

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
 Data File : BP017565.D
 Acq On : 05 Oct 2023 14:48
 Operator : MA/JU
 Sample : 04679-12
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PMW-7S(20230927)

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-BP100423.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP017565.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.287	30	34	37	rBV	24528	31236	0.49%	0.057%
2	3.323	37	40	45	rVB	48967	59166	0.93%	0.109%
3	3.728	106	109	124	rBV	154492	249265	3.90%	0.457%
4	4.028	156	160	164	rBV2	12102	17803	0.28%	0.033%
5	4.452	229	232	238	rVB3	13394	20260	0.32%	0.037%
6	5.193	352	358	370	rBV	319641	502121	7.86%	0.921%
7	5.870	467	473	475	rBV6	5177	6673	0.10%	0.012%
8	6.634	599	603	610	rBV	9536	18020	0.28%	0.033%
9	7.099	675	682	691	rBV	141424	231776	3.63%	0.425%
10	7.281	706	713	722	rBV	555571	860507	13.46%	1.579%
11	7.375	725	729	736	rVB2	9582	16662	0.26%	0.031%
12	7.458	736	743	754	rBV	557447	950321	14.87%	1.744%
13	7.816	797	804	814	rBV	796879	1244224	19.46%	2.283%
14	7.940	818	825	826	rBV	457312	599872	9.38%	1.101%
15	7.975	826	831	842	rVV	4062369	6392372	100.00%	11.730%
16	8.287	877	884	890	rBV	62020	96284	1.51%	0.177%
17	8.664	941	948	957	rBV	414619	697234	10.91%	1.279%
18	9.146	1021	1030	1037	rBV	694082	1107896	17.33%	2.033%
19	9.340	1054	1063	1067	rVB3	12163	24501	0.38%	0.045%
20	9.469	1078	1085	1091	rBV2	24095	40821	0.64%	0.075%
21	9.516	1091	1093	1101	rVB6	8070	14660	0.23%	0.027%
22	9.863	1145	1152	1167	rVB	572125	931334	14.57%	1.709%
23	10.069	1183	1187	1192	rVB3	21124	31294	0.49%	0.057%
24	10.263	1211	1220	1223	rBV10	4659	9012	0.14%	0.017%
25	10.393	1235	1242	1250	rBV	831839	1409911	22.06%	2.587%
26	10.463	1250	1254	1262	rVB2	33835	66282	1.04%	0.122%
27	10.775	1300	1307	1316	rVV	623914	1021880	15.99%	1.875%
28	10.946	1326	1336	1346	rBV	726698	1250110	19.56%	2.294%
29	11.422	1412	1417	1424	rBV6	6373	11616	0.18%	0.021%
30	11.546	1433	1438	1443	rBV8	5006	9515	0.15%	0.017%
31	11.810	1477	1483	1485	rBV6	11105	17392	0.27%	0.032%
32	12.016	1514	1518	1522	rVB6	4082	6497	0.10%	0.012%
33	12.163	1537	1543	1548	rVB10	3657	7755	0.12%	0.014%
34	12.369	1572	1578	1584	rVV3	14126	24940	0.39%	0.046%
35	12.822	1647	1655	1658	rBV10	4554	11870	0.19%	0.022%
36	12.869	1658	1663	1667	rVB8	4713	7433	0.12%	0.014%

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37	13.469	1760	1765	1772	rBV4	20435	32741	0.51%	0.060%
38	13.681	1797	1801	1806	rBV8	5266	9773	0.15%	0.018%
39	13.810	1818	1823	1827	rVB7	4322	7790	0.12%	0.014%
40	14.046	1854	1863	1870	rBV	1699947	2301117	36.00%	4.223%
41	14.234	1890	1895	1902	rBV	21635	32666	0.51%	0.060%
42	14.328	1904	1911	1921	rBV	1791553	2613052	40.88%	4.795%
43	14.416	1923	1926	1931	rVB	11614	19133	0.30%	0.035%
44	14.522	1938	1944	1949	rVB	77537	103790	1.62%	0.190%
45	14.634	1955	1963	1970	rBV	953367	1376302	21.53%	2.526%
46	14.828	1992	1996	2000	rBV	24367	31452	0.49%	0.058%
47	14.887	2000	2006	2014	rBV	96228	199525	3.12%	0.366%
48	15.016	2024	2028	2039	rVB8	19710	34787	0.54%	0.064%
49	15.216	2056	2062	2067	rBV	126741	191822	3.00%	0.352%
50	15.375	2084	2089	2094	rBV4	24709	35285	0.55%	0.065%
51	15.634	2127	2133	2143	rBV	2469473	3447314	53.93%	6.326%
52	15.775	2152	2157	2170	rBV	807602	1132003	17.71%	2.077%
53	15.875	2170	2174	2179	rVB4	11811	20729	0.32%	0.038%
54	16.551	2287	2289	2294	rVB6	5644	7651	0.12%	0.014%
55	17.334	2415	2422	2427	rVB6	15620	30883	0.48%	0.057%
56	17.422	2431	2437	2443	rBV	1297989	1743810	27.28%	3.200%
57	17.522	2447	2454	2464	rBV	2925879	4036079	63.14%	7.406%
58	17.910	2517	2520	2525	rVB4	13180	18247	0.29%	0.033%
59	18.051	2541	2544	2548	rBV6	8191	11530	0.18%	0.021%
60	18.269	2577	2581	2592	rBV	224344	349929	5.47%	0.642%
61	19.345	2760	2764	2768	rBV	36968	47952	0.75%	0.088%
62	19.410	2770	2775	2782	rVB3	48325	96176	1.50%	0.176%
63	19.516	2789	2793	2799	rBV2	94149	134040	2.10%	0.246%
64	19.775	2832	2837	2843	rBV	3949369	5289794	82.75%	9.707%
65	21.216	3078	3082	3087	rBV	165667	233280	3.65%	0.428%
66	21.557	3135	3140	3146	rBV	1635485	2099232	32.84%	3.852%
67	23.186	3411	3417	3425	rBV	1439212	2598914	40.66%	4.769%
68	23.969	3542	3550	3560	rVB2	2835615	5960945	93.25%	10.938%
69	24.139	3572	3579	3591	rVB	1063356	2249080	35.18%	4.127%

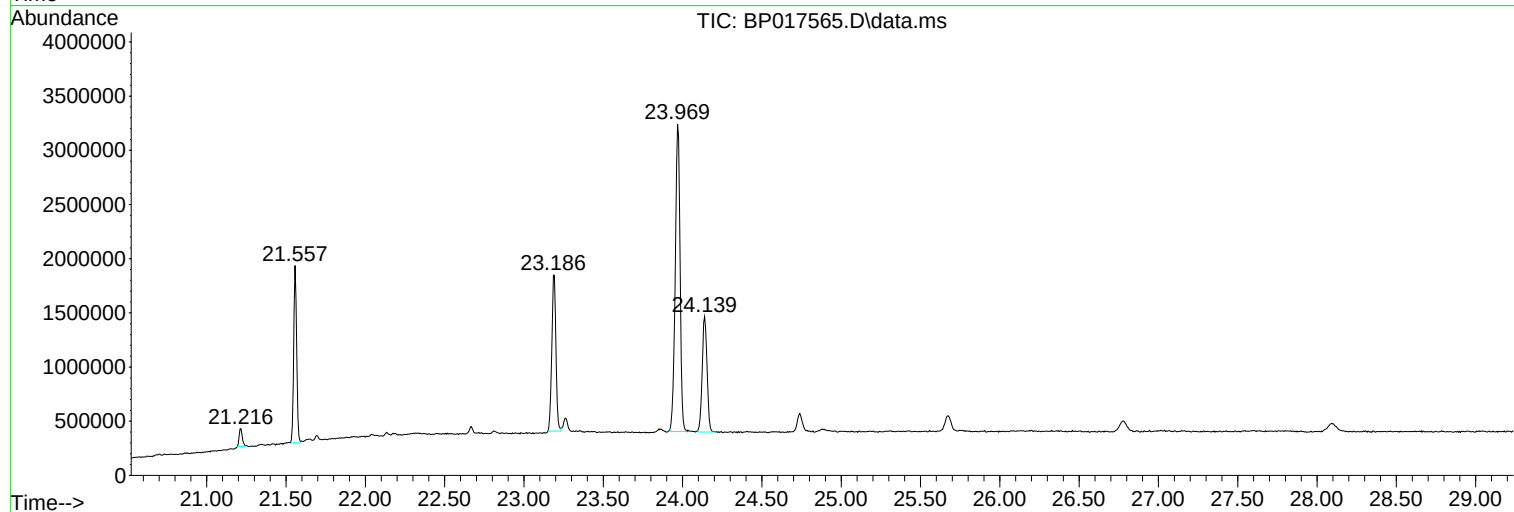
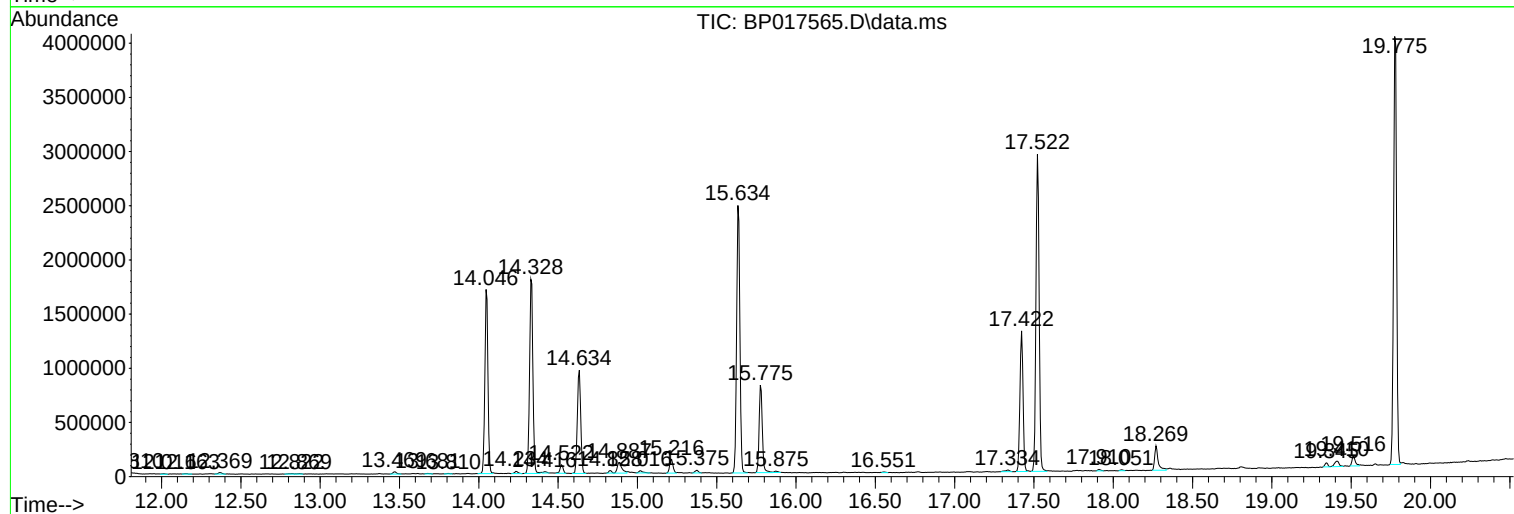
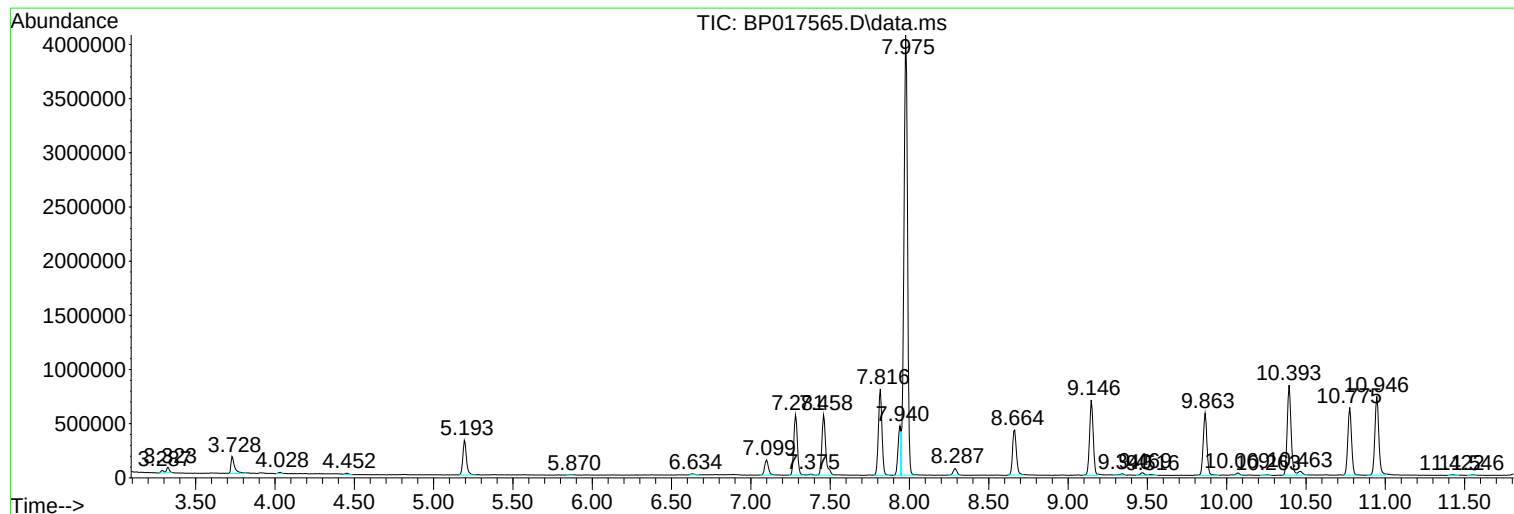
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
BNA_P
ClientSampleId :
PMW-7S(20230927)

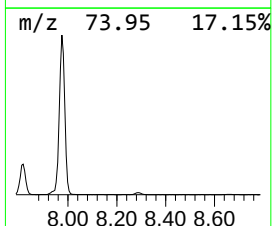
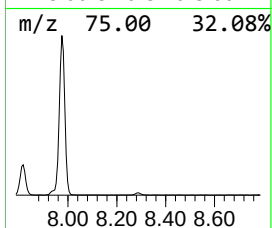
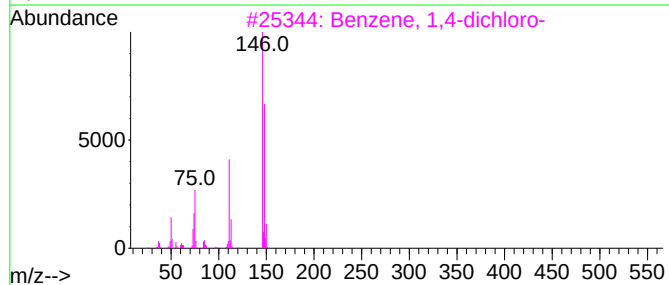
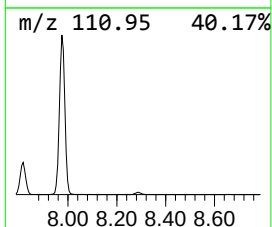
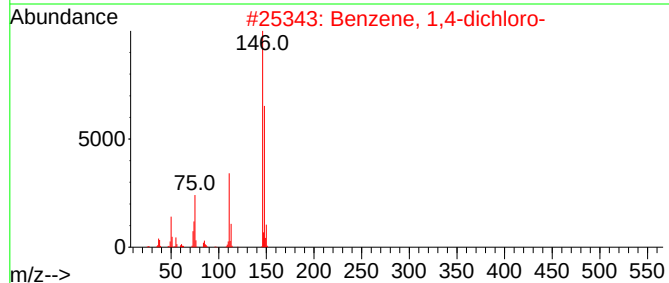
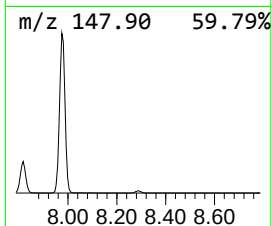
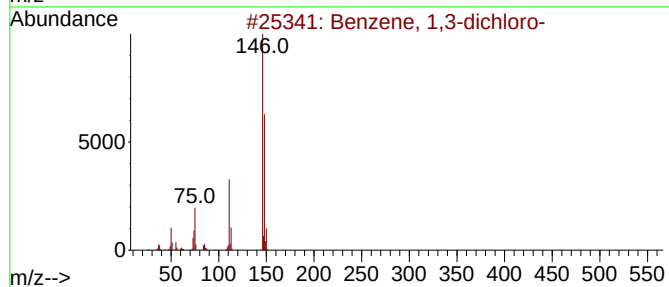
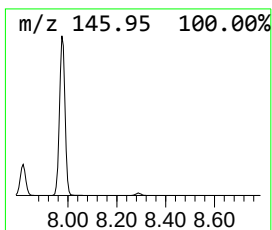
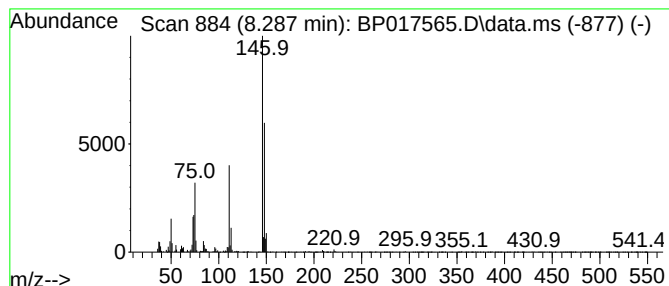
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Benzene, 1,3-dichloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.287	3.21 ng/ul	96284	1,4-Dichlorobenzene-d4	7.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dichloro-	146	C6H4Cl2	000541-73-1	97
2			Benzene, 1,4-dichloro-	146	C6H4Cl2	000106-46-7	96
3			Benzene, 1,4-dichloro-	146	C6H4Cl2	000106-46-7	96
4			Benzene, 1,3-dichloro-	146	C6H4Cl2	000541-73-1	95
5			Benzene, 1,3-dichloro-	146	C6H4Cl2	000541-73-1	95



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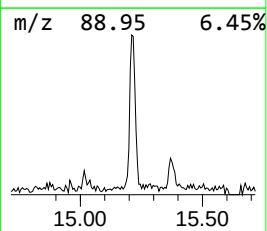
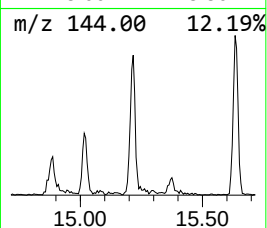
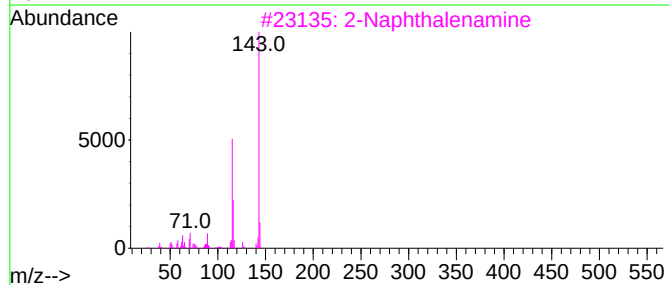
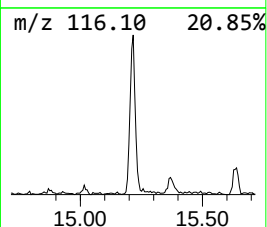
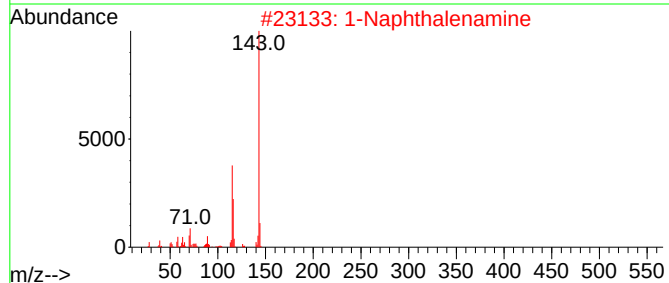
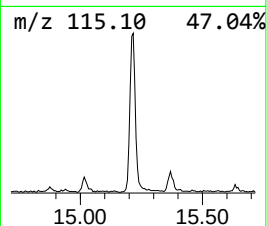
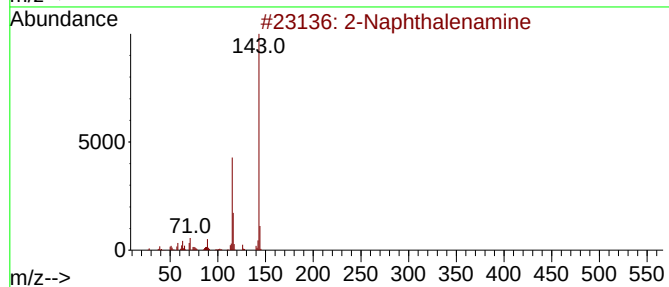
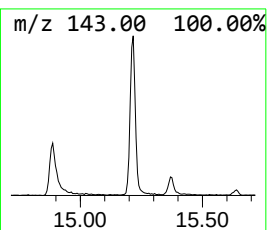
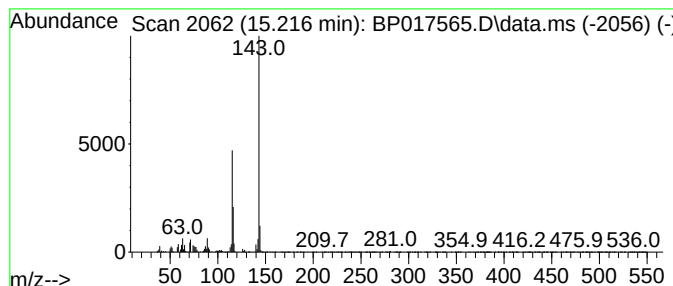
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 2-Naphthalenamine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.216	2.79 ng/ul	191822	Acenaphthene-d10	14.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Naphthalenamine			143	C10H9N	000091-59-8	95
2	1-Naphthalenamine			143	C10H9N	000134-32-7	95
3	2-Naphthalenamine			143	C10H9N	000091-59-8	94
4	2-Naphthalenamine			143	C10H9N	000091-59-8	94
5	1-Naphthalenamine			143	C10H9N	000134-32-7	91



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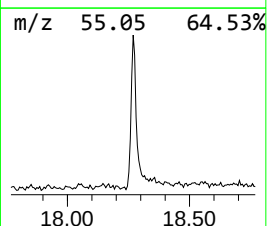
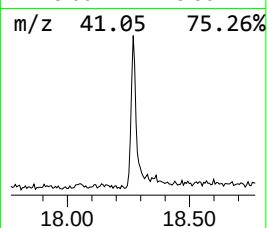
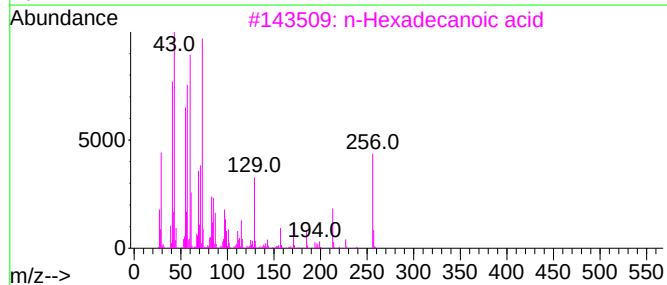
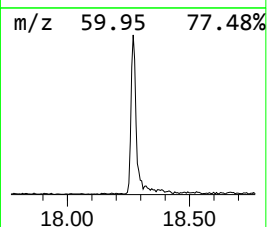
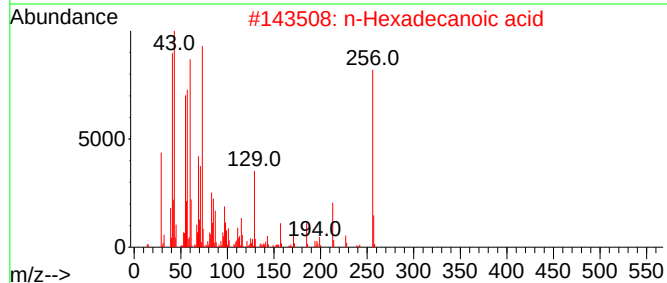
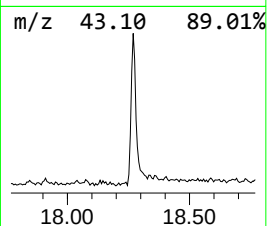
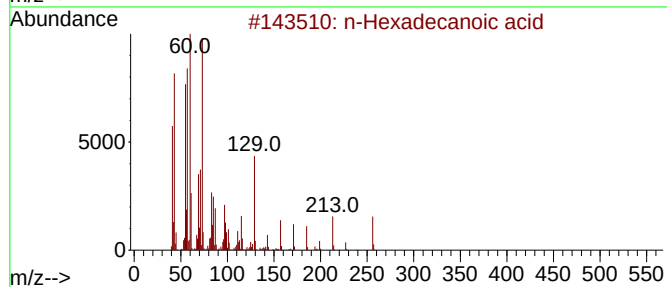
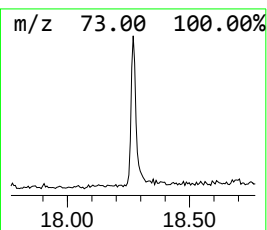
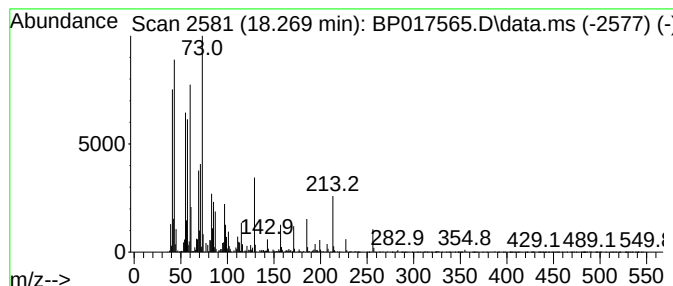
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TIC Library : C:\DATABASE\NIST20.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.269	4.01 ng/ul	349929	Phenanthrene-d10	17.422

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	97
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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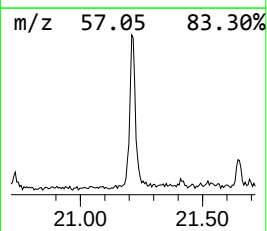
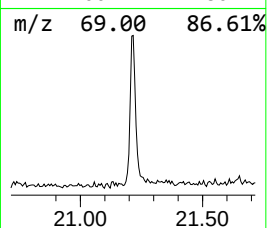
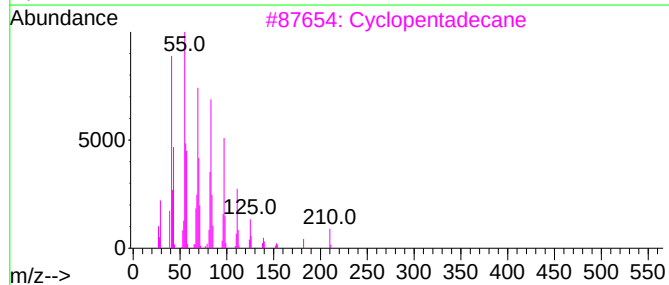
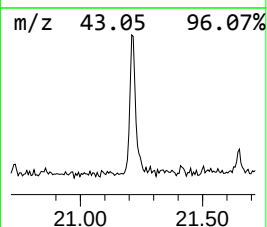
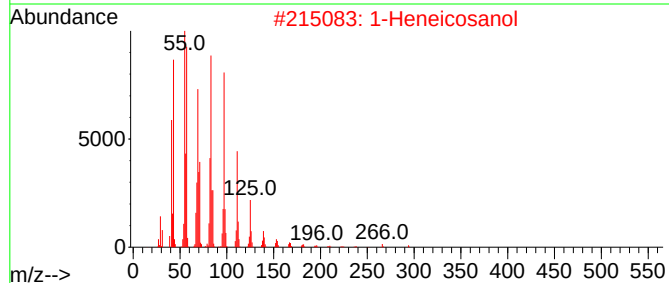
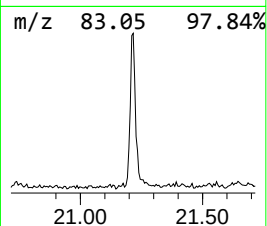
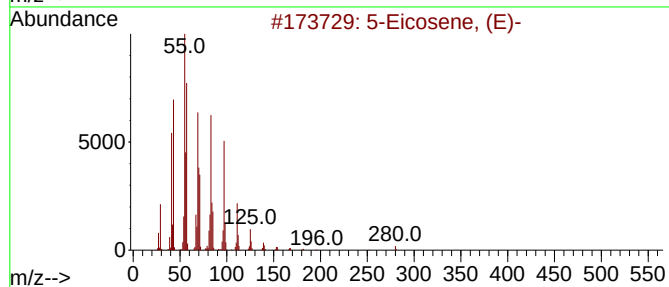
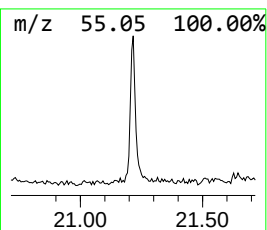
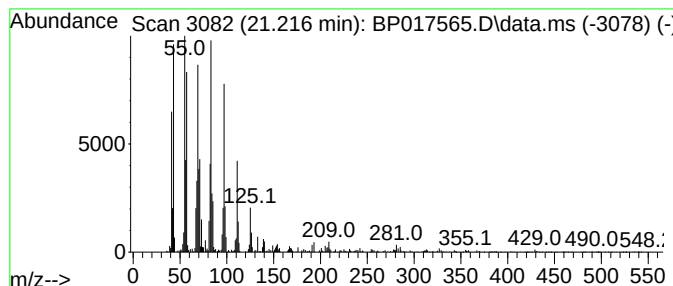
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.216	2.22 ng/ul	233280	Chrysene-d12	21.557

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Cyclopentadecane	210	C15H30	000295-48-7	95
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5		1-Octadecanol	270	C18H38O	000112-92-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017565.D
Acq On : 05 Oct 2023 14:48
Operator : MA/JU
Sample : 04679-12
Misc :
ALS Vial : 39 Sample Multiplier: 1

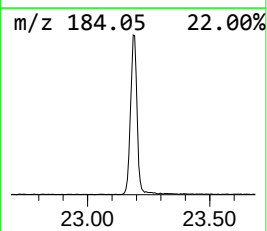
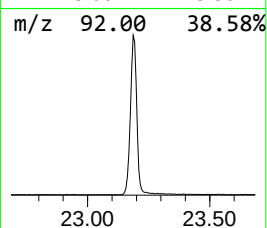
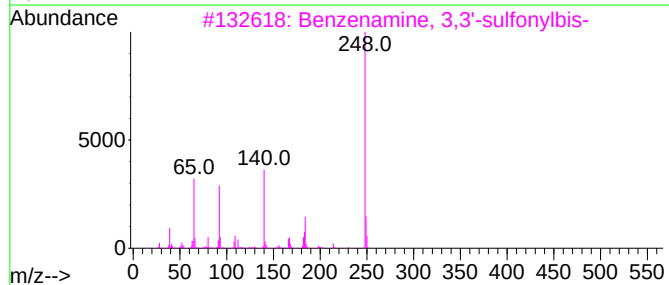
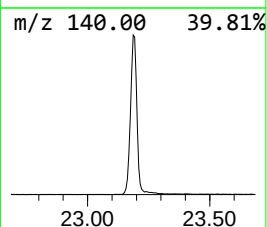
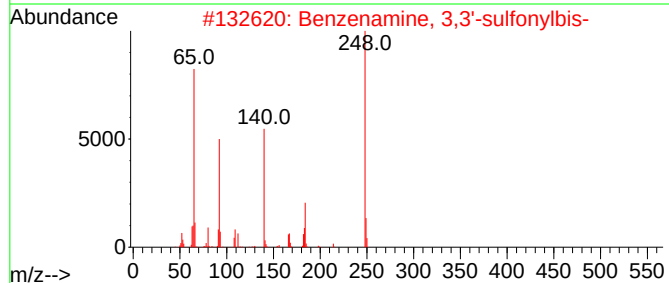
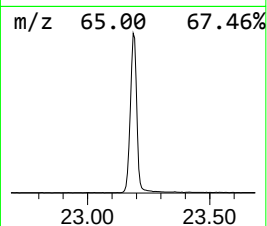
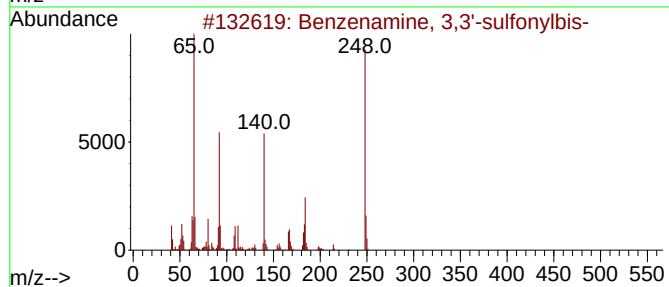
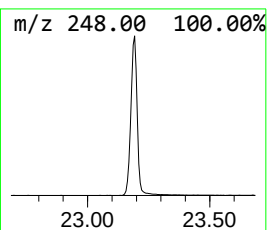
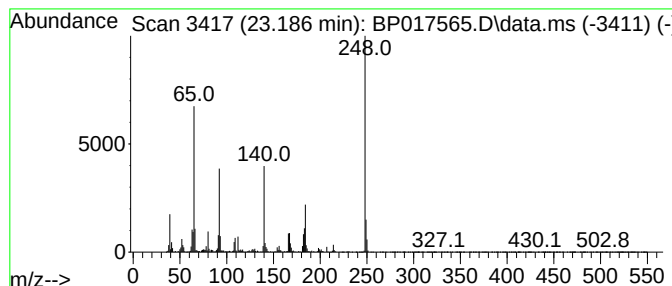
Instrument :
BNA_P
ClientSampleId :
PMW-7S(20230927)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 Benzenamine, 3,3'-sulfonylbis- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.186	23.11 ng/ul	2598910	Perylene-d12		24.139	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzenamine, 3,3'-sulfonylbis-		248	C12H12N2O2S	000599-61-1	99
2	Benzenamine, 3,3'-sulfonylbis-		248	C12H12N2O2S	000599-61-1	99
3	Benzenamine, 3,3'-sulfonylbis-		248	C12H12N2O2S	000599-61-1	96
4	3,4'-Diaminodiphenylsulfone		248	C12H12N2O2S	034262-32-3	64
5	2,3'-Diaminodiphenylsulfone		248	C12H12N2O2S	034262-29-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017565.D
Acq On : 05 Oct 2023 14:48
Operator : MA/JU
Sample : 04679-12
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-7S(20230927)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.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
Benzene, 1,3-di...	8.287	3.2	ng/ul	96284	1	7.940	599872	20.0
2-Naphthalenamine	15.216	2.8	ng/ul	191822	3	14.634	1376300	20.0
n-Hexadecanoic ...	18.269	4.0	ng/ul	349929	4	17.422	1743810	20.0
(DEL) Alkane: S...	21.216	2.2	ng/ul	233280	5	21.557	2099230	20.0
Benzenamine, 3,...	23.186	23.1	ng/ul	2598910	6	24.139	2249080	20.0