

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
 Data File : BP021153.D
 Acq On : 25 Jul 2024 18:49
 Operator : MA/JU
 Sample : P3263-17 5X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A4CK5

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-BP071024.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP021153.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.187	30	34	37	rVB5	8086	10727	0.51%	0.049%
2	3.481	81	84	90	rBV	12569	21690	1.04%	0.098%
3	3.640	108	111	114	rBV4	7796	10266	0.49%	0.047%
4	3.699	117	121	127	rVB	19906	29997	1.44%	0.136%
5	3.905	148	156	167	rVB	89772	143343	6.86%	0.650%
6	4.228	208	211	215	rVB3	8675	11128	0.53%	0.050%
7	4.452	245	249	255	rVB6	7285	11388	0.55%	0.052%
8	4.805	303	309	317	rVB2	11511	23651	1.13%	0.107%
9	5.252	381	385	389	rBV6	3849	6053	0.29%	0.027%
10	5.323	394	397	404	rVB4	6633	13432	0.64%	0.061%
11	5.675	452	457	463	rBV3	19571	34823	1.67%	0.158%
12	5.752	465	470	472	rBV6	4327	5862	0.28%	0.027%
13	6.199	542	546	551	rVB8	5552	8658	0.41%	0.039%
14	6.287	553	561	563	rBV8	5161	9891	0.47%	0.045%
15	6.540	598	604	612	rBV5	5647	9915	0.47%	0.045%
16	6.628	616	619	626	rBV7	5138	7226	0.35%	0.033%
17	6.687	626	629	634	rVB7	4451	6796	0.33%	0.031%
18	6.758	634	641	643	rBV8	7935	14164	0.68%	0.064%
19	6.828	648	653	657	rVV	56382	103572	4.96%	0.469%
20	6.875	657	661	678	rVV	97120	210688	10.09%	0.955%
21	7.005	678	683	693	rVV	86734	153108	7.33%	0.694%
22	7.122	699	703	710	rVB9	4935	9720	0.47%	0.044%
23	7.205	710	717	722	rBV	124178	210486	10.08%	0.954%
24	7.252	722	725	730	rVV	29844	50098	2.40%	0.227%
25	7.299	730	733	739	rVV5	16635	32964	1.58%	0.149%
26	7.352	739	742	746	rVV6	6248	9192	0.44%	0.042%
27	7.593	779	783	786	rBV3	7965	10729	0.51%	0.049%
28	7.652	786	793	806	rVV	756996	1202364	57.55%	5.448%
29	7.928	832	840	855	rBV6	19795	66318	3.17%	0.301%
30	8.187	879	884	890	rVB6	10499	20225	0.97%	0.092%
31	8.269	893	898	903	rBV6	11944	18150	0.87%	0.082%
32	8.387	911	918	933	rBV2	111114	271561	13.00%	1.230%
33	8.487	933	935	942	rVB5	8924	15509	0.74%	0.070%
34	8.728	971	976	983	rVB8	7708	16491	0.79%	0.075%
35	8.816	985	991	1004	rBV2	106769	259073	12.40%	1.174%
36	8.958	1010	1015	1021	rVB9	8649	19463	0.93%	0.088%

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
 Data File : BP021153.D
 Acq On : 25 Jul 2024 18:49
 Operator : MA/JU
 Sample : P3263-17 5X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A4CK5

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-BP071024.MA.M
 Title : SVOA CALIBRATION

37	9.528	1102	1112	1124	rBV	87818	189335	9.06%	0.858%
38	9.669	1134	1136	1144	rVB8	4650	8719	0.42%	0.040%
39	9.769	1144	1153	1166	rBV2	58952	227396	10.88%	1.030%
40	10.093	1199	1208	1219	rBV	97855	238177	11.40%	1.079%

41	10.281	1236	1240	1244	rVB5	5922	8397	0.40%	0.038%
42	10.363	1246	1254	1256	rBV	20995	32538	1.56%	0.147%
43	10.416	1256	1263	1269	rVV	882445	1599318	76.56%	7.247%
44	10.469	1269	1272	1284	rVB	90594	148162	7.09%	0.671%
45	10.558	1284	1287	1291	rVB5	4955	6109	0.29%	0.028%

46	10.599	1291	1294	1295	rBV3	5659	6830	0.33%	0.031%
47	11.057	1368	1372	1374	rBV5	5452	7652	0.37%	0.035%
48	11.181	1387	1393	1401	rBV3	24305	63495	3.04%	0.288%
49	11.263	1404	1407	1411	rVV6	9891	15903	0.76%	0.072%
50	11.310	1411	1415	1420	rVB8	6015	12333	0.59%	0.056%

51	11.410	1422	1432	1436	rVV5	9210	16467	0.79%	0.075%
52	11.816	1497	1501	1511	rVB3	17012	30262	1.45%	0.137%
53	11.969	1520	1527	1532	rBV7	5983	13322	0.64%	0.060%
54	12.093	1543	1548	1554	rBV	45148	71719	3.43%	0.325%
55	12.204	1561	1567	1580	rBV2	106549	294203	14.08%	1.333%

56	12.304	1581	1584	1594	rVB	25334	50920	2.44%	0.231%
57	12.740	1654	1658	1660	rBV4	4819	6087	0.29%	0.028%
58	12.793	1662	1667	1671	rVB5	7775	14398	0.69%	0.065%
59	13.081	1709	1716	1719	rBV2	16498	29411	1.41%	0.133%
60	13.110	1719	1721	1729	rVB	11874	24338	1.16%	0.110%

61	13.240	1738	1743	1751	rVV	8961	16891	0.81%	0.077%
62	13.310	1751	1755	1764	rVB3	10853	21940	1.05%	0.099%
63	13.451	1773	1779	1780	rBV3	14585	26421	1.26%	0.120%
64	13.604	1800	1805	1810	rBV3	25081	48586	2.33%	0.220%
65	13.657	1810	1814	1817	rBV2	20317	29408	1.41%	0.133%

66	13.699	1817	1821	1827	rBV	205872	309255	14.80%	1.401%
67	13.846	1842	1846	1849	rBV2	10698	17099	0.82%	0.077%
68	13.987	1861	1870	1874	rBV	295283	509709	24.40%	2.310%
69	14.099	1887	1889	1893	rVB5	8206	8361	0.40%	0.038%
70	14.175	1898	1902	1909	rVB2	19208	30637	1.47%	0.139%

71	14.299	1911	1923	1929	rBV	1320369	1956228	93.64%	8.864%
72	14.357	1929	1933	1943	rVB2	32185	71469	3.42%	0.324%
73	14.493	1949	1956	1957	rBV	802360	1083422	51.86%	4.909%
74	14.640	1976	1981	1987	rBV4	20862	47496	2.27%	0.215%
75	14.704	1987	1992	1996	rVV	60007	87871	4.21%	0.398%

76	14.775	2002	2004	2007	rVB3	10801	12353	0.59%	0.056%
----	--------	------	------	------	------	-------	-------	-------	--------

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
 Data File : BP021153.D
 Acq On : 25 Jul 2024 18:49
 Operator : MA/JU
 Sample : P3263-17 5X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A4CK5

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-BP071024.MA.M
 Title : SVOA CALIBRATION

77	14.922	2025	2029	2033	rVB5	13646	21029	1.01%	0.095%
78	14.975	2035	2038	2044	rVB2	11775	16228	0.78%	0.074%
79	15.098	2055	2059	2062	rVB6	11032	16004	0.77%	0.073%
80	15.151	2063	2068	2071	rVV3	20359	32523	1.56%	0.147%
81	15.187	2071	2074	2079	rVB	13592	18571	0.89%	0.084%
82	15.304	2088	2094	2100	rBV	346412	514557	24.63%	2.332%
83	15.363	2100	2104	2117	rVB4	40366	95606	4.58%	0.433%
84	15.487	2118	2125	2130	rBV3	46548	102369	4.90%	0.464%
85	15.663	2151	2155	2162	rVB4	27971	49729	2.38%	0.225%
86	15.828	2178	2183	2188	rBV2	25527	49373	2.36%	0.224%
87	16.045	2214	2220	2232	rVB7	42569	141319	6.76%	0.640%
88	16.769	2338	2343	2347	rBV3	58495	104719	5.01%	0.475%
89	16.928	2368	2370	2377	rVB	57260	75166	3.60%	0.341%
90	17.110	2395	2401	2405	rBV	1272984	1935542	92.65%	8.770%
91	17.151	2405	2408	2413	rVV	667207	939454	44.97%	4.257%
92	17.210	2414	2418	2422	rVV	323891	467402	22.37%	2.118%
93	17.251	2422	2425	2430	rVB	207620	280134	13.41%	1.269%
94	18.016	2552	2555	2556	rBV	89921	93365	4.47%	0.423%
95	18.045	2556	2560	2562	rVV	255679	294753	14.11%	1.336%
96	18.216	2585	2589	2593	rBV2	165473	324782	15.55%	1.472%
97	19.257	2761	2766	2770	rBV	1225936	1808419	86.56%	8.194%
98	19.604	2821	2825	2827	rBV2	580585	814702	39.00%	3.692%
99	19.634	2827	2830	2836	rVB	891482	1333005	63.81%	6.040%
100	21.563	3153	3158	3162	rVB2	1250314	2089099	100.00%	9.466%

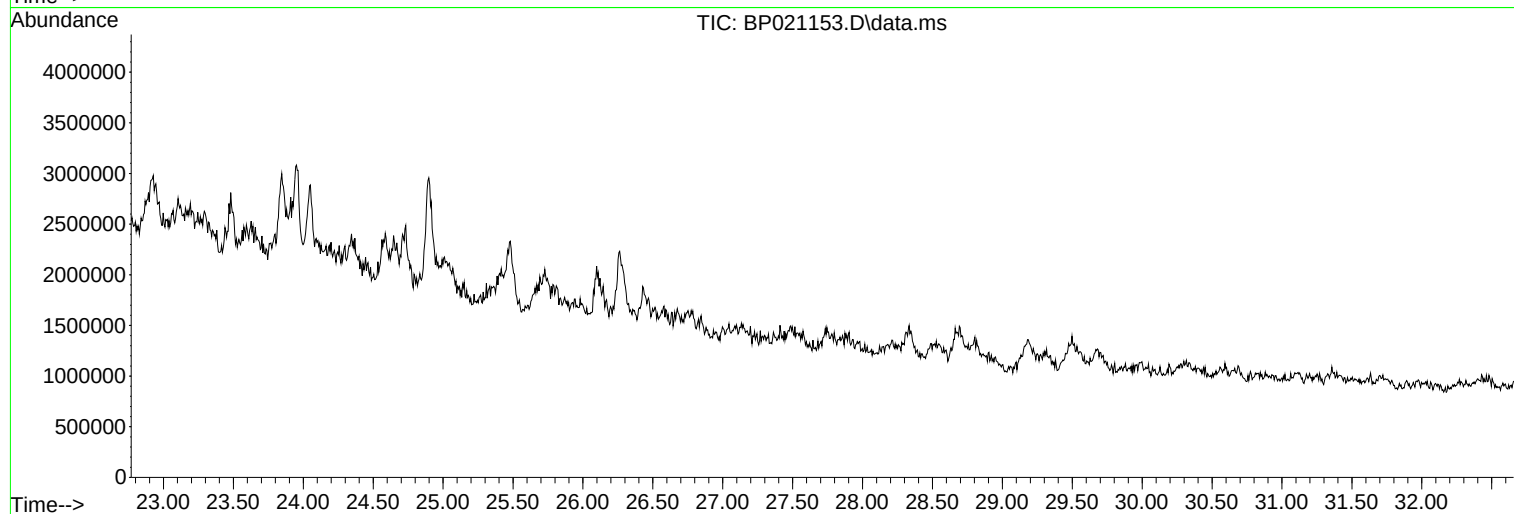
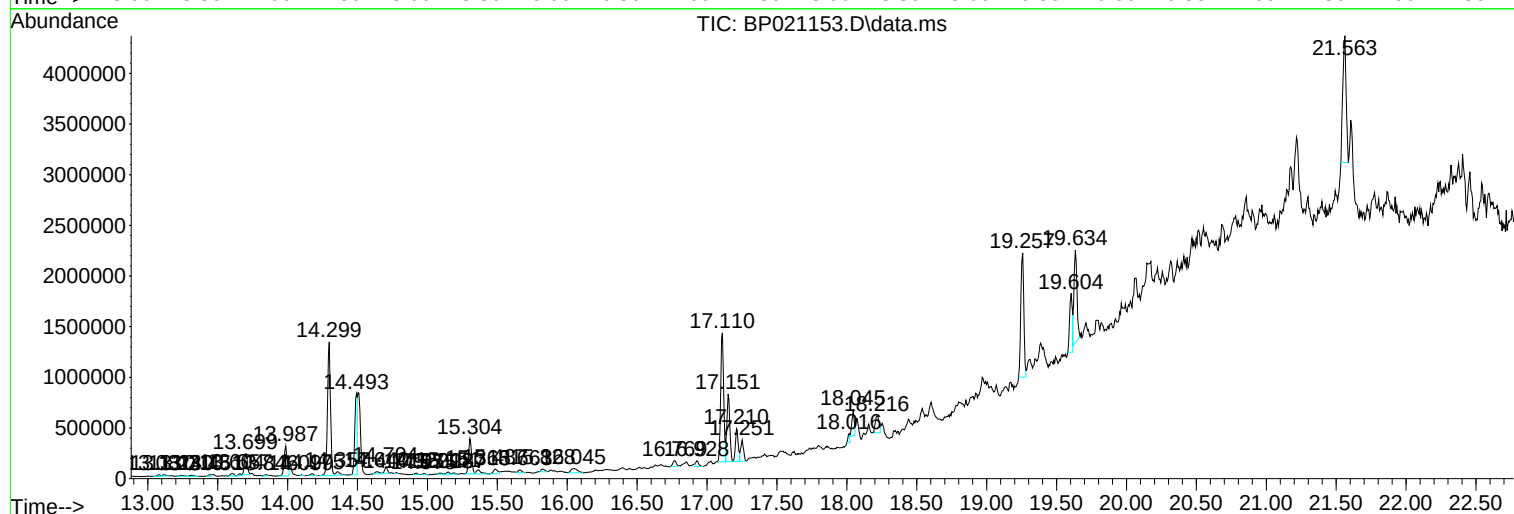
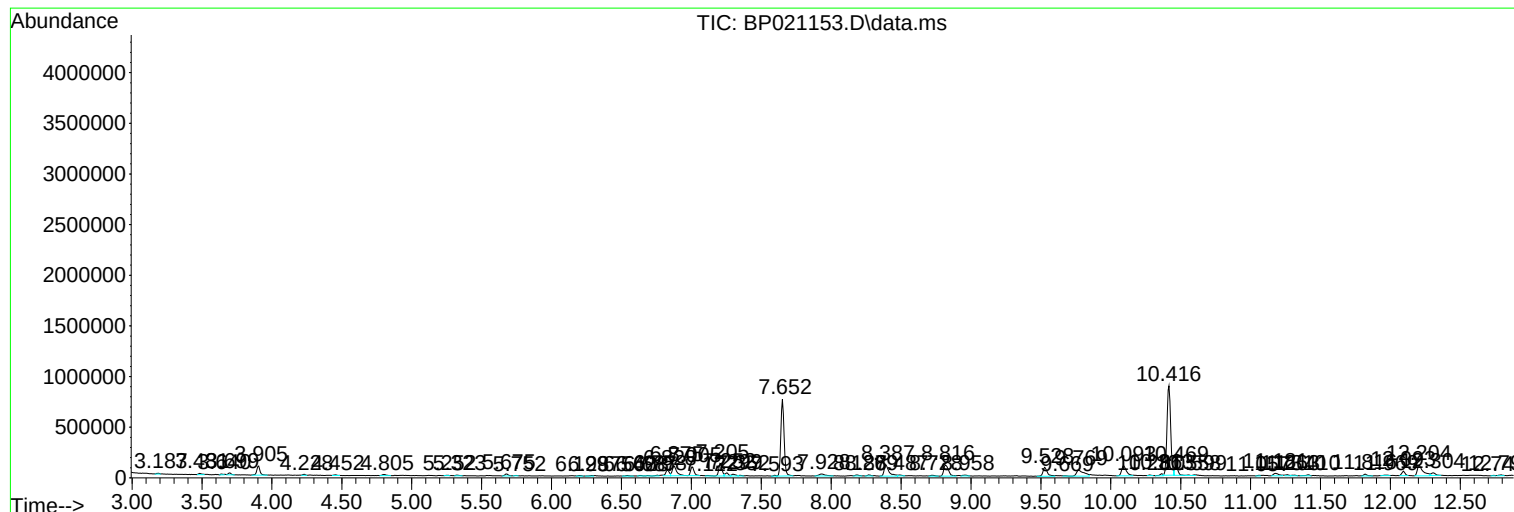
Sum of corrected areas: 22069208

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
Data File : BP021153.D
Acq On : 25 Jul 2024 18:49
Operator : MA/JU
Sample : P3263-17 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4CK5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
Data File : BP021153.D
Acq On : 25 Jul 2024 18:49
Operator : MA/JU
Sample : P3263-17 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4CK5

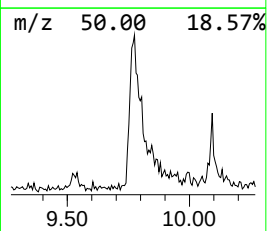
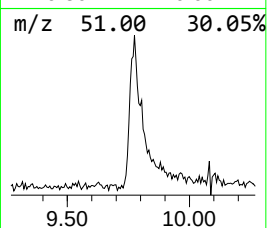
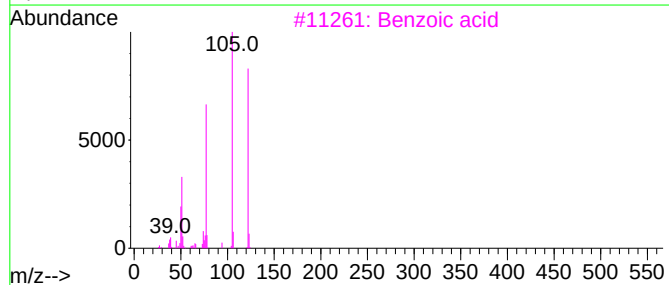
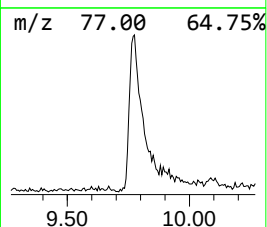
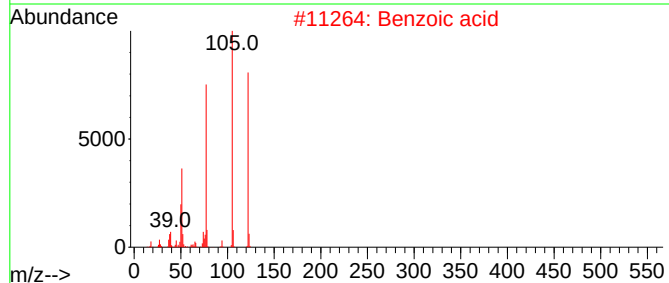
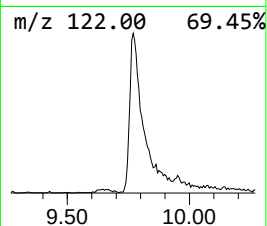
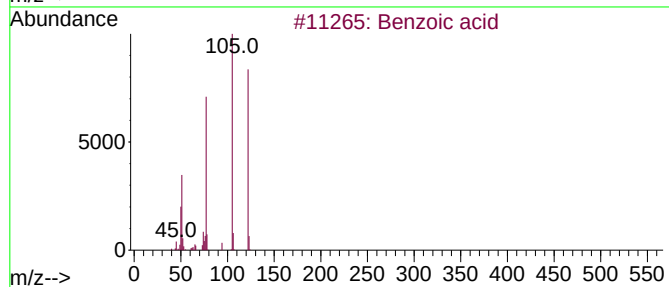
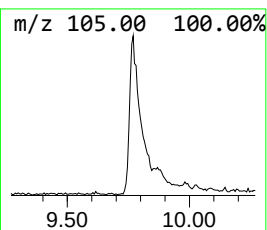
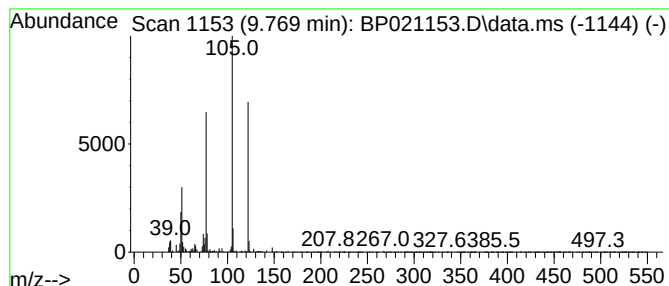
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.769	2.84 ng/ul	227396	Naphthalene-d8	10.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid	122	C7H6O2	000065-85-0	97
2			Benzoic acid	122	C7H6O2	000065-85-0	94
3			Benzoic acid	122	C7H6O2	000065-85-0	94
4			Benzoic acid	122	C7H6O2	000065-85-0	91
5			Benzoic acid, silver(1+) salt	228	C7H5AgO2	000532-31-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
Data File : BP021153.D
Acq On : 25 Jul 2024 18:49
Operator : MA/JU
Sample : P3263-17 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4CK5

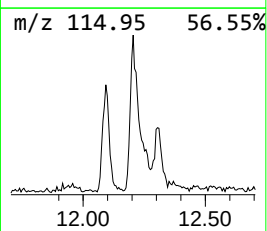
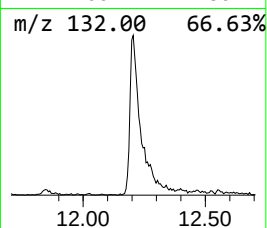
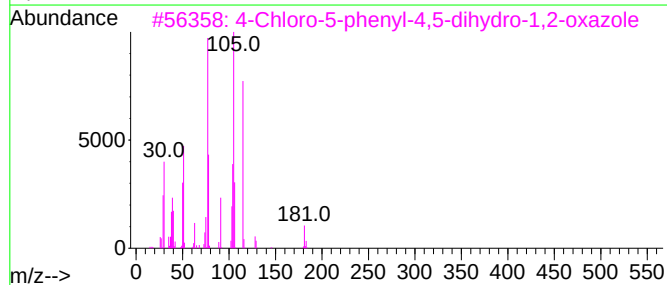
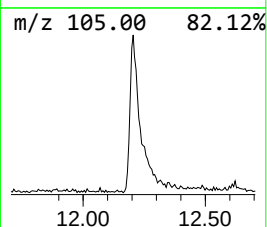
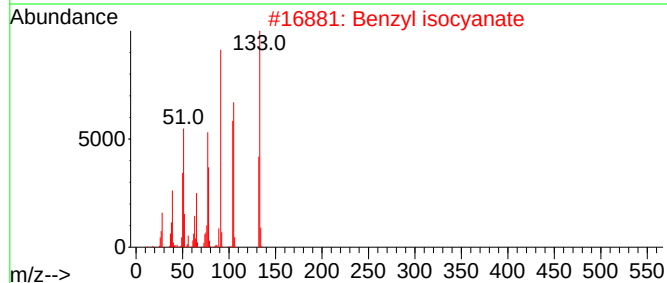
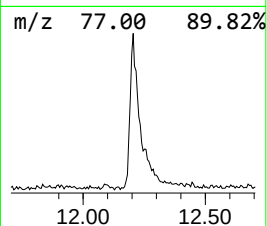
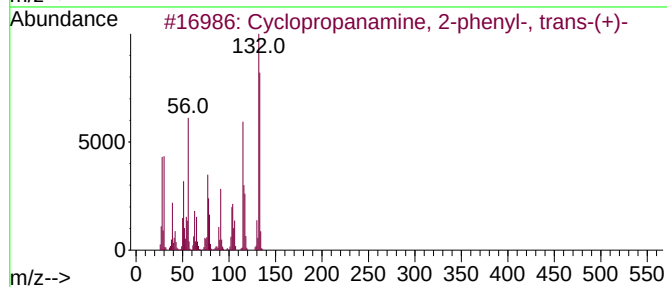
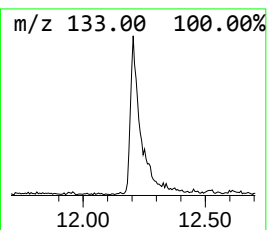
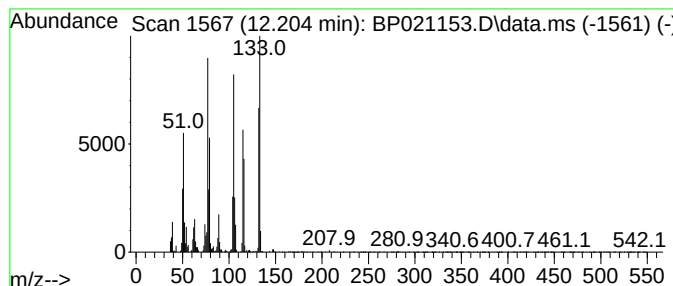
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.204	3.68 ng/ul	294203	Naphthalene-d8	10.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanamine, 2-phenyl-, tra...	133	C9H11N	003721-28-6	38
2			Benzyl isocyanate	133	C8H7NO	003173-56-6	30
3			4-Chloro-5-phenyl-4,5-dihydro-1,...	181	C9H8ClNO	1188906-47-9	27
4			Benzyl isocyanate	133	C8H7NO	003173-56-6	27
5			Benzeneacetonitrile, 3-hydroxy-	133	C8H7NO	025263-44-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
Data File : BP021153.D
Acq On : 25 Jul 2024 18:49
Operator : MA/JU
Sample : P3263-17 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4CK5

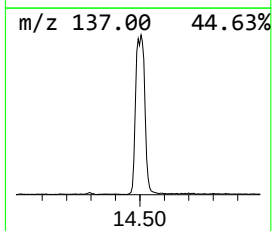
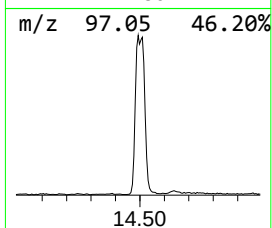
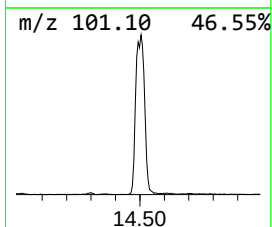
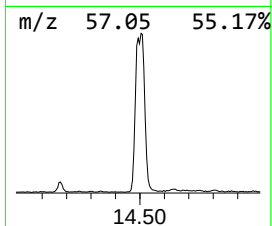
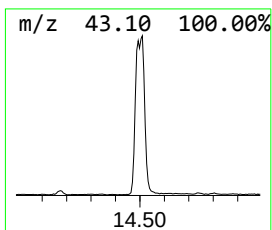
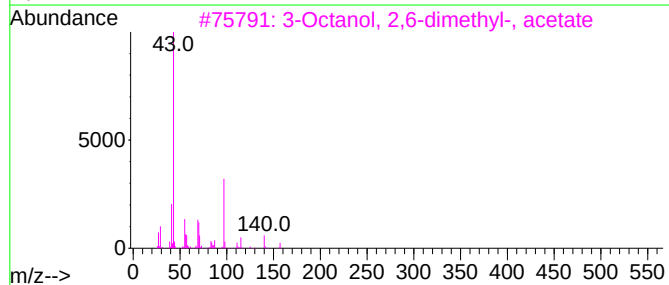
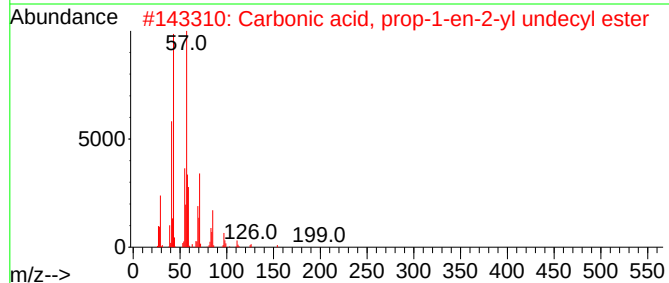
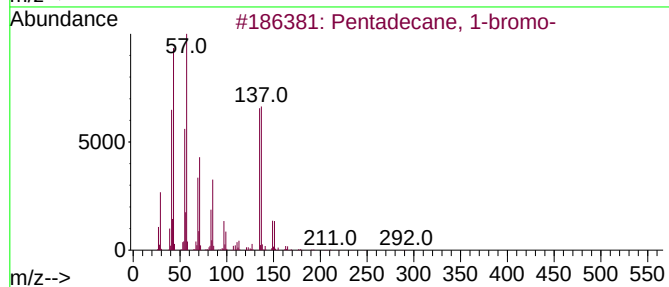
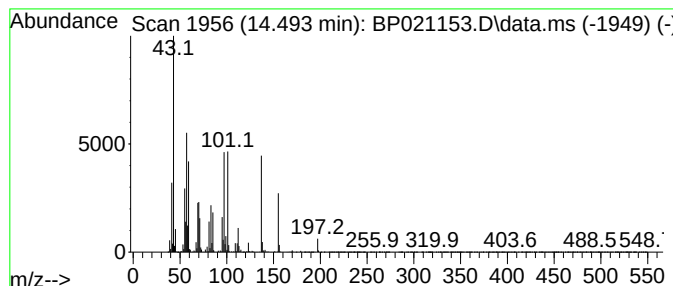
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.493	11.08 ng/ul	1083420	Acenaphthene-d10	14.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	15
2			Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	10
3			3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	10
4			6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	10
5			CH3C(O)OCH(CH2CH3)C(CH3)3	158	C9H18O2	039511-81-4	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
Data File : BP021153.D
Acq On : 25 Jul 2024 18:49
Operator : MA/JU
Sample : P3263-17 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4CK5

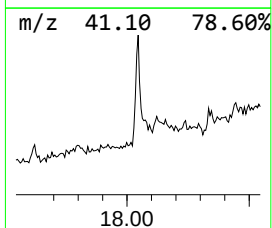
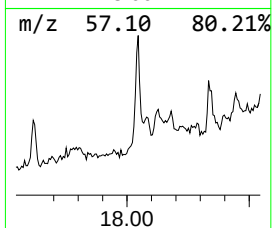
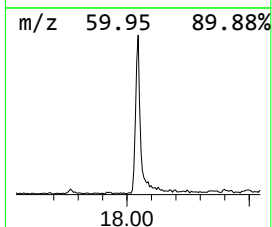
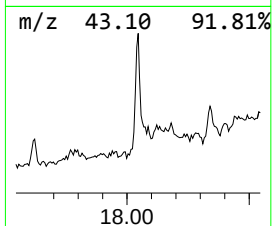
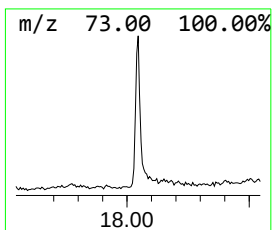
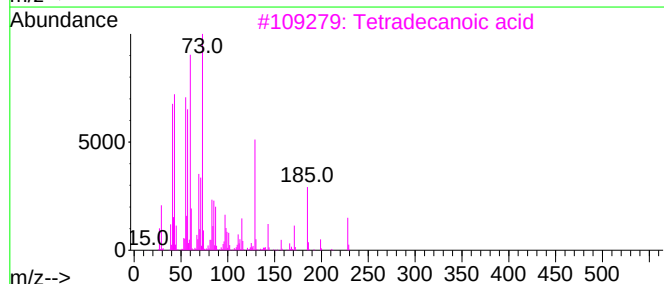
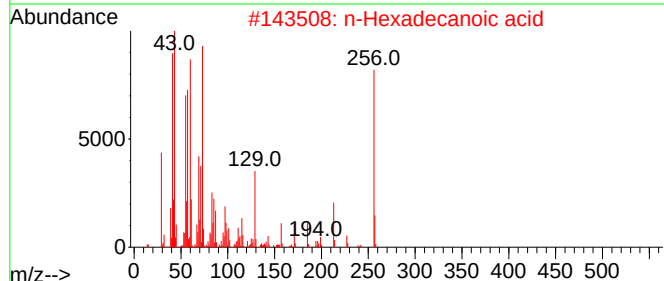
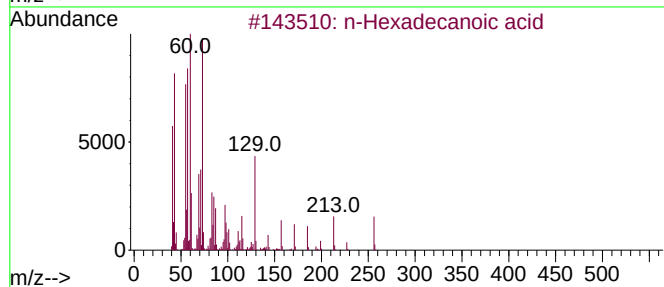
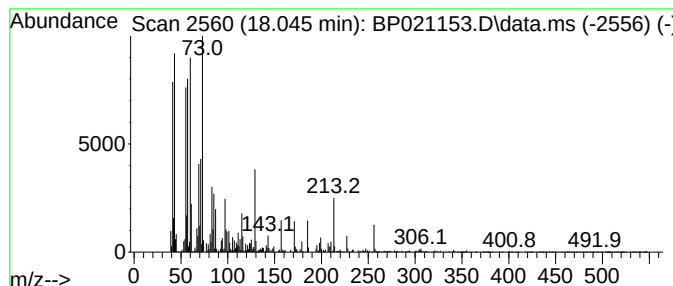
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	3.05 ng/ul	294753	Phenanthrene-d10	17.110

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	98
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Octadecanoic acid	284	C18H36O2	000057-11-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
Data File : BP021153.D
Acq On : 25 Jul 2024 18:49
Operator : MA/JU
Sample : P3263-17 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4CK5

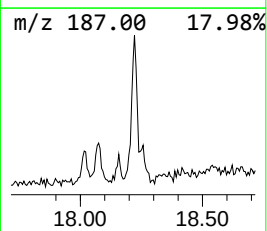
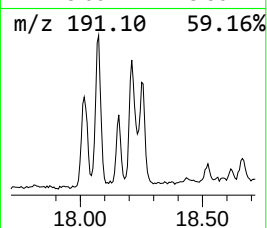
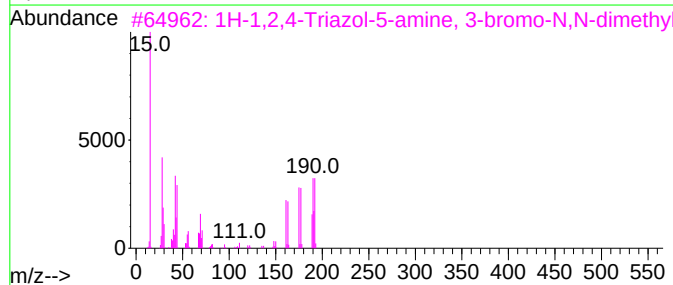
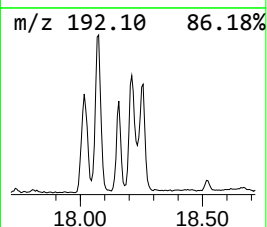
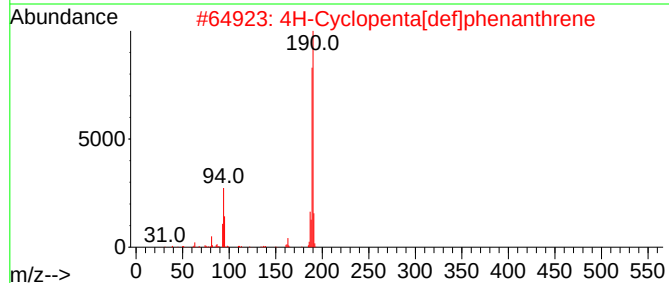
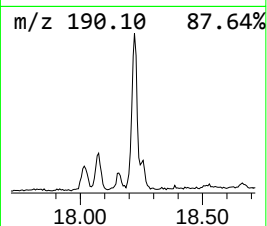
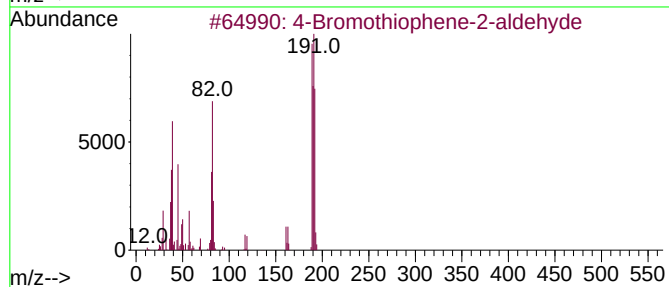
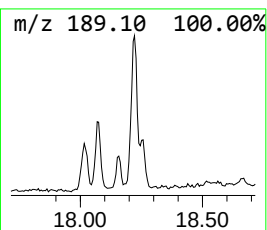
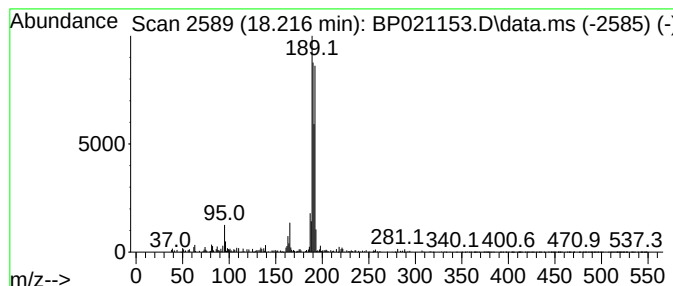
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 4-Bromothiophene-2-aldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	3.36 ng/ul	324782	Phenanthrene-d10	17.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	64
2			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
3			1H-1,2,4-Triazol-5-amine, 3-brom...	190	C4H7BrN4	1000460-85-7	59
4			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	43
5			5-Amino-3-bromo-2-fluoropyridine	190	C5H4BrFN2	209328-99-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072524\
Data File : BP021153.D
Acq On : 25 Jul 2024 18:49
Operator : MA/JU
Sample : P3263-17 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4CK5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.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
Benzoic acid	9.769	2.8	ng/ul	227396	2	10.416	1599320	20.0
unknown-01	12.204	3.7	ng/ul	294203	2	10.416	1599320	20.0
unknown-02	14.493	11.1	ng/ul	1083420	3	14.299	1956230	20.0
n-Hexadecanoic ...	18.045	3.0	ng/ul	294753	4	17.110	1935540	20.0
4-Bromothiophen...	18.216	3.4	ng/ul	324782	4	17.110	1935540	20.0