

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
 Data File : VX032588.D
 Acq On : 04 Nov 2022 19:44
 Operator : JC/MD
 Sample : N5387-03
 Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 32505

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_X\Method\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.947	297	305	313	rBV	11620	27105	1.39%	0.122%
2	5.391	696	706	719	rVV	63081	183020	9.38%	0.826%
3	5.550	721	732	750	rVB	115640	321795	16.49%	1.451%
4	5.952	789	798	813	rBV	74945	198116	10.15%	0.894%
5	6.757	920	930	943	rBV	173426	420973	21.57%	1.899%
6	8.647	1234	1240	1251	rBV	371708	570260	29.22%	2.572%
7	10.055	1466	1471	1483	rVB	363335	487052	24.96%	2.197%
8	11.085	1634	1640	1648	rBV	278805	407302	20.87%	1.837%
9	11.433	1692	1697	1701	rVV	32276	63314	3.24%	0.286%
10	11.476	1701	1704	1709	rVB	170649	206765	10.60%	0.933%
11	11.634	1727	1730	1733	rVB4	16301	21375	1.10%	0.096%
12	11.683	1733	1738	1740	rBV3	20142	25617	1.31%	0.116%
13	11.713	1740	1743	1746	rBV	87082	101258	5.19%	0.457%
14	11.750	1746	1749	1759	rVB4	65024	146006	7.48%	0.659%
15	11.841	1759	1764	1766	rBV2	34145	51712	2.65%	0.233%
16	11.890	1766	1772	1776	rVB4	51646	75064	3.85%	0.339%
17	11.945	1776	1781	1784	rBV2	139587	202281	10.37%	0.912%
18	11.975	1784	1786	1789	rVB2	44505	47848	2.45%	0.216%
19	12.024	1789	1794	1800	rBV2	397789	602864	30.89%	2.719%
20	12.073	1800	1802	1804	rBV2	75169	78759	4.04%	0.355%
21	12.104	1804	1807	1811	rVB2	107881	117644	6.03%	0.531%
22	12.171	1812	1818	1825	rVB4	129281	300296	15.39%	1.355%
23	12.268	1825	1834	1837	rBV5	91558	236636	12.13%	1.067%
24	12.311	1837	1841	1848	rBV8	219152	439114	22.50%	1.981%
25	12.427	1848	1860	1864	rBV	1432453	1951348	100.00%	8.802%
26	12.469	1864	1867	1873	rVB4	226324	387257	19.85%	1.747%
27	12.555	1875	1881	1883	rBV3	239503	424547	21.76%	1.915%
28	12.683	1898	1902	1905	rBV2	162160	216990	11.12%	0.979%
29	12.719	1905	1908	1912	rVV4	107703	209879	10.76%	0.947%
30	12.762	1912	1915	1918	rVV2	151292	244594	12.53%	1.103%
31	12.817	1920	1924	1931	rVV2	356895	531741	27.25%	2.398%
32	12.890	1931	1936	1943	rVV5	423620	845836	43.35%	3.815%
33	12.945	1943	1945	1947	rVV3	113782	149623	7.67%	0.675%
34	12.981	1947	1951	1956	rVV3	364962	569625	29.19%	2.569%
35	13.042	1957	1961	1964	rVB2	217293	249375	12.78%	1.125%
36	13.158	1975	1980	1986	rBV6	89301	244501	12.53%	1.103%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
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37	13.213	1986	1989	1991	rVV2	89802	124604	6.39%	0.562%
38	13.268	1994	1998	2000	rVV	878829	1055790	54.11%	4.762%
39	13.292	2000	2002	2007	rVV2	406101	569177	29.17%	2.567%
40	13.347	2007	2011	2014	rVV3	96858	145719	7.47%	0.657%
41	13.384	2014	2017	2019	rVV2	178214	227192	11.64%	1.025%
42	13.420	2020	2023	2033	rVB7	225655	550780	28.23%	2.484%
43	13.506	2033	2037	2041	rBV6	79823	136963	7.02%	0.618%
44	13.591	2047	2051	2055	rBV5	56004	97900	5.02%	0.442%
45	13.676	2061	2065	2068	rBV5	89266	157987	8.10%	0.713%
46	13.737	2072	2075	2078	rVV3	99275	148052	7.59%	0.668%
47	13.768	2078	2080	2083	rVV2	88827	109259	5.60%	0.493%
48	13.798	2083	2085	2088	rVV	94949	109140	5.59%	0.492%
49	13.841	2088	2092	2099	rVV4	123197	211920	10.86%	0.956%
50	13.908	2099	2103	2112	rVB8	66239	176325	9.04%	0.795%
51	14.036	2121	2124	2127	rVB2	99068	97938	5.02%	0.442%
52	14.103	2133	2135	2138	rVB3	36949	35455	1.82%	0.160%
53	14.164	2143	2145	2147	rBV2	44482	49686	2.55%	0.224%
54	14.225	2150	2155	2162	rVB5	113259	219011	11.22%	0.988%
55	14.438	2187	2190	2193	rVB2	103761	122844	6.30%	0.554%
56	14.487	2193	2198	2205	rBV5	134158	318839	16.34%	1.438%
57	14.554	2205	2209	2211	rBV3	85711	126516	6.48%	0.571%
58	14.615	2215	2219	2222	rBV	407634	545558	27.96%	2.461%
59	14.670	2225	2228	2232	rVB2	324883	392683	20.12%	1.771%
60	14.725	2233	2237	2239	rBV5	82823	127812	6.55%	0.577%
61	14.755	2239	2242	2244	rBV3	136399	141362	7.24%	0.638%
62	14.792	2244	2248	2251	rVV5	167076	221699	11.36%	1.000%
63	14.847	2254	2257	2261	rVB4	206693	258398	13.24%	1.166%
64	15.042	2284	2289	2293	rBV3	245271	405212	20.77%	1.828%
65	15.091	2293	2297	2301	rBV5	111921	205043	10.51%	0.925%
66	15.182	2309	2312	2314	rBV	125623	158469	8.12%	0.715%
67	15.207	2314	2316	2320	rVB3	150545	191304	9.80%	0.863%
68	15.316	2331	2334	2339	rVB5	124237	216296	11.08%	0.976%
69	15.377	2340	2344	2348	rBV	313769	479765	24.59%	2.164%
70	15.560	2370	2374	2379	rVB	896099	1197761	61.38%	5.403%
71	15.780	2407	2410	2415	rVB2	181000	265783	13.62%	1.199%
72	15.859	2419	2423	2433	rVB7	149406	392811	20.13%	1.772%
73	16.005	2441	2447	2456	rVB7	148778	470786	24.13%	2.124%
74	16.091	2456	2461	2477	rVB8	138528	350903	17.98%	1.583%

Sum of corrected areas: 22170234

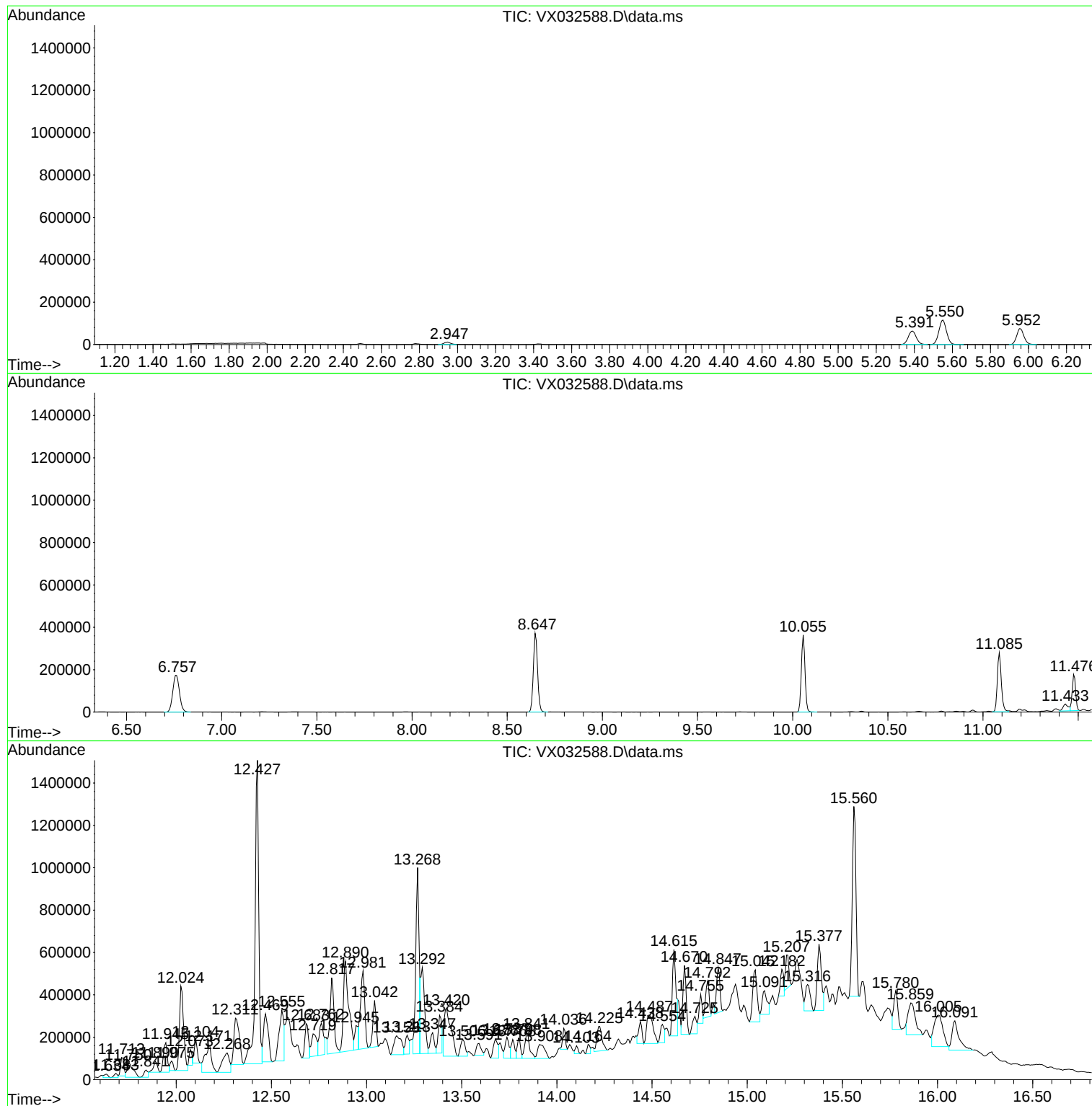
Instrument :
MSVOA_X
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

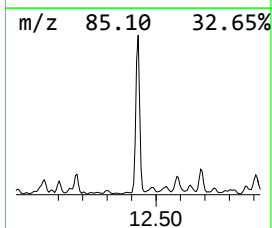
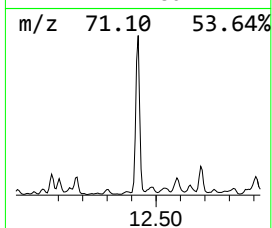
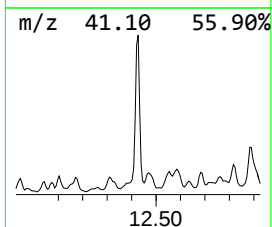
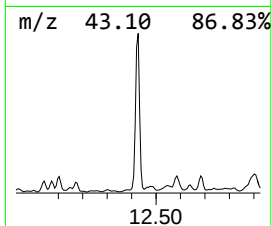
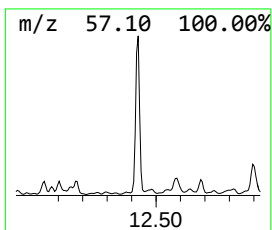
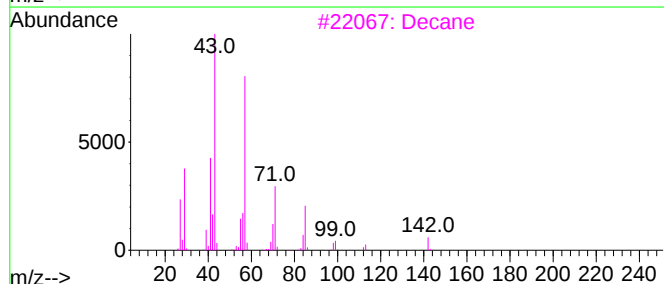
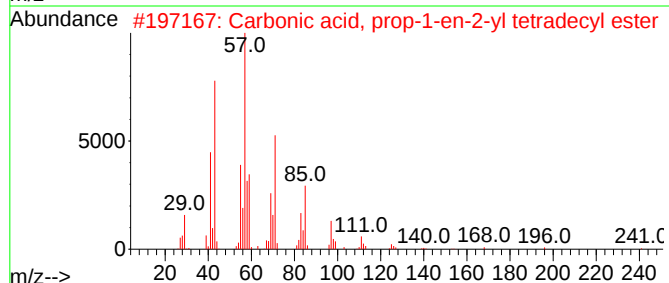
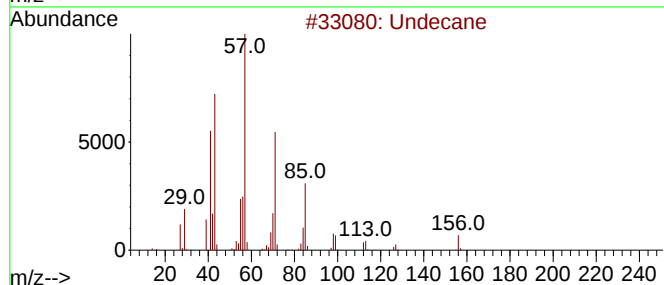
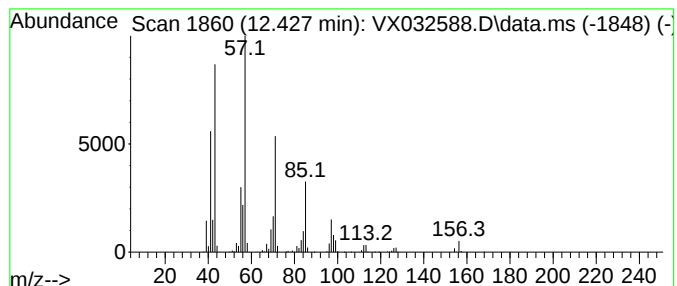
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	161.84 ug/l	1951350	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	96
2	Carbonic acid, prop-1-en-2-yl te...			298	C18H34O3	1000382-90-9	90
3	Decane			142	C10H22	000124-18-5	80
4	Carbonic acid, tetradecyl vinyl ...			284	C17H32O3	1000382-54-5	72
5	Carbonic acid, octadecyl prop-1-...			354	C22H42O3	1000383-11-5	72



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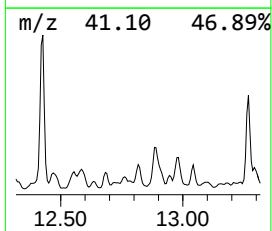
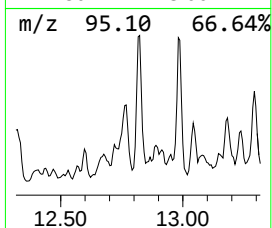
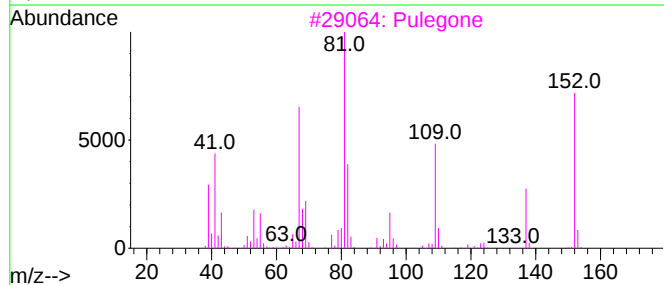
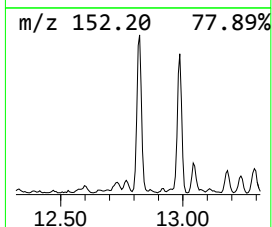
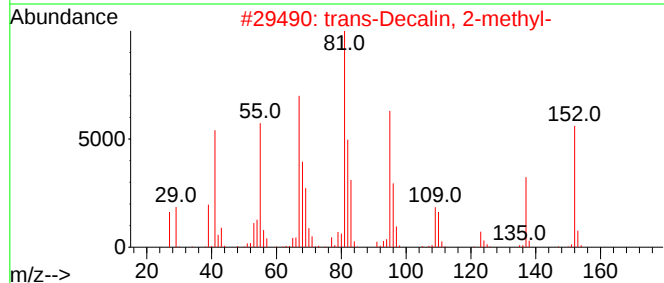
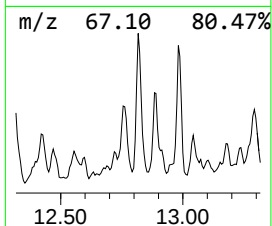
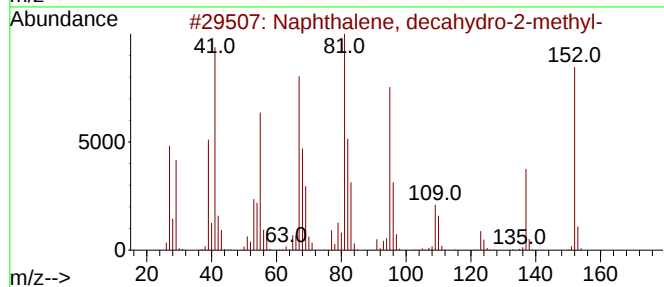
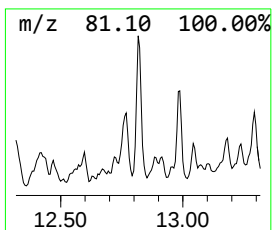
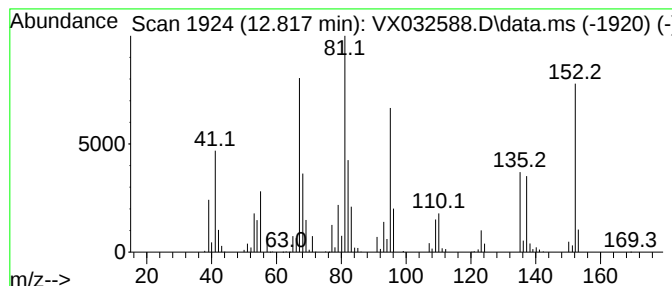
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Naphthalene, decahydro-2-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.817	44.10 ug/l	531741	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	96
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	93
3			Pulegone	152	C10H16O	000089-82-7	81
4			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	74
5			(+)-Dihydrocarvone	152	C10H16O	005524-05-0	64



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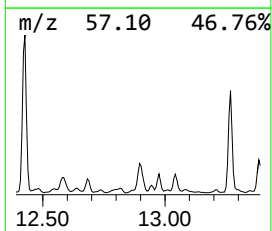
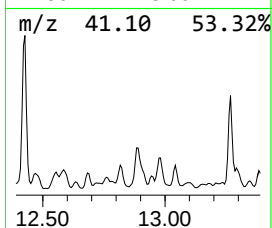
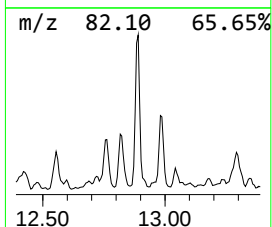
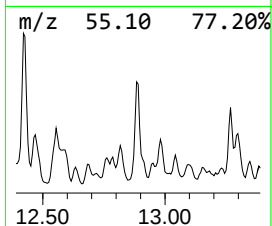
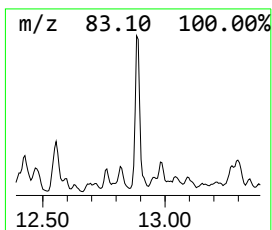
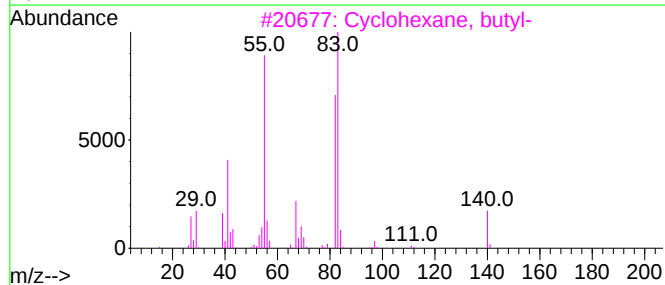
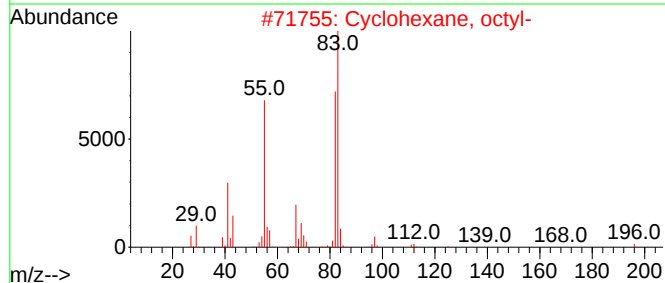
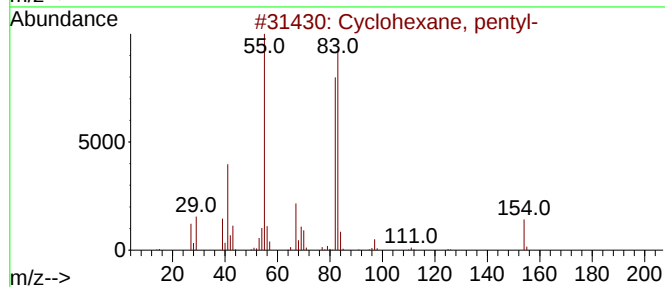
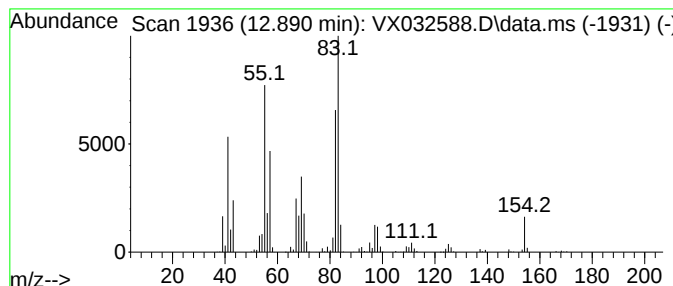
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclohexane, pentyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	70.15 ug/l	845836	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, pentyl-	154	C11H22	004292-92-6	87
2			Cyclohexane, octyl-	196	C14H28	001795-15-9	72
3			Cyclohexane, butyl-	140	C10H20	001678-93-9	64
4			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	62
5			Cyclohexane, propyl-	126	C9H18	001678-92-8	59



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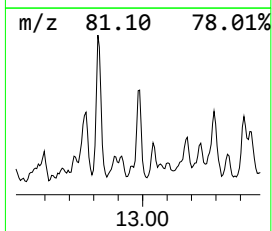
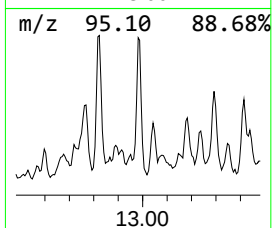
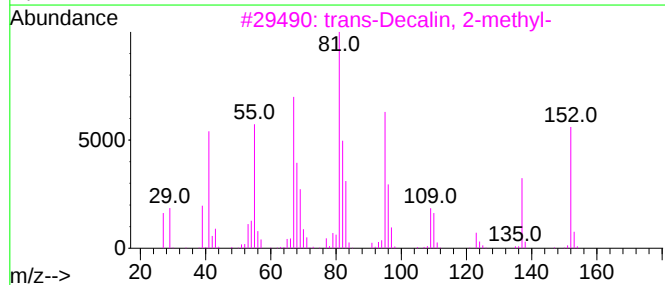
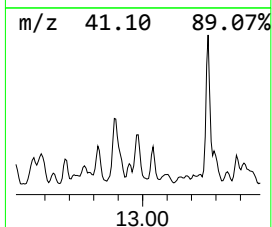
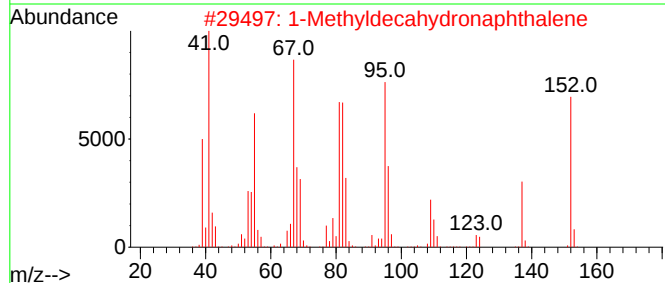
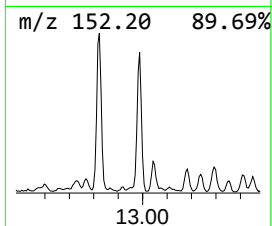
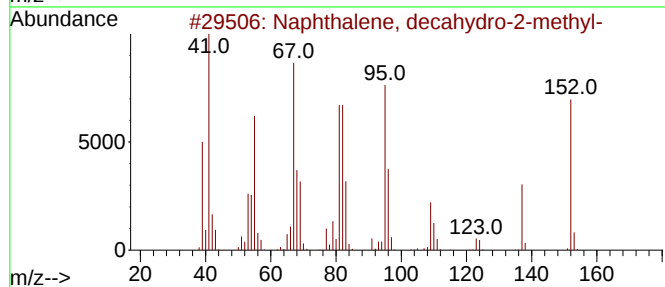
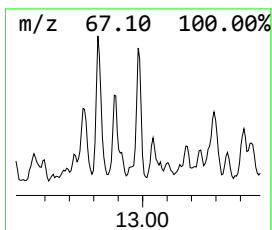
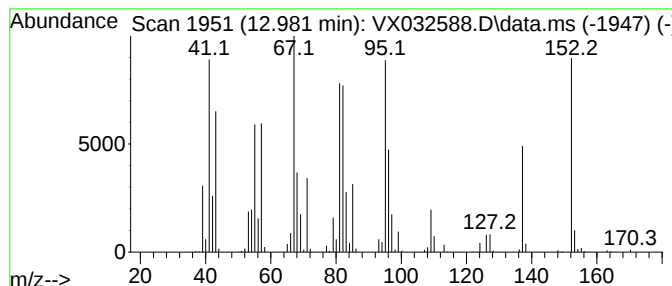
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Quant Title : SW846 8260

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

Peak Number 4 1-Methyldecahydronaphthalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.981	47.24 ug/l	569625	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	83
2			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	83
3			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	68
4			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	68
5			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032588.D
Acq On : 04 Nov 2022 19:44
Operator : JC/MD
Sample : N5387-03
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

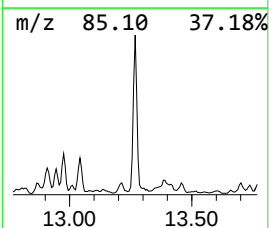
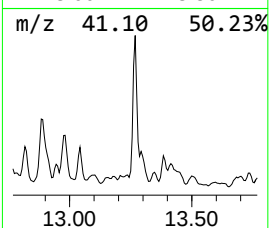
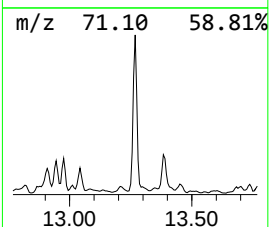
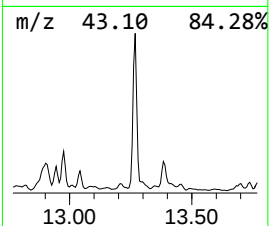
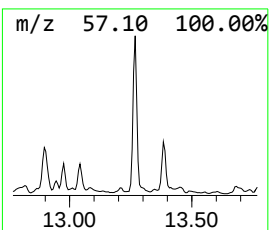
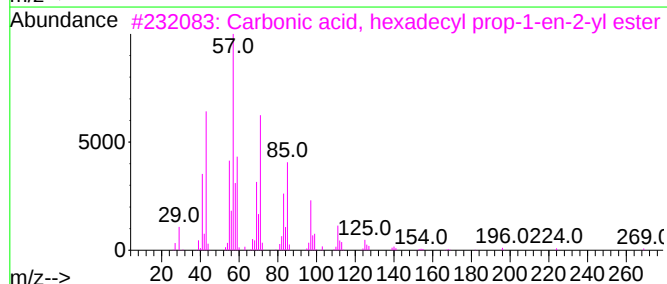
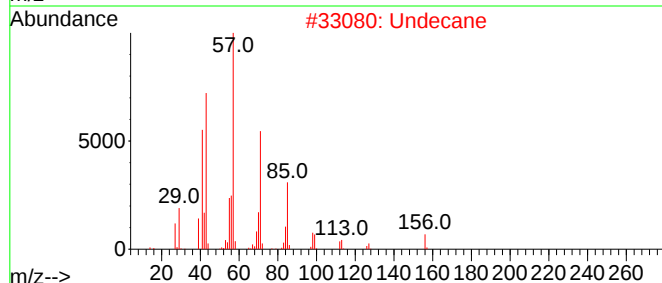
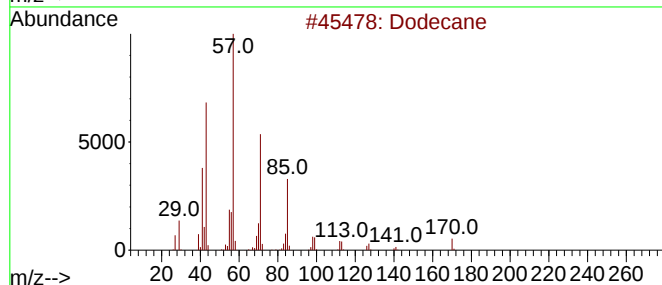
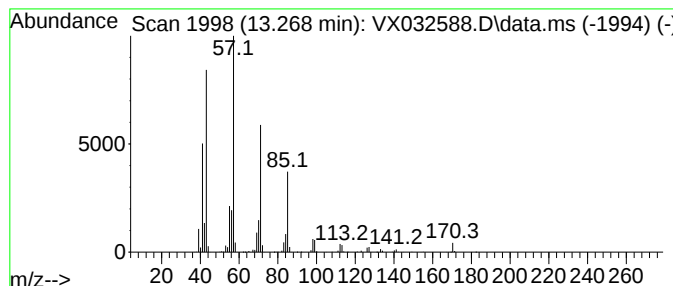
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Quant Title : SW846 8260

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

Peak Number 5 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	87.56 ug/l	1055790	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	97
2			Undecane	156	C11H24	001120-21-4	90
3			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	83
4			Tetradecane	198	C14H30	000629-59-4	80
5			Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032588.D
Acq On : 04 Nov 2022 19:44
Operator : JC/MD
Sample : N5387-03
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

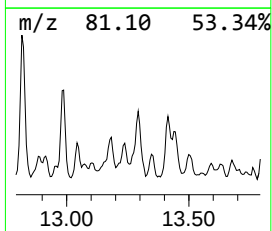
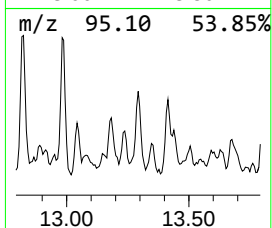
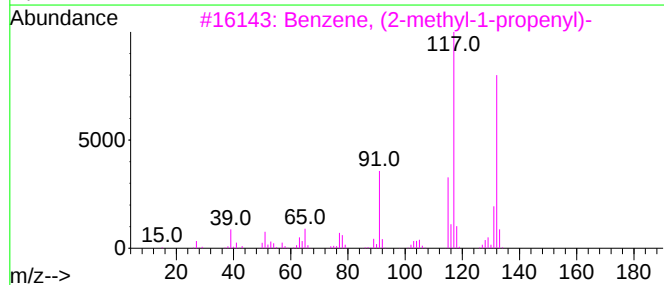
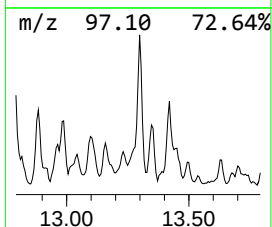
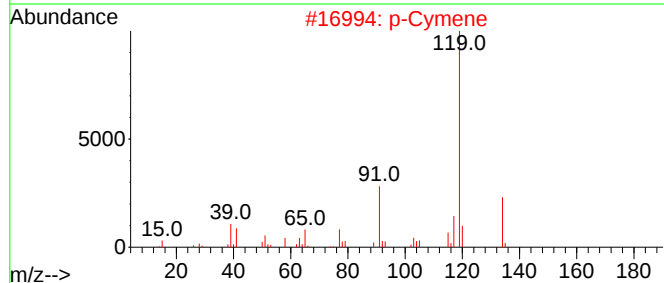
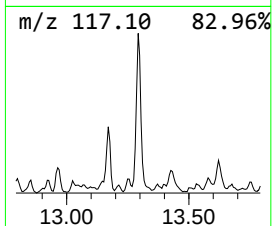
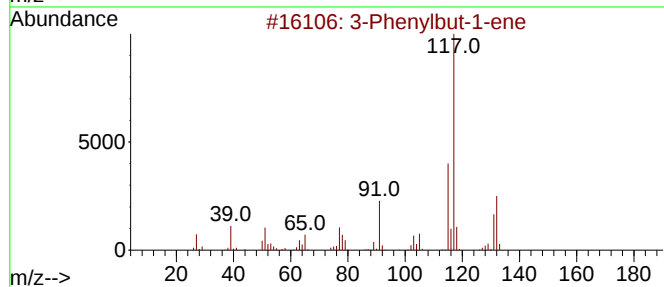
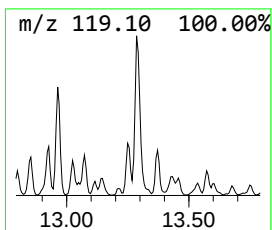
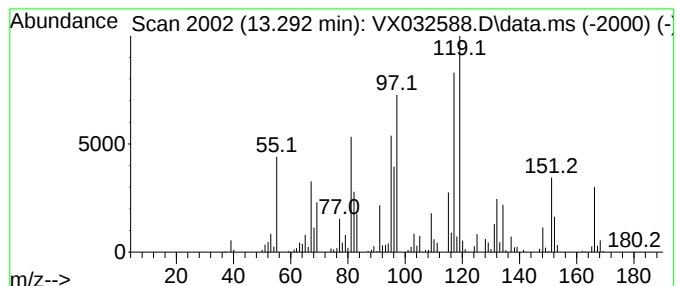
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.292 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	47.21 ug/l	569177	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Phenylbut-1-ene	132	C10H12	000934-10-1	25
2			p-Cymene	134	C10H14	000099-87-6	18
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	15
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	15
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	15



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032588.D
Acq On : 04 Nov 2022 19:44
Operator : JC/MD
Sample : N5387-03
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

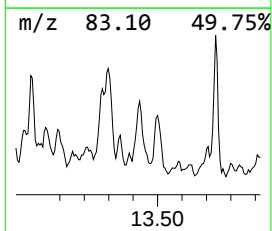
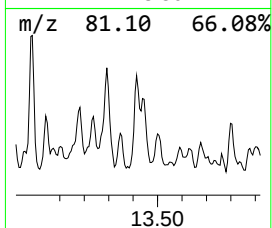
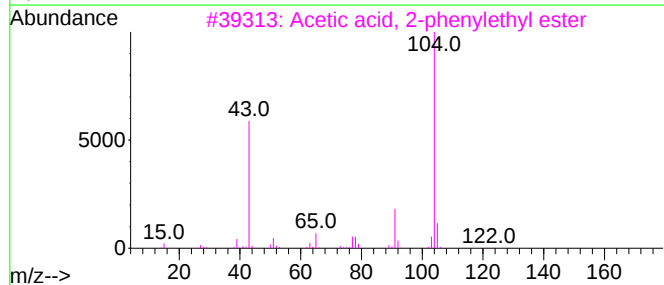
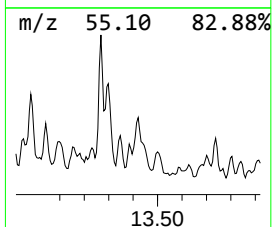
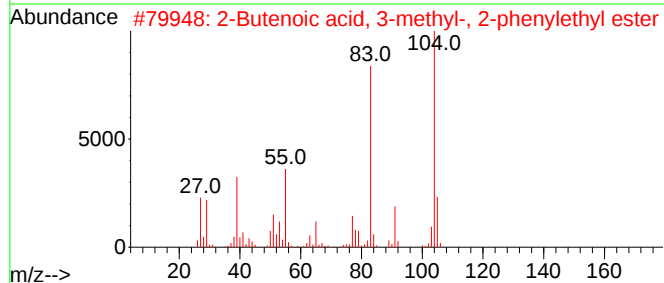
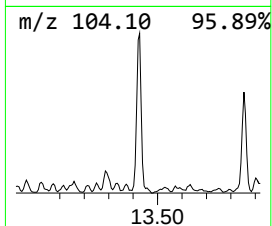
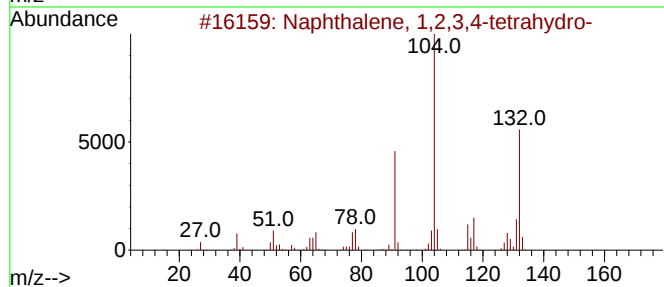
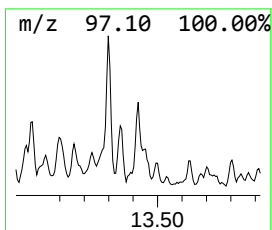
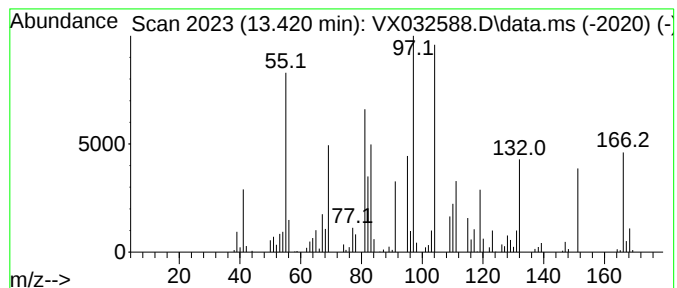
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	45.68 ug/l	550780	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	56
2			2-Butenoic acid, 3-methyl-, 2-ph...	204	C13H16O2	042078-65-9	10
3			Acetic acid, 2-phenylethyl ester	164	C10H12O2	000103-45-7	10
4			2-Azetidinone, 4-phenyl-	147	C9H9NO	005661-55-2	10
5			Glutaric acid, isobutyl 2-methyl...	292	C17H24O4	1000371-32-5	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032588.D
Acq On : 04 Nov 2022 19:44
Operator : JC/MD
Sample : N5387-03
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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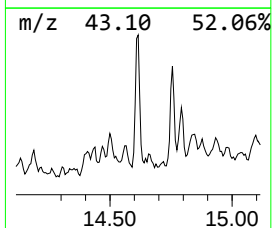
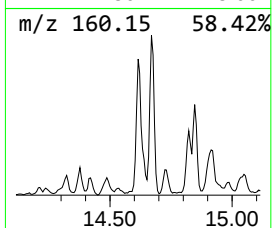
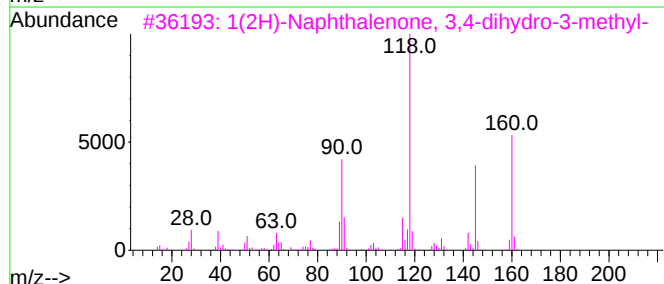
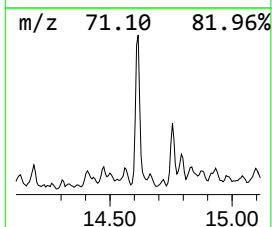
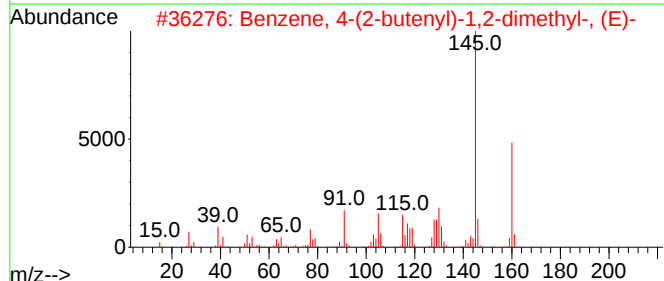
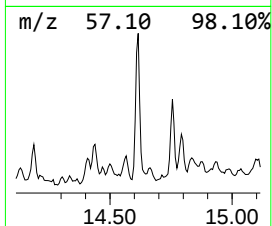
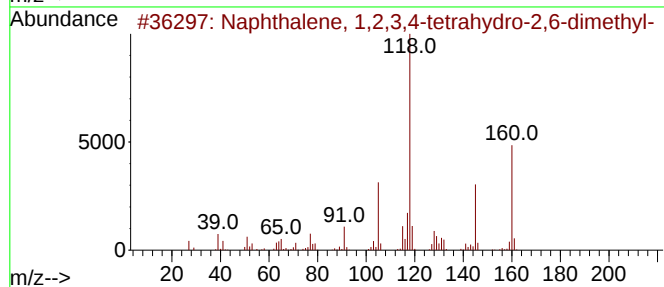
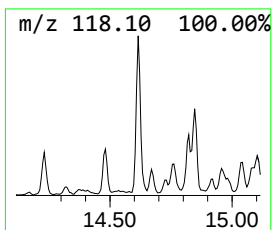
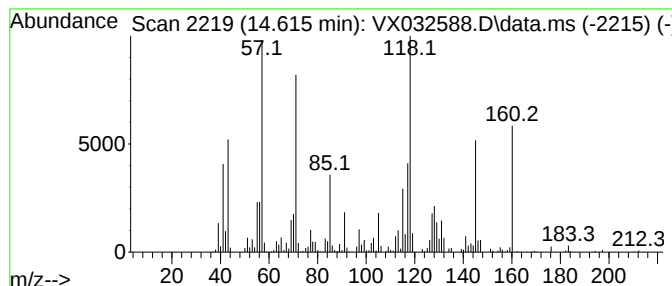
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Quant Title : SW846 8260

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

Peak Number 8 unknown14.615 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	45.25 ug/l	545558	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	49
2			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	43
3			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	43
4			Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	35
5			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032588.D
Acq On : 04 Nov 2022 19:44
Operator : JC/MD
Sample : N5387-03
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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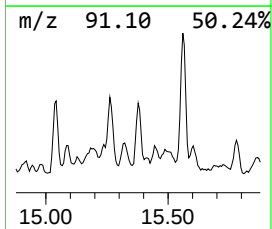
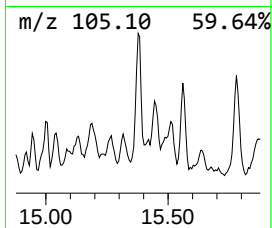
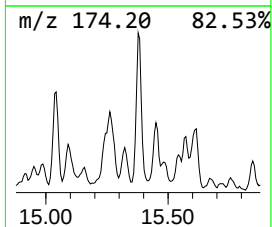
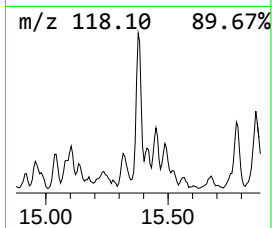
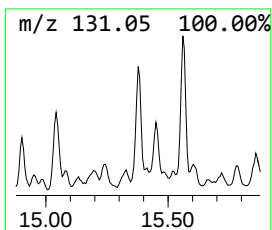
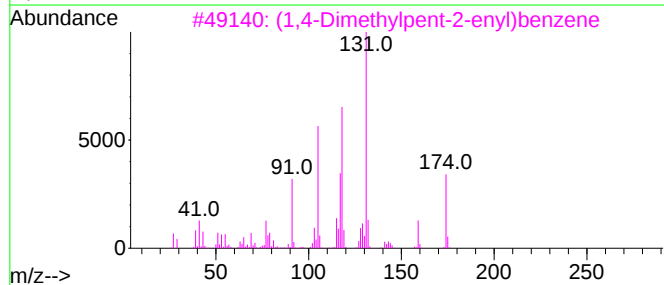
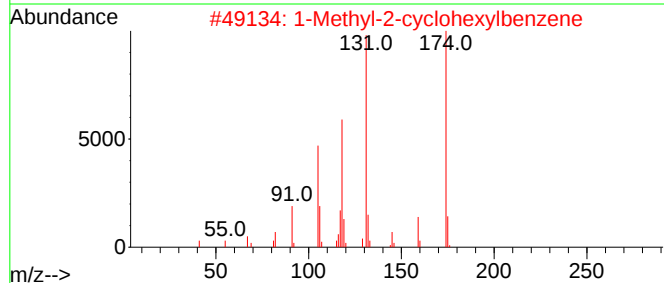
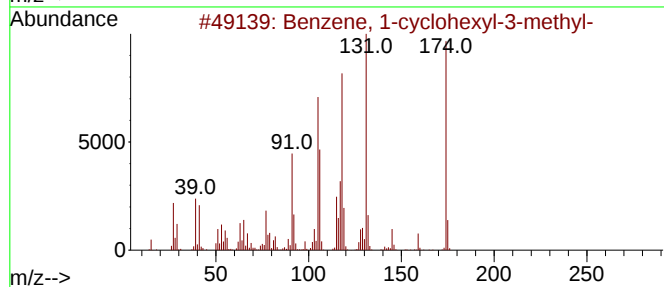
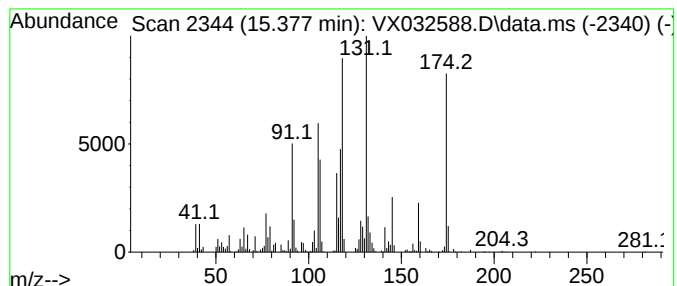
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-cyclohexyl-3-met... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.377	39.79 ug/l	479765	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	93
2			1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	87
3			(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	83
4			1H-1,3,2-Benzodiazaborole, 2-but...	174	C10H15BN2	031748-14-8	49
5			3-Amino-6-methoxyquinoline	174	C10H10N2O	029507-86-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032588.D
Acq On : 04 Nov 2022 19:44
Operator : JC/MD
Sample : N5387-03
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

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ClientSampleId :
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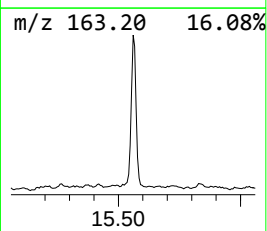
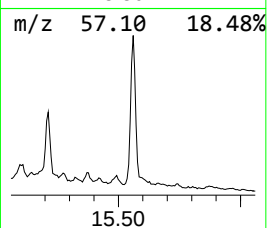
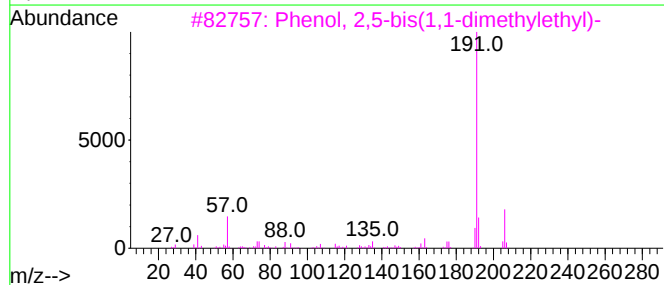
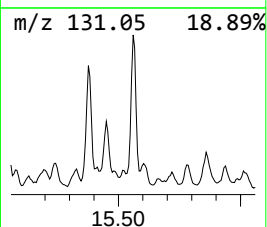
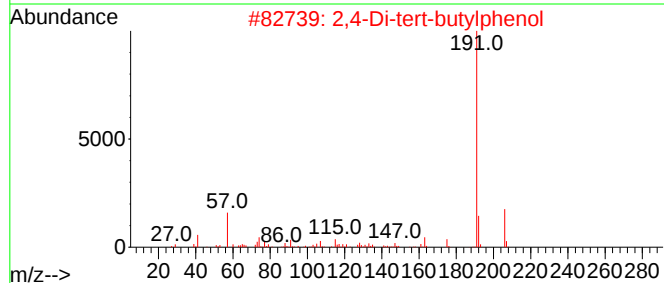
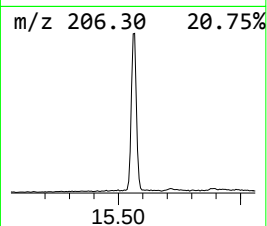
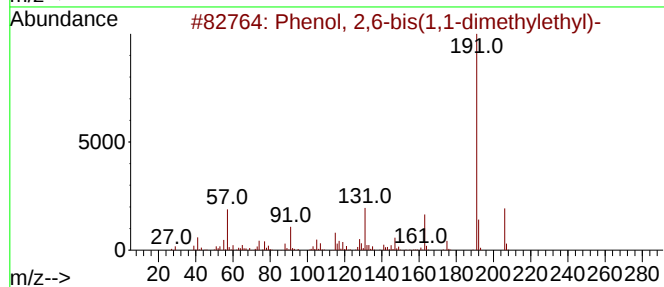
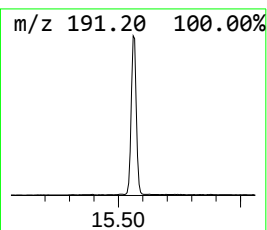
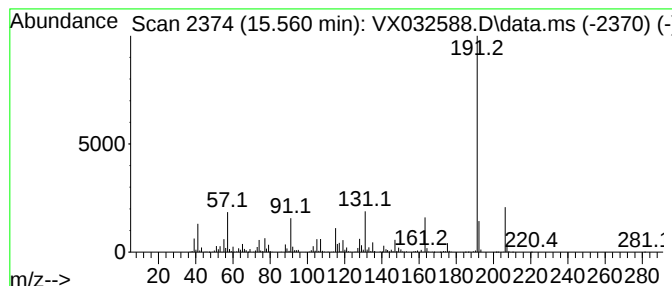
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Quant Title : SW846 8260

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

Peak Number 10 Phenol, 2,6-bis(1,1-dimethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	99.34 ug/l	1197760	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	95
2			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	87
3			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	81
4			4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	80
5			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032588.D
Acq On : 04 Nov 2022 19:44
Operator : JC/MD
Sample : N5387-03
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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
Undecane	12.427	161.8	ug/l	1951350	4	12.024	602864	50.0
Naphthalene, de...	12.817	44.1	ug/l	531741	4	12.024	602864	50.0
Cyclohexane, pe...	12.890	70.2	ug/l	845836	4	12.024	602864	50.0
1-Methyldecahyd...	12.981	47.2	ug/l	569625	4	12.024	602864	50.0
Dodecane	13.268	87.6	ug/l	1055790	4	12.024	602864	50.0
unknown13.292	13.292	47.2	ug/l	569177	4	12.024	602864	50.0
Naphthalene, 1,...	13.420	45.7	ug/l	550780	4	12.024	602864	50.0
unknown14.615	14.615	45.3	ug/l	545558	4	12.024	602864	50.0
Benzene, 1-cycl...	15.377	39.8	ug/l	479765	4	12.024	602864	50.0
Phenol, 2,6-bis...	15.560	99.3	ug/l	1197760	4	12.024	602864	50.0