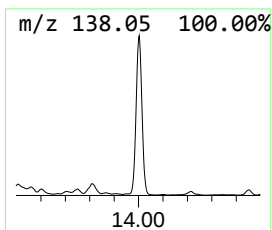
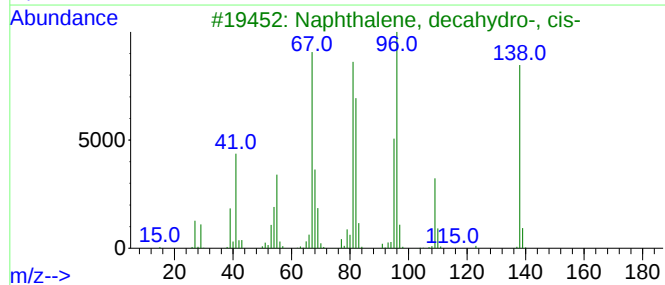
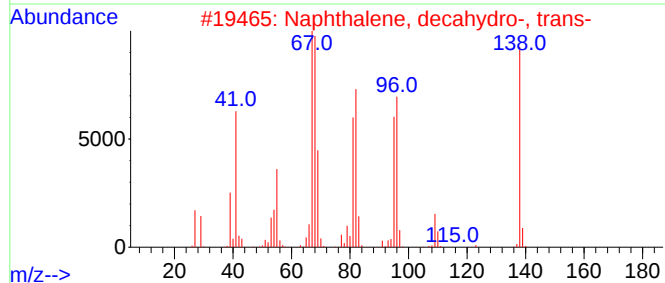
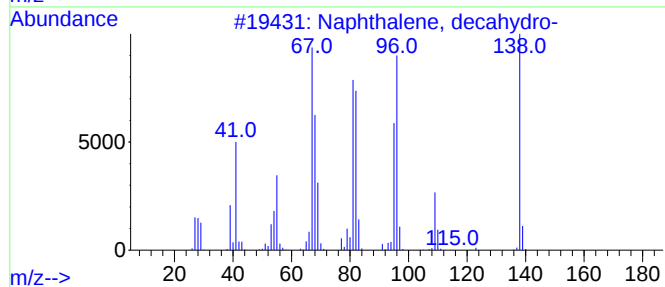
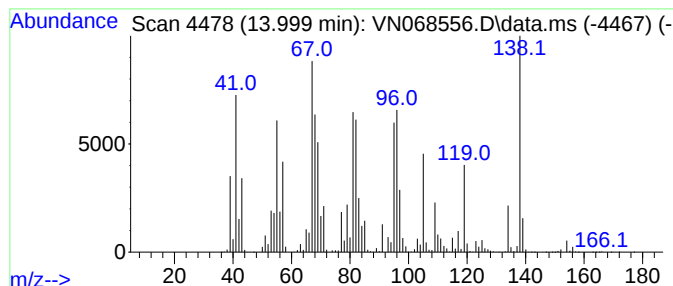
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, decahydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.999	165.90 ug/l	25290500	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	97
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	93
3			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	70
4			Spiro[4.5]decane	138	C10H18	000176-63-6	70
5			Cyclodecene	138	C10H18	003618-12-0	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068556.D
Acq On : 18 Sep 2021 7:44
Operator : JC/MD
Sample : M3798-09
Misc : 6.83g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(8-10)-END-POINT

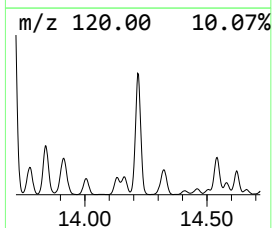
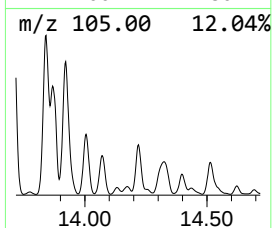
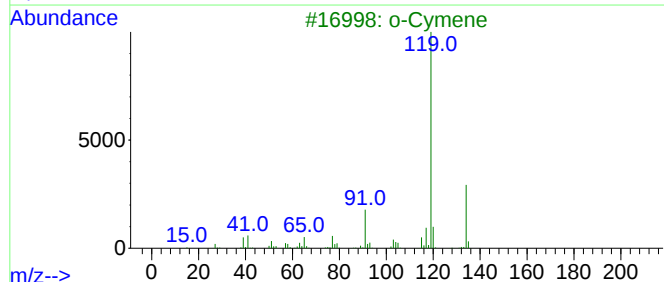
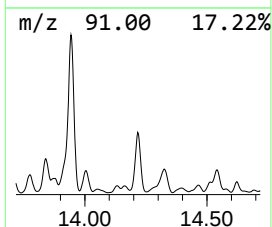
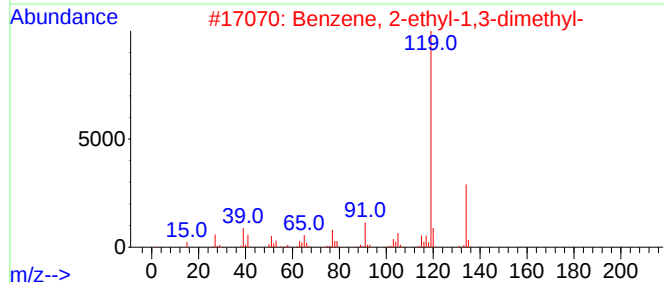
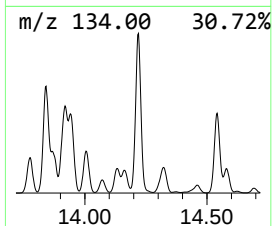
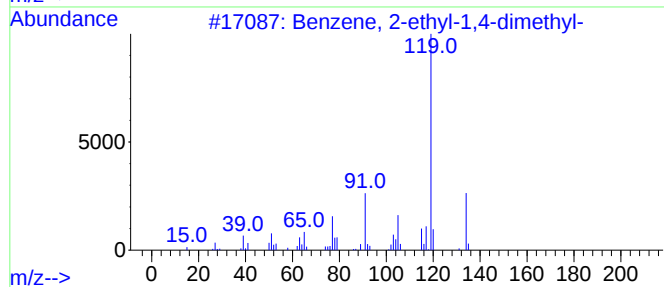
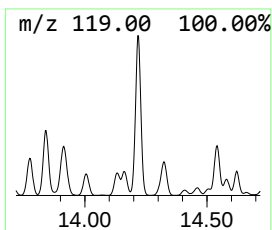
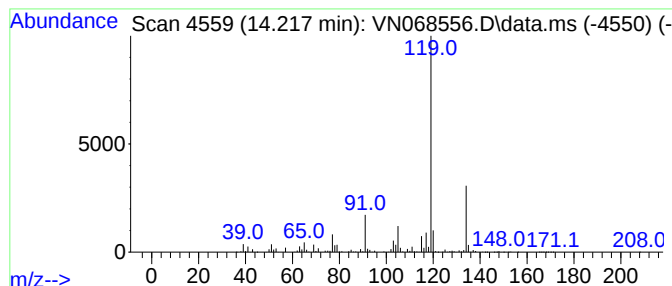
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	108.51 ug/l	16541900	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068556.D
Acq On : 18 Sep 2021 7:44
Operator : JC/MD
Sample : M3798-09
Misc : 6.83g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(8-10)-END-POINT

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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1-Ethyl-4-methy...	11.991	212.2	ug/l	16272700	3	11.749	3834510	50.0
4,4-Dimethyl oc...	12.181	140.8	ug/l	10800300	3	11.749	3834510	50.0
unknown12.256	12.256	542.5	ug/l	41607600	3	11.749	3834510	50.0
Octane, 2,6-dim...	12.374	356.2	ug/l	27317800	3	11.749	3834510	50.0
unknown12.457	12.457	417.3	ug/l	32003000	3	11.749	3834510	50.0
m-Menthane, (1S...	12.983	121.4	ug/l	18512400	4	13.675	7622030	50.0
Cyclohexane, 1-...	13.114	160.4	ug/l	24457500	4	13.675	7622030	50.0
Naphthalene, de...	13.999	165.9	ug/l	25290500	4	13.675	7622030	50.0
Benzene, 2-ethy...	14.217	108.5	ug/l	16541900	4	13.675	7622030	50.0