LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

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-BM120722.M
Title : SVOA CALIBRATION

Signal : TIC: BM038177.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	33	36	46	rVB	33057	56062	2.47%	0.151%
2	3.834	107	110	131	rBV	324113	557444	24.55%	1.499%
3	4.163	163	166	171	rVB3	11003	16607	0.73%	0.045%
4	5.116	323	328	334	rVB2	16724	29347	1.29%	0.079%
5	5.357	366	369	373	rBV5	3730	5959	0.26%	0.016%
6	5.851	451	453	457	rVB5	2842	3073	0.14%	0.008%
7	6.569	570	575	576	rBV4	2852	3218	0.14%	0.009%
8	6.934	635	637	641	rBV5	2262	2404	0.11%	0.006%
9	7.204	676	683	692	rVB	513944	829073	36.52%	2.230%
10	7.369	704	711	722	rVB	389735	606149	26.70%	1.630%
11	7.569	738	745	755	rBV	545607	853466	37.59%	2.295%
12	8.039	819	825	833	rBV	703454	1093324	48.15%	2.940%
13	8.104	834	836	838	rVV3	4581	3645	0.16%	0.010%
14	8.192	847	851	854	rVB4	1922	2734	0.12%	0.007%
15	8.422	886	890	894	rBV7	2390	4314	0.19%	0.012%
16	8.757	939	947	955	rBV	607408	985751	43.42%	2.651%
17	9.210	1017	1024	1034	rBV	496616	825103	36.34%	2.219%
18	9.275	1034	1035	1040	rVB5	3312	2723	0.12%	0.007%
19	9.363	1047	1050	1053	rBV4	5454	7118	0.31%	0.019%
20	9.598	1082	1090	1095	rVB3	10632	19184	0.84%	0.052%
21	9.863	1132	1135	1137	rVB2	2813	2340	0.10%	0.006%
22	9.939	1139	1148	1158	rVV	420967	708480	31.20%	1.905%
23	10.475	1232	1239	1251	rBV	685546	1134246	49.96%	3.050%
24	10.639	1262	1267	1271	rVB7	3394	5855	0.26%	0.016%
25	10.857	1297	1304	1315	rBV	968718	1598779	70.42%	4.300%
26	10.933	1315	1317	1320	rBV4	2074	2573	0.11%	0.007%
27	10.998	1320	1328	1339	rBV	622245	1053108	46.38%	2.832%
28	11.192	1357	1361	1367	rVB8	2359	4921	0.22%	0.013%
29	11.345	1384	1387	1390	rVB4	1904	2433	0.11%	0.007%
30	11.633	1432	1436	1440	rBV6	3357	5258	0.23%	0.014%
31	11.757	1450	1457	1458	rBV4	2397	3405	0.15%	0.009%
32	11.892	1479	1480	1485	rVB4	2035	2377	0.10%	0.006%
33	12.086	1506	1513	1518	rVB9	2814	6194	0.27%	0.017%
34	12.251	1536	1541	1548	rVV7	3770	6595	0.29%	0.018%
35	12.339	1553	1556	1560	rBV6	2590	3104	0.14%	0.008%
36	12.433	1567	1572	1578	rVB	12178	18634	0.82%	0.050%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

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-BM120722.M
Title : SVOA CALIBRATION

37	12.951	1654	1660	1662	rVB6	2101	4169	0.18%	0.011%
38	13.039	1671	1675	1678	rVV6	2240	3304	0.15%	0.009%
39	13.139	1687	1692	1693	rBV5	2486	2436	0.11%	0.007%
40	13.192	1697	1701	1705	rVB7	3947	5301	0.23%	0.014%
41	13.274	1711	1715	1721	rVB7	2053	2485	0.11%	0.007%
42	13.392	1733	1735	1738	rBV3	2540	2718	0.12%	0.007%
43	13.480	1745	1750	1755	rVB5	10563	15250	0.67%	0.041%
44	13.598	1767	1770	1771	rBV3	3208	3301	0.15%	0.009%
45	13.621	1773	1774	1777	rVB3	3279	2451	0.11%	0.007%
46	13.921	1823	1825	1831	rVV6	2070	3003	0.13%	0.008%
47	14.074	1843	1851	1858	rVV	1156908	1556310	68.55%	4.186%
48	14.139	1860	1862	1866	rVV5	3308	4405	0.19%	0.012%
49	14.186	1866	1870	1875	rVB8	3260	5277	0.23%	0.014%
50	14.363	1894	1900	1907	rVV	1302155	1889840	83.24%	5.083%
51	14.545	1928	1931	1937	rVB6	4669	6031	0.27%	0.016%
52	14.668	1942	1952	1959	rBV	1421580	2019236	88.94%	5.431%
53	14.868	1980	1986	1996	rBV	425070	642511	28.30%	1.728%
54	15.068	2016	2020	2029	rVB8	13558	22723	1.00%	0.061%
55	15.233	2045	2048	2053	rVB6	2744	3782	0.17%	0.010%
56	15.315	2056	2062	2063	rBV6	2116	3991	0.18%	0.011%
57	15.427	2079	2081	2082	rBV2	3973	3086	0.14%	0.008%
58	15.492	2088	2092	2097	rVB7	4116	5505	0.24%	0.015%
59	15.610	2108	2112	2114	rBV5	2861	3393	0.15%	0.009%
60	15.657	2114	2120	2127	rVV	1688480	2270454	100.00%	6.106%
61	15.774	2135	2140	2149	rBV	201173	284854	12.55%	0.766%
62	15.892	2155	2160	2165	rBV5	7540	11725	0.52%	0.032%
63	16.015	2176	2181	2190	rVB	60182	84092	3.70%	0.226%
64	16.227	2215	2217	2220	rVB3	3071	2604	0.11%	0.007%
65	16.345	2235	2237	2240	rBV4	4483	5779	0.25%	0.016%
66	16.568	2274	2275	2280	rVB5	2709	2952	0.13%	0.008%
67	16.657	2287	2290	2292	rBV4	2280	2619	0.12%	0.007%
68	16.745	2301	2305	2306	rBV4	2515	3231	0.14%	0.009%
69	16.792	2310	2313	2319	rBV6	9487	15869	0.70%	0.043%
70	16.845	2319	2322	2329	rVB8	6157	10774	0.47%	0.029%
71	16.898	2329	2331	2333	rBV3	2783	3231	0.14%	0.009%
72	17.021	2348	2352	2353	rBV3	2469	2689	0.12%	0.007%
73	17.139	2370	2372	2374	rBV3	4367	4197	0.18%	0.011%
74	17.192	2379	2381	2385	rVV5	5052	5615	0.25%	0.015%
75	17.286	2393	2397	2401	rBV6	9280	15763	0.69%	0.042%
76	17.351	2406	2408	2411	rVV4	4546	5875	0.26%	0.016%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

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-BM120722.M
Title : SVOA CALIBRATION

77	17.409	2411	2418	2424	rVV	1573701	2183698	96.18%	5.873%
78	17.504	2428	2434	2441	rVV	1579489	2194699	96.66%	5.903%
79	17.556	2441	2443	2446	rVV4	8757	11382	0.50%	0.031%
80	17.592	2446	2449	2454	rVB6	17816	26958	1.19%	0.073%
81	17.668	2457	2462	2467	rBV4	18843	37799	1.66%	0.102%
82	17.745	2473	2475	2477	rBV3	4051	3959	0.17%	0.011%
83	17.921	2501	2505	2509	rBV6	10033	14546	0.64%	0.039%
84	18.062	2526	2529	2531	rBV3	7823	9267	0.41%	0.025%
85	18.162	2542	2546	2553	rBV9	15783	38218	1.68%	0.103%
86	18.227	2554	2557	2562	rVB5	16760	19722	0.87%	0.053%
87	18.286	2562	2567	2576	rBV	514862	762193	33.57%	2.050%
88	18.633	2622	2626	2634	rVB4	16186	27839	1.23%	0.075%
89	18.703	2634	2638	2643	rBV	94755	110861	4.88%	0.298%
90	19.139	2709	2712	2718	rBV6	11528	19059	0.84%	0.051%
91	19.433	2755	2762	2765	rBV5	59738	135659	5.97%	0.365%
92	19.550	2778	2782	2792	rBV	178282	274532	12.09%	0.738%
93	19.792	2817	2823	2832	rBV	1676365	2268232	99.90%	6.100%
94	20.733	2971	2983	2984	rBV2	301640	772196	34.01%	2.077%
95	20.756	2984	2987	3006	rVB4	513887	1548688	68.21%	4.165%
96	21.262	3069	3073	3083	rBV	477051	600862	26.46%	1.616%
97	21.574	3121	3126	3131	rVB	1447112	1841860	81.12%	4.954%
98	23.868	3509	3516	3524	rVB2	1095715	2103142	92.63%	5.656%
99	24.027	3537	3543	3555	rVB2	944105	1911568	84.19%	5.141%
100	24.515	3621	3626	3634	rVB3	433518	857626	37.77%	2.307%

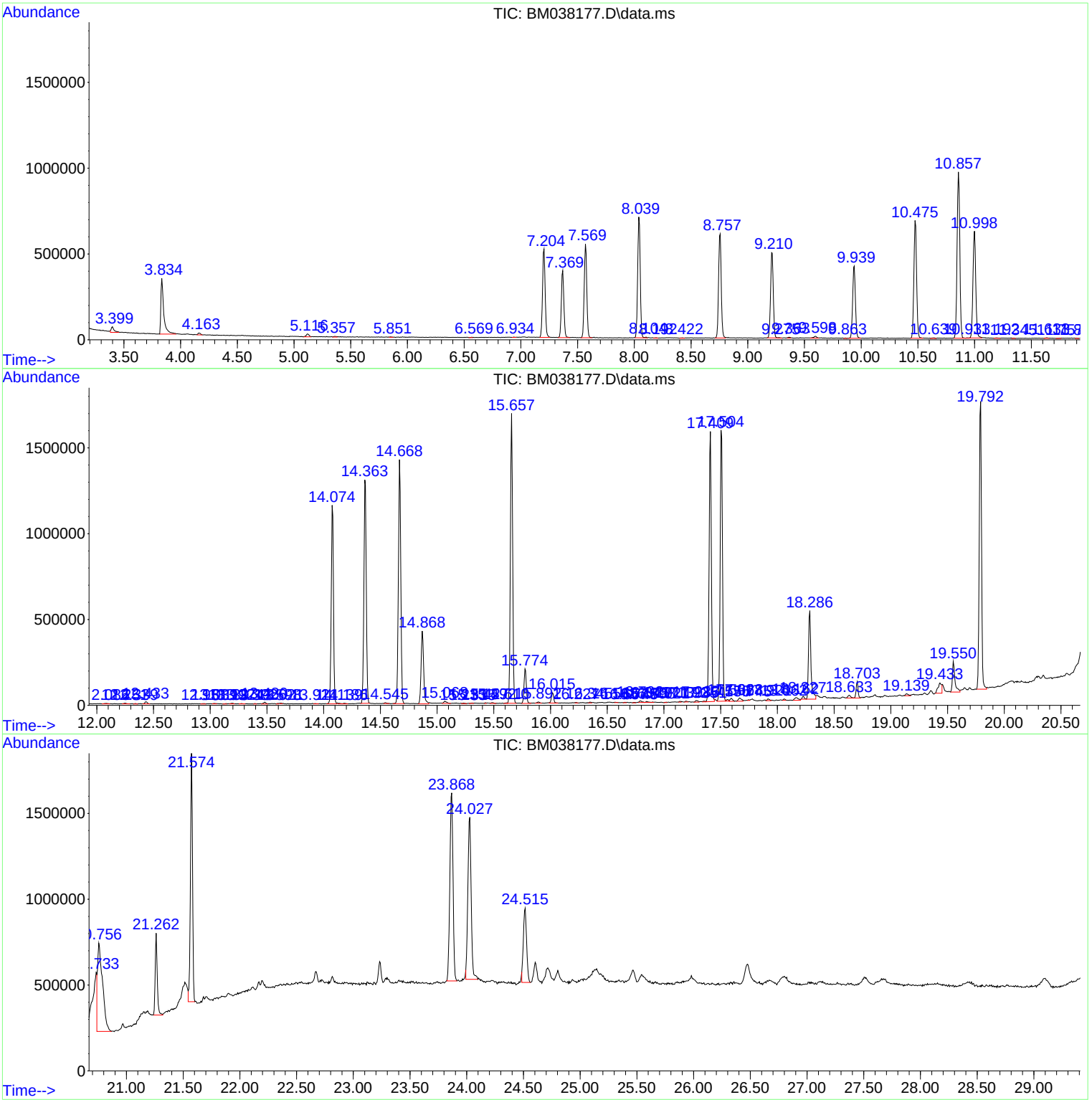
Sum of corrected areas: 37182396

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

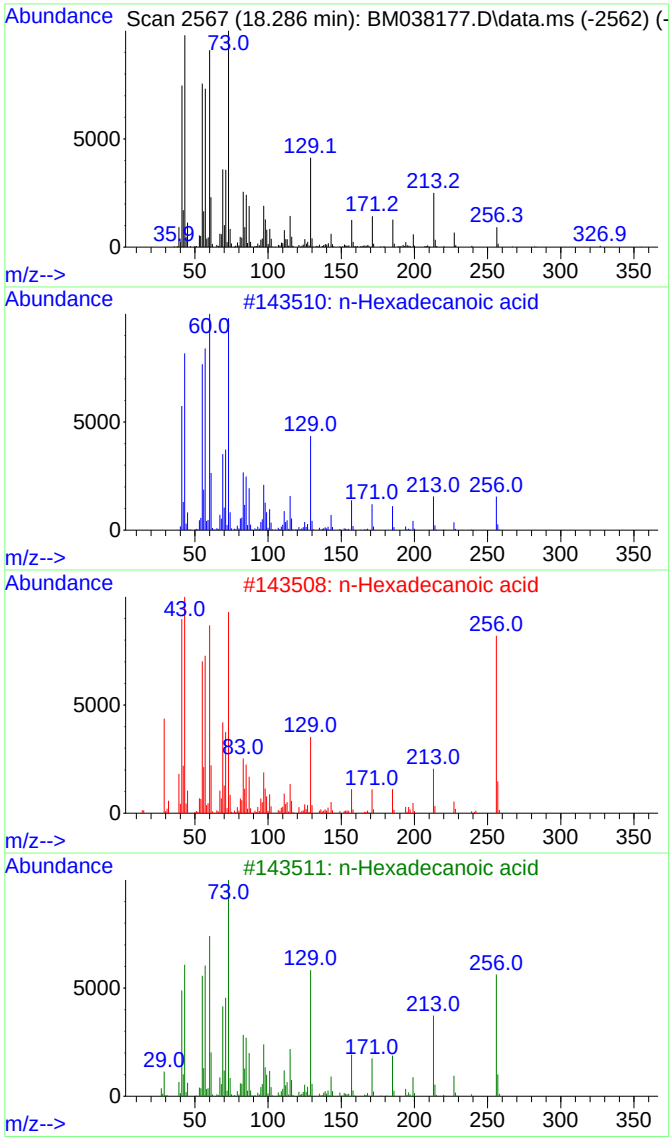
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

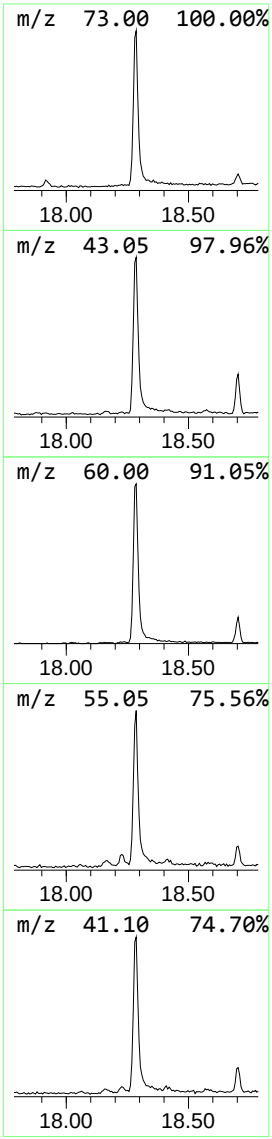
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	6.98 ng/ul	762193	Phenanthrene-d10	17.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

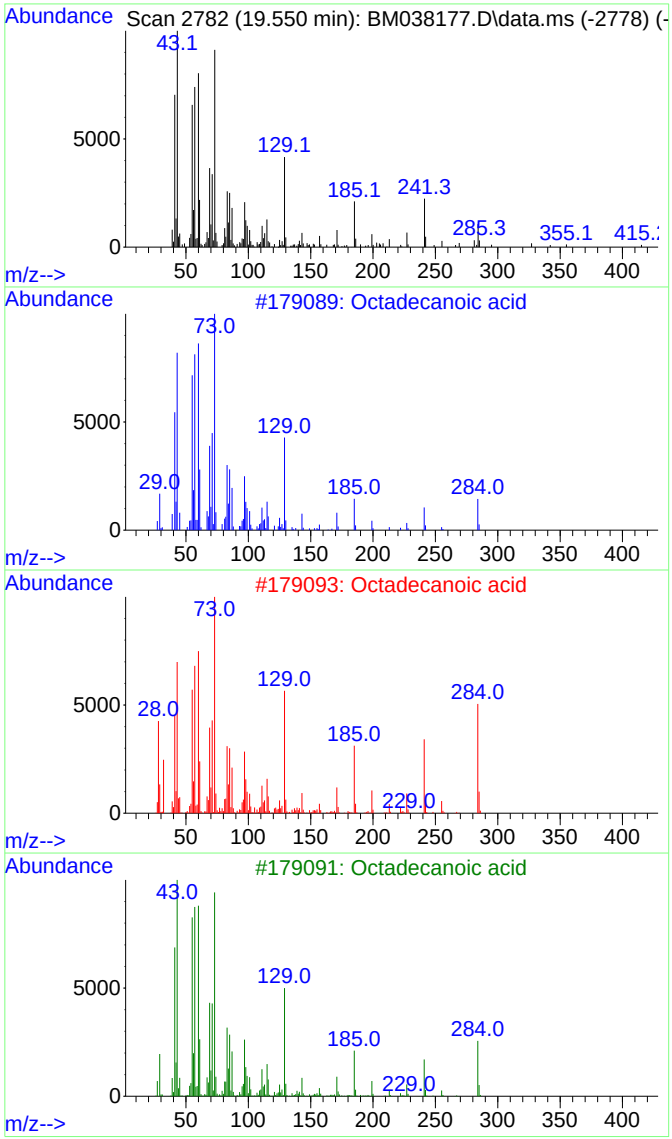
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

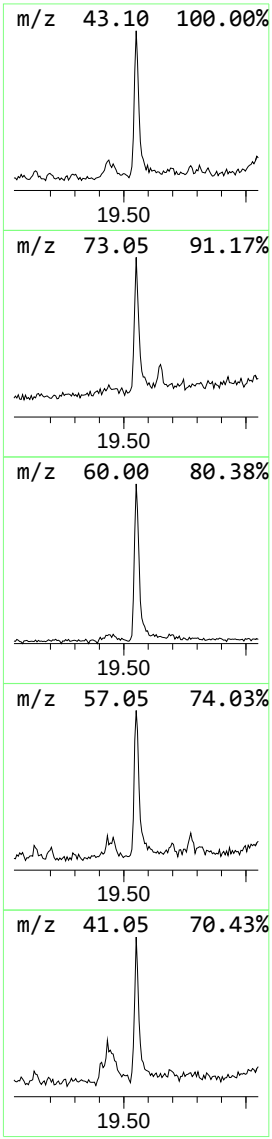
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.550	2.98 ng/ul	274532	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	96
4	Octadecanoic acid	284	C18H36O2	000057-11-4	95
5	Octadecanoic acid	284	C18H36O2	000057-11-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

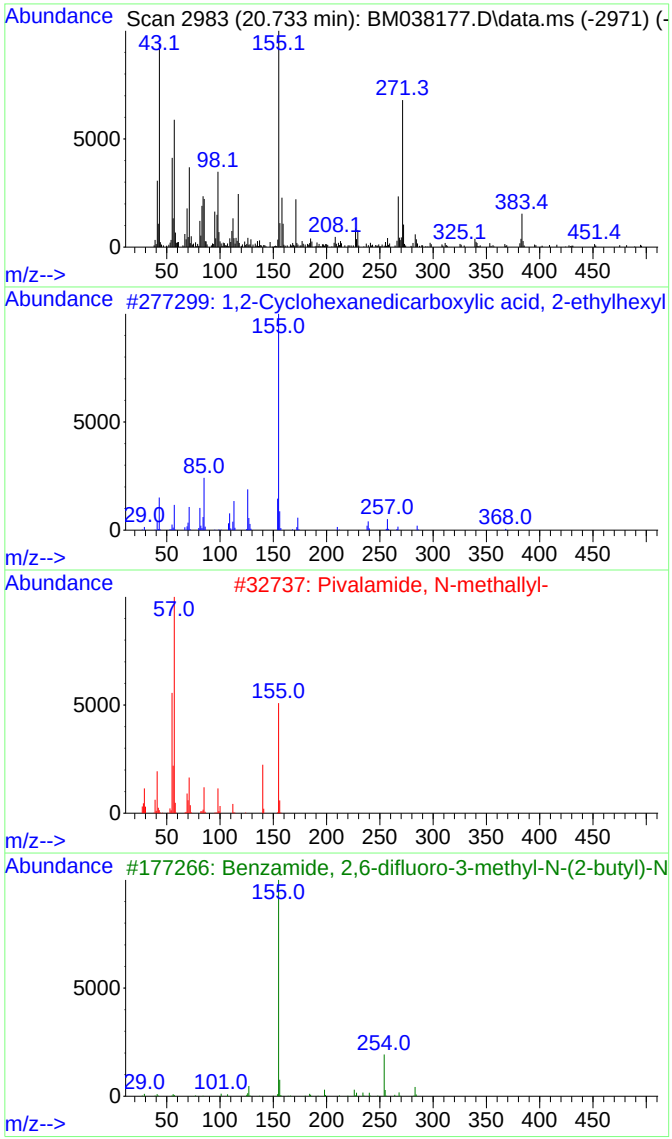
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

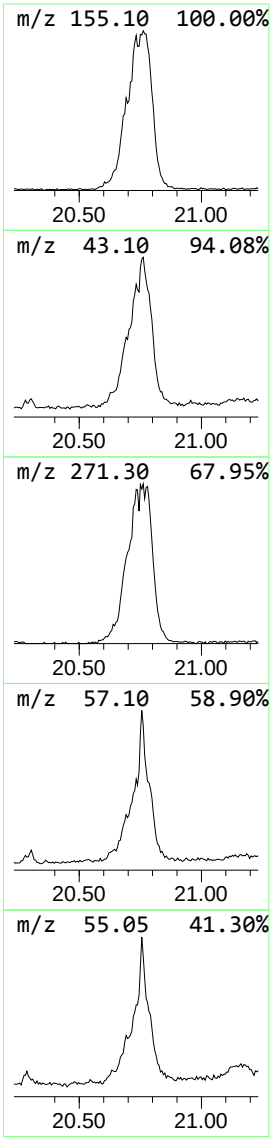
****

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.733	8.38 ng/ul	772196	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclohexanedicarboxylic acid...	368	C22H40O4	1000339-45-5	30
2	Pivalamide, N-methallyl-	155	C9H17NO	1000345-72-5	27
3	Benzamide, 2,6-difluoro-3-methyl...	283	C16H23F2NO	1000464-36-5	25
4	N-(1H-Tetrazol-5-yl)decanamide	239	C11H21N5O	186302-24-9	25
5	Benzamide, 2,6-difluoro-3-methyl...	283	C16H23F2NO	1000464-36-4	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

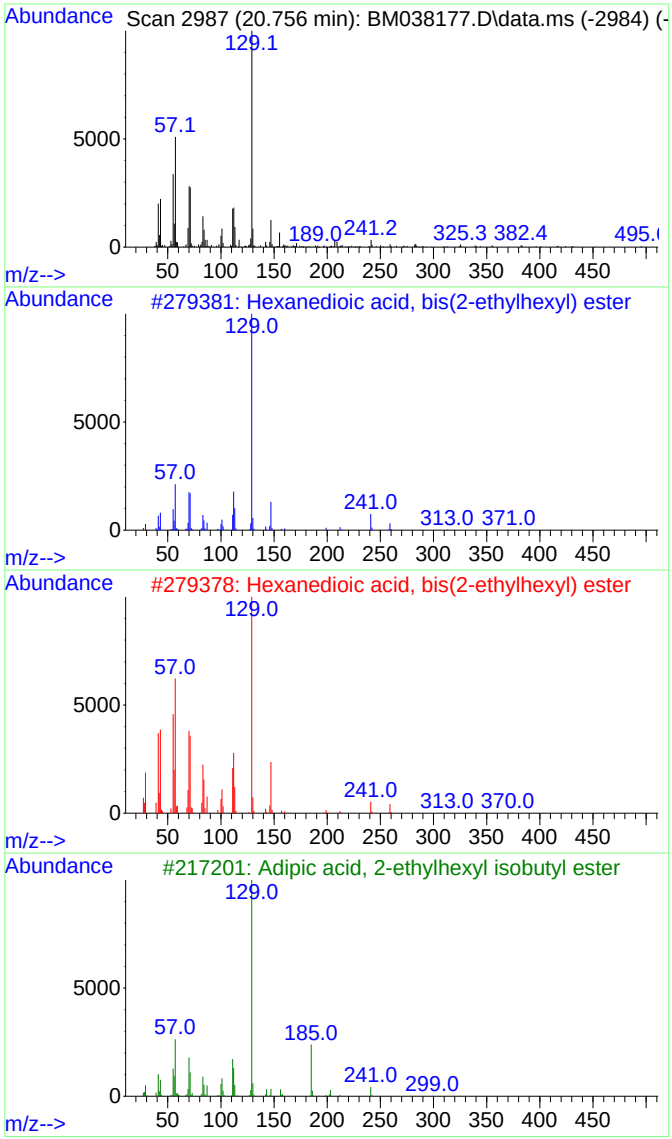
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

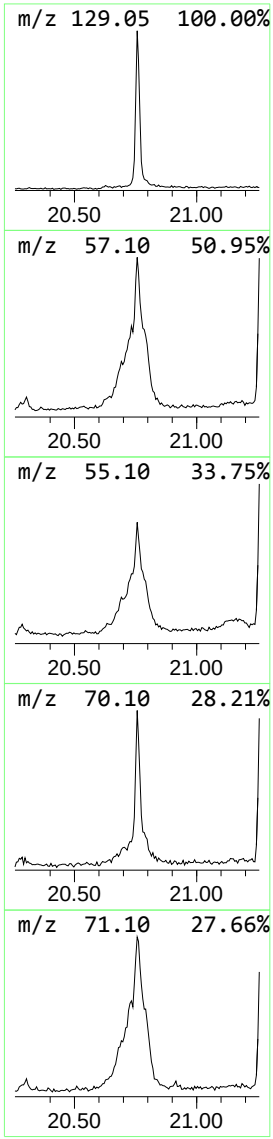
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	16.82 ng/ul	1548690	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	64
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	62
3	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	53
4	Adipic acid, pentadecyl pent-4-e...	424	C26H48O4	1000354-13-0	53
5	Adipic acid, 2-methylbutyl undec...	370	C22H42O4	1000324-68-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

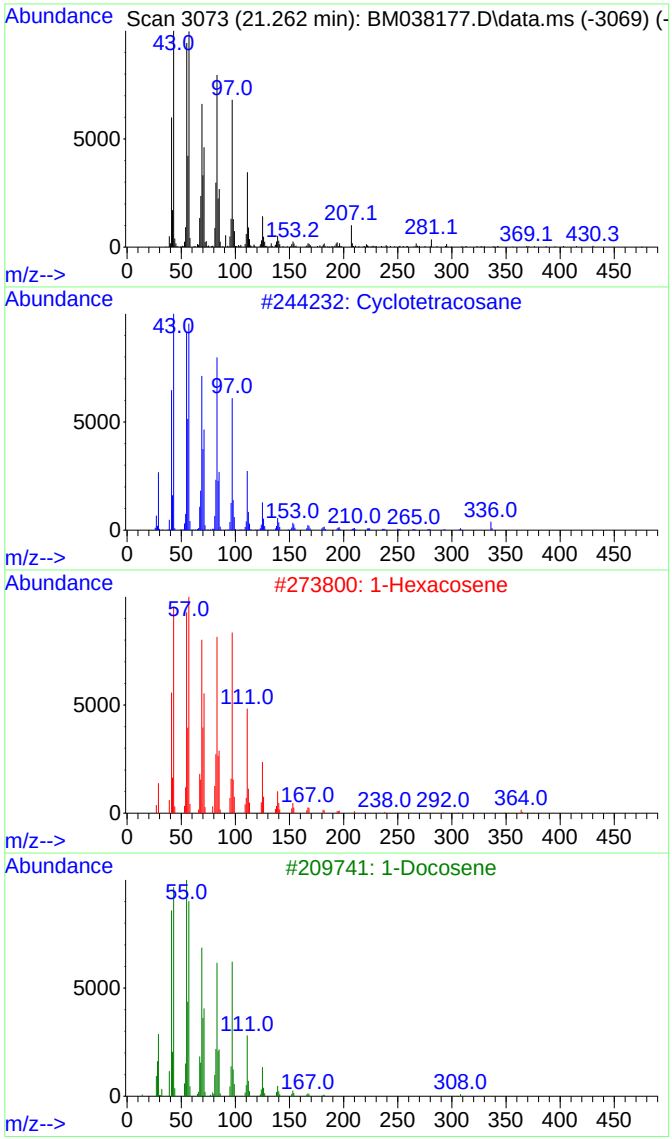
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

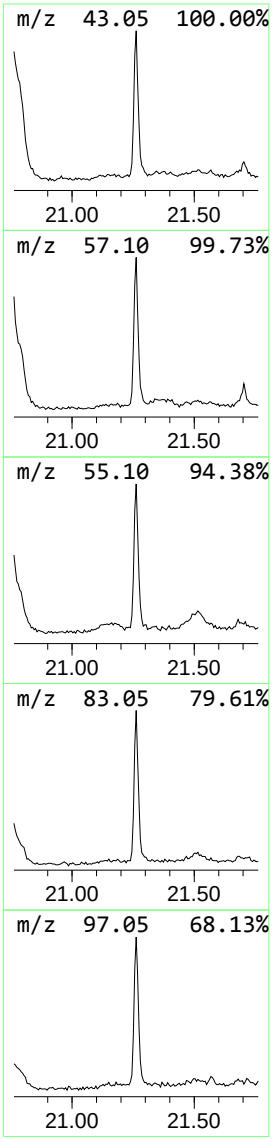
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic21.262 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.262	6.52 ng/ul	600862	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	94
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	1-Docosene	308	C22H44	001599-67-3	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	Pentacos-1-ene	350	C25H50	016980-85-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

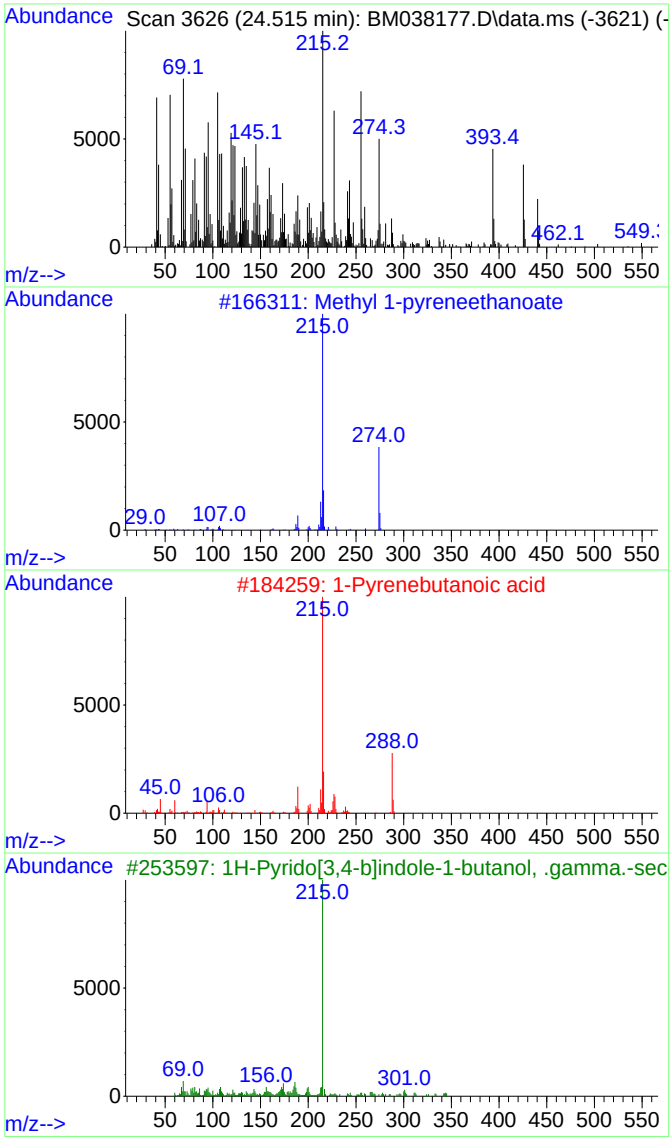
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

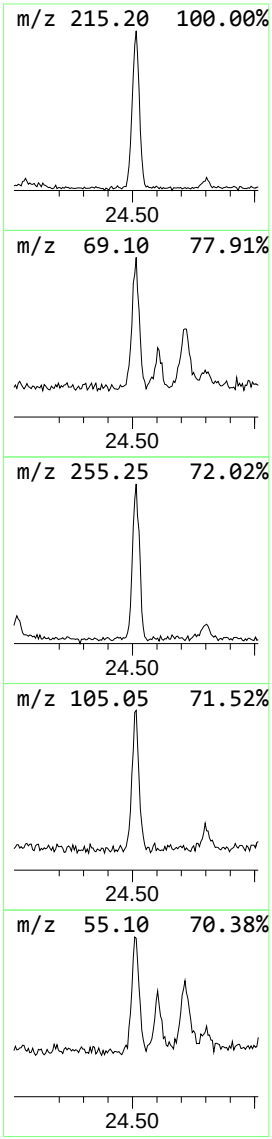
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Methyl 1-pyreneethanoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.515	8.97 ng/ul	857626	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 1-pyreneethanoate	274	C19H14O2	073654-19-0	53
2	1-Pyrenebutanoic acid	288	C20H16O2	003443-45-6	25
3	1H-Pyrido[3,4-b]indole-1-butanol...	344	C21H32N2O2	014358-60-2	25
4	6H-Benzo[d]pyrimido[5,4-b]thiopy...	215	C11H9N3S	1010267-44-6	15
5	Tricyclo[8.3.1.0(3,8)]tetradeca-...	215	C14H17NO	1000337-37-5	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038177.D
Acq On : 21 Dec 2022 18:14
Operator : CG/JU
Sample : N6014-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.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 ...	18.286	7.0	ng/ul	762193	4	17.409	2183700	20.0
Octadecanoic acid	19.550	3.0	ng/ul	274532	5	21.574	1841860	20.0
unknown-01	20.733	8.4	ng/ul	772196	5	21.574	1841860	20.0
Hexanedioic aci...	20.756	16.8	ng/ul	1548690	5	21.574	1841860	20.0
(DEL) Alkane: C...	21.262	6.5	ng/ul	600862	5	21.574	1841860	20.0
Methyl 1-pyrene...	24.515	9.0	ng/ul	857626	6	24.027	1911570	20.0