

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050917\
 Data File : BG026931.D
 Acq On : 10 May 2017 3:32
 Operator : SJ/MA
 Sample : I2884-01 5X
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 YAB34

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.1
 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: 1

Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG042717.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	7.188	692	698	713	rVB2	72127	169521	4.54%	0.547%
2	7.329	716	722	730	rVB	66960	117155	3.14%	0.378%
3	7.547	751	759	771	rVB2	85643	169589	4.54%	0.547%
4	8.005	829	837	848	rVB	685429	1154617	30.90%	3.723%
5	8.134	856	859	866	rVB7	4381	7480	0.20%	0.024%
6	8.722	952	959	974	rBV	83660	196740	5.27%	0.634%
7	9.168	1028	1035	1049	rBV	75157	156545	4.19%	0.505%
8	9.321	1057	1061	1065	rBV5	4054	7206	0.19%	0.023%
9	9.891	1147	1158	1168	rBV2	59507	123081	3.29%	0.397%
10	10.443	1245	1252	1271	rBV2	79228	188399	5.04%	0.607%
11	10.802	1304	1313	1331	rVV	1082143	1989862	53.25%	6.416%
12	10.954	1331	1339	1354	rVV6	16396	50993	1.36%	0.164%
13	11.959	1507	1510	1517	rVB4	3468	7148	0.19%	0.023%
14	12.459	1589	1595	1600	rVB3	15505	25912	0.69%	0.084%
15	12.676	1624	1632	1637	rVB2	19789	35367	0.95%	0.114%
16	13.140	1708	1711	1716	rBV5	3509	7003	0.19%	0.023%
17	13.222	1721	1725	1731	rVB4	8629	13057	0.35%	0.042%
18	13.434	1756	1761	1764	rBV4	6823	11421	0.31%	0.037%
19	13.481	1764	1769	1774	rVB5	10603	17675	0.47%	0.057%
20	13.651	1794	1798	1808	rVB9	2757	7933	0.21%	0.026%
21	13.798	1814	1823	1829	rBV8	8139	23126	0.62%	0.075%
22	13.857	1829	1833	1840	rBV5	5378	8837	0.24%	0.028%
23	13.945	1840	1848	1853	rBV6	13667	27728	0.74%	0.089%
24	14.016	1853	1860	1865	rVV	181822	296852	7.94%	0.957%
25	14.063	1865	1868	1876	rVV	81567	123288	3.30%	0.397%
26	14.174	1882	1887	1891	rVV7	7431	13299	0.36%	0.043%
27	14.204	1891	1892	1899	rVB6	6126	8151	0.22%	0.026%
28	14.309	1904	1910	1921	rBV	241030	397670	10.64%	1.282%
29	14.503	1937	1943	1952	rVB4	11807	23559	0.63%	0.076%
30	14.615	1952	1962	1970	rBV2	1485800	2431549	65.07%	7.840%
31	14.680	1970	1973	1979	rVB3	22115	33783	0.90%	0.109%
32	14.750	1982	1985	1994	rBV5	8341	14708	0.39%	0.047%
33	14.868	1996	2005	2014	rBV7	21049	63300	1.69%	0.204%
34	15.009	2024	2029	2039	rBV	32311	64974	1.74%	0.209%

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35	15.079	2039	2041	2046	rVV6	6012	9206	0.25%	0.030%
36	15.226	2063	2066	2071	rVB7	8216	13327	0.36%	0.043%
37	15.279	2071	2075	2080	rBV7	4726	8135	0.22%	0.026%
38	15.385	2087	2093	2094	rBV6	11893	15551	0.42%	0.050%
39	15.449	2101	2104	2109	rVB2	25021	28663	0.77%	0.092%
40	15.602	2120	2130	2135	rBV	296407	446100	11.94%	1.438%
41	15.661	2135	2140	2149	rVB4	58966	107262	2.87%	0.346%
42	15.743	2149	2154	2160	rBV9	18764	41578	1.11%	0.134%
43	15.855	2164	2173	2178	rVB9	15989	36825	0.99%	0.119%
44	15.949	2185	2189	2195	rVB5	21368	34169	0.91%	0.110%
45	16.013	2195	2200	2204	rBV8	7422	15469	0.41%	0.050%
46	16.101	2205	2215	2223	rBV7	17300	45510	1.22%	0.147%
47	16.201	2227	2232	2235	rBV7	8229	14126	0.38%	0.046%
48	16.307	2245	2250	2252	rBV3	32915	48376	1.29%	0.156%
49	16.331	2252	2254	2259	rVB4	34039	43471	1.16%	0.140%
50	16.466	2274	2277	2283	rVB8	8843	13944	0.37%	0.045%
51	16.548	2284	2291	2295	rVV10	6947	14033	0.38%	0.045%
52	16.660	2301	2310	2313	rBV10	14629	37786	1.01%	0.122%
53	16.707	2314	2318	2322	rVB7	12439	20391	0.55%	0.066%
54	16.748	2322	2325	2330	rBV6	9367	21521	0.58%	0.069%
55	16.806	2332	2335	2338	rVB6	8404	7487	0.20%	0.024%
56	16.889	2345	2349	2354	rBV8	8937	15418	0.41%	0.050%
57	17.006	2363	2369	2375	rBV2	40458	72131	1.93%	0.233%
58	17.094	2378	2384	2388	rBV3	24436	40880	1.09%	0.132%
59	17.171	2388	2397	2406	rVB3	32323	99843	2.67%	0.322%
60	17.253	2409	2411	2416	rVB5	8667	11796	0.32%	0.038%
61	17.353	2420	2428	2432	rBV	1624056	2457235	65.76%	7.922%
62	17.394	2432	2435	2441	rVV	563569	875076	23.42%	2.821%
63	17.453	2441	2445	2456	rVB3	268389	476607	12.76%	1.537%
64	17.635	2472	2476	2478	rBV5	6367	9198	0.25%	0.030%
65	17.758	2489	2497	2503	rBV	42741	91420	2.45%	0.295%
66	17.835	2505	2510	2512	rBV2	31790	45443	1.22%	0.147%
67	17.870	2513	2516	2520	rVB6	18747	24452	0.65%	0.079%
68	17.935	2523	2527	2534	rVB10	19161	36109	0.97%	0.116%
69	18.158	2561	2565	2566	rBV4	11393	14829	0.40%	0.048%
70	18.228	2572	2577	2581	rBV3	82931	148740	3.98%	0.480%
71	18.275	2581	2585	2591	rVB	78061	120924	3.24%	0.390%

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72	18.416	2604	2609	2613	rBV3	78170	140690	3.77%	0.454%
73	18.457	2614	2616	2622	rVB	47696	55133	1.48%	0.178%
74	18.522	2623	2627	2632	rBV6	31881	40429	1.08%	0.130%
75	18.716	2656	2660	2665	rBV	41537	58932	1.58%	0.190%
76	18.769	2665	2669	2674	rVB3	42700	69572	1.86%	0.224%
77	19.145	2727	2733	2737	rBV3	61471	117570	3.15%	0.379%
78	19.227	2745	2747	2751	rVB4	36968	39964	1.07%	0.129%
79	19.280	2751	2756	2760	rBV2	55013	116302	3.11%	0.375%
80	19.398	2771	2776	2782	rVB	552047	753698	20.17%	2.430%
81	19.497	2790	2793	2798	rVB7	26396	35156	0.94%	0.113%
82	19.727	2827	2832	2835	rBV2	369559	607627	16.26%	1.959%
83	19.756	2835	2837	2846	rVV	530523	735444	19.68%	2.371%
84	19.832	2846	2850	2855	rVB6	45429	74409	1.99%	0.240%
85	20.249	2916	2921	2928	rBV4	106823	171603	4.59%	0.553%
86	20.314	2929	2932	2936	rBV2	75733	97725	2.62%	0.315%
87	20.737	3002	3004	3013	rVB2	88007	130717	3.50%	0.421%
88	21.007	3046	3050	3056	rBV2	58697	114788	3.07%	0.370%
89	21.595	3142	3150	3155	rBV	1635261	2899851	77.61%	9.349%
90	21.642	3156	3158	3165	rVB	225686	300578	8.04%	0.969%
91	22.535	3307	3310	3327	rVB	118753	443014	11.86%	1.428%
92	23.040	3392	3396	3399	rBV2	107146	150648	4.03%	0.486%
93	23.745	3509	3516	3519	rBV6	210952	504270	13.50%	1.626%
94	24.074	3567	3572	3580	rVB4	313940	727636	19.47%	2.346%
95	24.768	3681	3690	3709	rVB	1116185	3736598	100.00%	12.047%
96	25.085	3736	3744	3760	rVB7	354551	1247797	33.39%	4.023%
97	25.379	3790	3794	3803	rVB3	285288	676619	18.11%	2.181%
98	25.925	3881	3887	3895	rBV6	234900	638571	17.09%	2.059%
99	26.466	3972	3979	3998	rVB7	350806	1360038	36.40%	4.385%
100	27.553	4157	4164	4182	rVB4	368806	1420517	38.02%	4.580%

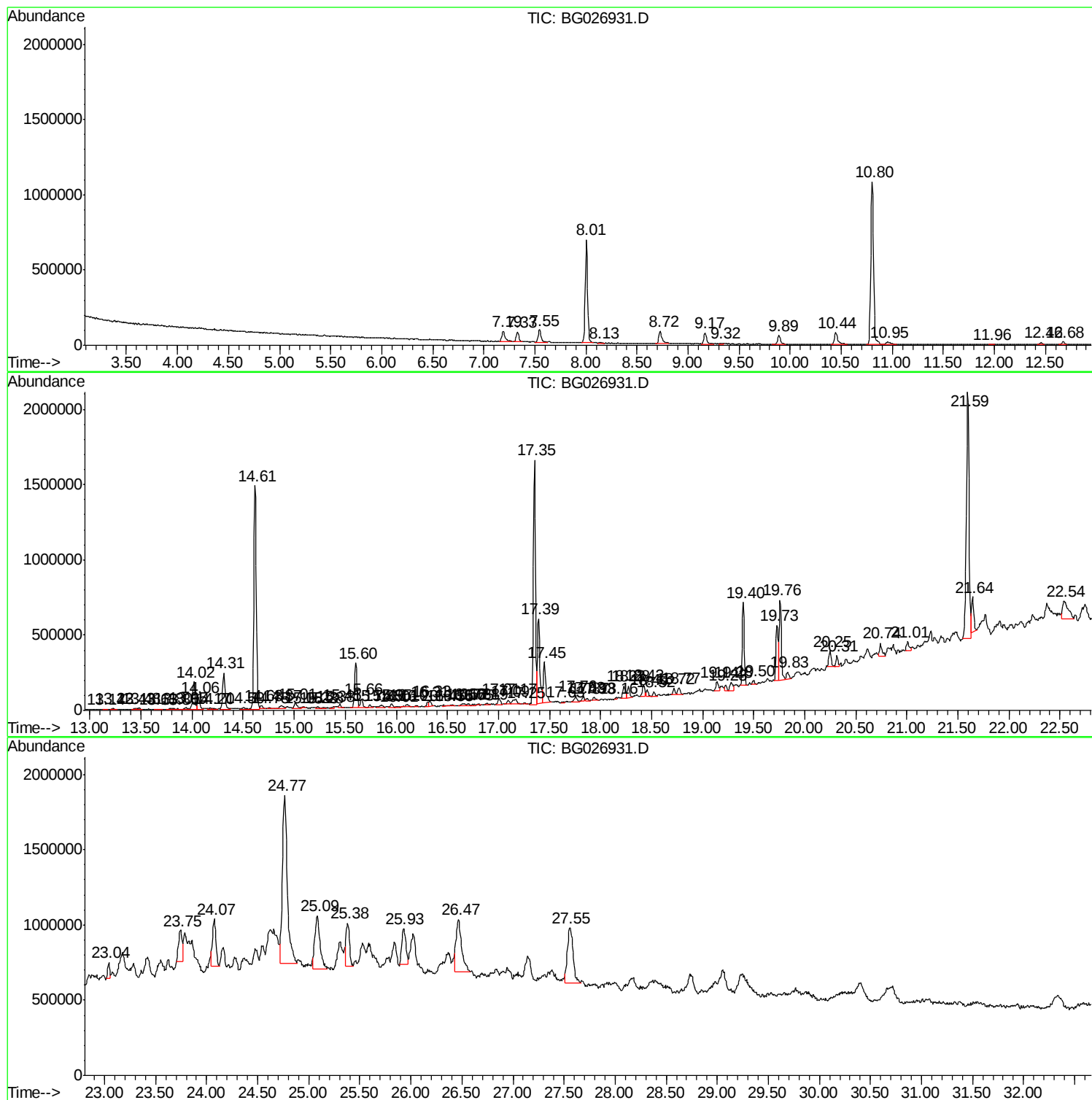
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Instrument :
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG042717.M
Quant Title : SVOA CALIBRATION

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



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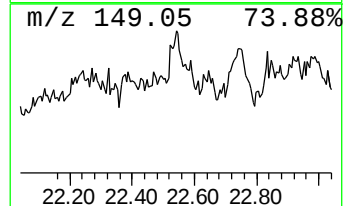
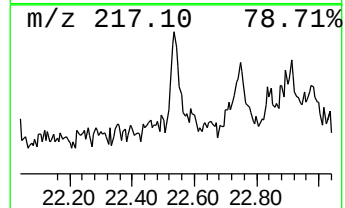
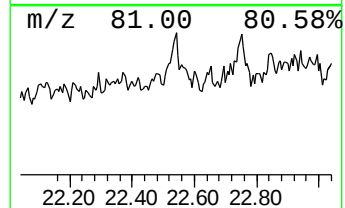
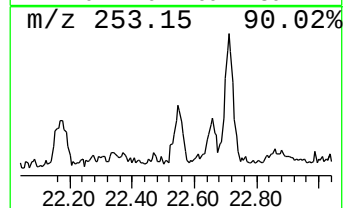
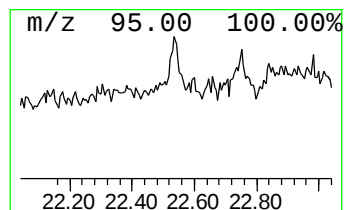
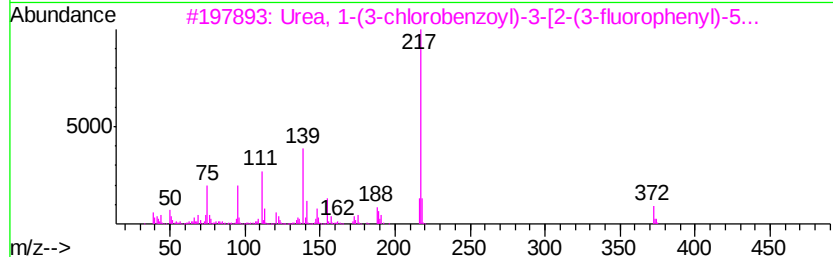
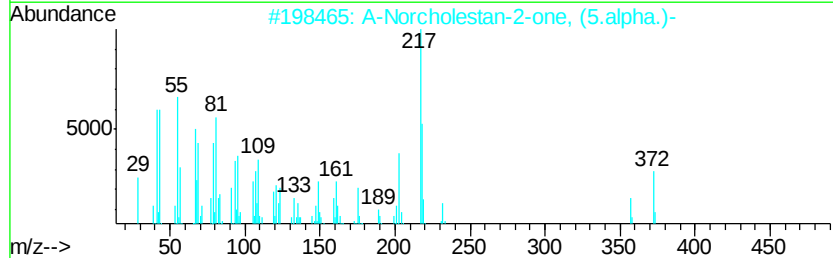
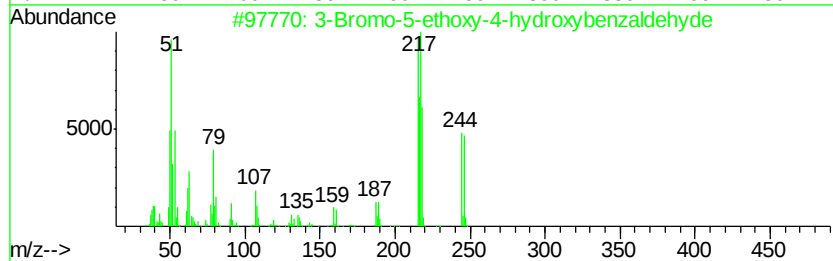
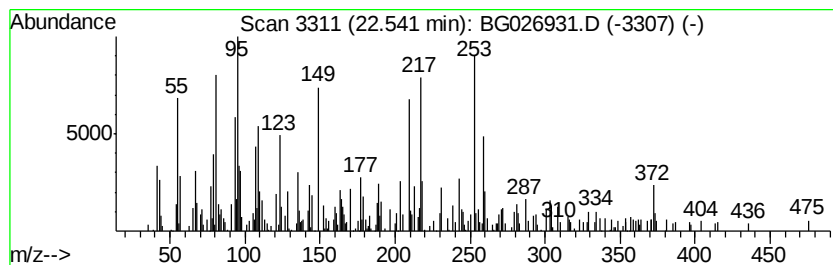
Instrument :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG042717.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 3-Bromo-5-ethoxy-4-hydroxyb... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
22.54	3.06 ng/ul	443014	Chrysene-d12	21.59		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Bromo-5-ethoxy-4-hydroxybenzal...	244	C9H9BrO3	003111-37-3	53	
2	A-Norcholestan-2-one, (5.alpha.)-	372	C26H44O	002310-36-3	49	
3	Urea, 1-(3-chlorobenzoyl)-3-[2-(...	372	C18H14ClFN4O2	1000317-02-0	14	
4	3-Ethyl-4-[(ethylaminocarbonyl)i...	261	C13H15N3O3	1000326-44-6	11	
5	Disiloxane, hexaethyl-	246	C12H30OSi2	000994-49-0	10	



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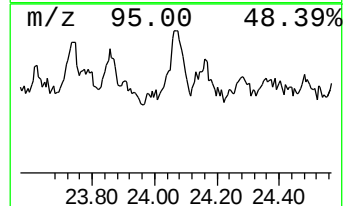
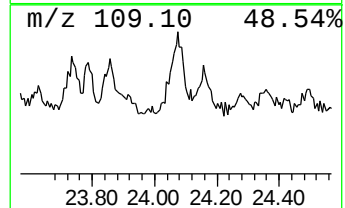
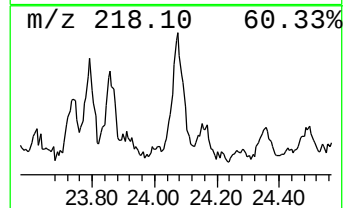
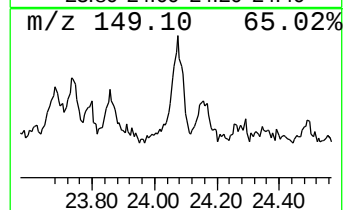
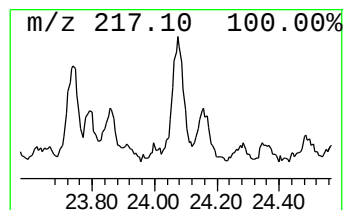
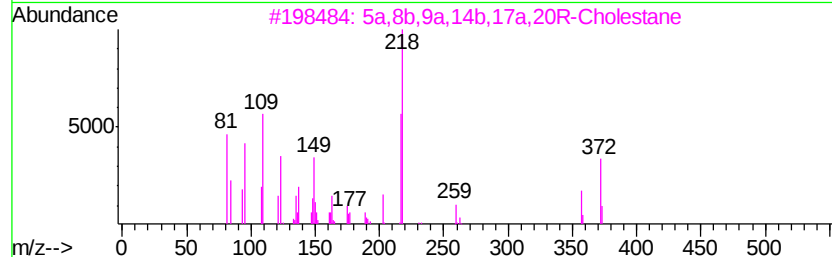
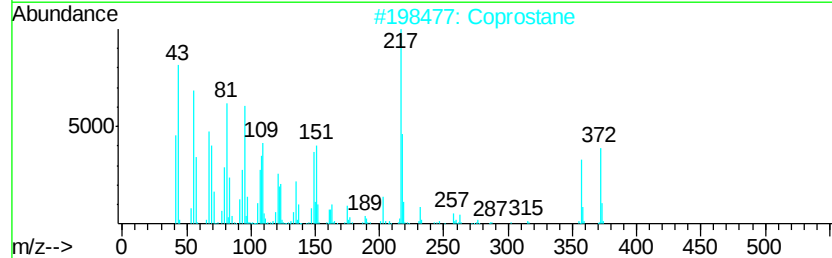
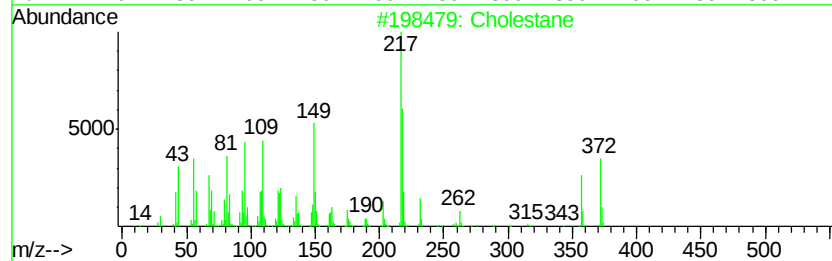
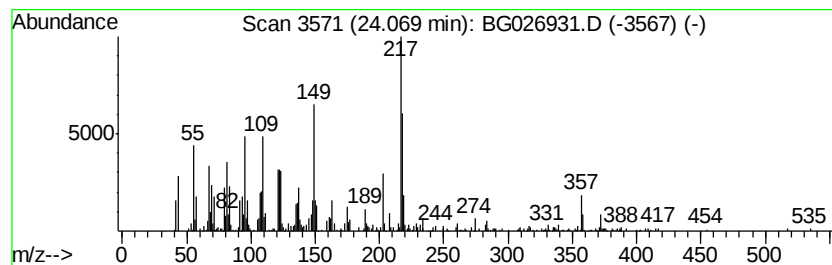
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Cholestane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.07	3.89 ng/ul	727636	Perylene-d12	24.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cholestane		372 C27H48	000481-21-0 87
2	Coprostone		372 C27H48	000481-20-9 59
3	5a,8b,9a,14b,17a,20R-Cholestane		372 C27H48	1000147-83-1 43
4	Cholestane		372 C27H48	000481-21-0 27
5	3-Bromo-5-ethoxy-4-hydroxybenzal...		244 C9H9BrO3	003111-37-3 25



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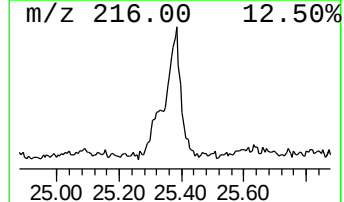
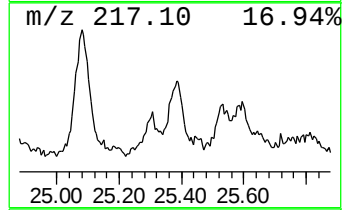
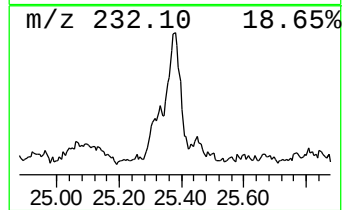
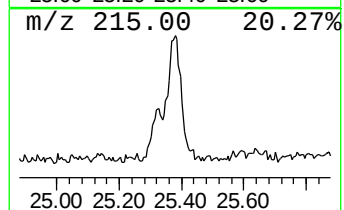
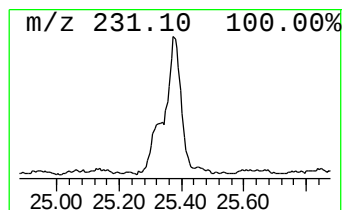
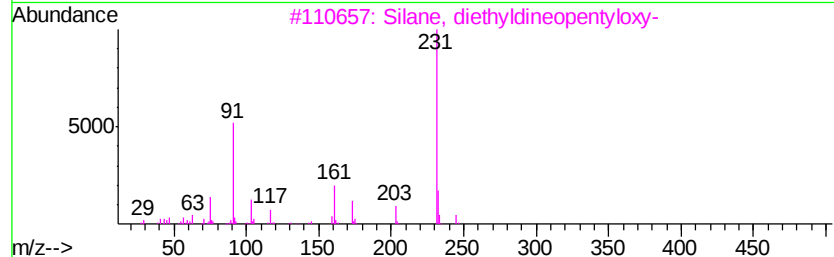
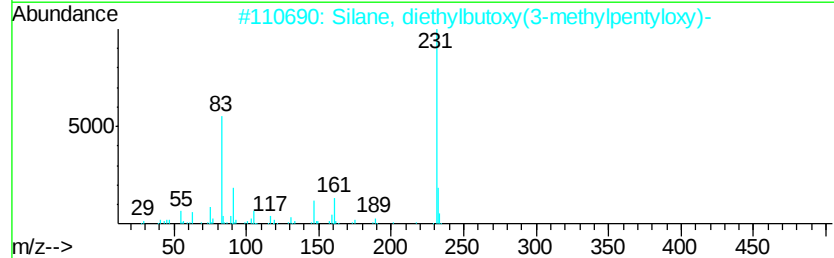
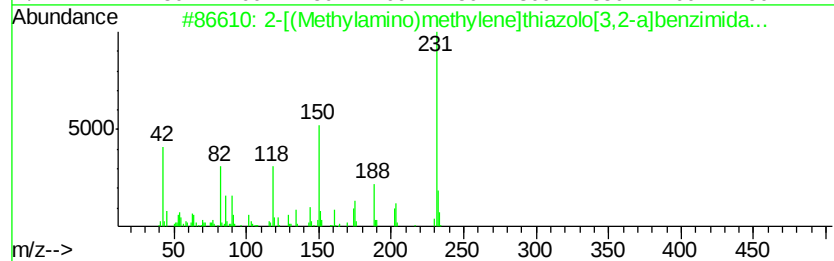
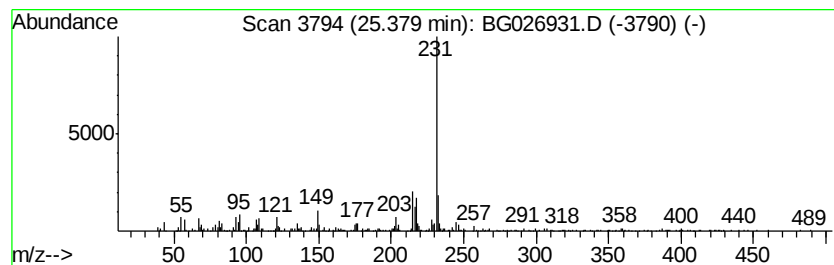
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.38	3.62 ng/ul	676619	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-[(Methylamino)methylene]thiazo...	231	C11H9N3OS	072740-41-1	49
2		Silane, diethylbutoxy(3-methylpe...	260	C14H32O2Si	1000363-48-4	47
3		Silane, diethyldineopentyloxy-	260	C14H32O2Si	1000363-94-9	47
4		2,6-Diphenylpyridine	231	C17H13N	003558-69-8	43
5		Cannabichromene	314	C21H30O2	020675-51-8	43



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050917\
Data File : BG026931.D
Acq On : 10 May 2017 3:32
Operator : SJ/MA
Sample : I2884-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
YAB34

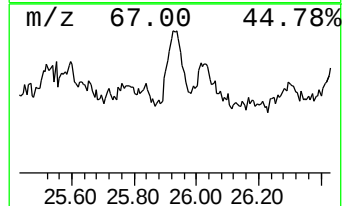
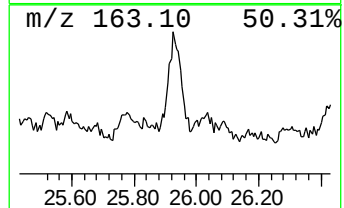
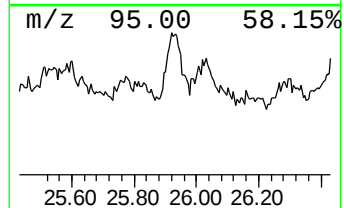
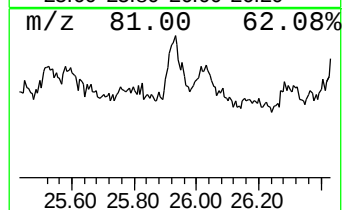
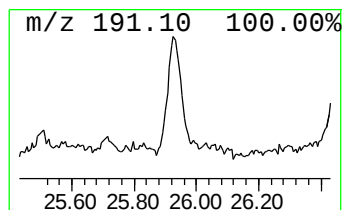
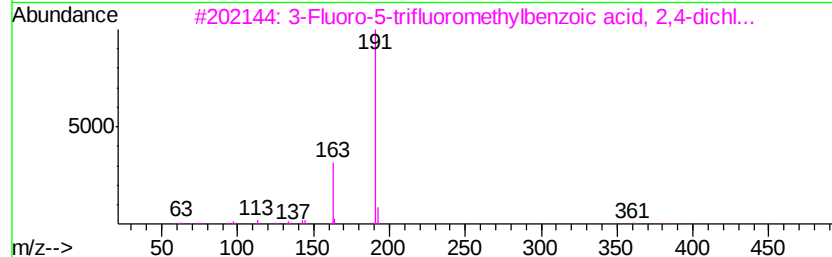
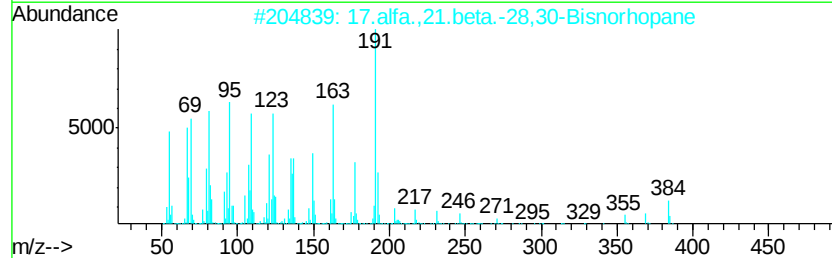
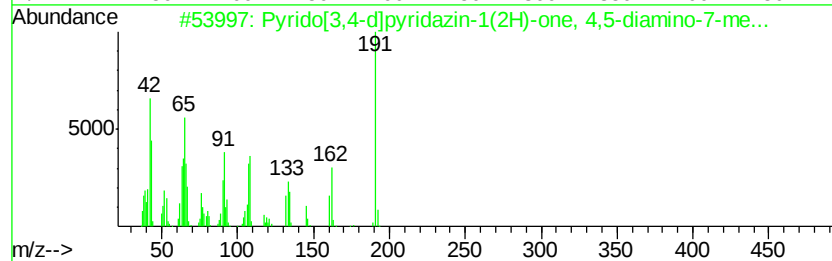
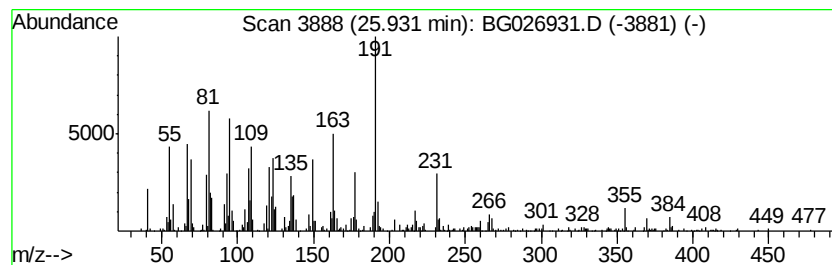
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Pyrido[3,4-d]pyridazin-1(2H)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.93	3.42 ng/ul	638571	Perylene-d12	24.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	74
2		17.alfa.,21.beta.-28,30-Bisnorho...	384	C28H48	1000360-26-1	42
3		3-Fluoro-5-trifluoromethylbenzoi...	380	C15H6Cl2F4O3	1000357-34-5	38
4		5-Fluoro-2-trifluoromethylbenzoi...	320	C14H6F6O2	1000357-62-5	38
5		Isophthalic acid, oct-3-en-2-yl ...	318	C19H26O4	1000343-89-0	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050917\
Data File : BG026931.D
Acq On : 10 May 2017 3:32
Operator : SJ/MA
Sample : I2884-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
YAB34

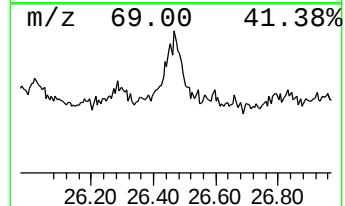
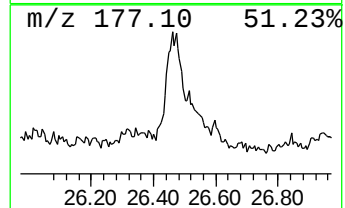
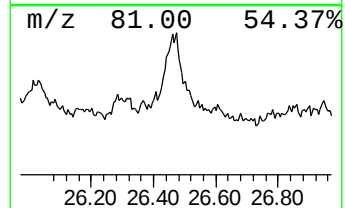
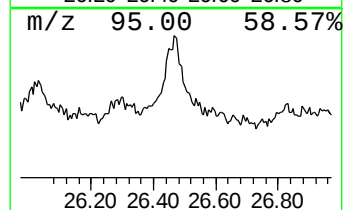
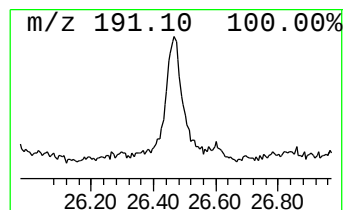
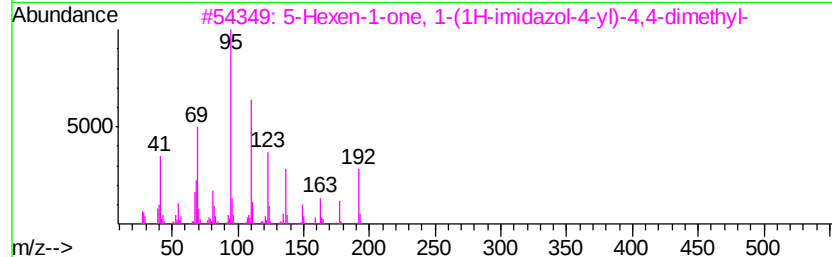
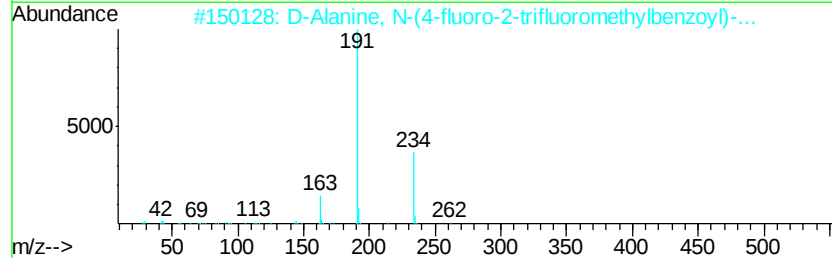
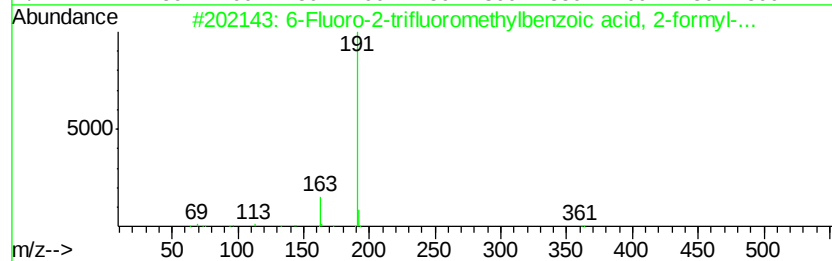
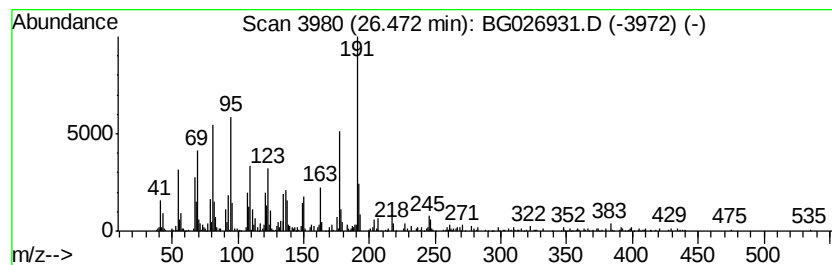
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG042717.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.47	7.28 ng/ul	1360040	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Fluoro-2-trifluoromethylbenzoi...	380	C15H6Cl2F4O3	1000343-74-4	22
2		D-Alanine, N-(4-fluoro-2-trifluo...	307	C13H13F4NO3	1000348-40-0	22
3		5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	20
4		p-Cyanophenyl p-(2-methylbutoxy)...	309	C19H19NO3	067951-45-5	18
5		3-Fluoro-5-trifluoromethylbenzoi...	329	C14H7F4NO4	1000357-96-3	18



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050917\
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Acq On : 10 May 2017 3:32
Operator : SJ/MA
Sample : I2884-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

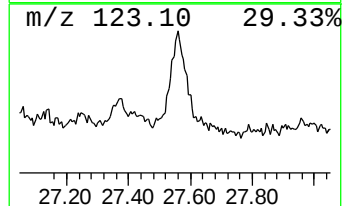
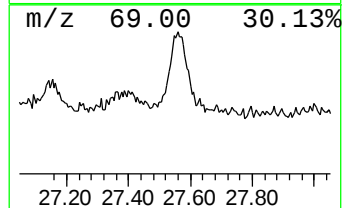
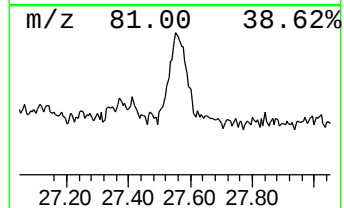
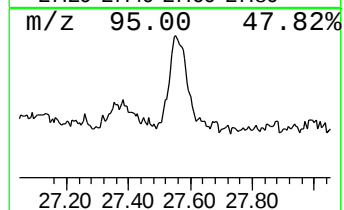
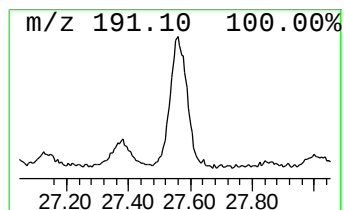
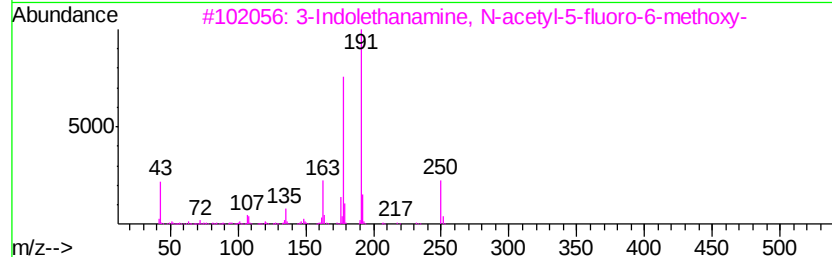
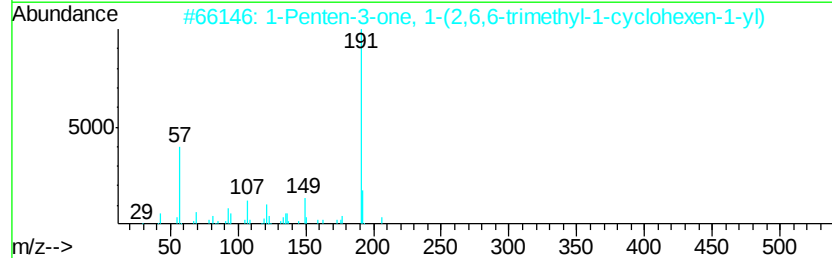
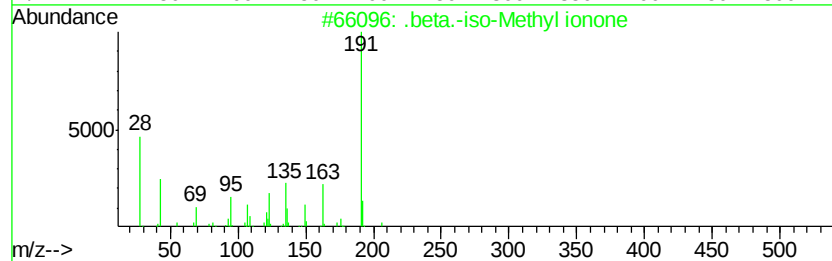
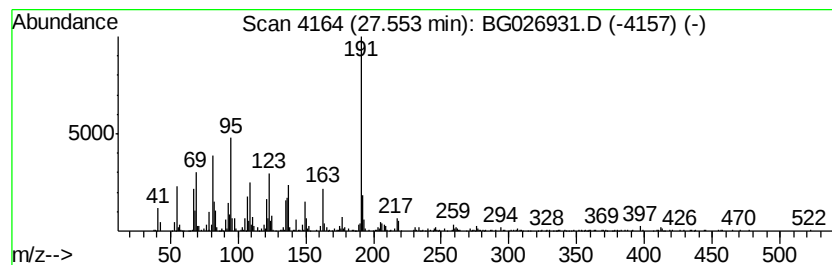
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG042717.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 .beta.-iso-Methyl ionone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
27.55	7.60 ng/ul	1420520	Perylene-d12	24.76		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	41
3		3-Indolethanamine, N-acetyl-5-fl...	250	C13H15FN2O2	1000116-27-1	38
4		4-Fluoro-2-trifluoromethylbenzoi...	278	C13H14F4O2	1000357-27-5	35
5		2-Amino-4-methyl-6-(2-thienyl)py...	191	C9H9N3S	026963-43-9	30



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050917\
Data File : BG026931.D
Acq On : 10 May 2017 3:32
Operator : SJ/MA
Sample : I2884-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
YAB34

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG042717.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
3-Bromo-5-ethoxy-...	22.54	3.1	ng/ul	443014	5	21.59	2899850	20.0
Cholestane	24.07	3.9	ng/ul	727636	6	24.76	3736600	20.0
unknown-01	25.38	3.6	ng/ul	676619	6	24.76	3736600	20.0
Pyrido[3,4-d]pyri...	25.93	3.4	ng/ul	638571	6	24.76	3736600	20.0
unknown-02	26.47	7.3	ng/ul	1360040	6	24.76	3736600	20.0
.beta.-iso-Methyl...	27.55	7.6	ng/ul	1420520	6	24.76	3736600	20.0