LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038144.D
Acq On : 20 Dec 2022 21:03
Operator : CG/JU
Sample : N6008-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXY3

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: BM038144.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	43	rVB3	9514	14804	0.27%	0.030%
2	3.840	108	111	125	rBV	103759	209761	3.76%	0.426%
3	4.163	163	166	172	rVB2	8546	12094	0.22%	0.025%
4	7.204	676	683	692	rBV	469575	741786	13.29%	1.508%
5	7.369	705	711	723	rVB	247726	379949	6.81%	0.772%
6	7.569	739	745	753	rBV	399435	637937	11.43%	1.297%
7	8.045	817	826	835	rBV	593147	921166	16.51%	1.872%
8	8.757	940	947	958	rBV	685826	1100949	19.73%	2.238%
9	9.216	1017	1025	1032	rBV	460565	723018	12.96%	1.470%
10	9.322	1036	1043	1048	rBV7	4180	9779	0.18%	0.020%
11	9.375	1048	1052	1057	rVB5	5478	7744	0.14%	0.016%
12	9.610	1086	1092	1097	rVB5	3601	7299	0.13%	0.015%
13	9.939	1138	1148	1156	rBV	424659	681005	12.20%	1.384%
14	10.157	1181	1185	1189	rVB6	5015	6488	0.12%	0.013%
15	10.480	1231	1240	1249	rBV	808019	1322912	23.71%	2.689%
16	10.863	1297	1305	1313	rBV	857522	1403191	25.15%	2.852%
17	10.998	1321	1328	1341	rBV	412382	726474	13.02%	1.477%
18	11.633	1430	1436	1443	rBV6	7420	15788	0.28%	0.032%
19	12.257	1538	1542	1549	rVB7	5636	10665	0.19%	0.022%
20	12.433	1568	1572	1578	rBV	14097	22329	0.40%	0.045%
21	13.486	1744	1751	1753	rBV4	8745	14118	0.25%	0.029%
22	14.080	1844	1852	1858	rBV	1647142	2128194	38.14%	4.326%
23	14.139	1860	1862	1866	rVV5	5773	6173	0.11%	0.013%
24	14.192	1866	1871	1874	rVV6	4680	6571	0.12%	0.013%
25	14.368	1894	1901	1913	rVB	1968045	2713541	48.63%	5.515%
26	14.545	1927	1931	1935	rVB5	8130	10518	0.19%	0.021%
27	14.674	1946	1953	1960	rVB	1309464	1867698	33.47%	3.796%
28	14.768	1965	1969	1976	rVB10	2953	6594	0.12%	0.013%
29	14.868	1980	1986	1999	rBV	544063	794704	14.24%	1.615%
30	15.027	2009	2013	2017	rBV5	13200	19463	0.35%	0.040%
31	15.068	2017	2020	2027	rVB5	19664	31201	0.56%	0.063%
32	15.445	2081	2084	2089	rVB6	5131	8101	0.15%	0.016%
33	15.492	2089	2092	2096	rVB5	7011	9890	0.18%	0.020%
34	15.598	2107	2110	2114	rBV6	5956	10139	0.18%	0.021%
35	15.662	2114	2121	2129	rVB	2465644	3441169	61.67%	6.994%
36	15.780	2134	2141	2150	rVV	601514	795140	14.25%	1.616%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038144.D
Acq On : 20 Dec 2022 21:03
Operator : CG/JU
Sample : N6008-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXY3

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	15.898	2157	2161	2166	rVB3	19614	30517	0.55%	0.062%
38	16.021	2174	2182	2190	rVB	95856	140495	2.52%	0.286%
39	16.209	2208	2214	2216	rBV6	3514	6810	0.12%	0.014%
40	16.227	2216	2217	2224	rVB7	6188	8989	0.16%	0.018%
41	16.357	2236	2239	2240	rBV2	9594	9360	0.17%	0.019%
42	16.374	2240	2242	2247	rVB4	17036	21735	0.39%	0.044%
43	16.504	2261	2264	2270	rVB6	7018	9963	0.18%	0.020%
44	16.798	2310	2314	2320	rBV6	26986	51869	0.93%	0.105%
45	17.145	2370	2373	2377	rBV4	7770	13629	0.24%	0.028%
46	17.198	2379	2382	2385	rVV3	10961	15581	0.28%	0.032%
47	17.292	2393	2398	2405	rBV2	49946	86026	1.54%	0.175%
48	17.356	2405	2409	2412	rBV4	21584	30108	0.54%	0.061%
49	17.409	2412	2418	2428	rBV	1673208	2335086	41.85%	4.746%
50	17.509	2429	2435	2441	rVV	2750342	3617456	64.83%	7.353%
51	17.751	2473	2476	2479	rBV4	19070	26707	0.48%	0.054%
52	17.921	2503	2505	2510	rVB5	14990	18827	0.34%	0.038%
53	18.168	2542	2547	2551	rBV3	43383	78313	1.40%	0.159%
54	18.233	2553	2558	2563	rBV	67860	105592	1.89%	0.215%
55	18.286	2563	2567	2578	rBV	787517	1088146	19.50%	2.212%
56	18.580	2613	2617	2623	rBV7	28917	60661	1.09%	0.123%
57	18.633	2623	2626	2631	rVB5	26761	37573	0.67%	0.076%
58	19.021	2689	2692	2698	rVB8	22313	32587	0.58%	0.066%
59	19.198	2719	2722	2729	rBV9	23674	45180	0.81%	0.092%
60	19.356	2746	2749	2754	rVB3	38816	51367	0.92%	0.104%
61	19.415	2755	2759	2761	rBV4	136225	200217	3.59%	0.407%
62	19.456	2764	2766	2777	rVV	183158	282852	5.07%	0.575%
63	19.556	2779	2783	2796	rVV	228955	358277	6.42%	0.728%
64	19.792	2817	2823	2834	rBV	3400482	4579835	82.07%	9.309%
65	20.286	2904	2907	2909	rBV3	48999	63039	1.13%	0.128%
66	20.756	2983	2987	2991	rBV2	279765	365501	6.55%	0.743%
67	21.262	3069	3073	3084	rVB	848358	1026962	18.40%	2.087%
68	21.574	3122	3126	3131	rVB	1742821	2330858	41.77%	4.738%
69	22.197	3229	3232	3241	rVB2	281542	419565	7.52%	0.853%
70	23.868	3510	3516	3524	rVB2	1786790	3377946	60.54%	6.866%
71	24.027	3537	3543	3551	rVB2	971521	1872799	33.56%	3.807%
72	28.550	4302	4312	4329	rVB3	1563236	5580071	100.00%	11.342%

Sum of corrected areas: 49198851

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
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Acq On : 20 Dec 2022 21:03
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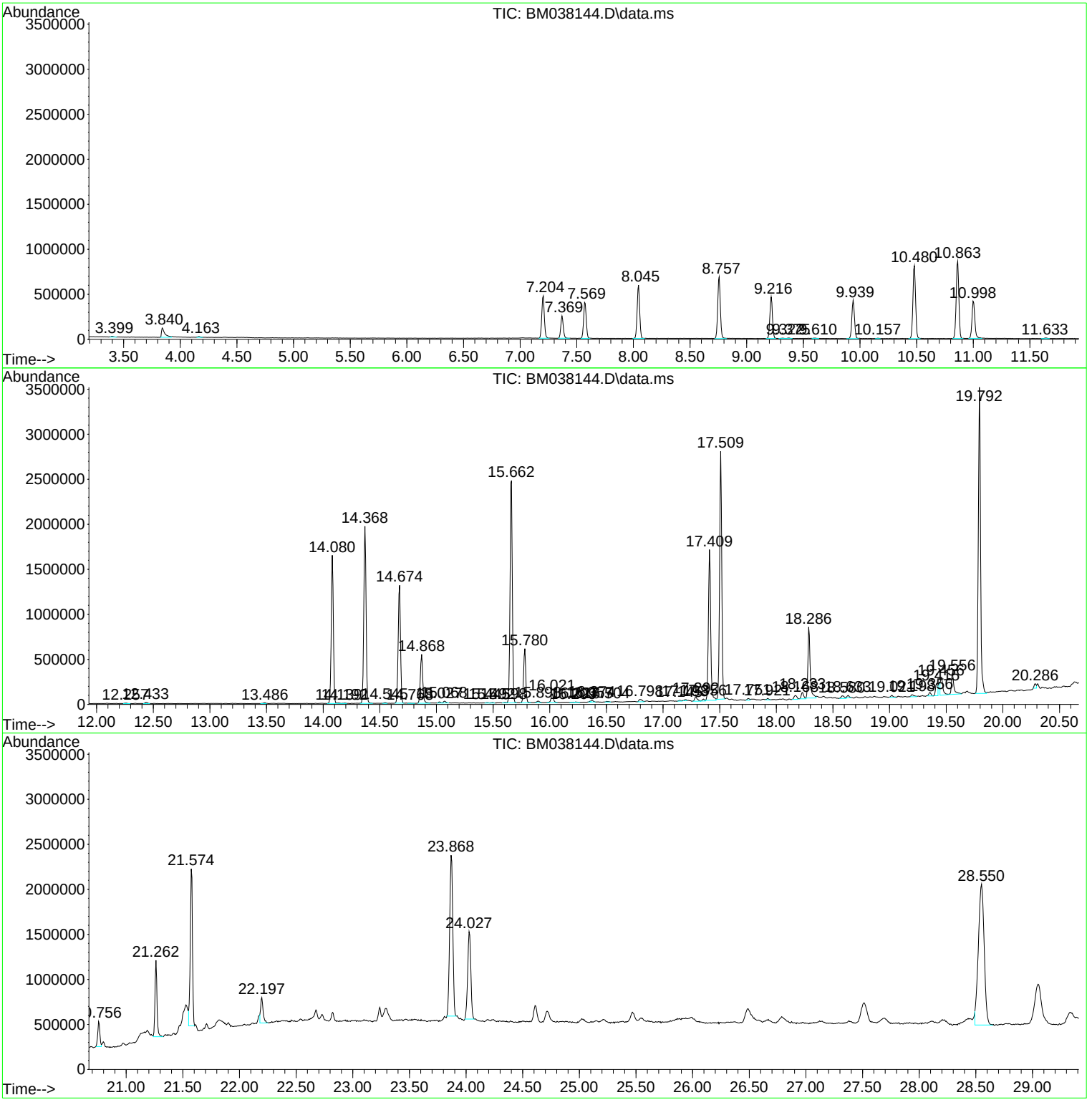
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXY3

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 : BM038144.D
Acq On : 20 Dec 2022 21:03
Operator : CG/JU
Sample : N6008-21
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

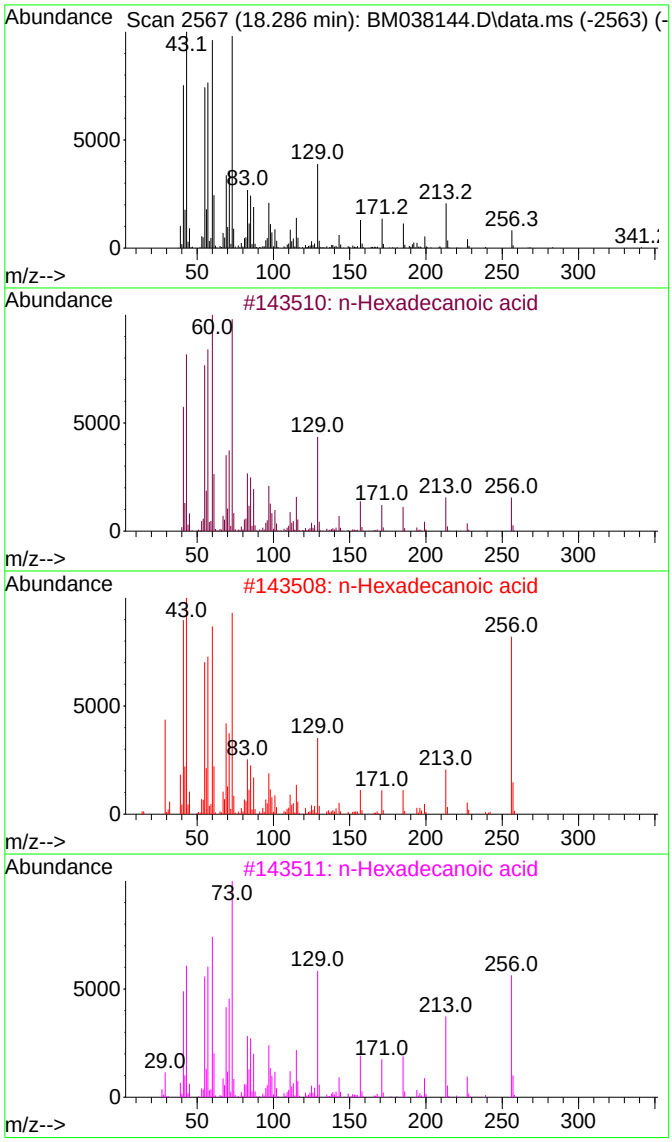
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

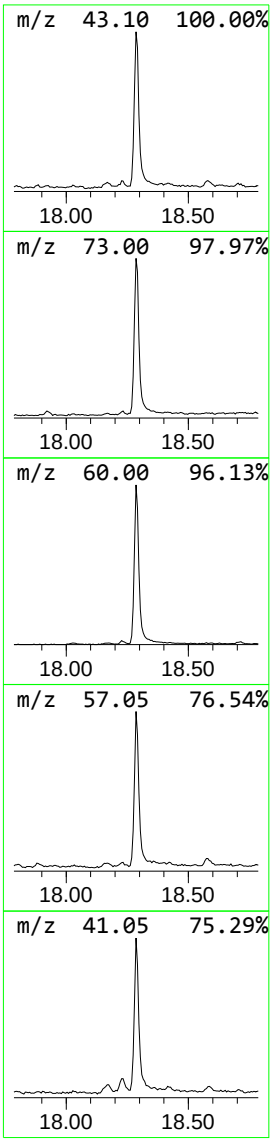
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	9.32 ng/ul	1088150	Phenanthrene-d10	17.409

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	97
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5	Tridecanoic acid	214	C13H26O2	000638-53-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038144.D
Acq On : 20 Dec 2022 21:03
Operator : CG/JU
Sample : N6008-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXY3

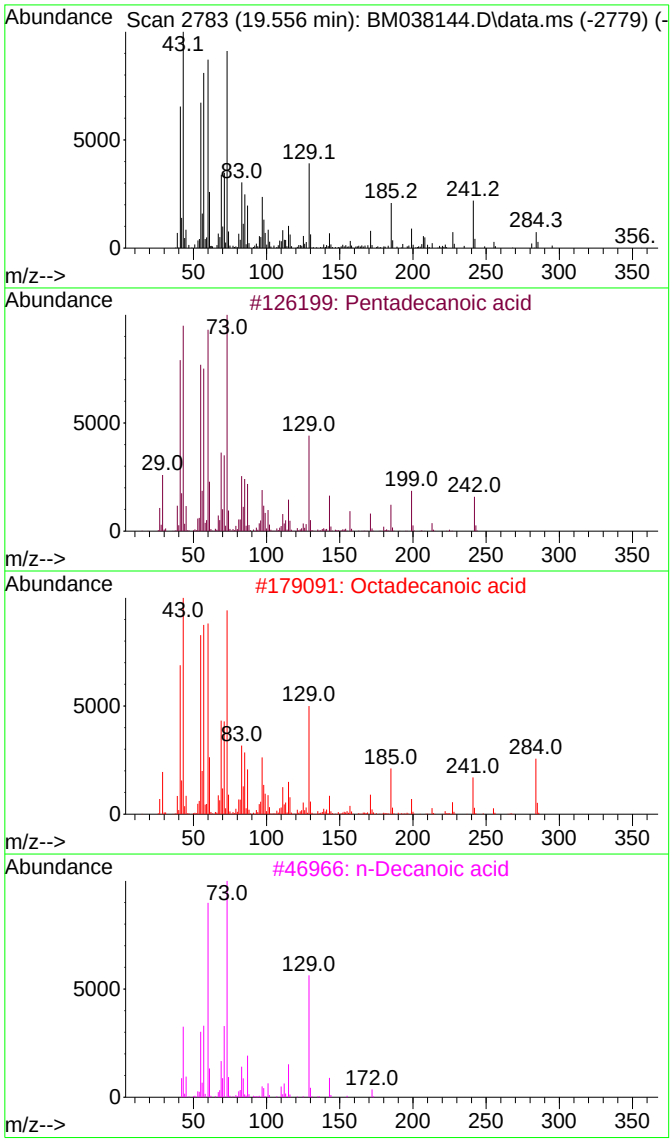
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

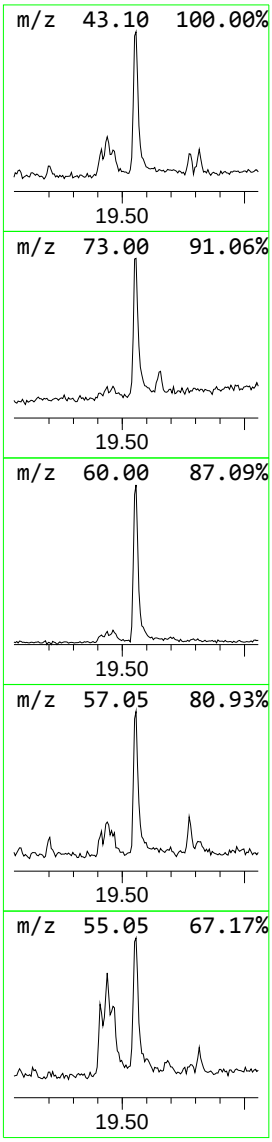
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.556	3.07 ng/ul	358277	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
2	Octadecanoic acid	284	C18H36O2	000057-11-4	94
3	n-Decanoic acid	172	C10H20O2	000334-48-5	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038144.D
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Operator : CG/JU
Sample : N6008-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXY3

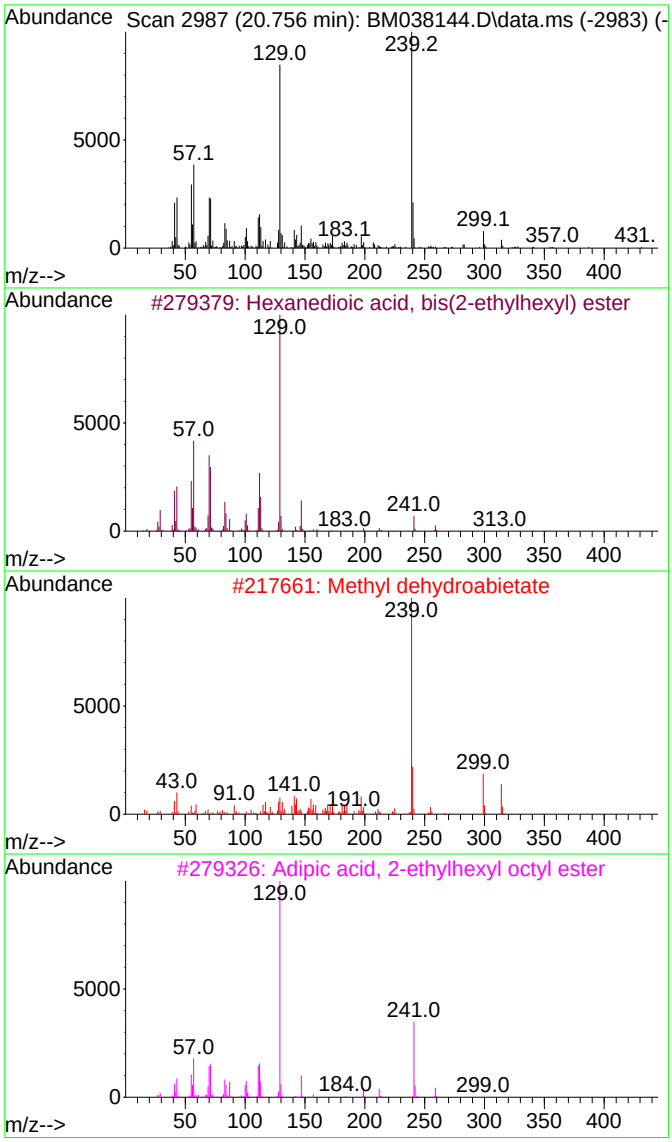
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

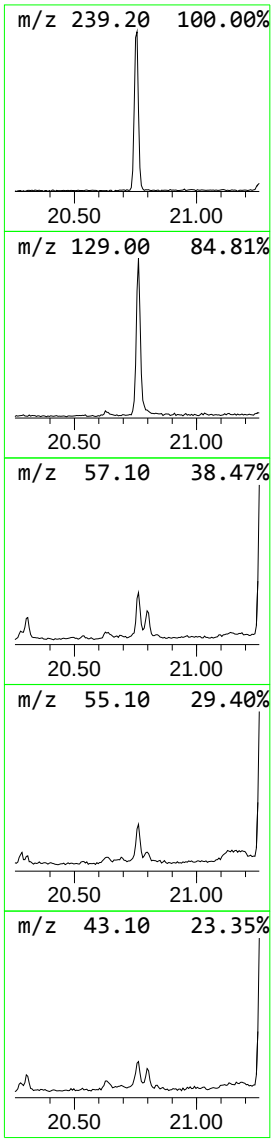
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexanedioic acid, bis(2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	3.14 ng/ul	365501	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	55
2	Methyl dehydroabietate	314	C21H30O2	001235-74-1	50
3	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	49
4	Adipic acid, 2-ethylhexyl nonyl ...	384	C23H44O4	1000324-48-7	46
5	Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
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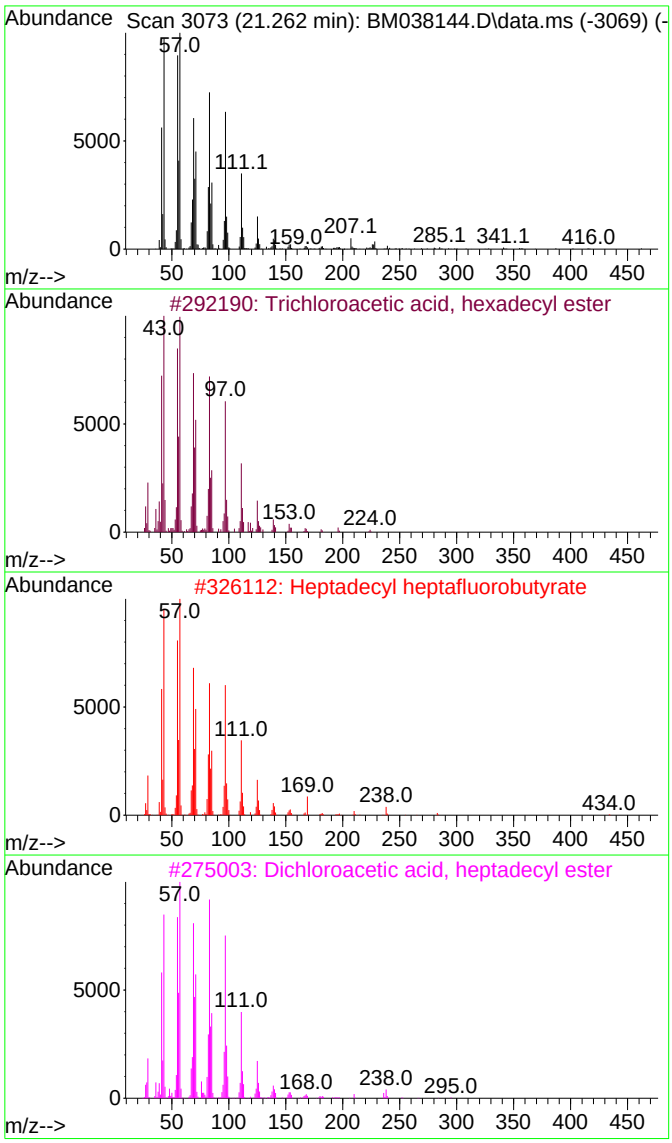
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

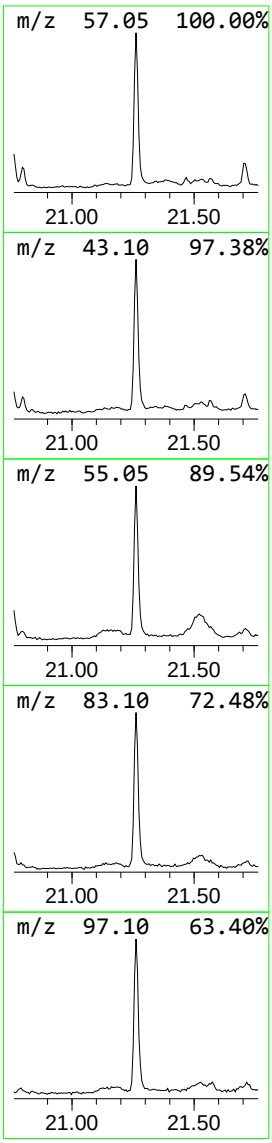
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.262	8.81 ng/ul	1026960	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





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Misc :
ALS Vial : 11 Sample Multiplier: 1

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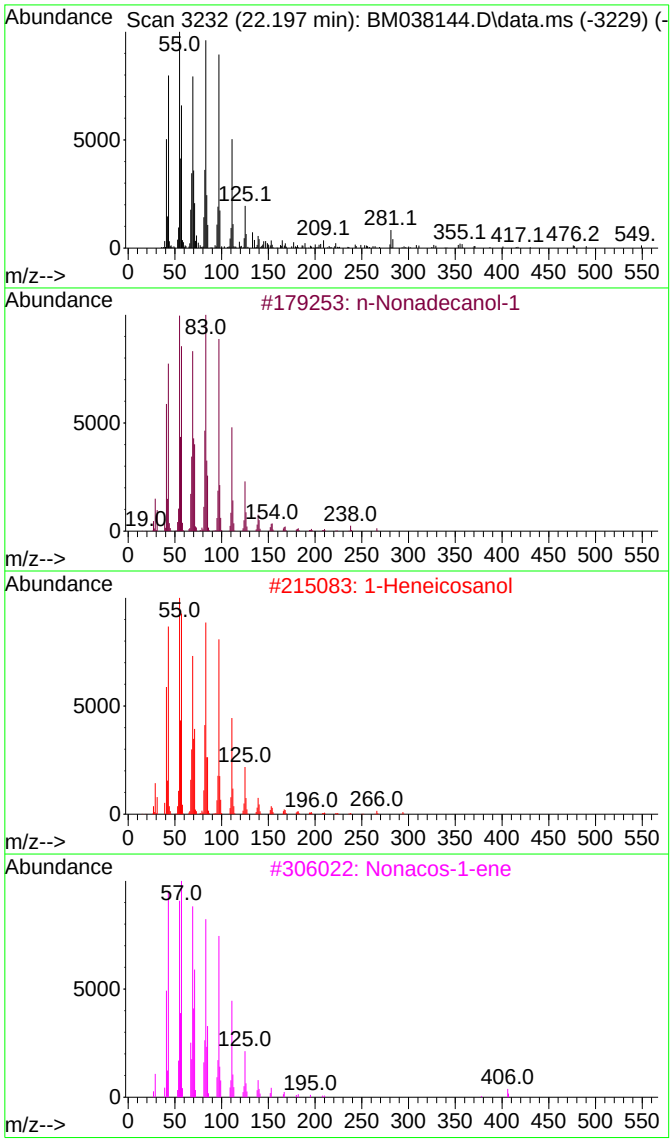
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

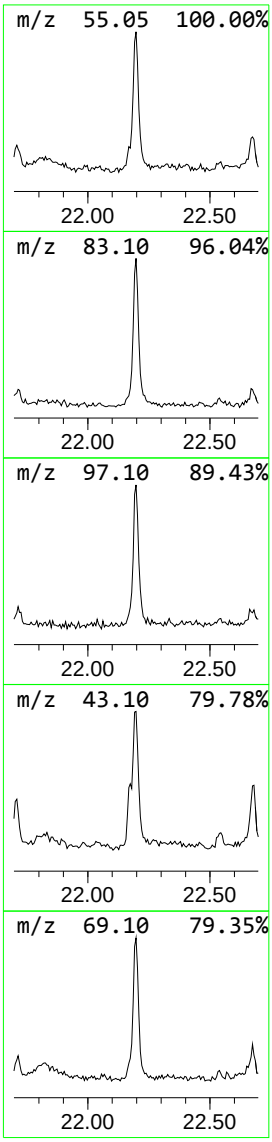
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.197	3.60 ng/ul	419565	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	Nonacos-1-ene	406	C29H58	018835-35-3	91
4	1-Tetracosene	336	C24H48	010192-32-2	83
5	1-Docosene	308	C22H44	001599-67-3	78





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Sample : N6008-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXY3

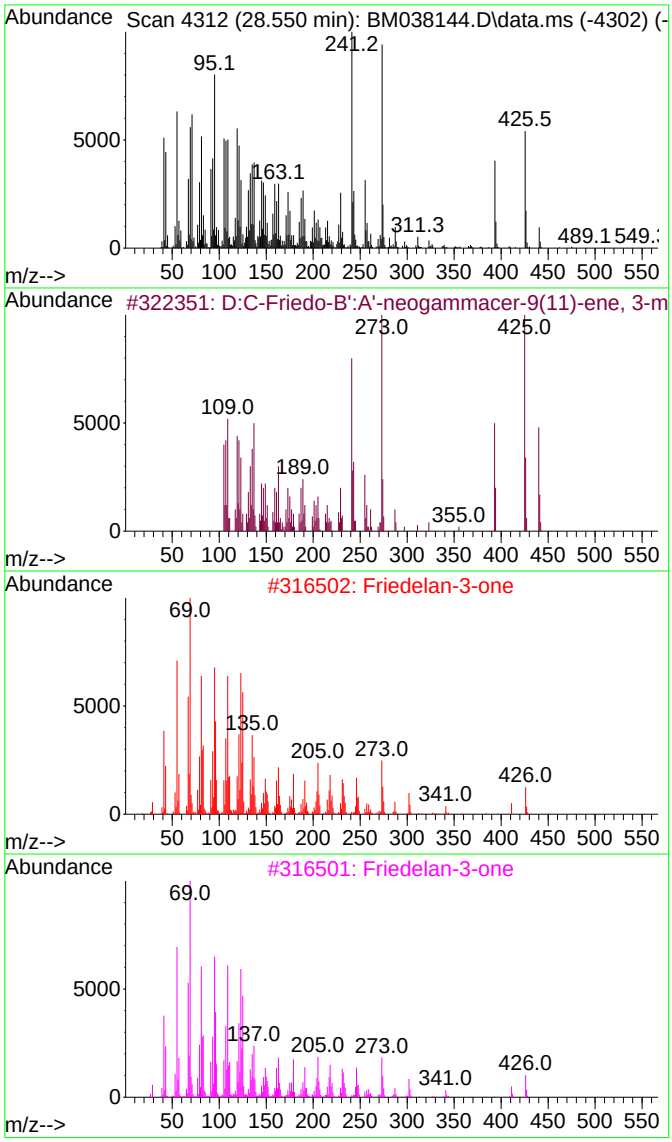
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

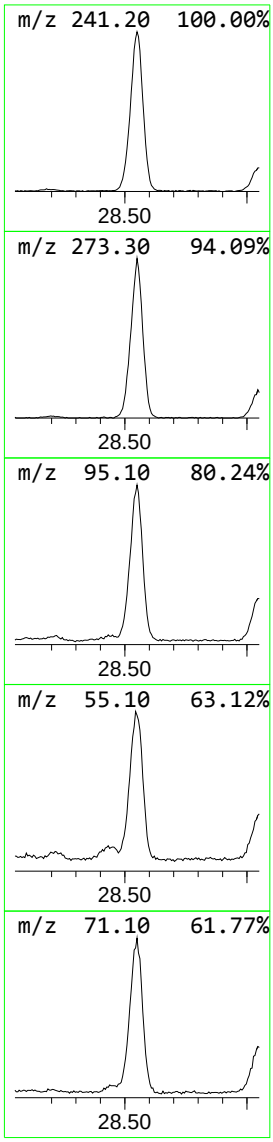
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.550	59.59 ng/ul	5580070	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	52
2	Friedelan-3-one	426	C30H50O	000559-74-0	38
3	Friedelan-3-one	426	C30H50O	000559-74-0	30
4	Tolcapone	273	C14H11NO5	134308-13-7	25
5	2-(Pentadec-14-yn-1-yl)furan	274	C19H30O	1000465-05-2	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038144.D
Acq On : 20 Dec 2022 21:03
Operator : CG/JU
Sample : N6008-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXY3

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	9.3	ng/ul	1088150	4	17.409	2335090	20.0
Pentadecanoic acid	19.556	3.1	ng/ul	358277	5	21.574	2330860	20.0
Hexanedioic aci...	20.756	3.1	ng/ul	365501	5	21.574	2330860	20.0
Trichloroacetic...	21.262	8.8	ng/ul	1026960	5	21.574	2330860	20.0
n-Nonadecanol-1	22.197	3.6	ng/ul	419565	5	21.574	2330860	20.0
D:C-Friedo-B':A...	28.550	59.6	ng/ul	5580070	6	24.027	1872800	20.0