LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBYD3

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: BP013302.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.328	21	24	32	rVB	214452	278454	1.23%	0.118%
2	3.628	72	75	81	rBV4	13301	24456	0.11%	0.010%
3	3.758	93	97	113	rBV	3049236	4475000	19.79%	1.889%
4	4.087	149	153	159	rVB	45279	60649	0.27%	0.026%
5	4.311	189	191	196	rVB3	23980	30789	0.14%	0.013%
6	5.034	308	314	319	rVB2	67138	114259	0.51%	0.048%
7	5.263	348	353	364	rBV2	23403	50439	0.22%	0.021%
8	6.540	565	570	573	rBV6	12378	22871	0.10%	0.010%
9	7.105	659	666	679	rBV	3978926	6273574	27.75%	2.648%
10	7.269	687	694	705	rVB	3197130	4819490	21.32%	2.034%
11	7.469	721	728	737	rBV	4088863	6266449	27.72%	2.645%
12	7.552	737	742	751	rVB6	21861	58540	0.26%	0.025%
13	7.940	801	808	815	rBV	2649082	4075324	18.03%	1.720%
14	8.651	922	929	941	rBV	4645746	7624480	33.72%	3.218%
15	9.110	999	1007	1022	rBV	3845058	6274648	27.75%	2.649%
16	9.263	1028	1033	1038	rVB6	20129	30613	0.14%	0.013%
17	9.504	1070	1074	1079	rBV	60468	89705	0.40%	0.038%
18	9.834	1122	1130	1142	rBV	3289345	5404928	23.91%	2.282%
19	10.051	1163	1167	1172	rBV8	13115	25346	0.11%	0.011%
20	10.257	1194	1202	1207	rBV5	20162	40942	0.18%	0.017%
21	10.375	1214	1222	1238	rBV	4981220	8367099	37.01%	3.532%
22	10.757	1277	1287	1297	rBV	3506031	5995292	26.52%	2.531%
23	10.893	1302	1310	1331	rBV	4286645	7289989	32.24%	3.077%
24	11.281	1371	1376	1383	rVB	12579	23541	0.10%	0.010%
25	11.540	1416	1420	1431	rVB	12358	24332	0.11%	0.010%
26	12.004	1495	1499	1504	rVB3	16350	26499	0.12%	0.011%
27	12.163	1520	1526	1531	rVB6	14998	28270	0.13%	0.012%
28	12.240	1535	1539	1544	rBV2	16927	28727	0.13%	0.012%
29	12.340	1550	1556	1563	rBV2	83869	138617	0.61%	0.059%
30	12.851	1636	1643	1647	rBV9	13008	27790	0.12%	0.012%
31	13.104	1680	1686	1694	rVB7	18694	35914	0.16%	0.015%
32	13.328	1718	1724	1728	rBV6	14186	32487	0.14%	0.014%
33	13.398	1728	1736	1741	rVB2	64680	111324	0.49%	0.047%
34	13.551	1757	1762	1765	rVB6	16474	29897	0.13%	0.013%
35	13.992	1828	1837	1851	rVV	8054242	11023306	48.76%	4.653%
36	14.104	1852	1856	1859	rVB6	19910	33340	0.15%	0.014%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

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	14.228	1872	1877	1879	rBV6	13888	24243	0.11%	0.010%
38	14.281	1879	1886	1896	rVV	9395205	13464816	59.56%	5.684%
39	14.469	1911	1918	1925	rVB2	45072	81661	0.36%	0.034%
40	14.586	1931	1938	1945	rVB	5007127	7425575	32.84%	3.134%
41	14.786	1965	1972	1989	rBV	2619410	4115009	18.20%	1.737%
42	14.992	2002	2007	2013	rBV3	70697	107863	0.48%	0.046%
43	15.363	2067	2070	2075	rBV3	13376	24974	0.11%	0.011%
44	15.422	2077	2080	2087	rVB3	24435	36945	0.16%	0.016%
45	15.581	2100	2107	2116	rBV	10980458	15675042	69.33%	6.617%
46	15.698	2121	2127	2141	rVV	2537117	3397856	15.03%	1.434%
47	15.816	2143	2147	2154	rVB2	57345	96537	0.43%	0.041%
48	15.945	2163	2169	2178	rVB	1029828	1396229	6.18%	0.589%
49	16.286	2224	2227	2233	rVB7	20112	33533	0.15%	0.014%
50	16.357	2234	2239	2245	rVB3	19163	40359	0.18%	0.017%
51	16.433	2248	2252	2254	rBV5	18546	24825	0.11%	0.010%
52	16.475	2256	2259	2262	rVV3	23465	29718	0.13%	0.013%
53	16.516	2262	2266	2272	rVB7	19876	32569	0.14%	0.014%
54	16.728	2297	2302	2309	rBV2	86109	127069	0.56%	0.054%
55	17.086	2359	2363	2367	rBV6	22756	40347	0.18%	0.017%
56	17.222	2382	2386	2394	rBV5	52995	88055	0.39%	0.037%
57	17.292	2394	2398	2400	rBV4	38115	44539	0.20%	0.019%
58	17.345	2400	2407	2417	rVV	5118375	7258038	32.10%	3.064%
59	17.445	2417	2424	2431	rVV	9463588	13442476	59.46%	5.674%
60	17.504	2431	2434	2436	rVV3	44593	59244	0.26%	0.025%
61	17.533	2437	2439	2447	rVB8	47501	92661	0.41%	0.039%
62	17.616	2451	2453	2460	rVB6	22129	42331	0.19%	0.018%
63	17.698	2463	2467	2470	rBV5	42285	64116	0.28%	0.027%
64	17.998	2516	2518	2522	rVB5	32913	35540	0.16%	0.015%
65	18.098	2530	2535	2540	rBV4	67559	131907	0.58%	0.056%
66	18.157	2541	2545	2550	rBV2	107321	142612	0.63%	0.060%
67	18.216	2550	2555	2565	rBV	1807736	2481219	10.97%	1.047%
68	18.463	2593	2597	2601	rBV	95282	128062	0.57%	0.054%
69	18.551	2608	2612	2619	rVB2	115032	192265	0.85%	0.081%
70	18.780	2647	2651	2656	rVB	191586	224583	0.99%	0.095%
71	19.122	2704	2709	2713	rBV2	131880	197753	0.87%	0.083%
72	19.251	2728	2731	2735	rVB	123720	141005	0.62%	0.060%
73	19.327	2737	2744	2747	rBV3	234065	518049	2.29%	0.219%
74	19.445	2760	2764	2773	rBV	454406	660277	2.92%	0.279%
75	19.674	2798	2803	2811	rBV	10177068	13942918	61.67%	5.886%
76	19.827	2824	2829	2836	rBV	1397248	1870665	8.27%	0.790%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
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Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

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

77	19.951	2846	2850	2857	rBV	200227	343725	1.52%	0.145%
78	20.174	2884	2888	2893	rVB4	230481	401443	1.78%	0.169%
79	20.668	2969	2972	2975	rVB	190241	206304	0.91%	0.087%
80	21.127	3045	3050	3054	rBV	1997092	3261936	14.43%	1.377%
81	21.433	3097	3102	3107	rBV	5055271	6892736	30.49%	2.910%
82	22.698	3314	3317	3323	rVB	602115	865469	3.83%	0.365%
83	23.127	3387	3390	3396	rVB	502830	706743	3.13%	0.298%
84	23.757	3490	3497	3512	rVB2	7788590	16393005	72.51%	6.920%
85	23.915	3517	3524	3536	rVB2	3556953	7529507	33.30%	3.178%
86	24.533	3624	3629	3637	rVB	827259	1656663	7.33%	0.699%
87	28.503	4293	4304	4325	rVB	5649657	22608144	100.00%	9.543%
88	29.003	4382	4389	4418	rVB8	2139209	8844549	39.12%	3.733%

Sum of corrected areas: 236901089

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
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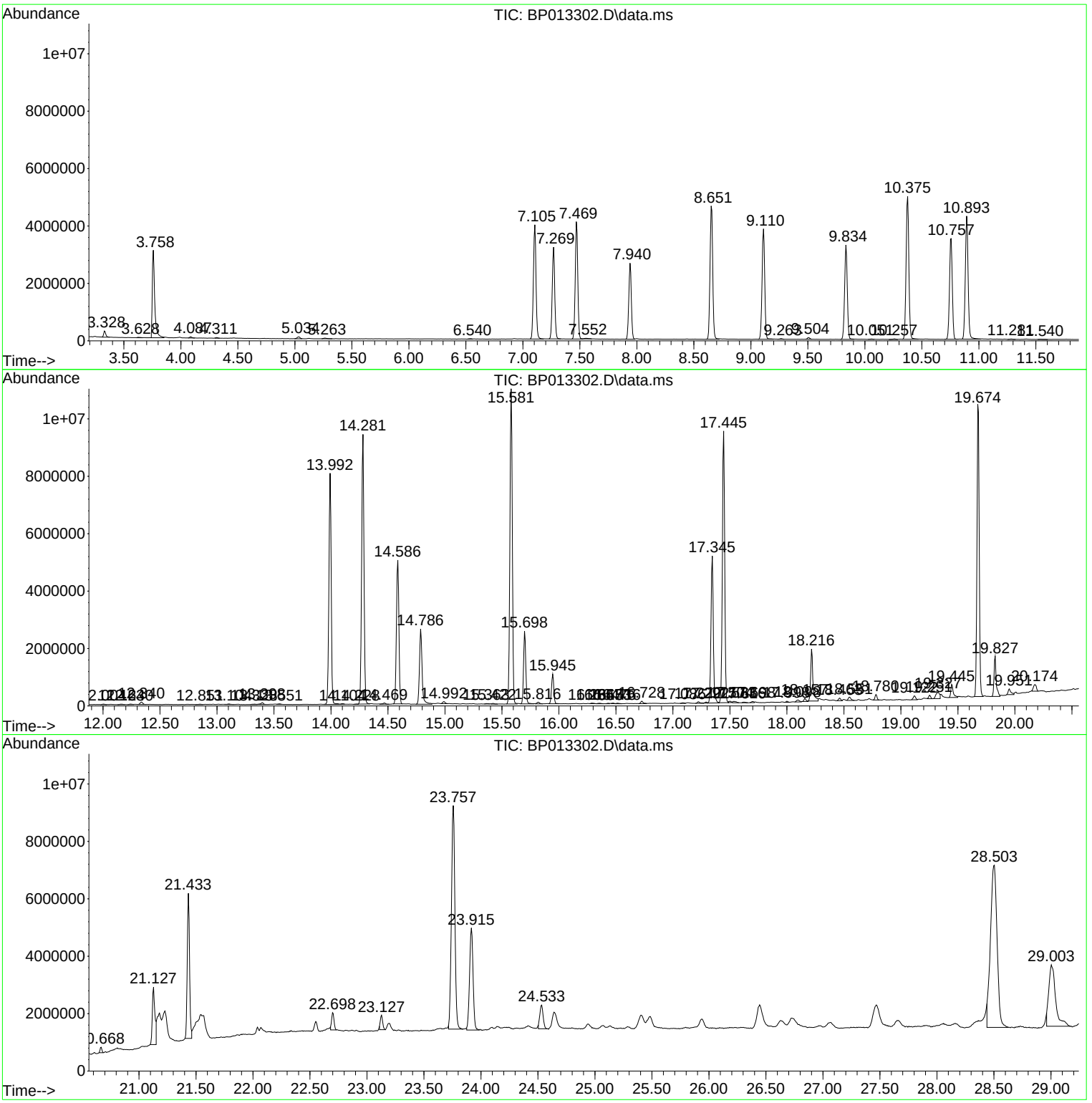
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

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\BP122422\
Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

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

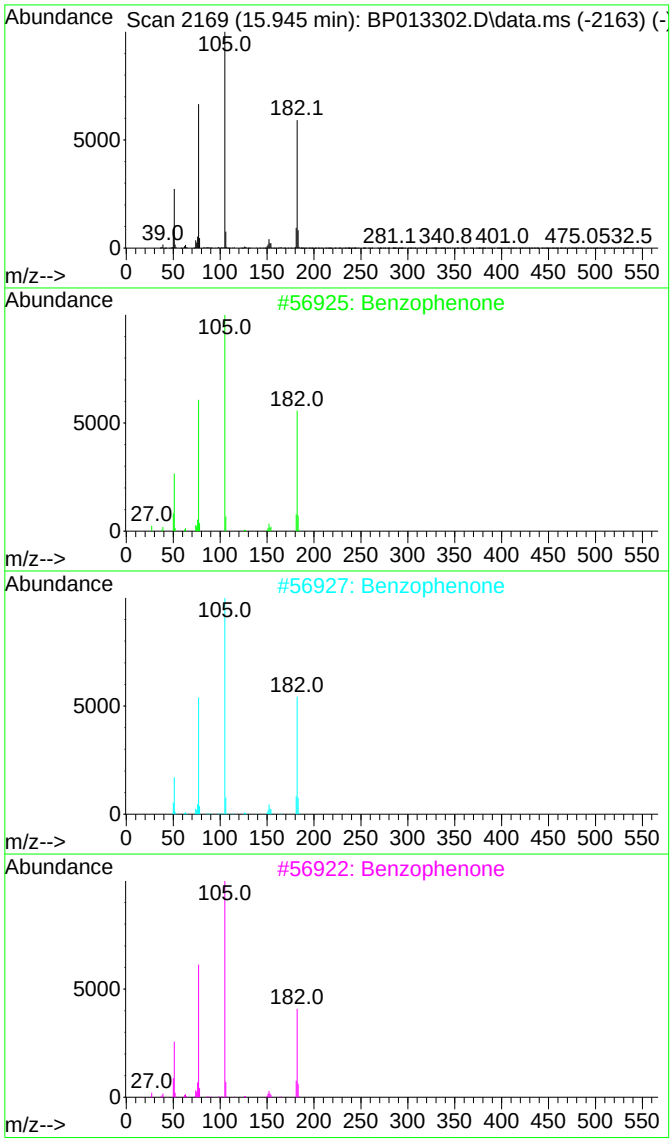
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

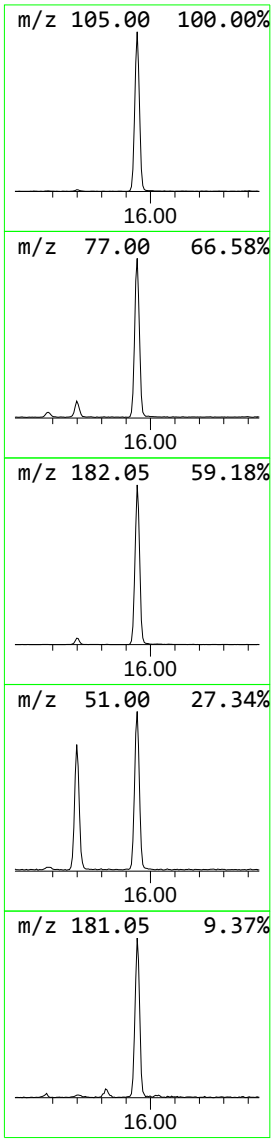
****

Peak Number 1 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	3.76 ng/ul	1396230	Acenaphthene-d10	14.586

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	90
5	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

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

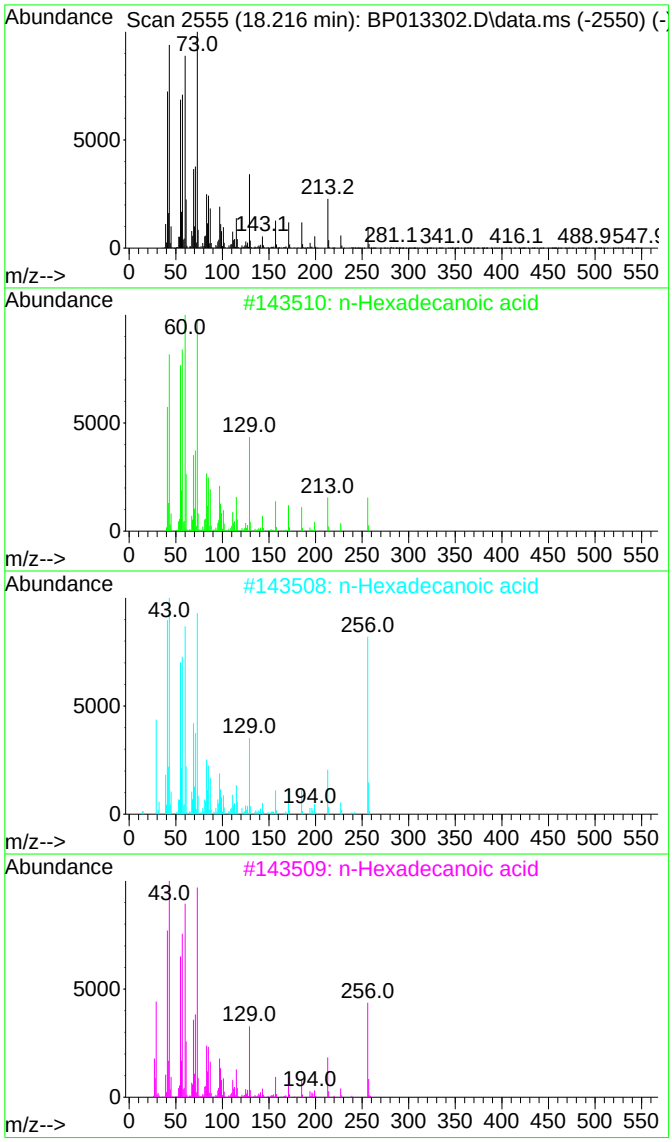
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

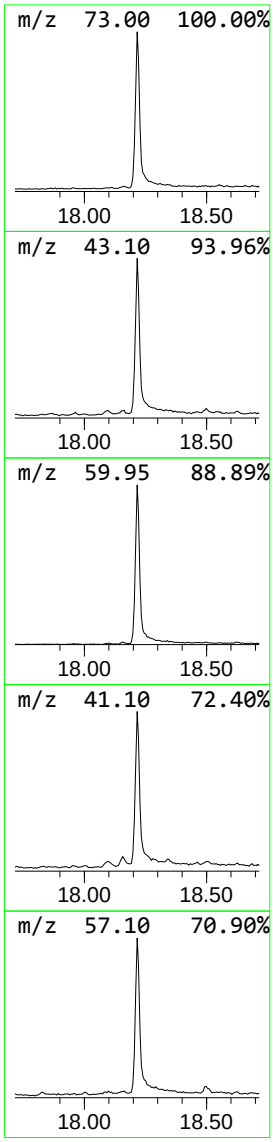
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	6.84 ng/ul	2481220	Phenanthrene-d10	17.345

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	96
5	Tridecanoic acid	214	C13H26O2	000638-53-9	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

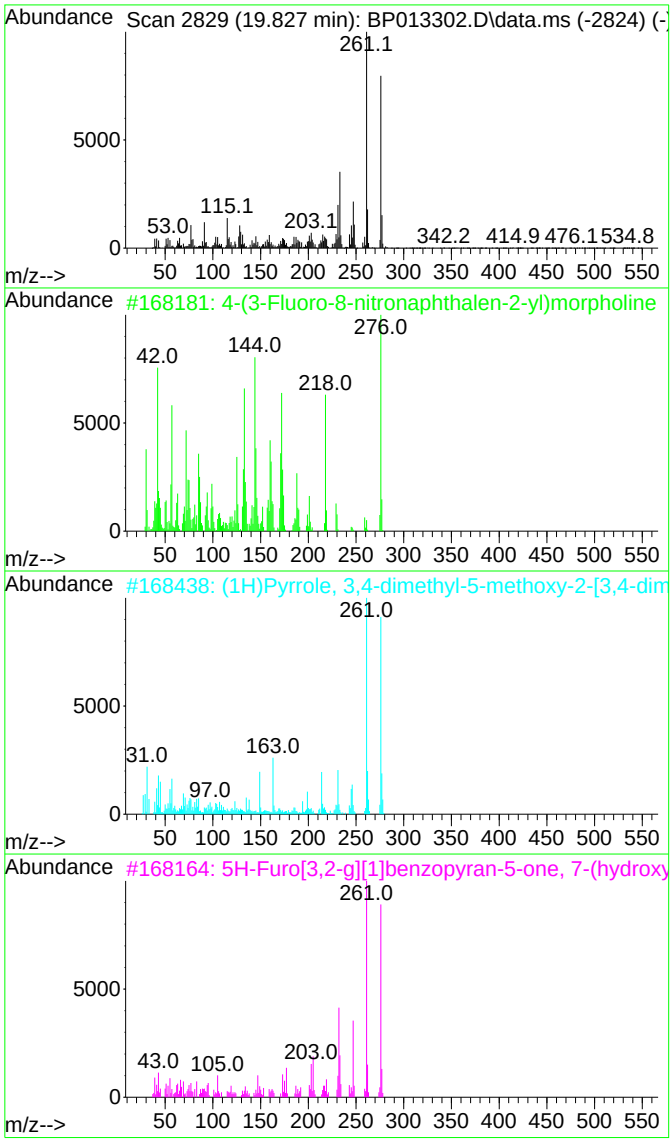
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

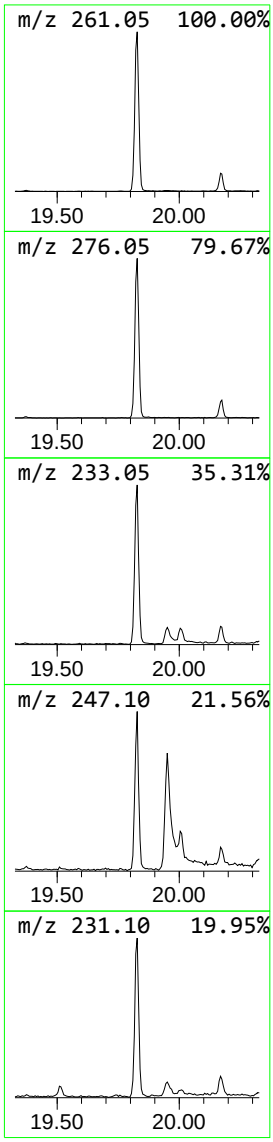
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4-(3-Fluoro-8-nitronaphthal... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.827	5.43 ng/ul	1870670	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(3-Fluoro-8-nitronaphthalen-2-...	276	C14H13FN2O3	1000409-37-1	91
2	(1H)Pyrrole, 3,4-dimethyl-5-meth...	276	C15H20N2OS	1000197-22-6	90
3	5H-Furo[3,2-g][1]benzopyran-5-on...	276	C14H12O6	000668-10-0	80
4	3,5-di-tert-Butyl-4-hydroxycinna...	276	C17H24O3	022014-01-3	70
5	5,6,7,8-Tetrahydrothieno[2,3-b]q...	276	C14H20N2SSi	1000496-40-4	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
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Acq On : 24 Dec 2022 16:23
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Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

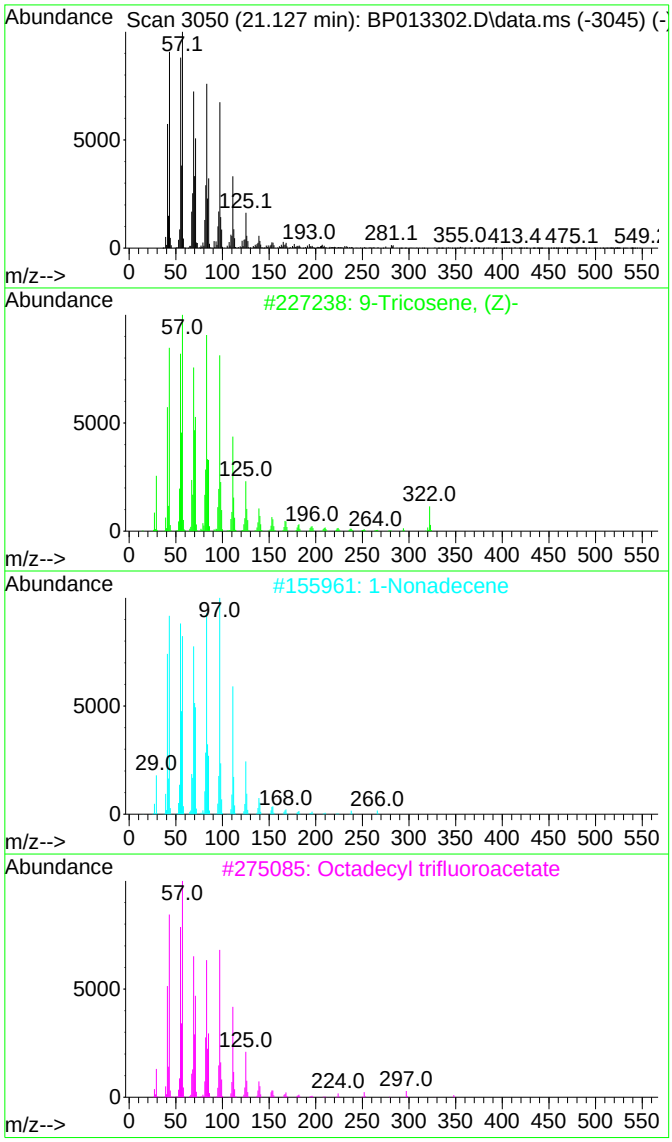
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

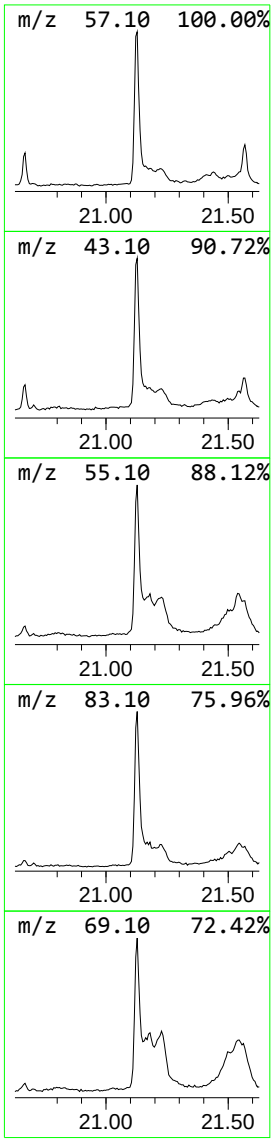
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	9.46 ng/ul	3261940	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	99
2	1-Nonadecene	266	C19H38	018435-45-5	97
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

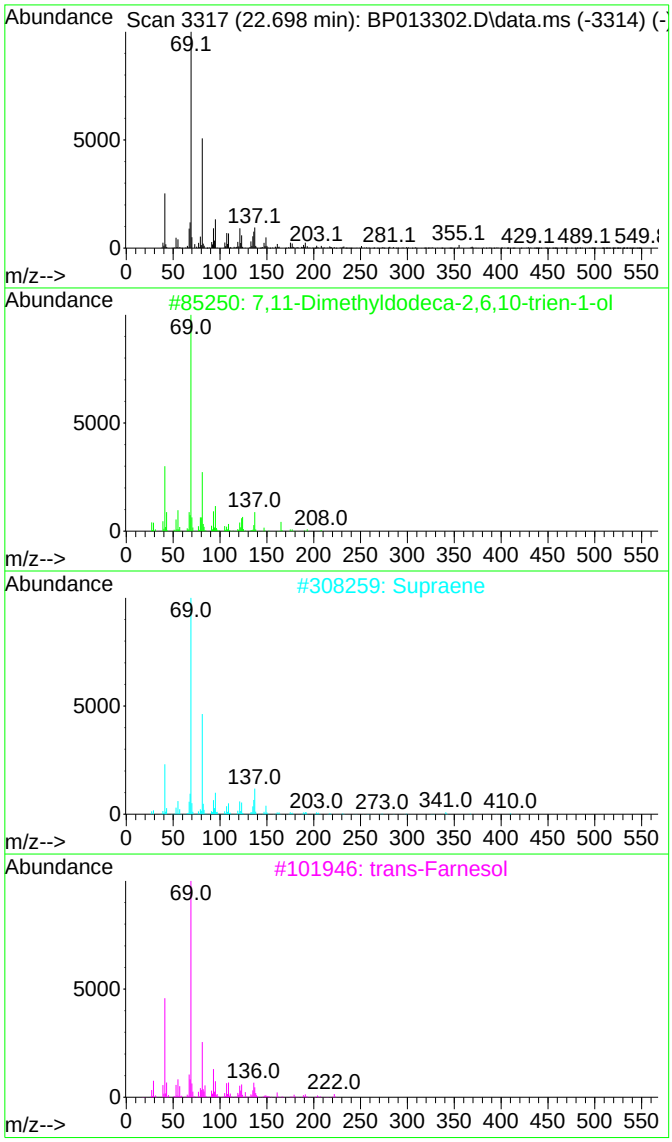
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

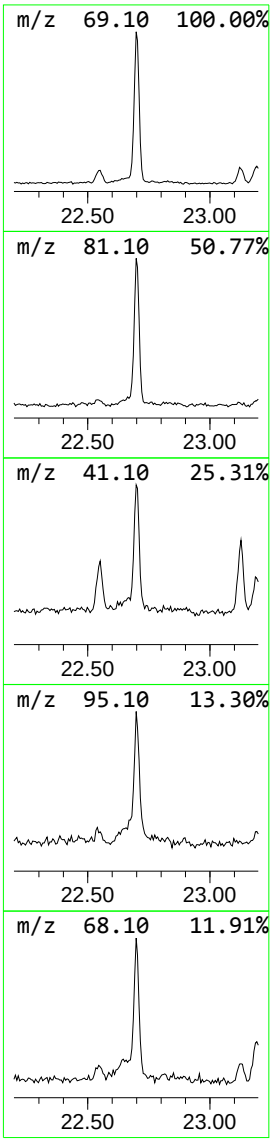
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 7,11-Dimethyldodeca-2,6,10-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.698	2.30 ng/ul	865469	Perylene-d12	23.915

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	87
2	Supraene	410	C30H50	007683-64-9	86
3	trans-Farnesol	222	C15H26O	000106-28-5	80
4	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
5	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

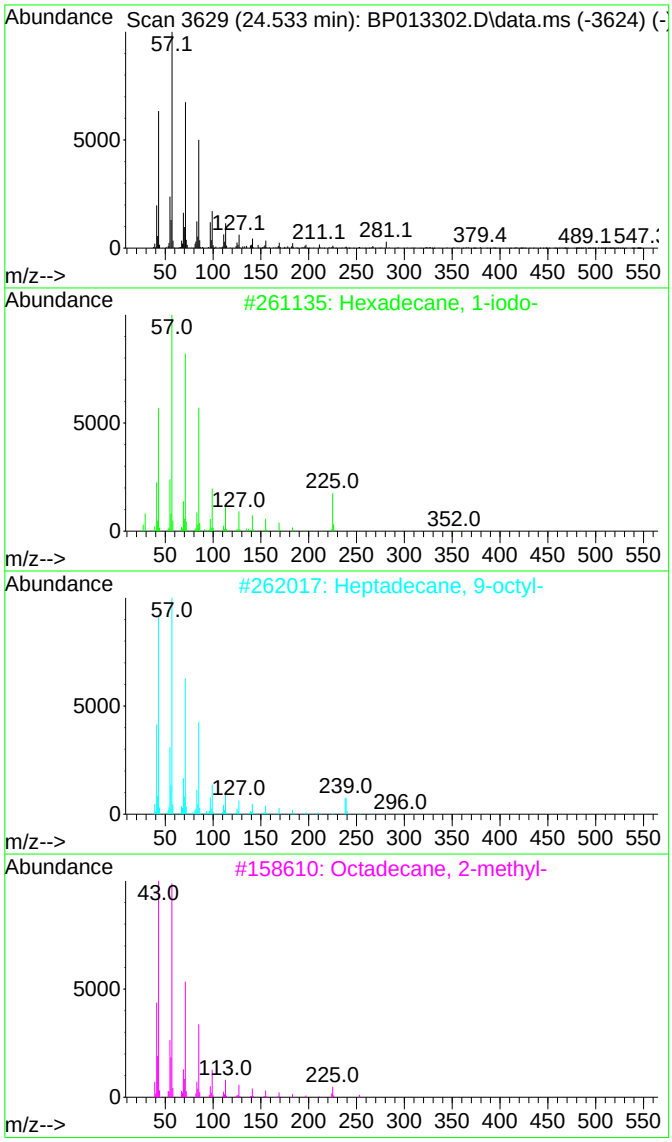
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

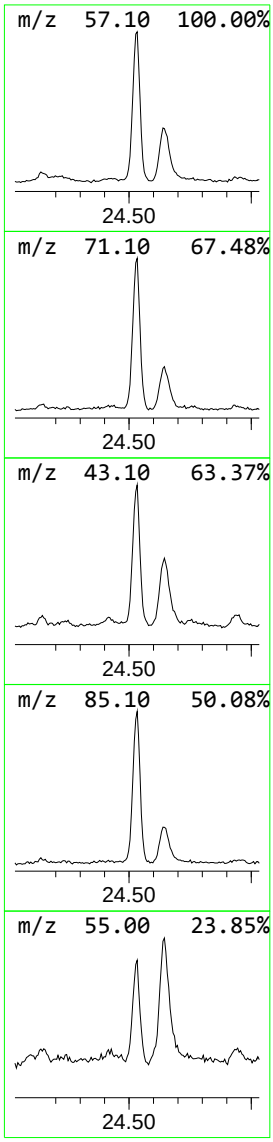
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexadecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.533	4.40 ng/ul	1656660	Perylene-d12	23.915

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	95
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
4	Tricosane	324	C23H48	000638-67-5	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90





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Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

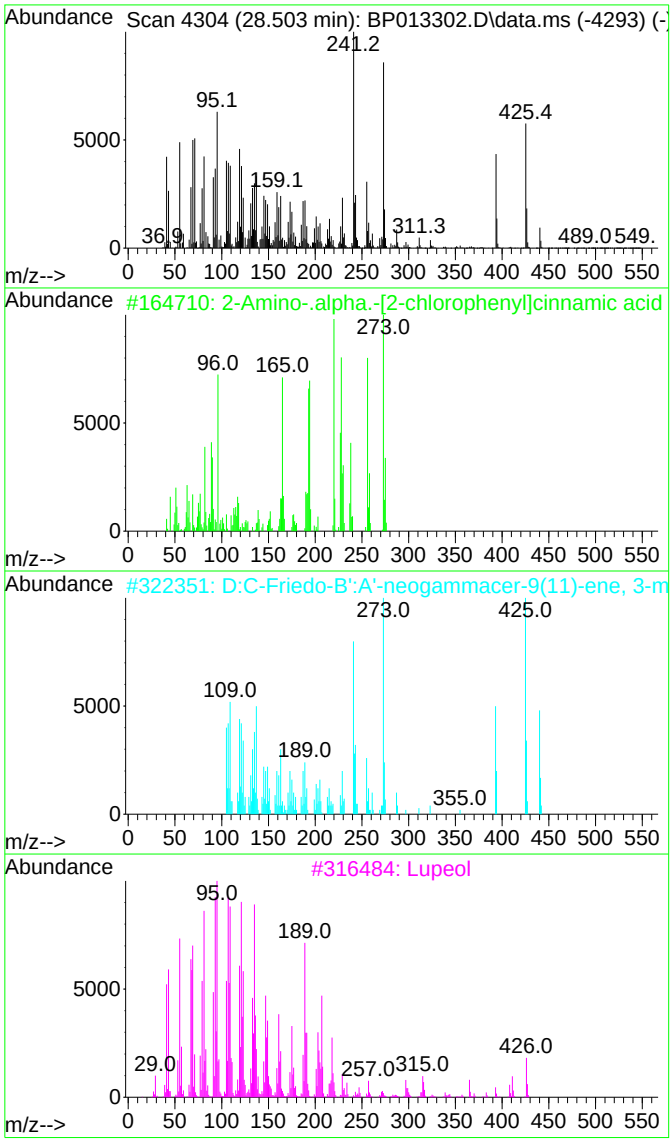
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

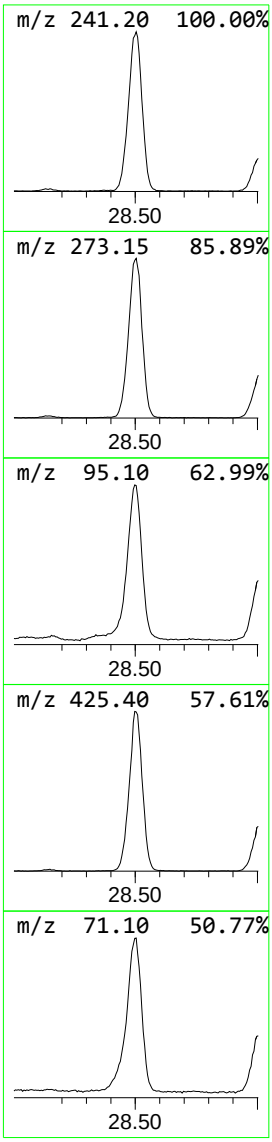
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Amino-.alpha.-[2-chloroph... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.503	60.05 ng/ul	22608100	Perylene-d12	23.915

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	59
2	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	50
3	Lupeol	426	C30H50O	000545-47-1	30
4	Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	25
5	2-(1H-Indol-3-ylmethylene)-1H-in...	273	C18H11NO2	031060-64-7	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

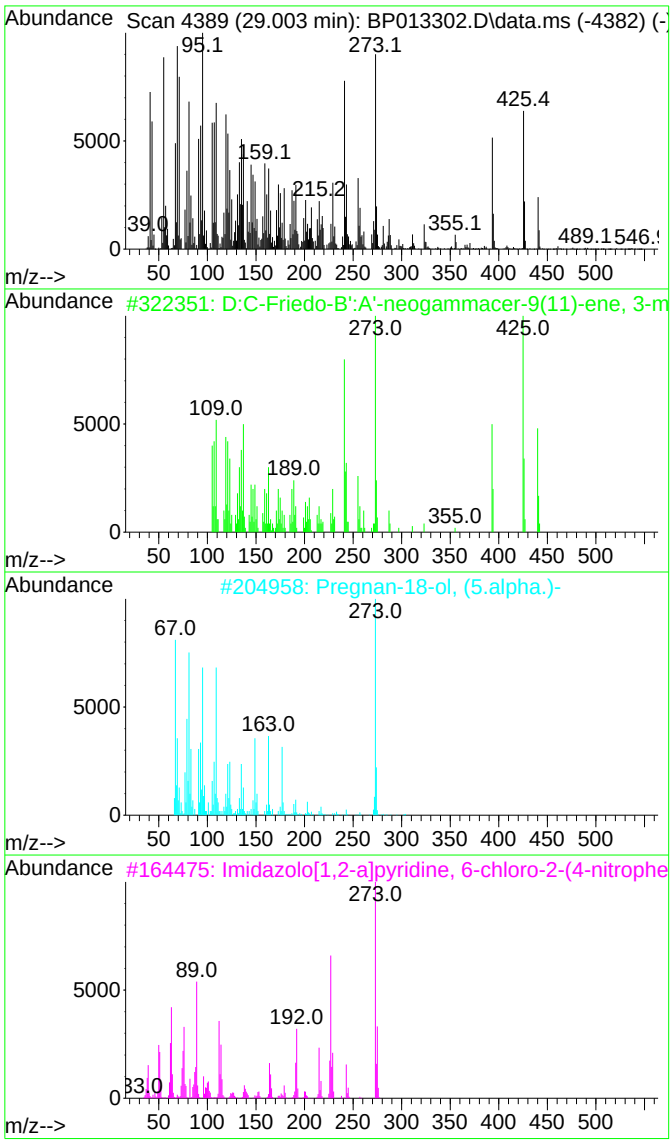
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

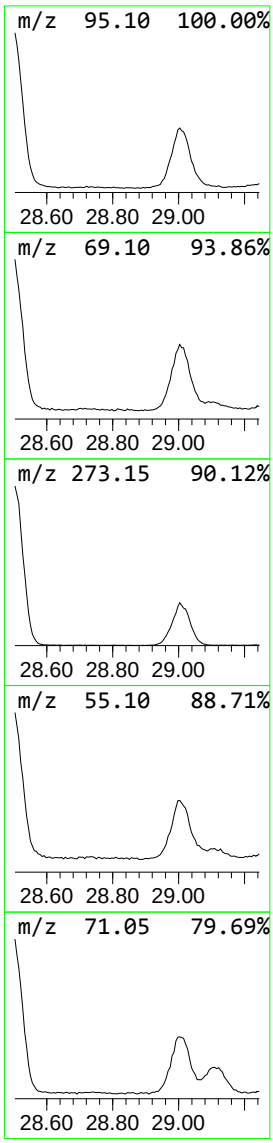
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 D:C-Friedo-B':A'-neogammace... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.003	23.49 ng/ul	8844550	Perylene-d12	23.915

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	86
2	Pregnan-18-ol, (5.alpha.)-	304	C21H36O	056053-09-9	60
3	Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	56
4	9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	38
5	3-Ethyl-2,8-dimethyl-4-quinolino...	273	C16H23NOSi	1000474-26-4	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013302.D
Acq On : 24 Dec 2022 16:23
Operator : CG/JU
Sample : N6016-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD3

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	15.945	3.8	ng/ul	1396230	3	14.586	7425580	20.0
n-Hexadecanoic ...	18.216	6.8	ng/ul	2481220	4	17.345	7258040	20.0
4-(3-Fluoro-8-n...	19.827	5.4	ng/ul	1870670	5	21.433	6892740	20.0
(DEL) Alkane: S...	21.127	9.5	ng/ul	3261940	5	21.433	6892740	20.0
7,11-Dimethyldo...	22.698	2.3	ng/ul	865469	6	23.915	7529510	20.0
Hexadecane, 1-i...	24.533	4.4	ng/ul	1656660	6	23.915	7529510	20.0
2-Amino-.alpha....	28.503	60.0	ng/ul	22608100	6	23.915	7529510	20.0
D:C-Friedo-B':A...	29.003	23.5	ng/ul	8844550	6	23.915	7529510	20.0