LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060424\
Data File : BM045853.D
Acq On : 05 Jun 2024 16:56
Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM045853.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.052	8	11	16	rBV	65694	84935	2.27%	0.135%
2	3.364	61	64	78	rBV2	70144	189376	5.06%	0.301%
3	3.464	78	81	104	rVV	684318	1355409	36.18%	2.157%
4	3.722	118	125	133	rBV	160758	317712	8.48%	0.506%
5	4.481	248	254	262	rBV3	27274	62401	1.67%	0.099%
6	4.616	271	277	286	rBV2	40051	90828	2.42%	0.145%
7	5.081	352	356	364	rBV2	20082	37509	1.00%	0.060%
8	5.287	387	391	395	rVB7	5525	10053	0.27%	0.016%
9	5.652	449	453	459	rBV2	19262	38044	1.02%	0.061%
10	5.758	469	471	475	rVB4	8169	9252	0.25%	0.015%
11	6.134	530	535	540	rVB9	6694	11212	0.30%	0.018%
12	6.605	609	615	622	rBV7	13362	34932	0.93%	0.056%
13	6.722	628	635	646	rBV	1303765	2190677	58.48%	3.486%
14	6.828	647	653	665	rVV	981434	1541686	41.16%	2.453%
15	7.028	680	687	695	rBV	1337161	2114357	56.45%	3.364%
16	7.463	755	761	771	rVB	1261589	1904287	50.84%	3.030%
17	7.581	777	781	784	rBV4	9778	13074	0.35%	0.021%
18	7.622	784	788	789	rBV4	8348	11214	0.30%	0.018%
19	7.781	808	815	821	rBV9	16948	34429	0.92%	0.055%
20	7.969	842	847	850	rBV6	7349	10244	0.27%	0.016%
21	8.234	883	892	898	rVV	1528165	2451039	65.43%	3.900%
22	8.287	898	901	911	rVB	69046	134813	3.60%	0.215%
23	8.628	952	959	974	rBV	1321492	2123393	56.69%	3.379%
24	8.722	974	975	980	rVB5	6093	8728	0.23%	0.014%
25	8.804	985	989	994	rBV6	11886	20004	0.53%	0.032%
26	9.204	1051	1057	1058	rBV5	6537	10366	0.28%	0.016%
27	9.240	1058	1063	1073	rVV	89274	154367	4.12%	0.246%
28	9.340	1073	1080	1091	rVB	1080797	1766681	47.16%	2.811%
29	9.675	1132	1137	1145	rVB9	16250	36396	0.97%	0.058%
30	9.887	1165	1173	1187	rVV	1456750	2443137	65.22%	3.887%
31	10.034	1193	1198	1206	rVB8	10964	19402	0.52%	0.031%
32	10.228	1224	1231	1240	rBV	1559823	2552516	68.14%	4.061%
33	10.410	1254	1262	1279	rBV	1151969	2224241	59.38%	3.539%
34	10.857	1328	1338	1347	rBV4	32860	69187	1.85%	0.110%
35	11.022	1358	1366	1379	rBV	121564	287940	7.69%	0.458%
36	11.122	1379	1383	1387	rBV7	7564	13469	0.36%	0.021%

LSC Area Percent Report

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Data File : BM045853.D
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Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Title : SVOA CALIBRATION

37	11.692	1475	1480	1484	rVB8	7252	11164	0.30%	0.018%
38	11.787	1489	1496	1498	rBV5	8571	13870	0.37%	0.022%
39	11.828	1498	1503	1508	rVB3	30206	50775	1.36%	0.081%
40	12.145	1548	1557	1577	rBV	377474	722234	19.28%	1.149%
41	12.363	1591	1594	1600	rVB8	10929	17240	0.46%	0.027%
42	12.545	1621	1625	1630	rVV7	4057	8515	0.23%	0.014%
43	12.957	1689	1695	1696	rVV6	15712	24504	0.65%	0.039%
44	12.981	1696	1699	1707	rVV5	16889	34404	0.92%	0.055%
45	13.069	1709	1714	1721	rVV9	17699	43418	1.16%	0.069%
46	13.439	1773	1777	1781	rBV7	6234	10571	0.28%	0.017%
47	13.557	1789	1797	1806	rBV	2016347	2887855	77.10%	4.595%
48	13.798	1829	1838	1848	rVV	2391114	3470503	92.65%	5.522%
49	13.886	1851	1853	1859	rVB7	6795	8548	0.23%	0.014%
50	14.028	1873	1877	1881	rVV7	12752	20500	0.55%	0.033%
51	14.104	1884	1890	1897	rVV	1951072	2800945	74.78%	4.457%
52	14.157	1897	1899	1905	rVV7	9554	16730	0.45%	0.027%
53	14.357	1927	1933	1934	rBV4	41522	51895	1.39%	0.083%
54	14.404	1934	1941	1958	rVB	783094	1339321	35.76%	2.131%
55	14.592	1970	1973	1978	rVV7	10496	15609	0.42%	0.025%
56	14.922	2026	2029	2032	rBV4	8725	10397	0.28%	0.017%
57	14.957	2032	2035	2037	rBV4	7558	8573	0.23%	0.014%
58	14.981	2037	2039	2043	rVB4	17196	21704	0.58%	0.035%
59	15.045	2047	2050	2054	rVB3	14637	16664	0.44%	0.027%
60	15.104	2054	2060	2068	rBV	2726922	3745794	100.00%	5.960%
61	15.245	2078	2084	2093	rBV	590935	791961	21.14%	1.260%
62	15.345	2097	2101	2106	rBV5	13193	20339	0.54%	0.032%
63	15.533	2124	2133	2142	rVB5	23556	67732	1.81%	0.108%
64	15.610	2142	2146	2148	rBV4	8012	12002	0.32%	0.019%
65	15.645	2148	2152	2159	rVV9	12014	24372	0.65%	0.039%
66	15.845	2182	2186	2190	rBV6	15250	19843	0.53%	0.032%
67	16.016	2211	2215	2217	rBV5	6182	9561	0.26%	0.015%
68	16.104	2227	2230	2235	rVB3	16586	21058	0.56%	0.034%
69	16.310	2259	2265	2270	rBV8	30460	57590	1.54%	0.092%
70	16.433	2281	2286	2290	rBV6	22426	32725	0.87%	0.052%
71	16.586	2309	2312	2315	rBV5	8384	9669	0.26%	0.015%
72	16.639	2317	2321	2323	rVV3	19624	24305	0.65%	0.039%
73	16.663	2323	2325	2330	rVV4	12601	20154	0.54%	0.032%
74	16.722	2330	2335	2340	rVB	32113	46423	1.24%	0.074%
75	16.798	2345	2348	2352	rBV5	14045	19067	0.51%	0.030%
76	16.851	2352	2357	2363	rVV	1940186	2698875	72.05%	4.294%

LSC Area Percent Report

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Acq On : 05 Jun 2024 16:56
Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

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

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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Title : SVOA CALIBRATION

77	16.892	2363	2364	2368	rVV	63769	63986	1.71%	0.102%
78	16.951	2368	2374	2385	rVB2	2528643	3415588	91.18%	5.435%
79	17.074	2389	2395	2399	rBV9	17041	36344	0.97%	0.058%
80	17.169	2409	2411	2416	rVB6	14663	21426	0.57%	0.034%
81	17.269	2424	2428	2435	rVB2	70958	104064	2.78%	0.166%
82	17.410	2449	2452	2456	rVB6	9529	13977	0.37%	0.022%
83	17.545	2473	2475	2479	rVB5	10690	11396	0.30%	0.018%
84	17.622	2485	2488	2491	rBV3	16862	18475	0.49%	0.029%
85	17.669	2491	2496	2502	rBV9	19380	35400	0.95%	0.056%
86	17.721	2503	2505	2511	rBV6	15296	18038	0.48%	0.029%
87	17.786	2511	2516	2529	rBV	385661	771700	20.60%	1.228%
88	18.086	2564	2567	2572	rVB5	24174	35366	0.94%	0.056%
89	18.321	2604	2607	2610	rBV	27212	33922	0.91%	0.054%
90	18.816	2688	2691	2695	rVB3	32322	40592	1.08%	0.065%
91	18.863	2696	2699	2701	rBV2	32850	37521	1.00%	0.060%
92	18.916	2705	2708	2711	rBV	108943	130043	3.47%	0.207%
93	19.068	2730	2734	2746	rBV3	129282	283195	7.56%	0.451%
94	19.251	2759	2765	2775	rBV	2775523	3680879	98.27%	5.857%
95	20.780	3022	3025	3036	rBV	304129	487651	13.02%	0.776%
96	21.062	3069	3073	3078	rVB	1791924	2285711	61.02%	3.637%
97	21.986	3226	3230	3238	rVB6	185784	305696	8.16%	0.486%
98	23.356	3457	3463	3473	rVB2	579582	1308908	34.94%	2.083%
99	23.603	3498	3505	3520	rVB2	1521016	3358791	89.67%	5.344%
100	23.786	3529	3536	3545	rVB	1207231	2743650	73.25%	4.366%

Sum of corrected areas: 62847038

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060424\
Data File : BM045853.D
Acq On : 05 Jun 2024 16:56
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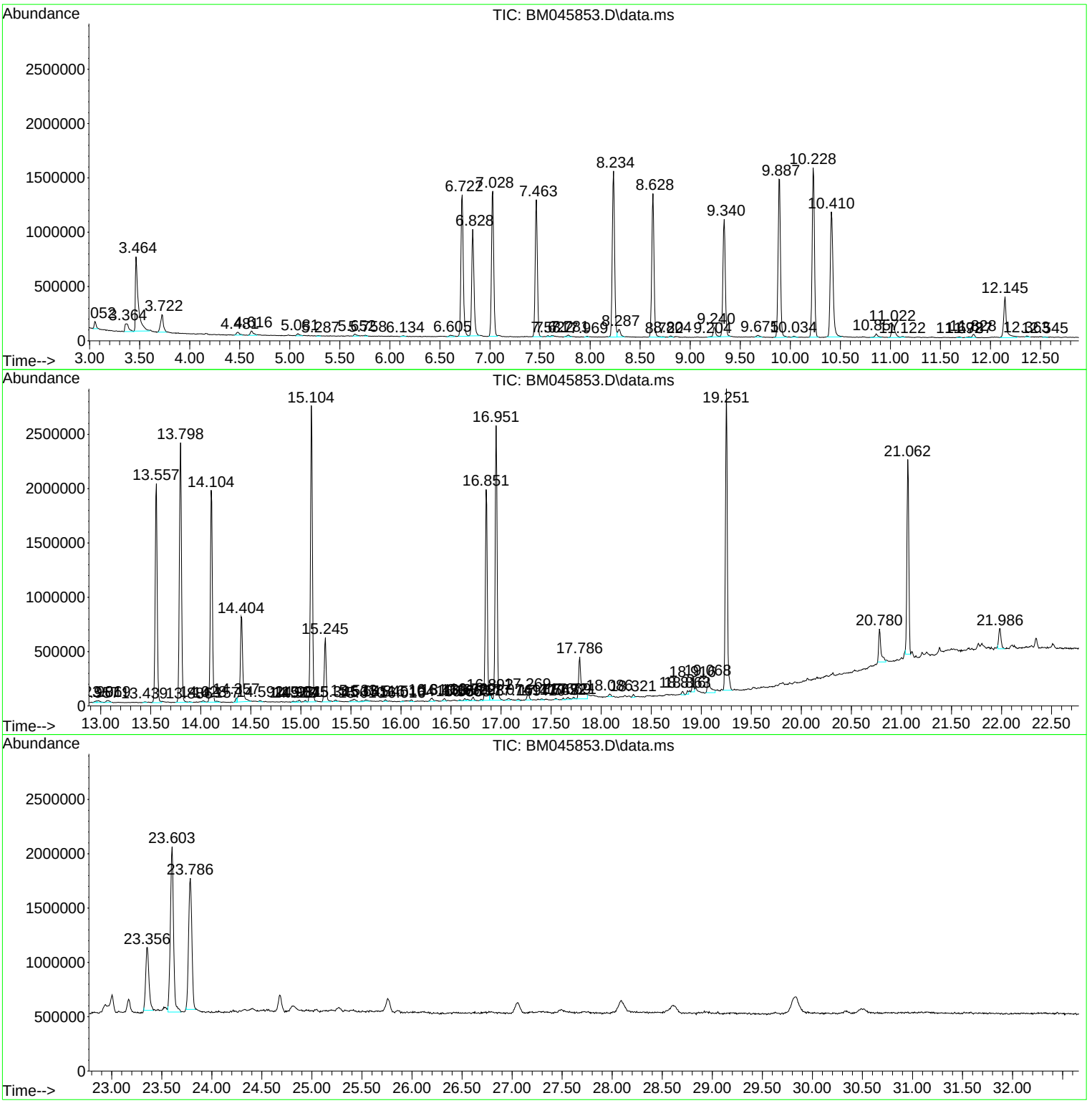
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060424\
Data File : BM045853.D
Acq On : 05 Jun 2024 16:56
Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

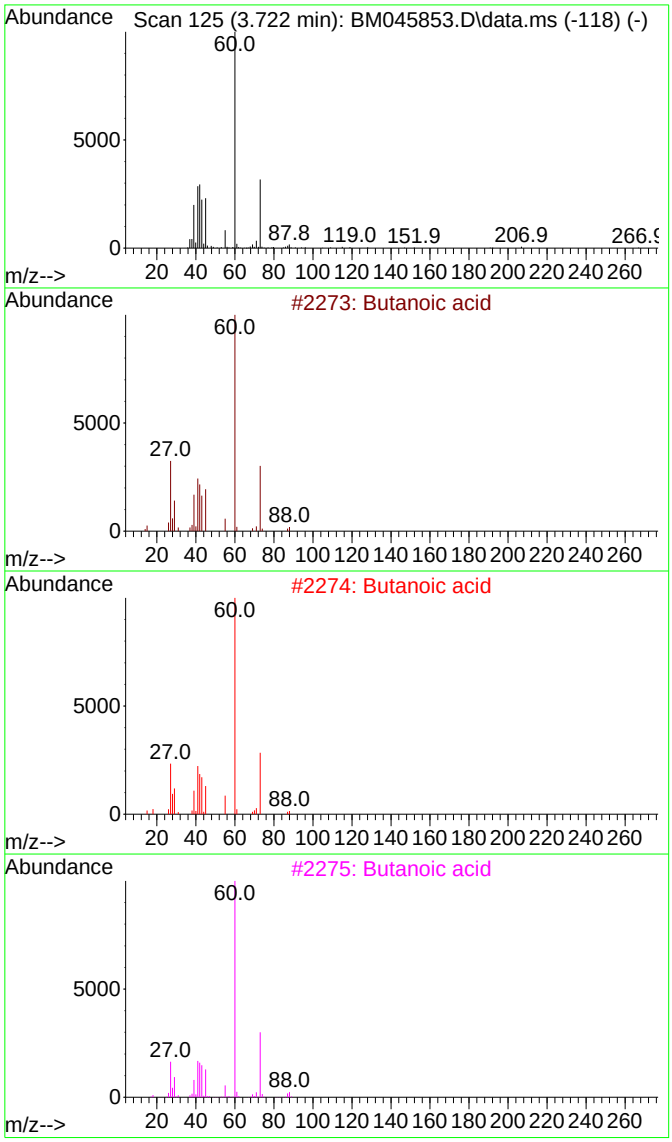
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

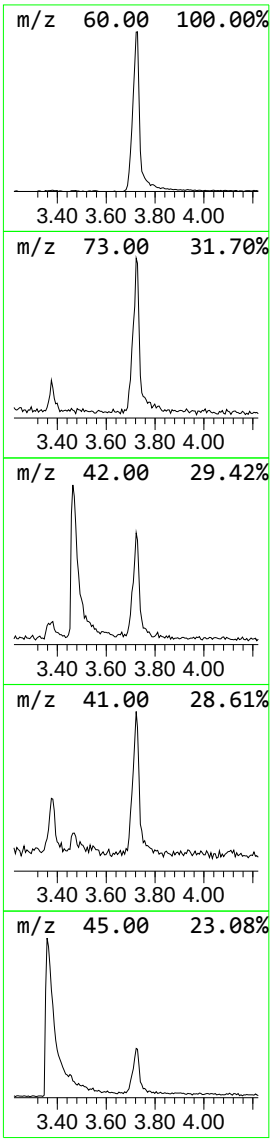
****

Peak Number 1 Butanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.722	3.34 ng/ul	317712	1,4-Dichlorobenzene-d4	7.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	91
2	Butanoic acid	88	C4H8O2	000107-92-6	72
3	Butanoic acid	88	C4H8O2	000107-92-6	10
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5	Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060424\
Data File : BM045853.D
Acq On : 05 Jun 2024 16:56
Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

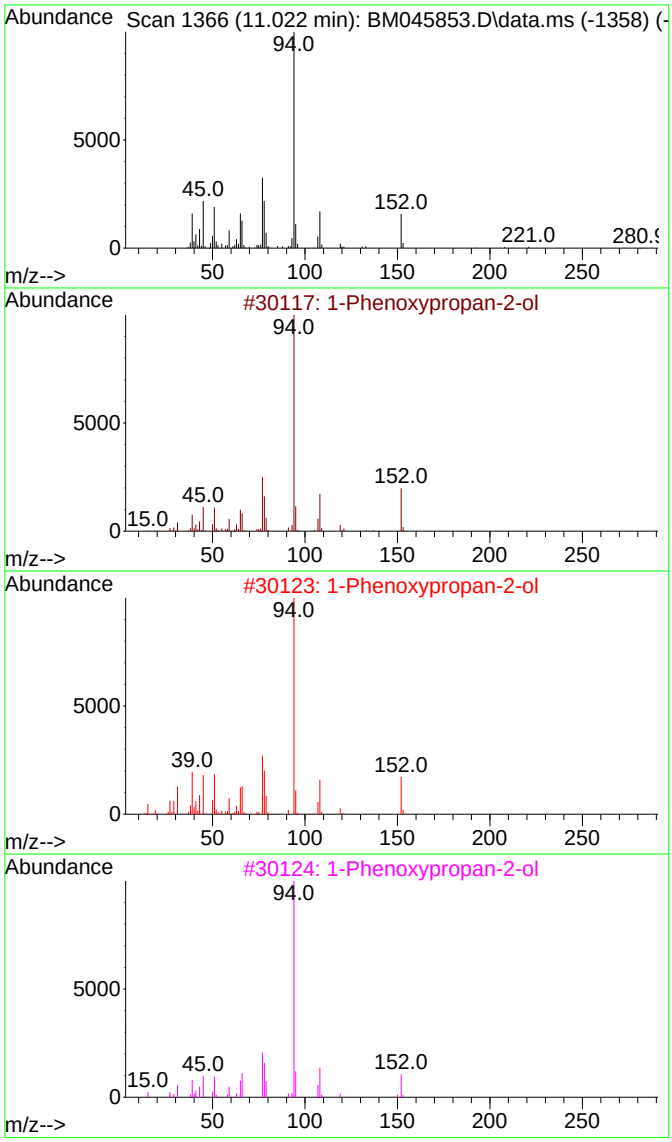
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

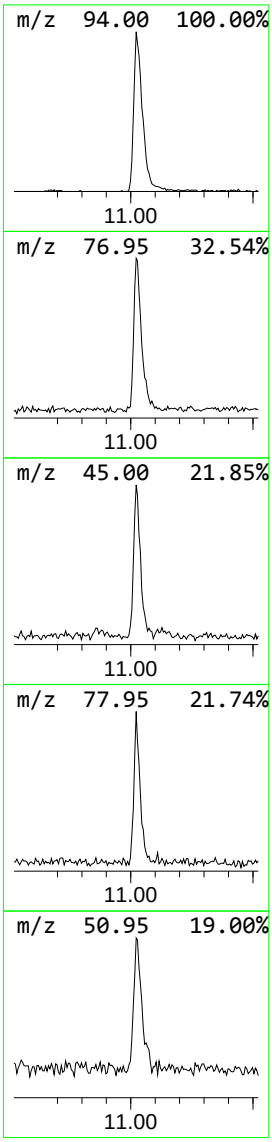
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.022	2.26 ng/ul	287940	Naphthalene-d8	10.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
5	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060424\
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Sample : P2586-19
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

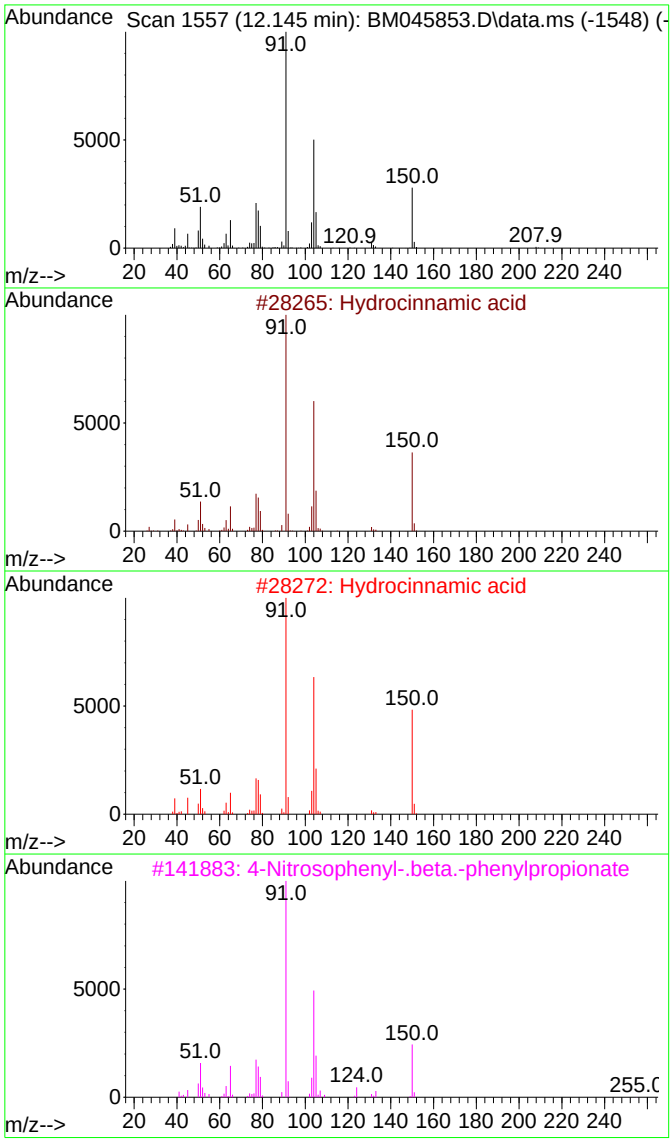
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

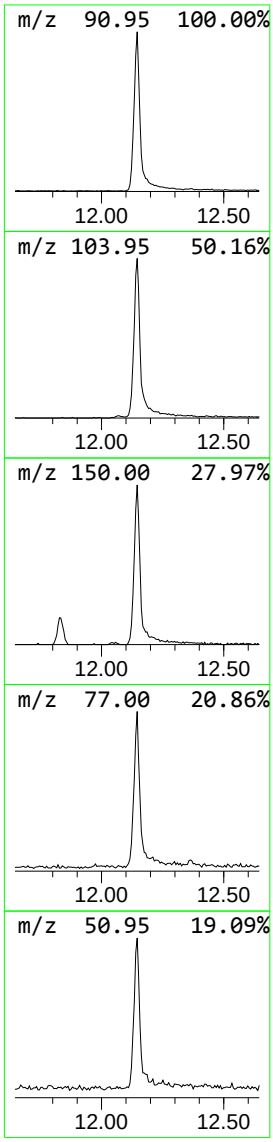
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hydrocinnamic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.145	5.66 ng/ul	722234	Naphthalene-d8	10.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	95
2	Hydrocinnamic acid	150	C9H10O2	000501-52-0	95
3	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	91
4	Hydrocinnamic acid	150	C9H10O2	000501-52-0	87
5	Hydrocinnamic acid	150	C9H10O2	000501-52-0	81





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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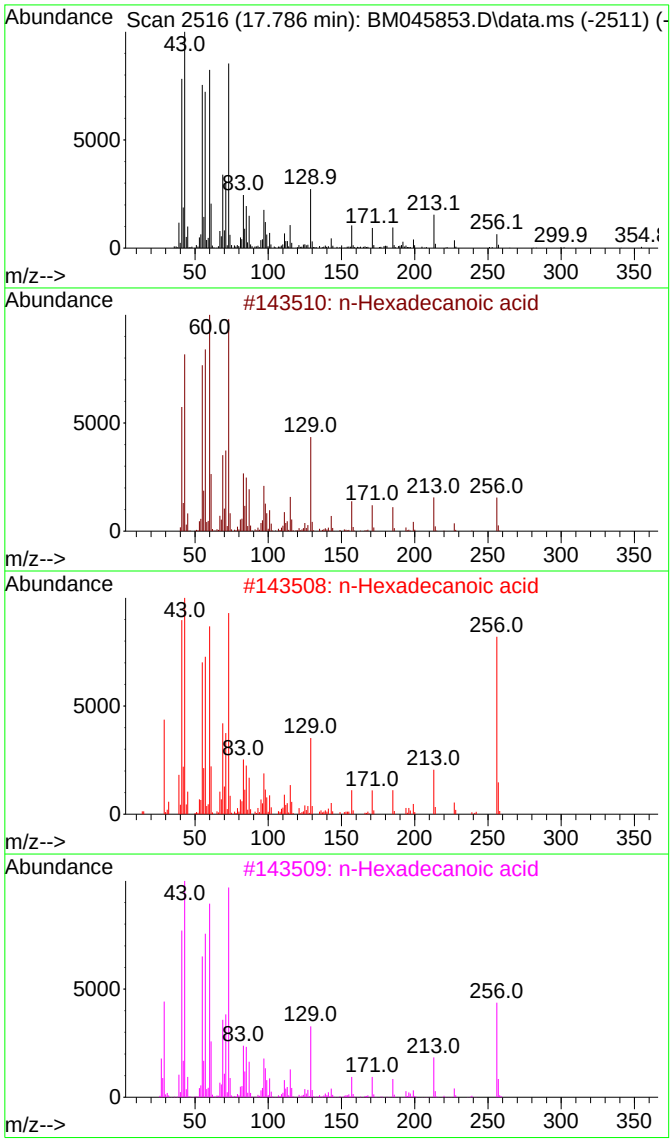
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

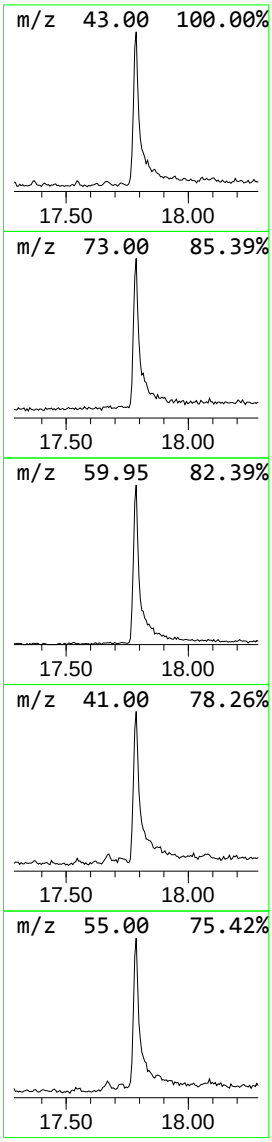
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.786	5.72 ng/ul	771700	Phenanthrene-d10	16.851

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	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060424\
Data File : BM045853.D
Acq On : 05 Jun 2024 16:56
Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

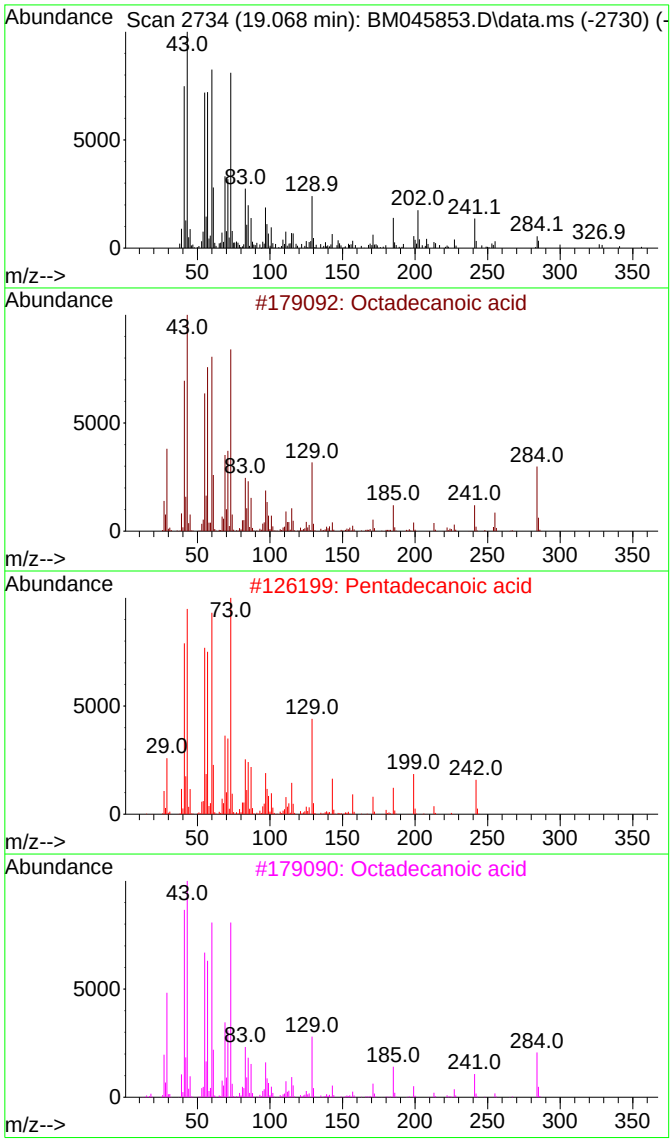
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

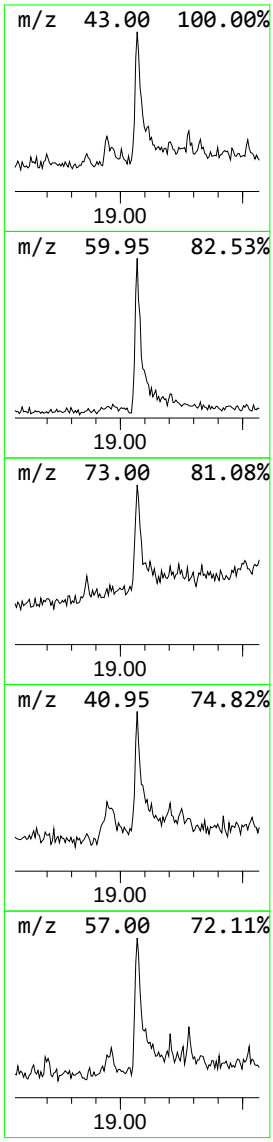
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.069	2.48 ng/ul	283195	Chrysene-d12	21.062

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	96
3	Octadecanoic acid	284	C18H36O2	000057-11-4	95
4	Octadecanoic acid	284	C18H36O2	000057-11-4	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	76





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Data File : BM045853.D
Acq On : 05 Jun 2024 16:56
Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

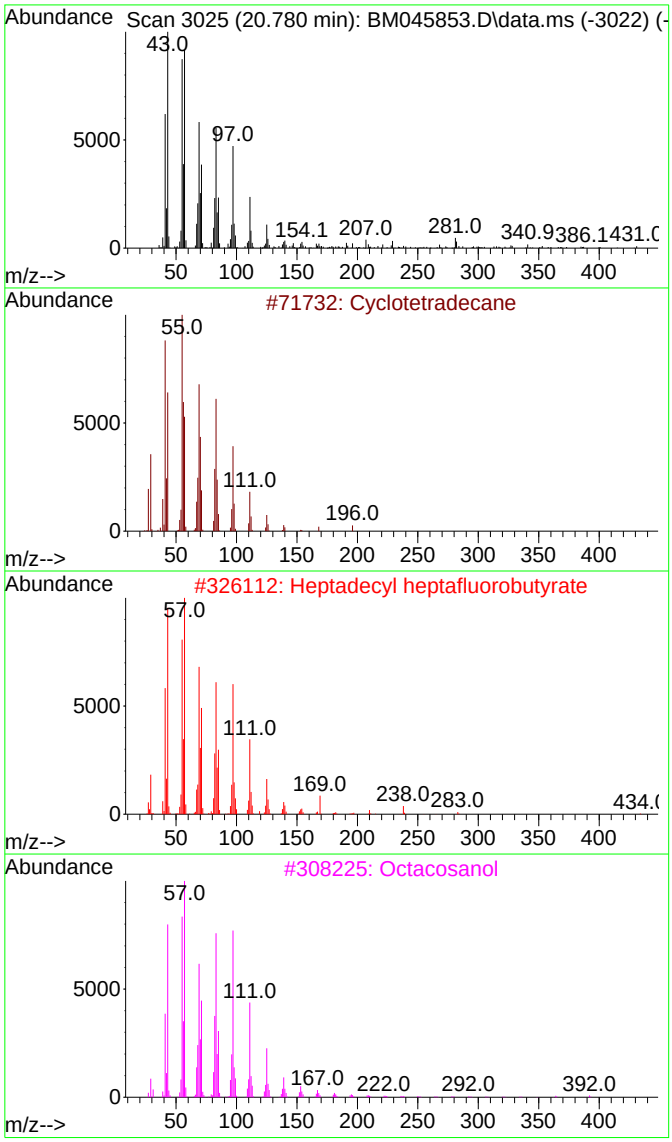
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

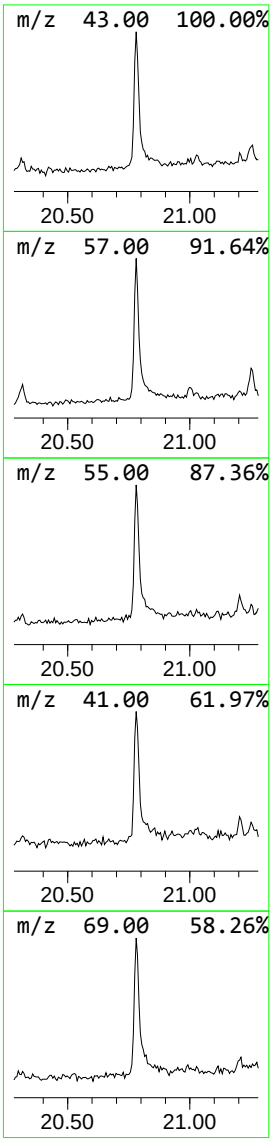
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Cyclic20.780 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.780	4.27 ng/ul	487651	Chrysene-d12	21.062

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Octacosanol	410	C28H58O	000557-61-9	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060424\
Data File : BM045853.D
Acq On : 05 Jun 2024 16:56
Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

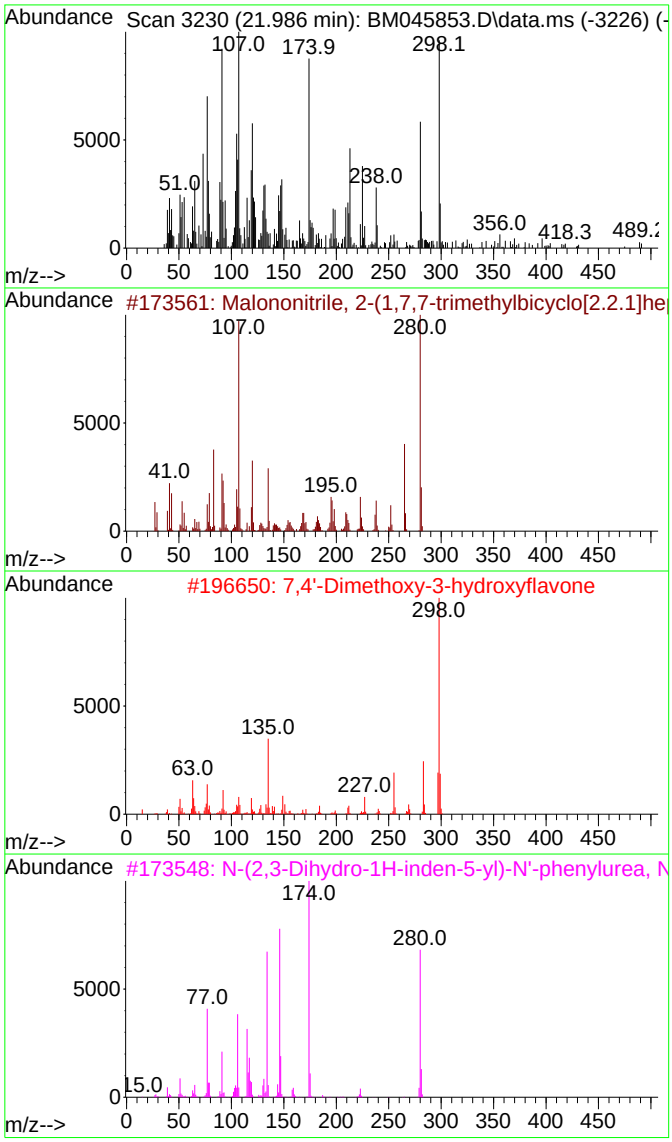
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

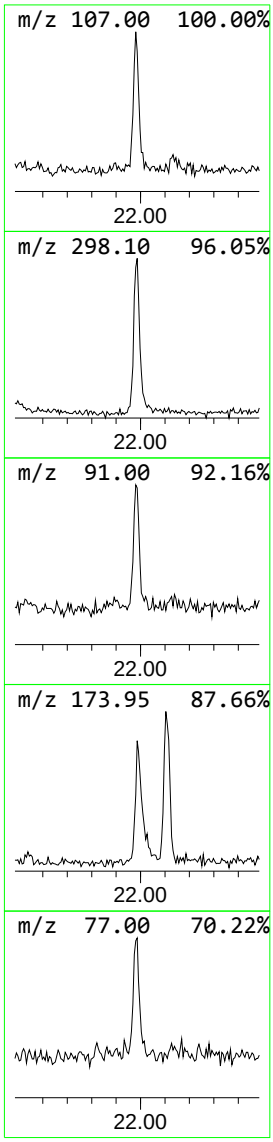
****

Peak Number 7 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.986	2.67 ng/ul	305696	Chrysene-d12	21.062

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Malononitrile, 2-(1,7,7-trimethy...	280	C18H20N2O	1000164-42-4	38
2	7,4'-Dimethoxy-3-hydroxyflavone	298	C17H14O5	013198-99-7	25
3	N-(2,3-Dihydro-1H-inden-5-yl)-N'...	280	C18H20N2O	1000492-22-0	20
4	[1,4,5]Thiadiazepine, 3,6-diphen...	298	C16H14N2O2S	1000305-12-2	15
5	N-(2-Amino-phenyl)-3-trifluorome...	280	C14H11F3N2O	1000277-75-3	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060424\
Data File : BM045853.D
Acq On : 05 Jun 2024 16:56
Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

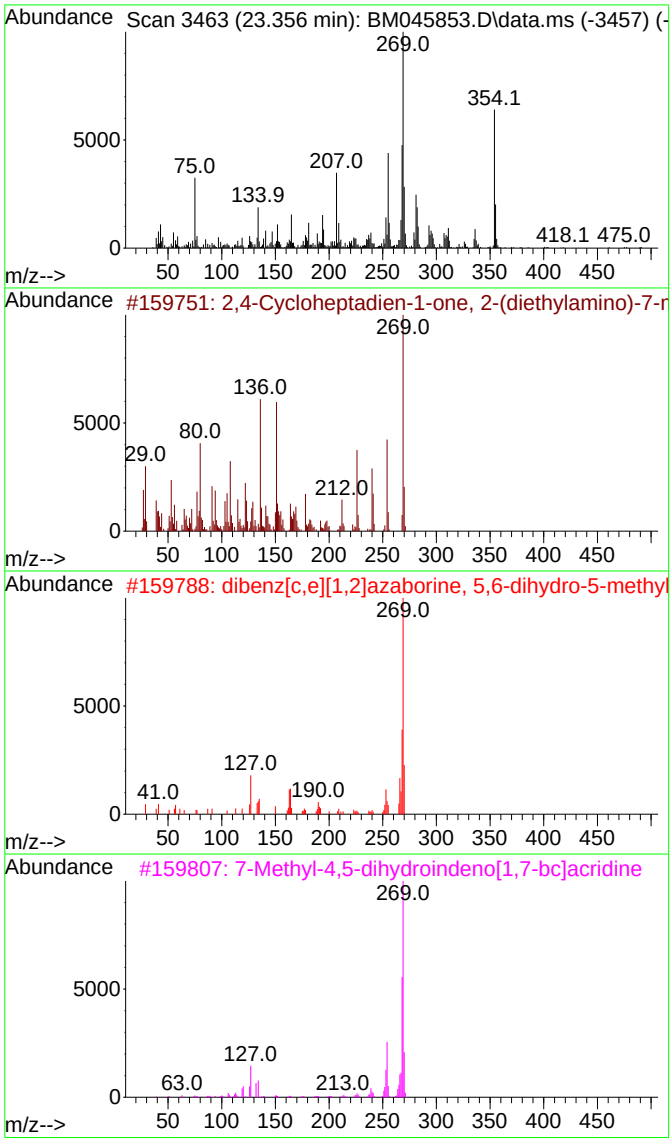
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

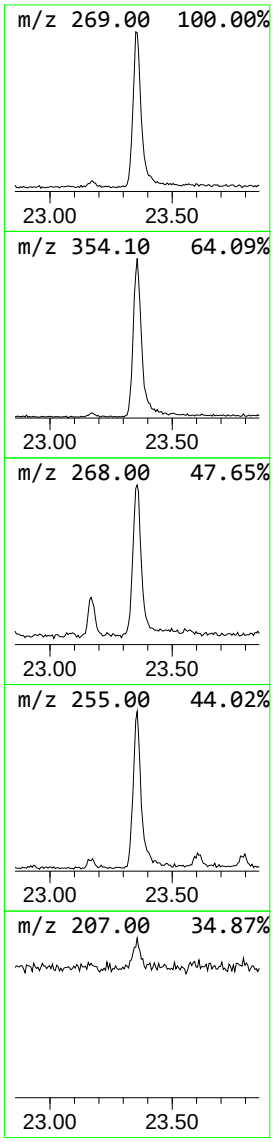
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,4-Cycloheptadien-1-one, 2... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.356	9.54 ng/ul	1308910	Perylene-d12	23.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Cycloheptadien-1-one, 2-(die...	269	C18H23NO	133436-07-4	74
2	dibenz[c,e][1,2]azaborine, 5,6-d...	269	C19H16BN	1000396-96-7	45
3	7-Methyl-4,5-dihydroindeno[1,7-b...	269	C20H15N	1000496-51-0	41
4	N,N-Di(2-naphthyl)amine	269	C20H15N	000532-18-3	41
5	2-(Benzylideneamino)fluorene	269	C20H15N	013924-50-0	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060424\
Data File : BM045853.D
Acq On : 05 Jun 2024 16:56
Operator : MA/JU
Sample : P2586-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4C44

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanoic acid	3.722	3.3	ng/ul	317712	1	7.463	1904290	20.0
1-Phenoxypropan...	11.022	2.3	ng/ul	287940	2	10.228	2552520	20.0
Hydrocinnamic acid	12.145	5.7	ng/ul	722234	2	10.228	2552520	20.0
n-Hexadecanoic ...	17.786	5.7	ng/ul	771700	4	16.851	2698880	20.0
Octadecanoic acid	19.069	2.5	ng/ul	283195	5	21.062	2285710	20.0
(DEL) Alkane: C...	20.780	4.3	ng/ul	487651	5	21.062	2285710	20.0
unknown-01	21.986	2.7	ng/ul	305696	5	21.062	2285710	20.0
2,4-Cycloheptad...	23.356	9.5	ng/ul	1308910	6	23.786	2743650	20.0