

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
 Data File : VX046457.D
 Acq On : 02 Jun 2025 20:39
 Operator : JC/MD
 Sample : Q2155-01
 Misc : 2.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 446

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\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046457.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	32	rBV	7466	7675	1.74%	0.169%
2	1.563	68	78	80	rBV6	5666	14305	3.25%	0.314%
3	1.630	80	89	90	rBV4	4210	10698	2.43%	0.235%
4	2.416	212	218	228	rBV	2551	6746	1.53%	0.148%
5	3.416	375	382	392	rVB3	2882	6673	1.51%	0.147%
6	5.385	695	705	720	rBV	48104	143319	32.53%	3.147%
7	5.544	720	731	746	rVB	75846	216293	49.09%	4.749%
8	5.952	788	798	815	rBV	57705	154489	35.06%	3.392%
9	6.385	860	869	872	rBV4	1648	4713	1.07%	0.103%
10	6.757	920	930	945	rBV	129222	320627	72.77%	7.040%
11	8.647	1233	1240	1251	rBV	276134	440594	100.00%	9.675%
12	9.543	1382	1387	1397	rBV4	1988	4416	1.00%	0.097%
13	10.055	1465	1471	1493	rVB	271224	393103	89.22%	8.632%
14	10.866	1598	1604	1614	rBV3	2832	5286	1.20%	0.116%
15	11.079	1634	1639	1648	rBV	226704	297821	67.60%	6.540%
16	11.482	1701	1705	1715	rVB5	3314	8364	1.90%	0.184%
17	11.969	1781	1785	1789	rVV2	18177	23340	5.30%	0.513%
18	12.018	1789	1793	1805	rVB	278044	369594	83.89%	8.116%
19	12.811	1919	1923	1927	rBV5	4489	6732	1.53%	0.148%
20	12.859	1927	1931	1935	rVV5	3416	5386	1.22%	0.118%
21	12.920	1937	1941	1945	rVV7	2439	4446	1.01%	0.098%
22	12.981	1945	1951	1954	rVV6	3248	6457	1.47%	0.142%
23	13.036	1956	1960	1964	rVB7	2607	4886	1.11%	0.107%
24	13.164	1975	1981	1985	rBV9	3257	6943	1.58%	0.152%
25	13.292	1998	2002	2006	rVB4	12411	17950	4.07%	0.394%
26	13.414	2016	2022	2033	rBV4	13190	42328	9.61%	0.929%
27	13.499	2033	2036	2040	rBV5	4518	7413	1.68%	0.163%
28	13.585	2046	2050	2054	rBV6	8922	16423	3.73%	0.361%
29	13.670	2061	2064	2069	rBV6	6958	14579	3.31%	0.320%
30	13.749	2071	2077	2082	rBV6	8180	20252	4.60%	0.445%
31	13.798	2082	2085	2088	rBV6	11857	14370	3.26%	0.316%
32	13.847	2089	2093	2099	rVB6	20002	34044	7.73%	0.748%
33	13.926	2099	2106	2111	rBV7	18759	46687	10.60%	1.025%
34	14.005	2117	2119	2121	rBV3	7212	8343	1.89%	0.183%
35	14.066	2126	2129	2132	rVB5	13186	17184	3.90%	0.377%
36	14.164	2142	2145	2148	rBV4	13685	19440	4.41%	0.427%

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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Title : SW846 8260

37	14.225	2149	2155	2160	rVV4	55363	107992	24.51%	2.371%
38	14.323	2168	2171	2174	rBV4	13824	21707	4.93%	0.477%
39	14.481	2193	2197	2204	rBV4	66014	125164	28.41%	2.748%
40	14.548	2205	2208	2210	rBV3	24291	30995	7.03%	0.681%
41	14.615	2215	2219	2225	rBV	135271	218464	49.58%	4.797%
42	14.670	2225	2228	2232	rVB2	94144	109483	24.85%	2.404%
43	14.755	2239	2242	2244	rBV4	44111	48249	10.95%	1.059%
44	14.786	2244	2247	2250	rVV4	32702	44618	10.13%	0.980%
45	14.847	2254	2257	2261	rVB2	73255	92624	21.02%	2.034%
46	15.036	2284	2288	2293	rBV5	78011	129499	29.39%	2.844%
47	15.091	2293	2297	2301	rBV5	42728	87305	19.82%	1.917%
48	15.182	2307	2312	2314	rBV2	78503	122573	27.82%	2.691%
49	15.377	2340	2344	2347	rBV2	117105	164248	37.28%	3.607%
50	15.414	2347	2350	2354	rVV	97149	124562	28.27%	2.735%
51	15.487	2358	2362	2367	rBV5	45190	111208	25.24%	2.442%
52	15.737	2400	2403	2407	rBV3	56969	86889	19.72%	1.908%
53	15.780	2407	2410	2414	rVB2	59296	76287	17.31%	1.675%
54	16.084	2456	2460	2466	rBV3	70906	130316	29.58%	2.862%

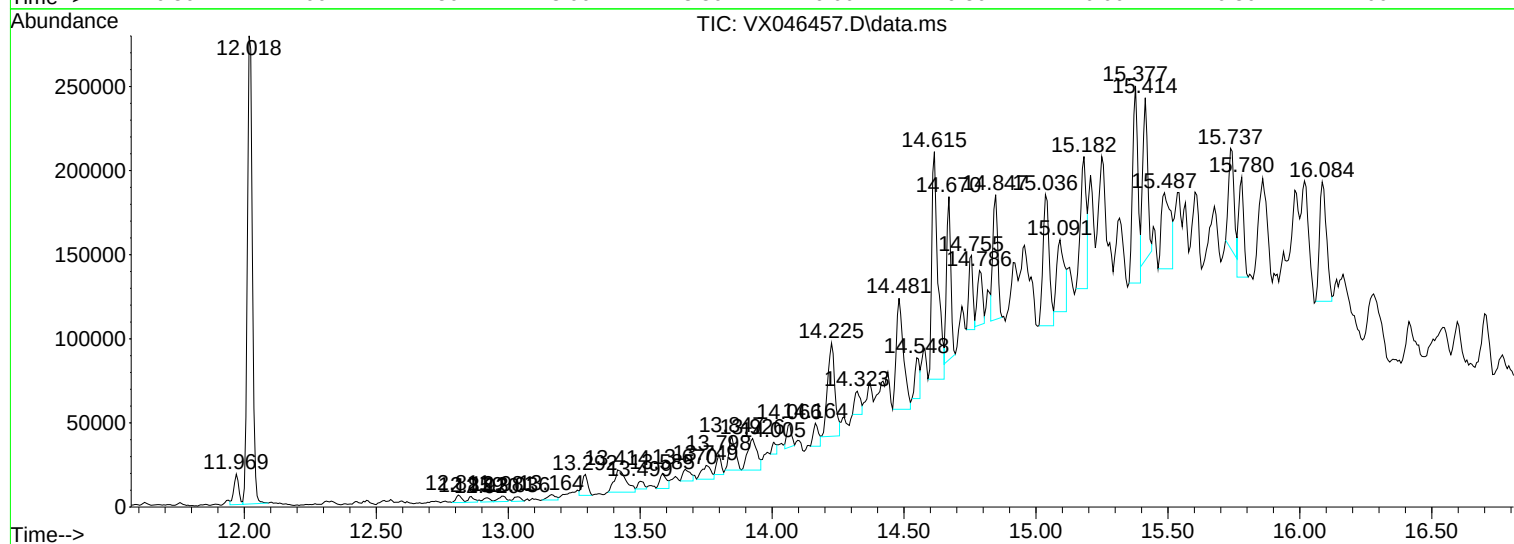
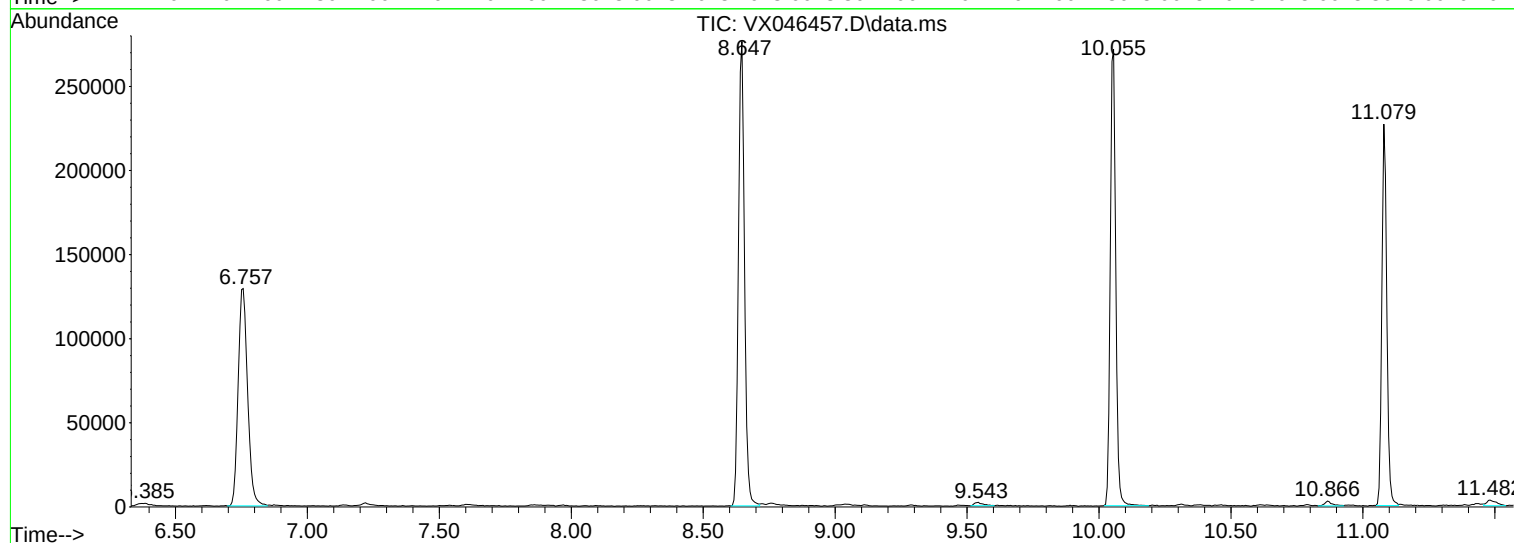
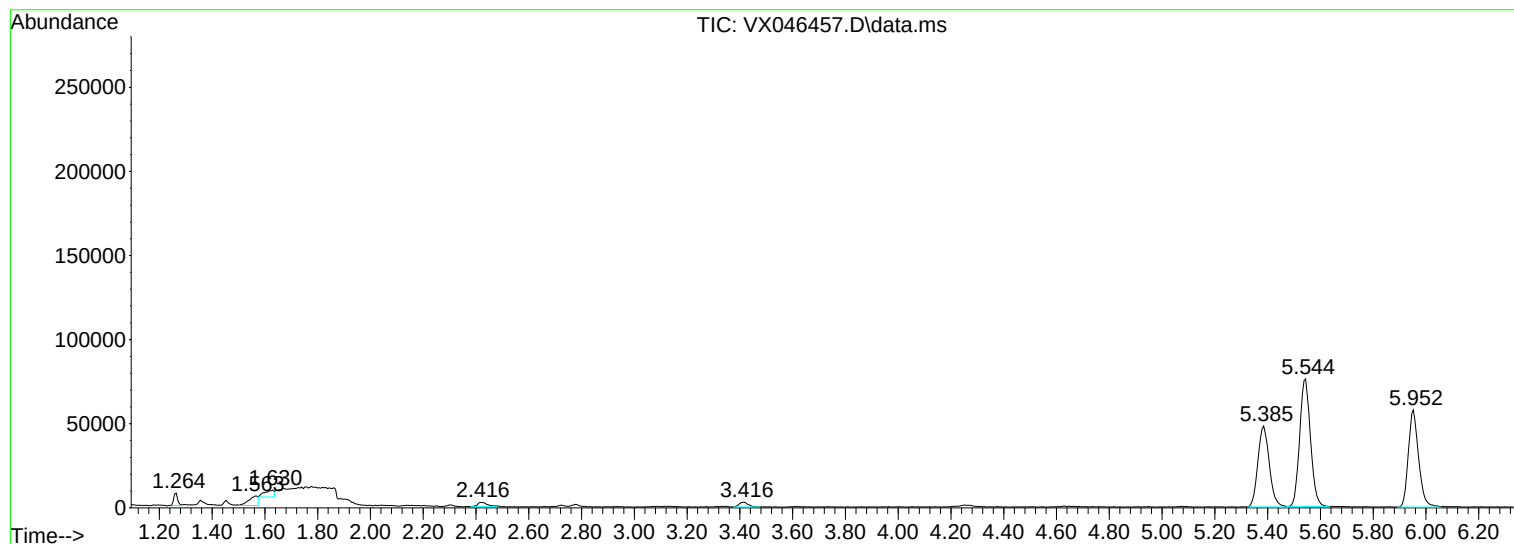
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TIC Integration Parameters: LSCINT.P



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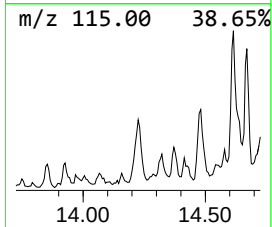
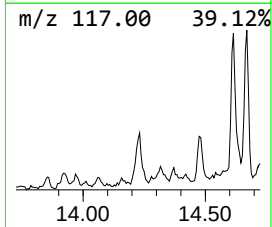
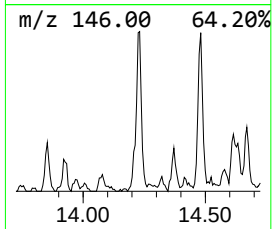
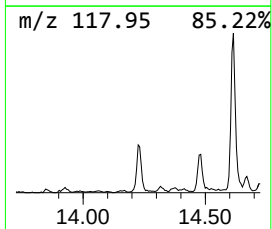
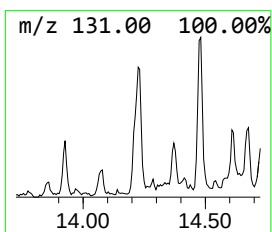
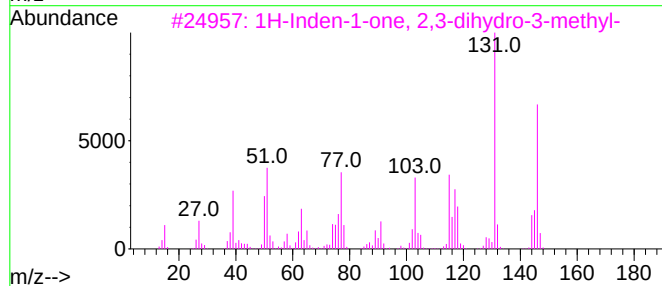
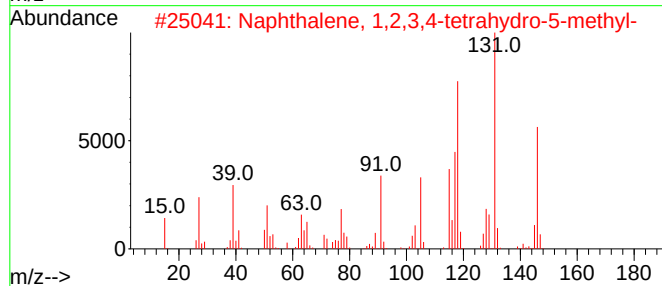
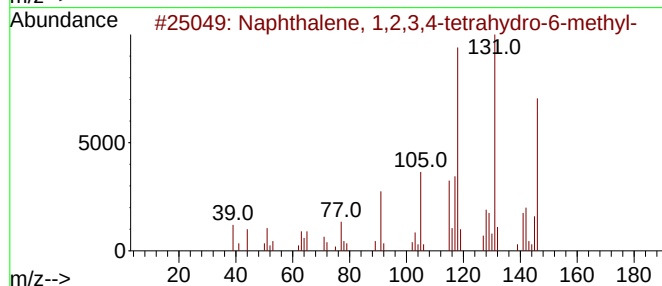
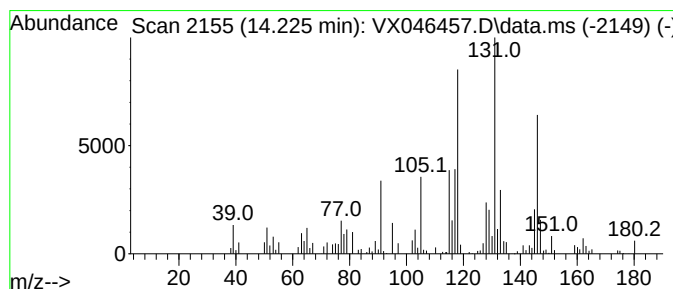
Instrument :
MSVOA_X
ClientSampleId :
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Quant Title :

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

Peak Number 1 Naphthalene, 1,2,3,4-tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.225	14.61 ug/l	107992	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
3	1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	53
4	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	52
5	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	52



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Misc : 2.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

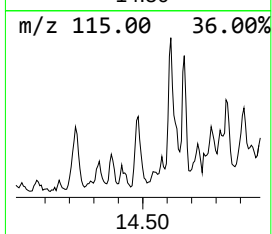
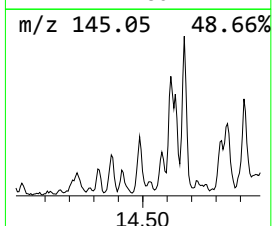
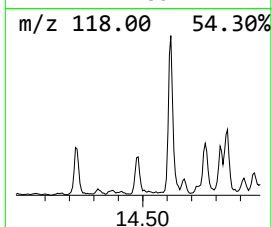
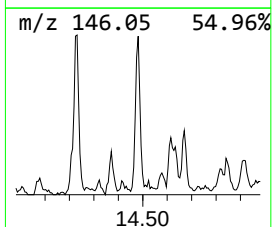
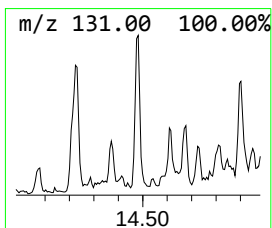
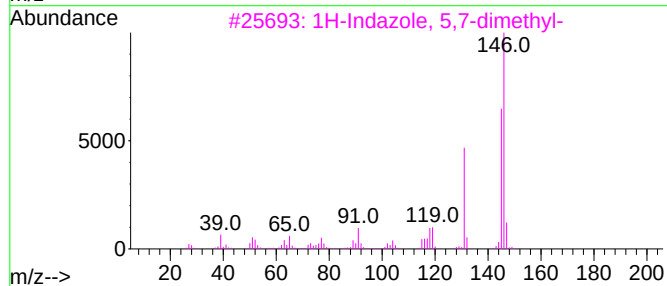
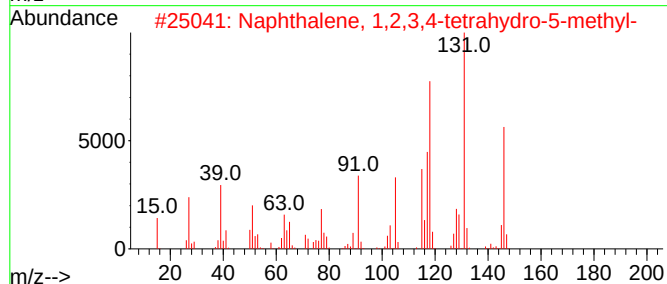
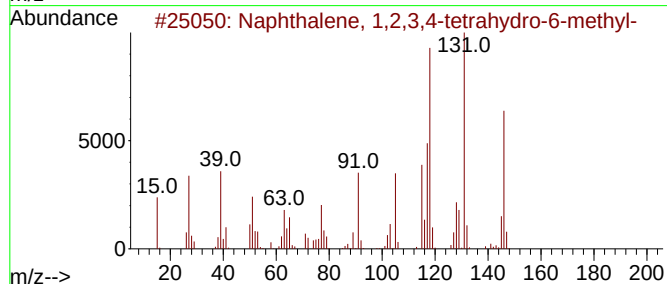
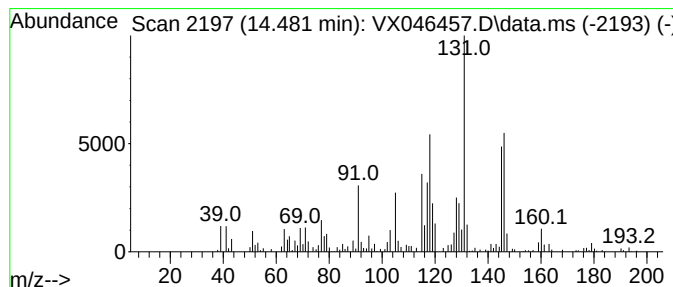
Instrument :
MSVOA_X
ClientSampleId :
446

Quant Title :

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

Peak Number 2 Naphthalene, 1,2,3,4-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.481	16.93 ug/l	125164	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	001680-51-9	70
2	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	002809-64-5	70
3	1H-Indazole, 5,7-dimethyl-		146	C9H10N2	043067-41-0	68
4	1H-Benzimidazole, 5,6-dimethyl-		146	C9H10N2	000582-60-5	64
5	2-Propyn-1-ol, 3-(4-methylphenyl)-		146	C10H10O	016017-24-6	58



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Misc : 2.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

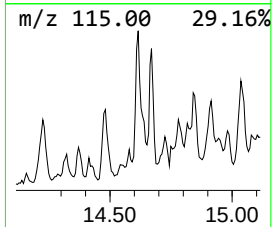
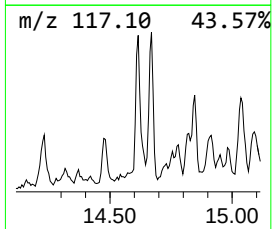
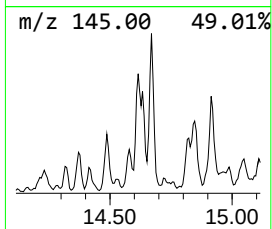
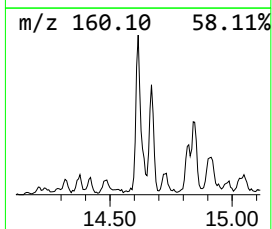
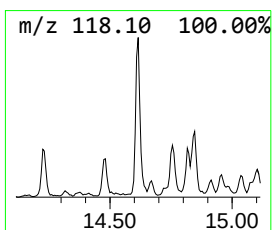
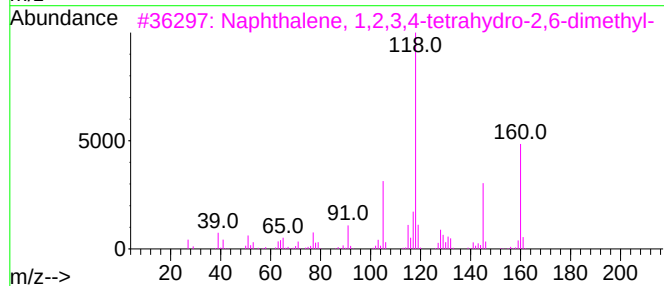
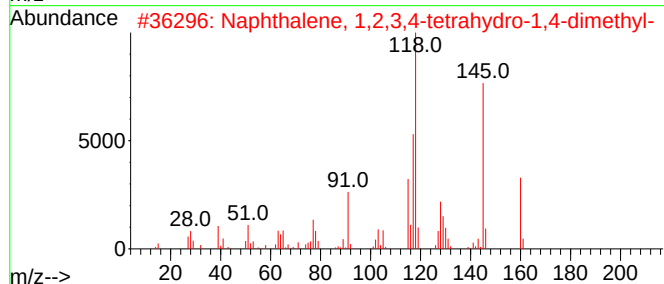
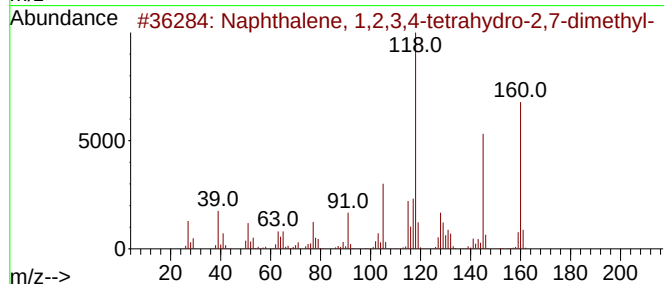
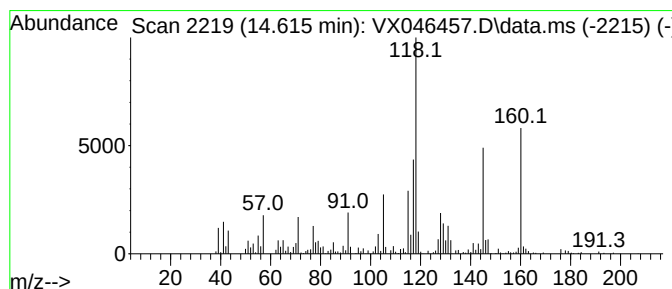
Instrument :
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Quant Title :

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.615	29.55 ug/l	218464	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	91
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	91
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	83
4	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	58
5	Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	58



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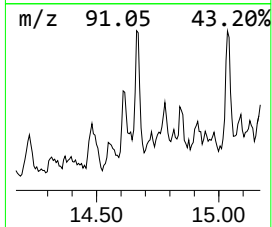
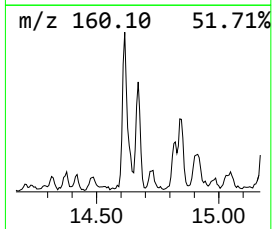
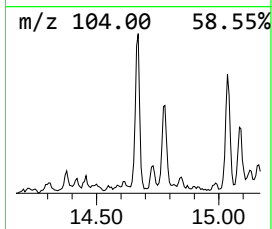
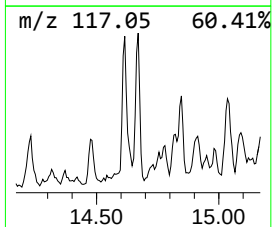
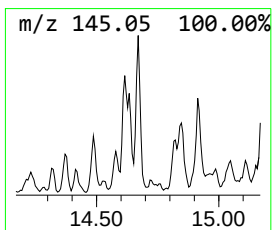
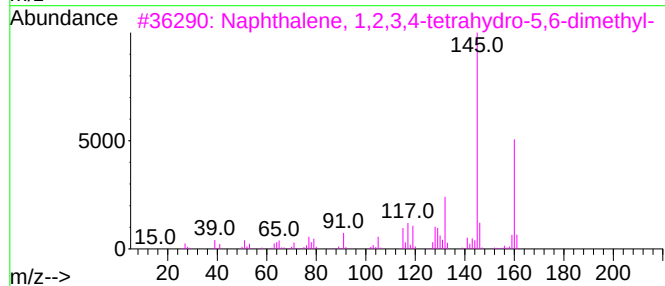
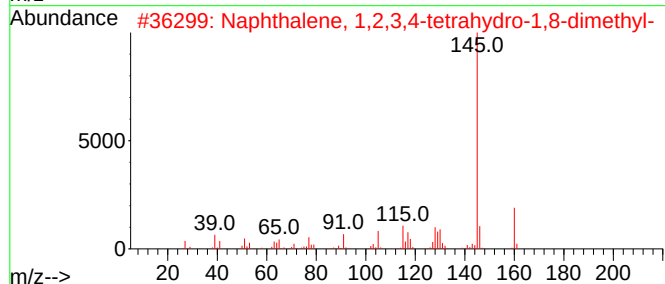
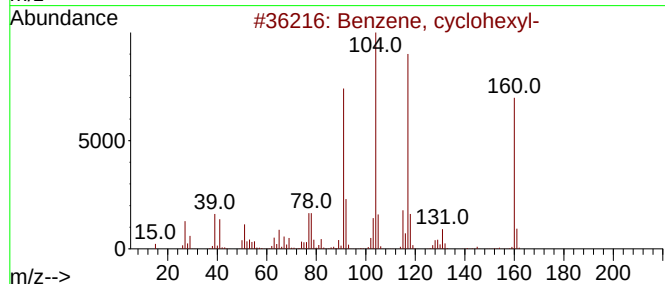
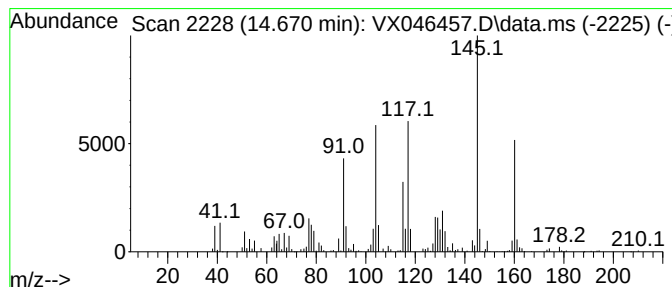
Instrument :
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Quant Title :

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzene, cyclohexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.670	14.81 ug/l	109483	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclohexyl-	160	C12H16	000827-52-1	86
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	025419-33-4	64
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	60
4	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	58
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	58



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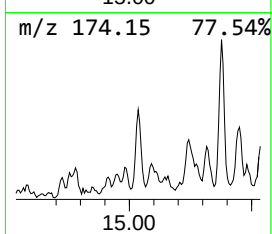
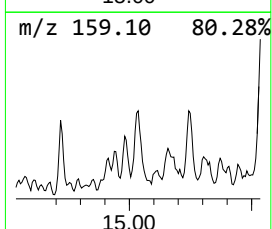
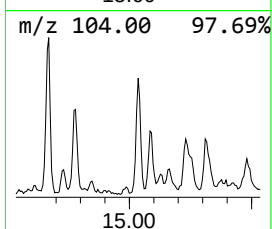
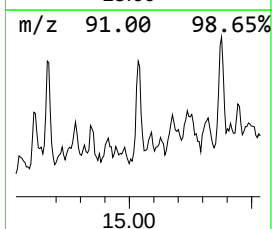
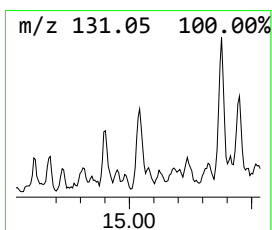
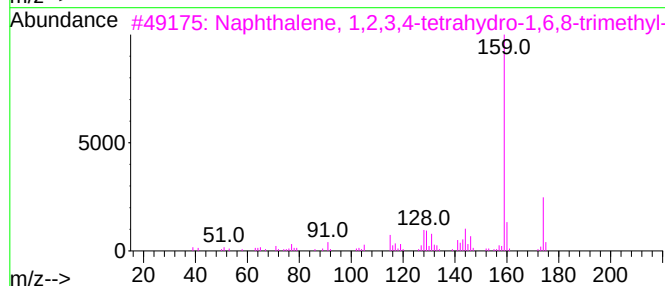
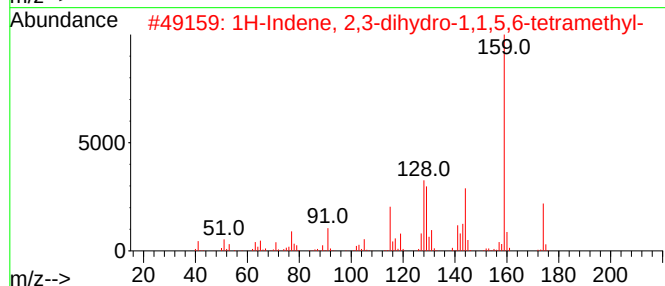
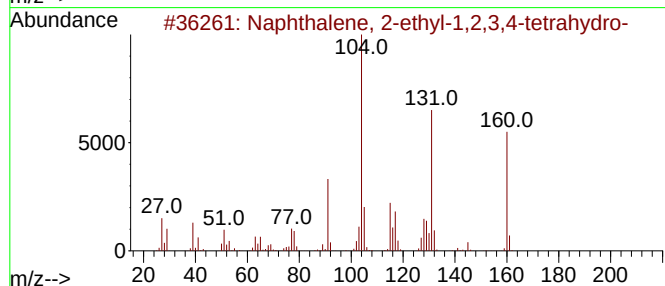
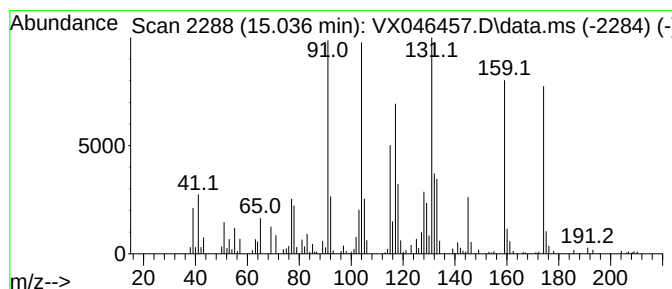
Instrument :
MSVOA_X
ClientSampleId :
446

Quant Title :

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

Peak Number 5 Naphthalene, 2-ethyl-1,2,3,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.036	17.52 ug/l	129499	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	50
2	1H-Indene, 2,3-dihydro-1,1,5,6-t...	174	C13H18	000942-43-8	46
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	46
4	4-Phenylcyclohexanone	174	C12H14O	004894-75-1	46
5	1-tert-Butyl-2-(prop-2-en-1-yl)b...	174	C13H18	1000486-84-0	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
Data File : VX046457.D
Acq On : 02 Jun 2025 20:39
Operator : JC/MD
Sample : Q2155-01
Misc : 2.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
446

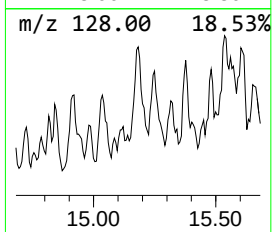
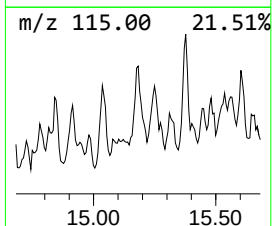
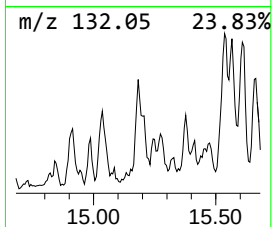
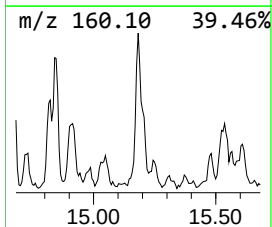
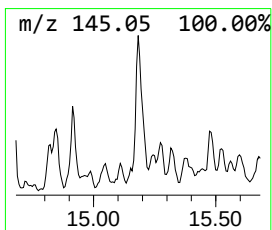
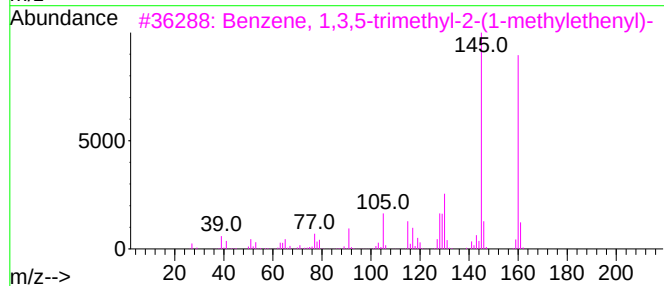
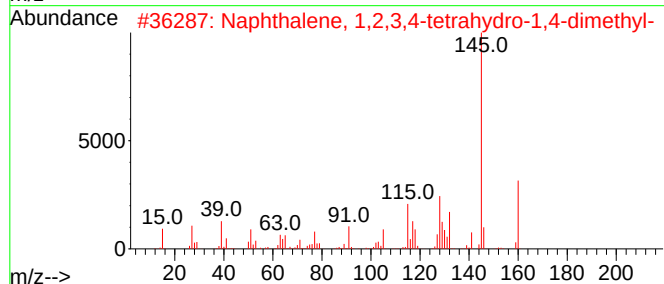
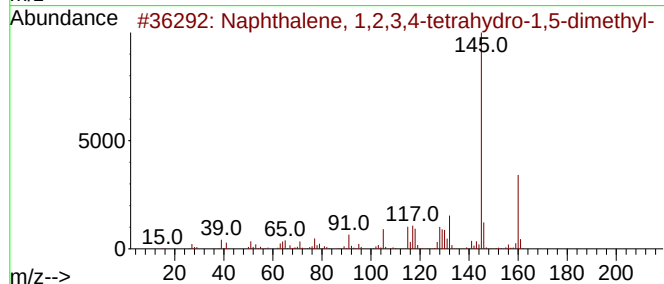
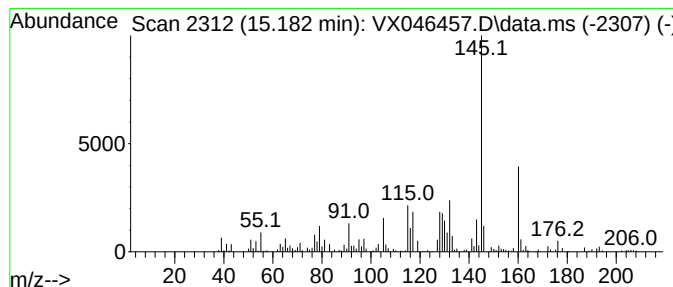
Quant Title :

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

Peak Number 6 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	16.58 ug/l	122573	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	90
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	83
3			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	76
4			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	76
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	025419-33-4	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
Data File : VX046457.D
Acq On : 02 Jun 2025 20:39
Operator : JC/MD
Sample : Q2155-01
Misc : 2.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
446

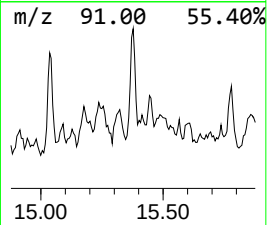
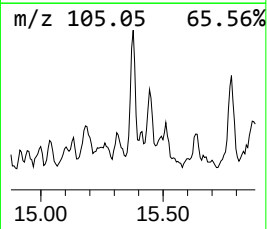
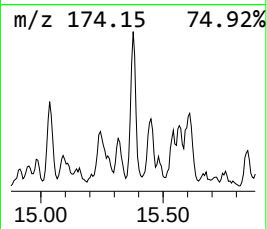
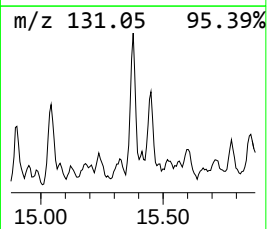
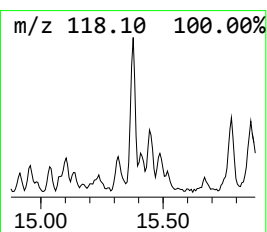
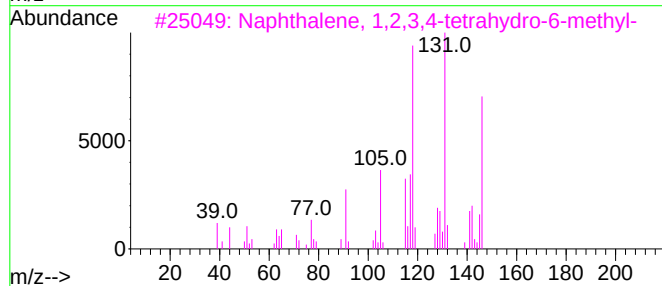
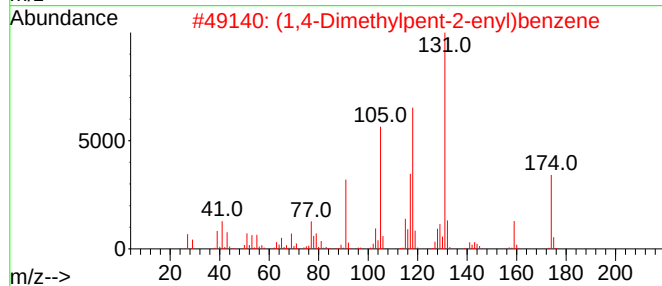
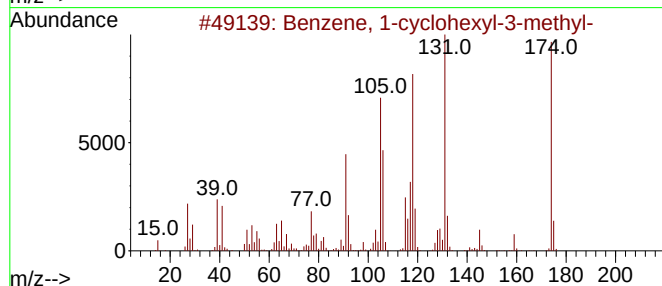
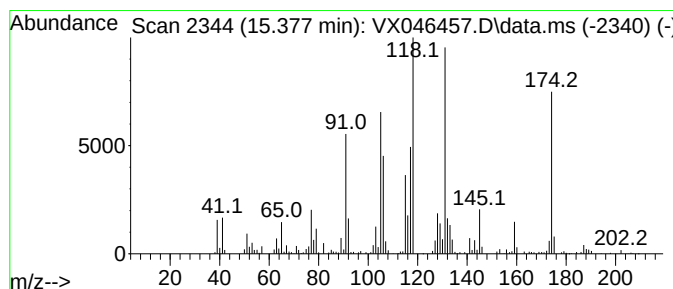
Quant Title :

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

Peak Number 7 Benzene, 1-cyclohexyl-3-met... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.377	22.22 ug/l	164248	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	87
2			(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	46
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	46
4			1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	38
5			Spiro(cyclohexane-1,2'-(1,3-dith...	174	C8H14S2	000177-16-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
Data File : VX046457.D
Acq On : 02 Jun 2025 20:39
Operator : JC/MD
Sample : Q2155-01
Misc : 2.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
446

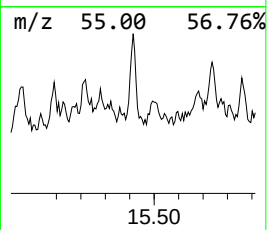
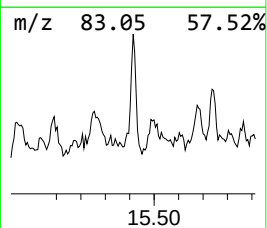
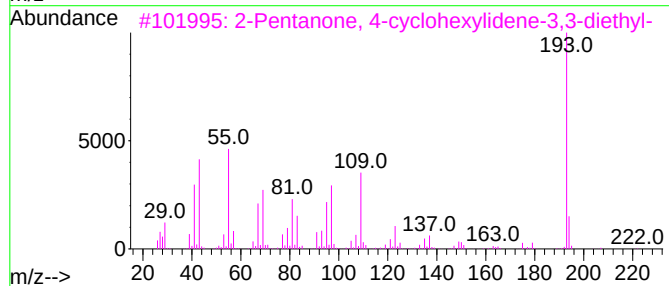
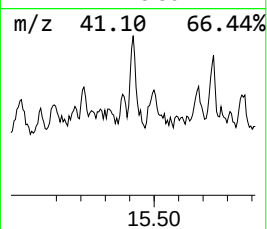
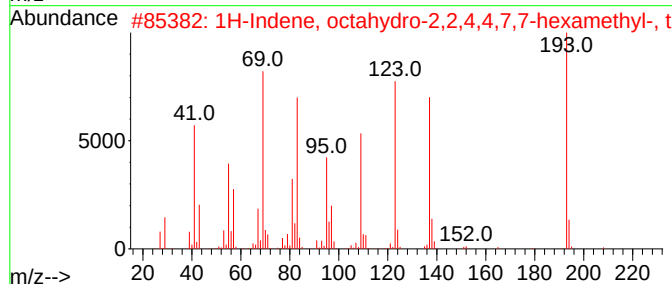
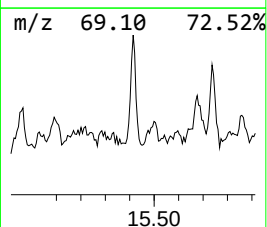
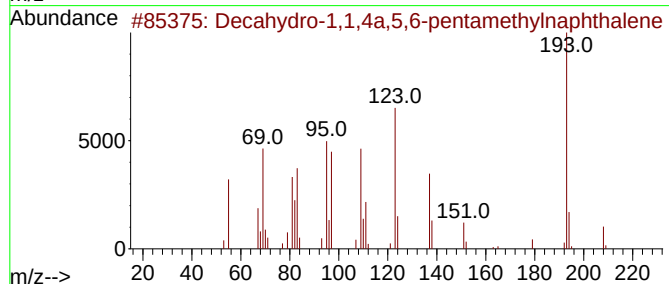
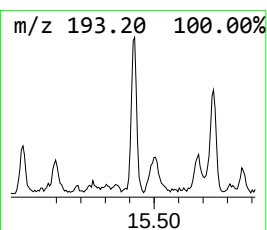
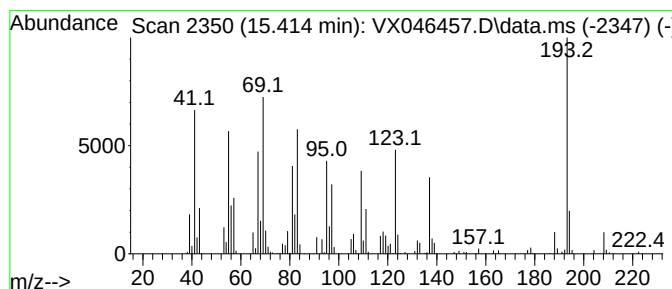
Quant Title :

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

Peak Number 8 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	16.85 ug/l	124562	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	90
2		1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	47
3		2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	40
4		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
5		Acridine, 9-methyl-	193	C14H11N	000611-64-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
Data File : VX046457.D
Acq On : 02 Jun 2025 20:39
Operator : JC/MD
Sample : Q2155-01
Misc : 2.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
446

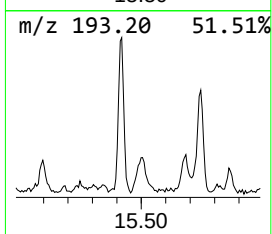
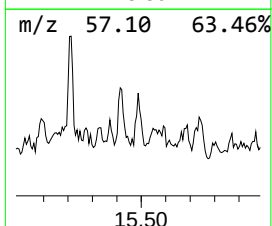
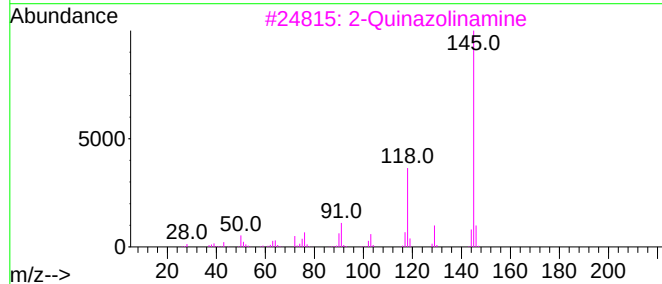
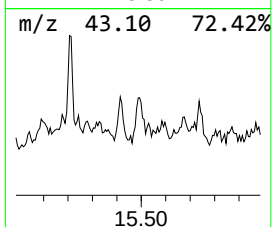
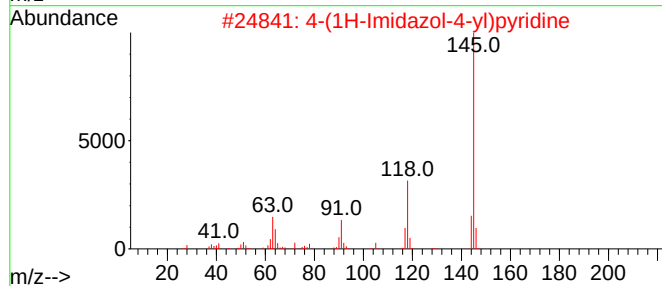
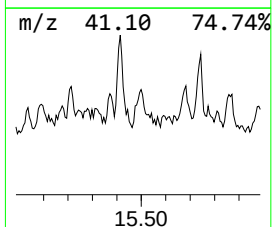
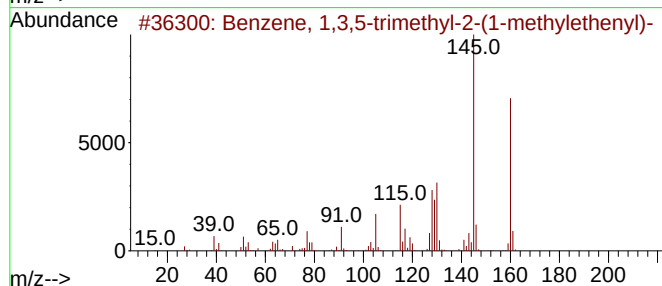
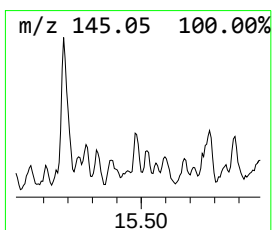
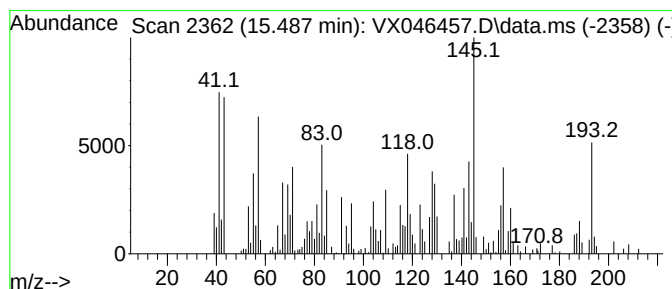
Quant Title :

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

Peak Number 9 unknown15.487 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.487	15.04 ug/l	111208	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	27
2			4-(1H-Imidazol-4-yl)pyridine	145	C8H7N3	051746-87-3	25
3			2-Quinazolinamine	145	C8H7N3	001687-51-0	22
4			2-Ethyl-3-methyl-1H-pyrrolo[2,3-...	160	C10H12N2	1000436-85-1	14
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	025419-33-4	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
Data File : VX046457.D
Acq On : 02 Jun 2025 20:39
Operator : JC/MD
Sample : Q2155-01
Misc : 2.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

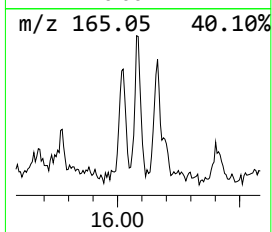
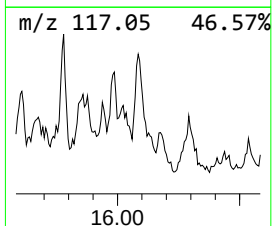
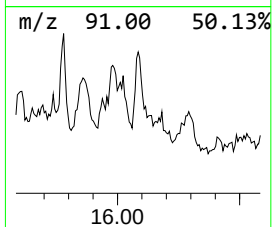
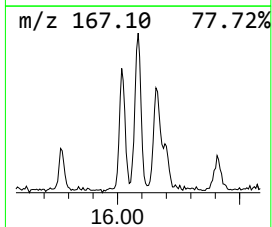
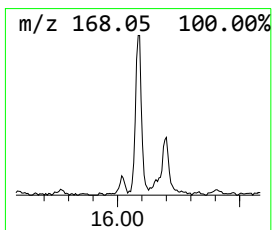
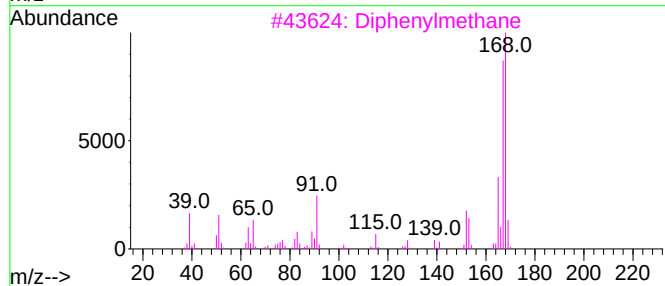
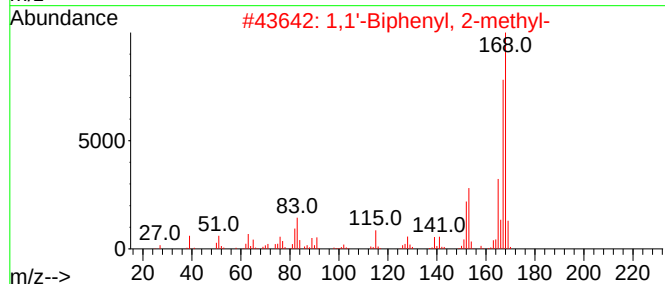
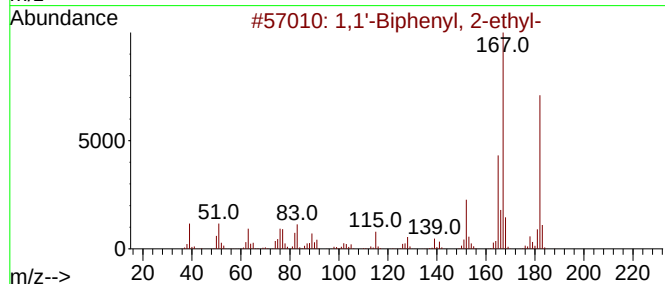
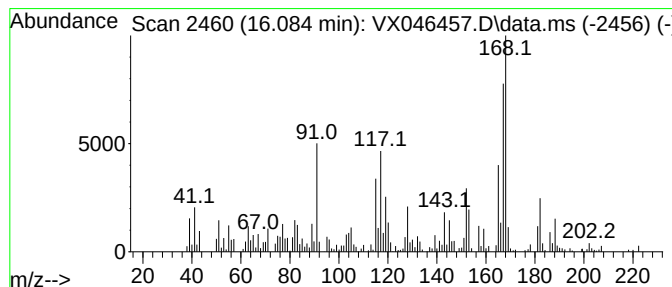
Instrument :
MSVOA_X
ClientSampleId :
446

Quant Title :

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

Peak Number 10 1,1'-Biphenyl, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.084	17.63 ug/l	130316	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2-ethyl-	182	C14H14	001812-51-7	90
2	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	87
3	Diphenylmethane	168	C13H12	000101-81-5	78
4	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	78
5	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
Data File : VX046457.D
Acq On : 02 Jun 2025 20:39
Operator : JC/MD
Sample : Q2155-01
Misc : 2.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
446

Quant Title :

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Naphthalene, 1,...	14.225	14.6	ug/l	107992	4	12.024	369594	50.0
Naphthalene, 1,...	14.481	16.9	ug/l	125164	4	12.024	369594	50.0
Naphthalene, 1,...	14.615	29.6	ug/l	218464	4	12.024	369594	50.0
Benzene, cycloh...	14.670	14.8	ug/l	109483	4	12.024	369594	50.0
Naphthalene, 2-...	15.036	17.5	ug/l	129499	4	12.024	369594	50.0
Naphthalene, 1,...	15.182	16.6	ug/l	122573	4	12.024	369594	50.0
Benzene, 1-cycl...	15.377	22.2	ug/l	164248	4	12.024	369594	50.0
Decahydro-1,1,4...	15.414	16.9	ug/l	124562	4	12.024	369594	50.0
unknown15.487	15.487	15.0	ug/l	111208	4	12.024	369594	50.0
1,1'-Biphenyl, ...	16.084	17.6	ug/l	130316	4	12.024	369594	50.0