LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038173.D
Acq On : 21 Dec 2022 15:48
Operator : CG/JU
Sample : N6014-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR2

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-BM120722.M
Title : SVOA CALIBRATION

Signal : TIC: BM038173.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.393	31	35	44	rBV	28448	48115	1.57%	0.106%
2	3.828	106	109	125	rBV	368953	639612	20.89%	1.408%
3	4.052	144	147	151	rVB5	5010	7241	0.24%	0.016%
4	4.163	162	166	172	rVB	15630	24393	0.80%	0.054%
5	5.122	324	329	334	rVB2	12972	19676	0.64%	0.043%
6	5.357	364	369	371	rBV5	4859	6993	0.23%	0.015%
7	5.587	400	408	414	rBV5	4227	11029	0.36%	0.024%
8	6.022	479	482	488	rBV6	3050	5414	0.18%	0.012%
9	6.704	591	598	604	rVV	126445	195918	6.40%	0.431%
10	7.028	648	653	656	rVV6	3724	6790	0.22%	0.015%
11	7.204	675	683	693	rVB	583002	932375	30.45%	2.053%
12	7.369	703	711	718	rBV	426866	666086	21.75%	1.466%
13	7.569	738	745	752	rBV	612159	946473	30.91%	2.084%
14	8.040	816	825	833	rBV	668595	1022729	33.40%	2.252%
15	8.751	938	946	955	rBV	657550	1088886	35.56%	2.397%
16	9.216	1017	1025	1031	rBV	568260	934681	30.52%	2.058%
17	9.369	1045	1051	1057	rVB7	9265	15900	0.52%	0.035%
18	9.592	1084	1089	1094	rVV3	12182	23801	0.78%	0.052%
19	9.628	1094	1095	1103	rVB7	5730	5613	0.18%	0.012%
20	9.939	1140	1148	1156	rVV	485165	800355	26.14%	1.762%
21	10.092	1168	1174	1181	rBV2	15922	31053	1.01%	0.068%
22	10.163	1181	1186	1190	rVV6	7705	12888	0.42%	0.028%
23	10.475	1230	1239	1247	rBV	796419	1292366	42.20%	2.845%
24	10.857	1296	1304	1311	rVV	915782	1493407	48.77%	3.288%
25	10.998	1321	1328	1338	rBV	662900	1124395	36.72%	2.475%
26	11.063	1338	1339	1347	rVB7	4371	6200	0.20%	0.014%
27	11.634	1430	1436	1441	rVB6	4400	8460	0.28%	0.019%
28	11.863	1468	1475	1480	rBV8	4372	8763	0.29%	0.019%
29	12.251	1537	1541	1545	rVB3	7012	10094	0.33%	0.022%
30	12.433	1568	1572	1577	rBV2	12803	19174	0.63%	0.042%
31	12.510	1580	1585	1590	rVV5	5693	8969	0.29%	0.020%
32	12.645	1602	1608	1613	rBV10	2941	5800	0.19%	0.013%
33	12.728	1618	1622	1625	rBV5	5788	7814	0.26%	0.017%
34	12.939	1655	1658	1664	rBV6	4182	7812	0.26%	0.017%
35	13.480	1744	1750	1756	rVV2	16308	26794	0.87%	0.059%
36	13.557	1759	1763	1766	rVB5	4746	7711	0.25%	0.017%

LSC Area Percent Report

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Operator : CG/JU
Sample : N6014-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR2

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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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Title : SVOA CALIBRATION

37	13.598	1766	1770	1775	rBV6	6837	12707	0.41%	0.028%
38	13.992	1832	1837	1842	rBV5	24798	41408	1.35%	0.091%
39	14.075	1842	1851	1858	rVV	1273453	1754731	57.30%	3.863%
40	14.139	1860	1862	1867	rVV6	9550	10772	0.35%	0.024%
41	14.369	1894	1901	1910	rVB	1458285	2191052	71.55%	4.824%
42	14.498	1917	1923	1926	rBV7	3817	7885	0.26%	0.017%
43	14.545	1926	1931	1934	rVB3	11029	17043	0.56%	0.038%
44	14.622	1940	1944	1946	rBV5	7585	11025	0.36%	0.024%
45	14.669	1946	1952	1959	rVB	1368379	1918052	62.64%	4.223%
46	14.733	1959	1963	1964	rBV4	5337	6011	0.20%	0.013%
47	14.869	1979	1986	1997	rBV	522858	805407	26.30%	1.773%
48	15.069	2016	2020	2025	rVB6	19695	25942	0.85%	0.057%
49	15.122	2025	2029	2032	rBV6	4368	5974	0.20%	0.013%
50	15.445	2078	2084	2087	rBV6	5299	9475	0.31%	0.021%
51	15.486	2088	2091	2096	rVB4	10412	15717	0.51%	0.035%
52	15.569	2098	2105	2107	rBV6	4620	8598	0.28%	0.019%
53	15.657	2113	2120	2127	rBV	2006909	2635518	86.07%	5.802%
54	15.774	2135	2140	2147	rBV	246620	347613	11.35%	0.765%
55	15.892	2154	2160	2165	rBV7	12064	18656	0.61%	0.041%
56	15.986	2171	2176	2177	rBV5	7346	10509	0.34%	0.023%
57	16.016	2177	2181	2190	rVB	44186	66091	2.16%	0.145%
58	16.110	2192	2197	2200	rBV7	4635	9010	0.29%	0.020%
59	16.221	2210	2216	2223	rVB10	5530	11991	0.39%	0.026%
60	16.351	2235	2238	2239	rBV2	13696	12685	0.41%	0.028%
61	16.433	2250	2252	2258	rVB8	4254	6782	0.22%	0.015%
62	16.498	2258	2263	2268	rBV2	52781	83724	2.73%	0.184%
63	16.545	2268	2271	2273	rVV2	11613	16193	0.53%	0.036%
64	16.574	2274	2276	2279	rVB4	9341	9027	0.29%	0.020%
65	16.792	2309	2313	2320	rVV3	27143	41557	1.36%	0.091%
66	16.851	2320	2323	2327	rVB5	6825	9486	0.31%	0.021%
67	17.057	2356	2358	2363	rVB5	6526	9027	0.29%	0.020%
68	17.139	2369	2372	2376	rBV5	15054	20229	0.66%	0.045%
69	17.192	2379	2381	2385	rVB5	7760	8811	0.29%	0.019%
70	17.286	2392	2397	2404	rBV	64528	102283	3.34%	0.225%
71	17.351	2404	2408	2412	rBV2	44269	63223	2.06%	0.139%
72	17.410	2412	2418	2423	rBV	1575439	2215164	72.34%	4.877%
73	17.504	2428	2434	2441	rVB	1872052	2664761	87.02%	5.866%
74	17.598	2447	2450	2455	rVB6	15534	28024	0.92%	0.062%
75	17.674	2459	2463	2473	rBV6	26873	53276	1.74%	0.117%
76	17.751	2473	2476	2478	rBV3	12205	14947	0.49%	0.033%

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Instrument :
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Integration Parameters: LSCINT.P
Integrator: RTE
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77	17.880	2495	2498	2501	rBV2	13554	19077	0.62%	0.042%
78	17.921	2502	2505	2512	rVB6	18964	28877	0.94%	0.064%
79	18.021	2520	2522	2525	rVB4	13202	11847	0.39%	0.026%
80	18.057	2526	2528	2533	rVB6	13454	15075	0.49%	0.033%
81	18.168	2541	2547	2553	rBV2	65601	124357	4.06%	0.274%
82	18.227	2553	2557	2562	rVV	148466	211483	6.91%	0.466%
83	18.286	2562	2567	2583	rVV	1146789	1657636	54.13%	3.649%
84	18.580	2613	2617	2622	rBV5	45533	73458	2.40%	0.162%
85	18.633	2622	2626	2630	rVB4	29896	41028	1.34%	0.090%
86	18.704	2634	2638	2642	rBV	107035	127262	4.16%	0.280%
87	19.198	2719	2722	2726	rBV5	31130	47848	1.56%	0.105%
88	19.298	2735	2739	2743	rBV3	29036	42290	1.38%	0.093%
89	19.415	2754	2759	2760	rBV2	104874	138497	4.52%	0.305%
90	19.457	2760	2766	2775	rVV2	205863	462844	15.11%	1.019%
91	19.551	2778	2782	2795	rBV	416436	644034	21.03%	1.418%
92	19.792	2817	2823	2835	rBV	2291891	3062216	100.00%	6.741%
93	20.756	2984	2987	2991	rBV2	176247	218533	7.14%	0.481%
94	21.262	3068	3073	3085	rVB2	946960	1548362	50.56%	3.409%
95	21.574	3122	3126	3131	rVB	1526476	2041252	66.66%	4.494%
96	23.239	3405	3409	3413	rBV	304232	433891	14.17%	0.955%
97	23.868	3510	3516	3523	rVB2	1257374	2383011	77.82%	5.246%
98	24.027	3538	3543	3551	rVB	863714	1655998	54.08%	3.646%
99	24.521	3620	3627	3635	rVB2	1383281	2799862	91.43%	6.164%
100	24.609	3637	3642	3652	rVB	425986	860519	28.10%	1.894%

Sum of corrected areas: 45423423

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Instrument :
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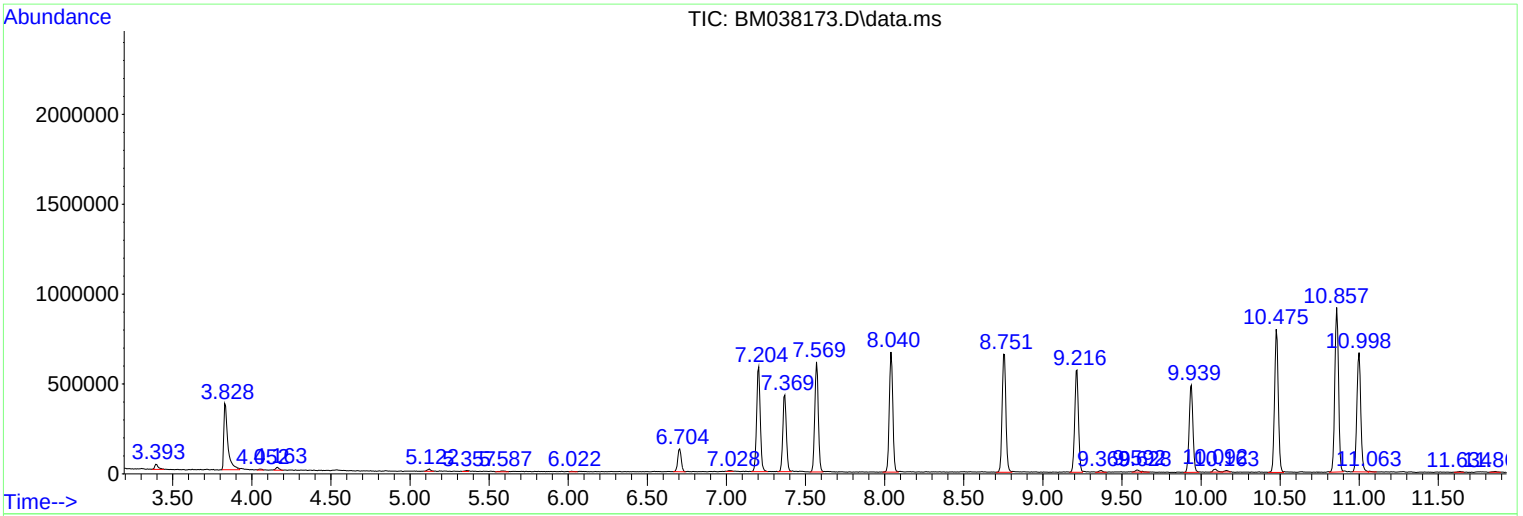
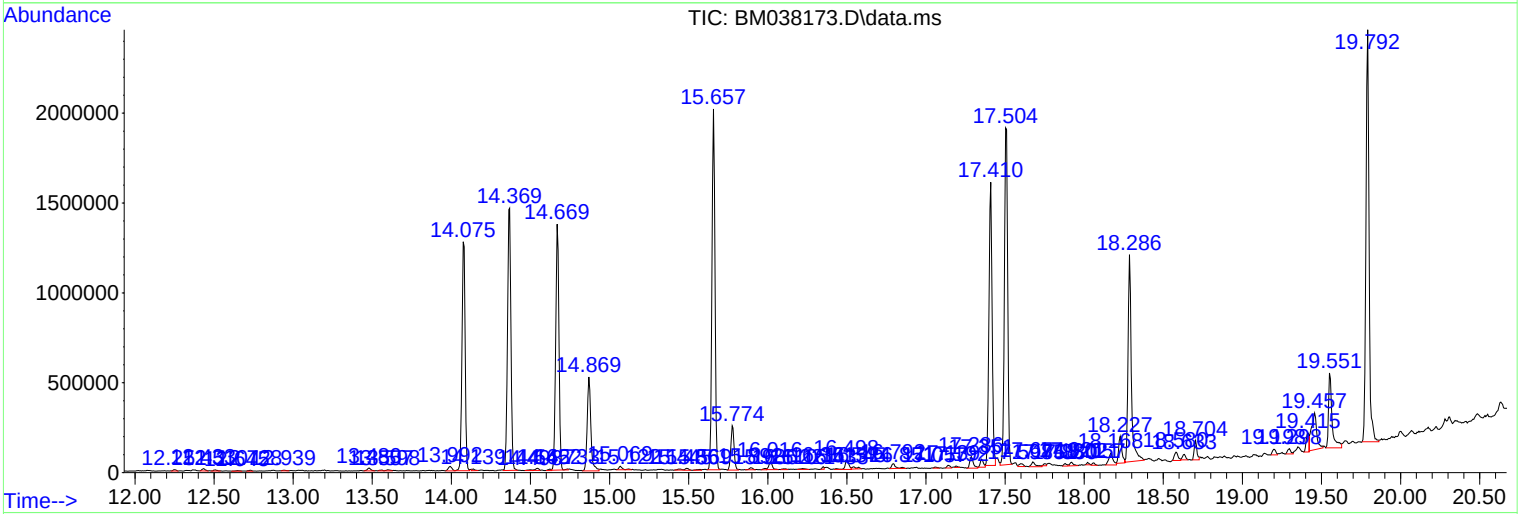
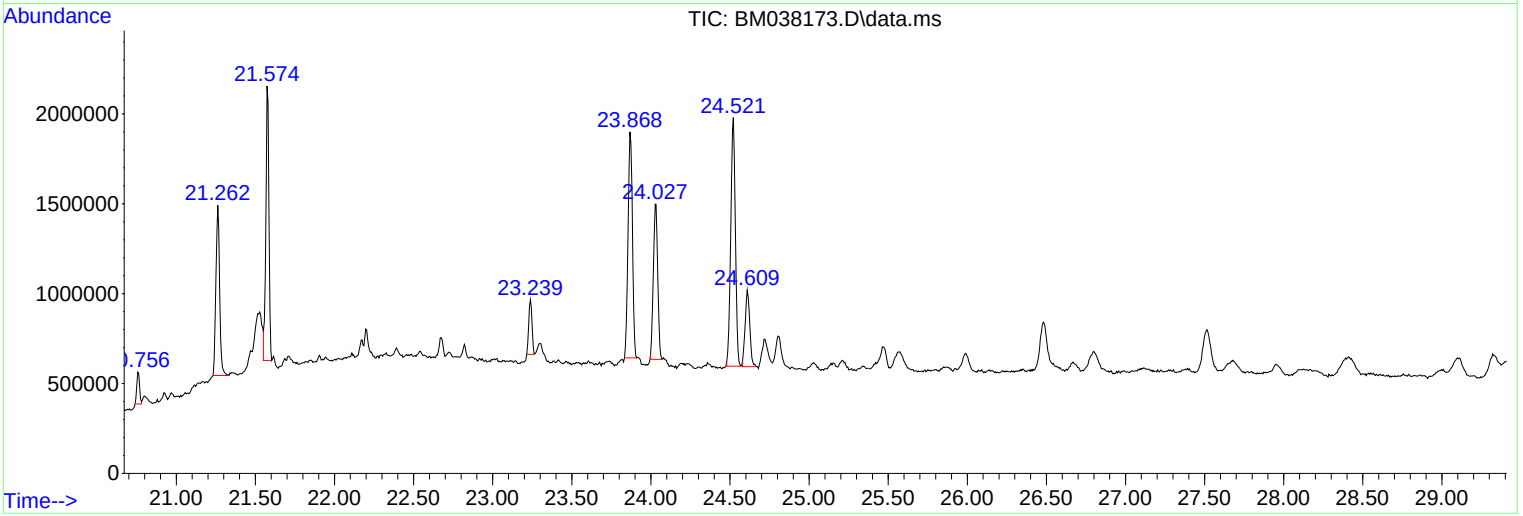
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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







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Instrument :
BNA_M
ClientSampleId :
DBXR2

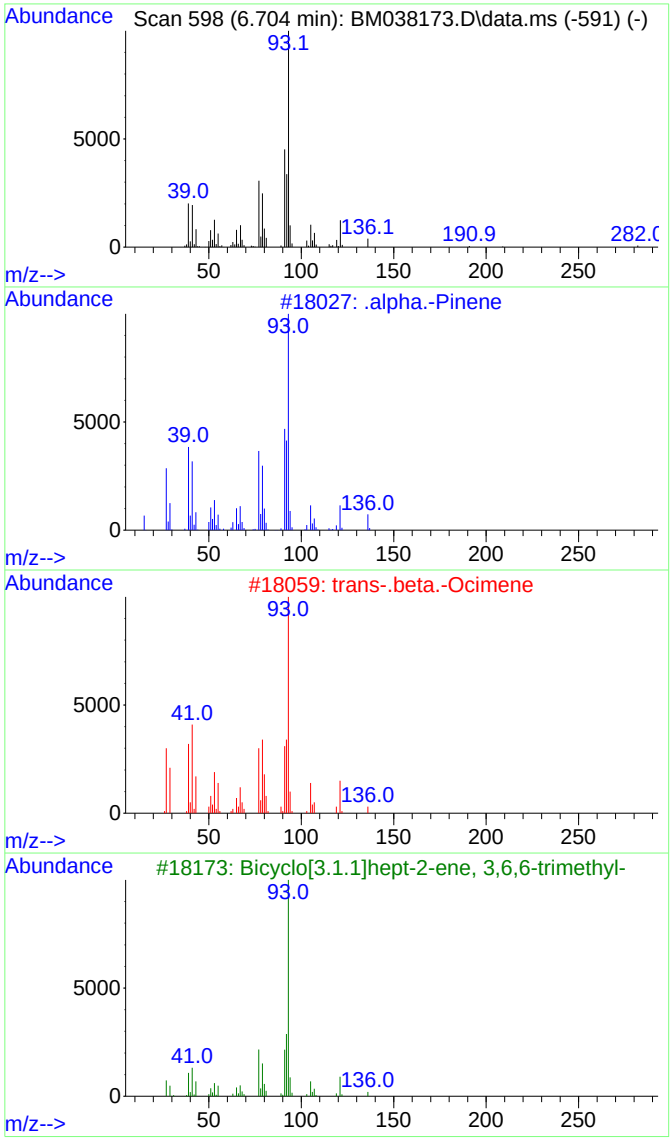
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

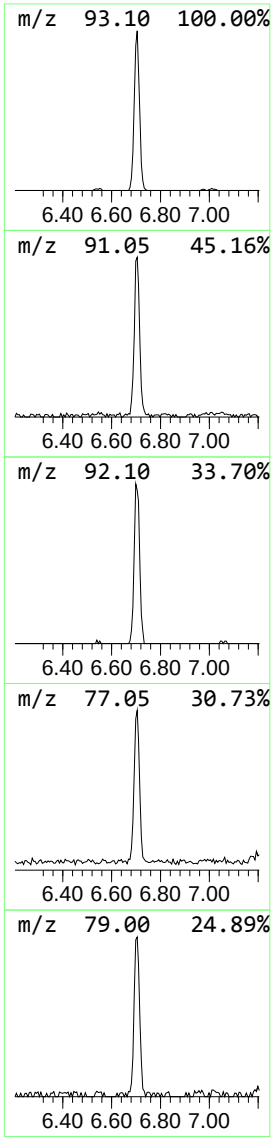
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 .alpha.-Pinene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	3.83 ng/ul	195918	1,4-Dichlorobenzene-d4	8.040

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	95
2	trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
4	.alpha.-Pinene	136	C10H16	000080-56-8	91
5	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

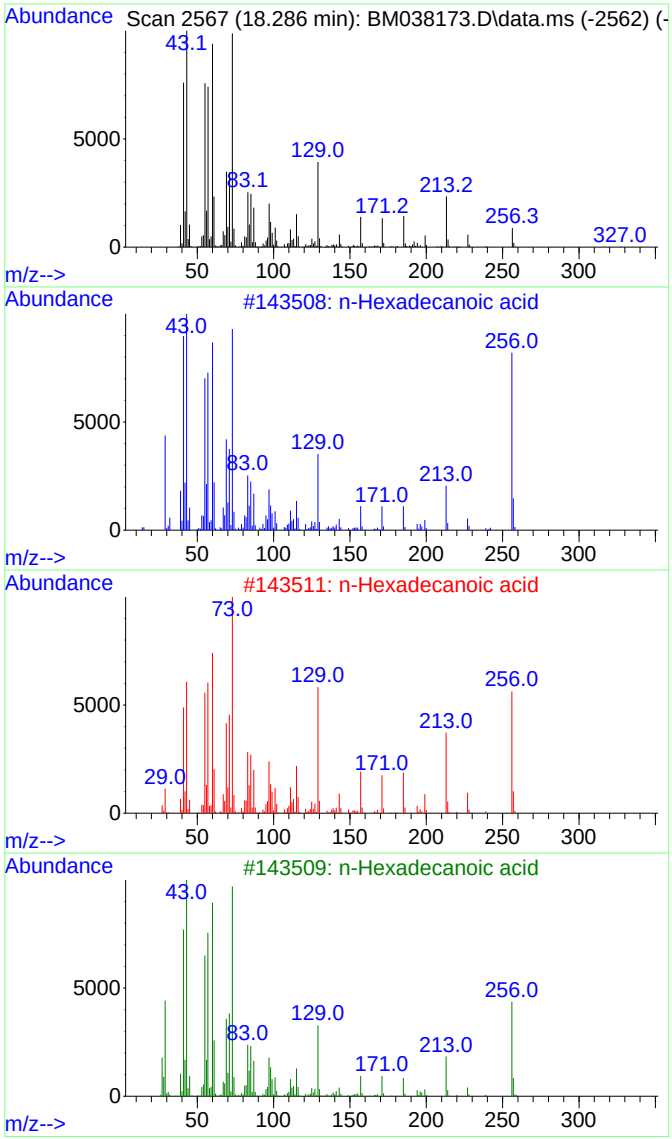
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

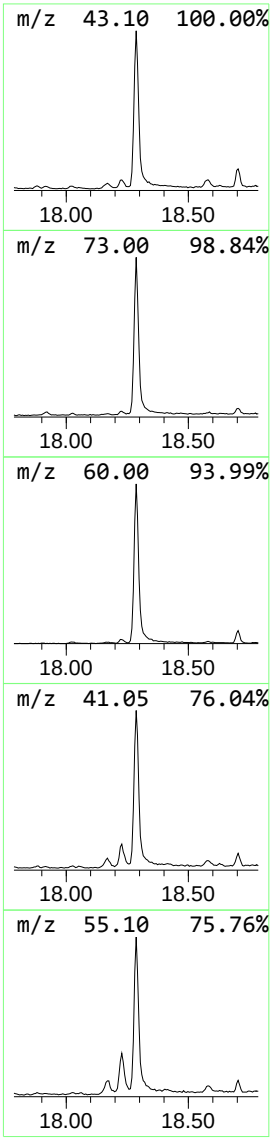
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	14.97 ng/ul	1657640	Phenanthrene-d10	17.410

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	95
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5	Tridecanoic acid	214	C13H26O2	000638-53-9	93





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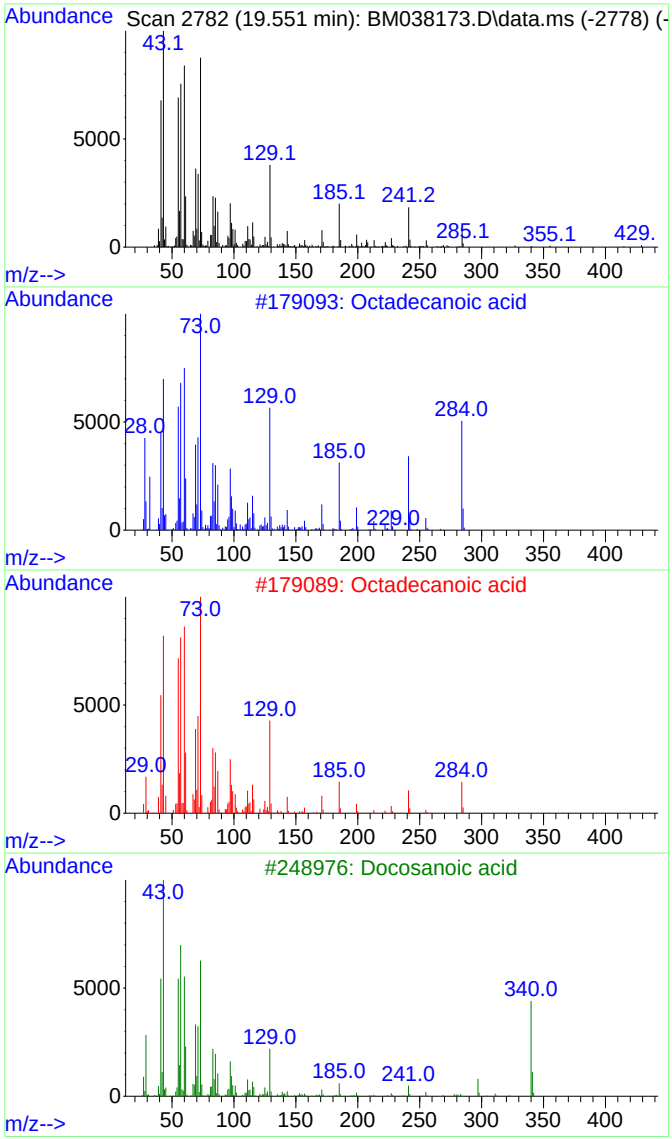
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

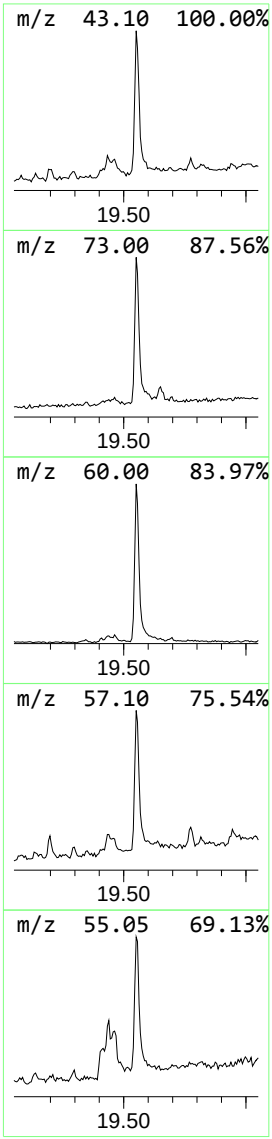
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	6.31 ng/ul	644034	Chrysene-d12	21.574

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	98
3	Docosanoic acid	340	C22H44O2	000112-85-6	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93





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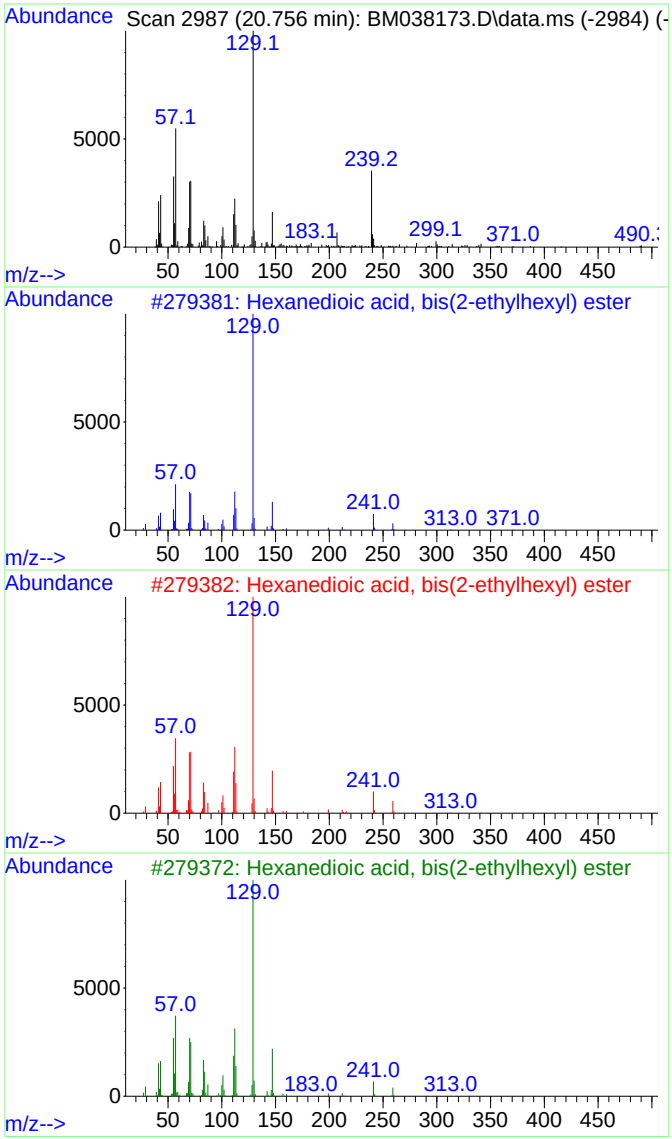
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

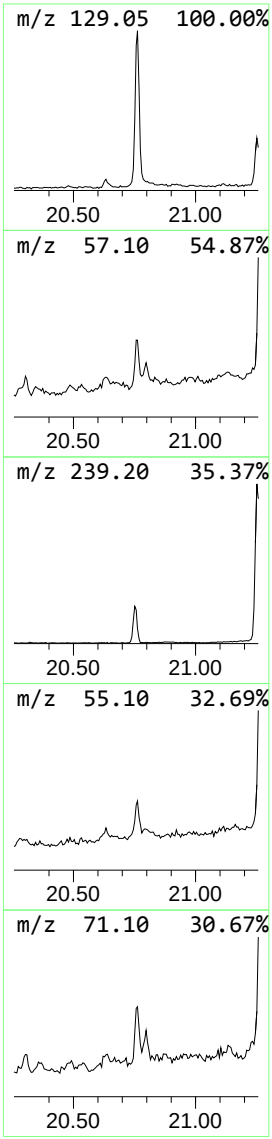
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	2.14 ng/ul	218533	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	83
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	83
3	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	72
4	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	64
5	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	64





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Data File : BM038173.D
Acq On : 21 Dec 2022 15:48
Operator : CG/JU
Sample : N6014-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DBXR2

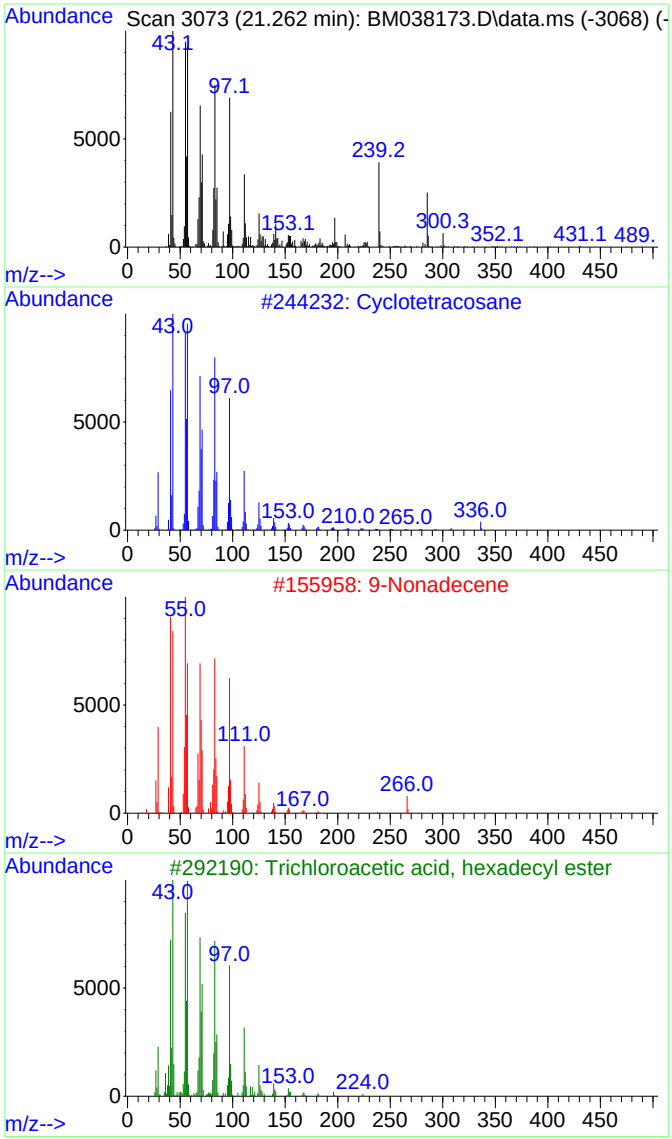
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

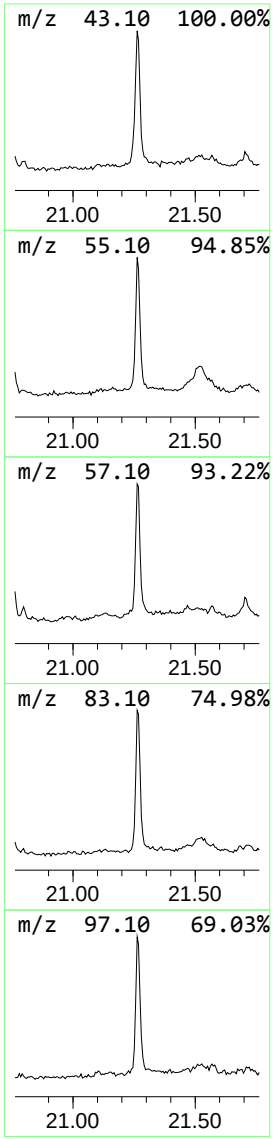
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic21.262 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.262	15.17 ng/ul	1548360	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	93
2	9-Nonadecene	266	C19H38	031035-07-1	86
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
4	Cyclooctacosane	392	C28H56	000297-24-5	81
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	81





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Data File : BM038173.D
Acq On : 21 Dec 2022 15:48
Operator : CG/JU
Sample : N6014-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR2

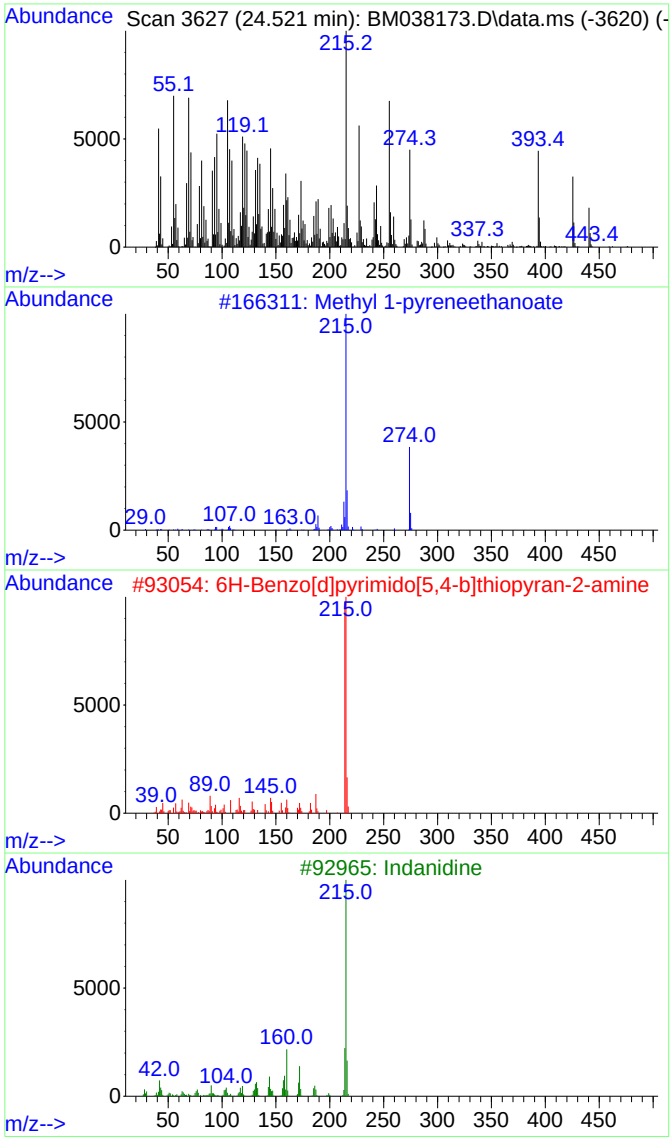
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

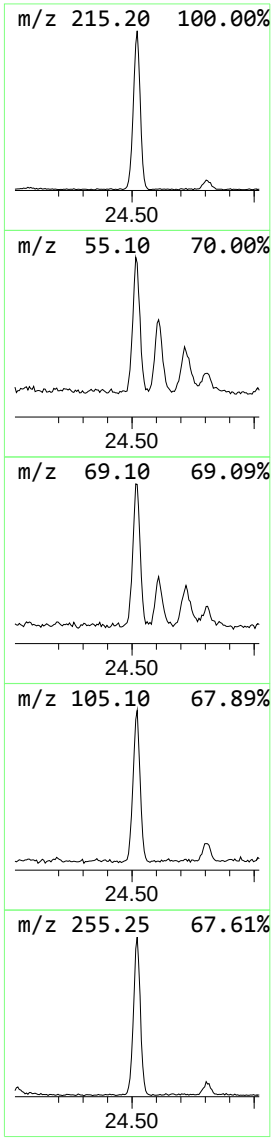
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.521	33.81 ng/ul	2799860	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 1-pyreneethanoate	274	C19H14O2	073654-19-0	49
2	6H-Benzo[d]pyrimido[5,4-b]thiopy...	215	C11H9N3S	1010267-44-6	20
3	Indanidine	215	C11H13N5	085392-79-6	20
4	1-Pyrenebutanoic acid	288	C20H16O2	003443-45-6	20
5	3-Pyrenylacetic acid	260	C18H12O2	064709-55-3	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038173.D
Acq On : 21 Dec 2022 15:48
Operator : CG/JU
Sample : N6014-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR2

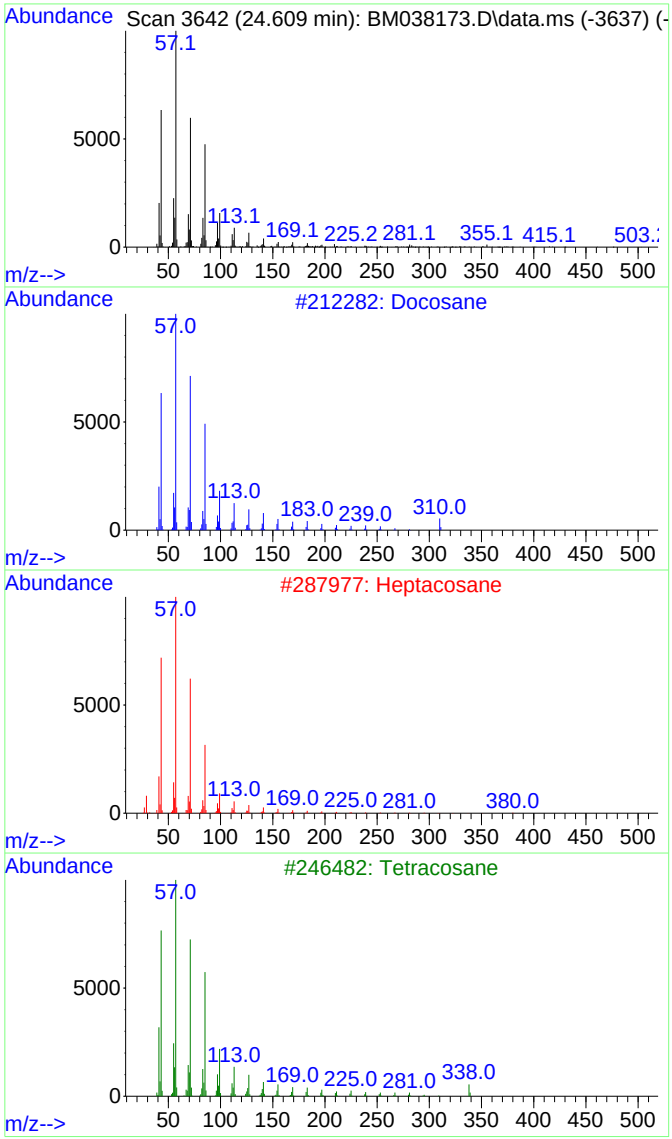
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

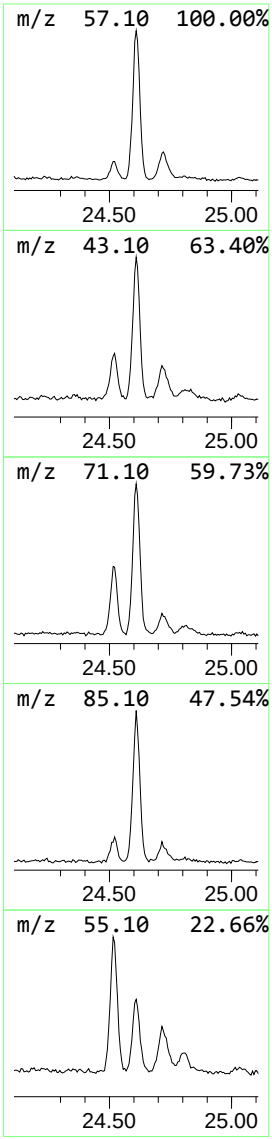
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.609	10.39 ng/ul	860519	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	97
2	Heptacosane	380	C27H56	000593-49-7	95
3	Tetracosane	338	C24H50	000646-31-1	94
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038173.D
Acq On : 21 Dec 2022 15:48
Operator : CG/JU
Sample : N6014-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXR2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.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
.alpha.-Pinene	6.704	3.8	ng/ul	195918	1	8.040	1022730	20.0
n-Hexadecanoic ...	18.286	15.0	ng/ul	1657640	4	17.410	2215160	20.0
Octadecanoic acid	19.551	6.3	ng/ul	644034	5	21.574	2041250	20.0
Hexanedioic aci...	20.756	2.1	ng/ul	218533	5	21.574	2041250	20.0
(DEL) Alkane: C...	21.262	15.2	ng/ul	1548360	5	21.574	2041250	20.0
unknown-01	24.521	33.8	ng/ul	2799860	6	24.027	1656000	20.0
(DEL) Alkane: S...	24.609	10.4	ng/ul	860519	6	24.027	1656000	20.0