LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
Acq On : 20 Dec 2022 18:12
Operator : CG/JU
Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXZ1

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-BP120722.M
Title : SVOA CALIBRATION

Signal : TIC: BP013172.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	22	25	31	rVB	87962	109627	0.88%	0.105%
2	3.629	72	75	84	rVB	33061	52633	0.42%	0.050%
3	3.776	97	100	113	rBV	275736	419696	3.36%	0.401%
4	3.870	113	116	125	rVB	86750	115321	0.92%	0.110%
5	3.999	134	138	142	rVB	54610	79820	0.64%	0.076%
6	4.093	151	154	162	rVB	35649	51191	0.41%	0.049%
7	4.470	216	218	225	rVB7	16945	27217	0.22%	0.026%
8	4.664	247	251	256	rVB3	32568	44543	0.36%	0.043%
9	5.040	309	315	323	rVB2	134242	223665	1.79%	0.214%
10	5.134	326	331	339	rBV5	19032	32337	0.26%	0.031%
11	7.111	660	667	683	rVV	1328522	2139768	17.11%	2.043%
12	7.281	690	696	710	rVB	1180274	1819013	14.54%	1.737%
13	7.481	723	730	741	rBV	1445367	2233623	17.86%	2.132%
14	7.569	741	745	748	rVB3	15319	20853	0.17%	0.020%
15	7.952	803	810	817	rBV	1439783	2277271	18.21%	2.174%
16	8.017	817	821	827	rVB3	13981	24960	0.20%	0.024%
17	8.664	923	931	941	rBV	1382219	2186800	17.48%	2.088%
18	8.787	945	952	958	rVB	85271	143546	1.15%	0.137%
19	9.122	1002	1009	1017	rBV	1328834	2148953	17.18%	2.052%
20	9.222	1023	1026	1032	rVV8	8618	13119	0.10%	0.013%
21	9.287	1032	1037	1042	rVB9	8213	15804	0.13%	0.015%
22	9.528	1072	1078	1083	rVB2	46708	77453	0.62%	0.074%
23	9.846	1125	1132	1142	rBV	1074660	1769746	14.15%	1.689%
24	10.075	1167	1171	1176	rVB7	8577	13466	0.11%	0.013%
25	10.328	1208	1214	1217	rBV3	24699	39582	0.32%	0.038%
26	10.387	1217	1224	1242	rVV	1684679	2741653	21.92%	2.617%
27	10.552	1245	1252	1257	rVB8	17750	37842	0.30%	0.036%
28	10.769	1279	1289	1295	rBV	1922890	3166249	25.31%	3.023%
29	10.816	1295	1297	1304	rVB	38890	58617	0.47%	0.056%
30	10.910	1304	1313	1329	rBV	901868	1638771	13.10%	1.564%
31	11.240	1365	1369	1373	rVB7	11753	17843	0.14%	0.017%
32	11.299	1373	1379	1387	rBV7	10918	22236	0.18%	0.021%
33	11.558	1414	1423	1429	rBV7	14246	36590	0.29%	0.035%
34	11.775	1455	1460	1466	rVV8	7629	15372	0.12%	0.015%
35	12.175	1523	1528	1534	rVB	30595	43753	0.35%	0.042%
36	12.352	1553	1558	1564	rVB2	29067	50734	0.41%	0.048%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
Acq On : 20 Dec 2022 18:12
Operator : CG/JU
Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXZ1

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-BP120722.M
Title : SVOA CALIBRATION

37	12.422	1564	1570	1580	rBV3	20002	38509	0.31%	0.037%
38	12.646	1600	1608	1612	rBV3	12795	20374	0.16%	0.019%
39	12.863	1638	1645	1651	rBV3	13354	28557	0.23%	0.027%
40	13.122	1685	1689	1694	rBV6	10129	12766	0.10%	0.012%
41	13.410	1732	1738	1746	rVB3	47989	78272	0.63%	0.075%
42	13.487	1746	1751	1754	rBV6	11579	19387	0.16%	0.019%
43	13.587	1765	1768	1773	rVB4	18379	24747	0.20%	0.024%
44	13.916	1819	1824	1830	rBV8	25767	44427	0.36%	0.042%
45	13.999	1830	1838	1846	rBV	2477396	3467306	27.72%	3.310%
46	14.116	1854	1858	1862	rBV6	9137	12736	0.10%	0.012%
47	14.293	1881	1888	1908	rVV	2877591	4341885	34.71%	4.145%
48	14.481	1916	1920	1926	rVB	29502	46449	0.37%	0.044%
49	14.593	1930	1939	1946	rBV	2456341	3687749	29.48%	3.521%
50	14.657	1946	1950	1957	rVB	50169	82785	0.66%	0.079%
51	14.793	1967	1973	1988	rBV	675594	1151906	9.21%	1.100%
52	14.946	1996	1999	2003	rBV6	21369	31040	0.25%	0.030%
53	14.999	2003	2008	2017	rVB	56621	103479	0.83%	0.099%
54	15.263	2049	2053	2058	rVB8	9100	14335	0.11%	0.014%
55	15.381	2067	2073	2075	rBV6	11815	17866	0.14%	0.017%
56	15.434	2079	2082	2086	rVB5	13272	16238	0.13%	0.016%
57	15.587	2101	2108	2115	rBV	3592830	5178490	41.40%	4.944%
58	15.646	2115	2118	2123	rVB4	56378	79557	0.64%	0.076%
59	15.704	2123	2128	2137	rBV	817423	1135507	9.08%	1.084%
60	15.834	2147	2150	2157	rVB7	18721	29785	0.24%	0.028%
61	15.957	2165	2171	2178	rVB	255269	374149	2.99%	0.357%
62	16.087	2189	2193	2200	rVB7	15815	35424	0.28%	0.034%
63	16.163	2204	2206	2210	rVB5	10931	13596	0.11%	0.013%
64	16.298	2226	2229	2230	rBV3	14284	15210	0.12%	0.015%
65	16.740	2299	2304	2308	rBV7	24834	40468	0.32%	0.039%
66	17.004	2345	2349	2353	rBV	44354	61183	0.49%	0.058%
67	17.098	2362	2365	2369	rVB5	18025	25000	0.20%	0.024%
68	17.169	2374	2377	2384	rVB	38755	56495	0.45%	0.054%
69	17.234	2384	2388	2393	rBV8	16636	31436	0.25%	0.030%
70	17.351	2402	2408	2412	rBV	2787307	3828267	30.61%	3.655%
71	17.392	2412	2415	2420	rVV	705681	985155	7.88%	0.940%
72	17.451	2420	2425	2437	rVB2	3377310	4870896	38.94%	4.650%
73	17.757	2470	2477	2482	rBV	79208	125201	1.00%	0.120%
74	17.840	2488	2491	2493	rBV4	10915	13749	0.11%	0.013%
75	18.163	2543	2546	2550	rBV2	63544	71371	0.57%	0.068%
76	18.222	2551	2556	2560	rBV2	573242	760603	6.08%	0.726%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
Acq On : 20 Dec 2022 18:12
Operator : CG/JU
Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ1

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

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Title : SVOA CALIBRATION

77	18.263	2560	2563	2567	rVB	79395	115087	0.92%	0.110%
78	18.410	2583	2588	2591	rBV2	51148	88643	0.71%	0.085%
79	18.634	2622	2626	2631	rBV	204568	237302	1.90%	0.227%
80	18.698	2634	2637	2640	rVV2	50604	66596	0.53%	0.064%
81	18.739	2641	2644	2649	rVB2	63296	84984	0.68%	0.081%
82	19.357	2739	2749	2755	rBV	1385560	1936668	15.48%	1.849%
83	19.457	2761	2766	2779	rBV	2125130	3140405	25.11%	2.998%
84	19.681	2799	2804	2808	rBV	4507569	6504502	52.00%	6.210%
85	21.128	3046	3050	3054	rBV	1179238	1532385	12.25%	1.463%
86	21.439	3096	3103	3107	rBV2	3411452	5558563	44.44%	5.307%
87	21.475	3107	3109	3114	rVB	645406	800174	6.40%	0.764%
88	23.133	3387	3391	3397	rBV2	826310	2252506	18.01%	2.150%
89	23.757	3491	3497	3504	rBV2	3296940	6449155	51.56%	6.157%
90	23.922	3519	3525	3531	rVB2	2361339	4451418	35.59%	4.250%
91	24.433	3607	3612	3622	rVB5	849073	1839103	14.70%	1.756%
92	24.539	3625	3630	3640	rVB	1070624	2302554	18.41%	2.198%
93	28.510	4296	4305	4325	rVB2	3425406	12507711	100.00%	11.941%

Sum of corrected areas: 104749778

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
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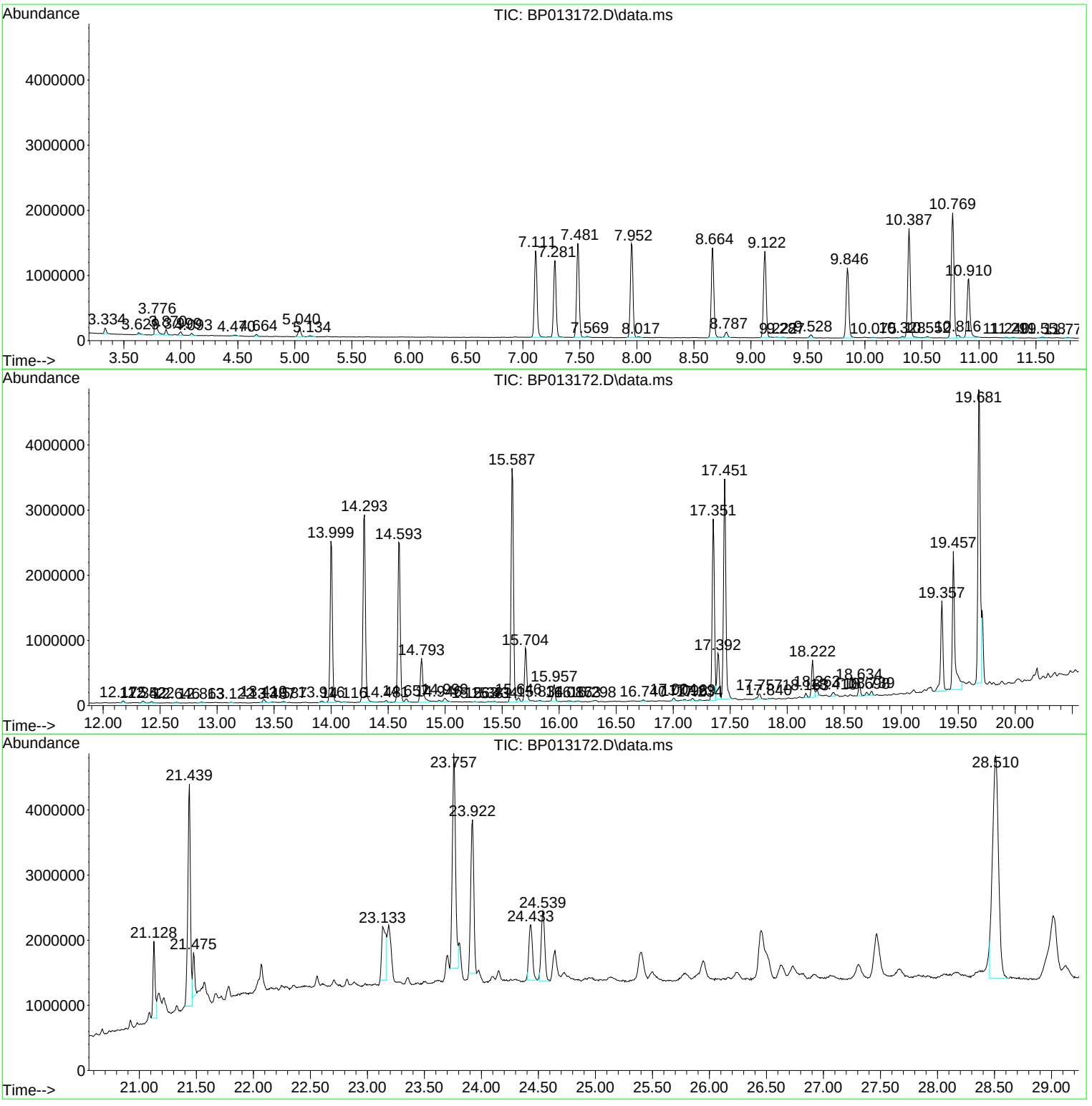
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
Acq On : 20 Dec 2022 18:12
Operator : CG/JU
Sample : N6009-03
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ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

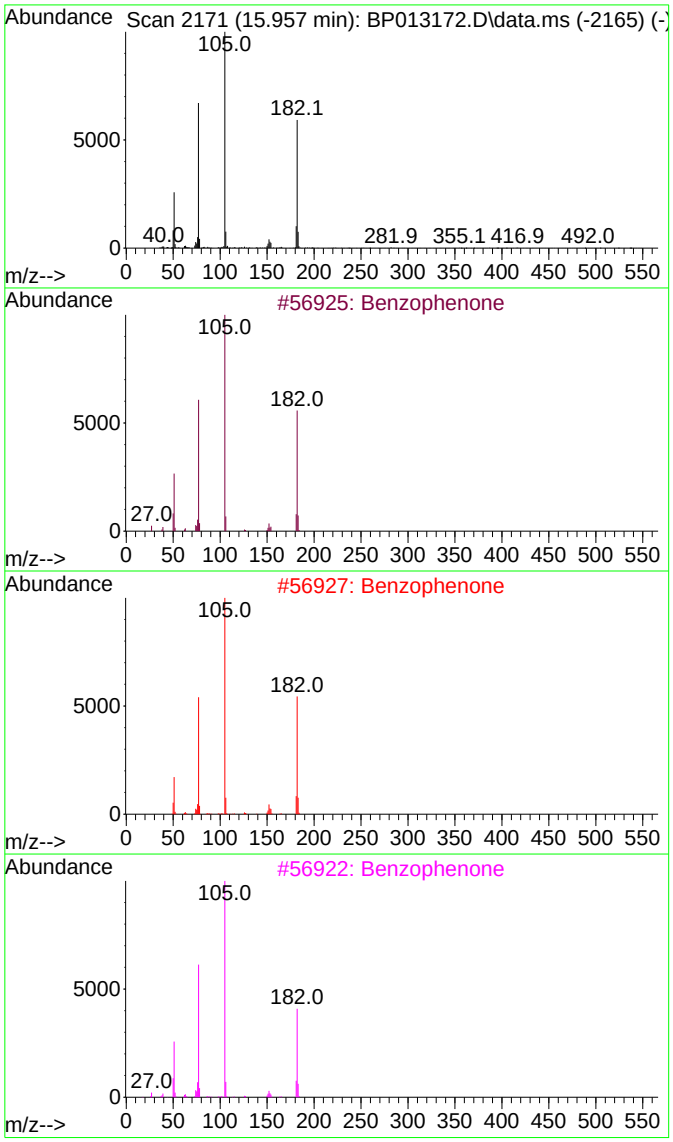
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

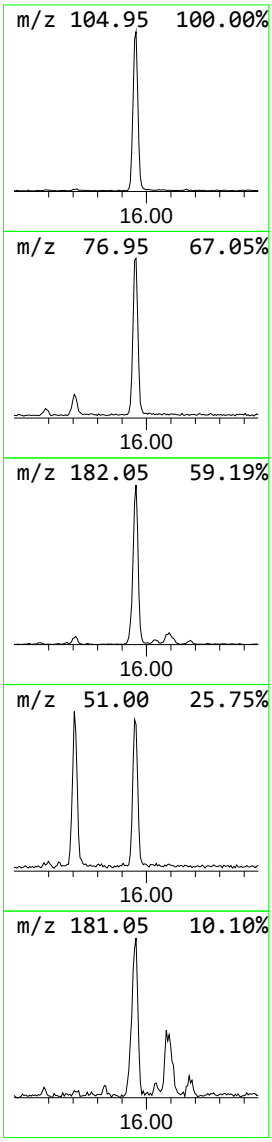
****

Peak Number 1 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	2.03 ng/ul	374149	Acenaphthene-d10	14.593

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	94
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
Acq On : 20 Dec 2022 18:12
Operator : CG/JU
Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

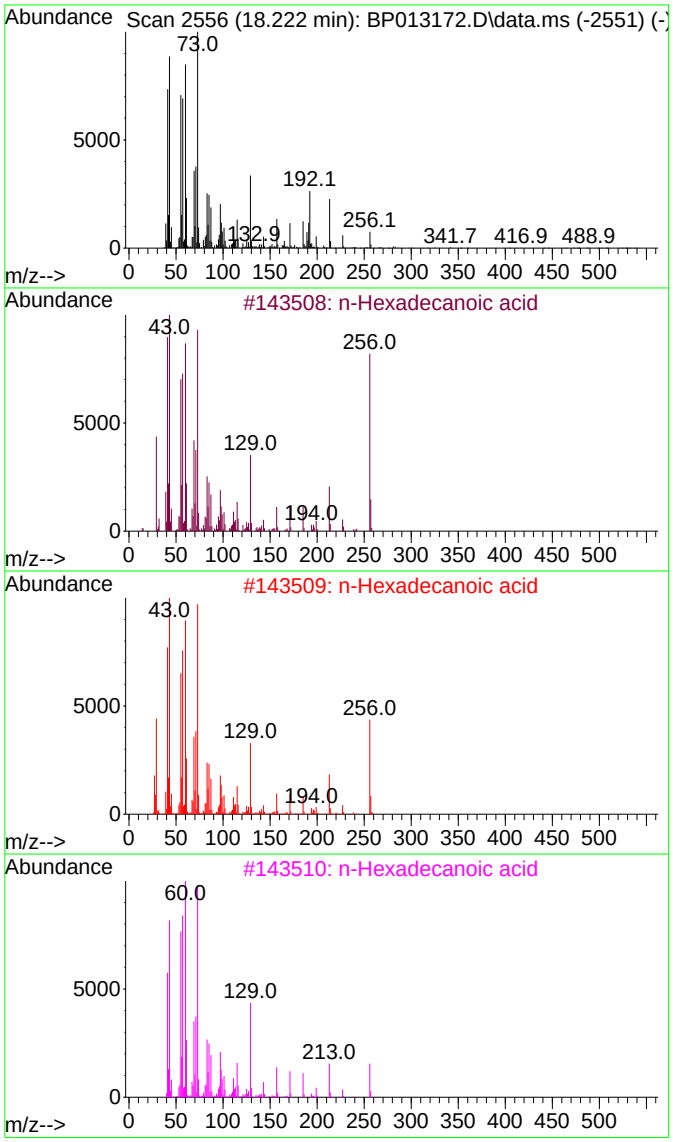
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

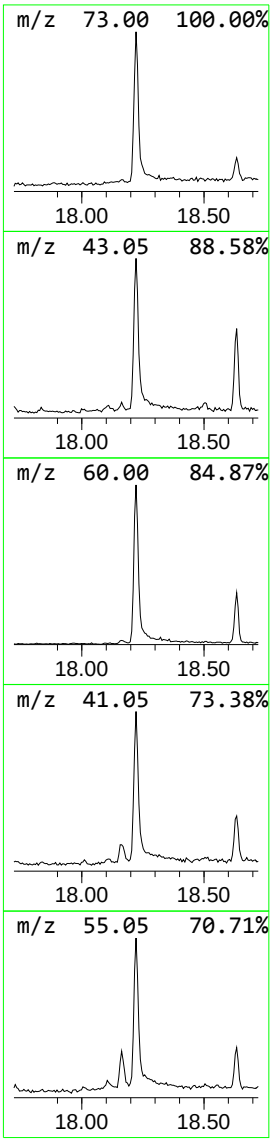
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	3.97 ng/ul	760603	Phenanthrene-d10	17.351

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	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
Acq On : 20 Dec 2022 18:12
Operator : CG/JU
Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

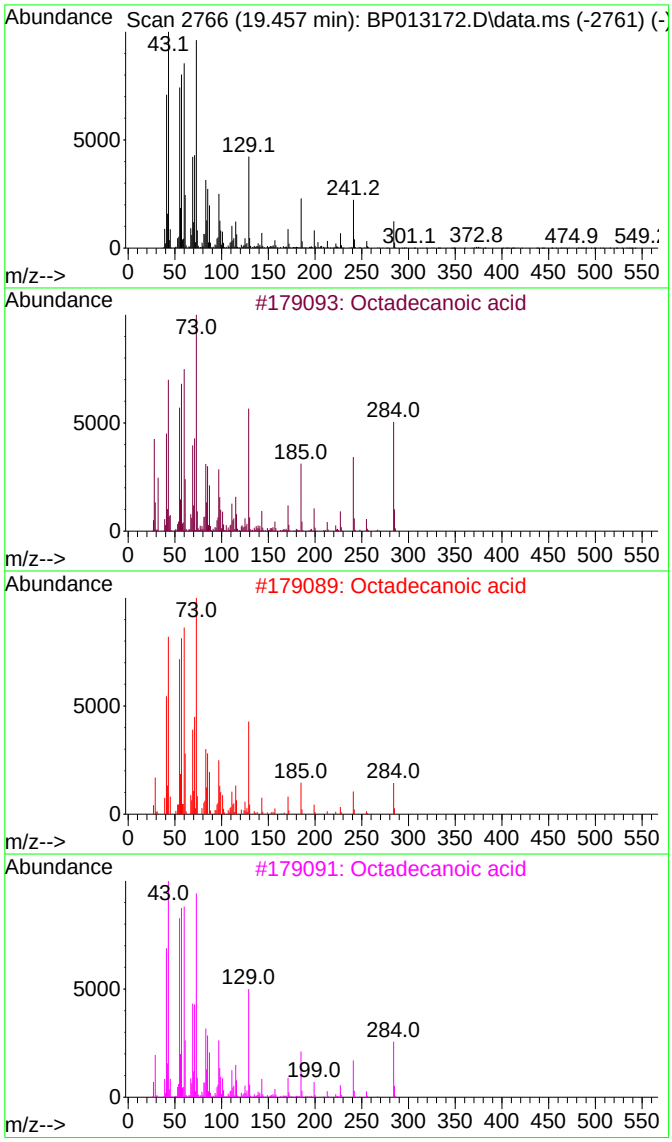
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

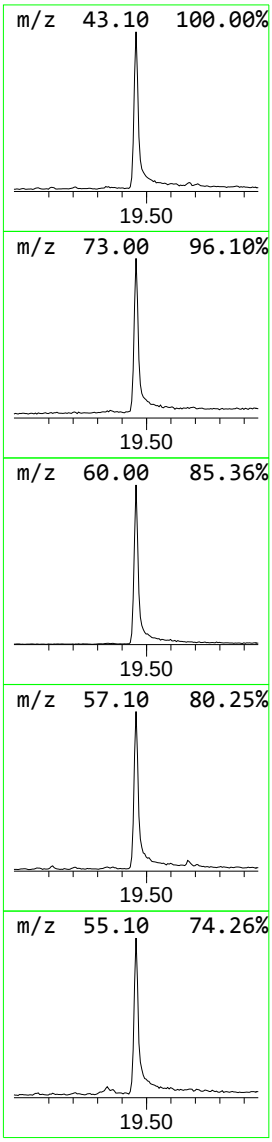
****

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.457	11.30 ng/ul	3140410	Chrysene-d12	21.439

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	99
4	Octadecanoic acid	284	C18H36O2	000057-11-4	98
5	Octadecanoic acid	284	C18H36O2	000057-11-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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Acq On : 20 Dec 2022 18:12
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Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ1

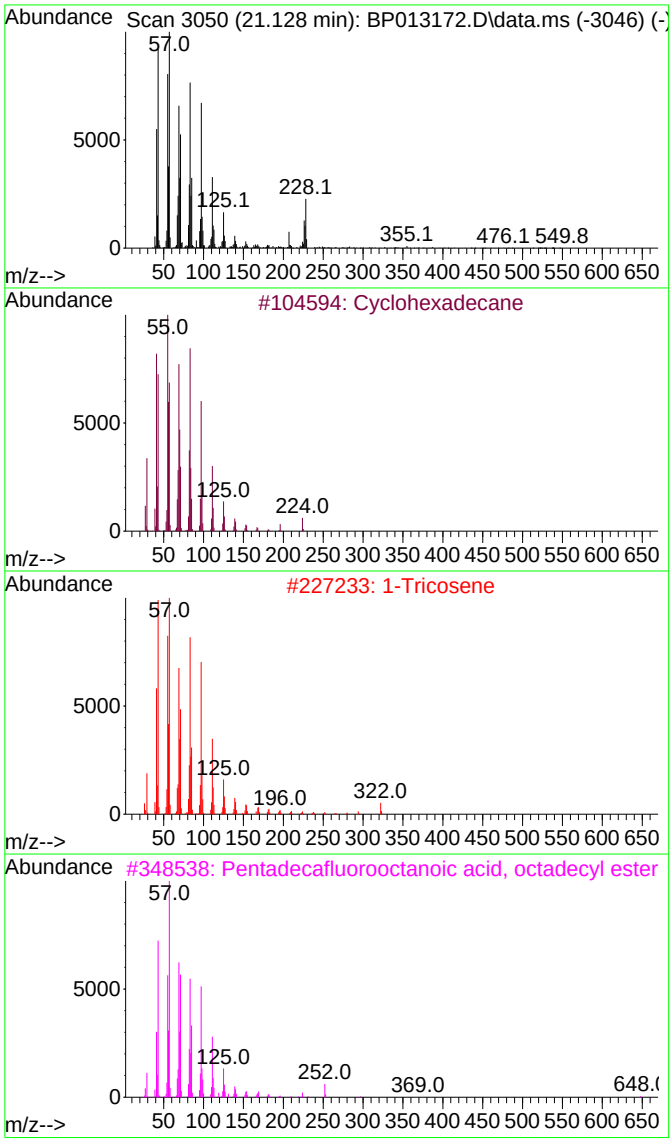
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

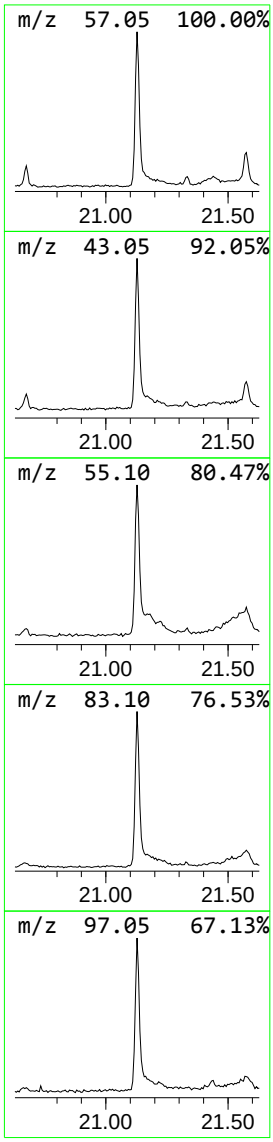
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Cyclic21.128 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	5.51 ng/ul	1532390	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	1-Tricosene	322	C23H46	018835-32-0	93
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
4	Heptacos-1-ene	378	C27H54	015306-27-1	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
Acq On : 20 Dec 2022 18:12
Operator : CG/JU
Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

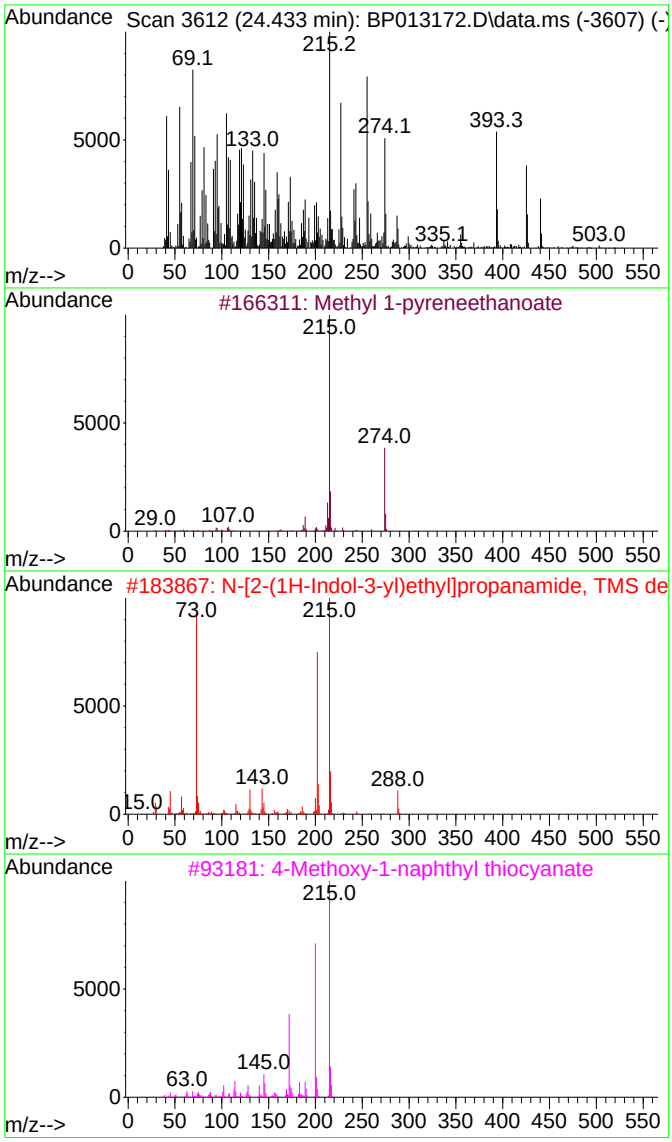
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

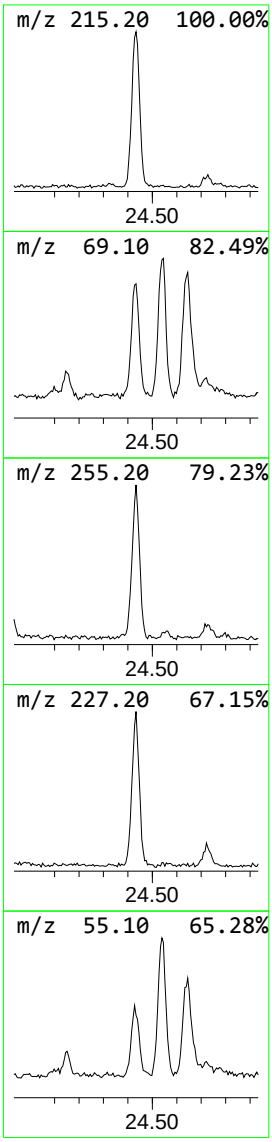
****

Peak Number 5 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.433	8.26 ng/ul	1839100	Perylene-d12	23.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 1-pyreneethanoate	274	C19H14O2	073654-19-0	43
2	N-[2-(1H-Indol-3-yl)ethyl]propan...	288	C16H24N2OSi	1000493-19-0	41
3	4-Methoxy-1-naphthyl thiocyanate	215	C12H9NOS	066231-77-4	15
4	6H-Benzo[d]pyrimido[5,4-b]thiopy...	215	C11H9N3S	1010267-44-6	15
5	.alpha.-Benzoylthioacetic acid a...	255	C15H13NOS	013196-40-2	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
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Operator : CG/JU
Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ1

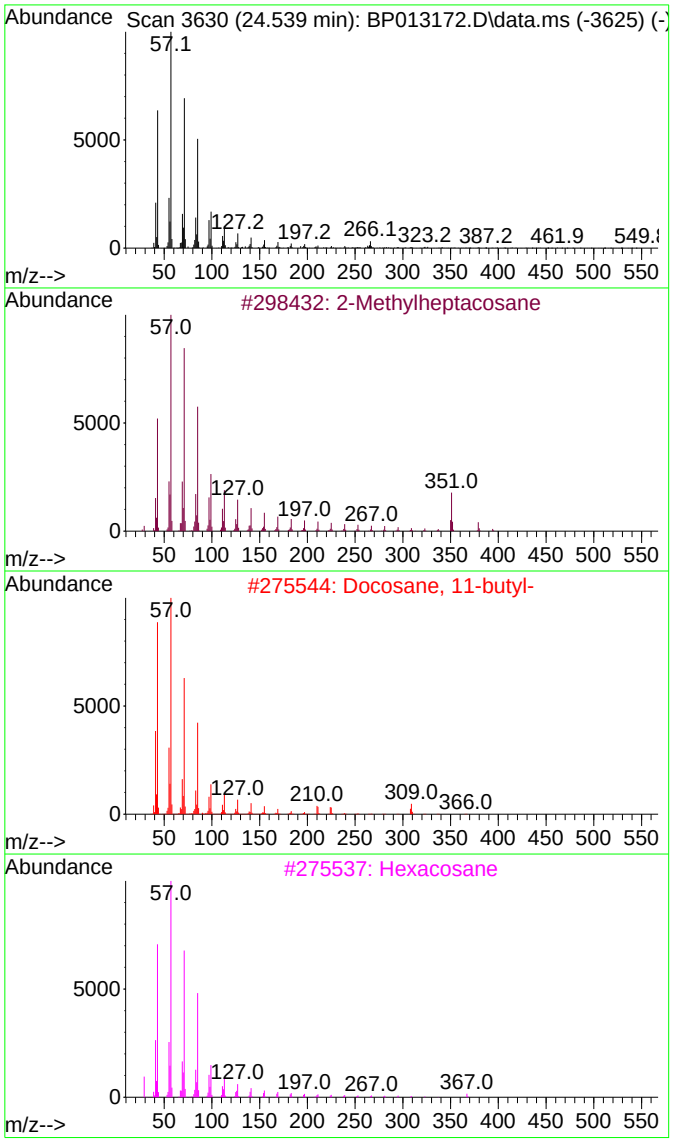
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

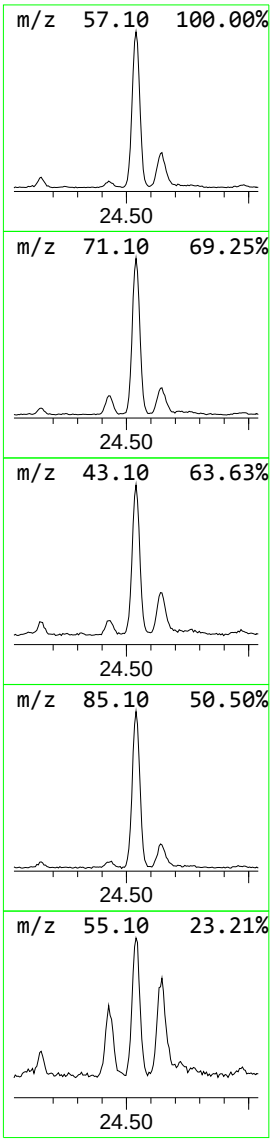
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.539	10.35 ng/ul	2302550	Perylene-d12	23.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylheptacosane	394	C28H58	001561-00-8	95
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
3	Hexacosane	366	C26H54	000630-01-3	93
4	Docosane, 9-butyl-	366	C26H54	055282-14-9	93
5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
Acq On : 20 Dec 2022 18:12
Operator : CG/JU
Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ1

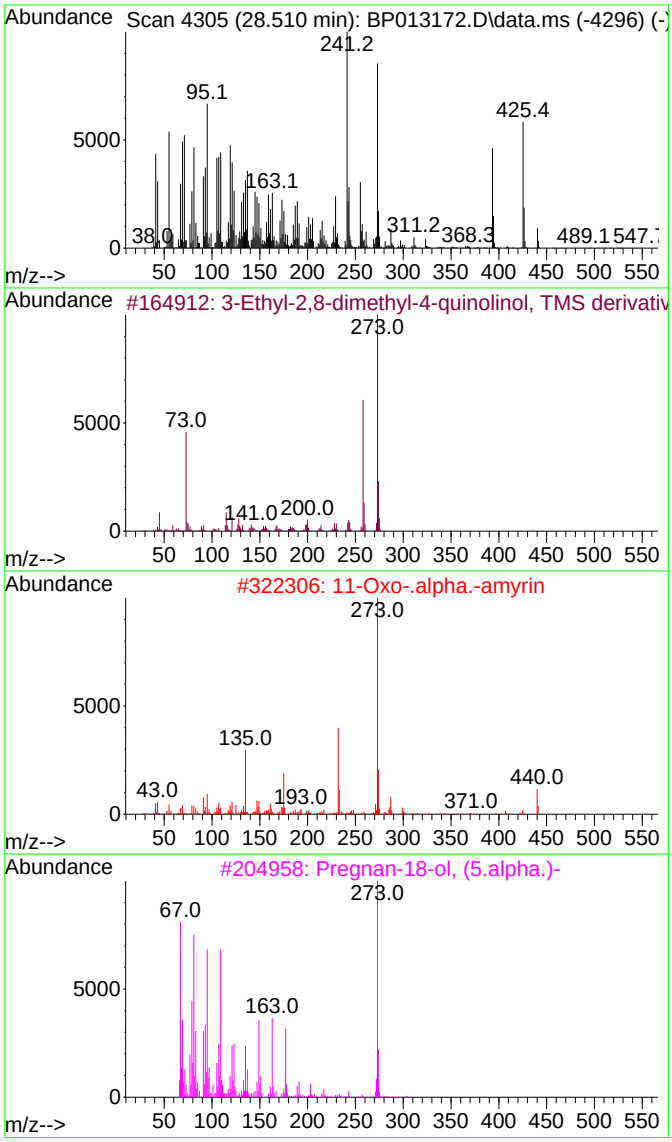
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

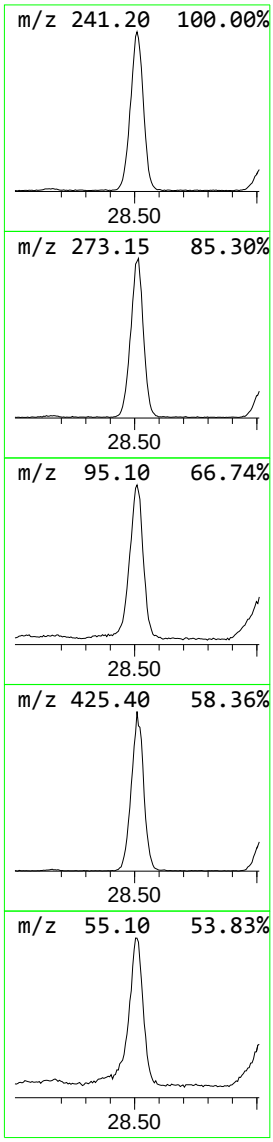
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.510	56.20 ng/ul	12507700	Perylene-d12	23.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethyl-2,8-dimethyl-4-quinolino...	273	C16H23NOSi	1000474-26-4	45
2	11-Oxo-.alpha.-amyrin	440	C30H48O2	002118-90-3	44
3	Pregnan-18-ol, (5.alpha.)-	304	C21H36O	056053-09-9	27
4	2-(1H-Indol-3-ylmethylene)-1H-in...	273	C18H11NO2	031060-64-7	25
5	8-Trifluoromethylcinchoninic acid	241	C11H6F3NO2	031009-01-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013172.D
Acq On : 20 Dec 2022 18:12
Operator : CG/JU
Sample : N6009-03
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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	15.957	2.0	ng/ul	374149	3	14.593	3687750	20.0
n-Hexadecanoic ...	18.222	4.0	ng/ul	760603	4	17.351	3828270	20.0
Octadecanoic acid	19.457	11.3	ng/ul	3140410	5	21.439	5558560	20.0
(DEL) Alkane: C...	21.128	5.5	ng/ul	1532390	5	21.439	5558560	20.0
unknown-01	24.433	8.3	ng/ul	1839100	6	23.922	4451420	20.0
(DEL) Alkane: S...	24.539	10.4	ng/ul	2302550	6	23.922	4451420	20.0
unknown-02	28.510	56.2	ng/ul	12507700	6	23.922	4451420	20.0