

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102824\
 Data File : BM048331.D
 Acq On : 30 Oct 2024 20:17
 Operator : RC/JU
 Sample : P4534-15
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 E1L88

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_M\Methods\SFAM-EPA-BM102624.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM048331.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.169	27	31	35	rBV	46565	59429	1.61%	0.136%
2	3.622	106	108	111	rBV3	5077	5610	0.15%	0.013%
3	3.910	153	157	160	rBV2	11657	16947	0.46%	0.039%
4	4.275	215	219	220	rBV4	4987	5257	0.14%	0.012%
5	4.840	310	315	319	rBV6	9748	16500	0.45%	0.038%
6	5.010	339	344	349	rVB8	4280	8436	0.23%	0.019%
7	6.745	636	639	640	rBV2	4577	4839	0.13%	0.011%
8	6.857	653	658	659	rBV2	14351	17484	0.47%	0.040%
9	6.892	659	664	680	rVB2	137674	279157	7.56%	0.638%
10	7.045	684	690	706	rBV	540020	886600	24.00%	2.026%
11	7.151	706	708	712	rVB4	2952	4022	0.11%	0.009%
12	7.245	717	724	735	rBV	585971	968186	26.21%	2.213%
13	7.334	737	739	743	rVB5	4978	7133	0.19%	0.016%
14	7.710	796	803	813	rBV	763277	1267341	34.30%	2.896%
15	7.792	813	817	822	rVB8	5056	10621	0.29%	0.024%
16	8.428	918	925	943	rBV	430914	775959	21.00%	1.773%
17	8.639	956	961	965	rVB7	3858	6829	0.18%	0.016%
18	8.869	993	1000	1009	rBV	591574	1011276	27.37%	2.311%
19	9.292	1063	1072	1077	rVB2	29953	53555	1.45%	0.122%
20	9.445	1093	1098	1106	rBV3	17771	31982	0.87%	0.073%
21	9.592	1115	1123	1138	rBV	465606	821075	22.22%	1.876%
22	10.133	1208	1215	1236	rBV	646729	1279541	34.63%	2.924%
23	10.498	1270	1277	1294	rVB	1063292	1827547	49.47%	4.176%
24	10.645	1294	1302	1322	rBV	284466	721435	19.53%	1.649%
25	10.798	1325	1328	1334	rVB7	2929	6234	0.17%	0.014%
26	11.086	1371	1377	1383	rBV9	5033	10905	0.30%	0.025%
27	11.339	1415	1420	1421	rBV5	3485	4534	0.12%	0.010%
28	11.786	1487	1496	1502	rBV	38418	62737	1.70%	0.143%
29	12.116	1546	1552	1563	rBV2	9920	21818	0.59%	0.050%
30	12.716	1650	1654	1658	rVB6	3303	5518	0.15%	0.013%
31	12.969	1690	1697	1702	rVB8	7317	13893	0.38%	0.032%
32	13.186	1730	1734	1738	rBV5	6459	9679	0.26%	0.022%
33	13.768	1826	1833	1844	rBV	1301202	1913883	51.80%	4.374%
34	14.045	1871	1880	1890	rBV	1464534	2272173	61.50%	5.192%
35	14.263	1915	1917	1922	rVB4	4230	5334	0.14%	0.012%
36	14.357	1926	1933	1941	rBV	1549722	2266212	61.34%	5.179%

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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\SFAM-EPA-BM102624.MA.M
Title : SVOA CALIBRATION

37	14.421	1941	1944	1952	rVV6	17023	41212	1.12%	0.094%
38	14.480	1952	1954	1960	rVB6	4853	7974	0.22%	0.018%
39	14.610	1970	1976	1990	rBV3	31239	113915	3.08%	0.260%
40	14.780	2001	2005	2007	rBV5	7187	8609	0.23%	0.020%
41	14.992	2039	2041	2044	rBV4	3178	3965	0.11%	0.009%
42	15.174	2065	2072	2077	rBV3	8665	23062	0.62%	0.053%
43	15.351	2095	2102	2118	rBV	1934849	2897834	78.44%	6.622%
44	15.474	2118	2123	2132	rBV	494069	775307	20.99%	1.772%
45	15.592	2139	2143	2148	rVB6	11016	18226	0.49%	0.042%
46	15.715	2158	2164	2174	rBV	870814	1213005	32.83%	2.772%
47	15.833	2182	2184	2189	rVB6	4052	6150	0.17%	0.014%
48	15.921	2193	2199	2202	rVB7	5004	8431	0.23%	0.019%
49	16.080	2222	2226	2232	rVB9	6590	14573	0.39%	0.033%
50	16.127	2232	2234	2240	rVB6	3649	5033	0.14%	0.012%
51	16.221	2243	2250	2252	rBV6	4482	7907	0.21%	0.018%
52	16.280	2252	2260	2267	rVB	226657	328279	8.89%	0.750%
53	16.380	2274	2277	2280	rVB5	3482	3830	0.10%	0.009%
54	16.509	2295	2299	2305	rBV6	20260	30170	0.82%	0.069%
55	16.592	2310	2313	2317	rVB5	6445	9695	0.26%	0.022%
56	16.704	2329	2332	2335	rBV5	5048	6893	0.19%	0.016%
57	16.862	2356	2359	2361	rBV4	6533	7894	0.21%	0.018%
58	16.974	2375	2378	2379	rBV2	3878	3987	0.11%	0.009%
59	17.027	2382	2387	2390	rVB6	10862	14885	0.40%	0.034%
60	17.098	2390	2399	2409	rBV	1761025	2515623	68.09%	5.749%
61	17.198	2409	2416	2426	rVV	2118901	3153368	85.35%	7.206%
62	17.274	2426	2429	2435	rVB7	18213	29035	0.79%	0.066%
63	17.392	2445	2449	2450	rBV4	3323	4339	0.12%	0.010%
64	17.504	2464	2468	2470	rVV5	4977	8176	0.22%	0.019%
65	17.604	2479	2485	2490	rBV8	8724	18442	0.50%	0.042%
66	17.733	2505	2507	2510	rVV4	4031	4548	0.12%	0.010%
67	17.768	2511	2513	2517	rVB5	5091	5631	0.15%	0.013%
68	17.868	2524	2530	2536	rBV5	33681	58456	1.58%	0.134%
69	17.998	2546	2552	2568	rBV	694325	1100493	29.79%	2.515%
70	18.180	2581	2583	2589	rVB5	14281	17430	0.47%	0.040%
71	18.292	2598	2602	2607	rBV2	35537	61911	1.68%	0.141%
72	18.445	2626	2628	2633	rVB4	17492	18735	0.51%	0.043%
73	18.715	2671	2674	2678	rBV5	14899	18909	0.51%	0.043%
74	18.845	2690	2696	2705	rVB	82115	154971	4.19%	0.354%
75	19.056	2728	2732	2735	rBV3	30087	40926	1.11%	0.094%
76	19.127	2740	2744	2746	rBV3	41887	53798	1.46%	0.123%

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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

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Title : SVOA CALIBRATION

77	19.274	2765	2769	2778	rBV	165442	282058	7.63%	0.645%
78	19.492	2800	2806	2814	rBV	2683720	3694529	100.00%	8.443%
79	20.180	2920	2923	2927	rVB4	95602	112565	3.05%	0.257%
80	21.009	3060	3064	3075	rBV	266937	545317	14.76%	1.246%
81	21.321	3112	3117	3129	rBV	1697154	2677503	72.47%	6.119%
82	22.868	3375	3380	3388	rVB	433108	727513	19.69%	1.663%
83	24.062	3575	3583	3594	rVB	1431043	3400555	92.04%	7.771%
84	24.268	3610	3618	3637	rVB	1110468	2823886	76.43%	6.453%

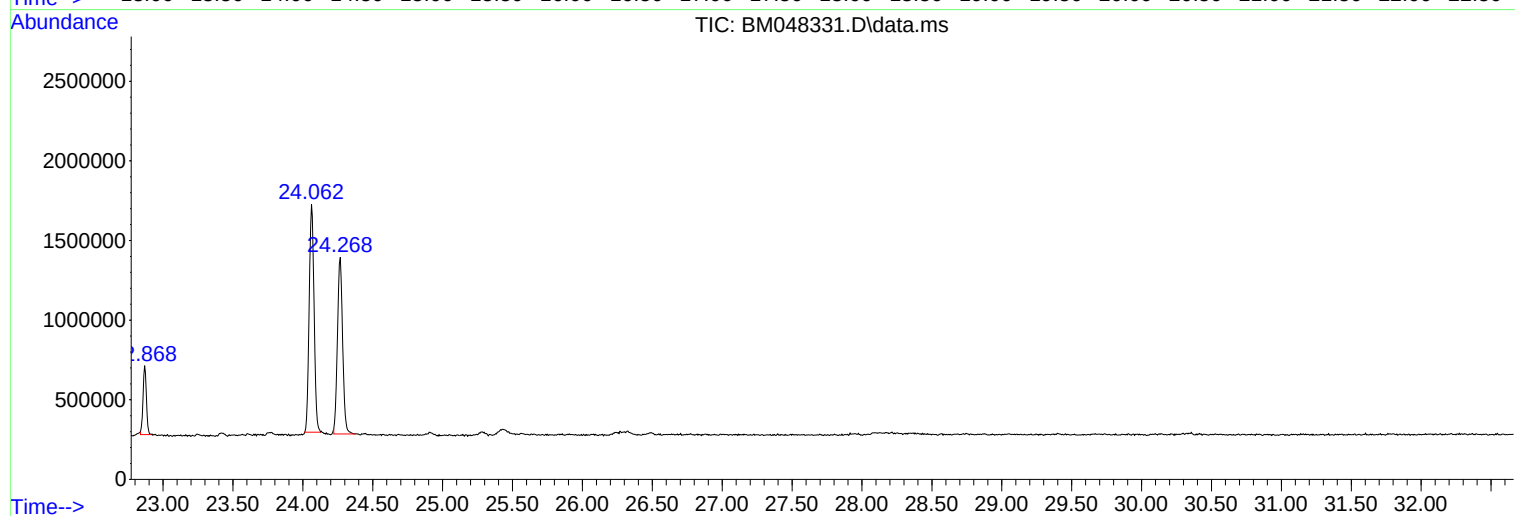
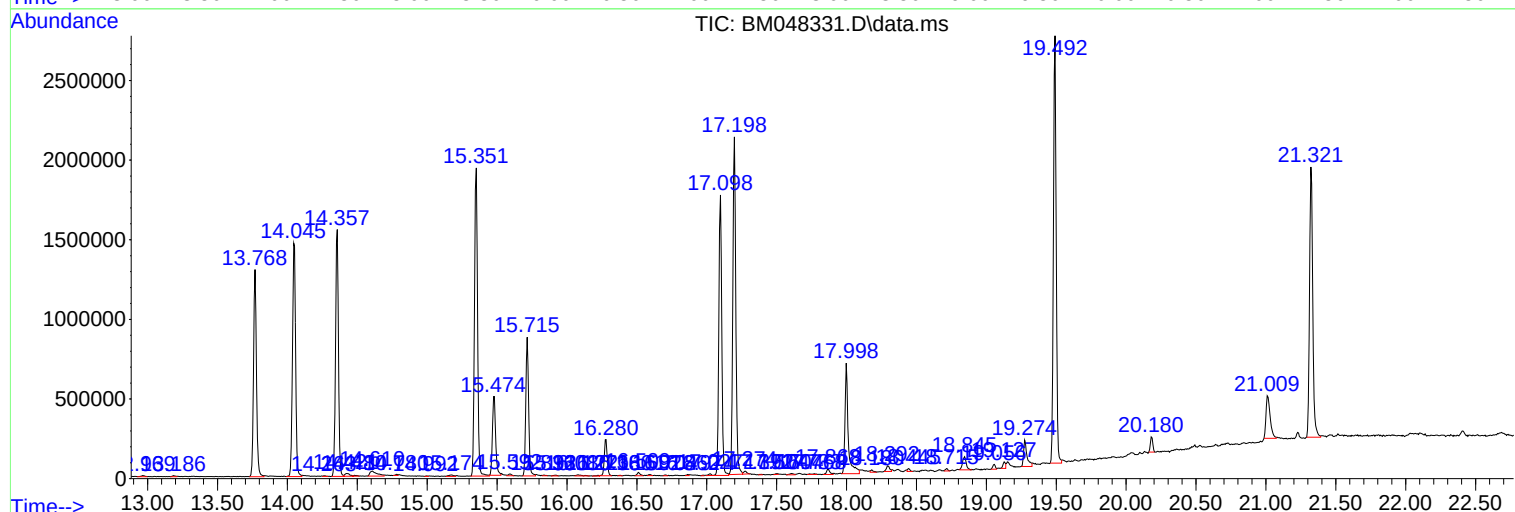
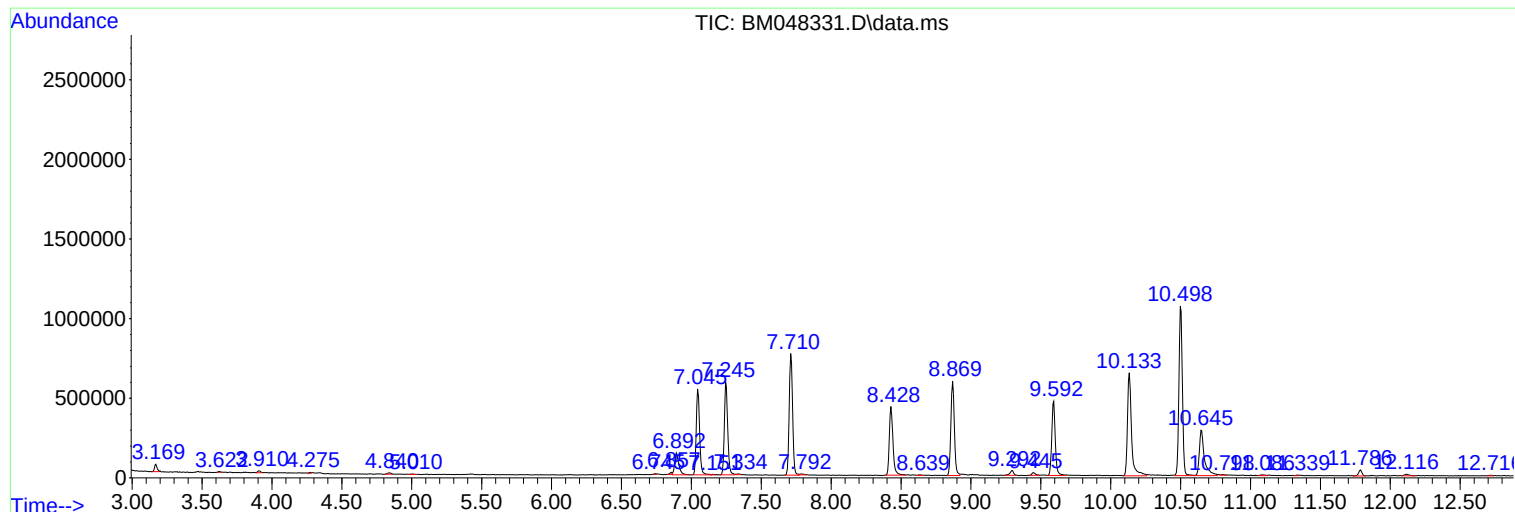
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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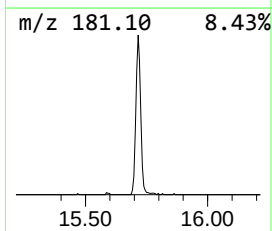
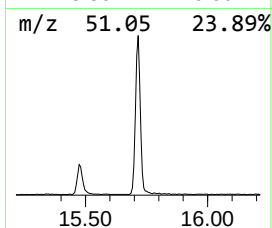
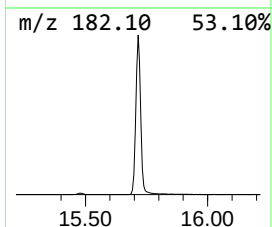
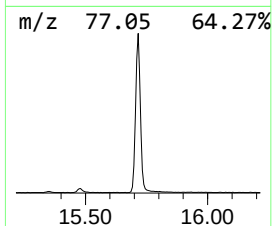
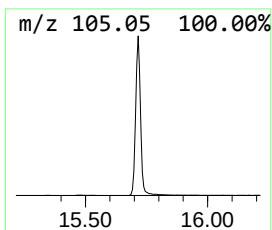
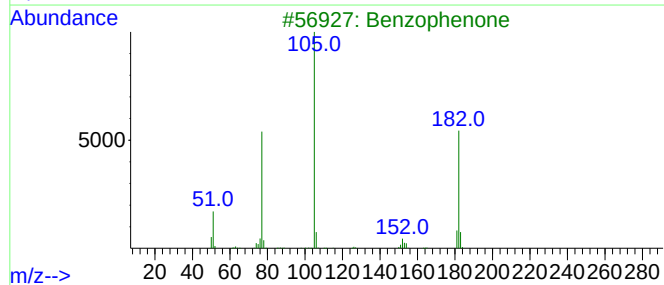
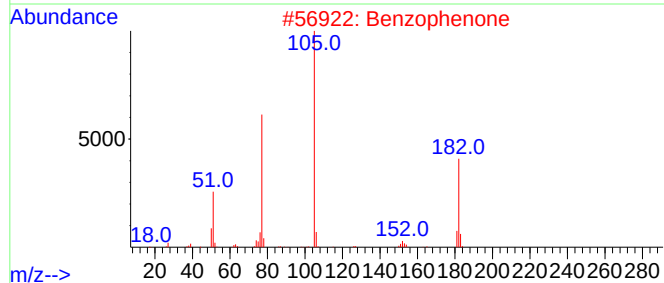
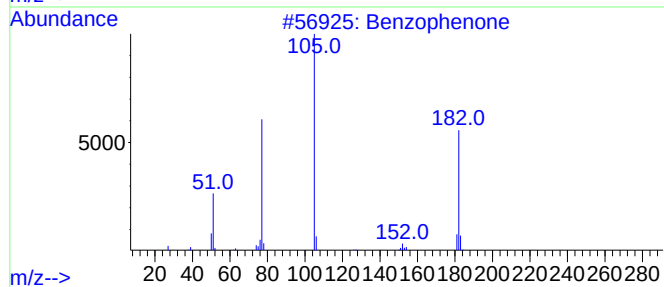
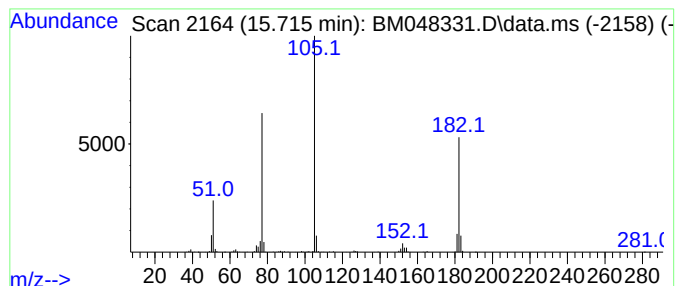
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.715	10.71 ng/ul	1213010	Acenaphthene-d10	14.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzophenone	182	C13H10O	000119-61-9	95
3			Benzophenone	182	C13H10O	000119-61-9	95
4			Benzophenone	182	C13H10O	000119-61-9	93
5			Benzophenone	182	C13H10O	000119-61-9	91



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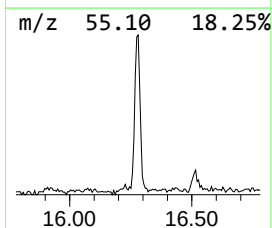
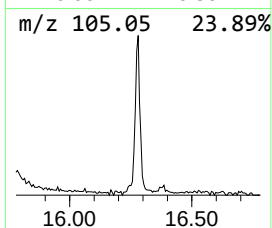
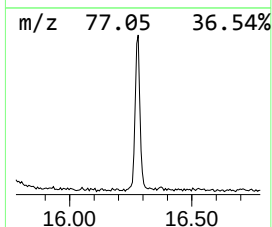
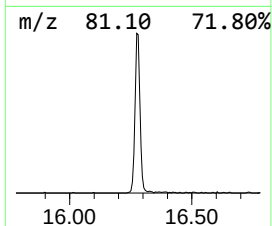
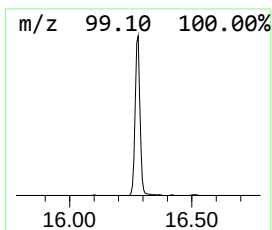
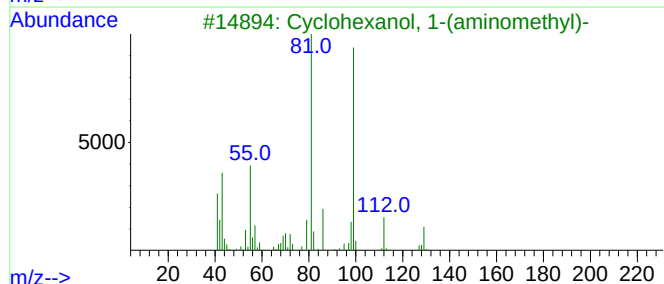
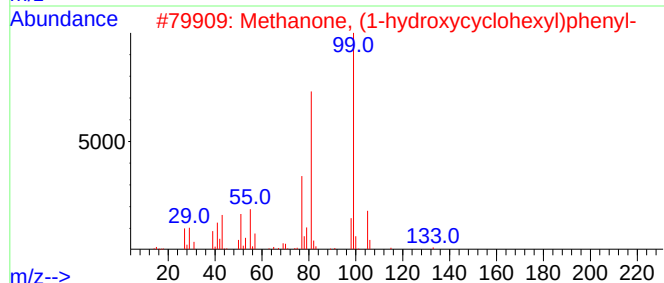
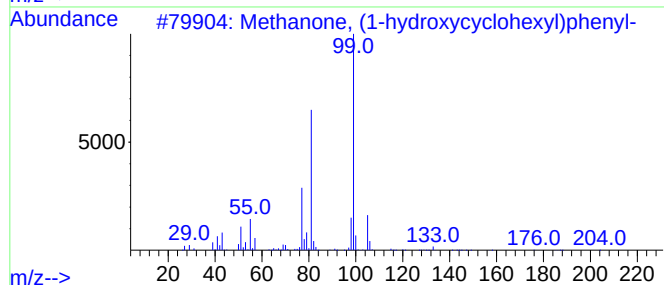
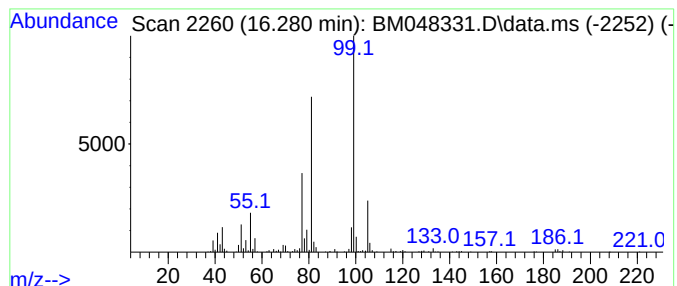
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.280	2.61 ng/ul	328279	Phenanthrene-d10	17.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	87
2			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	86
3			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	50
4			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	47
5			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	40



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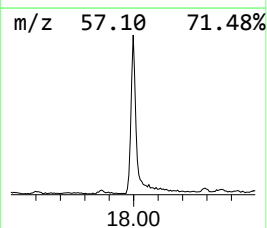
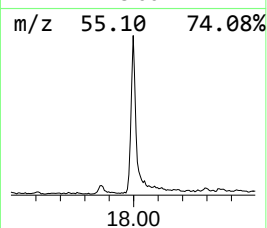
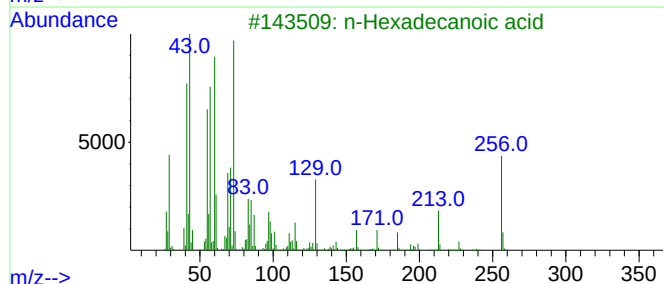
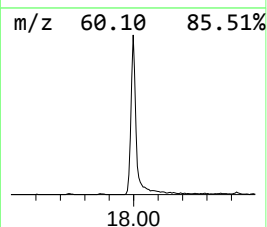
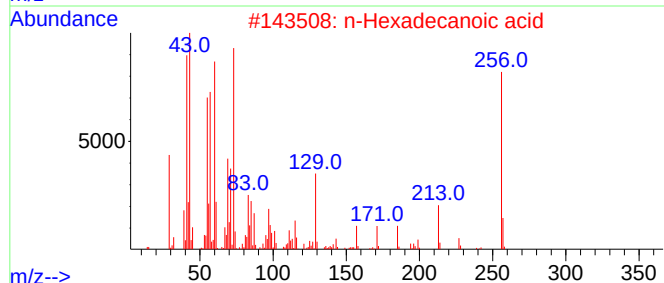
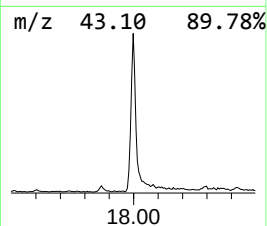
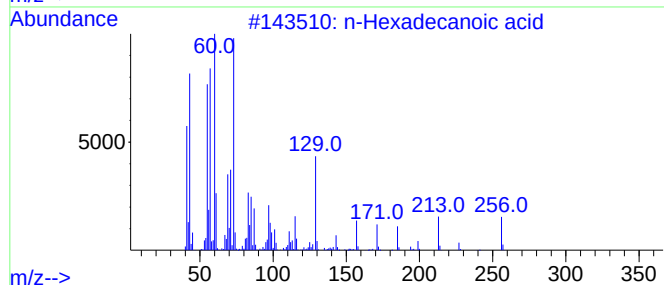
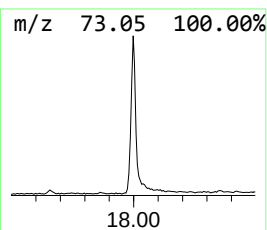
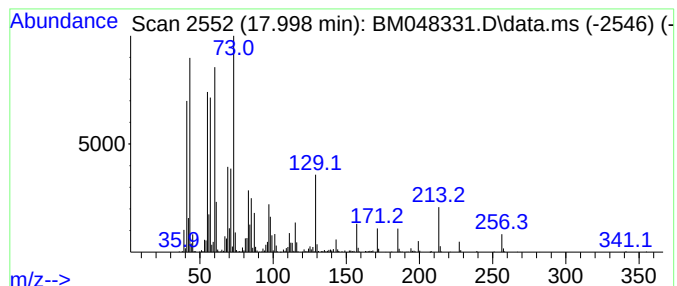
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.998	8.75 ng/ul	1100490	Phenanthrene-d10	17.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	93



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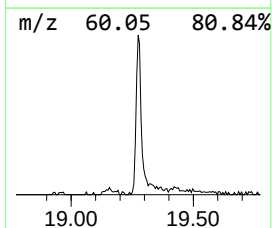
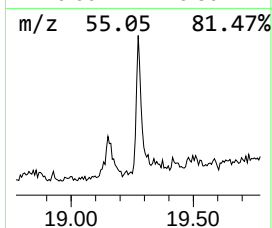
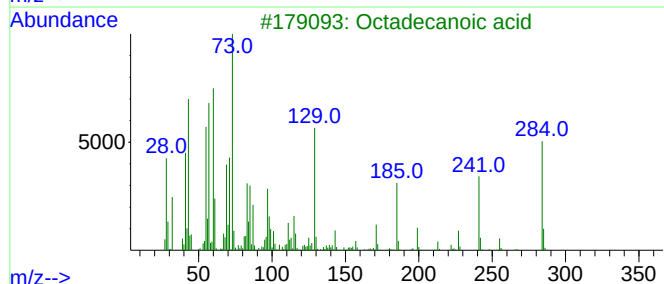
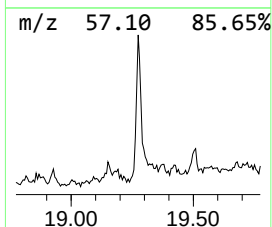
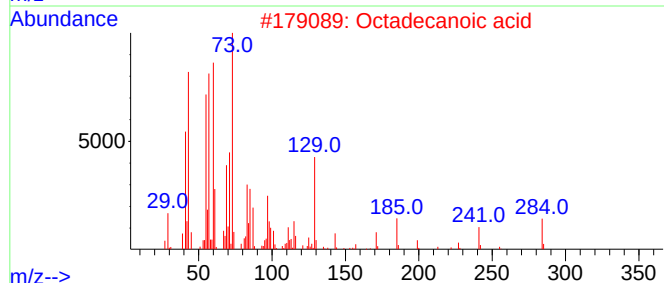
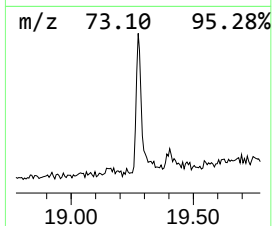
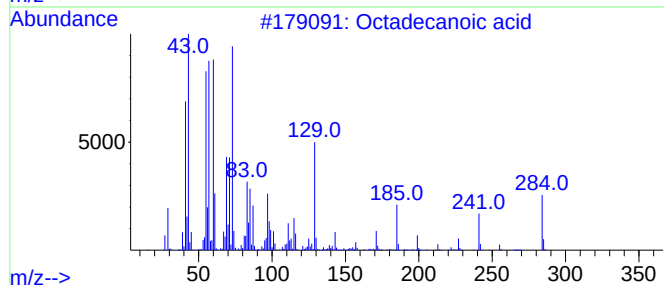
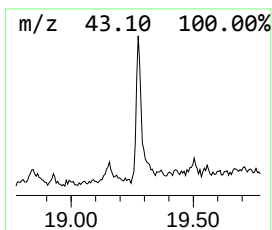
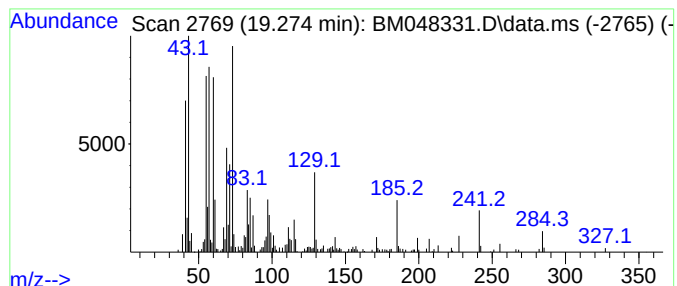
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.274	2.11 ng/ul	282058	Chrysene-d12	21.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	99
3			Octadecanoic acid	284	C18H36O2	000057-11-4	98
4			Octadecanoic acid	284	C18H36O2	000057-11-4	98
5			Octadecanoic acid	284	C18H36O2	000057-11-4	98



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102824\
Data File : BM048331.D
Acq On : 30 Oct 2024 20:17
Operator : RC/JU
Sample : P4534-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E1L88

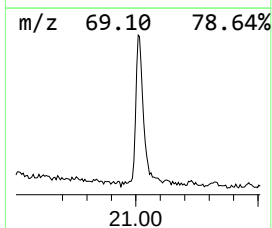
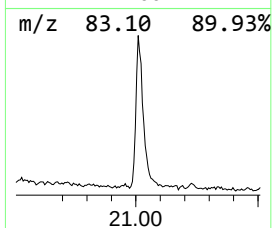
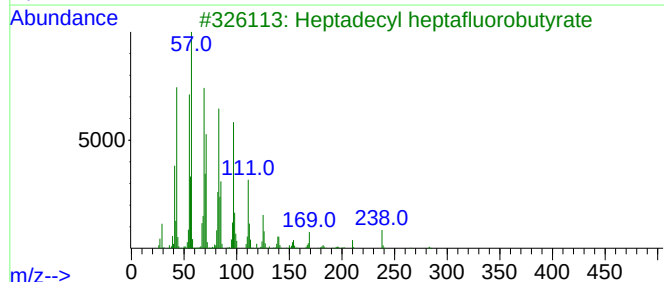
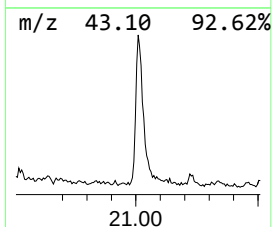
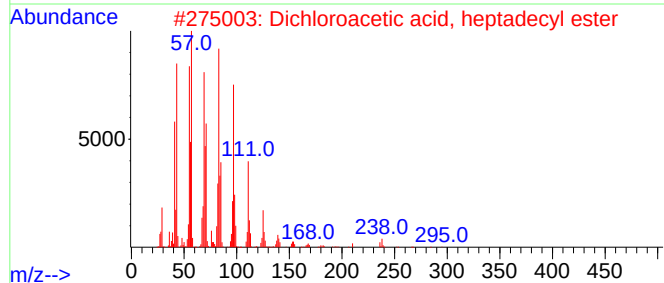
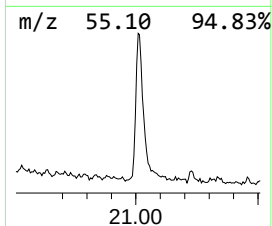
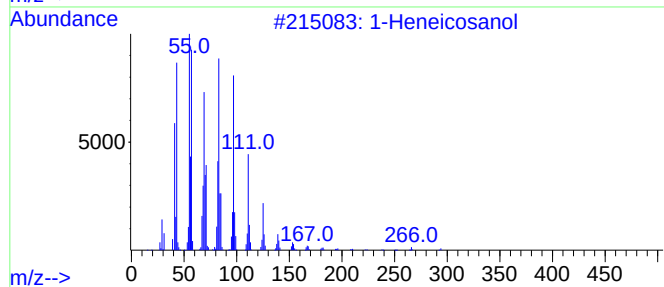
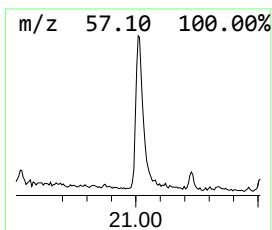
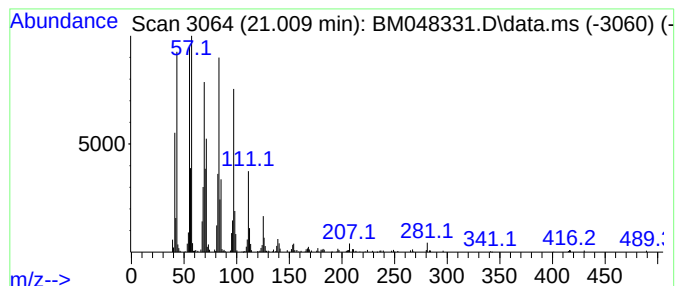
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.009	4.07 ng/ul	545317	Chrysene-d12	21.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102824\
Data File : BM048331.D
Acq On : 30 Oct 2024 20:17
Operator : RC/JU
Sample : P4534-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E1L88

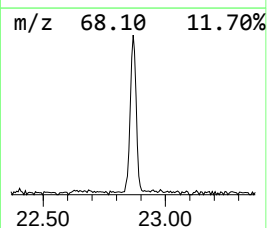
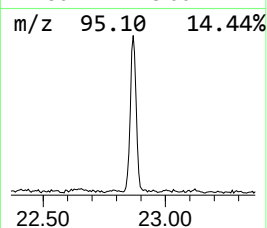
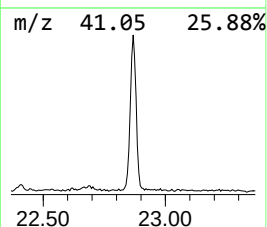
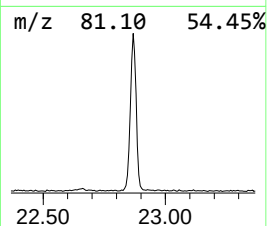
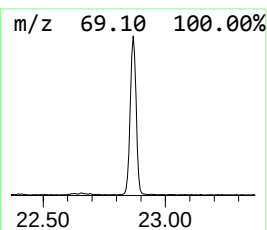
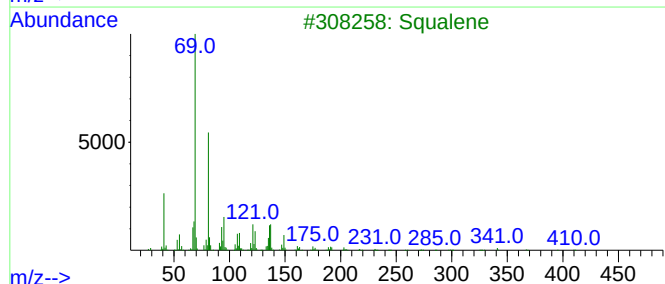
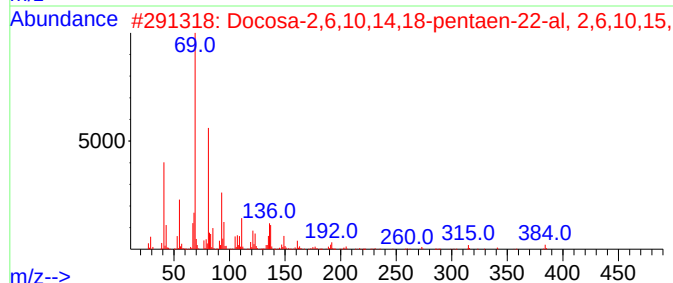
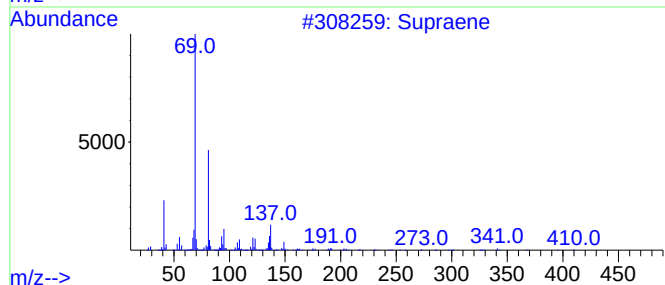
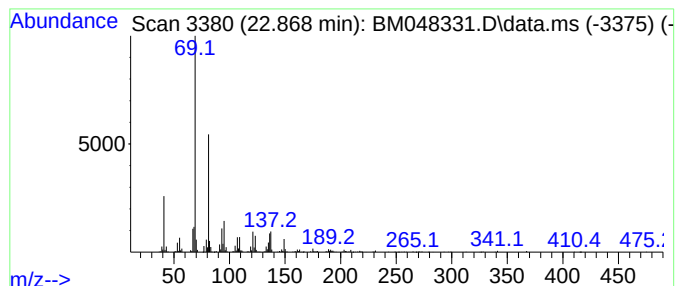
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.868	5.15 ng/ul	727513	Perylene-d12	24.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3			Squalene	410	C30H50	000111-02-4	89
4			Squalene	410	C30H50	000111-02-4	86
5			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102824\
Data File : BM048331.D
Acq On : 30 Oct 2024 20:17
Operator : RC/JU
Sample : P4534-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E1L88

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.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
Benzophenone	15.715	10.7	ng/ul	1213010	3	14.357	2266210	20.0
Methanone, (1-h...	16.280	2.6	ng/ul	328279	4	17.098	2515620	20.0
n-Hexadecanoic ...	17.998	8.8	ng/ul	1100490	4	17.098	2515620	20.0
Octadecanoic acid	19.274	2.1	ng/ul	282058	5	21.321	2677500	20.0
1-Heneicosanol	21.009	4.1	ng/ul	545317	5	21.321	2677500	20.0
Supraene	22.868	5.2	ng/ul	727513	6	24.268	2823890	20.0