LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101724\
Data File : BM048116.D
Acq On : 17 Oct 2024 21:42
Operator : RC/JU
Sample : P4380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E27H9

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-BM101724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM048116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.240	39	43	54	rVB	51401	86335	0.42%	0.100%
2	3.657	110	114	128	rBV	163834	307791	1.49%	0.356%
3	3.975	164	168	173	rVB	17161	24944	0.12%	0.029%
4	4.904	321	326	334	rVB3	20812	33906	0.16%	0.039%
5	5.293	386	392	400	rVB4	12037	23985	0.12%	0.028%
6	6.128	527	534	536	rBV6	13359	21983	0.11%	0.025%
7	6.157	536	539	544	rVB2	17809	27279	0.13%	0.032%
8	6.945	665	673	690	rBV	253038	506440	2.44%	0.585%
9	7.104	693	700	712	rBV	702169	1135810	5.48%	1.312%
10	7.304	728	734	745	rBV	838396	1409550	6.80%	1.629%
11	7.769	806	813	821	rBV	800615	1339921	6.47%	1.548%
12	7.839	821	825	831	rVB5	11903	23761	0.11%	0.027%
13	8.145	869	877	884	rBV	45159	77997	0.38%	0.090%
14	8.304	893	904	912	rBV2	49471	124743	0.60%	0.144%
15	8.481	927	934	942	rBV	739196	1269008	6.12%	1.466%
16	8.928	1002	1010	1018	rBV	739840	1293928	6.24%	1.495%
17	9.492	1101	1106	1111	rBV2	38883	59743	0.29%	0.069%
18	9.645	1124	1132	1142	rBV	658235	1118799	5.40%	1.293%
19	9.975	1182	1188	1196	rVB	10061	26867	0.13%	0.031%
20	10.186	1217	1224	1240	rBV	1029516	1889350	9.12%	2.183%
21	10.563	1280	1288	1291	rBV	1050107	1889541	9.12%	2.183%
22	10.616	1291	1297	1305	rVV	11403877	20725307	100.00%	23.948%
23	10.698	1305	1311	1331	rVB2	803500	1930111	9.31%	2.230%
24	11.839	1501	1505	1511	rBV4	14112	28749	0.14%	0.033%
25	12.145	1555	1557	1561	rVV	17717	25747	0.12%	0.030%
26	12.227	1561	1571	1585	rVV2	529374	1060665	5.12%	1.226%
27	12.374	1586	1596	1601	rVV5	49138	116263	0.56%	0.134%
28	12.445	1602	1608	1616	rVB	338917	561876	2.71%	0.649%
29	13.245	1733	1744	1754	rBV2	163678	299806	1.45%	0.346%
30	13.439	1773	1777	1785	rVV2	11449	23181	0.11%	0.027%
31	13.568	1791	1799	1808	rBV3	34362	102312	0.49%	0.118%
32	13.727	1819	1826	1832	rBV2	53563	111416	0.54%	0.129%
33	13.815	1832	1841	1851	rVB	1889284	2700109	13.03%	3.120%
34	13.963	1862	1866	1869	rBV	16907	23622	0.11%	0.027%
35	14.098	1879	1889	1901	rBV	2245257	3483924	16.81%	4.026%
36	14.404	1933	1941	1947	rBV	1578474	2423244	11.69%	2.800%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101724\
Data File : BM048116.D
Acq On : 17 Oct 2024 21:42
Operator : RC/JU
Sample : P4380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E27H9

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-BM101724.MA.M
Title : SVOA CALIBRATION

37	14.468	1947	1952	1961	rVB	1864465	2790285	13.46%	3.224%
38	14.539	1961	1964	1969	rVB	20363	28793	0.14%	0.033%
39	14.627	1972	1979	1992	rBV2	158704	369633	1.78%	0.427%
40	14.804	2004	2009	2020	rVB	500133	752078	3.63%	0.869%
41	14.951	2031	2034	2040	rVV	13311	21023	0.10%	0.024%
42	15.021	2040	2046	2052	rVB10	17753	37139	0.18%	0.043%
43	15.398	2104	2110	2115	rBV	2840564	3996913	19.29%	4.618%
44	15.451	2115	2119	2126	rVB	620074	922514	4.45%	1.066%
45	15.521	2126	2131	2139	rBV	902496	1287921	6.21%	1.488%
46	15.762	2165	2172	2178	rBV	740902	1049079	5.06%	1.212%
47	15.892	2191	2194	2202	rVB3	28764	64269	0.31%	0.074%
48	15.968	2203	2207	2213	rVB9	22710	35204	0.17%	0.041%
49	16.027	2214	2217	2224	rVB5	17129	24857	0.12%	0.029%
50	16.127	2224	2234	2239	rBV3	184911	372731	1.80%	0.431%
51	16.645	2317	2322	2329	rBV	172615	271395	1.31%	0.314%
52	16.780	2341	2345	2347	rBV3	20436	27465	0.13%	0.032%
53	16.968	2371	2377	2384	rVB2	66166	128996	0.62%	0.149%
54	17.098	2394	2399	2401	rBV	153591	217444	1.05%	0.251%
55	17.145	2401	2407	2411	rVV	1808978	2755953	13.30%	3.185%
56	17.186	2411	2414	2419	rVV	583564	822426	3.97%	0.950%
57	17.245	2419	2424	2435	rVV2	2992901	4501424	21.72%	5.201%
58	17.345	2438	2441	2451	rVB2	53045	91665	0.44%	0.106%
59	17.551	2471	2476	2483	rVB	322026	480007	2.32%	0.555%
60	18.039	2554	2559	2568	rBV	587191	938291	4.53%	1.084%
61	18.221	2585	2590	2599	rVB	128687	219163	1.06%	0.253%
62	19.097	2736	2739	2746	rVB2	55837	78457	0.38%	0.091%
63	19.174	2749	2752	2753	rVV	48951	57300	0.28%	0.066%
64	19.203	2753	2757	2764	rVB	379652	539765	2.60%	0.624%
65	19.292	2769	2772	2774	rVV	183779	250063	1.21%	0.289%
66	19.315	2774	2776	2787	rVB2	285263	450455	2.17%	0.521%
67	19.533	2808	2813	2827	rBV	3495046	5409834	26.10%	6.251%
68	21.044	3068	3070	3079	rVB3	176987	246163	1.19%	0.284%
69	21.374	3120	3126	3137	rBV	1844386	2840612	13.71%	3.282%
70	22.744	3355	3359	3367	rVB5	192160	375772	1.81%	0.434%
71	24.156	3590	3599	3609	rVB	1952156	4803124	23.18%	5.550%
72	24.356	3626	3633	3644	rVB	1217156	2975350	14.36%	3.438%

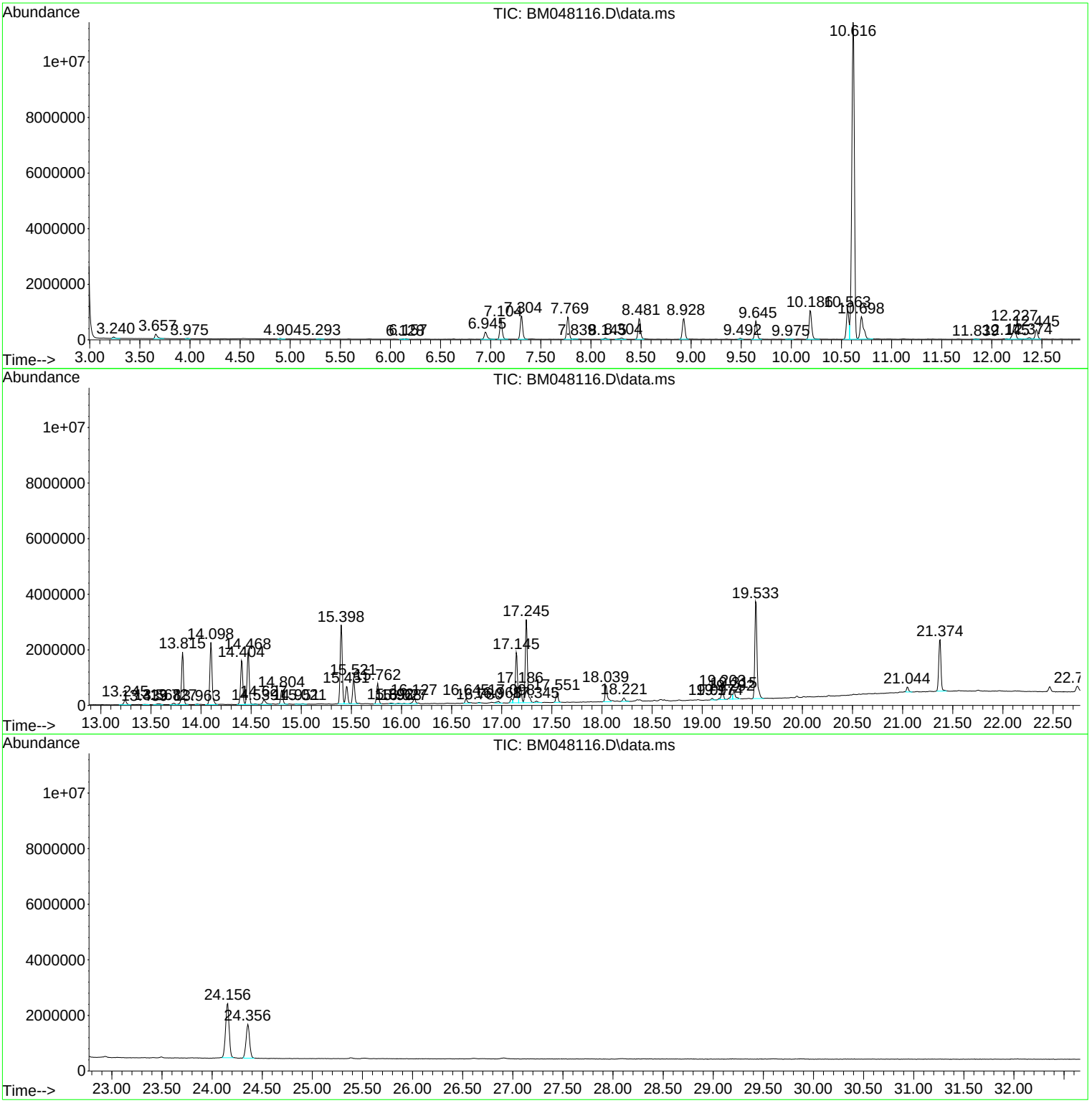
Sum of corrected areas: 86541576

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101724\
Data File : BM048116.D
Acq On : 17 Oct 2024 21:42
Operator : RC/JU
Sample : P4380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E27H9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101724.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\BM101724\
Data File : BM048116.D
Acq On : 17 Oct 2024 21:42
Operator : RC/JU
Sample : P4380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E27H9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101724.MA.M
Quant Title : SVOA CALIBRATION

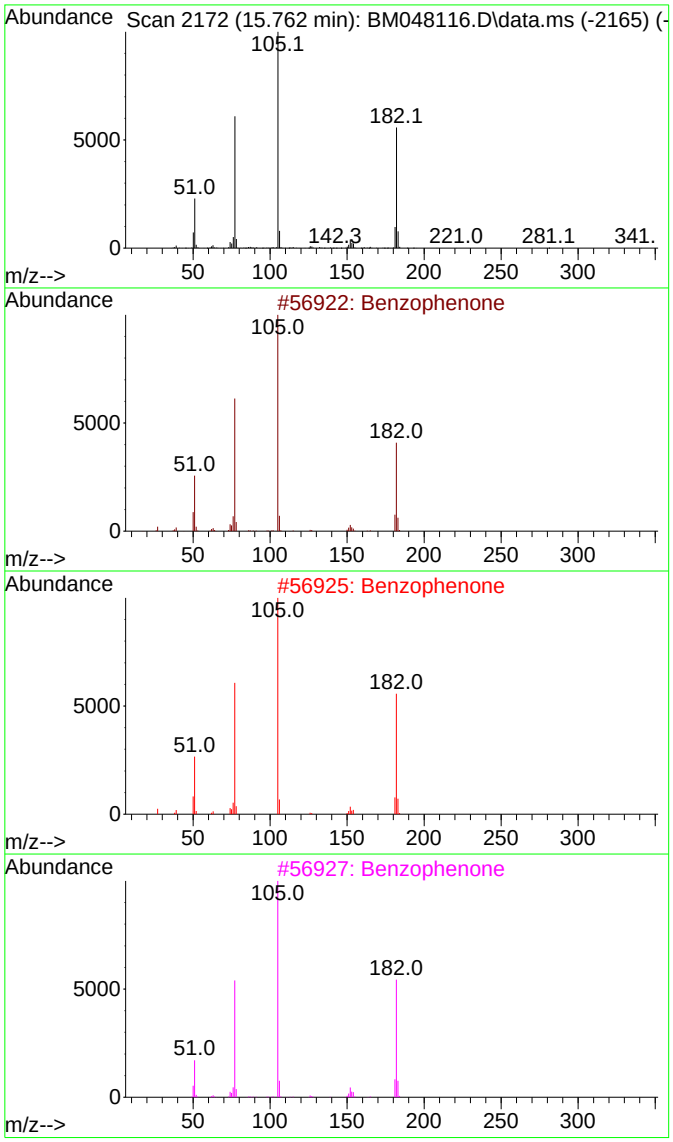
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

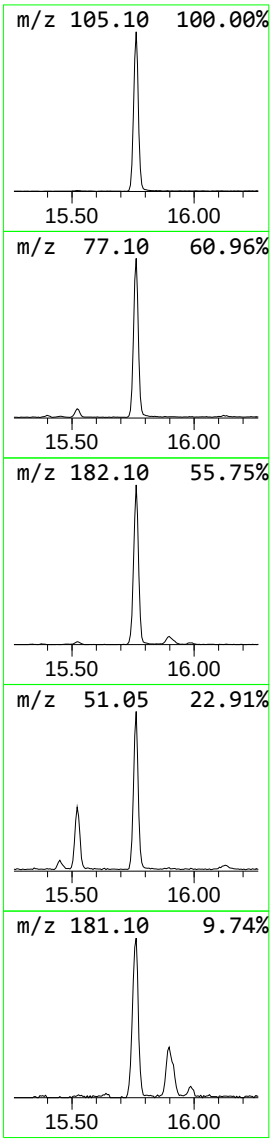
****

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	8.66 ng/ul	1049080	Acenaphthene-d10	14.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzophenone	182	C13H10O	000119-61-9	96
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	93
5	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101724\
Data File : BM048116.D
Acq On : 17 Oct 2024 21:42
Operator : RC/JU
Sample : P4380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E27H9

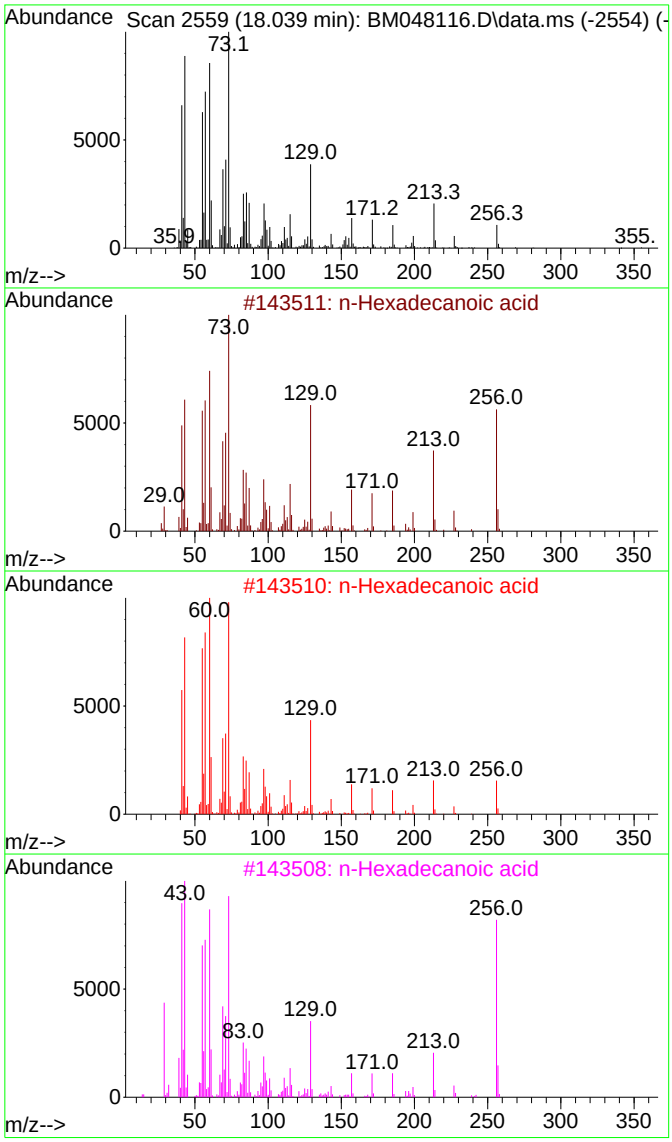
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101724.MA.M
Quant Title : SVOA CALIBRATION

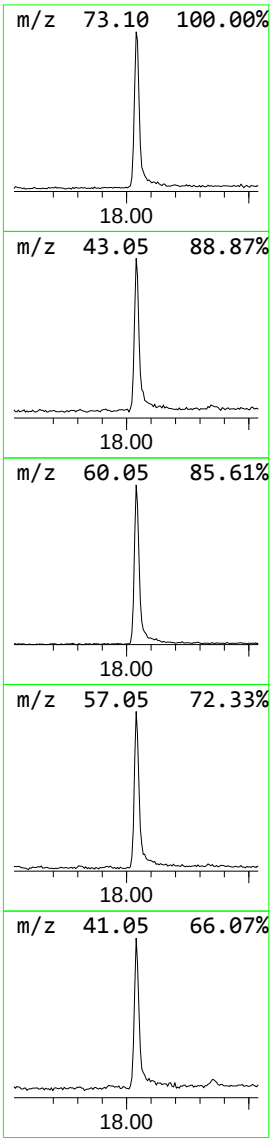
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	6.81 ng/ul	938291	Phenanthrene-d10	17.145

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	Tridecanoic acid	214	C13H26O2	000638-53-9	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101724\
Data File : BM048116.D
Acq On : 17 Oct 2024 21:42
Operator : RC/JU
Sample : P4380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E27H9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101724.MA.M
Quant Title : SVOA CALIBRATION

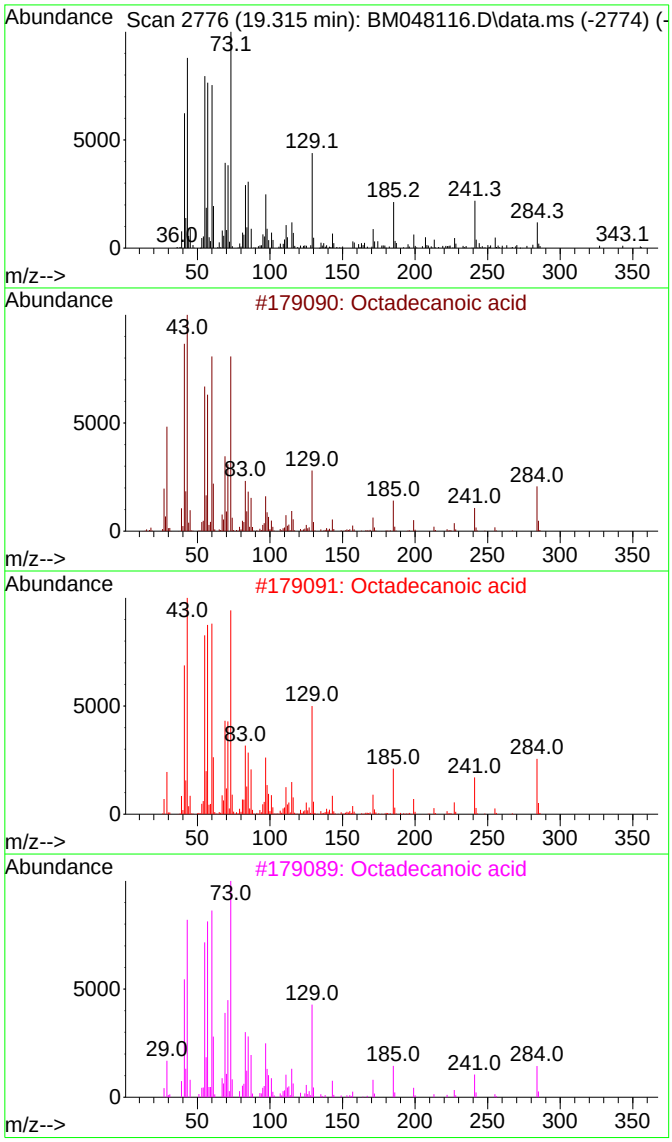
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

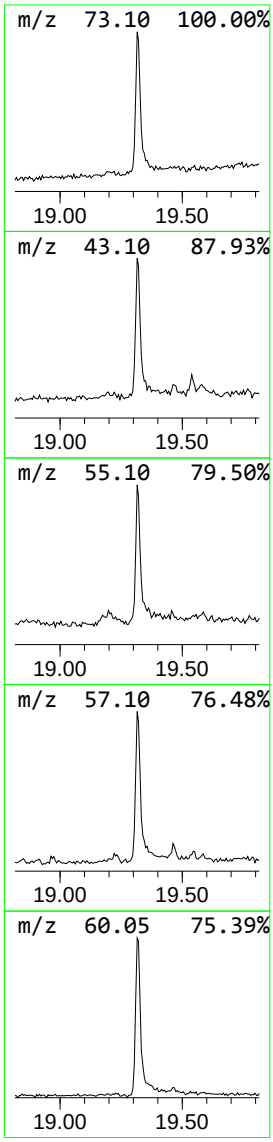
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.315	3.17 ng/ul	450455	Chrysene-d12	21.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Octadecanoic acid	284	C18H36O2	000057-11-4	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Octadecanoic acid	284	C18H36O2	000057-11-4	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101724\
Data File : BM048116.D
Acq On : 17 Oct 2024 21:42
Operator : RC/JU
Sample : P4380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E27H9

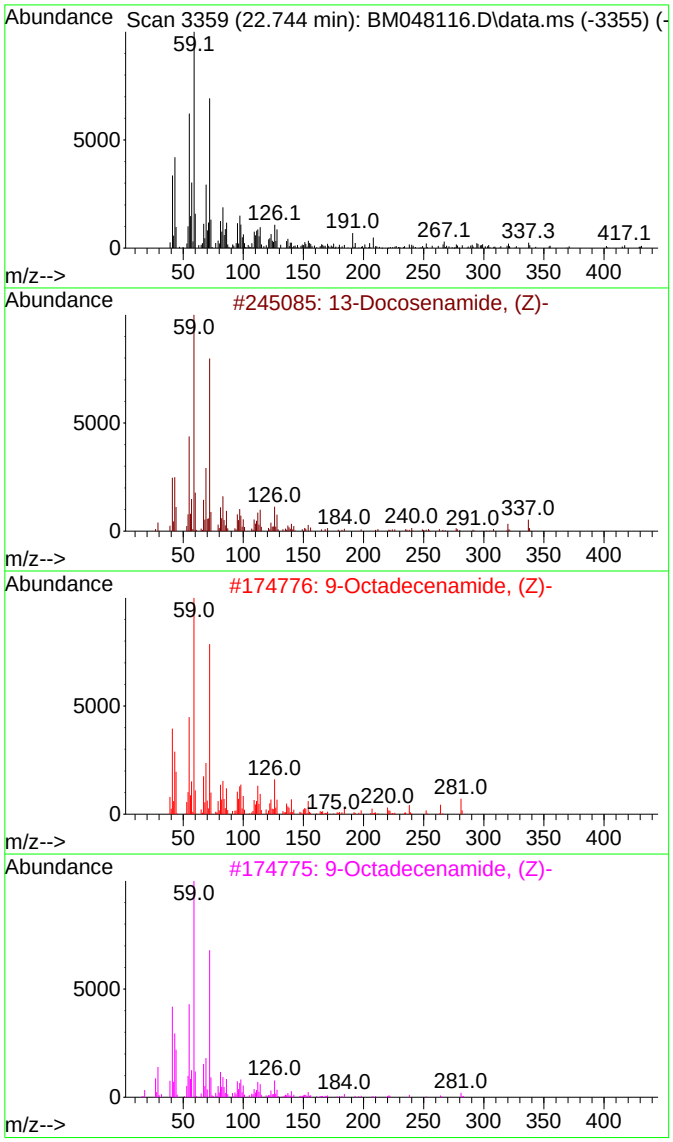
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101724.MA.M
Quant Title : SVOA CALIBRATION

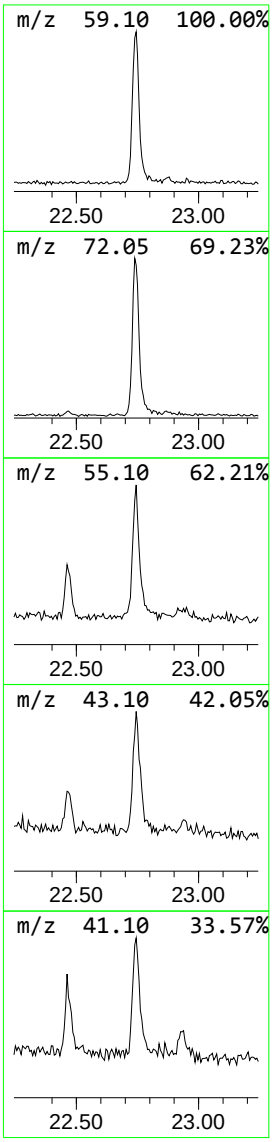
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.744	2.65 ng/ul	375772	Chrysene-d12	21.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	97
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101724\
Data File : BM048116.D
Acq On : 17 Oct 2024 21:42
Operator : RC/JU
Sample : P4380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E27H9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101724.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
Benzophenone	15.762	8.7	ng/ul	1049080	3	14.404	2423240	20.0
n-Hexadecanoic ...	18.039	6.8	ng/ul	938291	4	17.145	2755950	20.0
Octadecanoic acid	19.315	3.2	ng/ul	450455	5	21.374	2840610	20.0
13-Docosenamide...	22.744	2.6	ng/ul	375772	5	21.374	2840610	20.0