

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
 Data File : VX006095.D
 Acq On : 19 Nov 2018 17:00
 Operator : JC/MD
 Sample : J5951-01 10X
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FDSB-02(10-12)

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

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

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.500	699	713	723	rBV2	80029	221100	13.41%	0.486%
2	5.659	723	739	762	rVB2	140334	431781	26.18%	0.948%
3	6.067	794	806	826	rVV2	83104	220274	13.36%	0.484%
4	6.860	926	936	960	rBV	207786	498523	30.23%	1.095%
5	7.457	1022	1034	1045	rBV2	93294	222093	13.47%	0.488%
6	8.341	1173	1179	1183	rVV	122783	210362	12.76%	0.462%
7	8.664	1225	1232	1235	rBV	155391	267724	16.23%	0.588%
8	8.713	1235	1240	1252	rVB	393885	689845	41.83%	1.515%
9	8.975	1277	1283	1289	rBV	149649	233392	14.15%	0.513%
10	9.042	1289	1294	1305	rVB	120663	215072	13.04%	0.472%
11	9.445	1354	1360	1364	rBV	155508	223438	13.55%	0.491%
12	9.560	1374	1379	1385	rBV4	125069	268367	16.27%	0.589%
13	9.621	1385	1389	1393	rVB	215358	289867	17.58%	0.637%
14	9.676	1393	1398	1402	rBV	204897	314915	19.10%	0.692%
15	9.877	1426	1431	1437	rBV3	165559	396468	24.04%	0.871%
16	9.963	1440	1445	1449	rVB	330302	470291	28.52%	1.033%
17	10.066	1455	1462	1466	rBV	343950	476533	28.90%	1.047%
18	10.115	1466	1470	1474	rVB	361043	466957	28.32%	1.025%
19	10.335	1497	1506	1509	rBV2	142994	299628	18.17%	0.658%
20	10.377	1509	1513	1516	rVB	188116	241958	14.67%	0.531%
21	10.414	1516	1519	1529	rVB3	172679	335599	20.35%	0.737%
22	10.512	1529	1535	1543	rBV3	90507	165872	10.06%	0.364%
23	10.640	1550	1556	1564	rBV4	302857	547047	33.17%	1.201%
24	10.725	1564	1570	1575	rBV3	141095	249022	15.10%	0.547%
25	10.835	1580	1588	1592	rBV2	584410	913156	55.37%	2.005%
26	10.914	1592	1601	1604	rBV3	472129	807269	48.95%	1.773%
27	10.950	1604	1607	1612	rVB	238728	317071	19.23%	0.696%
28	11.011	1612	1617	1621	rBV3	90352	171288	10.39%	0.376%
29	11.085	1626	1629	1632	rVB	173102	196652	11.93%	0.432%
30	11.139	1632	1638	1640	rBV2	647604	899276	54.53%	1.975%
31	11.243	1648	1655	1658	rBV	361649	535601	32.48%	1.176%
32	11.274	1658	1660	1665	rVB4	246783	310084	18.80%	0.681%
33	11.396	1676	1680	1684	rVV2	110186	162287	9.84%	0.356%
34	11.444	1684	1688	1691	rVV3	135842	176810	10.72%	0.388%

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35	11.487	1691	1695	1699	rVV	356713	453790	27.52%	0.997%
36	11.536	1699	1703	1707	rVB3	195344	316548	19.20%	0.695%
37	11.682	1721	1727	1732	rVB7	172757	363579	22.05%	0.798%
38	11.737	1732	1736	1738	rBV2	170551	209825	12.72%	0.461%
39	11.767	1738	1741	1744	rBV	470432	480204	29.12%	1.055%
40	11.895	1758	1762	1763	rBV	126711	167937	10.18%	0.369%
41	11.944	1764	1770	1775	rVV5	329877	642466	38.96%	1.411%
42	11.999	1775	1779	1782	rVV	552080	724942	43.96%	1.592%
43	12.030	1782	1784	1788	rVV2	148700	166747	10.11%	0.366%
44	12.084	1788	1793	1797	rVV2	477042	870165	52.77%	1.911%
45	12.127	1797	1800	1803	rVV	218073	209378	12.70%	0.460%
46	12.158	1803	1805	1809	rVB3	171884	168147	10.20%	0.369%
47	12.225	1812	1816	1824	rVB3	341363	615701	37.34%	1.352%
48	12.304	1824	1829	1834	rBV2	384154	587477	35.62%	1.290%
49	12.371	1835	1840	1847	rBV3	533573	1050211	63.69%	2.306%
50	12.475	1847	1857	1862	rBV3	298029	768217	46.59%	1.687%
51	12.523	1862	1865	1871	rVB4	294588	496273	30.09%	1.090%
52	12.615	1873	1880	1881	rBV5	224100	444616	26.96%	0.976%
53	12.670	1886	1889	1892	rVB	432765	463431	28.10%	1.018%
54	12.755	1897	1903	1906	rBV2	301755	669315	40.59%	1.470%
55	12.822	1911	1914	1918	rVV6	102535	215131	13.05%	0.472%
56	12.877	1919	1923	1929	rVB3	589208	905853	54.93%	1.989%
57	12.944	1929	1934	1937	rBV3	686999	1124997	68.22%	2.471%
58	12.981	1937	1940	1946	rVV3	467413	769197	46.64%	1.689%
59	13.042	1946	1950	1954	rVV3	433392	549344	33.31%	1.206%
60	13.096	1954	1959	1963	rVB5	328259	571887	34.68%	1.256%
61	13.151	1965	1968	1973	rVB2	149167	221389	13.43%	0.486%
62	13.224	1978	1980	1984	rVV	155587	176777	10.72%	0.388%
63	13.346	1996	2000	2006	rVB2	1018151	1649062	100.00%	3.622%
64	13.401	2006	2009	2011	rBV3	132578	162211	9.84%	0.356%
65	13.438	2011	2015	2018	rVV2	368053	637191	38.64%	1.399%
66	13.474	2018	2021	2031	rVB7	455642	1204383	73.03%	2.645%
67	13.566	2032	2036	2039	rBV4	188911	296870	18.00%	0.652%
68	13.602	2039	2042	2045	rVV	197206	249687	15.14%	0.548%
69	13.639	2045	2048	2052	rVV2	298958	451812	27.40%	0.992%
70	13.688	2053	2056	2057	rVV2	116062	151363	9.18%	0.332%
71	13.730	2059	2063	2066	rVV2	308558	532098	32.27%	1.169%

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72	13.798	2070	2074	2080	rVB4	326474	591709	35.88%	1.299%
73	13.858	2080	2084	2087	rBV3	314044	387488	23.50%	0.851%
74	13.901	2087	2091	2098	rVB4	436690	630292	38.22%	1.384%
75	13.986	2098	2105	2109	rVB8	290723	693101	42.03%	1.522%
76	14.035	2109	2113	2115	rBV3	138212	225408	13.67%	0.495%
77	14.133	2124	2129	2132	rBV4	256528	404196	24.51%	0.888%
78	14.163	2132	2134	2137	rVV3	165540	177739	10.78%	0.390%
79	14.224	2141	2144	2146	rVV	142360	195797	11.87%	0.430%
80	14.273	2149	2152	2160	rVB2	371644	654245	39.67%	1.437%
81	14.432	2175	2178	2181	rVB2	177362	203588	12.35%	0.447%
82	14.480	2182	2186	2192	rVB6	159255	310022	18.80%	0.681%
83	14.547	2192	2197	2200	rBV4	218913	430900	26.13%	0.946%
84	14.675	2214	2218	2219	rBV2	360979	458023	27.77%	1.006%
85	14.700	2219	2222	2225	rVV	1281034	1516375	91.95%	3.330%
86	14.730	2225	2227	2231	rVB3	233030	267777	16.24%	0.588%
87	14.785	2231	2236	2239	rBV2	182647	278821	16.91%	0.612%
88	14.840	2241	2245	2253	rVV	819749	1117454	67.76%	2.454%
89	14.907	2253	2256	2260	rVB2	142732	161551	9.80%	0.355%
90	15.248	2308	2312	2314	rBV3	119956	181922	11.03%	0.400%
91	15.279	2314	2317	2320	rVB	166660	205657	12.47%	0.452%
92	15.450	2340	2345	2348	rBV2	277309	409715	24.85%	0.900%
93	15.486	2348	2351	2355	rVV3	116673	177763	10.78%	0.390%
94	15.553	2356	2362	2369	rVB	631602	996726	60.44%	2.189%
95	15.687	2379	2384	2388	rBV	560686	963101	58.40%	2.115%
96	15.724	2388	2390	2399	rVB	503442	759337	46.05%	1.668%
97	15.919	2418	2422	2432	rVB2	150224	373200	22.63%	0.820%
98	16.072	2443	2447	2458	rVB3	102377	224962	13.64%	0.494%
99	16.443	2503	2508	2516	rVB	88076	160259	9.72%	0.352%
100	16.693	2545	2549	2554	rVV	109424	194244	11.78%	0.427%

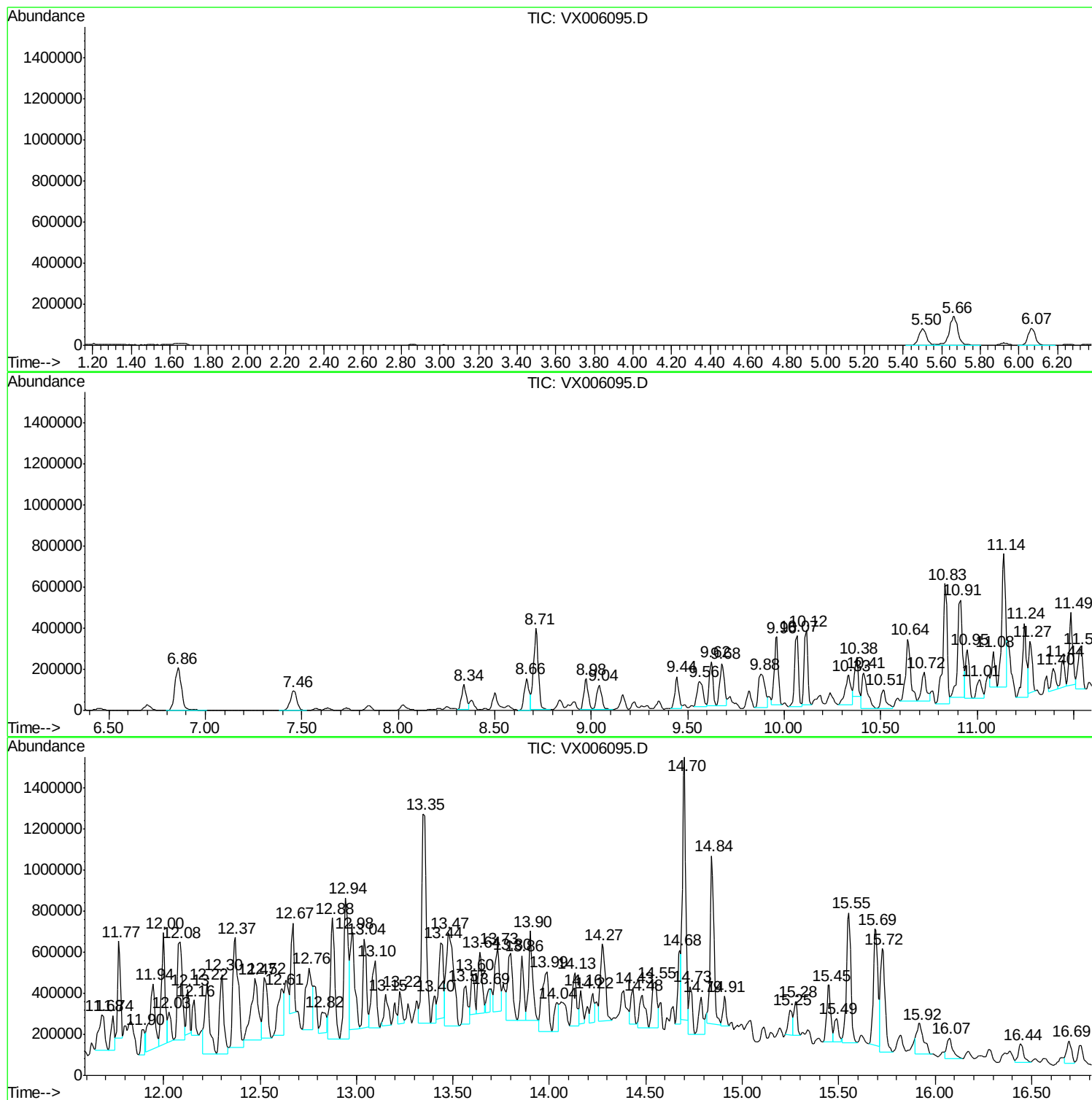
Sum of corrected areas: 45535215

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Instrument :
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ClientSampleId :
FDSB-02(10-12)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 18 Sample Multiplier: 1

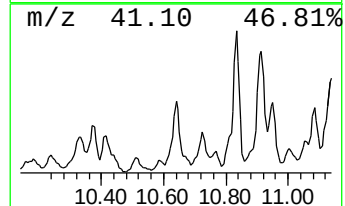
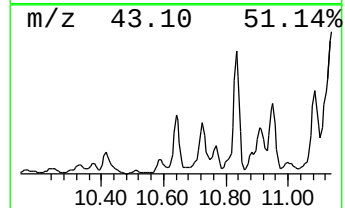
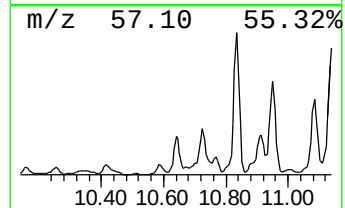
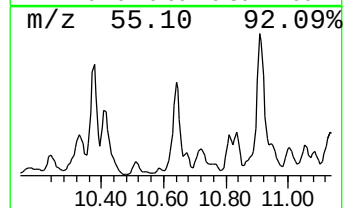
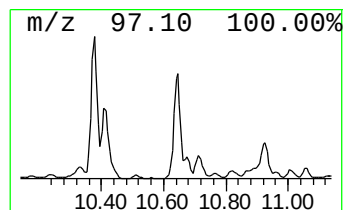
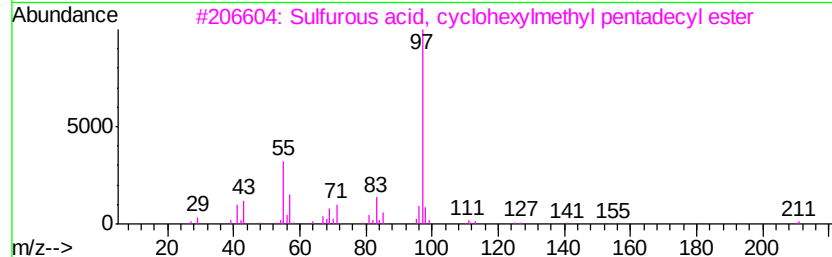
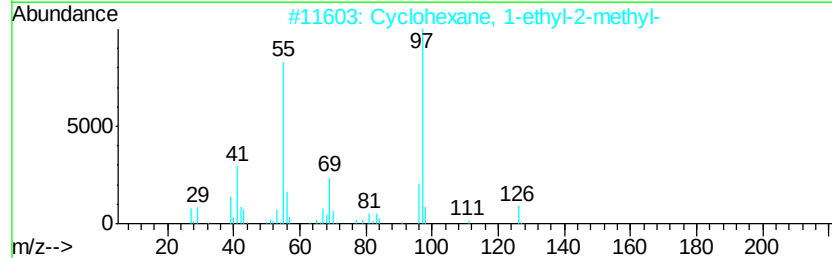
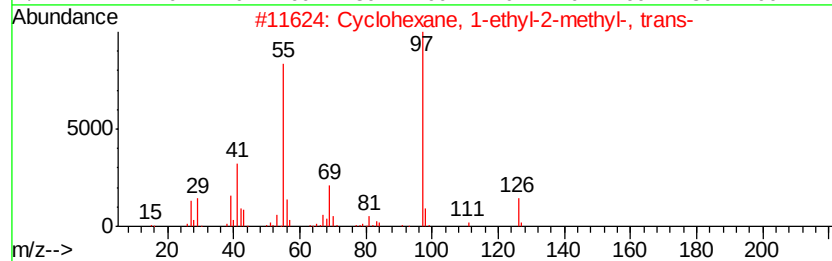
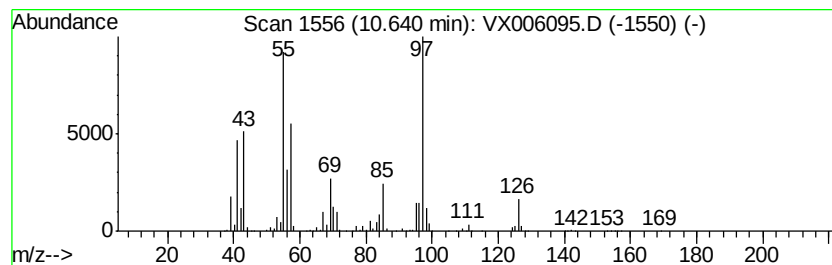
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.64	58.58 ug/l	547047	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	70
2		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	62
3		Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	59
4		Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	59
5		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	58



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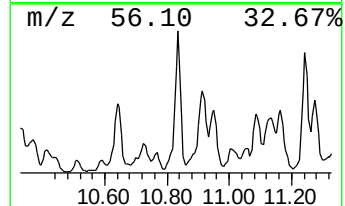
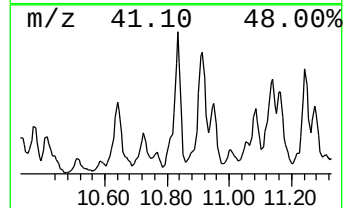
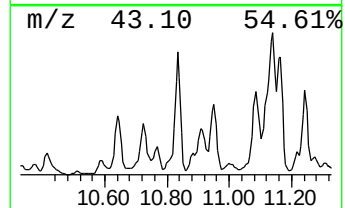
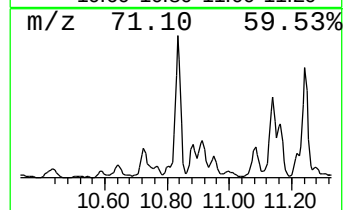
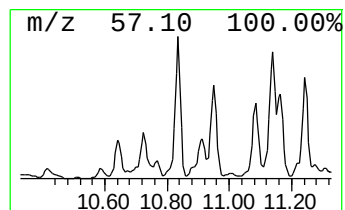
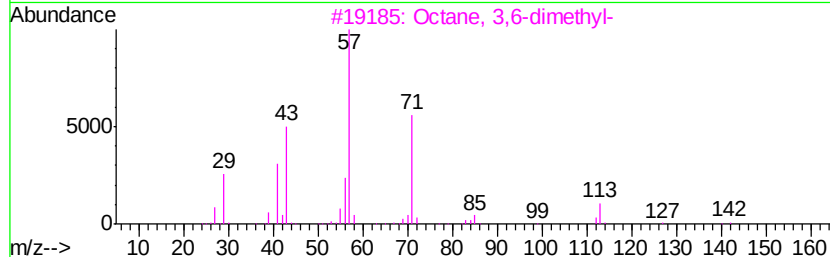
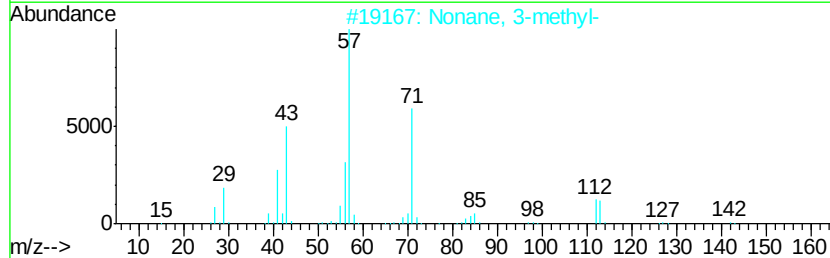
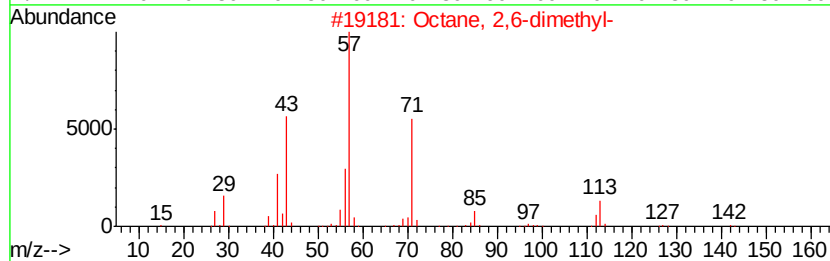
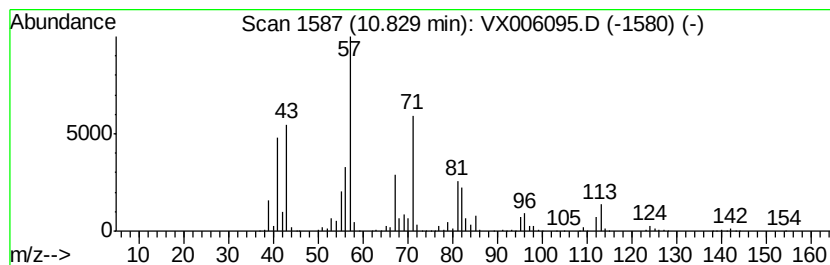
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.83	97.78 ug/l	913156	Chlorobenzene-d5	10.12	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	60
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	53
4	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	43
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	43



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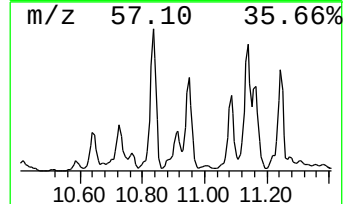
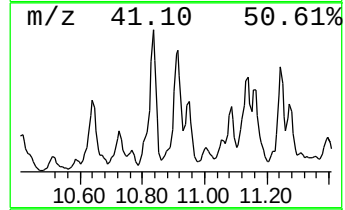
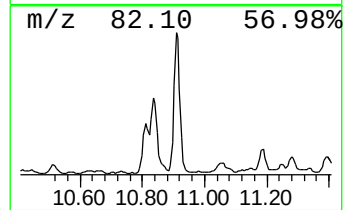
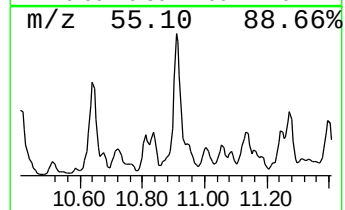
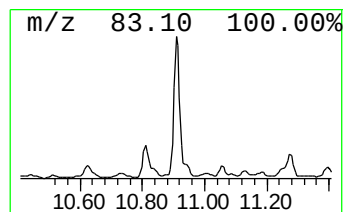
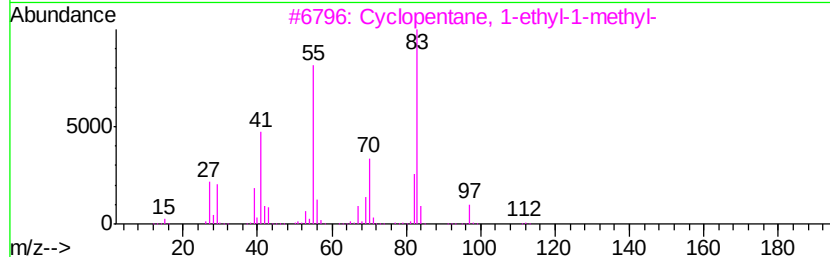
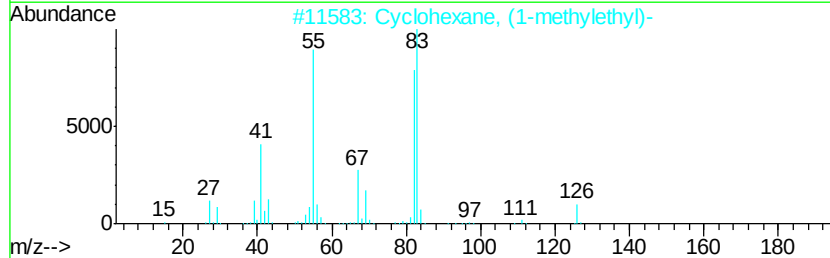
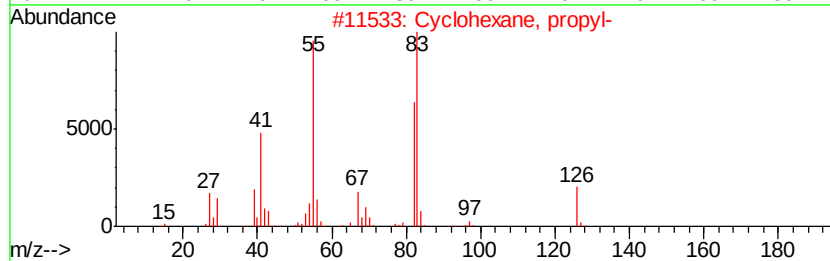
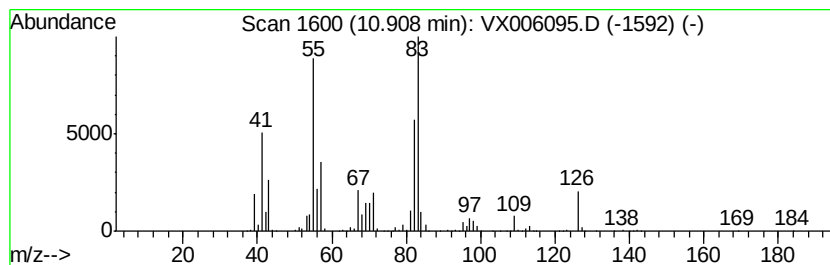
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MSVOA_X
ClientSampleId :
FDSB-02(10-12)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexane, propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.91	86.44 ug/l	807269	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, propyl-	126	C9H18	001678-92-8	64
2		Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	49
3		Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	49
4		Cyclohexane, methyl-	98	C7H14	000108-87-2	46
5		Cycloheptanone, 2-methyl-	126	C8H14O	000932-56-9	46



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006095.D
Acq On : 19 Nov 2018 17:00
Operator : JC/MD
Sample : J5951-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

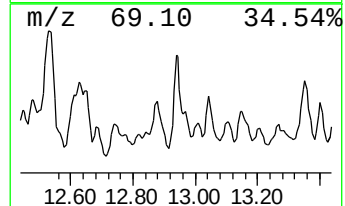
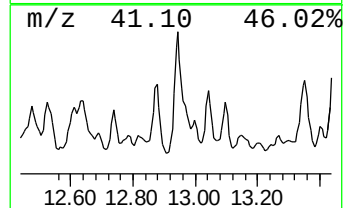
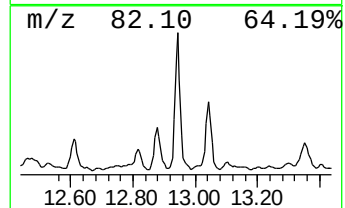
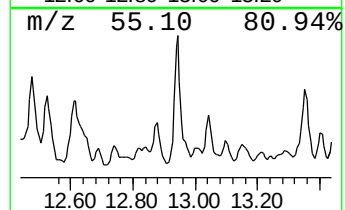
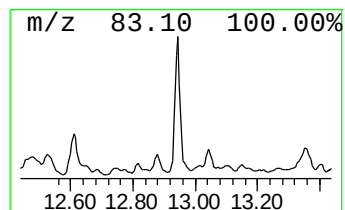
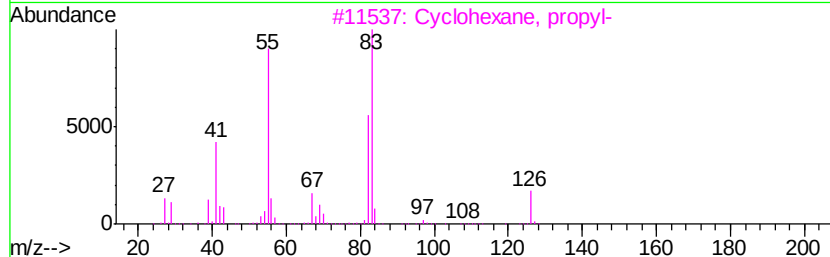
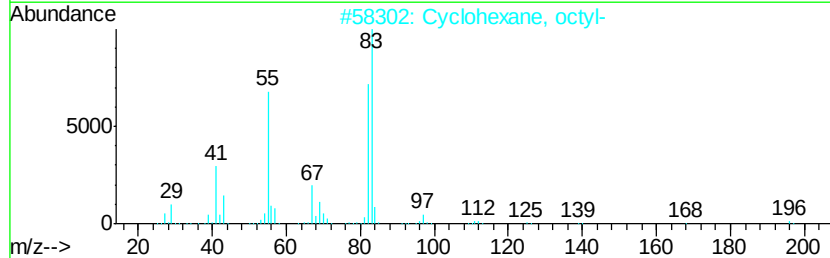
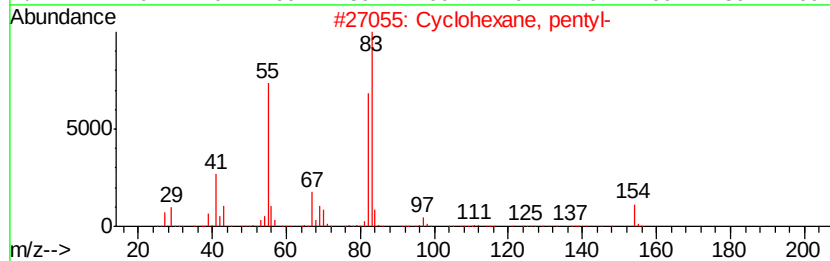
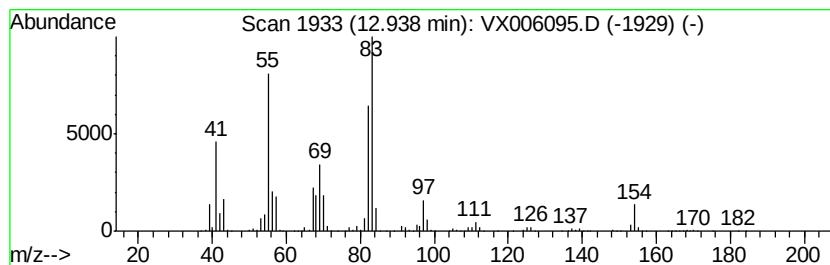
Instrument :
MSVOA_X
ClientSampled :
FDSB-02(10-12)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexane, pentyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.94	64.64 ug/l	1125000	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	90
2	Cyclohexane, octyl-	196	C14H28	001795-15-9	72
3	Cyclohexane, propyl-	126	C9H18	001678-92-8	64
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	64
5	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006095.D
Acq On : 19 Nov 2018 17:00
Operator : JC/MD
Sample : J5951-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

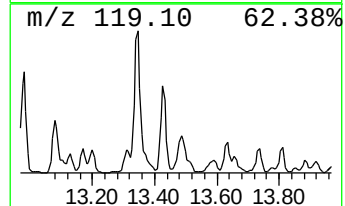
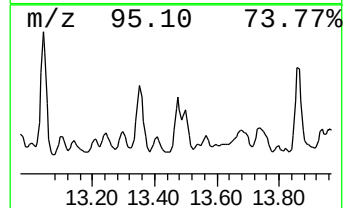
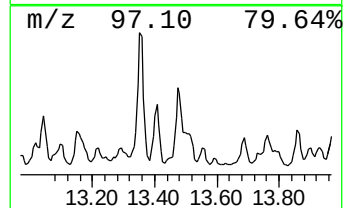
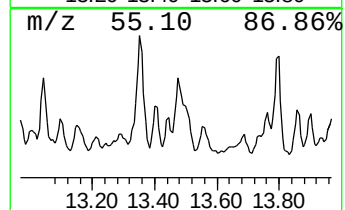
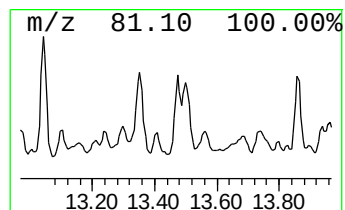
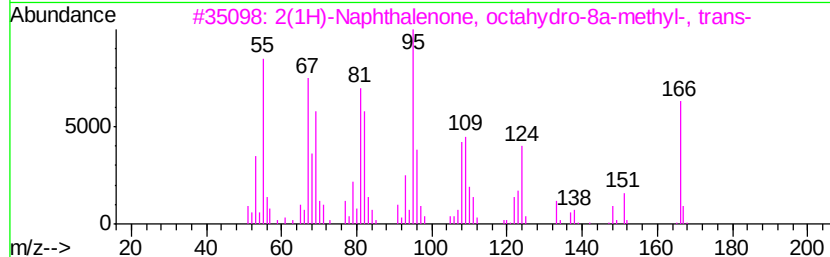
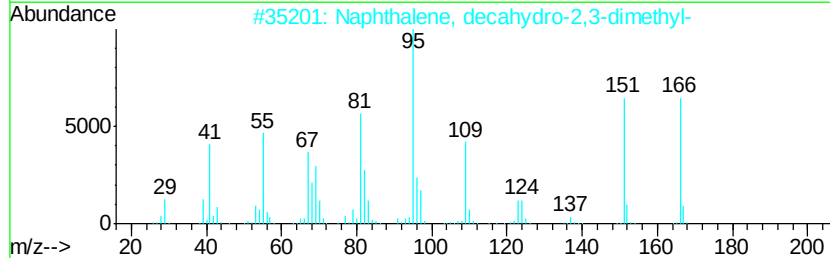
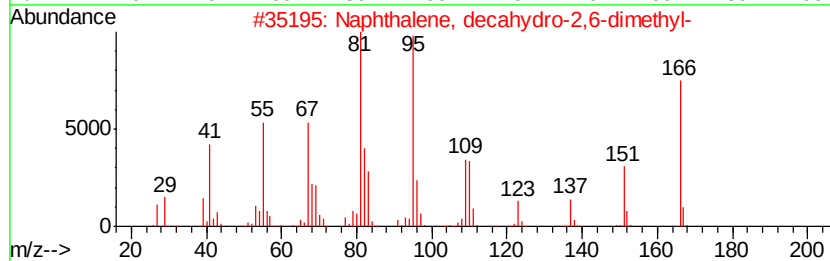
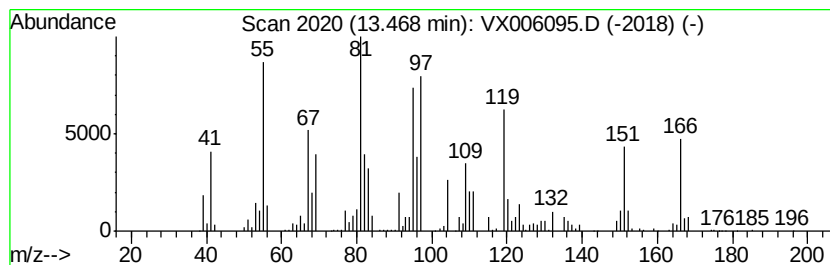
Instrument :
MSVOA_X
ClientSampleId :
FDSB-02(10-12)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, decahydro-2,6-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	69.20 ug/l	1204380	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, decahydro-2,6-dimet...	166 C12H22	001618-22-0 51
2		Naphthalene, decahydro-2,3-dimet...	166 C12H22	001008-80-6 25
3		2(1H)-Naphthalenone, octahydro-8...	166 C11H18O	001197-95-1 25
4		cis,trans-1,6-Dimethylspiro[4.5]...	166 C12H22	1000111-72-3 15
5		Cyclohexane, ethylidene-	110 C8H14	001003-64-1 15



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006095.D
Acq On : 19 Nov 2018 17:00
Operator : JC/MD
Sample : J5951-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FDSB-02(10-12)

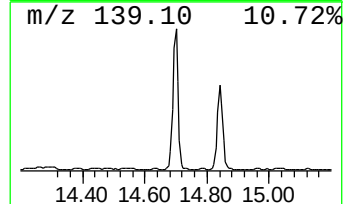
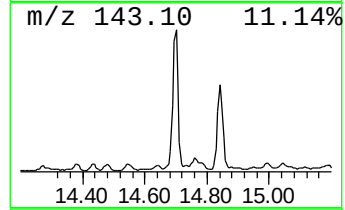
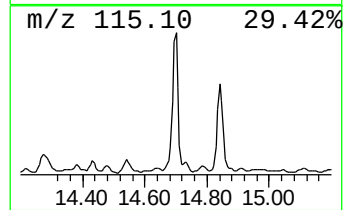
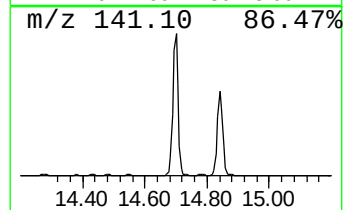
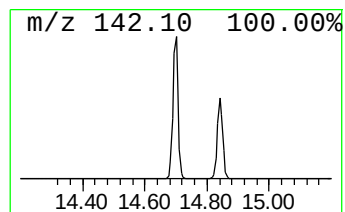
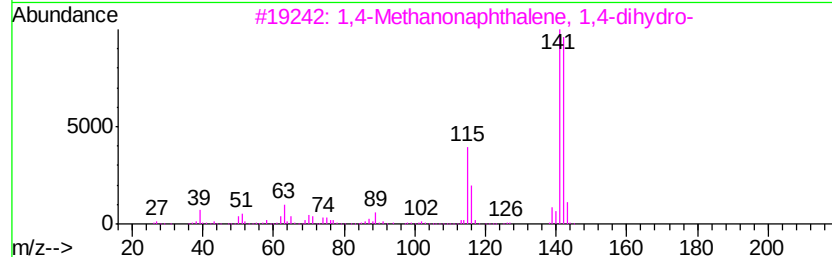
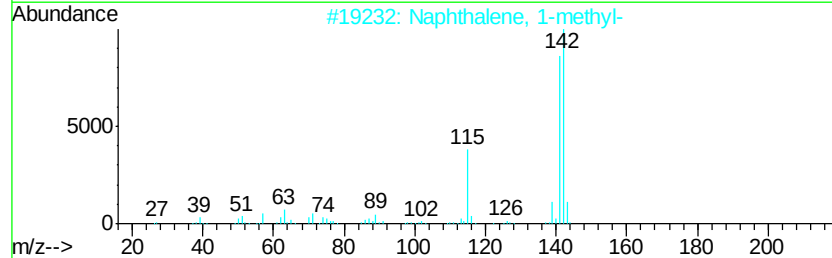
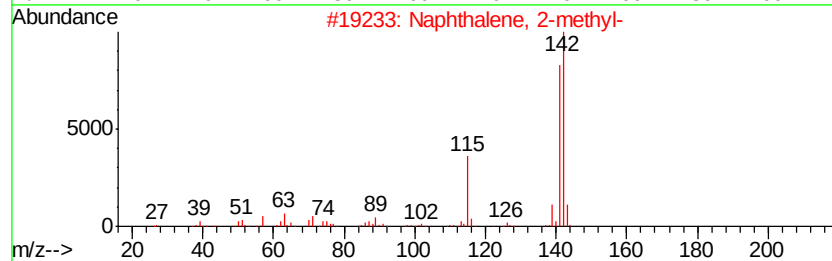
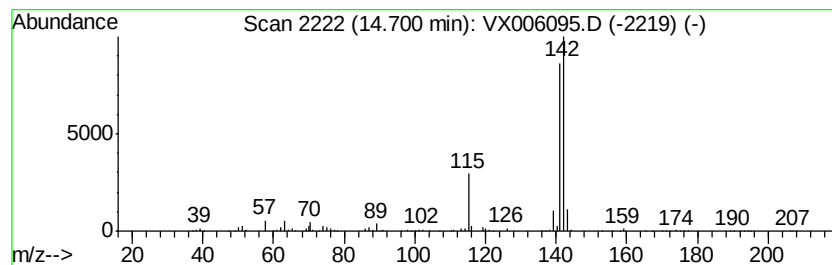
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	87.13 ug/l	1516380	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4		Benzocycloheptatriene	142	C11H10	000264-09-5	91
5		3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006095.D
Acq On : 19 Nov 2018 17:00
Operator : JC/MD
Sample : J5951-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

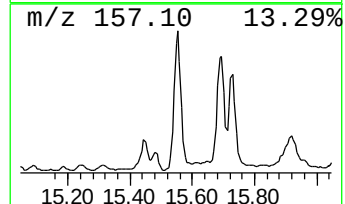
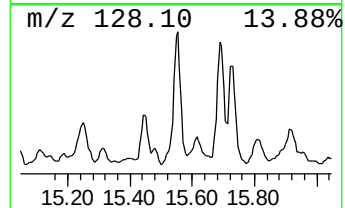
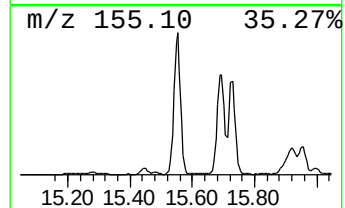
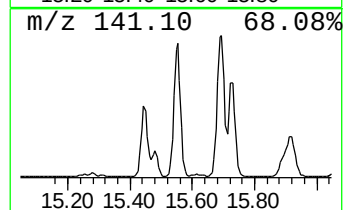
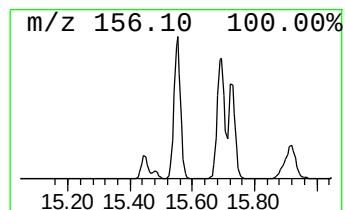
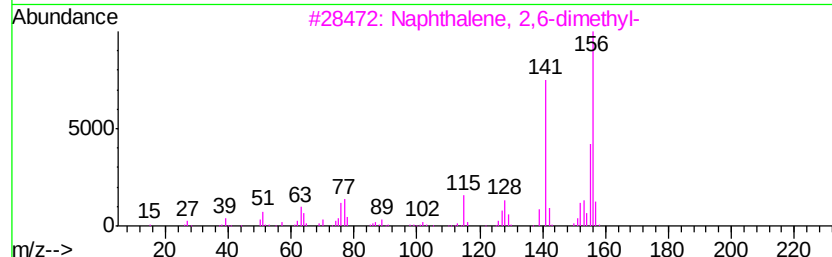
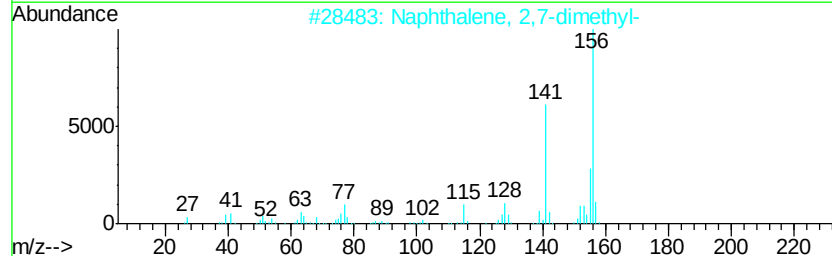
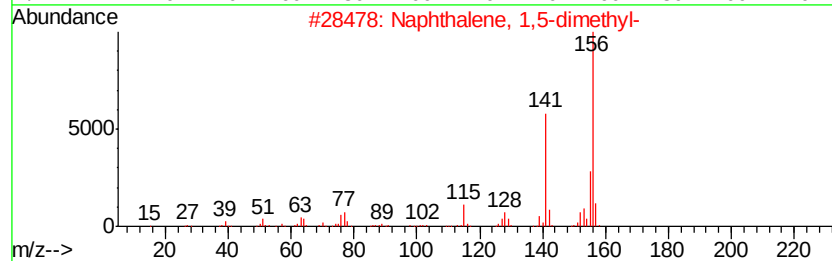
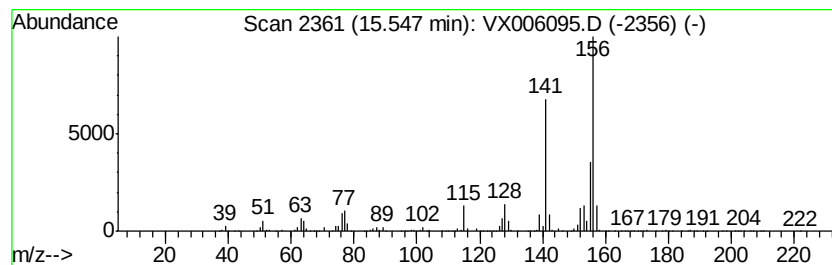
Instrument :
MSVOA_X
ClientSampleId :
FDSB-02(10-12)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Naphthalene, 1,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	57.27 ug/l	996726	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 1,5-dimethyl-	156 C12H12	000571-61-9 97
2		Naphthalene, 2,7-dimethyl-	156 C12H12	000582-16-1 97
3		Naphthalene, 2,6-dimethyl-	156 C12H12	000581-42-0 97
4		Naphthalene, 1,7-dimethyl-	156 C12H12	000575-37-1 97
5		Naphthalene, 1,6-dimethyl-	156 C12H12	000575-43-9 97



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006095.D
Acq On : 19 Nov 2018 17:00
Operator : JC/MD
Sample : J5951-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

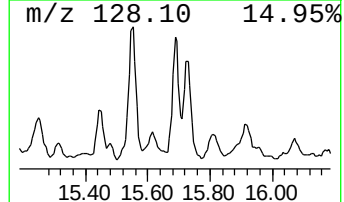
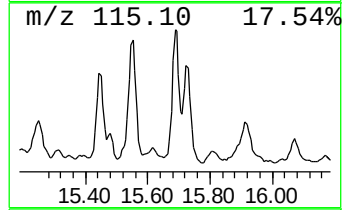
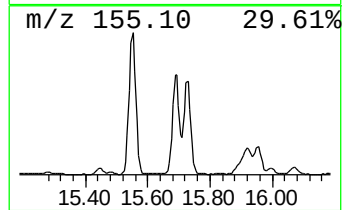
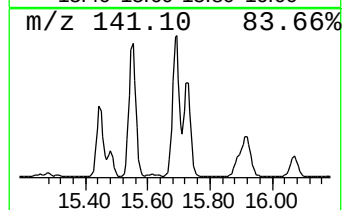
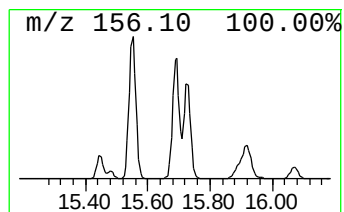
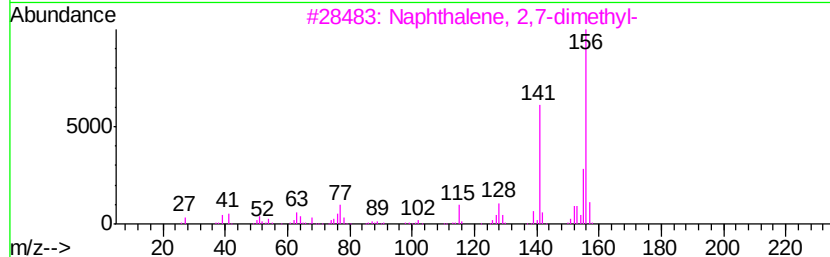
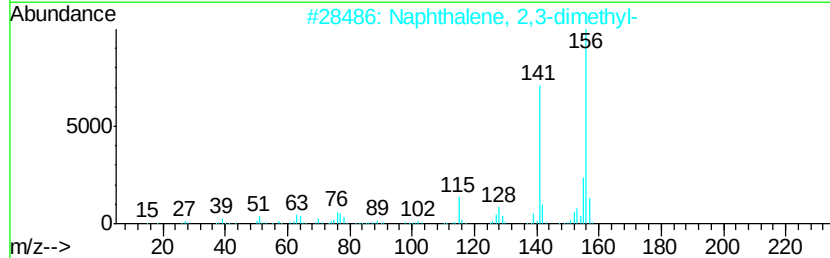
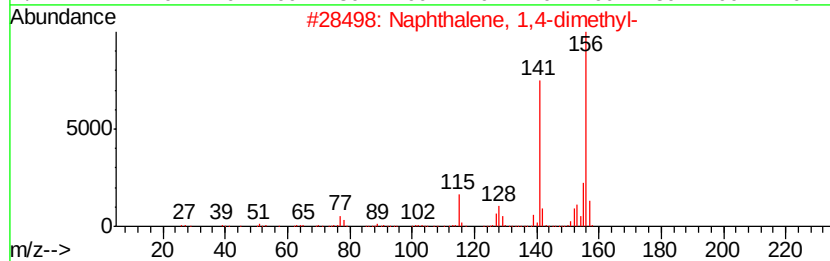
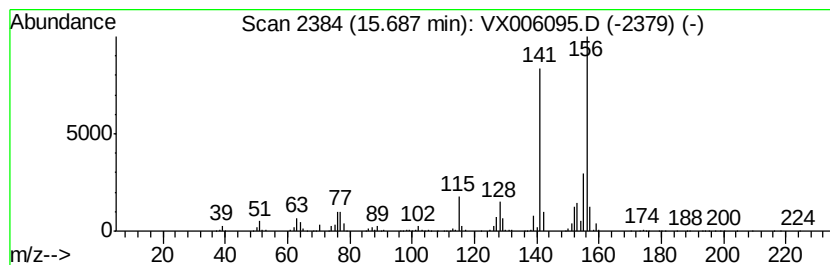
Instrument :
MSVOA_X
ClientSampleId :
FDSB-02(10-12)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Naphthalene, 1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.69	55.34 ug/l	963101	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
5	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	96



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006095.D
Acq On : 19 Nov 2018 17:00
Operator : JC/MD
Sample : J5951-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FDSB-02(10-12)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane, 1-et...	10.64	58.6	ug/l	547047	3	10.12	466957	50.0
Octane, 2,6-dimet...	10.83	97.8	ug/l	913156	3	10.12	466957	50.0
Cyclohexane, propyl-	10.91	86.4	ug/l	807269	3	10.12	466957	50.0
Cyclohexane, pentyl-	12.94	64.6	ug/l	1125000	4	12.08	870165	50.0
Naphthalene, deca...	13.47	69.2	ug/l	1204380	4	12.08	870165	50.0
Naphthalene, 1-me...	14.70	87.1	ug/l	1516380	4	12.08	870165	50.0
Naphthalene, 1,5-...	15.55	57.3	ug/l	996726	4	12.08	870165	50.0
Naphthalene, 1,4-...	15.69	55.3	ug/l	963101	4	12.08	870165	50.0