

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090324\
 Data File : VY019424.D
 Acq On : 03 Sep 2024 13:17
 Operator : SY/MD
 Sample : P3787-03
 Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-2

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_Y\methods\82Y082924S.M
 Title : SW846 8260

Signal : TIC: VY019424.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.634	960	970	975	rBV	64051	154686	3.99%	1.387%
2	7.707	975	982	995	rVB	104027	238618	6.16%	2.140%
3	8.061	1031	1040	1052	rBV2	63503	151730	3.92%	1.360%
4	8.609	1122	1130	1144	rBV	157074	319868	8.25%	2.868%
5	10.109	1368	1376	1382	rBV	252028	434926	11.22%	3.900%
6	10.170	1382	1386	1393	rVB	75686	122541	3.16%	1.099%
7	11.420	1583	1591	1598	rBV	229946	377235	9.73%	3.382%
8	11.518	1601	1607	1615	rBV	32725	53737	1.39%	0.482%
9	11.627	1615	1625	1636	rBV	182885	354250	9.14%	3.176%
10	11.956	1667	1679	1691	rBV	148602	250060	6.45%	2.242%
11	12.408	1747	1753	1758	rBV	159344	238122	6.14%	2.135%
12	12.664	1788	1795	1798	rBV	45860	80228	2.07%	0.719%
13	12.737	1802	1807	1813	rVB2	111557	173853	4.49%	1.559%
14	12.895	1826	1833	1841	rBV2	26783	55404	1.43%	0.497%
15	13.042	1851	1857	1863	rBV	156573	238108	6.14%	2.135%
16	13.346	1901	1907	1910	rBV	181971	299864	7.74%	2.689%
17	13.676	1955	1961	1965	rBV2	77239	106513	2.75%	0.955%
18	13.724	1965	1969	1976	rVV2	86468	144411	3.73%	1.295%
19	13.798	1976	1981	1984	rVV3	20493	40324	1.04%	0.362%
20	13.889	1992	1996	2001	rVB2	27525	40106	1.03%	0.360%
21	14.163	2031	2041	2044	rBV4	28941	67695	1.75%	0.607%
22	14.529	2097	2101	2106	rVB	122502	156701	4.04%	1.405%
23	14.596	2106	2112	2117	rBV3	43090	91378	2.36%	0.819%
24	14.651	2117	2121	2128	rVB4	33028	60426	1.56%	0.542%
25	14.956	2167	2171	2177	rBV5	20689	44508	1.15%	0.399%
26	15.047	2183	2186	2192	rVB3	40476	64847	1.67%	0.581%
27	15.145	2192	2202	2213	rBV	2376062	3875145	100.00%	34.746%
28	15.236	2213	2217	2224	rVB	55470	101334	2.61%	0.909%
29	15.340	2226	2234	2242	rBV	345303	506572	13.07%	4.542%
30	15.450	2243	2252	2256	rBV8	29502	76274	1.97%	0.684%
31	15.779	2301	2306	2309	rBV2	36491	66446	1.71%	0.596%
32	15.907	2323	2327	2334	rVV2	48068	80565	2.08%	0.722%
33	15.986	2334	2340	2346	rVB4	46609	94727	2.44%	0.849%
34	16.047	2346	2350	2356	rBV2	45625	77602	2.00%	0.696%
35	16.175	2364	2371	2378	rBV	378083	719440	18.57%	6.451%
36	16.248	2378	2383	2395	rVB	321924	560627	14.47%	5.027%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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37	16.370	2395	2403	2409	rBV	242587	545753	14.08%	4.893%
38	16.742	2455	2464	2469	rBV3	31782	88157	2.27%	0.790%

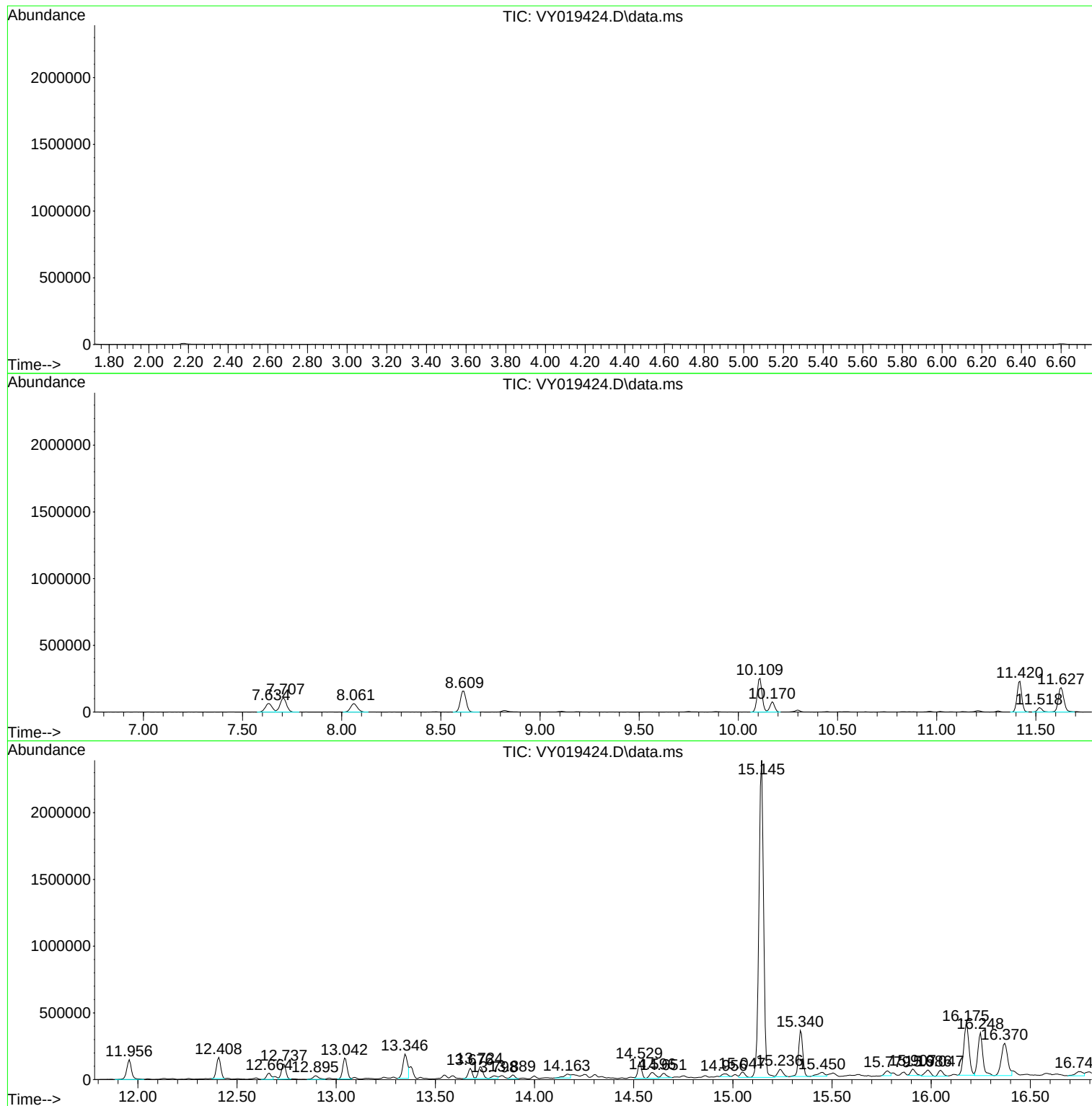
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082924S.M
Quant Title : SW846 8260

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



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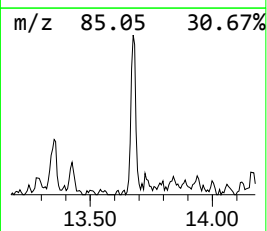
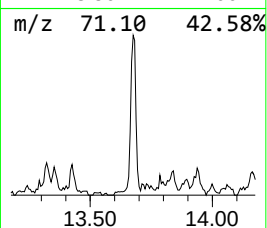
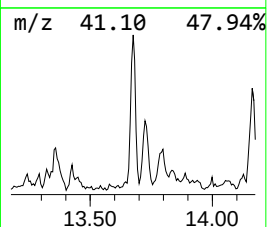
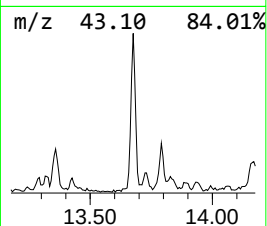
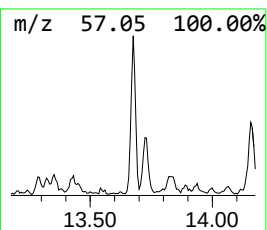
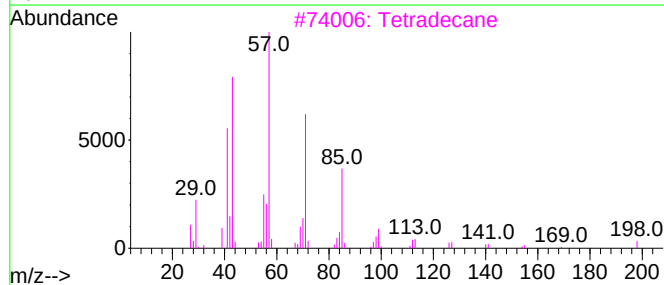
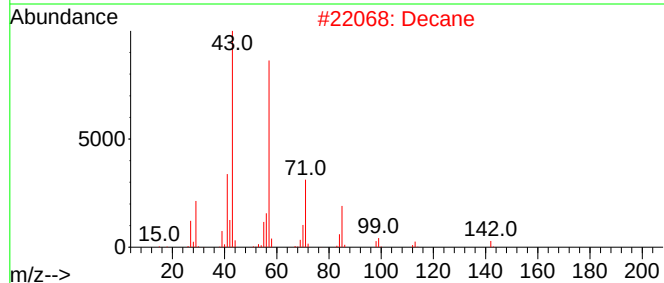
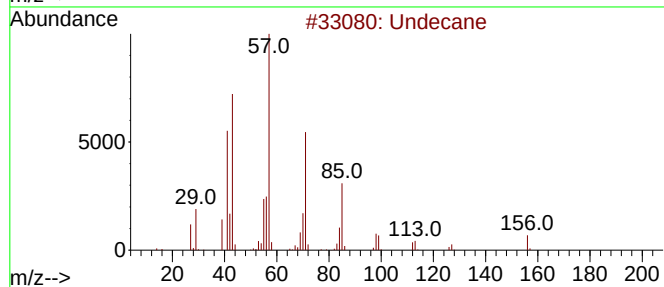
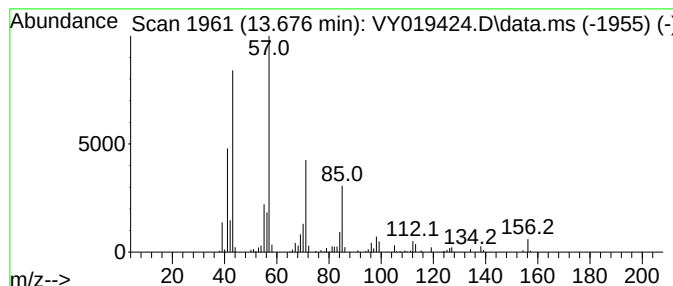
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082924S.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	17.76 ug/l	106513	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	96
2	Decane			142	C10H22	000124-18-5	80
3	Tetradecane			198	C14H30	000629-59-4	80
4	Carbonic acid, prop-1-en-2-yl te...			298	C18H34O3	1000382-90-9	78
5	Tridecane			184	C13H28	000629-50-5	72



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Instrument :
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ClientSampleId :
SB-2

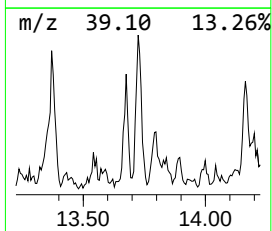
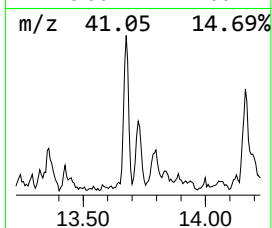
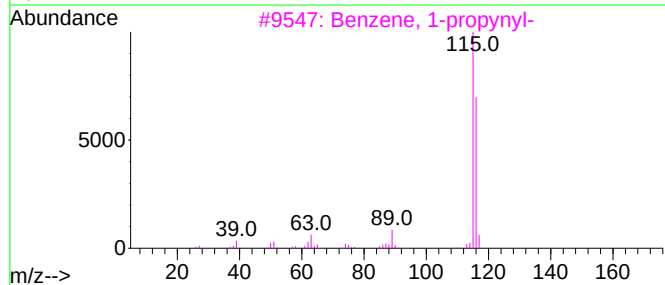
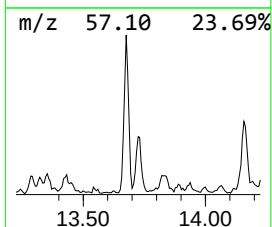
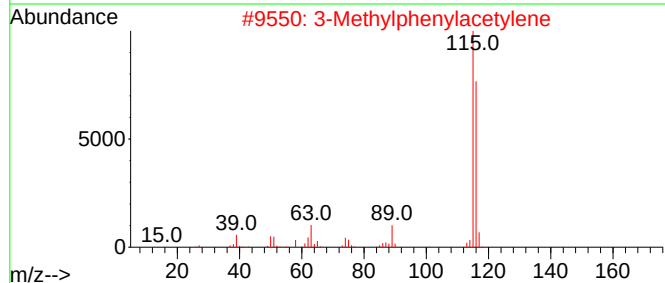
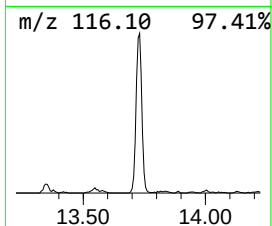
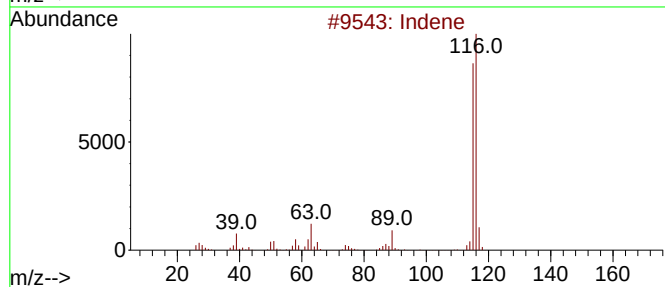
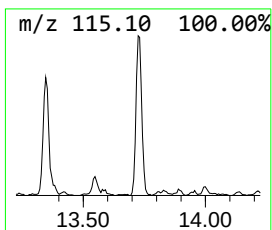
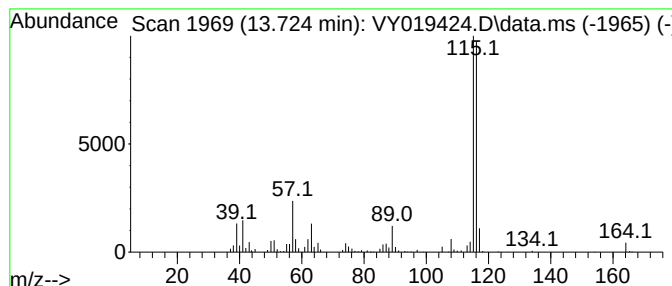
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082924S.M
Quant Title : SW846 8260

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

Peak Number 2 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.724	24.08 ug/l	144411	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	95
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



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Instrument :
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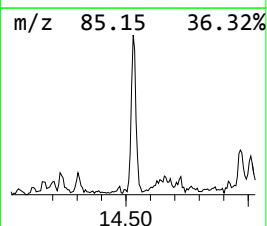
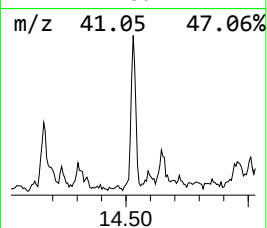
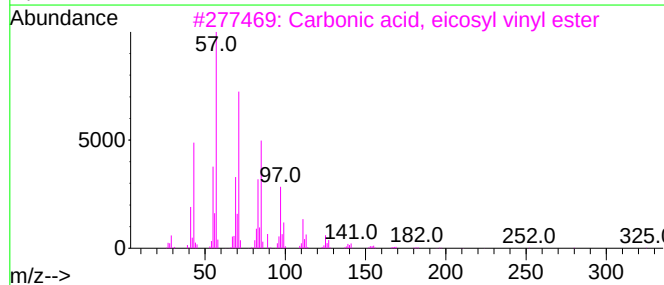
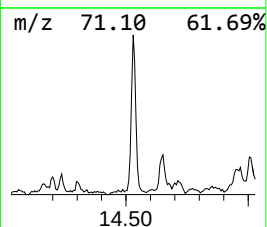
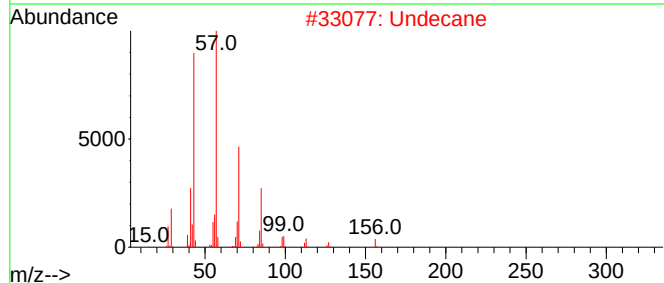
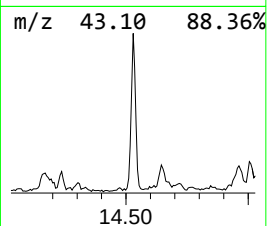
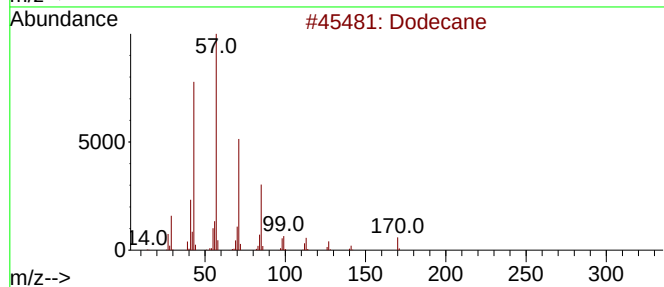
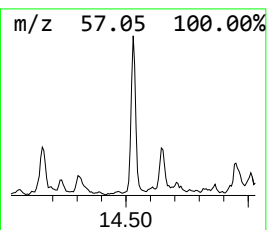
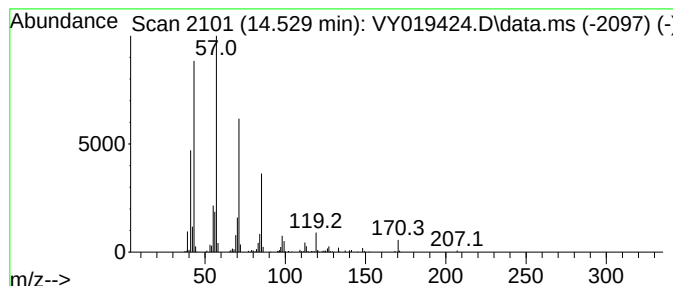
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082924S.M
Quant Title : SW846 8260

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

Peak Number 3 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.529	26.13 ug/l	156701	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	87
2			Undecane	156	C11H24	001120-21-4	72
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	72
4			Tridecane	184	C13H28	000629-50-5	64
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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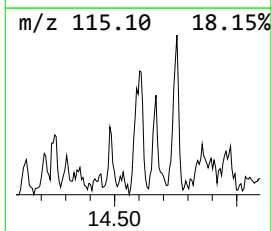
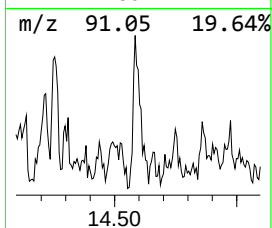
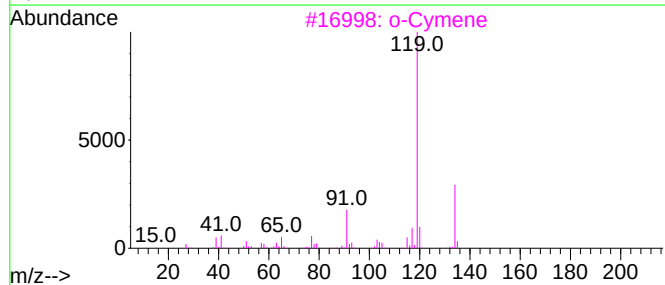
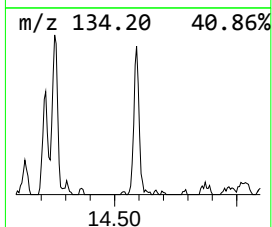
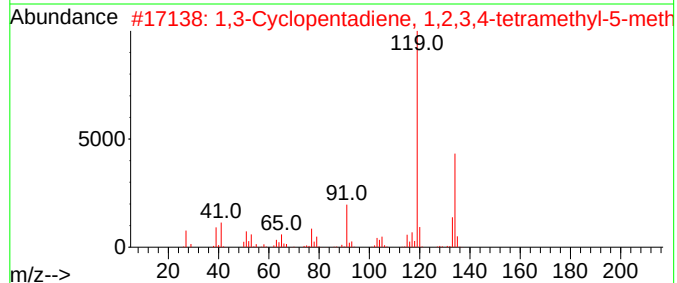
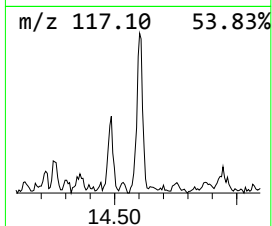
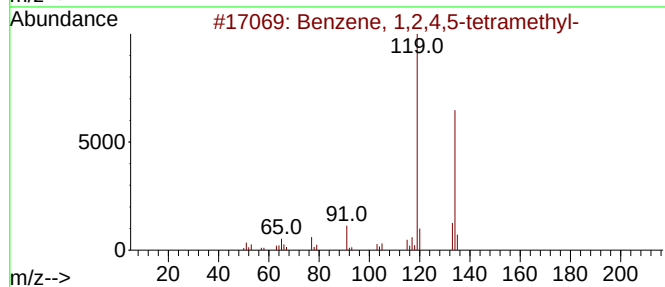
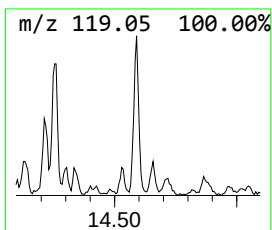
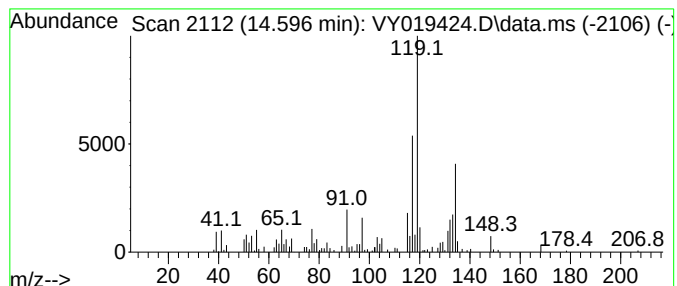
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082924S.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.596	15.24 ug/l	91378	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
2			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	64
3			o-Cymene	134	C10H14	000527-84-4	64
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	64
5			Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	60



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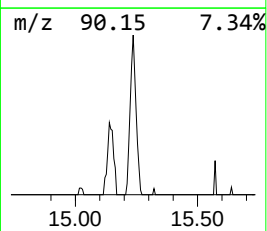
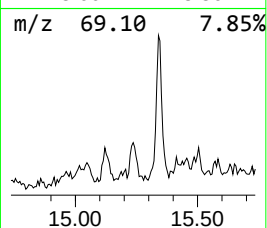
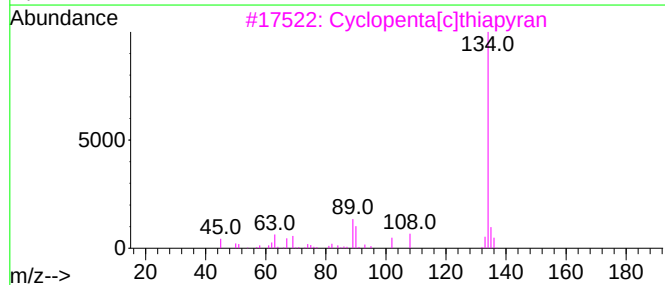
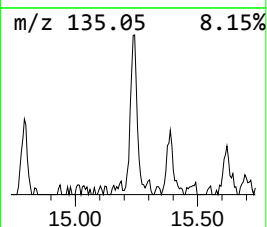
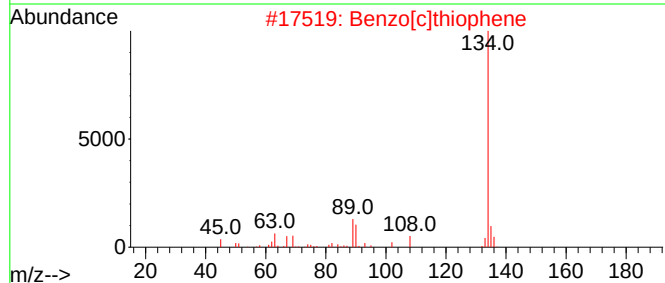
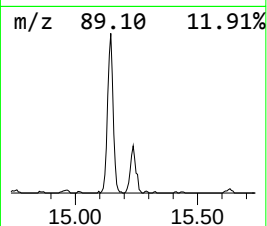
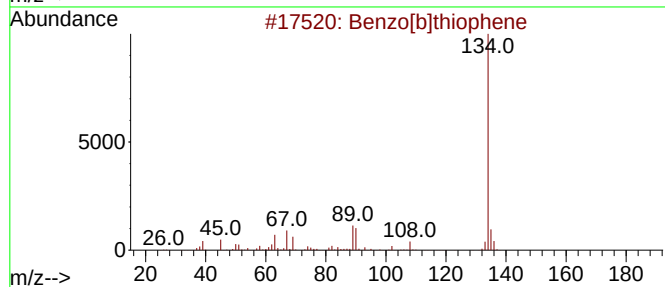
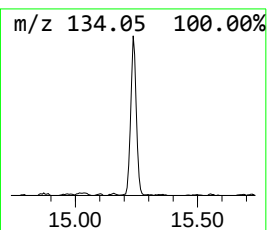
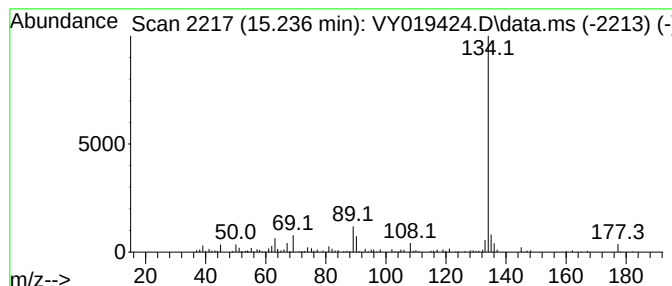
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082924S.M
Quant Title : SW846 8260

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

Peak Number 5 Benzo[b]thiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.236	16.90 ug/l	101334	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	90
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	86
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	83
4			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	64
5			3-Deazaadenine	134	C6H6N4	006811-77-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090324\
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Acq On : 03 Sep 2024 13:17
Operator : SY/MD
Sample : P3787-03
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-2

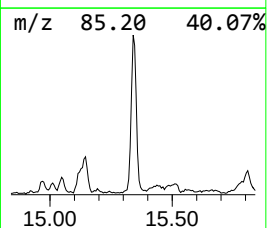
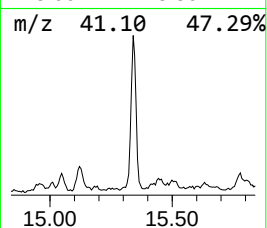
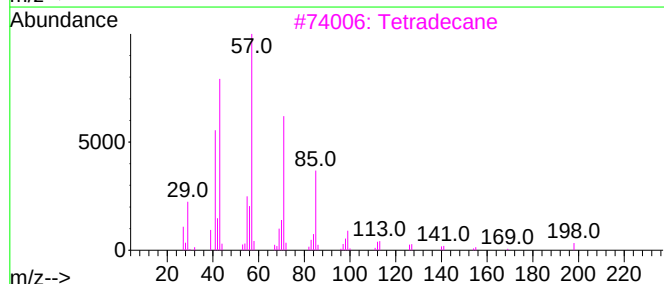
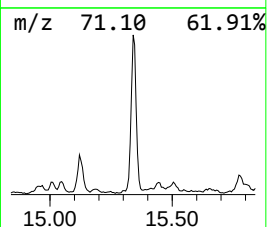
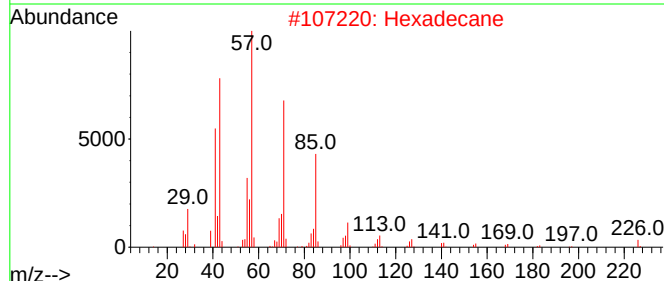
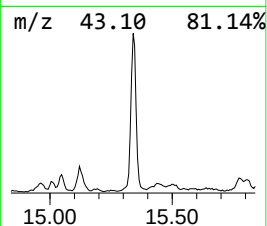
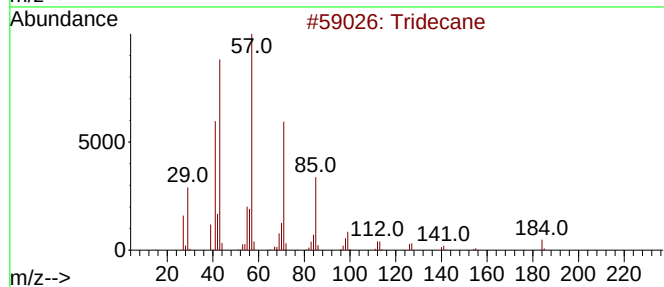
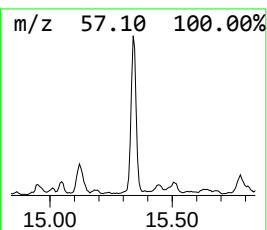
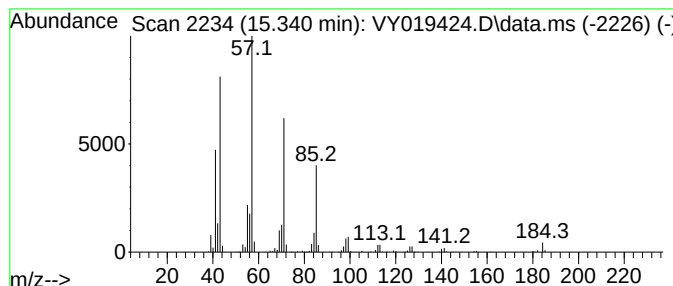
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Quant Title : SW846 8260

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

Peak Number 6 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.340	84.47 ug/l	506572	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	97
2			Hexadecane	226	C16H34	000544-76-3	91
3			Tetradecane	198	C14H30	000629-59-4	91
4			Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	86
5			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090324\
Data File : VY019424.D
Acq On : 03 Sep 2024 13:17
Operator : SY/MD
Sample : P3787-03
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-2

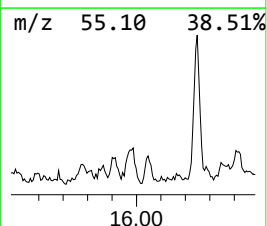
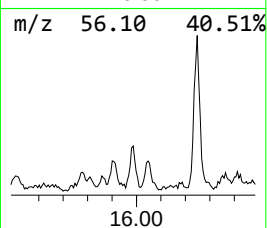
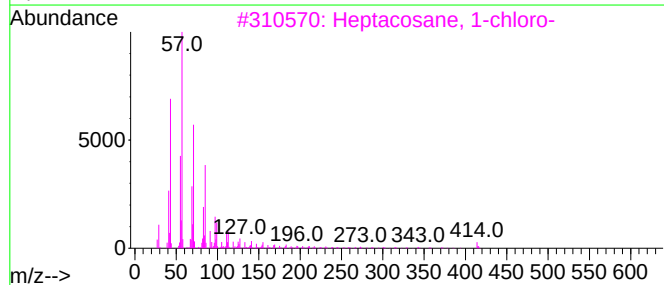
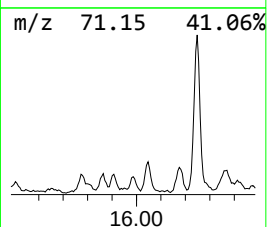
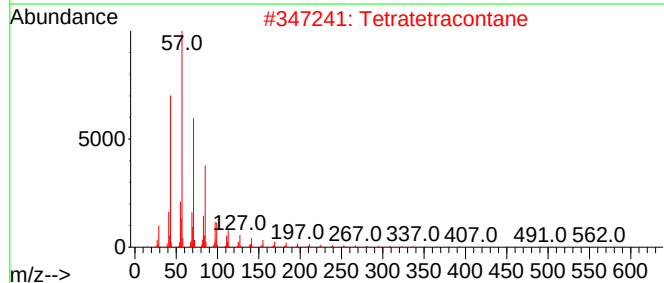
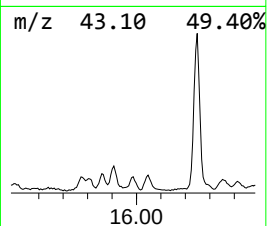
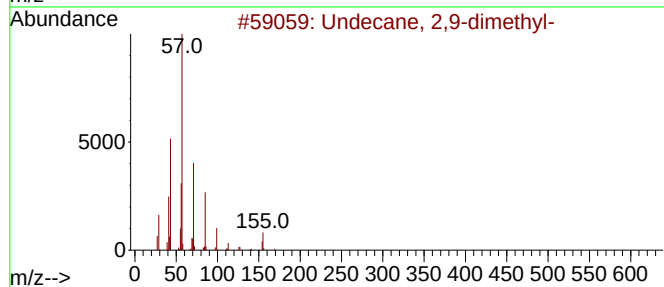
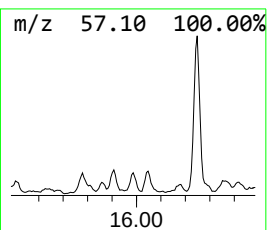
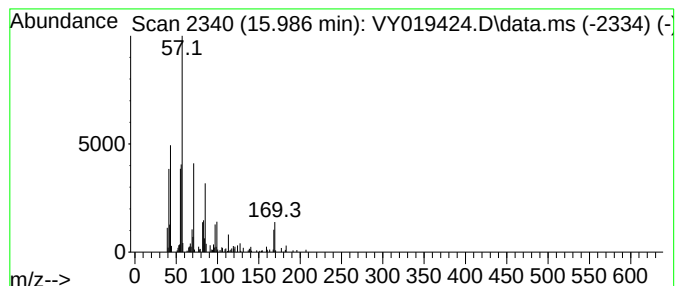
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Quant Title : SW846 8260

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

Peak Number 7 Undecane, 2,9-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.986	15.80 ug/l	94727	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	64
2			Tetratetracontane	619	C44H90	007098-22-8	53
3			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	49
4			Hexatriacontane	507	C36H74	000630-06-8	49
5			Cyclopentanol, 3-methyl-	100	C6H12O	018729-48-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090324\
Data File : VY019424.D
Acq On : 03 Sep 2024 13:17
Operator : SY/MD
Sample : P3787-03
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-2

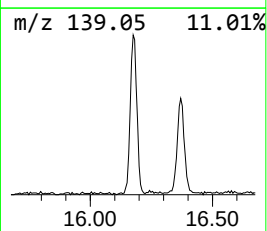
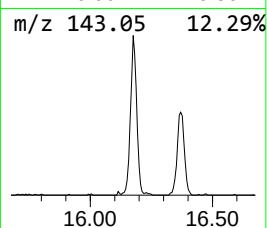
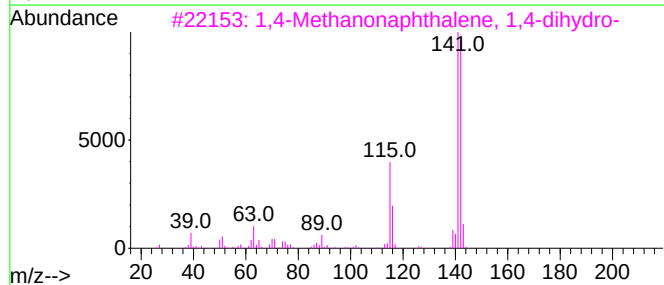
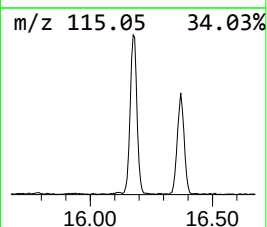
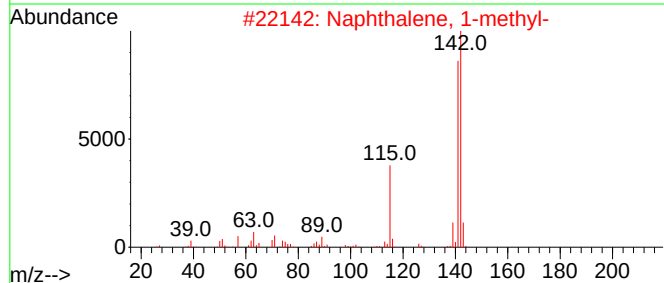
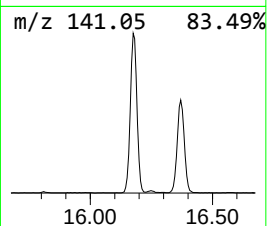
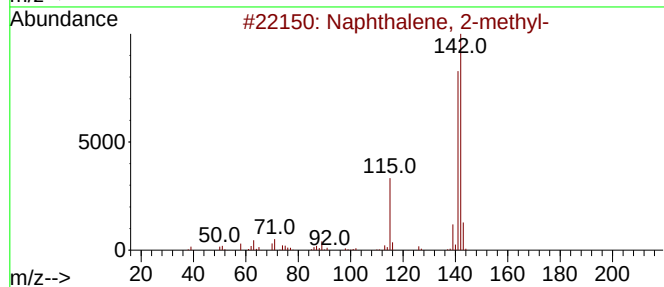
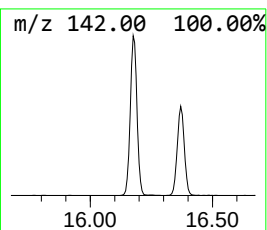
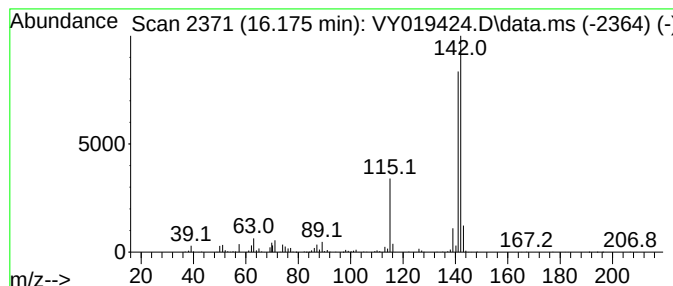
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.175	119.96 ug/l	719440	1,4-Dichlorobenzene-d4	13.347

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			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090324\
Data File : VY019424.D
Acq On : 03 Sep 2024 13:17
Operator : SY/MD
Sample : P3787-03
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-2

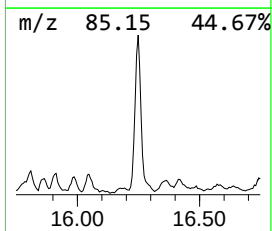
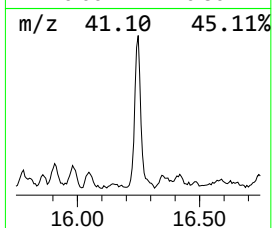
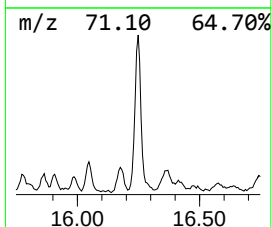
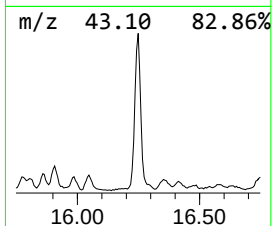
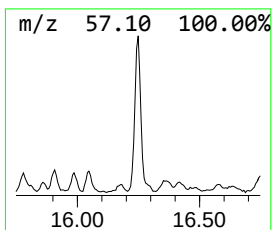
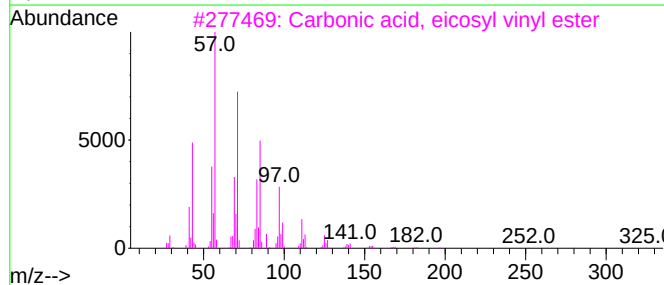
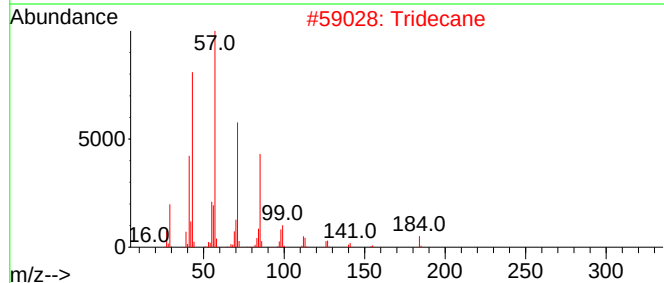
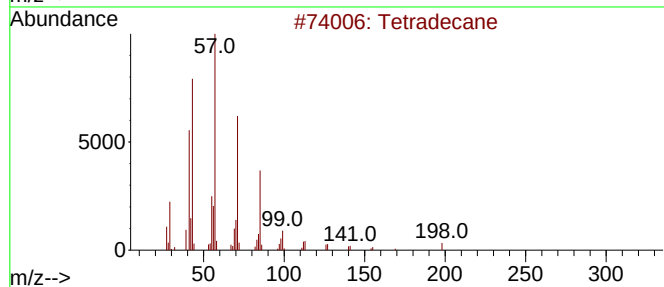
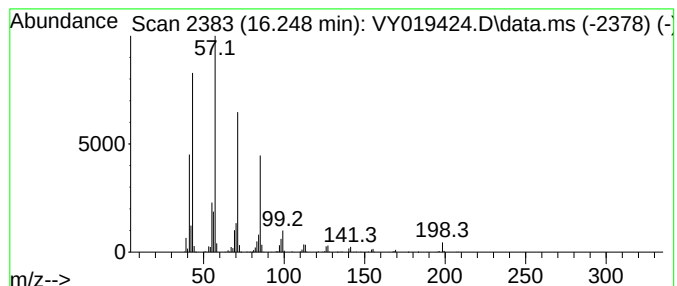
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Quant Title : SW846 8260

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

Peak Number 9 Carbonic acid, eicosyl vinyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.248	93.48 ug/l	560627	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	96
2			Tridecane	184	C13H28	000629-50-5	87
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	86
4			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	86
5			Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090324\
Data File : VY019424.D
Acq On : 03 Sep 2024 13:17
Operator : SY/MD
Sample : P3787-03
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-2

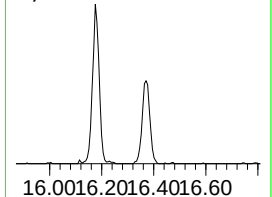
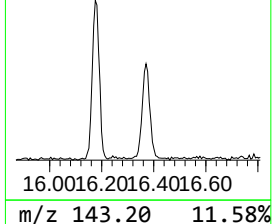
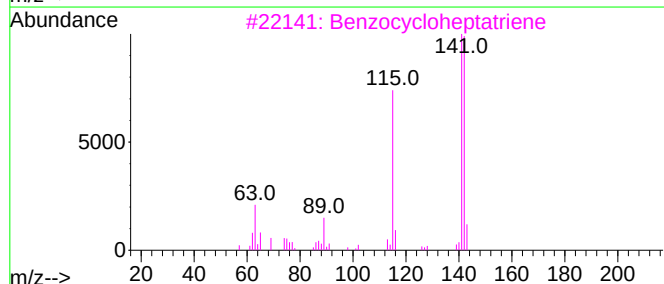
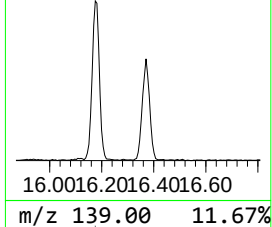
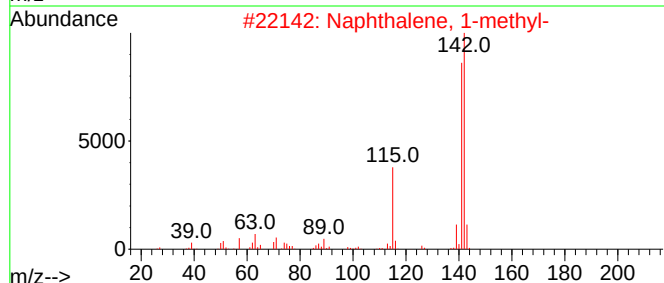
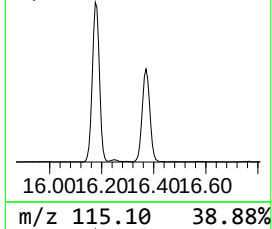
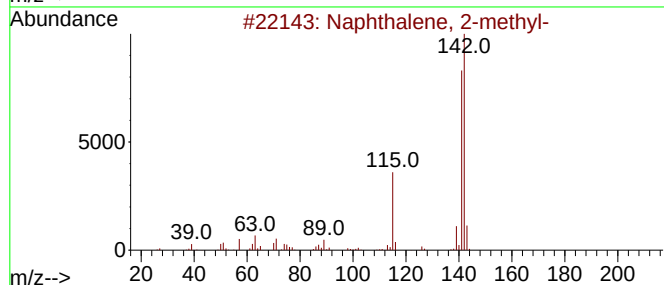
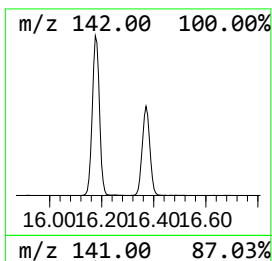
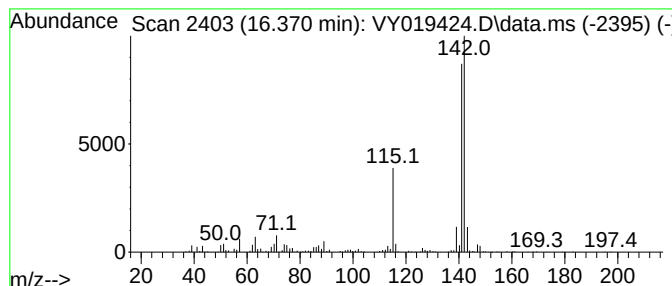
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Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.370	91.00 ug/l	545753	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	90
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87
5			1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090324\
Data File : VY019424.D
Acq On : 03 Sep 2024 13:17
Operator : SY/MD
Sample : P3787-03
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082924S.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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Indene	13.724	24.1	ug/l	144411	4	13.347	299864	50.0
Dodecane	14.529	26.1	ug/l	156701	4	13.347	299864	50.0
Benzene, 1,2,4,...	14.596	15.2	ug/l	91378	4	13.347	299864	50.0
Benzo[b]thiophene	15.236	16.9	ug/l	101334	4	13.347	299864	50.0
Tridecane	15.340	84.5	ug/l	506572	4	13.347	299864	50.0
Undecane, 2,9-d...	15.986	15.8	ug/l	94727	4	13.347	299864	50.0
Naphthalene, 1-...	16.175	120.0	ug/l	719440	4	13.347	299864	50.0
Carbonic acid, ...	16.248	93.5	ug/l	560627	4	13.347	299864	50.0
Benzocyclohepta...	16.370	91.0	ug/l	545753	4	13.347	299864	50.0