

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120621\
 Data File : BG051397.D
 Acq On : 8 Dec 2021 00:47
 Operator : CG/JU
 Sample : M4870-05
 Misc :
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BGKP2

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % 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

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
 Title : SVOA CALIBRATION

Signal : TIC: BG051397.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.523	3	6	14	rVB2	7370	12566	1.22%	0.113%
2	3.964	77	81	94	rVB	22760	40260	3.91%	0.362%
3	5.650	362	368	376	rBV	8011	14289	1.39%	0.128%
4	5.786	386	391	400	rBV	21926	47029	4.57%	0.422%
5	6.162	450	455	459	rBV2	6475	9432	0.92%	0.085%
6	6.784	555	561	569	rBV4	3968	7973	0.77%	0.072%
7	7.354	652	658	670	rVB3	33067	86392	8.39%	0.776%
8	7.501	676	683	691	rBV	101723	178750	17.37%	1.606%
9	7.583	694	697	704	rVB	5816	9765	0.95%	0.088%
10	7.719	712	720	733	rBV	100934	188718	18.34%	1.695%
11	7.818	733	737	742	rVB	8607	13163	1.28%	0.118%
12	8.189	793	800	806	rBV	107877	188346	18.30%	1.692%
13	8.717	884	890	894	rVB4	4435	7527	0.73%	0.068%
14	8.905	915	922	933	rBV2	87029	160814	15.63%	1.444%
15	9.017	937	941	950	rVV5	6074	10492	1.02%	0.094%
16	9.111	950	957	966	rVB4	3048	7194	0.70%	0.065%
17	9.364	993	1000	1009	rBV	123233	229284	22.28%	2.059%
18	9.704	1053	1058	1062	rVB2	5455	7815	0.76%	0.070%
19	10.092	1116	1124	1132	rBV	104722	192825	18.74%	1.732%
20	10.645	1211	1218	1228	rBV	151535	280695	27.28%	2.521%
21	10.756	1231	1237	1248	rBV2	32521	64095	6.23%	0.576%
22	11.015	1271	1281	1286	rVV	150722	279356	27.15%	2.509%
23	11.062	1286	1289	1296	rVV	35806	61604	5.99%	0.553%
24	11.156	1298	1305	1317	rVV	108868	214913	20.88%	1.930%
25	12.378	1509	1513	1521	rVB3	4873	8289	0.81%	0.074%
26	12.660	1554	1561	1571	rVB	22250	37374	3.63%	0.336%
27	12.877	1590	1598	1606	rVB2	16224	29711	2.89%	0.267%
28	13.606	1716	1722	1726	rBV2	9049	13268	1.29%	0.119%
29	13.659	1726	1731	1738	rBV3	8091	13863	1.35%	0.125%
30	13.988	1781	1787	1795	rBV8	5404	14355	1.39%	0.129%
31	14.140	1806	1813	1816	rBV4	13677	24934	2.42%	0.224%
32	14.211	1816	1825	1831	rVV	307483	484986	47.13%	4.356%
33	14.428	1856	1862	1870	rVV4	12307	27966	2.72%	0.251%
34	14.516	1870	1877	1887	rVV	334560	535861	52.07%	4.813%
35	14.822	1920	1929	1936	rVV	232219	380996	37.02%	3.422%
36	15.063	1964	1970	1985	rVV2	23889	62956	6.12%	0.565%

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
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37	15.210	1985	1995	2002	rVV9	8140	21900	2.13%	0.197%
38	15.427	2027	2032	2038	rVB4	7314	12058	1.17%	0.108%
39	15.580	2050	2058	2060	rBV3	10151	16700	1.62%	0.150%
40	15.615	2060	2064	2072	rVB5	11976	23865	2.32%	0.214%

41	15.809	2085	2097	2104	rBV2	585561	1004566	97.61%	9.023%
42	15.950	2115	2121	2131	rBV	129788	217093	21.09%	1.950%
43	16.238	2164	2170	2171	rBV	9215	14492	1.41%	0.130%
44	16.261	2171	2174	2179	rVV4	11887	19815	1.93%	0.178%
45	16.314	2179	2183	2187	rVV	11724	20149	1.96%	0.181%

46	16.355	2187	2190	2195	rVV3	6649	10159	0.99%	0.091%
47	16.426	2199	2202	2206	rVV5	5472	8403	0.82%	0.075%
48	16.479	2206	2211	2216	rVV8	7667	19543	1.90%	0.176%
49	16.532	2216	2220	2224	rVV	27156	38675	3.76%	0.347%
50	16.626	2231	2236	2240	rVV	55523	80734	7.84%	0.725%

51	16.679	2240	2245	2252	rVV2	102245	194921	18.94%	1.751%
52	16.743	2252	2256	2260	rVV2	88806	128594	12.50%	1.155%
53	16.790	2260	2264	2268	rVV	43864	65996	6.41%	0.593%
54	16.843	2268	2273	2274	rVV	17942	27493	2.67%	0.247%
55	16.867	2274	2277	2279	rVV	29316	41470	4.03%	0.372%

56	16.890	2279	2281	2284	rVV	20811	25868	2.51%	0.232%
57	16.943	2285	2290	2297	rVV3	60513	119628	11.62%	1.074%
58	17.014	2297	2302	2305	rVV	62709	92545	8.99%	0.831%
59	17.049	2305	2308	2311	rVV3	26245	42532	4.13%	0.382%
60	17.084	2311	2314	2322	rVB2	34016	51996	5.05%	0.467%

61	17.225	2332	2338	2342	rBV6	5144	7318	0.71%	0.066%
62	17.278	2342	2347	2350	rBV2	8311	14018	1.36%	0.126%
63	17.437	2368	2374	2377	rVB4	14803	19858	1.93%	0.178%
64	17.513	2382	2387	2391	rBV7	5366	10141	0.99%	0.091%
65	17.572	2391	2397	2402	rBV	298520	459844	44.68%	4.130%

66	17.613	2402	2404	2408	rVV	11279	13764	1.34%	0.124%
67	17.672	2408	2414	2422	rVB	530265	828244	80.48%	7.439%
68	17.848	2440	2444	2449	rBV7	5564	9580	0.93%	0.086%
69	18.195	2499	2503	2507	rVB2	30177	39415	3.83%	0.354%
70	18.289	2514	2519	2527	rBV2	4591	13026	1.27%	0.117%

71	18.418	2535	2541	2544	rBV2	8065	15173	1.47%	0.136%
72	18.453	2545	2547	2552	rVV6	5836	10499	1.02%	0.094%
73	18.494	2552	2554	2561	rVB3	8039	10324	1.00%	0.093%
74	18.594	2566	2571	2574	rBV6	5160	9127	0.89%	0.082%
75	18.835	2610	2612	2618	rVB4	8327	11860	1.15%	0.107%

76	18.958	2630	2633	2640	rVB7	5853	11471	1.11%	0.103%
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77	19.164	2663	2668	2673	rBV4	5560	11457	1.11%	0.103%
78	19.264	2681	2685	2688	rVB3	8423	9632	0.94%	0.087%
79	19.323	2692	2695	2698	rBV5	9097	14496	1.41%	0.130%
80	19.352	2698	2700	2704	rVB5	8965	11700	1.14%	0.105%
81	19.522	2723	2729	2735	rVB6	11033	19885	1.93%	0.179%
82	19.587	2735	2740	2744	rBV	10245	17758	1.73%	0.159%
83	19.804	2773	2777	2786	rVB6	10218	19255	1.87%	0.173%
84	19.951	2795	2802	2812	rBV	704912	1029121	100.00%	9.243%
85	20.210	2843	2846	2850	rVB	10571	12705	1.23%	0.114%
86	20.739	2931	2936	2939	rBV5	7088	13295	1.29%	0.119%
87	20.838	2948	2953	2958	rVB	57944	76980	7.48%	0.691%
88	21.185	3009	3012	3016	rVB2	10809	13140	1.28%	0.118%
89	21.450	3053	3057	3068	rBV5	40773	90590	8.80%	0.814%
90	21.555	3072	3075	3080	rVB	6829	9576	0.93%	0.086%
91	21.708	3099	3101	3105	rVB3	7423	7828	0.76%	0.070%
92	21.873	3123	3129	3137	rVB	276812	488240	47.44%	4.385%
93	22.648	3255	3261	3265	rBV5	8525	18522	1.80%	0.166%
94	23.365	3378	3383	3390	rVB4	12901	23062	2.24%	0.207%
95	23.565	3415	3417	3422	rVB4	9217	11580	1.13%	0.104%
96	24.205	3520	3526	3534	rVB5	13696	33775	3.28%	0.303%
97	25.039	3656	3668	3679	rVB2	310202	919919	89.39%	8.263%
98	25.198	3689	3695	3699	rBV4	15252	38823	3.77%	0.349%
99	25.274	3699	3708	3721	rVB3	161211	488480	47.47%	4.387%
100	26.379	3890	3896	3897	rBV6	14298	23071	2.24%	0.207%

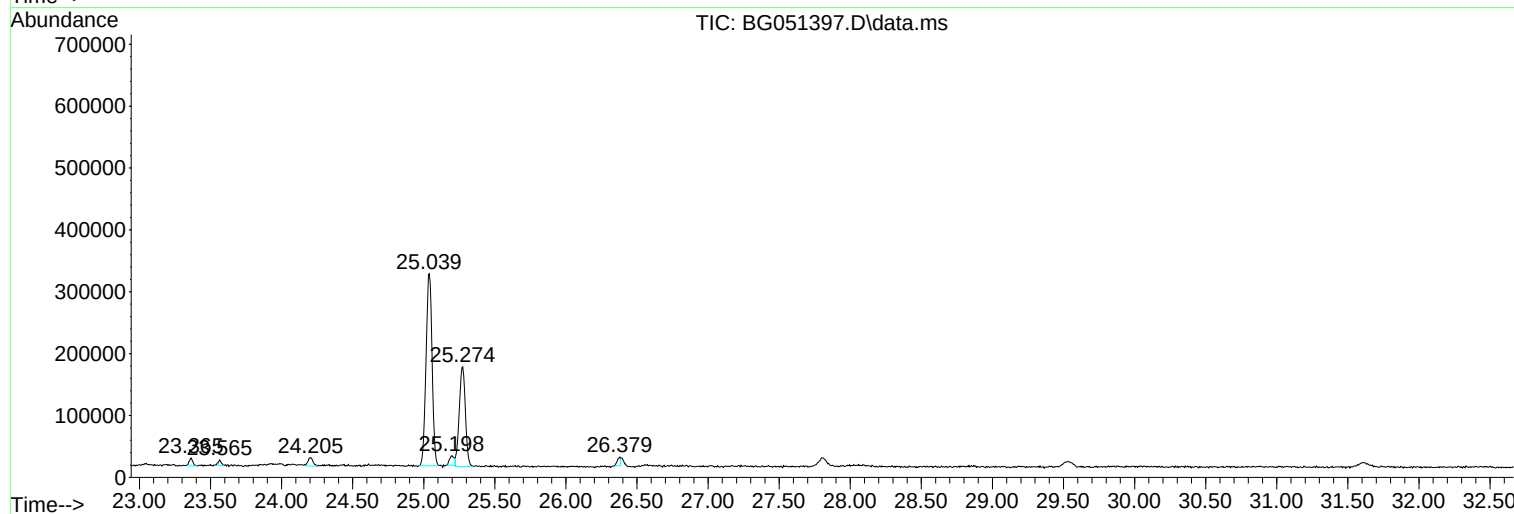
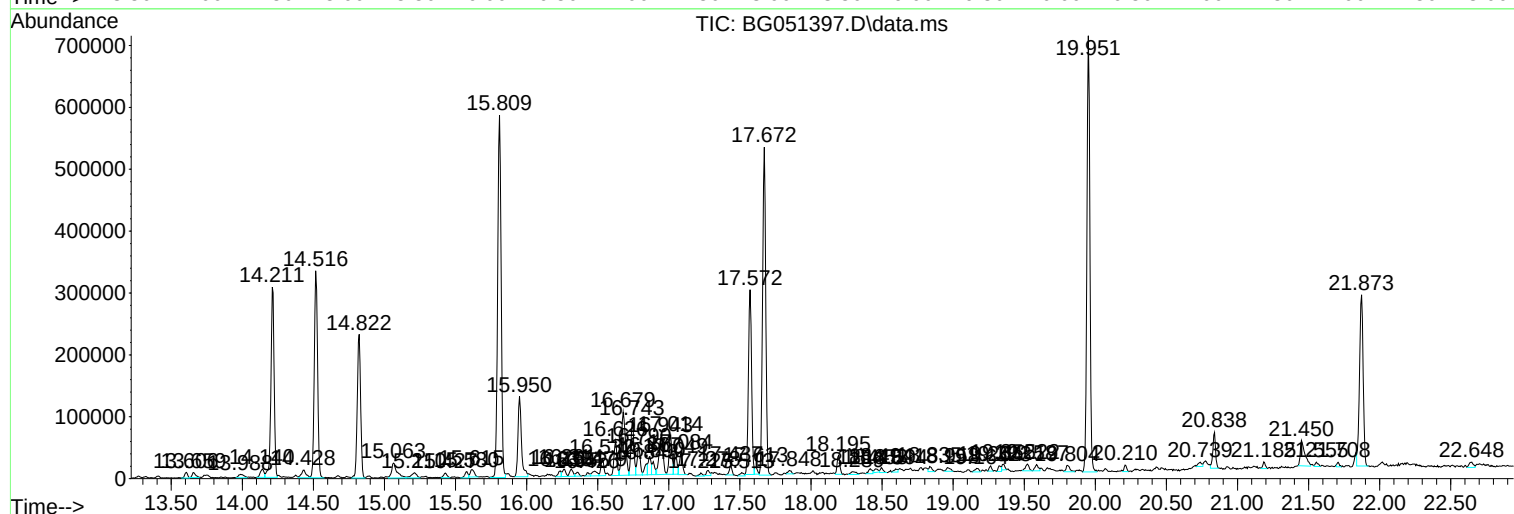
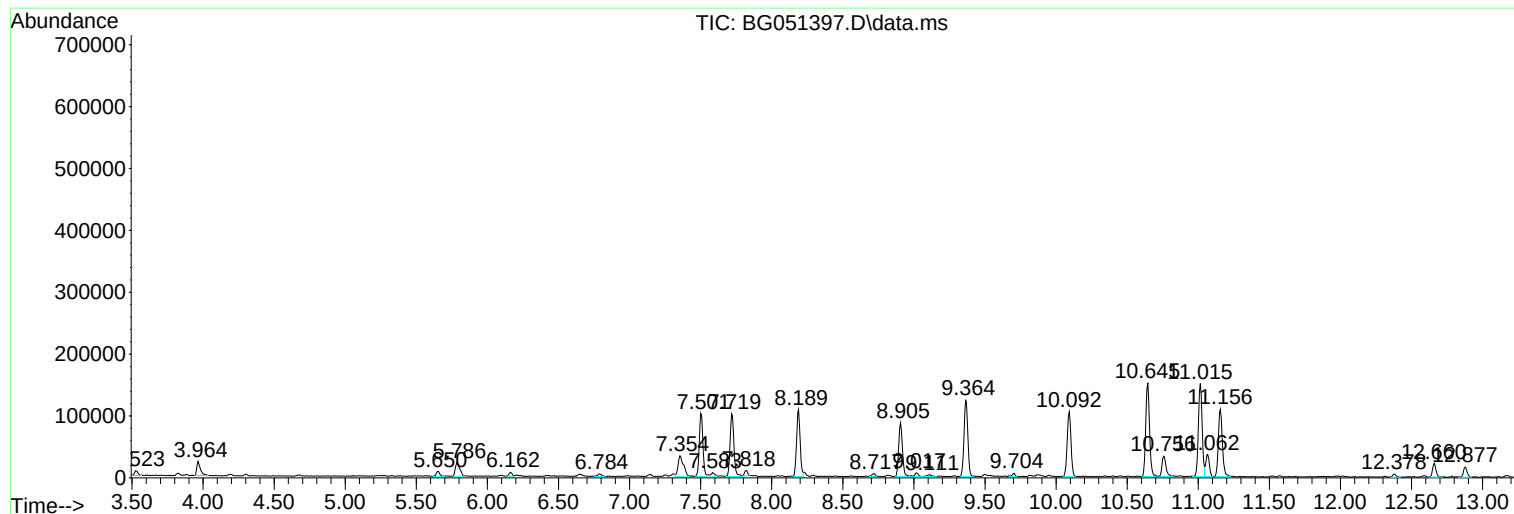
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

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



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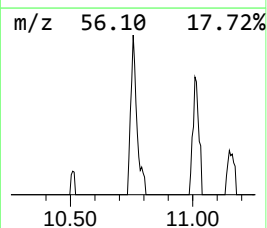
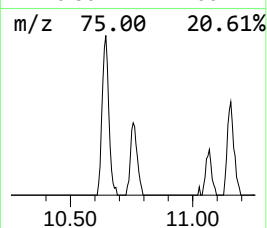
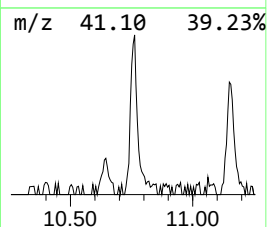
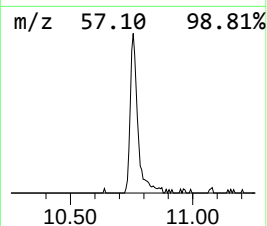
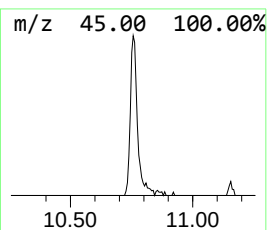
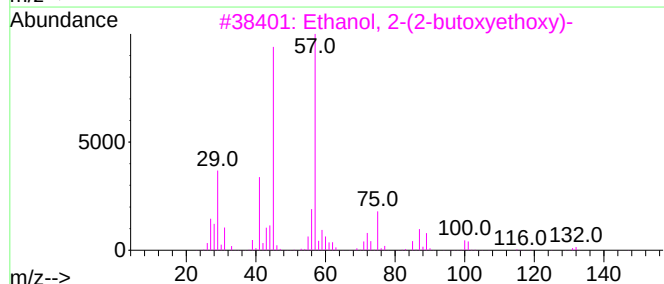
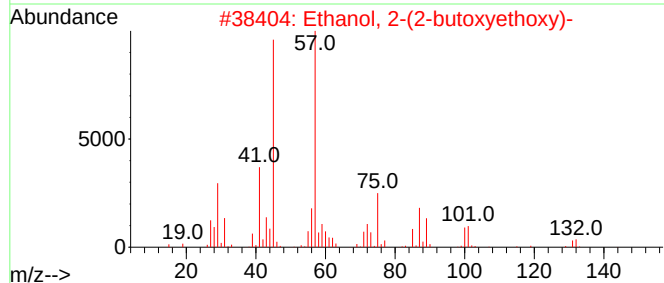
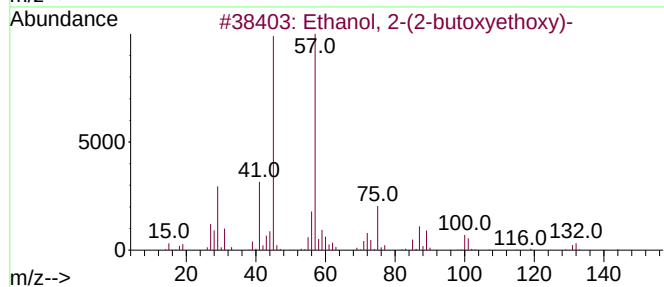
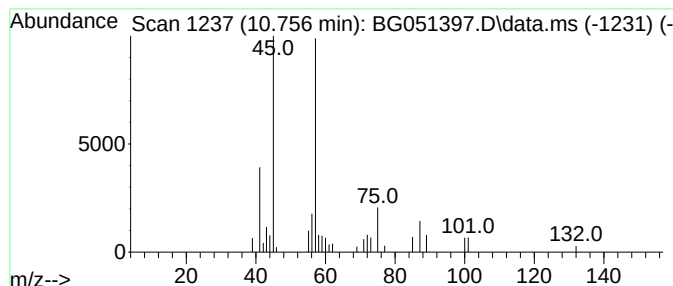
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	4.59 ng/ul	64095	Naphthalene-d8	11.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
5			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83



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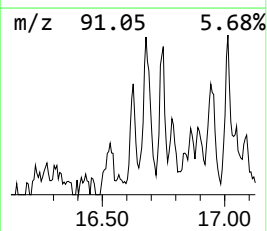
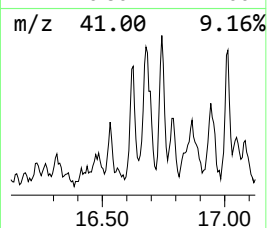
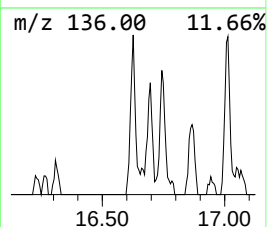
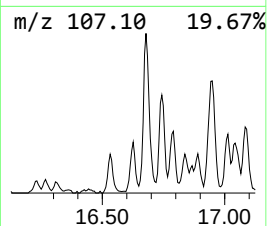
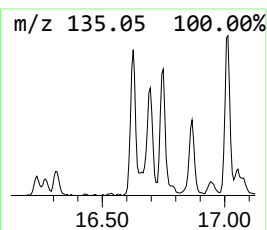
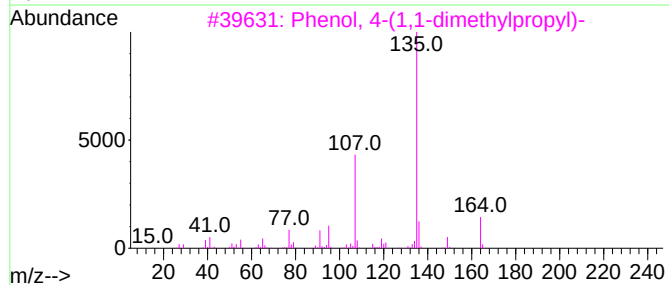
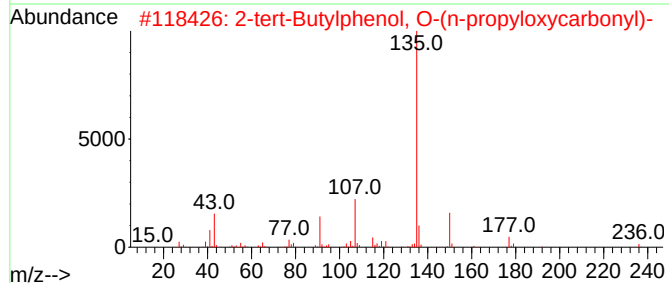
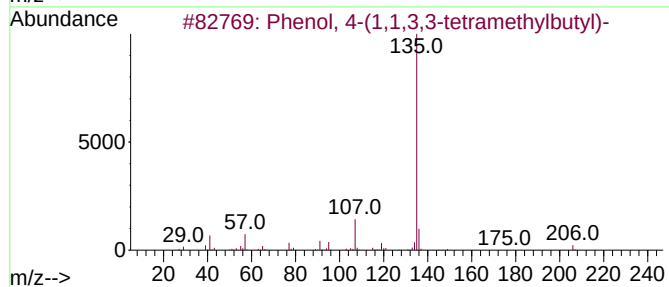
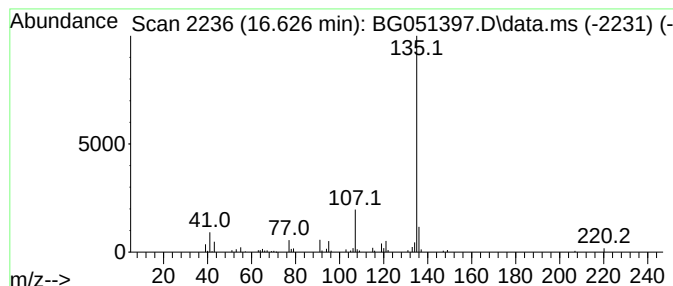
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.626	3.51 ng/ul	80734	Phenanthrene-d10	17.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	86
2			2-tert-Butylphenol, O-(n-propylo...	236	C14H20O3	1000487-37-9	78
3			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
4			4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
5			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	72



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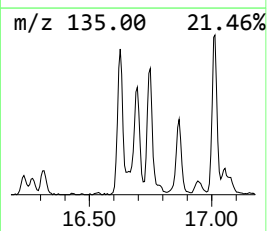
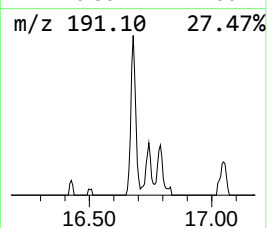
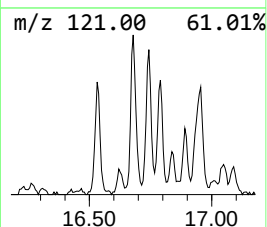
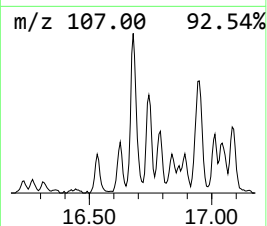
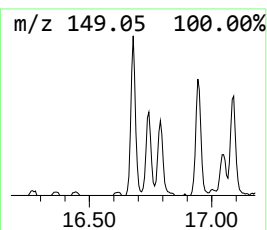
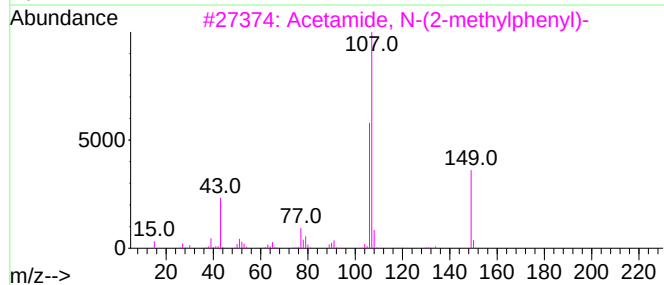
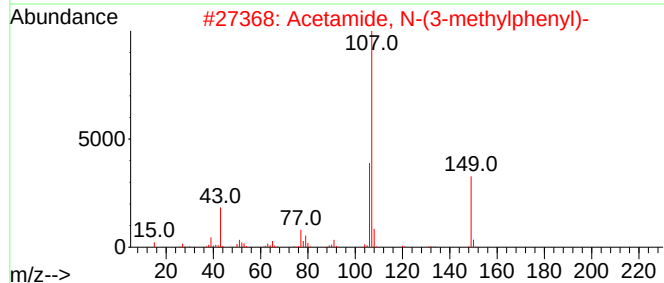
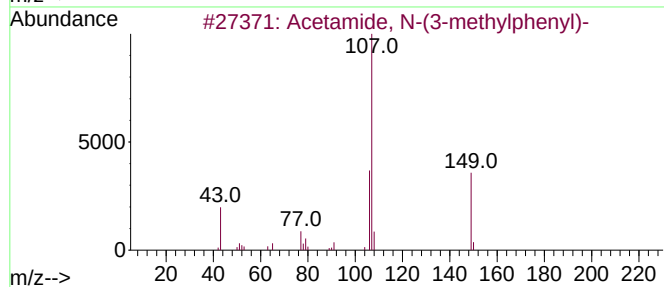
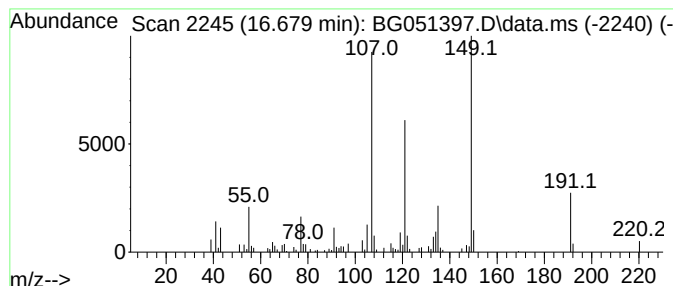
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 Acetamide, N-(3-methylphenyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.679	8.48 ng/ul	194921	Phenanthrene-d10	17.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	52
2			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	52
3			Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	50
4			Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	43
5			1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120621\
Data File : BG051397.D
Acq On : 8 Dec 2021 00:47
Operator : CG/JU
Sample : M4870-05
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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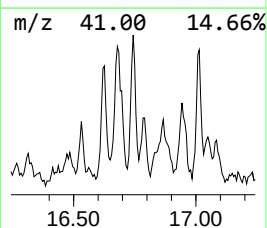
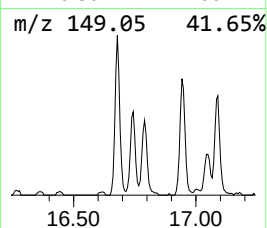
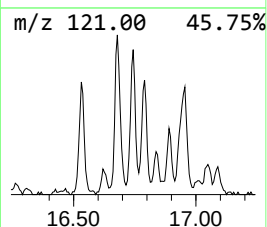
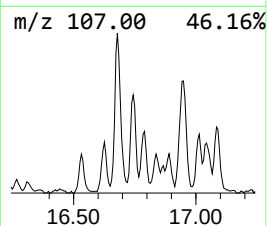
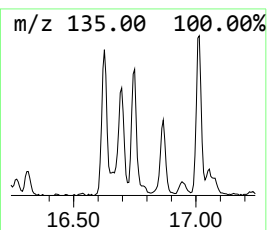
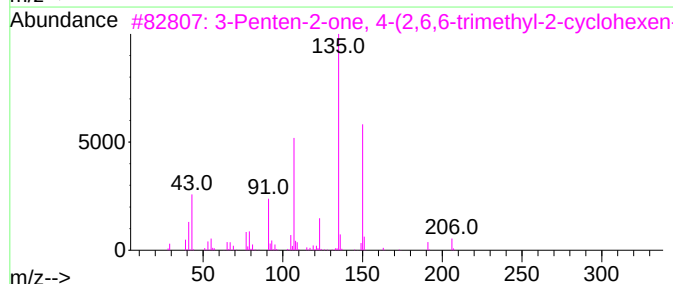
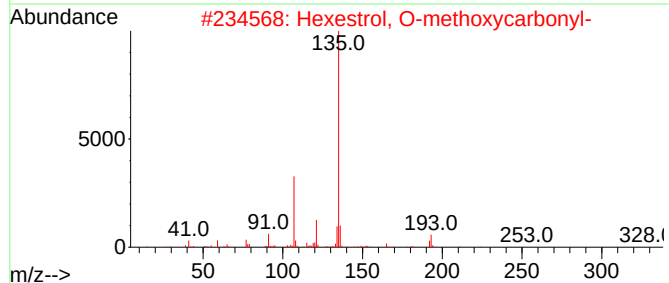
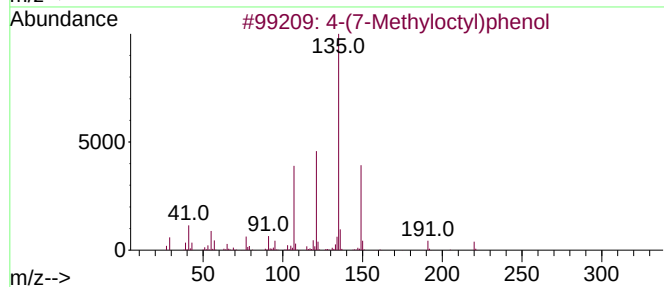
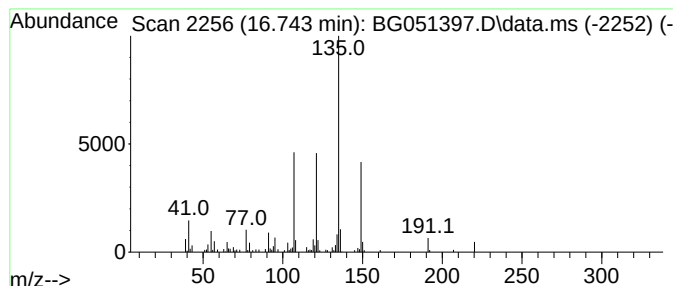
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 4-(7-Methyloctyl)phenol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.743	5.59 ng/ul	128594	Phenanthrene-d10	17.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	98
2			Hexestrol, O-methoxycarbonyl-	328	C20H24O4	1000487-66-3	53
3			3-Penten-2-one, 4-(2,6,6-trimeth...	206	C14H22O	114933-28-7	50
4			((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	50
5			6-Fluoroindole	135	C8H6FN	000399-51-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120621\
Data File : BG051397.D
Acq On : 8 Dec 2021 00:47
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Sample : M4870-05
Misc :
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Instrument :
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ClientSampleId :
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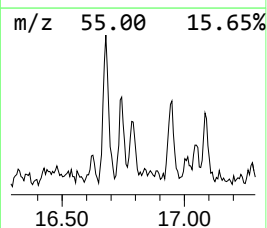
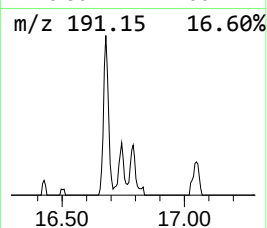
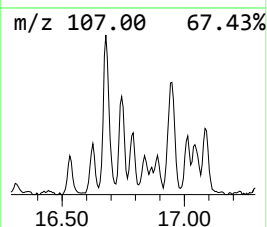
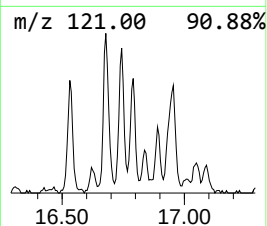
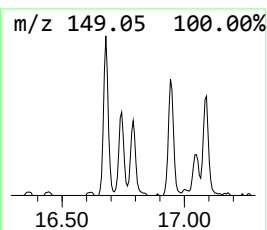
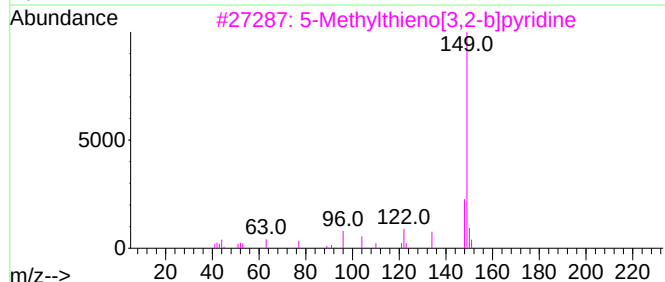
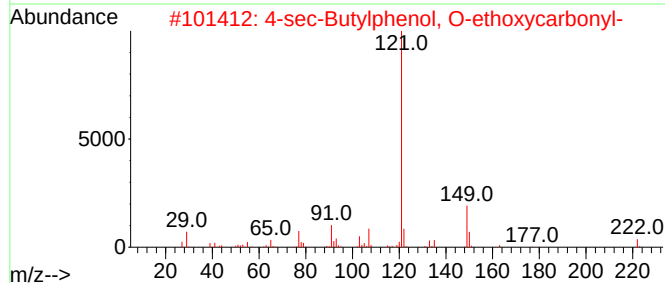
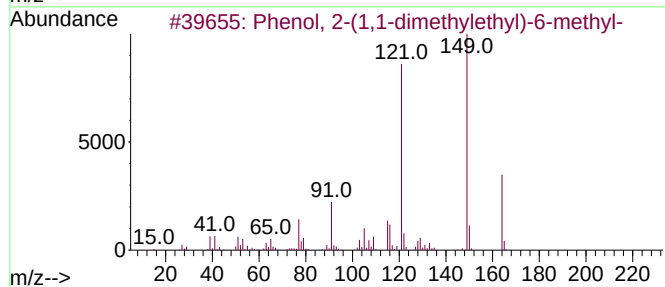
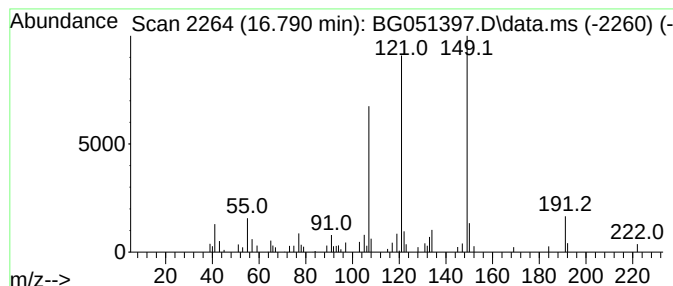
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Phenol, 2-(1,1-dimethylethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.790	2.87 ng/ul	65996	Phenanthrene-d10	17.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1-dimethylethyl)-6-...	164	C11H16O	002219-82-1	53
2			4-sec-Butylphenol, O-ethoxycarbo...	222	C13H18O3	1000487-30-7	41
3			5-Methylthieno[3,2-b]pyridine	149	C8H7NS	001759-29-1	38
4			p-Sec-butylphenyl acetate	192	C12H16O2	003245-24-7	38
5			2-Methyl-4-propylphenol	150	C10H14O	018441-56-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120621\
Data File : BG051397.D
Acq On : 8 Dec 2021 00:47
Operator : CG/JU
Sample : M4870-05
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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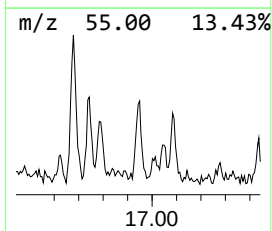
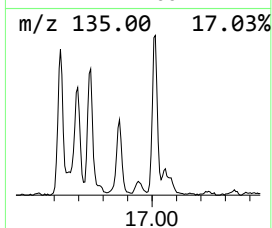
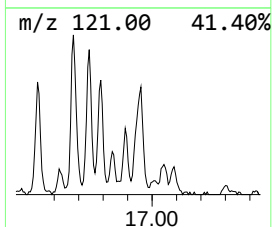
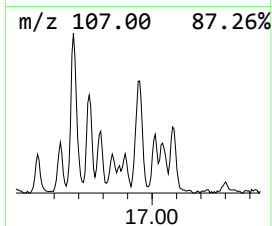
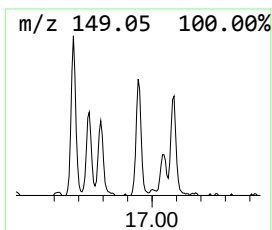
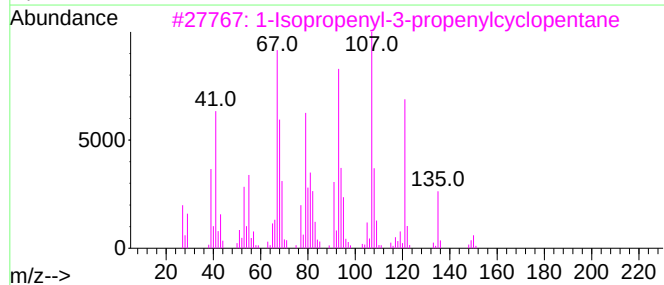
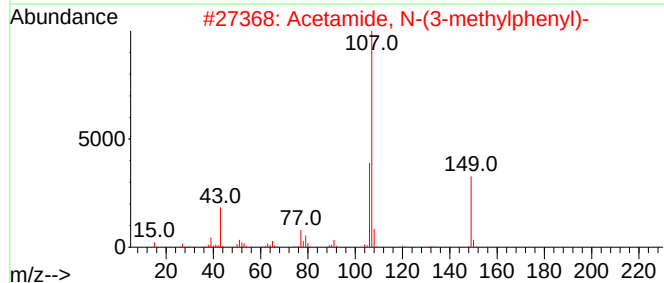
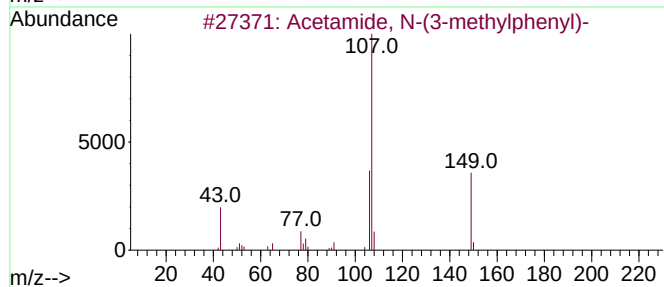
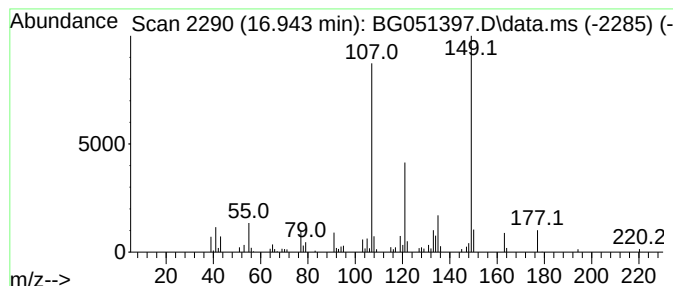
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-Isopropenyl-3-propenylcyc... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.943	5.20 ng/ul	119628	Phenanthrene-d10	17.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	68
2			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	64
3			1-Isopropenyl-3-propenylcyclopentane...	150	C11H18	1000192-81-2	50
4			Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	41
5			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120621\
Data File : BG051397.D
Acq On : 8 Dec 2021 00:47
Operator : CG/JU
Sample : M4870-05
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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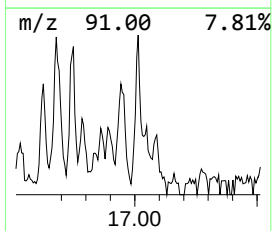
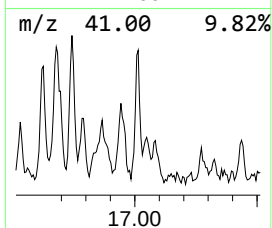
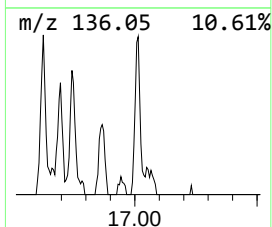
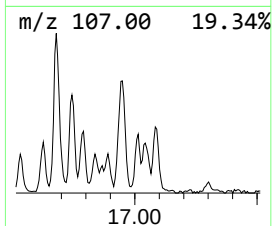
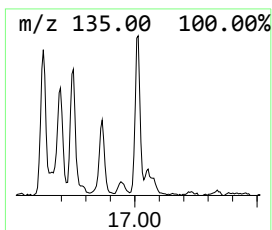
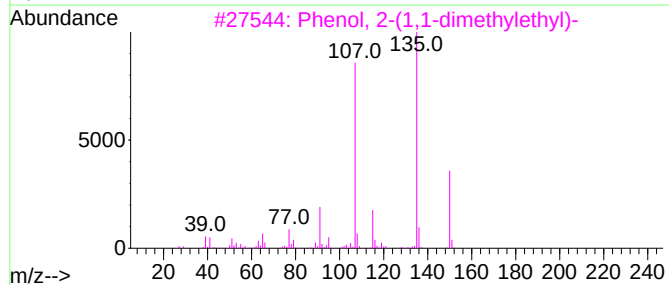
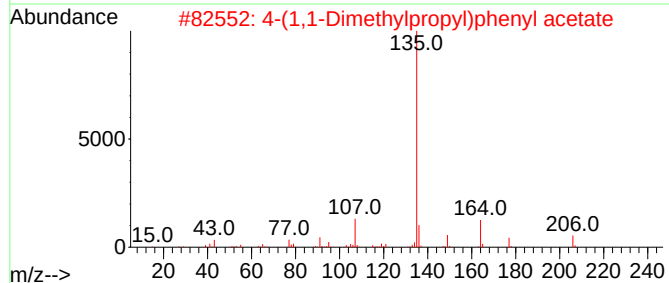
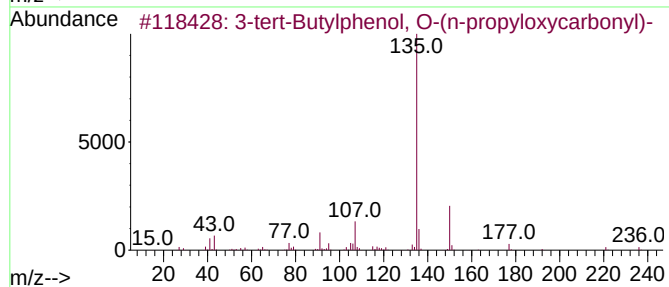
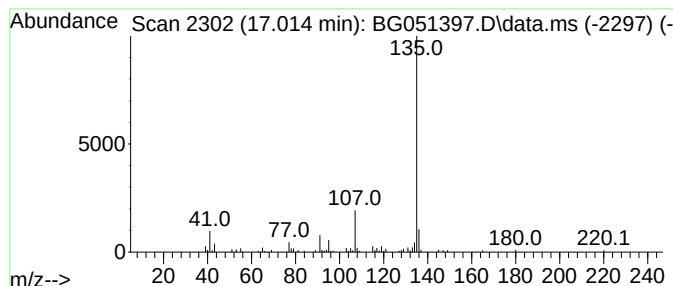
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 3-tert-Butylphenol, O-(n-pr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.014	4.03 ng/ul	92545	Phenanthrene-d10	17.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-tert-Butylphenol, O-(n-propylo...	236	C14H20O3	1000487-38-2	78
2			4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
3			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	72
4			Hexestrol, O-heptafluorobutyryl-	466	C22H21F7O3	1000365-31-9	72
5			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120621\
Data File : BG051397.D
Acq On : 8 Dec 2021 00:47
Operator : CG/JU
Sample : M4870-05
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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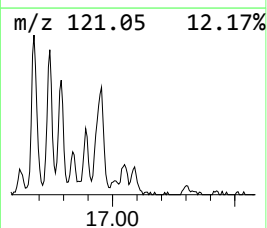
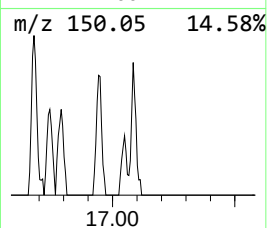
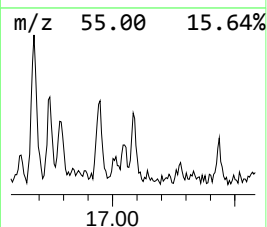
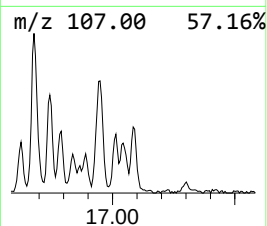
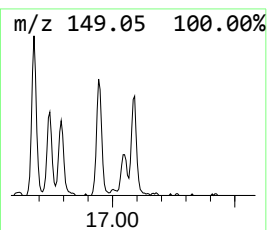
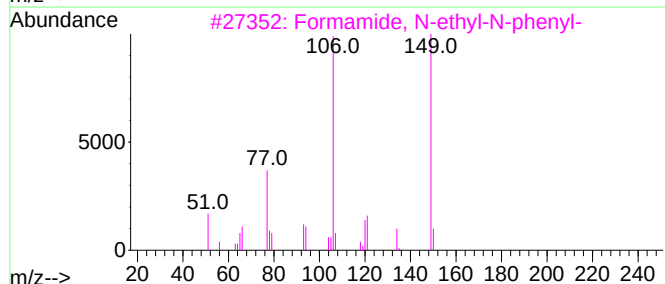
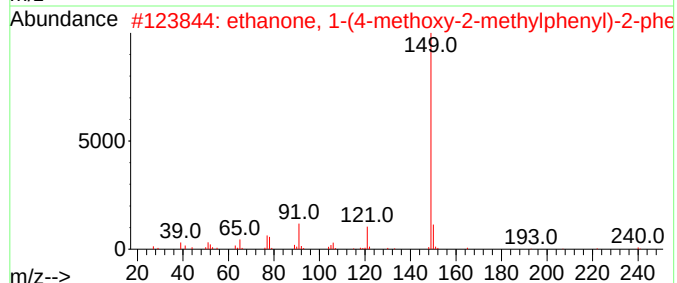
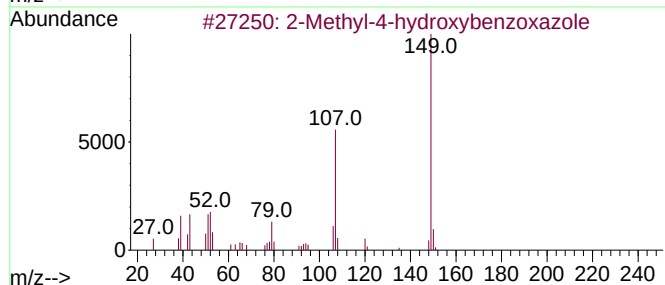
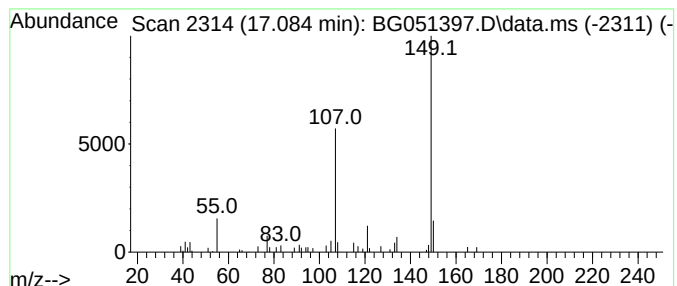
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 2-Methyl-4-hydroxybenzoxazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.084	2.26 ng/ul	51996	Phenanthrene-d10	17.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	72
2			ethanone, 1-(4-methoxy-2-methylp...	240	C16H16O2	1000401-19-7	47
3			Formamide, N-ethyl-N-phenyl-	149	C9H11NO	005461-49-4	40
4			2-t-Butyl-5-[hydroxy-(2,4,6-trim...	306	C18H26O4	092572-63-9	40
5			Benzene, 2-methoxy-4-methyl-1-(1...	164	C11H16O	001076-56-8	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120621\
Data File : BG051397.D
Acq On : 8 Dec 2021 00:47
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Sample : M4870-05
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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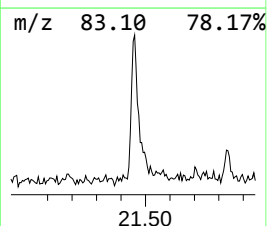
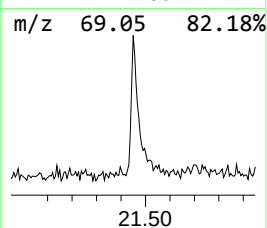
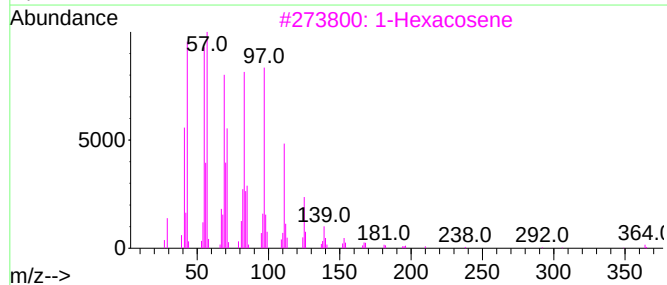
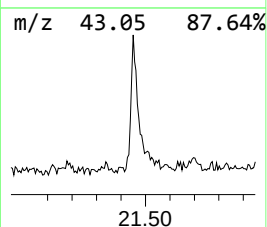
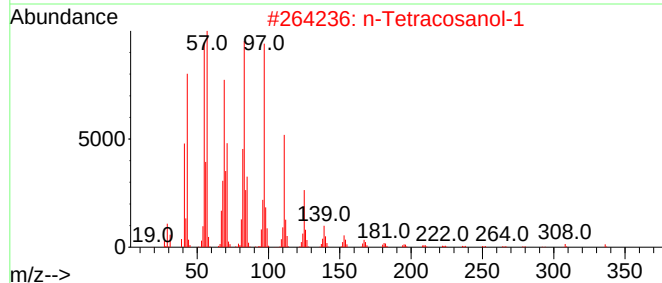
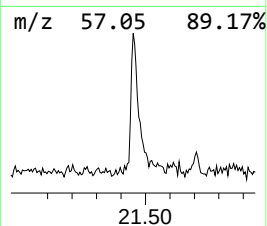
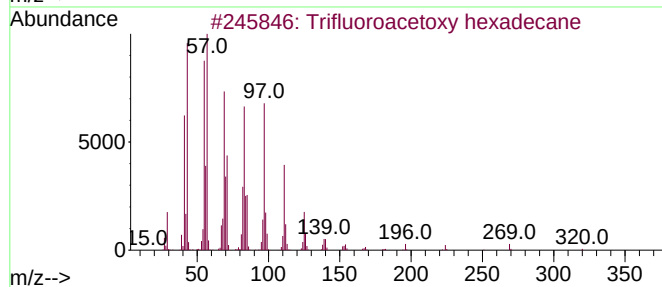
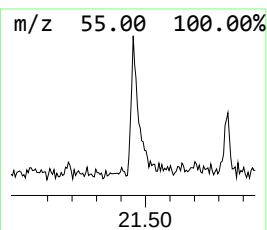
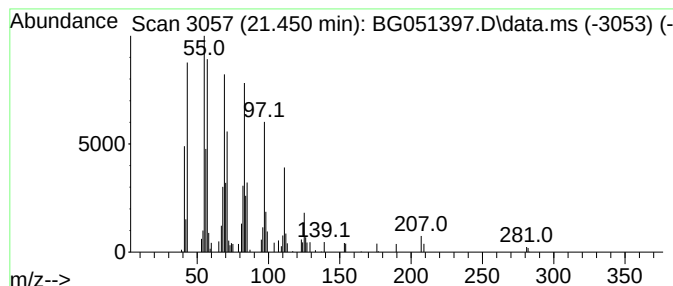
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.450	3.71 ng/ul	90590	Chrysene-d12	21.872

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			1-Hexacosene	364	C26H52	018835-33-1	90
4			Behenic alcohol	326	C22H46O	000661-19-8	87
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120621\
Data File : BG051397.D
Acq On : 8 Dec 2021 00:47
Operator : CG/JU
Sample : M4870-05
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BGKP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Phenol, 4-(1,1,...	16.626	3.5	ng/ul	80734	4	17.572	459844	20.0
Acetamide, N-(3...	16.679	8.5	ng/ul	194921	4	17.572	459844	20.0
4-(7-Methylocty...	16.743	5.6	ng/ul	128594	4	17.572	459844	20.0
Phenol, 2-(1,1-...	16.790	2.9	ng/ul	65996	4	17.572	459844	20.0
1-Isopropenyl-3...	16.943	5.2	ng/ul	119628	4	17.572	459844	20.0
3-tert-Butylphe...	17.014	4.0	ng/ul	92545	4	17.572	459844	20.0
2-Methyl-4-hydr...	17.084	2.3	ng/ul	51996	4	17.572	459844	20.0
Trifluoroacetox...	21.450	3.7	ng/ul	90590	5	21.872	488240	20.0