

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
 Data File : VN082269.D
 Acq On : 22 May 2024 03:33
 Operator : JC\MD
 Sample : P2494-09 40X
 Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 9

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\82N051524W.M
 Title : SW846 8260

Signal : TIC: VN082269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1046	1057	1061	rBV	154047	368741	10.06%	2.187%
2	8.224	1061	1066	1081	rVB	285385	639826	17.45%	3.795%
3	8.583	1117	1127	1139	rBV2	187650	466322	12.72%	2.766%
4	9.100	1205	1215	1228	rBV	426692	876307	23.90%	5.197%
5	10.571	1456	1465	1471	rBV	666466	1245783	33.98%	7.389%
6	10.630	1471	1475	1484	rVB2	77935	146920	4.01%	0.871%
7	11.865	1677	1685	1696	rBV	622002	1115175	30.42%	6.614%
8	11.965	1696	1702	1709	rVV	29025	48713	1.33%	0.289%
9	12.071	1712	1720	1732	rVV	157245	298489	8.14%	1.770%
10	12.400	1763	1776	1785	rBV	155472	291497	7.95%	1.729%
11	12.606	1795	1811	1812	rBV9	17879	54987	1.50%	0.326%
12	12.847	1846	1852	1863	rVB	500095	871366	23.77%	5.168%
13	13.100	1889	1895	1901	rBV	55794	116753	3.18%	0.692%
14	13.171	1901	1907	1913	rVB3	119781	222902	6.08%	1.322%
15	13.335	1920	1935	1942	rBV5	60034	216188	5.90%	1.282%
16	13.482	1953	1960	1966	rBV	203990	335958	9.16%	1.993%
17	13.671	1973	1992	2006	rBV5	98792	544895	14.86%	3.232%
18	13.794	2006	2013	2022	rBV2	605753	1174268	32.03%	6.965%
19	14.018	2034	2051	2059	rBV6	163863	629126	17.16%	3.731%
20	14.106	2060	2066	2073	rVV4	143493	315840	8.61%	1.873%
21	14.176	2073	2078	2084	rVB	159741	276357	7.54%	1.639%
22	14.329	2100	2104	2108	rVB2	28503	41814	1.14%	0.248%
23	14.441	2118	2123	2126	rBV4	28788	55609	1.52%	0.330%
24	14.576	2140	2146	2151	rVB5	40876	92253	2.52%	0.547%
25	14.629	2151	2155	2157	rBV3	32591	49589	1.35%	0.294%
26	14.659	2157	2160	2163	rVV3	37673	53898	1.47%	0.320%
27	14.694	2163	2166	2170	rVB	50142	61542	1.68%	0.365%
28	14.800	2177	2184	2187	rBV6	17415	41144	1.12%	0.244%
29	14.841	2188	2191	2202	rVB6	25713	74213	2.02%	0.440%
30	14.959	2202	2211	2218	rVB3	88151	164859	4.50%	0.978%
31	15.035	2218	2224	2233	rBV6	79717	259267	7.07%	1.538%
32	15.206	2248	2253	2261	rVB4	43023	82872	2.26%	0.492%
33	15.317	2268	2272	2282	rVB8	31329	67572	1.84%	0.401%
34	15.441	2287	2293	2298	rVB6	25027	55734	1.52%	0.331%
35	15.641	2314	2327	2338	rBV	1854933	3666416	100.00%	21.746%
36	15.747	2340	2345	2351	rVB	49104	97143	2.65%	0.576%

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Instrument :
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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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Title : SW846 8260

37	15.829	2356	2359	2371	rVB8	49335	101278	2.76%	0.601%
38	15.947	2371	2379	2386	rBV9	24295	73122	1.99%	0.434%
39	16.112	2400	2407	2413	rVB6	18685	49671	1.35%	0.295%
40	16.259	2428	2432	2439	rVB9	24061	51988	1.42%	0.308%
41	16.717	2503	2510	2513	rBV2	24196	52244	1.42%	0.310%
42	16.782	2513	2521	2522	rBV	895218	1411780	38.51%	8.373%

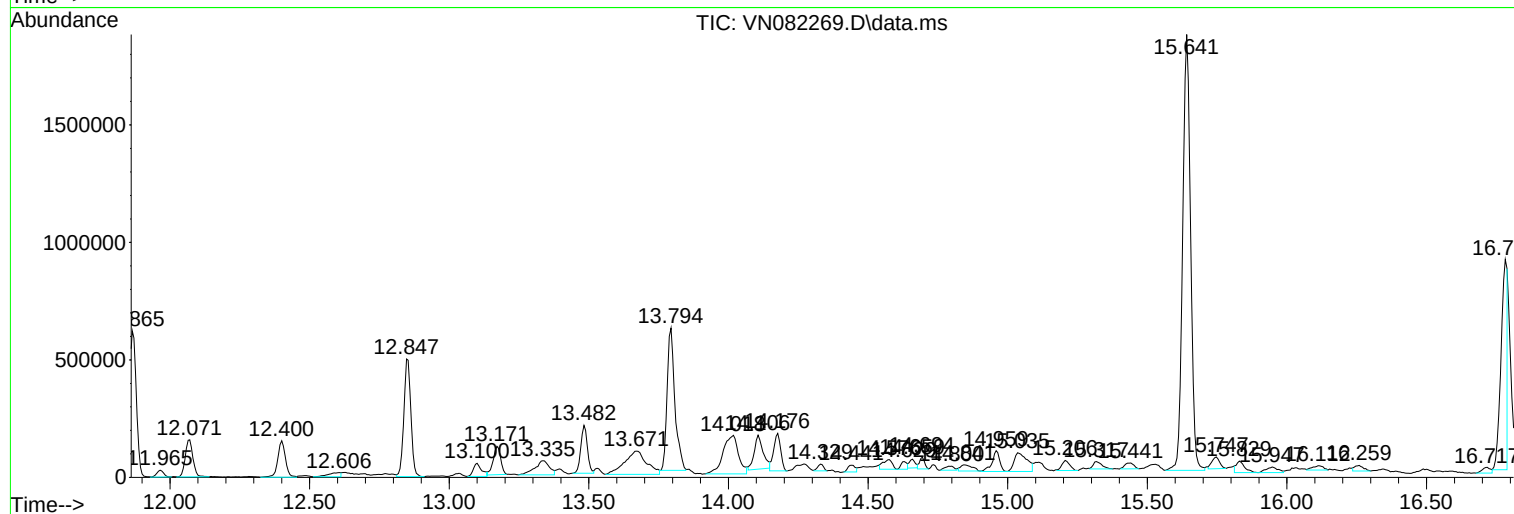
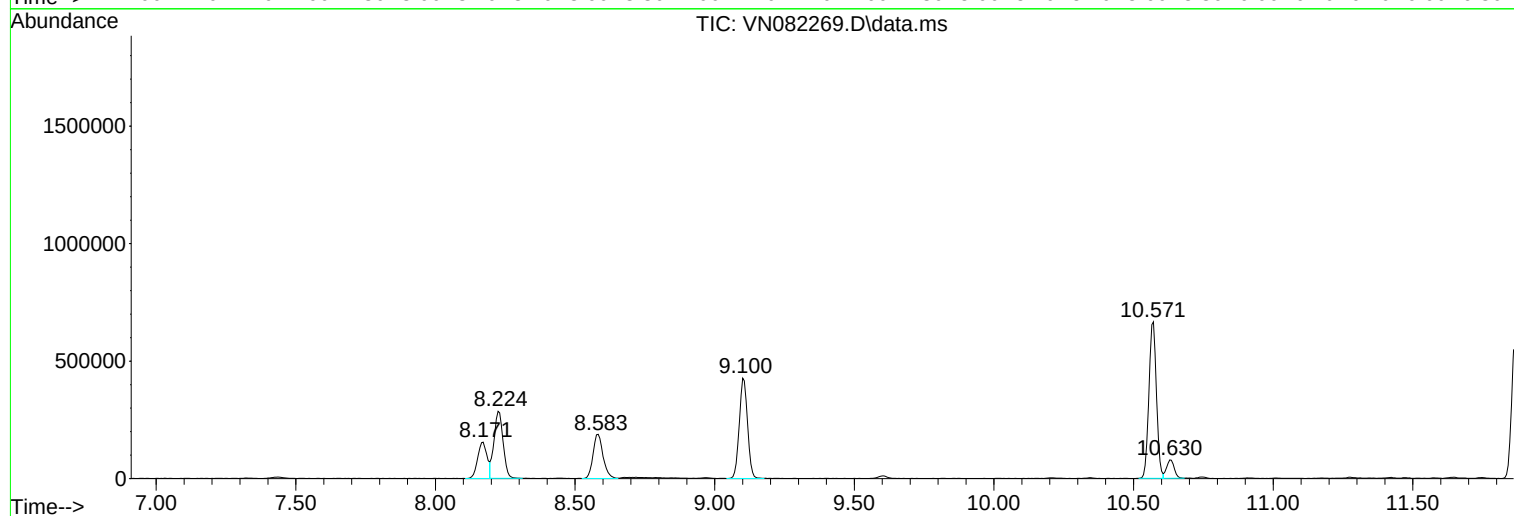
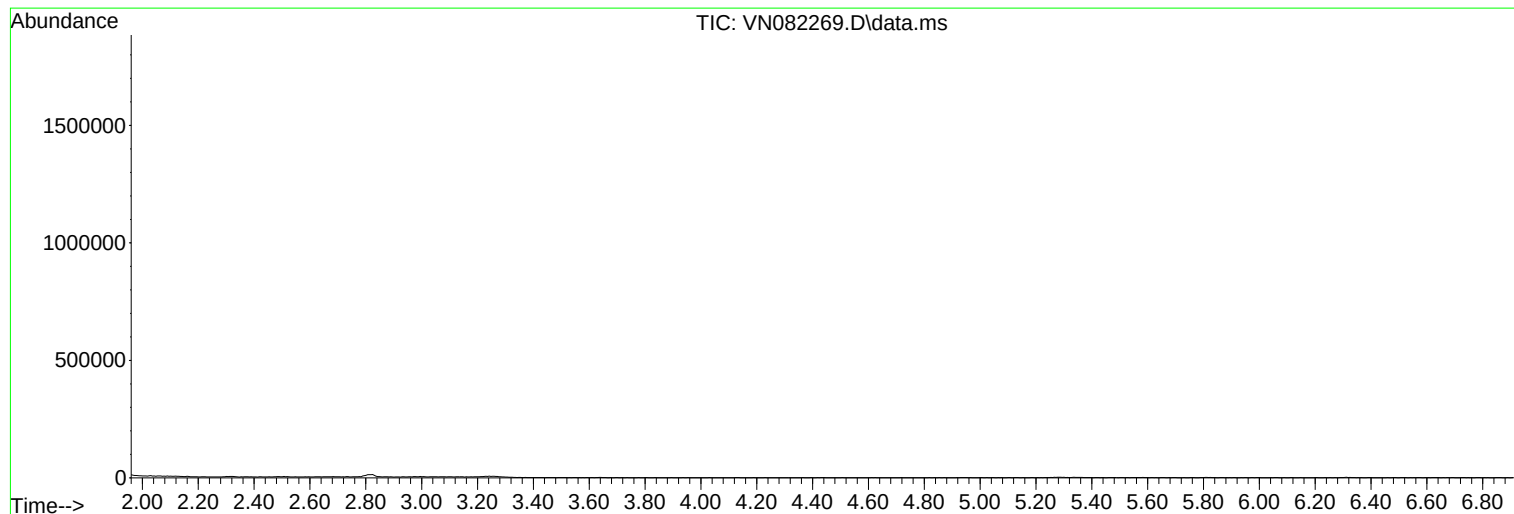
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
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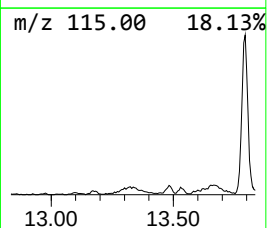
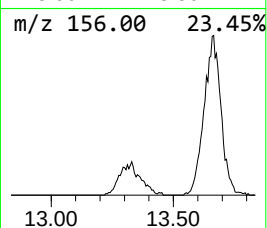
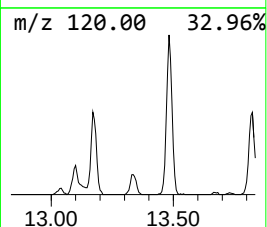
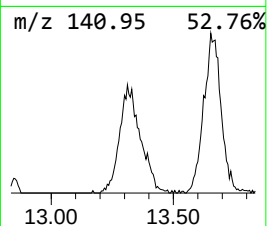
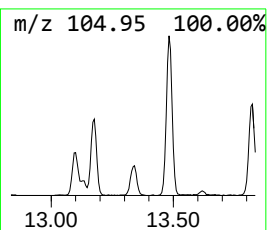
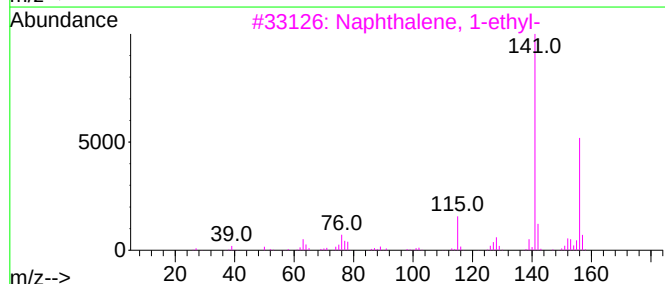
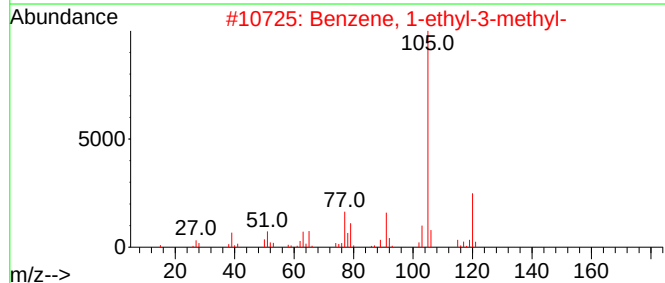
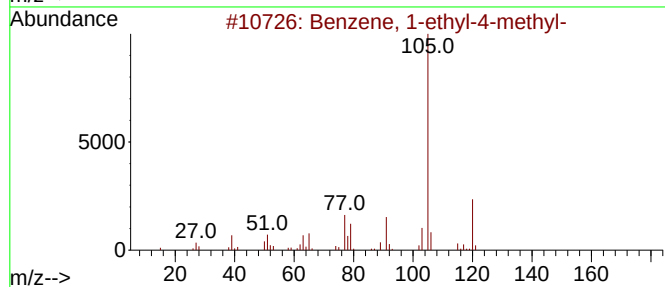
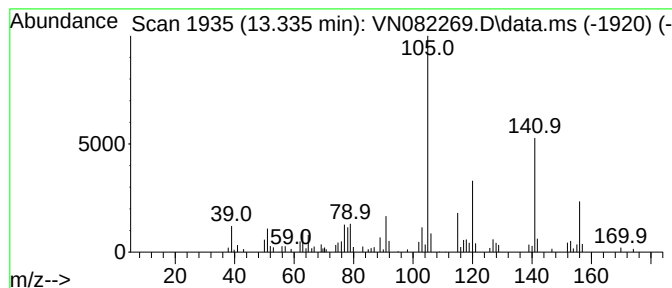
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	9.21 ug/l	216188	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	52
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	51
3			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	46
4			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	46
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	38



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Sample : P2494-09 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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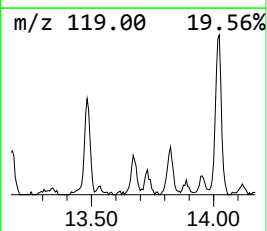
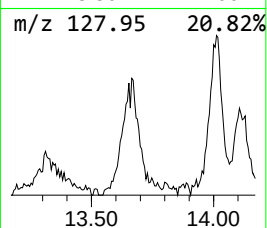
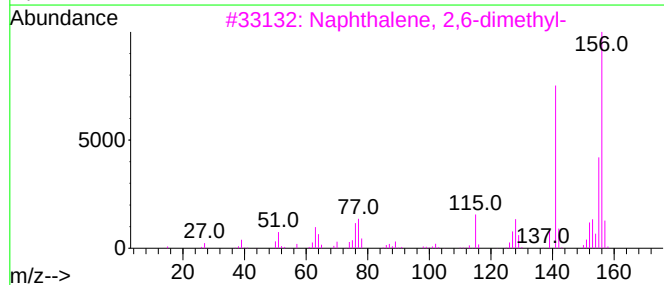
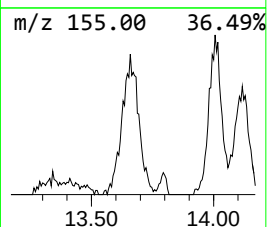
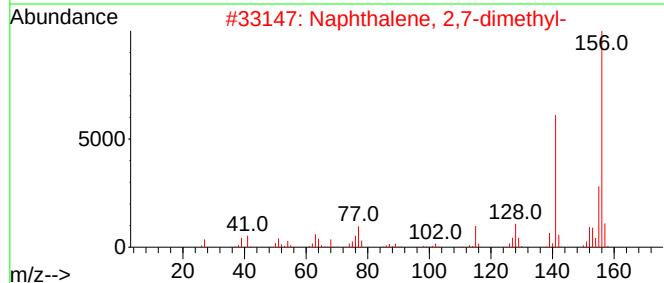
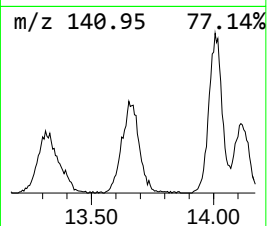
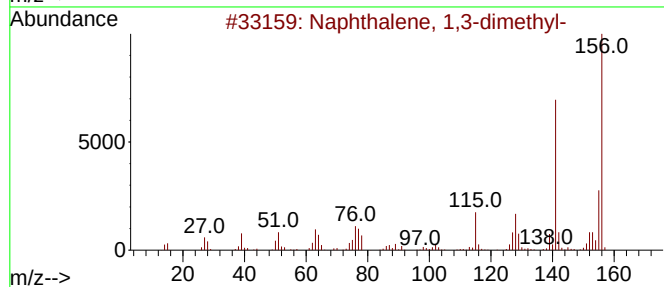
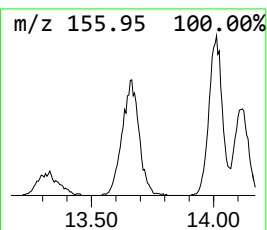
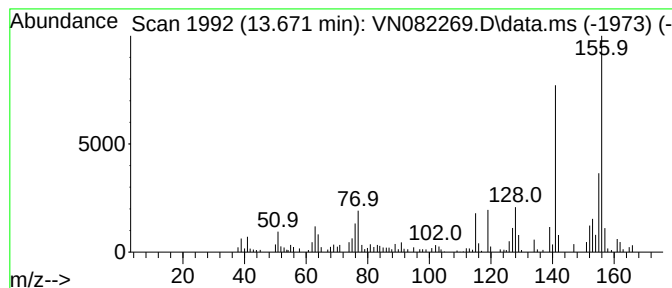
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 1,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.671	23.20 ug/l	544895	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96



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Data File : VN082269.D
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Operator : JC\MD
Sample : P2494-09 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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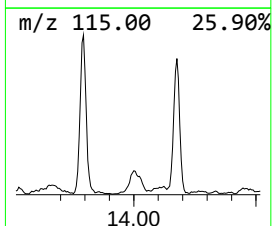
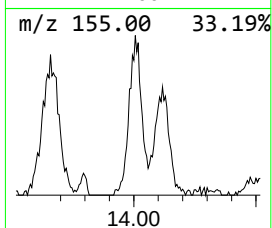
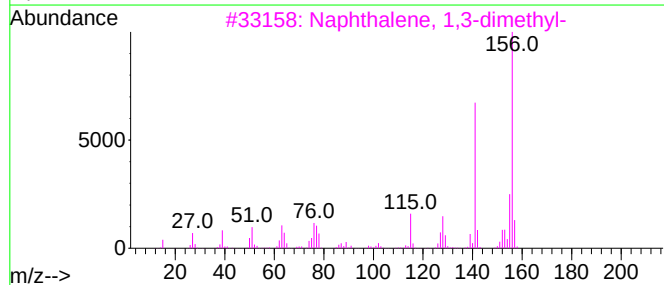
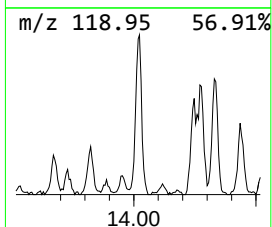
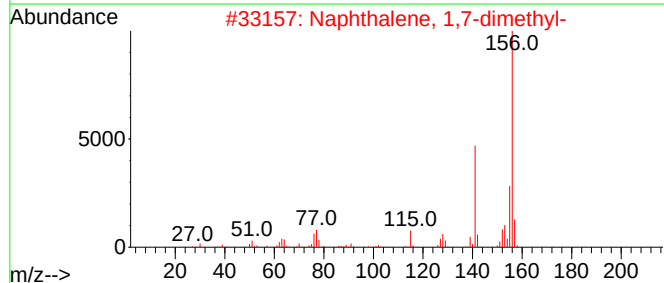
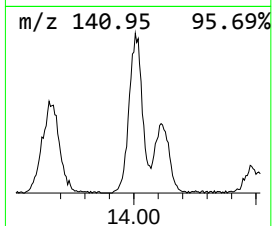
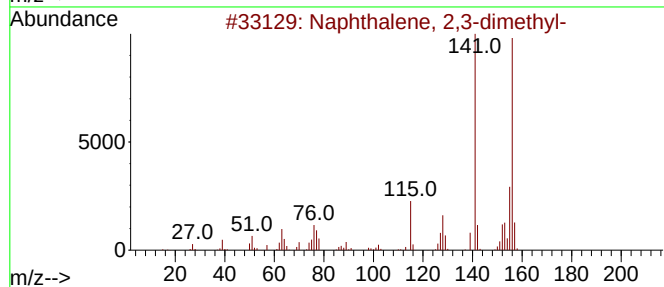
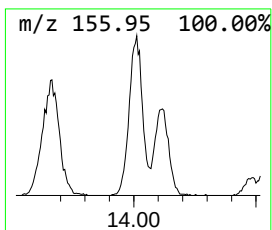
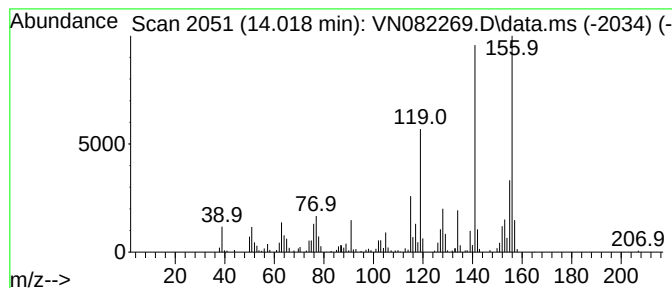
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.018	26.79 ug/l	629126	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96



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Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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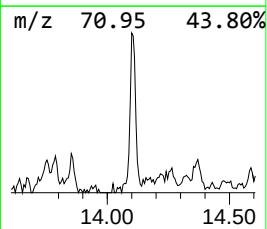
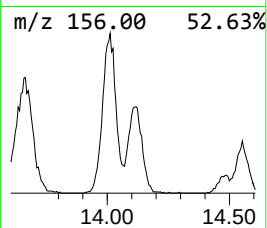
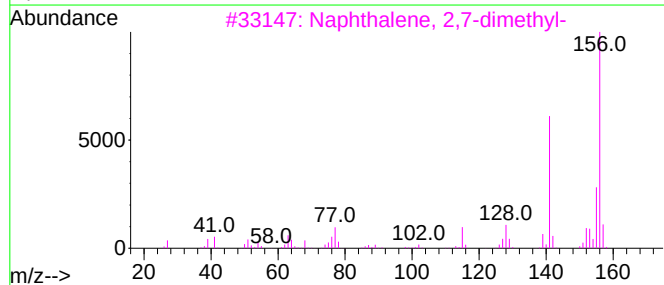
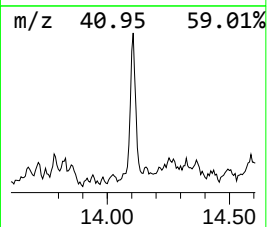
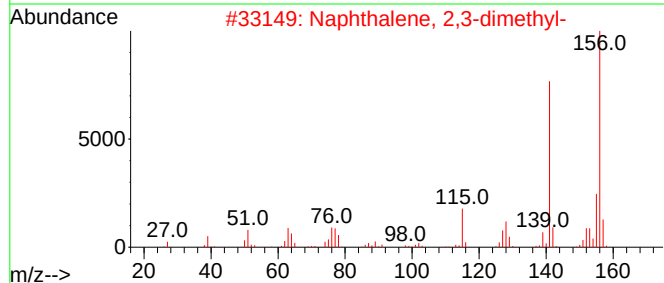
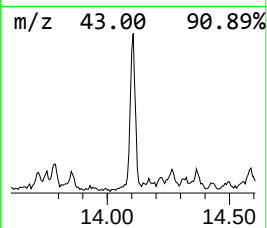
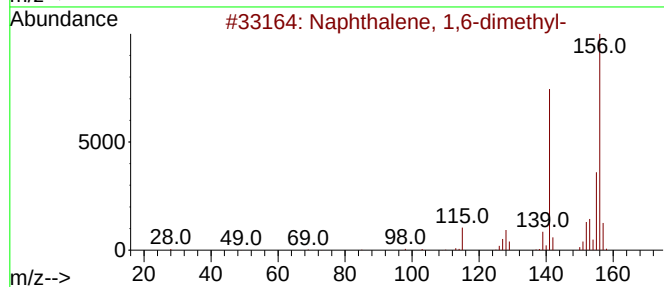
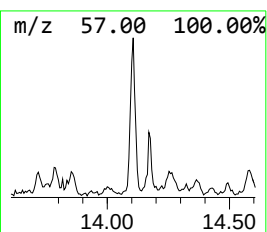
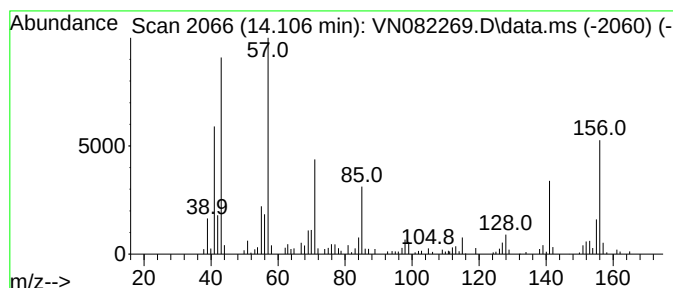
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	13.45 ug/l	315840	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	90
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	89
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	86
4			Decane	142	C10H22	000124-18-5	52
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	50



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Instrument :
MSVOA_N
ClientSampleId :
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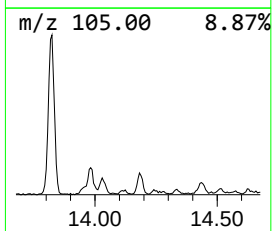
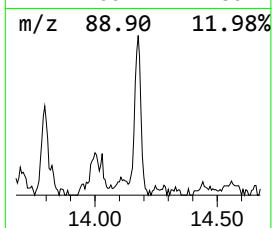
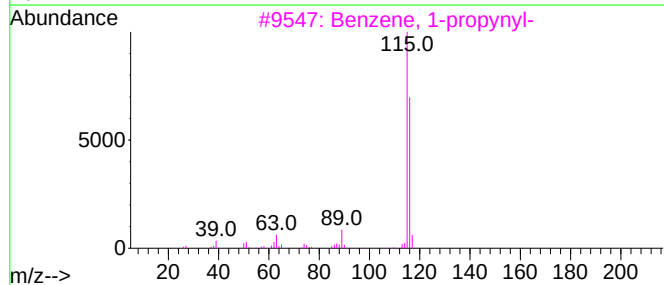
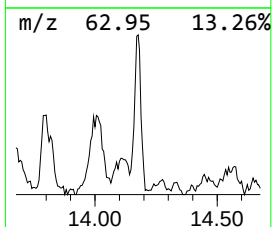
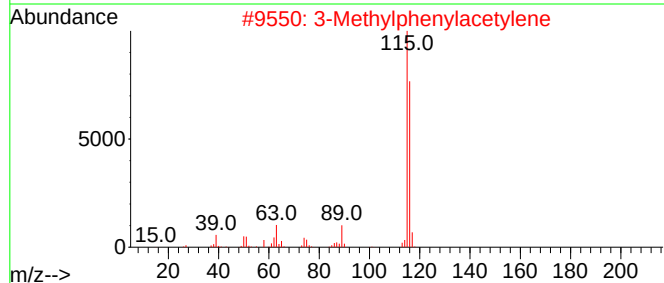
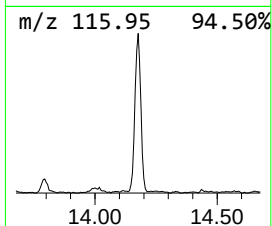
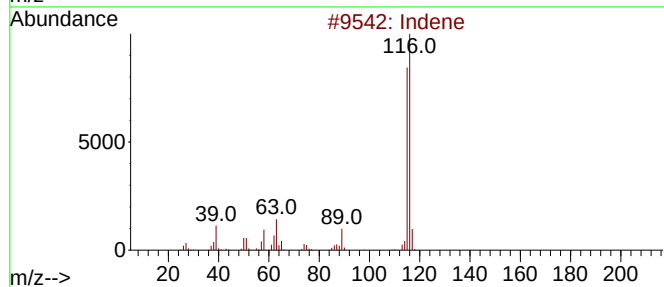
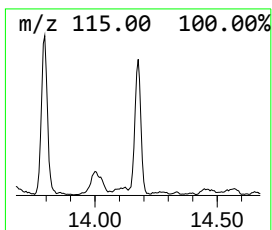
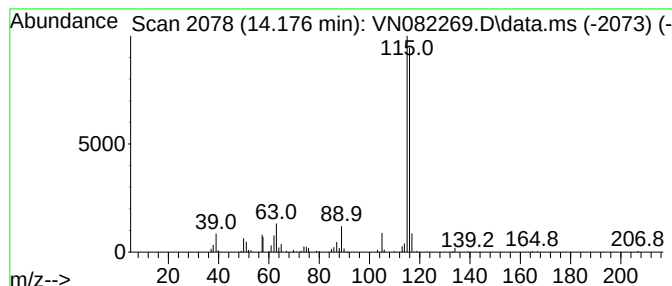
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Quant Title : SW846 8260

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

Peak Number 5 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	11.77 ug/l	276357	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	94
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	90
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082269.D
Acq On : 22 May 2024 03:33
Operator : JC\MD
Sample : P2494-09 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9

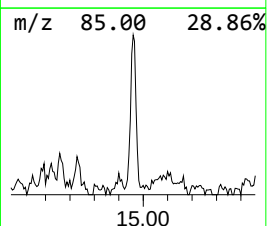
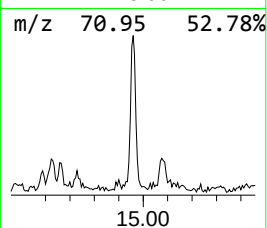
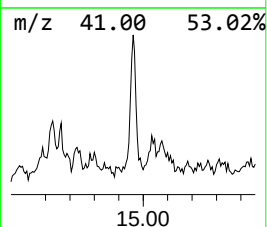
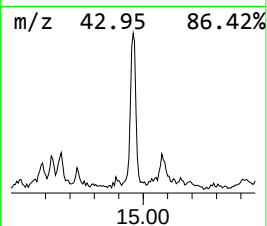
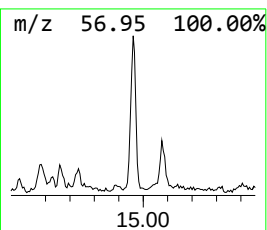
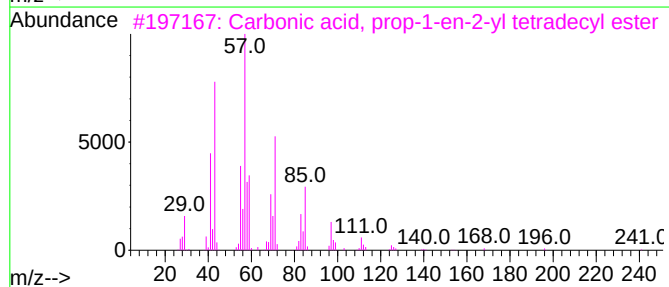
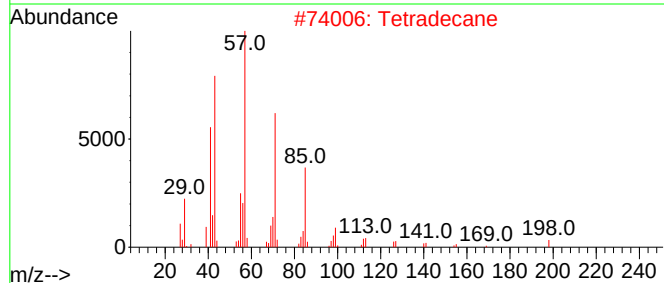
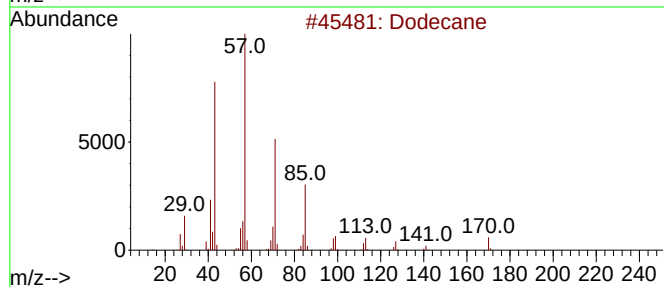
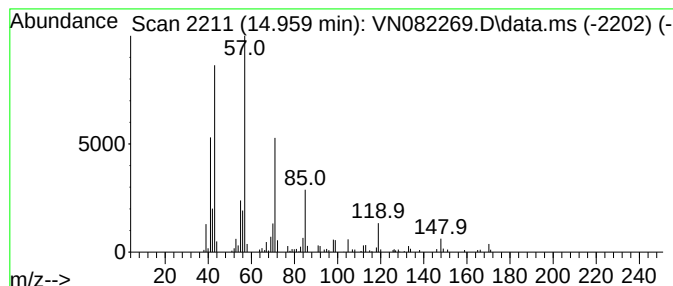
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	7.02 ug/l	164859	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	76
2			Tetradecane	198	C14H30	000629-59-4	72
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	59
4			Hexadecane	226	C16H34	000544-76-3	53
5			Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082269.D
Acq On : 22 May 2024 03:33
Operator : JC\MD
Sample : P2494-09 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9

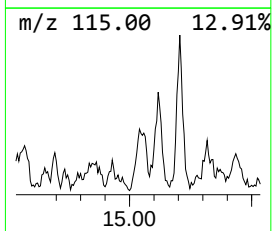
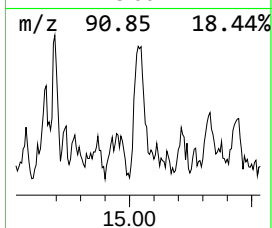
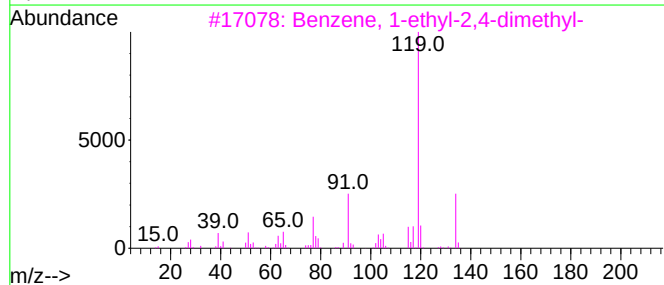
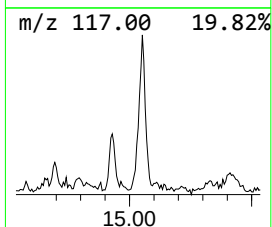
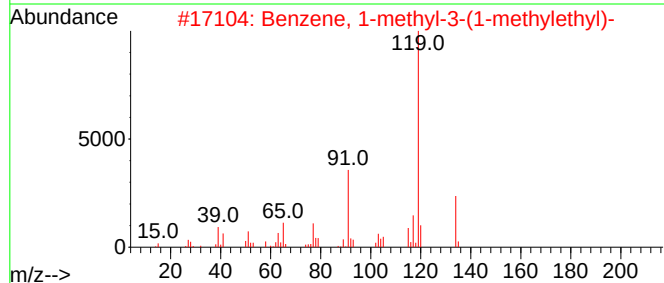
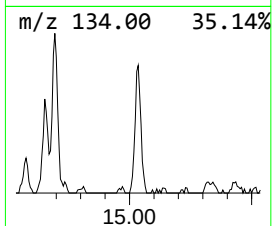
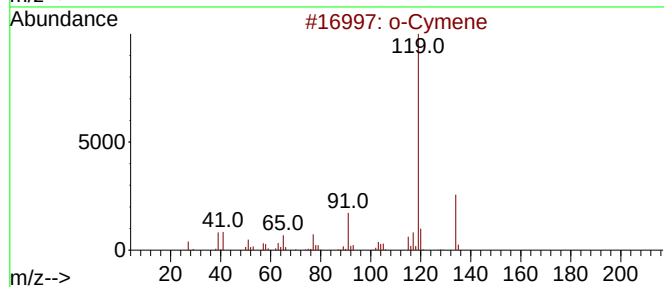
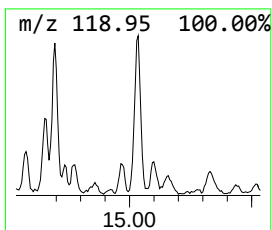
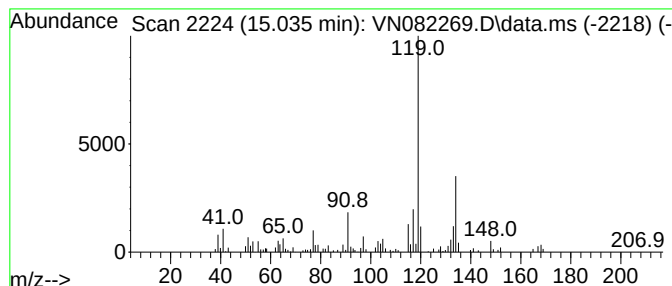
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Quant Title : SW846 8260

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

Peak Number 7 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	11.04 ug/l	259267	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	94
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	93
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082269.D
Acq On : 22 May 2024 03:33
Operator : JC\MD
Sample : P2494-09 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9

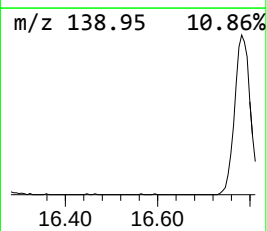
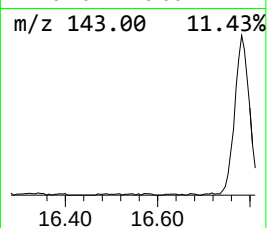
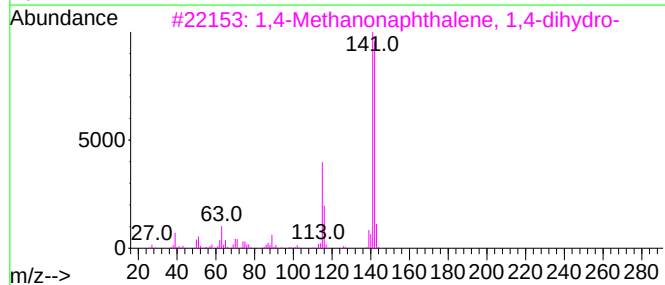
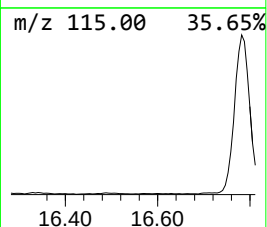
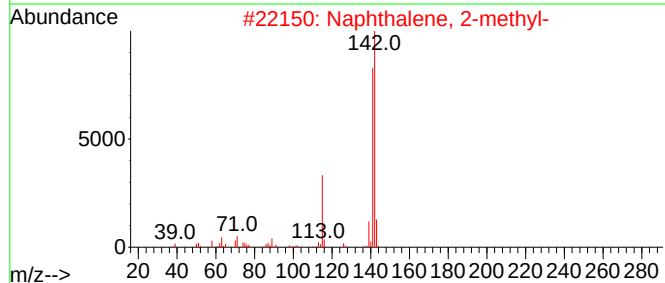
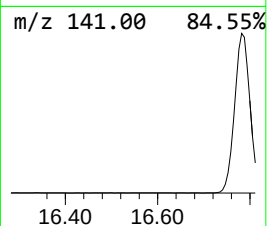
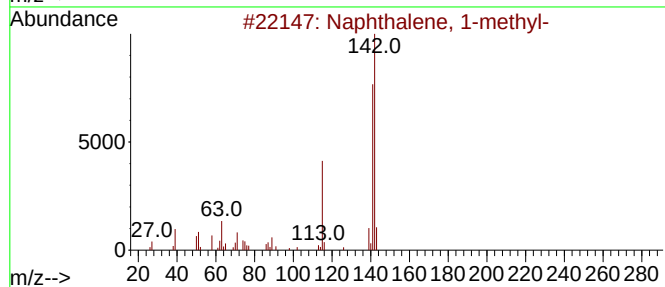
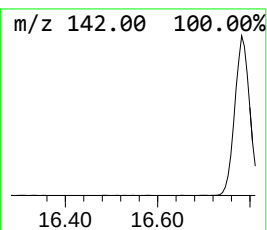
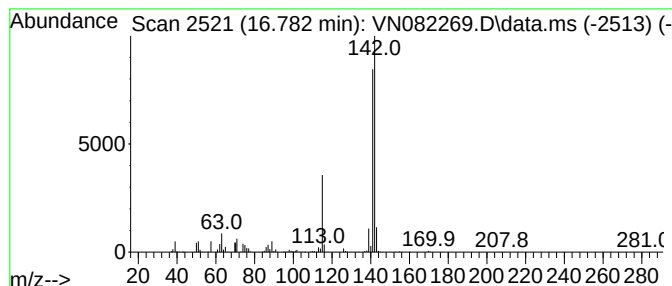
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Quant Title : SW846 8260

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.
16.782	60.11 ug/l	1411780	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	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	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082269.D
Acq On : 22 May 2024 03:33
Operator : JC\MD
Sample : P2494-09 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.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
Benzene, 1-ethy...	13.335	9.2	ug/l	216188	4	13.794	1174270	50.0
Naphthalene, 1,...	13.671	23.2	ug/l	544895	4	13.794	1174270	50.0
Naphthalene, 2,...	14.018	26.8	ug/l	629126	4	13.794	1174270	50.0
Naphthalene, 1,...	14.106	13.4	ug/l	315840	4	13.794	1174270	50.0
Indene	14.176	11.8	ug/l	276357	4	13.794	1174270	50.0
Dodecane	14.959	7.0	ug/l	164859	4	13.794	1174270	50.0
o-Cymene	15.035	11.0	ug/l	259267	4	13.794	1174270	50.0
Naphthalene, 1-...	16.782	60.1	ug/l	1411780	4	13.794	1174270	50.0