LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

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_P\Methods\SFAM-EPA-BP100724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP022680.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.187	30	34	40	rVB	24887	33011	0.90%	0.096%
2	3.599	99	104	114	rBV	281156	471833	12.87%	1.377%
3	3.911	153	157	163	rVB4	4946	8514	0.23%	0.025%
4	4.281	216	220	225	rVB7	2506	4682	0.13%	0.014%
5	4.464	247	251	255	rBV5	5161	7874	0.21%	0.023%
6	4.517	257	260	268	rVB3	4021	6983	0.19%	0.020%
7	4.828	309	313	317	rBV5	3169	5840	0.16%	0.017%
8	4.875	317	321	328	rVB8	4105	7314	0.20%	0.021%
9	5.493	420	426	437	rVB2	20957	42031	1.15%	0.123%
10	5.705	455	462	467	rBV5	6138	10945	0.30%	0.032%
11	5.811	476	480	486	rVB3	7999	13002	0.35%	0.038%
12	6.022	510	516	521	rBV	63125	104261	2.84%	0.304%
13	6.064	521	523	529	rVB5	12506	19900	0.54%	0.058%
14	6.193	542	545	549	rBV5	3449	5182	0.14%	0.015%
15	6.258	549	556	563	rVB4	12831	34787	0.95%	0.102%
16	6.428	578	585	587	rBV7	5074	8691	0.24%	0.025%
17	6.469	587	592	596	rVV	31738	50359	1.37%	0.147%
18	6.516	596	600	607	rVV2	44661	65614	1.79%	0.191%
19	6.599	607	614	619	rVB6	4866	9319	0.25%	0.027%
20	6.840	649	655	670	rVV	407249	700423	19.11%	2.044%
21	6.987	674	680	693	rVB	287981	475155	12.97%	1.387%
22	7.187	706	714	733	rVB	398475	662877	18.09%	1.935%
23	7.340	733	740	745	rBV8	2737	5111	0.14%	0.015%
24	7.646	785	792	800	rBV	329294	517368	14.12%	1.510%
25	7.722	801	805	809	rVB7	2814	4625	0.13%	0.013%
26	8.352	905	912	922	rBV	539669	880561	24.03%	2.570%
27	8.787	978	986	1002	rBV	407180	685874	18.72%	2.002%
28	8.952	1011	1014	1018	rVB6	3145	3962	0.11%	0.012%
29	9.187	1050	1054	1059	rBV4	9775	15751	0.43%	0.046%
30	9.346	1074	1081	1088	rBV2	29739	49393	1.35%	0.144%
31	9.499	1099	1107	1113	rBV	346660	612489	16.71%	1.788%
32	9.552	1113	1116	1123	rVB2	19693	35779	0.98%	0.104%
33	9.775	1148	1154	1160	rBV2	2011	5266	0.14%	0.015%
34	10.034	1191	1198	1221	rBV	513986	971699	26.51%	2.836%
35	10.399	1249	1260	1271	rBV	425329	698460	19.06%	2.038%
36	10.540	1277	1284	1303	rBV	454794	852346	23.26%	2.488%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

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_P\Methods\SFAM-EPA-BP100724.MA.M
Title : SVOA CALIBRATION

37	10.946	1346	1353	1364	rBV6	9566	22843	0.62%	0.067%
38	11.216	1395	1399	1403	rBV7	2853	4656	0.13%	0.014%
39	11.669	1469	1476	1480	rBV2	6303	10614	0.29%	0.031%
40	11.993	1525	1531	1542	rVB2	9952	17620	0.48%	0.051%
41	12.604	1629	1635	1641	rBV9	2260	4892	0.13%	0.014%
42	12.693	1646	1650	1660	rVB6	4517	7435	0.20%	0.022%
43	13.075	1710	1715	1722	rVB8	4027	7578	0.21%	0.022%
44	13.216	1735	1739	1748	rVB8	3784	7561	0.21%	0.022%
45	13.575	1792	1800	1802	rBV8	1956	3671	0.10%	0.011%
46	13.663	1808	1815	1825	rBV	1191714	1649214	45.00%	4.813%
47	13.946	1851	1863	1876	rBV	1167198	1770880	48.32%	5.168%
48	14.163	1896	1900	1904	rVB5	5464	6462	0.18%	0.019%
49	14.257	1908	1916	1925	rBV	734957	1075931	29.36%	3.140%
50	14.381	1933	1937	1940	rBV4	3014	4013	0.11%	0.012%
51	14.504	1952	1958	1974	rBV	312580	669138	18.26%	1.953%
52	14.698	1986	1991	1998	rVB8	14783	27406	0.75%	0.080%
53	15.069	2049	2054	2058	rBV7	3463	7318	0.20%	0.021%
54	15.263	2082	2087	2099	rVB	1915862	2376950	64.86%	6.937%
55	15.398	2104	2110	2126	rBV	415402	694789	18.96%	2.028%
56	15.522	2126	2131	2141	rVV7	9214	19951	0.54%	0.058%
57	15.640	2145	2151	2158	rVV	404176	480545	13.11%	1.402%
58	15.687	2158	2159	2165	rVB6	3353	3810	0.10%	0.011%
59	16.328	2261	2268	2270	rBV6	2278	4640	0.13%	0.014%
60	16.469	2289	2292	2297	rVB6	8154	11604	0.32%	0.034%
61	16.539	2299	2304	2308	rBV7	2978	5557	0.15%	0.016%
62	16.834	2350	2354	2360	rBV10	4159	8097	0.22%	0.024%
63	16.881	2360	2362	2367	rVB6	2639	3683	0.10%	0.011%
64	16.981	2373	2379	2385	rVB6	4080	7979	0.22%	0.023%
65	17.057	2385	2392	2399	rBV	1103866	1449850	39.56%	4.231%
66	17.163	2402	2410	2421	rBV	1667111	2731178	74.52%	7.971%
67	17.251	2421	2425	2427	rVV6	8382	12021	0.33%	0.035%
68	17.287	2427	2431	2435	rVB6	8520	13462	0.37%	0.039%
69	17.875	2527	2531	2537	rBV7	12036	17214	0.47%	0.050%
70	17.998	2547	2552	2562	rBV	691323	846953	23.11%	2.472%
71	18.310	2602	2605	2610	rVB3	10535	13509	0.37%	0.039%
72	18.698	2668	2671	2675	rBV6	9346	13296	0.36%	0.039%
73	19.098	2735	2739	2743	rBV2	25486	34775	0.95%	0.101%
74	19.175	2747	2752	2756	rBV2	35461	73133	2.00%	0.213%
75	19.216	2756	2759	2770	rVV6	50770	97701	2.67%	0.285%
76	19.333	2774	2779	2791	rBV	174657	259645	7.08%	0.758%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

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_P\Methods\SFAM-EPA-BP100724.MA.M
Title : SVOA CALIBRATION

77	19.545	2809	2815	2825	rBV	2300215	3336154	91.03%	9.737%
78	20.657	3002	3004	3008	rVB3	22863	21264	0.58%	0.062%
79	21.180	3088	3093	3108	rVB2	165891	379790	10.36%	1.108%
80	21.410	3128	3132	3137	rVB	49582	67074	1.83%	0.196%
81	21.504	3141	3148	3160	rVV	1013647	1779310	48.55%	5.193%
82	23.027	3402	3407	3418	rVB2	213803	448116	12.23%	1.308%
83	23.251	3440	3445	3454	rVB2	88751	189642	5.17%	0.553%
84	24.527	3653	3662	3673	rVB	1419687	3664781	100.00%	10.696%
85	24.757	3691	3701	3712	rVB2	575851	1812491	49.46%	5.290%

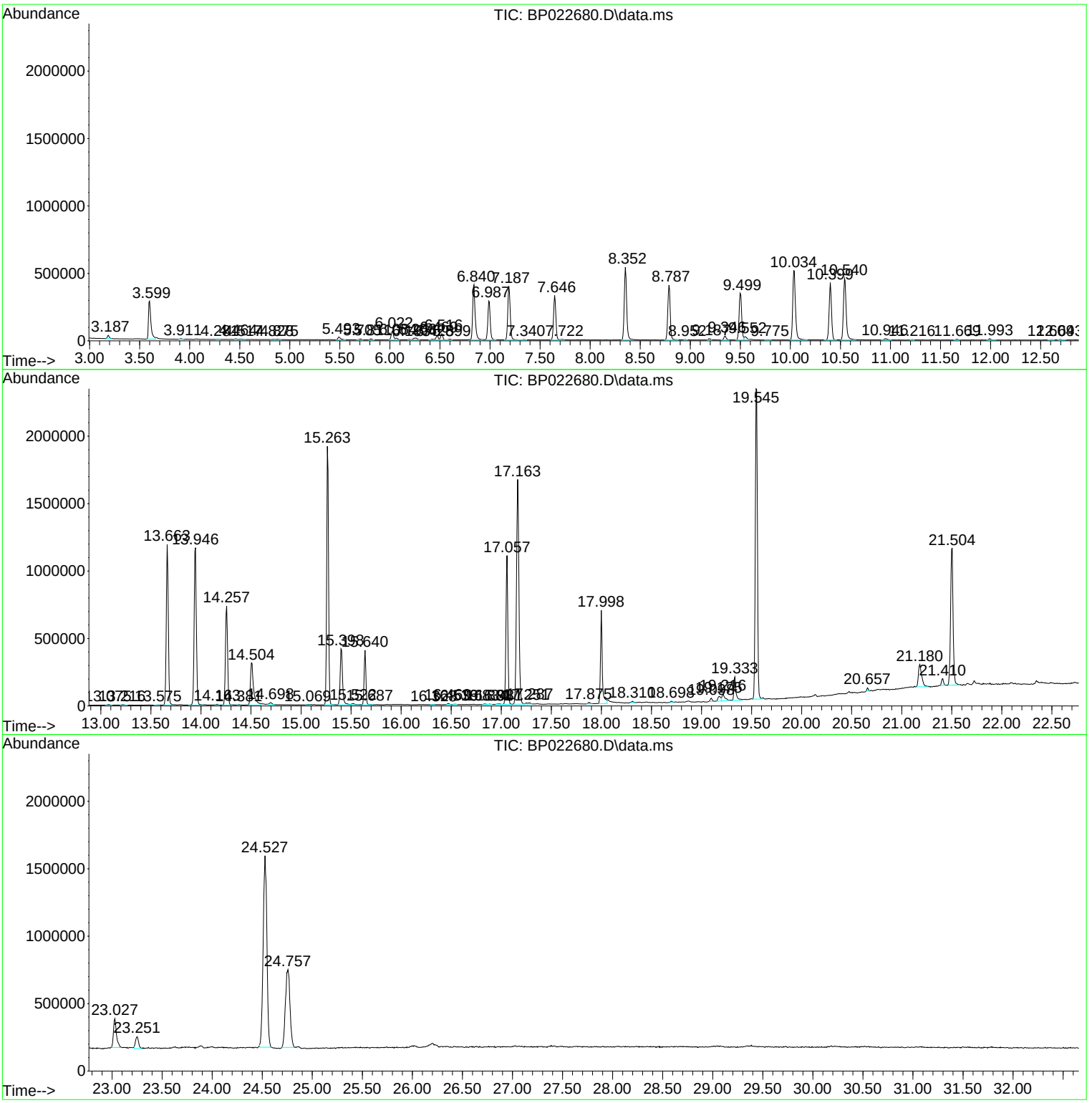
Sum of corrected areas: 34263477

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

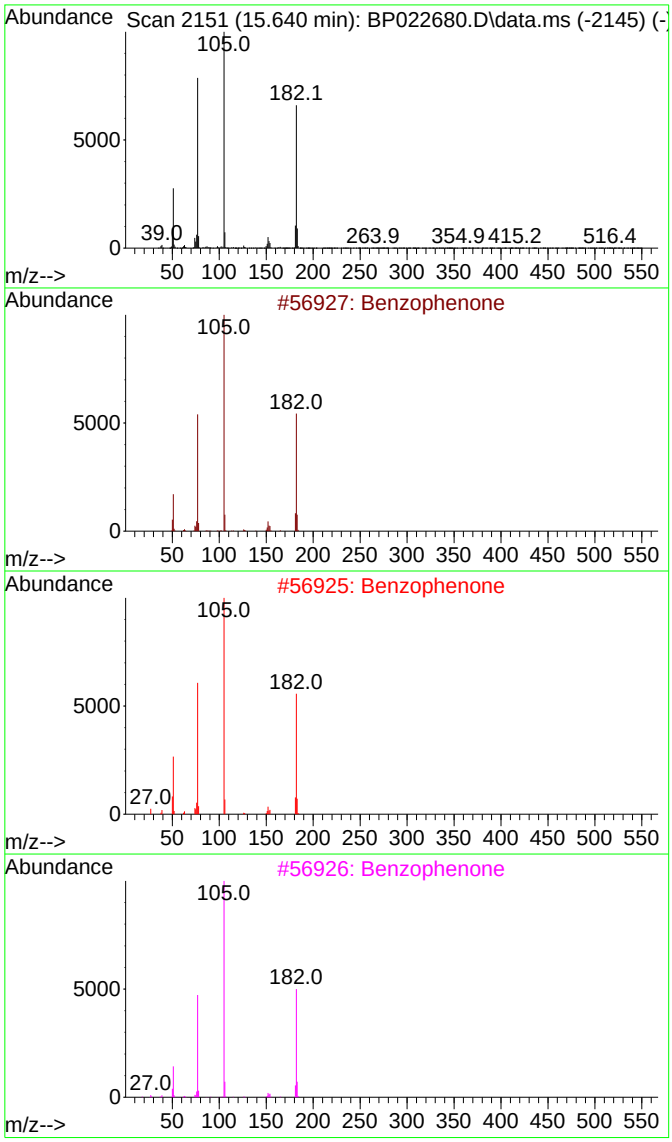
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

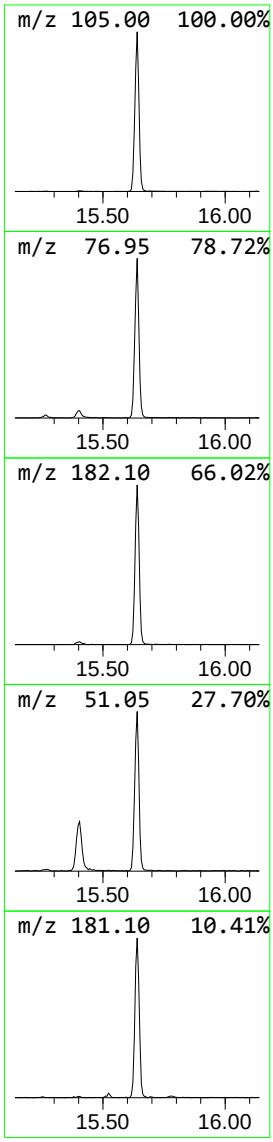
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.640	8.93 ng/ul	480545	Acenaphthene-d10	14.257

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	91
4	Benzophenone	182	C13H10O	000119-61-9	90
5	Benzophenone	182	C13H10O	000119-61-9	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

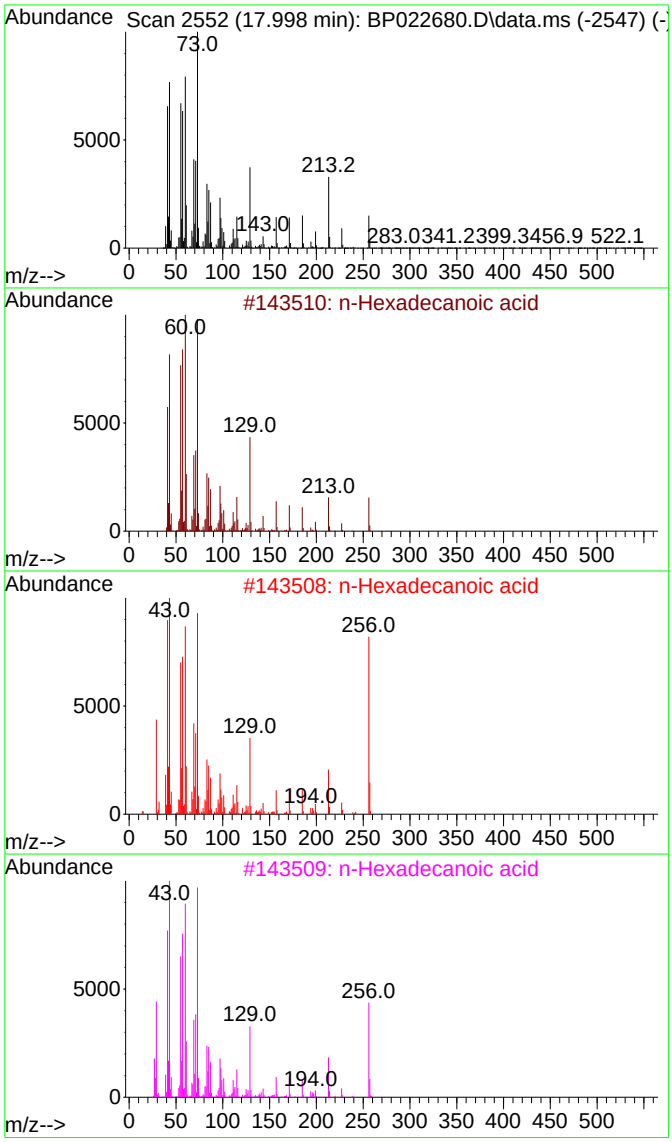
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

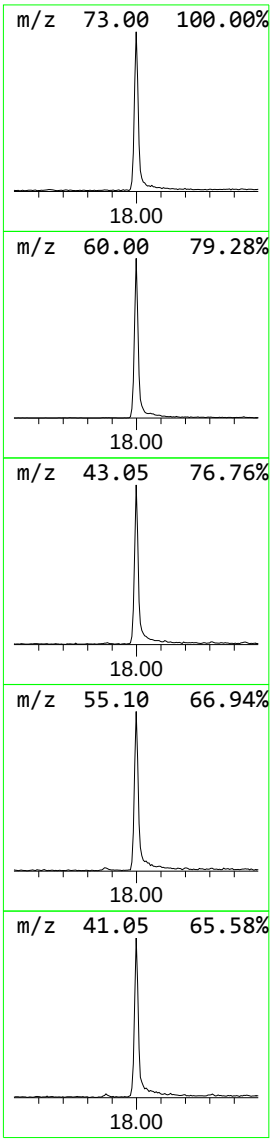
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.998	11.68 ng/ul	846953	Phenanthrene-d10	17.057

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	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

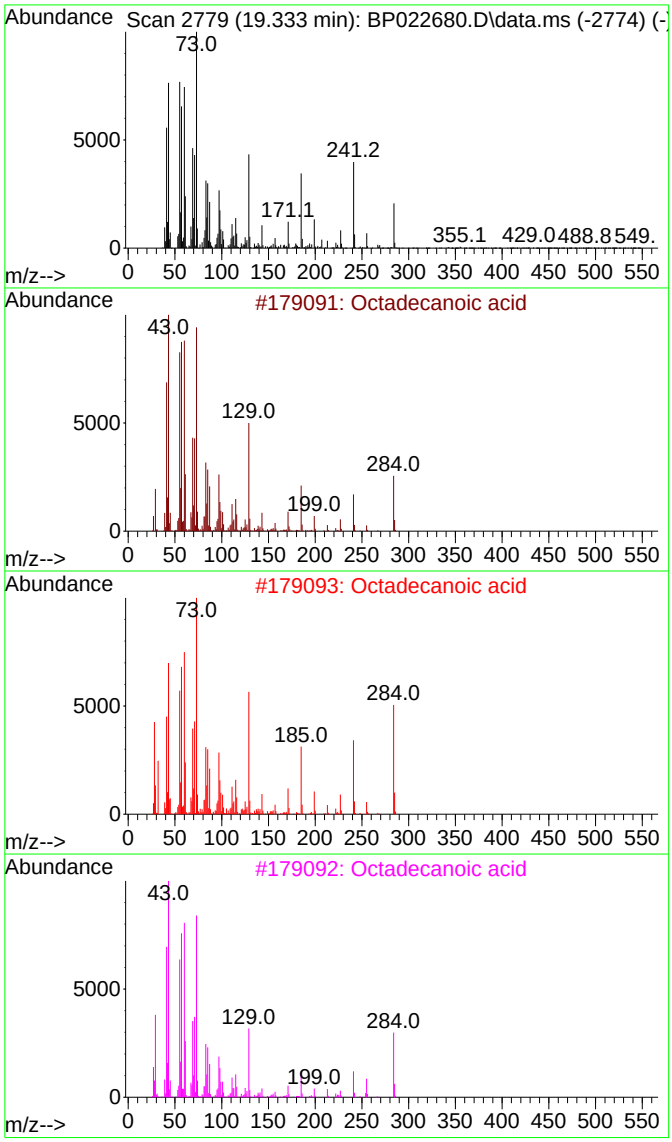
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

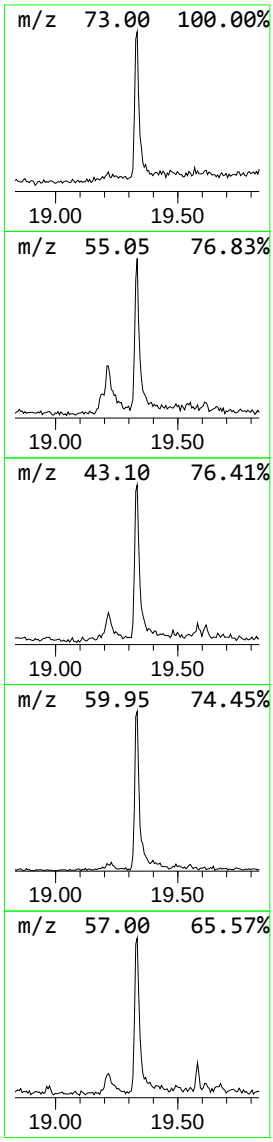
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.334	2.92 ng/ul	259645	Chrysene-d12	21.498

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	94
3	Octadecanoic acid	284	C18H36O2	000057-11-4	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	Octadecanoic acid	284	C18H36O2	000057-11-4	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

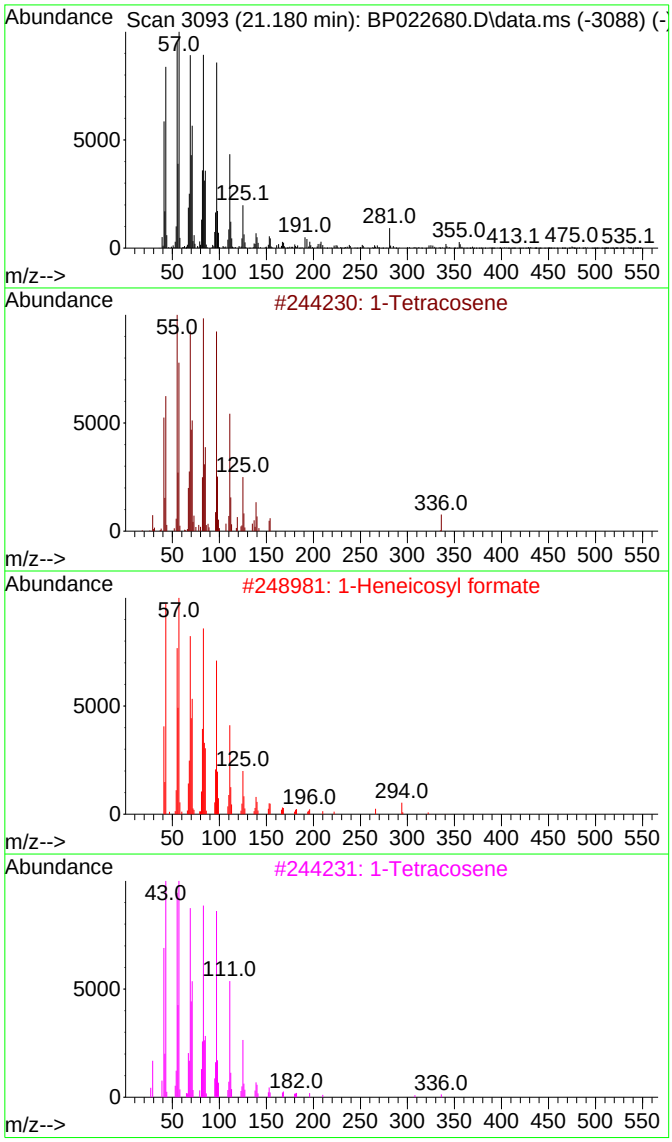
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

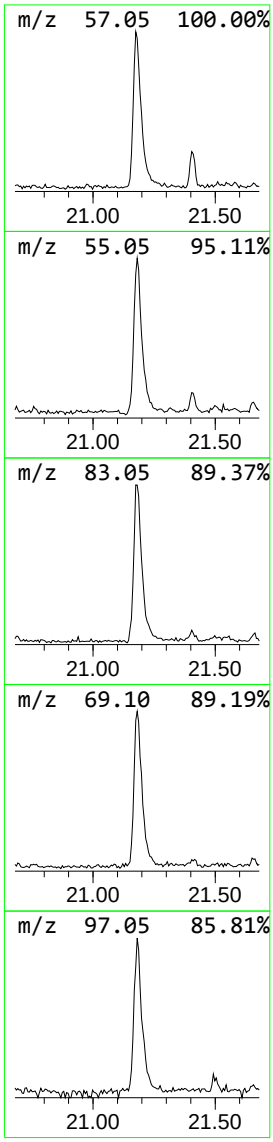
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	4.27 ng/ul	379790	Chrysene-d12	21.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	98
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
3	1-Tetracosene	336	C24H48	010192-32-2	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

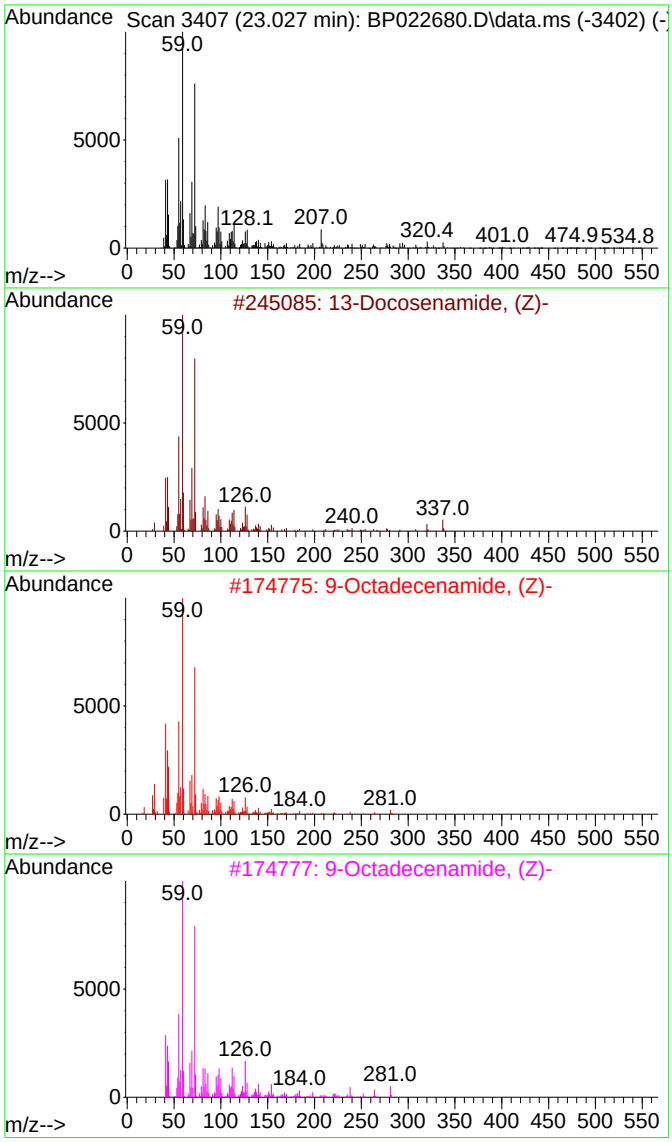
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

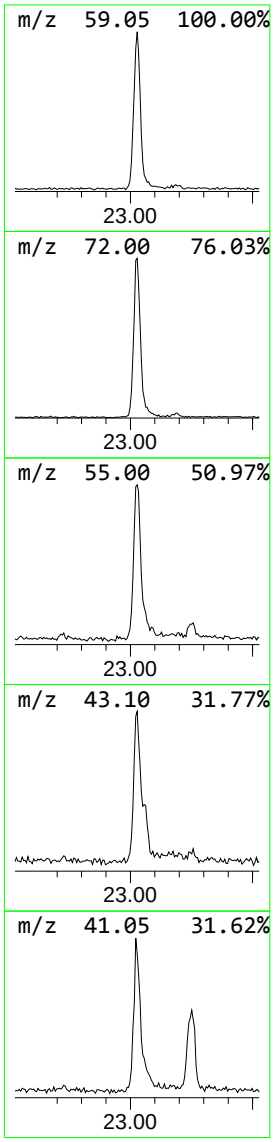
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.027	5.04 ng/ul	448116	Chrysene-d12	21.498

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	83
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
4	Tetradecanamide	227	C14H29NO	000638-58-4	50
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102824\
Data File : BP022680.D
Acq On : 28 Oct 2024 14:58
Operator : RC/JU
Sample : P4529-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
F7H12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.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	15.640	8.9	ng/ul	480545	3	14.257	1075930	20.0
n-Hexadecanoic ...	17.998	11.7	ng/ul	846953	4	17.057	1449850	20.0
Octadecanoic acid	19.334	2.9	ng/ul	259645	5	21.498	1779310	20.0
(DEL) Alkane: S...	21.180	4.3	ng/ul	379790	5	21.498	1779310	20.0
13-Docosenamide...	23.027	5.0	ng/ul	448116	5	21.498	1779310	20.0