

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102521\
 Data File : BP007688.D
 Acq On : 26 Oct 2021 20:43
 Operator : CG/JU
 Sample : M4291-18
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 P046-TW001-01

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_P\METHODS\SFAM-EPA-BP102521.M
 Title : SVOA CALIBRATION

Signal : TIC: BP007688.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.369	10	14	23	rVB	47297	66933	0.17%	0.074%
2	3.787	82	85	105	rBV	176782	296419	0.76%	0.328%
3	4.028	121	126	134	rVB2	29647	45483	0.12%	0.050%
4	7.099	641	648	656	rBV	210287	327125	0.84%	0.362%
5	7.263	669	676	684	rBV	608802	951209	2.45%	1.052%
6	7.463	703	710	719	rBV	639211	1018357	2.62%	1.126%
7	7.934	783	790	797	rBV	741885	1174426	3.02%	1.298%
8	8.640	903	910	924	rBV	540499	878433	2.26%	0.971%
9	9.093	977	987	998	rBV	694863	1156483	2.98%	1.279%
10	9.551	1003	1065	1068	rBV	3980739	38832363	100.00%	42.930%
11	9.816	1103	1110	1118	rVB	535910	895431	2.31%	0.990%
12	10.122	1147	1162	1178	rBV	627394	1887100	4.86%	2.086%
13	10.357	1194	1202	1211	rBV	873062	1455772	3.75%	1.609%
14	10.534	1226	1232	1241	rBV	36818	62992	0.16%	0.070%
15	10.740	1259	1267	1275	rBV	980222	1640064	4.22%	1.813%
16	10.869	1281	1289	1304	rBV	678608	1210841	3.12%	1.339%
17	11.651	1417	1422	1428	rBV2	40599	67380	0.17%	0.074%
18	12.481	1557	1563	1579	rBV	184585	314916	0.81%	0.348%
19	13.981	1812	1818	1835	rBV	1753865	2378433	6.12%	2.629%
20	14.263	1857	1866	1876	rVV	1900407	2779682	7.16%	3.073%
21	14.381	1880	1886	1901	rVV	252803	408596	1.05%	0.452%
22	14.569	1912	1918	1929	rVV	1528918	2321918	5.98%	2.567%
23	14.763	1944	1951	1960	rBV	199707	308508	0.79%	0.341%
24	14.845	1960	1965	1973	rVB	155150	234069	0.60%	0.259%
25	15.269	2030	2037	2047	rBV	126876	222538	0.57%	0.246%
26	15.563	2080	2087	2095	rBV	2452372	3612309	9.30%	3.993%
27	15.681	2099	2107	2118	rBV	712733	977098	2.52%	1.080%
28	17.328	2380	2387	2395	rBV	1923454	2830064	7.29%	3.129%
29	17.428	2397	2404	2417	rBV	2860734	4122442	10.62%	4.557%
30	18.222	2534	2539	2545	rBV	53132	82540	0.21%	0.091%
31	19.239	2708	2712	2718	rBV3	45671	62414	0.16%	0.069%
32	19.304	2719	2723	2728	rBV	46441	62763	0.16%	0.069%
33	19.657	2777	2783	2797	rBV	3790913	5260120	13.55%	5.815%
34	21.416	3077	3082	3095	rBV	2713558	3508127	9.03%	3.878%
35	23.704	3464	3471	3480	rVB2	2792496	5445874	14.02%	6.021%
36	23.862	3491	3498	3508	rVB2	1734995	3555531	9.16%	3.931%

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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_P\METHODS\SFAM-EPA-BP102521.M
Title : SVOA CALIBRATION

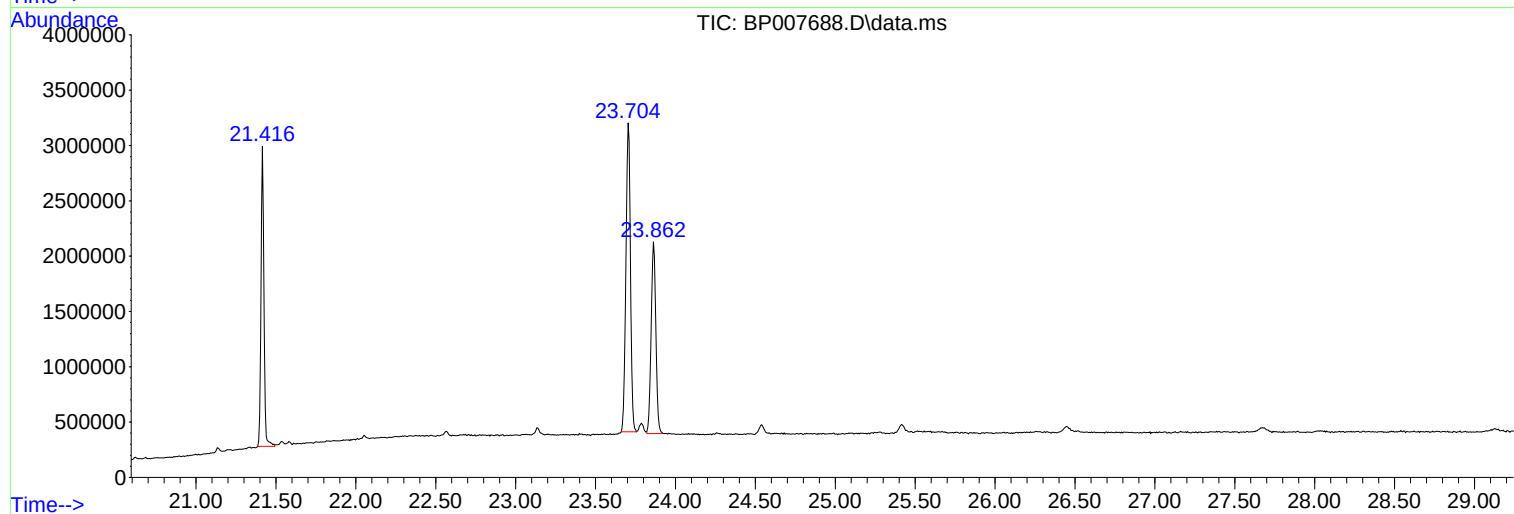
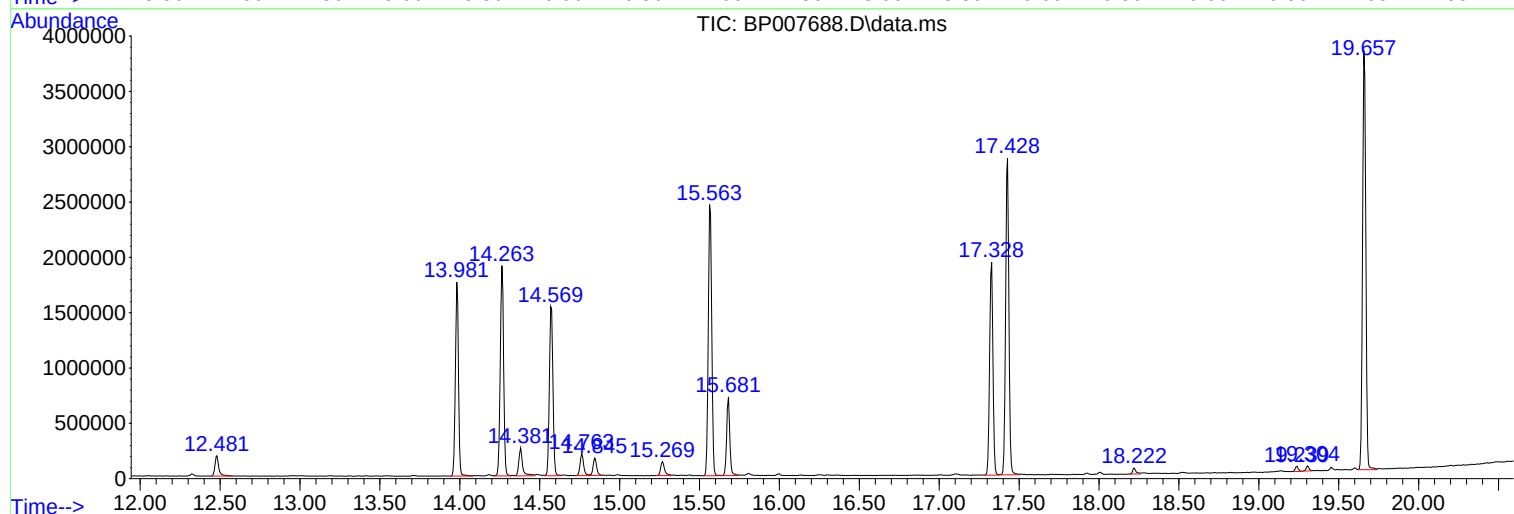
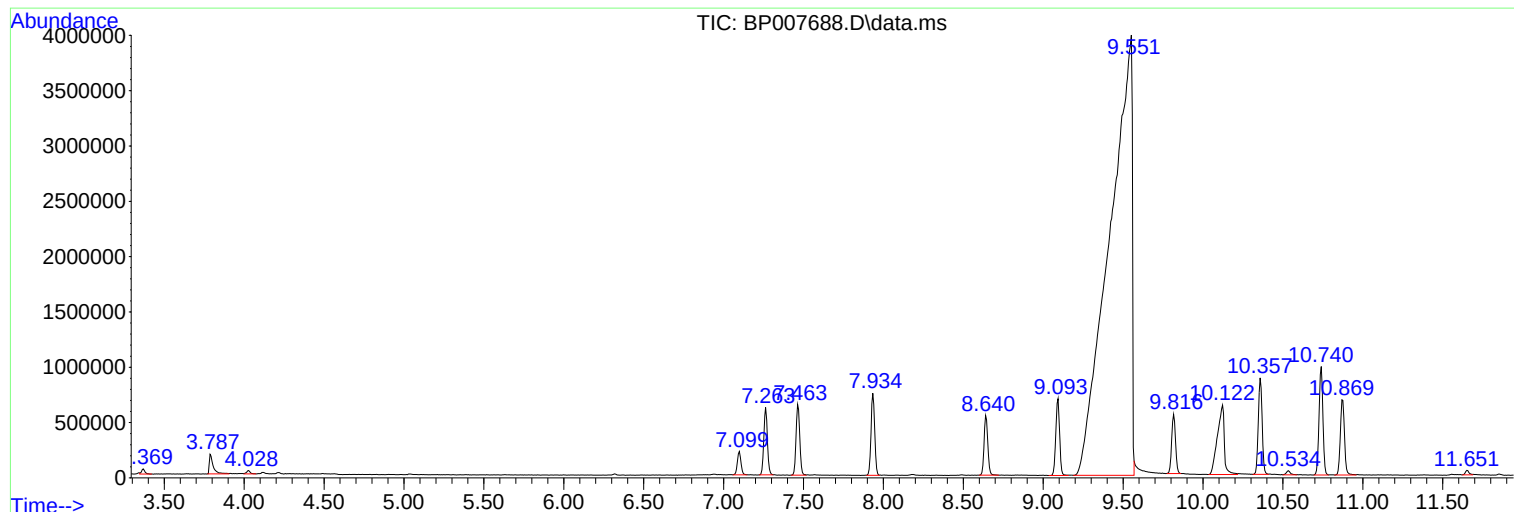
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

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



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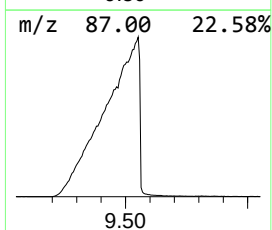
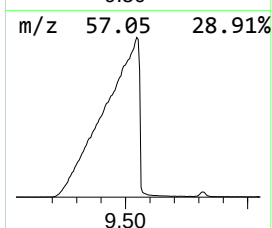
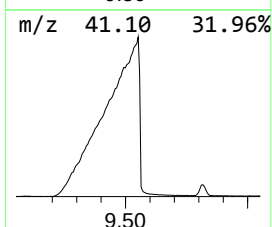
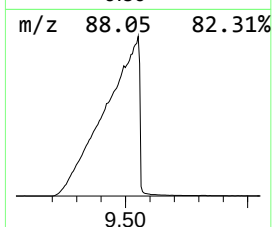
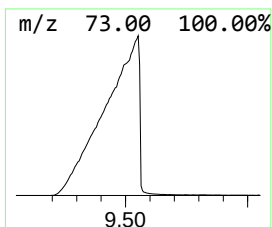
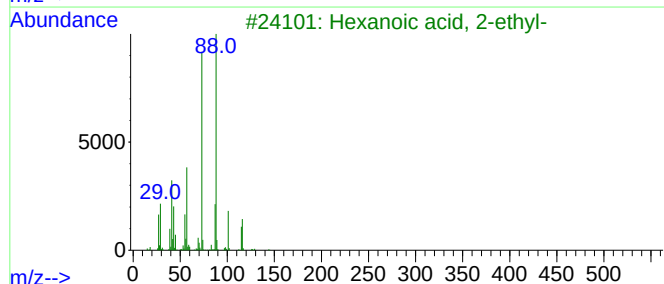
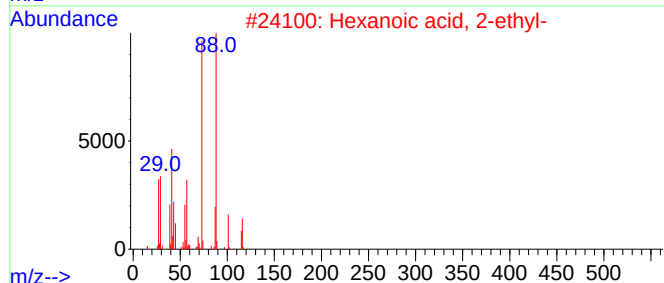
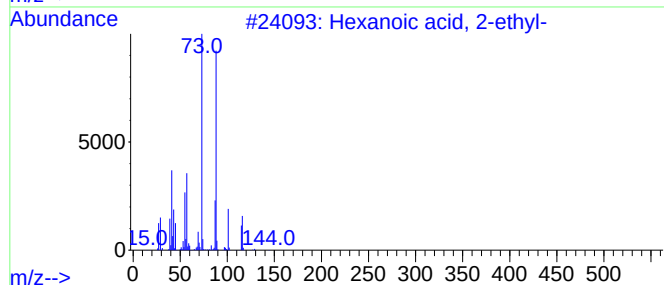
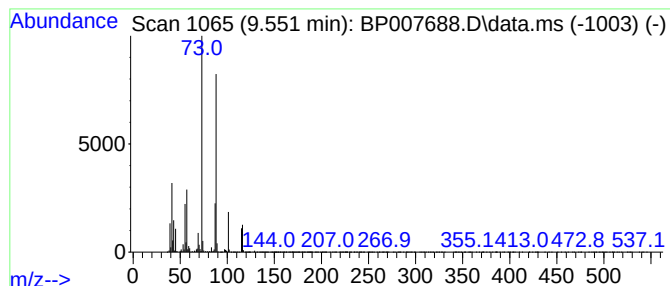
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.551	473.55 ng/ul	38832400	Naphthalene-d8	10.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
3			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
4			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
5			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72



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ALS Vial : 46 Sample Multiplier: 1

Instrument :
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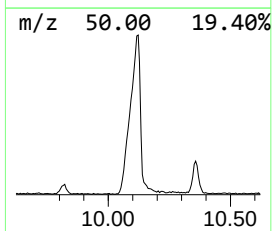
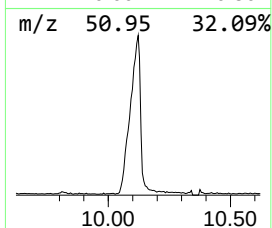
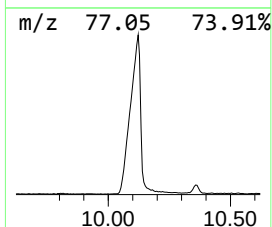
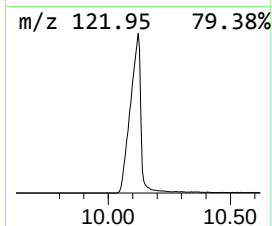
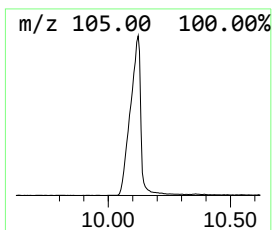
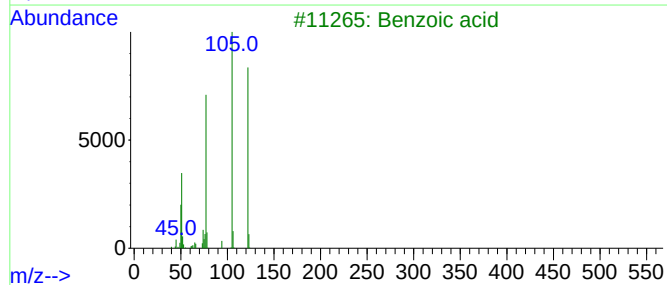
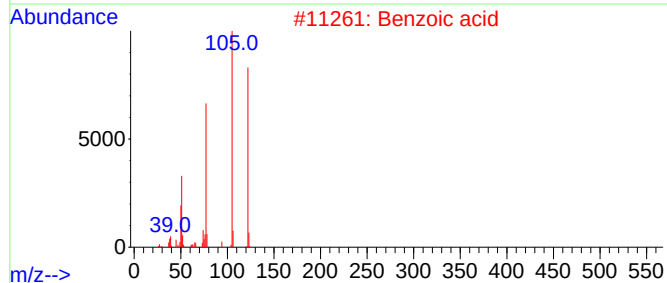
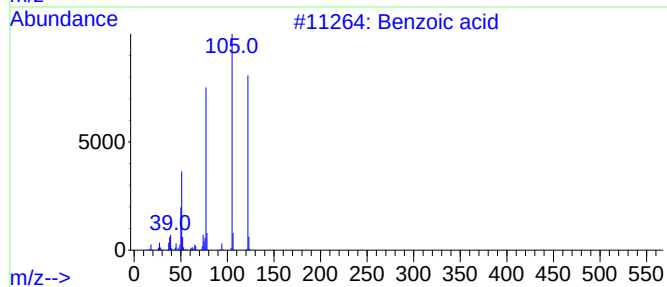
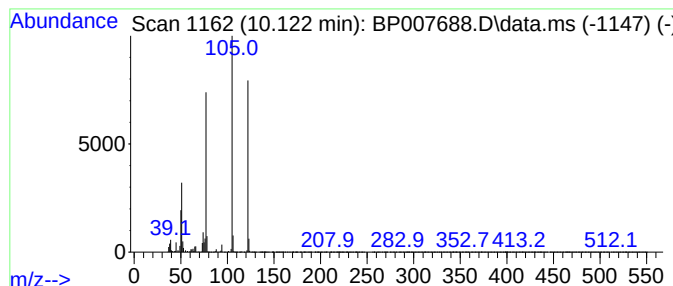
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.122	23.01 ng/ul	1887100	Naphthalene-d8	10.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid	122	C7H6O2	000065-85-0	96
2			Benzoic acid	122	C7H6O2	000065-85-0	96
3			Benzoic acid	122	C7H6O2	000065-85-0	96
4			Benzoic acid	122	C7H6O2	000065-85-0	94
5			Cyclobutane-1,1-dicarboxamide, N...	382	C20H18N2O6	1000253-25-3	91



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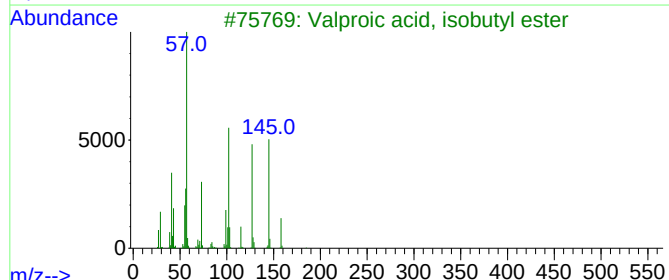
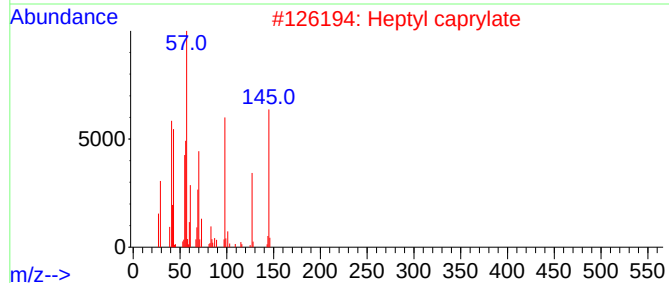
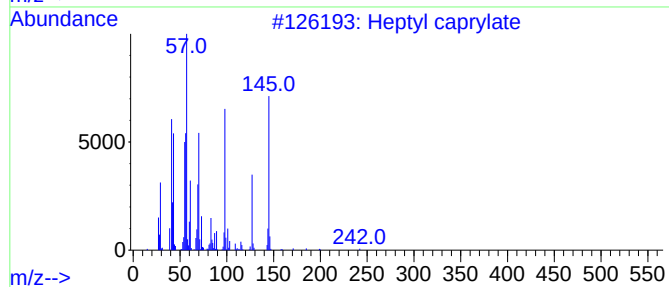
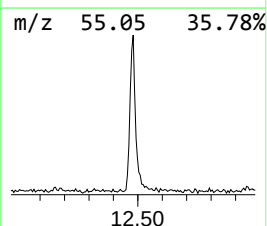
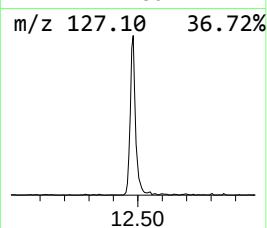
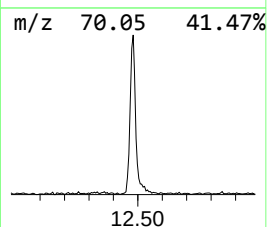
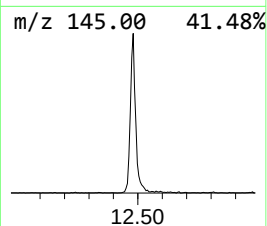
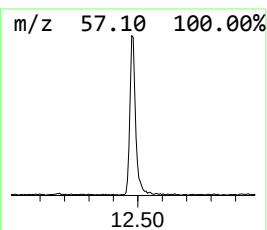
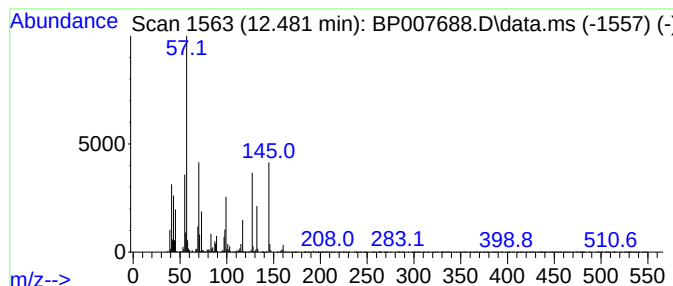
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.481	3.84 ng/ul	314916	Naphthalene-d8	10.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl caprylate	242	C15H30O2	004265-97-8	37
2			Heptyl caprylate	242	C15H30O2	004265-97-8	35
3			Valproic acid, isobutyl ester	200	C12H24O2	1000438-96-8	25
4			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	16
5			1-Hexanol, 2,2-dimethyl-	130	C8H18O	002370-13-0	14



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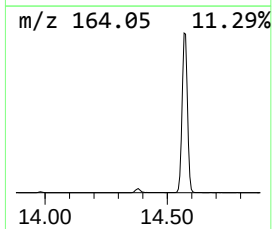
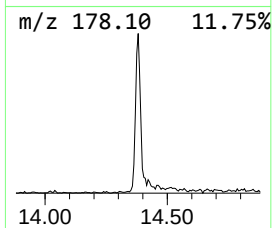
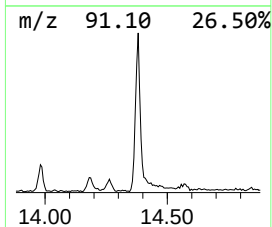
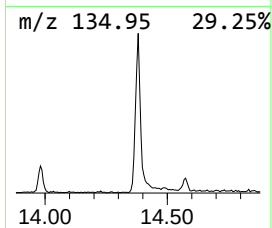
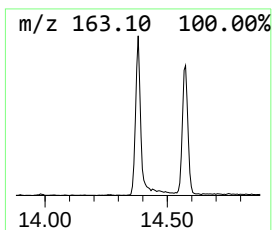
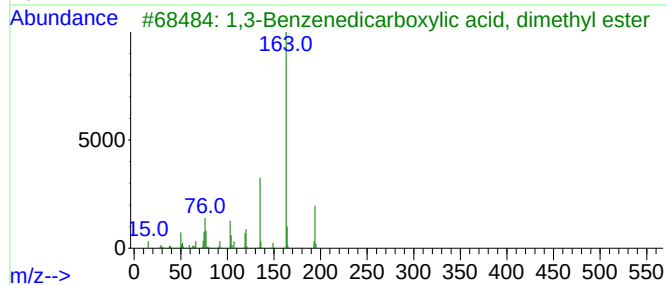
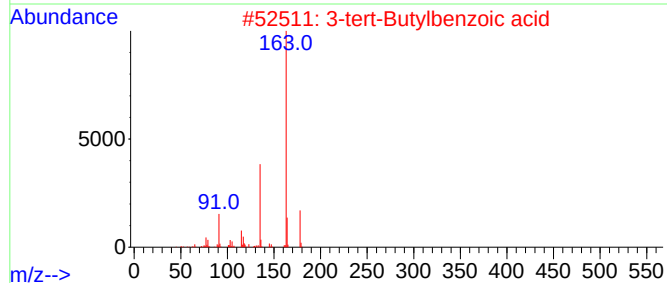
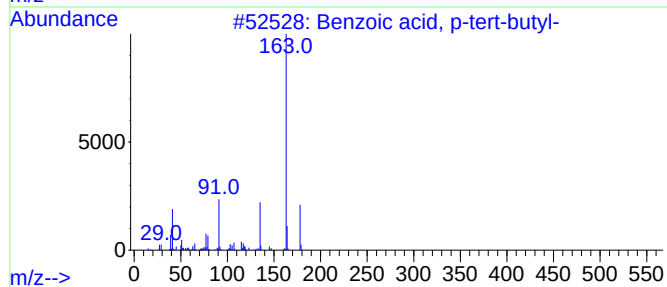
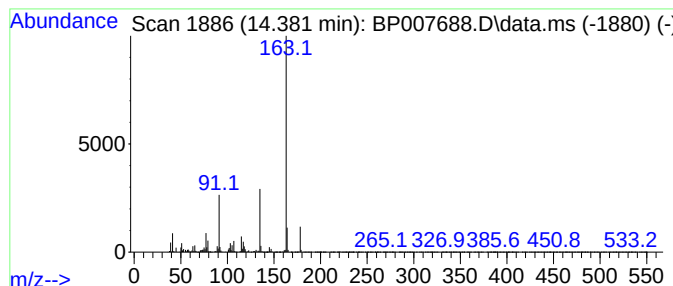
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Benzoic acid, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.381	3.52 ng/ul	408596	Acenaphthene-d10	14.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	91
2			3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	72
3			1,3-Benzenedicarboxylic acid, di...	194	C10H10O4	001459-93-4	64
4			5'-Hydroxy-2',3',4'-trimethylace...	178	C11H14O2	013667-28-2	64
5			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	60



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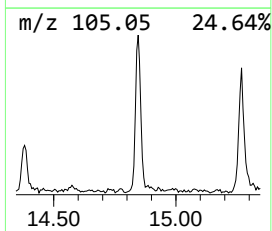
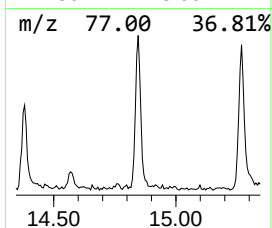
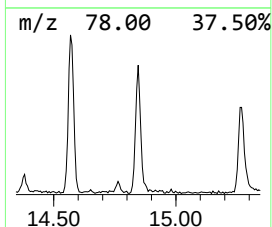
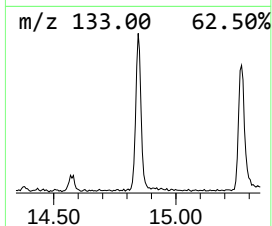
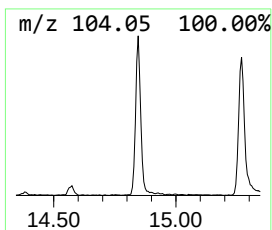
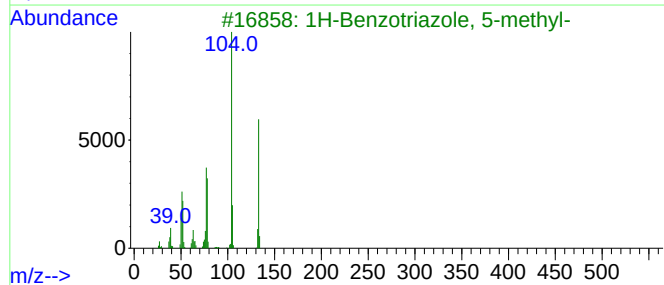
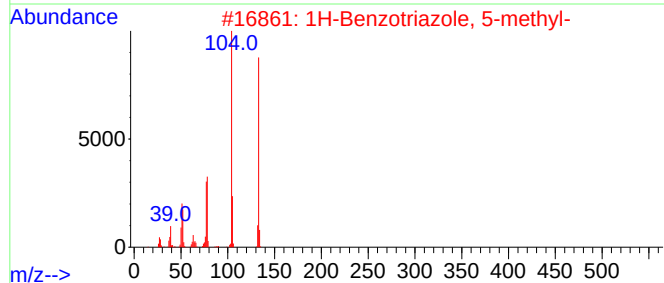
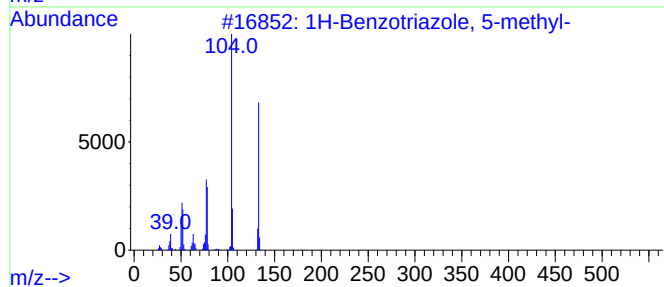
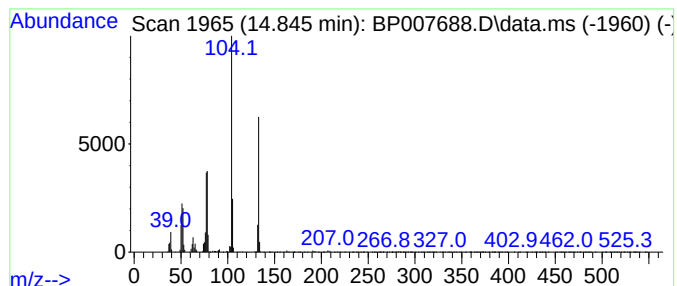
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1H-Benzotriazole, 5-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	2.02 ng/ul	234069	Acenaphthene-d10	14.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methyl-		133	C7H7N3		000136-85-6	97
2	1H-Benzotriazole, 5-methyl-		133	C7H7N3		000136-85-6	95
3	1H-Benzotriazole, 5-methyl-		133	C7H7N3		000136-85-6	94
4	1H-Benzotriazole, 4-methyl-		133	C7H7N3		029878-31-7	94
5	1H-Benzotriazole, 5-methyl-		133	C7H7N3		000136-85-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102521\
Data File : BP007688.D
Acq On : 26 Oct 2021 20:43
Operator : CG/JU
Sample : M4291-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
P046-TW001-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanoic acid, ...	9.551	473.6	ng/ul	38832400	2	10.740	1640060	20.0
Benzoic acid	10.122	23.0	ng/ul	1887100	2	10.740	1640060	20.0
unknown-01	12.481	3.8	ng/ul	314916	2	10.740	1640060	20.0
Benzoic acid, p...	14.381	3.5	ng/ul	408596	3	14.569	2321920	20.0
1H-Benzotriazol...	14.845	2.0	ng/ul	234069	3	14.569	2321920	20.0