LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

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-BN041924.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN031211.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.146	23	27	37	rVB	33042	52051	0.97%	0.065%
2	3.429	71	75	81	rVB2	9060	15065	0.28%	0.019%
3	3.552	93	96	110	rBV	259298	449181	8.33%	0.565%
4	3.652	110	113	123	rVB	54889	83139	1.54%	0.104%
5	3.864	145	149	156	rVB2	13916	23954	0.44%	0.030%
6	4.223	208	210	216	rVB5	9051	11900	0.22%	0.015%
7	4.411	239	242	246	rVB3	9997	13856	0.26%	0.017%
8	4.776	298	304	312	rVB3	12658	33540	0.62%	0.042%
9	4.864	315	319	325	rVB	11747	17760	0.33%	0.022%
10	5.287	387	391	400	rBV3	13046	33498	0.62%	0.042%
11	5.652	447	453	459	rBV5	12467	22212	0.41%	0.028%
12	5.728	464	466	473	rVB5	8963	12105	0.22%	0.015%
13	6.181	539	543	549	rBV7	5352	10154	0.19%	0.013%
14	6.622	615	618	623	rVB6	7189	10499	0.19%	0.013%
15	6.805	642	649	664	rVB	735031	1229486	22.81%	1.545%
16	6.970	670	677	686	rBV	584922	902792	16.75%	1.135%
17	7.158	702	709	719	rBV	752942	1196054	22.19%	1.503%
18	7.246	719	724	732	rVB7	10580	25338	0.47%	0.032%
19	7.322	732	737	741	rBV7	8002	13537	0.25%	0.017%
20	7.628	780	789	797	rBV	1038300	1659220	30.78%	2.085%
21	7.711	797	803	811	rVB7	14142	31333	0.58%	0.039%
22	8.334	902	909	921	rBV	849290	1401672	26.00%	1.762%
23	8.446	923	928	935	rVV	78262	133391	2.47%	0.168%
24	8.781	978	985	1000	rBV	718100	1177931	21.85%	1.480%
25	8.940	1006	1012	1022	rVB	69037	115638	2.15%	0.145%
26	9.175	1048	1052	1058	rVB2	13035	19110	0.35%	0.024%
27	9.352	1077	1082	1090	rVB	29451	50483	0.94%	0.063%
28	9.499	1099	1107	1121	rBV	589160	984190	18.26%	1.237%
29	9.646	1126	1132	1139	rVV3	13948	32255	0.60%	0.041%
30	9.728	1143	1146	1155	rVB9	5442	11067	0.21%	0.014%
31	9.863	1162	1169	1172	rBV6	7111	11758	0.22%	0.015%
32	10.028	1190	1197	1214	rBV	961927	1642962	30.48%	2.065%
33	10.199	1222	1226	1232	rVV8	5203	10042	0.19%	0.013%
34	10.252	1232	1235	1244	rVB8	5079	12271	0.23%	0.015%
35	10.405	1253	1261	1267	rBV	1542428	2592298	48.09%	3.258%
36	10.552	1276	1286	1305	rBV	493967	937570	17.39%	1.178%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

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-BN041924.MA.M
Title : SVOA CALIBRATION

37	10.952	1348	1354	1362	rBV	10832	24841	0.46%	0.031%
38	11.152	1383	1388	1393	rBV3	25214	48668	0.90%	0.061%
39	11.199	1393	1396	1403	rVB3	18687	31488	0.58%	0.040%
40	11.910	1512	1517	1522	rBV5	5460	10199	0.19%	0.013%
41	11.999	1524	1532	1538	rVV	18299	35859	0.67%	0.045%
42	12.075	1540	1545	1551	rVB2	10309	17830	0.33%	0.022%
43	12.299	1579	1583	1591	rVB2	7026	12724	0.24%	0.016%
44	12.505	1611	1618	1620	rBV8	3991	10489	0.19%	0.013%
45	13.093	1714	1718	1723	rBV3	13139	20609	0.38%	0.026%
46	13.169	1726	1731	1738	rVV	27095	41653	0.77%	0.052%
47	13.234	1738	1742	1751	rVV10	8800	15720	0.29%	0.020%
48	13.587	1798	1802	1808	rBV6	9058	15219	0.28%	0.019%
49	13.693	1813	1820	1827	rVV	1629976	2349841	43.60%	2.953%
50	13.751	1827	1830	1835	rVV6	10070	16383	0.30%	0.021%
51	13.963	1856	1866	1878	rBV	2042922	3041297	56.42%	3.822%
52	14.175	1898	1902	1907	rVB3	16071	21010	0.39%	0.026%
53	14.275	1911	1919	1925	rVV	2462748	3525577	65.41%	4.431%
54	14.334	1925	1929	1936	rVB	37153	63245	1.17%	0.079%
55	14.493	1948	1956	1976	rBV	663376	1224518	22.72%	1.539%
56	14.646	1976	1982	1985	rBV	50511	78231	1.45%	0.098%
57	15.069	2048	2054	2058	rBV7	10621	23026	0.43%	0.029%
58	15.128	2061	2064	2068	rVB2	18225	22645	0.42%	0.028%
59	15.269	2082	2088	2094	rBV	2627449	3761943	69.79%	4.728%
60	15.328	2094	2098	2103	rVB2	52288	81234	1.51%	0.102%
61	15.393	2103	2109	2118	rBV	616900	852080	15.81%	1.071%
62	15.510	2126	2129	2132	rBV4	9108	11081	0.21%	0.014%
63	15.622	2144	2148	2150	rBV2	11057	12463	0.23%	0.016%
64	15.763	2168	2172	2178	rBV3	12145	24730	0.46%	0.031%
65	15.828	2178	2183	2193	rVB5	16367	40950	0.76%	0.051%
66	16.004	2207	2213	2219	rBV4	38510	92879	1.72%	0.117%
67	16.057	2219	2222	2227	rVB6	10978	14571	0.27%	0.018%
68	16.540	2299	2304	2312	rBV	48014	89926	1.67%	0.113%
69	16.681	2324	2328	2336	rVB	35810	60283	1.12%	0.076%
70	16.787	2343	2346	2349	rBV2	20332	22817	0.42%	0.029%
71	16.840	2352	2355	2360	rVB2	58709	77477	1.44%	0.097%
72	17.028	2380	2387	2391	rBV	2942108	4418283	81.97%	5.553%
73	17.069	2391	2394	2398	rVV	874526	1130767	20.98%	1.421%
74	17.122	2398	2403	2413	rVV2	2897119	4280861	79.42%	5.380%
75	17.216	2416	2419	2424	rVB2	34741	58348	1.08%	0.073%
76	17.434	2451	2456	2464	rVB	138375	200560	3.72%	0.252%

LSC Area Percent Report

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Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

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-BN041924.MA.M
Title : SVOA CALIBRATION

77	17.528	2469	2472	2474	rBV	22119	28773	0.53%	0.036%
78	17.698	2498	2501	2506	rVB6	35797	44215	0.82%	0.056%
79	17.928	2531	2540	2550	rBV2	508657	982639	18.23%	1.235%
80	18.092	2562	2568	2572	rBV4	144982	252659	4.69%	0.318%
81	18.222	2587	2590	2593	rBV2	29667	32439	0.60%	0.041%
82	18.404	2618	2621	2625	rBV	78365	104107	1.93%	0.131%
83	18.445	2625	2628	2634	rVB	169304	232041	4.31%	0.292%
84	18.987	2714	2720	2724	rBV2	72428	161253	2.99%	0.203%
85	19.092	2733	2738	2746	rVB	2323688	3078007	57.11%	3.868%
86	19.216	2756	2759	2767	rBV3	176988	273276	5.07%	0.343%
87	19.375	2783	2786	2790	rBV	470071	550235	10.21%	0.692%
88	19.428	2790	2795	2798	rBV	3716095	5390020	100.00%	6.774%
89	19.457	2798	2800	2804	rVB	1899663	2070936	38.42%	2.603%
90	20.369	2951	2955	2956	rBV	2330034	2449272	45.44%	3.078%
91	20.386	2956	2958	2969	rVB	2764814	3416441	63.38%	4.294%
92	20.475	2970	2973	2978	rBV	447920	508209	9.43%	0.639%
93	20.957	3051	3055	3062	rBV2	630496	1012974	18.79%	1.273%
94	21.263	3100	3107	3111	rBV2	3035405	5264564	97.67%	6.617%
95	21.304	3111	3114	3123	rVB	882397	1260179	23.38%	1.584%
96	22.628	3332	3339	3348	rBV3	714695	1839269	34.12%	2.312%
97	23.245	3438	3444	3451	rBV	700985	1889928	35.06%	2.375%
98	23.892	3550	3554	3559	rBV	317013	587454	10.90%	0.738%
99	23.963	3559	3566	3572	rBV2	1485642	3268067	60.63%	4.107%
100	24.163	3592	3600	3608	rBV	1606372	4008210	74.36%	5.038%

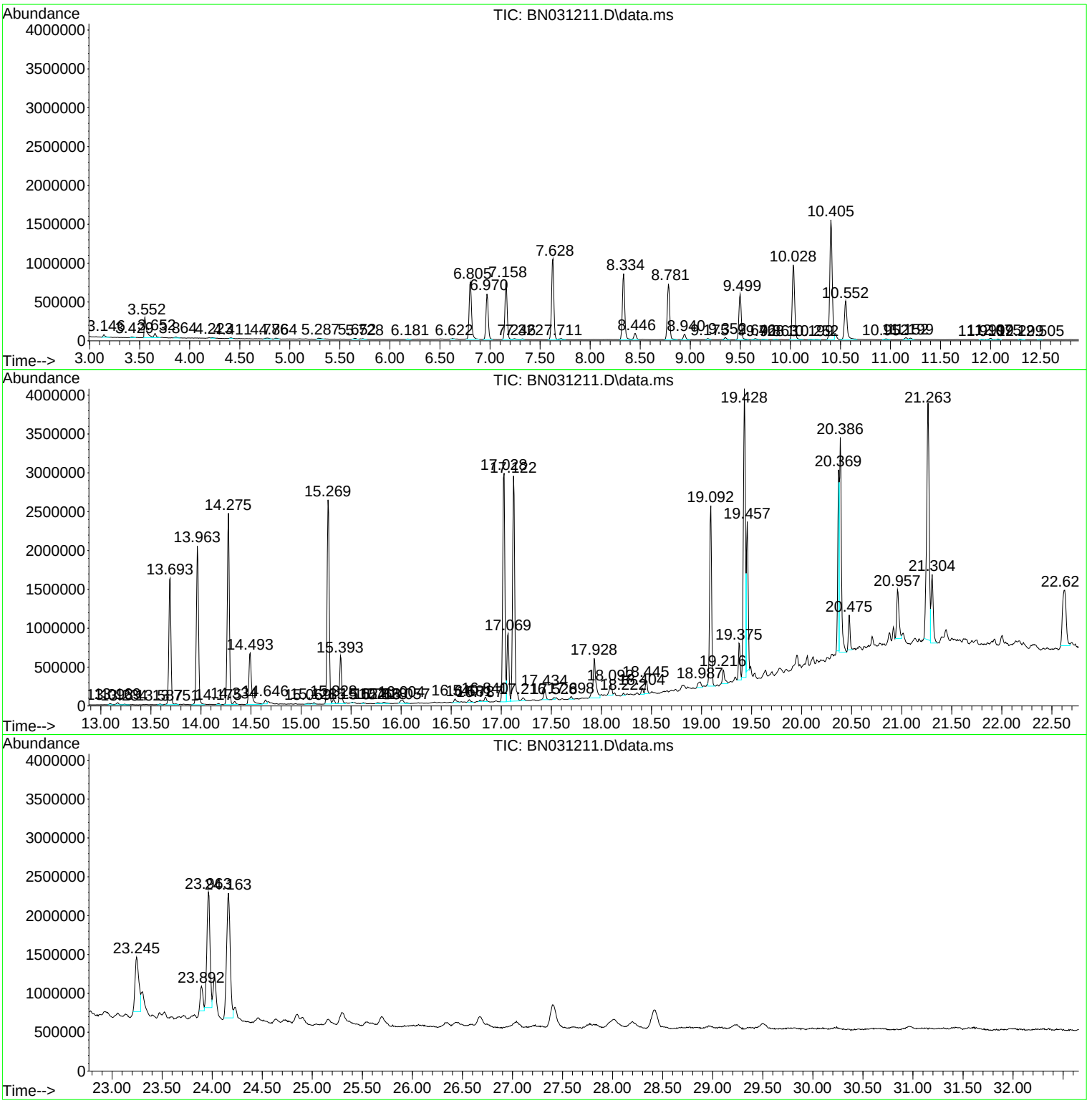
Sum of corrected areas: 79566804

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.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\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

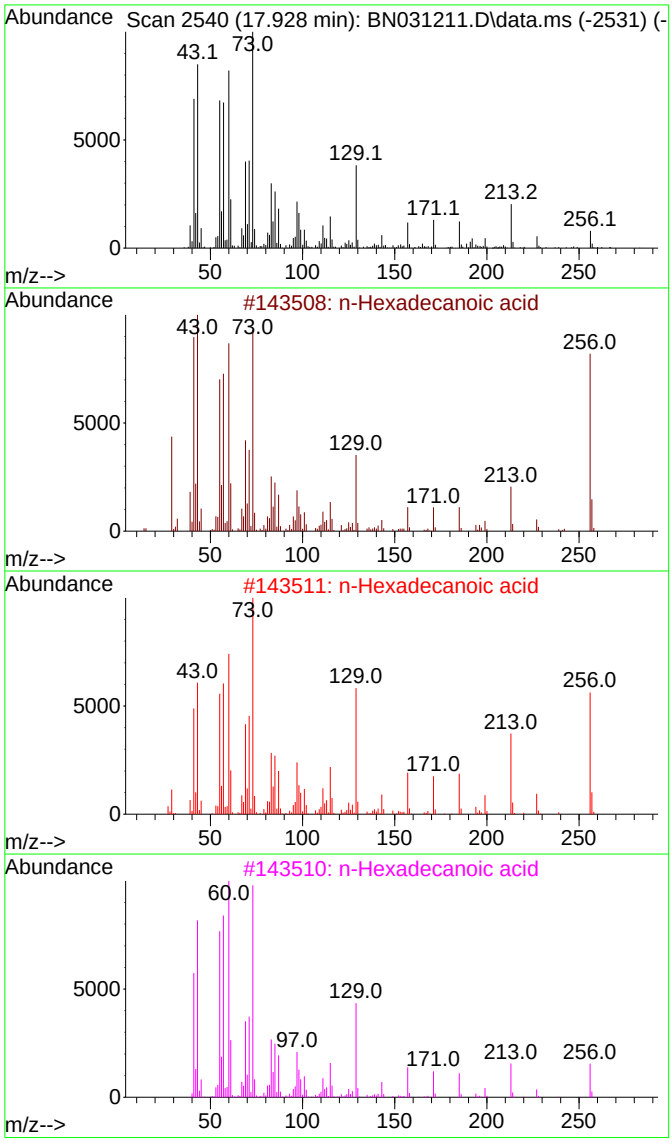
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

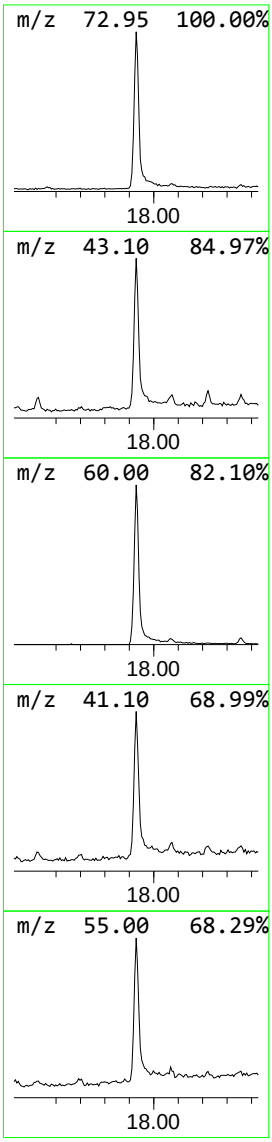
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.928	4.45 ng/ul	982639	Phenanthrene-d10	17.028

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	99
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

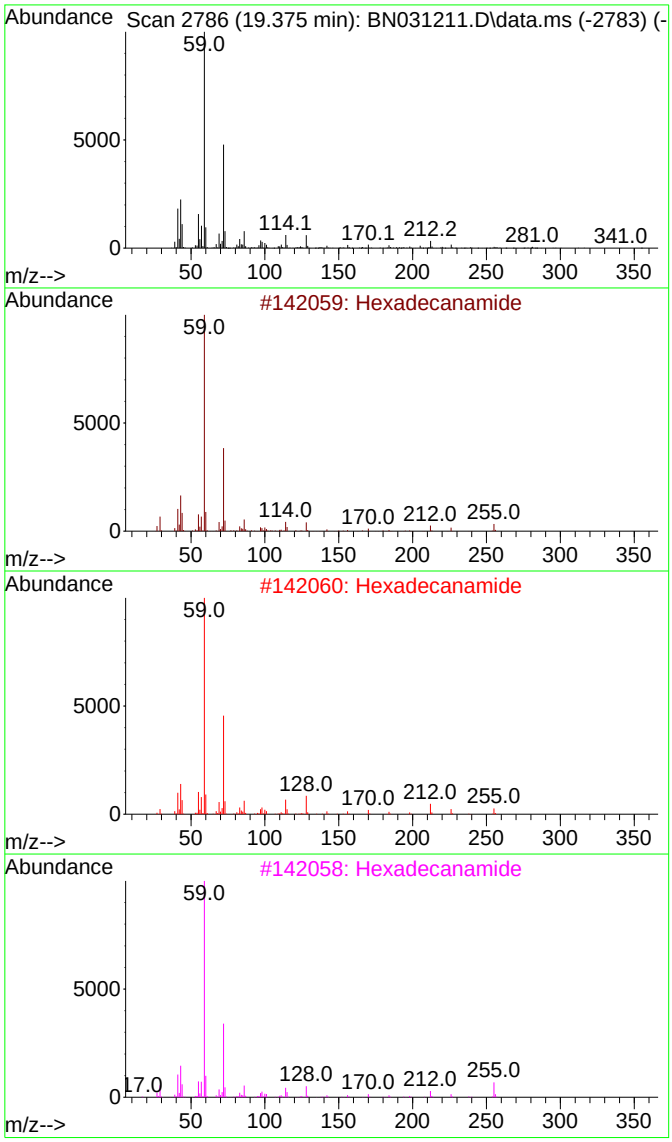
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

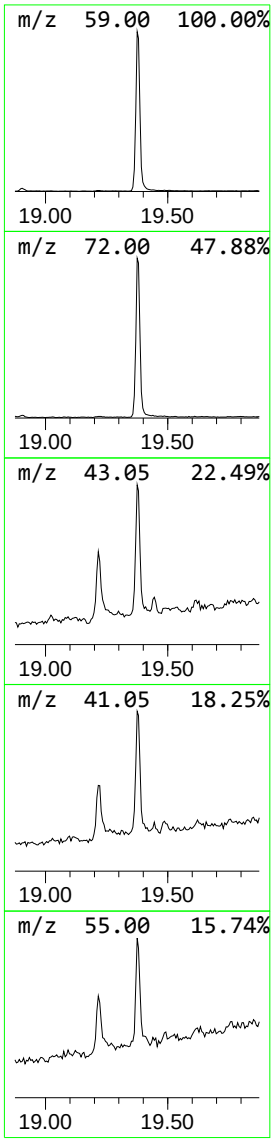
****

Peak Number 2 Hexadecanamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.375	2.09 ng/ul	550235	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	96
2	Hexadecanamide	255	C16H33NO	000629-54-9	95
3	Hexadecanamide	255	C16H33NO	000629-54-9	91
4	Tetradecanamide	227	C14H29NO	000638-58-4	83
5	Palmitoleamide	253	C16H31NO	106010-22-4	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

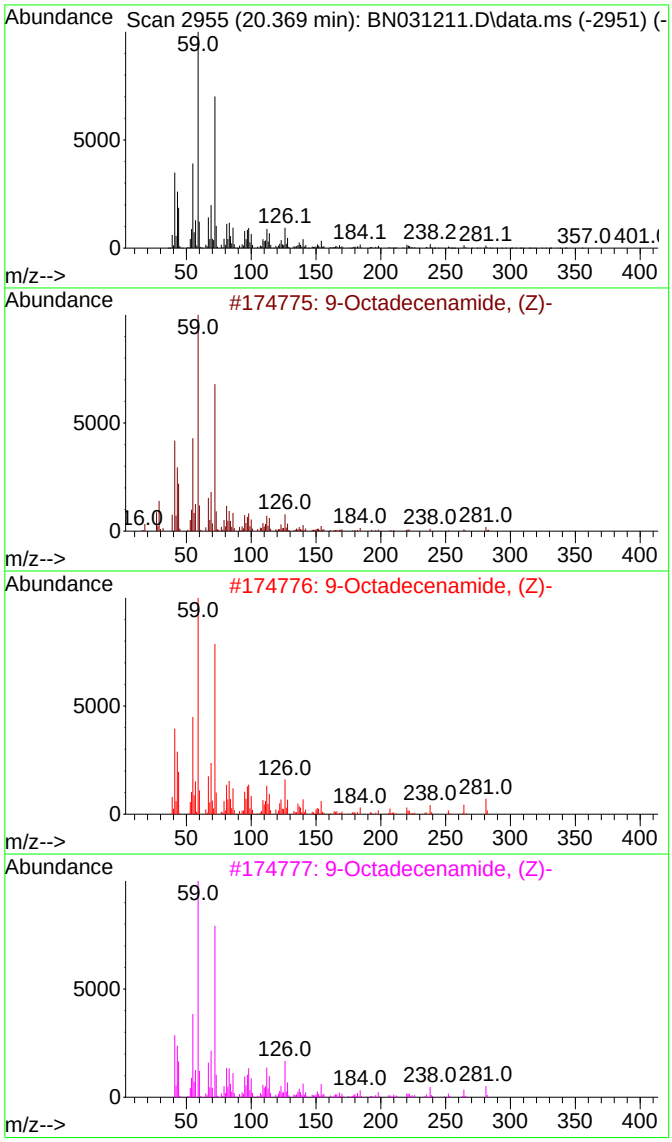
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

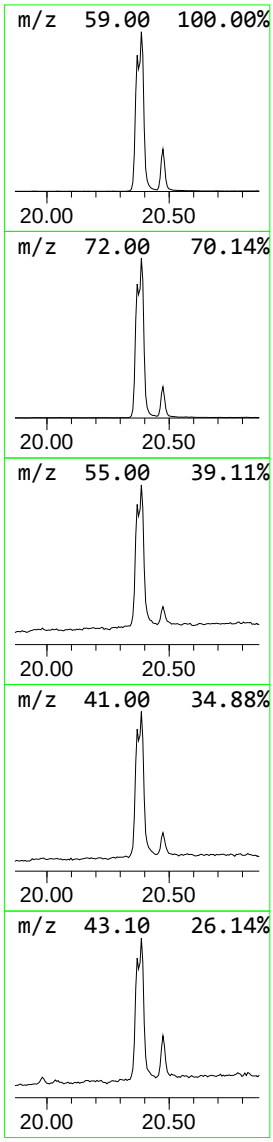
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.369	9.30 ng/ul	2449270	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
4	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
5	Palmitoleamide	253	C16H31NO	106010-22-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

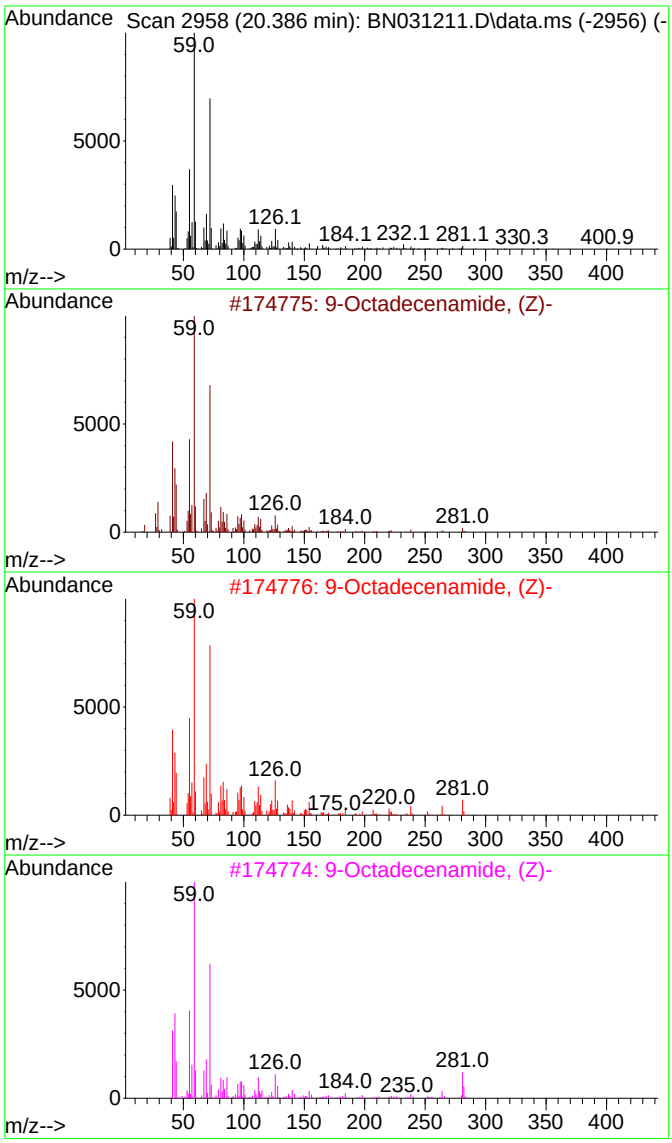
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

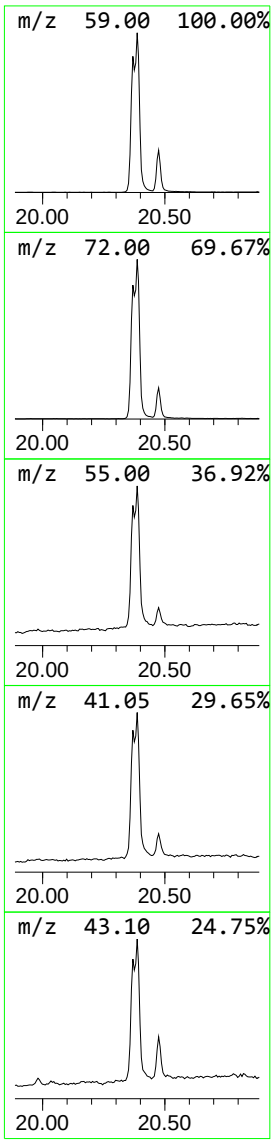
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Palmitoleamide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.386	12.98 ng/ul	3416440	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
4	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
5	Palmitoleamide	253	C16H31NO	106010-22-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

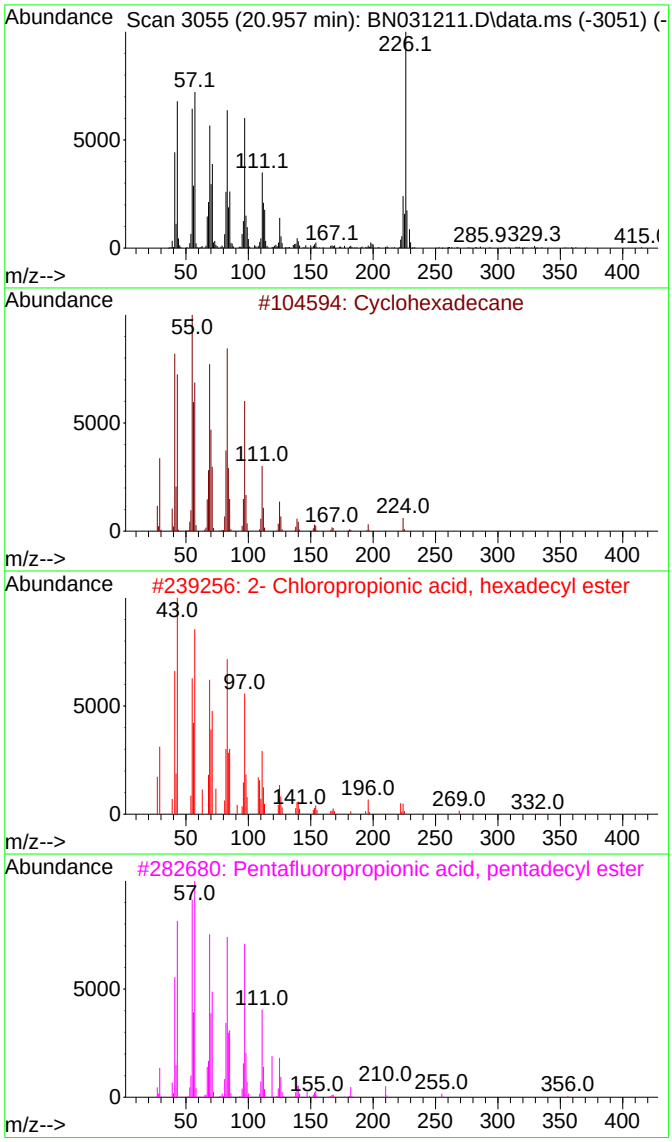
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

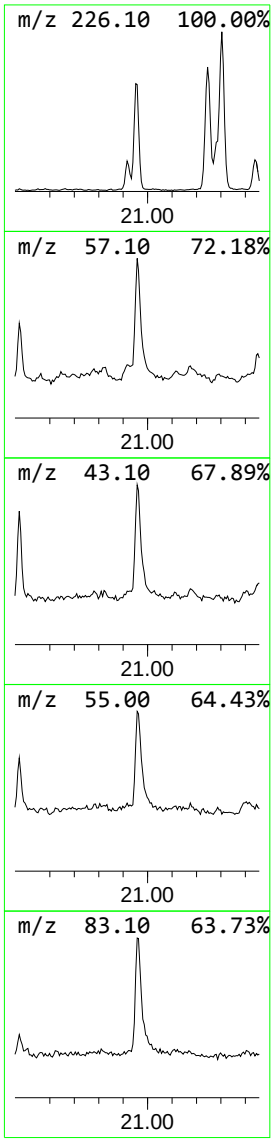
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic20.957 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	3.85 ng/ul	1012970	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	86
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	70
4	Heptacos-1-ene	378	C27H54	015306-27-1	70
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	70





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Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

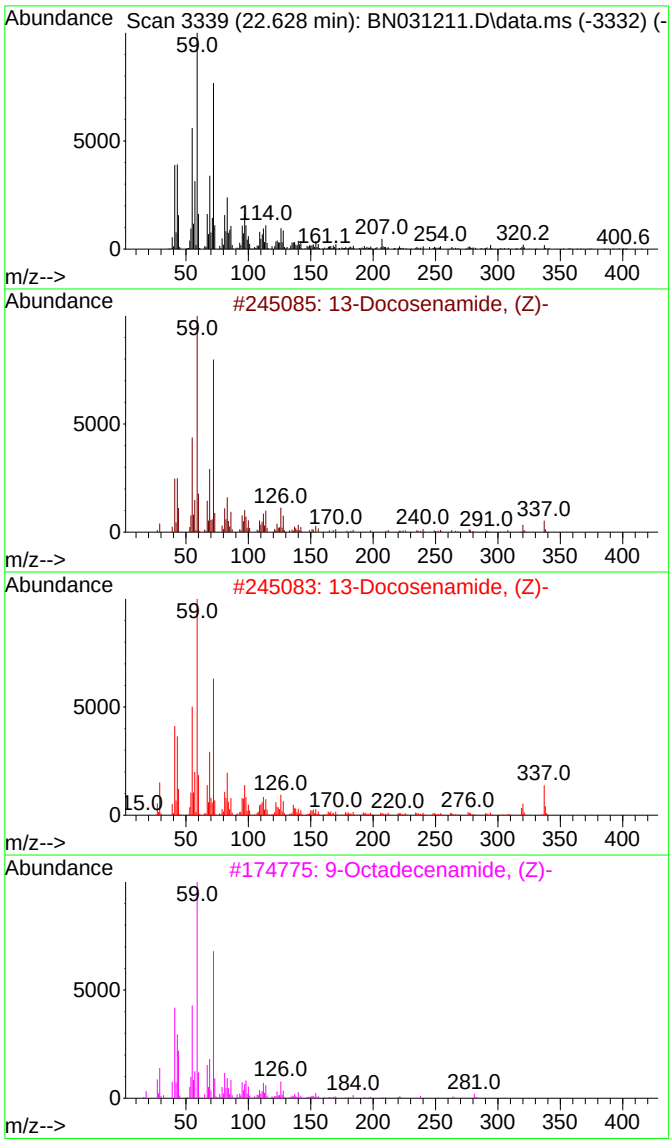
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

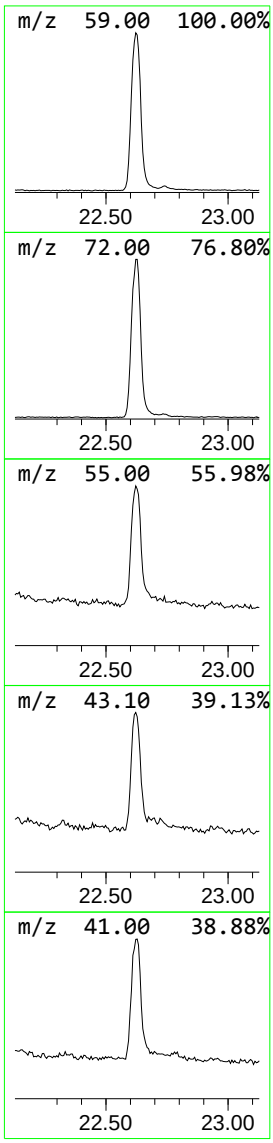
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.628	6.99 ng/ul	1839270	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	99
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
4	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

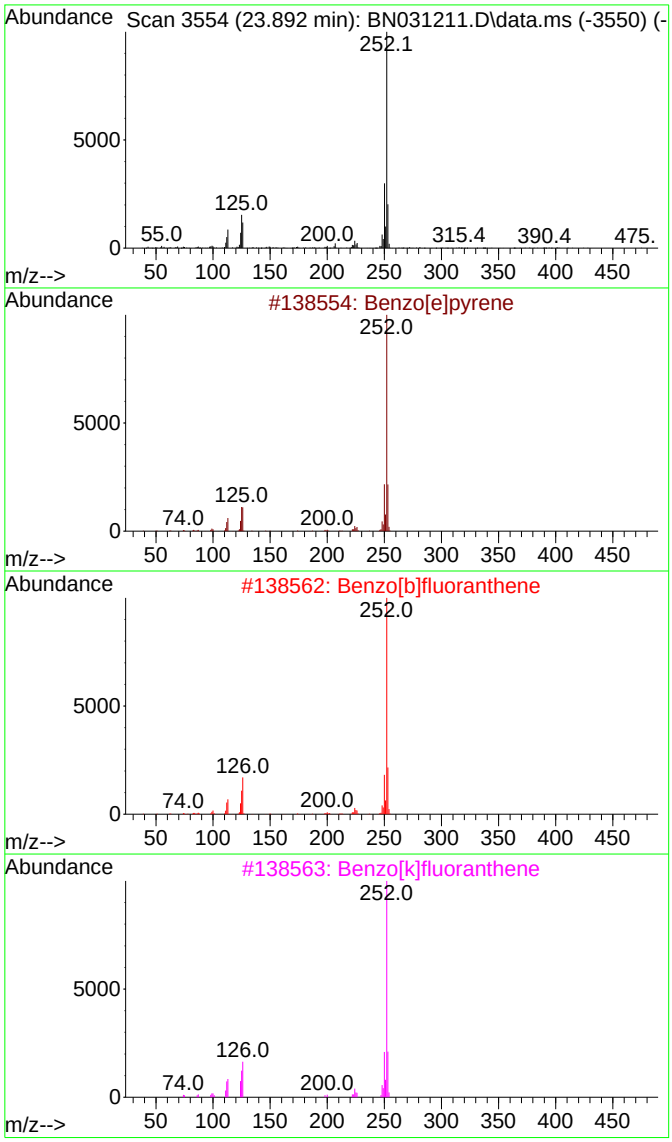
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

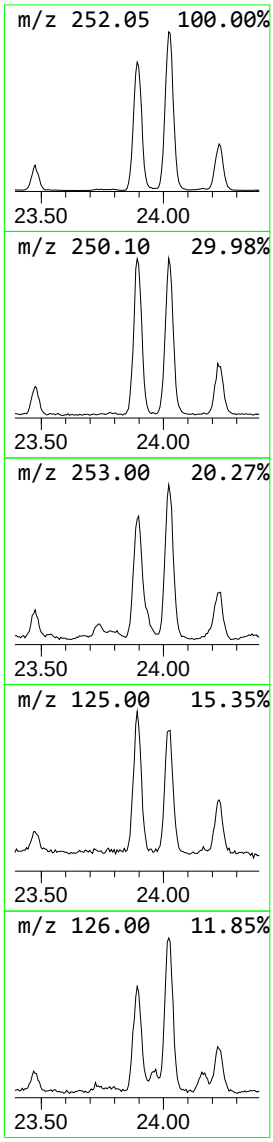
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.892	2.93 ng/ul	587454	Perylene-d12	24.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042424\
Data File : BN031211.D
Acq On : 25 Apr 2024 06:46
Operator : MA/JU
Sample : P2104-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AA3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.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
n-Hexadecanoic ...	17.928	4.5	ng/ul	982639	4	17.028	4418280	20.0
Hexadecanamide	19.375	2.1	ng/ul	550235	5	21.263	5264560	20.0
9-Octadecenamid...	20.369	9.3	ng/ul	2449270	5	21.263	5264560	20.0
Palmitoleamide	20.386	13.0	ng/ul	3416440	5	21.263	5264560	20.0
(DEL) Alkane: C...	20.957	3.9	ng/ul	1012970	5	21.263	5264560	20.0
13-Docosenamide...	22.628	7.0	ng/ul	1839270	5	21.263	5264560	20.0
Benzo[e]pyrene	23.892	2.9	ng/ul	587454	6	24.163	4008210	20.0