LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013175.D
Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBYB9

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: BP013175.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.340	23	26	32	rVB	79565	106526	1.17%	0.115%
2	3.781	98	101	114	rVV	176464	280079	3.09%	0.302%
3	3.875	114	117	122	rVB2	35983	45848	0.51%	0.049%
4	3.999	134	138	143	rVB	54795	76893	0.85%	0.083%
5	4.093	152	154	159	rVB	33741	37122	0.41%	0.040%
6	4.434	209	212	215	rBV3	11464	15742	0.17%	0.017%
7	5.040	309	315	325	rVB2	222586	355054	3.91%	0.383%
8	7.111	660	667	681	rBV	1263663	2043256	22.51%	2.201%
9	7.281	689	696	704	rBV	1087833	1674189	18.45%	1.804%
10	7.481	723	730	740	rBV	1357102	2115813	23.31%	2.279%
11	7.564	742	744	753	rVB6	16808	29236	0.32%	0.031%
12	7.764	776	778	786	rVB6	7187	13486	0.15%	0.015%
13	7.952	798	810	818	rBV	1445083	2263842	24.94%	2.439%
14	8.016	818	821	827	rVB3	10625	18172	0.20%	0.020%
15	8.663	924	931	941	rBV	1260298	1985627	21.88%	2.139%
16	8.781	946	951	961	rVB	61667	108484	1.20%	0.117%
17	9.122	1001	1009	1017	rBV	1246074	2005501	22.10%	2.161%
18	9.287	1032	1037	1040	rVB7	9513	13477	0.15%	0.015%
19	9.522	1070	1077	1085	rBV	41402	70433	0.78%	0.076%
20	9.846	1125	1132	1146	rBV	1036678	1685053	18.57%	1.815%
21	10.181	1183	1189	1200	rVB3	58226	106580	1.17%	0.115%
22	10.387	1214	1224	1233	rBV	1506949	2551529	28.11%	2.749%
23	10.546	1245	1251	1261	rVB5	35537	62575	0.69%	0.067%
24	10.769	1281	1289	1297	rBV	1859969	3127771	34.46%	3.370%
25	10.905	1304	1312	1328	rBV	1179627	2074068	22.85%	2.234%
26	11.134	1344	1351	1353	rBV8	5129	13200	0.15%	0.014%
27	11.240	1366	1369	1374	rVV6	6252	9744	0.11%	0.010%
28	11.299	1376	1379	1380	rVV3	7658	9100	0.10%	0.010%
29	11.310	1380	1381	1389	rVB8	10265	10887	0.12%	0.012%
30	11.557	1419	1423	1426	rBV6	5878	11150	0.12%	0.012%
31	12.175	1523	1528	1533	rBV8	12933	21587	0.24%	0.023%
32	12.352	1552	1558	1566	rVB2	27494	45282	0.50%	0.049%
33	12.557	1590	1593	1602	rVB2	4900	12140	0.13%	0.013%
34	12.987	1658	1666	1670	rVB2	6865	13217	0.15%	0.014%
35	13.410	1733	1738	1745	rVB	41646	58913	0.65%	0.063%
36	13.487	1746	1751	1754	rBV5	10927	17083	0.19%	0.018%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

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	13.581	1761	1767	1773	rVB5	14934	28503	0.31%	0.031%
38	13.763	1792	1798	1803	rBV9	15594	24421	0.27%	0.026%
39	13.916	1819	1824	1828	rBV7	13583	19771	0.22%	0.021%
40	13.998	1831	1838	1848	rBV	2514041	3621724	39.90%	3.902%
41	14.116	1853	1858	1863	rVB9	13527	28006	0.31%	0.030%
42	14.240	1874	1879	1880	rBV5	6249	9697	0.11%	0.010%
43	14.287	1880	1887	1901	rVV	2969525	4433862	48.85%	4.777%
44	14.481	1914	1920	1924	rVB3	23591	30896	0.34%	0.033%
45	14.593	1931	1939	1947	rBV	2591315	3958822	43.62%	4.265%
46	14.793	1966	1973	1987	rBV	783707	1356905	14.95%	1.462%
47	14.946	1996	1999	2004	rVB6	16563	22843	0.25%	0.025%
48	15.010	2004	2010	2015	rBV6	47080	76843	0.85%	0.083%
49	15.434	2080	2082	2087	rVB5	12429	14140	0.16%	0.015%
50	15.587	2101	2108	2118	rBV	3837463	5534625	60.98%	5.962%
51	15.704	2123	2128	2139	rVV	880288	1227641	13.53%	1.323%
52	15.828	2145	2149	2155	rVB3	21169	33653	0.37%	0.036%
53	15.951	2165	2170	2179	rVB	322418	450803	4.97%	0.486%
54	16.175	2204	2208	2212	rVB7	7955	12884	0.14%	0.014%
55	16.298	2226	2229	2231	rBV4	11478	13495	0.15%	0.015%
56	16.734	2300	2303	2307	rBV6	15362	19235	0.21%	0.021%
57	16.887	2325	2329	2336	rVB	24458	33351	0.37%	0.036%
58	17.234	2384	2388	2391	rBV5	23527	33100	0.36%	0.036%
59	17.298	2396	2399	2402	rBV5	17179	22402	0.25%	0.024%
60	17.351	2402	2408	2419	rVV	3173154	4511062	49.70%	4.860%
61	17.451	2419	2425	2433	rVV	3896678	5551867	61.17%	5.981%
62	17.539	2437	2440	2448	rVB3	51961	75340	0.83%	0.081%
63	17.728	2469	2472	2475	rVB5	17791	20818	0.23%	0.022%
64	18.004	2517	2519	2525	rVB7	21160	27619	0.30%	0.030%
65	18.163	2543	2546	2550	rBV5	21310	29458	0.32%	0.032%
66	18.222	2551	2556	2566	rBV	536386	790305	8.71%	0.851%
67	18.416	2586	2589	2593	rVB	62205	70258	0.77%	0.076%
68	18.469	2596	2598	2601	rVB2	28187	27029	0.30%	0.029%
69	18.634	2622	2626	2630	rBV	274977	319506	3.52%	0.344%
70	18.786	2648	2652	2659	rVB	146421	185950	2.05%	0.200%
71	19.257	2729	2732	2736	rVB2	71646	90465	1.00%	0.097%
72	19.334	2740	2745	2748	rBV2	110848	209021	2.30%	0.225%
73	19.451	2762	2765	2773	rBV4	145911	222071	2.45%	0.239%
74	19.681	2799	2804	2816	rBV	5614297	7430563	81.87%	8.005%
75	19.828	2825	2829	2837	rBV	744600	922723	10.17%	0.994%
76	21.128	3046	3050	3060	rBV	1226717	1653404	18.22%	1.781%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013175.D
Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

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	21.439	3098	3103	3114	rVB	4018127	5444653	59.99%	5.866%
78	23.133	3386	3391	3398	rBV	1588159	2593791	28.58%	2.794%
79	23.757	3490	3497	3512	rVB2	4299817	9076170	100.00%	9.778%
80	23.916	3518	3524	3536	rVB2	2961534	6277180	69.16%	6.762%
81	24.539	3624	3630	3638	rVB	1502576	3198437	35.24%	3.446%

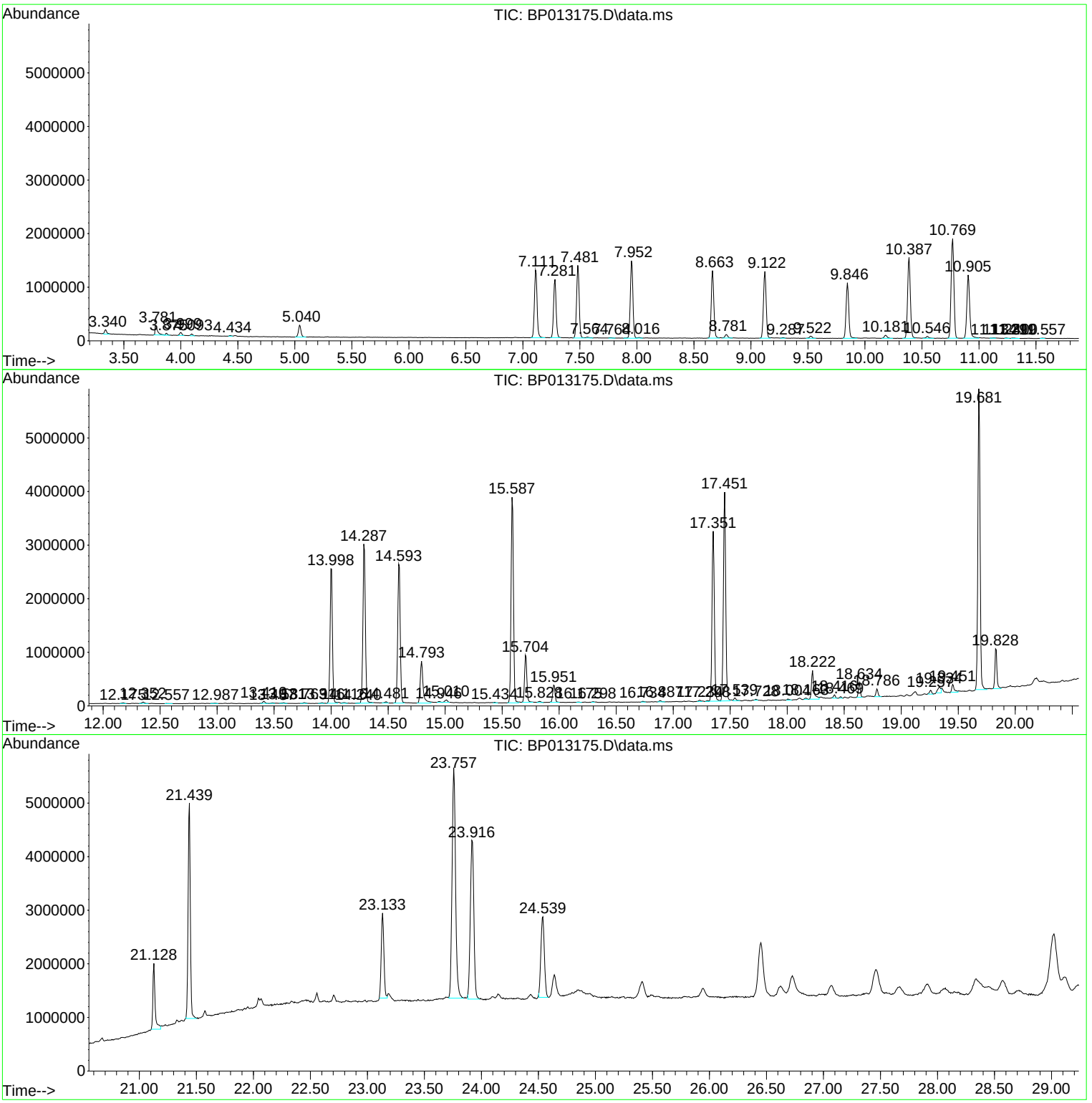
Sum of corrected areas: 92823971

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013175.D
Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

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 : BP013175.D
Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

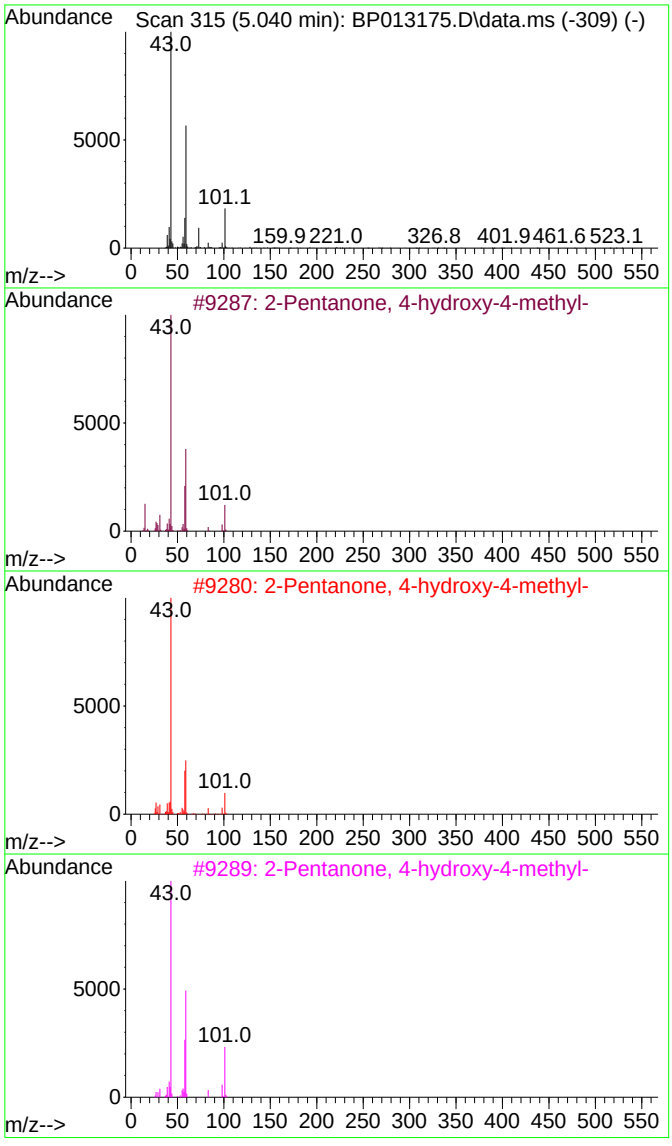
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

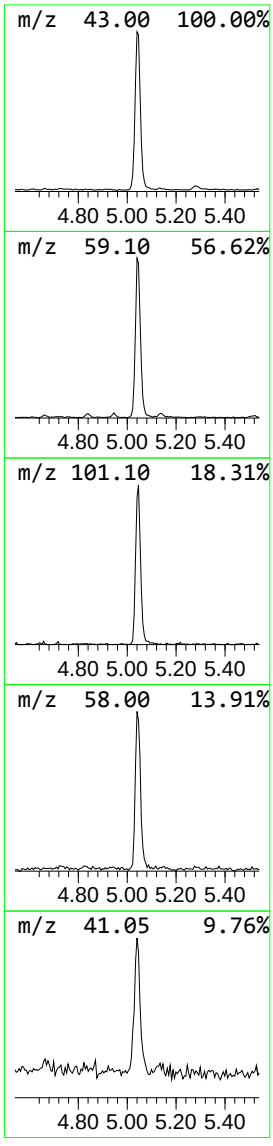
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	3.14 ng/ul	355054	1,4-Dichlorobenzene-d4	7.952

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
5	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013175.D
Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

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

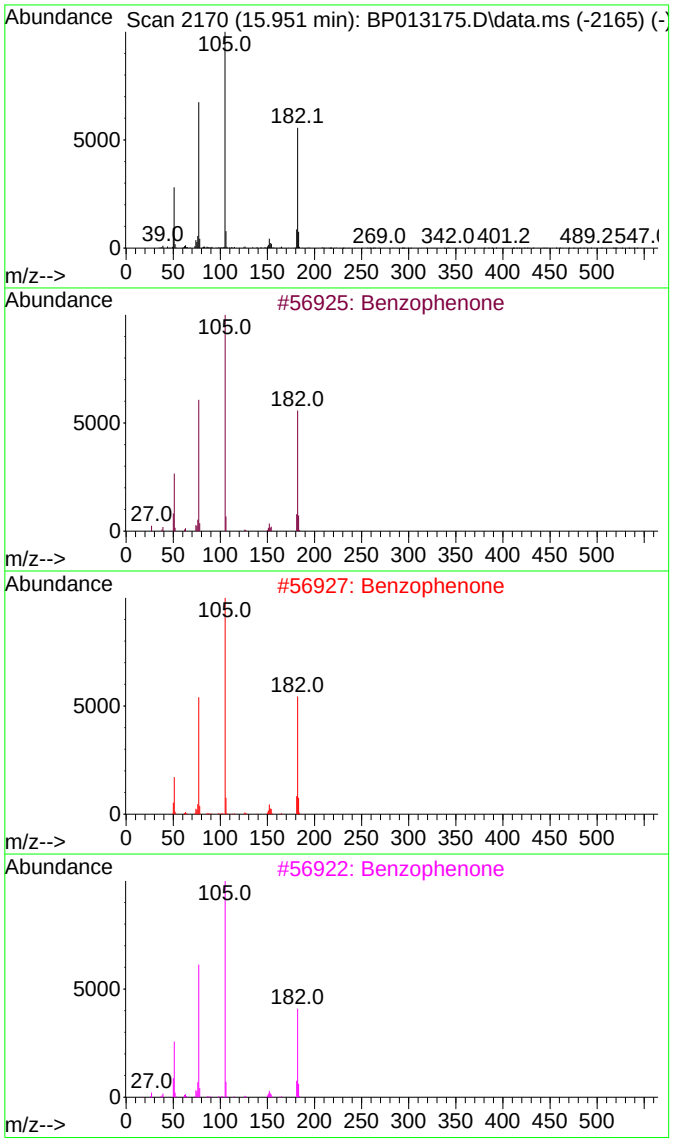
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

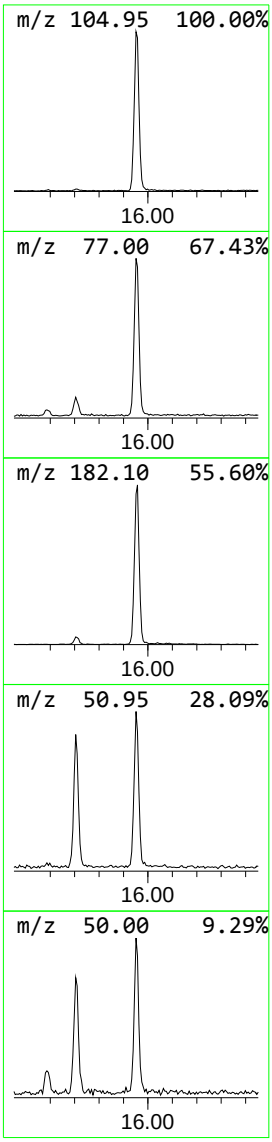
****

Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.28 ng/ul	450803	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	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013175.D
Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

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

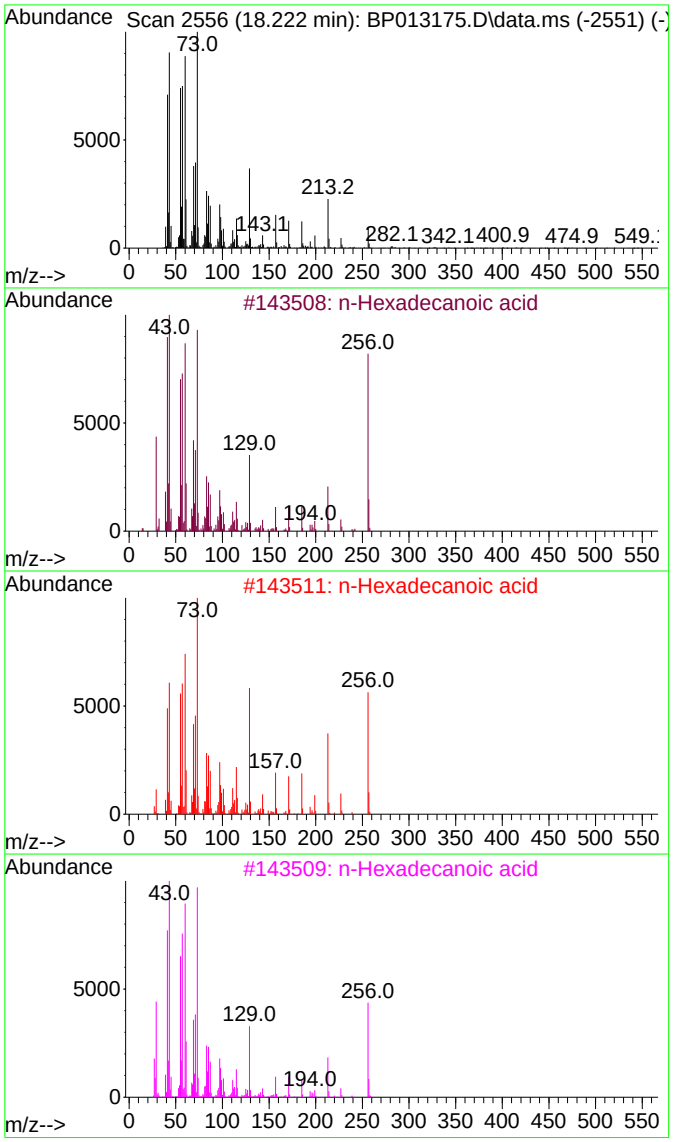
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

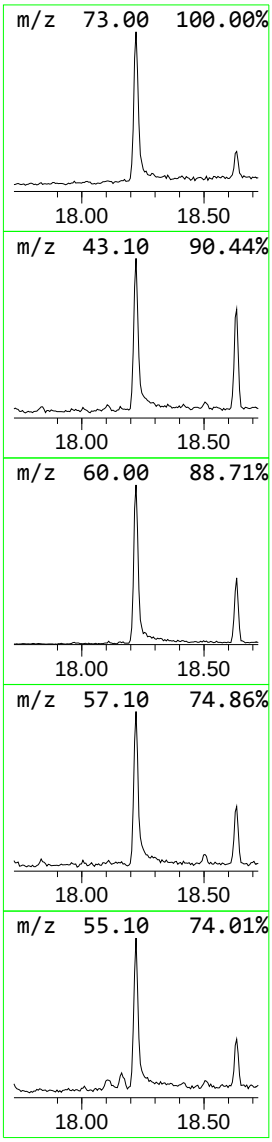
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	3.50 ng/ul	790305	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
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	98
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013175.D
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Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

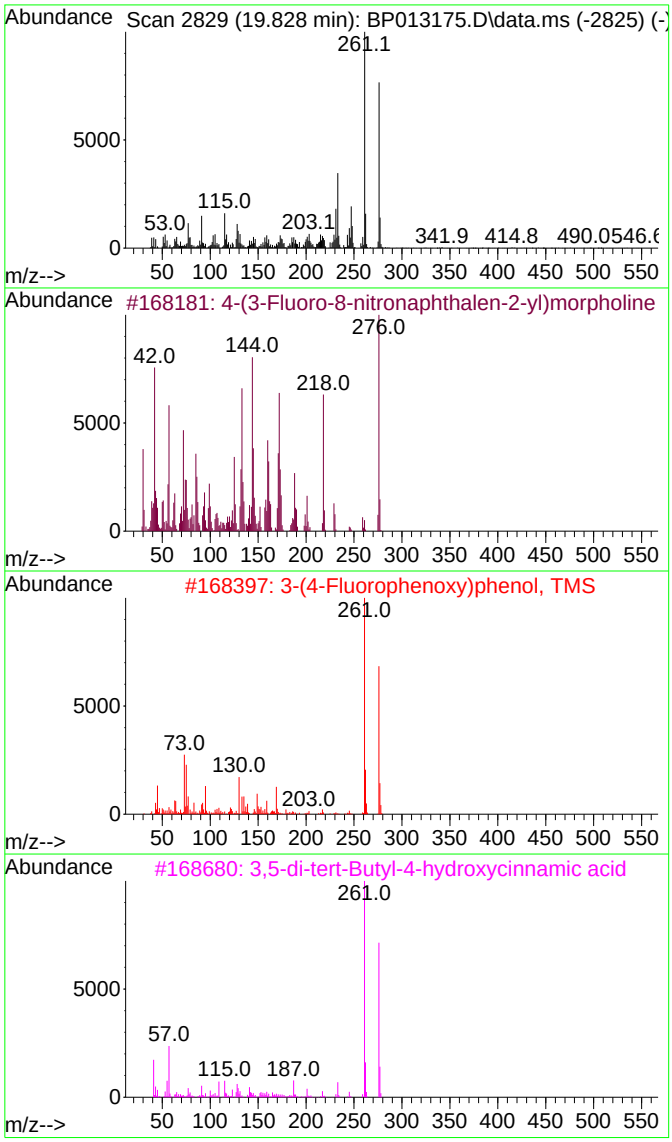
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

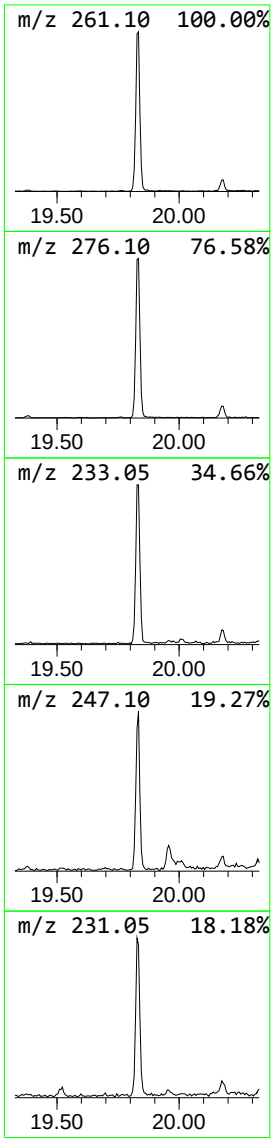
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.828	3.39 ng/ul	922723	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(3-Fluoro-8-nitronaphthalen-2-...	276	C14H13FN2O3	1000409-37-1	93
2	3-(4-Fluorophenoxy)phenol, TMS	276	C15H17FO2Si	1000495-60-9	70
3	3,5-di-tert-Butyl-4-hydroxycinna...	276	C17H24O3	022014-01-3	68
4	3-Methoxy-5-pentyl-2-prenylpheno...	276	C18H28O2	083036-53-7	64
5	(1H)Pyrrole, 3,4-dimethyl-5-meth...	276	C15H20N2OS	1000197-22-6	58





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Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

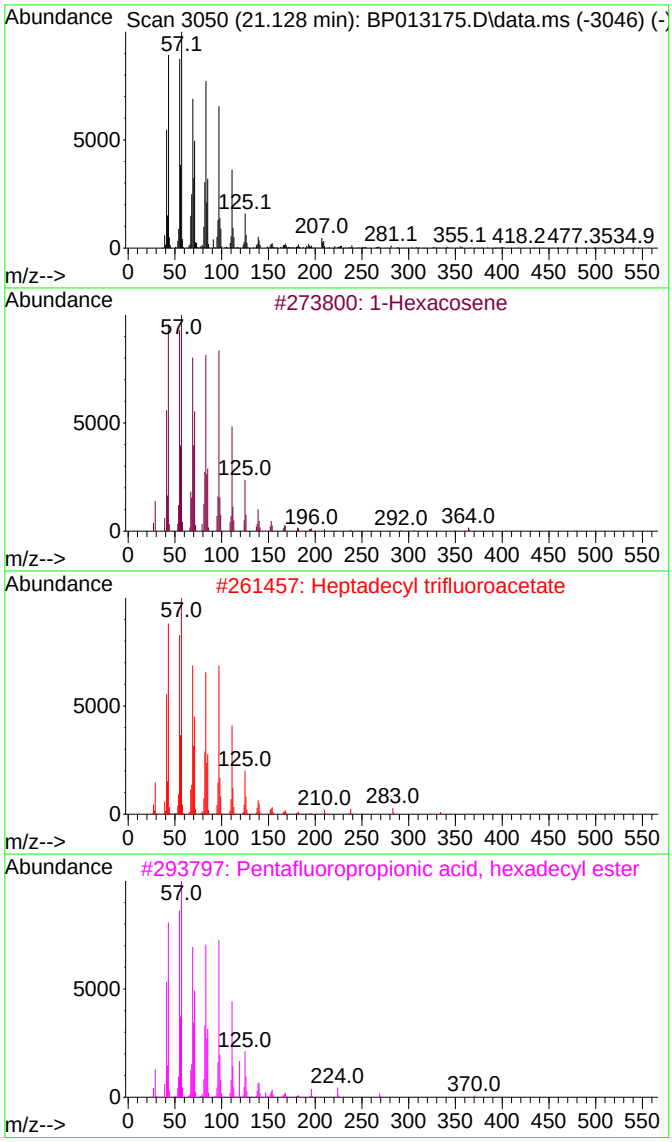
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

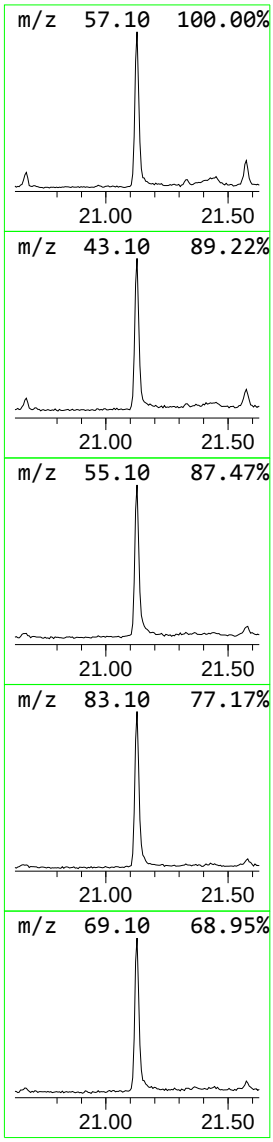
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	6.07 ng/ul	1653400	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	1-Tetracosene	336	C24H48	010192-32-2	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013175.D
Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

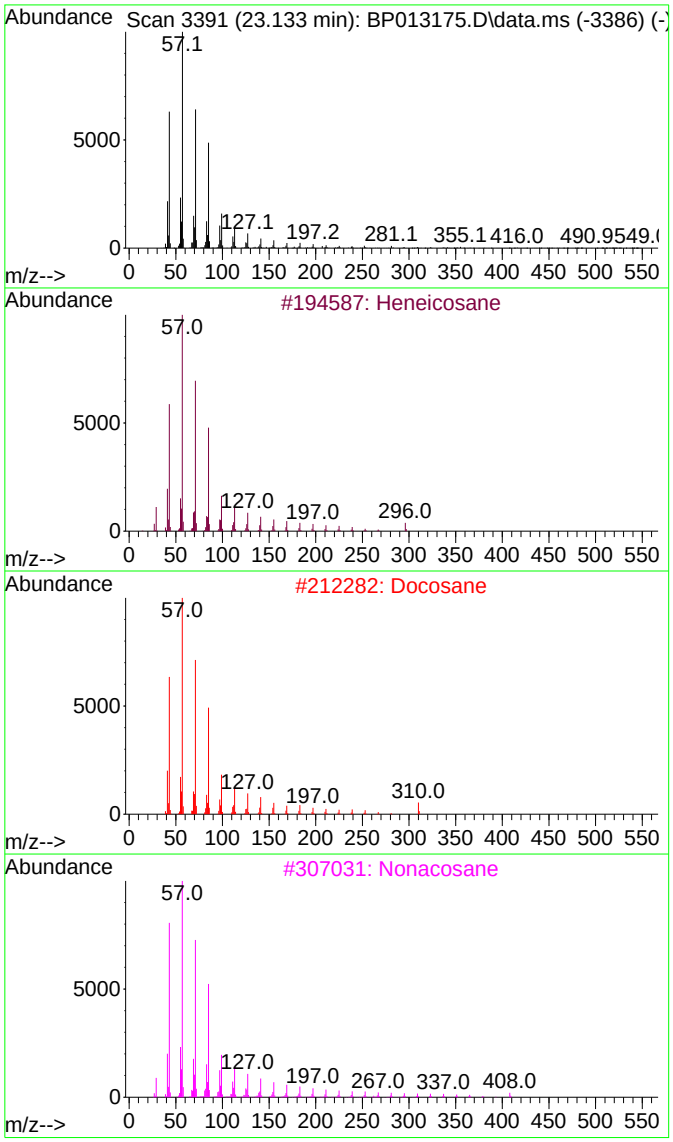
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

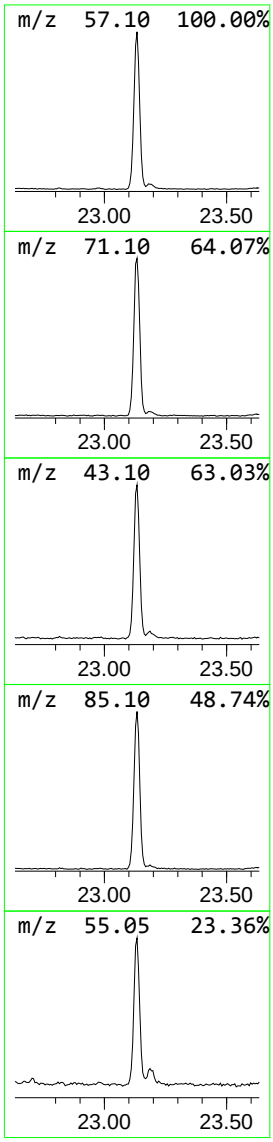
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.133	8.26 ng/ul	2593790	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Docosane	310	C22H46	000629-97-0	97
3	Nonacosane	408	C29H60	000630-03-5	97
4	Tetracosane	338	C24H50	000646-31-1	97
5	Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013175.D
Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

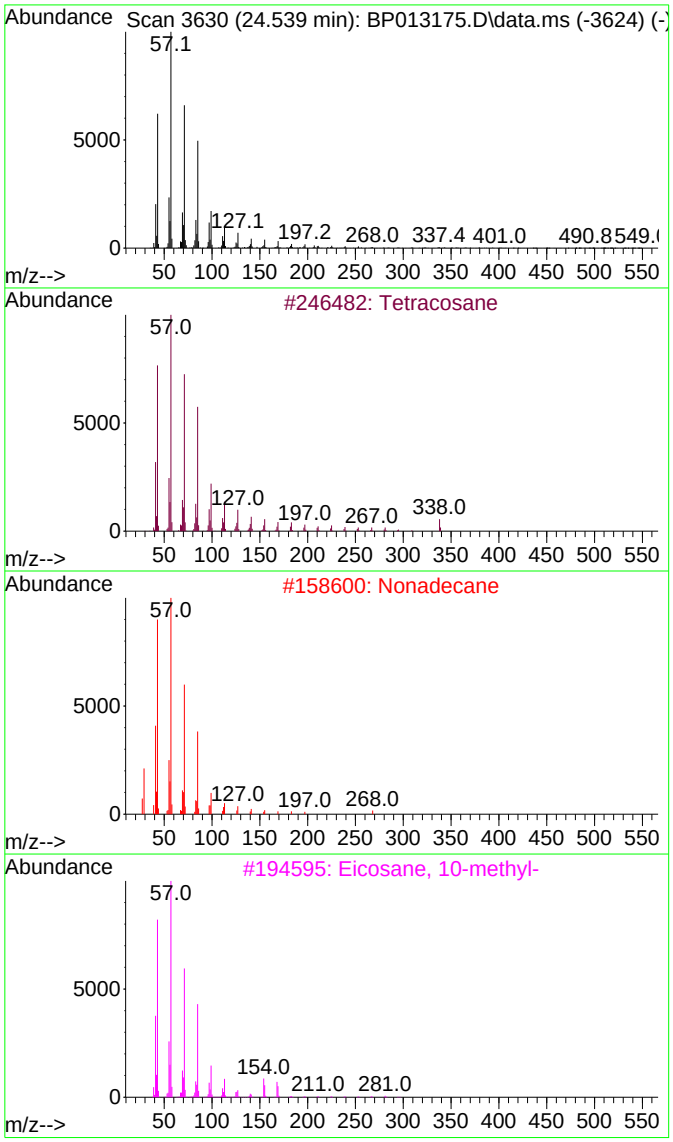
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

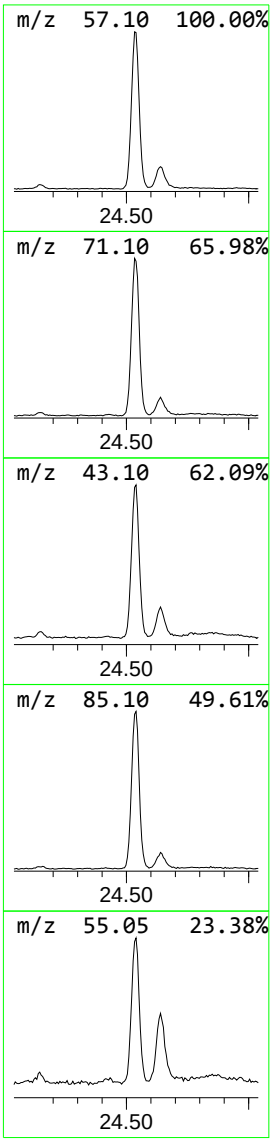
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.539	10.19 ng/ul	3198440	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Nonadecane	268	C19H40	000629-92-5	93
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013175.D
Acq On : 20 Dec 2022 19:55
Operator : CG/JU
Sample : N6009-06
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB9

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
2-Pentanone, 4-...	5.040	3.1	ng/ul	355054	1	7.952	2263840	20.0
Benzophenone	15.951	2.3	ng/ul	450803	3	14.593	3958820	20.0
n-Hexadecanoic ...	18.222	3.5	ng/ul	790305	4	17.351	4511060	20.0
4-(3-Fluoro-8-n...	19.828	3.4	ng/ul	922723	5	21.439	5444650	20.0
(DEL) Alkane: S...	21.128	6.1	ng/ul	1653400	5	21.439	5444650	20.0
(DEL) Alkane: S...	23.133	8.3	ng/ul	2593790	6	23.916	6277180	20.0
(DEL) Alkane: S...	24.539	10.2	ng/ul	3198440	6	23.916	6277180	20.0