

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071922\
 Data File : VD073862.D
 Acq On : 19 Jul 2022 15:40
 Operator : VA/SY
 Sample : N3688-03
 Misc : 5.02G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 VNJ-240

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_D\Method\82D071822S.M
 Title : SW846 8260

Signal : TIC: VD073862.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.221	45	51	53	rBV3	6324	12494	2.04%	0.289%
2	2.315	64	67	69	rBV3	7377	8833	1.44%	0.204%
3	2.491	93	97	101	rBV3	5130	7393	1.20%	0.171%
4	2.632	117	121	127	rBV7	4801	10743	1.75%	0.249%
5	4.956	506	516	529	rVB4	27987	91097	14.85%	2.107%
6	5.985	683	691	701	rVB8	8766	25476	4.15%	0.589%
7	7.197	888	897	902	rBV4	6172	16033	2.61%	0.371%
8	7.909	1008	1018	1023	rBV	100179	236617	38.57%	5.474%
9	7.967	1023	1028	1037	rVB	131997	284366	46.35%	6.578%
10	8.320	1079	1088	1101	rVB	83896	182098	29.68%	4.213%
11	8.856	1169	1179	1189	rBV	222786	464659	75.73%	10.749%
12	10.332	1422	1430	1438	rBV	344700	613538	100.00%	14.193%
13	10.720	1488	1496	1501	rBV5	4030	8368	1.36%	0.194%
14	11.632	1644	1651	1662	rBV	293686	520101	84.77%	12.032%
15	12.473	1787	1794	1799	rVB6	4905	9314	1.52%	0.215%
16	12.620	1811	1819	1826	rBV	220427	358234	58.39%	8.287%
17	12.802	1843	1850	1853	rBV5	3704	6172	1.01%	0.143%
18	12.938	1870	1873	1878	rVB5	6839	10022	1.63%	0.232%
19	13.138	1901	1907	1912	rBV4	17258	30580	4.98%	0.707%
20	13.402	1945	1952	1953	rBV6	6067	10047	1.64%	0.232%
21	13.426	1954	1956	1961	rVV6	7235	12864	2.10%	0.298%
22	13.479	1963	1965	1970	rVV5	4328	8116	1.32%	0.188%
23	13.561	1972	1979	1987	rVV	233691	389458	63.48%	9.010%
24	13.773	2011	2015	2018	rBV5	4572	7409	1.21%	0.171%
25	13.879	2027	2033	2038	rBV6	17963	36514	5.95%	0.845%
26	13.985	2046	2051	2056	rBV8	4765	9467	1.54%	0.219%
27	14.055	2059	2063	2064	rVV4	7310	7971	1.30%	0.184%
28	14.091	2067	2069	2074	rVB5	10123	12300	2.00%	0.285%
29	14.208	2086	2089	2093	rBV5	8945	14284	2.33%	0.330%
30	14.261	2095	2098	2105	rVB9	17426	32549	5.31%	0.753%
31	14.326	2106	2109	2114	rBV7	9340	16887	2.75%	0.391%
32	14.385	2115	2119	2121	rBV4	26970	38207	6.23%	0.884%
33	14.526	2139	2143	2146	rBV	16412	22114	3.60%	0.512%
34	14.602	2152	2156	2160	rVB6	18626	34353	5.60%	0.795%
35	14.738	2177	2179	2185	rVB6	10792	15824	2.58%	0.366%
36	14.814	2185	2192	2196	rBV8	24911	68133	11.10%	1.576%

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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

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Title : SW846 8260

37	14.861	2196	2200	2205	rVB6	32872	60241	9.82%	1.394%
38	14.926	2205	2211	2215	rBV9	13665	33512	5.46%	0.775%
39	14.985	2215	2221	2222	rBV5	32861	56085	9.14%	1.297%
40	15.008	2222	2225	2230	rVB4	48868	84669	13.80%	1.959%
41	15.079	2231	2237	2241	rBV4	48958	89018	14.51%	2.059%
42	15.138	2243	2247	2249	rBV4	37066	56317	9.18%	1.303%
43	15.426	2290	2296	2303	rBV7	66744	218347	35.59%	5.051%
44	15.885	2371	2374	2380	rBV6	47159	91892	14.98%	2.126%

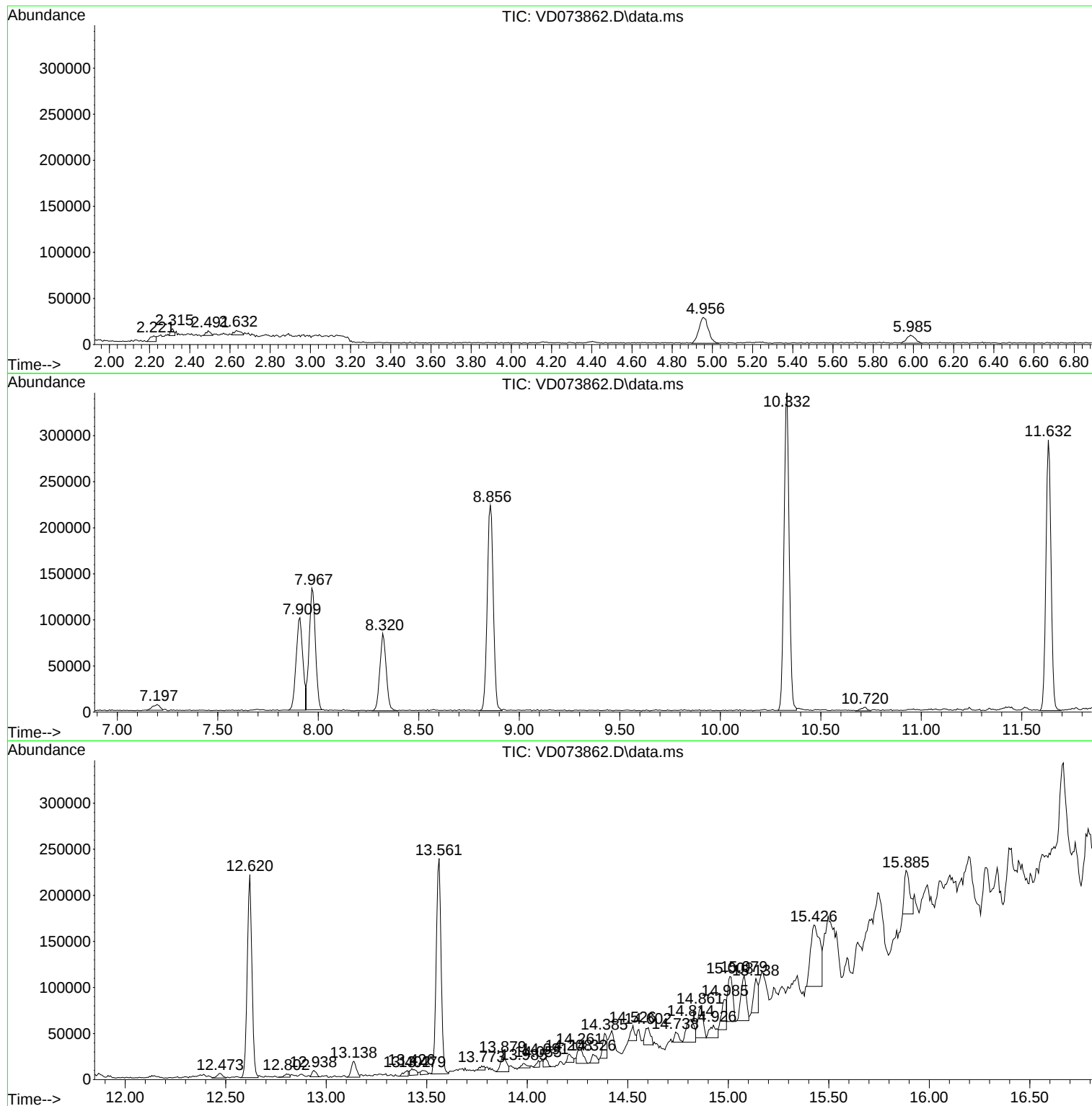
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071922\
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Instrument :
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ClientSampleId :
VNJ-240

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.M
Quant Title : SW846 8260

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



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Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
VNJ-240

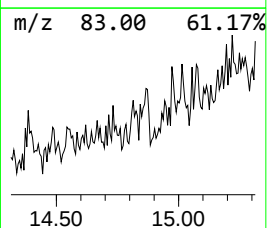
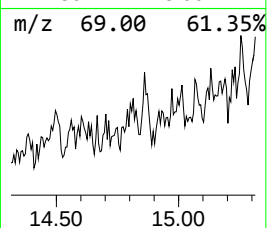
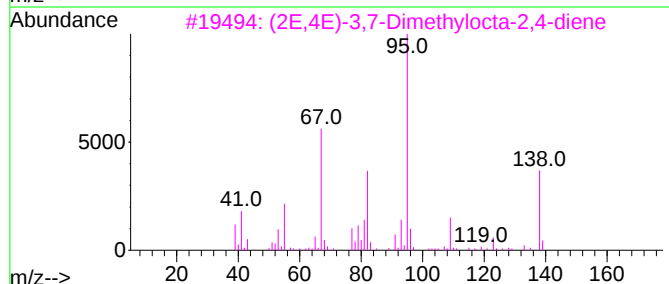
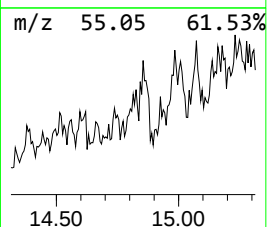
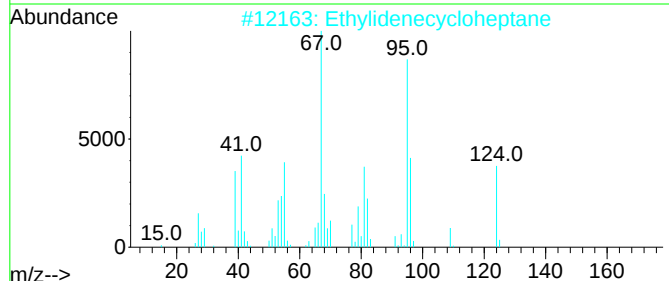
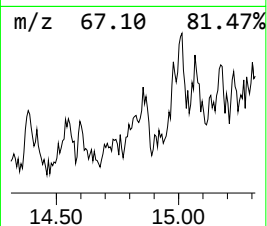
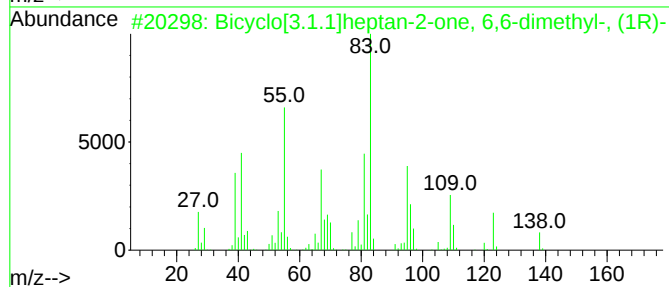
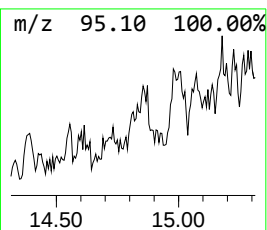
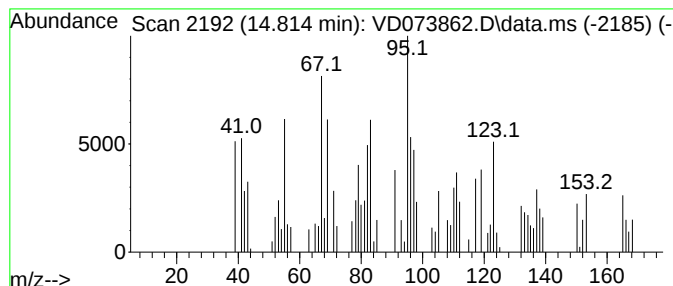
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.M
Quant Title : SW846 8260

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

Peak Number 2 Bicyclo[3.1.1]heptan-2-one,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.814	8.75 ug/l	68133	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-2-one, 6,6-...	138	C9H14O	038651-65-9	62
2			Ethylidenecycloheptane	124	C9H16	010494-87-8	45
3			(2E,4E)-3,7-Dimethylocta-2,4-diene	138	C10H18	006874-39-1	41
4			Cyclopropane, tetramethylmethylene-	110	C8H14	054376-39-5	38
5			2-Propanone, 1-(1-cyclohexen-1-yl)-	138	C9H14O	000768-50-3	38



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Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

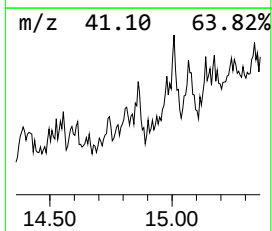
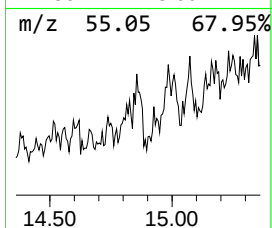
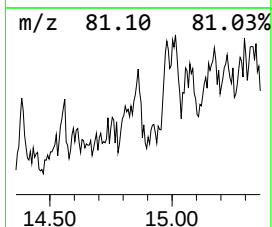
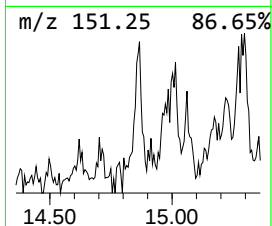
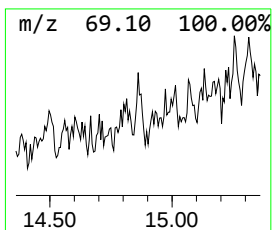
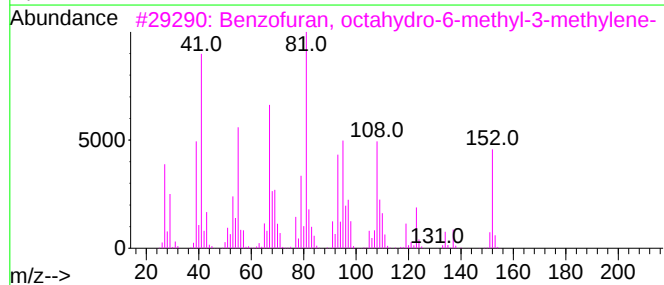
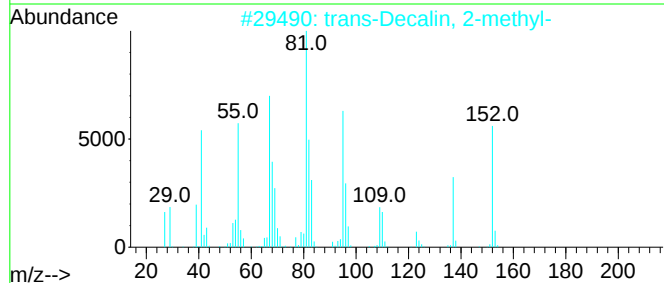
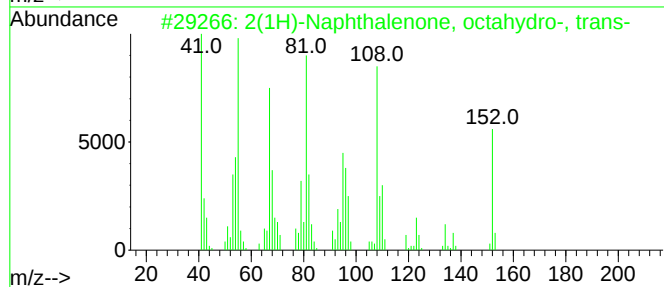
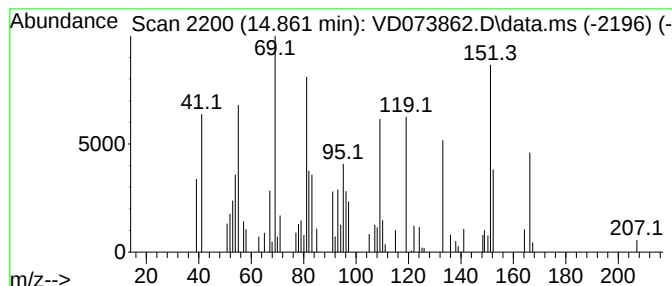
Instrument :
MSVOA_D
ClientSampleId :
VNJ-240

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown14.861 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.861	7.73 ug/l	60241	1,4-Dichlorobenzene-d4	13.561	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-,...	152	C10H16O	016021-08-2	30
2	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	25
3	Benzofuran, octahydro-6-methyl-3...	152	C10H16O	077954-13-3	25
4	3-(2-Hydroxycyclohexyl)-furan	166	C10H14O2	118959-04-9	20
5	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	029606-79-9	20



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071922\
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Acq On : 19 Jul 2022 15:40
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Sample : N3688-03
Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
VNJ-240

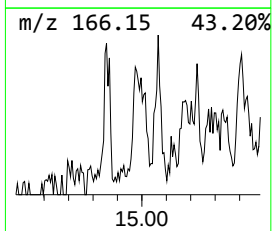
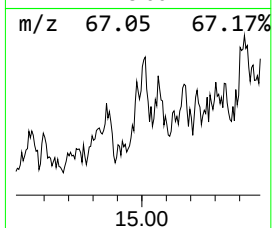
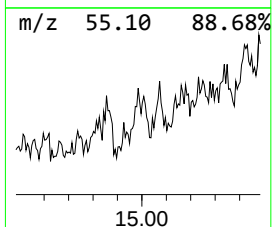
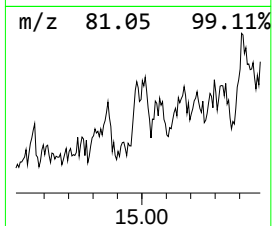
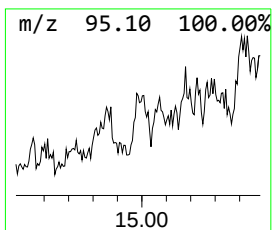
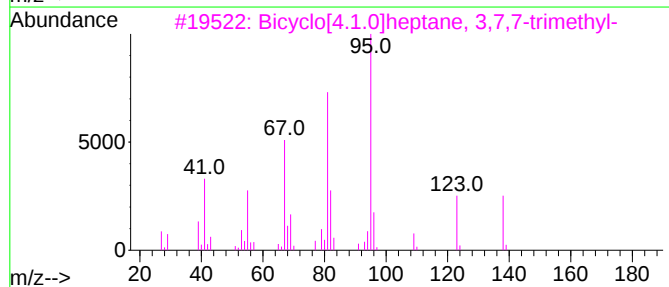
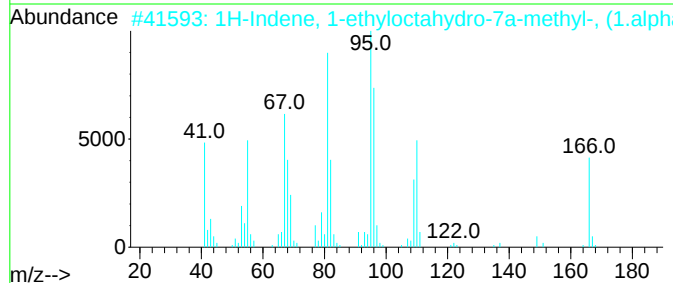
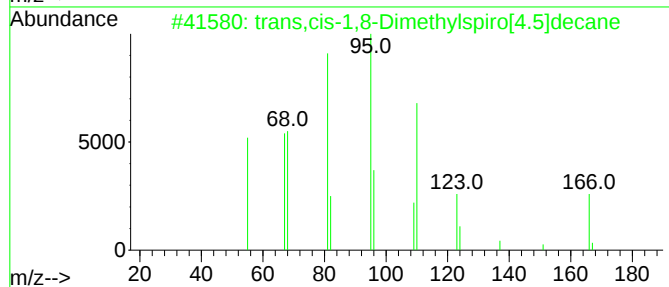
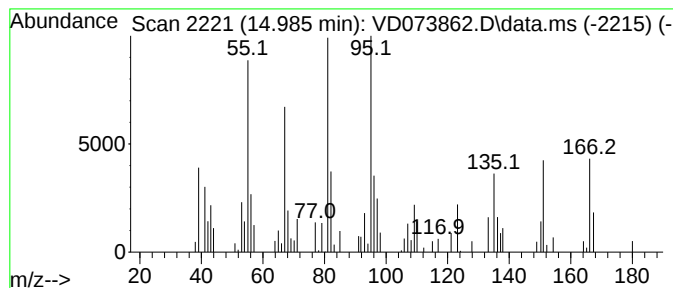
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.M
Quant Title : SW846 8260

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

Peak Number 4 trans,cis-1,8-Dimethylspiro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.985	7.20 ug/l	56085	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans,cis-1,8-Dimethylspiro[4.5]...	166	C12H22	1000111-72-9	64
2			1H-Indene, 1-ethyloctahydro-7a-m...	166	C12H22	056324-71-1	62
3			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	53
4			Cyclohexene,1-hexyl-	166	C12H22	003964-66-7	49
5			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	49



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VNJ-240

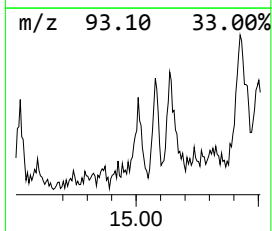
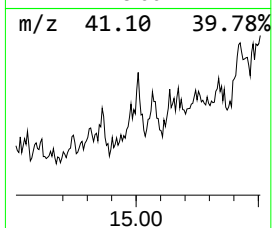
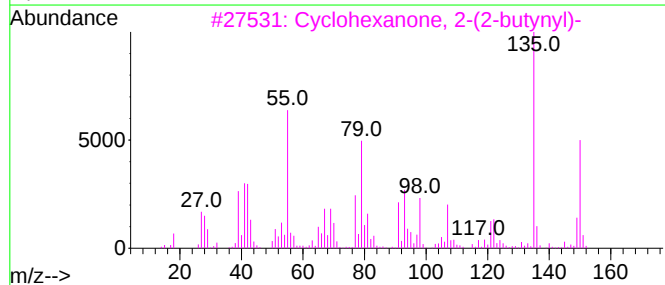
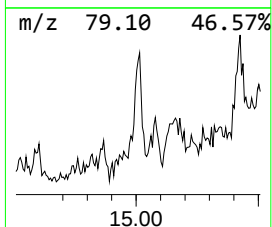
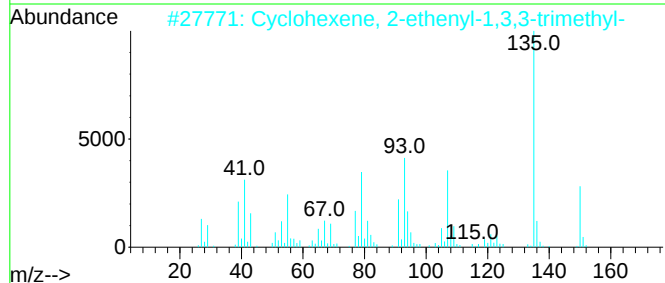
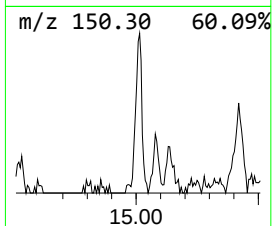
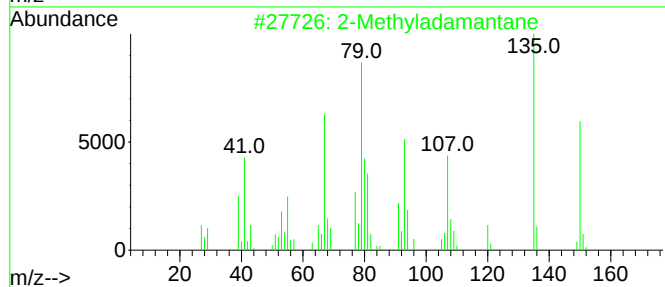
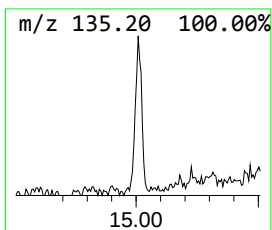
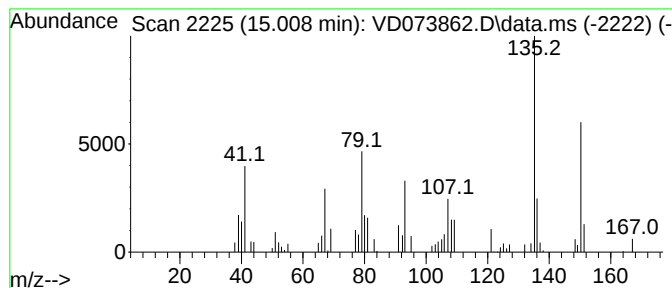
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.M
Quant Title : SW846 8260

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

Peak Number 5 2-Methyladamantane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.008	10.87 ug/l	84669	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyladamantane	150	C11H18	000700-56-1	87
2			Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	86
3			Cyclohexanone, 2-(2-butenyl)-	150	C10H14O	054166-48-2	80
4			Y-Methylbicyclo(4.3.0)non-6-en-8...	150	C10H14O	1000424-65-9	58
5			1-(Hydroxyamino)adamantane	167	C10H17NO	031463-23-7	52



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Instrument :
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ClientSampleId :
VNJ-240

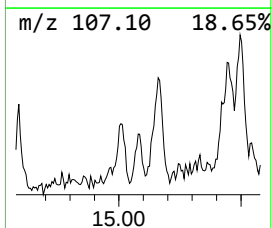
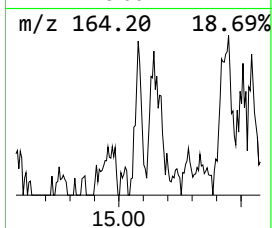
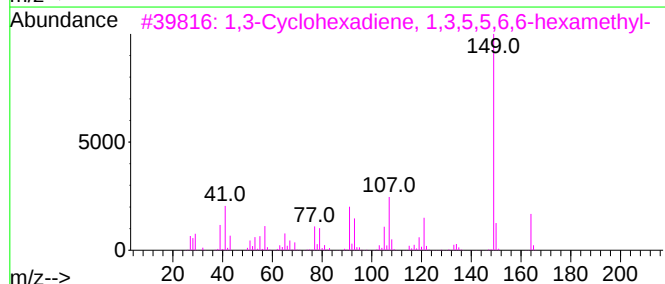
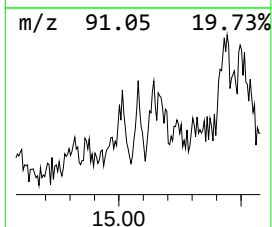
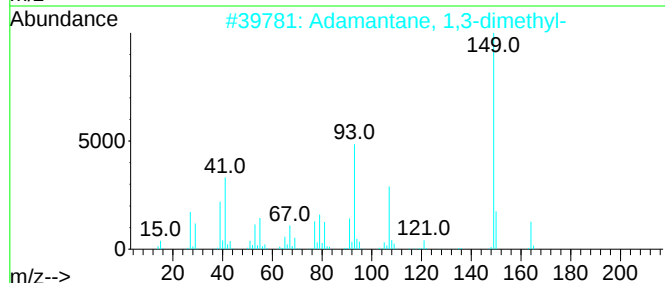
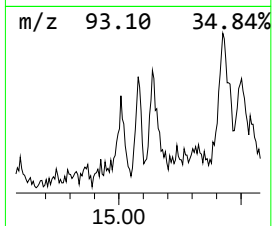
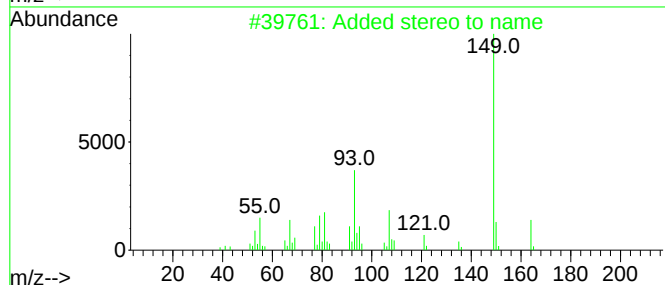
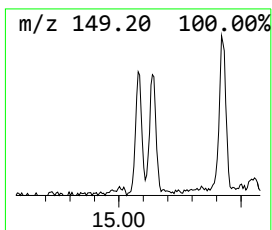
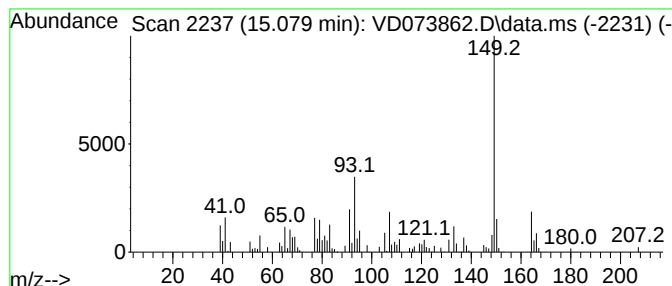
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Quant Title : SW846 8260

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

Peak Number 6 Adamantane, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.079	11.43 ug/l	89018	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-89-9	80
2	Adamantane, 1,3-dimethyl-			164	C12H20	000702-79-4	72
3	1,3-Cyclohexadiene, 1,3,5,5,6,6-...			164	C12H20	1000150-39-4	59
4	1,4-Dimethyladamantane (isomer 2)			164	C12H20	1000460-67-1	59
5	1,4-Dimethyladamantane (isomer 1)			164	C12H20	1000460-67-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071922\
Data File : VD073862.D
Acq On : 19 Jul 2022 15:40
Operator : VA/SY
Sample : N3688-03
Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
VNJ-240

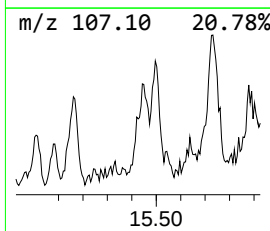
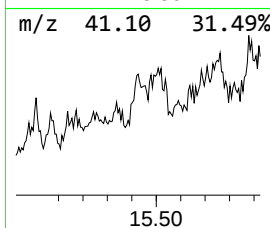
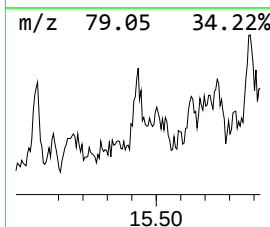
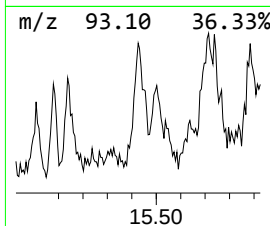
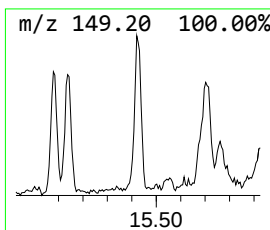
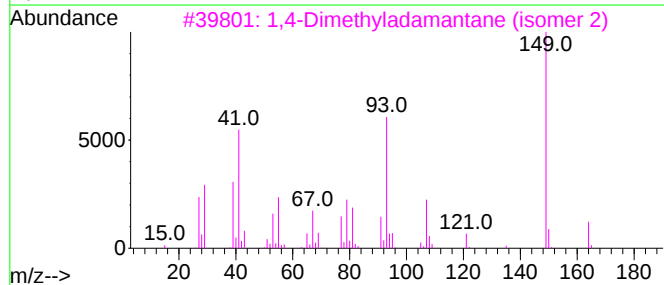
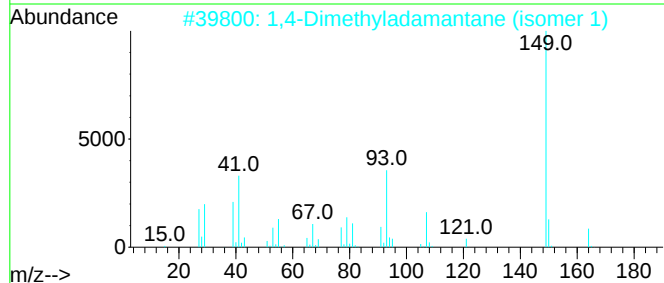
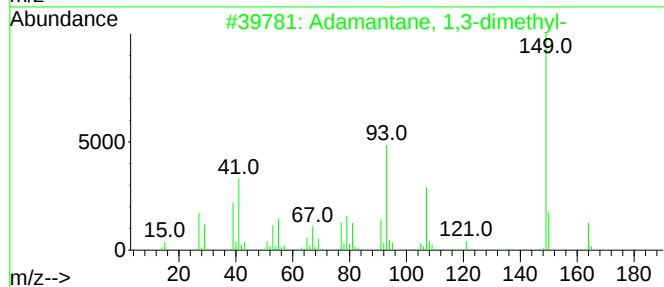
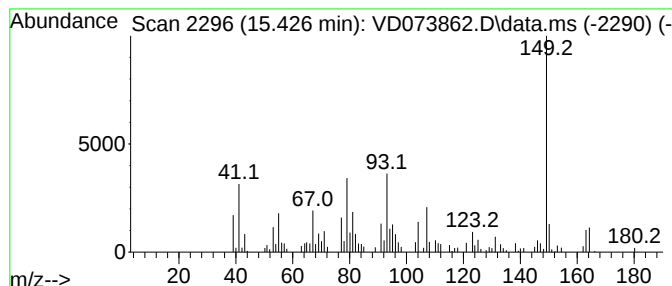
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Quant Title : SW846 8260

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

Peak Number 8 1,4-Dimethyladamantane (iso... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.426	28.03 ug/l	218347	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	76
2			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	64
3			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	58
4			Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	50
5			Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071922\
Data File : VD073862.D
Acq On : 19 Jul 2022 15:40
Operator : VA/SY
Sample : N3688-03
Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
VNJ-240

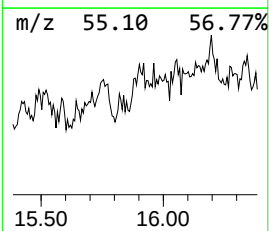
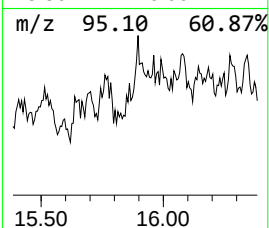
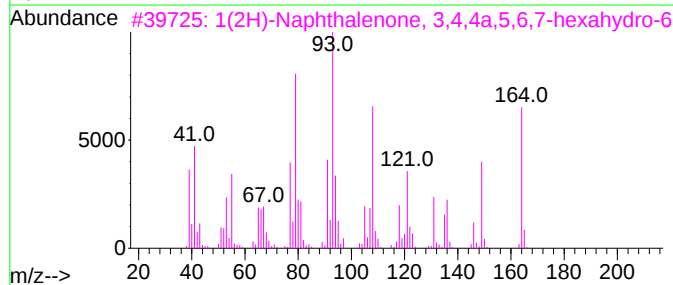
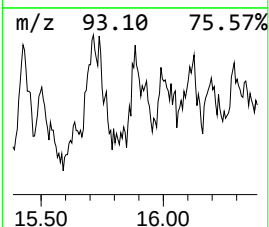
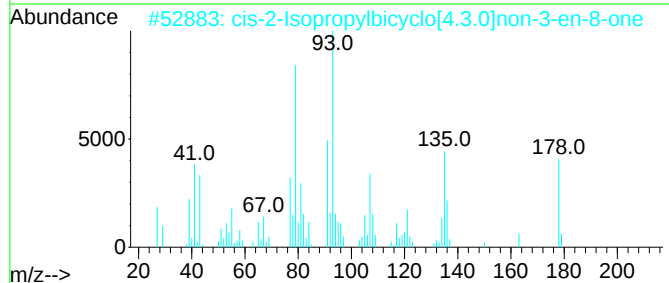
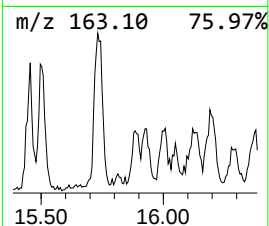
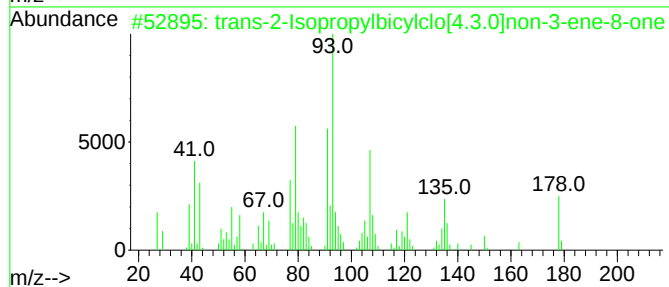
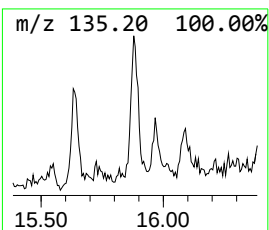
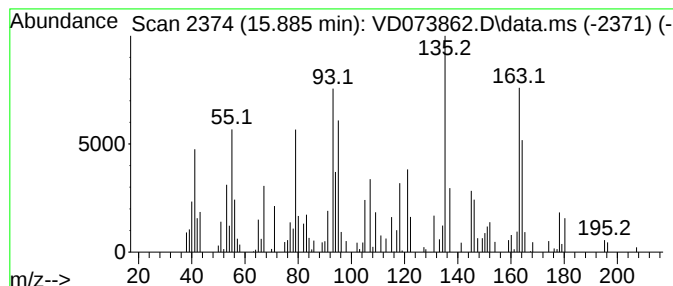
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown15.885 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.885	11.80 ug/l	91892	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Isopropylbicyclo[4.3.0]...	178	C12H18O	1000064-60-0	25
2			cis-2-Isopropylbicyclo[4.3.0]non...	178	C12H18O	1000064-59-9	22
3			1(2H)-Naphthalenone, 3,4,4a,5,6,...	164	C11H16O	1000221-37-6	22
4			2-(Adamantan-1-ylamino)-ethanol	195	C12H21NO	1000300-19-1	18
5			5,6,7,8-Tetrahydro-2-methyl-4H-c...	164	C10H12O2	014713-89-4	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071922\
Data File : VD073862.D
Acq On : 19 Jul 2022 15:40
Operator : VA/SY
Sample : N3688-03
Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
VNJ-240

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.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
Bicyclo[3.1.1]h...	14.814	8.8	ug/l	68133	4	13.561	389458	50.0
unknown14.861	14.861	7.7	ug/l	60241	4	13.561	389458	50.0
trans,cis-1,8-D...	14.985	7.2	ug/l	56085	4	13.561	389458	50.0
2-Methyladamantane	15.008	10.9	ug/l	84669	4	13.561	389458	50.0
Adamantane, 1,3...	15.079	11.4	ug/l	89018	4	13.561	389458	50.0
1,4-Dimethylada...	15.426	28.0	ug/l	218347	4	13.561	389458	50.0
unknown15.885	15.885	11.8	ug/l	91892	4	13.561	389458	50.0