LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DDCE2

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-BM092724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM047761.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.258	42	46	55	rVB	49252	69951	0.17%	0.063%
2	3.675	114	117	133	rBV	273530	450365	1.12%	0.405%
3	4.928	324	330	337	rBV	538454	766983	1.92%	0.690%
4	6.128	526	534	542	rBV	724193	1078375	2.69%	0.970%
5	6.975	671	678	687	rBV	767839	1239298	3.10%	1.114%
6	7.140	697	706	714	rBV	613298	987500	2.47%	0.888%
7	7.340	732	740	750	rBV	748473	1184623	2.96%	1.065%
8	7.440	750	757	763	rVB	37928	61579	0.15%	0.055%
9	7.810	813	820	827	rBV	1126237	1790923	4.47%	1.610%
10	8.045	855	860	869	rVB	175282	269412	0.67%	0.242%
11	8.510	932	939	948	rBV	1002472	1574521	3.93%	1.416%
12	8.957	1006	1015	1025	rBV	729866	1235354	3.09%	1.111%
13	9.528	1106	1112	1122	rBV2	82403	129706	0.32%	0.117%
14	9.681	1131	1138	1146	rBV	572993	955641	2.39%	0.859%
15	9.757	1146	1151	1157	rVV2	36674	67788	0.17%	0.061%
16	9.839	1160	1165	1170	rVV3	31661	50835	0.13%	0.046%
17	9.904	1170	1176	1182	rVB4	23282	40397	0.10%	0.036%
18	10.098	1201	1209	1223	rVB	55929	104370	0.26%	0.094%
19	10.222	1223	1230	1238	rBV	964588	1613653	4.03%	1.451%
20	10.481	1268	1274	1286	rBV	173072	290173	0.72%	0.261%
21	10.604	1286	1295	1304	rBV	1598830	2682698	6.70%	2.412%
22	10.734	1309	1317	1325	rBV	923662	1574619	3.93%	1.416%
23	10.804	1325	1329	1335	rVV4	37156	73401	0.18%	0.066%
24	10.892	1339	1344	1353	rVB2	45652	81560	0.20%	0.073%
25	11.139	1377	1386	1392	rBV3	32297	58477	0.15%	0.053%
26	12.022	1530	1536	1542	rBV6	21327	45032	0.11%	0.040%
27	12.128	1546	1554	1560	rBV2	65018	120108	0.30%	0.108%
28	12.192	1560	1565	1575	rVB5	22165	45504	0.11%	0.041%
29	12.686	1644	1649	1658	rBV7	22791	53361	0.13%	0.048%
30	13.433	1769	1776	1782	rBV8	19447	44303	0.11%	0.040%
31	13.851	1841	1847	1854	rVV	1785951	2518876	6.29%	2.265%
32	14.080	1876	1886	1889	rBV8	24982	54601	0.14%	0.049%
33	14.133	1889	1895	1902	rVB	2084245	3058176	7.64%	2.749%
34	14.351	1926	1932	1938	rBV	3026367	3814653	9.53%	3.430%
35	14.439	1941	1947	1954	rBV	2365274	3423423	8.55%	3.078%
36	14.586	1968	1972	1975	rBV	105254	128124	0.32%	0.115%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

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-BM092724.MA.M
Title : SVOA CALIBRATION

37	14.627	1975	1979	1993	rVB	792072	1189036	2.97%	1.069%
38	14.757	1995	2001	2005	rBV2	104752	170100	0.42%	0.153%
39	14.810	2006	2010	2014	rVB3	38654	56202	0.14%	0.051%
40	14.904	2020	2026	2031	rVB5	22622	48826	0.12%	0.044%
41	14.980	2032	2039	2045	rBV2	104326	222294	0.56%	0.200%
42	15.063	2048	2053	2062	rVB	721374	1046337	2.61%	0.941%
43	15.204	2072	2077	2084	rVV	103757	160714	0.40%	0.144%
44	15.280	2085	2090	2097	rVB2	131782	247471	0.62%	0.222%
45	15.433	2106	2116	2123	rBV	2680228	3870974	9.67%	3.480%
46	15.545	2128	2135	2149	rBV2	787756	1327451	3.32%	1.193%
47	15.680	2153	2158	2160	rBV4	31081	51512	0.13%	0.046%
48	15.792	2171	2177	2183	rBV	893568	1274141	3.18%	1.146%
49	15.845	2183	2186	2193	rVB4	65289	90012	0.22%	0.081%
50	16.069	2219	2224	2231	rBV6	37643	74566	0.19%	0.067%
51	16.157	2235	2239	2242	rBV	52422	71722	0.18%	0.064%
52	16.263	2253	2257	2262	rVB4	54703	78639	0.20%	0.071%
53	16.357	2267	2273	2277	rBV4	48101	97944	0.24%	0.088%
54	16.504	2293	2298	2305	rBV5	40638	71429	0.18%	0.064%
55	16.563	2305	2308	2315	rVB6	29287	47045	0.12%	0.042%
56	16.845	2345	2356	2370	rBV	23857076	40037887	100.00%	35.996%
57	16.945	2370	2373	2377	rVV	100560	176155	0.44%	0.158%
58	16.992	2379	2381	2392	rVB5	71312	131321	0.33%	0.118%
59	17.180	2407	2413	2422	rBV	2851727	4128743	10.31%	3.712%
60	17.280	2423	2430	2435	rVV	2850262	4118115	10.29%	3.702%
61	17.321	2435	2437	2445	rVB3	104812	141134	0.35%	0.127%
62	17.468	2458	2462	2470	rBV3	67162	130823	0.33%	0.118%
63	17.539	2470	2474	2477	rVV4	36999	62670	0.16%	0.056%
64	17.574	2478	2480	2487	rVB4	38545	58839	0.15%	0.053%
65	17.680	2494	2498	2502	rBV	45484	61372	0.15%	0.055%
66	17.757	2507	2511	2514	rVV	141298	193728	0.48%	0.174%
67	17.798	2514	2518	2525	rVB3	134708	200119	0.50%	0.180%
68	18.074	2560	2565	2572	rBV	368612	542865	1.36%	0.488%
69	18.462	2627	2631	2636	rVB4	32414	49558	0.12%	0.045%
70	19.004	2719	2723	2730	rVB4	39962	75168	0.19%	0.068%
71	19.127	2741	2744	2748	rVB4	33746	43322	0.11%	0.039%
72	19.198	2753	2756	2760	rVB	37757	44119	0.11%	0.040%
73	19.345	2778	2781	2786	rBV	73032	98812	0.25%	0.089%
74	19.392	2786	2789	2795	rVB6	27747	45936	0.11%	0.041%
75	19.562	2812	2818	2833	rBV	3730332	4817895	12.03%	4.332%
76	20.486	2972	2975	2978	rBV4	41906	48808	0.12%	0.044%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

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-BM092724.MA.M
Title : SVOA CALIBRATION

77	21.074	3072	3075	3086	rBV3	237700	360979	0.90%	0.325%
78	21.403	3125	3131	3139	rBV	2808144	4197090	10.48%	3.773%
79	24.197	3598	3606	3619	rVB	1949332	4772321	11.92%	4.291%
80	24.403	3633	3641	3655	rVB	1831075	4754691	11.88%	4.275%

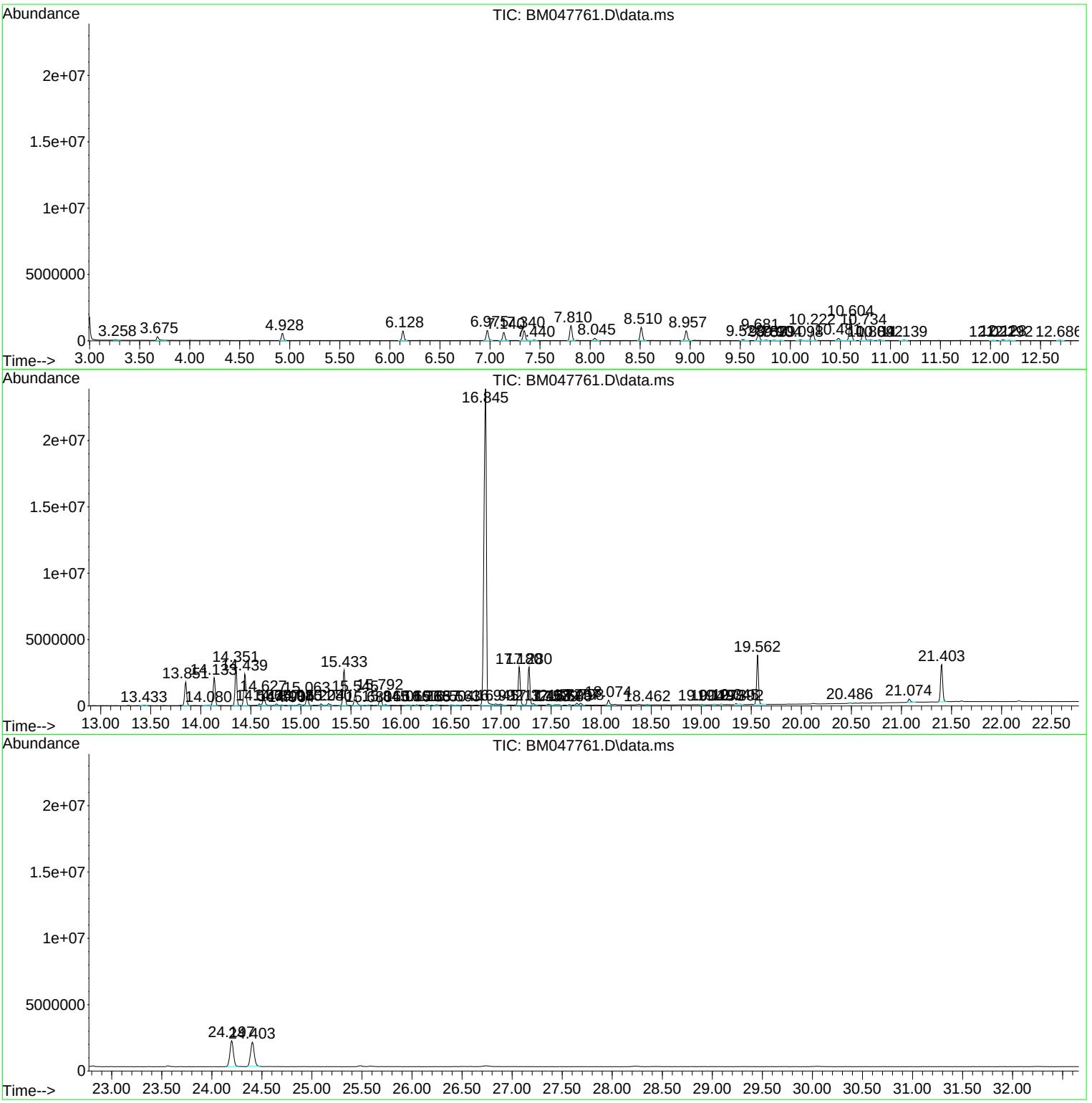
Sum of corrected areas: 111227248

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

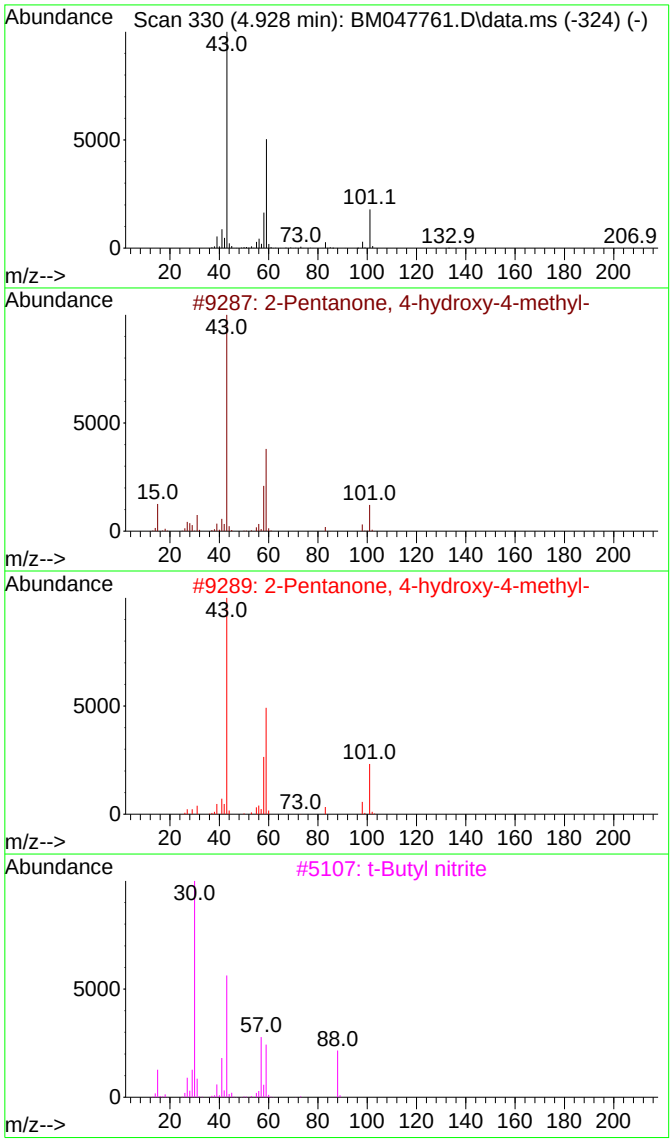
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

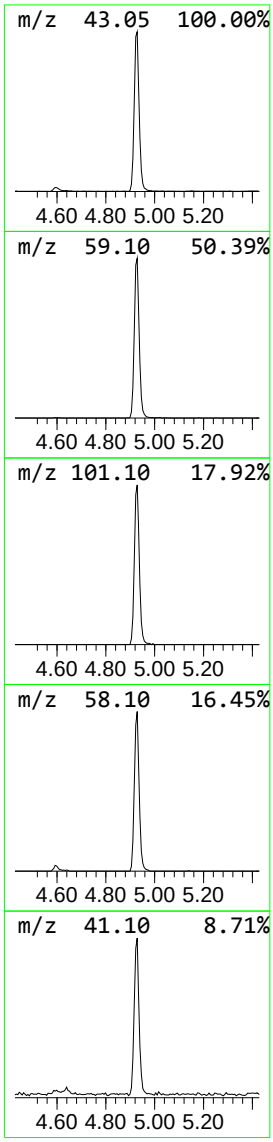
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	8.57 ng/ul	766983	1,4-Dichlorobenzene-d4	7.810

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	50
3	t-Butyl nitrite	103	C4H9NO2	000540-80-7	50
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

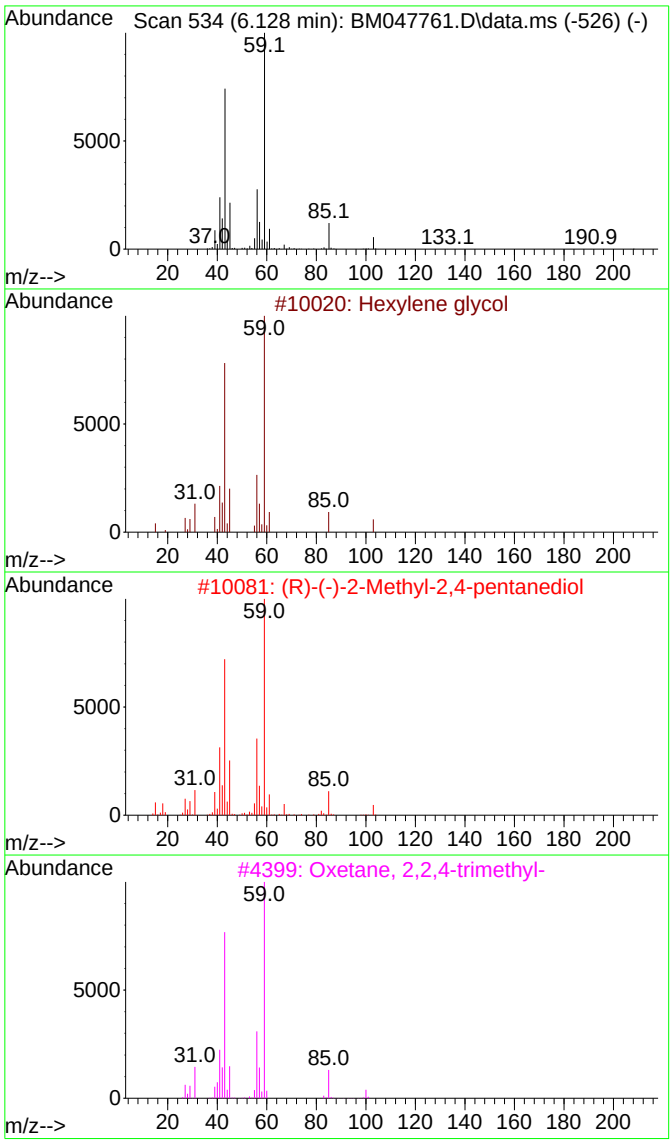
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

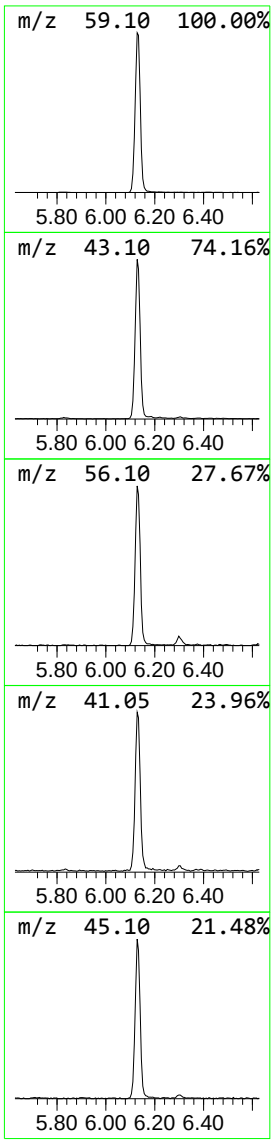
****

Peak Number 2 Hexylene glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.128	12.04 ng/ul	1078380	1,4-Dichlorobenzene-d4	7.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	90
2	(R)-(-)-2-Methyl-2,4-pentanediol	118	C6H14O2	099210-90-9	86
3	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	83
4	Hexylene glycol	118	C6H14O2	000107-41-5	83
5	Hexylene glycol	118	C6H14O2	000107-41-5	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

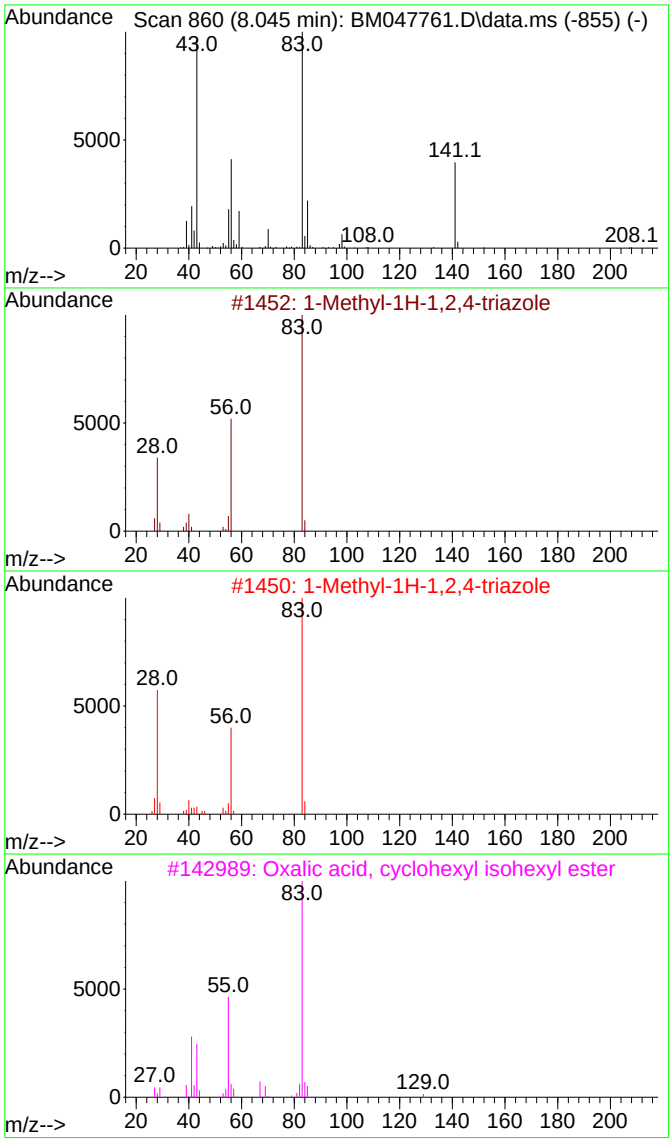
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

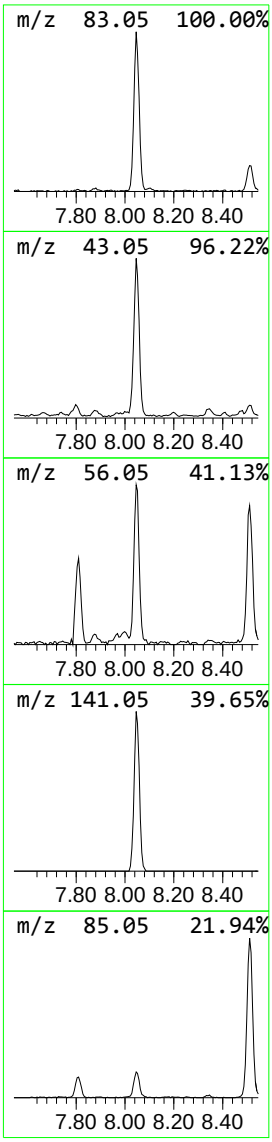
****

Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.045	3.01 ng/ul	269412	1,4-Dichlorobenzene-d4	7.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	37
2	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	37
3	Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	12
4	3-Methylbut-2-enoic acid, 4-nitr...	221	C11H11NO4	1000307-59-8	12
5	Glycine, N-methyl-N-(trifluoroac...	269	C11H18F3NO3	057983-78-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

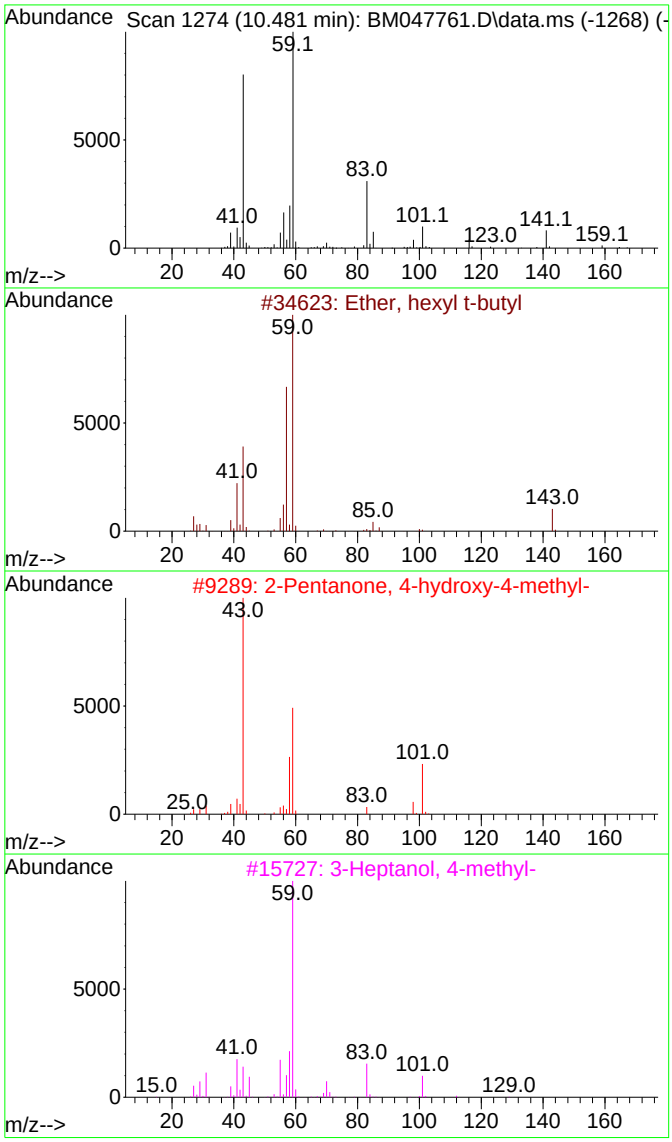
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

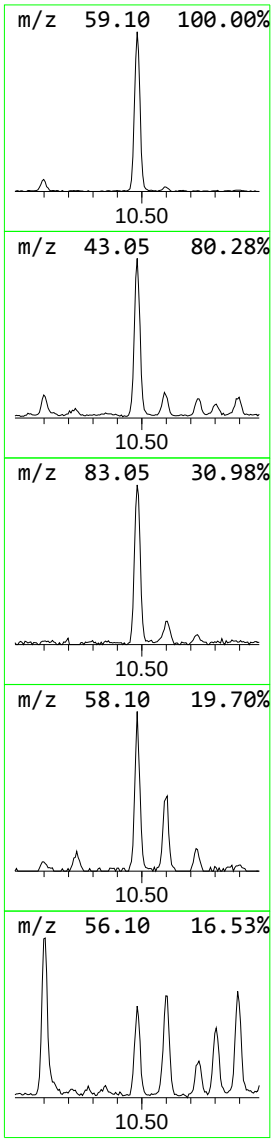
****

Peak Number 4 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.481	2.16 ng/ul	290173	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ether, hexyl t-butyl	158	C10H22O	069775-79-7	47
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	40
4	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	38
5	Guanidine	59	CH5N3	000113-00-8	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

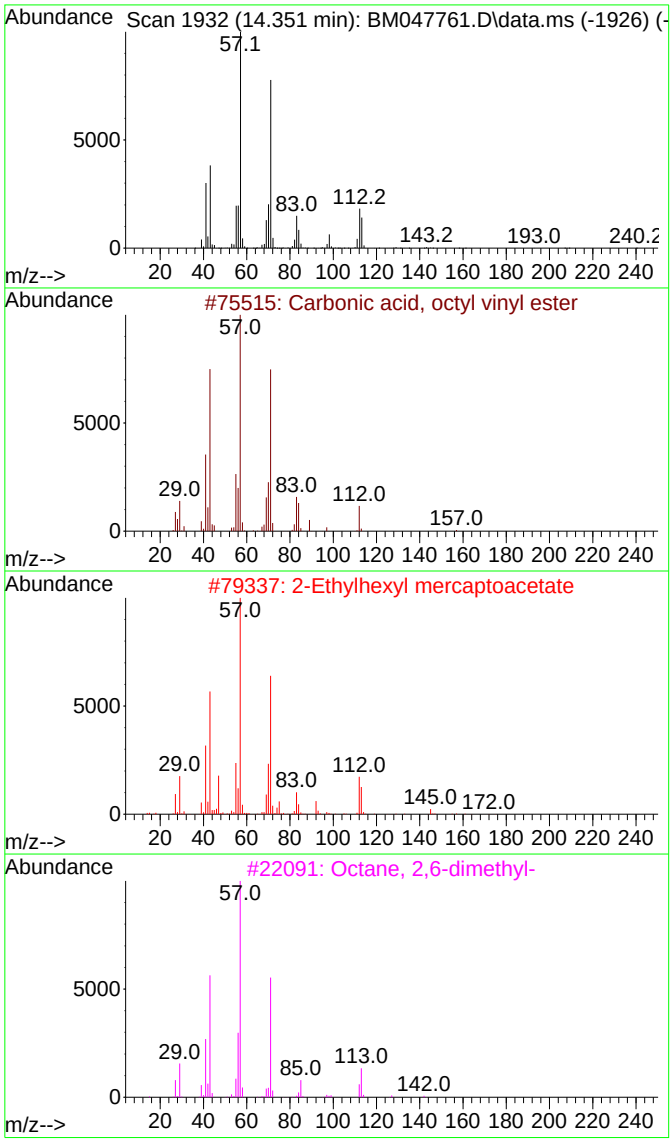
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

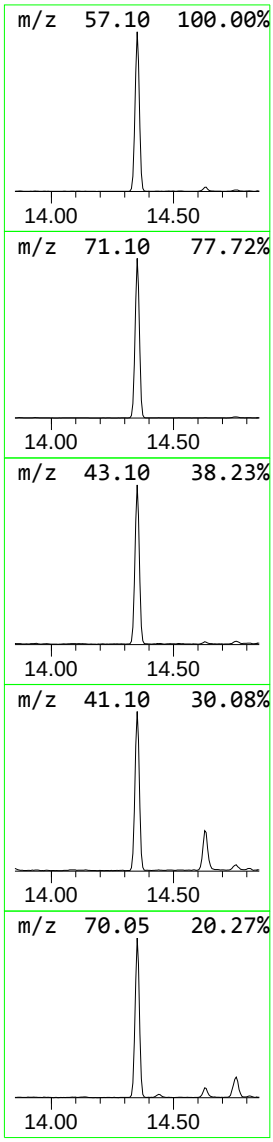
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Carbonic acid, octyl vinyl ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.351	22.29 ng/ul	3814650	Acenaphthene-d10	14.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	72
2	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	72
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
4	Tridecane, 7-methyl-	198	C14H30	026730-14-3	64
5	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

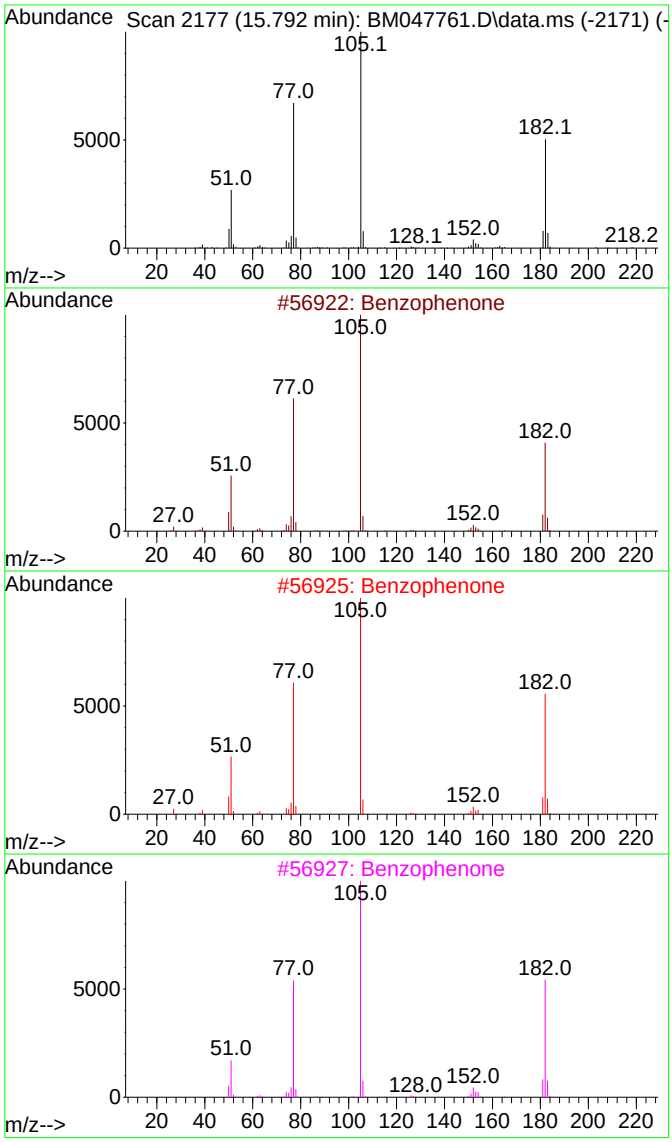
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

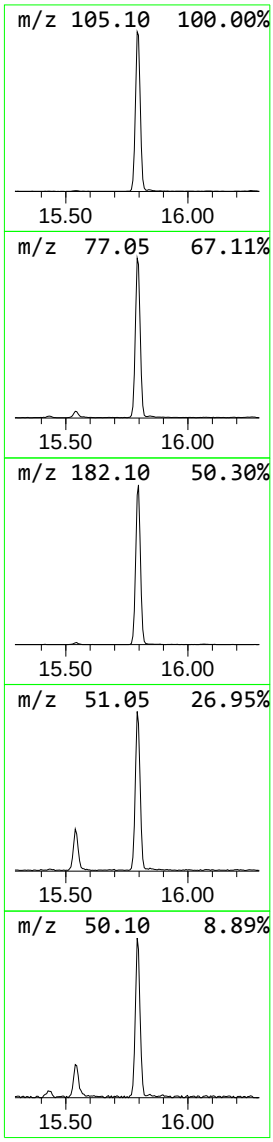
****

Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	7.44 ng/ul	1274140	Acenaphthene-d10	14.439

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





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

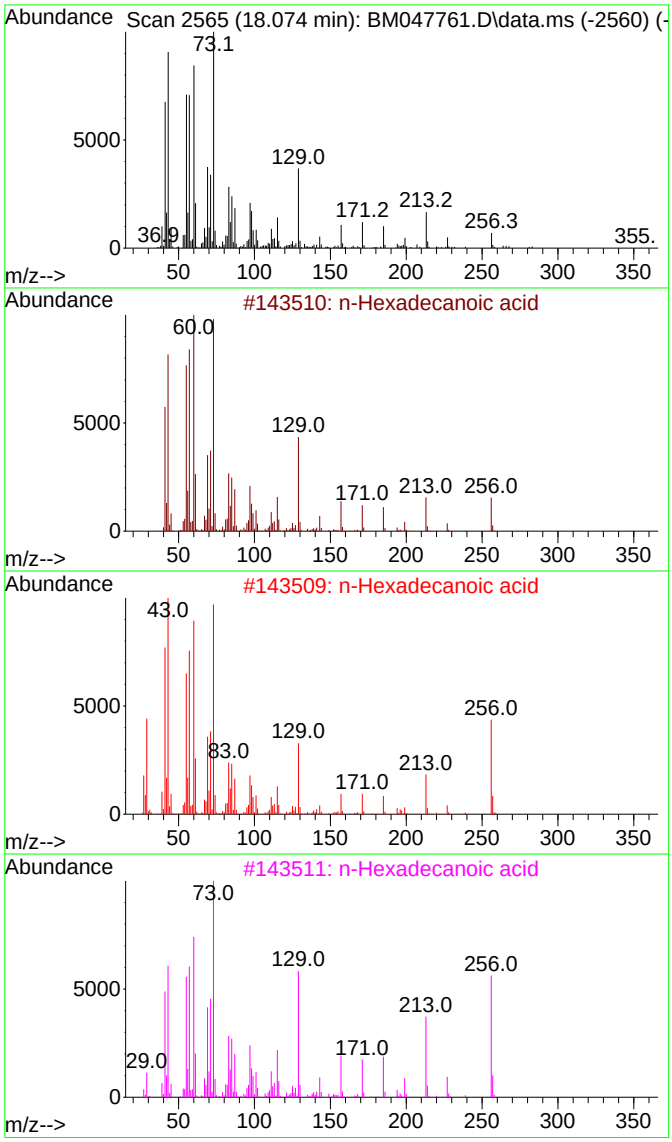
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

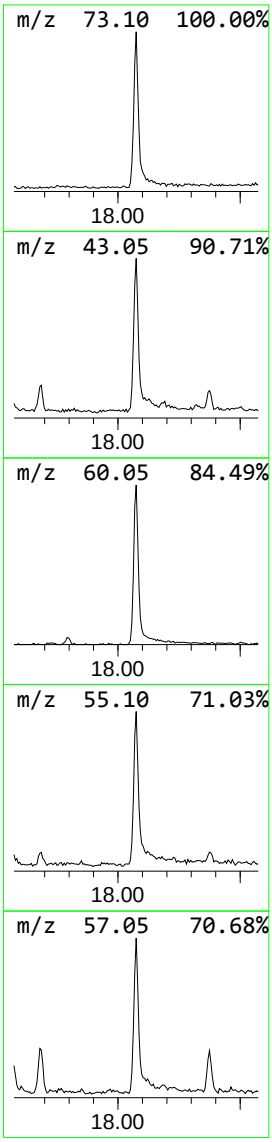
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	2.63 ng/ul	542865	Phenanthrene-d10	17.180

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	98
5	Tridecanoic acid	214	C13H26O2	000638-53-9	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100124\
Data File : BM047761.D
Acq On : 02 Oct 2024 03:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.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
2-Pentanone, 4-...	4.928	8.6	ng/ul	766983	1	7.810	1790920	20.0
Hexylene glycol	6.128	12.0	ng/ul	1078380	1	7.810	1790920	20.0
unknown-01	8.045	3.0	ng/ul	269412	1	7.810	1790920	20.0
unknown-02	10.481	2.2	ng/ul	290173	2	10.604	2682700	20.0
Carbonic acid, ...	14.351	22.3	ng/ul	3814650	3	14.439	3423420	20.0
Benzophenone	15.792	7.4	ng/ul	1274140	3	14.439	3423420	20.0
n-Hexadecanoic ...	18.074	2.6	ng/ul	542865	4	17.180	4128740	20.0