

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
 Data File : BN034667.D
 Acq On : 19 Oct 2024 03:06
 Operator : RC/JU
 Sample : P4380-08RX
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 E27J0RX

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_N\Methods\SFAM-EPA-BN101624.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BN034667.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.969	8	14	36	rVB	12357844	19286316	100.00%	15.155%
2	3.211	53	55	60	rVV	94841	120972	0.63%	0.095%
3	3.493	95	103	107	rBV2	85951	165722	0.86%	0.130%
4	3.611	118	123	137	rBV	666035	993694	5.15%	0.781%
5	3.928	172	177	190	rVB	793710	1128679	5.85%	0.887%
6	4.440	258	264	276	rBV	4517505	6973714	36.16%	5.480%
7	4.611	281	293	297	rVV	248220	582163	3.02%	0.457%
8	4.752	304	317	324	rBV	196833	435054	2.26%	0.342%
9	5.346	413	418	427	rBV	66136	117393	0.61%	0.092%
10	6.158	549	556	559	rBV	69482	119462	0.62%	0.094%
11	6.681	635	645	650	rBV	60393	130661	0.68%	0.103%
12	6.840	665	672	675	rBV	550562	997032	5.17%	0.783%
13	7.005	694	700	708	rVV	1428179	2163788	11.22%	1.700%
14	7.199	726	733	741	rVB	1619189	2502440	12.98%	1.966%
15	7.322	748	754	762	rVB3	55944	108493	0.56%	0.085%
16	7.575	792	797	805	rVV3	132756	232252	1.20%	0.183%
17	7.663	805	812	819	rVV	1351188	2144212	11.12%	1.685%
18	7.740	821	825	829	rVV	102534	180864	0.94%	0.142%
19	8.157	891	896	907	rVV	457775	786105	4.08%	0.618%
20	8.369	925	932	937	rVV	1331366	2147905	11.14%	1.688%
21	8.434	937	943	947	rVV	257657	499725	2.59%	0.393%
22	8.475	947	950	957	rVB2	67786	131124	0.68%	0.103%
23	8.552	957	963	971	rBV2	81727	174449	0.90%	0.137%
24	8.757	989	998	1001	rBV4	84784	167775	0.87%	0.132%
25	8.804	1001	1006	1012	rVV	1507657	2399767	12.44%	1.886%
26	8.875	1012	1018	1027	rVB3	178016	405492	2.10%	0.319%
27	9.075	1047	1052	1059	rVV3	171317	286307	1.48%	0.225%
28	9.199	1068	1073	1078	rBV6	46904	111346	0.58%	0.087%
29	9.263	1078	1084	1093	rVB5	84588	230258	1.19%	0.181%
30	9.369	1093	1102	1107	rBV3	61954	159012	0.82%	0.125%
31	9.522	1122	1128	1136	rVB	1188159	1912323	9.92%	1.503%
32	9.628	1139	1146	1148	rBV2	154625	250611	1.30%	0.197%
33	9.657	1148	1151	1155	rVB	109777	150847	0.78%	0.119%
34	9.857	1179	1185	1190	rBV4	97448	214771	1.11%	0.169%
35	9.934	1193	1198	1203	rVV2	148484	281053	1.46%	0.221%
36	9.999	1203	1209	1213	rVV3	183321	310759	1.61%	0.244%

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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_N\Methods\SFAM-EPA-BN101624.MA.M
 Title : SVOA CALIBRATION

37	10.063	1213	1220	1230	rVB	1782341	3225136	16.72%	2.534%
38	10.228	1243	1248	1254	rBV3	79785	138335	0.72%	0.109%
39	10.440	1274	1284	1288	rVV	1766975	2966262	15.38%	2.331%
40	10.487	1288	1292	1298	rVV	671809	1207422	6.26%	0.949%

41	10.569	1299	1306	1323	rVV2	1401404	2817147	14.61%	2.214%
42	10.998	1372	1379	1385	rVV	229020	409469	2.12%	0.322%
43	11.246	1414	1421	1423	rBV2	202137	394599	2.05%	0.310%
44	11.369	1437	1442	1447	rVB3	129096	227295	1.18%	0.179%
45	11.440	1447	1454	1462	rBV3	185816	354124	1.84%	0.278%

46	11.569	1470	1476	1479	rVV3	174142	317350	1.65%	0.249%
47	11.610	1479	1483	1490	rVB2	111762	199360	1.03%	0.157%
48	11.798	1507	1515	1516	rBV3	52878	113182	0.59%	0.089%
49	11.928	1532	1537	1546	rBV	325060	608906	3.16%	0.478%
50	12.034	1547	1555	1558	rVV5	75746	198756	1.03%	0.156%

51	12.075	1558	1562	1563	rVV2	114714	161028	0.83%	0.127%
52	12.104	1563	1567	1575	rVB	261237	420615	2.18%	0.331%
53	12.269	1591	1595	1599	rVV	78331	113093	0.59%	0.089%
54	12.322	1600	1604	1609	rVV	279330	408046	2.12%	0.321%
55	12.369	1609	1612	1616	rVB	114120	141885	0.74%	0.111%

56	12.440	1617	1624	1633	rBV4	215712	460562	2.39%	0.362%
57	12.593	1644	1650	1658	rBV7	145039	373517	1.94%	0.294%
58	12.657	1658	1661	1666	rVV6	59033	134907	0.70%	0.106%
59	12.834	1684	1691	1700	rVB5	270707	537154	2.79%	0.422%
60	13.034	1717	1725	1726	rBV2	107211	209803	1.09%	0.165%

61	13.169	1744	1748	1751	rVV2	183324	253476	1.31%	0.199%
62	13.210	1751	1755	1761	rVB	649192	943295	4.89%	0.741%
63	13.469	1794	1799	1806	rBV5	106172	216981	1.13%	0.171%
64	13.534	1806	1810	1813	rBV3	72802	110623	0.57%	0.087%
65	13.622	1817	1825	1829	rVV3	191444	434223	2.25%	0.341%

66	13.669	1830	1833	1835	rVV	105522	154456	0.80%	0.121%
67	13.716	1835	1841	1848	rVB	2121461	3095615	16.05%	2.433%
68	13.934	1874	1878	1881	rBV4	72658	119503	0.62%	0.094%
69	13.987	1881	1887	1897	rVB	3236670	4871130	25.26%	3.828%
70	14.157	1911	1916	1926	rVB	1134478	1558087	8.08%	1.224%

71	14.292	1933	1939	1945	rBV	2177826	3374977	17.50%	2.652%
72	14.357	1946	1950	1956	rVV	458475	692651	3.59%	0.544%
73	14.498	1969	1974	1979	rVB2	522510	728604	3.78%	0.573%
74	14.575	1984	1987	1994	rVB8	90713	146655	0.76%	0.115%
75	14.698	2005	2008	2016	rVB	158442	272818	1.41%	0.214%

76	14.775	2018	2021	2026	rVV6	91689	149043	0.77%	0.117%
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 ClientSampleId :
 E27J0RX

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_N\Methods\SFAM-EPA-BN101624.MA.M
 Title : SVOA CALIBRATION

77	14.828	2026	2030	2036	rVV2	179477	347601	1.80%	0.273%
78	15.222	2094	2097	2101	rVB	93034	119191	0.62%	0.094%
79	15.292	2103	2109	2115	rVV	3878754	5373241	27.86%	4.222%
80	15.345	2115	2118	2123	rVB	222297	296880	1.54%	0.233%
81	15.404	2123	2128	2136	rBV	1008575	1445813	7.50%	1.136%
82	15.557	2151	2154	2159	rBV5	80883	116586	0.60%	0.092%
83	15.628	2163	2166	2169	rBV	143899	192033	1.00%	0.151%
84	15.745	2182	2186	2192	rVB	637636	783999	4.07%	0.616%
85	15.969	2221	2224	2226	rBV	86869	116326	0.60%	0.091%
86	16.351	2284	2289	2294	rVB	1380891	1892596	9.81%	1.487%
87	16.439	2301	2304	2314	rVB5	227852	389215	2.02%	0.306%
88	16.692	2344	2347	2355	rVB2	148120	248761	1.29%	0.195%
89	16.922	2383	2386	2393	rVB3	144578	234882	1.22%	0.185%
90	17.039	2399	2406	2410	rBV	2445818	3540009	18.36%	2.782%
91	17.081	2410	2413	2416	rVV	540317	638350	3.31%	0.502%
92	17.139	2417	2423	2431	rVV2	4100598	5877678	30.48%	4.619%
93	17.428	2466	2472	2481	rVB4	242194	664190	3.44%	0.522%
94	18.080	2581	2583	2591	rVB6	181333	306826	1.59%	0.241%
95	19.433	2807	2813	2820	rBV	4620629	6389254	33.13%	5.021%
96	20.222	2944	2947	2951	rBV	354010	384511	1.99%	0.302%
97	20.939	3065	3069	3082	rVB	644262	909066	4.71%	0.714%
98	21.263	3119	3124	3135	rVB2	2457033	3580534	18.57%	2.814%
99	23.957	3573	3582	3598	rVB	3011385	7124417	36.94%	5.598%
100	24.151	3607	3615	3626	rVB	1651565	4024800	20.87%	3.163%

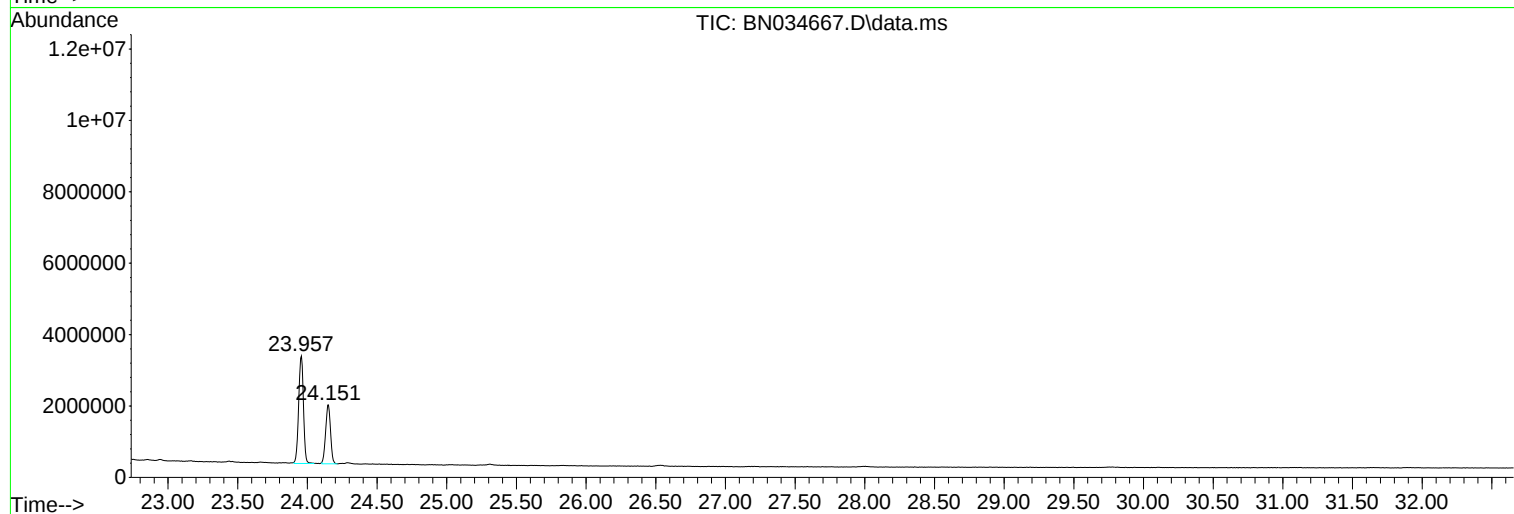
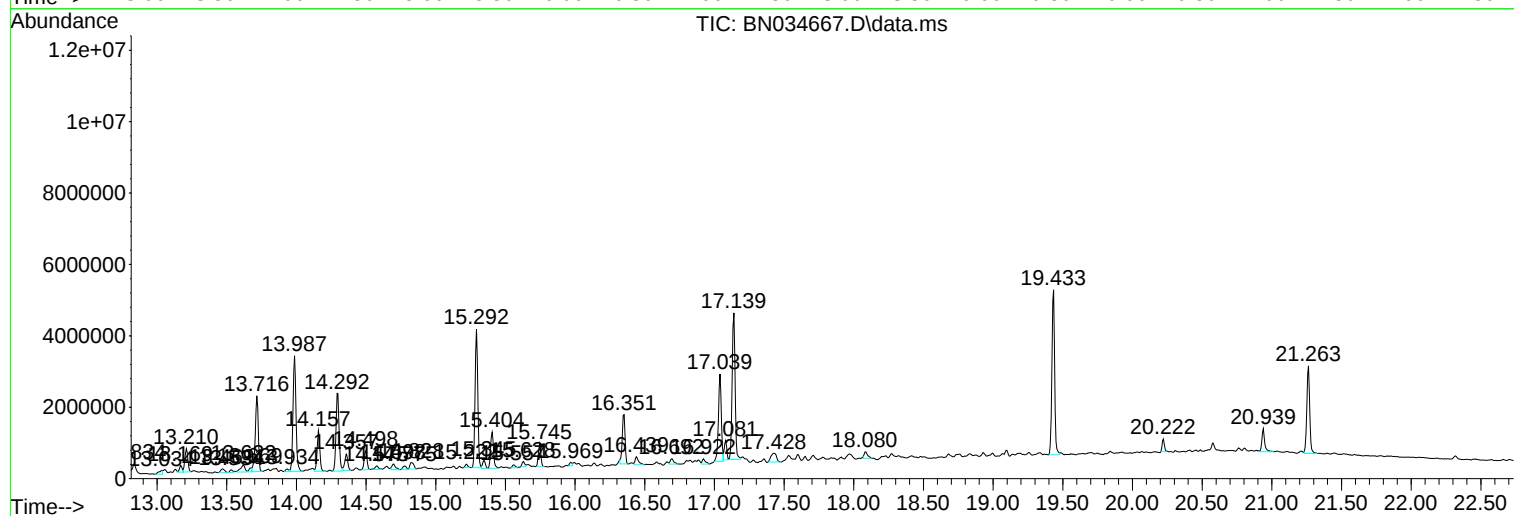
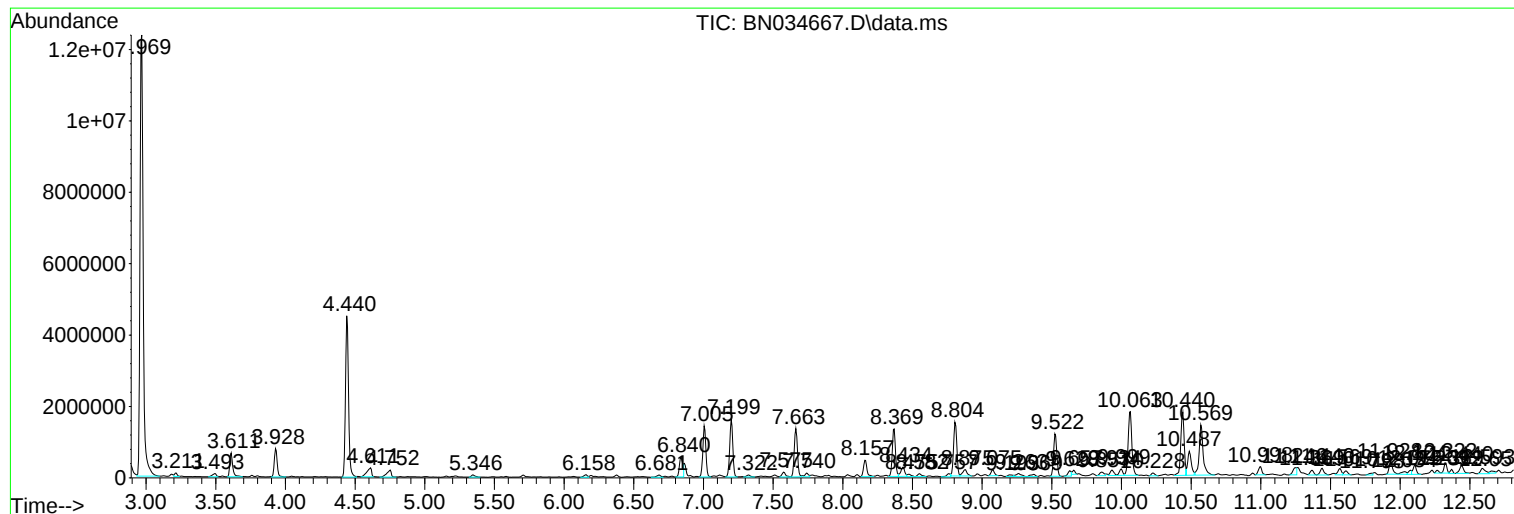
Sum of corrected areas: 127259389

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Instrument :
BNA_N
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101624.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
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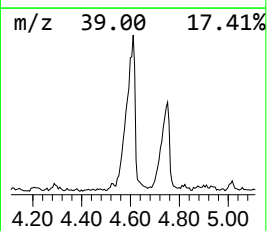
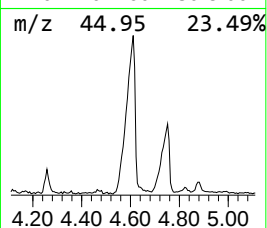
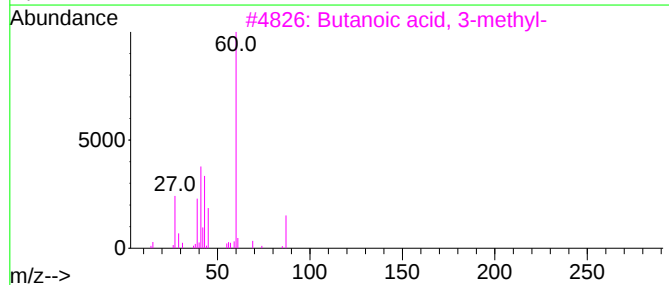
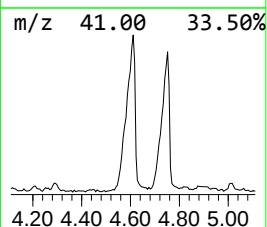
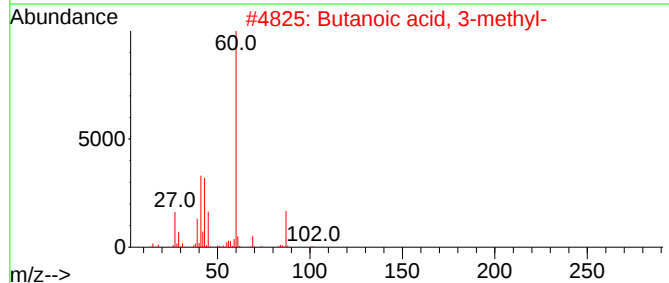
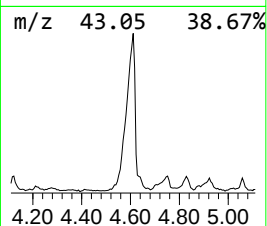
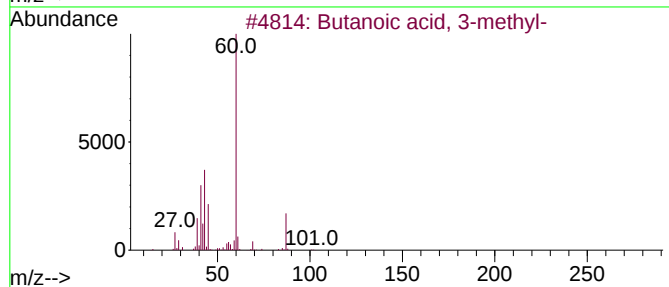
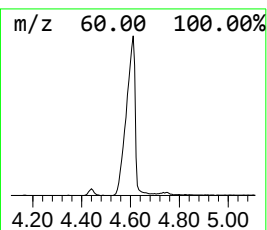
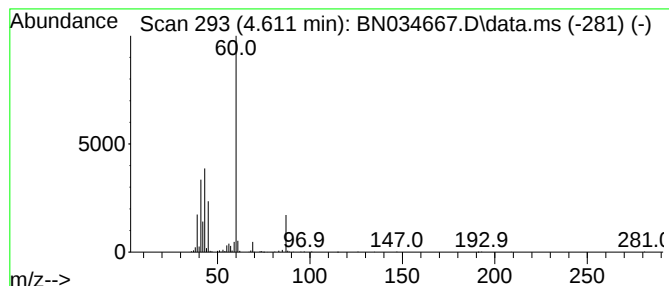
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 Butanoic acid, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.611	5.43 ng/ul	582163	1,4-Dichlorobenzene-d4	7.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	78
3			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	78
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	56



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ClientSampleId :
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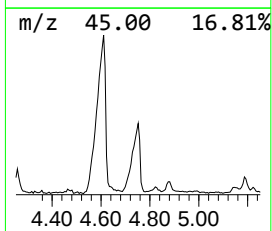
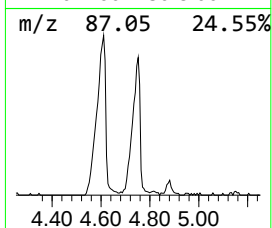
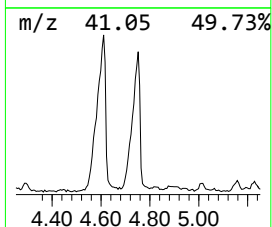
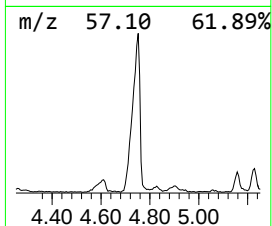
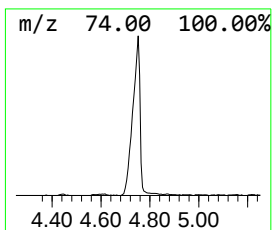
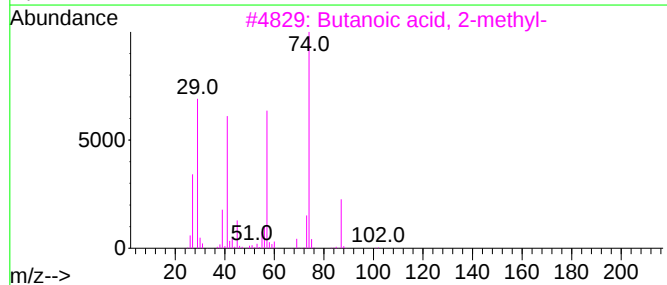
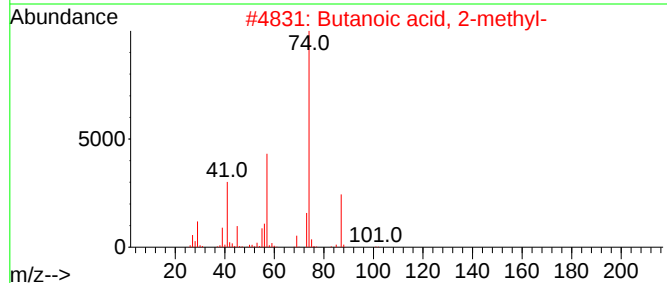
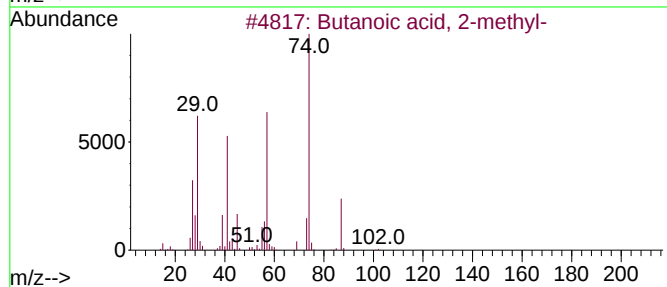
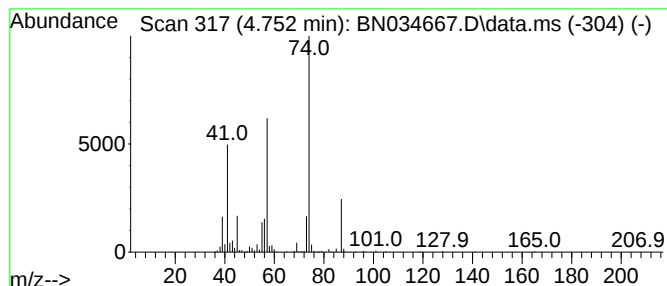
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 Butanoic acid, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.752	4.06 ng/ul	435054	1,4-Dichlorobenzene-d4	7.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	90
2			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
3			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
4			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
5			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72



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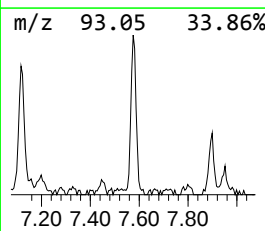
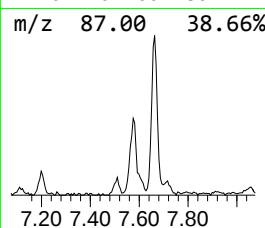
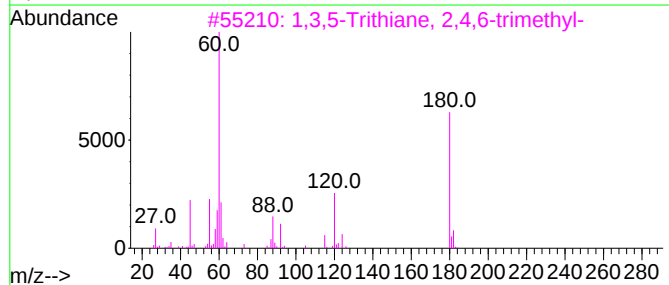
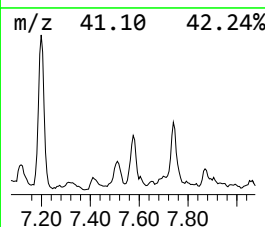
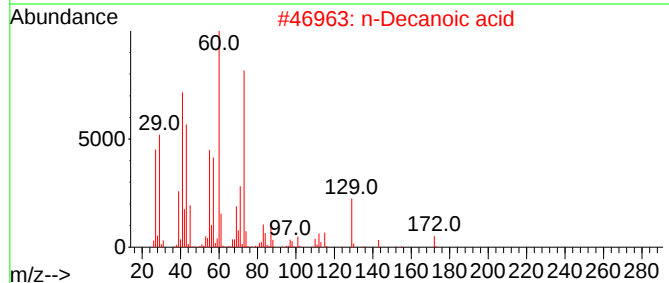
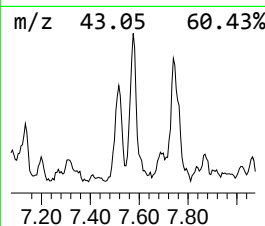
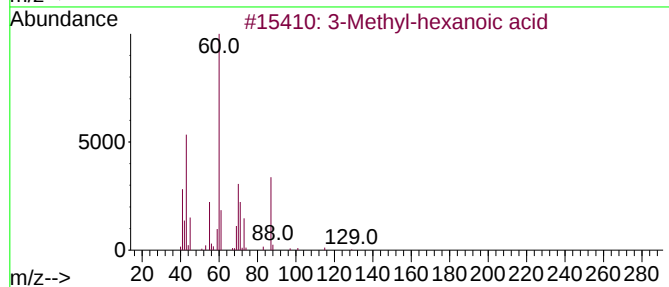
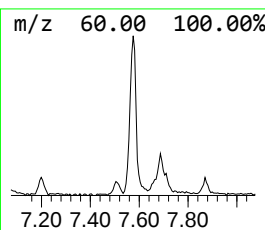
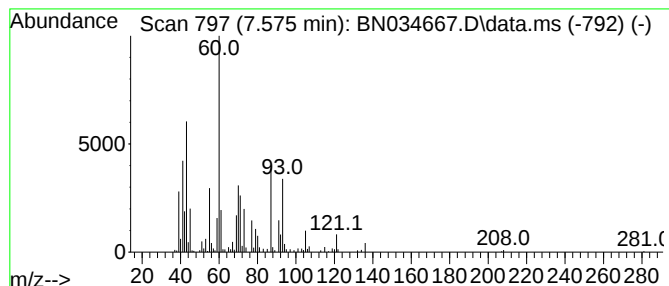
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 3-Methyl-hexanoic acid Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.575	2.17 ng/ul	232252	1,4-Dichlorobenzene-d4	7.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	86
2			n-Decanoic acid	172	C10H20O2	000334-48-5	25
3			1,3,5-Trithiane, 2,4,6-trimethyl-	180	C6H12S3	002765-04-0	23
4			.alpha.-L-Galactopyranoside, met...	178	C7H14O5	014687-15-1	23
5			Heptanoic acid	130	C7H14O2	000111-14-8	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E27J0RX

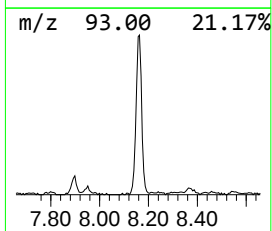
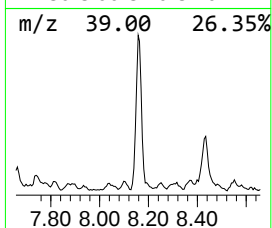
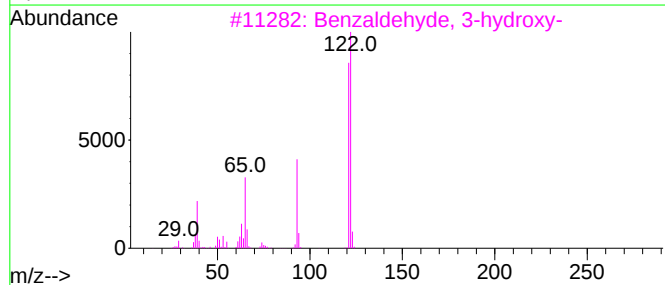
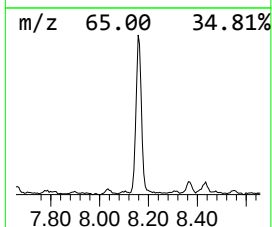
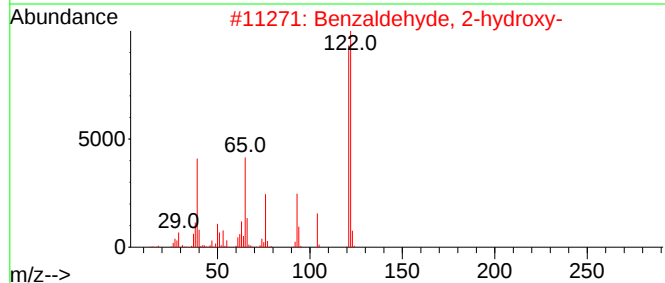
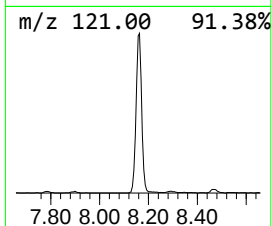
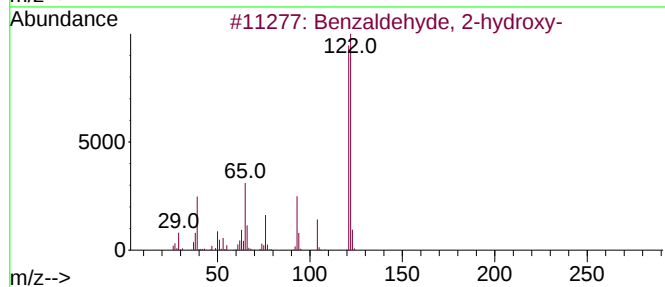
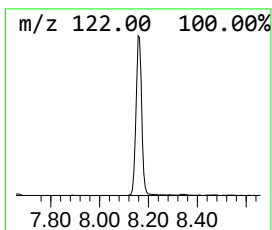
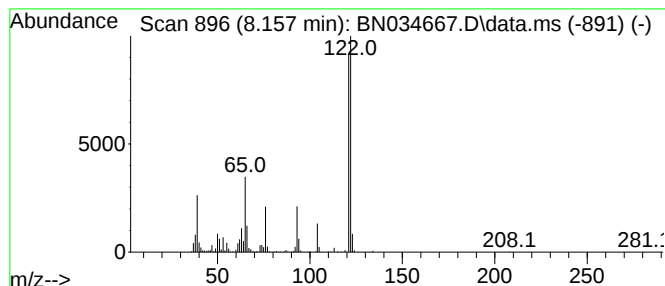
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Benzaldehyde, 2-hydroxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.157	7.33 ng/ul	786105	1,4-Dichlorobenzene-d4	7.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 2-hydroxy-	122	C7H6O2	000090-02-8	96
2			Benzaldehyde, 2-hydroxy-	122	C7H6O2	000090-02-8	95
3			Benzaldehyde, 3-hydroxy-	122	C7H6O2	000100-83-4	94
4			Benzaldehyde, 3-hydroxy-	122	C7H6O2	000100-83-4	89
5			Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
E27J0RX

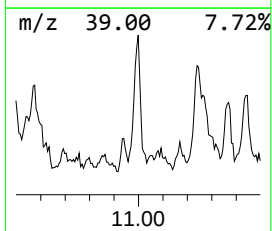
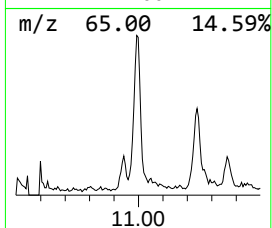
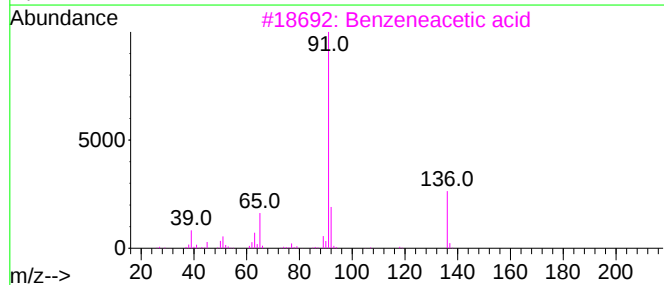
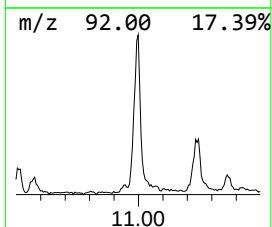
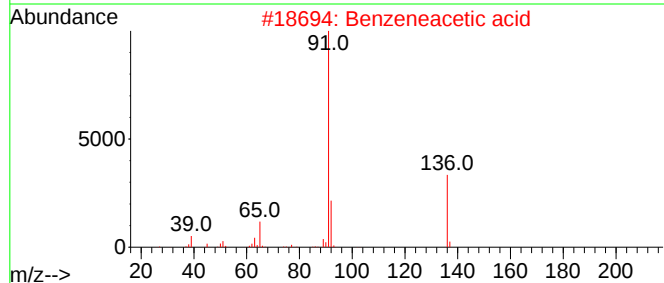
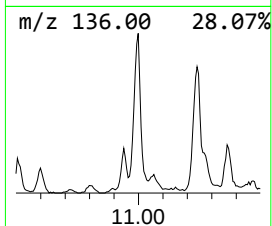
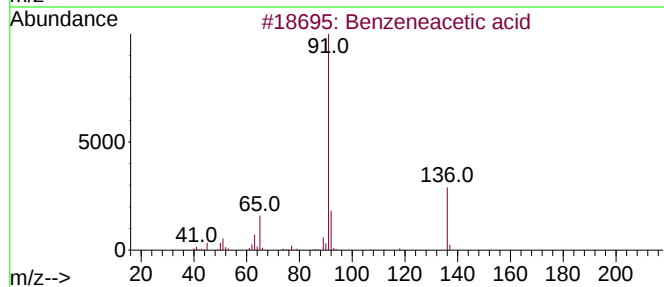
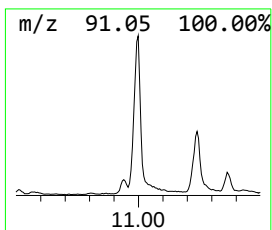
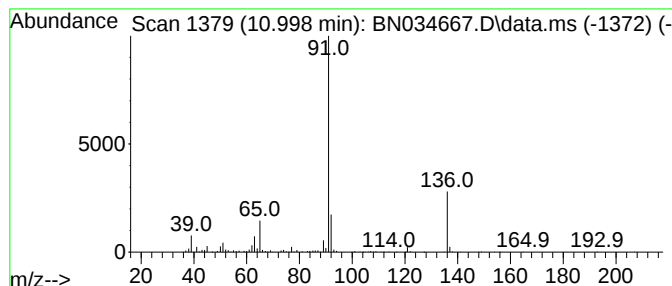
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 Benzeneacetic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.999	2.76 ng/ul	409469	Naphthalene-d8	10.440

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	90
2			Benzeneacetic acid	136	C8H8O2	000103-82-2	90
3			Benzeneacetic acid	136	C8H8O2	000103-82-2	90
4			Benzeneacetic acid	136	C8H8O2	000103-82-2	81
5			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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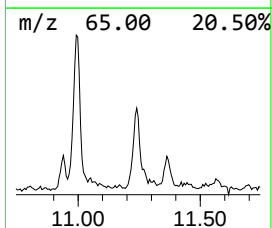
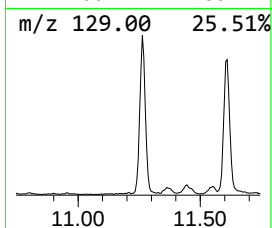
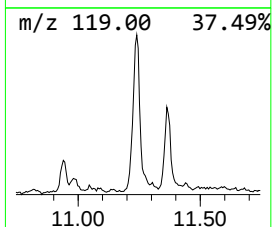
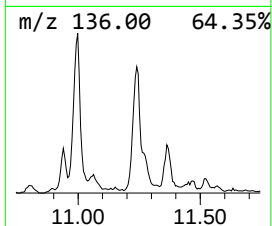
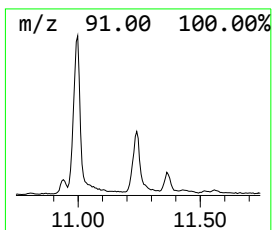
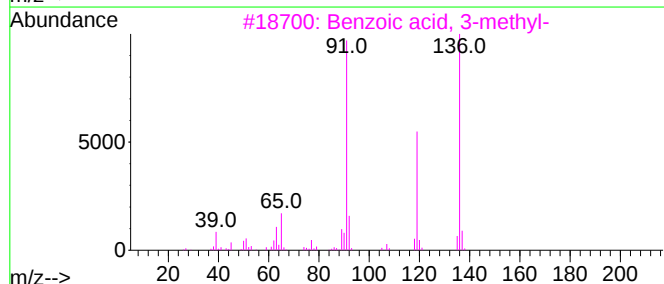
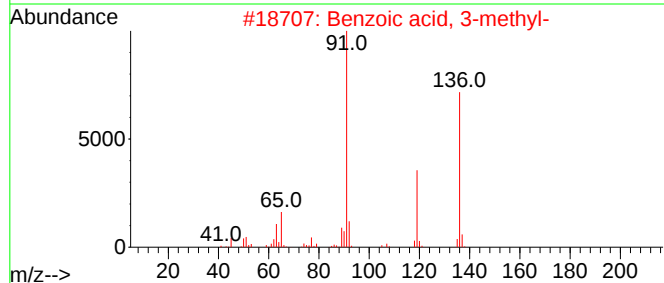
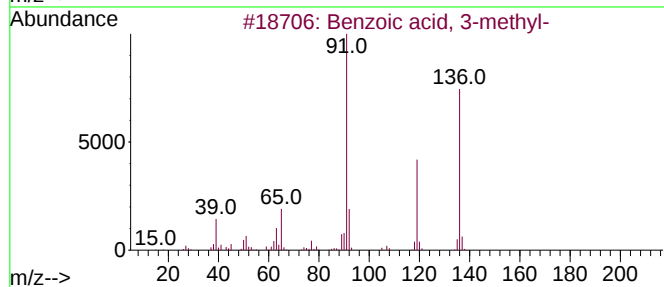
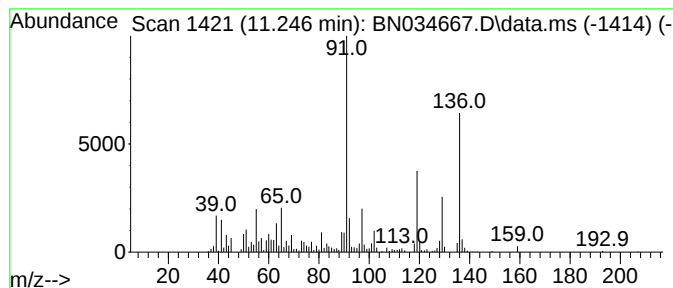
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 Benzoic acid, 3-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.246	2.66 ng/ul	394599	Naphthalene-d8	10.440

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	96
2			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	96
3			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	93
4			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	78
5			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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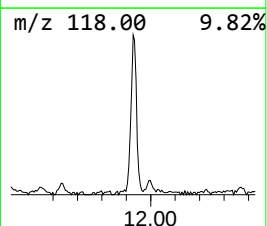
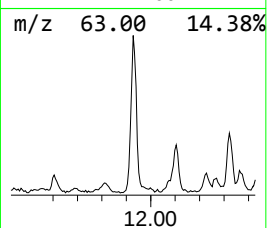
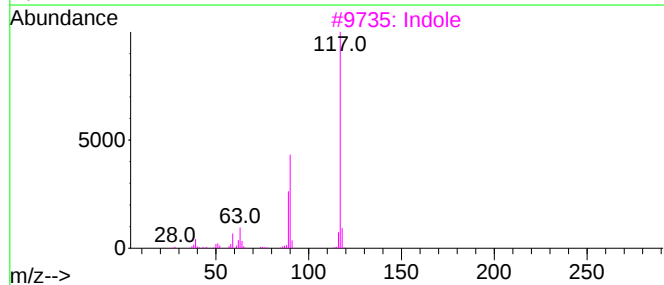
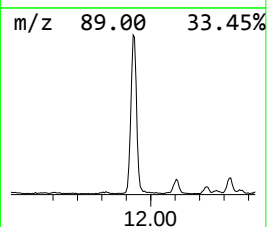
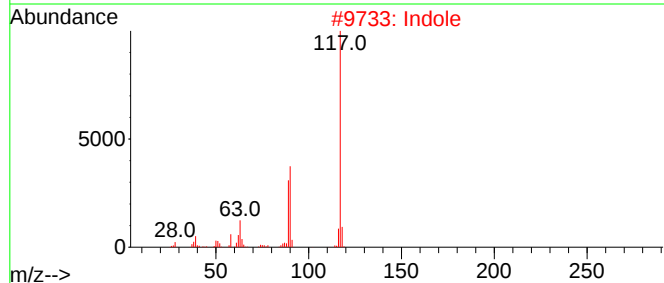
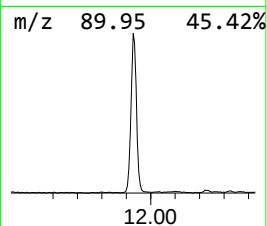
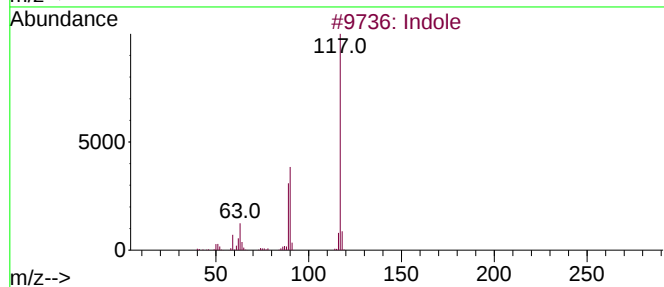
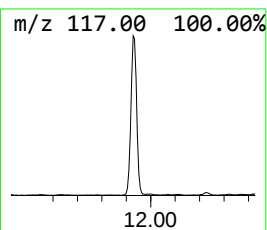
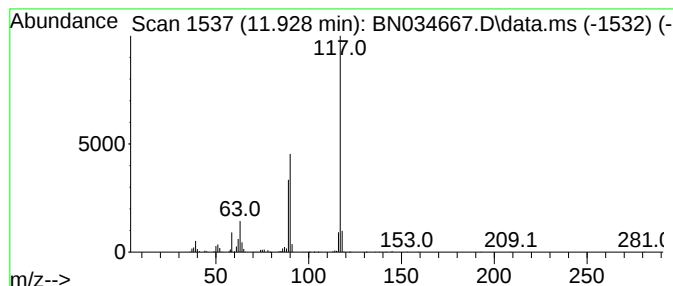
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Quant Title : SVOA CALIBRATION

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

Peak Number 14 Indole Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	4.11 ng/ul	608906	Naphthalene-d8	10.440

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole			117	C8H7N	000120-72-9	97
2	Indole			117	C8H7N	000120-72-9	96
3	Indole			117	C8H7N	000120-72-9	94
4	Indolizine			117	C8H7N	000274-40-8	90
5	Indole			117	C8H7N	000120-72-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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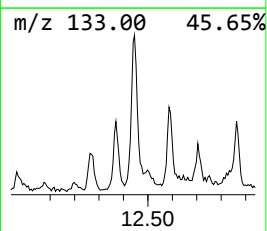
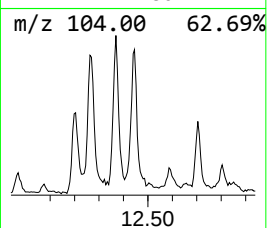
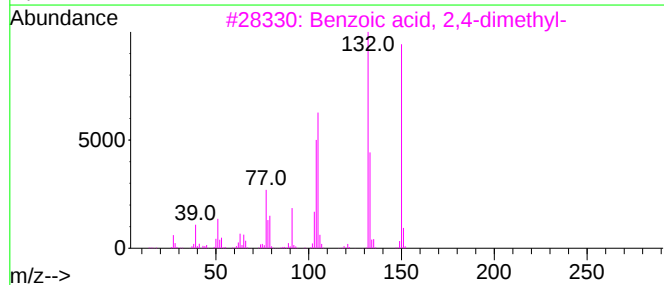
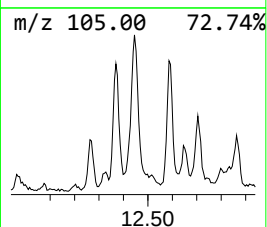
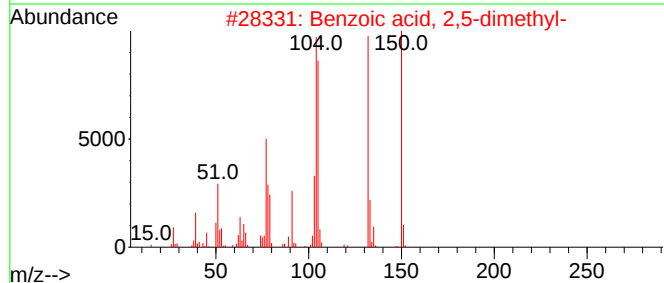
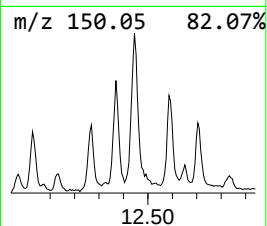
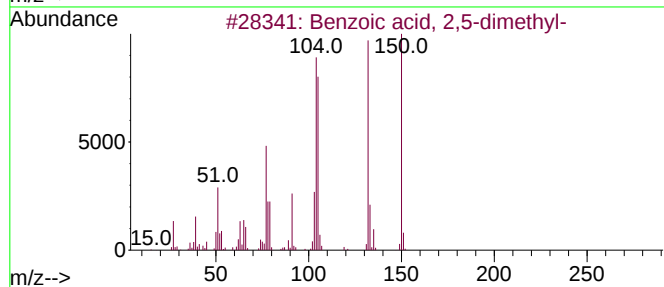
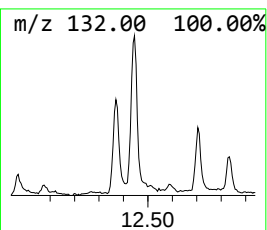
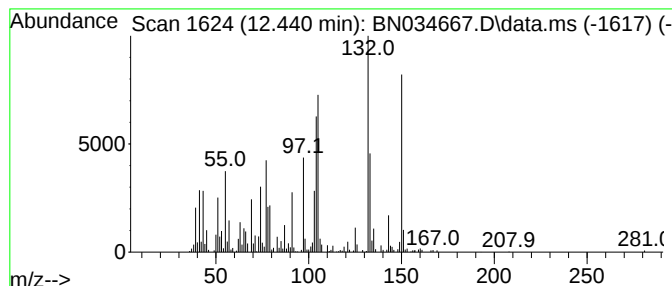
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Quant Title : SVOA CALIBRATION

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

Peak Number 15 Benzoic acid, 2,5-dimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.440	2.73 ng/ul	460562	Acenaphthene-d10	14.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	98
2			Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	96
3			Benzoic acid, 2,4-dimethyl-	150	C9H10O2	000611-01-8	94
4			Benzoic acid, 2,3-dimethyl-	150	C9H10O2	000603-79-2	93
5			Benzoic acid, 2,4-dimethyl-	150	C9H10O2	000611-01-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
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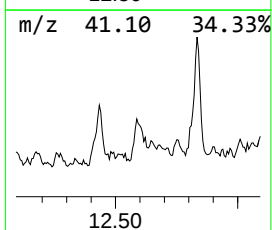
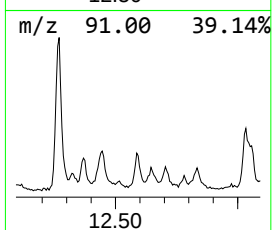
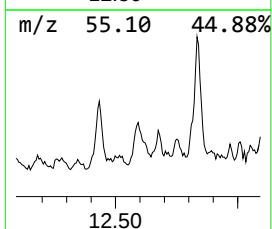
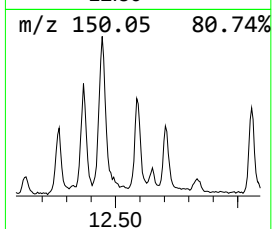
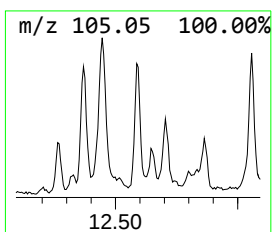
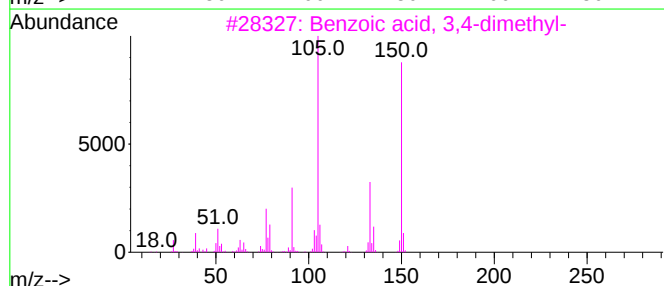
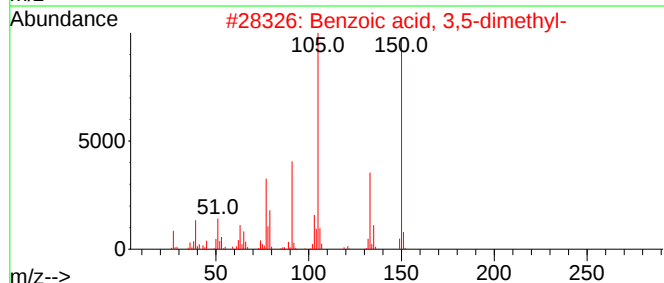
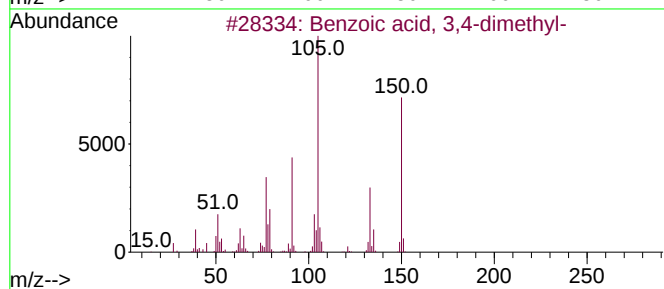
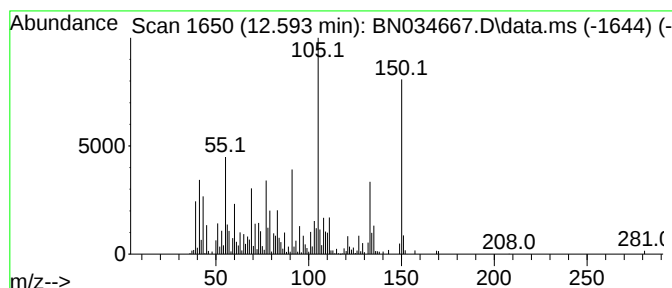
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Quant Title : SVOA CALIBRATION

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

Peak Number 16 Benzoic acid, 3,4-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.592	2.21 ng/ul	373517	Acenaphthene-d10	14.298	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 3,4-dimethyl-	150	C9H10O2	000619-04-5	95
2	Benzoic acid, 3,5-dimethyl-	150	C9H10O2	000499-06-9	95
3	Benzoic acid, 3,4-dimethyl-	150	C9H10O2	000619-04-5	91
4	Benzoic acid, 3,5-dimethyl-	150	C9H10O2	000499-06-9	91
5	Benzoic acid, 3,4-dimethyl-	150	C9H10O2	000619-04-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
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Misc :
ALS Vial : 29 Sample Multiplier: 1

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ClientSampleId :
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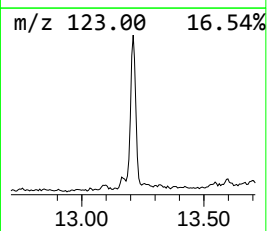
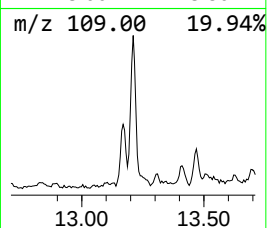
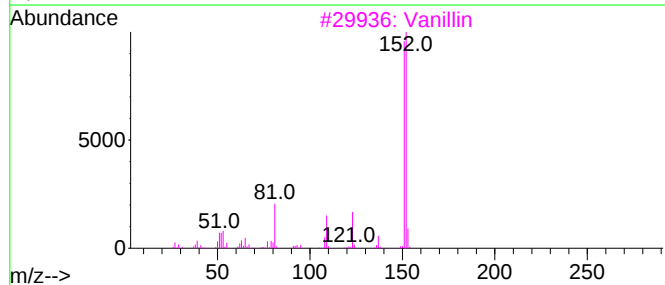
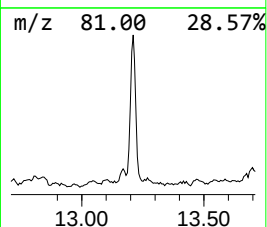
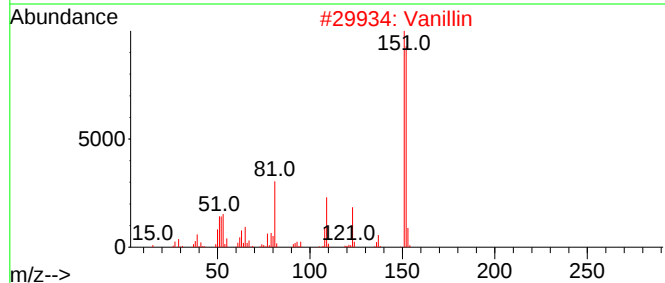
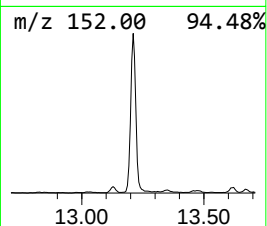
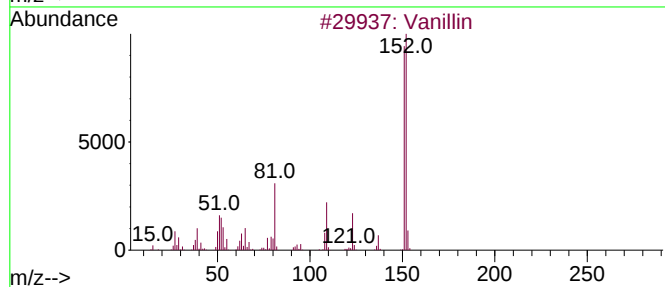
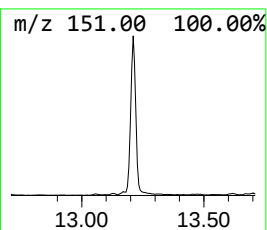
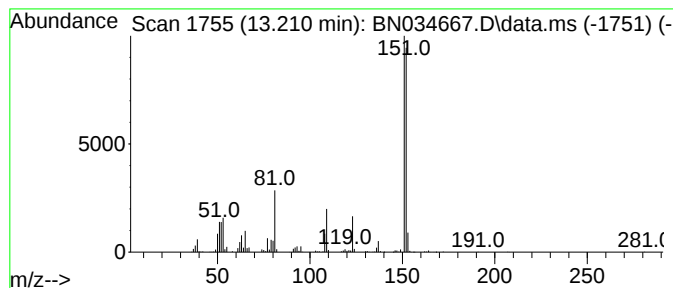
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Quant Title : SVOA CALIBRATION

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

Peak Number 18 Vanillin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.210	5.59 ng/ul	943295	Acenaphthene-d10	14.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin			152	C8H8O3	000121-33-5	97
2	Vanillin			152	C8H8O3	000121-33-5	97
3	Vanillin			152	C8H8O3	000121-33-5	97
4	Benzaldehyde, 3-hydroxy-4-methoxy-			152	C8H8O3	000621-59-0	96
5	Benzaldehyde, 3-hydroxy-4-methoxy-			152	C8H8O3	000621-59-0	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E27J0RX

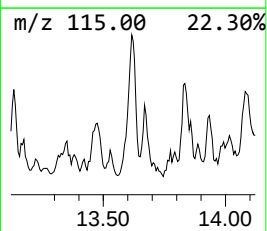
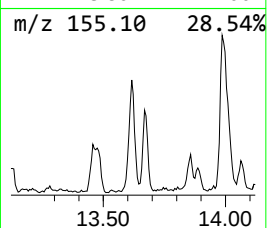
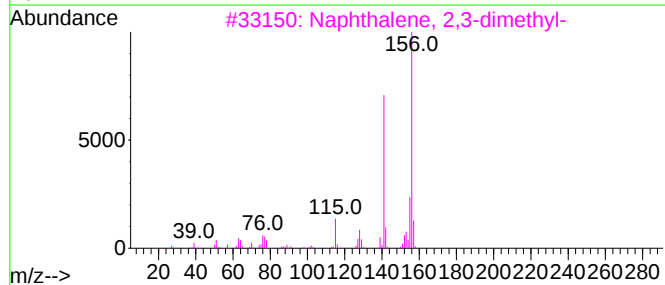
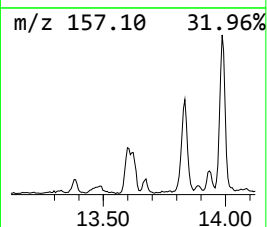
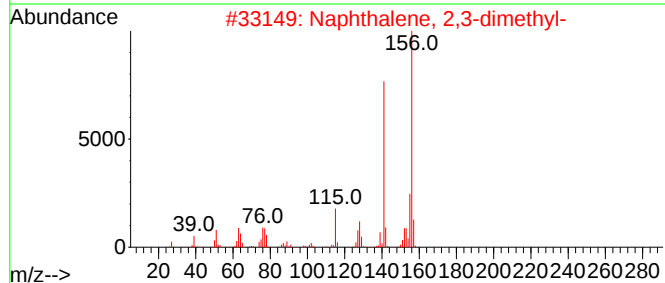
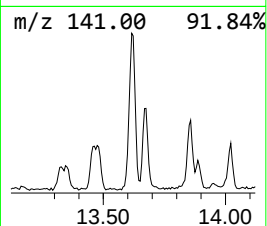
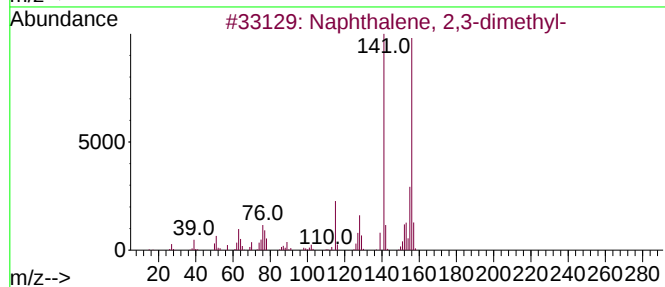
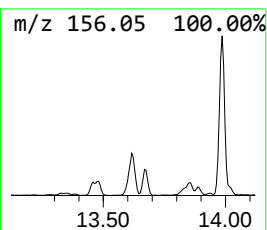
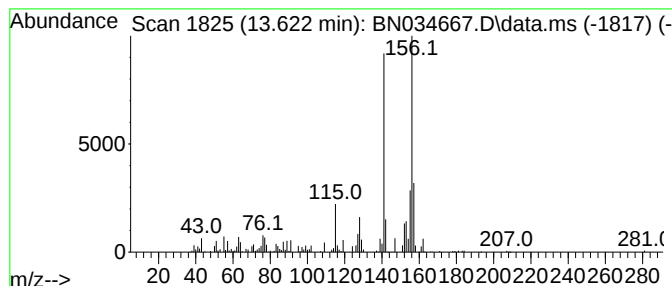
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Quant Title : SVOA CALIBRATION

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

Peak Number 19 Naphthalene, 2,3-dimethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.622	2.57 ng/ul	434223	Acenaphthene-d10	14.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	94
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	94
4			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	94
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E27J0RX

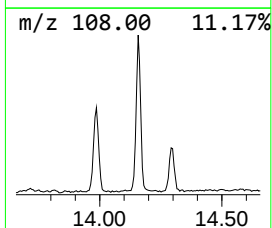
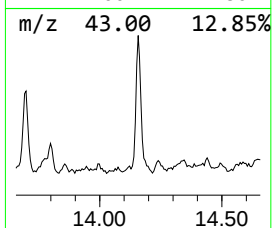
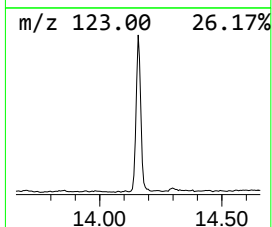
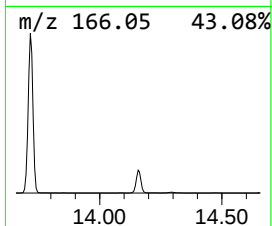
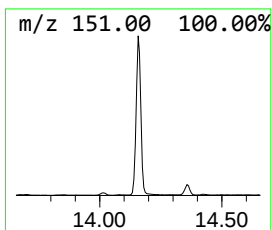
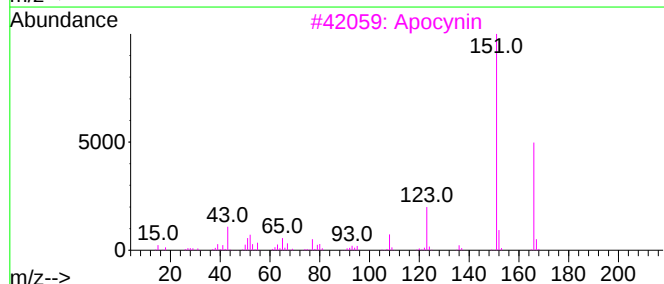
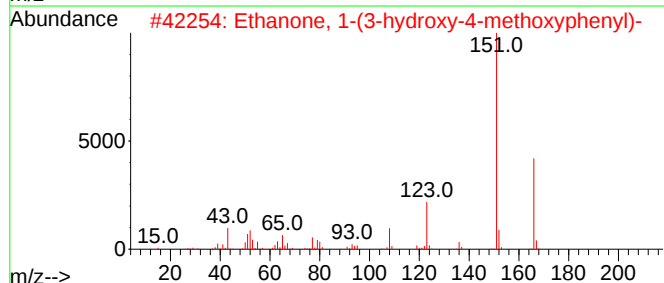
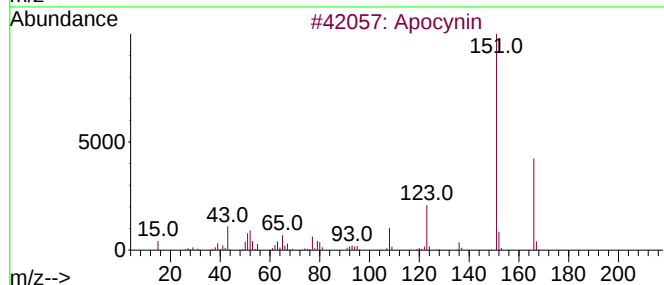
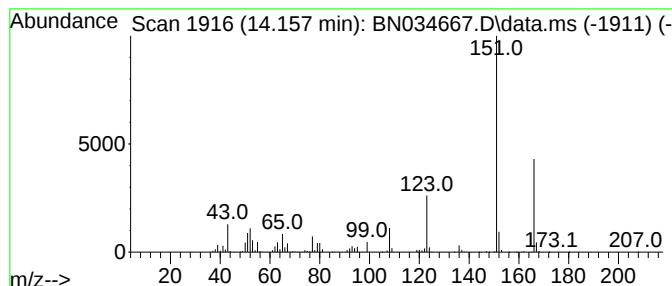
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Quant Title : SVOA CALIBRATION

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

Peak Number 20 Apocynin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	9.23 ng/ul	1558090	Acenaphthene-d10	14.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin			166	C9H10O3	000498-02-2	96
2	Ethanone, 1-(3-hydroxy-4-methoxy...			166	C9H10O3	006100-74-9	95
3	Apocynin			166	C9H10O3	000498-02-2	95
4	Ethanone, 1-(3-hydroxy-4-methoxy...			166	C9H10O3	006100-74-9	93
5	Apocynin			166	C9H10O3	000498-02-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

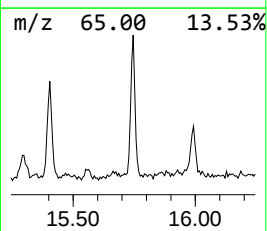
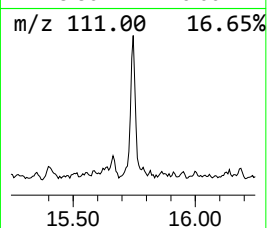
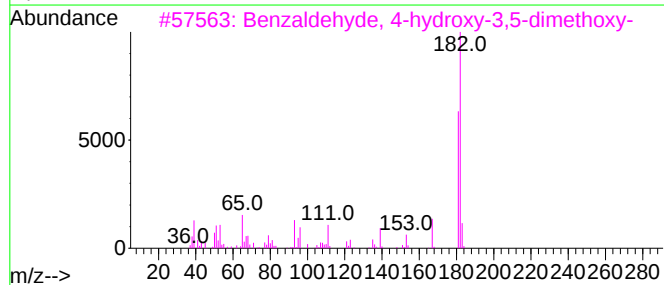
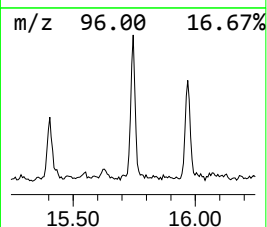
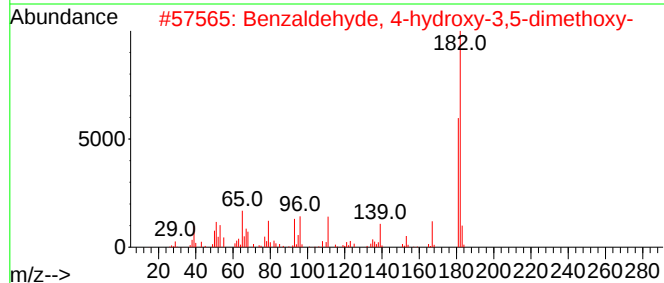
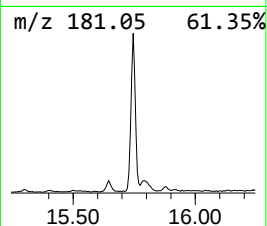
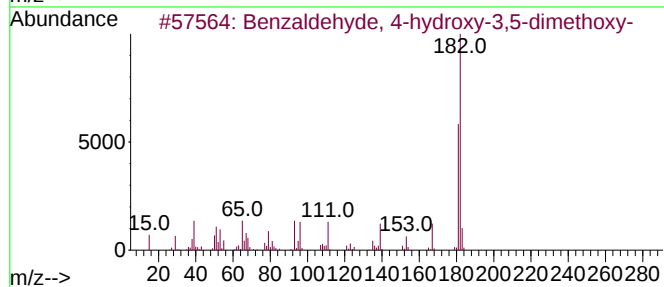
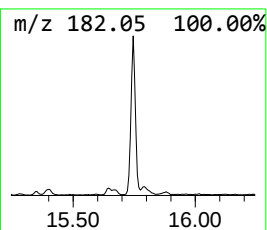
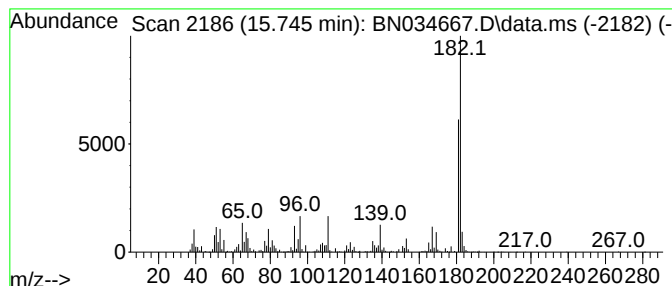
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 22 Benzaldehyde, 4-hydroxy-3,5... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
15.745	4.43 ng/ul	783999	Phenanthrene-d10			17.039
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzaldehyde, 4-hydroxy-3,5-dime...		182	C9H10O4	000134-96-3	98
2	Benzaldehyde, 4-hydroxy-3,5-dime...		182	C9H10O4	000134-96-3	98
3	Benzaldehyde, 4-hydroxy-3,5-dime...		182	C9H10O4	000134-96-3	98
4	Benzaldehyde, 4-hydroxy-3,5-dime...		182	C9H10O4	000134-96-3	96
5	Benzaldehyde, 4-hydroxy-3,5-dime...		182	C9H10O4	000134-96-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E27J0RX

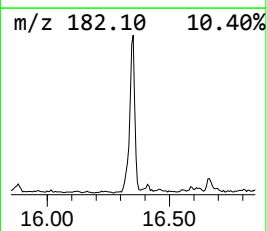
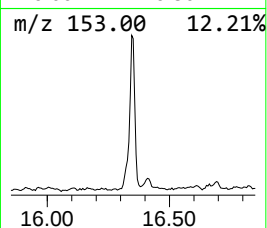
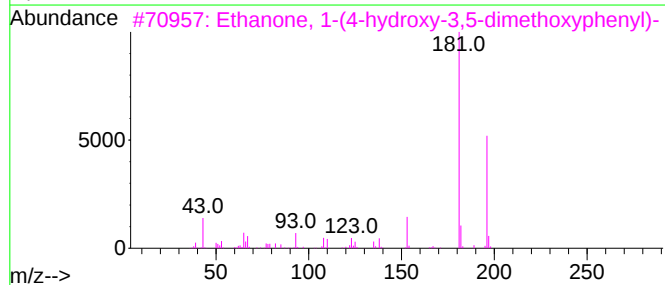
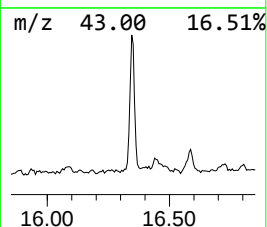
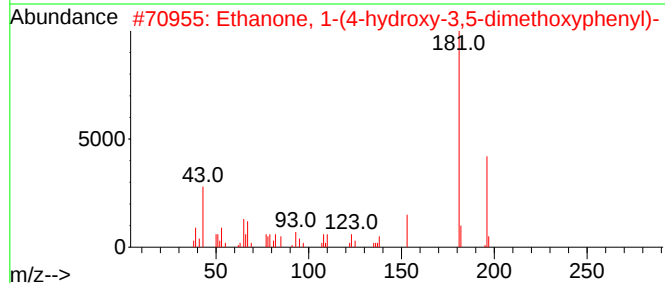
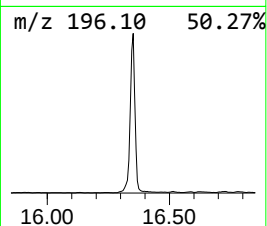
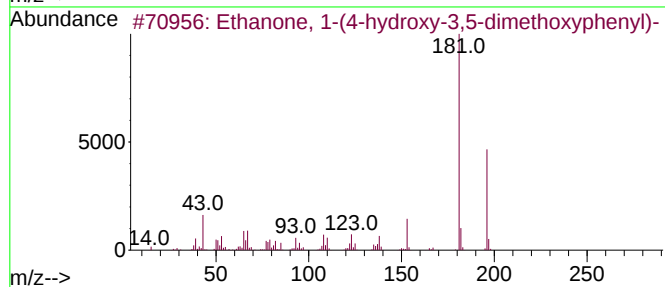
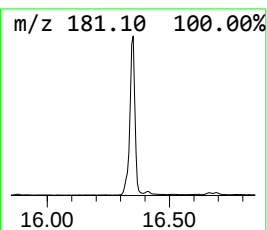
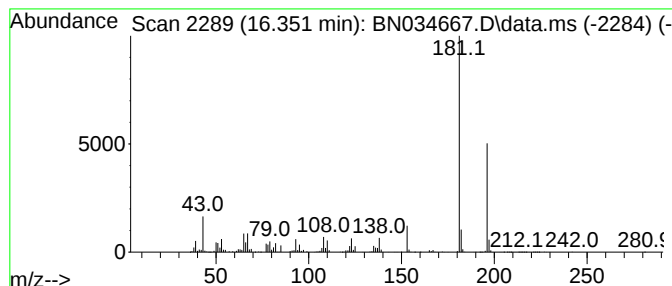
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Quant Title : SVOA CALIBRATION

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

Peak Number 23 Ethanone, 1-(4-hydroxy-3,5-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.351	10.69 ng/ul	1892600	Phenanthrene-d10	17.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(4-hydroxy-3,5-dimet...	196	C10H12O4	002478-38-8	97
2			Ethanone, 1-(4-hydroxy-3,5-dimet...	196	C10H12O4	002478-38-8	96
3			Ethanone, 1-(4-hydroxy-3,5-dimet...	196	C10H12O4	002478-38-8	96
4			Ethanone, 1-(4-hydroxy-3,5-dimet...	196	C10H12O4	002478-38-8	94
5			4,5-Dimethoxy-2-hydroxyacetophenone	196	C10H12O4	020628-06-2	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

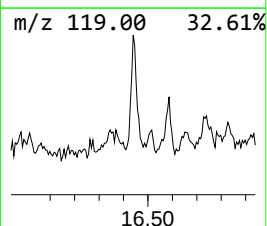
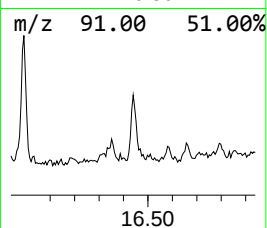
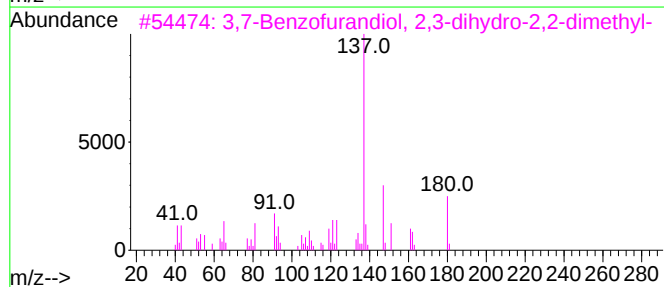
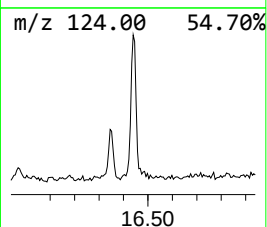
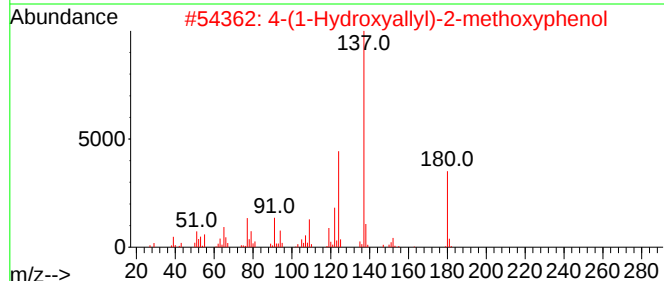
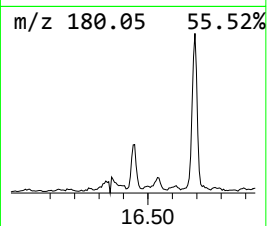
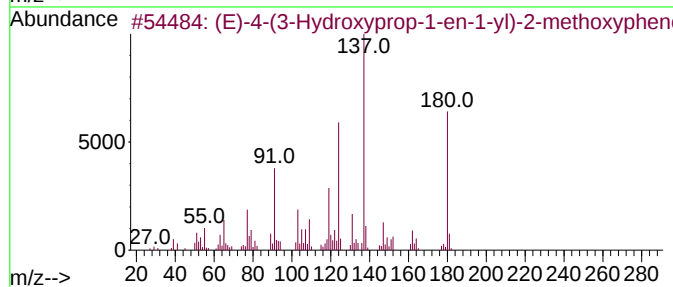
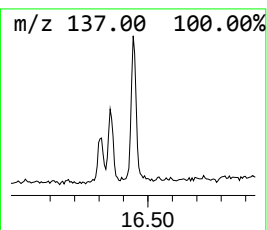
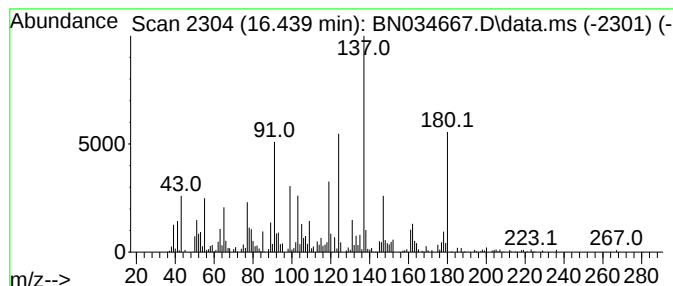
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 24 (E)-4-(3-Hydroxyprop-1-en-1-yl) Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.439	2.20 ng/ul	389215	Phenanthrene-d10		17.039	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...		180	C10H12O3	032811-40-8	95
2	4-(1-Hydroxyallyl)-2-methoxyphenol		180	C10H12O3	112465-50-6	60
3	3,7-Benzofurandiol, 2,3-dihydro-...		180	C10H12O3	017781-15-6	60
4	3,7-Benzofurandiol, 2,3-dihydro-...		180	C10H12O3	017781-15-6	49
5	3,7-Benzofurandiol, 2,3-dihydro-...		180	C10H12O3	017781-15-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
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Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

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BNA_N
ClientSampleId :
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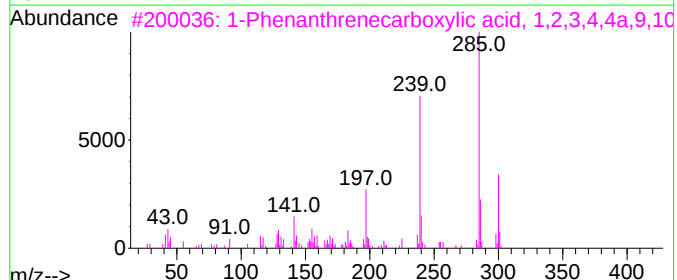
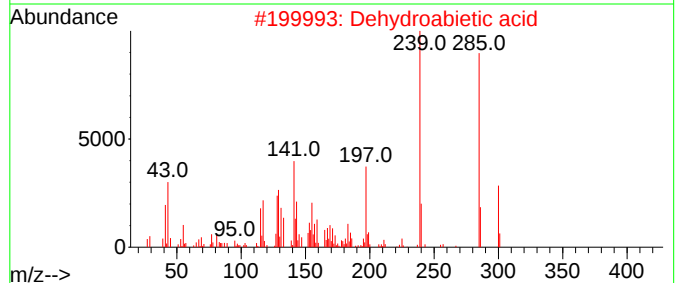
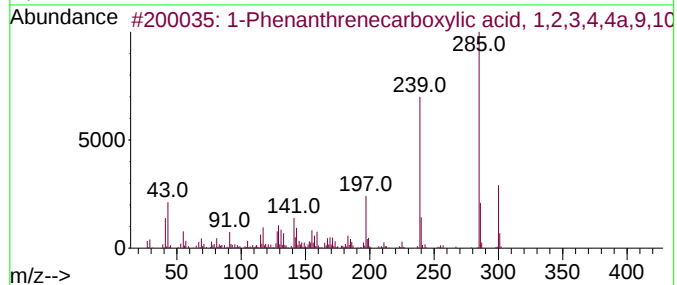
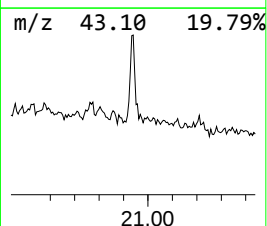
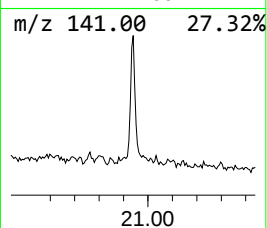
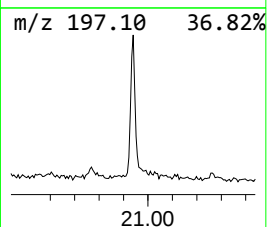
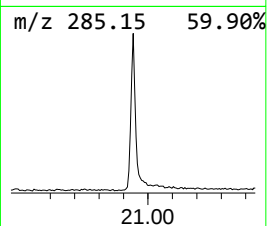
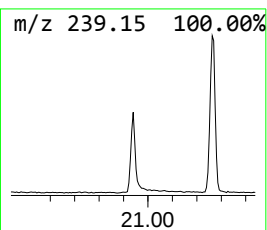
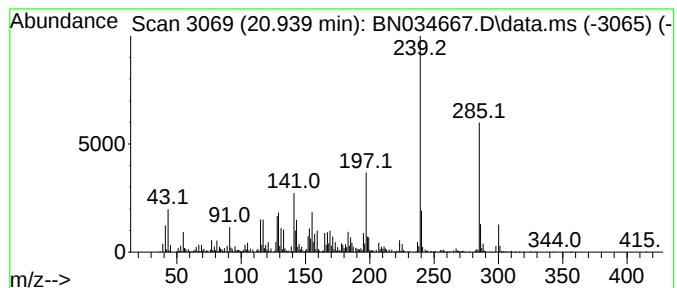
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Quant Title : SVOA CALIBRATION

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

Peak Number 26 1-Phenanthrenecarboxylic ac... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.939	5.08 ng/ul	909066	Chrysene-d12	21.263

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	99
2			Dehydroabietic acid	300	C20H28O2	001740-19-8	99
3			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	94
4			Dehydroabietic acid	300	C20H28O2	001740-19-8	94
5			Dehydroabietic acid	300	C20H28O2	001740-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101724\
Data File : BN034667.D
Acq On : 19 Oct 2024 03:06
Operator : RC/JU
Sample : P4380-08RX
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E27J0RX

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101624.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
Butanoic acid, ...	4.611	5.4	ng/ul	582163	1	7.663	2144210	20.0
Butanoic acid, ...	4.752	4.1	ng/ul	435054	1	7.663	2144210	20.0
3-Methyl-hexano...	7.575	2.2	ng/ul	232252	1	7.663	2144210	20.0
Benzaldehyde, 2...	8.157	7.3	ng/ul	786105	1	7.663	2144210	20.0
Benzeneacetic acid	10.999	2.8	ng/ul	409469	2	10.440	2966260	20.0
Benzoic acid, 3...	11.246	2.7	ng/ul	394599	2	10.440	2966260	20.0
Indole	11.928	4.1	ng/ul	608906	2	10.440	2966260	20.0
Benzoic acid, 2...	12.440	2.7	ng/ul	460562	3	14.298	3374980	20.0
Benzoic acid, 3...	12.592	2.2	ng/ul	373517	3	14.298	3374980	20.0
Vanillin	13.210	5.6	ng/ul	943295	3	14.298	3374980	20.0
Naphthalene, 2,...	13.622	2.6	ng/ul	434223	3	14.298	3374980	20.0
Apocynin	14.157	9.2	ng/ul	1558090	3	14.298	3374980	20.0
Benzaldehyde, 4...	15.745	4.4	ng/ul	783999	4	17.039	3540010	20.0
Ethanone, 1-(4-...	16.351	10.7	ng/ul	1892600	4	17.039	3540010	20.0
(E)-4-(3-Hydrox...	16.439	2.2	ng/ul	389215	4	17.039	3540010	20.0
1-Phenanthrenec...	20.939	5.1	ng/ul	909066	5	21.263	3580530	20.0