

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060717\
 Data File : BM010429.D
 Acq On : 07 Jun 2017 12:20
 Operator : SJ/MA
 Sample : I3490-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B0AC8

Integration Parameters: LSCINT.P

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

Filtering: 5
 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM052717.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.164	9	13	19	rBV	306785	355240	5.28%	0.595%
2	3.381	43	50	57	rBV2	54690	100243	1.49%	0.168%
3	4.422	223	227	241	rVB	812489	1080731	16.05%	1.810%
4	5.034	327	331	339	rBV	140703	205323	3.05%	0.344%
5	7.099	676	682	695	rBV	954921	1584269	23.53%	2.654%
6	7.252	701	708	716	rBV	634142	1005191	14.93%	1.684%
7	7.452	735	742	751	rBV	1109512	1787996	26.56%	2.995%
8	7.910	811	820	834	rBV	950864	1575409	23.40%	2.639%
9	8.634	935	943	954	rBV	1098088	1815748	26.97%	3.042%
10	9.093	1015	1021	1030	rBV	844878	1412715	20.99%	2.367%
11	9.810	1136	1143	1151	rBV	778501	1313204	19.51%	2.200%
12	10.340	1224	1233	1243	rBV	1224803	2094100	31.11%	3.508%
13	10.710	1289	1296	1307	rBV	1023595	1739053	25.83%	2.913%
14	10.881	1317	1325	1336	rBV	517773	987054	14.66%	1.653%
15	12.222	1546	1553	1560	rBV	866823	1421404	21.11%	2.381%
16	13.957	1841	1848	1852	rBV	2059504	2742161	40.73%	4.594%
17	14.004	1852	1856	1863	rVB	765960	1040974	15.46%	1.744%
18	14.245	1890	1897	1903	rBV	2100871	3002911	44.61%	5.030%
19	14.545	1941	1948	1958	rVB3	1411549	2177474	32.35%	3.648%
20	14.787	1981	1989	2001	rBV2	553506	1054293	15.66%	1.766%
21	15.145	2044	2050	2060	rBV3	56520	132743	1.97%	0.222%
22	15.539	2107	2117	2123	rBV	2601637	3759692	55.85%	6.298%
23	15.663	2133	2138	2144	rBV	617576	850391	12.63%	1.425%
24	16.186	2220	2227	2232	rBV6	51633	95516	1.42%	0.160%
25	17.292	2409	2415	2422	rBV	1763509	2445379	36.32%	4.096%
26	17.392	2425	2432	2440	rBV2	2729928	3985615	59.20%	6.677%
27	18.139	2554	2559	2566	rBV2	263046	386141	5.74%	0.647%
28	19.410	2771	2775	2781	rVB3	148193	215948	3.21%	0.362%
29	19.680	2815	2821	2828	rBV	3750109	4885293	72.57%	8.184%
30	20.139	2897	2899	2905	rBV7	54353	79570	1.18%	0.133%
31	21.457	3118	3123	3129	rBV	3142980	3649417	54.21%	6.113%
32	23.651	3490	3496	3503	rVB	3587582	6732020	100.00%	11.277%
33	23.804	3516	3522	3530	rVB	2116840	3982823	59.16%	6.672%

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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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

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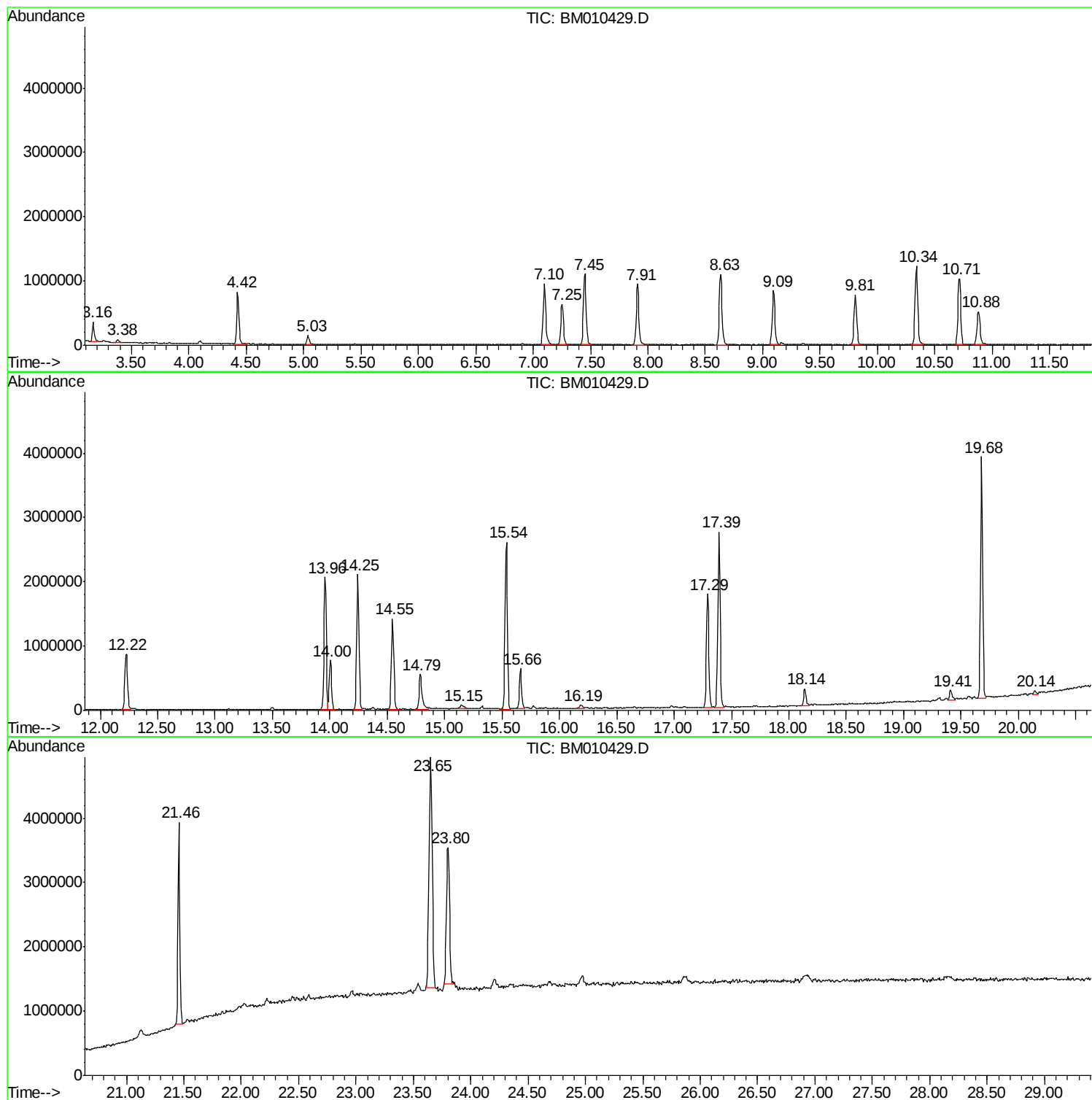
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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



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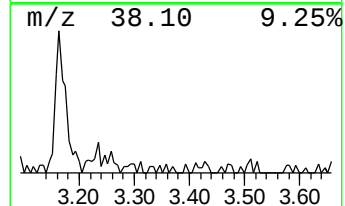
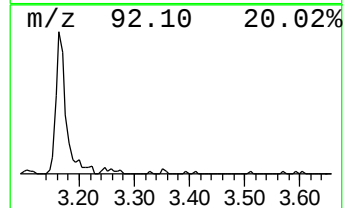
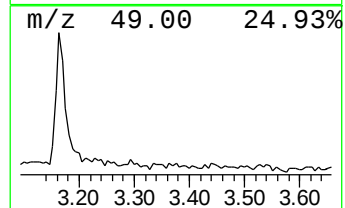
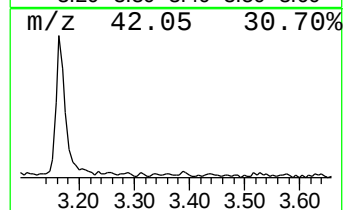
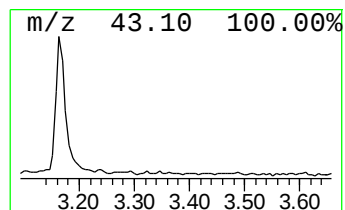
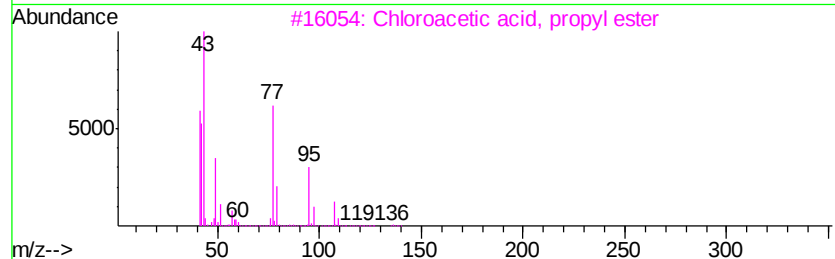
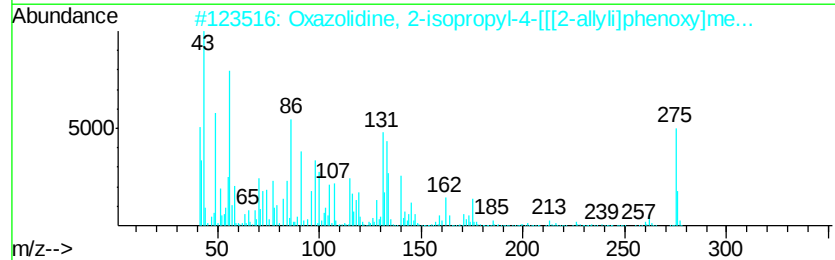
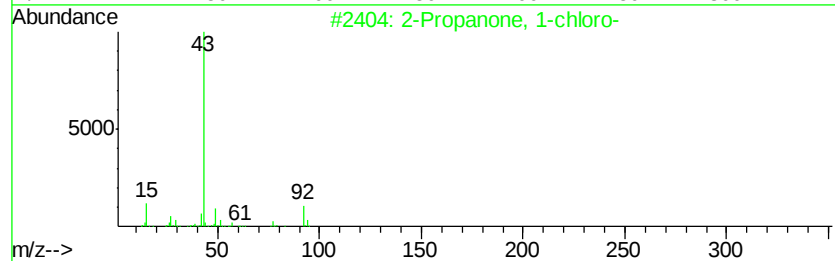
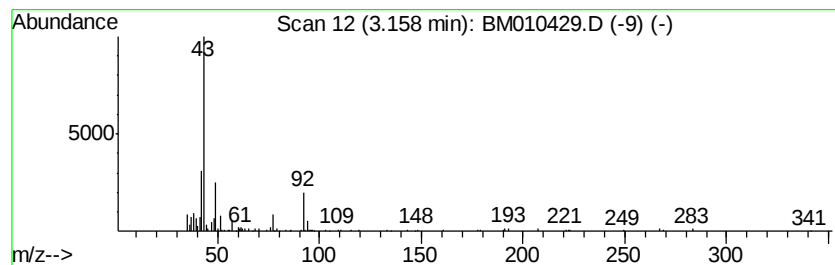
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	4.51 ng/ul	355240	1,4-Dichlorobenzene-d4	7.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanone, 1-chloro-	92	C3H5ClO	000078-95-5	40
2			Oxazolidine, 2-isopropyl-4-[[[2-...	275	C16H21NO3	070687-97-7	37
3			Chloroacetic acid, propyl ester	136	C5H9ClO2	005396-24-7	36
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	32
5			Xanthumin	306	C17H22O5	026791-72-0	28



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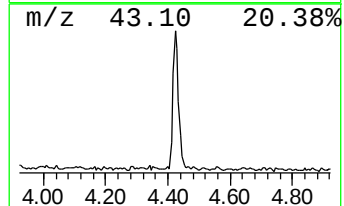
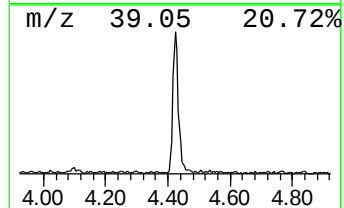
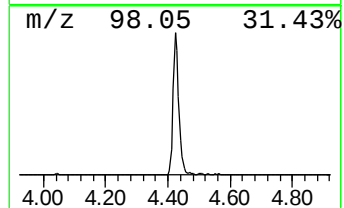
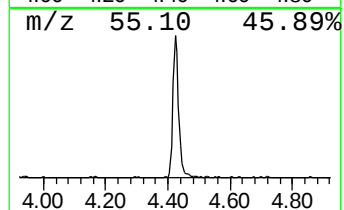
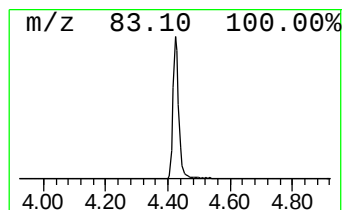
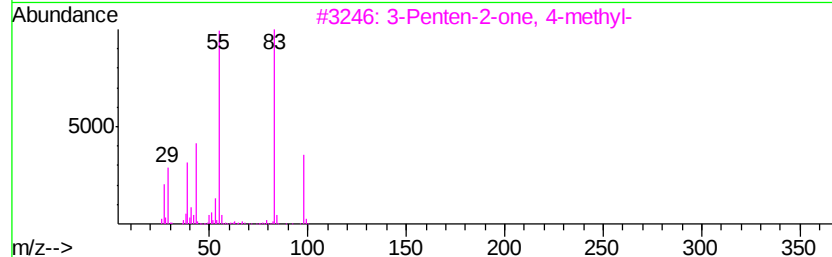
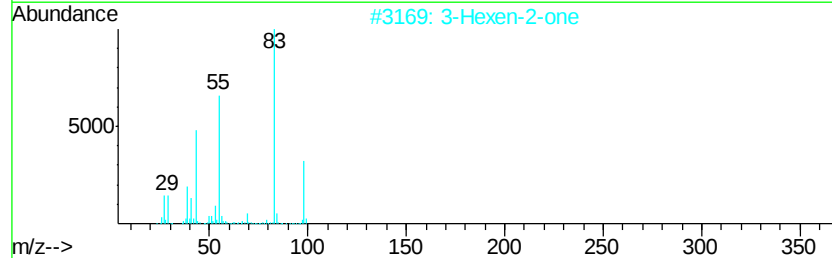
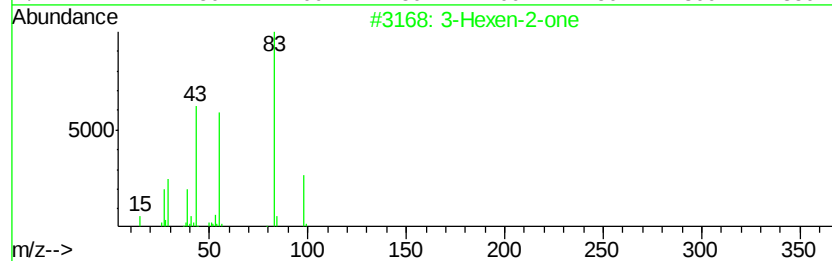
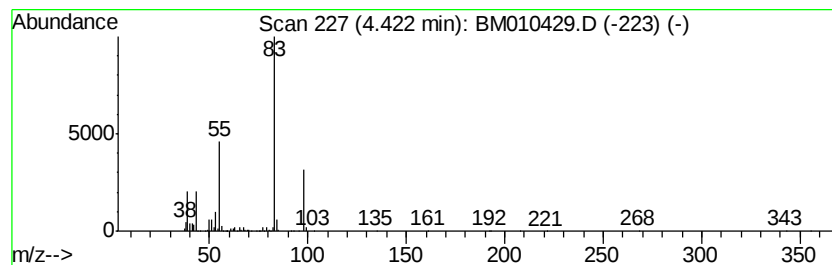
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	13.72 ng/ul	1080730	1,4-Dichlorobenzene-d4	7.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	86
2		3-Hexen-2-one	98	C6H10O	000763-93-9	80
3		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	80
4		3-Hexen-2-one	98	C6H10O	000763-93-9	78
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72



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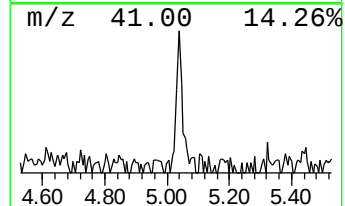
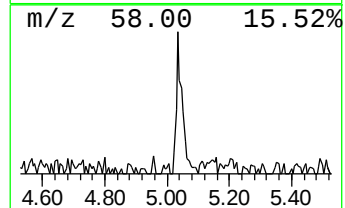
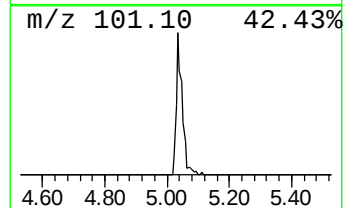
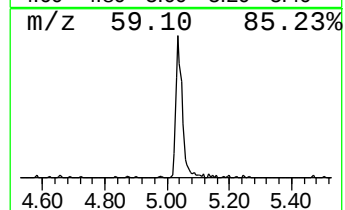
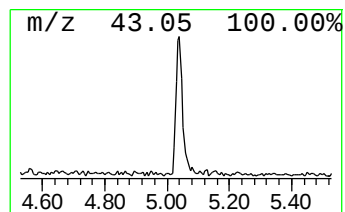
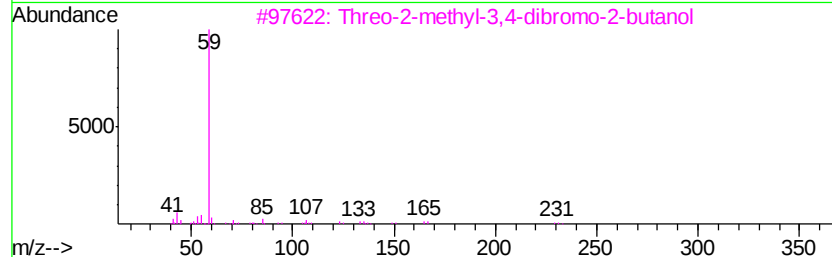
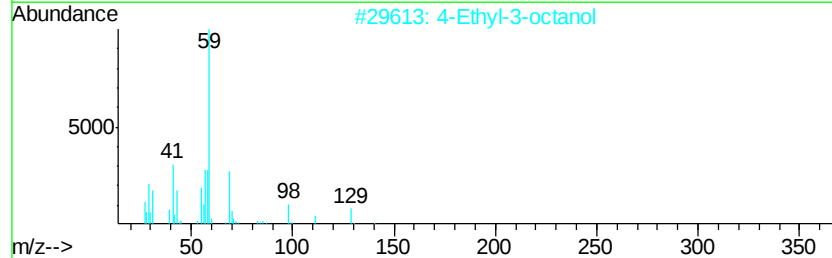
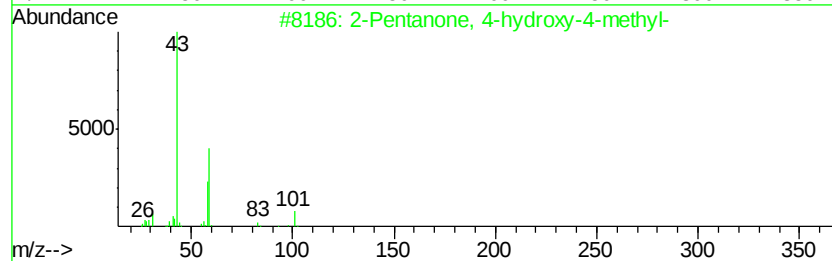
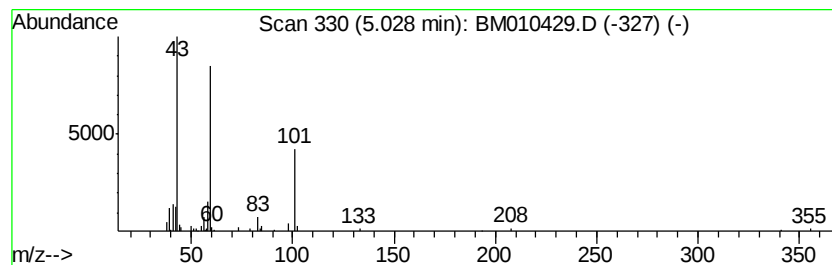
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	2.61 ng/ul	205323	1,4-Dichlorobenzene-d4	7.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2		4-Ethyl-3-octanol	158	C10H22O	019781-26-1	38
3		Threo-2-methyl-3,4-dibromo-2-but...	244	C5H10Br2O	1000288-19-2	35
4		Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	33
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32



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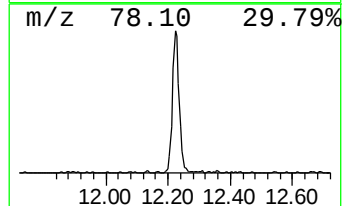
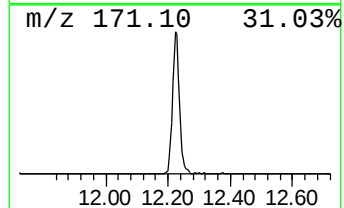
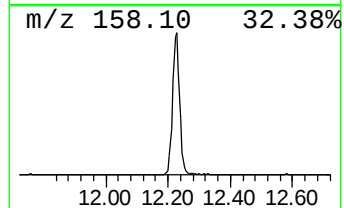
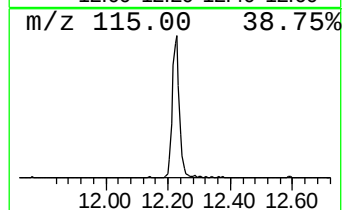
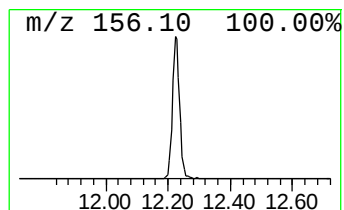
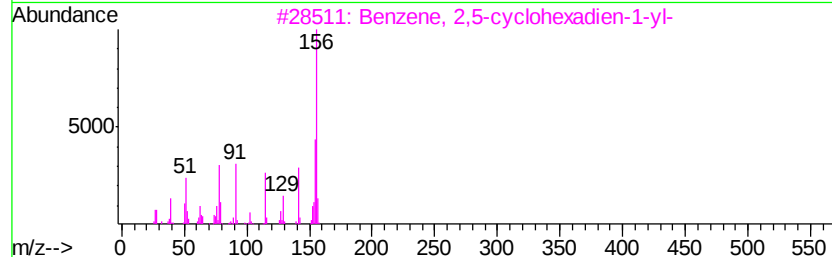
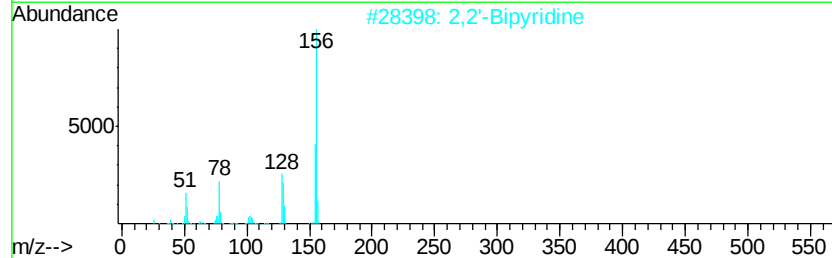
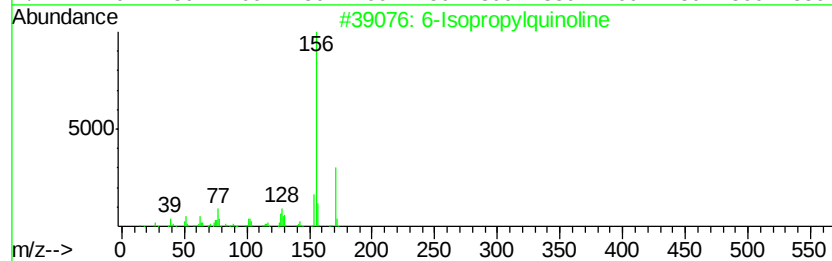
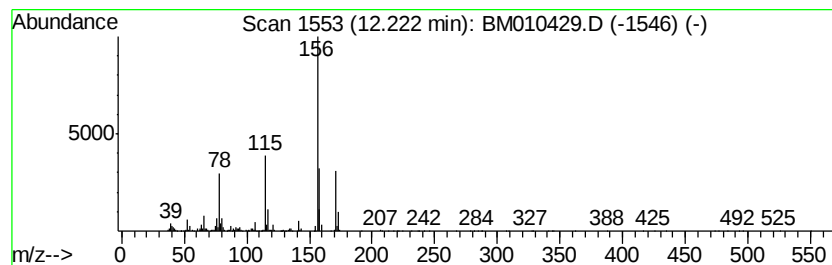
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.22	16.35 ng/ul	1421400	Naphthalene-d8	10.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Isopropylquinoline	171	C12H13N	000135-79-5	38
2		2,2'-Bipyridine	156	C10H8N2	000366-18-7	38
3		Benzene, 2,5-cyclohexadien-1-yl-	156	C12H12	004794-05-2	37
4		Chloroxyleneol	156	C8H9ClO	000088-04-0	32
5		Benzoic acid, 3-chloro-	156	C7H5ClO2	000535-80-8	32



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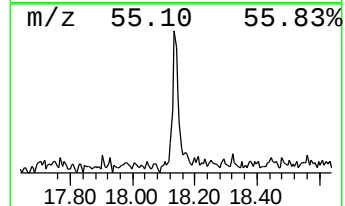
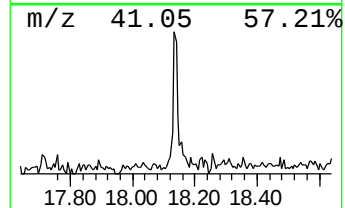
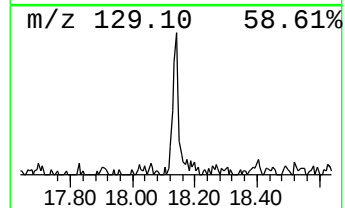
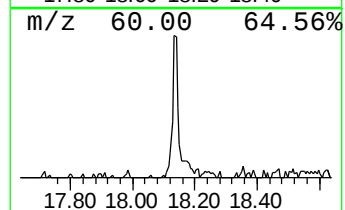
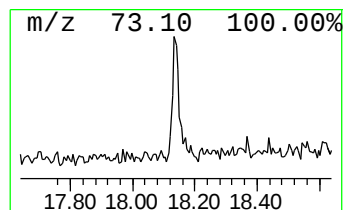
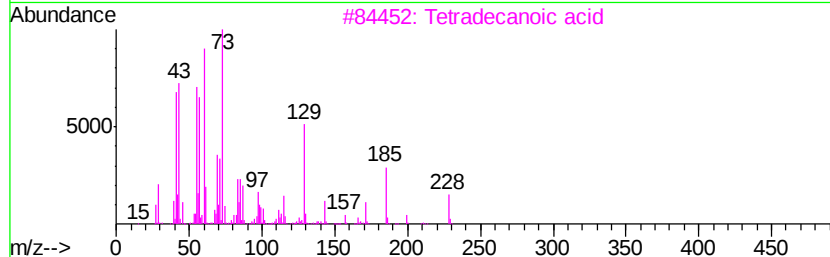
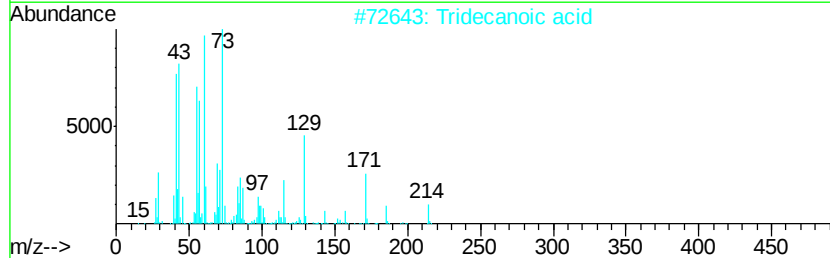
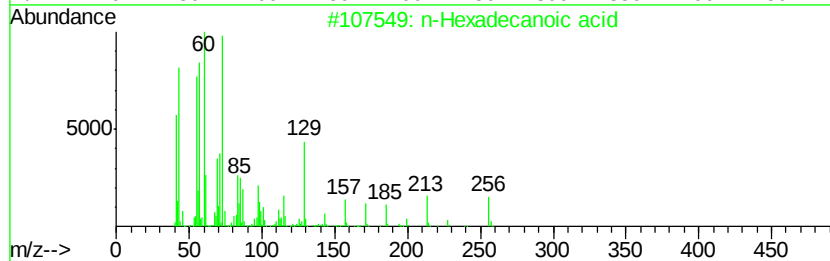
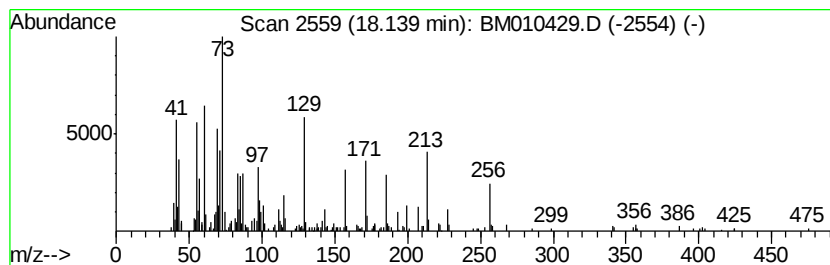
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.14	3.16 ng/ul	386141	Phenanthrene-d10	17.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Tridecanoic acid	214	C13H26O2	000638-53-9	43
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	38
4		n-Decanoic acid	172	C10H20O2	000334-48-5	38
5		Undecanoic acid	186	C11H22O2	000112-37-8	38



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	3.16	4.5	ng/ul	355240	1	7.91	1575410	20.0
3-Hexen-2-one	4.42	13.7	ng/ul	1080730	1	7.91	1575410	20.0
unknown-02	5.03	2.6	ng/ul	205323	1	7.91	1575410	20.0
unknown-03	12.22	16.4	ng/ul	1421400	2	10.71	1739050	20.0
n-Hexadecanoic acid	18.14	3.2	ng/ul	386141	4	17.29	2445380	20.0