

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121820\
 Data File : BM028183.D
 Acq On : 19 Dec 2020 06:41
 Operator : JU/CG
 Sample : L5068-11
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 A54G9

Integration Parameters: LSCINT.P

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

Filtering: 5
 Min Area: 0.1 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121520MA.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	3.416	35	39	45	rVB	17871	24475	0.67%	0.089%
2	3.993	132	137	144	rBV	10857	15873	0.43%	0.058%
3	4.228	173	177	181	rVB2	5689	7532	0.21%	0.028%
4	6.240	513	519	523	rBV2	5492	8818	0.24%	0.032%
5	6.287	523	527	535	rVB3	5626	10521	0.29%	0.038%
6	7.339	697	706	719	rBV2	309954	542678	14.87%	1.984%
7	7.516	729	736	744	rBV	241988	376746	10.32%	1.377%
8	7.728	765	772	778	rBV	320502	517244	14.17%	1.891%
9	7.798	778	784	793	rVB2	9530	20014	0.55%	0.073%
10	7.986	812	816	824	rVB3	2997	4954	0.14%	0.018%
11	8.204	844	853	860	rBV	423664	663926	18.19%	2.427%
12	8.257	860	862	868	rVB4	4104	5854	0.16%	0.021%
13	8.904	961	972	980	rBV	331969	544429	14.92%	1.991%
14	9.380	1046	1053	1061	rBV	275935	450030	12.33%	1.645%
15	9.533	1074	1079	1087	rBV5	3760	7217	0.20%	0.026%
16	9.775	1113	1120	1124	rBV	7321	11365	0.31%	0.042%
17	10.104	1163	1176	1183	rBV	215872	366020	10.03%	1.338%
18	10.645	1261	1268	1278	rVB	362534	578048	15.84%	2.113%
19	11.033	1326	1334	1341	rBV	555119	905626	24.81%	3.311%
20	11.163	1348	1356	1364	rBV	268010	456223	12.50%	1.668%
21	12.486	1578	1581	1587	rBV5	2758	4627	0.13%	0.017%
22	12.604	1596	1601	1605	rBV	5515	7760	0.21%	0.028%
23	13.198	1697	1702	1710	rVB7	4374	7973	0.22%	0.029%
24	13.439	1737	1743	1750	rVB4	8590	14079	0.39%	0.051%
25	13.645	1771	1778	1786	rBV2	3438	6703	0.18%	0.025%
26	13.716	1786	1790	1794	rVV3	3845	5475	0.15%	0.020%
27	14.074	1846	1851	1857	rVB	37815	55115	1.51%	0.202%
28	14.227	1871	1877	1882	rBV	591094	766256	20.99%	2.802%
29	14.274	1882	1885	1893	rVB	96642	122761	3.36%	0.449%
30	14.527	1921	1928	1947	rBV	682031	982716	26.92%	3.593%
31	14.704	1954	1958	1963	rVB4	4092	5033	0.14%	0.018%
32	14.833	1972	1980	1987	rBV	735058	1089845	29.86%	3.985%
33	14.957	1997	2001	2003	rBV	14380	17818	0.49%	0.065%
34	14.998	2003	2008	2014	rBV	166809	225910	6.19%	0.826%

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35	15.080	2014	2022	2042	rBV	2376564	3649951	100.00%	13.345%
36	15.651	2115	2119	2124	rVB4	9387	15532	0.43%	0.057%
37	15.809	2135	2146	2153	rBV	821401	1235391	33.85%	4.517%
38	15.921	2159	2165	2175	rBV	222278	322164	8.83%	1.178%
39	16.051	2182	2187	2194	rBV3	9576	13055	0.36%	0.048%
40	16.157	2201	2205	2207	rBV5	2950	3724	0.10%	0.014%
41	16.439	2248	2253	2262	rBV	118939	182622	5.00%	0.668%
42	16.586	2274	2278	2282	rBV5	3621	4863	0.13%	0.018%
43	16.686	2292	2295	2298	rVV3	5012	5628	0.15%	0.021%
44	16.715	2298	2300	2306	rVB5	4229	5303	0.15%	0.019%
45	16.774	2306	2310	2317	rVB4	4184	6226	0.17%	0.023%
46	16.998	2343	2348	2357	rBV6	14144	23364	0.64%	0.085%
47	17.145	2367	2373	2377	rVB4	9528	13320	0.36%	0.049%
48	17.280	2392	2396	2400	rBV4	6131	9489	0.26%	0.035%
49	17.339	2402	2406	2409	rVV3	4293	5893	0.16%	0.022%
50	17.368	2409	2411	2415	rVB4	3045	3790	0.10%	0.014%
51	17.551	2436	2442	2447	rBV	876916	1205553	33.03%	4.408%
52	17.592	2447	2449	2453	rVV	65650	73659	2.02%	0.269%
53	17.645	2453	2458	2469	rVB2	812432	1201071	32.91%	4.391%
54	17.809	2483	2486	2489	rBV4	2613	3754	0.10%	0.014%
55	17.898	2498	2501	2505	rBV6	2925	4855	0.13%	0.018%
56	17.939	2505	2508	2515	rVB2	4183	4907	0.13%	0.018%
57	18.121	2536	2539	2547	rVB7	4520	8188	0.22%	0.030%
58	18.274	2559	2565	2566	rBV3	4983	7540	0.21%	0.028%
59	18.345	2572	2577	2582	rBV2	18209	25367	0.69%	0.093%
60	18.403	2582	2587	2592	rVV2	93543	136279	3.73%	0.498%
61	18.462	2593	2597	2604	rVV2	24136	42567	1.17%	0.156%
62	18.539	2608	2610	2614	rVB4	4211	5013	0.14%	0.018%
63	18.603	2616	2621	2625	rVV4	16923	33779	0.93%	0.124%
64	18.639	2625	2627	2632	rVB	15878	20565	0.56%	0.075%
65	18.692	2634	2636	2639	rBV4	4170	4882	0.13%	0.018%
66	18.898	2667	2671	2675	rBV4	9334	13740	0.38%	0.050%
67	18.945	2675	2679	2684	rVB5	8333	12413	0.34%	0.045%
68	19.198	2719	2722	2724	rBV4	5698	6404	0.18%	0.023%
69	19.315	2737	2742	2746	rBV3	21520	35169	0.96%	0.129%
70	19.450	2761	2765	2768	rBV5	11195	17611	0.48%	0.064%
71	19.515	2774	2776	2778	rBV3	9158	10662	0.29%	0.039%

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72	19.545	2778	2781	2782	rVV2	21513	23903	0.65%	0.087%
73	19.574	2782	2786	2792	rVB	117526	156277	4.28%	0.571%
74	19.656	2797	2800	2807	rBV7	26762	41385	1.13%	0.151%
75	19.797	2821	2824	2834	rVB7	11481	23766	0.65%	0.087%
76	19.903	2836	2842	2853	rBV2	1085883	1609656	44.10%	5.885%
77	20.380	2920	2923	2925	rBV3	20368	25410	0.70%	0.093%
78	21.350	3084	3088	3093	rBV2	259741	359769	9.86%	1.315%
79	21.662	3135	3141	3145	rBV	967687	1359056	37.23%	4.969%
80	23.315	3418	3422	3434	rVB3	185098	431582	11.82%	1.578%
81	23.874	3511	3517	3524	rBV	716352	1368863	37.50%	5.005%
82	24.027	3536	3543	3562	rVB	671953	1413874	38.74%	5.169%
83	26.585	3972	3978	3993	rVB2	347180	982191	26.91%	3.591%
84	26.921	4027	4035	4051	rVB2	720405	2351183	64.42%	8.596%

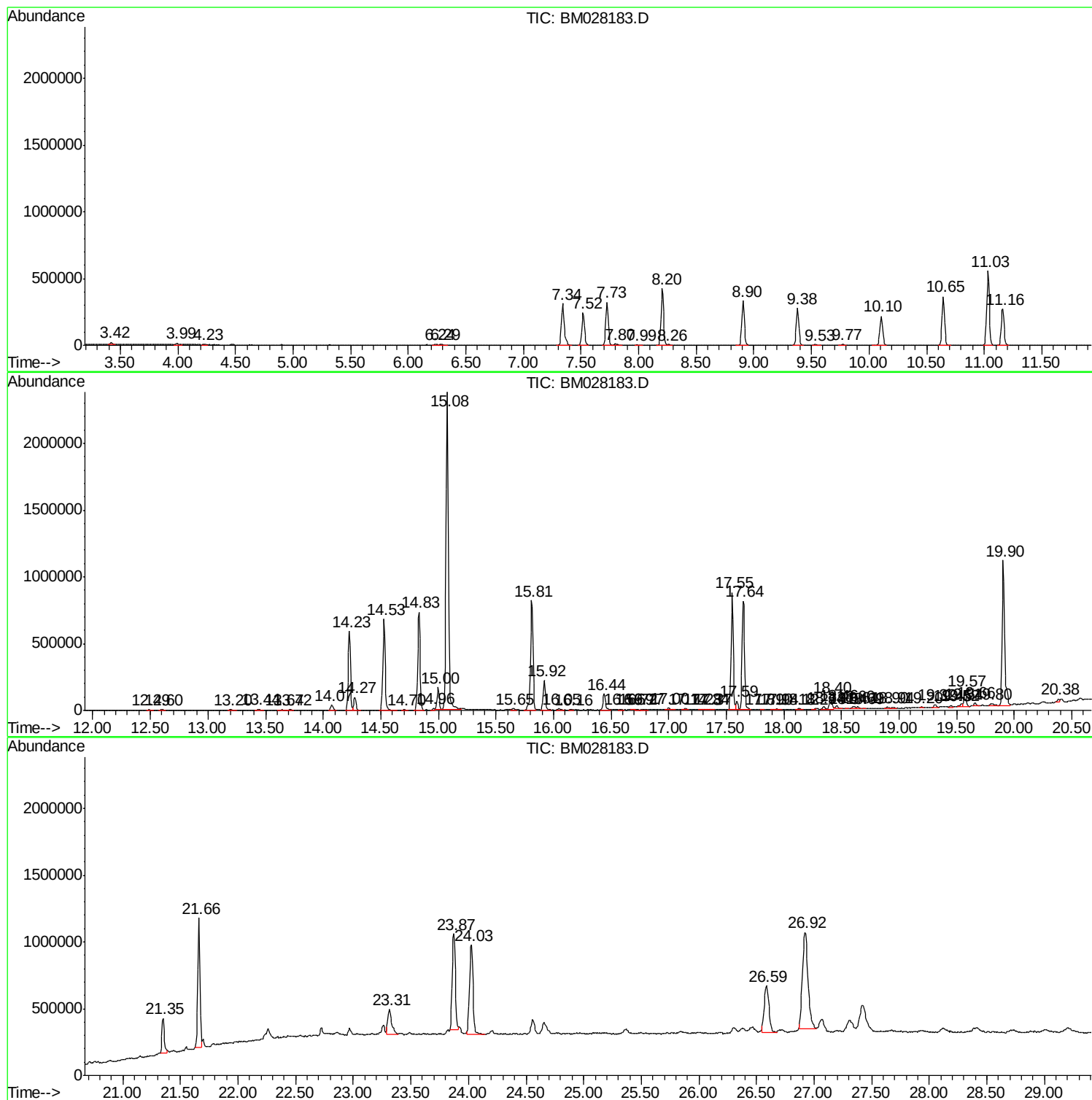
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121520MA.M
Quant Title : SVOA CALIBRATION

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



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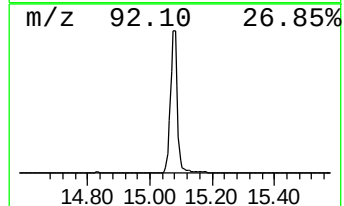
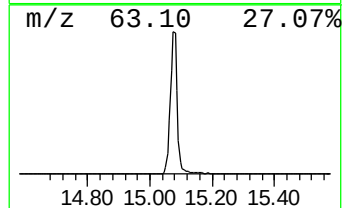
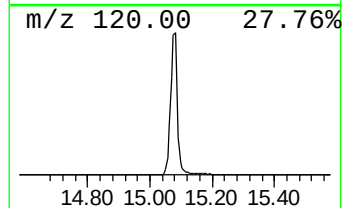
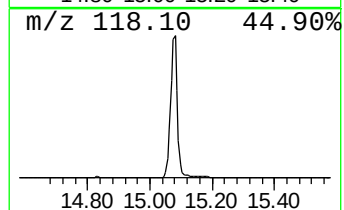
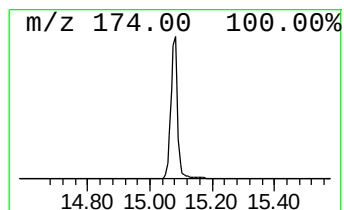
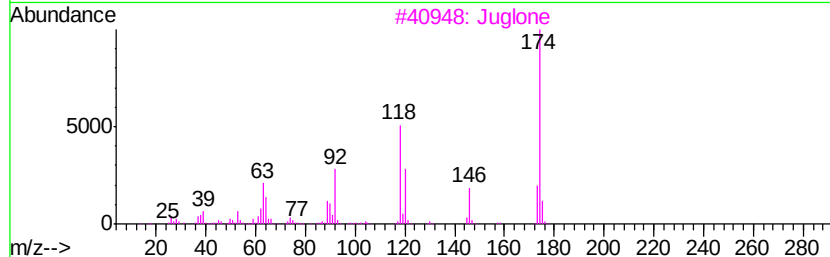
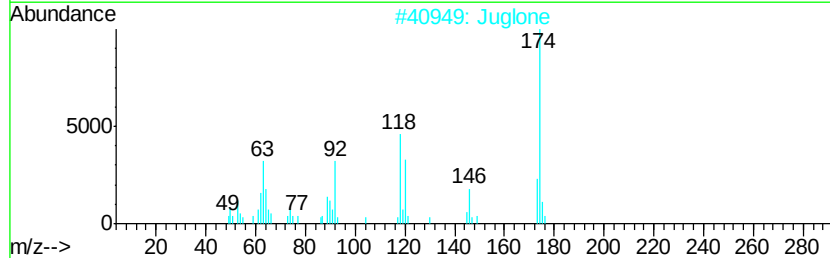
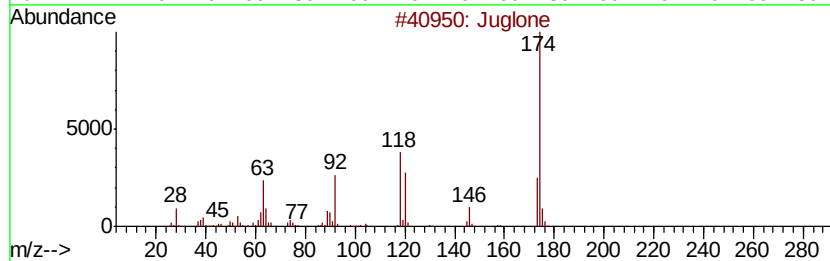
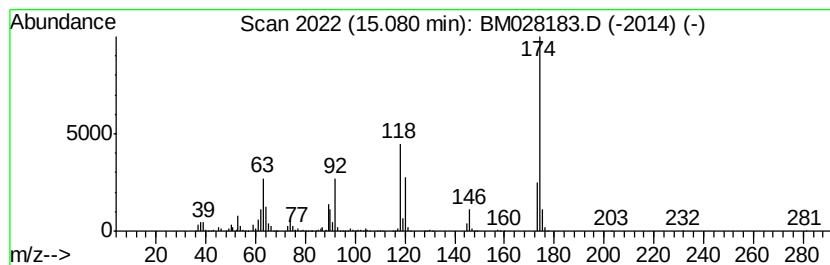
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121520MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Juglone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	66.98 ng/ul	3649950	Acenaphthene-d10	14.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Juglone	174	C10H6O3	000481-39-0	98
2		Juglone	174	C10H6O3	000481-39-0	94
3		Juglone	174	C10H6O3	000481-39-0	90
4		Benzene, 1,3-diisocyanato-2-methyl-	174	C9H6N2O2	000091-08-7	43
5		8-Quinolinol, 5-nitroso-	174	C9H6N2O2	003565-26-2	43



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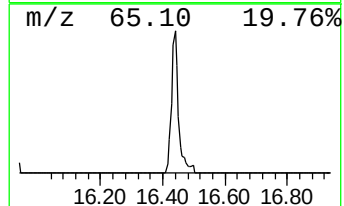
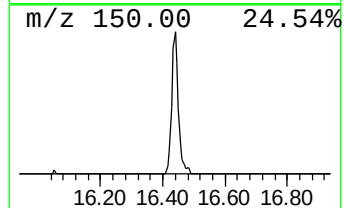
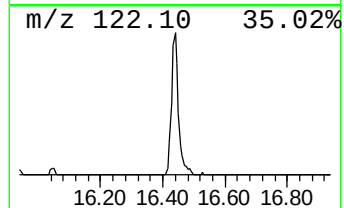
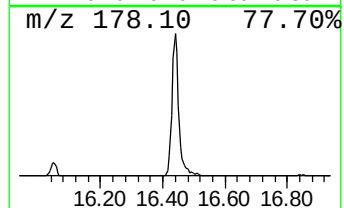
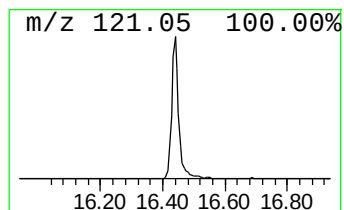
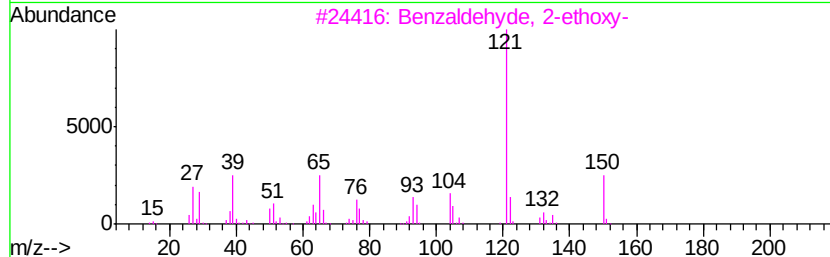
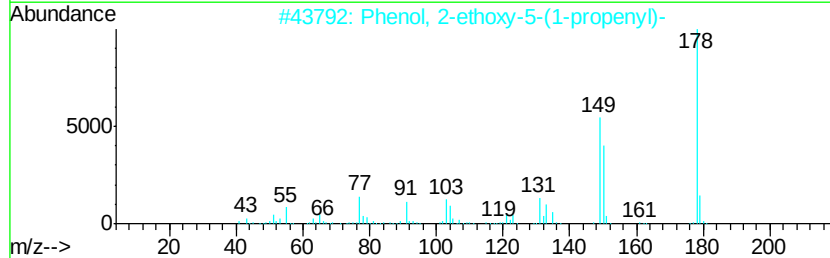
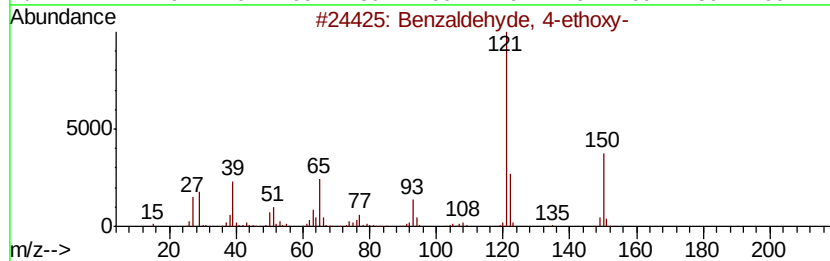
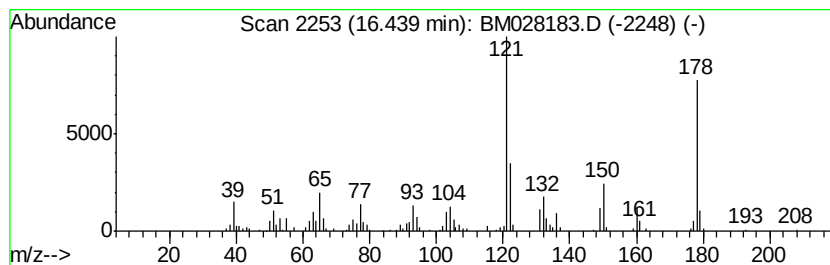
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	3.03 ng/ul	182622	Phenanthrene-d10	17.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzaldehyde, 4-ethoxy-	150	C9H10O2	010031-82-0	46
2		Phenol, 2-ethoxy-5-(1-propenyl)-	178	C11H14O2	000094-86-0	45
3		Benzaldehyde, 2-ethoxy-	150	C9H10O2	000613-69-4	45
4		1(2H)-Naphthalenone, 3,4-dihydro...	178	C10H10O3	054549-75-6	43
5		Benzaldehyde, 4-ethoxy-	150	C9H10O2	010031-82-0	38



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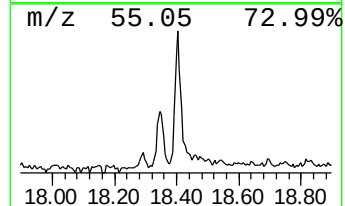
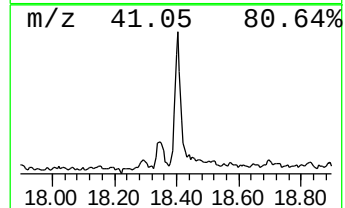
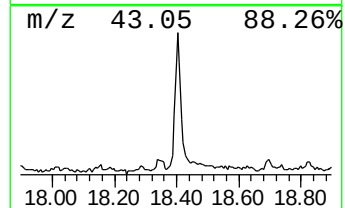
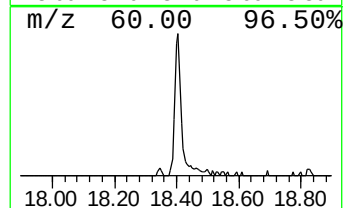
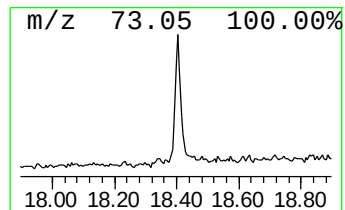
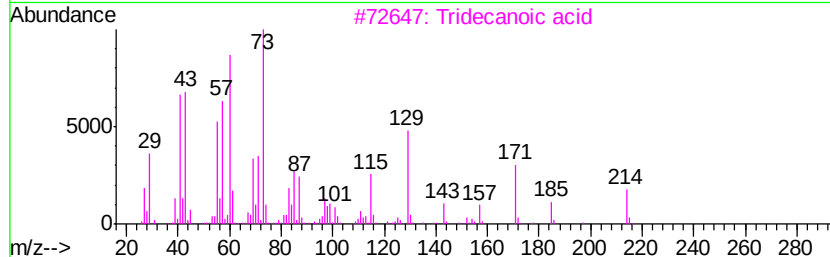
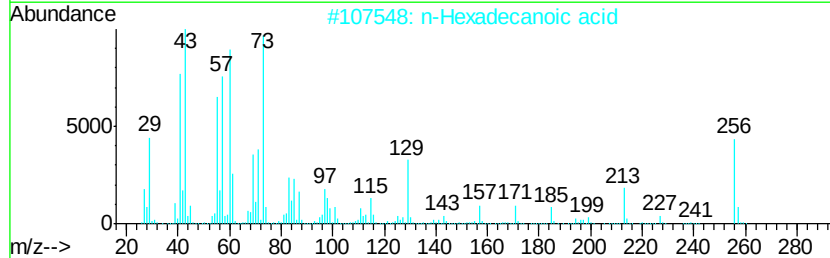
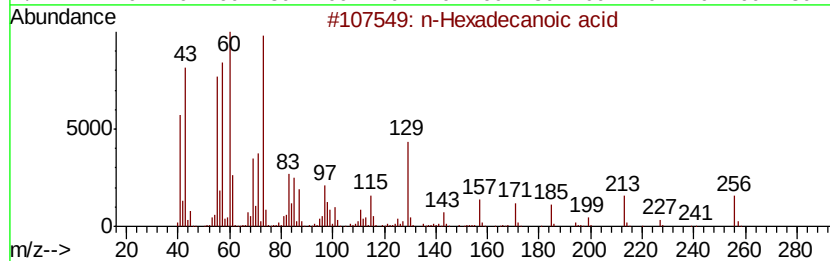
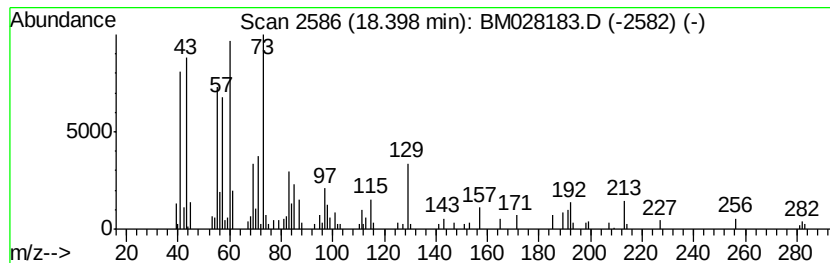
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	2.26 ng/ul	136279	Phenanthrene-d10	17.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3		Tridecanoic acid	214	C13H26O2	000638-53-9	93
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	62



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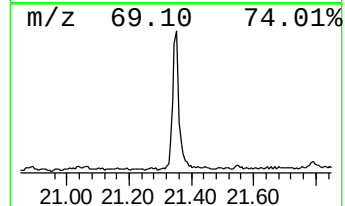
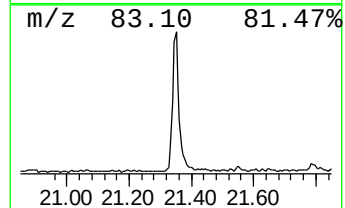
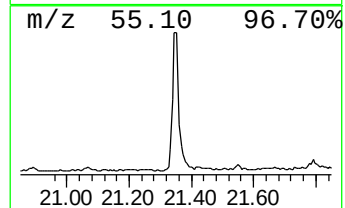
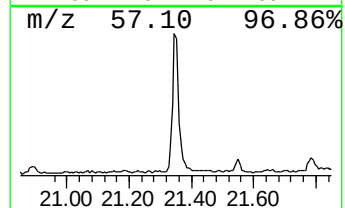
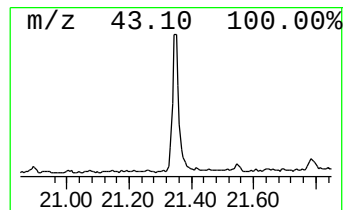
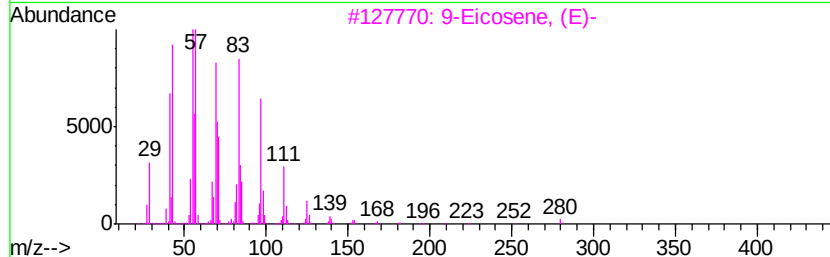
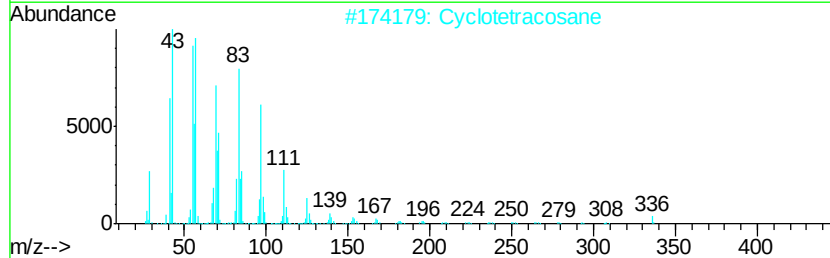
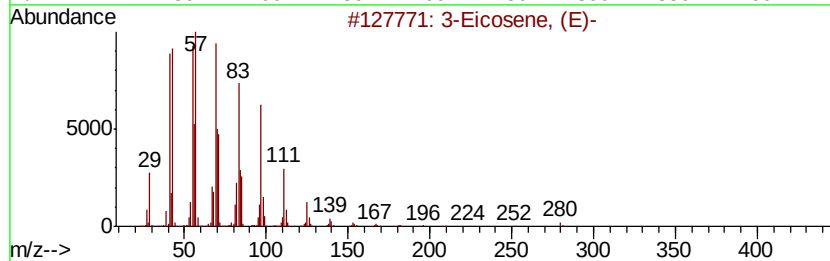
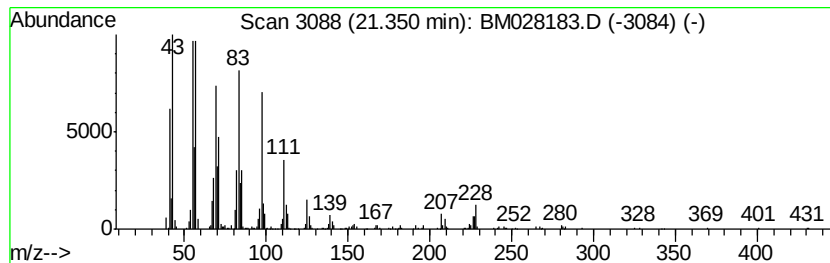
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	5.29 ng/ul	359769	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2		Cyclotetracosane	336	C24H48	000297-03-0	93
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121820\
Data File : BM028183.D
Acq On : 19 Dec 2020 06:41
Operator : JU/CG
Sample : L5068-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A54G9

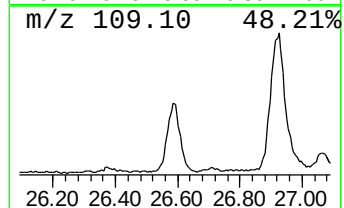
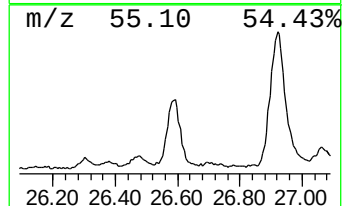
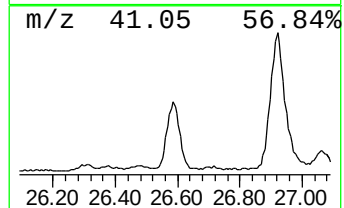
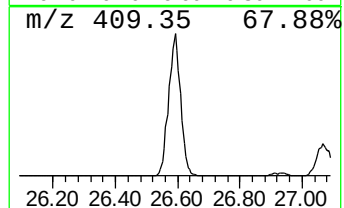
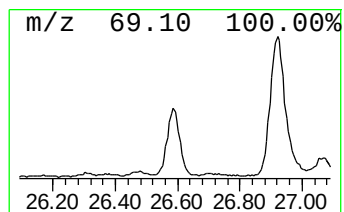
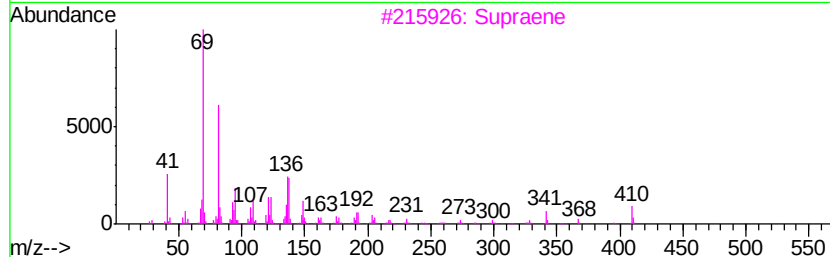
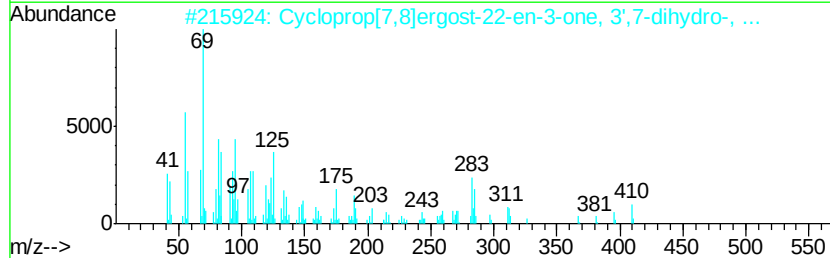
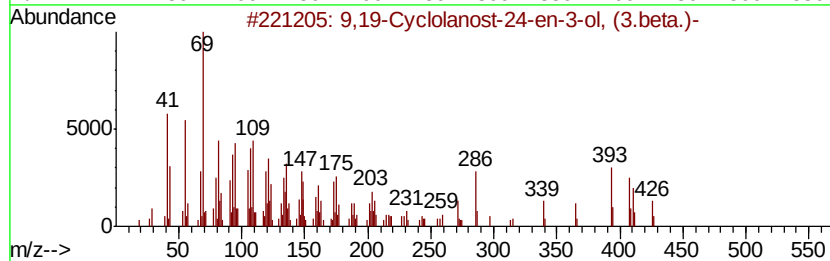
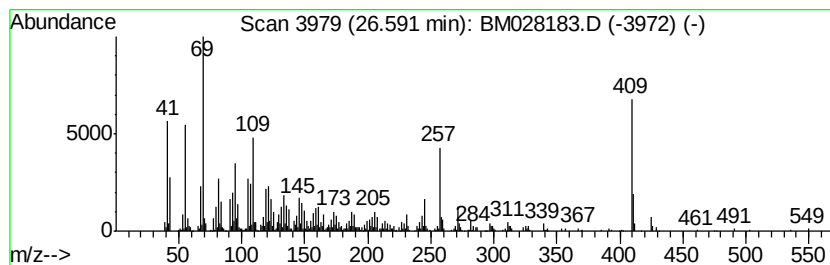
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.59	13.89 ng/ul	982191	Perylene-d12	24.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,19-Cyclolanost-24-en-3-ol, (3...	426	C30H50O	000469-38-5	38		
2	Cycloprop[7,8]ergost-22-en-3-one...	410	C29H46O	053755-18-3	37		
3	Supraene	410	C30H50	007683-64-9	25		
4	2,6,10,14-Hexadecatetraene, 1-be...	488	C33H44OS	1000194-30-4	16		
5	5-(Cyclopentanecarbonyl-amino)-3...	353	C17H23NO5S	1000300-90-0	16		



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121820\
Data File : BM028183.D
Acq On : 19 Dec 2020 06:41
Operator : JU/CG
Sample : L5068-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

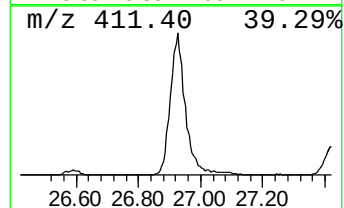
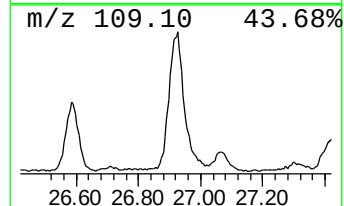
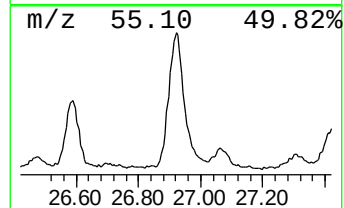
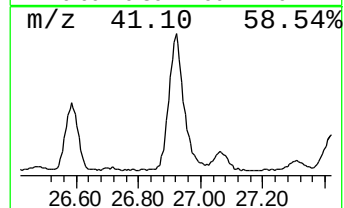
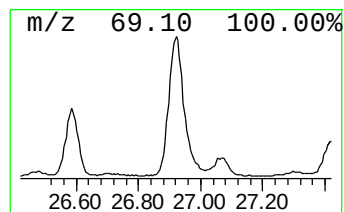
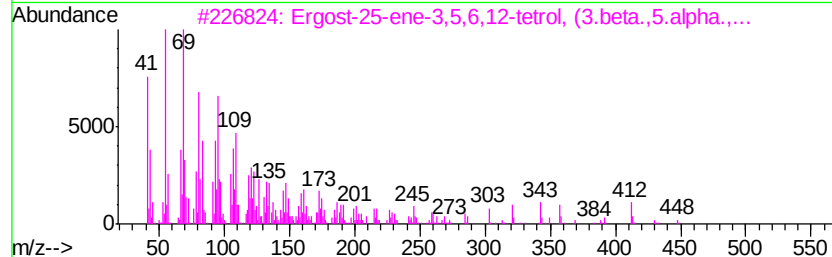
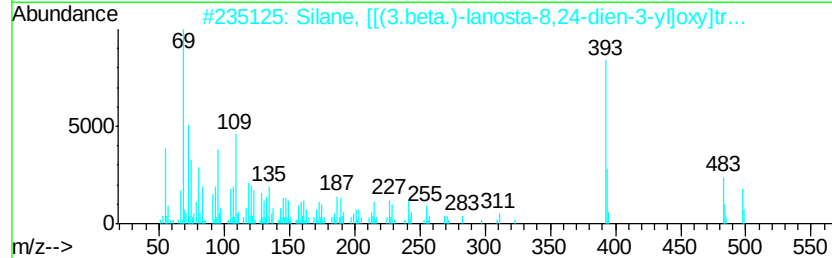
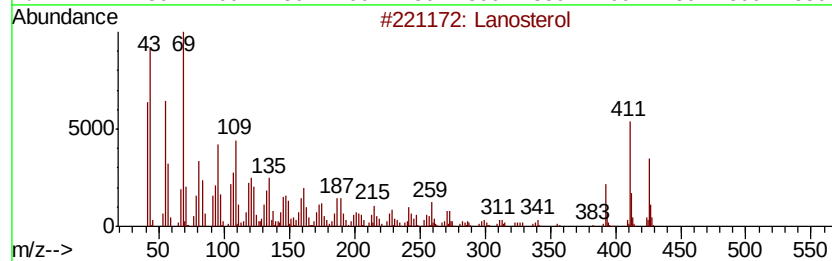
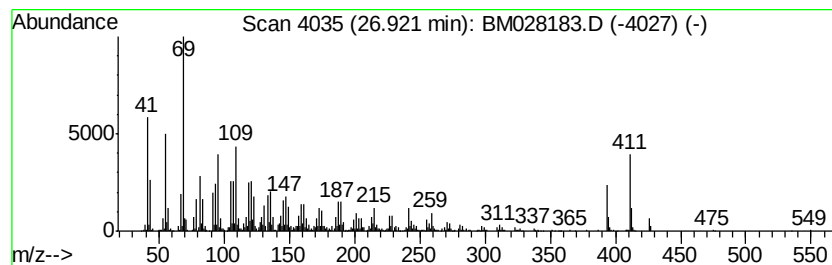
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121520MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 Lanosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.92	33.26 ng/ul	2351180	Perylene-d12	24.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Lanosterol	426 C30H50O	000079-63-0	87
2	Silane, [[(3.beta.)-lanosta-8,24...	498 C33H58OSi	055493-84-0	58
3	Ergost-25-ene-3,5,6,12-tetrol, (...	448 C28H48O4	056052-97-2	38
4	9,19-Cyclolanost-24-en-3-ol, (3....	426 C30H50O	000469-38-5	11
5	D:B-Friedo-18,19-secolup-19-ene,...	426 C30H50O	035060-26-5	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121820\
Data File : BM028183.D
Acq On : 19 Dec 2020 06:41
Operator : JU/CG
Sample : L5068-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A54G9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121520MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Juglone	15.08	67.0	ng/ul	3649950	3	14.83	1089850	20.0
unknown-01	16.44	3.0	ng/ul	182622	4	17.55	1205550	20.0
n-Hexadecanoic acid	18.40	2.3	ng/ul	136279	4	17.55	1205550	20.0
(DEL) Alkane: Str...	21.35	5.3	ng/ul	359769	5	21.66	1359060	20.0
unknown-02	26.59	13.9	ng/ul	982191	6	24.03	1413870	20.0
Lanosterol	26.92	33.3	ng/ul	2351180	6	24.03	1413870	20.0